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Topology features of the 4-amino- and -carboxyquinolines derivatives

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Abstract

The study results of the topology features of 4-amino and 4-carboxyquinolines derivatives are presented. The structure of the selected research objects differs by the nature of the functional group and substituents in positions 2 and 6, which facilitates the realization of various types of intermolecular interactions. To establish the relationship between structure and properties, including chromatographic retention as molecular structure descriptors, topological indices (connectivity indices and Wiener indices) are selected. These indices are possible to correlate with different physico-chemical characteristics and properties of molecules, so they are useful for identification and prognostic goals.

The values of the connectivity indices and Wiener indices for 15 quinoline derivatives are calculated. It is shown that for the compounds studied the values of topological indices vary within a relatively wide range. At the same time, the increase in the number of atoms in the molecule is accompanied by an increase in the values of the indices, and the replacement of carbon atoms by heteroatoms leads to decrease in the corresponding quantities. The relationship between the topological and electronic characteristics of quinoline derivatives was studied. It is established that topological indices correlate well with the size physicochemical characteristics of quinoline derivatives, however, the level of such correlations turns out to be different for different indices, connectivity indices of different orders and is determined, first of all, by the structure of analyte molecules. It was found that the maximum values of the regression coefficient correspond to the correlations between the polarizability, the surface area, the volume of the molecules of the quinoline derivatives and the zero-order connectivity indices ($^0\chi$). Increasing the order of such one leads to a significant decrease in the value of the correlation coefficient. The effect of the topology of the molecules of these compounds on their retention in conditions of reversed-phase high-performance liquid chromatography using nonpolar sorbents of various chemical nature was studied. It has been demonstrated that the most important is the effect of the molecular topology on the retention of a porous graphite carbon by a flat surface. On the basis of a good level of such correlations, an assumption is made about the predictive capabilities of the dependences obtained, which can be used to predict the retention of quinoline derivatives

References

[1] M.I. Stankevich, I.V. Stankevich, N.S. Zefirov. *The Success of Chemistry*. **1988**. Vol.57. No.3. P.337-366. (russian)
[2] Chemical applications of topology and graph theory. Ed. R. King. *Moscow: Mir*. **1987**. 568p. (russian)
[3] Yu.G. Papulov, T.I. Chernova, V.M. Smolyakov, M.N. Polyakov. *Russian Journal of Physical Chemistry*. **1993**. Vol.67. No.2. P.203-209. (russian)
[4] V.I. Minkin, B.Ya. Simkin, R.M. Minyaev. Theory of the molecules structure. *R.-D.: Phoenix*. **1997**. 557p. (russian)
[5] M. Randic´. *Journal of Molecular Graphics and Modelling*. **2001**. Vol.20. P.19-35.
[6] Chunhui Lu, Weimin Guo, Chunsheng Yin. *Analytica Chimica Acta*. **2006**. Vol.561. P.96-102.

[7] S.A. Dzhabieva, I.V. Skvortsova, S.V. Kurbatova, E.A. Kolosova, and E.E. Finkelshtein. Topology of benzotriazole derivatives. *Butlerov Communications.* **2014**. Vol.38. No.6. P.8-14. ROI: jbc-02/14-38-6-8
[8] J. D. Thompson, P.W. Carr. *Analytical Chemistry***. 2002**. Vol.74. P.4150-4154.
[9] A.S. Savchenkova, S.V. Kurbatova, M.N. Zemtsova. *Sorption and Chromatographic Processes*. **2014**. Vol.14. No.3. P.468-476. (russian)
[10] A.S. Savchenkova, A.K. Buryak, S.V. Kurbatova. *Russian Journal of Physical Chemistry*. **2015**. Vol.89. No.9. P.1450-1454. (russian)
[11] E. Estrada. *J. Phys. Chem*. **2002**. Vol.106. P.9085-9091.
[12] S.A. Djabieva, S.V. Kurbatova, Z.P. Belousova, and E.E. Finkelstein. Physico-chemical characteristics of triazole derivatives sorption from aqueous acetonitrile solution. *Butlerov Communications.* **2013**. Vol.34. No.4. P.95-101. ROI: jbc-02/13-34-4-95
[13] S.V. Kurbatova. Gas chromatography of adamantine derivatives. *Samara: Samara University.* **2006**. 168p. (russian)