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<p>(21) International Application Number: PCT/US95/10171</p> <p>(22) International Filing Date: 10 August 1995 (10.08.95)</p> <p>(30) Priority Data: 08/288,503 10 August 1994 (10.08.94) US</p> <p>(60) Parent Application or Grant (63) Related by Continuation US 08/288,503 (CIP) Filed on 10 August 1994 (10.08.94)</p> <p>(71) Applicant (for all designated States except US): PSI INTERNATIONAL, INC. [US/US]; Suite 300, 810 Gleneagles Court, Towson, MD 21286 (US).</p> <p>(71)(72) Applicants and Inventors: MOORE, Jeffrey [US/US]; 12 Breezy Tree Court, Timonimun, MD 21093 (US). BRAZIL, Joanne [US/US]; 4500 Jolly Acres Road, White Hall, MD 21161 (US). HOOVER, Jeffrey, R. [US/US]; 8639 Willow Oak Road, Baltimore, MD 21234 (US).</p> <p>(74) Agent: GROSSMAN, Jon, D.; Dickstein, Shapiro & Morin, L.L.P., Suite 400, 2101 L Street, N.W., Washington, DC 20037-1526 (US).</p>	<p>(81) Designated States: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN, European patent (AT, BE, CH, DE, DK, ES, 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), ARIPO patent (KE, MW, SD, SZ, UG).</p> <p>Published <i>With international search report. Before the expiration of the time limit for amending the claims and to be republished in the event of the receipt of amendments.</i></p> <p>(88) Date of publication of the international search report: 9 May 1996 (09.05.96)</p>	
(54) Title: RELATIONAL DATABASE MANAGEMENT SYSTEM FOR CHEMICAL STRUCTURE STORAGE, SEARCHING AND RETRIEVAL		
<p>(57) Abstract</p> <p>A chemical structure search system and method which capitalizes on the strengths of relational database technology, by allowing a user to optimally store (62) and search (66) chemical structure information, including information related to multi-valued atoms, multi-typed bonds, and Markush searching. The system provides a complete chemical information system, with capabilities for exact structure, substructure, key, chemical name and molecular formula searching, registration of new molecules, structure import/export and data editing. The system also has dynamic querying capabilities (68) which allow the user to be notified of any new chemicals that are entered into the database that are responsive to previously run queries. Furthermore, structure classes allow a user to store information about types of chemical structures, such as steroids, and to re-use the structure classes and queries without re-entry of the information.</p>	<pre> graph TD 60[60 USER PERFORMS SEARCH] --> 62[62 SYSTEM STORES RESULTS] 62 --> 64[64 SYSTEM TAGS RESULTS THAT ARE SEEN] 64 --> 66[66 NEW SEARCHES ADDED] 66 --> 68[68 SYSTEM PERFORMS DYNAMIC QUERIES] 68 --> 70[70 SYSTEM NOTIFIES USER OF MATCH] 70 --> 72[72 USER VIEWS UNSEEN RESULTS] </pre>	

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INTERNATIONAL SEARCH REPORT

International application No.
PCT/US95/10171

A. CLASSIFICATION OF SUBJECT MATTER
 IPC(6) :G06F 17/30
 US CL :395/600; 364/496, 497, 499
 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. : 395/600; 364/496, 497, 499

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 Extra Sheet.

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	US, A, 4,811,217 (TOKIZANE ET AL.) 07 March 1989, see whole document.	1-2
A	US, A, 5,025,388 (CRAMER, III ET AL.) 18 June 1991, see whole document.	1-2
A	US, A, 5,056,035 (FUJITA) 08 October 1991, see whole document.	1-2
A	US, A, 4,855,931 (SAUNDERS) 08 August 1989, see whole document.	1-2

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B. FIELDS SEARCHED

Electronic data bases consulted (Name of data base and where practicable terms used):

APS (USPAT file)

search terms: chemical, atoms, bonds, relational, database, search, query