Predicting Tautomeric Equilibria, II.

Basic problem: Compare pairs of tautomeric molecules to predict the most stable isomer. Since tautomeric equillbria are often finely poised and solvent dependent, this will act as a test of the capability of any given method to give an experimentally correct result for a gas phase molecular calculation.

Method: AM1 and 6-31G* are reasonable levels of theory for these comparisons. Optimize geometries and obtain heats of formation for the tautomeric molecules, and estimate the room temperature equilibrium constants that relate them (assume that $\Delta H \sim \Delta G$). How well do the computations reproduce experiment?

Literature: Use Beilstein Online, Chemical Abstracts, or the NIST database sites to get experimental heats of formation and literature references for them, wherever available.