

Supporting Information

**SYNTHESIS OF 4,5-DISUBSTITUTED
PYRANO[3,4-*b*]PYRROL-7(1*H*)-ONES VIA SONOGASHIRA–HAGIHARA
CROSS-COUPLING OF
N-BENZENESULFONYL-3-BROMO-1*H*-PYRROLE-2-CARBOXYLATE
AND SUBSEQUENT IODINE-MEDIATED CYCLIZATION**

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¹ H NMR, ¹³ C NMR, HMQC, and HMBC spectra	S2–S42
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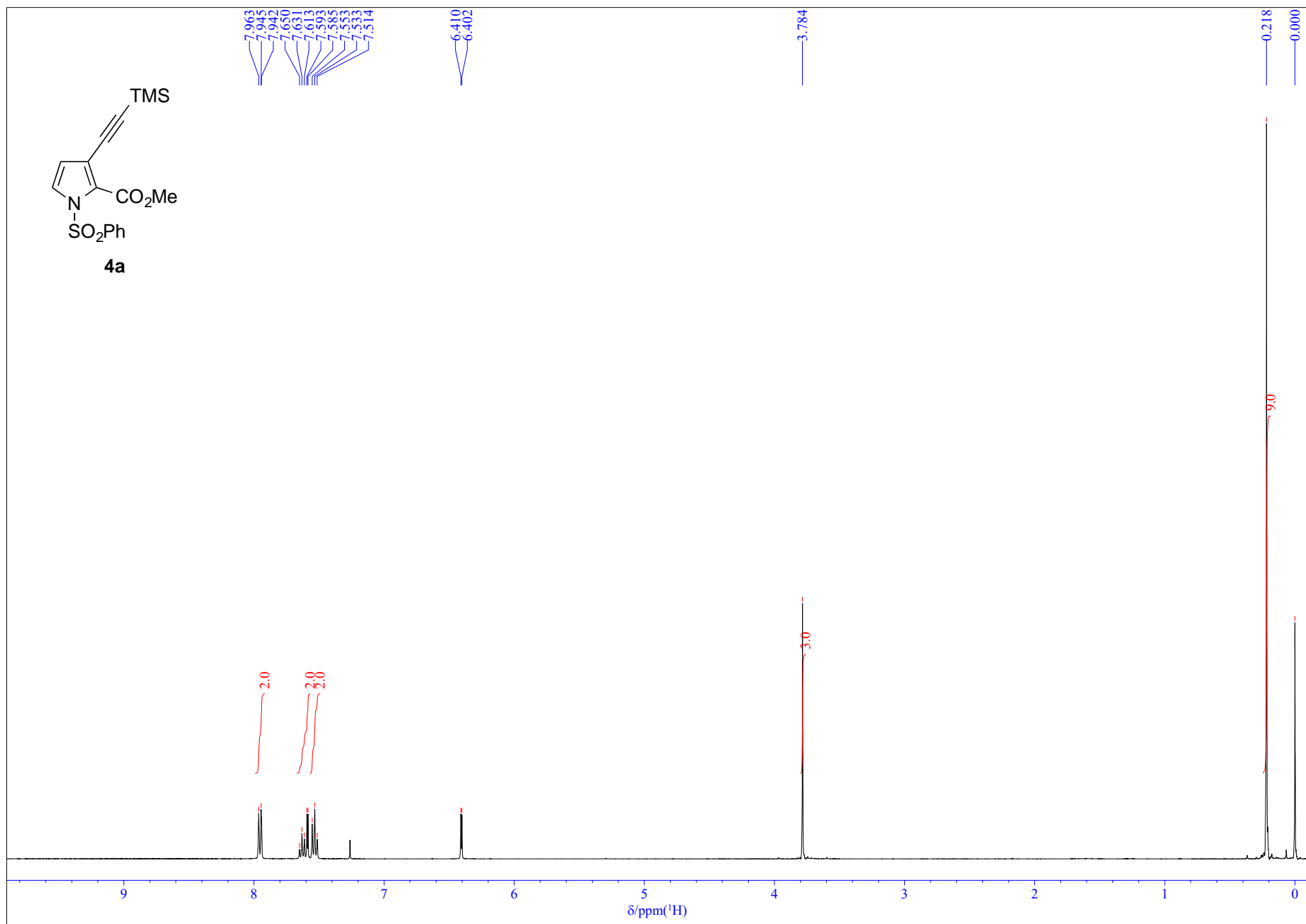


Figure S1. ¹H NMR spectrum of compound **4a** (400 MHz, CDCl₃).

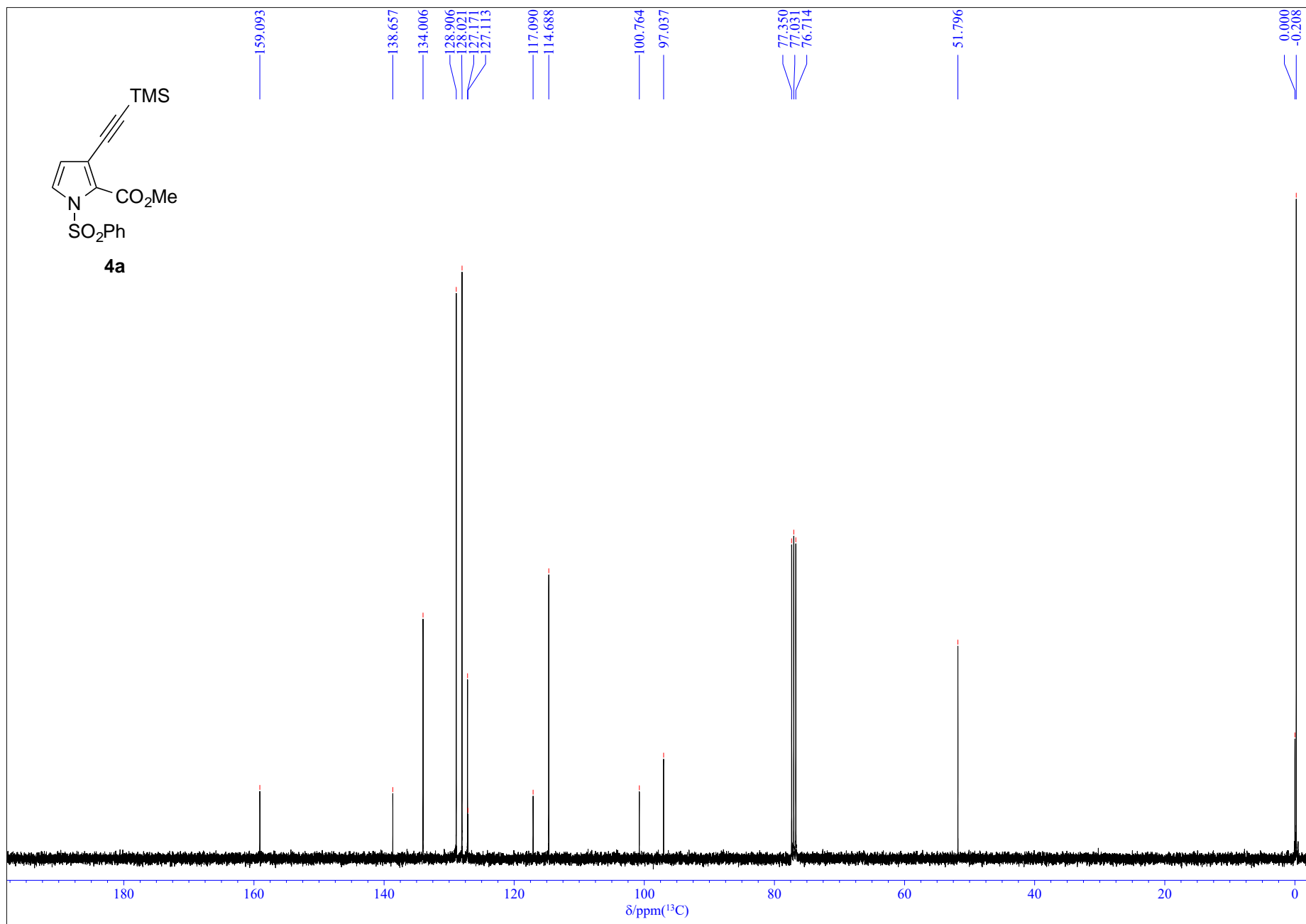


Figure S2. ¹³C NMR spectrum of compound **4a** (100 MHz, CDCl₃).

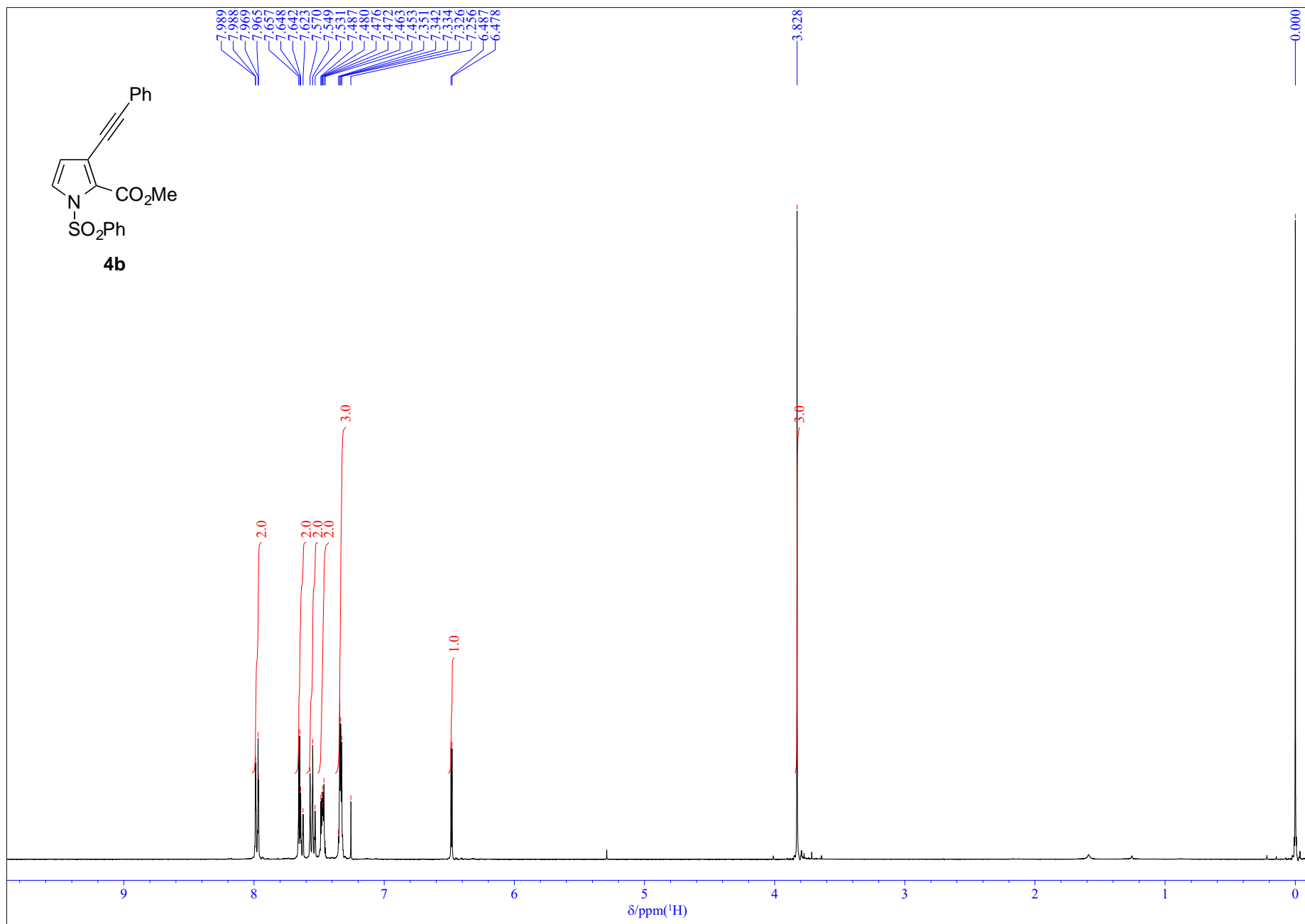


Figure S3. ¹H NMR spectrum of compound **4b** (400 MHz, CDCl₃).

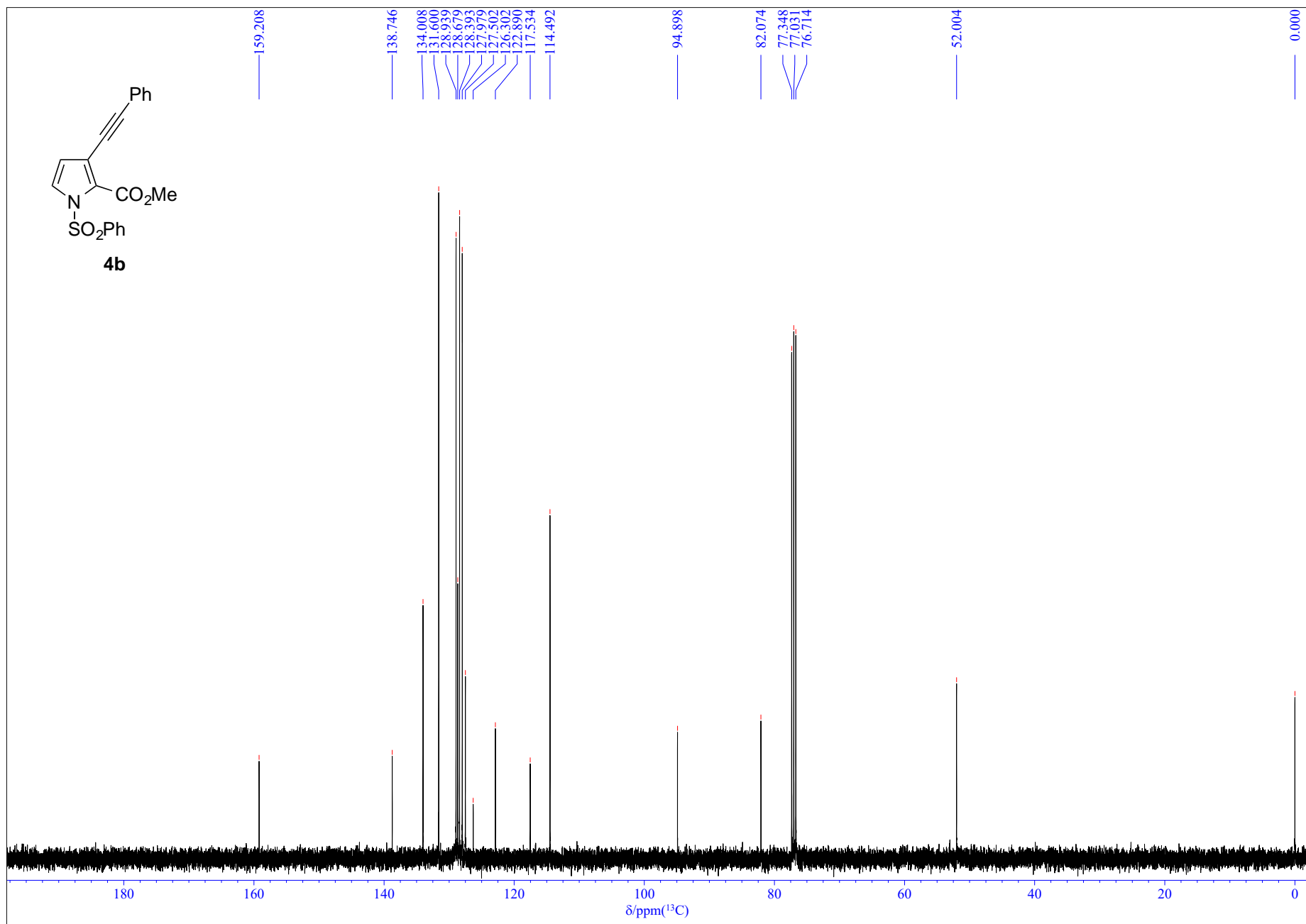


Figure S4. ^{13}C NMR spectrum of compound **4b** (100 MHz, CDCl_3).

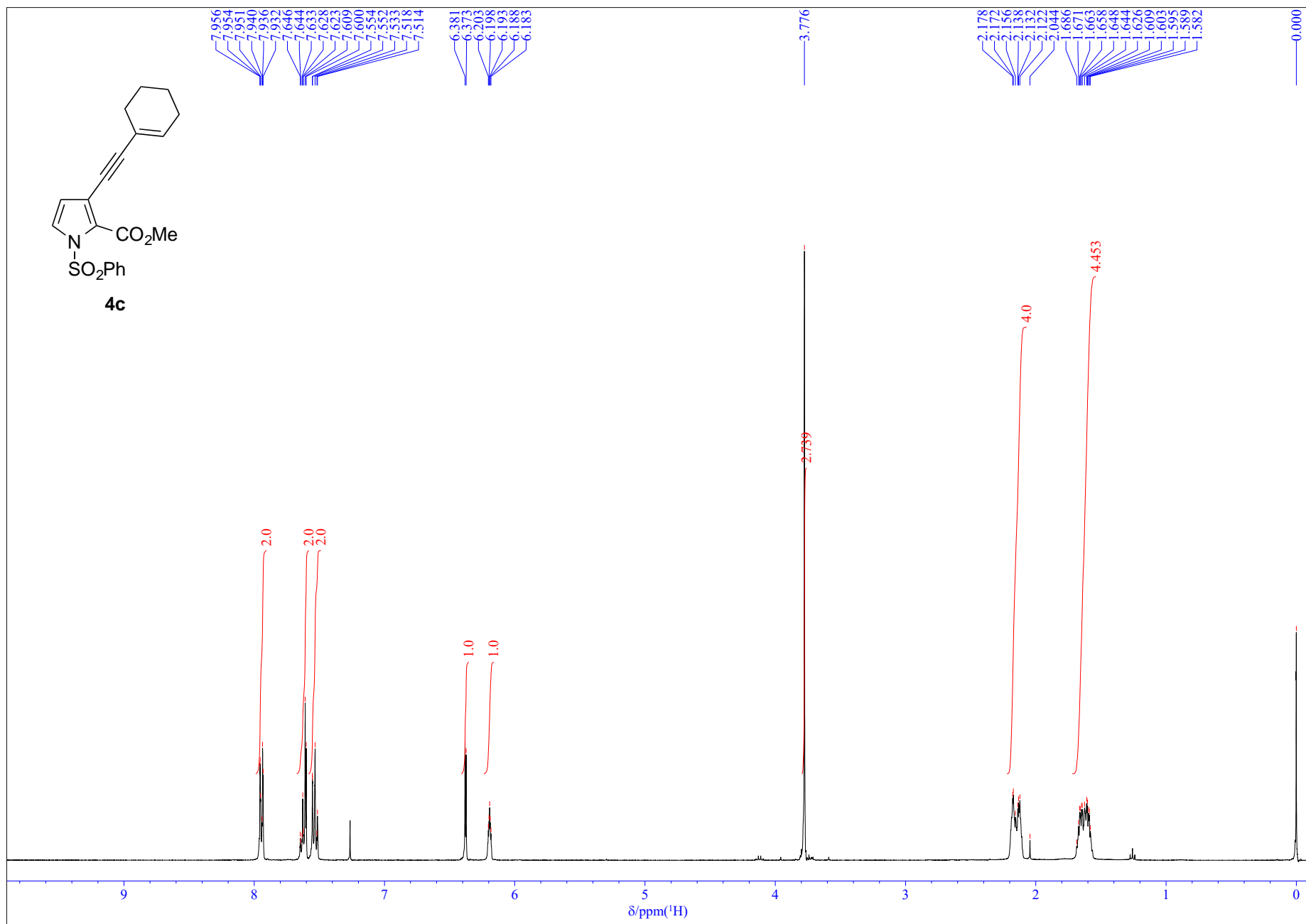


Figure S5. ¹H NMR spectrum of compound **4c** (400 MHz, CDCl₃).

