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INCLUDING ELECTROPHORESIS, MASS SPECTROMETRY AND OTHER SEPARATION AND DETECTION METHODS

JOURNAL OF CHROMATOGRAPHY B

ANALYTICAL TECHNOLOGIES IN THE BIOMEDICAL AND LIFE SCIENCES

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JOURNAL OF CHROMATOGRAPHY

INSTRUCTIONS TO AUTHORS

Scope

Journal of Chromatography A

including electrophoresis, mass spectrometry and other separation and detection methods

The *Journal of Chromatography A* publishes papers on all aspects of separation science including chromatography, electrophoresis, hyphenated and other multi-dimensional techniques, sample preparation as well as detection methods such as mass spectrometry. Contributions consist mainly of research papers dealing with chromatographic and electrophoretic theory, instrumental developments and their analytical and preparative applications.

Journal of Chromatography B analytical technologies in the biomedical and life sciences

The Journal of Chromatography B addresses advancements in and applications of analytical methodologies related to drugs, other biologically active compounds, metabolites, biomarkers as well as to bio-polymers such as proteins, peptides, nucleic acids and glycans. The areas considered include:

- clinical analysis, therapeutic drug monitoring, pharmaceutical analysis toxicological analysis, bio-environmental analysis and novel approaches to sample
 preparation in analysis of biological matrices
- the qualitative and quantitative analysis of biopolymers including proteins, peptides and their post-translational modifications as well as nucleic acids and glycans
- the screening and profiling of body fluids, tissues, biological matrices and system related to monitoring the level of active substances, including metabolities, biomarkers and toxicants
- the comparative analysis of biological systems using proteomics, genomics, metabonomics and other "omics" including novel ways of data handling and interpretation
- preparative aspects related to separation and isolation of bioactive compounds including biopolymers

Analytical techniques covered include the various facets of chromatography, electrophoresis and related methods, including mass spectrometry and affinity-based methodologies.

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- [4] A. Veide, C. Hassinen, D. Hallen, M. Eiteman, B. Lassen, K. Holmbert, in R.D. Rogers, M.A. Eiteman (Editors), Proceedings of the American Chemical Society Symposium on Aqueous Biophasic Separation. Plenum Publishers, New York, NY, 1995, p. 133.

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Appendix 1: Experimental conditions to be specified

Experimental conditions should preferably be given on a separate sheet, headed "Conditions". These conditions will, if appropriate, be printed in a block, directly following the heading "Experimental".

General

Chemicals. Supplier (+ city/town, state, country) and degree of purity of all less common chemicals; EC number of enzymes; optical purity of enantiomers. Equipment. Model and manufacturer (+ city/town, state, country) of commercial instruments (e.g. chromatographs and detectors). For instruments that are not commercially available, sufficient detail (or a reference) should be given to allow others to construct their own instrument. Detection parameters (e.g. type, wavelength, attenuation, linearity range, limit of detection at a specified signal-to-noise ratio).

Sample preparation. Application papers should contain full details (or a reference) of the method of sample preparation. For centrifugation steps, give details of g value and time. Injection device and volume and concentration of the injected sample should be specified.

Column liquid chromatography

Column. Column dimensions (length × internal diameter), manufacturer and location, packing material (for non-commercial columns or columns that are not widely used the chemical composition should be specified), particle diameter, pore diameter, column temperature.

Mobile phase. Complete and unambiguous description of the mobile phase composition or procedure for its preparation; pH; flow-rate; gradient programme. k values. When reporting values, the method for determining the hold-up time (t_0) must be described.

Gas chromatography and supercritical fluid chromatography

Column. In addition to the parameters mentioned for column liquid chromatography, specify type of column (packed, capillary, etc.) support material, film thickness of the stationary phase, and surface modification, if applicable.

Carrier gas. Type, purity, flow-rate or inlet pressure (bar or MPa).

Temperature. All relevant temperatures (or temperature programmes) should be detailed.

