This compound's CID is 51 and compound's name is 2-Oxoglutaric acid. There are 16 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 15, double bond between 2 and 8, double bond between 3 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 16, double bond between 5 and 10, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 14, single bond between attom at postion 8 and 10. The 3D x,y,z coordinates of the element at position 1 is 3.7402, -0.6979, 0.0666, . The 3D x,y,z coordinates of the element at position 2 is -1.2693, -1.6692, -0.0205, . The 3D x,y,z coordinates of the element at position 3 is 2.7936, 1.3637, -0.0282, . The 3D x,y,z coordinates
This compound's CID is 176 and compound's name is Acetic Acid. There are 8 attoms in the molecule and their positions in the order are O, O, C, C, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 8, double bond between 2 and 4, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7. The 3D x,y,z coordinates of the element at position 1 is -0.3035, 1.289, -2.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -0.98, -0.8878, -2.0E-4, . The 3D x,y,z coordinates of the
This compound's CID is 177 and compound's name is Acetaldehyde. There are 7 attoms in the molecule and their positions in the order are O, C, C, H, H, H, H. The bonds between them are: double bond between 1 and 3, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 6, single bond between attom at postion 3 and 7. The 3D x,y,z coordinates of the element at position 1 is 1.1443, 0.2412, 0.0, . The 3D x,y,z coordinates of the element at position 2 is -1.2574, 0.1815, 0.0, . The 3D x,y,z coordinates of the element at position 3 is 0.113, -0.4226, 0.0, . The
This compound's CID is 247 and compound's name is Betaine. There are 19 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, double bond between 2 and 8, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 19. The 3D x,y,z coordinates of the element at position 1 is 1.6647, 1.2167, -0.0588, . The 3D x,y,z coordinates of the element at position 2 is 2.262, -0.9886, -0.0737, . The 3D x,y,z coordinates of the
This compound's CID is 284 and compound's name is Formic Acid. There are 5 attoms in the molecule and their positions in the order are O, O, C, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 5, double bond between 2 and 3, single bond between attom at postion 3 and 4. The 3D x,y,z coordinates of the element at position 1 is -1.1685, 0.1825, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 1.1146, 0.2103, 0.0, . The 3D x,y,z coordinates of the element at position 3 is 0.0538, -

This compound's CID is 311 and compound's name is Citric Acid. There are 21 attoms in the molecule and their positions in the order are O, O, O, O, O, O, O, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 19, double bond between 3 and 11, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 20, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 21, double bond between 6 and 12, double bond between 7 and 13, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 17. The 3D x,y,z coordinates of the element at position 1 is 0.0296, 0.2095, 1.6069, . The 3D x,y,z coordinates of the element at position 2 is -0.8558, 1.7979, -1.4962, . The 3D x,y,z coordinates of the element at position 3 is -1.3554,
This compound's CID is 338 and compound's name is Salicylic Acid. There are 16 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 16, double bond between 3 and 10, single bond between attom at postion 4 and 5, double bond between 4 and 6, single bond between attom at postion 4 and 10, double bond between 5 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 12, double bond between 8 and 9, single bond between attom at postion 8 and 13, single bond between attom at postion 9 and 14. The 3D x,y,z coordinates of the element at position 1 is 0.2626, -2.1794, -0.1866, . The 3D x,y,z coordinates of the element at position 2 is 2.2319, 1.3945, -0.4792, . The 3D x,y,z coordinates of the element at position 3 is
This compound's CID is 525 and compound's name is Malic Acid. There are 15 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 15, double bond between 4 and 8, double bond between 5 and 9, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 12. The 3D x,y,z coordinates of the element at position 1 is 0.3372, -1.6121, 0.1837, . The 3D x,y,z coordinates of the element at position 2 is 2.1682, 1.3843, -0.5735, . The 3D x,y,z
This compound's CID is 564 and compound's name is Aminocaproic acid. There are 22 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 22, double bond between 2 and 9, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 20, single bond between attom at postion 3 and 21, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19. The 3D x,y,z coordinates of the element at position 1 is -3.9002, -0.72, -0.05, . The 3D x,y,z coordinates of the element at position 2 is -2.9187, 1.3278, -0.0187, . The 3D x,y,z coordinates of the element at position 3 is 4.6948, 0.4169, -0.0518, . The 3D x,y,z

This compound's CID is 612 and compound's name is Lactic Acid. There are 12 attoms in the molecule and their positions in the order are O, O, O, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 12, double bond between 3 and 6, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10. The 3D x,y,z coordinates of the element at position 1 is -1.3875, 1.1182, 0.1968, . The 3D x,y,z coordinates of the element at position 2 is 1.4877, -1.0368, 0.2617, . The 3D x,y,z coordinates of the element at
This compound's CID is 702 and compound's name is Ethanol. There are 9 attoms in the molecule and their positions in the order are O, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8. The 3D x,y,z coordinates of the element at position 1 is -1.1712, 0.2997, 0.0, . The 3D x,y,z coordinates of the element at position 2 is -0.0463, -0.5665, 0.0, . The 3D x,y,z coordinates of the element at position 3 is 1.2175, 0.2668, 0.0, .
This compound's CID is 753 and compound's name is Glycerin. There are 14 attoms in the molecule and their positions in the order are O, O, O, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 13, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 14, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11. The 3D x,y,z coordinates of the element at position 1 is 0.0235, -1.3493, 0.2499, . The 3D x,y,z coordinates of the element at position 2 is 2.3988, -0.0044, -0.2369, . The 3D x,y,z coordinates of the element at
This compound's CID is 784 and compound's name is Hydrogen Peroxide. There are 4 attoms in the molecule and their positions in the order are O, O, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 3, single bond between attom at postion 2 and 4. The 3D x,y,z coordinates of the element at position 1 is 0.7247, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is -0.7247, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 3 is 0.8233, -0.7, -0.6676, . The 3D x,y,z
This compound's CID is 785 and compound's name is Hydroquinone. There are 14 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 14, double bond between 3 and 5, single bond between attom at postion 3 and 7, double bond between 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 10, double bond between 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 12. The 3D x,y,z coordinates of the element at position 1 is 2.7558, 0.0, -1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -2.7561, -1.0E-4, -2.0E-4, . The 3D x,y,z coordinates of the element at

This compound's CID is 798 and compound's name is Indole. There are 16 attoms in the molecule and their positions in the order are N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 3, double bond between 2 and 5, single bond between attom at postion 3 and 4, double bond between 3 and 6, double bond between 4 and 7, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 14, double bond between 8 and 9, single bond between attom at postion 8 and 15, single bond between attom at postion 9 and 16. The 3D x,y,z coordinates of the element at position 1 is 1.561, 1.1123, -1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is 0.2536, 0.6808, 0.0, . The 3D x,y,z coordinates of the This compound's CID is 807 and compound's name is Iodine. There are 2 attoms in the molecule and their positions in the order are I, I. The bonds between them are: single bond between attom at postion 1 and 2. The 3D x,y,z coordinates of the element at position 1 is -1.326, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 1.326, 0.0, 0.0. There are 0 chiral atoms (stereocenters), 0 chiral centers, 0 undefined chiral centers, 0 chiral bonds, This compound's CID is 864 and compound's name is Thioctic acid. There are 26 attoms in the molecule and their positions in the order are S, S, O, O, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 5, single bond between attom at postion 2 and 10, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 26, double bond between 4 and 12, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 24, single bond between attom at postion 11 and 25. The 3D x,y,z coordinates of the element at position 1 is 2.587, -1.3583, -0.3603, . The 3D x,y,z coordinates of the element at position 2 is 4.6243, -1.1509, -0.4692, . The 3D x,y,z coordinates of the element at position 3 is -5.158, -

This compound's CID is 896 and compound's name is Melatonin. There are 33 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 17, double bond between 2 and 15, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 27, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, double bond between 5 and 9, double bond between 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22, double bond between 11 and 13, single bond between attom at postion 11 and 24, double bond between 12 and 14, single bond between attom at postion 12 and 25, single bond between attom at postion 13 and 14, single bond between attom at postion 14 and 26, single bond between attom at postion 15 and 16, single bond between attom at postion 16 and 28, single bond between attom at postion 16 and 29, single bond between attom at postion 16 and 30, single bond between attom at postion 17 and 31, single bond between attom at postion 17 and 32, single bond between attom at postion 17 and 33. The 3D x,y,z coordinates of the element at position 1 is -1.3636, 3.0246, 0.297, . The 3D x,y,z coordinates of the element at position 2 is 3.7267, 0.6738, 0.6109, . The 3D x,y,z coordinates of the element at position 3 is -2.0703, -
This compound's CID is 931 and compound's name is Naphthalene. There are 18 attoms in the molecule and their positions in the order are C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, double bond between 1 and 3, single bond between attom at postion 1 and 5, double bond between 2 and 4, single bond between attom at postion 2 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 12, double bond between 5 and 9, single bond between attom at postion 5 and 13, double bond between 6 and 10, single bond between attom at postion 6 and 14, double bond between 7 and 8, single bond between attom at postion 7 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 10 and 18. The 3D x,y,z coordinates of the element at position 1 is 0.0, -0.7076, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 0.0, 0.7076, 1.0E-4, . The 3D x,y,z coordinates of the element at position 3
This compound's CID is 936 and compound's name is Niacinamide. There are 15 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 8, single bond between attom at postion 2 and 6, double bond between 2 and 9, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 15, single bond between attom at postion 4 and 5, double bond between 4 and 6, single bond between attom at postion 4 and 8, double bond between 5 and 7, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 12, single bond between attom at postion 9 and 13. The 3D x,y,z coordinates of the element at position 1 is -2.394, 1.1116, -0.0088, . The 3D x,y,z coordinates of the element at position 2 is 1.7614, -1.2284, -0.0034, . The 3D x,y,z coordinates of the element at position 3 is -2.4052, -1.1814, 0.0027, . The 3D x,y,z coordinates of the element

This compound's CID is 938 and compound's name is Nicotinic acid. There are 14 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 14, double bond between 2 and 9, single bond between attom at postion 3 and 6, double bond between 3 and 8, single bond between attom at postion 4 and 5, double bond between 4 and 6, single bond between attom at postion 4 and 9, double bond between 5 and 7, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 13. The 3D x,y,z coordinates of the element at position 1 is -2.2827, -1.2029, -7.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -2.4704, 1.0624, 2.0E-4, . The 3D x,y,z coordinates of the element at position 3 is
This compound's CID is 944 and compound's name is Nitric Acid. There are 5 attoms in the molecule and their positions in the order are O, O, O, N, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 5, single bond between attom at postion 2 and 4, double bond between 3 and 4. The 3D x,y,z coordinates of the element at position 1 is -0.0416, -1.3017, 1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -1.1005, 0.6377, 1.0E-4, . The 3D x,y,z coordinates of the element at position 3 is
This compound's CID is 947 and compound's name is Nitrogen. There are 2 attoms in the molecule and their positions in the order are N, N. The bonds between them are: triple bond between 1 and 2. The 3D x,y,z coordinates of the element at position 1 is -0.556, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 0.556, 0.0, 0.0. There are 0 chiral atoms (stereocenters), 0 chiral centers, 0 undefined chiral centers, 0 chiral bonds, 0 chiral
This compound's CID is 948 and compound's name is Nitrous Oxide. There are 3 attoms in the molecule and their positions in the order are O, N, N. The bonds between them are: single bond between attom at postion 1 and 2, triple bond between 2 and 3. The 3D x,y,z coordinates of the element at position 1 is 1.3063, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is -0.1096, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 3 is -
This compound's CID is 962 and compound's name is Water. There are 3 attoms in the molecule and their positions in the order are O, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 3. The 3D x,y,z coordinates of the element at position 1 is 0.0, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 0.2774, 0.8929, 0.2544, . The 3D x,y,z coordinates of the element at
This compound's CID is 977 and compound's name is Oxygen. There are 2 attoms in the molecule and their positions in the order are O, O. The bonds between them are: double bond between 1 and 2. The 3D x,y,z coordinates of the element at position 1 is -0.616, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 0.616, 0.0, 0.0. There are 0 chiral atoms (stereocenters), 0 chiral centers, 0 undefined chiral centers, 0 chiral bonds, 0 chiral bonds
This compound's CID is 996 and compound's name is Phenol. There are 13 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 13, double bond between 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 8, double bond between 4 and 6, single bond between attom at postion 4 and 9, double bond between 5 and 7, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 12. The 3D x,y,z coordinates of the element at position 1 is -2.3622, 1.0E-4, -4.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -1.0011, 0.0, 3.0E-4, . The 3D x,y,z coordinates of the element at position 3 is -0.3037, 1.208, 2.0E-4, . The 3D x,y,z

This compound's CID is 1004 and compound's name is Phosphoric Acid. There are 8 attoms in the molecule and their positions in the order are P, O, O, O, O, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 4, double bond between 1 and 5, single bond between attom at postion 2 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 4 and 8. The 3D x,y,z coordinates of the element at position 1 is 0.0936, -2.0E-4, -0.0071, . The 3D x,y,z coordinates of the element at position 2 is -0.6464, -0.865, -1.1531, . The 3D This compound's CID is 1030 and compound's name is Propylene Glycol. There are 13 attoms in the molecule and their positions in the order are O, O, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 13, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11. The 3D x,y,z coordinates of the element at position 1 is -0.4721, -1.3536, -0.1558, . The 3D x,y,z coordinates of the element at position 2 is 1.934, 0.0013, 0.1076, . The 3D x,y,z coordinates of the element at position 3 is -0.4535, -0.0168, This compound's CID is 1046 and compound's name is Pyrazinamide. There are 14 attoms in the molecule and their positions in the order are O, N, N, N, C, C, C, C, C, H, H, H, H, H. The bonds between them are: double bond between 1 and 7, double bond between 2 and 5, single bond between attom at postion 2 and 8, double bond between 3 and 6, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 6 and 10, double bond between 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 12. The 3D x,y,z coordinates of the element at position 1 is -2.3259, 1.1655, -0.0083, . The 3D x,y,z coordinates of the element at position 2 is 0.3019, -1.1915, -0.0013, . The 3D x,y,z coordinates of the element at position 3 is 1.8445, This compound's CID is 1054 and compound's name is Pyridoxine. There are 23 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 21, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 22, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 23, double bond between 4 and 8, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 6, double bond between 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 10, double bond between 6 and 11, single bond between attom at postion 7 and 8, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 12 and 20. The 3D x,y,z coordinates of the element at position 1 is 1.638, 1.8421, -0.5091, . The 3D x,y,z coordinates of the element at position 2 is -1.3948, 2.4034, 0.9095, . The 3D x,y,z coordinates of the

This compound's CID is 1123 and compound's name is Taurine. There are 14 attoms in the molecule and their positions in the order are S, O, O, O, N, C, C, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, double bond between 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 6, single bond between attom at postion 2 and 14, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 11. The 3D x,y,z coordinates of the element at position 1 is 1.0051, -0.1135, 0.0174, . The 3D x,y,z coordinates of the element at position 2 is 1.8821, 1.2404, -0.2242, . The 3D x,y,z coordinates of the element at position 3 is 1.1465, -
This compound's CID is 1175 and compound's name is Uric Acid. There are 16 attoms in the molecule and their positions in the order are O, O, O, N, N, N, N, C, C, C, C, C, H, H, H, H. The bonds between them are: double bond between 1 and 10, double bond between 2 and 11, double bond between 3 and 12, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 15, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 16, double bond between 8 and 9, single bond between attom at postion 9 and 10. The 3D x,y,z coordinates of the element at position 1 is -0.7342, -2.6384, -6.0E-4, . The 3D x,y,z coordinates of the element at position 2 is 3.679, 0.3794, 0.0, . The 3D x,y,z
This compound's CID is 1176 and compound's name is Urea. There are 8 attoms in the molecule and their positions in the order are O, N, N, C, H, H, H, H. The bonds between them are: double bond between 1 and 4, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 6, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8. The 3D x,y,z coordinates of the element at position 1 is -1.3042, -8.0E-4, 1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is 0.6903, -1.1479, 1.0E-4, . The 3D x,y,z coordinates
This compound's CID is 1727 and compound's name is Dalfampridine. There are 13 attoms in the molecule and their positions in the order are N, N, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 13, double bond between 2 and 6, single bond between attom at postion 2 and 7, double bond between 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, double bond between 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 11. The 3D x,y,z coordinates of the element at position 1 is 2.402, 0.0, -2.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -1.8029, 1.0E-4, -1.0E-4, . The 3D x,y,z coordinates of the element at position 3 is 0.9924, -1.0E-4, 2.0E-4, . The 3D x,y,z coordinates of

This compound's CID is 1775 and compound's name is Phenytoin. There are 31 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 8, double bond between 2 and 9, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, double bond between 6 and 10, single bond between attom at postion 6 and 12, double bond between 7 and 11, single bond between attom at postion 7 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 23, double bond between 12 and 16, single bond between attom at postion 12 and 24, double bond between 13 and 17, single bond between attom at postion 13 and 25, double bond between 14 and 18, single bond between attom at postion 14 and 26, double bond between 15 and 19, single bond between attom at postion 15 and 27, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 28, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 29, single bond between attom at postion 18 and 30, single bond between attom at postion 19 and 31. The 3D x,y,z coordinates of the element at position 1 is -0.1232, 1.0446, 2.3893, . The 3D x,y,z coordinates of the element at position 2 is 0.0896, 3.8139, -1.2441, . The 3D x,y,z coordinates of the element at position 3 is 0.0499, This compound's CID is 1983 and compound's name is Acetaminophen. There are 20 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 20, double bond between 2 and 10, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 14, double bond between 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, double bond between 6 and 8, single bond between attom at postion 6 and 13, double bond between 7 and 9, single bond between attom at postion 7 and 15, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 16, single bond between attom at postion 10 and 11, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 19. The 3D x,y,z coordinates of the element at position 1 is 3.8509, 0.4516, 0.0012, . The 3D x,y,z coordinates of the element at position 2 is -2.5999, 1.4041, -0.0018, . The 3D x,y,z coordinates of the element at position 3 is -1.5705, -0.7171, 1.0E-4, . The 3D This compound's CID is 1986 and compound's name is Acetazolamide. There are 19 attoms in the molecule and their positions in the order are S, S, O, O, O, N, N, N, N, C, C, C, C, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 11, double bond between 5 and 12, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 9, double bond between 7 and 10, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, double bond between 9 and 11, single bond between attom at postion 12 and 13, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 19. The 3D x,y,z coordinates of the element at position 1 is -3.0413, 0.1096, -0.0849, . The 3D x,y,z coordinates of the element at position 2 is -0.3004, 1.2561, -0.0551, . The 3D x,y,z coordinates

This compound's CID is 2082 and compound's name is Albendazole. There are 33 attoms in the molecule and their positions in the order are S, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 17, single bond between attom at postion 2 and 18, double bond between 3 and 17, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 20, single bond between attom at postion 5 and 8, double bond between 5 and 12, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 30, double bond between 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 11, double bond between 9 and 10, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 19, double bond between 11 and 14, single bond between attom at postion 11 and 21, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 22, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 24, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 25, single bond between attom at postion 15 and 26, single bond between attom at postion 16 and 27, single bond between attom at postion 16 and 28, single bond between attom at postion 16 and 29, single bond between attom at postion 18 and 31, single bond between attom at postion 18 and 32, single bond between attom at postion 18 and 33. The 3D x,y,z coordinates of the element at position 1 is -4.1704, -0.1302, -1.2041, . The 3D x,y,z coordinates of the element at position 2 is 5.4796, 0.9561, 0.1191, . The 3D x,y,z coordinates of the element at position 3 is 4.4522, -0.9526,

This compound's CID is 2117 and compound's name is DL-alpha-Tocopherol acetate. There are 86 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 24, single bond between attom at postion 2 and 33, double bond between 3 and 33, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 35, single bond between attom at postion 5 and 36, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 37, single bond between attom at postion 6 and 38, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 39, single bond between attom at postion 7 and 40, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 41, single bond between attom at postion 9 and 42, single bond between attom at postion 9 and 43, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 44, single bond between attom at postion 10 and 45, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 46, single bond between attom at postion 11 and 47, single bond between attom at postion 12 and 48, single bond between attom at postion 12 and 49, single bond between attom at postion 12 and 50, double bond between 13 and 14, single bond between attom at postion 13 and 20, single bond between attom at postion 14 and 21, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 51, single bond between attom at postion 15 and 52, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 53, single bond between attom at postion 16 and 54, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 25, single bond between attom at postion 17 and 55, single bond between attom at postion 18 and 56, single bond between attom at postion 18 and 57, single bond between attom at postion 18 and 58, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 59, single bond between attom at postion 19 and 60, double bond between 20 and 24, single bond between attom at postion 20 and 27, double bond between 21 and 23, single bond between attom at postion 21 and 28, single bond between attom at postion 22 and 26, single bond between attom at postion 22 and 61, single bond between attom at postion 22 and 62, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 30, single bond between attom at postion 25 and 63, single bond between attom at

This compound's CID is 2118 and compound's name is Alprazolam. There are 35 attoms in the molecule and their positions in the order are CL, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 11, double bond between 3 and 9, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 5, double bond between 4 and 8, double bond between 5 and 11, double bond between 6 and 7, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 10, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 17, double bond between 12 and 15, single bond between attom at postion 12 and 25, double bond between 13 and 16, single bond between attom at postion 13 and 26, double bond between 14 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 27, single bond between attom at postion 17 and 28, single bond between attom at postion 17 and 29, single bond between attom at postion 17 and 30, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 31, double bond between 19 and 21, single bond between attom at postion 19 and 32, double bond between 20 and 22, single bond between attom at postion 20 and 33, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 34, single bond between attom at postion 22 and 35. The 3D x,y,z coordinates of the element at position 1 is -1.0909, 4.462, 0.7689, . The 3D x,y,z coordinates of the element at position 2 is 2.162, -0.4252, -0.0813, . The 3D x,y,z coordinates of the element at
This compound's CID is 2130 and compound's name is Amantadine. There are 28 attoms in the molecule and their positions in the order are N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 27, single bond between attom at postion 1 and 28, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 8, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 12, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26. The 3D x,y,z coordinates of the element at position 1 is 2.7385, 3.0E-4, -1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is 1.2768, -

This compound's CID is 2153 and compound's name is Theophylline. There are 21 attoms in the molecule and their positions in the order are O, O, N, N, N, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 9, double bond between 2 and 10, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 7, double bond between 6 and 13, double bond between 7 and 8, single bond between attom at postion 8 and 9, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 12 and 20, single bond between attom at postion 13 and 21. The 3D x,y,z coordinates of the element at position 1 is -0.4586, 2.7181, 3.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -2.4695, -
This compound's CID is 2159 and compound's name is Amisulpride. There are 52 attoms in the molecule and their positions in the order are S, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 4, double bond between 1 and 5, single bond between attom at postion 1 and 18, single bond between attom at postion 1 and 23, double bond between 2 and 16, single bond between attom at postion 3 and 20, single bond between attom at postion 3 and 25, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 37, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 48, single bond between attom at postion 8 and 49, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 26, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 27, single bond between attom at postion 10 and 28, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 29, single bond between attom at postion 11 and 30, single bond between attom at postion 12 and 31, single bond between attom at postion 12 and 32, single bond between attom at postion 13 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 35, single bond between attom at postion 14 and 36, single bond between attom at postion 15 and 38, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 17, double bond between 17 and 19, single bond between attom at postion 17 and 20, single bond between attom at postion 18 and 19, double bond between 18 and 21, single bond between attom at postion 19 and 41, double bond between 20 and 22, single bond between attom at postion 21 and 22, single bond between attom at postion 22 and 42, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 43, single bond between attom at postion 23 and 44, single bond between attom at postion 24 and 45, single bond between attom at postion 24 and 46, single bond between attom at postion 24 and 47, single bond between attom at postion 25 and 50, single bond between attom at postion 25 and 51, single bond between attom at postion 25 and 52. The 3D x,y,z coordinates of the element at position 1 is -3.9148, -1.5454, 0.237, . The 3D x,y,z coordinates of the element at position 2 is 1.1816, 1.5794, -1.4616, . The 3D x,y,z

This compound's CID is 2162 and compound's name is Amlodipine. There are 53 attoms in the molecule and their positions in the order are CL, O, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 15, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 27, double bond between 5 and 16, double bond between 6 and 18, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 52, single bond between attom at postion 8 and 53, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 29, double bond between 10 and 12, single bond between attom at postion 10 and 16, double bond between 11 and 13, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 19, double bond between 14 and 20, single bond between attom at postion 15 and 31, single bond between attom at postion 15 and 32, single bond between attom at postion 17 and 33, single bond between attom at postion 17 and 34, single bond between attom at postion 17 and 35, double bond between 19 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 36, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 37, double bond between 22 and 23, single bond between attom at postion 22 and 38, single bond between attom at postion 23 and 39, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 40, single bond between attom at postion 24 and 41, single bond between attom at postion 25 and 28, single bond between attom at postion 25 and 42, single bond between attom at postion 25 and 43, single bond between attom at postion 26 and 44, single bond between attom at postion 26 and 45, single bond between attom at postion 27 and 46, single bond between attom at postion 27 and 47, single bond between attom at postion 27 and 48, single bond between attom at postion 28 and 49, single bond between attom at postion 28 and 50, single bond between attom at postion 28 and 51. The 3D x,y,z coordinates of the element at position 1 is -2.9012, -2.3251, 1.3735, . The 3D x,y,z coordinates of the element at

This compound's CID is 2187 and compound's name is Anastrozole. There are 41 attoms in the molecule and their positions in the order are N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 14, single bond between attom at postion 1 and 21, double bond between 2 and 22, triple bond between 3 and 19, triple bond between 4 and 20, double bond between 5 and 21, single bond between attom at postion 5 and 22, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 19, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 20, double bond between 8 and 10, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 10, double bond between 9 and 13, single bond between attom at postion 10 and 23, double bond between 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 27, single bond between attom at postion 15 and 28, single bond between attom at postion 15 and 29, single bond between attom at postion 15 and 30, single bond between attom at postion 16 and 31, single bond between attom at postion 16 and 32, single bond between attom at postion 16 and 33, single bond between attom at postion 17 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 17 and 36, single bond between attom at postion 18 and 37, single bond between attom at postion 18 and 38, single bond between attom at postion 18 and 39, single bond between attom at postion 21 and 40, single bond between attom at postion 22 and 41. The 3D x,y,z coordinates of the element at position 1 is -3.3646, -0.2989, -0.4641, . The 3D x,y,z coordinates of the element at position 2 is -3.7453, -1.3975, 0.1786, . The 3D x,y,z coordinates This compound's CID is 2244 and compound's name is Aspirin. There are 21 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 21, double bond between 3 and 11, double bond between 4 and 12, single bond between attom at postion 5 and 6, double bond between 5 and 7, double bond between 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 14, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 15, double bond between 9 and 10, single bond between attom at postion 9 and 16, single bond between attom at postion 10 and 17, single bond between attom at postion 12 and 13, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 20. The 3D x,y,z coordinates of the element at position 1 is 1.2333, 0.554, 0.7792, . The 3D x,y,z coordinates of the element at position 2 is -0.6952, -2.7148, -0.7502, . The 3D x,y,z coordinates of the element at

This compound's CID is 2249 and compound's name is Atenolol. There are 41 attoms in the molecule and their positions in the order are O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 33, double bond between 3 and 19, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 19, single bond between attom at postion 5 and 40, single bond between attom at postion 5 and 41, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 20, single bond between attom at postion 6 and 21, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 22, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 23, single bond between attom at postion 9 and 25, single bond between attom at postion 9 and 26, single bond between attom at postion 10 and 27, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, double bond between 12 and 14, single bond between attom at postion 12 and 15, double bond between 13 and 16, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 18, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 34, double bond between 15 and 17, single bond between attom at postion 15 and 35, single bond between attom at postion 16 and 36, single bond between attom at postion 17 and 37, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 38, single bond between attom at postion 18 and 39. The 3D x,y,z coordinates of the element at position 1 is -1.0828, -1.5377, -0.3658, . The 3D x,y,z coordinates of the element at position 2 is -3.5748, -2.7555, -0.5623, . The 3D x,y,z

This compound's CID is 2265 and compound's name is Azathioprine. There are 26 attoms in the molecule and their positions in the order are S, O, O, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 9, double bond between 3 and 9, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 18, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 14, double bond between 6 and 15, double bond between 7 and 13, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 16, double bond between 8 and 18, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 16, double bond between 10 and 19, double bond between 11 and 14, single bond between attom at postion 12 and 13, double bond between 12 and 16, single bond between attom at postion 15 and 20, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 22, single bond between attom at postion 17 and 23, single bond between attom at postion 18 and 25, single bond between attom at postion 19 and 26. The 3D x,y,z coordinates of the element at position 1 is -0.3031, 0.3792, -1.6099, . The 3D x,y,z coordinates of the element at position 2 is -2.44, -1.8923, -1.2402, . The 3D x,y,z coordinates of the element at position 3 is -4.096, -

This compound's CID is 2266 and compound's name is Azelaic Acid. There are 29 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 28, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 29, double bond between 3 and 12, double bond between 4 and 13, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 20, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 26, single bond between attom at postion 11 and 27. The 3D x,y,z coordinates of the element at position 1 is 6.1587, -0.5503, 0.0634, . The 3D x,y,z coordinates of the element at position 2 is -6.1728, -0.5526, 0.0948, . The 3D x,y,z coordinates of the element at position 3 is 5.0195, 1.4228, 0.0409, . The 3D This compound's CID is 2284 and compound's name is Baclofen. There are 26 attoms in the molecule and their positions in the order are CL, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 26, double bond between 3 and 11, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 22, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 15, double bond between 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 20, double bond between 10 and 13, single bond between attom at postion 10 and 21, double bond between 12 and 14, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 25. The 3D x,y,z coordinates of the element at position 1 is -4.5473, 0.3707, 0.2496, . The 3D x,y,z coordinates of the element at position 2 is 2.0613, 2.7033, This compound's CID is 2337 and compound's name is Benzocaine. There are 23 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 11, double bond between 2 and 10, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 23, double bond between 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 13, double bond between 6 and 9, single bond between attom at postion 6 and 14, double bond between 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 8 and 15, single bond between attom at postion 9 and 16, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 12 and 20, single bond between attom at postion 12 and 21. The 3D x,y,z coordinates of the element at position 1 is -2.1131, -0.3568, 5.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -1.7062, 1.9089, 0.0, . The 3D x,y,z coordinates of the element at position

This compound's CID is 2375 and compound's name is Bicalutamide. There are 43 attoms in the molecule and their positions in the order are S, X, X, X, X, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 7, double bond between 1 and 8, single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 25, single bond between attom at postion 3 and 28, single bond between attom at postion 4 and 28, single bond between attom at postion 5 and 28, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 36, double bond between 9 and 15, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 35, triple bond between 11 and 29, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 30, single bond between attom at postion 13 and 31, single bond between attom at postion 14 and 32, single bond between attom at postion 14 and 33, single bond between attom at postion 14 and 34, double bond between 16 and 18, single bond between attom at postion 16 and 19, double bond between 17 and 20, single bond between attom at postion 17 and 23, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 37, double bond between 19 and 22, single bond between attom at postion 19 and 38, single bond between attom at postion 20 and 24, single bond between attom at postion 20 and 39, double bond between 21 and 25, single bond between attom at postion 21 and 40, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 41, double bond between 23 and 27, single bond between attom at postion 23 and 42, double bond between 24 and 26, single bond between attom at postion 24 and 28, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 29, single bond between attom at postion 27 and 43. The 3D x,y,z coordinates of the element at position 1 is 2.9018, 0.9317, -0.6541, . The 3D x,y,z coordinates of the element at position 2 is 6.4013, -3.7222, 0.1278, . The 3D x,y,z coordinates of the element at position 3 is -3.7862, -2.2514,

This compound's CID is 2391 and compound's name is Bisacodyl. There are 46 attoms in the molecule and their positions in the order are O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 1 and 24, single bond between attom at postion 2 and 20, single bond between attom at postion 2 and 25, double bond between 3 and 24, double bond between 4 and 25, single bond between attom at postion 5 and 9, double bond between 5 and 22, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 28, double bond between 7 and 10, single bond between attom at postion 7 and 12, double bond between 8 and 11, single bond between attom at postion 8 and 13, double bond between 9 and 14, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 30, double bond between 12 and 17, single bond between attom at postion 12 and 31, double bond between 13 and 18, single bond between attom at postion 13 and 32, single bond between attom at postion 14 and 21, single bond between attom at postion 14 and 33, double bond between 15 and 19, single bond between attom at postion 15 and 34, double bond between 16 and 20, single bond between attom at postion 16 and 35, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 36, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 37, double bond between 21 and 23, single bond between attom at postion 21 and 38, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 39, single bond between attom at postion 23 and 40, single bond between attom at postion 24 and 26, single bond between attom at postion 25 and 27, single bond between attom at postion 26 and 41, single bond between attom at postion 26 and 42, single bond between attom at postion 26 and 43, single bond between attom at postion 27 and 44, single bond between attom at postion 27 and 45, single bond between attom at postion 27 and 46. The 3D x,y,z coordinates of the element at position 1 is -4.2128, -2.5912, 0.3339, . The 3D x,y,z coordinates of the element at position 2 is 5.1849, -0.9634, -0.0734, . The 3D x,y,z

This compound's CID is 2471 and compound's name is Bumetanide. There are 45 attoms in the molecule and their positions in the order are S, O, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 19, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 45, double bond between 6 and 20, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 38, single bond between attom at postion 8 and 39, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 26, single bond between attom at postion 9 and 27, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 29, double bond between 11 and 12, single bond between attom at postion 11 and 15, single bond between attom at postion 12 and 13, double bond between 13 and 17, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 31, single bond between attom at postion 14 and 32, double bond between 15 and 16, single bond between attom at postion 15 and 33, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 20, single bond between attom at postion 17 and 34, single bond between attom at postion 18 and 35, single bond between attom at postion 18 and 36, single bond between attom at postion 18 and 37, double bond between 19 and 21, single bond between attom at postion 19 and 22, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 40, double bond between 22 and 24, single bond between attom at postion 22 and 41, double bond between 23 and 25, single bond between attom at postion 23 and 42, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 43, single bond between attom at postion 25 and 44. The 3D x,y,z coordinates of the element at position 1 is -2.9153, -2.0685, 0.4127, . The 3D x,y,z coordinates of the element at position 2 is -0.0266, -1.5191, 0.9881, . The 3D x,y,z coordinates of the element at position 3 is -2.1819, -2.9156,

This compound's CID is 2474 and compound's name is Bupivacaine. There are 49 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 10, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 9, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 13, single bond between attom at postion 3 and 37, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 22, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 23, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 25, single bond between attom at postion 6 and 26, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 27, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 33, single bond between attom at postion 11 and 34, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 35, single bond between attom at postion 12 and 36, double bond between 13 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 14 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 19, double bond between 16 and 18, single bond between attom at postion 16 and 20, double bond between 17 and 21, single bond between attom at postion 17 and 41, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 42, single bond between attom at postion 19 and 43, single bond between attom at postion 19 and 44, single bond between attom at postion 19 and 45, single bond between attom at postion 20 and 46, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 49. The 3D x,y,z coordinates of the element at position 1 is -0.0084, 0.0139, 1.4094, . The 3D x,y,z coordinates of the element at position 2 is -2.3135, 0.5416, 0.1259, . The 3D x,y,z coordinates This compound's CID is 2478 and compound's name is Busulfan. There are 28 attoms in the molecule and their positions in the order are S, S, O, O, O, O, O, O, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, double bond between 1 and 5, double bond between 1 and 6, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 4, double bond between 2 and 7, double bond between 2 and 8, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 12, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 16, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 18, single bond between attom at postion 11 and 19, single bond between attom at postion 11 and 20, single bond between attom at postion 12 and 21, single bond between attom at postion 12 and 22, single bond between attom at postion 13 and 23, single bond between attom at postion 13 and 24, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 27, single bond between attom at postion 14 and 28. The 3D x,y,z coordinates of the element at position 1 is -4.517, -0.1564, 0.0102, . The 3D x,y,z coordinates of the element at position 2 is 4.517, 0.1563, 0.0109, . The 3D x,y,z coordinates of the element at position 3 is -

This compound's CID is 2481 and compound's name is Butalbital. There are 32 attoms in the molecule and their positions in the order are O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 10, double bond between 2 and 11, double bond between 3 and 15, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 28, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 29, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 12 and 22, single bond between attom at postion 12 and 23, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 25, single bond between attom at postion 13 and 26, single bond between attom at postion 13 and 27, double bond between 14 and 16, single bond between attom at postion 14 and 30, single bond between attom at postion 16 and 31, single bond between attom at postion 16 and 32. The 3D x,y,z coordinates of the element at position 1 is -1.6378, -0.2416, -1.9532, . The 3D x,y,z coordinates of the element at position 2 is 0.9371, 0.7971, 1.8338, . The 3D x,y,z coordinates This compound's CID is 2519 and compound's name is Caffeine. There are 24 attoms in the molecule and their positions in the order are O, O, N, N, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 9, double bond between 2 and 10, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 12, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 8, double bond between 6 and 11, double bond between 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 11 and 15, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 20, single bond between attom at postion 13 and 21, single bond between attom at postion 14 and 22, single bond between attom at postion 14 and 23, single bond between attom at postion 14 and 24. The 3D x,y,z coordinates of the element at position 1 is 0.47, 2.5688, 6.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -3.1271, -0.4436, -3.0E-4, . The 3D x,y,z coordinates of the element at position 3 is -0.9686, -

This compound's CID is 2540 and compound's name is Candesartan Cilexetil. There are 79 attoms in the molecule and their positions in the order are O, O, O, O, O, O, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 19, single bond between attom at postion 2 and 22, double bond between 3 and 19, single bond between attom at postion 4 and 22, single bond between attom at postion 4 and 28, single bond between attom at postion 5 and 25, single bond between attom at postion 5 and 38, double bond between 6 and 28, single bond between attom at postion 7 and 20, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 23, double bond between 8 and 25, single bond between attom at postion 9 and 11, double bond between 9 and 44, double bond between 10 and 12, single bond between attom at postion 10 and 44, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 79, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 46, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 47, single bond between attom at postion 14 and 48, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 49, single bond between attom at postion 15 and 50, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 51, single bond between attom at postion 16 and 52, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 53, single bond between attom at postion 17 and 54, single bond between attom at postion 18 and 55, single bond between attom at postion 18 and 56, single bond between attom at postion 20 and 23, double bond between 20 and 24, single bond between attom at postion 21 and 26, single bond between attom at postion 21 and 57, single bond between attom at postion 21 and 58, single bond between attom at postion 22 and 32, single bond between attom at postion 22 and 59, double bond between 23 and 27, single bond between attom at postion 24 and 28, single bond between attom at postion 24 and 29, double bond between 26 and 30, single bond between attom at postion 26 and 31, single bond between attom at postion 27 and 33, single bond between attom at postion 27 and 60, double bond between 29 and 33, single bond between attom at postion 29 and 61, single bond between attom at postion 30 and 35, single bond between attom at postion 30 and 62, double bond between 31 and 36, single bond between attom at postion 31 and 63, single bond between attom at postion 32 and 65, single bond between attom at postion 32 and 66, single bond between attom at postion 32 and 67, single bond between attom at postion 33 and 64, double bond between 34 and 35, single bond

This compound's CID is 2554 and compound's name is Carbamazepine. There are 30 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 14, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 29, single bond between attom at postion 3 and 30, single bond between attom at postion 4 and 6, double bond between 4 and 10, single bond between attom at postion 5 and 7, double bond between 5 and 11, single bond between attom at postion 6 and 8, double bond between 6 and 12, single bond between attom at postion 7 and 9, double bond between 7 and 13, double bond between 8 and 9, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 24, double bond between 15 and 17, single bond between attom at postion 15 and 25, double bond between 16 and 18, single bond between attom at postion 16 and 26, single bond between attom at postion 17 and 27, single bond between attom at postion 18 and 28. The 3D x,y,z coordinates of the element at position 1 is 1.0649, 2.9296, -0.7569, . The 3D x,y,z coordinates of the element at position 2 is -3.0E-4, 0.8924, -

This compound's CID is 2576 and compound's name is Carisoprodol. There are 42 attoms in the molecule and their positions in the order are O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 16, double bond between 3 and 14, double bond between 4 and 16, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 34, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 41, single bond between attom at postion 6 and 42, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 11 and 27, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 28, single bond between attom at postion 12 and 29, single bond between attom at postion 13 and 30, single bond between attom at postion 13 and 31, single bond between attom at postion 13 and 32, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 33, single bond between attom at postion 17 and 35, single bond between attom at postion 17 and 36, single bond between attom at postion 17 and 37, single bond between attom at postion 18 and 38, single bond between attom at postion 18 and 39, single bond between attom at postion 18 and 40. The 3D x,y,z coordinates of the element at position 1 is 0.7138, -0.3398, 0.0876, . The 3D x,y,z coordinates of the element at position 2 is -
This compound's CID is 2578 and compound's name is Carmustine. There are 21 attoms in the molecule and their positions in the order are CL, CL, O, O, N, N, N, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 12, double bond between 3 and 10, double bond between 4 and 7, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 17, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 16, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 19, single bond between attom at postion 12 and 20, single bond between attom at postion 12 and 21. The 3D x,y,z coordinates of the element at position 1 is -4.2047, 1.429, -0.8042, . The 3D x,y,z coordinates of the element at position 2 is 3.6917, -0.4395, -1.6893, . The 3D x,y,z coordinates

