

SUPPORTING INFORMATION

A Systematic Series of BODIPY-Cyclotriphosphazene Conjugates: Exploring The Effect of BODIPY Number on Photophysical Properties

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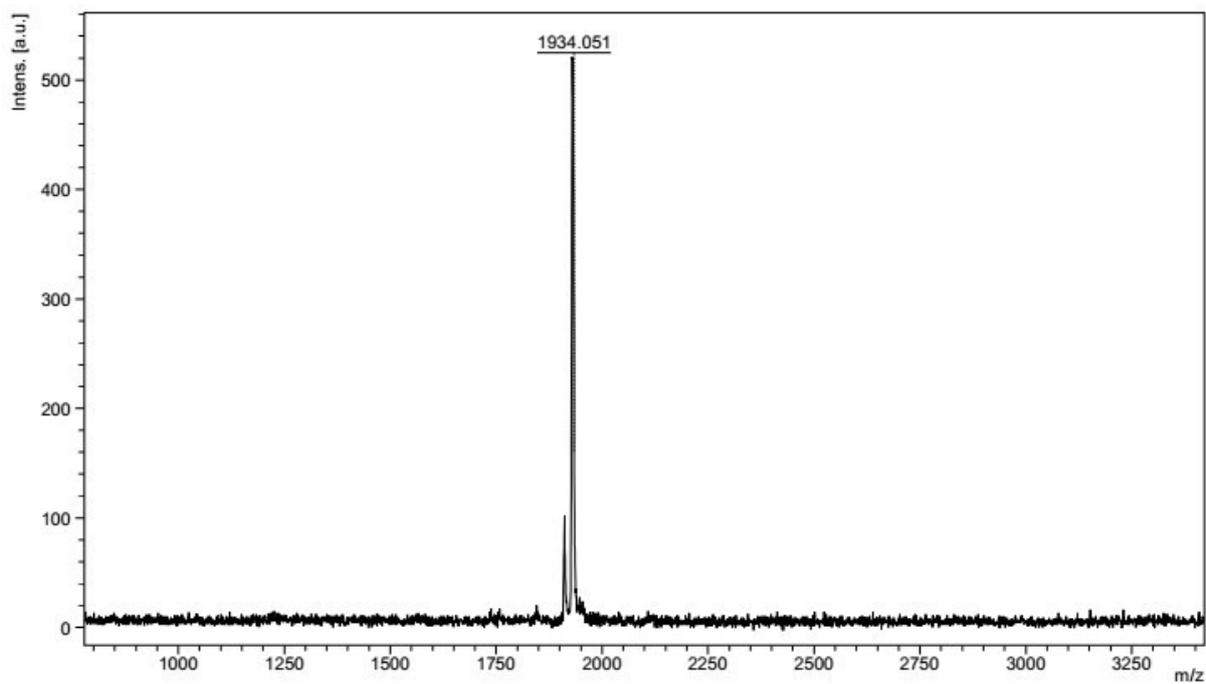


Fig. S1. MALDI TOF-MS spectrum of conjugate 6

MS (MALDI-TOF) (DIT) m/z Calc.: 1934.76; found: 1934.05 [M]⁺.

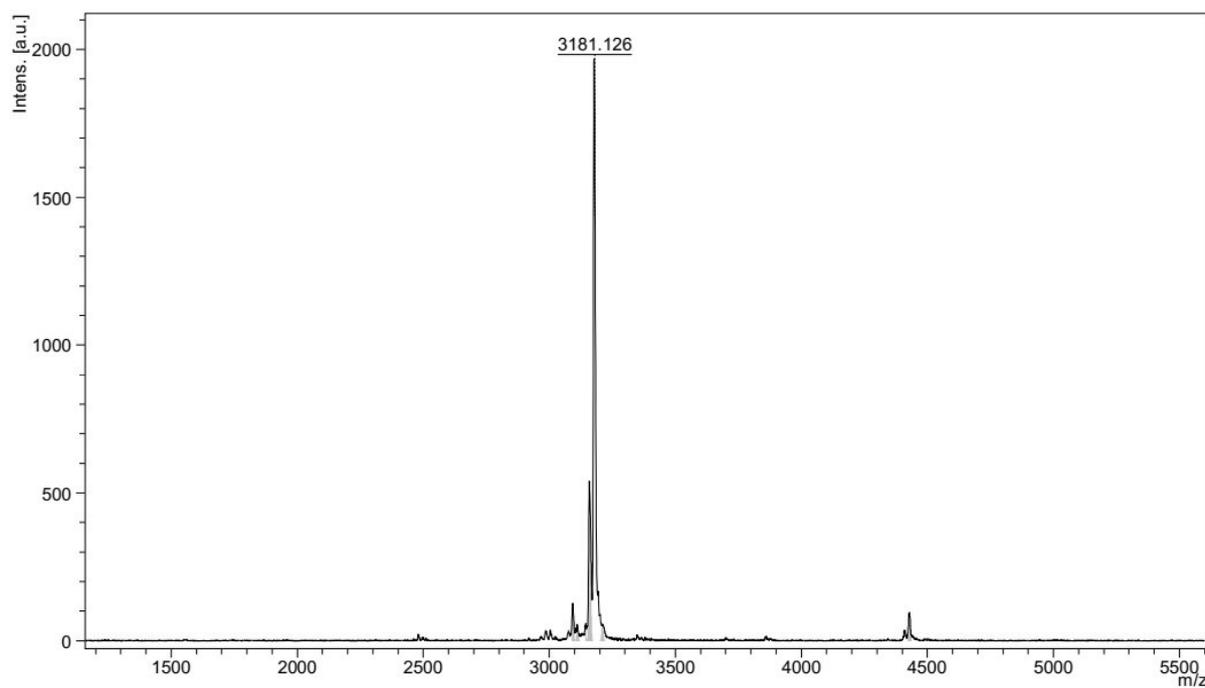


Fig. S2. MALDI TOF-MS spectrum of conjugate 7

MS (MALDI-TOF) (DIT) m/z Calc.: 3181.99; found: 3181.13 [M]⁺.

