

Molecular Coding Format examples

Author : Akira Yamaji Date : January 3, 2018

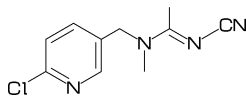
Located at : <http://www.ctan.org/pkg/mcf2graph>

** FM:Molecular formula calculated by mcf2graph

** MW:Molecular weight calculated by mcf2graph

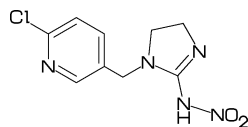
[1] Acetamiprid

MW:222.6740 / FM:C10H11ClN4
MW:222.676 (data)



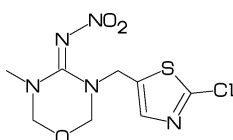
[2] Imidacloprid

MW:265.6609 / FM:C9H10ClN5O2
MW:265.662 (data)



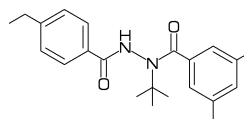
[3] Thiamethoxam

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



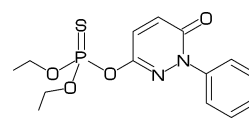
[4] Tebufenozide

MW:352.4697 / FM:C22H28N2O2
MW:352.478 (data)



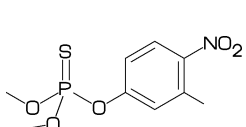
[5] Pyridaphenthion

MW:340.3344 / FM:C14H17N2O4PS
MW:340.334 (data)



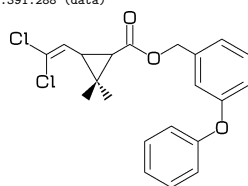
[6] Fenitrothion

MW:277.2339 / FM:C9H12NO5PS
MW:277.231 (data)



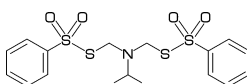
[7] Permethrin

MW:391.2875 / FM:C21H20Cl2O3
MW:391.288 (data)



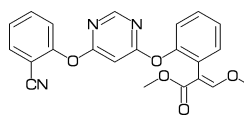
[8] Bensultap

MW:431.6128 / FM:C17H21N4O4S4
MW:431.598 (data)



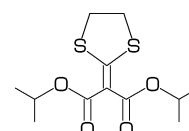
[9] Azoxytorbin

MW:403.3873 / FM:C22H17N3O5
MW:403.394 (data)



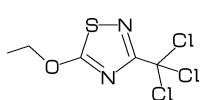
[10] Isoprothiolane

MW:290.3988 / FM:C18H18O4S2
MW:290.392 (data)



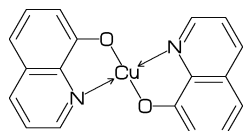
[11] Etridiazole

MW:247.5299 / FM:C5H5Cl3N2OS
MW:247.518 (data)



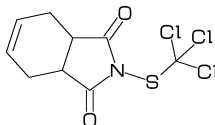
[12] Oxine-Copper

MW:351.8459 / FM:C18H12CuN2O2
MW:351.852 (data)



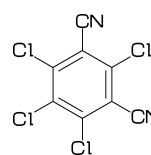
[13] Captan

MW:300.5892 / FM:C9H8Cl3NO2S
MW:300.578 (data)



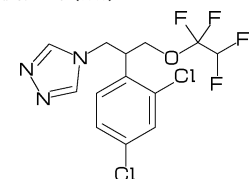
[14] Chlorothalonil

MW:265.9109 / FM:C8Cl4N2
MW:265.902 (data)



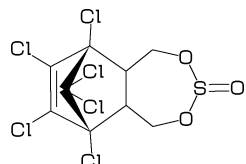
[15] Tetraconazole

MW:372.1454 / FM:C13H11Cl2F4N3O
MW:372.145 (data)



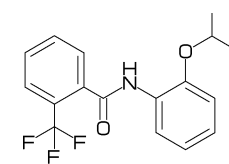
[16] Endosulfan

MW:406.9251 / FM:C9H6Cl3O3S
MW:406.904 (data)



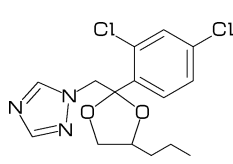
[17] Flutolanil

MW:323.3095 / FM:C17H16F3NO2
MW:323.315 (data)



