

Supporting Information

Synthesis and Photophysics of a Broadband Absorbing Texaphyrin Derivative with Attached Rhodamine 6G Motif

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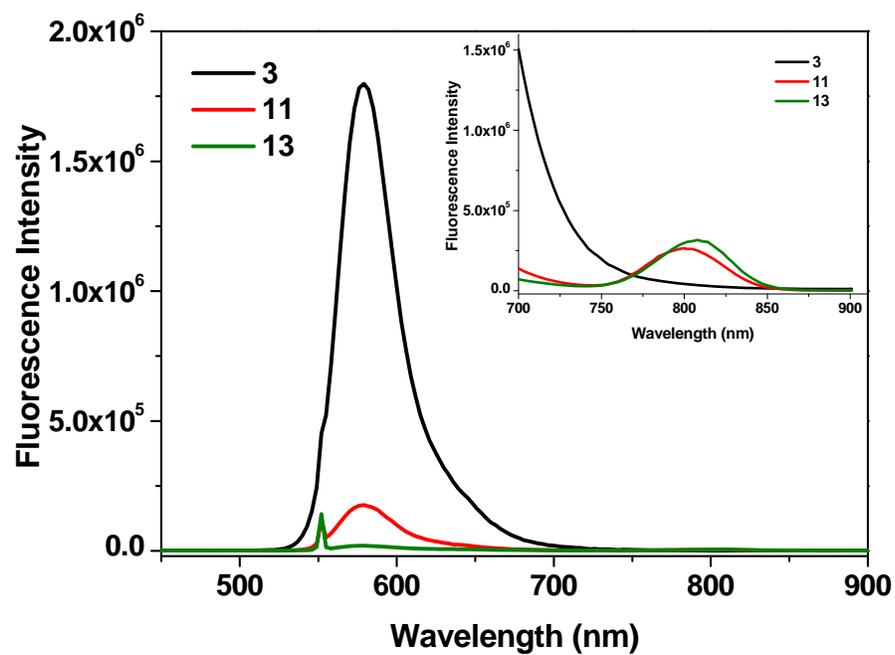
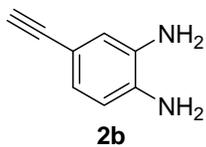
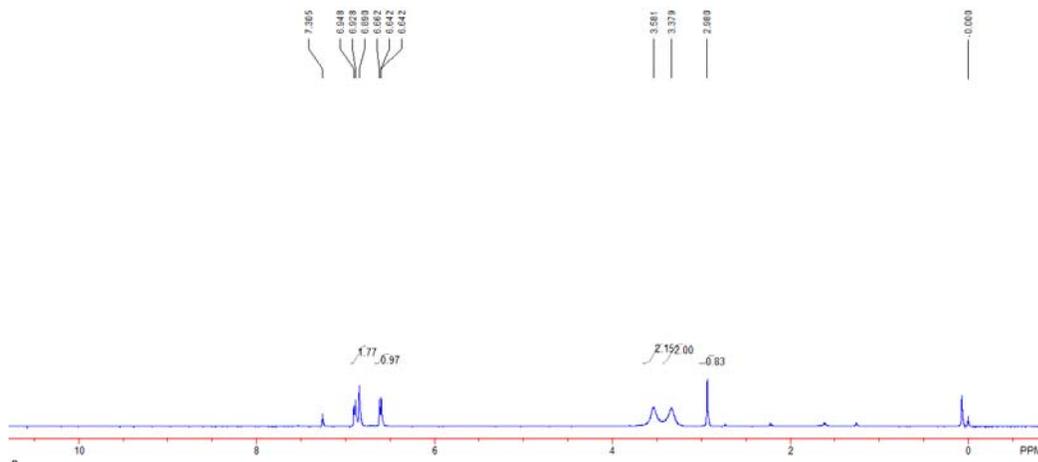


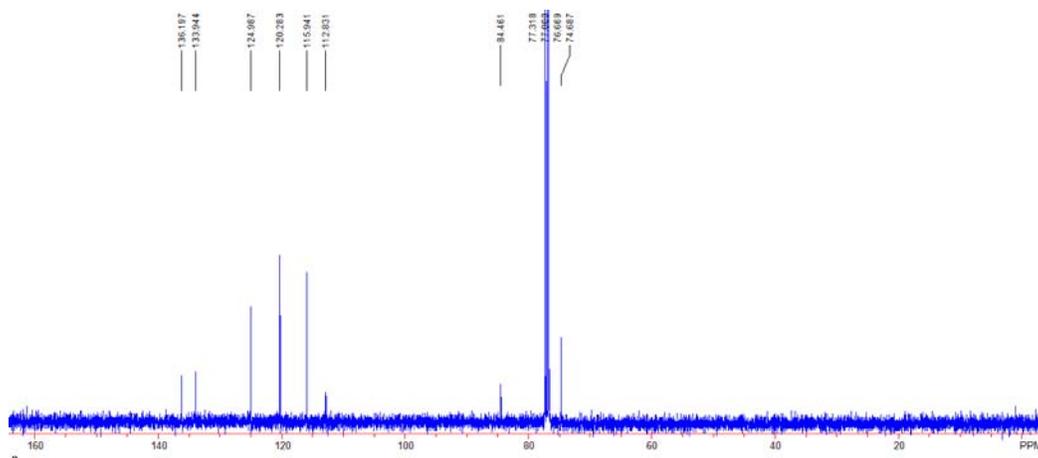
Figure S1. Fluorescence spectra of **3**, **11**, and **13** in acetone under the identical excitation condition of $A_{550\text{nm}} = 0.05$ in a 1-cm cuvette. $\lambda_{\text{ex}} = 550$ nm for all of the samples. The inset shows the NIR emission band at a larger slit width upon 550 nm excitation.

