Table 4. Keys to the descriptors used in the QSPR correlations

#	Descriptor designation	Descriptor explanation
1	$RPCS$	Relative positive charged surface area
2	$RNCS$	Relative negative charged surface area
3	$DPSA^{(1)}$	Difference in positively charged surface areas (PPSA1-PNSA1)
4	$FPSA^{(1)}$	Fractional partial positively charged surface area (PPSA-1/TMSA)
5	$WPSA^{(1)}$	Weighted partial positively charged surface area (PPSA1*TMSA/1000)
6	$WNSA^{(1)}$	Weighted partial negatively charged surface area (PNSA1*TMSA/1000)
7	$DPSA^{(2)}$	Difference in positively charged surface areas (PPSA2-PNSA2)
8	$FNSA^{(2)}$	Fractional partial negatively charged surface area (PNSA-2/TMSA)
9	$FPSA^{(2)}$	Fractional partial positively charged surface area (PPSA-2/TMSA)
10	$WNSA^{(2)}$	Weighted partial negatively charged surface area (PNSA2*TMSA/1000)
11	$WPSA^{(2)}$	Weighted partial positively charged surface area (PPSA2*TMSA/1000)
12	$PPSA^{(3)}$	Atomic charge weighted partial positively charged surface area
13	$FNSA^{(3)}$	Fractional partial negatively charged surface area (PNSA-3/TMSA)
14	$FPSA^{(3)}$	Fractional partial positively charged surface area (PPSA-3/TMSA)
15	$WNSA^{(3)}$	Weighted partial negatively charged surface area (PNSA3*TMSA/1000)
16	$WPSA^{(3)}$	Weighted partial positively charged surface area (PPSA3*TMSA/1000)
17	${}^{0}CIC$	Complementary Information content (order 0)
18	${}^{1}CIC$	Complementary Information content (order 1)
19	${}^{0}\overline{BIC}$	Average Bonding Information content (order 0)
20	${}^{0}\overline{CIC}$	Average Complementary Information content (order 0)
21	${}^{0}\overline{SIC}$	Average Structural Information content (order 0)
22	${}^{1}\overline{CIC}$	Average Complementary Information content (order 1)
23	${}^{1}\overline{BIC}$	Average Bonding Information content (order 1)

24	$^{2}\overline{IC}$	Average Information content (order 2)
25	^{2}SIC	Structural Information content (order 2)
26	$^{2}\overline{SIC}$	Average Structural Information content (order 2)
27	$q_A^{\min}$	Minimum partial charge for all atom types
28	$q_A^{\max}$	Maximum partial charge for all atom types
29	$q_C^{\max}$	Maximum net atomic charge (typed) for atom *C*
30	$q_C^{\min}$	Minimum net atomic charge (typed) for atom *C*
31	$q_{net}^{\min}$	Minimum net atomic charge
32	$V_C^{\min}$	Minimum valency for atom *C*
33	$V_H^{\min}$	Minimum valency for atom *H*
34	$\overline{V}_H$	Average valency for atom *H*
35	$P_H^{\min}$	Minimum bond order for atom *H*
36	$\overline{P}_C$	Average bond order for atom *C*
37	$R_C^{\min}$	Minimum one-electron reactivity index for atom *C*
38	$R_C^{\max}$	Maximum one-electron reactivity index for atom *C*
39	$E_{state}^{\min}(H)$	Minimum atomic state energy for atom *H*
40	$E_{exc}^{\min}(H-C)$	Minimum exchange energy for bond *H-C*
41	$E_{exc}^{\max}(H-C)$	Maximum exchange energy for bond *H-C*
42	$E_{en}^{\min}(H-C)$	Minimum electron-nuclear attraction for bond *H-C*
43	$E_{en}^{\max}(H-C)$	Maximum electron-nuclear attraction for bond *H-C*
44	$N_C^{\max}$	Maximum nucleophilic reactivity index for atom C
45	$\overline{E}_C$	Average electrophilic reactivity index for atom C
46	$T_H^{\min}$	Min atomic state energy for atom H
47	E_{tot}	Total molecular electrostatic interaction

