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INCLUDING ELECTROPHORESIS AND OTHER SEPARATION METHODS

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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, miRNAs, 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.

The study of modified nucleosides in biological matrices (blood, urine) is the major thrust of Part C. As potential biological markers of disease, and for the insight that the modified nucleosides in fluids provide into the catabolism of the nucleic acids, a number of advanced methods for modified nucleoside isolation, separation, detection, characterization and measurement have been developed world-wide. Part C provides the reader with a comprehensive treatment of modified nucleosides as biochemical signals of neoplasia and normal metabolism. The final volume, Part D, will present structural characterization of unknown nucleosides as well as extensive biochemical, chemical and physical properties of RNA and DNA nucleosides, as a "database" for researchers in the field. Chromatographic methodology will be described for analysis of total modification of tRNAs and DNAs.

The chapters are written by leading scientists in their respective fields and present an up-to-date review on the

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.

Contents: Introduction. Early development of nucleoside markers for cancer (*T.P. Waalkes, C.W. Gehrke*). 1. Progress and future prospects of modified nucleosides as biological markers of cancer (*R.W. Zumwalt et al.*). 2. Ribonucleosides in biological fluids by a high-resolution quantitative RPLC-UV method (*K.C. Kuo et al.*). 3. Ribonucleosides in body fluids: On-line chromatographic cleanup and analysis by a column switching technique (*E. Schlimme, K. Siegfried-Boos*). 4. High-performance liquid chromatography of free nucleotides, nucleosides, and their bases in biological samples (*P.R. Brown, Y.-N. Kim*). 5. Isolation and characterization of modified nucleosides from human urines (*G.B. Chheda et al.*). 6. High performance liquid chromatography of modified nucleosides in human serum (*E.P. Mitchell et al.*). 7. Modified nucleosides in human blood serum as biochemical signals for neoplasia (*F. Salvatore et al.*). 8. Biochemical correlations between pseudouridine excretion and neoplasias (*F. Cimino et al.*). 9. High-performance liquid chromatography analysis of nucleosides and bases in mucosa tissues and urine of gastrointestinal cancer patients (*K. Nakano*). 10. Modified nucleosides as biochemical markers of asbestos exposure and AIDS (*O.K. Sharma, A. Fischbein*). 11. RNA catabolites in health and disease (*I. Clark et al.*). 12. Serum nucleoside chromatography for classification of lung cancer and controls (*J.E. McEntire et al.*). 13. Modified nucleosides and nucleobases in urine and serum as selective markers for the whole-body turnover of tRNA, rRNA, and mRNA-cap - Future prospects and impact (*G. Schöch et al.*). Combined Subject Index for Parts A, B and C.

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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. Dunand). 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

troubleshooting HPLC assay methods (K. Tsuji & K.M. Jenkins). Uniform shell designs for optimization in reversed-phase LC (Y. Hu & D.L. Massart). Retention prediction of analytes in reversed-phase HPLC based on molecular structure (R.M. Smith & C.M. Burr). Cathie: expert interpretation of chromatographic data (R. Milne). Prediction of retention of metabolites in HPLC by an expert system approach (K. Valkó *et al.*). Reversed-phase chromatographic method development for peptide separations using the computer simulation program ProDigest-LC (C.T. Mant *et al.*). Rule-based approach for the determination of solute types in unknown sample mixtures as a first step of optimization parameter selection in reversed-phase ion-pair chromatography (A. Bartha & G. Vigh). Rationalization of the selection of the type of the organic modifier(s) for selectivity optimization in reversed-phase ion-pair chromatography (A. Bartha *et al.*). Predicting reversed-phase gradient elution separations by computer simulation (J. Schmidt). Computer-assisted optimization with NEMROD software (G. Mazerolles *et al.*). Multi-dimensional interpolation by the moving least squares approach for modelling of chromatographic retention data (M. Otto *et al.*). Microcomputer-assisted LC separation system (MCASYS) for method development and data handling (K. Jinno *et al.*). Objective functions in experimental and simulated chromatographic optimization (R. Cela *et al.*). Optimization strategies for solutes exhibiting peak tailing (S. Sekulic & P.R. Haddad). Computer-assisted selection of the optimum gradient programme in TLC (W. Markowski). Prediction of retention times in ion-exchange chromatography (T. Sasagawa *et al.*). Solvent modulation in LC: optimization strategies (J.H. Wahl & V.L. McGuffin). Recent advances in fuzzy peak tracking in HPLC (E.P. Lankmayr *et al.*). Peak tracking in HPLC based on normalized band areas. A ribosomal protein sample as an example (I. Molnar *et al.*). Development of a HPLC method for fluroxyppy herbicide and metabolites using computer simulation with Drylab G software (R.G. Lehmann & J.R. Miller). Computer-assisted optimization of a HPLC separation for chlorpromazine and thirteen metabolites (J.S. Kiel *et al.*). Practical approach for HPLC method development: assaying synthetic intermediates of a leukotriene inhibitor (J. Fulper). Computer-assisted development of a HPLC method for fractionating selected nitro derivatives of polyaromatic hydrocarbons (D.J. Thompson & W.D. Ellenson). Reversed-phase LC retention and selectivity surfaces. II. Deoxyribonucleosides (E. Grushka *et al.*). Effects of different organic modifiers in optimization of reversed-phase HPLC gradient elution of a mixture of natural secoiridoid compounds (F. Dondi *et al.*). Optimization of gradients in anion-exchange separations of oligonucleotides using computer-assisted retention prediction and a HPLC simulation system (Y. Baba & M.K. Ito). Separation of mixtures of *o*-phthalaldehyde-derivatized amino acids by reversed-phase gradient elution (J.D. Stuart *et al.*). Glossary of terms. Author index. Subject index.

