

Supplementary Information

Mechanochemistry Metal-Free Synthesis and Molecular Modeling Study of 4-Arylamino-1,2-naphthoquinones by C_{sp2}–C_{sp2} Bond Formation

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Spectra collection for the synthesized molecules

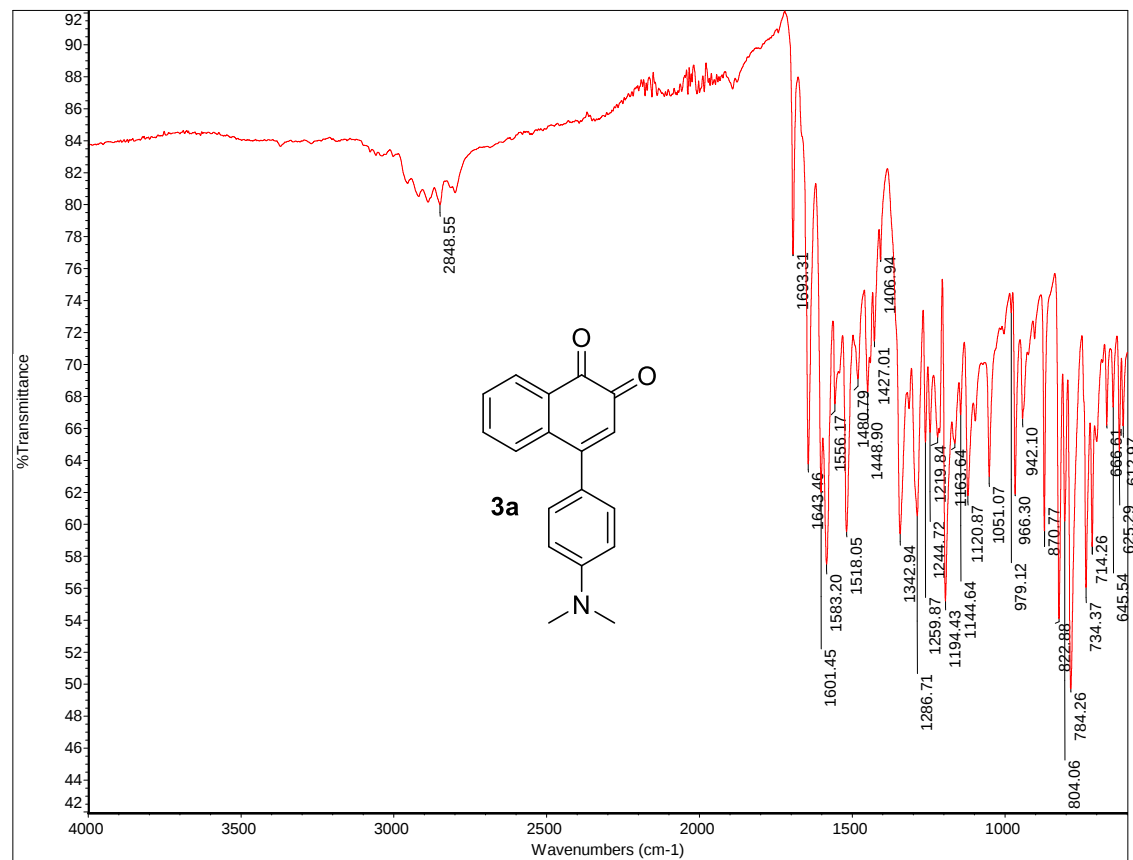


Figure S1. FTIR (neat) spectrum of compound **3a**.

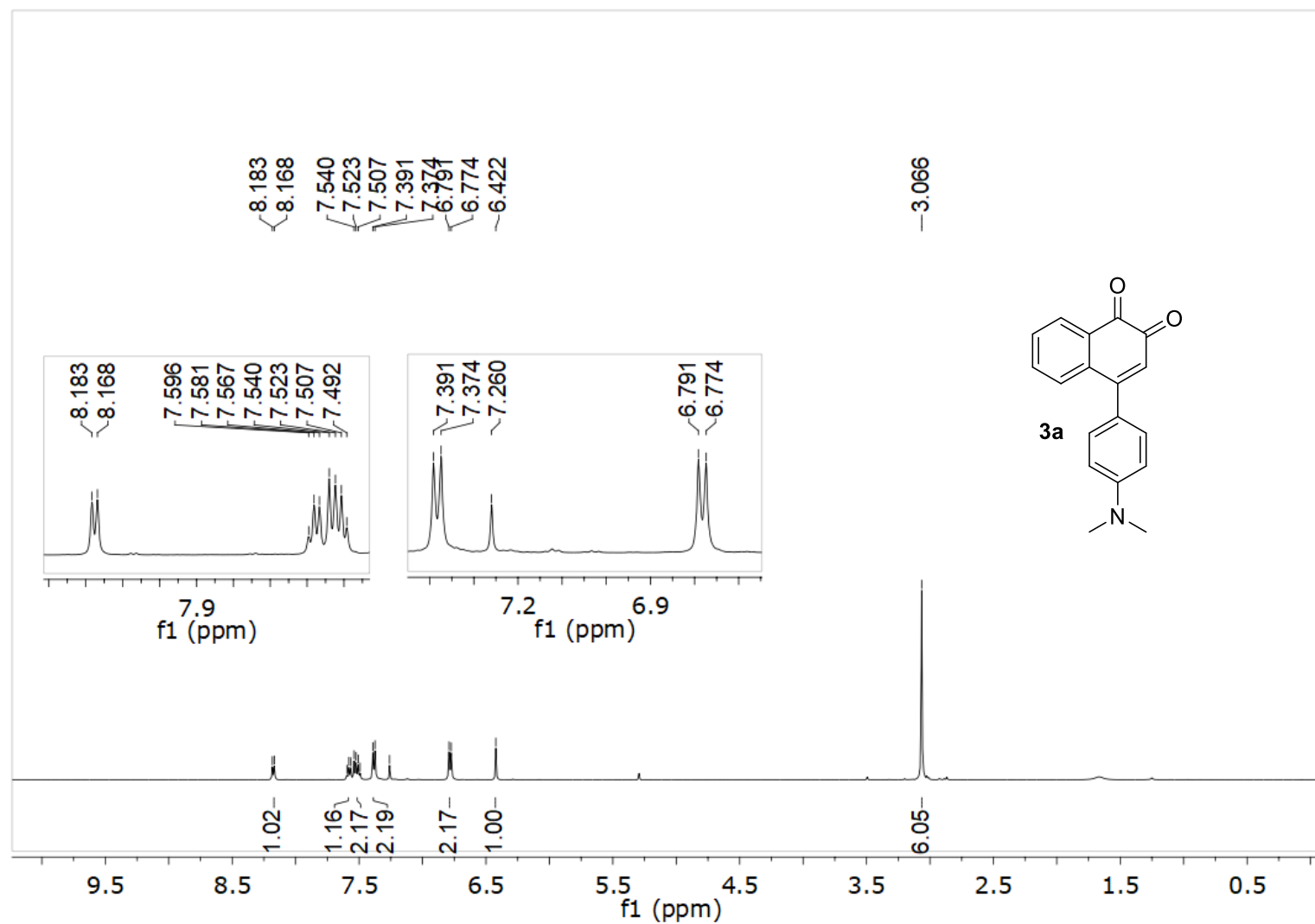


Figure S2. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **3a**.

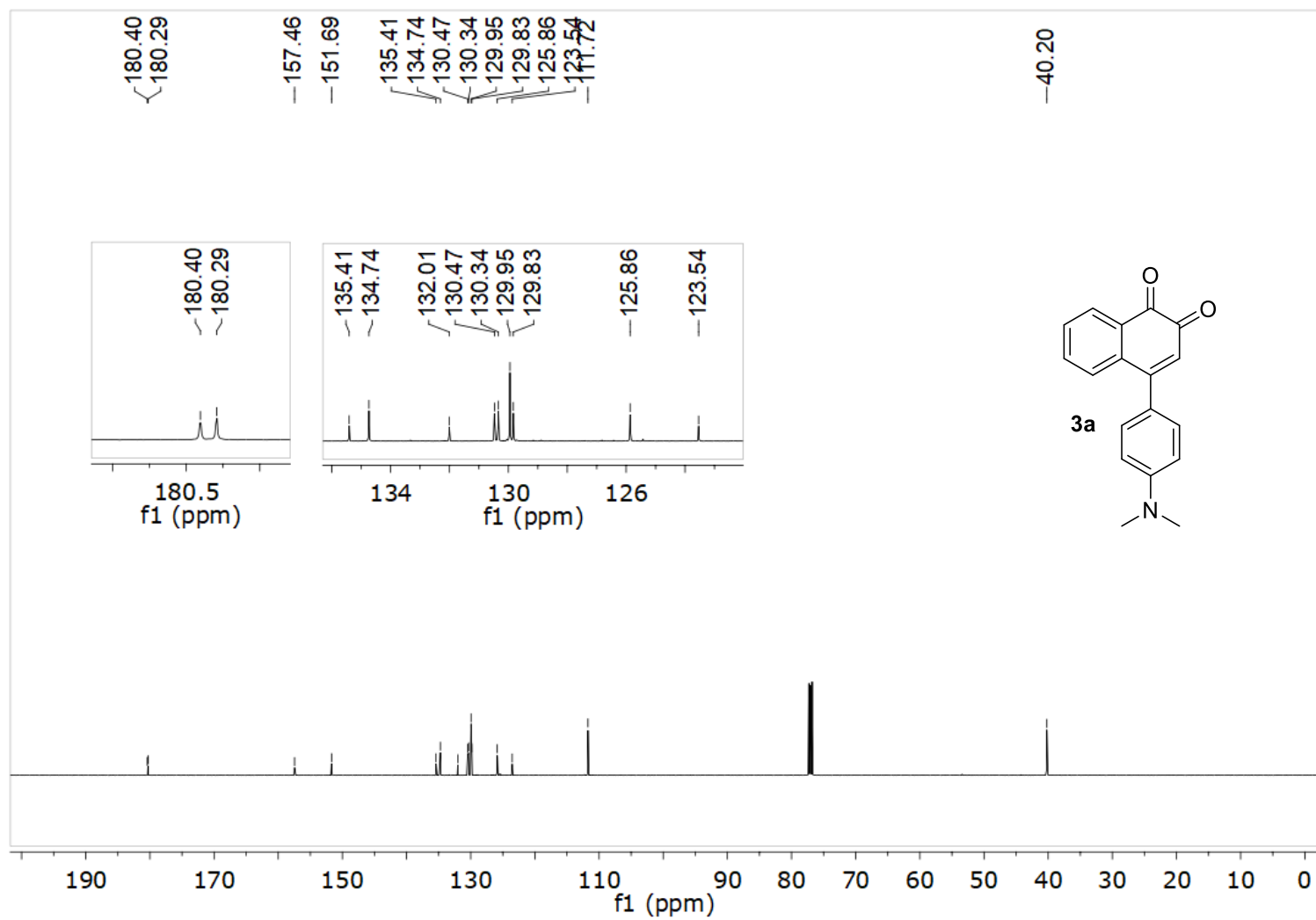


Figure S3. ¹³C NMR spectrum (125 MHz, CDCl₃) of compound **3a**.