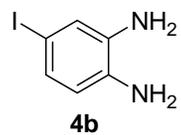


^1H NMR (400 MHz, CDCl_3): δ 6.85 (d, $J = 7.6$ Hz, 1H), 6.76 (s, 1H), 6.50 (d, $J = 7.6$ Hz, 1H), 3.47 (s, 4H), 2.97 (s, 1H).

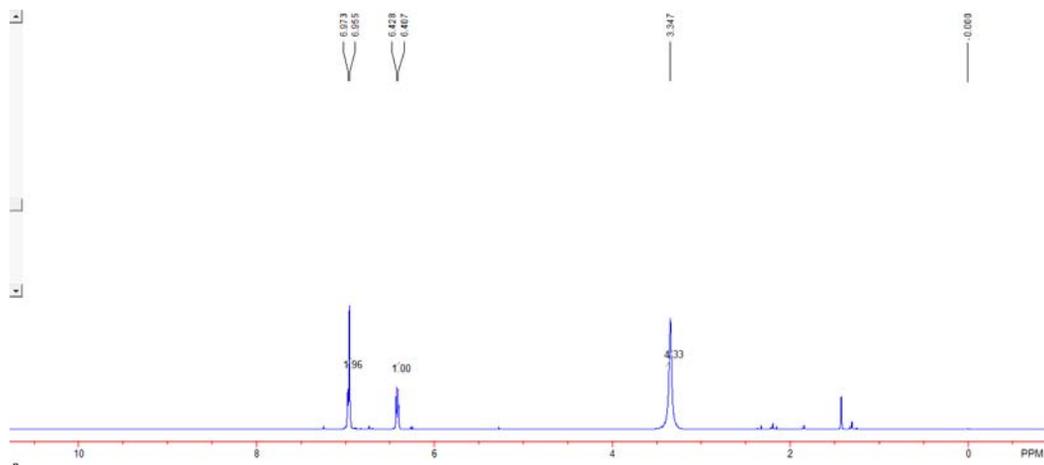


^{13}C NMR (CDCl_3 , 100 MHz, TMS): δ 74.5, 84.5, 112.8, 115.9, 120.3, 125.0, 133.9, 136.2.

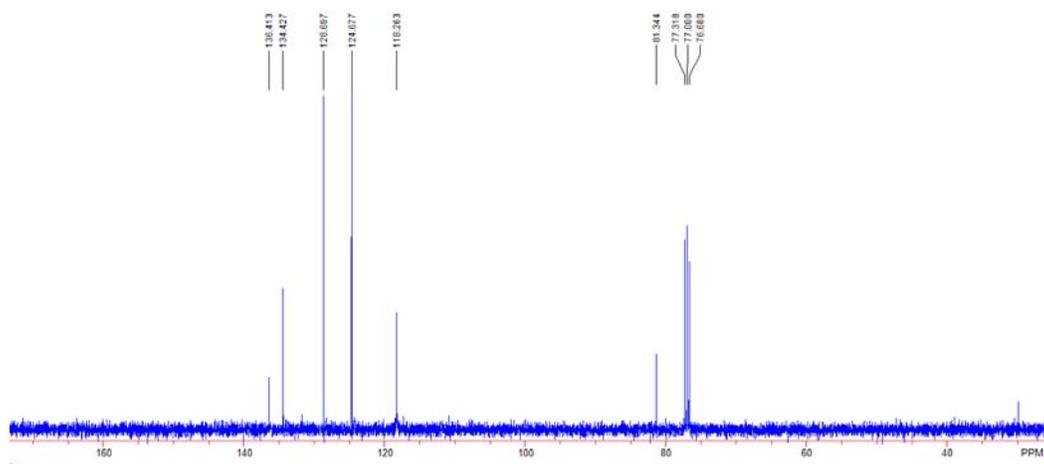


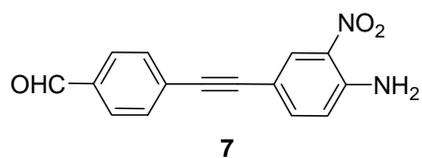


^1H NMR (500 MHz, CDCl_3): δ 6.98 (d, $J = 8.0$ Hz, 1H), 6.94 (s, 1H), 6.41 (d, $J = 8.0$ Hz, 1H), 3.42 (s, 4H).

