Molecular Coding Format examples
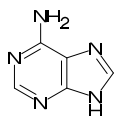
Author : Akira Yamaji   Date : September 20, 2021
Located at : http://www.ctan.org/pkg/mcf2graph

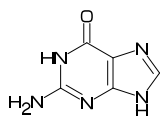** use molecular data base file 'mcf_data_base.mcf'

Adenine
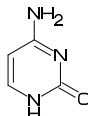MW:135.1267 / FM:C5H5N5
MW:135.13 (data) / [1]

Guanine
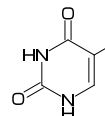MW:151.1261 / FM:C5H5N5O
MW:151.13 (data) / [2]

Cytosine
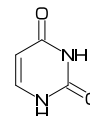MW:111.1019 / FM:C4H5N3O
MW:111.10 (data) / [3]

Thymine
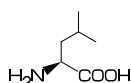MW:126.1133 / FM:C5H6N2O2
MW:126.11 (data) / [4]

Uracil
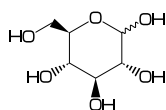MW:112.0867 / FM:C4H4N2O2
MW:112.09 (data) / [5]

L-Leucine
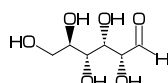MW:131.1729 / FM:C6H13NO2
MW:131.16 (data) / [6]

Glucose 1
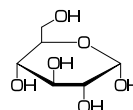MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [7]

Glucose 2
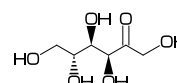MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [8]

D-Glucose
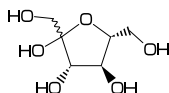MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [9]

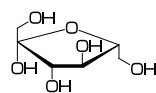**Fructose 1**
MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [10]
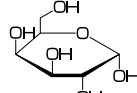
Fructose 2
MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [11]

D-Fluctose
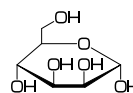MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [12]

D-Galactose
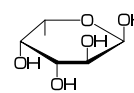MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [13]

D-Mannose
MW:180.1558 / FM:C6H12O6
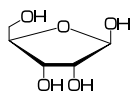MW:180.16 (data) / [14]

L-Fucose
MW:164.1564 / FM:C6H12O5
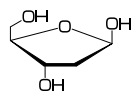MW:164.16 (data) / [15]

D-Ribose
MW:150.1299 / FM:C5H10O5
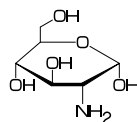MW:150.13 (data) / [16]

D-Deoxyribose
MW:134.1305 / FM:C5H10O4
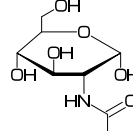MW:134.13 (data) / [17]

D-Glucosamine
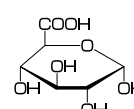MW:179.1711 / FM:C6H13NO5
MW:179.17 (data) / [18]

N-acetyl-Glucosamine
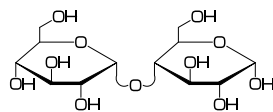MW:221.2077 / FM:C8H15NO6
MW:221.21 (data) / [19]

Glucuronic acid
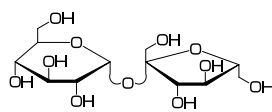MW:194.1393 / FM:C6H10O7
MW:194.14 (data) / [20]

Maltose
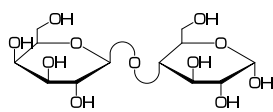MW:342.2964 / FM:C12H22O11
MW:342.3 (data) / [21]

Sucrose
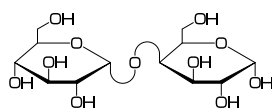MW:342.2964 / FM:C12H22O11
MW:342.3 (data) / [22]

Lactose
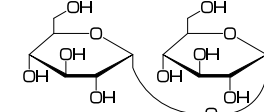MW:342.2964 / FM:C12H22O11
MW:342.3 (data) / [23]

Cellobiose
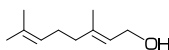MW:342.2964 / FM:C12H22O11
MW:342.3 (data) / [24]

Trehalose
MW:342.2964 / FM:C12H22O11
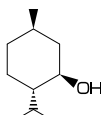MW:342.3 (data) / [25]

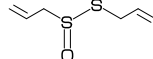**Geraniol**
MW:154.2493 / FM:C10H18O
MW:154.25 (data) / [26]

l-Menthol
MW:156.2652 / FM:C10H20O
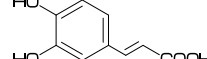MW:156.27 (data) / [27]

