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Effect of 1,2,4-triazole derivatives structure on their sorption by hypercarb under RP HPLC conditions

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Abstract

The results of 1,2,4-triazole derivatives studies by high-performance liquid chromatography using water-acetonitrile mixture in various volume ratios as eluent are presented. A porous graphitic carbon – hypercarb was used as a sorbent. It has been shown that the main physicochemical parameters determining the sorption of 1,2,4-triazole derivatives under the conditions of RP HPLC are the lipophilicity, polarizability and the volume of analyte molecules. At the same time, almost all the investigated substances are relatively polar, which contributes to their interaction with the components of the polar mobile phase. In general, among the derivatives of 1,2,4-triazole selected for the study, the values of the molecular volume, polarizability, lipophilicity and dipole moment vary within relatively wide limits, which leads to significant differences in the sorption characteristics of these compounds, which are also determined by the nature of the sorbent. At the same time, a symbiotic relationship was established in changing the values of the retention factor of the studied substances, their polarizability and lipophilicity. The observed deviations from the dependences obtained are due to specific interactions of sorbate molecules with the components of the mobile phase. The effect of temperature on the chromatographic retention of azoles was investigated. The sorption isotherm of 2-(1*H*-triazol-1-ylmethyl) phenol is obtained, which is almost linear in the initial part, which corresponds to the Henry region. The thermodynamic sorption characteristics of triazole derivatives have been experimentally determined. It is established that the values of changes in standard molar enthalpy and Gibbs energy of sorption during the transition of the molecules of the analyzed analytes from the bulk solution to the surface layer of the hypercarb are predominantly negative, which indicates the exothermic process and its spontaneous flow. At the same time, these values lie in a relatively narrow range and are determined mainly by the nature of the substituent and its position in the heterocycle.

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