

Table 5. Performance of leave-one-out cross-validation for LR and SVM models for 96 substances

Variable group	Accuracy (%)		Sensitivity (%)		Specificity (%)	
	LR	SVM	LR	SVM	LR	SVM
	A. Avg.Lys.Cys + h-CLAT + KeratinoSens + Toolbox + Log P	91	94	89	95	93
I. Avg.Lys.Cys + h-CLAT + KeratinoSens + Toolbox	92	94	92	95	90	90
K. Avg.Lys.Cys + h-CLAT + Toolbox	92	94	92	92	90	97

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; SVM, support vector machine; Toolbox, read-across using QSAR Toolbox. The data set of 96 substances contains 66 human sensitizers and 30 non-sensitizers.