

**Cross-Coupling as a Key Step in the Synthesis and Structure Revision of the Natural
Products Selagibenzophenones A and B.**

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Figure S1. Numbering of selagibenzophenone A and B, and key HMBC correlations for selagibenzophenone B

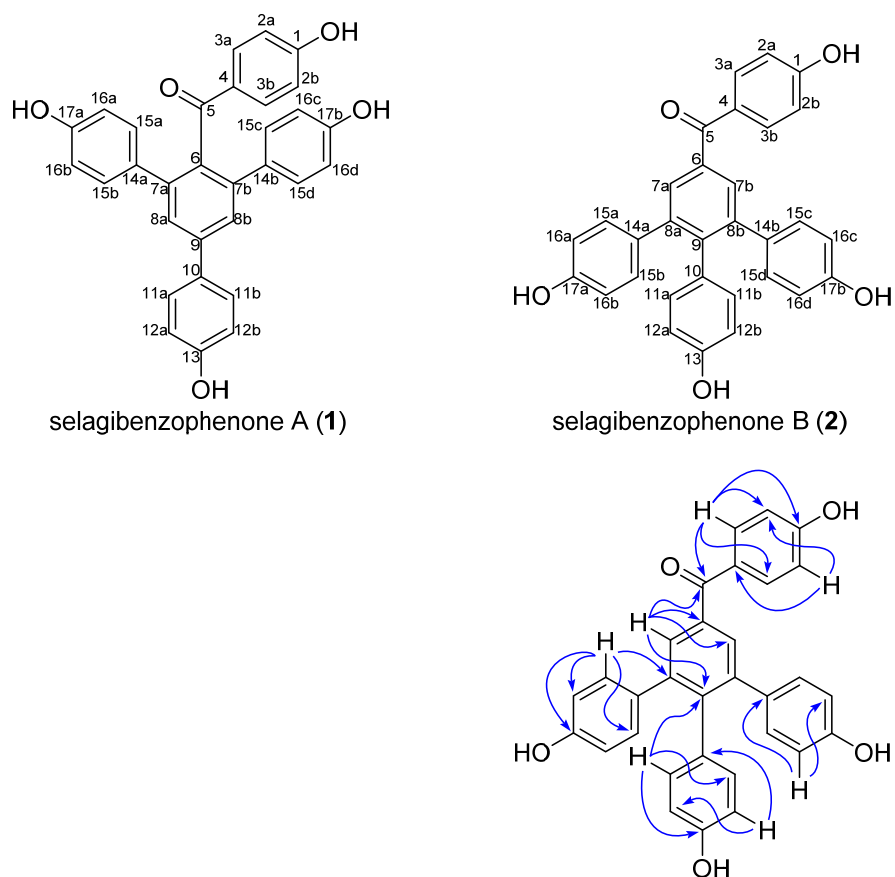


Table S1. Comparison of synthetic and isolated selagibenzophenone A and B

Position	Synthetic compounds				Reported values as was assigned in publications					
	Selagibenzophenone A		Selagibenzophenone B		Selagibenzophenone A (Liu, Tang, 2017)		Selagibenzophenone B			
	¹ H NMR	¹³ C NMR	¹ H NMR	¹³ C NMR	¹ H NMR	¹³ C NMR	Wang, Yao, 2018		Liu, Zou, 2020	
							¹ H NMR	¹³ C NMR	¹ H NMR	¹³ C NMR
1	-	163.8	-	170.5	-	165.9	-	163.6	-	162.2
2a/b	6.59	116.0	6.76	118.2	6.55	116.6	6.59	115.9	6.61	114.5
3a/b	7.41	133.2	7.77	134.6	7.38	133.6	7.37	133.5	7.42	132.0
4	-	131.6	-	126.5	-	130.6	-	131.6	-	130.2
5	-	200.7	-	197.5	-	200.5	-	200.7	-	199.2
6	-	137.6	-	138.8	-	137.8	-	137.5	-	136.2
7a/b	-	142.4	7.58	131.0	-	142.4	7.47	127.6	7.51	126.2
8a/b	7.50	127.6	-	143.4	7.49	127.6	-	142.4	-	141.0
9	-	143.0	-	143.7	-	142.9	-	132.7	-	141.6
10	-	132.8	-	131.9	-	132.8	-	143.0	-	131.4
11a/b	7.58	129.3	6.66	133.7	7.56	129.3	7.51	129.3	7.58	127.8
12a/b	6.90	116.8	6.48	115.4	6.89	116.8	6.87	116.8	6.91	115.4
13	-	158.8	-	156.9	-	158.7	-	158.7	-	157.3
14a/b	-	133.5	-	134.2	-	133.3	-	133.2	-	131.8
15a/b/c/d	7.10	131.5	6.91	132.0	7.10	131.4	7.07	131.4	7.11	130.0
16a/b/c/d	6.63	115.8	6.59	115.6	6.63	115.8	6.61	115.8	6.65	114.4
17a/b	-	157.9	-	157.2	-	157.8	-	157.8	-	156.4

Figure S2. ^1H NMR spectra of compound **10** in CDCl_3 (400 MHz)

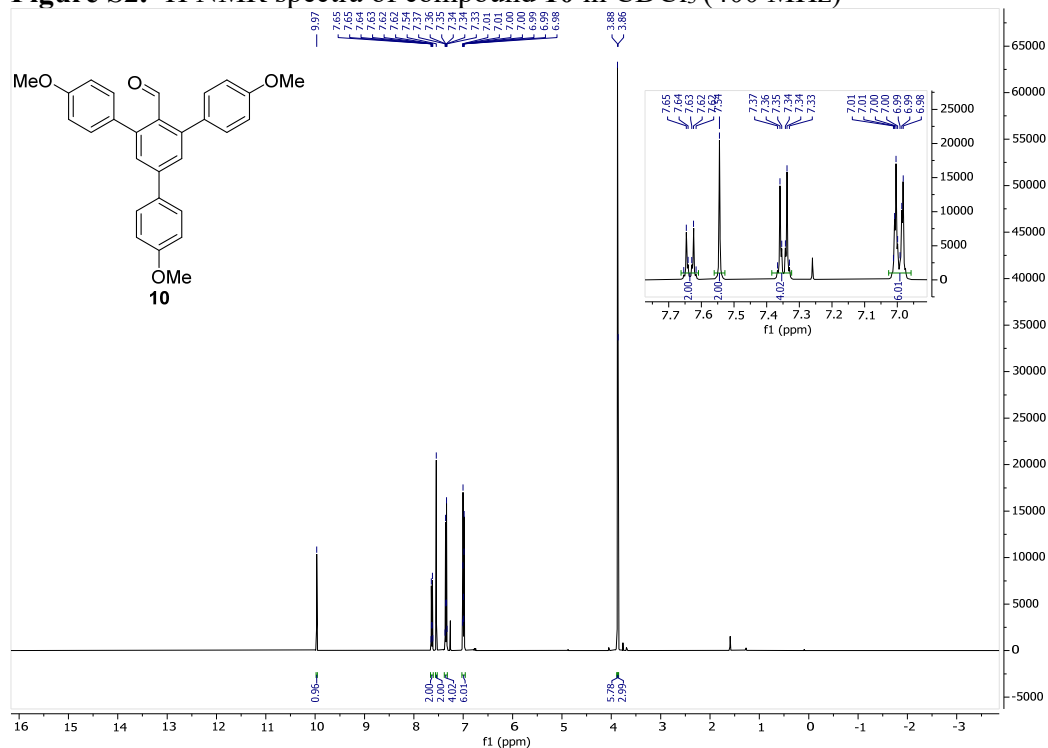
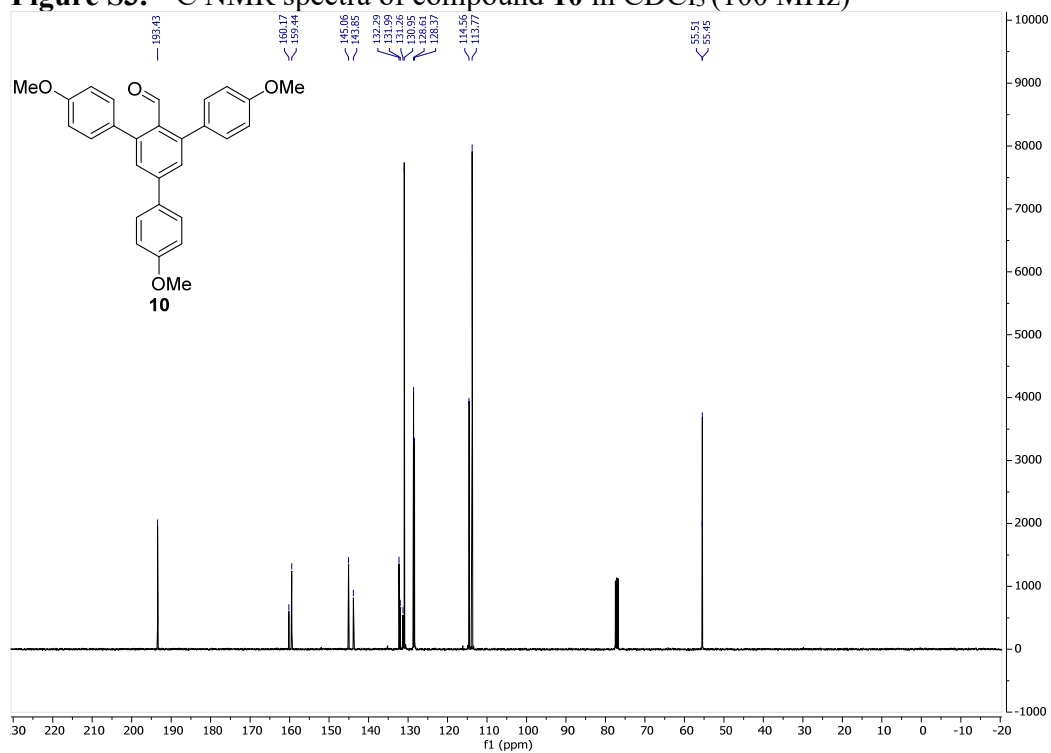


