The second sets of molecular descriptors, used frequently by Basak et al, are calculated by the software POLLY [8] and Triplet [9]. We use 98 and 100 descriptors calculated by these software, respectively. These 198 descriptors are generally referred to as topological indices (TIs), since they are derived from graph theoretical methods. TIs include both topostructural (TS) and topochemical (TC) subclasses. The former encode information strictly on molecular connectivity. The later include chemical features in addition to topological information. These chemical features include atom and bond type. Table 1 provides a list of the TIs from the Basak lab used in this study, along with brief descriptions.

Table 1. Symbols and definitions of topological indices (TIs).

|  |  |
| --- | --- |
|  | Topostructural (TS) |
| *IWD* | Information index for the magnitudes of distances between all possible pairs of vertices of a graph |
| *IWD* | 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 |
| *ID* | Degree complexity |
| *HV* | Graph vertex complexity |
| *HD* | Graph distance complexity |
| *IC* | Information content of the distance matrix partitioned by frequency of occurrences of distance *h* |
| *M1* | A Zagreb group parameter = sum of square of degree over all vertices |
| *M2* | A Zagreb group parameter = sum of cross-product of degrees over all neighboring (connected) vertices |
| *hχ* | Path connectivity index of order *h* = 0-6 |
| *hχC* | Cluster connectivity index of order *h* = 3-6 |
| *hχPC* | Path-cluster connectivity index of order *h* = 4-6 |
| *hχCh* | Chain connectivity index of order *h* = 3-6 |
| *Ph* | Number of paths of length *h* = 0-10 |
| DN2Sy | Triplet index from distance matrix, square of graph order, and distance sum; operation y = 1-5 |
| DN21y | Triplet index from distance matrix, square of graph order, and number 1; operation y = 1-5 |
| AS1y | Triplet index from adjacency matrix, distance sum, and number 1; operation y = 1-5 |
| DS1y | Triplet index from distance matrix, distance sum, and number 1; operation y = 1-5 |
| ASNy | Triplet index from adjacency matrix, distance sum, and graph order; operation y = 1-5 |
| DSNy | Triplet index from distance matrix, distance sum, and graph order; operation y = 1-5 |
| DN2Ny | Triplet index from distance matrix, square of graph order, and graph order; operation y = 1-5 |
| ANSy | Triplet index from adjacency matrix, graph order, and distance sum; operation y = 1-5 |
| AN1y | Triplet index from adjacency matrix, graph order, and number 1; operation y = 1-5 |
| ANNy | Triplet index from adjacency matrix, graph order, and graph order again; operation y = 1-5 |
| ASVy | Triplet index from adjacency matrix, distance sum, and vertex degree; operation y = 1-5 |
| DSVy | Triplet index from distance matrix, distance sum, and vertex degree; operation y = 1-5 |
| ANVy | Triplet index from adjacency matrix, graph order, and vertex degree; operation y = 1-5 |
| Topochemical (TC) | |
| O | Order of neighborhood when ICr reaches its maximum value for the hydrogen-filled graph |
| Oorb | Order of neighborhood when ICr reaches its maximum value for the hydrogen-suppressed graph |
| IORB | Information content or complexity of the hydrogen-suppressed graph at its maximum neighborhood of vertices |
| ICr | Mean information content or complexity of a graph based on the rth (r = 0-6) order neighborhood of vertices in a hydrogen-filled graph |
| SICr | Structural information content for rth (r = 0-6) order neighborhood of vertices in a hydrogen-filled graph |
| CICr | Complementary information content for rth (r = 0-6) order neighborhood of vertices in a hydrogen-filled graph |
| hχb | Bond path connectivity index of order h = 0-6 |
| hχbC | Bond cluster connectivity index of order h = 3-6 |
| hχbCh | Bond chain connectivity index of order h = 3- 6 |
| hχbPC | Bond path-cluster connectivity index of order h = 4-6 |
| hχv | Valence path connectivity index of order h = 0-6 |
| hχvC | Valence cluster connectivity index of order h = 3-6 |
| hχvCh | Valence chain connectivity index of order h = 3-6 |
| hχvPC | Valence path-cluster connectivity index of order h = 4-6 |
| AZVy | Triplet index from adjacency matrix, atomic number, and vertex degree; operation y = 1-5 |
| AZSy | Triplet index from adjacency matrix, atomic number, and distance sum; operation y = 1-5 |
| ASZy | Triplet index from adjacency matrix, distance sum, and atomic number; operation y = 1-5 |
| AZNy | Triplet index from adjacency matrix, atomic number, and graph order; operation y = 1-5 |
| ANZy | Triplet index from adjacency matrix, graph order, and atomic number; operation y = 1-5 |
| DSZy | Triplet index from distance matrix, distance sum, and atomic number; operation y = 1-5 |
| DN2Zy | Triplet index from distance matrix, square of graph order, and atomic number; operation  y = 1-5 |