Supplementary Information for

"Photogeneration of Quinone Methide from Adamantylphenol in an Ultrafast Non-adiabatic Dehydration Reaction"

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1. Deconvolution of rise time in transient absorption data

1.1 Results of transient absorption using THG of 120 fs at 800 nm as a pump pulse

Since the results of transient absorption measurements didn't show significant dynamics in first few picoseconds after excitation with 267 nm, 120 fs pulses we performed fitting of several kinetic profiles (at 425, 500 and 600 nm) focusing on first 10 ps. For the model function we used two exponential functions convoluted with identical Gaussian function to account for instrument response function (IRF) of our transient absorption spectrometer. Time constant of the first exponential function (t1) having negative amplitude then represented deconvoluted rise time of kinetic profile at that particular wavelength. In order to reduce number of free parameters, time constant for the exponential decay was fixed at 1 ns. Where needed, we expanded this model to account for coherent artifacts that could not be removed from the data without significantly affecting measured kinetic profiles. Hence, we included in the model function additional Gaussian in Figure S1 to account for two-photon absorption (TPA) signal around zero delay time, and two Gaussians were added to account for cross phase modulation signal (XPM) superimposed on exponential rise (Figures S7 to S10). It is known that, it the case of broadband chirped probe pulse, XPM signal splits in two, where the transient optical density will exhibit a gain (ΔOD<0) followed by a loss (ΔOD>0), i.e., a dispersion shape for the first XPM signal, while at increased delay times second XPM-induced pump-probe signal is present, which is out of phase with the first one.[1] In addition, loss and gain amplitudes in this case are not identical, and only the overall signal averages to zero. This prompted us to use two Gaussian functions with the position of the center of the peak and peak amplitude being free parameters for modelling XPM artifacts.

General model:

$$f(t) = A_1 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}\left[1+erf\left(\frac{t-p-\frac{1}{t_1}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_2 e^{-\frac{\left(t-p-\frac{\sigma^2}{2\cdot 10^6}\right)}{10^6}}\left[1+erf\left(\frac{t-p-\frac{1}{10^6}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_3 e^{-\frac{t^2}{2\sigma^2}}$$

Coefficients (with 95% confidence bounds):

A1 = -0.0003891 (-0.004005, 0.003227) A2 = 0.0003032 (0.0003006, 0.0003058)
A3 = 0.0006108 (0.0004117, 0.0008099)
p = 175.3 (-2646, 2997) sigma = 365.9 (334.5, 397.4)
t1 = 227.9 (-84.93, 540.6)

Goodness of fit:
SSE: 6.133e-08 R-square: 0.9942 Adjusted R-square: 0.994 RMSE: 2.071e-05

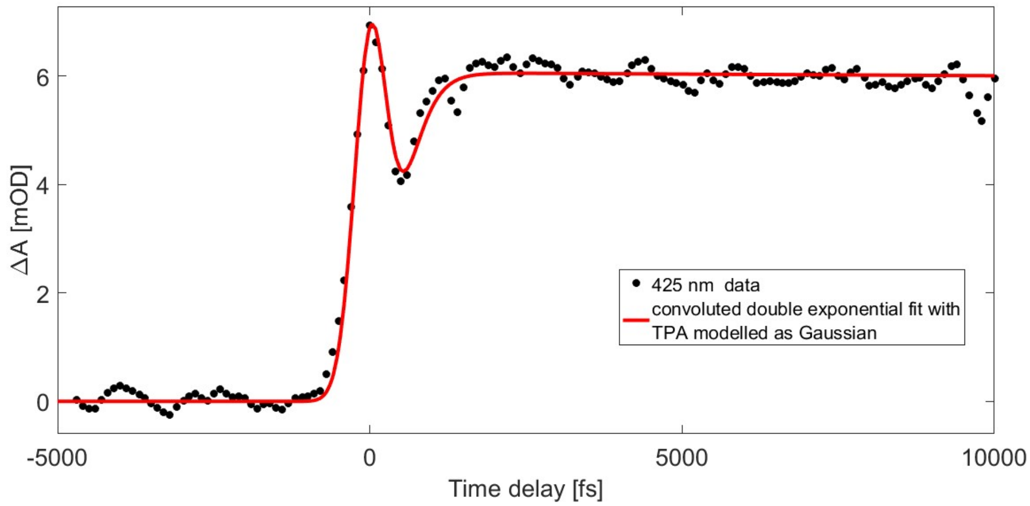


Figure S1

General model:

$$f(t) = A_1 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}\left[1+erf\left(\frac{t-p-\frac{1}{t_1}\sigma^2}{\sqrt{2\sigma}}\right)\right] + A_2 e^{-\frac{\left(t-p-\frac{\sigma^2}{2\cdot 10^6}\right)}{10^6}}\left[1+erf\left(\frac{t-p-\frac{1}{10^6}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_3 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}$$

Coefficients (with 95% confidence bounds):

A1 = -0.0003054 (-0.01061, 0.01) A2 = 0.000407 (0.0004037, 0.0004102)

p = -7.86 (-5054, 5038) sigma = 555.8 (159.8, 951.9)

t1 = 211.4 (-358, 780.7)

Goodness of fit:

SSE: 8.264e-08 R-square: 0.9958 Adjusted R-square: 0.9957 RMSE: 2.396e-05

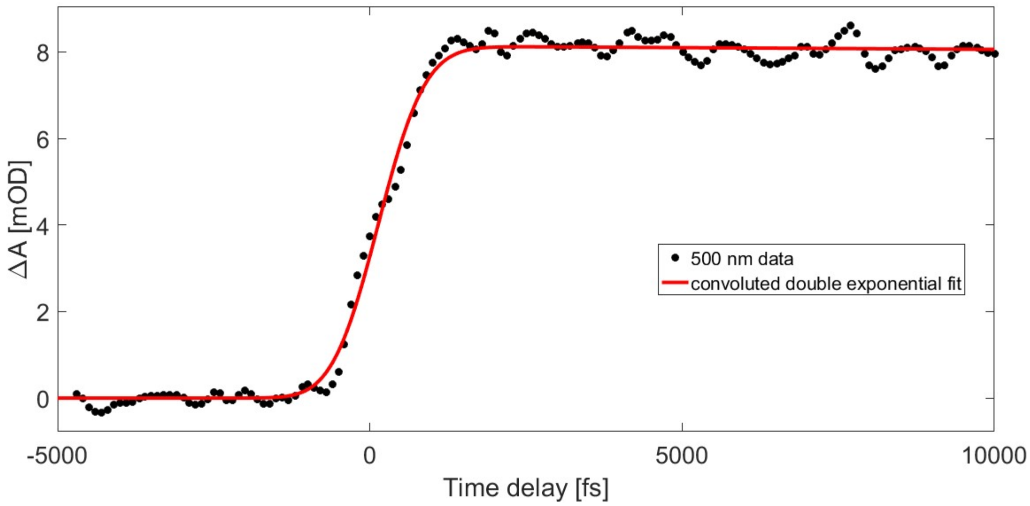


Figure S2

General model:

$$f(t) = A_1 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}\left[1+erf\left(\frac{t-p-\frac{1}{t_1}\sigma^2}{\sqrt{2\sigma}}\right)\right] + A_2 e^{-\frac{\left(t-p-\frac{\sigma^2}{2\cdot 10^6}\right)}{10^6}}\left[1+erf\left(\frac{t-p-\frac{1}{10^6}\sigma^2}{\sqrt{2\sigma}}\right)\right] + A_3 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}$$

Coefficients (with 95% confidence bounds):

A1 = -0.0004303 (-0.01574, 0.01488) A2 = 0.000353 (0.000349, 0.000357)

p = -86.56 (-1.016e+04, 9986) sigma = 553.4 (-699.3, 1806)

t1 = 248 (-409.5, 905.5)

Goodness of fit:

SSE: 6.651e-08 R-square: 0.9954 Adjusted R-square: 0.9953 RMSE: 2.18e-05

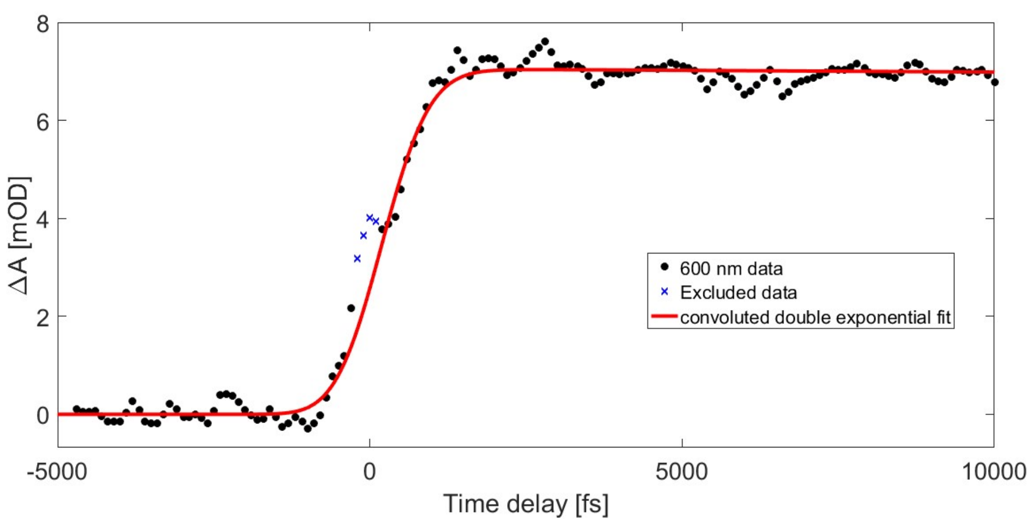


Figure S3

To evaluate slow decay of signal at longer wavelengths that we believe originates from solvated electrons we performed simple bi-exponential fitting for the entire range of time delay points (up to 1.1 ns) for kinetic profiles corresponding to 500, 550 and 600 nm.

General model:

$$f(t) = A_1 e^{b \cdot t} + A_2 e^{c \cdot t}$$

Coefficients (with 95% confidence bounds):

A1 = 0.001542 (0.00149, 0.001593)

b = -2.866e-05 (-3.18e-05, -2.553e-05) – 35 ps

A2 = 0.002615 (0.002577, 0.002654)

c = -6.328e-07 (-6.584e-07, -6.071e-07) – 1.5 ns

Goodness of fit:

SSE: 1.287e-05 R-square: 0.975 Adjusted R-square: 0.9749 RMSE: 0.000139

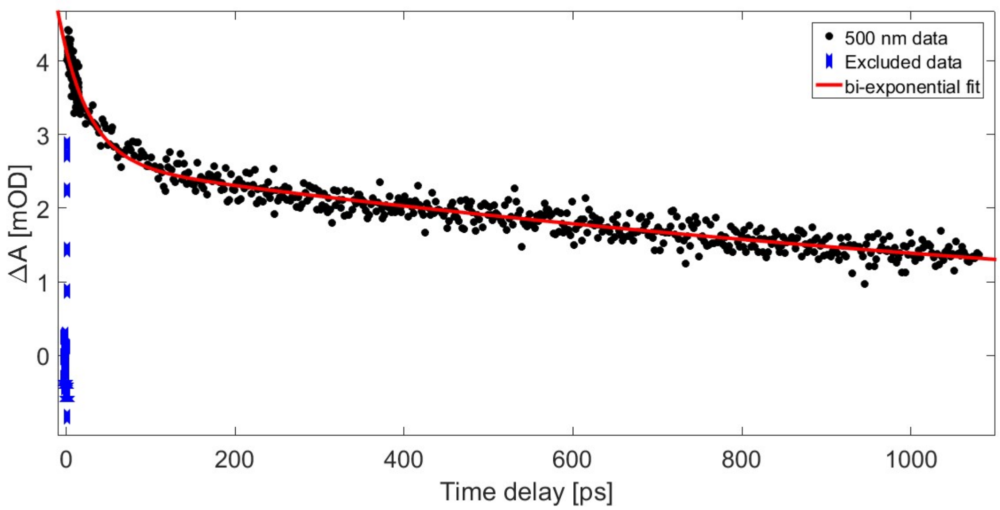


Figure S4

General model:

$$f(t) = A_1 e^{b \cdot t} + A_2 e^{c \cdot t}$$

Coefficients (with 95% confidence bounds):

A1 = 0.001125 (0.001071, 0.00118)

b = -2.801e-05 (-3.247e-05, -2.355e-05) – 35 ps

A2 = 0.002108 (0.002067, 0.002149)

c = -5.481e-07 (-5.809e-07, -5.153e-07) – 1.8 ns

Goodness of fit:

SSE: 1.511e-05 R-square: 0.9471 Adjusted R-square: 0.9469 RMSE: 0.0001504

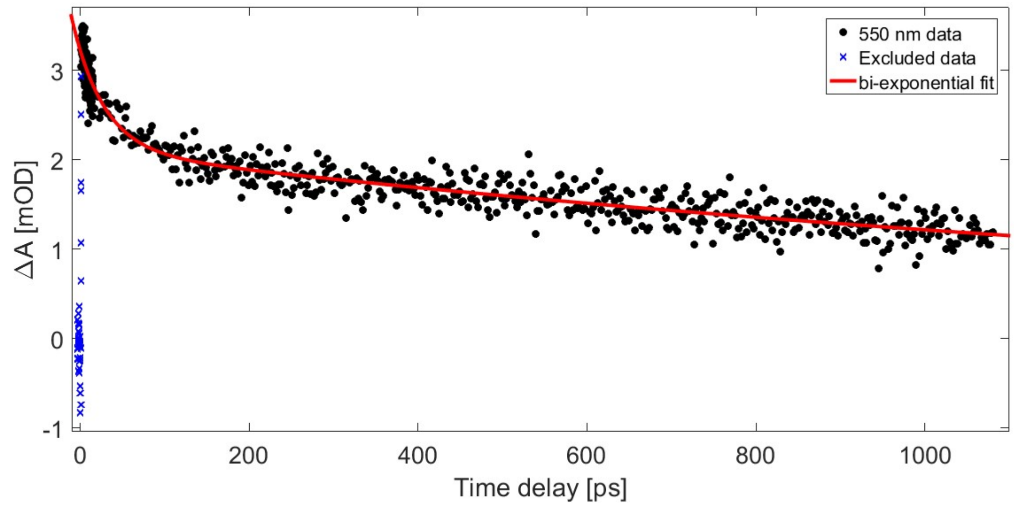


Figure S5

General model:
$f(t) = A_1 e^{b \cdot t} + A_2 e^{c \cdot t}$

Coefficients (with 95% confidence bounds):
A1 = 0.001514 (0.001479, 0.001549)
b = -3.506e-05 (-3.748e-05, -3.264e-05) – 28.5 ps
A2 = 0.002624 (0.002599, 0.002648)
c = -6.594e-07 (-6.764e-07, -6.425e-07) – 1.5 ns

Goodness of fit:
SSE: 6.179e-06 R-square: 0.9884 Adjusted R-square: 0.9883 RMSE: 9.505e-05

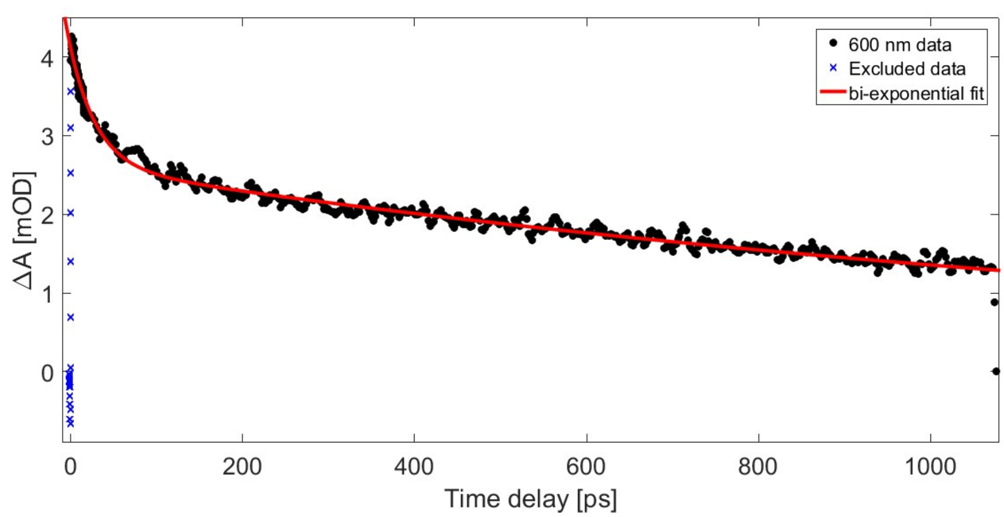


Figure S6

1.2 Results of transient absorption using sub-20-fs UV NOPA pump pulse

The same fitting procedure was used for extracting deconvoluted rise time of second set of measurements with better IRF due to the sub-20-fs UV pump pulse driving the photochemical reaction.

General model:

$$f(t) = A_1 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}\left[1+erf\left(\frac{t-p-\frac{1}{t_1}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_2 e^{-\frac{\left(t-p-\frac{\sigma^2}{2\cdot 10^6}\right)}{10^6}}\left[1+erf\left(\frac{t-p-\frac{1}{10^6}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_3 e^{-\frac{(t-r)^2}{2\sigma^2}} + A_4 e^{-\frac{(t-n)^2}{2\sigma^2}}$$

Coefficients (with 95% confidence bounds):

A1 = -0.001039 (-3.707, 3.705)
A2 = 0.001039 (0.0007483, 0.001329)
A3 = 0.001602 (0.0007051, 0.002499)
A4 = -0.0007747 (-0.0009405, -0.000609)
n = -47.11 (-50.94, -43.28)
p = -7.918 (-2.797e+05, 2.797e+05)
r = -4.96 (-7.359, -2.562)
σ= 21.59 (17.11, 26.07)
t1 = 78.4 (70.48, 86.33)

Goodness of fit:

SSE: 7.801e-07 R-square: 0.9954 Adjusted R-square: 0.9953 RMSE: 5.689e-05

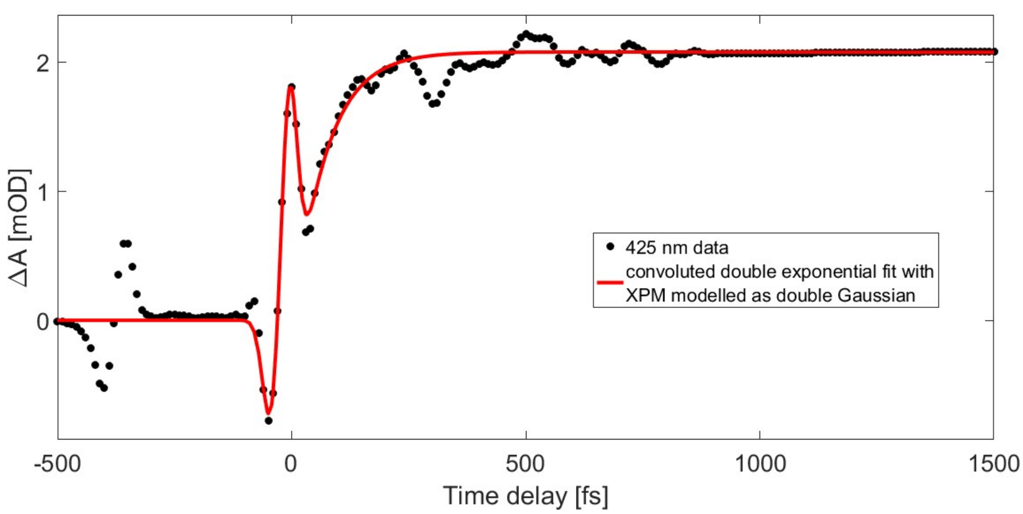


Figure S7

General model:

$$f(t) = A_1 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}\left[1+erf\left(\frac{t-p-\frac{1}{t_1}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_2 e^{-\frac{\left(t-p-\frac{\sigma^2}{2\cdot 10^6}\right)}{10^6}}\left[1+erf\left(\frac{t-p-\frac{1}{10^6}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_3 e^{-\frac{(t-r)^2}{2\sigma^2}} + A_4 e^{-\frac{(t-n)^2}{2\sigma^2}}$$

Coefficients (with 95% confidence bounds):

A1 = -0.0009393 (-0.05372, 0.05184) A2 = 0.000975 (0.0009683, 0.0009818)

