

Supporting Information

Photostable Orange-Red Fluorescent Unsymmetrical Diketopyrrolopyrrole-BF₂ Hybrids

David C. Young,^a Mariusz Tasior,^a Adèle D. Laurent,^b Łukasz Dobrzycki,^c Michał K. Cyrański,^{*c} Nikolai Tkachenko,^{*c} Denis Jacquemin,^{*b} Daniel T. Gryko^{*a}

^a*Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44–52, 01-224, Warsaw, Poland.*

^b*Université de Nantes, CNRS, CEISAM UMR 6230, F-44000 Nantes, France.*

^c*Chemistry and Advanced Materials Group, Faculty of Engineering and Natural Sciences, Tampere University, Korkeakoulunkatu 8, FI-33720 Tampere, Finland.*

Email: dtgryko@icho.edu.pl

Table of Contents

Section S1	General Information	S2
Section S2	Experimental Procedures	S2
Section S3	Photophysical Data	S9
Section S4	Absorption and Emission Spectra	S14
Section S5	Fluorescence Lifetime Measurements	S23
Section S6	X-Ray Analysis	S32
Section S7	Theoretical Methods	S33
Section S8	Photostability Measurements	S75
Section S9	NMR Spectra	S77
Section S10	References	S99

Section S1: General Information

All chemicals are from commercial sources and were used as received, unless otherwise noted. All reported NMR spectra were recorded on Varian 500 MHz or Varian 600 MHz spectrometers. Chemical shifts (δ ; ppm) for ^1H and ^{13}C NMR spectra were determined with TMS or residual solvent signals as the internal reference. J values are given in Hz. Spectroscopic-grade solvents were used in all fluorescence/absorption-spectroscopy measurements. Mass spectra were obtained with EI ion source and the EBE double focusing geometry mass analyzer or spectrometer equipped with electro-spray ion source with Q-TOF type mass analyzer. The synthesis of compounds **1a-1c**,¹ **2a**,² **2b** and **2c**³ have been described previously.

Absorption and fluorescence spectra were recorded on a Shimadzu UV-3600 spectrometer and an Edinburgh Instruments FLS1000 photoluminescence spectrometer, respectively. Optical densities at the excitation wavelengths for fluorescence measurements were maintained at around 0.1 to avoid reabsorption. Fluorescence lifetimes were measured using a time-correlated single photon counting (TCSPC) technique. Samples were excited at 485 nm by a LDH-P-C-485 laser diode (PicoQuant Germany). The emission was detected by a micro-channel photomultiplier (R3809U-50, Hamamatsu Inc.) coupled with a monochromator. The signals were processed by PicoHarp 300 electronic module (PicoQuant GmbH). The fluorescence decay was collected with a maximum peak count of 10000 counts with a time resolution of 16 ps. Photostability was determined using an Asahi Spectra Max-350 as a light source and a Perkin Elmer Lambda 25 UV/Vis spectrometer.

Section S2: Experimental Procedures

Imidazo[1,2-a]quinoline-4-carbonitrile (**2d**)

A solution of 2-nitrobenzaldehyde (5.00 g, 33.1 mmol), malononitrile (2.40 g, 36.4 mmol) and 2 drops of pyridine were refluxed in methanol (20 mL) for 3 hours. During this time a white precipitate formed in the still hot solution. This solid was filtered and washed with methanol. This solid together with iron powder (7.31g, 0.166 mol) was slurried in ethanol (50 mL) and stirred at 45 °C for 30 minutes, then an aqueous solution of FeCl_3 (0.3 g, FeCl_3 dissolved in 6 ml water) was added dropwise. The mixture was then heated to reflux and monitored by TLC (1:1 EtOAc:hexanes). Upon completion of the reaction, the still hot slurry was filtered through celite, and the volatiles removed *in vacuo*. Addition of water to the residue produced an ochre product which was isolated by filtration. This was then recrystallized from THF to yield 2-amino-3-cyanoquinoline (3.9 g, 23.2 mmol, 70%) with spectra consistent to the literature.⁴

2-Amino-3-cyanoquinoline (0.86g, 5.1 mmol) was dissolved in hot ethanol (50 mL), and a 50% solution of chloroacetaldehyde was added (0.65 mL, 10.2 mmol) slowly. Heating was continued for 5 hours at which point the solution was poured into a solution of sat. NaHCO_3 . The product was then extracted into DCM, dried with MgSO_4 , concentrated *in vacuo* and recrystallized from ethyl acetate to yield an off-white powder (0.312g, 1.61 mmol, 32%).

^1H NMR (500 MHz, CDCl_3); 8.14 (d, $J=1.5$ Hz, 1H), 8.03 (s, 1H), 7.98 (d, $J=8.3$ Hz, 1H), 7.91 (td, $J=8.3, 0.7$ Hz, 1H), 7.83 (td, $J=7.6, 1.5$ Hz, 1H), 7.79 (d, $J=1.5$ Hz, 1H), 7.58 (t, $J=7.6$ Hz, 1H). ^{13}C NMR (126 MHz,

CDCl₃); 140.5, 133.8, 133.8, 133.6, 132.1, 130.2, 125.8, 121.5, 115.5, 114.9, 112.4, 102.7. ESI-TOF MS (in MeCN) m/z: Calculated for C₁₂H₈N₃ 194.0718, found 194.0717.

Benzo[h]benzo[4,5]imidazo[1,2-a]quinoline-8-carbonitrile (**2f**)

(2-Benzimidazolyl)acetonitrile (2.25 g, 14.3 mmol) and 1-bromo-2-naphthaldehyde (3.37 g, 14.3 mmol) were combined in ethanol (50 mL) with 3 drops of piperidine and refluxed for 5 hours. The bright yellow precipitate that formed in this time was filtered from the still warm solution and washed with ethanol then diethyl ether. The solid was then directly suspended in sulfolane (12 mL) and heated to 250 °C until cyclization was complete (monitored by TLC 1:1 EtOAc:hexanes, approximately 2 hours). The brown solution was then cooled to 100 °C at which point it was added to a vigorously stirred solution of water (150 mL) in a dropwise manner. The yellow precipitate which formed was filtered, washed with water, ethanol then diethyl ether to yield the title compound (3.45 g, 11.8 mmol, 82%). Spectral data matches that of this compound prepared through a different procedure.⁵

¹H NMR (500 MHz, DMSO-*d*₆); 8.85 (d, *J*=2.9 Hz, 1H), 8.71 (dd, *J*=8.8, 0.7 Hz, 1H), 8.24 (d, *J*=8.3 Hz, 1H), 8.16 (d, *J*=8.8 Hz, 1H), 7.99 - 8.10 (m, 3H), 7.87 (t, *J*=7.6 Hz, 1H), 7.73 (t, *J*=7.6 Hz, 1H), 7.62 (t, *J*=7.8 Hz, 1H), 7.42 (t, *J*=7.8 Hz, 1H). ¹³C NMR (126 MHz, DMSO-*d*₆); 146.3, 144.1, 139.6, 135.0, 133.3, 132.2, 129.6, 128.6, 126.5, 125.6, 125.5, 125.3, 124.1, 121.5, 121.0, 120.4, 120.1, 115.6, 115.4, 101.0. ESI-TOF MS (in MeCN) m/z: Calculated for C₂₀H₁₂N₃ 294.1031, found 294.1024.

General procedure for the synthesis of DPP derivatives **3a-3i**

A mixture of nitrile **2** (1.2 eq) and lithium tert-butoxide (4 eq) was heated to 100 °C under argon. To this solid mixture, pyrrolodone **1** (1 eq) dissolved in a 1:1 mixture of toluene and *tert*-amyl alcohol was added in a dropwise manner. The resulting dark purple/blue solution was left to stir at this temperature overnight. It was then cooled, quenched with acetic acid and the volatiles removed. The residue was extracted into dichloromethane, dried with MgSO₄ then the solvent was removed *in vacuo*. The resulting residue was recrystallized from an appropriate solvent to yield the desired DPP product.

Synthesis of **3a**

2a (0.26 g, 1.8 mmol) and **1a** (0.61 g, 1.5 mmol) in 8 mL of combined solvent were used to produce **3a** as a dark red solid (0.38 g, 0.91 mmol, 61%). Recrystallized from ethyl acetate.

¹H NMR (500 MHz, CDCl₃); 11.19 (br. s, 1H), 9.18 (d, *J*=7.3 Hz, 1H), 8.23 (d, *J*=6.7 Hz, 1H), 7.89 (d, *J*=8.8 Hz, 2H), 7.66 (d, *J*=6.6 Hz, 2H), 7.04 - 7.10 (m, 3H), 3.91 (s, 3H), 3.88 (t, *J*=7.5 Hz, 2H), 1.68 (quin, *J*=7.5 Hz, 2H), 1.35 (sxt, 7.5 Hz, 2H), 0.91 (t, *J*=7.5 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃); 162.6, 161.9, 161.8, 147.8, 142.1, 141.7, 133.1, 130.7, 128.1, 127.7, 120.6, 116.8, 114.5, 113.3, 113.0, 110.7, 110.3, 55.5, 42.1, 31.6, 20.1, 13.6. ESI-TOF MS (in MeCN) m/z: Calculated for C₂₄H₂₃N₄O₃ 415.1770, found 415.1762. m.p 199 °C.

Synthesis of **3b**

2b (0.40 g, 2.0 mmol) and **1a** (0.68 g, 1.7 mmol) in 8 mL of combined solvent were used to produce **3b** as a dark red solid (0.35 g, 0.75 mmol, 45%). Recrystallized from diethyl ether.

¹H NMR (500 MHz, CDCl₃); 11.19 (br. s, 1H), 9.14 (d, *J*=7.3, 1H), 8.15 (d, *J*=6.4 Hz, 1H), 7.89 (d, *J*=8.7, 2H), 7.39 (s, 1H), 7.08 (d, *J*=8.7 Hz, 2H), 6.98 (dd, *J*=7.3, 6.4 Hz, 2H), 3.92 (s, 3H), 3.89 (t, *J*=7.7 Hz, 2H), 1.68 (quin, *J*=7.7 Hz, 2H), 1.42 (s, 9H), 1.35 (sxt, 7.5 Hz, 2H), 0.91 (t, *J*=7.5 Hz, 2H). ¹³C NMR (126 MHz, CDCl₃); 162.5, 162.0, 161.8, 157.4, 142.3, 141.7, 130.7, 127.8, 127.5, 120.7, 120.4, 116.0, 114.4, 114.1, 112.6, 107.22, 55.5, 42.1, 32.4, 31.7, 30.11, 20.1, 13.6. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₂₈H₃₁N₄O₃ 471.2396, found 471.2400. m.p 200 °C.

Synthesis of **3c**

2c (0.56 g, 2.6 mmol) and **1a** (0.87 g, 2.1 mmol) in 8 mL of combined solvent were used to produce **3c** as a dark red solid (0.61 g, 1.2 mmol, 59%). Recrystallized from ethyl acetate.

¹H NMR (500 MHz, CDCl₃); 11.15 (br. s, 1H), 9.17 (d, *J*=7.4, 1H), 8.20 (d, *J*=6.5 Hz, 1H), 7.99 (d, *J*=7.8, 2H), 7.89 (m, 3H), 7.47 (t, *J*=7.7 Hz, 1H), 7.38 (m, 1H), 7.09 (d, *J*=8.8 Hz, 2H), 7.01 (dd, *J*=7.0, 6.4 Hz, 2H), 3.92 (s, 3H), 3.87 (t, *J*=7.7 Hz, 2H), 1.68 (m, 2H), 1.34 (sxt, 7.3 Hz, 2H), 0.92 (t, *J*=7.3 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃); 162.5, 161.9, 161.8, 147.7, 145.7, 142.3, 141.7, 132.6, 130.7, 128.8, 128.5, 128.2, 127.4, 126.3, 120.6, 116.3, 114.5, 113.4, 110.7, 110.2, 108.4, 55.5, 42.1, 31.7, 20.1, 13.6. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₃₀H₂₇N₄O₃ 491.2083, found 491.2078. m.p 222 °C.

Synthesis of **3d**

2d (0.26 g, 1.3 mmol) and **1a** (0.40 g, 1.1 mmol) in 8 mL of combined solvent were used to produce **3d** as a dark purple solid (0.26 g, 0.55 mmol, 50%). Recrystallized from ethylacetate.

¹H NMR (500 MHz, CDCl₃); 11.34 (br. s, 1H), 9.62 (s, 1H), 8.12 (m, 2H), 7.91 (m, 3H), 7.73 (t, *J*=8.1 Hz, 1H), 7.68 (s, 1H), 7.54 (t, *J*=7.6 Hz, 1H), 7.09 (d, *J*=8.8 Hz, 2H), 3.92 (s, 3H), 3.91 (m, 2H), 1.71 (quin, *J*=7.7 Hz, 2H), 1.38 (qt, *J*=7.7, 7.4 Hz, 2H), 0.93 (t, *J*=7.4 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃); 162.6, 162.0, 161.9, 147.7, 141.9, 140.9, 132.9, 131.8, 131.2, 130.8, 130.7, 130.1, 125.6, 123.5, 120.7, 115.9, 115.1, 114.5, 111.5, 110.8, 110.4, 55.5, 42.1, 31.7, 20.1, 13.7. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₂₈H₂₅N₄O₃ 465.1927, found 465.1924. m.p 218 °C.

Synthesis of **3e**

2e (0.70 g, 2.9 mmol) and **1a** (0.98 g, 2.4 mmol) in 16 mL of combined solvent were used to produce **3e** as a dark purple solid (0.65 g, 1.3 mmol, 53%). Recrystallized from ethyl acetate.

¹H NMR (500 MHz, CDCl₃); 11.59 (br. s, 1H), 9.86 (s, 1H), 8.6 (d, *J*=8.6 Hz, 1H), 8.45 (d, *J*=8.4 Hz, 1H), 8.16 (d, *J*=7.8 Hz, 1H), 8.08 (d, *J*=8.61 Hz, 1H), 7.93 (d, *J*=8.6 Hz, 2H), 7.85 (m, 1H), 7.61 (m, 1H), 7.56 (m, 2H), 7.10 (d, *J*=8.6 Hz, 2H), 3.93 (s, 3H), 3.91 (m, 2H), 1.75 (m, 2H), 1.37 (m, 2H), 0.94 (t, *J*=7.3 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃); 162.6, 162.0, 161.9, 147.8, 145.2, 143.6, 141.9, 135.8, 134.9, 131.8, 131.7, 130.7, 130.4, 125.1, 124.9, 123.5, 123.4, 120.7, 120.6, 115.9, 115.1, 114.5, 114.1, 110.8, 110.4, 55.5, 42.2, 31.7, 20.1, 13.7. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₃₂H₂₇N₄O₃ 515.2083, found 515.2084. m.p 240 °C.

Synthesis of **3f**

2f (0.44 g, 1.5 mmol) and **1a** (0.50 g, 1.2 mmol) in 8 mL of combined solvent were used to produce **3f** as a dark green solid (77 mg, 0.14 mmol, 11%). Recrystallized from diethyl ether.

¹H NMR (500 MHz, CDCl₃); 11.53 (br. s, 1H), 9.80 (s, 1H), 8.74 (d, *J*=8.6 Hz, 1H), 7.96 - 8.10 (m, 4H), 7.88 - 7.94 (m, 2H), 7.72 (t, *J*=7.5 Hz, 1H), 7.58 (m, 2H), 7.35 (dd, *J*=8.4, 7.2 Hz, 1H), 7.11 (d, *J*=8.6 Hz, 2H), 3.93 (s, 3H), 3.91 (m, 2H), 1.72 (qt, *J*=7.7, 7.2 Hz, 2H), 1.39 (qt, *J*=7.7, 7.3 Hz, 2H), 0.94 (t, *J*=7.3 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃); 162.6, 162.0, 161.9, 147.8, 146.6, 143.9, 141.6, 135.1, 134.1, 132.7, 131.9, 130.7, 128.8, 128.6, 126.6, 126.5, 125.5, 124.9, 124.4, 122.5, 122.4, 120.7, 120.6, 120.6, 115.8, 115.6, 114.5, 111.0, 110.5, 55.5, 42.2, 31.7, 20.1, 13.7. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₃₆H₂₉N₄O₃ 565.2240, found 565.2245. m.p 304 °C.

Synthesis of **3g**

2a (0.22 g, 1.5 mmol) and **1b** (0.52 g, 1.3 mmol) in 8 mL of combined solvent were used to produce **3g** as a red solid (0.18 g, 0.42 mmol, 33%). Recrystallized from ethyl acetate.

¹H NMR (500 MHz, CDCl₃); 11.09 (br. s, 1H), 9.18 (d, *J*=7.2 Hz, 1H), 8.24 (d, *J*=6.8 Hz, 1H), 7.65 (s, 1H), 7.57 (dd, *J*=7.5, 1.2 Hz, 1H), 7.49 (td, *J*=7.8, 1.4 Hz), 7.12 (t, *J*=7.7 Hz, 1H), 7.04 (m, 2H), 3.89 (s, 3H), 3.64 (m, 2H), 1.50 (quin, *J*=7.5 Hz, 2H), 1.20 (sxt, *J*=7.5 Hz, 2H), 0.79 (t, *J*=7.4 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃); 161.9, 161.8, 156.9, 145.4, 142.7, 142.1, 133.1, 132.3, 131.2, 128.5, 127.9, 121.1, 117.6, 116.7, 113.3, 113.0, 111.4, 111.4, 110.6, 55.6, 41.9, 31.3, 20.0, 13.5. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₂₄H₂₃N₄O₃ 415.1770, found 415.1773. m.p 127 °C.

Synthesis of **3h**

2e (0.35 g, 1.4 mmol) and **1b** (0.49 g, 1.2 mmol) in 8 mL of combined solvent were used to produce **3h** as a red solid (0.30 g, 0.56 mmol, 48%). Recrystallized from ethyl acetate.

¹H NMR (500 MHz, CDCl₃); 11.32 (s, 1H), 9.69 (s, 1H), 8.48 (d, *J*=8.5 Hz, 1H), 8.32 (d, *J*=8.4 Hz, 1H), 8.05 (d, *J*=7.8 Hz, 1H), 7.93 (d, *J*=8.0 Hz, 1H), 7.76 (m, 1H), 7.60 (dd, *J*=7.4, 1.5 Hz, 1H), 7.53 (m, 4H), 7.17 (m, 1H), 7.09 (d, *J*=8.5 Hz, 1H), 3.94 (s, 3H), 3.69 (br. m, 2H), 1.56 (quin, *J*=7.5 Hz), 1.24 (m, 2H), 0.82 (t, *J*=7.4 Hz, 3H). ¹³C NMR (126 MHz, CDCl₃); 161.8, 161.8, 156.9, 145.3, 144.8, 143.4, 142.7, 135.7, 135.1, 132.4, 131.7, 131.7, 131.2, 130.2, 125.0, 124.8, 123.4, 123.1, 121.2, 120.6, 117.7, 115.5, 115.0, 114.0, 111.5, 110.6, 55.6, 41.9, 31.4, 20.0, 13.6. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₃₂H₂₇N₄O₃ 515.2083, found 515.2087. m.p 250 °C.

Synthesis of **3i**

2e (0.21 g, 0.86 mmol) and **1c** (0.30 g, 0.72 mmol) in 8 mL of combined solvent were used to produce **3i** as a green solid (0.22 g, 0.41 mmol, 57%). Recrystallized from ethyl acetate.

¹H NMR (500 MHz, CDCl₃); 11.49 (s, 1H), 9.74 (s, 1H), 8.54 (d, *J*=8.3 Hz, 1H), 8.38 (d, *J*=8.2 Hz, 1H), 8.09 (d, *J*=7.8 Hz, 1H), 8.02 (d, *J*=7.8 Hz, 1H), 7.97 (d, *J*=8.9 Hz, 2H), 7.78 (t, *J*=7.8 Hz, 1H), 7.56 (m, 1H), 7.50 (m, 2H), 6.83 (d, *J*=8.9 Hz, 2H), 3.93 (t, *J*=8.0 Hz, 2H), 1.78 (t, *J*=8.0, 7.5 Hz, 2H), 1.43 (qt, *J*=7.5, 7.4 Hz, 2H), 0.98 (t, *J*=7.4 Hz, 1H). ¹³C NMR (126 MHz, CDCl₃); 163.0, 161.8, 152.1, 149.3, 145.2, 143.6, 139.4, 135.5, 133.7, 131.5, 131.2, 130.8, 130.3, 124.9, 124.7, 123.5, 123.3, 120.7, 116.0, 115.2, 115.0, 114.0, 111.6, 111.2, 109.0, 42.5, 40.0, 31.8, 20.2, 13.8. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₃₃H₃₀N₅O₂ 528.2400, found 528.2405. m.p 216 °C.

General procedure A for the synthesis of **4** (using Et₃N)

To a solution of **3** (0.1 g) in dry DCM (10 mL) under argon was added Et₃N (10 eq) with no observable color change. Subsequently, BF₃·OEt₂ was added slowly at room temperature and stirring was continued overnight. The reaction was quenched with water and extracted into DCM. The residue was purified by column chromatography (DCM/MeOH).

General procedure B for the synthesis of **4** (using LiHMDS)

To a solution of **3** (0.1 g) in dry DCM (10 mL) under argon was added a 1.0M THF solution of LiHMDS (1.2 eq) which rapidly darkened the solution. Subsequently, BF₃·OEt₂ was added slowly at room temperature and stirring was continued overnight. The reaction was quenched with water and extracted into DCM. The residue was purified by column chromatography (DCM/MeOH).

Note - Despite many attempts in a range of solvents, the solubility of DPP-BF₂ compounds with large aromatic imidazopyridine substituents at levels required for well resolved ¹³CNMR spectra proved difficult. In these cases some quaternary carbon atoms are not observed.

Synthesis of **4a**

General Procedure B; Yield 37 %.

¹H NMR (500 MHz, DMSO-*d*₆); 8.96 (d, *J*=7.6 Hz, 1H), 8.90 (d, *J*=7.6 Hz, 1H), 8.40 (d, *J*=2.0 Hz, 1H), 8.20 (d, *J*=2.0 Hz, 1H), 7.92 (d, *J*=8.4 Hz, 2H), 7.65 (t, *J*=7.1 Hz, 1H), 7.16 (d, *J*=8.4 Hz, 2H), 3.88 (m, 5H), 1.48 (m, 2H), 1.21 (m, 2H), 0.80 (m, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆); 161.6, 161.5, 161.3, 147.1, 139.0, 137.5, 130.6, 130.1, 129.2, 124.3, 120.2, 117.3, 114.4, 113.0, 111.4, 110.6, 109.5, 55.5, 40.9, 30.8, 19.3, 13.4. ¹⁹F NMR (470 MHz, DMSO-*d*₆); -148.4. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₂₄H₂₁N₄O₃BF₂Na 485.1572, found 485.1579. m.p 155 °C.

Synthesis of **4b**

General Procedure B; Yield 50 %.

¹H NMR (500 MHz, DMSO-*d*₆); 8.98 (dd, *J*=7.2, 1.0 Hz, 1H), 8.79 (dd, *J*=6.7, 1.0 Hz, 1H), 8.22 (s, 1H), 7.90 (d, *J*=8.9 Hz, 2H), 7.61 (dd, *J*=7.2, 6.7 Hz, 1H), 7.14 (d, *J*=8.9 Hz, 2H), 3.86 (s, 3H), 3.82 (m, 2H), 1.48 (s, 6H), 1.45 (m, 2H), 1.21 (s, 3H), 1.18 (m, 2H), 0.78 (t, *J*=7.4 Hz, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆); 163.7, 161.4, 161.2, 149.7, 146.6, 139.2, 130.5, 129.7, 129.2, 120.2, 117.0, 144.4, 112.8, 111.5, 109.5, 105.9, 55.5, 32.4, 30.8, 29.5, 22.1, 19.29, 13.9, 13.4. ¹⁹F NMR (470 MHz, DMSO-*d*₆); -132.5, -148.3. ESI-TOF MS (in MeCN) *m/z*: Calculated for C₂₈H₂₉N₄O₃BF₂Na 541.2198, found 541.2207. decomp. at 200 °C.

Synthesis of **4c**

General Procedure B; Yield 44 %.

¹H NMR (500 MHz, DMSO-*d*₆); 9.03 (d, *J*=7.4 Hz, 1H), 8.91 (d, *J*=6.8 Hz, 1H), 8.63 (s, 1H), 7.96 (dd, *J*=7.4, 1.8 Hz, 2H), 7.91 (d, *J*=8.3 Hz, 2H), 7.68 (t, *J*=7.1 Hz, 1H), 7.56 (m, 3H), 7.15 (d, *J*=8.3 Hz, 2H), 3.88 (s, 3H), 3.85 (m, 2H), 1.48 (m, 2H), 1.21 (m, 2H), 0.80 (m, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆); 163.7, 161.4, 161.3, 146.9, 139.2, 130.6, 130.5, 129.8, 129.3, 129.0, 128.7, 127.9, 120.2, 120.1, 117.5, 114.5, 114.4, 113.0,

111.4, 109.5, 55.5, 40.9, 30.7, 19.3, 13.4. ESI-TOF MS (in MeCN) m/z: Calculated for C₃₀H₂₅N₄O₃BF₂Na 561.1885, found 561.1896. m.p 248 °C.

Synthesis of **4d**

General Procedure B; Yield 46 %.

¹H NMR (500 MHz, toluene-*d*₈); 9.81 (s, 1H), 7.98 (d, *J*=9.0 Hz, 2H), 7.68 (m, 1H), 7.33 (m, 2H), 7.21 (m, 1H), 7.06 (1, 2H), 6.96 (m, partially obscured by residual solvent), 6.76 (d, *J*=9.0 Hz, 2H), 3.83 (t, *J*=7.6 Hz, 2H), 3.26 (s, 3H), 1.64 (m, 2H), 1.26 (m, 2H), 0.81 (t, *J*=7.4 Hz, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆); 162.3, 161.6, 161.3, 146.7, 141.5, 140.8, 132.5, 131.3, 130.8, 130.6, 129.5, 128.9, 124.3, 123.6, 121.1, 116.1, 114.5, 114.1, 111.2, 110.9, 110.7, 54.4, 41.7, 31.6, 20.6, 13.4. ¹⁹F NMR (470 MHz, toluene-*d*₈); -147.5. ESI-TOF MS (in MeCN) m/z: Calculated for C₂₈H₂₃N₄O₃BF₂Na 535.1729, found 535.1736. decomp. at. 204 °C.

Synthesis of **4e**

General Procedure A; Yield 9 %. General Procedure B; Yield 62 %. Instead of column chromatography, residue was purified by slurrying in 2mL DMF, then filtering and washing with DMF then diethyl ether.

¹H NMR (500 MHz, CD₂Cl₂ + TFA); 9.68 (s, 1H), 8.77 (d, *J*=8.6 Hz, 1H), 8.61 (m, 1H), 8.34 (d, *J*=7.4 Hz, 1H), 8.21 (m, 1H), 8.12 (m, 1H), 7.97 (m, 1H), 7.87-7.80 (m, 4H), 7.10 (d, *J*=8.8 Hz, 2H), 3.92 (s, 3H), 3.89 (m, 2H), 1.68 (m, 2H), 1.35 (m, 2H), 0.91 (t, *J*=7.3 Hz, 3H). ¹³C NMR (126 MHz, CD₂Cl₂ + TFA); 167.0, 165.2, 163.4, 138.7, 136.9, 134.4, 133.4, 132.7, 131.9, 130.3, 129.6, 129.1, 128.4, 127.1, 124.1, 117.5, 116.9, 116.4, 116.1, 115.8, 115.4, 112.2, 110.6, 56.5, 43.2, 31.6, 20.5, 13.8. ¹⁹F NMR (470 MHz, CD₂Cl₂ + TFA); -146.3. ESI-TOF MS (in MeCN) m/z: Calculated for C₃₂H₂₅N₄O₃BF₂Na 585.1885, found 585.1889. m.p 239 °C.

Synthesis of **4g**

General Procedure A; Yield 5 %.

¹H NMR (500 MHz, DMSO-*d*₆); 8.95 (d, *J*=7.4 Hz, 1H), 8.93 (d, *J*=6.8 Hz, 1H), 8.41 (1H), 8.20 (1H), 7.66 (t, *J*=7.1 Hz, 1H), 7.57 (m, 1H), 7.50 (m, 1H), 7.25 (d, *J*=8.3 Hz, 1H), 7.13 (t, *J*=7.4 Hz, 1H), 3.86 (s, 3H), 3.52 (m, 2H), 1.35 (quin, *J*=7.0 Hz, 2H), 1.09 (td, *J*=7.4 Hz, *J*=7.0 Hz, 2H), 0.69 (t, *J*=7.4 Hz, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆); 163.6, 160.6, 156.6, 144.6, 140.3, 137.5, 132.5, 130.8, 130.4, 129.5, 124.3, 120.7, 117.3, 117.0, 116.92, 112.9, 112.5, 111.9, 110.2, 55.7, 40.7, 30.6, 19.1, 13.2. ¹⁹F NMR (470 MHz, DMSO-*d*₆); -140.4. ESI-TOF MS (in MeCN) m/z: Calculated for C₂₄H₂₁N₄O₃BF₂Na 485.1572, found 485.1576. decomp. at. 215 °C.

Synthesis of **4h**

General Procedure A; Yield 9 %. General Procedure B; Yield 41 %.

¹H NMR (500 MHz, DMSO-*d*₆); 9.68 (s, 1H), 9.12 (d, *J*=8.3 Hz, 1H), 9.07 (d, *J*=8.3 Hz, 1H), 8.36 (d, *J*=8.0 Hz, 1H), 8.12 (m, 2H), 7.89-7.78 (m, 3H), 7.60 (m, 1H), 7.56 (m, 1H), 7.28 (d, *J*=8.3 Hz, 1H), 7.16(t, *J*=7.4 Hz, 1H), 3.89 (s, 3H), 3.57 (m, 2H), 1.41 (m, 2H), 1.12 (m, 2H), 0.72 (t, *J*=7.4 Hz, 3H). ¹³C NMR (126 MHz, DMSO-*d*₆); 163.4, 160.6, 156.6, 144.6, 141.2, 140.6, 135.5, 134.0, 133.9, 133.2, 132.6, 131.9, 130.9, 129.4, 127.8, 127.3, 125.8, 123.9, 120.8, 117.4, 117.1, 116.5, 116.0, 112.4, 111.9, 111.8, 110.1, 55.7,

45.8, 30.6, 19.2, 13.3. ESI-TOF MS (in MeCN) m/z: Calculated for $C_{32}H_{25}N_4O_3BF_2Na$ 585.1885, found 585.1893. decomp. at. 240 °C.

Synthesis of **4i**

General Procedure A; Yield 10 %.

1H NMR (500 MHz, DMSO- d_6); 9.57 (s, 1H), 9.02 (m, 2H), 8.27 (m, 1H), 8.10 (m, 1H), 8.06, (m, 1H), 7.99 (d, $J=9.0$ Hz, 2H), 7.85 (m, 1H), 7.80 (m, 1H), 6.84 (d, $J=9.0$ Hz, 2H), 3.88 (m, 2H), 3.06 (s, 6H), 1.57 (m, 2H), 1.26 (m, 2H), 0.85 (m, 3H). Solubility prevented well resolved ^{13}C NMR. ^{19}F NMR (470 MHz, DMSO- d_6); 142.3. ESI-TOF MS (in MeCN) m/z: Calculated for $C_{33}H_{29}N_5O_2BF_2$ 576.2382, found 576.2401. decomp. at. 244 °C.

Section S3: Absorption and Emission Data

Most of emission decays could be fitted successfully to a single exponent accounting for a background due to the instruments dark counts. In some cases a bi-exponential decay model had to be used, but when the second component contribution was less than 5% it was ignored. Other case are marked in the table and discussed separately in the Table S1 footnote field.

Table S1. Photophysical data of DPPs and DPP-BF₂ hybrids in a range of solvents.

Dye	Solvent	$\max\lambda_{\text{abs}}$ [nm]	ϵ_{max} [M ⁻¹ cm ⁻¹]	$\max\lambda_{\text{ems}}$ [nm]	Stokes shift [cm-1]	$\Phi_{\text{fl}}^{\text{a}}$	τ_{F} [ns]	k_{r} [10 ⁸ s ⁻¹]	k_{nr} [10 ⁸ s ⁻¹]
3a	Toluene	512, 549	12900, 13700	573, 611	760	0.78	5.2	1.5	0.4
	THF	508, 546	14900, 15800	566, 611	650	0.72	5.4	1.3	0.5
	CHCl ₃	509, 544	15000, 15900	569, 614	810	0.63	5.5	1.1	0.7
	DMF	507, 542	12700, 13700	566, 611	780	0.70	5.4	1.3	0.6
	MeCN	503, 536	17400, 18100	562, 605	860	0.54	5.4	1.0	0.9
	MeOH	504, 530	14800, 17000	565, 604	1170	0.43	3.6	1.2	1.6
3b	Toluene	510, 549	13600, 14400	570, 617	670	0.79	5.1	1.5	0.4
	THF	510, 544	13500, 14100	565, 610	680	0.71	5.3	1.3	0.5
	CHCl ₃	509, 544	17400, 18500	568, 613	780	0.61	5.2	1.2	0.8
	DMF	507, 543	15400, 16500	565, 611	720	0.76	5.4	1.4	0.4
	MeCN	503, 537	13100, 13300	562, 605	830	0.73	5.4	1.4	0.5
	MeOH	504, 530	12500, 15200	562, 604	1070	0.59	3.7	1.6	1.1
3c	Toluene	516, 555	16800, 17800	576, 622	660	0.69	5.0	1.4	0.6
	THF	512, 549	20800, 21600	570, 616	670	0.62	5.2	1.2	0.7
	CHCl ₃	513, 548	24100, 25400	573, 618	800	0.58	5.1	1.1	0.8
	DMF	511, 546	19300, 20400	572, 614	830	0.71	5.3	1.3	0.5
	MeCN	506, 539	21200, 21400	567, 610	920	0.60	5.3	1.1	0.8
	MeOH	503, 535	16800, 19200	568, 611	1100	0.47	3.7	1.3	1.4
3d	Toluene	521, 561	17700, 18500	584, 633	700	0.71	4.9	1.4	0.6
	THF	517, 558	18900, 19700	580, 627	680	0.62	5.0	1.2	0.8
	CHCl ₃	517, 554	19600, 20400	581, 629	840	0.70	5.1	1.4	0.6
	DMF	516, 554	18200, 19200	580, 627	810	0.53	4.9	1.1	1.0

	MeCN	511, 546	16600, 16900	576, 620	950	0.59	4.8	1.2	0.9
	MeOH	508, 540	14800, 16500	579, 625	1250	0.43	3.2	1.3	1.8
3e	Toluene	534, 576	35700, 34600	601, 653	720	0.32	3.1	1.0	2.2
	THF	531, 572	30900, 30000	598, 646	760	0.36	3.4	1.1	1.9
	CHCl ₃	530, 567	25100, 24700	597, 646	890	0.36	3.3	1.1	1.9
	DMF	529, 567	31600, 31000	601, 645	1000	0.37	3.3	1.1	1.9
	MeCN	524, 560	28600, 27900	595, 640	1050	0.32	3.1	1.0	2.2
	MeOH	520, 550	26900, 28600	597, 645	1430	0.23	2.1	1.1	3.7
3f	Toluene	552, 595	34800, 32600	626, 678	830	0.27	2.7	1.0	2.7
	THF	549, 593	29300, 27700	620, 676	730	0.32	2.9	1.1	2.3
	CHCl ₃	547, 588	27100, 26200	618, 673	830	0.38	2.8	1.4	2.2
	DMF	546, 589	29600, 28700	623, 674	930	0.33	2.8	1.2	2.4
	MeCN	541, 577	31600, 30300	616, 670	1100	0.31	2.8	1.1	2.5
	MeOH	537, 572	24700, 26300	616, 669	1250	0.15	1.5	1.0	5.7
3g	Toluene	506, 536	14700, 12600	566, 611	920	0.60	5.4	1.1	0.7
	THF	502, 534	13900, 11800	560, 605	870	0.50	5.7	0.9	0.9
	CHCl ₃	501, 530	15600, 13800	566, 611	1200	0.50	5.5	0.9	0.9
	DMF	497, 529	14100, 12600	564, 604	1170	0.55	5.5	1.0	0.8
	MeCN	494, 521	15200, 13400	558, 603	1270	0.55	5.4	1.0	0.8
	MeOH	496, 505	16600, 16600	564, 604	2430	0.25	3.1	0.8	2.4
3h	Toluene	527, 564	25800, 20800	599, 648	1040	0.25	2.9	0.9	2.6
	THF	525, 562	27100, 21800	596, 644	1020	0.29	3.1	0.9	2.3
	CHCl ₃	521, 555	22400, 20100	595, 640	1210	0.27	3.1	0.9	2.4
	DMF	519, 554	28700, 23400	596, 637	1270	0.27	3.3	0.8	2.2
	MeCN	516, 546	26700, 22000	591, 634	1340	0.21	2.9	0.7	2.7
	MeOH	510, 535	21600, 19700	594, 641	1860	0.13	1.8	0.7	4.8
3i	Toluene	555, 602	25900, 33800	630, 684	740	0.97	4.1	2.4	0.1
	THF	555, 600	26700, 33600	646, 691	1190	0.66	4.3	1.5	0.8

	CHCl ₃	557, 596	27300, 35600	636, 687	1060	0.69	4.3	1.6	0.7
	DMF	559, 598	22700, 28900	667	1730	0.16	6.9, 1.0 ^b	-	-
	MeCN	553, 589	17200, 23000	654	1690	0.34	1.3	2.6	5.1
	MeOH	550, 586	19600, 27100	651	1700	0.01	- ^c	-	-
4a	Toluene	338, 545	58,006,800	613, 655	2040	0.44	5.4	0.8	1.0
	THF	550	8100	611	1820	0.48	5.5	0.9	0.9
	CHCl ₃	546	10100	608	1870	0.31	5.8	0.5	1.2
	DMF	517, 551	7400, 7900	599	1450	0.52	5.8	0.9	0.8
	MeCN	514, 542	8800, 5800	598	1730	0.45	5.8	0.8	0.9
	MeOH	537	9400	594	1790	0.35	4.5	0.8	1.4
4b	Toluene	540, 576	14600, 15100	612	1020	0.44	5.3	0.8	1.1
	THF	525, 563	12300, 12500	602	1150	0.25	5.4	0.5	1.4
	CHCl ₃	534, 570	13700, 14700	606	1040	0.42	5.8	0.7	1.0
	DMF	519, 556	14800, 16100	598	1260	0.52	6.0	0.9	0.8
	MeCN	514, 550	14900, 15900	594	1350	0.51	6.00	0.9	0.8
	MeOH	332, 540	10800, 18600	591	1600	0.38	4.3	0.9	1.4
4c	Toluene	541, 577	11700, 12000	617, 659	1120	0.44	5.5	0.8	1.0
	THF	531, 569	11500, 11800	611, 658	1210	0.46	5.7	0.8	0.9
	CHCl ₃	537, 574	11100, 11500	611, 655	1050	0.47	5.9	0.8	0.9
	DMF	523, 560	11500, 12200	604, 635	1300	0.51	5.9	0.9	0.8
	MeCN	519, 550	11700, 12200	600	1520	0.47	6.1	0.8	0.9
	MeOH	544	13500	598	1660	0.37	4.6	0.8	1.4
4d	Toluene	555, 598	20900, 19800	638	1050	0.42	4.9	0.9	1.2
	THF	547, 587	17600, 16600	626	1060	0.49	4.9	1.0	1.0
	CHCl ₃	546, 585	16300, 16200	625	1090	0.50	5.3	0.9	0.9
	DMF	536, 571	17400, 17800	621	1410	0.54	5.3	1.0	0.9
	MeCN	531, 562	15800, 15800	625	1790	0.59	5.7	1.0	0.7
	MeOH	555	19400	620	1890	0.35	3.6	1.0	1.8

4e	Toluene	573, 605	20300, 16200	664	1470	0.16	2.7	0.6	3.1
	THF	566, 590	15400, 13100	654	1660	0.16	2.9	0.6	2.9
	CHCl ₃	566, 603	24800, 20700	652	1250	0.22	3.0	0.7	2.6
	DMF	551	22400, 21200	659	2970	0.22	3.4	0.6	2.3
	MeCN	546	19700	657	3090	0.19	2.9	0.7	2.8
	MeOH	564	18200	657	2510	0.10	1.7	0.6	5.3
4g	Toluene	533, 565	17100, 14900	611, 656	1330	0.49	5.5	5.5	5.5
	THF	521, 554	21600, 19000	604, 640	1490	0.51	5.9	5.9	5.9
	CHCl ₃	525, 558	15000, 13700	604, 654	1360	0.51	6.0	6	6
	DMF	508, 541	21900, 19900	590, 628	1540	0.62	6.4	6.4	6.4
	MeCN	505, 531	22800, 21000	589, 629	1850	0.49	6.3	6.3	6.3
	MeOH	503, 521	25900, 25300	599	2500	0.25	3.9	3.9	3.9
4h	Toluene	568, 603	13100, 10600	667	1590	0.09	2.1	0.4	4.3
	THF	555, 592	12300, 10200	667	1900	0.09	1.9	0.5	4.8
	CHCl ₃	555, 583	10700, 9200	656	1910	0.07	2.5	0.3	3.7
	DMF	540, 573	13800, 11500	668	2480	0.15	2.8	0.5	3.0
	MeCN	531, 559	13600, 12000	665	2850	0.13	2.4	0.5	3.6
	MeOH	527	15100	660	3820	0.07	1.4	0.5	6.6
4i	Toluene	601, 650	16000, 15800	697	1040	0.19	2.5	0.8	3.2
	THF	602, 634	18200, 17500	706	1610	0.14	2.5	0.6	3.4
	CHCl ₃	601, 644	13300, 14400	702	1280	0.27	2.9	0.9	2.5
	DMF	619	17200	723	2320	0.15	5.6, 0.8 ^d	-	-
	MeCN	607	18100	717	2530	0.11	1.1	1.0	8.1
	MeOH	604	15900	710	2470	0.01	- ^e	-	-

^aQuantum yields determined using rhodamine 6g in EtOH. Quantum yields of selected samples were compared to those determined using an integrating sphere and negligible differences were observed.

^b bi-exponential decay **3i** in DMF was observed with dominating 1 ns decay component.

^c the emission intensity was very weak and the lifetime below the instrument resolution, which is attributed to specific interaction of **3i** with MeOH and strong molecule distortion resulting in the fast quenching of the excited state.

^d bi-exponential decay of **4i** in DMF was observed with dominating 0.8ns decay component.

^e the emission intensity was very weak and the lifetime below the instrument resolution, which is attributed to specific interaction of **4i** with MeOH and strong molecule distortion resulting in the fast quenching of the excited state.

Section S4: Absorption and Emission Spectra

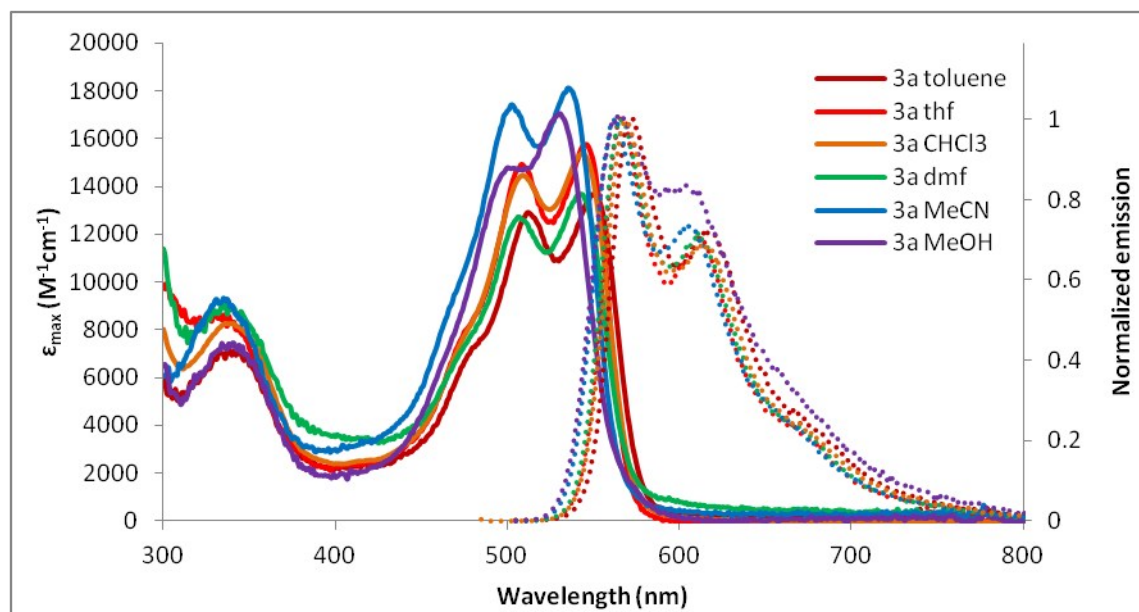


Figure S1. Absorption (solid lines) and emission (dashed lines) spectra of **3a** in various solvents.

