

Session: DevTox, Model: AMG_DevTox_Model_DTModel4

Fri May 13 2011, 11:34

Modeled property: Tox

Modeling technique: Decision Tree

Model statistics:

	Number	Kappa	Accuracy
TRN	227	0.7776	0.9119
VAL	58	0.6288	0.8621

Parameters used:

Descriptor pre-selection:

- Threshold for minimum occurrence: 4%
- Threshold for minimum standard deviation: 0.0005
- Threshold for maximum correlation between descriptors: 0.95

Descriptors remaining after pre-selection: 169

Descriptors used in the model: 11

Model details:

Data was classified into 2 classes

- class Toxic
- class Non-toxic

Confusion matrices

Training set

		Predicted	
		Toxic	Non-toxic
Observed	Toxic	156	1
	Non-toxic	19	51

- Sensitivity for Toxic : 0.994
- Specificity for Toxic : 0.891
- Sensitivity for Non-toxic : 0.729
- Specificity for Non-toxic : 0.981

Validation set

		Predicted	
		Toxic	Non-toxic
Observed	Toxic	40	1
	Non-toxic	7	10

- Sensitivity for Toxic : 0.976
- Specificity for Toxic : 0.851
- Sensitivity for Non-toxic : 0.588
- Specificity for Non-toxic : 0.909

Descriptors

Flex
AromaticRings
logP
CH2hetero
aminoethanol1
pyridine
nC(sp3)
HAS
HAO
N7
q458

Decision Tree

aminoethanol1 > 0

--> N7 > 0

--> Result: Non-toxic (Trn: 23/0 Val:7/0 Test:0/0) Leaf 1

N7 <= 0

--> AromaticRings > 0

--> nC(sp3) > 4

--> q458 > 6

--> Result: Non-toxic (Trn: 4/1 Val:2/1 Test:0/0) Leaf 2

q458 <= 6

--> Result: Toxic (Trn: 3/0 Val:0/0 Test:0/0) Leaf 3

nC(sp3) <= 4

--> Result: Toxic (Trn: 7/0 Val:4/1 Test:0/0) Leaf 4

AromaticRings <= 0

--> Result: Non-toxic (Trn: 5/0 Val:0/0 Test:0/0) Leaf 5

aminoethanol1 <= 0

--> q458 > 5

--> HAO > 0

--> Result: Toxic (Trn: 116/9 Val:32/5 Test:0/0) Leaf 6

HAO <= 0

--> HAS > 0

--> Result: Toxic (Trn: 6/0 Val:2/0 Test:0/0) Leaf 7

HAS <= 0

--> Flex > 0

--> Result: Toxic (Trn: 11/4 Val:5/0 Test:0/0) Leaf 8

Flex <= 0

--> Result: Non-toxic (Trn: 5/0 Val:0/0 Test:0/0) Leaf 9

q458 <= 5

--> CH2hetero > 2

--> Result: Non-toxic (Trn: 6/0 Val:0/0 Test:0/0) Leaf 10

CH2hetero <= 2

--> pyridine > 0

--> Result: Non-toxic (Trn: 4/0 Val:0/0 Test:0/0) Leaf 11

pyridine <= 0

--> logP > 0.059904

--> nC(sp3) > 1

--> Result: Toxic (Trn: 21/6 Val:4/1 Test:0/0) Leaf 12

nC(sp3) <= 1

--> Result: Non-toxic (Trn: 5/0 Val:2/0 Test:0/0) Leaf 13

logP <= 0.059904

--> Result: Toxic (Trn: 11/0 Val:0/0 Test:0/0) Leaf 14