A3 = -0.01123 (-316.9, 316.9) A4 = 0.01201 (-316.9, 316.9)

n = -13.97 (-2.436e+04, 2.433e+04) p = 19.84 (-4415, 4455)

r = -15.79 (-2.547e+04, 2.544e+04) σ = 26.4 (-544.6, 597.4)

t1 = 82.4 (68.44, 96.35)

Goodness of fit:

SSE: 1.273e-06 R-square: 0.9914 Adjusted R-square: 0.9911 RMSE: 7.267e-05

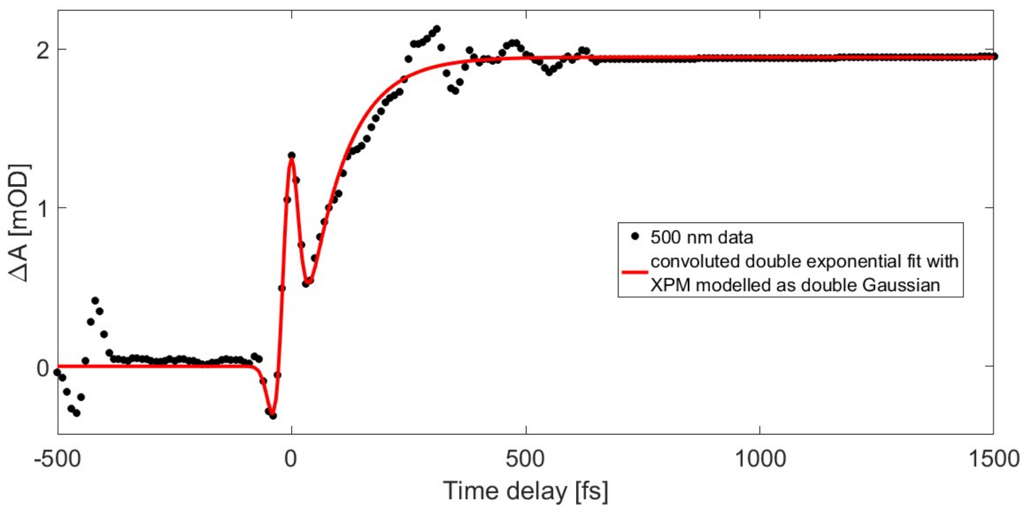


Figure S8

General model:

$$f(t) = A_1 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}\left[1+erf\left(\frac{t-p-\frac{1}{t_1}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_2 e^{-\frac{\left(t-p-\frac{\sigma^2}{2\cdot 10^6}\right)}{10^6}}\left[1+erf\left(\frac{t-p-\frac{1}{10^6}\sigma^2}{\sqrt{2}\sigma}\right)\right] + A_3 e^{-\frac{(t-r)^2}{2\sigma^2}} + A_4 e^{-\frac{(t-n)^2}{2\sigma^2}}$$

Coefficients (with 95% confidence bounds):

A1 = -0.0003732 (-0.0004635, -0.000283) A2 = 0.0008317 (0.000826, 0.0008375)

A3 = -0.000227 (-0.0003128, -0.0001413) A4 = 0.0007324 (0.0006103, 0.0008544)

n = 4.683 (1.515, 7.851) p = 39.37 (31.42, 47.33)

r = -45.3 (-54.89, -35.72) σ = 21.36 (17.14, 25.59)

t1 = 125.4 (98.21, 152.6)

Goodness of fit:

SSE: 1.23e-06 R-square: 0.9705 Adjusted R-square: 0.9693 RMSE: 7.727e-05

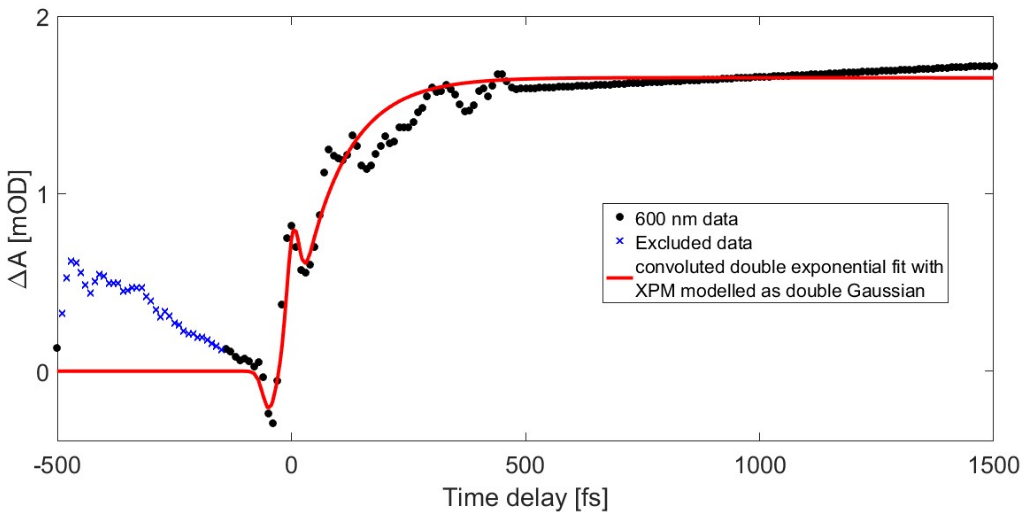


Figure S9

Finally, in order to reduce the noise in kinetic profiles we integrated the signal in 400-500 nm wavelength range. By doing so we also obtained better contrast for coherent artifacts. The XPM superimposed on the initial rise of the time trace was accounted for by two Gaussian functions of opposite sign. It is reasonable to assume that TPA, being stronger at shorter wavelengths, also contributes to this artifact additionally changing the shape and ratio between positive and negative amplitudes of XPM. For negative delay times we also observe a weaker replica of the XPM artifact visible at time zero, shifted in time due to dispersion of the first cuvette window.

General model:

$$f(t) = A_1 e^{-\frac{\left(t-p-\frac{\sigma^2}{2t_1}\right)}{t_1}}\left[1+erf\left(\frac{t-p-\frac{1}{t_1}\sigma^2}{\sqrt{2\sigma}}\right)\right] + A_2 e^{-\frac{\left(t-p-\frac{\sigma^2}{2\cdot 10^6}\right)}{10^6}}\left[1+erf\left(\frac{t-p-\frac{1}{10^6}\sigma^2}{\sqrt{2\sigma}}\right)\right] + A_3 e^{-\frac{(t-r)^2}{2\sigma^2}} + A_4 e^{-\frac{(t-n)^2}{2\sigma^2}}$$

Coefficients (with 95% confidence bounds):

A1 = -118.2 (-140.1, -96.41)	A2 = 199.8 (199.1, 200.6)
A3 = -108.7 (-133, -84.33)	A4 = 314.7 (298.4, 331)
n = -2.628 (-4.677, -0.5791)	p = 28.17 (18.37, 37.98)
r = -43.34 (-49.82, -36.86)	σ = 23.98 (20.97, 26.98)
t1 = 110 (98.23, 121.8)	

Goodness of fit:

SSE: 2.085e+04 R-square: 0.9966 Adjusted R-square: 0.9965 RMSE: 9.302

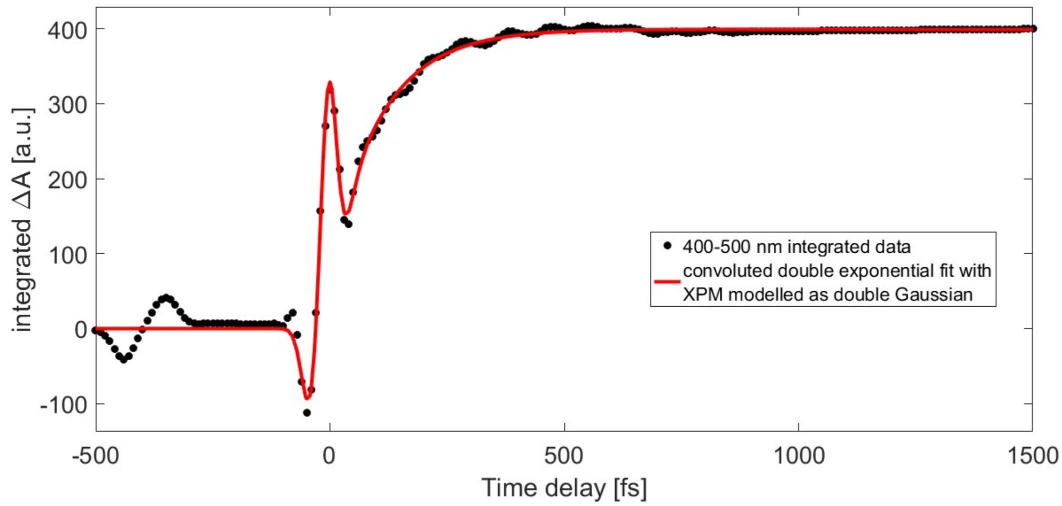


Figure S10

2. Intensity dependence of transient absorption spectra

In order to clarify the origin of the signal at longer wavelengths that we attributed to solvated electrons we measured excitation intensity dependence on the transient absorption spectra for both the sample and pure solvent at fixed delay of 10 ps that show quadratic dependence in the case of pure solvent as expected for two-photon ionization. Intensity dependence for sample is almost linear suggesting that it stems from free electrons resulting from radical cation formation which is one photon process as is shown in Figure 8. with only minor contribution of two-photon ionization of solvent molecules.

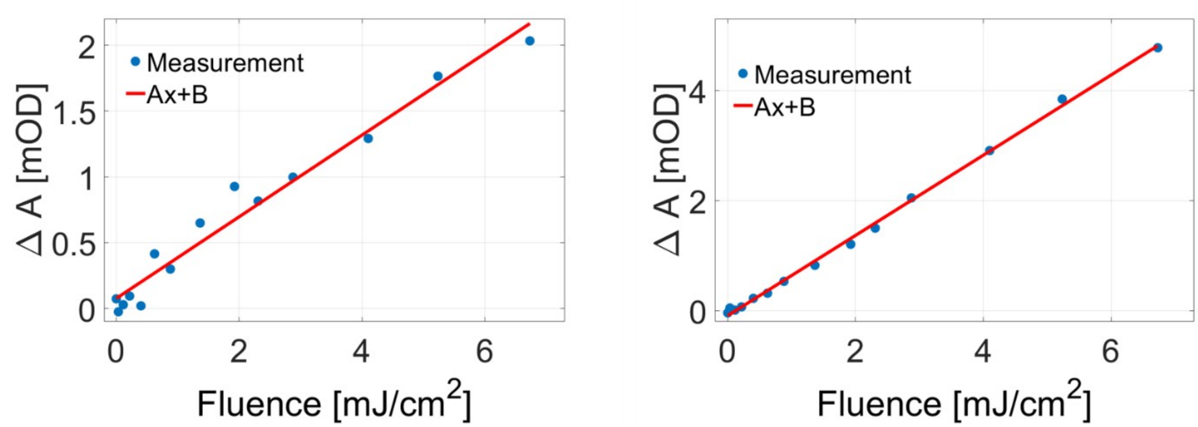


Figure S11 Excitation intensity dependence on the transient absorption spectra of adamantylphenol at fixed delay of 10 ps at 425 nm (left) and 600 nm (right) that show linear dependence.

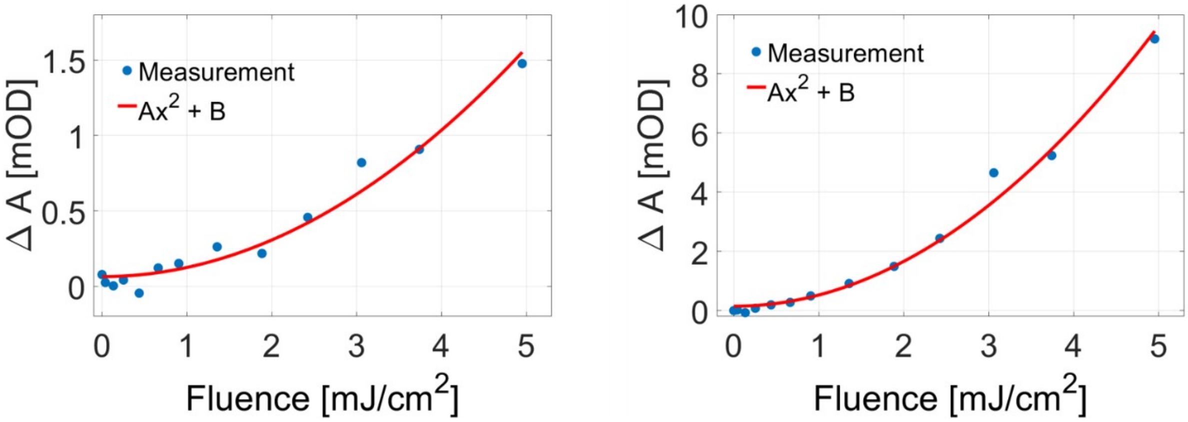


Figure S12 Excitation intensity dependence on the transient absorption spectra in pure solvent at fixed delay of 10 ps at 425 nm (left) and 600 nm (right) that show quadratic dependence as expected for two-photon ionization.

3. Absorption spectra and transient absorption spectra

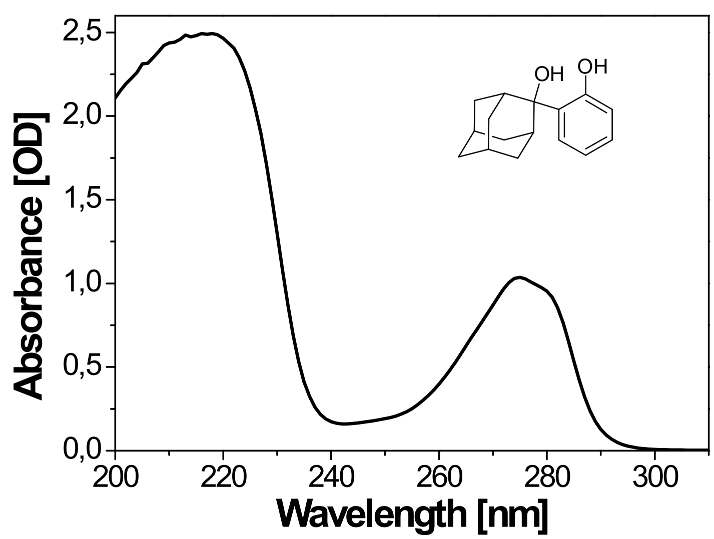


Figure S13 Absorption spectrum of **3** in CH_3CN-H_2O (1:1) (for the path of 1 mm), at concentration c = 5.0 × 10^{-3} M that was used for fs-TA experiment with 280 nm sub-20-fs pump pulses from SHG of NOPA.

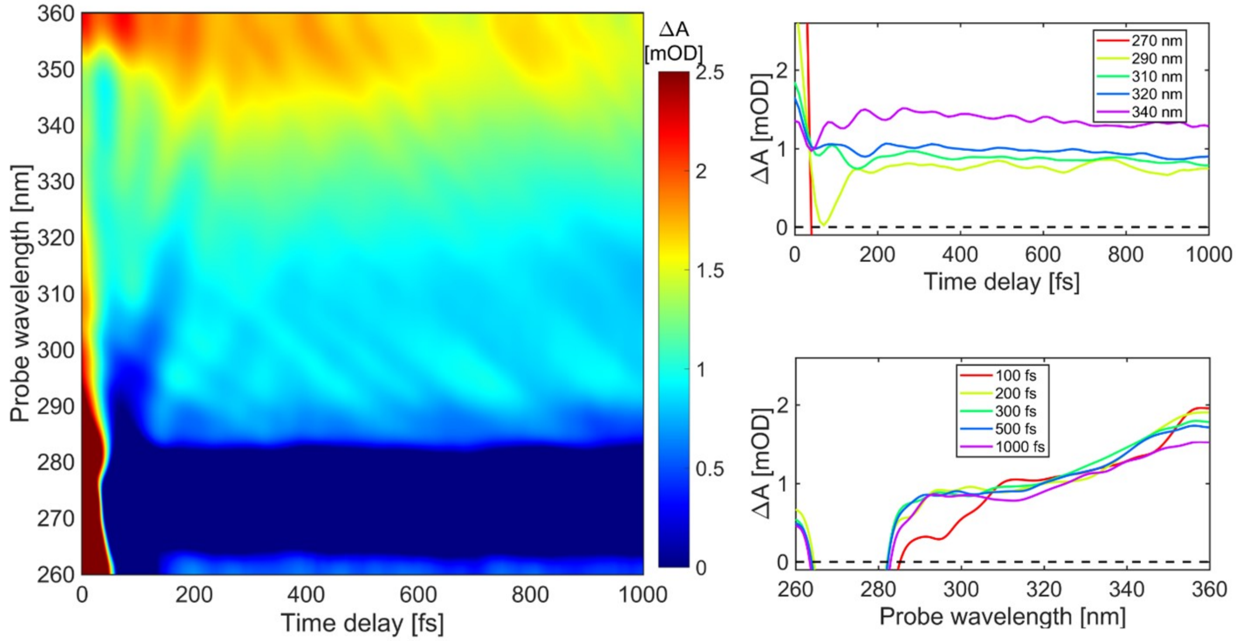


Figure S14 fs-TA data using sub-20-fs UV NOPA pump pulse and WLC driven by the SH of Ti:sapphire together with spectral and kinetic profiles for the selected wavelengths. Only strong ground state bleach is observed below 285nm.

4. Laser flash photolysis measurements

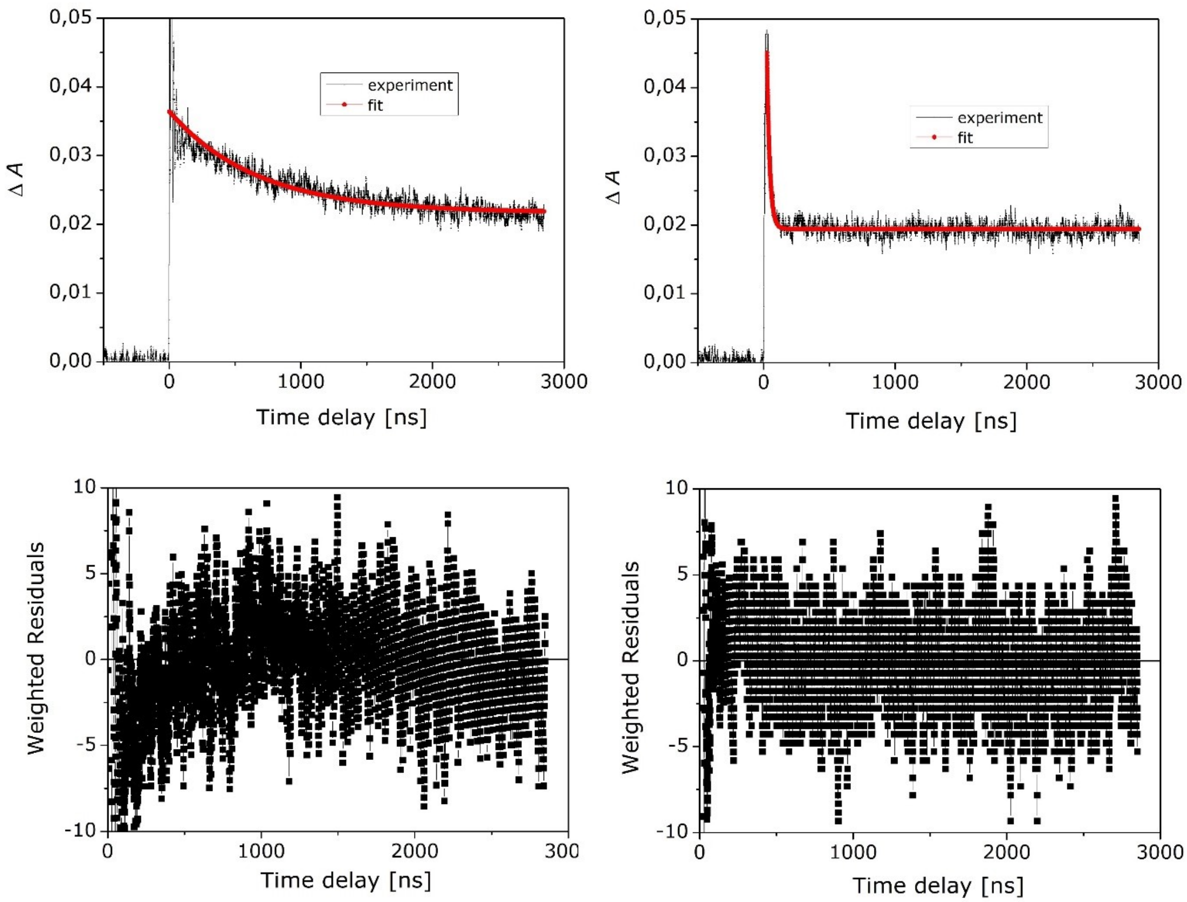


Figure S15 Nanosecond decay of transient absorption at 400 nm for Ar-purged (left) and O_2-purged (right) CH_3CN-H_2O (1:1 v/v) solution of **3** (2.0×10^{-4} M). The energy of the laser pulse at 266 nm was set to 17 mJ/pulse. The bottom panels correspond to the weighted residuals between the measured value and the calculated according to the single exponential decay model.

