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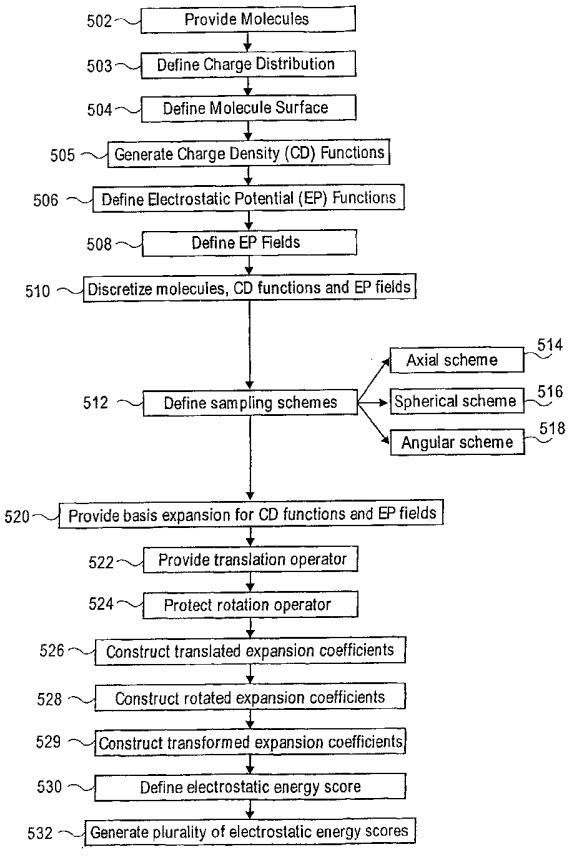
[Continued on next page]

(54) Title: METHOD AND APPARATUS FOR ESTIMATION OF THE ELECTROSTATIC AFFINITY BETWEEN MOLECULES USING A BASIS EXPANSION



(57) Abstract: A method and apparatus for analysis of molecular combinations featuring two or more molecular subsets is described. The computational method estimates the electrostatic affinity of the system (532) via utilization of a basis expansion (529) representing charge density and electrostatic potential functions associated with the first and second molecular subsets in a coordinate system. An electrostatic affinity (530), representing a correlation of the charge density (505) and electrostatic potential functions (506) of the first and second molecular subsets, is computed via suitable application of translation (522) and rotation (524) operators to the basis expansion coefficients (529) over a sequence of different sampled configurations for the molecular combination. The method may also be combined with other methods for computation of shape complementarity in determining a composite or augmented score reflecting both electrostatic affinity and shape complementarity for configurations of a molecular combination.

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INTERNATIONAL SEARCH REPORT

International application No.
PCT/US04/33817

A. CLASSIFICATION OF SUBJECT MATTER
IPC(7) : C12Q 1/00
US CL : 702/22
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. : 702/22, 19, 21, 23, 27-32

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched
NONE

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,E	US 2005/0055165 A1 (PURVIS, III) 10 March 2005 (10.03.2005), see entire document.	1-89
A,E	US 2005/0038610 A1 (MAYO et al) 17 February 2005 (17.02.2005), see entire document.	1-89
A,E	US 2005/0027458 A1 (MERZ, JR. et al) 03 February 2005 (03.02.2005), see entire document.	1-89
A,E	US 2005/0027457 A1 (MANDELL et al) 03 February 2005 (03.02.2005), see entire document.	1-89
A	US 2002/0133298 A1 (SILVERMAN) 19 September 2002 (19.09.2005), see entire document.	1-89
A	US 6,230,102 B1 (TIDOR et al) 08 May 2001 (08.05.2001), see entire document.	1-89
A	US 5,915,230 A (BERNE et al) 22 June 1999 (22.06.1999), see entire document.	1-89
A	US 5,703,792 A (CHAPMAN) 30 December 1997 (30.12.1997), see entire document.	1-89
A	US 5,424,963 A (TURNER et al) 13 June 1995 (13.06.1995), see entire document.	1-89

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

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

International application No.
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Continuation of Item 4 of the first sheet:
Long Title: New Title: METHOD AND APPARATUS FOR ESTIMATION OF THE ELECTROSTATIC AFFINITY BETWEEN MOLECULES USING A BASIS EXPANSION

Continuation of B. FIELDS SEARCHED Item 3:
US-PGPUB; USPAT; EPO; JPO; DERWENT;IBM_TDB
search terms: electrostatic adj affinity; electrostatic adj potential; electrostatic; electro-static; "electro static"; rotat$7; translat$7