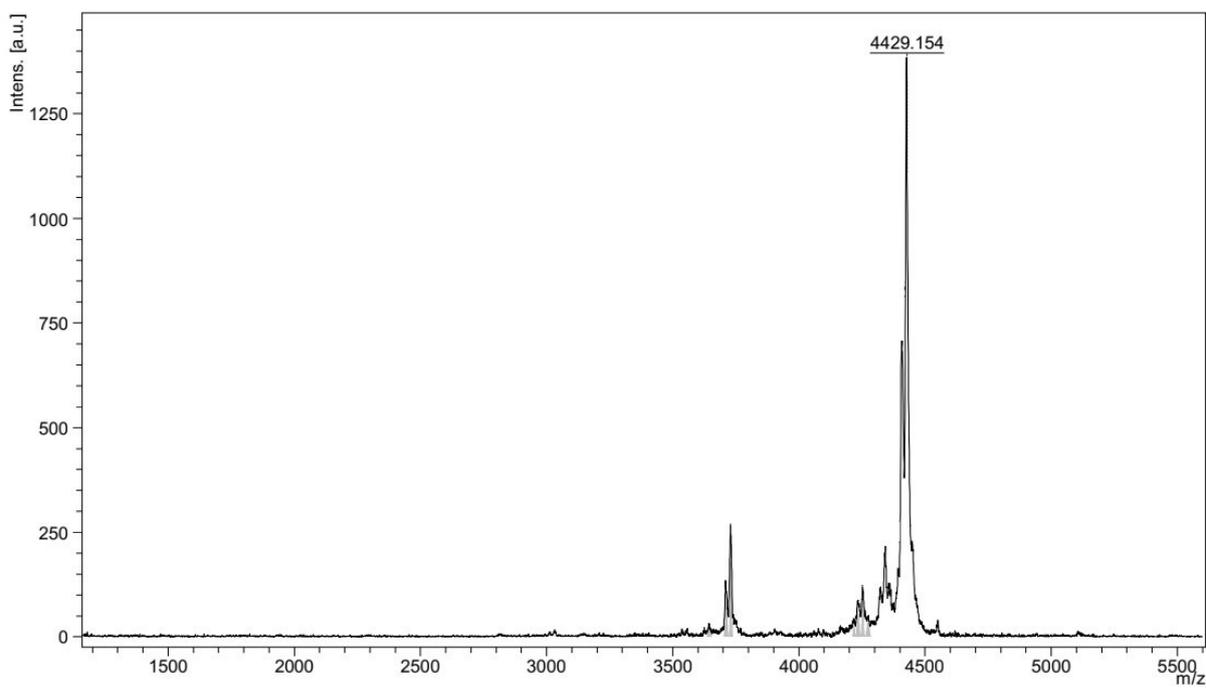


Fig. S3. MALDI TOF-MS spectrum of conjugate **8**

MS (MALDI-TOF) (DIT) m/z Calc.: 4429.22; found: 4429.15 [M]⁺.

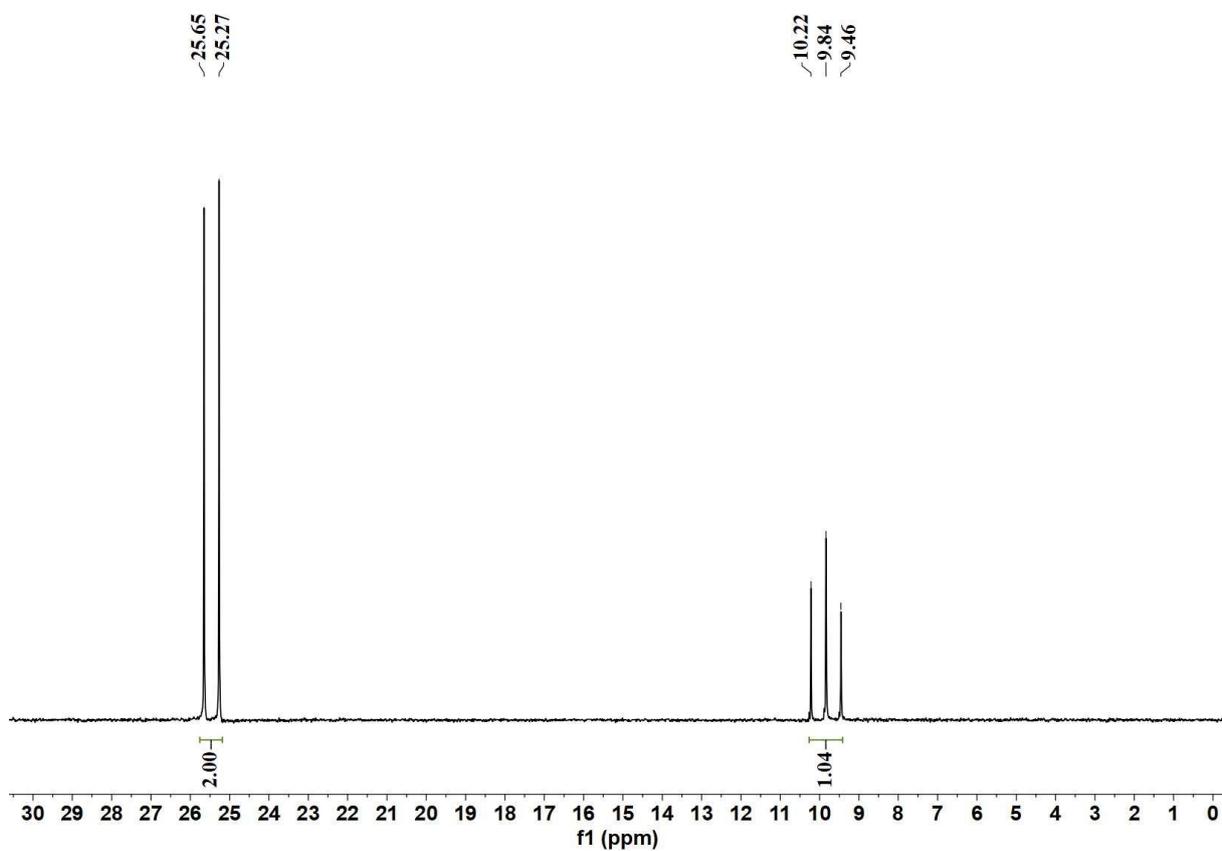


Fig. S4. The proton decoupled ^{31}P NMR spectrum of conjugate **6**

^{31}P NMR (243 MHz, CDCl_3 , δ ppm): 9.84 (t, $J = 92.2$ Hz, 1P), 25.46 (d, $J = 92.4$ Hz, 2P),
spin system: A_2X .

