

Phase 1

**We need the internet
What I did to get diplopterol built**

Start with PubChem

<https://pubchem.ncbi.nlm.nih.gov>

The screenshot shows the homepage of the PubChem website. At the top, there is a navigation bar with various icons and links. Below the navigation bar, the NIH National Library of Medicine logo is displayed. The main heading "Explore Chemistry" is prominently shown in large white text against a blue hexagonal background. Below this, a subtext reads "Quickly find chemical information from authoritative sources". A search bar contains the query "Diplopteron". To the right of the search bar, a table lists compound and gene results. At the bottom of the page, there are statistics: 112M Compounds, 25M Substances, 10M Bioactivities, 10M Literature, 12M Patents, and 884 Data Sources.

Compound	Gene
Diplopteron	sterol-C5-desaturase
2-methyldiplopteron	sterol 14-demethylase
2beta-Methyldiplopteron	Diacyl glycerol kinase
2-Hydroxydiplopteron	sterol 14 alpha-demethylase
Diploptene	Diacyl glycerol kinase epsilon
Ulopteron	diacylglycerol kinase eta
Dinosterol	diacylglycerol kinase iota
Propterol	diacylglycerol kinase zeta
DESMOSTEROL	diacylglycerol kinase beta
Notopteron	diacylglycerol lipase beta

112M Compounds 25M Substances 10M Bioactivities 10M Literature 12M Patents 884 Data Sources

Find your structure and click on 3D



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COMPOUND SUMMARY

Diploptero^l

Cite

Download

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11 Interactions and Pathways

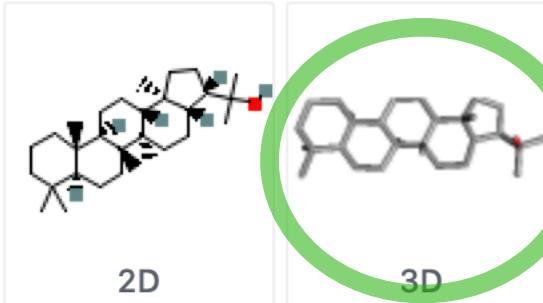
12 Taxonomy

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PubChem CID

164874



[Find Similar Structures](#)

Molecular Formula

C30H52O

Diploptero

Hopan-22-ol

1721-59-1

22-Hydroxyhopane

22-Hopanol

[More...](#)

Molecular Weight

428.7

Dates

Modify

Create
2022-11-19 2005-06-24

Download and save SDF

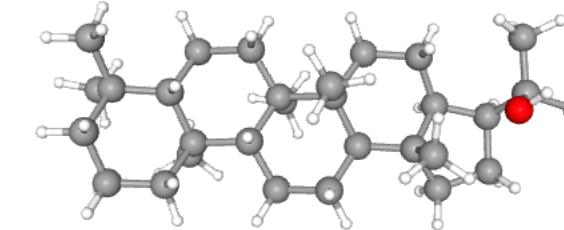
PubChem Diplopterol (Compound) ↑

1.2 3D Conformer ? ↗

Find Similar 3D Structure Download X

Interactive Chemical Structure Model

Ball and Stick Sticks Wire-Frame Space-Filling
 Show Hydrogens Animate



SDF Save Display
JSON Save Display
XML Save Display
ASNT Save Display

+ -

▶ PubChem

2 Names and Identifiers ? ↗

2.1 Computed Descriptors ? ↗

2.1.1 IUPAC Name ? ↗

2-[(3S,3aS,5aR,5bR,7aS,11aS,11bR,13aR,13bS)-5a,5b,8,8,11a,13b-hexamethyl-1,2,3,3a,4,5,6,7,7a,9,10,11,11b,12,13,13a-hexadecahydrocyclopenta[a]chrysene-3-yl]propan-2-ol

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

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That highlighted number? Change it to a 3-4 letter resname

164874												
-OEChem-11212216483D												
83	87	0	1	0	0	0	0	0999	V2000			
5.3334			-0.1568		-1.5790	0	0	0	0	0	0	0
0.5343			-0.5563		-0.1137	C	0	0	1	0	0	0
-0.9731			-0.5360		0.5313	C	0	0	1	0	0	0
1.2276			0.8282		0.2359	C	0	0	1	0	0	0
-1.7644			0.6928		-0.0825	C	0	0	1	0	0	0
2.7618			0.8953		-0.0545	C	0	0	2	0	0	0
-3.3342			0.7390		0.2028	C	0	0	2	0	0	0
3.4060			-0.2999		0.6848	C	0	0	1	0	0	0
-3.9250			-0.6555		-0.2317	C	0	0	1	0	0	0
1.3964			-1.7515		0.4328	C	0	0	0	0	0	0
0.4289			2.0251		-0.3039	C	0	0	0	0	0	0
-1.0252			2.0290		0.1778	C	0	0	0	0	0	0
-1.7410			-1.8551		0.2271	C	0	0	0	0	0	0
2.9147			-1.6455		0.1783	C	0	0	0	0	0	0
4.9049			0.0083		0.7775	C	0	0	2	0	0	0
3.4964			2.0427		0.6773	C	0	0	0	0	0	0
-3.2441			-1.8128		0.5238	C	0	0	0	0	0	0
-5.4906			-0.7531		-0.3047	C	0	0	0	0	0	0
0.4632			-0.7719		-1.6588	C	0	0	0	0	0	0
-0.8989			-0.4321		2.0873	C	0	0	0	0	0	0
-3.9813			1.8303		-0.7079	C	0	0	0	0	0	0
4.9554			1.5536		0.7953	C	0	0	0	0	0	0
3.1159			1.0061		-1.5569	C	0	0	0	0	0	0
-3.6450			1.1174		1.6715	C	0	0	0	0	0	0
-6.0251			0.4093		-1.1769	C	0	0	0	0	0	0
-5.5084			1.7811		-0.7693	C	0	0	0	0	0	0
5.7849			-0.6110		-0.3008	C	0	0	0	0	0	0
-6.1886			-0.7585		1.0673	C	0	0	0	0	0	0
-5.9114			-2.0665		-1.0156	C	0	0	0	0	0	0

