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(54) Title: MACROMOLECULE IDENTIFICATION MADE BY MASS SPECTROMETRY AND DATABASE SEARCHING

(57) Abstract: A method of determining the parent ion charge state of a tandem MS spectrum. The parent ion is labeled with a probe that is cleaved as a result of the MS. A candidate parent ion charge state is chosen and the spectrum is searched for a peak having a value F, where F is the ratio between (i) the mass of the parent ion minus the mass of the cleaved probe and (ii) the difference between the candidate parent ion charge state and the charge of the cleaved probe. A method of removing a parent ion mass dependence and a parent ion charge dependence from a cross correlation score between a predicted spectrum and an experimental spectrum. A method of computing a false positive gamma distribution curve for a data set of tandem MS spectra. A method of reducing a number of false positive assignments made to tandem microcopy spectra in a tandem MS data set. In this method, the spectra are processed in a manner that is based on the presence or absence of peak fragments within the spectra.

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INTERNATIONAL SEARCH REPORT

International application No.
PCT/US04/04016

A. CLASSIFICATION OF SUBJECT MATTER
 IPC(7) : G01N33/00; G06F17/11,50
 US CL : 438/89, 94,173, 702/19,23,30
 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)
 U.S. : 438/89, 94,173, 702/19,23,30

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 practicable, search terms used)
 Please See Continuation Sheet

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	US 5,073,713 (SMITH et al) December, 1991	1-13


Further documents are listed in the continuation of Box C. See patent family annex.

* Special categories of cited documents:	
"A" document defining the general state of the art which is not considered to be of particular relevance	"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
"E" earlier application or patent published on or after the international filing date	"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
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"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
"O" document referring to an oral disclosure, use, exhibition or other means	"&" document member of the same patent family
"P" document published prior to the international filing date but later than the priority date claimed	

Date of the actual completion of the international search
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INTERNATIONAL SEARCH REPORT

International application No.

PCT/US04/04016

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:
Please See Continuation Sheet

1. As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.
 2. As all searchable claims could be searched without effort justifying additional fees, this Authority did not invite payment of any additional fees.
 3. As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

 4. No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.: 1-13
- Remark on Protest**
- The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.
 - The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.
 - No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US04/04016

BOX III. OBSERVATIONS WHERE UNITY OF INVENTION IS LACKING

Group I, claims 1-13, drawn to method of determining parent ion charge state for MS spectrum.

Group II, claims 14-32, drawn to method for computing cross correlation score between MS spectra.

Group III, claims 33-39,50-55, drawn to method of computing false positive gamma distribution.

Group IV, claims 40-49, drawn to method for reducing false positive assignments.

The claims of Group II are individually or dependently directed to a two groups of disclosed patentably distinct species of the generic invention. The claims of the Group are individually or dependently directed to a plurality of disclosed patentably distinct species of method of calculation of correlation score (as in claims 14-24 and claims 25-29).

The inventions listed as Groups I-IV do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features for the following reasons: Each of the Groups I-IV claim a distinct and separate method (Gr. I - method of determining parent ion charge state; Group II -method for computing cross correlation score; Group III - method of computing false positive gamma distribution; Group IV - method for reducing false positive assignments). The methods do not share a special technical feature because each method contains specific and unique method steps which are not shared by each of the other methods and each method has a unique and distinct outcome. Thus, groups I-IV do not share a corresponding special technical feature.

The species listed above do not relate to a single inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, the species lack the same or corresponding special technical features for the following reasons:

The methods of 14-24 and 25-29 utilize different methods of calculating cross correlation score.

Continuation of B. FIELDS SEARCHED Item 3: