Quantitative Structure-Retention Relationships Applied to Reversed-Phase High-Performance Liquid Chromatography

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Quantitative structure retention relationships (QSRRs) derived by means of various statistical procedures are reviewed from the viewpoint of identifying retention affecting structural factors and understanding the mechanism of separations. A brief summary of the theoretical background of QSRRs is followed by presentation of reversed-phase high-performance liquid chromatographic (RP-HPLC) separation theories of relevance to the reported QSRRs. Reported QSRRs equations are critically reviewed, bearing in mind their statistical significance and physical meaning. Information on retention mechanism, as extracted by factorial methods of data analysis, is briefly analyzed. QSRRs studies are demonstrated to be of value in the search for new reliable and precise descriptors of the structures of solutes of relevance to their properties, including properties other than chromatographic, e.g., bioactivity.