Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Manipulating Triplet States: Tuning Energies, Absorption, Lifetimes, and Annihilation Rates in Anthanthrene Derivatives

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List of Figures and Tables

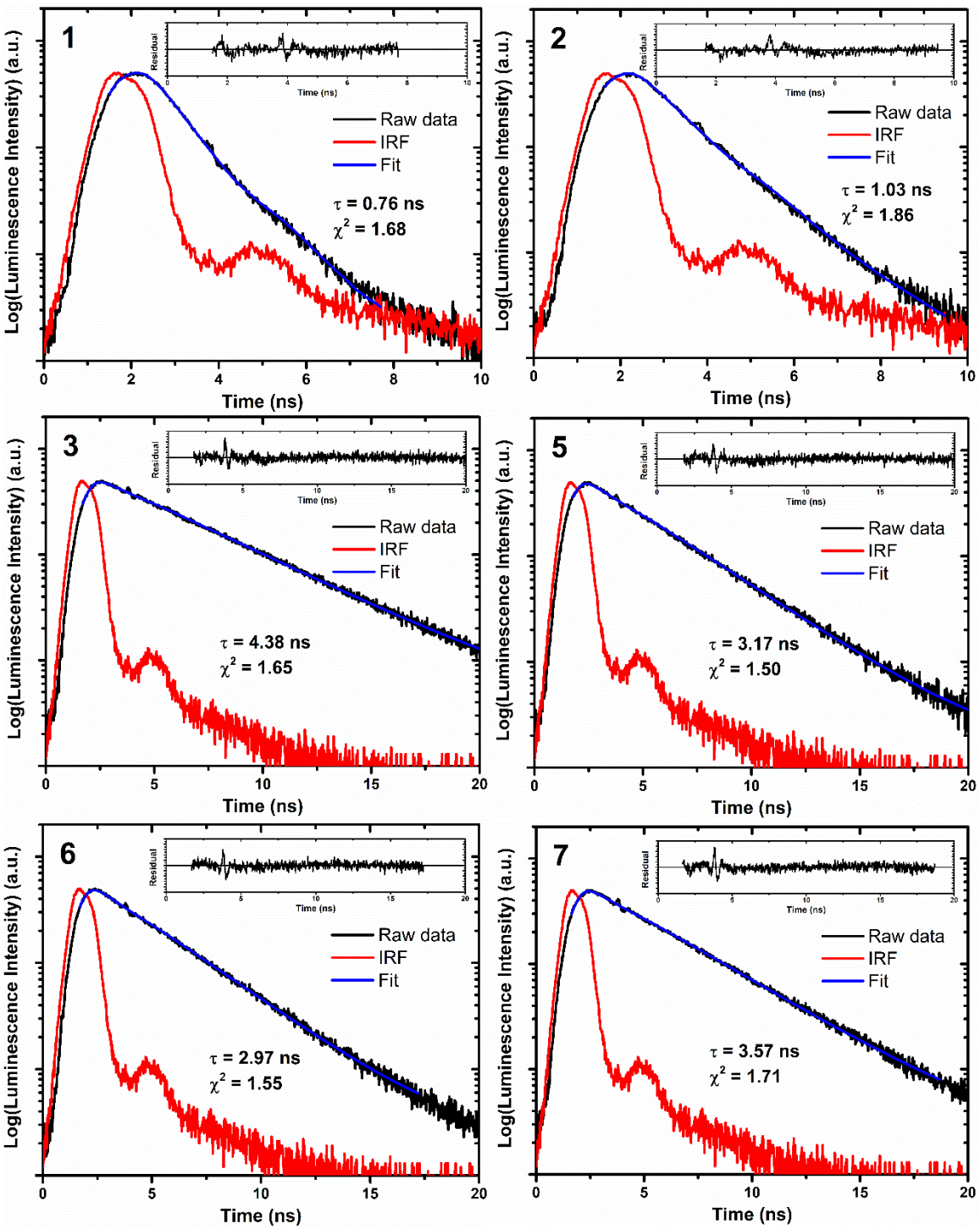

Figure S1. Time-resolved fluorescence decays of **1**-**3** and **5**-**7** in deaerated toluene. λ_{ex} = 404 nm, λ_{det} = fluorescence maximum (see Table 1). Raw data (black), instrument response function (IRF, red), and exponential fit (blue) are shown. Inset: residual as a function of time.

