

Table 3

Statistical characteristics of LLNA results vs. external QSAR predictions (5-fold external cross-validation) for predicting human skin sensitization.

Model	CCR	Sensitivity	PPV	Specificity	NPV	Coverage
QSAR model	0.71	0.65	0.79	0.76	0.61	1.00
LLNA result	0.63	0.83	0.67	0.43	0.65	1.00
Combined (QSAR + LLNA)	0.82	0.88	0.90	0.76	0.72	0.52