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Probing selectivity of mixed-mode reversed-phase / weak-anion-exchange liquid chromatography to advance method development

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Highlights

- Selectivity of mixed-mode reversed-phase/weak-anion-exchange columns were evaluated
- RP and IEX retention mechanisms were investigated for different compound classes
- A novel model combining mixed-mode retention mechanisms was proposed and validated

Abstract

The current study comprises a systematic investigation to assess retention properties and selectivity of a mixed-mode reversed-phase / weak-anion-exchange (RP/WAX) stationary phase to aid method development. Retention was investigated for different compound classes which vary in hydrophobicity, van der Waals surface area, and charge as function of organic content, pH, and ionic strength of the mobile phase. The linear-solvent-strength model was successfully applied for aromatic hydrocarbons to obtain retention-time predictions based on log *P* values and van der Waals surface area values. For phenols, predictions were based on log *P* values and data from a single scouting run performed in isocratic mode to estimate the *S* parameter; the deviations between experimental and predicted retention times were smaller than 6%. To describe the mixed-mode (RP/WAX) retention behavior of singly and doubly negatively-charged aromatic acids, a novel model combining the linear-solvent-strength and the empirical stoichiometric-displacement-net-charge models is proposed and validated. Using combinations of three scouting runs that are not linearly dependent, the maximum prediction error was 11% and changes in selectivity were correctly forecasted when altering the mobile-phase composition, *i.e.*, either organic modifier content or ionic strength. When using nine scouting runs in combination with a least-squares regression approach to determine the model parameters, the maximum prediction error was 6%.

Keywords: column characterization; retention mechanism; method development; retention-time modeling.

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