

Indole-Based Novel Small Molecules for the Modulation of Bacterial Signalling Pathways

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Supporting Information

- 1) Growth Inhibition Data
- 2) ¹H and ¹³C NMR Spectrums of Synthesised Compounds

1) Growth Inhibition Data

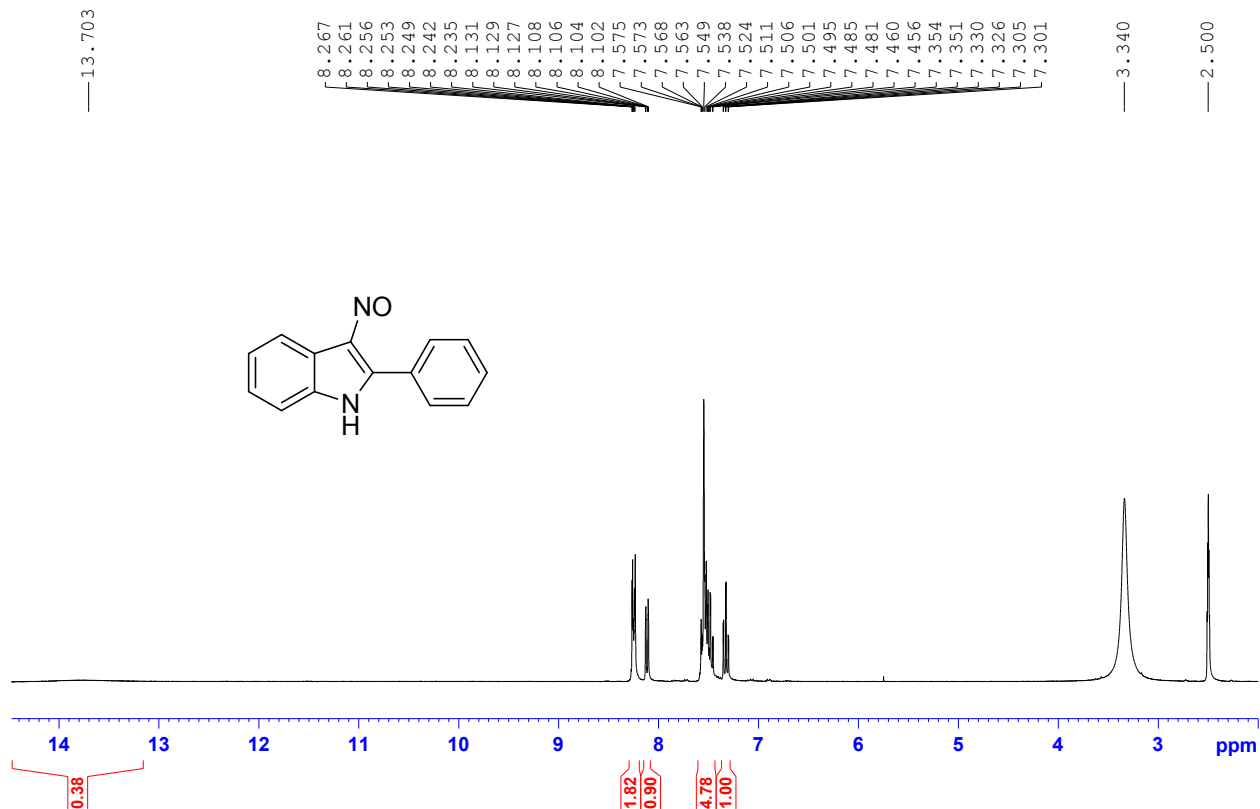
Table 1: Percentage growth inhibition of the indole based AHLs as determined by reduction in OD₆₀₀ in the P_{lasB}::gfp reporter strain

Compound	Concentration (μM)			
	250	125	62.5	31.25
11a	6.19 ± 3.21	3.18 ± 4.12	3.52 ± 3.9	3.87 ± 5.38
11b	7.50 ± 5.32	3.92 ± 4.65	5.39 ± 5.44	5.84 ± 2.93
11c	7.28 ± 3.41	6.52 ± 4.32	5.27 ± 4.93	4.91 ± 5.32
11d	14.99 ± 4.89	11.63 ± 4.87	9.52 ± 5.43	4.71 ± 1.75
11e	0	0	0	0
14a	0	0	0	0
14b	0	0	0	0
14c	0	0	0	0
16a	6.96 ± 3.89	0	0	0
16b	0	0	0	0
16c	0	0	0	0
16d	0	0	0	0
16e	0	0	0	0
17a	0	0	0	0
17b	0	0	0	0
17c	5.92 ± 1.88	5.34 ± 2.96	6.39 ± 4.67	4.28 ± 3.58
20a	0	0	0	0
20b	7.38 ± 2.12	0	0	0
20c	0	0	0	0
21a	0	0	0	0
21b	0	0	0	0
21c	0	0	0	0
Furanone 30	31.57 ± 3.87	5.85 ± 2.97	0	0

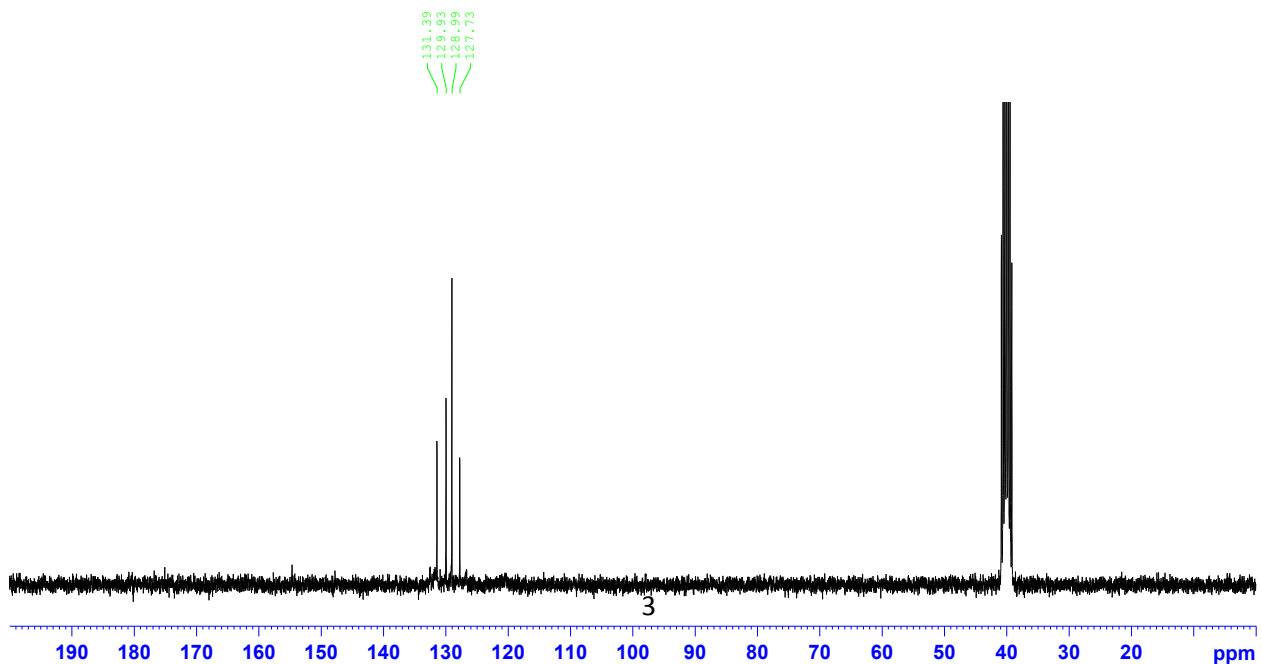
Growth inhibition ± standard deviation of mean from at least two independent experiments. Compounds tested twice in duplicate. 0 = No growth inhibition

