

Modeling Exercises, part 1

Name: _____

Please refer to the document titled “Introduction to Spartan” at this page: <http://global.oup.com/uk/orc/chemistry/patrick5e/student/exercises/>

Spartan Introduction (ungraded)

In the “Introduction to Spartan” document, exercises 2.1, 2.2 will be useful to familiarize yourself with basic functions as well as the computer interface.

Sections 2.8, 2.11, 3 and 4 include some more complex functions, and are highly recommended as preparation for the assignments. When we do have our second molecular modeling session later this semester, I'll recommend further introductory sections that will be relevant.

The following assignments will be graded. Underneath each Exercise, below, is a description of what you will turn in for grading.

1. Exercise 2.1 Study of CDK2 (the second 2.1 in the list under Chapter 2)

- Submit to me, by email, a screen-capture or JPG image of your TUBULAR rendering of CDK2. Your file should be named, “lastname_2.1”

2. Exercise 17.1 Adrenaline

- Measuring the C-C bond lengths
Choose Measure Distance from the Geometry Menu. Click on any two atoms that are linked together, or click on the bond connecting the two atoms. The bond length will appear in the window at the bottom right of the screen.

Measure BOTH of the C-N bonds _____ (enter your values here)

- Measuring the C-C-C bond angles
Choose Measure Angle from the Geometry Menu. Click on three atoms that are linked together, or on the two bonds involved. The bond angle will appear in the bottom right window.

Measure ANY of the C-O-H angles _____ (enter your value here)

Measure the C-N-C angle _____ (enter your value here)

- Measuring the torsion or dihedral angle (C-C-C-C)
Choose Measure Dihedral from the Geometry Menu. Click on 4 linked carbon atoms or the three connecting bonds and the value will appear in the bottom right window.

Measure the dihedral angle between H10 and the H on the Nitrogen

_____ (enter your value here)

- Measuring atom-atom distances
Choose Measure Distance from the Geometry Menu. Click on any two atoms. The separation between these is indicated in the bottom right window.

Measure the distance between the nitrogen and the oxygen atoms that is closest to it.

_____ (enter your value here)

Exercise 17.3 Histamine

- Part A: Submit your molecular rendering that mimics Figure 4. Send as either a screen-capture or JPG image. Your file should be named, "lastname_17.3_Part A".
- Section B: Submit to me, by email, your TRANSPARENT electrostatic potential map. Send as either a screen-capture or JPG image. Your file should be named, "lastname_17.3_Section B".