

Session: Nordquist CACO2_training_set_5, Model: Caco-2_log(Papp)_GPFVS

Sun October 14 2012, 21:30

Modeled property: caco2

Modeling technique: Gaussian Processes

Model statistics:

	Number	Rsqr	RMSE
TRN	77	0.6019	0.4711
VAL	23	0.6554	0.4996

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: 10

Descriptors used in the model: 8

Model details:

Theta1: 47.04102707

Theta2: 24.60710716

Theta3: 0.9800000191

Descriptor	Length scale
logP	23.01851
HBD-prof	20.68149
OverallCharge	16.79273
HBA-prof	32.60904
Flex	1.887514
NegativeCharge	5.582905
ERTLNotPSA	586.6201
PositiveCharge	16.80087