1) ¹H and ¹³C NMR Spectrums of Synthesised Compounds

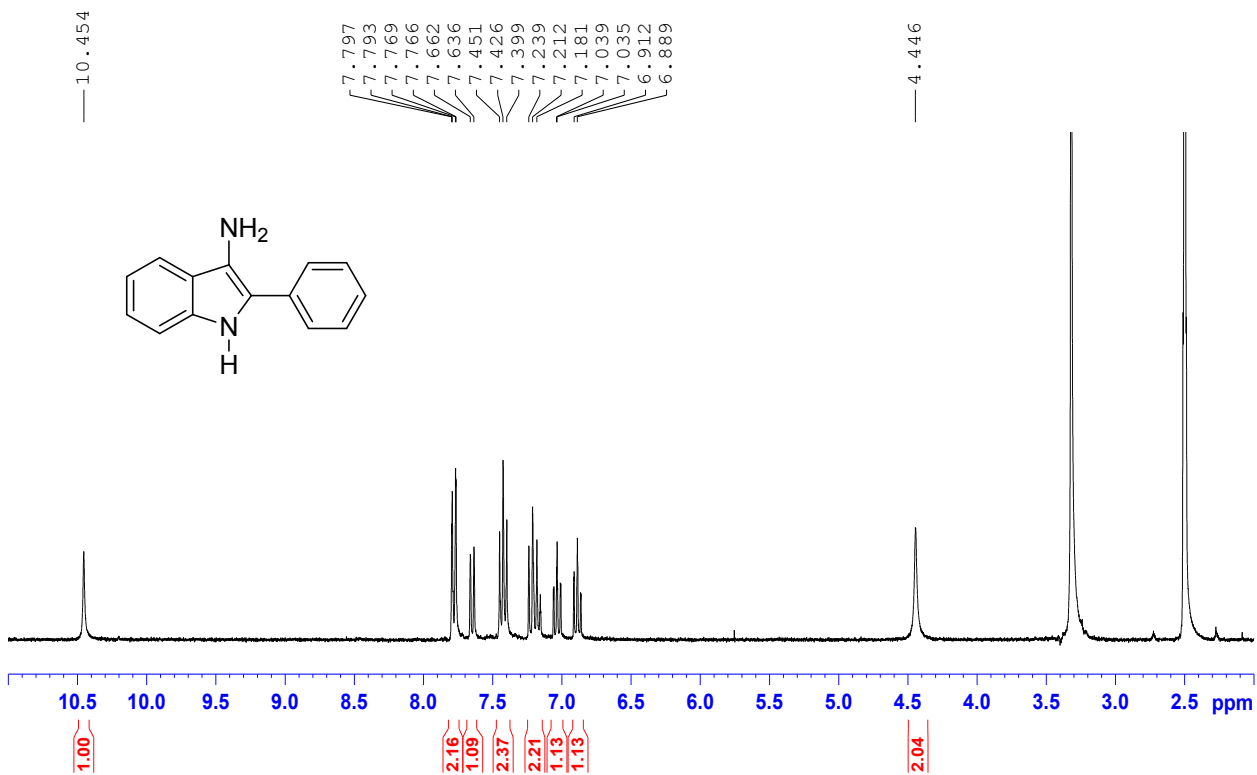
¹H NMR spectrum of Compound # 9



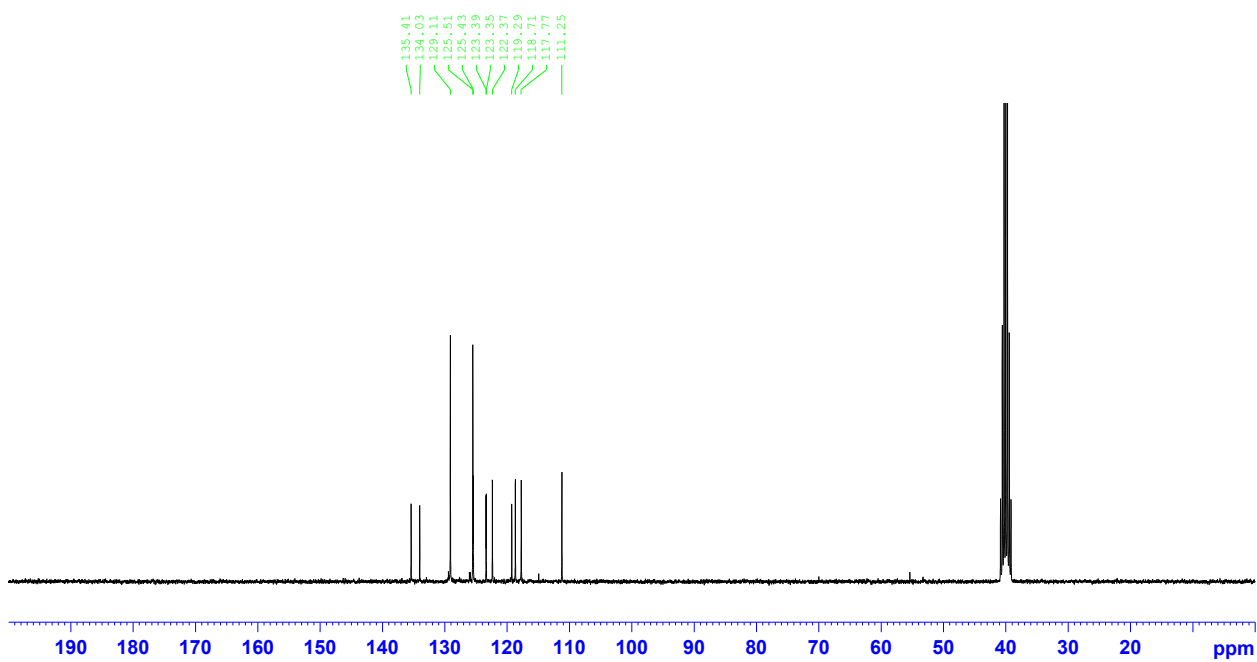
¹³C NMR spectrum of Compound # 9



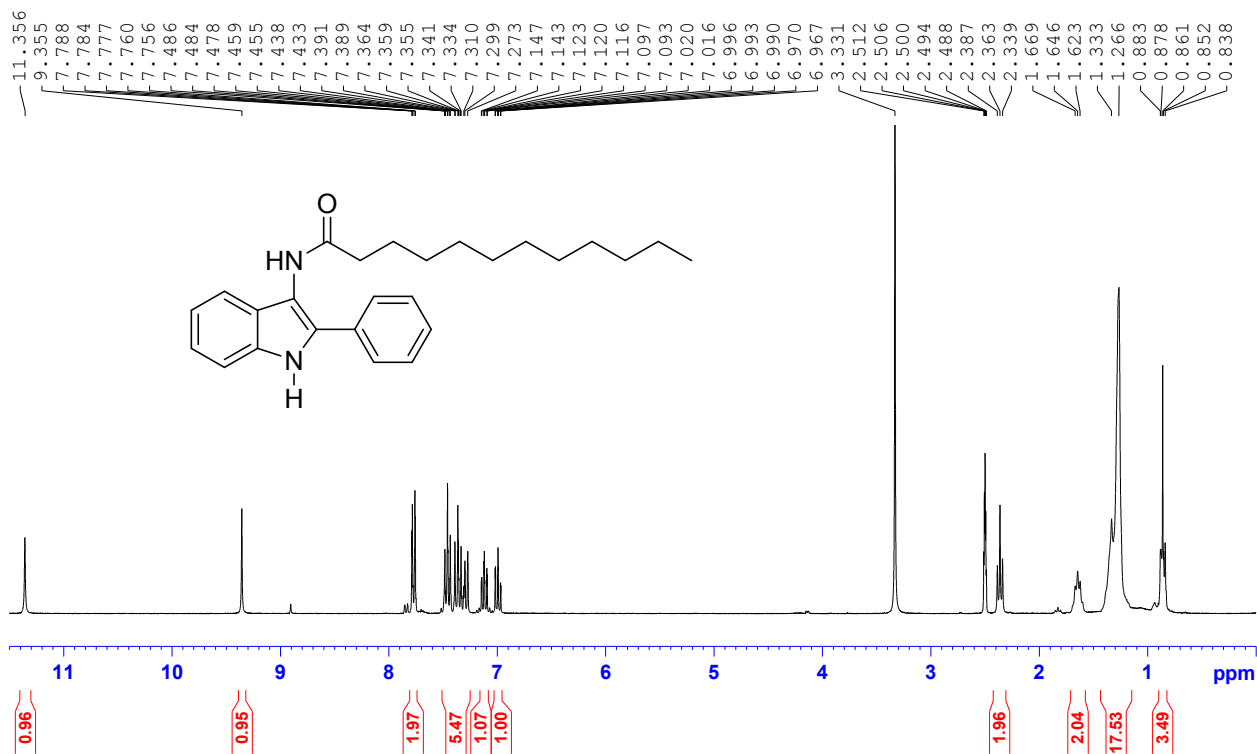
¹H NMR spectrum of Compound # 10



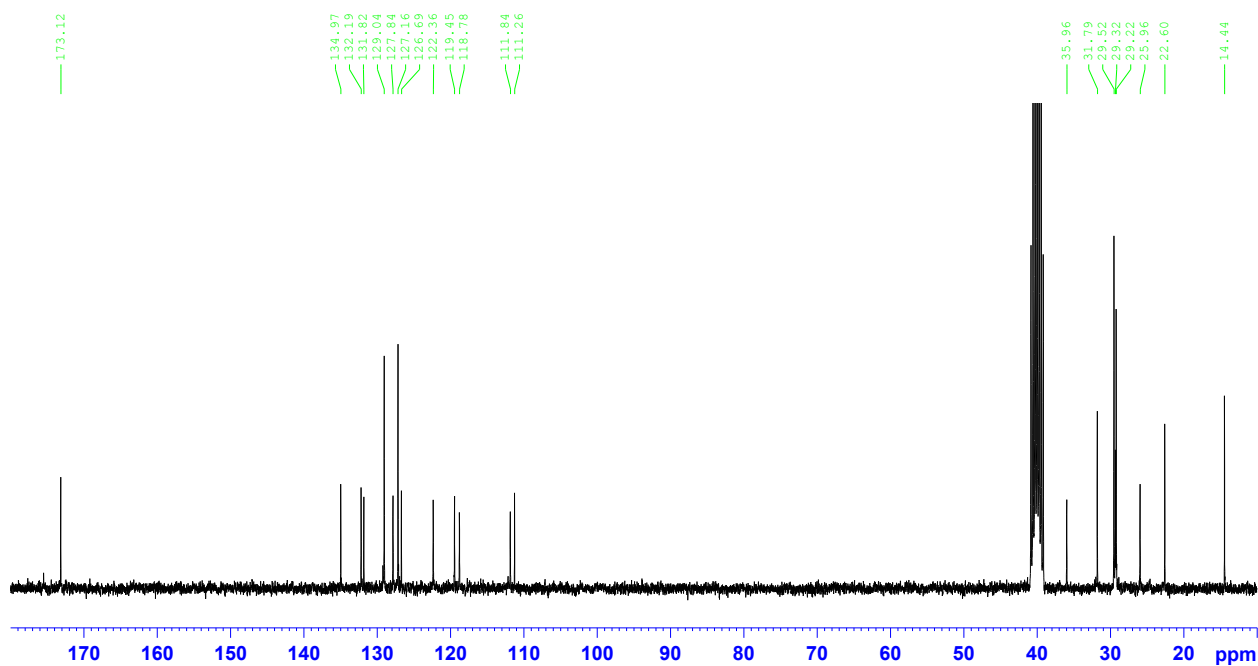
¹³C NMR spectrum of Compound # 10



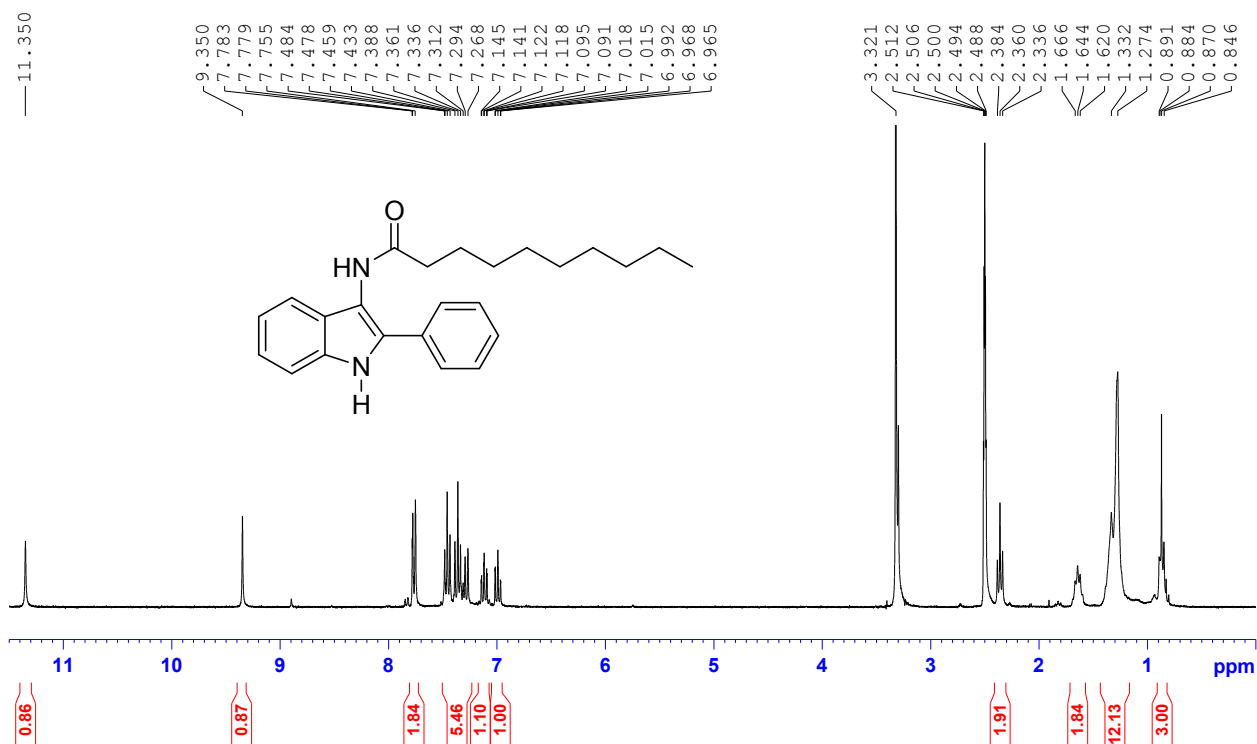
¹H NMR spectrum of Compound # 11a



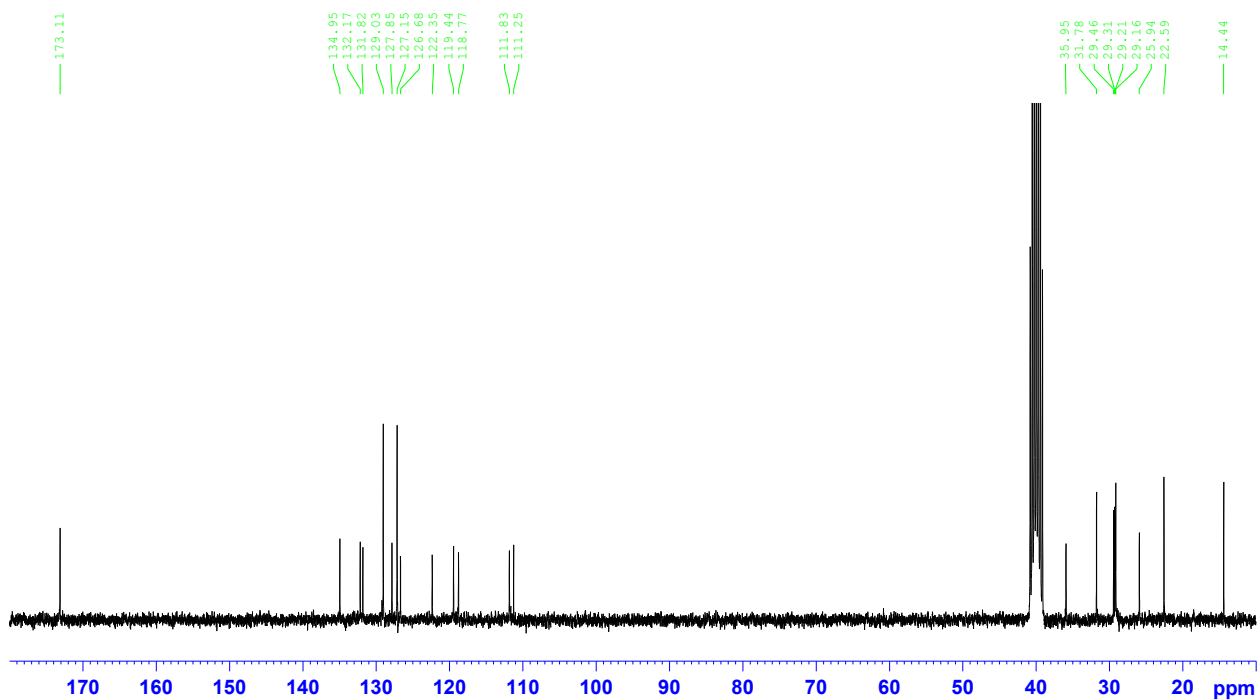
¹³C NMR spectrum of Compound # 11a



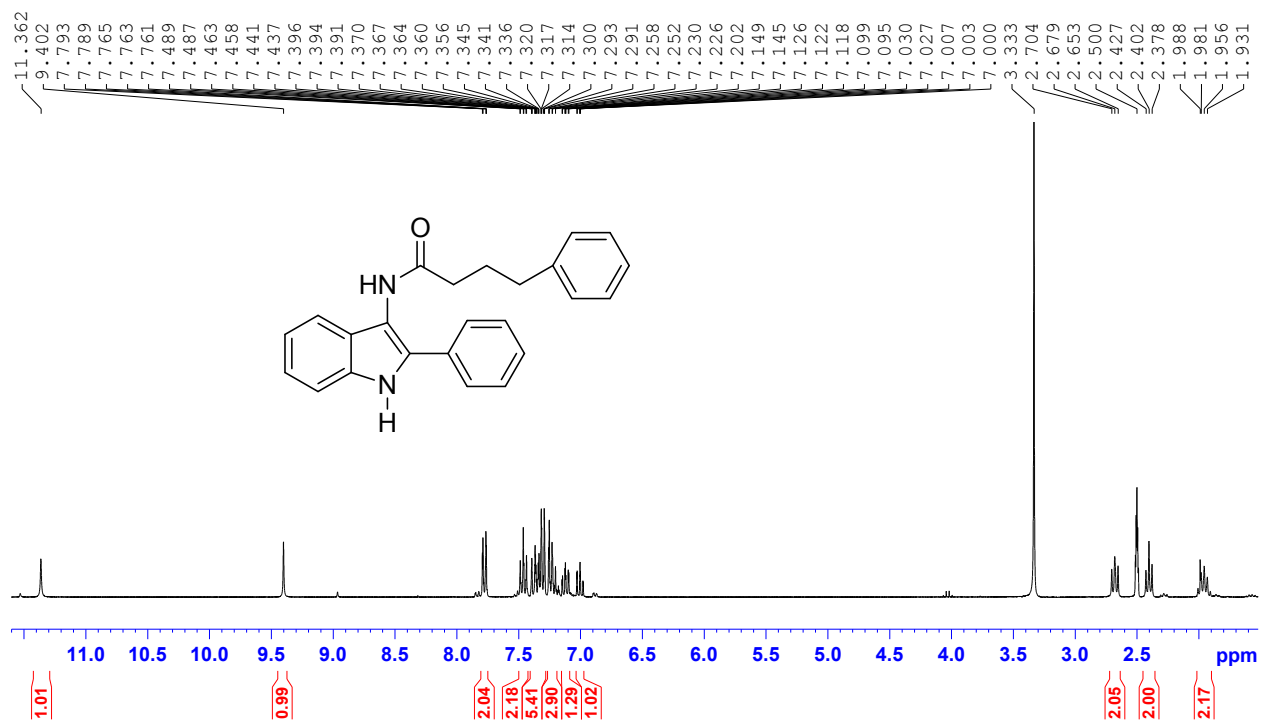
¹H NMR spectrum of Compound # 11b



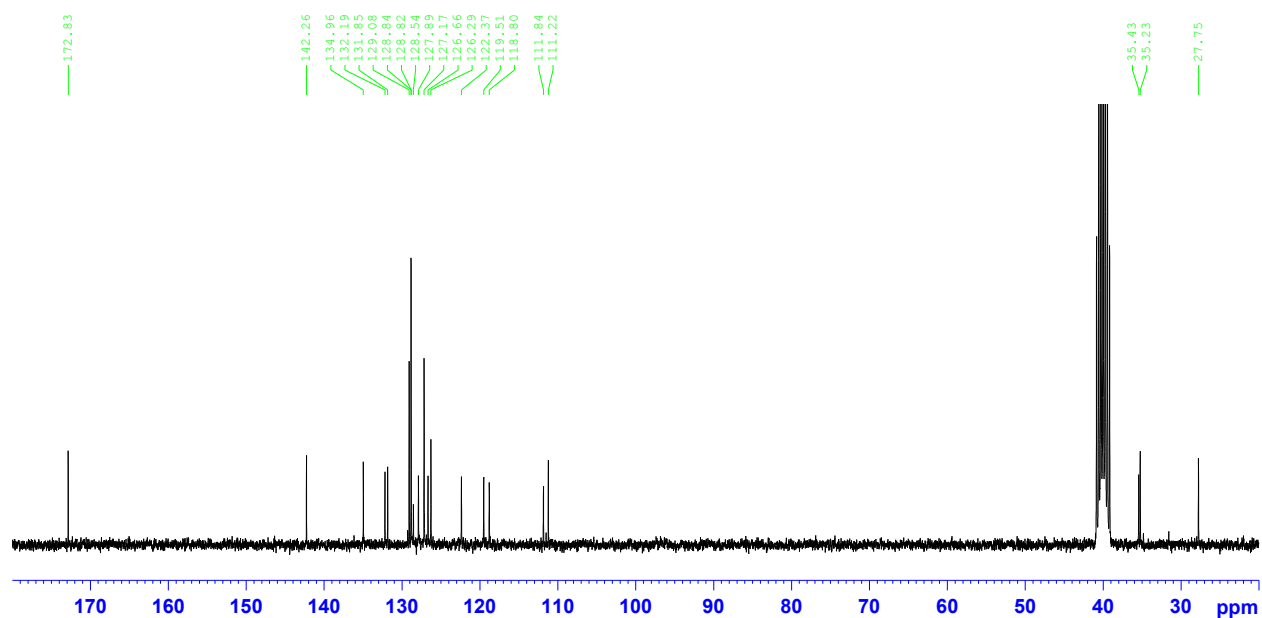