Allicin
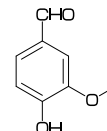MW:162.2729 / FM:C6H10OS2
MW:162.28 (data) / [28]

Caffeic acid
MW:180.1574 / FM:C9H8O4
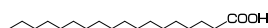MW:180.16 (data) / [29]

Vanillin
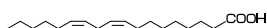MW:152.1473 / FM:C8H8O3
MW:152.15 (data) / [30]

Stearic acid
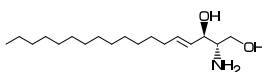MW:284.4772 / FM:C18H36O2
MW:284.48 (data) / [31]

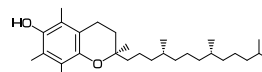**Linoleic acid**
MW:280.4454 / FM:C18H32O2
MW:280.45 (data) / [32]

Sphingosine
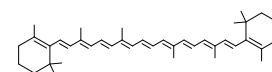MW:299.4918 / FM:C18H37NO2
MW:299.50 (data) / [33]

Tocopherol
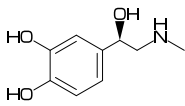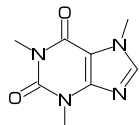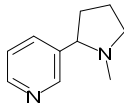MW:430.7060 / FM:C29H50O2
MW:430.717 (data) / [34]

Carotene
MW:536.8726 / FM:C40H56
MW:536.8726 (data) / [35]

Adrenalin
MW:183.2044 / FM:C9H13NO3
MW:183.21 (data) / [36]

Caffeine
MW:194.1905 / FM:C8H10N4O2
MW:194.194 (data) / [37]

Nicotine
MW:162.2315 / FM:C10H14N2
MW:162.23 (data) / [38]

