


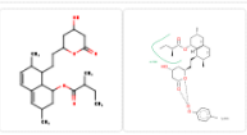
# Ligand PDB

2018年2月23日 下午 03:21

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Small Molecules

Ligands 2 Unique

ID	Chains	Name / Formula / InChI Key	2D Diagram & Interactions	3D Interactions
<a href="#">MG</a> <a href="#">Query on MG</a> <a href="#">Download SDF File</a> <a href="#">Download CCD File</a>	A, B	<b>MAGNESIUM ION</b> Mg JLVVSXFLKOJNIY-UHFFFAOYSA-N		<a href="#">Ligand Interaction</a>
<a href="#">803</a> <a href="#">Query on 803</a> <a href="#">Download SDF File</a> <a href="#">Download CCD File</a>	A, B	<b>LOVASTATIN</b> MK-803; LOVALIP; MEVACOR C <sub>24</sub> H <sub>36</sub> O <sub>5</sub> PCZOHLXUXFIOCF-BXMDZJMSA-N		<a href="#">Ligand Interaction</a>

External Ligand Annotations

ID	Binding Affinity (Sequence Identity %)
803	Kd: 12900 nM (99) <a href="#">BINDINGDB</a>
803	IC50: 2400 nM <a href="#">PDBBIND</a>

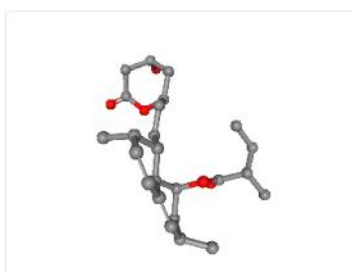
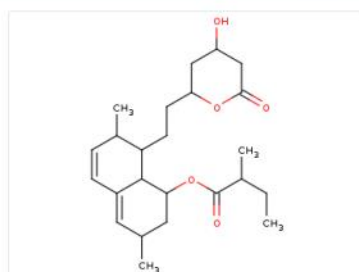
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137692 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

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## 803

### LOVASTATIN

803 as a free ligand exists in 1 entry. Examples include: 1CQP

Find related ligands: [Stereoisomers](#) [Similar ligands](#)  
[Chemical Structure Search](#)

[View summary at Ligand Expo](#)

[View / Download Files](#)

Chemical Component Summary	
<b>Name</b>	LOVASTATIN
<b>Identifiers</b>	[(1S,3R,7S,8S,8aR)-8-[2-[(2R,4R)-4-hydroxy-6-oxo-oxan-2-yl]ethyl]-3,7-dimethyl-1,2,3,7,8a-hexahydronaphthalen-1-yl] (2S)-2-methylbutanoate
<b>Formula</b>	C <sub>24</sub> H <sub>36</sub> O <sub>5</sub>
<b>Molecular Weight</b>	404.54
<b>Type</b>	NON-POLYMER
<b>Isomeric SMILES</b>	CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@H]12
<b>InChI</b>	InChI=1S/C24H36O5 /c1-5-15(3)24(27)29-21-11-14(2)10-17-7-6-16(4)20(23)(17)21)9-8-19-12-18(25)13-22(26)28-19 /h6-7-10-14-16-18-21-22-25H-5-8-9-11-13-14-15-16-18-19-20-22-23-24H2

Chemical Details	
<b>Formal Charge</b>	0
<b>Atom Count</b>	65
<b>Chiral Atom Count</b>	8
<b>Chiral Atoms</b>	C1, C12, C14, C16, C3, C7, C8, C9
<b>Bond Count</b>	67
<b>Aromatic Bond Count</b>	0
<b>Leaving Atoms</b>	n/a

[Chemical Details](#)

[Geometry](#)

[Atom Nomenclature](#)

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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

2018年2月23日 下午 03:22

## Convert Gaussian output to Amber

```
$ gaussian2LEaP LVA
```

The output files are:

```
frcmol.LVA  
LVA.lib
```

## Compare the atom name from LEaP and original compound pdb

Open xleap and source the new library just built.

