

Title (en)

METHOD OF DESIGNING CHEMICAL SUBSTANCES

Title (de)

METHODE ZUM ENTWURF VON CHEMISCHEN SUBSTANZEN

Title (fr)

PROCEDE D'IDENTIFICATION DE SUBSTANCES CHIMIQUES

Publication

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Application

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Abstract (en)

[origin: WO9926901A1] A method for designing chemical substances is disclosed, in which a plurality of sets of candidate elements are selected. From those sets of candidate elements, an array of all possible substances that can be made is generated. From this array, a smaller, sub-array is identified which includes all possible pairings of the elements within each set. The substances within that sub-array are then synthesised and their physical properties tested in each case. Based on the results of these tests, the physical properties of substances within the array of all possible substances but not within the sub-array may be predicted. The method allows a chemical substance, and particularly a pharmaceutical substance, having an optimised physical characteristic to be identified from a large array of possible substances more quickly and accurately.

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C07B 61/00; G06F 17/50

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