

Absorption spectra of biological systems from TDDFT

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www.tddft.org/programs/octopus/

Collaborators



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Our approach...

- Protein Data Bank (<http://www.pdb.org>)
- Optimization of starting geometry
 - (Small) basis sets
 - QM/MM methods
 - Molecular dynamics
- Calculation of linear absorption spectra using `octopus`
 - Quantities are discretized in real-space
 - TD Kohn-Sham equations are propagated in real-time
 - XC potential is approximated at the level of the ALDA or AGGA
 - Troullier-Martins pseudo-potentials

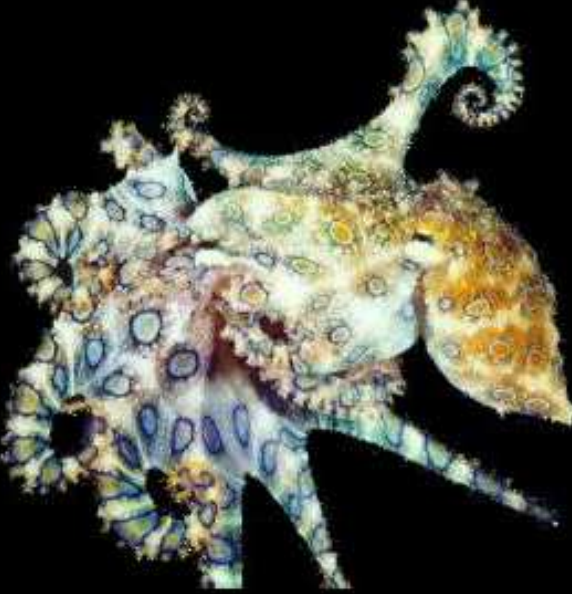


octopus

<http://www.tddft.org/programs/octopus>



OCTOPUS



- News**
- Download**
- Documentation**
- Pseudopotentials**
- Contributors**
- References**

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Green Fluorescent Protein - *Aequorea victoria*



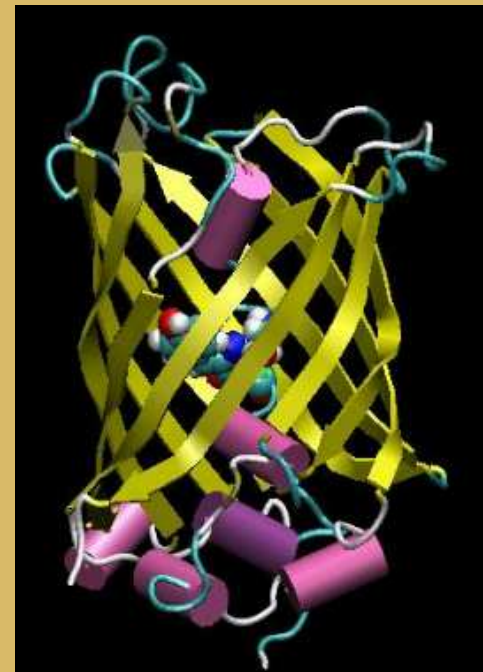
Aequorea victoria is an abundant jellyfish in Puget Sound, Washington State, from which the luminescent protein aequorin and the fluorescent molecule GFP have been extracted, purified, and eventually cloned. These two products have proved useful and popular in various kinds of biomedical research in the 1990s and 2000s and their value is likely to increase in coming years.

