

Template-based Screening

Date: 2022-07-01

Tags: *1_Drylab 3_Virtual Screening*

Created by: Jesko Kaiser

1 / 1

(_Written by Jesko Kaiser_)

(_Last update: 2022.08.18_)

The shape query of {suvorexant|ligand} was created using {ROCS|software} with {default settings|query generation settings} and the prepared database was subsequently screened using {default settings|screening settings}. The {best|number of stored hits} conformation for each compound was saved and {10|number of selected compounds} virtual hits were selected based on {their overall score|selection criteria}.