Planar chromatography

Chamber. Internal dimensions, manufacturer and location, saturation, temperature, humidity.

Thin layer or paper. Manufacturer and location, material, dimensions, type (laboratory-prepared or commercially precoated) and thickness of layer, additives (fluorescent indicator, binder), position of starting line, development mode, method of activation.

Solvent. Composition of solvent, monophasic or upper or lower phase of two-phase mixture, total volume.

Sample. Application method, size of spot or streak, solvent and amount of solute and volume of solution applied.

Detection. Spray reagent, wavelength, details of colours, R_F values.

Electrophoresis

Matrix. For example, cellulose acetate, agarose, polyacrylamide; gel concentration; percentage cross-linker; dimensions and material of tube, sheet, etc., surface modification, length between column inlet and detector, temperature.

Buffers. Complete and unambiguous description of buffers used, pH and how the pH was set or adjusted.

Other. Injection method, voltage, current. In electropherograms, anode and cathode should be indicated.

Mass spectrometry

Inlet system. Direct on-line, off-line, postcolumn splitting, postcolumn buffer or matrix addition.

Source. Ionization energy, temperature, trap current, reagent gas. For LC interfaces, complete and unambiguous description of the same and their operating parameters (vaporizer and capillary temperature, buffers, nebulizing, auxiliary or ionizing gases, gas pressures, source and interface voltages, up-front CID voltages.

Mass analyzer. Accelerating voltage, scan mode, collision gas for tendem MS work, collision gas pressure, collision energy, resolution and mass range. Detection. Electron multiplier voltage and/or electrometer gain, ions monitored in SIM and dwell times.

Appendix 2: Conversion table for the non-SI units most frequently used

The use of some non-SI units has been accepted for practical reasons; to this category belong units for time (min, h), volume (1), pressure (1 bar = 10^5 Pa), temperature (°C), energy (1 eV $\approx 160 \, 219 \cdot 10^{-21}$ J), mass (1 u $\approx 1.66053 \cdot 10^{-27}$ kg) and activity (1 Ci = $3.7 \cdot 10^{10}$ Bq). This journal also accepts Å (= 0.1 nm). Concentration should formally be expressed in mol dm⁻³ or mol 1⁻¹, but the symbol M is accepted; normality (N) should not be used, however. The frequently used "daltons" are not compatible with the SI system — the relative molecular mass (M_r) should be given as a value only (dimensionless). Gravitational force must be expressed in g; rpm is not allowed for centrifugation (but it is, e.g., for vortex mixing). The table below summarizes some conversion factors; to obtain the value in SI units, the value in non-SI units should be multiplied by the factor.

Physical quantity	Type of conversion	Factor
Length	in. \rightarrow cm	2.54
	$ft. \rightarrow cm$	30.4801
Area	$in.^2 \rightarrow cm^2$	6.451626
Mass	lb. \rightarrow kg	0.45359237
Volume	gallon (USA) $\rightarrow 1$	3.785332
	gallon $(UK) \rightarrow 1$	4.54609
Pressure	$atm \rightarrow Pa$	101 325
	mmHg or Torr \rightarrow Pa	133.322
	$mmH_2O \rightarrow Pa$	9.80665
	$kp cm^2 \rightarrow Pa$	98066.5
	lbs. in. $^{-2}$ or p.s.i. \rightarrow Pa	6894.76

Other frequently used non-SI "units" are ppm, ppb and ppt. When used in this journal, the American billion (10⁹) and trillion (10¹²) are meant. The use of ppm, ppb and ppt is only permitted if they refer to mass/mass or volume/volume ratios; they should **not** be used for mass/volume ratios. The first time such a "unit" appears in an article, it should be indicated whether it refers to mass/mass or to volume/volume.

Appendix 3: Abbreviations and symbols that may be used without definition

Abbreviations and symbols should not be used in article titles. Please note that most abbreviations should only be used in combination with a value, or in structural formulae.