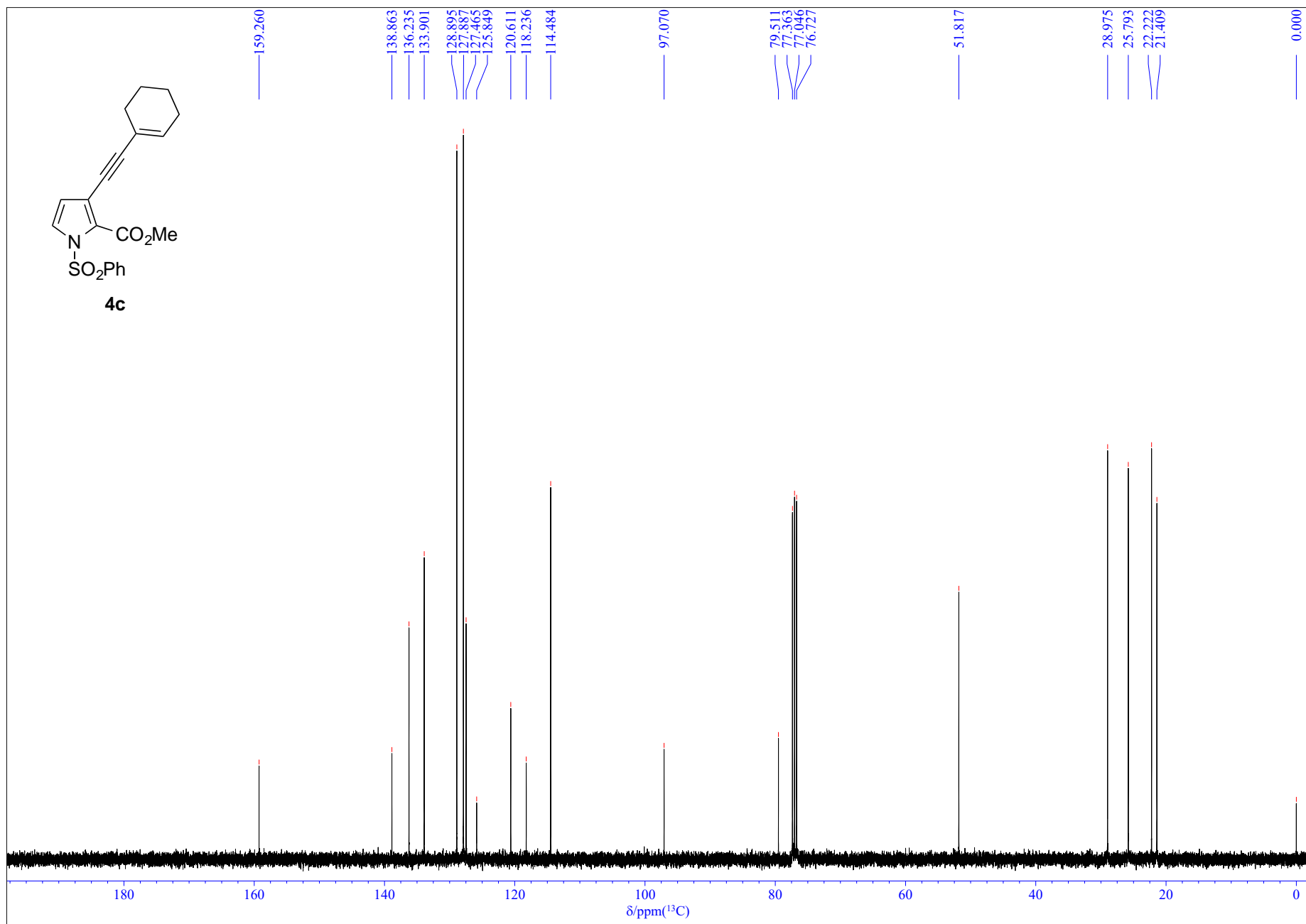


Figure S6. ^{13}C NMR spectrum of compound **4c** (100 MHz, CDCl_3).

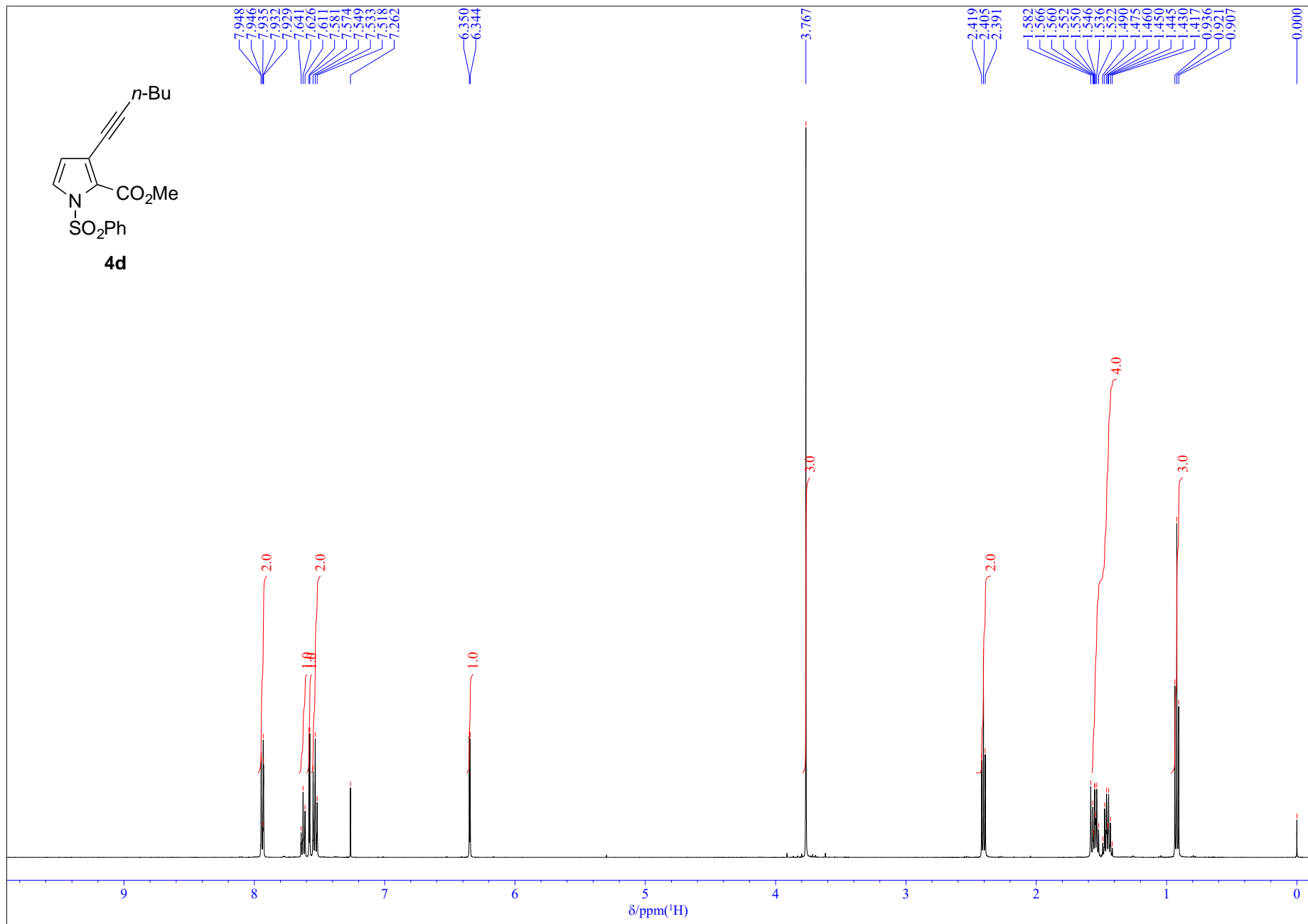


Figure S7. ¹H NMR spectrum of compound **4d** (500 MHz, CDCl₃).

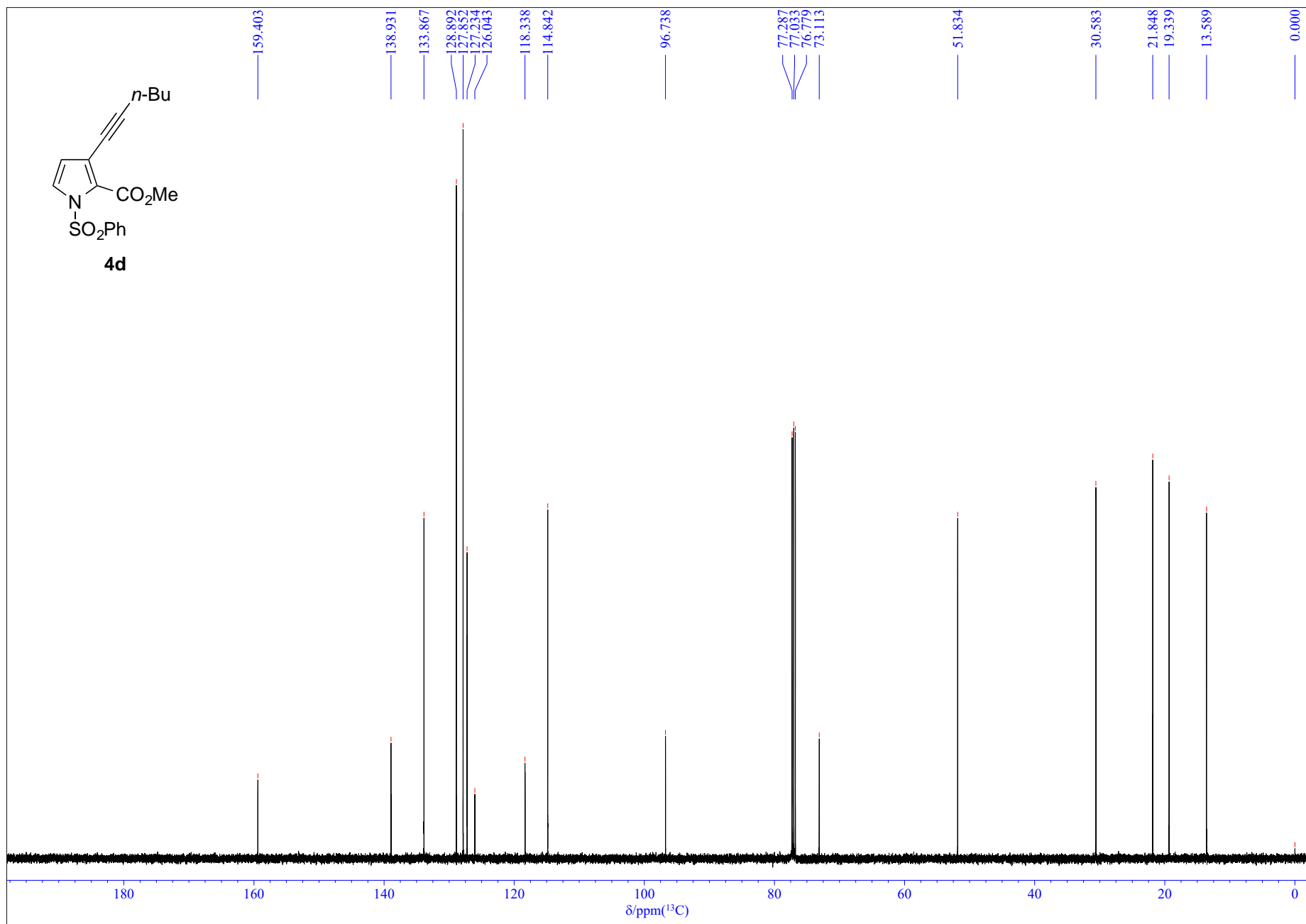


Figure S8. ${}^{13}\text{C}$ NMR spectrum of compound **4d** (126 MHz, CDCl_3).

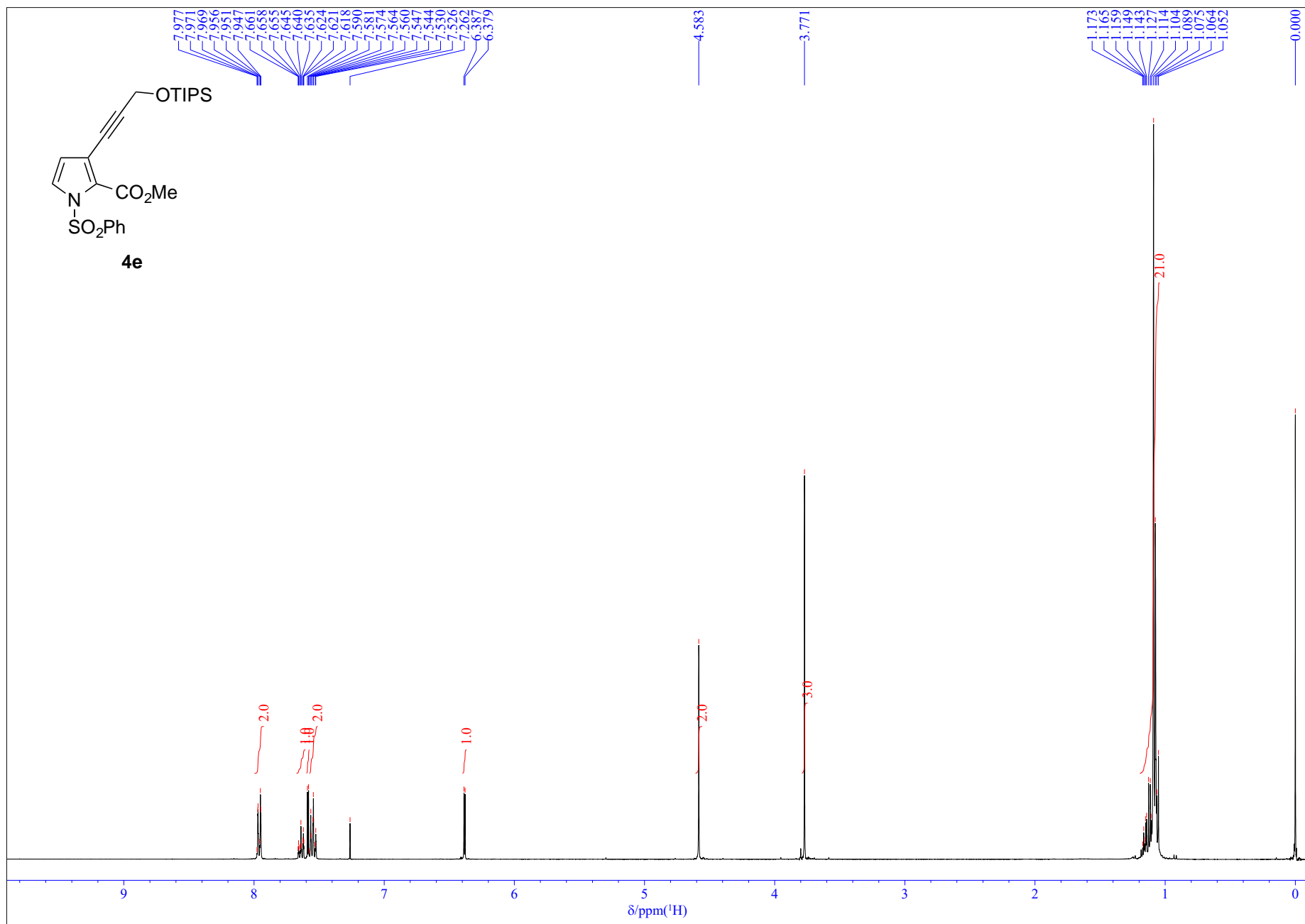


Figure S9. ^1H NMR spectrum of compound **4e** (400 MHz, CDCl_3).

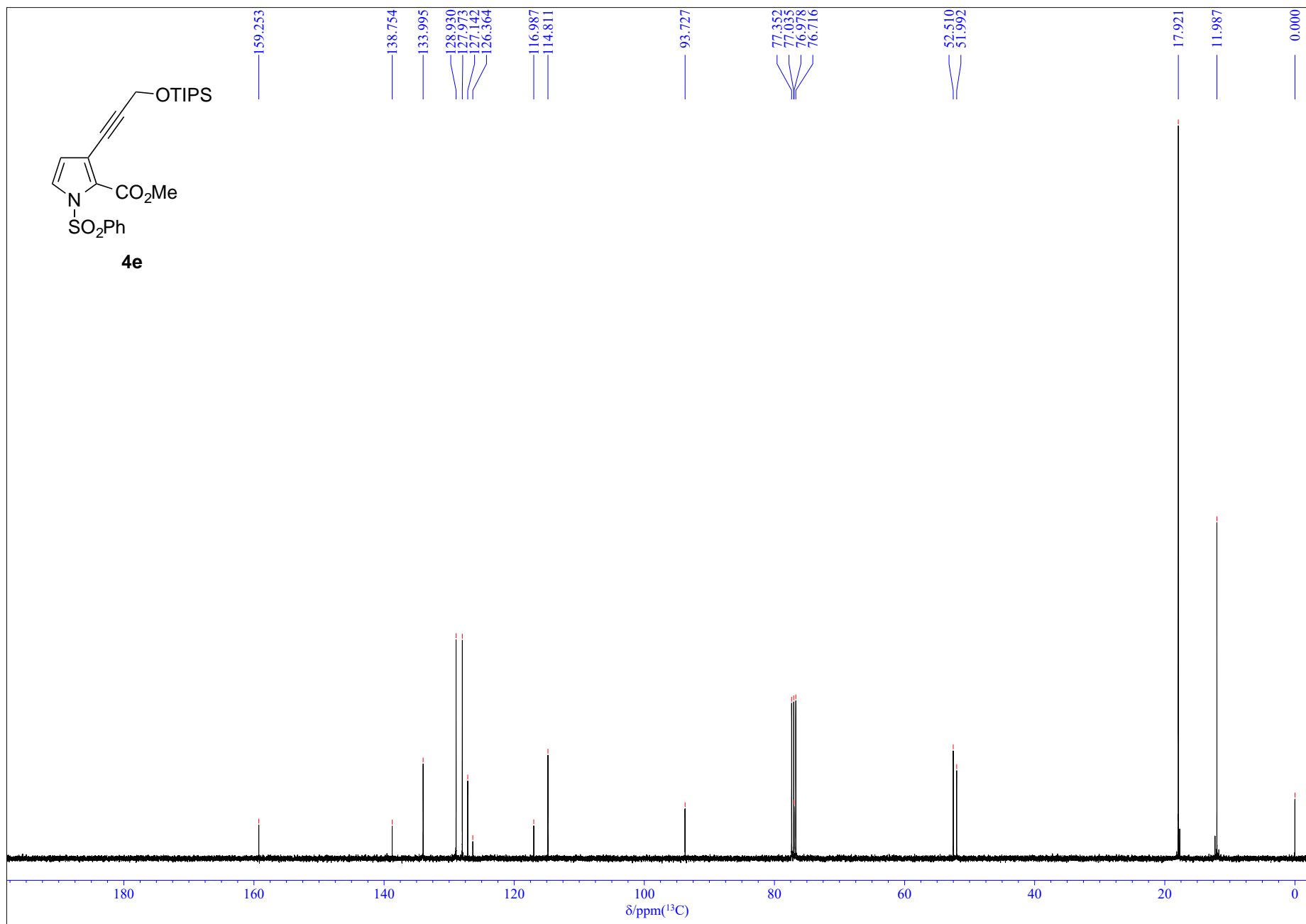


Figure S10. ^{13}C NMR spectrum of compound **4e** (100 MHz, CDCl_3).

