Overview

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  - 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

- I will describe how I docked the FDA approved drugs against HIV protease
  - 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
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15

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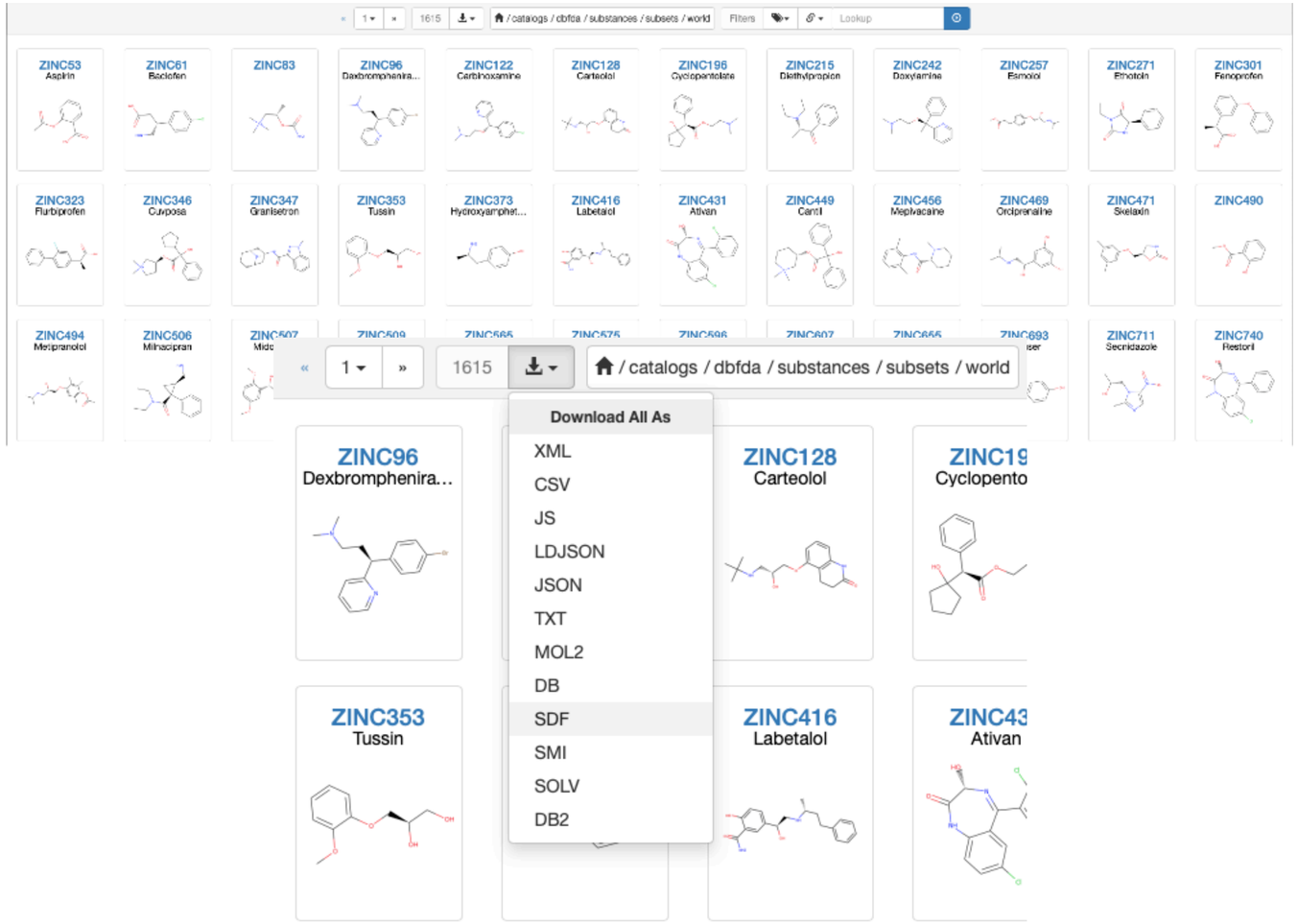
Preparing a chemical library

- 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/