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

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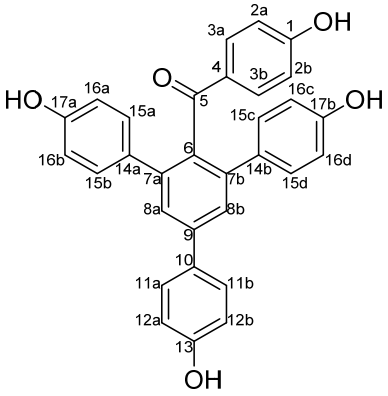
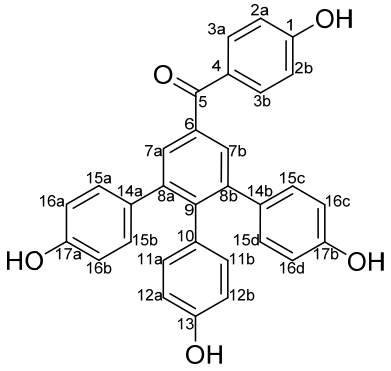
Figure S1. Numbering of selagibenzophenone A and B, and key HMBC correlations for selagibenzophenone B



selagibenzophenone A (**1**)



selagibenzophenone B (**2**)

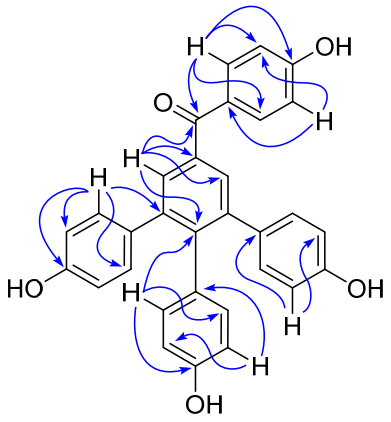


Table S1. Comparison of synthetic and isolated selagibenzophenone A and B

Position	Synthetic compounds				Reported values as was assigned in publications					
	Selagibenzophenone A		Selagibenzophenone B		Selagibenzophenone A (Liu, Tang, 2017)		Selagibenzophenone B			
							Wang, Yao, 2018		Liu, Zou, 2020	
	^{1}H NMR	^{13}C NMR	^{1}H NMR	^{13}C NMR	^{1}H NMR	^{13}C NMR	^{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. ^{1}H NMR spectra of compound **10** in $CDCl_3$ (400 MHz)

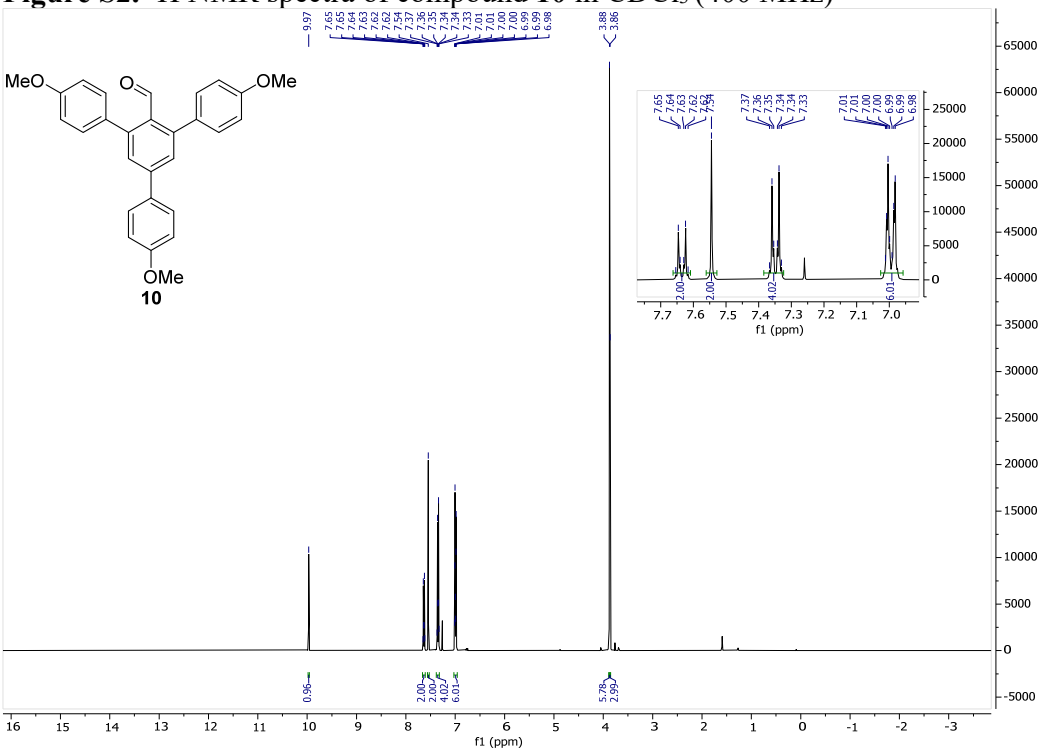


Figure S3. ^{13}C NMR spectra of compound **10** in $CDCl_3$ (100 MHz)

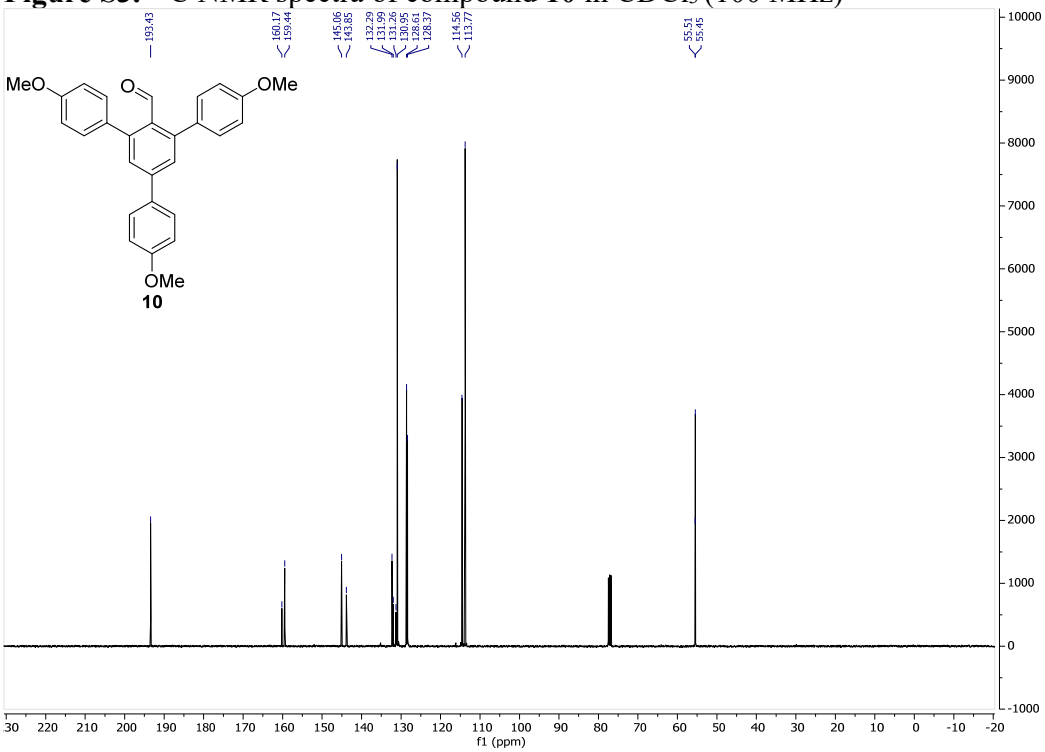


Figure S4. ^{1}H NMR spectra of compound **12** in $CDCl_3$ (400 MHz)

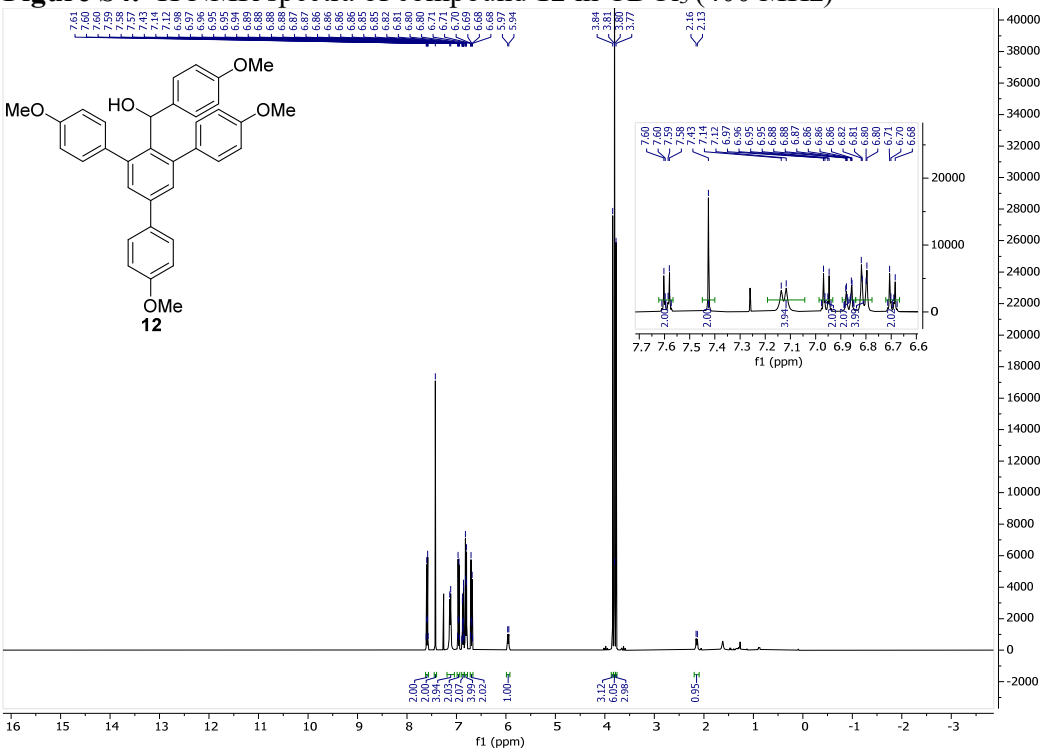


Figure S5. ^{13}C NMR spectra of compound **12** in $CDCl_3$ (100 MHz)

