

Table 5. Defined Approach (DA) performance in predicting human sensitizing potency.

Predicting Human Potency (Strong, Weak, Non-sensitizers)

Defined approach:	Kao STS	Kao ITS	Shiseido ANN (D_hC)	Shiseido ANN (D_hC_KS)	P&G BN ITS-3	LLNA
<i>N</i>	126	120	126	126	115	128
Accuracy (%)*	63.5	69.2	61.1	62.7	54.8	59.4
Over-predicted (%)	22.2	13.3	22.2	25.4	20.0	19.5
Under-predicted (%)	14.3	17.5	16.7	11.9	25.2	21.1

*Performance was assessed for prediction of three potency classes as described in the main text, and is shown against the maximum subset (*N*) out of 128 substances with all necessary DA features. With the exception of the P&G BN ITS-3, all misclassifications varied by one class only (i.e. no non-sensitizers were predicted as strong sensitizers or vice versa).

STS: sequential testing strategy; ITS: integrated testing strategy; SVM: support vector machine; ANN: artificial neural network; BN: Bayesian network; DKH and D_hC_KS: DPRA/h-CLAT/KeratinoSensTM; D_hC: DPRA/h-CLAT.