



## Supporting Information

for

### Deep-blue emitting 9,10-bis(perfluorobenzyl)anthracene

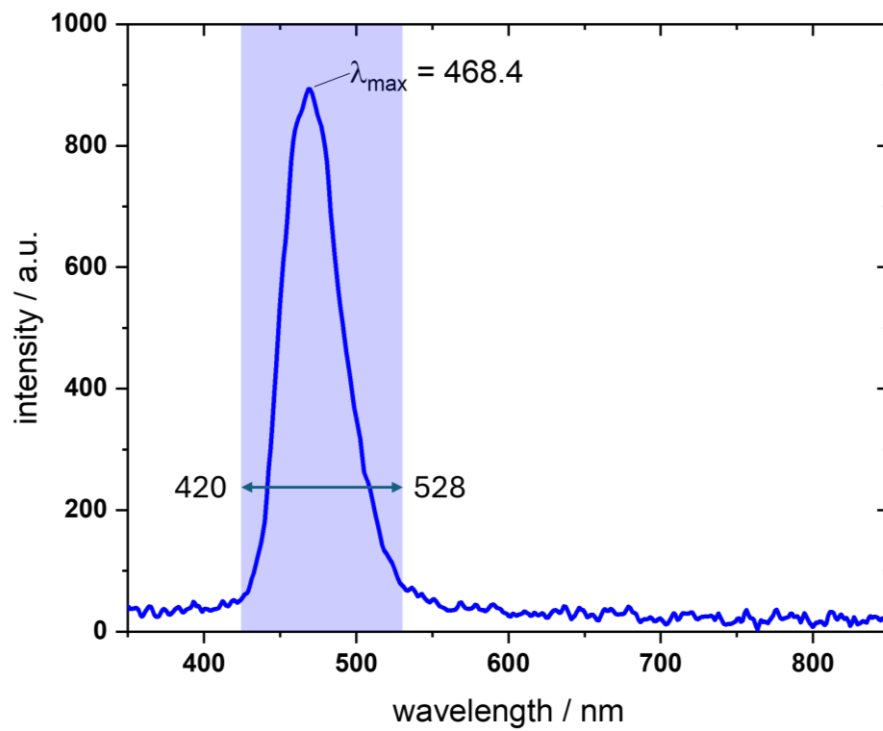
Long K. San, Sebastian Balser, Brian J. Reeves, Tyler T. Clikeman, Yu-Sheng Chen, Steven H. Strauss and Olga V. Boltalina

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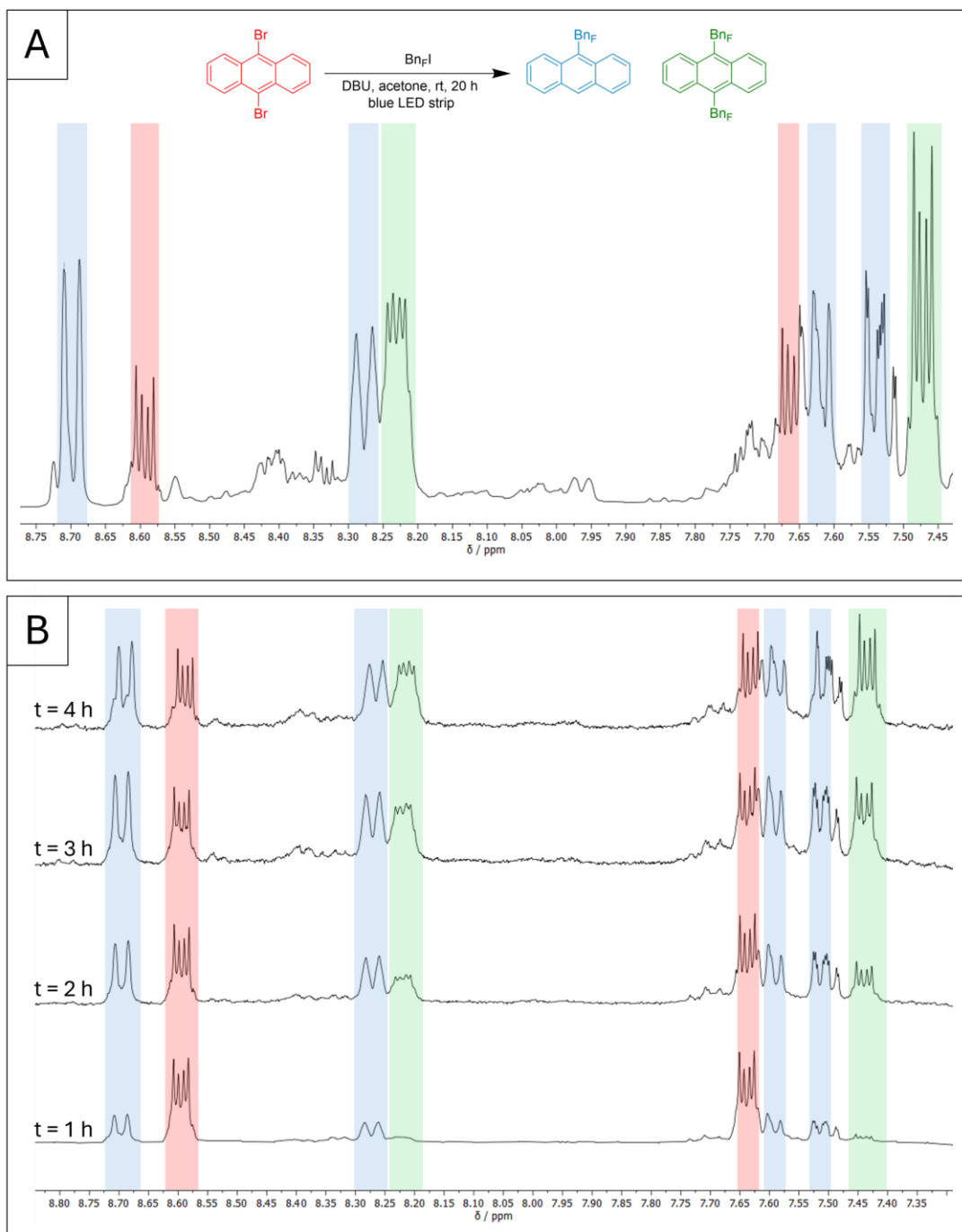
### Experimental details, spectroscopic data, and crystallographic data

