
Supplementary information

**Structure and flexibility in cortical
representations of odour space**

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Odor Set	Dragon No.	Name	Description	Block
Global	250	rGes	Relative number of symmetry classes (based on electrotopological state)	Information indices
Global	371	ChiA_X	average Randic-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(m)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass	2D matrix-based descriptors
Global	1071	GATS1i	Geary autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations
Global	1306	SpMAD_EA(ri)	spectral mean 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	2231	Mor07s	signal 07 / weighted by l-state	3D-MoRSE descriptors
Global	2240	Mor16s	signal 16 / weighted by l-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 polarizability	WHIM descriptors
Global	2331	E1s	1st component accessibility directional WHIM index / weighted by l-state	WHIM descriptors
Global	2516	RARS	R matrix average row sum	GETAWAY descriptors
Global	2607	RTP+	R maximal index / weighted by polarizability	GETAWAY descriptors
Global	4925	Hy	hydrophilic factor	Molecular properties
Clustered	260	IC2	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(v)	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 l-state	2D autocorrelations
Clustered	1317	SpMax_AEA(dm)	leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
Clustered	1321	SpMAD_AEA(dm)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
Clustered	1576	Eig01_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	PJl3	3D Petitjean shape index	Geometrical descriptors
Clustered	2199	Mor07i	signal 07 / weighted by ionization potential	3D-MoRSE descriptors
Clustered	2230	Mor06s	signal 06 / weighted by l-state	3D-MoRSE descriptors
Clustered	2237	Mor13s	signal 13 / weighted by l-state	3D-MoRSE descriptors
Clustered	2246	Mor22s	signal 22 / weighted by l-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	2331	E1s	1st component accessibility directional WHIM index / weighted by l-state	WHIM descriptors
Clustered	2362	Di	D total accessibility index / weighted by ionization potential	WHIM descriptors
Clustered	4946	DLS_02	modified drug-like score from Oprea et al. (6 rules)	Drug-like indices
Clustered	4947	DLS_03	modified drug-like score from Walters et al. (6 rules)	Drug-like indices
Tiled	272	SIC2	Structural Information Content index (neighborhood symmetry of 2-order)	Information indices
Tiled	368	AVS_X	average vertex sum from chi matrix	2D matrix-based descriptors
Tiled	371	ChiA_X	average Randic-like index from chi matrix	2D matrix-based descriptors
Tiled	633	Chi_Dz(p)	Randic-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	SpMax2_Bh(s)	largest eigenvalue n. 2 of Burden matrix weighted by l-state	Burden eigenvalues
Tiled	1288	SpMaxA_EA(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	Eig01_AEA(dm)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
Tiled	1614	PJl3	3D Petitjean 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	2226	Mor02s	signal 02 / weighted by l-state	3D-MoRSE descriptors
Tiled	2227	Mor03s	signal 03 / weighted by l-state	3D-MoRSE descriptors
Tiled	2265	E1u	1st component accessibility directional WHIM index / unweighted	WHIM descriptors
Tiled	2274	G2m	2nd component symmetry directional WHIM index / weighted by mass	WHIM descriptors
Tiled	2320	E1i	1st component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
Tiled	2326	P1s	1st component shape directional WHIM index / weighted by l-state	WHIM descriptors
Tiled	2589	RTe+	R maximal index / weighted by Sanderson electronegativity	GETAWAY descriptors
Tiled	2636	R2s+	R maximal autocorrelation of lag 2 / weighted by l-state	GETAWAY descriptors
Boutons	272	SIC2	Structural Information Content index (neighborhood symmetry of 2-order)	Information indices
Boutons	368	AVS_X	average vertex sum from chi matrix	2D matrix-based descriptors
Boutons	371	ChiA_X	average Randic-like index from chi matrix	2D matrix-based descriptors
Boutons	633	Chi_Dz(p)	Randic-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
Boutons	635	J_Dz(p)	Balaban-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors
Boutons	1149	SpMax2_Bh(s)	largest eigenvalue n. 2 of Burden matrix weighted by l-state	Burden eigenvalues
Boutons	1317	SpMax_AEA(dm)	leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
Boutons	1576	Eig01_AEA(dm)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices
Boutons	1614	PJl3	3D Petitjean shape index	Geometrical descriptors
Boutons	2137	Mor09e	signal 09 / weighted by Sanderson electronegativity	3D-MoRSE descriptors
Boutons	2201	Mor09i	signal 09 / weighted by ionization potential	3D-MoRSE descriptors
Boutons	2208	Mor16i	signal 16 / weighted by ionization potential	3D-MoRSE descriptors
Boutons	2265	E1u	1st component accessibility directional WHIM index / unweighted	WHIM descriptors
Boutons	2274	G2m	2nd component symmetry directional WHIM index / weighted by mass	WHIM descriptors
Boutons	2320	E1i	1st component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors
Boutons	2329	G2s	2nd component symmetry directional WHIM index / weighted by l-state	WHIM descriptors
Boutons	2330	G3s	3rd component symmetry directional WHIM index / weighted by l-state	WHIM descriptors
Boutons	2589	RTe+	R maximal index / weighted by Sanderson electronegativity	GETAWAY descriptors
Boutons	4948	DLS_04	modified drug-like score from Chen et al. (7 rules)	Drug-like indices
Boutons	4953	LLS_01	modified lead-like score from Congreve et al. (6 rules)	Drug-like indices