Caffeine

Caffeine is a central nervous system (CNS) stimulant. It is the world's most widely consumed psychoactive drug. Unlike many other psychoactive substances, it is legal and unregulated in nearly all parts of the world. There are several known mechanisms of action to explain the effects of caffeine. The most prominent is that it reversibly blocks the action of adenosine on its receptor and consequently prevents the onset of drowsiness induced by adenosine.

The caffeine molecule can be found on avogadro, or perhaps directly in Psi4.
Surely there is on https://pubchem.ncbi.nlm.nih.gov/

The results you should try to achive are:

1) optimize the structure and compute the molecular orbital energies with two or more different basis set discussing the differences you found.

2) what is the absolute value of the total energy? How compare with experimental one? Why?

3) minimize the structure with a classical force field within avogadro (UFF, for example). Plot in a graph the bond length and the angles to compare the obtained values with the ab inito ones

4) plot the electrostatic potential, the HOMO-LUMO orbitals. What are the positive and negative zones on the molecular potential map? Where are localized the HOMO and the LUMO orbitals?

5) compute the potential energy due to the rotation of one of the CH3 group (hint: perhaps 120 degree is sufficient...why?)

6) compute the mulliken charges and the dipole moment

Pay attention that if you minimize the structures with avogadro that the type of bond has to be explicitely set by clicking with the pencil on the bond.

The work have to be attacked as group, help each other!

A short (~ 10 slides) presentation of the work has to be presented at the exam and, as the exam is personal, also the presentation must be personal.

Good luck!