

Molecular Coding Format examples

Author : Akira Yamaji Date : January 3, 2019

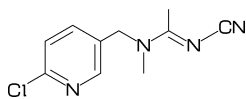
Located at : <http://www.ctan.org/pkg/mcf2graph>

** FM:Molecular formula calculated by mcf2graph

** MW:Molecular weight calculated by mcf2graph

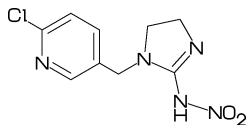
[1] Acetamiprid

MW:222.6741 / FM:C10H11ClN4
MW:222.676 (data)



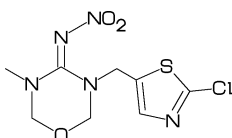
[2] Imidacloprid

MW:265.661 / FM:C9H10ClN5O2
MW:265.662 (data)



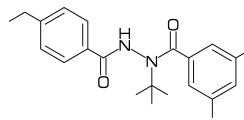
[3] Thiamethoxam

MW:291.7146 / FM:C8H10ClN5O3S
MW:291.71 (data)



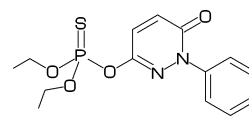
[4] Tebufenozide

MW:352.4699 / FM:C22H28N2O2
MW:352.478 (data)



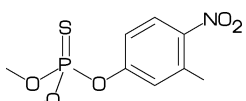
[5] Pyridaphenthion

MW:340.3345 / FM:C14H17N2O4PS
MW:340.334 (data)



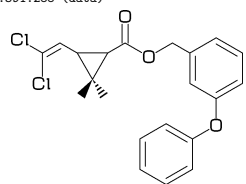
[6] Fenitrothion

MW:277.2340 / FM:C9H12NO5PS
MW:277.231 (data)



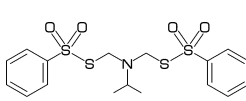
[7] Permethrin

MW:391.2876 / FM:C21H20Cl2O3
MW:391.288 (data)



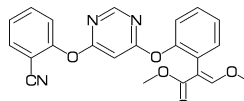
[8] Bensultap

MW:431.6129 / FM:C17H21N4S4
MW:431.598 (data)



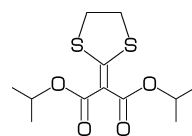
[9] Azoxystorbin

MW:403.3874 / FM:C22H17N3O5
MW:403.394 (data)



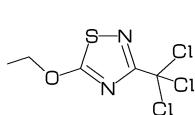
[10] Isoprothiolane

MW:290.3989 / FM:C12H18O4S2
MW:290.392 (data)



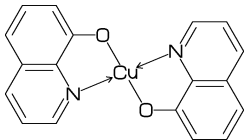
[11] Etridiazole

MW:247.53 / FM:C5H5Cl3N2OS
MW:247.518 (data)



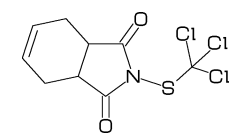
[12] Oxine-Copper

MW:351.8460 / FM:C18H12CuN2O2
MW:351.852 (data)



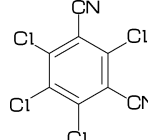
[13] Captan

MW:300.5893 / FM:C9H8Cl3NO2S
MW:300.578 (data)



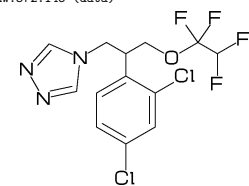
[14] Chlorothalonil

MW:265.911 / FM:C8Cl4N2
MW:265.902 (data)



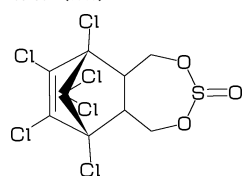
[15] Tetraconazole

MW:372.1455 / FM:C13H11Cl2F4N3O
MW:372.145 (data)



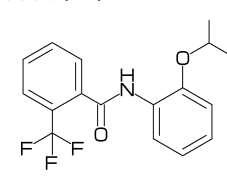
[16] Endosulfan

MW:406.9251 / FM:C9H6Cl3NO3S
MW:406.904 (data)



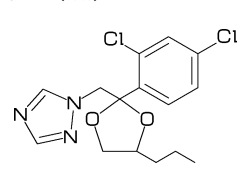
[17] Flutolanil

MW:323.3096 / FM:C17H16F3NO2
MW:323.315 (data)