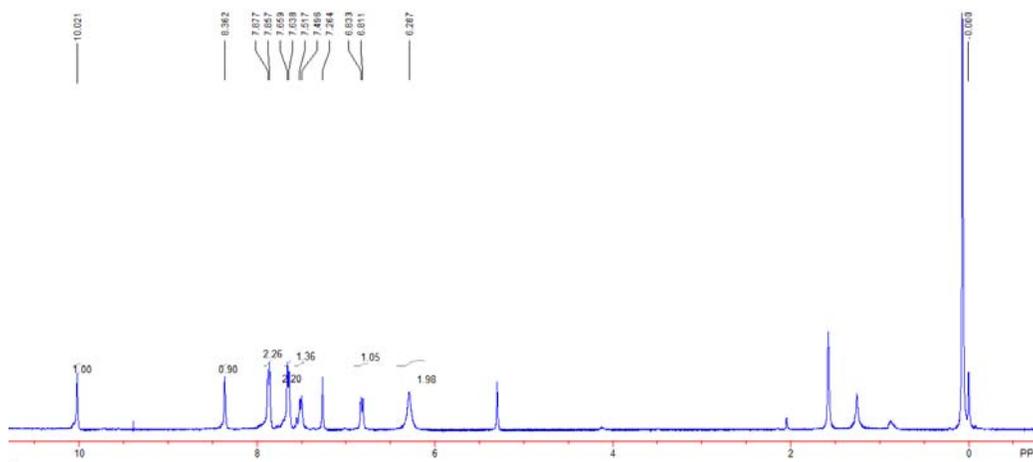


^{13}C NMR (CDCl_3 , 100 MHz, TMS): δ 81.3, 118.3, 124.7, 128.7, 134.4, 136.4.

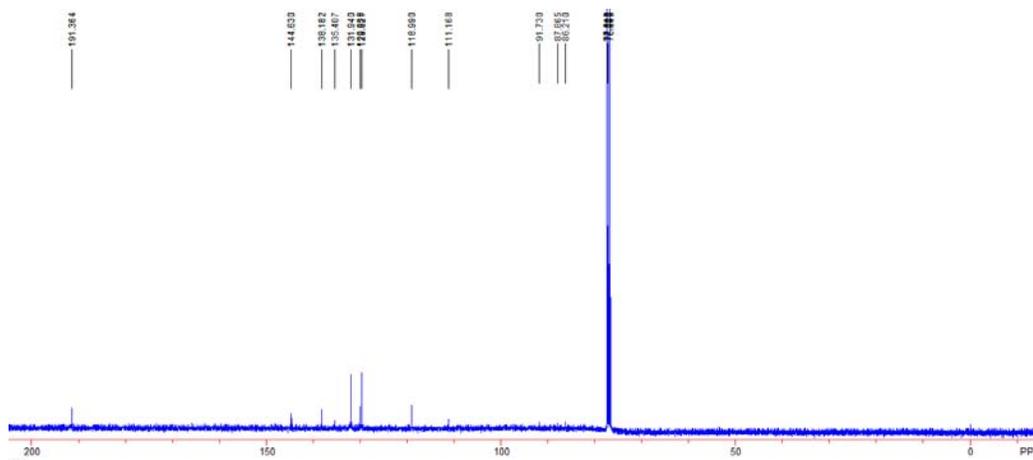


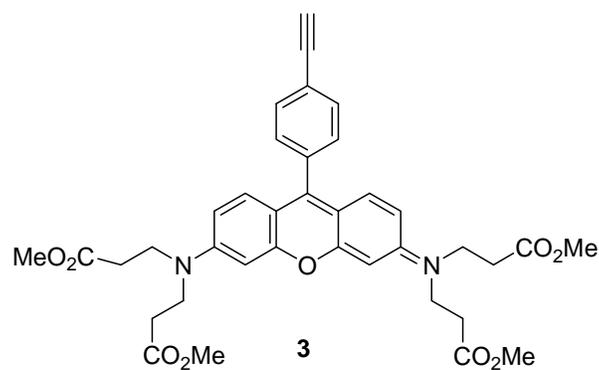


^1H NMR (400 MHz, CDCl_3): δ 9.99 (s, 1H), 8.34 (s, 1H), 7.84 (d, $J = 8$ Hz, 2H), 7.62 (d, $J = 8$ Hz, 2H), 7.48 (d, $J = 8.8$ Hz, 1H), 6.79 (d, $J = 8.8$ Hz, 1H), 6.26 (s, 2H).

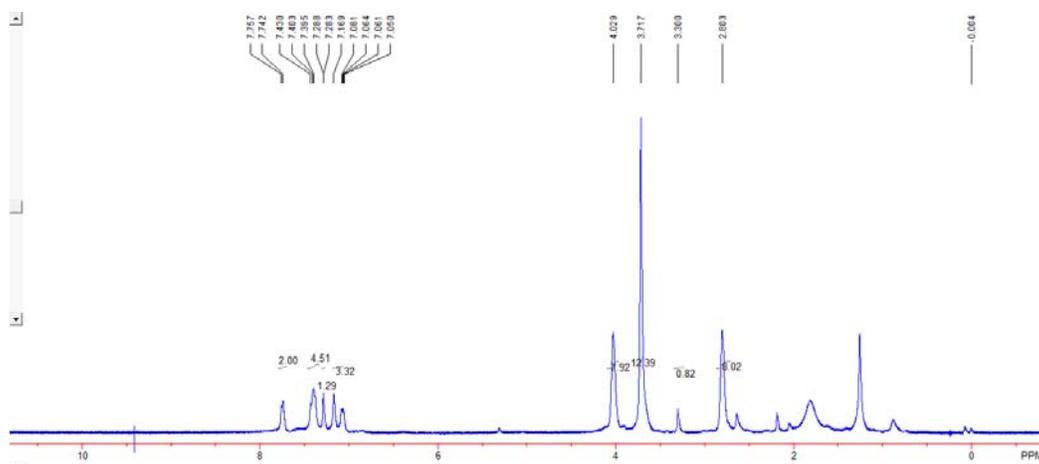


^{13}C NMR (CDCl_3 , 100 MHz, TMS): δ 86.2, 87.9, 91.7, 111.2, 119.0, 129.6, 130.0, 131.9, 135.4, 138.2, 144.6, 191.4