¹³C NMR spectrum of Compound # 11b



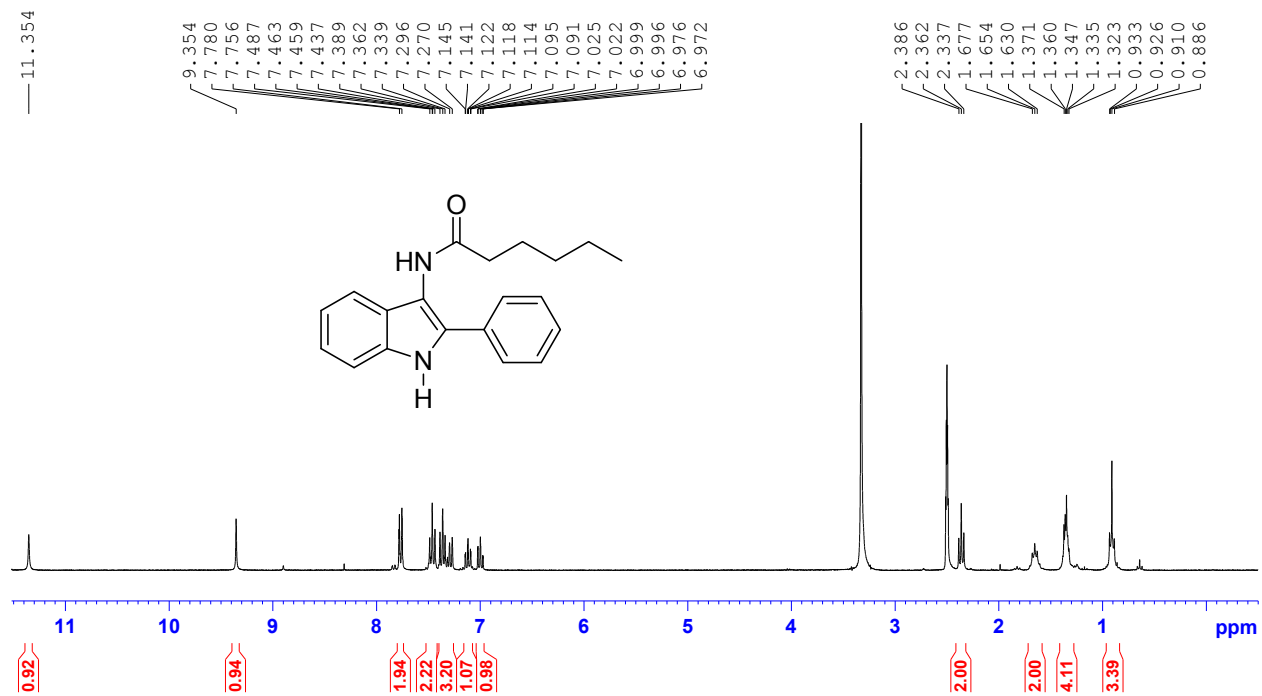
¹H NMR spectrum of Compound # 11c



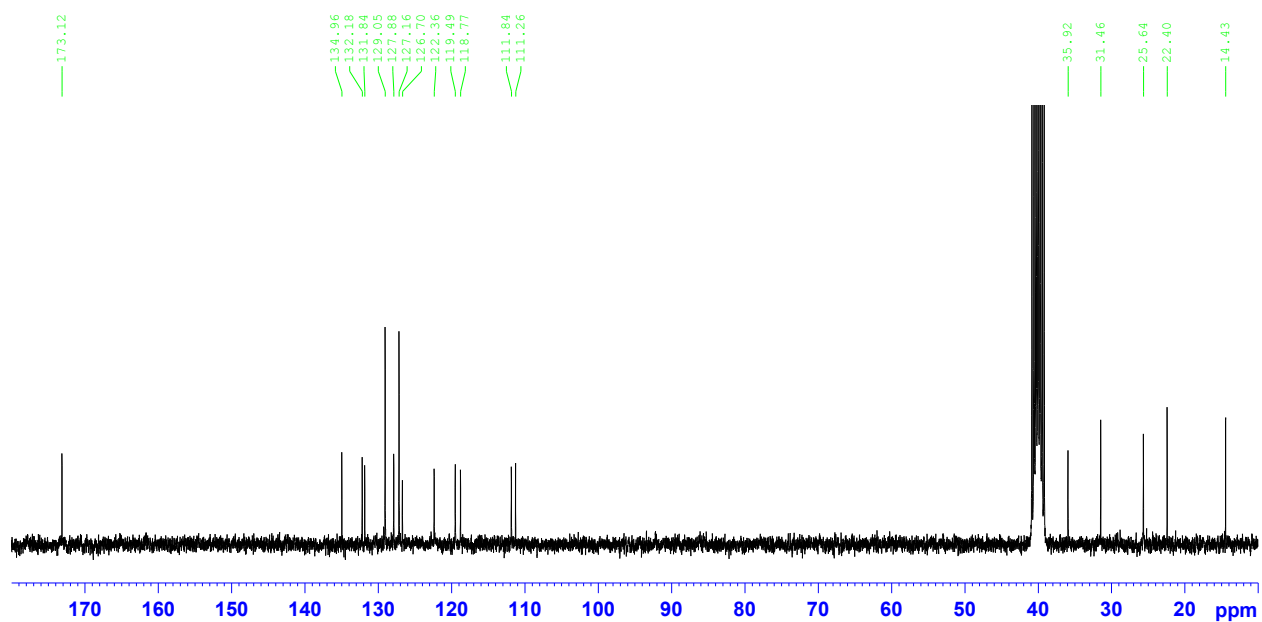
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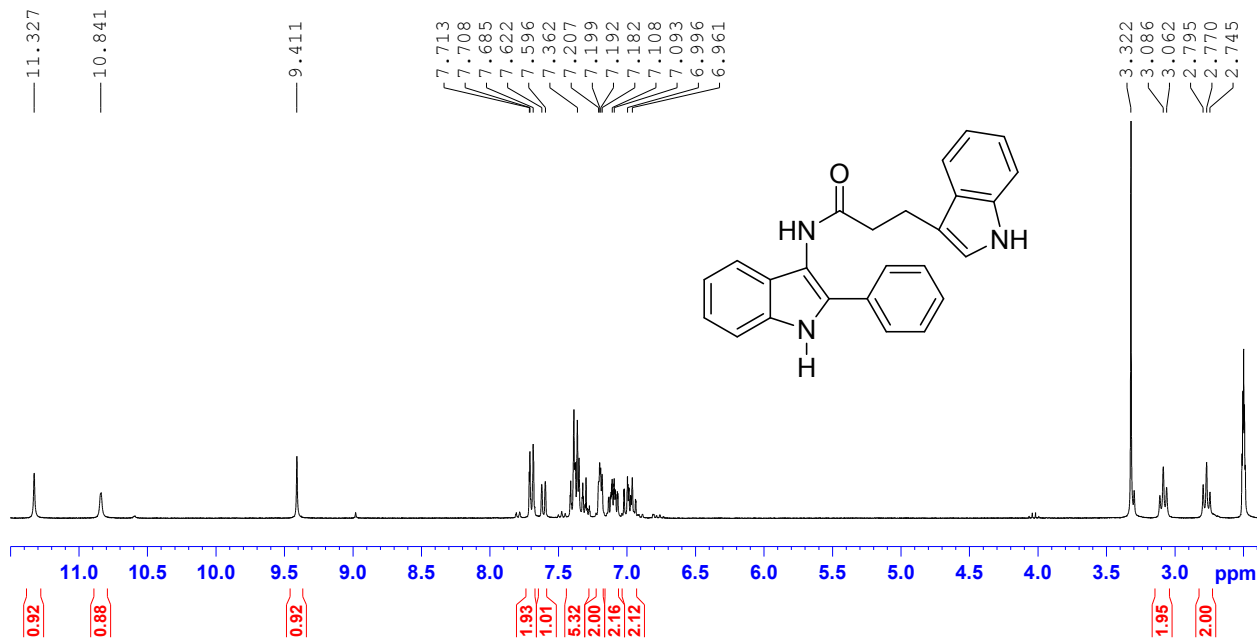
¹H NMR spectrum of Compound # 11d



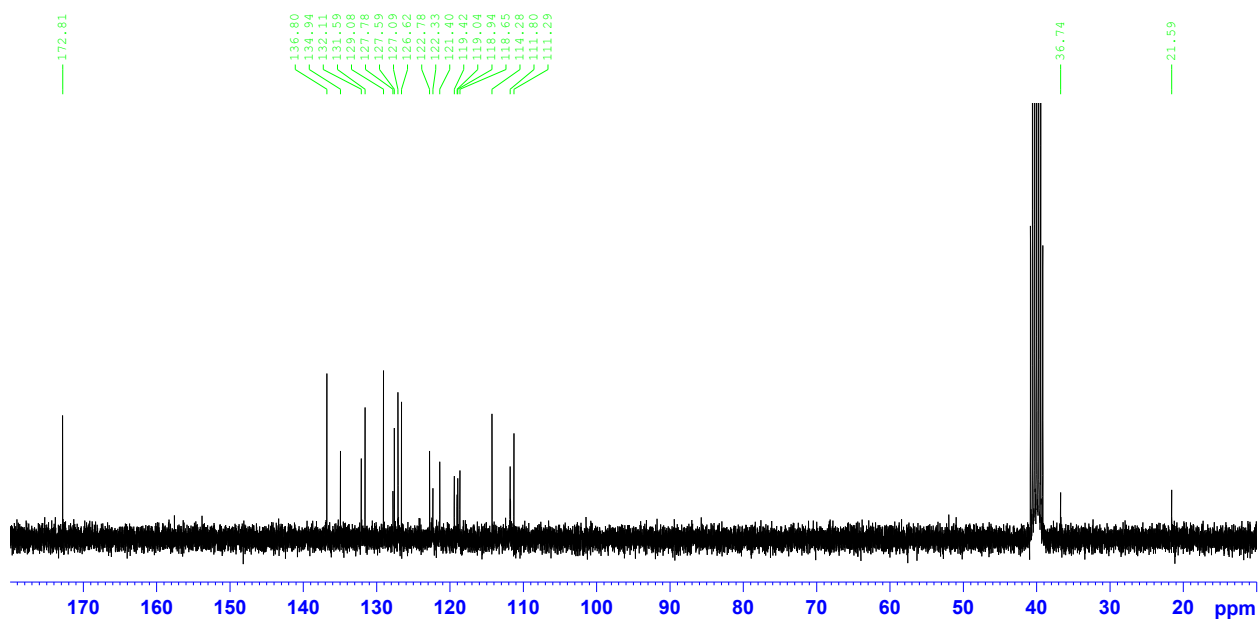
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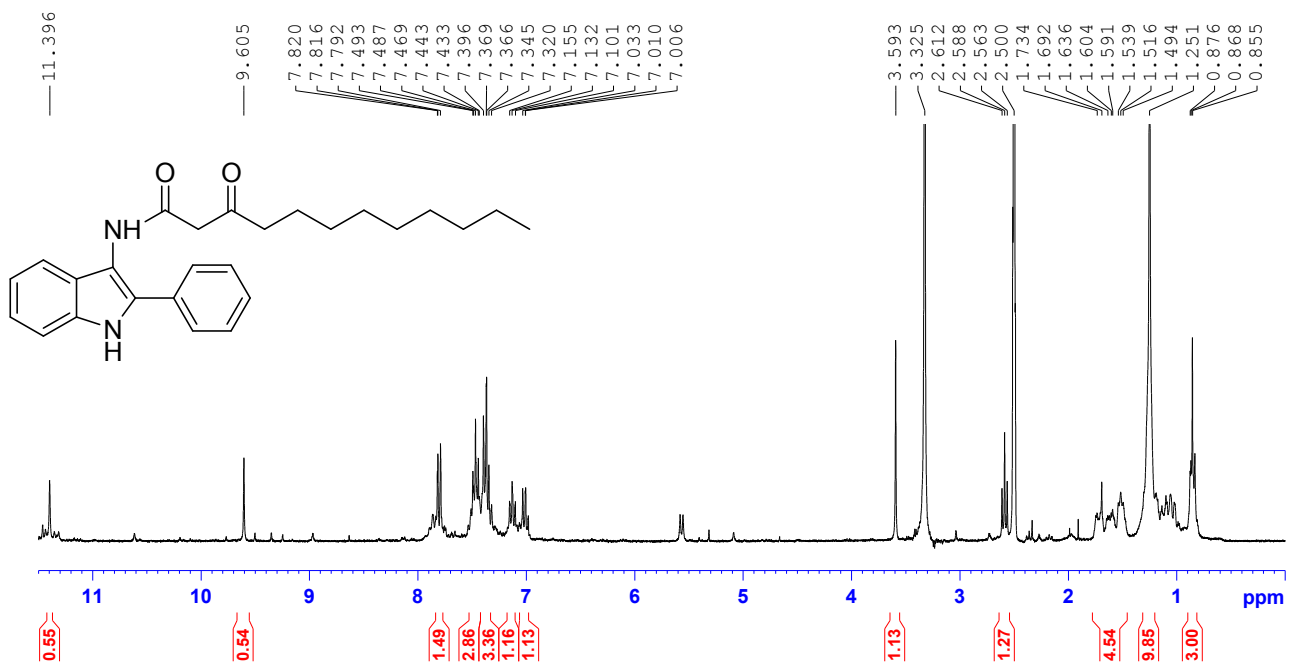
¹H NMR spectrum of Compound # 11e



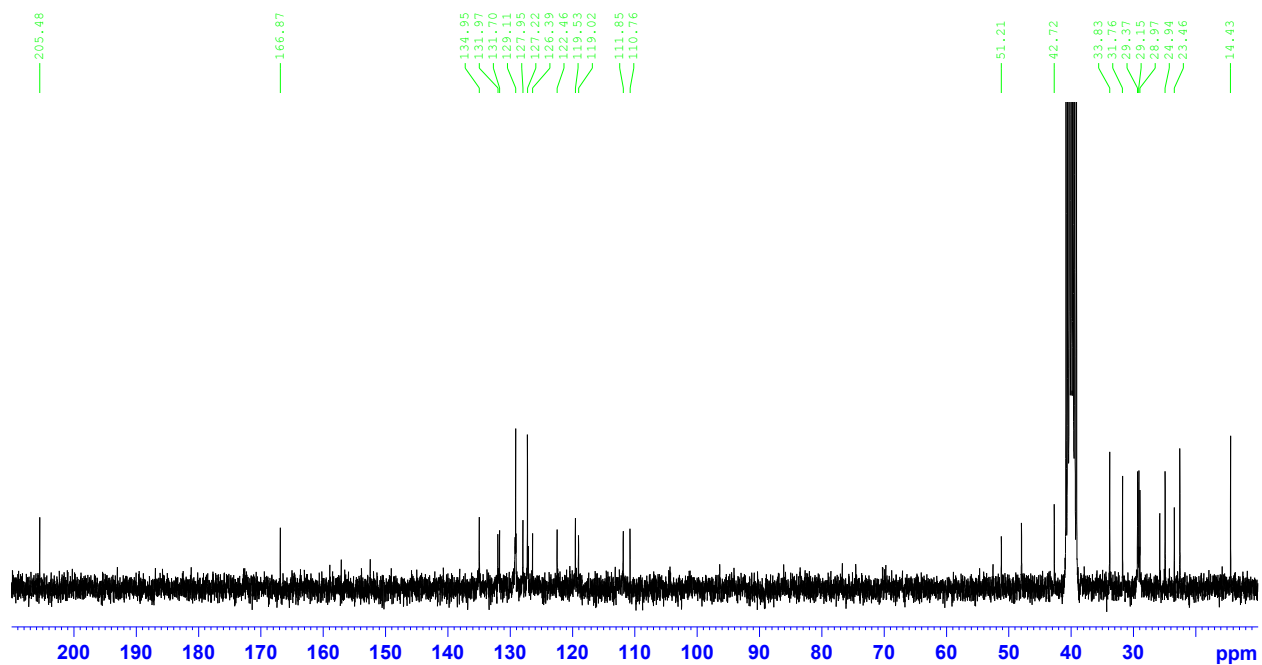
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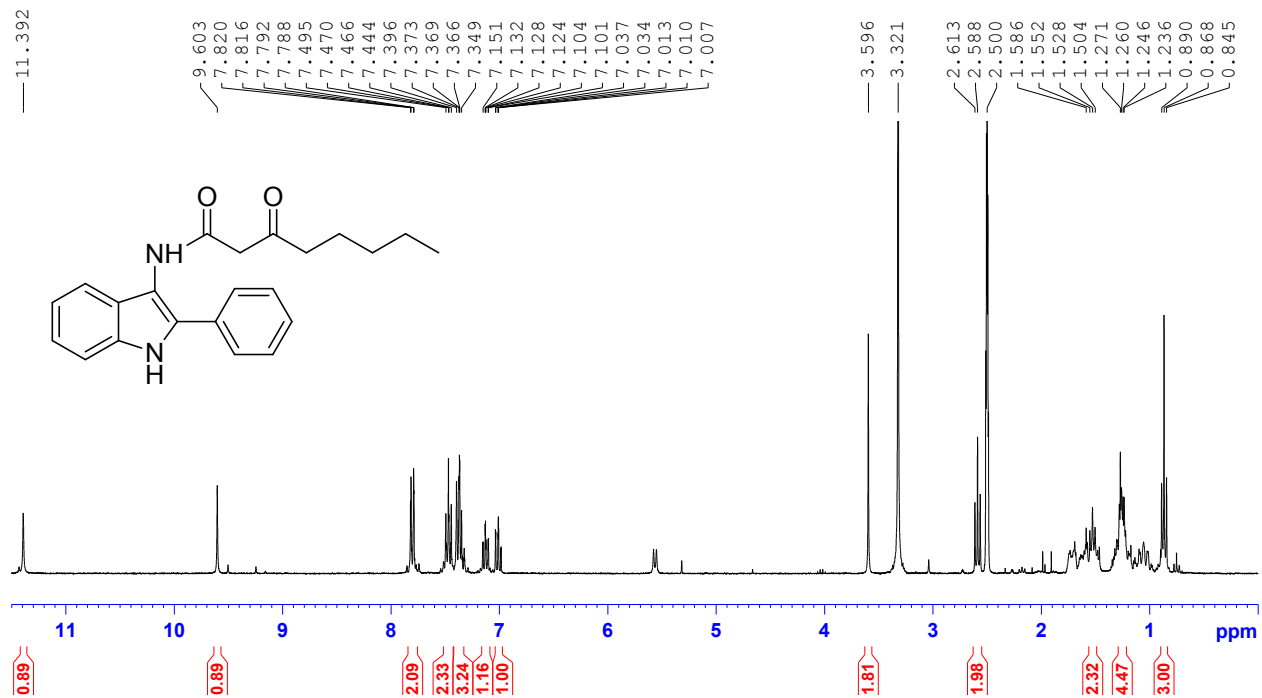
¹H NMR spectrum of Compound # 14a