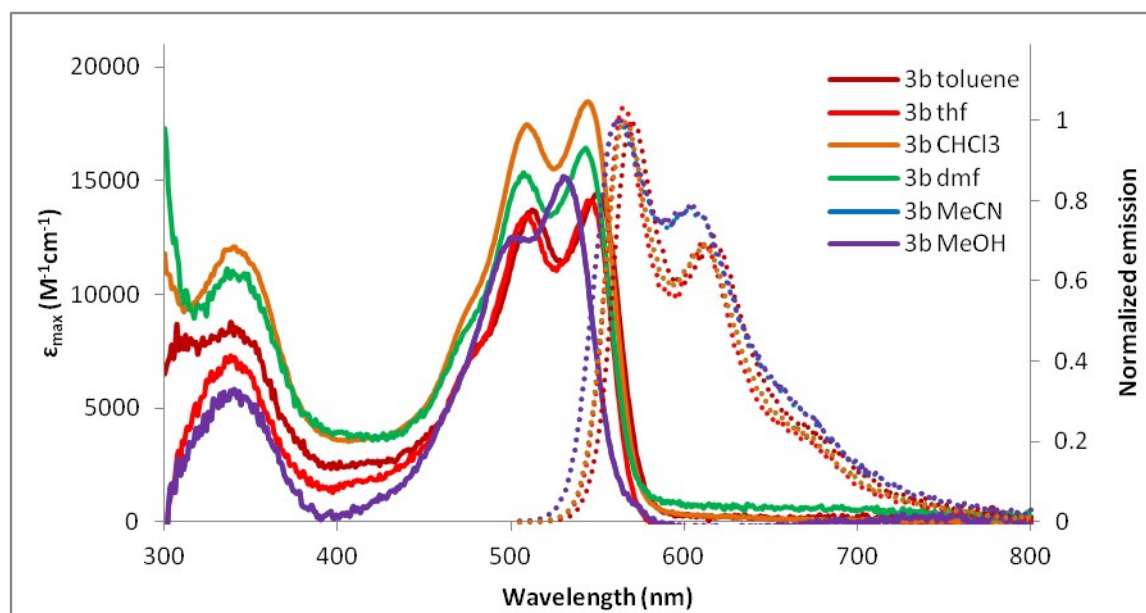


Figure S2. Absorption (solid lines) and emission (dashed lines) spectra of **3b** in various solvents.

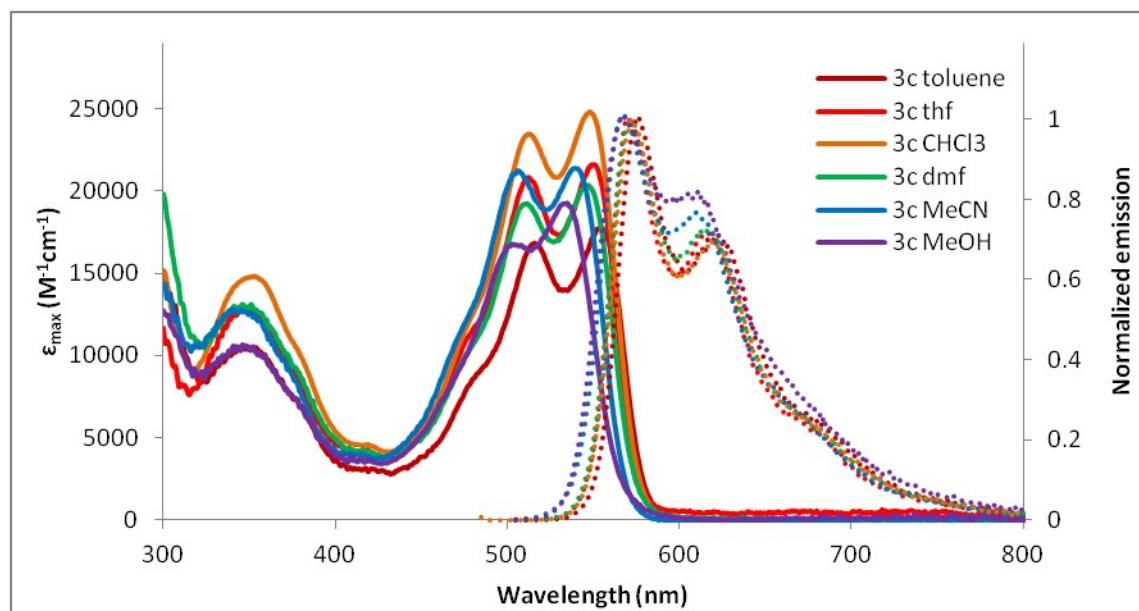


Figure S3. Absorption (solid lines) and emission (dashed lines) spectra of **3c** in various solvents.

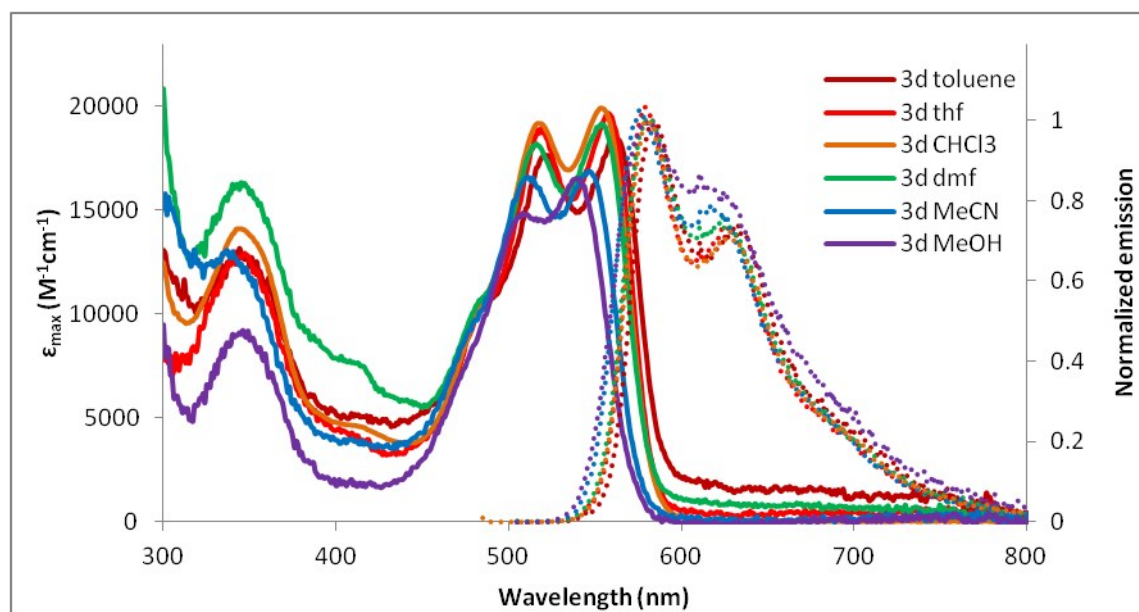


Figure S4. Absorption (solid lines) and emission (dashed lines) spectra of **3d** in various solvents.

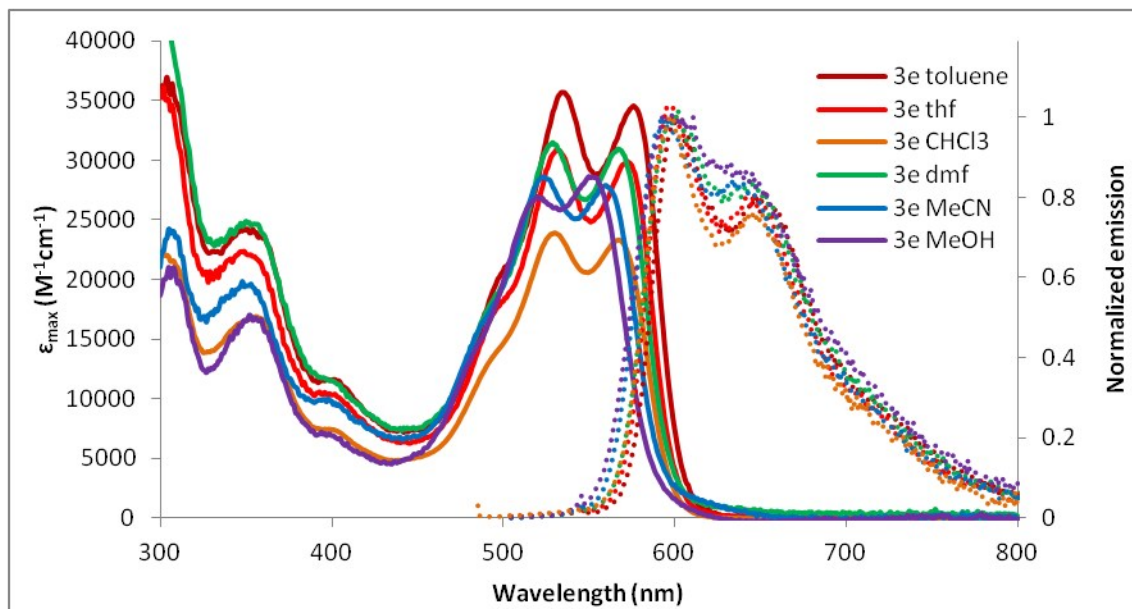


Figure S5. Absorption (solid lines) and emission (dashed lines) spectra of **3e** in various solvents.

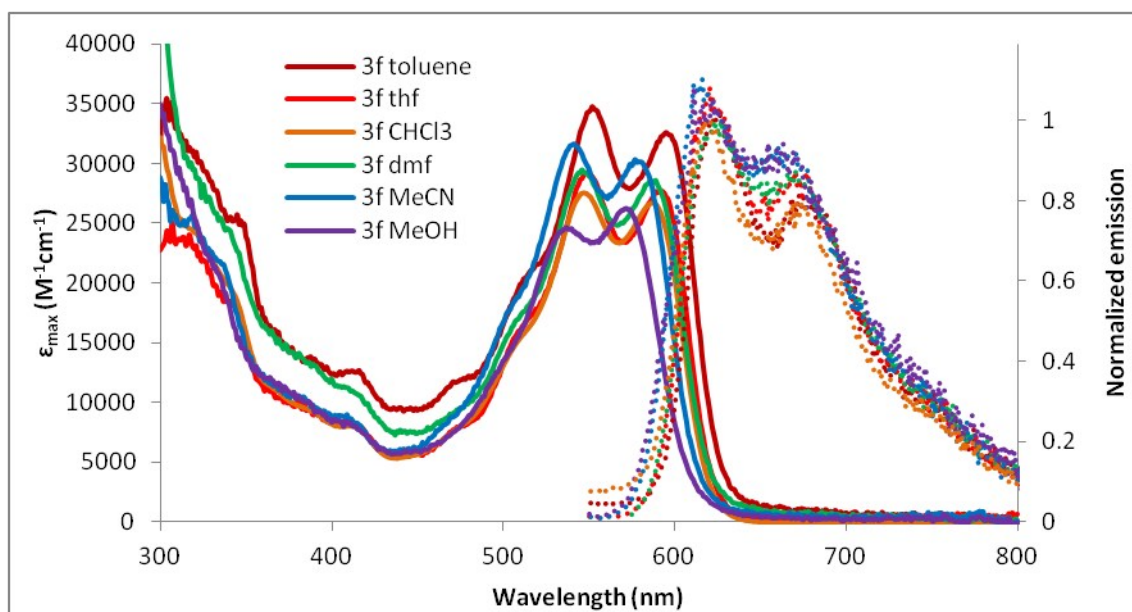


Figure S6. Absorption (solid lines) and emission (dashed lines) spectra of **3f** in various solvents.

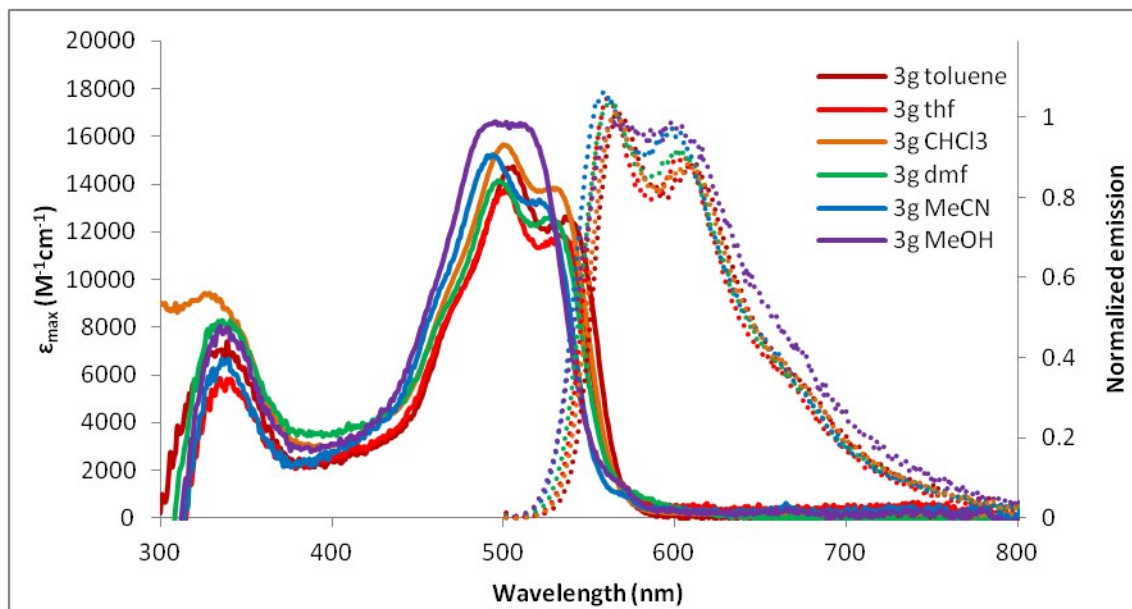


Figure S7. Absorption (solid lines) and emission (dashed lines) spectra of **3g** in various solvents.

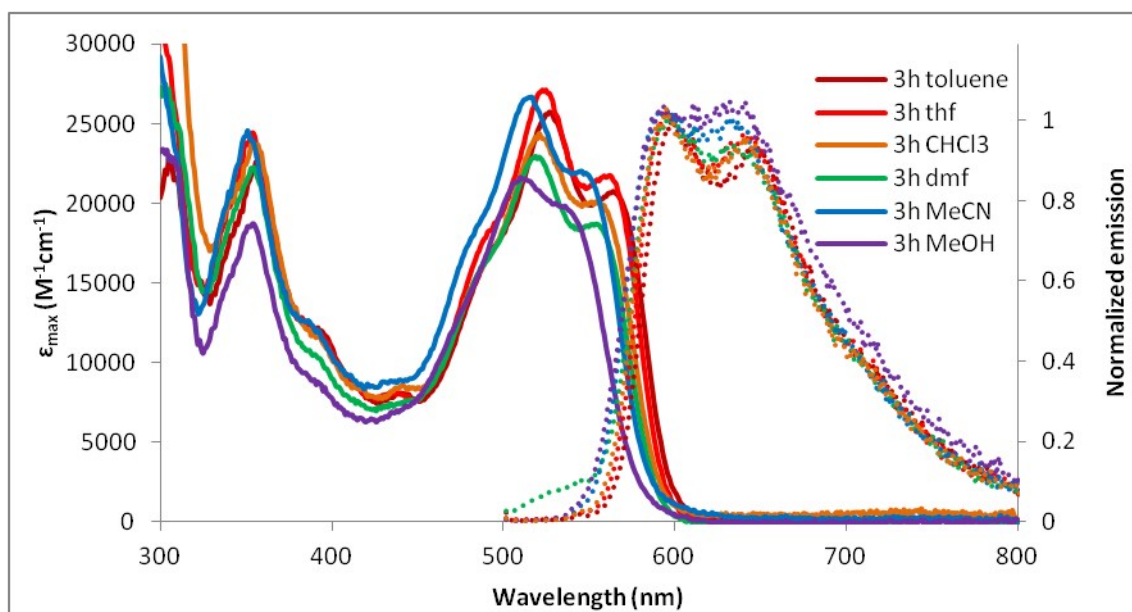


Figure S8. Absorption (solid lines) and emission (dashed lines) spectra of **3h** in various solvents.

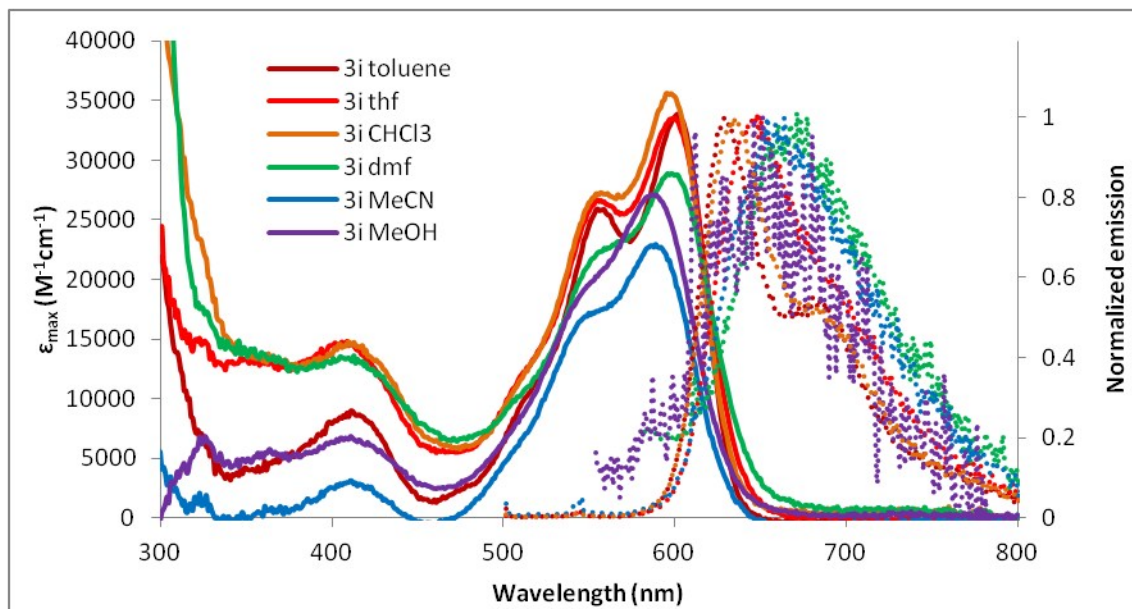


Figure S9. Absorption (solid lines) and emission (dashed lines) spectra of **3i** in various solvents.

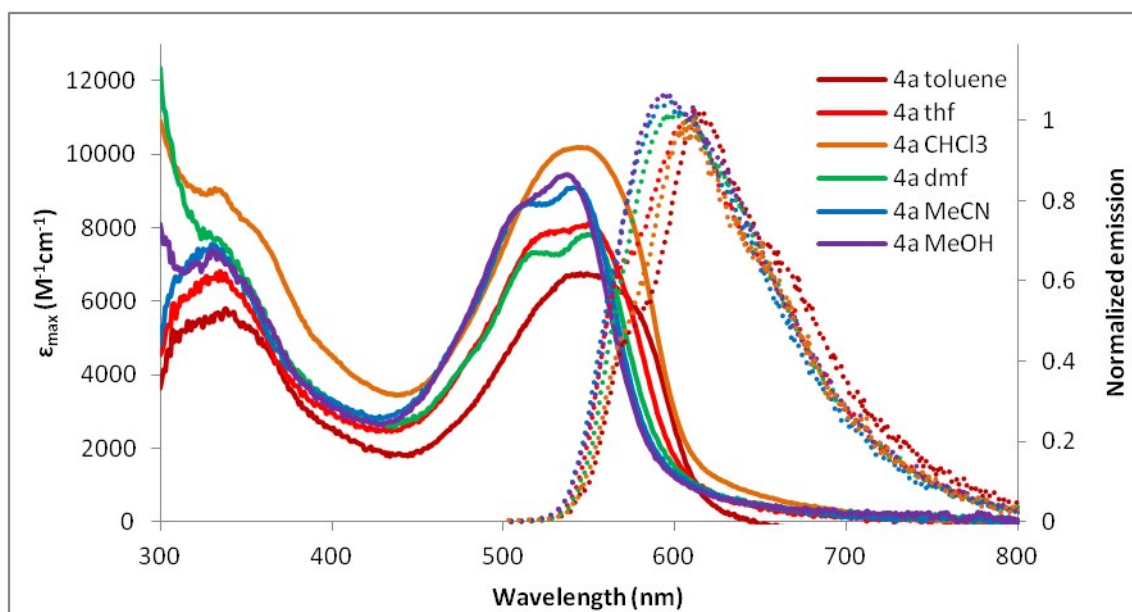


Figure S10. Absorption (solid lines) and emission (dashed lines) spectra of **4a** in various solvents.

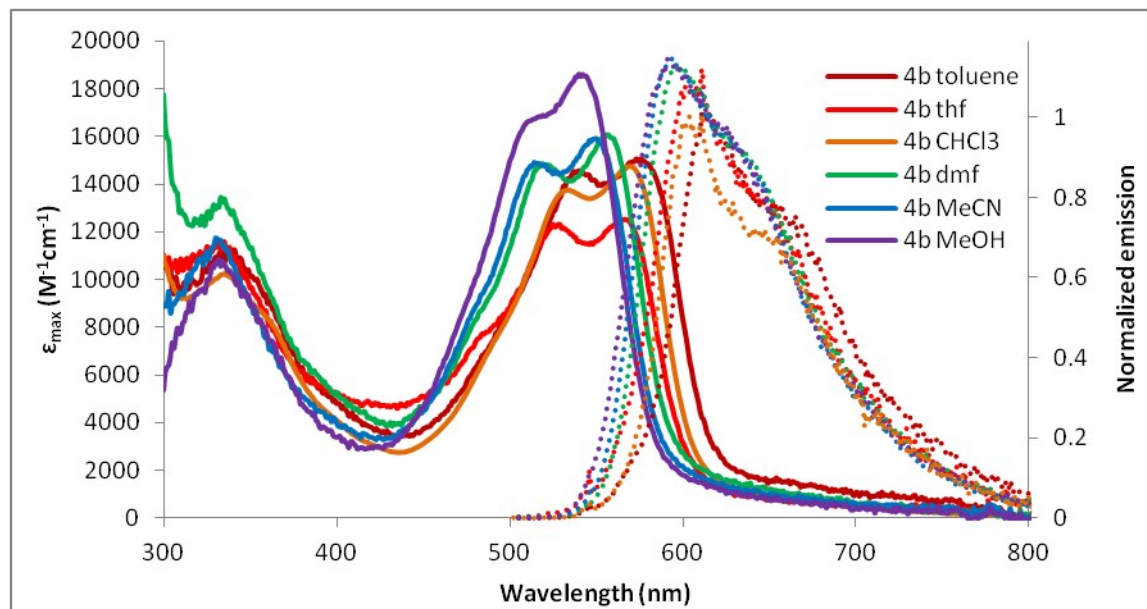


Figure S11. Absorption (solid lines) and emission (dashed lines) spectra of **4b** in various solvents.

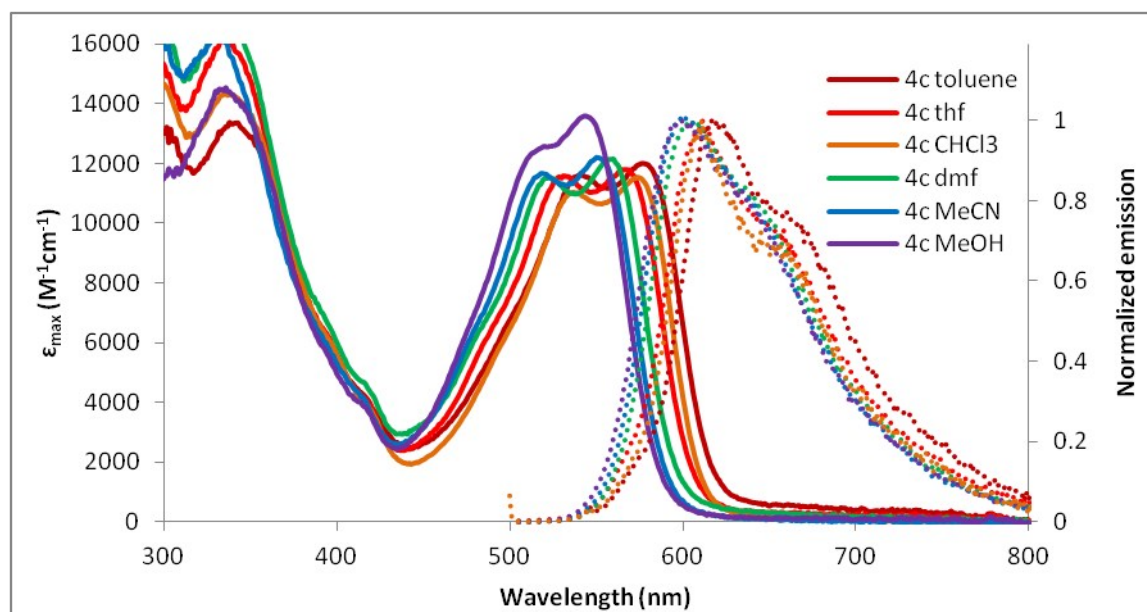


Figure S12. Absorption (solid lines) and emission (dashed lines) spectra of **4c** in various solvents.

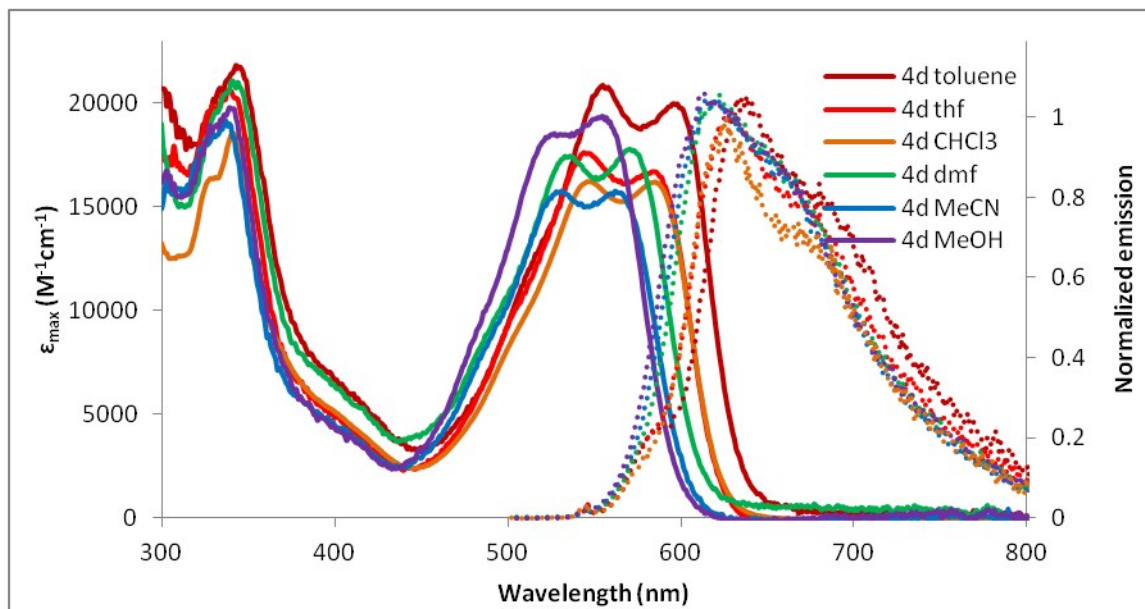


Figure S13. Absorption (solid lines) and emission (dashed lines) spectra of **4d** in various solvents.

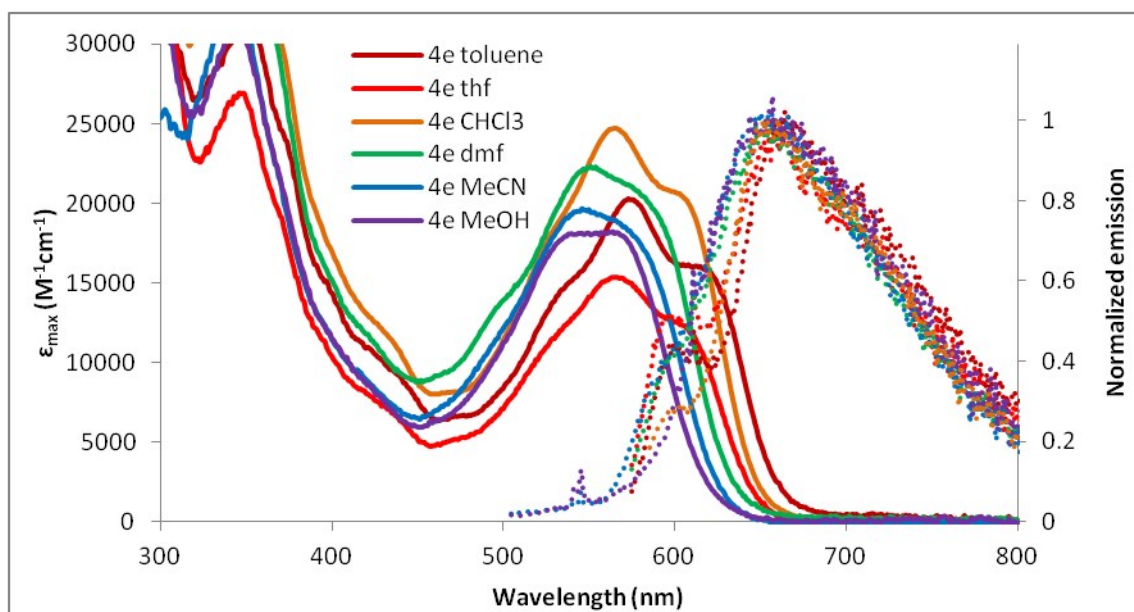


Figure S14. Absorption (solid lines) and emission (dashed lines) spectra of **4e** in various solvents.

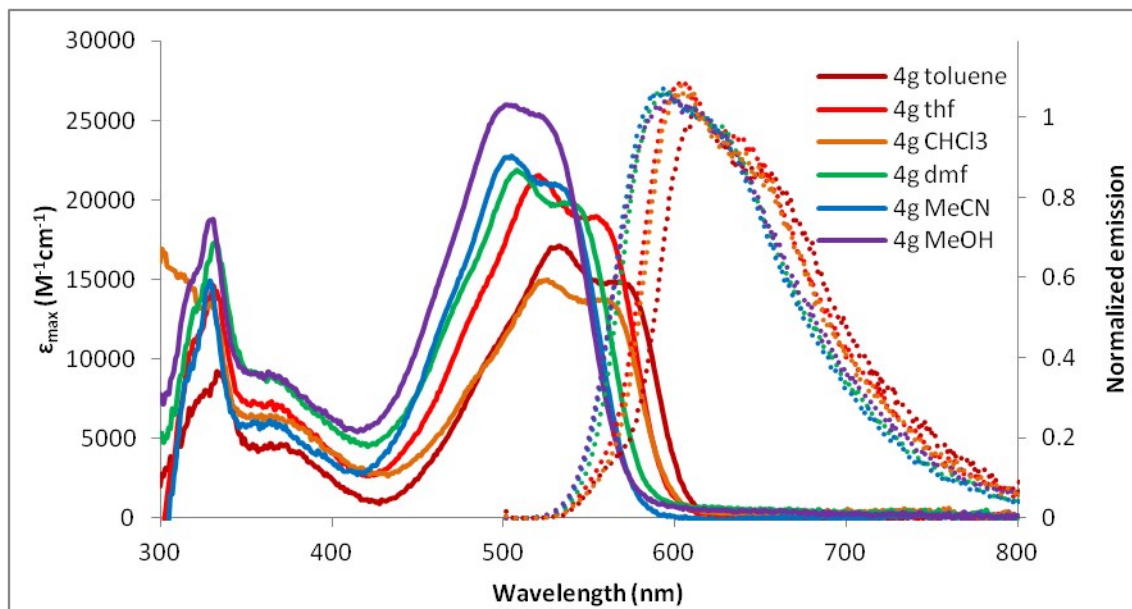


Figure S15. Absorption (solid lines) and emission (dashed lines) spectra of **4g** in various solvents.

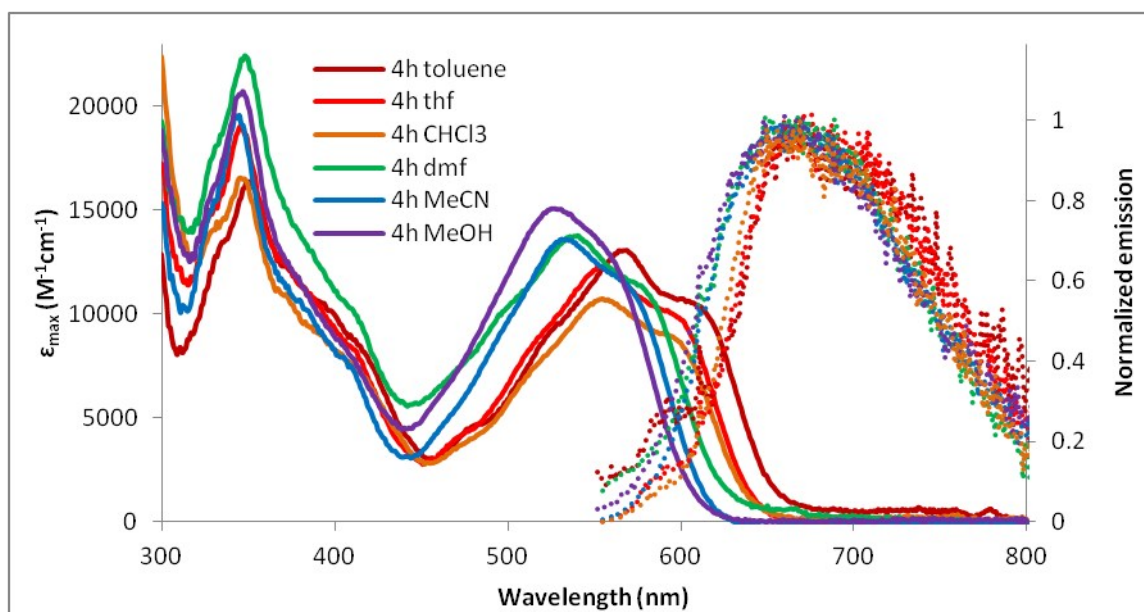


Figure S16. Absorption (solid lines) and emission (dashed lines) spectra of **4h** in various solvents.

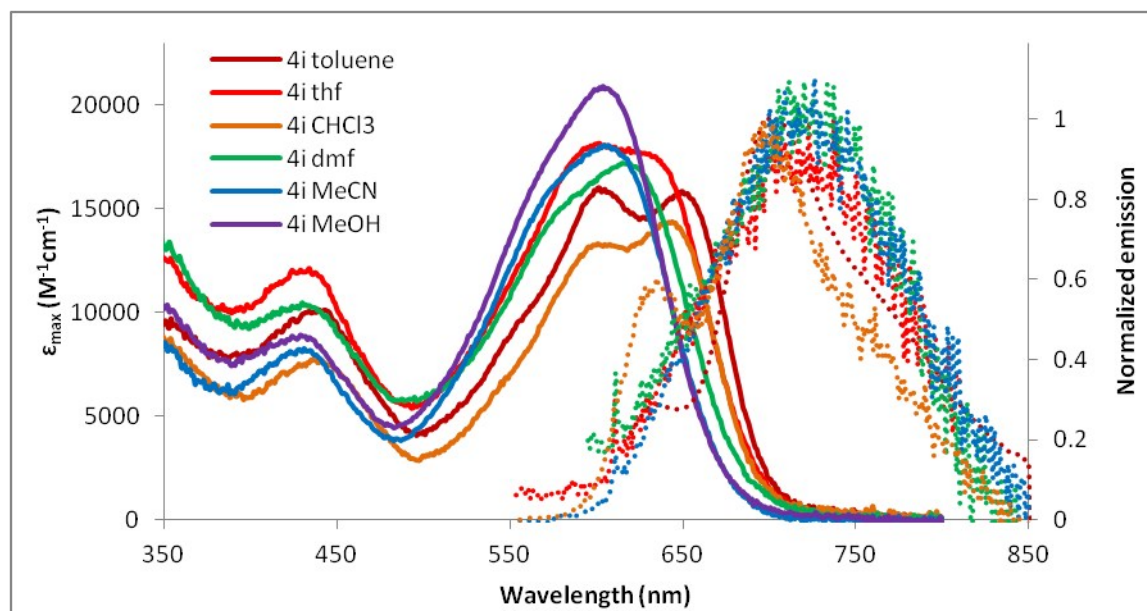


Figure S16. Absorption (solid lines) and emission (dashed lines) spectra of **4i** in various solvents.

Section S5: Fluorescence Lifetime Measurements

Where two emission maxima were present, fluorescence lifetimes were measured and determined for both but in all cases only a negligible difference could be observed. Only the data recorded for the most intense emission maxima are presented here.

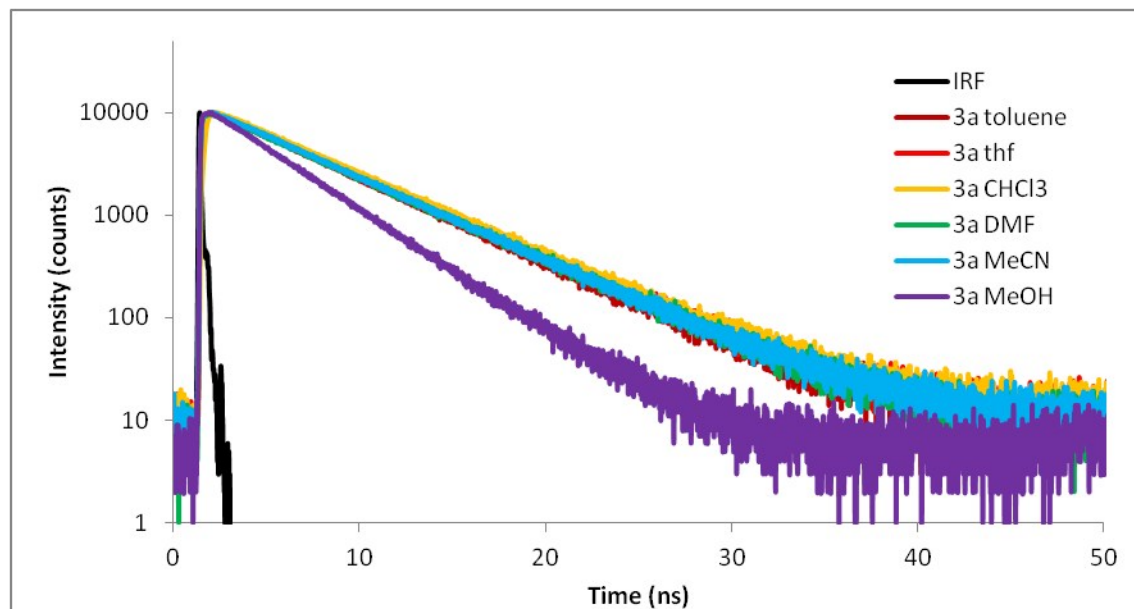


Figure S17. Fluorescence lifetime of **3a** in various solvents.

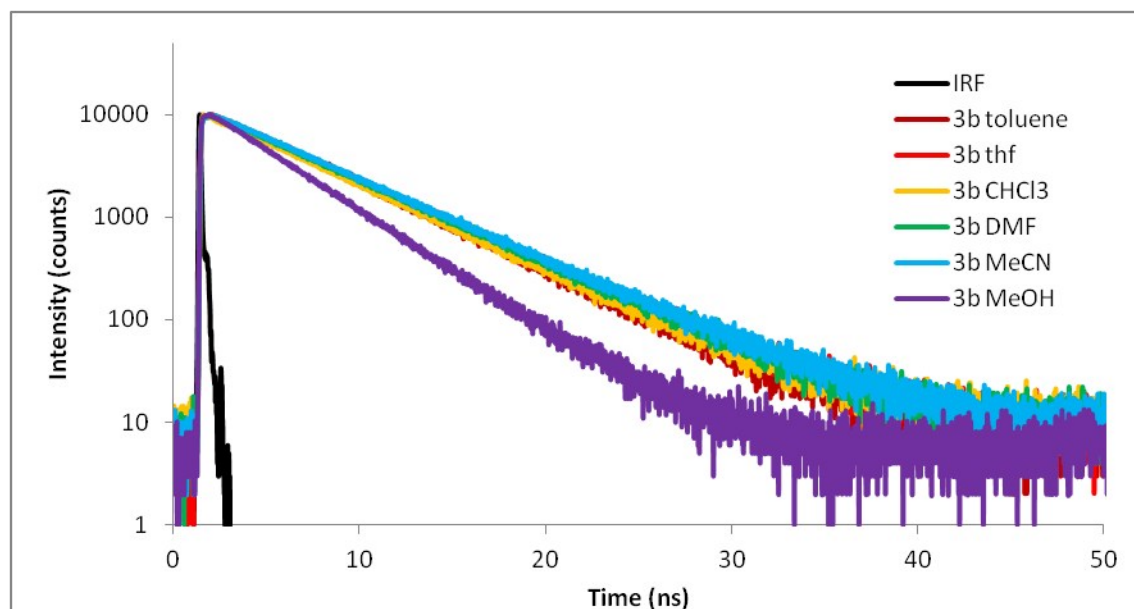


Figure S18. Fluorescence lifetime of **3b** in various solvents.

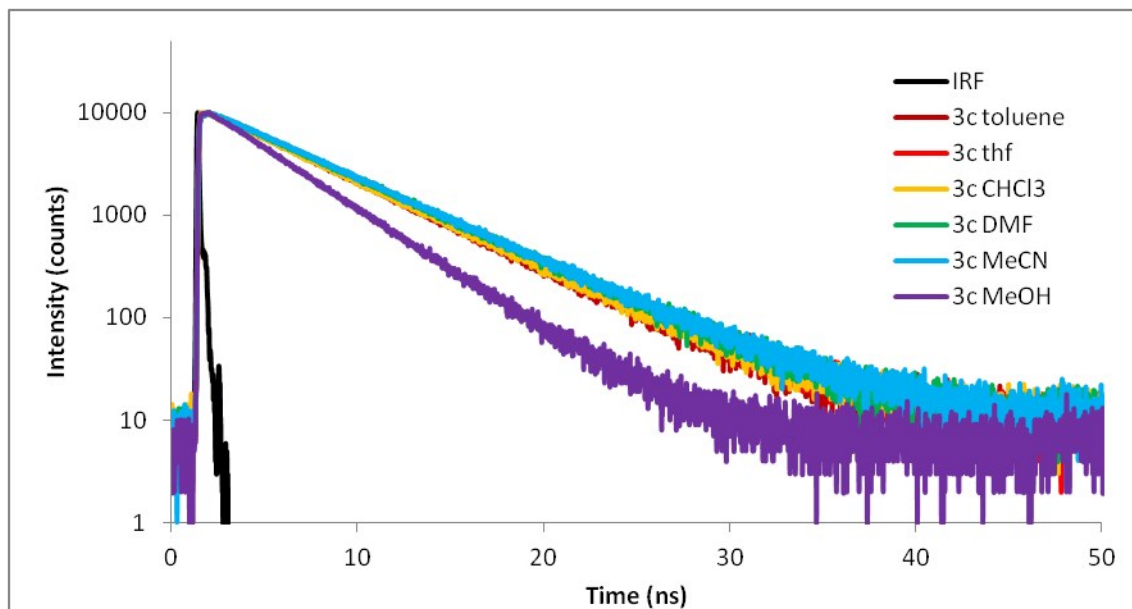


Figure S19. Fluorescence lifetime of **3c** in various solvents.

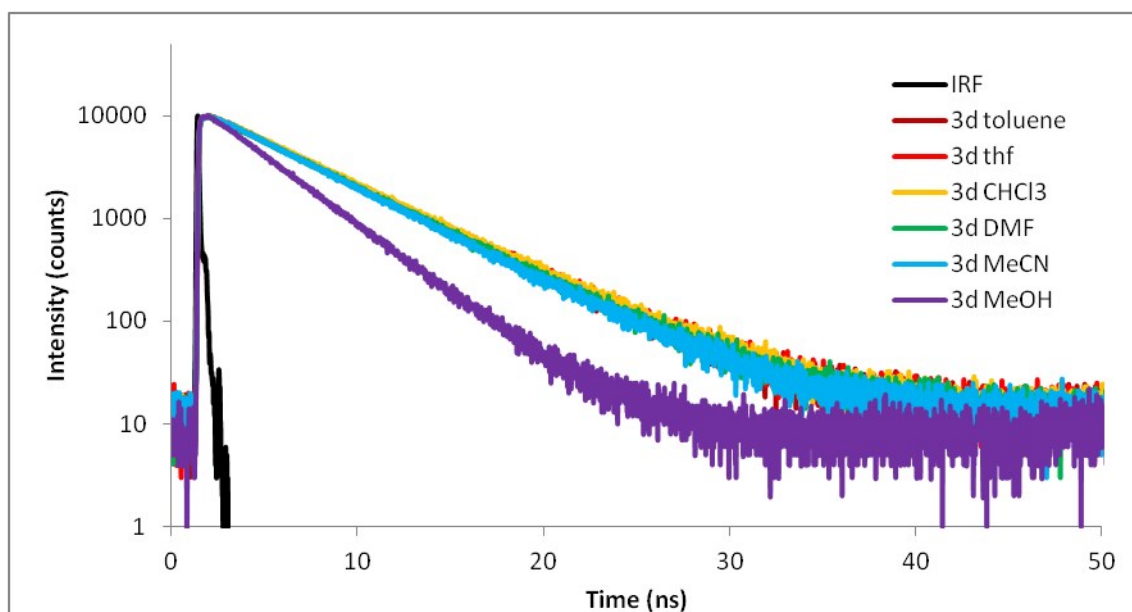


Figure S20. Fluorescence lifetime of **3d** in various solvents.