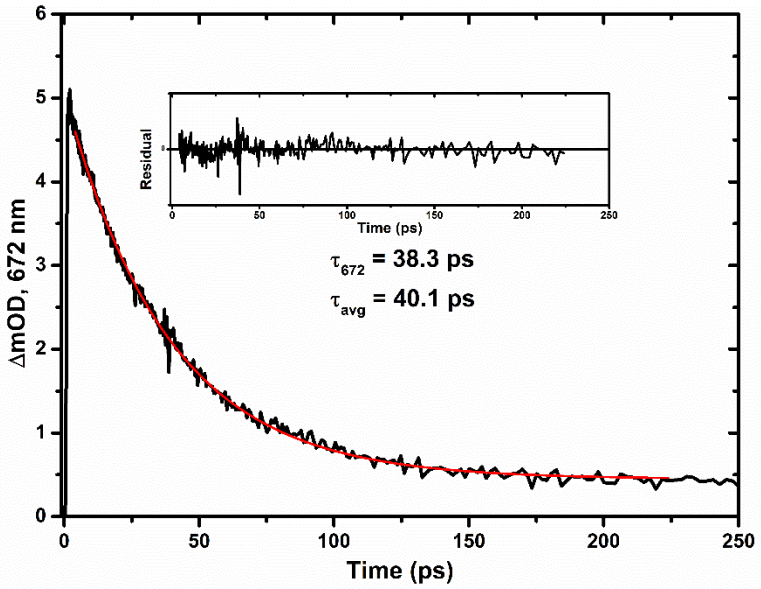

Figure S2. Transient absorption decay of **4** in aerated toluene monitored at 672 nm fit to a single exponential decay (red line). λ_{ex} = 400 nm. Inset: residual as a function of time. τ_{672} is the observed lifetime at 672 nm, while τ_{avg} is the average lifetime of seven different individual wavelength fits ranging from 639 – 701 nm.

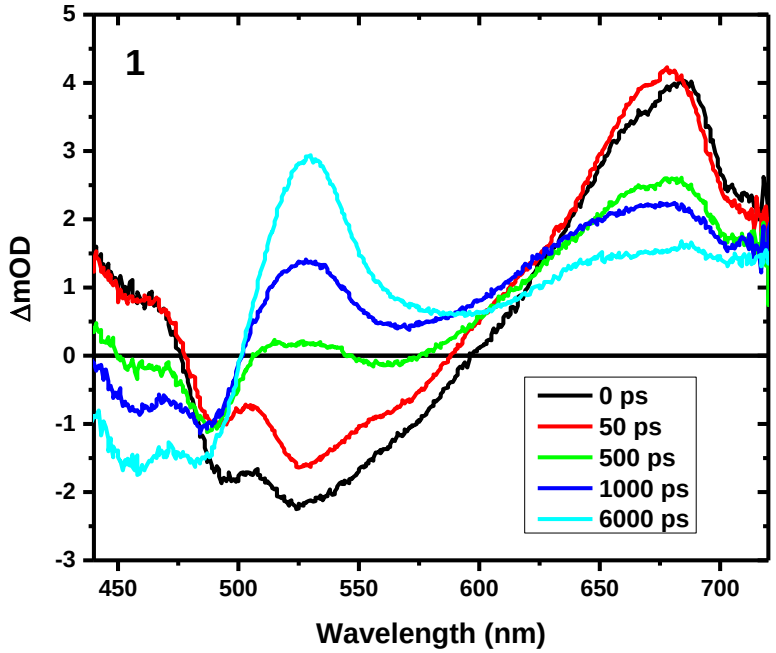

Figure S3. Ultrafast transient absorption difference spectra of **1** in toluene, λ_{ex} = 400 nm

