

Molecular Coding Format examples

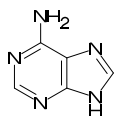
Author : Akira Yamaji Date : September 5, 2021

Located at : <http://www.ctan.org/pkg/mcf2graph>

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

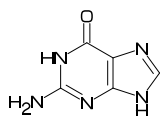
Adenine

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



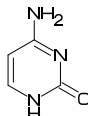
Guanine

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



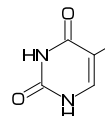
Cytosine

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



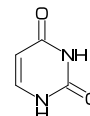
Thymine

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



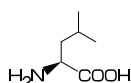
Uracil

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



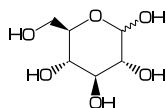
L-Leucine

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



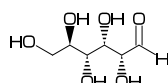
Glucose 1

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



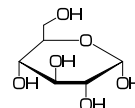
Glucose 2

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



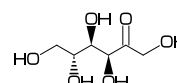
D-Glucose

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



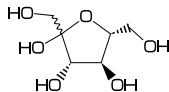
Fructose 1

MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [10]



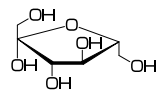
Fructose 2

MW:180.1558 / FM:C6H12O6
MW:180.16 (data) / [11]



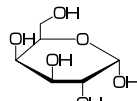
D-Fluctose

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



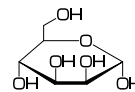
D-Galactose

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



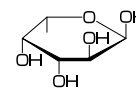
D-Mannose

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



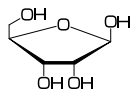
L-Fucose

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



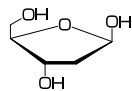
D-Ribose

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



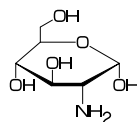
D-Deoxyribose

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



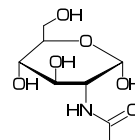
D-Glucosamine

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



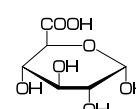
N-acetyl-Glucosamine

MW:221.2077 / FM:C8H15NO6
MW:221.21 (data) / [19]



