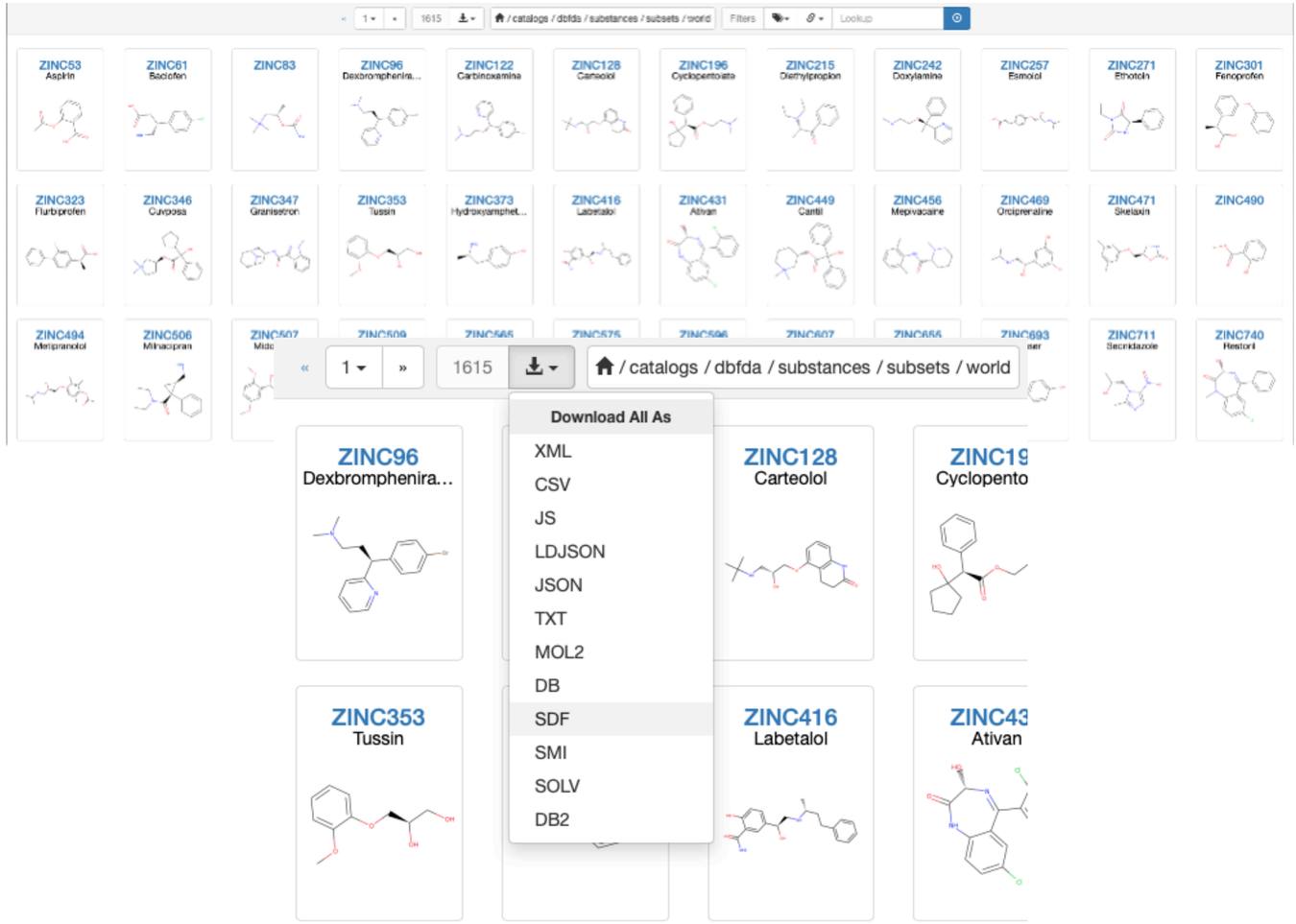
Preparing a chemical library

- 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/

File formatting

- ZINC provides the library in a file format that AutoDock Tools is unfamiliar with, SDF
- To convert to the format that AutoDock uses, I used Open Babel with the command
  - `obabel dbfda-world.sdf -O dbfda.pdbqt -m’
  - -m means that the molecule is split into multiple files
- This generated 1657 pdbqt files in the same directory