

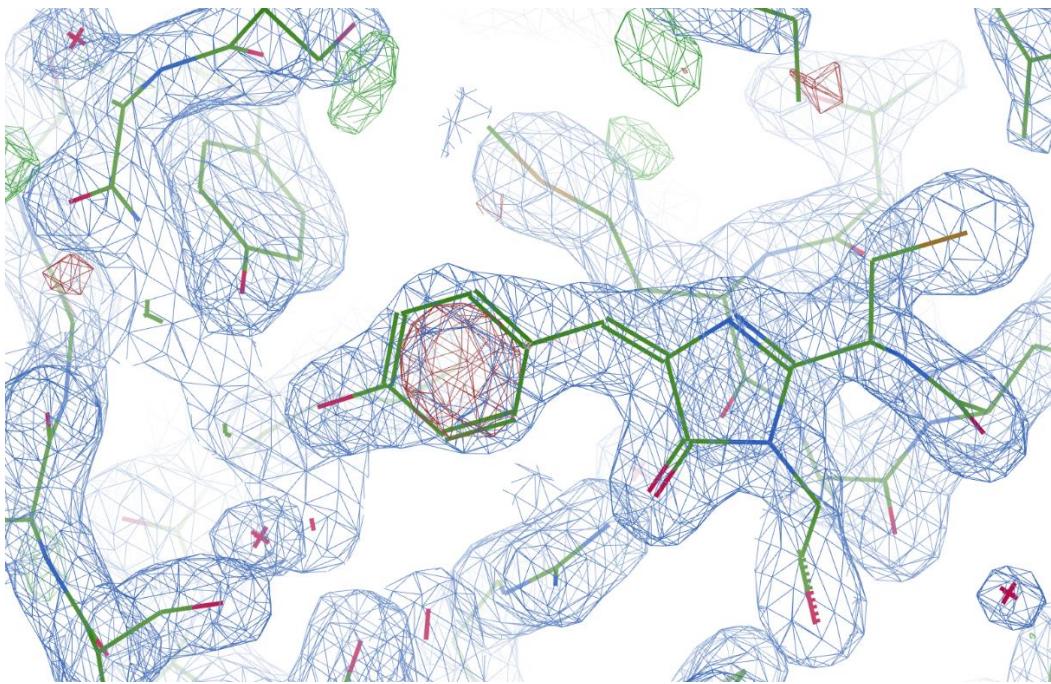
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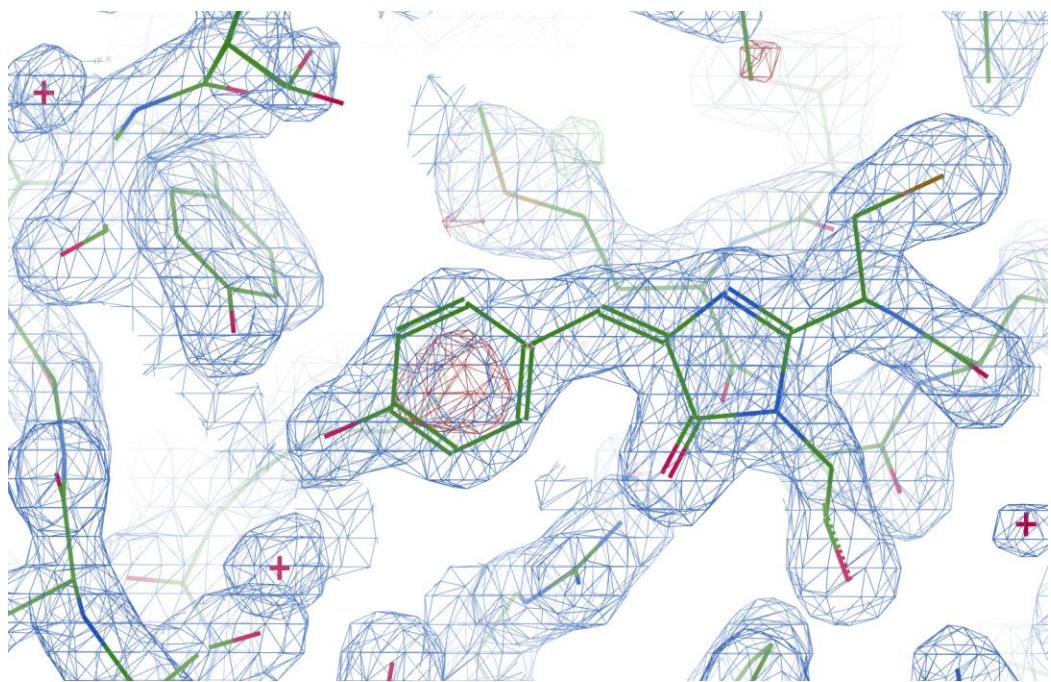
Supporting information for article:

