

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.

The screenshot displays the ZINC15 website interface. At the top, a navigation bar shows the path: / catalogs / dbfda / substances / subsets / world. Below this, a grid of chemical structures is visible, each labeled with a ZINC ID and a drug name. A download menu is open, showing options for downloading the entire catalog in various formats: XML, CSV, JS, LDJSON, JSON, TXT, MOL2, DB, SDF (highlighted), SMI, SOLV, and DB2. The SDF option is selected, indicating the format used for the download.

<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