Now converting the sdf to a mol2

- Tried openable and it didn't preserve chirality
- Convert <https://datascience.unm.edu/tomcat/biocomp/convert> had correct chirality
- I'd test both and see what happens for you though

The screenshot shows a web browser window with the URL <https://datascience.unm.edu/tomcat/biocomp/convert>. The page title is "Convert - molecule file format conversion (via ChemAxon JChem)". The interface is divided into sections: "Input" (format: sdf:V3 - MDL SDfile, upload: Choose File, no file selected, ...or paste: [large text area]), "Output" (format: mol2 - Tripos Mol2, smiles: [checkboxes for name, arom, stereo, uniq, r1, H, SDData, header], SDF: V3000, generic: +2D, +3D, +IUPAC name, gzip, parts2mols, enummarkush), and "Misc" (verbose). At the bottom, there is a "Results" section showing "mols in: 1", "mols out: 1", and "errors: 0", and a "download convert_out.mol2 (5.9KB)" button.

Mol2 file

```
@<TRIPOS>MOLECULE
DPOP
83 87 1
SMALL
USER_CHARGES
@<TRIPOS>ATOM
1  O1      5.3334   -0.1568   -1.5790  0.3 1  noname  -0.3900
2  C1      0.5343   -0.5563   -0.1137  C.3 1  noname  -0.0235
3  C2     -0.9731   -0.5360    0.5313  C.3 1  noname  -0.0235
4  C3      1.2276    0.8282    0.2359  C.3 1  noname  -0.0297
5  C4     -1.7644    0.6928   -0.0825  C.3 1  noname  -0.0297
6  C5      2.7618    0.8953   -0.0545  C.3 1  noname  -0.0260
7  C6     -3.3342    0.7390    0.2028  C.3 1  noname  -0.0258
8  C7      3.4060   -0.2999    0.6848  C.3 1  noname  -0.0301
9  C8     -3.9250   -0.6555   -0.2317  C.3 1  noname  -0.0305
10 C9      1.3964   -1.7515    0.4328  C.3 1  noname  -0.0467
11 C10     0.4289    2.0251   -0.3039  C.3 1  noname  -0.0491
12 C11     -1.0252    2.0290    0.1778  C.3 1  noname  -0.0491
13 C12     -1.7410   -1.8551    0.2271  C.3 1  noname  -0.0467
14 C13     2.9147   -1.6455    0.1783  C.3 1  noname  -0.0490
15 C14     4.9049    0.0083    0.7775  C.3 1  noname  -0.0095
16 C15     3.4964    2.0427    0.6773  C.3 1  noname  -0.0469
17 C16     -3.2441   -1.8128    0.5238  C.3 1  noname  -0.0488
18 C17     -5.4906   -0.7531   -0.3047  C.3 1  noname  -0.0320
19 C18     0.4632   -0.7719   -1.6588  C.3 1  noname  -0.0588
20 C19     -0.8989   -0.4321    2.0873  C.3 1  noname  -0.0588
21 C20     -0.0010    0.0000    0.7070  C.3 1  noname  -0.0470
Use sed 's/noname/<newname>/g' file.mol2 to fix
```

Paramchem

- Go to <https://cgenff.umaryland.edu>
- Make an account (may take 5 min to verify may take a day)

The screenshot shows a web browser window with the URL paramchem.org in the address bar. The page title is "New User Registration / Login". On the left, there is a logo featuring a molecular structure with the text "CGenFF" overlaid. The main content area is titled "New User Registration". A note at the top states: "This page is for new users to register an account with CGenFF. Once registered and activated, the user can submit files using the CGenFF web interface. Please fill out the following form to generate a CGenFF User name and Password. You will be sent an email link to activate your CGenFF User Account." Below this, a "Note" section says: "All fields are required. New account registration is currently restricted to educational and research institutions". The "Register Account" form contains fields for Name, Institution, Department, E-mail, Username, and Password. Each field has a corresponding note below it. There is also a "Check email & username availability" button.

New User Registration / Login

New User Registration

This page is for new users to register an account with CGenFF. Once registered and activated, the user can submit files using the CGenFF web interface. Please fill out the following form to generate a CGenFF User name and Password. You will be sent an email link to activate your CGenFF User Account.

