Molecular Coding Format examples

Author: Akira Yamaji Date: January 26, 2020 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:255.661 / FM:C9H10ClN502 MW:255.662 (data)

[3] Thiamethoxam
MW:291.7146 / FM:C8H10C1N503S
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)

`NO2

-Cl

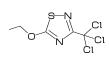
[6] Fenitrothion MW:277.2340 / FM:C9H12N05PS MW:277.231 (data) [7] Permethrin MW:391.2876 / FM:C21H20C12D3 MW:391.288 (data) [8] Bensultap MW:431.6129 / FM:C17H21N04S4 MW:431.598 (data)

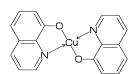
[9] Azoxystorbin MW:403.3874 / FM:C22H17N305 MW:403.394 (data) [10] Isoprothiolane MW:290.3989 / FM:C12H1804S2 MW:290.392 (data)

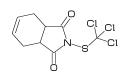
[11] Etridiazole MW:247.53 / FM:C5H5C13N2OS MW:247.518 (data) [12] Oxine-Copper MW:351.8460 / FM:C18H12CuN2O2 MW:351.852 (data)

[13] Captan MW:300.5893 / FM:C9H8C13N02S MW:300.578 (data) [14] Chlorothalonil MW:265.911 / FM:C8C14N2 MW:265.902 (data)

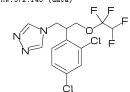
[15] Tetraconazole MW: 372.1455 / FM:C13H11Cl2F4N30 MW: 372.145 (data)









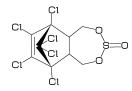


[16] Endosulfan MW:406.9251 / FM:C9H6C16D3S MW:406.904 (data) [17] Flutolanil MW:323.3096 / FM:C17H16F3NO2 MW:323.315 (data)

[18] Propiconazole MW: 342.2203 / FM:C15H17C12N302 MW: 342.22 (data)

[19] Pencycuron MW:328.8358 / FM:C19H21ClN20 MW:328.84 (data)

[20] Asulam MW:230.2409 / FM:C8H10N2D4S MW:230.238 (data)

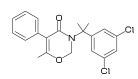


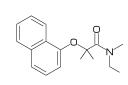
[21] Oxadiargyl MW:341.1892 / FM:C15H14C12N2O3 MW:341.19 (data)

[22] Oxaziclomefone MW:376.2763 / FM:C20H19C12N02 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:C17H21N02 MW: 271.36 (data)





[26] Pyributicarb MW:330.4444 / FM:C18H22N2O2S MW:330.446 (data) [27] Propyzamide MW: 256.1278 / FM: C12H11C12NO MW: 256.126 (data) [28] Pendimethalin
MW:281.3076 / FM:C13H19N304
MW:281.312 (data)

[29] Benfluralin MW:335.2790 / FM:C13H16F3N3O4 MW:335.283 (data)



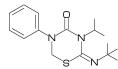
[31] Buprofezin MW:305.4383 / FM:C16H23N3OS MW:305.44 (data) [32] Tricyclazole MW:189.2369 / FM:C9H7N3S MW:189.236 (data)

[33] Phthalide MW:271.9122 / FM:C8H2C1402 MW:271.91 (data)

[34] Probenazole

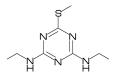
MW:223.2483 / FM:C10H9N03S MW:223.246 (data)

[35] Simetryn MW:213.3032 / FM:C8H15N5S MW:213.303 (data)









[36] Rifampicin
MW:822.9402 / FM:C43H58N4012
MW:822.94 (data)

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[41] Luciferin
MW:280.3228 / FM:C11H8N2O3S2
MW:280.33 (data)

[46] Tetrodotoxine

[51] Cromolyn

HOOC

MW:468.3665 / FM:C23H16011 MW:468.37 (data)

[56] Ibotenic acid
MW:158.1121 / FM:C5H6N2O4
MW:158.113 (data)

[61] Warfarin

[66] Rotenone

[71] Sesamine

MW:394.4171 / FM:C23H22O6 MW:394.423 (data)

MW:308.3279 / FM:C19H1604 MW:308.333 (data)

