

Molecular Coding Format examples

Author : Akira Yamaji Date : December 12, 2021

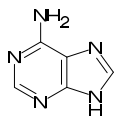
Located at : <http://www.ctan.org/pkg/mcf2graph>

* use molecular data base file 'mcf_data_base.mcf'

* FM(fm):molecular formula (calculated) * MW(mw):molecular weight (calculated)

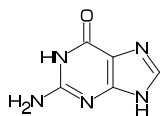
Adenine

mw:135.1267 / fm:C5H5N5
MW:135.13 / [1]



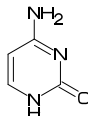
Guanine

mw:151.1261 / fm:C5H5N5O
MW:151.13 / [2]



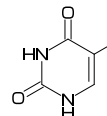
Cytosine

mw:111.1019 / fm:C4H5N3O
MW:111.10 / [3]



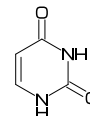
Thymine

mw:126.1133 / fm:C5H6N2O2
MW:126.11 / [4]



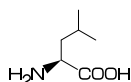
Uracil

mw:112.0867 / fm:C4H4N2O2
MW:112.09 / [5]



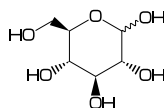
L-Leucine

mw:131.1729 / fm:C6H13NO2
MW:131.16 / [6]



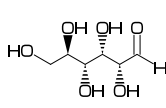
Glucose 1

mw:180.1558 / fm:C6H12O6
MW:180.16 / [7]



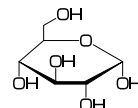
Glucose 2

mw:180.1558 / fm:C6H12O6
MW:180.16 / [8]



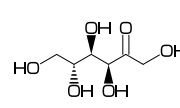
D-Glucose

mw:180.1558 / fm:C6H12O6
MW:180.16 / [9]



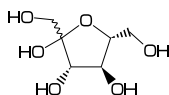
Fructose 1

mw:180.1558 / fm:C6H12O6
MW:180.16 / [10]



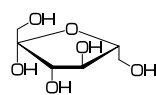
Fructose 2

mw:180.1558 / fm:C6H12O6
MW:180.16 / [11]



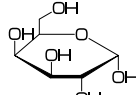
D-Fluctose

mw:180.1558 / fm:C6H12O6
MW:180.16 / [12]



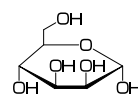
D-Galactose

mw:180.1558 / fm:C6H12O6
MW:180.16 / [13]



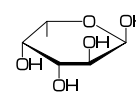
D-Mannose

mw:180.1558 / fm:C6H12O6
MW:180.16 / [14]



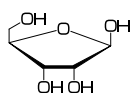
L-Fucose

mw:164.1564 / fm:C6H12O5
MW:164.16 / [15]



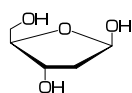
D-Ribose

mw:150.1299 / fm:C5H10O5
MW:150.13 / [16]



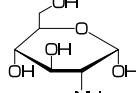
D-Deoxyribose

mw:134.1305 / fm:C5H10O4
MW:134.13 / [17]



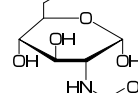
D-Glucosamine

mw:179.1711 / fm:C6H13NO5
MW:179.17 / [18]



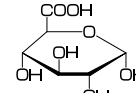
N-acetyl-Glucosamine

mw:221.2077 / fm:C8H15NO6
MW:221.21 / [19]



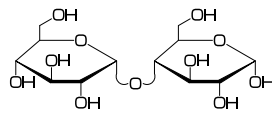
Glucuronic acid

mw:194.1393 / fm:C6H10O7
MW:194.14 / [20]



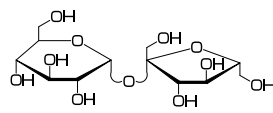
Maltose

mw:342.2964 / fm:C12H22O11
MW:342.3 / [21]



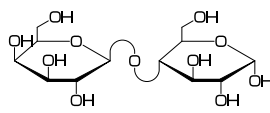
Sucrose

mw:342.2964 / fm:C12H22O11
MW:342.3 / [22]



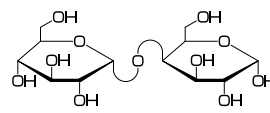
Lactose

mw:342.2964 / fm:C12H22O11
MW:342.3 / [23]