Note:
All fields are required.
New account registration is currently restricted to educational and research institutions

Register Account

*Name:

Note : Name should be at least 3 characters long. It must begin with a letter. Allowed characters: a-z, 0-9, hyphen and white space.

*Institution:

Note : Institution should be at least 2 characters long. Allowed characters: a-z, 0-9, hyphen, dot, single-quote, ampersand and white space.

*Department:

Note : Department should be at least 2 characters long. Allowed characters: a-z, 0-9, hyphen, dot, single-quote, ampersand and white space

*E-mail:

*Username:

[Check email & username availability](#)

Note : Username should be 3 - 12 characters long. It must begin with a letter and should not have spaces in between.

*Password:

Upload your mol2 file, and I leave default option

Output Data

THIS SITE IS VERIFIED TO WORK WITH FIREFOX 17 AND NEWER, CHROME 23 AND NEWER, AND INTERNET EXPLORER 10 AND NEWER. INTERNET EXPLORER 9 AND OLDER ARE KNOWN NOT TO WORK.

RESTRICTIONS

Please upload your molecule in mol2 format. It is important that all hydrogens are present, in the correct protonation and tautomeric states, and that the bond orders are correct. The xyz coordinates are not critical. The maximum number of atoms is 384, and there is a limit of 100 molecules per user per week.

Important notes:

** CGenFF should **NOT** be used for biological macromolecules! Only use CGenFF for small organic molecules; the highly optimized CHARMM force field for **Proteins, Nucleic Acids, Carbohydrates and Lipids** can be downloaded freely from the **CHARMM Force Field** page and can readily be combined with CGenFF.

** Apart from the mol2 format, it is also possible to upload files in sdf and pdb format. Such files are internally converted to mol2 using Open Babel 2.3.0. However, we cannot guarantee the correctness of this conversion; therefore, it is highly recommended to download the intermediary mol2 file and carefully inspect its connectivity and bond orders for errors.

** For more info, see the [summary of output data and its utilization](#), the [usage information for the CGenFF program](#) and the [FAQ](#).

Total number of files uploaded: 0 of 150 for the week ending November 27, 2022

[Click to upload new file](#)

Input
[convert_out.mol2](#)

Output
[convert_out.str](#)
Click to download/view atomtypes, charges and parameters

Error / Warning
No error/warnings found

Curl, or wget
Copy and paste is a LAST resort

str file

- We can split the str file into 2 other files
 - The rtf file and the prm file
- I'm not convinced you **need** to though
 - Once you get this file, you will need to manually read through and compare the bonds, angles, and dihedrals to at the atom types for another molecule using the charmm36 force field
 - CG301 has a more standard charmm atom type

