Title (en)

SYSTEM AND METHOD FOR PREDICTION OF DRUG METABOLISM, TOXICITY, MODE OF ACTION, AND SIDE EFFECTS OF NOVEL SMALL MOLECULE COMPOUNDS

Title (de)

SYSTEM UND VERFAHREN ZUR VORHERSAGE DES ARZNEIMITTELMETABOLISMUS, DER TOXIZITÄT, DER WIRKUNGSWEISE UND DER NEBENEFFEKTE NEUER KLEINMOLEKÜLVERBINDUNGEN

Title (fr)

SYSTEME ET PROCEDE POUR PREDIRE LE METABOLISME, LA TOXICITE, LE MODE D'ACTION, ET LES EFFETS SECONDAIRES DE NOUVEAUX COMPOSES CONSTITUES DE PETITES MOLECULES CHEZ L'ETRE HUMAIN

Publication

EP 1866824 A2 20071219 (EN)

Application

EP 06748475 A 20060317

Priority

- US 2006010053 W 20060317
- US 66269905 P 20050317

Abstract (en)

[origin: WO2006099624A2] A system is provided for the prediction of human drug metabolism and toxicity of novel compounds. The system enables the visualization of pre-clinical and clinical high- throughput data in the context of a complete biological organism. Substructure and similarity structure searches can be performed using the underlying databases of xenobiotics, active ligands, and endobiotics. The system also has an analytical component for the parsing, integration, and network analysis of genomics, proteomics, and metabolomics high-throughput data. From this information, the system further generates networks around proteins, genes and compounds to assess toxicity and drug-drug interactions.

IPC 8 full level

G01N 33/48 (2006.01); **G06F 19/00** (2011.01); **G06G 7/48** (2006.01); **G16B 5/00** (2019.01); **G16B 20/20** (2019.01); **G16B 45/00** (2019.01)

CPC (source: EP GB US)

G16B 5/00 (2019.01 - EP GB US); **G16B 20/20** (2019.01 - EP GB US); **G16B 35/00** (2019.01 - GB); **G16C 20/30** (2019.01 - EP); **G16C 20/60** (2019.01 - GB); G16B 20/00 (2019.01 - EP); G16B 45/00 (2019.01 - EP); G16C 20/80 (2019.01 - EP)

Designated contracting state (EPC)

AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HU IE IS IT LI LT LU LV MC NL PL PT RO SE SI SK TR

Designated extension state (EPC)

AL BA HR MK YU

DOCDB simple family (publication)

WO 2006099624 A2 20060921; **WO 2006099624 A3 20071206**; **WO 2006099624 A9 20061109**; EP 1866824 A2 20071219; EP 1866824 A4 20090805; GB 0719562 D0 20071114; GB 2439675 A 20080102

DOCDB simple family (application)

US 2006010053 W 20060317; EP 06748475 A 20060317; GB 0719562 A 20060317