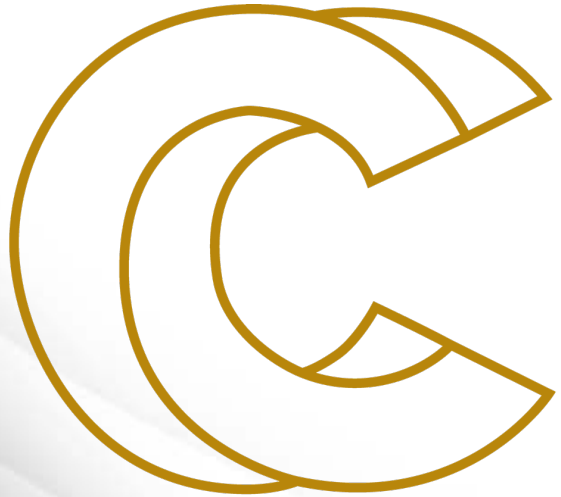

EURO^2

High throughput Virtual Screening with AutoDOCK vina program

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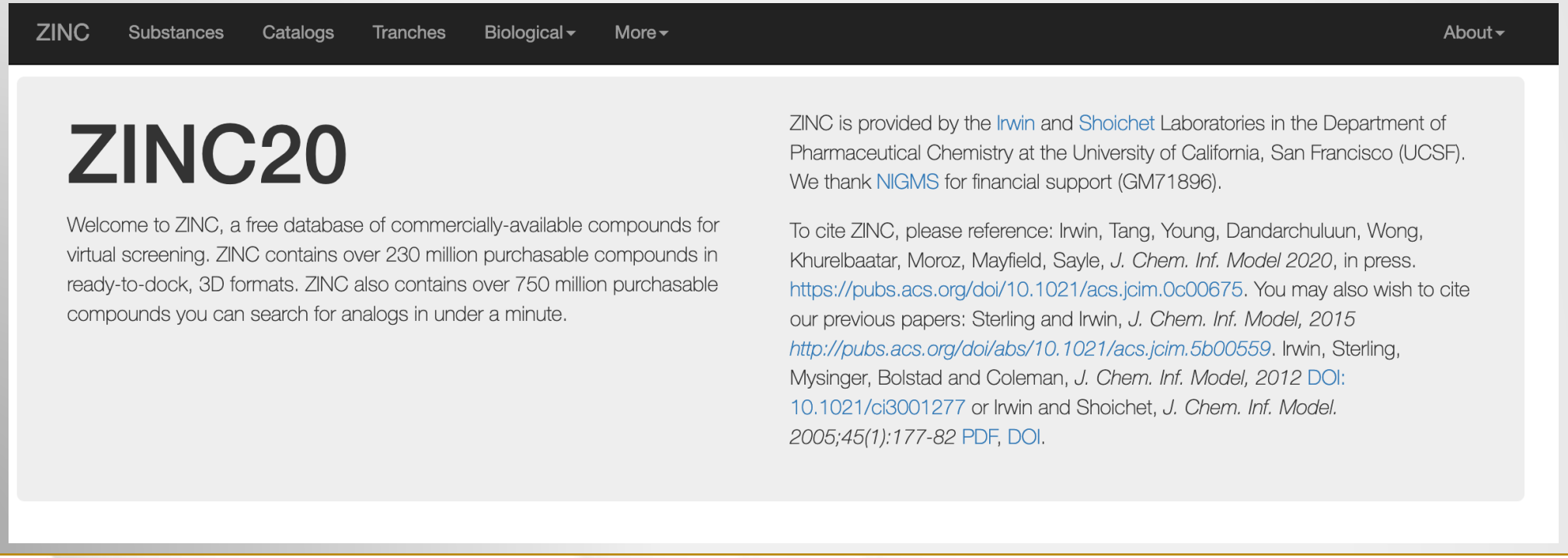
Lesson 2: Preparing a library of ligands for docking