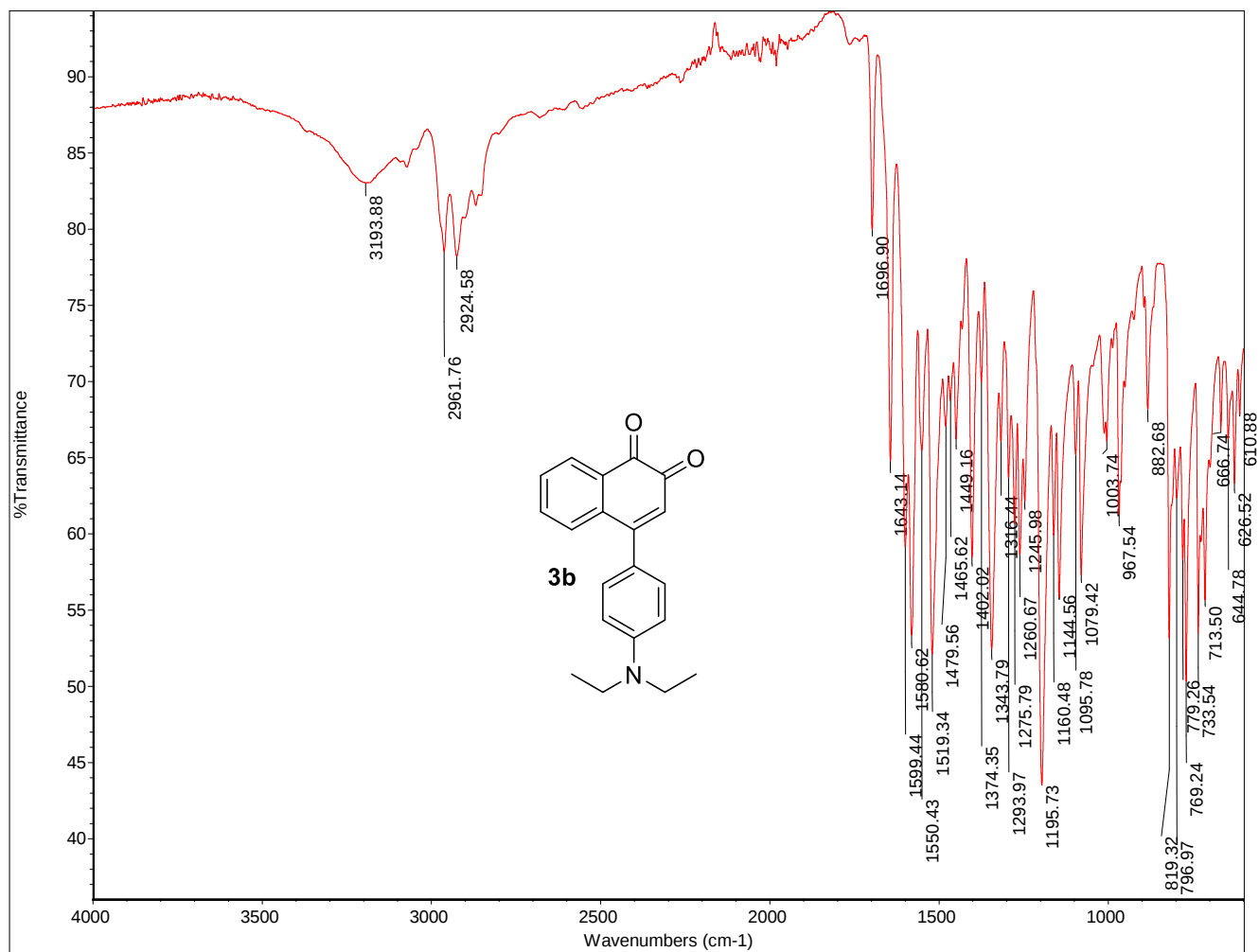


Figure S4. FTIR (neat) spectrum of compound **3b**.

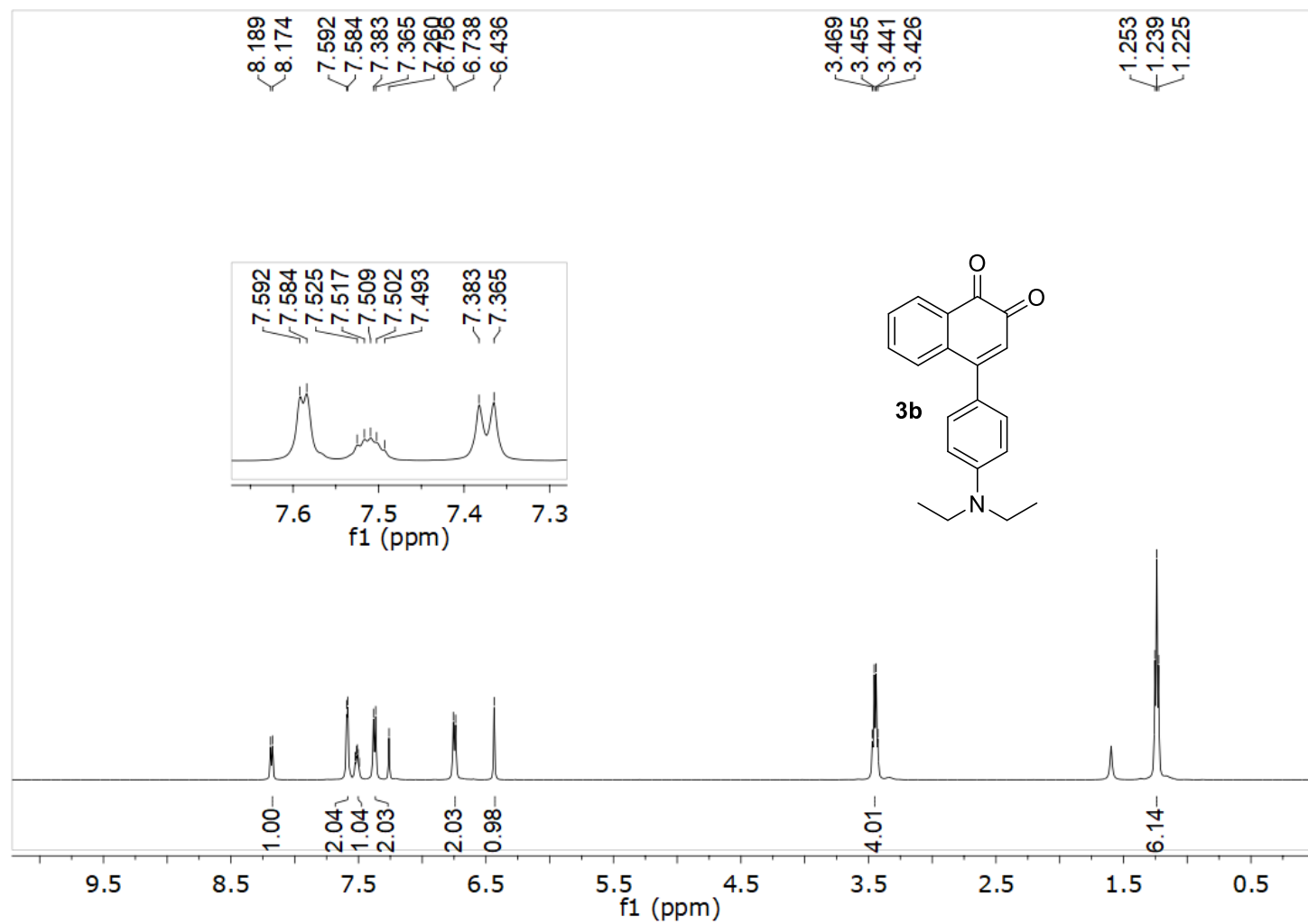


Figure S5. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **3b**.

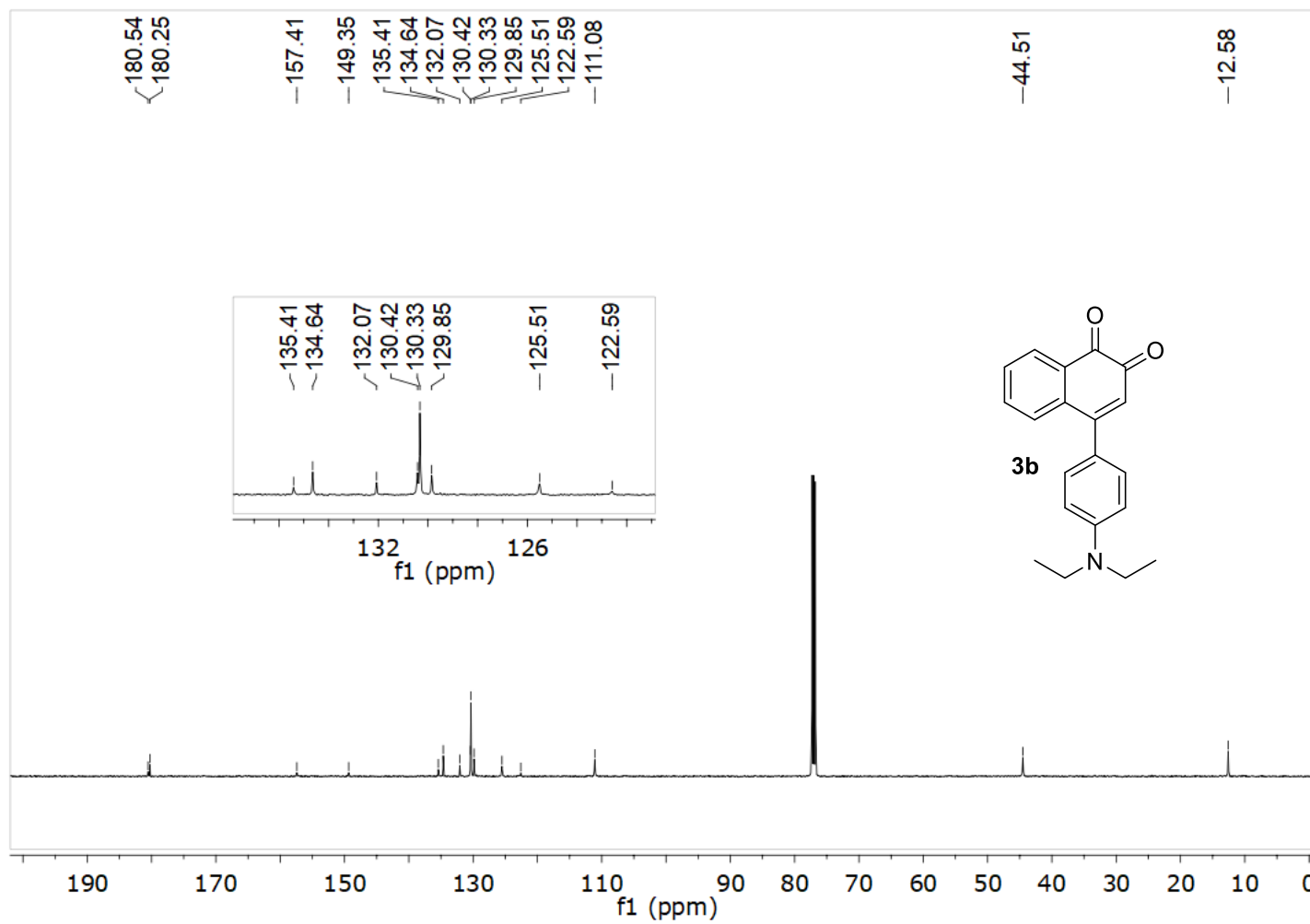


Figure S6. ^{13}C NMR spectrum (125 MHz, CDCl_3) of compound **3b**.