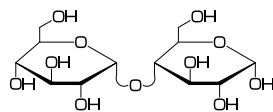
Glucuronic acid

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



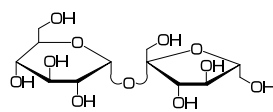
Maltose

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



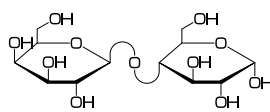
Sucrose

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



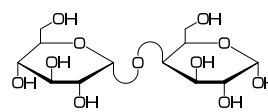
Lactose

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



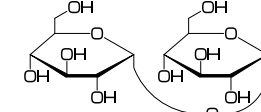
Cellobiose

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



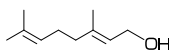
Trehalose

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



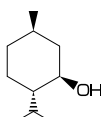
Geraniol

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



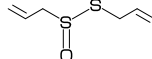
l-Menthol

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



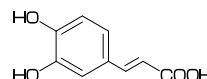
Allicin

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



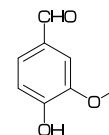
Caffeic acid

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



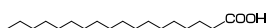
Vanillin

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



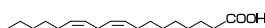
Stearic acid

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



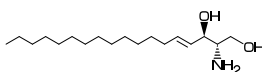
Linoleic acid

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



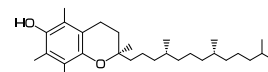
Sphingosine

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



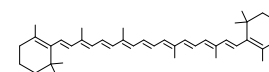
Tocopherol

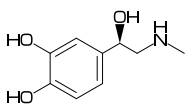
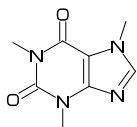
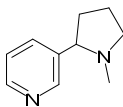
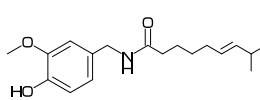
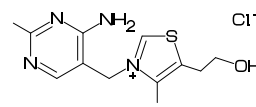
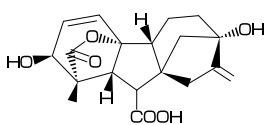
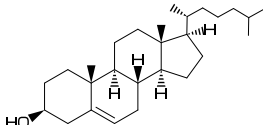
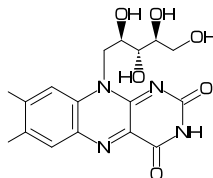
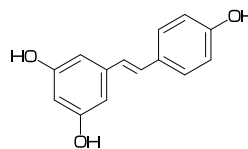
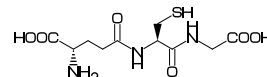
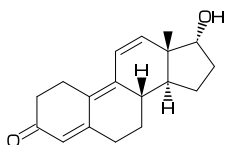
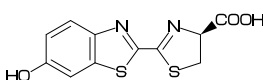
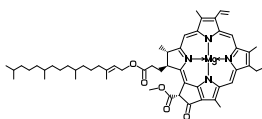
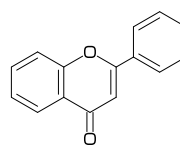
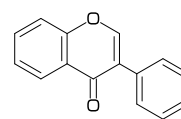
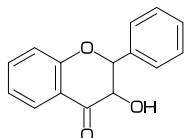
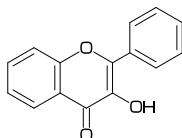
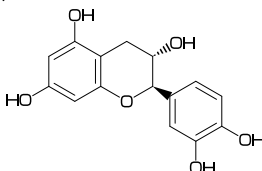
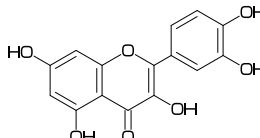
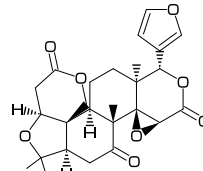
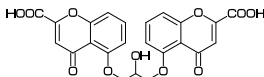
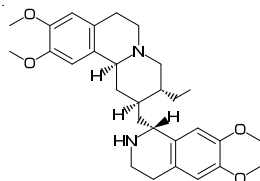
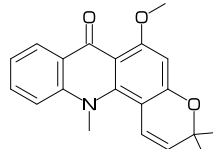
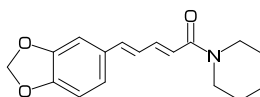
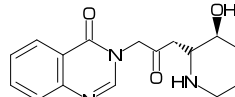
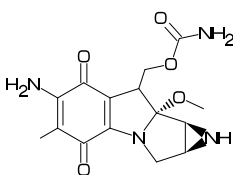
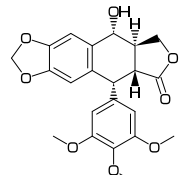
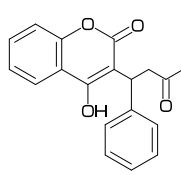
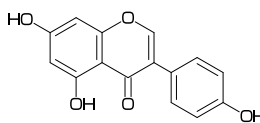
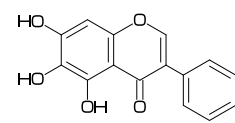
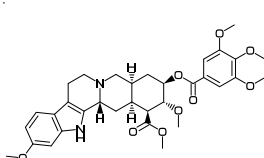
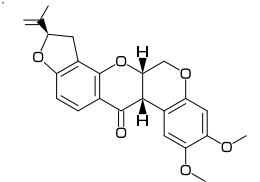
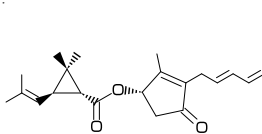
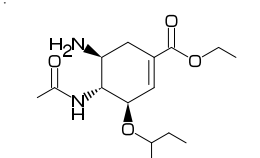
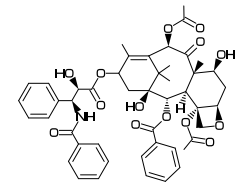
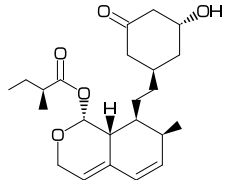
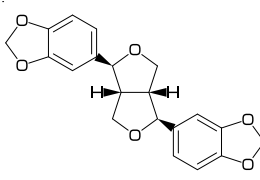
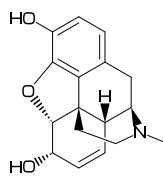
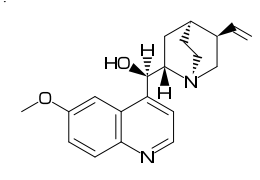
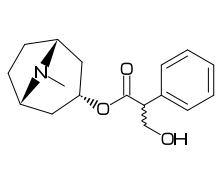
MW:430.7060 / FM:C29H50O2
MW:430.717 (data) / [34]

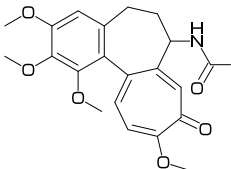
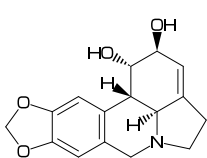
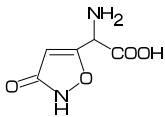
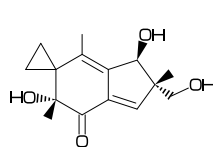
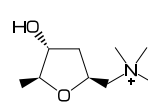
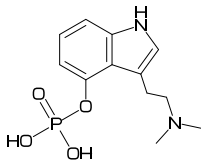
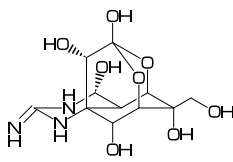
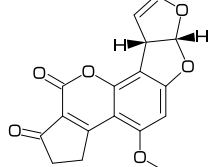
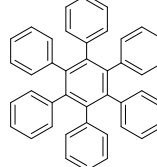
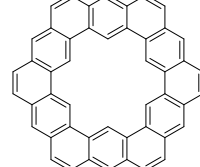
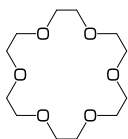
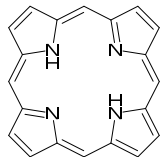
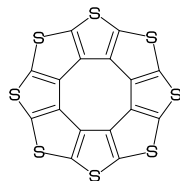
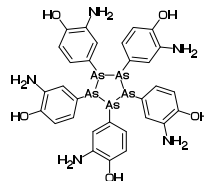
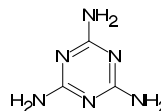
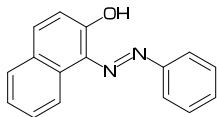
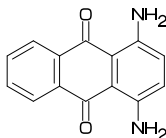
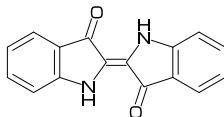
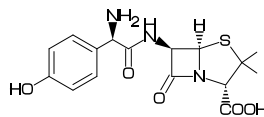
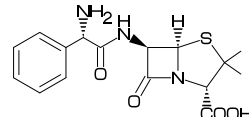
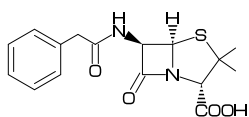
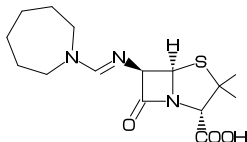
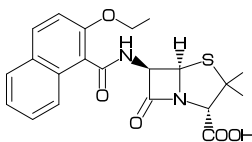
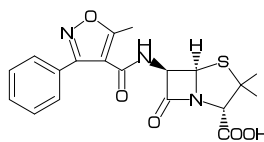
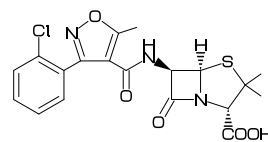
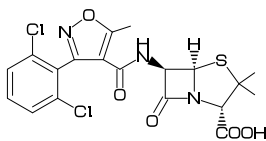
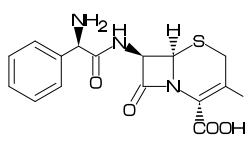
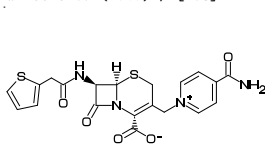
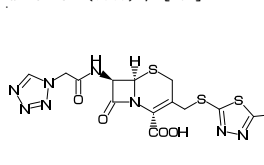
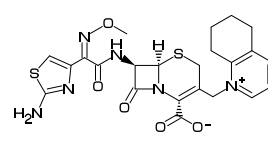
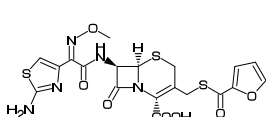
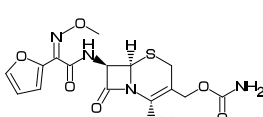
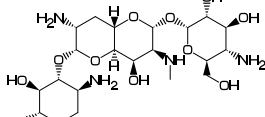
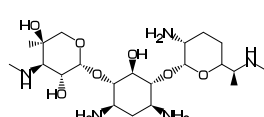
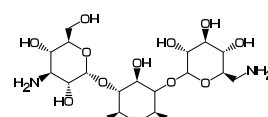
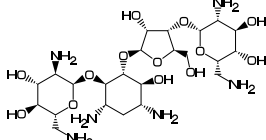
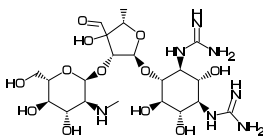
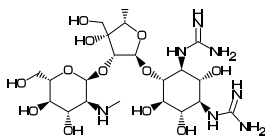
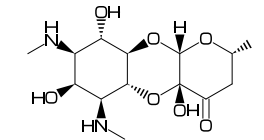
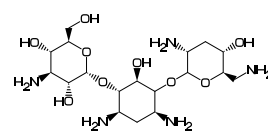