Abbreviations

A, C, G, T adenine, cytidine, guanine, thymine

Ac, OAc acetyl, acetate A/D analog-to-digital

ADP, AMP, ATP, and similar adenosine 5'-di-, -mono-, triphosphate, etc.

nucleoside phosphates

alternating current a.c.

standard 3- and 1-letter codes amino acids

absorbance units ΑU

BET Brunauer—Emmett—Teller

boiling point b.p. Bu butyl

cpm counts per minute CE capillary electrophoresis

d, m, p, r, t (in nucleosides/ deoxy, messenger, phosphate, recombinant/ ribosomal, transfer

nucleotides/nucleic acids)

direct current d.c.

DDD, DDT, DDE di-, trichloro-bis(chlorophenyl)ethane, -ethylene DEAE diethylaminoethyl

deoxyribonucleic acid, deoxyribonuclease DNA, DNase Dns, dansyl 5-dimethylaminonaphthalene-1-sulfonyl

DOPA 3,4-dihydroxyphenylalanine dpm desintegrations per minute

EC enzyme commission numbering system **EDTA** ethylenediaminetetraacetate, -acetic acid

equivalent equiv. Et ethyl FS full scale

FSOT fused-silica open tubular FT Fourier transform

GC, GLC, GSC gas chromatography, gas-liquid chromatography, gas-solid chromatography

HP... high-performance... internal diameter I.D. immunoglobulin G IgG intramuscular i.m. i.p. intraperitoneal IR infrared

I.S. internal standard I.U. international unit i.v. intravenous

LC liquid chromatography

LD lethal dose
Me methyl
m.p. melting point
MS mass spectrometry

NAD, NADH (NADP, NADPH) nicotinamide—adenine dinucleotide (phosphate)

NMR nuclear magnetic resonance

O.D. outer diameter Ph phenyl Pr propyl

PTFE poly(tetrafluoroethylene) RNA, RNase ribonucleic acid, ribonuclease

RP... reversed-phase... rpm revolutions per minute

RSD relative standard deviation (preferred over coefficient of variation)

SD standard deviation
TLC thin-layer chromatography
Tris tris(hydroxymethyl)aminomethane

u atomic mass units (reference to mass of ¹²C; preferred over a.m.u./amu:

reference to mass of ¹⁶O)

UV ultraviolet

vol., v/v volume, volume/volume

Vis visible

WCOT wall-coated open tubular wt., w/w, m/m mass, mass/mass

Symbols

 $\begin{array}{lll} A & & \text{peak area or absorbance} \\ \alpha & & \text{separation factor} \\ D & & \text{diffusion coefficient} \\ d_{\text{f}} & & \text{film thickness} \\ d_{\text{p}} & & \text{particle diameter} \end{array}$

 ε interparticle porosity or molar adsorptivity

F mobile phase flow-rate

 ΔG^0 standard Gibbs free energy change

 ΔH^0 standard enthalpy change

H plate height
h reduced plate height
J coupling constant
K equilibrium constant
k retention factor

 $K_{\rm c}$ distribution constant (preferred over partition coefficient)

L length λ wavelength

 $\begin{array}{ll} \textit{M}_{r} & \text{(relative) molecular mass} \\ \mu & \text{electrophoretic mobility} \\ \textit{N} & \text{number of plates} \\ \textit{n} & \text{number of determinations} \end{array}$

 η viscosity

p pressure or probability
P relative pressure

p... negative logarithm of... (as in pH, pI, p K_a) r relative retention or correlation coefficient

R molar gas constant R_F retardation factor R_M log $(1/R_F-1)$ R_S resolution ρ density

 ΔS^0 standard entropy change S/N signal-to-noise ratio T temperature

time

 t_0 retention time of unretained compound

 $t_{\rm R} \ (t'_{\rm R})$ (adjusted) retention time u mobile phase velocity

 V_0 retention volume of unretained compound

 $V_{\rm R}$ ($V_{\rm R}'$) (adjusted) retention volume $w_{\rm b}$ peak width at base $w_{\rm h}$ peak width at half height

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