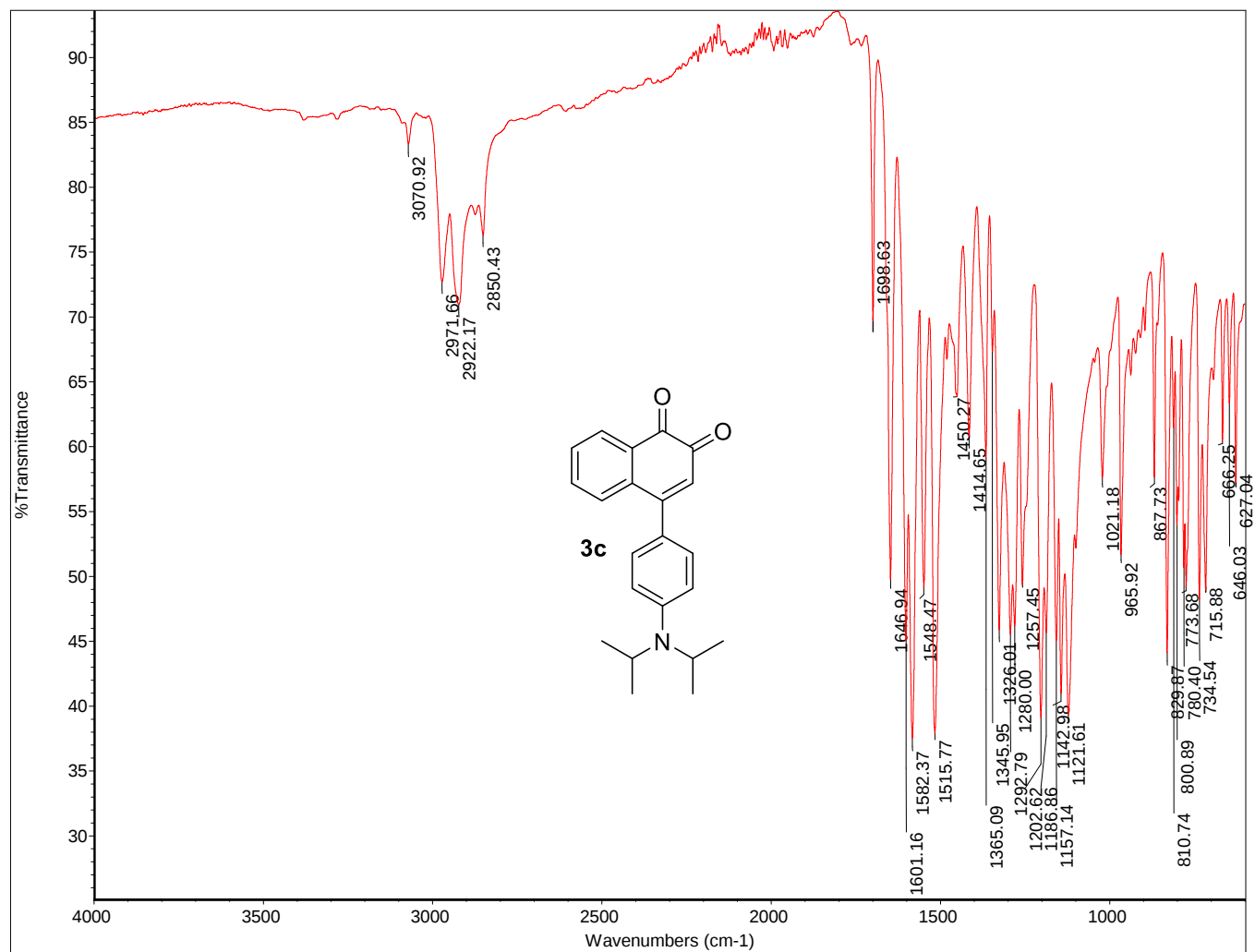


Figure S7. FTIR (neat) spectrum of compound **3c**.

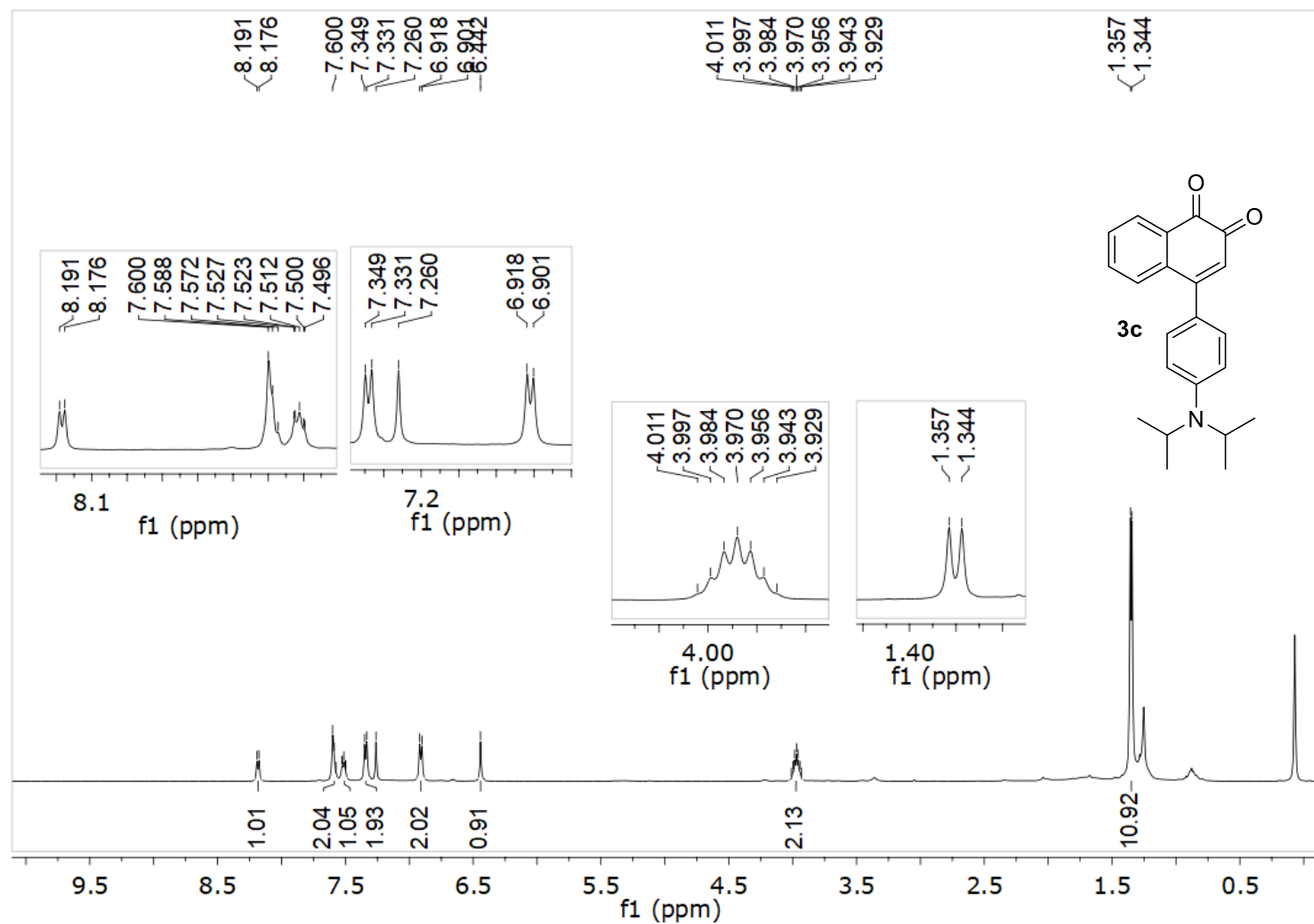
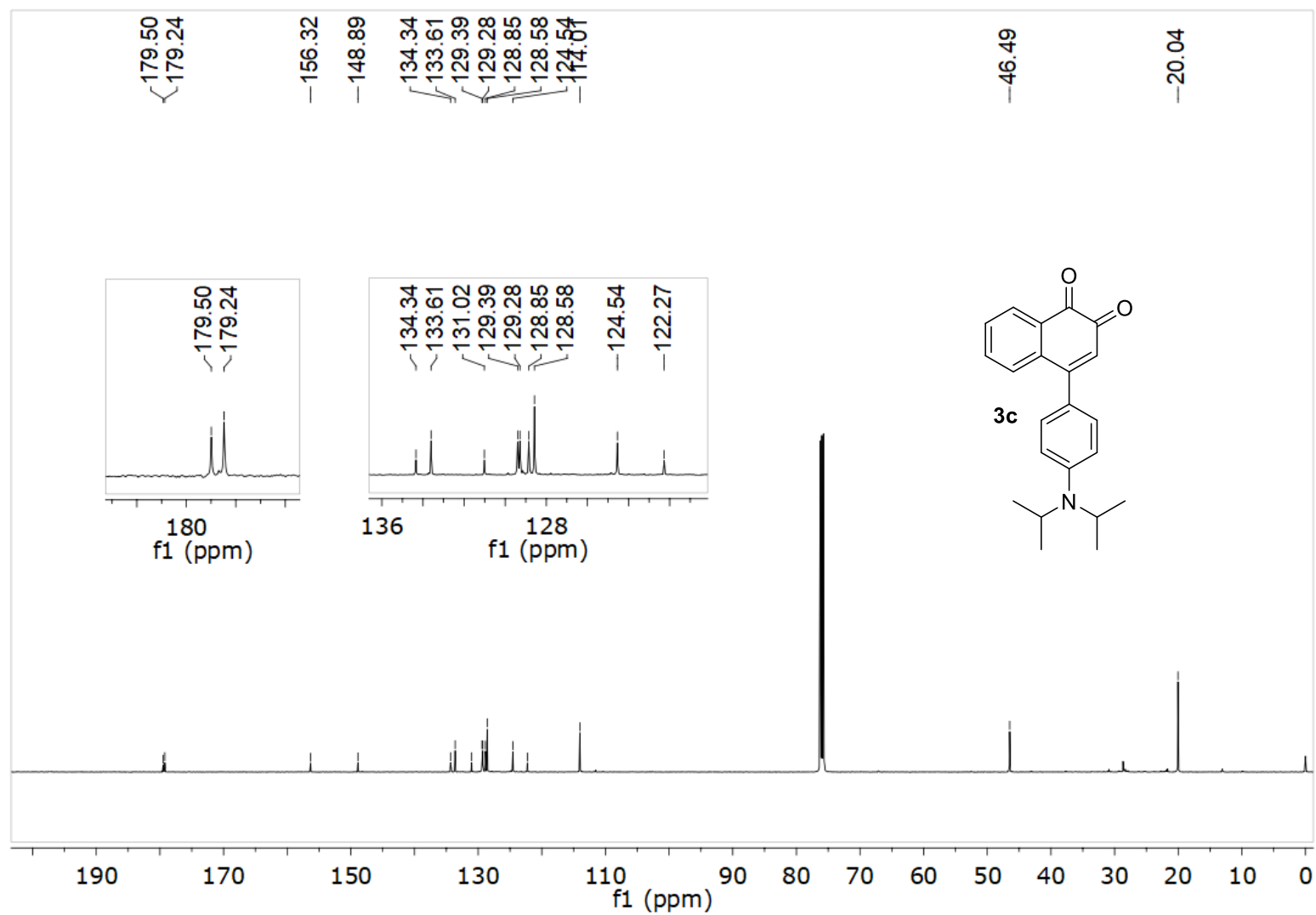
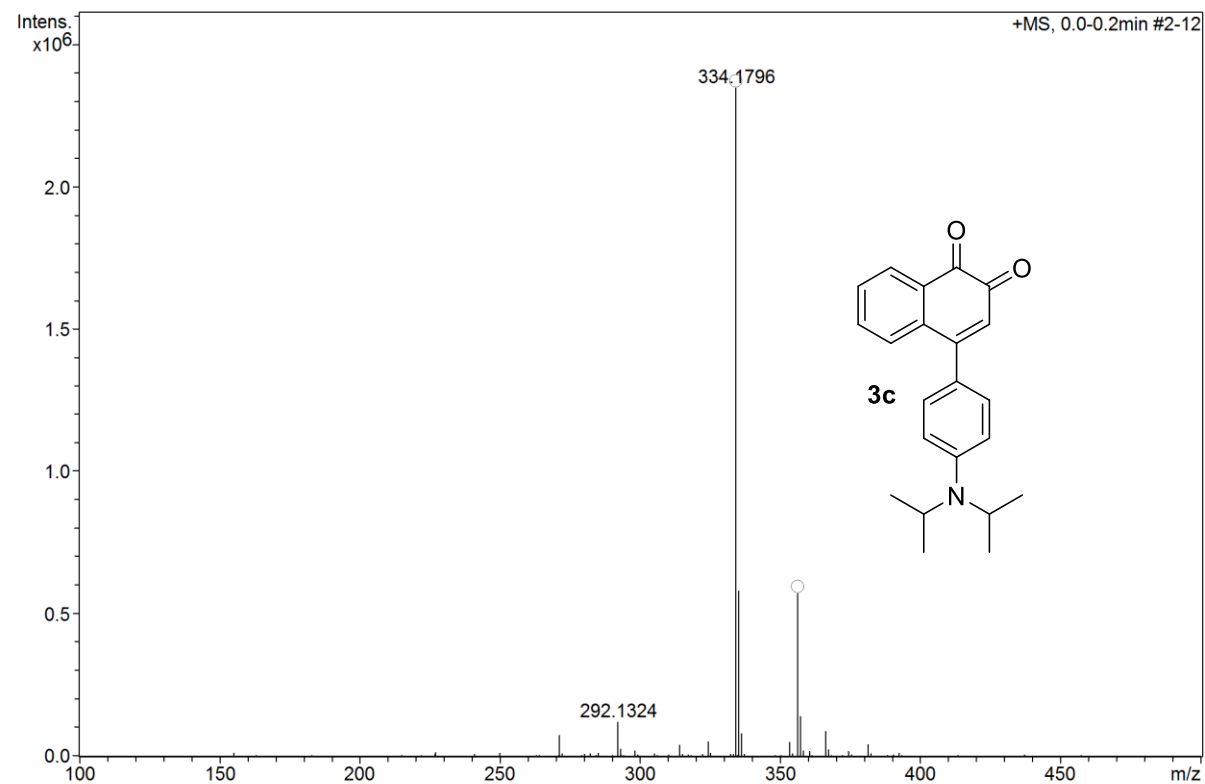