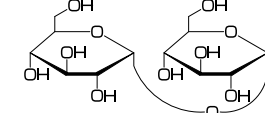
Cellobiose

mw:342.2964 / fm:C12H22O11
MW:342.3 / [24]



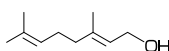
Trehalose

mw:342.2964 / fm:C12H22O11
MW:342.3 / [25]



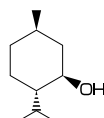
Geraniol

mw:154.2493 / fm:C10H18O
MW:154.25 / [26]



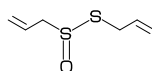
l-Menthol

mw:156.2652 / fm:C10H20O
MW:156.27 / [27]



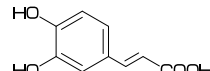
Allicin

mw:162.2729 / fm:C6H10OS2
MW:162.28 / [28]



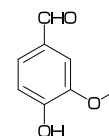
Caffeic acid

mw:180.1574 / fm:C9H8O4
MW:180.16 / [29]



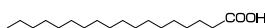
Vanillin

mw:152.1473 / fm:C8H8O3
MW:152.15 / [30]



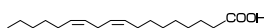
Stearic acid

mw:284.4772 / fm:C18H36O2
MW:284.48 / [31]



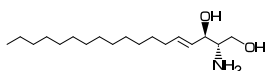
Linoleic acid

mw:280.4454 / fm:C18H32O2
MW:280.45 / [32]



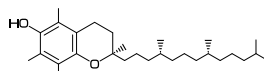
Sphingosine

mw:299.4918 / fm:C18H37NO2
MW:299.50 / [33]



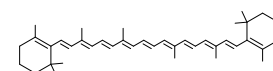
Tocopherol

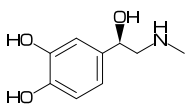
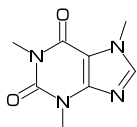
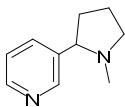
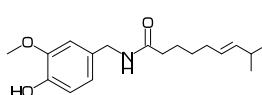
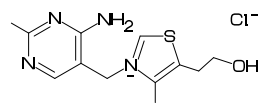
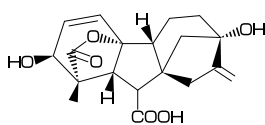
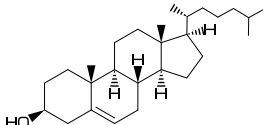
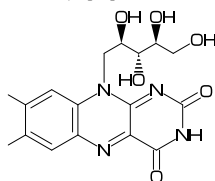
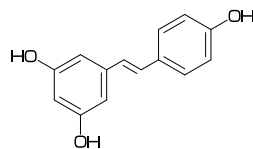
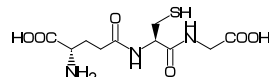
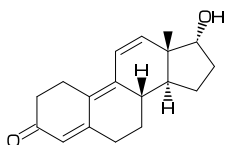
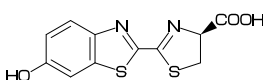
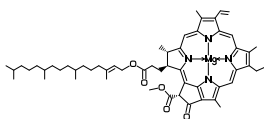
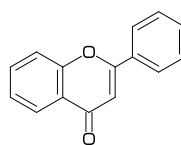
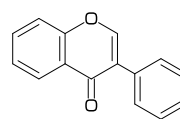
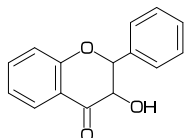
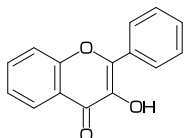
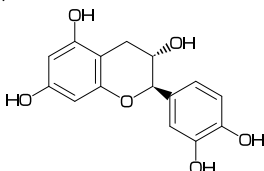
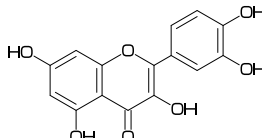
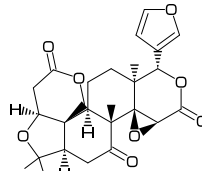
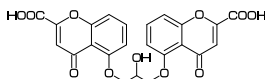
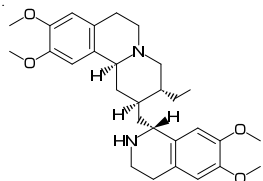
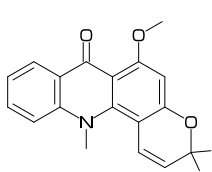
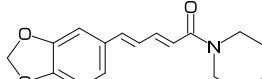
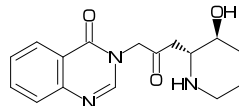
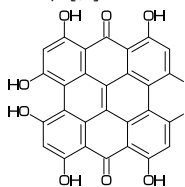
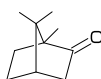
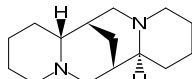
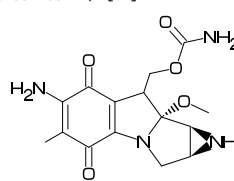
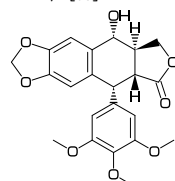
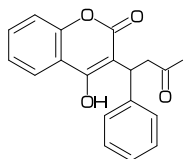
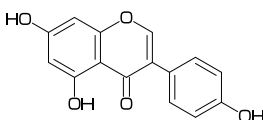
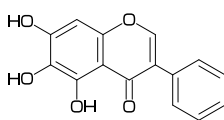
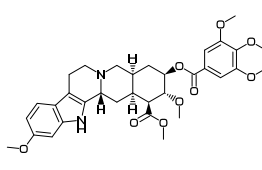
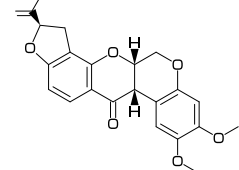
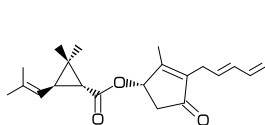
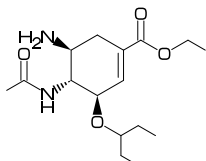
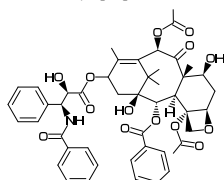
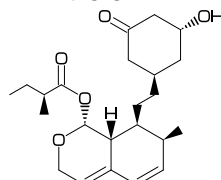
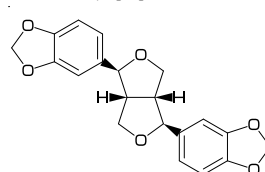
mw:430.7060 / fm:C29H50O2
MW:430.717 / [34]