Room-temperature photo-induced martensitic transformation in a protein crystal

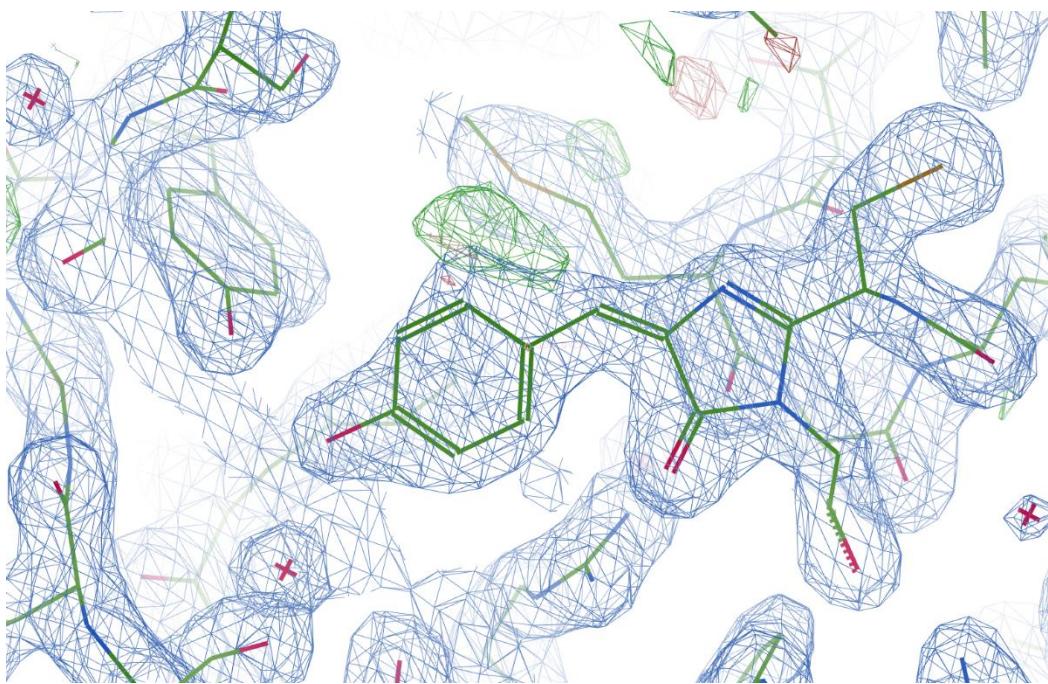
Steven Dajnowicz, Patricia S. Langan, Kevin L. Weiss, Ilia N. Ivanov and Andrey Kovalevsky