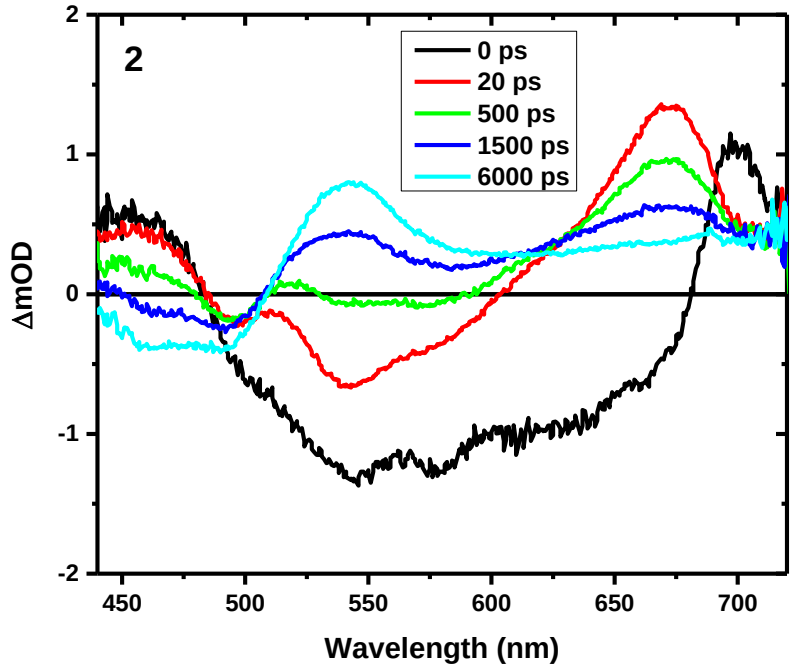

Figure S4. Ultrafast transient absorption difference spectra of **2** in toluene, λ_{ex} = 400 nm

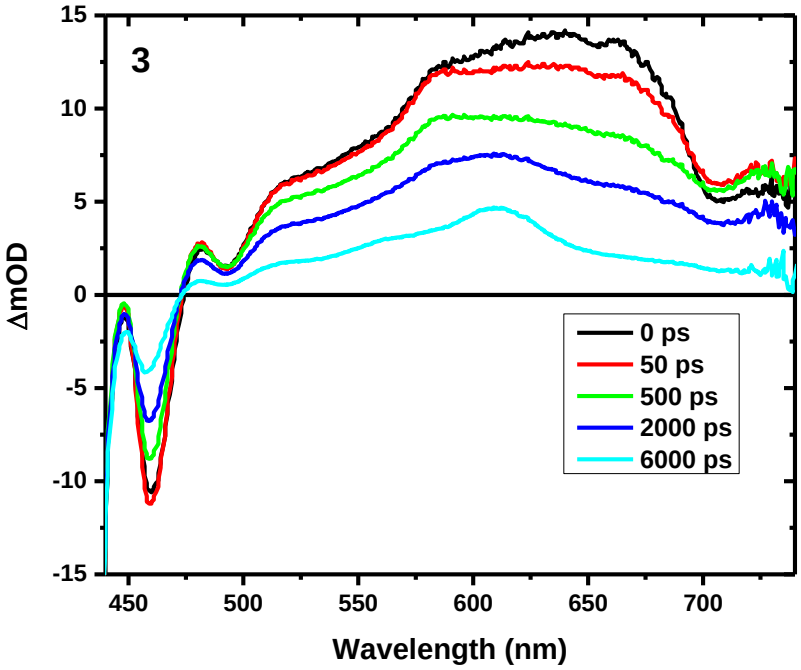

Figure S5. Ultrafast transient absorption difference spectra of **3** in toluene, λ_{ex} = 400 nm

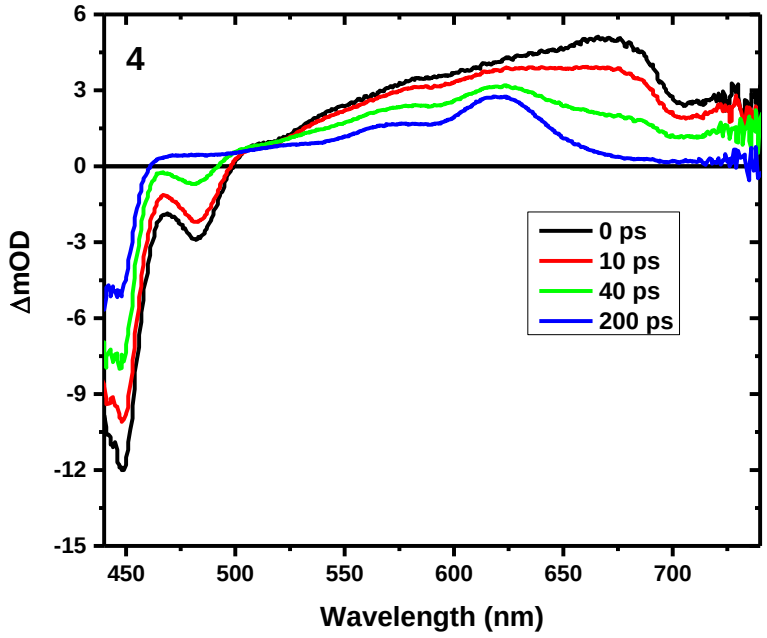

Figure S6. Ultrafast transient absorption difference spectra of **4** in toluene, λ_{ex} = 400 nm

