

POSTER PRESENTATION

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Targeting flexibility: a structure-based computational study revealing allosteric HIV-1 protease inhibitors

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From 9th German Conference on Chemoinformatics
Fulda, Germany. 10-12 November 2013

We present the discovery of innovative low molecular weight inhibitors against human immunodeficiency virus 1 (HIV-1) protease. Structure-based virtual screening focused on potential allosteric surface cavities revealed these compounds [1]. To identify and prioritize such cavities we performed a molecular dynamics simulation where we concentrated on flexible and transient potential binding sites. For several time-points of the simulation we computed receptor-derived pharmacophore models in the so-called hinge region ('Exo site') and screened a large screening compound library [2]. The most potent hit shows inhibition in a non-competitive mode of action.

Published: 11 March 2014

References

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doi:10.1186/1758-2946-6-S1-P48

Cite this article as: Kunze et al.: Targeting flexibility: a structure-based computational study revealing allosteric HIV-1 protease inhibitors. *Journal of Cheminformatics* 2014 **6**(Suppl 1):P48.

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