Figure S3. ^{13}C NMR spectra of compound **10** in CDCl_3 (100 MHz)



Chemical structure of compound **12** is shown in the top left. The ¹H NMR spectrum (CDCl₃) is displayed below, with the chemical shift (f1, ppm) on the x-axis (ranging from 16 to -3) and the intensity on the y-axis (ranging from -2000 to 38000). The spectrum shows several peaks in the aromatic region (6.5-7.8 ppm), a large peak at 3.8 ppm (methoxy protons), and a small peak at 2.1 ppm (hydroxyl proton). An inset shows the aromatic region (6.5-7.8 ppm) with peak labels and integrations.

Figure S5. ¹³C NMR spectra of compound 12 in CDCl₃ (100 MHz).

Chemical structure of compound 12 is shown. The spectrum displays peaks corresponding to the carbon atoms in the molecule, with the following chemical shifts (ppm) labeled above the peaks:

- 159.48
- 158.72
- 158.14
- 142.77
- 138.07
- 137.62
- 136.00
- 134.01
- 133.55
- 130.75
- 128.79
- 128.23
- 126.72
- 114.38
- 113.22
- 72.29
- 55.46
- 55.41

Figure S6. ^1H NMR spectra of compound **13** in CDCl_3 (400 MHz)

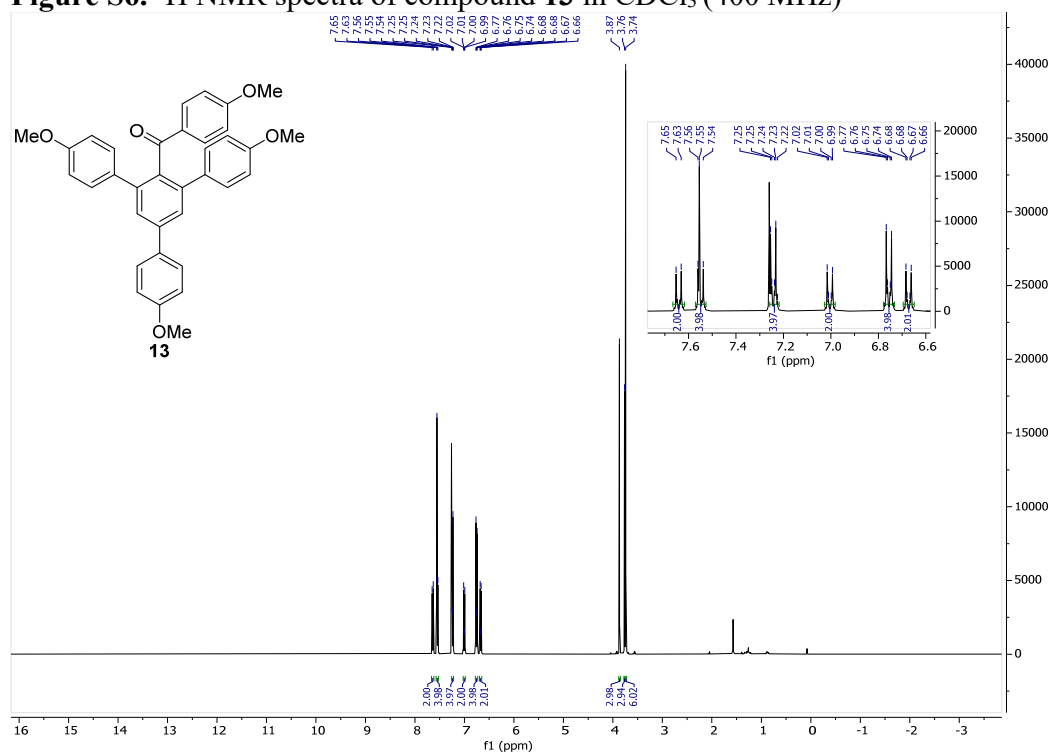


Figure S7. ^{13}C NMR spectra of compound **13** in CDCl_3 (100 MHz)

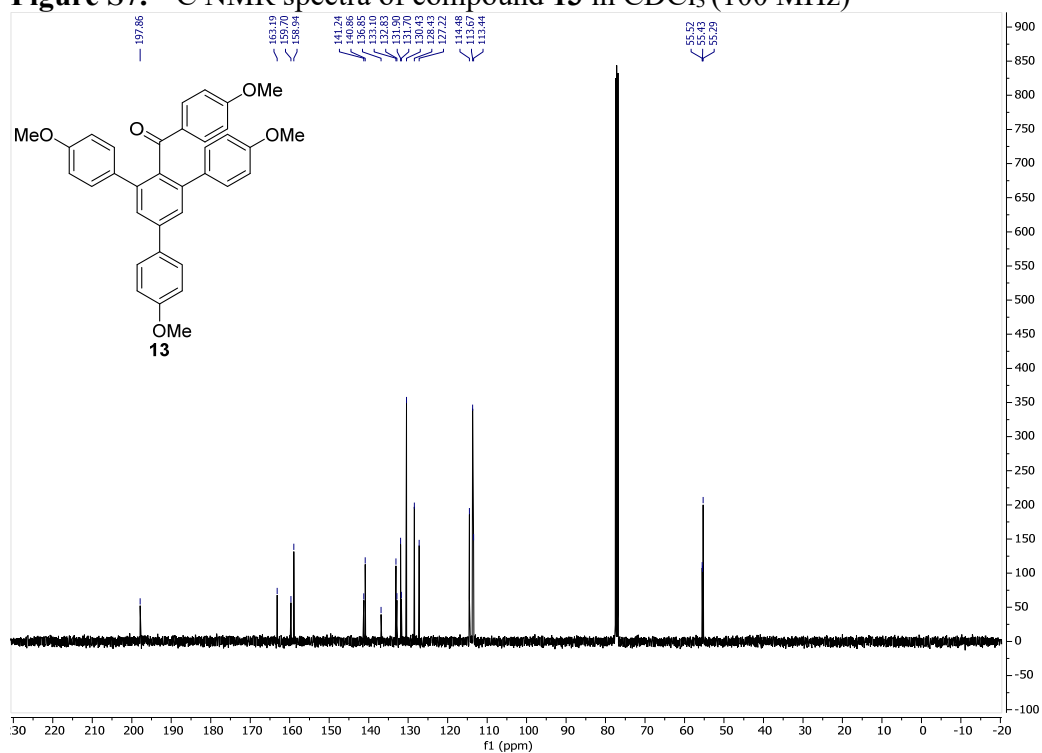


Figure S8. ^1H NMR spectra of compound **14** in $\text{MeOD-}d_4$ (600 MHz)

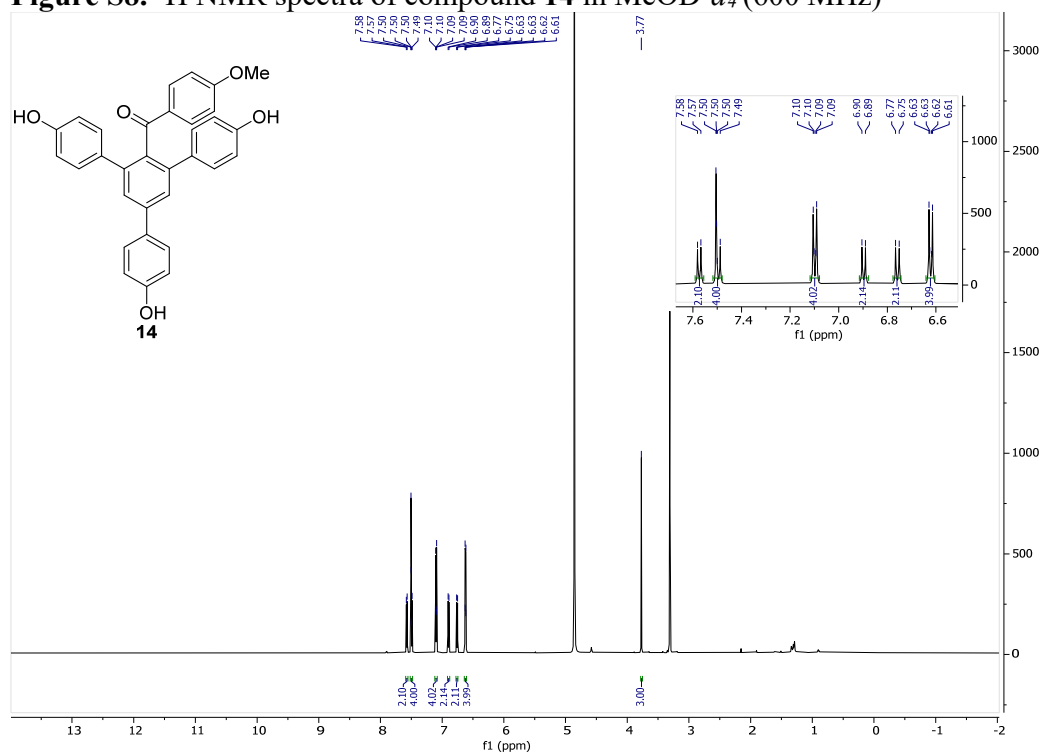


Figure S10. ^1H NMR spectra of selagibenzophenone A (**1**) in $\text{MeOD-}d_4$ (400 MHz)

