Prediction of the retention behaviors of purine and aromatic compounds in gradient-elution RP-HPLC

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The retention mechanism of solute under gradient conditions has been studied. Separation of a mixture of four purine compounds and five aromatic compounds in the binary mobile phases, water/methanol and water/acetonitrile, was considered as a practical case. Retention factors were experimentally correlated by the mobile phase composition in the mobile phase. The elution profiles were calculated by the plate theory based on the four retention mechanism of capacity factor, $\ln k = \ln k_w + SF$, $\ln k = L + MF + NF2$, $k = A + B/F$, $k = A/(1 + B*Fn)$. The experimental data expressed in terms of the calculated retention factor and peak width were used to predict the elution profile under gradient conditions. The calculated elution profiles considered by the gradient-deviation time have a good agreement with experimental data, and this mathematical model showed the feasibility of a predictive tool under gradient conditions.