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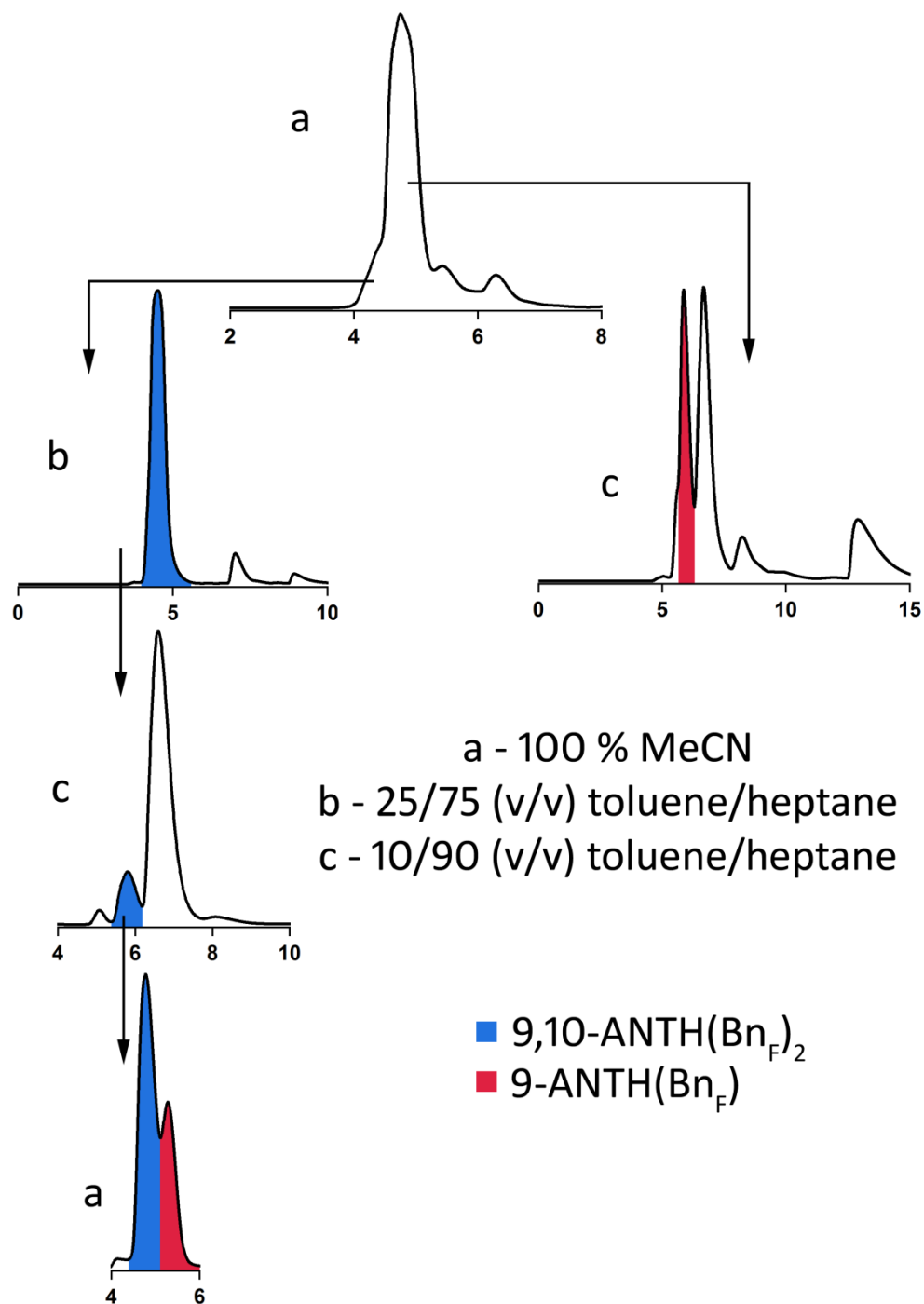
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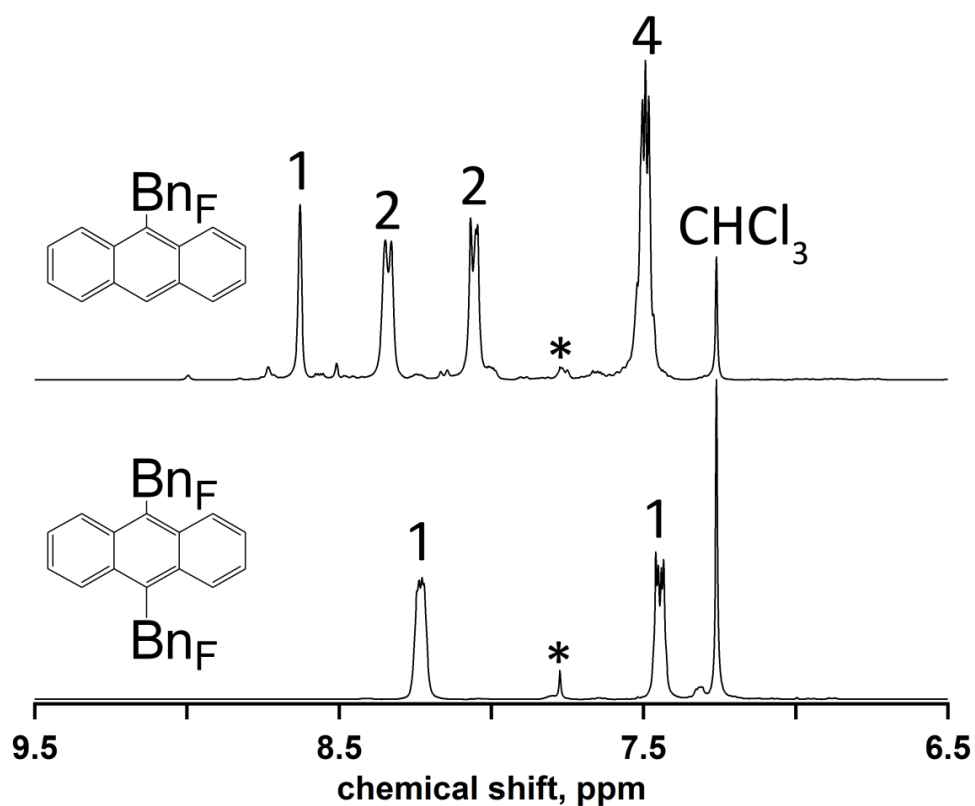
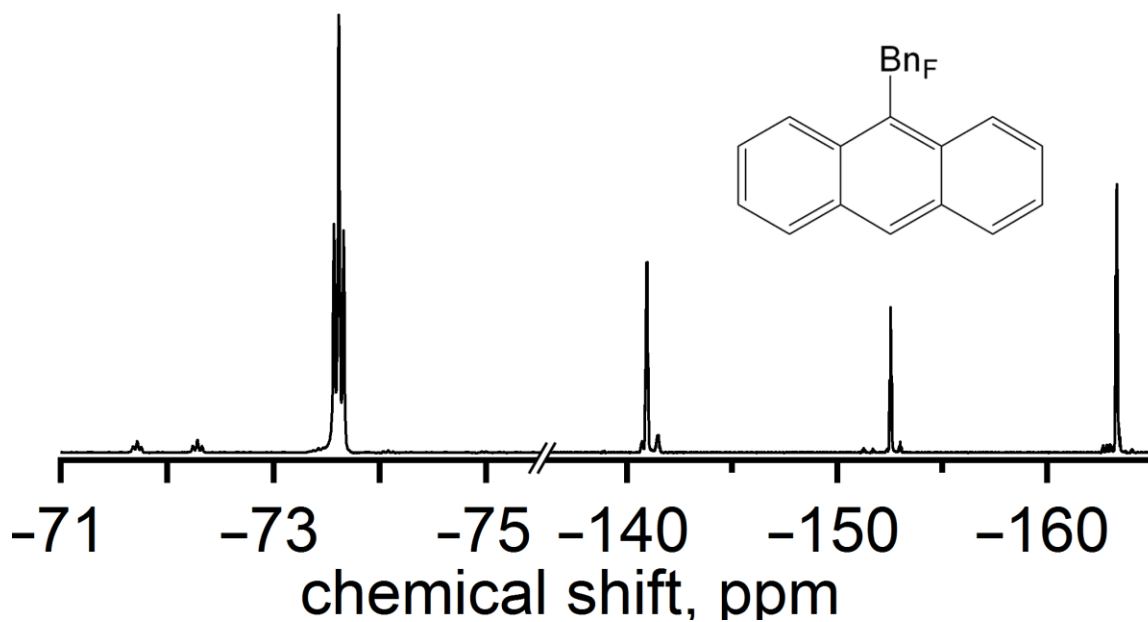
**Figure S1:** Emission spectrum of the blue LED strip (1.2 W, *Tenmiro*), used for the photochemical conversion of 9,10-ANTH(Br)<sub>2</sub> to 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub>.