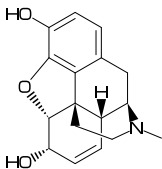
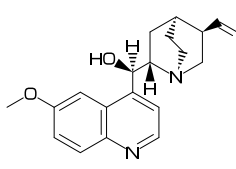
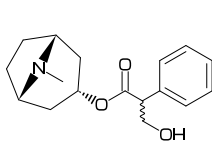
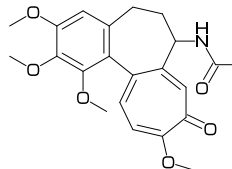
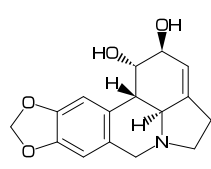
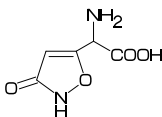
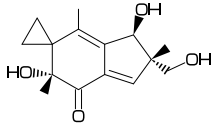
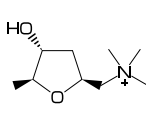
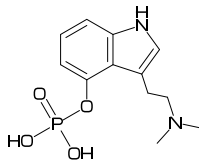
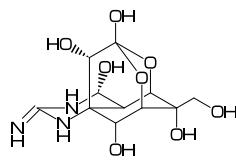
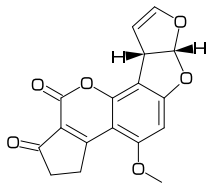
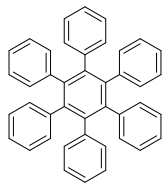
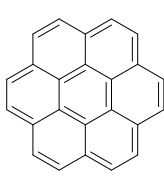
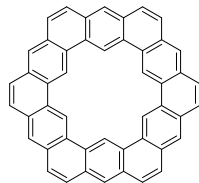
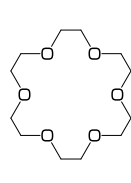
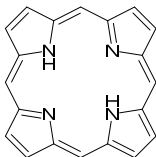
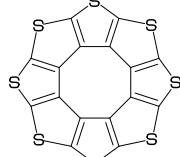
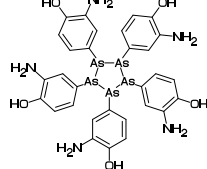
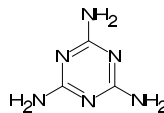
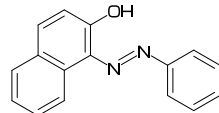
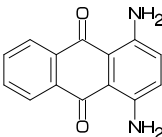
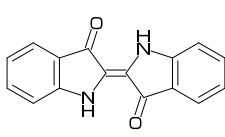
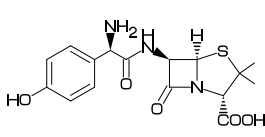
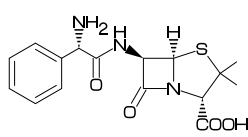
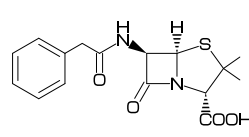
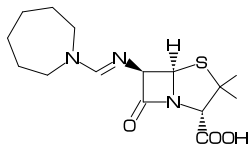
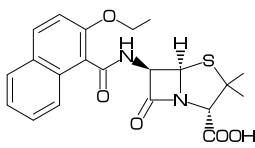
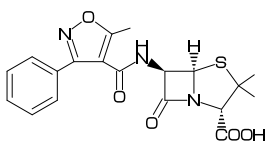
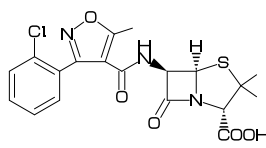
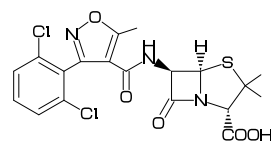
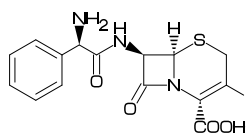
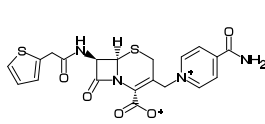
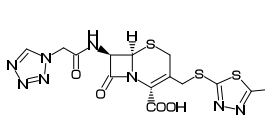
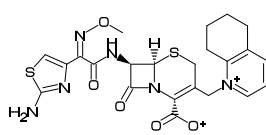
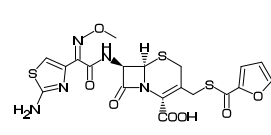
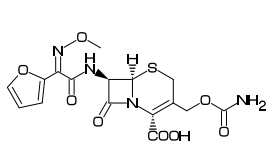
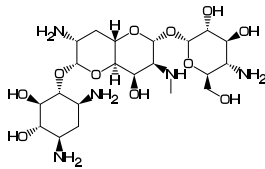
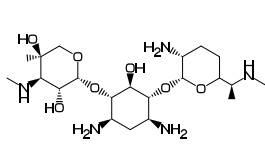
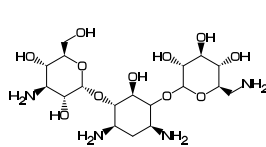
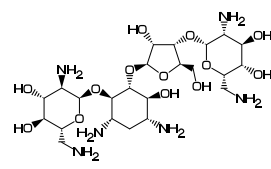


