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# Computer-Assisted Method Development for High-Performance Liquid Chromatography

edited by J.L. Glajch and L.R. Snyder

(Spin-off from the Journal of Chromatography Vol. 485 plus an additional chapter, index and glossary)

This book deals with the use of the computer as an aid in selecting adequate or optimum conditions for a given analytical separation. Originally published as Volume 485 of the Journal of Chromatography, it has now been reprinted in book form, since the information is so useful that many chromatographers want a copy readily available in the lab.

An extensive Introduction is added to the book edition. This surveys the field and refers to the pages where particular items are discussed in the book. The addition of a Glossary of Terms, an Author Index and a Subject Index make this book an invaluable source of easily consulted information for the practising chromatographer.

For the purpose of this book, computer-assisted method development will be limited to specific procedures which are intended to be used with a computer - rather than their manually applied precursors. In that sense, the subject can be considered to have begun around 1980.

The ongoing, intense research activity into various forms of computer assisted HPLC method development provides the assurance that this approach can really assist the practical chromatographer working in an industrial laboratory.

Contents. Introduction Chapter: Computer-assisted method development for HPLC (J.L. Glajch & L.R. Snyder). Foreword (G.L. Glajch & L.R. Snyder). Simplex optimization of HPLC separations (J.C. Berridge). Computer-assisted optimization in HPLC method development (S.N. Deming et al.). Selection of mobile phase parameters and their optimization in reversed-phase LC (H.A.H. Billiet & L. de Galan). Method development in HPLC using retention mapping and experimental design techniques (J.L. Glajch & J.J. Kirkland). Isocratic elution (L.R. Snyder et al.). Drylab computer simulation for HPLC method development. I. Isocratic elution (L.R. Snyder et al.). II. Gradient elution (J.W. Dolan et al.). Predictive calculation methods for optimization of gradient elution using binary and ternary solvent gradients (P. Jandera). Computer-assisted retention prediction for HPLC in the ion-exchange mode (Y. Baba). Multivariate calibration strategy for reversed-phase chromatographic systems based on the characterization of stationary-mobile phase combinations with markers (A.K. Smilde et al.). Computer-aided optimization of HPLC in the pharmaceutical industry (E.P. Lankmayr et al.). Comparison of optimization methods in reversed-phase HPLC using mixture designs and multi-criteria decision making (P.M.J. Coenegracht et al.). Explanations and advice provided by an expert system for system optimization in HPLC (P.J. Schoenmakers & N. Dunaand). Expert system for the selection of HPLC methods for the analysis of drugs (M. De Smet et al.). Expert system for the selection of initial HPLC conditions for the analysis of pharmaceuticals (R. Hindriks et al.). Expert system program for assistance in HPLC method development (S.S. Williams et al.). Expert system for method validation in chromatography (M. Mulholland et al.). Knowledge-based expert system for

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### 3. GENERAL TECHNIQUES

#### 3a. Apparatus and accessories

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See also 4237, 4366, 4394, 4429, 4483, 4508, 4559, 4562, 4569, 4626,  
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 194929j, 201682d, 204773v, 213556d, 218071b, 229033s,  
 229175q, 232271y, 233913w, 245341w.

See also 4230, 4236, 4239, 4242, 4248, 4272, 4373, 4374, 4379, 4380, 4381, 4385, 4388, 4396, 4406, 4567, 4638, 4686, 4823, 4915, 5072.

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## 4. SPECIAL TECHNIQUES

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## 4b. Combination of various chromatographic techniques

For additional information see:

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## 4c. Combination with other physico-chemical techniques (MS, IR etc.)

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## 19. PROTEINS

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## 3. GENERAL TECHNIQUES

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## 4. SPECIAL TECHNIQUES

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11. ORGANIC ACIDS AND LIPIDS

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See also 1964, 2052.

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## 15. TERPENES AND OTHER VOLATILE AROMATIC COMPOUNDS

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See also 2146.

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See also 2070.

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See also 1944, 2047, 2048, 2085.

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*32g. Other drug categories*

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See also 1889, 1919, 1959, 1998, 2004.

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See also 1932, 1940, 1970.

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see also 1769, 1881, 1884, 1913, 1924, 1927, 1928, 1929, 1941, 1975, 1984, 1996, 2006, 2021, 2033, 2128, 2132, 2153.

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See also 1882, 1887, 1990.

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See also 1890, 1905, 1907, 1936, 1937, 2016, 2024, 2032, 2154.

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See also 1916, 2007.

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See also 1879, 1888, 1903, 1914, 2166.

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See also 1934, 1946, 1991.

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See also 1781, 1791, 1809, 1924, 2167.

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See also 1954, 2052.

## Planar Chromatography

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See also 936.

