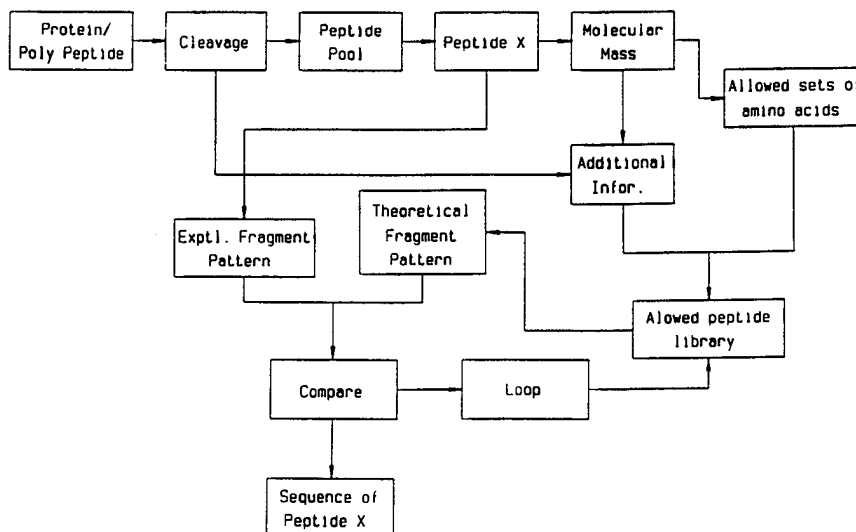




## INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

<p>(51) International Patent Classification <sup>6</sup> : <b>G01N 33/68</b></p>	<p><b>A3</b></p>	<p>(11) International Publication Number: <b>WO 98/53323</b></p> <p>(43) International Publication Date: 26 November 1998 (26.11.98)</p>
<p>(21) International Application Number: PCT/GB98/01486</p> <p>(22) International Filing Date: 22 May 1998 (22.05.98)</p> <p>(30) Priority Data: 9710582.9 22 May 1997 (22.05.97) GB</p> <p>(71) Applicant (for all designated States except US): OXFORD GLYCOSCIENCES (UK) LTD. [GB/GB]; 10 The Quadrant, Barton lane, Abingdon Science Park, Abingdon OX14 3YS (GB).</p> <p>(72) Inventors; and (75) Inventors/Applicants (for US only): PAREKH, Raj, Bhikhu [GB/GB]; Alchester House, Langford Lane, Nr Wendlebury, Oxfordshire OX6 0NS (GB). PRIME, Sally, Barbara [GB/GB]; Sunnybrook, 37 North Hinksey Village, Oxford OX2 0NA (GB). WEDD, Nick, Sinclair [GB/GB]; Sunnybrook, 37 North Hinksey Village, Oxford OX2 0NA (GB). TOWNSEND, Robert, Reid [US/GB]; 33 Norreys Avenue, Oxford OX1 4ST (GB).</p> <p>(74) Agent: GILL JENNINGS &amp; EVERY; Broadgate House, 7 Eldon Street, London EC2M 7LH (GB).</p>	<p>(81) Designated States: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG).</p> <p><b>Published</b> <i>With international search report.</i></p> <p>(88) Date of publication of the international search report: 11 March 1999 (11.03.99)</p>	

(54) Title: A METHOD FOR DE NOVO PEPTIDE SEQUENCE DETERMINATION



## (57) Abstract

A method for determining the amino acid sequence of an unknown peptide comprising (a) determining a molecular mass and an experimental fragmentation spectrum for the unknown peptide; (b) comparing the experimental fragmentation spectrum of the unknown peptide to theoretical fragmentation spectra calculated for a peptide library composed of all possible linear sequences of amino acids having a total mass that corresponds to the molecular mass of the unknown peptide; and (c) identifying a peptide in the peptide library having a theoretical fragmentation spectrum that matches most closely the fragmentation spectrum of the unknown peptide.