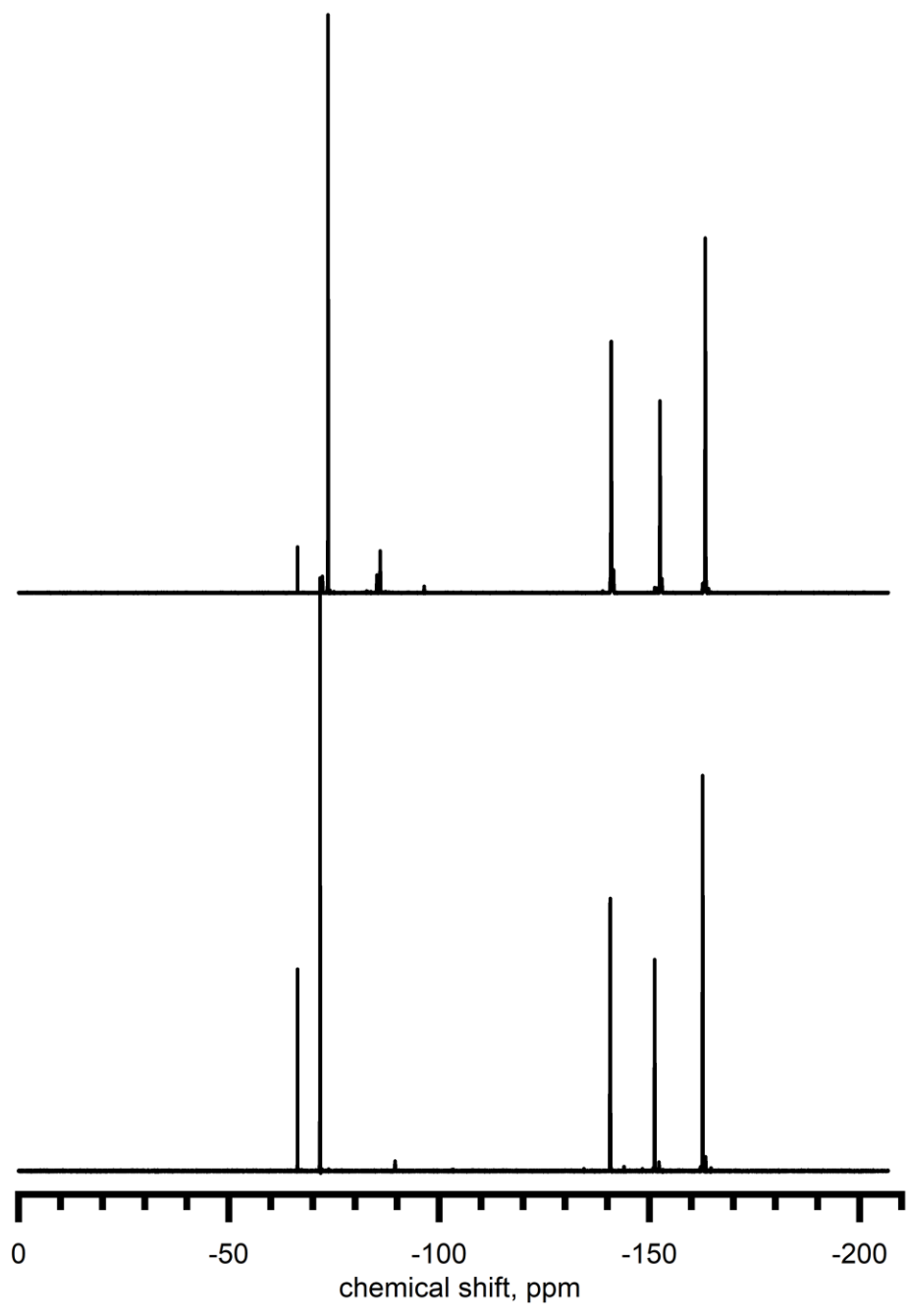
**Figure S2:** **A:**  $^1\text{H}$  NMR spectra of the crude reaction mixture at the end of the reaction (20 h) showing the signals of 9,10-ANTH(Br) $_2$  (red), 9-ANTH(Bn<sub>F</sub>) (blue) and 9,10-ANTH(Bn<sub>F</sub>) $_2$  (green) in CDCl $_3$ . **B:**  $^1\text{H}$  NMR spectra of the reaction mixture after 1, 2, 3, and 4 h (procedure: 1 mL from the reaction was taken out of the flask, the solvent was evaporated, and the residue was redissolved in CDCl $_3$ ).

