

Supporting Information

Comparative Evaluation of the Antibacterial and Antitumor

Activities of 9-Phenylfascaplysin and Its Analogs

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Table S1. Antimicrobial and antiproliferative activities (MIC* and IC₅₀ correspondingly) of fascaplysin (1) and its derivatives *in vitro*.**

Compound	MIC, µg/mL												IC ₅₀ , µM		
	<i>S. aureus</i> ATCC 29213	<i>B. cereus</i> ATCC 10702	<i>E. faecalis</i> ATCC 29212	<i>E. faecium</i> 132	<i>E. faecium</i> 130 (VRE)	<i>E. faecalis</i> 583 (VRE)	<i>S. aureus</i> 88 (MRSA)	<i>S. aureus</i> PE3R (MRSA)	<i>S. epidermidis</i> 2001 MR	<i>S. aureus</i> 21555	<i>M. smegmatis</i> ATCC 607	<i>E. coli</i> ATCC 25922	K-562	K-562/4	A-549
Van	0.5	1.0	2.0	0.5	>32	32.0	0.5	1.0	1.0	2.0	-	-	-	-	-
Rif	0.018	0.25	-	-	-	-	-	-	-	-	0.03	8.0	-	-	-
DOX	-	-	-	-	-	-	-	-	-	-	-	-	0.40±0.05	6.4±0.8	0.40±0.06
1	1.0	0.125	8.0	1.0	1.0	≥8.0	1.0	0.5	0.0075	0.03	0.03	8.0	0.19±0.03	0.30±0.05	0.20±0.03
7	0.03	0.03	0.25	4.0	2.0	0.25	0.015	0.03	0.00375	0.03	0.25	8.0	0.10±0.02	0.22±0.03	0.20±0.02
15	0.125	2.0	16.0	8.0	8.0	16.0	0.5	0.5	0.0075	0.25	2.0	>16.0	1.2±0.2	4.0±0.5	0.60±0.08
16	0.125	0.125	0.25	8.0	16.0	0.13	0.125	0.06	0.03	0.03	1.0	>16.0	0.60±0.08	3.2±0.4	2.1±0.3
25a	0.06	0.03	0.25	8.0	8.0	0.125	0.03	0.03	0.03	0.03	0.5	>16.0	1.6±0.2	1.3±0.2	0.50±0.06
25b	0.06	0.06	0.125	0.5	0.5	0.125	0.03	0.06	0.015	0.03	0.5	>16.0	1.1±0.2	1.5±0.2	0.60±0.07

25c	0.25	0.25	2.0	16	16	2.0	0.25	0.25	0.25	0.25	4.0	>16.0	0.60±0.06	0.8±0.1	0.30±0.04
25d	0.06	0.5	0.5	16	8.0	1.0	0.125	0.06	0.015	0.06	8.0	>16.0	2.2±0.3	2.3±0.3	1.4±0.2
25e	0.06	0.25	0.125	0.5	0.5	0.25	0.06	0.06	0.015	0.06	0.5	8.0	0.50±0.07	0.8±0.1	0.30±0.04
25f	0.25	1.0	0.25	0.25	0.25	0.25	0.5	0.25	0.03	0.06	16.0	>16.0	4.5±0.6	3.9±0.5	0.25±0.03
25g	0.5	0.125	>16.0	16.0	16.0	>16.0	1.0	0.5	0.06	0.25	8.0	>16.0	1.2±0.2	1.3±0.2	3.8±0.5
25h	4.0	0.25	>16.0	>16.0	>16.0	>16.0	8.0	2.0	0.25	0.5	4.0	>16.0	4.5±0.6	5.4±0.7	9.0±1.3

* Modal values of minimum inhibitory concentration (MIC).

** Mean 50% growth inhibitory concentration ($IC_{50} \pm S.D.$) of 3 independent experiments, MTT-test.

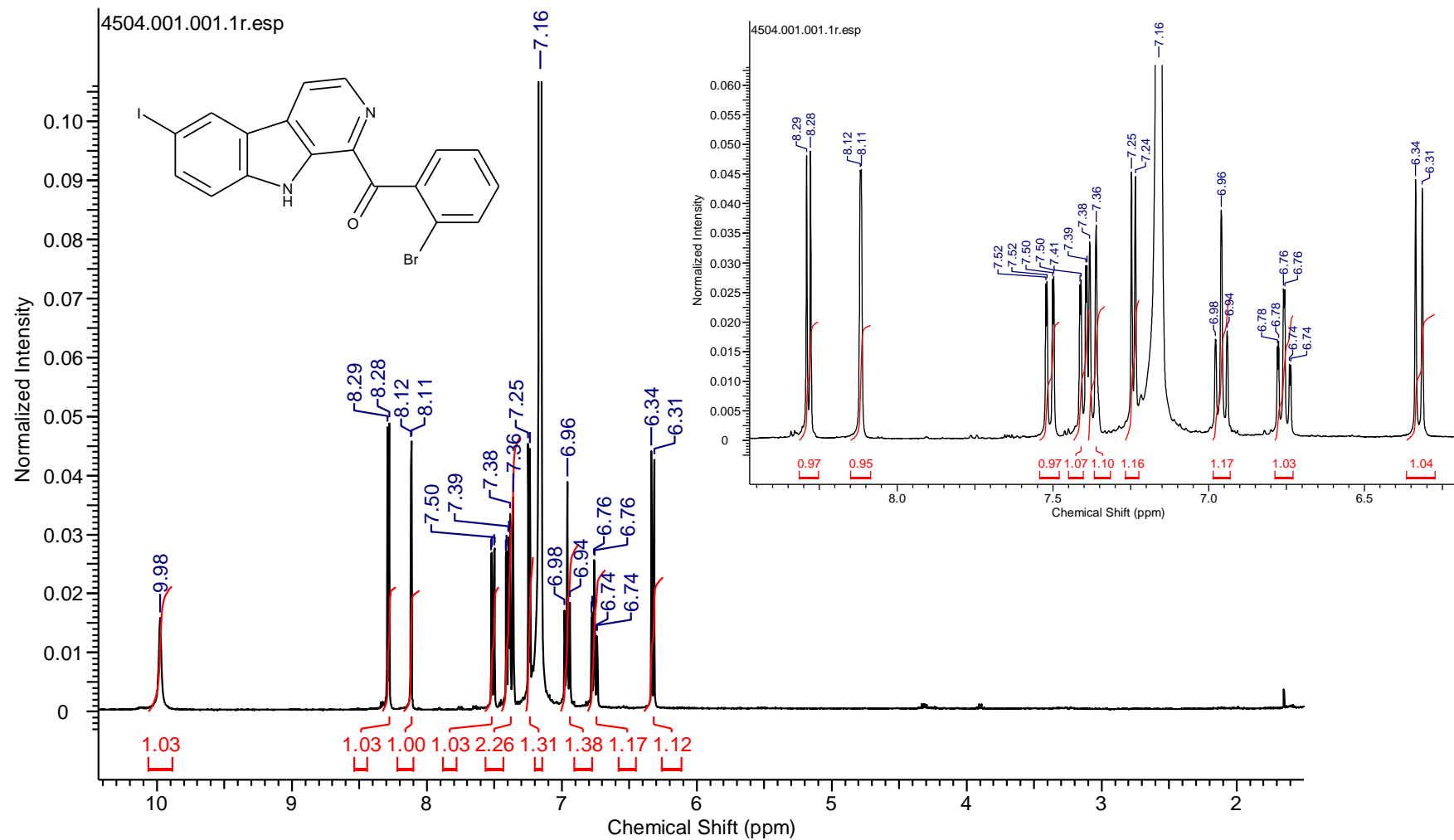
Table S2. Efficacy (ED₅₀ value, mg/kg) of 9-phenylfascaplysin (7), fascaplysin (1) and vancomycin (Van) on a mouse model of staphylococcal sepsis.

Compound	Dose, mg/kg	Survival*, %	ED ₅₀ , mg/kg
Fascaplysin (1)	0.10	20	0.55
	0.25	40	
	0.50	50	
	1.0	70	
	2.0	70	
	4.0	80	
9-Phenylfascaplysin (7)	0.10	30	0.48
	0.25	40	
	0.50	50	
	1.0	70	
	2.0	80	
	4.0	90	
Van	2.5	30	4.2
	3.5	40	
	4.5	50	
	5.5	70	
	6.5	90	
	7.5	100	
Control dose <i>S. aureus</i>	-	0	

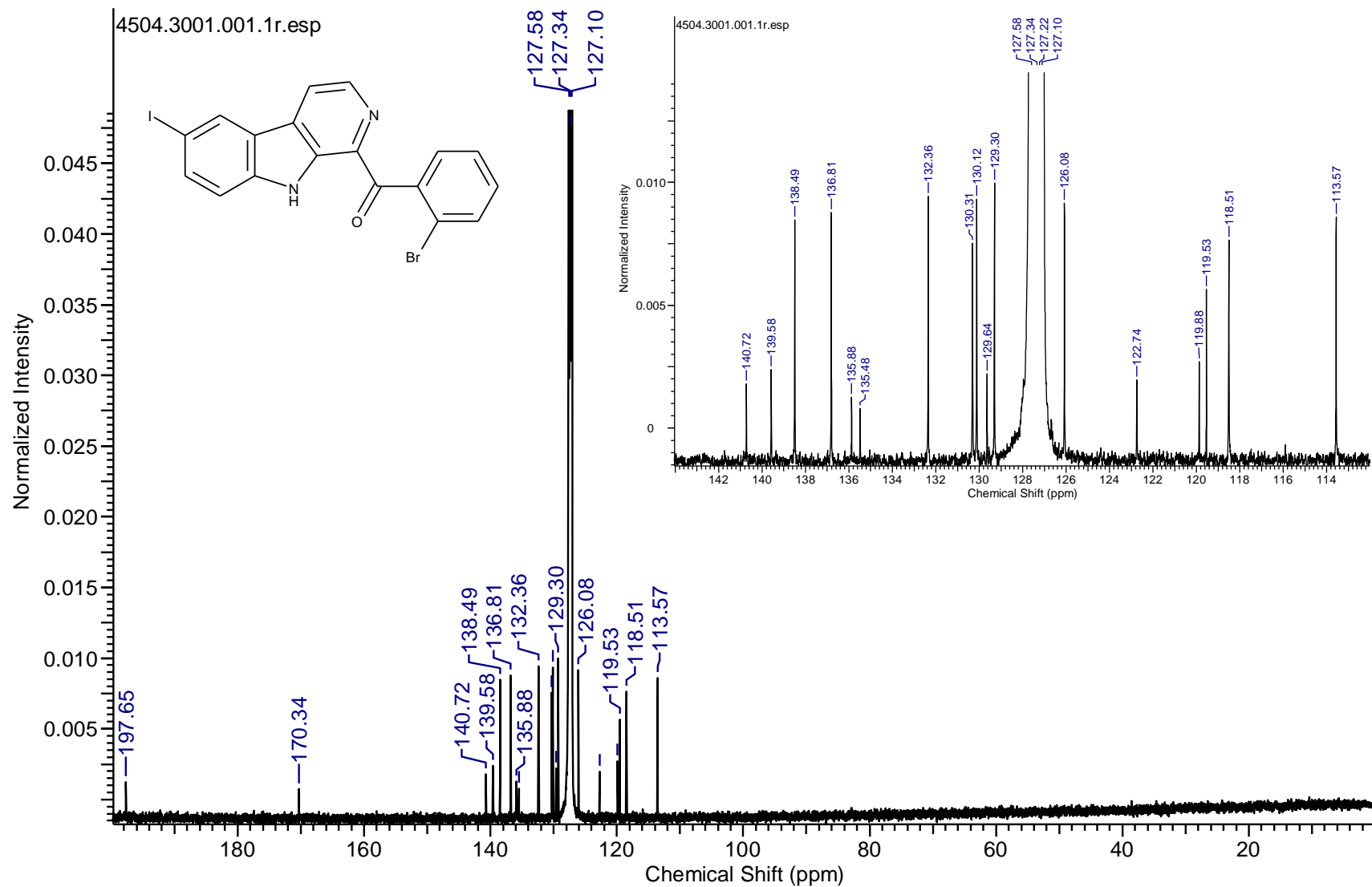
*n=10 for each group.

Spectra Data

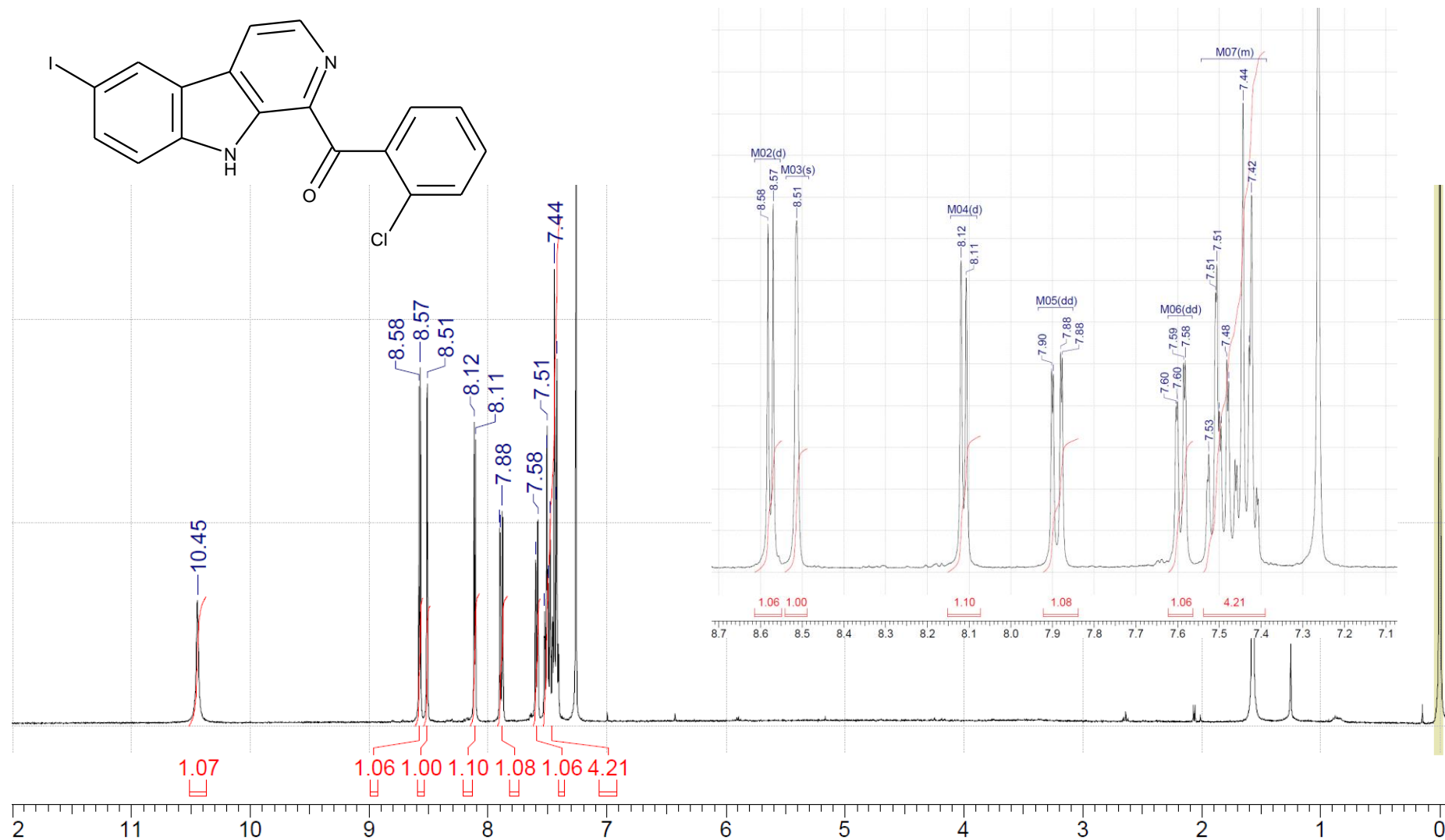
¹H NMR spectra of 1-(2'-bromobenzoyl)-6-iodo-β-carboline (9)



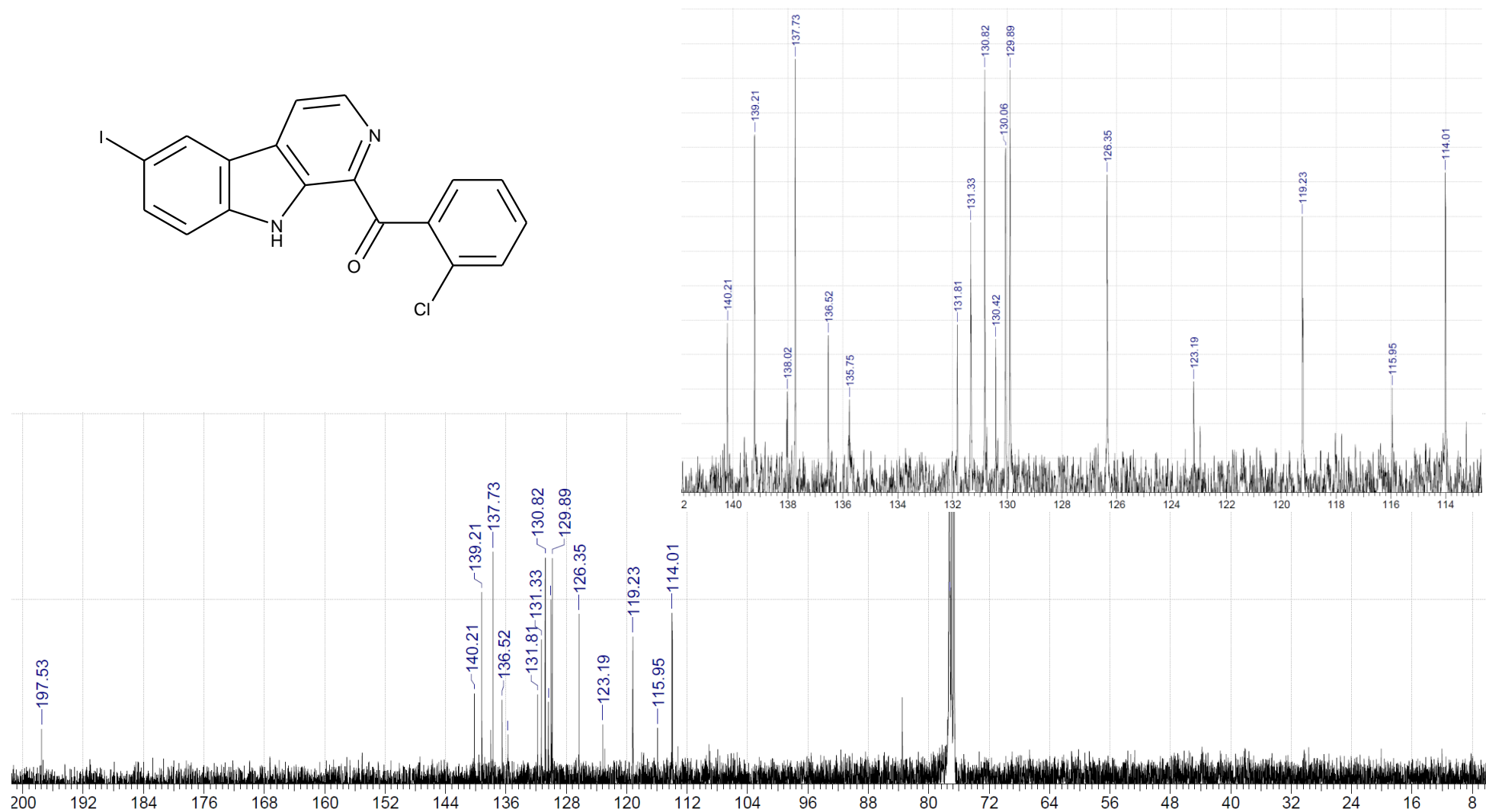
^{13}C NMR spectra of 1-(2'-bromobenzoyl)-6-iodo- β -carboline (9)