<http://faculty.washington.edu/cemills/Aequorea.html>

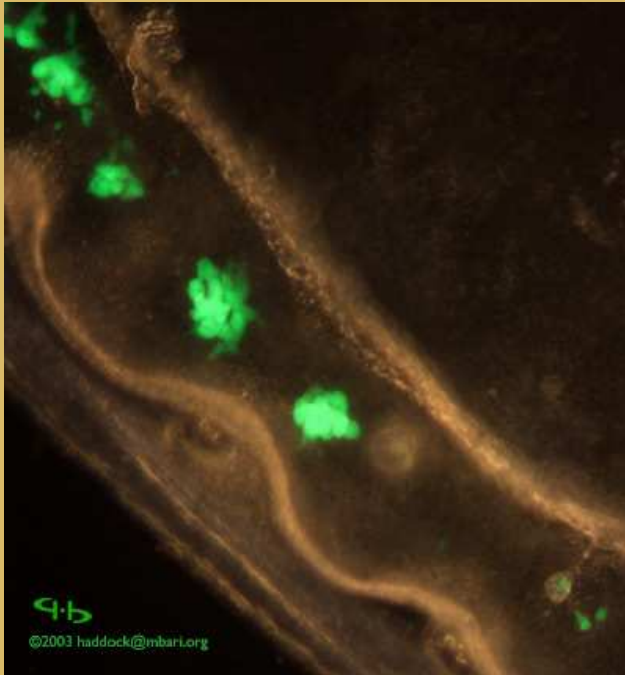


Green Fluorescent Protein - Data Sheet

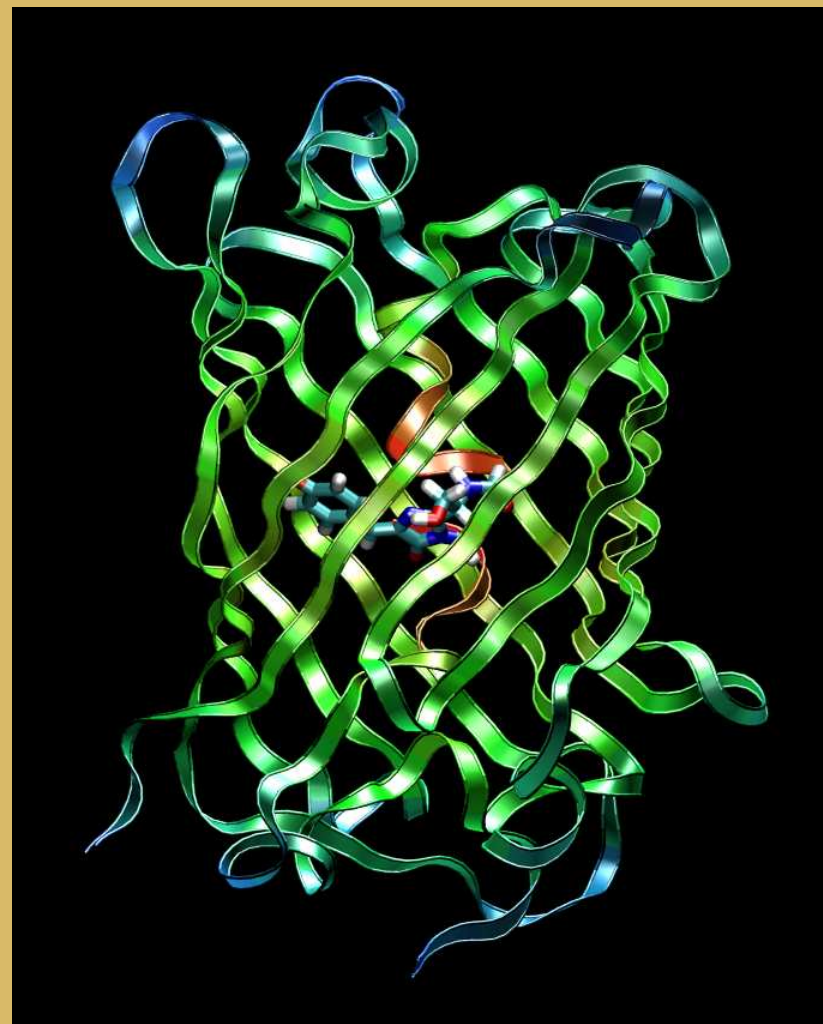
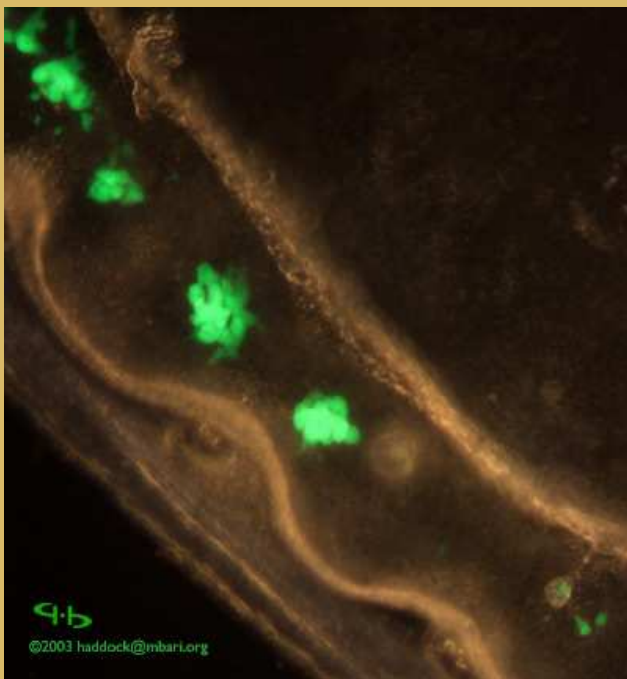
- 238 AA protein forming a β -barrel or β -can
- Chromophore located inside the β -barrel (shielded)
- Info to create the chromophore contained entirely in the gene
- High Stability: Wide pH, T, salt
- Long Half life: ≈ 20 years
- Resistant to most Proteases
- Active after peptide fusions: reporter protein
- Availability of chromophores variants



