Quantitative Structure-Retention Relationships in Reversed-Phase High-Performance Liquid Chromatography

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A quantitative structure-retention relationships (QSRR) approach, as one of the all-important areas in modern chemical science, gives knowledge that is practical and necessary for drug design, combinatorial, and medicinal chemistries. QSRR derived by means of various statistical procedures are reviewed from the viewpoint of identifying retention affecting various factors and understanding the mechanism of chromatographic separations. Structural and physicochemical descriptors derived by reversed-phase high-performance liquid chromatography (RP-HPLC) are discussed in relation to retention factors with special accent on properties of reversed-phase materials. QSRR approaches employing molecular descriptors can model fundamental intermolecular interactions. Numerous studies are already demonstrated their great potential in most essential areas of contemporary chemistry. A quantity of scientific publications steadily grows from year to year, this implyies that the QSRR enormous advantage and potential in chemistry, biology, and pharmacology.