DETERMINATION OF ELECTRONIC PROPERTIES OF TRIAZINE DERIVATIVES BY HARTREE-FOCK METHOD AND ESTIMATION OF THEIR INFLUENCE ON RETENTION BEHAVIOR IN RP-UHPLC SYSTEM

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Abstract
In this study, electronic properties of a series of *s*-triazine derivatives with acyclic and cyclic substituents were calculated by using Gaussian 16 software [1]. The Hartree-Fock method and 6-31G basis set were applied. The calculated electronic properties were the energy of Highest Occupied Molecular Orbital (HOMO), the energy of Lowest Unoccupied Molecular Orbital (LUMO) and the energy of optimal structure for each molecule. According to the HOMO energy, the compounds with acyclic and cyclic were clearly separated. Namely, compounds with cyclic substituents had higher values of HOMO energies than the compounds with acyclic substituents. Based on the LUMO energies, the compounds were not separated since the LUMO orbitals are only on the triazine ring and are energetically similar. The electronic properties were correlated with the retention parameters ($\log k_0$, $\log k$, S and C_0) of the studied compounds. The retention parameters were determined by using revered-phase ultra-high performance liquid chromatography (RP-UHPLC) with C_{18} stationary phase and mobile phase as a mixture of methanol and water [2]. The volume fraction of methanol in the mobile phase varied from 50 to 85 (v/v). The outstanding linear correlations between certain retention parameters and electronic properties were obtained, so the retention mechanism in the applied chromatographic system could be explained.

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References
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