

Molecular Coding Format examples

Author : Akira Yamaji Date : February 11, 2021

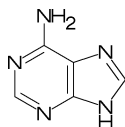
Located at : <http://www.ctan.org/pkg/mcf2graph>

** FM:Molecular formula calculated by mcf2graph

** MW:Molecular weight calculated by mcf2graph

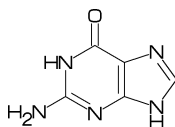
1:Adenine

MW:135.1267 / FM:C5H5N5
MW:135.13 (data)



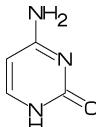
2:Guanine

MW:151.1261 / FM:C5H5N5O
MW:151.13 (data)



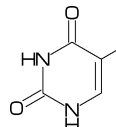
3:Cytosine

MW:111.1019 / FM:C4H5N3O
MW:111.10 (data)



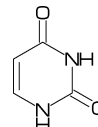
4:Thymine

MW:126.1133 / FM:C5H6N2O2
MW:126.11 (data)



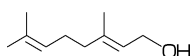
5:Uracil

MW:112.0867 / FM:C4H4N2O2
MW:112.09 (data)



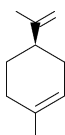
6:Geraniol

MW:154.2493 / FM:C10H18O
MW:154.25 (data)



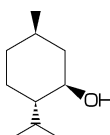
7:Limonene

MW:136.2340 / FM:C10H16
MW:136.24 (data)



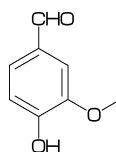
8:l-Menthol

MW:156.2652 / FM:C10H20O
MW:156.27 (data)



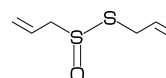
9:Vanillin

MW:152.1473 / FM:C8H8O3
MW:152.15 (data)



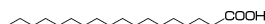
10:Allicin

MW:162.2729 / FM:C6H10OS2
MW:162.28 (data)



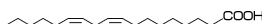
11:Stearic acid

MW:284.4772 / FM:C18H36O2
MW:284.48 (data)



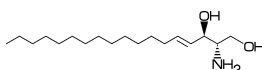
12:Linoleic acid

MW:280.4454 / FM:C18H32O2
MW:280.45 (data)



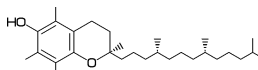
13:Sphingosine

MW:299.4918 / FM:C18H37NO2
MW:299.50 (data)



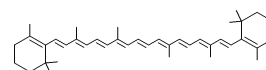
14:Tocopherol

MW:430.7060 / FM:C29H50O2
MW:430.717 (data)



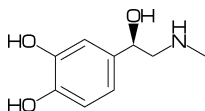
15:Carotene

MW:536.8726 / FM:C40H56
MW:536.8726 (data)



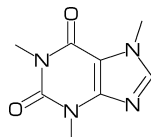
16:Adrenalin

MW:183.2044 / FM:C9H13NO3
MW:183.21 (data)



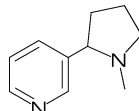
17:Caffeine

MW:194.1905 / FM:C8H10N4O2
MW:194.194 (data)



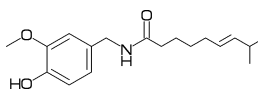
18:Nicotine

MW:162.2315 / FM:C10H14N2
MW:162.23 (data)



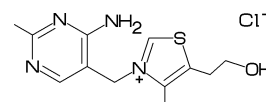
19:Capasaicin

MW:305.4118 / FM:C18H27NO3
MW:305.418 (data)



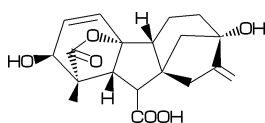
20:Thiamine

MW:265.3545 / FM:C12H17N4OS
MW:300.81 (data)



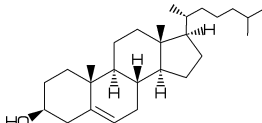
21:Gibberellin A3

MW:346.3743 / FM:C19H22O6
MW:346.379 (data)



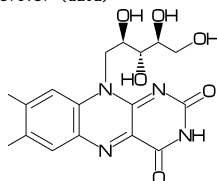
22:Cholesterol

MW:386.6535 / FM:C27H46O
MW:386.664 (data)



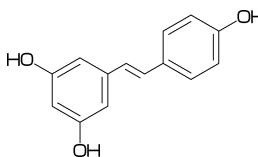
23:Riboflavin

MW:376.3638 / FM:C17H20N4O6
MW:376.37 (data)



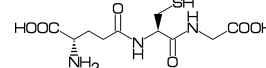
24:Resveratrol

MW:228.2432 / FM:C14H12O3
MW:228.24 (data)