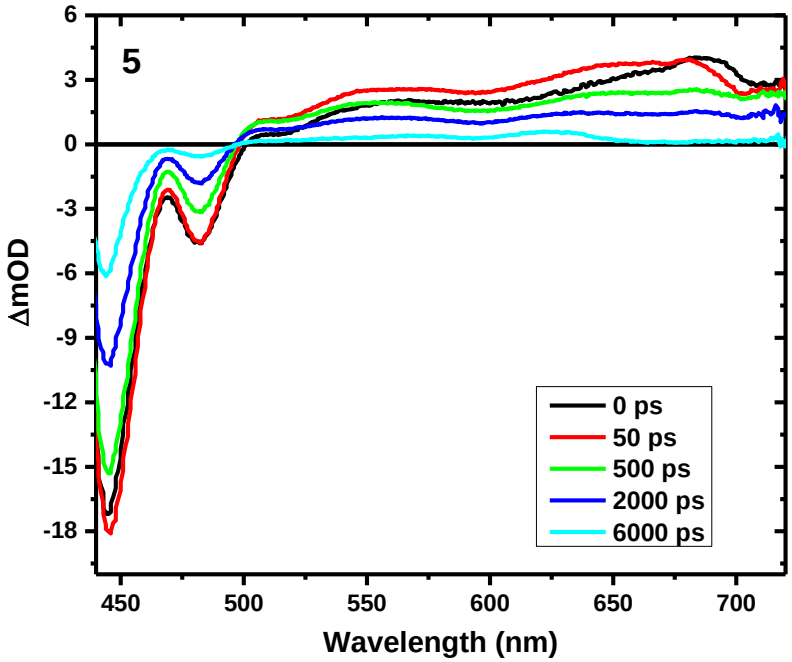

Figure S7. Ultrafast transient absorption difference spectra of **5** in toluene, λ_{ex} = 400 nm

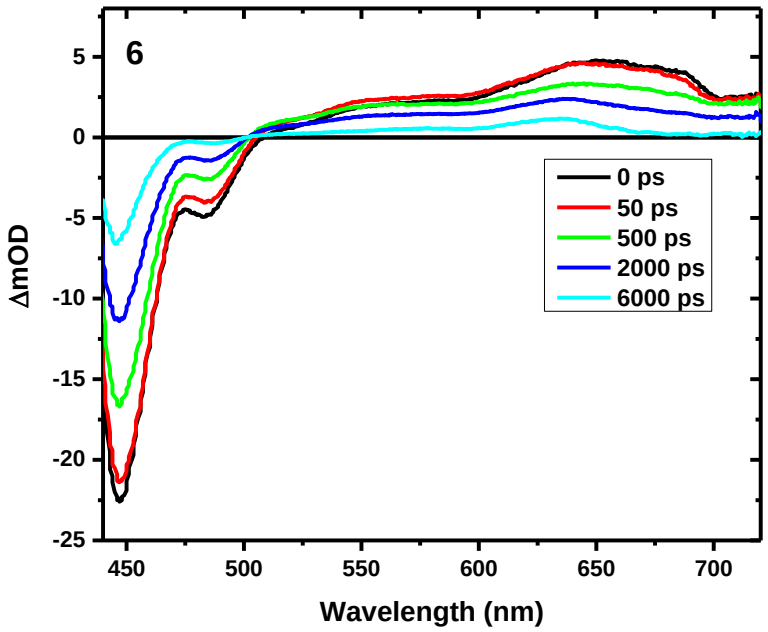

Figure S8. Ultrafast transient absorption difference spectra of **6** in toluene, λ_{ex} = 400 nm

