

Title (en)  
HIGH EFFICIENCY MAPPING OF MOLECULAR VARIATIONS TO FUNCTIONAL PROPERTIES

Title (de)  
HOCHLEISTUNGSFÄHIGE FESTSTELLUNG VON ÜBEREINSTIMMUNGEN ZWISCHENMOLEKULAREN VERÄNDERUNGEN UND FUNKTIONSEIGENSCHAFTEN

Title (fr)  
ETABLISSEMENT DE CORRESPONDANCES TRES EFFICACES ENTRE VARIATIONS MOLECULAIRES ET PROPRIETES FONCTIONNELLES

Publication  
**EP 1244909 A1 20021002 (EN)**

Application  
**EP 01901692 A 20010103**

Priority  
• US 0100150 W 20010103  
• US 17422500 P 20000103

Abstract (en)  
[origin: WO0150124A1] A method for the selective variation of a multi-variable molecular synthesis to optimize a reaction product functional property, including the steps of: constructing a first order library of functional property output data obtained by reacting all first order library input variable combinations for the multi-variable synthesis and measuring the functional property for every reaction product, wherein the first order library input variable combinations include all values selected for each variable taken one at a time; ordering the values for each input variable according to their effect upon functional property optimization; constructing a second order library of functional property output data obtained by reacting a set of second order library input variable combinations coarsely sampled two variables at a time from the ordered input variables and measuring the functional property for every reaction product; and interpolating among the functional property output data for functional property optimization.

IPC 1-7  
**G01N 31/00**; **G06F 19/00**

IPC 8 full level  
**C07B 61/00** (2006.01); **C40B 50/00** (2006.01); **G01N 31/00** (2006.01); **G06F 19/00** (2006.01); **G16B 20/20** (2019.01); **G06F 19/18** (2011.01)

CPC (source: EP US)  
**B82Y 5/00** (2013.01 - EP); **C40B 50/00** (2013.01 - EP); **G16B 20/20** (2019.01 - EP US); **G16C 20/30** (2019.01 - EP); **B01J 2219/007** (2013.01 - EP); **G01N 2500/00** (2013.01 - EP); **G16B 20/00** (2019.01 - EP)

Citation (search report)  
See references of WO 0150124A1

Designated contracting state (EPC)  
AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE TR

DOCDB simple family (publication)  
**WO 0150124 A1 20010712**; AU 2756801 A 20010716; EP 1244909 A1 20021002; JP 2003519201 A 20030617

DOCDB simple family (application)  
**US 0100150 W 20010103**; AU 2756801 A 20010103; EP 01901692 A 20010103; JP 2001550023 A 20010103