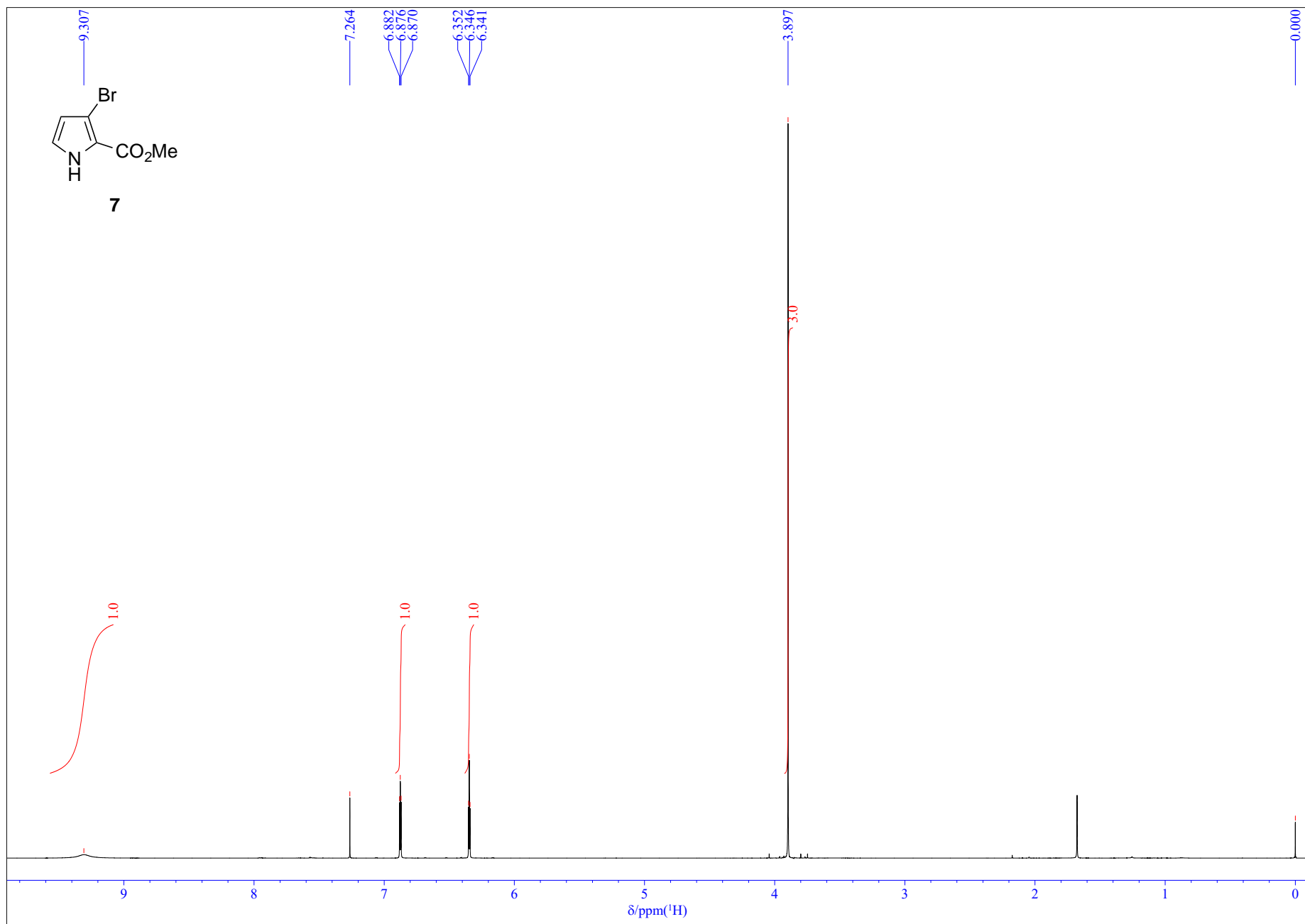


Figure S11. ^1H NMR spectrum of compound **7** (500 MHz, CDCl_3).

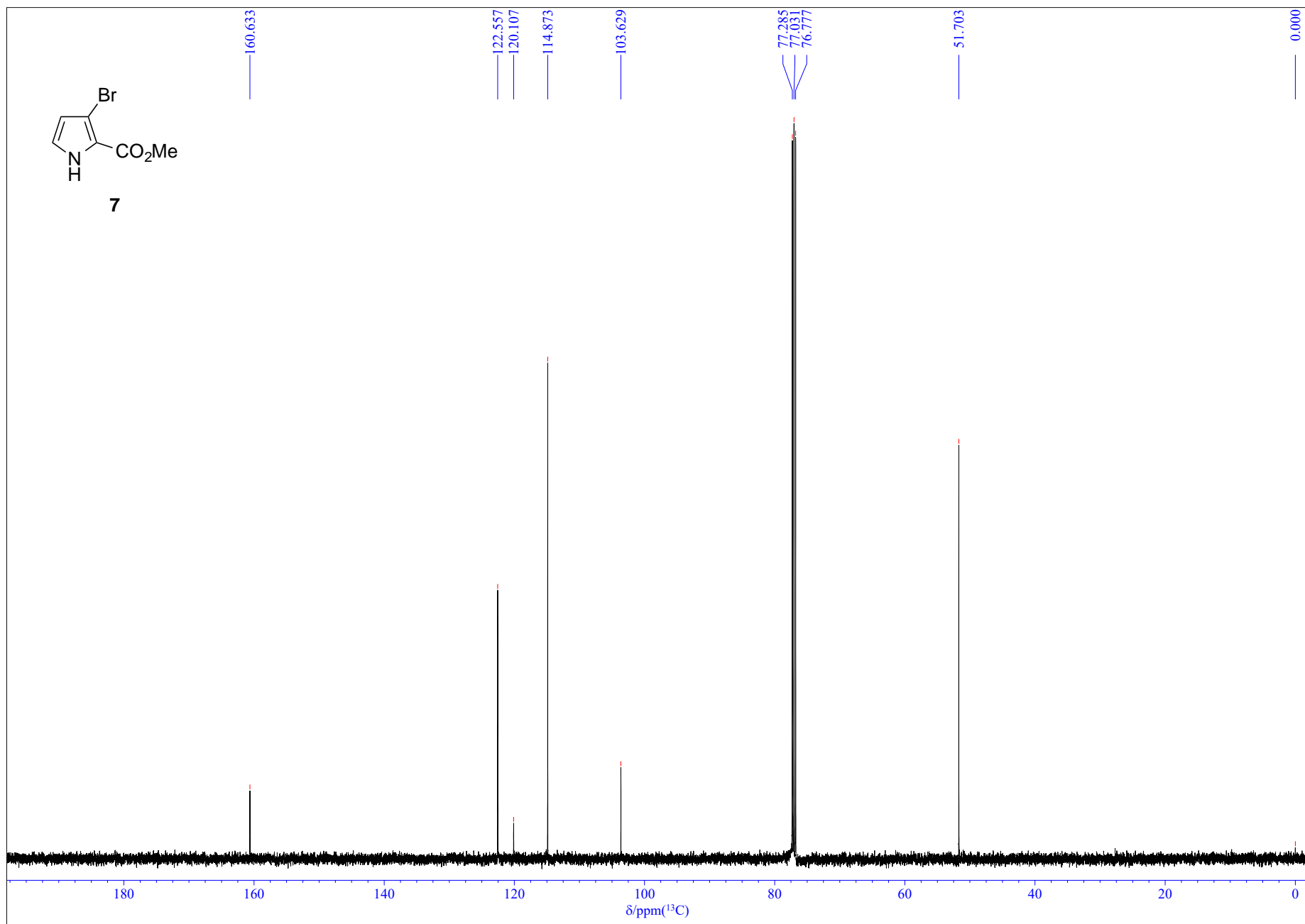


Figure S12. ^{13}C NMR spectrum of compound **7** (126 MHz, CDCl_3).

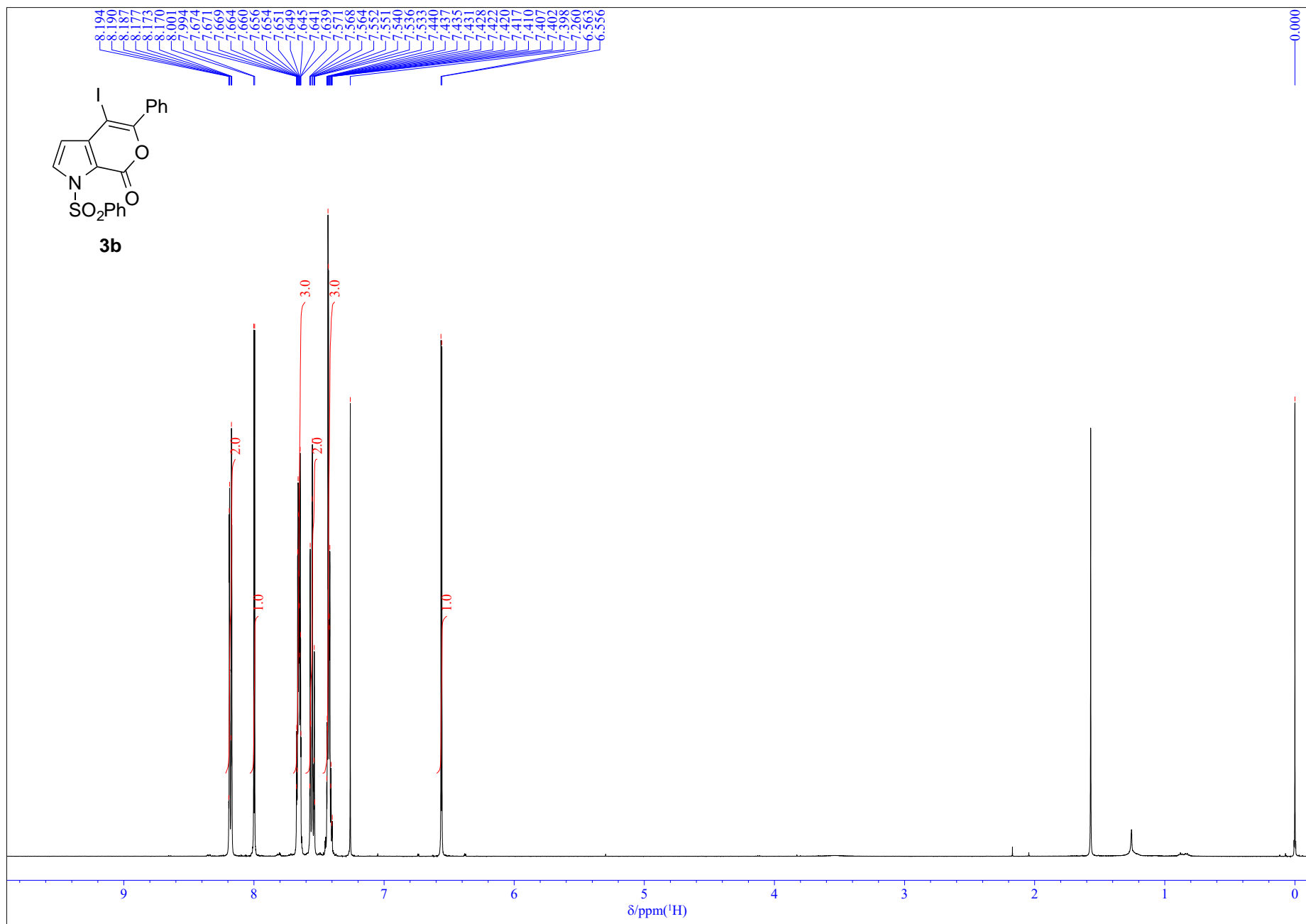


Figure S13. ¹H NMR spectrum of compound **3b** (500 MHz, CDCl₃).

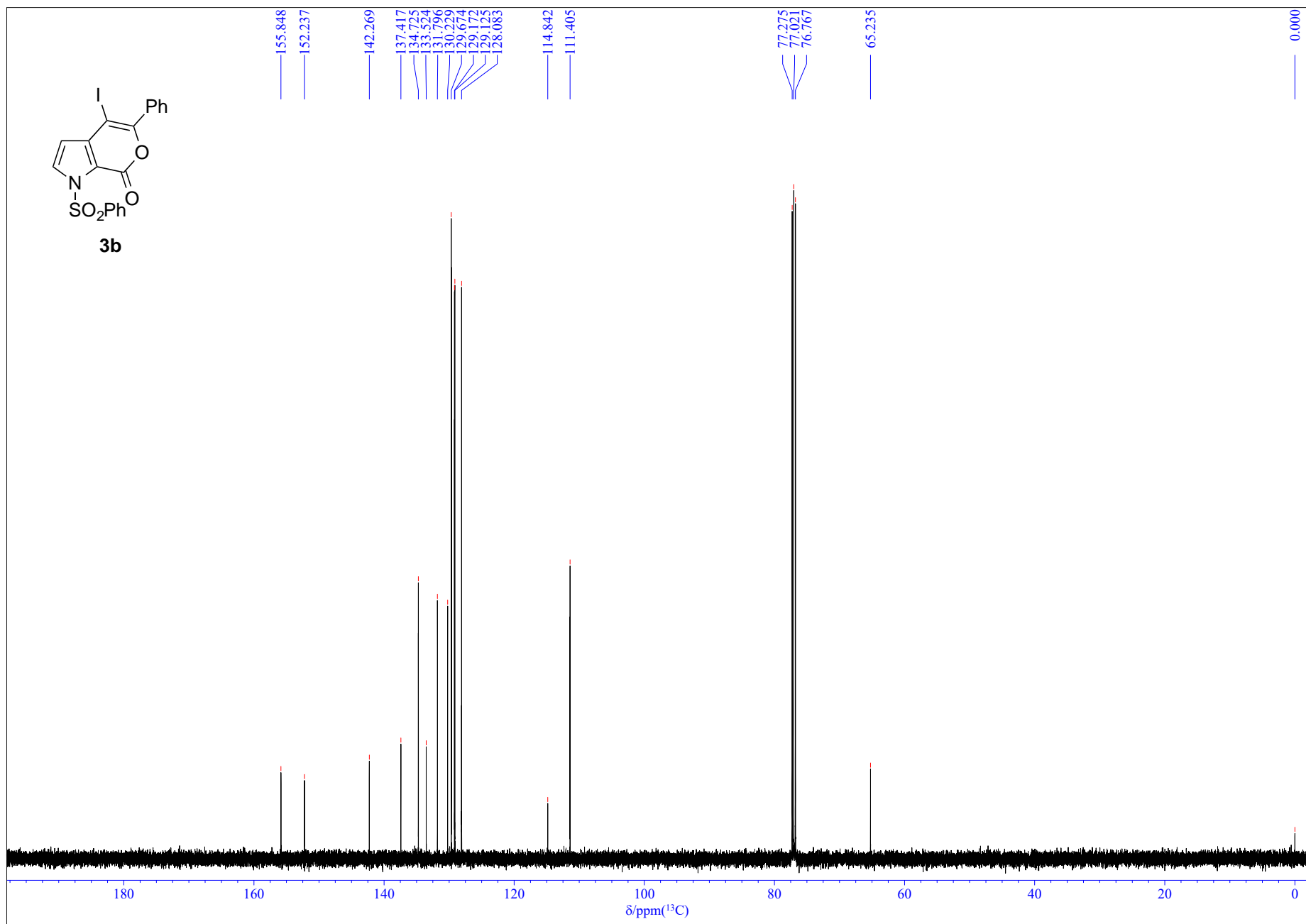


Figure S14. ^{13}C NMR spectrum of compound **3b** (126 MHz, CDCl_3).

