**Table S5.** Description of 189 molecular descriptors.

|  |  |  |
| --- | --- | --- |
| **Simple molecular properties(18)** | | |
| 1 | W mol | Molecular weight |
| 2 | nhyd | Count of hydrogen atoms |
| 3 | nhal | Count of halogen atoms |
| 4 | nhet | Count of hetero atoms |
| 5 | nhev | Count of heavy atoms |
| 6 | ncof | Count of F atoms |
| 7 | ncocl | Count of Cl atoms |
| 8 | ncobr | Count of Br atoms |
| 9 | ncoi | Count of I atoms |
| 10 | ncarb | Count of C atoms |
| 11 | nphos | Count of P atoms |
| 12 | nsulph | Count of S atoms |
| 13 | noxy | Count of O atoms |
| 14 | nnitro | Count of N atoms |
| 15 | nring | Numbers of rings |
| 16 | nrot | Number of rotatable bonds |
| 17 | ndonr | Number of H-bond donors |
| 18 | naccr | Number of H-bond acceptors |
| **Molecular connectivity and shape(27)** | | |
| 19 | 0χ | Simple molecular connectivity Chi indices for path order 0 |
| 20 | 1χ | Simple molecular connectivity Chi indices for path order 1 |
| 21 | 2χ | Simple molecular connectivity Chi indices for path order 2 |
| 22 | 3χP | Simple molecular connectivity Chi indices for path order 3 |
| 23 | 3χC | Simple molecular connectivity Chi indices for cluster |
| 24 | 4χPC | Simple molecular connectivity Chi indices for path/cluster |
| 25 | 3χCH | Simple molecular connectivity Chi indices for cycles of 3 atoms |
| 26 | 4χCH | Simple molecular connectivity Chi indices for cycles of 4 atom |
| 27 | 5χCH | Simple molecular connectivity Chi indices for cycles of 5 atom |
| 28 | 6χCH | Simple molecular connectivity Chi indices for cycles of 6 atom |
| 29 | 0χv | Valence molecular connectivity Chi indices for path order 0 |
| 30 | 1χv | Valence molecular connectivity Chi indices for path order 1 |
| 31 | 2χv | Valence molecular connectivity Chi indices for path order 2 |
| 32 | 3χvP | Valence molecular connectivity Chi indices for path order 3 |
| 33 | 3χvC | Valence molecular connectivity Chi indices for cluster |
| 34 | 4χvPC | Valence molecular connectivity Chi indices for path/cluster |
| 35 | 3χvCH | Valence molecular connectivity Chi indices for cycles of 3 atoms |
| 36 | 4χvCH | Valence molecular connectivity Chi indices for cycles of 4 atoms |
| 37 | 5χvCH | Valence molecular connectivity Chi indices for cycles of 5 atoms |
| 38 | 6χvCH | Valence molecular connectivity Chi indices for cycles of 6 atoms |
| 39 | 1κ | Molecular shape Kappa indices for one boned fragments |
| 40 | 2κ | Molecular shape Kappa indices for two boned fragments |
| 41 | 3κ | Molecular shape Kappa indices for three boned fragments |
| 42 | 1κ α | Kappa alpha indices for one boned fragments |
| 43 | 2κ α | Kappa alpha indices for two boned fragments |
| 44 | 3κ α | Kappa alpha indices for three boned fragments |
| 45 | phi | Kier molecular flexibility index |
| **Electrotopological state(97)** | | |
| 46 | S hev | Sum of electrotopological state (Estate) indices of heavy atoms |
| 47 | S car | Sum of Estate indices of carbon atoms |
| 48 | S het | Sum of Estate indices of hetero atoms |
| 49 | S hal | Sum of Estate indices of halogen atoms |
| 50 | S(1) | Atom-type H Estate sum for -O**H** |
| 51 | S(2) | Atom-type H Estate sum for =N**H** |
| 52 | S(3) | Atom-type H Estate sum for -S**H** |
| 53 | S(4) | Atom-type H Estate sum for -N**H** 2 |
| 54 | S(5) | Atom-type H Estate sum for > N**H** |
| 55 | S(6) | Atom-type H Estate sum for : N**H**: |