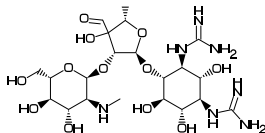
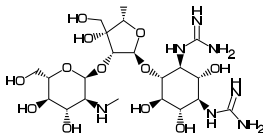
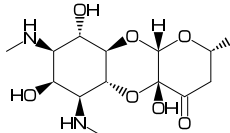
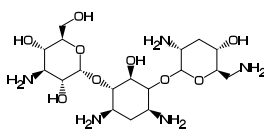
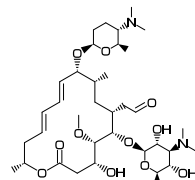
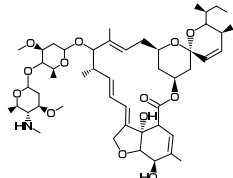
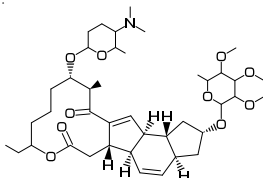
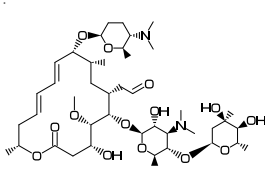
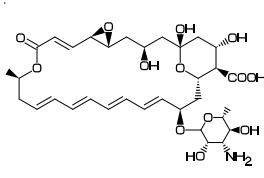
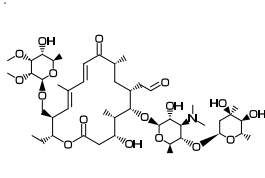
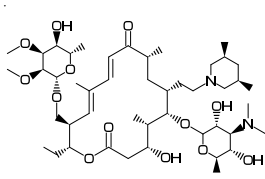
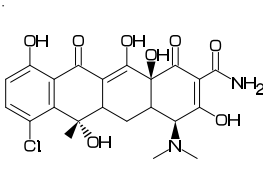
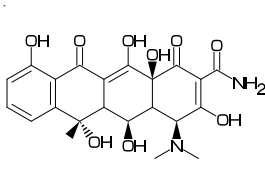
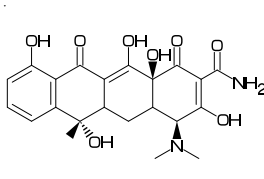
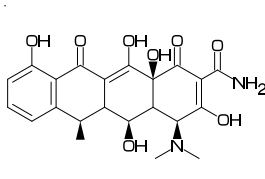
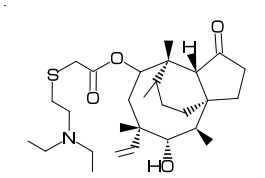
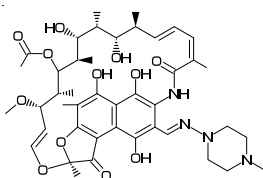
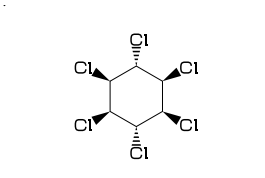
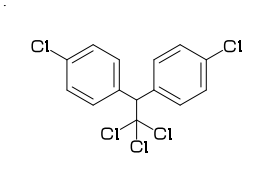
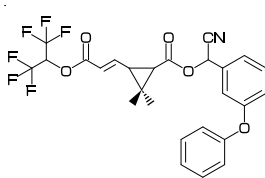