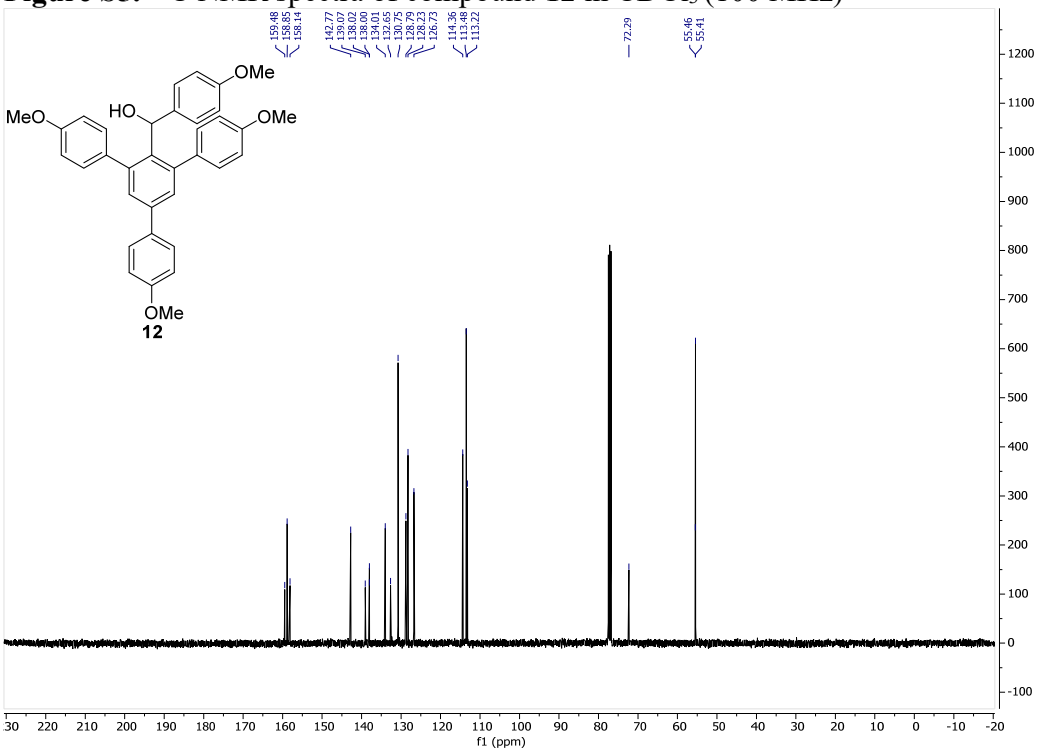


Figure S6. ^{1}H NMR spectra of compound **13** in $CDCl_3$ (400 MHz)

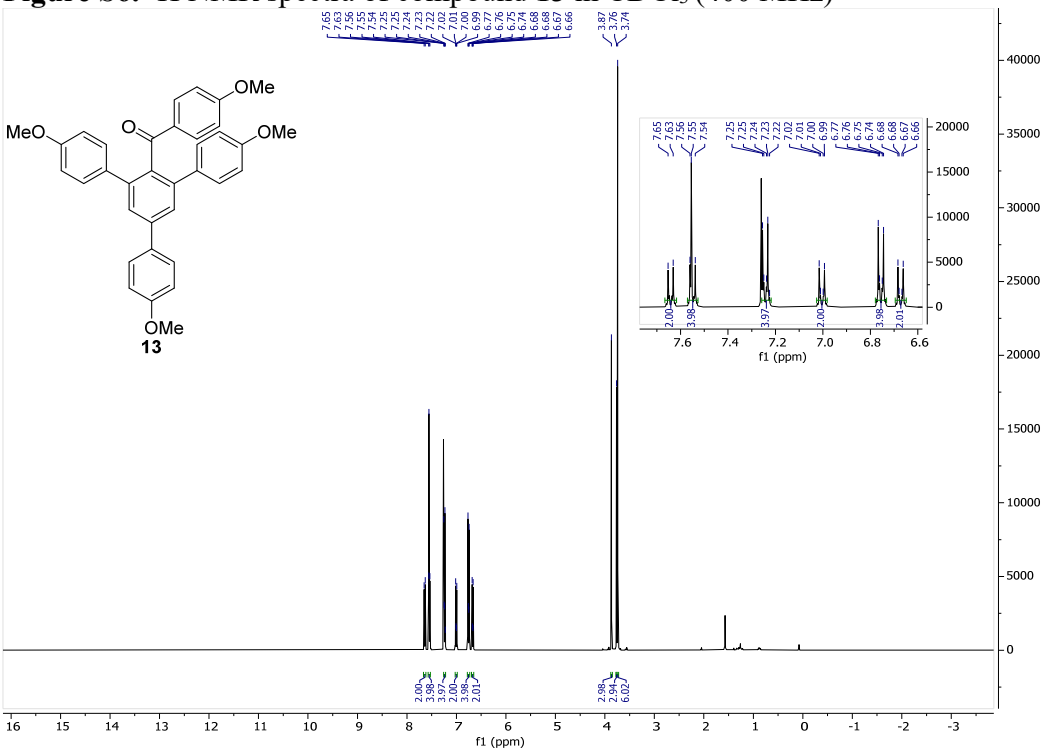


Figure S7. ^{13}C NMR spectra of compound **13** in $CDCl_3$ (100 MHz)

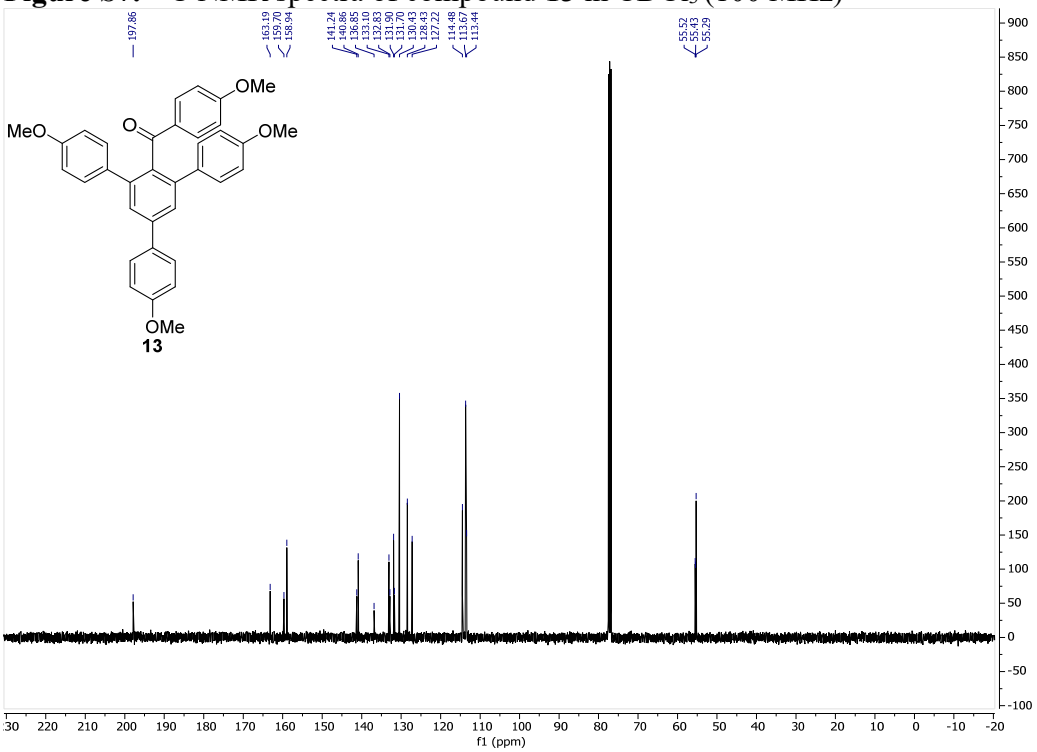


Figure S8. ^{1}H NMR spectra of compound **14** in MeOD-d_4 (600 MHz)

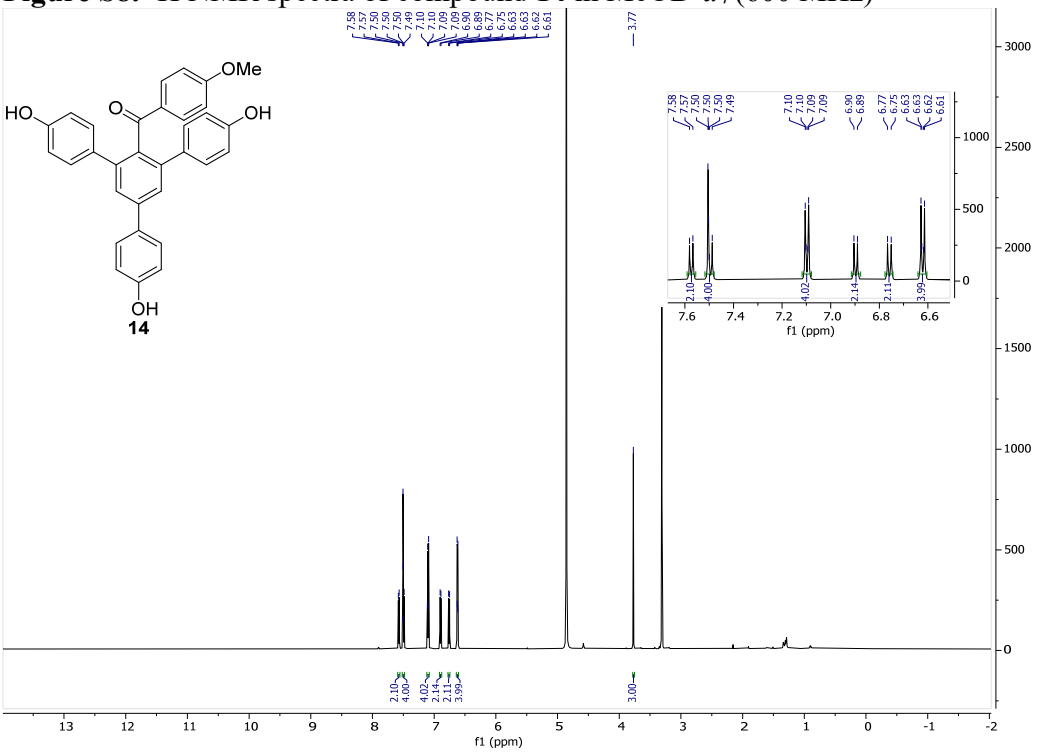


Figure S9. ^{13}C NMR spectra of compound **14** in MeOD-d_4 (150 MHz)

