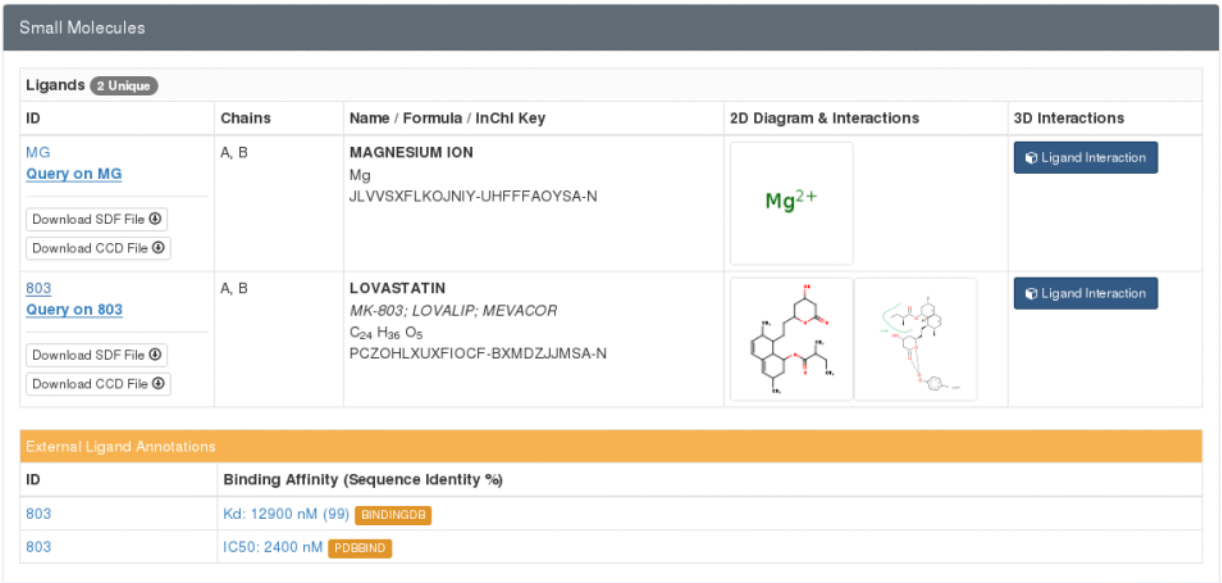
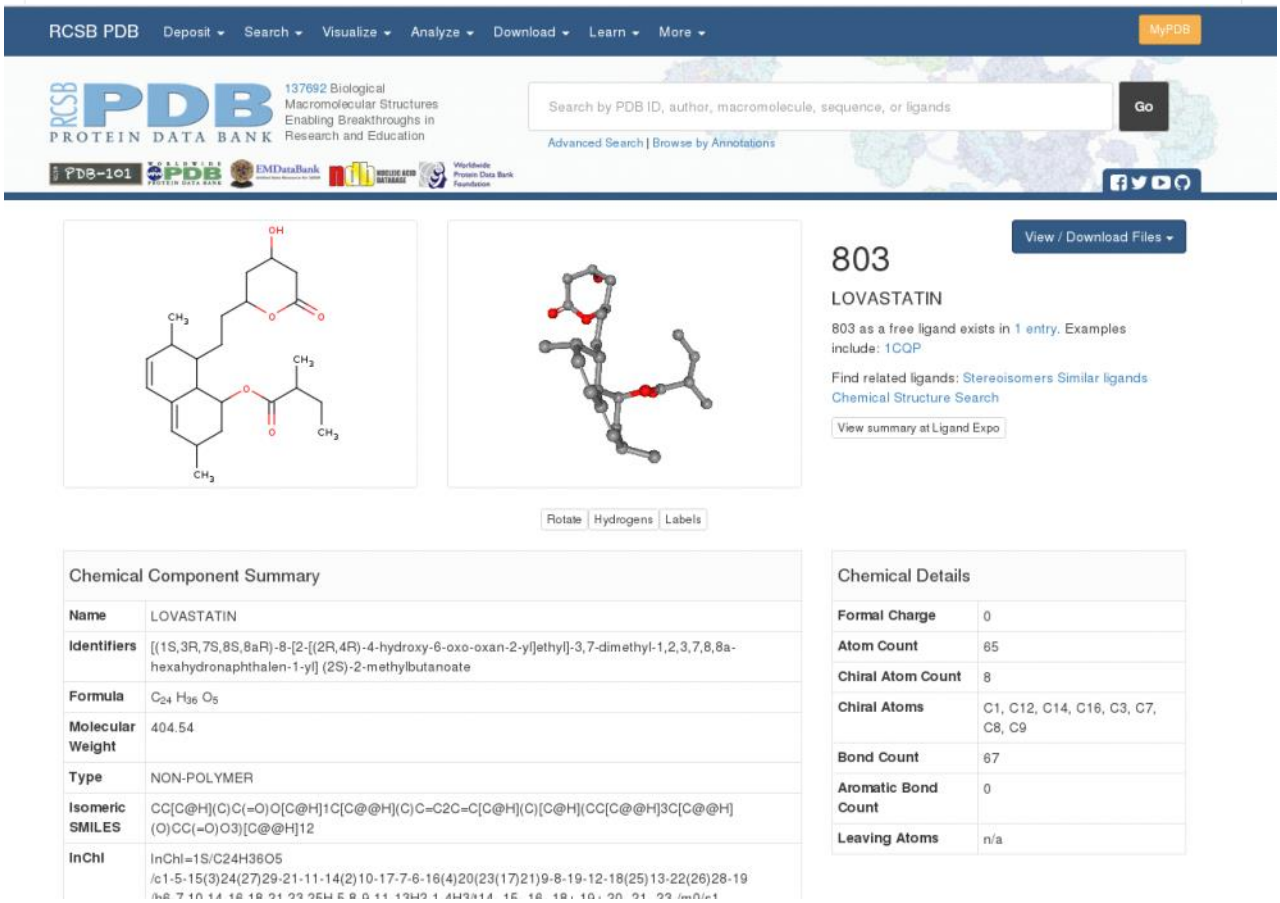
Ligand PDB

