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Sorption and topological characteristics of taurine derivatives

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Abstract

The results of the taurine derivatives study under high-performance liquid chromatography using water-acetonitrile and nonpolar sorbents of different chemical nature (octadecylsilica gel, hyper-cross-linked polystyrene, porous graphitized carbon) as eluent, were established within the framework of quantitative "structure-property" and "structure-chromatographic retention". It is noted that the establishment of quantitative relations "structure-property" creates the prerequisites for predicting many practically significant properties and, thus, forms the basis for creating the newest materials of a given structure with the required complex of properties. The choice of taurine derivatives as research objects is due to their wide use as medicaments, at the same time it is noted that the physico-chemical properties of these compounds have been studied insufficiently, and little data on the chromatographic behavior of these compounds. The effect of the structure of taurine derivatives on the chromatographic retention in reversed-phase high-performance liquid chromatography is investigated. The effect of the nature of the substituents associated with the sulfo group in the molecules of taurine derivatives is shown, which ultimately determines the features of their chromatographic behavior. The effect of sorbent nature on the retention of these substances has been studied. On the whole, for the taurine derivatives studied, the retention factor values were minimal for sorption by ODS and increased significantly when passing to the HCPS and PGC. In this case, the simbicity in the change in the values of the retention factor, polarizability, and volume characteristic of all sorbents used was noted. Topological indices of taurine derivatives are calculated, their close relationship with the physico-chemical parameters of the molecules of the investigated substances is shown.

References

[1] R. Kaliszan. *Chem. Rev*. **2007**. Vol.107. P.3212-3246.
[2] Yu. Polyakova, K.H. Row. *Med. Chem. Res*. **2005**. 14:8/9. P.488-522.
[3] The Cambridge Structural Database. https://www.ccdc.cam.ac.uk/
[4] D.A. Filimonov, V.V. Poroykov. *Rus. Chem. J. (Zh. Rus. Chem. Soc. named after D.I. Mendeleyev)*. **2006**. Vol.50. No.2. P.66-75. (russian)
[5] A.S. Savchenkova, S.V. Kurbatova, M.N. Zemtsova. *Sorption and chromatographic processes*. **2014**. Vol.14. No.3. P.468 476. (russian)
[6] S.A. Dzhabieva, S.V. Kurbatova, Z.P. Belousova. *Rus. Journ. Phys. Chem*. **2016**. Vol.90. No.2. P.264-271. (russian)
[7] F.H. Kudasheva. *Bulletin of Bashkir State University*. **2008**. Vol.13. No.2. P.265-269. (russian)
[8] F.J. Caruso. *Agric. Food Chem*. **2004**. Vol.52. P.7279-7285.
[9] M. Zhang. *Amino Acids*. **2004**. Vol. 26. P.203-207.
[10] T. Cataldi, G.Telesca, G. Bianco. *Talanta*. **2004**. Vol.64. P.626-630.
[11] E. Tessier, L. Neirinck, Z. Zhu. *J. Chromatogr*. B. **2003**. Vol.798. P.295-302.
[12] Chemical applications of topology and graph theory. Ed. R. King. *Moscow: Mir*. **1987**. 568p. (russian)
[13] O.V. Kharitonova. Physicochemical regularities of retention of some nitrogen-containing heterocyclic derivatives in liquid chromatography. *Diss. Cand. Chem. Sci. Samara*. **2009**. 130p. (russian)
[14] L. Sojak, I. Ostrovsky, J. Janak. *J. Chromatogr*. **1987**. Vol.406. P.43.
[15] L. Sojak. *Rus. Chem. J. (Zh. Rus. Chem. Soc. named after D.I. Mendeleyev)*. **2003**. Vol.47. No.2. P.51-69. (russian)

[16] V.D. Shatz, O.V. Sahartova. High performance liquid chromatography. *Riga: Zinatne*. **1988**. 390p.
[17] Z.O. Matkina, N.A. Nekrasova, A.S. Savchenkova, M.N. Zemtsova, and S.V. Kurbatova. Topology features of the 4-amino- and -carboxyquinolines derivatives. *Butlerov Communications.* **2017**. Vol.52. No.11. P.26-34. DOI: 10.37952/ROI-jbc-01/17-52-11-26