| 56 | S(7) | Atom-type H Estate sum for #C**H** (sp) |
| 57 | S(8) | Atom-type H Estate sum for =C**H** 2 (sp2) |
| 58 | S(9) | Atom-type H Estate sum for =C**H**- (sp2) |
| 59 | S(10) | Atom-type H Estate sum for :C**H**: (sp2, aromatic) |
| 60 | S(11) | Atom-type H Estate sum for C**H** n X (sp3, X= F, Cl, Br, I) |
| 61 | S(12) | Atom-type H Estate sum for C**H** n (Saturated) |
| 62 | S(13) | Atom-type H Estate sum for C**H** n (unsaturated) |
| 63 | S(14) | Atom-type H Estate sum for C**H** n (aromatic) |
| 64 | S(15) | Atom-type H Estate sum for A**H** n (not C, N, O, S) |
| 65 | S(16) | Atom-type Estate sum for -CH 3 |
| 66 | S(17) | Atom-type Estate sum for =CH 2 |
| 67 | S(18) | Atom-type Estate sum for >CH 2 |
| 68 | S(19) | Atom-type Estate sum for ≡CH |
| 69 | S(20) | Atom-type Estate sum for =CH- |
| 70 | S(21) | Atom-type Estate sum for : CH : (aromatic) |
| 71 | S(22) | Atom-type Estate sum for >CH- |
| 72 | S(23) | Atom-type Estate sum for =C= |
| 73 | S(24) | Atom-type Estate sum for ≡C- |
| 74 | S(25) | Atom-type Estate sum for =C< |
| 75 | S(26) | Atom-type Estate sum for : C:- |
| 76 | S(27) | Atom-type Estate sum for : C :: |
| 77 | S(28) | Atom-type Estate sum for >C< |
| 78 | S(29) | Atom-type Estate sum for -NH 2 |
| 79 | S(30) | Atom-type Estate sum for =NH |
| 80 | S(31) | Atom-type Estate sum for >NH |
| 81 | S(32) | Atom-type Estate sum for :NH: |
| 82 | S(33) | Atom-type Estate sum for ≡N |
| 83 | S(34) | Atom-type Estate sum for =N- |
| 84 | S(35) | Atom-type Estate sum for :N: |
| 85 | S(36) | Atom-type Estate sum for >N- |
| 86 | S(37) | Atom-type Estate sum for -N<< (NO2) |
| 87 | S(38) | Atom-type Estate sum for :N:- |
| 88 | S(39) | Atom-type Estate sum for -OH |
| 89 | S(40) | Atom-type Estate sum for =O |
| 90 | S(41) | Atom-type Estate sum for -O- |
| 91 | S(42) | Atom-type Estate sum for :O: |
| 92 | S(43) | Atom-type Estate sum for -F |
| 93 | S(44) | Atom-type Estate sum for -SiH 3 |
| 94 | S(45) | Atom-type Estate sum for -SiH2- |
| 95 | S(46) | Atom-type Estate sum for >SiH- |
| 96 | S(47) | Atom-type Estate sum for >Si< |
| 97 | S(48) | Atom-type Estate sum for -PH2 |
| 98 | S(49) | Atom-type Estate sum for -PH- |
| 99 | S(50) | Atom-type Estate sum for >P- |
| 100 | S(51) | Atom-type Estate sum for ->P= (P.O) |
| 101 | S(52) | Atom-type Estate sum for -=P= (P. O2) |
| 102 | S(53) | Atom-type Estate sum for - |
| 103 | S(54) | Atom-type Estate sum for -SH |
| 104 | S(55) | Atom-type Estate sum for =S |
| 105 | S(56) | Atom-type Estate sum for -S- |
| 106 | S(57) | Atom-type Estate sum for :S: |
| 107 | S(58) | Atom-type Estate sum for >S=O |
| 108 | S(59) | Atom-type Estate sum for >S<< |
| 109 | S(60) | Atom-type Estate sum for -Cl |
| 110 | S(61) | Atom-type Estate sum for GeH3 |
| 111 | S(62) | Atom-type Estate sum for -GeH 2- |
| 112 | S(63) | Atom-type Estate sum for >GeH- |
| 113 | S(64) | Atom-type Estate sum for>Ge< |
| 114 | S(65) | Atom-type Estate sum for -AsH2 |
| 115 | S(66) | Atom-type Estate sum for -AsH- |
| 116 | S(67) | Atom-type Estate sum for >As- |
| 117 | S(68) | Atom-type Estate sum for ->As= |
| 118 | S(69) | Atom-type Estate sum for -SeH |
| 119 | S(70) | Atom-type Estate sum for =Se |
| 120 | S(71) | Atom-type Estate sum for -Se- |
| 121 | S(72) | Atom-type Estate sum for :Se: |
| 122 | S(73) | Atom-type Estate sum for >Se= |
| 123 | S(74) | Atom-type Estate sum for -=Se=- |