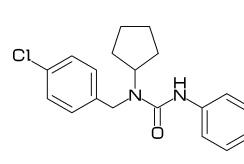
[18] Propiconazole

MW:342.2202 / FM:C15H17Cl2N3O2
MW:342.22 (data)



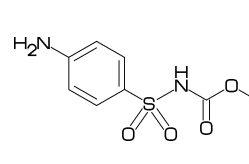
[19] Pencycuron

MW:328.8356 / FM:C19H21ClN2O2
MW:328.84 (data)



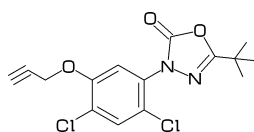
[20] Asulam

MW:230.2409 / FM:C8H10N2O4S
MW:230.238 (data)



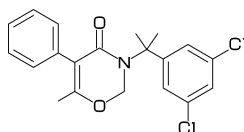
[21] Oxadiargyl

MW:341.1891 / FM:C15H14Cl2N2O3
MW:341.19 (data)



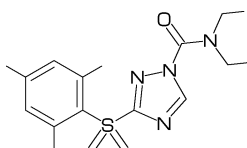
[22] Oxaziclomefone

MW:376.2762 / FM:C20H19Cl2N2O2
MW:376.277 (data)



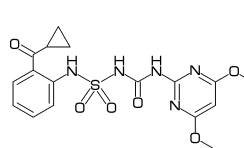
[23] Cafenstrole

MW:350.4357 / FM:C16H22ClN3O3S
MW:350.437 (data)



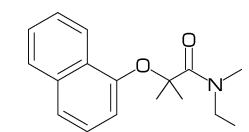
[24] Cyclosulfamuron

MW:421.4275 / FM:C17H19N5O6S
MW:421.428 (data)



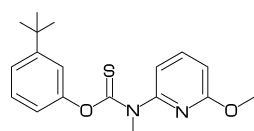
[25] Napropamide

MW:271.3539 / FM:C17H21N2O2
MW:271.36 (data)



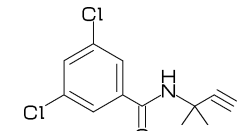
[26] Pyributicarb

MW:330.4443 / FM:C18H22N2O2S
MW:330.446 (data)



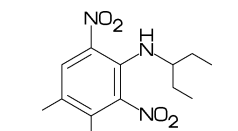
[27] Propyzamide

MW:256.1277 / FM:C12H11Cl2NO
MW:256.126 (data)



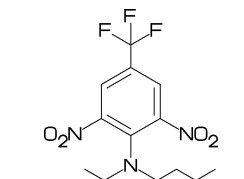
[28] Pendimethalin

MW:281.3075 / FM:C13H19N3O4
MW:281.312 (data)



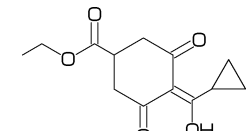
[29] Benfluralin

MW:335.2789 / FM:C13H16F3N3O4
MW:335.283 (data)



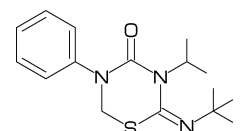
[30] Trinexapac-ethyl

MW:252.2630 / FM:C13H16O5
MW:252.266 (data)



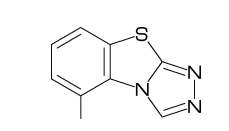
[31] Buprofezin

MW:305.4381 / FM:C16H23N3OS
MW:305.44 (data)



