

Title (en)

GENERATION OF VIRTUAL COMBINATORIAL LIBRARIES OF COMPOUNDS

Title (de)

ERZEUGUNG VIRTUELLER KOMBINATORISCHER BIBLIOTHEKEN VON VERBINDUNGEN

Title (fr)

ELABORATION DE LIBRAIRIES COMBINATOIRES VIRTUELLES DE COMPOSES

Publication

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Application

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Priority

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- US 7640598 A 19980512

Abstract (en)

[origin: WO9959061A1] Methods for the computer-generation of virtual libraries of compounds are disclosed, including methods for tracking the addition of fragments, use of reagents, and the transformations performed. A tracking table is generated for sample compound C1 and includes entries: (a) listing the order of fragments used, and (b) listing the transformations performed for each synthesis path.

IPC 1-7

G06F 9/455; **G06F 19/00**

IPC 8 full level

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CPC (source: EP)

G16B 15/30 (2019.01); **G16B 35/10** (2019.01); **G16C 20/62** (2019.01)

Citation (search report)

- [X] WO 9727559 A1 19970731 - PATTERSON DAVID E [US], et al
- [X] EP 0818744 A2 19980114 - PROTEUS MOLECULAR DESIGN [GB]
- See references of WO 9959061A1

Designated contracting state (EPC)

AT BE CH CY DE DK ES FI FR GB GR IE IT LI LU MC NL PT SE

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