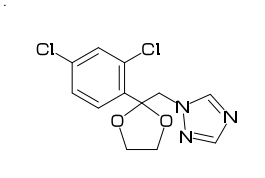
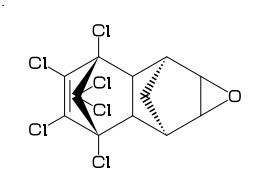
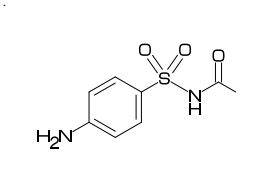
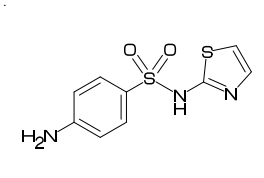
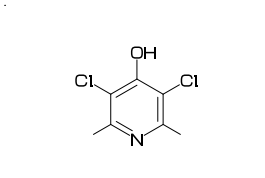
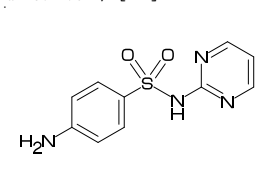
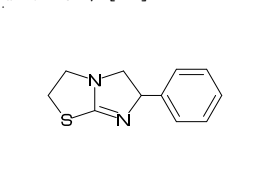
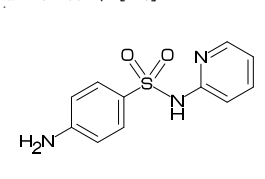
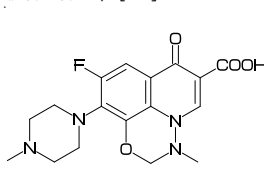
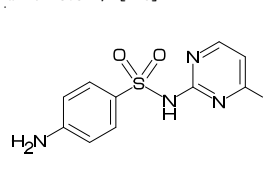
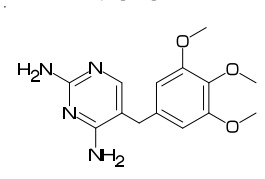
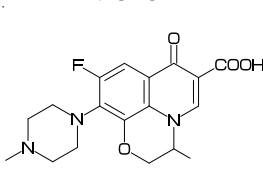
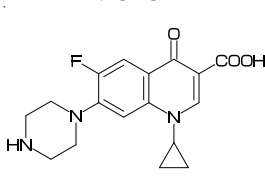
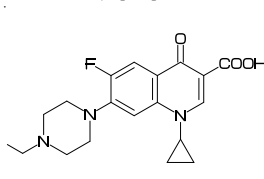
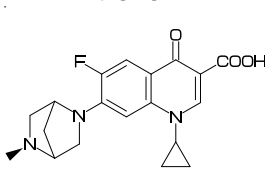
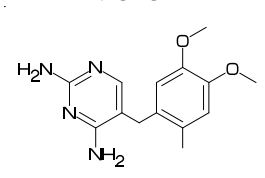
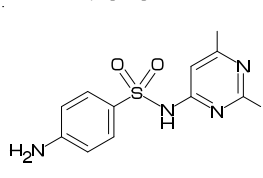
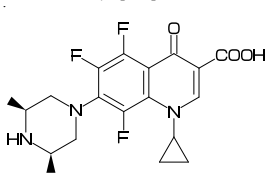
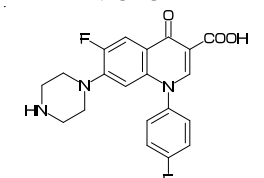
Carotene