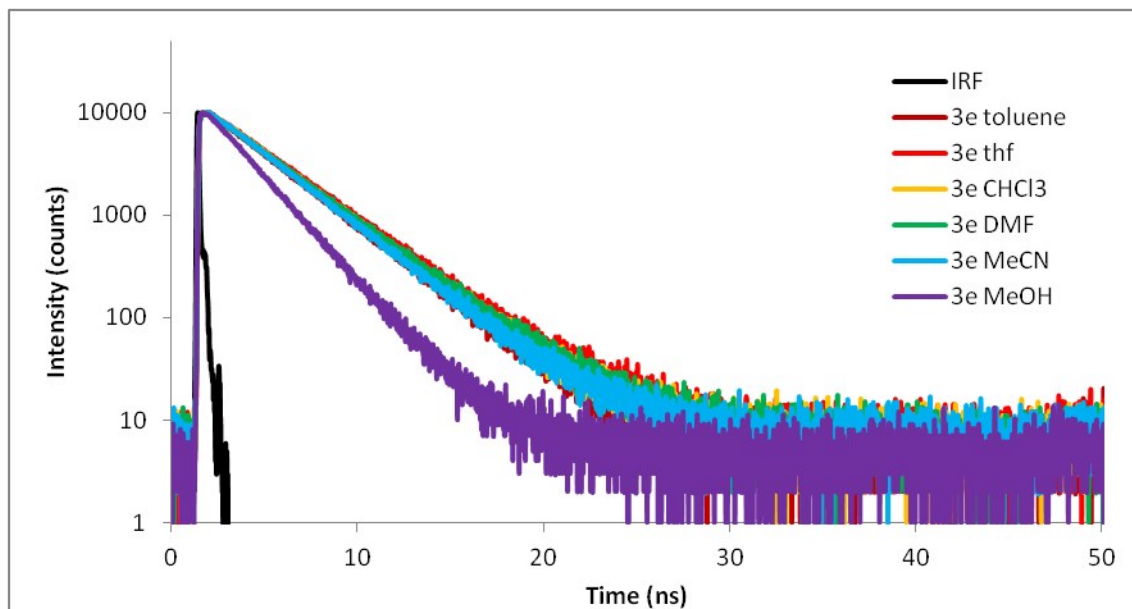


Figure S21. Fluorescence lifetime of **3e** in various solvents.

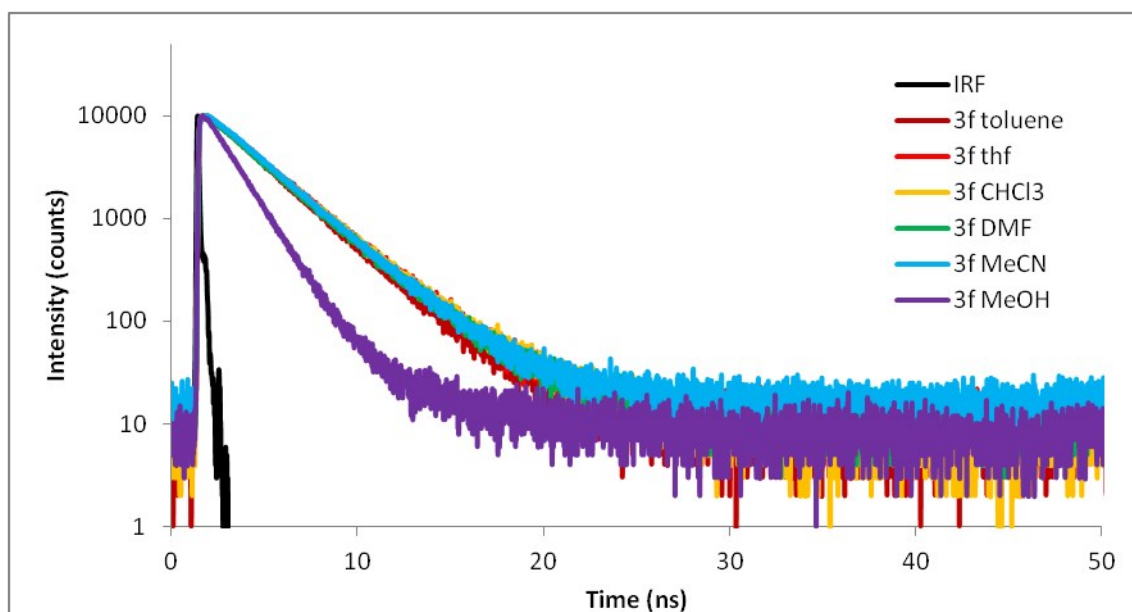


Figure S22. Fluorescence lifetime of **3f** in various solvents.

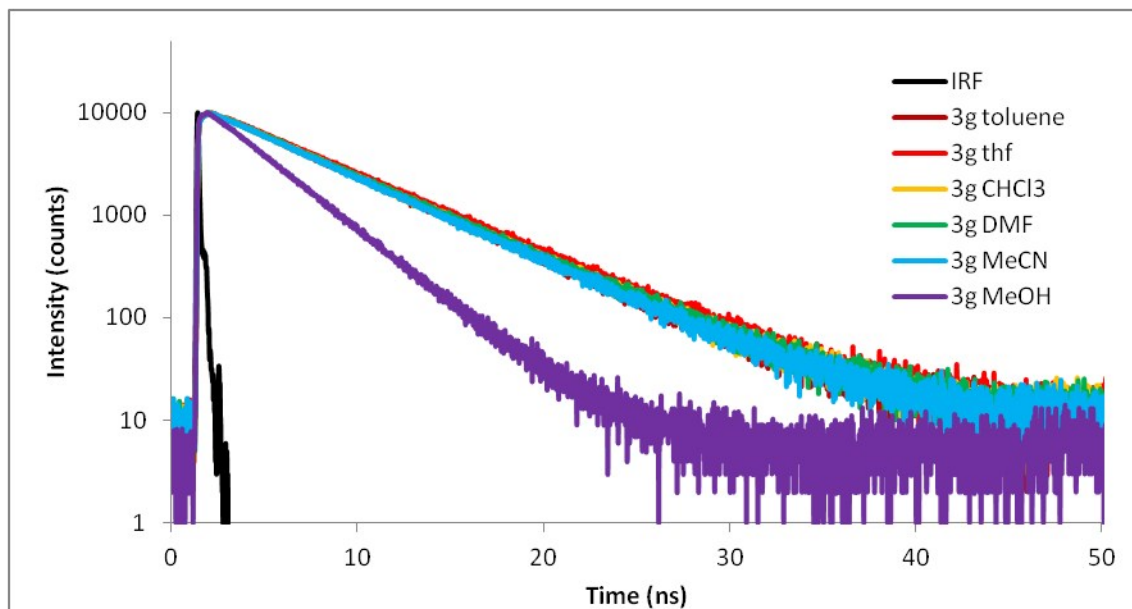


Figure S23. Fluorescence lifetime of **3g** in various solvents.

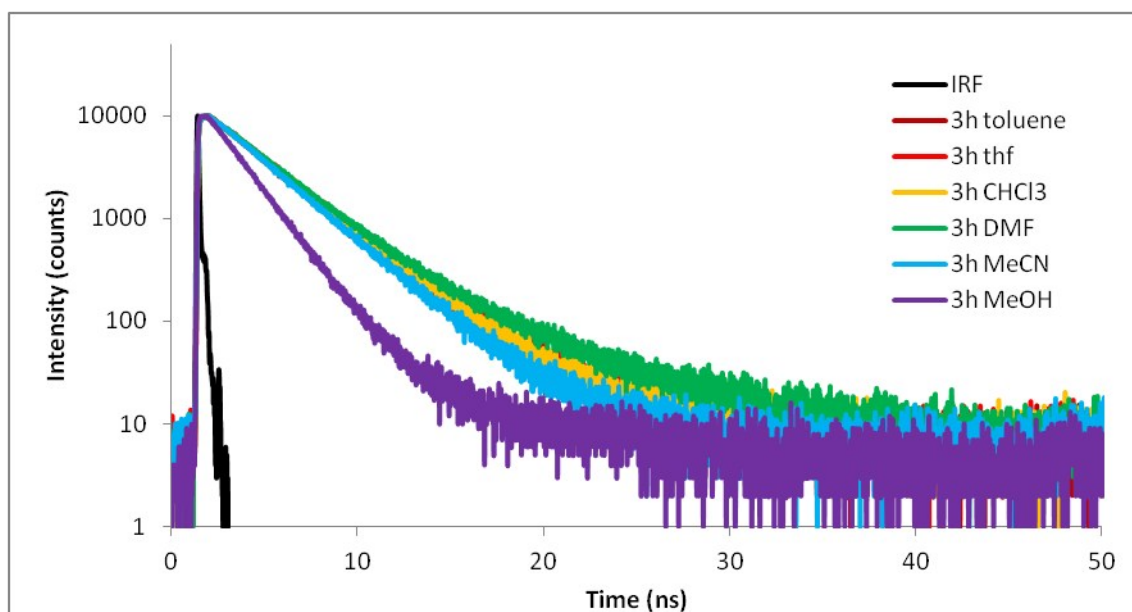


Figure S24. Fluorescence lifetime of **3h** in various solvents.

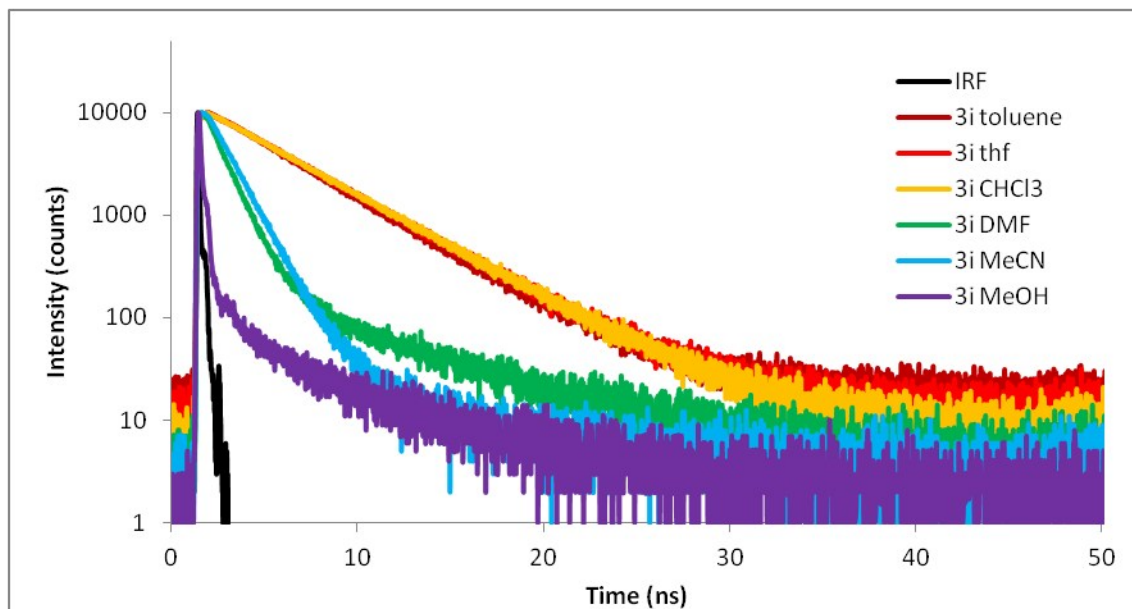


Figure S25. Fluorescence lifetime of **3i** in various solvents.

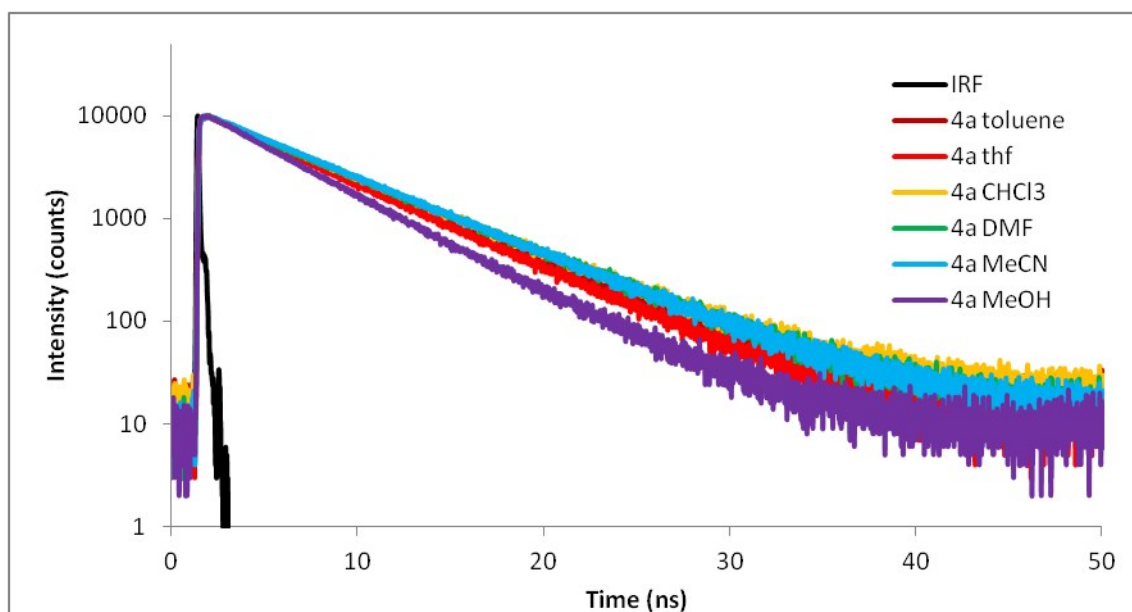


Figure S26. Fluorescence lifetime of **4a** in various solvents.

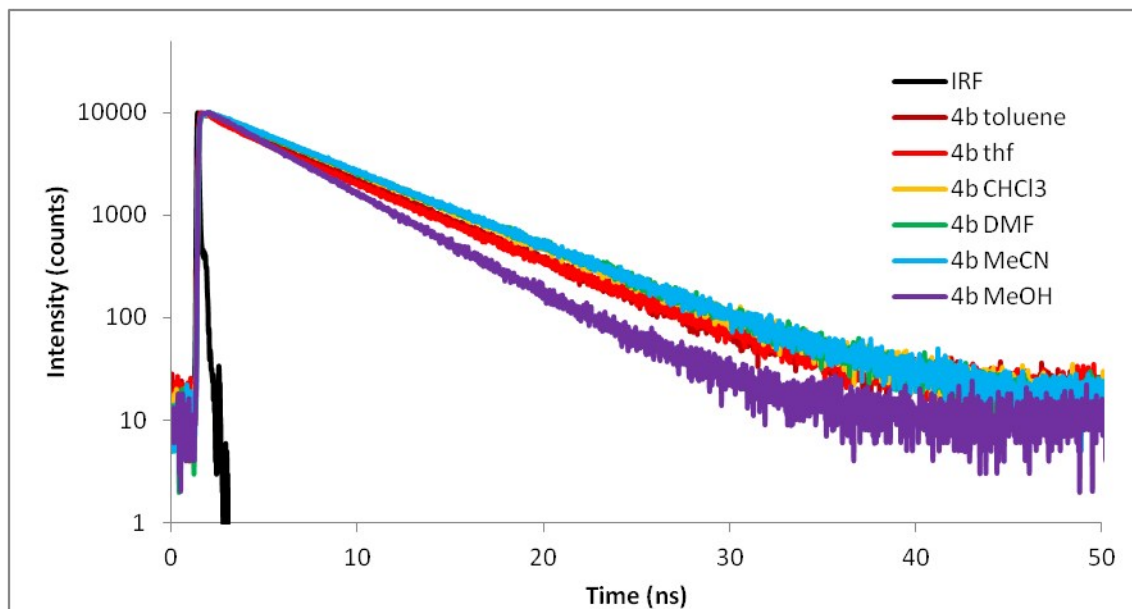


Figure S27. Fluorescence lifetime of **4b** in various solvents.

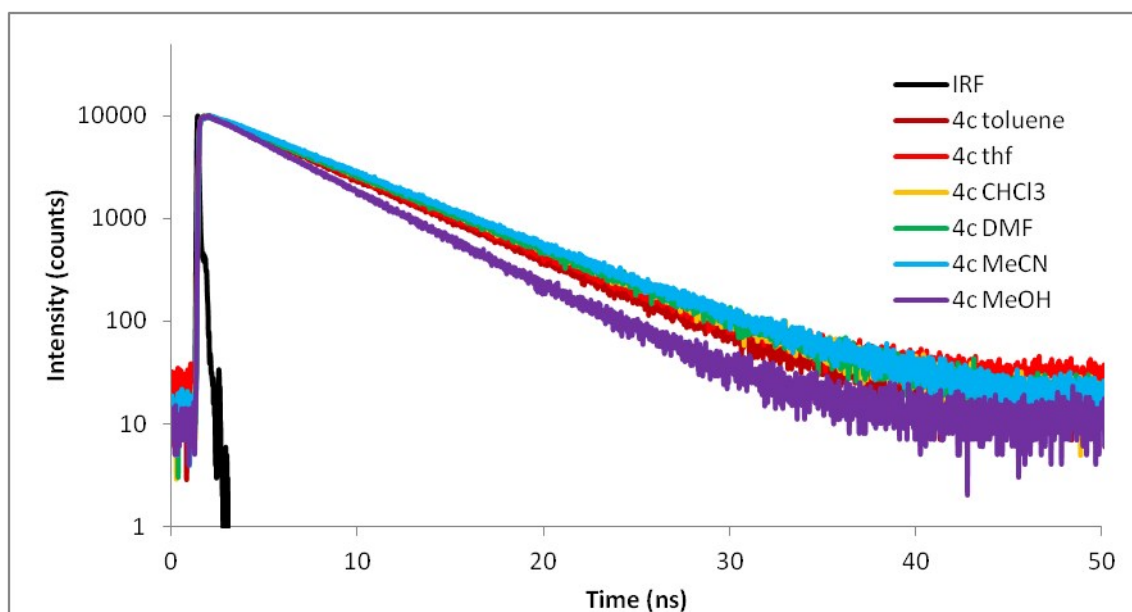


Figure S28. Fluorescence lifetime of **4c** in various solvents.

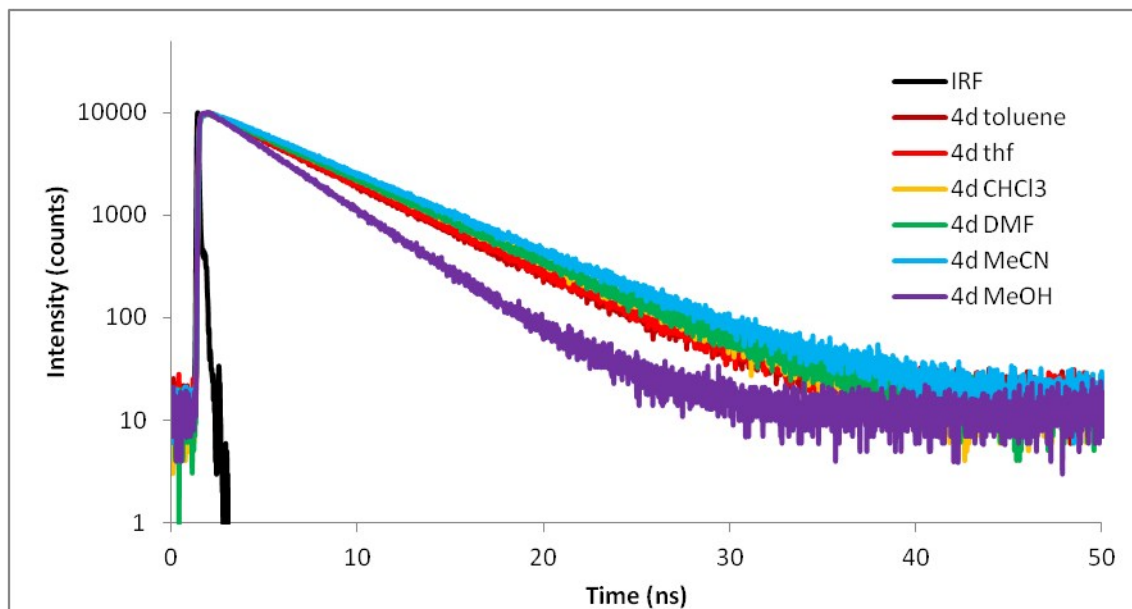


Figure S29. Fluorescence lifetime of **4d** in various solvents.

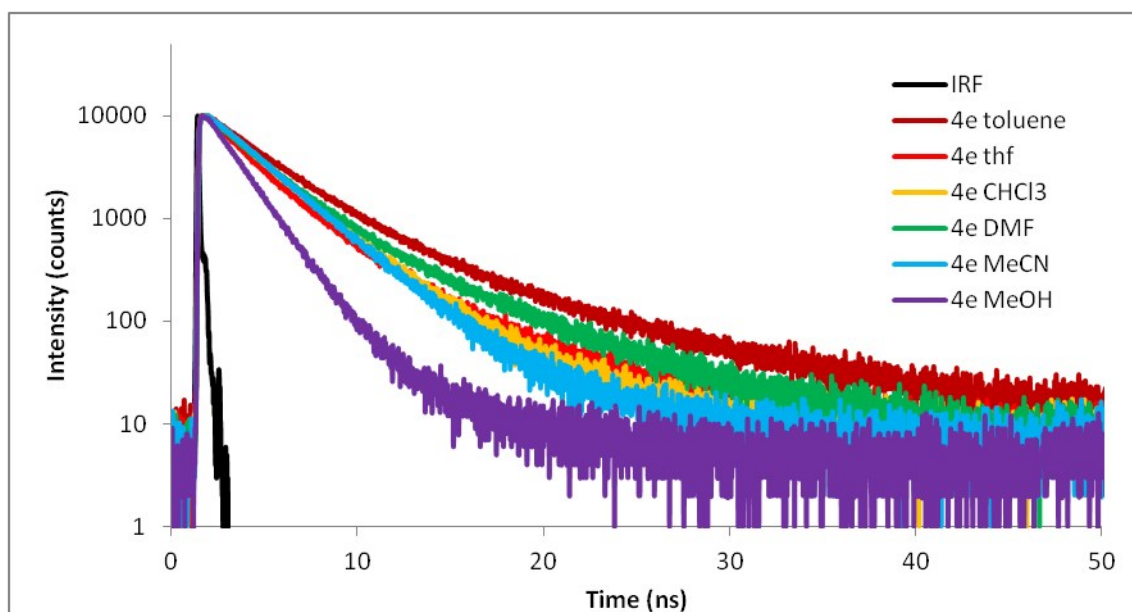


Figure S30. Fluorescence lifetime of **4e** in various solvents.

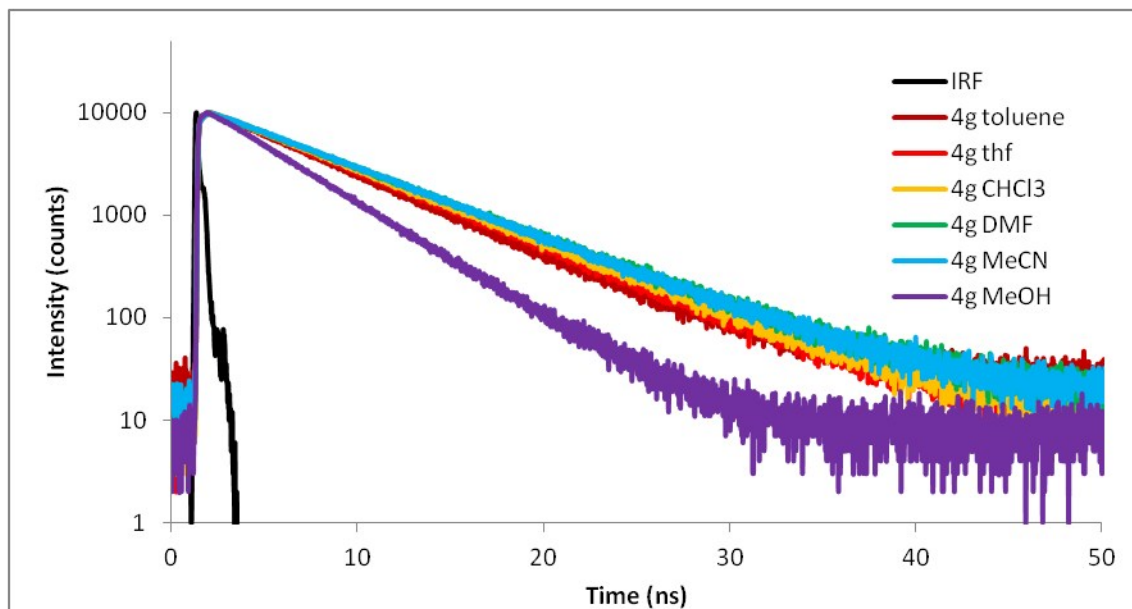


Figure S31. Fluorescence lifetime of **4g** in various solvents.

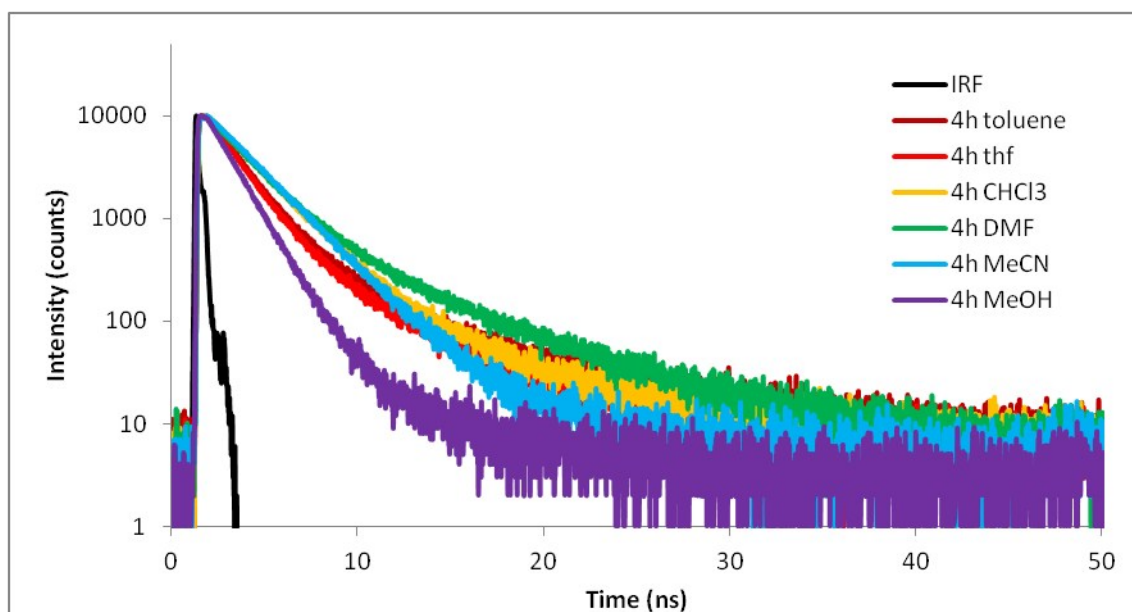


Figure 32 Fluorescence lifetime of **4h** in various solvents.

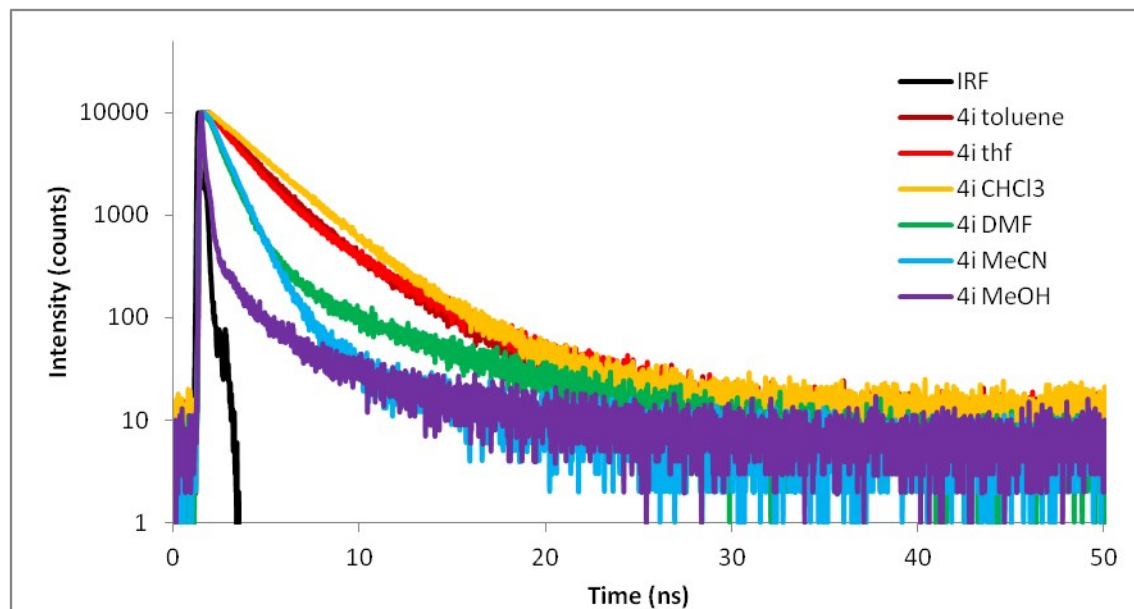


Figure S33. Fluorescence lifetime of **4i** in various solvents.

Section S6: X-Ray Analysis

Crystals of **3d** are very thin, easy to bend, dark red coloured plates. Crystals were grown through slow evaporation of a DCM/MeOH solution containing **3d**. A suitable sample was measured on a Bruker D8 Venture single crystal diffractometer. Data were processed with help of Bruker software⁶ and refined using the SHELX software package.^{7,8} CCDC 1983938 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures. The compound crystallizes in the monoclinic system $P2/c$ with two molecules in the asymmetric unit. Views along each of the crystallographic axes can be seen in Figure S34.

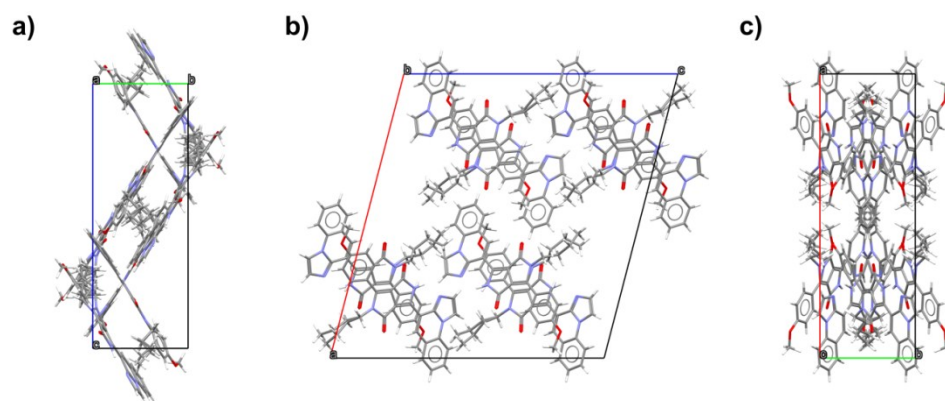


Figure S34. Views along the crystallographic a (a), b (b) and c (c) axes of **3d**.

In the asymmetric unit cell two molecules (denoted as A and B) of **3d** are present. Both of these species contain n butyl chains disordered over two alternative sites. In the molecule A, the alkyl substituted pyrrole skeleton also seems to be disordered. Both molecules A and B have similar geometry, however, slightly different orientations of the planar substituents around the diketopyrrolopyrrole (DPP) unit are observed. Indeed the angle between the LSQ mean planes⁹ fitted to all heavy atoms in the DPP core, imidazo[1,5 a]quinoline and p methoxyphenyl moieties are equal to 1.2°, 7.0° and 5.9°, 18.7° for the molecule A and B respectively. In the crystal lattice the molecules are arranged in ...ABAB... columns in the [010] direction. In these columns the shortest distances between DPP LSQ plane of molecule B and atoms in neighbouring molecules A yields 3.38 Å and 3.45 Å which is presented in Figure S35. The arrangement of the molecules in stacks is responsible for the elongated shape of the crystals in one direction.

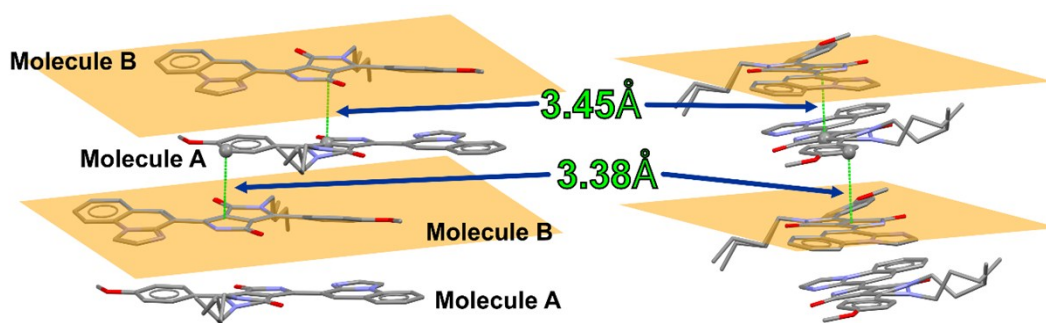


Figure S35. Stacking of molecules in the crystal structure of **3d**.

Section S7: Theoretical Methods

To model the ground and excited state properties of the compounds, we use a protocol based on Time-Dependent Density Functional Theory (TD-DFT) level to determine the transition energies as well as the geometries and vibrations of all states, whereas the environmental effects are accounted for using the well-known Polarizable Continuum Model (PCM). This protocol has been described and tested elsewhere.¹⁰ In all compounds the butyl chains on the DPP core are replaced by methyl groups during the calculations for decreased computational effort. No other simplification is made. All (TD-)DFT calculations are made with the Gaussian16.A03 program.¹¹ During these calculations, we use tightened self-consistent field (10^{-10} a.u.) and geometry optimization (10^{-5} a.u.) convergence thresholds, and a large DFT integration grid (so-called *ultrafine* grid, a pruned 99,590 grid). The DFT and TD-DFT calculations are performed with the M06-2X *meta*-GGA hybrid functional.¹² Given that the excited-states are not of cyanine nature, as in (isolated) BODIPYs, we have not applied post-Hartree-Fock corrections here.¹³ Following a published protocol,¹⁰ the 6-31+G(d) atomic basis set is used for geometries and vibrations whereas 6-311+G(2d,p) is used for the transition energies. The nature of the ground-state and excited-state stationary points is systematically confirmed by analytical Hessian calculations. The impact of the environment is taken into account at all DFT and TD-DFT steps by using the PCM model.¹⁴ For both absorption and emission the LR+cLR¹⁵ model in its *non-equilibrium* limit is applied. This model allows the recovery of both linear-response and state-specific solvent effects and is thus well suited for the bright transitions with a significant CT character as investigated here.

Table S2 displays additional theoretical results including computed vertical absorption and emission wavelengths as well as adiabatic energies and difference of zero-point vibrational energies between the ground and excited states.

Table S2: Computed vertical transition energies, adiabatic energies, zero point corrections and 0-0 energies at the cLR+LR-PCM(neq)-M06-2X/6-311+G(2d,p) level. All values are in eV.

Compound	ΔE^{abs}	ΔE^{ems}	ΔE^{adia}	$\Delta(\text{ZPVE})$	ΔE^{0-0}
3a	2.562	2.034	2.282	-0.060	2.221
4a	2.492	1.954	2.184	-0.057	2.127
3b	2.565	2.042	2.289	-0.061	2.227
4b	2.507	1.963	2.199	-0.058	2.141
3c	2.552	2.021	2.270	-0.060	2.210
4c	2.484	1.941	2.178	-0.054	2.124
3d	2.516				
4d	-	-	-	-	-
3e	2.486	1.947	2.198	-0.056	2.142
4e	2.411	1.846	2.093	-0.058	2.035
3f	2.417	1.878	2.128	-0.056	2.072
4f	2.352	1.774	2.026	-0.056	1.969
3g	2.594	2.050	2.302	-0.063	2.238
4g	2.524	1.966	2.202	-0.059	2.143
3h	2.516	1.960	2.216	-0.055	2.160
4h	2.440	1.853	2.108	-0.061	2.047
3i	2.373	1.853	2.091	-0.051	2.040
4i	2.278	1.736	1.970	-0.053	1.917

Table S3: Computed dipole moments for the ground and excited states of selected compounds on the ground-state geometry. All values are in D. At the right-hand side, we provide the change of dipole moment between the two states, as computed from the individual Cartesian components. These values correspond to $\mu^{\text{CT}} = q^{\text{CT}} \times d^{\text{CT}}$ in Le Bahers' model.

Compound	S_0				S_1				$\Delta\mu^{\text{CT}}$
	μ_x	μ_y	μ_z	μ_{tot}	μ_x	μ_y	μ_z	μ_{tot}	
3a	2.47	1.78	-0.45	3.08	0.41	1.30	-0.44	1.44	2.11
4a	6.70	5.73	-0.12	8.82	2.06	4.88	-0.18	5.30	4.73
3e	1.95	2.76	-0.44	3.41	-1.1	1.64	-0.44	2.04	3.28
4e	-7.45	6.47	0.15	9.88	-1.10	5.05	0.20	5.17	6.52

Below, we give the Cartesian coordinates (in Å), for all compounds, both the S_0 and S_1 as obtained with DFT and TD-DFT.

3a (ground state)

C	1.5379210	0.7621670	0.0771790
C	-0.3486650	2.1216670	0.1235240
C	-0.7434950	0.7243030	0.1308510
C	0.4440140	-0.0711210	0.1259620
C	-1.8326150	-0.1174860	0.0620860
C	0.0508310	-1.4803830	0.0696930
O	0.6848240	-2.5206660	0.0768690
O	-0.9821800	3.1672660	0.1657240
N	1.0690230	2.0763500	0.0834590
N	-1.3600170	-1.4129660	0.0305260
C	2.9476950	0.3954710	-0.0049450
C	3.9112770	1.1961180	-0.6470550
C	3.3510440	-0.8403360	0.5170840
C	5.2281210	0.7845250	-0.7382920
H	3.6237300	2.1328840	-1.1116720
C	4.6745860	-1.2609310	0.4351540
H	2.6145290	-1.4914750	0.9780170
C	5.6216430	-0.4440640	-0.1894570
H	5.9751410	1.3896160	-1.2416810
H	4.9480140	-2.2229690	0.8520350
C	7.3745580	-1.9960980	0.1949270
H	8.4414900	-2.0457690	-0.0197530
H	7.2150690	-2.0496780	1.2781400
H	6.8616660	-2.8318010	-0.2948210
C	-3.2516470	0.1952660	0.0171430
C	-4.2229880	-0.8523860	-0.0619200
C	-3.6947950	1.5011430	0.0520690
C	-5.0828790	1.7967490	0.0044690
H	-2.9708250	2.3104000	0.1159340
C	-6.0027940	0.7947050	-0.0732870
C	-6.2810050	-1.6869450	-0.1769590
C	-5.3330240	-2.6799870	-0.1733410
N	-5.5720550	-0.5064980	-0.1048760
N	-4.0708420	-2.1687730	-0.1026390
H	-1.9732990	-2.2246020	-0.0049960
C	1.8285080	3.2958490	0.2905000
H	2.6987950	3.0928880	0.9176030
H	2.1522540	3.7388760	-0.6564300
H	1.1682830	4.0065990	0.7910270
O	6.9325450	-0.7559130	-0.3223970
H	-5.4212410	2.8256200	0.0304300
H	-7.0750210	0.9465570	-0.1124260
H	-7.3588450	-1.7019070	-0.2218610
H	-5.5017760	-3.7468820	-0.2187140

3a (excited state)

C	-1.5754450	0.8151640	-0.0384660
C	0.3428020	2.1390410	-0.0811370
C	0.7297190	0.7458340	-0.0681030
C	-0.4284860	-0.0308600	-0.0609170
C	1.8688970	-0.1185830	-0.0218450
C	-0.0295380	-1.4509120	0.0034040
O	-0.6798520	-2.4825990	0.0344200
O	0.9655170	3.1935380	-0.1284670
N	-1.0905520	2.0989060	-0.0563220
N	1.3712530	-1.3985800	0.0128370
C	-2.9595170	0.4242950	0.0204570
C	-3.9906180	1.2551480	0.5249860
C	-3.3148270	-0.8736490	-0.4047990
C	-5.2974720	0.8169120	0.5734660
H	-3.7601670	2.2351460	0.9248440
C	-4.6283850	-1.3179040	-0.3607840
H	-2.5432710	-1.5488670	-0.7613300
C	-5.6328310	-0.4706270	0.1224010
H	-6.0869440	1.4451660	0.9734000
H	-4.8546100	-2.3219320	-0.7003250
C	-7.3271720	-2.0969570	-0.2139960
H	-8.4042050	-2.1503220	-0.0599270
H	-7.0989750	-2.2501630	-1.2749950
H	-6.8302550	-2.8677440	0.3860490
C	3.2486450	0.1881830	-0.0114090
C	4.2285520	-0.8628970	0.0410700
C	3.7130010	1.5123160	-0.0501890
C	5.0935850	1.7856510	-0.0358220
H	2.9933080	2.3272700	-0.0918540
C	6.0186780	0.7741510	0.0156810
C	6.2777570	-1.7137140	0.1052210
C	5.3271800	-2.7023480	0.1219000
N	5.5740060	-0.5272720	0.0530760
N	4.0648170	-2.1776370	0.0821750
H	1.9784710	-2.2176290	0.0453040
C	-1.8281690	3.3349510	-0.2391910
H	-2.6727340	3.1686120	-0.9112670
H	-2.1853600	3.7345950	0.7147260
H	-1.1358340	4.0565680	-0.6754250
O	-6.9398810	-0.8013550	0.2050500
H	5.4427480	2.8115030	-0.0657440
H	7.0919120	0.9179850	0.0292110
H	7.3564060	-1.7334280	0.1245770
H	5.4884300	-3.7704880	0.1607810

4a (ground state)

C	-1.8046050	1.0317010	-0.0823600
C	-0.0158680	2.5180130	-0.1238510
C	0.4623080	1.1493680	-0.1364480
C	-0.6568320	0.2726360	-0.1336210
C	1.5994850	0.3853100	-0.0673740
C	-0.1445750	-1.1063320	-0.0810730
O	-0.7140250	-2.1791430	-0.0952780
O	0.5649810	3.5948140	-0.1611230
N	-1.4245030	2.3804450	-0.0854420
N	1.2740210	-0.9565320	-0.0370850
C	-3.1847310	0.5694470	-0.0001180
C	-4.2123730	1.3110590	0.6136140
C	-3.4893580	-0.7069030	-0.4931570
C	-5.4953380	0.8038190	0.7045060
H	-4.0021120	2.2774650	1.0578860
C	-4.7780050	-1.2234290	-0.4107170
H	-2.7010210	-1.3138350	-0.9283610
C	-5.7900180	-0.4646060	0.1846490
H	-6.2905170	1.3631920	1.1865510
H	-4.9733040	-2.2143440	-0.8031470
C	-7.4162590	-2.1549360	-0.1711100
H	-8.4784120	-2.2797540	0.0366090
H	-7.2423980	-2.2250250	-1.2511090
H	-6.8461370	-2.9355740	0.3453640
C	2.9834580	0.8075410	-0.0143260
C	3.9324430	-0.2343260	0.0577330
C	3.4612090	2.1004240	-0.0277910
C	4.8639750	2.3275820	0.0359640
H	2.7611130	2.9319550	-0.0856590
C	5.7548790	1.2943630	0.1078540
C	5.9109880	-1.2301220	0.1787070
C	4.9188650	-2.1698130	0.1524400
N	5.2759570	0.0041670	0.1175720
N	3.7043920	-1.5445360	0.0779120
B	2.2238740	-2.1857590	0.0044590
F	2.1749560	-2.9355970	-1.1493300
F	2.0640270	-2.9441350	1.1407650
C	-2.2633300	3.5461610	-0.2961520
H	-3.1058700	3.2904220	-0.9417370
H	-2.6343730	3.9570340	0.6478670
H	-1.6447180	4.3053260	-0.7787150
O	-7.0746820	-0.8710610	0.3155430
H	4.9890490	-3.2470810	0.1815100
H	6.9842000	-1.3167340	0.2336730
H	6.8303080	1.4086110	0.1581550
H	5.2468000	3.3412940	0.0278540

4a (excited state)