This compound's CID is 2585 and compound's name is Carvedilol. There are 56 attoms in the molecule and their positions in the order are O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 49, single bond between attom at postion 3 and 23, single bond between attom at postion 3 and 24, single bond between attom at postion 4 and 25, single bond between attom at postion 4 and 30, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 32, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 20, single bond between attom at postion 6 and 41, single bond between attom at postion 7 and 8, double bond between 7 and 9, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 10, double bond between 8 and 16, single bond between attom at postion 9 and 15, double bond between 10 and 18, double bond between 11 and 17, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 31, single bond between attom at postion 13 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 35, single bond between attom at postion 14 and 36, double bond between 15 and 19, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 21, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 39, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 40, single bond between attom at postion 19 and 42, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 43, single bond between attom at postion 20 and 44, double bond between 21 and 22, single bond between attom at postion 21 and 45, single bond between attom at postion 22 and 46, single bond between attom at postion 23 and 47, single bond between attom at postion 23 and 48, single bond between attom at postion 24 and 25, double bond between 24 and 26, double bond between 25 and 27, single bond between attom at postion 26 and 28, single bond between attom at postion 26 and 50, single bond between attom at postion 27 and 29, single bond between attom at postion 27 and 51, double bond between 28 and 29, single bond between attom at postion 28 and 52, single bond between attom at postion 29 and 53, single bond between attom at postion 30 and 54, single bond between attom at postion 30 and 55, single bond between attom at postion 30 and 56. The 3D x,y,z coordinates of the element at position 1 is -2.4196, 1.7089, 0.1113, . The 3D x,y,z coordinates of the element at position 2 is -

This compound's CID is 2662 and compound's name is Celecoxib. There are 40 attoms in the molecule and their positions in the order are S, X, X, X, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 5, double bond between 1 and 6, single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 25, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 25, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 11, double bond between 8 and 14, single bond between attom at postion 9 and 39, single bond between attom at postion 9 and 40, single bond between attom at postion 10 and 12, double bond between 10 and 13, double bond between 11 and 15, single bond between attom at postion 11 and 16, double bond between 12 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 27, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 20, single bond between attom at postion 15 and 28, double bond between 16 and 21, single bond between attom at postion 16 and 29, double bond between 17 and 20, single bond between attom at postion 17 and 21, single bond between attom at postion 18 and 23, single bond between attom at postion 18 and 30, double bond between 19 and 24, single bond between attom at postion 19 and 31, single bond between attom at postion 20 and 32, single bond between attom at postion 21 and 33, double bond between 22 and 23, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 26, single bond between attom at postion 23 and 34, single bond between attom at postion 24 and 35, single bond between attom at postion 26 and 36, single bond between attom at postion 26 and 37, single bond between attom at postion 26 and 38. The 3D x,y,z coordinates of the element at position 1 is 4.7676, -1.6195, -0.0537, . The 3D x,y,z coordinates of the element at position 2 is -5.477, -1.1414, 0.059, . The 3D x,y,z coordinates of the element at position 3 is -4.4403, -2.7198, -

This compound's CID is 2678 and compound's name is Cetirizine. There are 52 attoms in the molecule and their positions in the order are CL, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 24, single bond between attom at postion 2 and 15, single bond between attom at postion 2 and 26, single bond between attom at postion 3 and 27, single bond between attom at postion 3 and 52, double bond between 4 and 27, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 37, single bond between attom at postion 12 and 38, double bond between 13 and 16, single bond between attom at postion 13 and 17, double bond between 14 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 41, double bond between 17 and 21, single bond between attom at postion 17 and 42, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 43, double bond between 19 and 23, single bond between attom at postion 19 and 44, double bond between 20 and 24, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 46, double bond between 22 and 25, single bond between attom at postion 22 and 47, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 48, single bond between attom at postion 25 and 49, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 50, single bond between attom at postion 26 and 51. The 3D x,y,z coordinates of the element at position 1 is -6.1023, 3.8582, 0.7111, . The 3D x,y,z coordinates of the element at position 2 is 5.702,

This compound's CID is 2708 and compound's name is Chlorambucil. There are 38 attoms in the molecule and their positions in the order are CL, CL, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 18, single bond between attom at postion 3 and 19, single bond between attom at postion 3 and 38, double bond between 4 and 19, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, double bond between 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 20, single bond between attom at postion 7 and 21, double bond between 8 and 14, single bond between attom at postion 8 and 15, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 26, single bond between attom at postion 11 and 27, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 28, double bond between 13 and 15, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 30, single bond between attom at postion 15 and 31, single bond between attom at postion 16 and 19, single bond between attom at postion 16 and 32, single bond between attom at postion 16 and 33, single bond between attom at postion 17 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 18 and 36, single bond between attom at postion 18 and 37. The 3D x,y,z coordinates of the element at position 1 is 4.1196, 3.7283, -0.9656, . The 3D x,y,z coordinates of the element at position 2 is 4.401, -3.5942, -0.6984, . The 3D x,y,z coordinates of the element at position 3 is -5.0294, -

This compound's CID is 2723 and compound's name is Chloroxylenol. There are 19 attoms in the molecule and their positions in the order are CL, O, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 19, double bond between 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 5, double bond between 4 and 7, single bond between attom at postion 4 and 10, double bond between 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 18. The 3D x,y,z coordinates of the element at position 1 is 2.8088, -4.0E-4, -0.0011, . The 3D x,y,z coordinates of the element at position 2 is -3.0735, 2.0E-4, -9.0E-4, . The 3D x,y,z coordinates

This compound's CID is 2732 and compound's name is Chlorthalidone. There are 33 attoms in the molecule and their positions in the order are CL, S, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 21, double bond between 2 and 5, double bond between 2 and 6, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 28, double bond between 4 and 13, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 32, single bond between attom at postion 8 and 33, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 10 and 12, double bond between 10 and 15, double bond between 11 and 14, single bond between attom at postion 11 and 16, single bond between attom at postion 12 and 13, double bond between 12 and 18, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 24, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 25, double bond between 16 and 20, single bond between attom at postion 16 and 26, double bond between 17 and 21, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 27, double bond between 19 and 22, single bond between attom at postion 19 and 30, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 29, single bond between attom at postion 22 and 31. The 3D x,y,z coordinates of the element at position 1 is -4.7187, -1.0015, 0.6077, . The 3D x,y,z coordinates of the element at position 2 is -3.1006, 1.6618, -0.2592, . The 3D x,y,z coordinates of the element at position 3 is 1.7196, -2.591, -
This compound's CID is 2733 and compound's name is Chlorzoxazone. There are 15 attoms in the molecule and their positions in the order are CL, O, O, N, C, C, C, C, C, C, C, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 10, double bond between 3 and 10, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 12, double bond between 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 6 and 8, double bond between 7 and 9, single bond between attom at postion 7 and 13, double bond between 8 and 11, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 11, single bond between attom at postion 11 and 15. The 3D x,y,z coordinates of the element at position 1 is 3.7901, 0.8156, 6.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -1.7579, -1.0498, 1.0E-4, . The 3D x,y,z coordinates of the element at position 3 is -3.5653,

This compound's CID is 2749 and compound's name is Ciclopirox. There are 32 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 32, double bond between 2 and 13, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 16, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 18, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 19, single bond between attom at postion 6 and 20, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 22, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 23, single bond between attom at postion 8 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 9 and 26, double bond between 10 and 11, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 27, double bond between 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 14, single bond between attom at postion 14 and 28, single bond between attom at postion 15 and 29, single bond between attom at postion 15 and 30, single bond between attom at postion 15 and 31. The 3D x,y,z coordinates of the element at position 1 is -0.612, 2.3795, -0.0558, . The 3D x,y,z coordinates of the element at position 2 is -
This compound's CID is 2754 and compound's name is Cilostazol. There are 54 attoms in the molecule and their positions in the order are O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 1 and 23, double bond between 2 and 25, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 14, double bond between 4 and 6, single bond between attom at postion 5 and 6, double bond between 5 and 14, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 25, single bond between attom at postion 7 and 52, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 29, single bond between attom at postion 9 and 30, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 31, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 33, single bond between attom at postion 11 and 34, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 35, single bond between attom at postion 12 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 15, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 41, single bond between attom at postion 16 and 42, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 20, double bond between 19 and 21, single bond between attom at postion 19 and 24, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 26, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 49, single bond between attom at postion 22 and 50, double bond between 23 and 24, single bond between attom at postion 23 and 27, single bond between attom at postion 24 and 51, double bond between 26 and 27, single bond between attom at postion 26 and 53, single bond between attom at postion 27 and 54. The 3D x,y,z coordinates of the element at position 1 is -0.0791, -2.1915, -0.7337, . The 3D x,y,z

This compound's CID is 2756 and compound's name is Cimetidine. There are 33 attoms in the molecule and their positions in the order are S, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 8, double bond between 4 and 14, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 30, double bond between 6 and 15, single bond between attom at postion 6 and 16, triple bond between 7 and 17, single bond between attom at postion 8 and 9, double bond between 8 and 12, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 19, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 12 and 13, single bond between attom at postion 13 and 26, single bond between attom at postion 13 and 27, single bond between attom at postion 13 and 28, single bond between attom at postion 14 and 29, single bond between attom at postion 16 and 31, single bond between attom at postion 16 and 32, single bond between attom at postion 16 and 33. The 3D x,y,z coordinates of the element at position 1 is 0.7415, -0.8471, -0.0546, . The 3D x,y,z coordinates of the element at position 2 is 4.9739, 0.8242, -0.6812, . The 3D x,y,z coordinates of the element at position 3 is -2.367, -0.4189, 0.3524, . The 3D This compound's CID is 2758 and compound's name is Eucalyptol. There are 29 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 4, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 12, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 11 and 27, single bond between attom at postion 11 and 28, single bond between attom at postion 11 and 29. The 3D x,y,z coordinates of the element at position 1 is -0.0266, -1.189, -1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -

This compound's CID is 2764 and compound's name is Ciprofloxacin. There are 42 attoms in the molecule and their positions in the order are X, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 23, double bond between 2 and 19, single bond between attom at postion 3 and 24, single bond between attom at postion 3 and 42, double bond between 4 and 24, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 20, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 41, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 26, single bond between attom at postion 9 and 27, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 13, double bond between 11 and 14, double bond between 12 and 18, single bond between attom at postion 12 and 30, single bond between attom at postion 13 and 19, double bond between 13 and 22, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 31, double bond between 15 and 23, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 32, single bond between attom at postion 16 and 33, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 24, single bond between attom at postion 20 and 36, single bond between attom at postion 20 and 37, single bond between attom at postion 21 and 38, single bond between attom at postion 21 and 39, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 40. The 3D x,y,z coordinates of the element at position 1 is -2.2164, 2.7826, 0.361, . The 3D x,y,z coordinates of the element at position 2 is 2.8091,

This compound's CID is 2771 and compound's name is Citalopram. There are 45 attoms in the molecule and their positions in the order are X, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 21, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 23, triple bond between 4 and 24, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 25, single bond between attom at postion 6 and 26, double bond between 7 and 8, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, double bond between 10 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 29, single bond between attom at postion 11 and 30, single bond between attom at postion 12 and 31, single bond between attom at postion 12 and 32, double bond between 13 and 17, single bond between attom at postion 13 and 33, double bond between 14 and 18, single bond between attom at postion 14 and 34, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 35, double bond between 16 and 20, single bond between attom at postion 16 and 36, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 37, single bond between attom at postion 18 and 24, double bond between 19 and 21, single bond between attom at postion 19 and 38, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 39, single bond between attom at postion 22 and 40, single bond between attom at postion 22 and 41, single bond between attom at postion 22 and 42, single bond between attom at postion 23 and 43, single bond between attom at postion 23 and 44, single bond between attom at postion 23 and 45. The 3D x,y,z coordinates of the element at position 1 is -2.0573, 5.0073, -0.1688, . The 3D x,y,z coordinates of the element at position 2 is -0.1141, -0.6063, This compound's CID is 2789 and compound's name is Clobazam. There are 34 attoms in the molecule and their positions in the order are CL, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, double bond between 2 and 9, double bond between 3 and 10, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 14, double bond between 6 and 7, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 22, single bond between attom at postion 8 and 23, double bond between 11 and 17, single bond between attom at postion 11 and 18, double bond between 12 and 15, single bond between attom at postion 12 and 24, double bond between 13 and 16, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 27, single bond between attom at postion 14 and 28, single bond between attom at postion 15 and 16, single bond between attom at postion 16 and 29, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 30, double bond between 18 and 20, single bond between attom at postion 18 and 31, double bond between 19 and 21, single bond between attom at postion 19 and 32, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 33, single bond between attom at postion 21 and 34. The 3D x,y,z coordinates of the element at position 1 is -0.0754, -4.4844, 0.9755, . The 3D x,y,z coordinates of the element at position 2 is -0.6431, 2.9072, 0.7473, . The 3D x,y,z

This compound's CID is 2802 and compound's name is Clonazepam. There are 32 attoms in the molecule and their positions in the order are CL, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, double bond between 2 and 16, single bond between attom at postion 3 and 7, double bond between 4 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 24, double bond between 6 and 10, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 15, double bond between 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 10 and 11, single bond between attom at postion 11 and 18, double bond between 11 and 19, double bond between 12 and 15, single bond between attom at postion 12 and 23, double bond between 13 and 17, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 27, single bond between attom at postion 15 and 17, single bond between attom at postion 17 and 28, double bond between 18 and 20, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 29, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 30, double bond between 21 and 22, single bond between attom at postion 21 and 31, single bond between attom at postion 22 and 32. The 3D x,y,z coordinates of the element at position 1 is 2.3382, 0.2449, -2.1583, . The 3D x,y,z coordinates of the element at position 2 is 1.3758, 4.3718, -0.0107, . The 3D x,y,z
This compound's CID is 2803 and compound's name is Clonidine. There are 23 attoms in the molecule and their positions in the order are CL, CL, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 19, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 20, single bond between attom at postion 5 and 7, double bond between 5 and 8, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, double bond between 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 10 and 12, double bond between 11 and 13, double bond between 12 and 14, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 22, single bond between attom at postion 14 and 23. The 3D x,y,z coordinates of the element at position 1 is -0.6943, -2.7291, -0.4532, . The 3D x,y,z coordinates of the element at position 2 is -0.7006, 2.7304, -

This compound's CID is 2812 and compound's name is Clotrimazole. There are 42 attoms in the molecule and their positions in the order are CL, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 15, double bond between 3 and 15, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 8, double bond between 5 and 9, double bond between 6 and 10, single bond between attom at postion 6 and 12, double bond between 7 and 11, single bond between attom at postion 7 and 13, double bond between 8 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 26, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 27, single bond between attom at postion 11 and 20, single bond between attom at postion 11 and 28, double bond between 12 and 21, single bond between attom at postion 12 and 29, double bond between 13 and 22, single bond between attom at postion 13 and 30, double bond between 14 and 16, single bond between attom at postion 14 and 31, single bond between attom at postion 15 and 32, single bond between attom at postion 16 and 33, single bond between attom at postion 17 and 23, single bond between attom at postion 17 and 34, double bond between 18 and 23, single bond between attom at postion 18 and 35, double bond between 19 and 24, single bond between attom at postion 19 and 36, double bond between 20 and 25, single bond between attom at postion 20 and 37, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 38, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 39, single bond between attom at postion 23 and 40, single bond between attom at postion 24 and 41, single bond between attom at postion 25 and 42. The 3D x,y,z coordinates of the element at position 1 is 0.6462, -0.1889, 2.763, . The 3D x,y,z coordinates of the element at position 2 is -0.4392, -0.0896, -1.7148, . The 3D x,y,z coordinates of the element at This compound's CID is 2907 and compound's name is Cyclophosphamide. There are 29 attoms in the molecule and their positions in the order are CL, CL, P, O, O, N, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 4, double bond between 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 4 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 24, single bond between attom at postion 12 and 25, single bond between attom at postion 13 and 26, single bond between attom at postion 13 and 27, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 29. The 3D x,y,z coordinates of the element at position 1 is 3.2423, 2.7414, -0.4539, . The 3D x,y,z coordinates of the element at position 2 is 3.0499, -3.109, -6.0E-4, . The 3D x,y,z

This compound's CID is 2913 and compound's name is Cyproheptadine. There are 43 attoms in the molecule and their positions in the order are N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, double bond between 2 and 7, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 23, single bond between attom at postion 3 and 24, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 25, single bond between attom at postion 4 and 26, single bond between attom at postion 5 and 27, single bond between attom at postion 5 and 28, single bond between attom at postion 6 and 29, single bond between attom at postion 6 and 30, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 8 and 11, double bond between 8 and 13, single bond between attom at postion 9 and 12, double bond between 9 and 14, single bond between attom at postion 10 and 31, single bond between attom at postion 10 and 32, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 15, double bond between 11 and 17, single bond between attom at postion 12 and 16, double bond between 12 and 18, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 20, single bond between attom at postion 14 and 35, double bond between 15 and 16, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 37, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 38, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 39, double bond between 19 and 21, single bond between attom at postion 19 and 40, double bond between 20 and 22, single bond between attom at postion 20 and 41, single bond between attom at postion 21 and 42, single bond between attom at postion 22 and 43. The 3D x,y,z coordinates of the element at position 1 is -4.0233, -0.2293, 0.2279, . The 3D x,y,z coordinates of This compound's CID is 2955 and compound's name is Dapsone. There are 29 attoms in the molecule and their positions in the order are S, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, double bond between 1 and 3, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 7, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 26, single bond between attom at postion 4 and 27, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 28, single bond between attom at postion 5 and 29, double bond between 6 and 8, single bond between attom at postion 6 and 10, double bond between 7 and 9, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 19, double bond between 10 and 14, single bond between attom at postion 10 and 20, double bond between 11 and 15, single bond between attom at postion 11 and 21, double bond between 12 and 16, single bond between attom at postion 12 and 22, double bond between 13 and 17, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 24, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 25. The 3D x,y,z coordinates of the element at position 1 is -0.0023, 1.619, 1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -0.0238, 2.35, -1.2592, . The 3D x,y,z coordinates of the element at position 3 is 0.0612, 2.349, 1.2596, .

This compound's CID is 2972 and compound's name is Deferiprone. There are 19 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 19, double bond between 2 and 9, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, double bond between 4 and 5, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 9, double bond between 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 14, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 10, single bond between attom at postion 10 and 18. The 3D x,y,z coordinates of the element at position 1 is -1.362, -1.992, 0.0052, . The 3D x,y,z coordinates of the element at position 2 is -2.7029, 0.4496, 0.0062, . The 3D x,y,z
This compound's CID is 3007 and compound's name is Amphetamine. There are 23 attoms in the molecule and their positions in the order are N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 19, single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 13, double bond between 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 17, double bond between 7 and 9, single bond between attom at postion 7 and 18, double bond between 8 and 10, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 23. The 3D x,y,z coordinates of the element at position 1 is -3.5849, -0.4599, 0.1218, . The 3D x,y,z coordinates of the element at position 2 is -2.2239, -0.1762, -0.3436, . The 3D x,y,z
This compound's CID is 3016 and compound's name is Diazepam. There are 33 attoms in the molecule and their positions in the order are CL, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, double bond between 2 and 9, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 13, double bond between 4 and 7, single bond between attom at postion 4 and 8, double bond between 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, double bond between 10 and 16, single bond between attom at postion 10 and 17, double bond between 11 and 14, single bond between attom at postion 11 and 23, double bond between 12 and 15, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 25, single bond between attom at postion 13 and 26, single bond between attom at postion 13 and 27, single bond between attom at postion 14 and 15, single bond between attom at postion 15 and 28, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 29, double bond between 17 and 19, single bond between attom at postion 17 and 30, double bond between 18 and 20, single bond between attom at postion 18 and 31, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 32, single bond between attom at postion 20 and 33. The 3D x,y,z coordinates of the element at position 1 is 0.2998, -4.4445, 0.8123, . The 3D x,y,z coordinates of the element at position 2 is 2.4289, 3.3083, -0.1483, . The 3D x,y,z coordinates of the element at position 3 is 2.3415,

This compound's CID is 3019 and compound's name is Diazoxide. There are 21 attoms in the molecule and their positions in the order are CL, S, O, O, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, double bond between 2 and 3, double bond between 2 and 4, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 15, double bond between 6 and 9, double bond between 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 14, double bond between 10 and 12, single bond between attom at postion 10 and 16, double bond between 11 and 13, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 13, single bond between attom at postion 13 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 14 and 20, single bond between attom at postion 14 and 21. The 3D x,y,z coordinates of the element at position 1 is 4.3022, -0.5652, -0.0011, . The 3D x,y,z coordinates of the element at position 2 is -1.0357, -1.4619, 5.0E-4, . The 3D x,y,z coordinates
This compound's CID is 3025 and compound's name is Dibucaine. There are 54 attoms in the molecule and their positions in the order are O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 1 and 19, double bond between 2 and 14, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 34, single bond between attom at postion 5 and 15, double bond between 5 and 18, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 26, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 14, double bond between 10 and 16, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 12 and 38, single bond between attom at postion 12 and 39, single bond between attom at postion 12 and 40, single bond between attom at postion 13 and 15, double bond between 13 and 21, double bond between 15 and 22, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 43, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 41, single bond between attom at postion 17 and 42, single bond between attom at postion 19 and 44, single bond between attom at postion 19 and 45, single bond between attom at postion 20 and 25, single bond between attom at postion 20 and 46, single bond between attom at postion 20 and 47, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 48, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 49, double bond between 23 and 24, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 54, single bond between attom at postion 25 and 51, single bond between attom at postion 25 and 52, single bond between attom at postion 25 and 53. The 3D x,y,z coordinates of the element at position 1 is 3.5524, -1.3311, -0.1336, . The 3D x,y,z coordinates of the element at position 2 is -1.6824, 0.1783, -1.7485, . The 3D x,y,z

This compound's CID is 3038 and compound's name is Dichlorphenamide. There are 22 attoms in the molecule and their positions in the order are CL, CL, S, S, O, O, O, O, N, N, C, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 16, double bond between 3 and 5, double bond between 3 and 6, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 11, double bond between 4 and 7, double bond between 4 and 8, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 12, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 13, double bond between 11 and 14, double bond between 12 and 13, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 16, double bond between 15 and 16, single bond between attom at postion 15 and 18. The 3D x,y,z coordinates of the element at position 1 is 2.7868, -1.8478, -5.0E-4, . The 3D x,y,z coordinates of the element at position 2 is 0.1858, -3.7158, -0.0511, . The 3D x,y,z coordinates of the element at position 3 is 2.4008, 1.3229, 0.1003, . The 3D x,y,z coordinates of the element at

This compound's CID is 3108 and compound's name is Dipyridamole. There are 76 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 33, single bond between attom at postion 1 and 73, single bond between attom at postion 2 and 34, single bond between attom at postion 2 and 74, single bond between attom at postion 3 and 35, single bond between attom at postion 3 and 75, single bond between attom at postion 4 and 36, single bond between attom at postion 4 and 76, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 23, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 24, double bond between 7 and 23, single bond between attom at postion 7 and 27, double bond between 8 and 24, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 25, double bond between 9 and 27, single bond between attom at postion 10 and 26, double bond between 10 and 28, single bond between attom at postion 11 and 27, single bond between attom at postion 11 and 29, single bond between attom at postion 11 and 30, single bond between attom at postion 12 and 28, single bond between attom at postion 12 and 31, single bond between attom at postion 12 and 32, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 45, single bond between attom at postion 17 and 46, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 47, single bond between attom at postion 18 and 48, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 49, single bond between attom at postion 19 and 50, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 51, single bond between attom at postion 20 and 52, single bond between attom at postion 21 and 53, single bond between attom at postion 21 and 54, single bond between attom at postion 22 and 55, single bond between attom at postion 22 and 56, single bond between attom at postion 23 and 26, single bond between attom at postion 24 and 25, double bond between 25 and 26, single bond between attom at postion 29 and 33, single bond between attom at postion 29 and 57, single bond between attom at

This compound's CID is 3117 and compound's name is Disulfiram. There are 36 attoms in the molecule and their positions in the order are S, S, S, S, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 16, double bond between 3 and 15, double bond between 4 and 16, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 11 and 27, single bond between attom at postion 12 and 28, single bond between attom at postion 12 and 29, single bond between attom at postion 12 and 30, single bond between attom at postion 13 and 31, single bond between attom at postion 13 and 32, single bond between attom at postion 13 and 33, single bond between attom at postion 14 and 34, single bond between attom at postion 14 and 35, single bond between attom at postion 14 and 36. The 3D x,y,z coordinates of the element at position 1 is 0.4366, 1.2142, 1.2884, . The 3D x,y,z coordinates of the element at position 2 is -0.8853, 1.8943, -0.1414, . The 3D x,y,z coordinates of the element at position 3 is 2.5634, 2.5308, -
This compound's CID is 3121 and compound's name is Valproic Acid. There are 26 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 26, double bond between 2 and 8, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 25. The 3D x,y,z coordinates of the element at position 1 is 0.0361, -2.0835, 0.9381, . The 3D x,y,z coordinates of the element at position 2 is -0.0363, -1.6209, -1.2811, . The 3D x,y,z

This compound's CID is 3168 and compound's name is Droperidol. There are 50 attoms in the molecule and their positions in the order are X, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 28, double bond between 2 and 16, double bond between 3 and 19, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 42, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 29, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 31, single bond between attom at postion 8 and 32, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 33, single bond between attom at postion 9 and 34, double bond between 10 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 37, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 38, single bond between attom at postion 13 and 39, single bond between attom at postion 14 and 17, double bond between 14 and 18, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, double bond between 17 and 20, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 43, single bond between attom at postion 19 and 23, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 44, double bond between 21 and 22, single bond between attom at postion 21 and 45, single bond between attom at postion 22 and 46, double bond between 23 and 24, single bond between attom at postion 23 and 25, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 47, double bond between 25 and 27, single bond between attom at postion 25 and 48, double bond between 26 and 28, single bond between attom at postion 26 and 49, single bond between attom at postion 27 and 28, single bond between attom at postion 27 and 50. The 3D x,y,z coordinates of the element at position 1 is -9.2014, -0.3477, 1.6246, . The 3D x,y,z coordinates of the element at This compound's CID is 3261 and compound's name is Estazolam. There are 32 attoms in the molecule and their positions in the order are CL, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 14, double bond between 3 and 8, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 5, double bond between 4 and 9, double bond between 5 and 14, double bond between 6 and 7, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 10, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, double bond between 11 and 17, single bond between attom at postion 11 and 18, double bond between 12 and 15, single bond between attom at postion 12 and 24, double bond between 13 and 16, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 27, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 28, double bond between 18 and 20, single bond between attom at postion 18 and 29, double bond between 19 and 21, single bond between attom at postion 19 and 30, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 31, single bond between attom at postion 21 and 32. The 3D x,y,z coordinates of the element at position 1 is -0.9872, 4.4647, 0.6744, . The 3D x,y,z coordinates of the element at position 2 is

This compound's CID is 3278 and compound's name is Ethacrynic acid. There are 31 attoms in the molecule and their positions in the order are CL, CL, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 13, single bond between attom at postion 3 and 18, double bond between 4 and 9, single bond between attom at postion 5 and 19, single bond between attom at postion 5 and 31, double bond between 6 and 19, single bond between attom at postion 7 and 9, double bond between 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, double bond between 8 and 17, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 14, double bond between 12 and 15, single bond between attom at postion 12 and 22, double bond between 13 and 14, single bond between attom at postion 13 and 15, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 24, single bond between attom at postion 16 and 25, single bond between attom at postion 16 and 26, single bond between attom at postion 17 and 27, single bond between attom at postion 17 and 28, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 29, single bond between attom at postion 18 and 30. The 3D x,y,z coordinates of the element at position 1 is 1.5998, 2.3519, 0.4371, . The 3D x,y,z coordinates of the element at position 2 is -1.5889, 2.5083, 0.3792, . The 3D x,y,z coordinates of the element at position 3 is -2.855, 0.0578, -0.698, . The 3D x,y,z coordinates of This compound's CID is 3291 and compound's name is Ethosuximide. There are 21 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 7, double bond between 2 and 9, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 18, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 14, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21. The 3D x,y,z coordinates of the element at position 1 is -0.2044, 2.3355, -0.2546, . The 3D x,y,z coordinates of the element at position 2 is 2.7476, -1.1847, -0.0754, . The 3D x,y,z

This compound's CID is 3308 and compound's name is Etodolac. There are 42 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 17, single bond between attom at postion 2 and 42, double bond between 3 and 17, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 30, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, double bond between 6 and 7, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 22, single bond between attom at postion 8 and 23, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 26, single bond between attom at postion 10 and 27, single bond between attom at postion 11 and 13, double bond between 11 and 16, single bond between attom at postion 12 and 28, single bond between attom at postion 12 and 29, double bond between 13 and 14, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 15 and 31, single bond between attom at postion 15 and 32, single bond between attom at postion 15 and 33, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 34, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 35, single bond between attom at postion 18 and 36, double bond between 19 and 20, single bond between attom at postion 19 and 37, single bond between attom at postion 20 and 38, single bond between attom at postion 21 and 39, single bond between attom at postion 21 and 40, single bond between attom at postion 21 and 41. The 3D x,y,z coordinates of the element at position 1 is -2.401, 1.1785, -0.6286, . The 3D x,y,z coordinates of the element at position 2 is -4.1917, -2.1084, 1.1506, . The 3D This compound's CID is 3324 and compound's name is Famciclovir. There are 42 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 20, double bond between 3 and 19, double bond between 4 and 20, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 16, double bond between 6 and 16, single bond between attom at postion 6 and 17, double bond between 7 and 15, single bond between attom at postion 7 and 21, single bond between attom at postion 8 and 18, double bond between 8 and 21, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 41, single bond between attom at postion 9 and 42, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 12 and 27, single bond between attom at postion 12 and 28, single bond between attom at postion 13 and 29, single bond between attom at postion 13 and 30, single bond between attom at postion 14 and 31, single bond between attom at postion 14 and 32, single bond between attom at postion 15 and 17, single bond between attom at postion 16 and 33, double bond between 17 and 18, single bond between attom at postion 18 and 34, single bond between attom at postion 19 and 22, single bond between attom at postion 20 and 23, single bond between attom at postion 22 and 35, single bond between attom at postion 22 and 36, single bond between attom at postion 22 and 37, single bond between attom at postion 23 and 38, single bond between attom at postion 23 and 39, single bond between attom at postion 23 and 40. The 3D x,y,z coordinates of the element at position 1 is 3.6199, 1.508, -0.0625, . The 3D x,y,z coordinates of the element at position 2 is 1.5277, -2.213, 0.095, . The 3D x,y,z coordinates of the element at position 3 is 5.2684,

This compound's CID is 3331 and compound's name is Felbamate. There are 31 attoms in the molecule and their positions in the order are O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 17, double bond between 3 and 16, double bond between 4 and 17, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 28, single bond between attom at postion 5 and 29, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 30, single bond between attom at postion 6 and 31, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 18, double bond between 8 and 11, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 23, double bond between 12 and 14, single bond between attom at postion 12 and 24, double bond between 13 and 15, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 26, single bond between attom at postion 15 and 27. The 3D x,y,z coordinates of the element at position 1 is -2.3963, 0.7925, 0.5031, . The 3D x,y,z coordinates of the element at position 2 is 2.4463, 0.7845, 0.3996, . The 3D x,y,z coordinates of the element at position 3 is -3.7613, 2.1738, -0.7331, . The 3D This compound's CID is 3333 and compound's name is Felodipine. There are 44 attoms in the molecule and their positions in the order are CL, CL, O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 17, single bond between attom at postion 4 and 24, double bond between 5 and 14, double bond between 6 and 17, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 26, double bond between 9 and 12, single bond between attom at postion 9 and 14, double bond between 10 and 13, single bond between attom at postion 10 and 17, double bond between 11 and 18, single bond between attom at postion 11 and 19, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 15 and 28, single bond between attom at postion 15 and 29, single bond between attom at postion 15 and 30, single bond between attom at postion 16 and 31, single bond between attom at postion 16 and 32, single bond between attom at postion 16 and 33, single bond between attom at postion 18 and 20, double bond between 19 and 21, single bond between attom at postion 19 and 34, double bond between 20 and 22, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 35, single bond between attom at postion 22 and 36, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 37, single bond between attom at postion 23 and 38, single bond between attom at postion 24 and 39, single bond between attom at postion 24 and 40, single bond between attom at postion 24 and 41, single bond between attom at postion 25 and 42, single bond between attom at postion 25 and 43, single bond between attom at postion 25 and 44. The 3D x,y,z coordinates of the element at position 1 is 0.4997, -2.0723, 2.1072, . The 3D x,y,z coordinates of the element at

This compound's CID is 3337 and compound's name is Fenfluramine. There are 32 attoms in the molecule and their positions in the order are X, X, X, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 20, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 17, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 19, double bond between 7 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, single bond between attom at postion 8 and 23, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 26, double bond between 11 and 13, single bond between attom at postion 11 and 27, double bond between 12 and 14, single bond between attom at postion 12 and 16, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 28, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 30, single bond between attom at postion 15 and 31, single bond between attom at postion 15 and 32. The 3D x,y,z coordinates of the element at position 1 is -4.3606, -0.5609, 0.4684, . The 3D x,y,z coordinates of the element at position 2 is -3.4072, -1.4373, -1.2713, . The 3D x,y,z

This compound's CID is 3339 and compound's name is Fenofibrate. There are 46 attoms in the molecule and their positions in the order are CL, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 25, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 10, double bond between 4 and 9, double bond between 5 and 19, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 32, double bond between 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 33, double bond between 13 and 18, single bond between attom at postion 13 and 34, double bond between 14 and 17, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 15 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 41, single bond between attom at postion 18 and 42, single bond between attom at postion 19 and 20, double bond between 20 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 43, double bond between 22 and 24, single bond between attom at postion 22 and 44, double bond between 23 and 25, single bond between attom at postion 23 and 45, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 46. The 3D x,y,z coordinates of the element at position 1 is -7.1677, -2.9104, -0.1781, . The 3D x,y,z coordinates of the element at position 2 is 2.289, 0.6715, -0.9147, . The 3D x,y,z

This compound's CID is 3345 and compound's name is Fentanyl. There are 53 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 12, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 9, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 26, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 27, single bond between attom at postion 5 and 28, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 29, single bond between attom at postion 6 and 30, single bond between attom at postion 7 and 31, single bond between attom at postion 7 and 32, single bond between attom at postion 8 and 33, single bond between attom at postion 8 and 34, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 35, single bond between attom at postion 9 and 36, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 37, single bond between attom at postion 10 and 38, double bond between 11 and 15, single bond between attom at postion 11 and 16, single bond between attom at postion 12 and 14, double bond between 13 and 18, single bond between attom at postion 13 and 19, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 20, single bond between attom at postion 15 and 41, double bond between 16 and 21, single bond between attom at postion 16 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 17 and 45, single bond between attom at postion 18 and 23, single bond between attom at postion 18 and 46, double bond between 19 and 24, single bond between attom at postion 19 and 47, double bond between 20 and 22, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 49, single bond between attom at postion 22 and 50, double bond between 23 and 25, single bond between attom at postion 23 and 51, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 52, single bond between attom at postion 25 and 53. The 3D x,y,z coordinates of the element at position 1 is -3.7, -2.9403, -0.0314, . The 3D x,y,z coordinates of the element at position 2 is 1.2909, -0.1114, -0.4784, . The 3D x,y,z coordinates of the element at

This compound's CID is 3365 and compound's name is Fluconazole. There are 34 attoms in the molecule and their positions in the order are X, X, O, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 27, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 18, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 19, double bond between 6 and 21, double bond between 7 and 22, double bond between 8 and 18, single bond between attom at postion 8 and 21, double bond between 9 and 19, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 13, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 12 and 25, single bond between attom at postion 12 and 26, double bond between 13 and 14, single bond between attom at postion 13 and 15, single bond between attom at postion 14 and 16, double bond between 15 and 17, single bond between attom at postion 15 and 28, double bond between 16 and 20, single bond between attom at postion 16 and 29, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 30, single bond between attom at postion 18 and 31, single bond between attom at postion 19 and 32, single bond between attom at postion 21 and 33, single bond between attom at postion 22 and 34. The 3D x,y,z coordinates of the element at position 1 is 0.1203, 0.8123, -2.3583, . The 3D x,y,z coordinates of the element at position 2 is 0.0743, 4.5194,
This compound's CID is 3366 and compound's name is Flucytosine. There are 13 attoms in the molecule and their positions in the order are X, O, N, N, N, C, C, C, C, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, double bond between 2 and 8, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 8, double bond between 5 and 9, double bond between 6 and 7, single bond between attom at postion 7 and 9, single bond between attom at postion 9 and 11. The 3D x,y,z coordinates of the element at position 1 is 2.3815, 0.9951, -2.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -2.7475, -0.4935, -6.0E-4, . The 3D x,y,z coordinates of the element at position 3 is -0.5463, -1.0798, 6.0E-4, . The 3D
This compound's CID is 3385 and compound's name is Fluorouracil. There are 12 attoms in the molecule and their positions in the order are X, O, O, N, N, C, C, C, C, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, double bond between 2 and 6, double bond between 3 and 7, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 10, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 8, double bond between 8 and 9, single bond between attom at postion 9 and 12. The 3D x,y,z coordinates of the element at position 1 is -2.4548, -0.8375, -7.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -1.6047, 1.7485, -4.0E-4, . The 3D x,y,z coordinates of the

This compound's CID is 3394 and compound's name is Flurbiprofen. There are 31 attoms in the molecule and their positions in the order are X, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 31, double bond between 3 and 13, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 19, double bond between 5 and 7, single bond between attom at postion 5 and 8, double bond between 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 20, double bond between 8 and 10, single bond between attom at postion 8 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 11 and 25, double bond between 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 26, double bond between 15 and 17, single bond between attom at postion 15 and 27, double bond between 16 and 18, single bond between attom at postion 16 and 28, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 29, single bond between attom at postion 18 and 30. The 3D x,y,z coordinates of the element at position 1 is -0.7173, -0.9249, 1.9199, . The 3D x,y,z coordinates of the element at position 2 is 5.435, -0.5394, -0.31, . The 3D x,y,z coordinates of the element at position 3 is 3.5304, -1.7672, -0.2791, . The 3D x,y,z
This compound's CID is 3397 and compound's name is Flutamide. There are 30 attoms in the molecule and their positions in the order are X, X, X, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 19, double bond between 4 and 11, single bond between attom at postion 5 and 8, double bond between 6 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 21, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 20, double bond between 10 and 13, single bond between attom at postion 10 and 17, single bond between attom at postion 12 and 13, double bond between 12 and 16, single bond between attom at postion 12 and 19, single bond between attom at postion 13 and 22, single bond between attom at postion 14 and 23, single bond between attom at postion 14 and 24, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 26, single bond between attom at postion 15 and 27, single bond between attom at postion 15 and 28, single bond between attom at postion 16 and 18, double bond between 17 and 18, single bond between attom at postion 17 and 29, single bond between attom at postion 18 and 30. The 3D x,y,z coordinates of the element at position 1 is 3.4234, -1.2904, 1.1363, . The 3D x,y,z coordinates of the element at position 2 is 2.1686, -2.7578, 0.136, . The 3D x,y,z coordinates of

This compound's CID is 3440 and compound's name is Furosemide. There are 32 attoms in the molecule and their positions in the order are CL, S, O, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, double bond between 2 and 4, double bond between 2 and 5, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 17, single bond between attom at postion 3 and 21, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 32, double bond between 7 and 18, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 12, double bond between 10 and 15, single bond between attom at postion 11 and 13, double bond between 11 and 16, double bond between 12 and 13, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 22, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 23, single bond between attom at postion 14 and 24, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 26, double bond between 17 and 19, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 27, double bond between 20 and 21, single bond between attom at postion 20 and 30, single bond between attom at postion 21 and 31. The 3D x,y,z coordinates of the element at position 1 is -2.5979, 2.9547, 0.0275, . The 3D x,y,z coordinates of the element at position 2 is -4.3876, 0.2607, 0.007, . The 3D x,y,z coordinates of the element at
This compound's CID is 3446 and compound's name is Gabapentin. There are 29 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 29, double bond between 2 and 12, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 27, single bond between attom at postion 3 and 28, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26. The 3D x,y,z coordinates of the element at position 1 is 2.3571, 1.7533, -0.2688, . The 3D x,y,z coordinates of the element at position 2 is 3.0687, -0.2795, 0.4674, . The 3D x,y,z coordinates of the

This compound's CID is 3463 and compound's name is Gemfibrozil. There are 40 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 31, double bond between 3 and 10, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 10, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 19, single bond between attom at postion 5 and 20, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 22, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 9 and 30, double bond between 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 17, double bond between 13 and 14, single bond between attom at postion 13 and 32, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 18, double bond between 15 and 16, single bond between attom at postion 15 and 33, single bond between attom at postion 16 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 17 and 36, single bond between attom at postion 17 and 37, single bond between attom at postion 18 and 38, single bond between attom at postion 18 and 39, single bond between attom at postion 18 and 40. The 3D x,y,z coordinates of the element at position 1 is -0.663, 0.1444, 0.8836, . The 3D x,y,z coordinates of the element at position 2 is 3.4432, -1.5237, 0.9762, . The 3D x,y,z coordinates of the element at position 3 is 4.8714, 0.2145,

