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FOREWORD

The present volume is a blend of review articles and new papers in the area of computer-assisted method development in chromatography. This general area is addressed in three recent books[1–3] and a special issue of the *Journal of Liquid Chromatography*[4]. Why, therefore another comprehensive treatment of the subject? The answer is that the field is moving quite rapidly with significant new developments since the last summary a year ago. Also, we are now beginning to see a broad acceptance of this approach among practical method-development laboratories. Most of the preceding literature dealing with applications of computer-assisted method development has come from laboratories that have developed these *procedures*, as opposed to groups whose primary responsibility is the development of *methods* for specific samples. For this reason, the editors sought various applications in the "real" world.

The 42 papers presented here can be divided into four main categories: optimization, expert systems, special techniques and applications. Under optimization are included several invited review articles from the various groups that have been the most active in developing computer-assisted method-development procedures. These articles refer generally to mobile phase mapping or computer simulation techniques. We believe that the major approaches to optimization are dealt with here; interested readers can compare these different strategies and draw their own conclusions as to which is "best" for a given problem. As an added help in this direction, some of the authors in this section on optimization have provided meaningful comparisons of their own; *e.g.* the papers of Berridge[5] and Snyder *et al.*[6].

Expert systems that deal with various chromatographic problems appear to constitute "an idea whose time has arrived". A few presentations on this topic can be found in the period 1984–1988, but it is only within the past year that most of these expert-system papers have appeared. Much of this recent activity has been stimulated by the European ESPRIT project, but several other groups are also active in this area —as illustrated by the 13 papers on expert systems in this volume. It is apparent that the field of expert systems in chromatography is still in its early stages and should be a fruitful area for new work. Therefore, several of the following presentations on expert systems must be considered fragmentary, and by current standards even premature for publication. That is, descriptions of work in progress without final results are sometimes evident. We debated whether to accept work that fell into this category, but eventually decided to proceed in spite of these limitations. Our feeling is that even preliminary work on expert systems has redeeming value, since it provides a formal dialogue among various groups working in this area. These papers should also furnish potential users with a valuable projection of future possibilities.

Special techniques are variations on previous optimization strategies, or further work on related problems such as peak tracking or the treatment of tailing bands. Finally, the applications papers include contributions from both types of laboratories referred to above: groups whose main concern is with developing method-development techniques, and working laboratories concerned with specific samples. We felt

that papers from the latter group would be especially interesting, because these workers offer an unbiased report of how different optimization procedures work in actual practice. Toward this end, we invited various companies who provide commercial method-development software to contact their users as possible authors for this volume. While the final response fell short of what we had hoped for, there are a few papers of this type represented here. Other application papers were also contributed by groups who have developed the original software.

It is hoped that the following collection of papers will prove useful to a broad range of users of high-performance liquid chromatography, both groups involved with the continuing development of optimization procedures and expert systems, and laboratories whose main responsibility is providing high-performance liquid chromatography methods for the analysis of various samples. We feel that this field is just beginning to justify the potential that first emerged a decade ago. A number of practical problems still stand in the way of computer-assisted optimization programs, but much can now be done using these procedures. A substantial expansion of the number of people using such techniques seems quite likely, and it will be interesting in a few years to see how much farther the field has advanced.

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