

## ELECTRONIC SUPPORTING INFORMATION

### A donor-acceptor pair for the real time study of vibrational energy transfer in proteins

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The supporting information contains additional spectra and structures of additional compounds used for band assignment. The analysis of time-resolved data and how transients for vibrational modes are calculated is described in the last part of this supporting information.

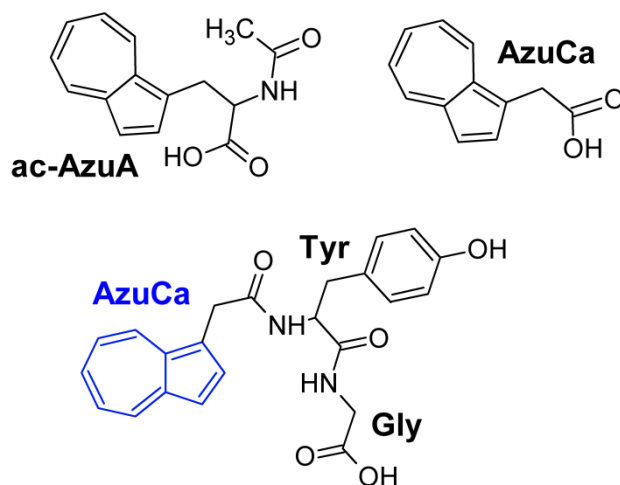


Figure S1: Structure of the monomeric azulene compounds ac-AzuA (Acetyl-azulenyl-alanine), AzuCa (Azulene-1-yl-acetic-acid) and the additional test peptide AzuP' (sequence AzuCa-Tyr-Gly).

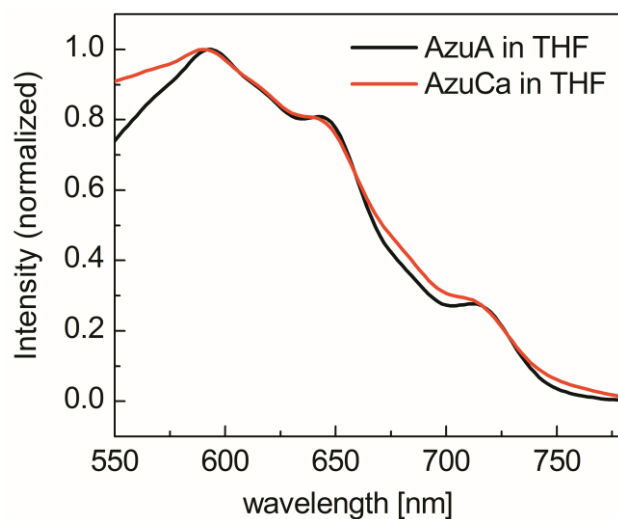


Figure S2: UV/Vis spectra of ac-AzuA and AzuCa in THF, covering the region of the  $S_0 \rightarrow S_1$  transition.

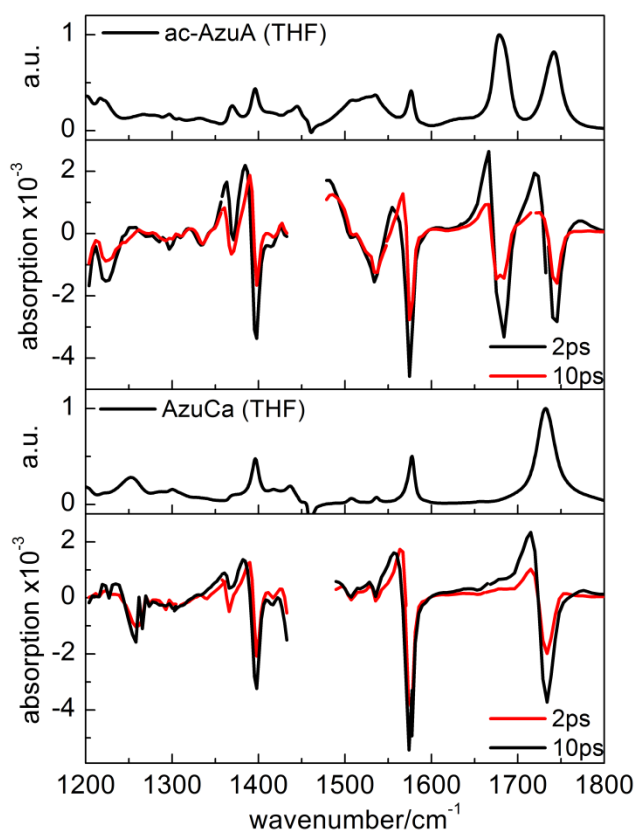


Figure S3: FTIR and transient IR spectra of ac-AzuA and AzuCa in THF. Note the break between data, no data were recorded between 1438 - 1486 cm<sup>-1</sup> due to high solvent absorption.