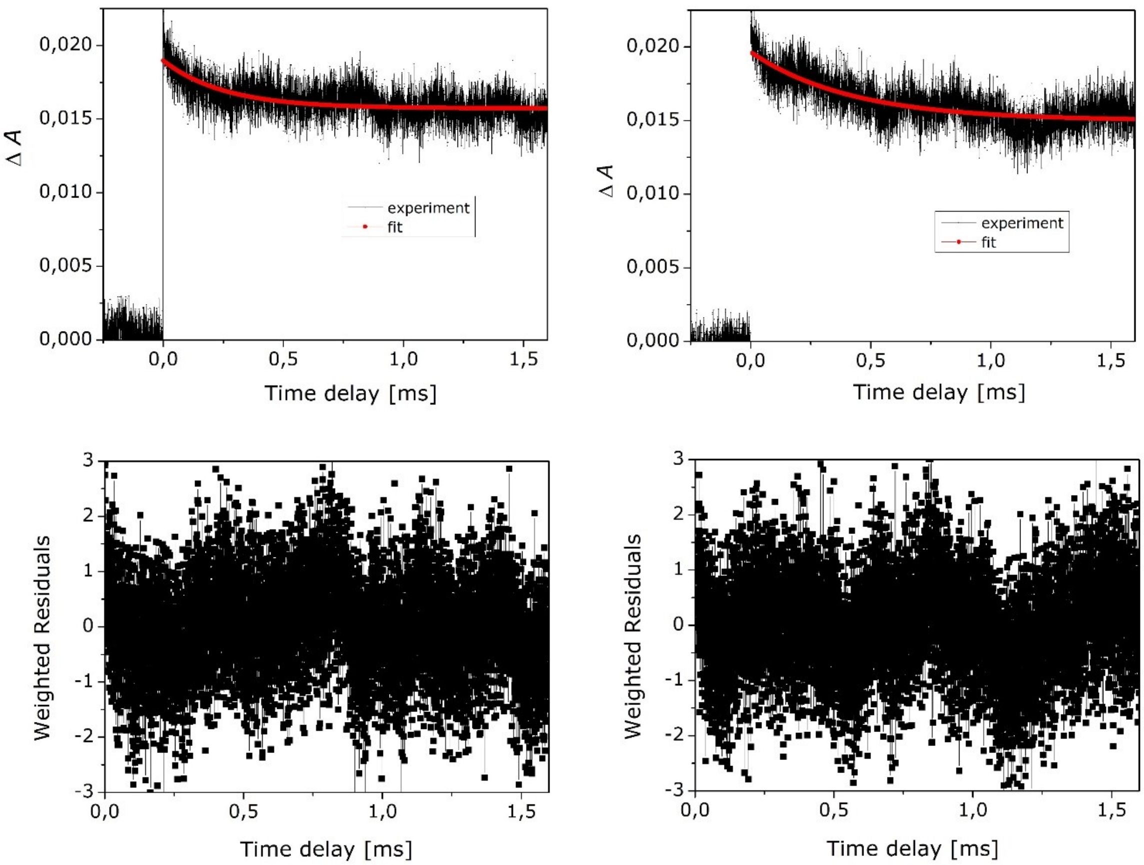


Figure S16 Milisecond decay of transient absorption at 400 nm for Ar-purged (left) and O_2-purged (right) CH_3CN-H_2O (1:1 v/v) solution of **3** (2.0×10^{-4} M). The energy of the laser pulse at 266 nm was set to 17 mJ/pulse. The bottom panels correspond to the weighted residuals between the measured value and the calculated according to the single exponential decay model.

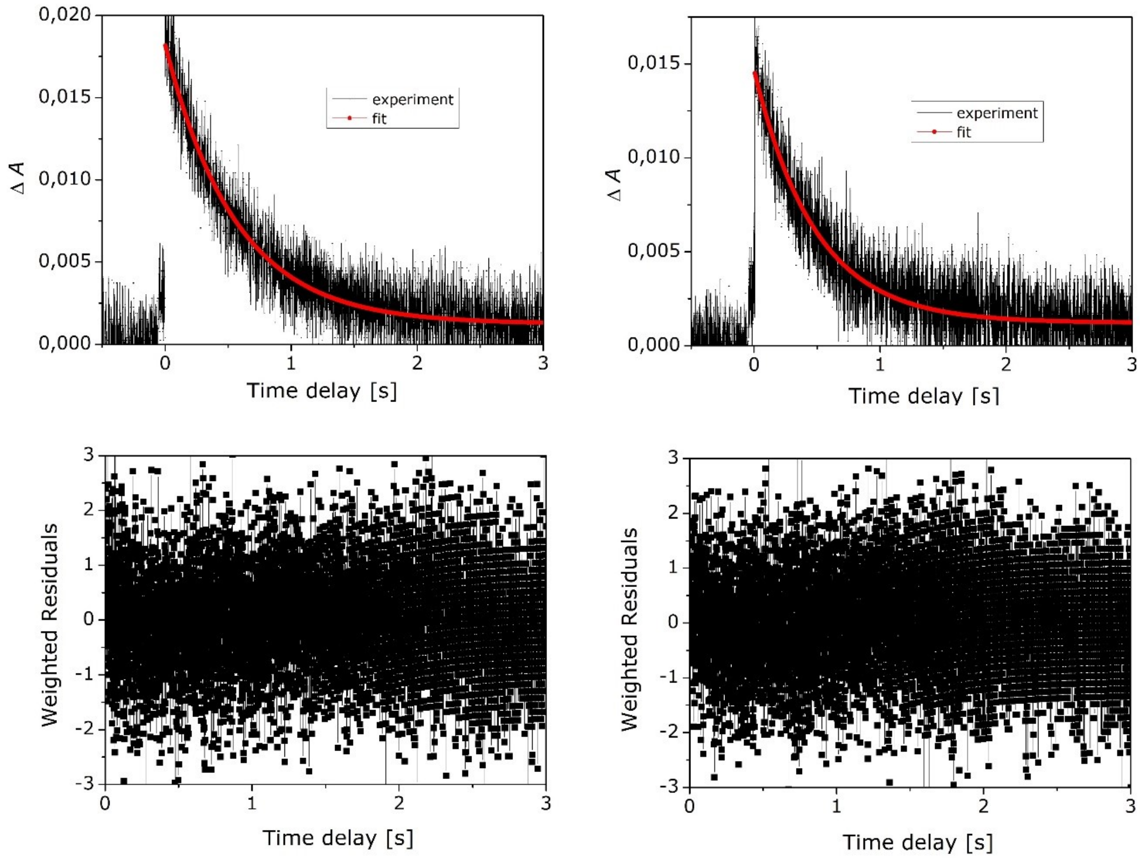


Figure S17 Decay of transient absorption at 420 nm for Ar-purged (left) and O_2-purged CH_3CN-H_2O (1:1 v/v) solution of **3** (2.0 × 10^{-4} M). The energy of the laser pulse at 266 nm was set to 17 mJ/pulse. The bottom panels correspond to the weighted residuals between the measured value and the calculated according to the single exponential decay model.

5. Fluorescence upconversion measurements

5.1 Instrument response function

Instrument response function measurement was taken with identical experimental conditions prior to FlUC measurments of adamantylphenol.

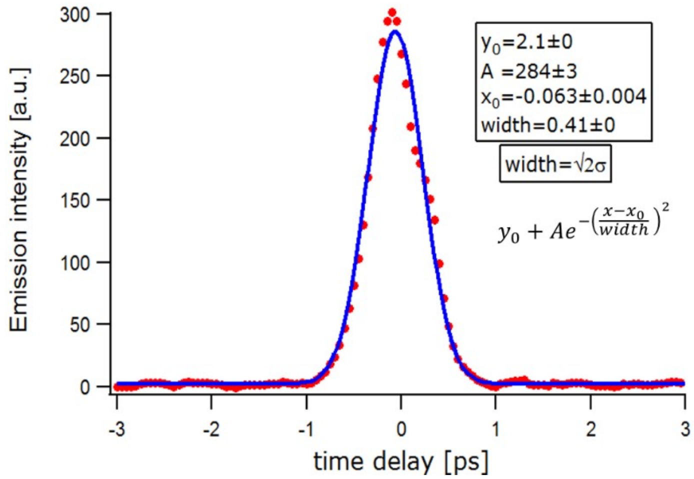


Figure S18. IRF of FlUC measurements with 272 nm excitation wavelength. IRF is equal to $2\sqrt{2ln2}\sigma$=680 fs.

5.2 Global analysis of FlUC data

The spectro-temporal signal can be describe by three components: the first describes a rise of the signal in 0.46 ps, the second describe a decay of ca, 1/3 of the total signal. The last component is set to 2 ns (infinity in our spanned time window). The presence of the first component is necessary because the rise of the signal is much slower than the measured IRF (630 fs). If we carry out the global fit procedure with free IRF we can remove the 0.5 ps component but the IRF would be 1.2 ps (and the time zero would be accordingly shifted). It is noteworthy that the first component equalizes the sum of the other two components. This speaks for a signal, which is delayed by 0.5 ps and is not directly populated upon excitation.

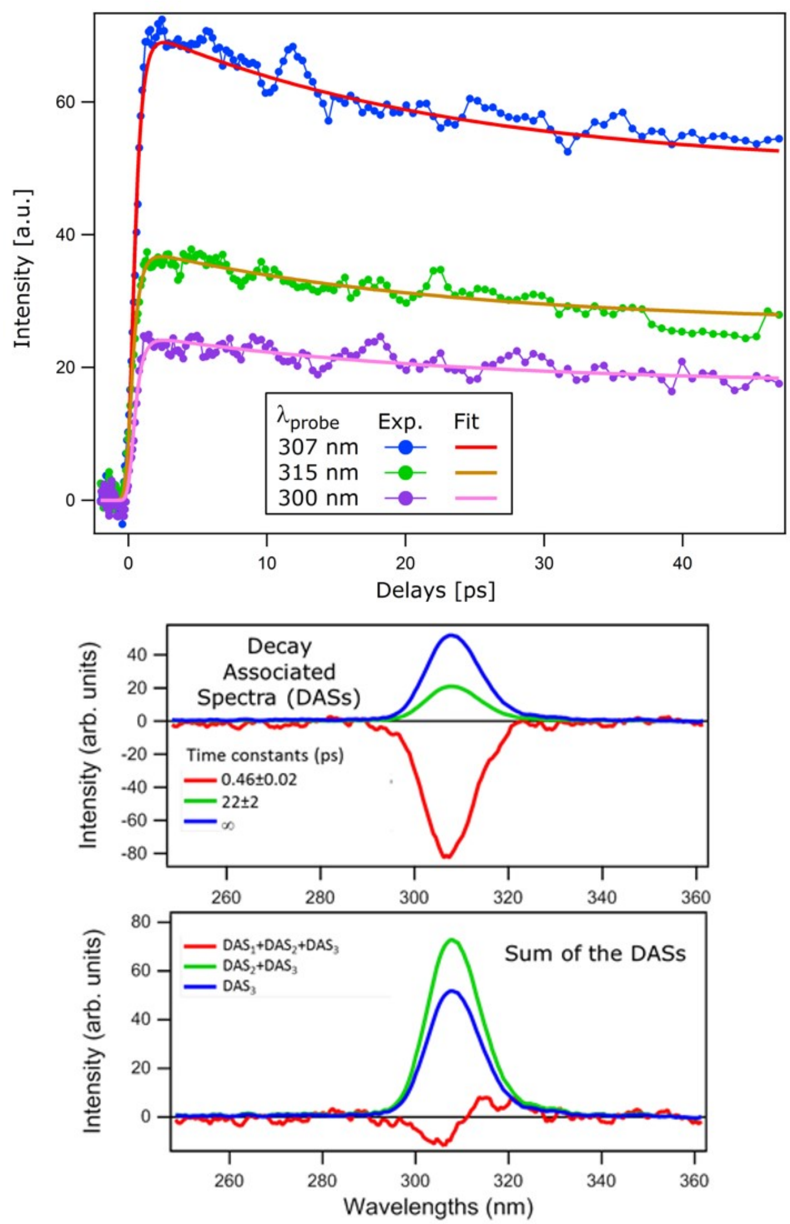


Figure S19. Results of global analysis using fixed value of 0.68 ps for the IRF.

Since FlUC measurements could not be performed at magic angle, it is possible to ascribe 22 ps decay to rotational anisotropy decay. Actually, 22 ps is too short for such processes (typically 100-200 ps in conventional solvents) but due to the limited scan range of 50 ps we cannot distinguish between 20 ps and 100 ps. In global analysis, the effect to change the time constant would be only to change the relative amplitude of the second and third DAS component (see Figure S19). To check this explanation, we carried out an analysis where we changed the second component in order to obtain a ratio 2:1 between the second and the third component. Indeed, a pure rotational anisotropy would induce a reduction by 2/3 of the initial signal with respect to the fully randomized one. The outcome of this analysis is shown in Figure S20. Under the 2:1 condition, the second time constant changed to 90 ps, which is compatible with a rotational diffusion process

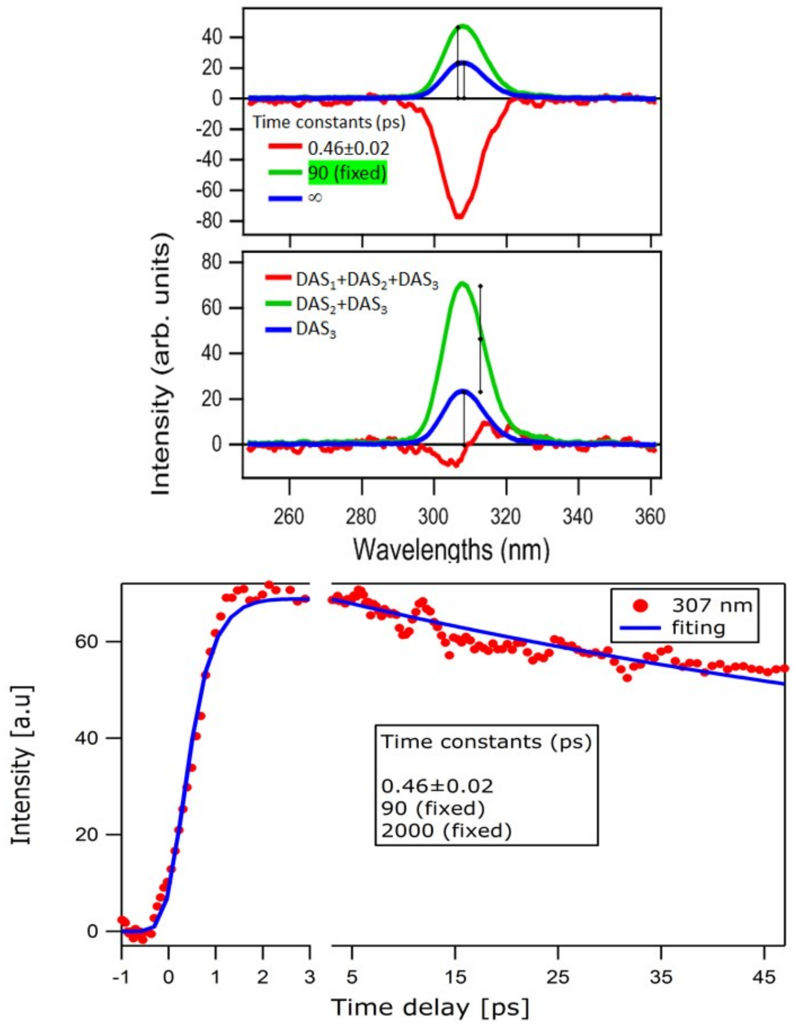


Figure S20. Results of global analysis with imposed rotational anisotropy decay.

5.3 FlUC of anisole molecule

In order to verify both IRF and the presence of the 0.5 ps rise in the adamantylphenol signal we performed additional FlUC measurements using anisole as a reference system. Only the two long components were necessary for the fitting of data. Any attempts to add a rise component or to impose 1 ps IRF were rejected by the fitting. When the IRF parameter was set free the fitting procedure gives 0.79±0.08 ps.

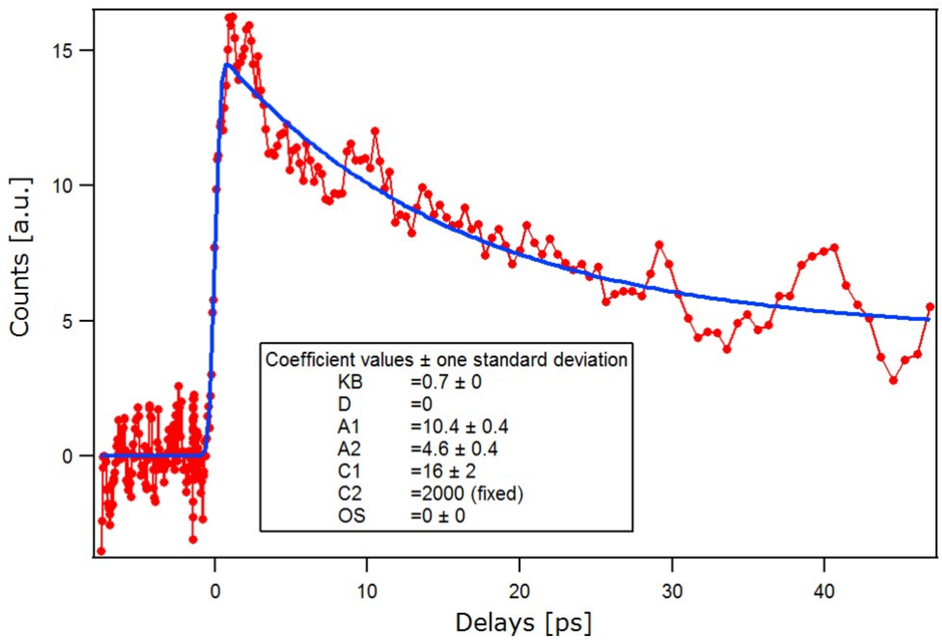


Figure S21. Fluorescence intensity kinetics of anisole in acetonitrile used as a reference molecule. IRF is represented by KB parameter.

6. Time-correlated single photon counting (TC-SPC) measurements

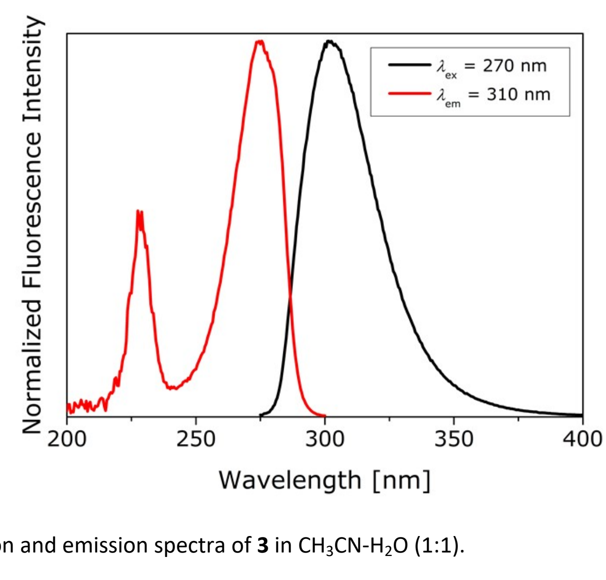


Figure S22. Normalized excitation and emission spectra of **3** in CH_3CN-H_2O (1:1).