<pre>* Toppar stream file generated by * CHARMM General Force Field (CGenFF) program version 2.5 * For use with CGenFF version 4.6 * read rtf card append * Topologies generated by * CHARMM General Force Field (CGenFF) program version 2.5 * 36 1 ! "penalty" is the highest penalty score of the associated parameters. ! Penalties lower than 10 indicate the analogy is fair; penalties between 10 ! and 50 mean some basic validation is recommended; penalties higher than ! 50 indicate poor analogy and mandate extensive validation/optimization. RESI 164874 0.000 ! param penalty= 13.100 ; charge penalty= 20.856 GROUP ! CHARGE CH_PENALTY ATOM 01 OG311 -0.598 ! 15.289 ATOM C1 CG301 -0.015 ! 11.913 ATOM C2 CG301 0.009 ! 8.615 ATOM C3 CG311 -0.083 ! 7.819 ATOM C4 CG311 -0.090 ! 3.938 ATOM C5 CG3RC1 0.054 ! 1.344 ATOM C6 CG301 0.013 ! 1.018 ATOM C7 CG3RC1 -0.150 ! 10.512 ATOM C8 CG311 -0.101 ! 0.853 ATOM C9 CG321 -0.174 ! 7.234 ATOM C10 CG321 -0.179 ! 0.379 ATOM C11 CG321 -0.185 ! 0.379 ATOM C12 CG321 -0.181 ! 5.413 ATOM C13 CG321 -0.188 ! 0.640 ATOM C14 CG3C51 -0.056 ! 20.856 ATOM C15 CG3C52 -0.163 ! 0.812 ATOM C16 CG321 -0.181 ! 0.512 ATOM C17 CG301 0.001 ! 0.764</pre>	<pre>read param card flex append * Parameters generated by analogy by * CHARMM General Force Field (CGenFF) program version 2.5 * ! Penalties lower than 10 indicate the analogy is fair; penalties between 10 ! and 50 mean some basic validation is recommended; penalties higher than ! 50 indicate poor analogy and mandate extensive validation/optimization. BONDS CG301 CG301 222.50 1.5000 ! 164874 , from CG301 CG311, penalty= 8 CG301 CG3C51 222.50 1.5280 ! 164874 , from CG311 CG3C51, penalty= 8 ANGLES CG301 CG301 CG311 58.35 113.50 11.16 2.56100 ! 164874 , from CG311 CG301 CG311, penalty= 1.2 CG301 CG301 CG321 58.35 113.50 11.16 2.56100 ! 164874 , from CG311 CG301 CG321, penalty= 1.2 CG301 CG301 CG331 58.35 113.50 11.16 2.56100 ! 164874 , from CG311 CG301 CG331, penalty= 1.2 CG331 CG301 CG3C51 53.35 108.50 8.00 2.56100 ! 164874 , from CG331 CG311 CG3C51, penalty= 8 CG3C51 CG301 OG311 75.70 110.10 ! 164874 , from CG3RC1 CG311 OG311, penalty= 9.5 CG301 CG311 CG301 52.00 108.00 ! 164874 , from CG301 CG311 CG311, penalty= 1.2 CG301 CG311 CG3RC1 53.35 103.70 8.00 2.56100 ! 164874 , from CG311 CG311 CG3RC1, penalty= 1.2 CG301 CG3C51 CG3C52 58.00 115.00 8.00 2.56100 ! 164874 , from CG311 CG3C51 CG3C52, penalty= 1.2 CG301 CG3C51 CG3RC1 52.00 108.00 ! 164874 , from CG311 CG3C51 CG3RC1, penalty= 1.2 CG301 CG3C51 HGA1 34.60 110.10 22.53 2.17900 ! 164874 , from CG311 CG3C51 HGA1, penalty= 1.2 CG331 CG3RC1 CG3C52 58.35 113.50 11.16 2.56100 ! 164874 , from CG331 CG3RC1 CG3C51, penalty= 0.4 DIHEDRALS CG311 CG301 CG301 CG311 0.2000 3 0.00 ! 164874 , from CG311 CG301 CG311 CG311, penalty= 8 CG311 CG301 CG301 CG321 0.2000 3 0.00 ! 164874 , from CG311 CG301 CG311 CG321, penalty= 8 CG311 CG301 CG301 CG331 0.2000 3 0.00 ! 164874 , from CG331 CG301 CG311 CG311, penalty= 8 CG321 CG301 CG301 CG321 0.2000 3 0.00 ! 164874 , from CG321 CG301 CG311 CG321, penalty= 8 CG321 CG301 CG301 CG331 0.2000 3 0.00 ! 164874 , from CG331 CG301 CG311 CG321, penalty= 8 CG331 CG301 CG301 CG331 0.2000 3 0.00 ! 164874 , from CG331 CG301 CG311 CG331, penalty= 8 CG301 CG301 CG311 CG301 0.2000 3 0.00 ! 164874 , from CG311 CG301 CG311 CG311, penalty= 2.4 CG301 CG301 CG311 CG321 0.2000 3 0.00 ! 164874 , from CG311 CG301 CG311 CG321, penalty= 1.2 CG301 CG301 CG311 CG3RC1 0.2000 3 0.00 ! 164874 , from CG301 CG311 CG311 CG3RC1, penalty= 8</pre>
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Phase 2

