Book Review

In liquid chromatography (LC), there remain a number of important issues which should be investigated and discussed, although so many applications have appeared and their information has indicated that LC is the most powerful separation technique of various chromatographic methods. The important issues are basically three, one is the retention mechanism, another is how to improve selectivity and the third is the optimization of separation conditions. These three are related to each other but systematic establishments are required at this time because the demand for LC for more and more difficult tasks is increasing with time. The book is concerned with just these three issues and the above reasons make this book so important and valuable in LC research fields.

The understanding of the retention mechanism in LC separation processes is most difficult because the interpretation of the molecular level interactions among solutes, stationary phase and mobile phase is almost impossible at this time even though super powerful computers can be useful for the purpose. Therefore alternative approaches for the interpretation of the retention mechanism have been proposed. The most famous and useful one is "Quantitative structure-retention relationships" (QSRR) approach. Using physicochemical properties or structural descriptors, the relationships between the retention and those descriptors are studied and from the results the most dominant descriptors for the retention can be found. The mechanism can be explained by the descriptors properties. This approach is the way to estimate the mechanism but also gives us the possi-

bility of using the relationships to predict the retention of any solutes of which descriptors are known. The optimization of the separation conditions is also possible based on such retention prediction. These are discussed in a part of this book.

Chapter 1 by Smith, the editor of this book, introduces such ideas and the basic approaches for rather standard basic compounds are discussed. Using an expert system, the approach is systemized. In Chapter 2, Valko also tries to realize such QSRR approach for pharmaceutical compounds. In her chapter, the topological descriptors which are calculable, such as van der Waals volume and connectivity index are used. She also uses a multiparameter approach for the retention prediction of pharmaceutical compounds. In these approaches, the most important criteria is how to indicate "retention". Generally, in LC the capacity factor (retention factor by IUPAC recommendation) k is used but the calculation of this value is a very difficult task, because one has to know the column dead volume or dead time t_0 and the measurement of t_0 is almost impossible although many methods have been proposed. In order to standardize the retention value, Smith has proposed a retention index scale such as the gas chromatography (GC) Kovats index. In Chapter 3, the proposal of the retention index is well described.

Smith extends his discussions to supercritical fluid chromatography (SFC) and showed the applications to the relationships between the retention and biological activity (QSAR). The index seems very useful even in LC as in GC. Using the retention

index value, one can identify the peaks in LC chromatograms under the certain separation conditions. This is described in Chapter 4 by Smith. He shows the method for identification of some compounds by using the retention index scale and in this chapter he has shown that the retention index scale can give us the excellent repeatability between different laboratories. In Chapter 5, Bogusz describes the usefulness of the retention index scale for forensic and clinical applications such as drug analysis. The approach has been applied in both normal-phase and reversed-phase separation modes with isocratic and gradient elution. He extends his concept to the toxicological screening procedures. Kuronen discusses the usefulness of retention index scale in gradient LC elution in Chapter 6. He shows how to choose the standard of retention index, examines the retention behavior of index standards under isocratic and gradient elution modes and concludes with the capability of the configuration for the identification of tricothecenes.

Selectivity is the indicator of the separation power of the chromatographic separation processes and high selectivity is always required for the separation of complex mixtures which are composed of very similar compounds groups. If one has very high selectivity for particular separation problems, one does not need high efficiency for the separation column because the high selectivity can give better separation results than those obtained by a highly efficient separation system. Enhancement or improvement of selectivity is therefore the most recent requirement in modern LC separation systems. In order to realize such high selectivity, the interpretation of the molecular level interactions among the solutes, the stationary phase and the mobile phase is required. Jandera introduces an interaction index for describing the retention based on the above concept in Chapter 7. He showed the interaction index approach for binary and ternary mobile phase systems and tries to predict the retention based on the concept. He extends his idea to relate the selectivity with the interaction indices for non-homologues and homologues series compounds in reversed-phase mode. However, the interaction index is the only indicator to show the interaction between the solutes and the mobile phase, although in LC, the more dominant interaction is between the solutes and the

stationary phase. Jandera discusses such interaction in Chapter 8, where he proposes lipophilic and polar indices for the description of the retention. In reversed-phase LC, the general idea on the retention mechanism is that the hydrophobic interaction between the solute and the stationary phase alkyl ligand and therefore the lipophilic nature of the solutes is the most important in describing the retention. Polar nature is also important because in the alkyl bonded silica phase there are still silanol groups remaining on the surface and this induces the polar interaction between the solute and the stationary phase. He discusses such things in this chapter and shows the usefulness of the indices for describing the retention and the retention prediction with binary, ternary mobile phase systems and the gradient elution. In Chapter 9, West describes the solvent selectivity and the retention prediction for benzene derivatives. He tries to explain why some failure occurs with the triangle selectivity approach and then extends this approach to GC separations.

Selectivity is also the word used to indicate the differences in the interactions between the solutes and the stationary phase ligand under the same mobile phase composition and the structure of the stationary phase contributes very much to this interaction. Molecular shape selectivity is induced by such structural recognition capability based on the stationary phase structures and Sander and Wise discuss the shape selectivity for polycyclic aromatic hydrocarbons (PAHs) with octadecylsilica stationary phases (ODS) in Chapter 10. The structural difference of various types of ODS phases produces the isomeric separation of PAHs based on their molecular shape and planarity. They have proposed that shape selectivity relates to the structure of ODS phases which are grouped into three categories, monomeric, oligomeric and polymeric ODS types. They also discuss the contribution of bonding density, ligand length and bonding chemistry to this shape selectivity in reversed-phase LC separations of PAHs. Structure of the stationary phases is indeed the key factor for the retention mechanism and the selectivity and, from this standpoint, the importance of the stationary phase structure has been acknowledged.

Pesek and Williamsen discuss three types of stationary phases, monomeric ODS, other silica

based materials and other solid materials in Chapter 11. They show characterization techniques for the stationary phase structures such as solid-state nuclear magnetic resonance, infrared, thermal analysis, elemental analysis and then chromatographic characterization. Details about the difference of the materials for the chromatographic properties are also discussed. In the final chapter, Chapter 12, characterization of the reversed-phase stationary phases by computer technique, the so-called multivariate method, is discussed. Bolck and Smilde introduce the multivariate characterization method for reversed-phase stationary phases using various computer calculation techniques such as principal components analysis. They also try to predict the properties of the stationary phases with partial least squares methods. This approach seems to be more important with the development of the computer technologies and availability of the software to general LC users.

The book has substantial contents on basic and important issues in LC and through these contents, the readers can access a number of factors which are still unknown in LC. The editor has succeeded in gathering important and valuable contributions from all over the world. The proposals by all authors in this book are still in the development stage but in the near future, with the development of computer technology and analytical instrumentation, the importance of these concepts will increase and increase. The book clearly indicates what will be most important in LC separations and chromatography in the future.

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