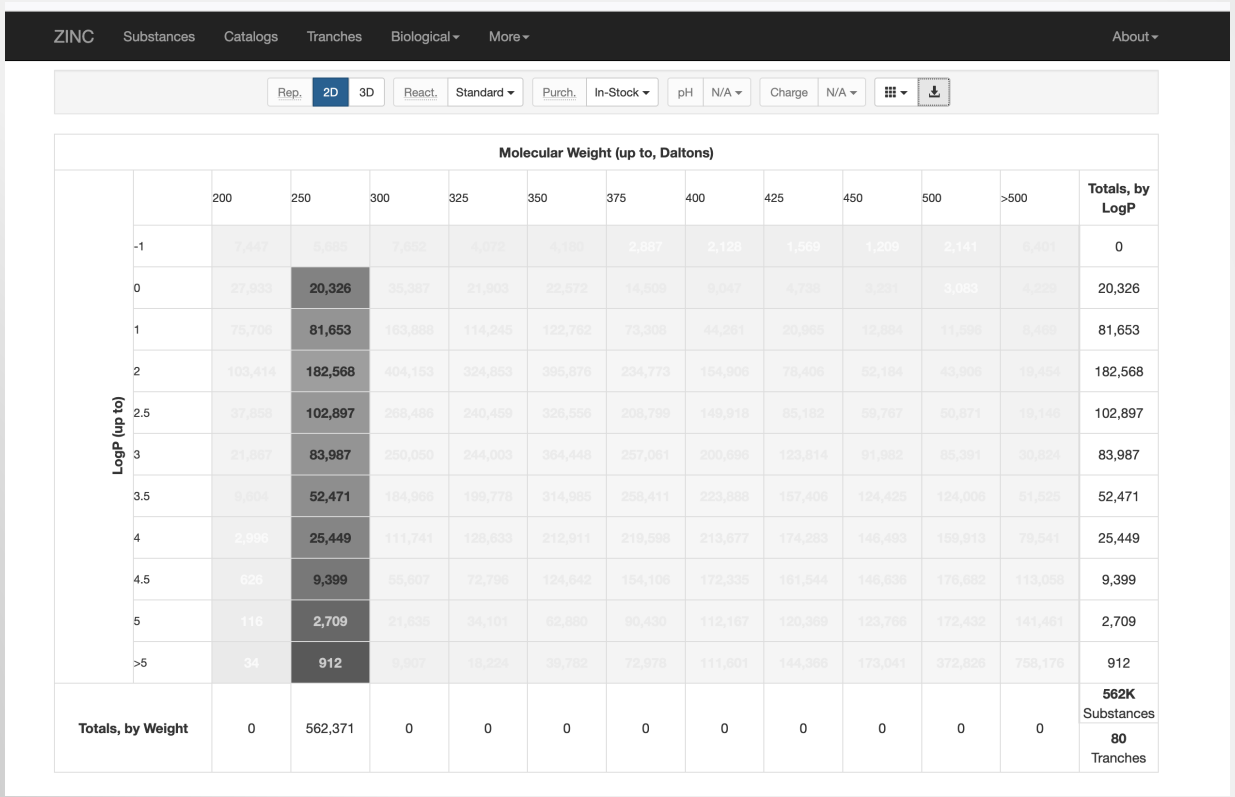
ZINC database offers a huge library of molecules that can be used in docking calculations.

https://zinc.docking.org/



Ligand pdbqt files can be downloaded from ZINC

- Molecule information can be downloaded as the PDBQT file on ZINC
- You can filter molecule based on various criteria like drug-like, lead-like, in-Stock, clean etc.