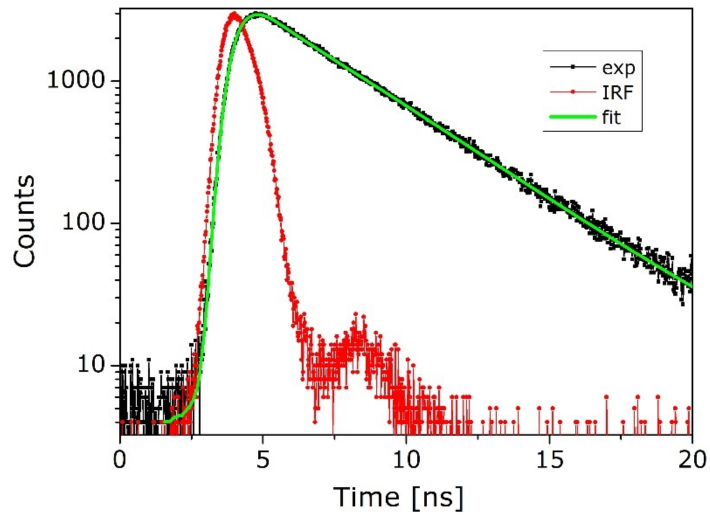


Figure S23. Decay of fluorescence of **3** in CH_3CN-H_2O (1:1) at 310 nm (λ_{exc} = 280 nm).

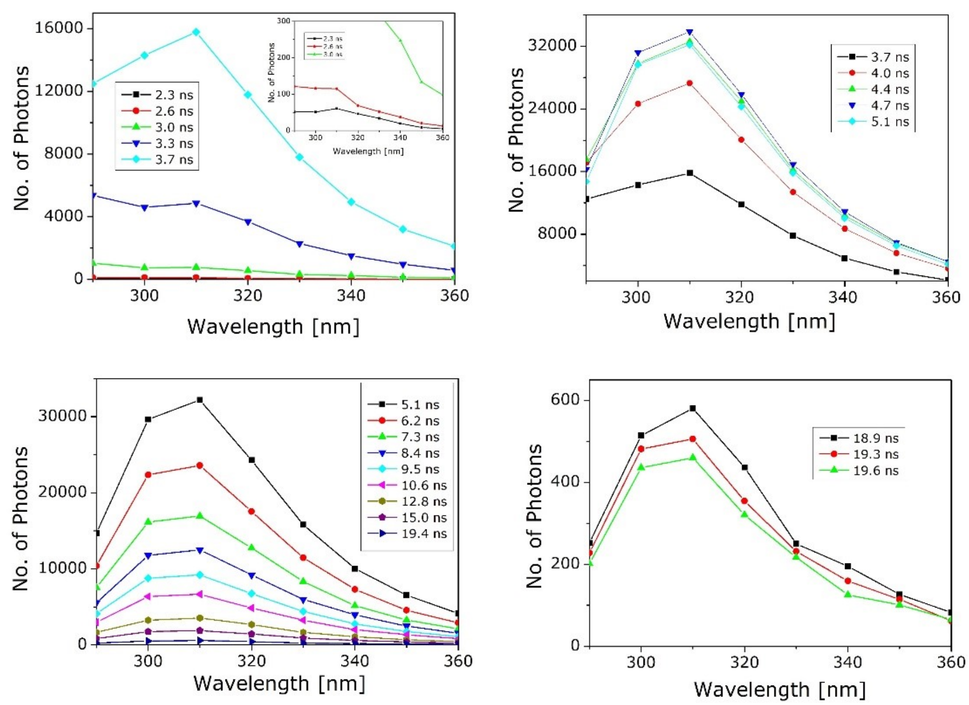
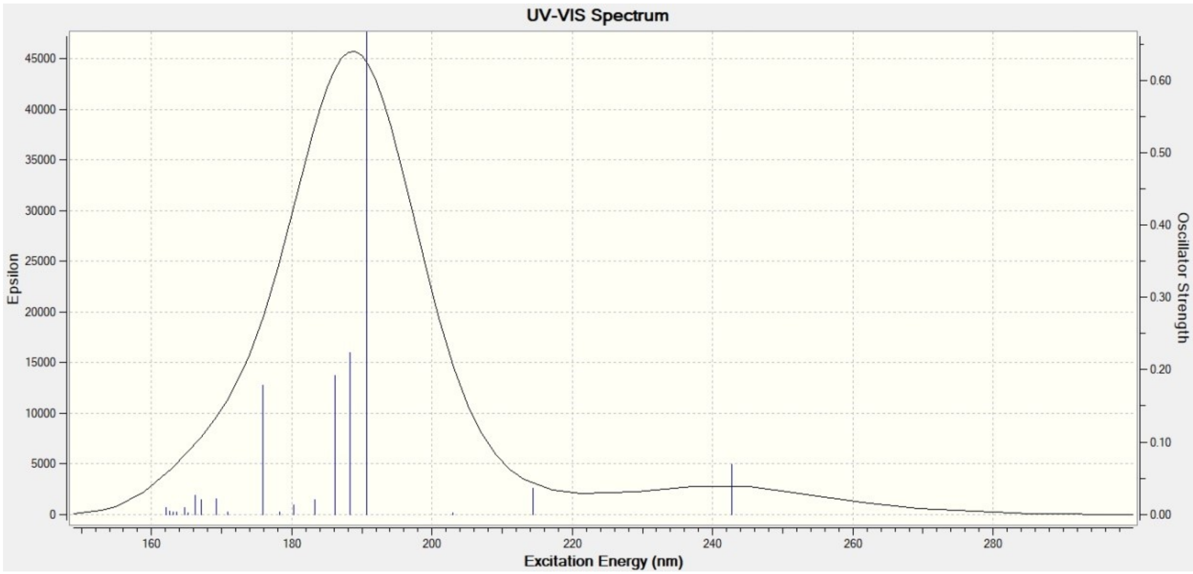
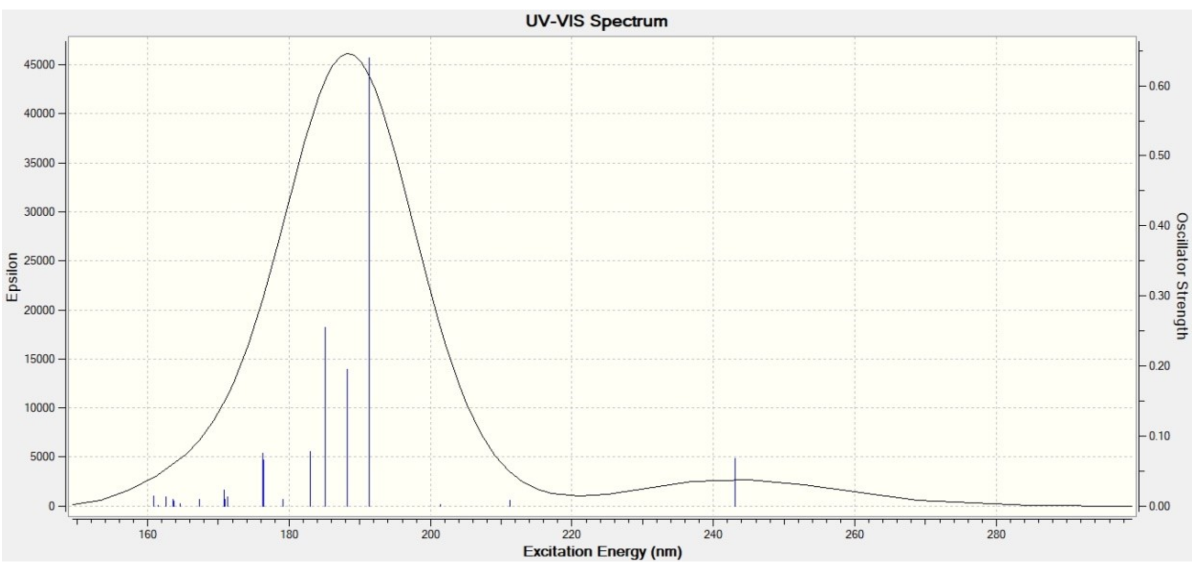


Figure S24. Time-resolved emission spectra (λ_{ex} = 280 nm) of **3** in CH_3CN-H_2O (1:1).

7. Computations



a)



b)

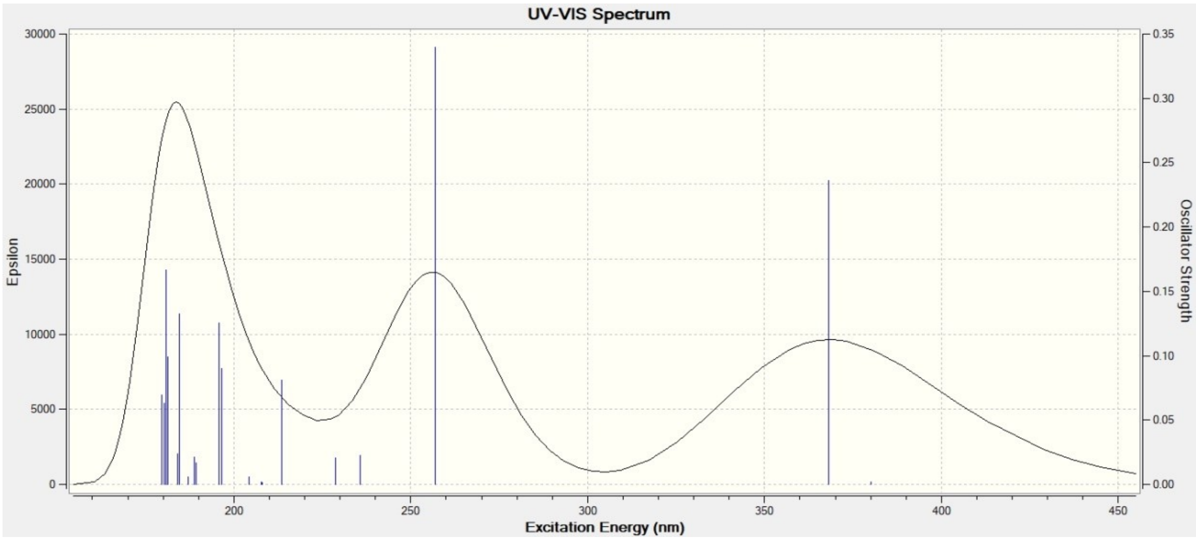
c)


Figure S25. Simulated spectra of **3**(S_0) (a), **3'**(S_0) (b) and **4**(S_0) (c) computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

Table S1. Vertical excitation of singlet **3**(S_0), **3'**(S_0) and **4**(S_0) computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

3(S_0)						
Excited State	1:	Singlet-A	5.1087 eV	242.69 nm	f=0.0686	<S**2>=0.000
65 -> 72	0.18262					
65 -> 73	-0.15138					
66 -> 67	0.16718					
66 -> 68	0.51394					
66 -> 69	-0.20974					
66 -> 70	0.10196					
66 -> 71	-0.18071					
66 -> 72	0.12491					
Excited State	2:	Singlet-A	5.7839 eV	214.36 nm	f=0.0363	<S**2>=0.000
65 -> 68	-0.283477					
65 -> 69	0.11648					
65 -> 71	0.10547					
66 -> 67	-0.12447					
66 -> 68	-0.11290					
66 -> 70	0.22629					
66 -> 72	0.40683					
66 -> 73	-0.28317					
66 -> 74	-0.10558					
66 -> 75	-0.12508					
Excited State	3:	Singlet-A	6.1077 eV	203.00 nm	f=0.0025	<S**2>=0.000
66 -> 67	0.44139					
66 -> 68	-0.21640					
66 -> 69	-0.32170					
66 -> 71	0.15996					
66 -> 73	-0.15506					

```
     66 -> 79         0.10660
     66 -> 80        -0.15515
     66 -> 87         0.12105
 Excited State   4:      Singlet-A      6.5006 eV  190.73 nm  f=0.6735  <S**2>=0.000
     65 -> 67         0.20094
     65 -> 68         0.38317
     65 -> 69        -0.18439
     65 -> 71        -0.14889
     65 -> 72        -0.17980
     65 -> 73         0.14288
     66 -> 68         0.16577
     66 -> 72         0.22198
     66 -> 73        -0.20566
 Excited State   5:      Singlet-A      6.5834 eV  188.33 nm  f=0.2238  <S**2>=0.000
     65 -> 68         0.29816
     65 -> 70         0.22921
     65 -> 72         0.29211
     65 -> 73        -0.17491
     66 -> 68        -0.28954
     66 -> 69        -0.10111
     66 -> 70         0.15612
     66 -> 71        -0.12467
     66 -> 72         0.18275
 Excited State   6:      Singlet-A      6.6599 eV  186.17 nm  f=0.1924  <S**2>=0.000
     65 -> 70         0.17454
     65 -> 72         0.24766
     65 -> 73        -0.16263
     66 -> 69         0.18771
     66 -> 70        -0.20373
     66 -> 71         0.33314
     66 -> 73        -0.25941
     66 -> 74         0.10692
     66 -> 77         0.11473
 Excited State   7:      Singlet-A      6.7638 eV  183.31 nm  f=0.0199  <S**2>=0.000
     65 -> 67        -0.24540
     65 -> 68         0.17010
     65 -> 69         0.17996
     66 -> 69        -0.11654
     66 -> 70         0.24439
     66 -> 71         0.30911
     66 -> 74         0.21175
     66 -> 75         0.13174
     66 -> 77        -0.15307
 Excited State   8:      Singlet-A      6.8752 eV  180.33 nm  f=0.0132  <S**2>=0.000
     65 -> 67         0.34962
     65 -> 68        -0.14467
     65 -> 69        -0.26185
     65 -> 80        -0.12008
     66 -> 70         0.27748
     66 -> 71         0.20187
     66 -> 77        -0.24350
```

66 -> 84 0.10756
Excited State 9: Singlet-A 6.9561 eV 178.24 nm f=0.0039 <S**2>=0.000
65 -> 67 -0.11889
65 -> 68 0.12482
66 -> 67 0.14771
66 -> 69 0.31207
66 -> 70 0.18337
66 -> 71 -0.14322
66 -> 72 -0.20247
66 -> 73 -0.18267
66 -> 74 -0.23626
66 -> 77 -0.23886
66 -> 80 -0.15244
Excited State 10: Singlet-A 7.0514 eV 175.83 nm f=0.1781 <S**2>=0.000
61 -> 67 0.13613
61 -> 68 0.28181
61 -> 69 -0.13513
64 -> 67 0.22713
64 -> 68 0.42523
64 -> 69 -0.18396
64 -> 71 -0.13788
Excited State 11: Singlet-A 7.2542 eV 170.91 nm f=0.0037 <S**2>=0.000
66 -> 67 0.25364
66 -> 69 0.10128
66 -> 74 -0.12555
66 -> 75 0.27907
66 -> 76 -0.27006
66 -> 77 0.10211
66 -> 78 0.10481
66 -> 80 0.30641
66 -> 85 -0.13211
66 -> 87 -0.13786
66 -> 91 -0.10806
Excited State 12: Singlet-A 7.3271 eV 169.21 nm f=0.0214 <S**2>=0.000
61 -> 70 -0.13078
64 -> 67 0.16672
64 -> 68 -0.14207
64 -> 70 -0.11157
65 -> 67 0.11754
65 -> 68 0.10175
65 -> 69 0.23738
65 -> 70 -0.23529
65 -> 73 -0.23757
65 -> 75 -0.10061
66 -> 74 0.14129
66 -> 76 0.13957
66 -> 79 -0.11357
Excited State 13: Singlet-A 7.4212 eV 167.07 nm f=0.0204 <S**2>=0.000
61 -> 72 -0.11630
64 -> 70 -0.13696
64 -> 72 -0.16005

```
     65 -> 68        0.13340
     65 -> 71        0.26197
     65 -> 74        0.12814
     66 -> 71        0.15442
     66 -> 73        0.16426
     66 -> 74       -0.25409
     66 -> 75       -0.15151
     66 -> 78        0.21682
     66 -> 79        0.17787
 Excited State  14:      Singlet-A      7.4573 eV  166.26 nm  f=0.0259  <S**2>=0.000
     61 -> 72        0.19530
     61 -> 73       -0.14194
     63 -> 67       -0.13802
     63 -> 68       -0.13154
     64 -> 70        0.17230
     64 -> 72        0.29671
     64 -> 73       -0.19253
     65 -> 69        0.10227
     65 -> 70       -0.10079
     65 -> 73       -0.15364
     66 -> 73        0.10313
     66 -> 74       -0.10137
     66 -> 75       -0.11640
     66 -> 78        0.12806
 Excited State  15:      Singlet-A      7.5018 eV  165.27 nm  f=0.0023  <S**2>=0.000
     60 -> 68        0.14916
     62 -> 68        0.12073
     63 -> 67        0.34432
     63 -> 68        0.32119
     66 -> 67        0.11612
     66 -> 73        0.14064
     66 -> 75       -0.14146
     66 -> 78        0.12643
 Excited State  16:      Singlet-A      7.5292 eV  164.67 nm  f=0.0098  <S**2>=0.000
     63 -> 67        0.19835
     63 -> 68        0.11297
     64 -> 67       -0.17400
     65 -> 67       -0.10996
     65 -> 68        0.12119
     65 -> 70       -0.10651
     65 -> 71        0.34525
     65 -> 73       -0.11673
     65 -> 74        0.14850
     66 -> 73       -0.11564
     66 -> 74        0.14847
     66 -> 75        0.13261
     66 -> 78       -0.15470
 Excited State  17:      Singlet-A      7.5808 eV  163.55 nm  f=0.0039  <S**2>=0.000
     63 -> 68       -0.15469
     65 -> 70        0.12542
     65 -> 71        0.23223
```

65 -> 73 0.11150
65 -> 74 0.13387
66 -> 67 0.21320
66 -> 69 0.14707
66 -> 72 0.13206
66 -> 74 0.11239
66 -> 76 0.28533
66 -> 78 0.12865
66 -> 79 -0.16330
Excited State 18: Singlet-A 7.6011 eV 163.11 nm f=0.0029 <S**2>=0.000
61 -> 67 0.12001
63 -> 67 0.23519
63 -> 69 0.15306
64 -> 67 -0.15972
65 -> 67 -0.10886
65 -> 69 -0.13605
65 -> 70 -0.19323
65 -> 71 -0.18505
65 -> 72 0.14640
65 -> 77 0.20131
66 -> 76 0.16363
66 -> 78 0.13182
Excited State 19: Singlet-A 7.6282 eV 162.53 nm f=0.0040 <S**2>=0.000
63 -> 68 0.12428
63 -> 69 -0.11100
65 -> 69 0.11178
66 -> 67 -0.14558
66 -> 74 -0.20689
66 -> 75 0.34096
66 -> 76 0.26619
66 -> 79 0.14981
66 -> 81 -0.17845
66 -> 82 0.13634
66 -> 87 0.11219
Excited State 20: Singlet-A 7.6470 eV 162.13 nm f=0.0092 <S**2>=0.000
62 -> 67 0.39720
62 -> 68 0.12847
62 -> 69 0.10331
63 -> 67 -0.21446
63 -> 69 -0.16449
65 -> 69 -0.12222
65 -> 72 0.18490
65 -> 73 0.11608
65 -> 77 0.12134
65 -> 80 0.10649

3'(S_0)

Excited State 1: Singlet-A 5.0995 eV 243.13 nm f=0.0675 <S**2>=0.000
65 -> 73 0.15256
65 -> 74 0.19317

```
      66 -> 67       -0.25325
      66 -> 68        0.57219
 Excited State   2:      Singlet-A      5.8683 eV  211.28 nm  f=0.0087  <S**2>=0.000
      65 -> 67       -0.19263
      65 -> 68        0.41669
      66 -> 67       -0.10915
      66 -> 71        0.16072
      66 -> 72       -0.20314
      66 -> 73       -0.27565
      66 -> 74       -0.31541
 Excited State   3:      Singlet-A      6.1549 eV  201.44 nm  f=0.0016  <S**2>=0.000
      66 -> 67        0.43542
      66 -> 68        0.20061
      66 -> 69        0.30906
      66 -> 70        0.19323
      66 -> 74       -0.13420
      66 -> 78        0.12510
      66 -> 80       -0.16780
 Excited State   4:      Singlet-A      6.4801 eV  191.33 nm  f=0.6394  <S**2>=0.000
      65 -> 67       -0.24549
      65 -> 68        0.41119
      65 -> 74       -0.11444
      66 -> 72        0.16839
      66 -> 73        0.24171
      66 -> 74        0.28727
      66 -> 75       -0.11811
 Excited State   5:      Singlet-A      6.5857 eV  188.26 nm  f=0.1956  <S**2>=0.000
      65 -> 67       -0.13360
      65 -> 68       -0.20975
      65 -> 71        0.19997
      65 -> 72       -0.17328
      65 -> 73       -0.20600
      65 -> 74       -0.20426
      66 -> 68        0.21143
      66 -> 69        0.27955
      66 -> 70       -0.18008
      66 -> 72       -0.15911
 Excited State   6:      Singlet-A      6.6969 eV  185.14 nm  f=0.2546  <S**2>=0.000
      65 -> 71        0.15593
      65 -> 72       -0.14587
      65 -> 73       -0.21562
      65 -> 74       -0.21331
      66 -> 68        0.10707
      66 -> 69       -0.27985
```