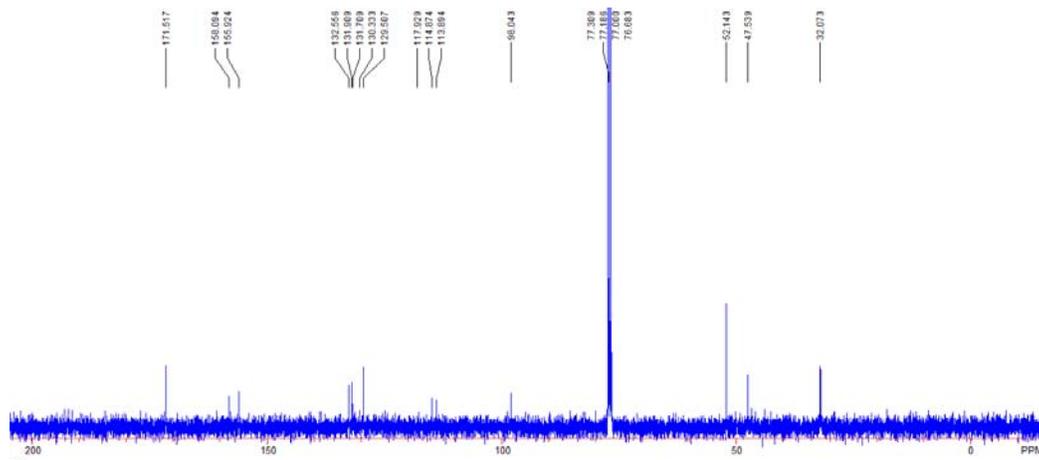


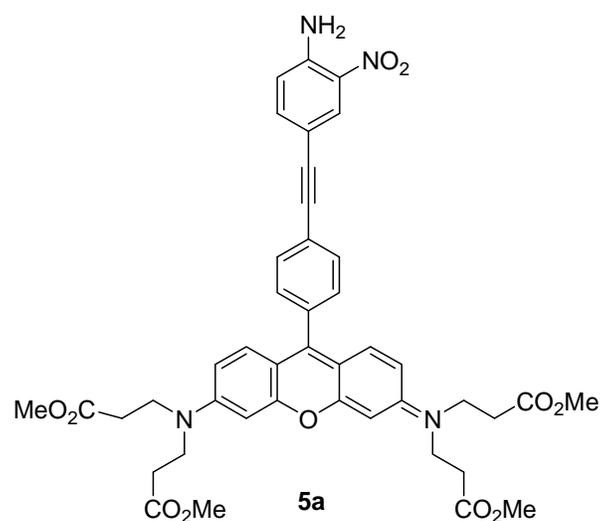


$^1\text{H NMR}$ (500 MHz, CDCl_3): δ 7.72 (d, $J = 7.5$ Hz, 2H), 7.39-7.36 (m, 4H), 7.06-7.02 (m, 4H), 3.99 (s, 8H), 3.68 (s, 12H), 3.29 (s, 1H), 2.78 (s, 8H).

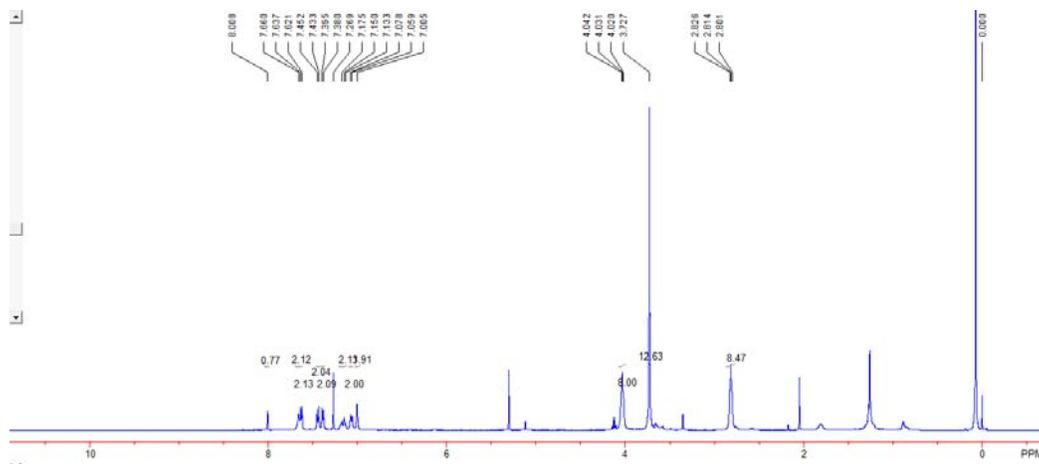


$^{13}\text{C NMR}$ (CDCl_3 , 100 MHz, TMS): δ 32.1, 47.5, 52.1, 77.2, 98.0, 113.9, 114.9, 117.9, 129.5, 130.3, 131.7, 131.9, 132.6, 155.9, 158.1, 171.5.