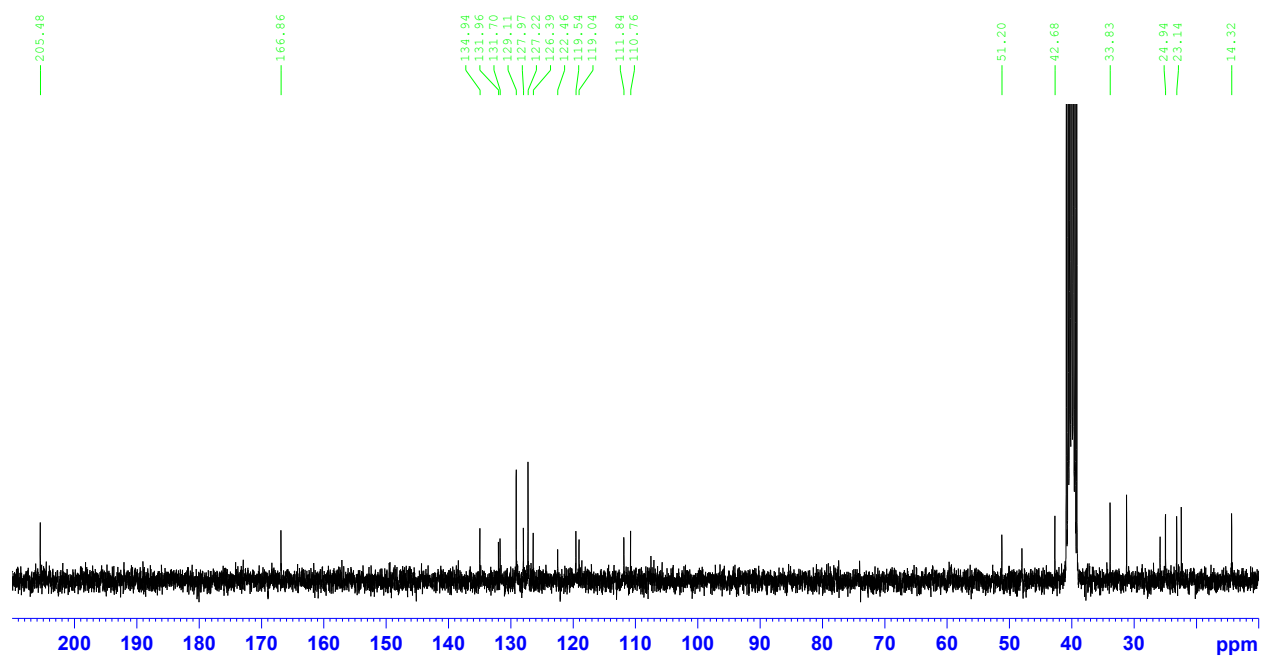
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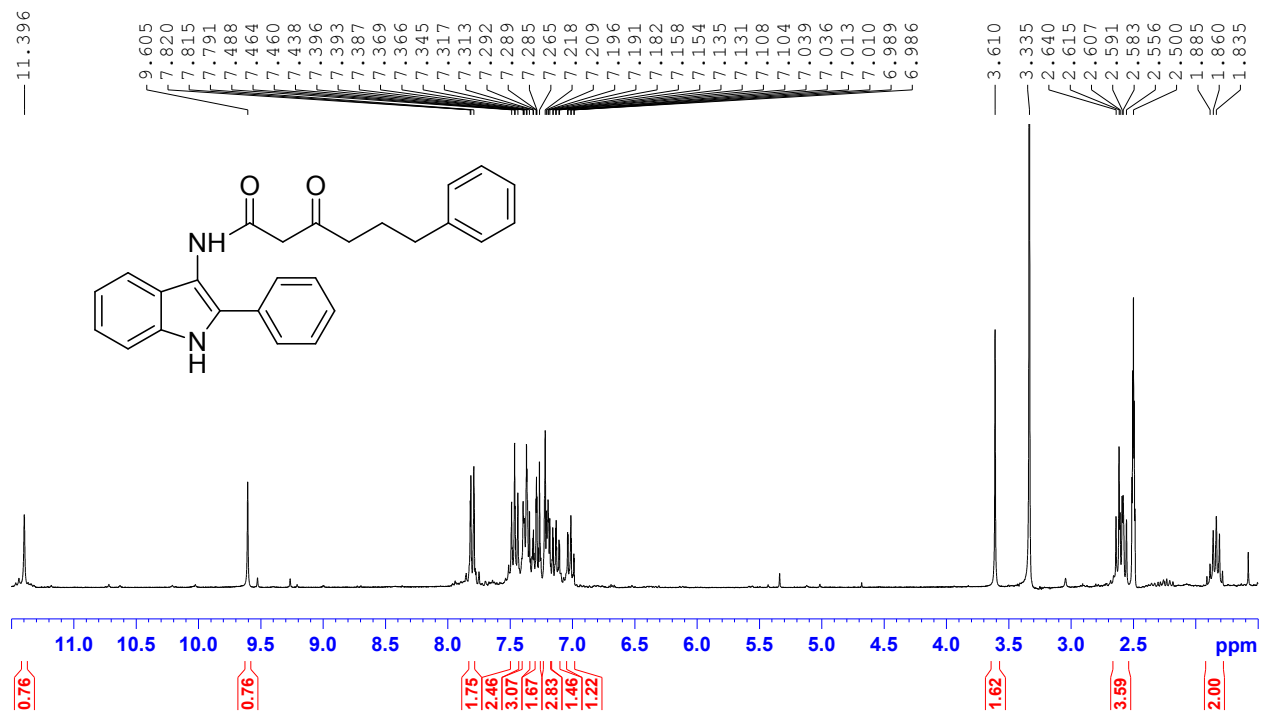
¹H NMR spectrum of Compound # 14b



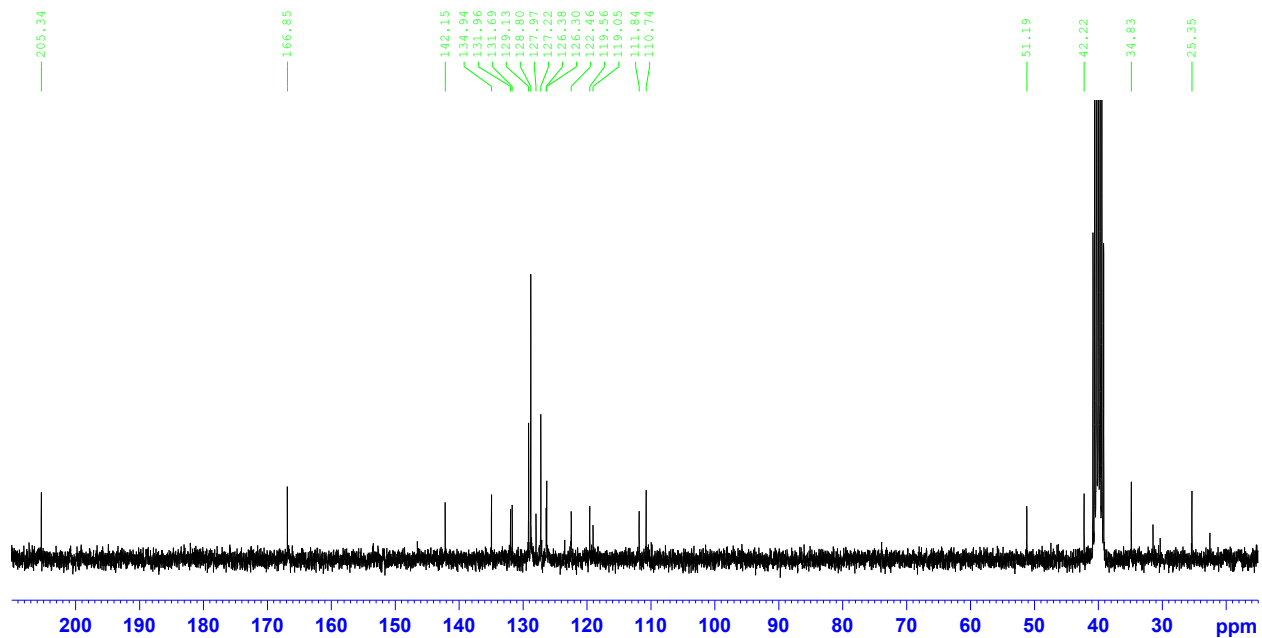
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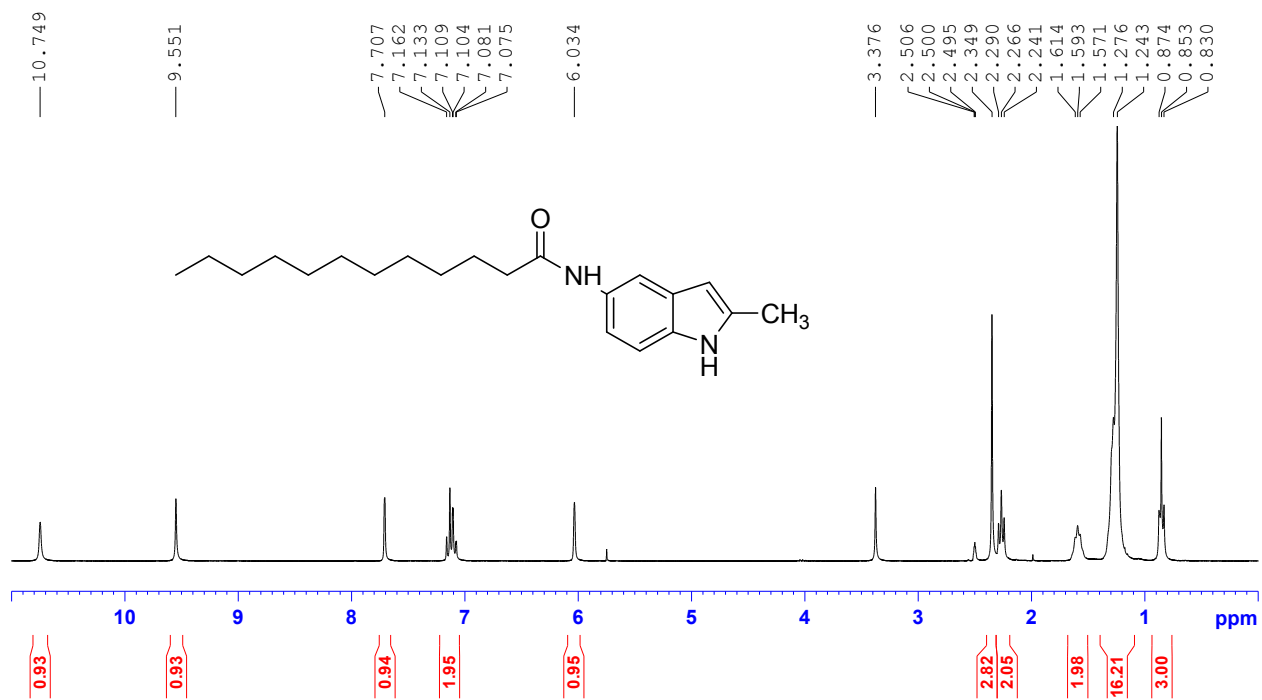
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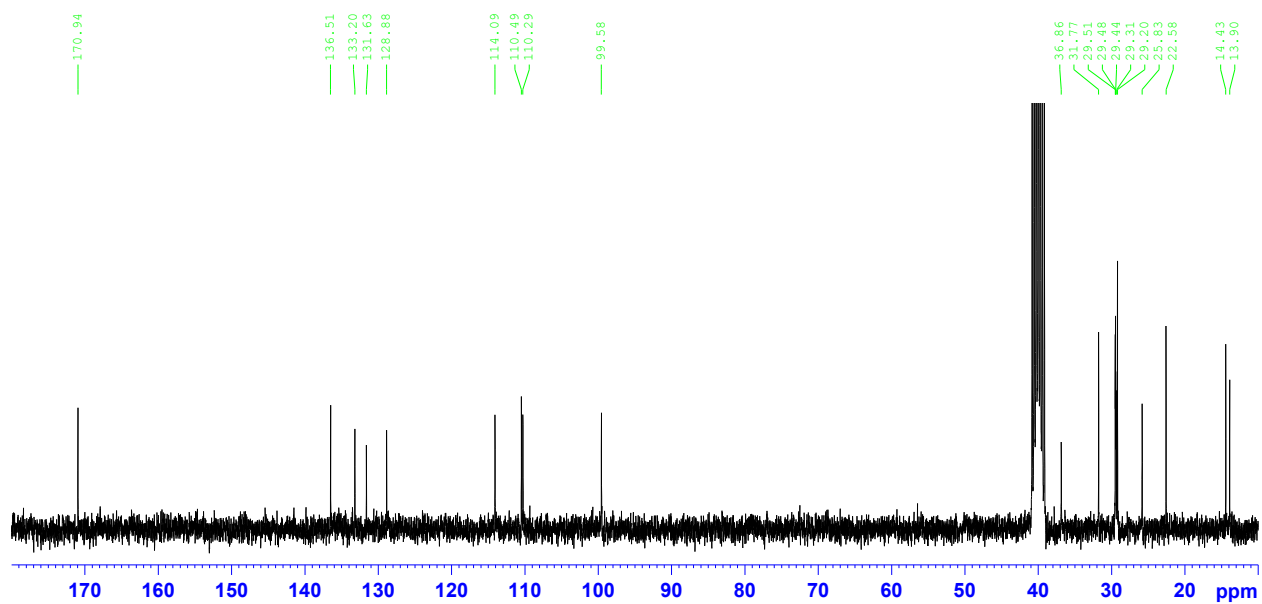
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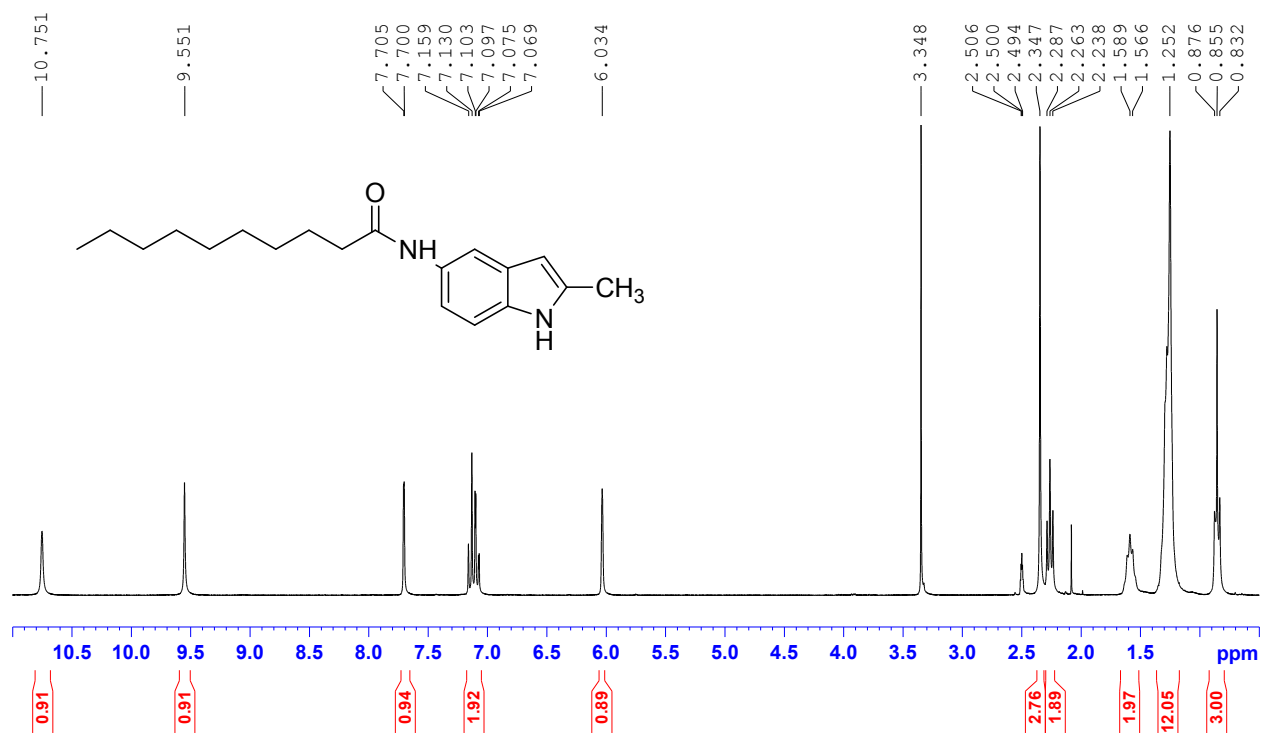
¹H NMR spectrum of Compound # 16a



