Chemistry of wonderful wet laundering

We use two types of laundries. One is dry-cleaning which is carried out using an organic solvent, and another is wet laundering is carried out using water and soap (surfactant). These observations are scientifically applied for the separation of a variety of compounds. The separation method is called “Chromatography” that was proposed by a Polish botanist Tswett in 1906. He observed that several color pigments from a vegetable extract in a glass tube packed with calcium carbonate. Such experiment can be performed at home. You prepare a piece of white cloth or paper, ink, and liqueur. Dot the ink at one corner of cloth or paper, then dip the end in the liqueur. Liqueur moves on the sheet; then the ink follows, and the components are separated, because an ink color is a mixture of a variety of dyes and paints. When you use a polyester cloth, which is water resident, add soap (surfactant) in water to observe the moving color. The latter approach is an example of a scientific experiment, called reversed-phase ion-pair liquid chromatography.

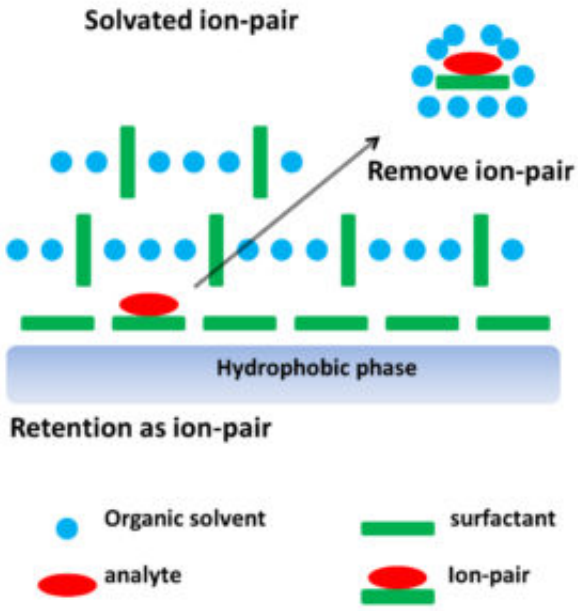

Fig. 1. Modeling of reversed-phase ion-pair liquid chromatography, where an analyte is retained by ion-pair formation; then, the paired-ion is removed by solvation.

On the other hand, the analysis of trace amounts of amino acids, the components of proteins, is a basic requirement for the biological study of human health. However, trace amount of amino acids cannot be detected, except trace amounts of sodium glutamate can be detected on our tongues. Therefore, the chemical structure of amino acids is modified with another chemical. A chemical that is often used for the continuous analysis of amino acids is phenylthiohydantoin (PTH). An automated amino acid analyzer was first developed by Edman in 1950.

The instrument used for separation of chemicals containing in biological, environmental, food, etc., is called as chromatograph. Chromatograph is a very popular analytical instrument. The separation mechanism was first proposed by Martin and Synge as “partition” in 1941, for which they later received the Nobel price. However, the chromatographic retention difference has not quantitatively explained. The basic retention mechanisms in chromatography should be “like dissolves likes” as in solution chemistry, which was proposed by Henry Freiser. However, the quantitative analysis of chromatographic retention mechanisms requires information regarding the molecular properties, which can be obtained using computational chemical calculation. Differences between chromatographic retention are based on differences in the molecular interactions between two molecules. The difference is calculated as molecular interaction energy. Comparison of molecular interaction energy values indicates which molecule is strongly retained. Molecules with stronger interactions move slowly on a sheet and/or a column either coated polymer or packed with adsorbent. This analytical method for chromatographic retention using a computational chemistry is called *in silico* chromatography.

In silico chromatography was applied for the quantitative analysis of PTH-derivatized amino acids retention in reversed-phase ion-pair liquid chromatography. Molecular interaction energy values were calculated using molecular mechanics (CAChe program from Fujitsu, Japan). The calculated molecular interaction energy values of PTH-amino acids and ion-pair reagent correlated well with the measured relative retention times (relative strength of molecular interactions) by the addition of molecular interaction energy values of a PTH-amino acid and solvent molecules. The correlation coefficient was 0.98 (n = 19). This is the first demonstration of the quantitative analysis of reversed-phase ion-pair liquid chromatographic retention mechanisms.

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