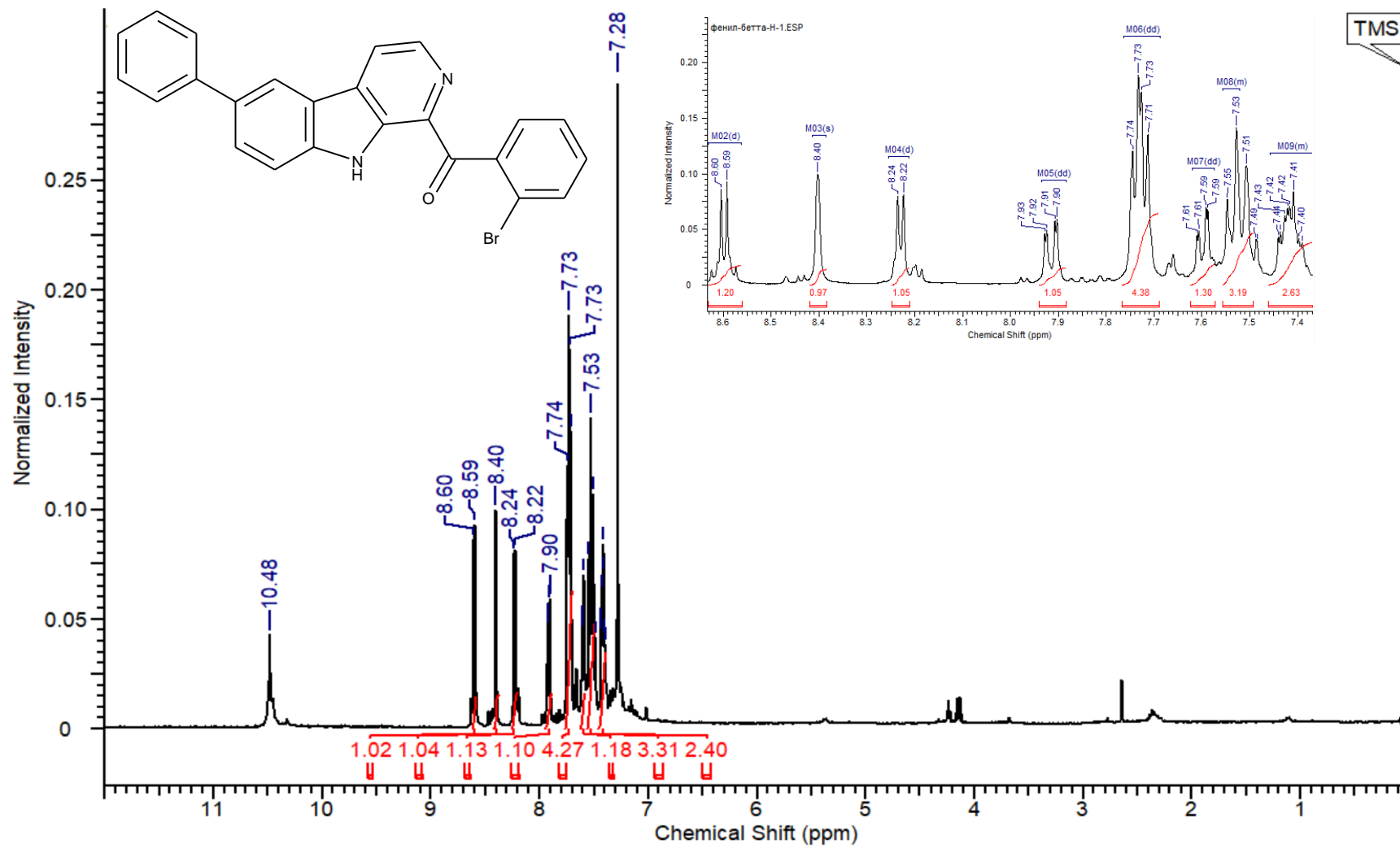
¹H NMR spectra of 1-(2'-chlorobenzoyl)-6-iodo-β-carboline (13)



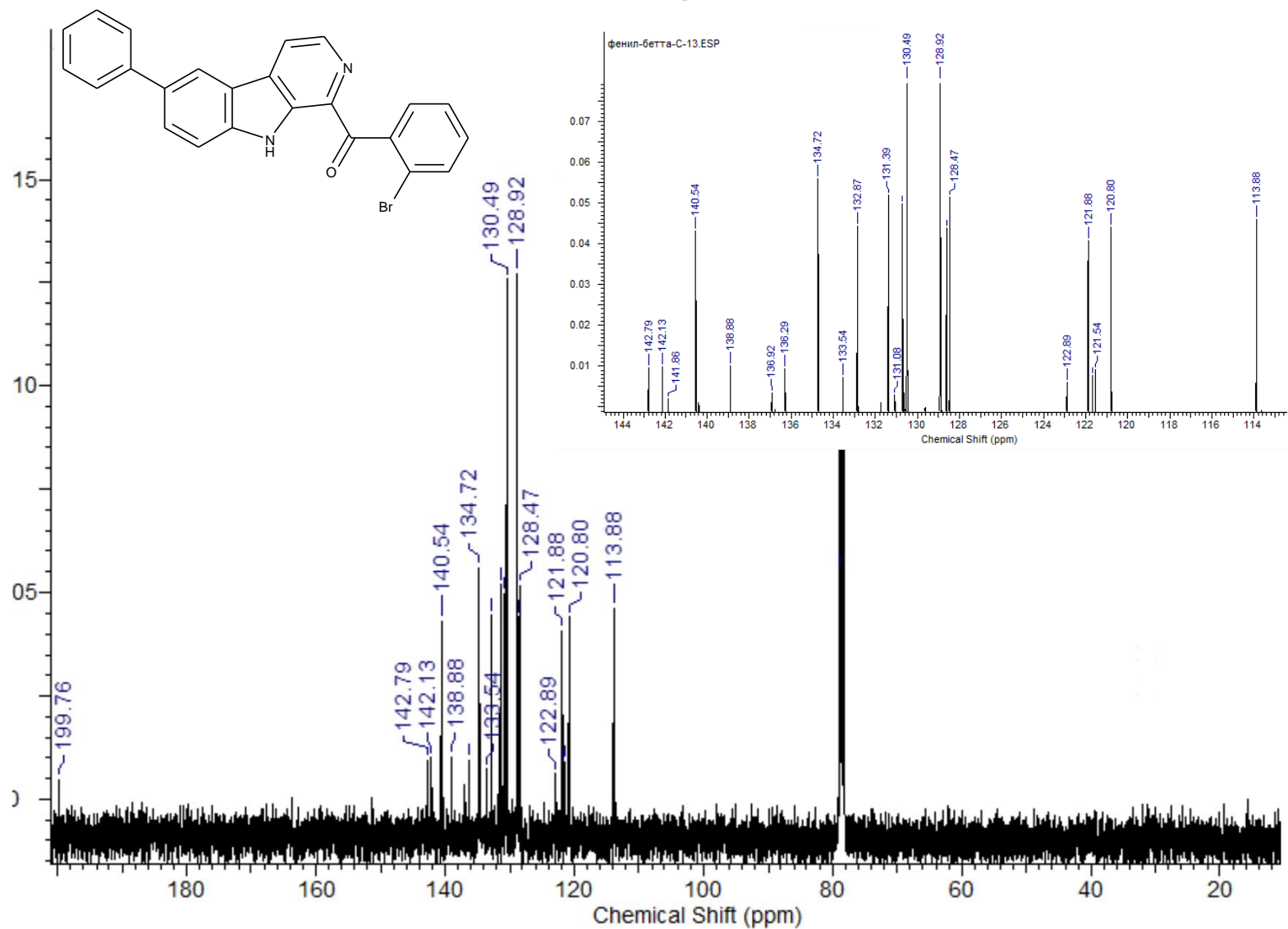
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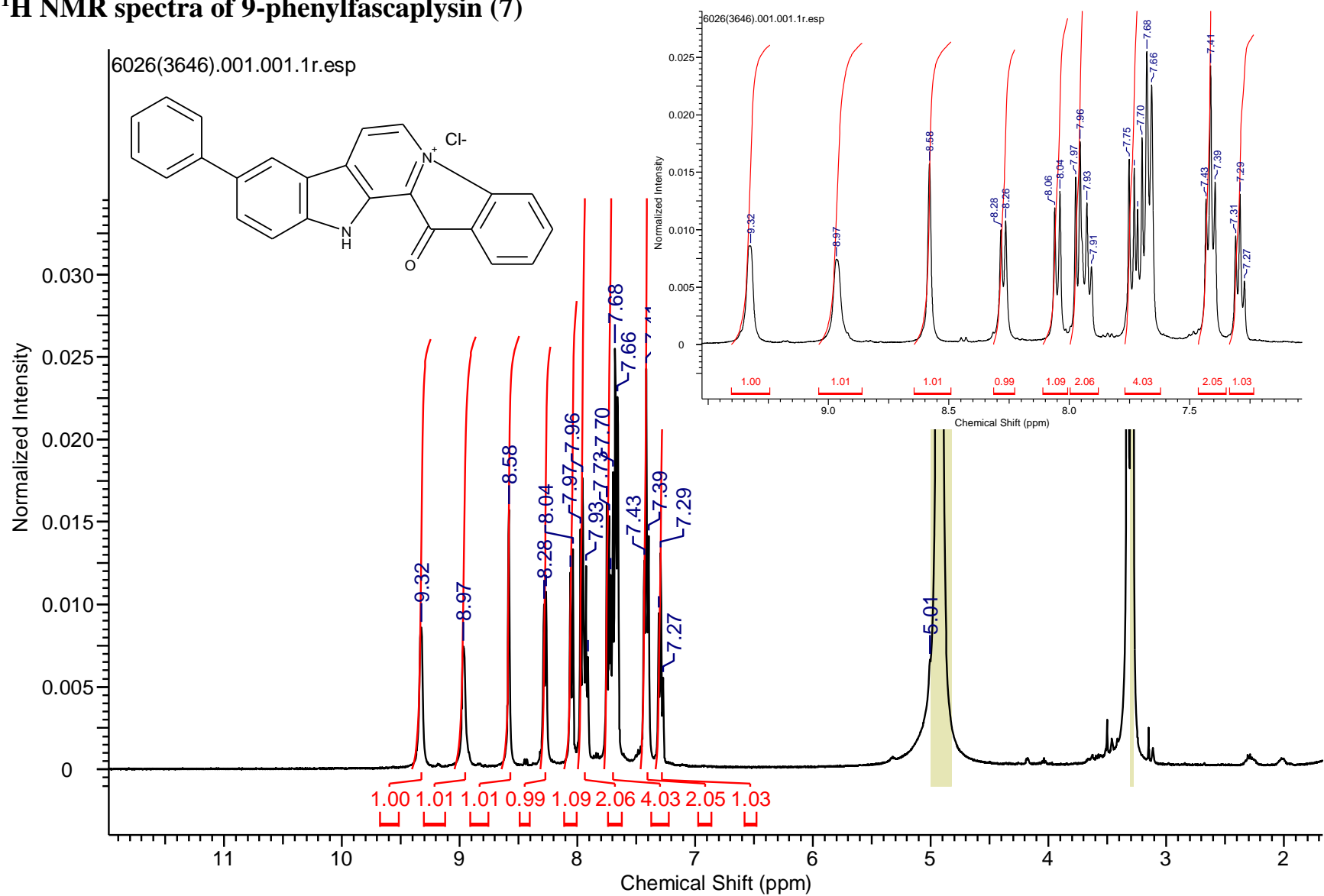
¹H NMR spectra of 1-(2'-bromobenzoyl)-6-phenyl-β-carboline (10)



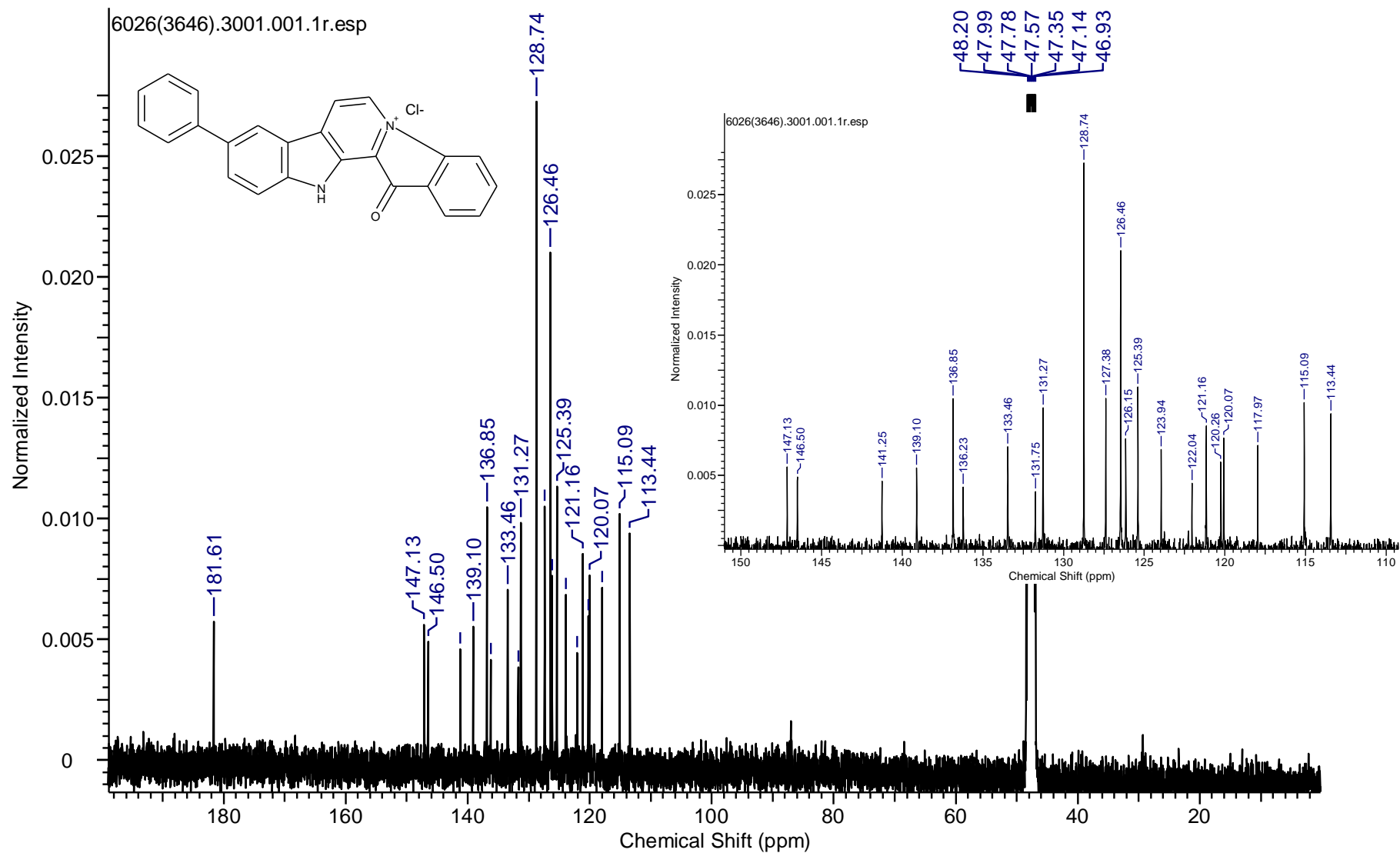
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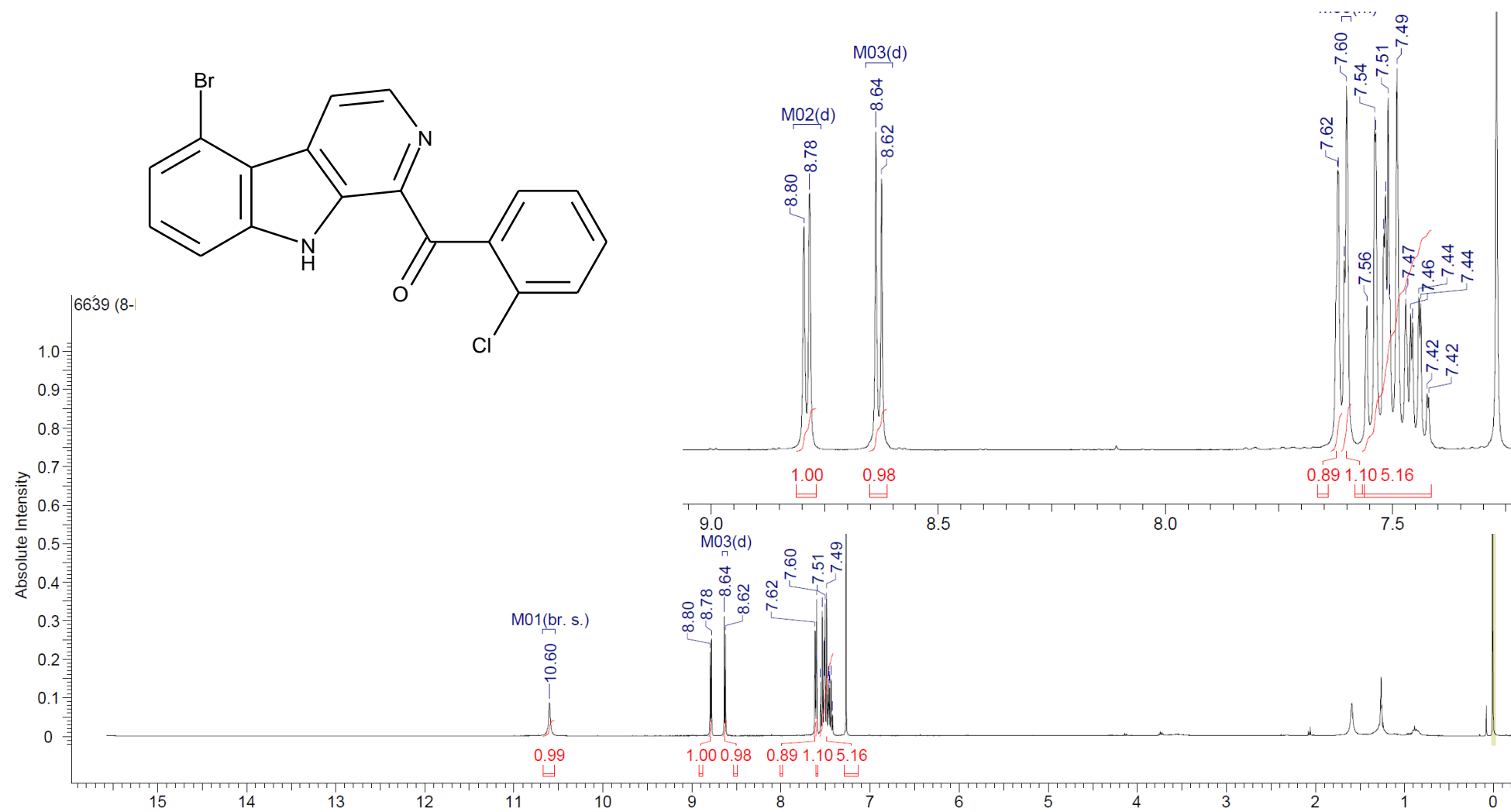
¹H NMR spectra of 9-phenylfascaplysin (7)



