

## Session: Daphnia magna toxicity -log(LC50) M, Model: AMG\_Daphnia magna toxicity -log(LC50) M\_Model\_GPRFVS

Fri May 13 2011, 18:45

Modeled property: Tox

Modeling technique: Gaussian Processes

### Model statistics:

	Number	Rsqr	RMSE
TRN	269	0.7839	0.8296
VAL	68	0.6793	0.9141

### 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: 138

Descriptors used in the model: 19

### Model details:

Theta1: 40.12356949

Theta2: 29.32440758

Theta3: 0.8999999762

Descriptor	Length scale
MW	1942.753
PositiveCharge	14.59426
logP	30.40908
ERTLNotPSA	561.3551
ERTLNoSPtPSA	659.6019
CH3hetero	13.57792
Pester	12.29012
RSR	7.334737
aliphOH-t6	5.394867
anycarbonyl	14.36183
di-widhraw-cx4	14.42716
ertl-33	7.673583
intraHbond6	4.309401
sp-carbons	5.451628
nC(sp2)	79.34677
NnH	12.53438
HAN	20.26996
C6	14.5717
C22	12.31685