Table 6. Misclassified substances [a] for the six LR and SVM models with the highest performance

Test method or model [b]	Training set					
	2-Methoxy-4-methylphenol	Sulfanilamide	Streptomycin sulfate	Penicillin G	Benzocaine	α-Amyl cinnamaldehyde
Human reference result	NEG	POS	POS	POS	POS	POS
DPRA	POS	NEG	NEG	POS	POS	NEG
KeratinoSens	NEG	NEG	NEG	NEG	POS	NEG
h-CLAT	POS	NEG	NEG	POS	POS	POS
Toolbox	POS	NEG	POS	NEG	NEG	POS
A. Avg.Lys.Cys + h-CLAT + KeratinoSens + Toolbox + Log P	**POS**	**NEG**	POS	**NEG**	POS/**NEG** [b]	**NEG**/POS [c]
I. Avg.Lys.Cys + h-CLAT + KeratinoSens + Toolbox	**POS**	**NEG**	**NEG**	**NEG**	**NEG**	POS
K. Avg.Lys.Cys + h-CLAT + Toolbox	**POS**	**NEG**	**NEG**	**NEG**	**NEG**	POS

Avg.Lys.Cys, average depletion for lysine and cysteine peptides from the direct peptide reactivity assay; h-CLAT, human cell line activation test; log P, log octanol/water partition coefficient; LR, logistic regression; NEG, negative; POS, positive; SVM, support vector machine; Toolbox, read-across using QSAR Toolbox.

a   Misclassifications, which disagree with the human outcomes, are bolded.

b   Correctly classified in the LR model but misclassified by the SVM model.

c   Misclassified by the LR model but correctly classified by the SVM model