66 -> 70 0.32346
66 -> 74 -0.23824
Excited State 7: Singlet-A 6.7772 eV 182.94 nm f=0.0783 <S**2>=0.000
65 -> 67 0.33259
65 -> 68 0.19870
65 -> 69 0.29945
65 -> 74 -0.19803
65 -> 75 0.12017
65 -> 80 -0.14156
66 -> 68 0.11899
66 -> 70 -0.17858
66 -> 71 -0.15733
66 -> 73 -0.11217
Excited State 8: Singlet-A 6.9186 eV 179.20 nm f=0.0100 <S**2>=0.000
65 -> 67 0.18919
65 -> 69 0.17178
66 -> 70 0.17018
66 -> 71 0.42500
66 -> 72 -0.13662
66 -> 73 0.18313
66 -> 75 -0.11608
66 -> 76 0.12946
66 -> 77 -0.25705
66 -> 83 -0.11232
Excited State 9: Singlet-A 7.0260 eV 176.46 nm f=0.0658 <S**2>=0.000
61 -> 67 -0.14314
61 -> 68 0.16102
63 -> 67 0.11650
63 -> 68 -0.13885
64 -> 67 -0.21718
64 -> 68 0.25631
66 -> 67 0.10259
66 -> 69 -0.15235
66 -> 70 -0.18836
66 -> 71 0.13879
66 -> 72 0.18240
66 -> 73 -0.16181
66 -> 77 -0.14700
66 -> 80 -0.11670
Excited State 10: Singlet-A 7.0320 eV 176.31 nm f=0.0750 <S**2>=0.000
61 -> 67 -0.10231
61 -> 68 0.17920
63 -> 68 -0.14882
64 -> 67 -0.20441

64 -> 68 0.25637
66 -> 69 0.20776
66 -> 70 0.20345
66 -> 72 -0.23590
66 -> 73 0.12123
66 -> 77 0.18222
66 -> 80 0.10465
Excited State 11: Singlet-A 7.2366 eV 171.33 nm f=0.0133 <S**2>=0.000
55 -> 68 -0.15961
60 -> 67 -0.11513
60 -> 68 0.24107
61 -> 67 0.11821
61 -> 68 -0.16330
63 -> 67 -0.20257
63 -> 68 0.25887
64 -> 67 -0.18815
64 -> 68 0.33184
66 -> 75 0.11665
Excited State 12: Singlet-A 7.2514 eV 170.98 nm f=0.0092 <S**2>=0.000
64 -> 68 -0.20236
65 -> 69 0.22270
65 -> 71 0.14561
65 -> 72 -0.13443
65 -> 74 0.12322
66 -> 67 -0.14993
66 -> 68 -0.11292
66 -> 73 0.15888
66 -> 75 0.26415
66 -> 80 -0.21744
Excited State 13: Singlet-A 7.2601 eV 170.77 nm f=0.0232 <S**2>=0.000
60 -> 68 -0.10687
61 -> 68 0.16187
63 -> 68 -0.19973
64 -> 67 0.10825
65 -> 69 -0.15887
65 -> 71 -0.15147
65 -> 72 0.10331
65 -> 74 -0.11254
66 -> 67 -0.11265
66 -> 73 0.16742
66 -> 75 0.31529
66 -> 80 -0.21649
Excited State 14: Singlet-A 7.4108 eV 167.30 nm f=0.0098 <S**2>=0.000
65 -> 69 -0.12106

```
      65 -> 70        0.47320
      65 -> 73        0.17172
      65 -> 74       -0.11268
      66 -> 70        0.14386
      66 -> 74        0.15735
      66 -> 76       -0.12780
      66 -> 79        0.14252
 Excited State  15:      Singlet-A      7.5333 eV  164.58 nm  f=0.0031  <S**2>=0.000
      64 -> 67        0.13254
      64 -> 68        0.10654
      65 -> 70       -0.17618
      65 -> 80        0.11319
      66 -> 72       -0.12135
      66 -> 73       -0.21156
      66 -> 74        0.28301
      66 -> 76       -0.23947
      66 -> 77       -0.11457
      66 -> 79        0.26173
 Excited State  16:      Singlet-A      7.5719 eV  163.74 nm  f=0.0068  <S**2>=0.000
      61 -> 67       -0.11376
      64 -> 67        0.26152
      64 -> 68        0.14580
      64 -> 69       -0.10235
      65 -> 67        0.15728
      65 -> 69       -0.17839
      65 -> 71        0.28824
      65 -> 75       -0.11415
      65 -> 77       -0.26176
      65 -> 83       -0.10543
      66 -> 67        0.11404
      66 -> 72       -0.10124
      66 -> 78       -0.10607
 Excited State  17:      Singlet-A      7.5772 eV  163.63 nm  f=0.0092  <S**2>=0.000
      63 -> 67       -0.14870
      64 -> 67       -0.23828
      64 -> 68       -0.17961
      64 -> 71        0.13944
      64 -> 72       -0.14016
      65 -> 69       -0.18265
      65 -> 70       -0.18351
      65 -> 72        0.25782
      65 -> 73       -0.12145
      65 -> 78        0.11904
      65 -> 80       -0.10321
```

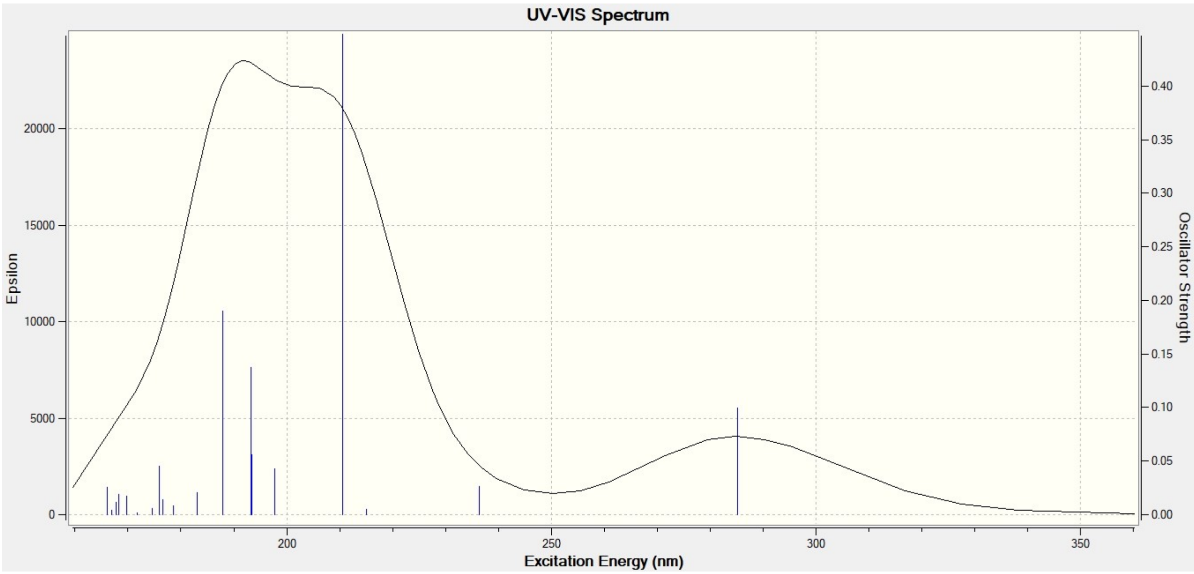
66 -> 74	0.10169
66 -> 76	-0.12977
Excited State 18: Singlet-A 7.6276 eV 162.55 nm f=0.0131 <S**2>=0.000	
61 -> 71	0.10592
63 -> 67	0.46116
63 -> 68	0.17404
63 -> 69	-0.20926
64 -> 67	0.10499
65 -> 72	0.14774
Excited State 19: Singlet-A 7.6772 eV 161.50 nm f=0.0009 <S**2>=0.000	
62 -> 67	0.31727
62 -> 69	-0.12550
63 -> 67	-0.11758
64 -> 67	0.11730
65 -> 72	0.14499
66 -> 67	-0.23226
66 -> 69	0.16054
66 -> 72	0.18055
66 -> 75	-0.12665
66 -> 78	0.24790
Excited State 20: Singlet-A 7.7080 eV 160.85 nm f=0.0139 <S**2>=0.000	
61 -> 67	-0.15936
61 -> 73	-0.11696
61 -> 74	-0.10807
62 -> 67	0.27369
63 -> 67	-0.19518
64 -> 67	0.17362
64 -> 70	-0.10517
64 -> 71	0.15711
64 -> 73	-0.13489
64 -> 74	-0.15896
65 -> 71	-0.10787
65 -> 77	0.17448
4(S_0)	
Excited State 1: Singlet-A 3.2613 eV 380.17 nm f=0.0020 <S**2>=0.000	
57 -> 62	-0.10971
60 -> 62	0.66874
60 -> 69	-0.10595
61 -> 62	-0.10442
Excited State 2: Singlet-A 3.3676 eV 368.17 nm f=0.2359 <S**2>=0.000	
60 -> 62	0.10158
61 -> 62	0.69571
Excited State 3: Singlet-A 4.8271 eV 256.85 nm f=0.3394 <S**2>=0.000	
56 -> 62	0.15489
59 -> 62	0.66611
Excited State 4: Singlet-A 5.2575 eV 235.82 nm f=0.0224 <S**2>=0.000	

55 -> 62 0.24020
57 -> 62 0.32750
58 -> 62 0.53123
Excited State 5: Singlet-A 5.4225 eV 228.65 nm f=0.0206 <S**2>=0.000
51 -> 62 -0.12394
57 -> 62 0.51068
58 -> 62 -0.38197
60 -> 62 0.12934
60 -> 75 0.11319
Excited State 6: Singlet-A 5.8104 eV 213.38 nm f=0.0811 <S**2>=0.000
60 -> 69 -0.10156
61 -> 65 0.11988
61 -> 66 -0.16479
61 -> 69 0.52261
61 -> 70 -0.25378
61 -> 71 -0.15760
61 -> 72 0.15804
Excited State 7: Singlet-A 5.9596 eV 208.04 nm f=0.0014 <S**2>=0.000
61 -> 63 0.48527
61 -> 64 -0.36774
61 -> 67 0.12908
61 -> 69 -0.12808
61 -> 76 -0.12077
61 -> 83 -0.13561
Excited State 8: Singlet-A 5.9707 eV 207.65 nm f=0.0021 <S**2>=0.000
50 -> 62 -0.10411
56 -> 62 0.61023
59 -> 62 -0.14914
60 -> 69 0.12243
61 -> 75 0.16080
Excited State 9: Singlet-A 6.0694 eV 204.28 nm f=0.0059 <S**2>=0.000
50 -> 62 -0.18077
56 -> 62 -0.15554
57 -> 62 -0.15774
60 -> 62 0.10106
60 -> 66 -0.11297
60 -> 69 0.44769
60 -> 70 -0.19398
60 -> 71 -0.15360
60 -> 72 0.15213
61 -> 69 0.12146
Excited State 10: Singlet-A 6.3117 eV 196.44 nm f=0.0898 <S**2>=0.000
48 -> 62 0.14601
52 -> 62 -0.19078
55 -> 62 0.37015
56 -> 62 0.11571
57 -> 62 -0.13399
58 -> 62 -0.11187
60 -> 69 -0.11986
61 -> 75 -0.34282
61 -> 76 0.10433

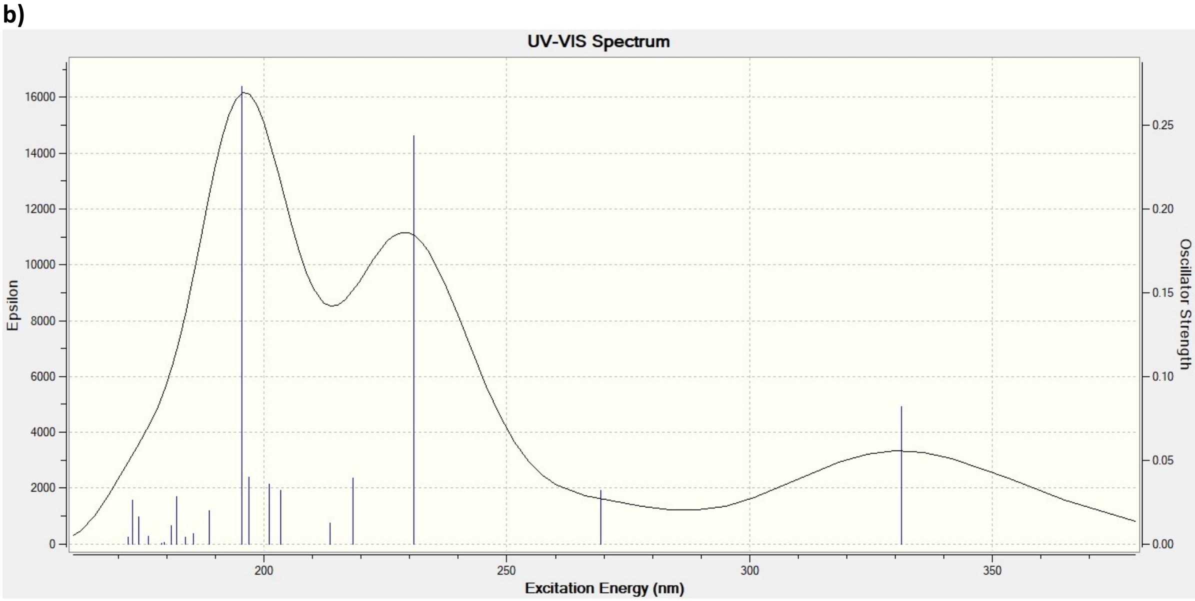
Excited State 11: Singlet-A 6.3361 eV 195.68 nm f=0.1254 <S**2>=0.000
48 -> 62 0.12844
52 -> 62 0.19441
55 -> 62 0.42813
56 -> 62 -0.15968
57 -> 62 -0.10203
58 -> 62 -0.13537
61 -> 65 -0.11486
61 -> 75 0.31378
Excited State 12: Singlet-A 6.5464 eV 189.39 nm f=0.0168 <S**2>=0.000
52 -> 62 0.11912
53 -> 62 -0.34185
61 -> 64 0.11707
61 -> 65 0.42694
61 -> 66 0.15668
61 -> 68 -0.24281
Excited State 13: Singlet-A 6.5664 eV 188.82 nm f=0.0210 <S**2>=0.000
52 -> 62 0.12283
53 -> 62 0.54445
54 -> 62 -0.15483
61 -> 65 0.27291
61 -> 66 0.10059
61 -> 68 -0.13274
Excited State 14: Singlet-A 6.6321 eV 186.95 nm f=0.0059 <S**2>=0.000
52 -> 62 0.21588
59 -> 63 -0.10968
61 -> 63 0.18125
61 -> 64 0.39381
61 -> 65 -0.18252
61 -> 67 0.35056
61 -> 76 -0.13161
Excited State 15: Singlet-A 6.7175 eV 184.57 nm f=0.1327 <S**2>=0.000
48 -> 62 0.12530
49 -> 62 -0.10176
50 -> 62 0.49735
51 -> 62 0.15506
52 -> 62 0.24300
60 -> 63 0.10024
60 -> 65 0.10055
60 -> 69 0.13337
61 -> 75 -0.12867
Excited State 16: Singlet-A 6.7323 eV 184.16 nm f=0.0240 <S**2>=0.000
50 -> 62 -0.11276
60 -> 63 0.38374
60 -> 64 -0.12947
60 -> 65 0.29853
60 -> 66 0.13797
60 -> 67 0.20315
60 -> 68 -0.18130
60 -> 74 0.15167
60 -> 75 -0.11365

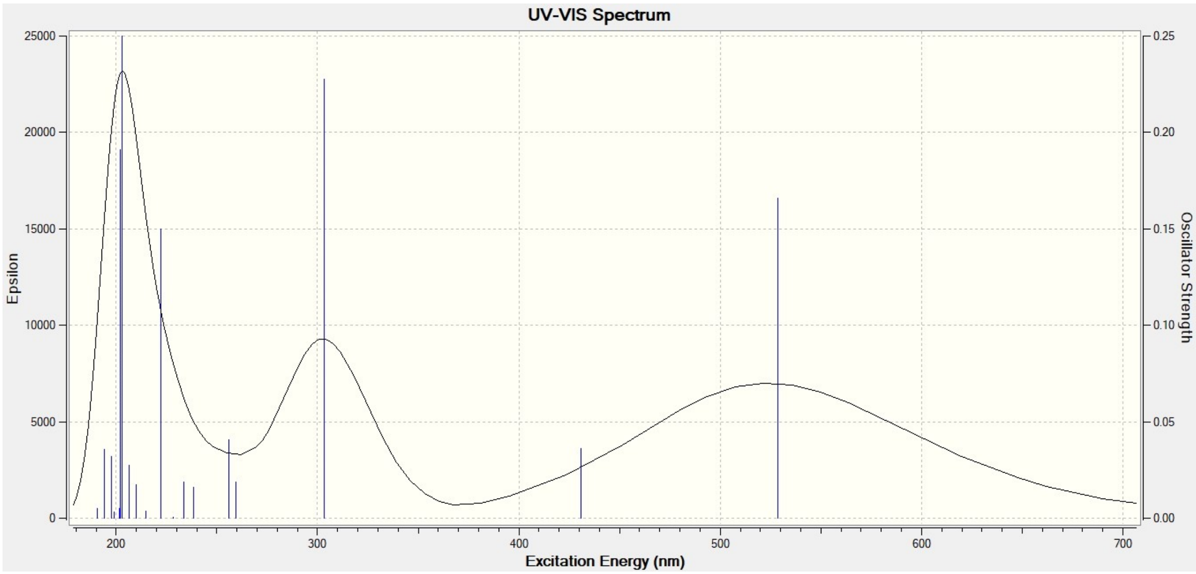
60 -> 82 0.10826
Excited State 17: Singlet-A 6.8377 eV 181.32 nm f=0.0990 <S**2>=0.000
51 -> 62 0.19809
52 -> 62 -0.13778
61 -> 65 0.12179
61 -> 66 -0.32045
61 -> 71 0.37277
61 -> 72 -0.10643
61 -> 75 0.18705
61 -> 82 -0.14116
Excited State 18: Singlet-A 6.8556 eV 180.85 nm f=0.1669 <S**2>=0.000
51 -> 62 0.23961
52 -> 62 -0.30597
53 -> 62 0.11174
54 -> 62 0.33444
61 -> 66 0.22523
61 -> 71 -0.21236
61 -> 72 0.10585
61 -> 75 0.12622
Excited State 19: Singlet-A 6.8710 eV 180.45 nm f=0.0631 <S**2>=0.000
50 -> 62 -0.10572
51 -> 62 -0.16944
52 -> 62 0.20051
53 -> 62 0.15656
54 -> 62 0.56134
61 -> 75 -0.10428
Excited State 20: Singlet-A 6.9067 eV 179.51 nm f=0.0692 <S**2>=0.000
48 -> 62 0.11683
50 -> 62 -0.29686
51 -> 62 0.33407
52 -> 62 0.25193
57 -> 62 0.14211
60 -> 75 -0.26983
60 -> 76 0.10816
61 -> 75 -0.11101

a)


UV-VIS Spectrum
Epsilon
Oscillator Strength
Excitation Energy (nm)
0
5000
10000
15000
20000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
200
250
300
350

b)


