*Article*

# New Pharmacokinetic and Microbiological Prediction Equations to Be Used as Models for the Search of Antibacterial Drugs

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# Supplementary Section S4: Symbols and Definitions of Topological Indices used with DESMOL13[a] and MOLCONN-Z[b] programs.

| Symbol | Name | Definition | Ref. |
|---|---|---|---|
| *Connectivity Indices* | | | |
| $^k\chi_t$<br><br>$k$=0-10<br>$t$=p,c,pc | Kier-Hall indices of order $k$ and type path (p), cluster (c) and path-cluster (pc) | $^k\chi_t = \sum_{j=1}^{^k n_t}\left(\prod_{i\in S_j}\delta_i\right)^{-1/2}$<br><br>$\delta_i$: number of bonds, $\sigma$ o $\pi$, of the atom $i$ to non-hydrogen atoms.<br>$S_j$: $j$th substructure of order $k$ and type $t$. | c |
| $^k\chi_t^v$<br><br>$k$=0-10<br>$t$=p,c,pc | Kier-Hall indices of order $k$ and type path (p), cluster (c) and path-cluster (pc) | $^k\chi_t^{\;v} = \sum_{j=1}^{^k n_t}\left(\prod_{i\in S_j}\delta_i^{\;v}\right)^{-1/2}$<br><br>$\delta_i^{\;v}$: Kier-Hall valence of the atom $i$.<br>$S_j$: $j$th substructure of order $k$ and type $t$. | b |
| $^k D_t$<br>$k$=0-10<br>$t$=p,c,pc | Connectivity differences of order $k$ and type path (p), cluster (c) and path-cluster (pc) | $^k D_t = {}^k\chi_t - {}^k\chi_t^{\;v}$ | b |
| $^k C_t$<br>$k$=0-10<br>$t$=p,c,pc | Connectivity ratios of order $k$ and type path (p), cluster (c) and path-cluster (pc) | $^k C_t = {}^k\chi_t / {}^k\chi_t^{\;v}$ | b |
| *Charge Indices* | | | |
| $G_k$<br><br>$k$=1-5 | Topological charge indices of order $k$ | $G_k = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left|M_{ij}-M_{ji}\right|\delta(k,D_{ij})$<br><br>$\mathbf{M}=\mathbf{A}.\mathbf{Q}$: product of the adjacency and inverse squared distance matrices for the hydrogen-depleted molecular graph.<br>$\mathbf{D}$: distance matrix.<br>$\delta$: Kronecker delta. | d |
| $G_k^v$<br><br>$k$=1-5 | Valence topological charge indices of order $k$ | $G_k^{\;v} = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\left|M_{ij}^{\;v}-M_{ji}^{\;v}\right|\delta(k,D_{ij})$<br><br>$\mathbf{M^v}=\mathbf{A^v}.\mathbf{Q}$: product of the electronegativity-modified adjacency and inverse squared distance matrices for the hydrogen-depleted molecular graph.<br>$\mathbf{D}$: distance matrix.<br>$\delta$: Kronecker delta. | d |
| $J_k$, $J_k^v$<br>$k$=1-5 | Pondered topological charge indices of order $k$ | $J_k = \dfrac{G_k}{N-1}$ $\qquad$ $J_k^{\;v} = \dfrac{G_k^{\;v}}{N-1}$ | d |
| *Electrotopological Indices* | | | |
| S(i) | Sum of electrotopological indices for a type of atom $i$ | $S_i = I_i + \Delta I_i$<br>$I_i$: intrinsic state value of atom $i$.<br>$\Delta I_i$: 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 electrotopological state of non-hydrogen atoms in the molecule. | f |
| 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, $\sigma$ or $\pi$, 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 $n$ | $^1\kappa = N(N-1)^2/(^1P)^2$ <br> $^2\kappa = (N-1)(N-2)^2/(^2P)^2$ <br> $^3\kappa = (N-3)(N-2)^2/(^3P)^2$ [N even; N>3] <br> $^3\kappa = (N-1)(N-3)^2/(^3P)^2$ [N odd; N>3] <br> N: number of non-hydrogen atoms. <br> $^{1,2,3}P$: number of type path subgraphs of order 1, 2, 3. | k |
| $^n\kappa_\alpha$ $n$=1-3 | Kappa-alpha index of order $n$ | $^1\kappa = N+\alpha(N+\alpha-1)^2/(^1P+\alpha)^2$ <br> $^2\kappa = (N+\alpha-1)(N+\alpha-2)^2/(^2P+\alpha)^2$ <br> $^3\kappa = (N+\alpha-3)(N+\alpha-2)^2/(^3P+\alpha)^2$ [N even; N>3] <br> $^3\kappa = (N+\alpha-1)(N+\alpha-3)^2/(^3P+\alpha)^2$ [N odd; N>3] <br> N: number of non-hydrogen atoms. <br> $^{1,2,3}P$: number of type path subgraphs of order 1, 2, 3. <br> $\alpha = \Sigma[(R_i / R_{Csp3})-1]$ <br> $R_i$: covalent radius for atom $i$. <br> $R_{Csp3}$: covalent radius for atom $Csp^3$. | l |
| $\Phi$ | Phia flexibility index | $\Phi = (^1\kappa_\alpha \cdot {}^2\kappa_\alpha) / N$ <br> N: number of non-hydrogen atoms. | m |
| *Global Topological Indices* | | |
| Sum-I | Sum of the intrinsic state values | $I_i = \dfrac{\delta_i^v + 1}{\delta_i}$ ; $\text{Sum} - I = \sum I_i$ <br><br> $\delta_i$, number of bonds, $\sigma$ o $\pi$, of the atom $i$ to non-hydrogen atoms. <br> $\delta_i^v$, Kier-Hall valence of the atom $i$. | e |
| Sum-$\Delta$I | Sum of the change in intrinsic state values | $\Delta I = \dfrac{I_i - I_j}{r_{ij}^2}$ ; $\text{Sum} - \Delta I = \sum \dfrac{I_i - I_j}{r_{ij}^2}$ <br><br> $r_{ij}$, 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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