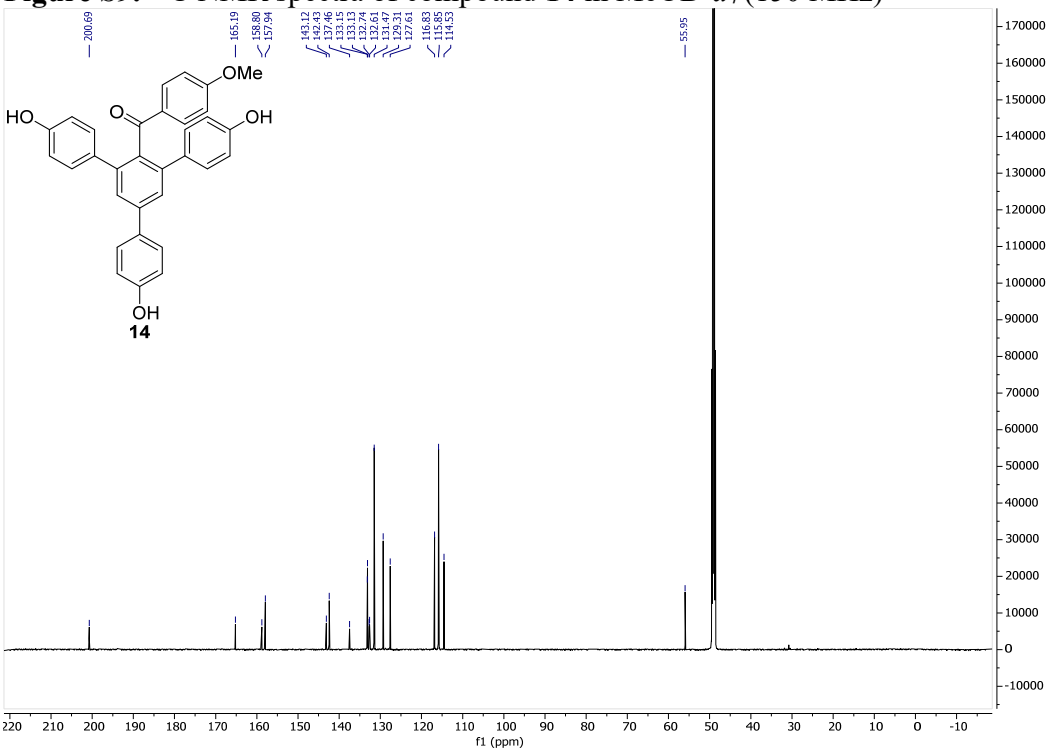


Figure S10. ^{1}H NMR spectra of selagibenzophenone A (**1**) in MeOD-d_4 (400 MHz)

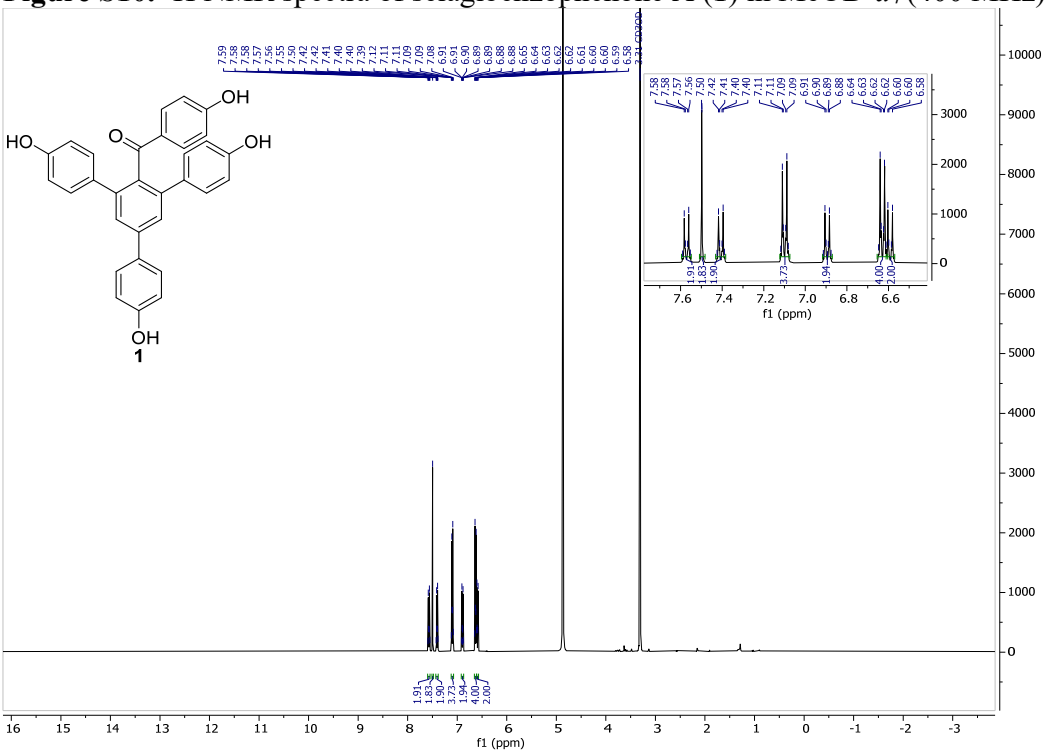


Figure S11. ^{13}C NMR spectra of selagibenzophenone A (**1**) in MeOD-d_4 (100 MHz)

