Electronic Supplementary Information

Unravelling the early photochemical behavior of (8-substituted-7-hydroxyquinolinyl)methyl acetates through electronic structure theory and ultrafast transient absorption spectroscopy

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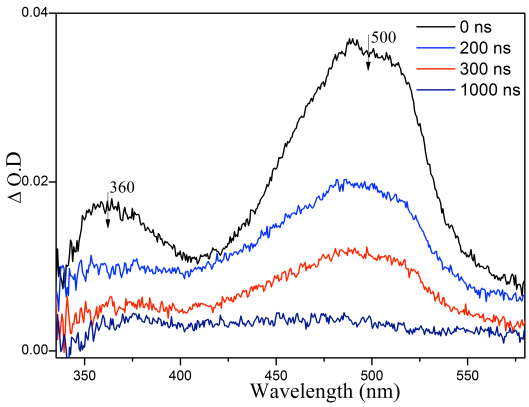

Figure S1. ns-TA spectra of BHQ-OAc obtained in acetonitrile.

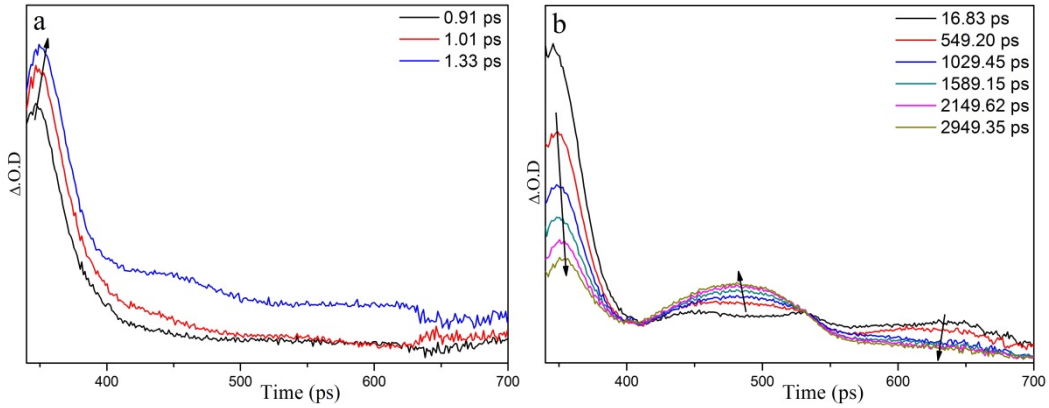

Figure S2. fs-TA spectra of CHQ-OAc obtained in acetonitrile at (a) early and (b) late times after irradiation at 267 nm.

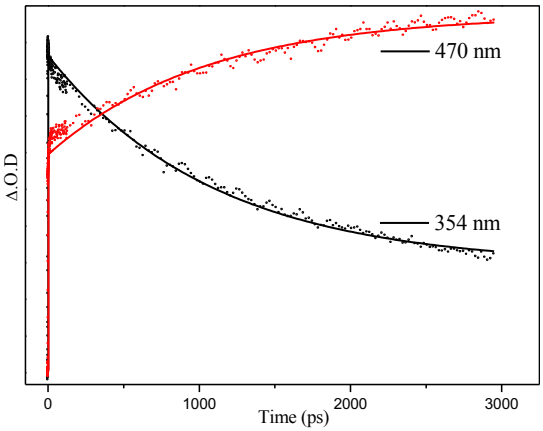

Figure S3. Time evolution fitted with one exponential at 354 and 470 nm of CHQ-OAc in acetonitrile. The dots are experimental data and the lines are fitted results. The growth time constant for the 354-nm band and the decay time constant for the 470-nm band were each 1055 ps.

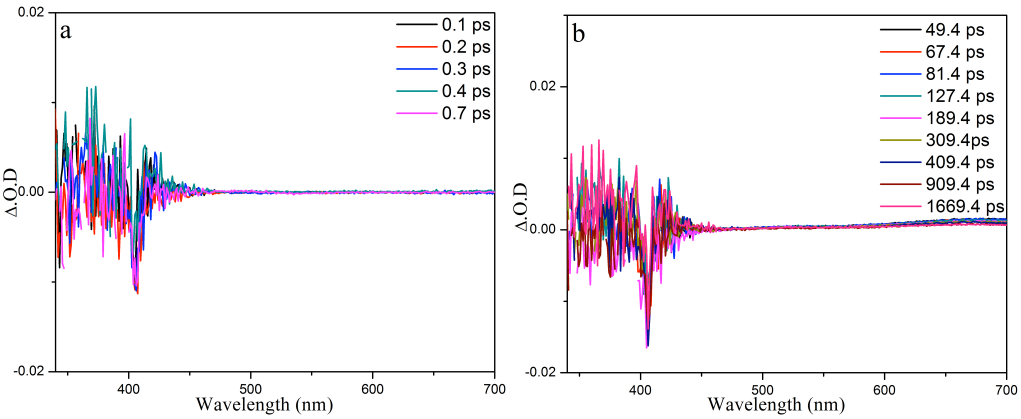

Figure S4 fs-TA spectra of 2:3 acetonitrile/water (pH 6-7).

Table S1 Absolute energies [eV] (with respect to the relaxed ground-state minimum) of the lowest singlet and triplet excited states as well as the ground state at the relaxed ground- (columns) and excited-state geometries (rows) for 8-bromo-7-hydroxyquinoline at the riCC2/SVP level of theory.

	S_0	$1\,^1A'$	$1\,^1A''$	$1\,^3A'$	$1\,^3A''$
S_0	0.00	4.19	4.48	3.29	4.10
$1\,^1A'$	0.22	**3.99**	4.46	3.08	4.13
$1\,^1A''$	0.68	4.60	**3.86**	3.53	3.58
$1\,^3A'$	0.39	—	—	**2.92**	4.14
$1\,^3A''$	0.61	—	—	—	**3.56**