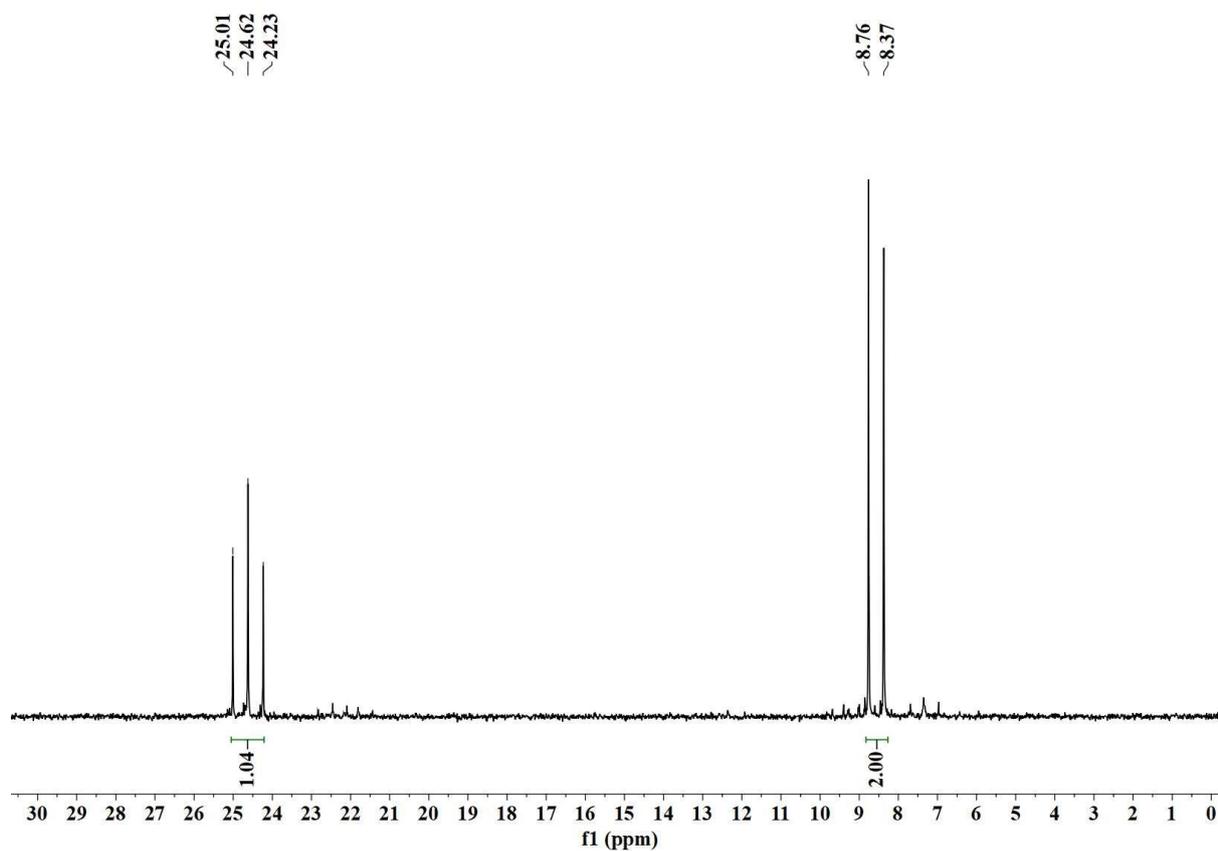


Fig. S5. The proton decoupled ^{31}P NMR spectrum of conjugate **7**

^{31}P NMR (243 MHz, CDCl_3 , δ ppm): 8.57 (d, $J = 94.7$ Hz, 2P), 24.62 (t, $J = 94.7$ Hz, 1P),
spin system: AX_2 .

