Suppl. Section S1: Symbols and Definitions of Topological Indices used with DESMOL13[a] and MOLCONN-Z[b] programs.

Symbol	Name	Definition	Ref.
		Connectivity Indices	
${}^k\chi_t$ k=0-10 t=p,c,pc	Kier-Hall indices of order k and type path (p), cluster (c) and path-cluster (pc)	${}^k\chi_t = \sum_{j=1}^{{}^k n_t} \left(\prod_{i \in S_j} \delta_i \right)^{-1/2}$ δ_i: number of bonds, σ o π, of the atom i to non-hydrogen atoms. S_j.: jth substructure of order k and type t.	c
${}^k\chi_t{}^v$ k=0-10 t=p,c,pc	Kier-Hall indices of order k and type path (p), cluster (c) and path-cluster (pc)	${}^k\chi_t{}^v = \sum_{j=1}^{{}^k n_t} \left(\prod_{i \in S_j} \delta_i{}^v \right)^{-1/2}$ $\delta_i{}^v$: Kier-Hall valence of the atom i. S_j.: jth substructure of order k and type t.	b
${}^kD_t$ k=0-10 t=p,c,pc	Connectivity differences of order k and type path (p), cluster (c) and path-cluster (pc)	${}^kD_t = {}^k\chi_t - {}^k\chi_t{}^v$	b
${}^kC_t$ k=0-10 t=p,c,pc	Connectivity ratios of order k and type path (p), cluster (c) and path-cluster (pc)	${}^kC_t = {}^k\chi_t / {}^k\chi_t{}^v$	b
		Charge Indices	
G_k k=1-5	Topological charge indices of order k	$G_k = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left\| \mathbf{M}_{ij} - \mathbf{M}_{ji} \right\| \delta(k, \mathbf{D}_{ij})$ **M**=**A.Q**: product of the adjacency and inverse squared distance matrices for the hydrogen-depleted molecular graph. **D**: distance matrix. δ: Kronecker delta.	d
$G_k{}^v$ k=1-5	Valence topological charge indices of order k	$G_k{}^v = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left\| \mathbf{M}_{ij}{}^v - \mathbf{M}_{ji}{}^v \right\| \delta(k, \mathbf{D}_{ij})$ $\mathbf{M}^v$=$\mathbf{A}^v$**.Q**: product of the electronegativity-modified adjacency and inverse squared distance matrices for the hydrogen-depleted molecular graph. **D**: distance matrix. δ: Kronecker delta.	d
J_k, $J_k{}^v$ k=1-5	Pondered topological charge indices of order k	$J_k = \frac{G_k}{N-1}$ $\quad$ $J_k{}^v = \frac{G_k{}^v}{N-1}$	d
		Electrotopological Indices	
S(i)	Sum of electrotopological indices for a type of atom i	$S_i = I_i + \Delta I_i$ I_i: intrinsic state value of atom i. ΔI_i: perturbation of I_j on I_i with the form as $\Delta I_{ij} = (I_i - I_j)/D^2_{ij}$	e
Gmaxpos	Gmaxpos index	Maximum positive value for the	f

		electrotopological state of non-hydrogen atoms in the molecule.	
Hmaxpos	Hmaxpos index	Maximum positive value for the electrotopological state of hydrogen atoms in the molecule.	c
Molecular Properties			
N	Molecular size	Number of non-hydrogen atoms.	g
L	Length	Maximum distance between atoms in terms of bonds.	h
PR_i	PR0 a PR3	Number of pairs of ramifications separated by *i* atoms.	f
R	Ramification	Number of simple structural branches.	f
V_k k=3,4	Vertexes of grade *k*	Number of atoms with *k* bonds, σ or π, with other atoms (hydrogens not included).	f
knotp	knotp index	Difference between ${}^3\chi_c$ and ${}^4\chi_{pc}$ indices	i
knotpv	knotpv index	Difference between ${}^3\chi^v_c$ and ${}^4\chi^v_{pc}$ indices	h
numhbd	numhbd index	Number of hydrogen-donating atoms in the molecule.	h
numhba	numhbd index	Number of hydrogen-accepting atoms in the molecule.	h
Information Indices			
$I_{Shannon}$	Shannon index	Index based on the atomic diversity of the molecule.	g
NI, NI2	NI, NI2 indices	Indices based on information theory.	g
BonIdW	Bonchev IdW(G) index	Index based in the distribution of topological distances in the molecule.	j
BonIdG	Bonchev Id(G) index	Index based on the number of order 2 subgraphs in the molecule.	i
Molecular Shape Indices			
${}^n\kappa$ n=1-3	Kappa index of order *n*	${}^1\kappa = N(N-1)^2/({}^1P)^2$ ${}^2\kappa = (N-1)(N-2)^2/({}^2P)^2$ ${}^3\kappa = (N-3)(N-2)^2/({}^3P)^2$ [N even; N>3] ${}^3\kappa = (N-1)(N-3)^2/({}^3P)^2$ [N odd; N>3] N: number of non-hydrogen atoms. ${}^{1,2,3}P$: number of type path subgraphs of order 1, 2, 3.	k
${}^n\kappa_\alpha$ n=1-3	Kappa-alpha index of order *n*	${}^1\kappa = N+\alpha(N+\alpha-1)^2/({}^1P+\alpha)^2$ ${}^2\kappa = (N+\alpha-1)(N+\alpha-2)^2/({}^2P+\alpha)^2$ ${}^3\kappa = (N+\alpha-3)(N+\alpha-2)^2/({}^3P+\alpha)^2$ [N even; N>3] ${}^3\kappa = (N+\alpha-1)(N+\alpha-3)^2/({}^3P+\alpha)^2$ [N odd; N>3] N: number of non-hydrogen atoms. ${}^{1,2,3}P$: number of type path subgraphs of order 1, 2, 3. $\alpha = \Sigma[(R_i / R_{Csp3})-1]$ R_i: covalent radius for atom *i*.	l

		R_{Csp3}: covalent radius for atom Csp^3.	
Φ	Phia flexibility index	$\Phi = ({}^1\kappa_\alpha \cdot {}^2\kappa_\alpha) / N$ N: number of non-hydrogen atoms.	m
Global Topological Indices			
Sum-I	Sum of the intrinsic state values	$I_i = \frac{\delta_i^v + 1}{\delta_i}$; $Sum - I = \sum I_i$ δ_i, number of bonds, σ o π, of the atom i to non-hydrogen atoms. δ_i^v, Kier-Hall valence of the atom i.	e
Sum-ΔI	Sum of the change in intrinsic state values	$\Delta I = \frac{I_i - I_j}{r_{ij}^2}$; $Sum - \Delta I = \sum \frac{I_i - I_j}{r_{ij}^2}$ r_{ij}, number of vertexes between i and j atoms.	e
TETS2	Total electrotopological state index	Sum of all the electrotopological indices in the molecule.	e
TTd4	TTd4 index	Sum of the intrinsic state of all the atoms in the molecule.	e
nclass	Nclass index	Maximum number of topological vertices of a graph by the shortest path	n
W	Wiener index	Sum of the topological distances between all the non-hydrogen atoms by the shortest path.	o
Wp	Wiener polarity index	Number of pairs of atoms with a distance of 3 bonds.	p
Ww	Hyper-Wiener index	Sum of the topological distances and the squared topological distances between all the non-hydrogen atoms by the shortest path.	q
Wt	Total Wiener index	Sum of the topological distances between all the non-hydrogen atoms by the longest path.	r
PlattF	PlattF index	Sum of the grades of the bonds.	s

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