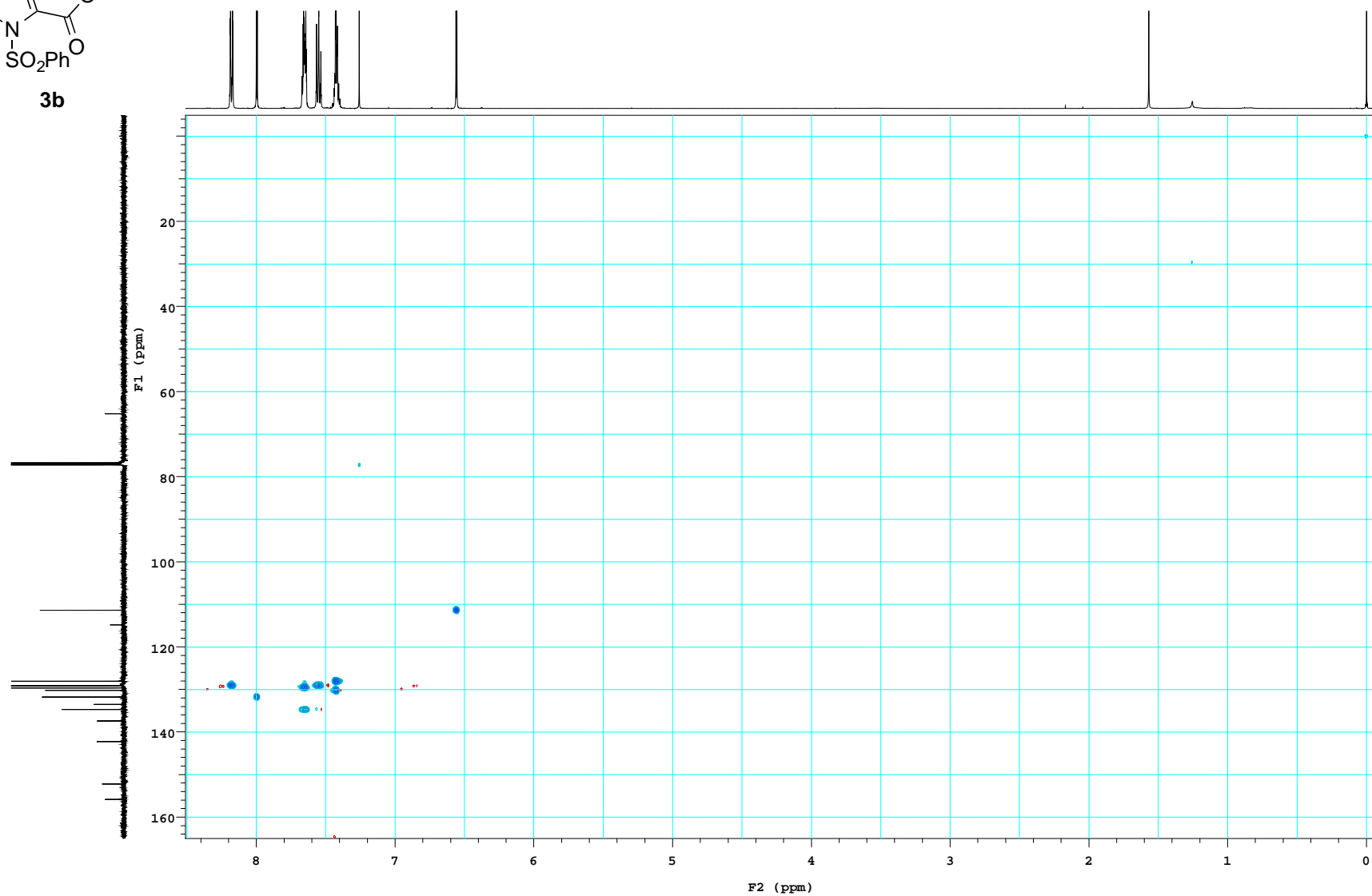
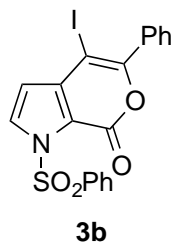


Figure S15. HMQC spectrum of compound **3b** (CDCl₃).

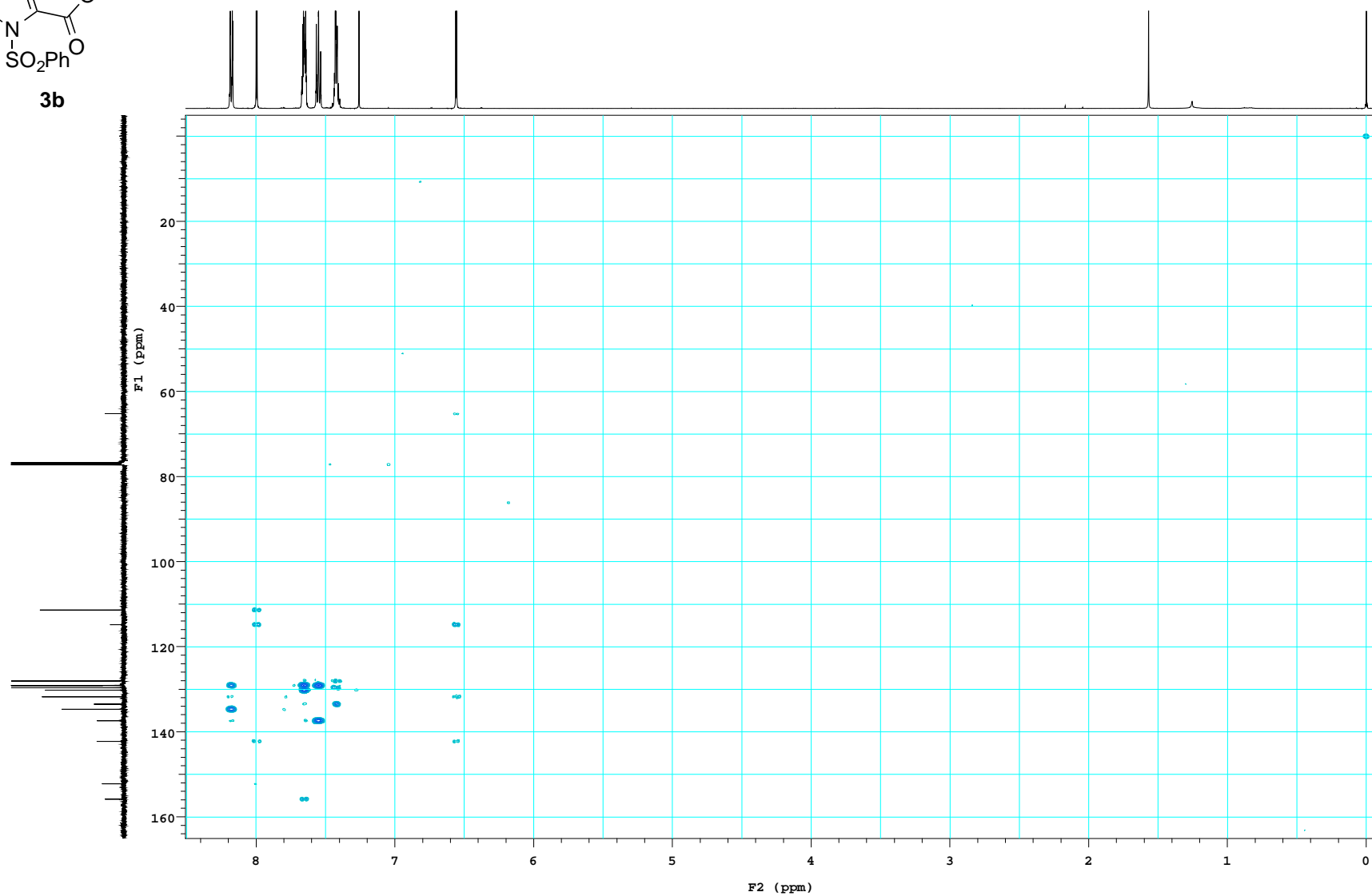
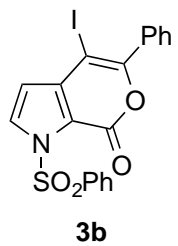
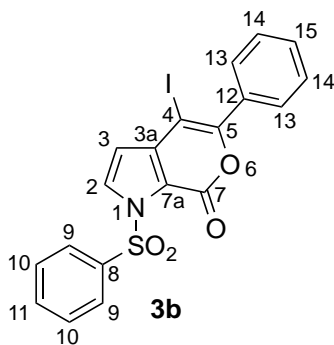


Figure S16. HMBC spectrum of compound **3b** (CDCl_3).

Table S1. NMR data for **3b** in CDCl₃.



C no.	δ_C	δ_H	HMBC (C no.)
2	131.8	8.00 (d, $J = 3.4$ Hz, 1H)	3, 3a, 7, 7a
3	111.4	6.56 (d, $J = 3.4$ Hz, 1H)	2, 3a, 4, 7a
3a	114.8		
4	65.2		
5	155.8		
7	152.2		
7a	142.3		
8	137.4		
9	129.1	8.16–8.20 (m, 2H)	8, 9, 11
10	129.2	7.53–7.57 (m, 2H)	8, 10
11	134.7	7.63–7.68 (m, 1H)	9
12	133.5		
13	129.7	7.63–7.68 (m, 2H)	5, 12, 15
14	128.1	7.39–7.46 (m, 2H)	12, 14
15	130.2	7.39–7.46 (m, 1H)	13

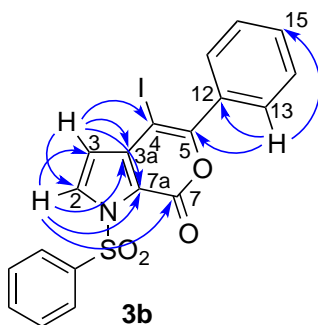


Figure S17. Key HMBC correlations in **3b**.

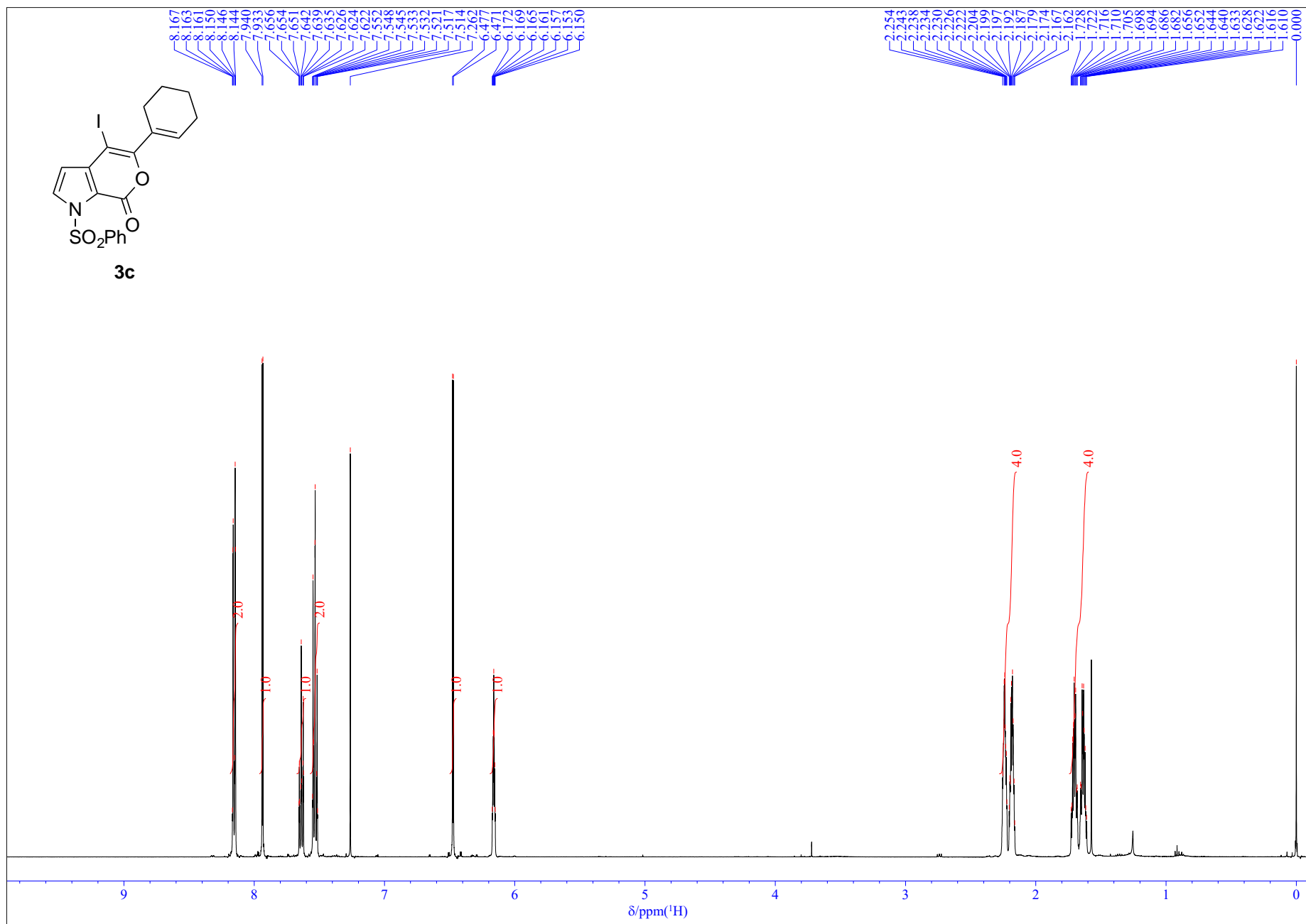


Figure S18. ^1H NMR spectrum of compound **3c** (500 MHz, CDCl_3).

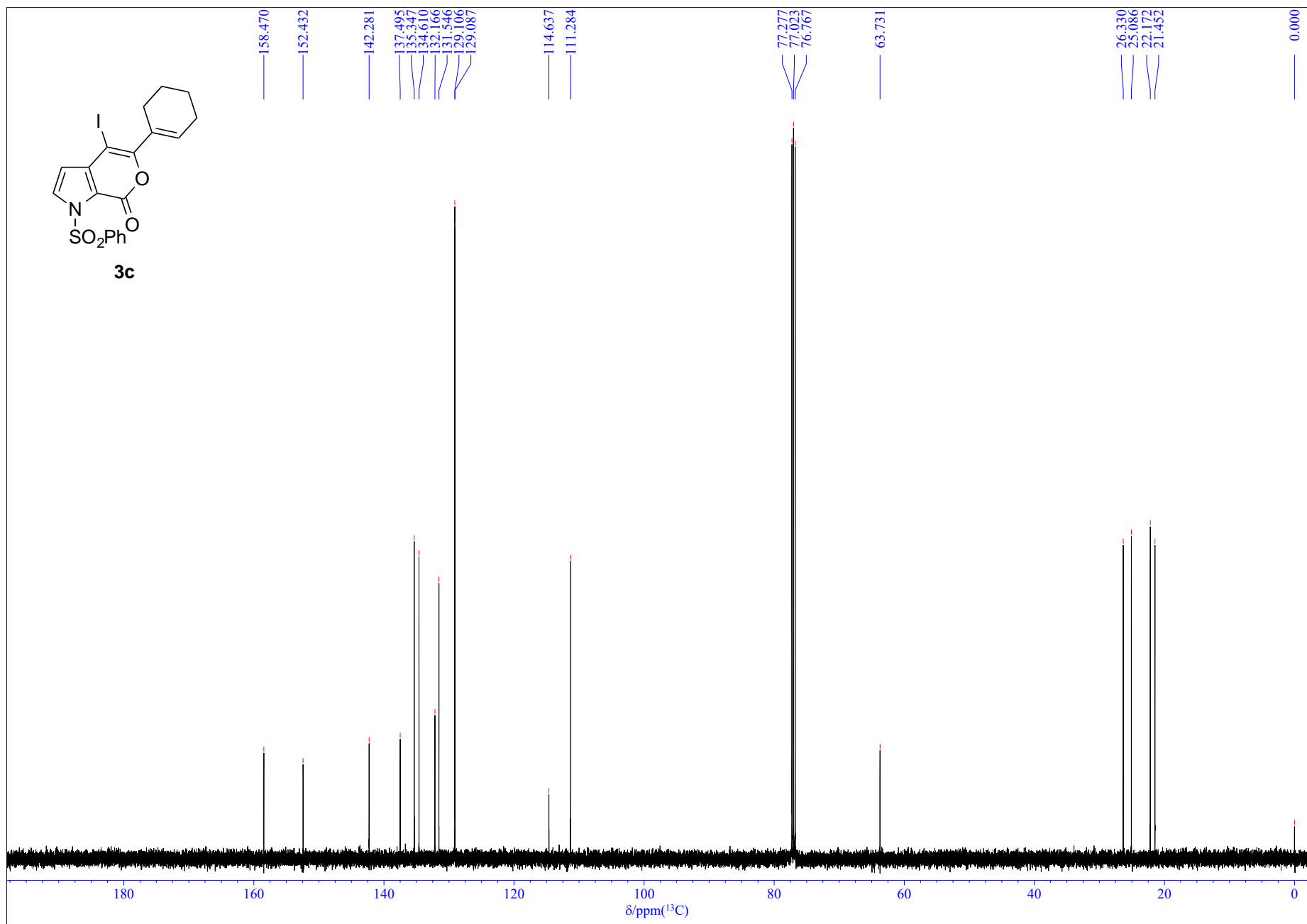


Figure S19. ^{13}C NMR spectrum of compound **3c** (126 MHz, CDCl_3).

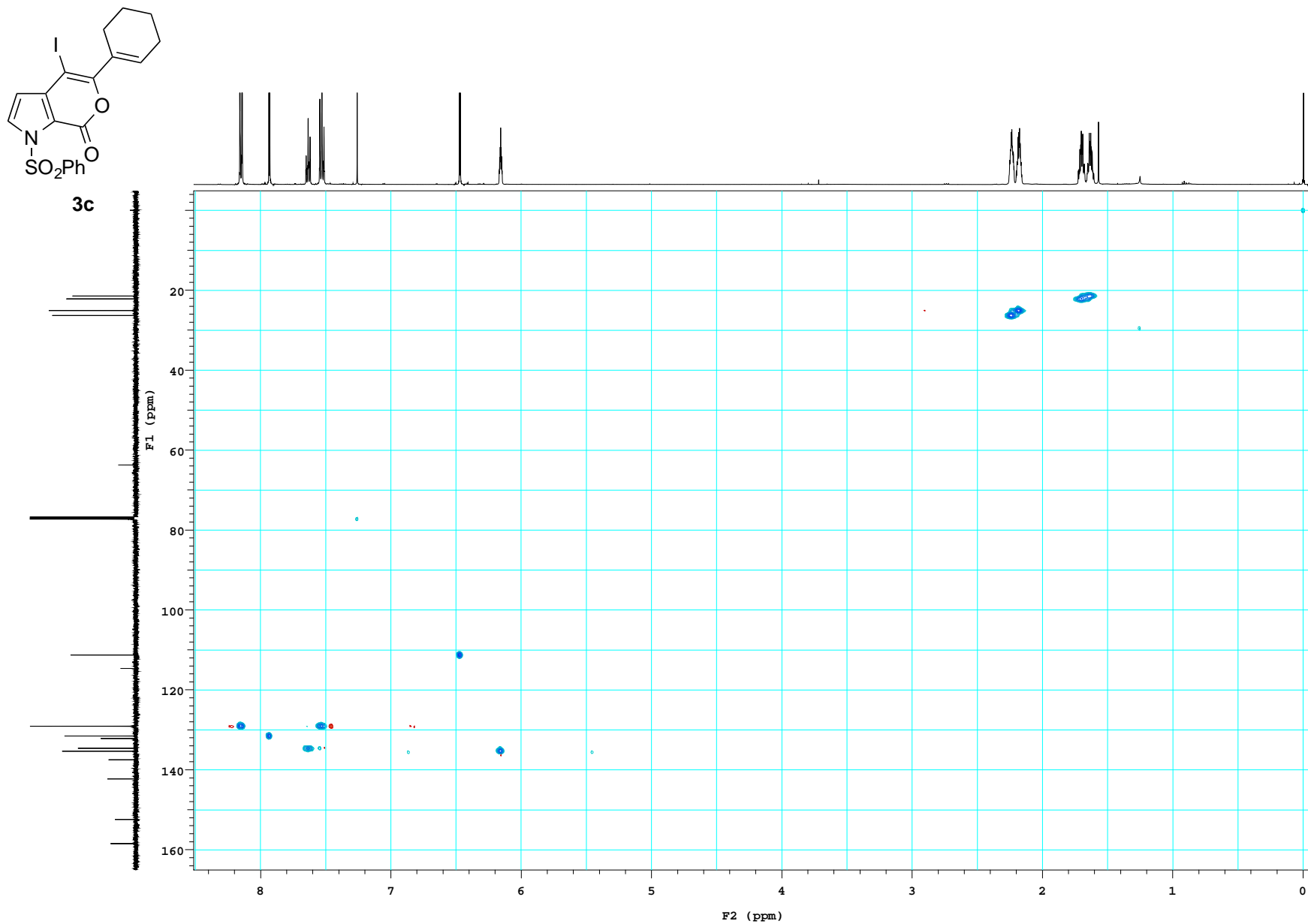


Figure S20. HMPC spectrum of compound **3c** (CDCl₃).