UV-VIS Spectrum
Epsilon
Oscillator Strength
Excitation Energy (nm)
0
2000
4000
6000
8000
10000
12000
14000
16000
0.00
0.05
0.10
0.15
0.20
0.25
200
250
300
350



c)

Figure S26. Simulated spectra of **3**(S_1) (a), **3'**(S_1) (b) and **4**(S_1) (c) computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

Table S2. Vertical excitation of singlet **3**(S_1), **3'**(S_1) and **4**(S_1) computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

3(S_1)					
Excited State 1:	Singlet-A	4.3469 eV	285.23 nm	f=0.0998	<S**2>=0.000
65 -> 67	-0.11363				
65 -> 73	0.10934				
66 -> 67	0.65474				
Excited State 2:	Singlet-A	5.2463 eV	236.33 nm	f=0.0264	<S**2>=0.000
65 -> 67	0.46561				
66 -> 67	0.16994				
66 -> 70	-0.17408				
66 -> 72	-0.20237				
66 -> 73	-0.31205				
66 -> 74	-0.15276				
66 -> 75	0.15631				
Excited State 3:	Singlet-A	5.7634 eV	215.12 nm	f=0.0048	<S**2>=0.000
66 -> 68	0.47585				
66 -> 69	-0.37595				
66 -> 71	-0.14595				
66 -> 80	-0.15398				
66 -> 87	-0.12117				
Excited State 4:	Singlet-A	5.8863 eV	210.63 nm	f=0.4484	<S**2>=0.000
65 -> 67	0.46580				
66 -> 70	0.16736				
66 -> 72	0.18975				
66 -> 73	0.34171				
66 -> 74	0.13735				
66 -> 75	-0.14492				

```
     66 -> 77       -0.12596
 Excited State   5:      Singlet-A      6.2675 eV  197.82 nm  f=0.0426  <S**2>=0.000
      65 -> 70        0.12932
      65 -> 72        0.12555
      65 -> 73        0.19766
      66 -> 67       -0.12152
      66 -> 69       -0.20436
      66 -> 71        0.41057
      66 -> 72        0.18798
      66 -> 73       -0.17547
      66 -> 74        0.15208
 Excited State   6:      Singlet-A      6.4080 eV  193.48 nm  f=0.0561  <S**2>=0.000
      61 -> 67        0.14385
      64 -> 67       -0.20472
      65 -> 68       -0.14395
      65 -> 69        0.11143
      65 -> 70        0.11491
      65 -> 72        0.12360
      65 -> 73        0.15590
      65 -> 74        0.11443
      66 -> 68       -0.12157
      66 -> 70        0.32943
      66 -> 71       -0.24352
      66 -> 74       -0.26581
      66 -> 77        0.11834
 Excited State   7:      Singlet-A      6.4175 eV  193.20 nm  f=0.1377  <S**2>=0.000
      64 -> 67        0.14356
      65 -> 70       -0.14660
      65 -> 72       -0.15875
      65 -> 73       -0.26765
      65 -> 74       -0.10182
      65 -> 75        0.12752
      66 -> 69       -0.11631
      66 -> 70        0.36989
      66 -> 71        0.10414
      66 -> 72        0.10341
      66 -> 77        0.24330
      66 -> 84        0.12723
 Excited State   8:      Singlet-A      6.5970 eV  187.94 nm  f=0.1235  <S**2>=0.000
      61 -> 67       -0.12471
      64 -> 67        0.17092
      65 -> 70        0.12128
      65 -> 72        0.11821
      65 -> 73        0.17285
      66 -> 68        0.14016
      66 -> 69        0.30049
      66 -> 70        0.15689
      66 -> 72       -0.28251
      66 -> 76        0.10776
      66 -> 77        0.21842
      66 -> 80       -0.15287
```

66 -> 84 0.10030
Excited State 9: Singlet-A 6.6004 eV 187.84 nm f=0.1897 <S**2>=0.000
61 -> 67 -0.30300
64 -> 67 0.42818
65 -> 73 0.11894
66 -> 68 -0.13877
66 -> 69 -0.13911
66 -> 71 -0.12698
66 -> 73 -0.11511
66 -> 74 -0.16987
Excited State 10: Singlet-A 6.7710 eV 183.11 nm f=0.0207 <S**2>=0.000
65 -> 68 0.45391
65 -> 69 -0.34749
65 -> 73 0.10001
65 -> 80 -0.15466
66 -> 69 -0.10706
66 -> 72 0.11878
Excited State 11: Singlet-A 6.9437 eV 178.56 nm f=0.0086 <S**2>=0.000
66 -> 68 -0.21695
66 -> 73 -0.13632
66 -> 75 -0.17644
66 -> 76 0.34725
66 -> 77 -0.12958
66 -> 80 -0.30965
66 -> 81 -0.11594
66 -> 84 -0.12717
66 -> 85 0.15169
66 -> 87 -0.16500
Excited State 12: Singlet-A 7.0235 eV 176.53 nm f=0.0140 <S**2>=0.000
63 -> 67 -0.15709
65 -> 70 -0.10887
66 -> 71 0.12159
66 -> 73 0.22796
66 -> 74 -0.28478
66 -> 75 0.30676
66 -> 76 0.11368
66 -> 77 -0.11672
66 -> 78 -0.17331
66 -> 79 -0.21277
66 -> 81 0.12179
Excited State 13: Singlet-A 7.0472 eV 175.93 nm f=0.0450 <S**2>=0.000
55 -> 67 -0.11101
60 -> 67 0.26021
61 -> 67 -0.15044
62 -> 67 0.25761
63 -> 67 0.46657
66 -> 74 -0.10537
Excited State 14: Singlet-A 7.1004 eV 174.62 nm f=0.0057 <S**2>=0.000
65 -> 69 0.17631
66 -> 68 0.20560
66 -> 69 0.11870

```
    66 -> 71       -0.15415
    66 -> 72        0.17782
    66 -> 73       -0.13888
    66 -> 75       -0.13660
    66 -> 76        0.31129
    66 -> 78        0.22880
    66 -> 79       -0.12806
    66 -> 87        0.14480
Excited State  15:      Singlet-A      7.2155 eV  171.83 nm  f=0.0017  <S**2>=0.000
    66 -> 71       -0.20008
    66 -> 74        0.22419
    66 -> 75        0.38263
    66 -> 76        0.19638
    66 -> 78        0.16542
    66 -> 79        0.12165
    66 -> 81        0.24879
Excited State  16:      Singlet-A      7.3037 eV  169.75 nm  f=0.0169  <S**2>=0.000
    65 -> 69       -0.16215
    65 -> 70        0.30400
    65 -> 71        0.15029
    65 -> 72        0.17054
    65 -> 73       -0.17442
    65 -> 77        0.17437
    66 -> 68        0.20215
    66 -> 69        0.13135
    66 -> 72        0.13251
    66 -> 74       -0.13651
    66 -> 79       -0.13793
Excited State  17:      Singlet-A      7.3705 eV  168.22 nm  f=0.0193  <S**2>=0.000
    62 -> 67        0.11427
    65 -> 70       -0.22265
    65 -> 71        0.42409
    65 -> 74        0.27313
    66 -> 74        0.11382
Excited State  18:      Singlet-A      7.3923 eV  167.72 nm  f=0.0112  <S**2>=0.000
    64 -> 68       -0.12555
    65 -> 68       -0.13176
    65 -> 69       -0.15819
    65 -> 71       -0.10978
    66 -> 68       -0.13009
    66 -> 69       -0.20535
    66 -> 70       -0.20280
    66 -> 73        0.17696
    66 -> 75       -0.14423
    66 -> 77        0.17420
    66 -> 84        0.26785
    66 -> 87        0.16371
    66 -> 89        0.13925
Excited State  19:      Singlet-A      7.4310 eV  166.85 nm  f=0.0042  <S**2>=0.000
    62 -> 67        0.55922
    63 -> 67       -0.30032
```

Excited State 20: Singlet-A 7.4654 eV 166.08 nm f=0.0253 <S**2>=0.000
57 -> 67 -0.15761
60 -> 67 -0.17293
61 -> 67 0.25564
61 -> 73 -0.12236
63 -> 67 0.20288
63 -> 68 0.10298
64 -> 67 0.16226
64 -> 70 0.12340
64 -> 72 0.13218
64 -> 73 0.12650
65 -> 69 0.17793
65 -> 71 -0.12829
65 -> 72 -0.15242
65 -> 73 0.10293

3'(S_1)

Excited State 1: Singlet-A 3.7412 eV 331.40 nm f=0.0819 <S**2>=0.000
65 -> 67 0.11014
66 -> 67 0.68106
Excited State 2: Singlet-A 4.6040 eV 269.30 nm f=0.0321 <S**2>=0.000
65 -> 67 0.56725
66 -> 67 -0.13870
66 -> 70 0.15196
66 -> 72 -0.28243
66 -> 73 0.12449
Excited State 3: Singlet-A 5.3692 eV 230.92 nm f=0.2437 <S**2>=0.000
65 -> 67 0.37328
66 -> 70 -0.25080
66 -> 71 0.14030
66 -> 72 0.43911
66 -> 73 -0.16359
Excited State 4: Singlet-A 5.6775 eV 218.38 nm f=0.0393 <S**2>=0.000
66 -> 68 0.48051
66 -> 69 0.21811
66 -> 71 0.27541
66 -> 72 -0.12093
66 -> 73 0.11966
66 -> 77 0.17748
66 -> 80 0.10231
66 -> 88 0.10301
Excited State 5: Singlet-A 5.8059 eV 213.55 nm f=0.0125 <S**2>=0.000
61 -> 67 0.21109
64 -> 67 0.63802
Excited State 6: Singlet-A 6.0982 eV 203.31 nm f=0.0321 <S**2>=0.000
60 -> 67 -0.13307
63 -> 67 0.18506

65 -> 70	-0.12143
65 -> 72	0.20124
65 -> 73	-0.10246
66 -> 68	0.15706
66 -> 69	0.36070
66 -> 71	-0.26549
66 -> 73	-0.15015
66 -> 74	-0.12278
66 -> 76	0.10893
66 -> 77	-0.10484
Excited State 7:	Singlet-A 6.1670 eV 201.04 nm f=0.0358 <S**2>=0.000
60 -> 67	-0.26696
61 -> 67	-0.16186
62 -> 67	-0.15570
63 -> 67	0.42936
65 -> 72	0.11257
66 -> 69	-0.19055
66 -> 71	0.22150
Excited State 8:	Singlet-A 6.2994 eV 196.82 nm f=0.0401 <S**2>=0.000
65 -> 70	0.12385
65 -> 72	-0.24075
65 -> 73	0.10344
66 -> 70	0.49776
66 -> 71	0.10848
66 -> 73	-0.19579
66 -> 75	-0.12318
Excited State 9:	Singlet-A 6.3456 eV 195.39 nm f=0.2732 <S**2>=0.000
63 -> 67	-0.21264
65 -> 68	0.10975
65 -> 70	-0.24777
65 -> 71	0.13797
65 -> 72	0.36066
65 -> 73	-0.15484
66 -> 70	0.16028
66 -> 71	0.20755
66 -> 72	0.12480
66 -> 73	-0.11107
Excited State 10:	Singlet-A 6.5740 eV 188.60 nm f=0.0201 <S**2>=0.000
66 -> 68	0.30228
66 -> 69	-0.27865
66 -> 70	0.10359
66 -> 71	-0.19299
66 -> 72	0.12831
66 -> 73	0.24538

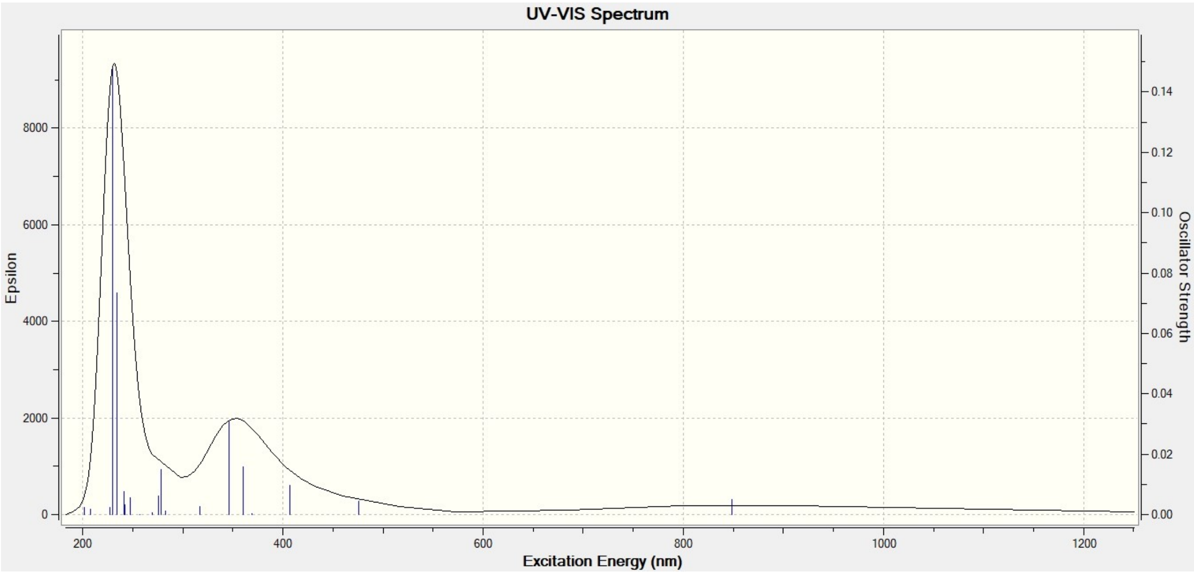
66 -> 75	-0.14560
66 -> 76	-0.12446
66 -> 77	-0.22338
66 -> 84	-0.17538
Excited State 11: Singlet-A 6.6881 eV 185.38 nm f=0.0064 <S**2>=0.000	
62 -> 67	0.14607
65 -> 68	0.40685
65 -> 69	0.24738
65 -> 71	0.13061
65 -> 72	-0.10338
65 -> 77	0.10362
66 -> 70	-0.11575
66 -> 71	-0.10106
66 -> 73	0.16537
66 -> 74	-0.14119
66 -> 75	-0.15116
Excited State 12: Singlet-A 6.7483 eV 183.73 nm f=0.0042 <S**2>=0.000	
62 -> 67	0.62910
63 -> 67	0.17944
Excited State 13: Singlet-A 6.8130 eV 181.98 nm f=0.0282 <S**2>=0.000	
61 -> 67	-0.10012
63 -> 67	-0.12369
65 -> 68	0.12509
65 -> 69	0.12284
65 -> 70	0.12369
66 -> 68	0.12233
66 -> 69	-0.13626
66 -> 74	0.34329
66 -> 75	0.19682
66 -> 76	0.25206
66 -> 77	-0.18646
66 -> 79	-0.17092
Excited State 14: Singlet-A 6.8574 eV 180.80 nm f=0.0109 <S**2>=0.000	
55 -> 67	-0.11540
60 -> 67	0.17397
61 -> 67	0.46889
63 -> 67	0.32212
64 -> 67	-0.11274
65 -> 68	0.13605
65 -> 69	0.13693
Excited State 15: Singlet-A 6.9119 eV 179.38 nm f=0.0011 <S**2>=0.000	
65 -> 68	-0.13985
65 -> 69	-0.19176
66 -> 73	0.20453

66 -> 74 0.10833
66 -> 75 -0.21682
66 -> 76 0.40416
66 -> 77 0.11735
66 -> 78 0.17223
Excited State 16: Singlet-A 6.9305 eV 178.90 nm f=0.0004 <S**2>=0.000
66 -> 71 -0.16976
66 -> 72 0.18127
66 -> 73 0.10820
66 -> 74 0.14913
66 -> 75 0.27533
66 -> 76 -0.17369
66 -> 77 0.11647
66 -> 80 0.29154
66 -> 82 -0.13630
66 -> 84 0.14874
66 -> 86 -0.22583
Excited State 17: Singlet-A 7.0404 eV 176.10 nm f=0.0045 <S**2>=0.000
54 -> 67 -0.27715
55 -> 67 -0.11471
57 -> 67 0.31587
58 -> 67 -0.13712
60 -> 67 0.27667
61 -> 67 -0.30157
63 -> 67 0.11875
64 -> 67 0.19074
Excited State 18: Singlet-A 7.1215 eV 174.10 nm f=0.0161 <S**2>=0.000
65 -> 71 0.21683
65 -> 77 0.10122
66 -> 70 -0.13827
66 -> 71 -0.21970
66 -> 73 -0.21152
66 -> 74 0.26985
66 -> 75 -0.20493
66 -> 76 -0.17266
66 -> 81 0.20995
66 -> 90 -0.13606
Excited State 19: Singlet-A 7.1697 eV 172.93 nm f=0.0264 <S**2>=0.000
64 -> 68 0.10086
65 -> 69 0.17893
65 -> 70 0.28654
65 -> 71 -0.15964
65 -> 73 -0.23539
65 -> 77 -0.13935

66 -> 68	-0.13585					
66 -> 69	0.13084					
66 -> 72	0.12834					
66 -> 75	-0.20559					
66 -> 81	0.10804					
Excited State 20:	Singlet-A	7.2095 eV	171.97 nm	f=0.0042	<S**2>=0.000	
64 -> 68	-0.13806					
65 -> 69	-0.13252					
65 -> 71	0.14455					
66 -> 68	-0.18201					
66 -> 69	0.28508					
66 -> 73	0.19676					
66 -> 74	0.13469					
66 -> 76	-0.14642					
66 -> 77	-0.12400					
66 -> 83	0.15222					
66 -> 84	-0.24489					
66 -> 86	0.11057					
66 -> 88	-0.12447					
4(S_1)						
Excited State 1:	Singlet-A	2.3459 eV	528.52 nm	f=0.1661	<S**2>=0.000	
60 -> 62	-0.18621					
61 -> 62	0.68148					
Excited State 2:	Singlet-A	2.8766 eV	431.00 nm	f=0.0361	<S**2>=0.000	
60 -> 62	0.66908					
61 -> 62	0.19065					
Excited State 3:	Singlet-A	4.0877 eV	303.31 nm	f=0.2274	<S**2>=0.000	
59 -> 62	0.68505					
Excited State 4:	Singlet-A	4.7746 eV	259.67 nm	f=0.0189	<S**2>=0.000	
51 -> 62	0.14423					
58 -> 62	0.67036					
Excited State 5:	Singlet-A	4.8437 eV	255.97 nm	f=0.0408	<S**2>=0.000	
52 -> 62	0.13798					
56 -> 62	-0.41228					
57 -> 62	0.49752					
Excited State 6:	Singlet-A	5.1966 eV	238.59 nm	f=0.0160	<S**2>=0.000	
57 -> 62	-0.14340					
61 -> 66	0.27143					
61 -> 69	0.57178					
61 -> 72	-0.15498					
Excited State 7:	Singlet-A	5.3029 eV	233.80 nm	f=0.0189	<S**2>=0.000	
56 -> 62	0.52475					
57 -> 62	0.39313					
61 -> 69	0.14111					
Excited State 8:	Singlet-A	5.4339 eV	228.17 nm	f=0.0003	<S**2>=0.000	
61 -> 63	0.47905					
61 -> 64	0.36519					
61 -> 65	0.14576					

61 -> 67 0.14216
61 -> 76 0.13001
61 -> 83 0.17026
Excited State 9: Singlet-A 5.5804 eV 222.18 nm f=0.1500 <S**2>=0.000
55 -> 62 -0.31583
56 -> 62 -0.12602
61 -> 70 -0.14320
61 -> 72 0.22840
61 -> 73 0.47730
Excited State 10: Singlet-A 5.7708 eV 214.85 nm f=0.0035 <S**2>=0.000
50 -> 62 -0.15939
51 -> 62 0.23323
52 -> 62 0.17753
53 -> 62 -0.12804
54 -> 62 -0.14978
57 -> 62 -0.11632
60 -> 66 0.14800
60 -> 69 0.39545
60 -> 70 -0.11521
60 -> 73 0.26464
Excited State 11: Singlet-A 5.9045 eV 209.98 nm f=0.0173 <S**2>=0.000
53 -> 62 0.35652
54 -> 62 0.50182
55 -> 62 -0.18985
60 -> 69 0.16870
60 -> 73 0.10076
Excited State 12: Singlet-A 6.0113 eV 206.25 nm f=0.0061 <S**2>=0.000
52 -> 62 -0.20073
61 -> 64 -0.24083
61 -> 65 0.44618
61 -> 66 0.18417
61 -> 67 0.13141
61 -> 68 -0.27645
Excited State 13: Singlet-A 6.0123 eV 206.22 nm f=0.0276 <S**2>=0.000
50 -> 62 -0.10822
52 -> 62 0.55875
57 -> 62 -0.10837
60 -> 69 -0.20184
61 -> 65 0.16749
61 -> 68 -0.10806
Excited State 14: Singlet-A 6.1127 eV 202.83 nm f=0.2500 <S**2>=0.000
54 -> 62 0.16439
55 -> 62 0.44749
61 -> 63 0.11166
61 -> 64 -0.21586
61 -> 65 -0.13353
61 -> 67 0.23774
61 -> 68 0.11114
61 -> 72 0.18228
61 -> 73 0.13056
Excited State 15: Singlet-A 6.1382 eV 201.99 nm f=0.1912 <S**2>=0.000

