

Supplementary S3: Value range of the most important descriptors for serotonergic activity  
model based on entire database

Descriptor	Active	Inactive
nBase	0 - 5	0 - 5
MATS1v	-0.15 - 0.35	-0.134 - 0.202
PEOE_VSA7	0.0 - 167.025	0.0 - 131.574
SlogP_VSA1	0.0 - 91.375	0.0 - 47.525
AXp-7dv	0.004 - 0.068	0.004 - 0.057
PEOE_VSA9	0.0 - 137.285	0.0 - 163.712
Xch-7dv	0.0 - 8.247	0.0 - 10.333
AATSC2dv	-0.662 - 2.213	-0.76 - 2.582
VSA_EState2	-1.306 - 87.06	-0.47 - 69.287
ATSC6v	-3489.32 - 3956.086	-3283.871 - 2862.563
SLogP	-3.24 - 9.445	-2.226 - 10.693
Kier2	2.939 - 41.981	2.146 - 44.684
ATSC5d	-101.306 - 22.712	-32.539 - 29.463
PEOE_VSA1	0.0 - 77.268	0.0 - 76.116
JGI2	0.031 - 0.144	0.028 - 0.156
SpMAD_Dzare	3.74 - 31.57	3.418 - 26.437
SaasC	-3.852 - 12.205	-4.633 - 14.035
MATS1se	-0.377 - 0.416	-0.396 - 0.459
IC3	2.969 - 6.109	3.303 - 6.127
SaaaC	-0.56 - 6.184	-0.699 - 6.396
VSA_EState7	-10.188 - 28.721	-10.783 - 22.081
ATSC7Z	-1023.77 - 709.752	-936.333 - 506.879
ZMIC3	15.555 - 88.704	15.542 - 108.155
JGI9	0.0 - 0.027	0.0 - 0.026
nFRing	0 - 3	0 - 3
Kier3	1.249 - 29.045	0.517 - 29.018
SsssN	0.0 - 13.116	0.0 - 10.038
GATS4i	0.429 - 1.433	0.54 - 1.536
PEOE_VSA6	0.0 - 110.967	0.0 - 130.584
MAXaasC	-0.572 - 1.709	-0.206 - 1.682
GGI9	0.0 - 1.413	0.0 - 1.084
GATS6v	0.382 - 1.925	0.111 - 1.628
GATS3i	0.553 - 2.01	0.564 - 1.633
TopoShapeIndex	0.0 - 1.0	0.0 - 1.0
SssO	0.0 - 77.604	0.0 - 79.125
PEOE_VSA10	0.0 - 60.131	0.0 - 62.373
GATS3v	0.294 - 1.999	0.693 - 1.442