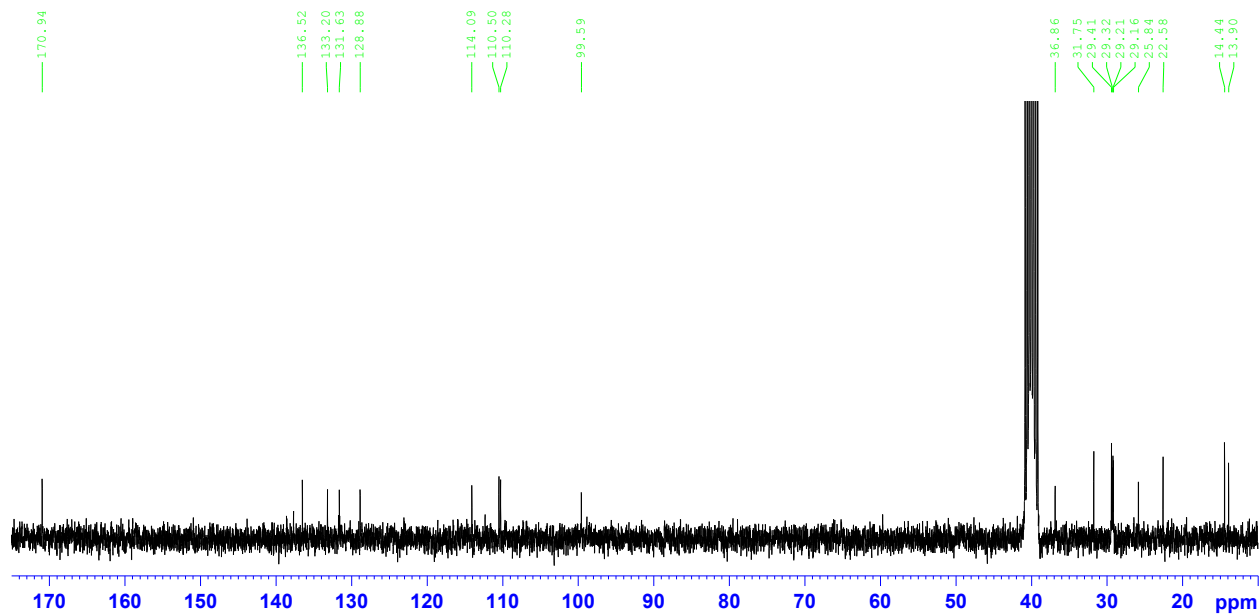
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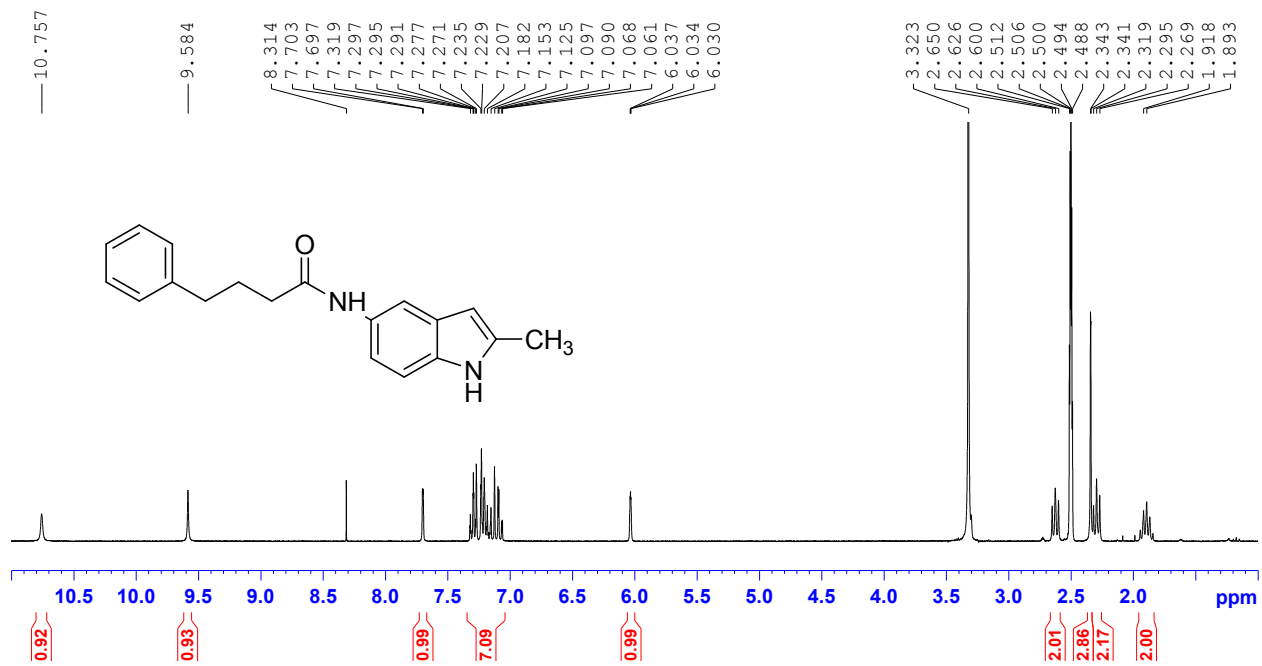
¹H NMR spectrum of Compound # 16b



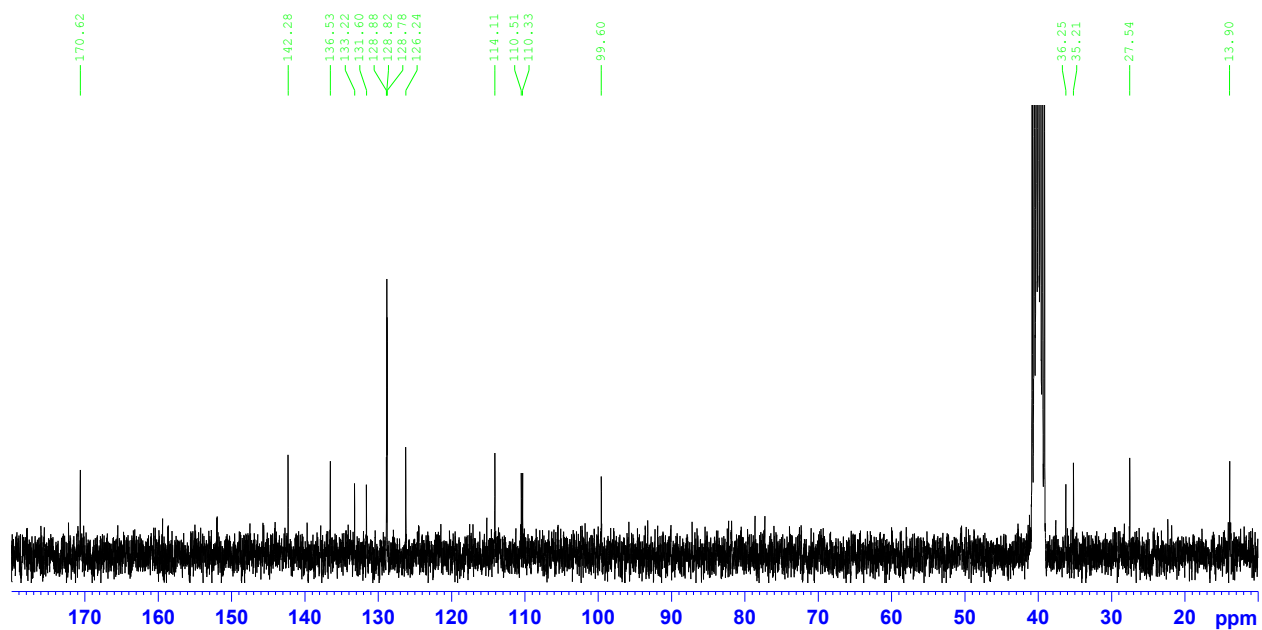
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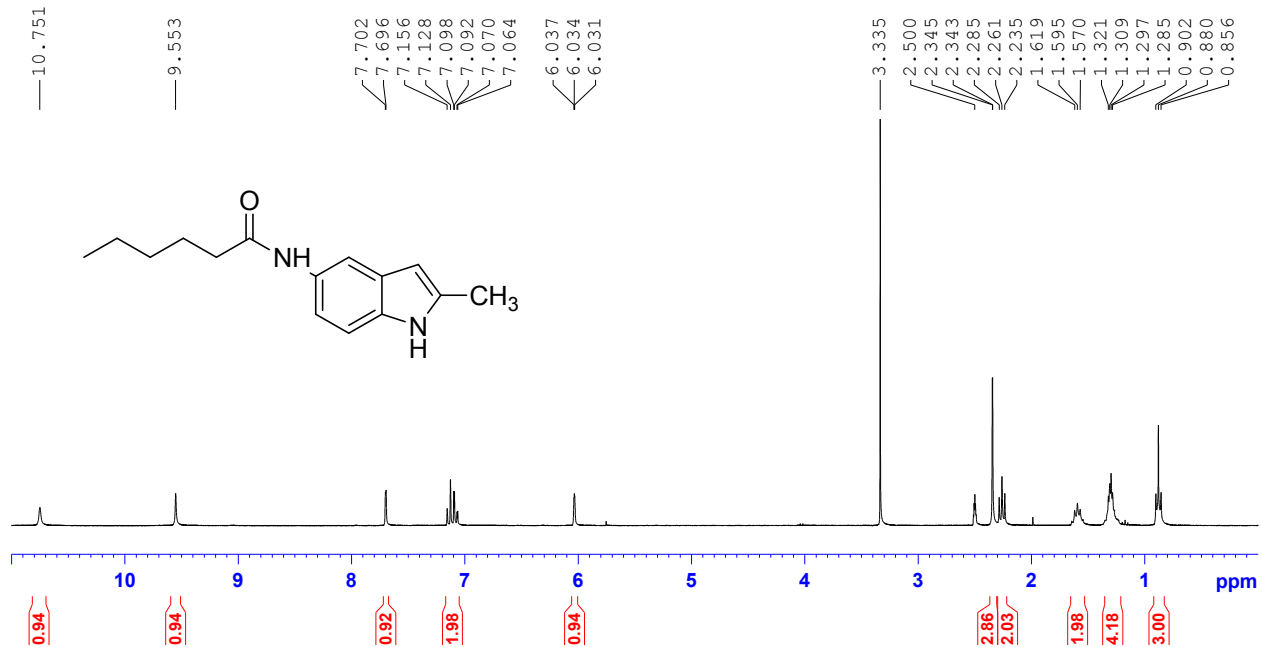
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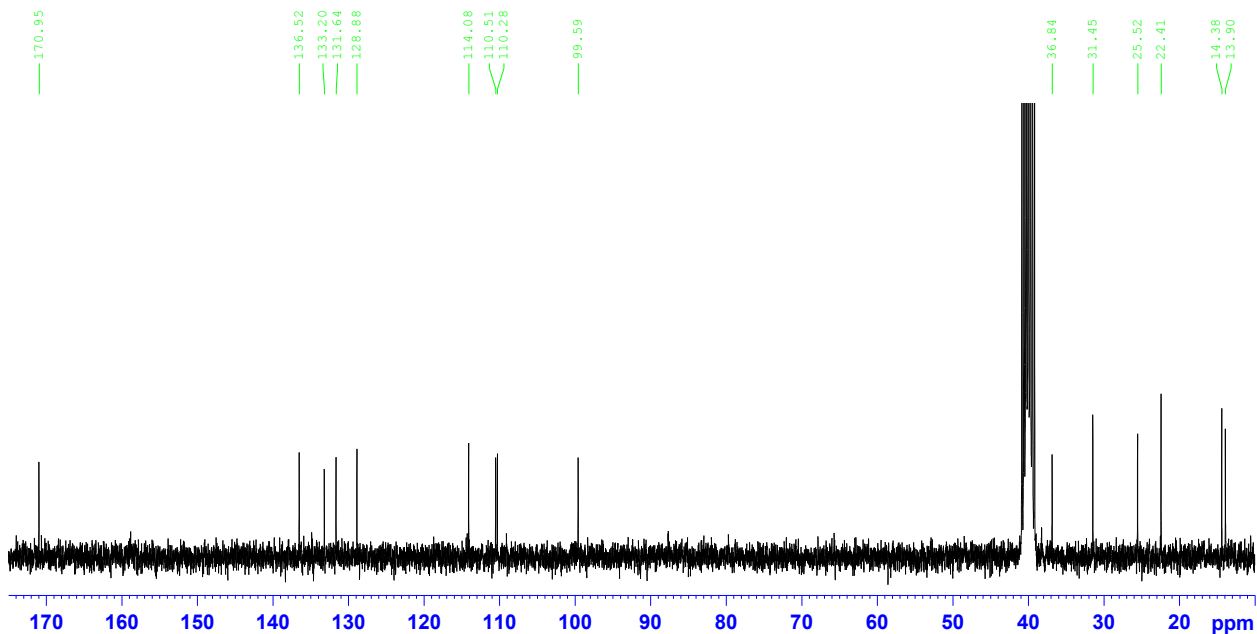
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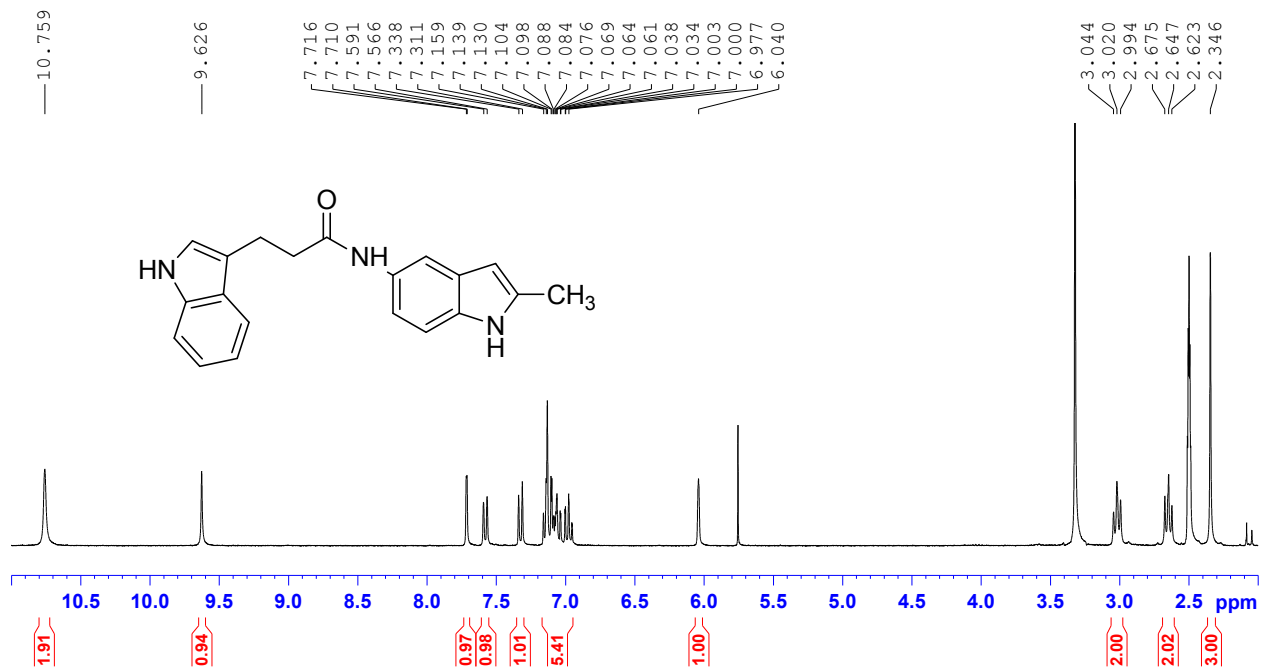
¹H NMR spectrum of Compound # 16d