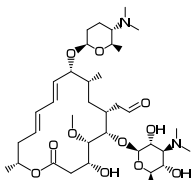
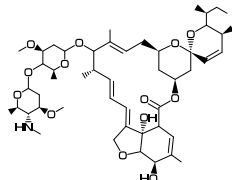
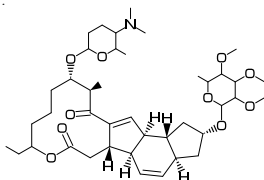
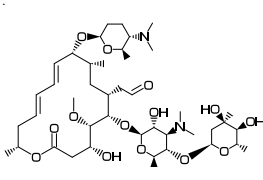
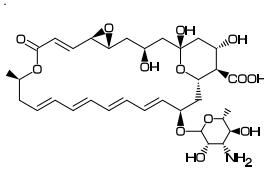
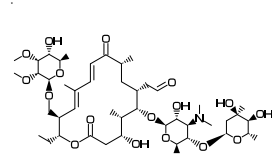
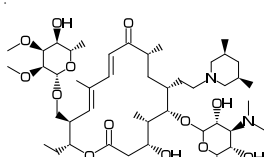
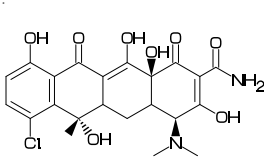
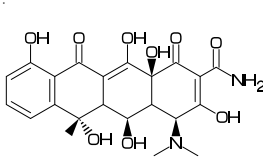
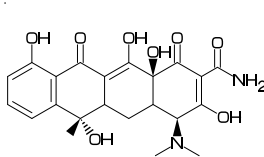
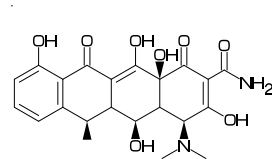
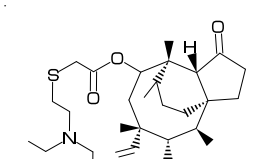
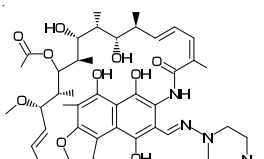
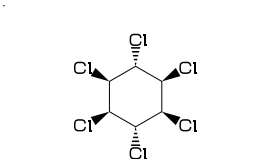
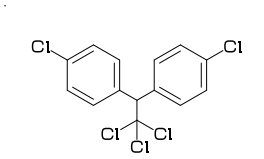
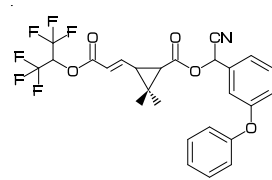
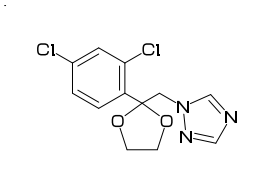
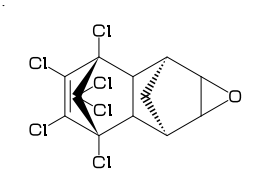
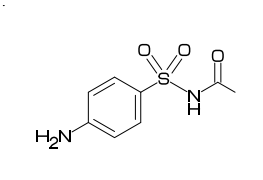
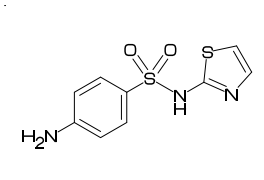
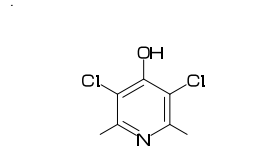
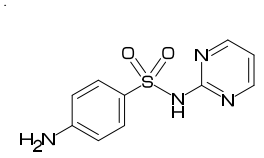
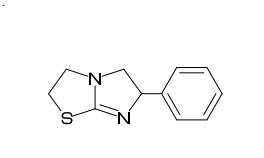
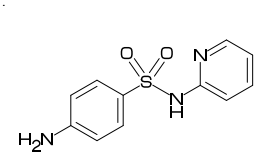
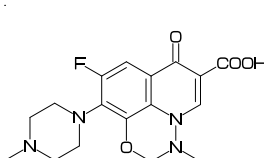
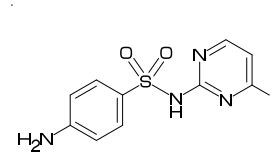
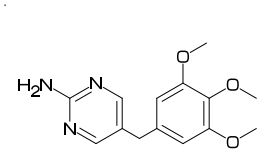
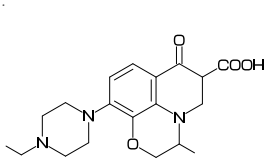
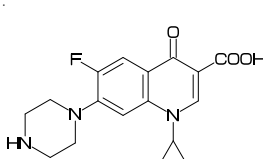
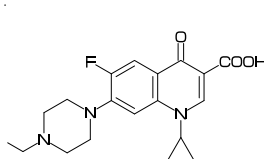
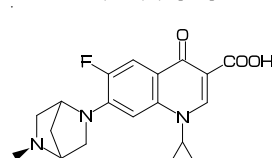
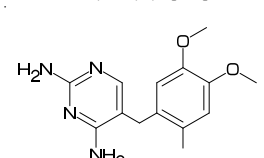
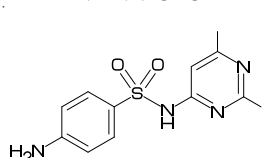
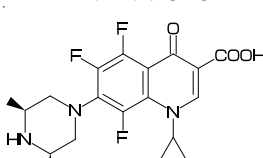
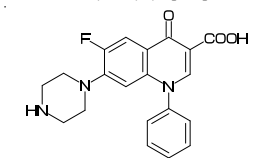
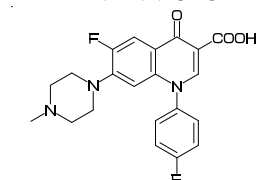
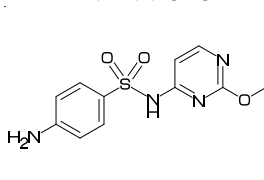
