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Structural properties governing retention mechanisms on RP-HPLC stationary phases used for lipophilicity measurement

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The objective of this study was to assess and compare the mechanisms of retention of two recent RP-HPLC stationary phases of interest in lipophilicity measurements, namely the silica-based Discovery RP Amide C16 phase and the polymer-based ODP-50 4B phase. A set of model solutes and drugs with well-defined solvatochromic parameters were selected to allow a broad distribution of property spaces. Linear solvation free-energy relationship (LSER) analyses have shown that the retention mechanisms of the two stationary phases are different, retention on the Discovery RP Amide C16 phase and partitioning in 1-octanol/water being controlled by the same balance of intermolecular forces (van der Waals volume V_w, H-bond acceptor basicity β and dipolarity/polarizability π^*). The chromatographic results showed that the lipophilicity index log k_w obtained with Discovery RP Amide C16 phase was more closely related to experimental log P_{oct} values than was log k_w obtained with the ODP-50 4B phase.