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

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Application
EP 03708827 A 20030110

Priority
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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.

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Citation (search report)
• [DXY] WO 9957253 A2 19991111 - VERTEX PHARMA [US], et al
• [DY] WO 0112621 A1 20010222 - VERTEX PHARMA [US], et al
• [DY] WO 0075118 A1 20001214 - VERTEX PHARMA [US], et al
• [DA] US 6274738 B1 20010814 - KOZLOWSKI MICHAEL R [US], et al
• [Y] WO 9942592 A1 19990826 - VERTEX PHARMA [US]
• [DA] US 6147080 A 20001114 - BEMIS GUY W [US], et al
• [A] WO 0070030 A1 20001123 - KINETIX PHARMACEUTICALS INC [US], et al
• See references of WO 03060102A2

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