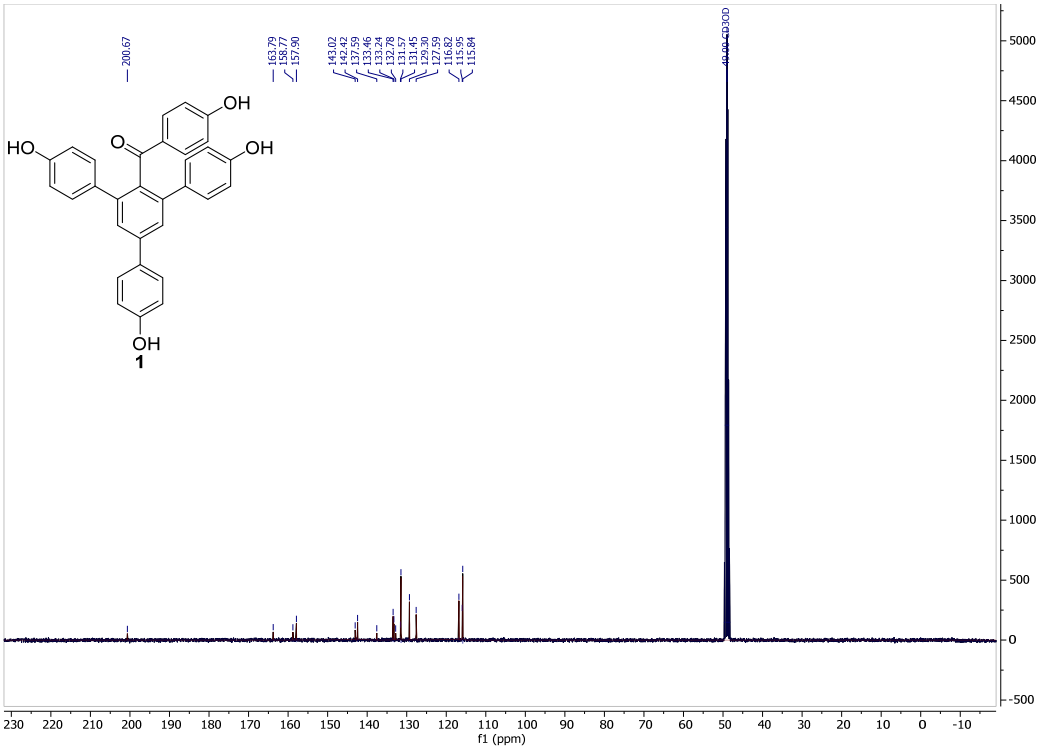


Figure S12. COSY spectra of selagibenzophenone A (**1**) in MeOD-d_4

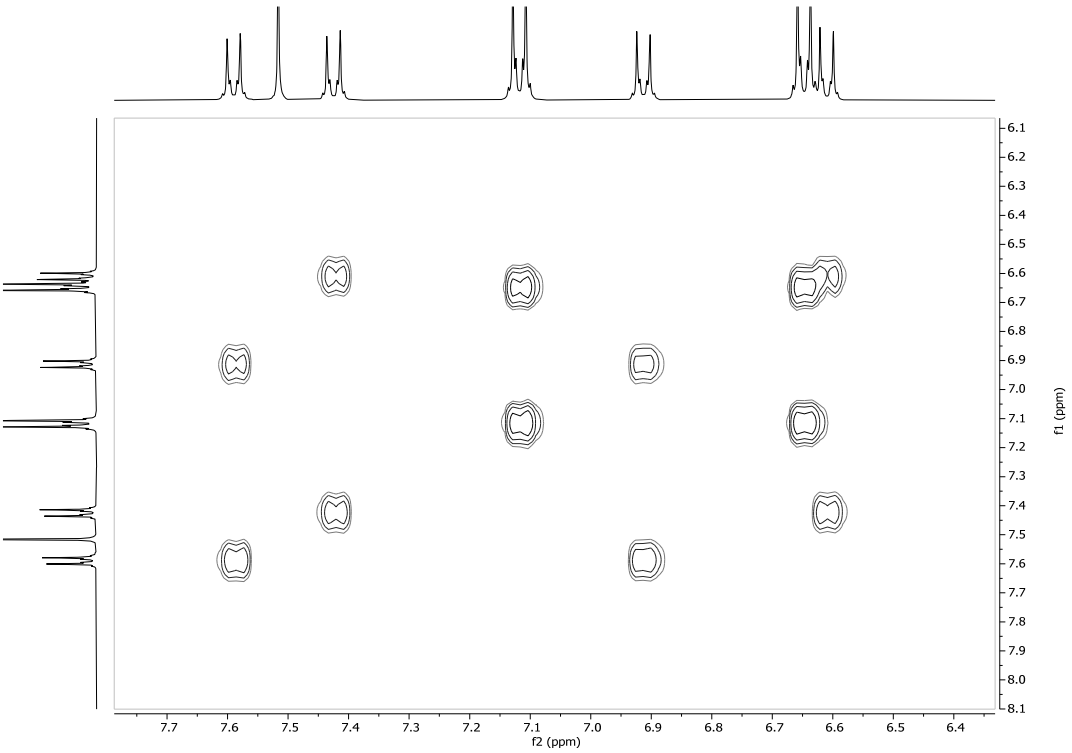


Figure S13. HSQC spectra of selagibenzophenone A (**1**) in MeOD-d_4

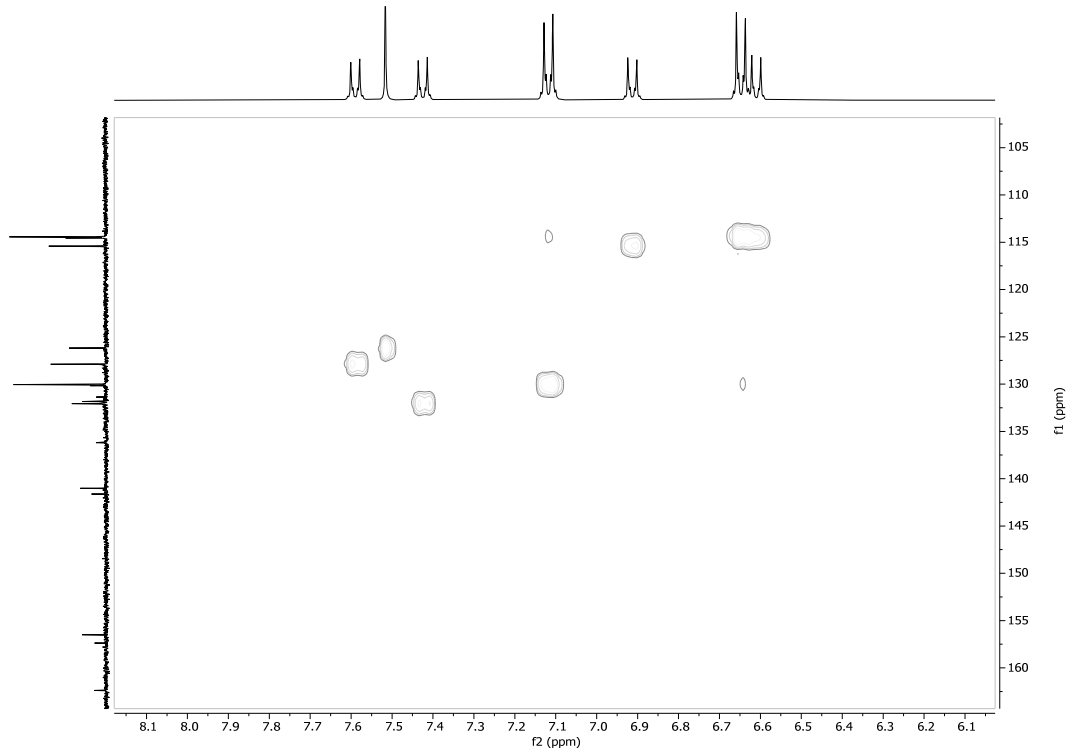


Figure S 14. HSQC spectra of selagibenzophenone A (**1**) in MeOD-d_4

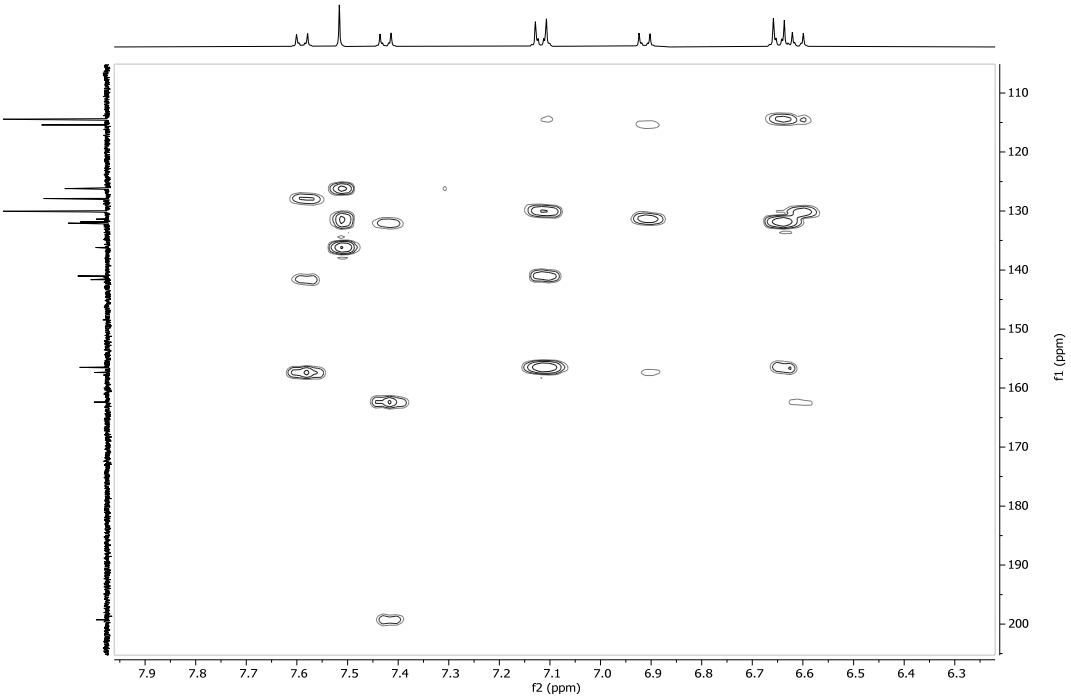


Figure S15. ^{1}H NMR spectra of compound **18** in $CDCl_3$ (400 MHz)

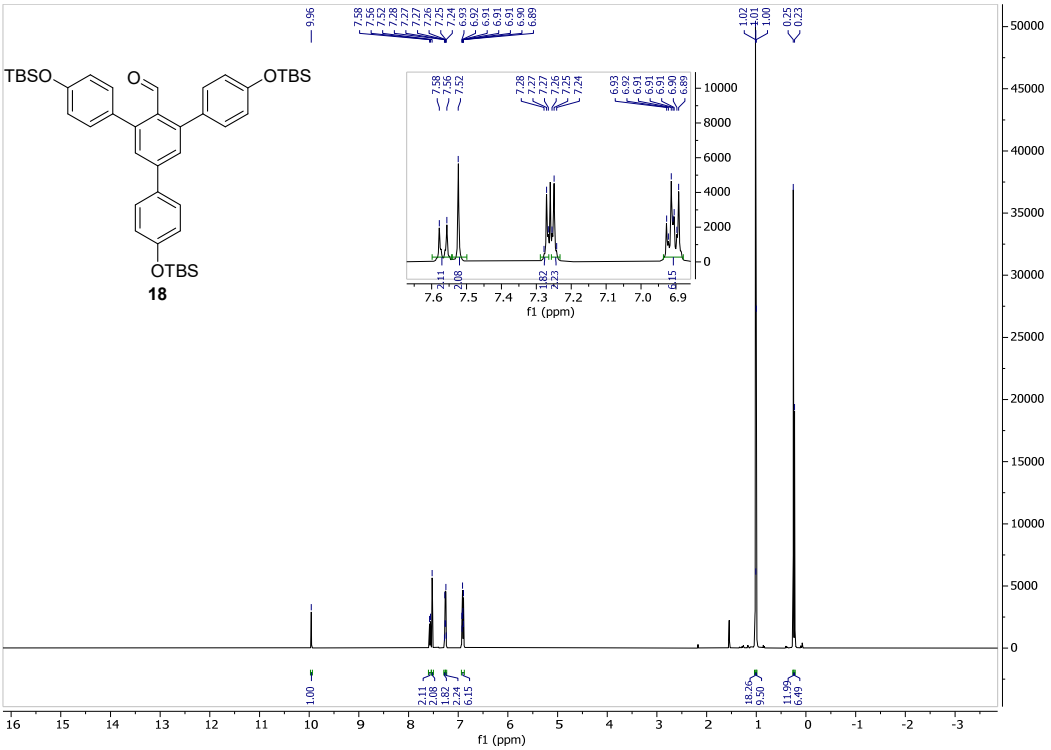


Figure S16. ^{13}C NMR spectra of compound **18** in $CDCl_3$ (100 MHz)

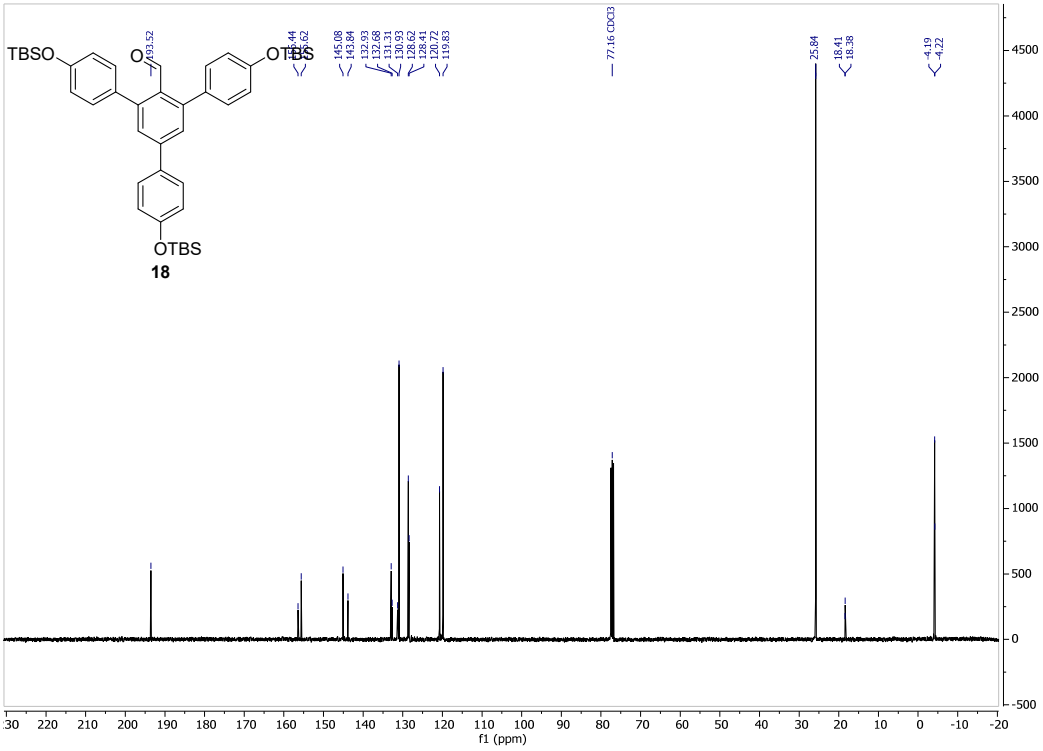


Figure S17. ^{1}H NMR spectra of compound **19** in $CDCl_3$ (400 MHz)

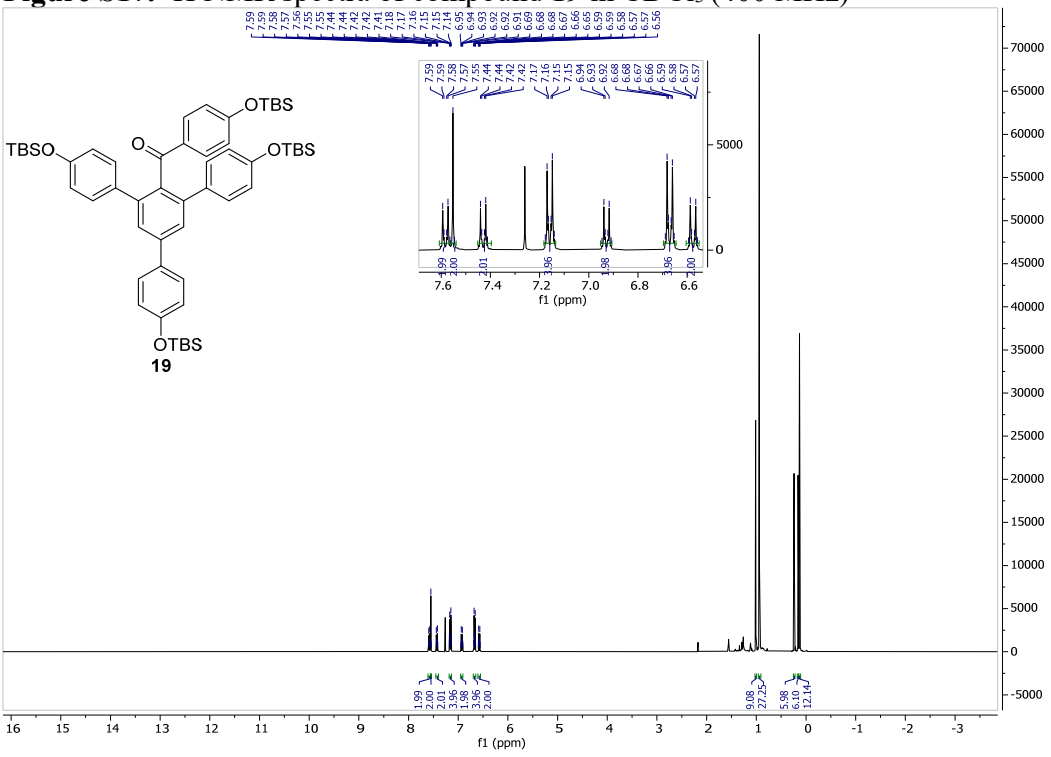


Figure S18. ^{13}C NMR spectra of compound **19** in $CDCl_3$ (100 MHz)