2018年2月23日　　下午 03:21

Download statin pdb from LigExpo





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PDB Chemical Component 803

Download Coordinate Files and Chemical Diagrams

Component definition in mmCIF format
Component definition in PDBML/XML format
SDF/MOL format (experimental model coordinates)
SDF/MOL format (ideal coordinates)
PDB format (experimental model coordinates)
Chemical diagram without atom labels
Chemical diagram with format V3 atom labels (heavy atoms)
Chemical diagram with format V3 atom labels (all atoms)
Chemical diagram with format V2 atom labels (heavy atoms)
Chemical diagram with format V2 atom labels (all atoms)

Gaussian Calculation

2018年2月23日　　下午 03:21

Prepare Gaussian input file

Input file: 803_model.pdb
Scripts: convert_pdb_2gaussian

$ ./convert_pdb_2_gaussian_input 803_model.pdb
　　Extract atom type and coordinates from the pdb

The input file will look as following:

Chk=LVA.1.g03.chk

%Mem=48000000

%nproc=4

#N hf/6-31g* iop(6/33=2) pop=mk scf=direct scfcon=6 opt

LVA.1.g03

0 1

C-1　　52.497　19.025　23.052

C0　　52.393　17.482　22.971

C1　　52.359　16.834　24.377

C2　　53.777　16.458　24.857

C3　　51.698　17.697　25.428

C4　　51.206　18.918　25.189

C5　　50.582　19.686　26.274

:

:

Launch Gaussian

$ source /opt/setup_Gaussian03.sh
$ g03 < LVA.1.g03.in > LVA.1.g03.out &

The tail of the output file will show as following:

:

:

Job cpu time:　0 days 13 hours 34 minutes 57.6 seconds.

File lengths (MBytes):　RWF=　172 Int=　0 D2E=　0 Chk=　25 Scr=　1

Normal termination of Gaussian 03 at Fri Feb 23 19:01:07 2018.

This shows the calculation is done successfully.