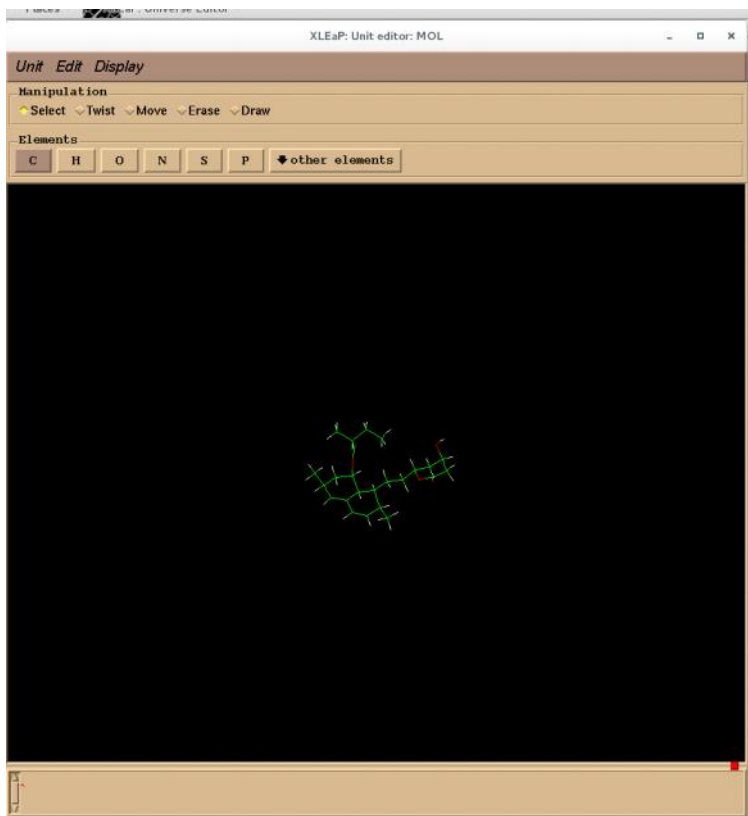
```
$ xleap
```

```
> source MOL_leap.in
```

```
> edit MOL
```

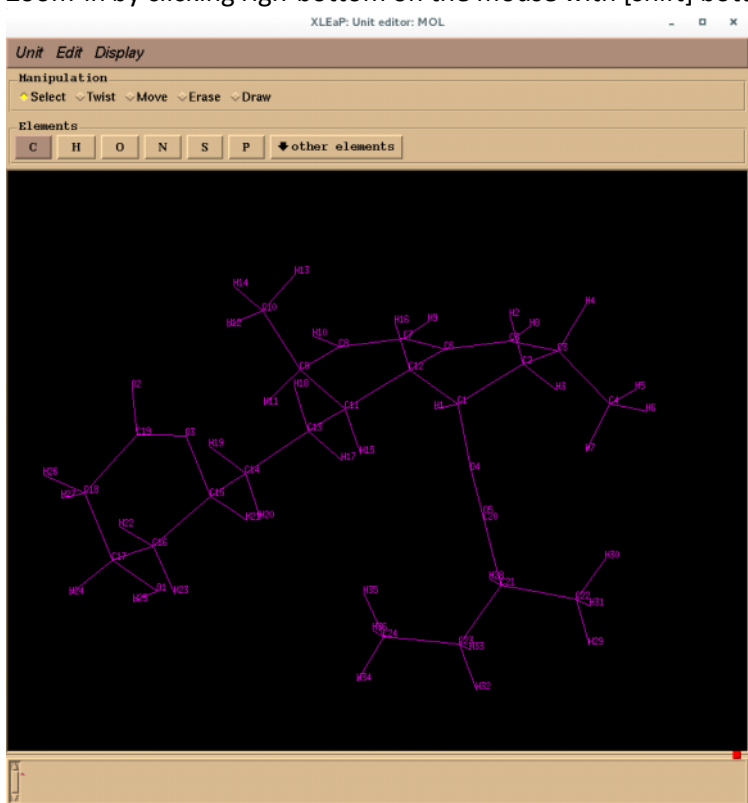


```
Applications ▾ Places ▾ LEaP: Universe Editor ▾  
  
File Edit Verbosity  
Please turn Num Lock off for the menus to function!  
Welcome to LEaP!  
(no leaprc in search path)  
> source MOL_leap.in  
----- Source: ./MOL_leap.in  
----- Source of ./MOL_leap.in done  
----- Source: ./leaprc.gaff  
----- Source of ./leaprc.gaff done  
Log file: ./leap.log  
Loading parameters: /opt/amber16/dat/leap/parm/gaff.dat  
Reading title:  
AMBER General Force Field for organic molecules (Version 1.8, Mar 2015)  
Loading parameters: /opt/amber16/dat/leap/parm/parm99.dat  
Reading title:  
PAR99 for DNA, RNA, AA, organic molecules, TIP3P wat. Polariz.& LP incl.02/04/99  
Loading library: /opt/amber16/dat/leap/lib/solvents.lib  
Loading parameters: ./frcmol.MOL  
Reading force field modification type file (frcmol)  
Reading title:  
remark goes here  
Loading Prep file: ./MOL.prepin  
Checking Unit.  
Building topology.  
Building atom parameters.  
Building bond parameters.  
Building angle parameters.  
Building proper torsion parameters.  
Building improper torsion parameters.  
old PREP-specified improper:  
<MOL 1>: C18 O2 C19 O3  
<MOL 1>: C9 C7 C8 H10  
<MOL 1>: C8 C6 C7 H9  
<MOL 1>: C5 C12 C6 C7  
<MOL 1>: C3 C6 C5 H8  
<MOL 1>: C21 O5 C20 O4  
total 6 improper torsions applied  
6 improper torsions in old prep form  
Building H-Bond parameters.  
Incorporating Non-Bonded adjustments.  
Not Marking per-residue atom chain types.  
Marking per-residue atom chain types.  
(no restraints)  
Building topology.  
Building atom parameters.  
>  
> ^
```