mw:536.8726 / fm:C40H56
MW:536.8726 / [35]



Adrenalinmw:183.2044 / fm:C9H13NO3
MW:183.21 / [36]**Caffeine**mw:194.1905 / fm:C8H10N4O2
MW:194.194 / [37]**Nicotine**mw:162.2315 / fm:C10H14N2
MW:162.23 / [38]**Capsaicin**mw:305.4118 / fm:C18H27NO3
MW:305.418 / [39]**Thiamine**mw:300.8075 / fm:C12H17ClN4OS
MW:300.81 / [40]**Gibberellin A3**mw:346.3743 / fm:C19H22O6
MW:346.379 / [41]**Cholesterol**mw:386.6535 / fm:C27H46O
MW:386.664 / [42]**Riboflavin**mw:376.3638 / fm:C17H20N4O6
MW:376.37 / [43]**Resveratrol**mw:228.2432 / fm:C14H12O3
MW:228.24 / [44]**Glutathione**mw:307.3234 / fm:C10H17N3O6S
MW:307.33 / [45]**Trenbolone**mw:270.3660 / fm:C18H22O2
MW:270.37 / [46]**Luciferin**mw:280.3228 / fm:C11H8N2O3S2
MW:280.33 / [47]**Chlorophyll a**mw:893.4889 / fm:C55H72MgN4O5
MW:893.509 / [48]**Flavone**mw:222.2386 / fm:C15H10O2
MW:222.24 / [49]**Isoflavone**mw:222.2386 / fm:C15H10O2
MW:222.24 / [50]**Flavanone**mw:240.2539 / fm:C15H12O3
MW:244.25 / [51]**Flavonol**mw:238.2381 / fm:C15H10O3
MW:238.24 / [52]**Cianidanol**mw:290.2680 / fm:C15H14O6
MW:290.27 / [53]**Quercetin**mw:302.2357 / fm:C15H10O7
MW:302.24 / [54]**Limonin**mw:470.5115 / fm:C26H30O8
MW:470.518 / [55]**Cromolyn**mw:468.3665 / fm:C23H16O11
MW:468.37 / [56]**Emetine**mw:480.6388 / fm:C29H40N2O4
MW:480.649 / [57]**Acronycine**mw:321.3697 / fm:C20H19NO3
MW:321.376 / [58]**Piperine**mw:285.3376 / fm:C17H19NO3
MW:285.343 / [59]**Febrifugine**mw:301.3403 / fm:C16H19N3O3
MW:301.34 / [60]**Hypericin**mw:504.4432 / fm:C30H16O8
MW:504.44 / [61]**Camphor**mw:152.2334 / fm:C10H16O
MW:152.23 / [62]**Sparteine**mw:234.3803 / fm:C15H26N2
MW:234.3803 / [63]**Mitomycine C**mw:334.3272 / fm:C15H18N4O5
MW:334.332 / [64]**Podophyllotoxin**mw:414.4052 / fm:C22H20O8
MW:414.41 / [65]**Warfarin**mw:308.3279 / fm:C19H16O4
MW:308.333 / [66]**Genistein**mw:270.2368 / fm:C15H10O5
MW:270.24 / [67]**Baicalein**mw:270.2368 / fm:C15H10O5
MW:270.24 / [68]**Reserpine**mw:608.6786 / fm:C33H40N2O9
MW:608.688 / [69]**Rotenone**mw:394.4171 / fm:C23H22O6
MW:394.423 / [70]**Pyrethrin I**mw:328.4452 / fm:C21H28O3
MW:328.452 / [71]**Oseltamivir**mw:312.4045 / fm:C16H28N2O4
MW:312.40 / [72]**Paclitaxel**mw:853.9061 / fm:C47H51NO14
MW:853.918 / [73]**Mevastatin**mw:390.5130 / fm:C23H34O5
MW:390.52 / [74]**Sesamine**mw:354.3533 / fm:C20H18O6
MW:354.35 / [75]

