

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
18 December 2003 (18.12.2003)

PCT

(10) International Publication Number
WO 2003/104824 A3

(51) International Patent Classification⁷: **G01N 33/53**

(21) International Application Number:
PCT/US2003/017739

(22) International Filing Date: 5 June 2003 (05.06.2003)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
60/386,896 5 June 2002 (05.06.2002) US
60/453,504 9 March 2003 (09.03.2003) US

(71) Applicant (for all designated States except US): **PHARMACIA & UPJOHN COMPANY** [US/US]; 301 Henrietta Street, Kalamazoo, MI 49001 (US).

(72) Inventor; and

(75) Inventor/Applicant (for US only): **DALVIT, Claudio** [IT/IT]; Via G.C. Procaccini, 23, I-20154 Milan (IT).

(74) Agent: **MUETING, Ann, M.**; Muetting, Raasch, Gebhardt, P.A., P.O. Box 581415, Minneapolis, MN 55458-1415 (US).

(81) Designated States (*national*): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, 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, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (*regional*): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR), OAPI patent (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:
26 August 2004

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: METHODS FOR IDENTIFYING LIGANDS USING WATERLOGSY NMR

(57) Abstract: A method of identifying a ligand to a target molecule that includes: providing a reference compound that interacts with the target molecule; collecting a WaterLOGSY nuclear magnetic resonance spectrum of the reference compound in the presence of the target molecule; providing a test sample comprising at least one test compound; collecting a WaterLOGSY nuclear magnetic resonance spectrum of the reference compound in the presence of the test sample and the target molecule; and comparing the WaterLOGSY spectra to determine if at least one test compound interacts with the target molecule with a binding affinity tighter than that of the reference compound.



WO 2003/104824 A3

INTERNATIONAL SEARCH REPORT

International application No.

PCT/US03/17739

A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) : G01N 33/53
US CL : 435/7.1

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. : 435/7.1

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)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X,E	US 6,677,160 A (STOCKMAN et al.) 13 January 2004, see entire document.	1-17
A	US 5,459,077 A (MOORE et al) 17 October 1995, see entire document	1-17

☐ 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

"E" earlier application or patent published on or after the international filing date

"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)

"O" document referring to an oral disclosure, use, exhibition or other means

"P" document published prior to the international filing date but later than 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

Date of the actual completion of the international search

22 June 2004 (22.06.2004)

Date of mailing of the international search report

30 JUN 2004

Name and mailing address of the ISA/US

Mail Stop PCT, Attn: ISA/US
Commissioner for Patents
P.O. Box 1450
Alexandria, Virginia 22313-1450

Facsimile No. (703) 305-3230

Authorized officer

Ann Y. Lam

Telephone No. (703) 308-0196