

Table S1: Description of the derived QSAR model with associated statistical parameters.

Variable	Parameter	T-STAT H0: parameter = 0	1-tail p-value
(Intercept)	-3.50589878934833	-5.0005	1.9e-05
Energy	-0.0627465444911588	-1.2961	0.103397
VDW	0.0527611680319246	1.1104	0.138689
HBond	0.0506522368831837	1.0481	0.152313
LUMO	0.267592026730564	5.1614	1.2e-05
SAA	-0.0077140063969647	-9.8597	0
SAG	0.00376956073219399	2.4999	0.009673
HE	0.0689803949322663	12.673	0
`Mass\r`	0.00628428271397869	7.1551	0