Predicting Human Hazard

BA: balanced accuracy; STS: sequential testing strategy; ITS: integrated testing strategy; SVM: support vector machine; ANN: artificial neural network; BN: Bayesian

78.6

95.4

41.0

68.2

78.6

30.8

65.4

100

75.6

81.3

64.1

74.2

85.2

50.0

67.6

Defined Approach:	BASF 2/3 (DKH)	Kao STS	Kao ITS	ICCVAM SVM (Human)	Shiseido ANN (D_hC)	Shiseido ANN (D_hC_KS)	P&G BN ITS-3	LLNA
N	127	126	120	120	126	126	119	128

81.7

86.4

71.8

79.1

Table 3. Defined Approach (DA) performance in predicting human hazard (sensitizer/non-sensitizer).

85.0

93.8

66.7

80.3

*Performance is shown against the maximum subset (N) out of 128 substances with all necessary DA features.

80.2

97.7

41.0

69.4

network: DKH and D hC KS: DPRA/h-CLAT/KeratinoSensTM: D hC: DPRA/h-CLAT.

Accuracy (%)*

Sensitivity (%)

Specificity (%)

BA (%)

77.2

79.3

72.5

75.9