Unselect NumLock.

Zoom-in by clicking right-bottom on the mouse with [shift] bottom on the keyboard



Show atom names by selecting "Display -> Name"



XLEaP: Edit selected atoms: MOL

**Table Operations**

NAME	TYPE	CHARGE	ELEMENT	unused	PERT.name	PERT.type	DELTA.char
O2	o	-0.574008	O				0.000000
C19	c	0.680126	C				0.000000
O3	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
O1	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	-0.009454	?				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".

XLEaP: Edit selected atoms: MOL

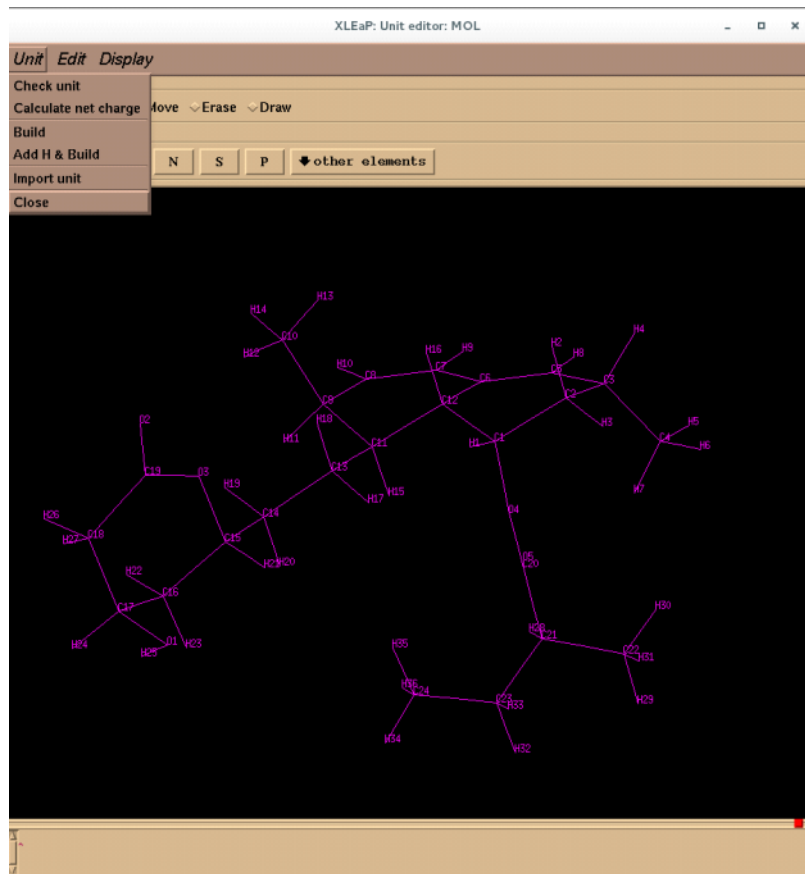
**Table Operations**

Save  
 Save and quit  
 Close table

NAME	TYPE	CHARGE	ELEMENT	unused	PERT.name	PERT.type	DELTA.char
O2	o	-0.574008	O				0.000000
C19	c	0.680126	C				0.000000
O3	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
O1	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	-0.009454	?				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.