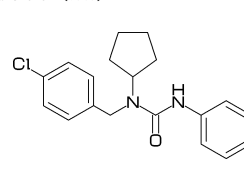
[18] Propiconazole

MW:342.2203 / FM:C15H17Cl2N3O2
MW:342.22 (data)



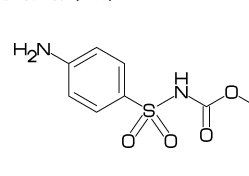
[19] Pencycuron

MW:328.8358 / FM:C19H21Cl2N2O
MW:328.84 (data)



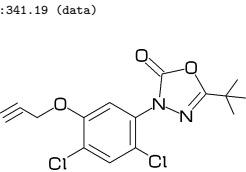
[20] Asulam

MW:230.2409 / FM:C13H10N2O4S
MW:230.238 (data)



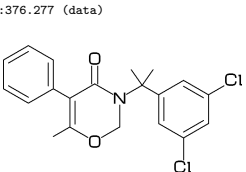
[21] Oxadiargyl

MW:341.1892 / FM:C15H14Cl2N2O3
MW:341.19 (data)



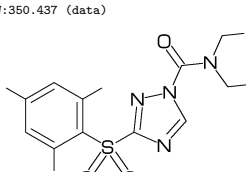
[22] Oxaziclomefone

MW:376.2763 / FM:C20H19Cl2N2O2
MW:376.277 (data)



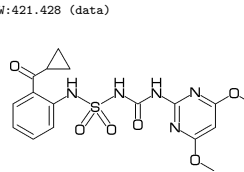
[23] Cafenstrole

MW:350.4358 / FM:C16H22N4O3S
MW:350.437 (data)



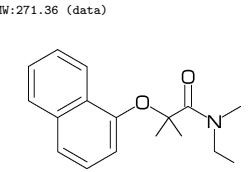
[24] Cyclosulfamuron

MW:421.4276 / FM:C17H19N5O6S
MW:421.428 (data)



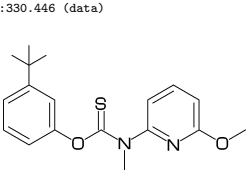
[25] Napropamide

MW:271.3541 / FM:C13H21N2O2
MW:271.36 (data)



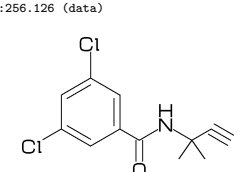
[26] Pyributicarb

MW:330.4444 / FM:C18H22N2O2S
MW:330.446 (data)



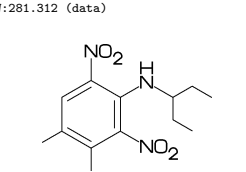
[27] Propyzamide

MW:256.1278 / FM:C12H11Cl2NO
MW:256.126 (data)



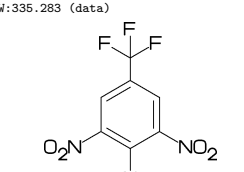
[28] Pendimethalin

MW:281.3076 / FM:C13H19N3O4
MW:281.312 (data)



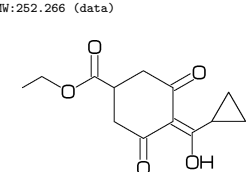
[29] Benfluralin

MW:335.2790 / FM:C13H16F3N3O4
MW:335.283 (data)



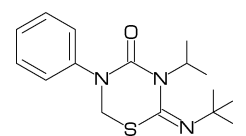
[30] Trinexapac-ethyl

MW:252.2631 / FM:C13H16O5
MW:252.266 (data)



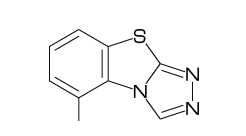
[31] Buprofezin

MW:305.4383 / FM:C16H23N3OS
MW:305.44 (data)



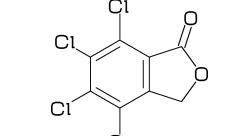
[32] Tricyclazole

MW:189.2369 / FM:C9H7N3S
MW:189.236 (data)



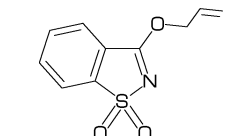
[33] Phthalide

MW:271.9122 / FM:C8H2Cl4O2
MW:271.91 (data)