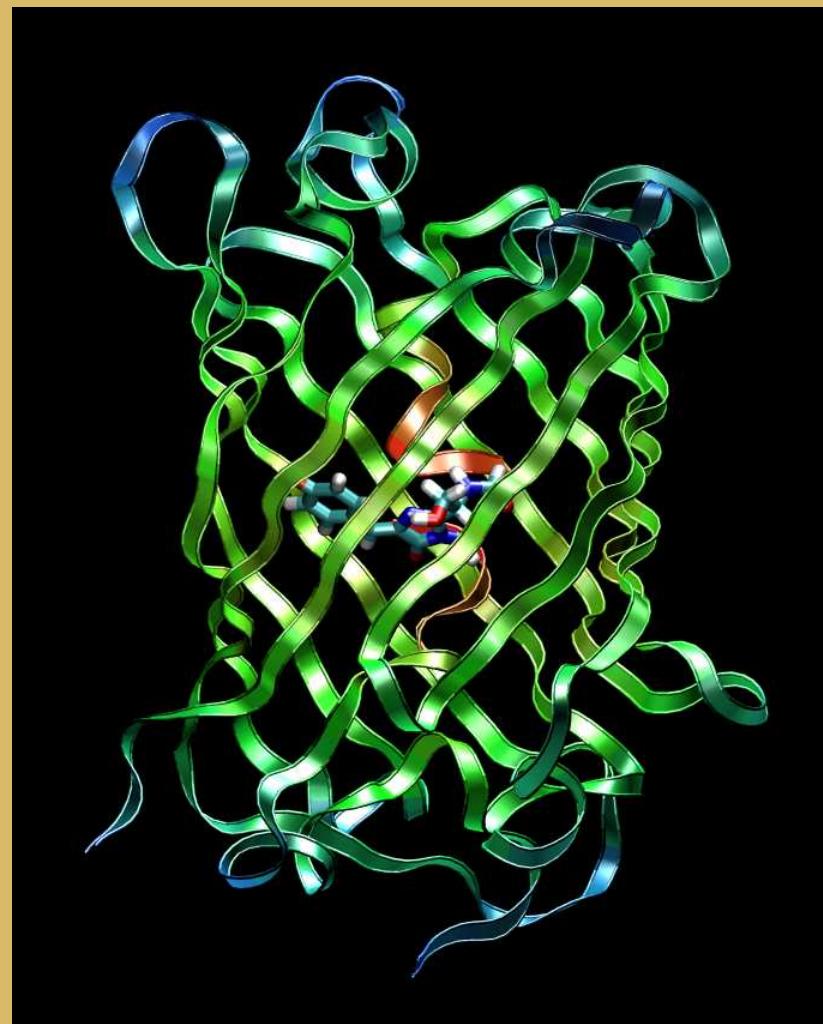
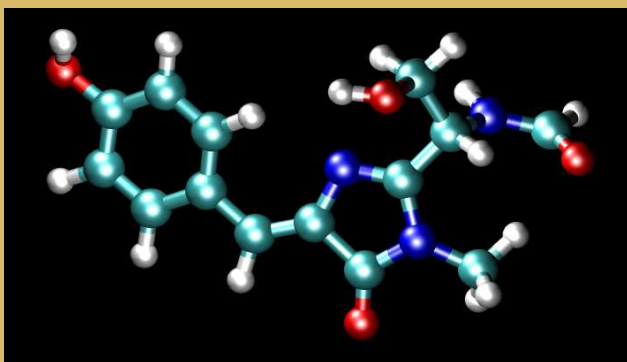
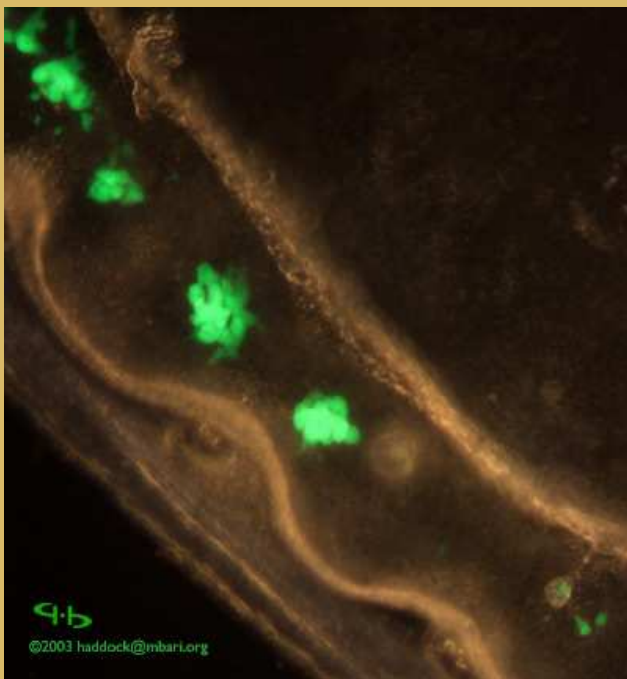
Green Fluorescent Protein - Chromophore



