Title (en)

SYSTEM AND METHOD FOR STRUCTURE-BASED DRUG DESIGN THAT INCLUDES ACCURATE PREDICTION OF BINDING FREE ENERGY

Title (de)

SYSTEM UND VERFAHREN ZUM AUF DER STRUKTUR BASIERENDEM ENTWURF VON ARZNEIMITTELN MIT GENAUER VORHERSAGE VON FREIEN BINDUNGSENERGIEN

Title (fr)

SYSTEME ET PROCEDE DE CONCEPTION RATIONNELLE DE MEDICAMENTS SUR LA BASE D'UNE STRUCTURE FAISANT INTERVENIR LA PREDICTION PRECISE DE L'ENERGIE LIBRE DE LIAISON

Publication

EP 1140737 A2 20011010 (EN)

Application

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Priority

- US 9930948 W 19991222
- US 22036398 A 19981224

Abstract (en)

[origin: WO0039751A2] A system and method for providing improved de novo structure-based drug design that includes a method for more accurately predicting binding free energy. The system and method use a coarse-graing model with corresponding knowledge-based potential data to grow ligand candidates and libraries of ligand candidates. In light of the present inventions using coarse-graining model, the novel growth method of the present invention uses a Metropolis Monte Carlo selection process which result in a low energy structure that is not necessarily the lowest energy structure, yet results in a better ligand candidate.

IPC 1-7

C07B 61/00; C07H 19/01; G06F 17/50

IPC 8 full level

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CPC (source: EP US)

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See references of WO 0039751A2

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