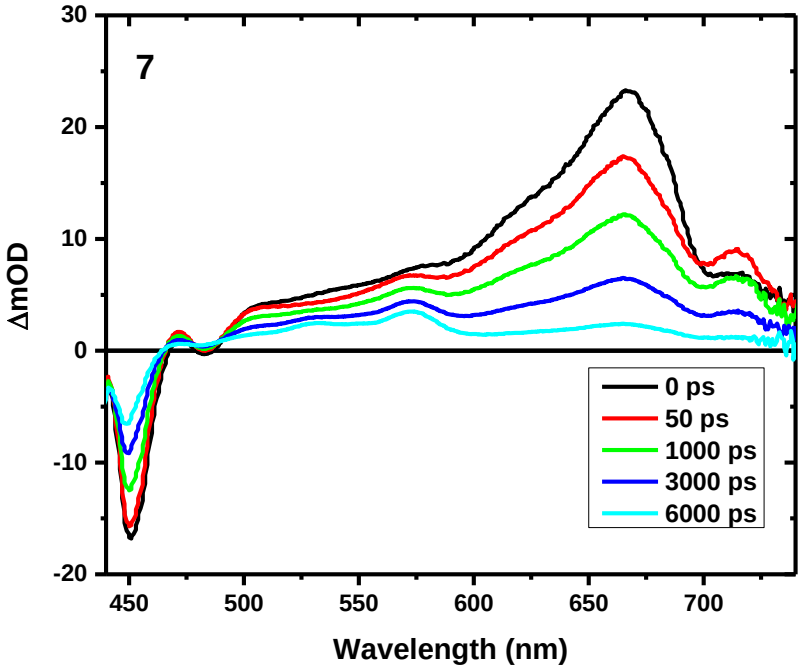

Figure S9. Ultrafast transient absorption difference spectra of **7** in toluene, λ_{ex} = 400 nm

Table S1. Ultrafast transient absorption properties in toluene.

Compound	λ_{max}/nm, t = 0	λ_{max}/nm, t = long[a]	τ_1/ps	τ_2/ps
1	684	529	4.17(2.49)	821(122)
2	684	529	5.43(2.05)	1090(10)
3	639	609	71.3(5.5)	4130(150)
4	669	619	40.1(3.6)	---
5	684	623	128(26)	3190(350)
6	652	635	262(75)	3290(260)
7	667	573	20.9(0.9)	3030(30)

[a]Taken from the longest time trace for each compound in Figures S3 – S9.

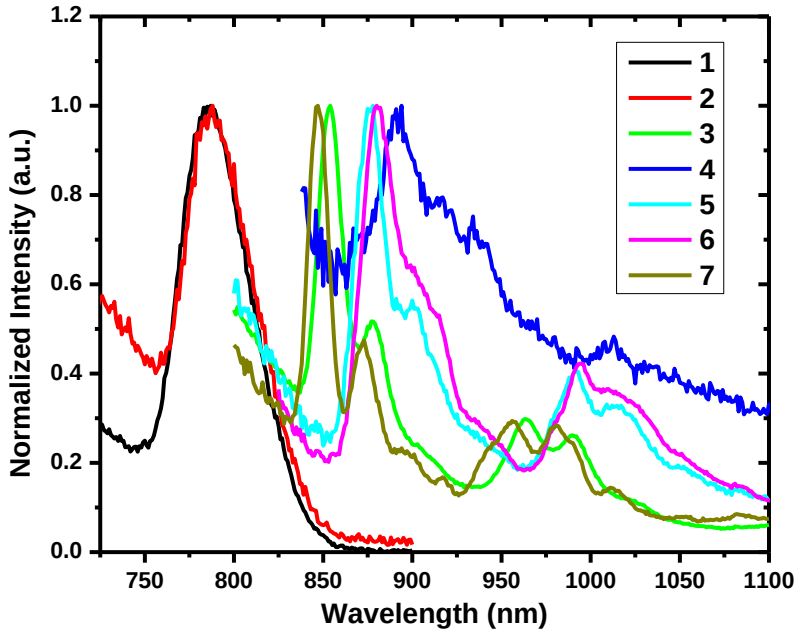

Figure S10. Phosphorescence spectra at 77 K in 2:2:1:1 diethyl ether:iodoethane:ethanol:toluene. λ_{ex} (nm): **1** (500), **2** (500), **3** (423), **4** (459), **5** (454), **6** (459), **7** (409). **1** and **2** were collected on a Cary Eclipse fluorometer (see experimental section in manuscript) using gated delay detection from 100 µs to 5 ms with a 595 nm long-pass filter. **3** – **7** were collected with the NIR PMT from an Edinburgh Instruments FLS980 with a 643 nm long-pass filter.