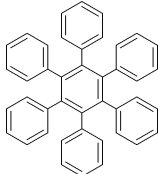
25:Glutathione

MW:307.3234 / FM:C10H17N3O6S
MW:307.33 (data)



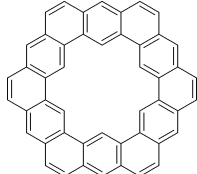
26:Hexaphenylbenzene

MW:534.6875 / FM:C42H30
MW:534.6876 (data)



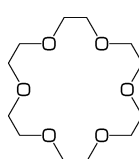
27:Kekulene

MW:600.7041 / FM:C48H24
MW:600.7 (data)



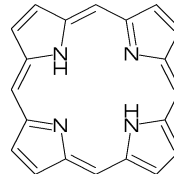
28:18-Crown-6

MW:264.3153 / FM:C12H24O6
MW:264.32 (data)



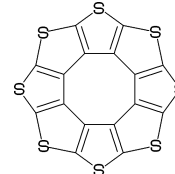
29:Porphyrin

MW:310.3519 / FM:C20H14N4
MW:310.4 (data)



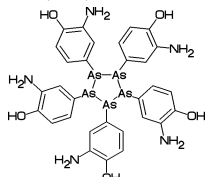
30:Sulfower

MW:448.6911 / FM:C16S8
MW:448.69 (data)



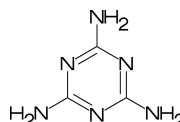
31:Arsphenamine x5

MW:915.1977 / FM:C30H30As5N5O5
MW:915.2 (data)



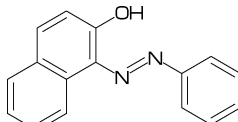
32:Melamine

MW:126.1199 / FM:C3H6N6
MW:126.12 (data)



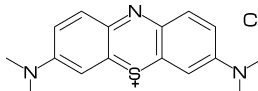
33:Sudan red 1

MW:248.2792 / FM:C16H12N2O
MW:248.28 (data)