Capsaicin
MW:305.4118 / FM:C18H27NO3
MW:305.418 (data) / [39]
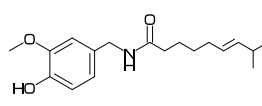
Thiamine
MW:300.8075 / FM:C12H17ClN4OS
MW:300.81 (data) / [40]
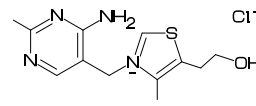
Gibberellin A3
MW:346.3743 / FM:C19H22O6
MW:346.379 (data) / [41]
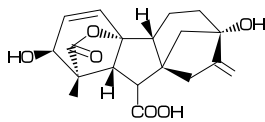
Cholesterol
MW:386.6535 / FM:C27H46O
MW:386.664 (data) / [42]
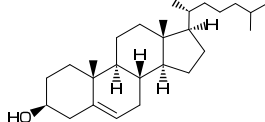
Riboflavin
MW:376.3638 / FM:C17H20N4O6
MW:376.37 (data) / [43]
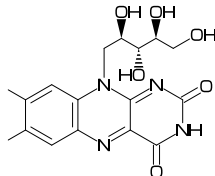
Resveratrol
MW:228.2432 / FM:C14H12O3
MW:228.24 (data) / [44]
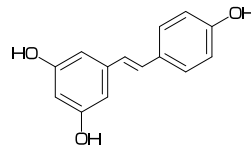
Glutathione
MW:307.3234 / FM:C10H17N3O6S
MW:307.33 (data) / [45]
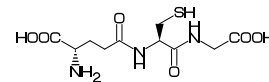
Trenbolone
MW:270.3660 / FM:C18H22O2
MW:270.37 (data) / [46]
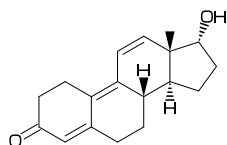
Luciferin
MW:280.3228 / FM:C11H8N2O3S2
MW:280.33 (data) / [47]
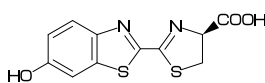
Chlorophyll a
MW:893.4889 / FM:C55H72MgN4O5
MW:893.509 (data) / [48]
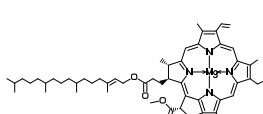
Flavone
MW:222.2386 / FM:C15H10O2
MW:222.24 (data) / [49]
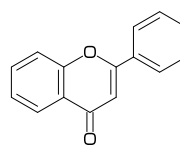
Isoflavone
MW:222.2386 / FM:C15H10O2
MW:222.24 (data) / [50]
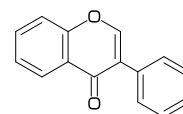
Flavanone
MW:240.2539 / FM:C15H12O3
MW:224.25 (data) / [51]
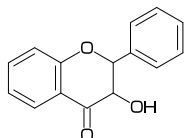
Flavonol
MW:238.2381 / FM:C15H10O3
MW:238.24 (data) / [52]
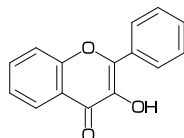
Cianidanol
MW:290.2680 / FM:C15H14O6
MW:290.27 (data) / [53]
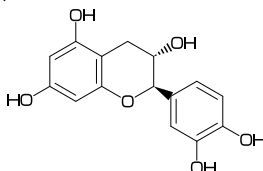
Quercetin
MW:302.2357 / FM:C15H10O7
MW:302.24 (data) / [54]
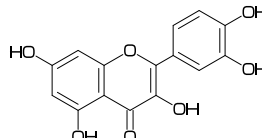
Limonin
MW:470.5115 / FM:C26H30O8
MW:470.518 (data) / [55]
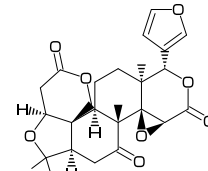
Cromolyn
MW:468.3665 / FM:C23H16O11
MW:468.37 (data) / [56]
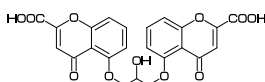
Emetine
MW:480.6388 / FM:C29H40N2O4
MW:480.649 (data) / [57]
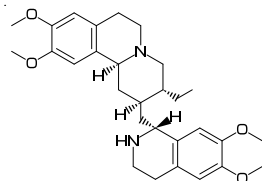
Acronycine
MW:321.3697 / FM:C20H19NO3
MW:321.376 (data) / [58]
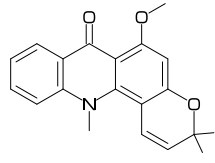