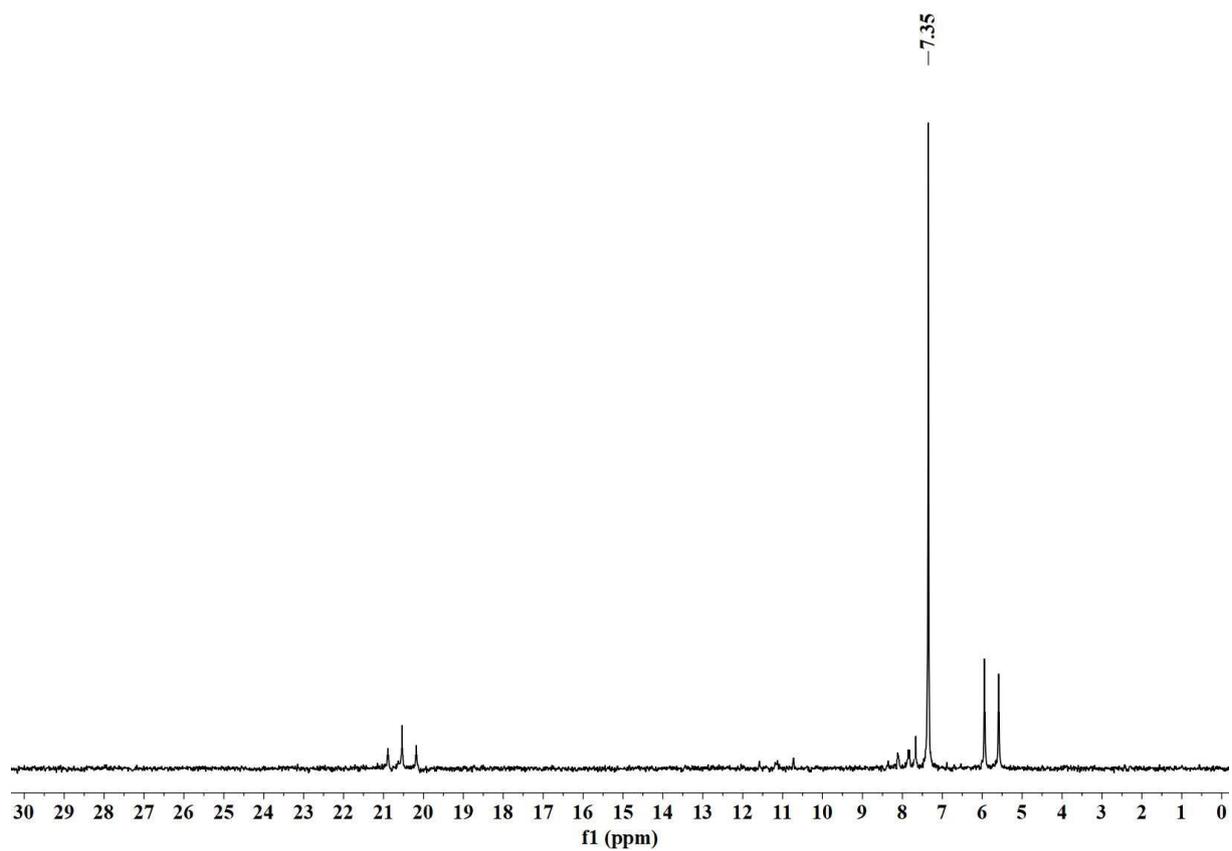


Fig. S6. The proton decoupled ^{31}P NMR spectrum of conjugate **8**
 ^{31}P NMR (243 MHz, CDCl_3 , δ ppm): 7.35 (s, 3P), spin system: A_3 .

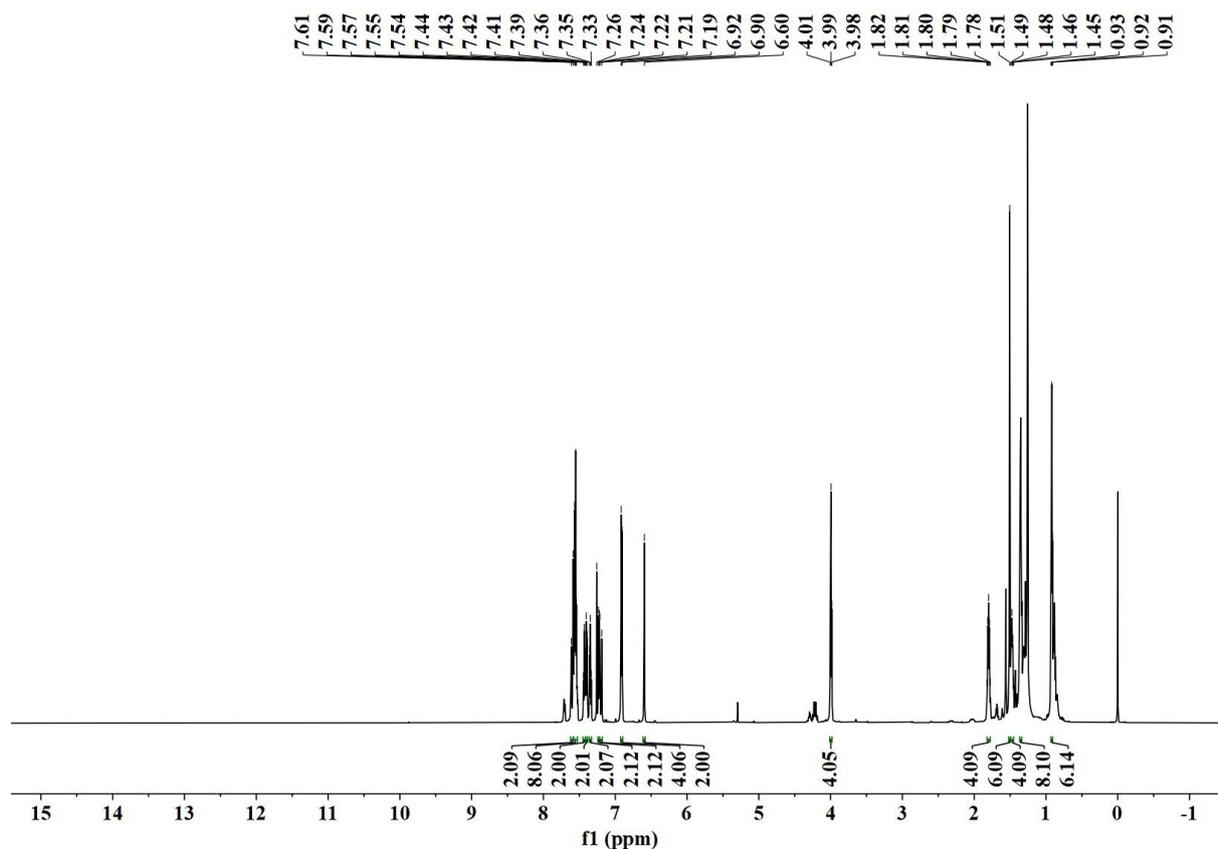


Fig. S7. ¹H- NMR spectrum of conjugate **6** in CDCl₃

¹H NMR (600 MHz, CDCl₃) δ 7.60 (d, *J* = 16.5 Hz, 2H), 7.57 – 7.55 (m, 8H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.23 (d, *J* = 8.3 Hz, 2H), 7.20 (d, *J* = 16.3 Hz, 2H), 6.91 (d, *J* = 8.5 Hz, 4H), 6.60 (s, 2H), 3.99 (t, *J* = 6.5 Hz, 4H), 1.80 (p, *J* = 6.8 Hz, 4H), 1.51 (s, 6H), 1.49 – 1.44 (m, 4H), 1.35 (m, 8H), 0.92 (t, *J* = 6.6 Hz, 6H).