This compound's CID is 3476 and compound's name is Glimepiride. There are 68 atoms in the molecule and their positions in the order are S, O, O, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 22, double bond between 2 and 18, double bond between 5 and 23, double bond between 6 and 27, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 48, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 49, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 27, single bond between attom at postion 10 and 27, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 63, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 35, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 36, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 17 and 45, single bond between attom at postion 17 and 46, single bond between attom at postion 17 and 47, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 50, single bond between attom at postion 19 and 51, double bond between 20 and 21, single bond between attom at postion 20 and 29, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 24, double bond between 22 and 30, single bond between attom at postion 22 and 31, single bond between attom at postion 24 and 34, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 28, single bond between attom at postion 25 and 54, single bond between attom at postion 25 and 55, double bond between 26 and 32, single bond between attom at postion 26 and 33, single bond between attom at postion 28 and 56, single bond between attom at postion 28 and 57, single bond between attom at postion 29 and 58, single bond between attom at postion 29 and 59, single bond between attom at postion 29 and 60, single bond between attom at postion 30 and 32, single bond between attom at postion 30 and 61, double bond

This compound's CID is 3478 and compound's name is Glipizide. There are 56 atoms in the molecule and their positions in the order are S, O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 18, double bond between 2 and 17, double bond between 5 and 26, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 43, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 44, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 53, double bond between 9 and 27, single bond between attom at postion 9 and 30, double bond between 10 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 41, single bond between attom at postion 16 and 42, double bond between 18 and 20, single bond between attom at postion 18 and 21, single bond between attom at postion 19 and 22, double bond between 19 and 23, single bond between attom at postion 19 and 24, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 47, double bond between 21 and 24, single bond between attom at postion 21 and 48, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 45, single bond between attom at postion 22 and 46, single bond between attom at postion 23 and 49, single bond between attom at postion 24 and 50, single bond between attom at postion 25 and 51, single bond between attom at postion 25 and 52, single bond between attom at postion 26 and 27, single bond between attom at postion 27 and 28, single bond between attom at postion 28 and 54, double bond between 29 and 30, single bond between attom at postion 29 and 31, single bond between attom at postion 30 and 55, single bond between attom at postion 31 and 56, single bond between attom at postion 31 and 57, single bond between attom at postion 31 and 58. The 3D x,y,z coordinates of the element at position 1 is -4.0331, 0.0044, -0.7568, . The 3D x,y,z coordinates of the element at position 2 is -1.6382, -1.6511, -1.8388, . The 3D x,y,z coordinates of the element at position 3 is -

This compound's CID is 3488 and compound's name is Glybunde. There are 61 attoms in the molecule and their positions in the order are CL, S, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 31, double bond between 2 and 4, double bond between 2 and 5, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 18, double bond between 3 and 17, double bond between 6 and 26, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 33, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 17, single bond between attom at postion 8 and 45, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 46, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 10 and 55, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 34, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 35, single bond between attom at postion 12 and 36, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, double bond between 18 and 21, single bond between attom at postion 18 and 22, single bond between attom at postion 19 and 20, double bond between 19 and 23, single bond between attom at postion 19 and 24, single bond between attom at postion 20 and 25, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 49, double bond between 22 and 24, single bond between attom at postion 22 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 24 and 52, single bond between attom at postion 25 and 53, single bond between attom at postion 25 and 54, single bond between attom at postion 26 and 27, double bond between 27 and 28, single bond between attom at postion 27 and 29, single bond between attom at postion 28 and 30, double bond between 29 and 31, single bond between attom at postion 29 and 56, double bond between 30 and 32, single bond between attom at postion 30 and 57, single bond between attom at postion 31 and 32, single bond between attom at postion 32 and 58, single bond between attom at postion 33 and 59, single bond between attom at postion 33 and 60, single bond between attom at postion 33 and 61. The 3D x,y,z coordinates of the element at position 1 is 3.147, This compound's CID is 3496 and compound's name is Glyphosate. There are 18 attoms in the molecule and their positions in the order are P, O, O, O, O, O, N, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 17, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 18, double bond between 6 and 10, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 15. The 3D x,y,z coordinates of the element at position 1 is -2.262, -0.0863, 0.078, . The 3D x,y,z coordinates of the element at position 2 is -2.2397, -0.8192, -1.3638, . The 3D x,y,z coordinates of the element at position 3 is -3.5361, 0.9054, -

This compound's CID is 3516 and compound's name is Guaifenesin. There are 28 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 22, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 9, double bond between 8 and 10, double bond between 9 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 21, double bond between 12 and 13, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 27, single bond between attom at postion 14 and 28. The 3D x,y,z coordinates of the element at position 1 is -0.6032, -0.2421, -0.4731, . The 3D x,y,z coordinates of the element at position 2 is -2.568, 0.3452, 1.4351, . The 3D This compound's CID is 3519 and compound's name is Guanfacine. There are 24 attoms in the molecule and their positions in the order are CL, CL, O, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 10, double bond between 3 and 13, single bond between attom at postion 4 and 13, double bond between 4 and 15, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 21, single bond between attom at postion 5 and 22, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 23, single bond between attom at postion 6 and 24, single bond between attom at postion 7 and 8, double bond between 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 11, double bond between 10 and 12, double bond between 11 and 14, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 19, single bond between attom at postion 14 and 20. The 3D x,y,z coordinates of the element at position 1 is 0.3268, -2.5685, -0.3483, . The 3D x,y,z coordinates of the element at position 2 is 1.5577, 2.7422, -0.4689, . The 3D x,y,z

This compound's CID is 3559 and compound's name is Haloperidol. There are 49 attoms in the molecule and their positions in the order are CL, X, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 26, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 39, double bond between 4 and 19, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 27, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, double bond between 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 40, double bond between 15 and 18, single bond between attom at postion 15 and 41, single bond between attom at postion 16 and 19, single bond between attom at postion 16 and 42, single bond between attom at postion 16 and 43, double bond between 17 and 20, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 21, double bond between 21 and 22, single bond between attom at postion 21 and 23, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 46, double bond between 23 and 25, single bond between attom at postion 23 and 47, double bond between 24 and 26, single bond between attom at postion 24 and 48, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 49. The 3D x,y,z coordinates of the element at position 1 is 9.1803, -0.0588, 0.2206, . The 3D x,y,z coordinates of the element at position 2 is -8.7674, 1.3659, 0.4286, . The 3D x,y,z

This compound's CID is 3639 and compound's name is Hydrochlorothiazide. There are 25 attoms in the molecule and their positions in the order are CL, S, S, O, O, O, O, N, N, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, double bond between 2 and 4, double bond between 2 and 5, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 11, double bond between 3 and 6, double bond between 3 and 7, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 15, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 11 and 12, double bond between 11 and 14, double bond between 12 and 16, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 19, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 20, double bond between 15 and 17, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 23. The 3D x,y,z coordinates of the element at position 1 is 2.701, -2.4152, -0.0041, . The 3D x,y,z coordinates of the element at position 2 is -2.3843, 1.239, 0.0262, . The 3D x,y,z coordinates of the element at

This compound's CID is 3657 and compound's name is Hydroxyurea. There are 9 attoms in the molecule and their positions in the order are O, O, N, N, C, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 9, double bond between 2 and 5, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8. The 3D x,y,z coordinates of the element at position 1 is 1.8879, -0.0095, -0.0027, . The 3D x,y,z coordinates of the element at position 2 is -0.4855, -1.3044, -3.0E-4, . The 3D x,y,z coordinates of the element at position 3 is 0.6761, 0.6946,
This compound's CID is 3672 and compound's name is Ibuprofen. There are 33 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 1 and 33, double bond between 2 and 15, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 17, single bond between attom at postion 4 and 18, double bond between 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 7, double bond between 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 26, double bond between 11 and 13, single bond between attom at postion 11 and 27, single bond between attom at postion 12 and 28, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 30, single bond between attom at postion 14 and 31, single bond between attom at postion 14 and 32. The 3D x,y,z coordinates of the element at position 1 is -4.4457, -1.0032, 0.4113, . The 3D x,y,z coordinates of the element at position 2 is -2.4005, -1.9114, 0.0531, . The 3D x,y,z coordinates of the element at position 3 is 3.9024, -0.4411, 0.0362, . The 3D x,y,z coordinates

This compound's CID is 3676 and compound's name is Lidocaine. There are 39 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 8, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 24, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 19, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 21, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 22, single bond between attom at postion 6 and 23, double bond between 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 15, double bond between 10 and 14, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 11 and 27, single bond between attom at postion 12 and 28, single bond between attom at postion 12 and 29, single bond between attom at postion 12 and 30, double bond between 13 and 17, single bond between attom at postion 13 and 31, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 32, single bond between attom at postion 15 and 33, single bond between attom at postion 15 and 34, single bond between attom at postion 15 and 35, single bond between attom at postion 16 and 36, single bond between attom at postion 16 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 39. The 3D x,y,z coordinates of the element at position 1 is 0.6658, -0.1341, 1.4612, . The 3D x,y,z coordinates of the element at position 2 is 3.0943, -0.0513, 0.1541, . The 3D x,y,z coordinates This compound's CID is 3690 and compound's name is Ifosfamide. There are 29 attoms in the molecule and their positions in the order are CL, CL, P, O, O, N, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 4, double bond between 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 4 and 10, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 24, single bond between attom at postion 12 and 25, single bond between attom at postion 13 and 26, single bond between attom at postion 13 and 27, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 29. The 3D x,y,z coordinates of the element at position 1 is -2.2988, 3.7376, 0.2524, . The 3D x,y,z coordinates of the element at position 2 is 4.9997, 0.8072, 0.2413, . The 3D x,y,z coordinates

This compound's CID is 3702 and compound's name is Indapamide. There are 40 attoms in the molecule and their positions in the order are CL, S, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 23, double bond between 2 and 4, double bond between 2 and 5, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 21, double bond between 3 and 18, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 31, single bond between attom at postion 8 and 39, single bond between attom at postion 8 and 40, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 26, single bond between attom at postion 10 and 27, single bond between attom at postion 11 and 12, double bond between 11 and 14, double bond between 12 and 15, single bond between attom at postion 13 and 28, single bond between attom at postion 13 and 29, single bond between attom at postion 13 and 30, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 32, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 33, double bond between 16 and 17, single bond between attom at postion 16 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 18 and 19, double bond between 19 and 20, single bond between attom at postion 19 and 22, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 36, double bond between 21 and 23, double bond between 22 and 24, single bond between attom at postion 22 and 37, single bond between attom at postion 23 and 24, single bond between attom at postion 24 and 38. The 3D x,y,z coordinates of the element at position 1 is 5.8085, -0.5802, -0.0632, . The 3D x,y,z coordinates of the element at position 2 is 3.7693, 1.8229, 0.6627, . The 3D x,y,z coordinates of the element at position 3 is -
This compound's CID is 3715 and compound's name is Indomethacin. There are 41 attoms in the molecule and their positions in the order are CL, O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 24, single bond between attom at postion 2 and 16, single bond between attom at postion 2 and 25, double bond between 3 and 15, single bond between attom at postion 4 and 19, single bond between attom at postion 4 and 41, double bond between 5 and 19, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 15, single bond between attom at postion 7 and 8, double bond between 7 and 10, single bond between attom at postion 7 and 11, double bond between 8 and 9, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 11 and 19, single bond between attom at postion 11 and 26, single bond between attom at postion 11 and 27, double bond between 12 and 16, single bond between attom at postion 12 and 28, double bond between 13 and 17, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 30, single bond between attom at postion 14 and 31, single bond between attom at postion 14 and 32, single bond between attom at postion 15 and 18, single bond between attom at postion 16 and 17, single bond between attom at postion 17 and 33, double bond between 18 and 20, single bond between attom at postion 18 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 34, double bond between 21 and 23, single bond between attom at postion 21 and 35, double bond between 22 and 24, single bond between attom at postion 22 and 36, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 37, single bond between attom at postion 25 and 38, single bond between attom at postion 25 and 39, single bond between attom at postion 25 and 40. The 3D x,y,z coordinates of the element at position 1 is -6.4605, -0.6873, -0.4755, . The 3D x,y,z coordinates of the element at position 2 is 1.6618, -4.1996, 0.1599, . The 3D x,y,z

This compound's CID is 3730 and compound's name is ionexol. There are 86 atoms in the molecule and their positions in the order are I, I, I, O, O, O, O, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 51, single bond between attom at postion 5 and 24, single bond between attom at postion 5 and 56, double bond between 6 and 25, single bond between attom at postion 7 and 30, single bond between attom at postion 7 and 57, single bond between attom at postion 8 and 31, single bond between attom at postion 8 and 58, double bond between 9 and 26, double bond between 10 and 27, single bond between attom at postion 11 and 33, single bond between attom at postion 11 and 59, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 60, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 46, single bond between attom at postion 15 and 27, single bond between attom at postion 15 and 29, single bond between attom at postion 15 and 47, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 35, single bond between attom at postion 16 and 36, double bond between 17 and 19, single bond between attom at postion 17 and 20, single bond between attom at postion 18 and 24, single bond between attom at postion 18 and 37, single bond between attom at postion 19 and 21, double bond between 20 and 22, double bond between 21 and 23, single bond between attom at postion 21 and 27, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 26, single bond between attom at postion 24 and 38, single bond between attom at postion 24 and 39, single bond between attom at postion 25 and 32, single bond between attom at postion 28 and 30, single bond between attom at postion 28 and 40, single bond between attom at postion 28 and 41, single bond between attom at postion 29 and 31, single bond between attom at postion 29 and 42, single bond between attom at postion 29 and 43, single bond between attom at postion 30 and 33, single bond between attom at postion 30 and 44, single bond between attom at postion 31 and 34, single bond between attom at postion 31 and 45, single bond between attom at postion 32 and 48, single bond between attom at postion 32 and 49, single bond between attom at postion 32 and 50, single bond between attom at postion 33 and 52, single bond between attom at postion 33 and 53, single bond between attom at postion 34 and 54, single bond between attom at postion 34 and 55. The 3D x,y,z coordinates of the element at position 1 is -2.9545, -1.9438, -0.5144, . The 3D x,y,z coordinates of the element at position 2 is

This compound's CID is 3731 and compound's name is Iomeprol. There are 53 attoms in the molecule and their positions in the order are I, I, I, O, O, O, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 23, single bond between attom at postion 4 and 49, single bond between attom at postion 5 and 24, single bond between attom at postion 5 and 50, double bond between 6 and 25, double bond between 7 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 8 and 51, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 52, double bond between 10 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 53, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 29, single bond between attom at postion 12 and 30, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 25, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 22, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 39, double bond between 15 and 18, single bond between attom at postion 15 and 19, double bond between 16 and 19, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 25, single bond between attom at postion 17 and 18, double bond between 17 and 20, single bond between attom at postion 17 and 26, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 32, single bond between attom at postion 21 and 33, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 34, single bond between attom at postion 22 and 35, single bond between attom at postion 23 and 27, single bond between attom at postion 23 and 36, single bond between attom at postion 24 and 28, single bond between attom at postion 24 and 37, single bond between attom at postion 27 and 40, single bond between attom at postion 27 and 41, single bond between attom at postion 28 and 42, single bond between attom at postion 28 and 43, single bond between attom at postion 29 and 44, single bond between attom at postion 29 and 45, single bond between attom at postion 29 and 46, single bond between attom at postion 30 and 31, single bond between attom at postion 31 and 47, single bond between attom at postion 31 and 48. The 3D x,y,z coordinates of the element at position 1 is 3.4229, -1.3112, 0.76, . The 3D x,y,z coordinates of the element at position 2 is -2.3, -3.4188, 0.5138, .

This compound's CID is 3741 and compound's name is loversol. There are 57 attoms in the molecule and their positions in the order are I, I, I, O, O, O, O, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 22, single bond between attom at postion 4 and 27, single bond between attom at postion 4 and 52, single bond between attom at postion 5 and 28, single bond between attom at postion 5 and 53, single bond between attom at postion 6 and 30, single bond between attom at postion 6 and 54, double bond between 7 and 25, double bond between 8 and 26, double bond between 9 and 29, single bond between attom at postion 10 and 31, single bond between attom at postion 10 and 55, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 56, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 57, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 23, single bond between attom at postion 14 and 25, single bond between attom at postion 14 and 42, single bond between attom at postion 15 and 24, single bond between attom at postion 15 and 26, single bond between attom at postion 15 and 43, double bond between 16 and 19, single bond between attom at postion 16 and 20, double bond between 17 and 20, single bond between attom at postion 17 and 22, single bond between attom at postion 17 and 25, single bond between attom at postion 18 and 19, double bond between 18 and 22, single bond between attom at postion 18 and 26, single bond between attom at postion 21 and 30, single bond between attom at postion 21 and 34, single bond between attom at postion 21 and 35, single bond between attom at postion 23 and 27, single bond between attom at postion 23 and 36, single bond between attom at postion 23 and 37, single bond between attom at postion 24 and 28, single bond between attom at postion 24 and 38, single bond between attom at postion 24 and 39, single bond between attom at postion 27 and 31, single bond between attom at postion 27 and 40, single bond between attom at postion 28 and 32, single bond between attom at postion 28 and 41, single bond between attom at postion 29 and 33, single bond between attom at postion 30 and 44, single bond between attom at postion 30 and 45, single bond between attom at postion 31 and 46, single bond between attom at postion 31 and 47, single bond between attom at postion 32 and 48, single bond between attom at postion 32 and 49, single bond between attom at postion 33 and 50, single bond between attom at postion 33 and 51. The 3D x,y,z coordinates of the element at position 1 is -2.9336, -1.6489, -1.0025, . The 3D x,y,z coordinates of the element at position 2 is 2.9561, -1.5564, 0.5964, . The 3D x,y,z coordinates

This compound's CID is 3749 and compound's name is Irbesartan. There are 60 attoms in the molecule and their positions in the order are O, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 13, single bond between attom at postion 2 and 8, double bond between 2 and 14, single bond between attom at postion 3 and 13, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 6, double bond between 4 and 31, double bond between 5 and 7, single bond between attom at postion 5 and 31, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 60, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 13, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 33, single bond between attom at postion 9 and 34, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 35, single bond between attom at postion 10 and 36, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 37, single bond between attom at postion 11 and 38, single bond between attom at postion 12 and 39, single bond between attom at postion 12 and 40, single bond between attom at postion 14 and 15, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 45, single bond between attom at postion 17 and 46, double bond between 18 and 20, single bond between attom at postion 18 and 21, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 49, double bond between 21 and 24, single bond between attom at postion 21 and 50, single bond between attom at postion 22 and 51, single bond between attom at postion 22 and 52, single bond between attom at postion 22 and 53, double bond between 23 and 25, single bond between attom at postion 23 and 54, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 55, single bond between attom at postion 25 and 26, single bond between attom at postion 26 and 27, double bond between 26 and 28, double bond between 27 and 29, single bond between attom at postion 27 and 31, single bond between attom at postion 28 and 30, single bond between attom at postion 28 and 56, single bond between attom at postion 29 and 32, single bond between attom at postion 29 and 57, double bond between 30 and 32, single bond between attom at postion 30 and 58, single bond between attom at postion 32 and 59. The 3D x,y,z coordinates of This compound's CID is 3763 and compound's name is Isoflurane. There are 12 attoms in the molecule and their positions in the order are CL, X, X, X, X, X, O, C, C, C, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 9, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 10 and 12. The 3D x,y,z coordinates of the element at position 1 is 0.6123, 2.2006, -0.2347, . The 3D x,y,z coordinates of the element at position 2 is 2.5543, -0.0301, -0.7397, . The 3D x,y,z coordinates

This compound's CID is 3767 and compound's name is Isoniazid. There are 17 attoms in the molecule and their positions in the order are O, N, N, N, C, C, C, C, C, C, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 8, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 15, double bond between 3 and 9, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 17, double bond between 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 11, double bond between 7 and 10, single bond between attom at postion 7 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 10 and 14. The 3D x,y,z coordinates of the element at position 1 is 1.8074, -1.451, 0.4097, . The 3D x,y,z coordinates of the element at position 2 is 2.1524, 0.751, -0.2342, . The 3D x,y,z coordinates of
This compound's CID is 3776 and compound's name is Isopropyl Alcohol. There are 12 attoms in the molecule and their positions in the order are O, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11. The 3D x,y,z coordinates of the element at position 1 is -4.0E-4, 1.3572, -0.1242, . The 3D x,y,z coordinates of the element at position 2 is 0.0, 0.0177, 0.3601, . The 3D x,y,z
This compound's CID is 3825 and compound's name is Ketoprofen. There are 33 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 33, double bond between 2 and 12, double bond between 3 and 13, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 20, double bond between 5 and 6, single bond between attom at postion 5 and 8, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 21, double bond between 7 and 10, single bond between attom at postion 7 and 12, double bond between 8 and 11, single bond between attom at postion 8 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 26, single bond between attom at postion 11 and 27, single bond between attom at postion 12 and 14, double bond between 14 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 28, double bond between 16 and 18, single bond between attom at postion 16 and 29, double bond between 17 and 19, single bond between attom at postion 17 and 30, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 31, single bond between attom at postion 19 and 32. The 3D x,y,z coordinates of the element at position 1 is 4.2053, -2.4798, 0.2885, . The 3D x,y,z coordinates of the element at position 2 is -1.6049, 1.749, 1.7885, . The 3D x,y,z coordinates of the element at position 3 is 2.1006, -2.1844, -0.4982, . The 3D x,y,z coordinates

This compound's CID is 3840 and compound's name is Kojic acid. There are 16 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 15, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 16, double bond between 4 and 8, double bond between 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 9, double bond between 9 and 10, single bond between attom at postion 10 and 14. The 3D x,y,z coordinates of the element at position 1 is -0.838, 1.0962, 0.2011, . The 3D x,y,z coordinates of the element at position 2 is -3.2819, 0.333, -0.5633, . The 3D x,y,z coordinates of the element at position 3 is 2.81, This compound's CID is 3869 and compound's name is Labetalol. There are 48 attoms in the molecule and their positions in the order are O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 41, single bond between attom at postion 2 and 20, single bond between attom at postion 2 and 46, double bond between 3 and 24, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 28, single bond between attom at postion 5 and 24, single bond between attom at postion 5 and 47, single bond between attom at postion 5 and 48, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 34, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, double bond between 12 and 14, single bond between attom at postion 12 and 15, double bond between 13 and 16, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 37, double bond between 15 and 19, single bond between attom at postion 15 and 38, single bond between attom at postion 16 and 21, single bond between attom at postion 16 and 39, double bond between 17 and 22, single bond between attom at postion 17 and 40, double bond between 18 and 20, single bond between attom at postion 18 and 24, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 42, double bond between 21 and 23, single bond between attom at postion 21 and 43, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 44, single bond between attom at postion 23 and 45. The 3D x,y,z coordinates of the element at position 1 is -2.5394, -1.7102, 2.646, . The 3D x,y,z coordinates of the element at position 2 is -3.2137, 2.6856, -1.7309, . The 3D x,y,z

This compound's CID is 3878 and compound's name is Lamotrigine. There are 23 attoms in the molecule and their positions in the order are CL, CL, N, N, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 13, double bond between 3 and 6, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 12, double bond between 4 and 16, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 21, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 22, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 9, double bond between 8 and 10, single bond between attom at postion 8 and 11, double bond between 9 and 12, single bond between attom at postion 10 and 13, double bond between 11 and 14, single bond between attom at postion 11 and 17, double bond between 13 and 15, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 19. The 3D x,y,z coordinates of the element at position 1 is -1.0017, 2.2965, -0.1127, . The 3D x,y,z coordinates of the element at position 2 is -4.1511, 1.7166, -0.0594, . The 3D x,y,z
This compound's CID is 3883 and compound's name is Lansoprazole. There are 39 attoms in the molecule and their positions in the order are S, X, X, X, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 6, single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 25, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 25, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 24, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 28, double bond between 8 and 13, single bond between attom at postion 8 and 15, double bond between 9 and 11, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 26, single bond between attom at postion 10 and 27, single bond between attom at postion 11 and 12, double bond between 12 and 16, single bond between attom at postion 12 and 17, single bond between attom at postion 14 and 15, double bond between 14 and 18, double bond between 15 and 20, single bond between attom at postion 16 and 19, single bond between attom at postion 17 and 29, single bond between attom at postion 17 and 30, single bond between attom at postion 17 and 31, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 32, double bond between 19 and 21, single bond between attom at postion 19 and 33, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 34, single bond between attom at postion 21 and 35, double bond between 22 and 23, single bond between attom at postion 22 and 36, single bond between attom at postion 23 and 37, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 38, single bond between attom at postion 24 and 39. The 3D x,y,z coordinates of the element at position 1 is -1.3874, -1.1002, 0.9641, . The 3D x,y,z coordinates of the element at position 2 is

This compound's CID is 3899 and compound's name is Leflunomide. There are 28 attoms in the molecule and their positions in the order are X, X, X, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 17, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 16, double bond between 5 and 15, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 22, double bond between 7 and 18, double bond between 8 and 11, single bond between attom at postion 8 and 12, double bond between 9 and 13, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 17, single bond between attom at postion 10 and 15, double bond between 10 and 16, single bond between attom at postion 10 and 18, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 20, double bond between 12 and 14, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 24, single bond between attom at postion 16 and 19, single bond between attom at postion 18 and 25, single bond between attom at postion 19 and 26, single bond between attom at postion 19 and 27, single bond between attom at postion 19 and 28. The 3D x,y,z coordinates of the element at position 1 is -5.0481, 1.4396, 0.033, . The 3D x,y,z coordinates of the element at position 2 is -5.3037, -0.4143, -
This compound's CID is 3902 and compound's name is Letrozole. There are 33 attoms in the molecule and their positions in the order are N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 13, double bond between 2 and 20, double bond between 3 and 13, single bond between attom at postion 3 and 20, triple bond between 4 and 21, triple bond between 5 and 22, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 23, double bond between 7 and 9, single bond between attom at postion 7 and 11, double bond between 8 and 10, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 24, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 25, double bond between 11 and 16, single bond between attom at postion 11 and 26, double bond between 12 and 17, single bond between attom at postion 12 and 27, single bond between attom at postion 13 and 28, double bond between 14 and 18, single bond between attom at postion 14 and 29, double bond between 15 and 19, single bond between attom at postion 15 and 30, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 31, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 32, single bond between attom at postion 18 and 21, single bond between attom at postion 19 and 22, single bond between attom at postion 20 and 33. The 3D x,y,z coordinates of the element at position 1 is 0.0488, 2.175, -0.1529, . The 3D x,y,z coordinates of the element at position 2 is 0.5991, 2.3578,

This compound's CID is 3950 and compound's name is Lomustine. There are 31 attoms in the molecule and their positions in the order are CL, O, O, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, double bond between 2 and 13, double bond between 3 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 27, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 12 and 25, single bond between attom at postion 12 and 26, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 30, single bond between attom at postion 15 and 31. The 3D x,y,z coordinates of the element at position 1 is 5.4639, 0.8671, 0.185, . The 3D x,y,z coordinates of the element at position 2 is 0.7531, 1.8292, -0.2064, . The 3D x,y,z coordinates of the element at
This compound's CID is 3957 and compound's name is Loratadine. There are 50 attoms in the molecule and their positions in the order are CL, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 23, single bond between attom at postion 2 and 19, single bond between attom at postion 2 and 26, double bond between 3 and 19, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 19, single bond between attom at postion 5 and 13, double bond between 5 and 25, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, double bond between 6 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 10 and 32, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 34, single bond between attom at postion 11 and 35, double bond between 12 and 14, single bond between attom at postion 12 and 18, double bond between 13 and 17, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 20, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 21, double bond between 18 and 22, single bond between attom at postion 18 and 40, double bond between 20 and 23, single bond between attom at postion 20 and 41, double bond between 21 and 24, single bond between attom at postion 21 and 42, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 43, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 44, single bond between attom at postion 25 and 45, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 46, single bond between attom at postion 26 and 47, single bond between attom at postion 27 and 48, single bond between attom at postion 27 and 49, single bond between attom at postion 27 and 50. The 3D x,y,z coordinates of the element at position 1 is -3.8155, -5.0246, 0.1273, . The 3D x,y,z

This compound's CID is 3958 and compound's name is Lorazepam. There are 31 attoms in the molecule and their positions in the order are CL, CL, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 31, double bond between 4 and 13, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 23, double bond between 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 8, double bond between 7 and 9, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 10, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 17, double bond between 10 and 18, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 22, double bond between 12 and 15, single bond between attom at postion 12 and 24, double bond between 14 and 16, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 16, single bond between attom at postion 16 and 26, double bond between 17 and 19, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 27, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 28, double bond between 20 and 21, single bond between attom at postion 20 and 29, single bond between attom at postion 21 and 30. The 3D x,y,z coordinates of the element at position 1 is 0.0085, 4.6295, -0.6891, . The 3D x,y,z coordinates of the element at position 2 is -1.2003, -1.2874, 2.3654, . The 3D x,y,z coordinates of the element at position 3 is 2.1122, -
This compound's CID is 3964 and compound's name is Loxapine. There are 41 attoms in the molecule and their positions in the order are CL, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 11, double bond between 5 and 10, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 24, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 28, single bond between attom at postion 8 and 29, single bond between attom at postion 9 and 30, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 12, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 11 and 34, double bond between 12 and 13, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 16, double bond between 14 and 20, double bond between 15 and 18, single bond between attom at postion 15 and 35, double bond between 16 and 21, double bond between 17 and 19, single bond between attom at postion 17 and 36, single bond between attom at postion 18 and 19, single bond between attom at postion 19 and 37, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 38, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 39, double bond between 22 and 23, single bond between attom at postion 22 and 40, single bond between attom at postion 23 and 41. The 3D x,y,z coordinates of the element at position 1 is 1.7518, 4.0271, 1.4608, . The 3D x,y,z

This compound's CID is 4021 and compound's name is Edaravone. There are 23 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 6, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 7, double bond between 3 and 5, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 8, double bond between 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 19, double bond between 10 and 12, single bond between attom at postion 10 and 20, double bond between 11 and 13, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 22, single bond between attom at postion 13 and 23. The 3D x,y,z coordinates of the element at position 1 is 0.7891, -2.3365, -0.3835, . The 3D x,y,z coordinates of the element at position 2 is 0.5753, -0.0063, 6.0E-4, . The 3D x,y,z
This compound's CID is 4030 and compound's name is Mebendazole. There are 35 attoms in the molecule and their positions in the order are O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 14, single bond between attom at postion 2 and 21, single bond between attom at postion 2 and 22, double bond between 3 and 21, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 8, double bond between 5 and 13, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 27, double bond between 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 11, double bond between 9 and 10, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 23, double bond between 11 and 12, single bond between attom at postion 11 and 25, single bond between attom at postion 12 and 26, single bond between attom at postion 14 and 15, double bond between 15 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 28, double bond between 17 and 19, single bond between attom at postion 17 and 29, double bond between 18 and 20, single bond between attom at postion 18 and 30, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 31, single bond between attom at postion 20 and 32, single bond between attom at postion 22 and 33, single bond between attom at postion 22 and 34, single bond between attom at postion 22 and 35. The 3D x,y,z coordinates of the element at position 1 is -3.3671, 2.1305, 0.9795, . The 3D x,y,z coordinates of the element at position 2 is 6.3541, -0.9229, 0.7268, . The 3D x,y,z coordinates of the element at position 3 is 5.4754, 0.0126, -1.1661, . The 3D
This compound's CID is 4033 and compound's name is Mechlorethamine. There are 19 attoms in the molecule and their positions in the order are CL, CL, N, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 2 and 8, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19. The 3D x,y,z coordinates of the element at position 1 is 3.9109, 0.6408, 0.1519, . The 3D x,y,z coordinates of the element at position 2 is -3.9089, 0.6512, 0.1363, . The 3D x,y,z

This compound's CID is 4044 and compound's name is Mefenamic Acid. There are 33 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 1 and 33, double bond between 2 and 18, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 19, single bond between attom at postion 4 and 5, double bond between 4 and 6, single bond between attom at postion 4 and 10, double bond between 5 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 12, double bond between 7 and 14, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 20, double bond between 9 and 11, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 25, double bond between 12 and 15, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 26, single bond between attom at postion 13 and 27, single bond between attom at postion 13 and 28, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 30, double bond between 16 and 17, single bond between attom at postion 16 and 31, single bond between attom at postion 17 and 32. The 3D x,y,z coordinates of the element at position 1 is 3.6687, 2.279, -0.1329, . The 3D x,y,z coordinates of the element at position 2 is 1.6167, 2.285, -1.0887, . The 3D x,y,z coordinates of the element at position 3 is 0.0318, 0.3523,
This compound's CID is 4055 and compound's name is Menadione. There are 21 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 6, double bond between 2 and 7, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 6, double bond between 3 and 9, single bond between attom at postion 4 and 7, double bond between 4 and 10, single bond between attom at postion 5 and 6, double bond between 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 7 and 8, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 19, double bond between 12 and 13, single bond between attom at postion 12 and 20, single bond between attom at postion 13 and 21. The 3D x,y,z coordinates of the element at position 1 is 1.3588, 2.3003, -0.0014, . The 3D x,y,z coordinates of the element at position 2 is 0.0774, -2.8887, 0.0, . The 3D x,y,z
This compound's CID is 4075 and compound's name is Mesalamine. There are 18 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 18, double bond between 3 and 11, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 16, single bond between attom at postion 5 and 7, double bond between 5 and 8, single bond between attom at postion 5 and 11, double bond between 6 and 7, single bond between attom at postion 6 and 9, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 10, double bond between 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 10 and 14. The 3D x,y,z coordinates of the element at position 1 is 1.3114, -2.0941, -0.1392, . The 3D x,y,z coordinates of the element at position 2 is 1.9128, 1.9352, -0.5015, . The 3D x,y,z coordinates of the element at position 3 is 2.8286, 0.1158,

This compound's CID is 4101 and compound's name is Methenamine. There are 22 attoms in the molecule and their positions in the order are N, N, N, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 7, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 9, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22. The 3D x,y,z coordinates of the element at position 1 is 0.9809, 1.0052, -0.5408, . The 3D x,y,z coordinates of the
This compound's CID is 4107 and compound's name is Methocarbamol. There are 32 attoms in the molecule and their positions in the order are O, O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 17, double bond between 5 and 16, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 31, single bond between attom at postion 6 and 32, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 11, double bond between 10 and 12, double bond between 11 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 25, double bond between 14 and 15, single bond between attom at postion 14 and 26, single bond between attom at postion 15 and 27, single bond between attom at postion 17 and 28, single bond between attom at postion 17 and 29, single bond between attom at postion 17 and 30. The 3D x,y,z coordinates of the element at position 1 is 0.8874, -0.1709, -0.7491, . The 3D x,y,z coordinates of the element at position 2 is -1.6689, -0.9312, -1.5925, . The 3D x,y,z
This compound's CID is 4133 and compound's name is Methyl Salicylate. There are 19 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 16, double bond between 3 and 10, single bond between attom at postion 4 and 5, double bond between 4 and 6, single bond between attom at postion 4 and 10, double bond between 5 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, double bond between 8 and 9, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 15, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 19. The 3D x,y,z coordinates of the element at position 1 is 2.1225, 0.8667, -0.3113, . The 3D x,y,z coordinates of the element at position 2 is -0.5276, -2.2538, -0.2299, . The 3D x,y,z

This compound's CID is 4170 and compound's name is Metolazone. There are 40 attoms in the molecule and their positions in the order are CL, S, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, double bond between 2 and 4, double bond between 2 and 5, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 17, double bond between 3 and 12, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 26, single bond between attom at postion 8 and 39, single bond between attom at postion 8 and 40, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 11, double bond between 10 and 16, single bond between attom at postion 11 and 12, double bond between 11 and 15, single bond between attom at postion 13 and 18, double bond between 13 and 20, single bond between attom at postion 14 and 27, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 30, single bond between attom at postion 16 and 19, single bond between attom at postion 16 and 31, double bond between 17 and 19, double bond between 18 and 21, single bond between attom at postion 18 and 22, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 32, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 33, single bond between attom at postion 22 and 34, single bond between attom at postion 22 and 35, single bond between attom at postion 22 and 36, double bond between 23 and 24, single bond between attom at postion 23 and 37, single bond between attom at postion 24 and 38. The 3D x,y,z coordinates of the element at position 1 is -4.7772, 1.7921, 0.731, . The 3D x,y,z coordinates of the element at position 2 is -4.485, -1.2855, -0.2154, . The 3D x,y,z coordinates of the element at position 3 is 0.7238, -

This compound's CID is 4173 and compound's name is Metronidazole. There are 21 attoms in the molecule and their positions in the order are O, O, O, N, N, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 21, single bond between attom at postion 2 and 6, double bond between 3 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, double bond between 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 14, single bond between attom at postion 8 and 12, double bond between 9 and 11, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 12 and 20. The 3D x,y,z coordinates of the element at position 1 is 3.2301, 1.6554, -0.2213, . The 3D x,y,z coordinates of the element at position 2 is -2.6598, 1.6655, -0.1573, . The 3D x,y,z

This compound's CID is 4189 and compound's name is Miconazole. There are 39 attoms in the molecule and their positions in the order are CL, CL, CL, CL, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 21, single bond between attom at postion 4 and 25, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, double bond between 7 and 16, single bond between attom at postion 7 and 20, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, double bond between 10 and 12, single bond between attom at postion 10 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 29, single bond between attom at postion 11 and 30, single bond between attom at postion 12 and 17, double bond between 13 and 18, single bond between attom at postion 13 and 31, double bond between 14 and 21, single bond between attom at postion 14 and 22, double bond between 15 and 20, single bond between attom at postion 15 and 32, single bond between attom at postion 16 and 33, double bond between 17 and 19, single bond between attom at postion 17 and 34, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 35, single bond between attom at postion 20 and 36, single bond between attom at postion 21 and 23, double bond between 22 and 24, single bond between attom at postion 22 and 37, double bond between 23 and 25, single bond between attom at postion 23 and 38, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 39. The 3D x,y,z coordinates of the element at position 1 is -2.6934, 0.0757, -2.6928, . The 3D x,y,z coordinates of the element at position 2 is -
This compound's CID is 4192 and compound's name is Midazolam. There are 36 attoms in the molecule and their positions in the order are CL, X, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 9, double bond between 4 and 10, double bond between 5 and 11, single bond between attom at postion 5 and 12, double bond between 6 and 8, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 9, double bond between 7 and 12, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 15, single bond between attom at postion 11 and 16, single bond between attom at postion 12 and 26, double bond between 13 and 17, single bond between attom at postion 13 and 27, double bond between 14 and 18, single bond between attom at postion 14 and 28, single bond between attom at postion 15 and 19, double bond between 15 and 20, single bond between attom at postion 16 and 29, single bond between attom at postion 16 and 30, single bond between attom at postion 16 and 31, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 32, double bond between 19 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 33, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 34, double bond between 22 and 23, single bond between attom at postion 22 and 35, single bond between attom at postion 23 and 36. The 3D x,y,z coordinates of the element at position 1 is -0.5811, -4.5922, 0.9239, . The 3D x,y,z coordinates of the element at position 2 is -2.8905, 2.1092,

This compound's CID is 4201 and compound's name is Minoxidil. There are 30 attoms in the molecule and their positions in the order are O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 30, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 12, double bond between 3 and 12, single bond between attom at postion 3 and 15, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 27, single bond between attom at postion 5 and 28, double bond between 6 and 15, single bond between attom at postion 6 and 29, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 12 and 13, double bond between 13 and 14, single bond between attom at postion 13 and 26. The 3D x,y,z coordinates of the element at position 1 is -3.9714, 0.0468, -0.236, . The 3D x,y,z coordinates of the This compound's CID is 4205 and compound's name is Mirtazapine. There are 39 attoms in the molecule and their positions in the order are N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 13, single bond between attom at postion 3 and 9, double bond between 3 and 20, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 22, single bond between attom at postion 5 and 23, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 24, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 10, double bond between 8 and 14, double bond between 9 and 12, single bond between attom at postion 10 and 11, double bond between 10 and 15, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 28, single bond between attom at postion 11 and 29, single bond between attom at postion 12 and 16, single bond between attom at postion 13 and 30, single bond between attom at postion 13 and 31, single bond between attom at postion 13 and 32, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 33, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 34, double bond between 16 and 19, single bond between attom at postion 16 and 35, double bond between 17 and 18, single bond between attom at postion 17 and 36, single bond between attom at postion 18 and 37, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 38, single bond between attom at postion 20 and 39. The 3D x,y,z coordinates of the element at position 1 is -0.4551, -1.186, -0.0216, . The 3D x,y,z coordinates of the element at position 2 is -3.3039, -1.0722, -0.0796, . The 3D x,y,z

This compound's CID is 4211 and compound's name is Mitotane. There are 28 attoms in the molecule and their positions in the order are CL, CL, CL, CL, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 8, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 19, double bond between 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 11, double bond between 7 and 12, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 21, double bond between 10 and 14, single bond between attom at postion 10 and 22, double bond between 11 and 15, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 23, double bond between 13 and 17, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 26, double bond between 16 and 18, single bond between attom at postion 16 and 27, single bond between attom at postion 18 and 28. The 3D x,y,z coordinates of the element at position 1 is -2.2541, -2.823, 0.4328, . The 3D x,y,z coordinates of the element at position 2 is 0.5311, -
This compound's CID is 4236 and compound's name is Modafinil. There are 34 attoms in the molecule and their positions in the order are S, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 8, double bond between 3 and 19, single bond between attom at postion 4 and 19, single bond between attom at postion 4 and 33, single bond between attom at postion 4 and 34, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 20, double bond between 6 and 9, single bond between attom at postion 6 and 11, double bond between 7 and 10, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 24, double bond between 11 and 15, single bond between attom at postion 11 and 25, double bond between 12 and 16, single bond between attom at postion 12 and 26, double bond between 13 and 17, single bond between attom at postion 13 and 27, double bond between 14 and 18, single bond between attom at postion 14 and 28, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 29, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 30, single bond between attom at postion 17 and 31, single bond between attom at postion 18 and 32. The 3D x,y,z coordinates of the element at position 1 is -0.9501, -1.3296, -0.4483, . The 3D x,y,z coordinates of the element at position 2 is -0.6587, -2.7047, 0.0393, . The 3D x,y,z coordinates of the element at position 3 is -