C	-1.8430030	1.0801520	-0.0467970
C	-0.0212570	2.5371610	-0.0819670
C	0.4506250	1.1767860	-0.0753720
C	-0.6445970	0.3176280	-0.0721300
C	1.6352790	0.3918190	-0.0313300
C	-0.1232980	-1.0692680	-0.0160560
O	-0.7062430	-2.1340250	0.0041660
O	0.5342350	3.6277730	-0.1212930
N	-1.4524590	2.3967510	-0.0596170
N	1.2883210	-0.9326060	-0.0006530
C	-3.1987140	0.5912580	0.0123700
C	-4.2808900	1.3420500	0.5307530
C	-3.4601840	-0.7236790	-0.4234820
C	-5.5525000	0.8102120	0.5851140
H	-4.1178030	2.3331670	0.9364360
C	-4.7375550	-1.2626020	-0.3752340
H	-2.6439790	-1.3370230	-0.7921310
C	-5.7963830	-0.4944050	0.1243980
H	-6.3824110	1.3758940	0.9961420
H	-4.8931050	-2.2771510	-0.7227640
C	-7.3697770	-2.2378930	-0.2137660
H	-8.4385940	-2.3701270	-0.0508850
H	-7.1407820	-2.3646520	-1.2779080
H	-6.8127510	-2.9749620	0.3753930
C	2.9936120	0.7970180	-0.0166510
C	3.9429800	-0.2501350	0.0308600
C	3.4944130	2.1088590	-0.0415910
C	4.8882570	2.3115280	-0.0159590
H	2.8026800	2.9475820	-0.0796990
C	5.7836330	1.2679240	0.0323320
C	5.9125780	-1.2632130	0.0998550
C	4.9205410	-2.2004370	0.1009830
N	5.2843740	-0.0250720	0.0549950
N	3.7049320	-1.5612870	0.0577510
B	2.2389030	-2.1824270	0.0323690
F	2.1127480	-2.9393040	-1.1109930
F	2.0653790	-2.9188330	1.1815030
C	-2.2759740	3.5787440	-0.2321260
H	-3.1077760	3.3594900	-0.9049810
H	-2.6588370	3.9450570	0.7252020
H	-1.6363490	4.3505750	-0.6631920
O	-7.0737030	-0.9203290	0.2138640
H	4.9846340	-3.2776210	0.1294020
H	6.9865780	-1.3543760	0.1262640
H	6.8601650	1.3695000	0.0539510
H	5.2834730	3.3211010	-0.0341150

3b (ground state)

C	-2.5880010	0.8811000	-0.0651200
C	-1.0478710	2.6243750	-0.0878300
C	-0.3549710	1.3495360	-0.1316290
C	-1.3378150	0.3112280	-0.1399100
C	0.8938640	0.7678400	-0.0894150
C	-0.6425870	-0.9771820	-0.1201570
O	-1.0304760	-2.1320910	-0.1491990
O	-0.6614540	3.7848510	-0.1074200
N	-2.4205390	2.2659760	-0.0413360
N	0.7181960	-0.6004840	-0.0868110
C	-3.8810830	0.2096290	0.0144420
C	-4.9918350	0.7614370	0.6803620
C	-4.0057300	-1.0723970	-0.5361500
C	-6.1837770	0.0658400	0.7674040
H	-4.9146960	1.7277160	1.1665820
C	-5.2021460	-1.7781260	-0.4584180
H	-3.1477690	-1.5330280	-1.0163970
C	-6.3004950	-1.2064660	0.1904610
H	-7.0413230	0.4785660	1.2888000
H	-5.2594560	-2.7670610	-0.8975120
C	-7.6692110	-3.0997570	-0.2234480
H	-8.6963670	-3.3900000	-0.0051820
H	-7.5124570	-3.0919510	-1.3083750
H	-6.9788680	-3.8116760	0.2434580
C	2.2111020	1.3800820	-0.0452790
C	3.3862650	0.5657810	0.0021210
C	2.3604440	2.7524880	-0.0509390
C	3.6507970	3.3403100	-0.0052210
H	1.4770180	3.3859650	-0.0902800
C	4.7662050	2.5569620	0.0426390
C	5.5754040	0.1923530	0.0847360
C	4.8735550	-0.9915800	0.0630650
N	4.6273770	1.1952620	0.0454080
N	3.5262400	-0.7509270	0.0118760
H	1.4976360	-1.2550700	-0.0746650
C	-3.4325560	3.2921360	-0.2125700
H	-4.2425230	2.9182220	-0.8419260
H	-3.8372580	3.6282740	0.7471470
H	-2.9502060	4.1438320	-0.6958430
O	-7.5082940	-1.8045730	0.3219480
H	3.7594480	4.4181900	-0.0083530
H	5.7808590	2.9360840	0.0786060
H	6.6304130	0.4157440	0.1232980
C	5.4071870	-2.4016510	0.0890790
C	4.8490330	-3.1202400	1.3273490
C	4.9412480	-3.1321410	-1.1799310
C	6.9371330	-2.3900520	0.1452470
H	5.1722690	-2.6209760	2.2474900
H	3.7552930	-3.1290140	1.3093140
H	5.2055160	-4.1563830	1.3529370
H	5.3312240	-2.6415000	-2.0785960
H	5.2984580	-4.1682970	-1.1694290
H	3.8491120	-3.1414740	-1.2419140
H	7.3176240	-3.4168270	0.1633460
H	7.3647260	-1.8898340	-0.7316220
H	7.2992360	-1.8828150	1.0471990

3b (excited state)

C	-2.6351990	0.9196190	-0.0314270
C	-1.0598420	2.6374070	-0.0560090
C	-0.3728600	1.3647850	-0.0709490
C	-1.3290860	0.3499530	-0.0746420
C	0.9310350	0.7756400	-0.0445010
C	-0.6239700	-0.9464450	-0.0384090
O	-1.0270090	-2.0982980	-0.0249140
O	-0.6858530	3.8042220	-0.0858860
N	-2.4474710	2.2798460	-0.0266210
N	0.7296860	-0.5834950	-0.0323820
C	-3.8972170	0.2306150	0.0268140
C	-5.0832800	0.8043370	0.5489490
C	-3.9592800	-1.1077360	-0.4174770
C	-6.2601010	0.0865730	0.5956680
H	-5.0728610	1.8049210	0.9637730
C	-5.1414120	-1.8326440	-0.3751270
H	-3.0597960	-1.5899540	-0.7874220
C	-6.3051530	-1.2363920	0.1252930
H	-7.1660360	0.5182380	1.0090280
H	-5.1420660	-2.8568190	-0.7296220
C	-7.5989670	-3.1928590	-0.2307600
H	-8.6362210	-3.4863450	-0.0739340
H	-7.3497580	-3.2759720	-1.2948700
H	-6.9392900	-3.8430290	0.3551420
C	2.2086250	1.3785590	-0.0329040
C	3.3953770	0.5672720	-0.0032890
C	2.3710520	2.7737660	-0.0485660
C	3.6571100	3.3425870	-0.0336390
H	1.4892800	3.4108260	-0.0726810
C	4.7815110	2.5552390	-0.0036940
C	5.5800640	0.1832340	0.0387070
C	4.8779940	-0.9987430	0.0399970
N	4.6330190	1.1900580	0.0108500
N	3.5271510	-0.7499840	0.0136640
H	1.5052170	-1.2457920	-0.0176860
C	-3.4421940	3.3241430	-0.1855450
H	-4.2331670	2.9858680	-0.8582690
H	-3.8730510	3.6188040	0.7761180
H	-2.9301910	4.1886320	-0.6108740
O	-7.5059630	-1.8501470	0.2076080
H	3.7738230	4.4202360	-0.0455840
H	5.7973880	2.9304970	0.0091440
H	6.6359990	0.4055880	0.0546280
C	5.4049780	-2.4108830	0.0656760
C	4.8689890	-3.1198100	1.3193220
C	4.9123400	-3.1495230	-1.1885980
C	6.9357660	-2.4056810	0.0920060
H	5.2127070	-2.6158780	2.2294000
H	3.7749670	-3.1232870	1.3234280
H	5.2207810	-4.1577560	1.3447160
H	5.2874980	-2.6671850	-2.0979670
H	5.2643920	-4.1876320	-1.1771620
H	3.8190970	-3.1536120	-1.2302240
H	7.3128440	-3.4338560	0.1100480
H	7.3476940	-1.9128320	-0.7964170
H	7.3169580	-1.8929240	0.9828600

4b (ground state)

C	-2.7502120	1.0362730	-0.0505850
C	-1.2963980	2.8525470	-0.0707400
C	-0.5553510	1.6100310	-0.1553170
C	-1.4768610	0.5263540	-0.1632770
C	0.7113130	1.0833670	-0.1366560
C	-0.7001660	-0.7235810	-0.1826750
O	-1.0473960	-1.8850990	-0.2555340
O	-0.9455610	4.0255500	-0.0771420
N	-2.6472870	2.4329710	-0.0035230
N	0.6616760	-0.2927310	-0.1390070
C	-4.0081330	0.3050410	0.0458980
C	-5.1360000	0.7996400	0.7281970
C	-4.0764140	-0.9810130	-0.5069770
C	-6.2909580	0.0460250	0.8282450
H	-5.1007990	1.7668800	1.2170900
C	-5.2355640	-1.7445660	-0.4156460
H	-3.2021470	-1.3984280	-0.9976540
C	-6.3523220	-1.2291160	0.2486830
H	-7.1609060	0.4144260	1.3621790
H	-5.2491680	-2.7344650	-0.8561200
C	-7.6308550	-3.1863980	-0.1546640
H	-8.6397240	-3.5276910	0.0748230
H	-7.4877550	-3.1675960	-1.2413090
H	-6.9005370	-3.8646680	0.3012710
C	1.9903780	1.7537150	-0.0825200
C	3.1266210	0.9172750	-0.0055580
C	2.1893570	3.1186980	-0.0735860
C	3.5081570	3.6351590	0.0140120
H	1.3288390	3.7837370	-0.1238770
C	4.5870210	2.8012560	0.0979690
C	5.2646690	0.3799450	0.1719890
C	4.5240930	-0.7736800	0.1252000
N	4.3814930	1.4435910	0.0901730
N	3.1864360	-0.4187790	0.0089530
B	1.8430540	-1.2800630	-0.3074660
F	1.9479370	-1.7078490	-1.6182930
F	1.7725350	-2.3187450	0.5905900
C	-3.7088120	3.4126670	-0.1448500
H	-4.5056390	3.0141530	-0.7759990
H	-4.1211890	3.7092920	0.8245460
H	-3.2718520	4.2962890	-0.6141690
O	-7.5275470	-1.8863500	0.3933920
H	6.3267120	0.5410900	0.2593940
H	5.6165170	3.1282100	0.1742010
H	3.6734150	4.7059390	0.0215690
C	5.0595070	-2.1828360	0.2590020
C	4.6750900	-2.7352310	1.6444820
C	4.5205840	-3.1043020	-0.8462100
C	6.5912150	-2.1363180	0.1563110
H	5.0985950	-2.1130490	2.4411540
H	3.5913950	-2.7798560	1.7657490
H	5.0784130	-3.7486010	1.7506980
H	4.7014610	-2.6804160	-1.8394740
H	5.0400430	-4.0667220	-0.7810580
H	3.4512490	-3.2874810	-0.7425420
H	6.9863470	-3.1521370	0.2518650
H	6.9190410	-1.7370160	-0.8102890
H	7.0362290	-1.5361340	0.9583660

4b (excited state)

C	-2.7994960	1.0740010	-0.0124940
C	-1.3102140	2.8693870	-0.0294870
C	-0.5738210	1.6328700	-0.0814280
C	-1.4725420	0.5707330	-0.0887810
C	0.7455000	1.0992260	-0.0844490
C	-0.6827410	-0.6847120	-0.0938520
O	-1.0422860	-1.8438740	-0.1250800
O	-0.9871620	4.0507730	-0.0410350
N	-2.6822590	2.4422320	0.0142230
N	0.6727800	-0.2648360	-0.0785810
C	-4.0277280	0.3213750	0.0559540
C	-5.2232050	0.8230880	0.6242160
C	-4.0346430	-1.0039250	-0.4248640
C	-6.3621690	0.0469870	0.6825930
H	-5.2489780	1.8124820	1.0647410
C	-5.1781050	-1.7878210	-0.3724970
H	-3.1228540	-1.4290200	-0.8327660
C	-6.3546860	-1.2634580	0.1764180
H	-7.2765730	0.4216460	1.1311760
H	-5.1385940	-2.8005620	-0.7560930
C	-7.5597570	-3.2723460	-0.1999010
H	-8.5762330	-3.6208860	-0.0217710
H	-7.3387190	-3.3139340	-1.2724720
H	-6.8518630	-3.9037760	0.3486840
C	1.9976010	1.7549130	-0.0789500
C	3.1399250	0.9181870	-0.0263390
C	2.2119860	3.1439050	-0.0868390
C	3.5274350	3.6383670	-0.0422550
H	1.3566210	3.8154560	-0.1186040
C	4.6161060	2.7996090	0.0172650
C	5.2754610	0.3668880	0.0966220
C	4.5356910	-0.7851430	0.0849170
N	4.3946970	1.4340150	0.0281130
N	3.1921290	-0.4204950	0.0018630
B	1.8580630	-1.2727600	-0.2497900
F	1.8825740	-1.7391170	-1.5510600
F	1.7777220	-2.2848650	0.6789500
C	-3.7306860	3.4379220	-0.1060100
H	-4.5185230	3.0725560	-0.7681940
H	-4.1546790	3.6951680	0.8693410
H	-3.2707200	4.3336580	-0.5264760
O	-7.5198430	-1.9381670	0.2735840
H	6.3400120	0.5262860	0.1524770
H	5.6489760	3.1180800	0.0594550
H	3.7026920	4.7082990	-0.0489960
C	5.0645600	-2.1958200	0.2240420
C	4.7267050	-2.7260280	1.6301990
C	4.4822110	-3.1330540	-0.8454100
C	6.5919010	-2.1623250	0.0667180
H	5.1838800	-2.0956590	2.4012480
H	3.6476980	-2.7578600	1.7920570
H	5.1238250	-3.7419730	1.7377770
H	4.6273870	-2.7255540	-1.8513050
H	4.9989300	-4.0974430	-0.7847010
H	3.4165540	-3.3107090	-0.6994690
H	6.9847570	-3.1788180	0.1668120
H	6.8868930	-1.7811990	-0.9175140
H	7.0676950	-1.5498230	0.8411420

3c (ground state)

C	-2.9516880	0.8176220	-0.0625540
C	-1.6102610	2.7177400	-0.0644130
C	-0.7830010	1.5261220	-0.1285980
C	-1.6472850	0.3876780	-0.1497240
C	0.5215420	1.0832550	-0.0961000
C	-0.8166680	-0.8179120	-0.1493070
O	-1.0765130	-2.0076370	-0.1933860
O	-1.3516770	3.9131940	-0.0688910
N	-2.9354690	2.2119850	-0.0193940
N	0.4953670	-0.2959390	-0.1131420
C	-4.1636890	0.0090500	0.0128840
C	-5.3239270	0.4290510	0.6906130
C	-4.1515650	-1.2721380	-0.5536850
C	-6.4327590	-0.3926840	0.7738660
H	-5.3491080	1.3919920	1.1887890
C	-5.2639810	-2.1042380	-0.4800710
H	-3.2514760	-1.6307800	-1.0436860
C	-6.4140970	-1.6630500	0.1809810
H	-7.3270980	-0.0821230	1.3042470
H	-5.2166300	-3.0879700	-0.9318700
C	-7.5724150	-3.6879980	-0.2520560
H	-8.5610060	-4.0901190	-0.0332330
H	-7.4236960	-3.6494440	-1.3374290
H	-6.8066260	-4.3270430	0.2023790
C	1.7637670	1.8354750	-0.0430320
C	3.0213880	1.1553780	-0.0001100
C	1.7615710	3.2160040	-0.0348250
C	2.9793370	3.9417400	0.0195070
H	0.8139570	3.7489180	-0.0696700
C	4.1749000	3.2872560	0.0599170
C	5.2380400	1.0297050	0.0783500
C	4.6704600	-0.2277660	0.0455710
N	4.1867740	1.9175330	0.0477200
N	3.3051830	-0.1371650	-0.0006130
H	1.3401550	-0.8626200	-0.1154770
C	-4.0536090	3.1246330	-0.1740190
H	-4.8223480	2.6714620	-0.8029020
H	-4.4858610	3.4049210	0.7915610
H	-3.6695180	4.0284340	-0.6506670
O	-7.5490500	-2.3899400	0.3097430
H	2.9680730	5.0250090	0.0281030
H	5.1415350	3.7753200	0.1006870
H	6.2598360	1.3716810	0.1338930
C	5.3556380	-1.5295040	0.0612460
C	6.7469050	-1.6139670	-0.0722320
C	4.6157390	-2.7071340	0.2127610
C	7.3861130	-2.8491750	-0.0475290
H	7.3357260	-0.7102460	-0.2066540
C	5.2563560	-3.9429310	0.2354280
H	3.5373570	-2.6429760	0.3156650
C	6.6423970	-4.0192220	0.1070090
H	8.4657810	-2.8991850	-0.1541490
H	4.6698470	-4.8491240	0.3548250
H	7.1407800	-4.9838840	0.1245960

3c (excited state)

C	3.0021080	-0.8514650	-0.0285440
C	1.6241150	-2.7316400	-0.0370930
C	0.8021940	-1.5423440	-0.0664780
C	1.6416560	-0.4289910	-0.0796410
C	-0.5581430	-1.0987870	-0.0463760
C	0.7989730	0.7831600	-0.0570240
O	1.0734750	1.9717380	-0.0550950
O	1.3813830	-3.9324590	-0.0545260
N	2.9650020	-2.2231840	-0.0100700
N	-0.5068030	0.2741970	-0.0476860
C	4.1805220	-0.0269060	0.0251180
C	5.4198310	-0.4608800	0.5580190
C	4.0965920	1.3047280	-0.4347950
C	6.5098900	0.3828880	0.6012140
H	5.5174610	-1.4520480	0.9838990
C	5.1911430	2.1562570	-0.3964420
H	3.1515210	1.6802470	-0.8144990
C	6.4108750	1.6976510	0.1159330
H	7.4558660	0.0585520	1.0228780
H	5.0807210	3.1701460	-0.7630170
C	7.4832010	3.7810700	-0.2569340
H	8.4807400	4.1885650	-0.0974740
H	7.2337850	3.8244060	-1.3233060
H	6.7518900	4.3607070	0.3177510
C	-1.7617970	-1.8372960	-0.0291520
C	-3.0302380	-1.1604700	-0.0048420
C	-1.7702240	-3.2427120	-0.0345880
C	-2.9854450	-3.9480680	-0.0161300
H	-0.8239980	-3.7792650	-0.0537830
C	-4.1910020	-3.2901500	0.0059610
C	-5.2436270	-1.0244660	0.0294290
C	-4.6756880	0.2320660	0.0245710
N	-4.1942730	-1.9162480	0.0098750
N	-3.3054430	0.1327480	0.0048140
H	-1.3494830	0.8477700	-0.0428490
C	4.0689330	-3.1539090	-0.1542090
H	4.8212810	-2.7380210	-0.8276830
H	4.5245430	-3.3895790	0.8122600
H	3.6566720	-4.0736000	-0.5719780
O	7.5355890	2.4408400	0.1964730
H	-2.9832050	-5.0320840	-0.0197420
H	-5.1591710	-3.7750130	0.0200350
H	-6.2668920	-1.3658960	0.0549100
C	-5.3526880	1.5355870	0.0414970
C	-6.7470060	1.6275130	-0.0619150
C	-4.6055710	2.7130220	0.1637330
C	-7.3793040	2.8659320	-0.0383110
H	-7.3437570	0.7253670	-0.1688590
C	-5.2395430	3.9521150	0.1858090
H	-3.5255590	2.6454950	0.2440580
C	-6.6276460	4.0348470	0.0860680
H	-8.4610010	2.9195260	-0.1208020
H	-4.6459770	4.8566000	0.2823150
H	-7.1210590	5.0020830	0.1032870

4c (ground state)

C	-3.0926010	0.9295220	-0.0876140
C	-1.8422070	2.8913920	-0.0882320
C	-0.9690580	1.7348160	-0.0883390
C	-1.7672060	0.5578980	-0.1124280
C	0.3456660	1.3507460	-0.0075750
C	-0.8607040	-0.5999710	-0.0545890
O	-1.0775210	-1.7949640	-0.0603640
O	-1.6190450	4.0948720	-0.1136430
N	-3.1423120	2.3295860	-0.0809450
N	0.4454940	-0.0234430	-0.0067390
C	-4.2681200	0.0680250	-0.0388880
C	-5.4842140	0.4552620	0.5556710
C	-4.1611050	-1.2345200	-0.5450030
C	-6.5543400	-0.4183780	0.6149030
H	-5.5859330	1.4345950	1.0096880
C	-5.2334890	-2.1187810	-0.4944660
H	-3.2172230	-1.5684360	-0.9653790
C	-6.4397970	-1.7098950	0.0817440
H	-7.4911610	-0.1323050	1.0819610
H	-5.1107800	-3.1176170	-0.8961230
C	-7.4687310	-3.8097850	-0.3189300
H	-8.4471040	-4.2532220	-0.1369320
H	-7.2588820	-3.8118220	-1.3948490
H	-6.6997030	-4.3866640	0.2074470
C	1.5403670	2.1632300	0.0511010
C	2.7634010	1.4587390	0.0866910
C	1.5915730	3.5416650	0.0315240
C	2.8513080	4.1958700	0.0439840
H	0.6643990	4.1109340	-0.0062850
C	4.0187600	3.4858080	0.0504670
C	4.9540080	1.1480850	0.0413170
C	4.3275480	-0.0746320	0.0556370
N	3.9624240	2.1127470	0.0598750
N	2.9617500	0.1386580	0.0978810
B	1.7130130	-0.8940720	0.1859070
F	1.8846330	-1.8270060	-0.8032550
F	1.7314950	-1.4442720	1.4582480
C	-4.2924690	3.1853360	-0.3074870
H	-5.0044930	2.6894030	-0.9701890
H	-4.7891070	3.4569080	0.6291820
H	-3.9257590	4.1003910	-0.7766180
O	-7.5431230	-2.4885370	0.1811990
H	6.0013810	1.4054820	0.0477270
H	5.0088450	3.9239560	0.0421770
H	2.9004670	5.2782470	0.0344470
C	4.9942910	-1.3861670	0.0020790
C	6.1787280	-1.4979730	-0.7391000
C	4.5043660	-2.5011480	0.6904110
C	6.8707680	-2.7034040	-0.7842070
H	6.5420100	-0.6448720	-1.3063250
C	5.2000990	-3.7058930	0.6373550
H	3.5876080	-2.4284660	1.2641010
C	6.3817830	-3.8116050	-0.0937270
H	7.7822830	-2.7805950	-1.3692200
H	4.8109890	-4.5671220	1.1715630
H	6.9162070	-4.7561880	-0.1326650

4c (excited state)

C	-3.1443800	0.9626500	-0.0580040
C	-1.8601030	2.9098830	-0.0537090
C	-0.9918870	1.7608040	-0.0374410
C	-1.7687420	0.6067470	-0.0577760
C	0.3766960	1.3758750	0.0279060
C	-0.8484980	-0.5536120	0.0119930
O	-1.0778890	-1.7451040	0.0426730
O	-1.6673310	4.1188320	-0.0794010
N	-3.1782780	2.3355390	-0.0611870
N	0.4531640	0.0117940	0.0375070
C	-4.2839250	0.0793860	-0.0298430
C	-5.5561410	0.4558900	0.4637630
C	-4.1179500	-1.2490130	-0.4721320
C	-6.6025700	-0.4424810	0.4884610
H	-5.7157050	1.4457230	0.8738600
C	-5.1675870	-2.1558240	-0.4536850
H	-3.1447240	-1.5782780	-0.8220830
C	-6.4222940	-1.7552480	0.0216730
H	-7.5751640	-0.1633740	0.8807050
H	-4.9951250	-3.1662200	-0.8053230
C	-7.3736640	-3.8964960	-0.3518890
H	-8.3524570	-4.3534260	-0.2119950
H	-7.0949250	-3.9395920	-1.4108530
H	-6.6284140	-4.4293630	0.2492250
C	1.5476210	2.1695990	0.0541060
C	2.7742960	1.4635800	0.0725310
C	1.6109110	3.5733920	0.0134820
C	2.8671620	4.2035880	-0.0164960
H	0.6886660	4.1499220	-0.0067690
C	4.0427400	3.4878050	-0.0248230
C	4.9584430	1.1368420	-0.0187390
C	4.3348290	-0.0842840	0.0287400
N	3.9723040	2.1059760	0.0085470
N	2.9656850	0.1404450	0.0990350
B	1.7330560	-0.8724880	0.2184270
F	1.8465690	-1.8197250	-0.7662110
F	1.7330950	-1.4144690	1.4939150
C	-4.3224230	3.2081730	-0.2469530
H	-5.0326780	2.7507700	-0.9391070
H	-4.8184240	3.4284890	0.7031250
H	-3.9432340	4.1439910	-0.6606100
O	-7.5078400	-2.5547710	0.0816610
H	6.0062460	1.3920340	-0.0408750
H	5.0349460	3.9167510	-0.0613260
H	2.9268350	5.2858100	-0.0447720
C	4.9912780	-1.3994040	-0.0159090
C	6.1694650	-1.5303270	-0.7651540
C	4.5015130	-2.5050950	0.6887900
C	6.8538810	-2.7403380	-0.8003750
H	6.5336810	-0.6864840	-1.3453640
C	5.1877740	-3.7155110	0.6436420
H	3.5925840	-2.4201090	1.2731260
C	6.3635330	-3.8383640	-0.0944940
H	7.7609910	-2.8294270	-1.3907550
H	4.7973840	-4.5675180	1.1918420
H	6.8917320	-4.7867370	-0.1262690

3e (ground state)

C	3.0553020	0.7563010	0.0563090
C	1.2137090	2.1759420	0.0666560
C	0.7742280	0.7943740	0.1315850
C	1.9356360	-0.0383050	0.1463890
C	-0.3431070	-0.0149090	0.1058440
C	1.4973530	-1.4347990	0.1482170
O	2.0966630	-2.4945950	0.1890640
O	0.6141560	3.2436480	0.0730210
N	2.6279910	2.0840470	0.0165990
N	0.0888210	-1.3234930	0.1201210
C	4.4515080	0.3407780	-0.0243420
C	5.4336670	1.0828300	-0.7074460
C	4.8196930	-0.8864630	0.5419710
C	6.7348280	0.6235470	-0.7963920
H	5.1720890	2.0100210	-1.2054840
C	6.1273060	-1.3545860	0.4626220
H	4.0674750	-1.4936060	1.0363040
C	7.0935470	-0.5954820	-0.2040660
H	7.4956020	1.1828960	-1.3311480
H	6.3733710	-2.3082790	0.9142670
C	8.7976560	-2.1905450	0.2213290
H	9.8595130	-2.2850470	-0.0031860
H	8.6499880	-2.1967630	1.3075200
H	8.2506440	-3.0264070	-0.2297150
C	-1.7495330	0.3555500	0.0631880
C	-2.7827290	-0.6556740	0.0292010
C	-2.1238640	1.6667090	0.0493320
C	-3.5050610	2.0510740	0.0223280
H	-1.3655990	2.4482830	0.0699460
C	-4.5239990	1.0695220	0.0021090
C	-4.8592200	-1.4612090	-0.0859140
C	-3.8859430	-2.4845160	-0.0401940
N	-4.1260860	-0.2705630	-0.0268870
N	-2.6183840	-1.9566000	0.0287290
C	-6.2205300	-1.7765320	-0.1982080
C	-6.5667470	-3.1200680	-0.2375030
H	-7.0029690	-1.0354360	-0.2718310
H	-7.6157640	-3.3849340	-0.3254480
C	-4.2541130	-3.8346530	-0.0790700
C	-5.5998420	-4.1405720	-0.1733940
H	-3.4883060	-4.6025670	-0.0401310
H	-5.9179420	-5.1778860	-0.2066690
C	-3.8649180	3.4125020	0.0376230
C	-5.1908880	3.7994500	0.0440470
H	-3.0680420	4.1512790	0.0494630
H	-5.4569760	4.8511960	0.0560370
C	-5.8664930	1.4683810	0.0286450
C	-6.1892660	2.8170050	0.0468690
H	-6.6611800	0.7398850	0.0525690
H	-7.2355000	3.1062370	0.0687640
H	-0.5522160	-2.1134610	0.1190160
C	3.4284460	3.2855490	0.1668790
H	4.2995210	3.0787920	0.7915960
H	3.7543770	3.6802290	-0.8004760
H	2.7978020	4.0364020	0.6464760
O	8.3914270	-0.9567750	-0.3390190

3e (excited state)

C	-1.2210080	2.1934900	-0.0061260
C	-0.7869230	0.8144450	-0.0598290
C	-1.9192140	0.0003560	-0.0837620
C	0.3815330	-0.0176750	-0.0559840
C	-1.4753450	-1.4069080	-0.0865430
O	-2.0892170	-2.4589350	-0.1029060
O	-0.6381800	3.2718150	-0.0073730
N	-2.6516970	2.1024590	0.0238600
N	-0.0746760	-1.3100530	-0.0785150
C	-4.4616550	0.3631280	0.0371630
C	-5.5079290	1.1303670	0.6045140
C	-4.7821030	-0.9178910	-0.4574910
C	-6.7996400	0.6483190	0.6484630
H	-5.2999930	2.0929170	1.0561280
C	-6.0801660	-1.4063580	-0.4195140
H	-3.9960130	-1.5451180	-0.8657170
C	-7.1018310	-0.6212360	0.1285070
H	-7.6013130	1.2266330	1.0963920
H	-6.2810460	-2.3955890	-0.8138430
C	-8.7497780	-2.2795120	-0.2764560
H	-9.8216770	-2.3760680	-0.1085870
H	-8.5359280	-2.3626530	-1.3481220
H	-8.2186240	-3.0675940	0.2692230
C	1.7446920	0.3469570	-0.0341320
C	2.7797060	-0.6611020	-0.0268170
C	2.1341950	1.6854510	-0.0036220
C	3.4995160	2.0533800	-0.0127490
H	1.3755650	2.4663500	0.0060090
C	4.5248720	1.0629790	-0.0373410
C	4.8546200	-1.4689640	0.0699790
C	3.8823840	-2.4942230	0.0312470
N	4.1209680	-0.2788060	0.0118160
N	2.6129830	-1.9636770	-0.0261790
C	6.2145160	-1.7810660	0.1904970
C	6.5640950	-3.1255350	0.2334520
H	6.9920660	-1.0358130	0.2753840
H	7.6132580	-3.3878370	0.3279750
C	4.2522500	-3.8419570	0.0723690
C	5.6004370	-4.1465570	0.1671910
H	3.4883010	-4.6120810	0.0377690
H	5.9193650	-5.1836220	0.2025250
C	3.8839960	3.4180470	-0.0297600
C	5.2108380	3.7878320	-0.0927900
H	3.0969070	4.1670020	-0.0017680
H	5.4858840	4.8377500	-0.1067660
C	5.8628990	1.4500670	-0.1326840
C	6.2030020	2.7981820	-0.1566540
H	6.6461630	0.7123860	-0.2133220
H	7.2491230	3.0777870	-0.2321360
H	0.5623240	-2.1066430	-0.0807030
C	-3.4342340	3.3185690	-0.0998430
H	-4.2843120	3.1479760	-0.7636520
H	-3.7876130	3.6696300	0.8743450
H	-2.7754800	4.0800230	-0.5199400
O	-8.3954450	-0.9986400	0.2123500

4e (ground state)

C	-3.1098310	1.0294330	-0.0777510
C	-1.3152110	2.5084260	-0.1261020
C	-0.8424610	1.1398900	-0.1539000
C	-1.9658020	0.2672700	-0.1456790
C	0.2930650	0.3689740	-0.1020320
C	-1.4593560	-1.1136500	-0.1088390
O	-2.0313460	-2.1848660	-0.1250900
O	-0.7316160	3.5857740	-0.1608260
N	-2.7233520	2.3764650	-0.0750670
N	-0.0393520	-0.9682540	-0.0784840
C	-4.4916140	0.5728850	0.0150210
C	-5.5074720	1.3121420	0.6504800
C	-4.8094400	-0.6952910	-0.4900150
C	-6.7922340	0.8108170	0.7508290
H	-5.2861320	2.2718540	1.1039560
C	-6.0999020	-1.2060350	-0.3978740
H	-4.0298870	-1.3005920	-0.9429360
C	-7.1003140	-0.4492960	0.2191600
H	-7.5782920	1.3685940	1.2494520
H	-6.3055030	-2.1909060	-0.8001700
C	-8.7401940	-2.1261640	-0.1375890
H	-9.8004570	-2.2481290	0.0813210
H	-8.5796980	-2.1838320	-1.2204300
H	-8.1681590	-2.9162940	0.3621350
C	1.6770310	0.7951910	-0.0607110
C	2.6562740	-0.2397490	-0.0038360
C	2.1185020	2.0851390	-0.0759170
C	3.5243210	2.3696800	-0.0212160
H	1.4006670	2.9042890	-0.1251290
C	4.4824820	1.3254300	0.0435370
C	4.6387240	-1.2510990	0.0776020
C	3.5981330	-2.1995250	0.0555810
N	4.0018060	0.0065370	0.0411720
N	2.3909050	-1.5331350	0.0051640
B	0.9191920	-2.1820610	-0.0537500
F	0.8668110	-2.9348320	-1.2080080
F	0.7826970	-2.9533110	1.0798810
C	5.9728330	-1.6729300	0.1194130
C	6.2068280	-3.0410290	0.1429380
H	6.8137470	-0.9953800	0.1299640
H	7.2333660	-3.3915020	0.1751840
C	3.8368500	-3.5744190	0.0798520
C	5.1593050	-3.9798510	0.1248110
H	3.0053080	-4.2706030	0.0626790
H	5.3950350	-5.0388200	0.1449620
C	3.9803870	3.7036120	-0.0248320
C	5.3274270	3.9982690	0.0363000
H	3.2388360	4.4959660	-0.0752950
H	5.6634310	5.0297990	0.0331860
C	5.8465140	1.6302890	0.1102150
C	6.2588110	2.9533240	0.1060130
H	6.5871360	0.8482410	0.1704260
H	7.3201900	3.1742110	0.1591350
C	-3.5597660	3.5470560	-0.2664410
H	-4.4123060	3.2989680	-0.9017960
H	-3.9161430	3.9531040	0.6853620
H	-2.9447670	4.3069240	-0.7524790
O	-8.3859480	-0.8504480	0.3607590

4e (excited state)

C	3.1458740	1.0744350	0.0563420
C	1.3268350	2.5303690	0.1005390
C	0.8565110	1.1661010	0.0979510
C	1.9554710	0.3113350	0.0900490
C	-0.3263600	0.3697700	0.0493380
C	1.4431700	-1.0755190	0.0299100
O	2.0205100	-2.1395020	0.0090810
O	0.7739560	3.6210060	0.1419520
N	2.7566390	2.3919060	0.0706460
N	0.0223030	-0.9405790	0.0136580
C	4.5050450	0.5904250	-0.0135510
C	5.5715790	1.3397610	-0.5623800
C	4.7805620	-0.7142280	0.4394220
C	6.8455610	0.8149320	-0.6308690
H	5.3936290	2.3234770	-0.9801510
C	6.0604450	-1.2463630	0.3790240
H	3.9749370	-1.3248770	0.8342910
C	7.1051720	-0.4801620	-0.1525100
H	7.6647190	1.3784430	-1.0655600
H	6.2289940	-2.2535030	0.7414550
C	8.6957970	-2.2078040	0.1882310
H	9.7623640	-2.3353840	0.0082790
H	8.4870410	-2.3168890	1.2583960
H	8.1336210	-2.9587540	-0.3779110
C	-1.6872030	0.7807000	0.0367640
C	-2.6517480	-0.2477650	-0.0115870
C	-2.1358100	2.1022840	0.0793390
C	-3.5252420	2.3731650	0.0410630
H	-1.4183210	2.9192450	0.1284270
C	-4.4890070	1.3183600	-0.0308760
C	-4.6393880	-1.2620370	-0.0311530
C	-3.6031630	-2.2172940	-0.0464780
N	-4.0001810	-0.0070560	-0.0212250
N	-2.3904220	-1.5512600	-0.0332480
B	-0.9411390	-2.1812330	-0.0182950
F	-0.8040120	-2.9444030	1.1211680
F	-0.7683640	-2.9172140	-1.1692890
C	-5.9731830	-1.6791890	-0.0052840
C	-6.2176520	-3.0494020	-0.0163330
H	-6.8087360	-0.9965400	0.0368910
H	-7.2469120	-3.3929240	0.0036390
C	-3.8497570	-3.5874010	-0.0586530
C	-5.1780980	-3.9903220	-0.0471960
H	-3.0240450	-4.2906530	-0.0715570
H	-5.4166630	-5.0488920	-0.0556710
C	-4.0101650	3.7060940	0.0521590
C	-5.3599120	3.9829220	-0.0202000
H	-3.2810980	4.5093800	0.1126200
H	-5.7047320	5.0121800	-0.0116970
C	-5.8473520	1.6110870	-0.1218260
C	-6.2833200	2.9336570	-0.1150700
H	-6.5767750	0.8213760	-0.2141920
H	-7.3456860	3.1420500	-0.1875210
C	3.5816210	3.5735720	0.2443610
H	4.4239320	3.3472370	0.9012970
H	3.9485150	3.9521180	-0.7143250
H	2.9490210	4.3396410	0.6954780
O	8.3826850	-0.8997530	-0.2572320

3f (ground state)

C	-3.7460690	-0.8141360	-0.0128160
C	-1.8160550	-2.0956010	-0.2159960
C	-1.4663420	-0.7038530	-0.0004610
C	-2.6779890	0.0405850	0.1385300
C	-0.4044130	0.1754190	0.0515270
C	-2.3304800	1.4538170	0.2983800
O	-2.9959980	2.4593750	0.4712990
O	-1.1480180	-3.1120570	-0.3562620
N	-3.2343870	-2.0961240	-0.2169940
N	-0.9185980	1.4408830	0.2361810
C	-5.1685610	-0.4897540	-0.0067820
C	-6.1244050	-1.2186660	-0.7396250
C	-5.5958010	0.6395160	0.7037680
C	-7.4554310	-0.8442110	-0.7381310
H	-5.8213110	-2.0647970	-1.3463560
C	-6.9333910	1.0214280	0.7157040
H	-4.8675380	1.2399710	1.2403800
C	-7.8716190	0.2743980	-0.0026950
H	-8.1969090	-1.3931990	-1.3094820
H	-7.2248850	1.9006240	1.2779850
C	-9.6602290	1.6912170	0.6475810
H	-10.7336360	1.7353610	0.4666290
H	-9.4730000	1.5896420	1.7228810
H	-9.1866390	2.6071420	0.2759520
C	1.0201900	-0.0903840	-0.0536560
C	1.9825240	0.9826490	0.0048300
C	1.4835910	-1.3543650	-0.2930300
C	2.8837010	-1.6478110	-0.3103270
H	0.7777650	-2.1747050	-0.4159190
C	3.8198710	-0.6359740	-0.0696220
C	3.9862810	1.9074510	-0.3015430
C	2.9633890	2.8719840	-0.1870610
N	3.3465270	0.6776650	-0.0956810
N	1.7400310	2.2734930	0.0022570
C	5.2795310	2.2658690	-0.7044860
C	5.5364660	3.6158610	-0.8868650
H	6.0506960	1.5288160	-0.8920910
H	6.5291930	3.9229500	-1.2007800
C	3.2468300	4.2351080	-0.3550740
C	4.5391310	4.5937160	-0.6919920
H	2.4537410	4.9683090	-0.2496040
H	4.7869590	5.6403850	-0.8391590
C	3.3345740	-2.9895330	-0.5010430
C	4.6550830	-3.3032940	-0.4025810
H	2.5914210	-3.7466100	-0.7353070
H	5.0018460	-4.3175850	-0.5790300
C	5.1713040	-0.9825740	0.2746420
C	5.5947630	-2.3224980	0.0377290
H	-0.3332060	2.2720190	0.2742320
C	-3.9481560	-3.3597100	-0.1895350
H	-4.8076250	-3.2895180	0.4799130
H	-4.2821960	-3.6597590	-1.1876070
H	-3.2522630	-4.1158520	0.1785060
O	-9.1946220	0.5569860	-0.0580140
C	6.0550100	-0.1125670	0.9664210
C	7.3299070	-0.5120230	1.2922440
H	5.7089290	0.8647490	1.2807260
H	7.9806720	0.1646170	1.8376630
C	6.9299400	-2.6882200	0.3395690

C	7.7896580	-1.7999960	0.9398310
H	7.2496770	-3.7034400	0.1190350
H	8.8055870	-2.0980780	1.1802630

3f (excited state)

C	-3.7724550	-0.8559000	-0.0398890
C	-1.8224290	-2.1104480	-0.2566920
C	-1.4755980	-0.7216090	-0.0447130
C	-2.6564190	0.0073490	0.1017340
C	-0.3638030	0.1789750	0.0283050
C	-2.3030960	1.4305660	0.2649680
O	-2.9820300	2.4299110	0.4163440
O	-1.1716470	-3.1386110	-0.4001780
N	-3.2556660	-2.1113620	-0.2467900
N	-0.8992690	1.4273950	0.2216280
C	-5.1714610	-0.5064180	-0.0137830
C	-6.1774270	-1.2656530	-0.6583460
C	-5.5625970	0.6774600	0.6436800
C	-7.4986770	-0.8707520	-0.6222220
H	-5.9167650	-2.1476030	-1.2310800
C	-6.8905490	1.0772880	0.6877870
H	-4.8094900	1.3003290	1.1157500
C	-7.8709440	0.2996270	0.0594880
H	-8.2709140	-1.4409260	-1.1285060
H	-7.1468890	1.9931570	1.2072720
C	-9.6142350	1.7785930	0.6951550
H	-10.6936650	1.8224460	0.5560020
H	-9.3821610	1.7411020	1.7655920
H	-9.1483040	2.6629590	0.2460240
C	1.0156680	-0.0848990	-0.0685870
C	1.9819400	0.9850370	-0.0109880
C	1.4952450	-1.3748930	-0.3346330
C	2.8739220	-1.6535680	-0.3401610
H	0.7876900	-2.1890370	-0.4826810
C	3.8192490	-0.6347370	-0.0729820
C	3.9848640	1.9079150	-0.3156640
C	2.9651870	2.8771130	-0.2063540
N	3.3420830	0.6809670	-0.1058500
N	1.7389600	2.2771920	-0.0152450
C	5.2812020	2.2587760	-0.7077270
C	5.5449100	3.6098230	-0.8918190
H	6.0507320	1.5163790	-0.8815200
H	6.5419680	3.9123490	-1.1965900
C	3.2530200	4.2362070	-0.3772120
C	4.5512470	4.5901980	-0.7081420
H	2.4626370	4.9735600	-0.2795540
H	4.8029420	5.6357620	-0.8568850
C	3.3510290	-2.9928060	-0.5442110
C	4.6664070	-3.2979160	-0.4035980
H	2.6222930	-3.7523080	-0.8144490
H	5.0248090	-4.3083290	-0.5812770
C	5.1525680	-0.9766310	0.3076770
C	5.5926960	-2.3171560	0.0778140
H	-0.3179370	2.2642890	0.2591610
C	-3.9561890	-3.3827090	-0.2534190
H	-4.7983890	-3.3474360	0.4406180
H	-4.3107720	-3.6413400	-1.2556780
H	-3.2402290	-4.1427650	0.0629930
O	-9.1879290	0.5960210	0.0432410
C	6.0241570	-0.1022270	1.0150780
C	7.2951580	-0.4975090	1.3639450
H	5.6694320	0.8745410	1.3220540
H	7.9336370	0.1841220	1.9181820
C	6.9162720	-2.6774760	0.4107110

C	7.7658850	-1.7843880	1.0272560
H	7.2438440	-3.6924700	0.1993010
H	8.7771500	-2.0801000	1.2890910

4f (ground state)

