| Odor Set | Dragon No. | Name | Description | Block |
|----------|------------|------|-------------|-------|
| Global   | 250        | rG6s | Relative number of symmetry classes (based on electropotential state) | Information indices |
| Global   | 371        | ChA_X | average Randić-like index from chi matrix | 2D matrix-based descriptors |
| Global   | 375        | SpPosA_X | normalized spectral positive sum from chi matrix | 2D matrix-based descriptors |
| Global   | 721        | VE1_B(r) | coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass | 2D matrix-based descriptors |
| Global   | 1071       | GATS | Geary autocorrelation of lag 1 weighted by ionization potential | 3D autocorrelations |
| Global   | 1306       | SpMad_E(A) | spectral absolute deviation from edge adjacency mat. weighted by resonance integral | Edge adjacency indices |
| Global   | 1611       | MEcc | molecular eccentricity | Geometrical descriptors |
| Global   | 1687       | SpPosA_RG | normalized spectral positive sum from reciprocal squared geometrical matrix | 3D matrix-based descriptors |
| Global   | 1693       | SpMad_RG | spectral mean absolute deviation from reciprocal squared geometrical matrix | 3D matrix-based descriptors |
| Global   | 1701       | VE1_RG | coefficient sum of the last eigenvector (absolute values) from reciprocal squared geometrical matrix | 3D matrix-based descriptors |
| Global   | 2221       | Mor07a | signal 07 / weighted by I-state | 3D-MoRSE descriptors |
| Global   | 2240       | Mor16a | signal 16 / weighted by I-state | 3D-MoRSE descriptors |
| Global   | 2284       | G1V | 1st component symmetry directional WHIM index / weighted by van der Waals volume | WHIM descriptors |
| Global   | 2285       | G2V | 2nd component symmetry directional WHIM index / weighted by van der Waals volume | WHIM descriptors |
| Global   | 2298       | E1e | 1st component accessibility directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |
| Global   | 2307       | G2p | 2nd component symmetry directional WHIM index / weighted by polarity | WHIM descriptors |
| Global   | 2331       | E1s | 1st component accessibility directional WHIM index / weighted by I-state | WHIM descriptors |
| Global   | 2351       | RARS | R matrix average row sum | GETAWAY descriptors |
| Global   | 2607       | RTp+ | R maximal index / weighted by polarization | GETAWAY descriptors |
| Global   | 4205       | Hy | hydrophilic factor | Molecular properties |
| Clustered | 260 | I2C | Information Content index (neighborhood symmetry of 2-order) | Information indices |
| Clustered | 284 | BiC2 | Bond Information Content index (neighborhood symmetry of 2-order) | Information indices |
| Clustered | 381 | SpMad_X | spectral mean absolute deviation from chi matrix | 2D matrix-based descriptors |
| Clustered | 739 | SpPosA_B(r) | normalized spectral positive sum from Burden matrix weighted by van der Waals volume | 2D matrix-based descriptors |
| Clustered | 1079 | GATS1s | Geary autocorrelation of lag 1 weighted by I-state | 3D autocorrelations |
| Clustered | 1317 | SpMax_AEA(dm) | leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment | Edge adjacency indices |
| Clustered | 1213 | SpMad_AEA(dm) | spectral mean absolute deviation from augmented edge adjacency mat. weighted by dipole moment | Edge adjacency indices |
| Clustered | 1576 | Exp01_AEA(dm) | eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment | Edge adjacency indices |
| Clustered | 1611 | MEcc | molecular eccentricity | Geometrical descriptors |
| Clustered | 1614 | Pj3 | 3D Pettayan shape index | Geometrical descriptors |
| Clustered | 2190 | Mor07i | signal 07 / weighted by ionization potential | 3D-MoRSE descriptors |
| Clustered | 2220 | Mor06s | signal 06 / weighted by I-state | 3D-MoRSE descriptors |
| Clustered | 2227 | Mor13a | signal 13 / weighted by I-state | 3D-MoRSE descriptors |
| Clustered | 2234 | Mor20b | signal 20 / weighted by I-state | 3D-MoRSE descriptors |
| Clustered | 2273 | G1m | 1st component symmetry directional WHIM index / weighted by mass | WHIM descriptors |
| Clustered | 2284 | G1v | 1st component symmetry directional WHIM index / weighted by van der Waals volume | WHIM descriptors |
| Clustered | 2323 | E1s | 1st component accessibility directional WHIM index / weighted by I-state | WHIM descriptors |
| Clustered | 2362 | D_2 | D total accessibility index / weighted by ionization potential | WHIM descriptors |
