Zinc(II) Sulfanyltribenzoporphyrazines with Bulky Peripheral Substituents—Synthesis, Photophysical Characterization, and Potential Photocytotoxicity

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Supplementary Materials

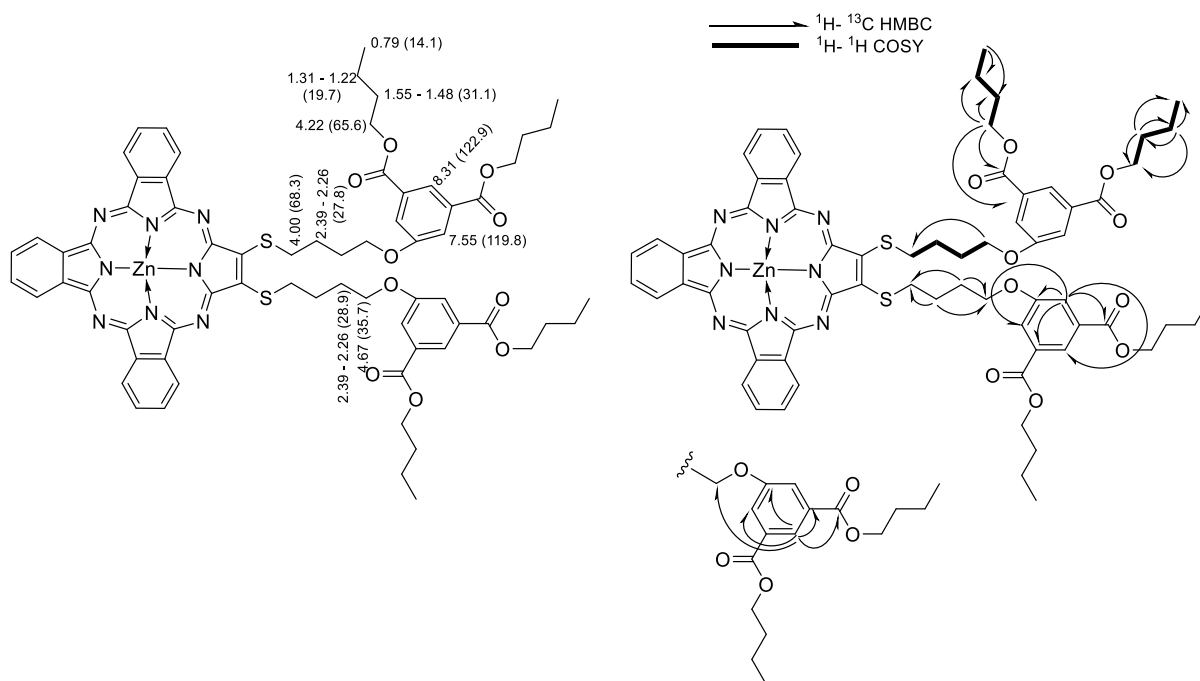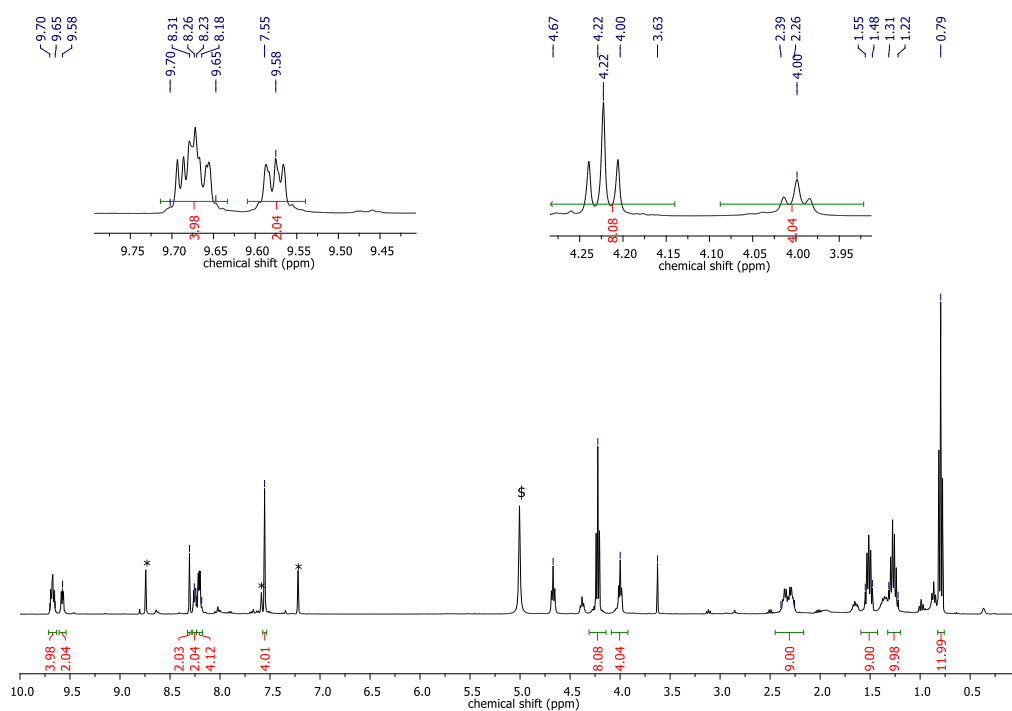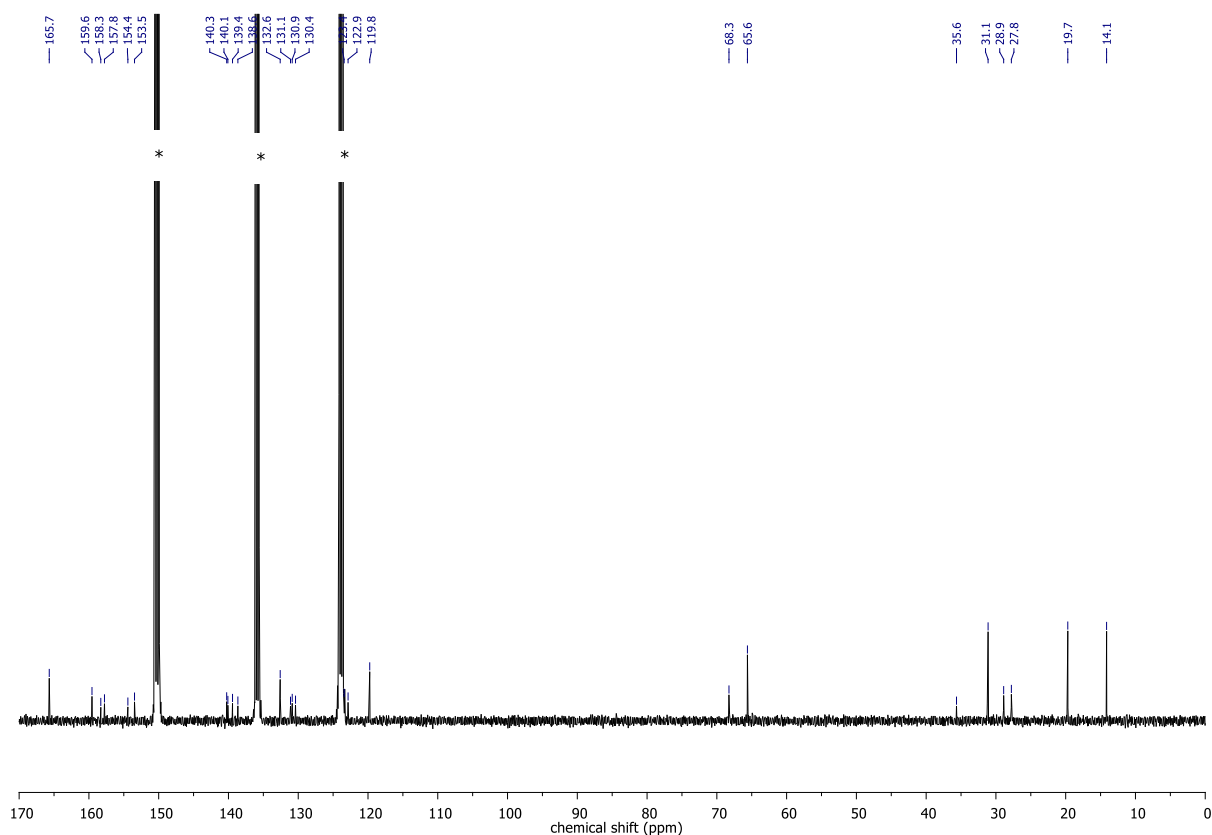NMR data for 22,23-bis[4-(3,5-dibutoxycarbonylphenoxy)butylthio]-tribenzo[b,g,l]porphyrazinato zinc (II) (6)