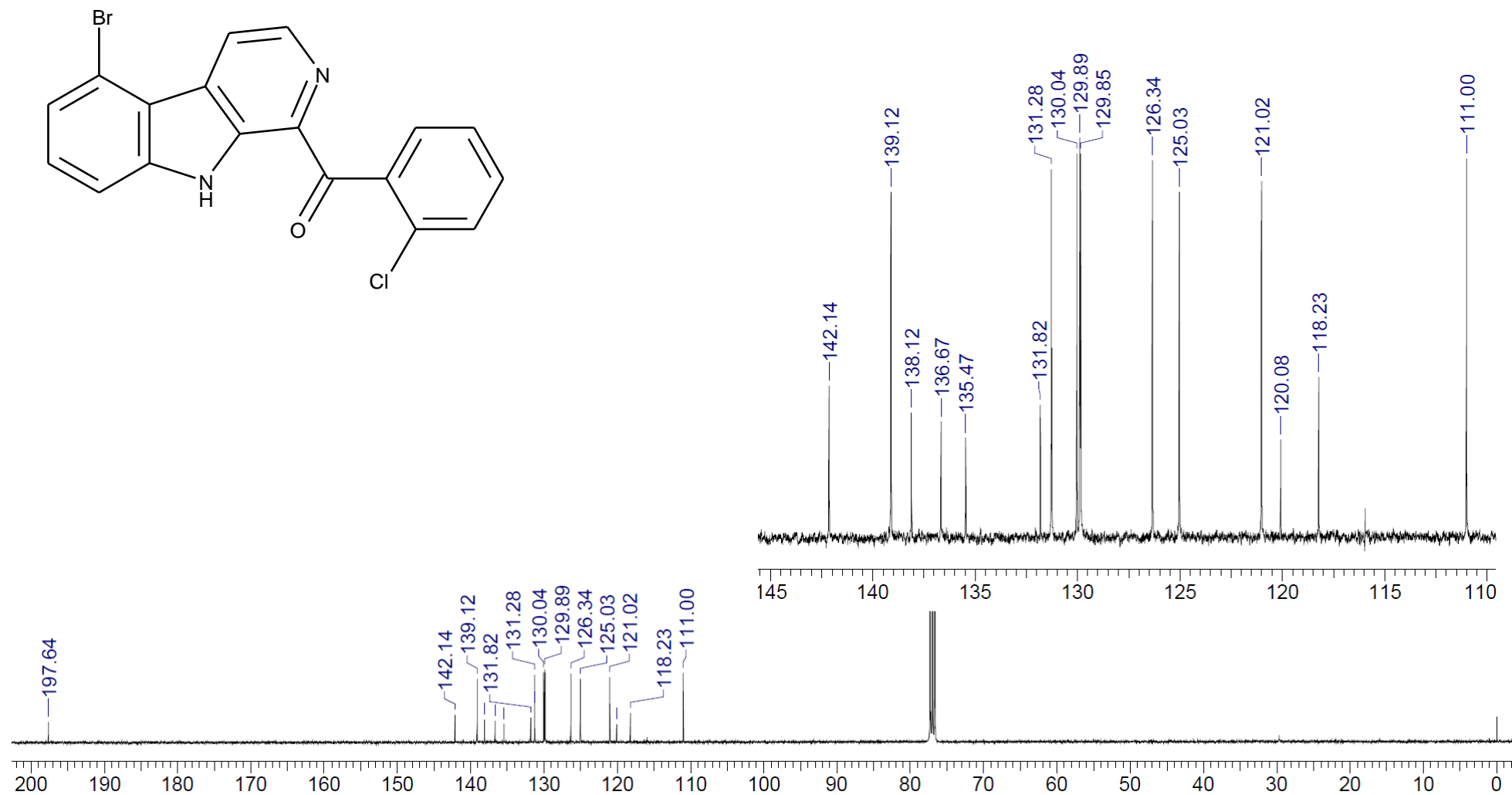
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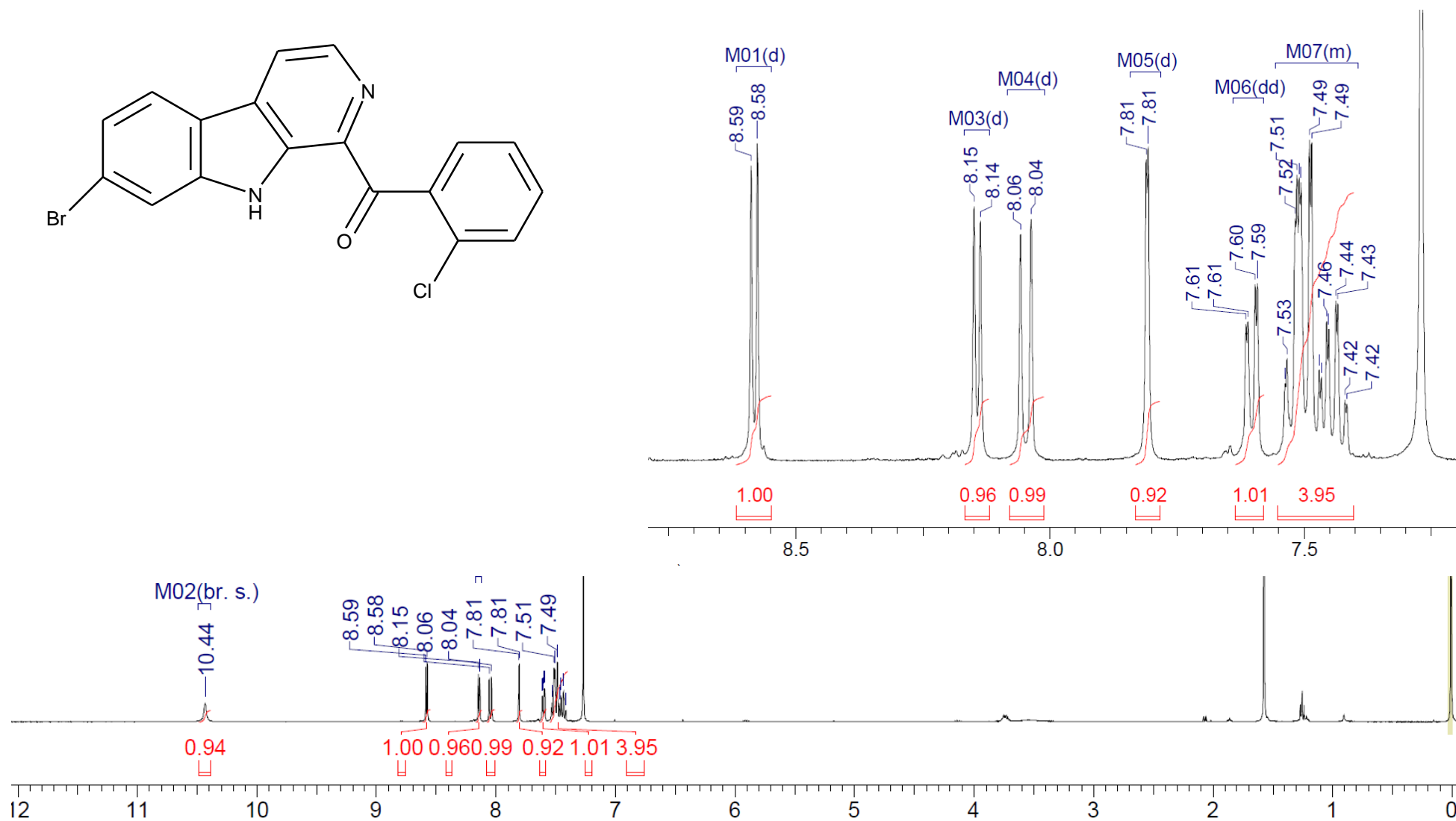
¹H NMR spectra of 5-bromo-1-(2-chlorobenzoyl)-β-carboline (20)



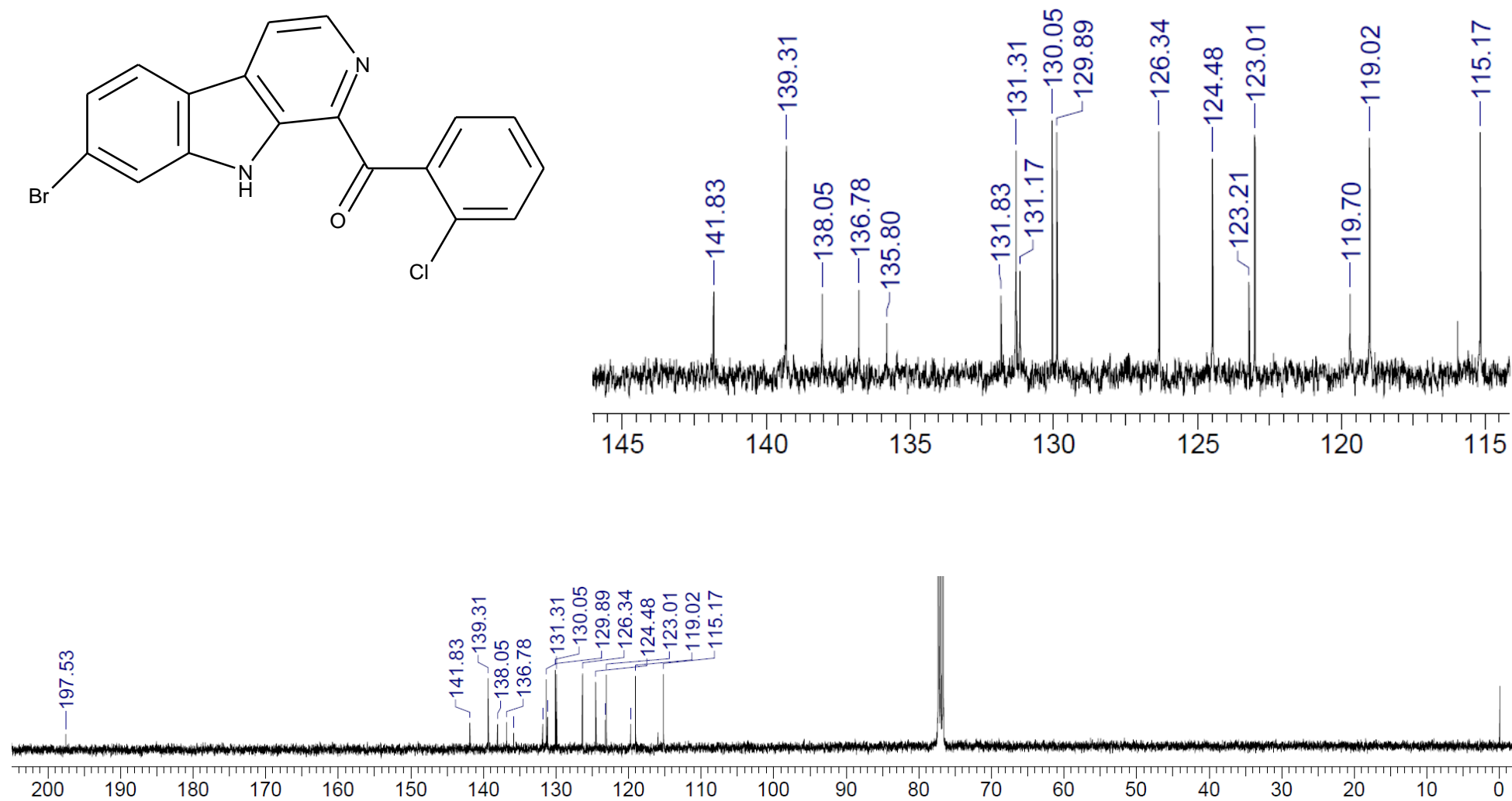
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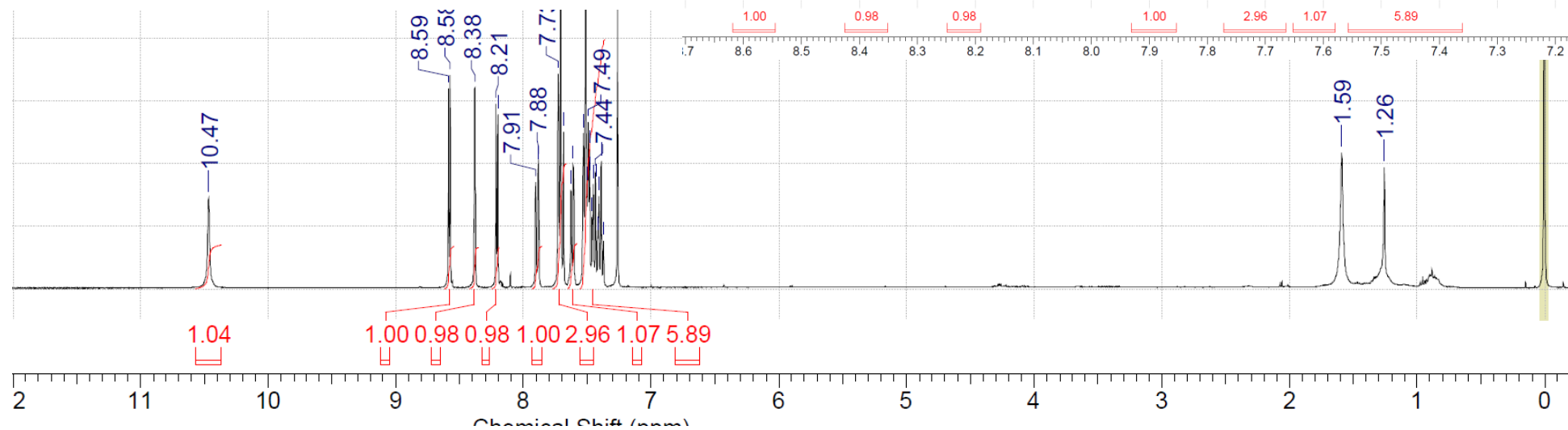
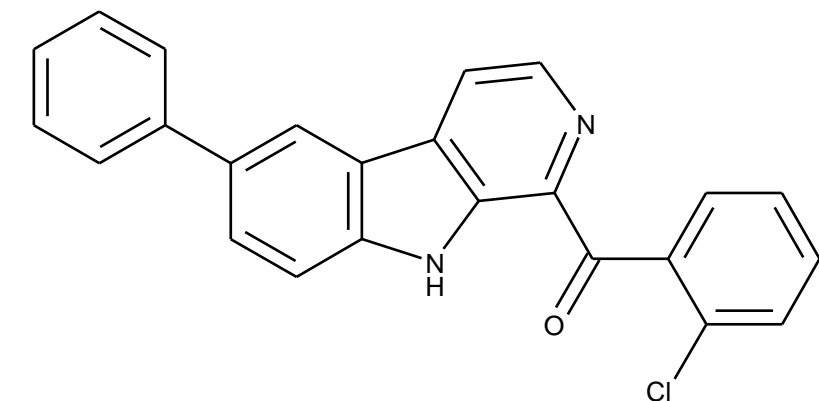
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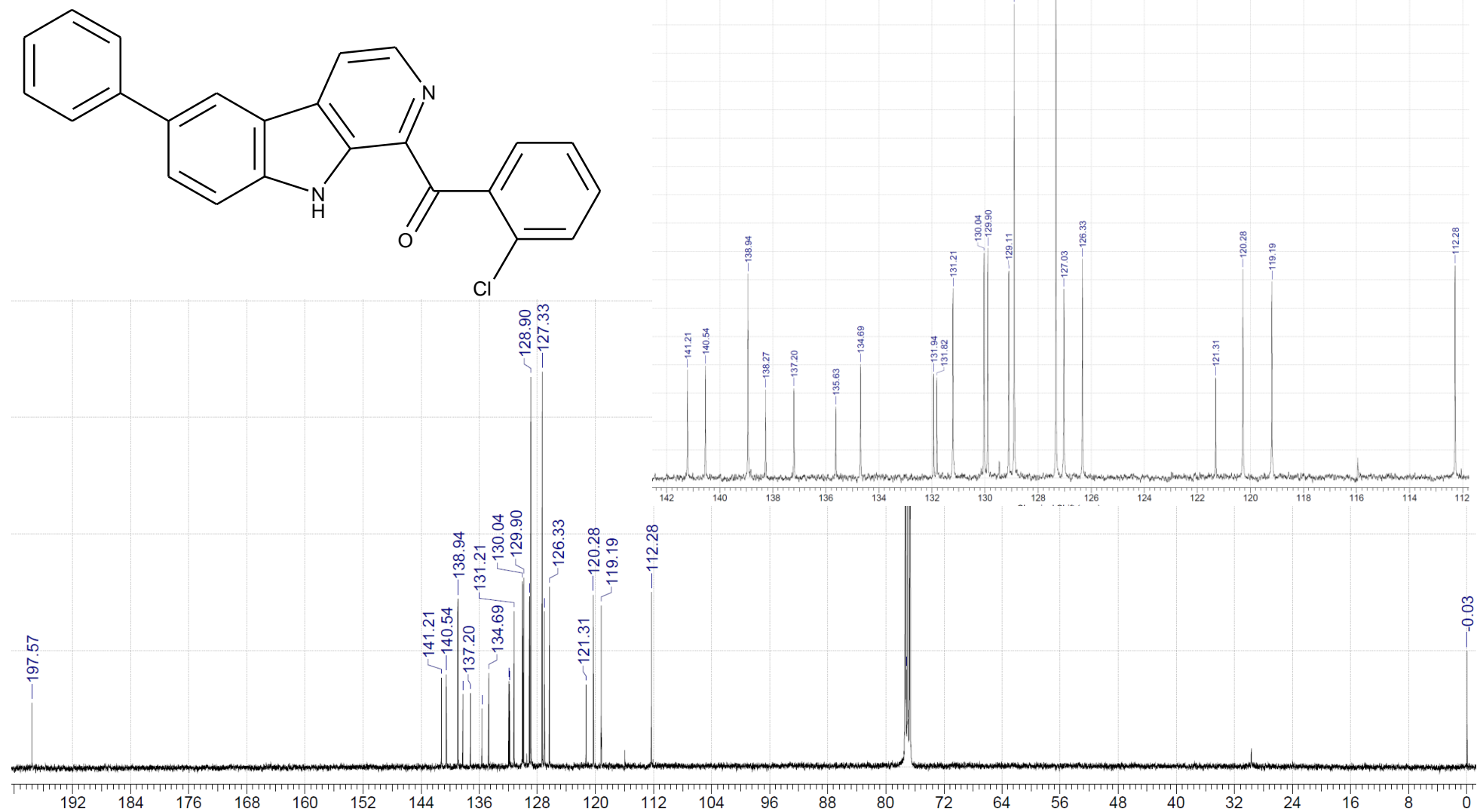
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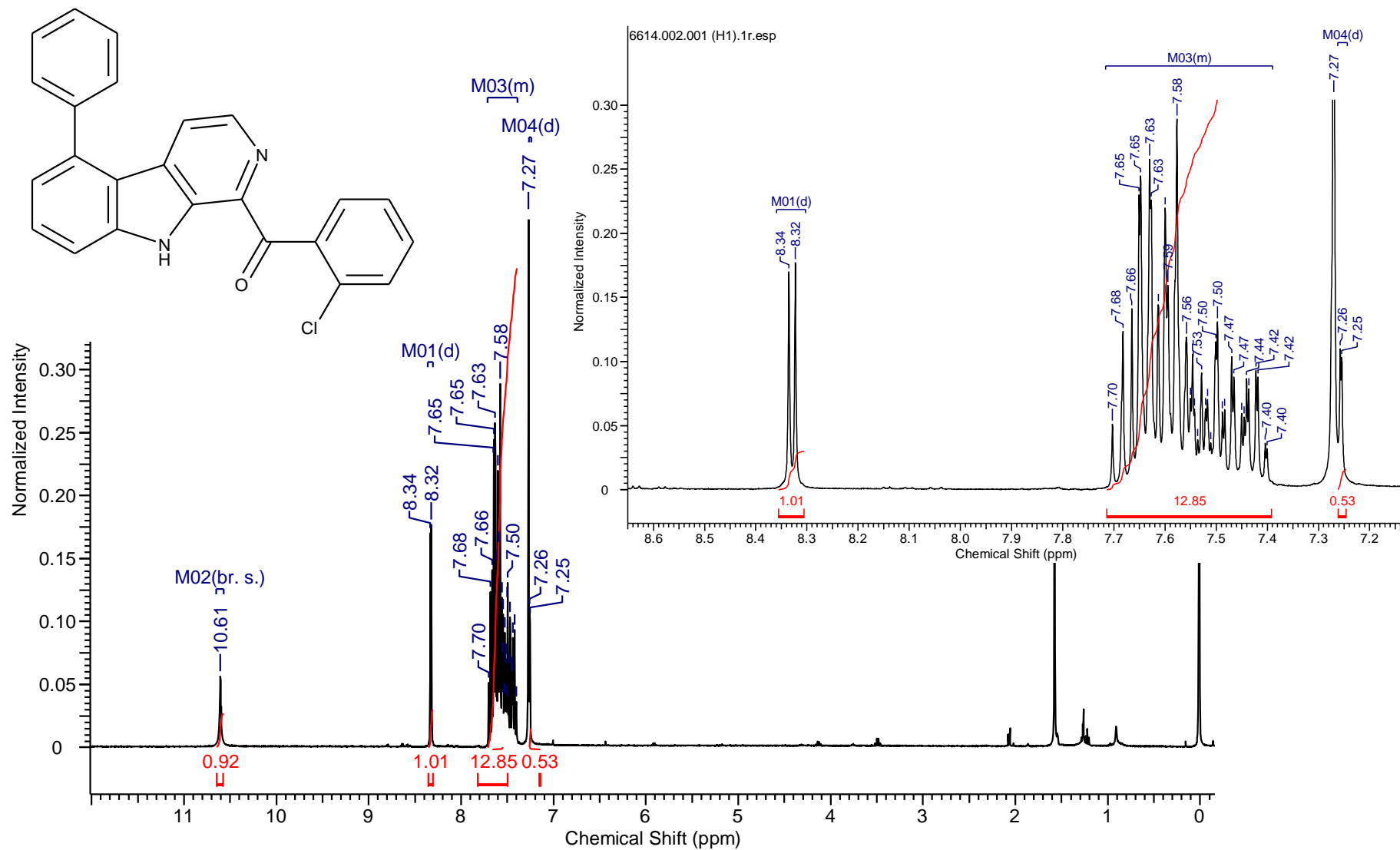
¹H NMR spectra of compound 14