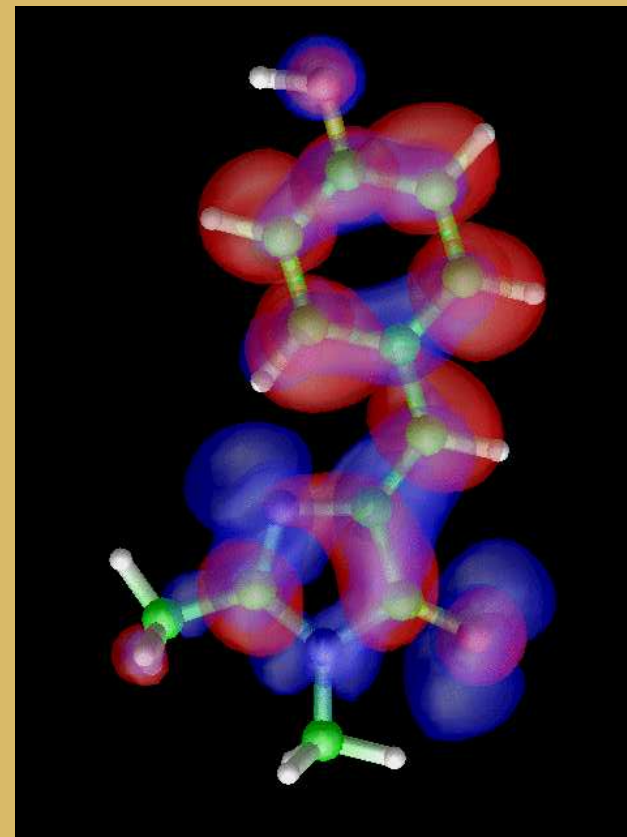
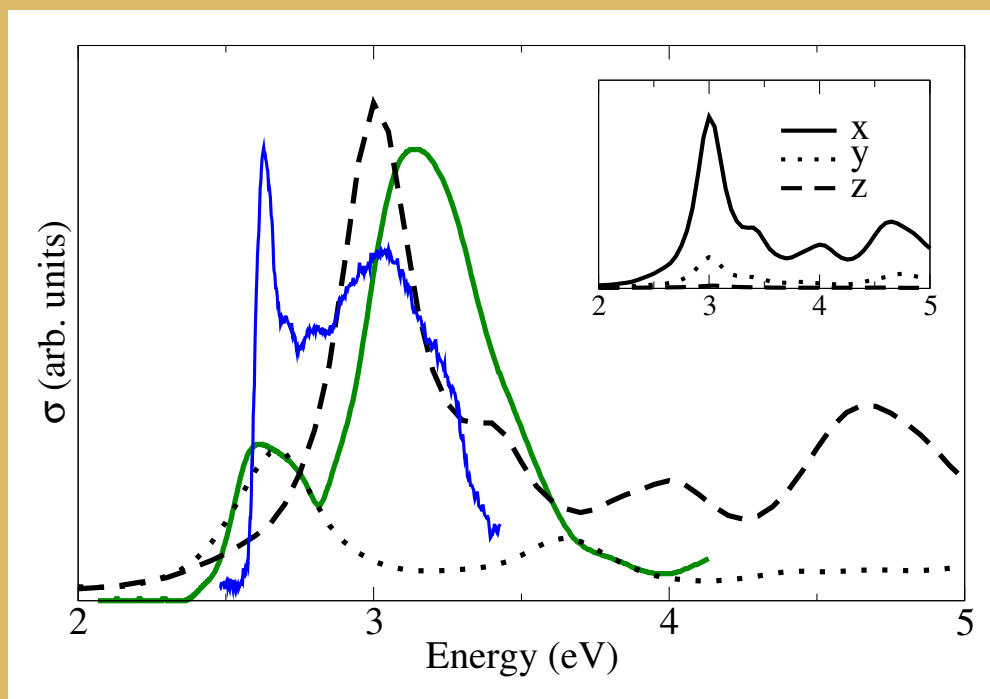
Green Fluorescent Protein - Chromophore