Figure S1. NMR data of **6**: ^{1}H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^{1}H-^{1}H COSY; Arrows: ^{1}H-^{13}C HMBC.

Table S1. ^{1}H and ^{13}C NMR data obtained for **6** including key correlations determined from ^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC spectra.

δ$_H$ (ppm)	Multiplicity (J$_{H-H}$ in Hz)	^{1}H-^{13}C HSQC δ$_C$ (ppm)	^{1}H-^{13}C HMBC δ$_C$ (ppm)
9.65 – 9.70	m	123.4	130.9, 131.1
9.58	2 × d (8)	122.9	130.4
8.31	s	122.9	140.1, 140.2, 165.7
8.26	2 × d (5.5)	130.9, 131.1	119.6, 139.4
8.18 – 8.23	m	130.4	122.9, 123.4, 138.7
7.55	s	119.8	122.9, 132.6, 159.6, 165.7
4.67	t (7)	35.7	27.8, 138.7
4.22	t (7)	65.6	19.7, 31.1, 165.7
4.00	t (6)	68.3	27.8, 28.9
2.26 – 2.39	m	27.8 28.9	35.7, 68.3
1.48 – 1.55	m	31.1	
1.22 – 1.31	m	19.7	14.1, 19.7, 65.6
0.79	t (7)	14.1	19.7, 31.1

^{1}H NMR spectrum of **6**. The symbols * and $ indicate pyridine-d_5 and water residual peaks, respectively.

^{13}C NMR spectrum recorded for **6**. The symbol * indicates pyridine-d_5 residual peaks.