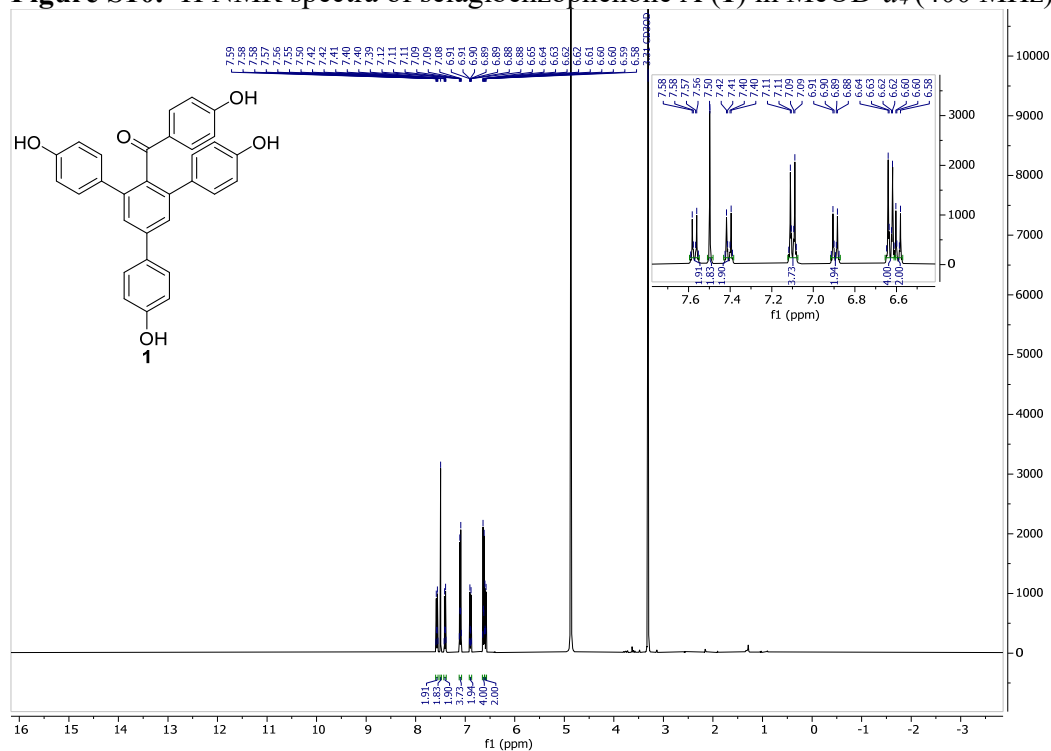


Figure S12. COSY spectra of selagibenzophenone A (**1**) in MeOD-*d*₄

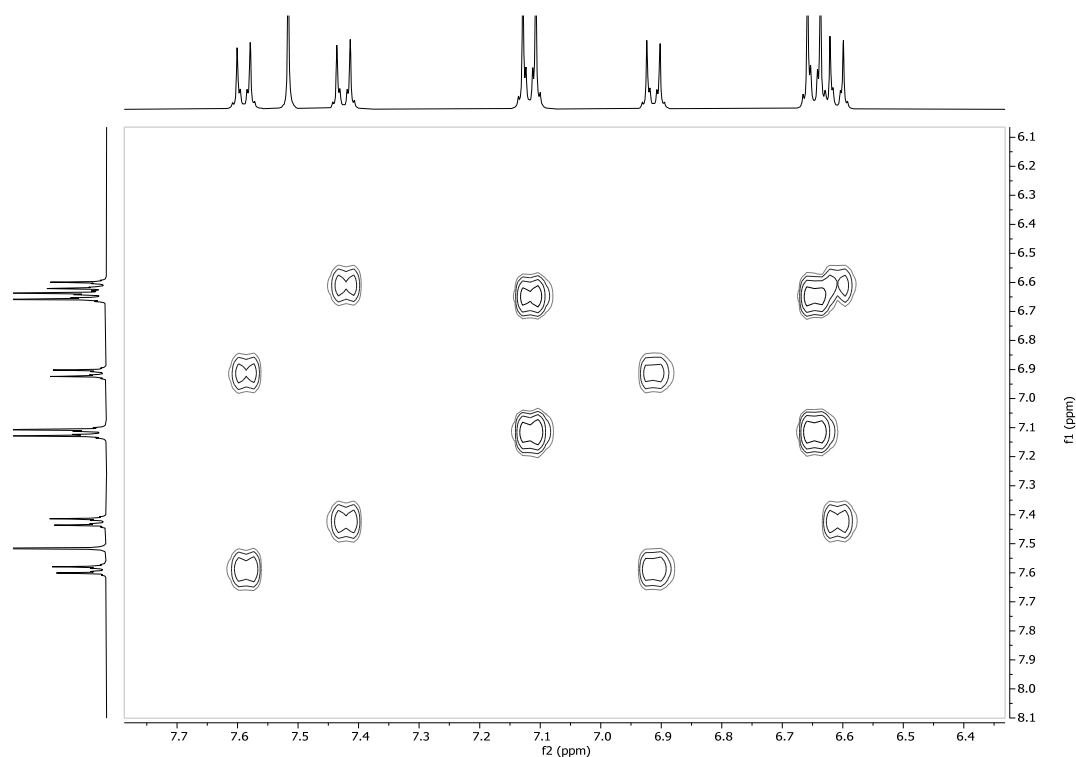


Figure S13. HSQC spectra of selagibenzophenone A (**1**) in MeOD-*d*₄

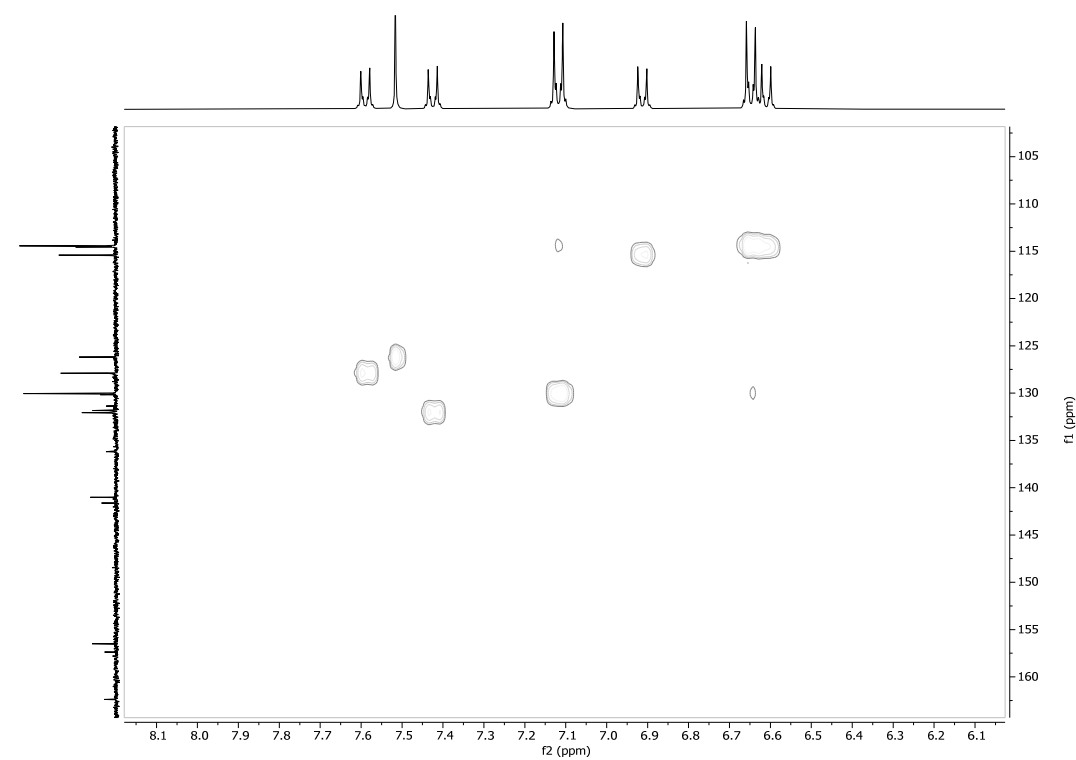


Figure S 14. HSQC spectra of selagibenzophenone A (**1**) in MeOD-*d*₄

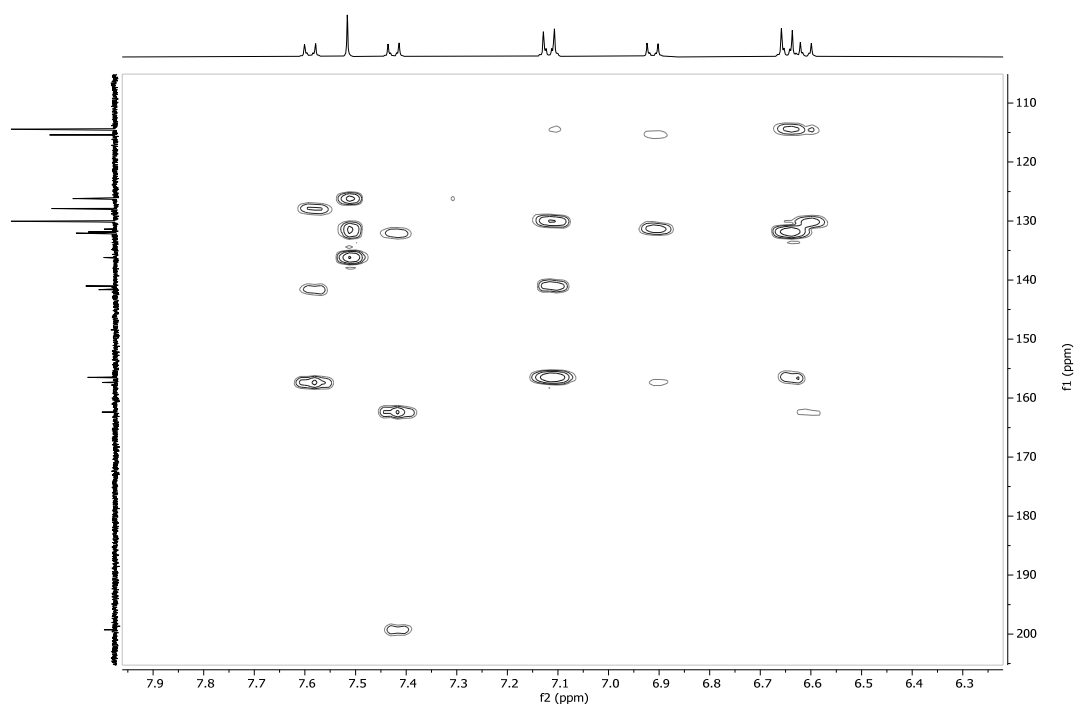
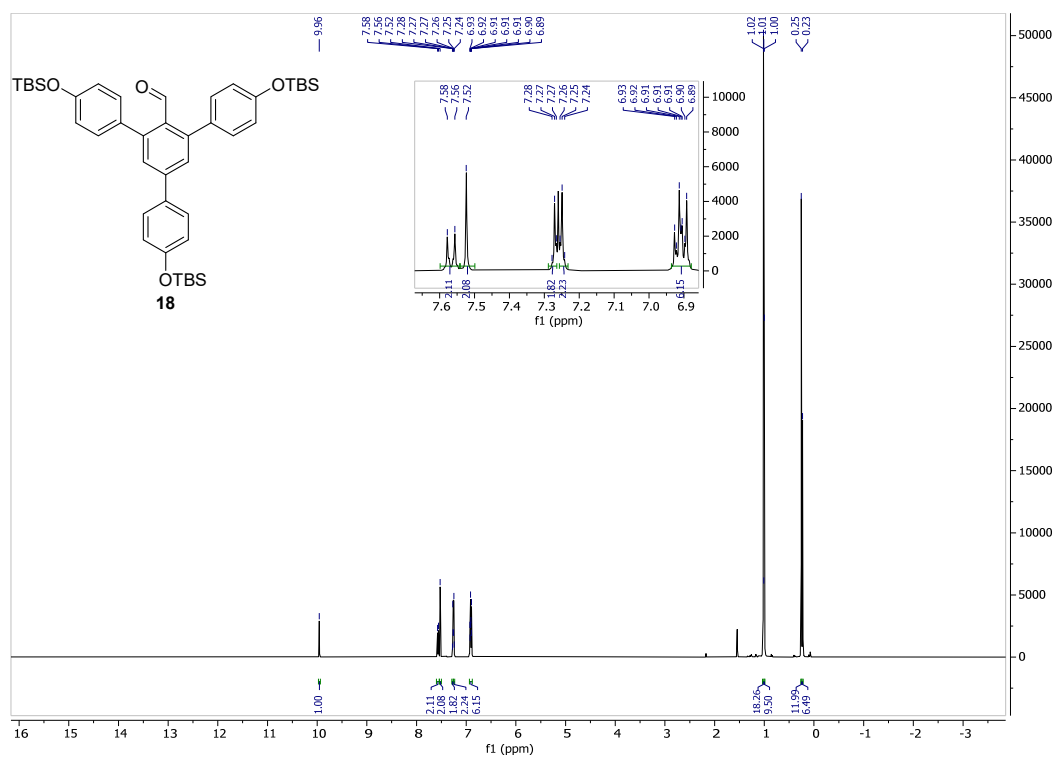


Figure S15. ¹H NMR spectra of compound **18** in CDCl₃ (400 MHz)



Chemical structure of compound **18** is shown above the spectrum. The structure is a substituted benzene ring with a vinyl group, a TBSO group, and two phenyl rings, one of which is substituted with a TBSO group.

