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Using docking and molecular dynamics to design potent and selective anticancer, anti-osteoclastogenic and anti-malarial compounds

Tuesday, 5 December 2017 11:30 (20 minutes)

Docking and molecular dynanmics simulations using Autodock Vina and Gromacs were used to identify selective inhibitors of cancer-, osteoclastogenic- and malaria-associated proteins. Selective benzotriazepine inhibitors of bromodomain 4 were identified and synthesized. The compounds show micromolar growth inhibition of several cancer cell lines, as well as potent inhibition of osteoclastogenesis without cytotoxicity against osteoclast progenators.

Potent inhibitors of malaria cytochrome bc1 proteins were identified and synthesized. The most potent compound inhibited in vitro asexual malaria parasite growth to 50% of the control at a concentration of 64nM. The compound showed no activity against human HepG2 cells at 5uM.

The present study will discuss how freely available docking and molecular dynamics tools are able to help researchers narrow down new, potent and selective pharmaceutically relevant compounds.

HPC content

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