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 A1 20070214 (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)

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DOCDB simple family (publication)
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