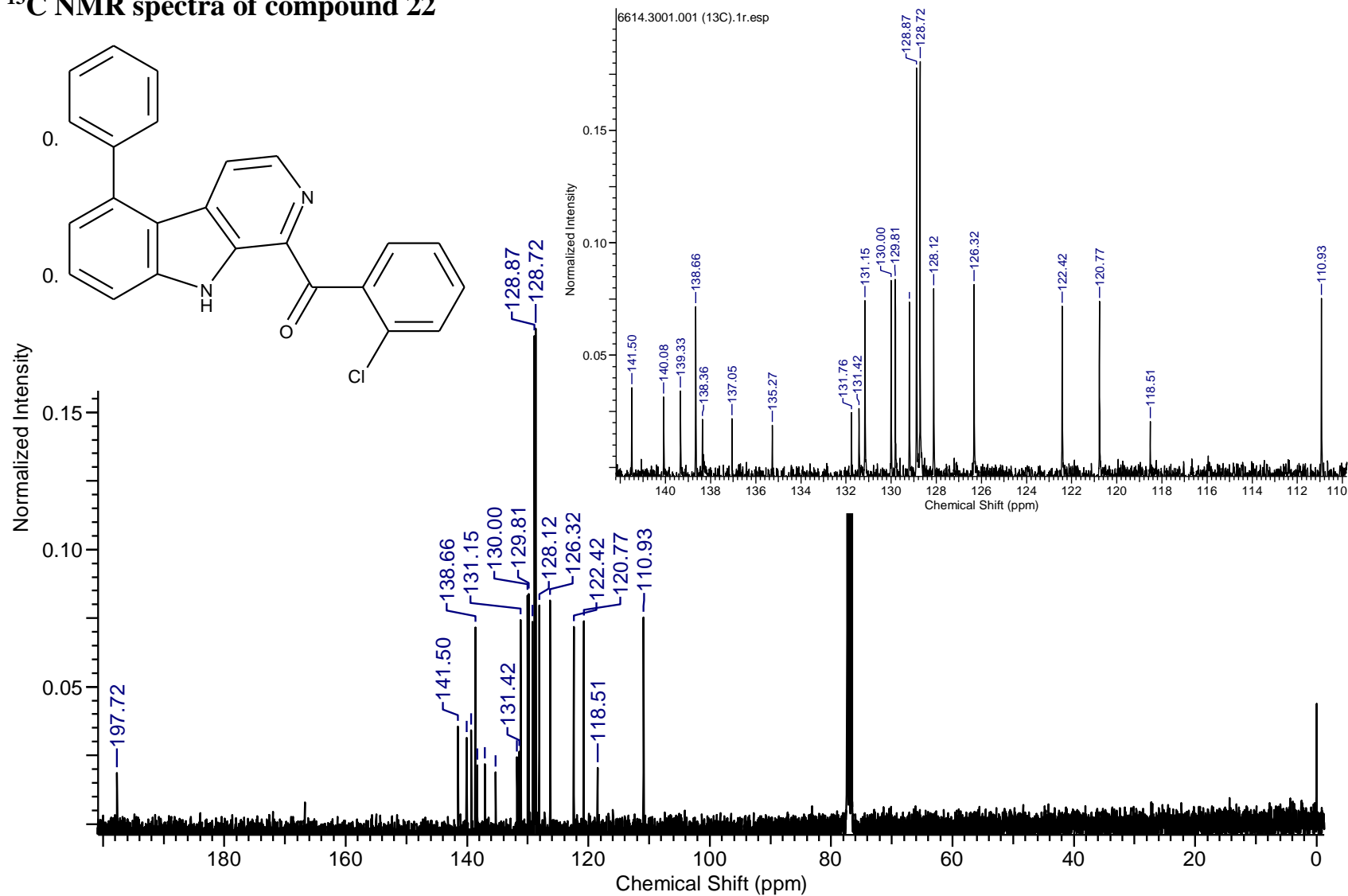
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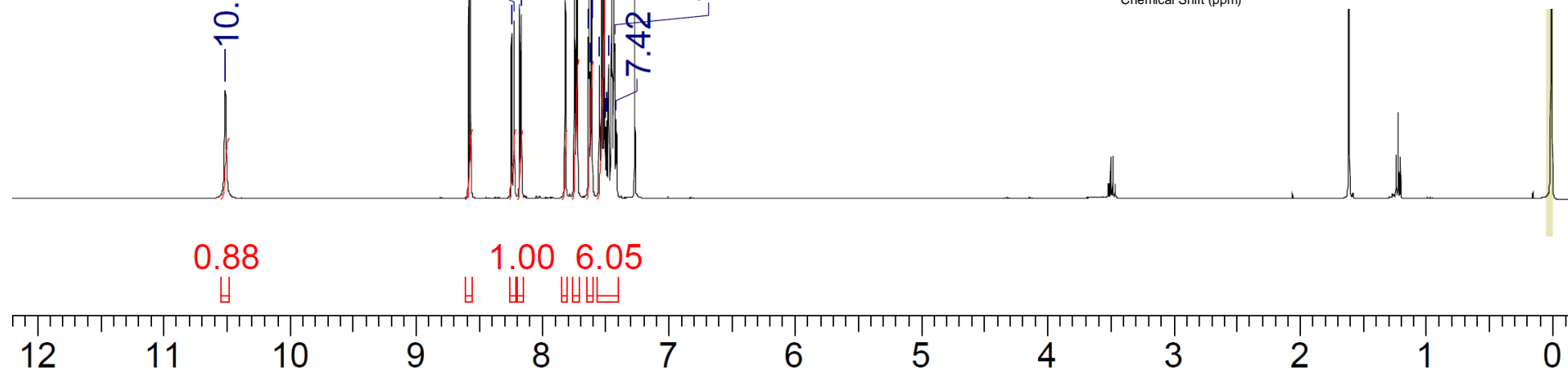
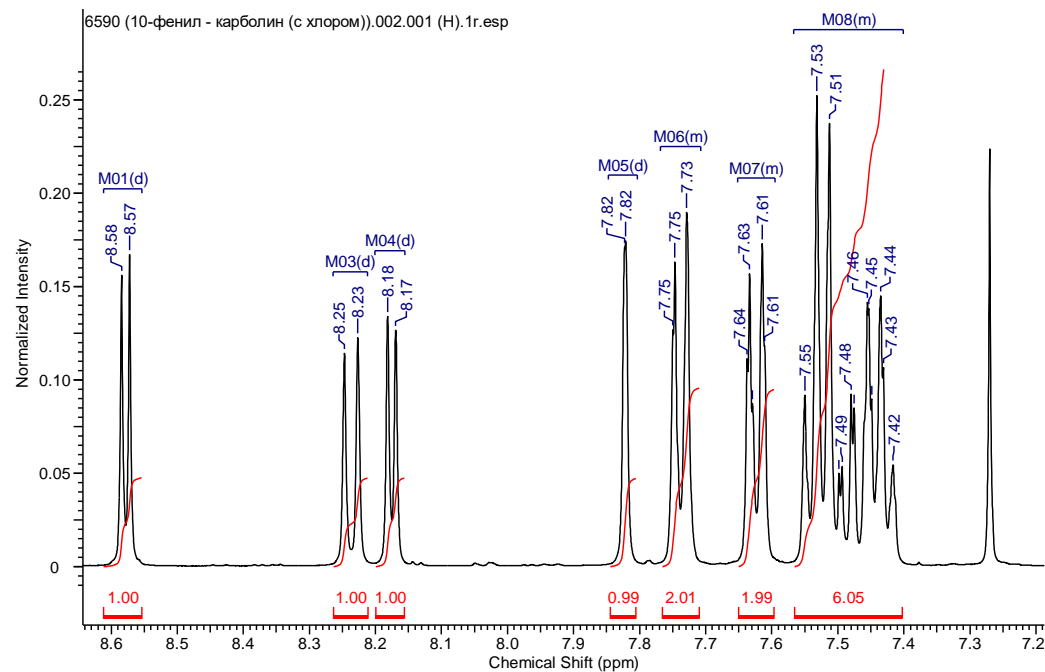
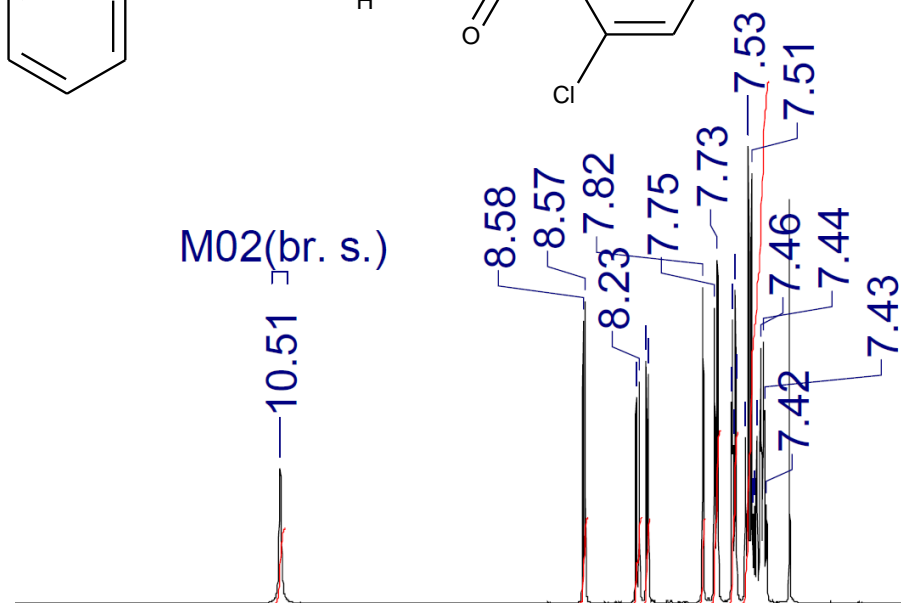
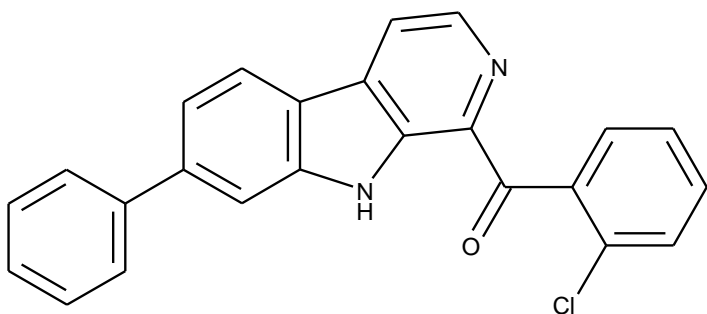
¹H NMR spectra of compound 22



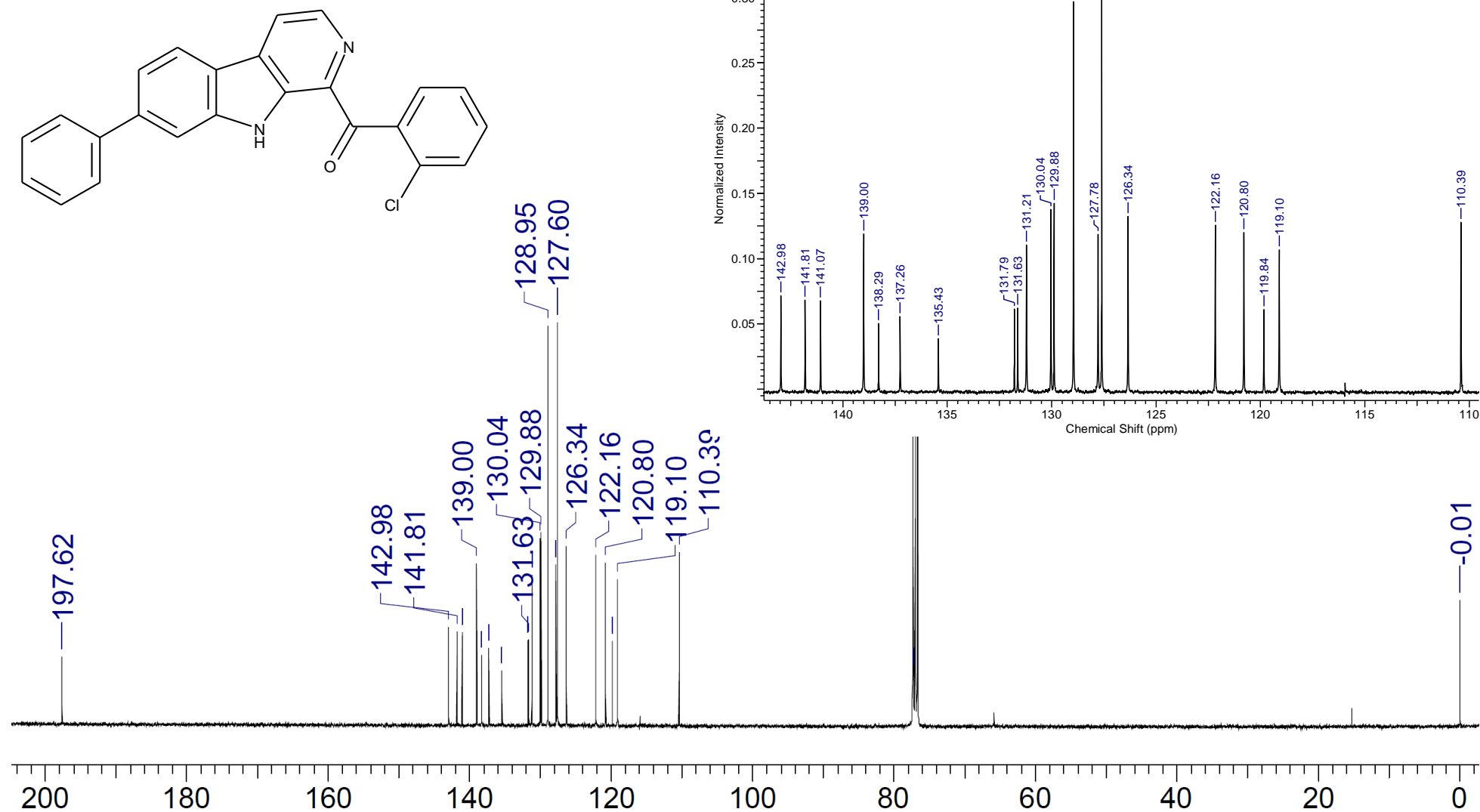
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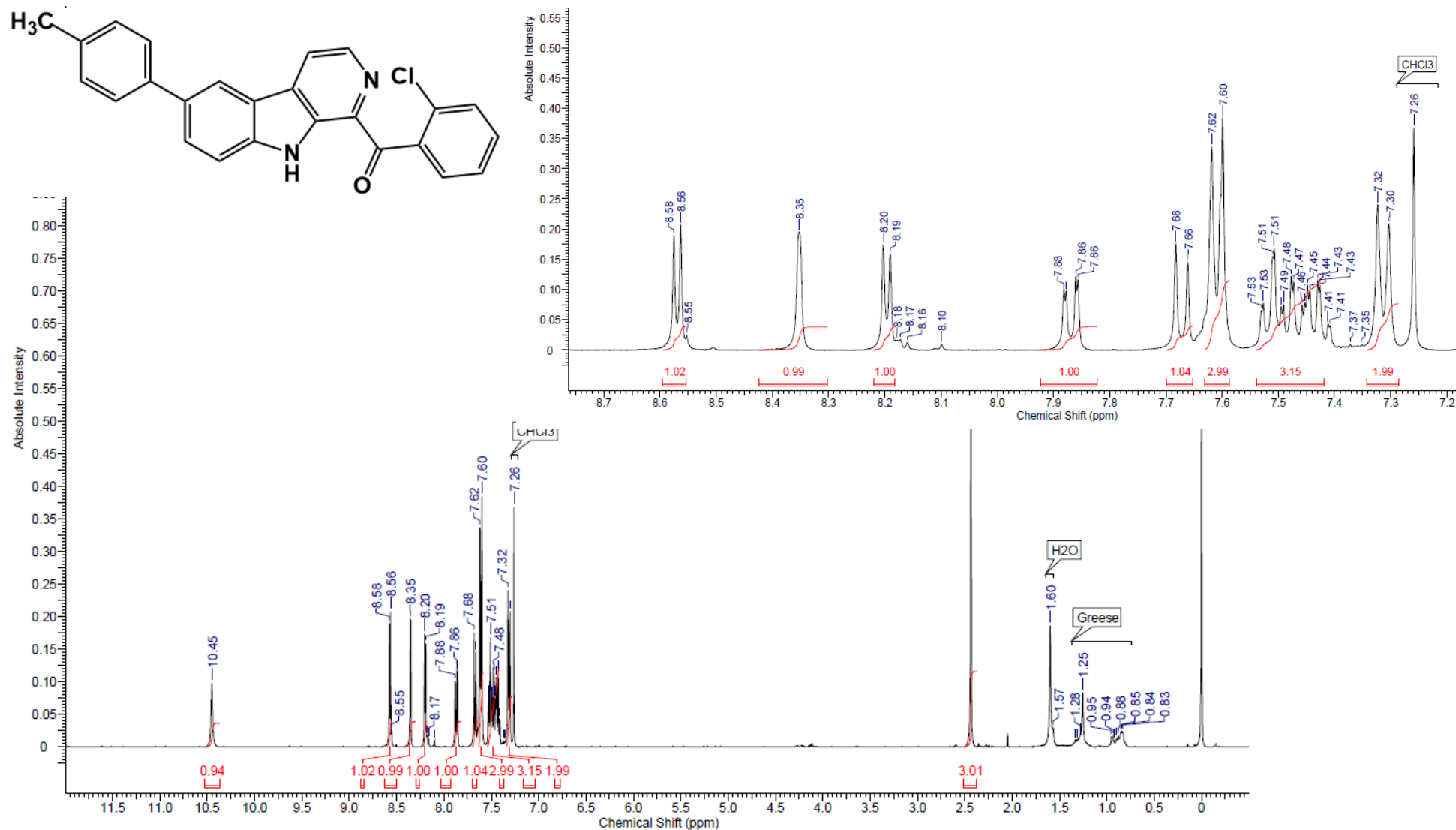
¹H NMR spectra of compound 23