Piperine
MW:285.3376 / FM:C17H19NO3
MW:285.343 (data) / [59]
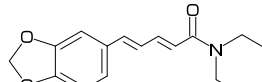
Febrifugine
MW:301.3403 / FM:C16H19N3O3
MW:301.346 (data) / [60]
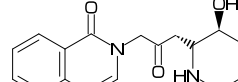
Mitomycine C
MW:334.3272 / FM:C15H18N4O5
MW:334.332 (data) / [61]
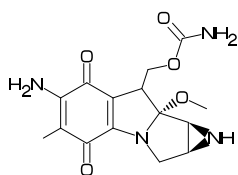
**Podophyllotoxin**
MW:414.4052 / FM:C22H22O8
MW:414.41 (data) / [62]
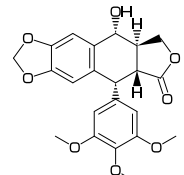
Warfarin
MW:308.3279 / FM:C19H16O4
MW:308.333 (data) / [63]
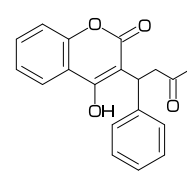
Genistein
MW:270.2368 / FM:C15H10O5
MW:270.24 (data) / [64]
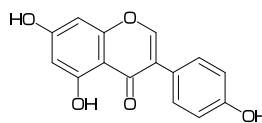
Baicalein
MW:270.2368 / FM:C15H10O5
MW:270.24 (data) / [65]
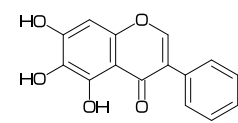
Reserpine
MW:608.6786 / FM:C33H40N2O9
MW:608.688 (data) / [66]
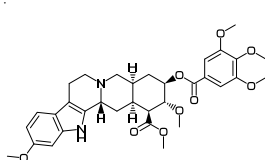
Rotenone
MW:394.4171 / FM:C23H22O6
MW:394.423 (data) / [67]
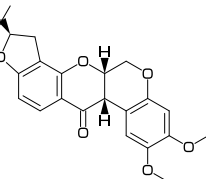
Pyrethrin I
MW:328.4452 / FM:C21H28O3
MW:328.452 (data) / [68]
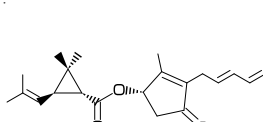
Oseltamivir
MW:312.4045 / FM:C16H28N2O4
MW:312.40 (data) / [69]
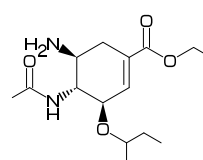
Paclitaxel
MW:853.9061 / FM:C47H51NO14
MW:853.918 (data) / [70]
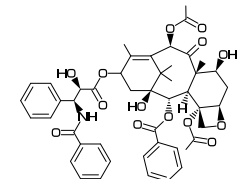
Mevastatin
MW:390.5130 / FM:C23H34O5
MW:390.52 (data) / [71]
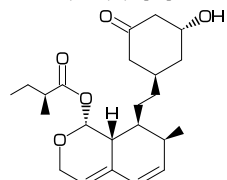
Sesamine
MW:354.3533 / FM:C20H18O6
MW:354.35 (data) / [72]
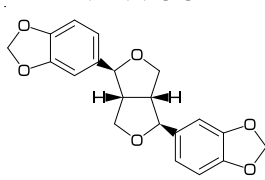
Morphine
MW:285.3376 / FM:C17H19NO3
MW:285.343 (data) / [73]
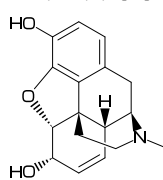
Quinine
MW:324.4167 / FM:C20H24N2O2
MW:324.424 (data) / [74]
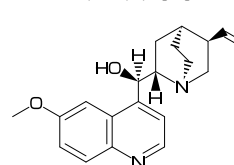
Atoropin
MW:289.3694 / FM:C17H23NO3
MW:289.375 (data) / [75]
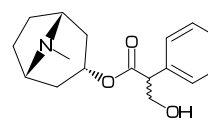
Colchicine
MW:399.4370 / FM:C22H25NO6
MW:399.443 (data) / [76]
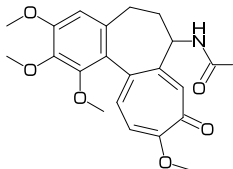
Lycorine
MW:287.3104 / FM:C16H17NO4
MW:287.315 (data) / [77]
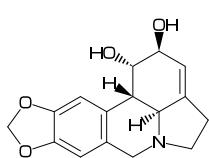
Ibotenic acid
MW:158.1121 / FM:C5H6N2O4
MW:158.113 (data) / [78]