Gaussian to Amber

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Convert Gaussian output to Amber

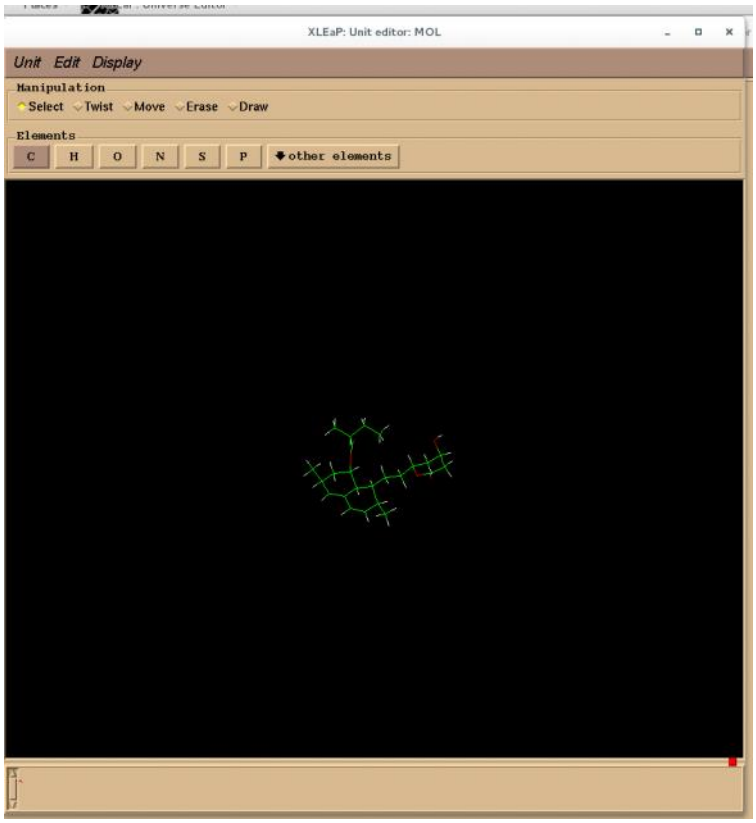
$ gaussian2LEaP LVA

The output files are:

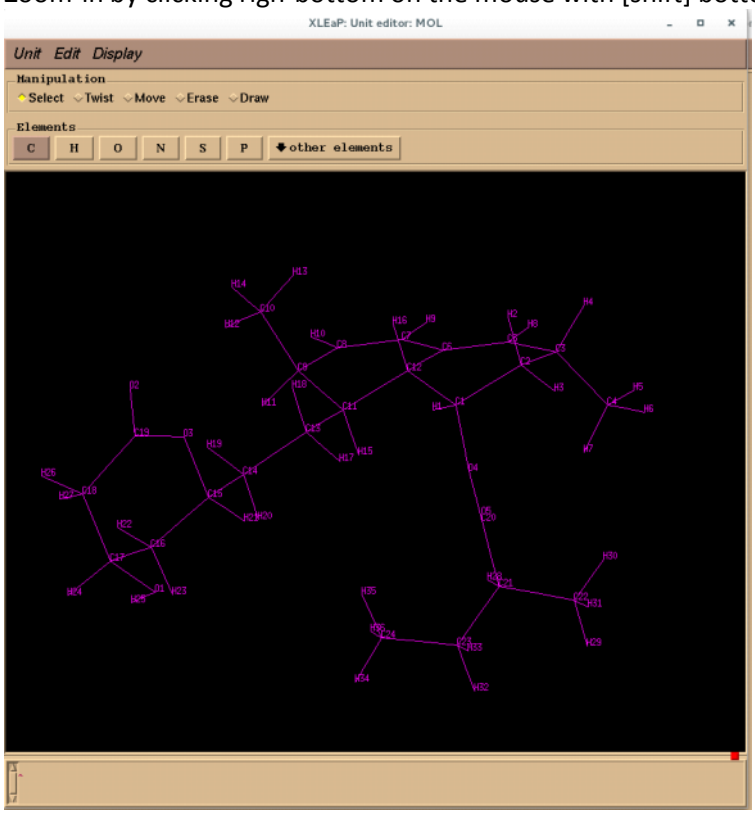
frcmod.LVA
LVA.lib

Compare the atom name from LEaP and original compound pdb

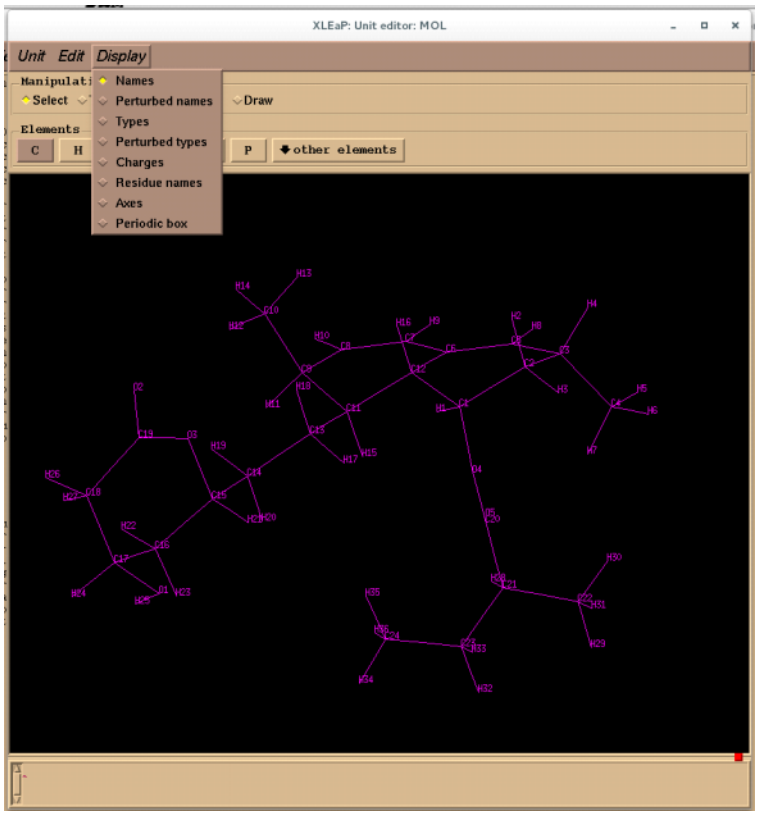
Open xleap and source the new library just built.
$ xleap
> source MOL_leap.in
> edit MOL



Unselect NumLock.
Zoom-in by clicking righ-bottom on the mouse with [shift] bottom on the keybroad