| 124 | S(75) | Atom-type Estate sum for -Br |
| 125 | S(76) | Atom-type Estate sum for -SnH3 |
| 126 | S(77) | Atom-type Estate sum for -SnH2- |
| 127 | S(78) | Atom-type Estate sum for >SnH- |
| 128 | S(79) | Atom-type Estate sum for >Sn< |
| 129 | S(80) | Atom-type Estate sum for -I |
| 130 | Twien | Weiner Index |
| 131 | Tcent | Centric Index |
| 132 | Talte | Altenburg Index |
| 133 | Tbala | Balaban Index |
| 134 | Thara | Harary Number |
| 135 | Tschl | Schultz Index |
| 136 | Tradi | PetitJohn R2 Index |
| 137 | Tdiam | PetitJohn D2 Index |
| 138 | Tbmdd | Mean Distance Index |
| 139 | Tpeti | PetitJohn I2 Index |
| 140 | Tiwie | Information Weiner |
| 141 | Trmsd | Balaban RMSD Index |
| 142 | Tigdi | Graph Distance Index |
| **Quantum chemical properties (22)** | | |
| 143 | π i | Polarizability index |
| 144 | μ | Molecular dipole moment |
| 145 | Q H, Max | Most positive charge on H atoms |
| 146 | Q C, Max | Most positive charge on C atoms |
| 147 | Q N, Max | Most positive charge on N atoms |
| 148 | Q O, Max | Most positive charge on O atoms |
| 149 | Q H, Min | Most negative charge on H atoms |
| 150 | Q C, Min | Most negative charge on C atoms |
| 151 | Q N, Min | Most negative charge on N atoms |
| 152 | Q O, Min | Most negative charge on O atoms |
| 153 | A Q, max | Most positive charge in a molecule |
| 154 | A Q, min | Most negative charge in a molecule |
| 155 | Q H, SS | Sum of squares of charges on H atoms |
| 156 | Q C, SS | Sum of squares of charges on C atoms |
| 157 | Q N, SS | Sum of squares of charges on N atoms |
| 158 | Q O, SS | Sum of squares of charges on O atoms |
| 159 | Q A, SS | Sum of squares of charges on all atoms |
| 160 | Mpc | Mean of positive charges |
| 161 | Mnc | Mean of negative charges |
| 162 | Mac | Mean absolute charge |
| 163 | Rpc | Relative positive charge |
| 164 | Rnc | Relative negative charge |
| **Geometrical properties(25)** | | |
| 165 | dis1 | Length vectors (longest distance) |
| 166 | dis2 | Length vectors (longest third atom) |
| 167 | dis3 | Length vectors (4th atom) |
| 168 | V mc | Van der Waals molecular volume |
| 169 | AS | Solvent accessible surface area |
| 170 | VS | van der Waals surface area |
| 171 | MS | Molecular surface area |
| 172 | PSA | Polar molecular surface area |
| 173 | Sapc | Sum of solvent accessible surface areas of positively charged atoms |
| 174 | Sanc | Sum of solvent accessible surface areas of negatively charged atoms |
| 175 | Sapcw | Sum of charge weighted solvent accessible surface areas of positively charged atoms |
| 176 | Sancw | Sum of charge weighted solvent accessible surface areas of negatively charged atoms |
| 177 | Svpc | Sum of van der Waals surface areas of positively charged atoms |
| 178 | Svnc | Sum of van der Waals surface areas of negatively charged atoms |
| 179 | Svpcw | Sum of charge weighted van der Waals surface areas of positively charged atoms |
| 180 | Svncw | Sum of charge weighted van der Waals surface areas of negatively charged atoms |
| 181 | Rugty | Molecular rugosity |
| 182 | Gloty | Molecular globularity |
| 183 | Shpl | Hydrophilic region |
| 184 | Shpb | Hydrophobic region |
| 185 | Capty | Capacity factor |
| 186 | Hlb | Hydrophilic-Hydrophobic balance |
| 187 | Hiwpl | Hydrophilic Intery Moment |
| 188 | Hiwpb | Hydrophobic Intery Moment |
| 189 | Hiwpa | Amphiphilic Moment |