Figure S8. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **3c**.



+MS, 0.0-0.2min #2-12



Meas. m/z #	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e ⁻ Conf	mSigm a	Std I	Std Mean m/z	Std VarNo	Std m/z	Std Comb
334.179559	1 C ₂₂ H ₂₄ NO ₂	334.180155	1.8	2.0	11.5	ok	even	1.8	3.1	n.a.	n.a.	n.a.	n.a.
356.161609	1 C ₂₀ H ₁₈ N ₇	356.161820	0.6	-0.5	15.5	ok	even	3.7	6.9	n.a.	n.a.	n.a.	n.a.
	2 C ₁₉ H ₂₂ N ₃ O ₄	356.160483	-3.2	-3.8	10.5	ok	even	14.9	24.2	n.a.	n.a.	n.a.	n.a.
	1 C ₂₂ H ₂₃ NNaO ₂	356.162100	1.4	1.3	11.5	ok	even	1.2	2.3	n.a.	n.a.	n.a.	n.a.

Figure S10. HRMS spectrum of compound **3c**.

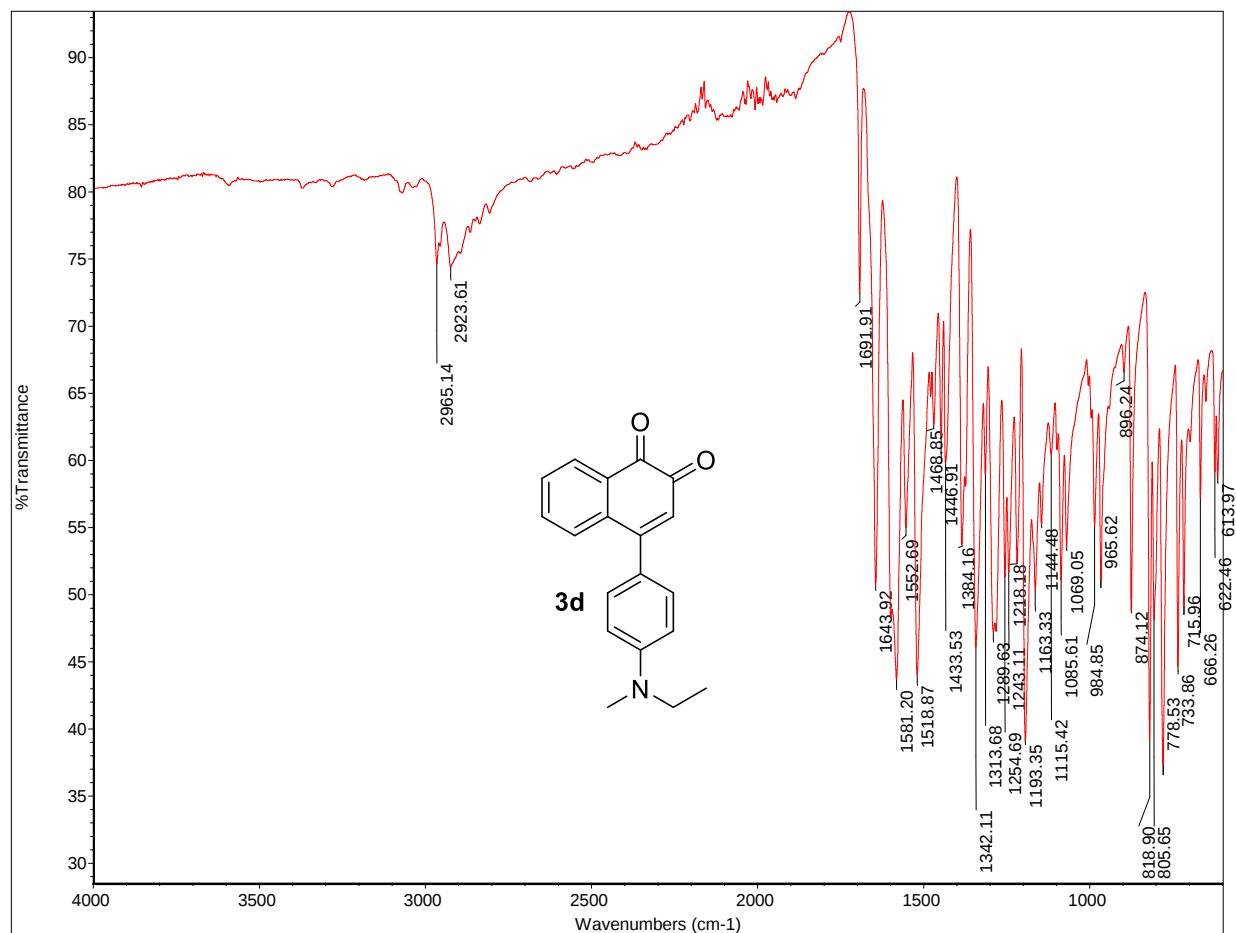


Figure S11. FTIR (neat) spectrum of compound **3d**.

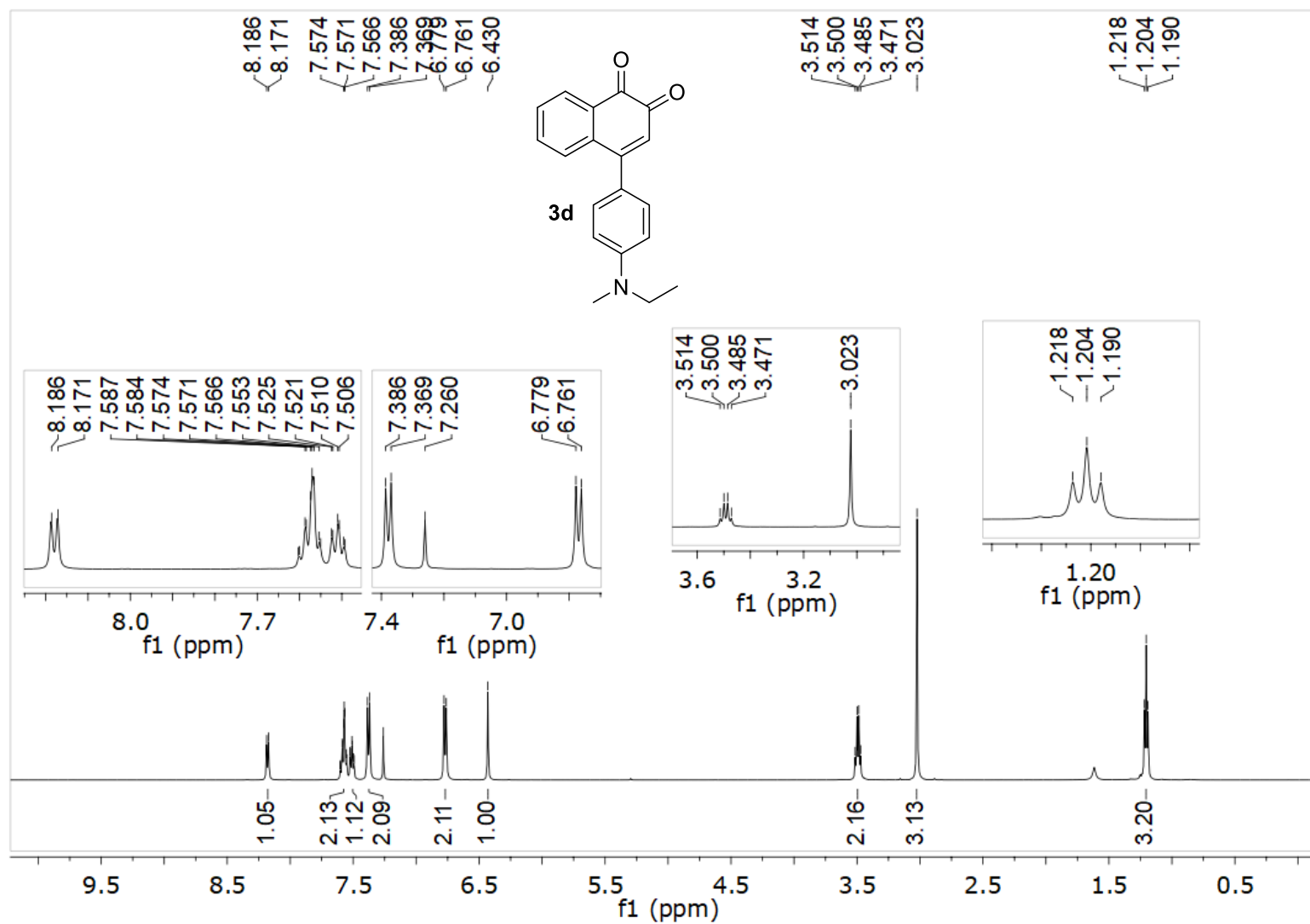


Figure S12. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **3d**.

