Supporting Information

Fig S1. Transient Spectra at selected delays (ps) of isolated Ac, $\lambda_{\text{exc}} = 330$ nm.

Fig S2. Kinetic traces of isolated Ac, with $\lambda_{\text{exc}}=330$ nm (black scatter) and with $\lambda_{\text{exc}}=400$ nm (red scatter).

Fig S3: 3D plots of MO of interest of Ac.
**Figure S4.** Ground electronic state (on the left) and first excited state (on the right) of Ac.

**Figure S5.** PCM cavity for the AAC conformation: solvent-accessible-surface (SAS).

**Figure S6.** Relevant conformations of Ac
**Figure S7**: 3D plots of relevant MO of AAC.

**Figure S8**: 3D plots of the electron density difference between the ground S0 and the first S1 (left-side picture), the fifth S5 (central picture) and sixth S6 (right-side picture) electronic state for AAC conformer. The zones where the electron density grows are mapped in light blue.
Figure S9: Theoretical $Dn$ population decay due to the energy transfer, calculated assuming a weighted sum of exponential function (red line). The pre-exponential factors in the sum are the relative population of the conformers calculated by DFT approach. The dashed line is the mono-exponential fit, with a time constant of 3.51 ps.