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#### Published

With international search report.

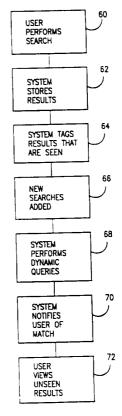
Before the expiration of the time limit for amending the claims and to be republished in the event of the receipt of amendments.

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(54) Title: RELATIONAL DATABASE MANAGEMENT SYSTEM FOR CHEMICAL STRUCTURE STORAGE, SEARCHING AND RETRIEVAL

#### (57) Abstract

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.



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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 :3	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)								
	95/600; 364/496, 497, 499							
Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched								
	ata base consulted during the international search (name Extra Sheet.	ne of data base and, where practicable,	search terms used)					
C. DOC	UMENTS CONSIDERED TO BE RELEVANT							
Category*	Citation of document, with indication, where ap	propriate, of the relevant passages	Relevant to claim No.					
X	US, A, 4,811,217 (TOKIZANE ET whole document.	AL.) 07 March 1989, see	1-2					
A	US, A, 5,025,388 (CRAMER, III E whole document.	1-2						
A	US, A, 5,056,035 (FUJITA) 08 October 1991, see whole document.							
A	US, A, 4,855,931 (SAUNDERS) 08 August 1989, see whole document.							
Furti	her documents are listed in the continuation of Box C	See patent family annex.						
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<b>6</b>	cument referring to an oral disclosure, use, exhibition or other cans	being obvious to a person skilled in to  document member of the same patent	he art					
th	e priority date claimed actual completion of the international search	Date of mailing of the international se						
	EMBER 1995	05 MAR 1996	•					
Box PCT	mailing address of the ISA/US oner of Patents and Trademarks on, D.C. 20231 No. (703) 305-3230	Authorized officer  WMARIA N. VON BUHR  Telephone No. (703) 305-9600	i Hell					

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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								