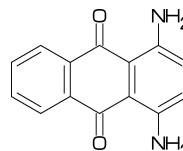
34:Basic blue 1

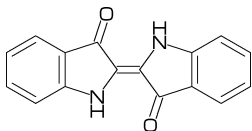
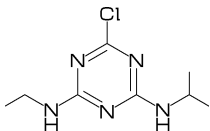
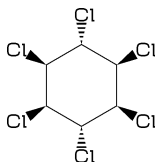
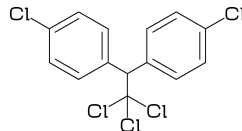
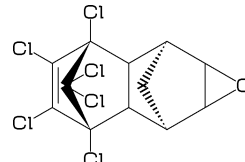
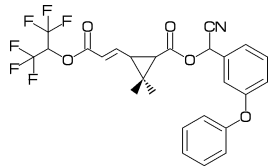
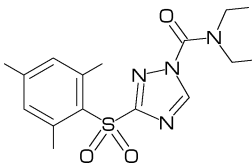
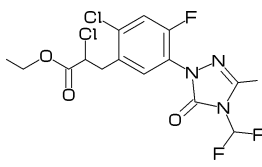
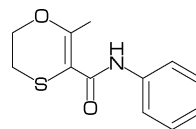
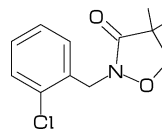
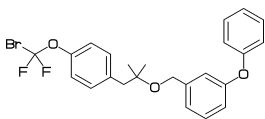
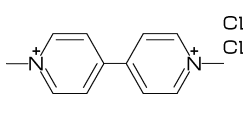
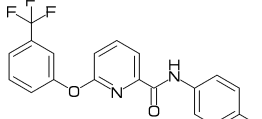
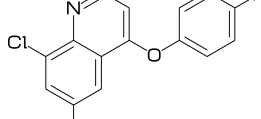
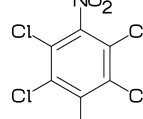
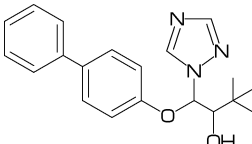
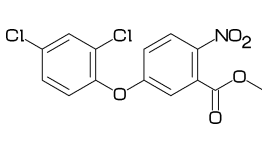
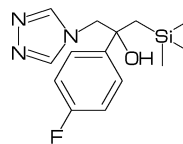
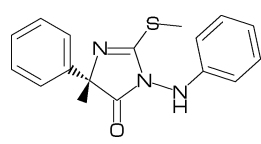
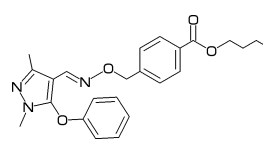
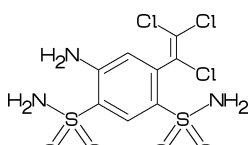
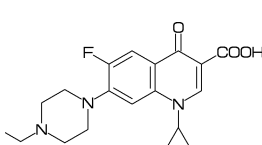
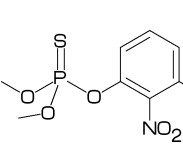
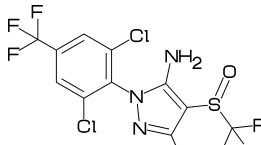
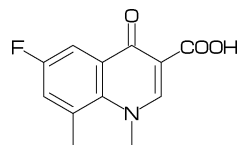
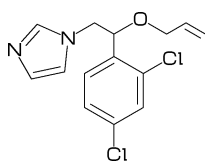
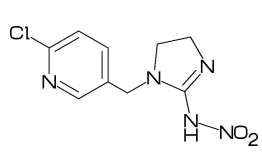
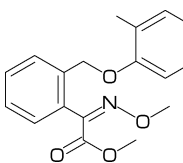
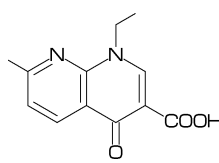
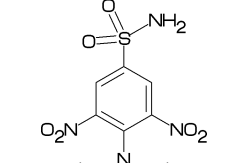
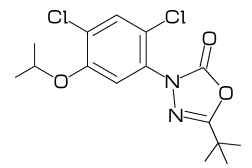
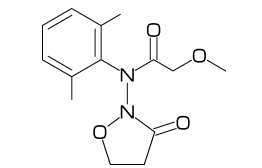
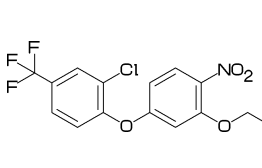
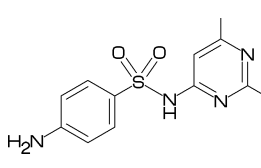
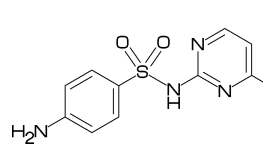
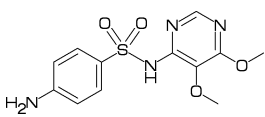
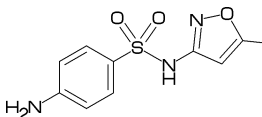
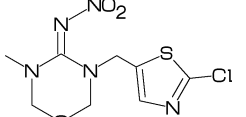
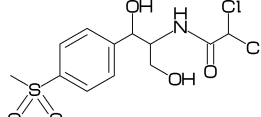
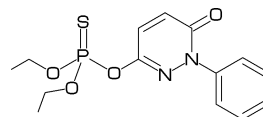
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MW:319.86 (data)