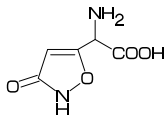
illudin S
MW:264.3168 / FM:C15H20O4
MW:264.3 (data) / [79]
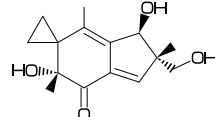
Muscarine
MW:174.2605 / FM:C9H20NO2
MW:174.26 (data) / [80]
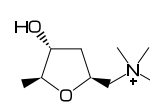
Psilocybin
MW:284.2481 / FM:C12H17N2O4P
MW:284.248 (data) / [81]
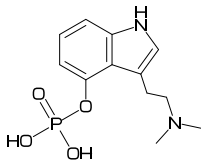
Tetrodotoxine
MW:319.2679 / FM:C11H17N3O8
MW:319.27 (data) / [82]
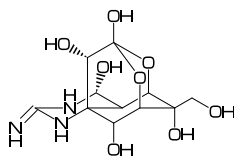
Aflatoxin B1
MW:312.2735 / FM:C17H12O6
MW:312.27 (data) / [83]
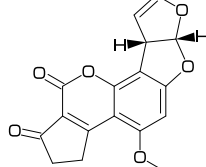
Hexaphenylbenzene
MW:534.6875 / FM:C42H30
MW:534.6876 (data) / [84]
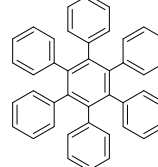
Kekulene
MW:600.7041 / FM:C48H24
MW:600.7 (data) / [85]
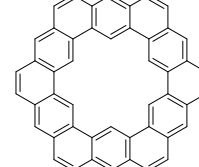
18-Crown-6
MW:264.3153 / FM:C12H24O6
MW:264.32 (data) / [86]
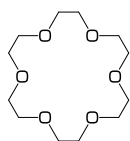
Porphyrin
MW:310.3519 / FM:C20H14N4
MW:310.4 (data) / [87]
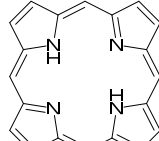
Sulflower
MW:448.6911 / FM:C16S8
MW:448.69 (data) / [88]
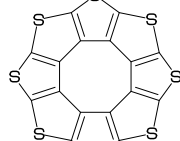
Arsphenamine x5
MW:915.1977 / FM:C30H30As5N5O5
MW:915.2 (data) / [89]
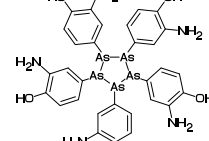
Melamine
MW:126.1199 / FM:C3H6N6
MW:126.12 (data) / [90]
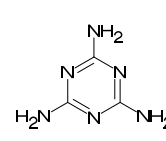
Sudan red 1
MW:248.2792 / FM:C16H12N2O
MW:248.28 (data) / [91]
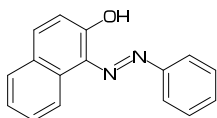
Disperse violet 1
MW:238.2413 / FM:C14H10N2O2
MW:238.25 (data) / [92]
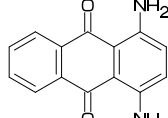
Vat blue 1
MW:262.2627 / FM:C16H10N2O2
MW:262.27 (data) / [93]
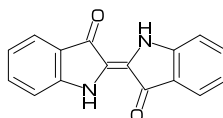
Amoxicillin
MW:365.4041 / FM:C16H19N3O5S
MW:365.4042 (data) / [94]
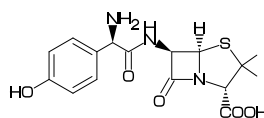
Ampicillin
MW:349.4047 / FM:C16H19N3O4S
MW:349.405 (data) / [95]
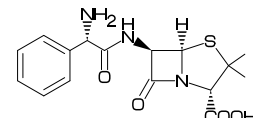
benzyl-Penicillin
MW:334.3901 / FM:C16H18N2O4S
MW:334.4 (data) / [96]
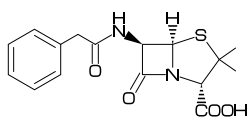
Mecillinam
MW:325.4264 / FM:C15H23N3O3S
MW:325.4264 (data) / [97]
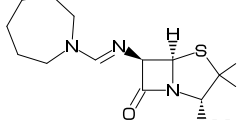
Nafcillin
MW:414.4747 / FM:C21H22N2O5S