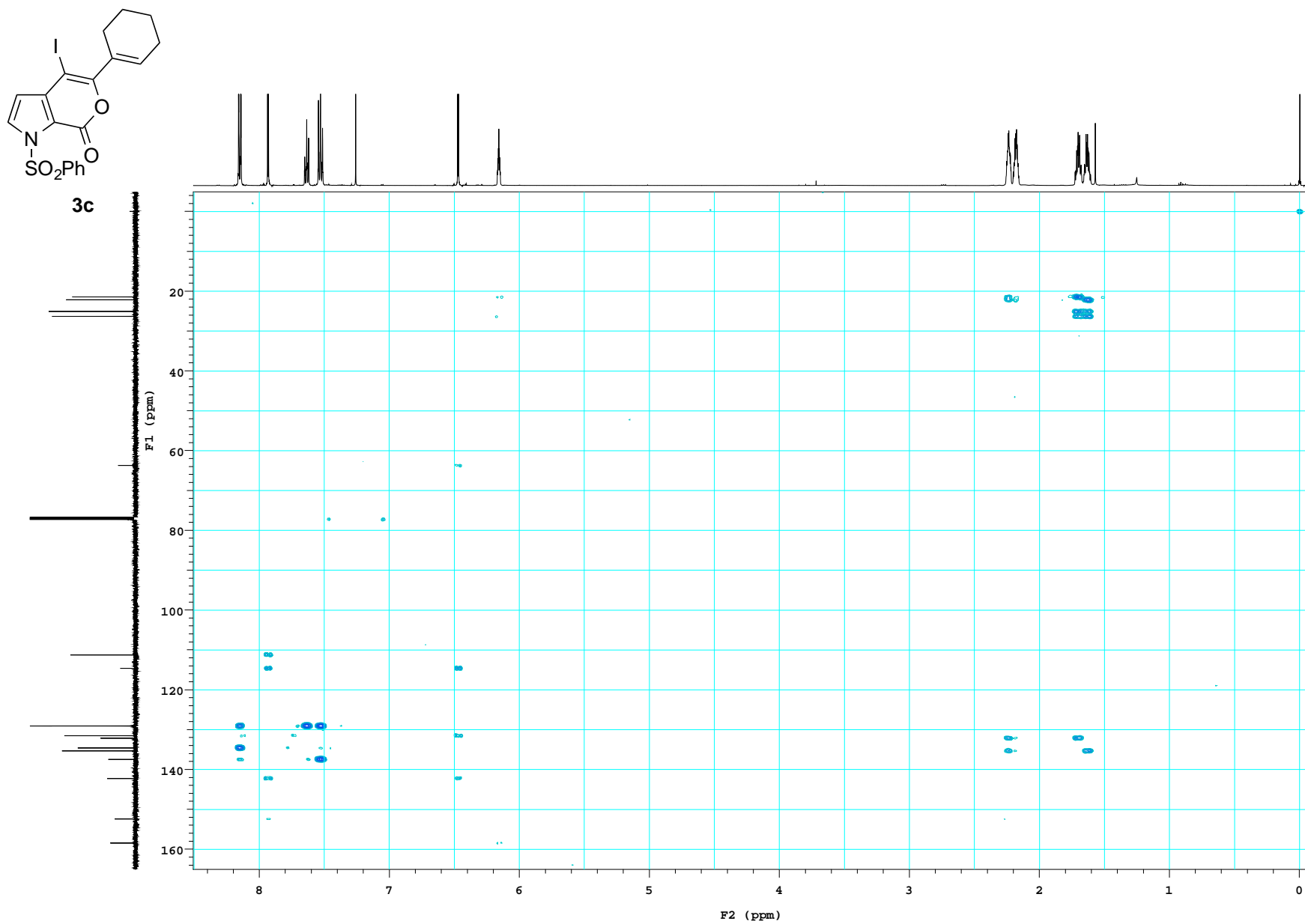
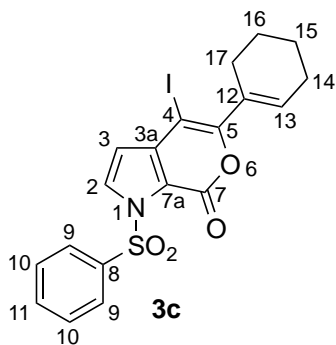


Figure S21. HMBC spectrum of compound **3c** (CDCl₃).

Table S2. NMR data for **3c** in CDCl₃.



C no.	δ_C	δ_H	HMBC (C no.)
2	131.5	7.94 (d, $J = 3.4$ Hz, 1H),	3, 3a, 7, 7a
3	111.3	6.47 (d, $J = 3.4$ Hz, 1H),	2, 3a, 4, 7a
3a	114.6		
4	63.7		
5	158.5		
7	152.4		
7a	142.3		
8	137.5		
9	129.1 (129.08)	8.14–8.17 (m, 2H).	8, 9, 11
10	129.1 (129.11)	7.51–7.56 (m, 2H),	8, 10
11	134.6	7.62–7.66 (m, 1H),	9
12	132.2		
13	135.3	6.14–6.18 (m, 1H),	5, 15, 17
14	25.1	2.15–2.21 (m, 2H),	12, 13, 16
15	21.5	1.60–1.67 (m, 2H),	13, 14, 16, 17
16	22.2	1.67–1.74 (m, 2H),	12, 14, 15, 17
17	26.3	2.22–2.27 (m, 2H),	12, 13, 15, 16

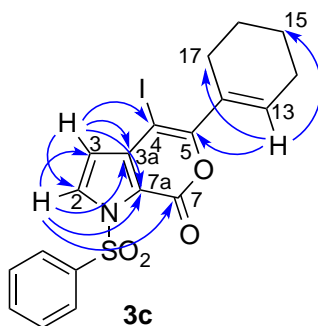


Figure S22. Key HMBC correlations in **3c**.

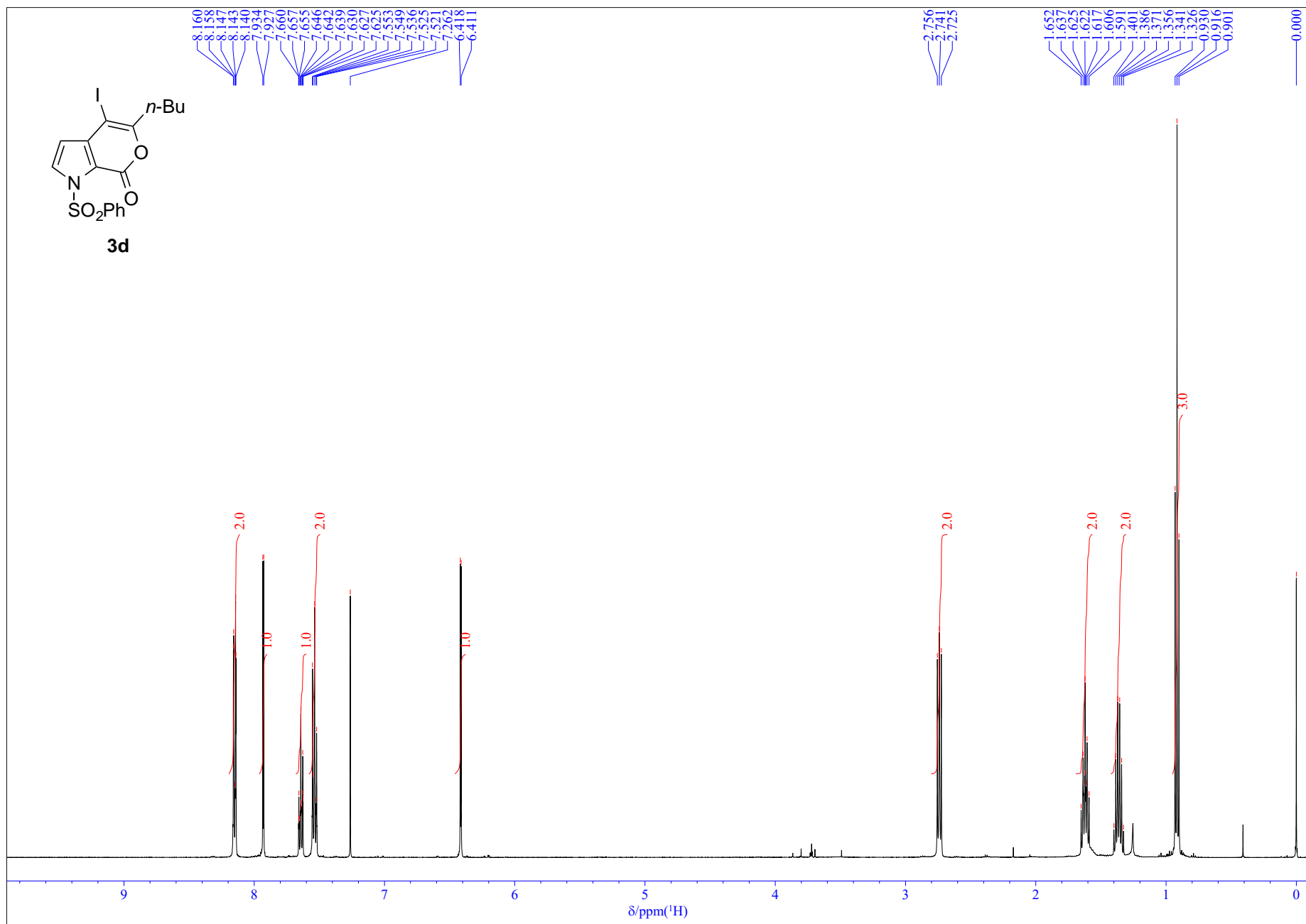


Figure S23. ^1H NMR spectrum of compound **3d** (500 MHz, CDCl_3).

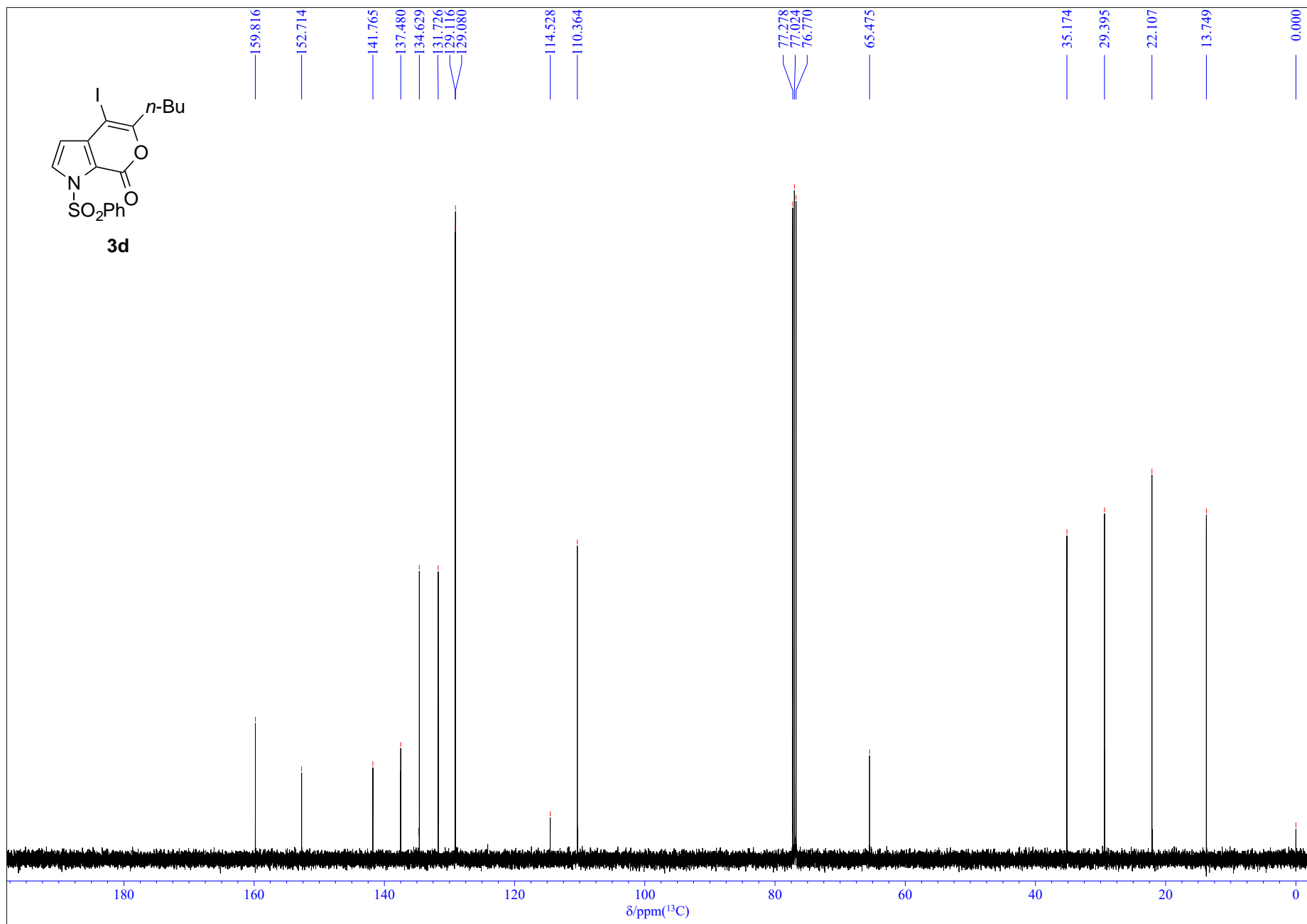


Figure S24. ^{13}C NMR spectrum of compound **3d** (126 MHz, CDCl_3).

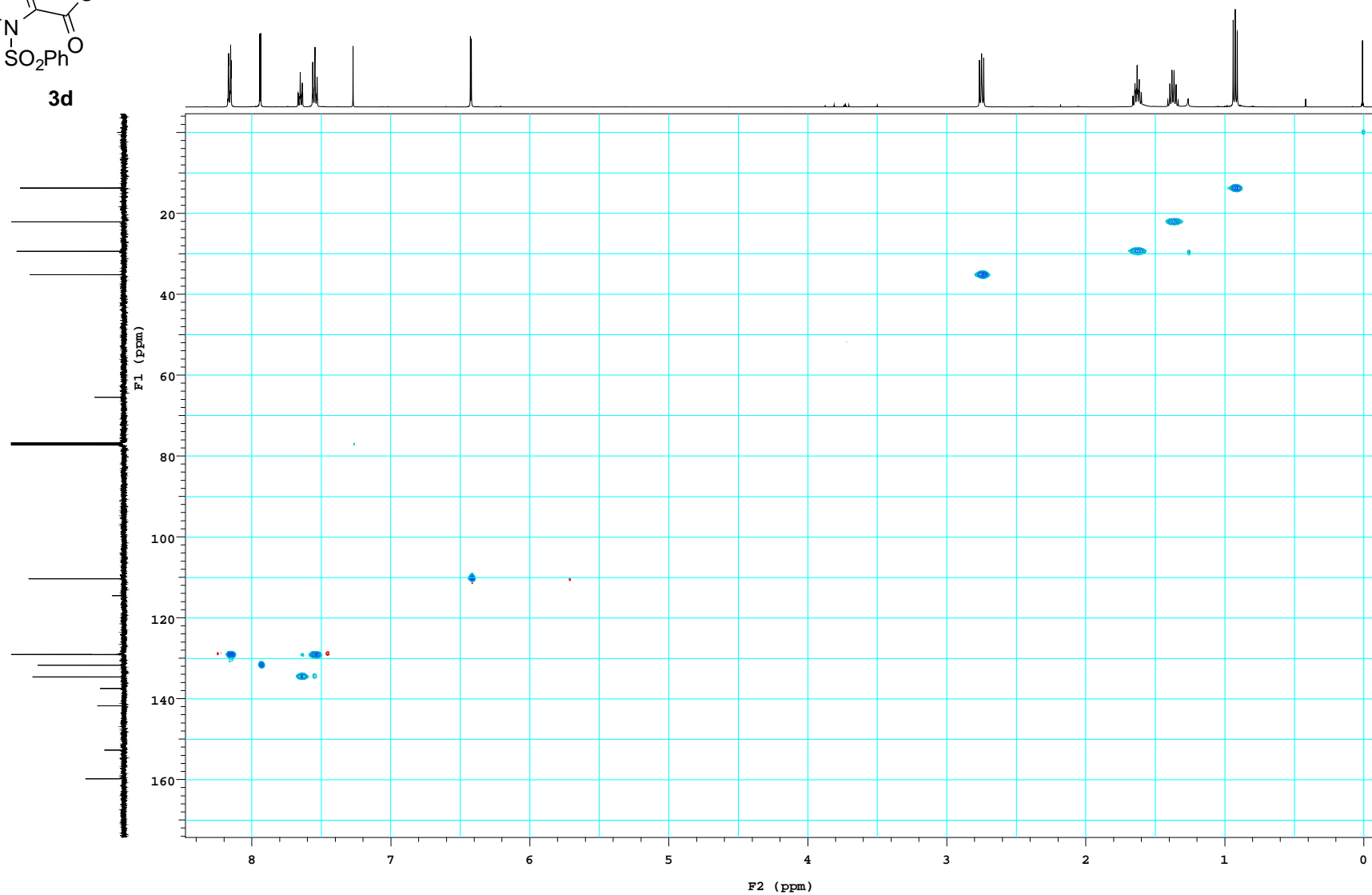
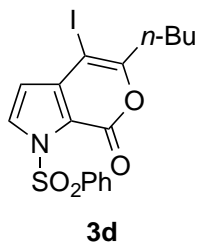


Figure S25. HMBC spectrum of compound **3d** ($CDCl_3$).