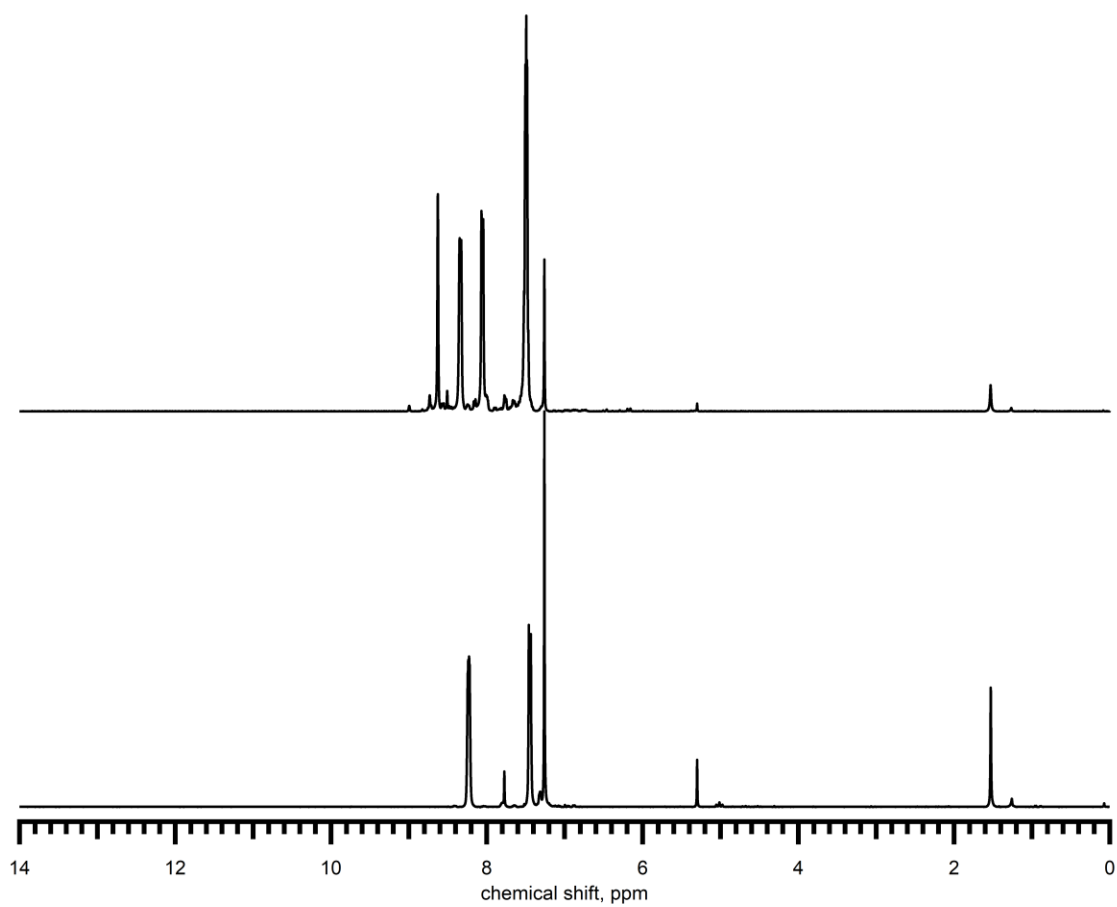


**Figure S3:** HPLC chromatograms for the separation of 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> and 9-ANTH(Bn<sub>F</sub>). The conditions are listed next to the chromatograms. All traces collected used a COSMOSIL Buckyprep semi-preparative stationary phase at a flow rate of 5 mL min<sup>-1</sup> and observed at 300 nm detection wavelength. The peaks in color are those collected and further separated in a subsequent separation stage. The blue color corresponds to 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> and the magenta color corresponds to 9-ANTH(Bn<sub>F</sub>). The *x*-axis for all chromatograms is the *t*<sub>R</sub> in minutes. Chromatogram a is of the crude product mixture.



