Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

ELECTRONIC SUPPLEMENTARY INFORMATION

Boron Functionalization of BODIPY by various Alcohols and Phenols

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Characterization of compounds 2-9, 11-16 : NMR and photophysical spectra

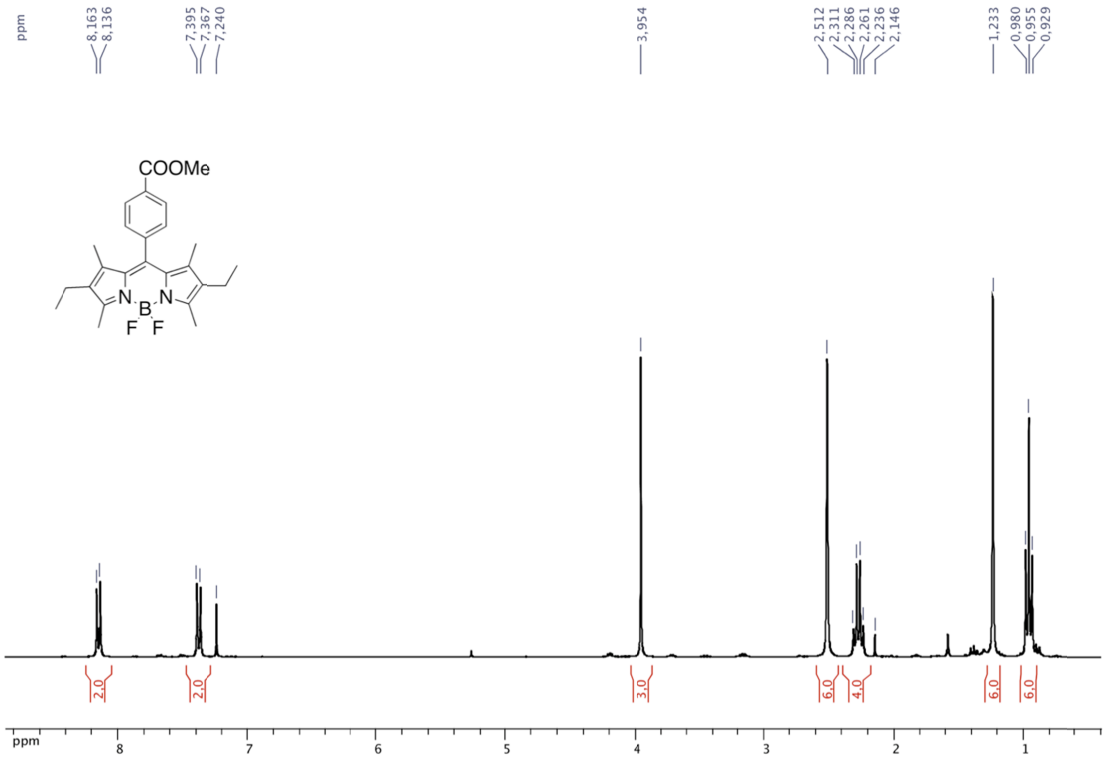

Figure 1: ^{1}H NMR spectrum of compound **1** in $CDCl_3$

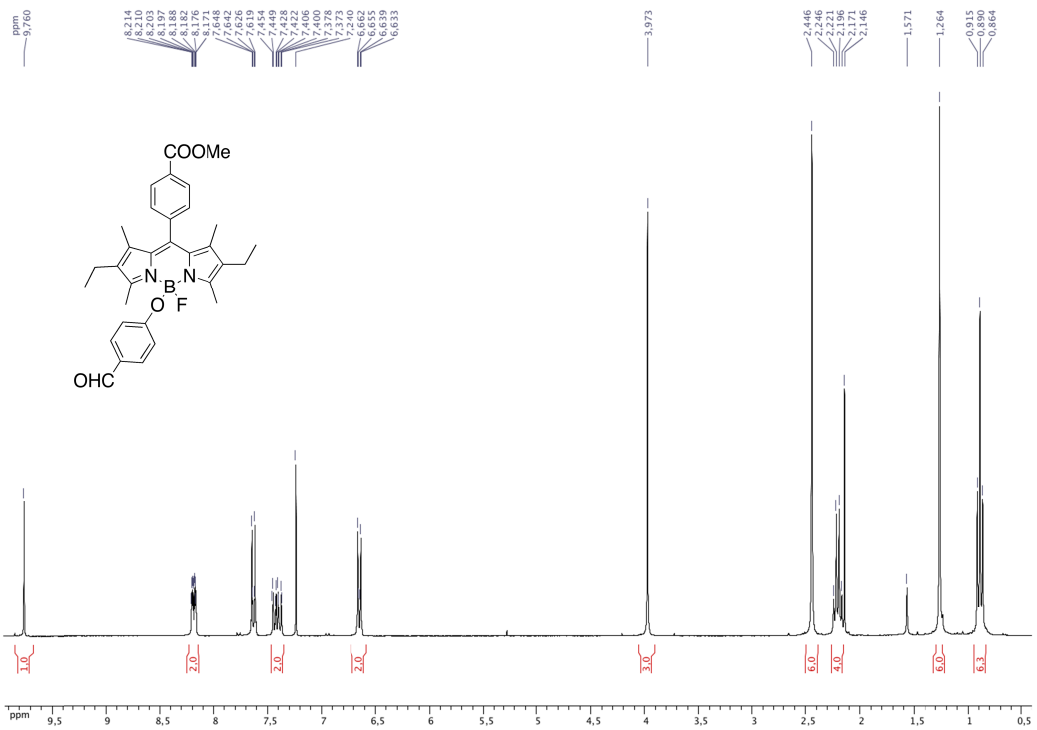

Figure 2: ^{1}H NMR spectrum of compound **2** in $CDCl_3$

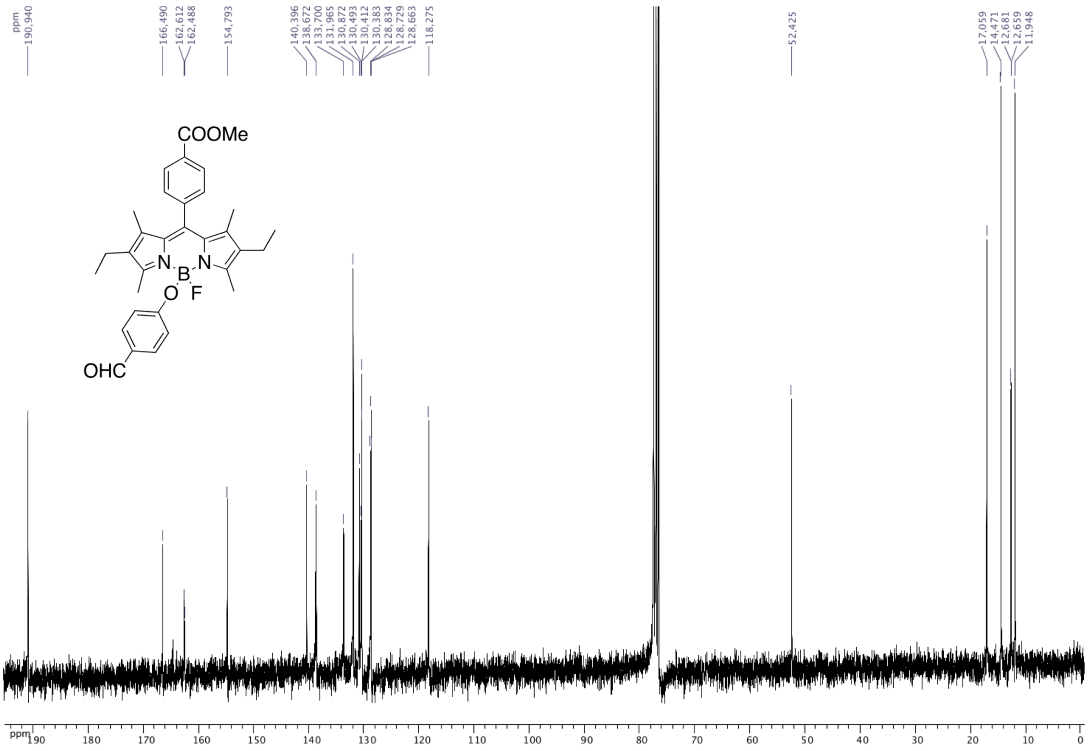

Figure 3: ^{13}C NMR spectrum of compound **2** in $CDCl_3$

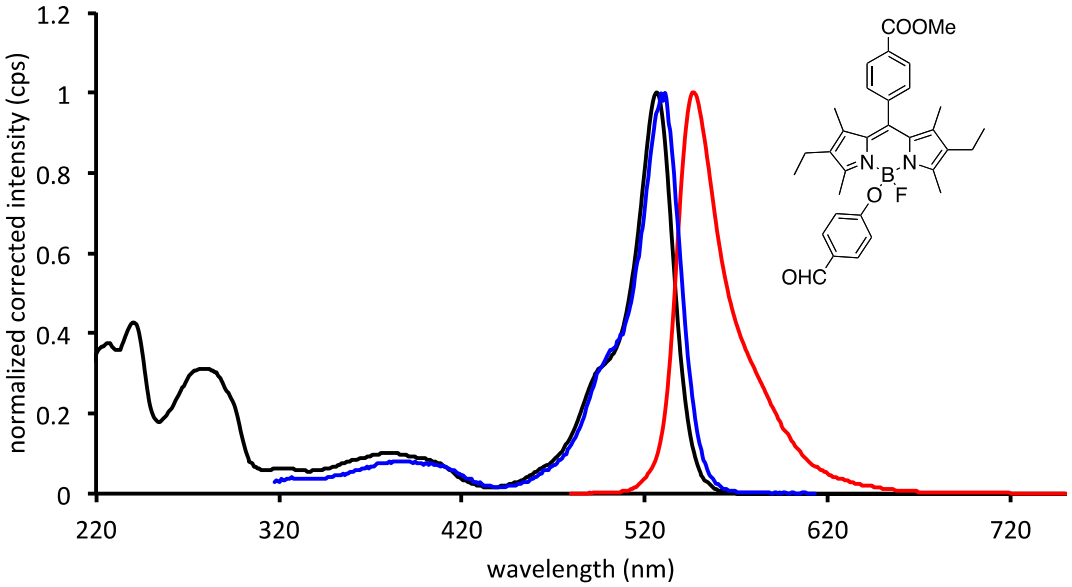

Figure 4: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 620 nm) spectra of **2** in 2-MeTHF at room temperature.

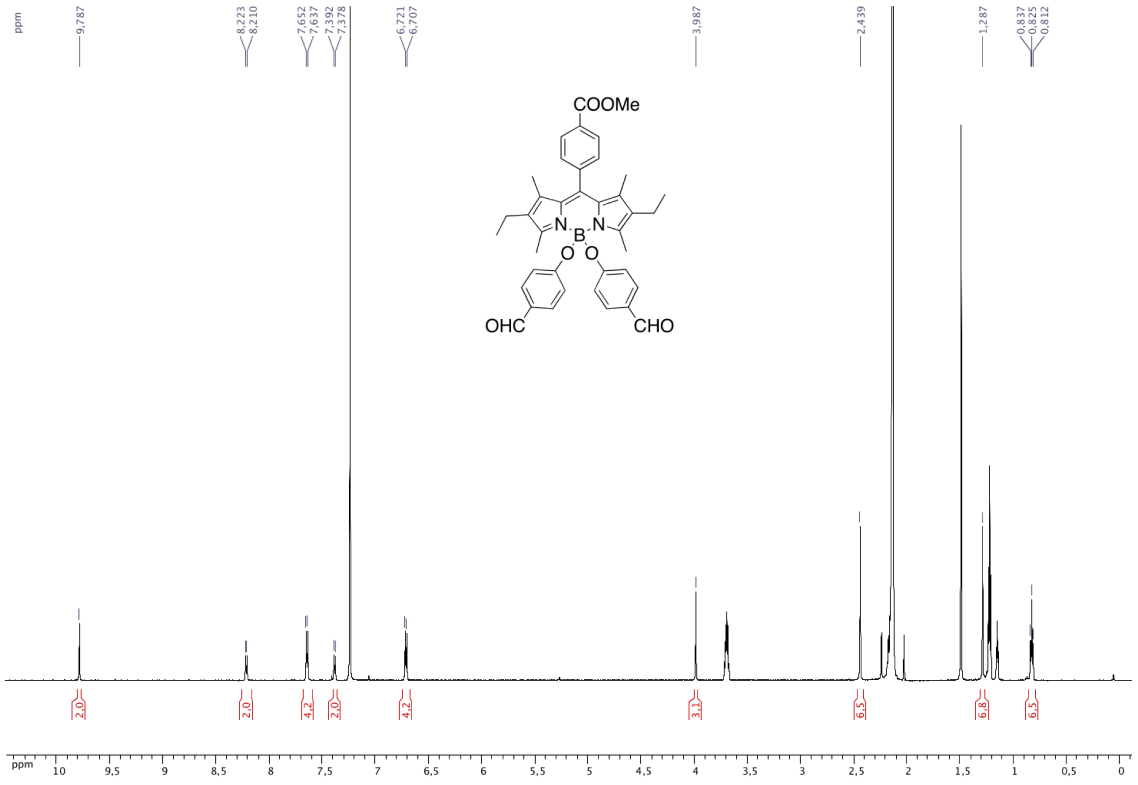

Figure 5: ^{1}H NMR spectrum of compound **3** in $CDCl_3$

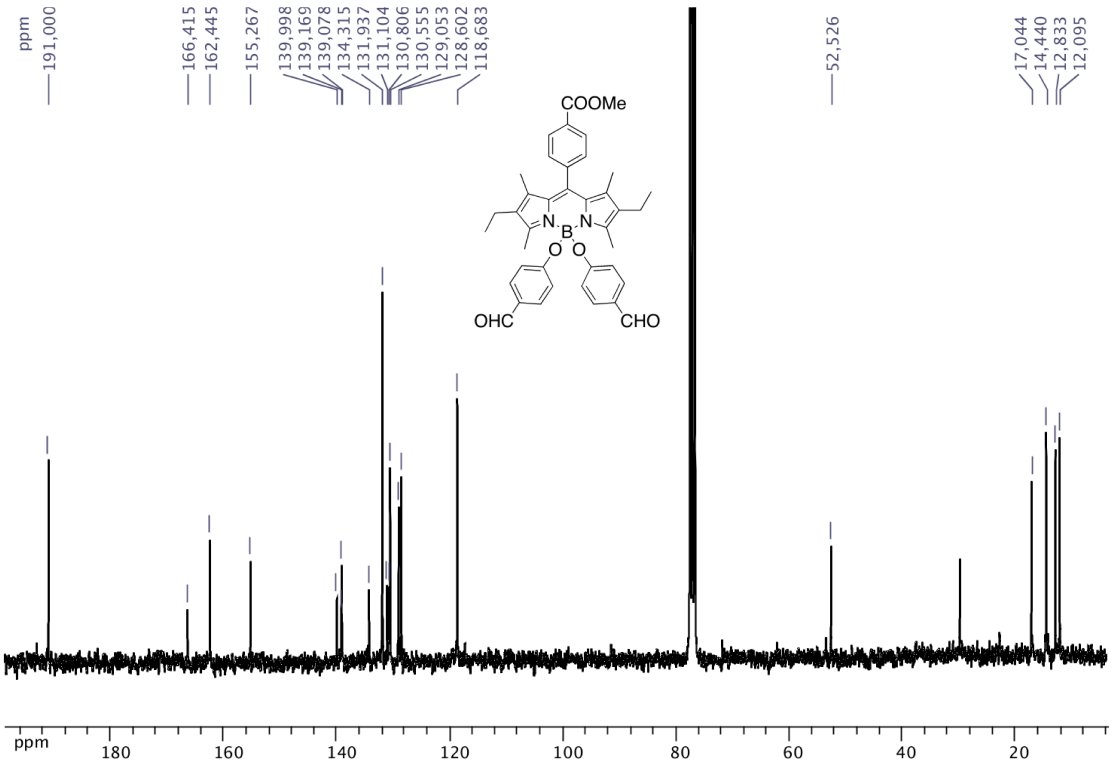

Figure 6: ^{13}C NMR spectrum of compound **3** in $CDCl_3$

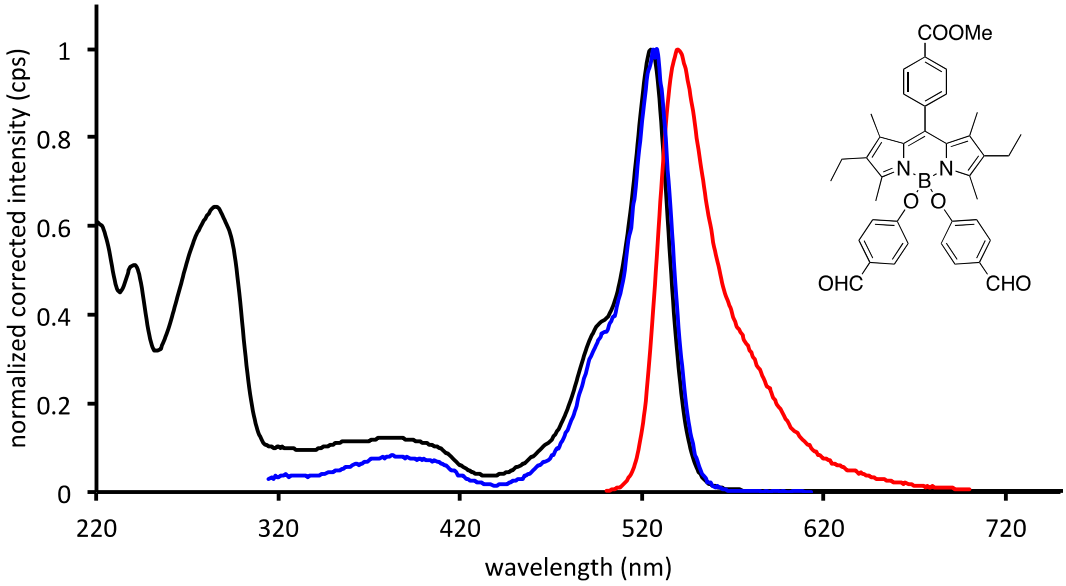

Figure 7: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 620 nm) spectra of **3** in 2-MeTHF at room temperature.

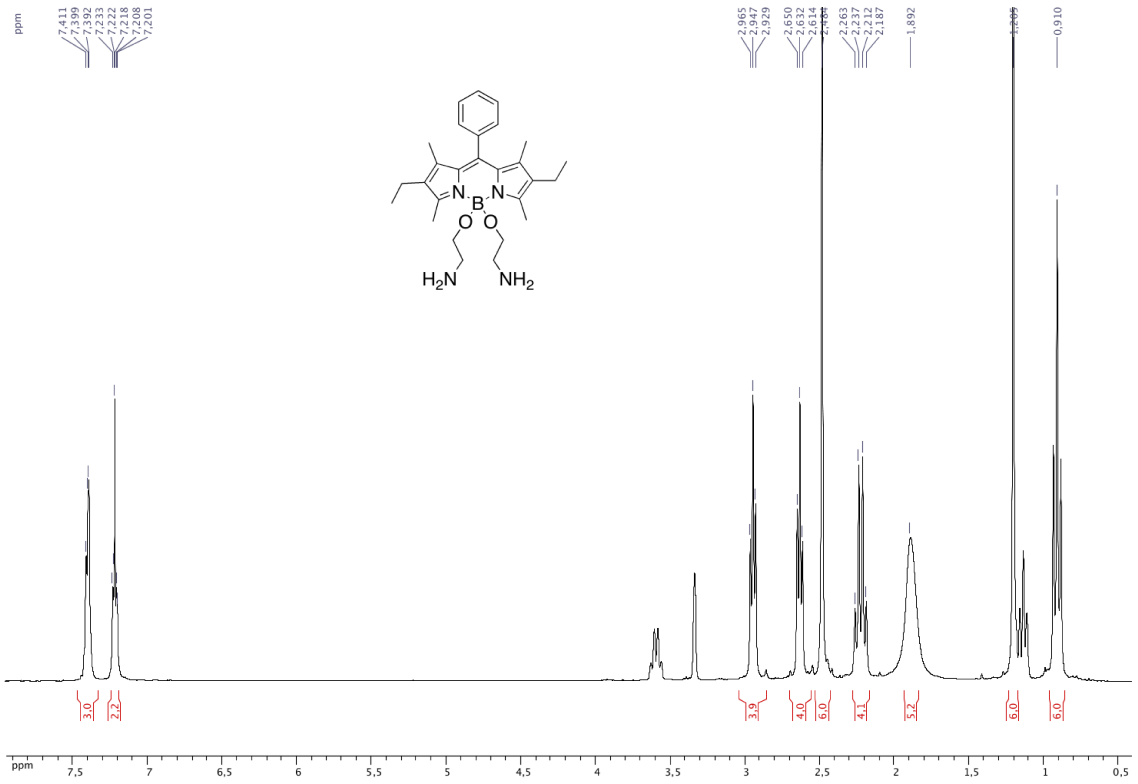

Figure 8: ^{1}H NMR spectrum of compound **4** in $CDCl_3$

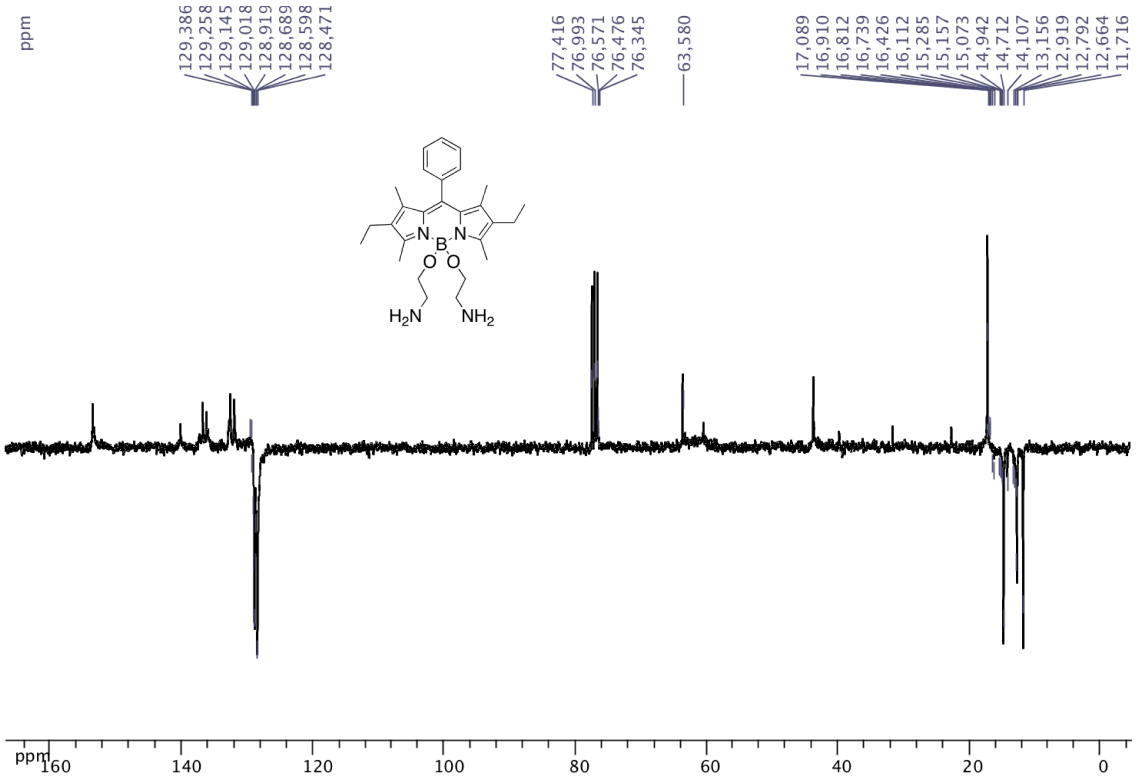

Figure 9: ^{13}C NMR spectrum of compound **4** in $CDCl_3$

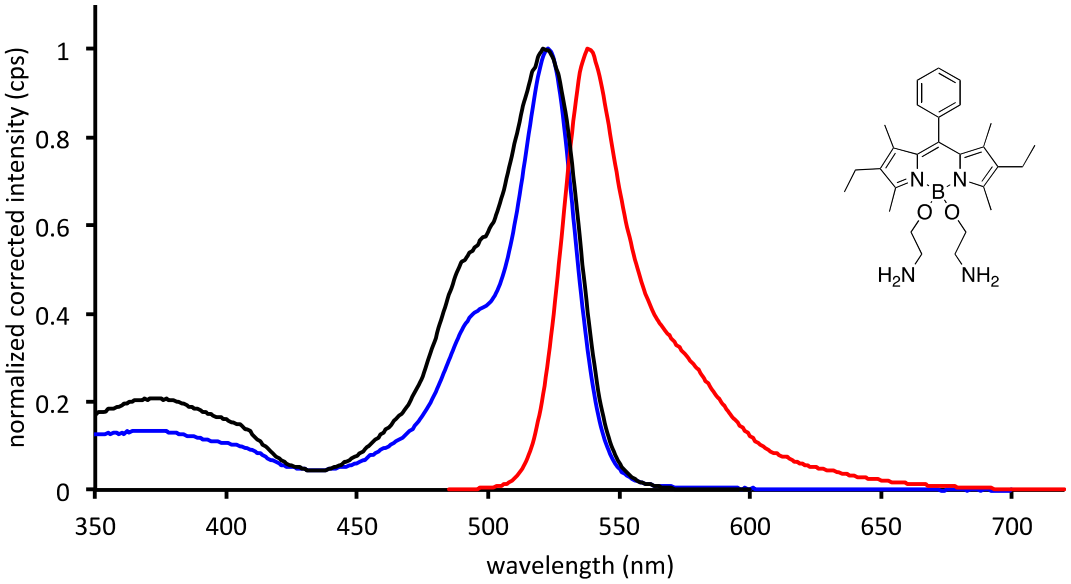

Figure 10: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 690 nm) spectra of **4** in 2-MeTHF at room temperature.