Green Fluorescent Protein - Chromophore

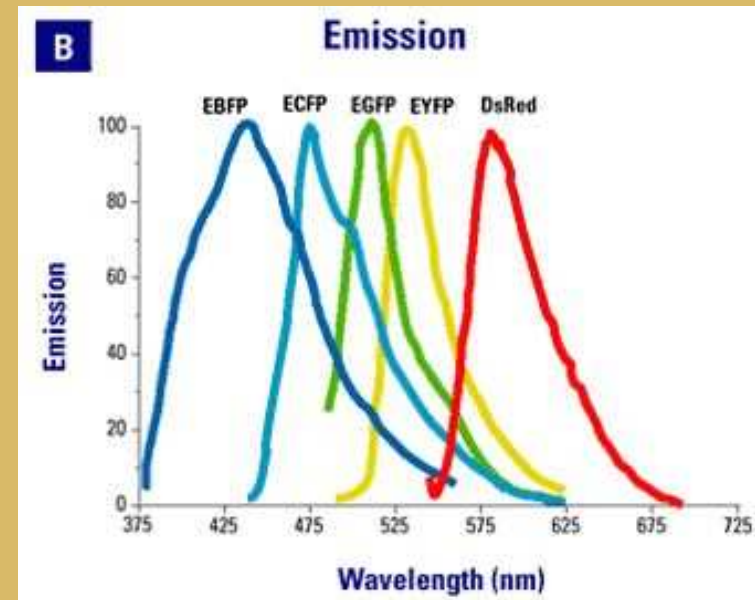
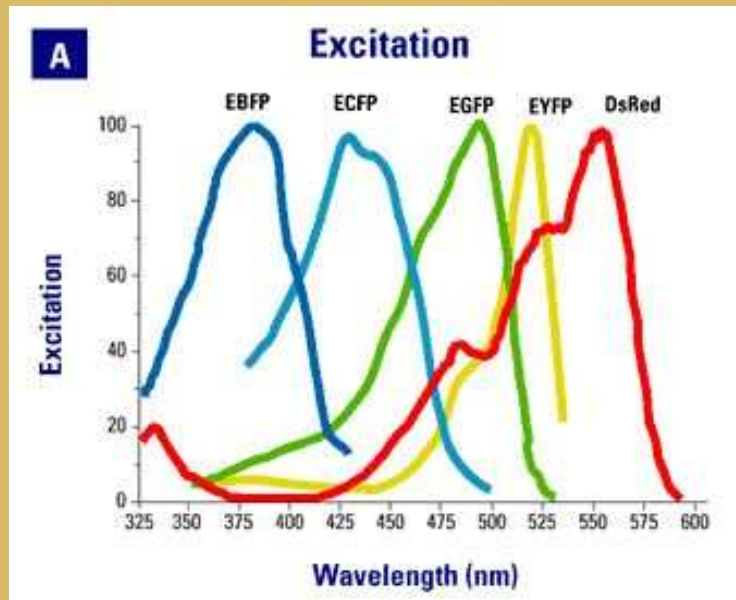