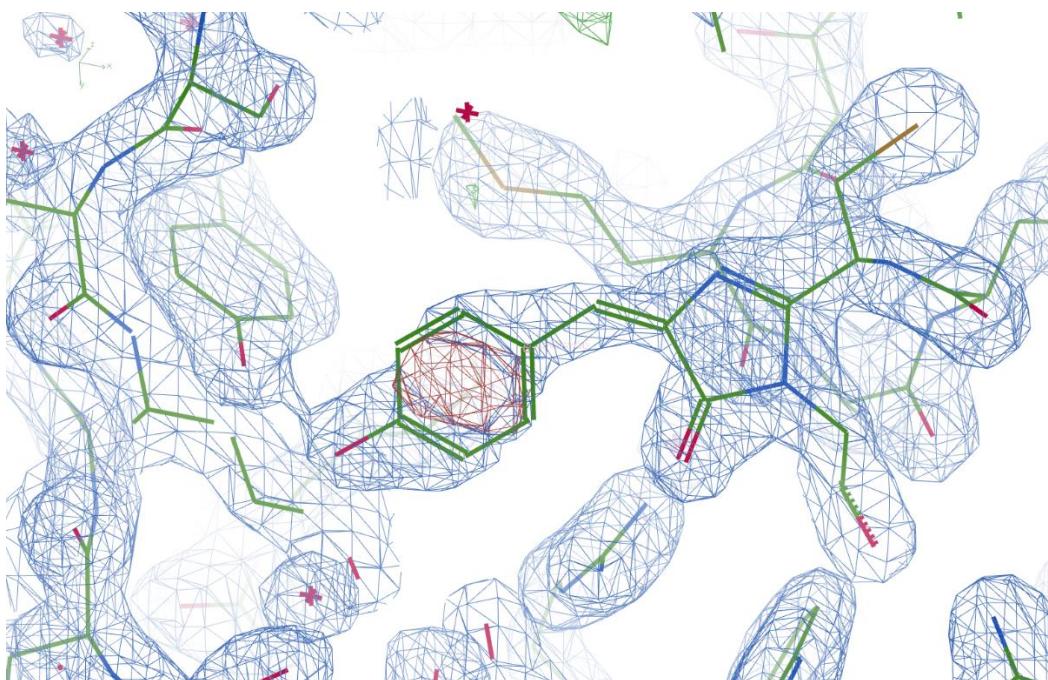
Molecule A



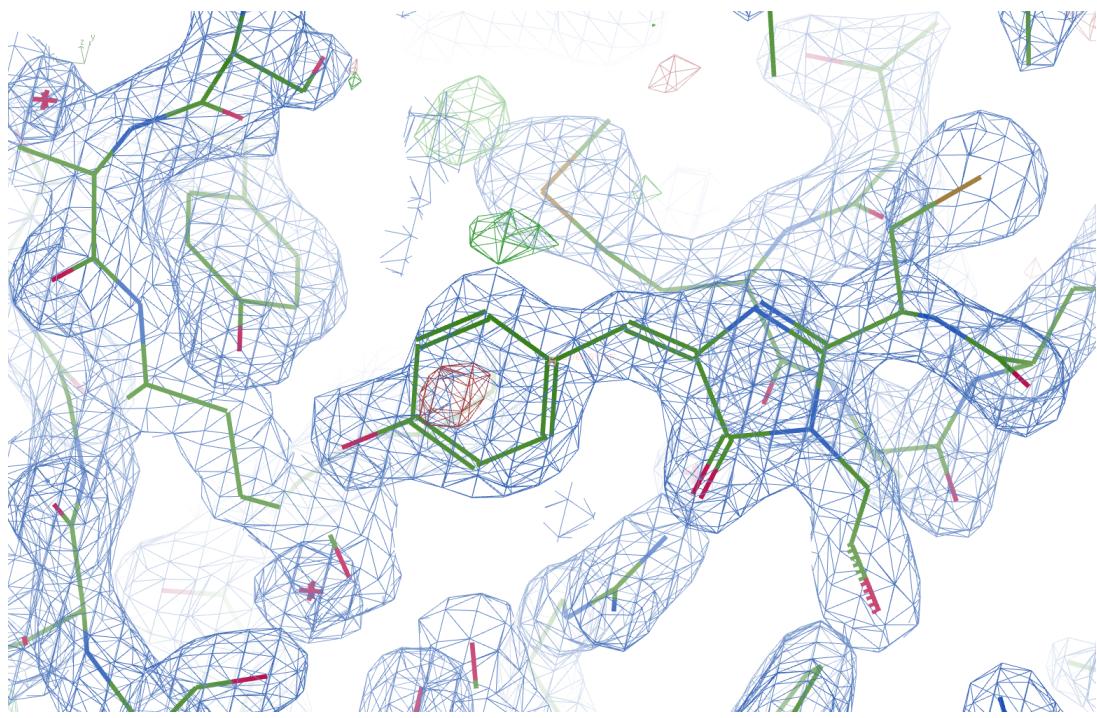
Molecule B



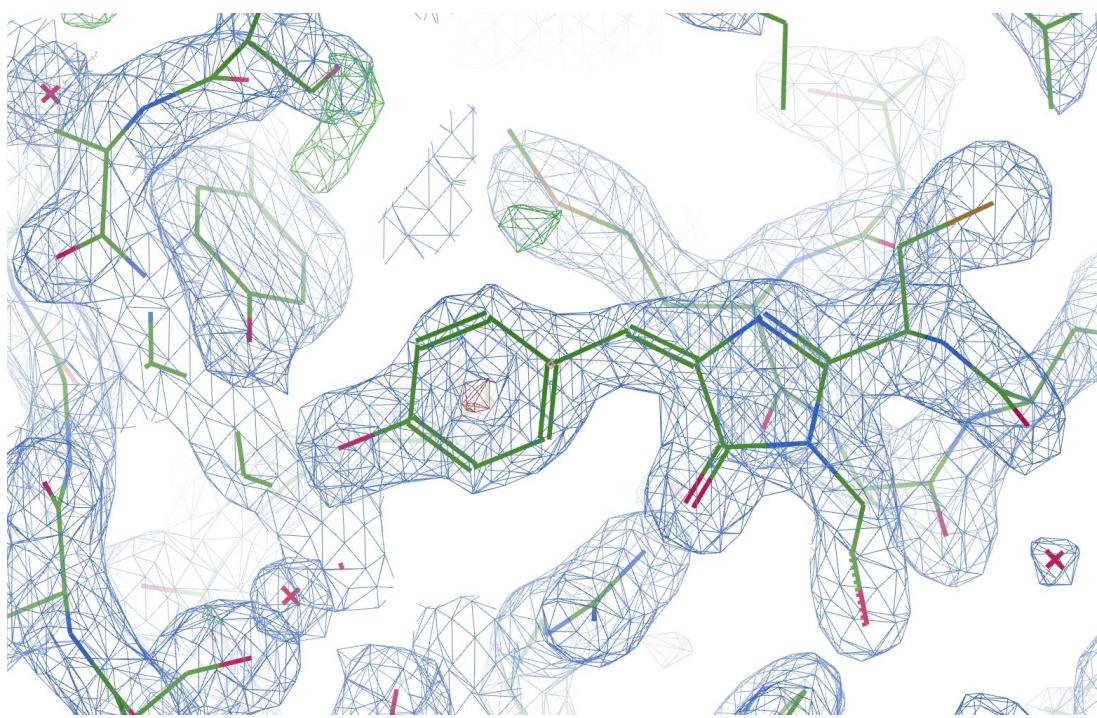
Molecule C