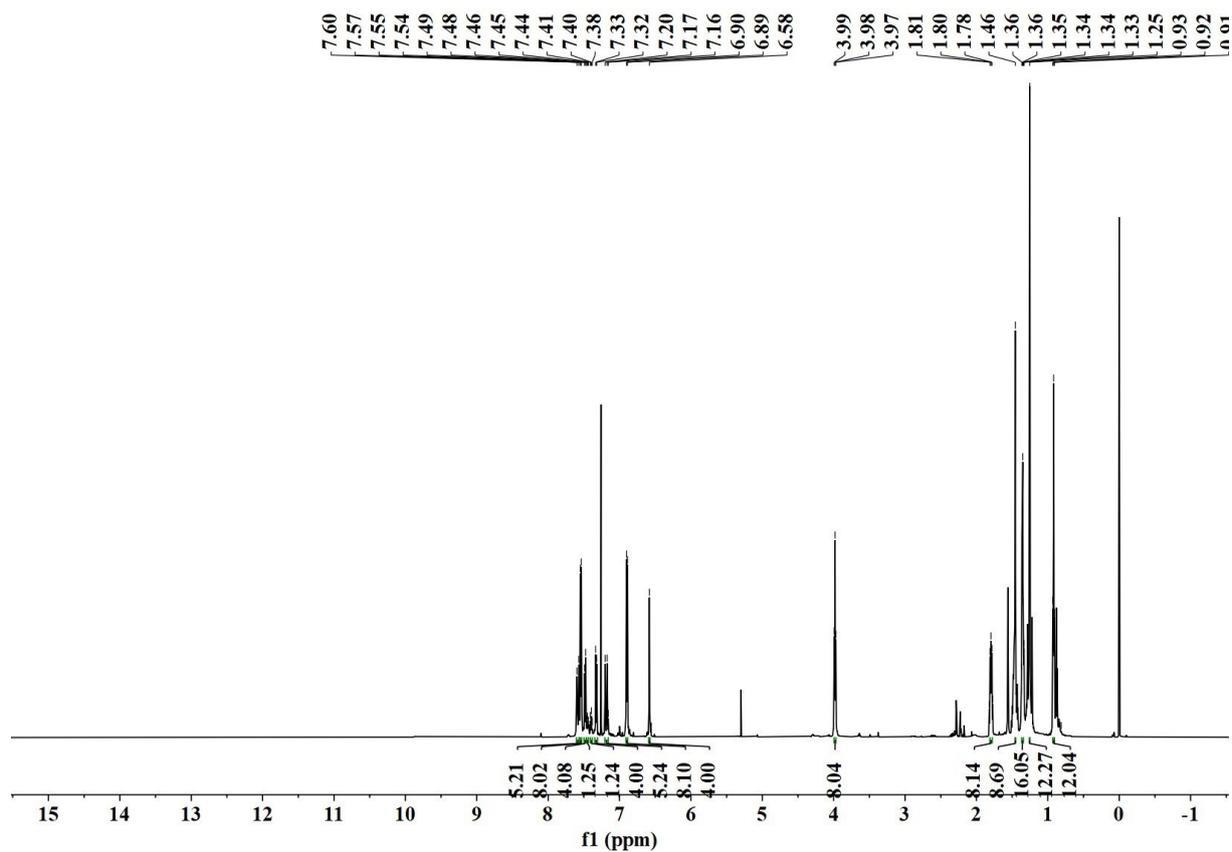


Fig. S8. ¹H- NMR spectrum of conjugate **7** in CDCl₃

¹H NMR (600 MHz, CDCl₃) δ 7.58 (m, 5H), 7.54 (d, *J* = 8.8 Hz, 8H), 7.48 (d, *J* = 8.4 Hz, 4H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 1H), 7.33 (d, *J* = 8.5 Hz, 4H), 7.19 (m, 5H), 6.90 (d, *J* = 8.8 Hz, 8H), 6.58 (s, 4H), 3.98 (t, *J* = 6.6 Hz, 8H), 1.80 (p, *J* = 6.5 Hz, 8H), 1.46(bs, 8H), 1.35 (m, 16H), 1.25 (m, 12H), 0.92 (t, *J* = 7.5 Hz, 12H).

