Title (en)

METHOD AND DEVICE FOR SELECTING A SUBASSEMBLY OF MOLECULES FOR USE IN PREDICTING AT LEAST ONE PROPERTY OF A MOLECULAR STRUCTURE

Title (de)

VERFAHREN UND VORRICHTUNG ZUR AUSWAHL EINER UNTERBAUGRUPPE VON MOLEKÜLEN ZUR VERWENDUNG IN DER VORHERSAGE VON MINDESTENS EINER EIGENSCHAFT EINER MOLEKULAREN STRUKTUR

Title (fr)

PROCÉDÉ ET DISPOSITIF DE SÉLECTION D'UN SOUS-ENSEMBLE DE MOLÉCULES DESTINÉES À ÊTRE UTILISÉES POUR PRÉDIRE AU MOINS UNE PROPRIÉTÉ D'UNE STRUCTURE MOLÉCULAIRE

Publication

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Application

EP 18749450 A 20180622

Priority

- FR 1700668 A 20170622
- FR 2018051529 W 20180622

Abstract (en)

[origin: WO2018234718A1] The selection method according to the invention is iterative and comprises an initialisation step (E10) associating with a molecule, referred to as the current molecule, a predetermined descriptor value of molecules associated with the target molecular structure, and, during each iteration (E20) of the selection method: — a step (E30), for each molecule of a database comprising a plurality of molecules each associated with a value of said descriptor, of evaluating a degree of similarity, referred to as overall similarity, between the value of the descriptor associated with said molecule and the value of the descriptor associated with the current molecule; — a step (E40) of selecting molecules of the database having a degree of overall similarity greater than a predetermined threshold, the selected molecules being added (E50) to the reference subassembly; and — a step (E60) of updating the value of the descriptor associated with the current molecule based on values of descriptors associated with at least one portion of the molecules belonging to the reference subassembly.

CPC (source: EP US)

G16C 20/30 (2019.01 - US); **G16C 20/40** (2019.01 - EP US); G16C 20/30 (2019.01 - EP); G16C 60/00 (2019.01 - US)

Citation (search report)

See references of WO 2018234718A1

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