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# **Modelling Absorption Spectra of Furimamide - Nanoluciferase** System



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Bioluminescence is a biological phenomenon of light production by living species with many applications[1], notably for the detection of cancer cells[2]. The present study deals with a ligand-protein bioluminescent system (furimazine – Nanoluciferase) derived from a shrimp called Oplophorus gracilirostri with a very high luminescence intensity[3]. A better understanding of this system will provide insights to tailor new devices with emission of a photon with a red color, and thus a light signal more easily detectable inside the human body. Simulations of the emission and absorption spectra are relevant tools to comply this goal[4]. We focus here on the absorption spectra of the light emitter system furimamide – Nanoluciferase. In order to take into account the protein environment and the system flexibility, we carry out classical molecular dynamics (MM) with AMBER software. Furimamide is a flexible molecule: standard force fields such as GAFF[5] (General Amber Force Field) are unable to reproduce correctly potential energy along torsion angles when compared to in vacuo DFT computations. Thus, we perform a multidimensional fit using 1D and 2D potential energy surface scans with several torsion angles of the molecule in order to parameterize a new force field. Then, we compute electronic transitions at a QM/MM level of theory on a set of 100 snapshots extracted from MM trajectory. As a perspective, we plan to use the same methodology to simulate emission spectra.









 $\mathbf{G}^{-}\mathbf{G}$ 

 $\theta = NCCC$ 

 $\varphi = CCCO$ 

The potential energies calculated using the GAFF2 force field doesn't match with the ones calculated using DFT scans of 7 dihedral angles of the molecule. The force field needs to be adjusted.

# **References**:

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# **Conclusion and perspectives:**

0.2

We have automatized the absorption spectra simulation, we need to compare our results with experimental data. The emission spectra are yet to be simulated in order to modelize the color of emission of this system.