Morphinemw:285.3376 / fm:C17H19N03
MW:285.343 / [76]**Quinine**mw:324.4167 / fm:C20H24N2O2
MW:324.424 / [77]**Atoropin**mw:289.3694 / fm:C17H23N03
MW:289.375 / [78]**Colchicine**mw:399.4370 / fm:C22H25N06
MW:399.443 / [79]**Lycorine**mw:287.3104 / fm:C16H17N04
MW:287.315 / [80]**Ibotenic acid**mw:158.1121 / fm:C5H6N2O4
MW:158.113 / [81]**illudin S**mw:264.3168 / fm:C15H20O4
MW:264.3 / [82]**Muscarine**mw:174.2605 / fm:C9H20N02
MW:174.26 / [83]**Psilocybin**mw:284.2481 / fm:C12H17N2O4P
MW:284.248 / [84]**Tetrodotoxine**mw:319.2679 / fm:C11H17N3O8
MW:319.27 / [85]**Aflatoxin B1**mw:312.2735 / fm:C17H12O6
MW:312.27 / [86]**Hexaphenylbenzene**mw:534.6875 / fm:C42H30
MW:534.6876 / [87]**Coronene**mw:300.3520 / fm:C24H12
MW:300.35 / [88]**Kekulene**mw:600.7041 / fm:C48H24
MW:600.7 / [89]**18-Crown-6**mw:264.3153 / fm:C12H24O6
MW:264.32 / [90]**Porphyrin**mw:310.3519 / fm:C20H14N4
MW:310.4 / [91]**Sulflower**mw:448.6911 / fm:C16S8
MW:448.69 / [92]**Arsphenamine x5**mw:915.1977 / fm:C30H30As5N5O5
MW:915.2 / [93]**Melamine**mw:126.1199 / fm:C3H6N6
MW:126.12 / [94]**Sudan red 1**mw:248.2792 / fm:C16H12N2O
MW:248.28 / [95]**Disperse violet 1**mw:238.2413 / fm:C14H10N2O2
MW:238.25 / [96]**Vat blue 1**mw:262.2627 / fm:C16H10N2O2
MW:262.27 / [97]**Amoxicillin**mw:365.4041 / fm:C16H19N3O5S
MW:365.4042 / [98]**Ampicillin**mw:349.4047 / fm:C16H19N3O4S
MW:349.405 / [99]**benzyl-Penicillin**mw:334.3901 / fm:C16H18N2O4S
MW:334.4 / [100]**Mecillinam**mw:325.4264 / fm:C15H23N3O3S
MW:325.4264 / [101]**Nafcillin**mw:414.4747 / fm:C21H22N2O5S
MW:414.4748 / [102]**Oxacillin**mw:401.4362 / fm:C19H19N3O5S
MW:401.4363 / [103]**Cloxacillin**mw:435.8813 / fm:C19H18ClN3O5S
MW:435.8813 / [104]**Dicloxacillin**mw:470.3263 / fm:C19H17Cl2N3O5S
MW:470.3264 / [105]**Cefalexin**mw:347.3888 / fm:C16H17N3O4S
MW:347.3889 / [106]**Cefalonium**mw:458.5107 / fm:C20H18N4O5S2
MW:458.5107 / [107]**Cefazorin**mw:454.5071 / fm:C14H14N8O4S3
MW:454.51 / [108]**Cefquinome**mw:528.6038 / fm:C23H24N6O5S2
MW:528.6 / [109]**Ceftiofur**mw:523.5625 / fm:C19H17N5O7S3
MW:523.5626 / [110]**Cefuroxime**mw:424.3852 / fm:C16H16N4O8S
MW:424.3852 / [111]**Apramycin**mw:539.5771 / fm:C21H41N5O11
MW:539.58 / [112]**Gentamycin**mw:477.5954 / fm:C21H43N5O7
MW:477.596 / [113]**Kanamycin**mw:484.4986 / fm:C18H36N4O11
MW:484.499 / [114]**Neomycin**mw:614.6437 / fm:C23H46N6O13
MW:614.644 / [115]

