[Building an explicit chloroform solvent shell around acetylacetone to predict keto-enol tautomer] *by Marcus Liebenthal*

The equilibrium concentration of the diketone and enol tautomer of acetylacetone as a function of solvent dielectricity is investigated by computational calculations. The percentage of enol at equilibrium is experimentally determined by NMR in a protic polar solvent (water), non-protic polar solvent (acetone), non-protic apolar solvent (chloroform). An explicit solvent study was carried out combining an effective fragment potential with a polarized continuum. [Previous results using the effective fragment potential (EFP2) method combined with a Monte-Carlo simulated annealing (MC/SA) is compared with a manual and intuitive building up of the solvent shell from one solvent molecule to four solvent molecules. Both methods are evaluated based on the ability to identify the minimum energy conformations of solvent-solute interactions and resource cost.] Full geometry optimizations and energy calculations with thermochemical corrections are done using a CPCM/M06-2X density functional with an extended basis. [The random placement of chloroform solvent molecules was as effective than the manual building of the solvent shell using chemical intuition. In addition the EFP required less human input but required significantly more computational resources.]