MY ff10 FROM AMBER11 vs MY FRIEND'S

my leap.log file with ff10 from **my amber11** package


```
elwing: ~/1HR2/starting_pdbs

amparo@elwing: /media/Amparo/Backup_Mar...  ✖  amparo@elw

Log started: Mon Feb  4 17:27:17 2013

Log file: ./leap.log
> #
> # ----- leaprc for loading the ff10 force field
> # ----- NOTE: this is designed for PDB format 3!
> #
> #      load atom type hybridizations
```

My **friend's** leap.log file with ff10 from his amber11 package


```
elwing: /media/Amparo/Backup_March2013/1N8R/MinoTauro/40C_1N8R_MinoTauro/replica.1/Nacho/muta

amparo@elwing: /media/Amparo/Backup_Mar...  ✖  amparo@elwing: /media/Amparo/Backup_Mar...  ✖

Log started: Mon May  6 15:26:10 2013

Log file: ./leap.log
>> #
>> # ----- leaprc for loading the ff10 force field
>> # ----- NOTE: this is designed for PDB format 3!
>> #      ff10 =  ff99SB for proteins; ff99bsc0 for DNA; ff99sbsc_chiOL3 for RNA
>> #      phosphoaa parms from N. Homeyer, A.H.C. Horn, H. Lanig, H. Sticht
>> #         J. Mol. Model. 2006, 12, 281-289.  OP vdW parameters modified
>> #         by T. Steinbrecher and J. Latzer.
>> #
>> #      load atom type hybridizations
```

my xleap loading ff10 from **my amber11** package


```
iverse Editor

⊗ ⊖ ▢   XLEaP: Universe Editor

File  Edit  Verbosity

Welcome to LEaP!
Sourcing: /usr/local/amber11/dat/leap/cmd/leaprc.ff10
Opening /usr/local/amber11/dat/leap/prep/leap.log: Permission denied
Opening /usr/local/amber11/dat/leap/lib/leap.log: Permission denied
Opening /usr/local/amber11/dat/leap/parm/leap.log: Permission denied
Opening /usr/local/amber11/dat/leap/cmd/leap.log: Permission denied
Could not open file leap.log: system error
Loading parameters: /usr/local/amber11/dat/leap/parm/parm10.dat
Reading title:
PARM99 + frcmod.ff99SB + frcmod.parmbsc0
Loading library: /usr/local/amber11/dat/leap/lib/all_amino10.lib
Loading library: /usr/local/amber11/dat/leap/lib/all_aminoct10.lib
Loading library: /usr/local/amber11/dat/leap/lib/all_aminont10.lib
Loading library: /usr/local/amber11/dat/leap/lib/all_nucleic10.lib
Loading library: /usr/local/amber11/dat/leap/lib/ions08.lib
Loading library: /usr/local/amber11/dat/leap/lib/solvents.lib
> ▪
```

Where is OL3?

ff10 FROM my AMBER11 vs ff10 FROM my AMBER12

Heading line of the leaprc.parm.10 file in my **amber11** package

```
@elwing: /usr/local/amber11/dat/leap/parm
amparo@elwing: /media/Amparo/Bac... ✖  amparo@elwing: /media/Amparo/Bac... ✖  amparo@elwing: /med
PARM99 + frcmod.ff99SB + frcmod.parmbsc0              ← Where is OL3?
C   12.01        0.616  !              sp2 C carbonyl group
CA 12.01         0.360                 sp2 C pure aromatic (benzene)
CB 12.01         0.360                 sp2 aromatic C, 5&6 membered ring junction
CC 12.01         0.360                 sp2 aromatic C, 5 memb. ring HIS
```

Heading line of the leaprc.parm.10 file in my **amber12** package

```
@elwing: /usr/local/amber12/dat/leap/parm
amparo@elwing: /media/Amparo/Bac... ✖  amparo@elwing: /media/Amparo/Bac... ✖  amparo@elwing: /me
PARM99 + frcmod.ff99SB + frcmod.parmbsc0 + OL3 for RNA  ←
C   12.01        0.616  !              sp2 C carbonyl group
CA 12.01         0.360                 sp2 C pure aromatic (benzene)
CB 12.01         0.360                 sp2 aromatic C, 5&6 membered ring junction
CC 12.01         0.360                 sp2 aromatic C, 5 memb. ring HIS
```

Heading line of the leaprc.ff10 file in my **amber11** package

```
elwing: /usr/local/amber11/dat/leap/cmd
amparo@elwing: /media/Amparo/Bac... ✖  amparo@elwing: /media/Am
LogFile leap.log
#
# ----- leaprc for loading the ff10 force field
# ----- NOTE: this is designed for PDB format 3!
#
#        load atom type hybridizations
#
```

Heading line of the leaprc.ff10 file in my **amber12** package

```
elwing: /usr/local/amber12/dat/leap/cmd
amparo@elwing: /media/Amparo/Bac... ✖  amparo@elwing: /media/Amparo/Bac... ✖  amparo@elwing: /
LogFile leap.log
#
# ----- leaprc for loading the ff10 force field
# ----- NOTE: this is designed for PDB format 3!
#        ff10 = ff99SB for proteins; ff99bsc0 for DNA; ff99sbsc_chiOL3 for RNA
#        phosphoaa parms from N. Homeyer, A.H.C. Horn, H. Lanig, H. Sticht
#           J. Mol. Model. 2006, 12, 281-289.  OP vdW parameters modified
#           by T. Steinbrecher and J. Latzer.
#
#        load atom type hybridizations
#
```

my xleap loading ff10 from my amber12 package

```
Loading parameters: ./parm10.dat
Reading title:
PARM99 + frcmod.ff99SB + frcmod.parmbsc0 + OL3 for RNA  ←
```