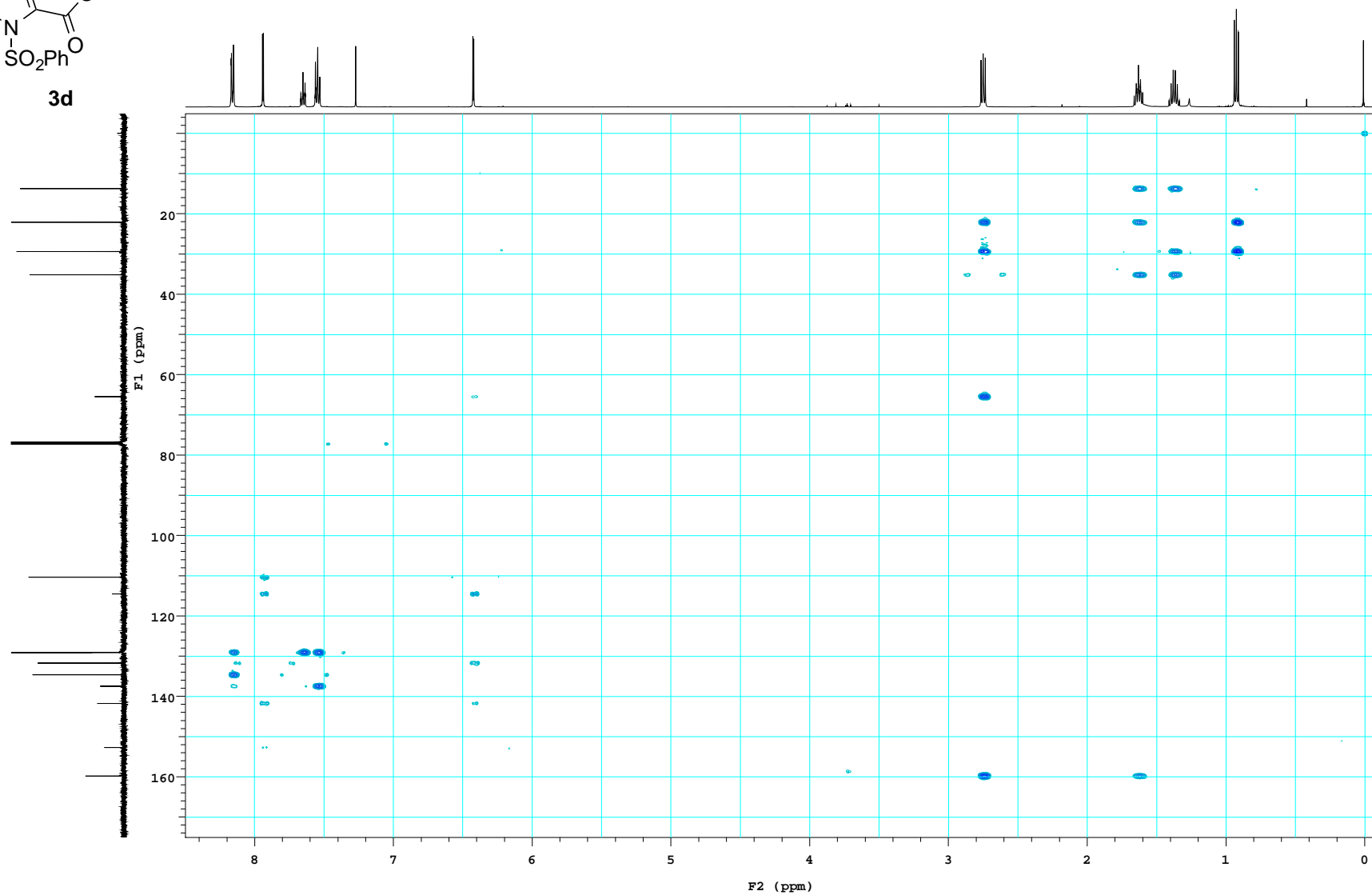
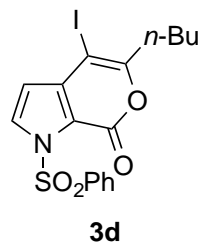
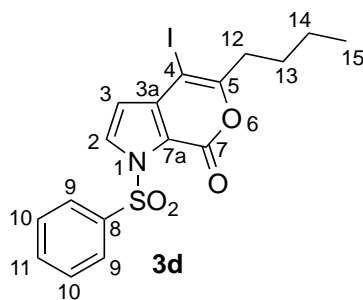


Figure S26. HMBC spectrum of compound **3d** (CDCl₃).

Table S3. NMR data for **3d** in CDCl₃.



C no.	δ_C	δ_H	HMBC (C no.)
2	131.7	7.93 (d, $J = 3.4$ Hz, 1H)	3, 3a, 7, 7a
3	110.4	6.41 (d, $J = 3.4$ Hz, 1H)	2, 3a, 4, 7a
3a	114.5		
4	65.5		
5	159.8		
7	152.7		
7a	141.8		
8	137.5		
9	129.1 (129.08)	8.13–8.17 (m, 2H)	8, 9, 11
10	129.1 (129.12)	7.51–7.56 (m, 2H)	8, 10
11	134.6	7.62–7.67 (m, 1H)	9
12	35.2	2.74 (t, $J = 7.7$ Hz, 2H)	4, 5, 13, 14
13	29.4	1.58–1.66 (m, 2H)	5, 12, 14, 15
14	22.1	1.32–1.41 (m, 2H)	12, 13, 15
15	13.7	0.92 (t, $J = 7.4$ Hz, 3H)	13, 14

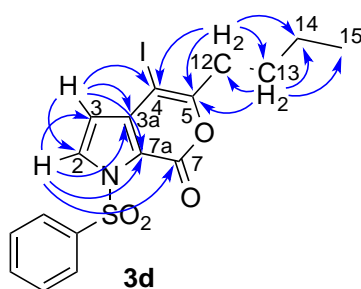


Figure S27. Key HMBC correlations in **3d**.

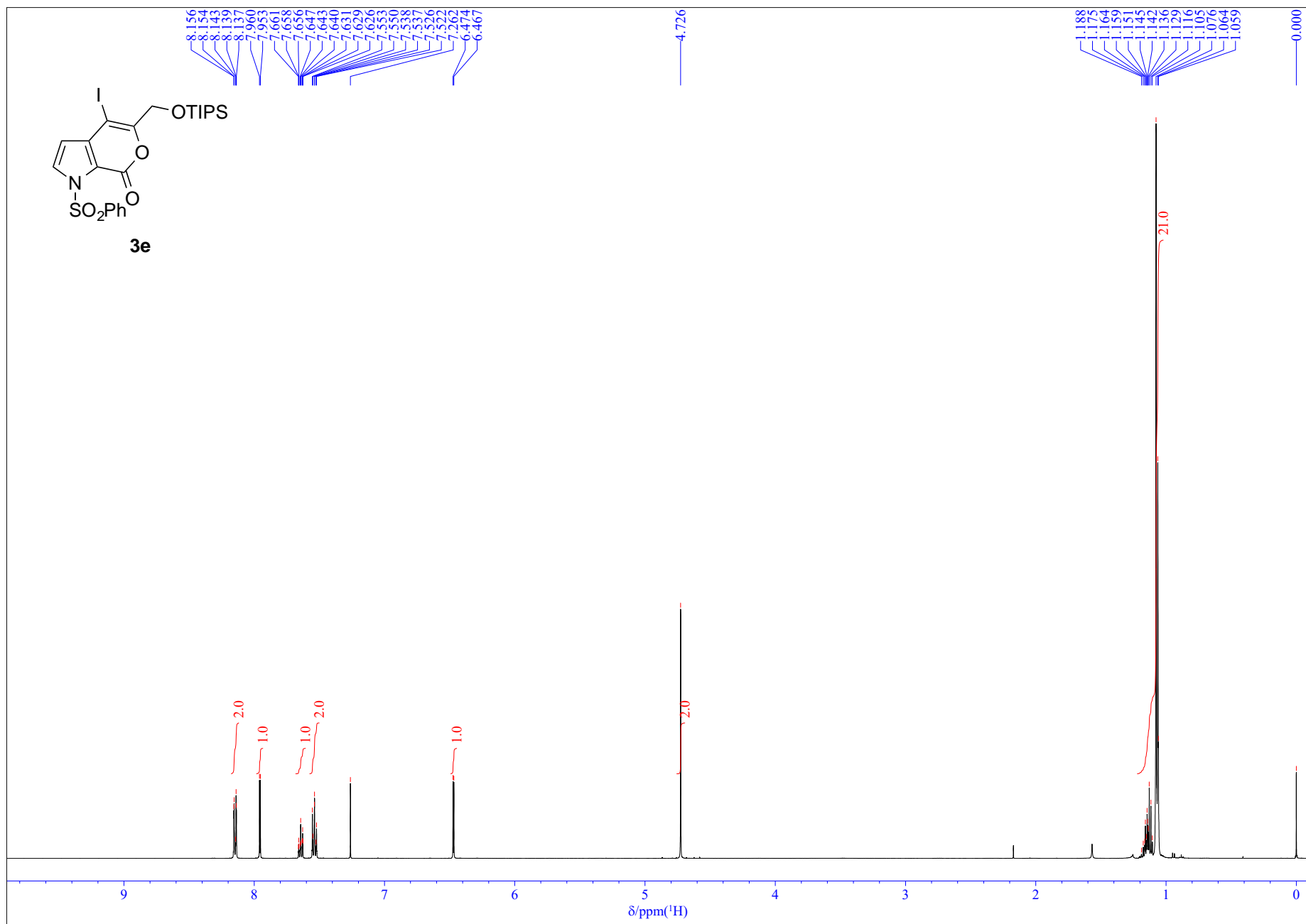


Figure S28. ^1H NMR spectrum of compound **3e** (500 MHz, CDCl_3).

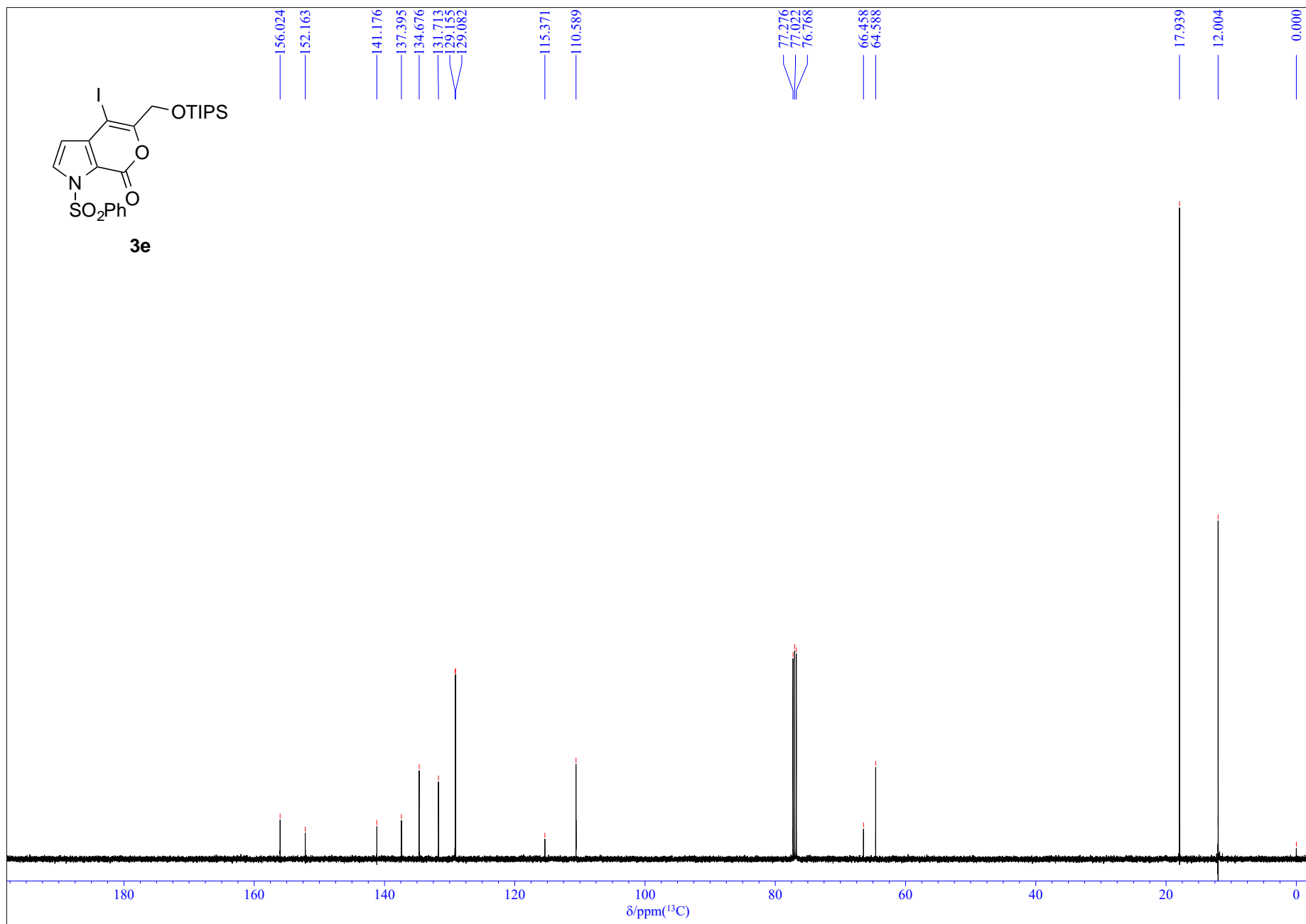
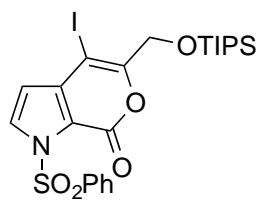


Figure S29. ^{13}C NMR spectrum of compound **3e** (126 MHz, CDCl_3).



3e

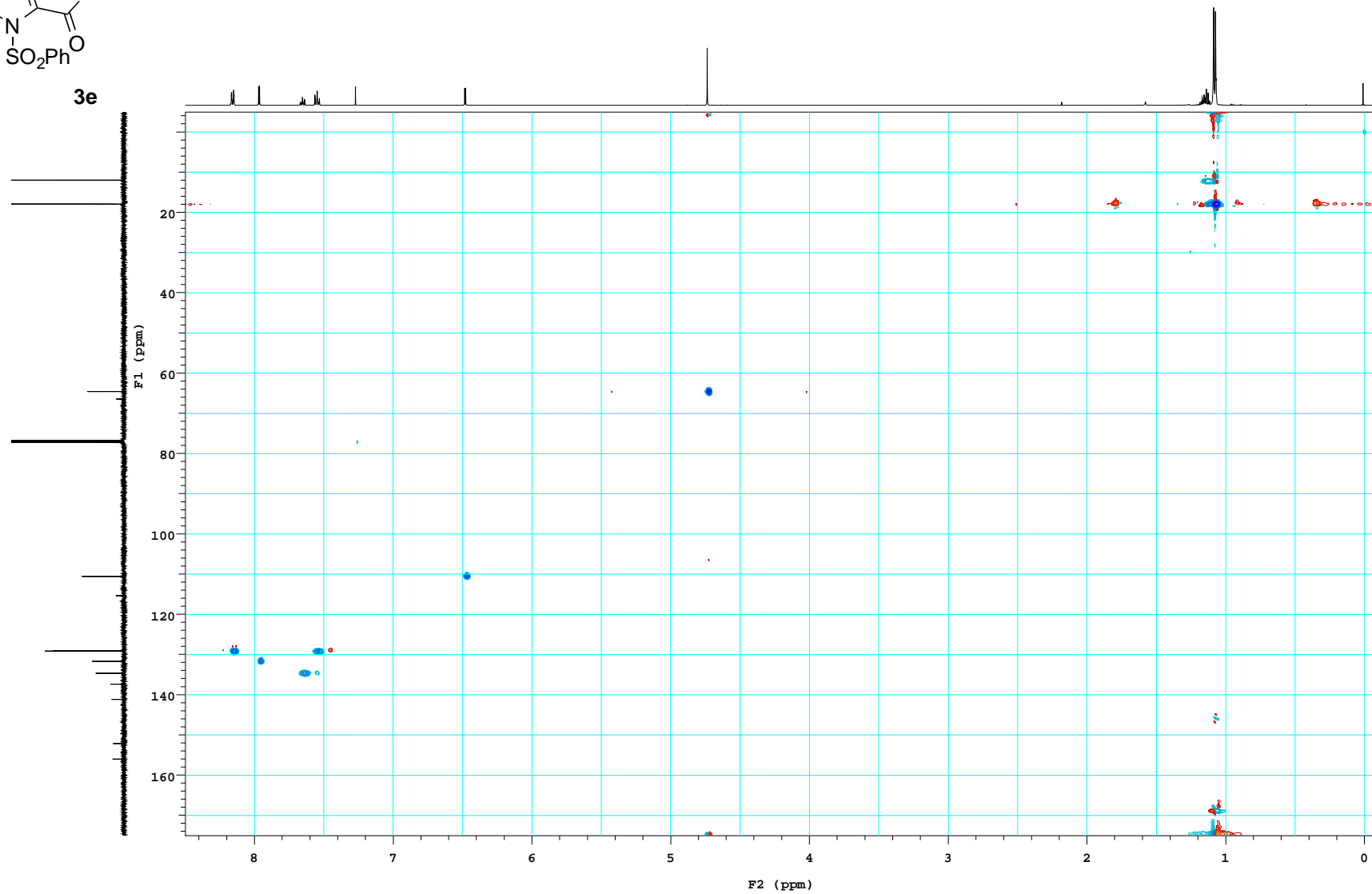
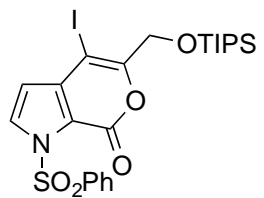


Figure S30. HMBC spectrum of compound **3e** (CDCl_3).