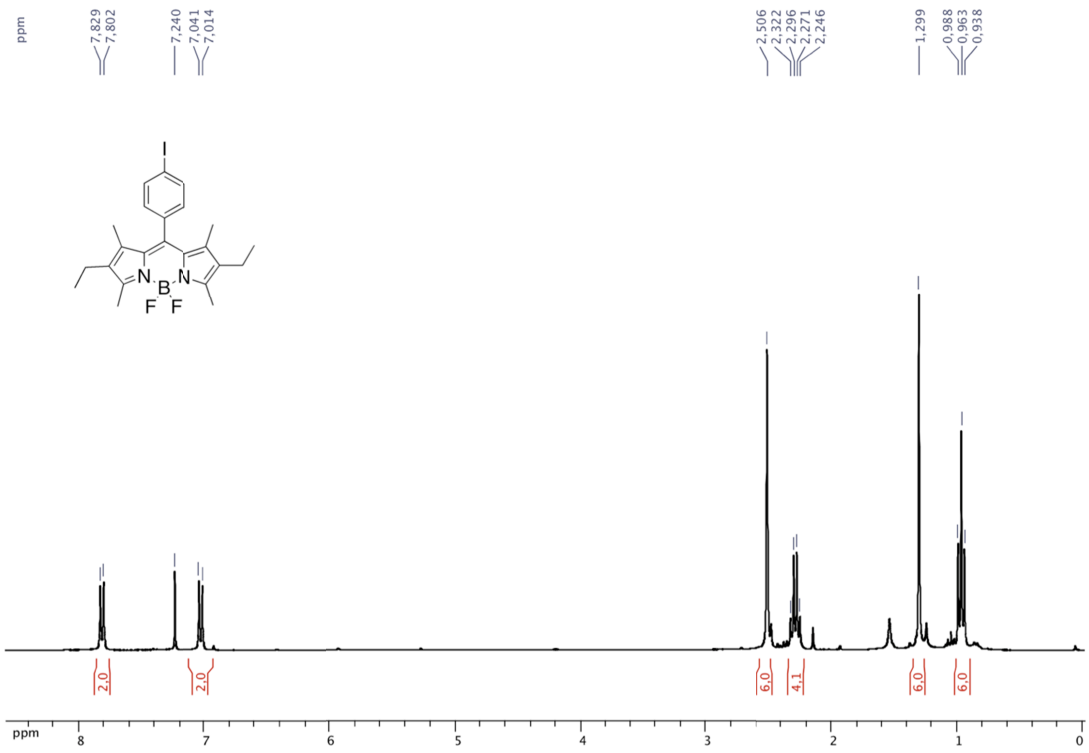

Figure 11: ^{1}H NMR spectrum of compound **5** in $CDCl_3$

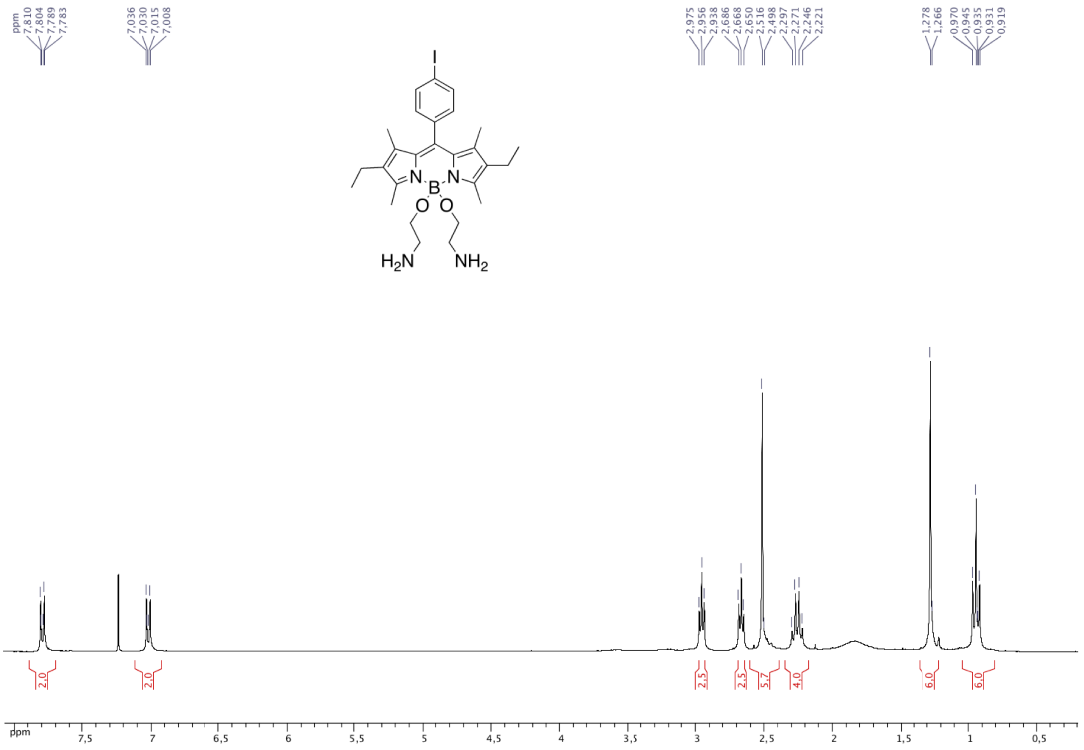

Figure 12: ^{1}H NMR spectrum of compound **6** in $CDCl_3$

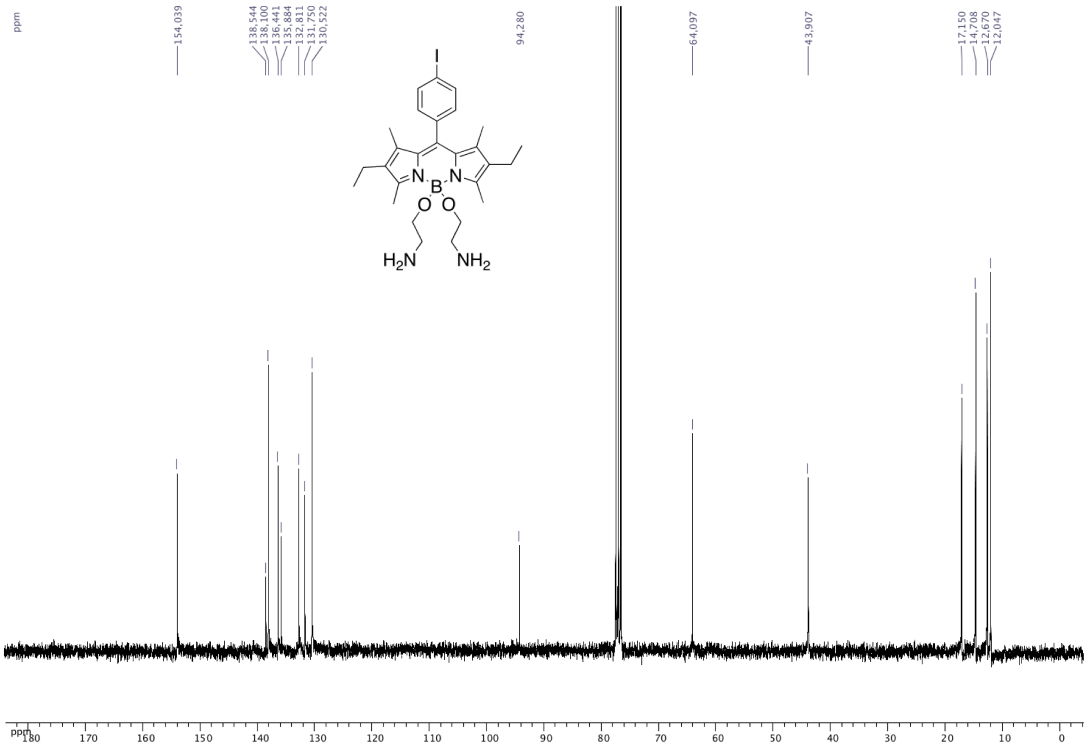

Figure 13: ^{13}C NMR spectrum of compound **6** in $CDCl_3$

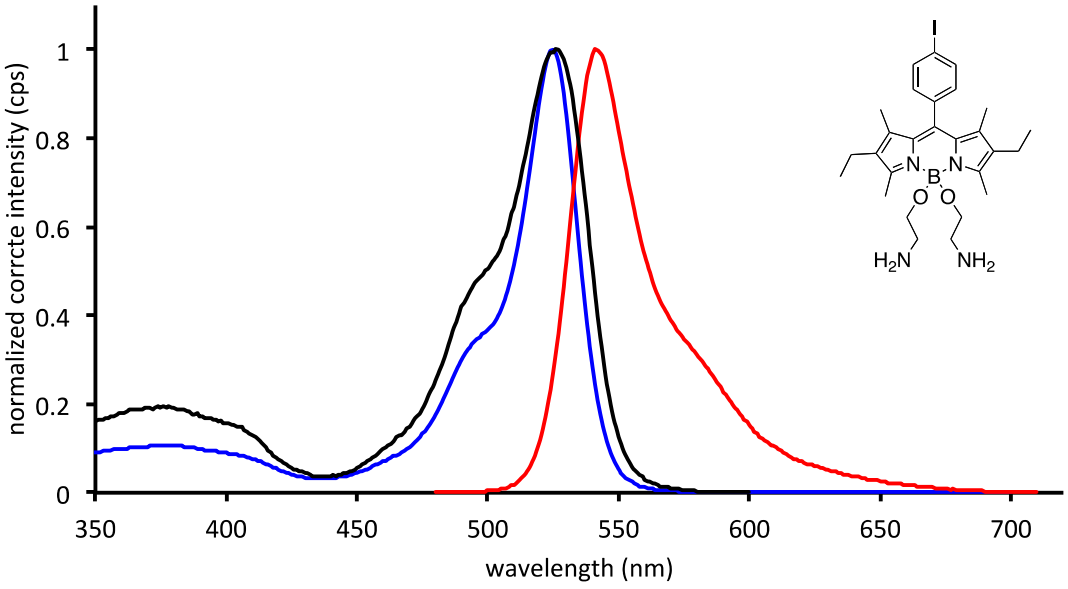

Figure 14: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 690 nm) spectra of **6** in 2-MeTHF at room temperature.