This compound's CID is 4409 and compound's name is Nabumetone. There are 33 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 17, double bond between 2 and 15, single bond between attom at postion 3 and 4, double bond between 3 and 7, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 19, double bond between 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 20, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, double bond between 9 and 10, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 24, double bond between 11 and 14, single bond between attom at postion 11 and 25, double bond between 12 and 13, single bond between attom at postion 12 and 26, single bond between attom at postion 13 and 14, single bond between attom at postion 14 and 27, single bond between attom at postion 15 and 16, single bond between attom at postion 16 and 28, single bond between attom at postion 16 and 29, single bond between attom at postion 16 and 30, single bond between attom at postion 17 and 31, single bond between attom at postion 17 and 32, single bond between attom at postion 17 and 33. The 3D x,y,z coordinates of the element at position 1 is -5.0038, -0.1941, 0.4359, . The 3D x,y,z coordinates of the element at position 2 is 5.5327, 0.2652, -0.843, . The 3D x,y,z coordinates of the element at position 3 is 1.3169, -0.4498, -0.4672, . The 3D This compound's CID is 4463 and compound's name is Nevirapine. There are 34 attoms in the molecule and their positions in the order are O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 14, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 10, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 26, double bond between 4 and 9, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 10, double bond between 5 and 18, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 21, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 22, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 24, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 11, double bond between 10 and 12, double bond between 11 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 19, double bond between 15 and 20, single bond between attom at postion 15 and 27, double bond between 16 and 17, single bond between attom at postion 16 and 28, single bond between attom at postion 17 and 29, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 30, single bond between attom at postion 19 and 31, single bond between attom at postion 19 and 32, single bond between attom at postion 19 and 33, single bond between attom at postion 20 and 34. The 3D x,y,z coordinates of the element at position 1 is 0.8987, -2.8388, -1.5122, . The 3D x,y,z coordinates of

This compound's CID is 4485 and compound's name is Nifedipine. There are 43 attoms in the molecule and their positions in the order are O, O, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 1 and 24, single bond between attom at postion 2 and 18, single bond between attom at postion 2 and 25, double bond between 3 and 17, double bond between 4 and 18, single bond between attom at postion 5 and 8, double bond between 6 and 8, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 15, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 26, double bond between 10 and 13, single bond between attom at postion 10 and 17, double bond between 11 and 14, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 15, double bond between 12 and 16, single bond between attom at postion 13 and 19, single bond between attom at postion 14 and 20, double bond between 15 and 21, single bond between attom at postion 16 and 22, single bond between attom at postion 16 and 28, single bond between attom at postion 19 and 29, single bond between attom at postion 19 and 30, single bond between attom at postion 19 and 31, single bond between attom at postion 20 and 32, single bond between attom at postion 20 and 33, single bond between attom at postion 20 and 34, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 35, double bond between 22 and 23, single bond between attom at postion 22 and 36, single bond between attom at postion 23 and 37, single bond between attom at postion 24 and 38, single bond between attom at postion 24 and 39, single bond between attom at postion 24 and 40, single bond between attom at postion 25 and 41, single bond between attom at postion 25 and 42, single bond between attom at postion 25 and 43. The 3D x,y,z coordinates of the element at position 1 is 3.0193, 0.8174, -1.7045, . The 3D x,y,z coordinates of the element at position 2 is -2.544, -1.3952, 0.4057, . The 3D x,y,z coordinates of the element at
This compound's CID is 4510 and compound's name is Nitroglycerin. There are 20 attoms in the molecule and their positions in the order are O, O, O, O, O, O, O, O, O, N, N, N, C, C, C, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 15, single bond between attom at postion 4 and 10, double bond between 5 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 12, double bond between 8 and 11, double bond between 9 and 12, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 20. The 3D x,y,z coordinates of the element at position 1 is 0.0424, -1.3569, 0.411, . The 3D x,y,z coordinates of the element at position 2 is 2.4896, -0.1938, -0.1771, . The 3D x,y,z coordinates of the element at position 3 is -1.5272, 0.9543, 0.2726, . The 3D x,y,z

This compound's CID is 4513 and compound's name is Nizatidine. There are 42 attoms in the molecule and their positions in the order are S, S, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 9, double bond between 4 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 18, double bond between 6 and 11, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 31, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 38, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 24, single bond between attom at postion 12 and 25, single bond between attom at postion 13 and 14, double bond between 13 and 16, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 26, single bond between attom at postion 15 and 27, single bond between attom at postion 16 and 30, single bond between attom at postion 17 and 32, single bond between attom at postion 17 and 33, single bond between attom at postion 17 and 34, single bond between attom at postion 18 and 35, single bond between attom at postion 18 and 36, single bond between attom at postion 18 and 37, double bond between 19 and 20, single bond between attom at postion 20 and 39, single bond between attom at postion 21 and 40, single bond between attom at postion 21 and 41, single bond between attom at postion 21 and 42. The 3D x,y,z coordinates of the element at position 1 is 0.2984, -2.263, 1.107, . The 3D x,y,z coordinates of the element at position 2 is 4.9348, -1.2239, -0.2744, . The 3D x,y,z coordinates of the element at position 3 is -4.421, 2.3178, -1.121, . The 3D x,y,z

This compound's CID is 4583 and compound's name is Ofloxacin. There are 46 attoms in the molecule and their positions in the order are X, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 17, double bond between 3 and 23, single bond between attom at postion 4 and 26, single bond between attom at postion 4 and 46, double bond between 5 and 26, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 20, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 24, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 14, double bond between 12 and 19, double bond between 13 and 14, single bond between attom at postion 13 and 18, single bond between attom at postion 15 and 32, single bond between attom at postion 15 and 33, single bond between attom at postion 16 and 34, single bond between attom at postion 16 and 35, single bond between attom at postion 17 and 36, single bond between attom at postion 17 and 37, double bond between 18 and 21, single bond between attom at postion 18 and 23, single bond between attom at postion 19 and 21, double bond between 20 and 25, single bond between attom at postion 20 and 38, single bond between attom at postion 21 and 39, single bond between attom at postion 22 and 40, single bond between attom at postion 22 and 41, single bond between attom at postion 22 and 42, single bond between attom at postion 23 and 25, single bond between attom at postion 24 and 43, single bond between attom at postion 24 and 44, single bond between attom at postion 24 and 45, single bond between attom at postion 25 and 26. The 3D x,y,z coordinates of the element at position 1 is -1.6951, -2.9042, 0.0812, . The 3D x,y,z coordinates of the element at position 2 is -1.0003, 1.7712, -

This compound's CID is 4594 and compound's name is Omeprazole. There are 43 attoms in the molecule and their positions in the order are S, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 3, single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 23, single bond between attom at postion 4 and 20, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 27, double bond between 6 and 11, single bond between attom at postion 6 and 14, double bond between 7 and 9, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 10, double bond between 10 and 13, single bond between attom at postion 10 and 16, double bond between 12 and 14, single bond between attom at postion 12 and 17, single bond between attom at postion 13 and 15, single bond between attom at postion 14 and 19, double bond between 15 and 18, single bond between attom at postion 15 and 22, single bond between attom at postion 16 and 28, single bond between attom at postion 16 and 29, single bond between attom at postion 16 and 30, double bond between 17 and 20, single bond between attom at postion 17 and 31, single bond between attom at postion 18 and 32, double bond between 19 and 21, single bond between attom at postion 19 and 33, single bond between attom at postion 20 and 21, single bond between attom at postion 21 and 34, single bond between attom at postion 22 and 35, single bond between attom at postion 22 and 36, single bond between attom at postion 22 and 37, single bond between attom at postion 23 and 38, single bond between attom at postion 23 and 39, single bond between attom at postion 23 and 40, single bond between attom at postion 24 and 41, single bond between attom at postion 24 and 42, single bond between attom at postion 24 and 43. The 3D x,y,z coordinates of the element at position 1 is 0.2799, 0.7535, -0.8523, . The 3D x,y,z coordinates of the element at position 2 is 5.6802, -1.1956, -

This compound's CID is 4595 and compound's name is Ondansetron. There are 41 attoms in the molecule and their positions in the order are O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 10, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 17, single bond between attom at postion 3 and 18, double bond between 4 and 17, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 23, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 24, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, double bond between 8 and 9, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 12, single bond between attom at postion 11 and 28, single bond between attom at postion 11 and 29, single bond between attom at postion 12 and 13, double bond between 12 and 15, double bond between 13 and 16, single bond between attom at postion 14 and 30, single bond between attom at postion 14 and 31, single bond between attom at postion 14 and 32, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 33, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 34, single bond between attom at postion 17 and 22, double bond between 18 and 21, single bond between attom at postion 18 and 35, double bond between 19 and 20, single bond between attom at postion 19 and 36, single bond between attom at postion 20 and 37, single bond between attom at postion 21 and 38, single bond between attom at postion 22 and 39, single bond between attom at postion 22 and 40, single bond between attom at postion 22 and 41. The 3D x,y,z coordinates of the element at position 1 is 0.8253, 1.0488, 1.3014, . The 3D x,y,z

This compound's CID is 4614 and compound's name is Oxaprozin. There are 37 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 7, single bond between attom at postion 2 and 20, single bond between attom at postion 2 and 37, double bond between 3 and 20, single bond between attom at postion 4 and 6, double bond between 4 and 7, double bond between 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 8, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 23, single bond between attom at postion 8 and 24, double bond between 9 and 12, single bond between attom at postion 9 and 13, double bond between 10 and 14, single bond between attom at postion 10 and 15, single bond between attom at postion 11 and 20, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 27, double bond between 13 and 17, single bond between attom at postion 13 and 28, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 29, double bond between 15 and 19, single bond between attom at postion 15 and 30, double bond between 16 and 21, single bond between attom at postion 16 and 31, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 32, double bond between 18 and 22, single bond between attom at postion 18 and 33, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 34, single bond between attom at postion 21 and 35, single bond between attom at postion 22 and 36. The 3D x,y,z coordinates of the element at position 1 is 1.1008, -0.8497, -0.4577, . The 3D x,y,z coordinates of the element at position 2 is 6.1955, 0.1563,
This compound's CID is 4616 and compound's name is Oxazepam. There are 31 attoms in the molecule and their positions in the order are CL, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 31, double bond between 3 and 13, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 22, double bond between 5 and 7, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 7, double bond between 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 9, single bond between attom at postion 8 and 12, double bond between 9 and 16, single bond between attom at postion 9 and 17, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 21, double bond between 11 and 14, single bond between attom at postion 11 and 23, double bond between 12 and 15, single bond between attom at postion 12 and 24, single bond between attom at postion 14 and 15, single bond between attom at postion 15 and 25, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 26, double bond between 17 and 19, single bond between attom at postion 17 and 27, double bond between 18 and 20, single bond between attom at postion 18 and 28, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 29, single bond between attom at postion 20 and 30. The 3D x,y,z coordinates of the element at position 1 is -0.1439, 4.4764, -1.08, . The 3D x,y,z coordinates of the element at position 2 is 2.0677, -3.18, -1.3667, . The 3D x,y,z coordinates of the element at position 3 is 2.9712, -

This compound's CID is 4632 and compound's name is Oxybenzone. There are 29 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 26, double bond between 3 and 5, single bond between attom at postion 4 and 5, double bond between 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 5 and 6, double bond between 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 10, double bond between 8 and 11, single bond between attom at postion 8 and 18, double bond between 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 20, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 21, double bond between 13 and 15, single bond between attom at postion 13 and 22, double bond between 14 and 16, single bond between attom at postion 14 and 23, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 24, single bond between attom at postion 16 and 25, single bond between attom at postion 17 and 27, single bond between attom at postion 17 and 28, single bond between attom at postion 17 and 29. The 3D x,y,z coordinates of the element at position 1 is 4.3765, 0.6456, 0.3982, . The 3D x,y,z coordinates of the element at position 2 is 0.4351, -1.5774, 1.8889, . The 3D x,y,z coordinates of the element at position 3 is -1.1022, -2.1355, -1.0958, . The This compound's CID is 4634 and compound's name is Oxybutynin. There are 57 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 38, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 19, double bond between 3 and 13, single bond between attom at postion 4 and 21, single bond between attom at postion 4 and 22, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 27, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 28, single bond between attom at postion 6 and 29, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 30, single bond between attom at postion 7 and 31, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 13, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 37, double bond between 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 39, double bond between 15 and 17, single bond between attom at postion 15 and 40, double bond between 16 and 18, single bond between attom at postion 16 and 41, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 44, single bond between attom at postion 19 and 45, triple bond between 20 and 24, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 46, single bond between attom at postion 21 and 47, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 48, single bond between attom at postion 22 and 49, single bond between attom at postion 23 and 26, single bond between attom at postion 23 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 25 and 52, single bond between attom at postion 25 and 53, single bond between attom at postion 25 and 54, single bond between attom at postion 26 and 55, single bond between attom at postion 26 and 56, single bond between attom at postion 26 and 57. The 3D x,y,z coordinates of the element at position 1 is -3.5726, -0.3106, 1.1643, . The 3D x,y,z coordinates of the element at

This compound's CID is 4678 and compound's name is Panthenol. There are 33 attoms in the molecule and their positions in the order are O, O, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 27, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 30, double bond between 3 and 11, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 33, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 25, single bond between attom at postion 12 and 26, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 28, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 31, single bond between attom at postion 14 and 32. The 3D x,y,z coordinates of the element at position 1 is -1.1368, -1.8058, 1.0716, . The 3D x,y,z coordinates of the element at position 2 is -4.0927, 1.1311, 0.229, . The 3D x,y,z coordinates of the element at position 3 is 0.1796, 0.4635, 1.7246, . The 3D This compound's CID is 4740 and compound's name is Pentoxifylline. There are 38 attoms in the molecule and their positions in the order are O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 12, double bond between 2 and 14, double bond between 3 and 19, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 17, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 13, double bond between 7 and 16, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 24, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 11 and 12, double bond between 11 and 13, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 27, single bond between attom at postion 15 and 28, single bond between attom at postion 16 and 29, single bond between attom at postion 17 and 30, single bond between attom at postion 17 and 31, single bond between attom at postion 17 and 32, single bond between attom at postion 18 and 33, single bond between attom at postion 18 and 34, single bond between attom at postion 18 and 35, single bond between attom at postion 19 and 20, single bond between attom at postion 20 and 36, single bond between attom at postion 20 and 37, single bond between attom at postion 20 and 38. The 3D x,y,z coordinates of the element at position 1 is 0.6376, 2.0245, 0.7478, . The 3D x,y,z coordinates of the element at position 2 is 0.2415, -2.6413, 0.4498, . The 3D x,y,z coordinates of the

This compound's CID is 4748 and compound's name is Perphenazine. There are 53 attoms in the molecule and their positions in the order are CL, S, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 24, single bond between attom at postion 2 and 18, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 50, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 38, single bond between attom at postion 12 and 39, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 40, single bond between attom at postion 13 and 41, single bond between attom at postion 14 and 42, single bond between attom at postion 14 and 43, single bond between attom at postion 15 and 44, single bond between attom at postion 15 and 45, double bond between 16 and 18, single bond between attom at postion 16 and 20, single bond between attom at postion 17 and 19, double bond between 17 and 21, single bond between attom at postion 18 and 22, double bond between 19 and 23, double bond between 20 and 24, single bond between attom at postion 20 and 46, single bond between attom at postion 21 and 25, single bond between attom at postion 21 and 47, double bond between 22 and 26, single bond between attom at postion 22 and 48, single bond between attom at postion 23 and 27, single bond between attom at postion 23 and 49, single bond between attom at postion 24 and 26, double bond between 25 and 27, single bond between attom at postion 25 and 51, single bond between attom at postion 26 and 52, single bond between attom at postion 27 and 53. The 3D x,y,z coordinates of the element at position 1 is 2.2203, -4.8841, -0.2752, . The 3D x,y,z coordinates of the element at

This compound's CID is 4763 and compound's name is Phenobarbital. There are 29 attoms in the molecule and their positions in the order are O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 9, double bond between 2 and 10, double bond between 3 and 14, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 19, double bond between 8 and 12, single bond between attom at postion 8 and 13, single bond between attom at postion 11 and 20, single bond between attom at postion 11 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 25, double bond between 13 and 16, single bond between attom at postion 13 and 26, double bond between 15 and 17, single bond between attom at postion 15 and 27, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 28, single bond between attom at postion 17 and 29. The 3D x,y,z coordinates of the element at position 1 is 0.5748, -0.7675, 2.3648, . The 3D x,y,z coordinates of the element at position 2 is 0.5804, -0.5584, -2.4243, . The 3D x,y,z coordinates of the element at position 3 is 3.4088,

This compound's CID is 4829 and compound's name is Pioglitazone. There are 45 attoms in the molecule and their positions in the order are S, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 15, double bond between 3 and 10, double bond between 4 and 19, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 19, single bond between attom at postion 5 and 37, double bond between 6 and 18, single bond between attom at postion 6 and 24, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 26, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 27, single bond between attom at postion 8 and 28, double bond between 9 and 11, single bond between attom at postion 9 and 12, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 29, double bond between 12 and 17, single bond between attom at postion 12 and 30, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 31, single bond between attom at postion 13 and 32, double bond between 14 and 16, single bond between attom at postion 14 and 17, single bond between attom at postion 15 and 33, single bond between attom at postion 15 and 34, single bond between attom at postion 16 and 35, single bond between attom at postion 17 and 36, single bond between attom at postion 18 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 23, double bond between 20 and 24, double bond between 21 and 23, single bond between attom at postion 21 and 38, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 39, single bond between attom at postion 22 and 40, single bond between attom at postion 23 and 41, single bond between attom at postion 24 and 42, single bond between attom at postion 25 and 43, single bond between attom at postion 25 and 44, single bond between attom at postion 25 and 45. The 3D x,y,z coordinates of the element at position 1 is -5.0292, 1.0875, 0.1775, . The 3D x,y,z coordinates of the element at position 2 is 1.6198, 1.7558, -0.9119, . The 3D x,y,z
This compound's CID is 4906 and compound's name is Prilocaine. There are 36 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 7, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 26, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 18, single bond between attom at postion 5 and 19, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 22, single bond between attom at postion 8 and 23, single bond between attom at postion 8 and 24, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 10, double bond between 9 and 12, double bond between 10 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 11 and 27, single bond between attom at postion 11 and 28, single bond between attom at postion 11 and 29, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 30, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 31, single bond between attom at postion 14 and 32, single bond between attom at postion 14 and 33, single bond between attom at postion 14 and 34, double bond between 15 and 16, single bond between attom at postion 15 and 35, single bond between attom at postion 16 and 36. The 3D x,y,z coordinates of the element at position 1 is -0.7432, 1.2197, -1.5006, . The 3D x,y,z coordinates of the element at position 2 is -3.0836, 0.5844, 0.0671, . The 3D x,y,z coordinates of the element at position 3 is

This compound's CID is 4909 and compound's name is Primidone. There are 30 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 8, double bond between 2 and 9, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 21, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 22, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 18, double bond between 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 26, double bond between 13 and 15, single bond between attom at postion 13 and 27, double bond between 14 and 16, single bond between attom at postion 14 and 28, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 29, single bond between attom at postion 16 and 30. The 3D x,y,z coordinates of the element at position 1 is -1.5353, 2.2626, -0.4939, . The 3D x,y,z coordinates of the element at position 2 is -1.4743, -2.3135, -
This compound's CID is 4917 and compound's name is Prochlorperazine. There are 49 attoms in the molecule and their positions in the order are CL, S, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 22, single bond between attom at postion 2 and 16, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 26, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 12 and 38, single bond between attom at postion 12 and 39, single bond between attom at postion 13 and 40, single bond between attom at postion 13 and 41, single bond between attom at postion 13 and 42, double bond between 14 and 16, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 17, double bond between 15 and 19, single bond between attom at postion 16 and 20, double bond between 17 and 21, double bond between 18 and 22, single bond between attom at postion 18 and 43, single bond between attom at postion 19 and 23, single bond between attom at postion 19 and 44, double bond between 20 and 24, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 25, single bond between attom at postion 21 and 46, single bond between attom at postion 22 and 24, double bond between 23 and 25, single bond between attom at postion 23 and 47, single bond between attom at postion 24 and 48, single bond between attom at postion 25 and 49. The 3D x,y,z coordinates of the element at position 1 is -1.4866, -4.8788, 0.2745, . The 3D x,y,z coordinates of

This compound's CID is 4943 and compound's name is Propofol. There are 31 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 31, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 15, double bond between 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 6, double bond between 5 and 8, double bond between 7 and 13, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 12 and 27, single bond between attom at postion 12 and 28, single bond between attom at postion 12 and 29, single bond between attom at postion 13 and 30. The 3D x,y,z coordinates of the element at position 1 is -0.0014, 1.9782, -2.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -2.5116, 0.6448, 1.0E-4, . The 3D x,y,z coordinates of the element at position 3 is 2.5118, 0.6452, 1.0E-
This compound's CID is 4993 and compound's name is Pyrimethamine. There are 30 attoms in the molecule and their positions in the order are CL, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 7, double bond between 2 and 14, double bond between 3 and 10, single bond between attom at postion 3 and 14, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 27, single bond between attom at postion 4 and 28, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 29, single bond between attom at postion 5 and 30, double bond between 6 and 7, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 8, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, double bond between 9 and 11, single bond between attom at postion 9 and 12, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 20, double bond between 12 and 16, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 22, single bond between attom at postion 13 and 23, single bond between attom at postion 13 and 24, double bond between 15 and 17, single bond between attom at postion 15 and 25, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 26. The 3D x,y,z coordinates of the element at position 1 is 5.3314, 0.1055, 0.0311, . The 3D x,y,z coordinates of the element at position 2 is -2.7207, -0.9466,

This compound's CID is 5002 and compound's name is Quetiapine. There are 52 attoms in the molecule and their positions in the order are S, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 25, single bond between attom at postion 3 and 52, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 12, double bond between 6 and 12, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 12 and 14, single bond between attom at postion 13 and 38, single bond between attom at postion 13 and 39, single bond between attom at postion 14 and 15, double bond between 14 and 16, double bond between 15 and 19, single bond between attom at postion 16 and 21, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 18, double bond between 17 and 23, double bond between 18 and 24, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 41, single bond between attom at postion 20 and 25, single bond between attom at postion 20 and 42, single bond between attom at postion 20 and 43, double bond between 21 and 22, single bond between attom at postion 21 and 44, single bond between attom at postion 22 and 45, single bond between attom at postion 23 and 26, single bond between attom at postion 23 and 46, single bond between attom at postion 24 and 27, single bond between attom at postion 24 and 47, single bond between attom at postion 25 and 48, single bond between attom at postion 25 and 49, double bond between 26 and 27, single bond between attom at postion 26 and 50, single bond between attom at postion 27 and 51. The 3D x,y,z coordinates of the element at position 1 is 4.0306, 0.6729, 1.5993,

This compound's CID is 5039 and compound's name is Ranitidine. There are 43 attoms in the molecule and their positions in the order are S, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 8, double bond between 4 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 18, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 19, single bond between attom at postion 6 and 38, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 39, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, double bond between 10 and 13, single bond between attom at postion 11 and 12, double bond between 11 and 14, single bond between attom at postion 12 and 24, single bond between attom at postion 12 and 25, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 26, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 27, single bond between attom at postion 15 and 28, single bond between attom at postion 16 and 30, single bond between attom at postion 16 and 31, single bond between attom at postion 17 and 32, single bond between attom at postion 17 and 33, single bond between attom at postion 17 and 34, single bond between attom at postion 18 and 35, single bond between attom at postion 18 and 36, single bond between attom at postion 18 and 37, double bond between 19 and 20, single bond between attom at postion 20 and 40, single bond between attom at postion 21 and 41, single bond between attom at postion 21 and 42, single bond between attom at postion 21 and 43. The 3D x,y,z coordinates of the element at position 1 is 0.3766, 2.2916, -1.0988, . The 3D x,y,z coordinates of the element at position 2 is 2.5877, 0.3402, 0.6973, . The 3D x,y,z coordinates This compound's CID is 5070 and compound's name is Riluzole. There are 20 attoms in the molecule and their positions in the order are S, X, X, X, O, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 15, single bond between attom at postion 3 and 15, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 9, double bond between 6 and 14, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 20, double bond between 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 9 and 12, double bond between 10 and 11, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 13, double bond between 12 and 13, single bond between attom at postion 12 and 17, single bond between attom at postion 13 and 18. The 3D x,y,z coordinates of the element at position 1 is -2.3641, -1.6594, -0.2511, . The 3D x,y,z coordinates of the element at position 2 is 2.617, -0.4337, 1.405, . The 3D x,y,z coordinates of

This compound's CID is 5073 and compound's name is Risperidone. There are 57 atoms in the molecule and their positions in the order are X, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 30, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 25, double bond between 3 and 23, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 18, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 23, double bond between 6 and 14, double bond between 7 and 20, single bond between attom at postion 7 and 24, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 12 and 38, single bond between attom at postion 12 and 39, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 40, single bond between attom at postion 13 and 41, single bond between attom at postion 14 and 17, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 42, single bond between attom at postion 15 and 43, single bond between attom at postion 16 and 23, double bond between 16 and 24, double bond between 17 and 25, single bond between attom at postion 17 and 26, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 22, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 48, single bond between attom at postion 21 and 49, single bond between attom at postion 22 and 50, single bond between attom at postion 22 and 51, single bond between attom at postion 24 and 27, single bond between attom at postion 25 and 28, double bond between 26 and 29, single bond between attom at postion 26 and 52, single bond between attom at postion 27 and 53, single bond between attom at postion 27 and 54, single bond between attom at postion 27 and 55, double bond between 28 and 30, single bond between attom at postion 28 and 56, single bond between attom at postion 29 and 30, single bond between attom at postion 29 and 57. The 3D x,y,z coordinates of the element at position 1 is 9.1912, -1.7833, 0.1494, . The 3D x,y,z coordinates of the element at

This compound's CID is 5095 and compound's name is Ropinirole. There are 43 attoms in the molecule and their positions in the order are O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 15, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 8, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 35, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 20, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 22, single bond between attom at postion 5 and 23, double bond between 6 and 9, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 29, double bond between 11 and 16, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 30, single bond between attom at postion 12 and 31, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 32, single bond between attom at postion 13 and 33, double bond between 14 and 17, single bond between attom at postion 14 and 34, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 36, single bond between attom at postion 17 and 37, single bond between attom at postion 18 and 38, single bond between attom at postion 18 and 39, single bond between attom at postion 18 and 40, single bond between attom at postion 19 and 41, single bond between attom at postion 19 and 42, single bond between attom at postion 19 and 43. The 3D x,y,z coordinates of the element at position 1 is -3.5619, 2.7899, -1.485, . The 3D x,y,z coordinates of the element at position 2 is 2.6471, This compound's CID is 5206 and compound's name is Sevoflurane. There are 15 attoms in the molecule and their positions in the order are X, X, X, X, X, X, X, O, C, C, C, C, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 10, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 15. The 3D x,y,z coordinates of the element at position 1 is 1.2852, -1.7729, -0.3891, . The 3D x,y,z coordinates of the element at position 2 is 0.0143, -1.3472, 1.3282, . The 3D x,y,z coordinates of the element at position 3 is -0.8714, -2.0796, -0.527, . The 3D

This compound's CID is 5215 and compound's name is Sulfadiazine. There are 27 attoms in the molecule and their positions in the order are S, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, double bond between 1 and 3, single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 8, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 20, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 23, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 14, double bond between 6 and 15, double bond between 7 and 14, single bond between attom at postion 7 and 16, double bond between 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 18, double bond between 10 and 13, single bond between attom at postion 10 and 19, double bond between 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 22, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 25, double bond between 16 and 17, single bond between attom at postion 16 and 26, single bond between attom at postion 17 and 27. The 3D x,y,z coordinates of the element at position 1 is 0.1398, 2.1322, -0.1283, . The 3D x,y,z coordinates of the element at position 2 is -0.4247, 3.2677, 0.5914, . The 3D x,y,z coordinates of the element at position 3 is 0.6069, This compound's CID is 5329 and compound's name is Sulfamethoxazole. There are 28 attoms in the molecule and their positions in the order are S, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 16, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 18, double bond between 6 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 27, single bond between attom at postion 7 and 28, double bond between 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 19, double bond between 10 and 14, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 15, double bond between 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 13 and 21, single bond between attom at postion 14 and 22, double bond between 15 and 16, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 17, single bond between attom at postion 17 and 24, single bond between attom at postion 17 and 25, single bond between attom at postion 17 and 26. The 3D x,y,z coordinates of the element at position 1 is 0.2645, -2.2031, -0.0845, . The 3D x,y,z coordinates of the element at position 2 is -2.6416, 0.9657, -

This compound's CID is 5339 and compound's name is Sulfasalazine. There are 42 attoms in the molecule and their positions in the order are S, O, O, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, double bond between 1 and 3, single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 11, single bond between attom at postion 4 and 22, single bond between attom at postion 4 and 41, single bond between attom at postion 5 and 28, single bond between attom at postion 5 and 42, double bond between 6 and 28, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 31, double bond between 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 17, double bond between 9 and 26, single bond between attom at postion 10 and 18, double bond between 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 29, double bond between 13 and 16, single bond between attom at postion 13 and 30, double bond between 14 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 15 and 32, single bond between attom at postion 16 and 33, double bond between 17 and 19, double bond between 18 and 21, single bond between attom at postion 18 and 23, single bond between attom at postion 19 and 25, single bond between attom at postion 19 and 34, single bond between attom at postion 20 and 21, double bond between 20 and 22, single bond between attom at postion 20 and 28, single bond between attom at postion 21 and 35, single bond between attom at postion 22 and 24, double bond between 23 and 24, single bond between attom at postion 23 and 36, single bond between attom at postion 24 and 37, double bond between 25 and 27, single bond between attom at postion 25 and 38, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 39, single bond between attom at postion 27 and 40. The 3D x,y,z coordinates of the element at position 1 is -4.7299, 1.4023, 0.5479, . The 3D x,y,z coordinates of the element at position 2 is -5.1626, 2.7369, 0.1509, . The 3D x,y,z coordinates This compound's CID is 5358 and compound's name is Sumatriptan. There are 41 attoms in the molecule and their positions in the order are S, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, double bond between 1 and 3, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 15, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 29, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 18, single bond between attom at postion 5 and 19, single bond between attom at postion 6 and 20, single bond between attom at postion 6 and 38, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, double bond between 7 and 14, double bond between 8 and 10, single bond between attom at postion 8 and 13, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 16, double bond between 11 and 13, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 23, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 15 and 27, single bond between attom at postion 15 and 28, double bond between 16 and 17, single bond between attom at postion 16 and 30, single bond between attom at postion 17 and 31, single bond between attom at postion 18 and 32, single bond between attom at postion 18 and 33, single bond between attom at postion 18 and 34, single bond between attom at postion 19 and 35, single bond between attom at postion 19 and 36, single bond between attom at postion 19 and 37, single bond between attom at postion 20 and 39, single bond between attom at postion 20 and 40, single bond between attom at postion 20 and 41. The 3D x,y,z coordinates of the element at position 1 is 3.1175, 1.1281, -0.4074, . The 3D x,y,z coordinates of the element at position 2 is 3.6898, 0.2319, -1.3999, . The 3D x,y,z

This compound's CID is 5381 and compound's name is Tazarotene. There are 46 attoms in the molecule and their positions in the order are S, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 23, single bond between attom at postion 2 and 24, double bond between 3 and 23, double bond between 4 and 18, single bond between attom at postion 4 and 22, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 26, single bond between attom at postion 6 and 27, double bond between 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 28, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 13, double bond between 12 and 14, single bond between attom at postion 12 and 36, double bond between 13 and 15, single bond between attom at postion 13 and 37, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 15 and 38, triple bond between 16 and 17, single bond between attom at postion 17 and 18, single bond between attom at postion 18 and 19, double bond between 19 and 21, single bond between attom at postion 19 and 39, single bond between attom at postion 20 and 21, double bond between 20 and 22, single bond between attom at postion 20 and 23, single bond between attom at postion 21 and 40, single bond between attom at postion 22 and 41, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 42, single bond between attom at postion 24 and 43, single bond between attom at postion 25 and 44, single bond between attom at postion 25 and 45, single bond between attom at postion 25 and 46. The 3D x,y,z coordinates of the element at position 1 is -6.534, 1.608, -0.1303, . The 3D x,y,z coordinates of the This compound's CID is 5391 and compound's name is Temazepam. There are 34 attoms in the molecule and their positions in the order are CL, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 33, double bond between 3 and 10, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 14, double bond between 5 and 8, single bond between attom at postion 5 and 9, double bond between 6 and 7, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 22, double bond between 11 and 17, single bond between attom at postion 11 and 18, double bond between 12 and 15, single bond between attom at postion 12 and 23, double bond between 13 and 16, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 27, single bond between attom at postion 15 and 16, single bond between attom at postion 16 and 28, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 29, double bond between 18 and 20, single bond between attom at postion 18 and 30, double bond between 19 and 21, single bond between attom at postion 19 and 31, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 32, single bond between attom at postion 21 and 34. The 3D x,y,z coordinates of the element at position 1 is -0.3452, 4.4948, -1.179, . The 3D x,y,z coordinates of the element at position 2 is 1.8787, -2.9811, -

This compound's CID is 5394 and compound's name is Temozolomide. There are 20 attoms in the molecule and their positions in the order are O, O, N, N, N, N, N, N, C, C, C, C, C, C, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 11, double bond between 2 and 14, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 10, double bond between 5 and 12, double bond between 6 and 7, single bond between attom at postion 6 and 9, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, double bond between 9 and 10, single bond between attom at postion 10 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 18. The 3D x,y,z coordinates of the element at position 1 is 2.6498, 1.6852, 0.0032, . The 3D x,y,z coordinates of the element at position 2 is -2.8126, -1.6976, 0.0114, . The 3D x,y,z coordinates of the This compound's CID is 5411 and compound's name is Tetracaine. There are 43 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 17, double bond between 2 and 17, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 26, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 19, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 21, single bond between attom at postion 6 and 22, single bond between attom at postion 6 and 23, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, double bond between 8 and 13, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, double bond between 12 and 15, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 17, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 34, double bond between 14 and 16, single bond between attom at postion 14 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 37, single bond between attom at postion 18 and 38, single bond between attom at postion 18 and 39, single bond between attom at postion 18 and 40, single bond between attom at postion 19 and 41, single bond between attom at postion 19 and 42, single bond between attom at postion 19 and 43. The 3D x,y,z coordinates of the element at position 1 is 2.6684, -0.0653, 0.1074, . The 3D x,y,z coordinates of the element at position 2 is 2.0965, -2.2942, 0.168, . The 3D x,y,z coordinates of

This compound's CID is 5426 and compound's name is Thalidomide. There are 29 attoms in the molecule and their positions in the order are O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 10, double bond between 2 and 11, double bond between 3 and 12, double bond between 4 and 15, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 20, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 24, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 13 and 14, double bond between 13 and 16, double bond between 14 and 17, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 26, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 27, double bond between 18 and 19, single bond between attom at postion 18 and 28, single bond between attom at postion 19 and 29. The 3D x,y,z coordinates of the element at position 1 is -1.3627, -0.0566, -2.1582, . The 3D x,y,z coordinates of the element at position 2 is 0.9379, 2.5651, -0.028, . The 3D x,y,z coordinates of This compound's CID is 5453 and compound's name is Thiotepa. There are 23 attoms in the molecule and their positions in the order are S, P, N, N, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 15, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 19, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 23. The 3D x,y,z coordinates of the element at position 1 is -0.3484, 0.9498, 2.1094, . The 3D x,y,z coordinates of the element at position 2 is -0.0615, 0.0526, 0.3907, . The 3D x,y,z coordinates

This compound's CID is 5482 and compound's name is Tioconazole. There are 36 attoms in the molecule and their positions in the order are CL, CL, CL, S, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 22, single bond between attom at postion 4 and 22, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 16, double bond between 7 and 16, single bond between attom at postion 7 and 20, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 9 and 26, double bond between 10 and 12, single bond between attom at postion 10 and 13, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 27, single bond between attom at postion 11 and 28, single bond between attom at postion 12 and 17, double bond between 13 and 18, single bond between attom at postion 13 and 29, double bond between 14 and 20, single bond between attom at postion 14 and 30, single bond between attom at postion 15 and 21, double bond between 15 and 22, single bond between attom at postion 16 and 31, double bond between 17 and 19, single bond between attom at postion 17 and 32, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 33, single bond between attom at postion 20 and 34, double bond between 21 and 23, single bond between attom at postion 21 and 35, single bond between attom at postion 23 and 36. The 3D x,y,z coordinates of the element at position 1 is -1.7343, -1.4552, -2.6992, . The 3D x,y,z coordinates of the element at position 2 is -5.8775, -0.338, 0.5497, . The 3D x,y,z This compound's CID is 5483 and compound's name is Tiopronin. There are 19 attoms in the molecule and their positions in the order are S, O, O, O, N, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 18, double bond between 2 and 7, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 19, double bond between 4 and 10, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 14. The 3D x,y,z coordinates of the element at position 1 is -2.2092, 1.8631, 0.0564, . The 3D x,y,z coordinates of the element at position 2 is -0.756, -1.0461, 1.1325, . The 3D x,y,z coordinates of the element at

This compound's CID is 5526 and compound's name is Tranexamic acid. There are 26 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 26, double bond between 2 and 11, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 24, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23. The 3D x,y,z coordinates of the element at position 1 is -3.4569, -0.5686, -0.6659, . The 3D x,y,z coordinates of the element at position 2 is -2.9214, 0.9529, 0.9238, . The 3D x,y,z coordinates of the element at position 3 is 4.0091, This compound's CID is 5546 and compound's name is Triamterene. There are 30 attoms in the molecule and their positions in the order are N, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 8, single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 11, double bond between 2 and 12, double bond between 3 and 11, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 13, double bond between 4 and 16, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 25, single bond between attom at postion 5 and 26, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 27, single bond between attom at postion 6 and 28, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 29, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 12, single bond between attom at postion 9 and 11, double bond between 9 and 13, double bond between 10 and 14, single bond between attom at postion 10 and 15, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 20, double bond between 15 and 18, single bond between attom at postion 15 and 21, double bond between 17 and 19, single bond between attom at postion 17 and 22, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 23, single bond between attom at postion 19 and 24. The 3D x,y,z coordinates of the element at position 1 is 0.0042, 0.72, 1.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -0.9418, -

This compound's CID is 5556 and compound's name is Triazolam. There are 35 attoms in the molecule and their positions in the order are CL, CL, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 12, double bond between 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 6, double bond between 5 and 9, double bond between 6 and 12, double bond between 7 and 8, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 15, single bond between attom at postion 9 and 11, single bond between attom at postion 10 and 14, single bond between attom at postion 11 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 12 and 18, double bond between 13 and 16, single bond between attom at postion 13 and 26, single bond between attom at postion 14 and 19, double bond between 14 and 20, double bond between 15 and 17, single bond between attom at postion 15 and 27, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 28, single bond between attom at postion 18 and 29, single bond between attom at postion 18 and 30, single bond between attom at postion 18 and 31, double bond between 19 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 32, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 33, double bond between 22 and 23, single bond between attom at postion 22 and 34, single bond between attom at postion 23 and 35. The 3D x,y,z coordinates of the element at position 1 is -1.0459, 4.6011, 0.2014, . The 3D x,y,z coordinates of the element at position 2 is -1.0166, -1.7941, -2.0306, . The 3D x,y,z

This compound's CID is 5564 and compound's name is Triclosan. There are 24 attoms in the molecule and their positions in the order are CL, CL, CL, O, O, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 17, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 24, double bond between 6 and 8, single bond between attom at postion 6 and 9, double bond between 7 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 12, double bond between 9 and 13, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 14, double bond between 11 and 15, single bond between attom at postion 11 and 19, double bond between 12 and 16, single bond between attom at postion 12 and 20, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 21, double bond between 14 and 17, single bond between attom at postion 14 and 22, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 23. The 3D x,y,z coordinates of the element at position 1 is -1.9929, 2.6476, 1.055, . The 3D x,y,z coordinates of the element at position 2 is 4.9959, -1.2993, 1.2086, . The 3D x,y,z coordinates of the element at position 3 is -4.975, -1.7896,

This compound's CID is 5578 and compound's name is Trimethoprim. There are 39 attoms in the molecule and their positions in the order are O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 21, double bond between 4 and 16, single bond between attom at postion 4 and 18, single bond between attom at postion 5 and 17, double bond between 5 and 18, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 27, single bond between attom at postion 6 and 28, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 38, single bond between attom at postion 7 and 39, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 22, single bond between attom at postion 8 and 23, double bond between 9 and 11, single bond between attom at postion 9 and 12, single bond between attom at postion 10 and 16, double bond between 10 and 17, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 24, double bond between 12 and 13, single bond between attom at postion 12 and 25, single bond between attom at postion 13 and 15, double bond between 14 and 15, single bond between attom at postion 17 and 26, single bond between attom at postion 19 and 29, single bond between attom at postion 19 and 30, single bond between attom at postion 19 and 31, single bond between attom at postion 20 and 32, single bond between attom at postion 20 and 33, single bond between attom at postion 20 and 34, single bond between attom at postion 21 and 35, single bond between attom at postion 21 and 36, single bond between attom at postion 21 and 37. The 3D x,y,z coordinates of the element at position 1 is -2.6987, 2.5018, 0.5331, . The 3D x,y,z coordinates of the element at position 2 is -2.7534, -2.1358, -
This compound's CID is 5665 and compound's name is Vigabatrin. There are 20 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 20, double bond between 2 and 8, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 17, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 14, double bond between 7 and 9, single bond between attom at postion 7 and 15, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 19. The 3D x,y,z coordinates of the element at position 1 is 2.4589, -1.1202, -0.0527, . The 3D x,y,z coordinates of the element at position 2 is 1.9133, 0.8595, -1.0276, . The 3D x,y,z coordinates of the element at position 3 is -2.398, 1.2971, -0.5037, . The 3D x,y,z coordinates of the