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The *Bibliography Section 1991* will be published in two volumes (560 and 561) of two issues each. Combined indexes to both volumes will appear in the last issue of the year, Vol. 561, No. 2.

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Editorial

As development is inherent to any evolving system, it is, perhaps, not surprising that our Bibliography Section must also occasionally undergo some changes. Beginning this year, the Bibliography Section will be published in two volumes per annum (Vols. 560 and 561). This will, we believe, make it more accessible. Because the various areas have changed in recent years, the individual entries can be more functionally classified and we have therefore introduced several minor changes into the classification scheme.

In the future, the classification scheme will always be included in the first issue of the first volume of the Bibliography Section in any particular year. On the other hand, the Indexes will appear only once per annum and will always form part of the last issue of the current year. We believe that most of our readers are interested in an annual survey of bibliographic data and this solution will therefore meet their demands. The sub-sections for individual entries will be preserved, according to the technique used, i.e. GC, LC, PC and ELPHO, as they have proven useful in the past.

Prague, January 1991

Z. Deyl, K. Macek

Brno, January 1991

J. Janák

CLASSIFICATION SCHEME FOR THE BIBLIOGRAPHY SECTION

Note, please, that there are considerable differences in subsections 1-4 in different techniques as these subsections deal with theory and technical aspects. Subsections 5 and beyond are identical for all different techniques.

LIQUID CHROMATOGRAPHY (LC)

1. Reviews and books
2. Fundamentals, theory and general
 - 2a. General
 - 2b. Thermodynamics and theoretical relationships
 - 2c. Relationship between structure and chromatographic behaviour
 - 2d. Measurement of physico-chemical and related values
3. General techniques
 - 3a. Apparatus and accessories
 - 3b. Detectors and detection reagents
 - 3c. Sorbents and columns, packing procedures
 - 3d. Quantitative analysis
 - 3e. Preparative scale chromatography
 - 3f. Programmed temperature, pressure, vapors, gradients
4. Special techniques
 - 4a. Automation
 - 4b. Computerization and modelling
 - 4c. Combination with other physico-chemical techniques (MS, IR etc.)
 - 4d. Affinity chromatography (advances)
 - 4e. Functional analysis
 - 4f. Trace analysis and preseparation techniques
 - 4g. Enantiomers, separation
 - 4h. Other special techniques

GAS CHROMATOGRAPHY (GC)

1. Reviews and books
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 - 2b. Thermodynamics and theoretical relationships
 - 2c. Relationship between structure and chromatographic behaviour
 - 2d. Measurement of physico-chemical and related values
3. General techniques
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 - 3b. Detectors and detection reagents
 - 3c. Sorbents and columns, packing procedures
 - 3d. Quantitative analysis
 - 3e. Preparative scale chromatography
 - 3f. Programmed temperature, pressure, vapors, gradients
4. Special techniques
 - 4a. Automation
 - 4b. Computerization and modelling
 - 4c. Combination with other physico-chemical techniques (MS, IR etc.)
 - 4d. Affinity chromatography (advances)
 - 4e. Functional analysis
 - 4f. Trace analysis and preseparation techniques
 - 4g. Enantiomers, separation
 - 4h. Other special techniques
 - 4i. Supercritical fluid chromatography

PLANAR CHROMATOGRAPHY (PC)

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 - 2d. Measurement of physico-chemical and related values
3. General techniques
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 - 3b. Detectors and detection reagents
 - 3c. Sorbents and columns, packing procedures
 - 3d. Quantitative analysis
 - 3e. Preparative scale chromatography
 - 3f. Programmed temperature, pressure, vapors, gradients
 - 3g. High performance procedures
4. Special techniques
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 - 4b. Computerization and modelling
 - 4c. Combination with other physico-chemical techniques (MS, IR etc.)
 - 4d. Affinity chromatography (advances)
 - 4e. Functional analysis
 - 4f. Trace analysis and pre-separation techniques
 - 4g. Enantiomers, separation
 - 4h. Other special techniques