C	3.7212940	-1.1305630	-0.0265050
C	1.8247890	-2.4726690	0.0900260
C	1.4508880	-1.0824320	-0.0667600
C	2.6332610	-0.2967810	-0.1516150
C	0.3740490	-0.2297780	-0.0819290
C	2.2274080	1.1149430	-0.2383160
O	2.8751330	2.1358210	-0.3530980
O	1.1654070	-3.5019050	0.1779880
N	3.2400010	-2.4394260	0.1086590
N	0.8011110	1.0765530	-0.1851470
C	5.1336050	-0.7684710	0.0037870
C	6.1075340	-1.5154500	0.6935960
C	5.5299490	0.4199500	-0.6246970
C	7.4262450	-1.1008630	0.7280500
H	5.8284780	-2.4093860	1.2400680
C	6.8548150	0.8426190	-0.5995790
H	4.7860840	1.0343530	-1.1230090
C	7.8116680	0.0776200	0.0738180
H	8.1809640	-1.6640380	1.2674020
H	7.1211470	1.7675680	-1.0971920
C	9.5575290	1.5919090	-0.4620700
H	10.6278140	1.6579270	-0.2694450
H	9.3803080	1.5594960	-1.5433620
H	9.0518910	2.4640600	-0.0320100
C	-1.0357720	-0.5461200	0.0070500
C	-1.9340390	0.5555570	-0.0321810
C	-1.5720480	-1.7824400	0.2387160
C	-2.9917300	-1.9592030	0.2811430
H	-0.9146420	-2.6446770	0.3522470
C	-3.8618630	-0.8765300	0.0806580
C	-3.8097060	1.7002790	0.3162140
C	-2.7157110	2.5741600	0.1865560
N	-3.2912820	0.4044500	0.0916400
N	-1.5755360	1.8289310	-0.0338020
B	-0.0641660	2.3605570	-0.1793220
F	0.0004970	3.0603050	-1.3645710
F	0.1784580	3.1627040	0.9161210
C	-5.0550510	2.1767340	0.7413540
C	-5.1756600	3.5450120	0.9324950
H	-5.8883960	1.5147850	0.9397440
H	-6.1287870	3.9435230	1.2649150
C	-2.8452060	3.9545840	0.3625960
C	-4.0951880	4.4251390	0.7237720
H	-1.9821180	4.6011160	0.2474880
H	-4.2405440	5.4890220	0.8808780
C	-3.5449140	-3.2626230	0.4815060
C	-4.8882810	-3.4680460	0.4314830
H	-2.8579910	-4.0789230	0.6849920
H	-5.3067190	-4.4533020	0.6166430
C	-5.2473330	-1.1098860	-0.2138790
C	-5.7658130	-2.4133450	0.0335100
C	3.9869210	-3.6809330	0.0262680
H	4.8421930	-3.5604050	-0.6416350
H	4.3323570	-4.0148880	1.0096320
H	3.3098270	-4.4387620	-0.3725780
O	9.1249690	0.3968970	0.1592470
C	-6.0838440	-0.1673880	-0.8671980
C	-7.3988670	-0.4621620	-1.1421150
H	-5.6730200	0.7784280	-1.1995980

H	-8.0141040	0.2668390	-1.6604760
C	-7.1356610	-2.6707100	-0.2166860
C	-7.9453810	-1.7116070	-0.7768180
H	-7.5257420	-3.6594090	0.0103050
H	-8.9902180	-1.9263060	-0.9783900

4f (excited state)

C	-3.7516260	-1.1721390	-0.0034900
C	-1.8354070	-2.4925190	-0.1151850
C	-1.4626690	-1.1064920	0.0355810
C	-2.6187420	-0.3353970	0.1181920
C	-0.3389090	-0.2307940	0.0842000
C	-2.2046420	1.0819140	0.2165380
O	-2.8552900	2.0981970	0.3126690
O	-1.2047850	-3.5376170	-0.1931950
N	-3.2710850	-2.4529650	-0.1368850
N	-0.7777480	1.0490200	0.1901750
C	-5.1420850	-0.7807500	-0.0199910
C	-6.1573890	-1.5371170	-0.6501800
C	-5.5048440	0.4423990	0.5761700
C	-7.4654880	-1.0989960	-0.6597450
H	-5.9141060	-2.4528030	-1.1757050
C	-6.8192890	0.8861200	0.5761620
H	-4.7409120	1.0604880	1.0367360
C	-7.8116820	0.1125530	-0.0385450
H	-8.2463430	-1.6661830	-1.1558200
H	-7.0552620	1.8319310	1.0492590
C	-9.5169470	1.6748450	0.4930610
H	-10.5911450	1.7460120	0.3280360
H	-9.3083940	1.6781570	1.5687980
H	-9.0131780	2.5221150	0.0147700
C	1.0461590	-0.5376610	0.0139120
C	1.9331160	0.5592780	0.0437650
C	1.5887780	-1.8022740	-0.2514470
C	2.9872720	-1.9664520	-0.3031870
H	0.9291120	-2.6591040	-0.3768650
C	3.8663450	-0.8756760	-0.0847420
C	3.8049200	1.6989130	-0.3506170
C	2.7212930	2.5848540	-0.2059590
N	3.2877360	0.4122940	-0.0986160
N	1.5794440	1.8421260	0.0495910
B	0.0940940	2.3578550	0.2128660
F	-0.0238790	3.0105490	1.4197180
F	-0.2053570	3.1700260	-0.8591530
C	5.0477450	2.1589120	-0.7922210
C	5.1813260	3.5284360	-0.9935230
H	5.8708240	1.4837040	-0.9900940
H	6.1354350	3.9150610	-1.3372710
C	2.8615830	3.9583240	-0.3947440
C	4.1146500	4.4171210	-0.7785660
H	2.0090720	4.6178210	-0.2745310
H	4.2654630	5.4789160	-0.9447960
C	3.5672140	-3.2640790	-0.5145750
C	4.9078310	-3.4592450	-0.4248720
H	2.8949080	-4.0849940	-0.7481380
H	5.3374210	-4.4404530	-0.6087420
C	5.2352770	-1.0993230	0.2398020
C	5.7740600	-2.4030300	0.0048090
C	-4.0103250	-3.7017550	-0.0997980
H	-4.8618040	-3.6115500	0.5778100
H	-4.3565370	-3.9939410	-1.0956300
H	-3.3227250	-4.4677100	0.2622760
O	-9.1160150	0.4500640	-0.0959400
C	6.0648660	-0.1448640	0.8933810
C	7.3793280	-0.4306450	1.1832240
H	5.6463580	0.8025780	1.2118350

H	7.9850050	0.3092970	1.6981710
C	7.1356980	-2.6500470	0.2792390
C	7.9382830	-1.6802710	0.8413330
H	7.5342400	-3.6389480	0.0661860
H	8.9813250	-1.8881850	1.0583020

3g (ground state)

C	1.9273480	0.7190670	-0.0120790
C	0.1083310	2.1408160	0.2498490
C	-0.3473650	0.7703470	0.0843890
C	0.8036890	-0.0650000	-0.0582580
C	-1.4717080	-0.0171880	-0.0407540
C	0.3529950	-1.4389050	-0.2895900
O	0.9390760	-2.4875690	-0.4806970
O	-0.4774200	3.1986440	0.4400330
N	1.5188560	2.0409390	0.1684950
N	-1.0570800	-1.3159560	-0.2480920
C	3.3279970	0.3427970	-0.2015400
C	4.1774390	1.1050770	-1.0122020
C	3.8151490	-0.8557610	0.3648250
C	5.4773110	0.6923760	-1.2820740
H	3.7923800	2.0115990	-1.4702630
C	5.1178070	-1.2773660	0.0816670
C	5.9380080	-0.5043490	-0.7361760
H	6.1161890	1.2875060	-1.9260760
H	5.4941880	-2.2020700	0.5037720
C	-2.8769660	0.3528590	0.0104250
C	-3.8951400	-0.6380930	-0.1579940
C	-3.2607100	1.6607340	0.2225320
C	-4.6354360	2.0138260	0.2688960
H	-2.4996980	2.4268320	0.3549520
C	-5.6003720	1.0657940	0.1060900
C	-5.9906360	-1.3702920	-0.2933230
C	-5.0876180	-2.3921360	-0.4519440
N	-5.2283820	-0.2371340	-0.1032930
N	-3.8024530	-1.9438410	-0.3689520
H	-1.7065000	-2.0887630	-0.3776130
C	2.3510000	3.1913210	0.4657340
H	3.2663490	2.8665140	0.9634890
H	2.6072260	3.7500180	-0.4401340
H	1.7812710	3.8493770	1.1246780
H	6.9476960	-0.8450720	-0.9462660
O	2.9802220	-1.5116910	1.1923540
C	3.2340740	-2.8806810	1.4541940
H	3.3599240	-3.4302500	0.5160090
H	4.1152850	-3.0014520	2.0956600
H	2.3496160	-3.2512280	1.9704090
H	-5.3047080	-3.4372570	-0.6234770
H	-7.0690070	-1.3371780	-0.2965130
H	-6.6656580	1.2629670	0.1298320
H	-4.9273540	3.0438620	0.4349080

3g (excited state)

C	1.9747160	0.7584240	0.0043040
C	0.1275350	2.1577870	0.2272490
C	-0.3248740	0.7906240	0.0939900
C	0.7950480	-0.0317880	-0.0246490
C	-1.5011260	-0.0145940	-0.0395350
C	0.3370270	-1.4106240	-0.2915470
O	0.9379380	-2.4431260	-0.5252070
O	-0.4350670	3.2335560	0.3960550
N	1.5575220	2.0533210	0.1480600
N	-1.0634040	-1.2994450	-0.2516580
C	3.3462740	0.3482750	-0.1837350
C	4.2519250	1.0974460	-0.9585130
C	3.7837870	-0.8865720	0.3638300
C	5.5306720	0.6281550	-1.2203720
H	3.9180210	2.0286260	-1.4057900
C	5.0632330	-1.3659200	0.0778940
C	5.9284540	-0.6097810	-0.7099530
H	6.2061270	1.2088670	-1.8400000
H	5.3923060	-2.3158970	0.4833880
C	-2.8650250	0.3510530	0.0173170
C	-3.8938600	-0.6382100	-0.1571860
C	-3.2655080	1.6781110	0.2401590
C	-4.6316400	2.0133310	0.2863160
H	-2.5074210	2.4472010	0.3739900
C	-5.6040640	1.0606250	0.1174320
C	-5.9816450	-1.3784810	-0.2990620
C	-5.0793490	-2.3980310	-0.4652630
N	-5.2218220	-0.2433630	-0.1003790
N	-3.7930220	-1.9415100	-0.3775350
H	-1.7092440	-2.0752910	-0.3973510
C	2.3764030	3.2252060	0.3933550
H	3.3031540	2.9265960	0.8866550
H	2.6078280	3.7503210	-0.5385050
H	1.8027100	3.8979060	1.0329950
H	6.9230400	-0.9910400	-0.9214630
O	2.9210440	-1.4993420	1.1937900
C	3.1098390	-2.8782850	1.4630650
H	3.2139760	-3.4374180	0.5282300
H	3.9817900	-3.0327360	2.1093690
H	2.2073810	-3.2048060	1.9785060
H	-5.2917270	-3.4426100	-0.6447040
H	-7.0601610	-1.3462280	-0.3021530
H	-6.6693540	1.2534480	0.1419050
H	-4.9316080	3.0408450	0.4578460

4g (ground state)

C	2.1887800	0.9057170	-0.0232680
C	0.5057170	2.4942640	0.1851630
C	-0.0600520	1.1622040	0.0729370
C	1.0001900	0.2216310	-0.0408060
C	-1.2433930	0.4726720	-0.0065240
C	0.4053280	-1.1133000	-0.2115830
O	0.9035340	-2.2082410	-0.3639480
O	-0.0035250	3.5980020	0.3353680
N	1.8991610	2.2703710	0.1055050
N	-1.0056190	-0.8777660	-0.1667690
C	3.5499040	0.3987900	-0.1865850
C	4.4745620	1.0499650	-1.0121320
C	3.9161120	-0.8219050	0.4236830
C	5.7307230	0.5062910	-1.2548350
H	4.1814810	1.9724860	-1.5049260
C	5.1746350	-1.3750130	0.1669900
C	6.0705410	-0.7109030	-0.6663440
H	6.4281890	1.0156070	-1.9115140
H	5.4566580	-2.3175110	0.6220920
C	-2.5992590	0.9782440	0.0518630
C	-3.6145330	0.0045760	-0.0564940
C	-2.9917140	2.2905430	0.2041590
C	-4.3786850	2.6046510	0.2404130
H	-2.2373450	3.0703410	0.2948220
C	-5.3359220	1.6361300	0.1303830
C	-5.6558680	-0.8583610	-0.1511300
C	-4.7252230	-1.8530320	-0.2637320
N	-4.9414620	0.3260520	-0.0187480
N	-3.4712050	-1.3095580	-0.2038240
B	-2.0312400	-2.0371200	-0.2845410
F	-1.9690010	-2.9114620	0.7787720
F	-1.9799440	-2.6772980	-1.5014140
C	2.8324030	3.3507850	0.3622840
H	3.7059910	2.9670280	0.8923920
H	3.1537650	3.8374990	-0.5640610
H	2.3181040	4.0908310	0.9786490
H	7.0443560	-1.1531280	-0.8557860
O	3.0180910	-1.3663590	1.2635860
C	3.1281860	-2.7479990	1.5639730
H	3.2122010	-3.3311250	0.6418220
H	3.9834160	-2.9376740	2.2237220
H	2.2019480	-3.0143150	2.0708450
H	-4.6954430	3.6341920	0.3584810
H	-6.4030770	1.8174470	0.1518730
H	-6.7338320	-0.8766840	-0.1521990
H	-4.8652240	-2.9171610	-0.3833960

4g (excited state)

C	2.2366500	0.9409750	-0.0057360
C	0.5234670	2.5110130	0.1693420
C	-0.0399140	1.1881390	0.0846230
C	0.9950180	0.2613370	-0.0077260
C	-1.2722650	0.4828480	-0.0016120
C	0.3899330	-1.0769180	-0.2084680
O	0.9007920	-2.1589910	-0.3977340
O	0.0525410	3.6343530	0.2965180
N	1.9420860	2.2741040	0.0948340
N	-1.0142330	-0.8515050	-0.1665730
C	3.5678490	0.3982260	-0.1708640
C	4.5351450	1.0280060	-0.9742160
C	3.8869580	-0.8473690	0.4288070
C	5.7652780	0.4330830	-1.2130110
H	4.2872450	1.9665010	-1.4605250
C	5.1184130	-1.4528260	0.1682520
C	6.0475660	-0.8126560	-0.6475920
H	6.4905130	0.9217870	-1.8551480
H	5.3581620	-2.4117080	0.6133730
C	-2.6013020	0.9723340	0.0603880
C	-3.6181020	-0.0034820	-0.0528380
C	-3.0126950	2.3057060	0.2200230
C	-4.3901690	2.5981890	0.2557920
H	-2.2658900	3.0915280	0.3113720
C	-5.3535980	1.6223740	0.1411660
C	-5.6512860	-0.8787440	-0.1529440
C	-4.7236030	-1.8727560	-0.2710500
N	-4.9418840	0.3075470	-0.0144550
N	-3.4675660	-1.3189420	-0.2068780
B	-2.0443250	-2.0273620	-0.2974970
F	-1.9333780	-2.9091380	0.7564260
F	-1.9536100	-2.6502780	-1.5211950
C	2.8661750	3.3745570	0.2917030
H	3.7613490	3.0146200	0.8022220
H	3.1457430	3.8339780	-0.6614250
H	2.3563750	4.1249950	0.8982510
H	7.0029590	-1.2919540	-0.8396100
O	2.9701230	-1.3466270	1.2741680
C	3.0213400	-2.7299540	1.5888160
H	3.0865670	-3.3253610	0.6732980
H	3.8646280	-2.9442990	2.2555130
H	2.0827340	-2.9526760	2.0946510
H	-4.7173780	3.6247540	0.3776260
H	-6.4212300	1.7937260	0.1623730
H	-6.7292910	-0.8989300	-0.1540740
H	-4.8595690	-2.9362130	-0.3967350

3i (ground state)

C	3.3580260	0.6656660	-0.0987220
C	1.5682690	2.1417610	0.0200860
C	1.0852140	0.7716290	0.0045030
C	2.2191540	-0.0961930	-0.0553360
C	-0.0560090	-0.0038630	-0.0239330
C	1.7409420	-1.4776280	-0.1323760
O	2.3042320	-2.5525770	-0.2135680
O	1.0038080	3.2264820	0.0993330
N	2.9752080	2.0068380	-0.0581860
N	0.3335710	-1.3235140	-0.0926470
C	4.7501470	0.2432670	-0.2501640
C	5.6110630	0.8944210	-1.1415710
C	5.2160690	-0.8952720	0.4436820
C	6.9017980	0.4290020	-1.3662010
H	5.2419520	1.7519110	-1.6968460
C	6.5094600	-1.3706880	0.2071640
C	7.3414980	-0.7087140	-0.6919780
H	7.5495860	0.9365750	-2.0731710
H	6.8694780	-2.2503910	0.7281190
C	-1.4505420	0.4108950	0.0051070
C	-2.5174310	-0.5634200	-0.0534000
C	-1.7806140	1.7317700	0.0804330
C	-3.1481980	2.1602420	0.1311900
H	-0.9958300	2.4863790	0.1172560
C	-4.1994240	1.2139270	0.0933600
C	-4.6226750	-1.2924870	-0.1533200
C	-3.6840740	-2.3473440	-0.2069460
N	-3.8479560	-0.1329190	-0.0385130
N	-2.3976080	-1.8661440	-0.1449380
C	-5.9965590	-1.5542630	-0.2471990
C	-6.3901570	-2.8798780	-0.3668960
H	-6.7537670	-0.7837960	-0.2508420
H	-7.4496100	-3.1037120	-0.4428550
C	-4.1000620	-3.6789620	-0.3252900
C	-5.4577180	-3.9334010	-0.3997420
H	-3.3607360	-4.4725070	-0.3624400
H	-5.8124130	-4.9550350	-0.4936840
C	-3.4613830	3.5283970	0.2460610
C	-4.7723350	3.9545510	0.3345100
H	-2.6403950	4.2400070	0.2695070
H	-5.0024990	5.0110990	0.4231060
C	-5.5255680	1.6508370	0.2064200
C	-5.8019040	3.0048800	0.3225910
H	-0.3330360	-2.0904350	-0.1377160
C	3.8313630	3.1662580	0.1066530
H	4.7434200	2.8800530	0.6333270
H	4.0925070	3.6161310	-0.8565360
H	3.2787520	3.9041620	0.6913550
H	8.3437760	-1.0899550	-0.8645800
O	4.3712110	-1.4406140	1.3387460
C	4.6016320	-2.7763490	1.7508720
H	4.7160270	-3.4288780	0.8795450
H	5.4820360	-2.8407190	2.4015080
H	3.7120120	-3.0716000	2.3053810
H	-6.3418040	0.9462090	0.2250040
H	-6.8358540	3.3241120	0.4111050

3i (excited state)

C	3.3984340	0.7043460	-0.0897020
C	1.5837560	2.1580860	-0.0160580
C	1.1039170	0.7927540	0.0121540
C	2.2079180	-0.0585760	-0.0188090
C	-0.0895870	-0.0048200	-0.0151800
C	1.7246970	-1.4500320	-0.1147970
O	2.3021480	-2.5137880	-0.2261230
O	1.0458600	3.2586260	0.0310600
N	3.0098750	2.0161250	-0.0924880
N	0.3240590	-1.3096360	-0.0769780
C	4.7623440	0.2476290	-0.2380290
C	5.6692170	0.8805760	-1.1076790
C	5.1844460	-0.9184000	0.4514840
C	6.9376780	0.3615110	-1.3226870
H	5.3444590	1.7559490	-1.6617570
C	6.4539360	-1.4496590	0.2155900
C	7.3215990	-0.8101870	-0.6668450
H	7.6149320	0.8502070	-2.0153500
H	6.7728210	-2.3486530	0.7305110
C	-1.4398730	0.4036640	0.0110430
C	-2.5082040	-0.5670930	-0.0430600
C	-1.7833810	1.7542500	0.0705980
C	-3.1348390	2.1660940	0.1284880
H	-0.9984450	2.5085800	0.0932790
C	-4.1926820	1.2101240	0.1108780
C	-4.6109350	-1.2956510	-0.1635860
C	-3.6747510	-2.3537260	-0.2088700
N	-3.8356870	-0.1381540	-0.0349760
N	-2.3868480	-1.8717050	-0.1341800
C	-5.9821630	-1.5511360	-0.2876700
C	-6.3796480	-2.8764560	-0.4190780
H	-6.7330530	-0.7746970	-0.3124100
H	-7.4382950	-3.0951990	-0.5184850
C	-4.0928370	-3.6817650	-0.3379340
C	-5.4519880	-3.9321620	-0.4358740
H	-3.3565190	-4.4785640	-0.3677270
H	-5.8077590	-4.9526070	-0.5390000
C	-3.4728740	3.5385790	0.2403870
C	-4.7850810	3.9460290	0.3568870
H	-2.6618020	4.2620380	0.2427270
H	-5.0242880	5.0012170	0.4438420
C	-5.5144520	1.6329190	0.2625200
C	-5.8084440	2.9870340	0.3809070
H	-0.3399000	-2.0819550	-0.1296940
C	3.8547090	3.1914530	0.0087770
H	4.7826340	2.9313530	0.5210920
H	4.0820920	3.6032650	-0.9792650
H	3.3041160	3.9436610	0.5760030
H	8.3077820	-1.2311160	-0.8388700
O	4.3194210	-1.4144630	1.3538390
C	4.4939460	-2.7523630	1.7893760
H	4.5815620	-3.4237840	0.9297140
H	5.3705740	-2.8383130	2.4419080
H	3.5931580	-3.0004480	2.3494100
H	-6.3198280	0.9167250	0.3156100
H	-6.8426110	3.2948070	0.4992200

4i (ground state)

C	3.4047090	0.9146360	-0.0694880
C	1.6724340	2.4577670	0.0644490
C	1.1481270	1.1069440	0.0155710
C	2.2377500	0.1950280	-0.0548040
C	-0.0142890	0.3764150	-0.0291270
C	1.6850440	-1.1638980	-0.1610740
O	2.2146540	-2.2498120	-0.2624810
O	1.1302120	3.5535630	0.1624490
N	3.0716700	2.2740560	-0.0045830
N	0.2672520	-0.9686640	-0.1250010
C	4.7815060	0.4432830	-0.2085800
C	5.6866310	1.0827070	-1.0642350
C	5.1854830	-0.7343170	0.4597690
C	6.9603790	0.5688230	-1.2794180
H	5.3651620	1.9703170	-1.6014390
C	6.4615710	-1.2584710	0.2310000
C	7.3379120	-0.6068940	-0.6326940
H	7.6425410	1.0681510	-1.9594790
H	6.7724660	-2.1685660	0.7310740
C	-1.3825750	0.8516020	0.0086790
C	-2.4004800	-0.1449020	-0.0505830
C	-1.7743640	2.1540700	0.1025420
C	-3.1698230	2.4894550	0.1278780
H	-1.0245770	2.9440800	0.1562970
C	-4.1676720	1.4832560	0.0616830
C	-4.4204230	-1.0816140	-0.0880530
C	-3.4155490	-2.0654720	-0.1597760
N	-3.7366180	0.1498860	-0.0210480
N	-2.1834760	-1.4447680	-0.1333170
B	-0.7345310	-2.1436910	-0.1873360
F	-0.6571360	-2.9763290	0.9107450
F	-0.6785280	-2.8422880	-1.3741320
C	-5.7696560	-1.4542510	-0.0890660
C	-6.0549800	-2.8105760	-0.1674600
H	-6.5845840	-0.7480950	-0.0294420
H	-7.0942210	-3.1229940	-0.1696040
C	-3.7058130	-3.4282770	-0.2392020
C	-5.0430720	-3.7849660	-0.2426770
H	-2.9003890	-4.1526870	-0.2938150
H	-5.3182770	-4.8328470	-0.3029420
C	-3.5757210	3.8366400	0.2154640
C	-4.9124340	4.1802840	0.2339520
H	-2.8038530	4.5994440	0.2666520
H	-5.2096680	5.2214940	0.3012050
C	-5.5211680	1.8377770	0.0770480
C	-5.8839010	3.1725970	0.1623580
C	3.9702080	3.3943630	0.1986920
H	4.8541520	3.0651300	0.7479640
H	4.2784690	3.8442880	-0.7504690
H	3.4314360	4.1476680	0.7769140
H	8.3258470	-1.0262090	-0.7998270
O	4.3030080	-1.2670110	1.3238790
C	4.4566050	-2.6282630	1.6898180
H	4.5599720	-3.2520450	0.7966230
H	5.3167610	-2.7594280	2.3573890
H	3.5388820	-2.8992640	2.2096120
H	-6.9377720	3.4321810	0.1724300
H	-6.2921090	1.0854600	0.0188780

4i (excited state)

C	3.4462190	0.9493990	-0.0477550
C	1.6926350	2.4747240	0.0691570
C	1.1677330	1.1299630	0.0300820
C	2.2317650	0.2343320	-0.0273900
C	-0.0441810	0.3771040	-0.0323620
C	1.6731650	-1.1270380	-0.1750040
O	2.2063610	-2.2017570	-0.3165550
O	1.1907210	3.5872710	0.1552620
N	3.1153560	2.2777890	0.0059690
N	0.2526400	-0.9397790	-0.1449230
C	4.7970160	0.4432680	-0.1893010
C	5.7404080	1.0741580	-1.0180990
C	5.1578120	-0.7641830	0.4600150
C	6.9926440	0.5163300	-1.2317240
H	5.4585820	1.9825540	-1.5417670
C	6.4129530	-1.3320880	0.2278980
C	7.3195300	-0.6919830	-0.6128350
H	7.7005000	1.0043580	-1.8933260
H	6.6876150	-2.2621480	0.7120520
C	-1.3889020	0.8376000	0.0122830
C	-2.3919950	-0.1502950	-0.0586680
C	-1.7835690	2.1717610	0.1338630
C	-3.1619770	2.4958520	0.1489130
H	-1.0335790	2.9576700	0.2015770
C	-4.1672300	1.4823480	0.0533710
C	-4.4172460	-1.0876810	-0.0692910
C	-3.4195930	-2.0789380	-0.1643690
N	-3.7301500	0.1405130	-0.0157830
N	-2.1818150	-1.4603090	-0.1533630
B	-0.7572510	-2.1396090	-0.2243240
F	-0.6108850	-2.9780930	0.8616030
F	-0.6469900	-2.8096900	-1.4224100
C	-5.7648230	-1.4554140	-0.0233970
C	-6.0630360	-2.8132280	-0.0966110
H	-6.5713290	-0.7448610	0.0796910
H	-7.1039460	-3.1183710	-0.0623490
C	-3.7199570	-3.4361180	-0.2392630
C	-5.0623390	-3.7893190	-0.2077530
H	-2.9232750	-4.1683610	-0.3140730
H	-5.3418300	-4.8363980	-0.2633710
C	-3.5945950	3.8435710	0.2390900
C	-4.9342750	4.1737710	0.2191360
H	-2.8337160	4.6151750	0.3175590
H	-5.2386570	5.2134870	0.2877860
C	-5.5150750	1.8295960	0.0156530
C	-5.8995920	3.1657360	0.0995310
C	4.0072550	3.4106850	0.1706990
H	4.9109750	3.0927970	0.6935660
H	4.2753180	3.8494530	-0.7951760
H	3.4754840	4.1637020	0.7546780
H	8.2927950	-1.1427970	-0.7828390
O	4.2545550	-1.2667190	1.3181080
C	4.3663870	-2.6299170	1.6980910
H	4.4614970	-3.2647320	0.8120050
H	5.2163150	-2.7754430	2.3746460
H	3.4374660	-2.8697150	2.2137200
H	-6.9547000	3.4167820	0.0676270
H	-6.2765240	1.0731080	-0.0946950

3j (ground state)

C	-2.7491260	0.7867660	-0.1240430
C	-0.8950000	2.1925940	-0.1047070
C	-0.4643710	0.8082670	-0.1687500
C	-1.6308750	-0.0164670	-0.2022500
C	0.6484460	-0.0063960	-0.1297870
C	-1.2014700	-1.4141550	-0.1993450
O	-1.8043290	-2.4730900	-0.2467970
O	-0.2869300	3.2558140	-0.1000840
N	-2.3096830	2.1117760	-0.0731770
N	0.2072590	-1.3119360	-0.1534550
C	-4.1454400	0.3856380	-0.0693550
C	-5.1452880	1.1403720	0.5651770
C	-4.5150420	-0.8593480	-0.6091620
C	-6.4551050	0.6960640	0.6333320
H	-4.8969840	2.0756960	1.0550190
C	-5.8208970	-1.3101460	-0.5557210
H	-3.7554310	-1.4909230	-1.0601520
C	-6.8358900	-0.5368280	0.0544860
H	-7.1826400	1.3073250	1.1534510
H	-6.0492760	-2.2782110	-0.9844630
N	-8.1394140	-0.9697790	0.0900190
C	-8.4569590	-2.3130250	-0.3541840
H	-9.5303790	-2.4750250	-0.2535970
H	-8.1945840	-2.4476730	-1.4092340
H	-7.9316210	-3.0783170	0.2347690
C	-9.1157810	-0.2330290	0.8665820
H	-8.8544300	-0.1962840	1.9342840
H	-9.2130690	0.7944100	0.4984400
H	-10.0877450	-0.7164590	0.7657240
C	2.0562220	0.3561290	-0.0674200
C	3.0834910	-0.6610550	-0.0223680
C	2.4390850	1.6647600	-0.0458710
C	3.8221970	2.0409190	-0.0014730
H	1.6860090	2.4509610	-0.0744760
C	4.8351840	1.0537070	0.0288520
C	5.1538770	-1.4787160	0.1179740
C	4.1753470	-2.4963330	0.0577520
N	4.4285100	-0.2839600	0.0514240
N	2.9119910	-1.9612100	-0.0263780
C	6.5116910	-1.8020770	0.2482410
C	6.8498820	-3.1476640	0.2896140
H	7.2970820	-1.0654290	0.3343340
H	7.8961220	-3.4186290	0.3912870
C	4.5354950	-3.8486190	0.0989180
C	5.8781240	-4.1624810	0.2104740
H	3.7658260	-4.6120100	0.0484020
H	6.1897930	-5.2017070	0.2458910
C	4.1907020	3.4000600	-0.0104390
C	5.5190390	3.7791250	-0.0014960
H	3.3984720	4.1436550	-0.0302100
H	5.7913210	4.8293690	-0.0088710
C	6.1803260	1.4443490	0.0174390
C	6.5117190	2.7909860	0.0048930
H	6.9706760	0.7109140	0.0002490
H	7.5598550	3.0739420	-0.0053900
H	0.8413110	-2.1069940	-0.1453000
C	-3.0959540	3.3200930	-0.2389750
H	-3.9501150	3.1238010	-0.8900800
H	-3.4471990	3.7120460	0.7206970

H -2.4453550 4.0685750 -0.6951000

3j (excited state)

C	-2.7812990	0.8307930	-0.0704560
C	-0.9016780	2.2104590	-0.0358810
C	-0.4763740	0.8289170	-0.0884770
C	-1.6146080	0.0203550	-0.1288940
C	0.6848870	-0.0071890	-0.0751210
C	-1.1767760	-1.3887160	-0.1309930
O	-1.7941330	-2.4401360	-0.1575650
O	-0.3091630	3.2845550	-0.0287140
N	-2.3302810	2.1301460	-0.0214170
N	0.2225920	-1.2988170	-0.1067550
C	-4.1509900	0.4034980	-0.0296920
C	-5.2088230	1.1830430	0.4932080
C	-4.4790100	-0.8951320	-0.4902010
C	-6.5065560	0.7146990	0.5303730
H	-5.0095160	2.1568350	0.9241880
C	-5.7723080	-1.3690980	-0.4636800
H	-3.6908180	-1.5425430	-0.8617150
C	-6.8344820	-0.5745260	0.0378790
H	-7.2727740	1.3467130	0.9632240
H	-5.9618530	-2.3701510	-0.8318440
N	-8.1205040	-1.0357910	0.0560500
C	-8.4117110	-2.3852950	-0.3899090
H	-9.4825480	-2.5659460	-0.2997530
H	-8.1285710	-2.5247320	-1.4401190
H	-7.8823950	-3.1327180	0.2152190
C	-9.1772820	-0.2183420	0.6190460
H	-9.0076860	-0.0144370	1.6848050
H	-9.2602300	0.7390220	0.0906270
H	-10.1263190	-0.7442410	0.5177340
C	2.0519100	0.3487630	-0.0382890
C	3.0804450	-0.6658170	-0.0232380
C	2.4499190	1.6838800	0.0004550
C	3.8177680	2.0438590	0.0043030
H	1.6960370	2.4693190	0.0052310
C	4.8373780	1.0478580	-0.0139840
C	5.1498410	-1.4856270	0.0944190
C	4.1722330	-2.5054350	0.0431150
N	4.4239430	-0.2917180	0.0299970
N	2.9068410	-1.9679690	-0.0269620
C	6.5064980	-1.8054770	0.2311340
C	6.8485770	-3.1518680	0.2760810
H	7.2865210	-1.0641570	0.3274840
H	7.8951100	-3.4199890	0.3830790
C	4.5347700	-3.8552050	0.0862650
C	5.8801480	-4.1674260	0.1964070
H	3.7670820	-4.6211340	0.0416120
H	6.1928700	-5.2063760	0.2337160
C	4.2116650	3.4058460	-0.0066370
C	5.5415030	3.7672890	-0.0590030
H	3.4293010	4.1599060	0.0167980
H	5.8228920	4.8156730	-0.0686160
C	6.1785230	1.4261020	-0.0994750
C	6.5282490	2.7720860	-0.1181940
H	6.9571390	0.6831060	-0.1773480
H	7.5766440	3.0450800	-0.1860630
H	0.8549320	-2.0986050	-0.1047490
C	-3.1007090	3.3511850	-0.1601500
H	-3.9317780	3.1911220	-0.8506990
H	-3.4815180	3.7005210	0.8045190

H -2.4245270 4.1105330 -0.5559500

4j (ground state)

C	-2.8261210	1.0552400	-0.1473410
C	-1.0199950	2.5231590	-0.1665920
C	-0.5548920	1.1518840	-0.1920640
C	-1.6824860	0.2856580	-0.2021100
C	0.5771810	0.3772780	-0.1247220
C	-1.1840320	-1.0965130	-0.1574100
O	-1.7592630	-2.1671620	-0.1784970
O	-0.4286410	3.5967700	-0.1907090
N	-2.4287730	2.4005420	-0.1345440
N	0.2359840	-0.9587680	-0.1081130
C	-4.2078730	0.6109750	-0.0804430
C	-5.2408490	1.3582740	0.5085310
C	-4.5265240	-0.6730700	-0.5596100
C	-6.5339470	0.8691290	0.5891920
H	-5.0328360	2.3248820	0.9539950
C	-5.8150200	-1.1689500	-0.4923870
H	-3.7394420	-1.2986210	-0.9705700
C	-6.8635220	-0.4044840	0.0703000
H	-7.2881170	1.4777230	1.0733010
H	-6.0026640	-2.1659490	-0.8717200
N	-8.1507220	-0.8838630	0.1182090
C	-8.4118880	-2.2610240	-0.2535060
H	-9.4796530	-2.4580410	-0.1547650
H	-8.1322560	-2.4430200	-1.2967870
H	-7.8648770	-2.9721040	0.3818580
C	-9.1578020	-0.1505750	0.8577570
H	-8.9042230	-0.0571660	1.9240100
H	-9.2906540	0.8553250	0.4442150
H	-10.1108560	-0.6734460	0.7740280
C	1.9616680	0.7968760	-0.0632930
C	2.9347050	-0.2436510	0.0050560
C	2.4121910	2.0841790	-0.0707780
C	3.8188520	2.3599440	0.0031840
H	1.7003660	2.9078390	-0.1286190
C	4.7700840	1.3101350	0.0787830
C	4.9099100	-1.2671350	0.1097010
C	3.8638040	-2.2090770	0.0730490
N	4.2811990	-0.0057420	0.0675810
N	2.6616310	-1.5354620	0.0085230
B	1.1863140	-2.1766170	-0.0684450
F	1.1478500	-2.9331990	-1.2212690
F	1.0337410	-2.9460460	1.0651070
C	6.2407510	-1.6975140	0.1672970
C	6.4659840	-3.0671150	0.1915140
H	7.0856610	-1.0252080	0.1889720
H	7.4898940	-3.4239910	0.2357630
C	4.0937080	-3.5854810	0.0981030
C	5.4129330	-3.9993420	0.1589700
H	3.2578970	-4.2761360	0.0693060
H	5.6417800	-5.0598170	0.1803440
C	4.2837260	3.6909520	0.0080710
C	5.6316470	3.9771830	0.0878200
H	3.5478990	4.4880510	-0.0508970
H	5.9738210	5.0067290	0.0910110
C	6.1349600	1.6063220	0.1645300
C	6.5558570	2.9266520	0.1682660
H	6.8696760	0.8194120	0.2335760
H	7.6177690	3.1408250	0.2361460
C	-3.2524080	3.5770250	-0.3413900

H	-4.0883930	3.3379380	-1.0018970
H	-3.6331420	3.9796220	0.6024960
H	-2.6191500	4.3360240	-0.8048960

4j (excited state)

C	-2.8593460	1.0975140	-0.1154010
C	-1.0298790	2.5444150	-0.1359700
C	-0.5680290	1.1771890	-0.1330720
C	-1.6731990	0.3267340	-0.1405140
C	0.6071280	0.3779660	-0.0727040
C	-1.1667300	-1.0618550	-0.0775200
O	-1.7473570	-2.1258190	-0.0654820
O	-0.4662330	3.6309720	-0.1695020
N	-2.4570410	2.4163050	-0.1201820
N	0.2527990	-0.9333710	-0.0444690
C	-4.2164980	0.6257220	-0.0574290
C	-5.2959700	1.3861940	0.4443400
C	-4.4981970	-0.6975150	-0.4714390
C	-6.5759160	0.8737470	0.5083070
H	-5.1280780	2.3816560	0.8377490
C	-5.7732780	-1.2162800	-0.4206140
H	-3.6893990	-1.3275870	-0.8277560
C	-6.8595220	-0.4431460	0.0633600
H	-7.3618270	1.4925570	0.9243010
H	-5.9291750	-2.2350750	-0.7537590
N	-8.1261040	-0.9498860	0.1092480
C	-8.3722770	-2.3227260	-0.2927390
H	-9.4347450	-2.5390230	-0.1849440
H	-8.0947940	-2.4837840	-1.3412190
H	-7.8101240	-3.0306940	0.3293530
C	-9.2096100	-0.1505370	0.6480200
H	-9.0409640	0.1000290	1.7036650
H	-9.3312490	0.7817920	0.0836640
H	-10.1387570	-0.7149230	0.5742690
C	1.9720140	0.7819600	-0.0421590
C	2.9298730	-0.2513200	0.0160510
C	2.4283140	2.1003350	-0.0750540
C	3.8188410	2.3639110	-0.0195990
H	1.7153690	2.9209520	-0.1304820
C	4.7763550	1.3041040	0.0607460
C	4.9119680	-1.2766040	0.0600200
C	3.8699750	-2.2261280	0.0600910
N	4.2802420	-0.0183630	0.0433710
N	2.6616450	-1.5539080	0.0320870
B	1.2087120	-2.1763090	-0.0020700
F	1.0857570	-2.9404500	-1.1435460
F	1.0211310	-2.9153230	1.1458970
C	6.2435690	-1.7016120	0.0525660
C	6.4802600	-3.0733740	0.0652040
H	7.0835490	-1.0237310	0.0236850
H	7.5078040	-3.4226370	0.0594200
C	4.1089240	-3.5976280	0.0738900
C	5.4350860	-4.0082550	0.0801790
H	3.2789080	-4.2958860	0.0747040
H	5.6674230	-5.0682380	0.0905730
C	4.3114160	3.6941790	-0.0220890
C	5.6618330	3.9636050	0.0655480
H	3.5873320	4.5014970	-0.0887270
H	6.0120100	4.9911670	0.0632240
C	6.1353700	1.5892810	0.1663150
C	6.5789310	2.9094560	0.1673610
H	6.8594850	0.7952800	0.2635660
H	7.6416430	3.1118990	0.2510570
C	-3.2702510	3.6023380	-0.3105710

H	-4.0936670	3.3851060	-0.9945940
H	-3.6649020	3.9787400	0.6381420
H	-2.6203920	4.3677370	-0.7379560

Section S8: Photostability measurements

Photostability was determined through the variation in absorption of each sample at the appropriate absorption maximum wavelength (λ_{abs}) with respect to irradiation time. Methanol was selected as the solvent in all cases as this is closest solvent to aqueous media (important for biological imaging) that these compounds are soluble in. Concentrations giving similar optical densities ($A \approx 1$) were used. Quartz cuvettes of samples were irradiated with a 300 W Xe lamp (Asahi spectra, MAX-350) equipped with a UV/vis mirror module through a glass fiber. The absorption spectra were measured at appropriate times during the irradiation. BODIPY (Difluoro{2-[1-(3,5-dimethyl-2*H*-pyrrol-2-ylidene-*N*)ethyl]-3,5-dimethyl-1*H*-pyrrolato-*N*}boron) and DPP (2,5-dibutyl-3,6-bis(3,5-dimethoxyphenyl)pyrrolo[3,4-*c*]pyrrole-1,4(2*H*,5*H*)-dione) were used as references.