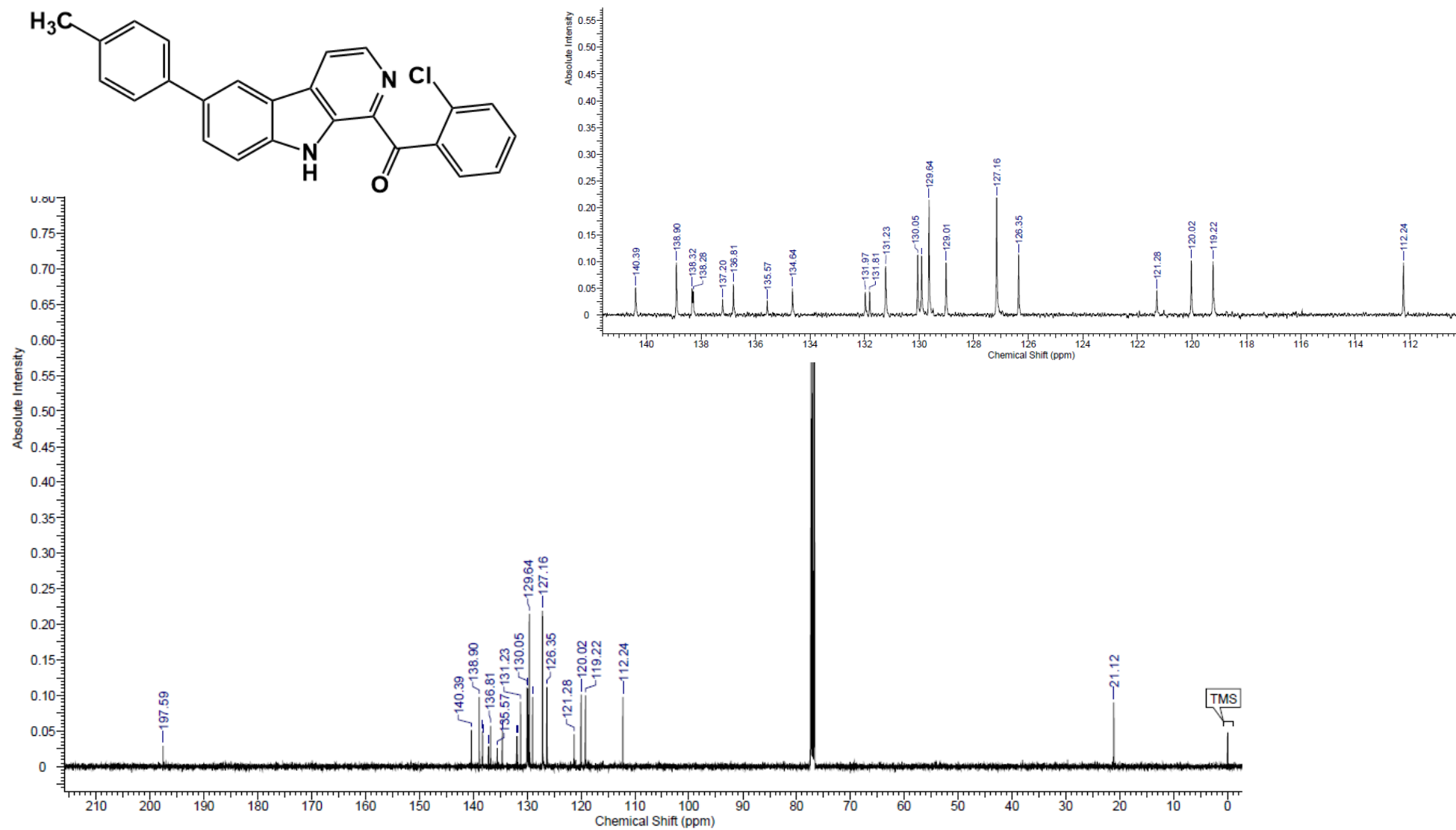
¹³C NMR spectra of compound 23



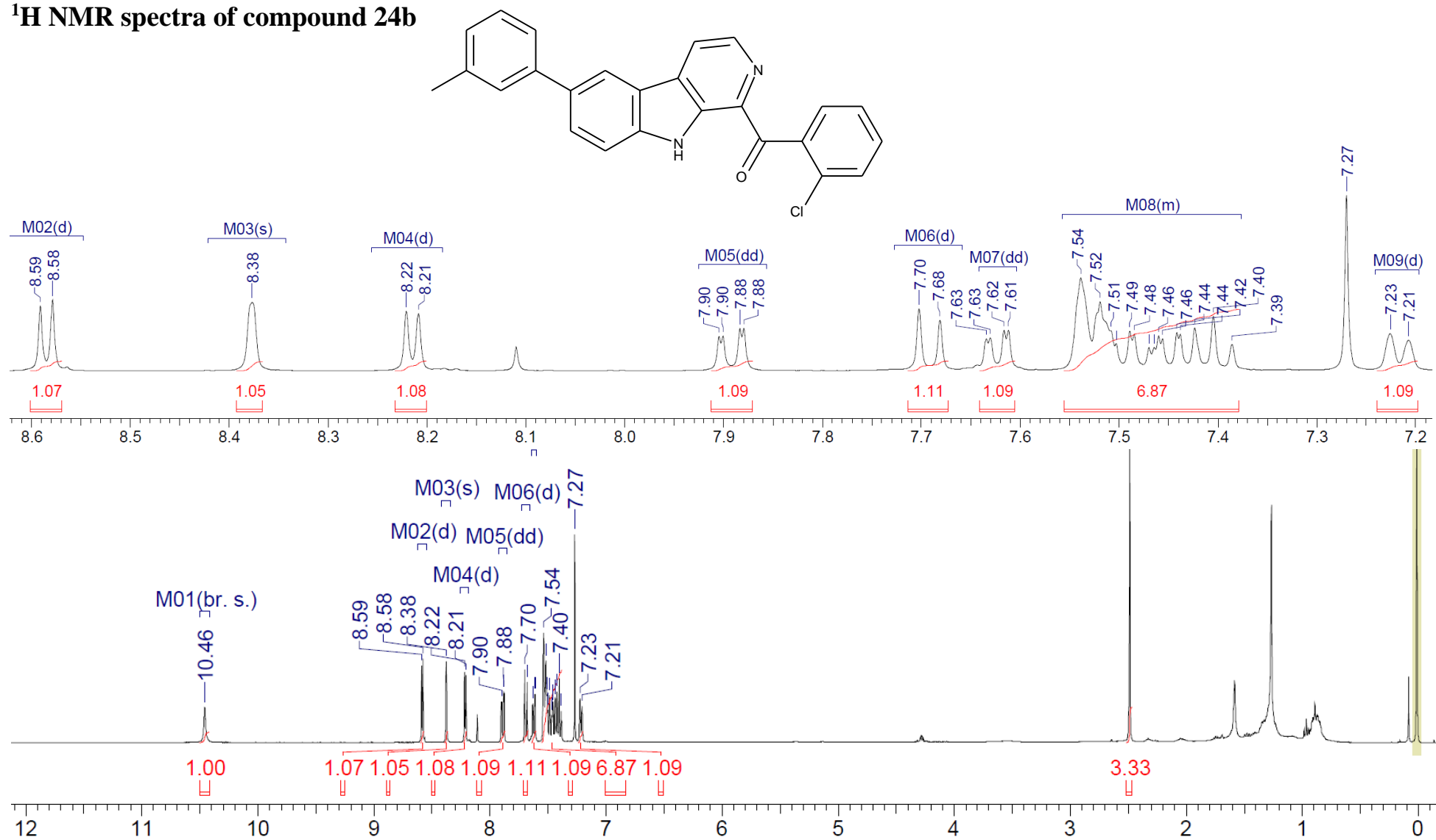
¹H NMR spectra of compound 24a



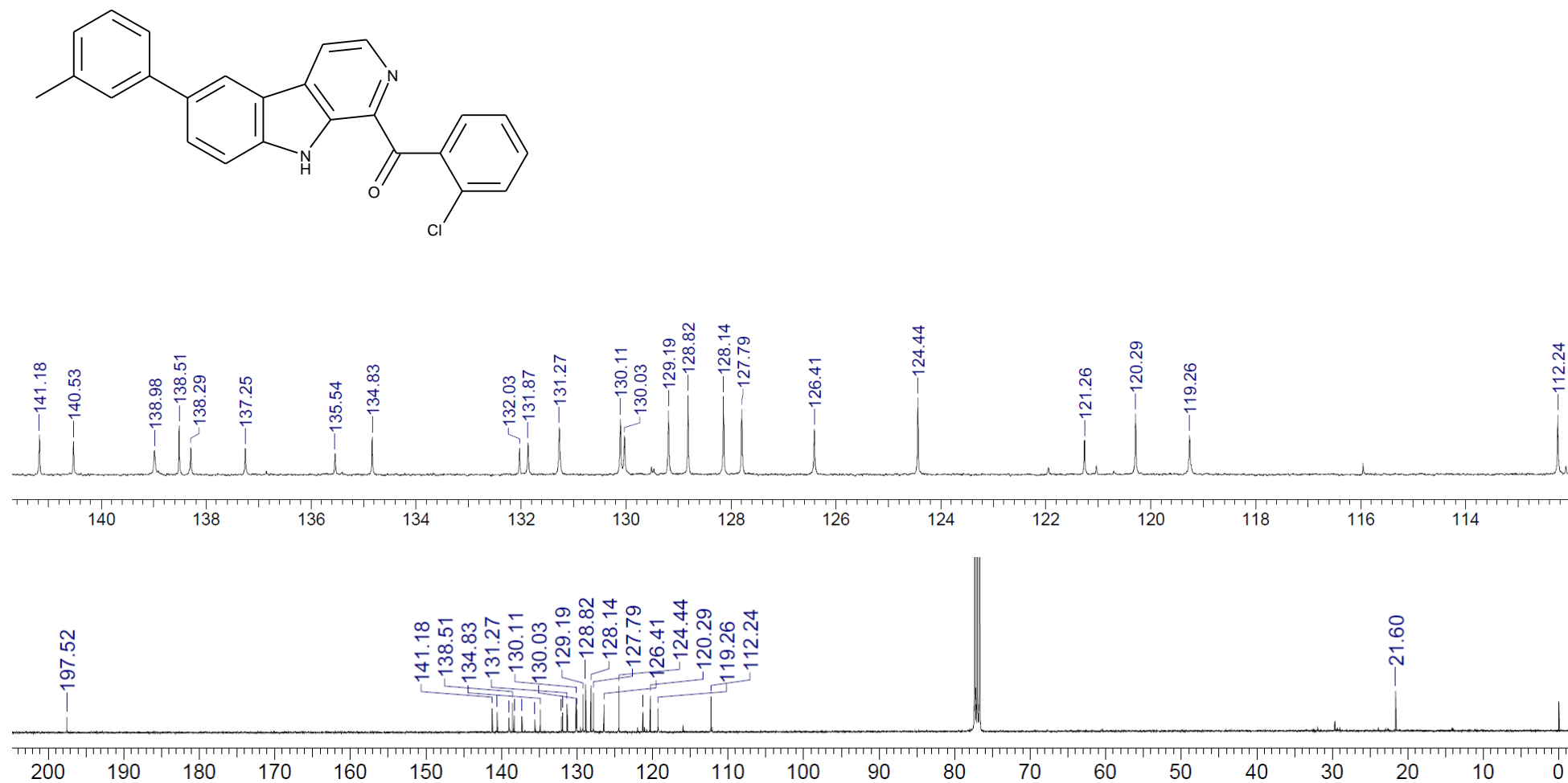
^{13}C NMR spectra of compound 24a



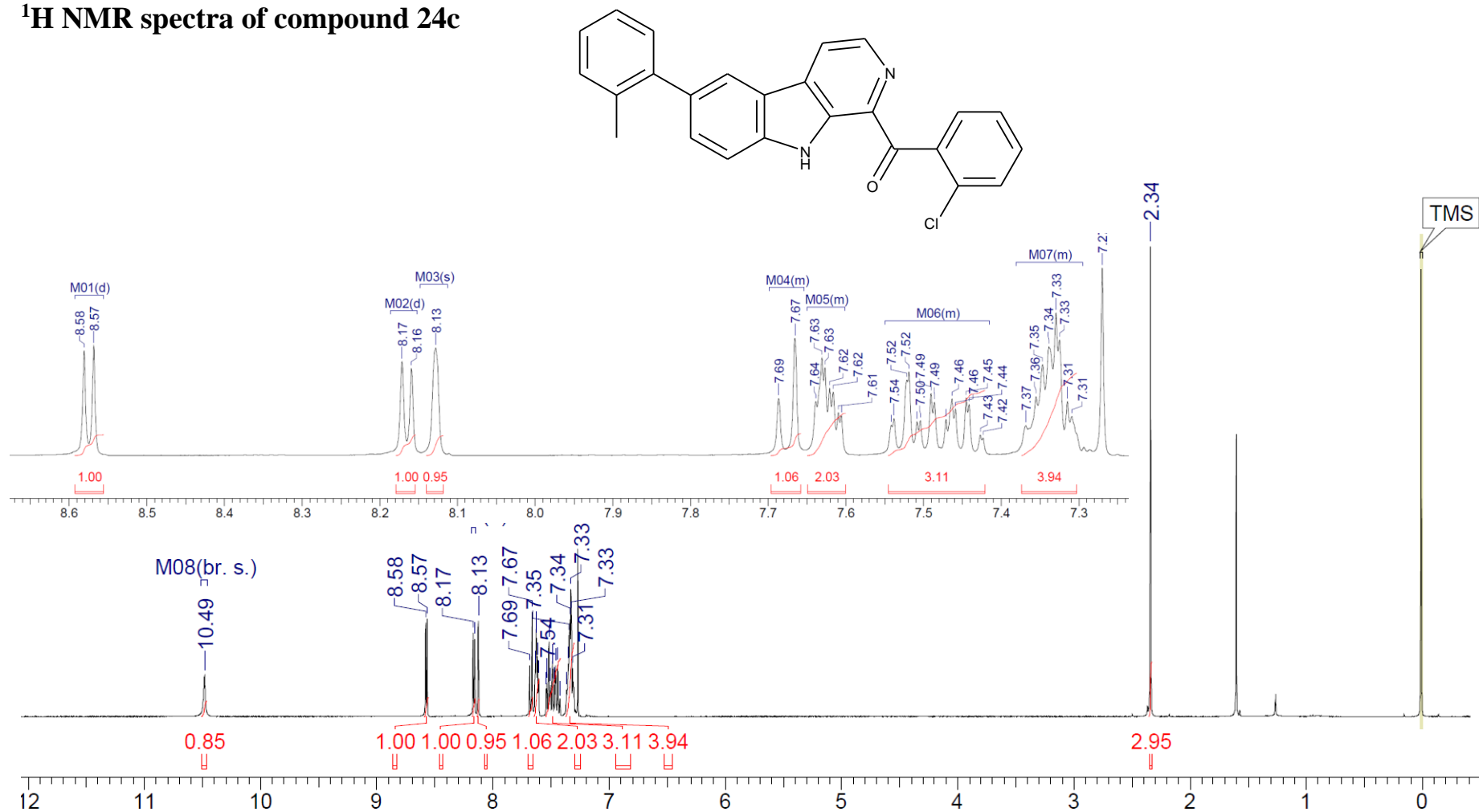
¹H NMR spectra of compound 24b



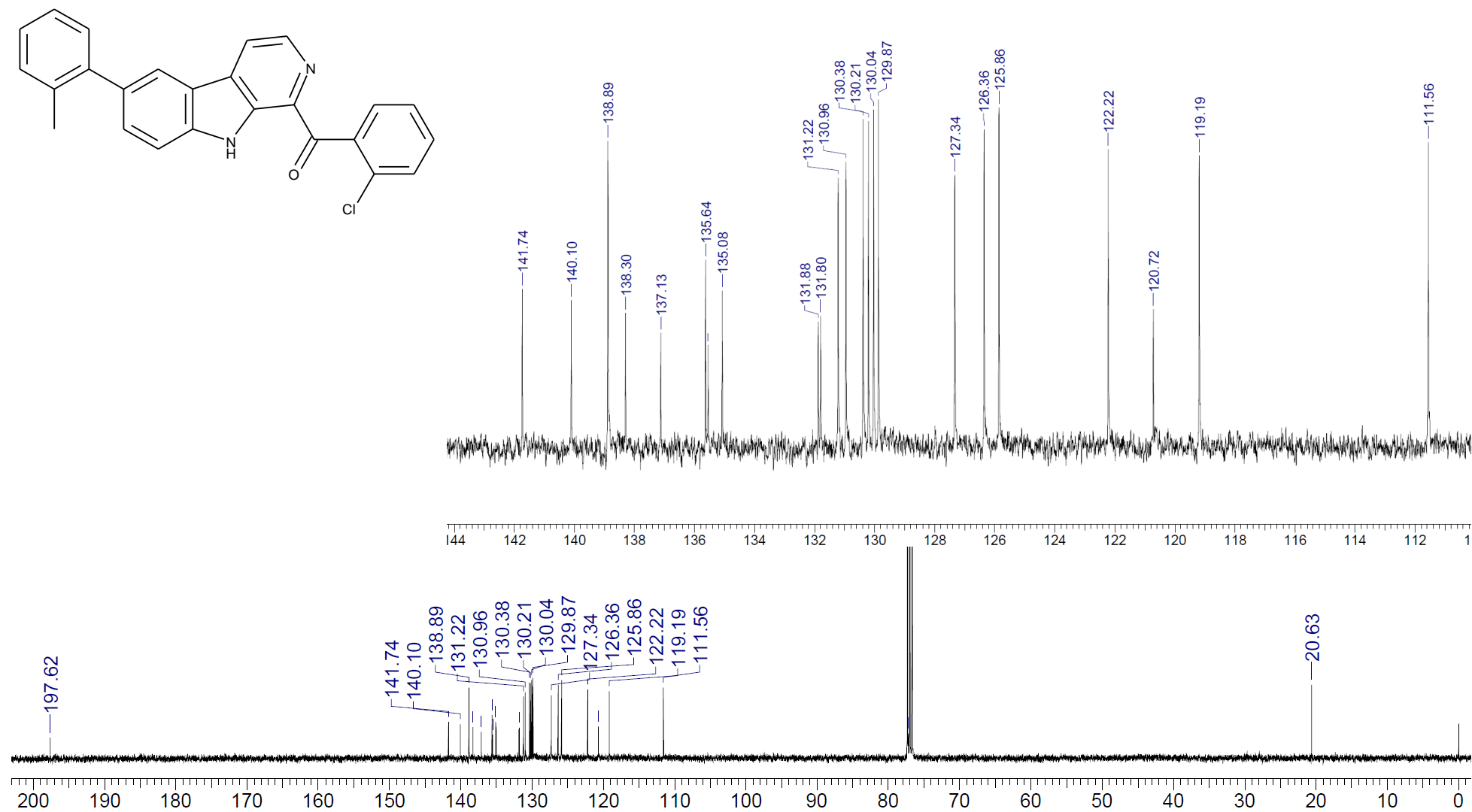
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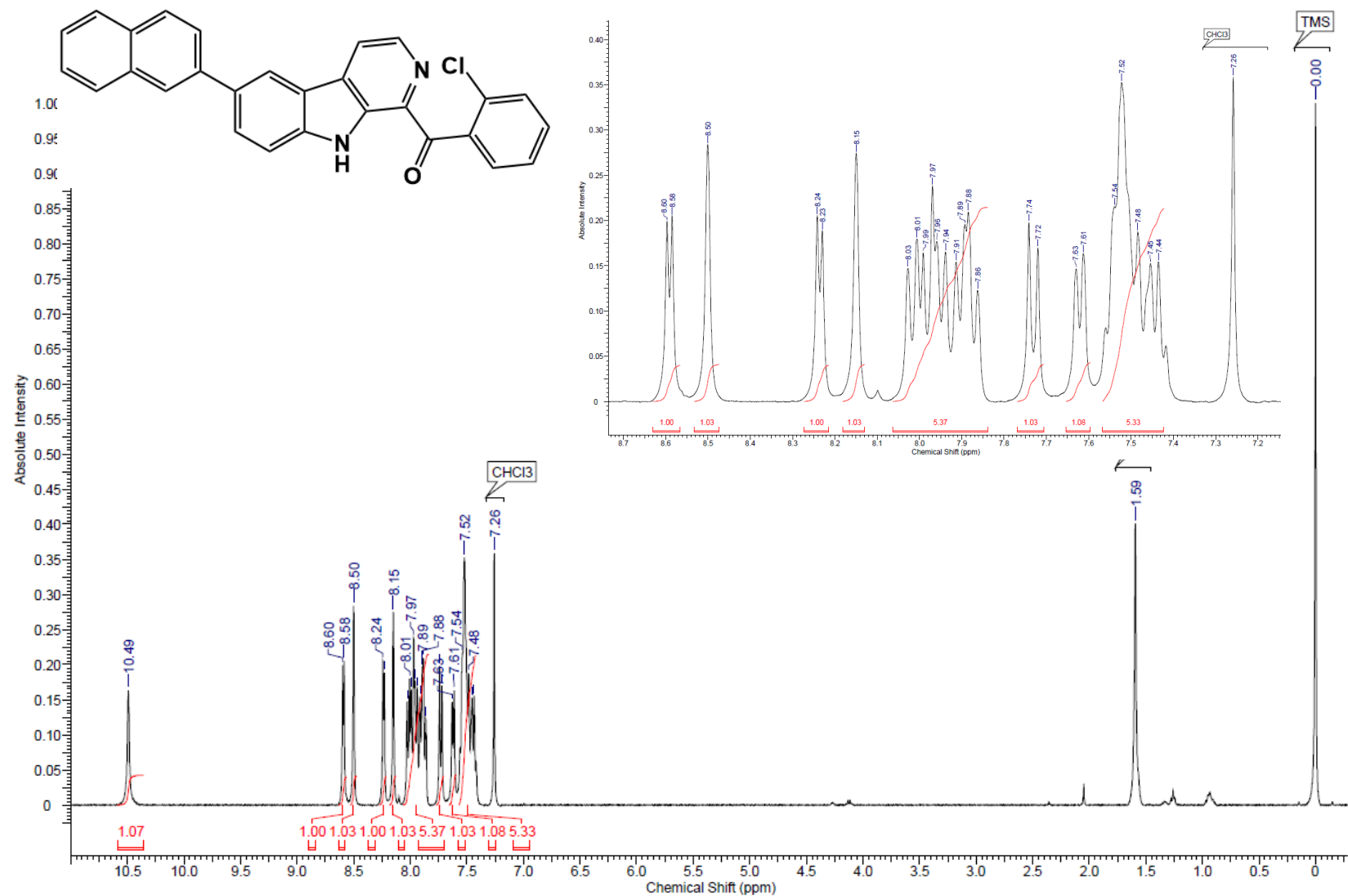