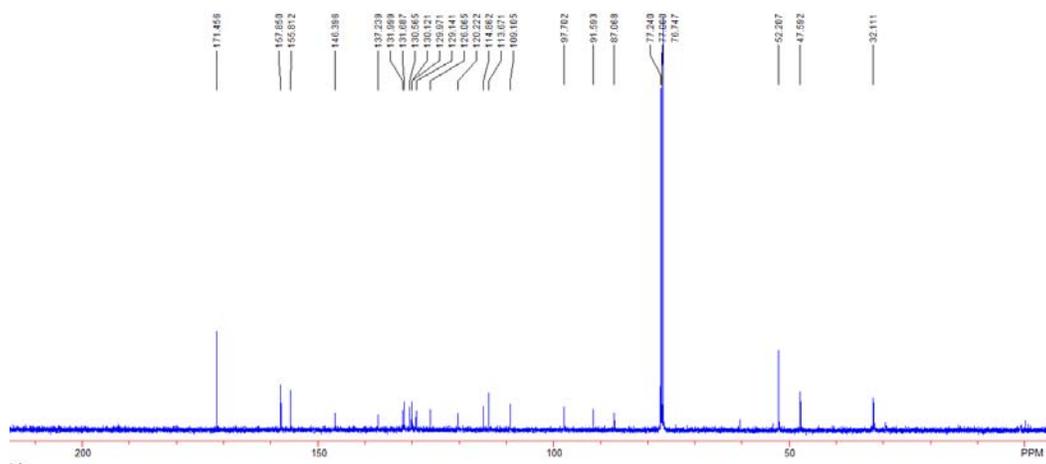


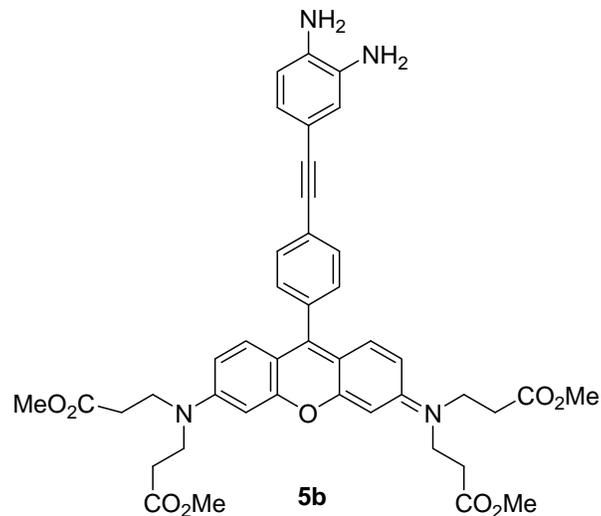


^1H NMR (CDCl_3 , 500 MHz, TMS): δ 8.01 (s, 1H), 7.66 (s, 2H), 7.65 (d, $J = 7.5$ Hz, 2H), 7.43 (d, $J = 9.5$ Hz, 2H), 7.39 (d, $J = 7.5$ Hz, 2H), 7.13-7.18 (m, 2H), 7.07 ($J = 9.5$ Hz, 2H), 7.00 (s, 2H), 4.03 (t, $J = 6.0$ Hz, 8H), 3.73 (s, 12H), 2.81 (t, $J = 6.0$ Hz, 8H).