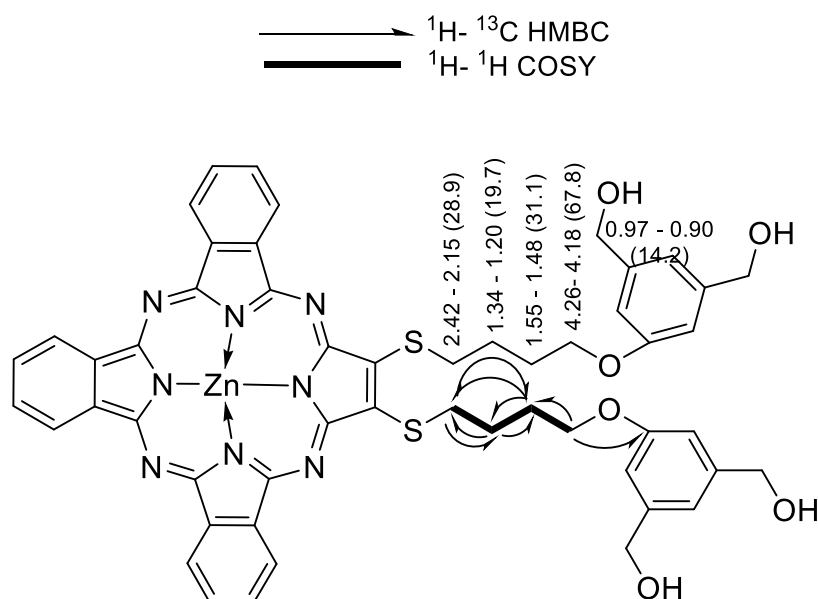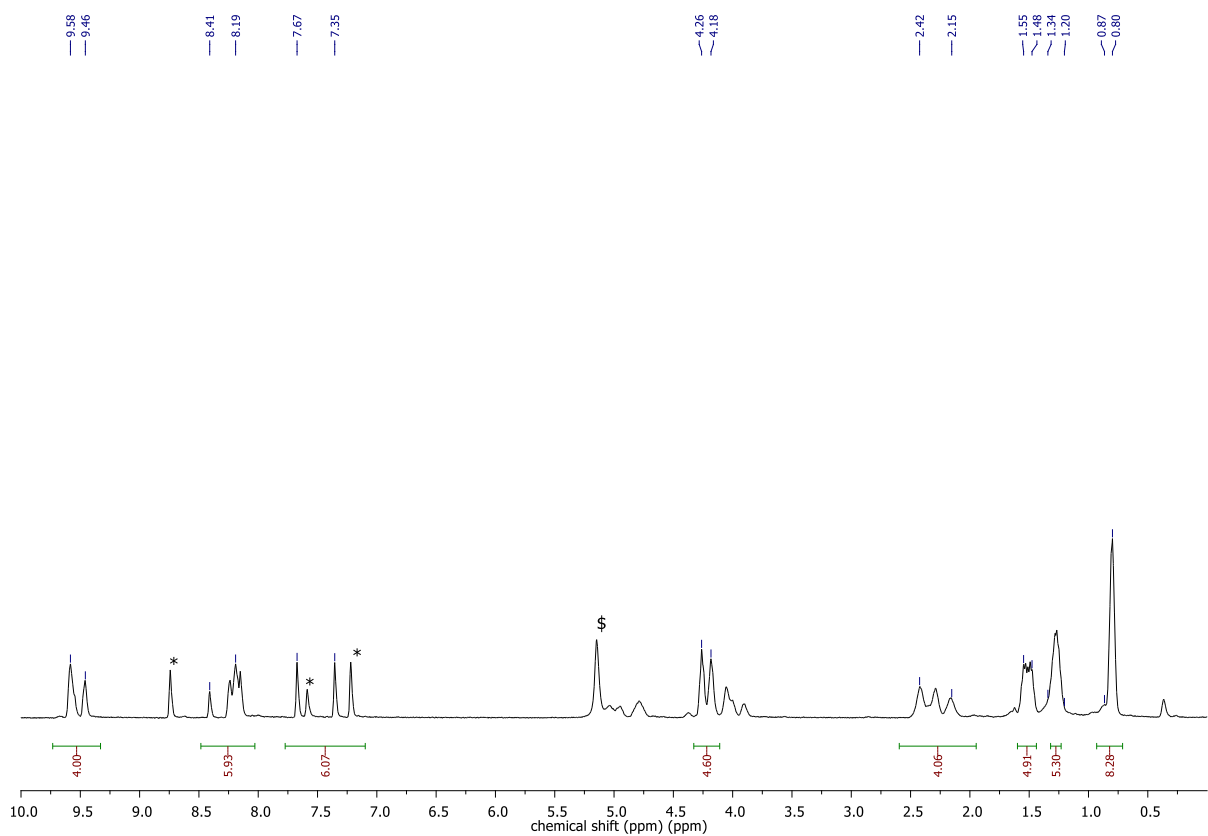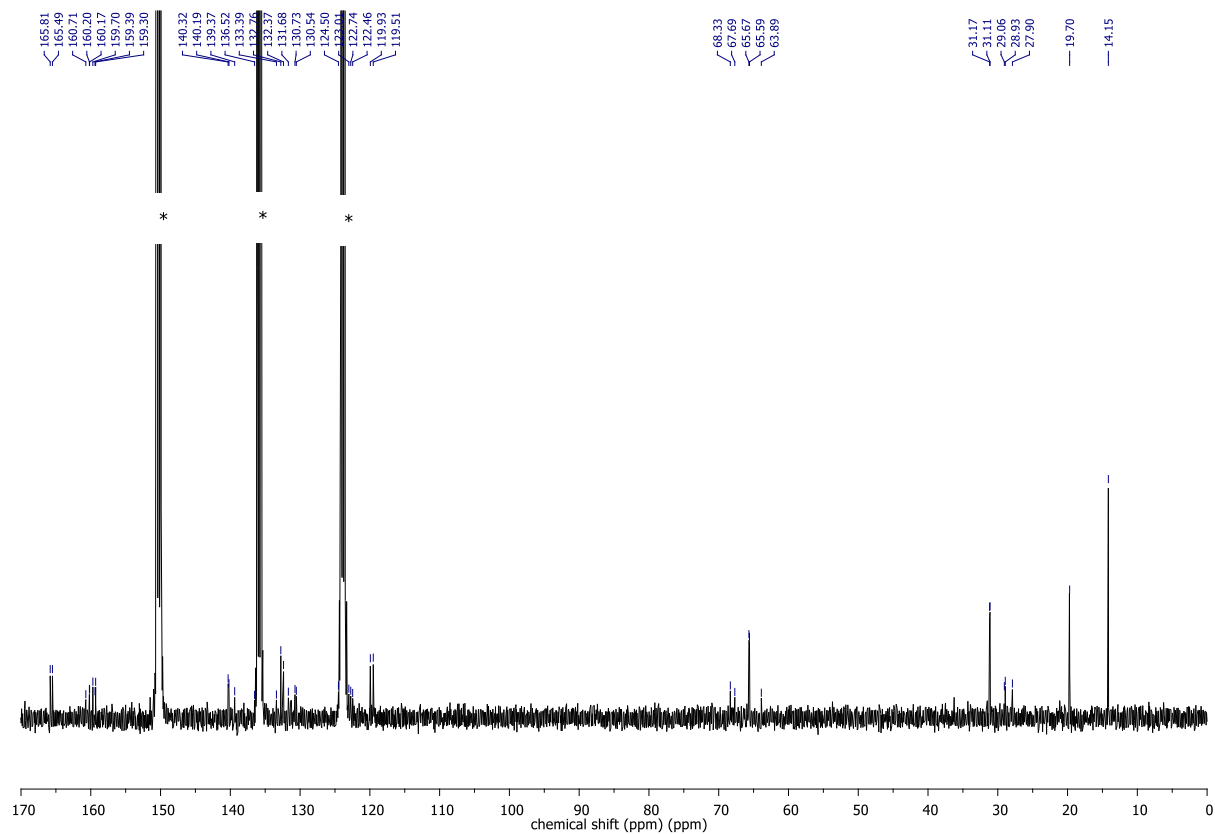NMR data for 22,23-bis{4-[3,5-di(hydroxymethyl)phenoxy]butylthio}tribenzo[b,g,l]porphyrazinato zinc (II) **7**

