Jverview

 Clinical trials have already been performed Demonstrated safety Understanding of pharmacokinetics

against a new target

In terms of clinical impact, there are many advantages of docking an existing drug

- Even before a new clinical trial, doctors can prescribe an existing drug for off-label

- use

 Protease is not a new target, but the same procedure can be followed for a new target The steps include downloading the library, converting to AutoDock's ligand format, transferring files to XSEDE Bridges, submitting a job that runs AutoDock Vina, transferring files back to my computer, and performing some analysis

I will describe how I docked the FDA approved drugs against HIV protease

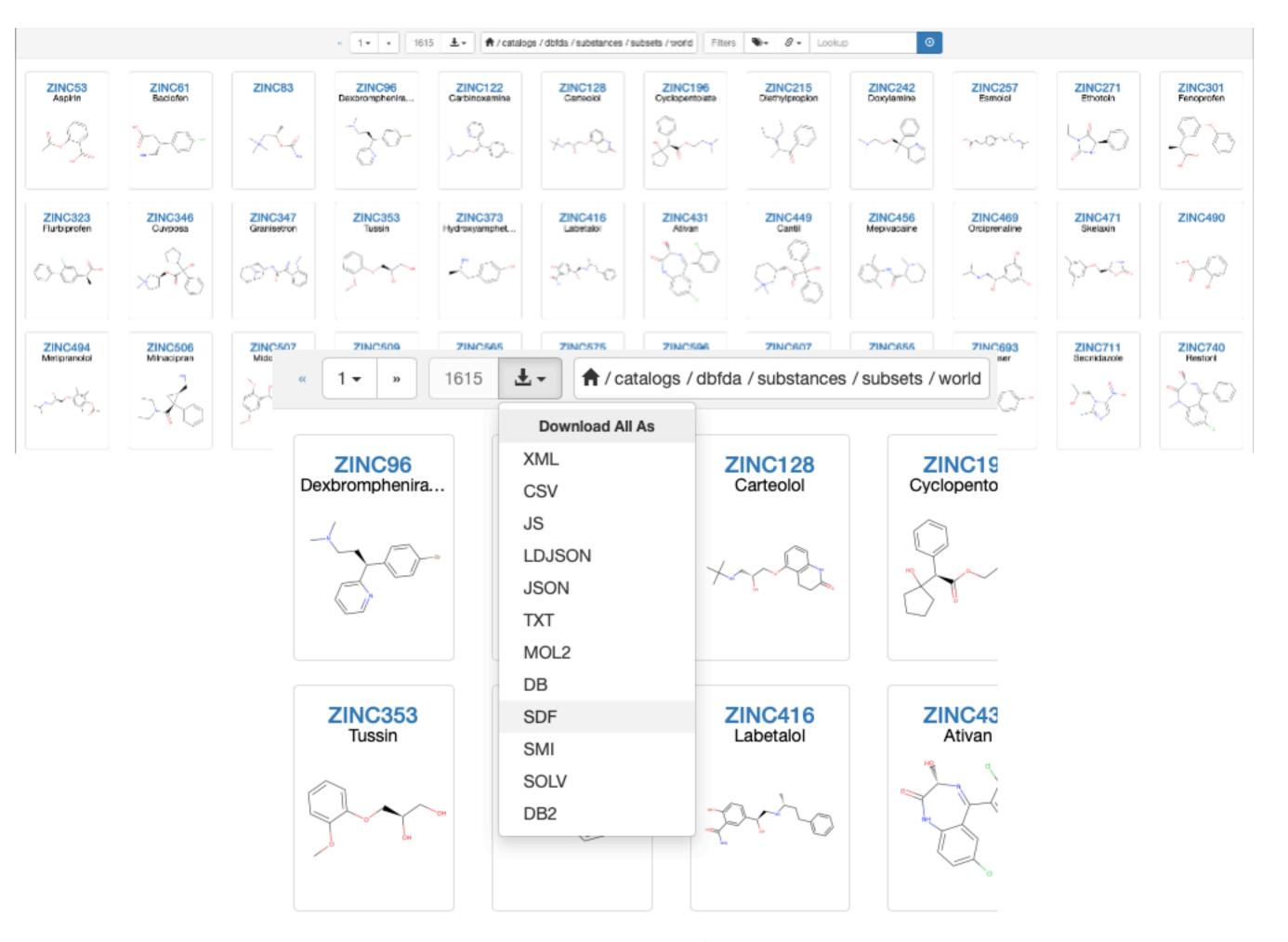
• Files for this tour are on GitHub

Overview

- In terms of clinical impact, there are many advantages of docking an existing drug against a new target
 - Clinical trials have already been performed
 - Demonstrated safety
 - Understanding of pharmacokinetics
 - Even before a new clinical trial, doctors can prescribe an existing drug for off-label use
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Preparing a chemical library

 First, I went to the ZINC15 web site and downloaded all substances in the "DrugBank FDA only" catalog in SDF format. It was a 3.8 MB file.



http://zinc15.docking.org/catalogs/dbfda/substances/subsets/world/