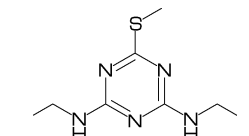
[34] Probenazole

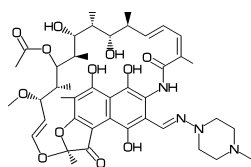
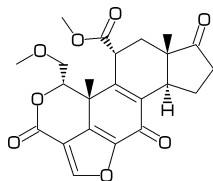
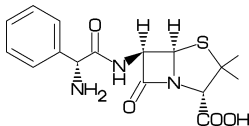
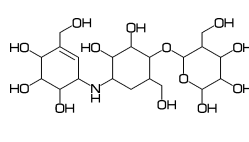
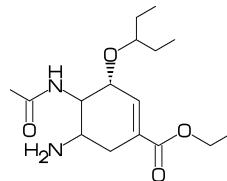
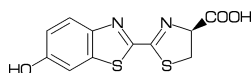
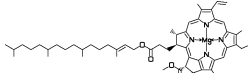
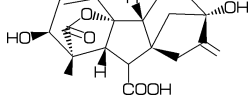
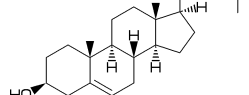
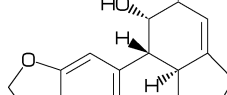
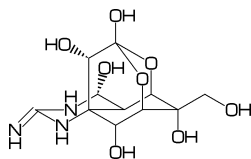
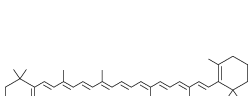
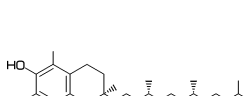
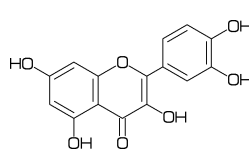
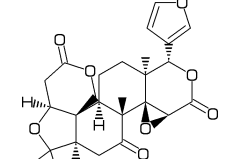
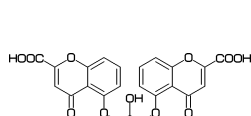
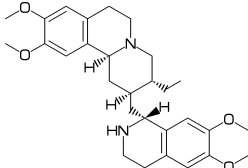
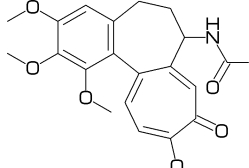
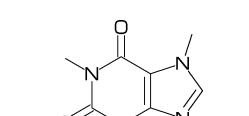
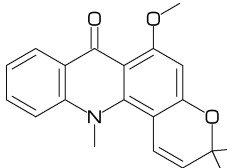
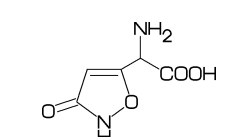
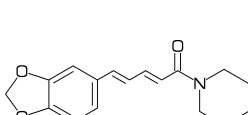
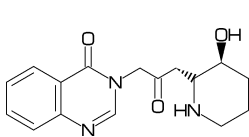
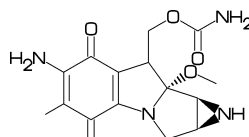
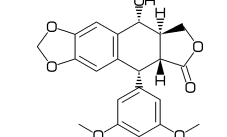
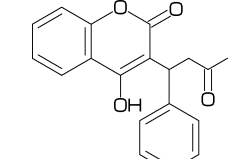
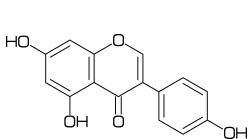
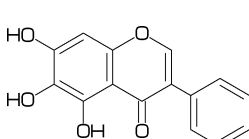
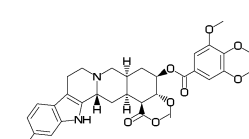
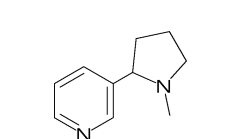
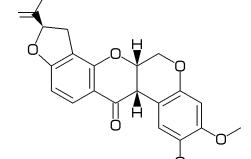
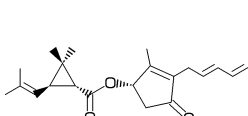
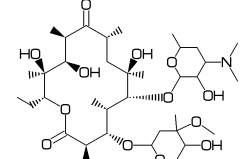
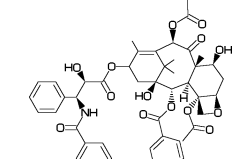
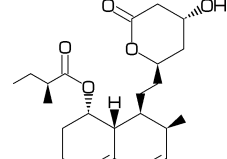
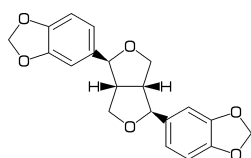
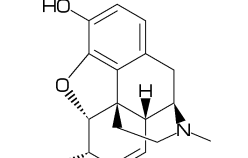
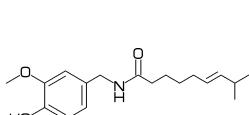
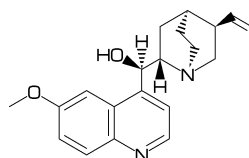
MW:223.2483 / FM:C10H9N3OS
MW:223.246 (data)