Molecule D



Molecule E



Molecule F

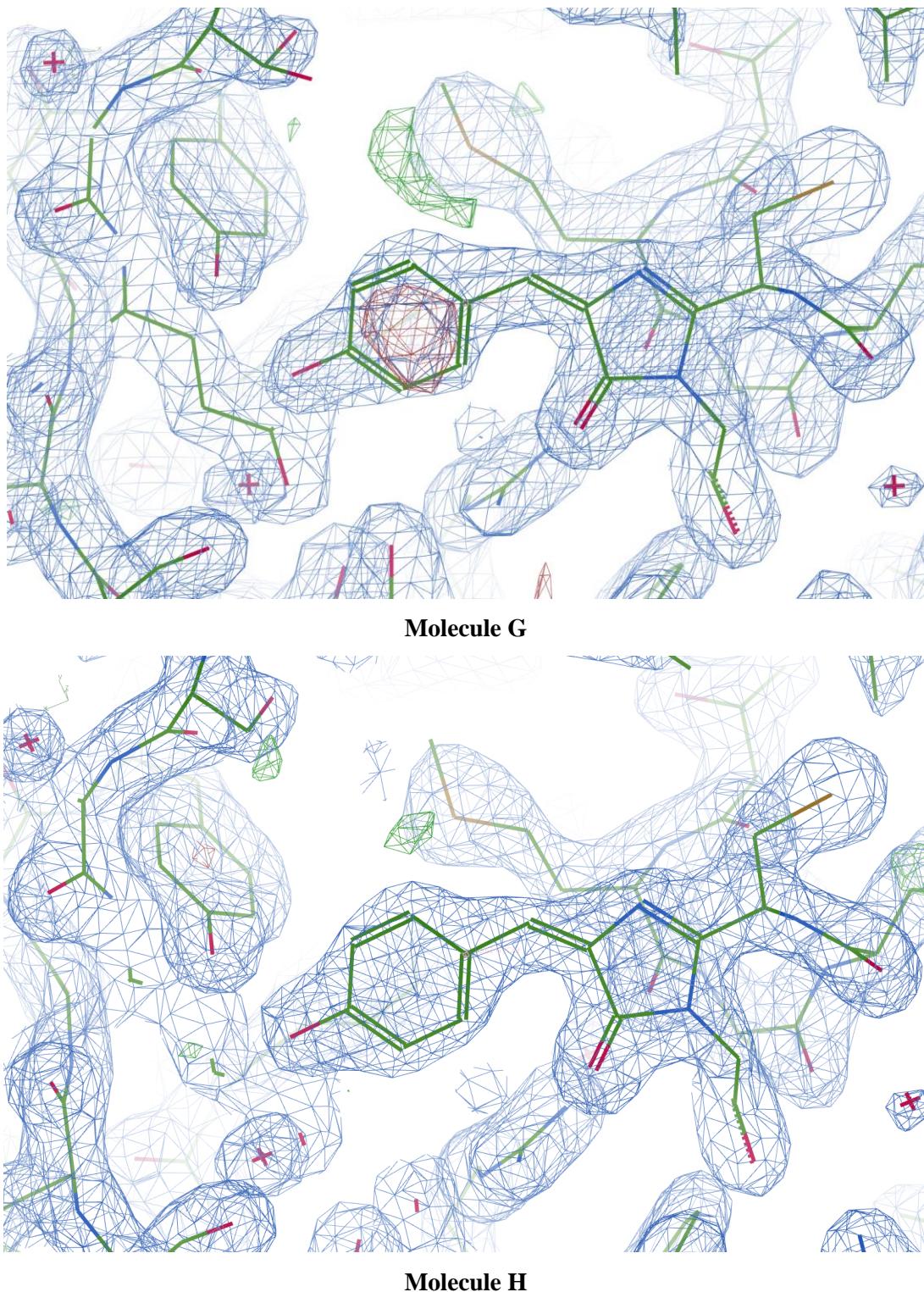
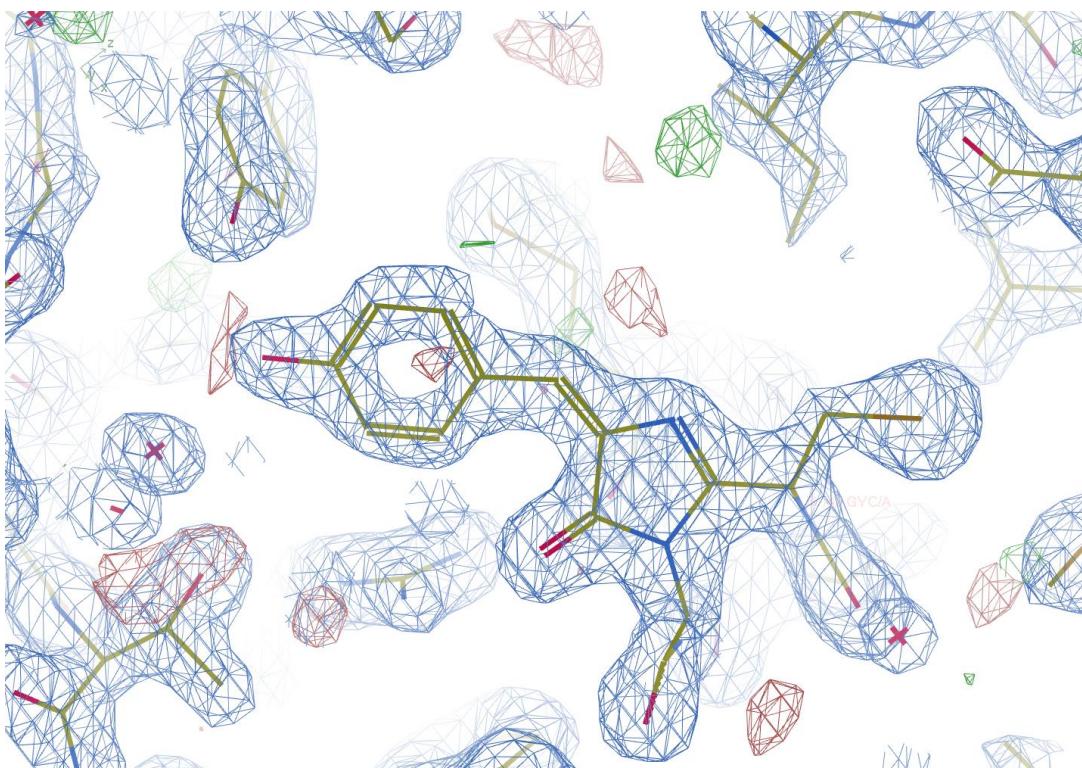
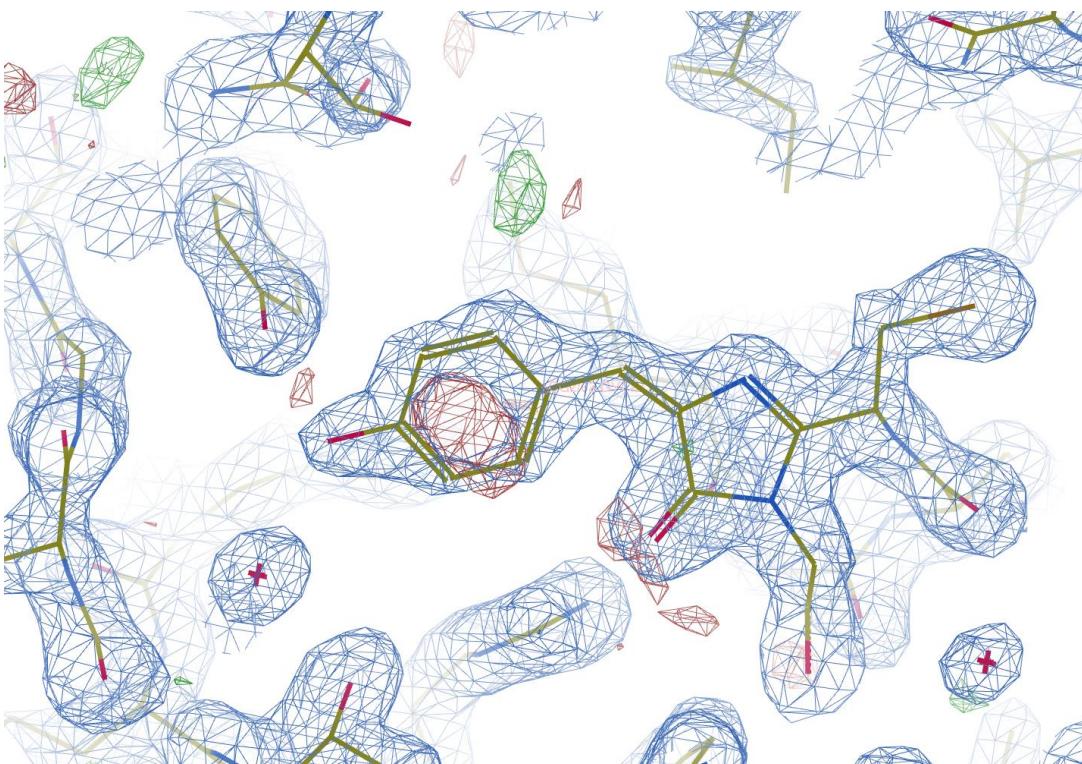