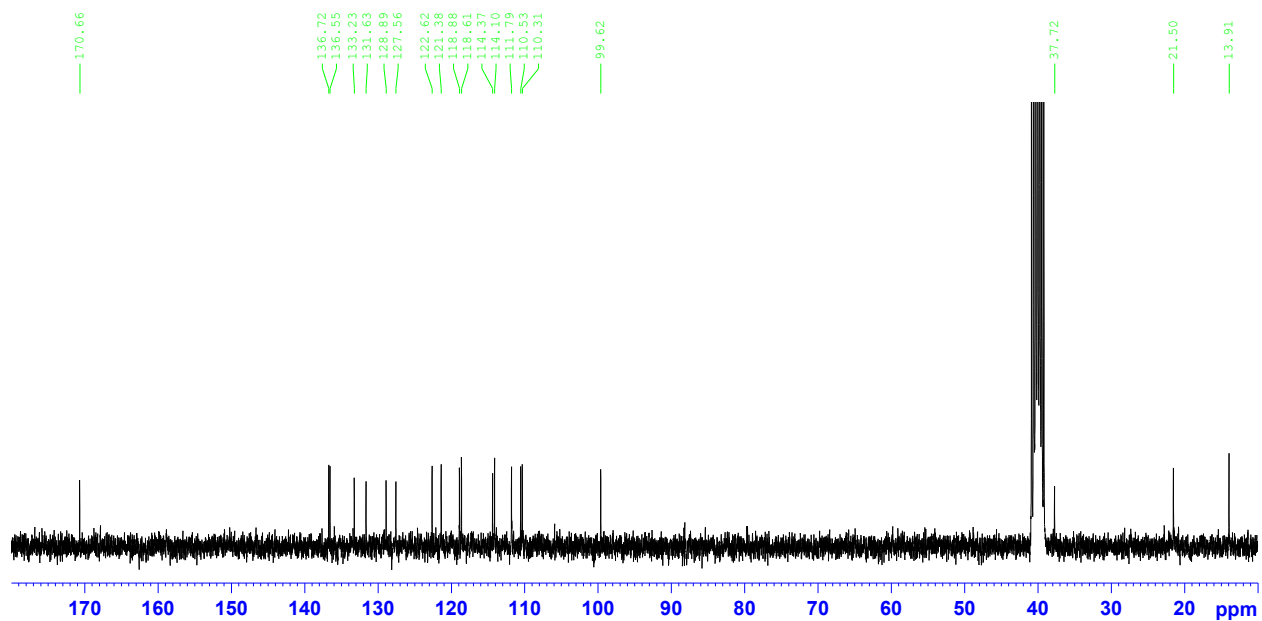
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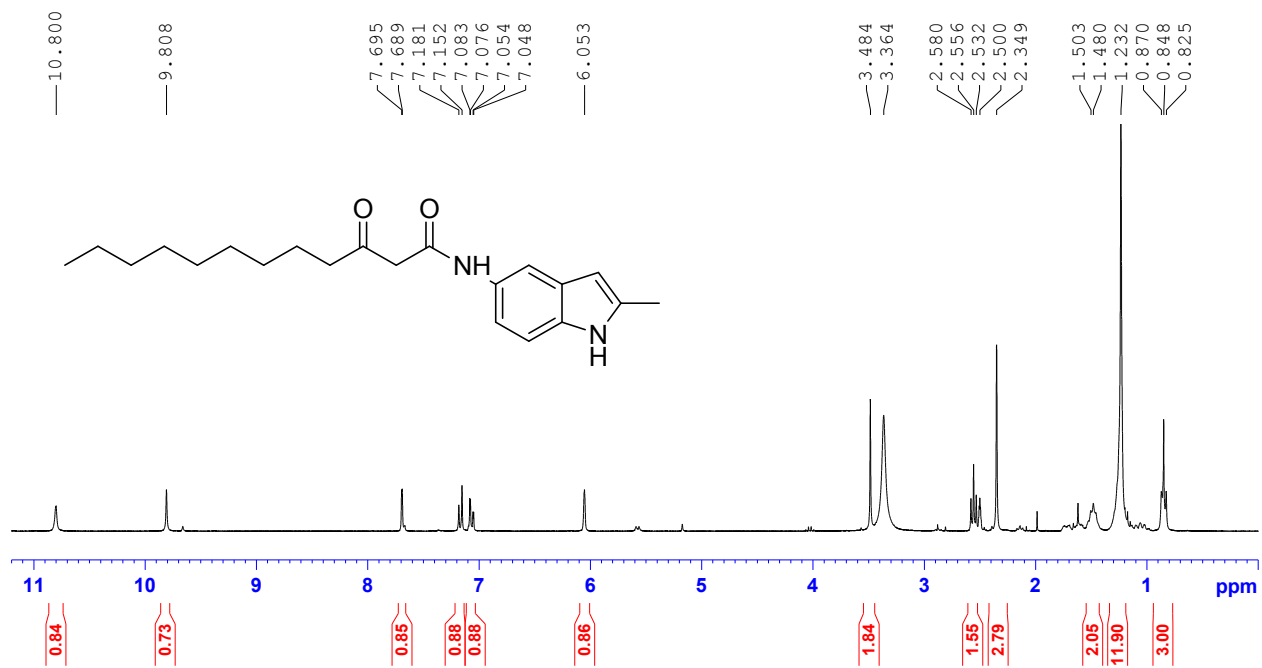
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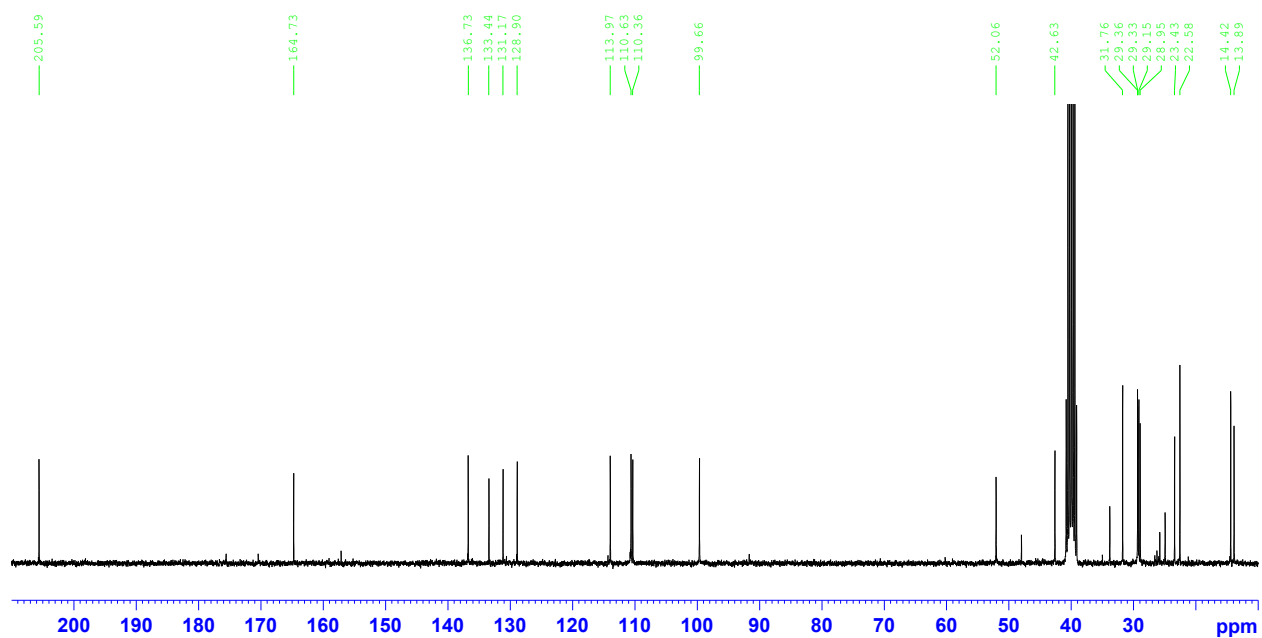
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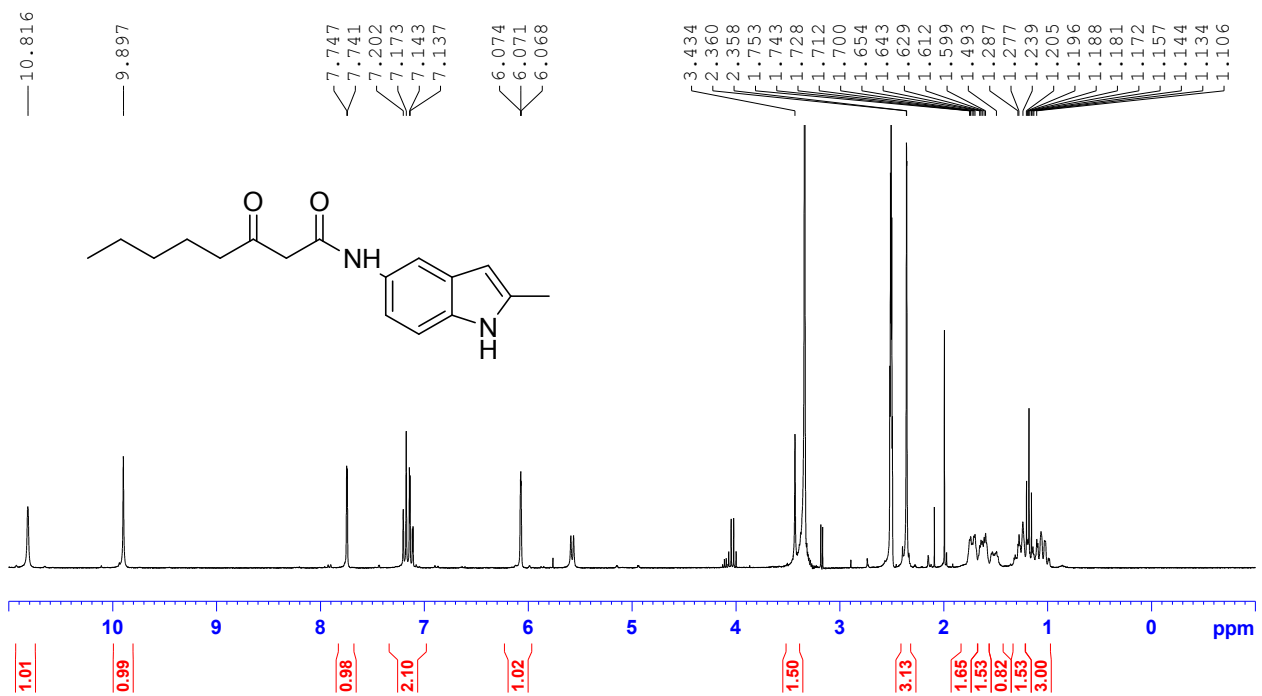
¹H NMR spectrum of Compound # 17a



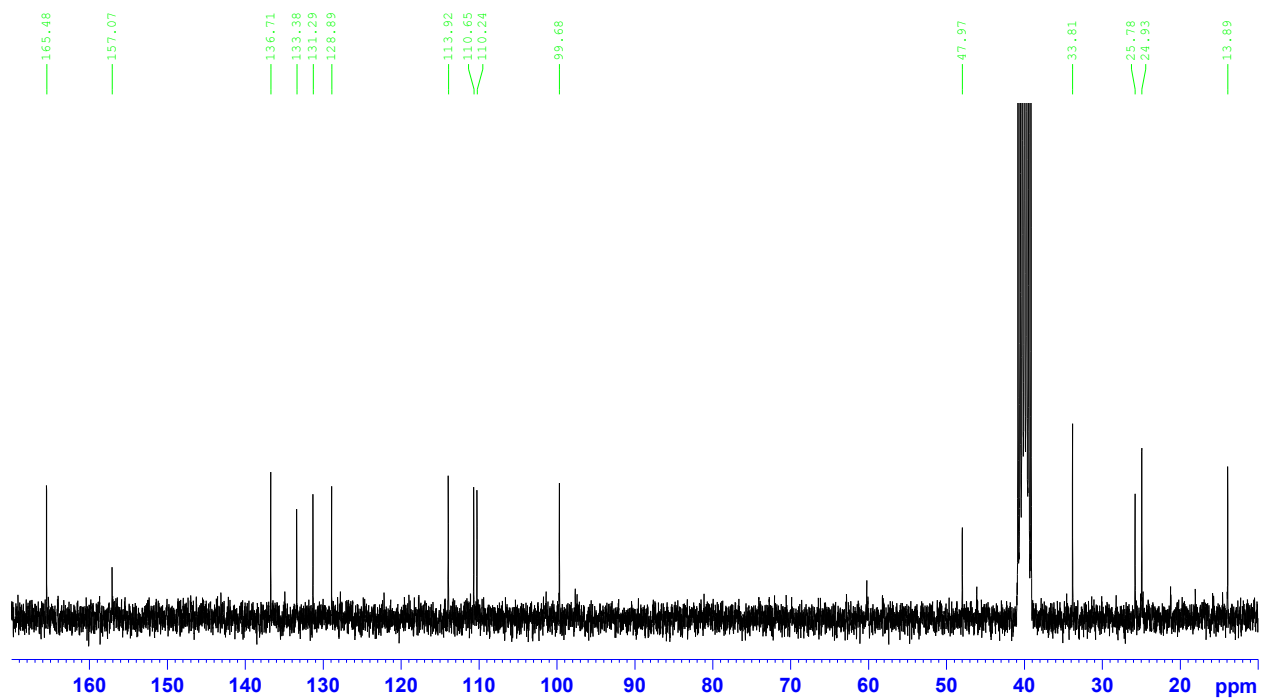
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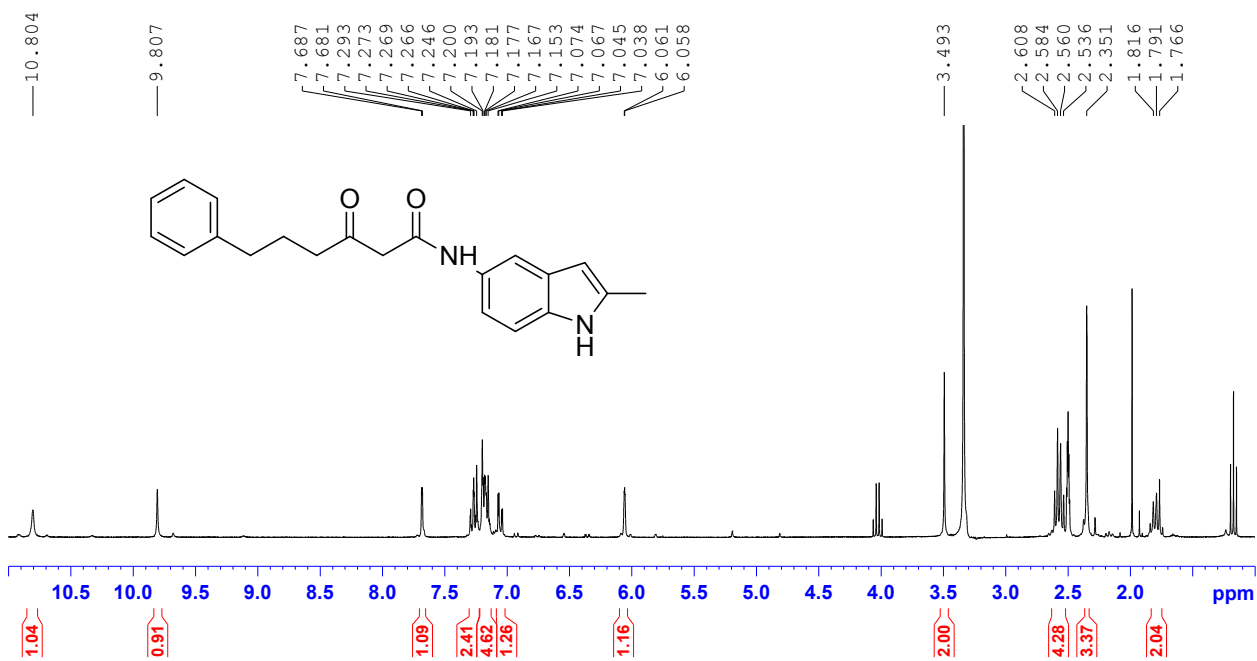
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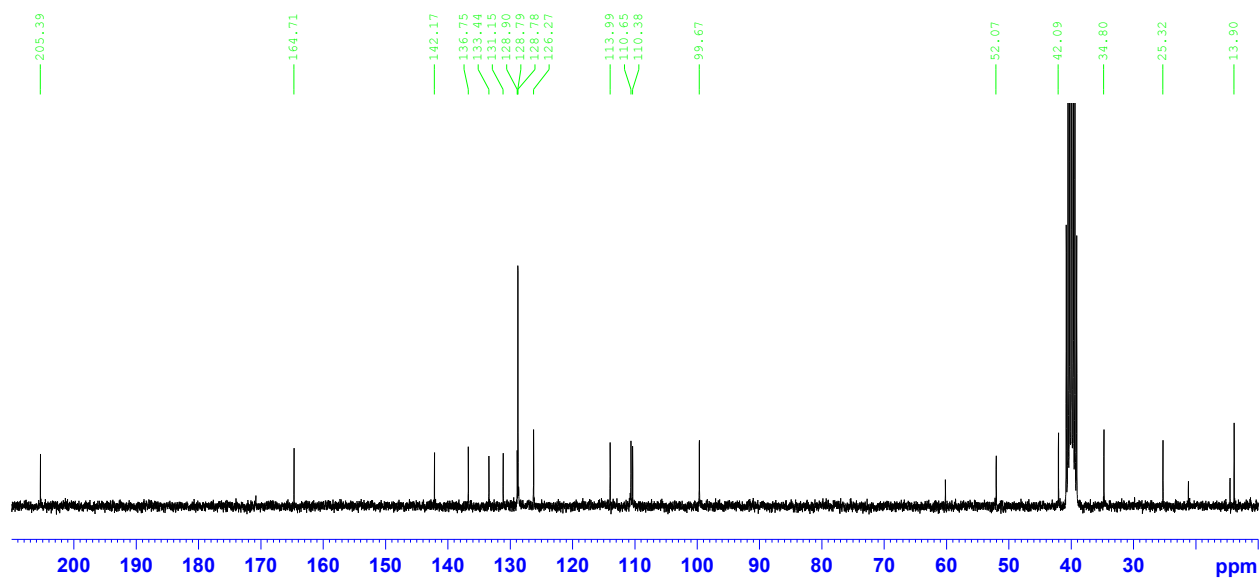
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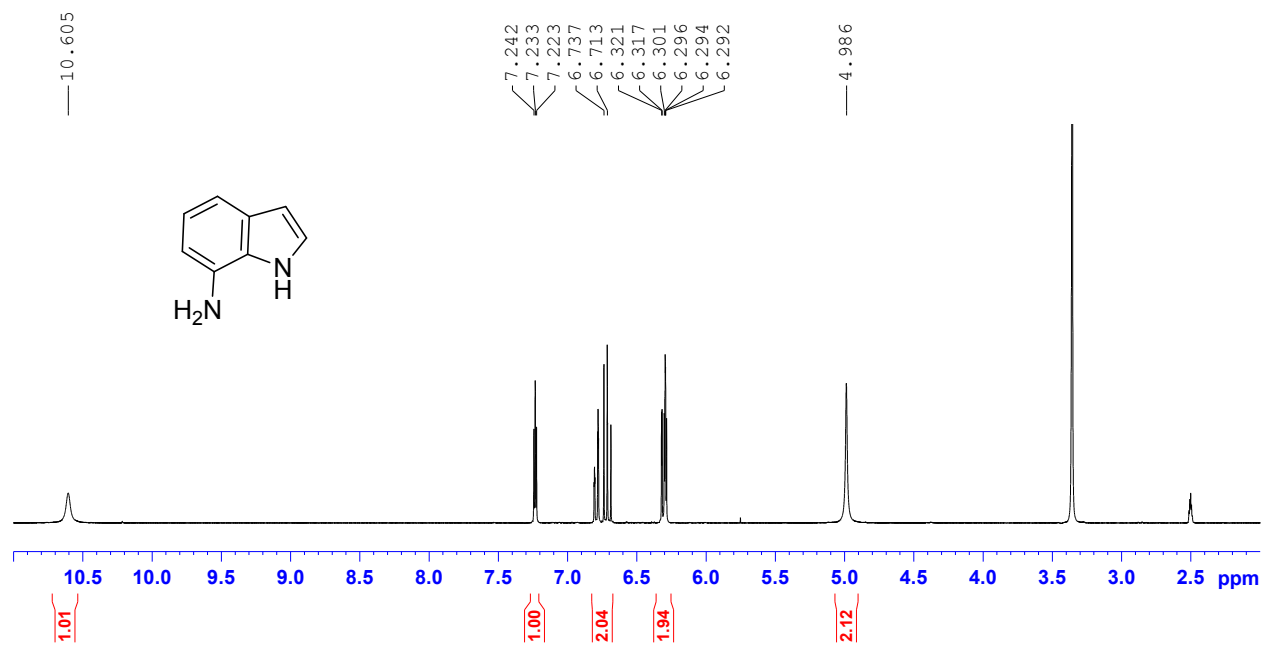
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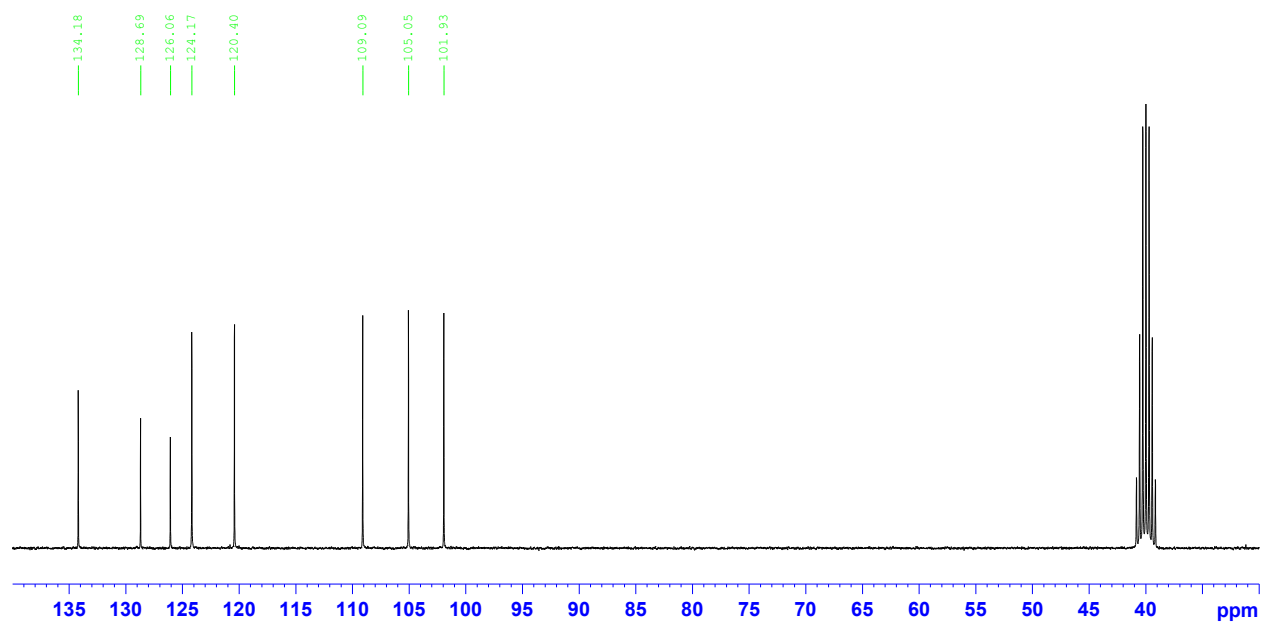
¹³C NMR spectrum of Compound # 17c



