

Supplementary Information-1

List of molecular descriptors computed to assign weights (δ) for the substituents

Graph theoretical descriptors

I^W_D	Information index for the magnitudes of distances between all possible pairs of vertices of a graph
$I_h^W_D$	Mean information index for the magnitude of distance
W	Wiener index = half-sum of the off-diagonal elements of the distance matrix of a graph
H	Harary index = half-sum of reciprocal square of the elements of the distance matrix of a graph
J	Balaban index = sum of the reciprocal square root of degree of all adjacent pairs
I_C^D	Information content of the distance matrix
IC	Information content of the distance matrix partitioned by frequency of occurrences of distance
O	Order of neighbourhoods when IC_r reaches its maximum value for the hydrogen-filled graph
$M1$	Zagreb group parameter = sum of square of degree over all vertices
$M2$	Zagreb group parameter = sum of cross-product of degrees over all neighbouring (connected) vertices $M2$

Topo-structural descriptors

$^h\chi$	Path connectivity index of order $h = 0-6$
$^h\chi_c$	Cluster connectivity index of order $h = 3-6$
$^h\chi_{ch}$	Chain connectivity index of order $h = 3-6$
$^h\chi_{pc}$	Path-cluster connectivity index of order $h = 4-6$
P_h	Number of paths of length $h = 0-10$

Topo-chemical descriptors (bond-order connectivity)

$^h\chi^b$	Bond path connectivity index of order $h = 0-9$
$^h\chi_c^b$	Bond cluster connectivity index of order $h = 3-6$
$^h\chi_{ch}^b$	Bond chain connectivity index of order $h = 3-6$
$^h\chi_{pc}^b$	Bond path-cluster connectivity index of order $h = 4-6$

Topo-chemical descriptors (valence connectivity)

$^h\chi^v$	Valence path connectivity index of order $h = 0-9$
$^h\chi_c^v$	Valence cluster connectivity index of order $h = 3-6$
$^h\chi_{ch}^v$	Valence chain connectivity index of order $h = 3-6$
$^h\chi_{pc}^v$	Valence path-cluster connectivity index of order $h = 4-6$

Information theoretic descriptors

I_{ORB}	Information content or complexity of the hydrogen suppressed graph at its maximum neighbourhood of vertices
O_{ORB}	Order of neighbourhoods when IC _r reaches its maximum value for the hydrogen suppressed graph
IC_r	Mean information content or complexity of a graph based on the r^{th} ($r = 0-6$) order neighbourhood of vertices in a hydrogen-filled graph
SIC_r	Structural information content for r^{th} ($r = 0-6$) order neighbourhood of vertices in a hydrogen-filled graph
CIC_r	Complementary information content for r^{th} ($r = 0-6$) order neighbourhood of vertices in a hydrogen-filled graph
TIC_r	Total information content for r^{th} ($r = 0-6$) order neighbourhood of vertices in a hydrogen-filled graph
BIC_r	Bond information content for r^{th} ($r = 0-6$) order neighbourhood of vertices in a hydrogen-filled graph

Overall connectivity indices

SumR	Sum of connectivity indices of all orders ($\Sigma^h \chi$)
VSumR	Sum of valence connectivity indices of all orders ($\Sigma^h \chi^v$)
BSumR	Sum of bond order connectivity indices of all orders ($\Sigma^h \chi^b$)
OPM	Overall path multiplicity $\Sigma^h \chi \times P_h$
VOPM	Overall path multiplicity of valence connectivity $\Sigma^h \chi^v \times P_h$
BOPM	Overall path multiplicity of bond order connectivity $\Sigma^h \chi^b \times P_h$
MPC	Mean path connectivity index $\Sigma^h \chi \div P_h$
VMPC	Mean path connectivity index based on valence connectivity $\Sigma^h \chi^v \div P_h$
BMPC	Mean path connectivity index based on bond connectivity $\Sigma^h \chi^b \div P_h$
SumK	Sum of all paths of length 1 to h ΣP_h

Triplet indices – Topo-structural (connectivity)

DN²S_y	Triplet index from distance matrix, square of graph order, and distance sum; operation y=1–5
DN₂1_y	Triplet index from distance matrix, square of graph order, and number 1; operation y=1–5
AS1_y	Triplet index from adjacency matrix, distance sum, and number 1; operation y=1–5
DS1_y	Triplet index from distance matrix, distance sum, and number 1; operation y=1–5
ASN_y	Triplet index from adjacency matrix, distance sum, and graph order; operation y=1–5
DSN_y	Triplet index from distance matrix, distance sum, and graph order; operation y=1–5
DN²N_y	Triplet index from distance matrix, square of graph order, and graph order; operation y=1–5

ANS_y	Triplet index from adjacency matrix, graph order, and distance sum; operation y=1–5
AN1_y	Triplet index from adjacency matrix, graph order, and number 1; operation y=1–5
ANN_y	Triplet index from adjacency matrix, graph order, and graph order again; operation y=1–5
ASV_y	Triplet index from adjacency matrix, distance sum, and vertex degree; operation y=1–5
DSV_y	Triplet index from distance matrix, distance sum, and vertex degree; operation y=1–5
ANV_y	Triplet index from adjacency matrix, graph order, and vertex degree; operation y=1–5

Triplet Indices - Topochemical

AZV_y	Triplet index from adjacency matrix, atomic number, and vertex degree; operation y=1–5
AZS_y	Triplet index from adjacency matrix, atomic number, and distance sum; operation y=1–5
ASZ_y	Triplet index from adjacency matrix, distance sum, and atomic number; operation y=1–5
AZN_y	Triplet index from adjacency matrix, atomic number, and graph order; operation y=1–5
ANZ_y	Triplet index from adjacency matrix, graph order, and atomic number; operation y=1–5
DSZ_y	Triplet index from distance matrix, distance sum, and atomic number; operation y=1–5
DN²Z_y	Triplet index from distance matrix, square of graph order, and atomic number; operation y=1–5