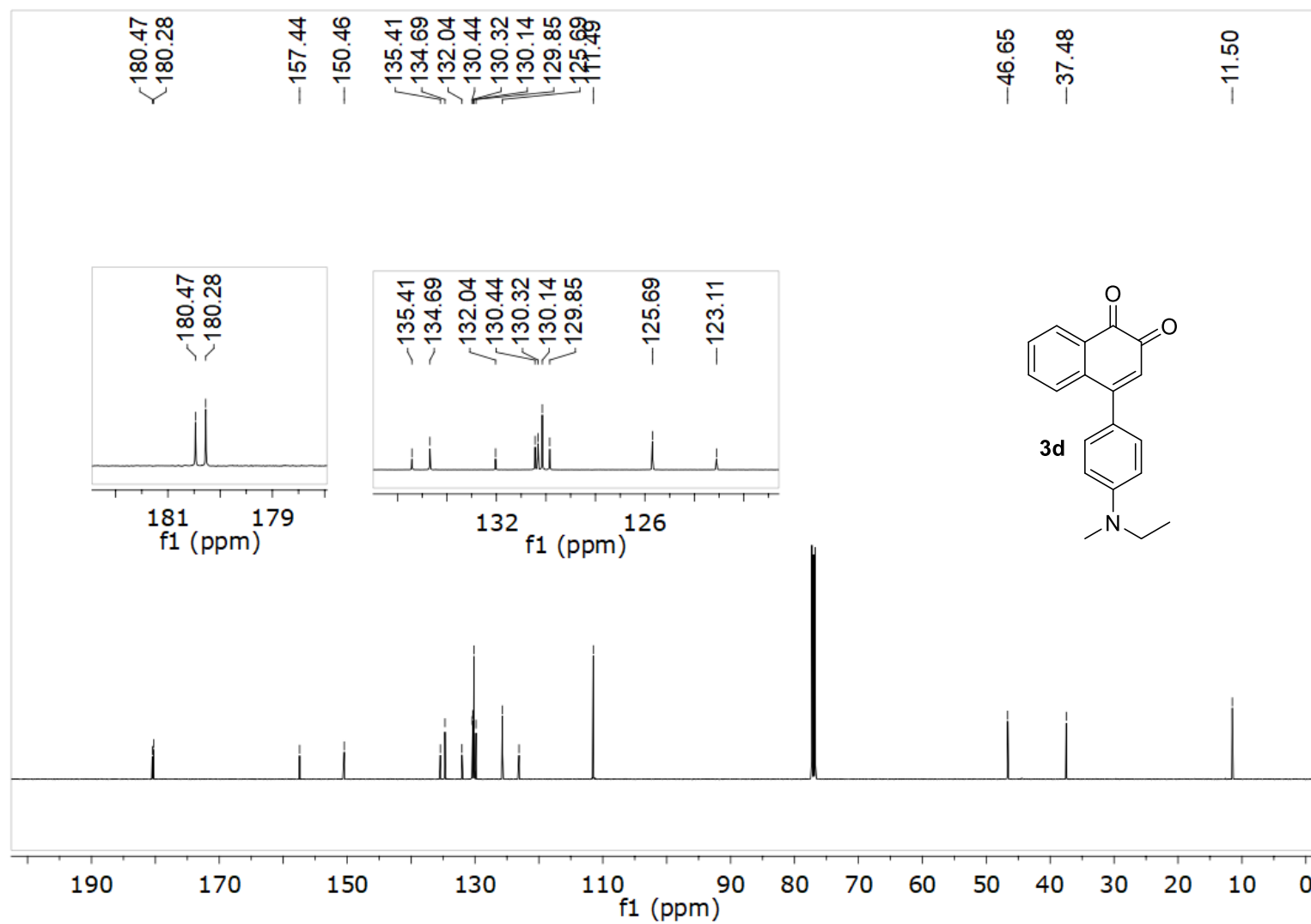
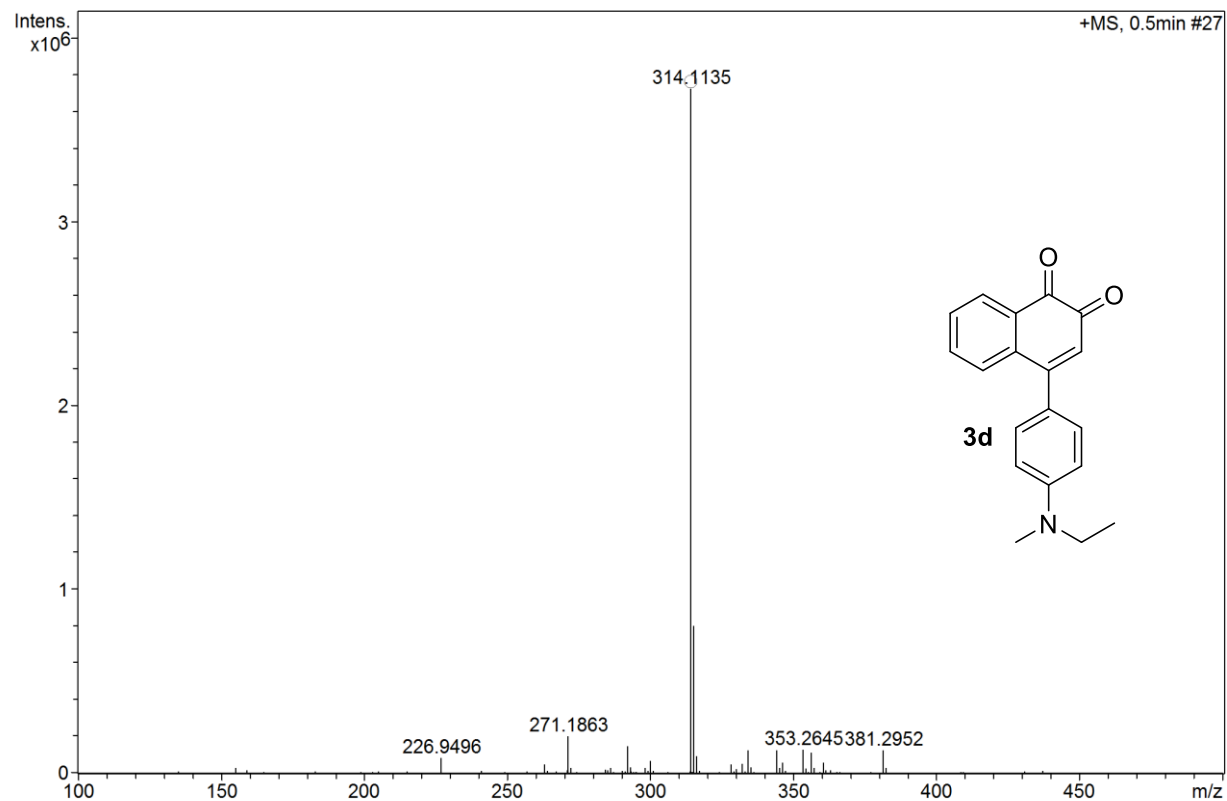


Figure S13. ^{13}C NMR spectrum (125 MHz, CDCl_3) of compound **3d**.

+MS, 0.5min #27



Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e ⁻ Conf	mSigm	Std I a	Std Mean m/z	Std VarNo	Std I rm	Std m/z Diff	Std Comb Dev
314.113507	1	C17H12N7	314.114870	4.3	3.3	15.5		ok even	3.5	6.7	n.a.	n.a.	n.a.	n.a.	n.a.
	2	C16H16N3O4	314.113532	0.1	-0.5	10.5		ok even	16.5	27.1	n.a.	n.a.	n.a.	n.a.	n.a.
	1	C19H17NNaO2	314.115149	5.2	5.4	11.5		ok even	2.4	3.6	n.a.	n.a.	n.a.	n.a.	n.a.

Figure S14. HRMS spectrum of compound **3d**.

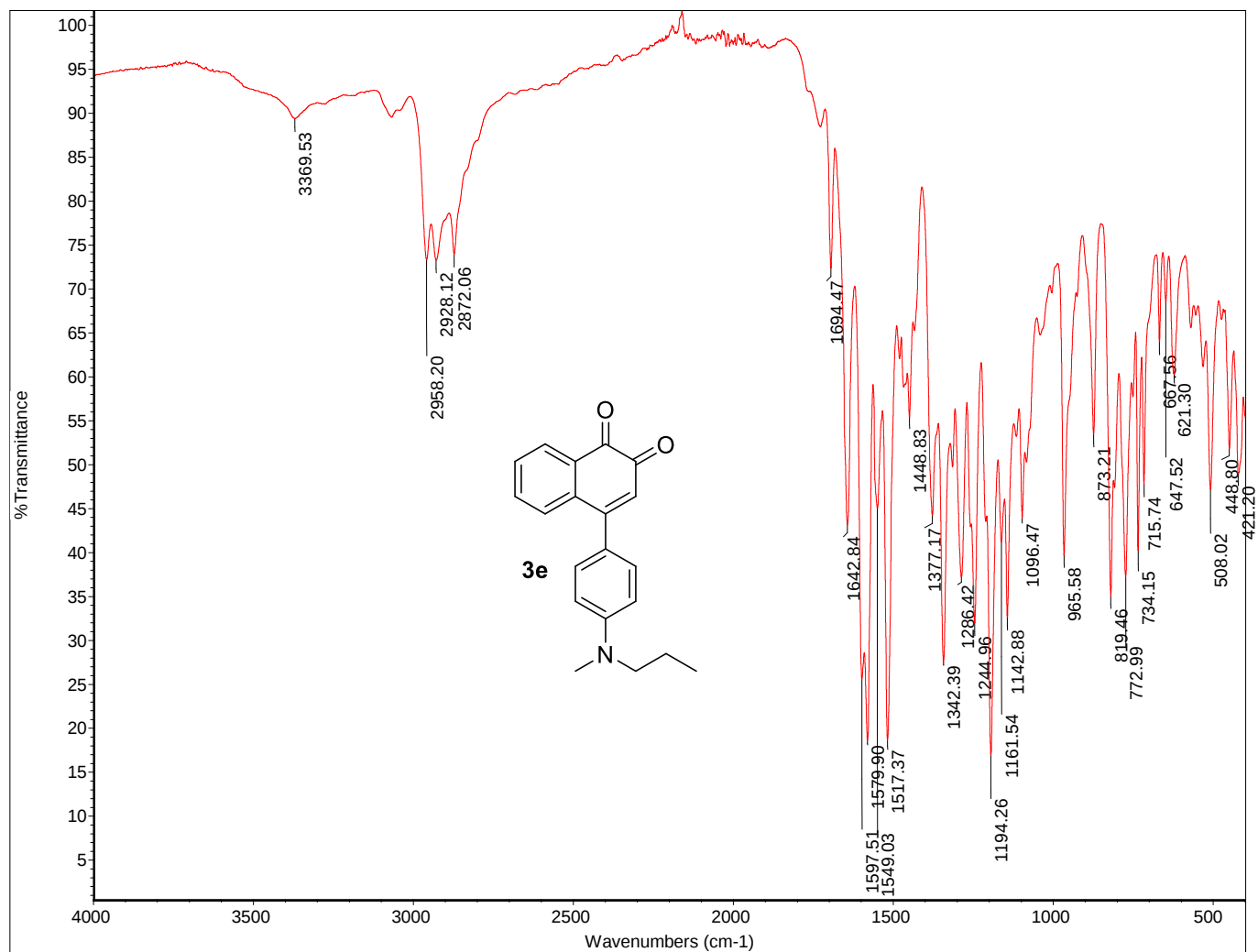


Figure S15. FTIR (neat) spectrum of compound **3e**.