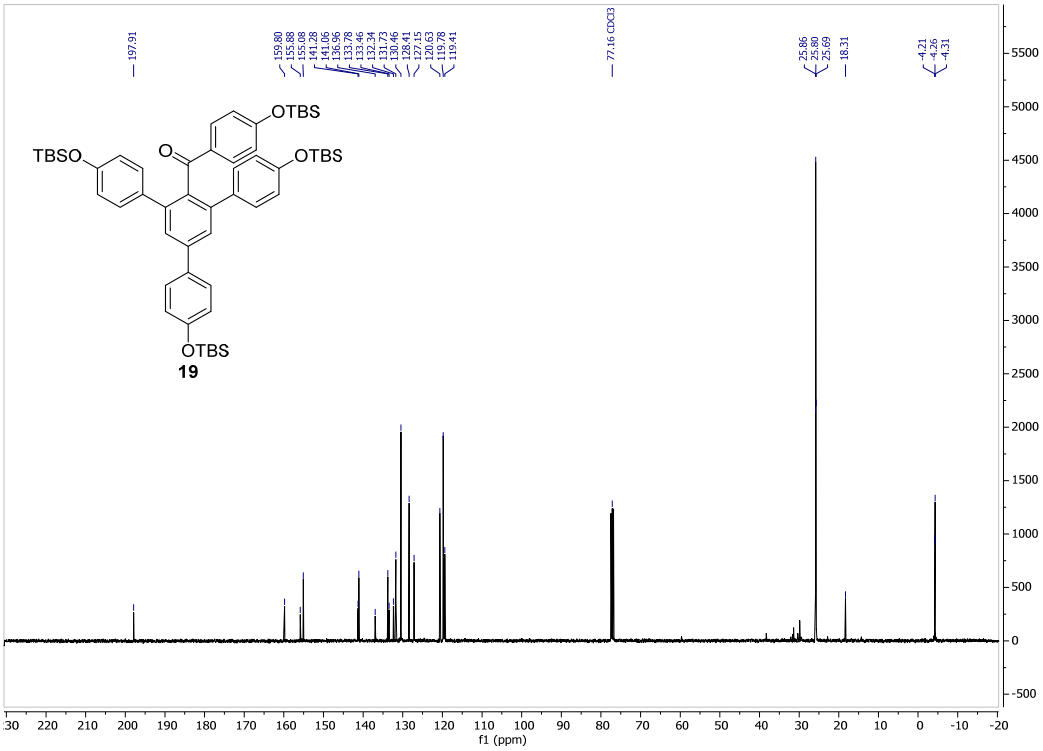


Figure S19. ^{1}H NMR spectra of compound **20** in $CDCl_3$ (300 MHz)

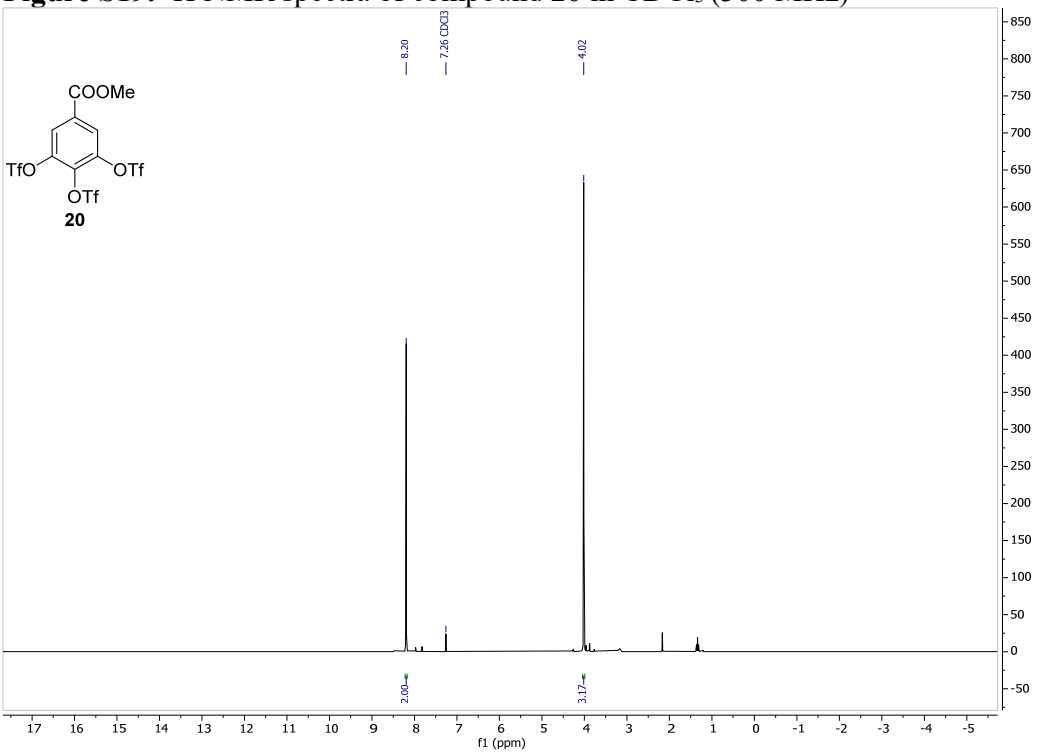


Figure S20. ^{13}C NMR spectra of compound **20** in $CDCl_3$ (75 MHz)

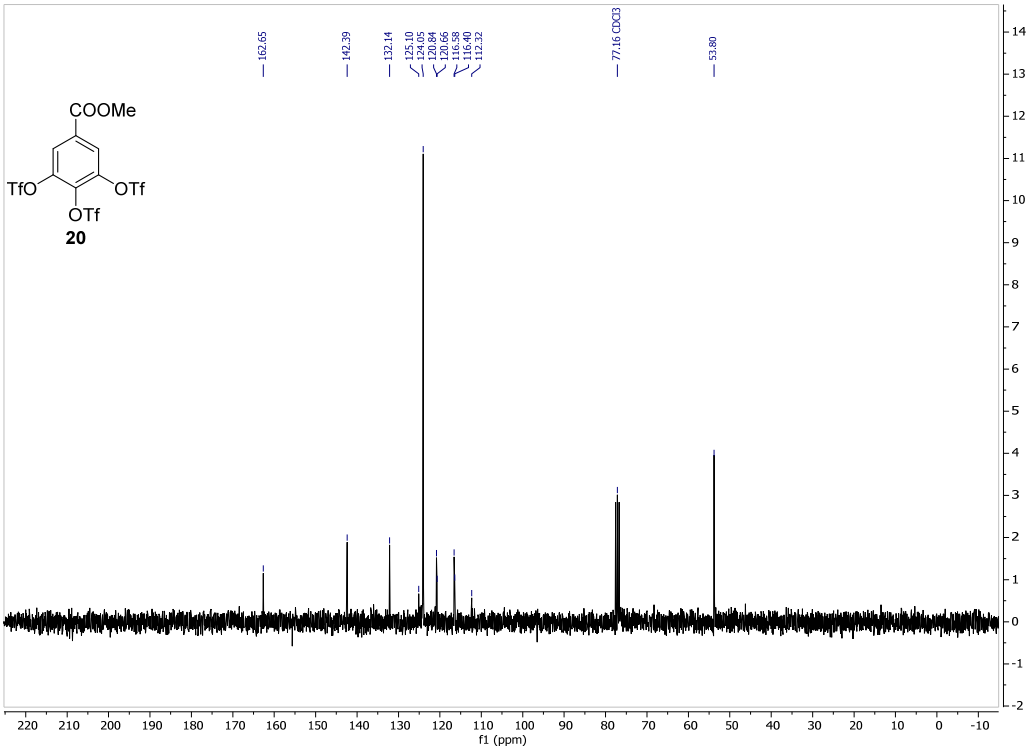


Figure S21. ^{1}H NMR spectra of compound **21** in $CDCl_3$ (400 MHz)

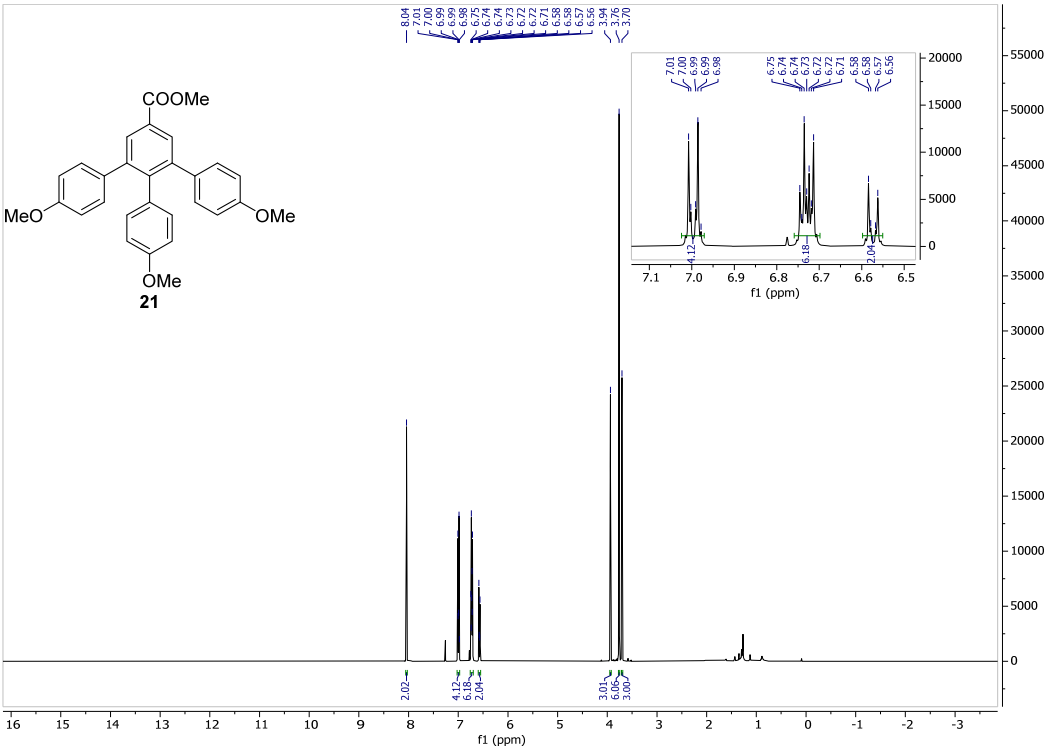


Figure S22. ^{13}C NMR spectra of compound **21** in $CDCl_3$ (100 MHz)

