

Session: BCF_training, Model: AMG_BCF_training_Model_GPOPT

Fri May 13 2011, 10:57

Modeled property: Tox

Modeling technique: Gaussian Processes

Model statistics:

| | Number | Rsqr | RMSE |
|-----|--------|--------|--------|
| TRN | 541 | 0.8511 | 0.5299 |
| VAL | 136 | 0.7597 | 0.6509 |

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: 139

Descriptors used in the model: 35

Model details:

Theta1: 42.57894897

Theta2: 31.96836853

Theta3: 0.3799999952

| Descriptor | Length scale | Normalised scale |
|-------------------|--------------|------------------|
| Vx | 3304.222 | 1.000467 |
| MW | 5393.45 | 1.000046 |
| NegativeCharge | 5.098043 | 0.3696294 |
| AromaticRings | 50.12748 | 1.057376 |
| logP | 3.810418 | 0.04320898 |
| ERTLNotPSA | 1564.718 | 1.002203 |
| ERTLNoSPtPSA | 1806.365 | 0.9990329 |
| CH2Aa | 177.3487 | 1.267419 |
| CH3Aa | 94.3506 | 1.240067 |
| NRB | 297.3539 | 1.118404 |
| allylic-oxyd-t10 | 19.52954 | 0.8764307 |
| di-widhraw-cx4 | 68.29613 | 1.100664 |
| lipovolume | 174.456 | 0.8713527 |
| nonring-at | 311.3122 | 1.152347 |
| ringat | 294.6872 | 1.18437 |
| nC(sp3) | 254.0392 | 1.151915 |
| nOS | 55.38563 | 1.116567 |
| aaCH | 150.8076 | 0.9010111 |
| UB | 301.0393 | 1.094908 |
| HAT | 38.20439 | 0.3683445 |
| HAO | 61.62174 | 0.8350424 |
| C1 | 203.2856 | 1.147647 |
| AroRingAttachment | 122.9827 | 1.066644 |
| HydrophobicGroup | 215.5376 | 1.291199 |
| C22 | 49.51698 | 1.324167 |
| ew10 | 11.8071 | 0.1628365 |
| f007 | 31.17941 | 0.424325 |
| f015 | 38.3765 | 0.9294281 |
| f390 | 68.03609 | 0.3982671 |
| f393 | 48.77765 | 0.2763648 |
| q017 | 411.8774 | 1.096074 |
| q039 | 220.4578 | 1.252809 |
| q137 | 372.7947 | 1.137262 |

q300
q453

80.49852
340.3046

1.161252
1.2485