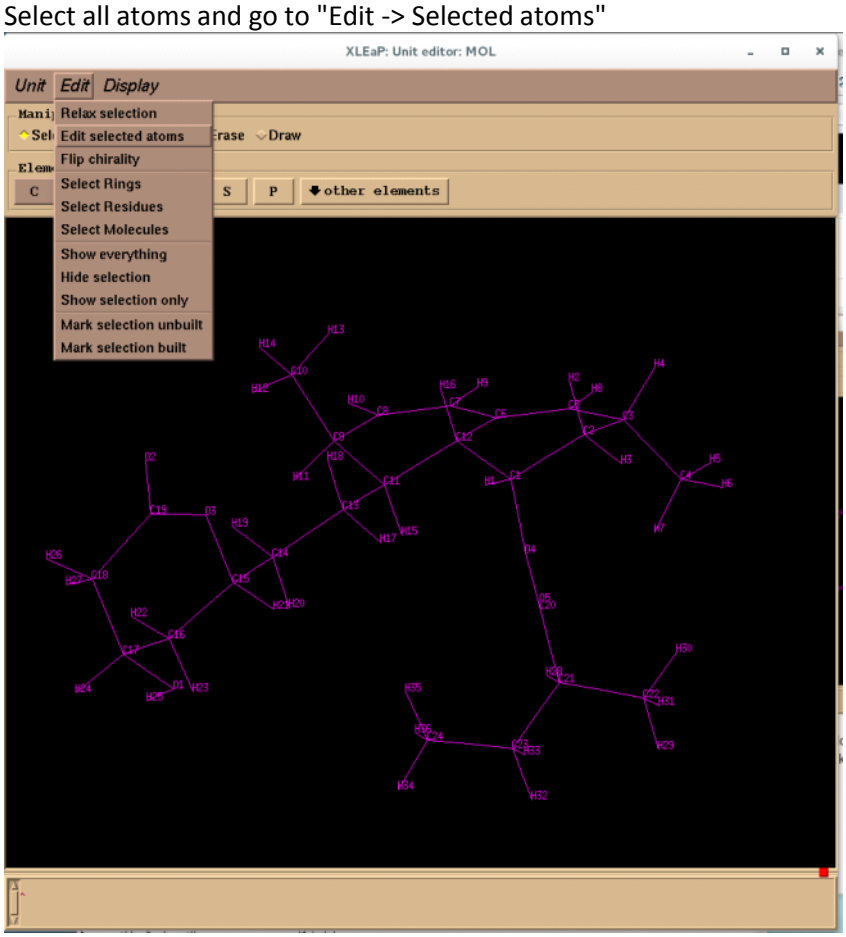


Show atom names by selecting "Display -> Name"

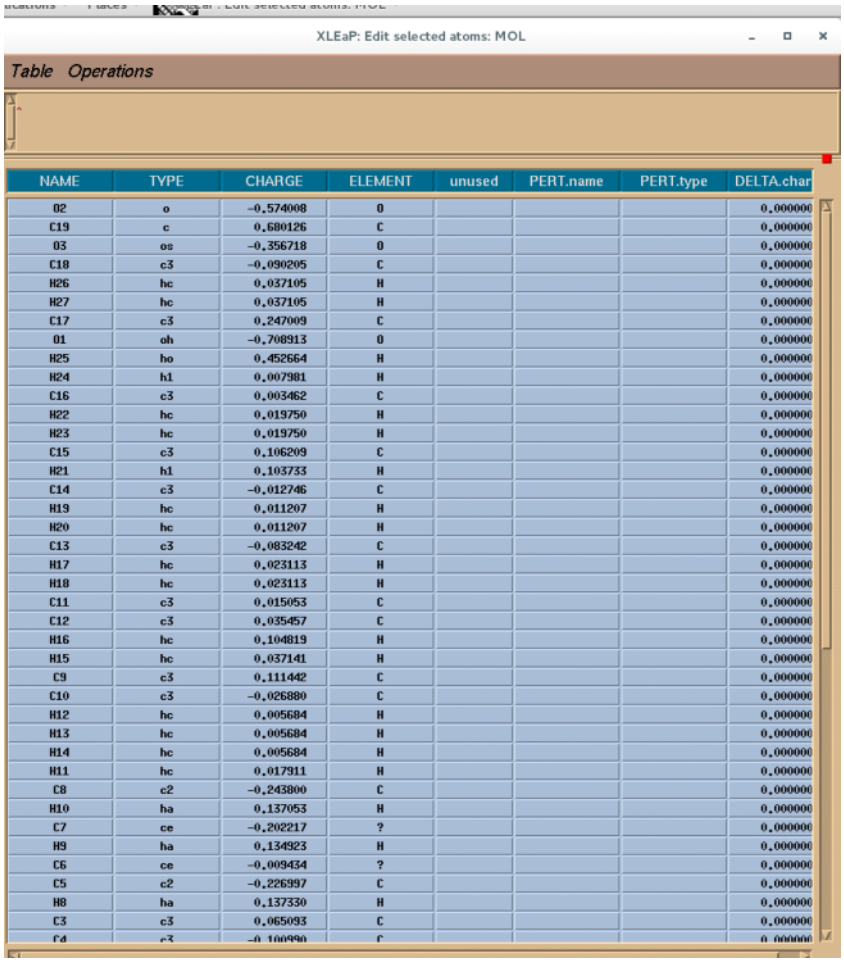


Compare those name with the atom name in the download pdb. The atom names have been renamed by LEaP. You need to change these atom name back according to the atom name in PDB.