This compound's CID is 5719 and compound's name is Zaleplon. There are 38 attoms in the molecule and their positions in the order are O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 17, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 14, double bond between 4 and 21, single bond between attom at postion 5 and 14, double bond between 5 and 20, triple bond between 6 and 23, single bond between attom at postion 7 and 9, double bond between 7 and 10, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 10, double bond between 8 and 13, double bond between 9 and 16, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, double bond between 12 and 15, single bond between attom at postion 12 and 27, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 28, double bond between 14 and 19, single bond between attom at postion 15 and 29, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 30, single bond between attom at postion 17 and 22, single bond between attom at postion 18 and 31, single bond between attom at postion 18 and 32, single bond between attom at postion 18 and 33, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 23, single bond between attom at postion 20 and 34, single bond between attom at postion 21 and 35, single bond between attom at postion 22 and 36, single bond between attom at postion 22 and 37, single bond between attom at postion 22 and 38. The 3D x,y,z coordinates of the element at position 1 is -2.3117, 2.4669, -0.1697, . The 3D x,y,z coordinates of the element at position 2 is -3.6728, 0.5603, 0.117, . The 3D x,y,z coordinates of the element at
This compound's CID is 5734 and compound's name is Zonisamide. There are 22 attoms in the molecule and their positions in the order are S, O, O, O, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 3, double bond between 1 and 4, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 7, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 10, double bond between 5 and 8, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 22, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 9, single bond between attom at postion 9 and 10, double bond between 9 and 11, double bond between 10 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 18, double bond between 13 and 14, single bond between attom at postion 13 and 19, single bond between attom at postion 14 and 20. The 3D x,y,z coordinates of the element at position 1 is -2.699, 0.3331, -0.3064, . The 3D x,y,z coordinates of the element at position 2 is 1.1605, -2.0306, -0.1297, . The 3D x,y,z coordinates of the element at position 3 is -2.1144, 1.4984, -

This compound's CID is 5743 and compound's name is Dexamethasone. There are 57 atoms in the molecule and their positions in the order are X, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 50, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 52, double bond between 4 and 21, single bond between attom at postion 5 and 26, single bond between attom at postion 5 and 57, double bond between 6 and 28, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 29, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 30, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 31, single bond between attom at postion 12 and 32, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 22, single bond between attom at postion 14 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 23, single bond between attom at postion 16 and 24, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 37, single bond between attom at postion 17 and 38, single bond between attom at postion 18 and 39, single bond between attom at postion 18 and 40, single bond between attom at postion 18 and 41, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 42, single bond between attom at postion 19 and 43, double bond between 20 and 25, single bond between attom at postion 21 and 26, single bond between attom at postion 22 and 44, single bond between attom at postion 22 and 45, single bond between attom at postion 22 and 46, single bond between attom at postion 23 and 47, single bond between attom at postion 23 and 48, single bond between attom at postion 23 and 49, double bond between 24 and 27, single bond between attom at postion 24 and 51, single bond between attom at postion 25 and 28, single bond between attom at postion 25 and 53, single bond between attom at postion 26 and 54, single bond between attom at postion 26 and 55, single bond between attom at postion 27 and 28, single bond between attom at postion 27 and 56. The 3D x,y,z coordinates of the element at position 1 is 1.3287, 0.0906, 1.2721, . The 3D x,y,z coordinates of the

This compound's CID is 5744 and compound's name is Hydrocortisone Acetate. There are 61 atoms in the molecule and their positions in the order are O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 52, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 55, double bond between 3 and 23, single bond between attom at postion 4 and 27, single bond between attom at postion 4 and 28, double bond between 5 and 26, double bond between 6 and 28, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 23, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 22, single bond between attom at postion 14 and 35, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 40, single bond between attom at postion 17 and 41, single bond between attom at postion 18 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 19 and 20, double bond between 19 and 25, single bond between attom at postion 20 and 45, single bond between attom at postion 20 and 46, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 47, single bond between attom at postion 21 and 48, single bond between attom at postion 22 and 49, single bond between attom at postion 22 and 50, single bond between attom at postion 22 and 51, single bond between attom at postion 23 and 27, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 56, single bond between attom at postion 27 and 57, single bond between attom at postion 27 and 58, single bond between attom at postion 28 and 29, single bond between attom at postion 29 and

This compound's CID is 5745 and compound's name is Cortisone Acetate. There are 59 atoms in the molecule and their positions in the order are O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 51, double bond between 2 and 17, double bond between 3 and 22, single bond between attom at postion 4 and 27, single bond between attom at postion 4 and 28, double bond between 5 and 26, double bond between 6 and 28, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 19, single bond between attom at postion 12 and 21, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 35, single bond between attom at postion 14 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 15 and 38, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 18 and 41, single bond between attom at postion 18 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 19 and 20, double bond between 19 and 25, single bond between attom at postion 20 and 44, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 46, single bond between attom at postion 21 and 47, single bond between attom at postion 22 and 27, single bond between attom at postion 23 and 48, single bond between attom at postion 23 and 49, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 54, single bond between attom at postion 27 and 55, single bond between attom at postion 27 and 56, single bond between attom at postion 28 and 29, single bond between attom at postion 29 and 57, single bond between attom at postion 29 and 58, single bond between attom at postion 29 and 59. The 3D x,y,z coordinates of

This compound's CID is 5746 and compound's name is Mitomycin. There are 42 attoms in the molecule and their positions in the order are O, O, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 17, single bond between attom at postion 2 and 24, double bond between 3 and 18, double bond between 4 and 19, double bond between 5 and 24, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 15, single bond between attom at postion 8 and 22, single bond between attom at postion 8 and 39, single bond between attom at postion 8 and 40, single bond between attom at postion 9 and 24, single bond between attom at postion 9 and 41, single bond between attom at postion 9 and 42, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 25, single bond between attom at postion 11 and 14, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 26, single bond between attom at postion 13 and 28, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 30, double bond between 15 and 16, single bond between attom at postion 15 and 18, single bond between attom at postion 16 and 19, single bond between attom at postion 17 and 31, single bond between attom at postion 17 and 32, single bond between attom at postion 18 and 21, single bond between attom at postion 19 and 22, single bond between attom at postion 20 and 33, single bond between attom at postion 20 and 34, single bond between attom at postion 20 and 35, double bond between 21 and 22, single bond between attom at postion 21 and 23, single bond between attom at postion 23 and 36, single bond between attom at postion 23 and 37, single bond between attom at postion 23 and 38. The 3D x,y,z coordinates of the element at position 1 is 1.1403, -1.6348, -2.0164, . The 3D x,y,z coordinates of

This compound's CID is 5754 and compound's name is Hydrocortisone. There are 56 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 49, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 52, double bond between 3 and 22, single bond between attom at postion 4 and 26, single bond between attom at postion 4 and 56, double bond between 5 and 25, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 20, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 32, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 33, single bond between attom at postion 14 and 34, single bond between attom at postion 15 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 19, single bond between attom at postion 16 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 39, single bond between attom at postion 17 and 40, single bond between attom at postion 17 and 41, single bond between attom at postion 18 and 19, double bond between 18 and 24, single bond between attom at postion 19 and 42, single bond between attom at postion 19 and 43, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 44, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 46, single bond between attom at postion 21 and 47, single bond between attom at postion 21 and 48, single bond between attom at postion 22 and 26, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 53, single bond between attom at postion 26 and 54, single bond between attom at postion 26 and 55. The 3D x,y,z coordinates of the element at

This compound's CID is 5755 and compound's name is Prednisolone. There are 54 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 48, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 49, double bond between 3 and 20, single bond between attom at postion 4 and 24, single bond between attom at postion 4 and 54, double bond between 5 and 26, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 19, single bond between attom at postion 14 and 21, single bond between attom at postion 14 and 22, single bond between attom at postion 15 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 39, single bond between attom at postion 17 and 40, single bond between attom at postion 17 and 41, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 42, single bond between attom at postion 18 and 43, double bond between 19 and 23, single bond between attom at postion 20 and 24, single bond between attom at postion 21 and 44, single bond between attom at postion 21 and 45, single bond between attom at postion 21 and 46, double bond between 22 and 25, single bond between attom at postion 22 and 47, single bond between attom at postion 23 and 26, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 51, single bond between attom at postion 24 and 52, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 53. The 3D x,y,z coordinates of the element at

This compound's CID is 5757 and compound's name is Estradiol. There are 44 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 40, single bond between attom at postion 2 and 20, single bond between attom at postion 2 and 44, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 22, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 23, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 24, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, double bond between 14 and 16, single bond between attom at postion 14 and 17, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 38, single bond between attom at postion 15 and 39, single bond between attom at postion 16 and 18, double bond between 17 and 19, single bond between attom at postion 17 and 41, double bond between 18 and 20, single bond between attom at postion 18 and 42, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 43. The 3D x,y,z coordinates of the element at position 1 is 5.0614, 1.1501, 0.2674, . The 3D x,y,z This compound's CID is 5816 and compound's name is Epinephrine. There are 26 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 21, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 25, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 26, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 19, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 14, double bond between 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 17, double bond between 9 and 11, single bond between attom at postion 9 and 18, double bond between 10 and 12, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 20, single bond between attom at postion 13 and 22, single bond between attom at postion 13 and 23, single bond between attom at postion 13 and 24. The 3D x,y,z coordinates of the element at position 1 is 1.7394, -2.1169, -1.0894, . The 3D x,y,z coordinates of the element at position 2 is -2.2941, 1.0781, -

This compound's CID is 5819 and compound's name is Levothyroxine. There are 35 attoms in the molecule and their positions in the order are I, I, I, I, O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 22, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 19, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 34, double bond between 7 and 18, single bond between attom at postion 8 and 24, single bond between attom at postion 8 and 35, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 30, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 27, double bond between 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 28, double bond between 14 and 16, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 16, double bond between 15 and 17, double bond between 19 and 20, single bond between attom at postion 19 and 21, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 32, double bond between 21 and 22, single bond between attom at postion 21 and 33, single bond between attom at postion 22 and 24, double bond between 23 and 24. The 3D x,y,z coordinates of the element at position 1 is 0.1456, -0.7021, -3.2374, . The 3D x,y,z coordinates of the element at position 2 is
This compound's CID is 5826 and compound's name is Dextroamphetamine. There are 23 attoms in the molecule and their positions in the order are N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 19, single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 13, double bond between 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 17, double bond between 7 and 9, single bond between attom at postion 7 and 18, double bond between 8 and 10, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 23. The 3D x,y,z coordinates of the element at position 1 is -3.5842, -0.4594, 0.1201, . The 3D x,y,z coordinates of the element at position 2 is -2.2228, -0.1767, -0.3441, . The 3D x,y,z

This compound's CID is 5832 and compound's name is Norethindrone Acetate. There are 53 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 23, double bond between 2 and 22, double bond between 3 and 23, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 26, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 29, single bond between attom at postion 9 and 30, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 31, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 11 and 34, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, double bond between 17 and 21, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, triple bond between 19 and 24, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 49, single bond between attom at postion 23 and 25, single bond between attom at postion 24 and 50, single bond between attom at postion 25 and 51, single bond between attom at postion 25 and 52, single bond between attom at postion 25 and 53. The 3D x,y,z coordinates of the element at position 1 is 3.9268, -0.5148, -0.5887, . The 3D x,y,z

This compound's CID is 5833 and compound's name is Spironolactone. There are 61 atoms in the molecule and their positions in the order are S, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 1 and 28, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 24, double bond between 3 and 24, double bond between 4 and 27, double bond between 5 and 28, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 33, single bond between attom at postion 11 and 34, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 35, single bond between attom at postion 12 and 36, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 22, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 41, single bond between attom at postion 17 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 23, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 20, double bond between 19 and 26, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 25, single bond between attom at postion 21 and 49, single bond between attom at postion 21 and 50, single bond between attom at postion 22 and 51, single bond between attom at postion 22 and 52, single bond between attom at postion 22 and 53, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 54, single bond between attom at postion 23 and 55, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 56, single bond between attom at postion 25 and 57, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 58, single bond between attom at postion 28 and 29, single bond

This compound's CID is 5884 and compound's name is Prednisolone Acetate. There are 59 atoms in the molecule and their positions in the order are O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 51, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 52, double bond between 3 and 21, single bond between attom at postion 4 and 25, single bond between attom at postion 4 and 28, double bond between 5 and 27, double bond between 6 and 28, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 37, single bond between attom at postion 15 and 20, single bond between attom at postion 15 and 22, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 40, single bond between attom at postion 17 and 41, single bond between attom at postion 18 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 45, single bond between attom at postion 19 and 46, double bond between 20 and 24, single bond between attom at postion 21 and 25, single bond between attom at postion 22 and 47, single bond between attom at postion 22 and 48, single bond between attom at postion 22 and 49, double bond between 23 and 26, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 27, single bond between attom at postion 24 and 53, single bond between attom at postion 25 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 56, single bond between attom at postion 28 and 29, single bond between attom at postion 29 and 57, single bond between attom at postion 29 and 58, single bond between attom at postion 29 and 59. The 3D x,y,z

This compound's CID is 5865 and compound's name is Prednisone. There are 52 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 47, double bond between 2 and 16, double bond between 3 and 20, single bond between attom at postion 4 and 24, single bond between attom at postion 4 and 52, double bond between 5 and 26, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 13 and 35, single bond between attom at postion 14 and 19, single bond between attom at postion 14 and 21, single bond between attom at postion 14 and 22, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 17 and 38, single bond between attom at postion 17 and 39, single bond between attom at postion 17 and 40, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 41, single bond between attom at postion 18 and 42, double bond between 19 and 23, single bond between attom at postion 20 and 24, single bond between attom at postion 21 and 43, single bond between attom at postion 21 and 44, single bond between attom at postion 21 and 45, double bond between 22 and 25, single bond between attom at postion 22 and 46, single bond between attom at postion 23 and 26, single bond between attom at postion 23 and 48, single bond between attom at postion 24 and 49, single bond between attom at postion 24 and 50, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 51. The 3D x,y,z coordinates of the element at position 1 is 3.0953, -

This compound's CID is 5877 and compound's name is Methylprednisolone Acetate. There are 62 atoms in the molecule and their positions in the order are O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 51, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 52, double bond between 3 and 21, single bond between attom at postion 4 and 26, single bond between attom at postion 4 and 29, double bond between 5 and 28, double bond between 6 and 29, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 20, single bond between attom at postion 15 and 22, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 41, single bond between attom at postion 17 and 42, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 24, single bond between attom at postion 18 and 43, single bond between attom at postion 19 and 44, single bond between attom at postion 19 and 45, single bond between attom at postion 19 and 46, double bond between 20 and 25, single bond between attom at postion 21 and 26, single bond between attom at postion 22 and 47, single bond between attom at postion 22 and 48, single bond between attom at postion 22 and 49, double bond between 23 and 27, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 24 and 55, single bond between attom at postion 25 and 28, single bond between attom at postion 25 and 56, single bond between attom at postion 26 and 57, single bond between attom at postion 26 and 58, single bond between attom at postion 27 and 28, single bond between attom at postion 27 and 59, single bond between attom at postion 29 and

This compound's CID is 5881 and compound's name is Prasterone. There are 49 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 14, single bond between attom at postion 2 and 21, single bond between attom at postion 2 and 49, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 22, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, double bond between 12 and 16, single bond between attom at postion 12 and 19, single bond between attom at postion 13 and 20, single bond between attom at postion 13 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 15, single bond between attom at postion 15 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 37, single bond between attom at postion 17 and 38, single bond between attom at postion 17 and 39, single bond between attom at postion 17 and 40, single bond between attom at postion 18 and 41, single bond between attom at postion 18 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 44, single bond between attom at postion 19 and 45, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 46, single bond between attom at postion 20 and 47, single bond between attom at postion 21 and 48. The 3D x,y,z coordinates of the element at position 1 is 5.0456, This compound's CID is 5920 and compound's name is Liothyronine. There are 35 attoms in the molecule and their positions in the order are I, I, I, O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 21, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 18, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 34, double bond between 6 and 17, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 35, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 24, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 26, double bond between 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 27, double bond between 13 and 15, single bond between attom at postion 13 and 28, single bond between attom at postion 14 and 15, double bond between 14 and 16, double bond between 18 and 19, single bond between attom at postion 18 and 20, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 31, double bond between 20 and 22, single bond between attom at postion 20 and 32, double bond between 21 and 23, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 33. The 3D x,y,z coordinates of the element at position 1 is 0.3791, -0.695, -3.2651, . The 3D x,y,z coordinates of the element at position 2 is 0.9319,

This compound's CID is 5944 and compound's name is Cantharidin. There are 26 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 12, double bond between 3 and 11, double bond between 4 and 12, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 15, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 20, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 22, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 24, single bond between attom at postion 14 and 25, single bond between attom at postion 14 and 26. The 3D x,y,z coordinates of the element at position 1 is 0.9284, -0.0027, 1.5427, . The 3D x,y,z coordinates of the element at position 2 is -2.0625, 4.0E-4,
This compound's CID is 5961 and compound's name is Glutamine. There are 20 attoms in the molecule and their positions in the order are O, O, O, N, N, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 20, double bond between 2 and 9, double bond between 3 and 10, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 18, single bond between attom at postion 5 and 19, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 15. The 3D x,y,z coordinates of the element at position 1 is -2.1389, 1.637, 0.5099, . The 3D x,y,z coordinates of the element at position 2 is -2.6773, 0.2475, -1.1973, . The 3D x,y,z coordinates of the element at position 3 is 2.9039, 0.2551, 1.0351, . The 3D x,y,z

This compound's CID is 5988 and compound's name is Sucrose. There are 45 attoms in the molecule and their positions in the order are O, O, O, O, O, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 38, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 39, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 40, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 41, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 42, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 43, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 44, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 45, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 22, single bond between attom at postion 15 and 26, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 27, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 28, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 29, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 30, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 31, single bond between attom at postion 21 and 32, single bond between attom at postion 21 and 33, single bond between attom at postion 22 and 34, single bond between attom at postion 22 and 35, single bond between attom at postion 23 and 36, single bond between attom at postion 23 and 37. The 3D x,y,z coordinates of the element at position 1 is -1.468, 0.4385, -

This compound's CID is 5991 and compound's name is Ethinyl Estradiol. There are 46 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 41, single bond between attom at postion 2 and 21, single bond between attom at postion 2 and 46, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, double bond between 14 and 16, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 19, triple bond between 17 and 22, double bond between 18 and 20, single bond between attom at postion 18 and 42, double bond between 19 and 21, single bond between attom at postion 19 and 43, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 44, single bond between attom at postion 22 and 45. The 3D x,y,z coordinates of the element at position 1 is -4.6386, 0.7554, -1.1201, . The 3D x,y,z coordinates of the element at

This compound's CID is 5994 and compound's name is Progesterone. There are 53 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 19, double bond between 2 and 22, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 24, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 25, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 26, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 27, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 14 and 16, double bond between 14 and 21, single bond between attom at postion 15 and 38, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 41, single bond between attom at postion 16 and 42, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 18 and 47, single bond between attom at postion 19 and 23, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 23 and 52, single bond between attom at postion 23 and 53. The 3D x,y,z coordinates of the element at position 1 is 5.5193, -0.1943, -0.6738, . The 3D x,y,z

This compound's CID is 5997 and compound's name is Cholesterol. There are 74 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 22, single bond between attom at postion 1 and 65, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 29, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 30, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 31, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 32, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 33, single bond between attom at postion 7 and 34, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 35, single bond between attom at postion 9 and 36, single bond between attom at postion 10 and 37, single bond between attom at postion 10 and 38, single bond between attom at postion 11 and 39, single bond between attom at postion 11 and 40, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 41, single bond between attom at postion 12 and 42, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 23, single bond between attom at postion 13 and 43, single bond between attom at postion 14 and 44, single bond between attom at postion 14 and 45, single bond between attom at postion 14 and 46, double bond between 15 and 17, single bond between attom at postion 15 and 19, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 47, single bond between attom at postion 16 and 48, single bond between attom at postion 17 and 49, single bond between attom at postion 18 and 50, single bond between attom at postion 18 and 51, single bond between attom at postion 18 and 52, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 53, single bond between attom at postion 19 and 54, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 55, single bond between attom at postion 20 and 56, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 57, single bond between attom at postion 21 and 58, single bond between attom at postion 22 and 59, single bond between attom at postion 23 and 60, single bond between attom at postion 23 and

This compound's CID is 6010 and compound's name is Methyltestosterone. There are 52 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 49, double bond between 2 and 22, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 14, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 19, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 34, single bond between attom at postion 13 and 35, single bond between attom at postion 14 and 36, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 16, double bond between 15 and 21, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 41, single bond between attom at postion 17 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 50, single bond between attom at postion 20 and 51, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 52. The 3D x,y,z coordinates of the element at position 1 is -5.0212, -0.9419, 0.1614, . The 3D x,y,z coordinates of

This compound's CID is 6013 and compound's name is Testosterone. There are 49 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 49, double bond between 2 and 21, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 22, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 16, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 23, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 24, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 13 and 35, single bond between attom at postion 14 and 15, double bond between 14 and 20, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 41, single bond between attom at postion 17 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 48. The 3D x,y,z coordinates of the element at position 1 is -5.1688, This compound's CID is 6047 and compound's name is Levodopa. There are 25 attoms in the molecule and their positions in the order are O, O, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 23, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 25, double bond between 4 and 12, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 21, single bond between attom at postion 5 and 22, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 17, double bond between 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 18, double bond between 10 and 13, single bond between attom at postion 10 and 19, double bond between 11 and 14, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 20. The 3D x,y,z coordinates of the element at position 1 is 2.5189, -2.0482, 0.5529, . The 3D x,y,z coordinates of the element at position 2 is -1.8525, -1.4781, -1.2114, . The 3D x,y,z coordinates of the element at

This compound's CID is 6140 and compound's name is Phenylalanine. There are 23 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 23, double bond between 2 and 9, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 18, single bond between attom at postion 3 and 19, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 15, double bond between 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 16, double bond between 8 and 11, single bond between attom at postion 8 and 17, double bond between 10 and 12, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 22. The 3D x,y,z coordinates of the element at position 1 is -1.5606, -1.548, -1.0372, . The 3D x,y,z coordinates of the element at position 2 is -3.1863, -1.0236, 0.4554, . The 3D x,y,z coordinates of the element at This compound's CID is 6167 and compound's name is Colchicine. There are 54 attoms in the molecule and their positions in the order are O, O, O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 1 and 26, single bond between attom at postion 2 and 19, single bond between attom at postion 2 and 27, single bond between attom at postion 3 and 20, single bond between attom at postion 3 and 28, single bond between attom at postion 4 and 24, single bond between attom at postion 4 and 29, double bond between 5 and 21, double bond between 6 and 22, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 22, single bond between attom at postion 7 and 35, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 14, double bond between 11 and 17, single bond between attom at postion 12 and 13, double bond between 12 and 16, single bond between attom at postion 13 and 14, double bond between 13 and 15, double bond between 14 and 18, single bond between attom at postion 15 and 19, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 36, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 37, single bond between attom at postion 18 and 23, single bond between attom at postion 18 and 38, double bond between 19 and 20, single bond between attom at postion 21 and 24, single bond between attom at postion 22 and 25, double bond between 23 and 24, single bond between attom at postion 23 and 39, single bond between attom at postion 25 and 40, single bond between attom at postion 25 and 41, single bond between attom at postion 25 and 42, single bond between attom at postion 26 and 43, single bond between attom at postion 26 and 44, single bond between attom at postion 26 and 45, single bond between attom at postion 27 and 46, single bond between attom at postion 27 and 47, single bond between attom at postion 27 and 48, single bond between attom at postion 28 and 49, single bond between attom at postion 28 and 50, single bond between attom at postion 28 and 51, single bond between attom at postion 29 and 52, single bond between attom at postion 29 and 53, single bond between attom at postion 29 and 54. The 3D x,y,z coordinates of the element at position 1 is 0.7092, 1.9623, -1.4223, . The 3D x,y,z coordinates of the element at position 2 is 3.4256, 2.1447, -

This compound's CID is 6213 and compound's name is Fluocinolone Acetonide. There are 62 atoms in the molecule and their positions in the order are X, X, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 21, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 51, double bond between 6 and 22, single bond between attom at postion 7 and 27, single bond between attom at postion 7 and 62, double bond between 8 and 32, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 19, single bond between attom at postion 11 and 34, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 22, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 18, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 40, single bond between attom at postion 18 and 24, single bond between attom at postion 18 and 25, single bond between attom at postion 18 and 26, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 41, single bond between attom at postion 19 and 42, single bond between attom at postion 20 and 43, single bond between attom at postion 20 and 44, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 46, single bond between attom at postion 22 and 27, single bond between attom at postion 23 and 28, single bond between attom at postion 23 and 29, double bond between 24 and 30, single bond between attom at postion 25 and 47, single bond between attom at postion 25 and 48, single bond between attom at postion 25 and 49, double bond between 26 and 31, single bond between attom at postion 26 and 50, single bond between attom at postion 27 and 52, single bond between attom at postion 27 and 53, single bond between attom at postion 28 and 54, single bond between attom at postion 28 and 55, single bond between attom at postion 28 and 56, single bond between attom at postion 29 and 57, single bond between attom at postion 29 and 58, single bond between attom at postion 29 and

This compound's CID is 6230 and compound's name is Norethindrone. There are 48 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 44, double bond between 2 and 21, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, double bond between 16 and 20, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 42, single bond between attom at postion 17 and 43, triple bond between 18 and 22, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 45, single bond between attom at postion 19 and 46, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 47, single bond between attom at postion 22 and 48. The 3D x,y,z coordinates of the element at position 1 is 4.6613, -0.6933, -0.6765, . The 3D x,y,z coordinates of the element at This compound's CID is 6234 and compound's name is Cycloserine. There are 13 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 6, double bond between 2 and 7, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10. The 3D x,y,z coordinates of the element at position 1 is -1.7919, 0.0017, 0.0374, . The 3D x,y,z coordinates of the element at position 2 is 1.3808, 1.4506, -0.0254, . The 3D x,y,z coordinates of the element at position 3 is -0.9168,

This compound's CID is 6251 and compound's name is Mannitol. There are 26 attoms in the molecule and their positions in the order are O, O, O, O, O, O, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 21, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 22, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 25, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 26, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 12 and 20. The 3D x,y,z coordinates of the element at position 1 is 0.5166, 1.3302, -1.1366, . The 3D x,y,z coordinates of the element at position 2 is -
This compound's CID is 6253 and compound's name is Cytarabine. There are 30 attoms in the molecule and their positions in the order are O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 27, double bond between 5 and 15, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 7 and 15, double bond between 7 and 17, single bond between attom at postion 8 and 17, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 20, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 22, single bond between attom at postion 13 and 23, double bond between 14 and 16, single bond between attom at postion 14 and 26, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 28. The 3D x,y,z coordinates of the element at position 1 is -1.3618, -0.3949, 0.9647, . The 3D x,y,z coordinates of

This compound's CID is 6256 and compound's name is Trifluridine. There are 31 attoms in the molecule and their positions in the order are X, X, X, O, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 29, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 31, double bond between 7 and 17, double bond between 8 and 19, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 17, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 22, single bond between attom at postion 13 and 23, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 26, single bond between attom at postion 15 and 27, double bond between 16 and 18, single bond between attom at postion 16 and 28, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 20. The 3D x,y,z coordinates of the element at position 1 is -3.4855, 1.5611, 0.8746, . The 3D x,y,z coordinates of the element at position 2 is -1.798, 2.5059, -0.1315, . The 3D x,y,z

This compound's CID is 6279 and compound's name is Medroxyprogesterone acetate. There are 62 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 27, double bond between 2 and 21, double bond between 3 and 25, double bond between 4 and 27, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 18, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 29, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 24, single bond between attom at postion 16 and 42, double bond between 17 and 23, single bond between attom at postion 18 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 20 and 50, single bond between attom at postion 21 and 26, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 51, single bond between attom at postion 22 and 52, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 24 and 55, single bond between attom at postion 24 and 56, single bond between attom at postion 26 and 57, single bond between attom at postion 26 and 58, single bond between attom at postion 26 and 59, single bond between attom at
This compound's CID is 6305 and compound's name is Tryptophan. There are 27 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 27, double bond between 2 and 13, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 24, single bond between attom at postion 4 and 25, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, double bond between 5 and 10, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 7 and 9, double bond between 7 and 11, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 18, double bond between 9 and 12, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 22, double bond between 14 and 15, single bond between attom at postion 14 and 23, single bond between attom at postion 15 and 26. The 3D x,y,z coordinates of the element at position 1 is 1.4762, -0.8154, 1.7282, . The 3D x,y,z coordinates of the element at position 2 is 2.5598, -1.9472, 0.0879, . The 3D x,y,z coordinates of the element at

This compound's CID is 6432 and compound's name is Perflutren. There are 11 attoms in the molecule and their positions in the order are X, X, X, X, X, X, X, X, C, C, C. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 9, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 10, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11. The 3D x,y,z coordinates of the element at position 1 is 0.0, 1.4092, 1.0818, . The 3D x,y,z coordinates of the element at position 2 is 1.0E-4, 1.4014, -1.0965, . The 3D x,y,z coordinates of the element at position 3 is 1.3335, -1.0243, -

This compound's CID is 6436 and compound's name is Triamcinolone Acetonide. There are 82 attoms in the molecule and their positions in the order are X, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 21, single bond between attom at postion 3 and 13, single bond between attom at postion 3 and 21, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 51, double bond between 5 and 22, single bond between attom at postion 6 and 26, single bond between attom at postion 6 and 62, double bond between 7 and 31, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 18, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 17, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 35, single bond between attom at postion 14 and 36, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 37, single bond between attom at postion 15 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 23, single bond between attom at postion 17 and 24, single bond between attom at postion 17 and 25, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 40, single bond between attom at postion 18 and 41, single bond between attom at postion 19 and 42, single bond between attom at postion 19 and 43, single bond between attom at postion 19 and 44, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 45, single bond between attom at postion 20 and 46, single bond between attom at postion 21 and 27, single bond between attom at postion 21 and 28, single bond between attom at postion 22 and 26, double bond between 23 and 29, single bond between attom at postion 24 and 47, single bond between attom at postion 24 and 48, single bond between attom at postion 24 and 49, double bond between 25 and 30, single bond between attom at postion 25 and 50, single bond between attom at postion 26 and 52, single bond between attom at postion 26 and 53, single bond between attom at postion 27 and 54, single bond between attom at postion 27 and 55, single bond between attom at postion 27 and 56, single bond between attom at postion 28 and 57, single bond between attom at postion 28 and 58, single bond between attom at

This compound's CID is 6503 and compound's name is Tromethamine. There are 19 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 18, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 19, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 16, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 14. The 3D x,y,z coordinates of the element at position 1 is -2.4461, 0.3527, 0.068, . The 3D x,y,z coordinates of the element at position 2 is 0.028, -2.1555, 0.0907, . The 3D x,y,z
This compound's CID is 6613 and compound's name is Pantothenic Acid. There are 32 attoms in the molecule and their positions in the order are O, O, O, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 26, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 29, double bond between 3 and 12, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 32, double bond between 5 and 15, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 27, single bond between attom at postion 13 and 28, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 30, single bond between attom at postion 14 and 31. The 3D x,y,z coordinates of the element at position 1 is -2.7529, -1.6944, 0.3338, . The 3D x,y,z coordinates of the element at position 2 is -1.1073, 2.8794, -0.1963, . The 3D x,y,z coordinates

This compound's CID is 6623 and compound's name is Bisphenol A. There are 33 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 1 and 32, single bond between attom at postion 2 and 17, single bond between attom at postion 2 and 33, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, double bond between 4 and 8, single bond between attom at postion 4 and 10, double bond between 5 and 9, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 19, single bond between attom at postion 6 and 20, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 22, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 24, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 25, double bond between 10 and 14, single bond between attom at postion 10 and 26, double bond between 11 and 15, single bond between attom at postion 11 and 27, double bond between 12 and 16, single bond between attom at postion 12 and 28, double bond between 13 and 17, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 30, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 31. The 3D x,y,z coordinates of the element at position 1 is -4.6727, 1.7597, 0.1081, . The 3D x,y,z coordinates of the element at position 2 is 4.7037, 1.7341, -0.1083, . The 3D x,y,z coordinates of the element at position 3 is 0.0069, -1.3899, -4.0E-4, . The 3D This compound's CID is 6736 and compound's name is Skatole. There are 19 attoms in the molecule and their positions in the order are N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, double bond between 2 and 6, double bond between 3 and 7, double bond between 4 and 5, single bond between attom at postion 4 and 8, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 14, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, double bond between 9 and 10, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 19. The 3D x,y,z coordinates of the element at position 1 is -0.8227, 1.7267, 0.0, . The 3D x,y,z coordinates of the element at position 2 is -0.2141, -

This compound's CID is 6741 and compound's name is Methylprednisolone. There are 57 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 48, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 49, double bond between 3 and 20, single bond between attom at postion 4 and 25, single bond between attom at postion 4 and 57, double bond between 5 and 27, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 29, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 30, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 34, single bond between attom at postion 13 and 35, single bond between attom at postion 14 and 19, single bond between attom at postion 14 and 21, single bond between attom at postion 14 and 22, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 23, single bond between attom at postion 17 and 40, single bond between attom at postion 18 and 41, single bond between attom at postion 18 and 42, single bond between attom at postion 18 and 43, double bond between 19 and 24, single bond between attom at postion 20 and 25, single bond between attom at postion 21 and 44, single bond between attom at postion 21 and 45, single bond between attom at postion 21 and 46, double bond between 22 and 26, single bond between attom at postion 22 and 47, single bond between attom at postion 23 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 23 and 52, single bond between attom at postion 24 and 27, single bond between attom at postion 24 and 53, single bond between attom at postion 25 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 56. The 3D x,y,z coordinates of the element at position 1 is 3.1525, 0.1126, 1.9964, . The 3D x,y,z coordinates of the element This compound's CID is 6883 and compound's name is Isosorbide Dinitrate. There are 24 attoms in the molecule and their positions in the order are O, O, O, O, O, O, O, O, N, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 10, double bond between 7 and 9, double bond between 8 and 10, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 19, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 20, single bond between attom at postion 15 and 21, single bond between attom at postion 15 and 22, single bond between attom at postion 16 and 23, single bond between attom at postion 16 and 24. The 3D x,y,z coordinates of the element at position 1 is 0.5145, 0.0895, -1.3888, . The 3D x,y,z coordinates of the element at position 2 is -0.3832, -1.9992,

This compound's CID is 6989 and compound's name is Thymol. There are 25 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 25, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 12, double bond between 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 18, single bond between attom at postion 6 and 9, double bond between 7 and 10, single bond between attom at postion 7 and 19, double bond between 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24. The 3D x,y,z coordinates of the element at position 1 is -0.4292, 2.3458, 2.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -2.1355, 0.0547, 0.0, . The 3D x,y,z coordinates of the element at position This compound's CID is 7027 and compound's name is Gluconolactone. There are 22 attoms in the molecule and their positions in the order are O, O, O, O, O, O, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 22, double bond between 6 and 12, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 18. The 3D x,y,z coordinates of the element at position 1 is -0.3286, 1.438, -0.1234, . The 3D x,y,z coordinates of the element at position 2 is -1.464, -2.0541, -0.6056, . The 3D x,y,z coordinates of the element at This compound's CID is 7187 and compound's name is Benzoyl Peroxide. There are 28 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 18, double bond between 3 and 17, double bond between 4 and 18, double bond between 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 17, double bond between 6 and 8, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 20, double bond between 9 and 13, single bond between attom at postion 9 and 21, double bond between 10 and 14, single bond between attom at postion 10 and 22, double bond between 11 and 15, single bond between attom at postion 11 and 23, double bond between 12 and 16, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 26, single bond between attom at postion 15 and 27, single bond between attom at postion 16 and 28. The 3D x,y,z coordinates of the element at position 1 is 0.686, 0.2752, -0.001, . The 3D x,y,z coordinates of the element at position 2 is -0.6672, -0.2683, -8.0E-4, . The 3D x,y,z coordinates of the

This compound's CID is 7697 and compound's name is Chlorphenesin. There are 24 attoms in the molecule and their positions in the order are CL, O, O, O, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 8, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 21, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, double bond between 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 19, double bond between 10 and 12, single bond between attom at postion 10 and 20, double bond between 11 and 13, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 23. The 3D x,y,z coordinates of the element at position 1 is -5.0723, 0.6033, -0.3525, . The 3D x,y,z coordinates of the element at position 2 is 0.6065, -0.6995, 0.3757, . The 3D x,y,z coordinates of the element at position 3 is 3.3788, -1.0738, This compound's CID is 7896 and compound's name is Butylene Glycol. There are 16 attoms in the molecule and their positions in the order are O, O, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 14. The 3D x,y,z coordinates of the element at position 1 is 1.2637, -1.3081, 0.2225, . The 3D x,y,z coordinates of the element at position 2 is -2.6897, 0.2382, 0.1788, . The 3D x,y,z coordinates of the element at This compound's CID is 8027 and compound's name is Pyrrole. There are 10 attoms in the molecule and their positions in the order are N, C, C, C, C, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 6, double bond between 2 and 4, single bond between attom at postion 2 and 7, double bond between 3 and 5, single bond between attom at postion 3 and 8, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 9, single bond between attom at postion 5 and 10. The 3D x,y,z coordinates of the element at position 1 is 0.0032, -1.158, -2.0E-4, . The 3D x,y,z coordinates of the element at position 2 is -1.1187, -0.3708, 2.0E-4, . The

This compound's CID is 8362 and compound's name is Homosalate. There are 41 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 13, double bond between 2 and 13, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 41, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 21, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 22, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 24, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 26, single bond between attom at postion 9 and 27, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 12 and 36, single bond between attom at postion 13 and 14, single bond between attom at postion 14 and 15, double bond between 14 and 16, double bond between 15 and 17, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 37, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 38, double bond between 18 and 19, single bond between attom at postion 18 and 39, single bond between attom at postion 19 and 40. The 3D x,y,z coordinates of the element at position 1 is 0.0956, 0.7757, -0.5488, . The 3D x,y,z coordinates of the element at position 2 is
This compound's CID is 8364 and compound's name is 2-Ethylhexyl salicylate. There are 40 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 12, double bond between 2 and 12, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 40, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 19, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 21, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 22, single bond between attom at postion 6 and 23, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 11 and 34, single bond between attom at postion 11 and 35, single bond between attom at postion 12 and 13, single bond between attom at postion 13 and 14, double bond between 13 and 15, double bond between 14 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 37, double bond between 17 and 18, single bond between attom at postion 17 and 38, single bond between attom at postion 18 and 39. The 3D x,y,z coordinates of the element at position 1 is 0.2475, -0.1361, 0.0345, . The 3D x,y,z coordinates of the element at position 2 is 1.3686, -1.8608, 1.0679, . The 3D x,y,z coordinates of the element at position 3 is 3.7984, -

This compound's CID is 9416 and compound's name is Testosterone Enanthate. There are 69 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 23, double bond between 2 and 22, double bond between 3 and 23, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 30, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 31, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 32, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 33, single bond between attom at postion 9 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 10 and 36, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 37, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 38, single bond between attom at postion 12 and 39, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 40, single bond between attom at postion 13 and 41, single bond between attom at postion 14 and 42, single bond between attom at postion 14 and 43, single bond between attom at postion 15 and 17, double bond between 15 and 21, single bond between attom at postion 16 and 44, single bond between attom at postion 16 and 45, single bond between attom at postion 16 and 46, single bond between attom at postion 17 and 47, single bond between attom at postion 17 and 48, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 49, single bond between attom at postion 18 and 50, single bond between attom at postion 19 and 51, single bond between attom at postion 19 and 52, single bond between attom at postion 19 and 53, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 54, single bond between attom at postion 20 and 55, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 56, single bond between attom at postion 23 and 24, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 57, single bond between attom at postion 24 and 58, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 59, single bond between attom at postion 25 and 60, single bond between attom at postion 26 and 27, single bond
This compound's CID is 9444 and compound's name is Azacitidine. There are 29 attoms in the molecule and their positions in the order are O, O, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 27, double bond between 5 and 15, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 15, double bond between 7 and 17, double bond between 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 18, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 19, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 21, single bond between attom at postion 13 and 20, single bond between attom at postion 14 and 22, single bond between attom at postion 14 and 23, single bond between attom at postion 16 and 26. The 3D x,y,z coordinates of the element at position 1 is -1.361, -0.5442, 1.0197, . The 3D x,y,z coordinates of the element at position 2 is -1.2258, 2.352, -