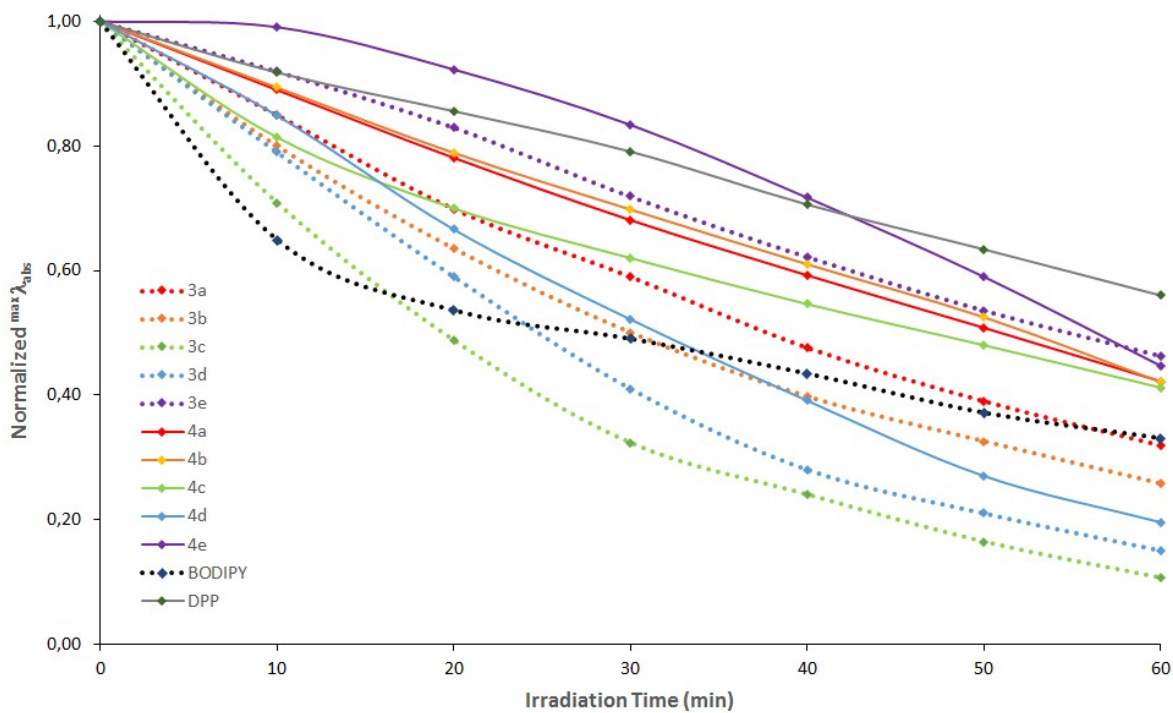
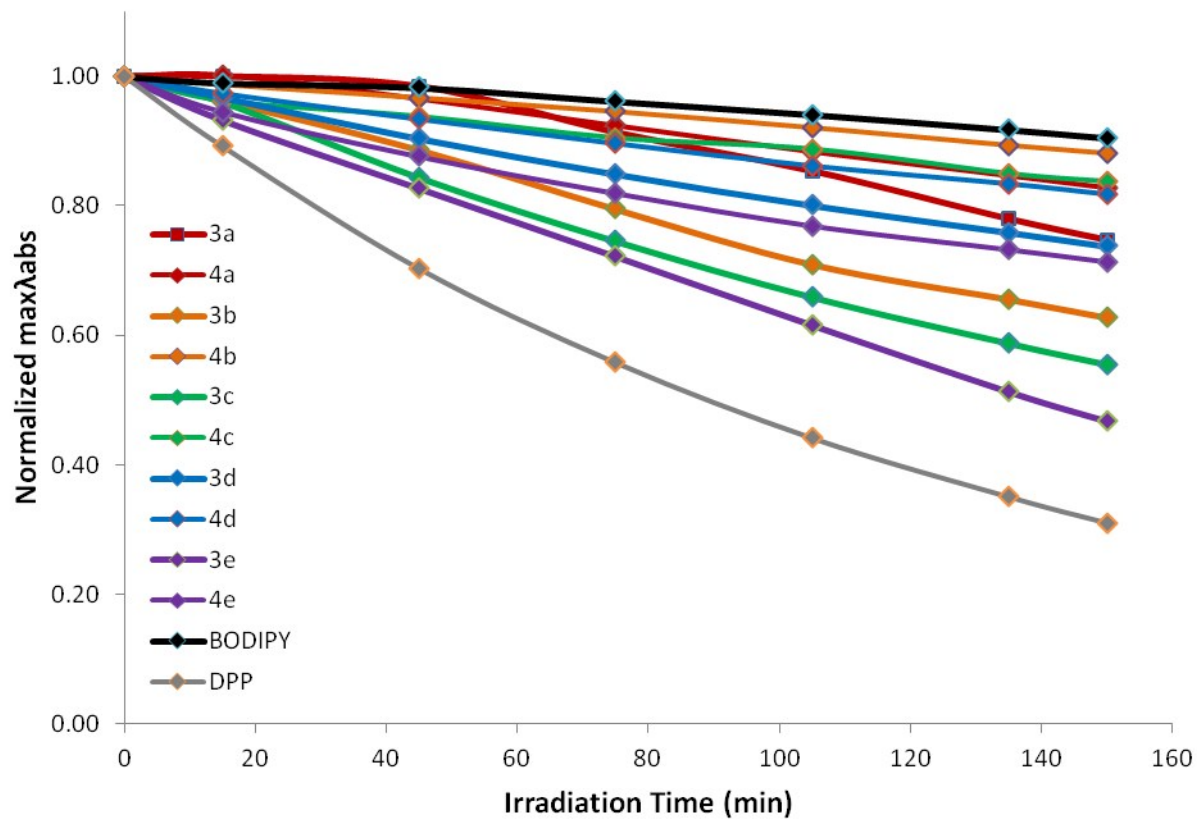
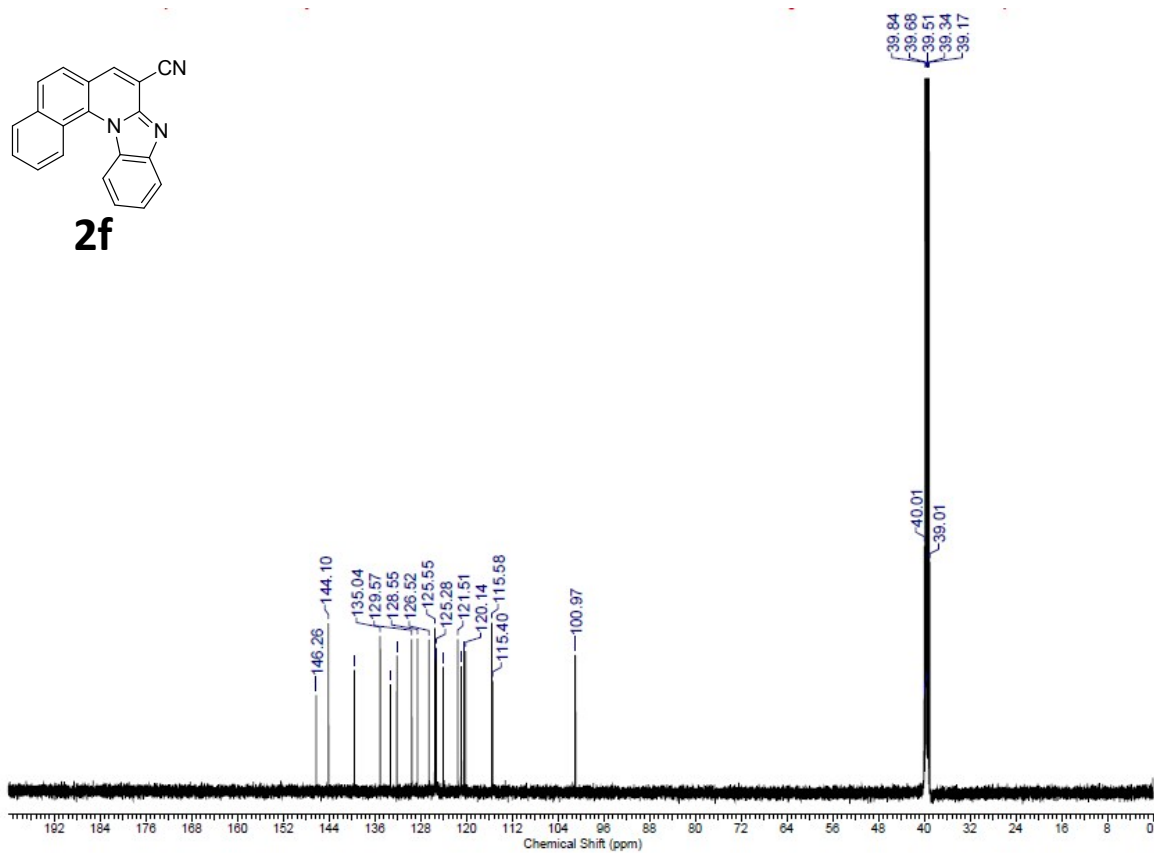
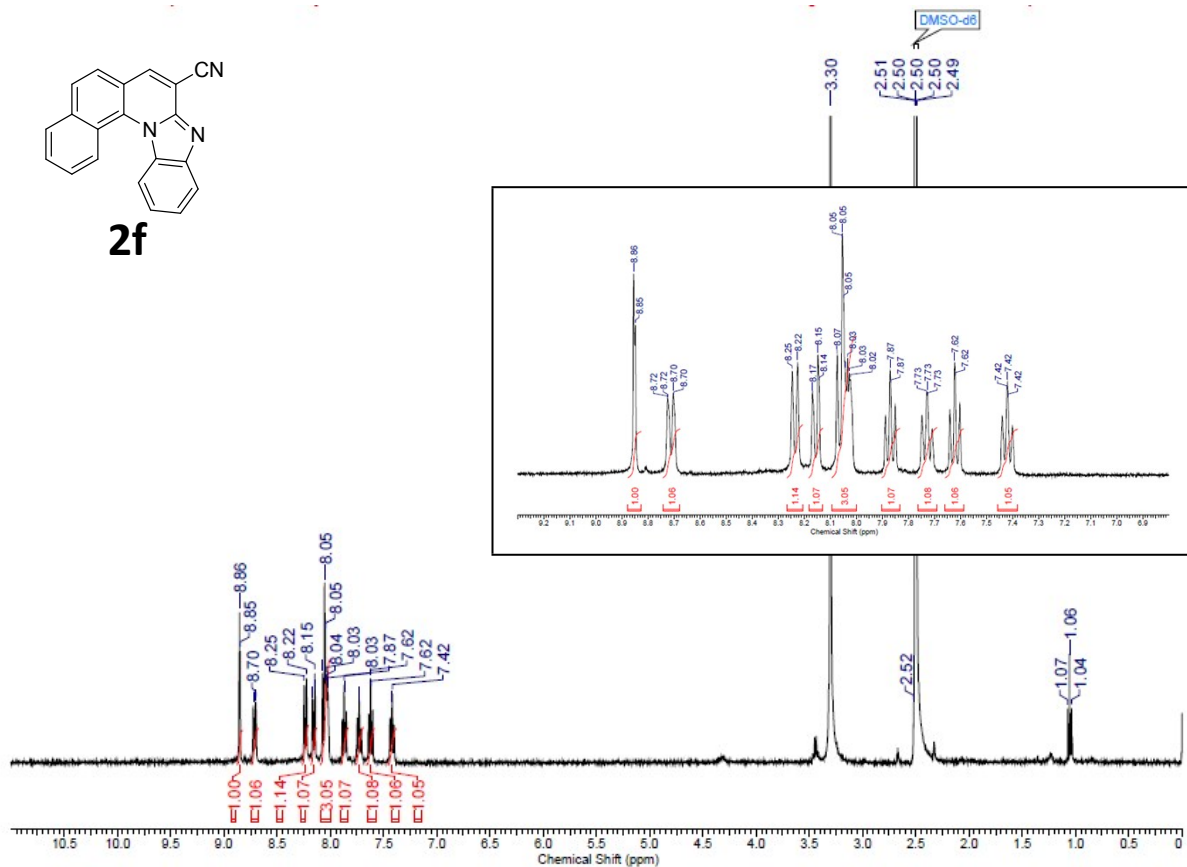
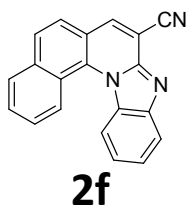
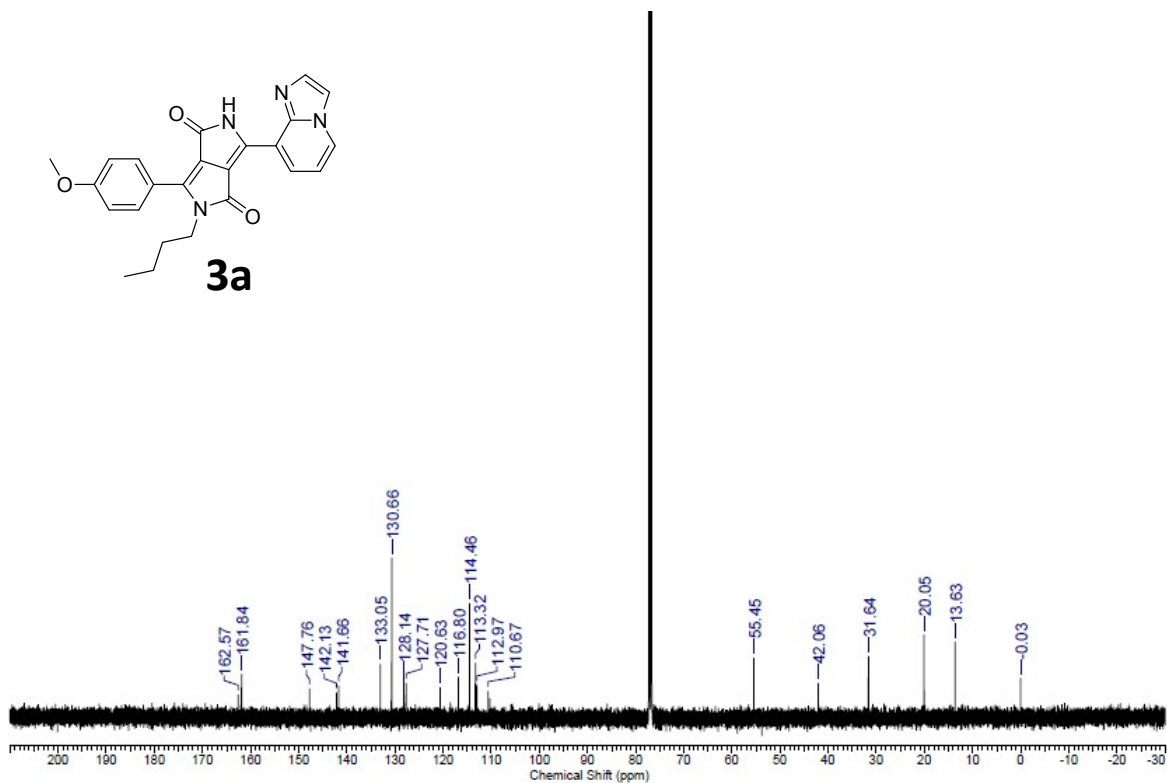
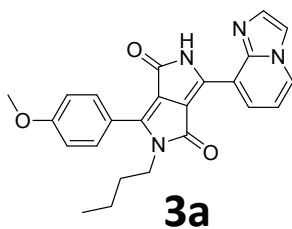
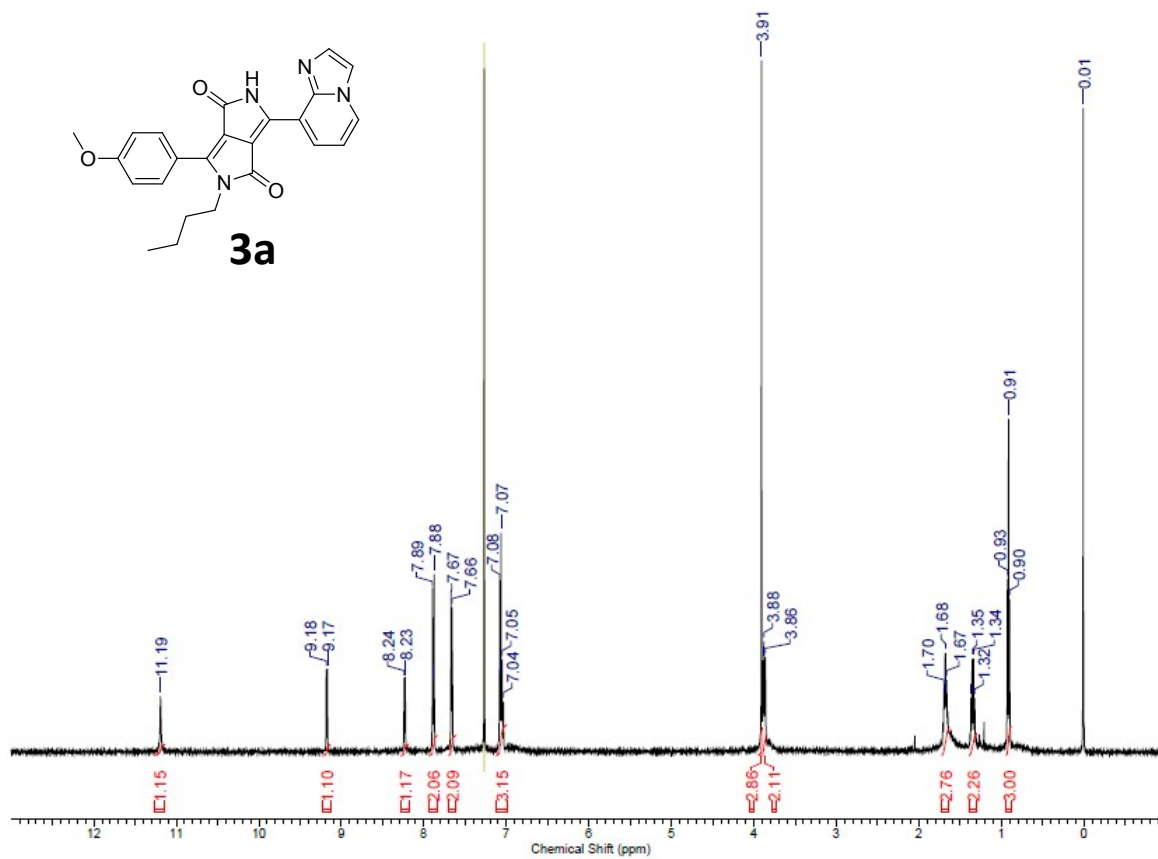
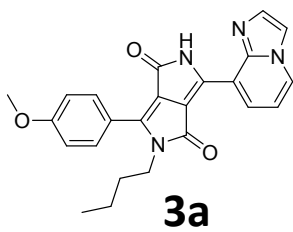
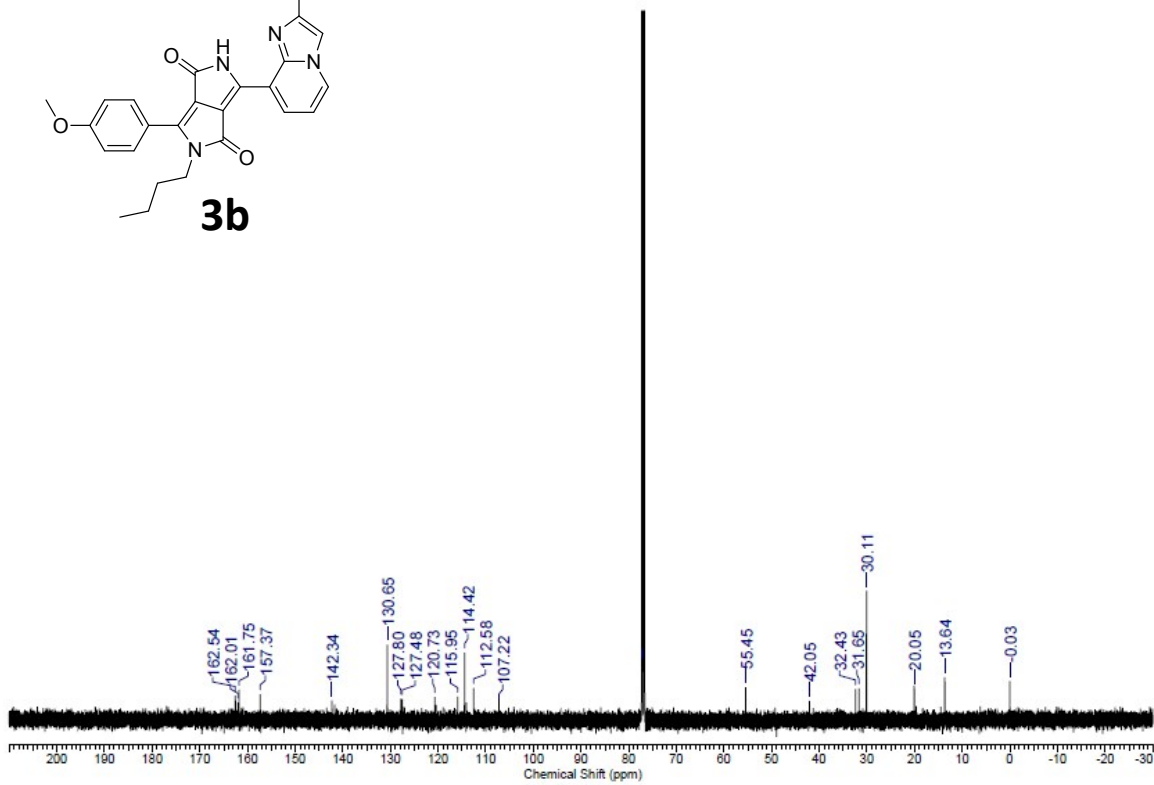
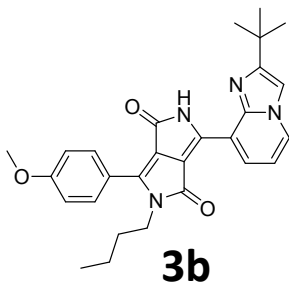
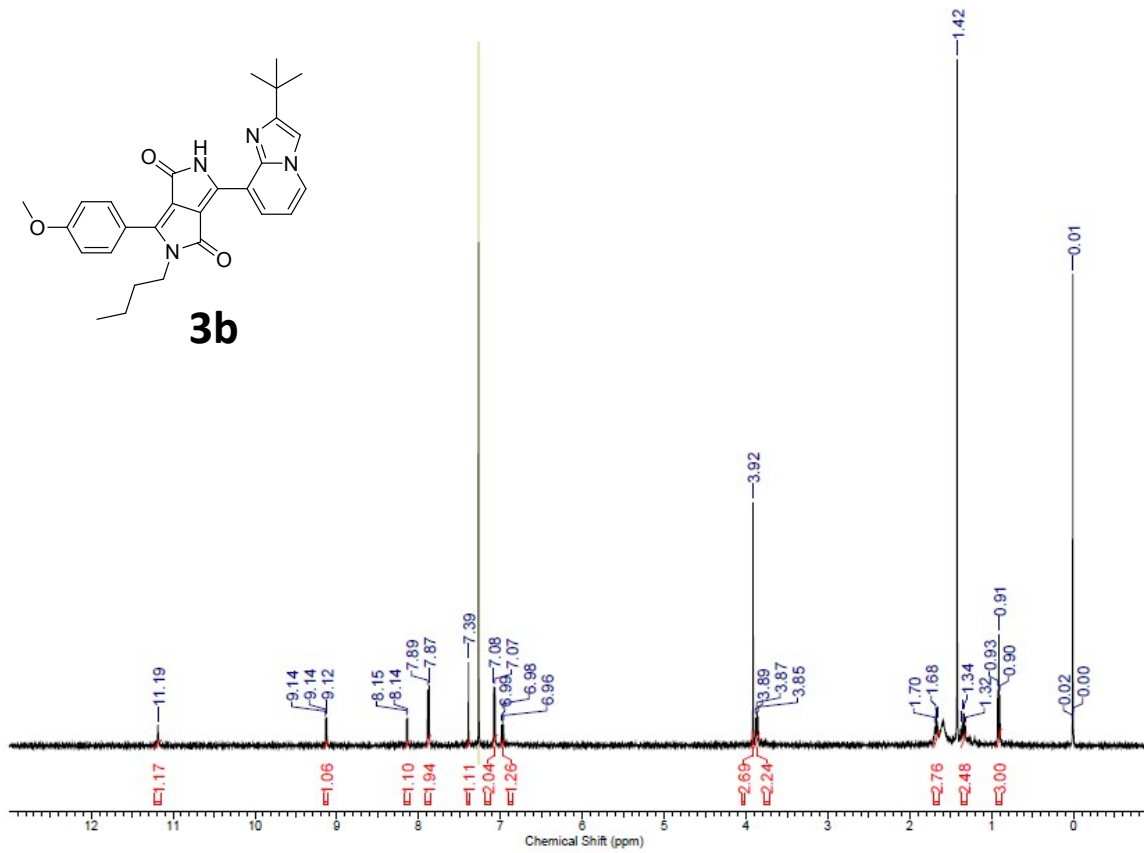
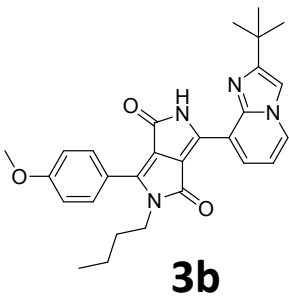
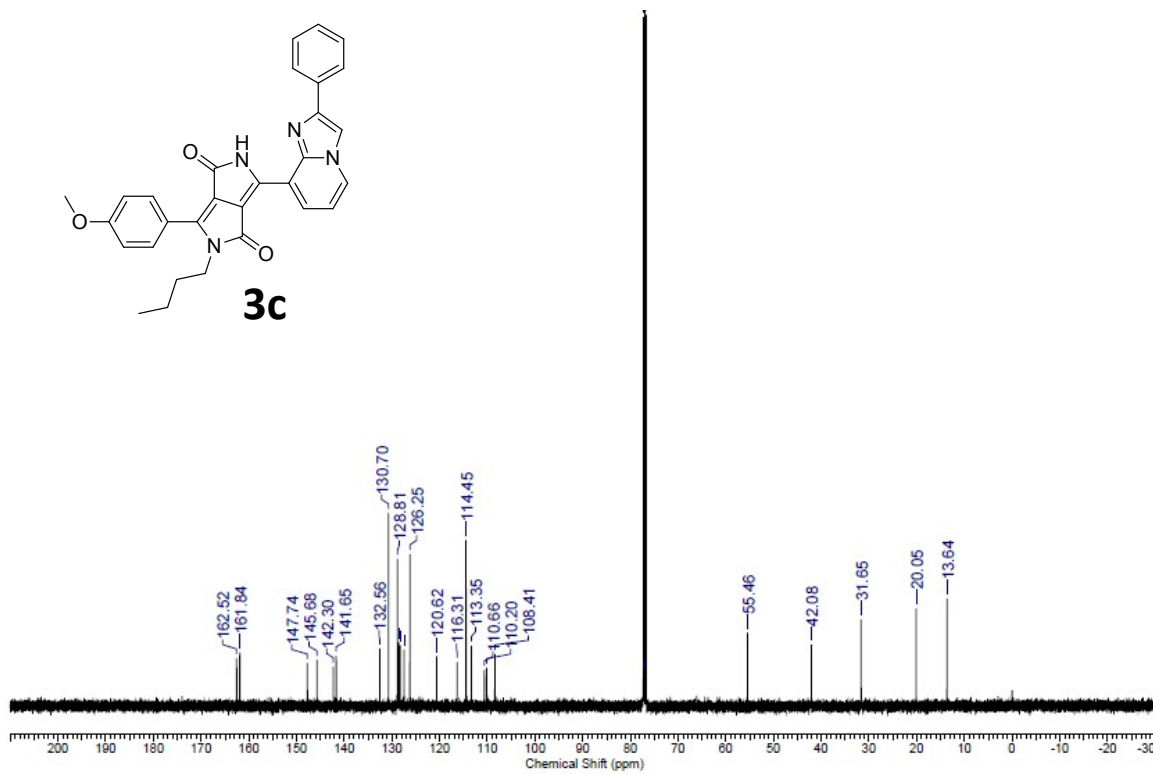
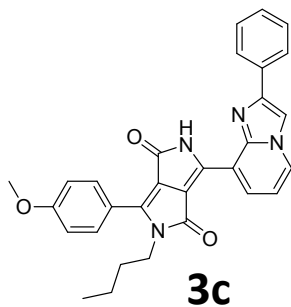
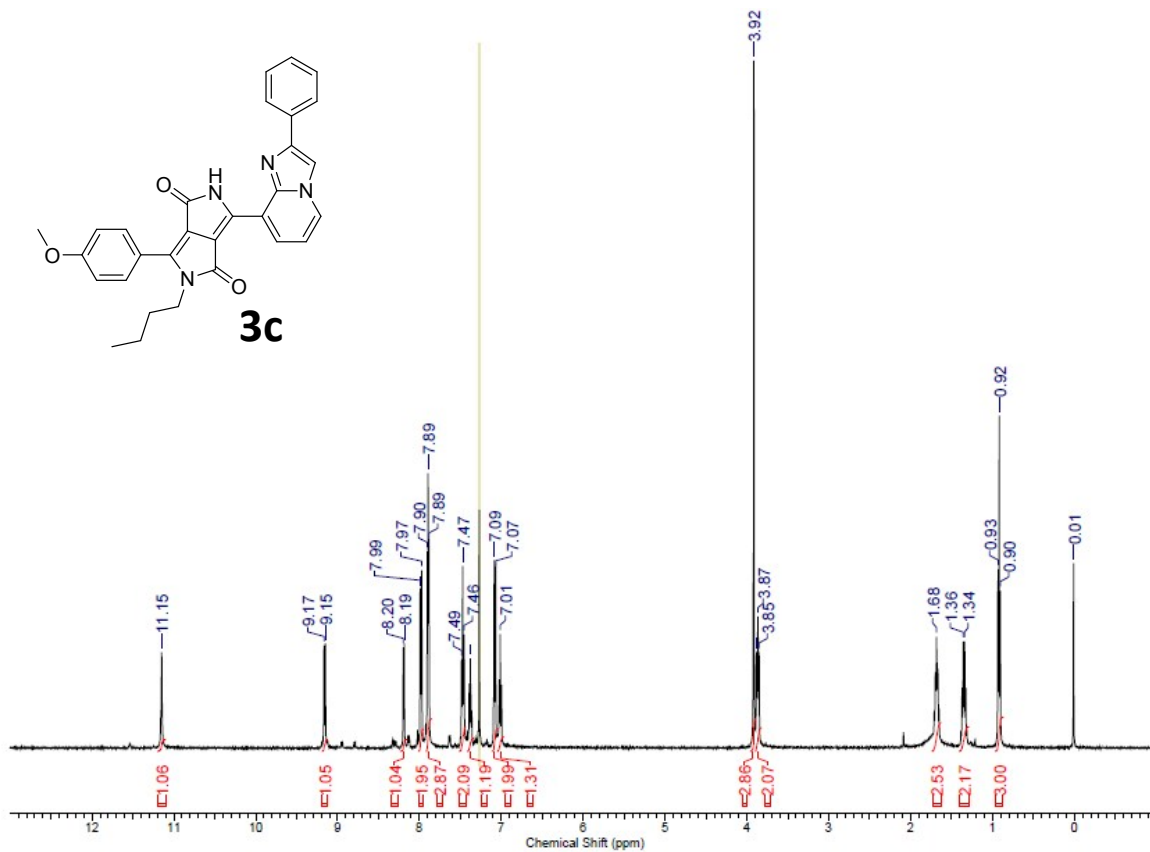
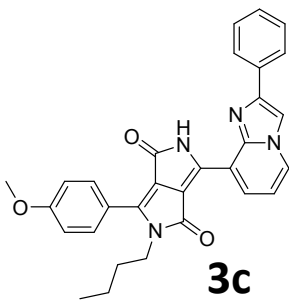


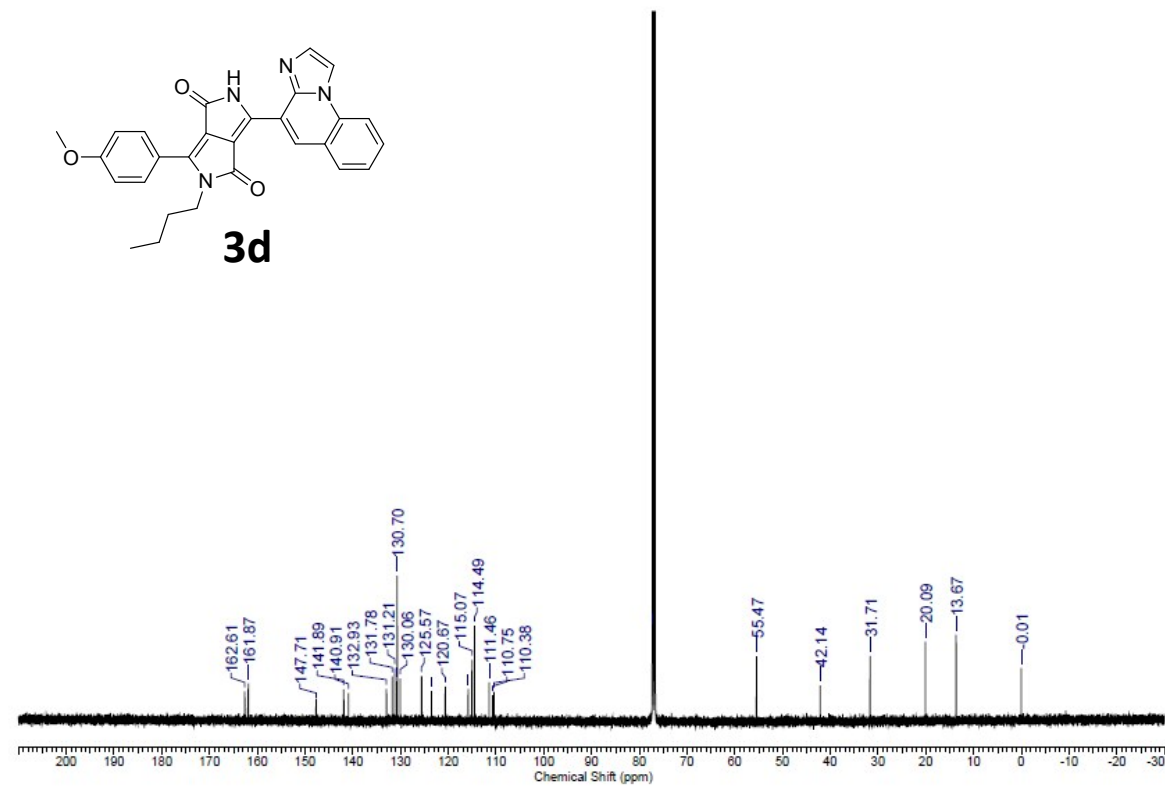
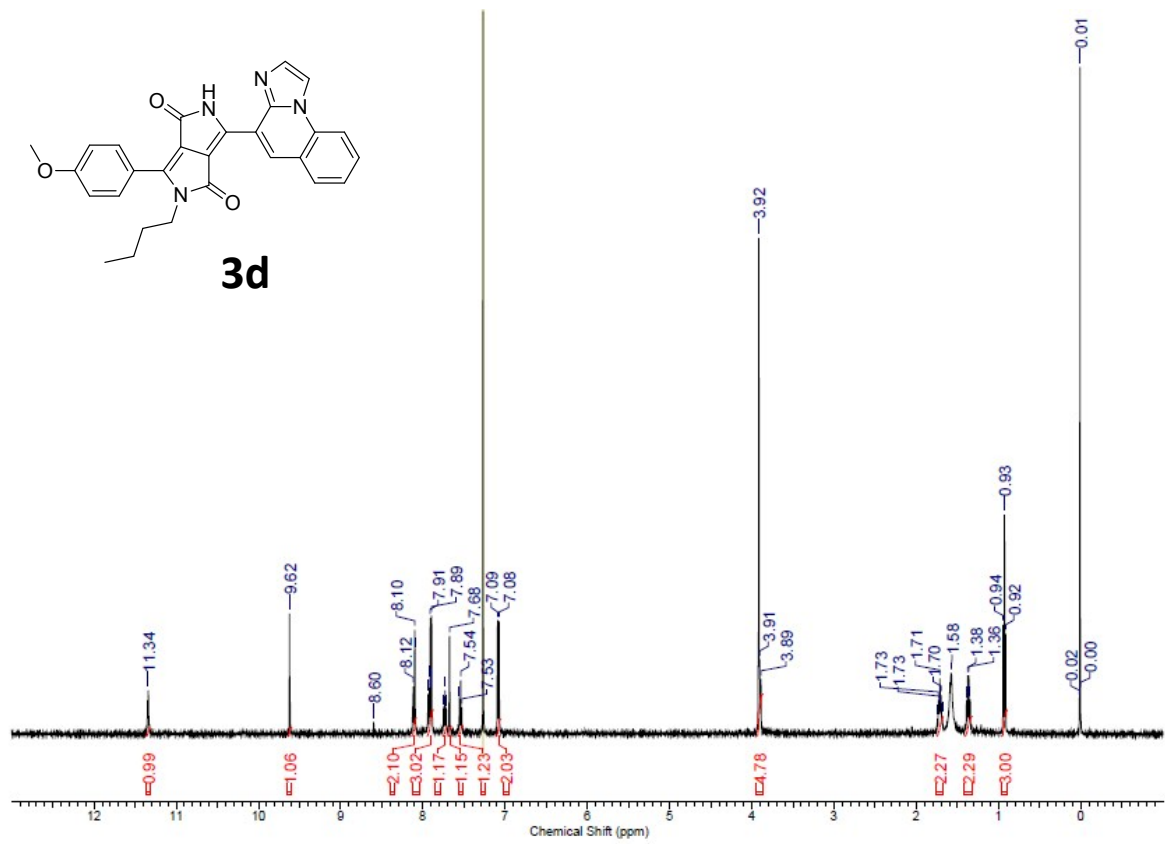
Figure 36. Photostability of free base DPPs **3a-3e** (dashed lines), DPP-BF₂ hybrids **4a-4e** (solid lines) and reference standards in MeOH (top) and DMF (bottom).

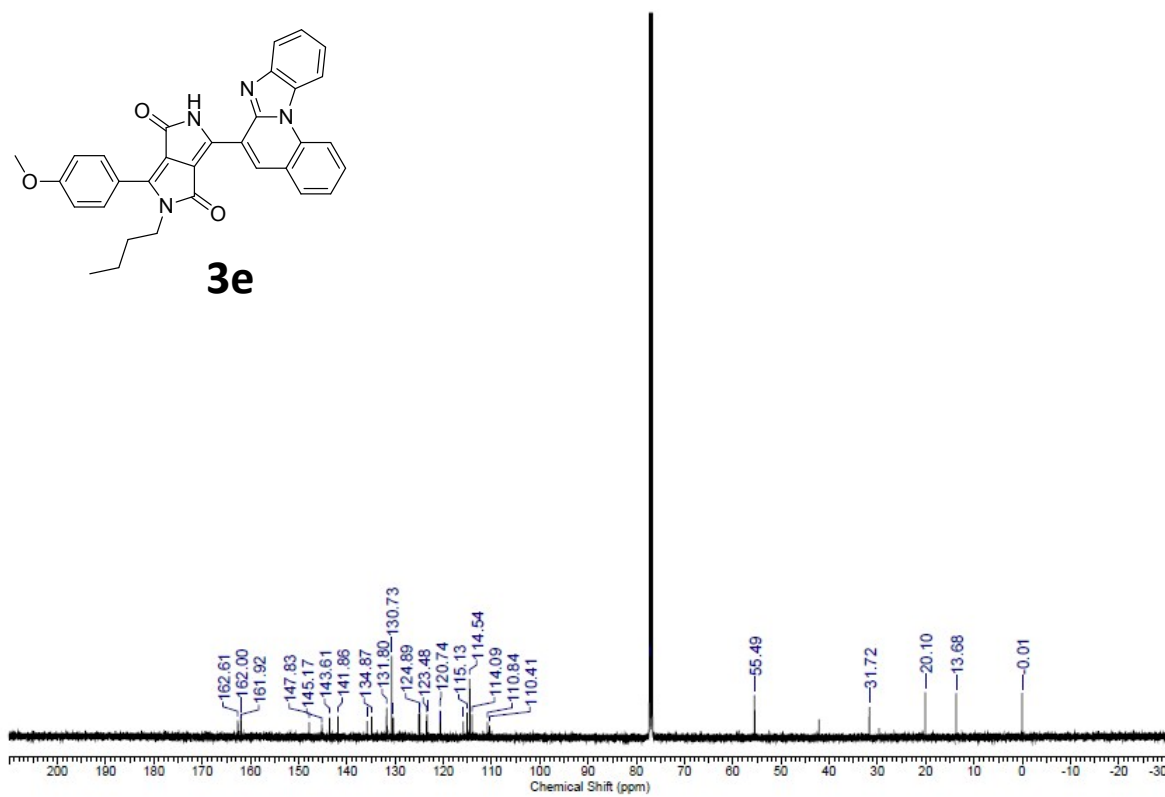
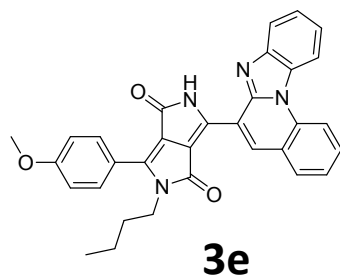
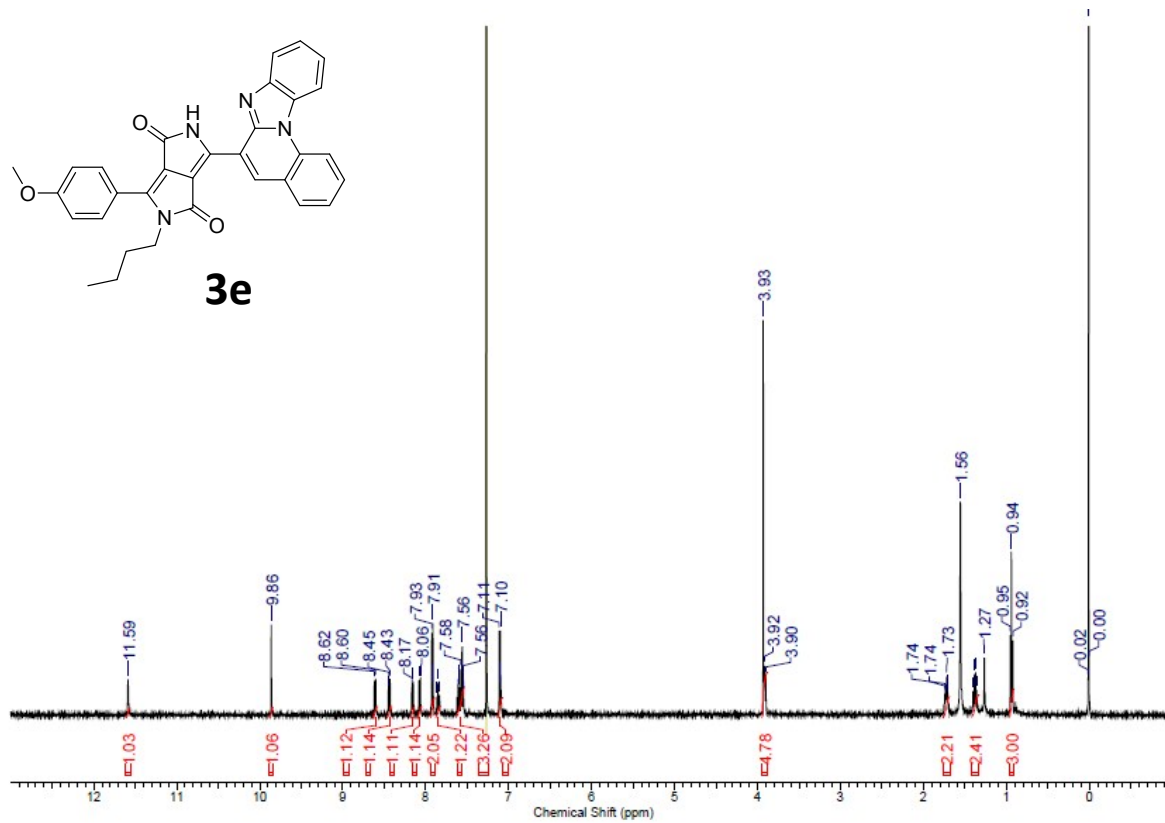
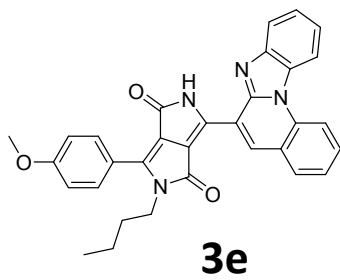


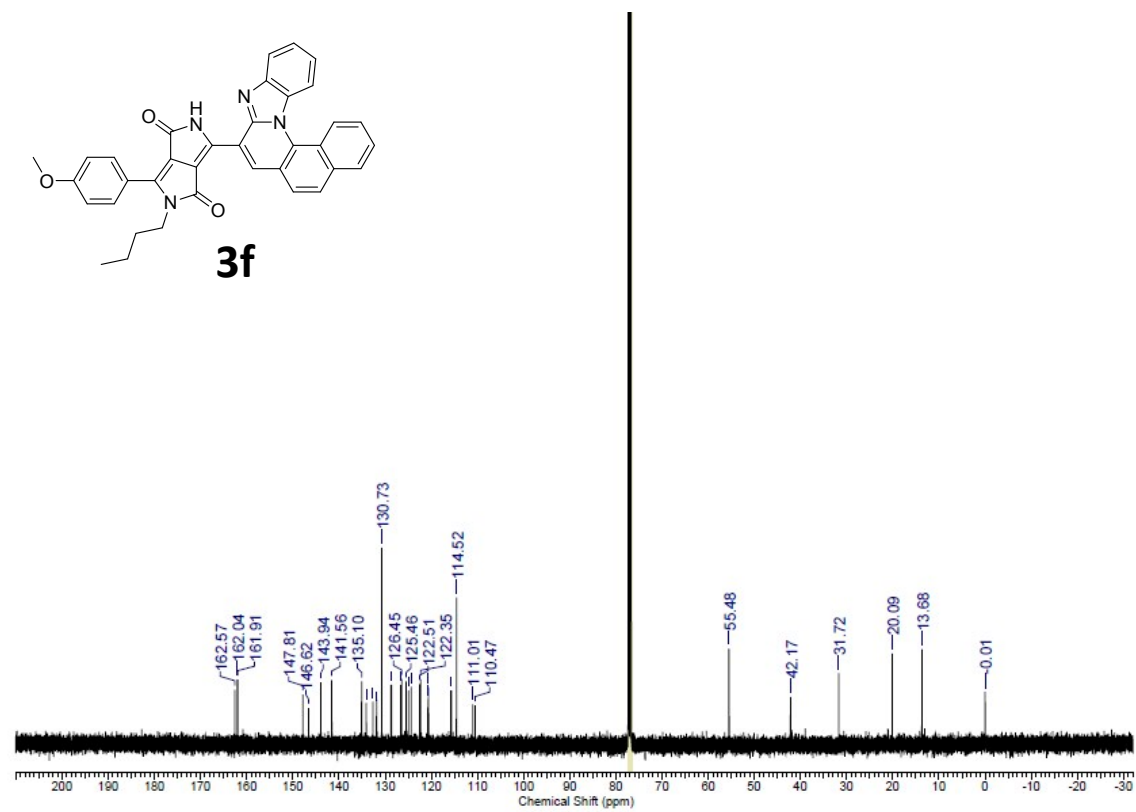
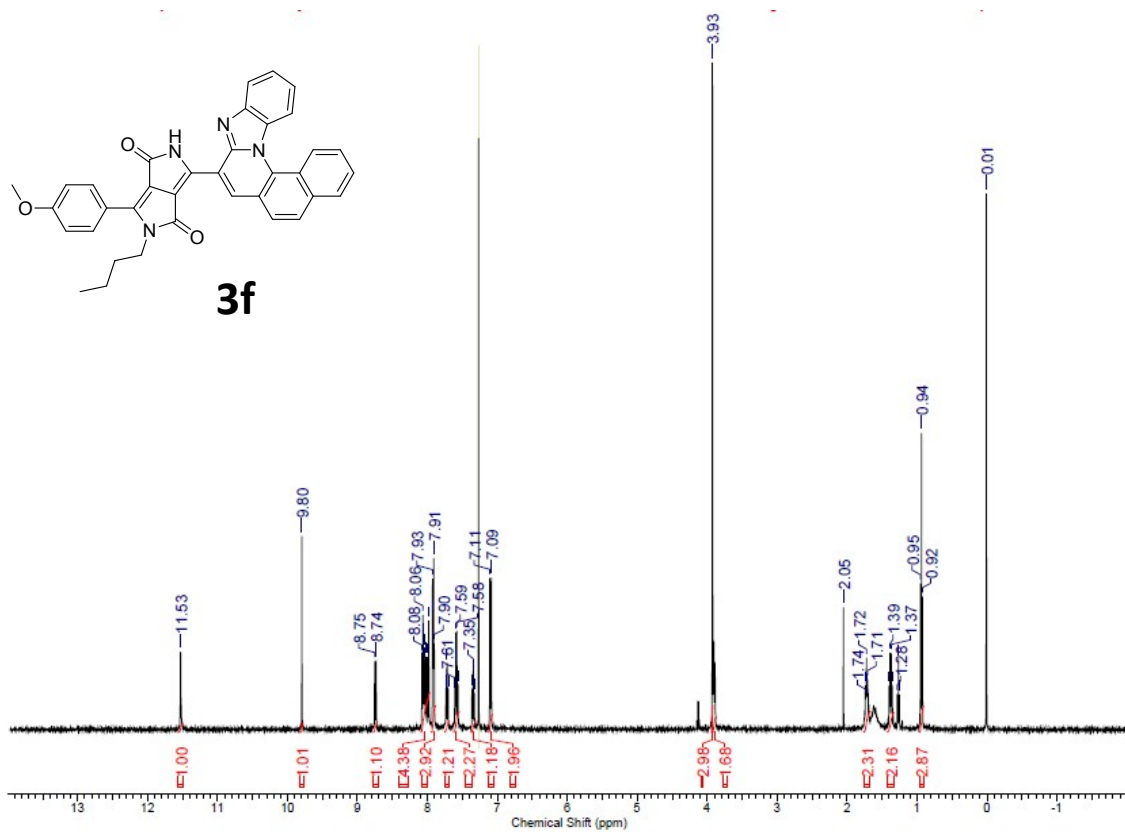


