

Table 2. Data ranges of input variables

Name	Description	Range ^a
DPRA	Average lysine and cysteine peptide depletion measurement (%)	0–95
h-CLAT	Minimum induction threshold [smallest value for CD54 EC ₂₀₀ and CD86 EC ₁₅₀] ($\mu\text{g ml}^{-1}$)	0.54–2001
KeratinoSens	EC _{1.5} (μM)	0.50–2001
LogP	Octanol/water partition coefficient	–8.28 to 6.46 ^b
LogS	Water solubility (mol l^{-1})	–6.39 to 1.92 ^b
LogVP	Vapor pressure (mmHg)	–28.47 to 5.89 ^b
MP	Melting point ($^{\circ}\text{C}$)	–148.50 to 288.00
BP	Boiling point ($^{\circ}\text{C}$)	–19.10 to 932.20
MW	Molecular weight (g mol^{-1})	30.03–581.57

BP, boiling point; DPRA, direct peptide reactivity assay; EC_{1.5}, concentration producing a 1.5-fold induction of luciferase controlled by the antioxidant response element; EC₁₅₀, estimated concentration inducing a 150% increase for CD86; EC₂₀₀, estimated concentration inducing a 200% increase for CD54; h-CLAT, human cell line activation test; LogP, log octanol/water partition coefficient; LogS, log water solubility; LogVP, log vapor pressure; MP, melting point; MW, molecular weight.

a Human data set with 87 substances is a subset of LLNA data set with 120 substances; the two data sets cover the same range.

b Range for base 10 logarithm of these measurements.