Donor-Acceptor Substituted Benzo-, Naphtho- and Phenanthro-fused Norbornadienes

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SUPPORTING INFORMATION

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NMR spectra

Compound 2



Supplementary Figure 1: ¹H NMR (400 MHz) spectrum of 2 in CDCl₃.



Supplementary Figure 2: ¹³C NMR (100 MHz) of 2 in CDCl₃.



Supplementary Figure 3: ¹H NMR (400 MHz) of 3 in CDCl₃.



175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 ppm

Supplementary Figure 4: ¹³C NMR (100 MHz) of 3 in CDCl₃.



Supplementary Figure 5: ¹H NMR (400 MHz) of 4 in CDCl₃.



Supplementary Figure 6: COSY NMR (400 MHz) of 4 in CDCl₃.



Supplementary Figure 7: ¹³C NMR (126 MHz) of 4 in CDCl₃.



Supplementary Figure 8: ¹H NMR (500 MHz) of 7 in CDCl₃.



Supplementary Figure 9: COSY NMR (400 MHz) of 7 in CDCl₃.



Supplementary Figure 10: ¹³C NMR (100 MHz) of 7 in CDCl₃.



Supplementary Figure 11: ¹H NMR (500 MHz) of 8 in CDCl₃.



Supplementary Figure 12: COSY NMR (500 MHz) of 8 in CDCl₃.



Supplementary Figure 13: ¹³C NMR APT (126 MHz) of 8 in CDCl₃.



Supplementary Figure 14: ¹H NMR (400 MHz) of 9 in CDCl₃.





Supplementary Figure 16: COSY NMR (400 MHz) of 9 in CDCl₃.



Supplementary Figure 17: HSQC NMR of 9 in CDCl₃.



Supplementary Figure 18: HMBC NMR of 9 in CDCl₃.



Supplementary Figure 19: NOESY NMR (500 MHz) of 9 in CDCl₃, zoomed in the aromatic region.



Supplementary Figure 20: ¹H NMR (400 MHz) of 10 in CDCl₃.



Supplementary Figure 21: ¹³C NMR (100 MHz) of 10 in CDCl₃.



Supplementary Figure 23: HSQC NMR of 10 in CDCl₃.



Supplementary Figure 24: HMBC NMR of 10 in CDCl₃.



Supplementary Figure 25: NOESY NMR of 10 in CDCl₃.



Supplementary Figure 26: ¹H NMR (400 MHz) of 13 in CDCl₃.



Supplementary Figure 27: ¹³C NMR (100 MHz) of 13 in CDCl₃.



Supplementary Figure 28: COSY NMR (400 MHz) of 13 in CDCl₃.



Supplementary Figure 29: ¹H NMR (400 MHz) of 14 in CDCl₃.



Supplementary Figure 30: ¹³C NMR (400 MHz) of 14 in CDCl₃.



Supplementary Figure 31: COSY NMR (400 MHz) of 14 in CDCl₃.



Supplementary Figure 32: ¹H NMR (500 MHz) of 15 in CDCl₃.



Supplementary Figure 33: COSY NMR (500 MHz) of 15 in CDCl₃.



Supplementary Figure 34: ¹³C NMR (126 MHz) of 15 in CDCl₃.



Supplementary Figure 35: ¹H NMR (500 MHz) of 17 in CDCl₃.



Supplementary Figure 36: ¹³C NMR (126 MHz) of 17 in CDCl₃.



Supplementary Figure 37: COSY NMR (500 MHz) of 17 in CDCl₃.





Supplementary Figure 38:¹H NMR (500 MHz) of 18 in CDCl₃.



Supplementary Figure 39: ¹³C NMR (126 MHz) of 18 in CDCl₃.



Supplementary Figure 40: COSY NMR (500 MHz) of 18 in CDCl₃.



Supplementary Figure 41: ¹H NMR (500 MHz) of 19 in CDCl₃.



Supplementary Figure 42: COSY NMR (500 MHz) of 19 in CDCl₃.



Supplementary Figure 43: ¹³C NMR (126 MHz) of 19 in CDCl₃.



Supplementary Figure 44: ¹H NMR (500 MHz) of 21 in CDCl₃.



Supplementary Figure 45: COSY NMR (500 MHz) of 21 in CDCl₃.



Supplementary Figure 46: ¹³C APT NMR (126 MHz) of 21 in CDCl₃.



Supplementary Figure 47: ¹H NMR (500 MHz) of 22 in CDCl₃.



Supplementary Figure 48: COSY NMR (500 MHz) of 22 in CDCl₃.



Supplementary Figure 49: ¹³C APT NMR (126 MHz) of 22 in CDCl₃.



Supplementary Figure 50: ¹H NMR (500 MHz) of 23 in CDCl₃.



Supplementary Figure 52: ¹³C APT NMR (126 MHz) of 23 in CDCl₃.

Photosensitizer Experiments

Compound **22** (2.3 mg) was dissolved in toluene- d_8 (600 µL) in an NMR tube; about the same weight of the Michler's ketone sensitizer was then added. The sample was then irradiated with a 300 nm LED light source from Thorlabs overnight (M300L4, minimum power output 32 mW). The NMR spectrum of the pure sample with Michler's ketone sensitizer before irradiation and after irradiation overnight was taken (Supplementary Figure 50).



Supplementary Figure 50. NMR spectra of 22 together with Michler's ketone in toluene-d₈ before (top) and after (bottom) irradiation.

Compound **23** (2.6 mg) was dissolved in toluene- d_8 (600 µL) in an NMR tube; about the same weight of the Michler's ketone sensitizer was then added. The sample was then irradiated with a 300 nm LED light source from Thorlabs overnight (M300L4, minimum power output 32 mW). The NMR spectrum of the pure sample with Michler's ketone sensitizer before irradiation and after irradiation overnight was taken (Supplementary Figure 51).



Supplementary Figure 51. NMR spectra of 23 together with Michler's ketone in toluene-d₈ before (top) and after (bottom) irradiation.