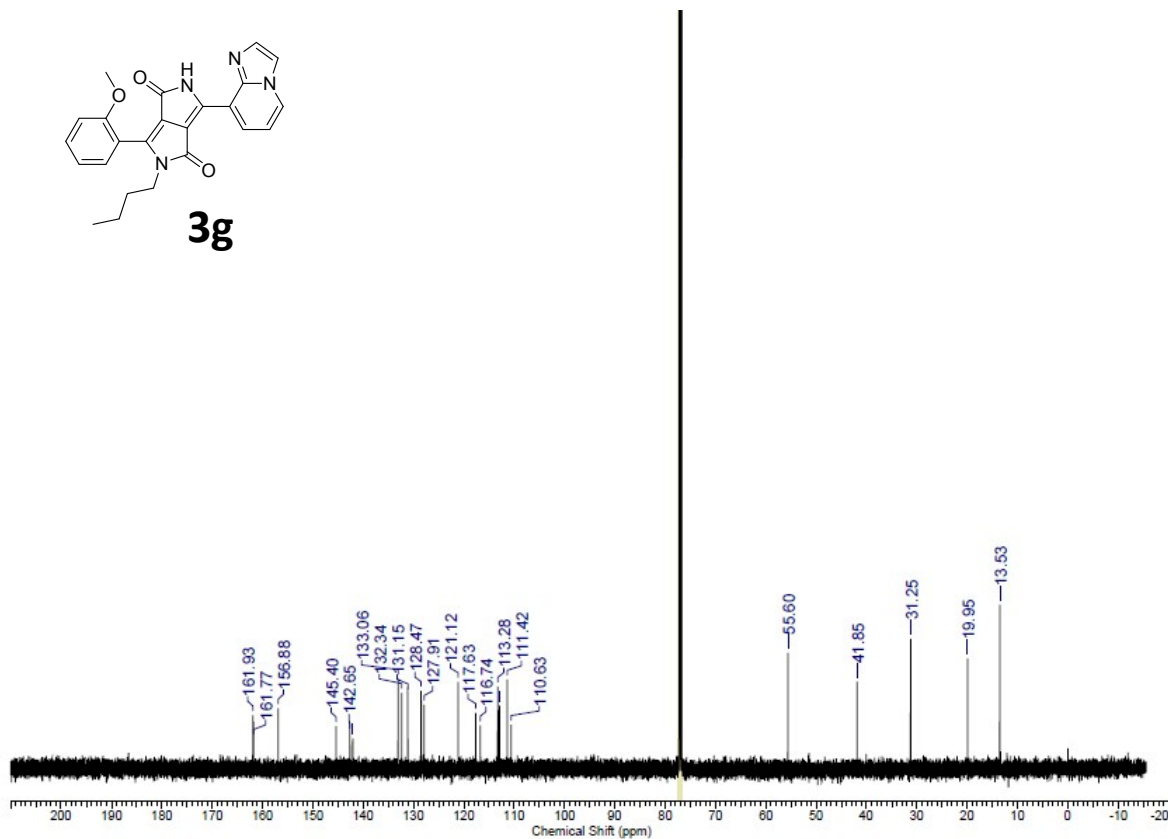
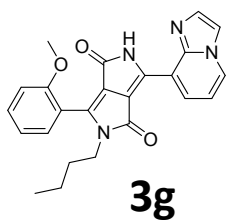
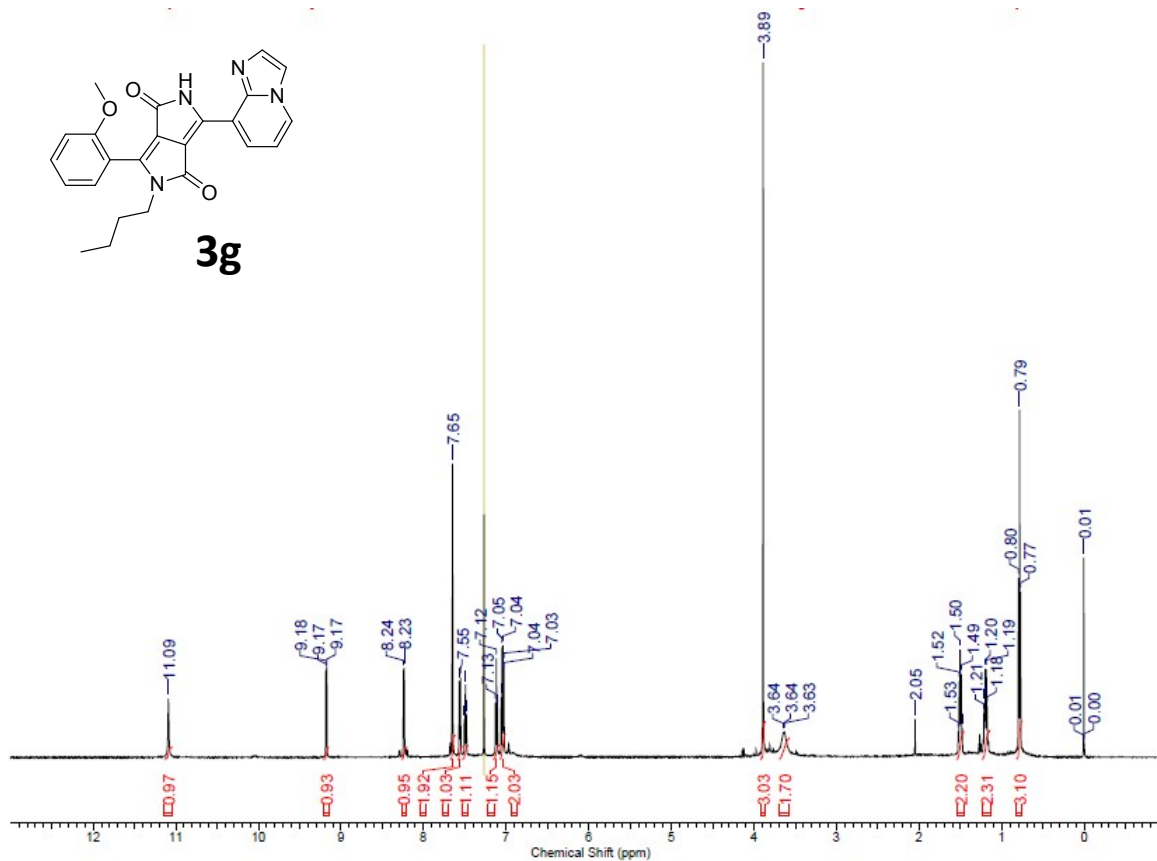
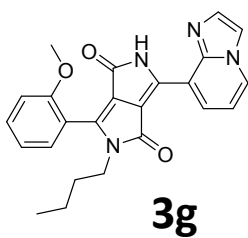


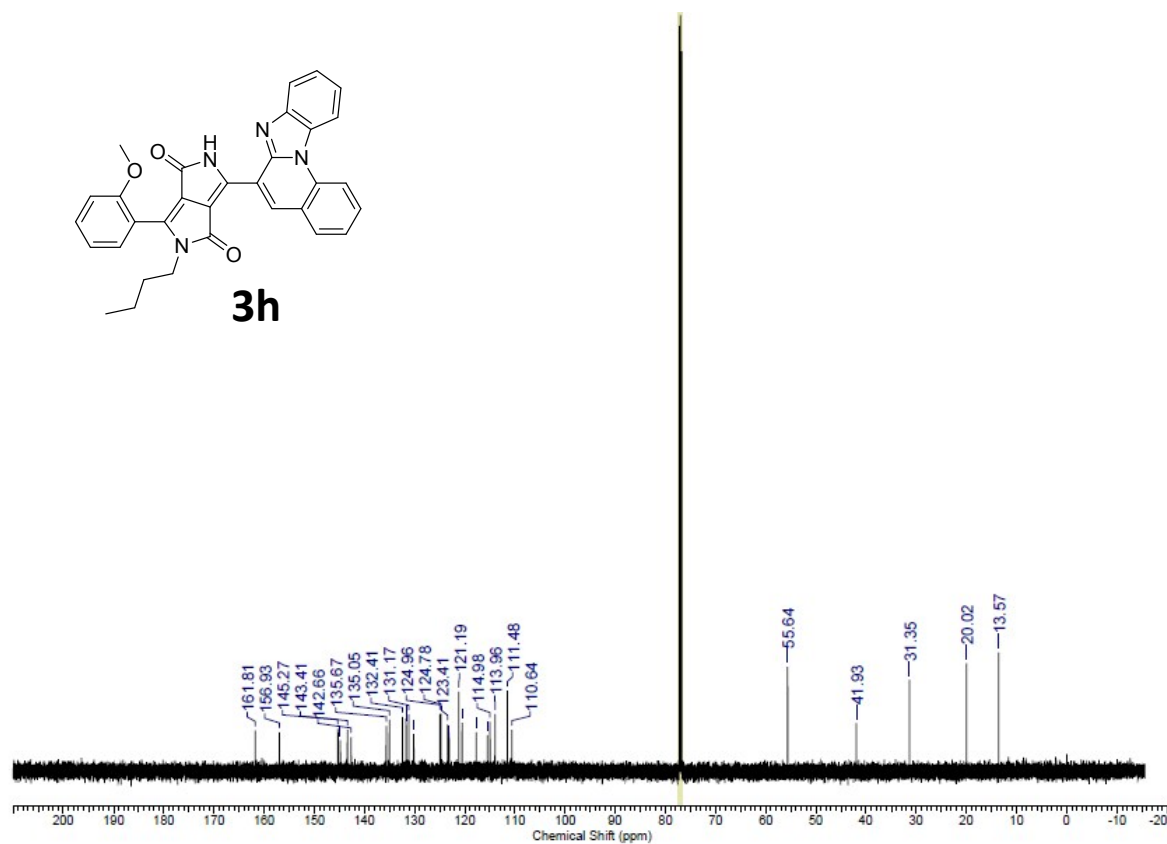
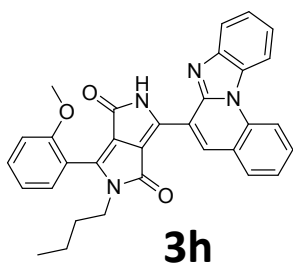
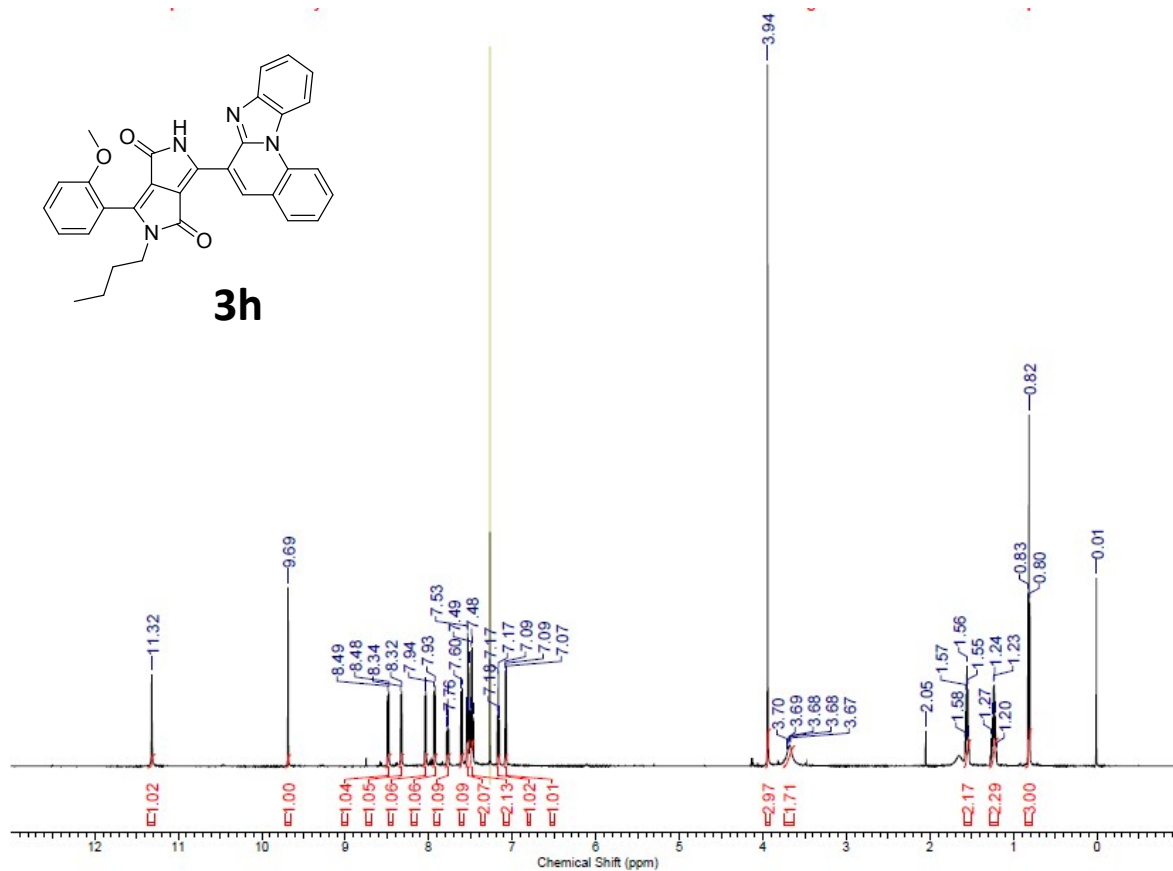
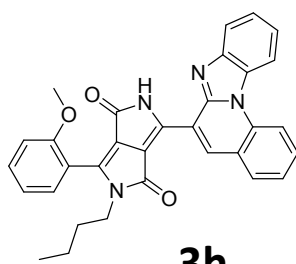


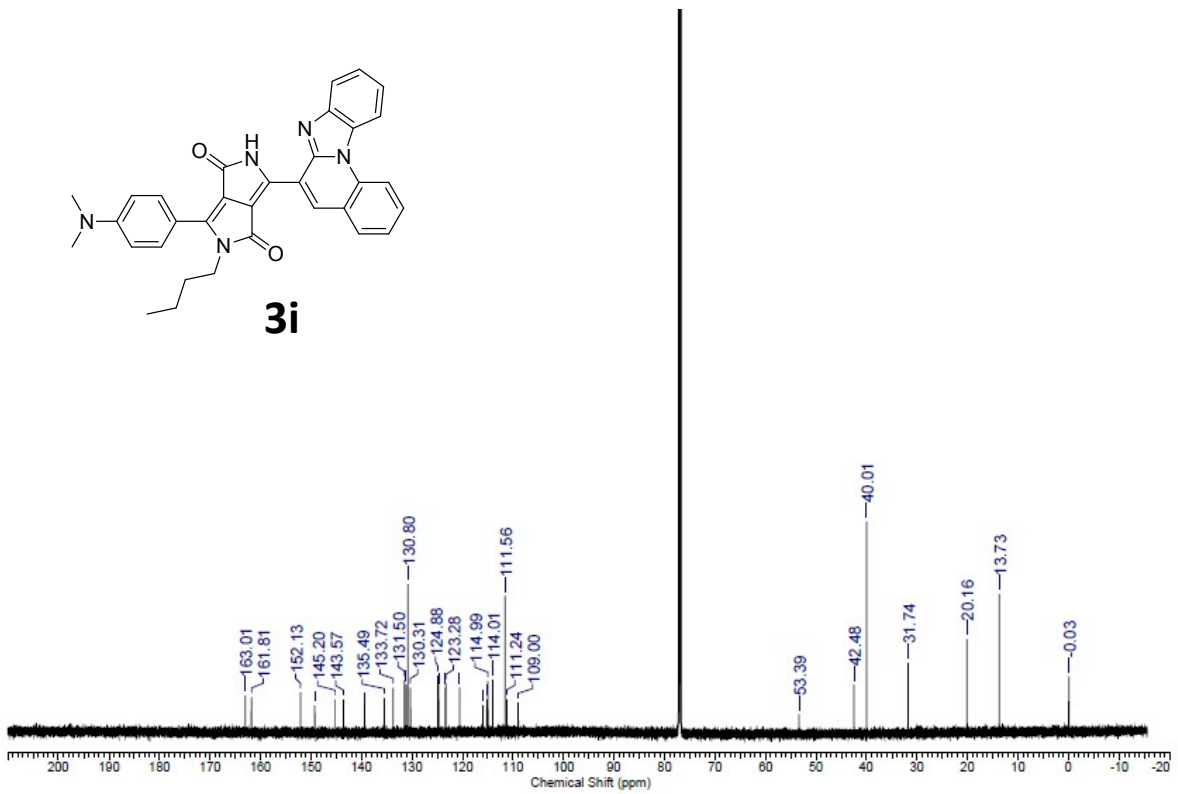
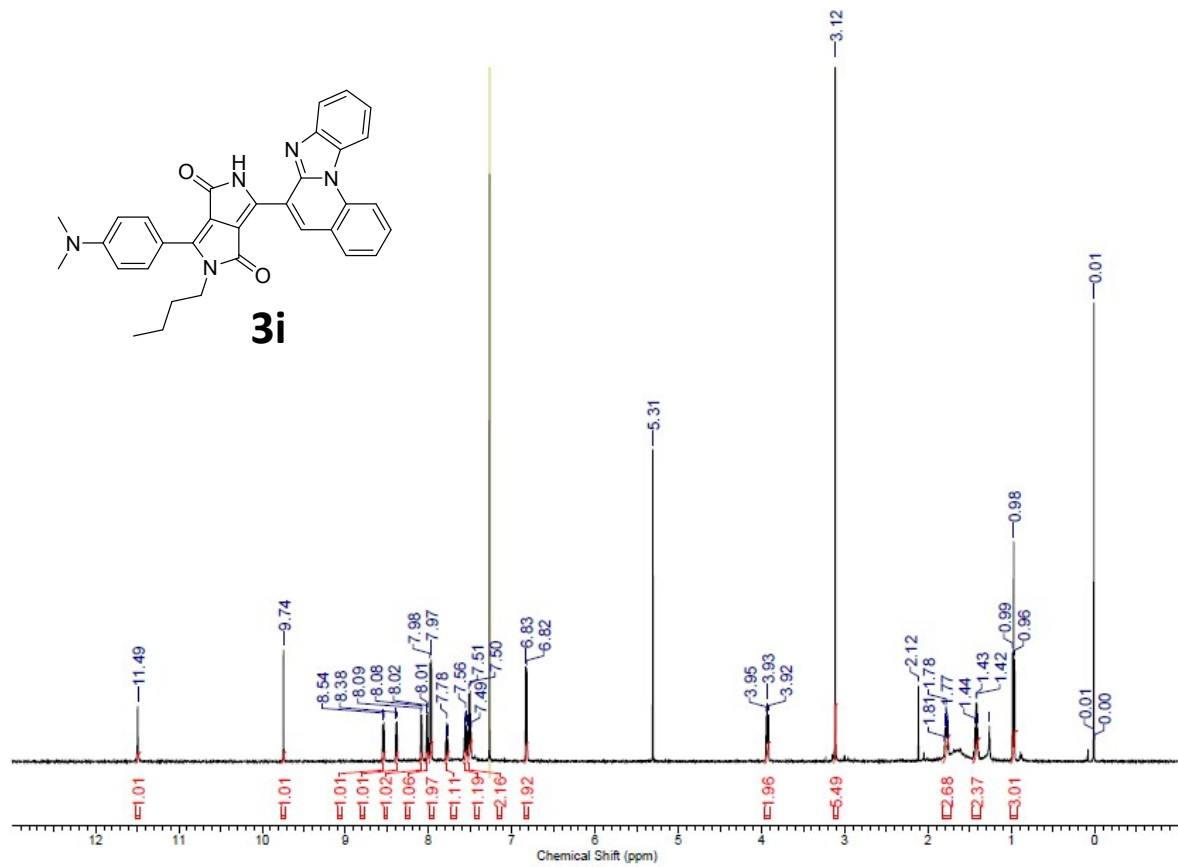


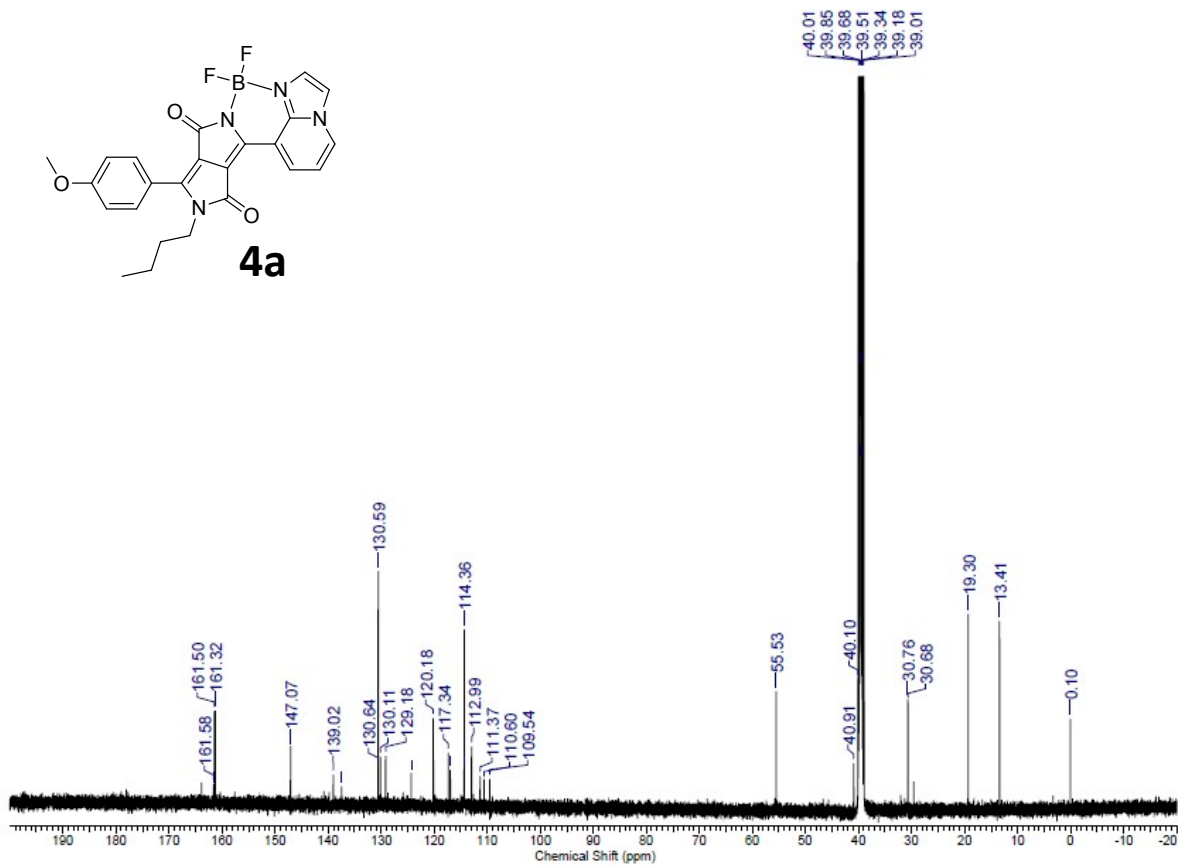
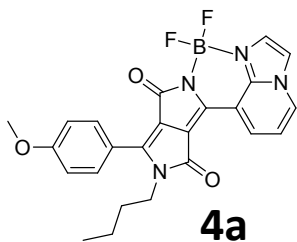
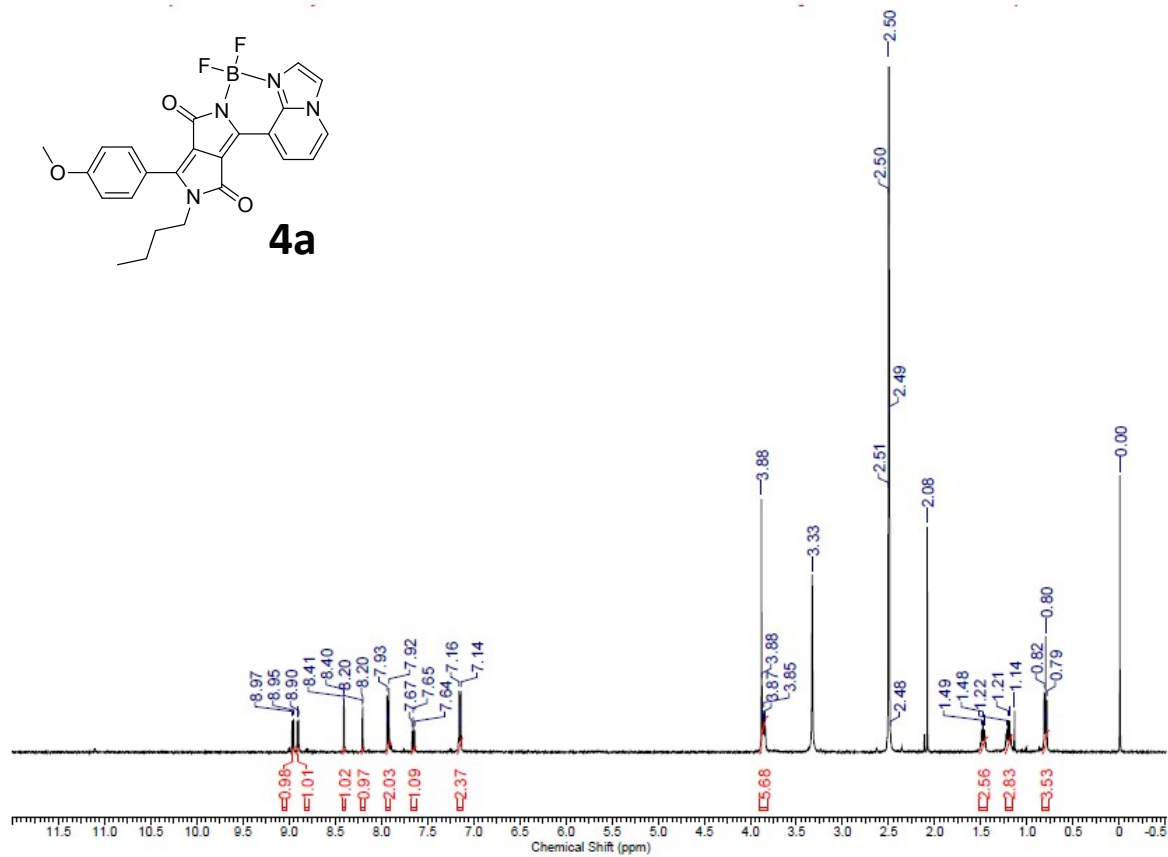
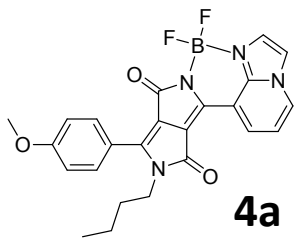


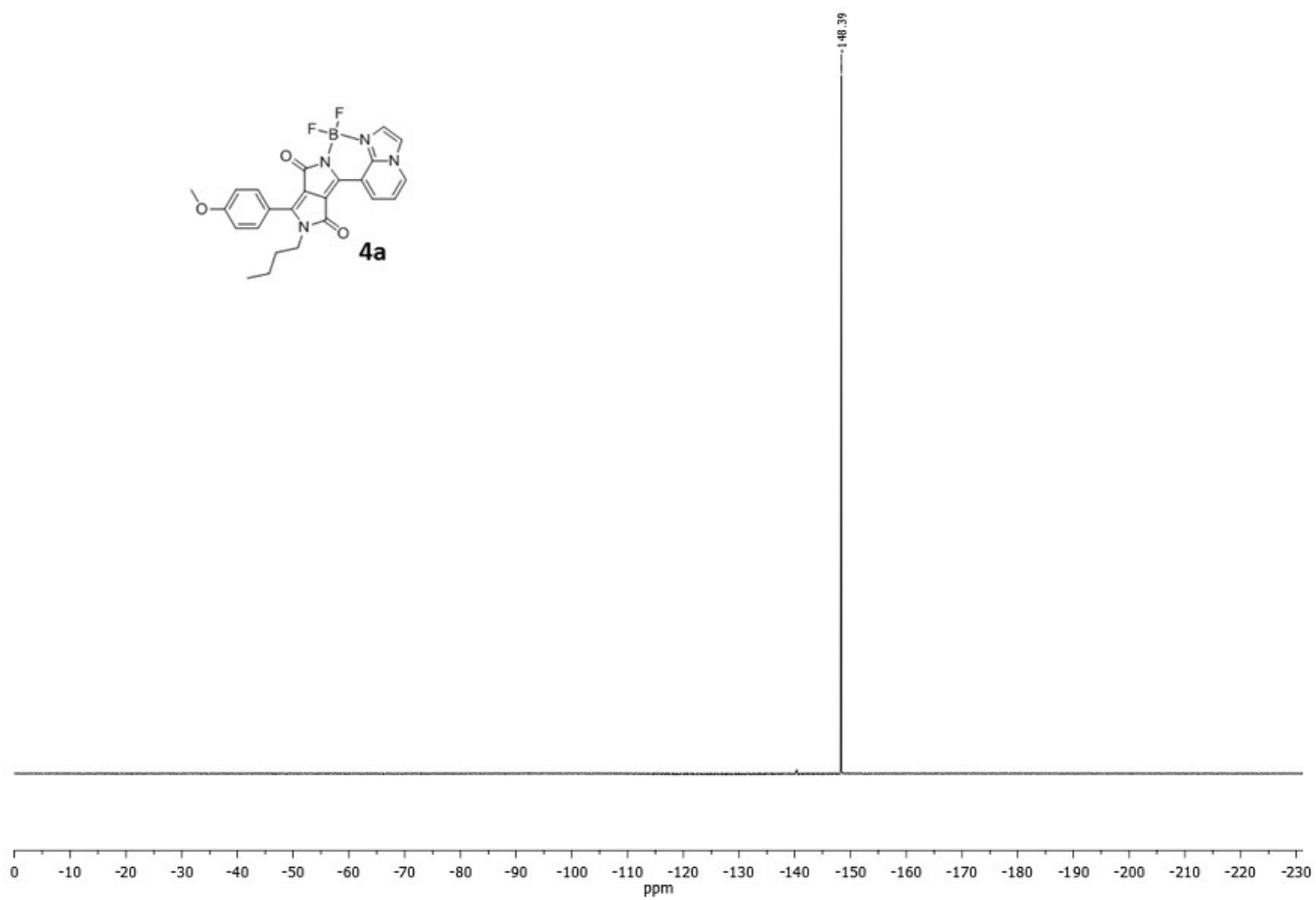
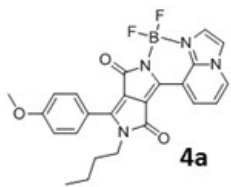


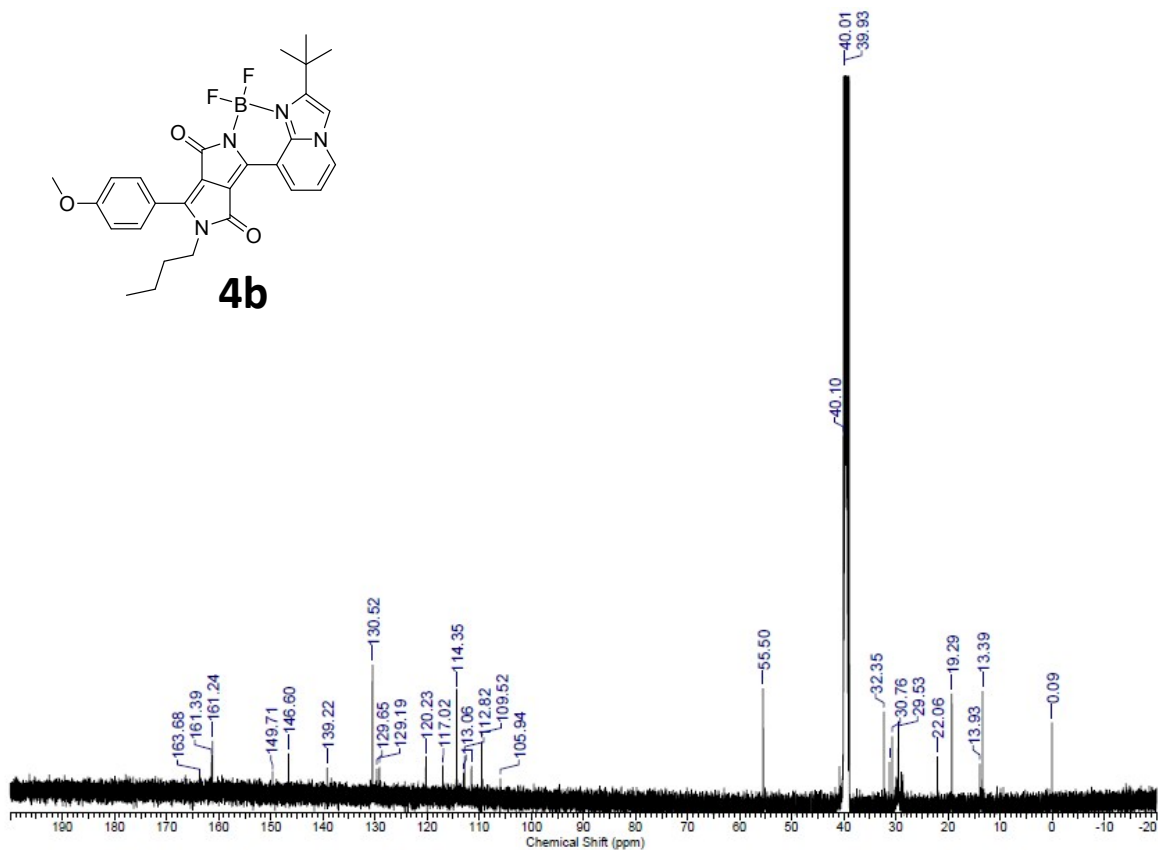
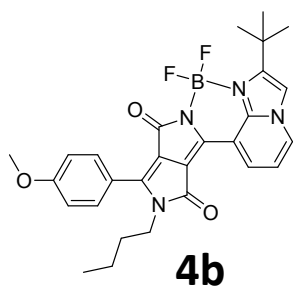
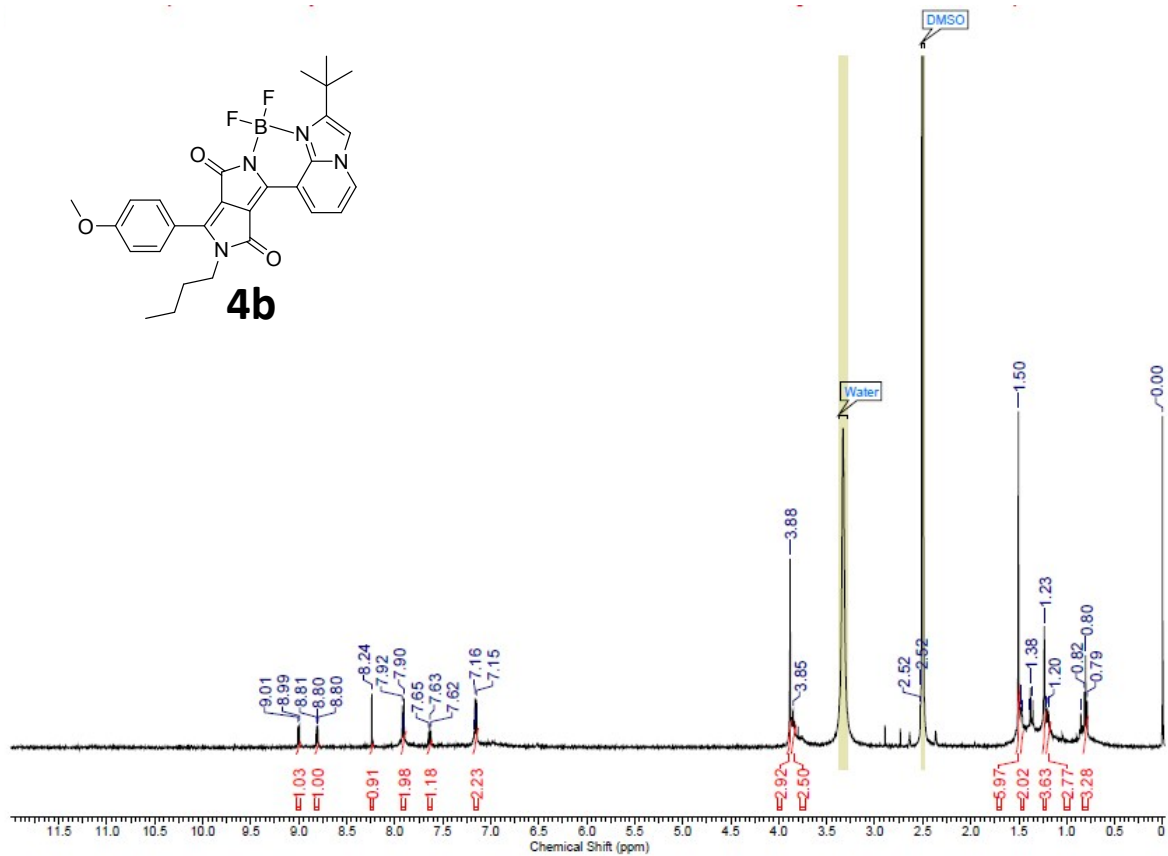
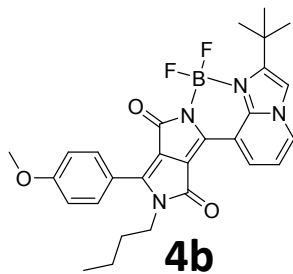


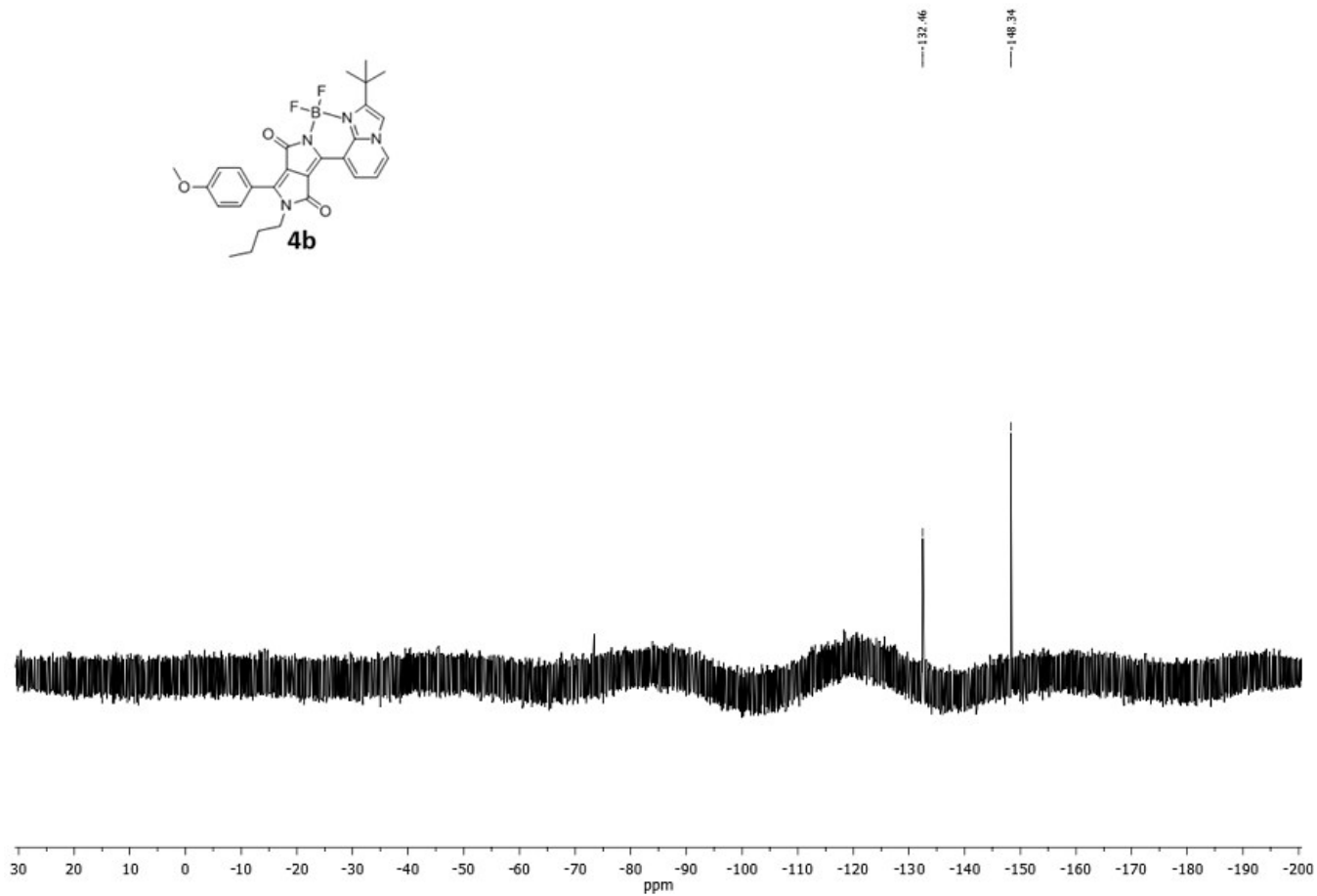
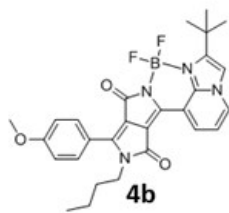