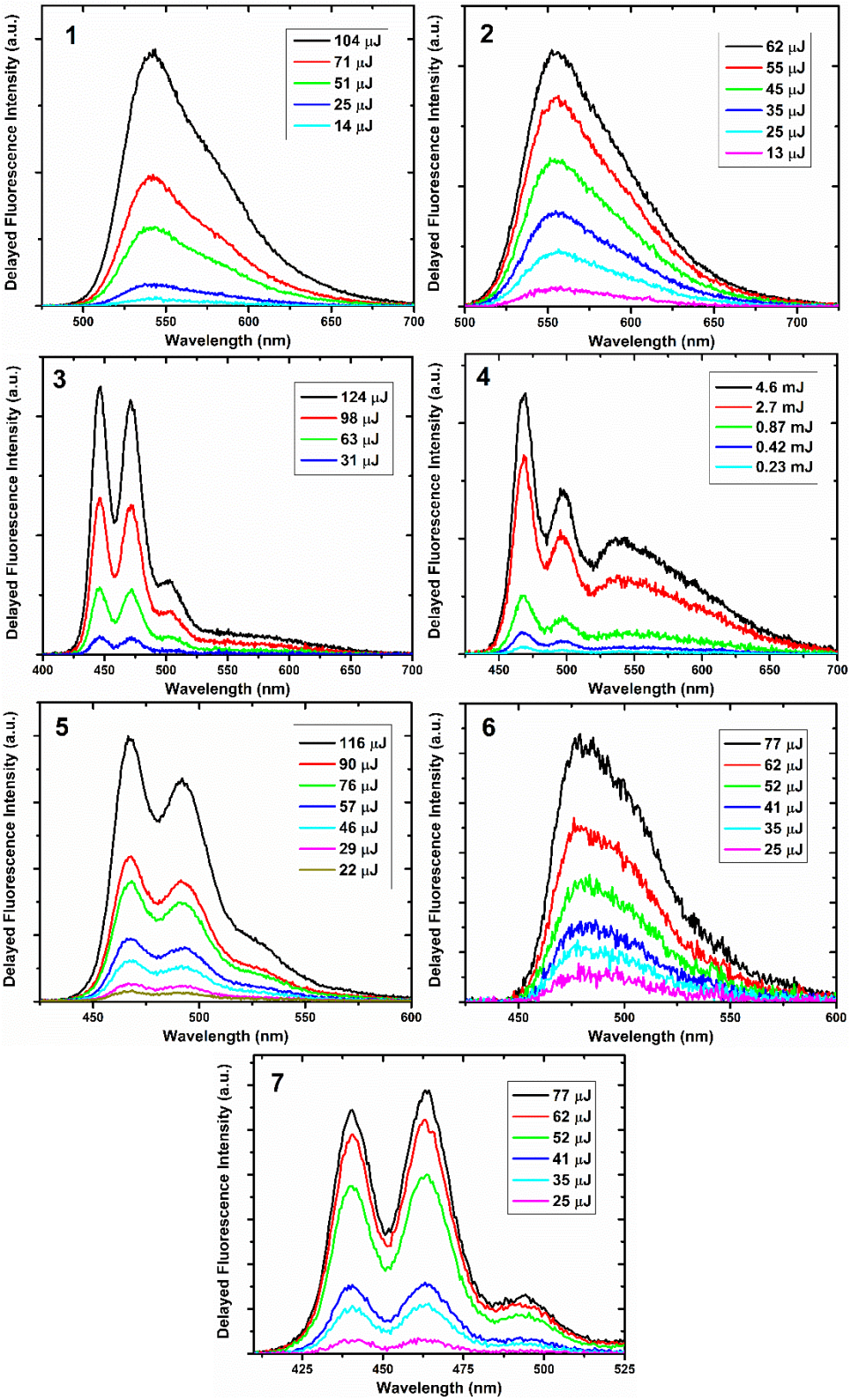

Figure S11. Delayed fluorescence spectra at 25 (**4**) or 50 (**1-3**, **5-7**) μs after excitation as a function of laser excitation energy. Gate widths were 49 (**4**) or 99 (**1-3**, **5-7**) μs. λ_{ex} = 478 nm (**1**,**2**), 422 nm (**3**), 442 nm (**4-6**), 418 nm (**7**)