ELECTROPHORESIS (ELPHO)

1. Reviews and books
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 - 2c. Relationship between structure and electrophoretic behaviour
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 - 3c. Stabilization media for electrophoresis
 - 3d. Quantitative analysis
 - 3e. Preparative scale electrophoresis
 - 3f. Programmed voltage and buffer gradients
4. Special techniques
 - 4a. Automation
 - 4b. Computerization and modelling
 - 4c. Combination with other physicochemical techniques, (MS, IR etc.)
 - 4d. Affinity electrophoresis
 - 4e. Capillary zone electrophoresis and electrokinetic chromatography
 - 4f. Isotachophoresis
 - 4g. Enantiomers, separation
 - 4h. Two dimensional electrophoresis
 - 4i. Other special techniques

SECTIONS COMMON TO ALL TECHNIQUES (LC, GC, PC and ELPHO)

For classification to sections 1-4 see individual techniques

5. Hydrocarbons and halogen derivatives
 - 5a. Aliphatic hydrocarbons
 - 5b. Cyclic hydrocarbons
 - 5c. Halogen derivatives
 - 5d. Complex hydrocarbon mixtures (incl. analysis of tars, bitumens and mineral oils)
6. Alcohols
7. Phenols
8. Substances containing heterocyclic oxygen
 - 8a. Flavonoids
 - 8b. Aflatoxins and other mycotoxins
 - 8c. Other compounds with heterocyclic oxygen (incl. tannins)
9. Oxo compounds, ethers, epoxides and quinones
10. Carbohydrates
 - 10a. Mono and oligosaccharides. Structural studies
 - 10b. Polysaccharides, mucopolysaccharides, lipopolysaccharides
 - 10c. Glycoproteins and their constituents
11. Organic acids and lipids
 - 11a. Organic acids and simple esters
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Chromatography and Modification of Nucleosides

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C.A., 113 (1990) 81636p, 81656v.

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17. AMINES, AMIDES AND RELATED NITROGEN COMPOUNDS

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18. AMINO ACIDS AND PEPTIDES; CHEMICAL STRUCTURE OF PROTEINS

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18c. Elucidation of structure of proteins and enzymes

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C.A., 113 (1990) 55044z.

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20. ENZYMES AND ENZYME ACTIVITY ESTIMATION

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C.A., 113 (1990) 55042x.

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C.A., 113 (1990) 73502b.

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5. HYDROCARBONS AND HALOGEN DERIVATIVES

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33. CLINICO-CHEMICAL APPLICATIONS

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Planar Chromatography

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19. PROTEINS

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See 100.

19f. *Structural and muscle proteins*

See 135.

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21f. *Complex mixtures of nucleic acids and their fragments*

See 388.

22. ALKALOIDS

See 20, 45.

24. ORGANIC SULPHUR COMPOUNDS (INCL. GLUCOSINOLATES)

See 20.

25. ORGANIC PHOSPHORUS COMPOUNDS (INCL. SUGAR PHOSPHATES)

See 71, 334.

26. ORGANOMETALLIC AND RELATED COMPOUNDS

26a. Organometallic compounds

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26c. Coordination compounds

See 460.

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28. ANTIBIOTICS

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32a. Drug analysis, general techniques

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See also 46.

32c. Autonomic and cardiovascular drugs

See 45, 72.

32d. *Central nervous system drugs*

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32e. *Chemotherapeutics (exc. cytostatics and antibiotics)*

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32g. *Other drug categories*

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33. CLINICO-CHEMICAL APPLICATIONS

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

- see 101, 103, 107, 109, 111, 113, 117, 120, 124, 214, 227, 249, 287, 315, 331, 341, 417.

34. FOOD ANALYSIS

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

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See also 194.

36. SOME TECHNICAL PRODUCTS AND COMPLEX MIXTURES

36c. *Complex mixtures, technical products and unidentified compounds*

See 62.

37. CELLS, CELLULAR PARTICLES AND SUPRAMOLECULAR STRUCTURES

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38. INORGANIC COMPOUNDS

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38d. Volatile inorganic compounds

See 120.

PUBLICATION SCHEDULE FOR 1991

Journal of Chromatography and Journal of Chromatography, Biomedical Applications

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Artificial Intelligence in Chemistry

Structure Elucidation and Simulation of Organic Reactions

by **Z. Hippe**, *Department of Physical and Computer Chemistry,
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(Studies in Physical and Theoretical Chemistry, 73)

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