^1H NMR spectra of compound 24c



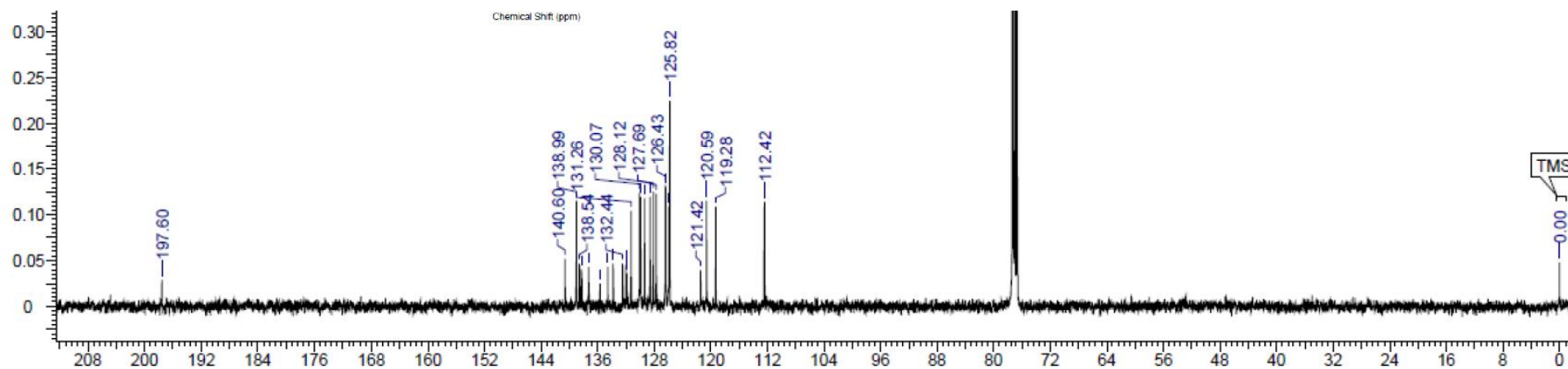
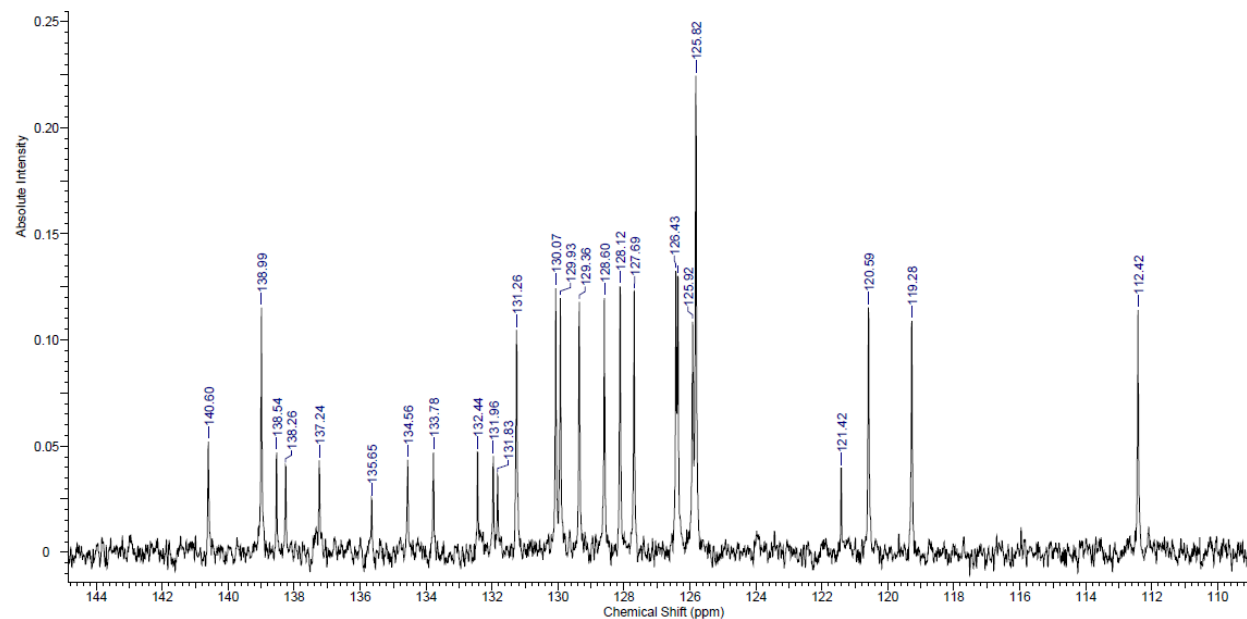
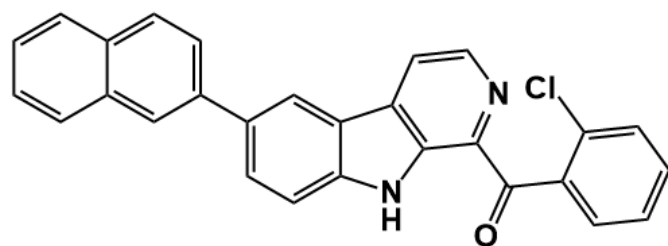
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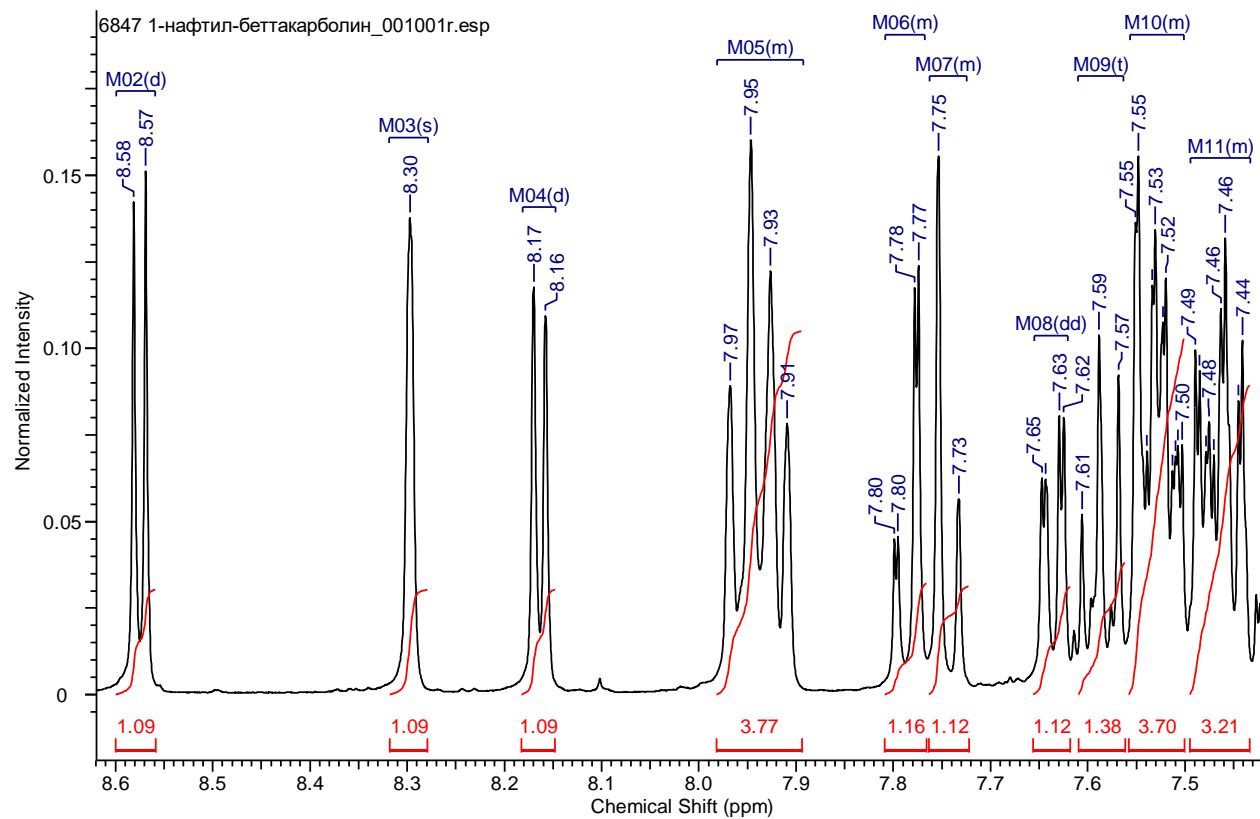
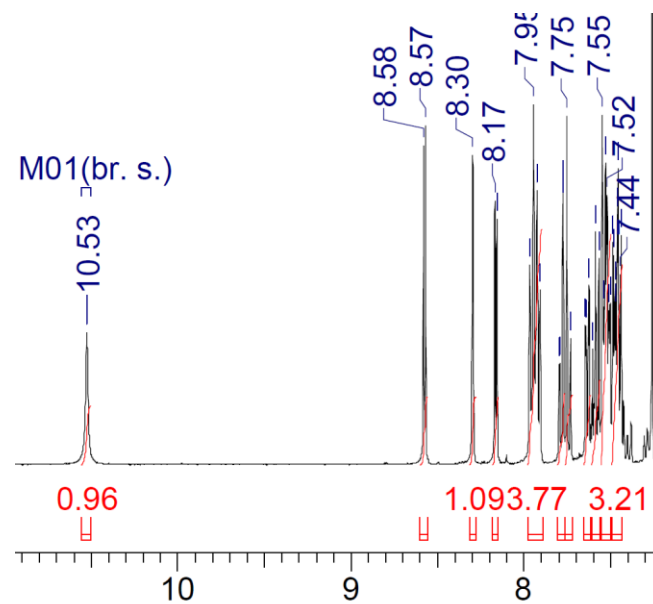
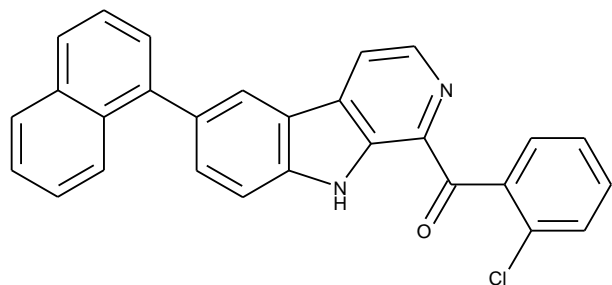
¹H NMR spectra of compound 24d



