Effect of the Protein Environment on the Electronic Properties of the **Oxyluciferin/Luciferase System**

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Motivation



- The oxyluciferin/luciferase complex has many applications in bioimaging¹ and biosensing²
- Goal: to determine the structural characteristics that affect the electronic transition properties of the oxyluciferin/luciferase system





- Only spectra from QM/MM MD present the expected red-shift and hypochromism

GAFF leads to a wrong description of the torsion energy and to an unphysical behaviour during the simulation

Conclusions

- The torsional motion of the OLU is hampered by the enzyme, reducing the intramolecular CT nature of the emitting state.
- The parametrization of a new FF is required to perform classical MD simulations.

