

Table 6. UPPS 2D-QSAR output

QuaSAR-Model (PLS) : /Volumes/hudock/MOE/UPPS/122106/qsar_5_122106-v1.mdb
Tue Jan 9 15:53:14 2007

Activity Field : UPPC_pIC50
Weight Field :
Condition Limit : 1e+06
Component Limit : 0

Observations : 29
Descriptors : 4
Components Used : 4
Condition Number : 7207.2837

ROOT MEAN SQUARE ERROR (RMSE) : 0.32774
CORRELATION COEFFICIENT (R2) : 0.85352
CROSS-VALIDATED RMSE : 0.43369
CROSS-VALIDATED R2 : 0.75871

ESTIMATED LINEAR MODEL

UPPC_pIC50 =
1.40017
-0.00044 * CASA-
-0.03311 * PEOE_VSA+3
-0.03824 * SlogP_VSA8
+0.01470 * VSA

ESTIMATED NORMALIZED LINEAR MODEL (SD = Standard Deviation)

UPPC_pIC50 / SD(UPPC_pIC50) =
1.63509
-0.34334 * CASA- / SD(CASA-)
-0.68892 * PEOE_VSA+3 / SD(PEOE_VSA+3)
-0.49988 * SlogP_VSA8 / SD(SlogP_VSA8)
+1.02660 * VSA / SD(VSA)

RELATIVE IMPORTANCE OF DESCRIPTORS

0.334438 CASA-
0.671064 PEOE_VSA+3
0.486927 SlogP_VSA8
1.000000 VSA

MOE Descriptor	Brief description
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CASA-	Negative charge weighted surface area
PEOE_VSA+3	Sub divided surface area partial charge descriptor (Gasteiger method). Sub divided surface area descriptors are based on approximate assessable van der Waals surface area for each atom v_i along with another property p_i . The descriptor is defined as the sum of the v_i over all atoms such that p_i is in a specified range. In this case, p_i is partial charge in range [0.15,0.20].
SLogP_VSA8	Sub divided surface area SLogP descriptor. In this case, p_i is SLogP in range [0.30, 0.40].
VSA	van der Waals surface area calculated by using polyhedral representation of each atom.