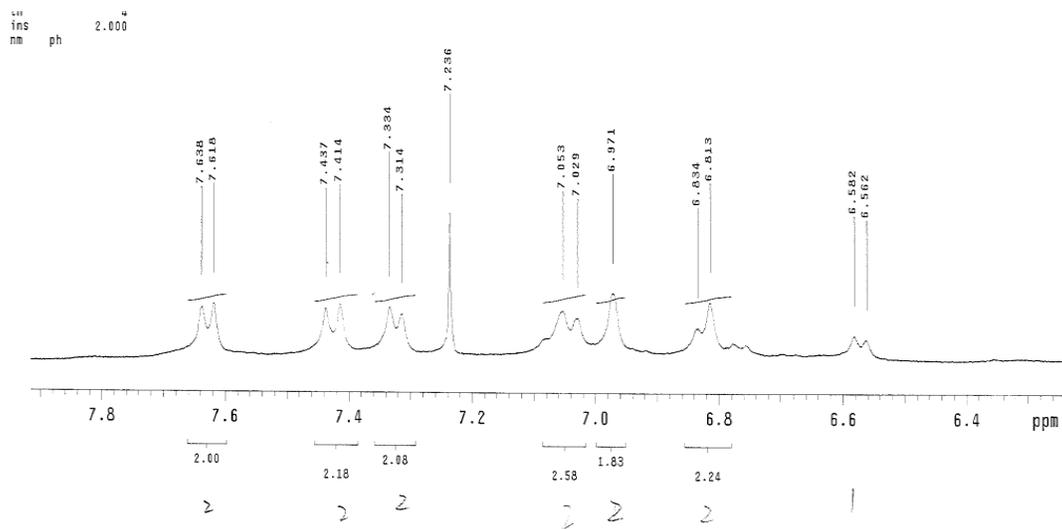


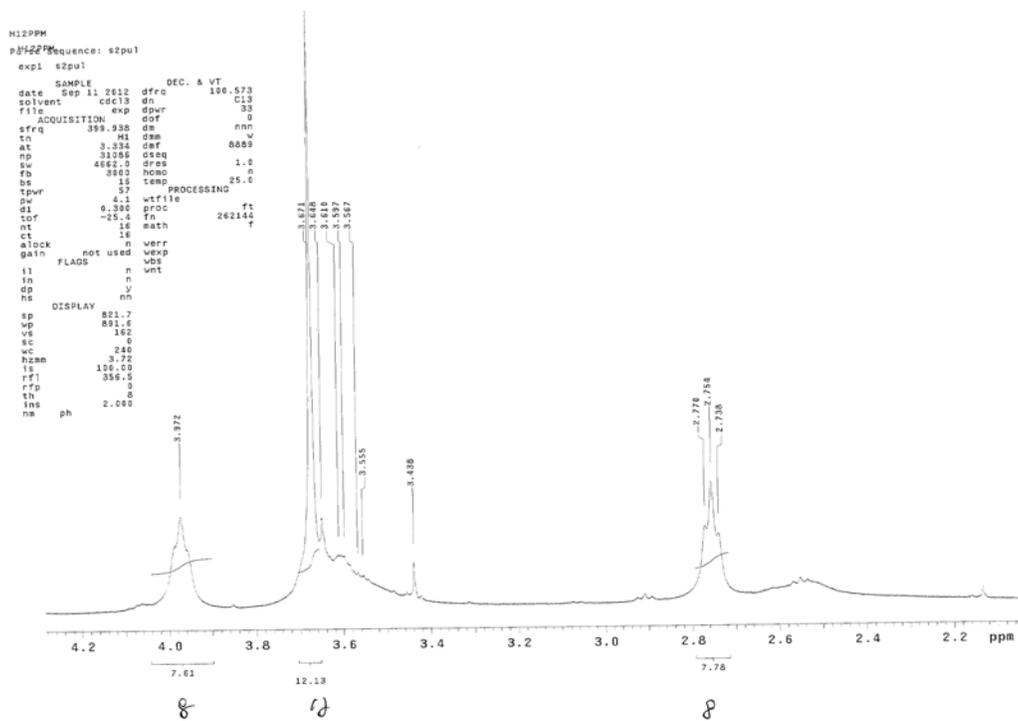
^{13}C NMR (CDCl_3 , 125 MHz, TMS): δ 32.1, 47.6, 52.2, 87.1, 91.6, 97.7, 109.1, 113.7, 114.9, 120.2, 126.1, 129.1, 130.0, 130.1, 130.6, 132.0, 137.2, 146.4, 155.8, 157.9, 171.5.