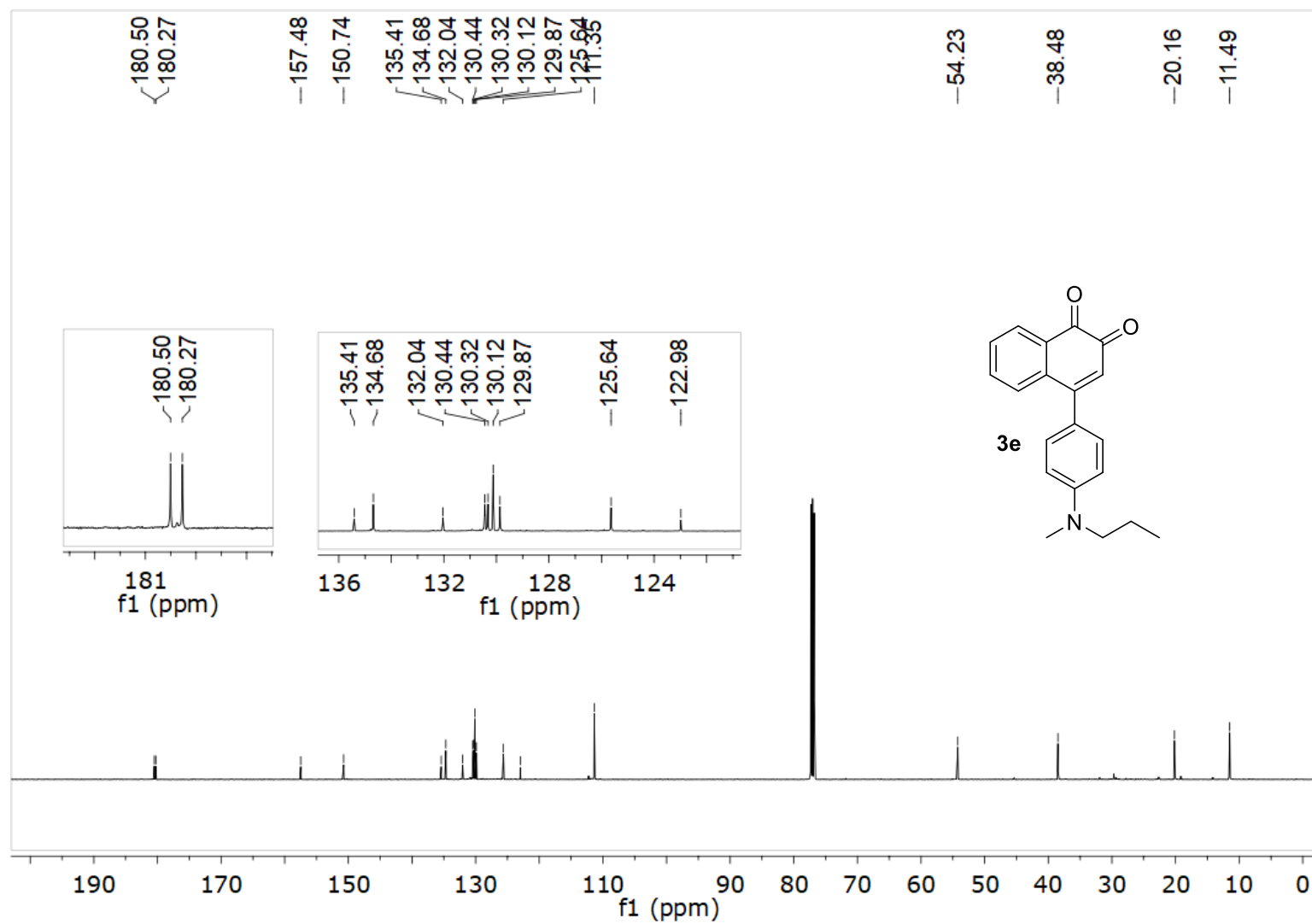
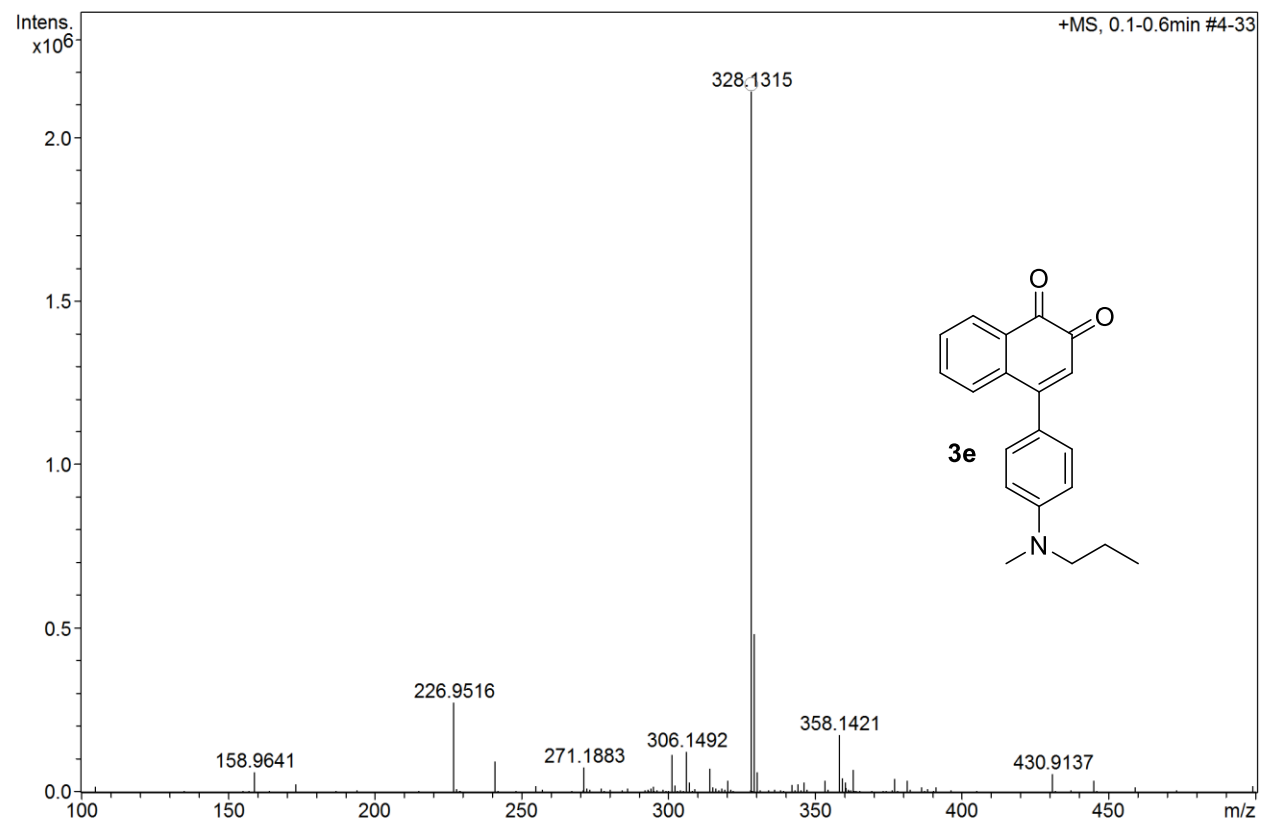


Figure S17. ^{13}C NMR spectrum (125 MHz, CDCl_3) of compound **3e**.

+MS, 0.1-0.6min #4-33



Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e ⁻ Conf	mSigm	Std I a	Std Mean m/z	Std VarNo rm	Std m/z Diff	Std Comb Dev
328.1315	36	1 C ₁₈ H ₁₄ N ₇	328.130520	-3.1	-3.9	15.5		ok even	3.8	7.4	n.a.	n.a.	n.a.	n.a.
	1	C ₂₀ H ₁₉ NNaO ₂	328.130800	-2.2	-2.0	11.5		ok even	2.0	3.4	n.a.	n.a.	n.a.	n.a.

Figure S18. HRMS spectrum of compound **3e**.

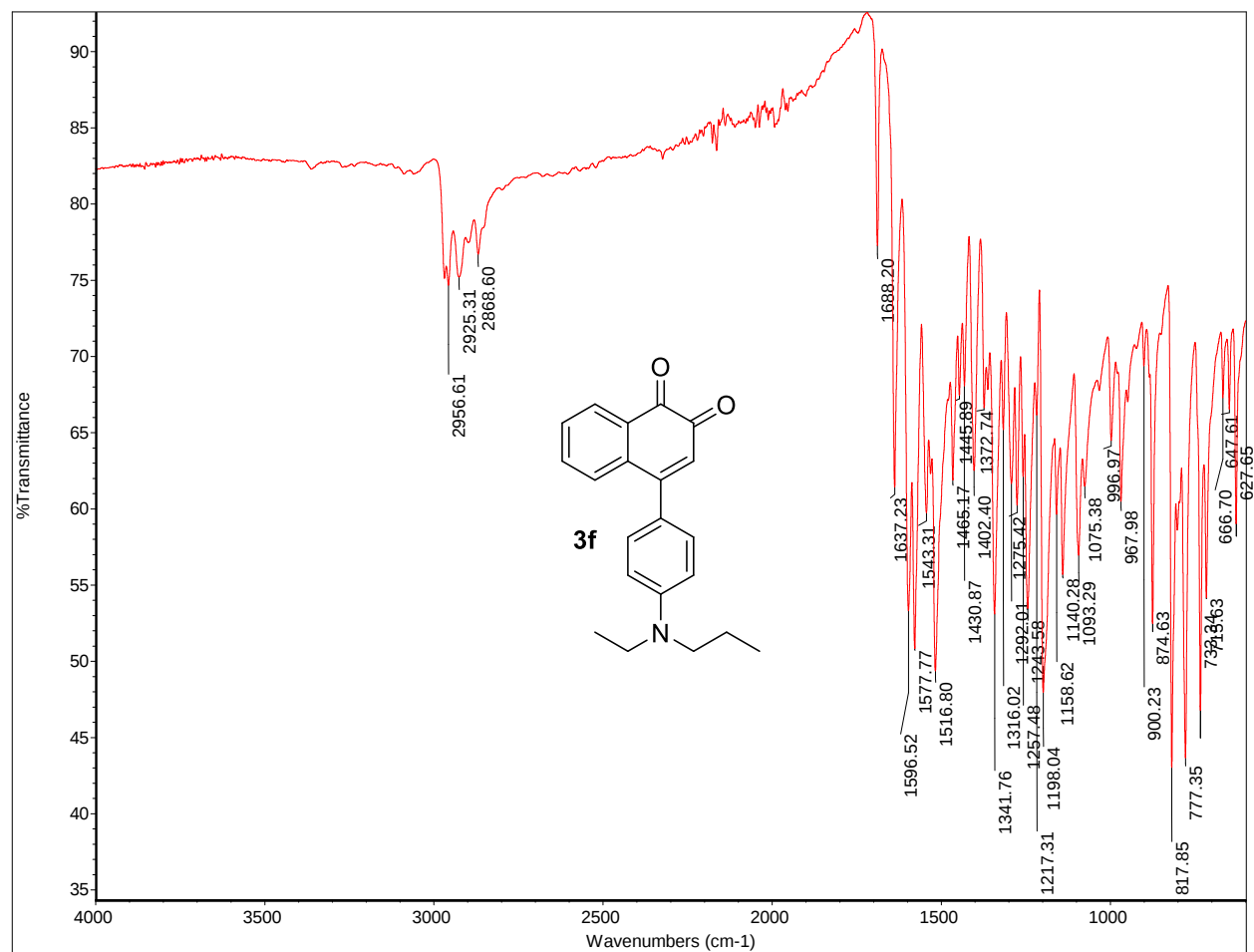


Figure S19. FTIR (neat) spectrum of compound **3f**.

