

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, there is a navigation bar with a search bar and a 'LookUp' button. Below the navigation bar, a grid of chemical structures is shown, each with a ZINC ID and a name. A 'Download All As' menu is open, showing various file formats: XML, CSV, JS, LDJSON, JSON, TXT, MOL2, DB, SDF (highlighted), SMI, SOLV, and DB2. The background shows a grid of chemical structures, including ZINC53 (Aspirin), ZINC81 (Baclofen), ZINC83, ZINC96 (Dexbrompheniramine), ZINC122 (Carbinoxamine), ZINC128 (Carteolol), ZINC196 (Cyclopentolate), ZINC215 (Dietylpropion), ZINC242 (Doxylamine), ZINC257 (Esmolol), ZINC271 (Ethotoin), ZINC301 (Fenoprofen), ZINC323 (Flurbiprofen), ZINC346 (Cuvposa), ZINC347 (Granisetron), ZINC353 (Tussin), ZINC373 (Hydroxymphet...), ZINC416 (Labetalol), ZINC431 (Ativan), ZINC449 (Cantil), ZINC456 (Mepivacaine), ZINC469 (Orciprenaline), ZINC471 (Skelaxin), ZINC490, ZINC494 (Metipranolol), ZINC506 (Minoxipran), ZINC507 (Mido), ZINC509, ZINC545, ZINC575, ZINC596, ZINC607, ZINC655, ZINC693 (Ser), ZINC711 (Slemdazole), and ZINC740 (Restoril).

<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