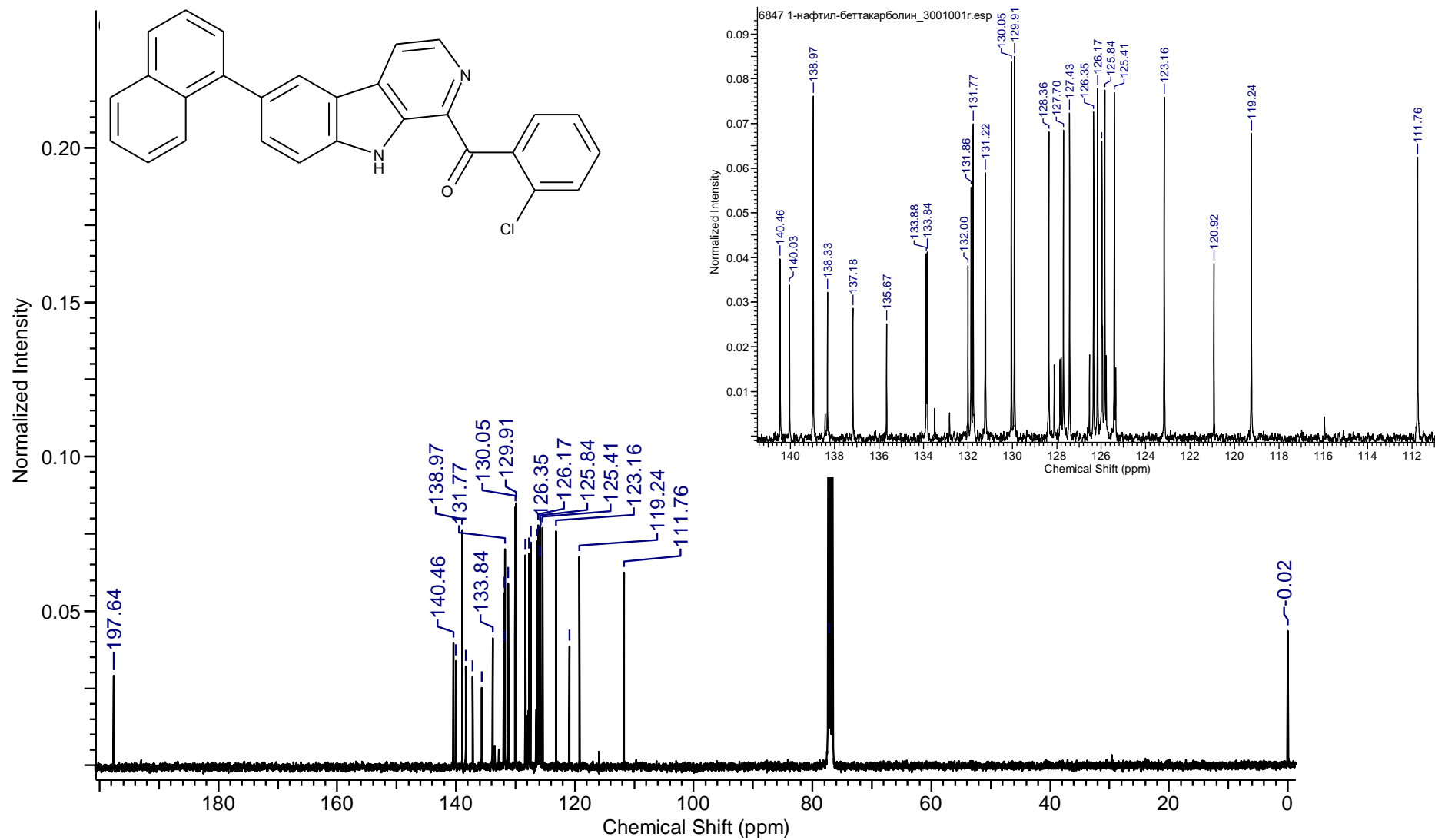
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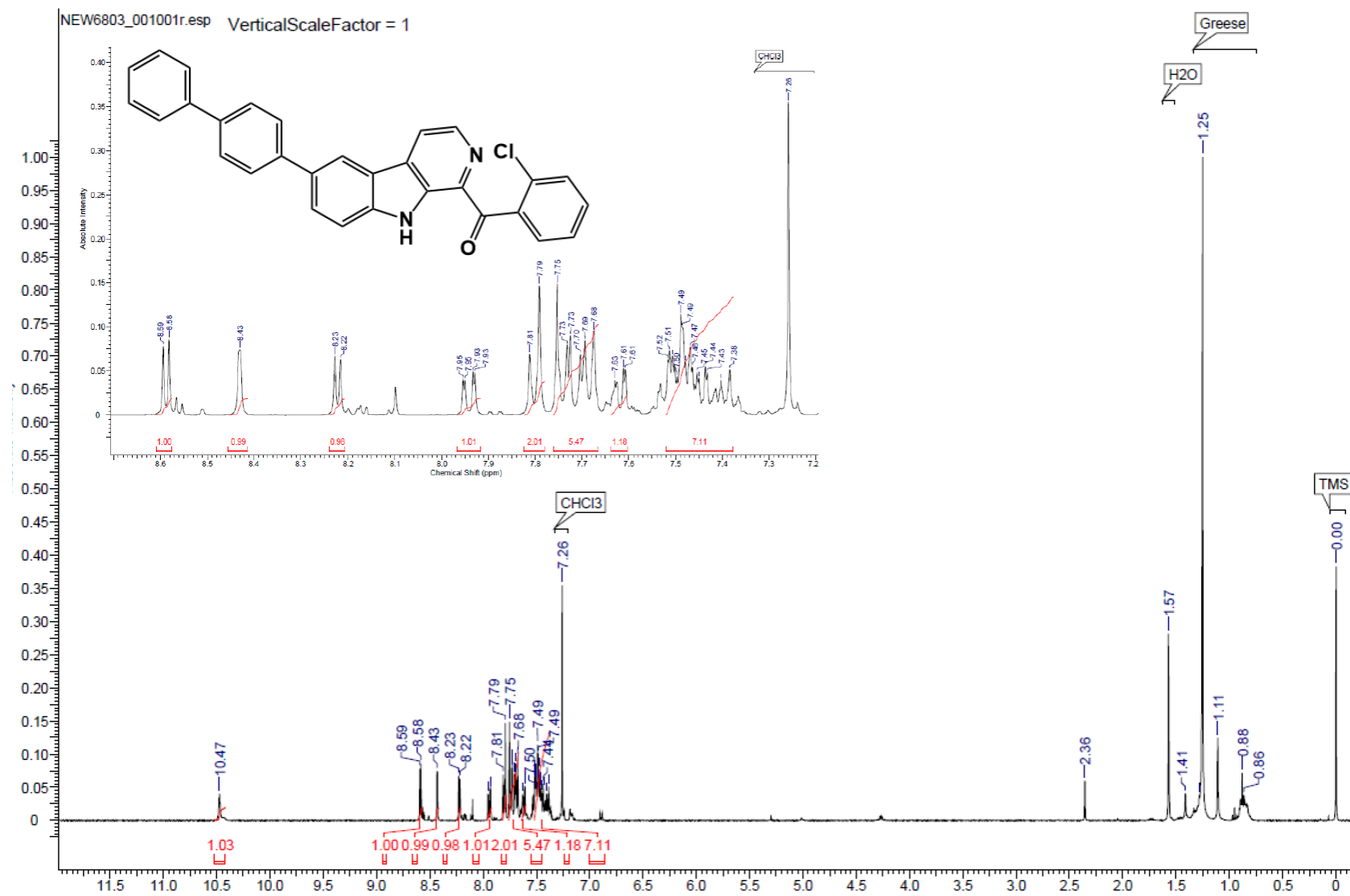
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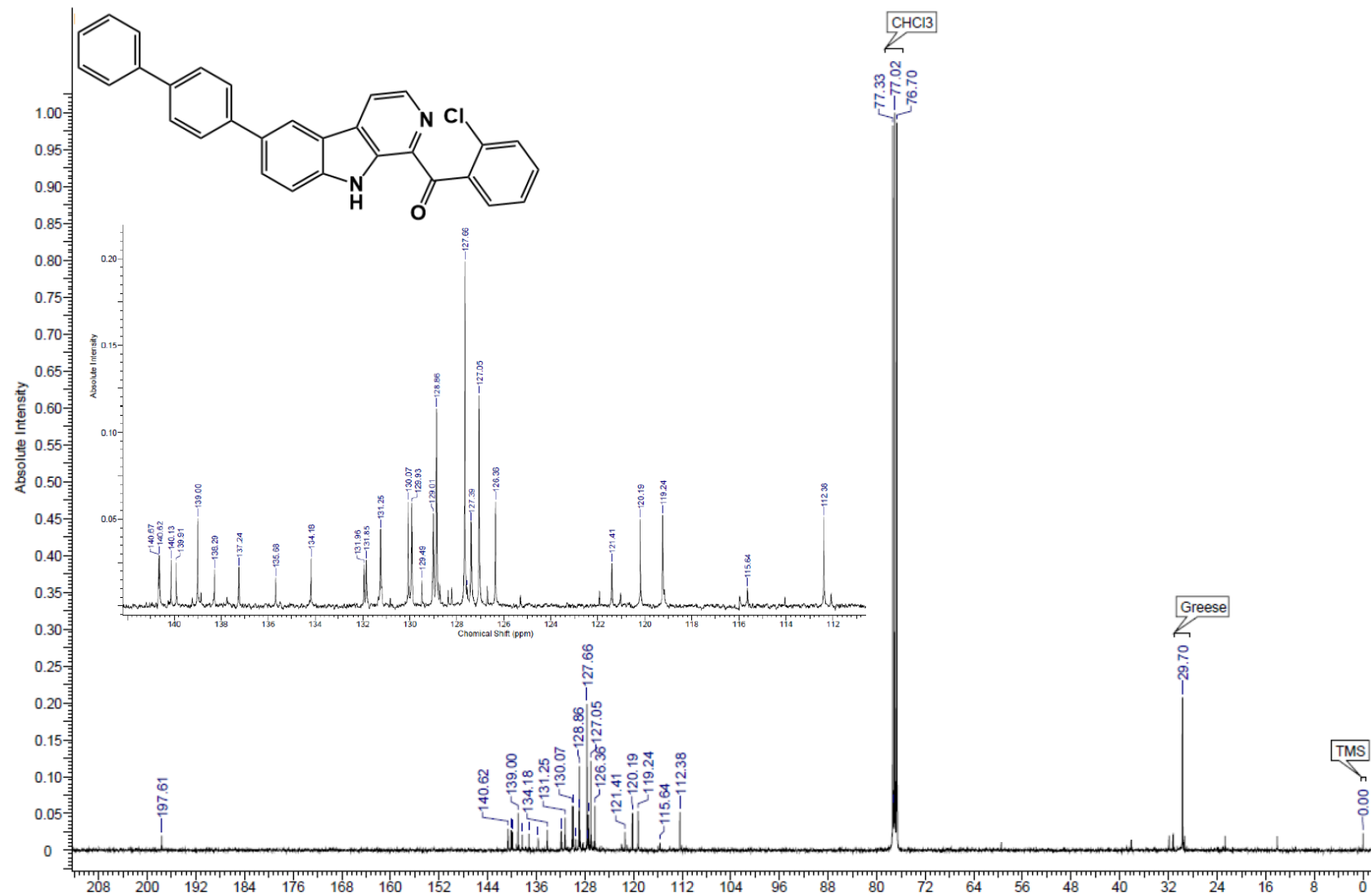
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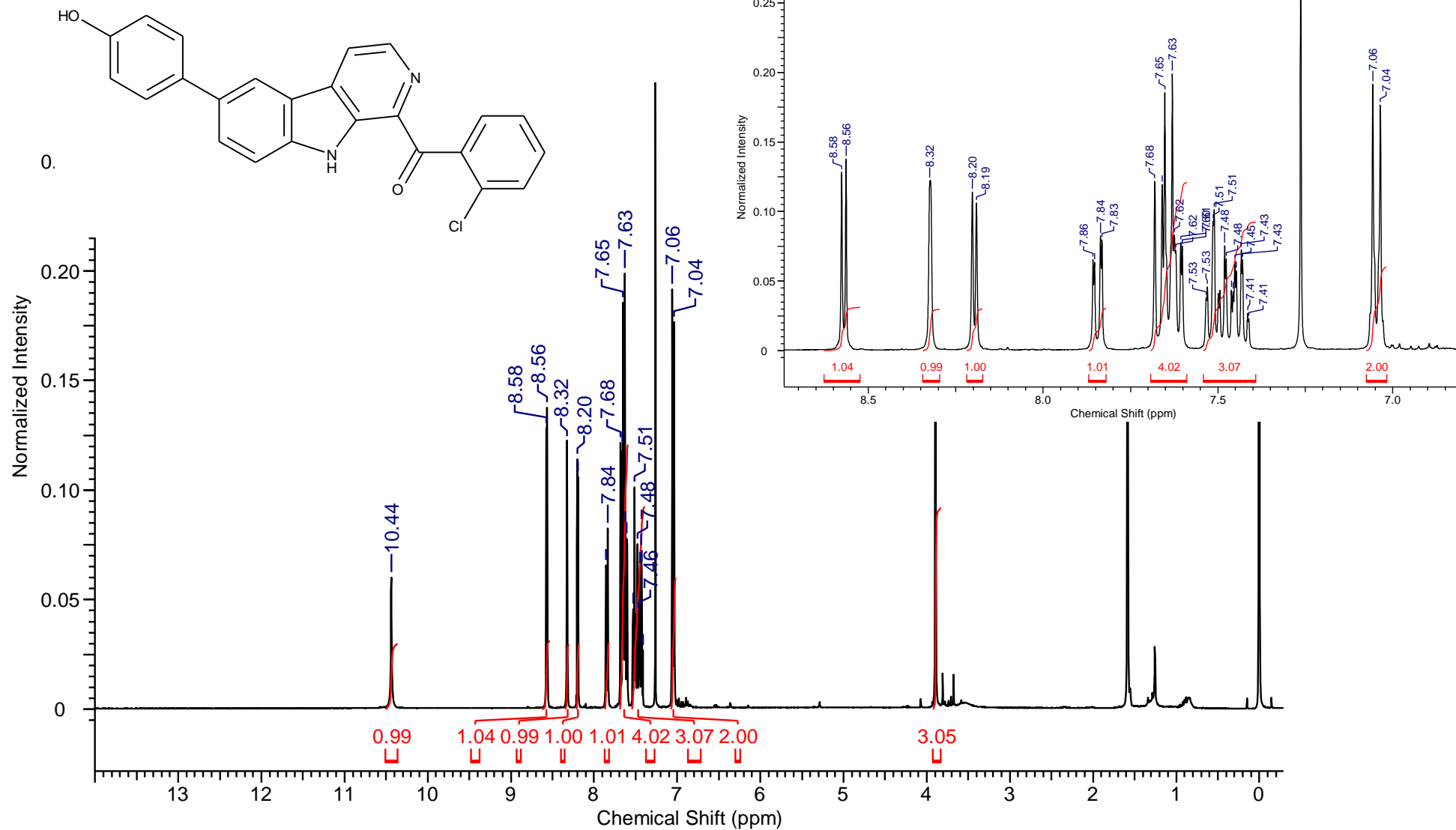
¹H NMR spectra of compound 24f



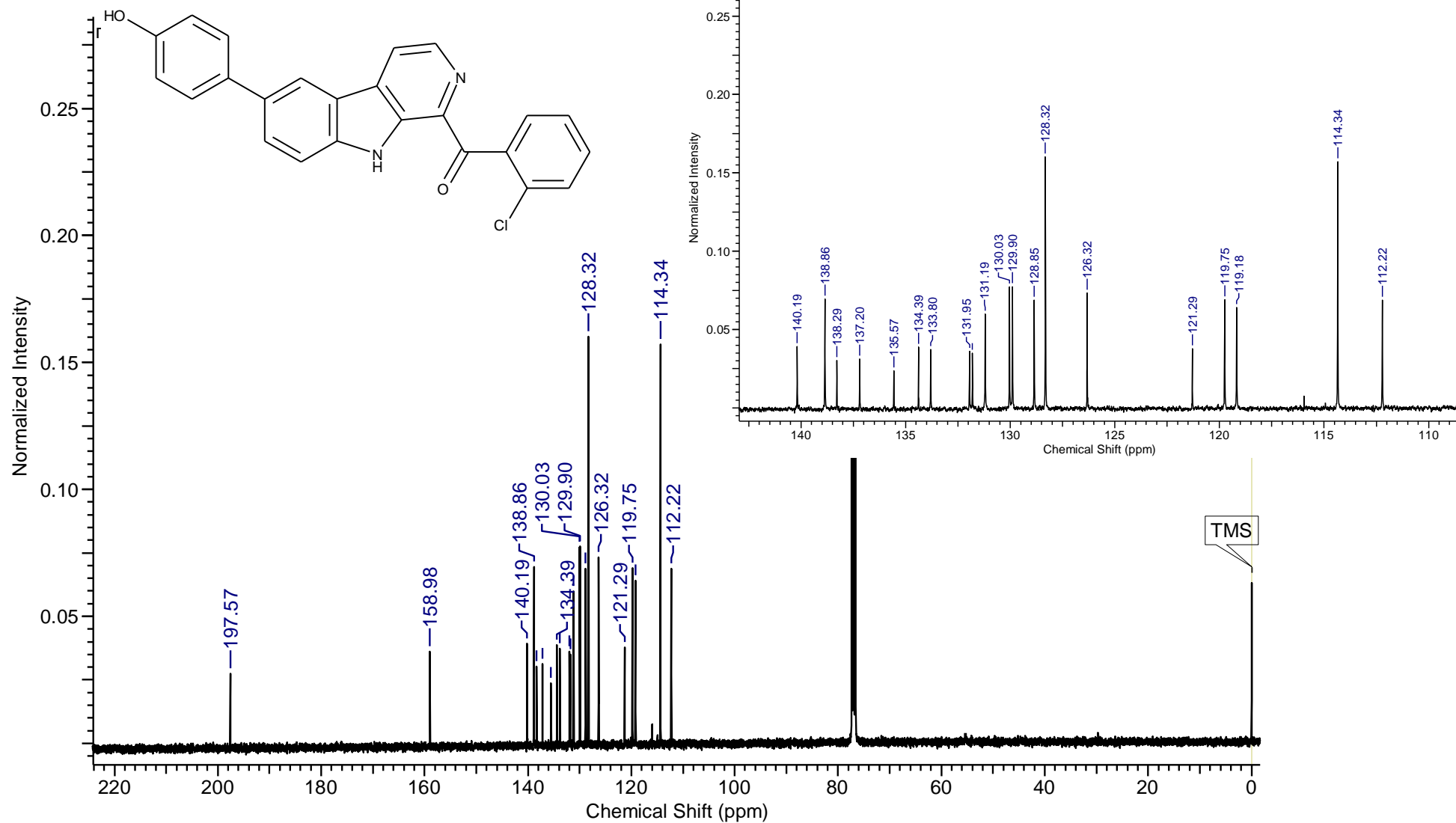
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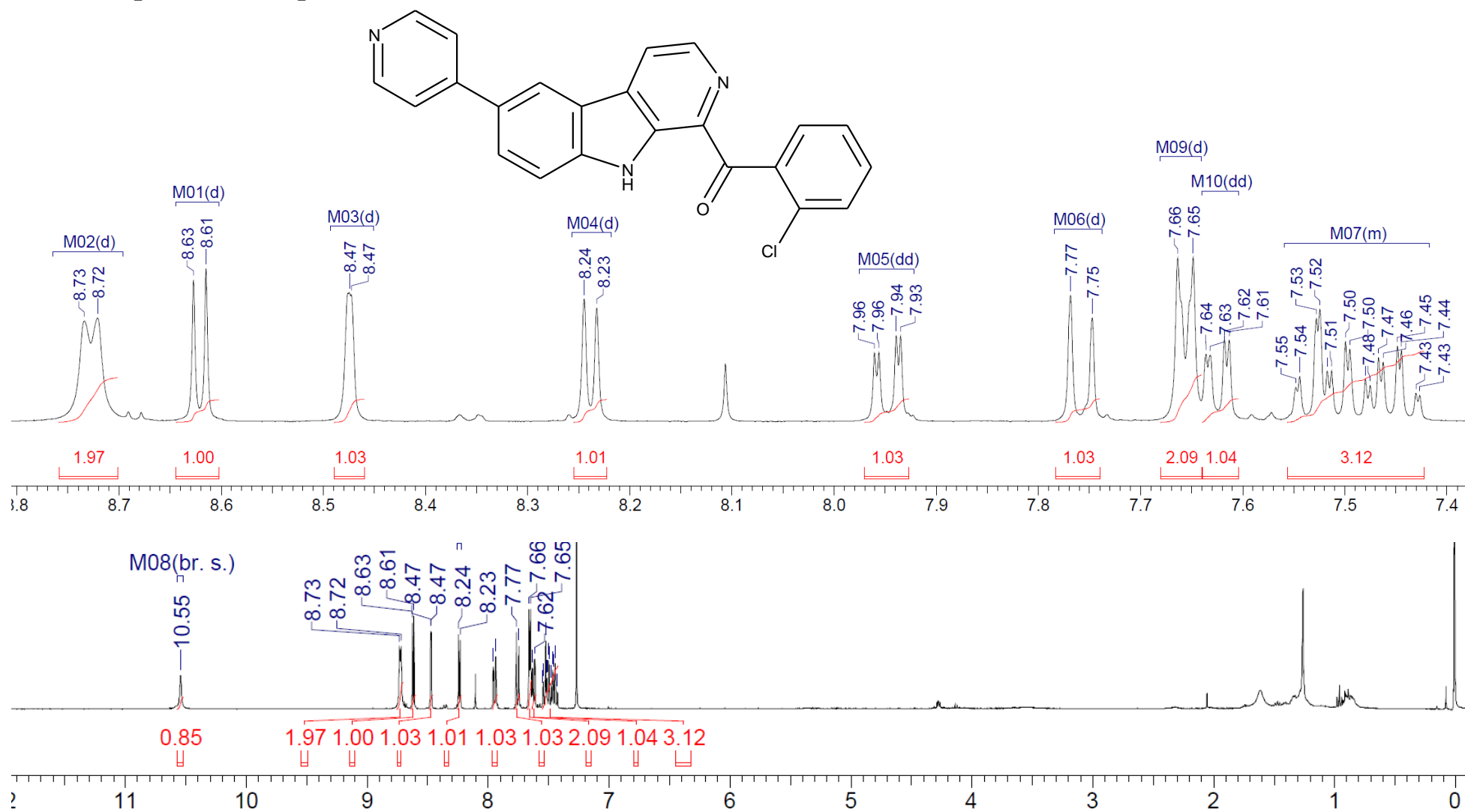
¹H NMR spectra of compound 24g