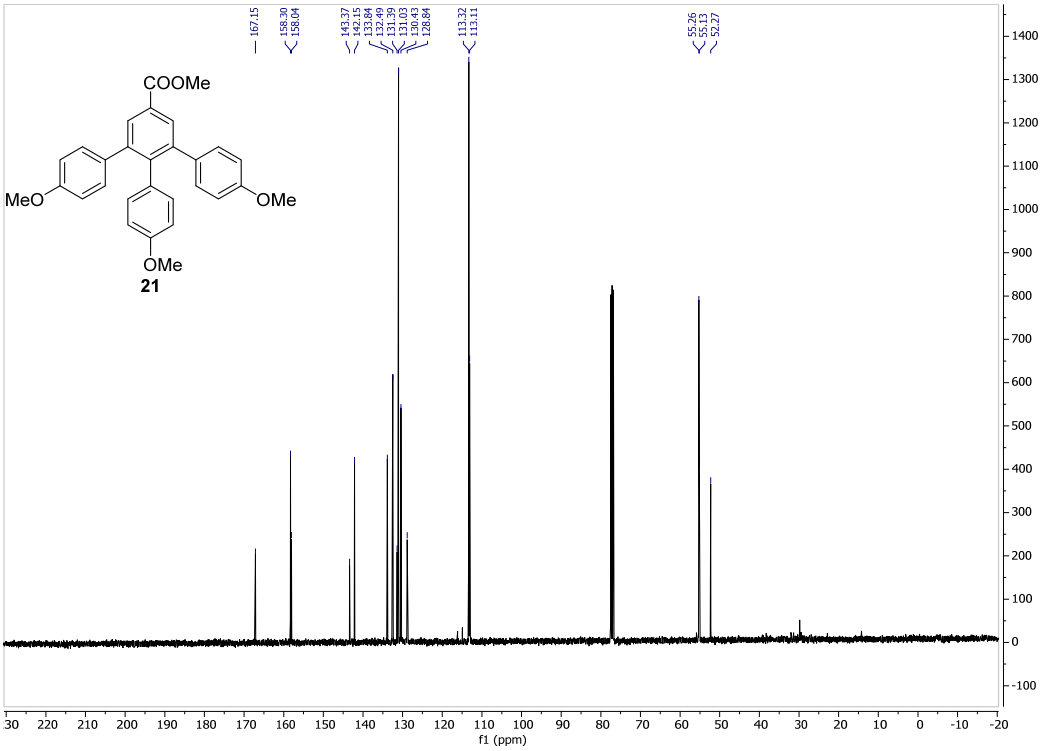


Figure S23. ^{1}H NMR spectra of compound **22** in $CDCl_3$ (400 MHz)

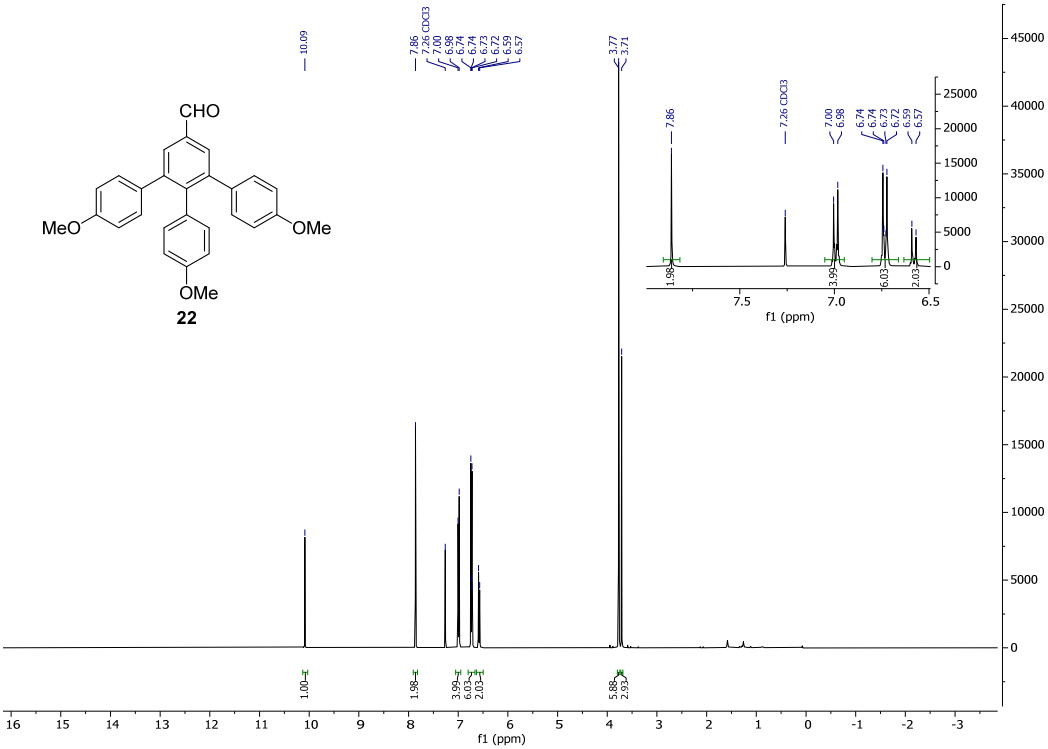


Figure S24. ^{13}C NMR spectra of compound **22** in $CDCl_3$ (100 MHz)

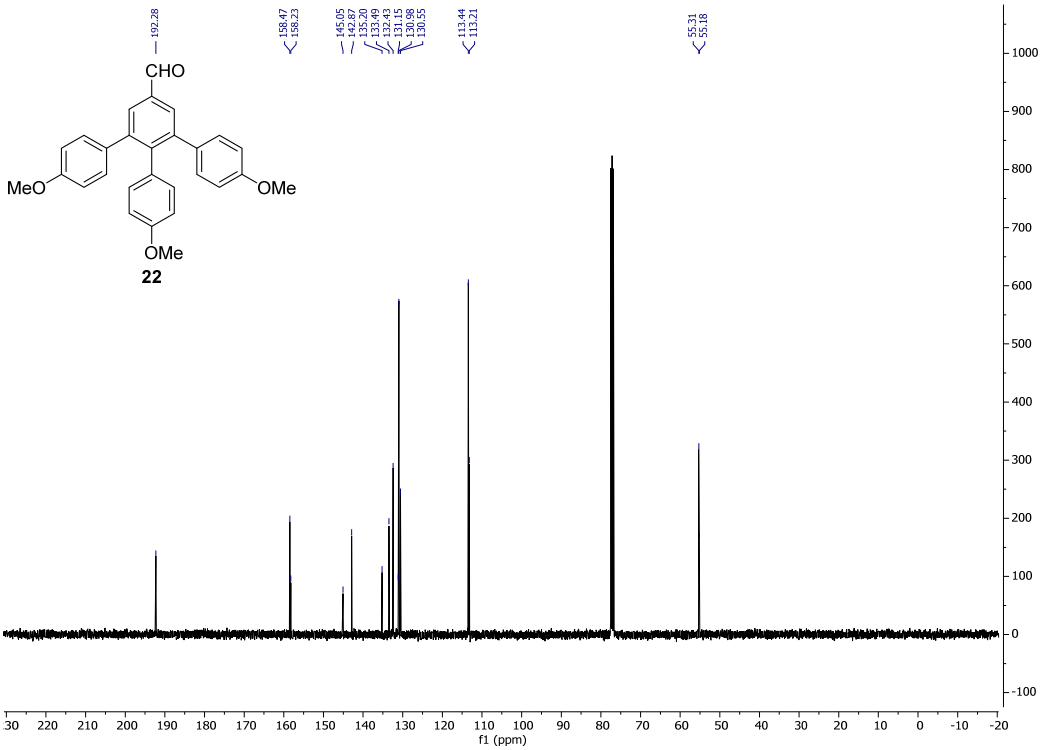


Figure S25. ^{1}H NMR spectra of compound **23** in $CDCl_3$ (400 MHz)

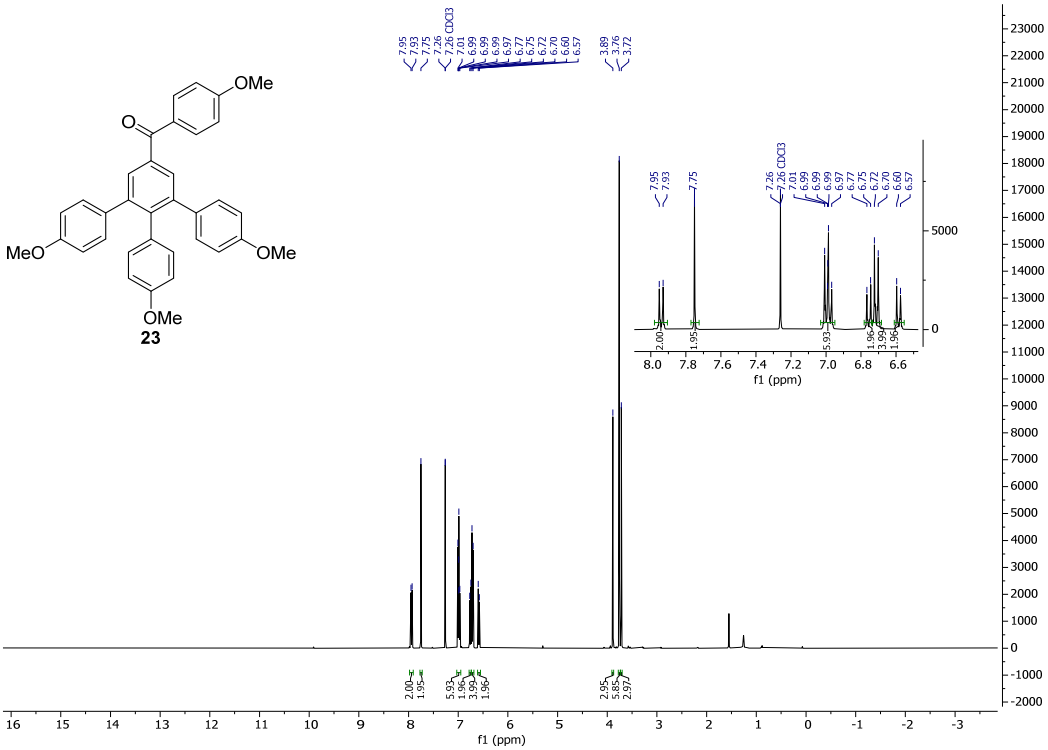


Figure S26. ^{13}C NMR spectra of compound **23** in $CDCl_3$ (100 MHz)

