

MCF example for luamplib(Lua $\text{L}^{\text{A}}\text{T}_{\text{E}}\text{X}$)

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

FM(C) : molecular formula calculated by mcf2graph

MW(C) : molecular weight calculated by mcf2graph

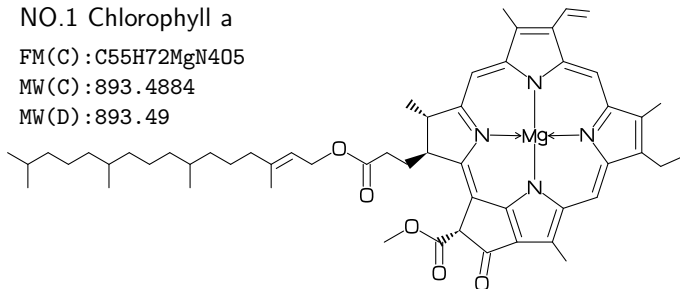
MW(D) : molecular weight from literature data

NO.1 Chlorophyll a

FM(C) : C₅₅H₇₂MgN₄O₅

MW(C) : 893.4884

MW(D) : 893.49

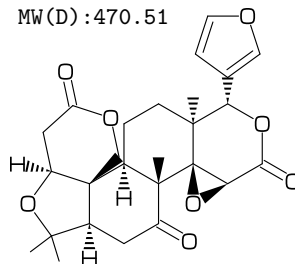


NO.2 Limonin

FM(C) : C₂₆H₃₀O₈

MW(C) : 470.51138

MW(D) : 470.51

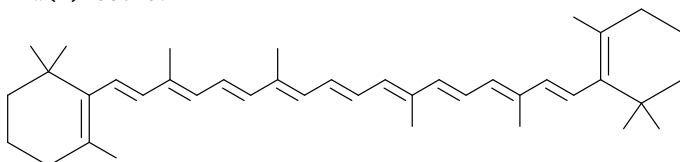


NO.3 beta-carotene

FM(C) : C₄₀H₅₆

MW(C) : 536.8722

MW(D) : 536.87

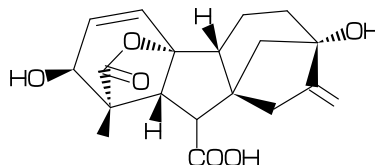


NO.4 Gibberellin A3

FM(C) : C₁₉H₂₂O₆

MW(C) : 346.37422

MW(D) : 346.37

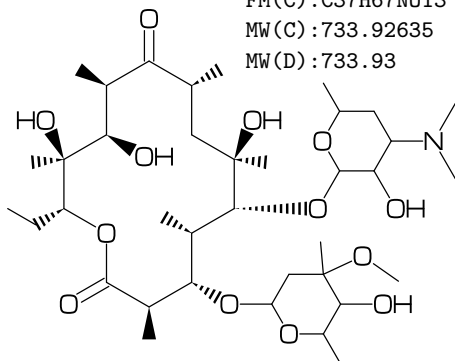


NO.5 Erythromycin

FM(C) : C₃₇H₆₇N₀O₁₃

MW(C) : 733.92635

MW(D) : 733.93

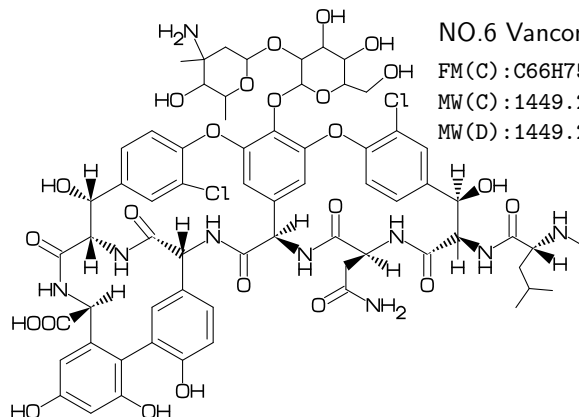


NO.6 Vancomycin

FM(C) : C₆₆H₇₅Cl₁₂N₉O₂₄

MW(C) : 1449.25307

MW(D) : 1449.25



NO.7 Maitotoxin

FM(C) : C₁₆₄H₂₅₆Na₂₀S₂

MW(C) : 3425.85455

MW(D) : 3425.86