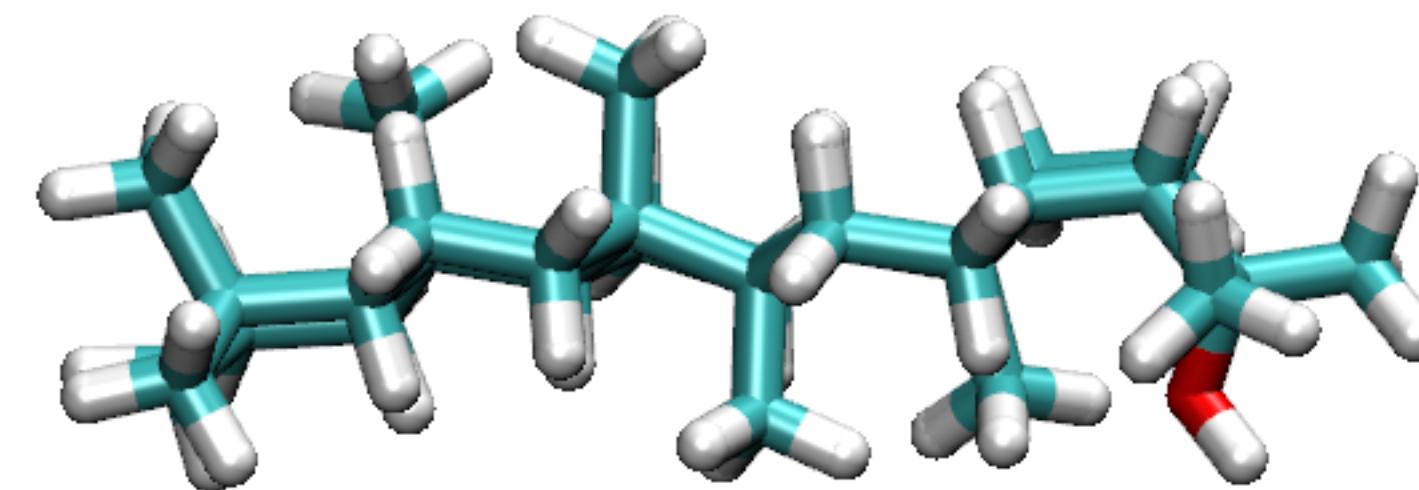
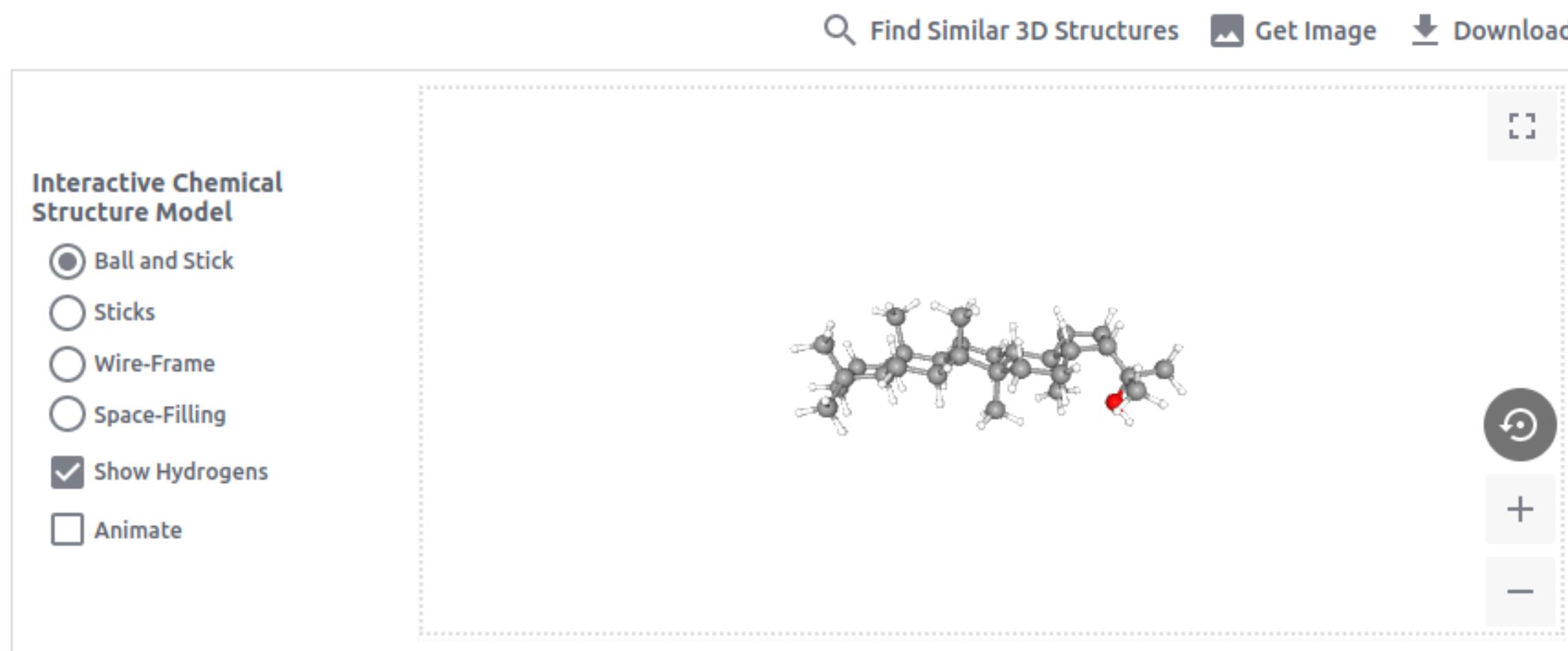
VMD

Pymol might also work, really don't know how to use it

- Go to https://www.ks.uiuc.edu/Research/vmd/script_library/scripts/write_charmm_crd/ and download the write_charmm_crd.tcl file

VMD Chirality Check

- Load your mol2 file into VMD
- First, check chirality
- If the pubchem structure and our structure do not match, there's something wrong converting the sdf to mol2 file, I'd do a google search..

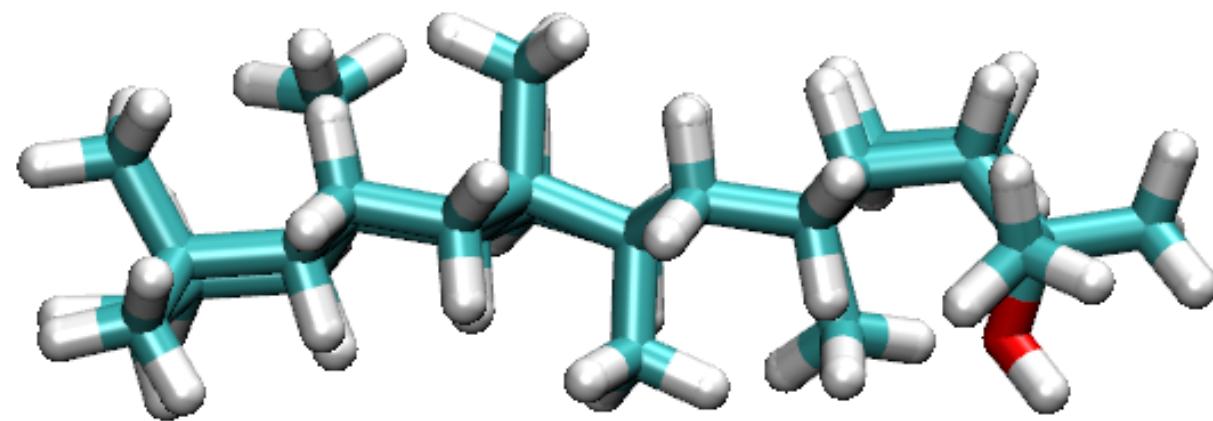


Names and Identifiers



VMD The atom names

- The structure has a “default” naming scheme
- To get these on charmm-gui, it needs an update
- Take a look at cholesterol’s naming scheme and try to implement it
 - I do not have a script for this, you’ll need to do it manually, but the oxygen should be O3 (used for orientation I think)