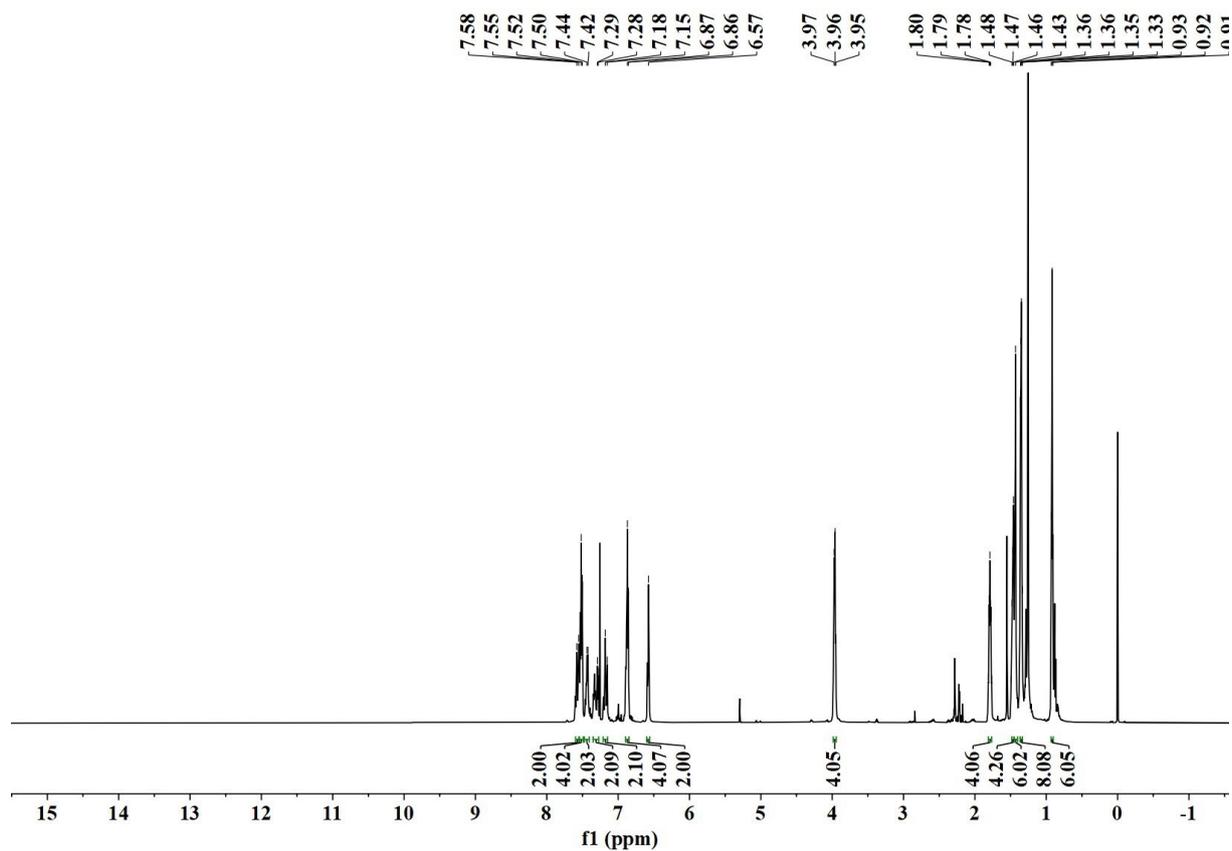


Fig. S9. ¹H- NMR spectrum of conjugate **8** in CDCl₃

¹H NMR (600 MHz, CDCl₃) δ 7.57 (d, *J* = 16.2 Hz, 2H), 7.51 (d, *J* = 8.9 Hz, 4H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 16.1 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 4H), 6.57 (s, 2H), 3.96 (t, *J* = 7.1 Hz, 4H), 1.79 (t, *J* = 6.5 Hz, 4H), 1.48 – 1.45 (m, 4H), 1.43 (s, 6H), 1.35 (m, 8H), 0.92 (t, *J* = 6.9 Hz, 6H).

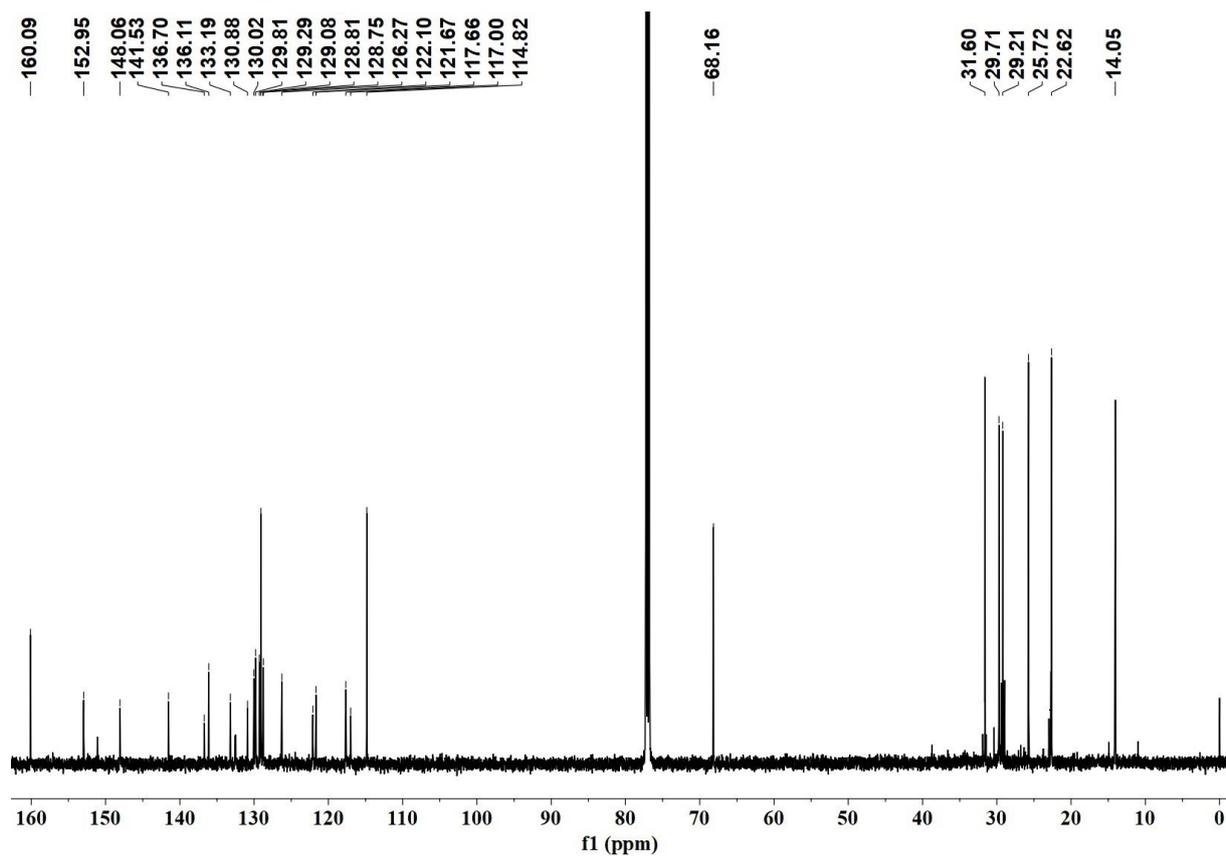


Fig. S10. ^{13}C - NMR spectrum of conjugate **6** in CDCl_3

^{13}C NMR (151 MHz, CDCl_3) δ 160.09, 152.95, 148.06, 141.53, 136.70, 136.11, 133.19, 130.88, 130.02, 129.81, 129.29, 129.08, 128.81, 128.75, 126.27, 122.10, 121.67, 117.66, 117.00, 114.82, 68.16, 31.60, 29.71, 25.72, 22.62, 14.93, 14.05.

