Title (en)

COMPOUND SCREENING SYSTEM

Title (de)

GEMISCHTES SICHTUNGSSYSTEM

Title (fr)

SYSTEME DE TAMISAGE DE COMPOSES

Publication

EP 1010094 A4 20010307 (EN)

Application

EP 98941143 A 19980903

Priority

- AU 9800715 W 19980903
- AU PO892197 A 19970903
- AU PP119297 A 19971231

Abstract (en)

[origin: WO9912118A1] The present application relates to a number of aspects of a compound and/or molecular screening system, including: 1) finding relationships between molecular structure and useful properties of molecules, more particularly using a virtual or mathematical analogue or model of a biological receptor or active site (a "virtual receptor") or other biological activity, such as toxicity; 2) creating a virtual receptor by use of Minimum Message Length or Maximum Entropy method (MEM) principles such as by applying a Bayesian regularised artificial neural network (BRANN); 3) using a virtual receptor to screen a database, the database may be real or virtual, may apply to existing or hypothetical molecules or compounds; 4) use of virtual receptors as fitness functions; 5) a method of mutating structures by modifying a SMILES string representation; 6) an improved molecular multipole moment representation; 7) an improved molecular eigenvalue index as a representation. Other aspects are also disclosed.

IPC 1-7

G06F 17/50

IPC 8 full level

G16C 20/64 (2019.01); **B01J 19/00** (2006.01); **G06F 17/50** (2006.01)

CPC (source: EP US)

B01J 19/0046 (2013.01 - EP); **G16B 35/00** (2019.01 - EP); **G16C 20/60** (2019.01 - EP); **G16C 20/64** (2019.01 - EP US); B01J 2219/00601 (2013.01 - EP); B01J 2219/007 (2013.01 - EP); B01J 2219/00702 (2013.01 - EP); B01J 2219/0072 (2013.01 - EP)

Citation (search report)

- [DX] US 5434796 A 19950718 - WEININGER DAVID [US]
- [PA] F.R. BURDEN ET AL.: "Predicting maximum bioactivity by effective inversion of neural networks using genetic algorithms", CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS, vol. 38, no. 2, 1 October 1997 (1997-10-01), Amsterdam, NL, pages 127 - 137, XP004097524, ISSN: 0169-7439
- [A] D.E. WALTERS ET AL.: "GENETICALLY EVOLVED RECEPTOR MODELS: A COMPUTATIONAL APPROACH TO CONSTRUCTION OF RECEPTOR MODELS", JOURNAL OF MEDICINAL CHEMISTRY, vol. 37, no. 16, 5 August 1994 (1994-08-05), Washington, DC, US, pages 2527 - 2536, XP000608151, ISSN: 0022-2623
- [A] J. B. MOON ET AL.: "Computer Design of Bioactive Molecules: A Method for Receptor-Based de Novo Ligand Design", PROTEINS: STRUCTURE, FUNCTION AND GENETICS, vol. 11, 1991, pages 314 - 328, XP000560842
- See references of WO 9912118A1

Cited by

WO2023123021A1

Designated contracting state (EPC)

DE FR GB IT

DOCDB simple family (publication)

WO 9912118 A1 19990311; EP 1010094 A1 20000621; EP 1010094 A4 20010307

DOCDB simple family (application)

AU 9800715 W 19980903; EP 98941143 A 19980903