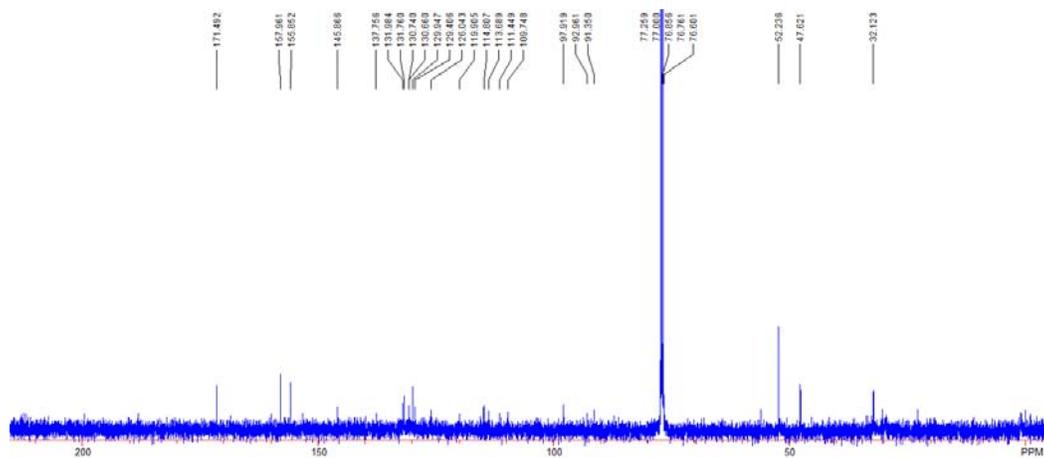


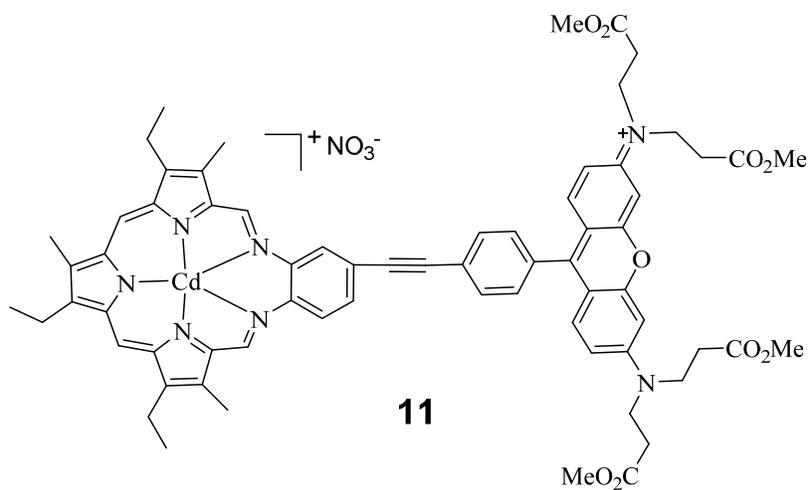
$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.63 (d, $J = 8$ Hz, 2H), 7.43 (d, $J = 9.2$ Hz, 2H), 7.32 (d, $J = 8$ Hz, 2H), 7.04 (d, $J = 9.6$ Hz, 2H), 6.97 (s, 2H), 6.82 (d, $J = 8.4$ Hz, 2H), 6.57 (d, $J = 8$ Hz, 1H), 3.97 (s, 8H), 3.67 (s, 12H), 2.75 (t, $J = 6.4$ Hz, 8H).