¹³C NMR spectrum (CDCl₃) of compound **18**. The x-axis represents the chemical shift in ppm (f1), ranging from 30 to -20. The y-axis represents intensity, ranging from -500 to 4500. The spectrum shows several peaks, with the following chemical shifts (ppm) labeled:

- 193.52
- 145.08
- 143.84
- 132.93
- 132.65
- 131.93
- 130.93
- 128.62
- 128.42
- 120.72
- 119.83
- 77.16 CDCl₃
- 25.84
- 18.41
- 18.36
- 4.19
- 4.22

Figure S18. ^{13}C NMR spectra of compound **19** in CDCl_3 (100 MHz)

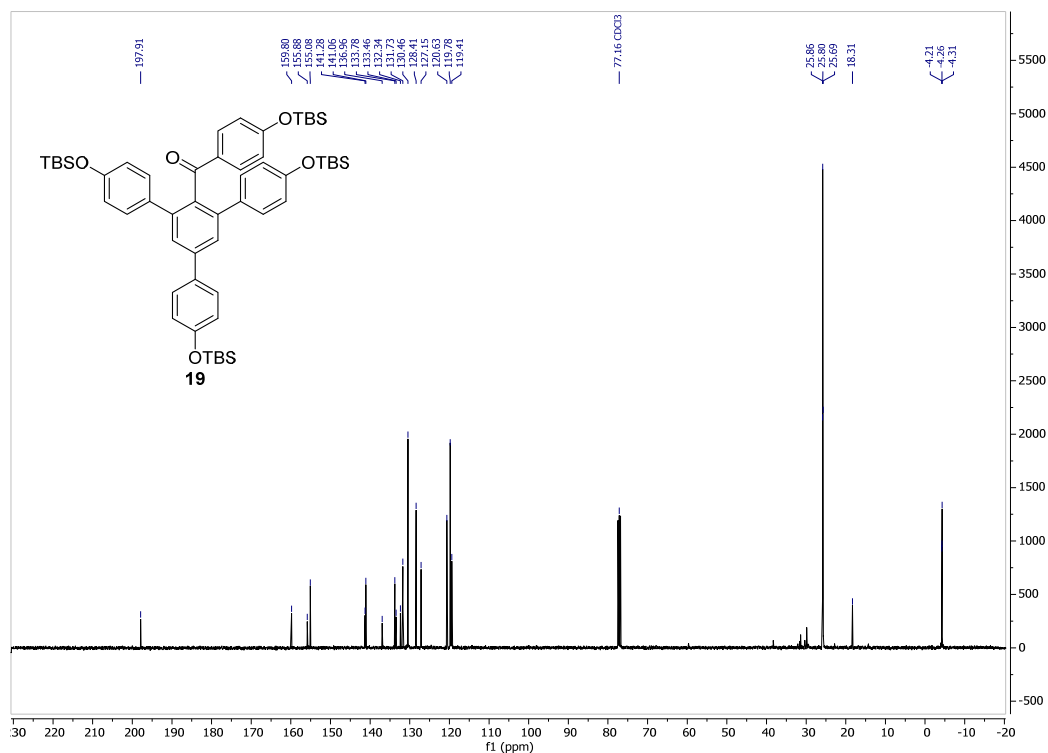


Figure S19. ^1H NMR spectra of compound **20** in CDCl_3 (300 MHz)