Streptomycinmw:581.5740 / fm:C21H39N7O12
MW:581.574 / [116]**dihydro-Streptomycin**mw:583.5899 / fm:C21H41N7O12
MW:583.574 / [117]**Spectinomycin**mw:332.3495 / fm:C14H24N2O7
MW:332.35 / [118]**Tobramycin**mw:467.5144 / fm:C18H37N5O9
MW:467.51 / [119]**Neospiramycin**mw:698.8842 / fm:C36H62N2O11
MW:698.9 / [120]**Emamectine**mw:886.1187 / fm:C49H75N013
MW:886.133 / [121]**Spinosad**mw:731.9555 / fm:C41H65N010
MW:731.968 / [122]**Spiramycin**mw:843.0526 / fm:C43H74N2O14
MW:843.1 / [123]**Natamycin**mw:665.7251 / fm:C33H47N013
MW:665.733 / [124]**Tylocin**mw:916.1000 / fm:C46H77N017
MW:916.10 / [125]**Tilmicosin**mw:869.1330 / fm:C46H80N2O13
MW:869.133 / [126]**Chlortetracycline**mw:478.8796 / fm:C22H23ClN2O8
MW:478.88 / [127]**Oxytetracycline**mw:460.4339 / fm:C22H24N2O9
MW:460.434 / [128]**Tetracycline**mw:444.4345 / fm:C22H24N2O8
MW:444.435 / [129]**Doxycycline**mw:444.4345 / fm:C22H24N2O8
MW:444.43 / [130]**Tiamulin**mw:493.7420 / fm:C28H47N04S
MW:493.74 / [131]**Rifampicin**mw:822.9402 / fm:C43H58N4O12
MW:822.94 / [132]**BHC**mw:290.8298 / fm:C6H6Cl6
MW:290.83 / [133]**pp-DDT**mw:354.4862 / fm:C14H9Cl5
MW:354.49 / [134]**Acrinathrin**mw:541.4390 / fm:C26H21F6NO5
MW:541.45 / [135]**Azaconazole**mw:300.1406 / fm:C12H11Cl2N3O2
MW:300.139 / [136]**Endrin**mw:380.9093 / fm:C12H8Cl6O
MW:380.91 / [137]**Sulfacetamide**mw:214.2415 / fm:C8H10N2O3S
MW:214.239 / [138]**Sulfatiazole**mw:255.3166 / fm:C9H9N3O2S2
MW:255.31 / [139]**Chlolidol**mw:192.0425 / fm:C7H7Cl2NO
MW:192.039 / [140]**Sulfadiadine**mw:250.2769 / fm:C10H10N4O2S
MW:250.276 / [141]**Levamisole**mw:204.2913 / fm:C11H12N2S
MW:204.29 / [142]**Sulfapyridine**mw:249.2889 / fm:C11H11N3O2S
MW:249.288 / [143]**Marbofloxacin**mw:362.3555 / fm:C17H19FN4O4
MW:362.361 / [144]**Sulfamerazine**mw:264.3035 / fm:C11H12N4O2S
MW:264.303 / [145]**Trimethoprim**mw:290.3177 / fm:C14H18N4O3
MW:290.323 / [146]**Ofloxacin**mw:361.3675 / fm:C18H20FN3O4
MW:361.373 / [147]**Ciprofloxacin**mw:331.3415 / fm:C17H18FN3O3
MW:331.347 / [148]**Enrofloxacin**mw:359.3946 / fm:C19H22FN3O3
MW:359.401 / [149]**Danofloxacin**mw:357.3788 / fm:C19H20FN3O3
MW:357.385 / [150]**Ormetoprim**mw:274.3183 / fm:C14H18N4O2
MW:274.324 / [151]**Sulfadimidine**mw:278.3301 / fm:C12H14N4O2S
MW:278.33 / [152]**Orbifloxacin**mw:395.3756 / fm:C19H20F3N3O3
MW:395.382 / [153]**Sarafloxacin**mw:385.3640 / fm:C20H17F2N3O3
MW:385.371 / [154]**Difloxacin**mw:399.3906 / fm:C21H19F2N3O3
MW:399.398 / [155]