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Prediction and mechanism elucidation of analyte retention on phospholipid stationary phases (IAM-HPLC) by in silico calculated physico-chemical descriptors

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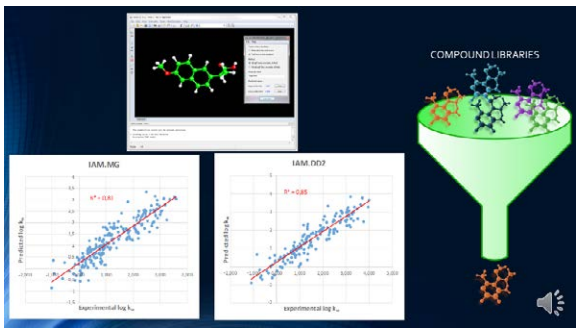
The present study proposes a method for an in silico calculation of phospholipophilicity. Phospholipophilicity is intended as the measure of analyte affinity for phospholipids; it is currently assessed by HPLC measures of analyte retention on phosphatidylcholine-like stationary phases (IAM-Immobilized Artificial Membrane) resulting in log kWIAM values. Due to the amphipathic and electrically charged nature of phospholipids, retention on these stationary phases results from complex mechanisms, being affected not only by lipophilicity (as measured by n-octanol/aqueous phase partition coefficients, log P) but also by the occurrence of polar and/or electrostatic intermolecular interaction forces. Differently from log P, to date no method has been proposed for in silico calculation of log kWIAM. The study is aimed both at shedding new light into the retention mechanism on IAM stationary phases and at offering a high-throughput method to achieve such values. A wide set of physico-chemical and topological properties were taken into account, yielding a robust final model including four in silico calculated parameters (lipophilicity, hydrophilic/lipophilic balance, molecular size, and molecule flexibility). The presented model was based on the analysis of 205 experimentally determined values, taken from the literature and measured by a single research group to minimize the inter laboratory variability; such model is able to predict phospholipophilicity values on both the two IAM stationary phases to date marketed, i.e., IAM.PC.MG and IAM.PC.DD2, with a fairly good degree (r2=0.85) of accuracy. The present work allowed the development of a free on-line service aimed at calculating log kWIAM values of any molecule included in the PubChem database, which is freely available at http://nova.disfarm.unimi.it/logkwiam.html



Biography

Giacomo Russo is a Post-doctoral Scientist in Pharmaceutical Sciences. His research field is intended to elucidate the mechanisms of drug interactions with biological membranes involved in bioavailability and distribution processes. His additional interest is in the development and validation of analytical methods aimed at determining endocrine disrupting agents in food/beverage and biological matrices.

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