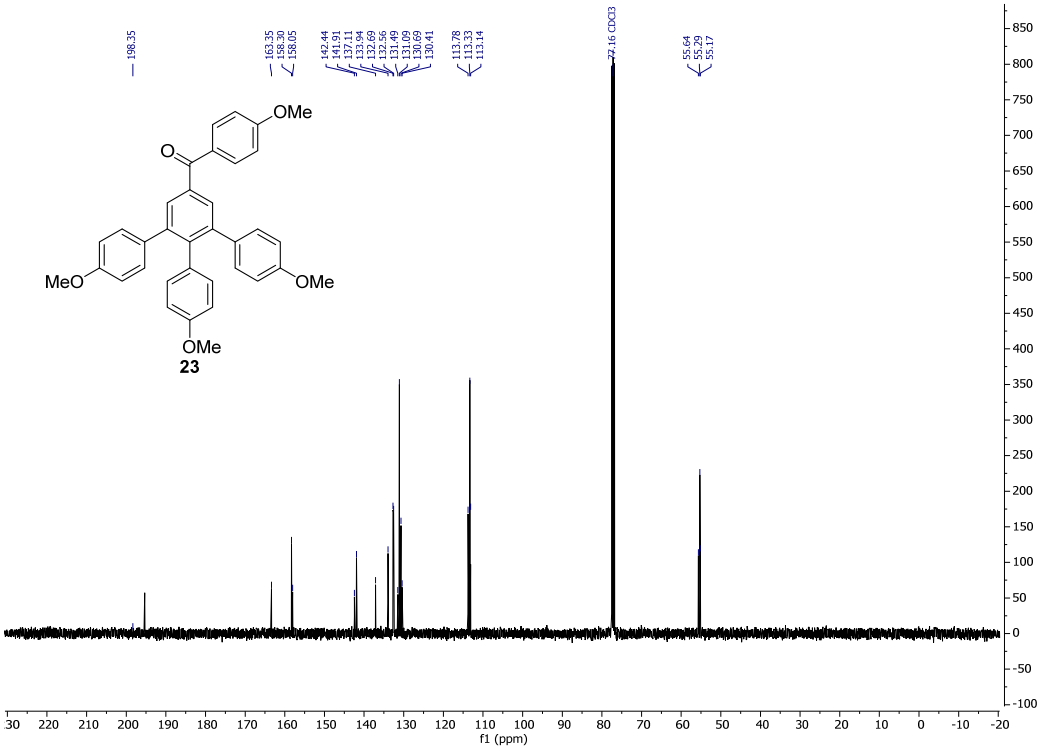


Figure S27. ^{1}H NMR spectra of selagibenzophenone B (**2**) in MeOD-d_4 (400 MHz)

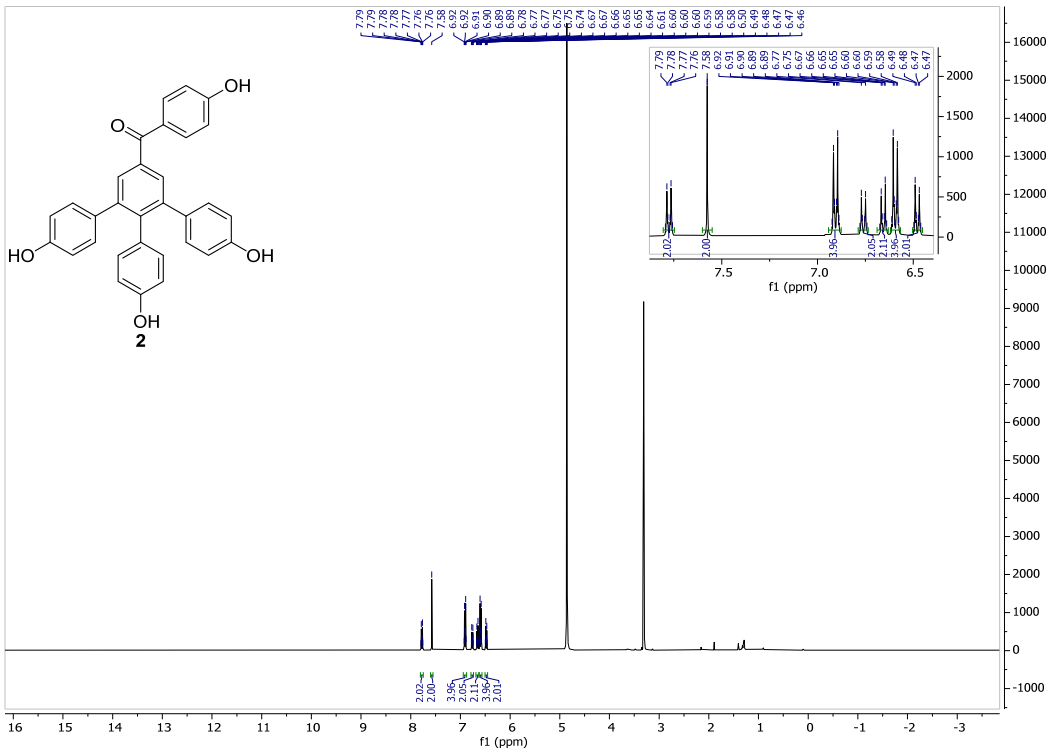


Figure S28. ^{13}C NMR spectra of selagibenzophenone B (**2**) in MeOD-*d*$_4$ (100 MHz)