### 2. FUNDAMENTALS, THEORY AND GENERAL

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### 3. GENERAL TECHNIQUES

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See also 933, 953, 1003, 1004.

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3d. *Quantitative analysis*

See 935.

3g. *High performance procedures*

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4. SPECIAL TECHNIQUES

4a. *Automation and computerization*

See 935.

7. PHENOLS

See 937.

8. SUBSTANCES CONTAINING HETEROCYCLIC OXYGEN

8a. *Flavonoids*

See 1028, 1029.

9. OXO COMPOUNDS, ETHERS, EPOXIDES AND QUINONES

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See also 993, 1030.

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See also 947, 955.

11d. *Lipoproteins and their constituents*

See 977.

12. ORGANIC PEROXIDES

See 1007.

13. STEROIDS

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See also 1027.

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See 960.

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See also 1021.

25. ORGANIC PHOSPHORUS COMPOUNDS (INCLUDING SUGAR PHOSPHATES)

See 990.

26. ORGANOMETALLIC AND RELATED COMPOUNDS

26a. Organometallic compounds

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#### 30b. Chloroplast and other natural pigments

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See 1027.

#### 32c. Autonomic and cardiovascular drugs

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*32i. Plant extracts*

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See also 988.

## 33. CLINICO-CHEMICAL APPLICATIONS

33b. *Complex mixtures and profiling (single compounds by cross-reference only)*

See 979, 983.

## 34. FOOD ANALYSIS

34b. *Complex mixtures (single compounds by cross-reference only)*

See 1014.

## 37. CELLS, CELLULAR PARTICLES AND SUPRAMOLECULAR STRUCTURES

See 965.

## 38. INORGANIC COMPOUNDS

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## 21. PURINES, PYRIMIDINES, NUCLEIC ACIDS AND THEIR CONSTITUENTS

## 21a. Purines, pyrimidines, nucleosides, nucleotides

See 1571, 1797.

## 21b. Nucleic acids, RNA

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## 30. SYNTHETIC AND NATURAL DYES

## 30b. Chloroplast and other natural pigments

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## 32. DRUG ANALYSIS

## 32a. Drug analysis, general techniques

See 1496.

## 33. CLINICO-CHEMICAL APPLICATIONS

## 33b. Complex mixtures and profiling (single compounds by cross-reference only)

See 1525, 1714, 1757, 1758, 1795, 1832.

## 34. FOOD ANALYSIS

## 34b. Complex mixtures (single compounds by cross-reference only)

See 1518.

## 36. SOME TECHNICAL PRODUCTS AND COMPLEX MIXTURES

## 36c. Various technical products

- 1851 Dulog, L. and Hilt, M.: (Mass transport electrophoresis of aqueous dispersions of binders and pigments). *Farbe Lack*, 95 (1989) 395-400; *C.A.*, 112 (1990) 181436w.
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## 38. INORGANIC COMPOUNDS

## 38a. Cations

See 1481.

## 38b. Anions

- 1855 Wang, D. et al.: (Determination of chloride, nitrite and iodide in water by isotachopheresis). *Shanghai Huanjing Kexue*, 8 (1989) 24-29; *C.A.*, 112 (1990) 204329e.

## 39. RADIOACTIVE AND OTHER ISOTOPE COMPOUNDS

See 1490, 1564.



## PUBLICATION SCHEDULE FOR 1990

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# Chromatography and Modification of Nucleosides

## Part C

### Modified Nucleosides in Cancer and Normal Metabolism - Methods and Applications

*Journal of Chromatography Library, 45C*

edited by **C.W. Gehrke** and **K.C.T. Kuo**, Department of Biochemistry, University of Missouri-Columbia, and Cancer Research Center, P.O. Box 1268, Columbia, MO, USA

Chromatography and Modification of Nucleosides is a four-volume work which provides state-of-the-art chromatography and analytical methods for use in a wide spectrum of nucleic acid modification research.

The focus of Part A is the presentation of advanced methods for modification research on tRNAs, mRNAs, mtRNAs, tRNAs and DNAs. HPLC-UV, GC-MS, NMR, FT-IR and affinity chromatography approaches to nucleic acid modification studies are presented, as are nucleoside, oligonucleotide and nucleic acid isolation techniques. Part B has as its central theme the modified nucleosides of tRNA and the current analytical means for studying rRNA modifications. Modified nucleoside synthesis, function, structural conformation, biological regulation, and occurrence of modification in a wide range of tRNAs are presented, as is a chapter on DNA modification and a chapter on solid phase immunoassay for determining a particular modification.

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roles of modified nucleosides in nucleic acids which will be extremely useful for workers in chromatography, molecular biology, genetics, biochemistry, biotechnology and the pharmaceutical industry.

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1. Progress and future prospects of modified nucleosides as biological markers of cancer (*R.W. Zumwalt et al.*).
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