Characterizing 3,5-difluoro-4-hydroxybenzylidene imidazolinone (DFHBI) Electron Distribution and its Effect on Fluorescence

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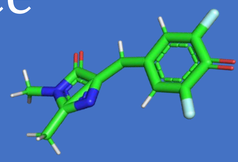
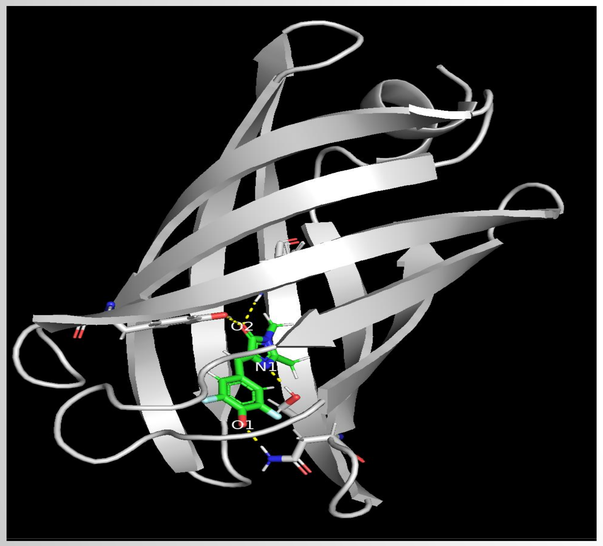


Introduction

The DFHBI ligand has a -1 net charge, and its partial charges vary from one ring to another. And since the electron distribution changes amongst the chromophore, electron distribution must also affect its brightness. Using existing quantum mechanics simulations in Professor Smith's lab, I researched how the partial charges are changed amongst different QM methods. By simulating electrons in the ground and excited states, we can change the partial charges on the DFHBI ligand to observe the shift in electrons. The study's overarching goal is to understand better how the protein movement is remotely controlled by nature and allows rational manipulation for therapeutic or synthetic applications.



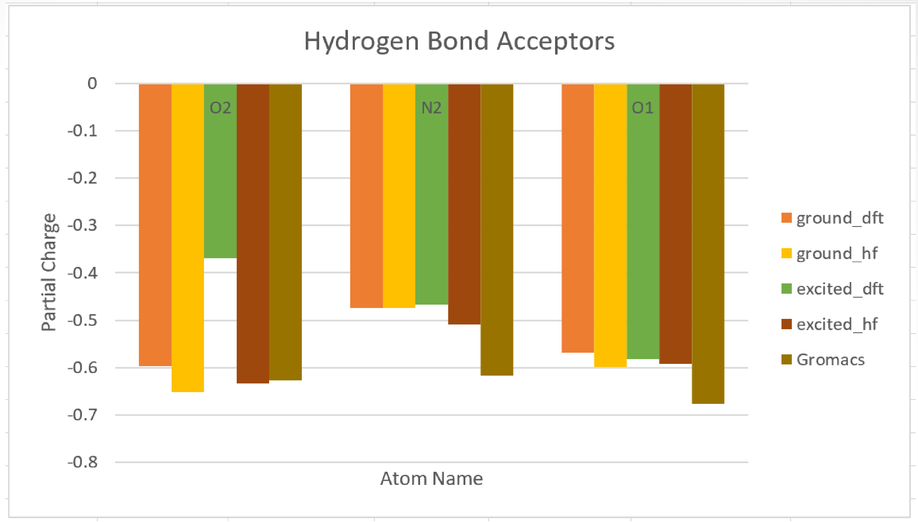
Central Question

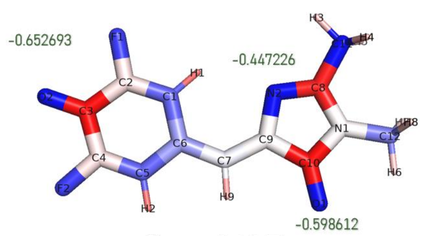
Is there a significant difference in the charge distribution in the ground and excited states when compared to the existing method in the Smith Lab?

Methods

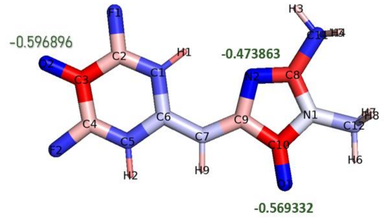
We used Antechamber, a set of auxiliary programs for molecular mechanic (MM) studies, to run MD simulations on cottontail (UNIX) to gather our output files to find the partial charges on each atom type DFHBI in the ground and excited states. We used Excel to gather the partial charges for each atom in the DFHBI ligand. We used data visualizations in excel to understand the difference in each QM methodology. And PyMol was used to represent the difference in charges on the molecule visually.

Results

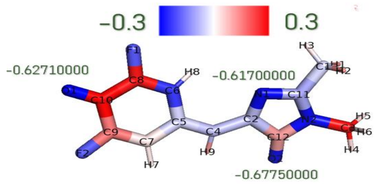




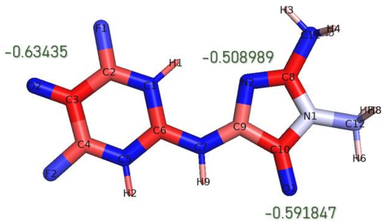
Ground_hf Figure



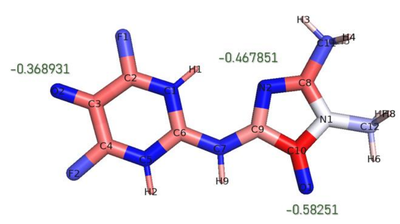
Ground_dft Figure



Gromacs Figure



Excited_hf Figure



Excited_dft Figure

Outcomes

The Gromacs model, the DFHBI molecule found in the smith lab, had most of its charge's distribution around the hydrogen bond acceptors found in the Phenyl and Imidazole group. And compared to the other models, we could see each QM method(Gaussian Output) from AM1-BCC also had many of its charges around the hydrogen bond acceptors. When comparing the differences, we found that AM1-BCC, the technique that optimizes to reproduce the hf calculated energies, works best to give us the partial charges close to the existing Gromacs partial charges found in the Smith Lab.

Conclusions

The strength of the potential charges of the terminal groups that make hydrogen bonds increases on the imidazole group in the excited states of each QM method. With the existing DFHBI molecule in the smith lab, we can tell that the O2 molecule in the Imidazole group has the most potent effect on hydrogen bonding.

Acknowledgements

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Future Directions

Edit the amber ff to include both excited state DFHBI partial charges and ground state and run MD simulations on the partial charges from the AM1-BCC methods

References

Wang, J. (n.d.). *Antechamber*. antechamber package. http://ambermd.org/antechamber/ac.html#antechamber.