Green Fluorescent Protein - Results

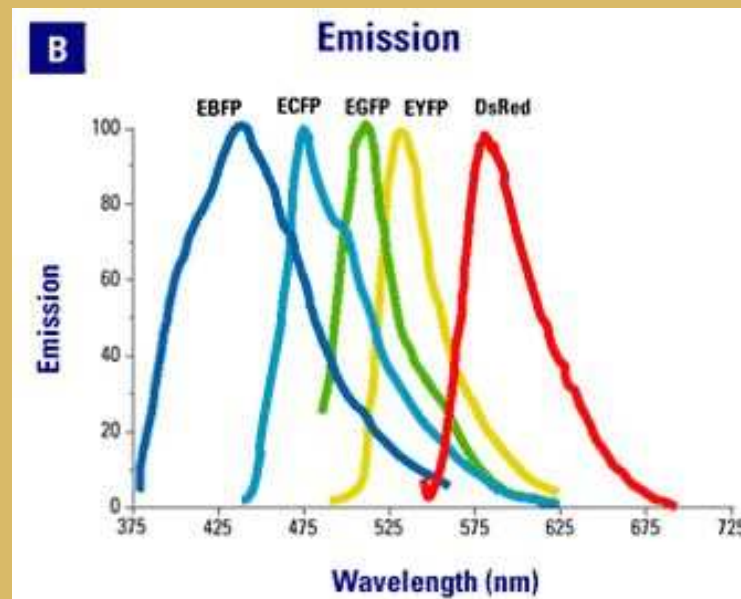
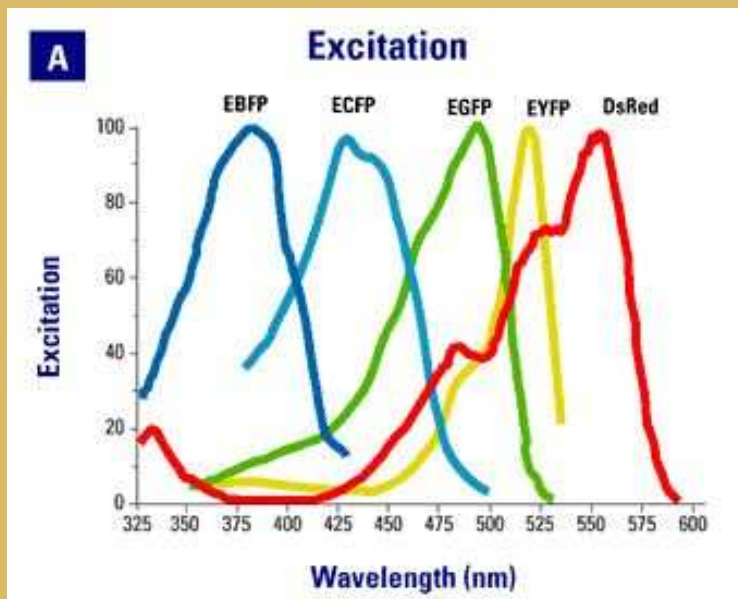


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Phys. Rev. Lett. **90**, 258101 (2003)