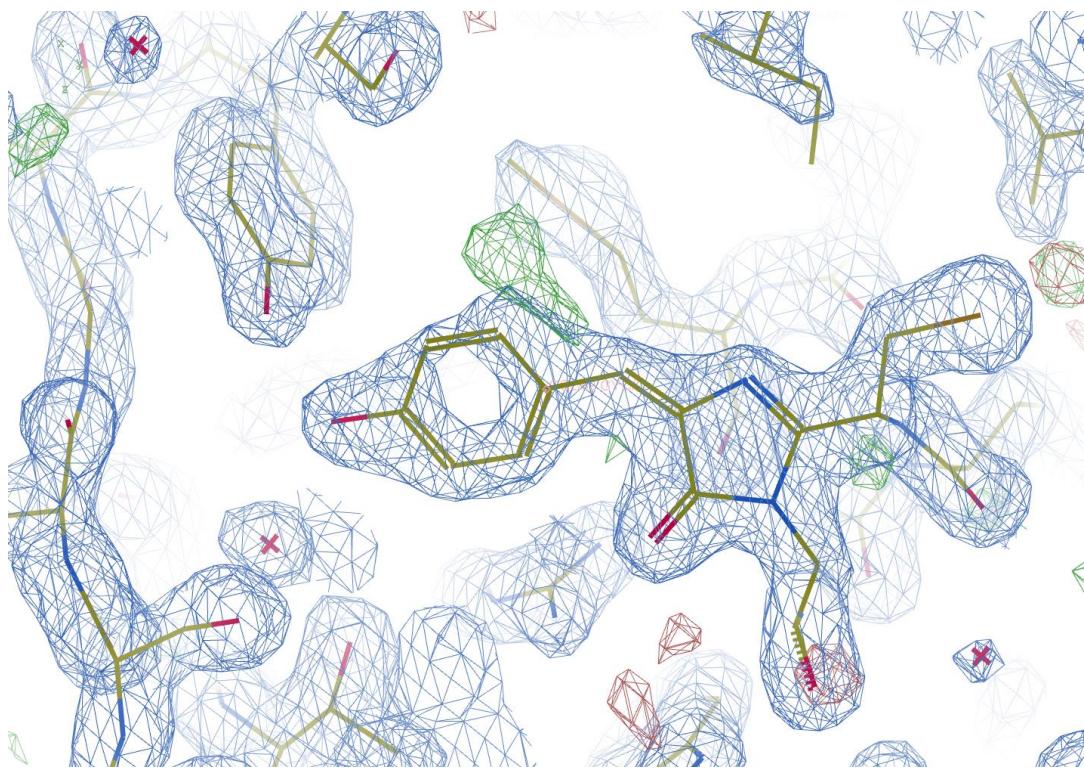
Figure S1 Electron density maps in the vicinity of the chromophore in hydrogenous Tetdrone, demonstrating that all 8 symmetry-independent molecules contain the trans configuration. $2\text{Fo}-\text{Fc}$ map is shown at 1.5σ level (blue mesh); the difference $\text{Fo}-\text{Fc}$ map is shown at 3 and -3σ levels (green and red meshes respectively).