Select all atoms and go to "Edit -> Selected atoms"



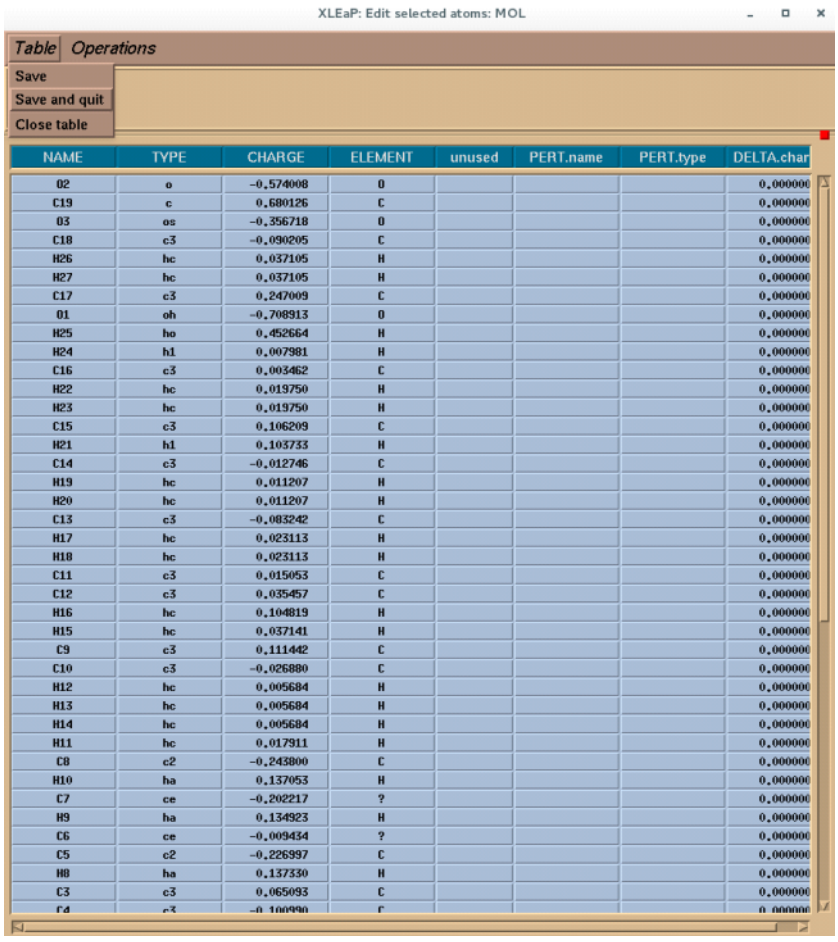
A new window will pop out.



NAME	TYPE	CHARGE	ELEMENT	unused	PERT.name	PERT.type	DELTA.char
02	o	-0.574008	O				0.000000
C19	c	0.680126	C				0.000000
03	os	-0.356718	O				0.000000
C18	c3	-0.090205	C				0.000000
H26	hc	0.037105	H				0.000000
H27	hc	0.037105	H				0.000000
C17	c3	0.247009	C				0.000000
01	oh	-0.708913	O				0.000000
H25	ho	0.452664	H				0.000000
H24	h1	0.007981	H				0.000000
C16	c3	0.003462	C				0.000000
H22	hc	0.019750	H				0.000000
H23	hc	0.019750	H				0.000000
C15	c3	0.106209	C				0.000000
H21	h1	0.103733	H				0.000000
C14	c3	-0.012746	C				0.000000
H19	hc	0.011207	H				0.000000
H20	hc	0.011207	H				0.000000
C13	c3	-0.083242	C				0.000000
H17	hc	0.023113	H				0.000000
H18	hc	0.023113	H				0.000000
C11	c3	0.015053	C				0.000000
C12	c3	0.035457	C				0.000000
H16	hc	0.104819	H				0.000000
H15	hc	0.037141	H				0.000000
C9	c3	0.111442	C				0.000000
C10	c3	-0.026880	C				0.000000
H12	hc	0.005684	H				0.000000
H13	hc	0.005684	H				0.000000
H14	hc	0.005684	H				0.000000
H11	hc	0.017911	H				0.000000
C8	c2	-0.243800	C				0.000000
H10	ha	0.137053	H				0.000000
C7	ce	-0.202217	?				0.000000
H9	ha	0.134923	H				0.000000
C6	ce	-0.009434	?				0.000000
C5	c2	-0.226997	C				0.000000
H8	ha	0.137330	H				0.000000
C3	c3	0.065093	C				0.000000
C4	c3	-0.100990	C				0.000000

The calculated partial charges and names are shown there.
Edit the atom name and make these name consistent with the name in 803_model.pdb.

