Liquid Chromatography: Chapter 17. Quantitative Structure Property (Retention) Relationships in Liquid Chromatography

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In view of linear free-energy relationships, LFER, chromatographic systems are "free-energy transducers," translating differences in the structure of analytes into quantitative differences in physicochemical properties, like retention parameters. Hence, quantitative structure property (retention) relationships, QSP(R)R, bear valuable information on analytes and the separation systems involved. We illustrate here what can be achieved from the statistically valid and physically meaningful quantitative structure-retention relationships, QSRR. In particular, one can predict retention data, confirm identification, and optimize conditions of separation of given structurally defined analytes. Also, QSPR can shed light on the molecular mechanism of separation operating on specific stationary phases. Additionally, one can assess such properties of drug analytes of pharmacokinetic importance, like lipophilicity and acidity. Also, differences in interactions of xenobiotics with biomacromolecule components of chromatographic systems can conveniently be quantified. By means of QSRR, the chromatographic behavior of analytes in diverse separation systems can be related to their pharmacological properties.

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