MW:414.4748 (data) / [98]
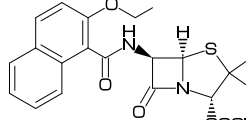
Oxacillin
MW:401.4362 / FM:C19H19N3O5S
MW:401.4363 (data) / [99]
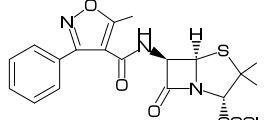
Cloxacillin
MW:435.8813 / FM:C19H18ClN3O5S
MW:435.8813 (data) / [100]
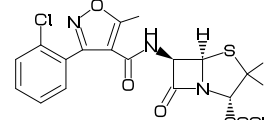
Dicloxacillin
MW:470.3263 / FM:C19H17Cl2N3O5S
MW:470.3264 (data) / [101]
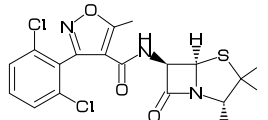
Cefalexin
MW:347.3888 / FM:C16H17N3O4S
MW:347.3889 (data) / [102]
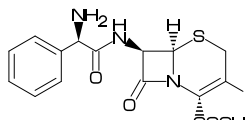
Cefalonium
MW:458.5107 / FM:C20H18N4O5S2
MW:458.5107 (data) / [103]
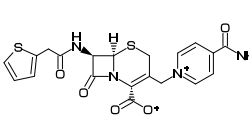
Cefazorin
MW:454.5071 / FM:C14H14N8O4S3
MW:454.51 (data) / [104]
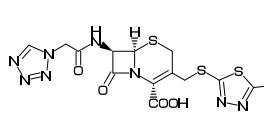
Cefquinome
MW:528.6038 / FM:C23H24N6O5S2
MW:528.6 (data) / [105]
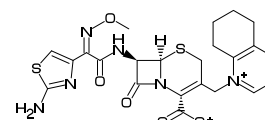
Ceftiofur
MW:523.5625 / FM:C19H17N5O7S3
MW:523.5626 (data) / [106]
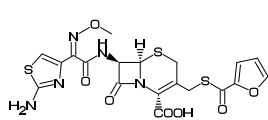
Cefuroxime
MW:424.3852 / FM:C16H16N4O8S
MW:424.3852 (data) / [107]
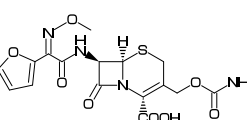
Apramycin
MW:539.5771 / FM:C21H41N5O11
MW:539.58 (data) / [108]
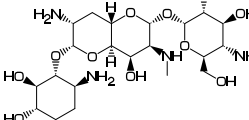
Gentamycin
MW:477.5954 / FM:C21H43N5O7
MW:477.596 (data) / [109]
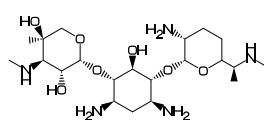
Kanamycin
MW:484.4986 / FM:C18H36N4O11
MW:484.499 (data) / [110]
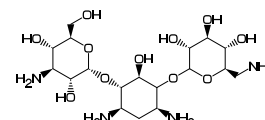
Neomycin
MW:614.6437 / FM:C23H46N6O13
MW:614.644 (data) / [111]
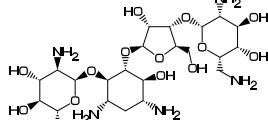
Streptmycin
MW:581.5740 / FM:C21H39N7O12
MW:581.574 (data) / [112]
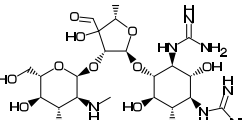
dihydro-Streptmycin
MW:583.5899 / FM:C21H41N7O12
MW:583.574 (data) / [113]
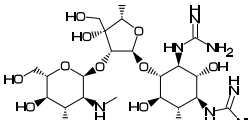
Spectinomycin
MW:332.3495 / FM:C14H24N2O7
MW:332.35 (data) / [114]
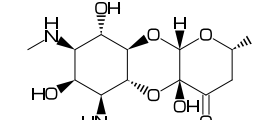
Tobramycin
MW:467.5144 / FM:C18H37N5O9
MW:467.51 (data) / [115]
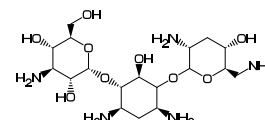
Neospiramycin
MW:698.8842 / FM:C36H62N2O11
MW:698.9 (data) / [116]
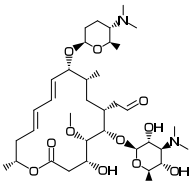
Emamectine
MW:886.1187 / FM:C49H75NO13