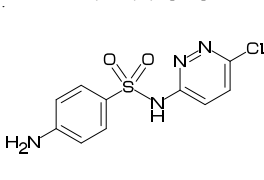
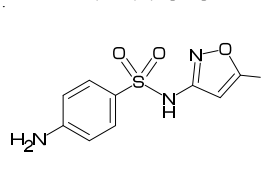
Carotene

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



AdrenalinMW: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:244.25 (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]**Mitomycin 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]**Baicalin**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:C20H24N2O7
MW:324.424 (data) / [74]**Atoropin**MW:289.3694 / FM:C17H23NO3
MW:289.375 (data) / [75]

ColchicineMW: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]**Sulfower**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:C16H12NO2
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]**Cefazolin**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]**Streptomycin**MW:581.5740 / FM:C21H39N7O12
MW:581.574 (data) / [112]**dihydro-Streptomycin**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]

NeospiramycinMW: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]**Chlortetracycline**MW:478.8796 / FM:C22H23ClN2O8
MW:478.88 (data) / [123]**Oxytetracycline**MW:460.4339 / FM:C22H24N2O9
MW:460.434 (data) / [124]**Tetracycline**MW:444.4345 / FM:C22H24N2O8
MW:444.435 (data) / [125]**Doxycycline**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]**Sulfapyridine**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:C19H20FN3O3
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]**Pyrimethamin**MW:233.6967 / FM:C12H12ClN3
MW:248.714 (data) / [155]