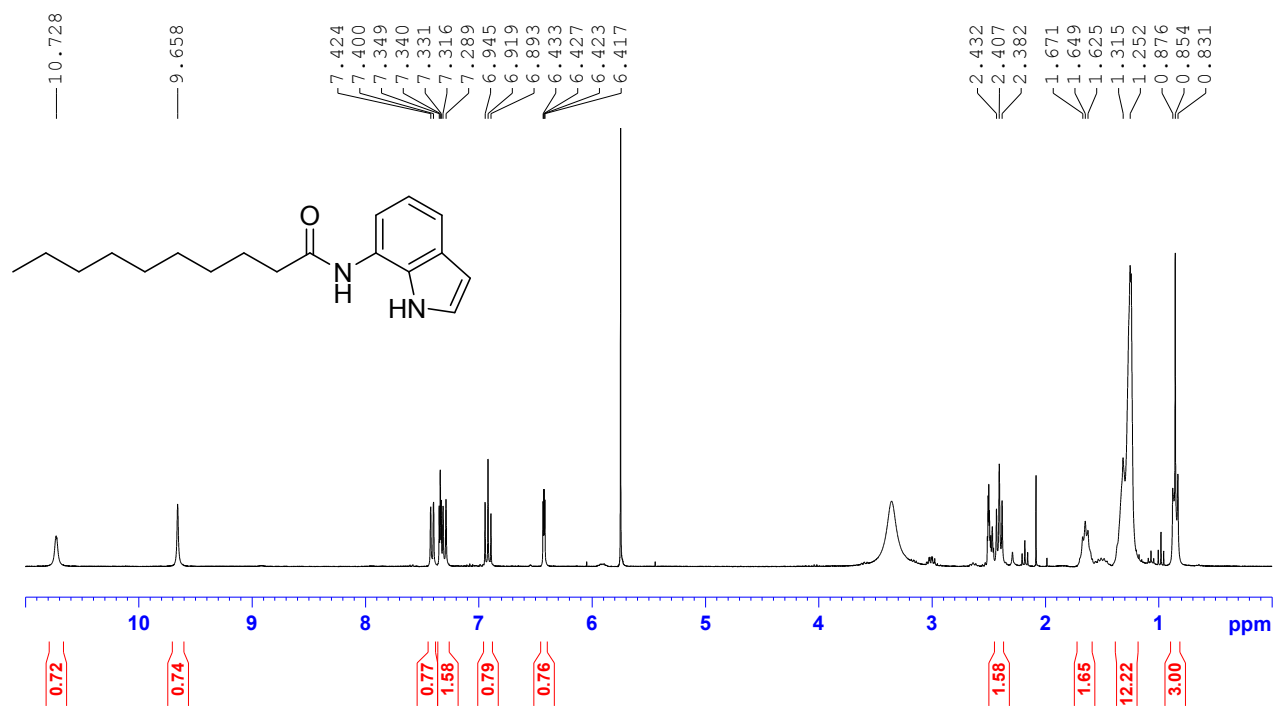
¹H NMR spectrum of Compound # 19



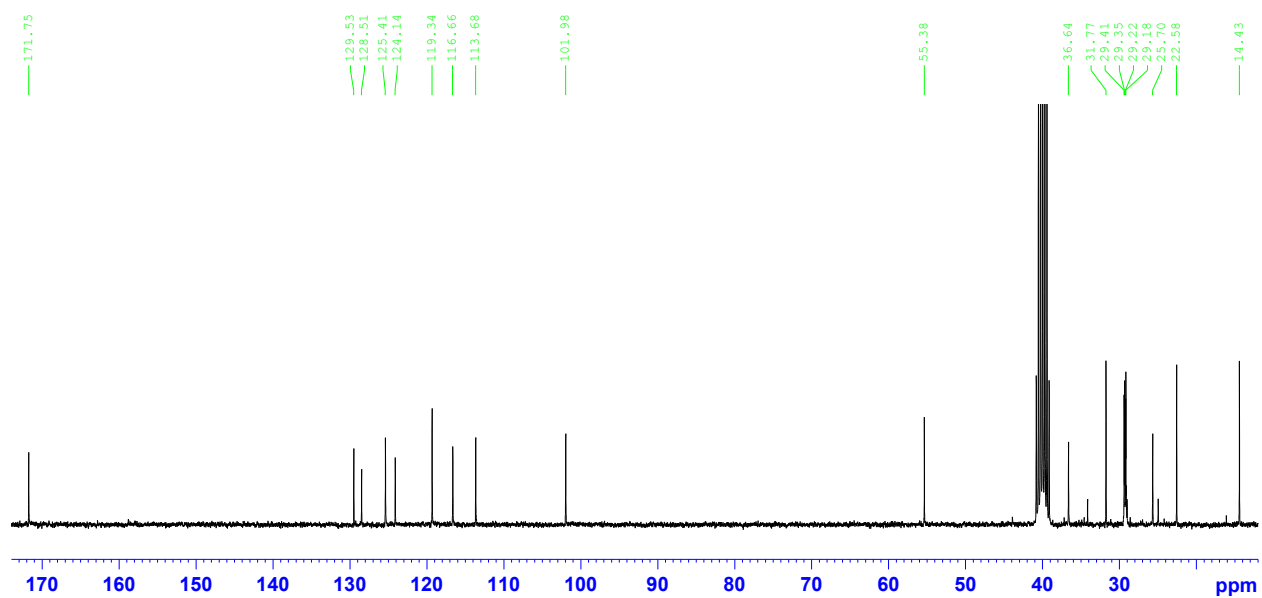
¹³C NMR spectrum of Compound # 19



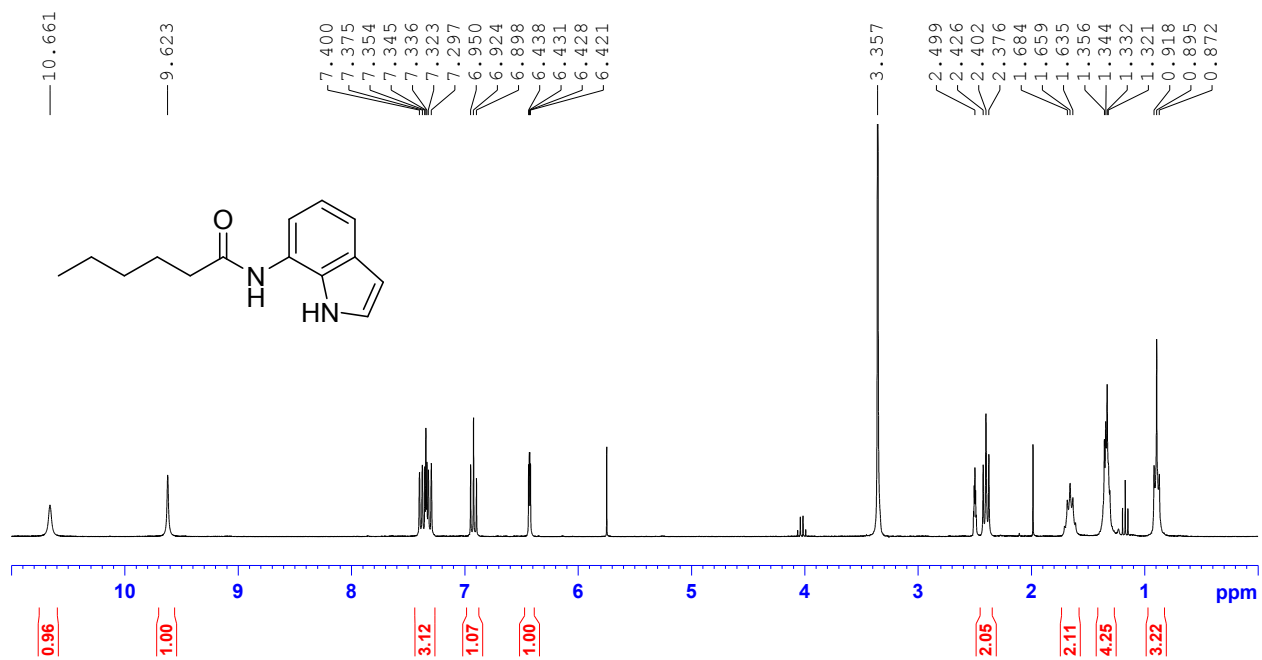
¹H NMR spectrum of Compound # 20a



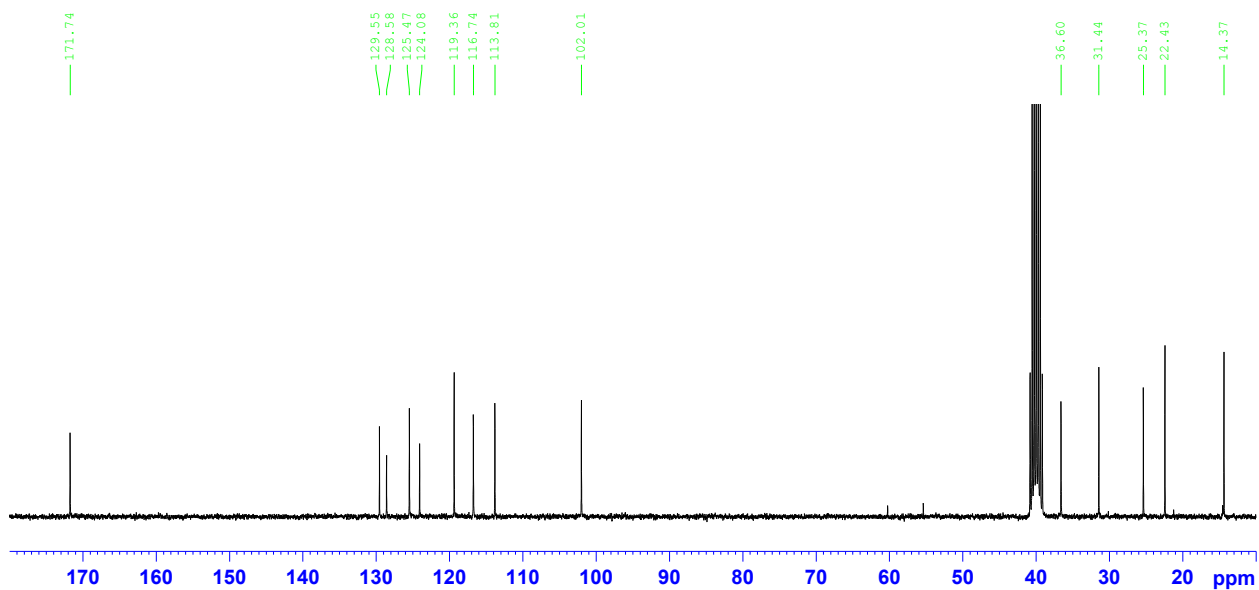
¹³C NMR spectrum of Compound # 20a



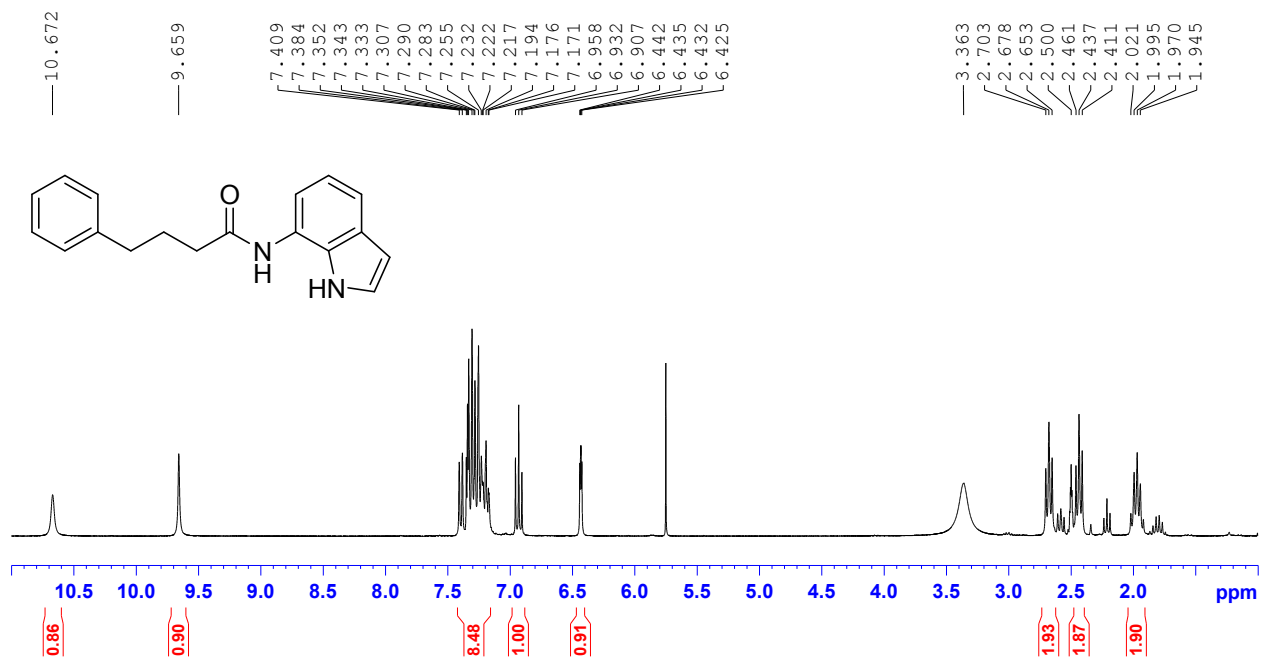
¹H NMR spectrum of Compound # 20b



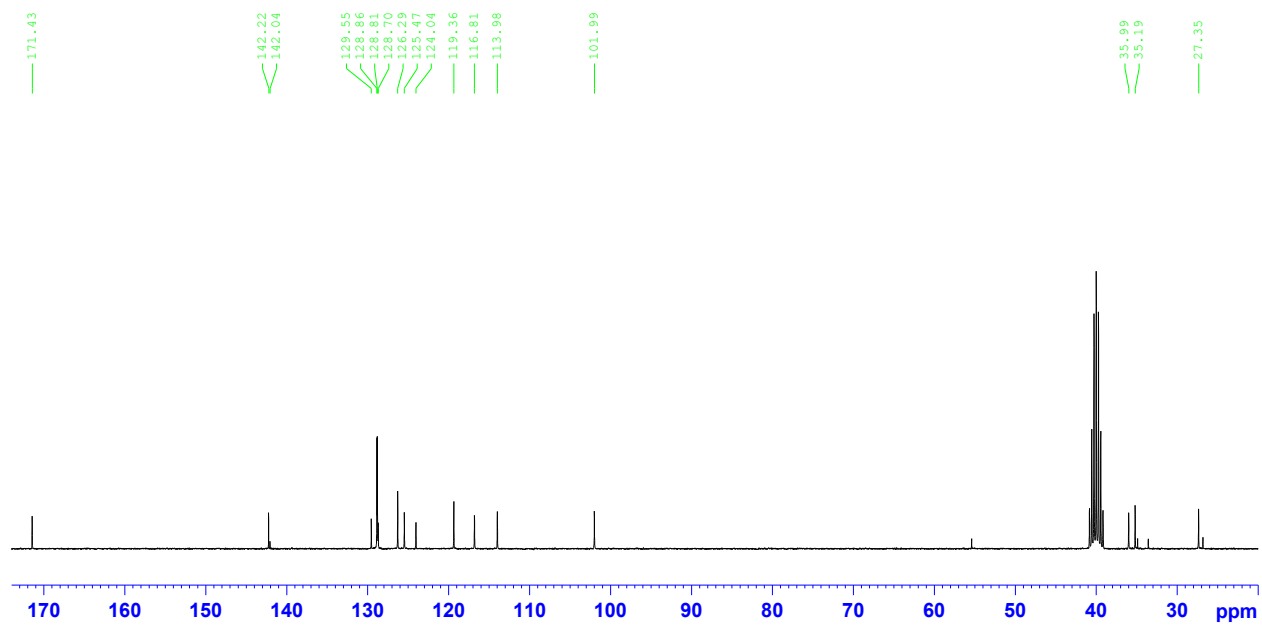
¹³C NMR spectrum of Compound # 20b



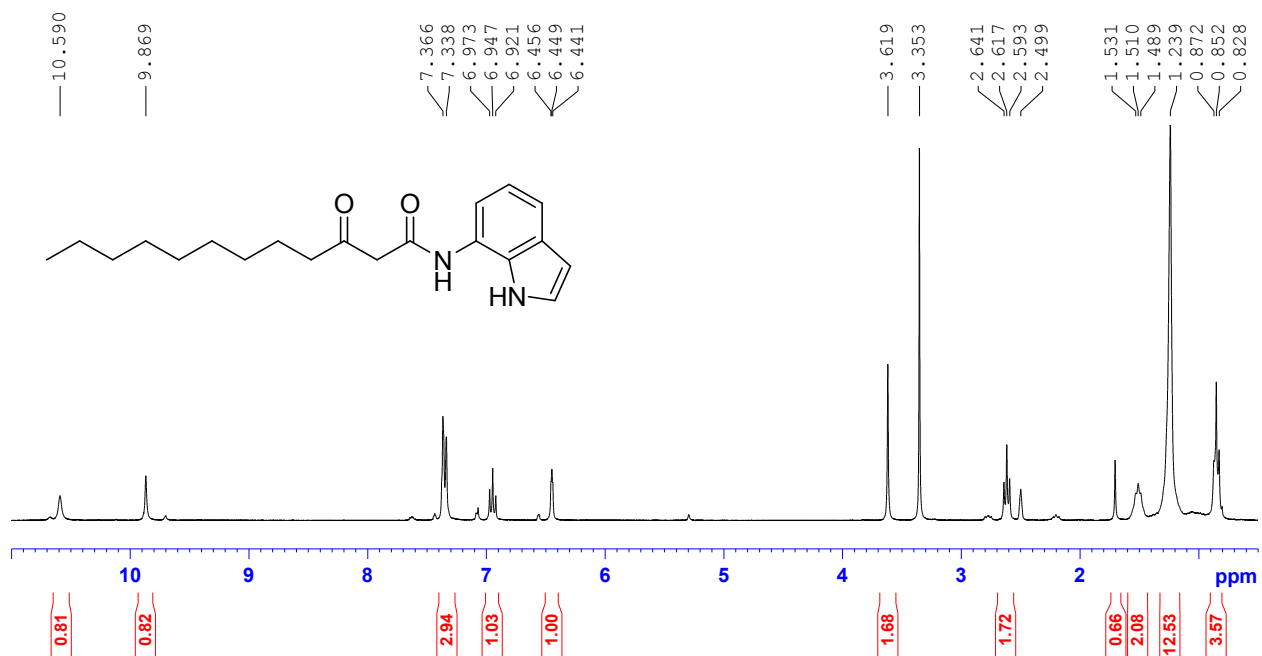