MW:886.133 (data) / [117]
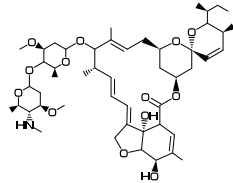
Spinosad
MW:731.9555 / FM:C41H65NO10
MW:731.968 (data) / [118]
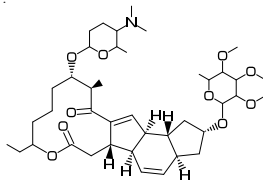
Spiramycin
MW:843.0526 / FM:C43H74N2O14
MW:843.1 (data) / [119]
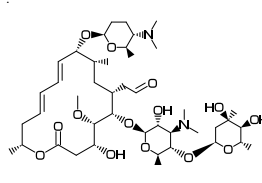
Natamycin
MW:665.7251 / FM:C33H47NO13
MW:665.733 (data) / [120]
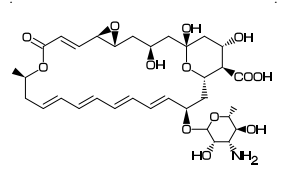
Tylocin
MW:916.1000 / FM:C46H77NO17
MW:916.10 (data) / [121]
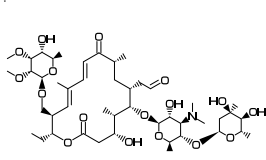
Tilmicosin
MW:869.1330 / FM:C46H80N2O13
MW:869.133 (data) / [122]
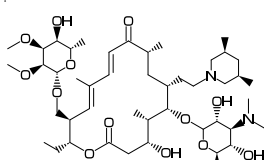
Chlortetracyclin
MW:478.8796 / FM:C22H23ClN2O8
MW:478.88 (data) / [123]
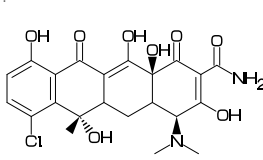
Oxytetracyclin
MW:460.4339 / FM:C22H24N2O9
MW:460.434 (data) / [124]
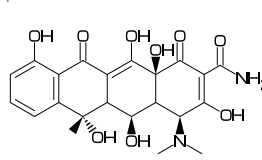
Tetracyclin
MW:444.4345 / FM:C22H24N2O8
MW:444.435 (data) / [125]
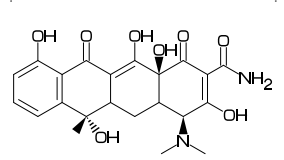
Doxycyclin
MW:444.4345 / FM:C22H24N2O8
MW:444.43 (data) / [126]
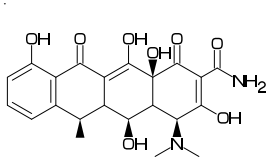
Tiamulin
MW:493.7420 / FM:C28H47NO4S
MW:493.74 (data) / [127]
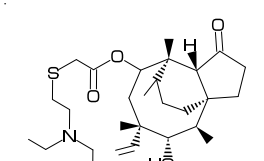
Rifampicin
MW:822.9402 / FM:C43H58N4O12
MW:822.94 (data) / [128]
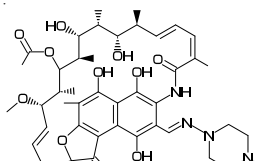
BHC
MW:290.8298 / FM:C6H6Cl6
MW:290.83 (data) / [129]
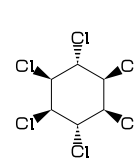
pp-DDT
MW:354.4862 / FM:C14H9Cl5
MW:354.49 (data) / [130]
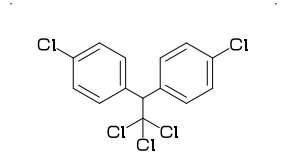
Acrinathrin
MW:541.4390 / FM:C26H21F6NO5
MW:541.45 (data) / [131]
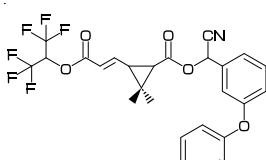
Azaconazole
MW:300.1406 / FM:C12H11Cl2N3O2
MW:300.139 (data) / [132]
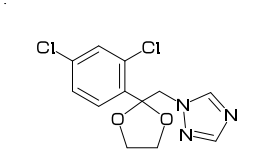
Endrin
MW:380.9093 / FM:C12H8Cl6O
MW:380.91 (data) / [133]
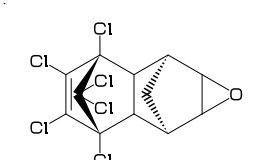
Sulfacetamide
MW:214.2415 / FM:C8H10N2O3S
MW:214.239 (data) / [134]
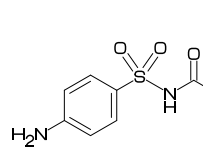
Sulfatiazole
MW:255.3166 / FM:C9H9N3O2S2
MW:255.31 (data) / [135]
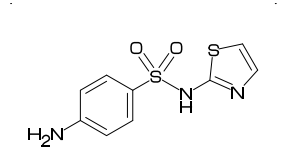
Chlopidol
MW:192.0425 / FM:C7H7Cl2NO
MW:192.039 (data) / [136]
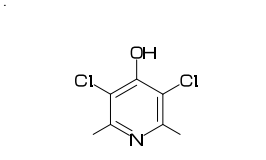
