Prediction of the retention time of purine compounds in linear gradient-elution RP-HPLC

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Mathematical modeling and simulation of chromatographic performances have become a necessary part of the development and design of processes. So retention models have been developed and used to predict the retention behaviors of solutes in high performance liquid chromatography. Two kinds of organic modifier, methanol and acetonitrile, are used and four purine compounds are also used as solutes. The elution profile were calculated by the plate theory based on the four retention mechanism of capacity factor, lnk=lnkw+ SF(1), lnk=L+ MF+ NF2(2), k=A+ B/F(3), k=A/(1+ B*Fn)(4). The analytical expression in terms of the calculated retention factor and peak width was presented to predict the elution profile under linear gradient conditions. From the final calculated results, the equation(3) of retention factor shows the best agreements with experimental data, and this mathematical model showed the feasibility of a predictive tool under gradient conditions.