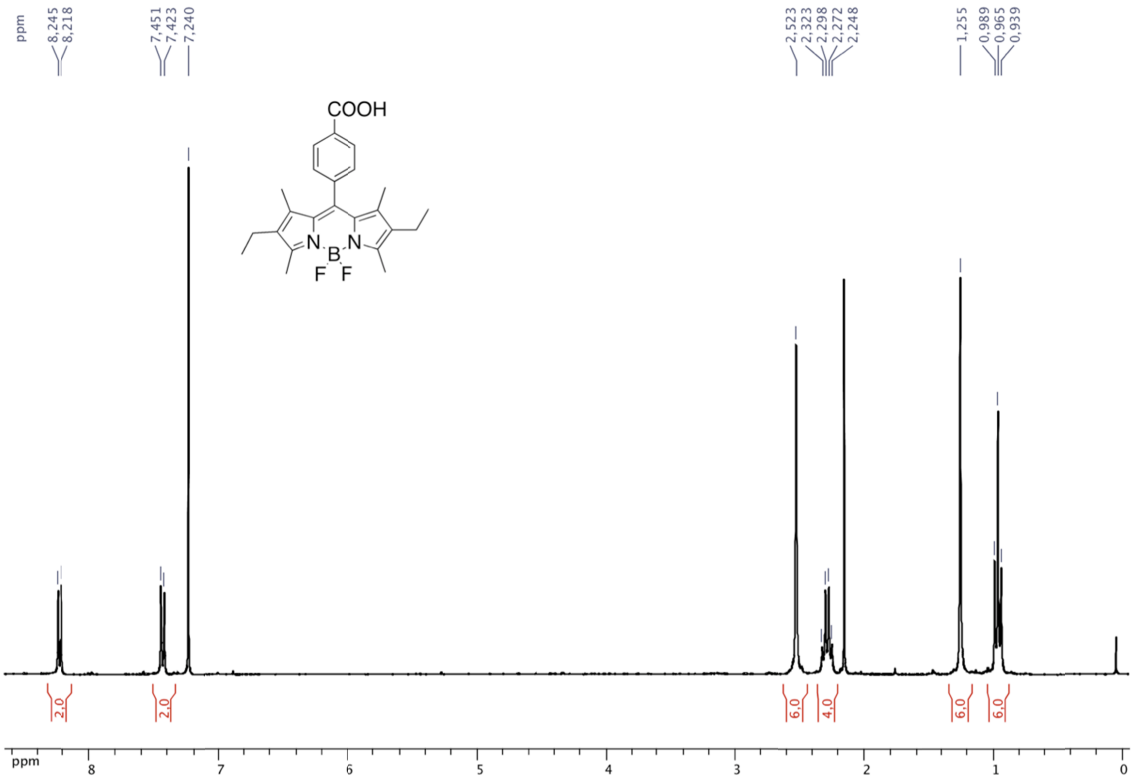

Figure 15: ^{1}H NMR spectrum of compound **7** in $CDCl_3$

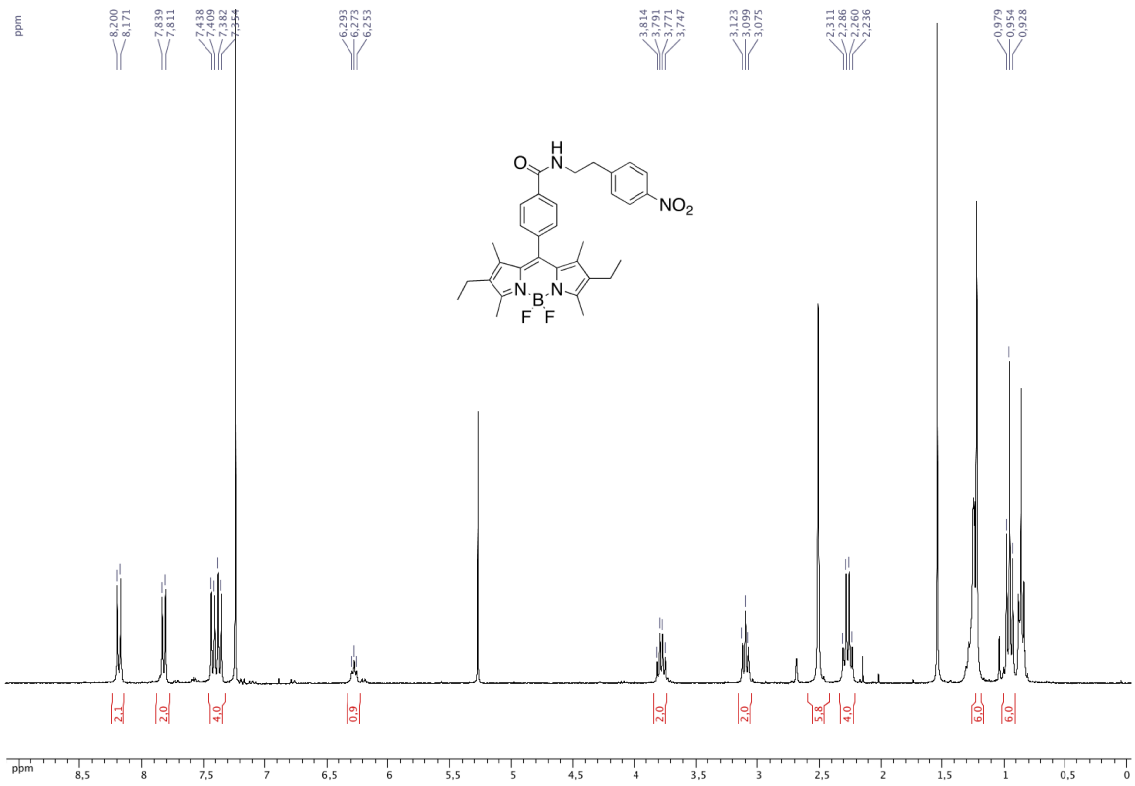

Figure 16: ^{1}H NMR spectrum of compound **8** in $CDCl_3$

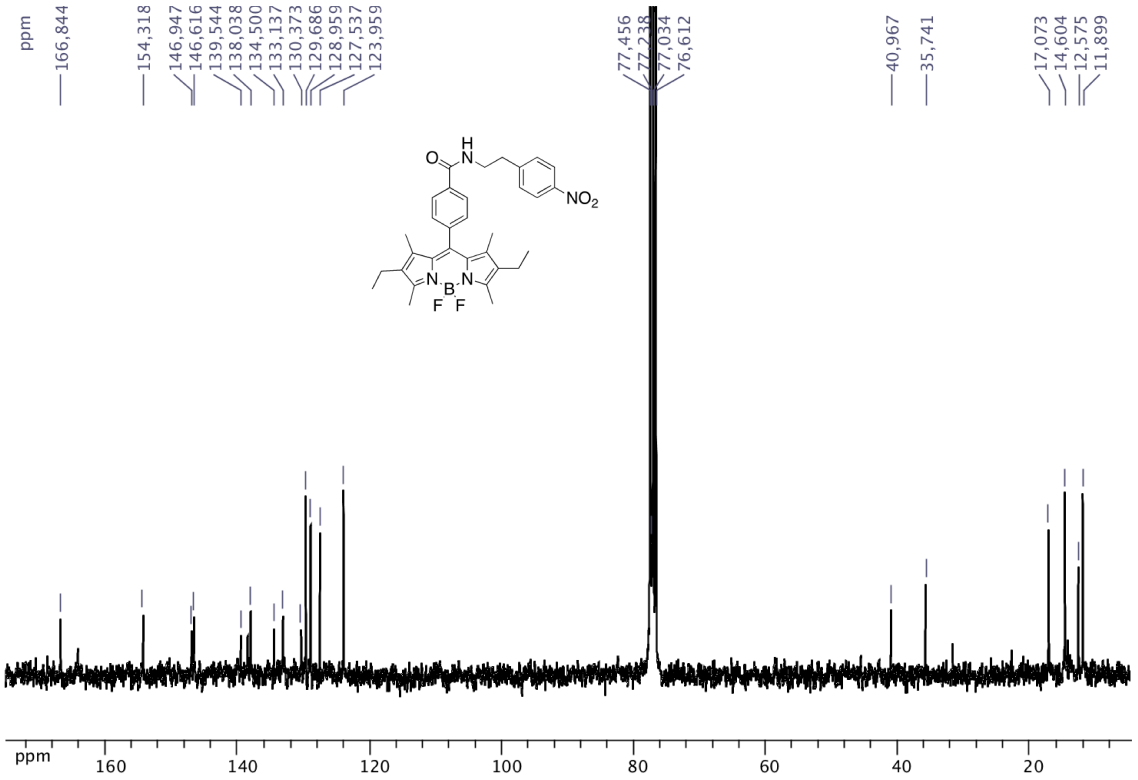

Figure 17: ^{13}C NMR spectrum of compound **8** in $CDCl_3$

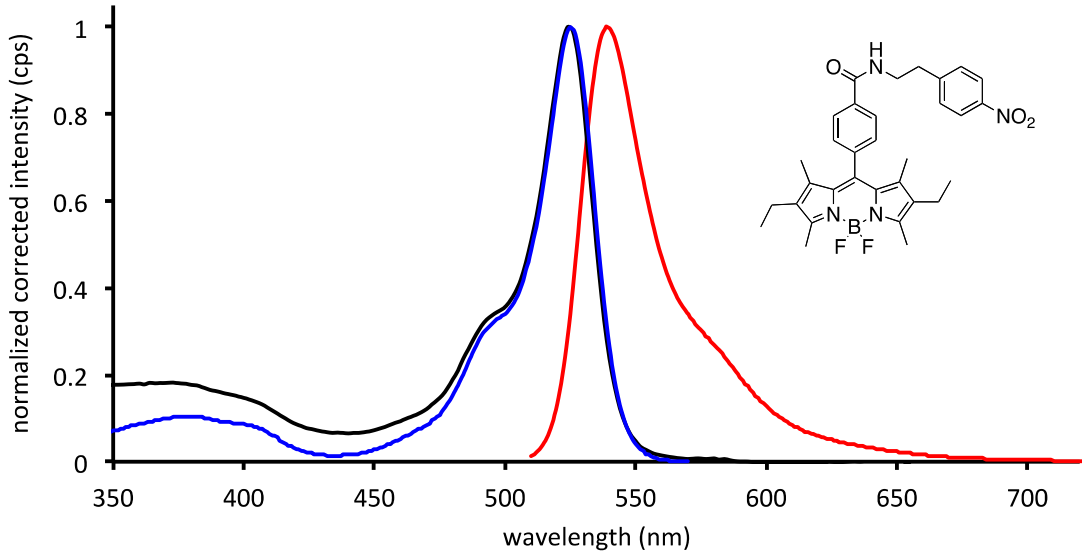

Figure 18: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 620 nm) spectra of **8** in 2-MeTHF at room temperature.

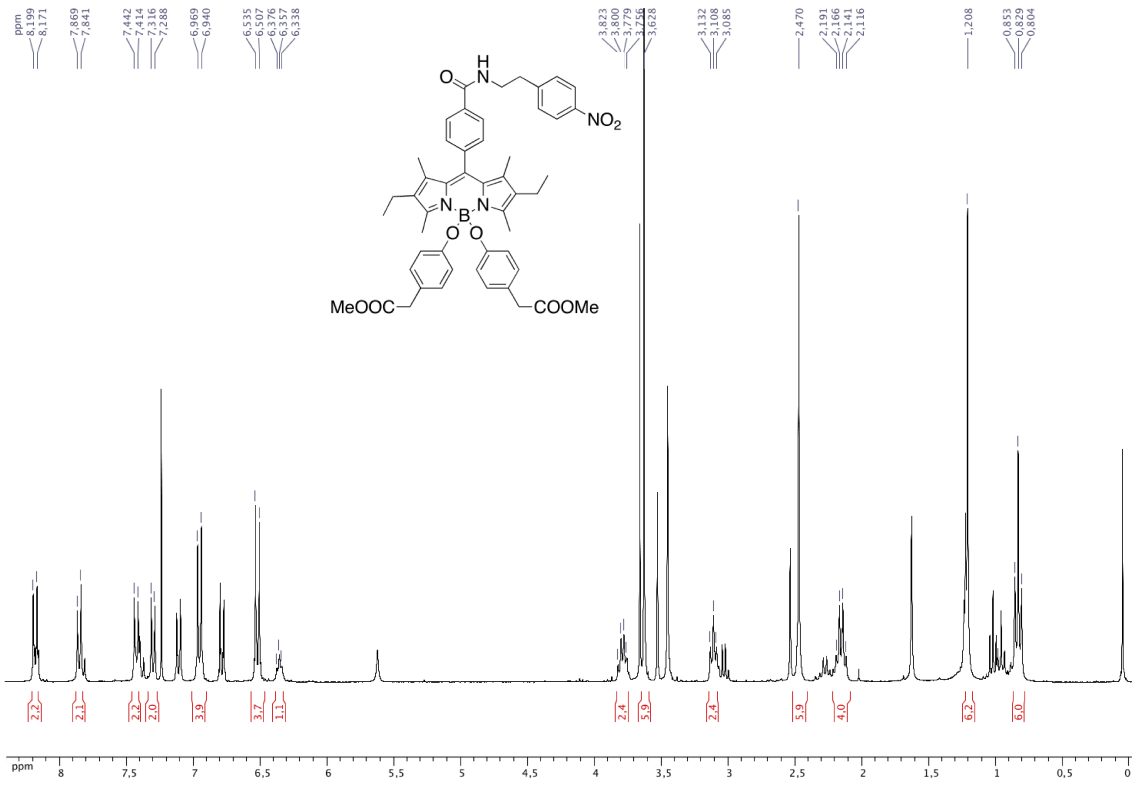

Figure 19: ^{1}H NMR spectrum of compound **9** in $CDCl_3$

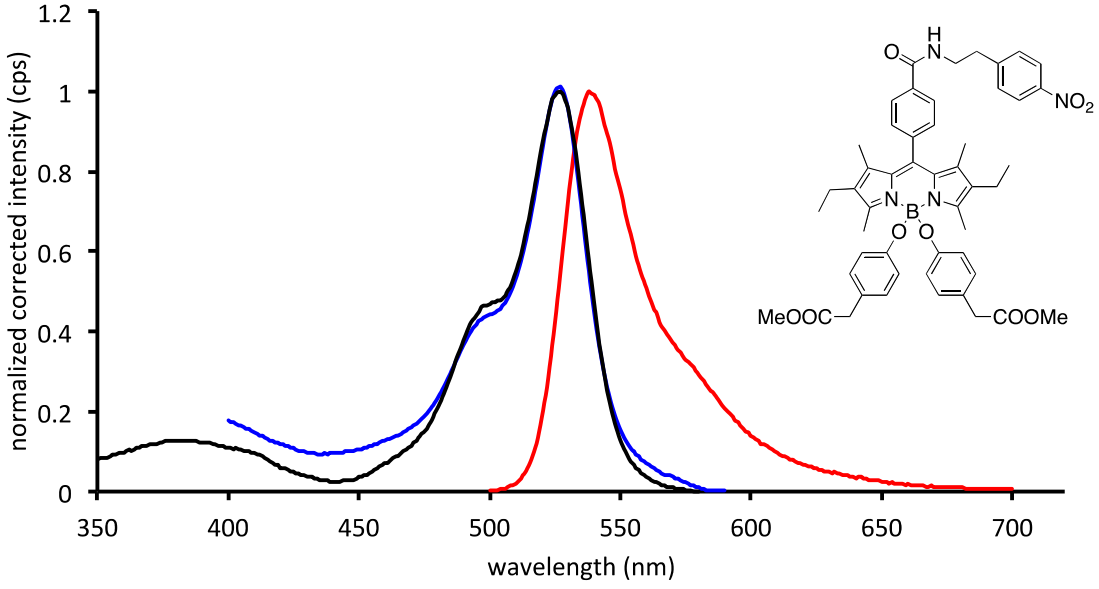

Figure 20: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 620 nm) spectra of **9** in 2-MeTHF at room temperature.