51 -> 62 -0.22118
52 -> 62 0.10061
55 -> 62 0.28296
61 -> 63 -0.14966
61 -> 64 0.27928
61 -> 65 0.16527
61 -> 67 -0.26724
61 -> 70 -0.12944
61 -> 73 0.17849
61 -> 76 -0.10539
Excited State 16: Singlet-A 6.1486 eV 201.65 nm f=0.0051 <S**2>=0.000
48 -> 62 -0.11183
51 -> 62 0.52817
54 -> 62 0.10506
58 -> 62 -0.11743
60 -> 69 -0.18880
61 -> 64 0.14988
61 -> 67 -0.15403
Excited State 17: Singlet-A 6.2347 eV 198.86 nm f=0.0033 <S**2>=0.000
53 -> 62 0.57193
54 -> 62 -0.38602
Excited State 18: Singlet-A 6.2767 eV 197.53 nm f=0.0319 <S**2>=0.000
61 -> 65 -0.10372
61 -> 66 0.41365
61 -> 69 -0.10218
61 -> 71 0.17161
61 -> 72 0.36576
61 -> 73 -0.20471
61 -> 80 0.15270
61 -> 82 -0.10904
Excited State 19: Singlet-A 6.3842 eV 194.21 nm f=0.0356 <S**2>=0.000
60 -> 65 0.11075
60 -> 66 -0.11895
60 -> 69 -0.27219
60 -> 72 0.31547
60 -> 73 0.45674
Excited State 20: Singlet-A 6.5064 eV 190.56 nm f=0.0051 <S**2>=0.000
50 -> 62 0.57666
52 -> 62 0.10920
60 -> 63 -0.15351
60 -> 65 -0.14740



a)

b)

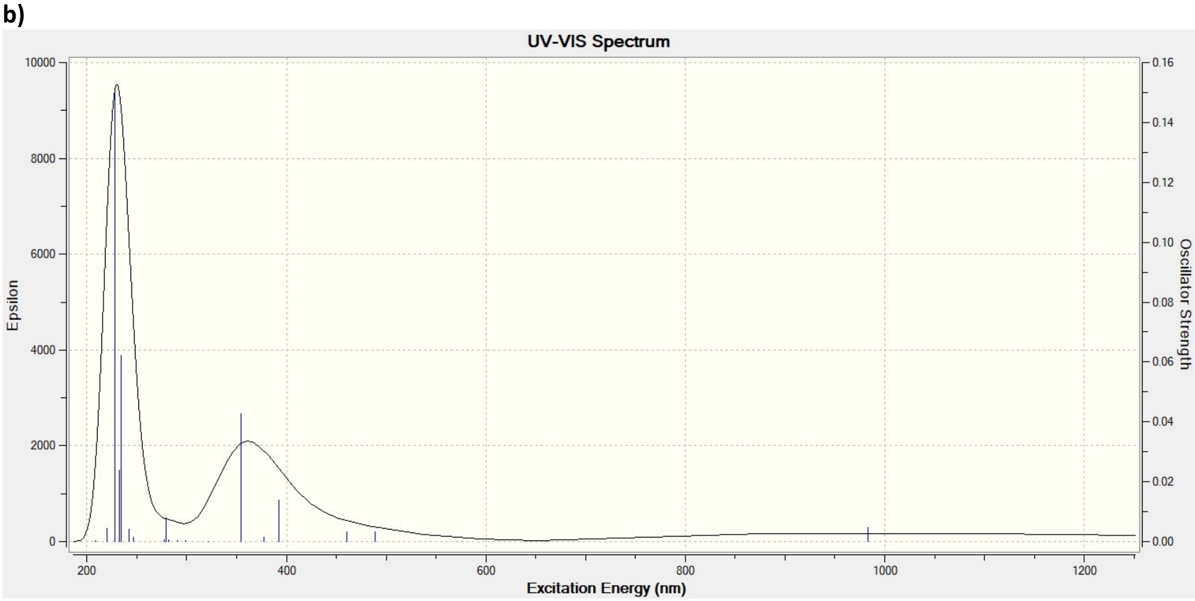


Figure S27. Simulated spectra of (a) **3rc**(S_0) and (b) **3'rc**(S_0) radical cation computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

Table S3. Vertical excitation of singlet **3rc**(S_0) and **3'rc**(S_0) radical cation computed at the PCM(water)/TD-ωB97XD/6-311++G(d,p) level of theory.

3rc(S_1)					
Excited State 1:	2.037-A	1.4604 eV	848.97 nm	f=0.0050	<S**2>=0.787
59B -> 66B	-0.15457				
61B -> 66B	0.11944				
62B -> 66B	0.77524				
63B -> 66B	0.20536				
64B -> 66B	0.16174				
65B -> 66B	-0.51803				

```
Excited State   2:  2.049-A      2.6073 eV  475.53 nm  f=0.0043  <S**2>=0.800
    54B -> 66B       -0.16827
    56B -> 66B        0.22734
    61B -> 66B        0.66706
    62B -> 66B        0.27386
    64B -> 66B       -0.20340
    65B -> 66B        0.54240
Excited State   3:  2.046-A      3.0481 eV  406.76 nm  f=0.0098  <S**2>=0.796
    59B -> 66B        0.35213
    62B -> 66B       -0.15439
    63B -> 66B        0.65081
    64B -> 66B        0.58119
    65B -> 66B        0.12863
Excited State   4:  2.042-A      3.3568 eV  369.35 nm  f=0.0004  <S**2>=0.793
    55B -> 66B        0.17292
    61B -> 66B        0.17387
    63B -> 66B       -0.63809
    64B -> 66B        0.69643
Excited State   5:  2.081-A      3.4391 eV  360.52 nm  f=0.0159  <S**2>=0.833
    62A -> 68A       -0.10679
    66A -> 67A        0.13291
    50B -> 66B       -0.11636
    55B -> 66B        0.39005
    56B -> 66B       -0.29338
    59B -> 66B        0.12802
    61B -> 66B        0.52952
    62B -> 66B       -0.32440
    64B -> 66B       -0.17803
    65B -> 66B       -0.46640
Excited State   6:  2.131-A      3.5818 eV  346.15 nm  f=0.0308  <S**2>=0.885
    62A -> 68A        0.16429
    63A -> 67A       -0.12385
    66A -> 67A       -0.18677
    66A -> 68A       -0.10662
    53B -> 66B        0.10487
    55B -> 66B       -0.37466
    56B -> 66B        0.53430
    57B -> 66B        0.16803
    59B -> 66B       -0.12228
    61B -> 66B        0.24285
    62B -> 66B       -0.34918
    62B -> 67B       -0.11541
    64B -> 66B        0.10463
    65B -> 66B       -0.38238
Excited State   7:  2.072-A      3.9117 eV  316.96 nm  f=0.0025  <S**2>=0.823
    48B -> 66B        0.14317
    49B -> 66B        0.13649
    50B -> 66B        0.23466
    51B -> 66B       -0.14343
    53B -> 66B        0.21999
    54B -> 66B        0.62193
```

56B -> 66B 0.10362
58B -> 66B -0.16168
59B -> 66B 0.50713
61B -> 66B 0.17831
62B -> 66B 0.10544
63B -> 66B -0.21946
64B -> 66B -0.14012
Excited State 8: 2.087-A 4.3912 eV 282.35 nm f=0.0012 <S**2>=0.839
50B -> 66B -0.18931
53B -> 66B -0.38536
54B -> 66B -0.17680
55B -> 66B -0.13869
56B -> 66B 0.12573
57B -> 66B -0.16561
58B -> 66B 0.57773
59B -> 66B 0.49795
61B -> 66B -0.10623
62B -> 66B 0.14692
63B -> 66B -0.17057
Excited State 9: 2.779-A 4.4499 eV 278.62 nm f=0.0148 <S**2>=1.680
59A -> 68A -0.10646
61A -> 68A -0.10297
62A -> 68A 0.43649
63A -> 67A 0.20615
63A -> 68A 0.13339
65A -> 68A -0.14689
66A -> 67A 0.52827
58B -> 66B 0.40475
62B -> 67B -0.29432
62B -> 68B 0.10327
65B -> 67B 0.17668
Excited State 10: 2.204-A 4.4982 eV 275.63 nm f=0.0062 <S**2>=0.964
62A -> 68A -0.19120
66A -> 67A -0.23618
50B -> 66B 0.15732
53B -> 66B 0.24720
54B -> 66B 0.37184
56B -> 66B -0.14143
57B -> 66B 0.11316
58B -> 66B 0.65050
59B -> 66B -0.30466
62B -> 67B 0.12239
65B -> 66B 0.12153
Excited State 11: 2.040-A 4.6066 eV 269.14 nm f=0.0007 <S**2>=0.790
60B -> 66B 0.97732
61B -> 66B -0.11019
Excited State 12: 2.051-A 4.8197 eV 257.25 nm f=0.0001 <S**2>=0.801
46B -> 66B 0.15237
48B -> 66B -0.49192
49B -> 66B -0.21740
54B -> 66B -0.10092

57B -> 66B 0.69885
59B -> 66B 0.32923
Excited State 13: 2.099-A 5.0035 eV 247.79 nm f=0.0057 <S**2>=0.851
66A -> 67A 0.13182
45B -> 66B -0.12784
46B -> 66B 0.20940
47B -> 66B 0.37042
48B -> 66B 0.65446
52B -> 66B -0.11522
53B -> 66B 0.15524
54B -> 66B -0.13360
55B -> 66B 0.11876
56B -> 66B 0.14783
57B -> 66B 0.36188
61B -> 66B -0.15275
Excited State 14: 2.471-A 5.1126 eV 242.51 nm f=0.0032 <S**2>=1.276
59A -> 67A 0.11047
62A -> 67A -0.53612
63A -> 67A -0.21843
63A -> 68A 0.26775
65A -> 67A 0.23229
65A -> 68A -0.14195
66A -> 68A 0.63073
46B -> 66B -0.10668
57B -> 66B 0.11779
Excited State 15: 2.145-A 5.1379 eV 241.31 nm f=0.0077 <S**2>=0.900
62A -> 67A -0.19297
66A -> 68A 0.10228
42B -> 66B -0.17897
45B -> 66B -0.12779
46B -> 66B 0.50161
47B -> 66B 0.20705
48B -> 66B -0.16430
49B -> 66B -0.18811
51B -> 66B 0.10966
52B -> 66B -0.12757
53B -> 66B 0.42344
54B -> 66B -0.11721
55B -> 66B -0.20756
57B -> 66B -0.42510
59B -> 66B 0.12921
Excited State 16: 2.916-A 5.2953 eV 234.14 nm f=0.0735 <S**2>=1.876
62A -> 67A -0.35163
62A -> 68A -0.29781
63A -> 68A -0.24917
65A -> 68A 0.20239
66A -> 67A 0.46677
66A -> 68A -0.28987
55B -> 66B -0.19426
57B -> 66B 0.11132
62B -> 68B -0.38066

65B -> 68B 0.23116
Excited State 17: 2.557-A 5.4042 eV 229.42 nm f=0.1478 <S**2>=1.385
62A -> 67A 0.27060
63A -> 67A 0.25988
63A -> 68A 0.14453
65A -> 67A -0.20114
66A -> 67A 0.35312
66A -> 68A 0.40979
43B -> 66B 0.10326
48B -> 66B -0.14884
54B -> 66B 0.13013
55B -> 66B -0.32511
56B -> 66B 0.19865
62B -> 67B 0.35054
65B -> 67B -0.21507
Excited State 18: 2.106-A 5.4678 eV 226.75 nm f=0.0024 <S**2>=0.859
66A -> 67A 0.13507
43B -> 66B -0.16258
48B -> 66B -0.20047
50B -> 66B -0.13973
51B -> 66B 0.11153
54B -> 66B 0.16481
55B -> 66B 0.55417
56B -> 66B 0.61455
57B -> 66B -0.13966
61B -> 66B -0.18492
64B -> 66B -0.12045
Excited State 19: 2.151-A 5.9710 eV 207.64 nm f=0.0018 <S**2>=0.906
41B -> 66B 0.26294
42B -> 66B 0.24036
45B -> 66B 0.33961
46B -> 66B -0.28339
50B -> 66B 0.27153
51B -> 66B -0.10625
52B -> 66B 0.30699
53B -> 66B 0.43632
54B -> 66B -0.36982
59B -> 66B 0.14373
62B -> 67B 0.14822
65B -> 67B -0.11373
Excited State 20: 2.207-A 6.1384 eV 201.98 nm f=0.0023 <S**2>=0.967
61A -> 67A 0.10155
40B -> 66B -0.29064
43B -> 66B 0.47438
44B -> 66B -0.34797
45B -> 66B 0.21840
46B -> 66B -0.20010
50B -> 66B -0.30662
51B -> 66B 0.12750
52B -> 66B -0.40828
53B -> 66B 0.24077

62B -> 67B	-0.11735

3'rc(S_1)					
Excited State 1: 2.037-A	1.2612 eV	983.04 nm	f=0.0048	<S**2>=0.788
61B -> 66B	-0.37552			
62B -> 66B	-0.59218			
63B -> 66B	-0.27225			
65B -> 66B	0.62854			
Excited State 2: 2.053-A	2.5370 eV	488.70 nm	f=0.0033	<S**2>=0.804
53B -> 66B	-0.10949			
56B -> 66B	0.14036			
60B -> 66B	0.17586			
61B -> 66B	0.69199			
63B -> 66B	0.33847			
64B -> 66B	0.12450			
65B -> 66B	0.51300			
Excited State 3: 2.045-A	2.6908 eV	460.78 nm	f=0.0034	<S**2>=0.795
53B -> 66B	-0.16022			
54B -> 66B	0.13841			
60B -> 66B	0.28493			
61B -> 66B	-0.20303			
62B -> 66B	-0.28924			
63B -> 66B	0.17091			
64B -> 66B	0.78941			
65B -> 66B	-0.23405			
Excited State 4: 2.061-A	3.1589 eV	392.50 nm	f=0.0139	<S**2>=0.812
54B -> 66B	0.11661			
55B -> 66B	0.12316			
56B -> 66B	-0.34150			
61B -> 66B	-0.27441			
62B -> 66B	-0.11823			
63B -> 66B	0.79912			
64B -> 66B	-0.27371			
Excited State 5: 2.042-A	3.2857 eV	377.35 nm	f=0.0014	<S**2>=0.793
51B -> 66B	-0.10045			
57B -> 66B	-0.10179			
60B -> 66B	-0.11972			
61B -> 66B	-0.33874			
62B -> 66B	0.67159			
64B -> 66B	0.35438			
65B -> 66B	0.49016			
Excited State 6: 2.185-A	3.4940 eV	354.85 nm	f=0.0426	<S**2>=0.943
61A -> 68A	0.14687			
62A -> 68A	0.18217			
63A -> 67A	-0.17879			

66A -> 67A	-0.13059	
66A -> 68A	-0.11756	
49B -> 66B	0.11168	
54B -> 66B	-0.40072	
55B -> 66B	-0.44605	
56B -> 66B	0.47550	
57B -> 66B	0.21343	
61B -> 66B	-0.25605	
61B -> 67B	0.10751	
63B -> 66B	0.31725	
Excited State 7:	2.046-A	3.8489 eV 322.12 nm f=0.0001 <S**2>=0.797
49B -> 66B	-0.13763	
50B -> 66B	0.20956	
51B -> 66B	0.23093	
53B -> 66B	-0.34263	
54B -> 66B	0.27182	
55B -> 66B	-0.18459	
57B -> 66B	-0.23932	
58B -> 66B	0.13503	
59B -> 66B	-0.14284	
60B -> 66B	0.57512	
61B -> 66B	-0.16551	
62B -> 66B	0.23817	
64B -> 66B	-0.33481	
Excited State 8:	2.051-A	4.1493 eV 298.81 nm f=0.0003 <S**2>=0.802
49B -> 66B	0.10160	
50B -> 66B	-0.20862	
51B -> 66B	-0.22644	
53B -> 66B	0.57192	
54B -> 66B	-0.12918	
56B -> 66B	-0.12663	
57B -> 66B	0.15116	
58B -> 66B	0.23685	
59B -> 66B	0.12809	
60B -> 66B	0.62274	
Excited State 9:	2.068-A	4.2589 eV 291.12 nm f=0.0004 <S**2>=0.819
48B -> 66B	-0.14441	
49B -> 66B	0.11507	
51B -> 66B	0.20374	
53B -> 66B	-0.12608	
55B -> 66B	0.16445	
57B -> 66B	0.22916	
58B -> 66B	0.85351	
60B -> 66B	-0.20701	

