Title (en)

DEVELOPMENT OF PRODRUGS POSSESSING A NITRIC OXIDE DONOR DIAZEN-1-IUM-1,2-DIOLATE MOIETY USING IN VITRO/IN SILICO PREDICTIONS

Title (de)

ENTWICKLUNG VON PRODRUGS MIT EINEM STICKOXIDSPENDER-DIAZEN-1-IUM-1,2-DIOLAT-TEIL UNTER VERWENDUNG VON IN-VITRO-/IN-SILICO-PROGNOSEN

Title (fr)

DÉVELOPPEMENT DE PROMÉDICAMENTS POSSÉDANT UNE ENTITÉ 1,2-DIOLATE DE DIAZÉN-1-IUM DONNEUSE D'OXYDE NITRIQUE EN UTILISANT DES PRÉDICTIONS IN VITRO/IN SILICO

Publication

EP 1934872 A2 20080625 (EN)

Application

EP 06826028 A 20061013

Priority

- US 2006040382 W 20061013
- US 72653005 P 20051013
- US 73012005 P 20051021
- US 75644606 P 20060105
- US 81223006 P 20060609

Abstract (en)

[origin: WO2007044963A2] The present invention provides a method of using a physiologically-based pharmacokinetic model to select a prodrug molecule (NO-X) comprising a therapeutic agent X (e.g. nonsteroidal anti- inflammatory drug, (NSAID)) and an appropriate nitric oxide donor NO. The NSAID can be a non- selective or selective cyclooxygenase inhibitor or other biocompatible compound comprising a carboxyl group. The pharmacokinetic model uses in vitro and/or in silico data to estimate an optimal set of parameters that can predict whether a particular NO-X candidate is capable of producing desirable therapeutic effects, e.g. enhanced antiif lammatory activity, reduced intestinal, cardiac and renal toxicity. Accordingly, the present invention can greatly enhance proper selection of an appropriate candidate for drug development, thereby minimizing development time and conserving costs.

IPC 8 full level

A61K 49/10 (2006.01)

CPC (source: EP)

A61K 47/55 (2017.07); **A61P 43/00** (2017.12); **G01N 33/94** (2013.01); **G01N 33/9486** (2013.01)

Citation (search report)

See references of WO 2007044963A2

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 RS

DOCDB simple family (publication)

WO 2007044963 A2 20070419; **WO 2007044963 A3 20090430**; **WO 2007044963 A8 20070614**; AU 2006299818 A1 20070419; CA 2622150 A1 20070419; EP 1934872 A2 20080625; JP 2009515824 A 20090416

DOCDB simple family (application)

US 2006040382 W 20061013; AU 2006299818 A 20061013; CA 2622150 A 20061013; EP 06826028 A 20061013; JP 2008535771 A 20061013