This compound's CID is 3642 and compound's name is Paclitaxel. There are 97 atoms in the molecule and their positions in the order are X, X, O, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 2 and 22, single bond between attom at postion 3 and 13, single bond between attom at postion 3 and 24, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 18, single bond between attom at postion 5 and 54, double bond between 6 and 23, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 34, double bond between 8 and 33, double bond between 9 and 34, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 20, single bond between attom at postion 12 and 37, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 41, single bond between attom at postion 17 and 42, single bond between attom at postion 18 and 43, single bond between attom at postion 19 and 25, single bond between attom at postion 19 and 26, single bond between attom at postion 19 and 27, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 44, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 46, single bond between attom at postion 21 and 47, single bond between attom at postion 21 and 48, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 49, single bond between attom at postion 23 and 28, single bond between attom at postion 24 and 29, single bond between attom at postion 24 and 30, double bond between 25 and 31, single bond between attom at postion 26 and 50, single bond between attom at postion 26 and 51, single bond between attom at postion 26 and 52, double bond between 27 and 32, single bond between attom at postion 27 and 53, single bond between attom at postion 28 and 55, single bond between attom at postion 28 and 56, single bond between attom at postion 29 and 57, single bond between attom at postion 29 and 58, single bond between attom at postion 29 and 59, single bond between attom at postion 30 and 60, single bond between attom at postion 30 and 61, single bond

This compound's CID is 9878 and compound's name is Fluorometholone. There are 56 attoms in the molecule and their positions in the order are X, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 47, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 48, double bond between 4 and 20, double bond between 5 and 27, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 29, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 32, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 14 and 19, single bond between attom at postion 14 and 21, single bond between attom at postion 14 and 22, single bond between attom at postion 15 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 23, single bond between attom at postion 17 and 39, single bond between attom at postion 18 and 40, single bond between attom at postion 18 and 41, single bond between attom at postion 18 and 42, double bond between 19 and 24, single bond between attom at postion 20 and 26, single bond between attom at postion 21 and 43, single bond between attom at postion 21 and 44, single bond between attom at postion 21 and 45, double bond between 22 and 25, single bond between attom at postion 22 and 46, single bond between attom at postion 23 and 49, single bond between attom at postion 23 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 24 and 27, single bond between attom at postion 24 and 52, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 53, single bond between attom at postion 26 and 54, single bond between attom at postion 26 and 55, single bond between attom at postion 26 and 56. The 3D x,y,z coordinates of the element at
This compound's CID is 10917 and compound's name is Levocarnitine. There are 26 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 26, single bond between attom at postion 2 and 11, double bond between 3 and 11, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 25. The 3D x,y,z coordinates of the element at position 1 is -0.0831, -1.588, -0.3056, . The 3D x,y,z coordinates of the element at position 2 is -3.4296, 1.0108,

This compound's CID is 11688 and compound's name is Megestrol Acetate. There are 66 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 27, double bond between 2 and 19, double bond between 3 and 25, double bond between 4 and 27, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 29, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 19, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 32, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 34, single bond between attom at postion 11 and 35, single bond between attom at postion 12 and 36, single bond between attom at postion 12 and 37, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 21, single bond between attom at postion 14 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, double bond between 16 and 20, single bond between attom at postion 16 and 43, single bond between attom at postion 17 and 20, double bond between 17 and 23, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 24, single bond between attom at postion 20 and 26, single bond between attom at postion 21 and 46, single bond between attom at postion 21 and 47, single bond between attom at postion 21 and 48, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 49, single bond between attom at postion 22 and 50, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 51, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 26 and 55, single bond between attom at postion 26 and 56, single bond between attom at postion 26 and 57, single bond between attom at postion 27 and 28, single bond between attom at postion 28 and 58, single bond between attom at postion 28 and 59, single bond between attom at postion 28 and This compound's CID is 12035 and compound's name is Acetylcysteine. There are 19 attoms in the molecule and their positions in the order are S, O, O, O, N, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 19, double bond between 3 and 8, double bond between 4 and 9, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 9 and 10, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 17. The 3D x,y,z coordinates of the element at position 1 is -1.408, 2.1982, -1.044, . The 3D x,y,z coordinates of the element at position 2 is -1.3703, -1.5653, -0.973, . The 3D x,y,z coordinates of the element at

This compound's CID is 13109 and compound's name is Norgestrel. There are 51 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 47, double bond between 2 and 22, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 14, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 25, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 26, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 27, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 29, single bond between attom at postion 9 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, double bond between 16 and 21, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, triple bond between 19 and 23, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 50, single bond between attom at postion 23 and 51. The 3D x,y,z coordinates of the element at position 1 is 4.6433, -0.7052, -

This compound's CID is 13791 and compound's name is Estradiol Valerate. There are 58 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 20, double bond between 2 and 20, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 53, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 27, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 28, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 37, single bond between attom at postion 12 and 38, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 39, single bond between attom at postion 13 and 40, single bond between attom at postion 14 and 41, single bond between attom at postion 14 and 42, single bond between attom at postion 14 and 43, double bond between 15 and 17, single bond between attom at postion 15 and 18, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 44, single bond between attom at postion 16 and 45, single bond between attom at postion 17 and 19, double bond between 18 and 21, single bond between attom at postion 18 and 46, double bond between 19 and 22, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 23, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 48, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 49, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 51, single bond between attom at postion 24 and 52, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 26 and 56, single bond between attom at postion 26 and 57, single bond between attom at postion 26 and 58. The 3D x,y,z coordinates of the element at position 1 is 3.2264,
This compound's CID is 13842 and compound's name is (Hydroxymethyl)urea. There are 12 attoms in the molecule and their positions in the order are O, O, N, N, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 12, double bond between 2 and 6, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8. The 3D x,y,z coordinates of the element at position 1 is 2.2169, 0.1217, -0.6231, . The 3D x,y,z coordinates of the element at position 2 is -0.9633, 1.3089, 0.0859, . The 3D x,y,z coordinates of the
This compound's CID is 14917 and compound's name is Hydrofluoric Acid. There are 2 attoms in the molecule and their positions in the order are X, H. The bonds between them are: single bond between attom at postion 1 and 2. The 3D x,y,z coordinates of the element at position 1 is 0.0, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 0.4358, -0.1477, -0.8188. There are 0 chiral atoms (stereocenters), 0 chiral centers, 0 undefined chiral centers,

This compound's CID is 15459 and compound's name is Metaxalone. There are 31 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 9, double bond between 3 and 8, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 22, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 17, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 19, single bond between attom at postion 7 and 20, single bond between attom at postion 7 and 21, double bond between 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 23, double bond between 11 and 13, single bond between attom at postion 11 and 24, double bond between 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 16, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 26, single bond between attom at postion 15 and 27, single bond between attom at postion 15 and 28, single bond between attom at postion 16 and 29, single bond between attom at postion 16 and 30, single bond between attom at postion 16 and 31. The 3D x,y,z coordinates of the element at position 1 is -2.6201, 0.932, -0.2804, . The 3D x,y,z coordinates of the element at position 2 is -0.1533, -0.0033, -1.3256, . The 3D x,y,z coordinates of the element at This compound's CID is 16078 and compound's name is Dronabinol. There are 53 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 46, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 24, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 25, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 26, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 11, double bond between 7 and 14, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 28, single bond between attom at postion 8 and 29, double bond between 9 and 10, single bond between attom at postion 9 and 30, single bond between attom at postion 10 and 16, double bond between 11 and 15, single bond between attom at postion 12 and 31, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, double bond between 17 and 18, single bond between attom at postion 17 and 19, single bond between attom at postion 18 and 41, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 42, single bond between attom at postion 19 and 43, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 44, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 47, single bond between attom at postion 21 and 48, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 49, single bond between attom at postion 22 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 23 and 52, single bond between attom at postion 23 and 53. The 3D x,y,z coordinates of the element at position 1 is -0.5787, -1.9919, 0.499, . The 3D x,y,z coordinates of the element at position 2 is -0.3951, 2.6957, -

This compound's CID is 16333 and compound's name is Betamethasone Valerate. There are 71 atoms in the molecule and their positions in the order are X, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 29, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 57, double bond between 4 and 22, single bond between attom at postion 5 and 27, single bond between attom at postion 5 and 64, double bond between 6 and 29, double bond between 7 and 30, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 35, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 18, single bond between attom at postion 10 and 36, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 22, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 23, single bond between attom at postion 15 and 41, single bond between attom at postion 16 and 42, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 24, single bond between attom at postion 17 and 25, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 19 and 45, single bond between attom at postion 19 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, double bond between 21 and 26, single bond between attom at postion 22 and 27, single bond between attom at postion 23 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 23 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 24 and 55, double bond between 25 and 28, single bond between attom at postion 25 and 56, single bond between attom at postion 26 and 30, single bond between attom at postion 26 and 58, single bond between attom at postion 27 and 59, single bond between attom at postion 27 and 60, single bond between attom at postion 28 and 30, single bond between attom at postion 28 and 61, single bond between attom at

This compound's CID is 16666 and compound's name is l-Menthol. There are 31 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 31, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 12, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 20, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 10 and 27, single bond between attom at postion 11 and 28, single bond between attom at postion 11 and 29, single bond between attom at postion 11 and 30. The 3D x,y,z coordinates of the element at position 1 is 0.4167, 2.3656, 0.4212, . The 3D x,y,z coordinates of the element at position 2 is 0.7056, -0.0351, 0.4283, . The 3D x,y,z
This compound's CID is 20279 and compound's name is Cladribine. There are 31 attoms in the molecule and their positions in the order are CL, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 13, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 28, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 29, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 16, double bond between 6 and 16, single bond between attom at postion 6 and 17, double bond between 7 and 15, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 18, double bond between 8 and 19, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 30, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 22, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 15 and 17, single bond between attom at postion 16 and 27, double bond between 17 and 18. The 3D x,y,z coordinates of the element at position 1 is 1.633, 3.3744, 0.3086, . The 3D x,y,z coordinates of the element at position 2 is -1.7996,

This compound's CID is 21700 and compound's name is Beclomethasone Dipropionate. There are 75 atoms in the molecule and their positions in the order are CL, O, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 30, single bond between attom at postion 3 and 17, single bond between attom at postion 3 and 59, double bond between 4 and 23, single bond between attom at postion 5 and 28, single bond between attom at postion 5 and 34, double bond between 6 and 30, double bond between 7 and 31, double bond between 8 and 34, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 37, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 19, single bond between attom at postion 11 and 38, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 24, single bond between attom at postion 16 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 25, single bond between attom at postion 18 and 26, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 45, single bond between attom at postion 19 and 46, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 50, single bond between attom at postion 21 and 51, double bond between 22 and 27, single bond between attom at postion 23 and 28, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 25 and 56, single bond between attom at postion 25 and 57, double bond between 26 and 29, single bond between attom at postion 26 and 58, single bond between attom at postion 27 and 31, single bond between attom at postion 27 and 60, single bond between attom at postion 28 and 61, single bond between attom at postion 28 and 62, single bond between attom at postion 29 and 31, single bond between attom at postion 29 and

This compound's CID is 21800 and compound's name is Betamethasone Dipropionate. There are 73 attoms in the molecule and their positions in the order are X, O, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 30, single bond between attom at postion 3 and 17, single bond between attom at postion 3 and 59, double bond between 4 and 23, single bond between attom at postion 5 and 28, single bond between attom at postion 5 and 34, double bond between 6 and 30, double bond between 7 and 31, double bond between 8 and 34, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 37, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 19, single bond between attom at postion 11 and 38, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 24, single bond between attom at postion 16 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 25, single bond between attom at postion 18 and 26, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 45, single bond between attom at postion 19 and 46, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 50, single bond between attom at postion 21 and 51, double bond between 22 and 27, single bond between attom at postion 23 and 28, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 25 and 56, single bond between attom at postion 25 and 57, double bond between 26 and 29, single bond between attom at postion 26 and 58, single bond between attom at postion 27 and 31, single bond between attom at postion 27 and 60, single bond between attom at postion 28 and 61, single bond between attom at postion 28 and 62, single bond between attom at postion 29 and 31, single bond between attom at postion 29 and

This compound's CID is 22571 and compound's name is Octocrylene. There are 54 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 12, double bond between 2 and 12, triple bond between 3 and 21, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 28, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 29, single bond between attom at postion 5 and 30, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 31, single bond between attom at postion 6 and 32, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 33, single bond between attom at postion 7 and 34, single bond between attom at postion 8 and 35, single bond between attom at postion 8 and 36, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 37, single bond between attom at postion 9 and 38, single bond between attom at postion 10 and 39, single bond between attom at postion 10 and 40, single bond between attom at postion 10 and 41, single bond between attom at postion 11 and 42, single bond between attom at postion 11 and 43, single bond between attom at postion 11 and 44, single bond between attom at postion 12 and 13, double bond between 13 and 14, single bond between attom at postion 13 and 21, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 16, double bond between 15 and 17, single bond between attom at postion 15 and 19, double bond between 16 and 18, single bond between attom at postion 16 and 20, single bond between attom at postion 17 and 22, single bond between attom at postion 17 and 45, single bond between attom at postion 18 and 23, single bond between attom at postion 18 and 46, double bond between 19 and 24, single bond between attom at postion 19 and 47, double bond between 20 and 25, single bond between attom at postion 20 and 48, double bond between 22 and 26, single bond between attom at postion 22 and 49, double bond between 23 and 27, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 51, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 52, single bond between attom at postion 26 and 53, single bond between attom at postion 27 and 54. The 3D x,y,z coordinates of the element at position 1 is 1.0866, 0.8012, 0.5469, . The 3D x,y,z coordinates of the element at position 2 is 0.255, 0.3423, 2.6499, . The 3D x,y,z coordinates of the element at position 3 is -1.924, 3.5392, 0.9979, This compound's CID is 24261 and compound's name is Silicon Dioxide. There are 3 attoms in the molecule and their positions in the order are Si, O, O. The bonds between them are: double bond between 1 and 2, double bond between 1 and 3. The 3D x,y,z coordinates of the element at position 1 is 0.0, -0.5548, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 1.2172, 0.2774, 0.0, . The 3D x,y,z coordinates of the element at position 3 is -1.2171, This compound's CID is 24408 and compound's name is Bromine. There are 2 attoms in the molecule and their positions in the order are Br, Br. The bonds between them are: single bond between attom at postion 1 and 2. The 3D x,y,z coordinates of the element at position 1 is -1.146, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 1.146, 0.0, 0.0. There are 0 chiral atoms (stereocenters), 0 chiral centers, 0 undefined chiral centers, 0 chiral This compound's CID is 24526 and compound's name is Chlorine. There are 2 attoms in the molecule and their positions in the order are CL, CL. The bonds between them are: single bond between attom at postion 1 and 2. The 3D x,y,z coordinates of the element at position 1 is -1.0061, 0.0, 0.0, . The 3D x,y,z coordinates of the element at position 2 is 1.0061, 0.0, 0.0. There are 0 chiral atoms (stereocenters), 0 chiral centers, 0 undefined chiral centers, 0

This compound's CID is 26133 and compound's name is Hydrocortisone Butyrate. There are 67 attoms in the molecule and their positions in the order are O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 28, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 56, double bond between 3 and 23, single bond between attom at postion 4 and 27, single bond between attom at postion 4 and 62, double bond between 5 and 26, double bond between 6 and 28, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 32, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 23, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 35, single bond between attom at postion 12 and 36, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 22, single bond between attom at postion 14 and 37, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 38, single bond between attom at postion 15 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 16 and 41, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 20, double bond between 19 and 25, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 49, single bond between attom at postion 21 and 50, single bond between attom at postion 22 and 51, single bond between attom at postion 22 and 52, single bond between attom at postion 22 and 53, single bond between attom at postion 23 and 27, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 54, single bond between attom at postion 24 and 55, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 57, single bond between attom at postion 27 and 58, single bond between attom at postion 27 and 59, single bond between attom at postion 28 and 29, single bond between attom at

This compound's CID is 26757 and compound's name is Selegiline. There are 31 attoms in the molecule and their positions in the order are N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 7, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 15, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 17, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 19, single bond between attom at postion 4 and 20, double bond between 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 22, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 26, double bond between 9 and 11, single bond between attom at postion 9 and 27, double bond between 10 and 12, single bond between attom at postion 10 and 28, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 29, single bond between attom at postion 12 and 30, triple bond between 13 and 14, single bond between attom at postion 14 and 31. The 3D x,y,z coordinates of the element at position 1 is -2.0759, -0.1101, -0.2416, . The 3D x,y,z coordinates of the element at position 2 is -0.7117, 0.1461, 0.2301, . The 3D x,y,z coordinates of the element at position 3 is 0.2983, -0.4049, -0.7929, . The 3D x,y,z coordinates This compound's CID is 27661 and compound's name is Isosorbide Mononitrate. There are 22 attoms in the molecule and their positions in the order are O, O, O, O, O, O, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 12, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 13, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 22, single bond between attom at postion 5 and 7, double bond between 6 and 7, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 13 and 20, single bond between attom at postion 13 and 21. The 3D x,y,z coordinates of the element at position 1 is -1.4908, -1.7744, -0.0017, . The 3D x,y,z coordinates of the element at position 2 is -

This compound's CID is 28417 and compound's name is Danazol. There are 52 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 50, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 23, double bond between 3 and 24, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 26, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 29, single bond between attom at postion 9 and 30, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 17, double bond between 15 and 21, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 16 and 41, single bond between attom at postion 17 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 19 and 48, triple bond between 20 and 25, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 49, double bond between 22 and 23, single bond between attom at postion 22 and 24, single bond between attom at postion 24 and 51, single bond between attom at postion 25 and 52. The 3D x,y,z coordinates of the element at position 1 is 5.2669, -0.9766, -0.7049, . The 3D x,y,z coordinates of

This compound's CID is 30751 and compound's name is Fludarabine Phosphate. There are 37 attoms in the molecule and their positions in the order are P, X, O, O, O, O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 8, double bond between 1 and 9, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 17, single bond between attom at postion 3 and 18, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 31, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 32, single bond between attom at postion 6 and 19, single bond between attom at postion 7 and 36, single bond between attom at postion 8 and 37, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21, double bond between 11 and 21, single bond between attom at postion 11 and 22, double bond between 12 and 20, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 23, double bond between 13 and 24, single bond between attom at postion 14 and 23, single bond between attom at postion 14 and 34, single bond between attom at postion 14 and 35, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 25, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 26, single bond between attom at postion 17 and 27, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 28, single bond between attom at postion 19 and 29, single bond between attom at postion 19 and 30, single bond between attom at postion 20 and 22, single bond between attom at postion 21 and 33, double bond between 22 and 23. The 3D x,y,z coordinates of the element at position 1 is 3.4324, 1.9535, 0.2623, . The 3D x,y,z coordinates of the element at position 2 is -0.3683, 3.0519, -0.5428, . The 3D x,y,z
This compound's CID is 31236 and compound's name is Phenoxyethanol. There are 20 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 4, single bond between attom at postion 2 and 5, single bond between attom at postion 2 and 20, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 12, double bond between 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 15, double bond between 7 and 9, single bond between attom at postion 7 and 16, double bond between 8 and 10, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 19. The 3D x,y,z coordinates of the element at position 1 is 1.0591, -0.3353, 0.2678, . The 3D x,y,z coordinates of the element at position 2 is 3.8513, -0.4617, 0.451, . The 3D x,y,z coordinates of the element at position 3 is 1.8807, 0.7397, -

This compound's CID is 31401 and compound's name is Ursodiol. There are 68 attoms in the molecule and their positions in the order are O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 1 and 61, single bond between attom at postion 2 and 24, single bond between attom at postion 2 and 65, single bond between attom at postion 3 and 28, single bond between attom at postion 3 and 68, double bond between 4 and 28, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 29, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 19, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 21, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 16 and 41, single bond between attom at postion 16 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 23, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 19 and 49, single bond between attom at postion 20 and 25, single bond between attom at postion 20 and 26, single bond between attom at postion 20 and 50, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 51, single bond between attom at postion 21 and 52, single bond between attom at postion 22 and 53, single bond between attom at postion 22 and 54, single bond between attom at postion 22 and 55, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 56, single bond between attom at postion 23 and

This compound's CID is 32758 and compound's name is Globetasol Propionate. There are 64 atoms in the molecule and their positions in the order are CL, X, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 27, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 29, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 55, double bond between 5 and 22, double bond between 6 and 29, double bond between 7 and 30, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 18, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 22, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 23, single bond between attom at postion 15 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 24, single bond between attom at postion 17 and 25, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 41, single bond between attom at postion 18 and 42, single bond between attom at postion 19 and 43, single bond between attom at postion 19 and 44, single bond between attom at postion 19 and 45, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 46, single bond between attom at postion 20 and 47, double bond between 21 and 26, single bond between attom at postion 22 and 27, single bond between attom at postion 23 and 48, single bond between attom at postion 23 and 49, single bond between attom at postion 23 and 50, single bond between attom at postion 24 and 51, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, double bond between 25 and 28, single bond between attom at postion 25 and 54, single bond between attom at postion 26 and 30, single bond between attom at postion 26 and 56, single bond between attom at postion 27 and 57, single bond between attom at postion 27 and 58, single bond between attom at postion 28 and 30, single bond between attom at postion 28 and 59, single bond between attom at postion 29 and 31, single bond between attom at postion 31 and 32, single bond

This compound's CID is 34312 and compound's name is Oxcarbazepine. There are 31 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 10, double bond between 2 and 15, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 15, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 30, single bond between attom at postion 4 and 31, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, double bond between 5 and 11, double bond between 6 and 12, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 20, single bond between attom at postion 7 and 21, single bond between attom at postion 8 and 9, double bond between 8 and 13, single bond between attom at postion 9 and 10, double bond between 9 and 14, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 19, single bond between attom at postion 14 and 25, double bond between 16 and 17, single bond between attom at postion 16 and 26, single bond between attom at postion 17 and 27, double bond between 18 and 19, single bond between attom at postion 18 and 28, single bond between attom at postion 19 and 29. The 3D x,y,z coordinates of the element at position 1 is 1.096, -3.0625, -1.0128, . The 3D x,y,z coordinates of the element at position 2 is 0.7617, 3.0768, -1.044, . The 3D x,y,z coordinates of the element at
This compound's CID is 35370 and compound's name is Zidovudine. There are 32 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 14, single bond between attom at postion 2 and 29, double bond between 3 and 16, double bond between 4 and 18, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 16, double bond between 6 and 8, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 28, double bond between 8 and 9, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 22, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 25, single bond between attom at postion 14 and 26, double bond between 15 and 17, single bond between attom at postion 15 and 27, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 19, single bond between attom at postion 19 and 30, single bond between attom at postion 19 and 31, single bond between attom at postion 19 and 32. The 3D x,y,z coordinates of the element at position 1 is 0.9179, 0.5315, 1.0162, . The 3D x,y,z coordinates of the element at position 2 is 1.434, 3.2516, 0.6483,

This compound's CID is 36294 and compound's name is Tobramycin. There are 69 attoms in the molecule and their positions in the order are O, O, O, O, O, O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 1 and 21, single bond between attom at postion 2 and 16, single bond between attom at postion 2 and 22, single bond between attom at postion 3 and 17, single bond between attom at postion 3 and 55, single bond between attom at postion 4 and 21, single bond between attom at postion 4 and 27, single bond between attom at postion 5 and 22, single bond between attom at postion 5 and 30, single bond between attom at postion 6 and 23, single bond between attom at postion 6 and 64, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 65, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 66, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 69, single bond between attom at postion 10 and 18, single bond between attom at postion 10 and 49, single bond between attom at postion 10 and 50, single bond between attom at postion 11 and 19, single bond between attom at postion 11 and 51, single bond between attom at postion 11 and 52, single bond between attom at postion 12 and 24, single bond between attom at postion 12 and 60, single bond between attom at postion 12 and 61, single bond between attom at postion 13 and 25, single bond between attom at postion 13 and 62, single bond between attom at postion 13 and 63, single bond between attom at postion 14 and 32, single bond between attom at postion 14 and 67, single bond between attom at postion 14 and 68, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 33, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 19, single bond between attom at postion 16 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 36, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 37, single bond between attom at postion 20 and 38, single bond between attom at postion 20 and 39, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 40, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 41, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 42, single bond between attom at postion 24 and 28, single bond between attom at postion 24 and 43, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 44, single bond between attom at postion 26 and 27, single bond between attom at postion 26 and 45, single bond between attom at postion 27 and 31, single bond between attom at postion 27 and 46, single bond

This compound's CID is 36462 and compound's name is Etoposide. There are 74 attoms in the molecule and their positions in the order are O, O, O, O, O, O, O, O, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 1 and 22, single bond between attom at postion 2 and 20, single bond between attom at postion 2 and 21, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 27, single bond between attom at postion 4 and 25, single bond between attom at postion 4 and 35, double bond between 5 and 21, single bond between attom at postion 6 and 24, single bond between attom at postion 6 and 61, single bond between attom at postion 7 and 30, single bond between attom at postion 7 and 35, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 62, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 38, single bond between attom at postion 10 and 32, single bond between attom at postion 10 and 38, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 41, single bond between attom at postion 12 and 37, single bond between attom at postion 12 and 42, single bond between attom at postion 13 and 39, single bond between attom at postion 13 and 68, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 20, single bond between attom at postion 14 and 43, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 21, single bond between attom at postion 15 and 44, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 45, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 23, single bond between attom at postion 17 and 46, single bond between attom at postion 18 and 19, double bond between 18 and 28, double bond between 19 and 29, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 49, double bond between 23 and 33, single bond between attom at postion 23 and 34, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 50, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 51, single bond between attom at postion 26 and 52, single bond between attom at postion 27 and 30, single bond between attom at postion 27 and 53, single bond between attom at postion 28 and 31, single bond between attom at postion 28 and 54, single bond between attom at postion 29 and 32, single bond between attom at postion 29 and 55, single bond between attom at postion 30 and 56, single bond between attom at postion 30 and 57, double bond between 31 and 32, single bond between attom at postion 33 and This compound's CID is 37542 and compound's name is Ribavirin. There are 29 attoms in the molecule and their positions in the order are O, O, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 27, double bond between 5 and 17, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 15, double bond between 7 and 16, double bond between 8 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 20, single bond between attom at postion 13 and 21, single bond between attom at postion 14 and 22, single bond between attom at postion 14 and 23, single bond between attom at postion 15 and 26, single bond between attom at postion 16 and 17. The 3D x,y,z coordinates of the element at position 1 is 1.3923, -0.5531, -1.0023, . The 3D x,y,z coordinates of the element at position 2 is 1.888, 2.3434,

This compound's CID is 37768 and compound's name is Amikacin. There are 83 attoms in the molecule and their positions in the order are O, O, O, O, O, O, O, O, O, O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 1 and 25, single bond between attom at postion 2 and 20, single bond between attom at postion 2 and 26, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 59, single bond between attom at postion 4 and 25, single bond between attom at postion 4 and 32, single bond between attom at postion 5 and 26, single bond between attom at postion 5 and 34, single bond between attom at postion 6 and 27, single bond between attom at postion 6 and 69, single bond between attom at postion 7 and 29, single bond between attom at postion 7 and 70, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 71, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 72, single bond between attom at postion 10 and 33, single bond between attom at postion 10 and 73, double bond between 11 and 35, single bond between attom at postion 12 and 36, single bond between attom at postion 12 and 78, single bond between attom at postion 13 and 38, single bond between attom at postion 13 and 79, single bond between attom at postion 14 and 21, single bond between attom at postion 14 and 35, single bond between attom at postion 14 and 50, single bond between attom at postion 15 and 23, single bond between attom at postion 15 and 54, single bond between attom at postion 15 and 55, single bond between attom at postion 16 and 28, single bond between attom at postion 16 and 66, single bond between attom at postion 16 and 67, single bond between attom at postion 17 and 37, single bond between attom at postion 17 and 76, single bond between attom at postion 17 and 77, single bond between attom at postion 18 and 40, single bond between attom at postion 18 and 82, single bond between attom at postion 18 and 83, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 41, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 42, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 43, single bond between attom at postion 22 and 44, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 45, single bond between attom at postion 24 and 46, single bond between attom at postion 24 and 47, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 48, single bond between attom at postion 26 and 29, single bond between attom at postion 26 and 49, single bond between attom at postion 27 and 28, single bond between attom at postion 27 and 51, single bond between attom at postion 28 and

This compound's CID is 39147 and compound's name is Nadolol. There are 49 attoms in the molecule and their positions in the order are O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 38, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 39, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 17, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 49, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 33, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 23, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 24, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, double bond between 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 11 and 14, double bond between 12 and 18, single bond between attom at postion 13 and 20, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 22, double bond between 14 and 19, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 30, single bond between attom at postion 16 and 31, single bond between attom at postion 16 and 32, single bond between attom at postion 17 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 36, single bond between attom at postion 19 and 37, single bond between attom at postion 20 and 40, single bond between attom at postion 20 and 41, single bond between attom at postion 20 and 42, single bond between attom at postion 21 and 43, single bond between attom at postion 21 and 44, single bond between attom at postion 21 and 45, single bond between attom at postion 22 and 46, single bond between attom at postion 22 and 47, single bond between attom at postion 22 and 48. The 3D x,y,z coordinates of the element at position 1 is -0.9271, -3.2972, 1.0267, . The 3D x,y,z coordinates of the element at position 2 is -2.3839, -2.5948, -

This compound's CID is 40632 and compound's name is Pirfenidone. There are 25 attoms in the molecule and their positions in the order are O, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 6, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 6, double bond between 3 and 9, single bond between attom at postion 3 and 10, double bond between 4 and 5, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 8, double bond between 7 and 8, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 18, double bond between 10 and 13, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 20, single bond between attom at postion 11 and 21, single bond between attom at postion 11 and 22, double bond between 12 and 14, single bond between attom at postion 12 and 23, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 25. The 3D x,y,z coordinates of the element at position 1 is 0.3145, 2.4122, -0.3762, . The 3D x,y,z coordinates of the element at position 2 is 0.3897, 0.0736, -0.003, . The 3D x,y,z coordinates of the element at

This compound's CID is 41693 and compound's name is Sufentanil. There are 57 attoms in the molecule and their positions in the order are S, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 1 and 27, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 20, double bond between 3 and 14, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 38, single bond between attom at postion 12 and 39, double bond between 13 and 17, single bond between attom at postion 13 and 18, single bond between attom at postion 14 and 16, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 16 and 21, single bond between attom at postion 16 and 42, single bond between attom at postion 16 and 43, single bond between attom at postion 17 and 22, single bond between attom at postion 17 and 44, double bond between 18 and 23, single bond between attom at postion 18 and 45, double bond between 19 and 24, single bond between attom at postion 20 and 46, single bond between attom at postion 20 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 49, single bond between attom at postion 21 and 50, single bond between attom at postion 21 and 51, double bond between 22 and 25, single bond between attom at postion 22 and 52, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 53, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 54, single bond between attom at postion 25 and 55, double bond between 26 and 27, single bond between attom at postion 26 and 56, single bond between attom at postion 27 and 57. The 3D x,y,z coordinates of the element at position 1 is -6.6212, -0.828, -1.2347, . The 3D x,y,z

This compound's CID is 41781 and compound's name is Torsemide. There are 44 attoms in the molecule and their positions in the order are S, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, double bond between 1 and 3, single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 10, double bond between 4 and 15, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 26, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 28, double bond between 8 and 16, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 25, double bond between 10 and 11, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 18, double bond between 12 and 20, single bond between attom at postion 13 and 29, single bond between attom at postion 13 and 30, single bond between attom at postion 13 and 31, single bond between attom at postion 14 and 32, single bond between attom at postion 14 and 33, single bond between attom at postion 14 and 34, single bond between attom at postion 16 and 35, double bond between 17 and 21, single bond between attom at postion 17 and 36, double bond between 18 and 19, single bond between attom at postion 18 and 37, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 24, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 38, single bond between attom at postion 21 and 39, double bond between 22 and 23, single bond between attom at postion 22 and 40, single bond between attom at postion 23 and 41, single bond between attom at postion 24 and 42, single bond between attom at postion 24 and 43, single bond between attom at postion 24 and 44. The 3D x,y,z coordinates of the element at position 1 is 1.4943, -1.6191, 1.4458, . The 3D x,y,z coordinates of the element at position 2 is 2.7815, -2.2857, 1.4048, . The 3D x,y,z

This compound's CID is 42113 and compound's name is Desflurane. There are 12 attoms in the molecule and their positions in the order are X, X, X, X, X, X, O, C, C, C, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 9, single bond between attom at postion 3 and 9, single bond between attom at postion 4 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 10 and 12. The 3D x,y,z coordinates of the element at position 1 is 0.2057, -1.5419, 0.6357, . The 3D x,y,z coordinates of the element at position 2 is 1.6754, 1.2532, -0.9049, . The 3D x,y,z coordinates of the

This compound's CID is 44093 and compound's name is Captopril. There are 29 attoms in the molecule and their positions in the order are S, O, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 29, double bond between 2 and 10, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 28, double bond between 4 and 12, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 15, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 11, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 22, single bond between attom at postion 13 and 23, single bond between attom at postion 13 and 24, single bond between attom at postion 14 and 25, single bond between attom at postion 14 and 26, single bond between attom at postion 14 and 27. The 3D x,y,z coordinates of the element at position 1 is -3.5125, 0.2892, 1.7967, . The 3D x,y,z coordinates of the element at position 2 is -0.9991, 1.5602, 0.2378, . The 3D x,y,z coordinates of the element at

This compound's CID is 47576 and compound's name is Ketoconazole. There are 64 attoms in the molecule and their positions in the order are CL, CL, O, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 22, single bond between attom at postion 2 and 34, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 13, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 24, double bond between 6 and 25, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 21, single bond between attom at postion 8 and 19, single bond between attom at postion 8 and 20, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, double bond between 10 and 29, single bond between attom at postion 10 and 35, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 15, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 13 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 14 and 41, double bond between 15 and 22, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 42, single bond between attom at postion 16 and 43, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 44, single bond between attom at postion 17 and 45, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 46, single bond between attom at postion 18 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 19 and 49, single bond between attom at postion 20 and 50, single bond between attom at postion 20 and 51, double bond between 21 and 26, single bond between attom at postion 21 and 27, single bond between attom at postion 22 and 32, double bond between 23 and 33, single bond between attom at postion 23 and 52, double bond between 24 and 30, single bond between attom at postion 24 and 31, single bond between attom at postion 25 and 36, single bond between attom at postion 26 and 30, single bond between attom at postion 26 and 53, double bond between 27 and 31, single bond between attom at postion 27 and 54, double bond between 28 and 35, single bond between attom at postion 28 and 55, single bond between attom at postion 29 and 56, single bond between attom at postion 30 and 57, single bond between attom at postion 31 and 58, double bond between 32 and 34, single bond between attom at postion 32 and 59, single bond between attom at postion 33 and 34, single bond between attom at

This compound's CID is 51040 and compound's name is Avobenzone. There are 45 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 14, double bond between 2 and 16, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, double bond between 5 and 9, single bond between attom at postion 5 and 10, single bond between attom at postion 6 and 24, single bond between attom at postion 6 and 25, single bond between attom at postion 6 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 8 and 32, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 33, double bond between 10 and 13, single bond between attom at postion 10 and 34, double bond between 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 15, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 37, single bond between attom at postion 15 and 38, single bond between attom at postion 16 and 17, double bond between 17 and 18, single bond between attom at postion 17 and 19, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 39, double bond between 19 and 21, single bond between attom at postion 19 and 40, double bond between 20 and 22, single bond between attom at postion 20 and 41, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 42, single bond between attom at postion 23 and 43, single bond between attom at postion 23 and 44, single bond between attom at postion 23 and 45. The 3D x,y,z coordinates of the element at position 1 is -0.4151, 2.5485, 0.4235, . The 3D x,y,z coordinates of the element at position 2 is 2.0774, 2.4614, -0.7022, . The 3D x,y,z coordinates of the element at position 3 is 6.5843, -

This compound's CID is 53232 and compound's name is Lovastatin. There are 65 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 23, single bond between attom at postion 2 and 19, single bond between attom at postion 2 and 26, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 59, double bond between 4 and 23, double bond between 5 and 26, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 30, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 31, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 32, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, double bond between 11 and 14, single bond between attom at postion 11 and 17, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 36, single bond between attom at postion 12 and 37, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 20, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, double bond between 16 and 17, single bond between attom at postion 16 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 20 and 50, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 51, single bond between attom at postion 21 and 52, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 53, single bond between attom at postion 23 and 25, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 54, single bond between attom at postion 24 and 55, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 28, single bond between attom at postion 25 and 56, single bond between attom at postion 27 and 29, single bond between attom at postion 27 and 57, single bond between attom at postion 27 and 58, single bond between attom at postion 28 and

This compound's CID is 54454 and compound's name is Simvastatin. There are 68 attoms in the molecule and their positions in the order are O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 22, single bond between attom at postion 2 and 19, single bond between attom at postion 2 and 26, single bond between attom at postion 3 and 23, single bond between attom at postion 3 and 65, double bond between 4 and 22, double bond between 5 and 26, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 31, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 32, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 33, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 34, double bond between 10 and 14, single bond between attom at postion 10 and 17, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 37, single bond between attom at postion 12 and 38, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 20, single bond between attom at postion 13 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, double bond between 16 and 17, single bond between attom at postion 16 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 18 and 47, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 20 and 50, single bond between attom at postion 20 and 51, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 52, single bond between attom at postion 21 and 53, single bond between attom at postion 22 and 24, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 54, single bond between attom at postion 24 and 27, single bond between attom at postion 24 and 28, single bond between attom at postion 24 and 29, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 55, single bond between attom at postion 25 and 56, single bond between attom at postion 27 and 30, single bond between attom at postion 27 and 57, single bond between attom at postion 27 and 58, single bond between attom at postion 28 and

This compound's CID is 54746 and compound's name is Cabergoline. There are 70 attoms in the molecule and their positions in the order are O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 18, double bond between 2 and 26, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 13, single bond between attom at postion 3 and 17, single bond between attom at postion 4 and 19, single bond between attom at postion 4 and 21, single bond between attom at postion 4 and 47, single bond between attom at postion 5 and 18, single bond between attom at postion 5 and 25, single bond between attom at postion 5 and 26, single bond between attom at postion 6 and 26, single bond between attom at postion 6 and 30, single bond between attom at postion 6 and 59, single bond between attom at postion 7 and 29, single bond between attom at postion 7 and 31, single bond between attom at postion 7 and 32, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 34, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 35, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 36, single bond between attom at postion 10 and 37, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 38, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 39, single bond between attom at postion 12 and 40, single bond between attom at postion 13 and 41, single bond between attom at postion 13 and 42, double bond between 14 and 15, single bond between attom at postion 14 and 20, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 19, double bond between 16 and 21, single bond between attom at postion 17 and 24, single bond between attom at postion 17 and 43, single bond between attom at postion 17 and 44, double bond between 19 and 22, double bond between 20 and 23, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 46, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 48, single bond between attom at postion 23 and 49, double bond between 24 and 28, single bond between attom at postion 24 and 50, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 51, single bond between attom at postion 25 and 52, single bond between attom at postion 27 and 29, single bond between attom at postion 27 and 53, single bond between attom at postion 27 and 54, single bond between attom at postion 28 and 55, single bond between attom at postion 28 and 56, single bond between attom at postion 29 and 57, single bond between attom at postion 29 and 58, single bond between attom at postion 30 and 33, single bond between attom at

This compound's CID is 55245 and compound's name is Mifepristone. There are 67 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 49, double bond between 2 and 25, single bond between attom at postion 3 and 29, single bond between attom at postion 3 and 31, single bond between attom at postion 3 and 32, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 33, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 34, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 35, single bond between attom at postion 8 and 36, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 37, single bond between attom at postion 9 and 38, single bond between attom at postion 10 and 40, single bond between attom at postion 10 and 41, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 39, double bond between 12 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 42, single bond between attom at postion 13 and 43, single bond between attom at postion 14 and 44, single bond between attom at postion 14 and 45, single bond between attom at postion 14 and 46, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 20, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 47, single bond between attom at postion 16 and 48, double bond between 17 and 23, single bond between attom at postion 17 and 24, double bond between 18 and 21, triple bond between 19 and 26, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 50, single bond between attom at postion 20 and 51, single bond between attom at postion 21 and 25, single bond between attom at postion 21 and 52, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 53, single bond between attom at postion 22 and 54, single bond between attom at postion 23 and 27, single bond between attom at postion 23 and 55, double bond between 24 and 28, single bond between attom at postion 24 and 56, single bond between attom at postion 26 and 30, double bond between 27 and 29, single bond between attom at postion 27 and 57, single bond between attom at postion 28 and 29, single bond between attom at postion 28 and 58, single bond between attom at postion 30 and

This compound's CID is 55283 and compound's name is itraconazole. There are 67 atoms in the molecule and their positions in the order are CL, CL, O, O, O, O, N, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 27, single bond between attom at postion 2 and 43, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 24, single bond between attom at postion 5 and 31, double bond between 6 and 44, single bond between attom at postion 7 and 18, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 20, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 41, single bond between attom at postion 10 and 36, single bond between attom at postion 10 and 44, single bond between attom at postion 10 and 47, double bond between 11 and 46, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 42, single bond between attom at postion 12 and 44, double bond between 13 and 41, single bond between attom at postion 13 and 46, double bond between 14 and 47, single bond between attom at postion 15 and 22, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 24, single bond between attom at postion 16 and 50, single bond between attom at postion 17 and 51, single bond between attom at postion 17 and 52, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 53, single bond between attom at postion 18 and 54, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 55, single bond between attom at postion 19 and 56, single bond between attom at postion 20 and 57, single bond between attom at postion 20 and 58, single bond between attom at postion 21 and 59, single bond between attom at postion 21 and 60, single bond between attom at postion 22 and 61, single bond between attom at postion 22 and 62, double bond between 23 and 27, single bond between attom at postion 23 and 28, single bond between attom at postion 24 and 63, single bond between attom at postion 24 and 64, double bond between 25 and 29, single bond between attom at postion 25 and 30, double bond between 26 and 32, single bond between attom at postion 26 and 33, single bond between attom at postion 27 and 39, double bond between 28 and 40, single bond between attom at postion 28 and 65, single bond between attom at postion 29 and 34, single bond between attom at postion 29 and 66, double bond between 30 and 35, single bond between attom at postion 30 and 67, double bond