Excited State 10:	2.048-A	4.4003 eV	281.76 nm	f=0.0007	<S**2>=0.799
47B -> 66B	0.14612				
48B -> 66B	-0.33461				
49B -> 66B	0.36365				
51B -> 66B	0.30559				
54B -> 66B	0.10859				
55B -> 66B	0.15705				
57B -> 66B	0.51448				
58B -> 66B	-0.32004				
59B -> 66B	-0.40031				
60B -> 66B	0.15133				
65B -> 66B	0.10725				
Excited State 11:	2.990-A	4.4385 eV	279.34 nm	f=0.0081	<S**2>=1.985
61A -> 68A	0.28855				
62A -> 68A	0.43726				
63A -> 67A	0.33434				
63A -> 68A	0.20722				
64A -> 67A	-0.19752				
66A -> 67A	0.36980				
66A -> 68A	-0.20514				
58B -> 66B	0.12781				
59B -> 66B	-0.18199				
61B -> 67B	0.20988				
62B -> 67B	0.27637				
63B -> 67B	0.12681				
65B -> 67B	-0.26481				
Excited State 12:	2.088-A	4.4654 eV	277.65 nm	f=0.0005	<S**2>=0.840
47B -> 66B	0.12215				
48B -> 66B	-0.18226				
50B -> 66B	0.15428				
51B -> 66B	0.17031				
57B -> 66B	0.17200				
58B -> 66B	-0.19185				
59B -> 66B	0.85732				
Excited State 13:	2.068-A	5.0359 eV	246.20 nm	f=0.0014	<S**2>=0.820
42B -> 66B	-0.15138				
47B -> 66B	-0.33117				
48B -> 66B	0.27144				
49B -> 66B	-0.37077				
51B -> 66B	-0.22820				
53B -> 66B	-0.26749				
54B -> 66B	0.17086				
57B -> 66B	0.65111				
Excited State 14:	2.873-A	5.1203 eV	242.14 nm	f=0.0042	<S**2>=1.814

```
61A -> 67A        0.33881
62A -> 67A        0.58344
63A -> 67A        0.25217
63A -> 68A       -0.31264
64A -> 68A        0.19241
66A -> 67A       -0.33498
66A -> 68A       -0.38109
62B -> 68B       -0.12323
65B -> 68B        0.11993
Excited State  15:  2.083-A      5.1302 eV  241.67 nm  f=0.0011  <S**2>=0.835
41B -> 66B        0.10736
42B -> 66B       -0.10400
43B -> 66B        0.22578
45B -> 66B        0.37641
46B -> 66B        0.50323
47B -> 66B        0.43739
50B -> 66B        0.22278
51B -> 66B       -0.27983
52B -> 66B       -0.20159
54B -> 66B        0.28220
55B -> 66B       -0.11613
Excited State  16:  2.331-A      5.2868 eV  234.52 nm  f=0.0623  <S**2>=1.108
61A -> 67A        0.10377
62A -> 67A        0.17429
63A -> 68A        0.35061
64A -> 68A       -0.19009
66A -> 67A       -0.16018
66A -> 68A        0.34215
42B -> 66B       -0.10244
45B -> 66B       -0.12381
53B -> 66B        0.25275
54B -> 66B        0.37815
55B -> 66B        0.15153
56B -> 66B        0.45129
61B -> 66B       -0.11162
61B -> 68B       -0.14105
62B -> 68B       -0.18825
65B -> 68B        0.17834
Excited State  17:  2.385-A      5.3379 eV  232.27 nm  f=0.0240  <S**2>=1.172
62A -> 67A       -0.13218
62A -> 68A       -0.14702
63A -> 67A        0.11709
63A -> 68A       -0.36842
64A -> 67A       -0.10574
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64A -> 68A 0.18340
66A -> 67A 0.31320
66A -> 68A -0.28368
53B -> 66B 0.18014
54B -> 66B 0.28481
55B -> 66B 0.12030
56B -> 66B 0.50002
61B -> 68B 0.13707
62B -> 68B 0.19720
65B -> 68B -0.19895
Excited State 18: 2.409-A 5.4462 eV 227.65 nm f=0.1498 <S**2>=1.201
62A -> 67A 0.18839
63A -> 67A 0.47459
63A -> 68A 0.10622
64A -> 67A -0.23160
66A -> 67A 0.38035
66A -> 68A 0.22436
42B -> 66B 0.14048
45B -> 66B 0.15333
54B -> 66B -0.32742
55B -> 66B -0.14789
56B -> 66B 0.18286
61B -> 67B -0.16202
62B -> 67B -0.23994
63B -> 67B -0.12210
65B -> 67B 0.25340
Excited State 19: 2.069-A 5.6420 eV 219.75 nm f=0.0043 <S**2>=0.820
45B -> 66B 0.25819
49B -> 66B -0.12940
51B -> 66B -0.12361
53B -> 66B -0.25253
54B -> 66B -0.34425
55B -> 66B 0.72058
56B -> 66B 0.26557
60B -> 66B 0.17286
Excited State 20: 2.126-A 5.9459 eV 208.52 nm f=0.0003 <S**2>=0.880
40B -> 66B 0.19836
41B -> 66B -0.30164
42B -> 66B 0.19691
43B -> 66B 0.48693
44B -> 66B 0.19552
49B -> 66B -0.42957
50B -> 66B 0.23779
51B -> 66B 0.31633

52B -> 66B	0.12039
53B -> 66B	0.31043
53B -> 67B	-0.12340
54B -> 66B	-0.10424

Table S4. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of **3**, **3'**, **TS**, and **4** in hartree computed at the PCM(water)/(TD-)ωB97XD/6-311++G(d,p) level of theory.

compound	***E***	***ZPVE***	***H***	***G***
3(S_0)	-772.200043	0.336145	-771.849724	-771.902342
3(S_1)	-772.024240	0.330859	-771.678357	-771.732814
3'(S_0)	-772.188675	0.335160	-771.838757	-771.892762
3'(S_1)	-772.013289	0.329769	-771.668068	-771.723800
TS(S_0)	-772.151188	0.332666	-771.804330	-771.857011
TS(S_1) s.p.	-772.034317	n.a.	n.a.	n.a.
4(S_0)	-695.722207	0.306650	-695.402073	-695.454941
4(S_1)	-695.620555	0.303339	-695.303578	-695.356520

Table S5. Conical intersection optimization scan for **4(S_0)** formation in hartree computed at the (TD-)ωB97X/6-311++G(d,p) level of theory using ORCA 4.2.0.

	Geometry convergence		
Item	Value	Tolerance	Converged
Energy change	0.0125993207	0.0000050000	NO
E diff. (CI)	0.0053210067	0.0001000000	NO 3.3 kcal mol^{-1}
RMS gradient	0.0069959798	0.0001000000	NO
MAX gradient	0.0535645244	0.0003000000	NO
RMS step	0.0188608384	0.0020000000	NO
MAX step	0.2071330471	0.0040000000	NO
Max(Bonds)	0.0478	Max(Angles)	3.30
Max(Dihed)	11.87	Max(Improp)	0.00

Coordinates (S_0)			
6	-2.619962000	0.936194000	-1.541115000
6	-3.353689000	0.334400000	-0.337393000
6	-2.334823000	-0.236073000	0.655523000
6	-1.516082000	-1.334427000	-0.035649000
6	-0.751072000	-0.720567000	-1.229701000
6	-1.773569000	-0.143109000	-2.223765000
6	-1.693317000	2.055895000	-1.060384000
6	-1.397629000	0.885734000	1.125734000
6	0.163352000	0.373857000	-0.713762000
6	-0.642371000	1.494680000	-0.082754000
8	1.912303000	3.418723000	-3.133119000
6	1.536491000	0.057559000	-0.380632000
6	1.913592000	-1.306688000	-0.226545000
6	3.115048000	-1.698651000	0.338602000
6	4.036883000	-0.742457000	0.761624000
6	3.756777000	0.599562000	0.535724000
6	2.578311000	0.996823000	-0.076826000
8	2.483042000	2.346581000	-0.349619000
1	-3.350930000	1.336829000	-2.255212000
1	-3.965027000	1.102304000	0.153733000
1	-4.037066000	-0.455346000	-0.672651000
1	-2.860140000	-0.659268000	1.519704000
1	-2.176972000	-2.137610000	-0.390416000
1	-0.808706000	-1.780962000	0.673152000
1	-0.178473000	-1.497579000	-1.741647000
1	-1.252007000	0.273367000	-3.092330000
1	-2.418925000	-0.951197000	-2.591704000
1	-1.208020000	2.517524000	-1.913648000
1	-2.278430000	2.835661000	-0.553734000
1	-1.975161000	1.674408000	1.629974000
1	-0.673805000	0.500594000	1.852362000
1	-0.002241000	2.286133000	0.287064000
1	1.993128000	4.223809000	-3.631316000
1	1.194741000	-2.075513000	-0.488370000
1	3.324261000	-2.756808000	0.471251000
1	4.971934000	-1.035870000	1.225745000
1	4.477713000	1.370579000	0.786131000
1	2.311124000	2.516069000	-1.254736000

Table S6. Geometries of **3**, **3'**, **TS**, and **4** in Cartesian coordinates in Å computed at the PCM(water)/(TD-)ωB97XD/6-311++G(d,p) level of theory.

3(S_0)			
6	3.022032000	0.554475000	0.215546000
6	3.313150000	-0.645124000	-0.695941000
6	1.997613000	-1.363718000	-1.021863000
6	1.341297000	-1.839709000	0.277351000
6	1.010649000	-0.628990000	1.176939000
6	2.342791000	0.073405000	1.508367000

6	2.088489000	1.522285000	-0.522893000
6	1.028666000	-0.405984000	-1.727214000
6	0.069685000	0.387018000	0.480485000
6	0.757903000	0.820101000	-0.842180000
8	-0.016505000	1.592541000	1.283490000
6	-1.374823000	-0.075507000	0.258922000
6	-1.838865000	-1.358724000	0.549549000
6	-3.147810000	-1.750260000	0.289752000
6	-4.038234000	-0.840218000	-0.265522000
6	-3.628625000	0.463683000	-0.503528000
6	-2.323232000	0.853939000	-0.217648000
8	-2.022904000	2.168633000	-0.401904000
1	3.957199000	1.064875000	0.466001000
1	3.797850000	-0.305363000	-1.618444000
1	4.002266000	-1.339285000	-0.201507000
1	2.194939000	-2.225945000	-1.666078000
1	2.022506000	-2.498181000	0.827124000
1	0.459251000	-2.431816000	0.033633000
1	0.538474000	-0.971804000	2.104950000
1	2.175821000	0.916763000	2.181477000
1	2.992784000	-0.637491000	2.029832000
1	1.910463000	2.416208000	0.077956000
1	2.551410000	1.844142000	-1.462453000
1	1.453802000	-0.066140000	-2.677415000
1	0.091591000	-0.923438000	-1.959861000
1	0.104372000	1.509327000	-1.380653000
1	-0.400014000	1.359358000	2.134106000
1	-1.171496000	-2.081135000	0.997505000
1	-3.464233000	-2.760375000	0.521781000
1	-5.058469000	-1.133029000	-0.487063000
1	-4.317989000	1.207592000	-0.886624000
1	-1.249373000	2.366306000	0.152326000

3(S_1)			
6	3.031351000	0.505052000	-0.012337000
6	3.197768000	-0.827434000	-0.756111000
6	1.832315000	-1.518081000	-0.874611000
6	1.266796000	-1.772357000	0.526982000
6	1.072070000	-0.433212000	1.267161000
6	2.446659000	0.250272000	1.386145000
6	2.075554000	1.404043000	-0.807195000
6	0.853040000	-0.619974000	-1.643853000
6	0.101144000	0.488666000	0.496716000
6	0.700093000	0.725832000	-0.919726000
8	0.089431000	1.832896000	1.109599000
6	-1.328180000	0.020469000	0.463808000
6	-1.856390000	-1.197863000	0.957699000
6	-3.053520000	-1.712780000	0.428225000
6	-3.839939000	-1.004314000	-0.520120000
6	-3.532314000	0.358757000	-0.717400000
6	-2.314264000	0.857398000	-0.212717000

8	-2.111220000	2.164701000	-0.289804000
1	4.003595000	0.998073000	0.085047000
1	3.619319000	-0.649576000	-1.752174000
1	3.896991000	-1.476984000	-0.217118000
1	1.943247000	-2.471730000	-1.399853000
1	1.959819000	-2.391584000	1.107088000
1	0.330190000	-2.326401000	0.447690000
1	0.666631000	-0.617425000	2.268763000
1	2.361901000	1.191029000	1.935196000
1	3.114845000	-0.402760000	1.958029000
1	1.979161000	2.379720000	-0.327133000
1	2.471354000	1.570516000	-1.815801000
1	1.222501000	-0.438004000	-2.658604000
1	-0.120046000	-1.114800000	-1.734375000
1	0.023886000	1.369344000	-1.490123000
1	-0.215525000	1.727676000	2.017498000
1	-1.321097000	-1.783216000	1.694825000
1	-3.391897000	-2.687658000	0.768261000
1	-4.754205000	-1.433889000	-0.906232000
1	-4.250921000	1.064620000	-1.120281000
1	-1.278530000	2.365422000	0.204937000

3'(S_0)			
6	-3.095590000	-0.271846000	0.373440000
6	-3.217436000	0.321386000	-1.036577000
6	-1.815760000	0.597791000	-1.597765000
6	-1.076848000	1.587822000	-0.688163000
6	-0.936867000	0.980263000	0.722257000
6	-2.346478000	0.708043000	1.280278000
6	-2.295917000	-1.576253000	0.314937000
6	-1.012342000	-0.707969000	-1.654335000
6	-0.104697000	-0.333936000	0.679499000
6	-0.890362000	-1.305473000	-0.244378000
8	-0.094745000	-0.942274000	1.979397000
6	1.374977000	-0.209047000	0.230977000
6	2.041567000	-1.417171000	-0.038649000
6	3.369047000	-1.493098000	-0.418378000
6	4.108627000	-0.319567000	-0.537332000
6	3.505626000	0.885984000	-0.243281000
6	2.165380000	0.952374000	0.157600000
8	1.761965000	2.220268000	0.455157000
1	-4.091838000	-0.463424000	0.783601000
1	-3.752141000	-0.375180000	-1.692238000
1	-3.797430000	1.250795000	-1.005510000
1	-1.896110000	1.024093000	-2.602074000
1	-1.631687000	2.529172000	-0.617893000
1	-0.104054000	1.821738000	-1.128869000
1	-0.485650000	1.685953000	1.432745000
1	-2.275378000	0.308261000	2.294084000
1	-2.883377000	1.660972000	1.338364000
1	-2.226189000	-2.024500000	1.308665000

1	-2.796900000	-2.299726000	-0.337902000
1	-1.513622000	-1.431607000	-2.305627000
1	-0.020308000	-0.523063000	-2.079236000
1	-0.361740000	-2.257220000	-0.296960000
1	0.479483000	-0.423272000	2.547857000
1	1.493653000	-2.344170000	0.066612000
1	3.821616000	-2.457451000	-0.616806000
1	5.148687000	-0.345629000	-0.842103000
1	4.058246000	1.816861000	-0.300506000
1	0.859421000	2.227630000	0.776595000

3'(S_1)			
6	-3.039237000	-0.139118000	0.074436000
6	-2.882258000	0.158536000	-1.423278000
6	-1.391258000	0.291498000	-1.764789000
6	-0.777232000	1.432622000	-0.945380000
6	-0.918984000	1.132095000	0.556707000
6	-2.413916000	0.997700000	0.893941000
6	-2.316224000	-1.449396000	0.411494000
6	-0.661195000	-1.013601000	-1.418194000
6	-0.177975000	-0.181253000	0.921335000
6	-0.822592000	-1.317999000	0.078121000
8	-0.430266000	-0.538070000	2.298084000
6	1.332950000	-0.137672000	0.738170000
6	2.075892000	-1.360304000	0.750827000
6	3.009723000	-1.585276000	-0.256645000
6	3.443834000	-0.548750000	-1.132933000
6	3.074007000	0.762866000	-0.830050000
6	2.102090000	0.967467000	0.158031000
8	2.034873000	2.198260000	0.679542000
1	-4.101083000	-0.228327000	0.324589000
1	-3.332106000	-0.647071000	-2.015047000
1	-3.408379000	1.085069000	-1.680643000
1	-1.273018000	0.506628000	-2.831303000
1	-1.283402000	2.378315000	-1.168079000
1	0.270939000	1.565300000	-1.234236000
1	-0.519132000	1.964278000	1.146970000
1	-2.540352000	0.807080000	1.962292000
1	-2.912962000	1.946015000	0.665689000
1	-2.448713000	-1.696562000	1.467300000
1	-2.739293000	-2.273591000	-0.175004000
1	-1.076876000	-1.843587000	-1.999820000
1	0.399656000	-0.933427000	-1.679124000
1	-0.306951000	-2.249683000	0.324268000
1	0.157289000	0.000753000	2.836621000
1	1.774575000	-2.178109000	1.395931000
1	3.409000000	-2.587098000	-0.390086000
1	4.185589000	-0.754991000	-1.893773000
1	3.645391000	1.613705000	-1.188053000
1	1.437221000	2.187292000	1.439752000

TS(S_0)			
6	-2.967272000	0.602205000	-0.258292000
6	-3.360304000	-0.626338000	0.573406000
6	-2.096892000	-1.415280000	0.942843000
6	-1.387047000	-1.873018000	-0.334266000
6	-0.959896000	-0.628733000	-1.167231000
6	-2.235042000	0.156288000	-1.530734000
6	-2.038921000	1.496688000	0.570132000
6	-1.137767000	-0.530206000	1.746991000
6	-0.038992000	0.187396000	-0.295698000
6	-0.753884000	0.731645000	0.922377000
8	0.121074000	1.939582000	-1.297437000
6	1.373459000	-0.118308000	-0.206931000
6	1.888673000	-1.354742000	-0.653217000
6	3.196322000	-1.715217000	-0.420655000
6	4.044349000	-0.813546000	0.249331000
6	3.605452000	0.434394000	0.621677000
6	2.274679000	0.863430000	0.347230000
8	1.914793000	2.085659000	0.497865000
1	-3.863923000	1.163319000	-0.536604000
1	-3.885788000	-0.311335000	1.481405000
1	-4.044306000	-1.265873000	0.004974000
1	-2.366449000	-2.292246000	1.538310000
1	-2.054734000	-2.476395000	-0.956576000
1	-0.526036000	-2.494435000	-0.080786000
1	-0.441935000	-0.947039000	-2.073658000
1	-1.982011000	1.020290000	-2.146992000
1	-2.877311000	-0.499388000	-2.127175000
1	-1.796141000	2.409501000	0.025667000
1	-2.531365000	1.787853000	1.503670000
1	-1.609075000	-0.188174000	2.673210000
1	-0.239201000	-1.089905000	2.023331000
1	-0.077990000	1.352483000	1.506018000
1	0.590089000	1.727100000	-2.111115000
1	1.236195000	-2.060446000	-1.152224000
1	3.562869000	-2.684183000	-0.736459000
1	5.071194000	-1.099924000	0.455031000
1	4.276521000	1.145304000	1.091941000
1	0.830961000	2.221638000	-0.627174000

4(S_0)			
6	2.581119000	-0.313743000	1.278099000
6	3.494395000	0.019886000	0.088506000
6	2.643828000	0.286424000	-1.163041000
6	1.803307000	-0.952127000	-1.485415000
6	0.881141000	-1.293869000	-0.289651000
6	1.747080000	-1.557395000	0.958918000
6	1.623294000	0.851554000	1.533545000
6	1.698357000	1.464797000	-0.906564000
6	-0.026857000	-0.107877000	-0.058586000
6	0.765211000	1.131425000	0.278660000

6	-1.396181000	-0.169954000	-0.133585000
6	-2.082209000	-1.451941000	-0.229508000
6	-3.415710000	-1.576570000	-0.067960000
6	-4.221741000	-0.414934000	0.198980000
6	-3.677798000	0.819858000	0.234060000
6	-2.262446000	1.045484000	-0.045975000
8	-1.855445000	2.194721000	-0.239630000
1	3.187464000	-0.496954000	2.170111000
1	4.102465000	0.901065000	0.320917000
1	4.183555000	-0.811117000	-0.098317000
1	3.295624000	0.516357000	-2.011128000
1	2.446177000	-1.816766000	-1.680588000
1	1.201070000	-0.782681000	-2.383961000
1	0.325851000	-2.195625000	-0.533430000
1	1.107543000	-1.817593000	1.808642000
1	2.393662000	-2.418268000	0.759399000
1	0.973759000	0.631339000	2.387288000
1	2.179399000	1.763551000	1.775123000
1	2.264895000	2.369229000	-0.661287000
1	1.105111000	1.681478000	-1.800783000
1	0.103348000	1.969173000	0.463374000
1	-1.500323000	-2.348169000	-0.392562000
1	-3.885948000	-2.551137000	-0.116213000
1	-5.287016000	-0.541855000	0.363397000
1	-4.281809000	1.704103000	0.404166000

4(S_1)			
6	2.501209000	-0.799054000	1.085320000
6	3.485442000	-0.087762000	0.145069000
6	2.705573000	0.663548000	-0.944414000
6	1.857008000	-0.328205000	-1.748160000
6	0.855194000	-1.039236000	-0.808065000
6	1.660884000	-1.800366000	0.287922000
6	1.576786000	0.231572000	1.744938000
6	1.783290000	1.698516000	-0.293741000
6	0.001579000	-0.032506000	-0.108862000
6	0.776180000	0.990607000	0.642559000
6	-1.416537000	-0.157429000	-0.054520000
6	-2.032200000	-1.400149000	0.000261000
6	-3.438158000	-1.560666000	0.004653000
6	-4.260964000	-0.447979000	0.003847000
6	-3.694404000	0.828218000	-0.003341000
6	-2.284956000	1.050334000	-0.008129000
8	-1.790204000	2.204484000	-0.001181000
1	3.055380000	-1.332828000	1.864113000
1	4.104158000	0.614614000	0.713994000
1	4.159697000	-0.819486000	-0.313145000
1	3.406382000	1.167888000	-1.616771000
1	2.492721000	-1.083536000	-2.221981000
1	1.311290000	0.189620000	-2.542865000
1	0.245385000	-1.739070000	-1.381937000

1	0.975241000	-2.339898000	0.948637000
1	2.300398000	-2.541747000	-0.203804000
1	0.883729000	-0.258452000	2.435504000
1	2.156599000	0.962895000	2.318021000
1	2.366554000	2.415626000	0.294228000
1	1.236273000	2.261212000	-1.055839000
1	0.106985000	1.713658000	1.106639000
1	-1.416497000	-2.290577000	0.067608000
1	-3.856151000	-2.560087000	-0.000416000
1	-5.338644000	-0.561519000	0.000101000
1	-4.323422000	1.709139000	-0.074671000

[1] K. Ekvall, P. van der Meulen, C. Dhollande, L.-E. Berg, S. Pommeret, R. Naskrecki, J.-C. Mialocq, *J. Appl. Phys.* 2000, **87**, 2340-2352.