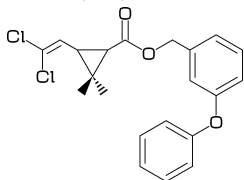
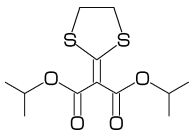
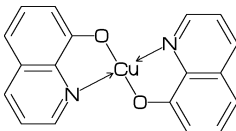
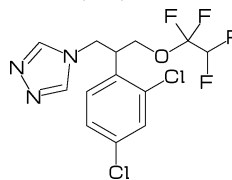
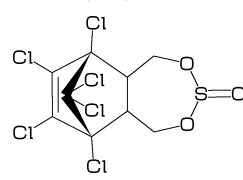
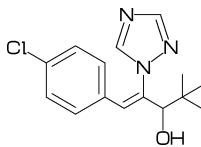
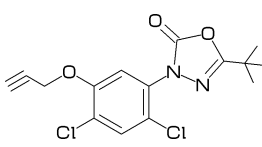
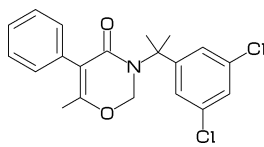
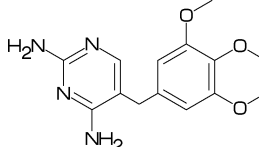
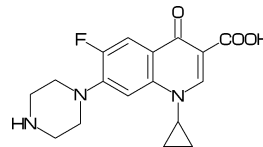
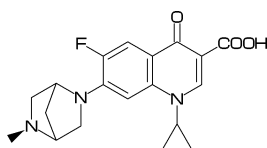
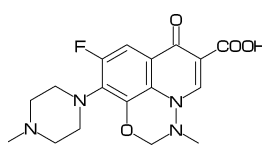
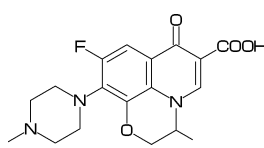
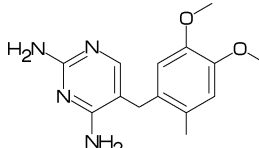
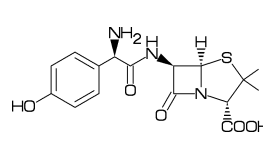
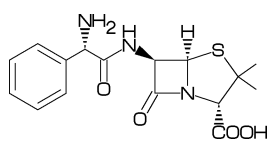
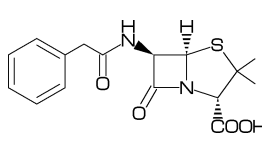
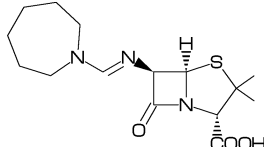
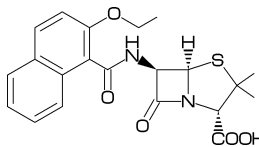
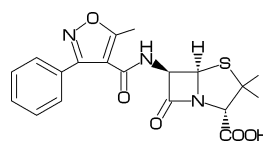
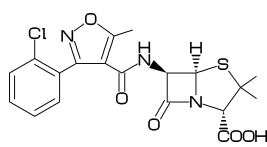
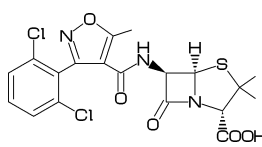
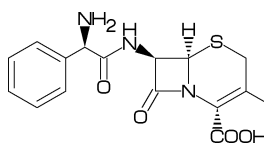
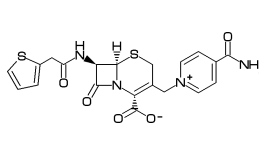
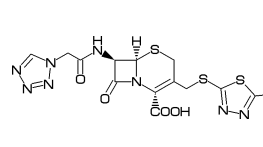
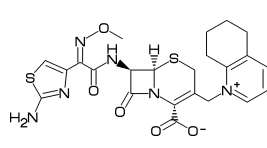
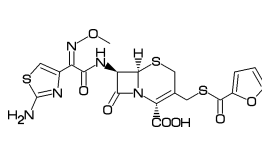
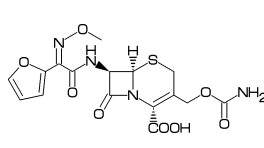
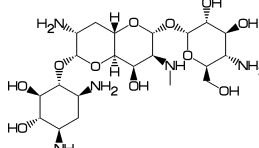
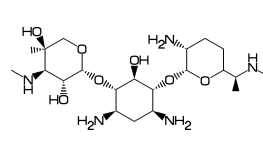
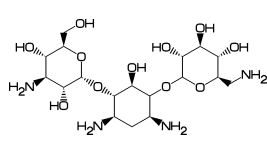
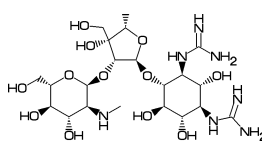
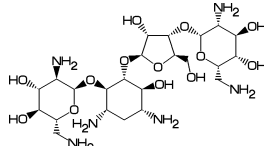
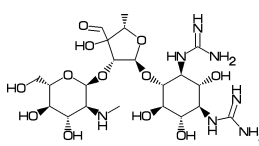
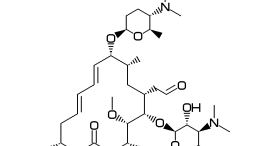
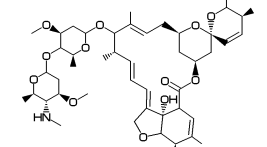
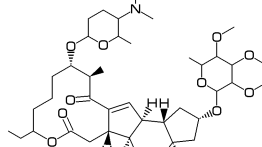
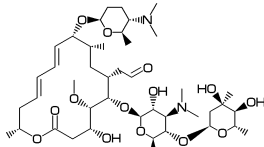
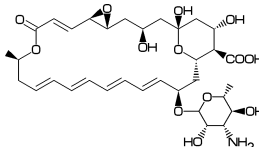
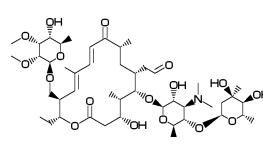


