The Enterprise of Synthesis: Strategies, Targets and Challenges

POSTER ABSTRACTS

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HPLC Enantioseparation of Structurally Related Chiral Compounds on Seven Chiral Stationary Phases and Computational Analysis of the Analyte Structures

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Today, high-performance liquid chromatographic (HPLC) analytical methods for controlling enantiomeric purity of natural or synthetic organic compounds play a key role in a research plan development. Moreover, semipreparative methods can represent a practical tool to resolve racemic mixtures. The development of a chiral method for HPLC enantioseparation can be a difficult process because the enantioselectivity of a given chiral stationary phase (CSP) for a given compound is unknown before the analysis. In addition, many types of CSPs are commercially available and some of them are very expensive. A range of strategies has been developed in order to help users in selecting the optimal operation conditions and to collect information about the chiral recognition mechanisms.

In this experimental and computational study, the chromatographic method has appeared friendly and suitable to test enantioseparability of three families of structurally related compounds (atropisomeric biphenyls, bridged polycyclic compounds and stilbene derivatives), which have been used as test probes on five polysaccharide-based, one synthetic polymer-based and one brush-type CSPs. In this context, the computational DFT geometry optimization of the analytes and the subsequent evaluation of computed electrostatic potentials proved to be able to furnish a useful rationalization of the chromatographic behaviour. This type of computational evaluation could be used to a priori collect information on the enantioseparability of a given analyte (enantio phore capability) on a given CSP.