VMD Atom Name Change

- In vmd we can map the existing atom names to updated names

```
set sel [atomselect top " all " ]
```

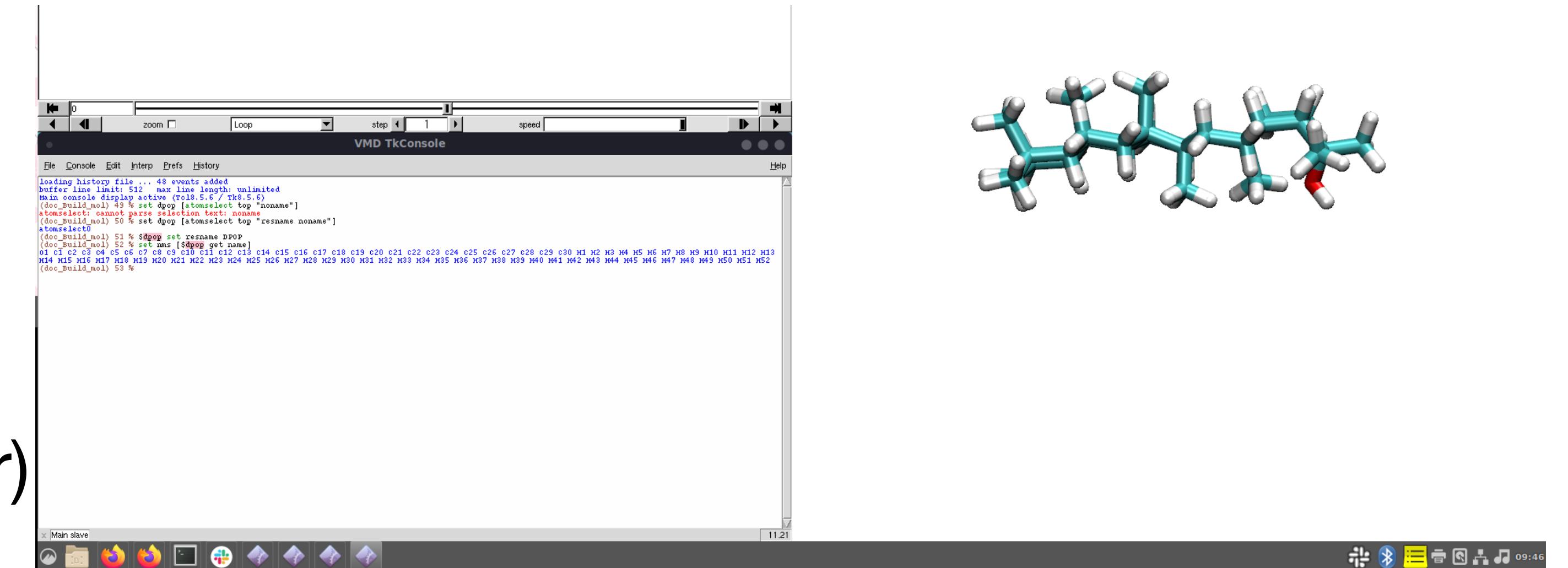
```
set name_list [$sel get name]
```

```
set new_name [list <new names>]
```

```
;#(MUST be in the same order)
```

```
$sel set name ${new_name}
```

Save the updated naming scheme as a new mol2 file



VMD Make a crd file

- Now we need a crd file with the updated names
- Load in the new mol2 file
- You will need the write_charmm_crd.tcl file

```
source $PATH/  
write_charmm_crd.tcl
```

```
writecharmmcoor " name.crd "  
top expanded;#/normal (I think  
expanded is the better option)
```

- You can use the coord file for the next step but I think the mol2 file should be fine..

```
wrong # args: should be "writecharmmcoor filename usemolid outtype"  
(doc_Build_mol) 55 % writecharmmcoor "dpop.crd" 0 extend  
Done with conversion  
(doc_Build_mol) 56 % writecharmmcoor "dpop.crd" 0 ext  
Done with conversion  
(doc_Build_mol) 57 % writecharmmcoor "dpop.crd" 0 extended  
Done with conversion  
(doc_Build_mol) 58 % writecharmmcoor "dpop.crd" 0 expanded  
Done with conversion  
/A...@...:14 mol1 co e
```

VMD Make psf file

- With VMD, we'll use psfgen the crd file and the str file
- Open psfgen (under extension>model)
- Load the str file into psfgen
- Select all
- Check the output psf file