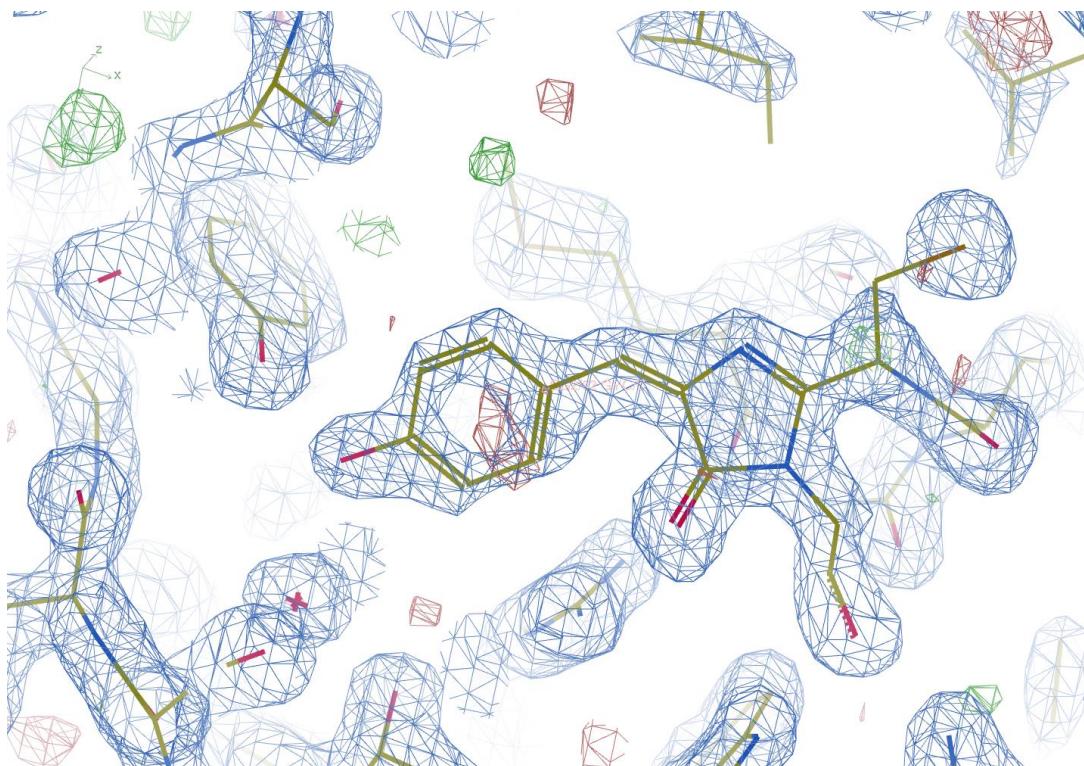
Molecule A



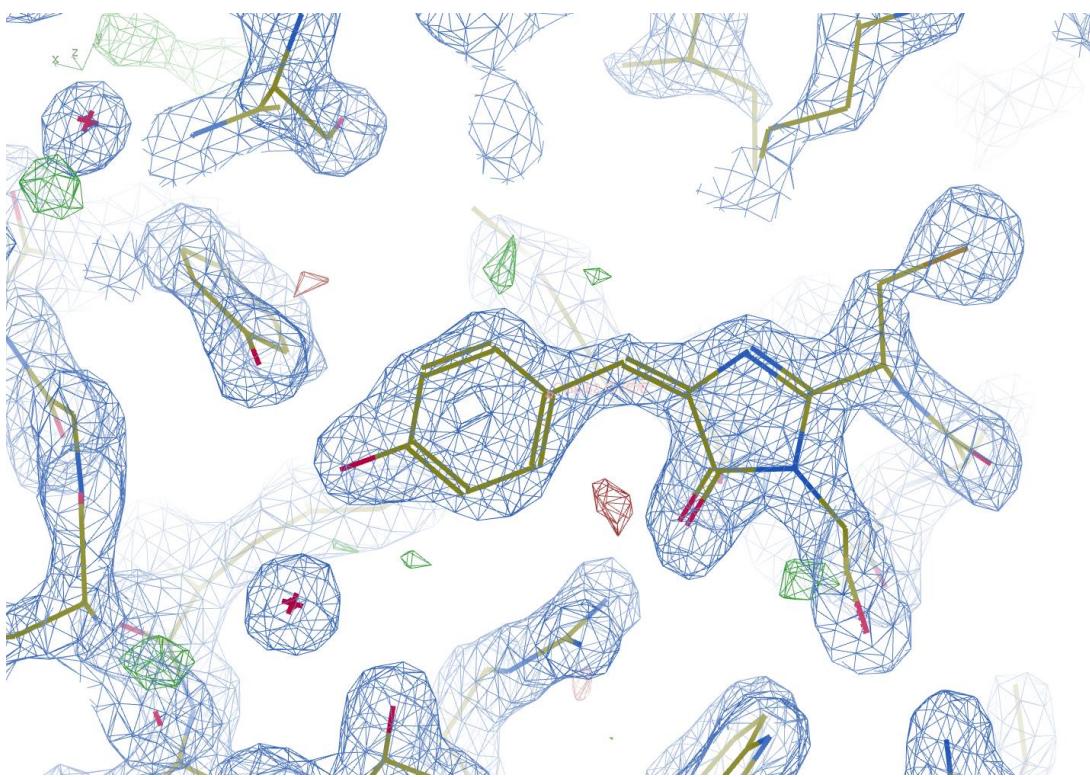
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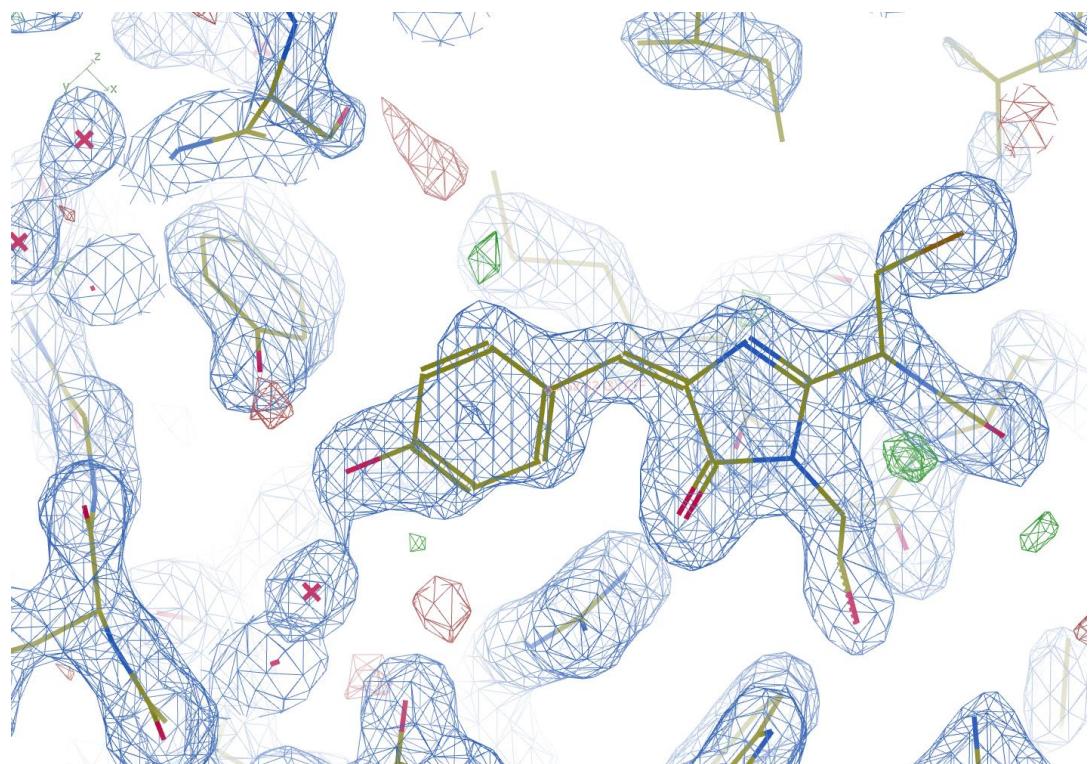
Molecule C