Sulfadiadine
MW:250.2769 / FM:C10H10N4O2S
MW:250.276 (data) / [137]
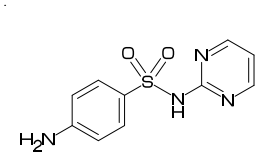
Levamisole
MW:204.2913 / FM:C11H12N2S
MW:204.29 (data) / [138]
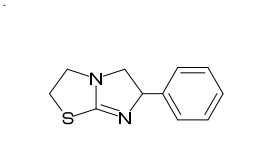
Sulfapyrizine
MW:249.2889 / FM:C11H11N3O2S
MW:249.288 (data) / [139]
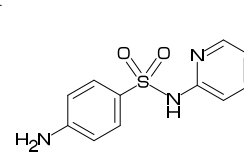
Marbofloxacin
MW:362.3555 / FM:C17H19FN4O4
MW:362.361 (data) / [140]
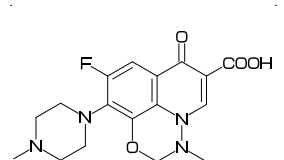
Sulfamerazine
MW:264.3035 / FM:C11H12N4O2S
MW:264.303 (data) / [141]
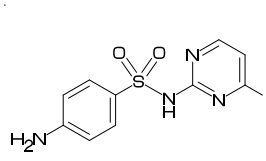
Trimetoprim
MW:275.3030 / FM:C14H17N3O3
MW:290.323 (data) / [142]
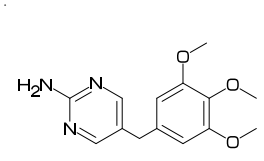
Ofloxacin
MW:359.4194 / FM:C19H25N3O4
MW:361.373 (data) / [143]
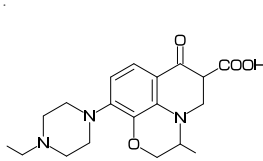
Ciprofloxacin
MW:331.3415 / FM:C17H18FN3O3
MW:331.347 (data) / [144]
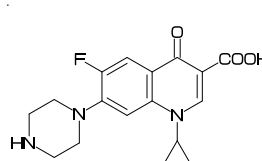
Enrofloxacin
MW:359.3946 / FM:C19H22FN3O3
MW:359.401 (data) / [145]
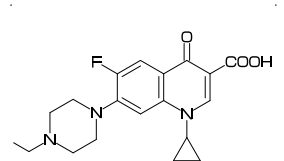
Danofloxacin
MW:357.3788 / FM:C19H20FN3O3
MW:357.385 (data) / [146]
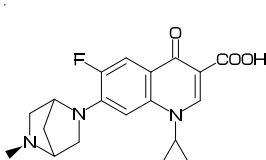
Ormetoprim
MW:274.3183 / FM:C14H18N4O2
MW:274.324 (data) / [147]
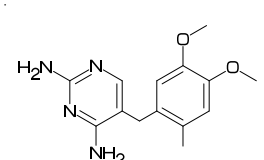
Sulfadimidine
MW:278.3301 / FM:C12H14N4O2S
MW:278.33 (data) / [148]
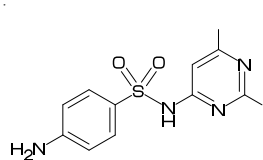
Orbifloxacin
MW:395.3756 / FM:C19H20F3N3O3
MW:395.382 (data) / [149]
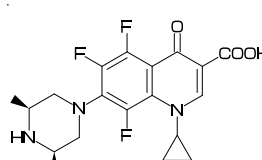
Sarafloxacin
MW:385.3640 / FM:C20H17F2N3O3
MW:385.371 (data) / [150]
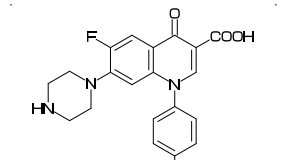
Difloxacin
MW:399.3906 / FM:C21H19F2N3O3
MW:399.398 (data) / [151]
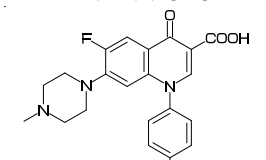
Sulfamonomethoxine
MW:280.3029 / FM:C11H12N4O3S
MW:280.302 (data) / [152]
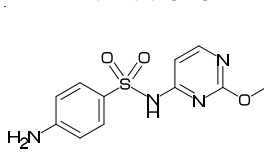
Sulfachlorpyridazine
MW:284.7220 / FM:C10H9ClN4O2S
MW:284.723 (data) / [153]
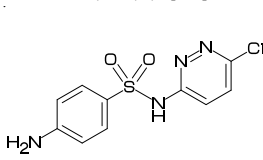
Sulfamethoxazole
MW:253.2776 / FM:C10H11N3O3S
MW:253.276 (data) / [154]
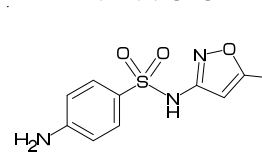
Pirimethamin
MW:233.6967 / FM:C12H12ClN3
MW:248.714 (data) / [155]