Phase 3

Check files and debug

Check PSF

I'd use sed -i "s/input/new/g" name.psf to fix everything up

```
lmm@MORIUS: ~/ODE1/ODE_BUILD_MOL          lmm@MORIUS: ~/CENSER/ODE1/ODE_BUILD_MOL
SF EXT                                         SF EXT CMAP XPLOR

 3 !NTITLE
REMARKS original generated structure x-plor psf file
REMARKS topology dpop_autopsf-temp.top
REMARKS segment X01 { first none; last none; auto angles dihedrals }

83 !NATOM
 1 X01   1     DPOP   O1    OG311  -0.598000  15.9994  0
 2 X01   1     DPOP   C1    CG301  -0.015000  12.0110  0
 3 X01   1     DPOP   C2    CG301  0.009000  12.0110  0
 4 X01   1     DPOP   C3    CG311  -0.083000  12.0110  0
 5 X01   1     DPOP   C4    CG311  -0.090000  12.0110  0
 6 X01   1     DPOP   C5    CG3RC1 0.054000  12.0110  0
 7 X01   1     DPOP   C6    CG301  0.013000  12.0110  0
 8 X01   1     DPOP   C7    CG3RC1 -0.150000  12.0110  0
 9 X01   1     DPOP   C8    CG311  -0.101000  12.0110  0
10 X01   1     DPOP   C9    CG321  -0.174000  12.0110  0
11 X01   1     DPOP   C10   CG321  -0.179000  12.0110  0
12 X01   1     DPOP   C11   CG321  -0.185000  12.0110  0
13 X01   1     DPOP   C12   CG321  -0.181000  12.0110  0
14 X01   1     DPOP   C13   CG321  -0.188000  12.0110  0
15 X01   1     DPOP   C14   CG3C51 -0.056000  12.0110  0
16 X01   1     DPOP   C15   CG3C52 -0.163000  12.0110  0
17 X01   1     DPOP   C16   CG321  -0.181000  12.0110  0
18 X01   1     DPOP   C17   CG301  0.001000  12.0110  0
19 X01   1     DPOP   C18   CG331  -0.266000  12.0110  0
20 X01   1     DPOP   C19   CG331  -0.271000  12.0110  0
21 X01   1     DPOP   C20   CG321  -0.182000  12.0110  0
22 X01   1     DPOP   C21   CG3C52 -0.204000  12.0110  0
23 X01   1     DPOP   C22   CG331  -0.272000  12.0110  0
24 X01   1     DPOP   C23   CG331  -0.271000  12.0110  0
```

```
3 !NTITLE
* GENERATED BY CHARMM-GUI (HTTP://WWW.CHARMM-GUI.ORG) V3.7 ON AUG, 30. 2022. JOB
* READ PDB, MANIPULATE STRUCTURE IF NEEDED, AND GENERATE TOPOLOGY FILE
* DATE: 8/30/22 17:51:40 CREATED BY USER: apache

83 !NATOM
 1 HETA   1     DPO   O1    OG311  -0.598000  15.9994  0
 2 HETA   1     DPO   C12   CG301  -0.150000E-01 12.0110  0
 3 HETA   1     DPO   C13   CG301  0.900000E-02 12.0110  0
 4 HETA   1     DPO   C11   CG311  -0.830000E-01 12.0110  0
 5 HETA   1     DPO   C16   CG311  -0.900000E-01 12.0110  0
 6 HETA   1     DPO   C8    CG3RC1 0.540000E-01 12.0110  0
 7 HETA   1     DPO   C20   CG301  0.130000E-01 12.0110  0
 8 HETA   1     DPO   C7    CG3RC1 -0.150000 12.0110  0
 9 HETA   1     DPO   C19   CG311  -0.101000 12.0110  0
10 HETA   1     DPO   C9    CG321  -0.174000 12.0110  0
11 HETA   1     DPO   C14   CG321  -0.179000 12.0110  0
12 HETA   1     DPO   C15   CG321  -0.185000 12.0110  0
13 HETA   1     DPO   C18   CG321  -0.181000 12.0110  0
14 HETA   1     DPO   C10   CG321  -0.188000 12.0110  0
15 HETA   1     DPO   C6    CG3C51 -0.560000E-01 12.0110  0
16 HETA   1     DPO   C4    CG3C52 -0.163000 12.0110  0
17 HETA   1     DPO   C17   CG321  -0.181000 12.0110  0
18 HETA   1     DPO   C21   CG301  0.100000E-02 12.0110  0
19 HETA   1     DPO   C26   CG331  -0.266000 12.0110  0
20 HETA   1     DPO   C27   CG331  -0.271000 12.0110  0
21 HETA   1     DPO   C22   CG321  -0.182000 12.0110  0
22 HETA   1     DPO   C5    CG3C52 -0.204000 12.0110  0
23 HETA   1     DPO   C25   CG331  -0.272000 12.0110  0
24 HETA   1     DPO   C28   CG331  -0.271000 12.0110  0
25 HETA   1     DPO   C24   CG321  -0.186000 12.0110  0
26 HETA   1     DPO   C23   CG321  -0.175000 12.0110  0
27 HETA   1     DPO   C3    CG301  0.210000 12.0110  0
28 HETA   1     DPO   C29   CG331  -0.271000 12.0110  0
```

Check Crd

Didn't grab the file before the change.. HETA was originally {}
So sed ... s/{}-/HETA/g ...