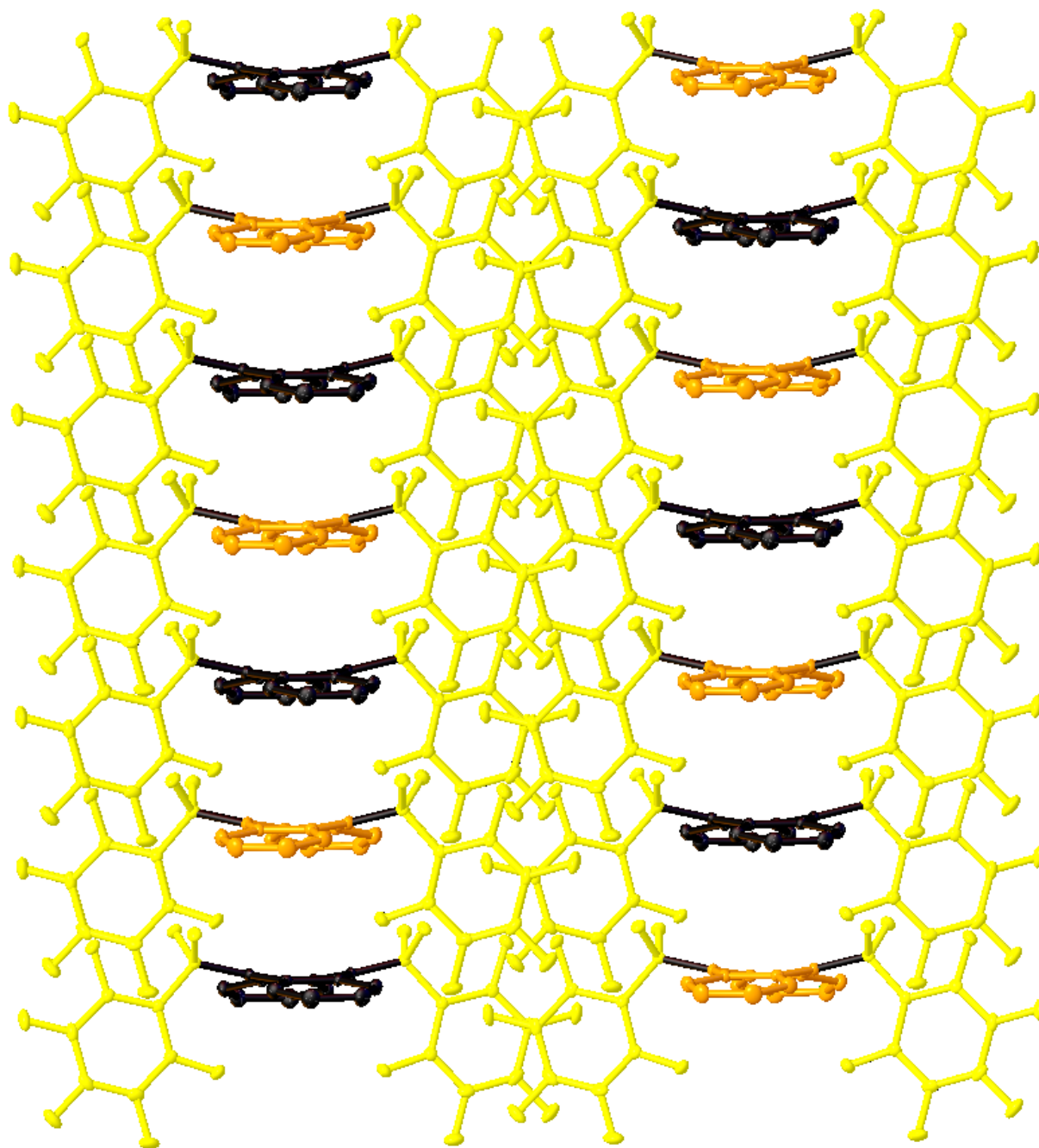
**Figure S4:** top:  $^{19}\text{F}$  NMR spectrum (379 MHz) of 9-ANTH( $\text{Bn}_\text{F}$ ) in  $\text{CDCl}_3$  with molecular structure drawing. **Bottom:**  $^1\text{H}$  NMR spectra of 9-ANTH( $\text{Bn}_\text{F}$ ) and 9,10-ANTH( $\text{Bn}_\text{F}$ ) $_2$  in  $\text{CDCl}_3$  (residual resonance  $\delta$  7.26 ppm). The internal standard 1,4-bis(trifluoromethyl)benzene is marked by an asterisk at  $\delta$  7.77 ppm).



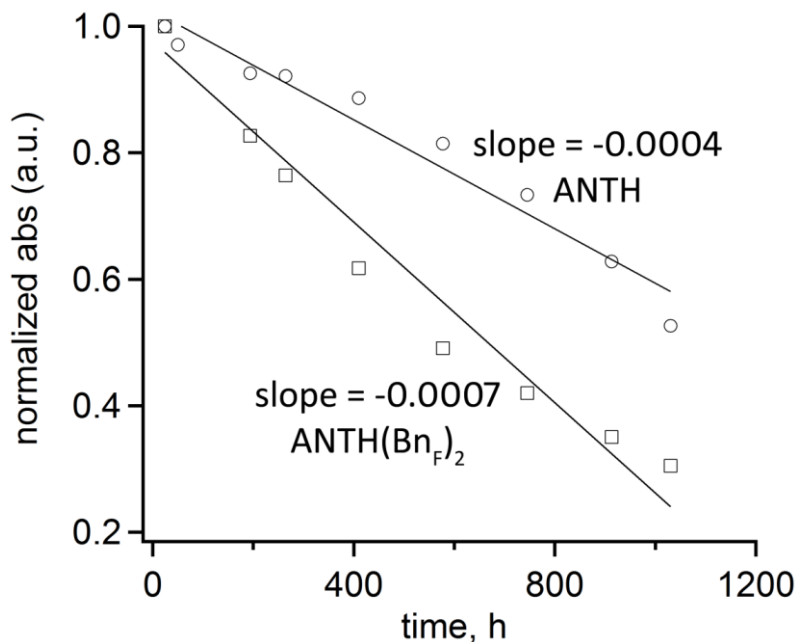


**Figure S4a expanded full spectra:** top panel:  $^{19}\text{F}$  NMR spectra (379 MHz) of 9-ANTH( $\text{Bn}_\text{F}$ ) (top) and 9,10-ANTH( $\text{Bn}_\text{F}$ ) $_2$  (bottom) in  $\text{CDCl}_3$ . Bottom panel:  $^1\text{H}$  NMR spectra of 9-ANTH( $\text{Bn}_\text{F}$ ) and 9,10-ANTH( $\text{Bn}_\text{F}$ ) $_2$  in  $\text{CDCl}_3$  (residual resonance  $\delta$  7.26 ppm).