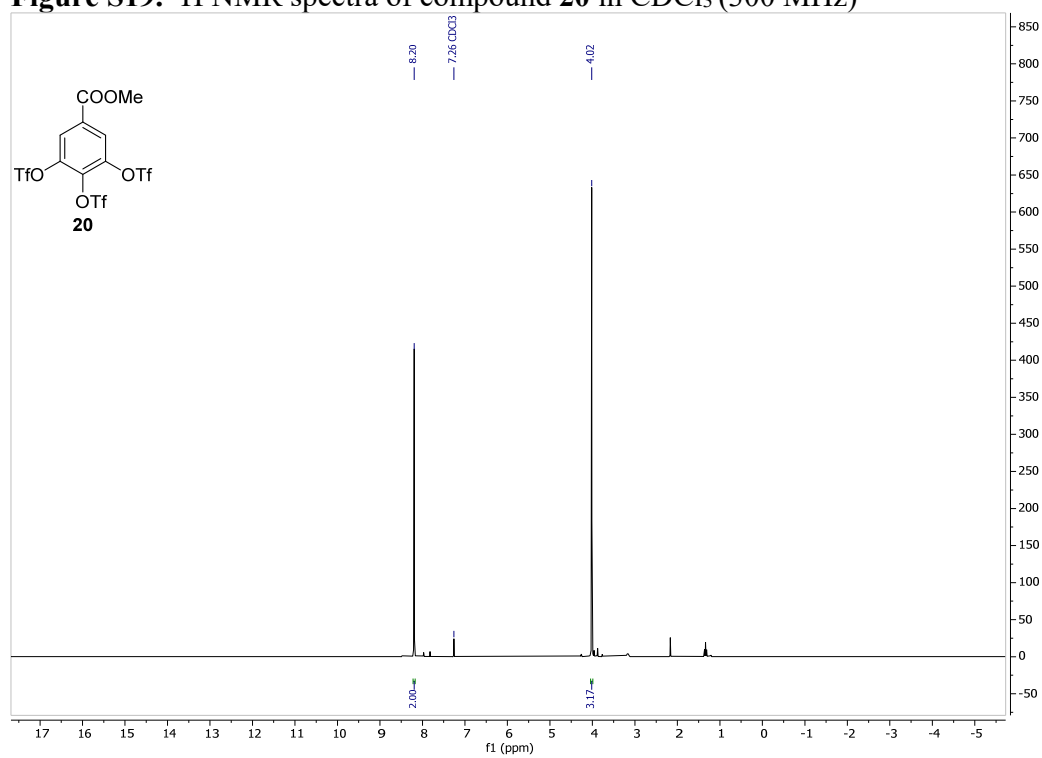


Figure S20. ^{13}C NMR spectra of compound **20** in CDCl_3 (75 MHz)

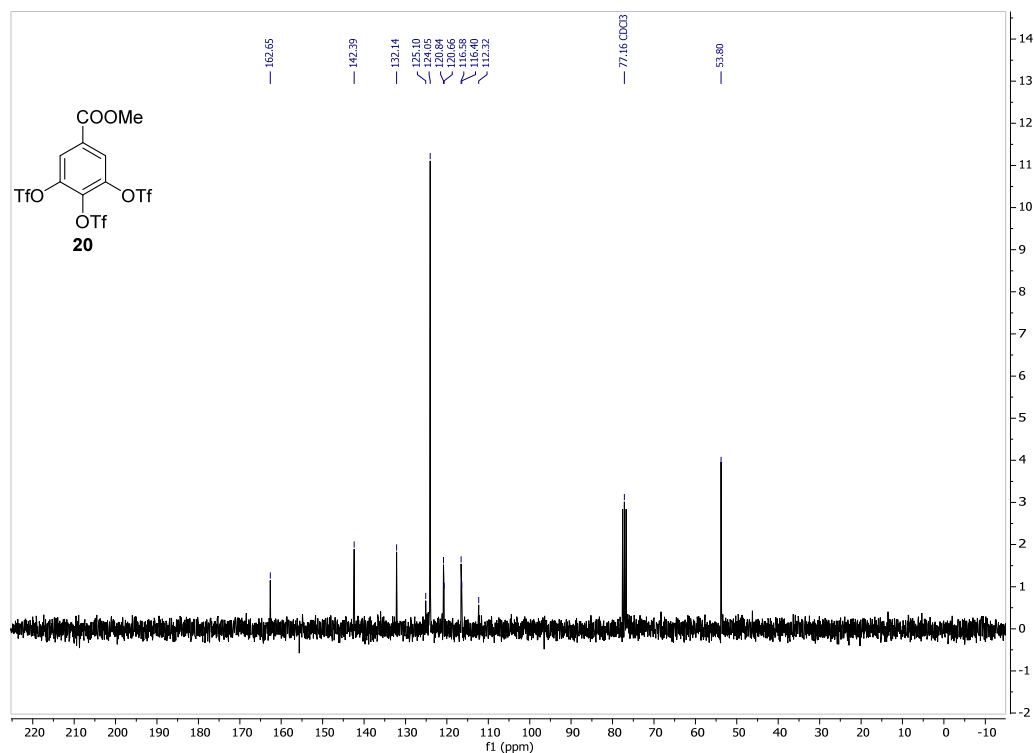


Figure S21. ^1H NMR spectra of compound **21** in CDCl_3 (400 MHz)

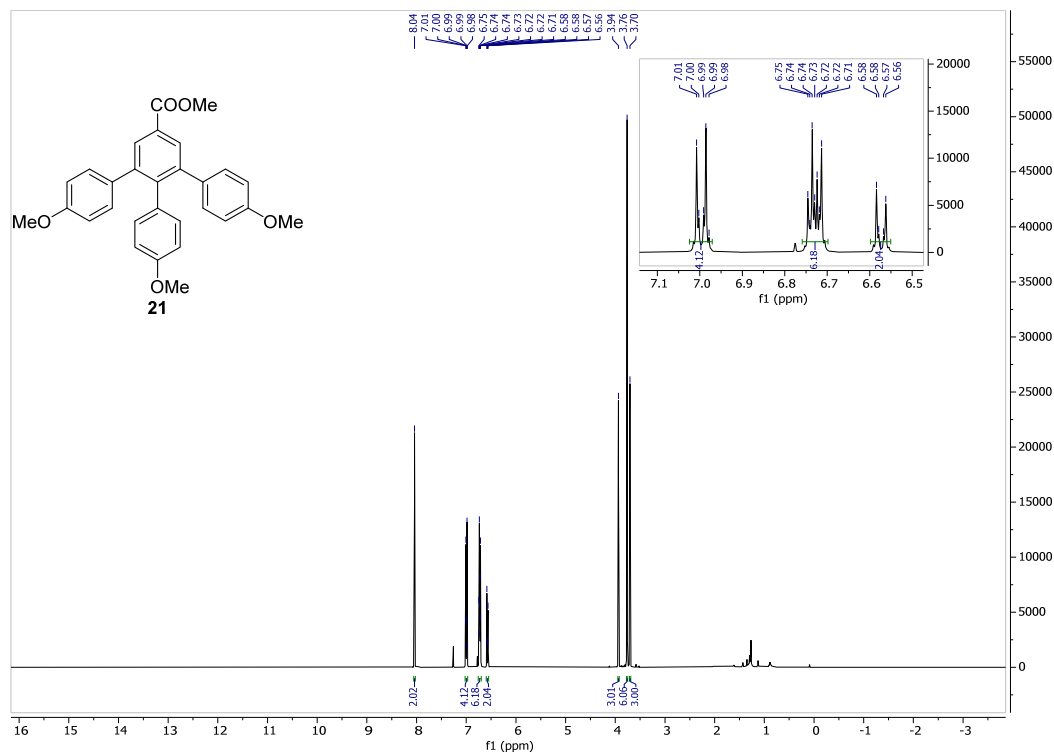


Figure S22. ^{13}C NMR spectra of compound **21** in CDCl_3 (100 MHz)

