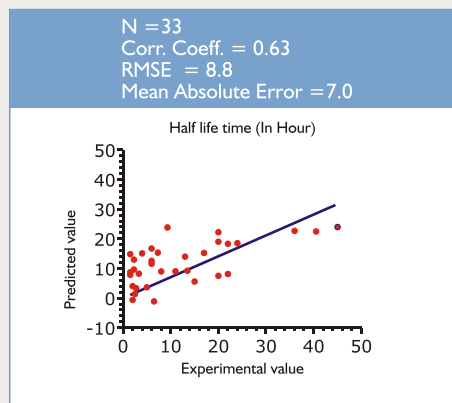
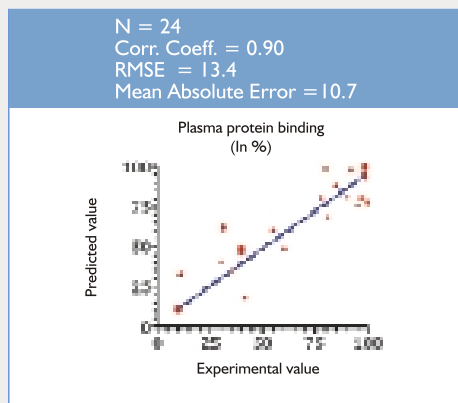
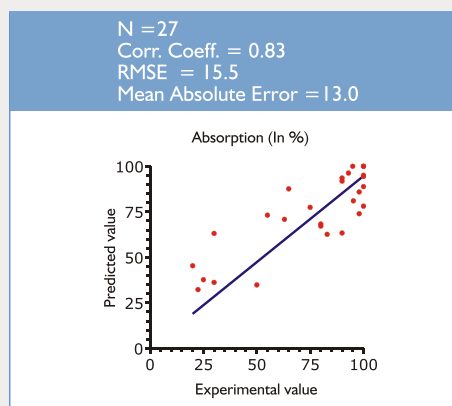
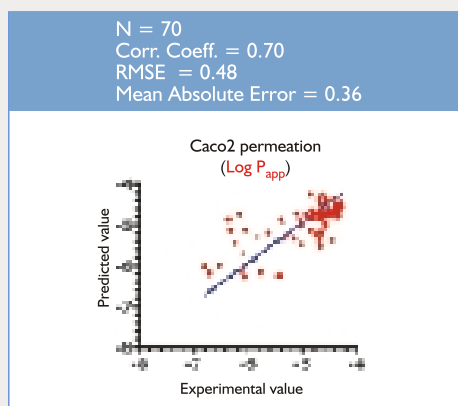
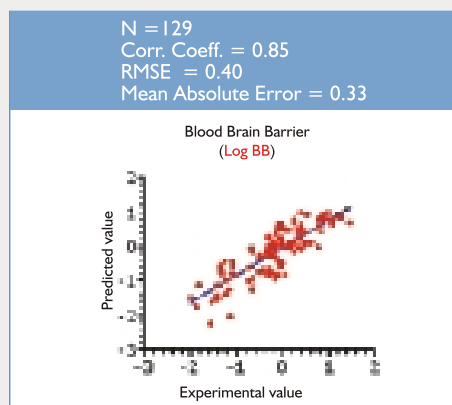
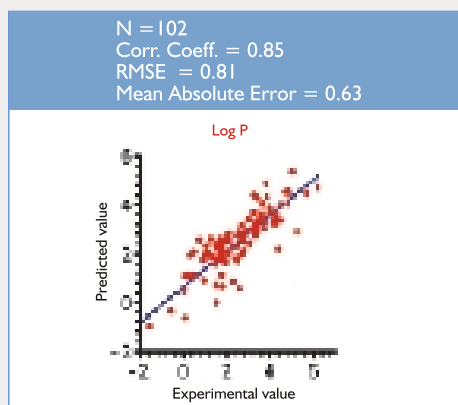
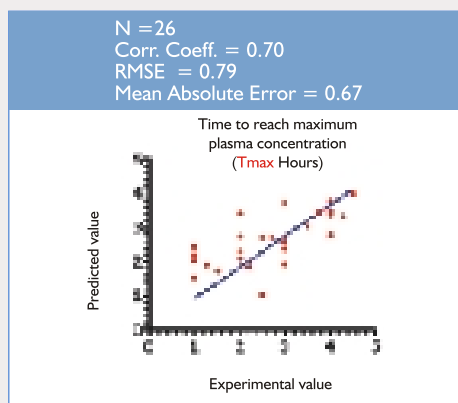


Predictive ADME/PK/DLS:

In-Silico predictions of ADME/PK or related properties are believed to provide useful guidance in identifying drug-like compounds with acceptable ADME/PK properties before their actual chemical synthesis and testing. Chembiotek has developed such predictive tools based upon QSPR approach using Neural Network methods. Currently, we can predict four ADME related properties (logP, logBB, logP_{app} and logS) and four PK properties (%Absorption, % plasma binding, T_{1/2} and T_{max}). Additionally, we assign some overall oral drug-likeness score (DLS) to each compound. Some results are given below





DATA GENERATED BY IN-HOUSE TOOL ADME06
Molecular Modeling Group, BIOLAB.
Chembiotek
Calcutta, India.

Compound Number = 1

LogP = 3.53 logBB = -1.33 logC = -4.12 logS = -5.25
Tmax = 2.04 ABSO = 36.79 thaf = 20.11 PLASM = 100.00
DLS = 0.63

Compound Number = 2

LogP = 3.64 logBB = -0.38 logC = -4.36 logS = -6.04
Tmax = 2.81 ABSO = 78.21 thaf = 17.07 PLASM = 100.00
DLS = 0.67

Compound Number = 3

LogP = 3.02 logBB = -0.37 logC = -4.38 logS = -4.73
Tmax = 2.79 ABSO = 67.66 thaf = 14.30 PLASM = 100.00
DLS = 0.72

Compound Number = 4

LogP = 3.96 logBB = -0.19 logC = -4.44 logS = -5.19
Tmax = 3.88 ABSO = 80.83 thaf = 23.04 PLASM = 100.00
DLS = 0.61

P = Octanol/Water partitioning coefficient. Uncertainty range for logP(± 0.63).
BB = Brain / Blood partitioning coefficient. Uncertainty range for logBB(± 0.33).
C = Permeability (cm/sec) through Caco2 monolayer. Uncertainty range for logC(± 0.36).
S = Aqueous solubility (micro gm/mL). Uncertainty range for logS(± 0.70).
Abso = Oral absorption (%). Uncertainty range (± 20%).
Plasm. = Plasma binding (%). Uncertainty range (± 18%).
tm = Time (Hours) required to reach the peak concentration.
thaf = Time (Hours) in which the concentration falls to half the peak value.
DLS = Overall drug-likeness score in the range (0.0 - 1.0).