Table 4. Variable sets for model building

Variable set	Combination of input variables
I	DPRA + h-CLAT + KeratinoSens
II	LogP + LogS + LogVP + MP + BP + MW
III	DPRA + h-CLAT + KeratinoSens + LogP + LogS + LogVP + MP + BP + MW
IV	DPRA + h-CLAT + KeratinoSens + LogP

BP, boiling point; DPRA, direct peptide reactivity assay; 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.