

Title (en)

IN-SILICO-SCREENING FOR DOCKING ON SUB-DOMAIN IIID OF HCV-IRES

Title (de)

IN-SILICO SCREENING VERFAHREN FÜR ANLEGEN AN DIE SUB-DOMÄNE IIID DES HCV-IRES

Title (fr)

AJUSTEMENT AU SOUS-DOMAIN IIID DU HCV-IRES PAR CRIBLAGE IN SILICO

Publication

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Application

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Abstract (en)

[origin: WO0181627A2] A model structure of sub-domain IIId of the hepatitis C virus internal ribosome entry site has been elucidated. The invention provides an *in silico* method for identifying a compound that interacts with sub-domain IIId, comprising the steps of: a) providing atomic co-ordinates of said sub-domain IIId in a storage medium on a computer; and b) using said computer to apply molecular modelling techniques to said co-ordinates. Suitable methods include *de novo* compound design, use of a pharmacophore, and automated docking algorithms.

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