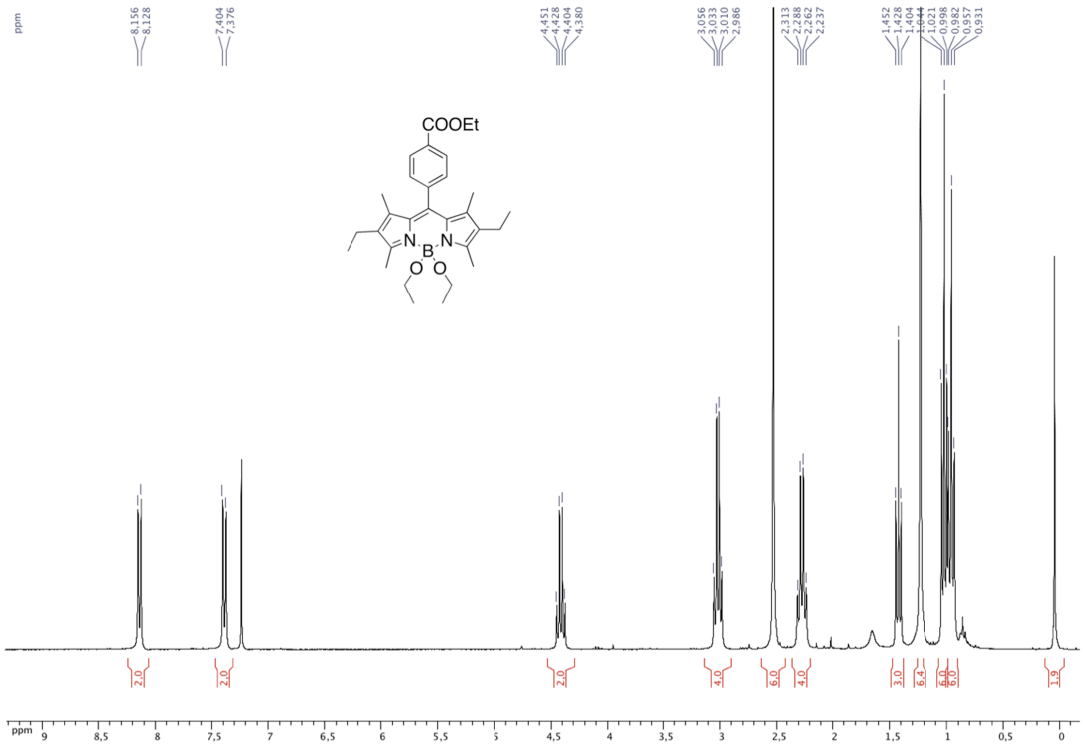

Figure 21: ^{1}H NMR spectrum of compound **10** in $CDCl_3$

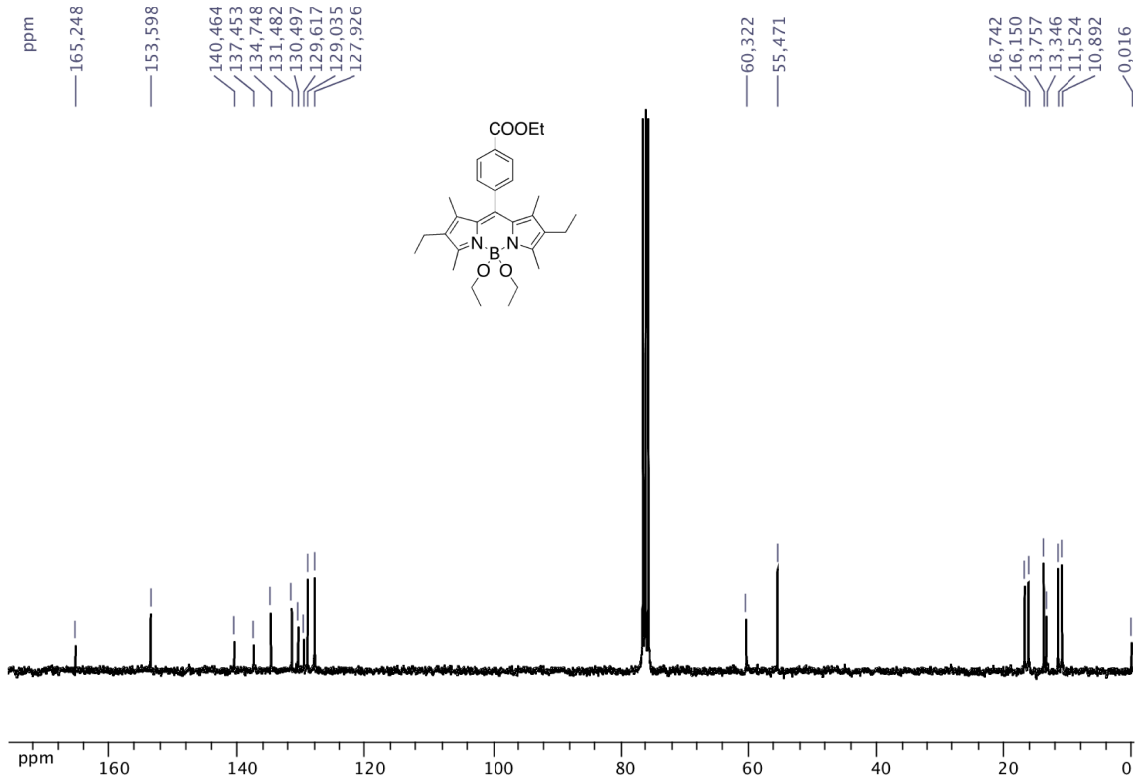

Figure 22: ^{13}C NMR spectrum of compound **11** in $CDCl_3$

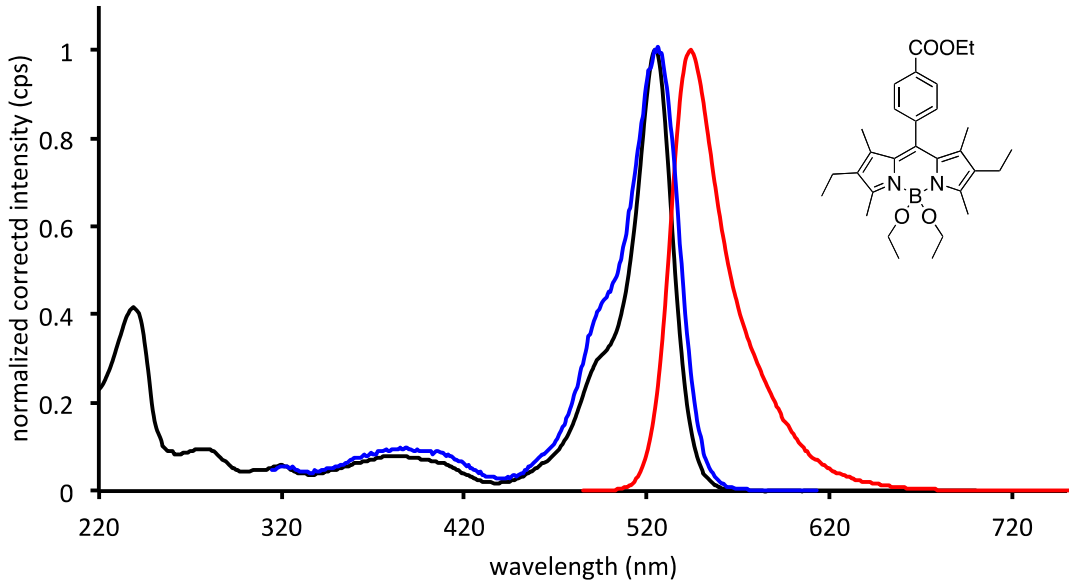

Figure 23: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 620 nm) spectra of **11** in 2-MeTHF at room temperature.

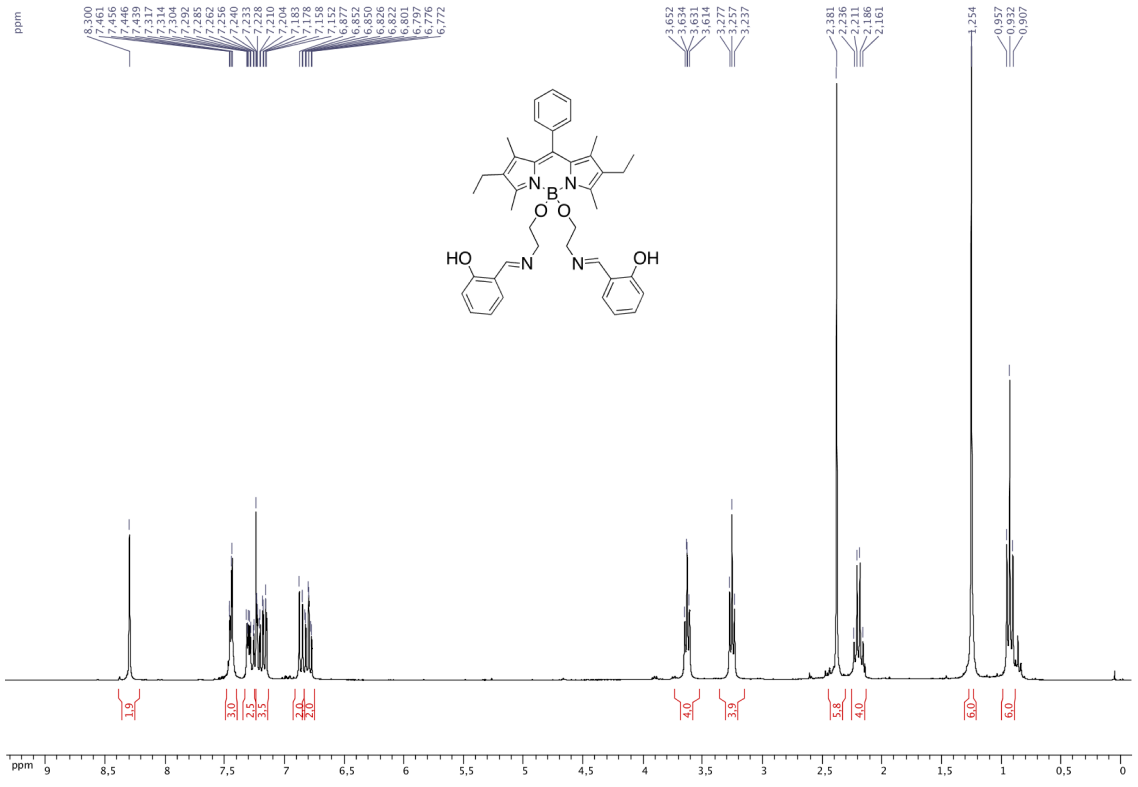

Figure 24: ^{1}H NMR spectrum of compound **12** in $CDCl_3$

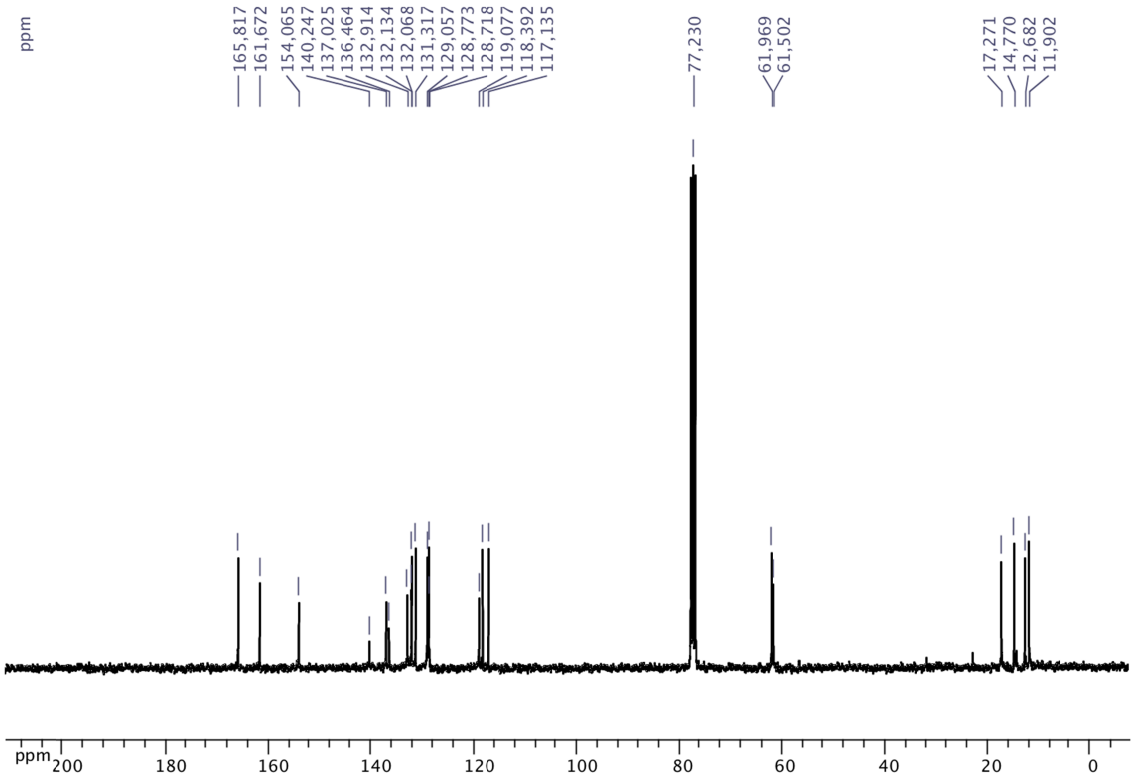

Figure 25: ^{13}C NMR spectrum of compound **12** in $CDCl_3$

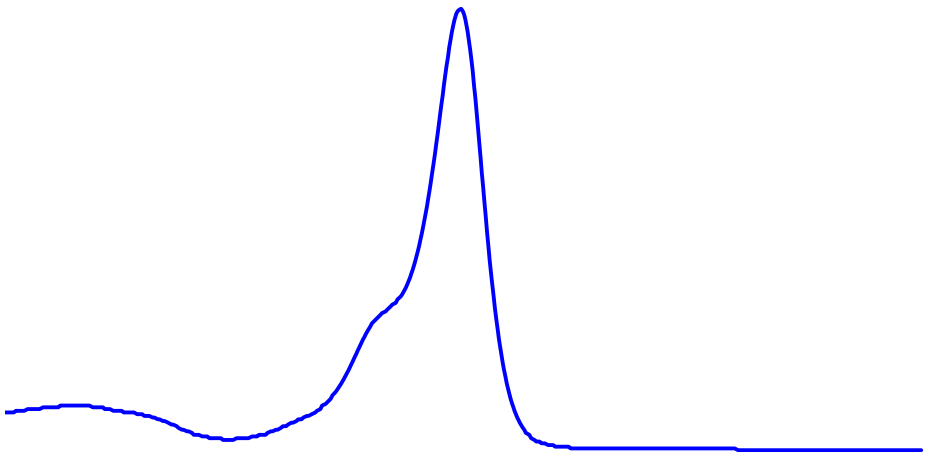

Figure 26: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 690 nm) spectra of **12** in 2-MeTHF at room temperature.

