# 25th Umbrella Symposium

For the development of Joint Cooperation Ideas
"Modeling and Simulation with emphasis on high performance computing and grid computing"

## Investigating the optical properties of fluorescence probes in Rhodamine-PBP

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Fluorescence probes are routinely used to investigate the structural basis of biochemical processes *in vitro* and *in vivo*. A rhodamine adduct with the phosphate binding protein has been developed previously for use as a fluorescent reagentless biosensor inorganic phosphate. Binding of inorganic phosphate to the protein causes a distinct structural change in the protein. This is associated with a large change in the absorption and fluorescence emission spectra of the rhodamines, along with an enhancement in the emission intensity of about 18-fold. The structural basis of these spectral changes is not clear: developing an understanding will not only provide a basis for how chromophores interact on protein surfaces, but also help future design of these types of biosensor. We are using a variety of computational approaches, including QM/MM simulations and TDDFT calculations to obtain theoretical optical spectra and determine how interactions between rhodamines and amino acids modulate these spectra.
Our results are being validated against experimental data from mutational and other studies.