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# INTERNATIONAL SEARCH REPORT

International Application No

PCT/GB 98/01486

**A. CLASSIFICATION OF SUBJECT MATTER**

IPC 6 G01N33/68

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)

IPC 6 G01N

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)

**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	US 5 470 753 A (SEPETOV NIKOLAI ET AL) 28 November 1995 see column 1, line 53 - column 2, line 32 see column 3, line 32 - line 39 ---	1-16
X	US 5 538 897 A (YATES III JOHN R ET AL) 23 July 1996 cited in the application see the whole document ----- -/--	1-16



Further documents are listed in the continuation of box C.



Patent family members are listed in annex.

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- "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.
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Date of the actual completion of the international search

26 October 1998

Date of mailing of the international search report

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## INTERNATIONAL SEARCH REPORT

International Application No

PCT/GB 98/01486

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	MEDZIHRADSKY K F ET AL: "Peptide Sequence Determination by Matrix-Assisted Laser Desorption Ionization Employing a Tandem Double Focusing Magnetic-Orthogonal Acceleration Time-of-Flight Mass Spectrometer" JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY, vol. 7, no. 1, January 1996, page 1-10 XP004051936 see page 7 - page 8 ---	1-16
A	MEDZIHRADSKY K F ET AL: "Protein sequence and structural studies employing matrix-assisted laser desorption ionization-high energy collision-induced dissociation" INTERNATIONAL JOURNAL OF MASS SPECTROMETRY AND ION PROCESSES, vol. 160, no. 1, January 1997, page 357-369 XP004058842 see the whole document ---	1-16
A	MANN M ET AL: "ERROR-TOLERANT IDENTIFICATION OF PEPTIDES IN SEQUENCE DATABASES BY PEPTIDE SEQUENCE TAGS" ANALYTICAL CHEMISTRY, vol. 66, no. 24, 15 December 1994, pages 4390-4399, XP000573399 see the whole document ---	1-16
A	WO 95 25737 A (PENN STATE RES FOUND ;BENKOVIC STEPHEN J (US); WINOGRAD NICHOLAS ( ) 28 September 1995 see the whole document ---	11
A	J A BOUTIN, P HENNIG, P-H LAMBERT, S BERTIN, L PETIT, J-P MAHIEU, B SERKIZ, J-P VOLLAND, J-L FAUCHÈRE: "Combinatorial Peptide Libraries: Robotic Synthesis and Analysis by Nuclear Magnetic Resonance, Mass Spectrometry, Tandem Mass Spectrometry, and High-Performance Capillary Electrophoresis Techniques" ANALYTICAL BIOCHEMISTRY, vol. 234, 1996, pages 126-141, XP002081905 see the whole document ---	1-16
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**INTERNATIONAL SEARCH REPORT**

International Application No  
PCT/GB 98/01486

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT		
Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>R S YOUNGQUIST, G R FUENTES, M P LACEY, T KEOUGH: "Generation and Screening of Combinatorial Peptide Libraries Designed for Rapid Sequencing by Mass Spectrometry" JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, vol. 117, no. 14, 1995, pages 3900-3906, XP002081906 see the whole document -----</p>	1-16
A	<p>M A KELLY, H LIANG, I-I SYTWU, I VLATTAS, N L LYONS, B R BOWEN, L P WENNOGLE: "Characterization of SH2-Ligand Interactions via Library Affinity Selection with Mass Spectrometric Detection" BIOCHEMISTRY, vol. 35, no. 36, 1996, pages 17747-11755, XP002081907 see the whole document -----</p>	1-16

# INTERNATIONAL SEARCH REPORT

International application No.

PCT/GB 98/ 01486

## Box I Observations where certain claims were found unsearchable (Continuation of item 1 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.: 17, 18  
because they relate to subject matter not required to be searched by this Authority, namely:  
Rule 39.1(v) PCT-Presentation of information  
Rule 39.1(iii) PCT-Scheme, rules and method for performing mental acts  
Rule 39.1(vi) PCT -
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 II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

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 an additional fee, this Authority did not invite payment of any additional fee.
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.:

### Remark on Protest

- The additional search fees were accompanied by the applicant's protest.
- No protest accompanied the payment of additional search fees.

# INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No PCT/GB 98/01486
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Patent document cited in search report	Publication date	Patent family member(s)	Publication date
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