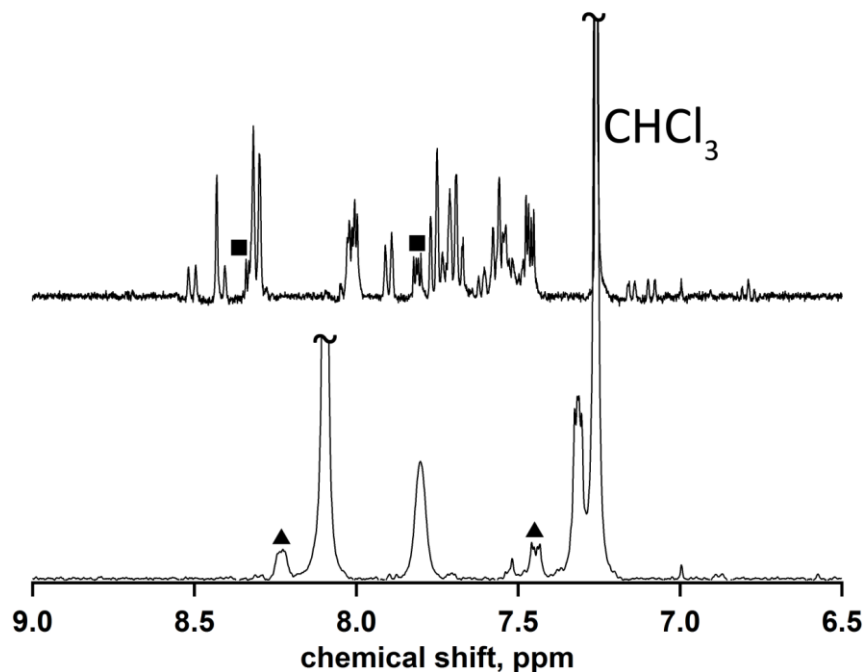




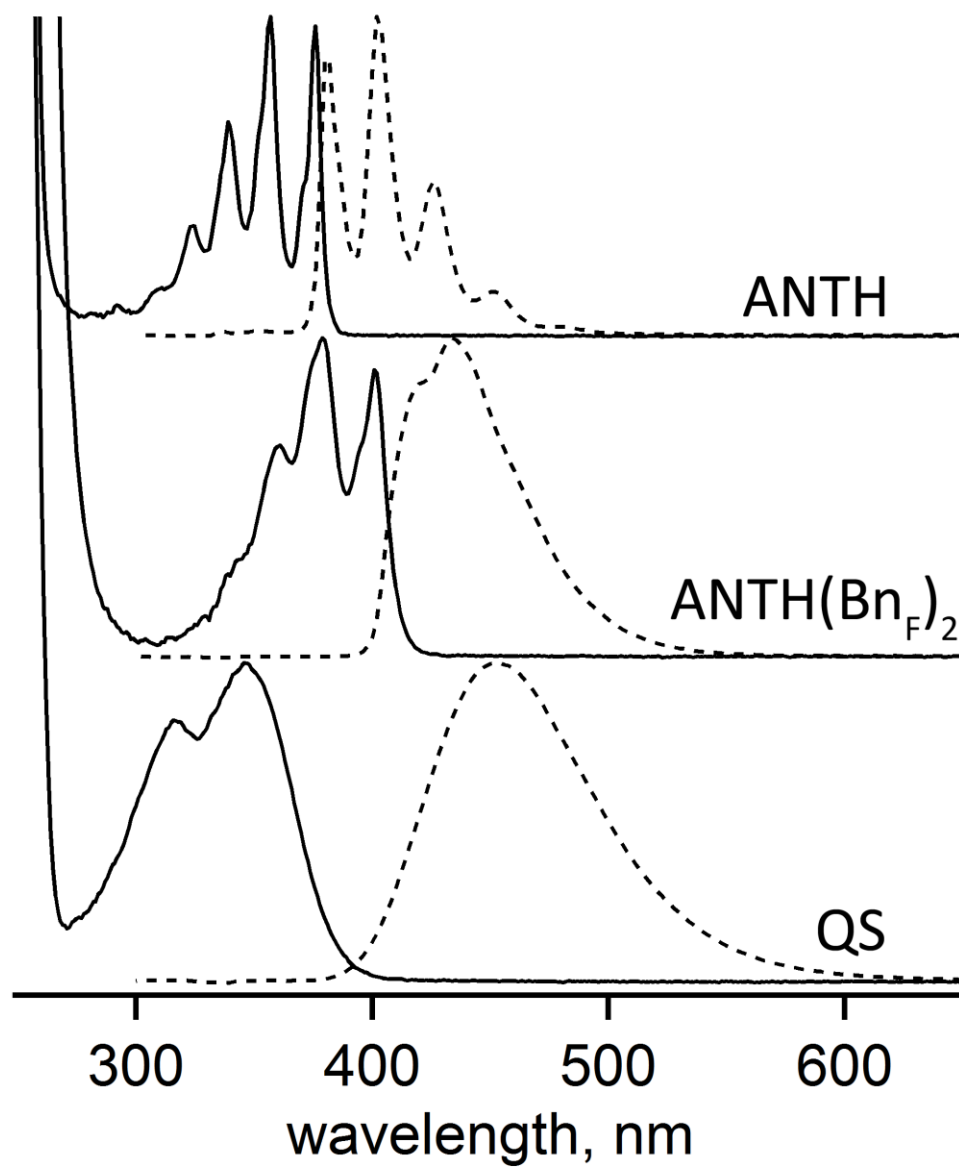
**Figure S5:** Solid-state packing of 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> viewed along the major axis of ANTH core. Two different stacked columns are colored in orange and black, and the Bn<sub>F</sub> groups are colored in yellow. The Bn<sub>F</sub> groups are shown to interact the ANTH core. Hydrogen atoms are omitted for clarity.



