Table 6. Individual category accuracy and overall accuracy of sensitizer classification [a] from tier 2 of strategy B using four machine learning approaches

LLNA/human [a]	Approach	Variable set [b]	Data set	Sensitivity (1A %)	Specificity (1B %)	Accuracy (%)
LLNA	CART	III/IV	Training	86 ± 13	88 ± 10	87 ± 8
			Test	57 ± 37	75 ± 25	68 ± 21
	LDA	I	Training	71 ± 17	75 ± 13	74 ± 10
			Test	71 ± 34	83 ± 21	79 ± 18
	LR	I	Training	82 ± 14	73 ± 14	77 ± 10
			Test	86 ± 26	67 ± 27	74 ± 20
	SVM	III	Training	89 ± 12	88 ± 10	88 ± 8
			Test	86 ± 26	92 ± 15	89 ± 14
Human	CART	I/III/IV	Training	68 ± 21	86 ± 15	78 ± 13
			Test	43 ± 37	100 ± 0	75 ± 21
	LDA	I	Training	79 ± 18	73 ± 19	76 ± 13
			Test	71 ± 34	78 ± 27	75 ± 21
	LR	III	Training	84 ± 17	64 ± 20	73 ± 14
			Test	57 ± 37	78 ± 27	69 ± 23
	SVM	III/IV	Training	90 ± 14	77 ± 18	83 ± 11
			Test	86 ± 26	78 ± 27	81 ± 19

CART, classification and regression tree; LDA, linear discriminant analysis; LR, logistic regression; LLNA, murine local lymph node assay; SVM, support vector machine.

Values after "±" indicate 95% confidence limits of proportion for correct classification rate.

a   Chemicals predicted to be sensitizers using the Strickland *et al*. (2016a,b), models were used in tier 2. LLNA and human data sets respectively included 84 (34 1A and 50 1B) and 53 (26 1A and 27 1B) chemicals predicted to be sensitizers.

b   Variable sets are defined in Table 4.