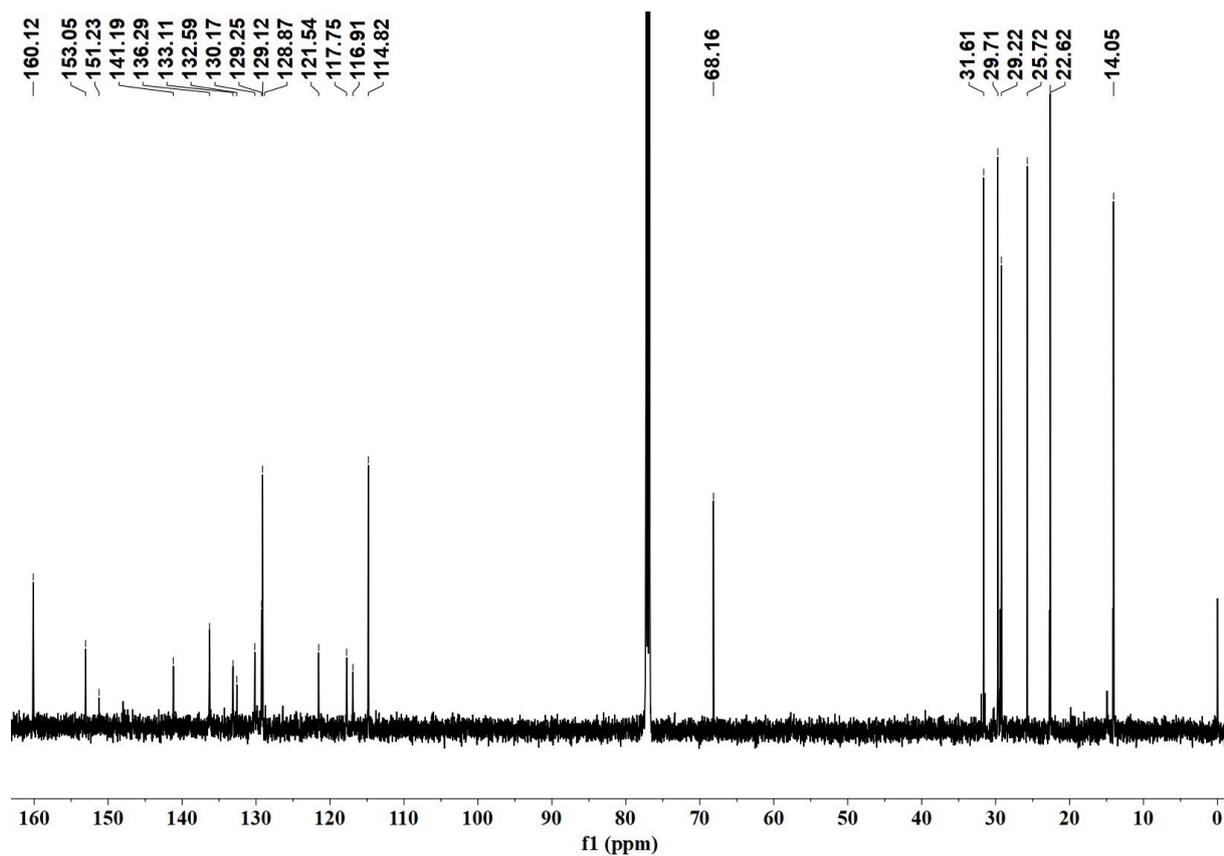


Fig. S11. ^{13}C - NMR spectrum of conjugate **7** in CDCl_3

^{13}C NMR (151 MHz, CDCl_3) δ 160.12, 153.05, 151.23, 141.19, 136.29, 133.11, 132.59, 130.17, 129.25, 129.12, 128.87, 121.54, 117.75, 116.91, 114.82, 68.16, 31.61, 29.71, 29.22, 25.72, 22.62, 14.05.

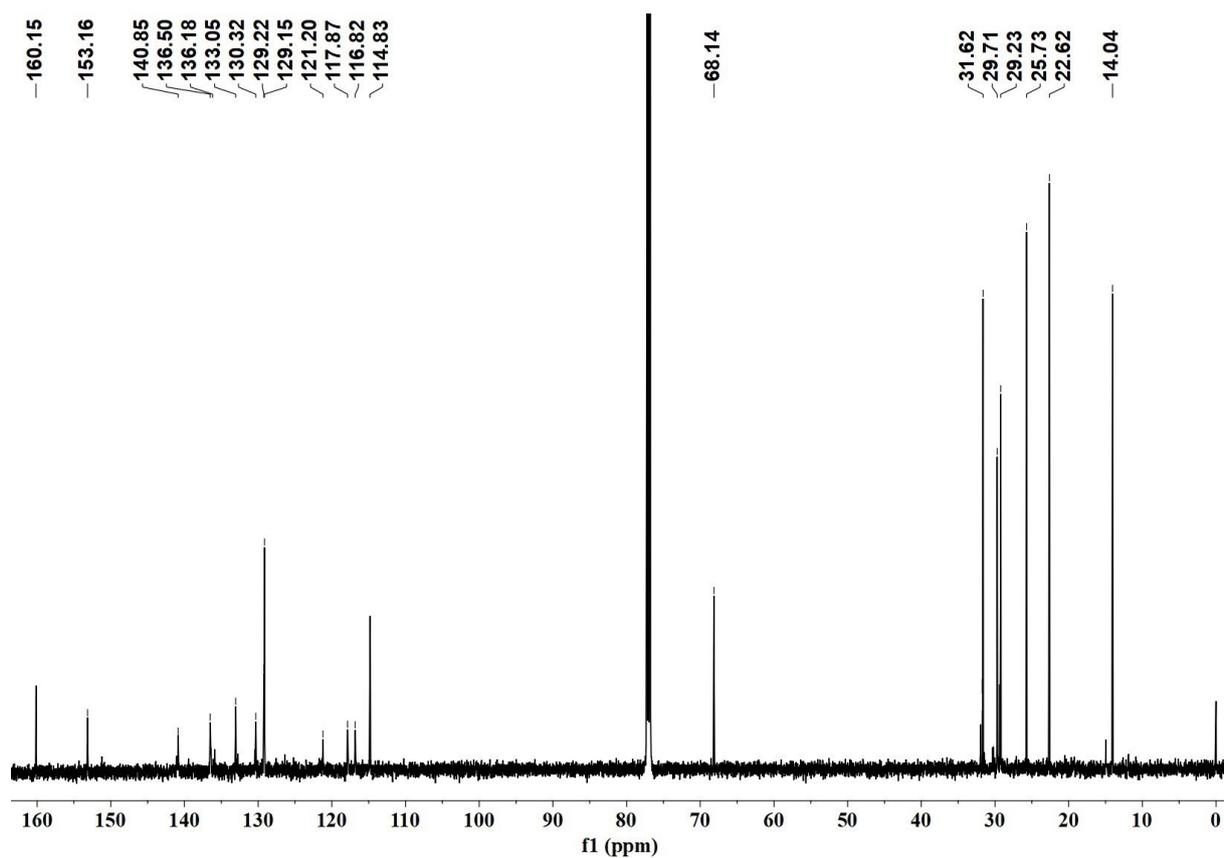


Fig. S12. ^{13}C - NMR spectrum of conjugate **8** in CDCl_3

^{13}C NMR (151 MHz, CDCl_3) δ 160.15, 153.16, 140.85, 136.50, 136.18, 133.05, 130.32, 129.22, 129.15, 121.20, 117.87, 116.82, 114.83, 68.14, 31.62, 29.71, 29.23, 25.73, 22.62, 14.04.