3e

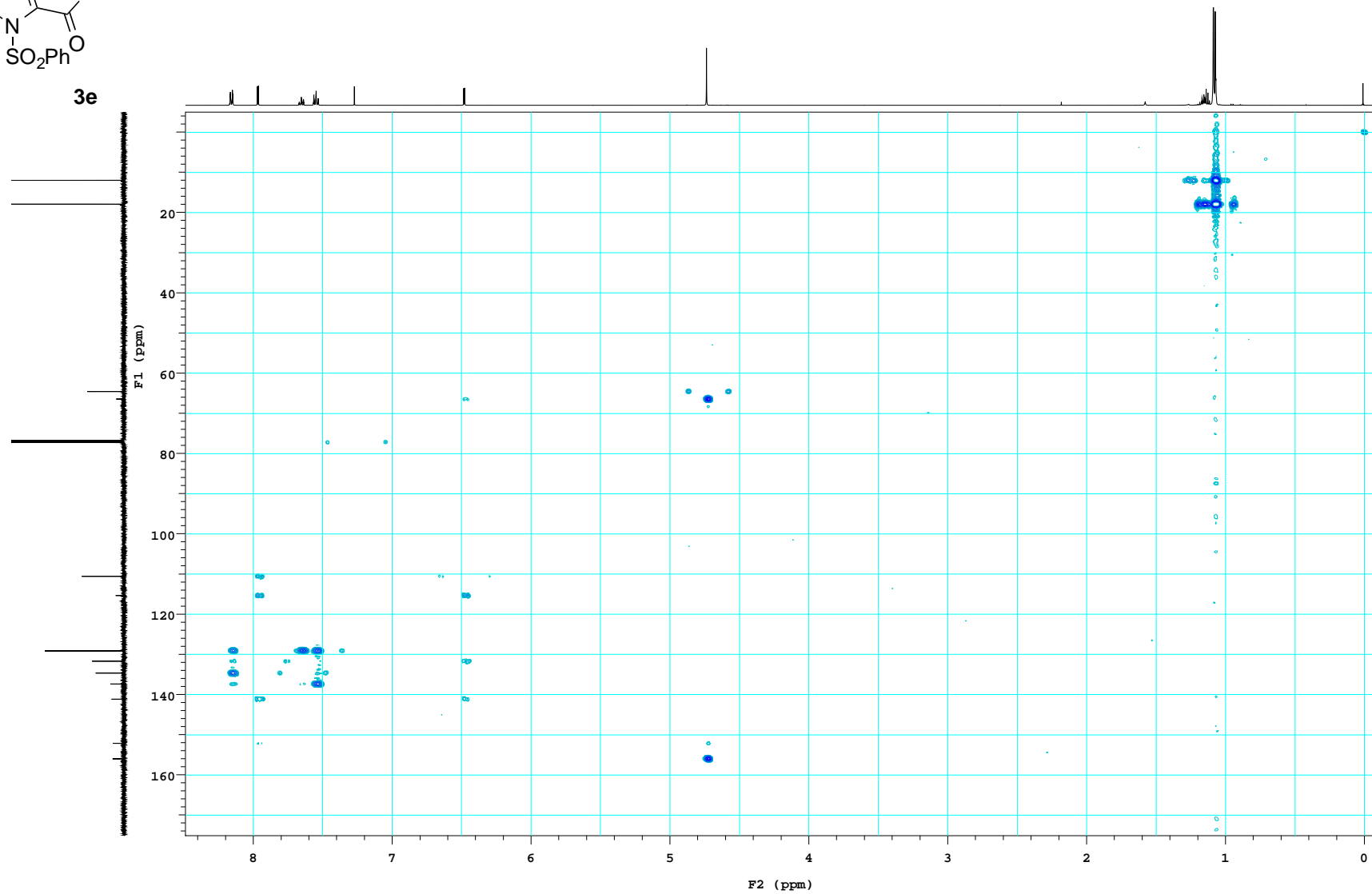
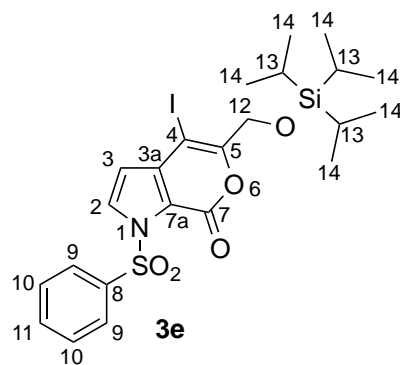


Figure S31. HMBC spectrum of compound **3e** (CDCl_3).

Table S4. NMR data for **3e** in CDCl₃.



C no.	δ_C	δ_H	HMBC (C no.)
2	131.7	7.96 (d, $J = 3.4$ Hz, 1H)	3, 3a, 7, 7a
3	110.6	6.47 (d, $J = 3.4$ Hz, 1H)	2, 3a, 4, 7a
3a	115.4		
4	66.5		
5	156.0		
7	152.2		
7a	141.2		
8	137.4		
9	129.1	8.13–8.17 (m, 2H)	8, 9, 11
10	129.2	7.51–7.56 (m, 2H)	8, 10
11	134.7	7.62–7.67 (m, 1H)	9
12	64.6	4.73 (s, 2H)	4, 5, 7
13	12.0	1.10–1.20 (m, 3H)	14
14	17.9	1.05–1.09 (m, 18H)	13, 14

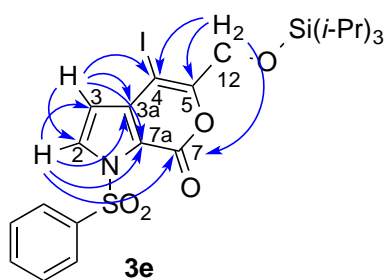


Figure S32. Key HMBC correlations in **3e**.

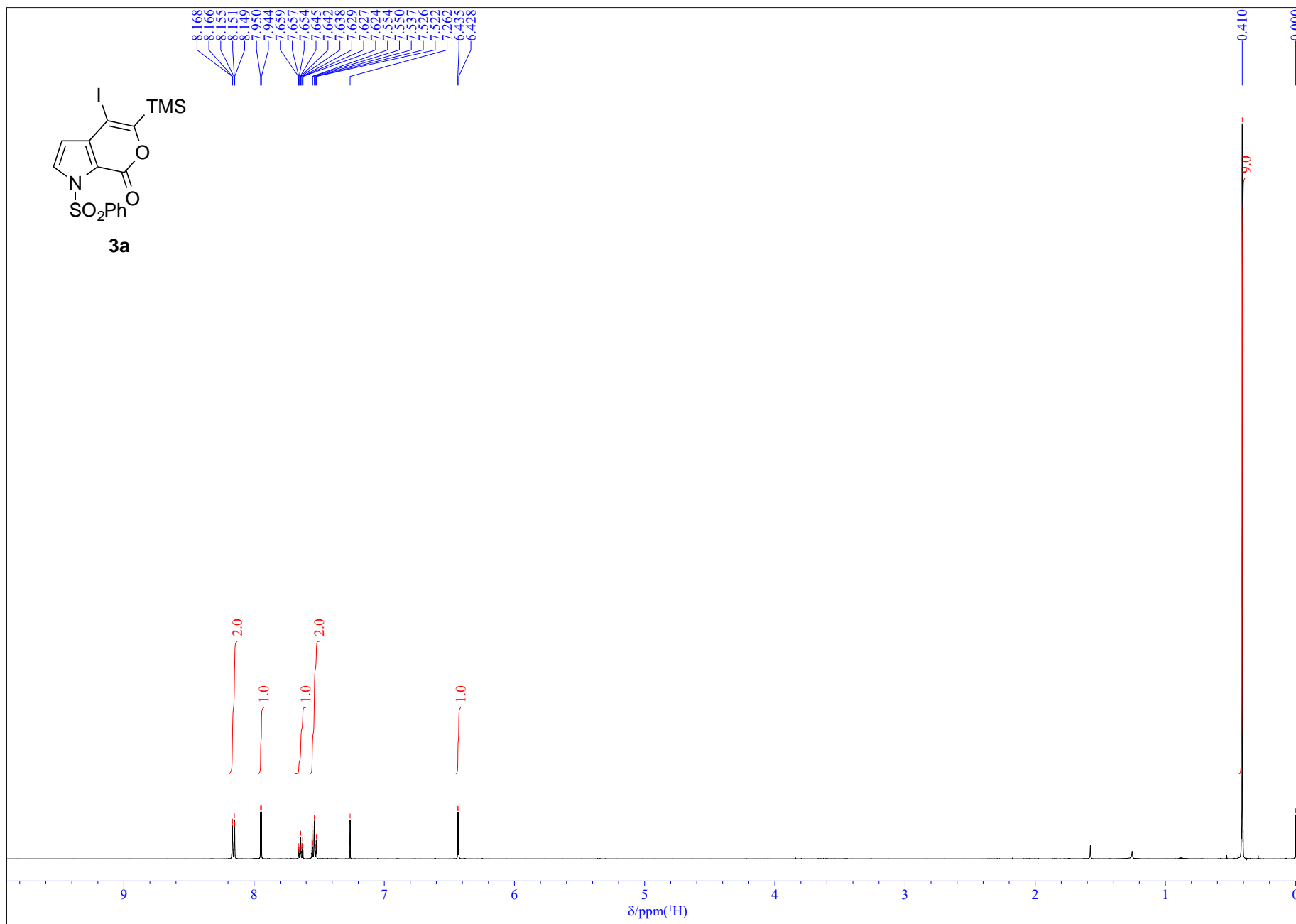


Figure S33. ^1H NMR spectrum of compound **3a** (500 MHz, CDCl_3).

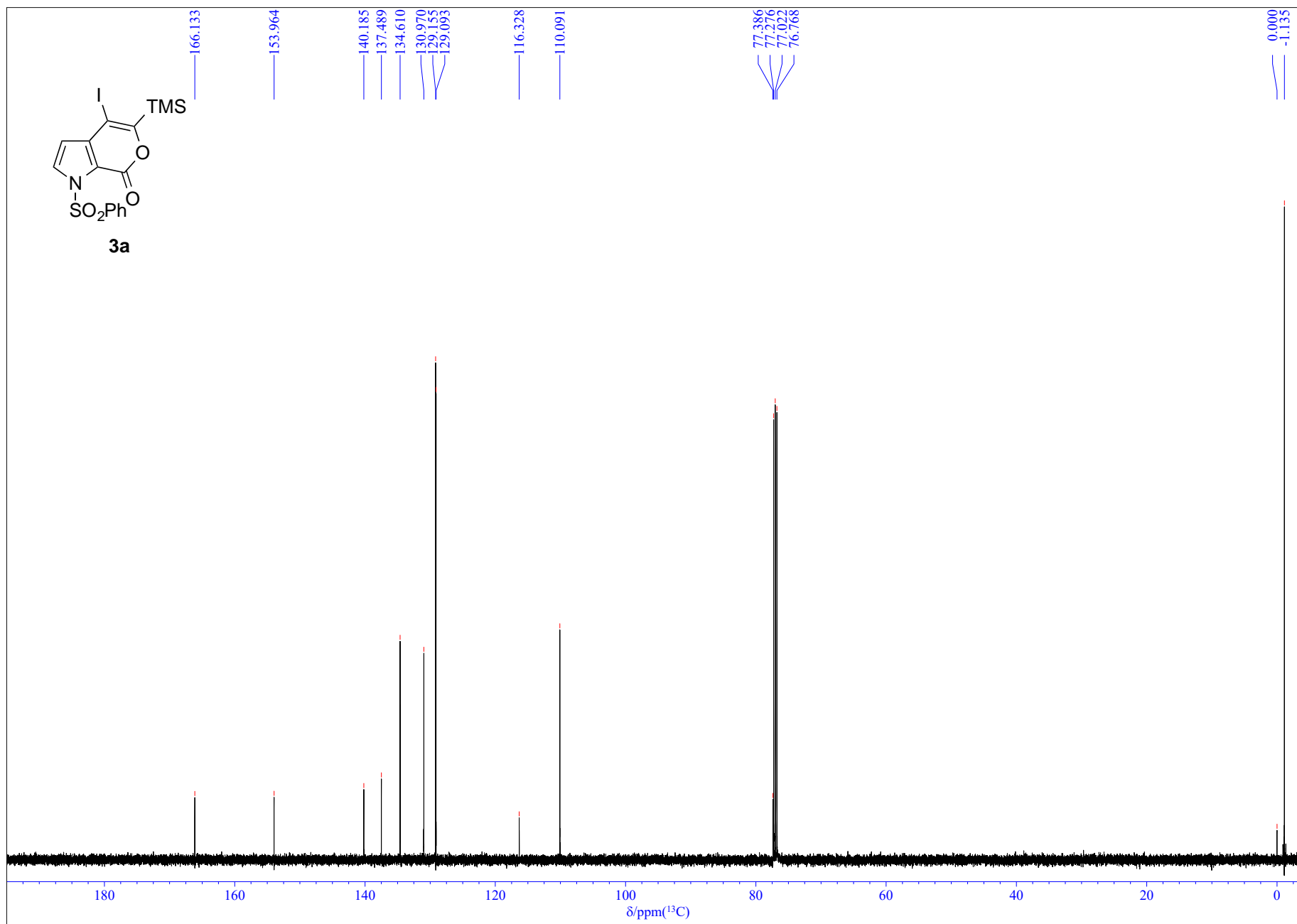


Figure S34. ${}^{13}\text{C}$ NMR spectrum of compound **3a** (126 MHz, CDCl_3).

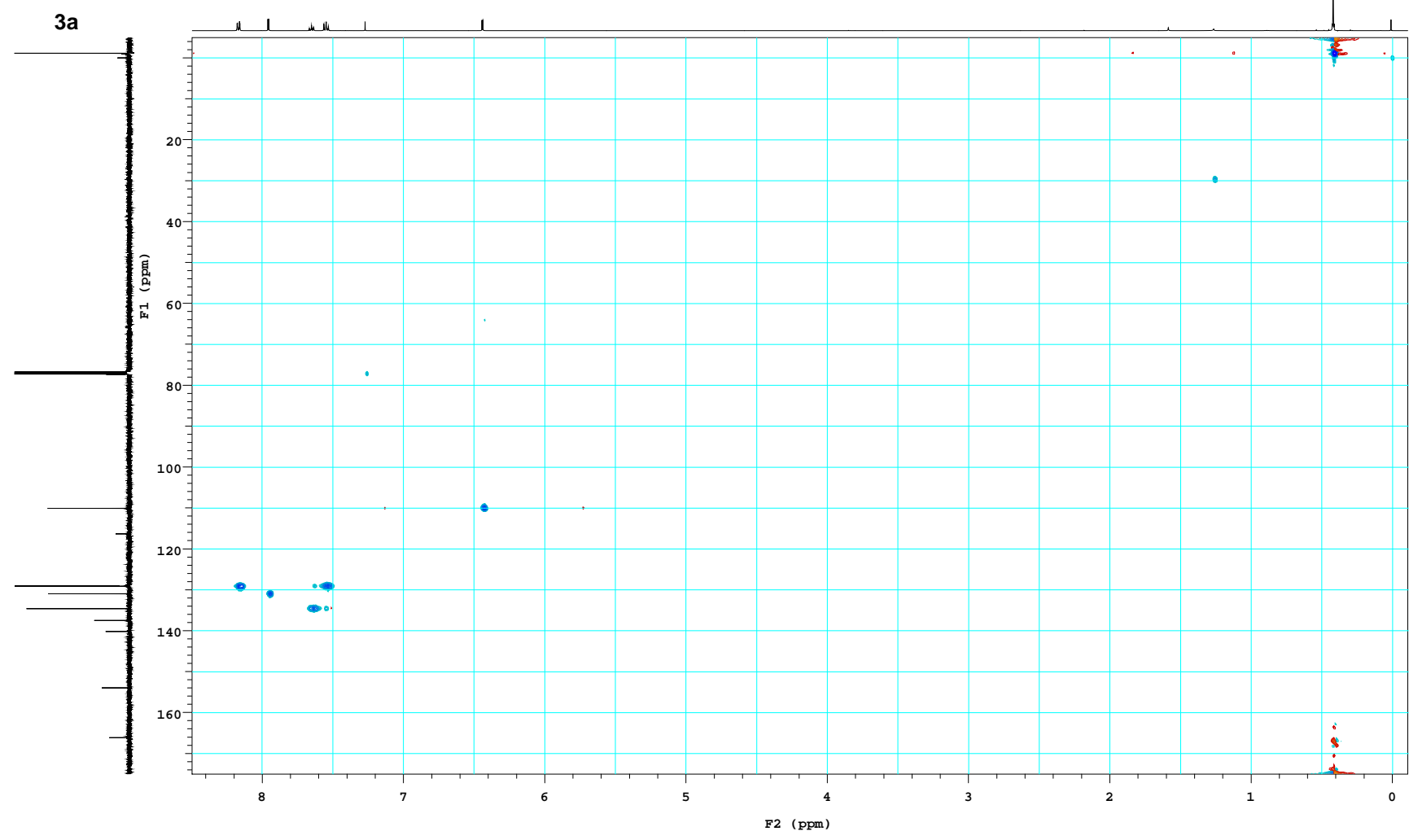
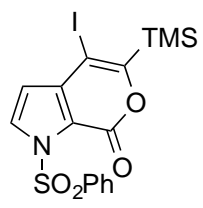


Figure S35. HMQC spectrum of compound 3a (CDCl₃).

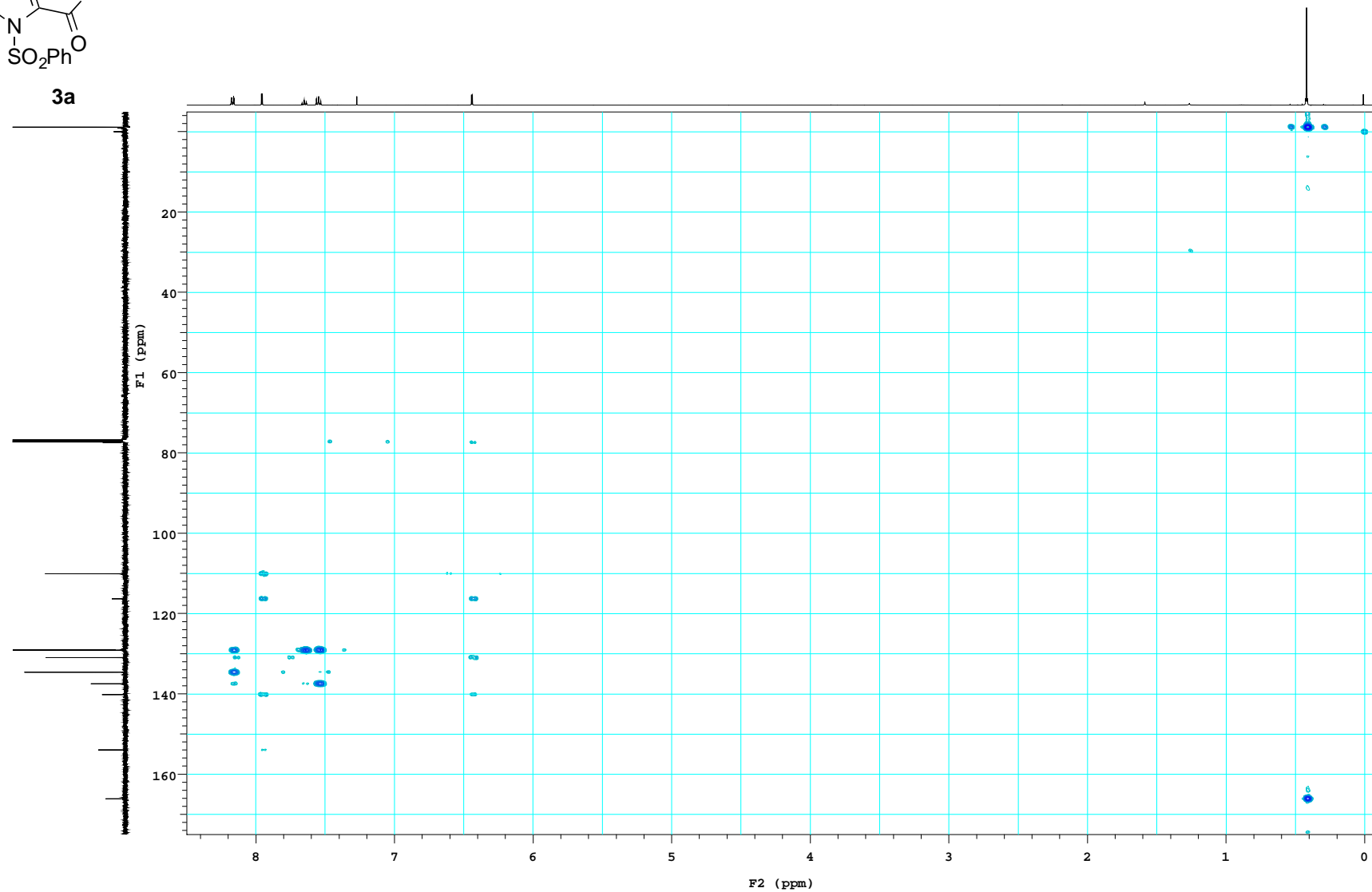
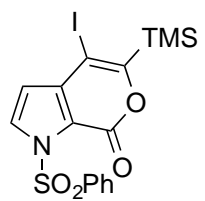
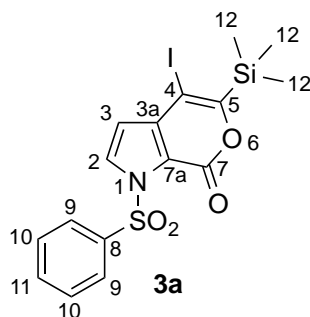


Figure S36. HMBC spectrum of compound **3a** (CDCl₃).