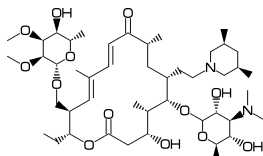
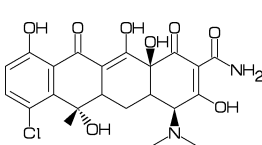
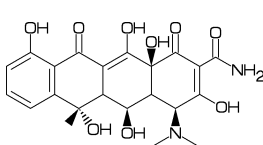
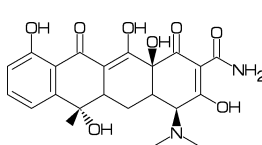
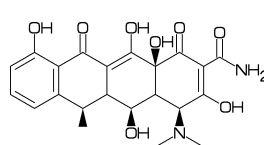
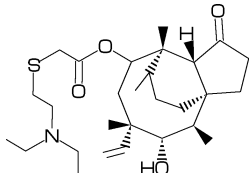
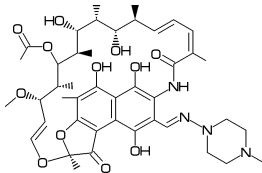
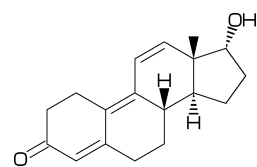
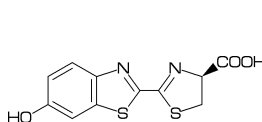
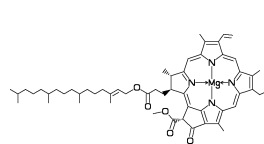
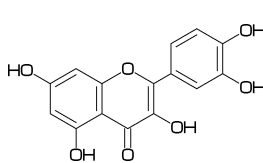
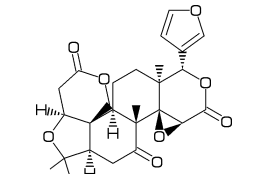
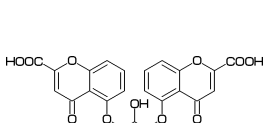
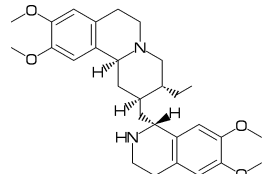
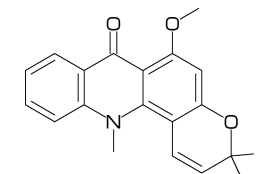
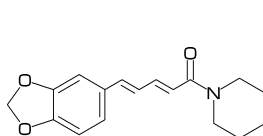
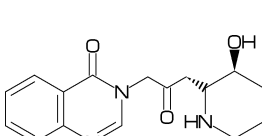
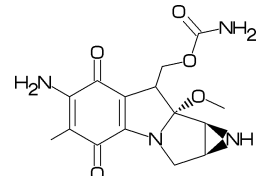
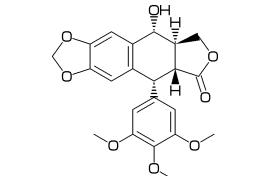
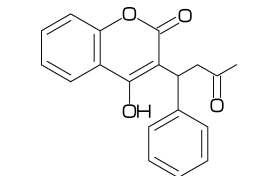
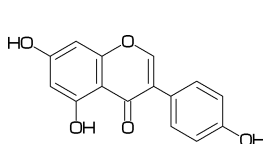
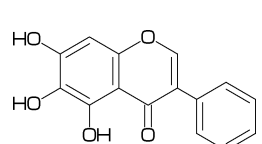
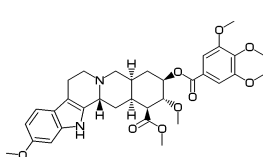
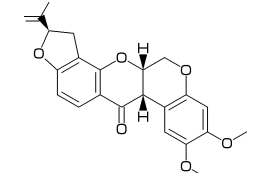
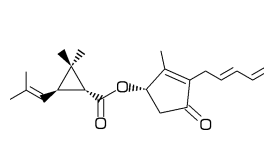
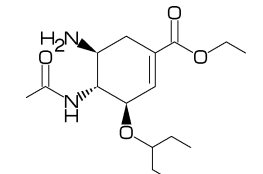
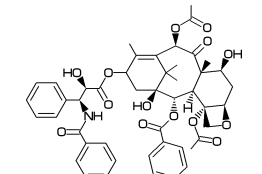
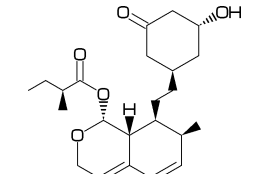
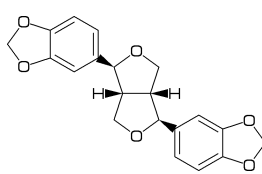
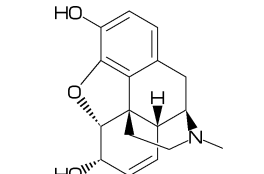
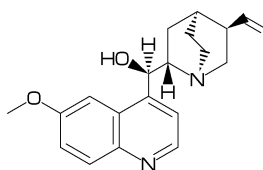
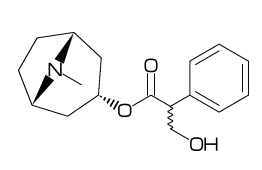
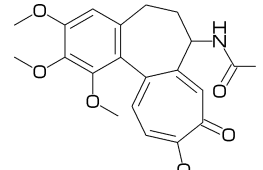
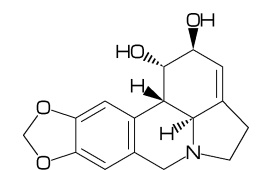
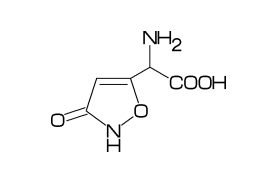
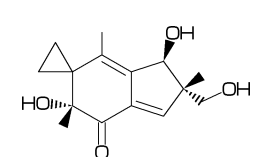
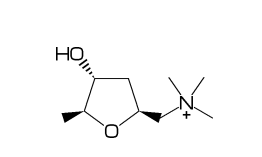
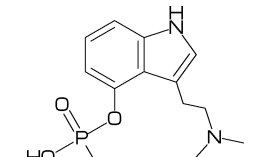
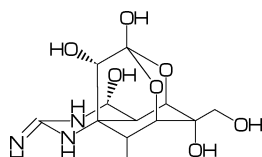
35:Disperse violet 1

