

Title (en)
COMPUTATIONAL PROTEIN PROBING TO IDENTIFY BINDING SITES

Title (de)
RECHNERISCHE PROTEIN-SONDIERUNG ZUM IDENTIFIZIEREN VON BINDUNGSSTELLEN

Title (fr)
SONDAGE INFORMATIQUE DE PROTEINES POUR IDENTIFIER DES SITES DE LIAISON

Publication
EP 1751669 A4 20081105 (EN)

Application
EP 04822039 A 20040506

Priority
US 2004014069 W 20040506

Abstract (en)
[origin: WO2005114458A1] Provided is a method of identifying binding sites on a macromolecule comprising: (a) for at least one organic fragment (ORF), conducting, at separate values of parameter B, two or more simulated annealing of chemical potential calculations using the ORF as the inserted solvent; and (b) comparing converged solutions from step (a) to identify first locations at which the relevant ORF is strongly bound, thereby identifying candidate sites for binding ligand molecules.

IPC 8 full level
G16B 20/30 (2019.01); **G06F 17/00** (2006.01); **G06F 19/00** (2011.01); **G16B 20/50** (2019.01)

CPC (source: EP US)
G16B 15/30 (2019.01 - EP US); **G16B 20/00** (2019.01 - EP); **G16B 20/30** (2019.01 - EP US); **G16C 20/50** (2019.01 - EP);
G16B 15/00 (2019.01 - EP); **G16B 20/50** (2019.01 - EP US)

Citation (search report)
• [E] US 6735530 B1 20040511 - GUARNIERI FRANK [US]
• [E] US 2004267509 A1 20041230 - BRUNNER STEPHAN [CH], et al
• [DXY] GUARNIERI F ET AL: "SIMULATED ANNEALING OF CHEMICAL POTENTIAL: A GENERAL PROCEDURE FOR LOCATING BOUND WATERS. APPLICATION TO THE STUDY OF THE DIFFERENTIAL HYDRATION PROPENSITIES FOR THE MAJOR AND MINOR GROOVES OF DNA", JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, AMERICAN CHEMICAL SOCIETY, WASHINGTON, DC.; US, US, vol. 118, no. 35, 1 January 1996 (1996-01-01), pages 8493 - 8494, XP009061246, ISSN: 0002-7863
• [AY] TOMIOKA N ET AL: "GREEN: A PROGRAM PACKAGE FOR DOCKING STUDIES IN RATIONAL DRUG DESIGN", JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN, ESCOM SCIENCE PUBLISHERS BV, XX, vol. 8, 1 January 1994 (1994-01-01), pages 347 - 366, XP002911172, ISSN: 0920-654X
• [A] EISENSTEIN M ET AL: "On proteins, grids, correlations, and docking", COMPTES RENDUS - BIOLOGIES, ELSEVIER, PARIS, FR, vol. 327, no. 5, 1 May 2004 (2004-05-01), pages 409 - 420, XP004512381, ISSN: 1631-0691
• See references of WO 2005114458A1

Designated contracting state (EPC)
AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IT LI LU MC NL PL PT RO SE SI SK TR

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