Table S5. NMR data for **3a** in CDCl₃.



C no.	δ_C	δ_H	HMBC (C no.)
2	131.0	7.95 (d, $J = 3.4$ Hz, 1H)	3, 3a, 7, 7a
3	110.1	6.43 (d, $J = 3.4$ Hz, 1H)	2, 3a, 4, 7a
3a	116.3		
4	77.4		
5	166.1		
7	154.0		
7a	140.2		
8	137.5		
9	129.2	8.14–8.18 (m, 2H).	8, 9, 11
10	129.1	7.51–7.56 (m, 2H),	8, 10
11	134.6	7.62–7.66 (m, 1H),	9
12	-1.1	0.41 (s, 9H)	5, 12

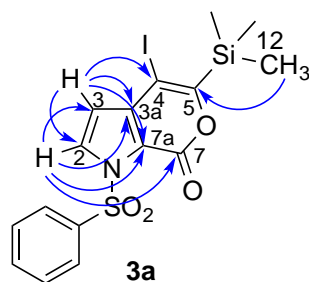


Figure S37. Key HMBC correlations in **3a**.

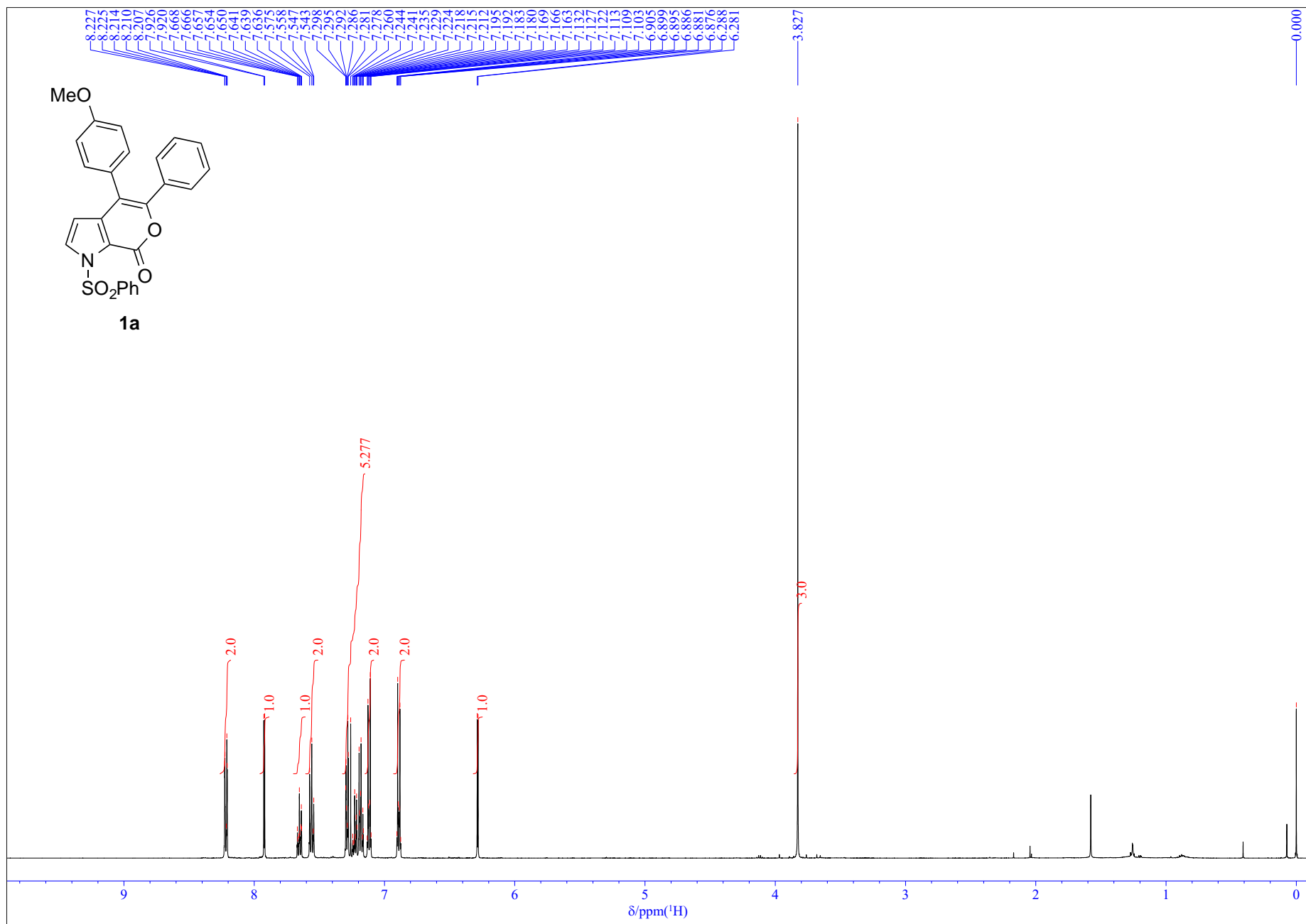


Figure S38. ^1H NMR spectrum of compound **1a** (500 MHz, CDCl_3).

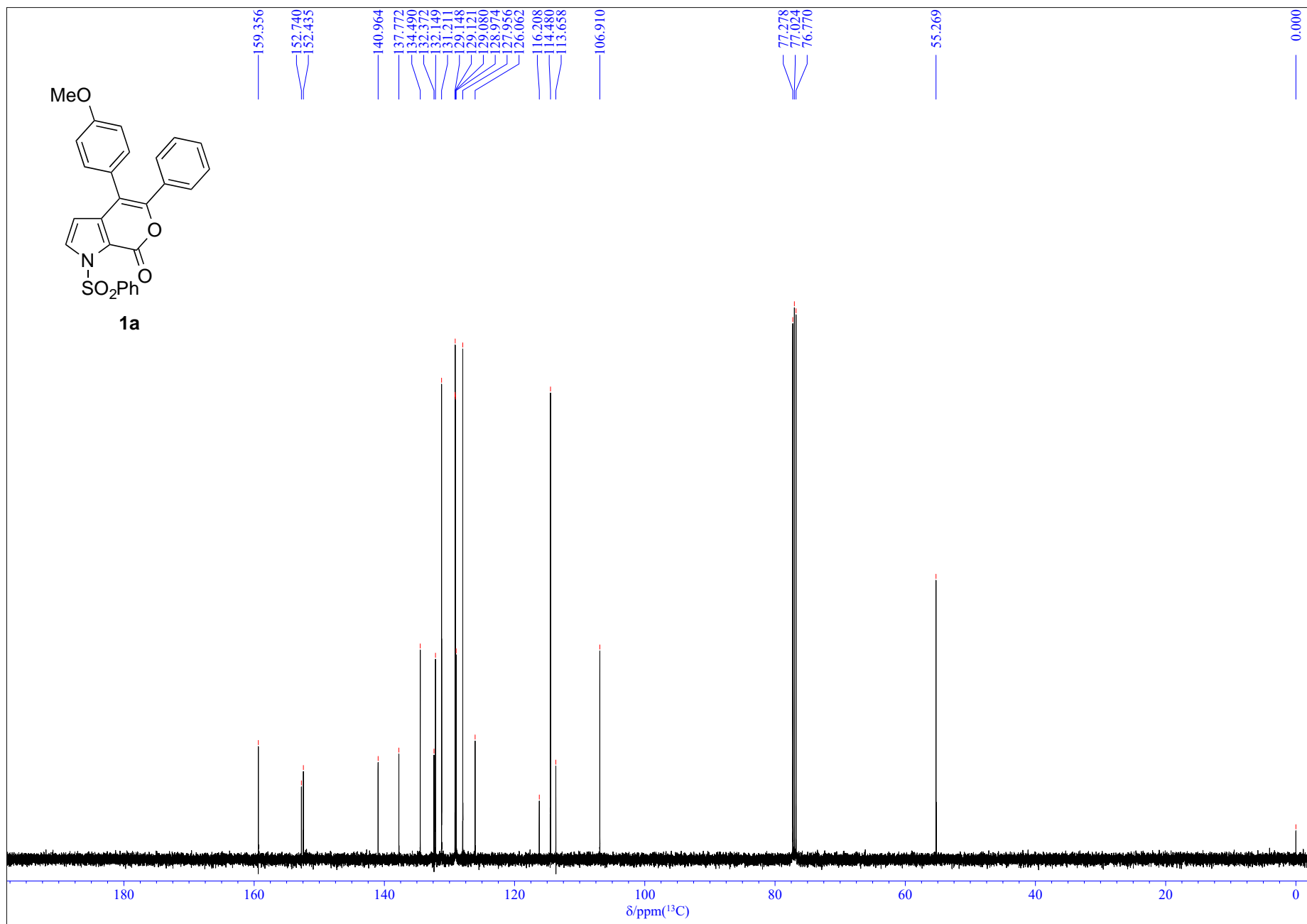


Figure S39. ¹³C NMR spectrum of compound **1a** (126 MHz, CDCl₃).

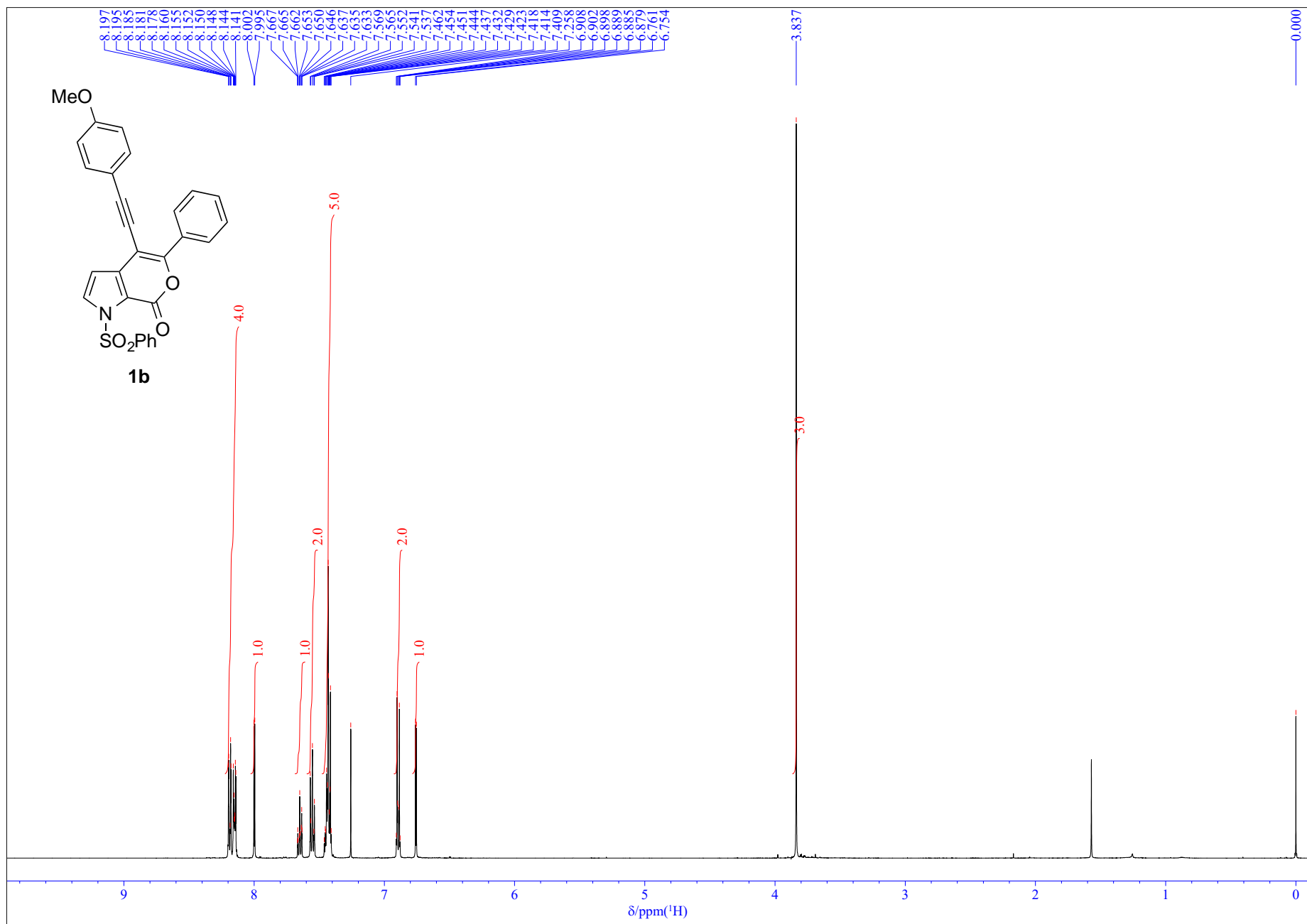


Figure S40. ¹H NMR spectrum of compound **1b** (500 MHz, CDCl₃).

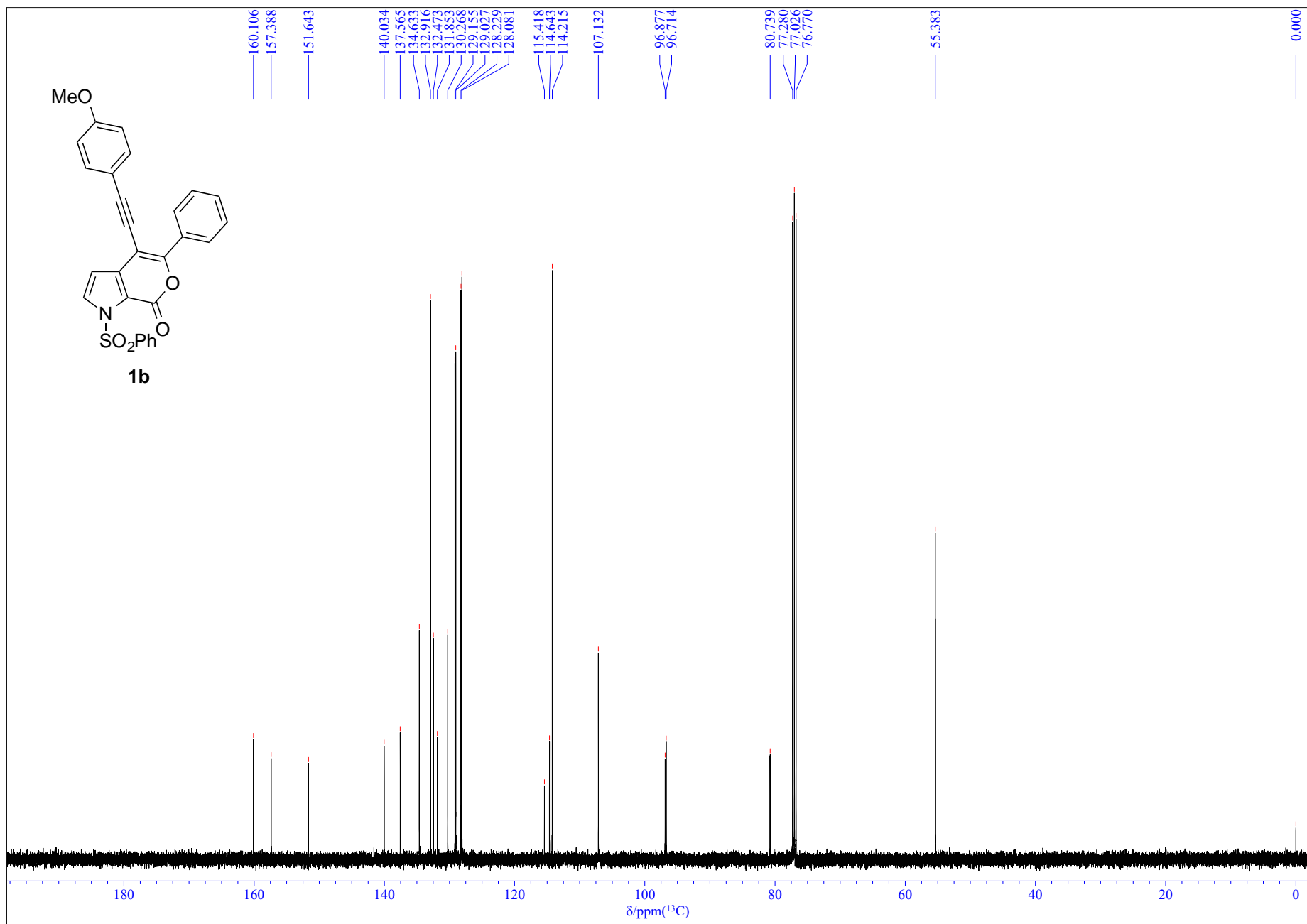


Figure S41. ¹³C NMR spectrum of compound **1b** (126 MHz, CDCl₃).