

Title (en)

CRYSTAL STRUCTURES OF JNK-INHIBITOR COMPLEXES AND BINDING POCKETS THEREOF

Title (de)

KRISTALLSTRUKTUREN VON JNK-INHIBITORKOMPLEXEN UND BINDE-POCKETS DAFÜR

Title (fr)

STRUCTURES CRISTALLINES DE COMPLEXES D'INHIBITION DE LA JNK ET POCHES DE LIAISON DE CEUX-CI

Publication

EP 1476840 A2 20041117 (EN)

Application

EP 03708827 A 20030110

Priority

- US 0300899 W 20030110
- US 34800202 P 20020111

Abstract (en)

[origin: WO03060102A2] The invention relates to crystalline molecules or molecular complexes that comprise binding pockets of c-Jun N-terminal kinase 3 (JNK3) or its homologues. The invention also relates to crystals comprising JNK3 and an inhibitor. The present invention also relates to a computer comprising a data storage medium encoded with the structural coordinates of JNK3 binding pockets and methods of using a computer to evaluate the ability of a compound to bind to the molecule or molecular complex. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen for, design and optimize compounds, including agonists and antagonists, which bind to JNK3 or homologues thereof.

IPC 1-7

G06F 19/00; **A01N 61/00**; **C12N 9/12**

IPC 8 full level

A01N 61/00 (2006.01); **C12N 9/12** (2006.01); **G01N 19/00** (2006.01)

CPC (source: EP)

C12N 9/1205 (2013.01); **C07K 2299/00** (2013.01)

Designated contracting state (EPC)

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

DOCDB simple family (publication)

WO 03060102 A2 20030724; **WO 03060102 A3 20031127**; AU 2003212796 A1 20030730; AU 2003212796 A8 20030730; EP 1476840 A2 20041117; EP 1476840 A4 20070509

DOCDB simple family (application)

US 0300899 W 20030110; AU 2003212796 A 20030110; EP 03708827 A 20030110