Modeling properties of the chromophore from the green fluorescent protein
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What did we learn from the literature?

Current hypothesis
The neutral form is responsible for absorption at 395 nm
The anionic form is responsible for emission at 508 nm

Motivation
We intend to verify by computational experiments the current hypothesis on the fluorescence process in GFP and suggest our own viewpoint

Minimum energy conical intersections (MECI) have been located by using the CASSCF(12,11)/cc-pVDZ approach
The shape of the excited state potential energy surface along the torsion angles is essential

In the gas phase the GFP chromophore does not emit due to the conical intersections for all protonation forms. This is consistent with experimental observations.

Modeling cis-trans isomerization of the anionic form of the GFP chromophore in the gas phase and aqueous solution

CONCLUSION:
the NEUTRAL form absorbs and the CATIONIC form emits

The CASSCF energy profile is consistent with the experimental data