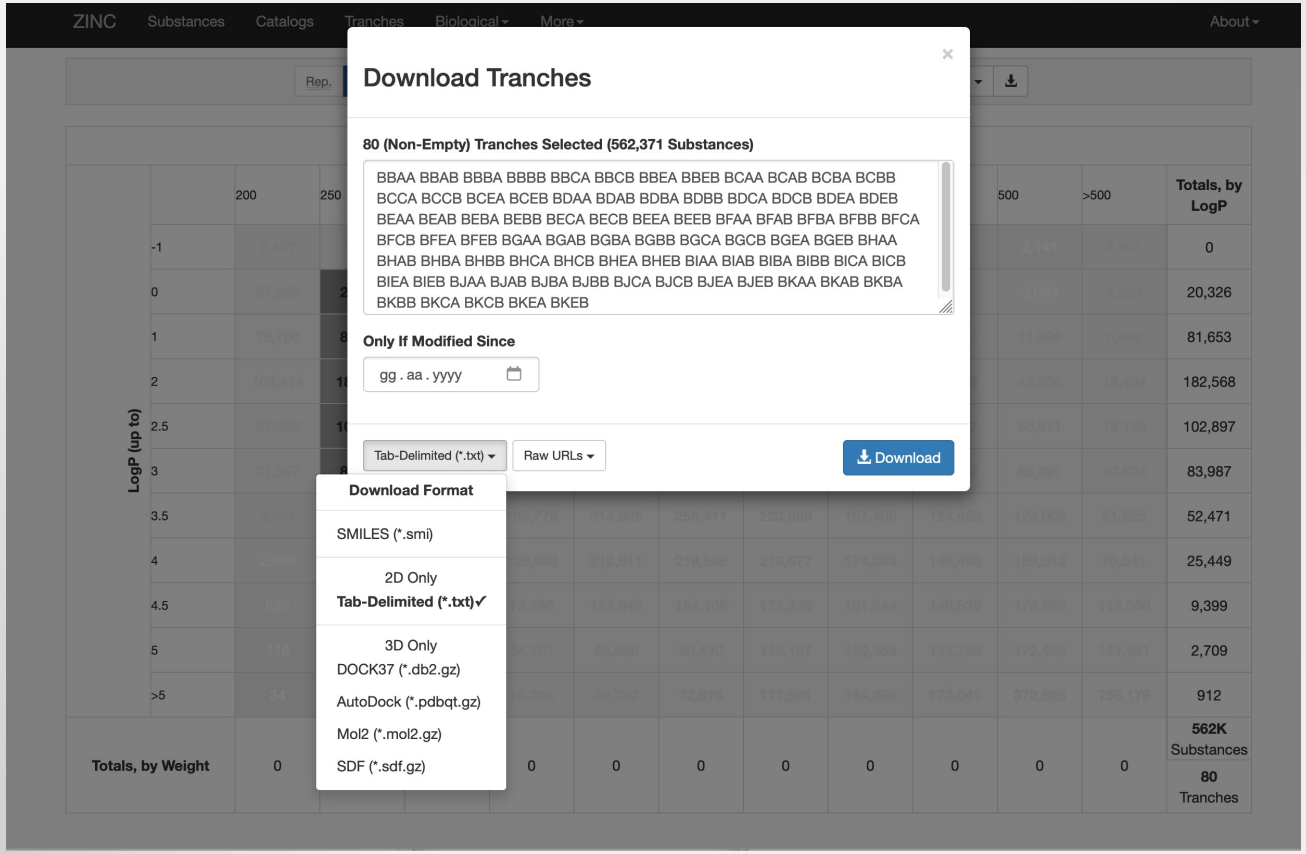


Molecular Weight (up to, Daltons)

LogP (up to)	200	250	300	325	350	375	400	425	450	500	>500	Totals, by LogP
-1	7,447	5,686	7,852	4,072	4,160	2,687	2,128	1,569	1,209	2,141	5,401	0
0	27,933	**20,326**	35,387	21,903	22,572	14,509	8,047	4,738	3,031	3,063	4,329	20,326
1	75,706	**81,653**	163,888	114,245	122,782	73,308	44,261	20,963	12,884	11,596	5,169	81,653
2	103,414	**182,568**	404,153	324,853	395,876	234,773	154,906	78,406	52,184	43,906	19,454	182,568
2.5	37,858	**102,897**	268,486	240,459	326,556	208,799	149,918	85,182	59,767	50,871	19,146	102,897
3	21,867	**83,987**	250,050	244,003	364,448	257,061	200,696	123,814	91,982	85,391	30,824	83,987
3.5	9,604	**52,471**	184,966	199,778	314,985	258,411	223,888	157,406	124,425	124,006	51,525	52,471
4	2,996	**25,449**	111,741	126,633	212,911	219,598	213,677	174,283	146,493	159,913	79,541	25,449
4.5	626	**9,399**	55,607	72,796	124,642	154,106	172,335	161,544	146,636	176,882	113,058	9,399
5	116	**2,709**	21,535	34,101	62,690	90,430	112,167	120,369	123,766	172,432	141,461	2,709
>5	34	**912**	9,807	18,224	39,782	72,978	111,601	144,366	173,041	372,826	758,176	912
Totals, by Weight	0	562,371	0	0	0	0	0	0	0	0	0	**562K** Substances **80** Tranches

