

Table 6. Defined Approach (DA) performance in predicting LLNA sensitizing potency.

Predicting LLNA 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
<i>N</i>	126	120	126	126	115
Accuracy (%)*	67.5	66.7	65.1	69.8	67.8
Over-predicted (%)	21.4	14.2	21.4	23.0	12.2
Under-predicted (%)	11.1	19.2	13.5	7.1	20.0

*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 DA human potency predictions were off by one class only (i.e. no non-sensitizers predicted as strong or vice versa).

LLNA: local lymph node assay; 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.