48	$E_{ee}^{1-center}(tot)$	Total molecular one-center electron-electron repulsion
49	E_{res}^{tot}	Tot molecular 2-center resonance energy
50	E_{exc}^{tot}	Tot molecular 2-center exchange energy
51	$P_{\sigma-\sigma}^{\max}$	Maximum SIGMA- SIGMA bond order
52	$P_{\sigma-\pi}^{\max}$	Maximum SIGMA-PI bond order
53	$P_{\pi-\pi}^{\max}$	Maximum PI-PI bond order
54	$N^{occ.el.lev}$	Number of occupied electronic levels
55	$N^{occ.el.lev} / N_A$	Number of occupied electronic levels / number of atoms
56	$n_A^{\max}$	Maximum atomic orbital electronic population
57	$k_A^{\max}$	Max atomic force constant
58	$\varphi_{bond}^{\max}$	Maximum bonding contribution of a molecular orbital
59	$\varphi_{antibond}^{\max}$	Maximum antibonding contribution of a molecular orbital
60	E^{HOMO}	Energy of the highest occupied molecular orbital
61	E^{LUMO}	Energy of the lowest unoccupied molecular orbital
62	ΔE_{HOMO}^{LUMO}	HOMO-LUMO energy gap
63	${}^{0}\chi$	Randic index (order 0)
64	${}^{0}\chi^{v}$	Kier&Hall index (order 0)
65	${}^{1}\chi$	Randic index (order 1)
66	${}^{1}\chi^{v}$	Kier&Hall index (order 1)
67	${}^{3}\chi$	Randic index (order 3)
68	${}^{2}\kappa$	Kier shape index (order 2)
69	J	Balaban index
70	W	Wiener index
71	Φ	Kier flexibility index
72	N^{HA}	Count of *H*-acceptor sites

73	N^{HD}	Count of *H*-donor sites
74	$(HA, HD)^{\min}$	Minimum value of N^{HA} and N^{HD}
75	$(HA, HD)^{\max/\min}$	Maximum/minimum values ratio between N^{HA} and N^{HD}
76	*HDCA*	*H*-donors charged surface area
77	*HACA*	*H*-acceptors charged surface area
78	*HASA*	*H*-acceptors surface area
79	*FHACA*	Fractional *H*-acceptor charged surface area (HACA/TMSA)
80	*FHASA*	Fractional *H*-acceptors surface area (HASA/TMSA)
81	*FHBCA*	Fractional *H*-donor charged surface area (HACA/TMSA)
82	*FHDCA*	Fractional HDCA (HDCA/TMSA)
83	*FHBSA*	Fractional *H*-bonding surface area (HBSA/TMSA)
84	${}^{HA}HDCA^{(1)}$	Hydrogen acceptor dependent HDCA-1/TMSA
85	$HACA^{(2)}$	HACA-2
86	${}^{HA}PSA^{(2)}$	New *H*-acceptors PSA
87	${}^{HA}HDCA^{(2)}$	Hydrogen acceptor dependent HDCA-2
88	${}^{HA}HDSA^{(2)}$	HA dependent HDSA-2/TMSA
89	${}^{HD}CPSA^{(2)}$	New *H*-donors CPSA
90	${}^{HA}FPSA^{(2)}$	New *H*-acceptors FPSA
91	${}^{HD}FPSA^{(2)}$	New *H*-donors FPSA
92	${}^{HA}FCPSA^{(2)}$	New *H*-acceptors FCPSA
93	${}^{HD}FCPSA^{(2)}$	New *H*-donors FCPSA
94	S_{ZX}	Shadow plane ZX
95	S_{YZ}	Shadow plane YZ
96	S_{XY} / R_{XY}	XY Shadow / XY Rectangle
97	S_{YZ} / R_{YZ}	YZ Shadow / YZ Rectangle

98	V_M / V_{XYZ}	Molecular volume / XYZ Box
99	I_B	Moments of inertia B
100	I_A / N_A	Relative principal moment of inertia A
101	I_B / N_A	Relative principal moment of inertia B
102	I_C / N_A	Relative principal moment of inertia C
103	G_b	Gravitation index (all bonds)
104	G_p	Gravitation index (all atoms' pairs)
105	T^E	Topographic electronic index (all atoms' pairs)
106	T_b^E	Topographic electronic index (all bonds)
107	α	Alfa polarizability
108	$1/2\beta$	1/2 * BetaA polarizability
109	$1/6\gamma$	1/6 * Gamma polarizability
110	μ	Total dipole of the molecule
111	μ^2 / MW	Image of the Onsager-Kirkwood solvation energy
112	μ_{hyb}	Total hybridization component of the molecular dipole
113	μ_{pch}	Total point-charge component of the molecular dipole
114	S_M	Total molecular surface area
115	ΔH_f^0	Thermodynamic heat of formation of the molecule at 300K
116	$\Delta H_f^0 / N_A$	Thermodynamic heat of formation of the molecule at 300K / number of atoms
117	$\Delta H_{vib} / N_A$	Vibration enthalpy (300K) / number of atoms
118	ΔS_{tot}	Total entropy (300K)
119	ΔS_{trans}	Translational entropy (300K)
120	$\Delta S_{\text{int}} / N_A$	Internal entropy (300K) /number of atoms
121	$\Delta S_{vib} / N_A$	Vibration entropy (300K) /number of atoms

122	c_p^{tot} / N_A	Total heat capacity (300K) /natoms
123	c_p^{int} / N_A	Internal heat capacity (300K) / number of atoms
124	c_p^{vib} / N_A	Vibrational heat capacity (300K) / number of atoms
125	V_{TD}^h	Highest normal mode vibration transition dipole
126	P	Polarity parameter
127	P_f^2	Polarity parameter / square distance