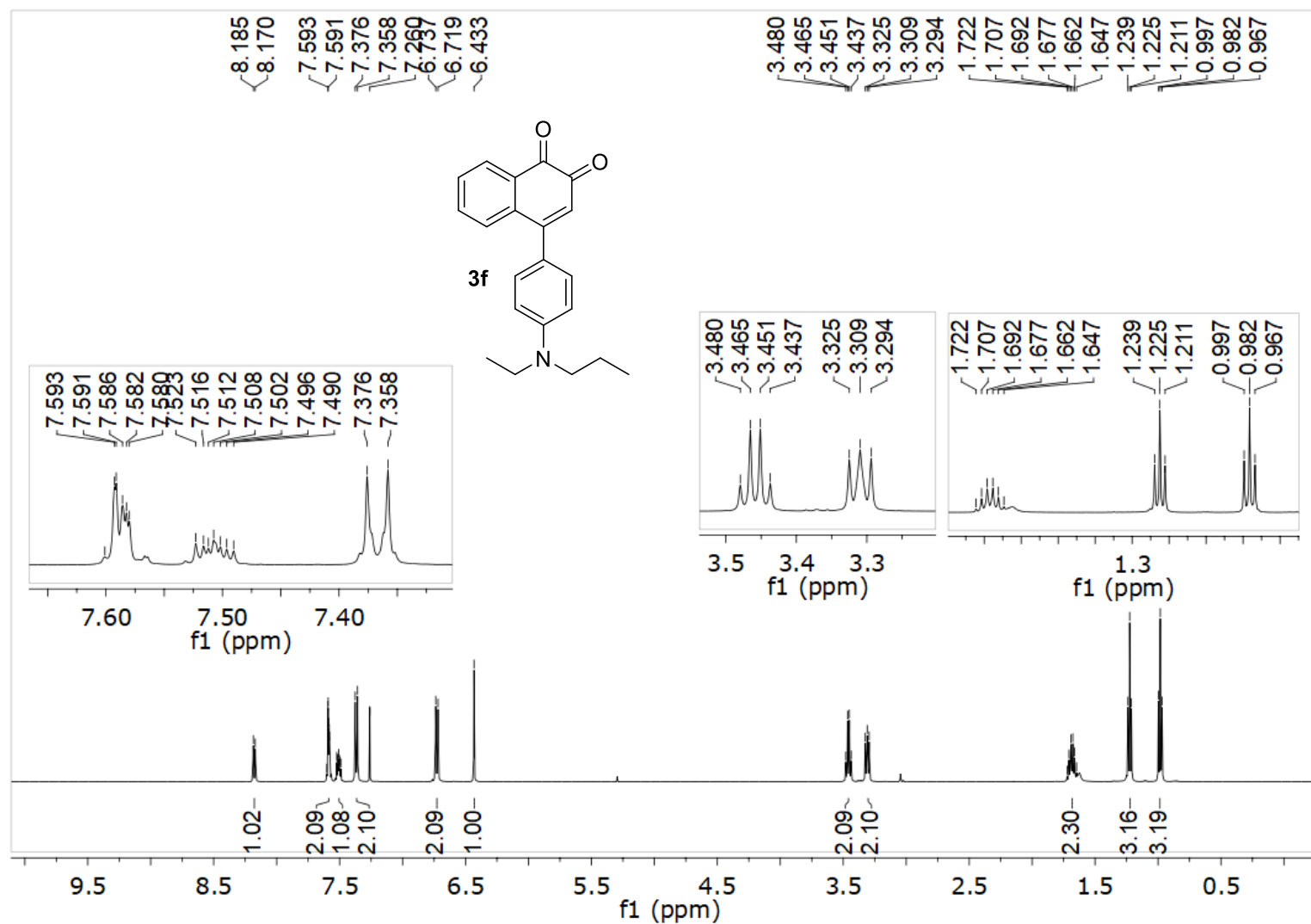


Figure S20. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **3f**.

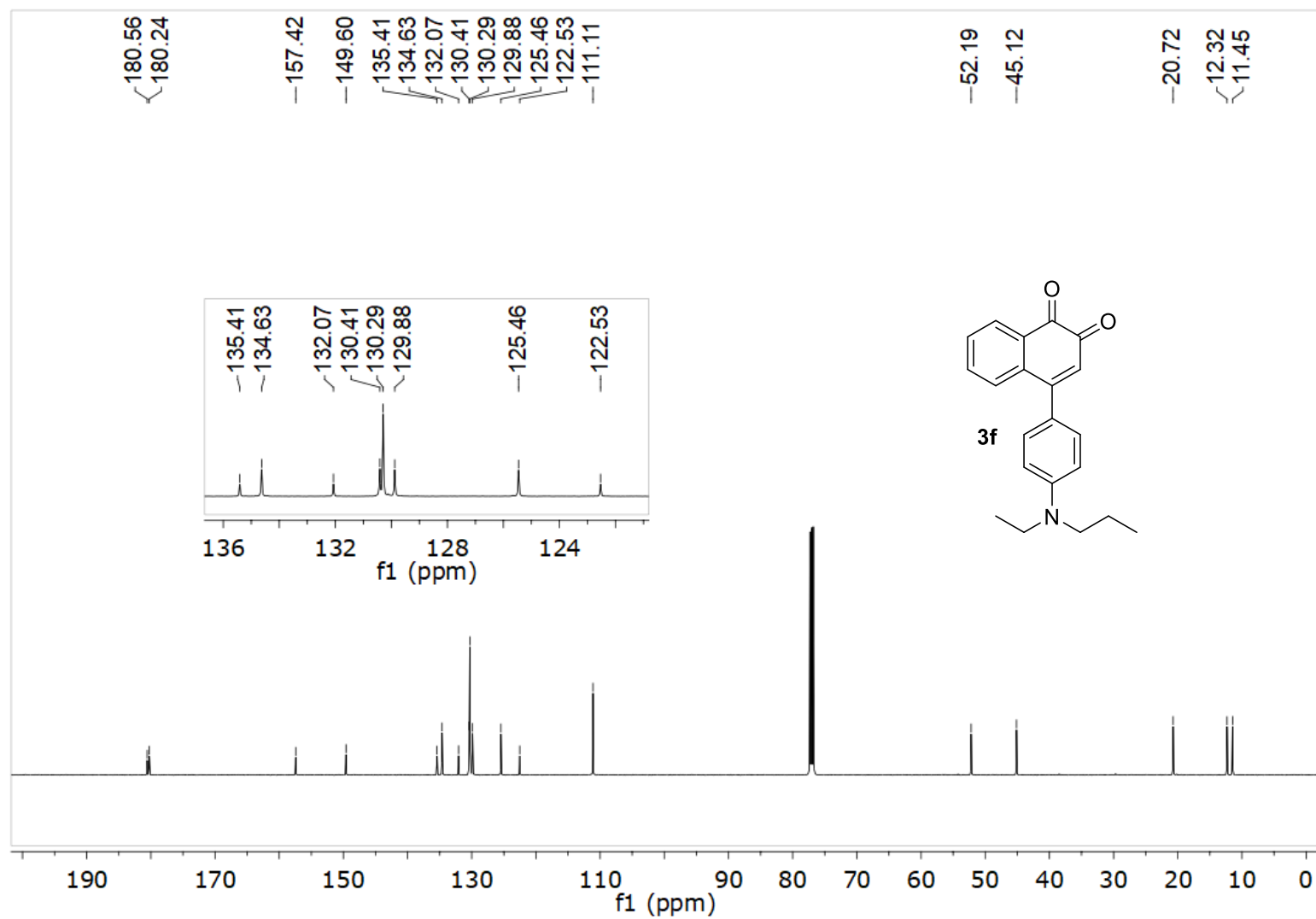
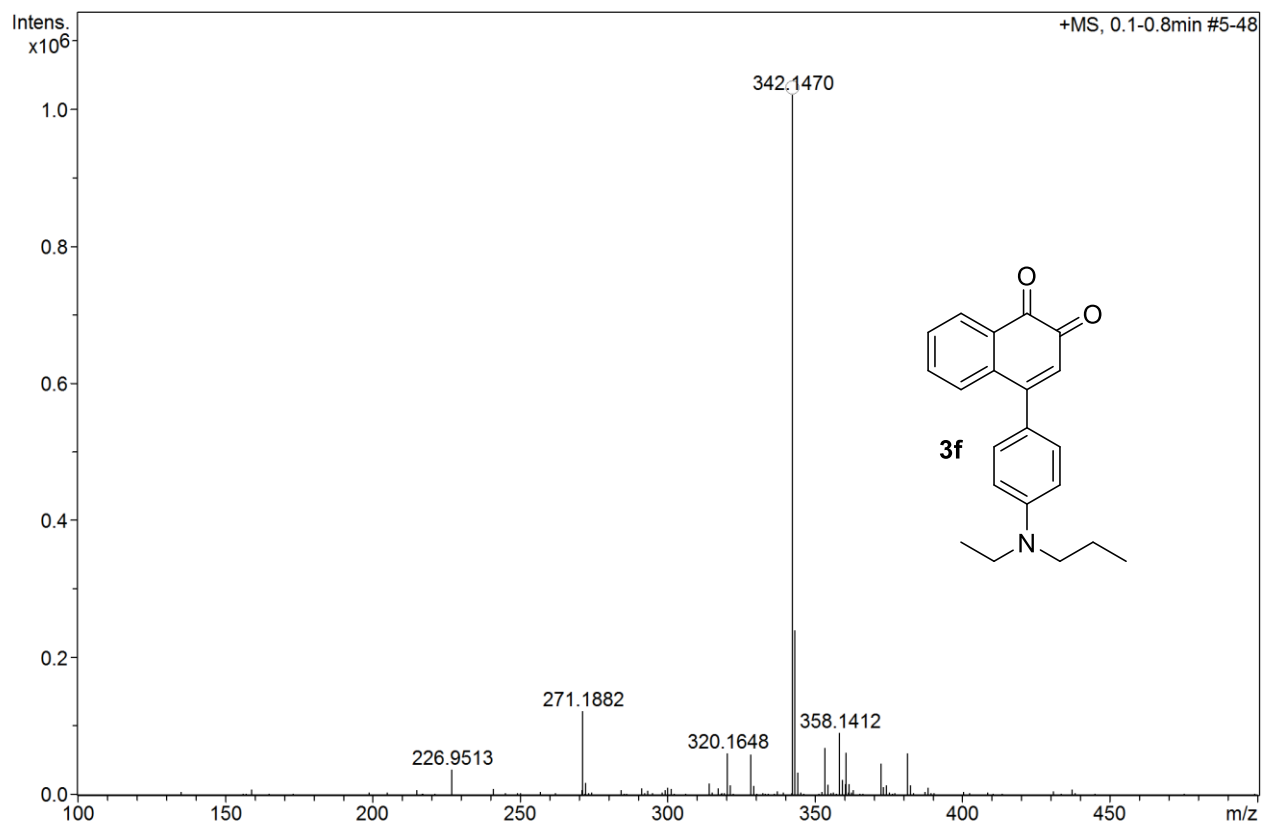


Figure S21. ^{13}C NMR spectrum (125 MHz, CDCl_3) of compound **3f**.

+MS, 0.1-0.8min #5-48



Meas. m/z	# Ion	Formula	m/z	err [ppm]	Mean err [ppm]	rdB	N-Rule	e ⁻ Conf	mSigm	Std I a	Std Mean m/z	Std VarNo	Std m/z Diff	Std Comb Dev
342.1470	46	1 C ₁₉ H ₁₆ N ₇	342.146170	-2.6	-2.7	15.5	ok	even	3.9	7.3	n.a.	n.a.	n.a.	n.a.
	1	C ₂₁ H ₂₁ NNaO ₂	342.146450	-1.7	-0.9	11.5	ok	even	1.4	2.7	n.a.	n.a.	n.a.	n.a.