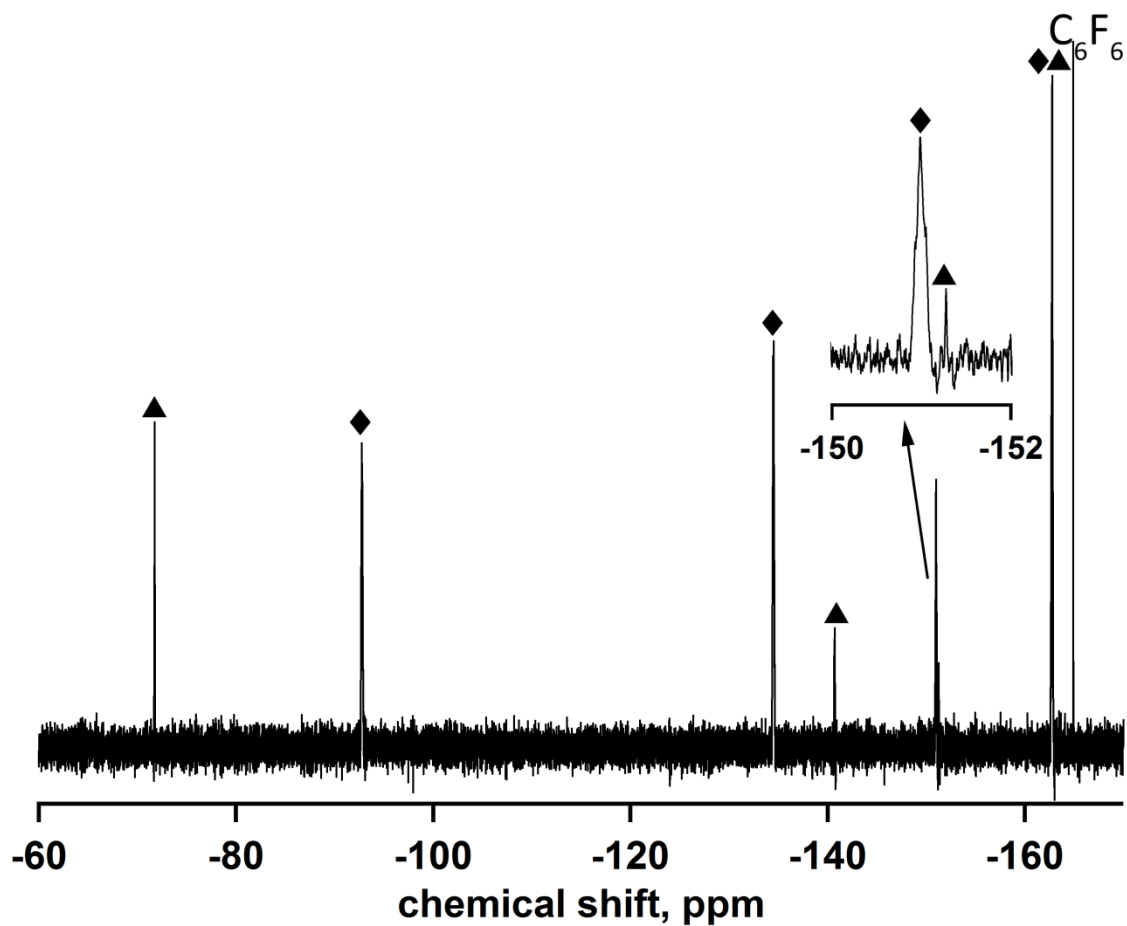
**Figure S6:** Normalized absorbance decay over time for ANTH and 9,10-ANTH(BnF)<sub>2</sub> under aerobic conditions and irradiated with 34 W ambient fume hood light bulb. Samples were dissolved in CH<sub>2</sub>Cl<sub>2</sub> and placed into a quartz sample holder.



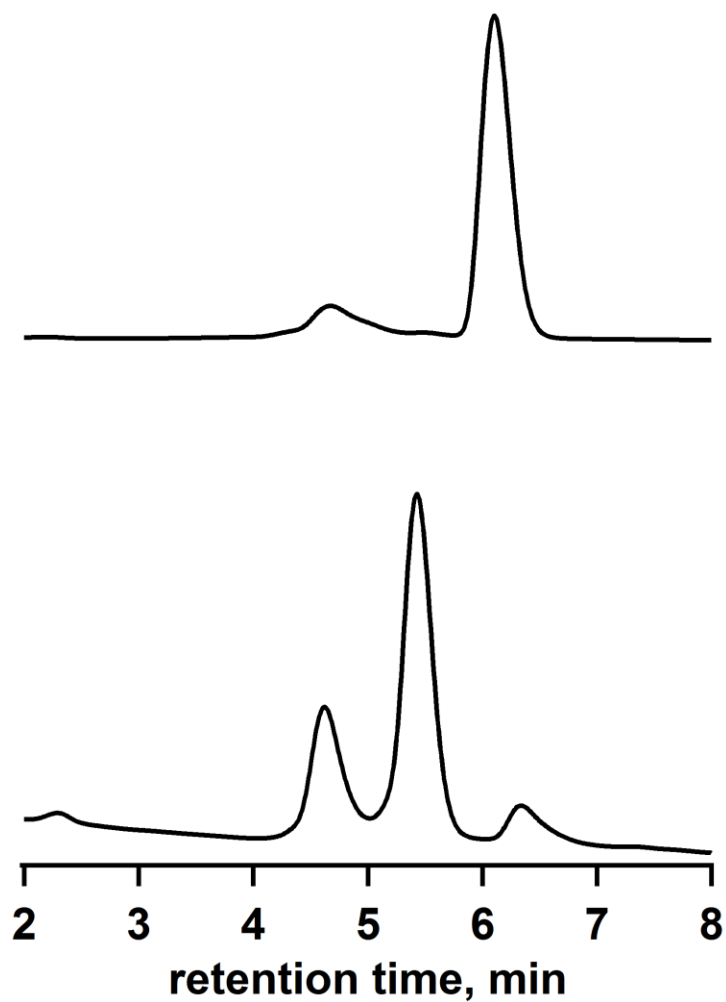
**Figure S7:** <sup>1</sup>H NMR spectra of ANTH (top) and 9,10-ANTH(BnF)<sub>2</sub> (bottom) post aerobic photostability in CDCl<sub>3</sub> (residual resonance δ 7.26 ppm). The black squares represent resonances corresponding to anthraquinone and the black triangles represent resonances corresponding to 9,10-ANTH(BnF)<sub>2</sub>. Unidentified solvent impurity at δ 8.1 ppm.



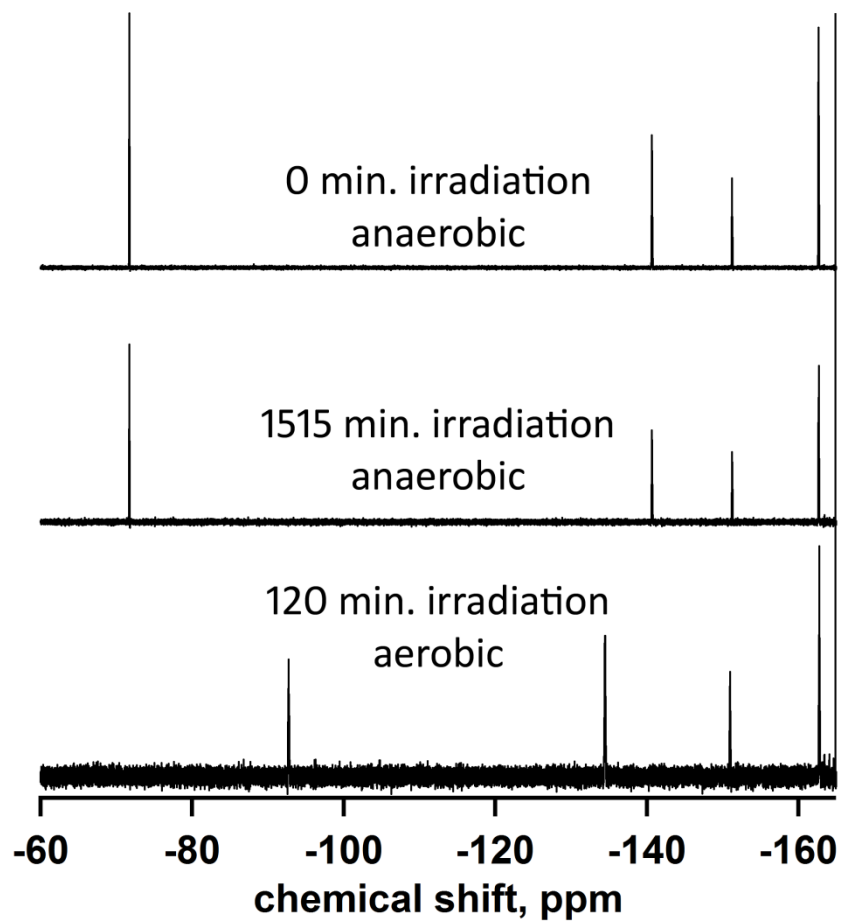
**Figure S8:** Absorption and emission spectra of ANTH and 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> in cyclohexane, and quinine sulfate (QS) in 0.1 M aqueous H<sub>2</sub>SO<sub>4</sub>. Samples were under aerobic (absorption, solid line) and anaerobic (emission, dashed line) conditions.



