

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

- 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
 - Files for this tour are [on GitHub](#)

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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.

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/>