

Review questions for Final Exam on material not covered on other tests

1. What does QSAR stand for?
2. How does one go about developing a QSAR for a series of compounds? In your response, be sure to address examples of typical variables (descriptors) that are incorporated, and the minimum ratio of structures to variables.
3. List 10 descriptors that are sometimes used in a QSAR.
4. Describe 3-dimensional QSAR.
5. In remote computing, describe the difference between **ftp** and **telnet**. What is each used for?
6. In setting up a *Gaussian* calculation on a UNIX machine, tell what each of the symbols in the route sections below means: (no need to duplicate your answers)

```
# HF/6-31+G** nosymm opt
```

```
# HF/6-31+G** geom=allcheckpoint nosymm nmr pop=npa
```

7. What command (in UNIX) can be used to open a file and scan rapidly through it. (This command is most useful to look at the end of a file, then scroll back up into the file)
8. What command (in UNIX) can be used to determine the location (path) of the directory you are currently in?
9. What command (in UNIX) can be used to copy a file (filenameA.zzz) and save it as a different name (filenameB.zzz)?
10. What command (in UNIX) can be used to change the name of a file from filenameA.zzz to filenameB.zzz?