

Title (en)
RECEPTOR SELECTIVITY MAPPING

Title (de)
REZEPTOR SELEKTIVITÄTSABBILDUNG

Title (fr)
REPRESENTATION DE LA SELECTIVITE DE RECEPTEURS

Publication
EP 1360560 A4 20070718 (EN)

Application
EP 00928364 A 20000426

Priority
• US 0011073 W 20000426
• US 13099299 P 19990426

Abstract (en)
[origin: WO0065421A2] A computer system comprising a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of the plurality of chemical compounds on biological systems and a second database containing records corresponding to a plurality of molecular targets. The computer system further comprises a third database containing records corresponding to tests of interaction between compounds in the first database and molecular targets in the second database, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target. Means for setting an interaction test threshold corresponding to said effect and means for selecting the compound when its use results in a test meeting the interaction test threshold are also included in the computer system. A user interface is provided to allow a user to view the selected compound and to selectively view information from the first database, the second database, the third database as it relates to a compound record in the first database or as it relates to a molecular target in the second database.

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G06F 1/00

IPC 8 full level
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Citation (search report)
• [X] SHI L M ET AL: "Mining the NCI anticancer drug discovery databases: genetic function approximation for the QSAR study of anticancer ellipticine analogues.", March 1998, JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES 1998 MAR-APR, VOL. 38, NR. 2, PAGE(S) 189 - 199, ISSN: 0095-2338, XP002436117
• [X] BROWN F K: "CHEMOINFORMATICS: WHAT IS IT AND HOW DOES IT IMPACT DRUG DISCOVERY", 1998, ANNUAL REPORTS IN MEDICINAL CHEMISTRY, SAN DIEGO, US, PAGE(S) 375-384, ISSN: 0065-7743, XP008035536
• [A] GOTO SUSUMU ET AL: "LIGAND database for enzymes, compounds and reactions", 1 January 1999, NUCLEIC ACIDS RESEARCH, VOL. 27, NR. 1, PAGE(S) 377-379, ISSN: 0305-1048, XP002436118
• [A] BURBAUM J J ET AL: "NEW TECHNOLOGIES FOR HIGH-THROUGHPUT SCREENING", CURRENT OPINION IN CHEMICAL BIOLOGY, CURRENT BIOLOGY LTD, LONDON, GB, vol. 1, no. 1, June 1997 (1997-06-01), pages 72 - 78, XP001029043, ISSN: 1367-5931
• [A] HEMM K ET AL: "Constituting a receptor-ligand information base from quality-enriched data.", 1995, PROCEEDINGS / ... INTERNATIONAL CONFERENCE ON INTELLIGENT SYSTEMS FOR MOLECULAR BIOLOGY ; ISMB. INTERNATIONAL CONFERENCE ON INTELLIGENT SYSTEMS FOR MOLECULAR BIOLOGY 1995, VOL. 3, PAGE(S) 170 - 178, ISSN: 1553-0833, XP002436119
• See references of WO 0065421A2

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