* CHARMM coordinates generated from VM								
83	EXT							
1	1	DPOP	O1	5.3333997726	-0.1568000019	-1.5789999962	HETA	1 0.0000000000
2	1	DPOP	C1	0.5343000293	-0.5562999845	-0.1137000024	HETA	1 0.0000000000
3	1	DPOP	C2	-0.9731000066	-0.5360000134	0.5313000083	HETA	1 0.0000000000
4	1	DPOP	C3	1.2275999784	0.8281999826	0.2358999997	HETA	1 0.0000000000
5	1	DPOP	C4	-1.7644000053	0.6927999854	-0.0825000033	HETA	1 0.0000000000
6	1	DPOP	C5	2.7618000507	0.8952999711	-0.0544999987	HETA	1 0.0000000000
7	1	DPOP	C6	-3.3341999054	0.7390000224	0.2028000057	HETA	1 0.0000000000
8	1	DPOP	C7	3.4059998989	-0.2998999953	0.6848000288	HETA	1 0.0000000000
9	1	DPOP	C8	-3.9249999523	-0.6554999948	-0.2317000031	HETA	1 0.0000000000
10	1	DPOP	C9	1.3963999748	-1.7515000105	0.4327999949	HETA	1 0.0000000000
11	1	DPOP	C10	0.4289000034	2.0250999928	-0.3039000034	HETA	1 0.0000000000
12	1	DPOP	C11	-1.0252000093	2.0290000439	0.1777999997	HETA	1 0.0000000000
13	1	DPOP	C12	-1.7410000563	-1.8551000357	0.2270999998	HETA	1 0.0000000000
14	1	DPOP	C13	2.9147000313	-1.6454999447	0.1782999933	HETA	1 0.0000000000
15	1	DPOP	C14	4.9049000740	0.0082999999	0.7774999738	HETA	1 0.0000000000
16	1	DPOP	C15	3.4964001179	2.0427000523	0.6772999763	HETA	1 0.0000000000
17	1	DPOP	C16	-3.2441000938	-1.8128000498	0.5238000154	HETA	1 0.0000000000
18	1	DPOP	C17	-5.4906001091	-0.7530999780	-0.3046999872	HETA	1 0.0000000000
19	1	DPOP	C18	0.4632000029	-0.7718999982	-1.6588000059	HETA	1 0.0000000000
20	1	DPOP	C19	-0.8988999724	-0.4320999980	2.0873000622	HETA	1 0.0000000000
21	1	DPOP	C20	-3.9813001156	1.8302999735	-0.7078999877	HETA	1 0.0000000000
22	1	DPOP	C21	4.9553999901	1.5535999537	0.7953000069	HETA	1 0.0000000000
23	1	DPOP	C22	3.1159000397	1.0061000586	-1.5569000244	HETA	1 0.0000000000
24	1	DPOP	C23	-3.6449999809	1.1174000502	1.6714999676	HETA	1 0.0000000000
25	1	DPOP	C24	-6.0251002312	0.4092999995	-1.1769000292	HETA	1 0.0000000000
26	1	DPOP	C25	-5.5083999634	1.7811000347	-0.7692999840	HETA	1 0.0000000000

Final Check using Charmm-Gui

Some [lectures](#), [job postings](#), and [FAQ](#) are now available. See [update log](#) for update history and [giving](#) for donation. [Contact](#) info is given below.

[Log In](#) [User P](#)

Input Generator

Force Field Converter

Force Field Converter takes CHARMM PSF and CRD files and produces input files with the selected force field.

Please note that

- The uploaded PSF and CRD files should be CHARMM FF compatible.
- Force Field Converter uses the latest version of FFs for the conversion / input generation.
- If the system contains ligand molecule(s), the corresponding ligand FF should be uploaded.
- Currently, Force Field Converter is limited to:
 - CHARMM FF: NAMD, GROMACS, Amber, OpenMM, GENESIS, Desmond, and LAMMPS input generation
 - Amber FF: GROMACS, Amber, and OpenMM input generation
 - OPLS-AA/M FF: NAMD and GROMACS input generation

Reference for Force Field Converter:

S. Jo, T. Kim, V.G. Iyer, and W. Im (2008)
CHARMM-GUI: A Web-based Graphical User Interface for CHARMM. *J. Comput. Chem.* 29:1859-1865
J. Lee, M. Hitzenberger, M. Rieger, N.R. Kern, M. Zacharias, and W. Im (2020)
CHARMM-GUI supports the Amber force fields. *J. Chem. Phys.* 153:035103

Upload PSF File: no file selected

Upload Coord. File: no file selected
Coordinate File Format: CHARMM CRD

Upload Additional Topology and Parameter Files:
File Type: STR no file selected

Setup PBC:

Next Step: [Check System Components](#) 

- Input your psf, crd, and str file (all should have the same file name)
- If not, you may have a naming, spacing, or I've missed something here
- If it works, charmm-gui will compile and you're good!
- These are the files you can request to have uploaded to charmm-gui