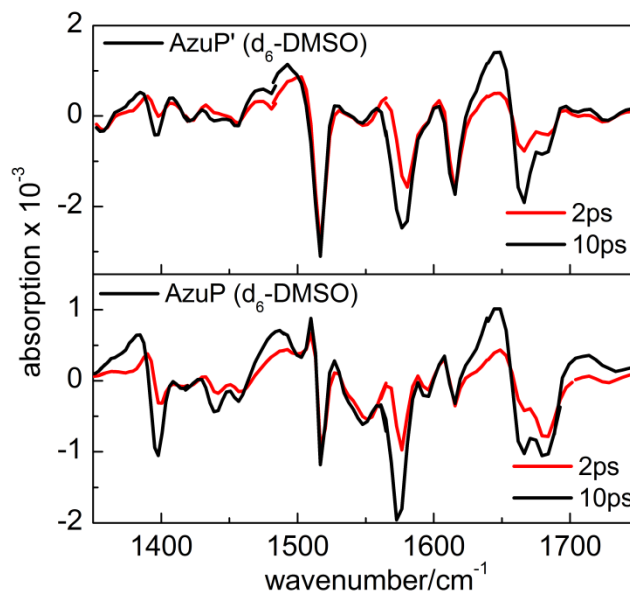


Figure S4: Transient IR data of the investigated model peptide AzuP in comparison to spectra of a shorter peptide AzuP' (upper panel) that were collected to obtain additional support for assignment.

### Data Analysis

Data were recorded as transient pump-probe spectra at a fixed pump wavelength of 600 nm. Resulting example spectra are plotted in figure S5. For the shown transients, that were used to analyze peak times  $t_{\max}$  and to help with band assignment, typically the bleach signal at one pixel was plotted. For small signals or broad signals, data are integrated by adding up several pixels. For some very weak signals the amplitude of the signal is shown, calculated from the intensity of the excited state absorption minus the intensities for the bleach signal.

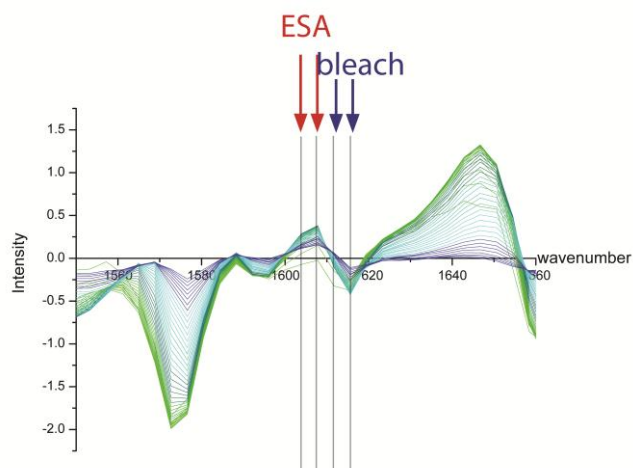


Figure S5: Example for data analysis. Shown are transient IR data for AzuP in the amide I region. Transients are either plotted as change of bleach intensity on one pixel, integrated bleach intensity (sum over more pixel) or in case of very small signals the amplitude, calculated from bleach signal and excited state absorption is shown.

### Shown transients in figure 3

- 2098  $\text{cm}^{-1}$  bleach, single pixel at 2098  $\text{cm}^{-1}$
- 1728  $\text{cm}^{-1}$  amplitude, (ESA[1710 + 1714]) - (bleach[1723 + 1728])
- 1678  $\text{cm}^{-1}$  bleach, single pixel at 1678  $\text{cm}^{-1}$
- 1670  $\text{cm}^{-1}$  integrated bleach signal, sum of signal at 1668  $\text{cm}^{-1}$  + 1672  $\text{cm}^{-1}$
- 1615  $\text{cm}^{-1}$  amplitude, (ESA[1604  $\text{cm}^{-1}$  + 1608  $\text{cm}^{-1}$ ]) - (bleach[1612  $\text{cm}^{-1}$  + 1616  $\text{cm}^{-1}$ ])
- 1516  $\text{cm}^{-1}$  bleach, single pixel at 1516  $\text{cm}^{-1}$
- 1398  $\text{cm}^{-1}$  bleach, single pixel at 1398  $\text{cm}^{-1}$