

# Supplementary Materials

## **QSPR Model for Caco-2 Cell Permeability Prediction using a Combination of HQPSO and Dual-RBF Neural Network**

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**Table S1 Details of 50 selected descriptors**

NO.	Descriptor name	Type	Description	Extended Class
1	maxHssNH	ElectrotopologicalStateAtomTypeDescriptor	Maximum atom-type H E-State: -NH-	E-state descriptors
2	maxHBint6	ElectrotopologicalStateAtomTypeDescriptor	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 6	E-state descriptors
3	EE_Dt	DetourMatrixDescriptor	Estrada-like index from detour matrix	Topological descriptors
4	hmax	ElectrotopologicalStateAtomTypeDescriptor	Maximum H E-State	E-state descriptors
5	ATSC1s	Centered Broto-Moreau AutocorrelationDescriptor	Centered Broto-Moreau autocorrelation - lag 1 / weighted by I-state	Autocorrelation descriptors
6	AATS1i	Average Broto-Moreau AutocorrelationDescriptor	Average Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential	Autocorrelation descriptors
7	SHsOH	ElectrotopologicalStateAtomTypeDescriptor	Sum of atom-type H E-State: -OH	E-state descriptors
8	maxHBint2	ElectrotopologicalStateAtomTypeDescriptor	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 2	E-state descriptors
9	ETA_Epsilon_5	ExtendedTopochemicalAtomDescriptor	A measure of electronegative atom count	Topological descriptors
10	maxHBint7	ElectrotopologicalStateAtomTypeDescriptor	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 7	E-state descriptors
11	Khs.aaN	ElectrotopologicalStateAtomTypeDescriptor	Count of atom-type E-State: :N:	E-state
12	nHBa	ElectrotopologicalStateAtomTypeDescriptor	Count of E-States for (strong) Hydrogen Bond acceptors	E-state descriptors
13	nHCsats	ElectrotopologicalStateAtomTypeDescriptor	Count of atom-type H E-State: H?bonded to B, Si, P, Ge, As, Se, Sn or Pb	E-state descriptors
14	MDEN-13	MDEDescriptor	Molecular distance edge between all primary and tertiary nitrogens	Topological descriptors
15	nAcid	AcidicGroupCountDescriptor	by these SMARTS "\$([O;H1]-[C,S,P]=O)", "\$([*];-;!\$(*~[*];+)))", "\$([NH](S(=O)=O)C(F)(F)F)", and "\$ (n1nnnc1)" originally presented in JOELib	Constitutional descriptors
16	minsssc	ElectrotopologicalStateAtomTypeDescriptor	Minimum atom-type E-State: >C<	E-state descriptors
17	ATSC3c	Centered Broto-Moreau AutocorrelationDescriptor	Centered Broto-Moreau autocorrelation - lag 3 / weighted by charges	Autocorrelation descriptors
18	C1SP3	CarbonTypesDescriptor	Singly bound carbon bound to one other carbon	Topological descriptors
19	ETA_Epsilon_2	ExtendedTopochemicalAtomDescriptor	A measure of electronegative atom count	Topological descriptors
20	C1SP2	CarbonTypesDescriptor	Doubly bound carbon bound to one other carbon	Topological descriptors
21	minaaCH	ElectrotopologicalStateAtomTypeDescriptor	Minimum atom-type E-State: :CH:	E-state descriptors
22	nHBint4	ElectrotopologicalStateAtomTypeDescriptor	Count of E-State descriptors of	E-state descriptors

		criptor	strength for potential Hydrogen Bonds of path length 4	
23	C3SP3	CarbonTypesDescriptor	Singly bound carbon bound to three other carbons	Topological descriptors
24	ETA_EtaP_F	ExtendedTopochemicalAtomDescriptor	Functionality index EtaF relative to molecular size	Topological descriptors
25	nHBint3	ElectrotopologicalStateAtomTypeDescriptor	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 3	E-state descriptors
26	SddssS	ElectrotopologicalStateAtomTypeDescriptor	Sum of atom-type E-State: >S==	E-state descriptors
27	nAtomP	LargestPiSystemDescriptor	Number of atoms in the largest pi system	Constitutional descriptors
28	JGT	TopologicalChargeDescriptor	Global topological charge index	Topological descriptors
29	minHBd	ElectrotopologicalStateAtomTypeDescriptor	Minimum E-States for (strong) Hydrogen Bond donors	E-state descriptors
30	GATS2p	Geary AutocorrelationDescriptor	Geary autocorrelation - lag 2 / weighted by polarizabilities	Autocorrelation descriptors
31	IC5	InformationContentDescriptor	Information content index (neighborhood symmetry of 5-order)	Basak descriptors
32	n7Ring	RingCountDescriptor	Number of 7-membered rings	Constitutional descriptors
33	AATS5s	Average Broto-Moreau AutocorrelationDescriptor	Average Broto-Moreau autocorrelation - lag 5 / weighted by I-state	Autocorrelation descriptors
34	JGI6	TopologicalChargeDescriptor	Mean topological charge index of order 6	Topological descriptors
35	GATS3s	Geary AutocorrelationDescriptor	Geary autocorrelation - lag 3 / weighted by I-state	Autocorrelation descriptors
36	CIC2	ComplementaryInformationContentDescriptor	Complementary information content index (neighborhood symmetry of 2-order)	Basak descriptors
37	maxHother	ElectrotopologicalStateAtomTypeDescriptor	Maximum atom-type H E-State: H?on aaCH, dCH2 or dsCH	E-state descriptors
38	ETA_EtaP	ExtendedTopochemicalAtomDescriptor	Composite index Eta relative to molecular size	Topological descriptors
39	GATS1p	Geary AutocorrelationDescriptor	Geary autocorrelation - lag 1 / weighted by polarizabilities	Autocorrelation descriptors
40	MDEC-33	MDEDescriptor	Molecular distance edge between all tertiary carbons	Topological descriptors
41	naasC	ElectrotopologicalStateAtomTypeDescriptor	Count of atom-type E-State: :C:-	E-state descriptors
42	SsF	ElectrotopologicalStateAtomTypeDescriptor	Sum of atom-type E-State: -F	E-state descriptors
43	minHBint5	ElectrotopologicalStateAtomTypeDescriptor	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 5	E-state descriptors
44	SHBint4	ElectrotopologicalStateAtomTypeDescriptor	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 4	E-state descriptors
45	ATSC1p	Centered Broto-Moreau AutocorrelationDescriptor	Centered Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities	Centered Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities
46	ATSC3p	Centered Broto-Moreau	Centered Broto-Moreau	Autocorrelation

		AutocorrelationDescriptor	autocorrelation - lag 3 / weighted by polarizabilities	descriptors
47	BCUTp-1h	BCUTDescriptor	nlow highest polarizability weighted BCUTS	BCUT descriptors
48	AATSC0i	Average centered Broto-Moreau AutocorrelationDescriptor	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential	Autocorrelation descriptors
49	nHBAcc	HBondAcceptorCountDescriptor	Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm)	Molecular property descriptors
50	SHCsatu	ElectrotopologicalStateAtomTypeDescriptor	Sum of atom-type H E-State: H?on C sp3 bonded to unsaturated C	E-state descriptors