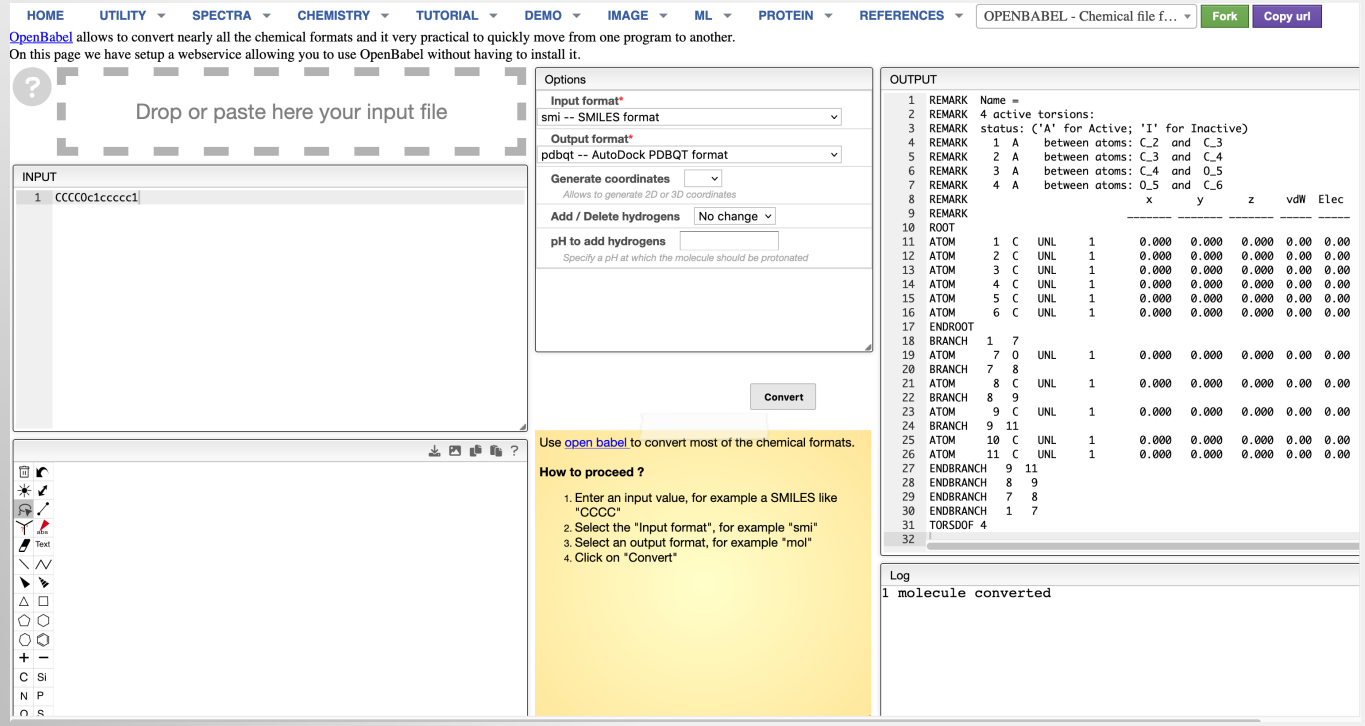
Ligand pdbqt files can be downloaded from ZINC

- You can download molecule information in different formats.



Creating pdbqt files using openbabel program

- PDBQT file format is not a common file format among the molecule databases.
- Another database might not return PDBQT files.
- In this case you can use openbabel program to create pdbqt files
- https://www.cheminfo.org/Chemistry/Cheminformatics/FormatConverter/index.html



Converting a large library of molecules into pdbqt

- If you want to create pdbqts for a large library of molecules you should run openbabel on your local computer or a HPC
- A script in bash environment can be used:
- This assumes you downloaded molecule as mol2.gz files.

```
for file in *.mol2.gz;
 do
 b=`basename $file .mol2.gz` ;
echo $b; mkdir ${b}_pdbqt ;
 cd ${b}_pdbqt;
obabel -i mol2 ../$file  -h --DelNonPolarH  -O new.pdbqt   ---errorlevel 1 -m ;
 cd ./../ ;
done
```

References

- https://zinc.docking.org/
- https://open-babel.readthedocs.io/en/latest/Installation/install.html

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None

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