

Session: Viscosity_training, Model: Viscosity GARBF

Wed September 14 2011, 08:23

Modeled property: Tox

Modeling technique: Radial Basis Function

Model statistics:

	Number	Rsqr	RMSE
TRN	346	0.9857	0.0633
VAL	87	0.9449	0.125

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: 107

Descriptors used in the model: 22

Model details:

No GA performed

Descriptors

Vx
MW
logP
HBD-lip
HBD-prof
CH2long
HaloC
RSR
anycarbonyl
aromF
ether
ringat
sF
sBr
nNneutral
N6
O3
O9
C22
ew10
f456
q458