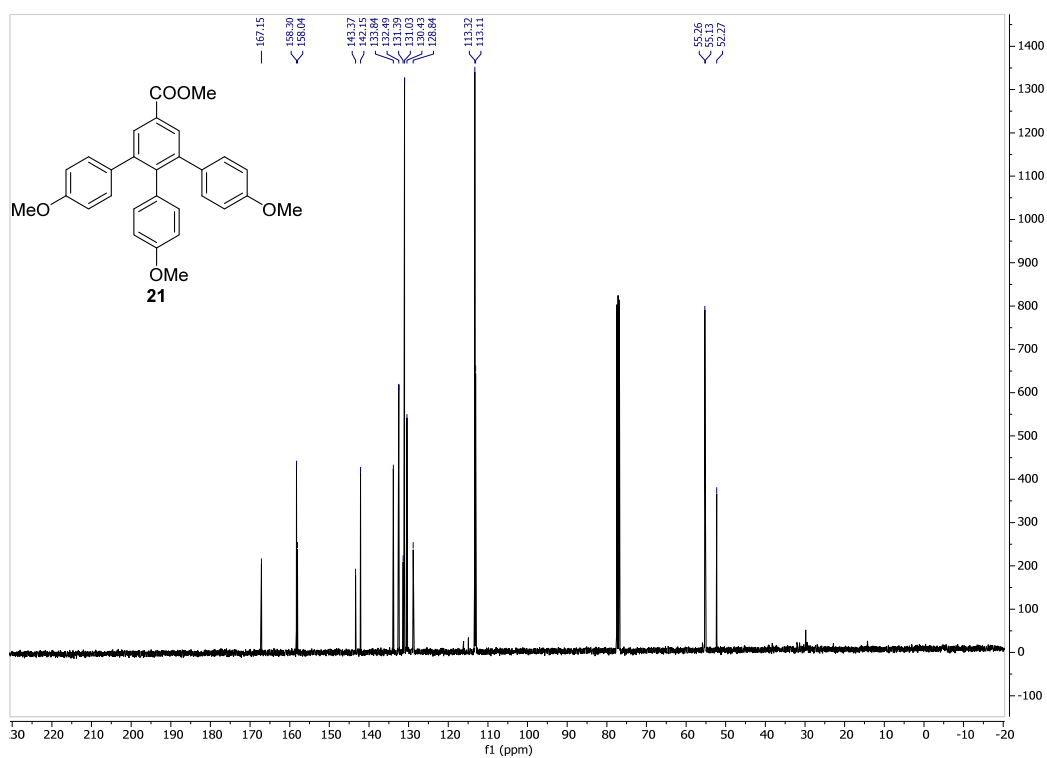


Figure S23. ¹H NMR spectra of compound **22** in CDCl₃ (400 MHz)

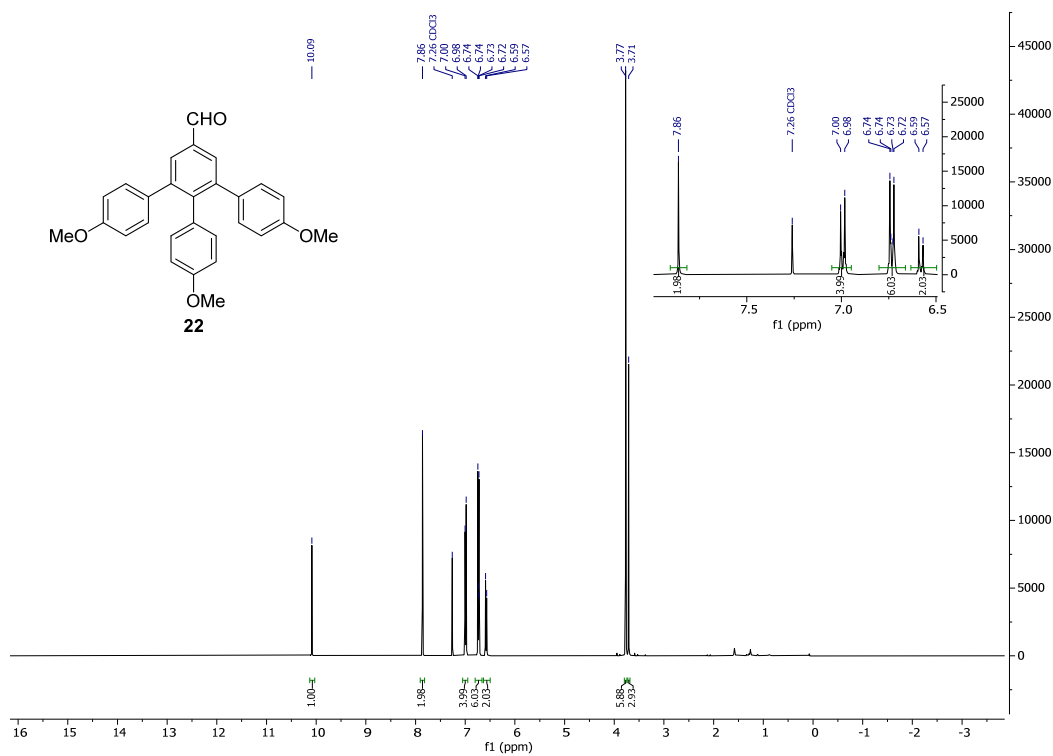


Figure S24. ^{13}C NMR spectra of compound **22** in CDCl_3 (100 MHz)

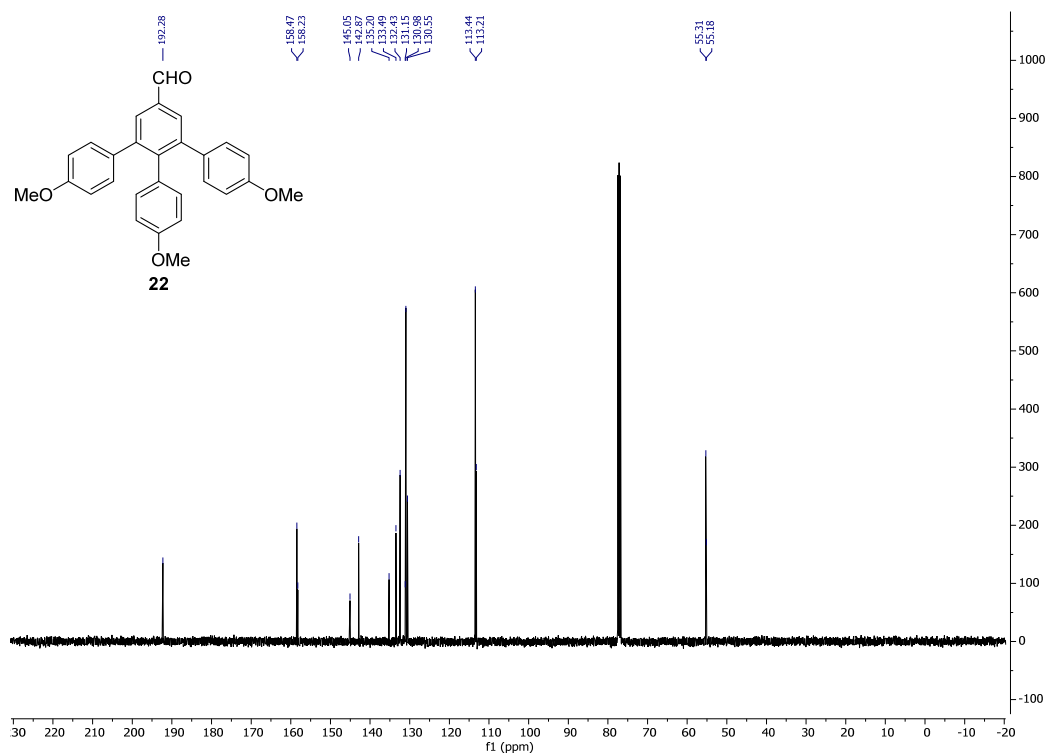


Figure S25. ^1H NMR spectra of compound **23** in CDCl_3 (400 MHz)

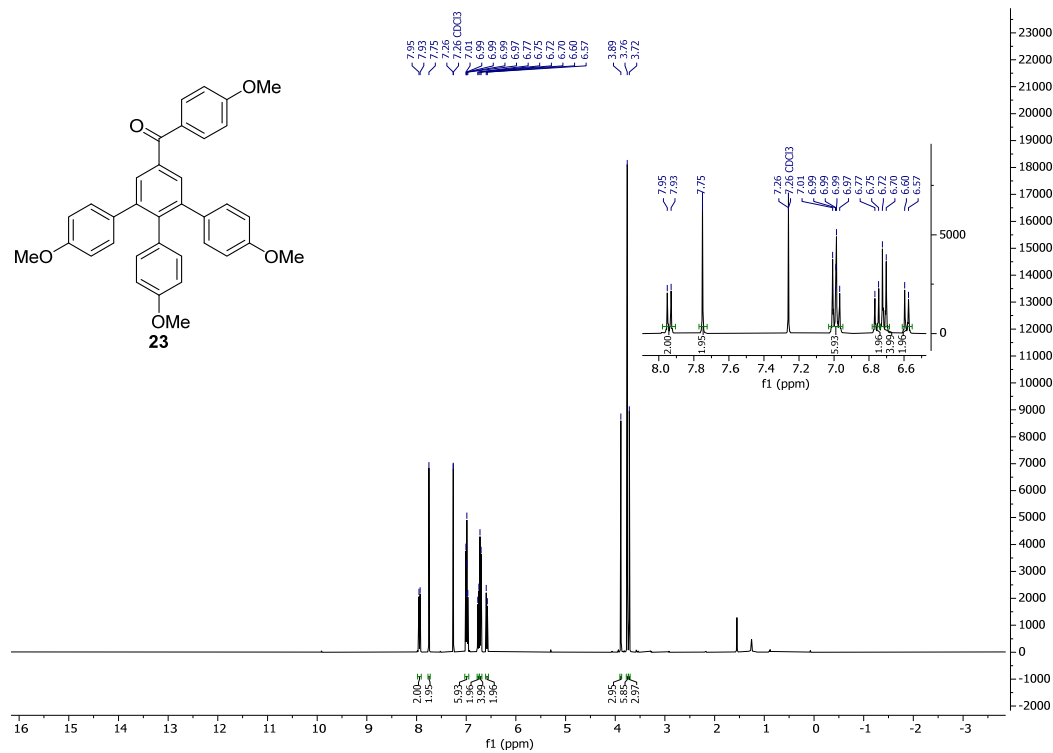


Figure S26. ^{13}C NMR spectra of compound **23** in CDCl_3 (100 MHz)