Figure S2. NMR data of **7**: ^{1}H and (^{13}C) chemical shift values [ppm] and key correlations observed in NMR spectra. Bold lines: ^{1}H-^{1}H COSY; Arrows: ^{1}H-^{13}C HMBC.

Table S2. ^{1}H and ^{13}C NMR data obtained for **7** including key correlations determined from ^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC spectra.

δ_H (ppm)	Multiplicity (J_{H-H} in Hz)	^{1}H-^{13}C HSQC δ_C (ppm)	^{1}H-^{13}C HMBC δ_C (ppm)
9.46 – 9.58	m	123.0, 124.5	14.2, 130.6, 130.7, 139.4
8.19 – 8.41	m	122.5, 122.7	19.7, 65.8, 139.4, 140.1, 140.3, 165.5
7.35 – 7.67	m	119.5, 119.9	122.5, 122.7, 132.3, 159.3, 159.7, 165.5, 165.8
4.18 – 4.26	m	67.8	65.6, 68.3
2.15 – 2.42	m	27.9, 28.9, 29.1	19.7, 31.1, 165.5, 165.8
1.48 – 1.55	m	31.2	14.2, 19.7, 65.6, 155.0
1.20 – 1.34	m	19.7	14.2, 31.1, 65.6
0.90 - 0.97	m	14.2	19.7, 31.1
Other carbon atoms: 160.7, 160.2, 159.4, 136.5, 133.4, 132.8, 131.7, 63.9.			

^{1}H NMR spectrum of **7**. The symbols * and $ indicate pyridine-d_5 and water residual peaks, respectively.

^{13}C NMR spectrum recorded for **7**. The symbol * indicates pyridine-d_5 residual peaks.