

Database Preparation

Date: 2022-07-07

Tags: *1_Drylab 3_Virtual Screening*

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The {Lead Like Now|:subset:} of the {ZINC20|:database:}, containing {3.500.000|number of compounds} compounds was downloaded as {SMILES strings|format}. For each compound {200|number of conformers} were generated using using {Open Eye OMEGA2|software} with {default|:settings:}.

The {Lead Like Now|:subset:} of the {ZINC20|:database:}, containing {3.500.000|number of compounds} compounds was downloaded as {db2.gzformat|file format}.