After finishing editing, click "save and quit".



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H27	hc	0.037105	H				0.000000
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01	oh	-0.708913	O				0.000000
H25	ho	0.452664	H				0.000000
H24	h1	0.007981	H				0.000000
C16	c3	0.003462	C				0.000000
H22	hc	0.019750	H				0.000000
H23	hc	0.019750	H				0.000000
C15	c3	0.106209	C				0.000000
H21	h1	0.103733	H				0.000000
C14	c3	-0.012746	C				0.000000
H19	hc	0.011207	H				0.000000
H20	hc	0.011207	H				0.000000
C13	c3	-0.083242	C				0.000000
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H18	hc	0.023113	H				0.000000
C11	c3	0.015053	C				0.000000
C12	c3	0.035457	C				0.000000
H16	hc	0.104819	H				0.000000
H15	hc	0.037141	H				0.000000
C9	c3	0.111442	C				0.000000
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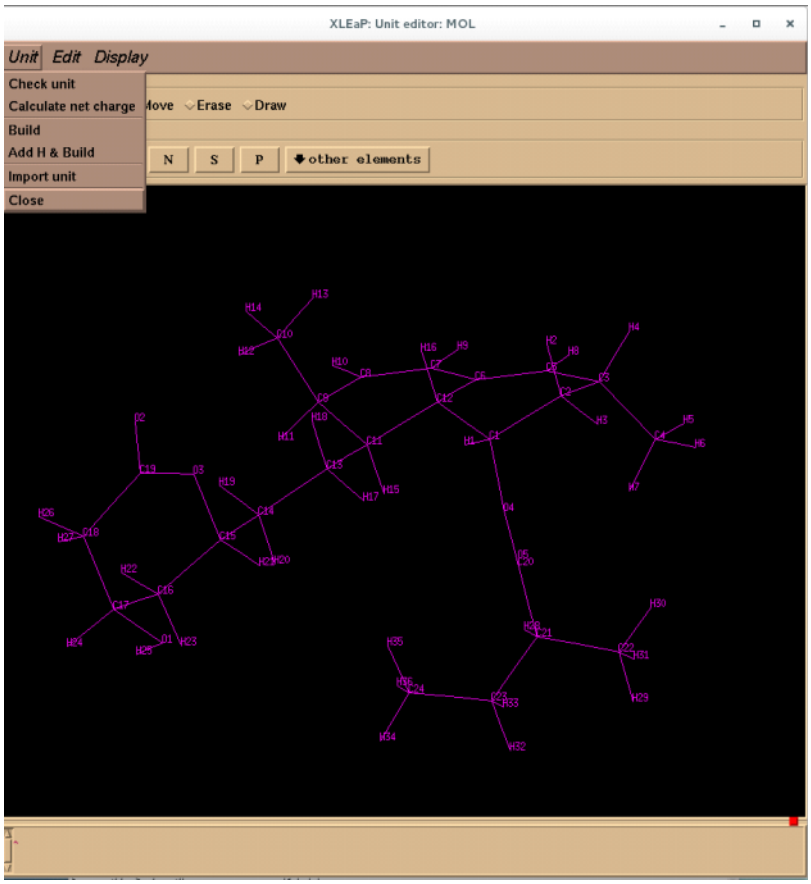
H14	hc	0.005684	H				0.000000
H11	hc	0.017911	H				0.000000
C8	c2	-0.243800	C				0.000000
H10	ha	0.137053	H				0.000000
C7	ce	-0.202217	?				0.000000
H9	ha	0.134923	H				0.000000
C6	ce	-0.009434	?				0.000000
C5	c2	-0.226997	C				0.000000
H8	ha	0.137330	H				0.000000
C3	c3	0.065093	C				0.000000
C4	c3	-0.100990	C				0.000000

Close "unit"



Back to the main terminal of xLEaP and updated name to MOL.lib.
> saveoff MOL MOL.lib
> quit

MOL.lib and frcmod.MOL are ready for LEaP input.