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Strategies, Targets and
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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

Paola Peluso,^a Davide Fabbri,^a Maria Antonietta Dettori,^a
Giovanna Delogu,^a and Sergio Cossu^b

^a *Istituto di Chimica Biomolecolare ICB CNR – UOS di Sassari, Traversa La Crucca 3, Regione Balduca, I-07100 Li Punti - Sassari, Italy*

^b *Dipartimento di Chimica, Università Ca' Foscari di Venezia, Dorsoduro 2137, I-30123 Venezia, Italy
e-mail: p.peluso@icb.cnr.it*

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.¹ 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 method² 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.³ This type of computational evaluation could be used to *a priori* collect information on the enantioseparability of a given analyte (*enantiochore capability*) on a given CSP.

¹ Lämmerhofer, M. Chiral recognition by enantioselective liquid chromatography: mechanism and modern chiral stationary phases. *J. Chromatogr. A*, **2010**, *1217*, 814-856.

² Peluso, P.; Cossu, S.; Moretto, F.; Marchetti, M. High performance liquid chromatographic enantioseparation of chiral bridged polycyclic compounds on Chiralcel OD-H and Chiralpak OT(+). *Chirality*, **2009**, *21*, 507-518.

³ Peluso, P.; Fabbri, D.; Dettori, M.A.; Delogu, G.; Zambrano, V.; Cossu, S. High-Performance liquid chromatographic enantioseparation of atropisomeric biphenyls on seven chiral stationary phases. *Current Organic Chemistry*, submitted.