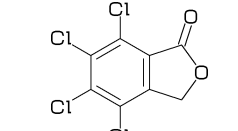
[32] Tricyclazole

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



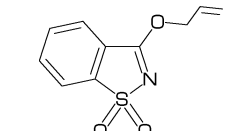
[33] Phthalide

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



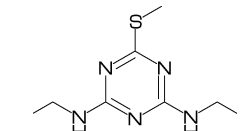
[34] Probenazole

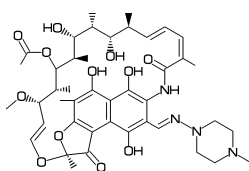
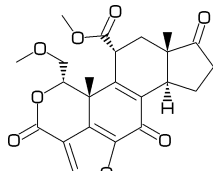
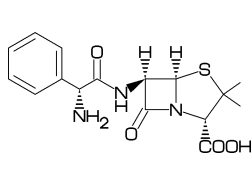
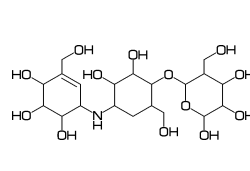
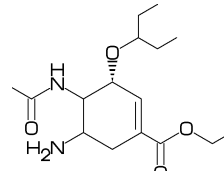
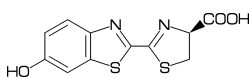
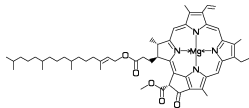
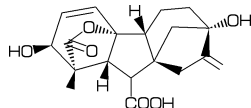
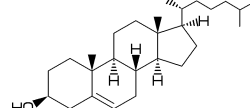
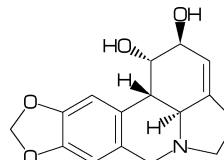
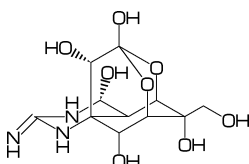
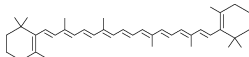
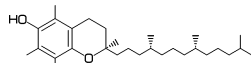
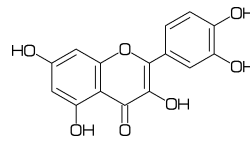
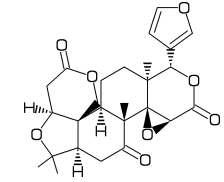
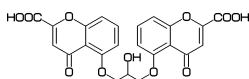
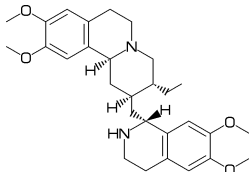
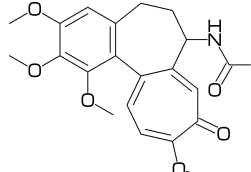
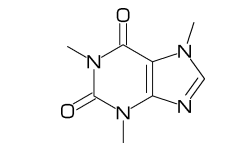
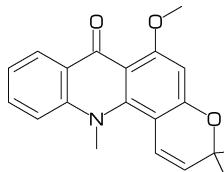
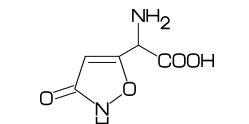
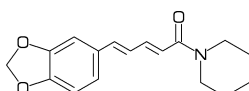
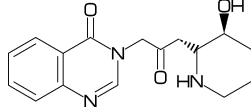
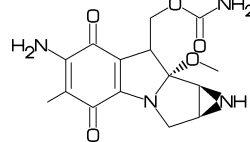
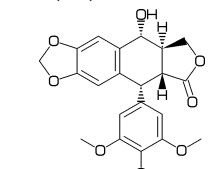
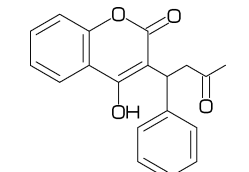
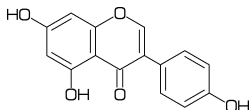
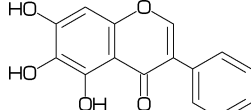
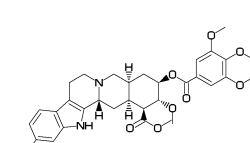
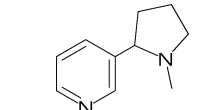
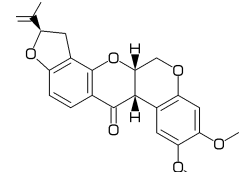
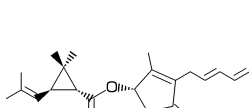
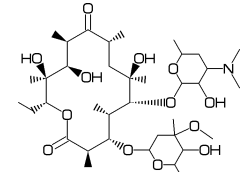
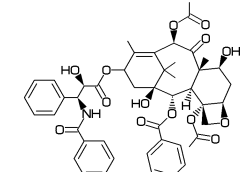
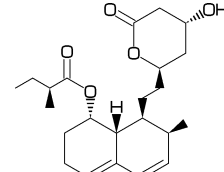
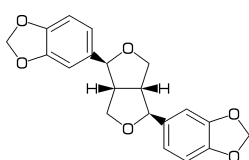
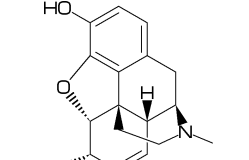
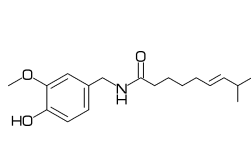
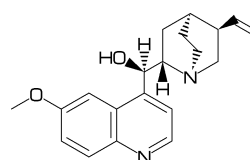
MW:223.2482 / FM:C10H9N3O3S
MW:223.246 (data)