MW:238.2413 / FM:C14H10N2O2
MW:238.25 (data)



36:Vat blue 1MW:262.2627 / FM:C16H10N2O2
MW:262.27 (data)**37:Atrazine**MW:215.6832 / FM:C8H14ClN5
MW:215.7 (data)**38:BHC**MW:290.8298 / FM:C6H6Cl6
MW:290.83 (data)**39:pp-DDT**MW:354.4862 / FM:C14H9Cl5
MW:354.49 (data)**40:Endrin**MW:380.9093 / FM:C12H8Cl16O
MW:380.91 (data)**41:Acrinathrin**MW:541.4390 / FM:C26H21F6NO5
MW:541.45 (data)**42:Cafenstrole**MW:350.4358 / FM:C16H22N4O3S
MW:350.4 (data)**43:Carfentrazone-ethyl**MW:412.1911 / FM:C15H14Cl2F3N3O3
MW:412.19 (data)**44:Carboxin**MW:235.3021 / FM:C12H13NO2S
MW:235.301 (data)**45:Clomazone**MW:239.6980 / FM:C12H14ClN02
MW:239.7 (data)**46:Halfenprox**MW:477.3384 / FM:C24H23BrF2O3
MW:477.4 (data)**47:Paraquat**MW:186.2529 / FM:C12H14N2
MW:257.16 (data)**48:Picolinafen**MW:376.3043 / FM:C19H12F4N2O2
MW:376.331 (data)**49:Quinoxifen**MW:308.1345 / FM:C15H8Cl2FN0
MW:308.13 (data)**50:Quitozene**MW:295.3347 / FM:C6Cl5NO2
MW:295.3 (data)**51:Bitertanol**MW:337.4155 / FM:C20H23N3O2
MW:337.4 (data)**52:Bifenox**MW:342.1309 / FM:C14H9Cl2NO5
MW:342.14 (data)**53:Simeconazole**MW:293.4120 / FM:C14H20FN3OSi
MW:293.417 (data)**54:Fenamidone**MW:311.4013 / FM:C17H17N3O5
MW:311.403 (data)**55:Fenpyroximate**MW:421.4888 / FM:C24H27N3O4
MW:421.49 (data)**56:Chlorsulron**MW:380.6558 / FM:C8H8Cl3N3O4S2
MW:380.648 (data)**57:Enrofloxacin**MW:359.3946 / FM:C19H22FN3O3
MW:359.401 (data)**58:Fenitrothion**MW:277.2340 / FM:C9H12NO5PS
MW:277.23 (data)**59:Fipronil**MW:437.1477 / FM:C12H4Cl2F6N4O5
MW:437.2 (data)**60:Flumequine**MW:261.2483 / FM:C14H12FN3O3
MW:261.225 (data)**61:Imazalil**MW:297.1797 / FM:C14H14Cl2N2O
MW:297.2 (data)**62:Imidacloprid**MW:255.661 / FM:C9H10ClN5O2
MW:255.662 (data)**63:Kresoxim-Methyl**MW:313.3477 / FM:C18H19NO4
MW:313.348 (data)**64:Nalidixic acid**MW:232.2352 / FM:C12H12N2O3
MW:232.239 (data)**65:Oryzalin**MW:346.3595 / FM:C12H18N4O6S
MW:346.4 (data)**66:Oxadiazon**MW:345.2210 / FM:C15H18Cl2N2O3
MW:345.2 (data)**67:Oxadixyl**MW:278.3037 / FM:C14H18N2O4
MW:278.3 (data)**68:Oxyfluorfen**MW:361.7003 / FM:C15H11ClF3NO4
MW:361.701 (data)**69:Sulfadimidine**MW:278.3301 / FM:C12H14N4O2S
MW:278.33 (data)**70:Sulfamerazine**MW:264.3035 / FM:C11H12N4O2S
MW:264.303 (data)**71:Sulfadoxine**MW:310.3289 / FM:C12H14N4O4S
MW:310.328 (data)**72:Sulfamethoxazole**MW:253.2776 / FM:C10H11N3O3S
MW:253.276 (data)**73:Thiamethoxam**MW:291.7146 / FM:C8H10ClN5O3S
MW:291.71 (data)**74:Thiamphenicol**MW:356.2221 / FM:C12H15Cl2N05S
MW:355 (data)**75:Pyridaphenthion**MW:340.3345 / FM:C14H17N2O4PS
MW:340.334 (data)