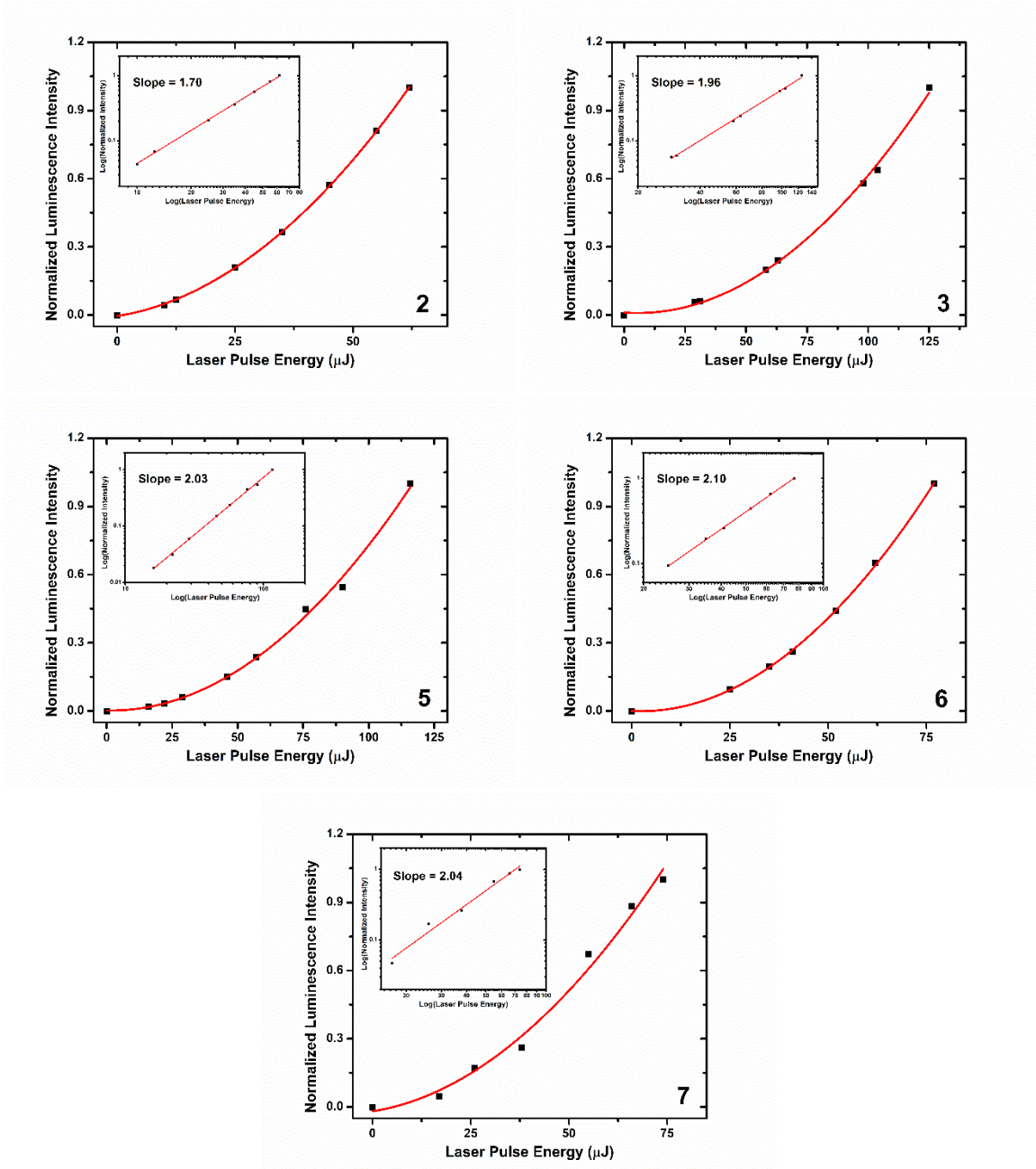

Figure S12. Normalized delayed integrated fluorescence intensity as a function of incident pulse energy in deaerated toluene. The data were integrated over the range shown in Figure S11 and normalized to the highest integrated intensity. The solid line is the best quadratic fit. Inset: double logarithm plot of the same data, with slopes listed.

