

# Chemistry software hints

For help with SciFinder and other library related material, see [this](#) wonderful resource.

**MestreNova** is a wonderful tool for manipulating NMR files. The manual for 6.0.4 is [here](#)

For X-Ray Chrystalography analysis, we have installed apex2 on laue, the manual is can be [downloaded](#).

You will need to login to laue: `ssh -Y laue.coby.edu`

and then type: `apex &`

to run it.

Gaussian is available on nsc, all 17 Macintosh in the schupf lab, and on all

wet lab imaged macs in Keyes. These macs run spartan remotely from schupflab over

an X windows connection. Under Mac OS you may need to install [XQuartz](#).

<http://www.ks.uiuc.edu/Training/Tutorials/Reference/macosxprimer.html>

**MOE** short hints (PDF)

**Gaussian** 03 online manual is [here](#), with Gaussian 09 [here](#).

After you submit a job, that is going to take a while (>3 hour), you can quit out of gview. If you leave gview open, after the job is done, it uses on full cpu at 100%.

Personally I think this is a bug, but they don't.

Here is was top would report:

```
top - 13:37:20 up 63 days, 2:23, 3 users, load average: 8.40, 8.81, 8.95
Tasks: 215 total, 2 running, 213 sleeping, 0 stopped, 0 zombie
Cpu(s): 49.9%us, 0.3%sy, 49.8%ni, 0.0%id, 0.0%wa, 0.0%hi, 0.0%si, 0.0%st
Mem: 32502784k total, 2481692k used, 30021092k free, 36136k buffers
Swap: 2031608k total, 256k used, 2031352k free, 682076k cached
  PID USER      PR  NI  VIRT  RES  SHR  S %CPU  %MEM  TIME+  COMMAND
21587 rhdowner 15   0 174m 40m 14m  S 100.0  0.1 69:24.58 gview.exe
```

**Spartan** command line options:

`spartan --help`

```
--monitor          : Run the Spartan Monitor
--arch             : Display the CPU architecture of this machine
--submit [opt] <path> : Submit backend jobs
  --background
  --foreground
  --external-default-queue
  --external-queue <queue_name>
  --verbose <level>
--foreground-submit : Submit backend jobs waiting for job to complete
--process-commands  : Process job command file
--unpack           : Unpack a .spartan file to Unix style format
--convert <old> <new> : Command line conversion utility
--select           : Return graphics mode
--inuse [-status]   : Inuse status
--inuse [-add|-remove] : Modify inuse state
--library-path     : Print LD_LIBRARY_PATH
--root-path        : Print the spartan root path
--ldd              : Print the spartan GUI library dependencies
```

--ldd-analysis <???)> : Print module library dependencies  
--ldd-so <lib???.so> : Print library dependencies

The following needs to be set to use **mm3** in the schupflab:

add these two lines to your .cshrc

```
setenv MM32000ROOT /export/local/src  
source $MM32000ROOT/mm32000/mm32000.cnf
```

An excellent resource for Varian Vnmr(j) can be found [here](#).

If vnmrJ does not start correctly, close it, open a terminal and delete the lock file:

```
rm vnmrsys/lock*
```

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```
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```

```
apex &
```

WebMO: available at <http://schupflab.colby.edu/cgi-bin/webmo/login.cgi>

you will need a login to use this service, check with [rhdowner@colby.edu](mailto:rhdowner@colby.edu).

You may need to adjust your java settings ([http://www.java.com/en/download/help/jcp\\_security.xml](http://www.java.com/en/download/help/jcp_security.xml))

to enable <http://schupflab.colby.edu> to dowload and run the java based builder.