76:PermethrinMW:391.2876 / FM:C21H20C12O3
MW:391.288 (data)**77:Isoprothiolane**MW:290.3989 / FM:C12H18O4S2
MW:290.392 (data)**78:Oxine-Copper**MW:351.8460 / FM:C18H12CuN2O2
MW:351.852 (data)**79:Tetraconazole**MW:372.1455 / FM:C13H11C12F4N3O
MW:372.145 (data)**80:Endosulfan**MW:406.9251 / FM:C9H6C16O3S
MW:406.904 (data)**81:Uniconazole-P**MW:291.7759 / FM:C15H18C1N3O
MW:291.779 (data)**82:Oxadiargyl**MW:341.1892 / FM:C15H14C12N2O3
MW:341.19 (data)**83:Oxaziclomefone**MW:376.2763 / FM:C20H19C12N2O2
MW:376.277 (data)**84:Trimetoprim**MW:290.3177 / FM:C14H18N4O3
MW:290.323 (data)**85:Ciprofloxacin**MW:331.3415 / FM:C17H18FN3O3
MW:331.347 (data)**86:Danofloxacin**MW:357.3788 / FM:C19H20FN3O3
MW:357.385 (data)**87:Marbofloxacin**MW:362.3555 / FM:C17H19FN4O4
MW:362.361 (data)**88:Ofloxacin**MW:361.3675 / FM:C18H20FN3O4
MW:361.373 (data)**89:Ormetoprim**MW:274.3183 / FM:C14H18N4O2
MW:274.324 (data)**90:Amoxicillin**MW:365.4041 / FM:C16H19N3O5S
MW:365.4042 (data)**91:Ampicillin**MW:349.4047 / FM:C16H19N3O4S
MW:349.405 (data)**92:Benzyl-Penicillin**MW:334.3901 / FM:C16H18N2O4S
MW:334.4 (data)**93:Mecillinam**MW:325.4264 / FM:C15H23N3O3S
MW:325.4264 (data)**94:Nafcillin**MW:414.4747 / FM:C21H22N2O5S
MW:414.4748 (data)**95:Oxacillin**MW:401.4362 / FM:C19H19N3O5S
MW:401.4363 (data)**96:Cloxacillin**MW:435.8813 / FM:C19H18C1N3O5S
MW:435.8813 (data)**97:Dicloxacillin**MW:470.3263 / FM:C19H17C12N3O5S
MW:470.3264 (data)**98:Cefalexin**MW:347.3888 / FM:C16H17N3O4S
MW:347.3889 (data)**99:Cefalonium**MW:458.5107 / FM:C20H18N4O5S2
MW:458.5107 (data)**100:Cefazorin**MW:454.5071 / FM:C14H14N8O4S3
MW:454.51 (data)**101:Cefquinome**MW:528.6038 / FM:C23H24N6O5S2
MW:528.6 (data)**102:Ceftiofur**MW:523.5625 / FM:C19H17N5O7S3
MW:523.5626 (data)**103:Cefuroxime**MW:424.3852 / FM:C16H16N4O8S
MW:424.3852 (data)**104:Apramycin**MW:539.5771 / FM:C21H41N5O11
MW:539.58 (data)**105:Gentamycin**MW:477.5954 / FM:C21H43N5O7
MW:477.596 (data)**106:Kanamycin**MW:484.4986 / FM:C18H36N4O11
MW:484.499 (data)**107:DihydroStreptomycin**MW:583.5899 / FM:C21H41N7O12
MW:583.574 (data)**108:Fradiomycin**MW:614.6437 / FM:C23H46N6O13
MW:614.644 (data)**109:Streptomycin**MW:581.5740 / FM:C21H39N7O12
MW:581.574 (data)**110:Neospiramycin**MW:698.8842 / FM:C36H62N2O11
MW:698.9 (data)**111:Emamectine**MW:886.1187 / FM:C49H75N1O13
MW:886.133 (data)**112:Spinosad**MW:731.9555 / FM:C41H65N1O10
MW:731.968 (data)**113:Spiramycin**MW:843.0526 / FM:C43H74N2O14
MW:843.1 (data)**114:Natamycin**MW:665.7251 / FM:C33H47N1O13
MW:665.733 (data)**115:Tylocin**MW:916.1000 / FM:C46H77N1O17
MW:916.10 (data)