| Clustered | 4946 | DLS_02 | modified drug-like score from Opmea et al. (8 rules) | Drug-like indices |
| Clustered | 4947 | DLS_03 | modified drug-like score from Walleers et al. (6 rules) | Drug-like indices |
| Tiled    | 272 | C2 | Structural Information Content index (neighborhood symmetry of 2-order) | Information indices |
| Tiled    | 368 | AV5s | average vertex sum from chi matrix | 2D matrix-based descriptors |
| Tiled    | 371 | ChA_X | average Randić-like index from chi matrix | 2D matrix-based descriptors |
| Tiled    | 633 | Ch_Dz(p) | Randić-like index from Barysz matrix weighted by polarizability | 2D matrix-based descriptors |
| Tiled    | 635 | J_Dz(p) | Balaban-like index from Barysz matrix weighted by polarizability | 2D matrix-based descriptors |
| Tiled    | 1149 | SpMax0_Bh(s) | largest eigenvalue n. 2 of Burden matrix weighted by I-state | Burden eigenvalues |
| Tiled    | 1288 | SpMax0_AEA(ed) | normalized leading eigenvalue from edge adjacency mat. weighted by edge degree | Edge adjacency indices |
| Tiled    | 1317 | SpMax_AEA(dm) | leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment | Edge adjacency indices |
| Tiled    | 1576 | Exp01_AEA(dm) | eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment | Edge adjacency indices |
| Tiled    | 1614 | Pj3 | 3D Pettayan shape index | Geometrical descriptors |
| Tiled    | 2201 | Mor09i | signal 09 / weighted by ionization potential | 3D-MoRSE descriptors |
| Tiled    | 2208 | Mor16i | signal 16 / weighted by ionization potential | 3D-MoRSE descriptors |
| Tiled    | 2222 | Mor02s | signal 02 / weighted by I-state | 3D-MoRSE descriptors |
| Tiled    | 2227 | Mor03a | signal 03 / weighted by I-state | 3D-MoRSE descriptors |
| Tiled    | 2285 | E1s | 1st component accessibility directional WHIM index / unweighted | WHIM descriptors |
| Tiled    | 2271 | G2m | 2nd component symmetry directional WHIM index / weighted by mass | WHIM descriptors |
| Tiled    | 2326 | E1i | 1st component accessibility directional WHIM index / weighted by Sanderson electronegativity | WHIM descriptors |
| Tiled    | 2326 | Pt1 | 1st component shape directional WHIM index / weighted by I-state | WHIM descriptors |
| Tiled    | 2589 | RS+ | R maximal index / weighted by Sanderson electronegativity | GETAWAY descriptors |
| Tiled    | 2636 | R2s+ | R maximal autocorrelation of lag 2 / weighted by I-state | GETAWAY descriptors |
| Boutsions | 272 | Si2 | Structural Information Content index (neighborhood symmetry of 2-order) | Information indices |
| Boutsions | 368 | AV5s | average vertex sum from chi matrix | 3D matrix-based descriptors |
| Boutsions | 371 | ChA_X | average Randić-like index from chi matrix | 2D matrix-based descriptors |
| Boutsions | 633 | Ch_Dz(p) | Randić-like index from Barysz matrix weighted by polarizability | 2D matrix-based descriptors |
| Boutsions | 635 | J_Dz(p) | Balaban-like index from Barysz matrix weighted by polarizability | 2D matrix-based descriptors |
| Boutsions | 1149 | SpMax0_Bh(s) | largest eigenvalue n. 2 of Burden matrix weighted by I-state | Burden eigenvalues |
| Boutsions | 1317 | SpMax_AEA(dm) | leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment | Edge adjacency indices |
| Boutsions | 1576 | Exp01_AEA(dm) | eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment | Edge adjacency indices |
| Boutsions | 1614 | Pj3 | 3D Pettayan shape index | Geometrical descriptors |
| Boutsions | 2201 | Mor09i | signal 09 / weighted by ionization potential | 3D-MoRSE descriptors |
| Boutsions | 2208 | Mor16i | signal 16 / weighted by ionization potential | 3D-MoRSE descriptors |
| Boutsions | 2285 | E1u | 1st component accessibility directional WHIM index / unweighted | WHIM descriptors |
| Boutsions | 2271 | G2m | 2nd component symmetry directional WHIM index / weighted by mass | WHIM descriptors |
| Boutsions | 2320 | E1i | 1st component accessibility directional WHIM index / weighted by ionization potential | WHIM descriptors |
| Boutsions | 2320 | G2s | 2nd component symmetry directional WHIM index / weighted by I-state | WHIM descriptors |
| Boutsions | 2320 | G3s | 3rd component symmetry directional WHIM index / weighted by I-state | WHIM descriptors |
| Boutsions | 2589 | RS+ | R maximal index / weighted by Sanderson electronegativity | GETAWAY descriptors |
| Boutsions | 4948 | DLS_04 | modified drug-like score from Chen et al. (7 rules) | Drug-like indices |
| Boutsions | 4953 | LLS_01 | modified lead-like score from Congreve et al. (8 rules) | Drug-like indices |