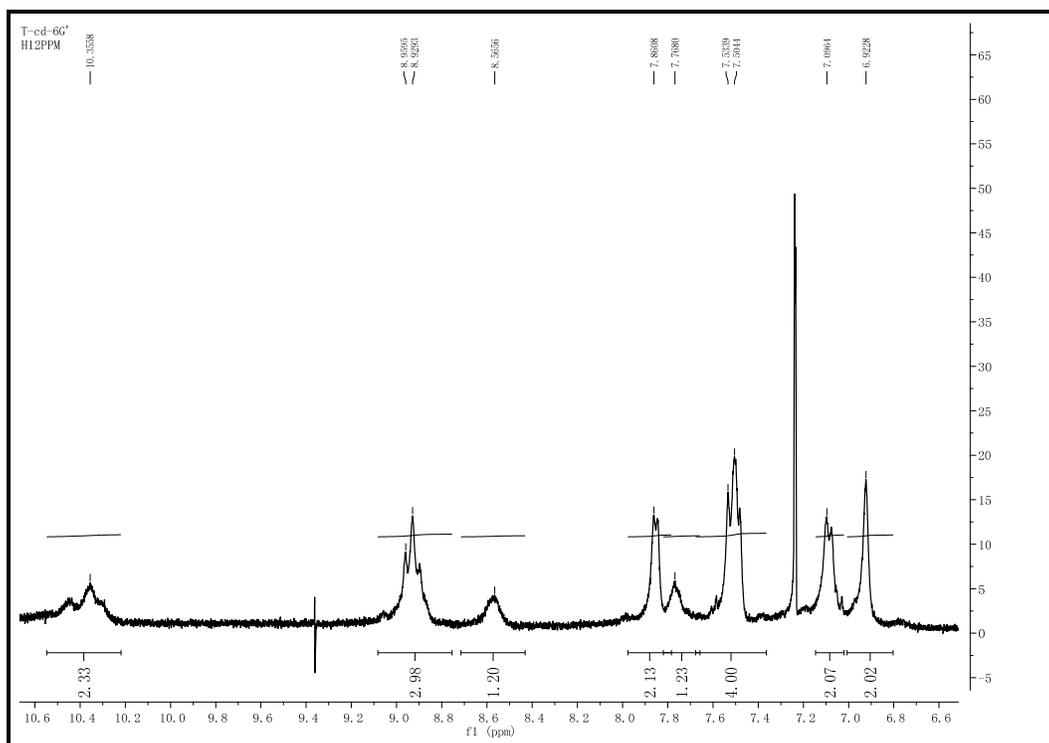


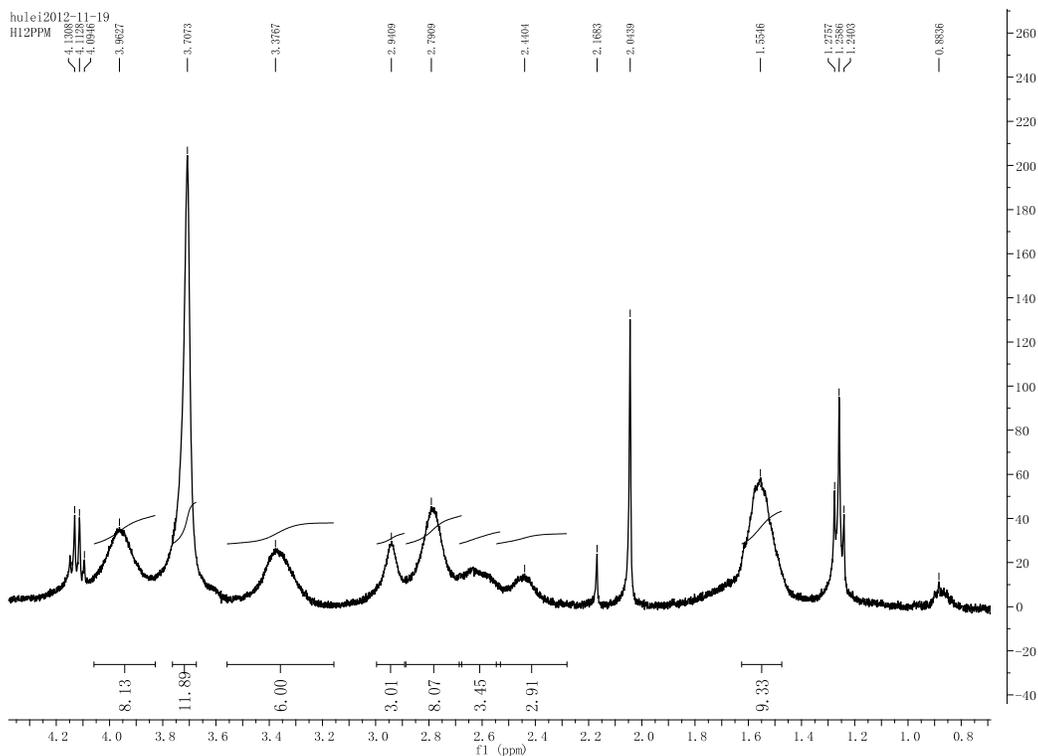
¹³C NMR (CDCl₃, 125 MHz, TMS): δ 32.1, 47.6, 52.2, 91.4, 93.0, 97.9, 109.7, 111.4, 113.7, 114.8, 119.9, 126.0, 129.4, 129.9, 130.66, 130.7, 131.8, 132.0, 137.8, 145.9, 155.9, 158.0, 171.5.



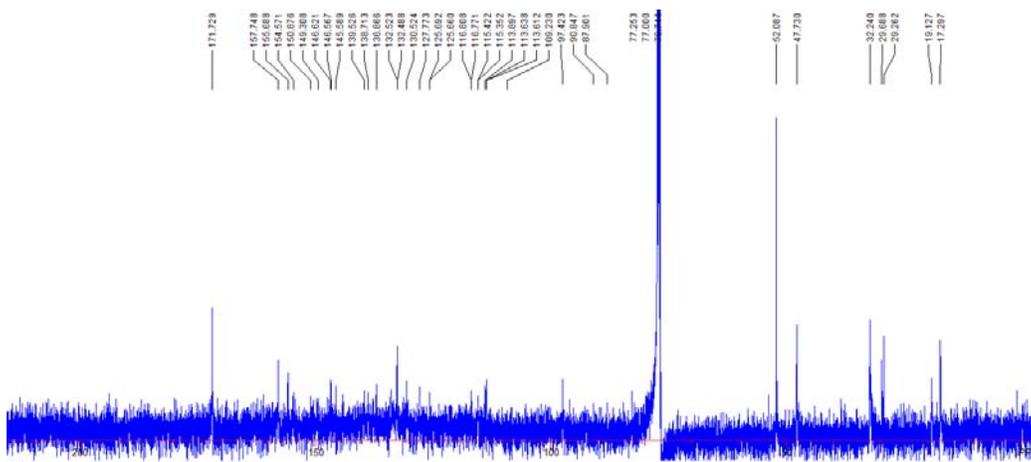


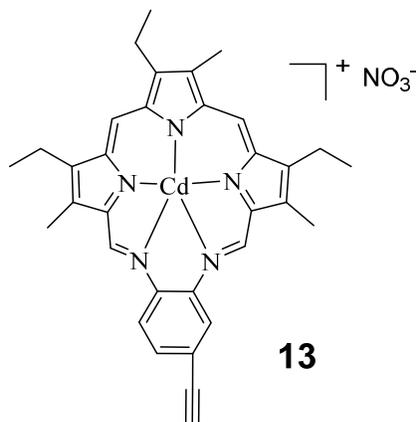
^1H NMR (400 MHz, CDCl_3): δ 10.58 (s, 1H), 10.50 (s, 1H), 9.02 (s, 3H), 8.72 (s, 1H), 7.89 (s, 2H), 7.77 (s, 1H), 7.51 (s, 4H), 7.14 (s, 2H), 6.99 (s, 2H), 3.94 (s, 8H), 3.68 (s, 12H), 3.35 (s, 6H), 2.92 (s, 3H), 2.77 (s, 8H), 2.61 (s, 3H), 2.42 (s, 3H), 1.53 (m, 9H).





^{13}C NMR (CDCl_3 , 125 MHz, TMS): δ 17.3, 19.1, 29.3, 2.7, 32.2, 47.7, 52.1, 87.9, 90.8, 97.4, 109.2, 113.61, 113.64, 113.9, 115.35, 115.42, 116.77, 116.81, 125.66, 125.69, 127.8, 130.5, 132.5, 136.9, 138.7, 139.5, 145.6, 146.56, 146.62, 149.3, 150.9, 154.6, 155.7, 157.7, 171.7.





^1H NMR (500 MHz, CDCl_3): δ 11.28 (s, 2H), 9.58 (m, 1H), 9.41 (m, 1H), 9.28 (d, 1H), 8.38 (m, 2H), 3.55-3.50 (m, 12H), 3.08-3.07 (m, 4H), 1.66-1.52 (m, 9H).