COOH

MW:319.2679 / FM:C11H17N308 MW:319.27 (data) [37] Wortmannin
MW:428.4318 / FM:C23H2408
MW:428.43 (data)

[42] Chlorophyll a
MW:893.4889 / FM:C55H72MgN405
MW:893.509 (data)

[47] beta-Carotene

MW:536.8726 / FM:C40H56 MW:536.888 (data)

[52] Emetine

MW:480.6388 / FM:C29H40N2O4 MW:480.649 (data)

[57] Piperine MW:285.3376 / FM:C17H19N03 MW:285.343 (data)

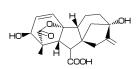
[62] Genistein

MW: 270.2368 / FM:C15H1005 MW: 270.24 (data) NH₂

MW: 349.4047 / FM:C16H19N304S MW:349.405 (data)

[38] Ampicillin

[43] Gibberellin A3
MW:346.3743 / FM:C19H2206
MW:346.379 (data)



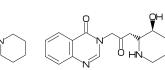
[48] alfa-Tocopherol MW:430.7060 / FM:C29H5002 MW:430.717 (data)

HO

[53] Colchicine

MW:399.4370 / FM:C22H25ND6 MW:399.443 (data)

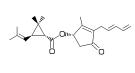
[58] Febrifugine
MW:301.3403 / FM:C16H19N303
MW:301.346 (data)



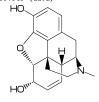
[63] Baicalein
MW:270.2368 / FM:C15H1005
MW:270.24 (data)

H0 0H 0

[67] Pyrethrin I [68] Erythromycin
MW:328.4452 / FM:C21H2803 MW:733.9267 / FM:C37H67N013
MW:328.452 (data) MW:733.937 (data)



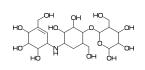
[72] Morphine
MW:285.3376 / FM:C17H19N03
MW:285.343 (data)



[73] Capsaicin MW:305.4118 / FM:C18H27N03 MW:305.418 (data)

HO

[39] Validamycin
MW:497.4908 / FM:C20H35N013
MW:497.494 (data)



[44] Cholesterol
MW:386.6535 / FM:C27H460
MW:386.664 (data)

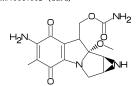
[49] Quercetin
MW:302.2357 / FM:C15H1007
MW:302.24 (data)

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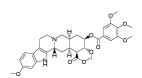
[54] Caffeine MW:194.1905 / FM:C8H10N402 MW:194.194 (data)



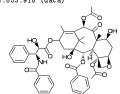
[59] Mitomycine C MW:334.3272 / FM:C15H18N405 MW:334.332 (data)



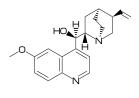
[64] Reserpine
MW:608.6786 / FM:C33H40N2D9
MW:608.688 (data)



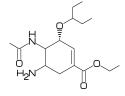
[69] Paclitaxel
MW:853.9061 / FM:C47H51N014
MW:853.918 (data)



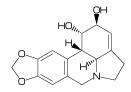
[74] Quinine MW:324.4167 / FM:C20H24N202 MW:324.424 (data)



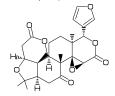
[40] Oceltamivir
MW:312.4045 / FM:C16H28N204
MW:312.41 (data)



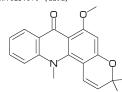
[45] Lycorine
MW:287.3104 / FM:C16H17N04
MW:287.315 (data)



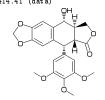
[50] Limonin MW:470.5115 / FM:C26H3008 MW:470.518 (data)



[55] Acronycine
MW:321.3697 / FM:C20H19N03
MW:321.376 (data)



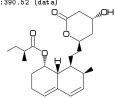
[60] Podophyllotoxin
MW:414.4052 / FM:C22H2208
MW:414.41 (data)



[65] Nicotine
MW:162.2315 / FM:C10H14N2
MW:162.23 (data)



[70] Mevastatin
MW:390.5130 / FM:C23H3405
MW:390.52 (data)



[75] Atoropin
MW:289.3694 / FM:C17H23N03
MW:289.375 (data)