116:TilmicosinMW:869.1330 / FM:C46H80N2O13
MW:869.133 (data)**117:Chlortetracycline**MW:478.8796 / FM:C22H23ClN2O8
MW:478.88 (data)**118:Oxytetracycline**MW:460.4339 / FM:C22H24N2O9
MW:460.434 (data)**119:Tetracycline**MW:444.4345 / FM:C22H24N2O8
MW:444.435 (data)**120:Doxycycline**MW:444.4345 / FM:C22H24N2O8
MW:444.43 (data)**121:Tiamulin**MW:493.7420 / FM:C28H47NO4S
MW:493.74 (data)**122:Rifampicin**MW:822.9402 / FM:C43H58N4O12
MW:822.94 (data)**123:Trenbolone**MW:270.3660 / FM:C18H22O2
MW:270.37 (data)**124:Luciferin**MW:280.3228 / FM:C11H8N2O3S2
MW:280.33 (data)**125:Chlorophyll a**MW:893.4889 / FM:C55H72MgN4O5
MW:893.509 (data)**126:Quercetin**MW:302.2357 / FM:C15H10O7
MW:302.24 (data)**127:Limonin**MW:470.5115 / FM:C26H30O8
MW:470.518 (data)**128:Cromolyn**MW:468.3665 / FM:C23H16O11
MW:468.37 (data)**129:Emetine**MW:480.6388 / FM:C29H40N2O4
MW:480.649 (data)**130:Acronycine**MW:321.3697 / FM:C20H19NO3
MW:321.376 (data)**131:Piperine**MW:285.3376 / FM:C17H19NO3
MW:285.343 (data)**132:Febrifugine**MW:301.3403 / FM:C16H19N3O3
MW:301.346 (data)**133:Mitomycine C**MW:334.3272 / FM:C15H18N4O5
MW:334.332 (data)**134:Podophyllotoxin**MW:414.4052 / FM:C22H22O8
MW:414.41 (data)**135:Warfarin**MW:308.3279 / FM:C19H16O4
MW:308.333 (data)**136:Genistein**MW:270.2368 / FM:C15H10O5
MW:270.24 (data)**137:Baicalein**MW:270.2368 / FM:C15H10O5
MW:270.24 (data)**138:Reserpine**MW:608.6786 / FM:C33H40N2O9
MW:608.688 (data)**139:Rotenone**MW:394.4171 / FM:C23H22O6
MW:394.423 (data)**140:Pyrethrin I**MW:328.4452 / FM:C21H28O3
MW:328.452 (data)**141:Oseltamivir**MW:312.4045 / FM:C16H28N2O4
MW:312.40 (data)**142:Paclitaxel**MW:853.9061 / FM:C47H51NO14
MW:853.918 (data)**143:Mevastatin**MW:390.5130 / FM:C23H34O5
MW:390.52 (data)**144:Sesamine**MW:354.3533 / FM:C20H18O6
MW:354.35 (data)**145:Morphine**MW:285.3376 / FM:C17H19NO3
MW:285.343 (data)**146:Quinine**MW:324.4167 / FM:C20H24N2O2
MW:324.424 (data)**147:Atoropin**MW:289.3694 / FM:C17H23NO3
MW:289.375 (data)**148:Colchicine**MW:399.4370 / FM:C22H25NO6
MW:399.443 (data)**149:Lycorine**MW:287.3104 / FM:C16H17NO4
MW:287.315 (data)**150:Ibotenic acid**MW:158.1121 / FM:C5H6N2O4
MW:158.113 (data)**151:illudin S**MW:264.3168 / FM:C15H20O4
MW:264.3 (data)**152:Muscarine**MW:174.2605 / FM:C9H20NO2
MW:174.26 (data)**153:Psilocybin**MW:284.2481 / FM:C12H17N2O4P
MW:284.248 (data)**154:Tetrodotoxine**MW:319.2679 / FM:C11H17N3O8
MW:319.27 (data)**155:Aflatoxin B1**MW:312.2735 / FM:C17H12O6
MW:312.27 (data)