Computational software, *Gaussian*, was used to study γ-butyrolactone*water complexes by using Density Functional Theory type calculations. The specific types of calculations performed were geometry optimizations, frequencies and excited states. Different conformers of the complex as well as the corresponding hydroxy acid, γ-hydroxybutyric acid, were analyzed for stability. Total electronic energy and enthalpy values for each complex were analyzed to predict stability. Infrared spectra were obtained for each complex to be able to distinguish between each stable complex. Frequency calculations were also performed on the isotopic forms of the stable complexes to obtain infrared spectra to assist in distinguishing the identity of complexes. The most stable hydroxy acid was determined to be one which was cyclic in nature with intramolecular hydrogen bonding. This acid was found to be more stable than the separated lactone and water by 28.54 kJ/mol. Similarly, the most stable GBL*water complex was determined to be one which had hydrogen bonds to the carbonyl and both α hydrogens. This complex was found to be more stable than the separated lactone and water by 25.05 kJ/mol.