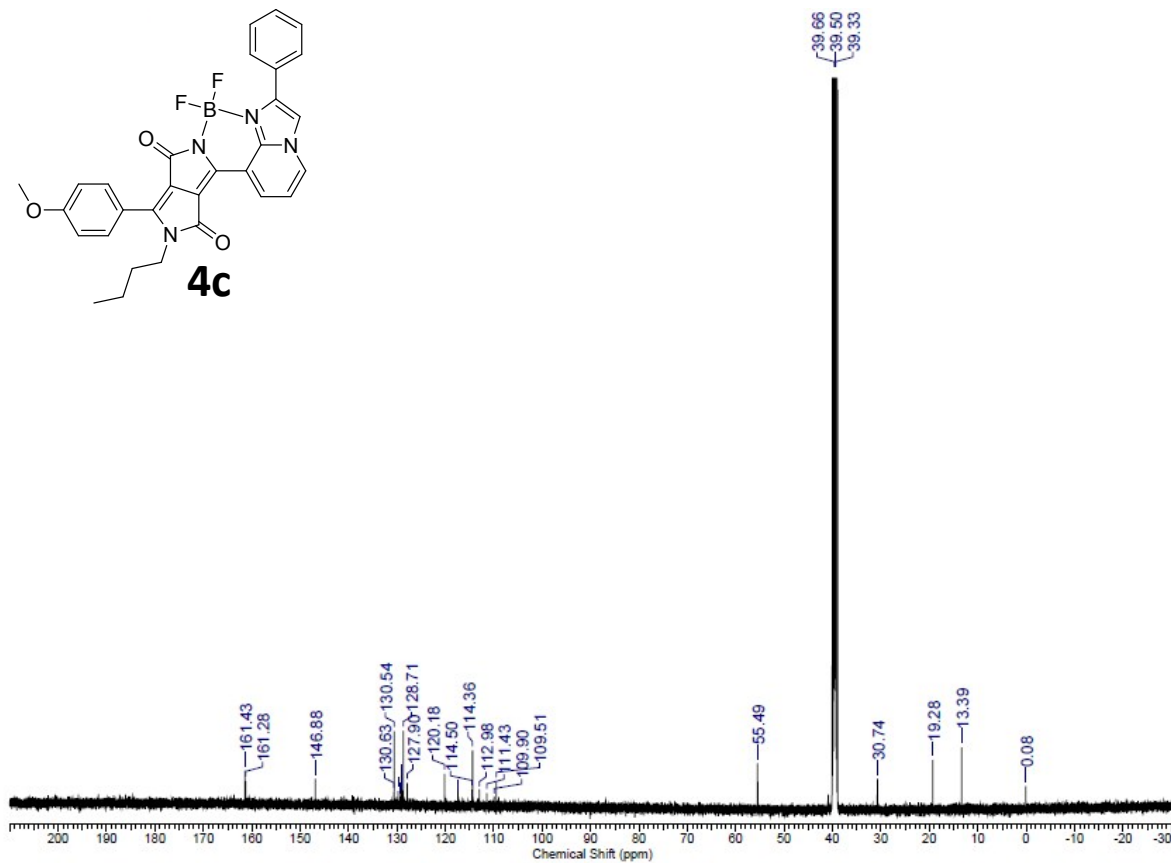
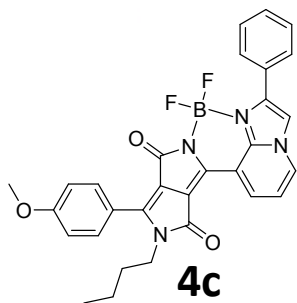
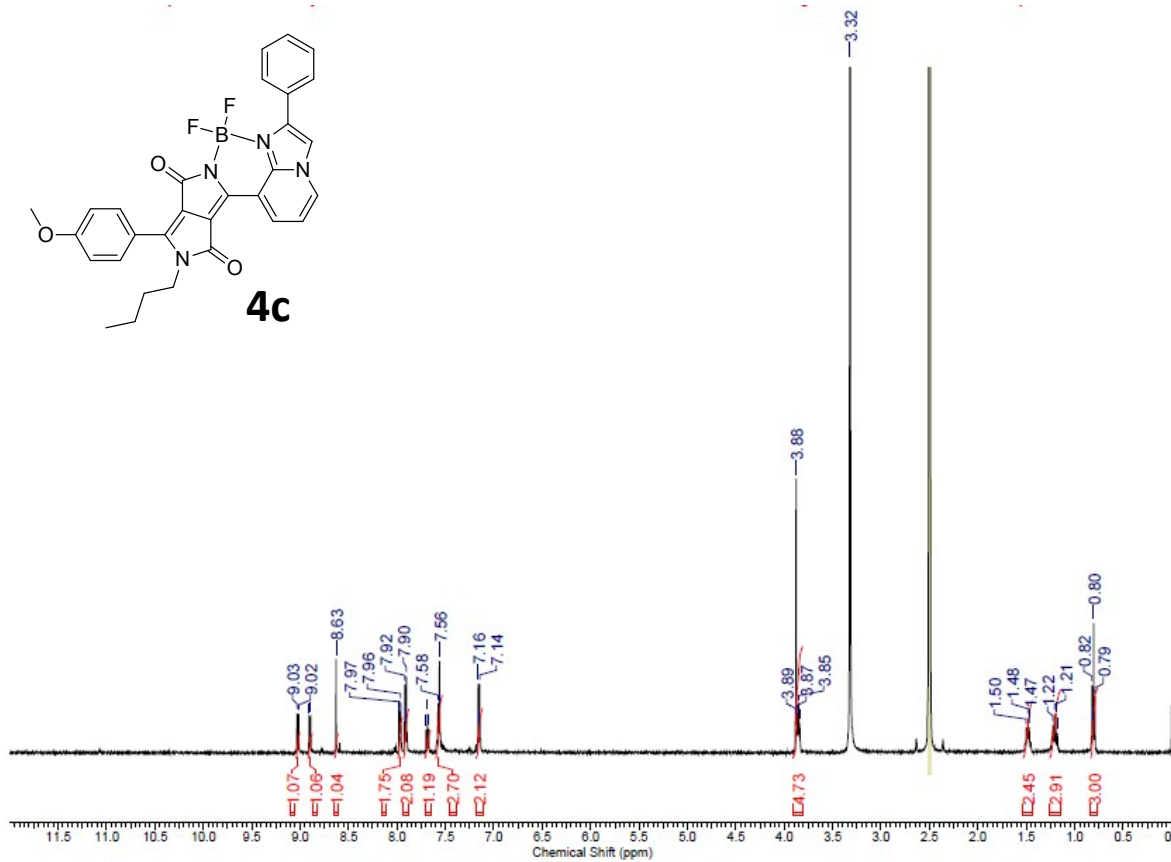
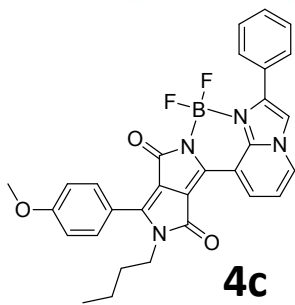


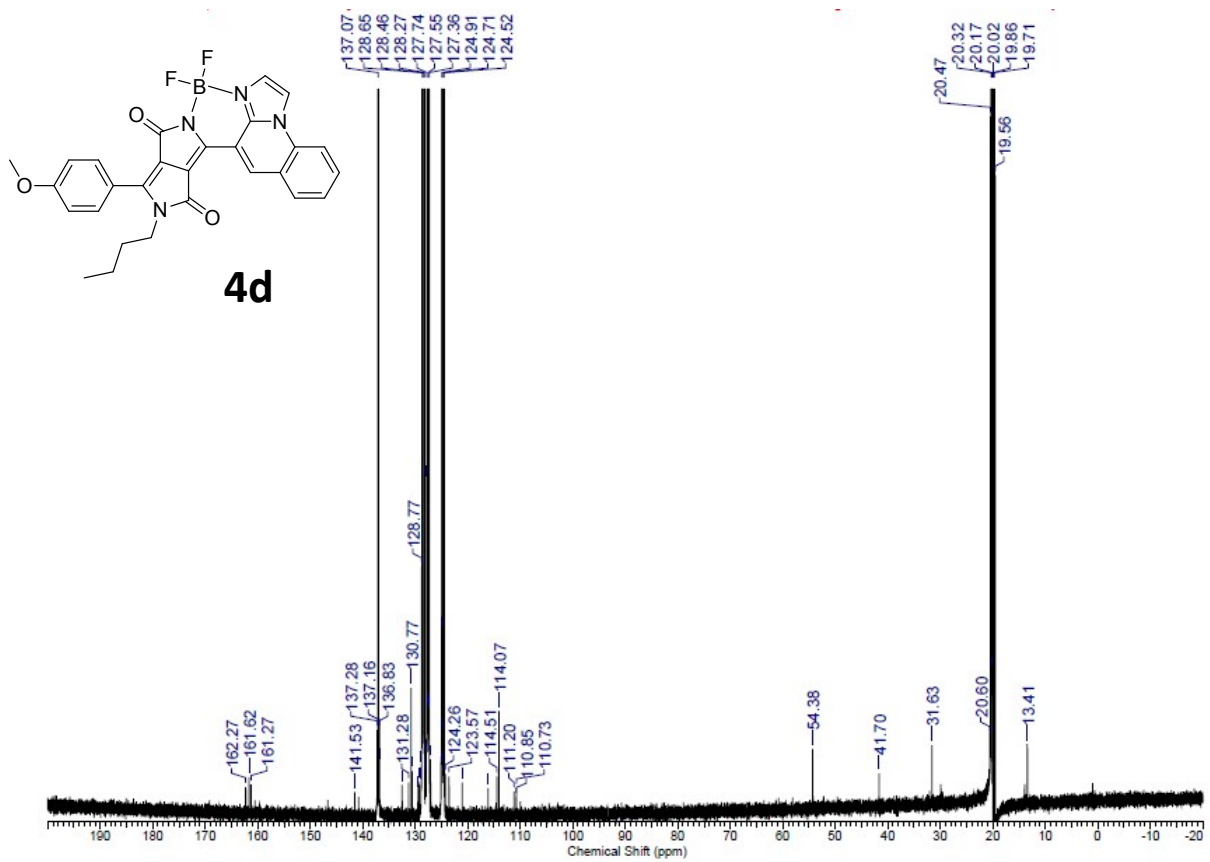
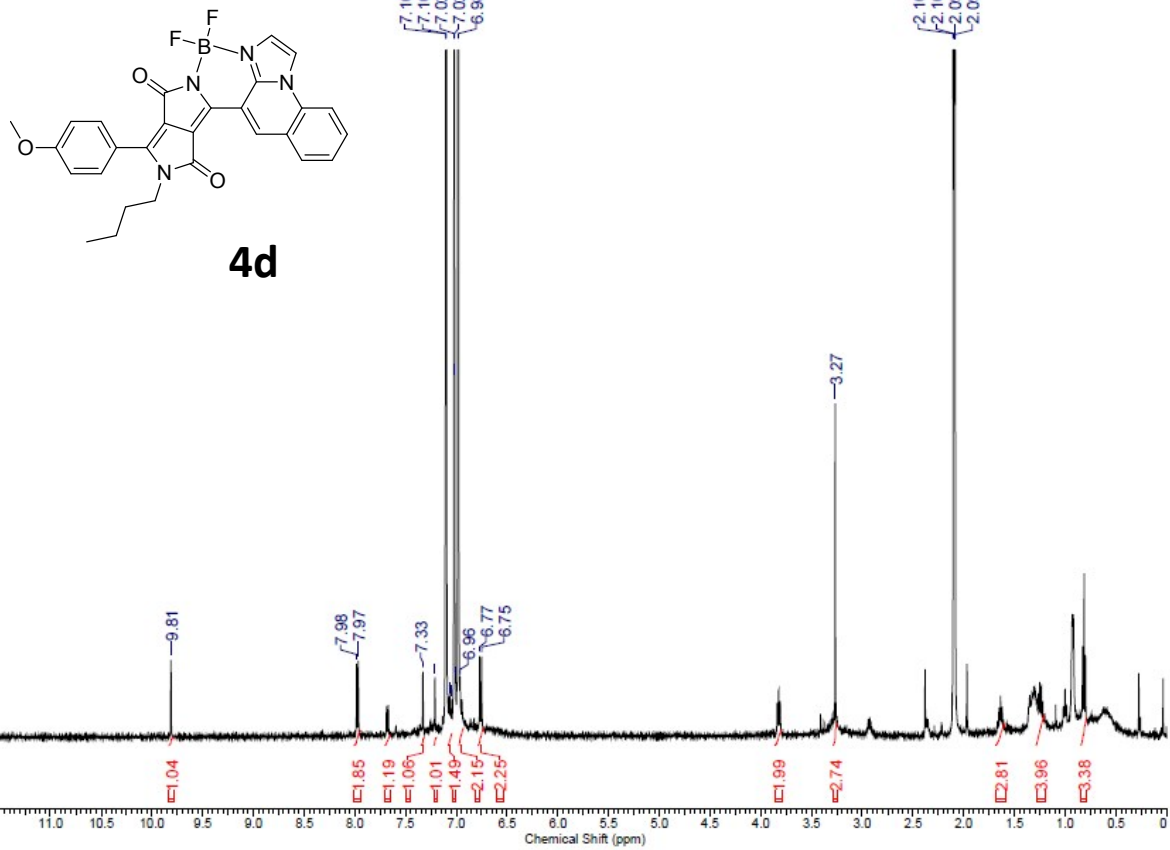


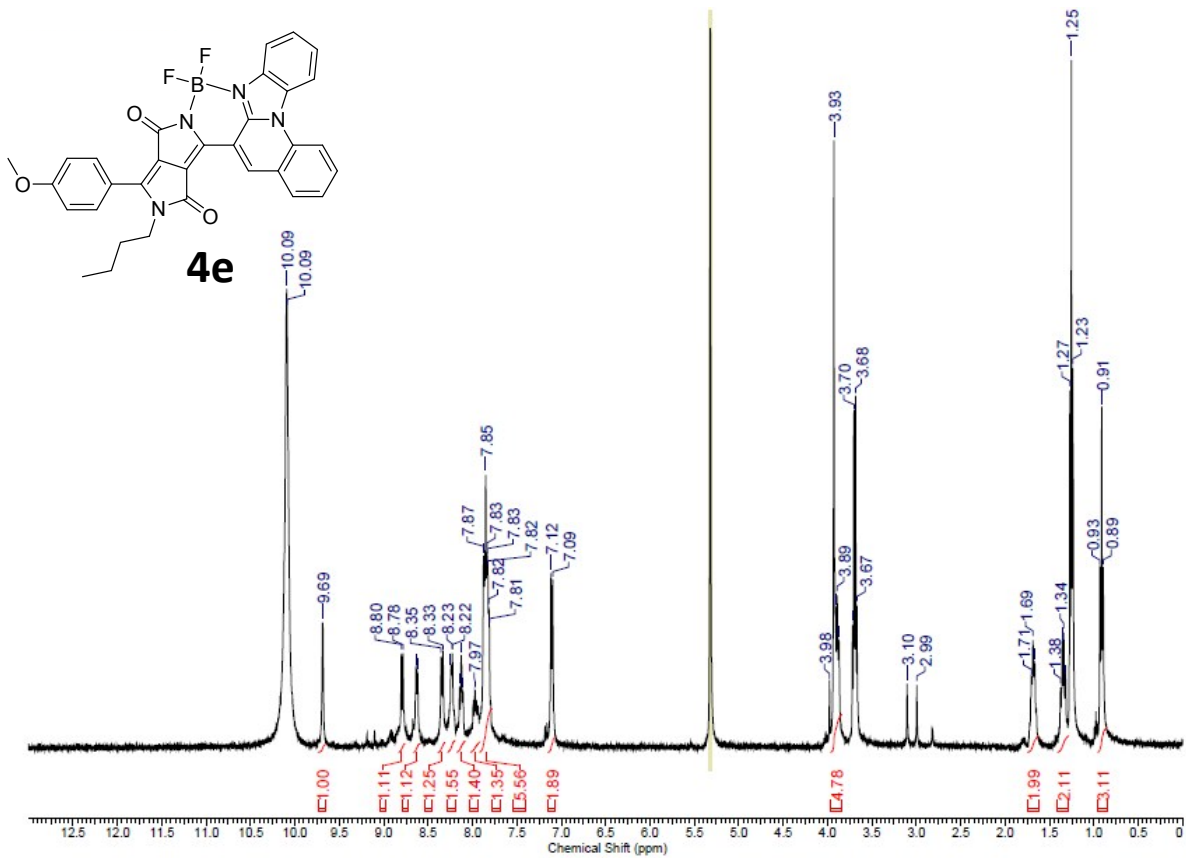
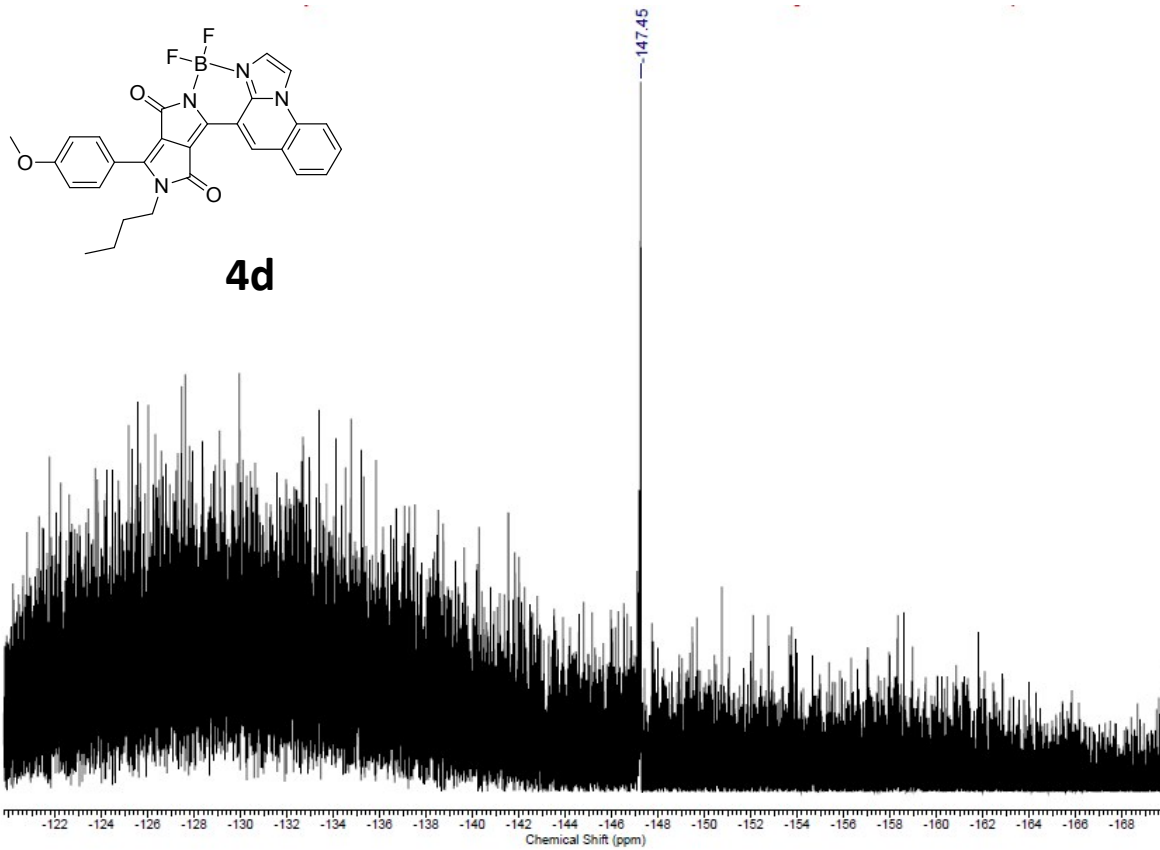


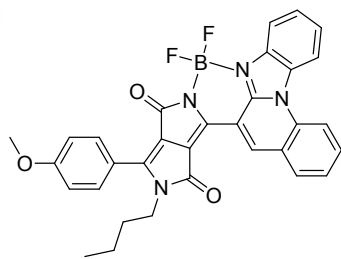




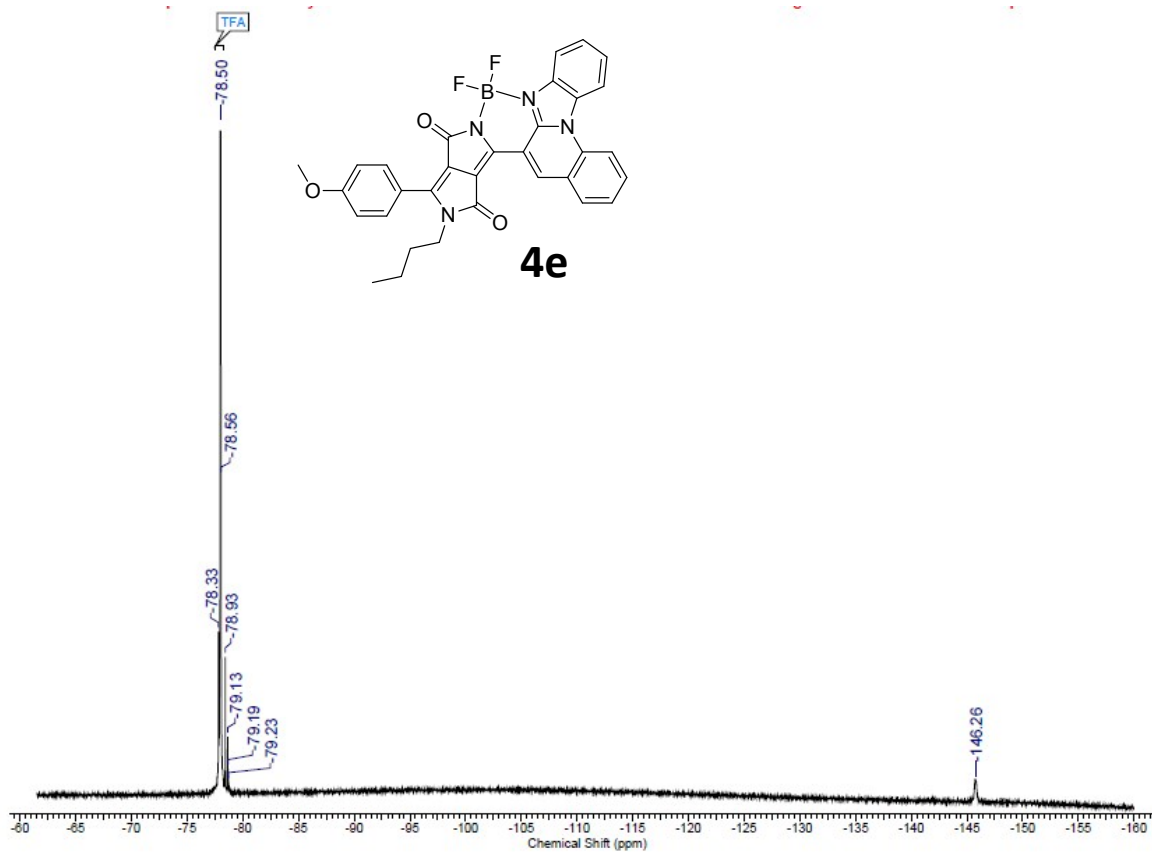
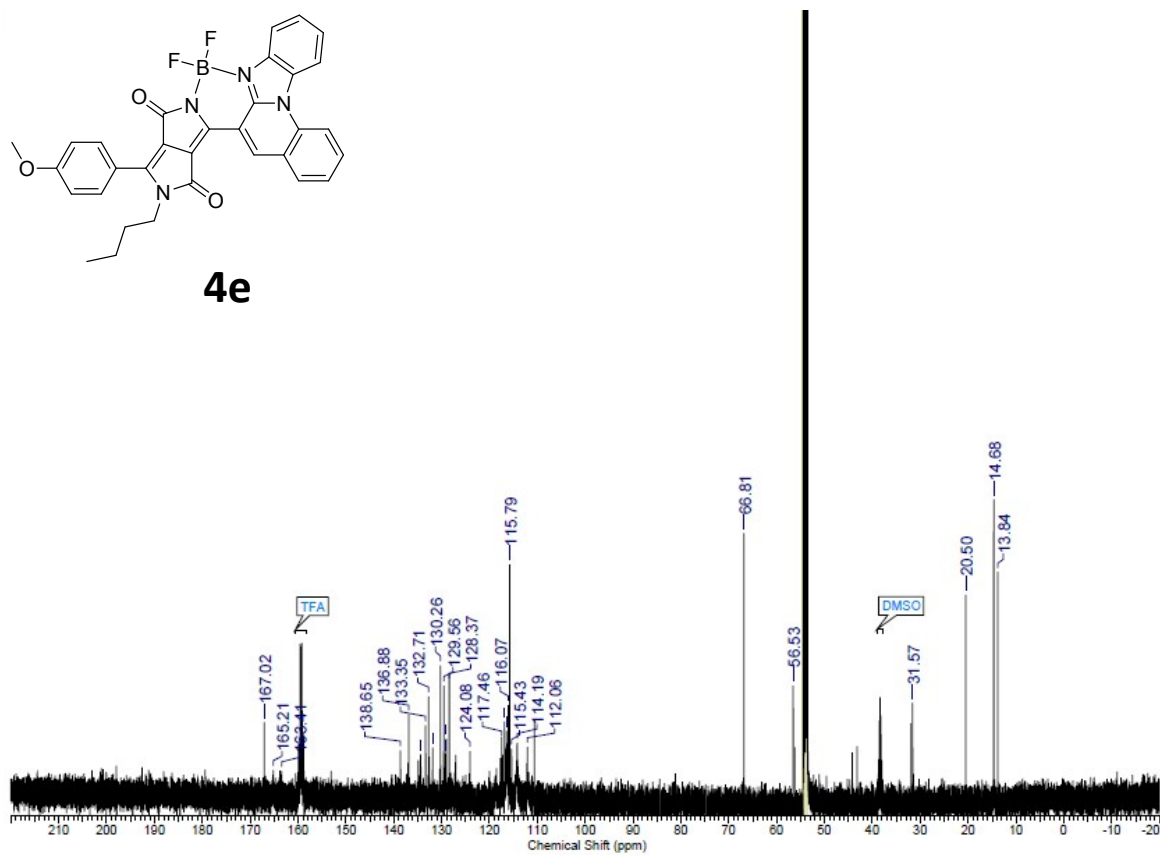


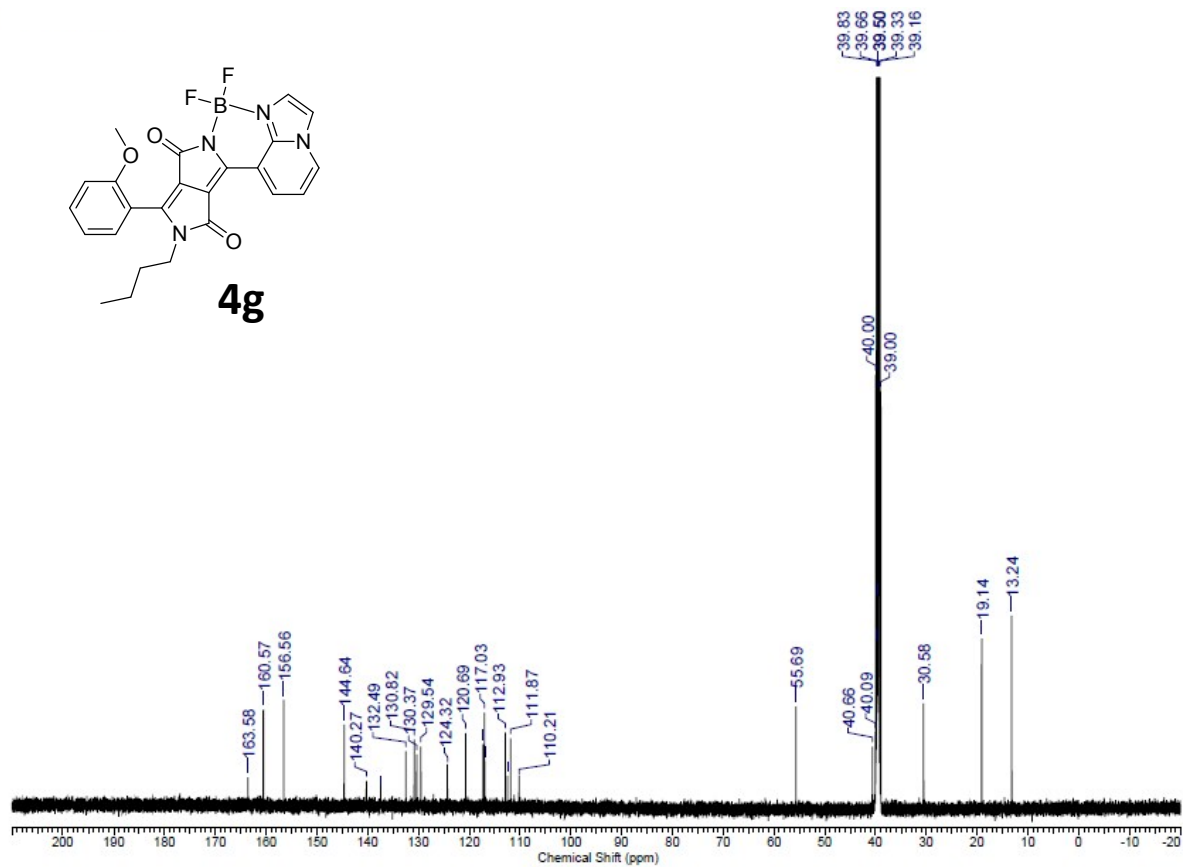
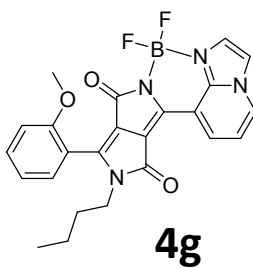
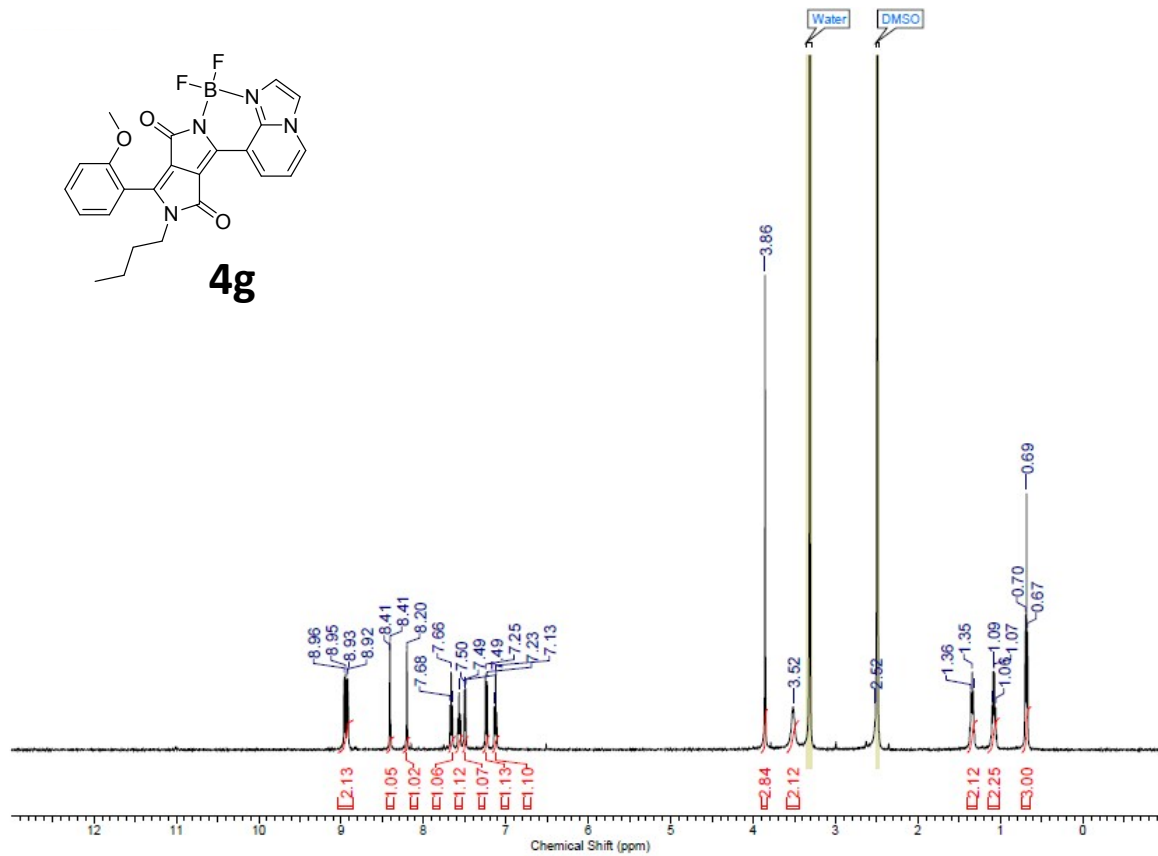
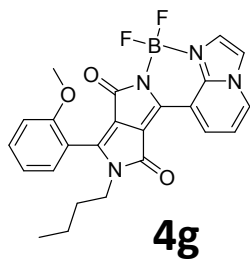


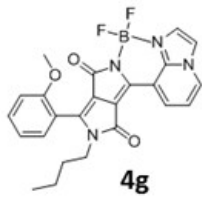




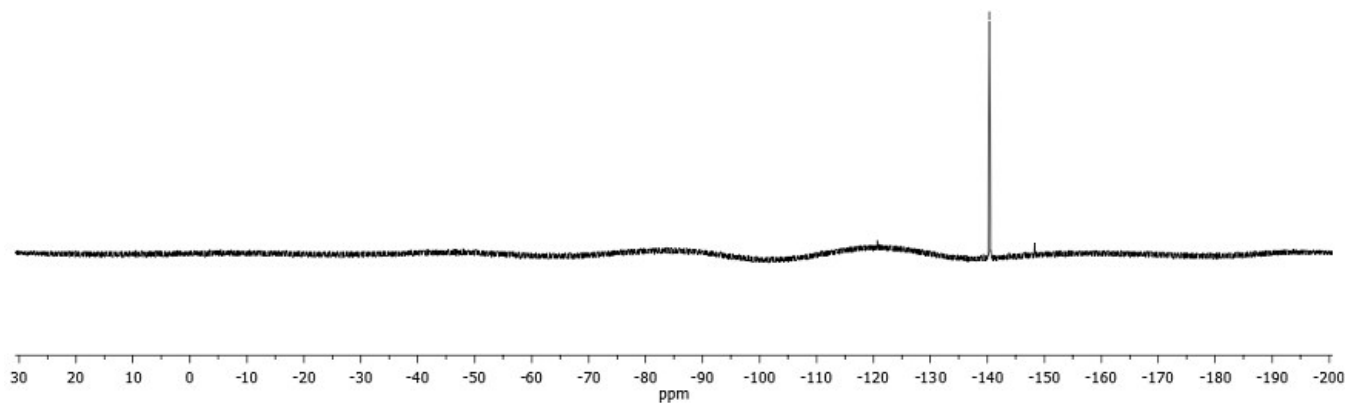
4e

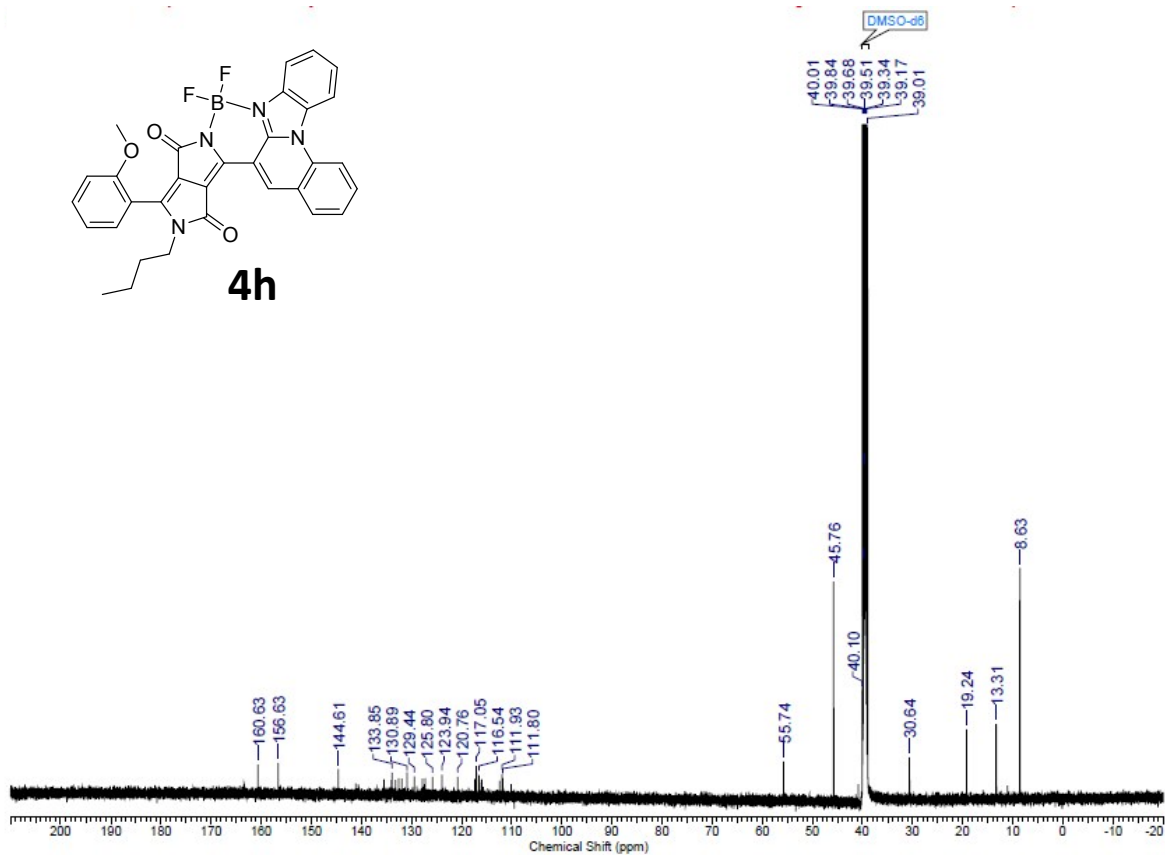
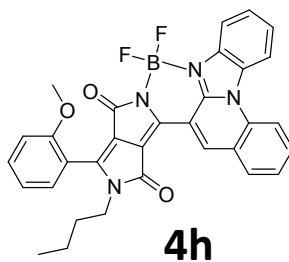
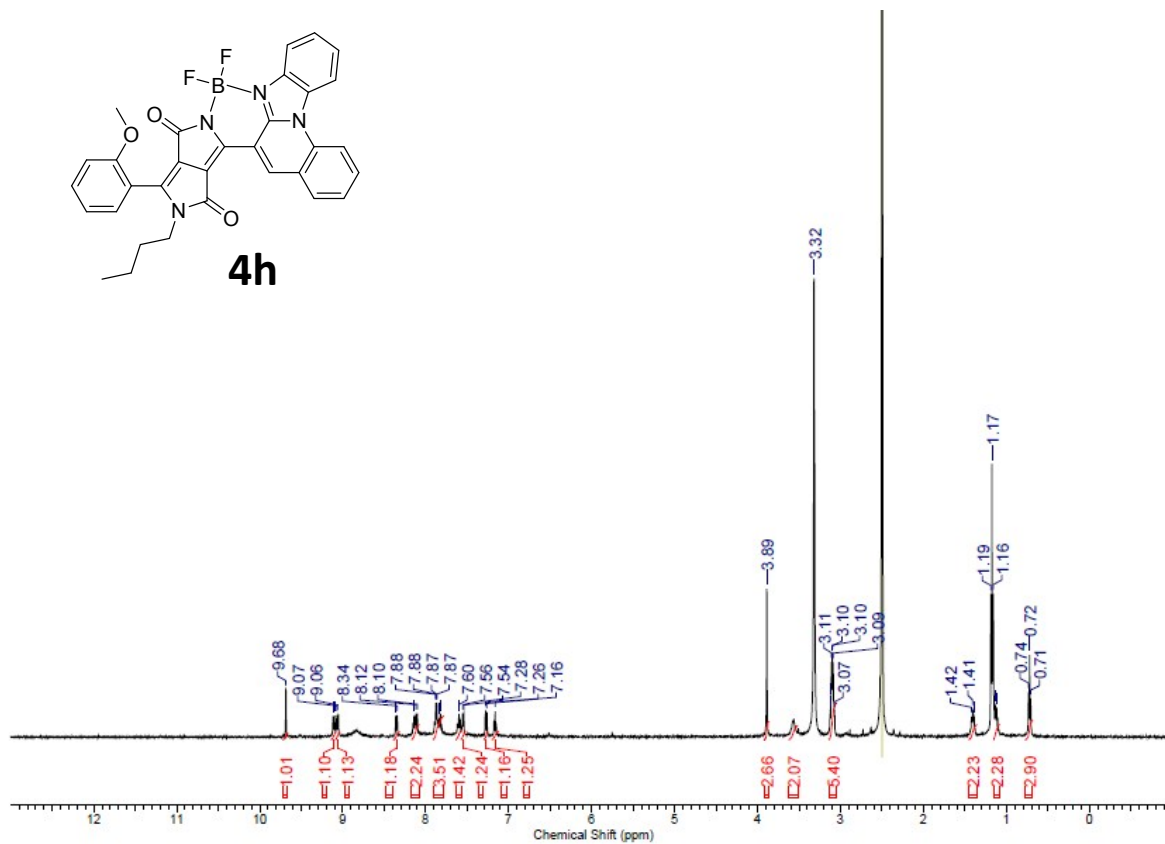
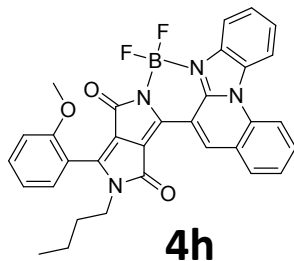


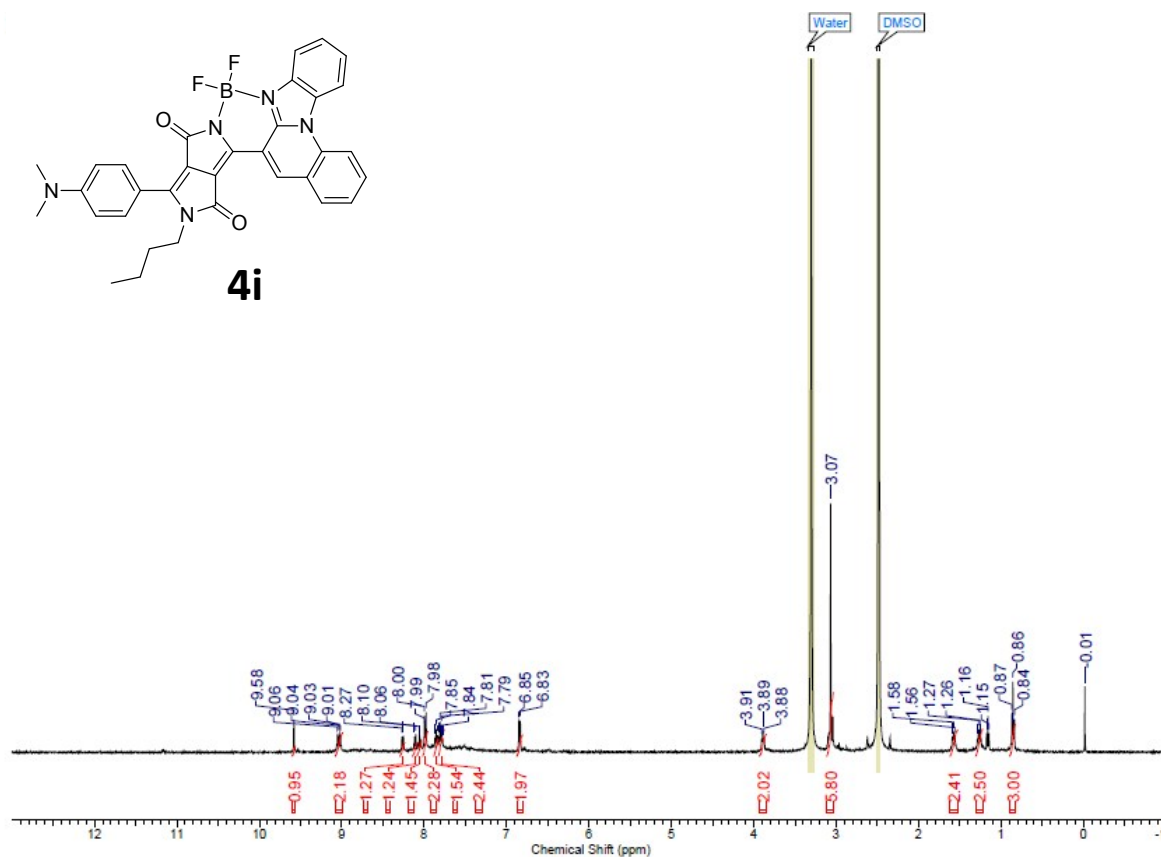




140.37







Section S8: References

1. M. Pieczykolan, B. Sadowski and D. T. Gryko, *Angew. Chem. Int. Ed.*, 2020, ahead of press.
2. S. H. Reich, P. A. Sprengeler, G. G. Chiang, J. R. Appleman, J. Chen, J. Clarine, B. Eam, J. T. Ernst, Q. Han, V. K. Goel, E. Z. R. Han, V. Huang, I. N. J. Hung, A. Jemison, K. A. Jessen, J. Molter, D. Murphy, M. Neal, G. S. Parker, M. Shaghafi, S. Sperry, J. Staunton, C. R. Stumpf, P. A. Thompson, C. Tran, S. E. Webber, C. J. Wegerski, H. Zheng and K. R. Webster, *J. Med. Chem.*, 2018, **61**, 3516-3540.
3. N. D. Kushwaha, S. Mondal, R. Sharma and N. Kumar, *Asian J. Chem.*, 2017, **29**, 1495-1498.
4. B. S. Rane, M. A. Kazi, S. M. Bagul, D. P. Shelar, R. B. Toche and M. N. Jachak, *J. Fluoresc.*, 2010, **20**, 415-420.
5. Q. Cai, Z. Li, J. Wei, L. Fu, C. Ha, D. Pei and K. Ding, *Org. Lett.*, 2010, **12**, 1500-1503.
6. , APEX3 V2019, Bruker Nano, Inc., 2019; SAINT V2018.2040A, Bruker Nano, Inc., 2019; SADABS V2016/2012, Bruker Nano, Inc., 2019.
7. G. Sheldrick, *Acta Crystallographica Section A*, 2015, **71**, 3-8.
8. G. Sheldrick, *Acta Crystallographica Section C*, 2015, **71**, 3-8.
9. C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek and P. A. Wood, *J. Appl. Crystallogr.*, 2008, **41**, 466-470.
10. D. Jacquemin, A. Planchat, C. Adamo and B. Mennucci, *J. Chem. Theory Comput.*, 2012, **8**, 2359-2372.

11. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Gaussian 16 Rev. B.01*, Wallingford, CT, 2016.
12. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
13. B. Le Guennic and D. Jacquemin, *Acc. Chem. Res.*, 2015, **48**, 530-537.
14. J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.*, 2005, **105**, 2999-3094.
15. P. M. Vérité, C. A. Guido and D. Jacquemin, *PCCP*, 2019, **21**, 2307-2317.