Model 997

Class = 0.05428 + 0.26464*NaasN - 32.77330*JGI6 + 0.07801*J_D/Dt - 0.01735*ATSC4m - 0.44701*F04[N-N] + 0.11065*Eig15_AEA(ed) + 0.20216*F04[N-S] -0.15403*B06[N-O]

NaasN: It is an atom-type E-state index representing the number of aasN E-states.

JGI6: Indicates the mean topological charge index of order 6.

J_D/Dt: is a Balaban-like index derived from the distance/detour matrix.

ATSC4m: Represent the centered Broto-Moreau autocorrelation of lag 4 weighted by atomic mass.

F04[N-N]: Symbolizes the frequency of Nitrogen - Nitrogen at a topological distance of 4.

Eig15_AEA(ed): Denotes the 15th eigenvalue from the augmented edge adjacency matrix weighted by edge degree.

F04[N-S] : Symbolizes the frequency of Nitrogen - Sulfur at a topological distance of 4.

B06[N-O] : Symbolizes the presence/absence of Nitrogen - Oxygen at a topological distance of 6.

Model 177

Class = 1.841914 + 0.078309*CATS2D_06_NL + 0.210243*SaasN - 0.088337*SM13_EA(bo) + 0.497195*F03[S-S] + 0.014034*CATS2D_06_LL - 0.003877 *T(N..O) -0.003744*P_VSA_MR_5 + 0.022183*X%

CATS2D_06_NL: Indicates the CATS2D (Chemically Advanced Template Search) Negative-Lipophilic at lag 06

SaasN: It is an atom-type E-state index representing the sum of aasN E-states.

SM13_EA(bo): Correspond to the spectral moment of order 13 from edge adjacency matrix weighted by bond order.

F03[S-S]: Symbolizes the frequency of Nitrogen - Nitrogen atom pairs at a topological distance of 3

CATS2D_06_LL: Indicates the CATS2D (Chemically Advanced Template Search) Lipophilic-Lipophilic at lag 06

T(N..O): Represent the sum of topological distances between N..O

P_VSA_MR_5: These are molecular descriptors defined as the amount of van der Waals surface area (VSA) having a property P in a certain range. In this case it is the P_VSA-like on Molar Refractivity, bin 5.

X%: Indicates the percentage of halogen atoms.

Model 1

Class = 0.76817 + 0.31916*NaasN - 0.03873*F07[C-N] -7.14022*JGI2 + 0.50412*B03[S-S] + 0.02543*CATS2D_02_LL - 0.02852*CATS2D_06_AL - 0.06139*H-051 + 0.23898*CATS2D_03_AN

NaasN: It is an atom-type E-state index representing the number of aasN E-states.

F07[C-N]: Symbolizes the frequency of Carbon – Nitrogen atom pairs at a topological distance of 7

JGI2: Indicates the mean topological charge index of order 2

B03[S-S]: Symbolizes the presence/absence of Sulfur – sulfur atom pairs at a topological distance of 3.

CATS2D_02_LL: Indicates the CATS2D (Chemically Advanced Template Search) Lipophilic-Lipophilic at lag 02.

CATS2D_06_AL: Indicates the CATS2D (Chemically Advanced Template Search) Acceptor-Lipophilic at lag 06.

H-051: Indicates the number of H attached to alpha-C.

CATS2D_03_AN: Indicates the CATS2D (Chemically Advanced Template Search) Acceptor-Negative at lag 03.

Model 556

Class = 1.376275 + 0.224271*SaasN - 0.137772*CATS2D_04_AA + 0.099137*C-016 - 0.314956*B06[C-N] - 5.140100*VE2_A + 0.474381*F03[S-S] - 0.016253*T(N..S) + 0.072411*SpMax_EA(dm) - 0.001143*ATSC5s

SaasN: It is an atom-type E-state index representing the sum of aasN E-states.

CATS2D_04_AA: Indicates the CATS2D (Chemically Advanced Template Search) Acceptor-Acceptor at lag 04

C-016: Indicates the number of =CHR in the molecule.

B06[C-N]: Symbolizes the presence/absence of Carbon - Nitrogen at a topological distance of 6

VE2_A: Represent the average coefficient of the last eigenvector from adjacency matrix.

F03[S-S]: Symbolizes the frequency of Sulfur - Sulfur at a topological distance of 3

T(N..S): Represent the sum of topological distances between N..S

SpMax_EA(dm): It denotes the leading eigenvalue from edge adjacency matrix weighted by dipole moment.

ATSC5s: It is a centred Broto-Moreau autocorrelation of lag 5 weighted by I-state.

Model 893

Class = 0.83218 + 0.29187*NaasN - 0.10621*NsCH3 + 0.02618*CATS2D_05_LL - 0.23414*B06[C-N] + 0.38038*nThiophenes - 2.23506*Eta_FL_A + 0.11009*F03[N-F]

NaasN: It is an atom-type E-state index representing the number of aasN E-states.

NsCH3: It is an atom-type E-state index representing the number of atoms of type sCH3.

CATS2D_05_LL: Indicates the CATS2D (Chemically Advanced Template Search) Lipophilic-Lipophilic at lag 05.

B06[C-N]: Symbolizes the presence/absence of Carbon - Nitrogen at topological distance 6

nThiophenes: Indicates the number of Thiophenes in the molecule.

Eta_FL_A: It is the eta average local functionality index.

F03[N-F]: Symbolizes the frequency of N - F at a topological distance of 3.