

Impurity Profiling Module

ACD/Percepta

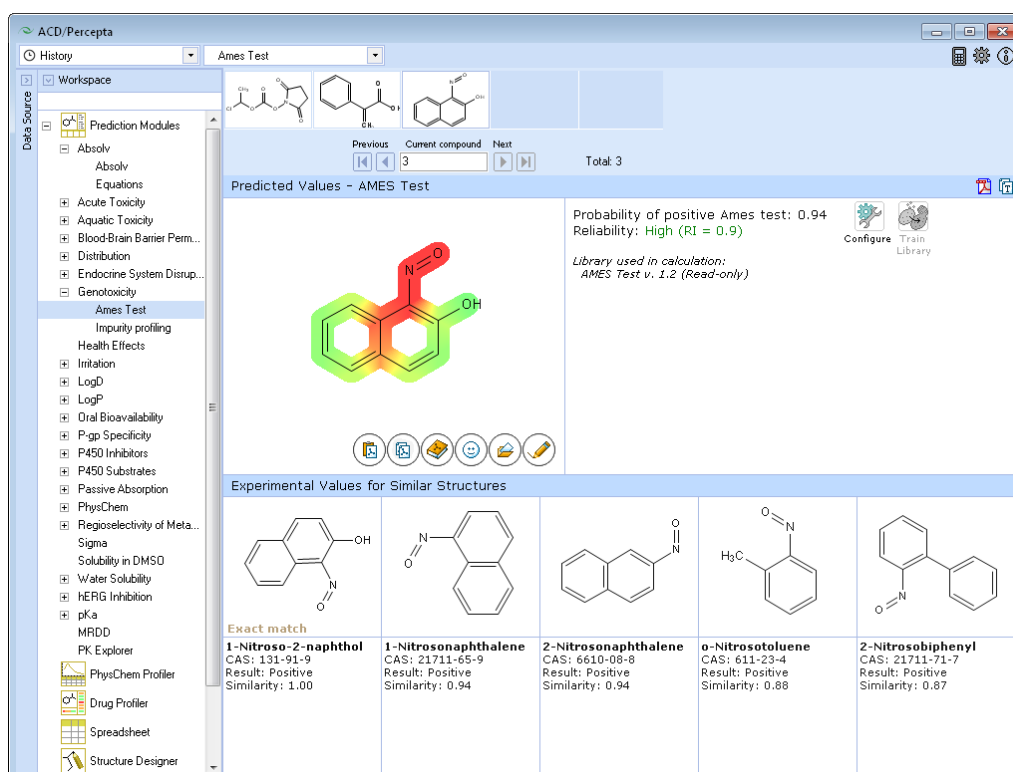
Model Performance

The predictive performance of Ames test (bacterial composite) mutagenicity model is summarized in Table 2. The accuracy of predictions is very high with almost 90% of the validation set compounds falling within Model Applicability Domain ($RI \geq 0.3$), and almost 90% of these – classified correctly. A high/moderate reliability index was reported for 65% of compounds in the validation set, and in this case the observed number of misclassifications is even lower.

Table 2. Statistical characteristics of the obtained Ames test classification model.

Accuracy testing		Calculated probability		Statistical parameters	Overall accuracy
		<0.5	≥ 0.5		
Test set ($RI \geq 0.3$) 1483 compounds (86.6% covered)	Safe	392 (26.4%)	96 (6.5%)	Specificity	80.3%
	Mutagenic	67 (4.5%)	928 (62.6%)	Sensitivity	93.3%
Test set ($RI \geq 0.5$) 1117 compounds (65.2% covered)	Safe	257 (23.0%)	51 (4.6%)	Specificity	83.4%
	Mutagenic	23 (2.0%)	786 (70.4%)	Sensitivity	97.2%

Performance of the derived models for other genotoxicity/carcinogenicity endpoints is given in Table 1 along with the data set sizes.



ACD/Percepta
History: Ames Test

Prediction Modules:
Absolv
Equations
Acute Toxicity
Aquatic Toxicity
Blood-Brain Barrier Perm...
Distribution
Endocrine System Disrup...
Genotoxicity
Ames Test
Impurity profiling
Health Effects
Irritation
LogD
LogP
Oral Bioavailability
P-gp Specificity
P450 Inhibitors
P450 Substrates
Passive Absorption
PhysChem
Regioselectivity of Meta...
Sigma
Solubility in DMSO
Water Solubility
HERG Inhibition
pKa
MRDD
PK Explorer
PhysChem Profiler
Drug Profiler
Spreadsheet
Structure Designer

Previous Current compound Next Total: 3

Predicted Values - AMES Test

Probability of positive Ames test: 0.94
Reliability: High ($RI = 0.9$)

Library used in calculation:
AMES Test v. 1.2 (Read-only)

Experimental Values for Similar Structures

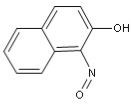
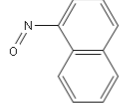
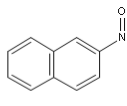
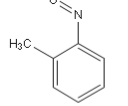
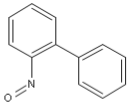
				
Exact match 1-Nitroso-2-naphthol CAS: 131-91-9 Result: Positive Similarity: 1.00	1-Nitrosonaphthalene CAS: 21711-65-9 Result: Positive Similarity: 0.94	2-Nitrosonaphthalene CAS: 6610-08-8 Result: Positive Similarity: 0.94	o-Nitrosotoluene CAS: 611-23-4 Result: Positive Similarity: 0.88	2-Nitrosobiphenyl CAS: 21711-71-7 Result: Positive Similarity: 0.87

Figure 2. Screenshot of ACD/Percepta Ames test module