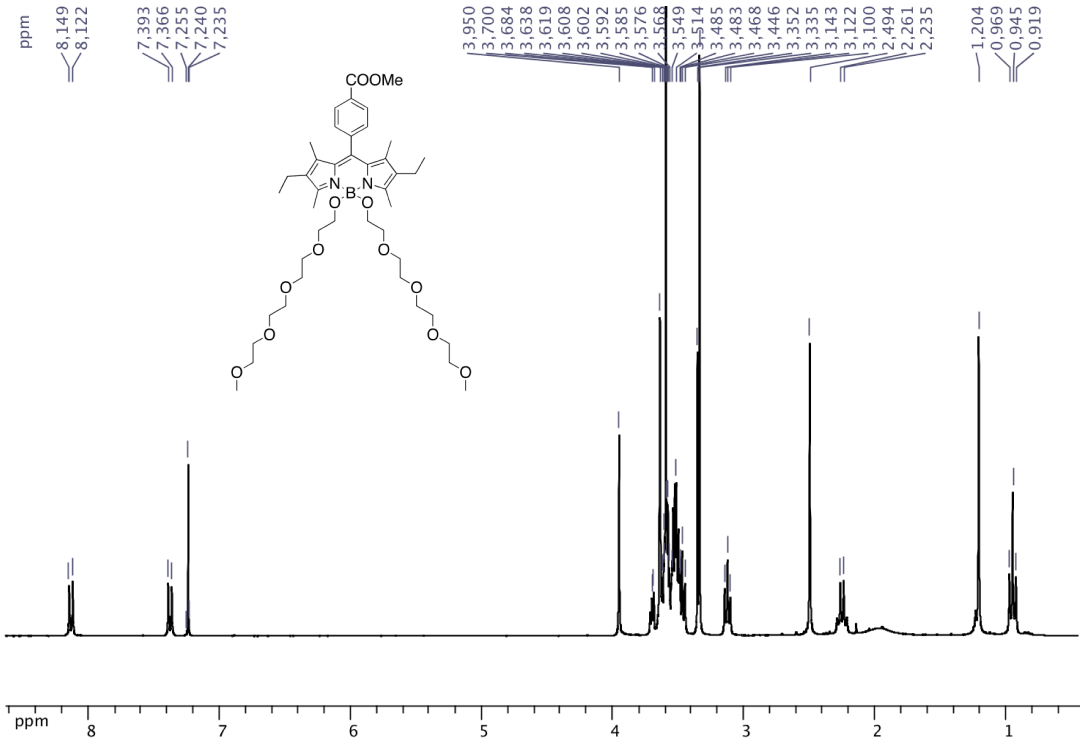

Figure 27: ^{1}H NMR spectrum of compound **13** in $CDCl_3$

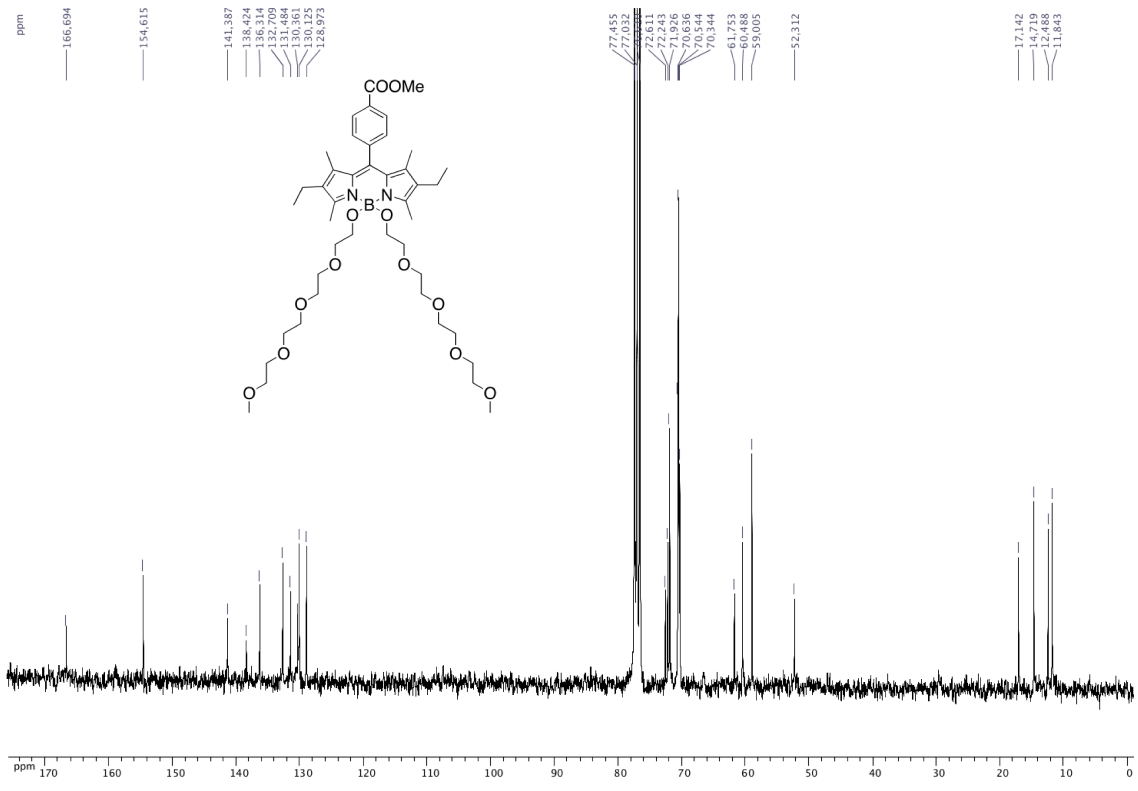

Figure 28: ^{13}C NMR spectrum of compound **13** in $CDCl_3$

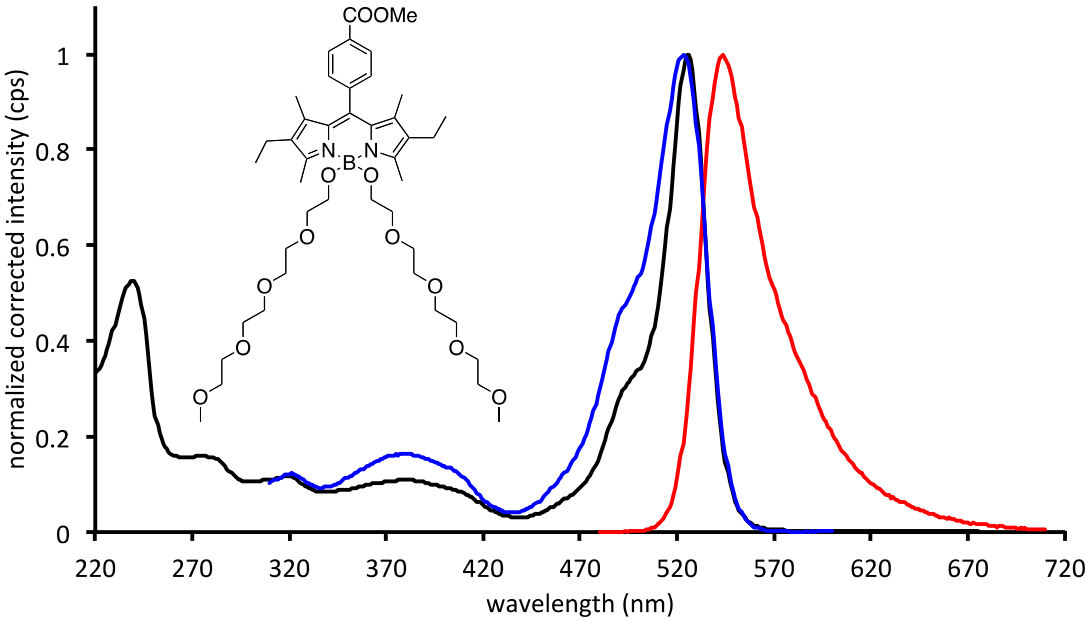

Figure 29: Absorption (black), fluorescence (red, λ_{ex}= 470 nm) and excitation (blue, λ_{em}= 620 nm) spectra of **13** in 2-MeTHF at room temperature.

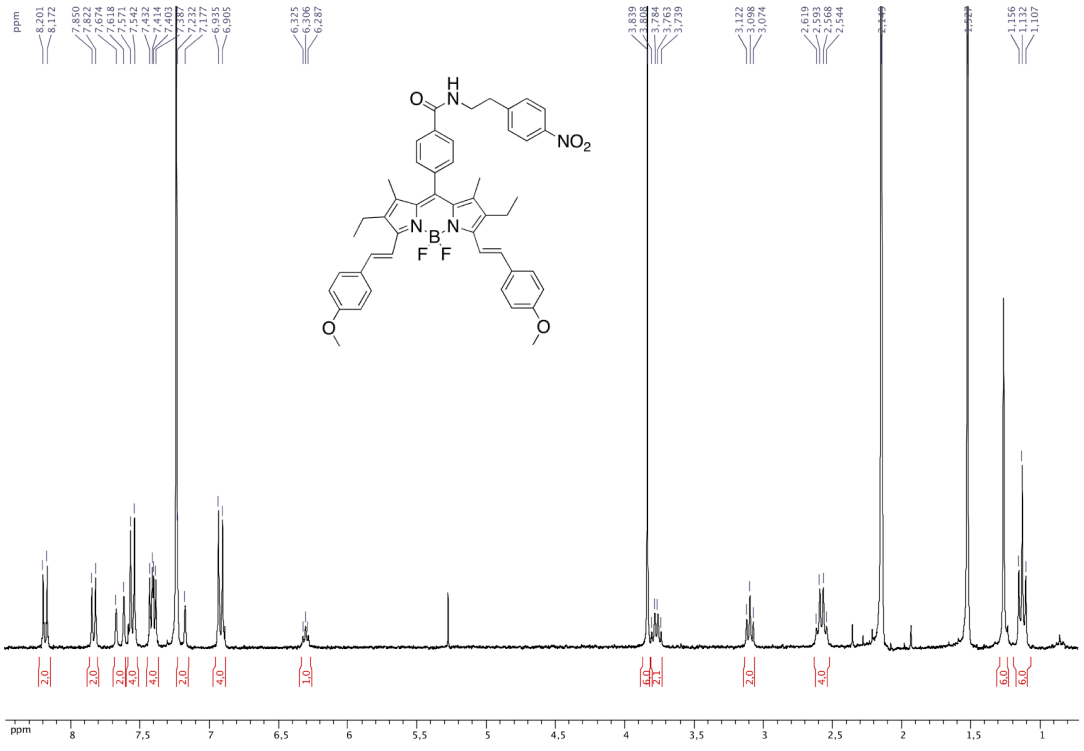

Figure 30: ^{1}H NMR spectrum of compound **14** in $CDCl_3$

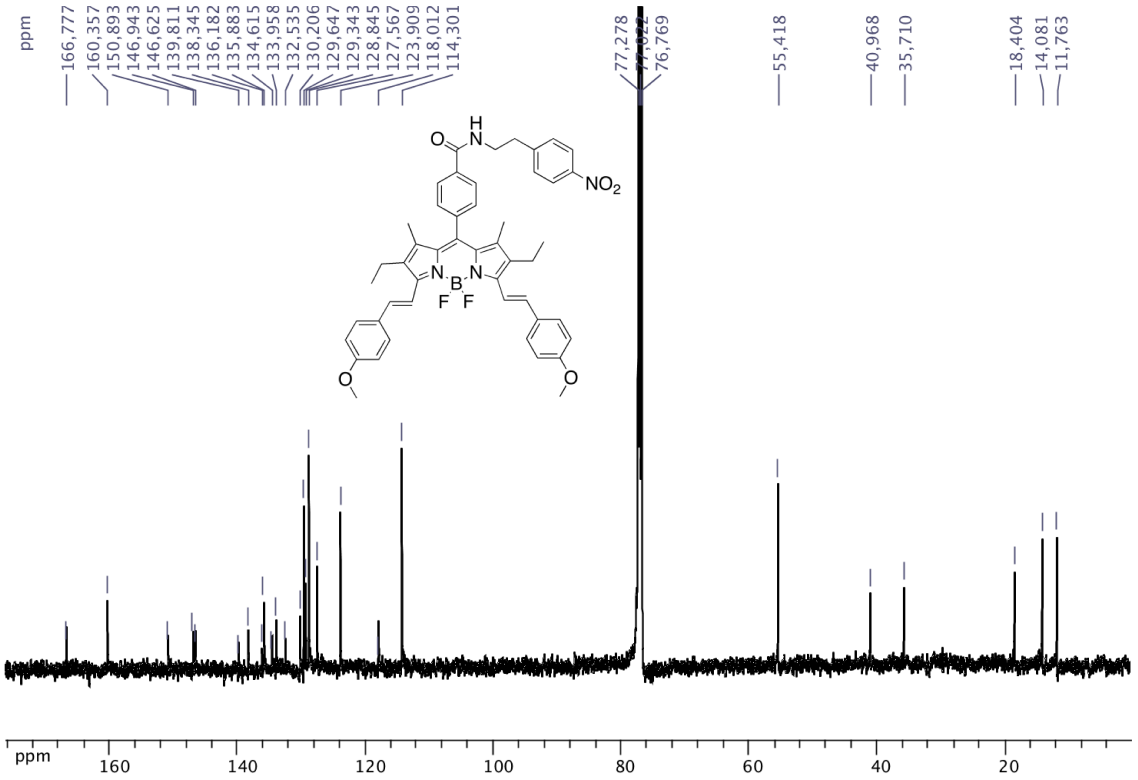

Figure 31: ^{13}C NMR spectrum of compound **14** in $CDCl_3$

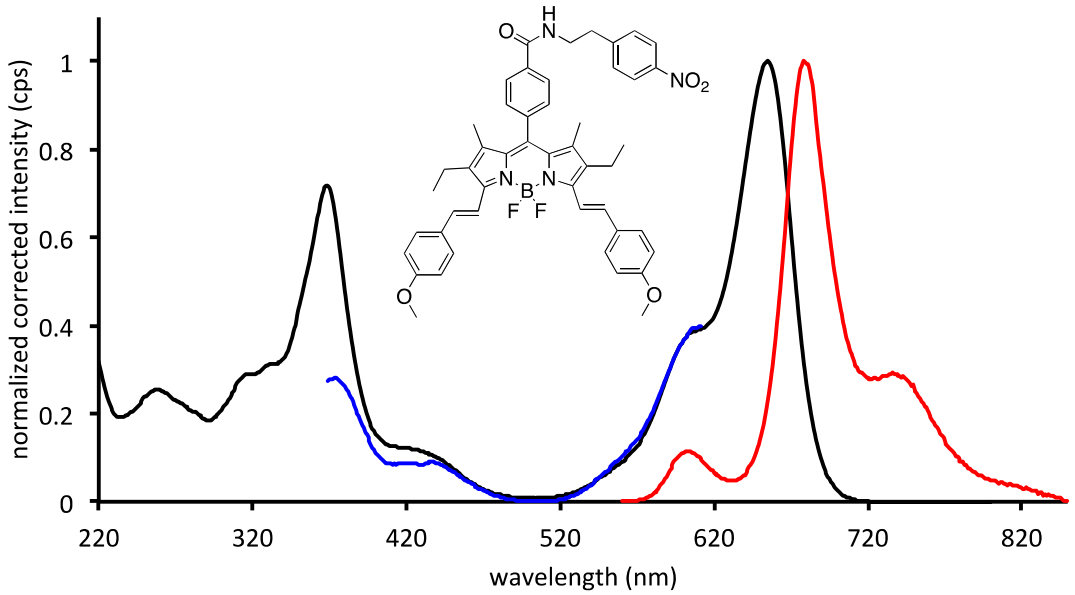

Figure 32: Absorption (black), fluorescence (red, λ_{ex}= 550 nm) and excitation (blue, λ_{em}= 700 nm) spectra of **14** in 2-MeTHF at room temperature.