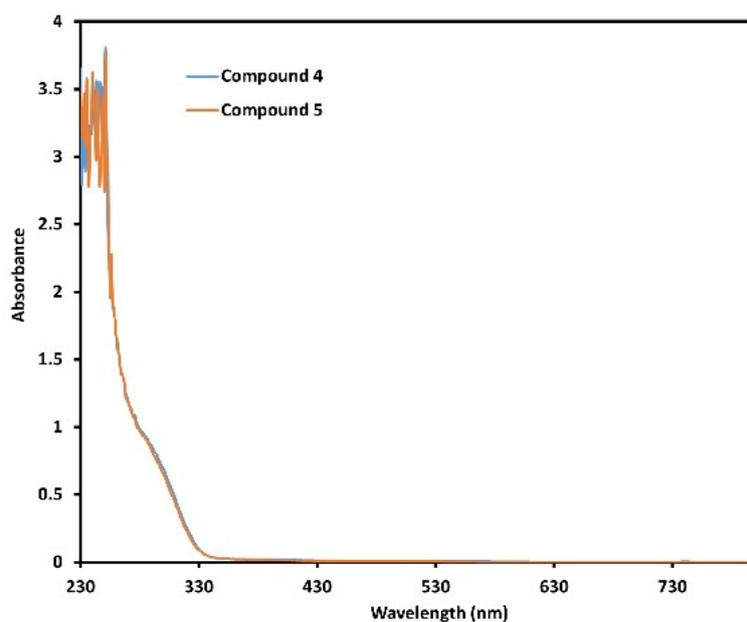


Fig. S13. UV-Vis absorption spectra of Compounds **4** and **5** (6×10^{-7} M in THF)



Fig. S14. Solubility of compounds in methanol

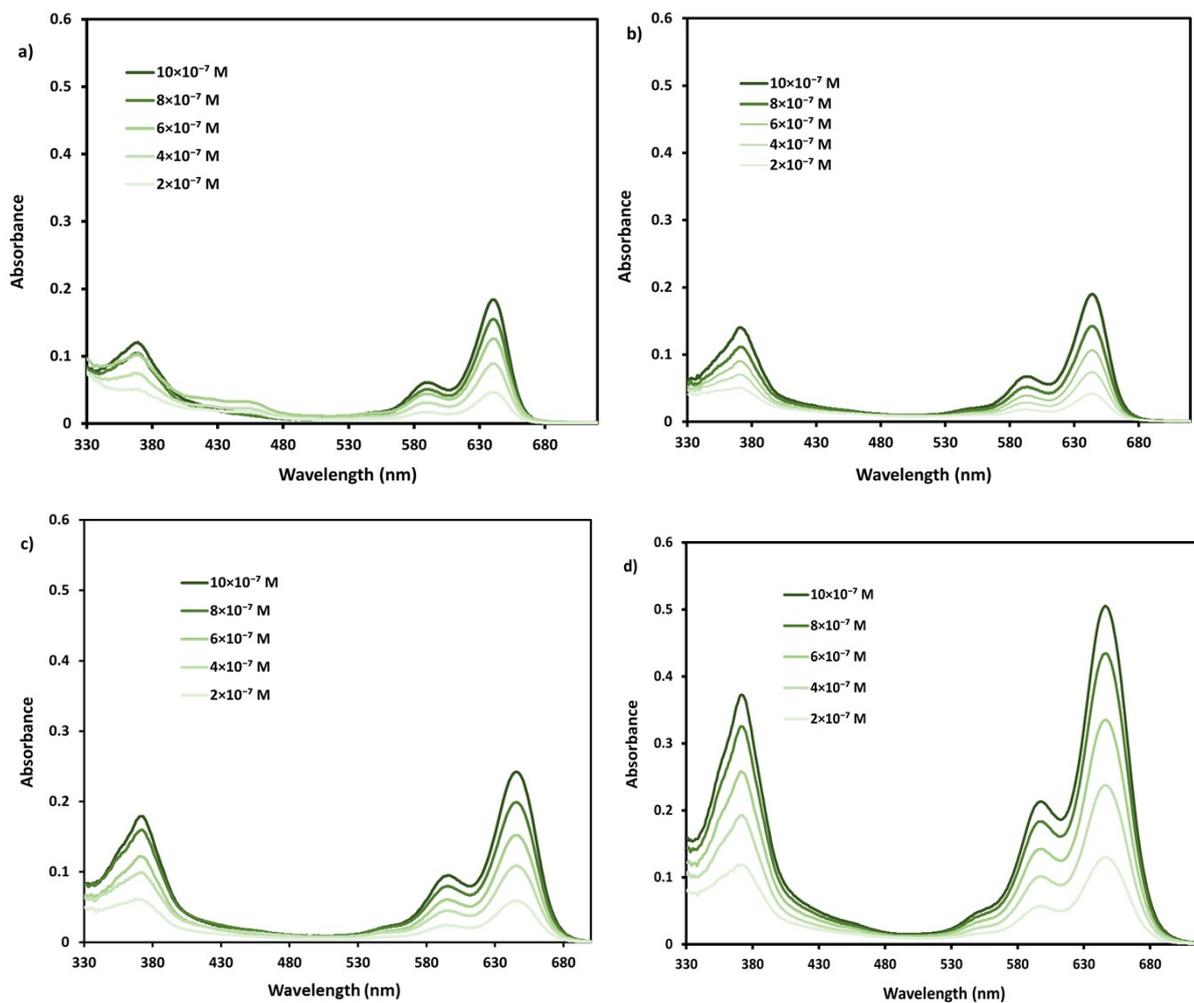


Fig. S15. UV-Vis absorption spectra of a) Compound **3**, b) Conjugate **6**, c) Conjugate **7**, d) Conjugate **8** in various concentrations.