|  |  |  |  |
| --- | --- | --- | --- |
| SN | Ligands | Pubchem CID | SMILES |
| 1 | Thujole | 261491 | C[C@@H]1[C@H]2C[C@]2(CC1=O)C(C)C |
| SN | COMPOUND | PubChem CID | SMILES |
| 2 | Camphor | 2537 | CC1(C2CCC1(C(=O)C2)C)C |
| 3 | * 1,8-Cineole | 2758 | CC1(C2CCC(O1)(CC2)C)C |
| 4 | α-Pinene | 6654 | CC1=CCC2CC1C2(C)C |
| 5 | β-Pinene | 14896 | CC1(C2CCC(=C)C1C2)C |
| 6 | Limonene | 440917 | CC1=CC[C@@H](CC1)C(=C)C |
| 7 | Linalool | 67179 | CC(=CCC[C@@](C)(C=C)O)C |
| 8 | Bornyl acetate | 6448 | CC(=O)OC1CC2CCC1(C2(C)C)C |
| 9 | Terpinen-4-ol | 2724161 | CC1=CC[C@@](CC1)(C(C)C)O |
| 10 | α-Terpinene | 7462 | CC1=CC=C(CC1)C(C)C |
| 11 | γ-Terpinene | 7461 | CC1=CCC(=CC1)C(C)C |
| 12 | p-Cymene | 7463 | CC1=CC=C(C=C1)C(C)C |
| 13 | Terpinolene | 11463 | CC1=CCC(=C(C)C)CC1 |
| 14 | Myrcene | 3253 | CC(=CCCC(=C)C=C)C |
| 15 | α-Phellandrene | 7460 | CC1=CCC(C=C1)C(C)C |
| 16 | Quercetin | 5280343 | C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O |
| 17 | Kaempferol | 5280863 | C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O |
| 18 | Isorhapontigenin | 5318650 | COC1=C(C=CC(=C1)/C=C/C2=CC(=CC(=C2)O)O)O |
| 19 | Luteolin | 5280445 | C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O |
| 20 | Apigenin | 5280443 | C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O |
| 21 | Myricetin | 5281672 | C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O |
| 22 | Fisetin | 5281614 | C1=CC(=C(C=C1C2=C(C(=O)C3=C(O2)C=C(C=C3)O)O)O)O |
| 23 | Galangin | 5281616 | C1=CC=C(C=C1)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O |
| 24 | Chrysin | 5281607 | C1=CC=C(C=C1)C2=CC(=O)C3=C(C=C(C=C3O2)O)O |
| 25 | Artemetin | 5320351 | COC1=C(C=C(C=C1)C2=C(C(=O)C3=C(C(=C(C=C3O2)OC)OC)O)OC)OC |
| 26 | Caffeic acid | 689043 | C1=CC(=C(C=C1/C=C/C(=O)O)O)O |
| 27 | Ferulic acid | 445858 | COC1=C(C=CC(=C1)/C=C/C(=O)O)O |
| 28 | p-Coumaric acid | 637542 | C1=CC(=CC=C1/C=C/C(=O)O)O |
| 29 | Gallic acid | 370 | C1=C(C=C(C(=C1O)O)O)C(=O)O |
| 30 | Chlorogenic acid | 1794427 | C1[C@H]([C@H]([C@@H](C[C@@]1(C(=O)O)O)OC(=O)/C=C/C2=CC(=C(C=C2)O)O)O)O |
| 31 | Artemisinin | 68827 | C[C@@H]1CC[C@H]2[C@H](C(=O)O[C@H]3[C@@]24[C@H]1CC[C@](O3)(OO4)C)C |
| 32 | β-Sitosterol | 222284 | CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C |
| 33 | Stigmasterol | 5280794 | CC[C@H](/C=C/[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C |
| 34 | Ursolic acid | 64945 | C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]2[C@H]1C)C)C(=O)O |
