Table 5. Accuracy of individual category and overall classification predictions using strategy A [a] and SVM

LLNA/human [b]	Variable set	Data set	1A [c] (%)	1B [c] (%)	Neg (%)	Accuracy (%)
LLNA	I	Training	79 ± 15	63 ± 15	85 ± 14	73 ± 9
		Test	86 ± 26	50 ± 28	71 ± 34	65 ± 18
		LOOCV	83 ± 12	62 ± 13	73 ± 15	71 ± 8
	II	Training	82 ± 14	75 ± 13	65 ± 18	75 ± 9
		Test	71 ± 34	58 ± 28	43 ± 37	58 ± 19
		LOOCV	68 ± 15	60 ± 13	55 ± 17	61 ± 9
	III	Training	96 ± 7	80 ± 12	96 ± 8	89 ± 6
		Test	86 ± 26	67 ± 27	86 ± 26	77 ± 16
		LOOCV	83 ± 12	69 ± 12	85 ± 12	78 ± 7

LLNA/human	Variable set	Data set	1A (%)	1B (%)	Neg (%)	Accuracy (%)

LLNA/human	Variable set	Data set	1A (%)	1B (%)	Neg (%)	Accuracy (%)
Human	IV	Training	96 ± 7	73 ± 14	96 ± 8	86 ± 7
		Test	71 ± 34	58 ± 28	86 ± 26	69 ± 18
		LOOCV	83 ± 12	60 ± 13	85 ± 12	73 ± 8
	I	Training	79 ± 18	55 ± 21	95 ± 9	76 ± 11
		Test	71 ± 34	56 ± 32	75 ± 30	67 ± 19
		LOOCV	77 ± 16	58 ± 17	80 ± 14	71 ± 10
	II	Training	58 ± 22	64 ± 20	77 ± 18	67 ± 12
		Test	43 ± 37	44 ± 32	50 ± 35	46 ± 20
		LOOCV	58 ± 19	65 ± 17	57 ± 18	60 ± 10
	III	Training	89 ± 13	59 ± 21	82 ± 16	76 ± 11
		Test	86 ± 26	56 ± 32	75 ± 30	71 ± 18

	LOOCV	85 ± 14	61 ± 17	80 ± 14	75 ± 9
IV	Training	84 ± 16	64 ± 20	82 ± 16	76 ± 11
	Test	86 ± 26	56 ± 32	75 ± 30	71 ± 18
	LOOCV	88 ± 13	58 ± 17	80 ± 14	75 ± 9

LLNA, murine local lymph node assay; LOOCV, leave-one-out cross-validation; SVM, support vector machine.

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

a   Strategy A modeled all three categories of response simultaneously.

b   LLNA data set contained 120 substances: 35 strong sensitizers, 52 weak sensitizers and 33 non-sensitizers. Human data set contained 87 substances: 26 strong sensitizers, 31 weak sensitizers and 30 non-sensitizers.

c   1A (strong) and 1B (weak) are subcategories for sensitizers in the Globally Harmonized System of Classification and Labeling of Chemicals (UN, 2015).