

Session: TC_training, Model: AMG_TC_training_Model_GPRFVS

Sun September 11 2011, 13:05

Modeled property: Tox

Modeling technique: Gaussian Processes

Model statistics:

	Number	Rsqr	RMSE
TRN	275	0.9435	7.291
VAL	71	0.8289	13.11

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: 80

Descriptors used in the model: 30

Model details:

Theta1: 746.7439575

Theta2: 509.537262

Theta3: 0.9800000191

Descriptor	Length scale
Vx	1745.055
MW	2039.435
Flex	6.470295
logP	39.87208
OverallCharge	6.206018
ERTLNotPSA	383.9765
HBA-prof	25.87426
HBD-lip	10.72719
CH2long	99.09561
CH3Aa	25.62762
CH3hetero	7.278405
branchedCnotRing	16.52631
di-widhraw-cx4	38.64464
ether	9.047541
ketone-t14	5.324257
nX	54.29404
dsCH	13.81635
dssC	11.45546
sOH	10.37705
sCl	19.15968
sBr	7.706907
NbN	6.58163
UB	71.2337
HAT	25.80178
C6	15.86191
AroRingAttachment	23.40606
H1a	18.14781
f245	19.14305
f407	28.52789
f444	28.91823