

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

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Application

EP 99967640 A 19991222

Priority

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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-graining 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.

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IPC 8 full level

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CPC (source: EP US)

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Citation (search report)

See references of WO 0039751A2

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