This compound's CID is 56959 and compound's name is Ranolazine. There are 64 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 1 and 47, single bond between attom at postion 2 and 15, single bond between attom at postion 2 and 18, double bond between 3 and 16, single bond between attom at postion 4 and 23, single bond between attom at postion 4 and 31, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 48, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 32, single bond between attom at postion 8 and 33, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 34, single bond between attom at postion 9 and 35, single bond between attom at postion 10 and 36, single bond between attom at postion 10 and 37, single bond between attom at postion 11 and 38, single bond between attom at postion 11 and 39, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 40, single bond between attom at postion 12 and 41, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 42, single bond between attom at postion 13 and 43, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 44, single bond between attom at postion 15 and 45, single bond between attom at postion 15 and 46, double bond between 17 and 19, single bond between attom at postion 17 and 20, single bond between attom at postion 18 and 23, double bond between 18 and 26, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 24, double bond between 20 and 22, single bond between attom at postion 20 and 25, double bond between 21 and 27, single bond between attom at postion 21 and 49, single bond between attom at postion 22 and 27, single bond between attom at postion 22 and 50, double bond between 23 and 28, single bond between attom at postion 24 and 51, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 25 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 25 and 56, single bond between attom at postion 26 and 29, single bond between attom at postion 26 and 57, single bond between attom at postion 27 and 58, single bond between attom at postion 28 and 30, single bond between attom at postion 28 and 59, double bond between 29 and 30, single bond between attom at postion 29 and 60, single bond between attom at postion 30 and

This compound's CID is 57363 and compound's name is Finasteride. There are 63 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 21, double bond between 2 and 23, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 23, single bond between attom at postion 3 and 52, single bond between attom at postion 4 and 21, single bond between attom at postion 4 and 24, single bond between attom at postion 4 and 54, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 28, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 29, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 31, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, single bond between attom at postion 14 and 17, single bond between attom at postion 14 and 38, single bond between attom at postion 14 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 17 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 18 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 19 and 49, single bond between attom at postion 19 and 50, double bond between 20 and 22, single bond between attom at postion 20 and 51, single bond between attom at postion 22 and 23, single bond between attom at postion 22 and 53, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 27, single bond between attom at postion 25 and 55, single bond between attom at postion 25 and 56, single bond between attom at postion 25 and 57, single bond between attom at postion 26 and 58, single bond between attom at postion 26 and

This compound's CID is 57469 and compound's name is Imiquimod. There are 34 attoms in the molecule and their positions in the order are N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 5, single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 9, double bond between 2 and 10, single bond between attom at postion 3 and 13, double bond between 3 and 14, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 33, single bond between attom at postion 4 and 34, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 19, single bond between attom at postion 5 and 20, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 21, single bond between attom at postion 7 and 8, double bond between 7 and 9, single bond between attom at postion 8 and 13, double bond between 8 and 15, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 12 and 26, single bond between attom at postion 12 and 27, single bond between attom at postion 12 and 28, double bond between 13 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 29, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 30, double bond between 17 and 18, single bond between attom at postion 17 and 31, single bond between attom at postion 18 and 32. The 3D x,y,z coordinates of the element at position 1 is 1.5378, 0.3937, -0.6366, . The 3D x,y,z coordinates of the element at
This compound's CID is 59227 and compound's name is Rotigotine. There are 47 attoms in the molecule and their positions in the order are S, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 1 and 22, single bond between attom at postion 2 and 15, single bond between attom at postion 2 and 44, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 23, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 24, single bond between attom at postion 5 and 25, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 26, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 29, double bond between 8 and 9, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 36, single bond between attom at postion 13 and 37, double bond between 14 and 16, single bond between attom at postion 14 and 38, double bond between 15 and 17, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 40, double bond between 18 and 20, single bond between attom at postion 19 and 41, single bond between attom at postion 19 and 42, single bond between attom at postion 19 and 43, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 45, double bond between 21 and 22, single bond between attom at postion 21 and 46, single bond between attom at postion 22 and 47. The 3D x,y,z coordinates of the element at position 1 is -4.8756, -0.5824, 1.3179, . The 3D x,y,z coordinates of the element at position 2 is

This compound's CID is 60164 and compound's name is Adapalene. There are 93 atoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 1 and 21, single bond between attom at postion 2 and 31, single bond between attom at postion 2 and 59, double bond between 3 and 31, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 32, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 33, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 12, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 34, single bond between attom at postion 8 and 35, single bond between attom at postion 8 and 36, single bond between attom at postion 9 and 37, single bond between attom at postion 9 and 38, single bond between attom at postion 10 and 39, single bond between attom at postion 10 and 40, single bond between attom at postion 11 and 41, single bond between attom at postion 11 and 42, single bond between attom at postion 12 and 43, single bond between attom at postion 12 and 44, single bond between attom at postion 13 and 45, single bond between attom at postion 13 and 46, double bond between 14 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 15 and 18, double bond between 16 and 17, single bond between attom at postion 16 and 47, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 20, double bond between 18 and 19, single bond between attom at postion 18 and 48, single bond between attom at postion 19 and 49, double bond between 20 and 22, single bond between attom at postion 20 and 23, single bond between attom at postion 21 and 50, single bond between attom at postion 21 and 51, single bond between attom at postion 21 and 52, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 53, double bond between 23 and 25, single bond between attom at postion 23 and 54, double bond between 24 and 26, single bond between attom at postion 24 and 27, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 55, single bond between attom at postion 26 and 28, double bond between 27 and 29, single bond between attom at postion 27 and 56, double bond between 28 and 30, single bond between attom at postion 28 and 57, single bond between attom at postion 29 and 30, single bond between attom at postion 29 and 58, single bond between attom at postion 30 and

This compound's CID is 60198 and compound's name is Exemestane. There are 46 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 12, double bond between 2 and 22, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 23, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 28, single bond between attom at postion 8 and 29, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 11 and 16, single bond between attom at postion 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 13, single bond between attom at postion 13 and 34, single bond between attom at postion 13 and 35, single bond between attom at postion 14 and 36, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 16, double bond between 15 and 19, double bond between 16 and 21, single bond between attom at postion 17 and 39, single bond between attom at postion 17 and 40, single bond between attom at postion 17 and 41, double bond between 18 and 20, single bond between attom at postion 18 and 42, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 43, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 44, single bond between attom at postion 21 and 45, single bond between attom at postion 21 and 46. The 3D x,y,z coordinates of the element at position 1 is 5.0126, -1.1769, 0.7793, . The 3D x,y,z coordinates of the element at position 2 is -

This compound's CID is 60606 and compound's name is Clopidogrel. There are 37 attoms in the molecule and their positions in the order are CL, S, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 15, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 21, double bond between 4 and 14, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 22, single bond between attom at postion 6 and 23, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, double bond between 10 and 11, single bond between attom at postion 10 and 13, single bond between attom at postion 12 and 16, double bond between 12 and 17, double bond between 13 and 15, single bond between attom at postion 13 and 29, single bond between attom at postion 15 and 30, double bond between 16 and 18, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 31, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 32, double bond between 19 and 20, single bond between attom at postion 19 and 33, single bond between attom at postion 20 and 34, single bond between attom at postion 21 and 35, single bond between attom at postion 21 and 36, single bond between attom at postion 21 and 37. The 3D x,y,z coordinates of the element at position 1 is 3.1828, 0.3367, -2.3503, . The 3D x,y,z coordinates of the element at position 2 is -4.966, -0.039, 0.3676, . The 3D x,y,z coordinates of the element at position 3 is 1.4377, -

This compound's CID is 60700 and compound's name is Topotecan. There are 54 attoms in the molecule and their positions in the order are O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 43, double bond between 3 and 17, double bond between 4 and 20, single bond between attom at postion 5 and 28, single bond between attom at postion 5 and 54, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 17, double bond between 7 and 15, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 31, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 20, double bond between 10 and 13, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 15, double bond between 11 and 16, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 19, single bond between attom at postion 14 and 15, double bond between 14 and 21, single bond between attom at postion 16 and 34, single bond between attom at postion 18 and 25, single bond between attom at postion 18 and 35, single bond between attom at postion 18 and 36, single bond between attom at postion 19 and 37, single bond between attom at postion 19 and 38, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 39, double bond between 22 and 23, single bond between attom at postion 22 and 24, single bond between attom at postion 23 and 27, single bond between attom at postion 24 and 26, double bond between 24 and 28, single bond between attom at postion 25 and 40, single bond between attom at postion 25 and 41, single bond between attom at postion 25 and 42, single bond between attom at postion 26 and 44, single bond between attom at postion 26 and 45, double bond between 27 and 29, single bond between attom at postion 27 and 46, single bond between attom at postion 28 and 29, single bond between attom at postion 29 and 47, single bond between attom at postion 30 and 48, single bond between attom at postion 30 and 49, single bond between attom at postion 30 and 50, single bond between attom at postion 31 and 51, single bond between attom at postion 31 and 52, single bond between attom at postion 31 and 53. The 3D x,y,z coordinates of the element at position 1 is -5.8987, -1.0731,
This compound's CID is 60750 and compound's name is Gemcitabine. There are 29 attoms in the molecule and their positions in the order are X, X, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 24, single bond between attom at postion 5 and 14, single bond between attom at postion 5 and 26, double bond between 6 and 16, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 16, double bond between 8 and 18, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 20, single bond between attom at postion 13 and 21, single bond between attom at postion 14 and 22, single bond between attom at postion 14 and 23, double bond between 15 and 17, single bond between attom at postion 15 and 25, single bond between attom at postion 17 and 18, single bond between attom at postion 17 and 27. The 3D x,y,z coordinates of the element at position 1 is 0.3741, -1.9974, -1.0754, . The 3D x,y,z coordinates of the element at position 2 is 1.9988, -2.2753,

This compound's CID is 60795 and compound's name is Aripiprazole. There are 57 atoms in the molecule and their positions in the order are CL, CL, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 23, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 22, double bond between 4 and 30, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 12, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 30, single bond between attom at postion 7 and 57, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 31, single bond between attom at postion 8 and 32, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 33, single bond between attom at postion 9 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 10 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 11 and 38, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 39, single bond between attom at postion 12 and 40, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 41, single bond between attom at postion 13 and 42, double bond between 14 and 17, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 43, single bond between attom at postion 15 and 44, single bond between attom at postion 16 and 45, single bond between attom at postion 16 and 46, single bond between attom at postion 17 and 23, double bond between 18 and 24, single bond between attom at postion 18 and 47, single bond between attom at postion 19 and 20, double bond between 19 and 21, single bond between attom at postion 19 and 28, single bond between attom at postion 20 and 25, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 21 and 26, double bond between 22 and 26, single bond between attom at postion 22 and 29, double bond between 23 and 27, single bond between attom at postion 24 and 27, single bond between attom at postion 24 and 52, single bond between attom at postion 25 and 30, single bond between attom at postion 25 and 50, single bond between attom at postion 25 and 51, single bond between attom at postion 26 and 53, single bond between attom at postion 27 and 55, double bond between 28 and 29, single bond between attom at postion 28 and 54, single bond between attom at postion 29 and 56. The 3D x,y,z coordinates of the element at position 1 is -7.0404, 1.8323, -1.0756, . The 3D x,y,z coordinates of the element at position 2 is -10.0814, 0.8103, -

This compound's CID is 60823 and compound's name is Atorvastatin. There are 76 attoms in the molecule and their positions in the order are X, O, O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 33, single bond between attom at postion 2 and 16, single bond between attom at postion 2 and 61, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 67, double bond between 4 and 23, single bond between attom at postion 5 and 35, single bond between attom at postion 5 and 73, double bond between 6 and 35, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 23, single bond between attom at postion 8 and 34, single bond between attom at postion 8 and 64, single bond between attom at postion 9 and 12, double bond between 9 and 14, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 42, single bond between attom at postion 10 and 43, double bond between 11 and 15, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 19, single bond between attom at postion 12 and 20, single bond between attom at postion 12 and 44, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 45, single bond between attom at postion 13 and 46, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 23, single bond between attom at postion 15 and 21, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 47, single bond between attom at postion 17 and 22, single bond between attom at postion 17 and 48, single bond between attom at postion 17 and 49, double bond between 18 and 25, single bond between attom at postion 18 and 26, single bond between attom at postion 19 and 50, single bond between attom at postion 19 and 51, single bond between attom at postion 19 and 52, single bond between attom at postion 20 and 53, single bond between attom at postion 20 and 54, single bond between attom at postion 20 and 55, double bond between 21 and 27, single bond between attom at postion 21 and 28, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 56, single bond between attom at postion 24 and 35, single bond between attom at postion 24 and 57, single bond between attom at postion 24 and 58, single bond between attom at postion 25 and 29, single bond between attom at postion 25 and 59, double bond between 26 and 30, single bond between attom at postion 26 and 60, single bond between attom at postion 27 and 31, single bond between attom at postion 27 and 62, double bond between 28 and 32, single bond between attom at postion 28 and 63, double bond between 29 and 33, single bond between attom at postion 29 and 65, single bond between attom at postion 30 and 33, single bond between attom at postion 30 and
This compound's CID is 60825 and compound's name is Lamivudine. There are 26 attoms in the molecule and their positions in the order are S, O, O, O, N, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 10, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 24, double bond between 4 and 13, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 13, double bond between 6 and 15, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 25, single bond between attom at postion 7 and 26, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 20, single bond between attom at postion 11 and 21, double bond between 12 and 14, single bond between attom at postion 12 and 22, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 23. The 3D x,y,z coordinates of the element at position 1 is -3.1049, -1.2086, -0.8358, . The 3D x,y,z coordinates of the element at position 2 is -1.5844, 0.204, 0.8145, . The 3D x,y,z coordinates of the element at

This compound's CID is 60846 and compound's name is Valsartan. There are 61 atoms in the molecule and their positions in the order are O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 1 and 56, double bond between 2 and 12, double bond between 3 and 16, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 7, double bond between 5 and 31, double bond between 6 and 8, single bond between attom at postion 6 and 31, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 61, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 14, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 15, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 13 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 14 and 41, single bond between attom at postion 14 and 42, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 43, single bond between attom at postion 15 and 44, double bond between 17 and 20, single bond between attom at postion 17 and 21, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 25, single bond between attom at postion 19 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 20 and 23, single bond between attom at postion 20 and 49, double bond between 21 and 24, single bond between attom at postion 21 and 50, double bond between 22 and 23, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 26, single bond between attom at postion 23 and 51, single bond between attom at postion 24 and 52, single bond between attom at postion 25 and 53, single bond between attom at postion 25 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 26 and 27, double bond between 26 and 28, double bond between 27 and 29, single bond between attom at postion 27 and 31, single bond between attom at postion 28 and 30, single bond between attom at postion 28 and 57, single bond between attom at postion 29 and 32, single bond between attom at postion 29 and 58, double bond between 30 and 32, single bond between attom at postion 30 and 59, single bond between attom at postion 32 and 60. The 3D x,y,z coordinates of the element at position 1 is -0.4458,

This compound's CID is 60854 and compound's name is Ziprasidone. There are 49 attoms in the molecule and their positions in the order are CL, S, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 22, double bond between 3 and 24, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 14, double bond between 6 and 14, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 45, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 37, single bond between attom at postion 12 and 38, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 39, single bond between attom at postion 13 and 40, single bond between attom at postion 14 and 16, single bond between attom at postion 15 and 18, double bond between 15 and 20, single bond between attom at postion 16 and 22, double bond between 16 and 25, double bond between 17 and 18, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 21, single bond between attom at postion 18 and 41, double bond between 19 and 23, single bond between attom at postion 20 and 23, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 42, single bond between attom at postion 21 and 43, double bond between 22 and 26, single bond between attom at postion 23 and 44, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 46, single bond between attom at postion 26 and 28, single bond between attom at postion 26 and 47, double bond between 27 and 28, single bond between attom at postion 27 and 48, single bond between attom at postion 28 and 49. The 3D x,y,z coordinates of the element at position 1 is -3.7598, -3.2474, 0.7298, . The 3D x,y,z

This compound's CID is 60857 and compound's name is Zolmitriptan. There are 42 attoms in the molecule and their positions in the order are O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 19, double bond between 2 and 19, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 19, single bond between attom at postion 3 and 30, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 17, single bond between attom at postion 4 and 36, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 21, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 22, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 24, double bond between 8 and 13, single bond between attom at postion 8 and 15, single bond between attom at postion 9 and 10, double bond between 9 and 12, single bond between attom at postion 9 and 13, single bond between attom at postion 10 and 14, double bond between 10 and 17, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 27, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 29, double bond between 15 and 18, single bond between attom at postion 15 and 31, single bond between attom at postion 16 and 32, single bond between attom at postion 16 and 33, single bond between attom at postion 17 and 34, single bond between attom at postion 18 and 35, single bond between attom at postion 20 and 37, single bond between attom at postion 20 and 38, single bond between attom at postion 20 and 39, single bond between attom at postion 21 and 40, single bond between attom at postion 21 and 41, single bond between attom at postion 21 and 42. The 3D x,y,z coordinates of the element at position 1 is -5.1307, 1.1877, -0.0377, . The 3D x,y,z coordinates of the element at position 2 is -4.1463, 2.6925, -1.4593, . The 3D x,y,z
This compound's CID is 60877 and compound's name is Emtricitabine. There are 26 attoms in the molecule and their positions in the order are S, X, O, O, O, N, N, N, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 15, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 24, double bond between 5 and 14, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 14, double bond between 7 and 16, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 17, single bond between attom at postion 10 and 18, single bond between attom at postion 10 and 19, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 20, single bond between attom at postion 12 and 21, single bond between attom at postion 12 and 22, double bond between 13 and 15, single bond between attom at postion 13 and 23, single bond between attom at postion 15 and 16. The 3D x,y,z coordinates of the element at position 1 is -3.3375, -1.0942, -0.8826, . The 3D x,y,z coordinates of the element at position 2 is 2.3201, 2.5586, -0.2266, . The 3D x,y,z coordinates of the element at

This compound's CID is 60953 and compound's name is Capecitabine. There are 47 attoms in the molecule and their positions in the order are X, O, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 33, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 34, double bond between 5 and 17, single bond between attom at postion 6 and 23, single bond between attom at postion 6 and 24, double bond between 7 and 24, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 17, double bond between 9 and 19, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 40, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 26, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 27, single bond between attom at postion 13 and 28, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 30, single bond between attom at postion 15 and 31, single bond between attom at postion 15 and 32, double bond between 16 and 18, single bond between attom at postion 16 and 35, single bond between attom at postion 18 and 19, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 36, single bond between attom at postion 20 and 37, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 38, single bond between attom at postion 21 and 39, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 41, single bond between attom at postion 22 and 42, single bond between attom at postion 23 and 43, single bond between attom at postion 23 and 44, single bond between attom at postion 25 and 45, single bond between attom at postion 25 and 46, single bond between attom at postion 25 and 47. The 3D x,y,z coordinates of the element at position 1 is -0.1418, -2.6904, -0.1559, . The 3D x,y,z coordinates of the element at position 2 is -4.4218, -0.7029, This compound's CID is 60961 and compound's name is Adenosine. There are 32 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 26, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 27, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 29, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 15, single bond between attom at postion 5 and 16, double bond between 6 and 16, single bond between attom at postion 6 and 17, double bond between 7 and 15, single bond between attom at postion 7 and 19, single bond between attom at postion 8 and 18, double bond between 8 and 19, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 21, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 22, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 23, single bond between attom at postion 14 and 24, single bond between attom at postion 14 and 25, single bond between attom at postion 15 and 17, single bond between attom at postion 16 and 28, double bond between 17 and 18, single bond between attom at postion 19 and 30. The 3D x,y,z coordinates of the element at position 1 is 1.9998, -0.5205, -0.9524, . The 3D x,y,z

This compound's CID is 64139 and compound's name is Efavirenz. There are 30 attoms in the molecule and their positions in the order are CL, X, X, X, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 16, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 16, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 19, double bond between 6 and 19, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 22, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 16, triple bond between 12 and 14, double bond between 13 and 15, single bond between attom at postion 13 and 17, single bond between attom at postion 15 and 18, double bond between 17 and 20, single bond between attom at postion 17 and 27, double bond between 18 and 21, single bond between attom at postion 18 and 29, single bond between attom at postion 20 and 21, single bond between attom at postion 21 and 30. The 3D x,y,z coordinates of the element at position 1 is -1.8517, -4.1698, -0.4699, . The 3D x,y,z coordinates of the element at position 2 is 0.6247, -0.2557, -2.3268, . The 3D x,y,z coordinates of the element at

This compound's CID is 65015 and compound's name is Plerixafor. There are 90 attoms in the molecule and their positions in the order are N, N, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 13, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 14, single bond between attom at postion 3 and 19, single bond between attom at postion 3 and 27, single bond between attom at postion 3 and 65, single bond between attom at postion 4 and 20, single bond between attom at postion 4 and 28, single bond between attom at postion 4 and 66, single bond between attom at postion 5 and 21, single bond between attom at postion 5 and 31, single bond between attom at postion 5 and 75, single bond between attom at postion 6 and 22, single bond between attom at postion 6 and 32, single bond between attom at postion 6 and 76, single bond between attom at postion 7 and 33, single bond between attom at postion 7 and 35, single bond between attom at postion 7 and 89, single bond between attom at postion 8 and 34, single bond between attom at postion 8 and 36, single bond between attom at postion 8 and 90, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 37, single bond between attom at postion 9 and 38, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 39, single bond between attom at postion 10 and 40, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 41, single bond between attom at postion 11 and 42, single bond between attom at postion 12 and 18, single bond between attom at postion 12 and 43, single bond between attom at postion 12 and 44, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 45, single bond between attom at postion 13 and 46, single bond between attom at postion 14 and 20, single bond between attom at postion 14 and 47, single bond between attom at postion 14 and 48, single bond between attom at postion 15 and 21, single bond between attom at postion 15 and 49, single bond between attom at postion 15 and 50, single bond between attom at postion 16 and 22, single bond between attom at postion 16 and 51, single bond between attom at postion 16 and 52, double bond between 17 and 23, single bond between attom at postion 17 and 25, double bond between 18 and 24, single bond between attom at postion 18 and 26, single bond between attom at postion 19 and 53, single bond between attom at postion 19 and 54, single bond between attom at postion 20 and 55, single bond between attom at postion 20 and 56, single bond between attom at postion 21 and 57, single bond between attom at postion 21 and 58, single bond between attom at postion 22 and 59, single bond between attom at postion 22 and

This compound's CID is 65157 and compound's name is Testosterone Undecanoate. There are 81 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 23, double bond between 2 and 22, double bond between 3 and 23, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 12, single bond between attom at postion 4 and 34, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 35, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 36, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 37, single bond between attom at postion 9 and 38, single bond between attom at postion 10 and 39, single bond between attom at postion 10 and 40, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 41, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 42, single bond between attom at postion 12 and 43, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 44, single bond between attom at postion 13 and 45, single bond between attom at postion 14 and 46, single bond between attom at postion 14 and 47, single bond between attom at postion 15 and 17, double bond between 15 and 21, single bond between attom at postion 16 and 48, single bond between attom at postion 16 and 49, single bond between attom at postion 16 and 50, single bond between attom at postion 17 and 51, single bond between attom at postion 17 and 52, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 53, single bond between attom at postion 18 and 54, single bond between attom at postion 19 and 55, single bond between attom at postion 19 and 56, single bond between attom at postion 19 and 57, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 58, single bond between attom at postion 20 and 59, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 60, single bond between attom at postion 23 and 24, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 61, single bond between attom at postion 24 and 62, single bond between attom at postion 25 and 26, single bond between attom at postion 25 and 63, single bond between attom at postion 25 and 64, single bond between attom at

This compound's CID is 65492 and compound's name is Iopamidol. There are 53 attoms in the molecule and their positions in the order are I, I, I, O, O, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 21, single bond between attom at postion 3 and 22, single bond between attom at postion 4 and 25, single bond between attom at postion 4 and 46, single bond between attom at postion 5 and 26, single bond between attom at postion 5 and 47, single bond between attom at postion 6 and 27, single bond between attom at postion 6 and 48, single bond between attom at postion 7 and 28, single bond between attom at postion 7 and 49, double bond between 8 and 23, double bond between 9 and 24, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 53, double bond between 11 and 29, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 23, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 24, single bond between attom at postion 13 and 35, single bond between attom at postion 14 and 20, single bond between attom at postion 14 and 29, single bond between attom at postion 14 and 44, single bond between attom at postion 15 and 25, single bond between attom at postion 15 and 26, single bond between attom at postion 15 and 32, single bond between attom at postion 16 and 27, single bond between attom at postion 16 and 28, single bond between attom at postion 16 and 33, double bond between 17 and 19, single bond between attom at postion 17 and 22, single bond between attom at postion 17 and 23, single bond between attom at postion 18 and 19, double bond between 18 and 21, single bond between attom at postion 18 and 24, single bond between attom at postion 20 and 21, double bond between 20 and 22, single bond between attom at postion 25 and 36, single bond between attom at postion 25 and 37, single bond between attom at postion 26 and 38, single bond between attom at postion 26 and 39, single bond between attom at postion 27 and 40, single bond between attom at postion 27 and 41, single bond between attom at postion 28 and 42, single bond between attom at postion 28 and 43, single bond between attom at postion 29 and 30, single bond between attom at postion 30 and 31, single bond between attom at postion 30 and 45, single bond between attom at postion 31 and 50, single bond between attom at postion 31 and 51, single bond between attom at postion 31 and 52. The 3D x,y,z coordinates of the element at position 1 is -0.4398, -3.2598, 0.3259, . The 3D x,y,z coordinates of the element at position 2 is -2.698, 2.1566, -

This compound's CID is 65981 and compound's name is Repaglinide. There are 69 attoms in the molecule and their positions in the order are O, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 23, single bond between attom at postion 2 and 28, single bond between attom at postion 2 and 32, single bond between attom at postion 3 and 31, single bond between attom at postion 3 and 69, double bond between 4 and 31, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 23, single bond between attom at postion 6 and 49, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 34, single bond between attom at postion 7 and 35, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 36, single bond between attom at postion 8 and 37, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 38, single bond between attom at postion 9 and 39, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 40, single bond between attom at postion 10 and 41, single bond between attom at postion 11 and 42, single bond between attom at postion 11 and 43, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 44, single bond between attom at postion 13 and 14, double bond between 13 and 17, double bond between 14 and 18, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 45, single bond between attom at postion 15 and 46, single bond between attom at postion 16 and 19, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 47, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 48, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 50, single bond between attom at postion 19 and 51, single bond between attom at postion 19 and 52, single bond between attom at postion 19 and 53, single bond between attom at postion 20 and 54, single bond between attom at postion 20 and 55, single bond between attom at postion 20 and 56, double bond between 21 and 22, single bond between attom at postion 21 and 57, single bond between attom at postion 22 and 58, single bond between attom at postion 23 and 24, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 59, single bond between attom at postion 24 and 60, double bond between 25 and 26, single bond between attom at postion 25 and 27, single bond between attom at postion 26 and 28, single bond between attom at postion 26 and 61, double bond between 27 and 29, single bond between attom at postion 27 and 62, double bond between 28 and 30, single bond between attom at postion 29 and 30, single bond

This compound's CID is 65999 and compound's name is Telmisartan. There are 83 attoms in the molecule and their positions in the order are O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 39, single bond between attom at postion 1 and 69, double bond between 2 and 39, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 10, double bond between 4 and 8, single bond between attom at postion 4 and 9, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 25, double bond between 6 and 16, single bond between attom at postion 6 and 21, double bond between 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 11, single bond between attom at postion 9 and 14, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 40, single bond between attom at postion 10 and 41, single bond between attom at postion 11 and 18, single bond between attom at postion 11 and 42, single bond between attom at postion 11 and 43, double bond between 12 and 13, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 16, single bond between attom at postion 13 and 44, double bond between 14 and 15, single bond between attom at postion 14 and 19, single bond between attom at postion 15 and 45, double bond between 17 and 22, single bond between attom at postion 17 and 23, single bond between attom at postion 18 and 24, single bond between attom at postion 18 and 46, single bond between attom at postion 18 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 19 and 49, single bond between attom at postion 19 and 50, single bond between attom at postion 20 and 21, double bond between 20 and 29, double bond between 21 and 30, single bond between attom at postion 22 and 27, single bond between attom at postion 22 and 51, double bond between 23 and 28, single bond between attom at postion 23 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 24 and 54, single bond between attom at postion 24 and 55, single bond between attom at postion 25 and 56, single bond between attom at postion 25 and 57, single bond between attom at postion 25 and 58, double bond between 26 and 27, single bond between attom at postion 26 and 28, single bond between attom at postion 26 and 31, single bond between attom at postion 27 and 59, single bond between attom at postion 28 and 60, single bond between attom at postion 29 and 32, single bond between attom at postion 29 and 61, single bond between attom at postion 30 and 33, single bond between attom at postion 30 and 62, single bond between attom at postion 31 and 34, double bond between 31 and 35, double bond between 32 and 33, single bond between attom at postion 32 and 63, single bond between attom at postion 33 and This compound's CID is 66348 and compound's name is Octathiocane. There are 8 attoms in the molecule and their positions in the order are S, S, S, S, S, S, S, S. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 3 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 7 and 8. The 3D x,y,z coordinates of the element at position 1 is 0.0238, 2.3163, -0.5082, . The 3D x,y,z coordinates of the element at position 2 is -1.6211, 1.6547, 0.508, . The 3D x,y,z coordinates of the element at position 3 is 1.6548,

This compound's CID is 68614 and compound's name is Fludeoxyglucose F-18. There are 23 attoms in the molecule and their positions in the order are X, O, O, O, O, O, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 19, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 9, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 23, double bond between 6 and 12, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 15, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 16, single bond between attom at postion 11 and 17, single bond between attom at postion 11 and 18, single bond between attom at postion 12 and 22. The 3D x,y,z coordinates of the element at position 1 is -2.0594, 1.371, 0.0599, . The 3D x,y,z coordinates of the element at position 2 is 0.4373, 1.6493, -0.2054, . The 3D x,y,z coordinates of the
This compound's CID is 68844 and compound's name is Brinzolamide. There are 44 attoms in the molecule and their positions in the order are S, S, S, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 4, double bond between 1 and 5, single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 15, single bond between attom at postion 2 and 19, double bond between 3 and 7, double bond between 3 and 8, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 19, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 23, single bond between attom at postion 9 and 13, single bond between attom at postion 9 and 16, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 40, single bond between attom at postion 11 and 41, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 25, single bond between attom at postion 13 and 26, double bond between 14 and 15, single bond between attom at postion 14 and 17, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 27, single bond between attom at postion 16 and 28, double bond between 17 and 19, single bond between attom at postion 17 and 30, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 31, single bond between attom at postion 18 and 32, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 33, single bond between attom at postion 20 and 34, single bond between attom at postion 21 and 35, single bond between attom at postion 21 and 36, single bond between attom at postion 22 and 37, single bond between attom at postion 22 and 38, single bond between attom at postion 22 and 39, single bond between attom at postion 23 and 42, single bond between attom at postion 23 and 43, single bond between attom at postion 23 and 44. The 3D x,y,z coordinates of the element at position 1 is 0.3779, 1.9156, 0.2123, . The 3D x,y,z coordinates of the element at position 2 is -2.4299, 1.2981, -0.5663, . The 3D x,y,z coordinates of the element at position 3 is -4.8382, -0.3542, -0.7189, . The

This compound's CID is 71329 and compound's name is Dofetilide. There are 56 attoms in the molecule and their positions in the order are S, S, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 4, double bond between 1 and 5, single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 28, double bond between 2 and 6, double bond between 2 and 7, single bond between attom at postion 2 and 10, single bond between attom at postion 2 and 29, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 22, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 16, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 45, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 50, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 34, single bond between attom at postion 13 and 35, double bond between 14 and 17, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 41, double bond between 18 and 21, single bond between attom at postion 18 and 42, double bond between 19 and 20, single bond between attom at postion 19 and 21, single bond between attom at postion 20 and 43, single bond between attom at postion 21 and 44, double bond between 22 and 24, single bond between attom at postion 22 and 25, double bond between 23 and 26, single bond between attom at postion 23 and 27, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 46, double bond between 25 and 27, single bond between attom at postion 25 and 47, single bond between attom at postion 26 and 48, single bond between attom at postion 27 and 49, single bond between attom at postion 28 and 51, single bond between attom at postion 28 and 52, single bond between attom at postion 28 and 53, single bond between attom at postion 29 and 54, single bond between attom at postion 29 and 55, single bond between attom at postion 29 and 56. The 3D x,y,z coordinates of the element at position 1 is 0.7787, -2.9475, -0.6362, . The 3D x,y,z coordinates of the element at position 2 is 5.3516, 0.3437, 0.5875, . The 3D x,y,z coordinates of the element at position 3 is -1.008, 1.7306, -0.3653, . The 3D

This compound's CID is 71616 and compound's name is Voriconazole. There are 39 attoms in the molecule and their positions in the order are X, X, X, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 2 and 18, single bond between attom at postion 3 and 22, single bond between attom at postion 4 and 10, single bond between attom at postion 4 and 32, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 21, double bond between 6 and 15, single bond between attom at postion 6 and 24, double bond between 7 and 25, double bond between 8 and 21, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 23, double bond between 9 and 24, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 13, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 26, single bond between attom at postion 12 and 27, single bond between attom at postion 12 and 28, double bond between 13 and 16, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 29, single bond between attom at postion 14 and 30, single bond between attom at postion 14 and 31, single bond between attom at postion 15 and 18, single bond between attom at postion 16 and 19, double bond between 17 and 20, single bond between attom at postion 17 and 33, double bond between 18 and 23, double bond between 19 and 22, single bond between attom at postion 19 and 34, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 35, single bond between attom at postion 21 and 36, single bond between attom at postion 23 and 37, single bond between attom at postion 24 and 38, single bond between attom at postion 25 and 39. The 3D x,y,z coordinates of the element at position 1 is -0.9996, 1.2212, -1.9654, . The 3D x,y,z coordinates of the element at position 2 is
This compound's CID is 74989 and compound's name is Atovaquone. There are 45 attoms in the molecule and their positions in the order are CL, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 23, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 42, double bond between 3 and 14, double bond between 4 and 18, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 27, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 28, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 29, single bond between attom at postion 7 and 30, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 31, single bond between attom at postion 8 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 9 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 10 and 36, double bond between 11 and 13, single bond between attom at postion 11 and 14, double bond between 12 and 15, single bond between attom at postion 12 and 16, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 18, single bond between attom at postion 15 and 20, single bond between attom at postion 15 and 37, double bond between 16 and 21, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 19, double bond between 17 and 22, single bond between attom at postion 18 and 19, double bond between 19 and 24, double bond between 20 and 23, single bond between attom at postion 20 and 39, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 40, single bond between attom at postion 22 and 25, single bond between attom at postion 22 and 41, single bond between attom at postion 24 and 26, single bond between attom at postion 24 and 43, double bond between 25 and 26, single bond between attom at postion 25 and 44, single bond between attom at postion 26 and 45. The 3D x,y,z coordinates of the element at position 1 is 8.6389, -0.4437, 0.0493, . The 3D x,y,z coordinates of the element at

This compound's CID is 76262 and compound's name is Triethoxyoctylsilane. There are 50 attoms in the molecule and their positions in the order are Si, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 2, single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 7, single bond between attom at postion 2 and 12, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 14, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 19, single bond between attom at postion 5 and 20, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 22, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 24, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 35, single bond between attom at postion 13 and 36, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 37, single bond between attom at postion 14 and 38, single bond between attom at postion 15 and 39, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 16 and 42, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 17 and 45, single bond between attom at postion 17 and 46, single bond between attom at postion 17 and 47, single bond between attom at postion 18 and 48, single bond between attom at postion 18 and 49, single bond between attom at postion 18 and 50. The 3D x,y,z coordinates of the element at position 1 is 2.2477, 0.0017, 0.0109, . The 3D x,y,z coordinates of the element at position 2 is 2.3894, -1.3591, 0.9874, . The 3D x,y,z

This compound's CID is 77991 and compound's name is Rivastigmine. There are 40 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 12, single bond between attom at postion 1 and 16, double bond between 2 and 16, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 10, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 19, double bond between 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 7 and 20, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 22, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 23, double bond between 9 and 13, single bond between attom at postion 9 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 10 and 27, single bond between attom at postion 11 and 28, single bond between attom at postion 11 and 29, single bond between attom at postion 11 and 30, double bond between 12 and 14, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 31, single bond between attom at postion 14 and 32, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 33, single bond between attom at postion 15 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 17 and 36, single bond between attom at postion 17 and 37, single bond between attom at postion 18 and 38, single bond between attom at postion 18 and 39, single bond between attom at postion 18 and 40. The 3D x,y,z coordinates of the element at position 1 is -1.6626, 0.3976, -0.5173, . The 3D x,y,z coordinates of the element at position 2 is -1.6859, -0.7248, 1.5073, . The 3D x,y,z coordinates of the element at position 3 is 3.2616, -1.3728,

This compound's CID is 82146 and compound's name is Bexarotene. There are 54 attoms in the molecule and their positions in the order are O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 26, single bond between attom at postion 1 and 54, double bond between 2 and 26, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 27, single bond between attom at postion 5 and 28, single bond between attom at postion 6 and 29, single bond between attom at postion 6 and 30, double bond between 7 and 8, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 9 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 10 and 35, single bond between attom at postion 10 and 36, single bond between attom at postion 11 and 37, single bond between attom at postion 11 and 38, single bond between attom at postion 11 and 39, single bond between attom at postion 12 and 40, single bond between attom at postion 12 and 41, single bond between attom at postion 12 and 42, double bond between 13 and 15, single bond between attom at postion 13 and 43, double bond between 14 and 16, single bond between attom at postion 14 and 44, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 16 and 18, single bond between attom at postion 17 and 19, double bond between 17 and 20, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 18 and 47, double bond between 19 and 21, single bond between attom at postion 19 and 22, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 50, double bond between 22 and 24, single bond between attom at postion 22 and 51, double bond between 23 and 25, single bond between attom at postion 23 and 52, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 53, single bond between attom at postion 25 and 26. The 3D x,y,z coordinates of the element at position 1 is 6.1672, -1.9222, -1.033, . The 3D x,y,z coordinates of the element at position 2 is 6.6076, 0.2152, -1.6689, . The 3D x,y,z

This compound's CID is 84951 and compound's name is 1,6-di-O-phosphono-D-fructose. There are 34 attoms in the molecule and their positions in the order are P, P, O, O, O, O, O, O, O, O, O, O, O, O, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 10, double bond between 1 and 11, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 13, double bond between 2 and 14, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 28, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 29, single bond between attom at postion 5 and 17, single bond between attom at postion 5 and 30, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 20, double bond between 8 and 19, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 13 and 34, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 21, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 22, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 23, single bond between attom at postion 18 and 24, single bond between attom at postion 18 and 25, single bond between attom at postion 19 and 20, single bond between attom at postion 20 and 26, single bond between attom at postion 20 and 27. The 3D x,y,z coordinates of the element at position 1 is -5.2807, -0.8752, -0.0804, . The 3D x,y,z coordinates of the element at position 2 is 4.9762, -1.3029, 0.0025, . The 3D x,y,z coordinates of the element at position 3 is -
This compound's CID is 89594 and compound's name is Nicotine. There are 26 attoms in the molecule and their positions in the order are N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 6, single bond between attom at postion 1 and 8, single bond between attom at postion 2 and 10, double bond between 2 and 12, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 17, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 19, single bond between attom at postion 7 and 9, double bond between 7 and 10, single bond between attom at postion 8 and 20, single bond between attom at postion 8 and 21, single bond between attom at postion 8 and 22, double bond between 9 and 11, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 25, single bond between attom at postion 12 and 26. The 3D x,y,z coordinates of the element at position 1 is -1.7023, -0.7962, -0.0339, . The 3D x,y,z coordinates of the element at position 2 is 2.2968, -0.7091, 1.2171, . The 3D x,y,z coordinates of the element at position 3 is -

This compound's CID is 92974 and compound's name is Droxidopa. There are 26 attoms in the molecule and their positions in the order are O, O, O, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 23, single bond between attom at postion 2 and 12, single bond between attom at postion 2 and 24, single bond between attom at postion 3 and 13, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 26, double bond between 5 and 12, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 20, single bond between attom at postion 6 and 21, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 16, single bond between attom at postion 8 and 12, single bond between attom at postion 8 and 17, double bond between 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 18, double bond between 11 and 14, single bond between attom at postion 11 and 19, double bond between 13 and 15, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 22. The 3D x,y,z coordinates of the element at position 1 is 1.8471, 0.3146, -2.12, . The 3D x,y,z coordinates of the element at position 2 is 3.0438,

This compound's CID is 94599 and compound's name is [3-(Dodecanoylamino)propyl](hydroxy)dimethylammonium. There are 57 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, double bond between 2 and 18, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 19, single bond between attom at postion 3 and 20, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 48, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 22, single bond between attom at postion 5 and 23, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 24, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 28, single bond between attom at postion 8 and 29, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 30, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 32, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 34, single bond between attom at postion 11 and 35, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 36, single bond between attom at postion 12 and 37, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 38, single bond between attom at postion 13 and 39, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 40, single bond between attom at postion 14 and 41, single bond between attom at postion 15 and 18, single bond between attom at postion 15 and 42, single bond between attom at postion 15 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 16 and 45, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 46, single bond between attom at postion 17 and 47, single bond between attom at postion 19 and 49, single bond between attom at postion 19 and 50, single bond between attom at postion 19 and 51, single bond between attom at postion 20 and 52, single bond between attom at postion 20 and 53, single bond between attom at postion 20 and 54, single bond between attom at postion 21 and 55, single bond between attom at postion 21 and 56, single bond between attom at postion 21 and 57. The 3D x,y,z coordinates of the element at position 1 is 2.174, -

