Title (en)

METHOD AND SYSTEM FOR PLANNING, PERFORMING, AND ASSESSING HIGH-THROUGHPUT SCREENING OF MULTICOMPONENT CHEMICAL COMPOSITIONS AND SOLID FORMS OF COMPOUNDS

Title (de)

VERFAHREN UND SYSTEM ZUR PLANUNG, DURCHFÜHRUNG UND BEURTEILUNG EINES HIGH-THROUGHPUT-SCREENING CHEMISCHER ZUSAMMENSETZUNGEN MIT MEHREREN KOMPONENTEN SOWIE FESTER FORMEN VON VERBINDUNGEN

Title (fr)

PROCEDE ET SYSTEME SERVANT A PLANIFIER, EXECUTER ET EVALUER UN CRIBLAGE A HAUT RENDEMENT DE COMPOSITIONS CHIMIQUES A CONSTITUANTS MULTIPLES ET DE FORMES SOLIDES DE COMPOSES

Publication

EP 1381857 A2 20040121 (EN)

Application

EP 02733893 A 20020325

Priority

- US 0209274 W 20020325
- US 27840101 P 20010323

Abstract (en)

[origin: WO02077772A2] The present application is directed to the use of computerized date processing to plan, perform, and assess the results of high-throughput screening of multicomponent chemical compositions and solid forms of compounds. Systems utilized include databases of molecular descriptors and related compounds and their properties as determined empirically and through simulation, along with multidimensional visualization tools. Methods include methods for determining chemical compositions by performing steps including selecting a plurality of combinations of values of experimental parameters that can be varied by an automated experiment apparatus, determining a set of experimental results, and determining a second plurality of combinations of values based on the set of experimental results. Additional methods include selecting values of parameters that produce a composition, the values being relatively far from areas of rapid change or boundaries between solid forms.

IPC 1-7

G01N 31/00

IPC 8 full level

B01J 19/00 (2006.01); **G01N 31/00** (2006.01); **G16C 20/64** (2019.01); C40B 40/06 (2006.01); C40B 40/10 (2006.01); C40B 50/08 (2006.01); C40B 60/14 (2006.01)

IPC 8 main group level

G06F (2006.01)

CPC (source: EP US)

B01J 19/0046 (2013.01 - EP); **G16C 20/30** (2019.01 - EP); **G16C 20/64** (2019.01 - EP US); B01J 2219/00315 (2013.01 - EP); B01J 2219/00585 (2013.01 - EP); B01J 2219/00587 (2013.01 - EP); B01J 2219/00599 (2013.01 - EP); B01J 2219/00659 (2013.01 - EP); B01J 2219/00689 (2013.01 - EP); B01J 2219/00695 (2013.01 - EP); B01J 2219/007 (2013.01 - EP); B01J 2219/00707 (2013.01 - EP); B01J 2219/00722 (2013.01 - EP); B01J 2219/00725 (2013.01 - EP); B01J 2219/00756 (2013.01 - EP); C40B 40/06 (2013.01 - EP); C40B 40/10 (2013.01 - EP); C40B 50/08 (2013.01 - EP); C40B 60/14 (2013.01 - EP); G16B 35/00 (2019.01 - EP); G16C 20/60 (2019.01 - EP); G16C 20/70 (2019.01 - EP)

Cited by

US12005127B2

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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 02077772 A2 20021003; **WO 02077772 A3 20030821**; **WO 02077772 A9 20030109**; **WO 02077772 B1 20040708**; AU 2002305092 A1 20021008; CA 2441931 A1 20021003; EP 1381857 A2 20040121; EP 1381857 A4 20070328

DOCDB simple family (application)

US 0209274 W 20020325; AU 2002305092 A 20020325; CA 2441931 A 20020325; EP 02733893 A 20020325