Redox properties of green fluorescent proteins and their chromophores

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The redox properties of chromophores of different fluorescent proteins from green fluorescent protein family were studied in different solvent atmospheres using density functional theory (with a long-range corrected functional) and implicit solvation models. Redox potential of the chromophores were calculated using a thermodynamic cycle. We studied the effect of conjugation length, resonance stabilization and presence of heteroatoms in the electron-donating abilities of these chromophores. We also investigated the effect of protein atmosphere in the redox potential. The computation of redox potential of the protein was performed using linear response approach (LRA). We use QM/MM electrostatic embedding scheme to describe the protein atmosphere, where the chromophore was included in QM part and rest of the protein was described by point charges. The photo-switchable protein DRONPA in it's ON state was studied for calculating redox potential in protein atmosphere.