**Figure S9:**  $^{19}\text{F}$  NMR spectrum of 9,10-ANTH( $\text{BnF}$ ) $_2$  post aerobic photostability in  $\text{CDCl}_3$ . The internal standard  $\text{C}_6\text{F}_6$  ( $\delta$   $-164.9$  ppm) is shown. The black triangles represent resonances corresponding to 9,10-ANTH( $\text{BnF}$ ) $_2$  and the black diamonds represent resonances corresponding to the new symmetric compound.



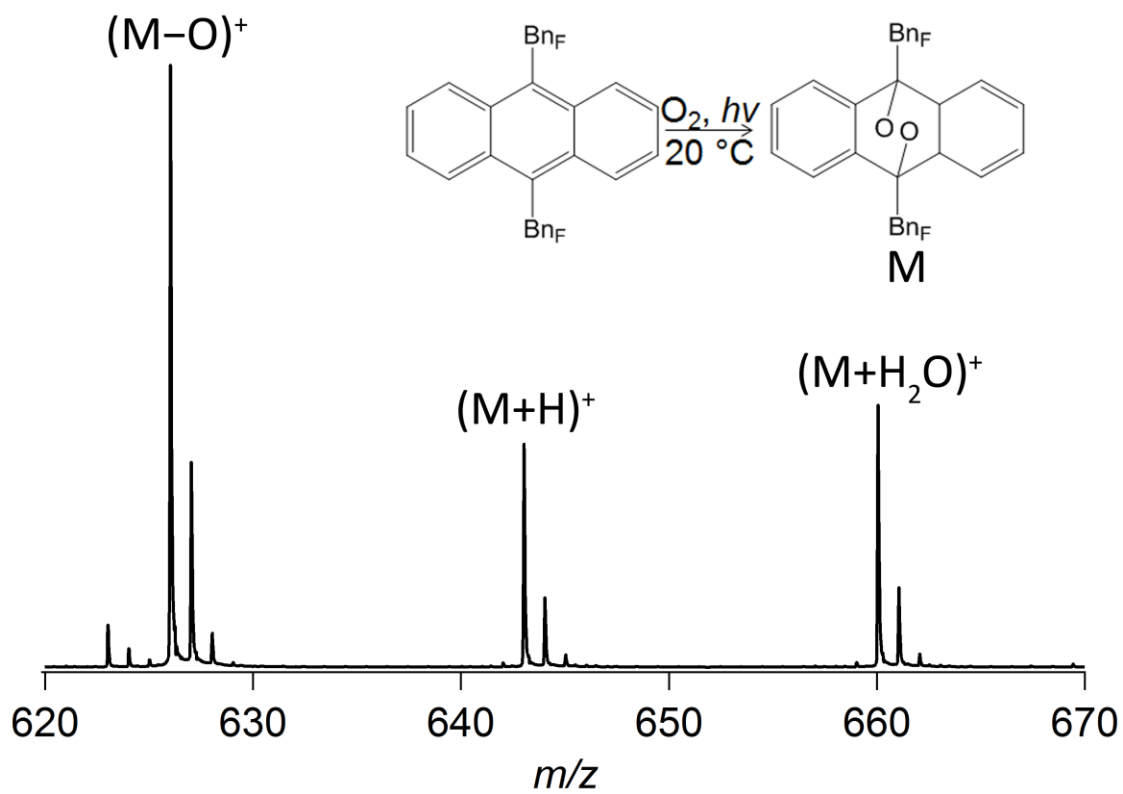
**Figure S10:** HPLC chromatograms of ANTH (bottom) and 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> (top) post aerobic photostability experiments in 100% MeCN at a flow rate of 5 mL min<sup>-1</sup>. The compounds ANTH and 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> have retention times of 5.5 minutes and 4.6 minutes, respectively. Note: ANTH co-elutes with anthraquinone (major peak in bottom chromatogram).



**Figure S11:**  $^{19}\text{F}$  NMR spectra of 9,10-ANTH( $\text{BnF}$ ) $_2$  irradiated for 0 min. (top), 1515 min. (middle), and after exposure to air with additional 120 min irradiation (bottom). Internal standard  $\text{C}_6\text{F}_6$  shown at  $\delta -164.9$  ppm.



**Figure S12:** The fluorescence of 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> in CH<sub>2</sub>Cl<sub>2</sub> under a 405 nm illumination.



**Figure S13:** DART-MS analysis of the photo irradiated 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> sample.

time (min)	% remaining, ANTH	% remaining, ANTH(Bn <sub>F</sub> ) <sub>2</sub>
30	100.0	100.0
60	85.0	94.6
90	79.4	88.9
180	58.8	85.9
240	54.0	79.3
300	51.2	73.2
540	22.3	50.3
720	20.8	41.5
960	16.3	31.5
1275	13.1	25.5

**Table S1:** Time of irradiation and % of ANTH and 9,10-ANTH(Bn<sub>F</sub>)<sub>2</sub> remaining based on the  $\delta(^1\text{H})$  7.48 and  $\delta(^1\text{H})$  7.46, respectively.