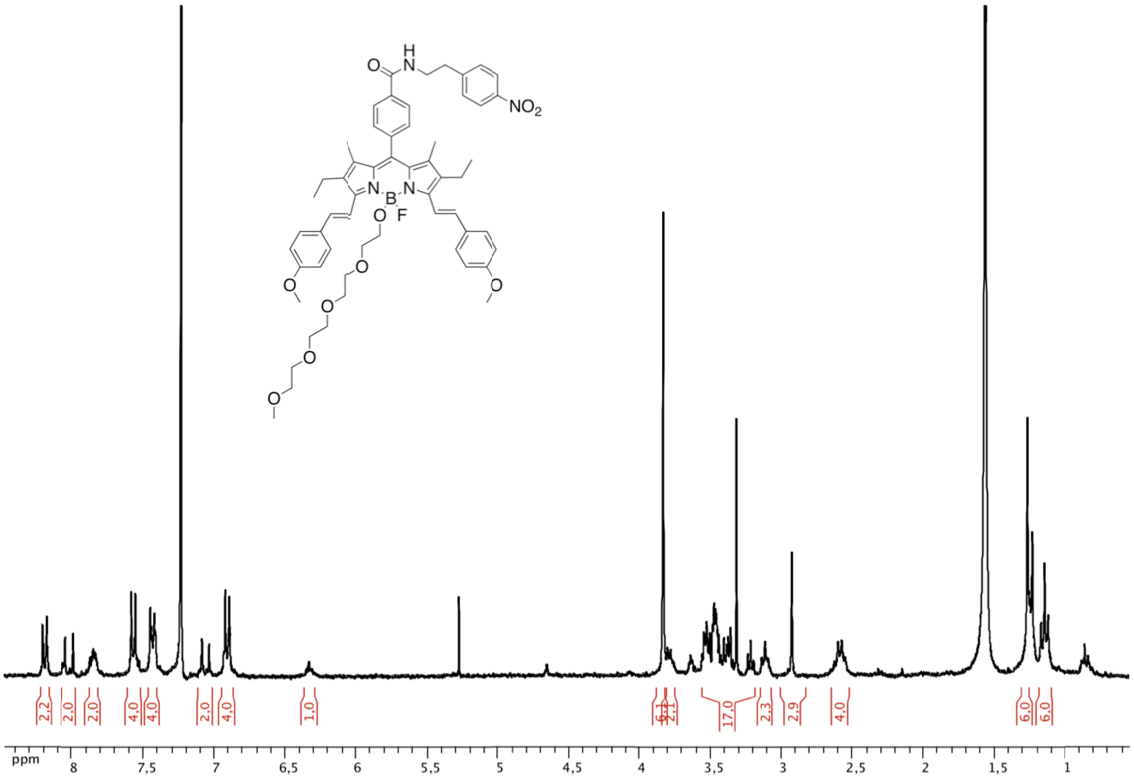

Figure 33: ^{1}H NMR spectrum of compound **15** in $CDCl_3$

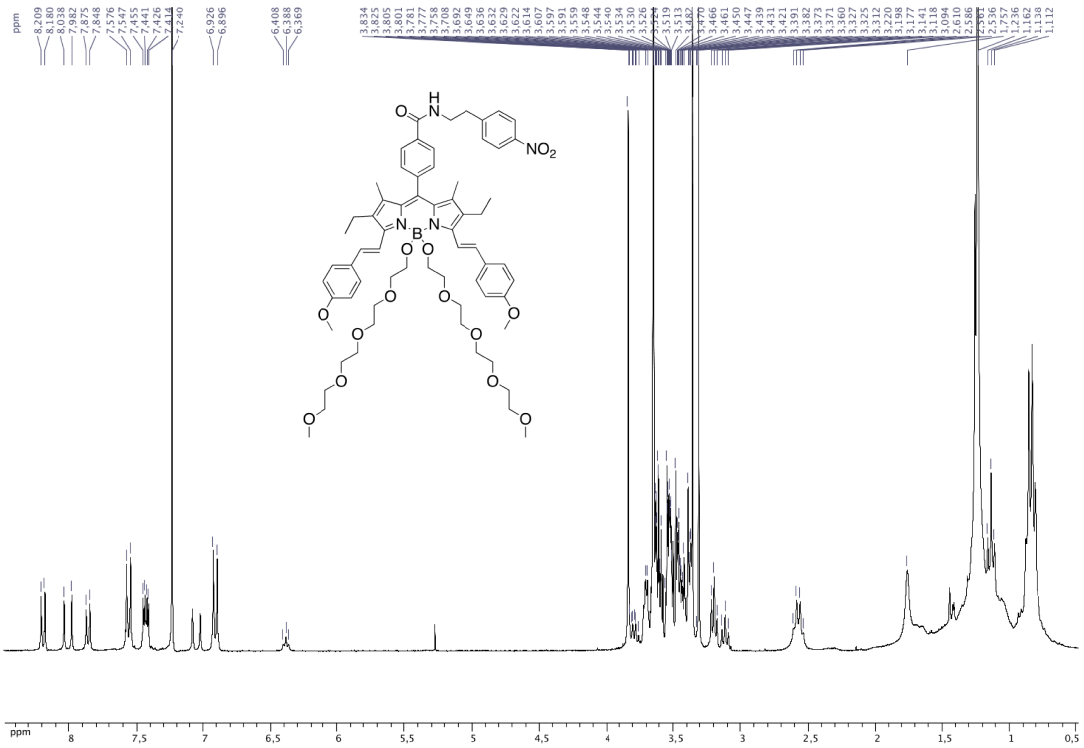

Figure 34: ^{1}H NMR spectrum of compound **16** in $CDCl_3$

X-Ray data of compound 3

X-ray equipment and refinement: diffraction data were collected on a Nonius Kappa Apex II diffractometer equipped with a nitrogen jet stream low-temperature system (Oxford Cryosystems). The X-ray source was graphite monochromated Mo-Kα1 radiation (λ = 0.71073 Å) from a sealed tube. The lattice parameters were obtained by least-squares fit to the optimized setting angles of the entire set of collected reflections. No significant temperature drift was observed during the data collections. Data were reduced by using DENZO software without applying absorption corrections, the missing absorption corrections were partially compensated by the data scaling procedure in the data reduction. The structure was solved by direct method using the SIR92 program. Refinements were carried out by full-matrix least-squares on F^2, using the SHELXL program on the complete set of reflections. Anisotropic thermal parameters were used for non-hydrogen atoms. All H atoms, on carbon atom or oxygen atom, were placed at calculated positions using a riding model with C-H = 0.95 (aromatic), 0.99 (methylene) or 0.98 (methyle) with $U_{iso}(H) = 1.2U_{eq}(CH)$, $U_{iso}(H) = 1.2U_{eq}(CH_2)$ or $U_{iso}(H) = 1.2U_{eq}(CH_3)$.

Table S1 Crystal data and structure refinement for **3**

Empirical formula	$C_{39}H_{39}N_2O_6B$
Formula weight	642.53
Temperature/K	115
Crystal system	triclinic
Space group	P-1
a/Å	10.8262(3)
b/Å	12.7507(4)
c/Å	14.1556(4)
α/°	86.5400(10)
β/°	68.923(2)
γ/°	65.630(2)
Volume/$Å^3$	1651.94(9)
Z	2
ρ_{calc}mg/mm^3	1.292
m/mm^{-1}	0.086
F(000)	680.0
Crystal size/mm^3	0.25 × 0.25 × 0.12
2Θ range for data collection	3.1 to 55.06°
Index ranges	$-14 \le h \le 14$, $-16 \le k \le 16$, $-18 \le l \le 18$
Reflections collected	14266
Independent reflections	7527[R(int) = 0.0305]
Data/restraints/parameters	7527/0/440
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	$R_1 = 0.0521$, $wR_2 = 0.1073$
Final R indexes [all data]	$R_1 = 0.0681$, $wR_2 = 0.1172$
Largest diff. peak/hole / e $Å^{-3}$	0.31/-0.22

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
C1	666.3(18)	3511.9(15)	1759.8(13)	18.5(3)
C2	-560.1(18)	4418.9(15)	2449.4(13)	18.2(3)
C3	-730.5(17)	4080.4(14)	3425.5(12)	16.8(3)
C4	403.7(17)	2953.7(14)	3314.9(12)	15.9(3)
C5	755.2(17)	2183.0(14)	4023.2(12)	15.8(3)
C6	1929.6(17)	1095.0(14)	3723.0(12)	16.5(3)
C7	2501.0(17)	179.9(14)	4290.7(12)	17.0(3)
C8	3720.7(18)	-690.0(14)	3592.2(13)	17.6(3)
C9	3870.2(17)	-316.8(14)	2612.5(13)	17.4(3)
C10	4998.9(19)	-982.9(15)	1622.5(13)	21.4(4)
C11	4752.5(19)	-1799.5(15)	3816.8(14)	21.1(4)
C12	5857(2)	-1623.6(17)	4150.3(16)	29.6(4)
C13	1932.9(19)	114.8(15)	5418.7(12)	20.9(4)
C14	-1889.3(19)	4787.0(15)	4394.7(13)	21.2(4)
C15	-1498.3(19)	5515.1(15)	2132.4(14)	22.8(4)
C16	-2637(2)	5375.6(18)	1819.1(16)	30.9(4)
C17	1321(2)	3515.8(17)	634.0(13)	24.7(4)
C18	-127.4(17)	2525.5(14)	5135.9(12)	16.1(3)
C19	-1334.2(18)	2276.8(15)	5595.5(13)	19.5(3)
C20	-2118.0(19)	2553.1(15)	6633.2(13)	20.2(3)
C21	-1716.1(18)	3093.1(14)	7222.0(12)	16.9(3)
C22	-512.4(19)	3350.2(16)	6760.4(13)	21.9(4)
C23	275.7(19)	3064.0(16)	5726.7(13)	20.6(4)
C24	-2578.1(19)	3453.7(15)	8335.3(13)	20.0(3)
C25	-4630(2)	3465.4(17)	9725.1(13)	28.2(4)
C26	4278.4(18)	2284.3(15)	2019.5(12)	17.8(3)
C27	3623.7(19)	3478.1(16)	2271.9(13)	22.6(4)
C28	4055(2)	3958.9(16)	2879.1(14)	23.9(4)
C29	5135.3(19)	3259.7(16)	3240.6(13)	22.4(4)
C30	5785(2)	2067.8(16)	2986.2(14)	25.1(4)
C31	5366.5(19)	1576.7(15)	2381.1(13)	22.2(4)
C32	5572(2)	3786.5(19)	3888.0(14)	28.7(4)
C33	1876.6(18)	329.2(15)	1032.4(12)	18.0(3)
C34	607.4(19)	474.5(16)	1869.0(13)	23.4(4)
C35	-142(2)	-173.6(17)	1858.3(14)	24.8(4)
C36	326.5(19)	-963.9(16)	1031.5(14)	23.2(4)
C37	1580(2)	-1097.0(16)	198.9(14)	25.1(4)
C38	2352.2(19)	-461.2(16)	205.3(13)	22.1(4)
C39	-480(2)	-1643.9(18)	1016.0(17)	31.5(4)
N1	1236.4(15)	2631.7(12)	2273.6(10)	16.5(3)
N2	2799.2(14)	746.2(12)	2691.1(10)	16.2(3)
O1	-2308.8(14)	3972.3(12)	8866.6(9)	26.4(3)
O2	-3689.8(14)	3145.4(11)	8662.5(9)	24.6(3)
O3	2695.5(13)	918.8(10)	956.1(8)	18.8(2)
O4	3925.1(12)	1797.1(10)	1379.7(8)	17.7(2)
O5	6458.3(19)	3246.2(15)	4271.3(12)	42.7(4)
O6	-1586.9(17)	-1592.8(14)	1694.3(13)	41.2(4)
B1	2665(2)	1513.9(16)	1809.0(14)	16.7(4)

Table S3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	19.2(8)	20.0(9)	18.6(8)	4.7(6)	-8.9(7)	-9.1(7)
C2	19.2(8)	17.8(8)	19.5(8)	3.8(6)	-8.7(7)	-8.5(7)
C3	15.8(8)	17.4(8)	18.2(8)	2.6(6)	-6.7(6)	-7.6(6)
C4	16.2(8)	18.1(8)	13.7(7)	1.0(6)	-4.1(6)	-8.4(6)
C5	15.2(8)	19.0(8)	15.1(8)	1.0(6)	-4.5(6)	-9.7(6)
C6	16.4(8)	19.0(8)	14.4(8)	1.3(6)	-4.3(6)	-8.6(7)
C7	16.7(8)	18.8(8)	17.2(8)	4.6(6)	-6.8(6)	-8.8(7)
C8	16.5(8)	16.5(8)	20.1(8)	3.2(6)	-6.2(6)	-8.0(7)
C9	16.2(8)	16.6(8)	19.9(8)	1.3(6)	-5.6(6)	-8.2(7)
C10	19.3(8)	19.7(9)	19.9(8)	-1.0(7)	-2.8(7)	-6.6(7)
C11	20.0(8)	15.6(8)	24.7(9)	3.1(7)	-8.8(7)	-4.3(7)
C12	26.2(10)	24.8(10)	37.2(11)	2.2(8)	-17.8(9)	-4.8(8)
C13	22.8(9)	20.6(9)	16.8(8)	5.6(7)	-7.1(7)	-7.4(7)
C14	22.5(9)	16.9(8)	20.9(8)	0.8(7)	-6.2(7)	-6.6(7)
C15	23.9(9)	19.0(9)	23.0(9)	6.3(7)	-9.6(7)	-6.4(7)
C16	28.6(10)	33.2(11)	32.8(11)	10.3(9)	-17.4(9)	-10.5(9)
C17	27.5(9)	26.6(10)	17.0(8)	6.4(7)	-7.6(7)	-9.8(8)
C18	16.3(8)	15.7(8)	14.3(8)	2.7(6)	-5.2(6)	-5.5(6)
C19	19.5(8)	23.4(9)	17.6(8)	0.6(7)	-6.2(7)	-11.1(7)
C20	19.8(8)	24.4(9)	17.7(8)	1.5(7)	-3.2(7)	-13.6(7)
C21	18.0(8)	16.7(8)	13.9(8)	2.6(6)	-5.3(6)	-6.0(6)
C22	24.1(9)	25.4(9)	18.7(8)	-0.5(7)	-7.2(7)	-12.9(7)
C23	19.2(8)	26.4(9)	18.4(8)	1.7(7)	-3.9(7)	-14.0(7)
C24	22.7(8)	17.8(8)	15.4(8)	3.2(6)	-5.7(7)	-6.1(7)
C25	29.8(10)	30.2(10)	16.2(9)	-2.4(7)	3.6(7)	-14.4(8)
C26	16.9(8)	22.1(9)	13.0(7)	1.8(6)	-1.6(6)	-10.2(7)
C27	22.1(9)	21.4(9)	23.4(9)	5.0(7)	-9.7(7)	-7.7(7)
C28	26.6(9)	19.0(9)	24.6(9)	0.4(7)	-9.6(7)	-8.0(7)
C29	23.8(9)	28.7(10)	18.5(8)	4.4(7)	-7.1(7)	-15.4(8)
C30	25.1(9)	25.4(10)	26.9(9)	8.1(7)	-14.5(8)	-9.1(8)
C31	22.7(9)	18.6(9)	23.4(9)	3.7(7)	-8.6(7)	-7.0(7)
C32	35.5(11)	38.8(11)	21.8(9)	7.9(8)	-10.9(8)	-25.2(9)
C33	17.3(8)	19.6(8)	17.8(8)	5.3(6)	-7.2(7)	-8.3(7)
C34	22.4(9)	29(1)	16.1(8)	-0.4(7)	-3.1(7)	-11.3(8)
C35	20.3(9)	33.8(11)	20.7(9)	6.4(7)	-5.3(7)	-14.2(8)
C36	22.7(9)	23.6(9)	27.9(9)	8.7(7)	-13.4(8)	-11.4(7)
C37	26.1(9)	22.0(9)	26.4(9)	-1.7(7)	-9.3(8)	-9.2(8)
C38	21.0(8)	23.8(9)	19.2(8)	0.1(7)	-4.7(7)	-9.3(7)
C39	32.1(10)	32.1(11)	40.9(11)	11.9(9)	-21.0(9)	-18.0(9)
N1	17.6(7)	17.3(7)	13.9(6)	1.7(5)	-5.0(5)	-7.4(6)
N2	14.8(6)	15.7(7)	15.4(7)	1.1(5)	-2.9(5)	-6.1(5)
O1	31.8(7)	29.4(7)	17.5(6)	-1.9(5)	-5.8(5)	-14.5(6)
O2	25.9(7)	30.6(7)	13.6(6)	-1.0(5)	0.7(5)	-14.5(6)
O3	19.7(6)	21.1(6)	14.2(5)	0.4(5)	-2.6(5)	-10.3(5)
O4	18.2(6)	21.0(6)	13.1(5)	1.1(5)	-2.5(5)	-10.1(5)
O5	62.0(11)	56.5(11)	43.3(9)	26.3(8)	-38.4(8)	-42.9(9)
O6	35.9(8)	49.7(10)	52.2(10)	18.7(8)	-20.0(7)	-29.8(8)
B1	15.8(8)	16.3(9)	14.4(8)	1.9(7)	-3.2(7)	-5.3(7)