Molecule D



Molecule E



Molecule F

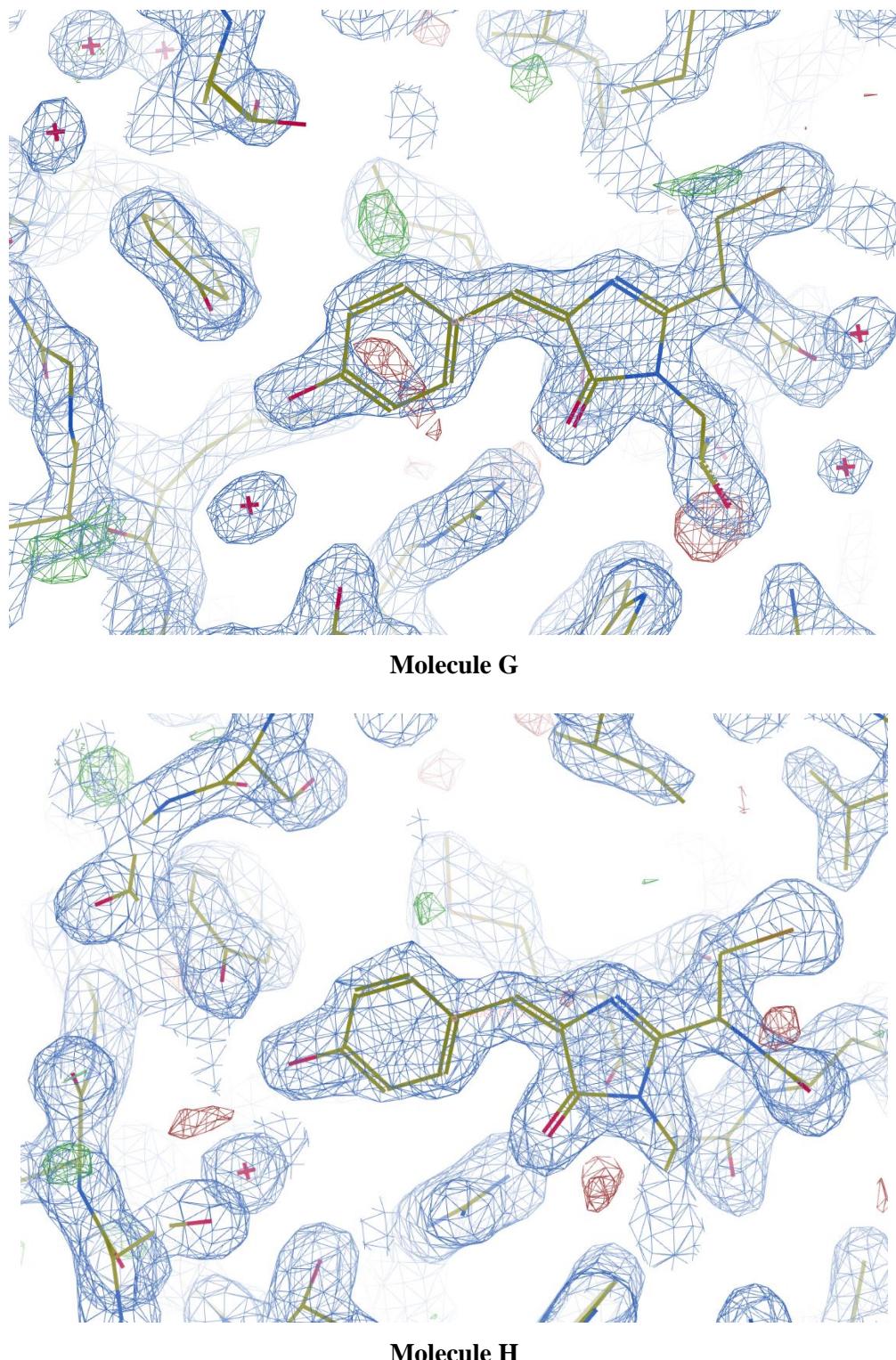


Figure S2 Electron density maps in the vicinity of the chromophore in perdeuterated Tetron, demonstrating that all 8 symmetry-independent molecules contain the trans configuration. $2\text{Fo}-\text{Fc}$ map is shown at 1.5σ level (blue mesh); the difference $\text{Fo}-\text{Fc}$ map is shown at 3σ and -3σ levels (green and red meshes respectively).

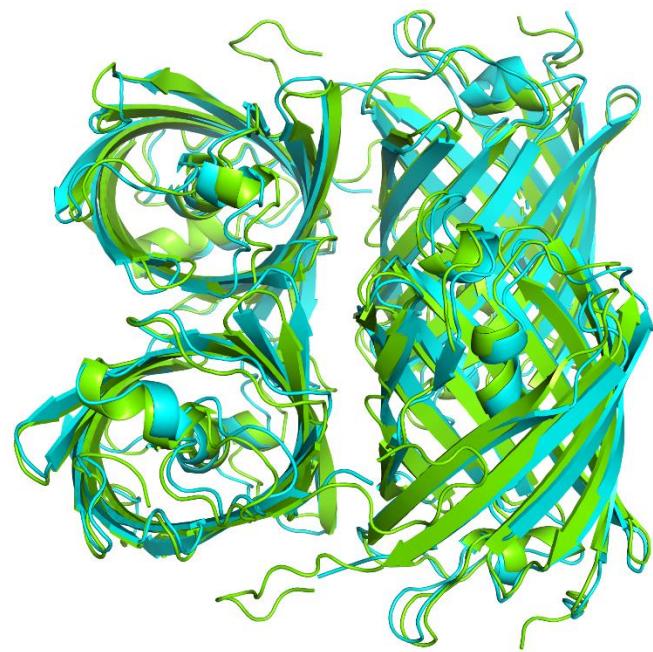


Figure S3 Structural alignment of Tetdrone in the 400 nm irradiated state (cyan) and the GFP from *Anemonia sulcata* (green).

