

Table 3. Variable groups used to build models for predicting human skin sensitization hazard

Variable group	Input variables				
	Avg.Lys.Cys from DPRA	KeratinoSens	h-CLAT	QSAR Toolbox	Log P or six physicochemical properties
A	X	X	X	X	X
B	–	–	X	X	X
C	–	X	–	X	X
D	X	–	–	X	X
E	–	–	X	–	X
F	–	X	–	–	X
G	X	–	–	–	X
H	–	–	–	–	X
I	X	X	X	X	–
J	–	X	X	X	–
K	X	–	X	X	–
L	X	X	–	X	–

Avg.Lys.Cys, average depletion for lysine and cysteine peptides from the DPRA; Cys, average depletion of cysteine peptide from the DPRA; DPRA, direct peptide reactivity assay; h-CLAT, human cell line activation test; log P, log octanol/water partition coefficient; log S, log water solubility; log VP, log vapor pressure; Lys, average depletion of lysine peptide from the DPRA; Toolbox, read-across using QSAR Toolbox.

“X” denotes the input variables included in each variable group. Dashes indicate that the variable is not included in the designated group. The six physicochemical properties are log octanol/water partition coefficient; log water solubility; log vapor pressure, melting point, boiling point and molecular weight.