¹H NMR spectrum of Compound # 20c



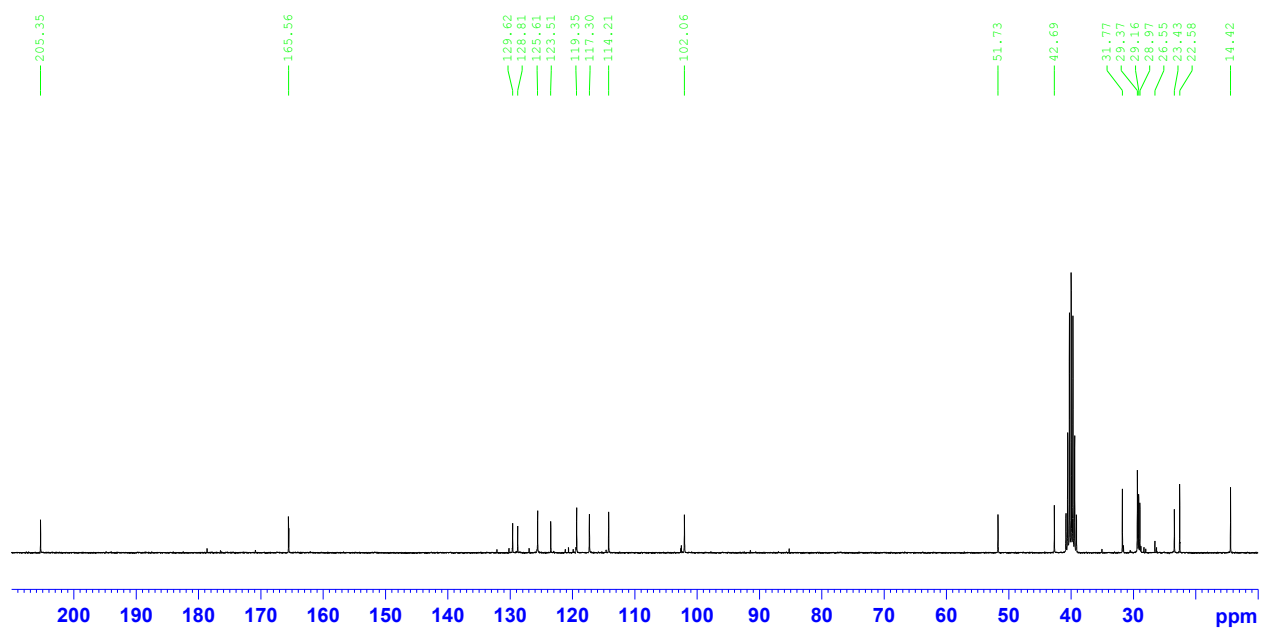
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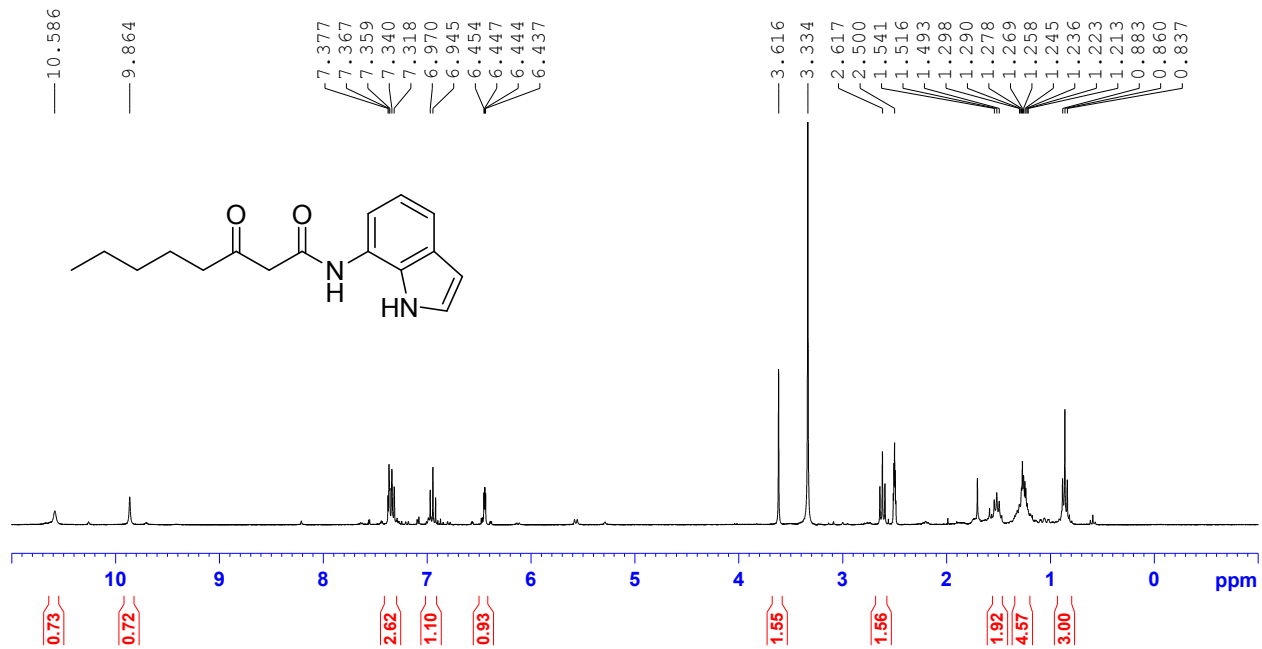
¹H NMR spectrum of Compound # 21a



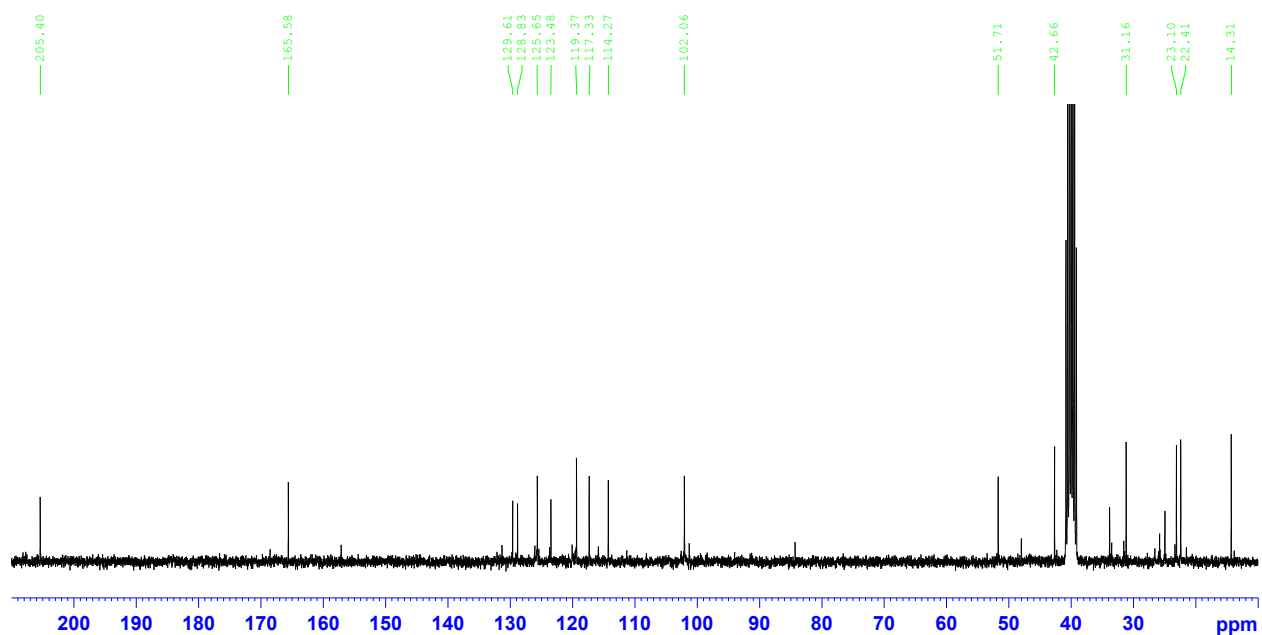
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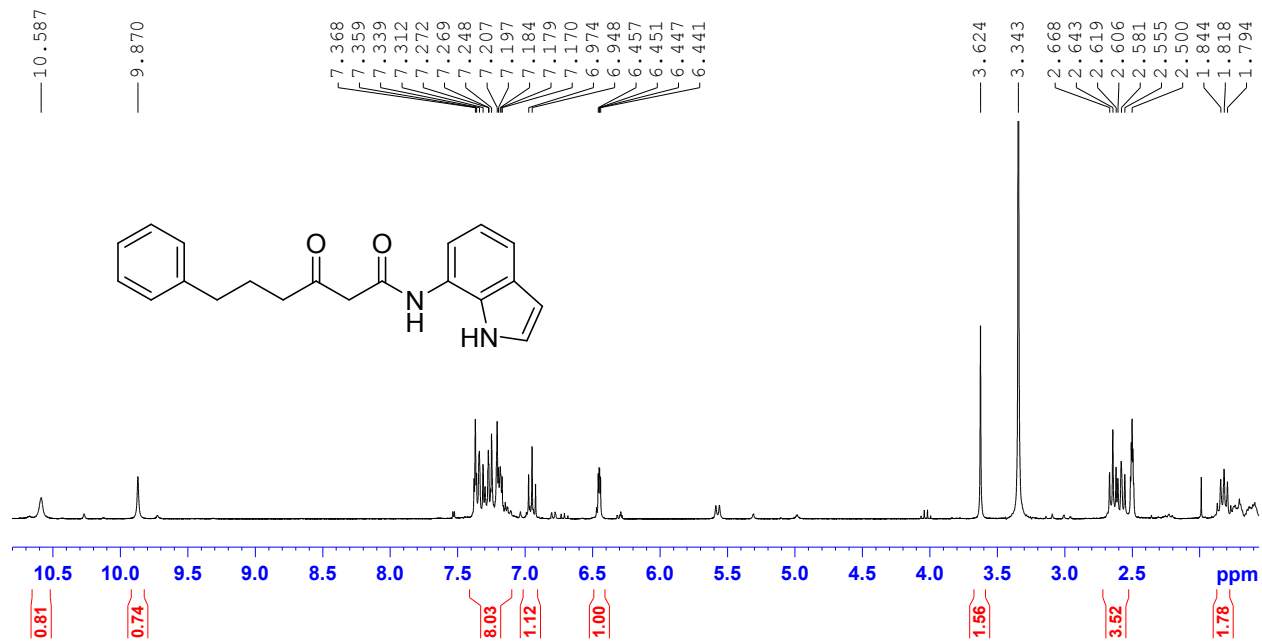
¹H NMR spectrum of Compound # 21b



¹³C NMR spectrum of Compound # 21b



¹H NMR spectrum of Compound # 21c



¹³C NMR spectrum of Compound # 21c