[35] Simetryn

MW:213.3030 / FM:C8H15N5S
MW:213.303 (data)



[36] RifampicinMW: 822.9398 / FM: C43H58N4O12
MW: 822.94 (data)**[37] Wortmannin**MW: 428.4316 / FM: C23H24O8
MW: 428.43 (data)**[38] Ampicillin**MW: 349.4046 / FM: C16H19N3O4S
MW: 349.405 (data)**[39] Validamycin**MW: 497.4906 / FM: C20H35N13
MW: 497.494 (data)**[40] Oceltamivir**MW: 312.4043 / FM: C16H28N2O4
MW: 312.41 (data)**[41] Luciferin**MW: 280.3227 / FM: C11H8N2O3S2
MW: 280.33 (data)**[42] Chlorophyll a**MW: 893.4884 / FM: C55H72MgN4O5
MW: 893.509 (data)**[43] Gibberellin A3**MW: 346.3742 / FM: C19H22O6
MW: 346.379 (data)**[44] Cholesterol**MW: 386.6532 / FM: C27H46O
MW: 386.664 (data)**[45] Lycorine**MW: 287.3103 / FM: C16H17NO4
MW: 287.315 (data)**[46] Tetrodotoxine**MW: 319.2678 / FM: C11H17N3O8
MW: 319.27 (data)**[47] beta-Carotene**MW: 536.8722 / FM: C40H56
MW: 536.888 (data)**[48] alpha-Tocopherol**MW: 430.7057 / FM: C29H50O2
MW: 430.717 (data)**[49] Quercetin**MW: 302.2356 / FM: C15H10O7
MW: 302.24 (data)**[50] Limonin**MW: 470.5113 / FM: C26H30O8
MW: 470.518 (data)**[51] Cromolyn**MW: 468.3664 / FM: C23H16O11
MW: 468.37 (data)**[52] Emetine**MW: 480.6386 / FM: C29H40N2O4
MW: 480.649 (data)**[53] Colchicine**MW: 399.4368 / FM: C22H25N5O6
MW: 399.449 (data)**[54] Caffeine**MW: 194.1905 / FM: C8H10N4O2
MW: 194.194 (data)**[55] Acronycine**MW: 321.3696 / FM: C20H19N3O
MW: 321.376 (data)**[56] Ibotenic acid**MW: 158.1121 / FM: C5H8N2O4
MW: 158.113 (data)**[57] Piperine**MW: 285.3375 / FM: C17H19NO3
MW: 285.343 (data)**[58] Febrifugine**MW: 301.3402 / FM: C16H19N3O3
MW: 301.346 (data)**[59] Mitomycin C**MW: 334.3270 / FM: C15H18N4O5
MW: 334.332 (data)**[60] Podophyllotoxin**MW: 414.4051 / FM: C26H22O6
MW: 414.41 (data)**[61] Warfarin**MW: 308.3278 / 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: 608.6784 / FM: C33H40N2O9
MW: 608.688 (data)**[65] Nicotine**MW: 162.2314 / FM: C10H14N2
MW: 162.23 (data)**[66] Rotenone**MW: 394.417 / FM: C23H22O6
MW: 394.423 (data)**[67] Pyrethrin I**MW: 328.445 / FM: C21H28O3
MW: 328.452 (data)**[68] Erythromycin**MW: 733.9263 / FM: C37H67N13
MW: 733.937 (data)**[69] Paclitaxel**MW: 853.9057 / FM: C47H51NO14
MW: 853.918 (data)**[70] Mevastatin**MW: 390.5128 / FM: C23H34O5
MW: 390.52 (data)**[71] Sesamine**MW: 354.3531 / FM: C20H18O6
MW: 354.35 (data)**[72] Morphine**MW: 285.3375 / FM: C17H19NO3
MW: 285.343 (data)**[73] Capsaicin**MW: 305.4116 / FM: C18H27NO3
MW: 305.418 (data)**[74] Quinine**MW: 324.4165 / FM: C20H24N2O2
MW: 324.424 (data)**[75] Atoropin**MW: 289.3692 / FM: C17H23NO3
MW: 289.375 (data)