Table S4 Bond Lengths for **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.411(2)	C22	C23	1.383(2)
C1	C17	1.494(2)	C24	O1	1.210(2)
C1	N1	1.350(2)	C24	O2	1.336(2)
C2	C3	1.393(2)	C25	O2	1.447(2)
C2	C15	1.506(2)	C26	C27	1.393(2)
C3	C4	1.425(2)	C26	C31	1.402(2)
C3	C14	1.499(2)	C26	O4	1.366(2)
C4	C5	1.401(2)	C27	C28	1.386(2)
C4	N1	1.402(2)	C28	C29	1.392(3)
C5	C6	1.396(2)	C29	C30	1.391(3)
C5	C18	1.497(2)	C29	C32	1.471(2)
C6	C7	1.428(2)	C30	C31	1.382(3)
C6	N2	1.401(2)	C32	O5	1.214(2)
C7	C8	1.391(2)	C33	C34	1.404(2)
C7	C13	1.502(2)	C33	C38	1.390(2)
C8	C9	1.414(2)	C33	O3	1.354(2)
C8	C11	1.499(2)	C34	C35	1.380(2)
C9	C10	1.495(2)	C35	C36	1.392(3)
C9	N2	1.350(2)	C36	C37	1.394(3)
C11	C12	1.531(2)	C36	C39	1.468(3)
C15	C16	1.527(3)	C37	C38	1.386(2)
C18	C19	1.392(2)	C39	O6	1.216(2)
C18	C23	1.393(2)	N1	B1	1.555(2)
C19	C20	1.386(2)	N2	B1	1.551(2)
C20	C21	1.391(2)	O3	B1	1.448(2)
C21	C22	1.395(2)	O4	B1	1.465(2)
C21	C24	1.497(2)			

Table S5 Bond Angles for **3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	C17	126.61(15)	O1	C24	O2	124.44(16)
N1	C1	C2	109.76(14)	O2	C24	C21	111.50(14)
N1	C1	C17	123.55(15)	C27	C26	C31	119.90(16)
C1	C2	C15	123.92(15)	O4	C26	C27	120.71(15)
C3	C2	C1	107.46(15)	O4	C26	C31	119.31(15)
C3	C2	C15	128.59(16)	C28	C27	C26	119.69(16)
C2	C3	C4	106.78(14)	C27	C28	C29	120.63(17)
C2	C3	C14	125.70(15)	C28	C29	C32	119.78(17)
C4	C3	C14	127.52(15)	C30	C29	C28	119.42(16)
C5	C4	C3	132.27(15)	C30	C29	C32	120.80(17)
C5	C4	N1	119.78(15)	C31	C30	C29	120.58(17)
N1	C4	C3	107.94(14)	C30	C31	C26	119.78(17)
C4	C5	C18	119.93(14)	O5	C32	C29	124.5(2)
C6	C5	C4	121.76(15)	C38	C33	C34	119.37(16)
C6	C5	C18	118.30(14)	O3	C33	C34	124.69(16)
C5	C6	C7	131.98(15)	O3	C33	C38	115.94(14)
C5	C6	N2	120.23(14)	C35	C34	C33	119.46(17)
N2	C6	C7	107.79(14)	C34	C35	C36	121.44(16)
C6	C7	C13	128.53(15)	C35	C36	C37	118.85(16)
C8	C7	C6	106.83(14)	C35	C36	C39	121.41(17)
C8	C7	C13	124.64(15)	C37	C36	C39	119.74(18)
C7	C8	C9	107.47(15)	C38	C37	C36	120.27(17)
C7	C8	C11	127.33(15)	C37	C38	C33	120.59(16)
C9	C8	C11	125.13(15)	O6	C39	C36	125.3(2)
C8	C9	C10	126.62(15)	C1	N1	C4	108.05(14)
N2	C9	C8	109.60(14)	C1	N1	B1	126.11(14)
N2	C9	C10	123.76(15)	C4	N1	B1	125.52(13)
C8	C11	C12	112.12(14)	C6	N2	B1	125.45(14)
C2	C15	C16	112.89(15)	C9	N2	C6	108.29(13)
C19	C18	C5	120.19(14)	C9	N2	B1	125.85(14)
C19	C18	C23	119.38(15)	C24	O2	C25	117.02(14)
C23	C18	C5	120.40(14)	C33	O3	B1	124.62(13)
C20	C19	C18	120.21(15)	C26	O4	B1	118.69(12)
C19	C20	C21	120.34(15)	N2	B1	N1	106.39(13)
C20	C21	C22	119.47(15)	O3	B1	N1	112.95(14)
C20	C21	C24	121.78(15)	O3	B1	N2	112.34(14)
C22	C21	C24	118.70(15)	O3	B1	O4	104.07(13)
C23	C22	C21	120.07(16)	O4	B1	N1	110.57(13)
C22	C23	C18	120.52(15)	O4	B1	N2	110.60(13)
O1	C24	C21	124.05(16)				

Table S6 Torsion Angles for **3**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	-0.39(18)	C17	C1	C2	C15	5.9(3)
C1	C2	C3	C14	179.22(15)	C17	C1	N1	C4	176.04(15)
C1	C2	C15	C16	82.2(2)	C17	C1	N1	B1	2.3(3)
C1	N1	B1	N2	-176.71(14)	C18	C5	C6	C7	0.2(3)
C1	N1	B1	O3	-53.0(2)	C18	C5	C6	N2	-178.97(14)
C1	N1	B1	O4	63.2(2)	C18	C19	C20	C21	0.8(3)
C2	C1	N1	C4	-0.86(18)	C19	C18	C23	C22	0.0(3)
C2	C1	N1	B1	-174.63(14)	C19	C20	C21	C22	-0.3(3)
C2	C3	C4	C5	-178.50(17)	C19	C20	C21	C24	177.10(16)
C2	C3	C4	N1	-0.12(18)	C20	C21	C22	C23	-0.3(3)
C3	C2	C15	C16	-95.5(2)	C20	C21	C24	O1	-176.47(17)
C3	C4	C5	C6	178.78(17)	C20	C21	C24	O2	2.7(2)
C3	C4	C5	C18	-2.0(3)	C21	C22	C23	C18	0.4(3)
C3	C4	N1	C1	0.61(18)	C21	C24	O2	C25	-178.78(14)
C3	C4	N1	B1	174.42(14)	C22	C21	C24	O1	0.9(3)
C4	C5	C6	C7	179.38(16)	C22	C21	C24	O2	-179.93(15)
C4	C5	C6	N2	0.2(2)	C23	C18	C19	C20	-0.6(3)
C4	C5	C18	C19	90.7(2)	C24	C21	C22	C23	-177.78(16)
C4	C5	C18	C23	-91.2(2)	C26	C27	C28	C29	-0.1(3)
C4	N1	B1	N2	10.6(2)	C26	O4	B1	N1	63.96(18)
C4	N1	B1	O3	134.27(15)	C26	O4	B1	N2	-53.62(19)
C4	N1	B1	O4	-109.57(16)	C26	O4	B1	O3	-174.48(13)
C5	C4	N1	C1	179.23(14)	C27	C26	C31	C30	0.0(3)
C5	C4	N1	B1	-7.0(2)	C27	C26	O4	B1	-86.23(19)
C5	C6	C7	C8	-177.95(17)	C27	C28	C29	C30	0.1(3)
C5	C6	C7	C13	2.7(3)	C27	C28	C29	C32	-179.70(16)
C5	C6	N2	C9	178.37(14)	C28	C29	C30	C31	0.0(3)
C5	C6	N2	B1	5.3(2)	C28	C29	C32	O5	176.92(18)
C5	C18	C19	C20	177.48(16)	C29	C30	C31	C26	0.0(3)
C5	C18	C23	C22	-178.07(16)	C30	C29	C32	O5	-2.9(3)
C6	C5	C18	C19	-90.09(19)	C31	C26	C27	C28	0.1(3)
C6	C5	C18	C23	88.0(2)	C31	C26	O4	B1	97.08(18)
C6	C7	C8	C9	-1.09(18)	C32	C29	C30	C31	179.74(17)
C6	C7	C8	C11	175.94(16)	C33	C34	C35	C36	-0.5(3)
C6	N2	B1	N1	-9.7(2)	C33	O3	B1	N1	-71.55(19)
C6	N2	B1	O3	-133.81(15)	C33	O3	B1	N2	48.8(2)
C6	N2	B1	O4	110.38(17)	C33	O3	B1	O4	168.49(13)
C7	C6	N2	C9	-0.97(18)	C34	C33	C38	C37	0.4(3)
C7	C6	N2	B1	-174.01(14)	C34	C33	O3	B1	19.4(3)
C7	C8	C9	C10	-177.91(15)	C34	C35	C36	C37	-0.1(3)
C7	C8	C9	N2	0.52(19)	C34	C35	C36	C39	-179.32(17)
C7	C8	C11	C12	-79.2(2)	C35	C36	C37	C38	0.8(3)
C8	C9	N2	C6	0.29(18)	C35	C36	C39	O6	-0.3(3)
C8	C9	N2	B1	173.30(14)	C36	C37	C38	C33	-1.0(3)
C9	C8	C11	C12	97.4(2)	C37	C36	C39	O6	-179.54(19)
C9	N2	B1	N1	178.42(14)	C38	C33	C34	C35	0.3(3)
C9	N2	B1	O3	54.3(2)	C38	C33	O3	B1	-161.22(15)
C9	N2	B1	O4	-61.5(2)	C39	C36	C37	C38	-179.90(17)
C10	C9	N2	C6	178.77(15)	N1	C1	C2	C3	0.79(19)
C10	C9	N2	B1	-8.2(2)	N1	C1	C2	C15	-177.33(15)
C11	C8	C9	C10	5.0(3)	N1	C4	C5	C6	0.6(2)
C11	C8	C9	N2	-176.60(15)	N1	C4	C5	C18	179.74(14)
C13	C7	C8	C9	178.24(15)	N2	C6	C7	C8	1.27(18)
C13	C7	C8	C11	-4.7(3)	N2	C6	C7	C13	-178.03(15)
C14	C3	C4	C5	1.9(3)	O1	C24	O2	C25	0.3(3)

C14	C3	C4	N1	-179.72(15)	O3	C33	C34	C35	179.71(16)
C15	C2	C3	C4	177.61(16)	O3	C33	C38	C37	-179.00(16)
C15	C2	C3	C14	-2.8(3)	O4	C26	C27	C28	-176.59(15)
C17	C1	C2	C3	-175.99(16)	O4	C26	C31	C30	176.68(15)

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3**.

Atom	***x***	***y***	***z***	**U(eq)**
H10A	4773	-1601	1456	32
H10B	5960	-1322	1678	32
H10C	5003	-462	1084	32
H11A	5282	-2362	3200	25
H11B	4188	-2130	4362	25
H12A	6469	-1353	3593	44
H12B	6472	-2359	4326	44
H12C	5337	-1046	4745	44
H13A	2496	-656	5573	31
H13B	904	256	5651	31
H13C	2028	702	5768	31
H14A	-2523	5527	4237	32
H14B	-1432	4931	4827	32
H14C	-2471	4365	4753	32
H15A	-866	5762	1554	27
H15B	-2001	6133	2705	27
H16A	-2147	4764	1253	46
H16B	-3199	6106	1606	46
H16C	-3295	5167	2398	46
H17A	2076	2741	331	37
H17B	1756	4074	486	37
H17C	560	3735	346	37
H19	-1622	1916	5197	23
H20	-2934	2373	6944	24
H22	-234	3722	7157	26
H23	1099	3236	5417	25
H25A	-4055	3450	10130	42
H25B	-5070	2916	9957	42
H25C	-5400	4247	9808	42
H27	2885	3961	2029	27
H28	3610	4773	3050	29
H30	6523	1587	3231	30
H31	5815	762	2211	27
H32	5131	4607	4015	34
H34	267	1015	2438	28
H35	-996	-78	2428	30
H37	1907	-1626	-375	30
H38	3214	-567	-361	26
H39	-107	-2166	428	38

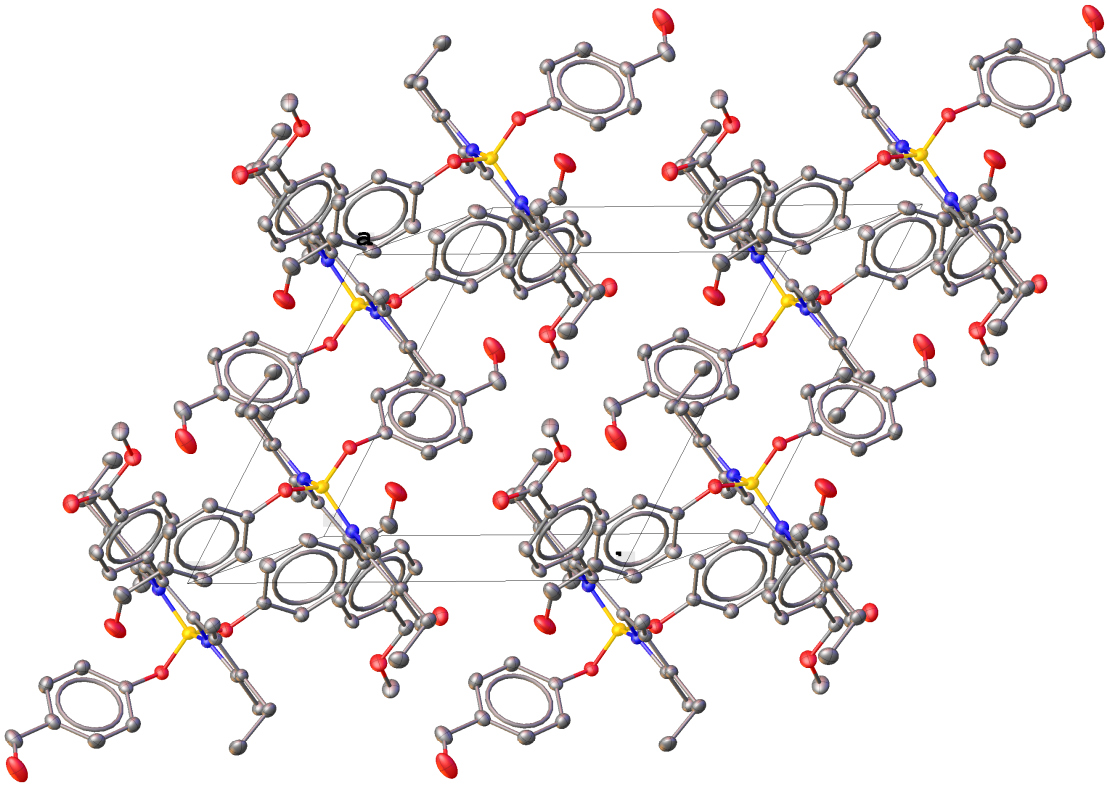

Figure 35: View of crystal packing in **3**.