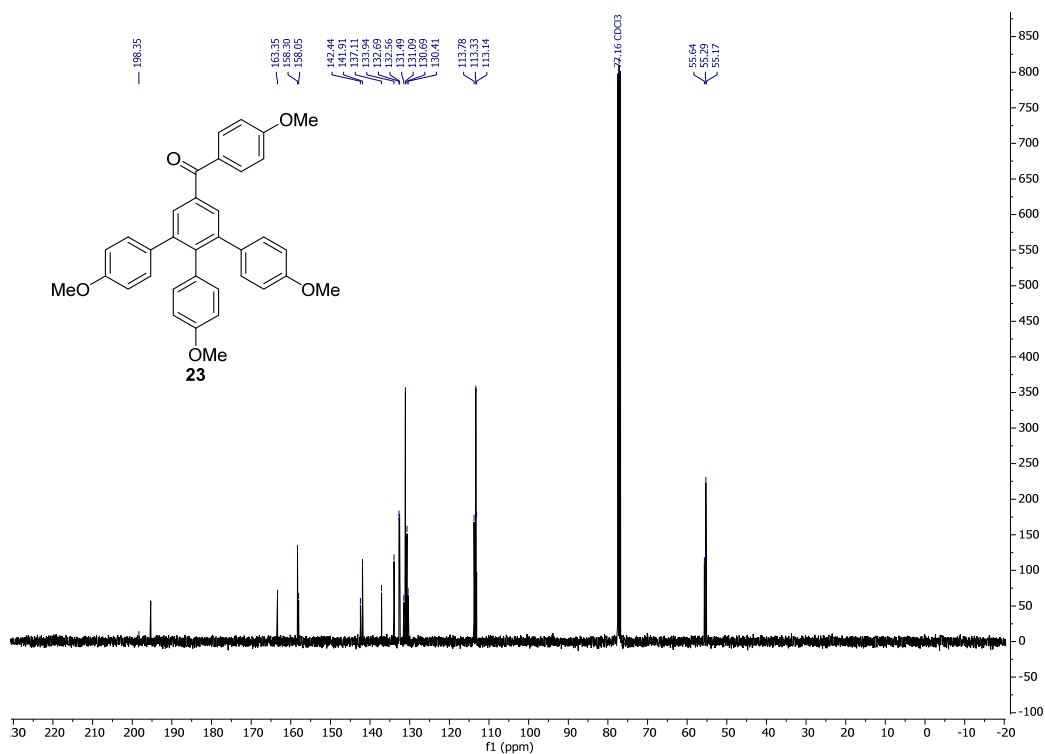


Figure S27. ^1H NMR spectra of selagibenzophenone B (**2**) in $\text{MeOD-}d_4$ (400 MHz)

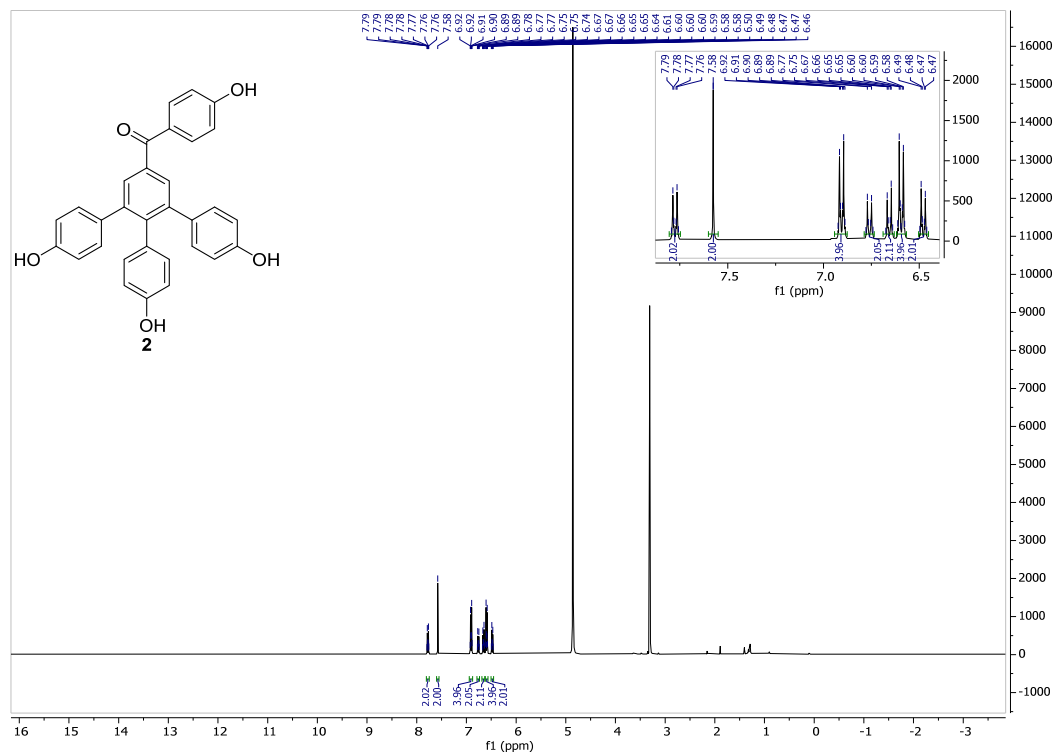


Figure S28. ^{13}C NMR spectra of selagibenzophenone B (**2**) in $\text{MeOD-}d_4$ (100 MHz)

