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# C EURO<sup>2</sup>

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/>

A screenshot of the ZINC database website. The top navigation bar is dark with white text for "ZINC", "Substances", "Catalogs", "Tranches", "Biological", "More", and "About". The main content area has a large "ZINC20" heading. Below it is a welcome message and a paragraph of text. To the right is a paragraph of text and a list of references with hyperlinks.

ZINC

Substances Catalogs Tranches Biological More About

## ZINC20

Welcome to ZINC, a free database of commercially-available compounds for virtual screening. ZINC contains over 230 million purchasable compounds in ready-to-dock, 3D formats. ZINC also contains over 750 million purchasable compounds you can search for analogs in under a minute.

ZINC is provided by the [Irwin](#) and [Shoichet](#) Laboratories in the Department of Pharmaceutical Chemistry at the University of California, San Francisco (UCSF). We thank [NIGMS](#) for financial support (GM71896).

To cite ZINC, please reference: Irwin, Tang, Young, Dandarchuluun, Wong, Khurelbaatar, Moroz, Mayfield, Sayle, *J. Chem. Inf. Model* 2020, in press. <https://pubs.acs.org/doi/10.1021/acs.jcim.0c00675>. You may also wish to cite our previous papers: Sterling and Irwin, *J. Chem. Inf. Model*, 2015 <http://pubs.acs.org/doi/abs/10.1021/acs.jcim.5b00559>. Irwin, Sterling, Mysinger, Bolstad and Coleman, *J. Chem. Inf. Model*, 2012 DOI: [10.1021/ci3001277](https://doi.org/10.1021/ci3001277) or Irwin and Shoichet, *J. Chem. Inf. Model*. 2005;45(1):177-82 [PDF](#), [DOI](#).

# 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.

ZINC Substances Catalogs Tranches Biological More About

Rep. 2D 3D React. Standard Purch. In-Stock pH N/A Charge N/A [Grid Icon] [Download Icon]

Molecular Weight (up to, Daltons)

	200	250	300	325	350	375	400	425	450	500	>500	Totals, by LogP
-1	7,447	5,585	7,852	4,072	4,190	2,897	2,129	1,959	1,209	2,141	5,401	0
0	27,933	<b>20,326</b>	35,397	21,903	22,572	14,508	8,047	4,736	3,231	3,083	4,229	20,326
1	75,708	<b>81,653</b>	163,888	114,245	122,762	73,308	44,261	20,365	12,594	11,596	6,469	81,653
2	103,414	<b>182,568</b>	404,153	324,953	395,876	234,773	154,906	78,406	52,184	43,906	18,454	182,568
2.5	97,958	<b>102,897</b>	258,486	240,459	326,556	208,799	148,918	85,182	59,787	50,871	19,146	102,897
3	21,867	<b>83,987</b>	250,050	244,003	364,448	257,061	206,896	123,814	91,862	85,391	30,824	83,987
3.5	9,804	<b>52,471</b>	184,966	199,775	314,985	258,411	223,888	157,406	124,425	124,006	51,525	52,471
4	2,996	<b>25,449</b>	111,741	128,633	212,911	219,598	213,677	174,283	146,493	159,913	78,541	25,449
4.5	626	<b>9,399</b>	55,607	72,796	124,942	154,106	172,335	161,544	146,636	176,682	113,058	9,399
5	116	<b>2,709</b>	21,635	34,101	62,880	80,430	112,167	120,369	123,786	172,432	141,461	2,709
>5	34	<b>912</b>	9,907	15,224	35,782	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



# 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>

HOME UTILITY SPECTRA CHEMISTRY TUTORIAL DEMO IMAGE ML PROTEIN REFERENCES OPENBABEL - Chemical file f... Fork Copy url

OpenBabel allows to convert nearly all the chemical formats and it very practical to quickly move from one program to another. On this page we have setup a webservice allowing you to use OpenBabel without having to install it.

Drop or paste here your input file

Options

Input format\*  
smi -- SMILES format

Output format\*  
pdbqt -- AutoDock PDBQT format

Generate coordinates  
Allows to generate 2D or 3D coordinates

Add / Delete hydrogens No change

pH to add hydrogens  
Specify a pH at which the molecule should be protonated

Convert

Use open babel to convert most of the chemical formats.

How to proceed ?

1. Enter an input value, for example a SMILES like "CCCC"
2. Select the "Input format", for example "smi"
3. Select an output format, for example "mol"
4. Click on "Convert"

OUTPUT

```
1 REMARK Name =
2 REMARK 4 active torsions:
3 REMARK status: ('A' for Active; 'I' for Inactive)
4 REMARK 1 A between atoms: C_2 and C_3
5 REMARK 2 A between atoms: C_3 and C_4
6 REMARK 3 A between atoms: C_4 and O_5
7 REMARK 4 A between atoms: O_5 and C_6
8 REMARK
9 REMARK
10 REMARK
11 ATOM 1 C UNL 1 0.000 0.000 0.000 0.00 0.00
12 ATOM 2 C UNL 1 0.000 0.000 0.000 0.00 0.00
13 ATOM 3 C UNL 1 0.000 0.000 0.000 0.00 0.00
14 ATOM 4 C UNL 1 0.000 0.000 0.000 0.00 0.00
15 ATOM 5 C UNL 1 0.000 0.000 0.000 0.00 0.00
16 ATOM 6 C UNL 1 0.000 0.000 0.000 0.00 0.00
17 ENDRROOT
18 BRANCH 1 7
19 ATOM 7 O UNL 1 0.000 0.000 0.000 0.00 0.00
20 BRANCH 7 8
21 ATOM 8 C UNL 1 0.000 0.000 0.000 0.00 0.00
22 BRANCH 8 9
23 ATOM 9 C UNL 1 0.000 0.000 0.000 0.00 0.00
24 BRANCH 9 11
25 ATOM 10 C UNL 1 0.000 0.000 0.000 0.00 0.00
26 ATOM 11 C UNL 1 0.000 0.000 0.000 0.00 0.00
27 ENDBRANCH 9 11
28 ENDBRANCH 8 9
29 ENDBRANCH 7 8
30 ENDBRANCH 1 7
31 TORSDOF 4
32
```

Log

```
1 molecule converted
```

# 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>

Copyright



*None*





# Thanks.



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