This compound's CID is 104741 and compound's name is Fulvestrant. There are 88 attoms in the molecule and their positions in the order are S, X, X, X, X, X, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 9, single bond between attom at postion 1 and 36, single bond between attom at postion 1 and 37, single bond between attom at postion 2 and 40, single bond between attom at postion 3 and 40, single bond between attom at postion 4 and 41, single bond between attom at postion 5 and 41, single bond between attom at postion 6 and 41, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 62, single bond between attom at postion 8 and 30, single bond between attom at postion 8 and 74, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 42, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 20, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 17, single bond between attom at postion 12 and 43, single bond between attom at postion 13 and 18, single bond between attom at postion 13 and 21, single bond between attom at postion 13 and 44, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 45, single bond between attom at postion 14 and 46, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 47, single bond between attom at postion 16 and 19, single bond between attom at postion 16 and 48, single bond between attom at postion 16 and 49, single bond between attom at postion 17 and 22, single bond between attom at postion 17 and 23, single bond between attom at postion 17 and 50, single bond between attom at postion 18 and 51, single bond between attom at postion 18 and 52, single bond between attom at postion 19 and 53, single bond between attom at postion 19 and 54, single bond between attom at postion 20 and 55, single bond between attom at postion 20 and 56, single bond between attom at postion 20 and 57, double bond between 21 and 24, single bond between attom at postion 21 and 26, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 58, single bond between attom at postion 22 and 59, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 60, single bond between attom at postion 23 and 61, single bond between attom at postion 24 and 27, single bond between attom at postion 25 and 28, single bond between attom at postion 25 and 63, single bond between attom at postion 25 and 64, double bond between 26 and 29, single bond between attom at postion 26 and 65, double bond between 27 and 30, single bond between attom at postion 27 and 66, single bond between attom at postion 28 and 31, single bond between attom at postion 28 and

This compound's CID is 104838 and compound's name is Imipenem. There are 37 attoms in the molecule and their positions in the order are S, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 15, single bond between attom at postion 1 and 18, single bond between attom at postion 2 and 13, single bond between attom at postion 2 and 29, double bond between 3 and 12, single bond between attom at postion 4 and 17, single bond between attom at postion 4 and 32, double bond between 5 and 17, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 14, single bond between attom at postion 7 and 19, double bond between 7 and 20, single bond between attom at postion 8 and 20, single bond between attom at postion 8 and 36, single bond between attom at postion 8 and 37, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 22, single bond between attom at postion 11 and 15, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 25, double bond between 14 and 15, single bond between attom at postion 14 and 17, single bond between attom at postion 16 and 26, single bond between attom at postion 16 and 27, single bond between attom at postion 16 and 28, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 30, single bond between attom at postion 18 and 31, single bond between attom at postion 19 and 33, single bond between attom at postion 19 and 34, single bond between attom at postion 20 and 35. The 3D x,y,z coordinates of the element at position 1 is -1.9571, -0.7478, -1.0576, . The 3D x,y,z coordinates of

This compound's CID is 104865 and compound's name is Bosentan. There are 68 attoms in the molecule and their positions in the order are S, O, O, O, O, O, O, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 2, double bond between 1 and 3, single bond between attom at postion 1 and 8, single bond between attom at postion 1 and 20, single bond between attom at postion 4 and 24, single bond between attom at postion 4 and 27, single bond between attom at postion 5 and 25, single bond between attom at postion 5 and 29, single bond between attom at postion 6 and 30, single bond between attom at postion 6 and 39, single bond between attom at postion 7 and 33, single bond between attom at postion 7 and 68, single bond between attom at postion 8 and 23, single bond between attom at postion 8 and 53, single bond between attom at postion 9 and 23, double bond between 9 and 26, double bond between 10 and 25, single bond between attom at postion 10 and 26, double bond between 11 and 28, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 28, double bond between 12 and 37, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 17, double bond between 14 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 15 and 40, single bond between attom at postion 15 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 16 and 45, single bond between attom at postion 17 and 46, single bond between attom at postion 17 and 47, single bond between attom at postion 17 and 48, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 49, double bond between 19 and 22, single bond between attom at postion 19 and 50, double bond between 20 and 21, single bond between attom at postion 20 and 22, single bond between attom at postion 21 and 51, single bond between attom at postion 22 and 52, double bond between 23 and 24, single bond between attom at postion 24 and 25, single bond between attom at postion 26 and 28, single bond between attom at postion 27 and 30, double bond between 27 and 31, single bond between attom at postion 29 and 33, single bond between attom at postion 29 and 54, single bond between attom at postion 29 and 55, double bond between 30 and 32, single bond between attom at postion 31 and 34, single bond between attom at postion 31 and 56, single bond between attom at postion 32 and 35, single bond between attom at postion 32 and 57, single bond between attom at postion 33 and 58, single bond between attom at postion 33 and 59, double bond between 34 and 35, single bond between attom at postion 34 and 60, single bond between attom at postion 35 and 61, double bond between 36 and 38, single bond between attom at postion 36 and 62, single bond This compound's CID is 107689 and compound's name is Lactic Acid, L-. There are 12 attoms in the molecule and their positions in the order are O, O, O, C, C, C, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 6, single bond between attom at postion 2 and 12, double bond between 3 and 6, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 10. The 3D x,y,z coordinates of the element at position 1 is -1.3875, 1.1182, 0.1968, . The 3D x,y,z coordinates of the element at position 2 is 1.4877, -1.0368, 0.2617, . The 3D x,y,z coordinates of the element at

This compound's CID is 107970 and compound's name is Fingolimod. There are 55 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 51, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 52, single bond between attom at postion 3 and 4, single bond between attom at postion 3 and 41, single bond between attom at postion 3 and 42, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 8, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 23, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 12, single bond between attom at postion 6 and 25, single bond between attom at postion 6 and 26, single bond between attom at postion 7 and 27, single bond between attom at postion 7 and 28, single bond between attom at postion 8 and 29, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 31, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, double bond between 12 and 17, single bond between attom at postion 12 and 18, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 37, single bond between attom at postion 13 and 38, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 39, single bond between attom at postion 14 and 40, double bond between 15 and 19, single bond between attom at postion 15 and 20, single bond between attom at postion 16 and 21, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 45, double bond between 18 and 20, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 48, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 49, single bond between attom at postion 21 and 50, single bond between attom at postion 22 and 53, single bond between attom at postion 22 and 54, single bond between attom at postion 22 and 55. The 3D x,y,z coordinates of the element at position 1 is -5.8225, -0.7507, 2.3133, . The 3D x,y,z coordinates of the element at position 2 is -

This compound's CID is 110635 and compound's name is Tadalafil. There are 48 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 13, double bond between 2 and 15, single bond between attom at postion 3 and 24, single bond between attom at postion 3 and 29, single bond between attom at postion 4 and 28, single bond between attom at postion 4 and 29, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 15, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 34, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 30, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 16, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 32, single bond between attom at postion 10 and 33, double bond between 11 and 12, single bond between attom at postion 12 and 14, single bond between attom at postion 14 and 18, double bond between 14 and 19, single bond between attom at postion 15 and 17, double bond between 16 and 20, single bond between attom at postion 16 and 21, single bond between attom at postion 17 and 35, single bond between attom at postion 17 and 36, double bond between 18 and 22, single bond between attom at postion 19 and 25, single bond between attom at postion 19 and 38, single bond between attom at postion 20 and 24, single bond between attom at postion 20 and 37, double bond between 21 and 26, single bond between attom at postion 21 and 39, single bond between attom at postion 22 and 27, single bond between attom at postion 22 and 40, single bond between attom at postion 23 and 41, single bond between attom at postion 23 and 42, single bond between attom at postion 23 and 43, double bond between 24 and 28, double bond between 25 and 27, single bond between attom at postion 25 and 44, single bond between attom at postion 26 and 28, single bond between attom at postion 26 and 45, single bond between attom at postion 27 and 46, single bond between attom at postion 29 and 47, single bond between attom at postion 29 and 48. The 3D x,y,z coordinates of the element at position 1 is -0.7505, 3.2326, 2.1493, . The 3D x,y,z coordinates of the

This compound's CID is 115237 and compound's name is Pulipendone. There are 58 attoms in the molecule and their positions in the order are X, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 31, single bond between attom at postion 2 and 7, single bond between attom at postion 2 and 26, single bond between attom at postion 3 and 19, single bond between attom at postion 3 and 56, double bond between 4 and 24, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 22, single bond between attom at postion 6 and 24, double bond between 7 and 15, double bond between 8 and 22, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 33, single bond between attom at postion 10 and 34, single bond between attom at postion 11 and 13, single bond between attom at postion 11 and 35, single bond between attom at postion 11 and 36, single bond between attom at postion 12 and 37, single bond between attom at postion 12 and 38, single bond between attom at postion 13 and 39, single bond between attom at postion 13 and 40, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 41, single bond between attom at postion 14 and 42, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 17, single bond between attom at postion 16 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 17 and 24, double bond between 17 and 25, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 45, single bond between attom at postion 18 and 46, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 22, single bond between attom at postion 19 and 47, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 21 and 50, single bond between attom at postion 21 and 51, double bond between 23 and 26, single bond between attom at postion 23 and 27, single bond between attom at postion 25 and 28, single bond between attom at postion 26 and 29, double bond between 27 and 30, single bond between attom at postion 27 and 52, single bond between attom at postion 28 and 53, single bond between attom at postion 28 and 54, single bond between attom at postion 28 and 55, double bond between 29 and 31, single bond between attom at postion 29 and 57, single bond between attom at postion 30 and 31, single bond between attom at postion 30 and 58. The 3D x,y,z coordinates of the element at position 1 is -9.6854, This compound's CID is 121396 and compound's name is Carglumic Acid. There are 23 attoms in the molecule and their positions in the order are O, O, O, O, O, N, N, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 20, double bond between 2 and 11, single bond between attom at postion 3 and 12, single bond between attom at postion 3 and 23, double bond between 4 and 12, double bond between 5 and 13, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 19, single bond between attom at postion 7 and 13, single bond between attom at postion 7 and 21, single bond between attom at postion 7 and 22, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 14, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 16, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 18. The 3D x,y,z coordinates of the element at position 1 is -0.2462, 2.8626, 0.8366, . The 3D x,y,z coordinates of the element at position 2 is -1.2009, 2.2944, -1.1424, . The 3D x,y,z coordinates of the element at position 3 is 3.748, -

This compound's CID is 123631 and compound's name is Gefitinib. There are 55 attoms in the molecule and their positions in the order are CL, X, O, O, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 29, single bond between attom at postion 2 and 31, single bond between attom at postion 3 and 14, single bond between attom at postion 3 and 15, single bond between attom at postion 4 and 16, single bond between attom at postion 4 and 17, single bond between attom at postion 5 and 20, single bond between attom at postion 5 and 26, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 48, single bond between attom at postion 8 and 21, double bond between 8 and 25, double bond between 9 and 23, single bond between attom at postion 9 and 25, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 32, single bond between attom at postion 10 and 33, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 34, single bond between attom at postion 11 and 35, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 36, single bond between attom at postion 12 and 37, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 38, single bond between attom at postion 13 and 39, single bond between attom at postion 14 and 40, single bond between attom at postion 14 and 41, single bond between attom at postion 15 and 42, single bond between attom at postion 15 and 43, single bond between attom at postion 16 and 44, single bond between attom at postion 16 and 45, single bond between attom at postion 17 and 19, double bond between 17 and 20, double bond between 18 and 19, single bond between attom at postion 18 and 21, single bond between attom at postion 18 and 23, single bond between attom at postion 19 and 46, single bond between attom at postion 20 and 22, double bond between 21 and 22, single bond between attom at postion 22 and 47, double bond between 24 and 27, single bond between attom at postion 24 and 28, single bond between attom at postion 25 and 49, single bond between attom at postion 26 and 52, single bond between attom at postion 26 and 53, single bond between attom at postion 26 and 54, single bond between attom at postion 27 and 29, single bond between attom at postion 27 and 50, double bond between 28 and 30, single bond between attom at postion 28 and 51, double bond between 29 and 31, single bond between attom at postion 30 and 31, single bond between attom at postion 30 and 55. The 3D x,y,z coordinates of the element at position 1 is -5.7668, 0.3787, 2.1969, . The 3D x,y,z coordinates of the element at position 2 is -6.5134, -0.4026, -0.5639, . The 3D x,y,z

This compound's CID is 124087 and compound's name is Desloratadine. There are 41 attoms in the molecule and their positions in the order are CL, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 35, single bond between attom at postion 3 and 11, double bond between 3 and 22, double bond between 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 10, single bond between attom at postion 5 and 11, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 23, single bond between attom at postion 6 and 24, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 25, single bond between attom at postion 7 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 9 and 30, double bond between 10 and 13, single bond between attom at postion 10 and 16, double bond between 11 and 15, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 31, single bond between attom at postion 12 and 32, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 33, single bond between attom at postion 14 and 34, single bond between attom at postion 15 and 18, double bond between 16 and 19, single bond between attom at postion 16 and 36, double bond between 17 and 20, single bond between attom at postion 17 and 37, double bond between 18 and 21, single bond between attom at postion 18 and 38, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 39, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 40, single bond between attom at postion 22 and 41. The 3D x,y,z coordinates of the element at position 1 is 5.6939, 0.3386, -0.2228, . The 3D x,y,z coordinates of the element at position 2 is -2.0074, -3.8596, 0.6975, . The 3D x,y,z coordinates

This compound's CID is 124886 and compound's name is Glutathione. There are 37 attoms in the molecule and their positions in the order are S, O, O, O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 16, single bond between attom at postion 1 and 35, double bond between 2 and 15, double bond between 3 and 17, single bond between attom at postion 4 and 18, single bond between attom at postion 4 and 36, double bond between 5 and 18, single bond between attom at postion 6 and 20, single bond between attom at postion 6 and 37, double bond between 7 and 20, single bond between attom at postion 8 and 13, single bond between attom at postion 8 and 15, single bond between attom at postion 8 and 27, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 30, single bond between attom at postion 9 and 31, single bond between attom at postion 10 and 17, single bond between attom at postion 10 and 19, single bond between attom at postion 10 and 32, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 23, single bond between attom at postion 12 and 24, single bond between attom at postion 13 and 16, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 25, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 26, single bond between attom at postion 16 and 28, single bond between attom at postion 16 and 29, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 33, single bond between attom at postion 19 and 34. The 3D x,y,z coordinates of the element at position 1 is -1.7509, -1.5088, -2.1175, . The 3D x,y,z coordinates of the element at position 2 is 1.2983, 2.0308, -0.8892, . The 3D x,y,z coordinates of the element at

This compound's CID is 125017 and compound's name is Desvenlafaxine. There are 44 attoms in the molecule and their positions in the order are O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 4, single bond between attom at postion 1 and 33, single bond between attom at postion 2 and 19, single bond between attom at postion 2 and 44, single bond between attom at postion 3 and 11, single bond between attom at postion 3 and 15, single bond between attom at postion 3 and 16, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 20, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 21, single bond between attom at postion 6 and 22, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 23, single bond between attom at postion 7 and 24, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, double bond between 12 and 13, single bond between attom at postion 12 and 14, single bond between attom at postion 13 and 17, single bond between attom at postion 13 and 34, double bond between 14 and 18, single bond between attom at postion 14 and 35, single bond between attom at postion 15 and 36, single bond between attom at postion 15 and 37, single bond between attom at postion 15 and 38, single bond between attom at postion 16 and 39, single bond between attom at postion 16 and 40, single bond between attom at postion 16 and 41, double bond between 17 and 19, single bond between attom at postion 17 and 42, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 43. The 3D x,y,z coordinates of the element at position 1 is -1.3482, 0.591, -1.4914, . The 3D x,y,z coordinates of the element at position 2 is 4.4342, 2.2329, -0.2134, . The 3D x,y,z coordinates

This compound's CID is 126941 and compound's name is Methotrexate. There are 55 attoms in the molecule and their positions in the order are O, O, O, O, O, N, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 23, single bond between attom at postion 1 and 50, double bond between 2 and 20, double bond between 3 and 23, single bond between attom at postion 4 and 28, single bond between attom at postion 4 and 51, double bond between 5 and 28, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 18, single bond between attom at postion 6 and 27, single bond between attom at postion 7 and 14, single bond between attom at postion 7 and 20, single bond between attom at postion 7 and 39, single bond between attom at postion 8 and 26, double bond between 8 and 30, single bond between attom at postion 9 and 29, double bond between 9 and 31, single bond between attom at postion 10 and 31, double bond between 10 and 33, double bond between 11 and 32, single bond between attom at postion 11 and 33, single bond between attom at postion 12 and 32, single bond between attom at postion 12 and 52, single bond between attom at postion 12 and 53, single bond between attom at postion 13 and 33, single bond between attom at postion 13 and 54, single bond between attom at postion 13 and 55, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 23, single bond between attom at postion 14 and 34, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 35, single bond between attom at postion 15 and 36, double bond between 16 and 21, single bond between attom at postion 16 and 22, single bond between attom at postion 17 and 28, single bond between attom at postion 17 and 37, single bond between attom at postion 17 and 38, single bond between attom at postion 18 and 26, single bond between attom at postion 18 and 40, single bond between attom at postion 18 and 41, single bond between attom at postion 19 and 20, double bond between 19 and 24, single bond between attom at postion 19 and 25, single bond between attom at postion 21 and 24, single bond between attom at postion 21 and 42, double bond between 22 and 25, single bond between attom at postion 22 and 43, single bond between attom at postion 24 and 44, single bond between attom at postion 25 and 45, double bond between 26 and 29, single bond between attom at postion 27 and 46, single bond between attom at postion 27 and 47, single bond between attom at postion 27 and 48, single bond between attom at postion 29 and 49, single bond between attom at postion 30 and 31, single bond between attom at postion 30 and 32. The 3D x,y,z coordinates of the element at position 1 is 6.6948, -0.364, -2.1205, . The 3D x,y,z coordinates of the element at position 2 is 4.0713, This compound's CID is 129228 and compound's name is Rufinamide. There are 25 attoms in the molecule and their positions in the order are X, X, O, N, N, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 2 and 12, double bond between 3 and 17, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 10, double bond between 5 and 6, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 18, single bond between attom at postion 8 and 19, double bond between 9 and 11, single bond between attom at postion 9 and 12, double bond between 10 and 13, single bond between attom at postion 10 and 20, single bond between attom at postion 11 and 14, double bond between 12 and 15, single bond between attom at postion 13 and 17, double bond between 14 and 16, single bond between attom at postion 14 and 21, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 22, single bond between attom at postion 16 and 23. The 3D x,y,z coordinates of the element at position 1 is -1.3962, 2.2795, -0.8993, . The 3D x,y,z coordinates of the element at position 2 is -2.1272, -2.3436, -0.1035, . The 3D x,y,z

This compound's CID is 130881 and compound's name is Olmesartan Medoxomil. There are 71 attoms in the molecule and their positions in the order are O, O, O, O, O, O, N, N, N, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 13, single bond between attom at postion 1 and 54, single bond between attom at postion 2 and 23, single bond between attom at postion 2 and 31, double bond between 3 and 23, single bond between attom at postion 4 and 34, single bond between attom at postion 4 and 41, single bond between attom at postion 5 and 38, single bond between attom at postion 5 and 41, double bond between 6 and 41, single bond between attom at postion 7 and 15, single bond between attom at postion 7 and 16, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 14, double bond between 8 and 16, single bond between attom at postion 9 and 11, double bond between 9 and 37, double bond between 10 and 12, single bond between attom at postion 10 and 37, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 71, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 19, single bond between attom at postion 13 and 20, double bond between 14 and 15, single bond between attom at postion 15 and 23, single bond between attom at postion 16 and 18, single bond between attom at postion 17 and 21, single bond between attom at postion 17 and 42, single bond between attom at postion 17 and 43, single bond between attom at postion 18 and 22, single bond between attom at postion 18 and 44, single bond between attom at postion 18 and 45, single bond between attom at postion 19 and 46, single bond between attom at postion 19 and 47, single bond between attom at postion 19 and 48, single bond between attom at postion 20 and 49, single bond between attom at postion 20 and 50, single bond between attom at postion 20 and 51, double bond between 21 and 24, single bond between attom at postion 21 and 25, single bond between attom at postion 22 and 26, single bond between attom at postion 22 and 52, single bond between attom at postion 22 and 53, single bond between attom at postion 24 and 28, single bond between attom at postion 24 and 55, double bond between 25 and 29, single bond between attom at postion 25 and 56, single bond between attom at postion 26 and 57, single bond between attom at postion 26 and 58, single bond between attom at postion 26 and 59, double bond between 27 and 28, single bond between attom at postion 27 and 29, single bond between attom at postion 27 and 30, single bond between attom at postion 28 and 60, single bond between attom at postion 29 and 61, single bond between attom at postion 30 and 32, double bond between 30 and 33, single bond between attom at postion 31 and 34, single bond between attom at postion 31 and 62, single bond between attom at postion 31 and 63, double bond between 32 and 35, single bond between attom at postion 32 and 37, single bond between attom at

This compound's CID is 131204 and compound's name is Dexpanthenol. There are 33 attoms in the molecule and their positions in the order are O, O, O, O, N, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 7, single bond between attom at postion 1 and 27, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 30, double bond between 3 and 11, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 33, single bond between attom at postion 5 and 11, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 9, single bond between attom at postion 6 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 7 and 15, single bond between attom at postion 8 and 16, single bond between attom at postion 8 and 17, single bond between attom at postion 9 and 18, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 12 and 13, single bond between attom at postion 12 and 25, single bond between attom at postion 12 and 26, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 28, single bond between attom at postion 13 and 29, single bond between attom at postion 14 and 31, single bond between attom at postion 14 and 32. The 3D x,y,z coordinates of the element at position 1 is 1.1437, -2.2261, -0.448, . The 3D x,y,z coordinates of the element at position 2 is 3.2891, 2.1521, -0.077, . The 3D x,y,z coordinates of the element at position 3 is -0.2801, -1.1191, 1.5659, . The 3D x,y,z

This compound's CID is 134018 and compound's name is Febuxostat. There are 38 attoms in the molecule and their positions in the order are S, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 1 and 19, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 11, single bond between attom at postion 3 and 22, single bond between attom at postion 3 and 38, double bond between 4 and 22, double bond between 5 and 17, single bond between attom at postion 5 and 18, triple bond between 6 and 21, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 23, single bond between attom at postion 8 and 24, single bond between attom at postion 8 and 25, single bond between attom at postion 9 and 26, single bond between attom at postion 9 and 27, single bond between attom at postion 9 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, double bond between 11 and 13, single bond between attom at postion 11 and 14, double bond between 12 and 15, single bond between attom at postion 12 and 16, single bond between attom at postion 12 and 17, single bond between attom at postion 13 and 15, single bond between attom at postion 13 and 21, double bond between 14 and 16, single bond between attom at postion 14 and 32, single bond between attom at postion 15 and 33, single bond between attom at postion 16 and 34, double bond between 18 and 19, single bond between attom at postion 18 and 20, single bond between attom at postion 19 and 22, single bond between attom at postion 20 and 35, single bond between attom at postion 20 and 36, single bond between attom at postion 20 and 37. The 3D x,y,z coordinates of the element at position 1 is -2.7288, 0.9775, -0.3464, . The 3D x,y,z coordinates of the element at position 2 is 3.6923, -0.2719, 0.5275, . The 3D x,y,z coordinates of the element at position 3 is -

This compound's CID is 134780 and compound's name is Pomalidomide. There are 31 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 11, double bond between 2 and 12, double bond between 3 and 13, double bond between 4 and 16, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 12, single bond between attom at postion 5 and 13, single bond between attom at postion 6 and 11, single bond between attom at postion 6 and 16, single bond between attom at postion 6 and 26, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 30, single bond between attom at postion 7 and 31, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 10, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 12 and 14, single bond between attom at postion 13 and 15, double bond between 14 and 15, single bond between attom at postion 14 and 17, single bond between attom at postion 15 and 18, double bond between 17 and 19, double bond between 18 and 20, single bond between attom at postion 18 and 27, single bond between attom at postion 19 and 20, single bond between attom at postion 19 and 28, single bond between attom at postion 20 and 29. The 3D x,y,z coordinates of the element at position 1 is -1.5507, -0.05, 2.1528, . The 3D x,y,z coordinates of the element at position 2 is 0.89, 2.3869, -0.0163, . The 3D x,y,z coordinates of the
This compound's CID is 150311 and compound's name is Ezetimibe. There are 51 attoms in the molecule and their positions in the order are X, X, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 27, single bond between attom at postion 2 and 30, double bond between 3 and 10, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 44, single bond between attom at postion 5 and 22, single bond between attom at postion 5 and 51, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 13, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 31, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 32, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 33, single bond between attom at postion 9 and 34, double bond between 11 and 15, single bond between attom at postion 11 and 16, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 35, single bond between attom at postion 12 and 36, double bond between 13 and 17, single bond between attom at postion 13 and 18, single bond between attom at postion 14 and 19, single bond between attom at postion 14 and 37, single bond between attom at postion 15 and 20, single bond between attom at postion 15 and 38, double bond between 16 and 21, single bond between attom at postion 16 and 39, single bond between attom at postion 17 and 23, single bond between attom at postion 17 and 40, double bond between 18 and 24, single bond between attom at postion 18 and 41, double bond between 19 and 25, single bond between attom at postion 19 and 26, double bond between 20 and 22, single bond between attom at postion 20 and 42, single bond between attom at postion 21 and 22, single bond between attom at postion 21 and 43, double bond between 23 and 27, single bond between attom at postion 23 and 45, single bond between attom at postion 24 and 27, single bond between attom at postion 24 and 46, single bond between attom at postion 25 and 28, single bond between attom at postion 25 and 47, double bond between 26 and 29, single bond between attom at postion 26 and 48, double bond between 28 and 30, single bond between attom at postion 28 and 49, single bond between attom at postion 29 and 30, single bond between attom at postion 29 and 50. The 3D x,y,z coordinates of the element at position 1 is -7.0846, -1.4757, 1.9034, . The 3D x,y,z coordinates of the element at position 2 is 7.9957, 0.9111, 0.9707, . The 3D x,y,z

This compound's CID is 151075 and compound's name is Nepafenac. There are 33 attoms in the molecule and their positions in the order are O, O, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 11, double bond between 2 and 14, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 25, single bond between attom at postion 3 and 26, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 32, single bond between attom at postion 4 and 33, double bond between 5 and 6, single bond between attom at postion 5 and 8, single bond between attom at postion 5 and 9, single bond between attom at postion 6 and 7, double bond between 7 and 10, single bond between attom at postion 7 and 11, single bond between attom at postion 8 and 14, single bond between attom at postion 8 and 20, single bond between attom at postion 8 and 21, double bond between 9 and 12, single bond between attom at postion 9 and 22, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 23, single bond between attom at postion 11 and 13, single bond between attom at postion 12 and 24, double bond between 13 and 15, single bond between attom at postion 13 and 16, single bond between attom at postion 15 and 17, single bond between attom at postion 15 and 27, double bond between 16 and 18, single bond between attom at postion 16 and 28, double bond between 17 and 19, single bond between attom at postion 17 and 29, single bond between attom at postion 18 and 19, single bond between attom at postion 18 and 30, single bond between attom at postion 19 and 31. The 3D x,y,z coordinates of the element at position 1 is -1.7282, -1.9653, -1.4652, . The 3D x,y,z coordinates of the element at position 2 is 2.9732, 1.949,
This compound's CID is 153994 and compound's name is Clevidipine. There are 53 attoms in the molecule and their positions in the order are CL, CL, O, O, O, O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 20, single bond between attom at postion 2 and 22, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 25, single bond between attom at postion 4 and 19, single bond between attom at postion 4 and 26, double bond between 5 and 16, double bond between 6 and 19, single bond between attom at postion 7 and 25, single bond between attom at postion 7 and 29, double bond between 8 and 29, single bond between attom at postion 9 and 14, single bond between attom at postion 9 and 15, single bond between attom at postion 9 and 32, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 10 and 13, single bond between attom at postion 10 and 31, double bond between 11 and 14, single bond between attom at postion 11 and 16, double bond between 12 and 15, single bond between attom at postion 12 and 19, double bond between 13 and 20, single bond between attom at postion 13 and 21, single bond between attom at postion 14 and 17, single bond between attom at postion 15 and 18, single bond between attom at postion 17 and 33, single bond between attom at postion 17 and 34, single bond between attom at postion 17 and 35, single bond between attom at postion 18 and 36, single bond between attom at postion 18 and 37, single bond between attom at postion 18 and 38, single bond between attom at postion 20 and 22, double bond between 21 and 23, single bond between attom at postion 21 and 39, double bond between 22 and 24, single bond between attom at postion 23 and 24, single bond between attom at postion 23 and 40, single bond between attom at postion 24 and 41, single bond between attom at postion 25 and 42, single bond between attom at postion 25 and 43, single bond between attom at postion 26 and 44, single bond between attom at postion 26 and 45, single bond between attom at postion 26 and 46, single bond between attom at postion 27 and 28, single bond between attom at postion 27 and 29, single bond between attom at postion 27 and 47, single bond between attom at postion 27 and 48, single bond between attom at postion 28 and 30, single bond between attom at postion 28 and 49, single bond between attom at postion 28 and 50, single bond between attom at postion 30 and 51, single bond between attom at postion 30 and 52, single bond between attom at postion 30 and 53. The 3D x,y,z coordinates of the element at position 1 is 0.3833, -1.886, 1.8815, . The 3D x,y,z coordinates of the element at position 2 is 2.3481, -

This compound's CID is 156391 and compound's name is Naproxen. There are 31 attoms in the molecule and their positions in the order are O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 14, single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 15, single bond between attom at postion 2 and 28, double bond between 3 and 15, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 11, single bond between attom at postion 4 and 15, single bond between attom at postion 4 and 18, double bond between 5 and 8, single bond between attom at postion 5 and 9, double bond between 6 and 7, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 12, single bond between attom at postion 7 and 10, single bond between attom at postion 7 and 13, single bond between attom at postion 8 and 19, double bond between 9 and 10, single bond between attom at postion 9 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 11 and 24, double bond between 12 and 16, single bond between attom at postion 12 and 25, double bond between 13 and 14, single bond between attom at postion 13 and 26, single bond between attom at postion 14 and 16, single bond between attom at postion 16 and 27, single bond between attom at postion 17 and 29, single bond between attom at postion 17 and 30, single bond between attom at postion 17 and 31. The 3D x,y,z coordinates of the element at position 1 is -4.6881, -0.1815, -0.2526, . The 3D x,y,z coordinates of the element at position 2 is 5.0783, 0.7631, -0.4703, . The 3D x,y,z coordinates of the element at position 3 is 3.0804, 1.2333, -

This compound's CID is 157920 and compound's name is Lubiprostone. There are 59 attoms in the molecule and their positions in the order are X, X, O, O, O, O, O, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 9, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 13, single bond between attom at postion 4 and 43, double bond between 5 and 15, single bond between attom at postion 6 and 27, single bond between attom at postion 6 and 59, double bond between 7 and 27, single bond between attom at postion 8 and 9, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 28, single bond between attom at postion 9 and 12, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 15, single bond between attom at postion 10 and 16, single bond between attom at postion 10 and 30, single bond between attom at postion 11 and 14, single bond between attom at postion 11 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 15, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 13 and 14, single bond between attom at postion 13 and 17, single bond between attom at postion 14 and 35, single bond between attom at postion 14 and 36, single bond between attom at postion 16 and 18, single bond between attom at postion 16 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 19, single bond between attom at postion 18 and 20, single bond between attom at postion 18 and 39, single bond between attom at postion 18 and 40, single bond between attom at postion 19 and 21, single bond between attom at postion 19 and 41, single bond between attom at postion 19 and 42, single bond between attom at postion 20 and 22, single bond between attom at postion 20 and 44, single bond between attom at postion 20 and 45, single bond between attom at postion 21 and 23, single bond between attom at postion 21 and 46, single bond between attom at postion 21 and 47, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 48, single bond between attom at postion 22 and 49, single bond between attom at postion 23 and 26, single bond between attom at postion 23 and 50, single bond between attom at postion 23 and 51, single bond between attom at postion 24 and 25, single bond between attom at postion 24 and 52, single bond between attom at postion 24 and 53, single bond between attom at postion 25 and 27, single bond between attom at postion 25 and 54, single bond between attom at postion 25 and 55, single bond between attom at postion 26 and 56, single bond between attom at postion 26 and 57, single bond between attom at postion 26 and 58. The 3D x,y,z coordinates of the element at position 1 is 4.6832, -0.0979,

This compound's CID is 159055 and compound's name is Camphor (synthetic). There are 27 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: double bond between 1 and 8, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 9, single bond between attom at postion 2 and 10, single bond between attom at postion 3 and 5, single bond between attom at postion 3 and 8, single bond between attom at postion 3 and 11, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 14, single bond between attom at postion 6 and 15, single bond between attom at postion 6 and 16, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 17, single bond between attom at postion 7 and 18, single bond between attom at postion 9 and 19, single bond between attom at postion 9 and 20, single bond between attom at postion 9 and 21, single bond between attom at postion 10 and 22, single bond between attom at postion 10 and 23, single bond between attom at postion 10 and 24, single bond between attom at postion 11 and 25, single bond between attom at postion 11 and 26, single bond between attom at postion 11 and 27. The 3D x,y,z coordinates of the element at position 1 is -2.5236, 0.3669, 0.2597, . The 3D x,y,z coordinates of the element at

This compound's CID is 163091 and compound's name is Asenapine. There are 36 attoms in the molecule and their positions in the order are CL, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 17, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 12, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 7, single bond between attom at postion 3 and 10, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 8, single bond between attom at postion 4 and 21, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 22, single bond between attom at postion 6 and 23, single bond between attom at postion 6 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 7 and 26, double bond between 8 and 11, single bond between attom at postion 8 and 13, single bond between attom at postion 9 and 12, double bond between 9 and 14, single bond between attom at postion 10 and 27, single bond between attom at postion 10 and 28, single bond between attom at postion 10 and 29, single bond between attom at postion 11 and 15, double bond between 12 and 16, double bond between 13 and 17, single bond between attom at postion 13 and 30, single bond between attom at postion 14 and 18, single bond between attom at postion 14 and 31, double bond between 15 and 19, single bond between attom at postion 15 and 32, single bond between attom at postion 16 and 20, single bond between attom at postion 16 and 33, single bond between attom at postion 17 and 19, double bond between 18 and 20, single bond between attom at postion 18 and 34, single bond between attom at postion 19 and 35, single bond between attom at postion 20 and 36. The 3D x,y,z coordinates of the element at position 1 is -5.0684, 0.3077, -1.0753, . The 3D x,y,z coordinates of This compound's CID is 165675 and compound's name is (+)-Menthol. There are 31 attoms in the molecule and their positions in the order are O, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 3, single bond between attom at postion 1 and 31, single bond between attom at postion 2 and 3, single bond between attom at postion 2 and 4, single bond between attom at postion 2 and 8, single bond between attom at postion 2 and 12, single bond between attom at postion 3 and 6, single bond between attom at postion 3 and 13, single bond between attom at postion 4 and 7, single bond between attom at postion 4 and 14, single bond between attom at postion 4 and 15, single bond between attom at postion 5 and 6, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 16, single bond between attom at postion 6 and 17, single bond between attom at postion 6 and 18, single bond between attom at postion 7 and 19, single bond between attom at postion 7 and 20, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 11, single bond between attom at postion 8 and 21, single bond between attom at postion 9 and 22, single bond between attom at postion 9 and 23, single bond between attom at postion 9 and 24, single bond between attom at postion 10 and 25, single bond between attom at postion 10 and 26, single bond between attom at postion 10 and 27, single bond between attom at postion 11 and 28, single bond between attom at postion 11 and 29, single bond between attom at postion 11 and 30. The 3D x,y,z coordinates of the element at position 1 is -0.4171, 2.3655, 0.4211, . The 3D x,y,z coordinates of the element at position 2 is -0.7057, -0.0352, 0.4282, . The 3D x,y,z

This compound's CID is 171548 and compound's name is Biotin. There are 32 attoms in the molecule and their positions in the order are S, O, O, O, N, N, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 9, single bond between attom at postion 1 and 10, double bond between 2 and 13, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 32, double bond between 4 and 16, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 24, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 13, single bond between attom at postion 6 and 25, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 9, single bond between attom at postion 7 and 17, single bond between attom at postion 8 and 10, single bond between attom at postion 8 and 18, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 19, single bond between attom at postion 10 and 20, single bond between attom at postion 10 and 21, single bond between attom at postion 11 and 12, single bond between attom at postion 11 and 22, single bond between attom at postion 11 and 23, single bond between attom at postion 12 and 14, single bond between attom at postion 12 and 26, single bond between attom at postion 12 and 27, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 28, single bond between attom at postion 14 and 29, single bond between attom at postion 15 and 16, single bond between attom at postion 15 and 30, single bond between attom at postion 15 and 31. The 3D x,y,z coordinates of the element at position 1 is -2.4613, 1.9562, 1.0264, . The 3D x,y,z coordinates of the element at
This compound's CID is 174174 and compound's name is Atropine. There are 44 attoms in the molecule and their positions in the order are O, O, O, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 11, single bond between attom at postion 1 and 13, double bond between 2 and 13, single bond between attom at postion 3 and 16, single bond between attom at postion 3 and 41, single bond between attom at postion 4 and 5, single bond between attom at postion 4 and 6, single bond between attom at postion 4 and 12, single bond between attom at postion 5 and 7, single bond between attom at postion 5 and 9, single bond between attom at postion 5 and 22, single bond between attom at postion 6 and 8, single bond between attom at postion 6 and 10, single bond between attom at postion 6 and 23, single bond between attom at postion 7 and 8, single bond between attom at postion 7 and 24, single bond between attom at postion 7 and 25, single bond between attom at postion 8 and 26, single bond between attom at postion 8 and 27, single bond between attom at postion 9 and 11, single bond between attom at postion 9 and 28, single bond between attom at postion 9 and 29, single bond between attom at postion 10 and 11, single bond between attom at postion 10 and 30, single bond between attom at postion 10 and 31, single bond between attom at postion 11 and 32, single bond between attom at postion 12 and 33, single bond between attom at postion 12 and 34, single bond between attom at postion 12 and 35, single bond between attom at postion 13 and 14, single bond between attom at postion 14 and 15, single bond between attom at postion 14 and 16, single bond between attom at postion 14 and 36, double bond between 15 and 17, single bond between attom at postion 15 and 18, single bond between attom at postion 16 and 37, single bond between attom at postion 16 and 38, single bond between attom at postion 17 and 19, single bond between attom at postion 17 and 39, double bond between 18 and 20, single bond between attom at postion 18 and 40, double bond between 19 and 21, single bond between attom at postion 19 and 42, single bond between attom at postion 20 and 21, single bond between attom at postion 20 and 43, single bond between attom at postion 21 and 44. The 3D x,y,z coordinates of the element at position 1 is -0.3627, 0.3694, 0.8291, . The 3D x,y,z coordinates of the element at position 2 is 0.6817, -0.5873, -0.987, . The 3D x,y,z

This compound's CID is 176870 and compound's name is Erlotinib. There are 52 attoms in the molecule and their positions in the order are O, O, O, O, N, N, N, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, C, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H, H. The bonds between them are: single bond between attom at postion 1 and 10, single bond between attom at postion 1 and 15, single bond between attom at postion 2 and 11, single bond between attom at postion 2 and 17, single bond between attom at postion 3 and 19, single bond between attom at postion 3 and 26, single bond between attom at postion 4 and 20, single bond between attom at postion 4 and 27, single bond between attom at postion 5 and 13, single bond between attom at postion 5 and 16, single bond between attom at postion 5 and 32, single bond between attom at postion 6 and 9, double bond between 6 and 18, double bond between 7 and 13, single bond between attom at postion 7 and 18, single bond between attom at postion 8 and 9, double bond between 8 and 12, single bond between attom at postion 8 and 13, double bond between 9 and 14, double bond between 10 and 11, single bond between attom at postion 10 and 12, single bond between attom at postion 11 and 14, single bond between attom at postion 12 and 30, single bond between attom at postion 14 and 31, single bond between attom at postion 15 and 19, single bond between attom at postion 15 and 33, single bond between attom at postion 15 and 34, single bond between attom at postion 16 and 21, double bond between 16 and 22, single bond between attom at postion 17 and 20, single bond between attom at postion 17 and 35, single bond between attom at postion 17 and 36, single bond between attom at postion 18 and 37, single bond between attom at postion 19 and 38, single bond between attom at postion 19 and 39, single bond between attom at postion 20 and 40, single bond between attom at postion 20 and 41, double bond between 21 and 23, single bond between attom at postion 21 and 42, single bond between attom at postion 22 and 24, single bond between attom at postion 22 and 43, single bond between attom at postion 23 and 25, single bond between attom at postion 23 and 28, double bond between 24 and 25, single bond between attom at postion 24 and 44, single bond between attom at postion 25 and 45, single bond between attom at postion 26 and 46, single bond between attom at postion 26 and 47, single bond between attom at postion 26 and 48, single bond between attom at postion 27 and 49, single bond between attom at postion 27 and 50, single bond between attom at postion 27 and 51, triple bond between 28 and 29, single bond between attom at postion 29 and 52. The 3D x,y,z coordinates of the element at position 1 is -2.4158, -1.4991, -0.9374, . The 3D x,y,z coordinates of the element at position 2 is -3.7833, 0.8252, -