Figure S22. HRMS spectrum of compound **3f**.

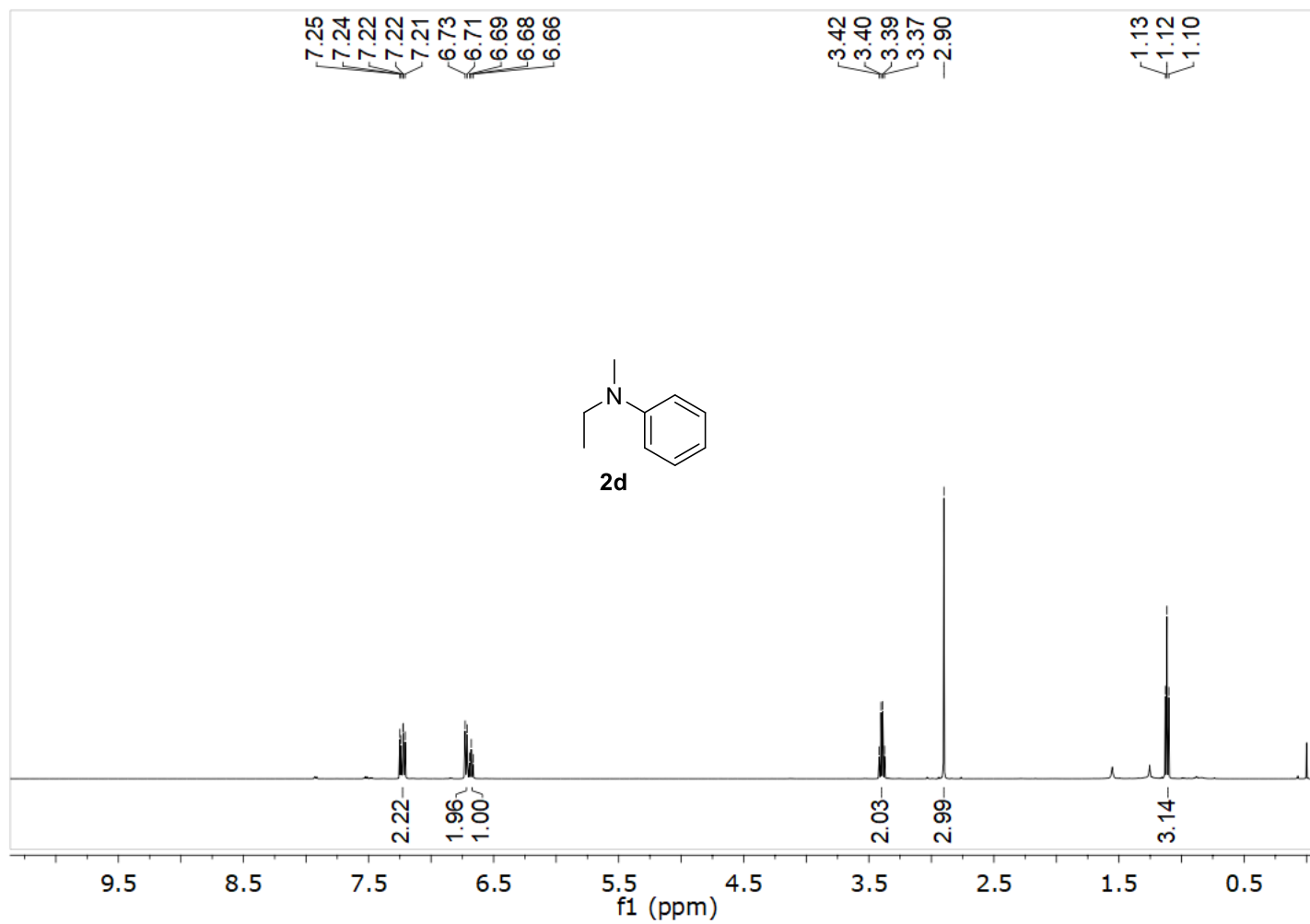


Figure S23. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **2d**.

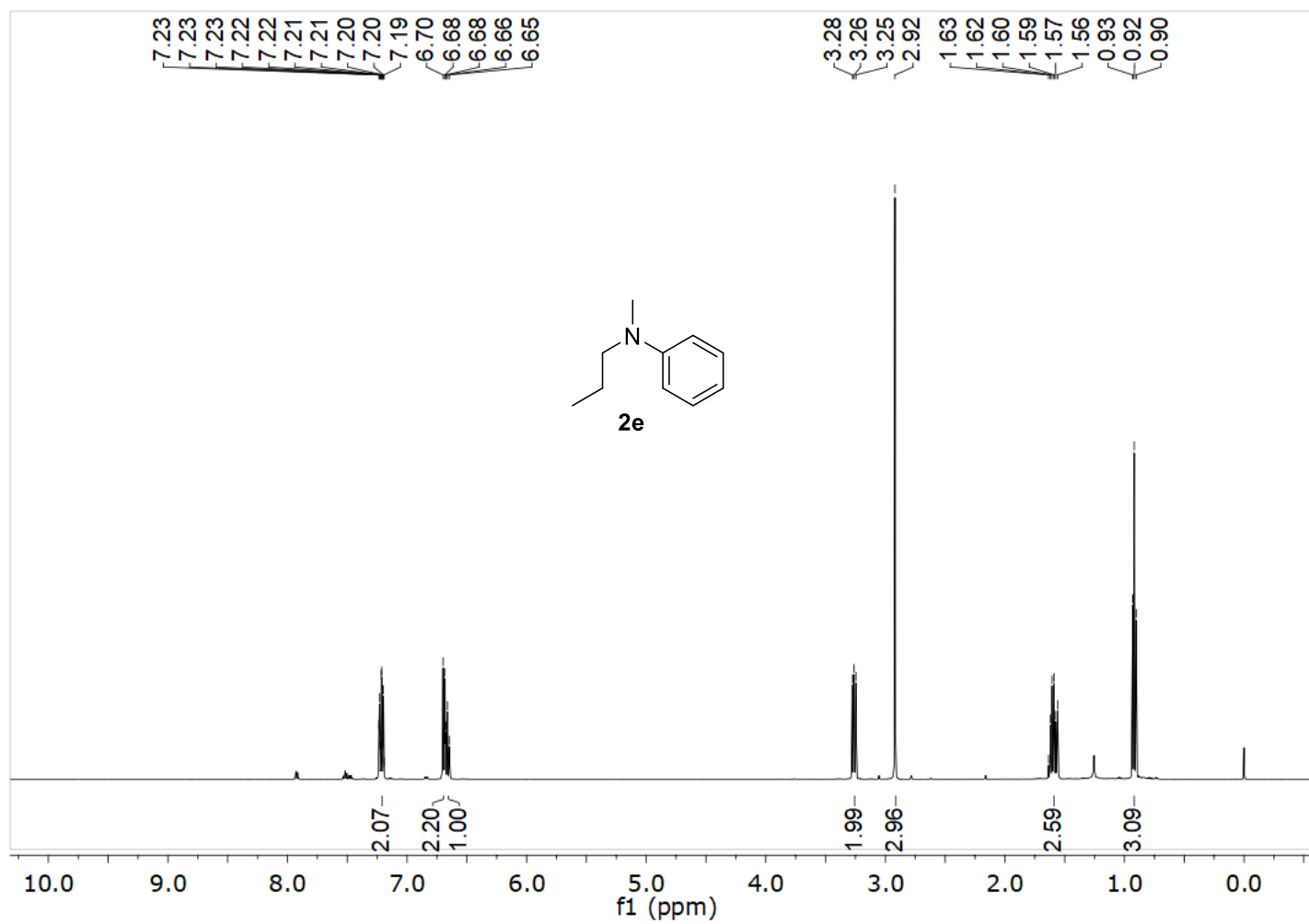


Figure S24. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **2e**.

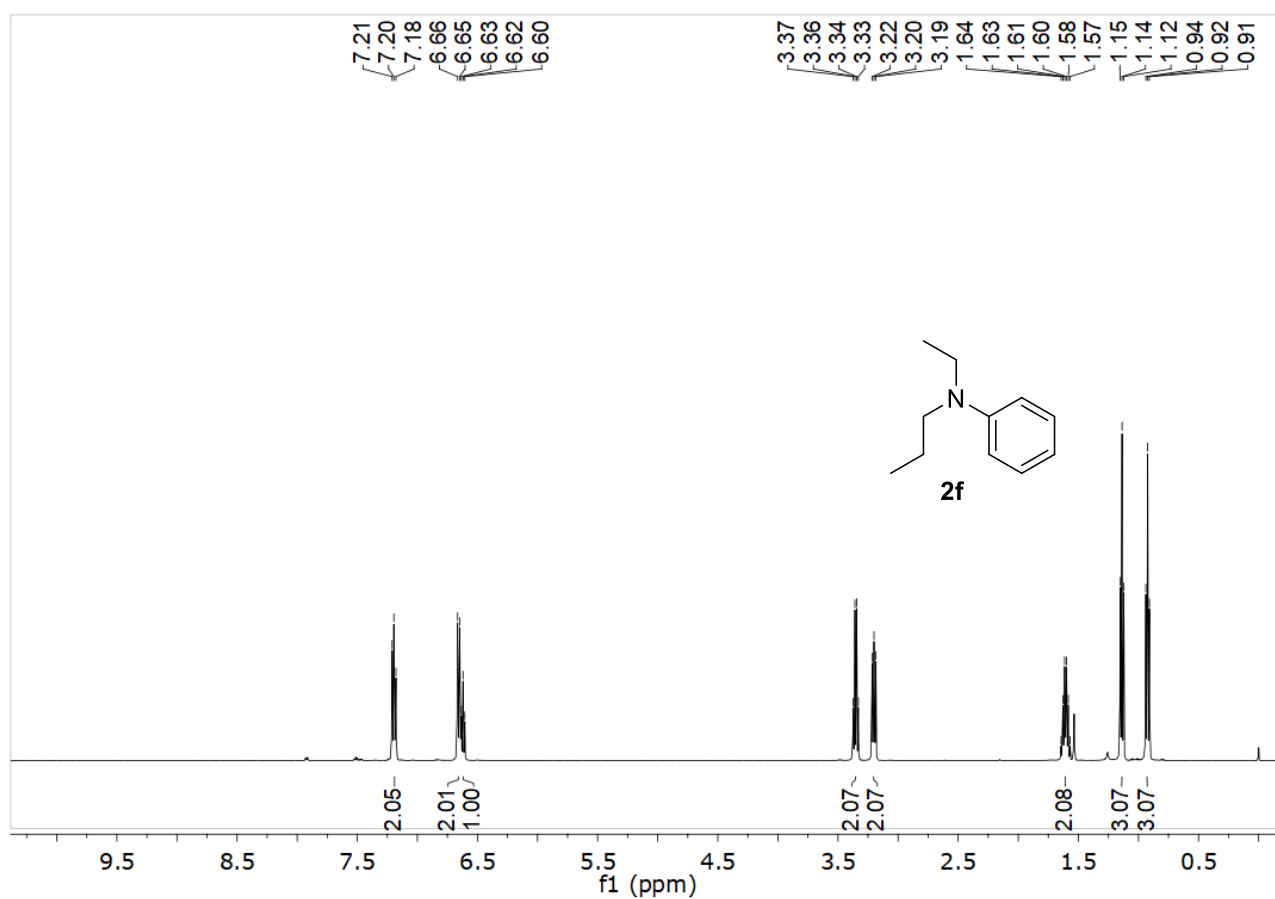


Figure S25. ¹H NMR spectrum (500 MHz, CDCl₃) of compound **2f**