[35] Simetryn

MW:213.3032 / FM:C8H15N5S
MW:213.303 (data)



[36] RifampicinMW:822.9402 / FM:C43H58N4O12
MW:822.94 (data)**[37] Wortmannin**MW:428.4318 / FM:C23H24O8
MW:428.43 (data)**[38] Ampicillin**MW:349.4047 / FM:C16H19N3O4S
MW:349.405 (data)**[39] Validamycin**MW:497.4908 / FM:C20H35N013
MW:497.494 (data)**[40] Oceltamivir**MW:312.4045 / FM:C16H28N04
MW:312.41 (data)**[41] Luciferin**MW:280.3228 / FM:C11H8N2O3S2
MW:280.33 (data)**[42] Chlorophyll a**MW:893.4889 / FM:C55H72MgN4O5
MW:893.509 (data)**[43] Gibberellin A3**MW:346.3743 / FM:C19H22O6
MW:346.379 (data)**[44] Cholesterol**MW:386.6535 / FM:C27H46O
MW:386.664 (data)**[45] Lycorine**MW:287.3104 / FM:C16H17N04
MW:287.315 (data)**[46] Tetrodotoxine**MW:319.2679 / FM:C11H17N3O8
MW:319.27 (data)**[47] beta-Carotene**MW:536.8726 / FM:C40H56
MW:536.888 (data)**[48] alfa-Tocopherol**MW:430.7060 / FM:C29H50O2
MW:430.717 (data)**[49] Quercetin**MW:302.2357 / FM:C15H10O7
MW:302.24 (data)**[50] Limonin**MW:470.5115 / FM:C26H38O8
MW:470.518 (data)**[51] Cromolyn**MW:468.3665 / FM:C23H16O11
MW:468.37 (data)**[52] Emetine**MW:480.6388 / FM:C29H40N2O4
MW:480.649 (data)**[53] Colchicine**MW:399.4370 / FM:C22H25N06
MW:399.443 (data)**[54] Caffeine**MW:194.1905 / FM:C8H10N4O2
MW:194.194 (data)**[55] Acronycine**MW:321.3697 / FM:C20H19N03
MW:321.376 (data)**[56] Ibotenic acid**MW:158.1121 / FM:C5H6N2O4
MW:158.113 (data)**[57] Piperine**MW:285.3376 / FM:C17H19N03
MW:285.343 (data)**[58] Febrifugine**MW:301.3403 / FM:C16H19N3O3
MW:301.346 (data)**[59] Mitomycin C**MW:334.3272 / FM:C15H18N4O5
MW:334.332 (data)**[60] Podophyllotoxin**MW:414.4052 / FM:C20H14N02
MW:414.41 (data)**[61] Warfarin**MW:308.3279 / FM:C19H16O4
MW:308.333 (data)**[62] Genistein**MW:270.2368 / FM:C15H10O5
MW:270.24 (data)**[63] Baicalein**MW:270.2368 / FM:C15H10O5
MW:270.24 (data)**[64] Reserpine**MW:608.6786 / FM:C33H40N2O9
MW:608.688 (data)**[65] Nicotine**MW:162.2315 / FM:C10H14N2
MW:162.23 (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] Erythromycin**MW:733.9267 / FM:C37H67N13
MW:733.937 (data)**[69] Paclitaxel**MW:853.9061 / FM:C47H51N014
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:C17H19N03
MW:285.343 (data)**[73] Capsaicin**MW:305.4118 / FM:C18H27N03
MW:305.418 (data)**[74] Quinine**MW:324.4167 / FM:C20H24N2O2
MW:324.424 (data)**[75] Atoropin**MW:289.3694 / FM:C17H23N03
MW:289.375 (data)