### ${\bf (19)}\ World\ Intellectual\ Property\ Organization$

International Bureau



# ) | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1881 | 1

(43) International Publication Date 25 November 2004 (25.11.2004)

**PCT** 

# (10) International Publication Number WO 2004/102180 A3

(51) International Patent Classification H01J 49/00

(21) International Application Number:

PCT/GB2004/002059

(22) International Filing Date: 13 May 2004 (13.05.2004)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:

0311225.7 15 May 2003 (15.05.2003) GB 0312095.3 27 May 2003 (27.05.2003) GB

(71) Applicant (for all designated States except US): ELECTROPHORETICS LIMITED [GB/GB]; Coveham House, Downside Bridge Road, Cobham, Surrey KT11 3EP (GB).

(72) Inventors; and

- (75) Inventors/Applicants (for US only): BAUER, Ute [DE/DE]; Sandweg 129, 60316 Frankfurt am Main (DE). MORAGA-MARTINEZ, Roger, Alfonso [ES/DE]; Bleichstrasse 6, 60313 Frankfurt am Main (DE). SCHWARZ, Josef [DE/DE]; Voelklinger Weg 7, 60529 Frankfurt (DE).
- (74) Agents: HILL, Christopher, Michael et al.; Page White & Farrer, 54 Doughty Street, London WC1N 2LS (GB).
- (81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM,

AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

#### **Published:**

- with international search report
- before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments
- (88) Date of publication of the international search report: 19 January 2006

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: MASS SPECTROMETRY

(57) Abstract: Provided is a method for processing data from a mass spectrum generated from a sample, which method comprises: (a) selecting a first peak in the mass spectrum; (b) selecting a first monoisotopic reference ion having a first charge state, which first reference ion could contribute to the first peak; (c) for one or more other isotopic forms of the first reference ion determining one or more further expected peaks in the mass spectrum; (d) comparing one or more of the determined further expected peaks with the mass spectrum to determine whether there are one or more peaks present in the spectrum that match the one or more determined further expected peaks; (e) if one or more of the determined further expected peaks match one or more of the peaks in the mass spectrum, designating the first peak as a data peak, and optionally designating the one or more peaks present in the spectrum that match the one or more determined further expected peaks as data peaks; (f) if the determined further expected peaks do not match peaks in the mass spectrum, repeating steps (b) to (e) with one or more further reference ions in one or more further charge states; (g) optionally if the first peak cannot be designated as a data peak for a reference ion in the first charge state, or for a further reference ion in the further charge states, designating the first peak as a non-data peak; (h) optionally repeating steps (a) - (g) for one or more further peaks in the mass spectrum.



WO 2004/102180

#### INTERNATIONAL SEARCH REPORT

al Application No PCT/GB2004/002059

# A. CLASSIFICATION OF SUBJECT MATTER H01J49/00

According to International Patent Classification (IPC) or to both national classification and IPC

#### **B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols) H01J

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, INSPEC, COMPENDEX

	ENTS CONSIDERED TO BE RELEVANT		Delevent to plain No		
Category °	Citation of document, with indication, where appropriate, of the	relevant passages	Relevant to claim No.		
X	WEHOFSKY M ET AL: "Automated deconvolution and deisotoping of electrospray mass spectra"  JOURNAL OF MASS SPECTROMETRY, WICHICHESTER, GB, vol. 37, 2002, pages 223-229, XISSN: 1076-5174  pages 223-225; figures 1,2	ILEY,	1-3,5-8, 11-24,26		
X Furt	her documents are listed in the continuation of box C.	χ Patent family members are listed	in annex.		
"A" docume consic "E" earlier (filing c) "L" docume which citatio "O" docume other ("P" docume)	ent defining the general state of the art which is not lered to be of particular relevance document but published on or after the international date ent which may throw doubts on priority claim(s) or is cited to establish the publication date of another n or other special reason (as specified) ent referring to an oral disclosure, use, exhibition or means ent published prior to the international filling date but han the priority date claimed	"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention  "X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone  "Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.  "&" document member of the same patent family			
	actual completion of the international search  1 November 2005	Date of mailing of the international sea 25/11/2005	Date of mailing of the international search report 25/11/2005		
Name and i	mailing address of the ISA  European Patent Office, P.B. 5818 Patentlaan 2  NL – 2280 HV Rijswijk  Tel. (+31–70) 340–2040, Tx. 31 651 epo nl,  Fax: (+31–70) 340–3016	Authorized officer  Loiseleur, P			

### INTERNATIONAL SEARCH REPORT

1 31 Application No PCT/GB2004/002059

Category °	ation) DOCUMENTS CONSIDERED TO BE RELEVANT  Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Calegory *	Organori or document, with indication, where appropriate, or the rolevant passages	
X	ZHANG Z ET AL: "A Universal Algorithm for Fast and Automated Charge State Deconvolution of Electrospray Mass-to-Charge Ratio Spectra" JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY, ELSEVIER SCIENCE INC, US, vol. 9, no. 3, March 1998 (1998-03), pages 225-233, XP004112012 ISSN: 1044-0305 pages 228-229; figure 3	1,23
(	BREEN E J ET AL: "AUTOMATIC POISSON PEAK HARVESTING FOR HIGH THROUGHPUT PROTEIN IDENTIFICATION" ELECTROPHORESIS, WEINHEIM, DE, vol. 21, June 2000 (2000-06), pages 2243-2251, XP001040008 ISSN: 0173-0835 the whole document	1,9,10,
X	US 6 147 344 A (ANNIS ET AL) 14 November 2000 (2000-11-14) columns 4-7 columns 9-10; figure 9	1,4,23,

## INTERNATIONAL SEARCH REPORT

Information on patent family members

PCT/GB2004/002059

	Patent document cited in search report		Publication date		Patent family member(s)	Publication date
	US 6147344	A	14-11-2000	AU CA EP JP WO US	6429199 A 2346959 A1 1138056 A1 2002527756 T 0022649 A1 6581013 B1	01-05-2000 20-04-2000 04-10-2001 27-08-2002 20-04-2000 17-06-2003
-						