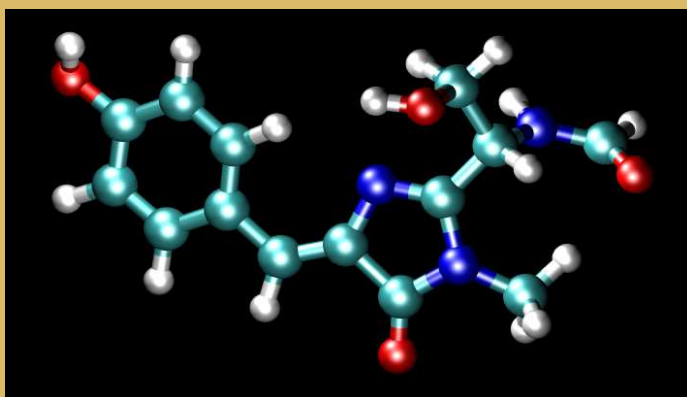
Blue Fluorescent Protein - Mutants



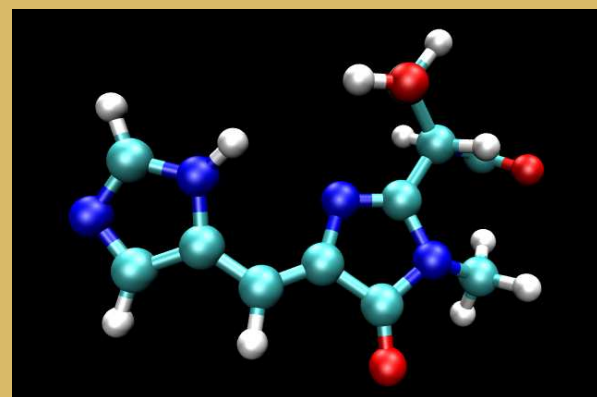
Blue Fluorescent Protein - Mutants



Green

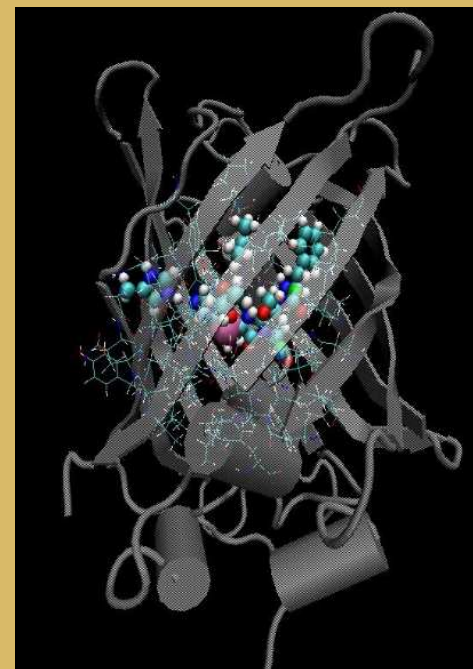


Blue

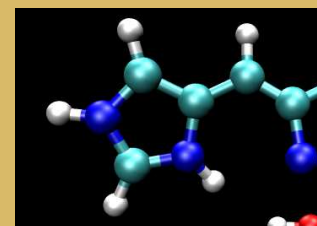
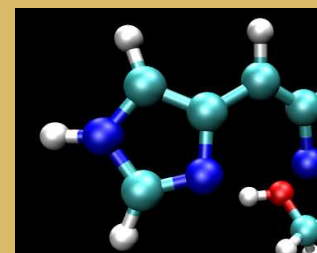
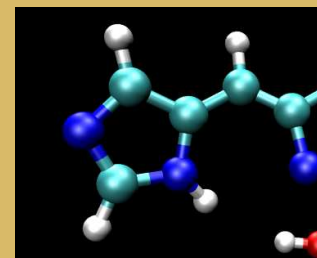
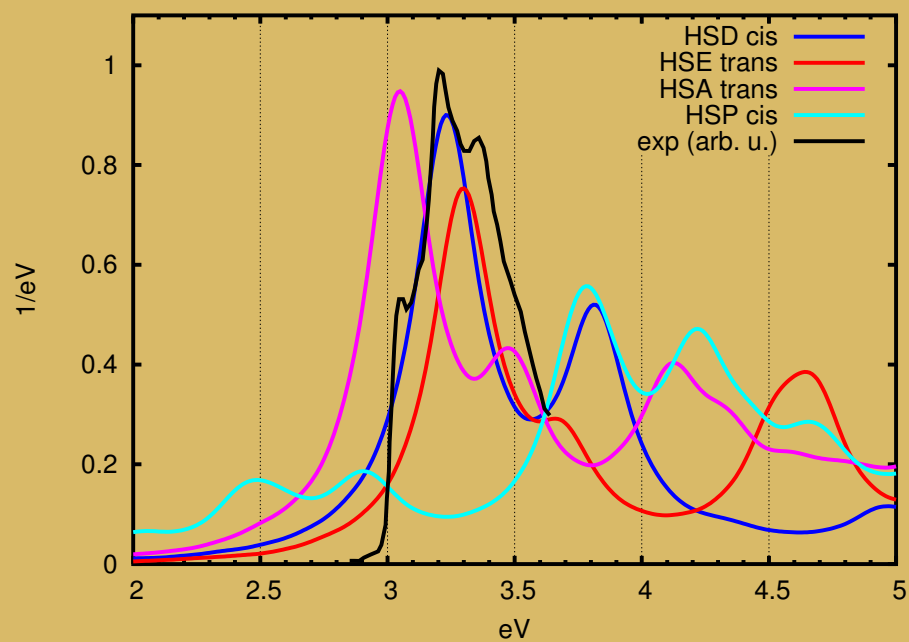