| 35 | Oleanolic acid | 10494 | C[C@]12CC[C@@H](C([C@@H]1CC[C@@]3([C@@H]2CC=C4[C@]3(CC[C@@]5([C@H]4CC(CC5)(C)C)C(=O)O)C)C)(C)C)O |
| 36 | β-Amyrin | 73145 | C[C@@]12CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]1CC(CC2)(C)C)C |
| 37 | α-Amyrin | 73170 | C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]2[C@H]1C)C)C |
| 38 | Lupeol | 259846 | CC(=C)[C@@H]1CC[C@]2([C@H]1[C@H]3CC[C@@H]4[C@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC2)C)C)(C)C)O)C)C |
| 39 | Taraxasterol | 115250 | C[C@H]1[C@@H]2[C@H]3CC[C@@H]4[C@]5(CC[C@@H](C([C@@H]5CC[C@]4([C@@]3(CC[C@]2(CCC1=C)C)C)C)(C)C)O)C |
| 40 | Psiloternol | 3779 | CC(C)NCC(C1=CC(=C(C=C1)O)O)O |
| 41 | Artemidine | 5945155 | CC/C=C/C1=CC2=CC=CC=C2C(=O)O1 |
| 42 | Afrafoline | 393601 | COC1=CC=C(C=C1)[C@]23[C@@H]([C@H]([C@H]([C@]2(C4=C(O3)C=C(C=C4OC)OC)O)O)C(=O)OC)C5=CC=CC=C5 |
| 43 | Aframide | 10843163 | C[C@H](CCCCC#C)C(=O)N(C)[C@@H](C)C(=O)N(C)[C@@H](C(C)C)C(=O)N(C)[C@@H](C(C)C)C(=O)N(C)[C@@H](C(C)C)C(=O)N(C)[C@@H](C(C)C)C(=O)N1CCC[C@H]1C2=NC=CS2 |
| 44 | Artemisinine | 68827 | C[C@@H]1CC[C@H]2[C@H](C(=O)O[C@H]3[C@@]24[C@H]1CC[C@](O3)(OO4)C)C |
| 45 | artabsin | 442146 | C[C@H]1[C@@H]2CC[C@](C3=CCC(=C3[C@H]2OC1=O)C)(C)O |
| 46 | apiol | 10659 | COC1=C2C(=C(C(=C1)CC=C)OC)OCO2 |
| 47 | Umbelliferone | 5281426 | C1=CC(=CC2=C1C=CC(=O)O2)O |
| 48 | Jatamansone | 10198387 | CC(C)[C@@H]1CC[C@@]2(CCCC(=O)[C@@]2(C1)C)C |
| 49 | Borneol | 6552009 | C[C@@]12CC[C@@H](C1(C)C)C[C@@H]2O |
| 50 | Scopoletin | 5280460 | COC1=C(C=C2C(=C1)C=CC(=O)O2)O |
| 51 | Entinostat | 4261 | C1=CC=C(C(=C1)N)NC(=O)C2=CC=C(C=C2)CNC(=O)OCC3=CN=CC=C3 |
| 52 | Vorinostat | 5311 | C1=CC=C(C=C1)NC(=O)CCCCCCC(=O)NO |
| 53 | Romidepsin | 5352062 | C/C=C\1/C(=O)N[C@H](C(=O)O[C@H]\2CC(=O)N[C@@H](C(=O)N[C@H](CSSCC/C=C2)C(=O)N1)C(C)C)C(C)C |
| 54 | Mocetinostat | 9865515 | C1=CC=C(C(=C1)N)NC(=O)C2=CC=C(C=C2)CNC3=NC=CC(=N3)C4=CN=CC=C4 |
| 55 | Givinostat | 9804992 | CCN(CC)CC1=CC2=C(C=C1)C=C(C=C2)COC(=O)NC3=CC=C(C=C3)C(=O)NO |
| 56 | Tubastatin A | 49850262 | CN1CCC2=C(C1)C3=CC=CC=C3N2CC4=CC=C(C=C4)C(=O)NO |
| 57 | LMK-235 | 71520717 | CC1=CC(=CC(=C1)C(=O)NOCCCCCC(=O)NO)C |
| 58 | PCI-34051 | 24753719 | COC1=CC=C(C=C1)CN2C=CC3=C2C=C(C=C3)C(=O)NO |
| 59 | Panobinostat | 6918837 | CC1=C(C2=CC=CC=C2N1)CCNCC3=CC=C(C=C3)/C=C/C(=O)NO |
| 60 | ST80 | 139378194 | CCOC(=O)NC(CCCCC(=O)NC1=CC=CC=C1N)C(=O)NC2=CC(=CC=C2)Br |
| 61 | FT985 | 134492522 | CC1(C2=CC=CC(=C2CN1C3=NC=C(N=C3)C(F)(F)F)C(=O)NO)C |