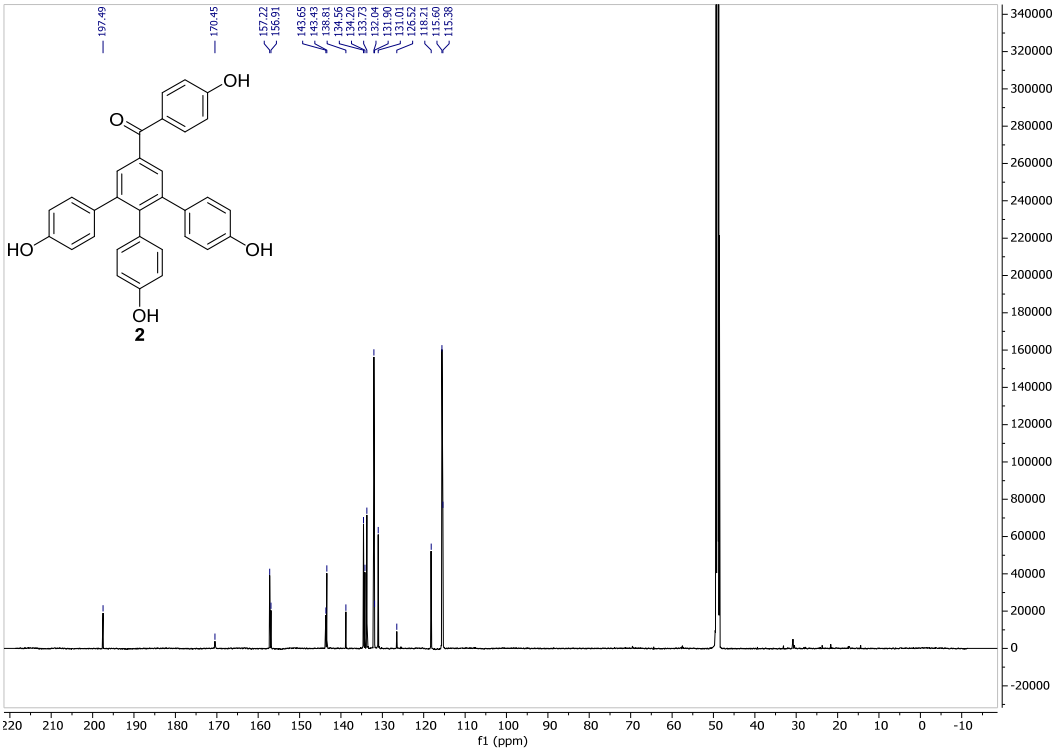


Figure S29. COSY spectra of selagibenzophenone B (**2**) in MeOD-*d*$_4$

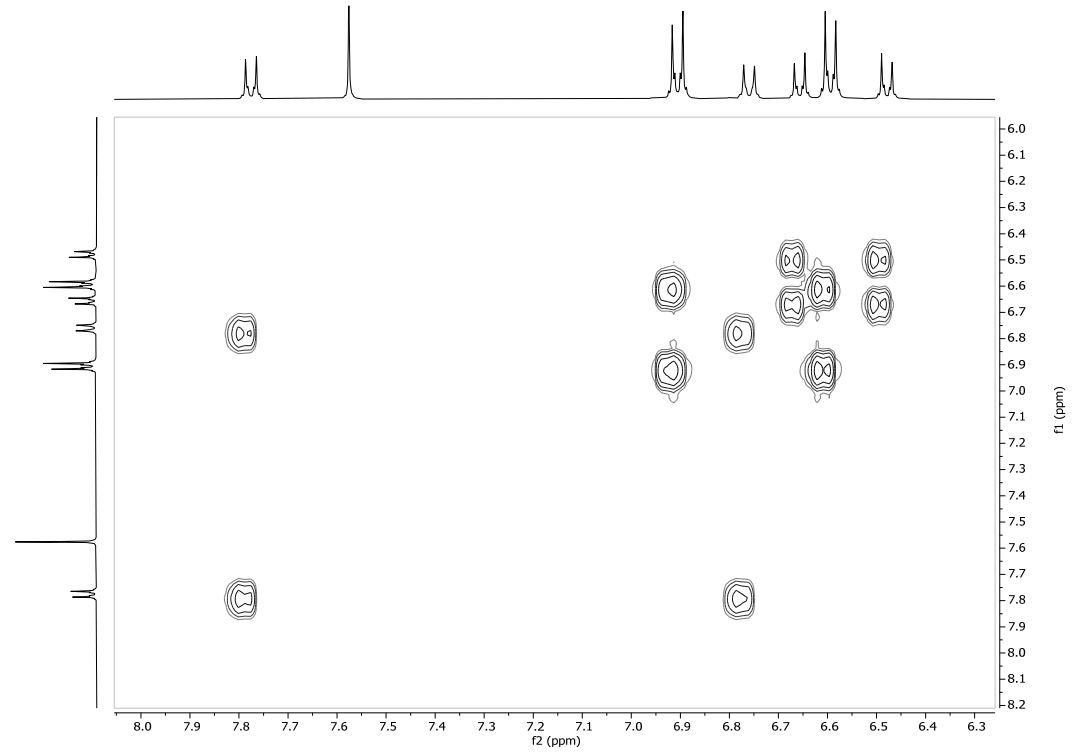


Figure S30. HSQC spectra of selagibenzophenone B (**2**) in MeOD-d_4

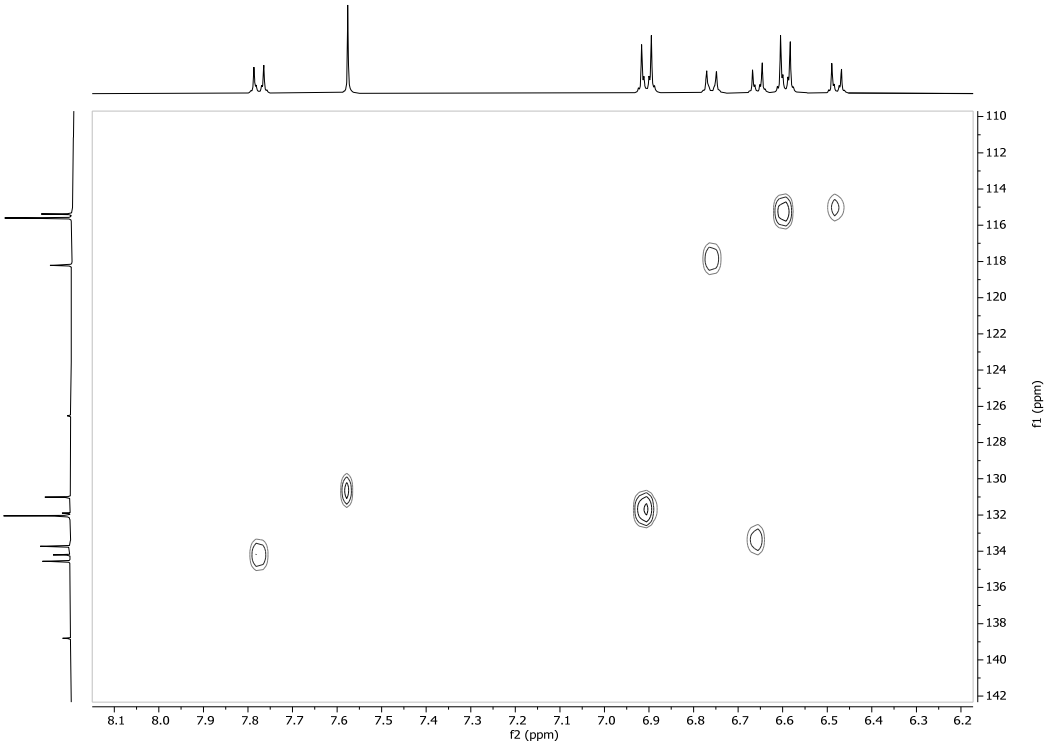


Figure S31. HMBC spectra of selagibenzophenone B (**2**) in MeOD-d_4

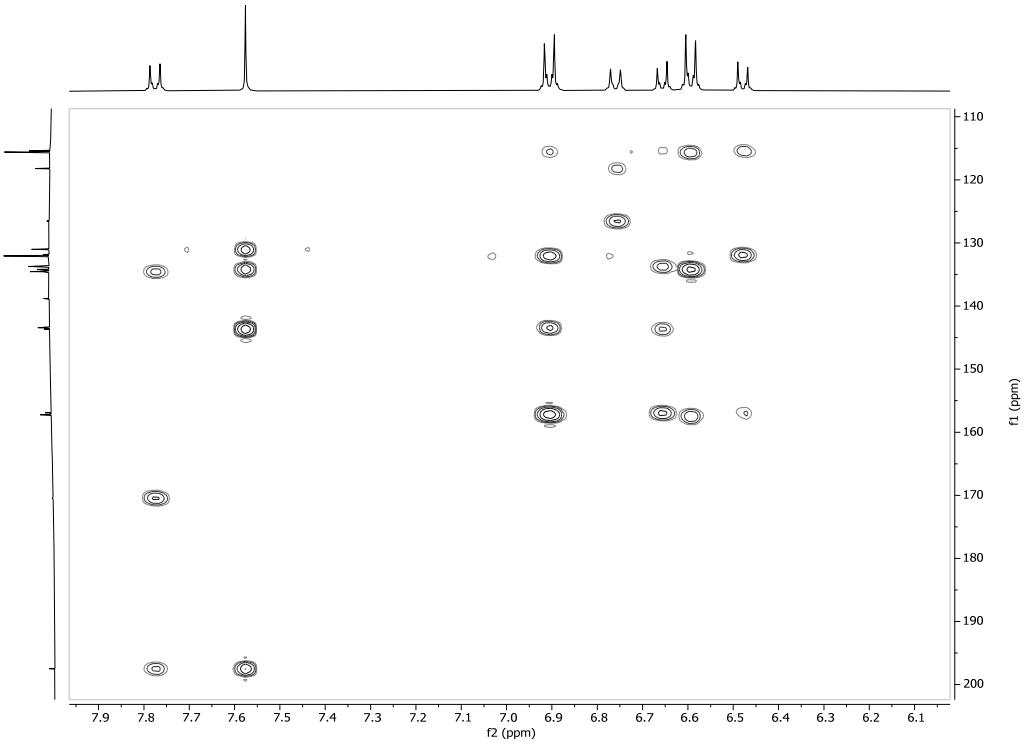


Figure S32. [1]H NMR spectra of monomethoxy-selagibenzophenone B in MeOD-*d*$_4$ (400 MHz)

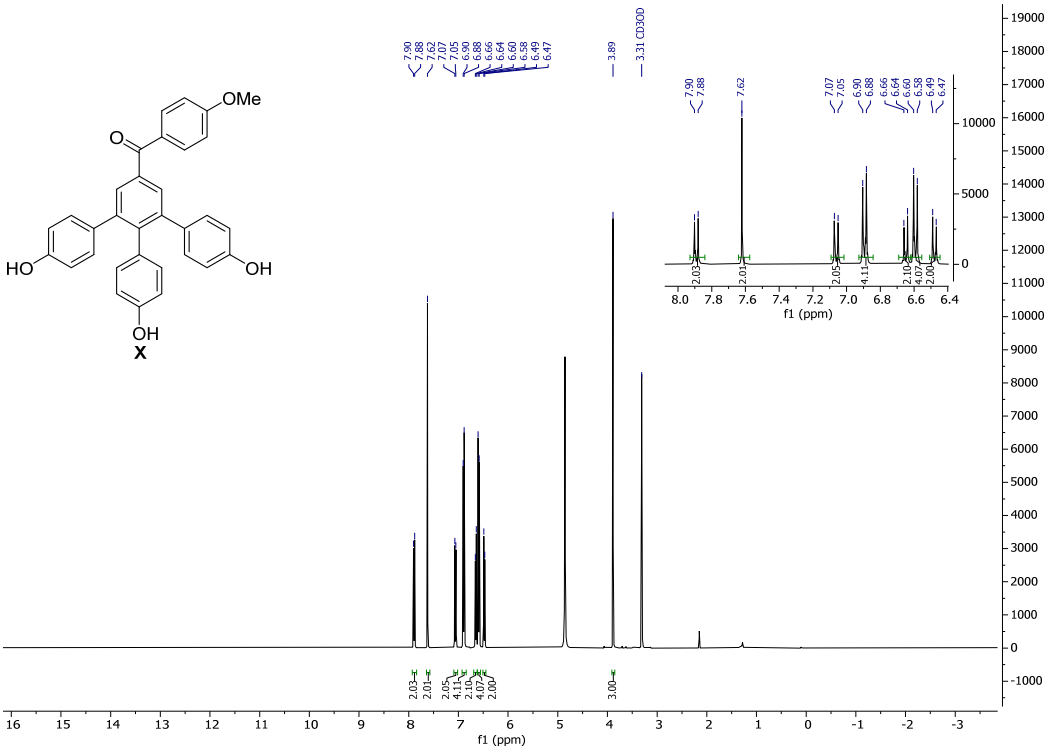


Figure S33. [13]C NMR spectra of monomethoxy-selagibenzophenone B in MeOD-*d*$_4$ (100 MHz)

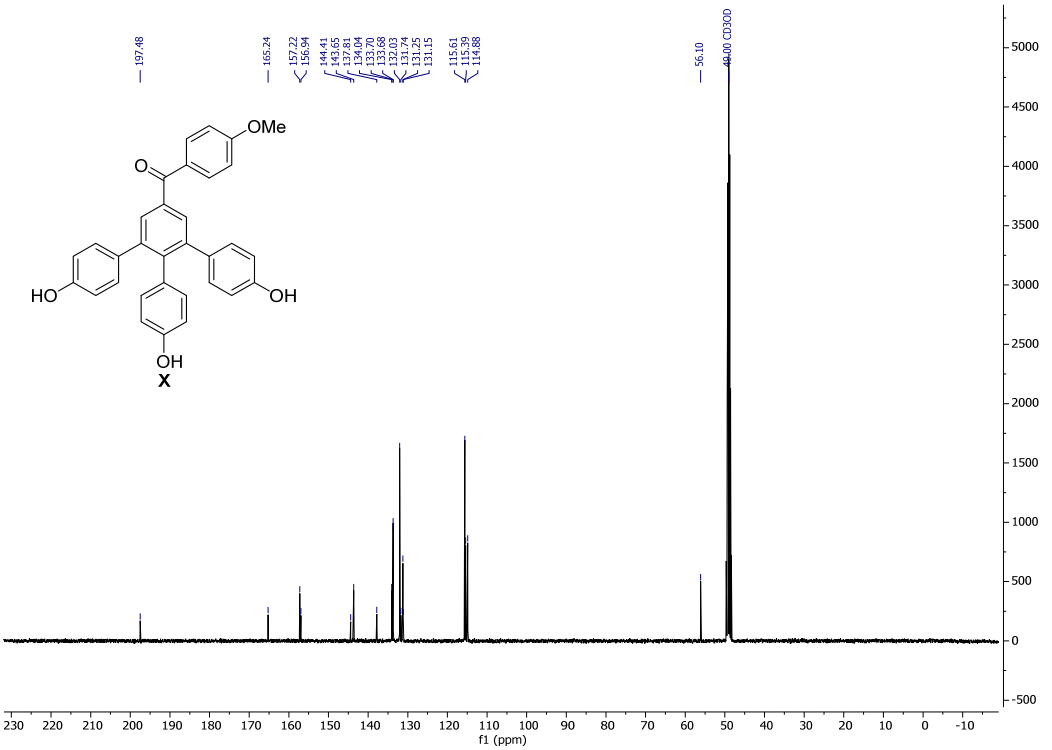


Figure S34. COSY spectra of monomethoxy-selagibenzophenone B in MeOD-d_4 (100 MHz)