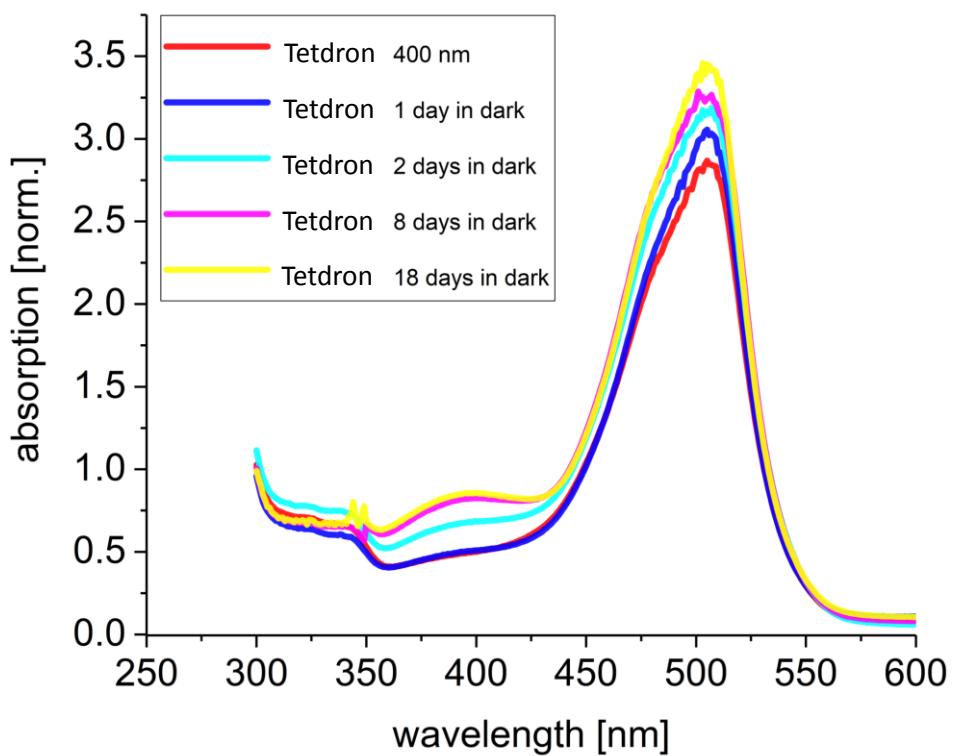


Figure S4 Crystal UV-Vis absorption spectra of Tetdrone irradiated with 400 nm light (red line), followed by relaxation in the dark (blue→yellow lines).

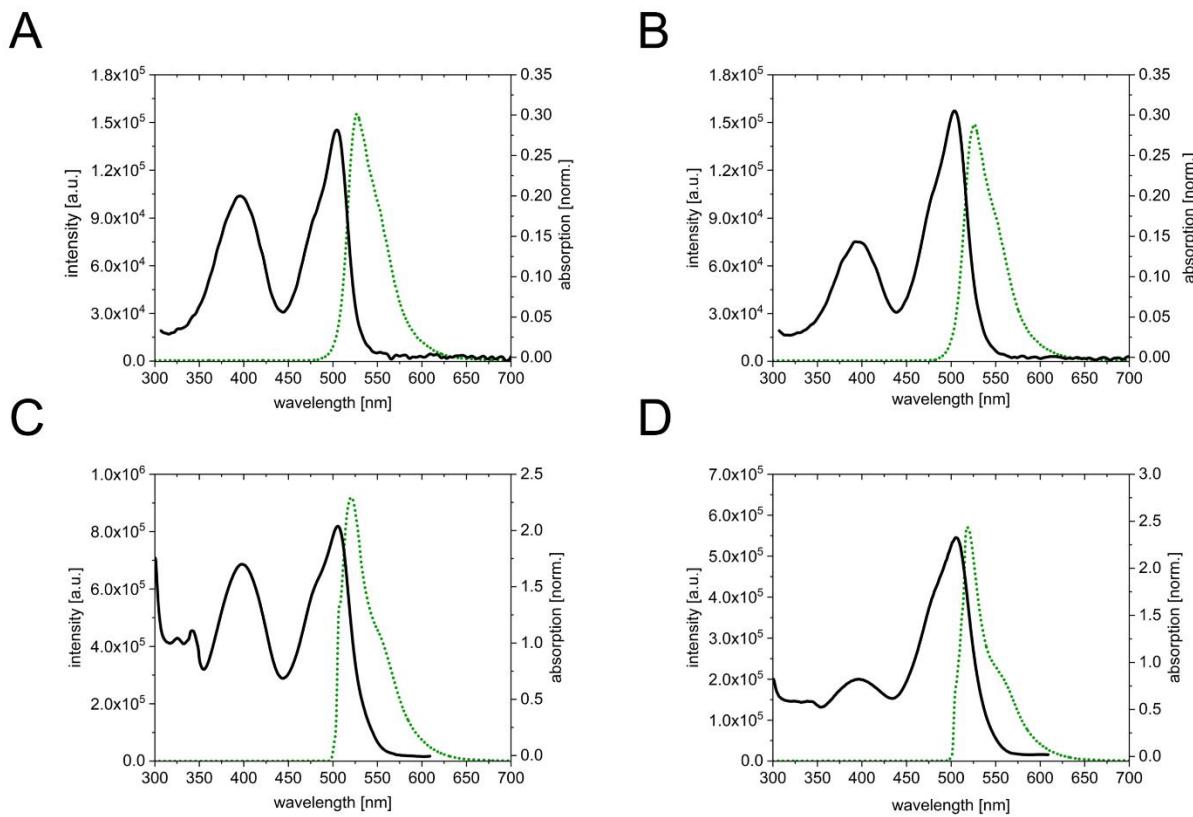


Figure S5 Tetdron UV-Vis absorption spectra and superimposed emission spectra. Emission spectra are one-dimensional slices at 500nm excitation wavelength of the corresponding fluorescence maps on Figure 7 Solution measurements of hydrogenated (**A**) and deuterated (**B**) Tetdron. Crystal measurements of hydrogenated (**C**) and deuterated (**D**) Tetdron.