Blue Fluorescent Protein - Data Sheet

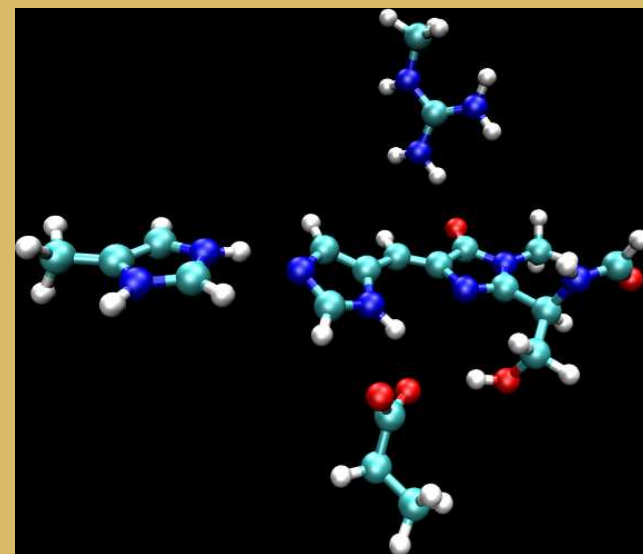
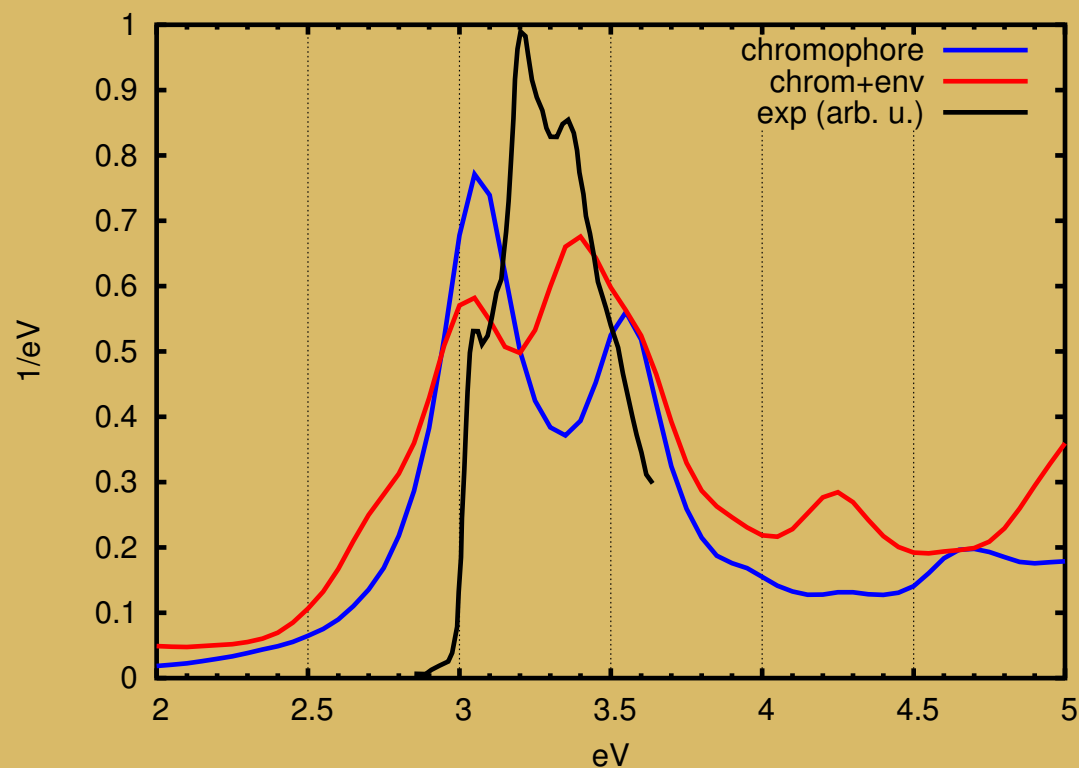
- Chromophore is composed of -Ser-His-Gly-
- Added Complexity due to the higher number of possible protonation states
- No proton information from X-Ray
- Experimental pKa's estimations suggest that HSA should be ruled out
- In addition, there are various conformers for each protonation state
- In vacuum, the global minimum in the neutral state cis-HSD



Blue Fluorescent Protein - Results



Blue Fluorescent Protein - Environment



- Inclusion of the micro-environment shifts only one of the peaks and the complexity of the shape increases
- Less satisfactory results than for the GFP (LDA?)