Table 4. Explanation of descriptors used in Table 2.

#	Descriptor designation	Descriptor explanation
1	*RPCS*	Relative positive charged surface area
2	$DPSA^{(1)}$	Difference in charged partial surface areas (Partial Positively charged Surface Area 1 - Partial Negatively charged Surface Area 1)
3	$FPSA^{(1)}$	Fractional partial positively charged surface area (PPSA1/ Total molecular surface area)
4	$WPSA^{(1)}$	Weighted partial positively charged surface area (PPSA1* Total molecular surface area /1000)
5	$WNSA^{(1)}$	Weighted partial negatively charged surface area (PNSA1* Total molecular surface area /1000)
6	$DPSA^{(2)}$	Difference in charged partial surface areas (PPSA2-PNSA2)
7	$FNSA^{(2)}$	Fractional partial negatively charged surface area (PNSA-2/ Total molecular surface area)
8	$FPSA^{(2)}$	Fractional partial positively charged surface area (PPSA-2/ Total molecular surface area)
9	$WNSA^{(2)}$	Weighted partial negatively charged surface area (PNSA2* Total molecular surface area /1000)
10	$WPSA^{(2)}$	Weighted partial positively charged surface area (PPSA2* Total molecular surface area /1000)
11	$PPSA^{(3)}$	Atomic charge weighted partial positively charged surface area
12	$FNSA^{(3)}$	Fractional partial negatively charged surface area (PNSA3/ Total molecular surface area)
13	$FPSA^{(3)}$	Fractional partial positively charged surface area (PPSA3/ Total molecular surface area)
14	$WNSA^{(3)}$	Weighted partial negatively charged surface area (PNSA3* Total molecular surface area /1000)
15	$WPSA^{(3)}$	Weighted partial positively charged surface area (PPSA3* Total molecular surface area /1000)
16	${}^{0}CIC$	Complementary Information content (order 0)
17	${}^{0}\overline{CIC}$	Average Complementary Information content (order 0)

18	${}^{0}\overline{BIC}$	Average Bonding Information content (order 0)
19	${}^{0}\overline{SIC}$	Average Structural Information content (order 0)
20	${}^{1}CIC$	Complementary Information content (order 1)
21	${}^{1}\overline{CIC}$	Average Complementary Information content (order 1)
22	${}^{1}\overline{BIC}$	Average Bonding Information content (order 1)
23	${}^{2}\overline{IC}$	Average Information content (order 2)
24	${}^{2}SIC$	Structural Information content (order 2)
25	${}^{2}\overline{SIC}$	Average Structural Information content (order 2)
26	$q_A^{\min}$	Minimum partial charge for all atom types
27	$q_A^{\max}$	Maximum partial charge for all atom types
28	$q_C^{\max}$	Maximum net atomic charge (typed) for atom *C*
29	$q_C^{\min}$	Minimum net atomic charge (typed) for atom *C*
30	$q_{net}^{\min}$	Minimum net atomic charge
31	$V_C^{\min}$	Minimum valency for atom *C*
32	$V_H^{\min}$	Minimum valency for atom *H*
33	$\overline{V}_H$	Average valency for atom *H*
34	$P_H^{\min}$	Minimum bond order for atom *H*
35	$\overline{P}_C$	Average bond order for atom *C*
36	$R_C^{\min}$	Minimum one-electron reactivity index for atom *C*
37	E_{tot}	Total molecular electrostatic interaction
38	$E_{exc}^{\min}(H-C)$	Minimum exchange energy for bond *H-C*
39	$E_{state}^{\min}(H)$	Minimum atomic state energy for atom *H*
40	$N^{occ.el.lev}$	Number of occupied electronic levels
41	$N^{occ.el.lev} / N_A$	Number of occupied electronic levels / number of atoms

42	$n_A^{\max}$	Maximum atomic orbital electronic population
43	$HOMO$	Energy of the highest occupied molecular orbital
44	${}^0\chi$	Randic index (order 0)
45	${}^0\chi^v$	Kier&Hall index (order 0)
46	${}^1\chi$	Randic index (order 1)
47	${}^1\chi^v$	Kier&Hall index (order 1)
48	${}^3\chi$	Randic index (order 3)
49	J	Balaban index
50	W	Wiener index
51	Φ	Kier flexibility index
52	N^{HA}	Count of *H*-acceptor sites
53	N^{HD}	Count of *H*-donor sites
54	$(HA, HD)^{\min}$	Minimum value of N^{HA} and N^{HD}
55	$(HA, HD)^{\max/\min}$	Maximum/minimum ratio between N^{HA} and N^{HD} values
56	$HDCA$	Hydrogen donors charged surface area
57	$HASA$	Hydrogen acceptors surface area
58	$FHACA$	Fractional hydrogen acceptor charged surface area (HACA/ Total molecular surface area)
59	$FHASA$	Fractional hydrogen acceptors surface area (HASA/ Total molecular surface area)
60	$FHBSA$	Fractional hydrogen bonding surface area (HBSA/ Total molecular surface area)
61	${}^{HA}HDCA^{(1)}$	Hydrogen acceptor dependent Hydrogen donors charged surface area -1
62	$HACA^{(1)}$	Hydrogen acceptors charged surface area - 1
63	$HACA^{(2)}$	Hydrogen acceptors charged surface area -2
64	${}^{HA}PSA^{(2)}$	New hydrogen acceptors partial surface area
65	${}^{HA}HDCA^{(2)}$	Hydrogen acceptor dependent HDCA-2

66	${}^{HA}HDSA^{(2)}$	Hydrogen acceptor dependent Hydrogen donors surface area-2
67	${}^{HD}CPSA^{(2)}$	New hydrogen donors charged partial surface area
68	${}^{HA}FPSA^{(2)}$	New hydrogen acceptors fractional partial surface area
69	${}^{HD}FPSA^{(2)}$	New hydrogen donors fractional partial surface area
70	${}^{HA}FCPSA^{(2)}$	New hydrogen acceptors fractional charged partial surface area
71	${}^{HD}FCPSA^{(2)}$	New hydrogen donors fractional charged partial surface area
72	S_{ZX}	Shadow plane ZX
73	S_{YZ}	Shadow plane YZ
74	S_{XY} / R_{XY}	XY Shadow / XY Rectangle
75	S_{YZ} / R_{YZ}	YZ Shadow / YZ Rectangle
76	V_M / V_{XYZ}	Molecular volume / XYZ Box
77	G_b	Gravitation index (all bonds)
78	G_p	Gravitation index (all atoms' pairs)
79	T^E	Topographic electronic index (all atoms' pairs)
80	T_b^E	Topographic electronic index (all bonds)
81	α	Alfa polarizability
82	μ	Total dipole of the molecule
83	μ_{hyb}	Total hybridization component of the molecular dipole
84	μ_{pch}	Total point-charge component of the molecular dipole
85	S_M	Total molecular surface area
86	ΔH_f^0	Thermodynamic heat of formation of the molecule at 300K
87	$\Delta H_f^0 / N_A$	Thermodynamic heat of formation of the molecule at 300K / number of atoms
88	ΔS_{tot}	Total entropy (300K)
89	$\Delta S_{vib} / N_A$	Vibration entropy (300K) /number of atoms

90	c_p^{int} / N_A	Internal heat capacity (300K) / number of atoms
100	ν_{TD}^h	Highest normal mode vibration transition dipole
101	P_f^2	Polarity parameter / (square distance)^2