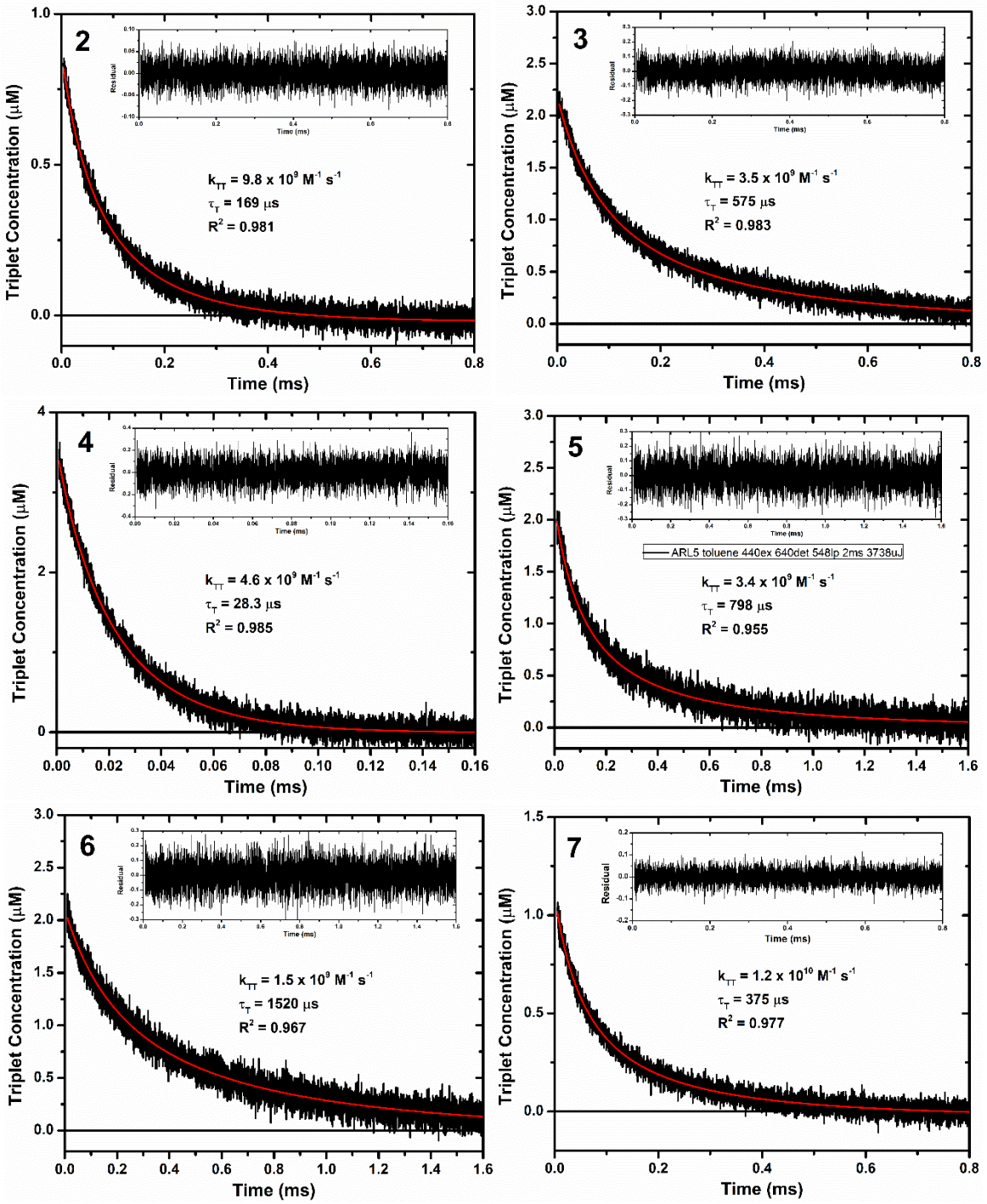

Figure S13. Triplet concentration as a function of time fit to eq 2. λ_{ex} = 468 (**2**), 422 (**3**), 442 (**4**), 440 (**5**), 442 (**6**), 418 (**7**); λ_{det} = 560 (**2**), 623 (**3**), 633 (**4**), 640 (**5**), 646 (**6**), 585 (**7**). Insets: residuals as a function of time.