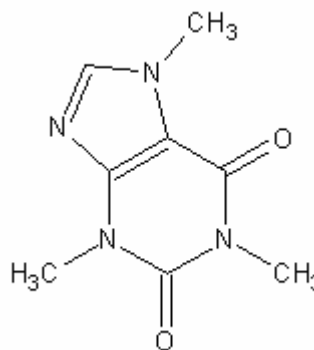
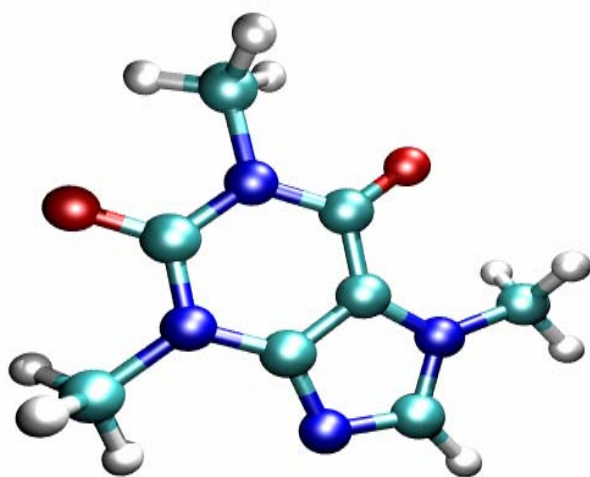


## PC\_Model set I

Your assigned molecule is CAFFEINE. The PC MODEL program contains a library of templates, CAFFEINE is very similar to the nucleotide ADENOSINE. You could start building from there. Hydrogens can be added or deleted by clicking on **H/AD**. Atoms can be changed from hydrogen to any other atom in the periodic table by clicking on **PT** then choosing the atom.



Molecular Formula:  $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$

8 green Carbons

10 white Hydrogens

4 blue Nitrogens

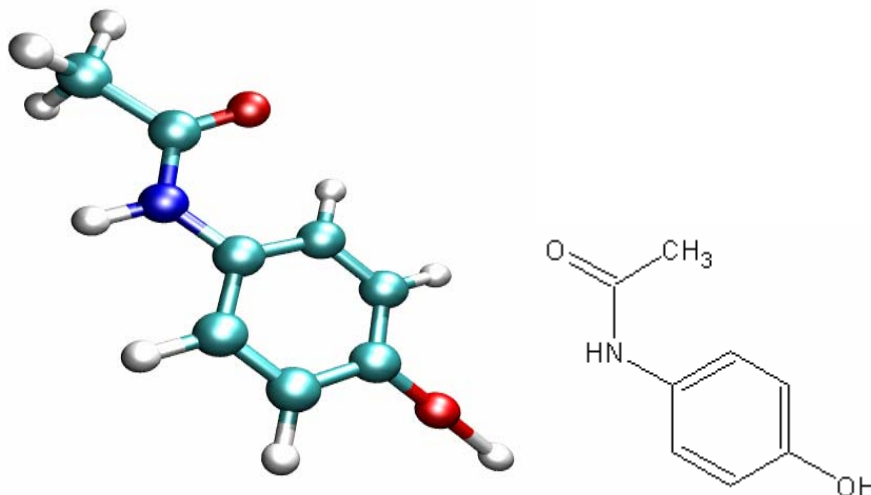
2 red Oxygens

Determine the value of each of the five inner angles of the pentameric ring. Are the values consistent with a planar ring geometry? First you must figure out the sum of inner angles for a perfect pentagon.

This ring has two oxygen atoms. What is the orientation of these atoms with respect to the ring plane. You can use the torsional angle values to answer this question if the ring is flat.

## PC\_Model set II

Your assigned molecule is ACETAMINOPHEN. The PC MODEL program contains a library of templates, ACETAMINOPHEN is very similar to the amino acid TYROSINE. You could start building from there. Hydrogens can be added or deleted by clicking on **H/AD**. Atoms can be changed from hydrogen to any other atom in the periodic table by clicking on **PT** then choosing the atom.



Molecular Formula:  $C_8H_9NO_2$

8 green Carbons

9 white Hydrogens

1 blue Nitrogen

2 red Oxygens

Determine the value of each of the six inner angles of the hexameric ring. Are the values consistent with a planar ring geometry? First you must figure out the sum of inner angles for a perfect hexagon.

There are two oxygen atoms in the molecule. Determine the Carbon-Oxygen bond length for each of them. Why is one of the bonds longer than the other? The bond order might have something to do with that.