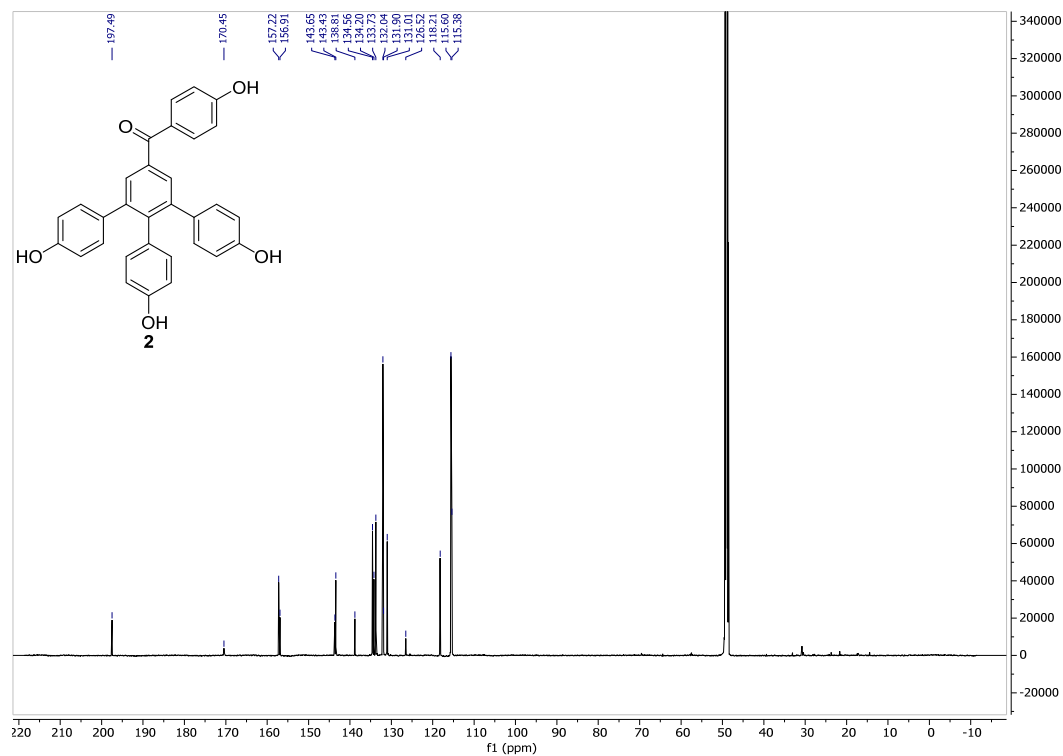


Figure S29. COSY spectra of selagibenzophenone B (**2**) in $\text{MeOD-}d_4$

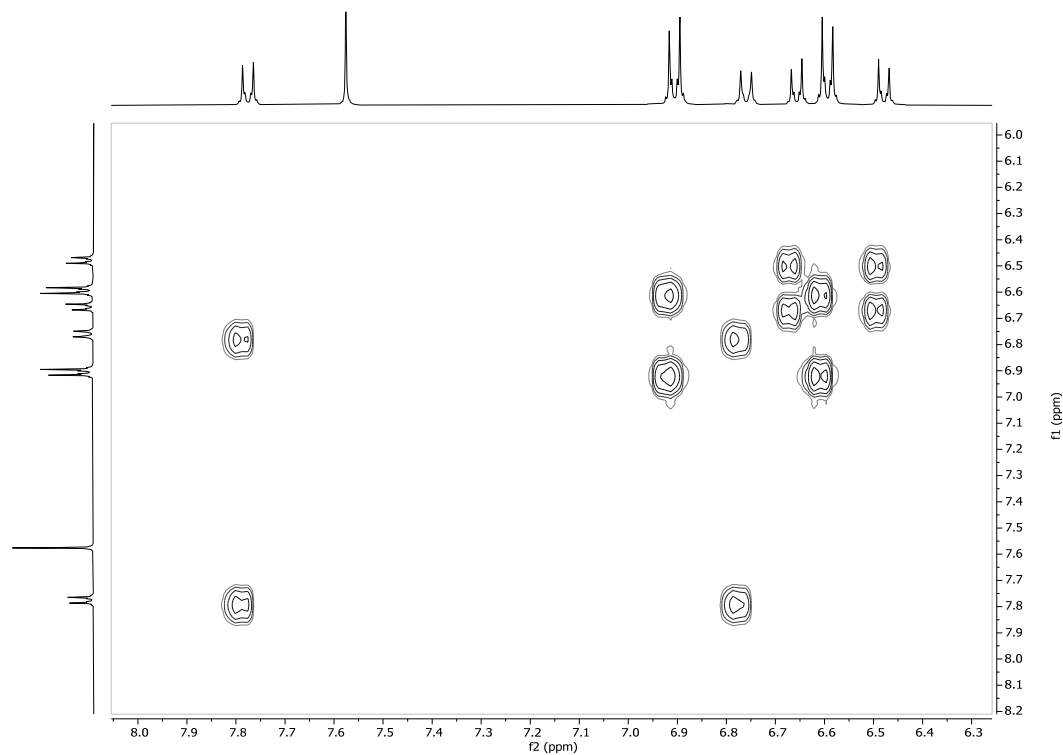


Figure S30. HSQC spectra of selagibenzophenone B (**2**) in MeOD-*d*₄

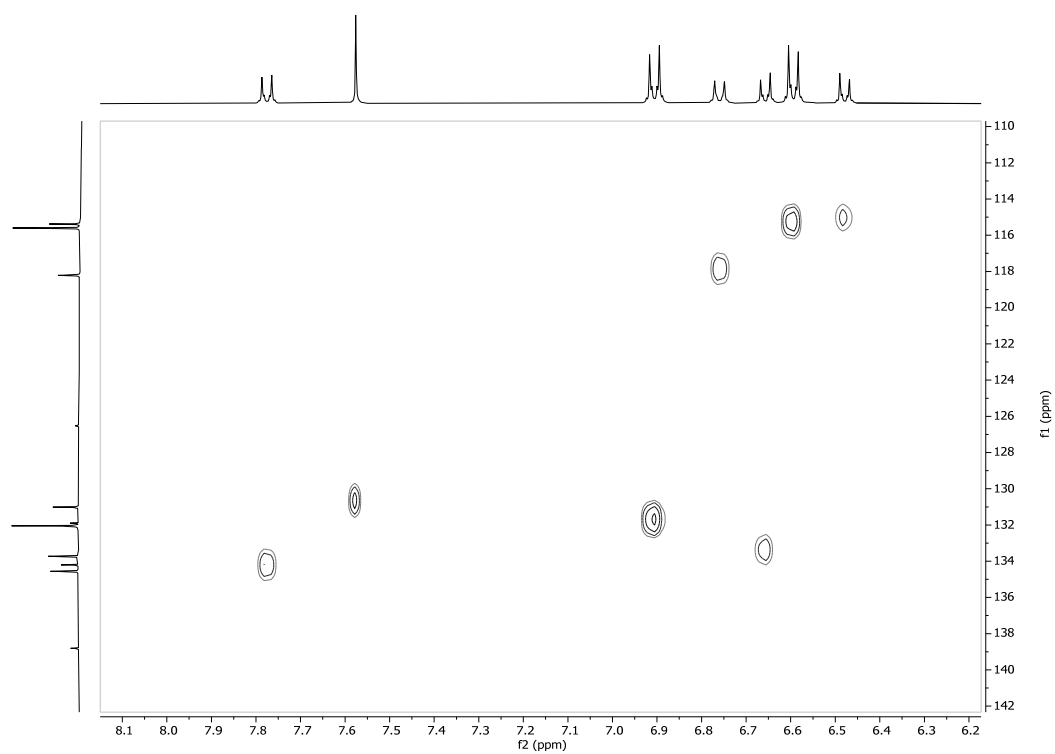
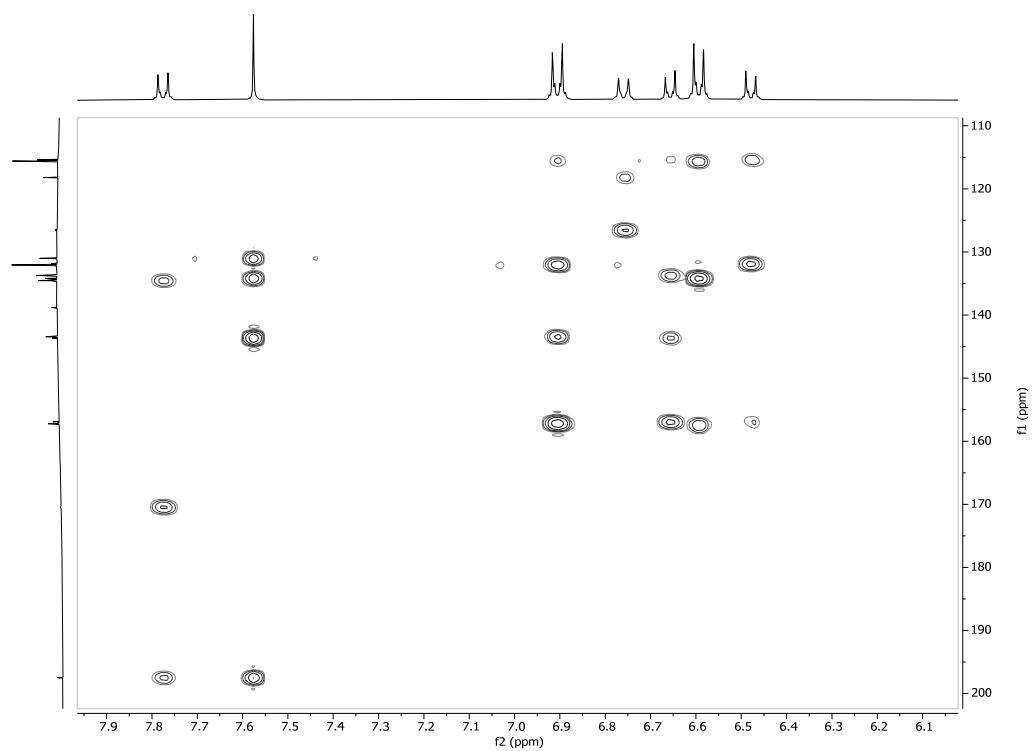


Figure S31. HMBC spectra of selagibenzophenone B (**2**) in MeOD-*d*₄



Chemical structure of compound 10: COc1ccc(cc1)C(=O)c2cc(cc(c2Oc3ccc(O)cc3)c4ccc(O)cc4)c5ccc(O)cc5

¹H NMR spectrum (DMSO-d₆) of compound 10. The x-axis represents the chemical shift in ppm (f1), ranging from 16 to -3. The y-axis represents the intensity, ranging from -1000 to 19000. The spectrum shows several peaks, with integration values provided below the baseline and above the peaks.

Peak list (ppm): 7.93, 7.88, 7.62, 7.07, 6.90, 6.88, 6.65, 6.64, 6.60, 6.58, 6.57, 6.47, 3.89, 3.31 (CD3OD).

Integration values (from left to right): 2.02, 2.01, 2.05, 2.11, 4.07, 2.00, 3.00, 2.03, 2.01, 2.05, 4.11, 2.10, 2.04, 2.00.

Inset spectrum (f1 ppm): 8.0, 7.8, 7.6, 7.4, 7.2, 7.0, 6.8, 6.6, 6.4. Integration values (from left to right): 2.03, 2.01, 2.05, 4.11, 2.10, 2.04, 2.00.

Chemical structure of compound 10 is shown. The spectrum displays peaks corresponding to the structure, with the following chemical shifts (ppm) labeled:

- 157.22
- 156.94
- 144.41
- 143.65
- 138.84
- 134.04
- 133.70
- 133.68
- 133.63
- 131.74
- 131.25
- 131.15
- 115.61
- 115.39
- 114.88
- 56.10
- 40.00 (CD3OD)

Figure S34. COSY spectra of monomethoxy-selagibenzophenone B in MeOD- d_4 (100 MHz)

