CNS MPO
Multi-Parameter Optimization
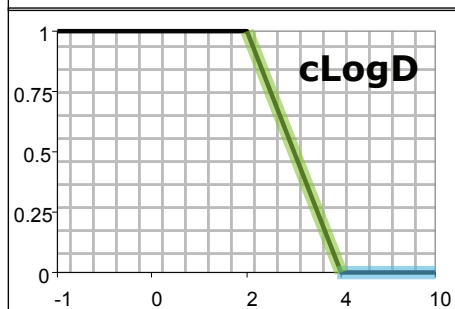
MPO = $\sum$Score (clogP + clogD + PSA + MW + HBD + pKa); $\qquad$ MPO_{max} = 6
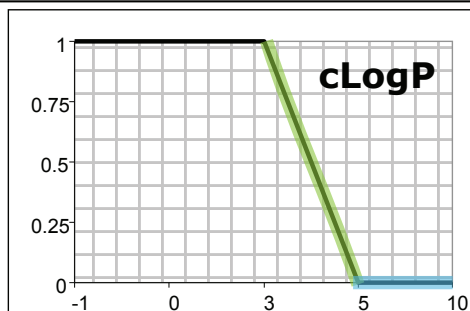
LogP

If clogP <= 3 $\qquad$ then mpo_clogP = 1
elseif clogP >= 5 $\qquad$ then mpo_clogP = 0 (color = blue)
else mpo_clogP = - 0.5*clogP + 2.5 (color = green)

LogD

If clogD <= 2 $\qquad$ then mpo_clogD = 1
elseif clogD >= 4 $\qquad$ then mpo_clogD = 0 (color = blue)
else mpo_clogD = - 0.5*clogD + 2.0 (color = green)
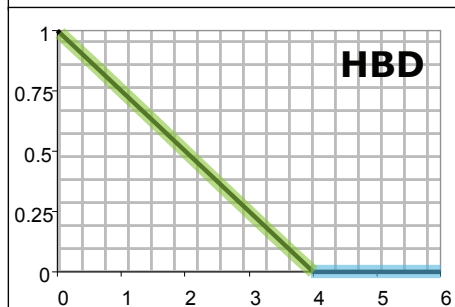
Hydrogen Bond Donors (HBD)

If HBD == 0 $\qquad$ then mpo_HBD = 1
elseif HBD >= 4 $\qquad$ then mpo_HBD = 0 (color = blue)
else mpo_HBD = - 0.25*HBD + 1.0 (color = green)
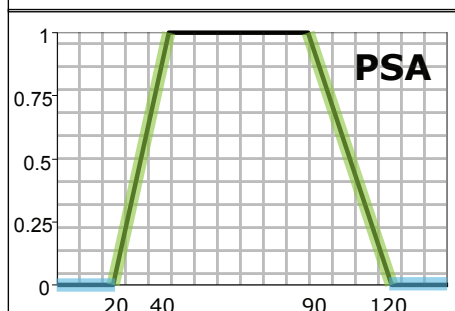
Polar Surface Area (PSA)

If PSA <= 20 or PSA >=120 $\quad$ then mpo_PSA = 0 (color = blue)
elseif PSA > 40 and PSA <90 $\quad$ then mpo_PSA = 1
elseif PSA > 20 and PSA <40 $\quad$ then mpo_PSA = 0.05*PSA -1 (color = green)
elseif PSA > 90 and PSA <120 then mpo_PSA = - 0.0333*PSA + 4.0 (color = green)
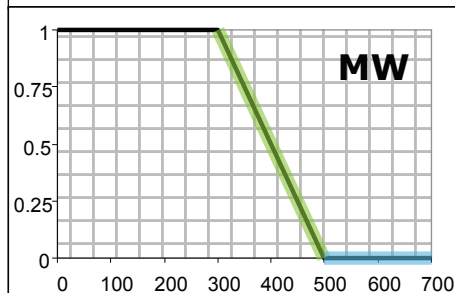
Molecular Weight (MW)

If MW <= 300 $\qquad$ then mpo_MW = 1
elseif MW >= 500 $\qquad$ then mpo_MV = 0 (color = blue)
else mpo_MV = - 0.005*MV + 2.5 (color = green)
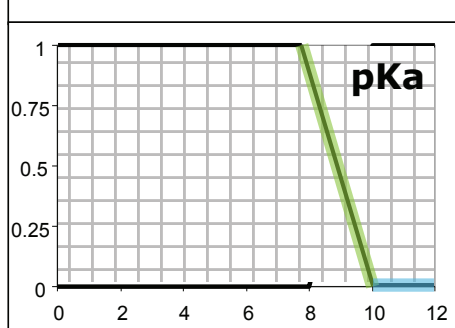
Base pKa

If pKa <= 8 $\qquad$ then mpo_pKa = 1
elseif pKa >= 10 $\qquad$ then mpo_pKa = 0 (color = blue)
else mpo_pKa = - 0.5*pKa + 5.0 (color = green)