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# Molecular Simulation of Peptide Retention in Reversed-Phase Liquid Chromatography

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Reversed-phase high-performance liquid chromatography (HPLC) is a fundamental tool for the purification and analysis of peptides. Peptides are separated on a hydrophobic stationary phase and eluted with a gradient of increasing organic solvent concentration. The nonpolar stationary phases are most often spherical porous silica particles that have been surface derivatized with hydrocarbon chains [1]. The conditions of reversed-phase chromatography require a nonpolar stationary phase, but this condition can be met by many different ligands. In fact, there are commercially available columns of at least C1, C2, C4, Cg, C18, phenyl, and cyano functionalities, where the carbon numbers refer to the length of a fully saturated hydrocarbon chain. The most popular stationary phase for this purpose is an octadecyl carbon chain (C18)-bonded silica [2].

Here, we employ advanced molecular simulation techniques to explore the effect of surface density of the bonded stationary phase chains and mobile phase composition on the retention coefficients of peptides over C18-bonded silica. Chromatographic retention involves a process of solute transfer from a mobile phase into or onto a stationary phase. The association of the solute with the stationary phase can involve partitioning, adsorption, or both. In either case, transfer is characterized by an exchange of the environment at the surface of the solute molecule: solute is initially surrounded by neighboring mobile phase molecules and is finally surrounded, fully or partially, by neighboring molecules of the stationary phase. Our aim here is to consider how the standard-state chemical potentials may be predicted from the molecular structures of the peptide chain and solvents and external thermodynamic variables (silica surface derivatized with hydrocarbon chains.).

[1] J. G. Dorsey, K. A. Dill, Chem. Rev. 89, 331 (1989).
[2] C. A. Browne, H. P. J. Bennett, S. Solomon, Anal. Biochem. 124, 201 (1982)

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