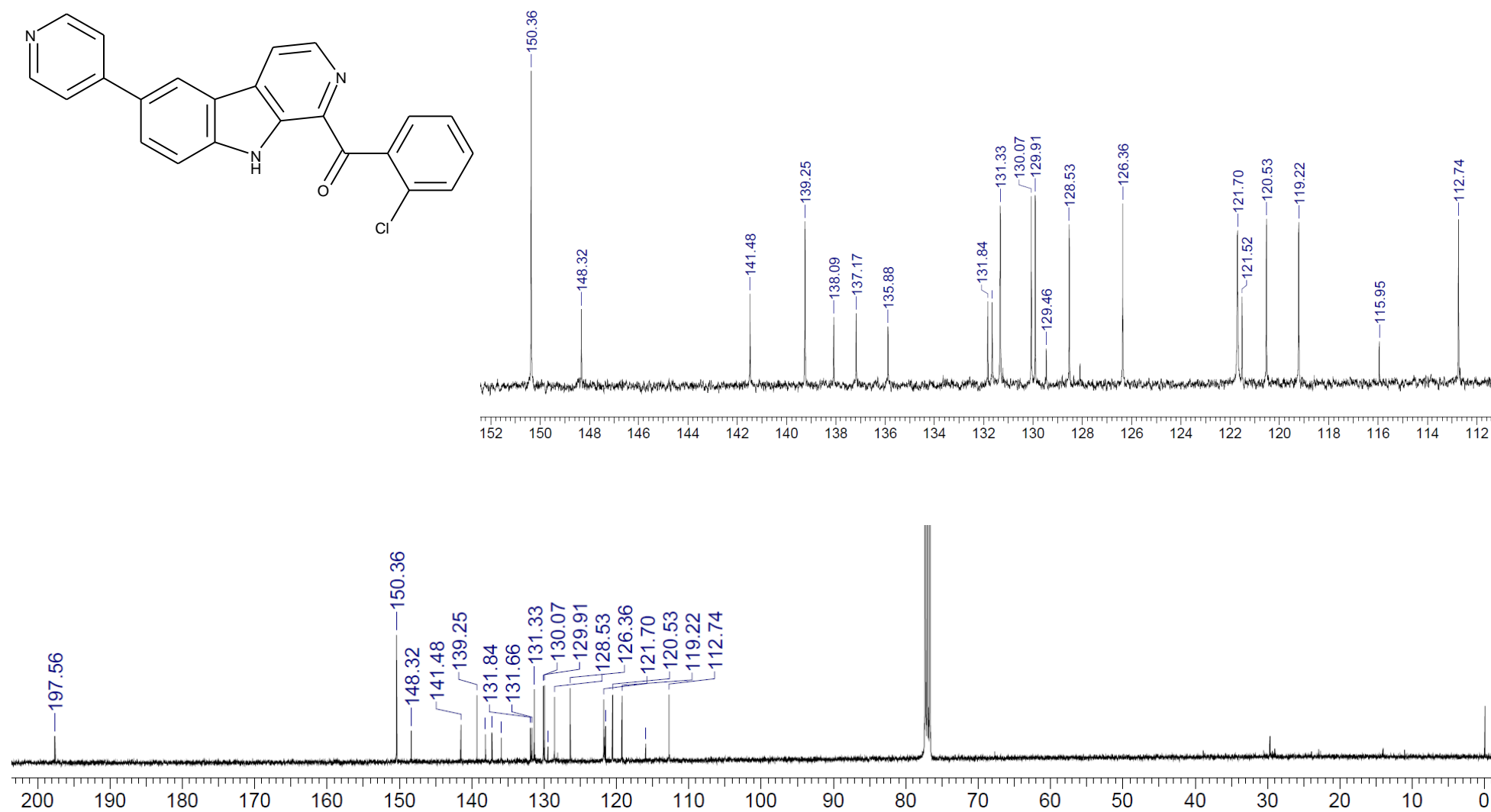
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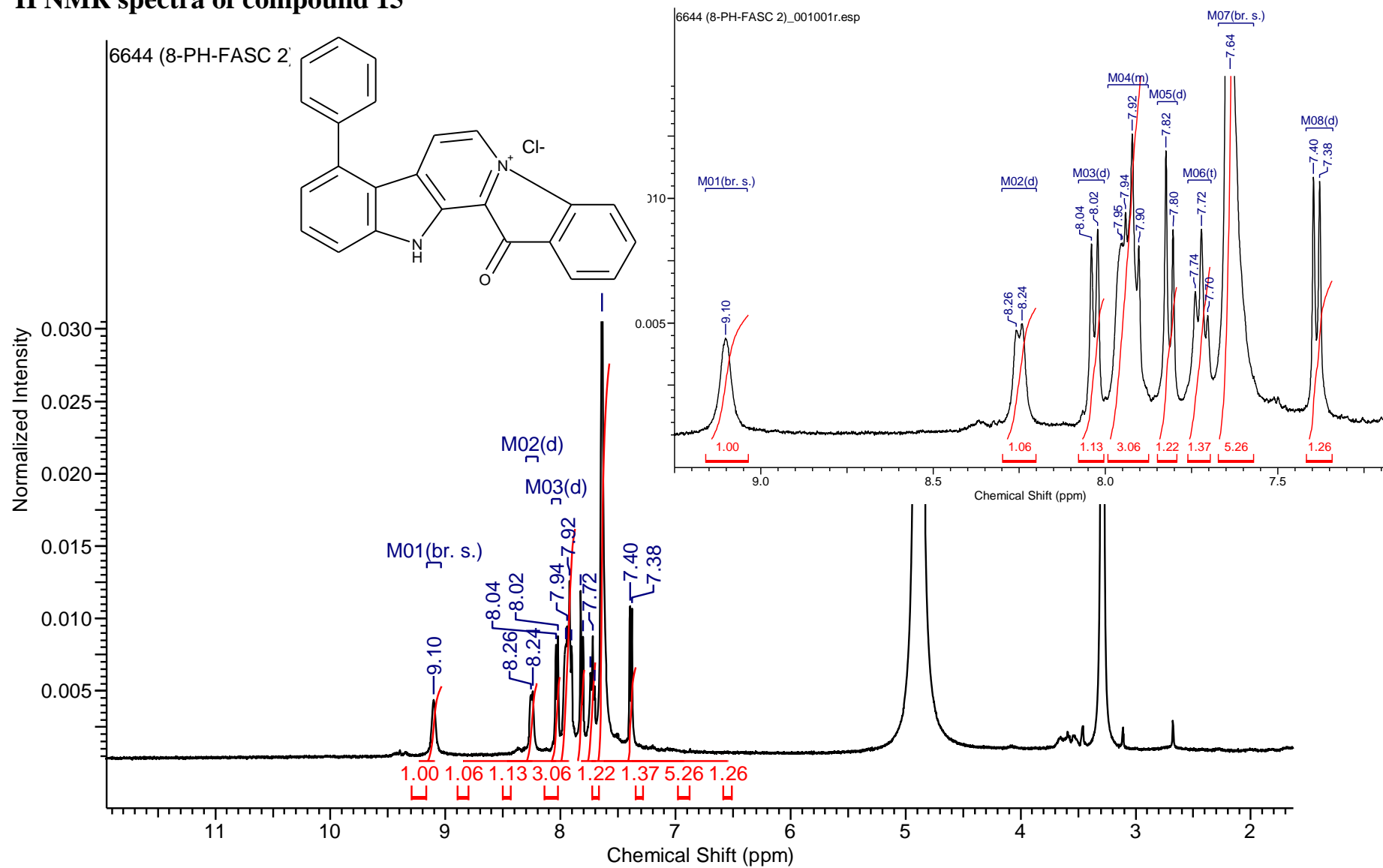
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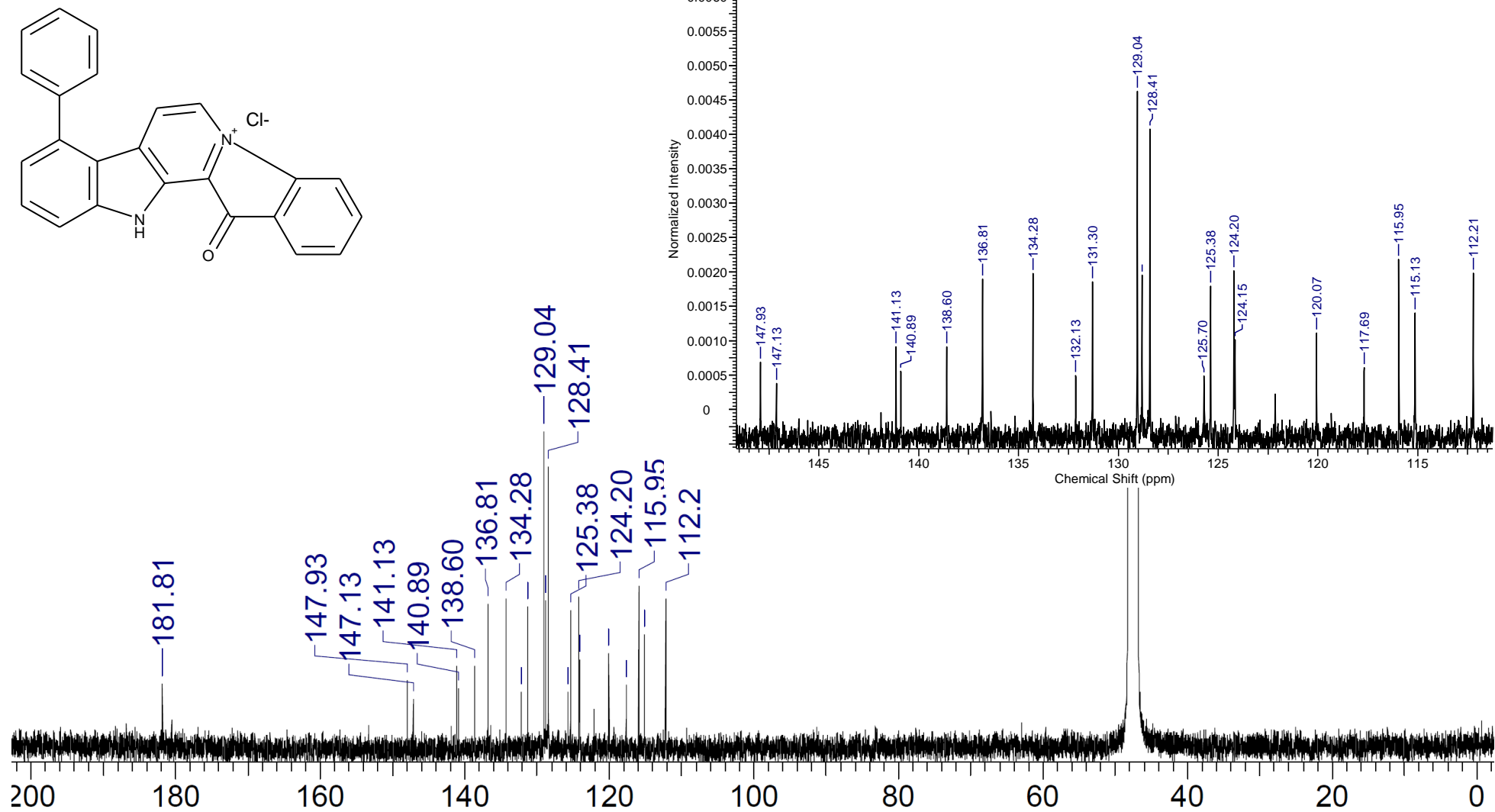
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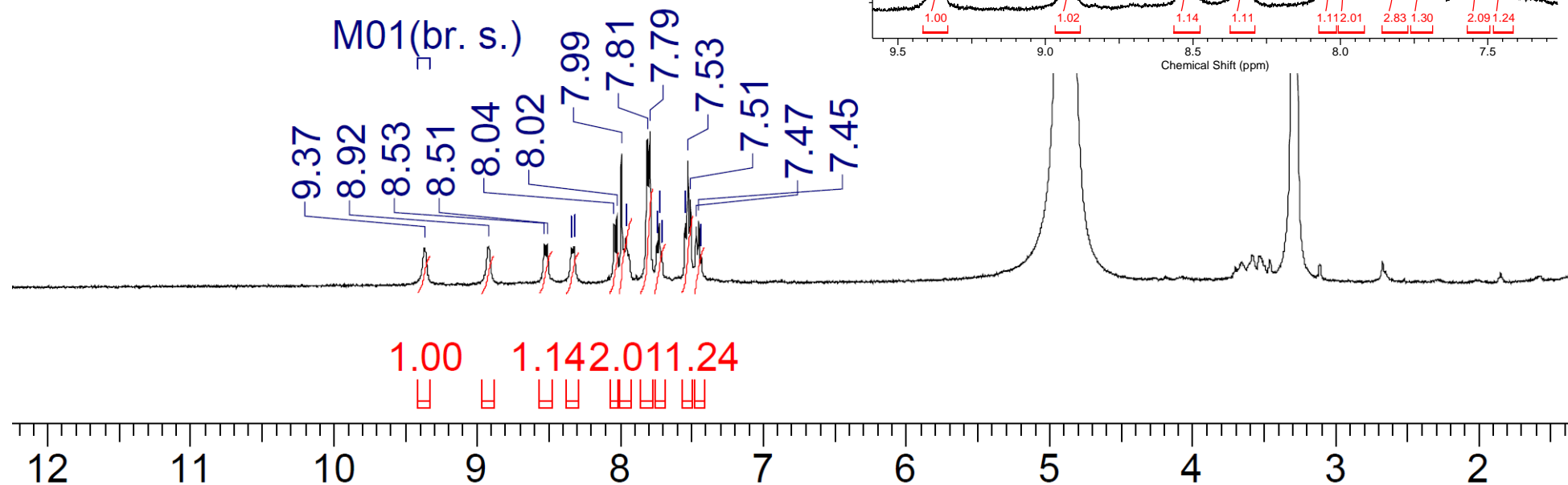
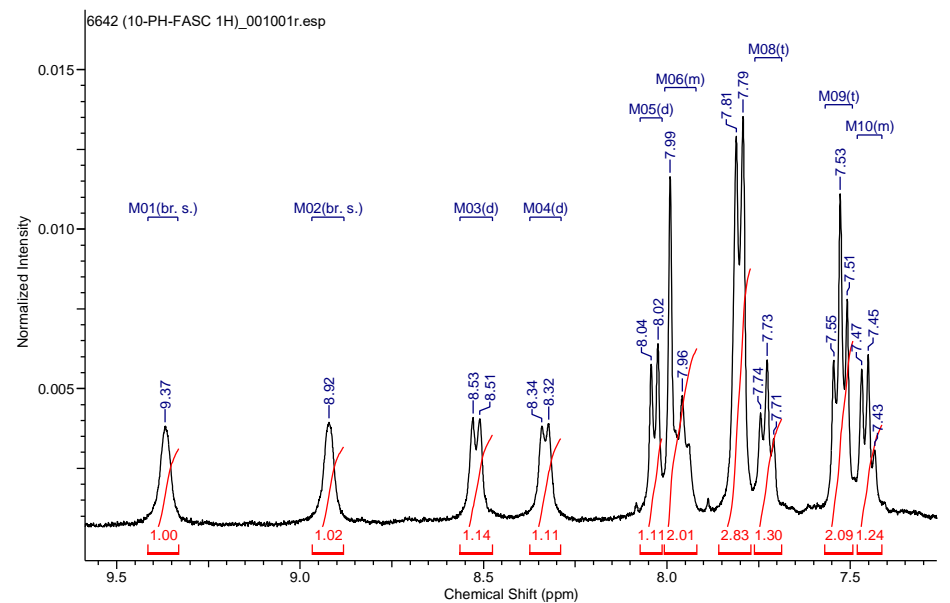
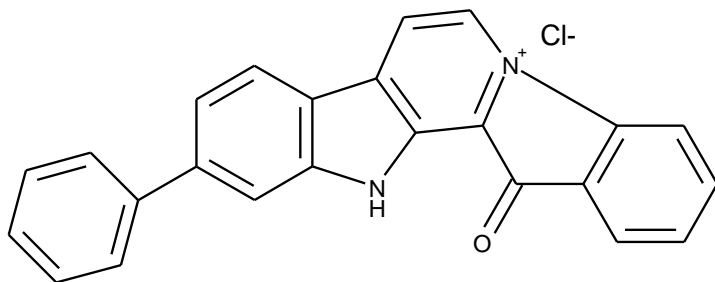
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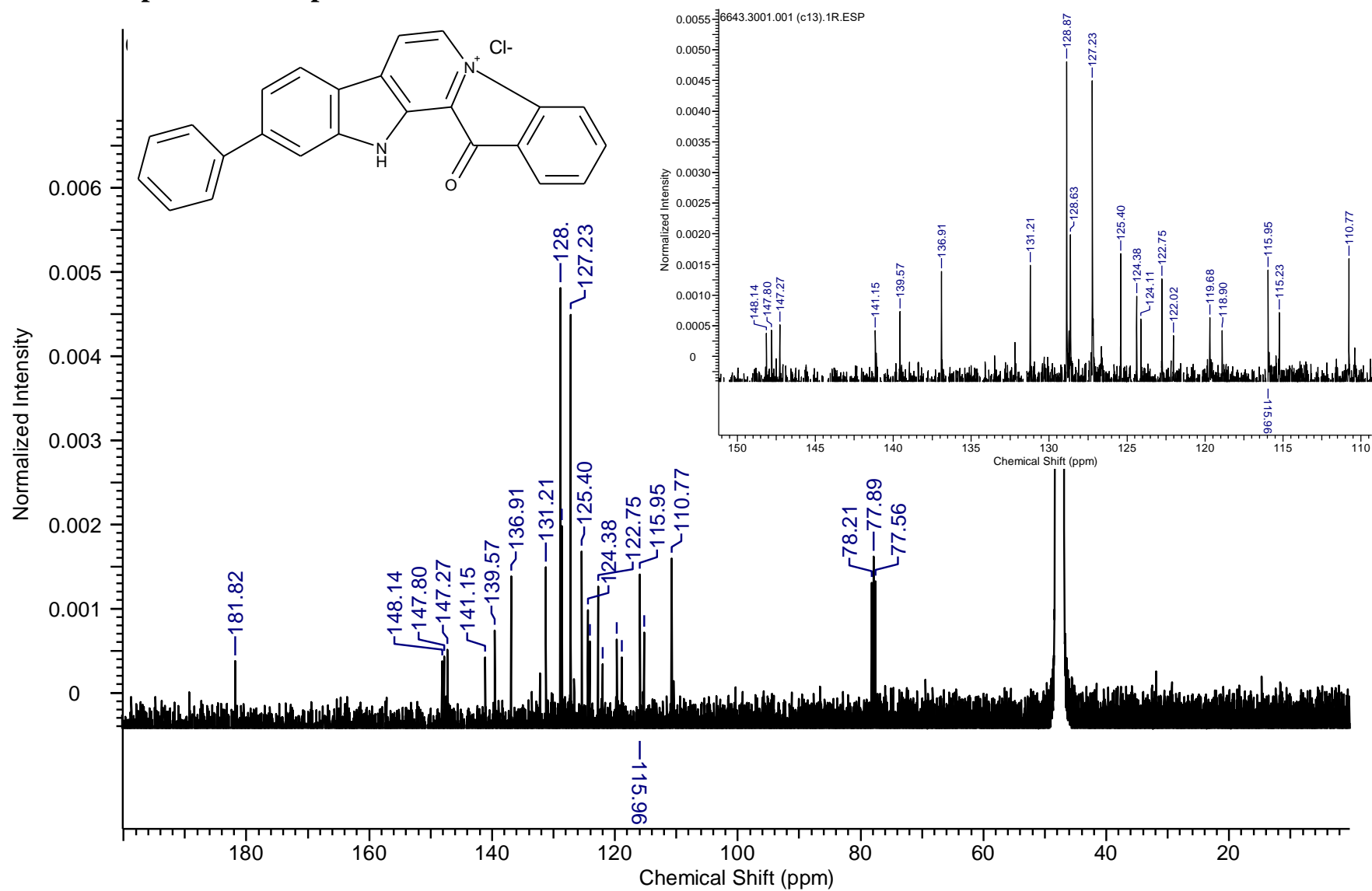
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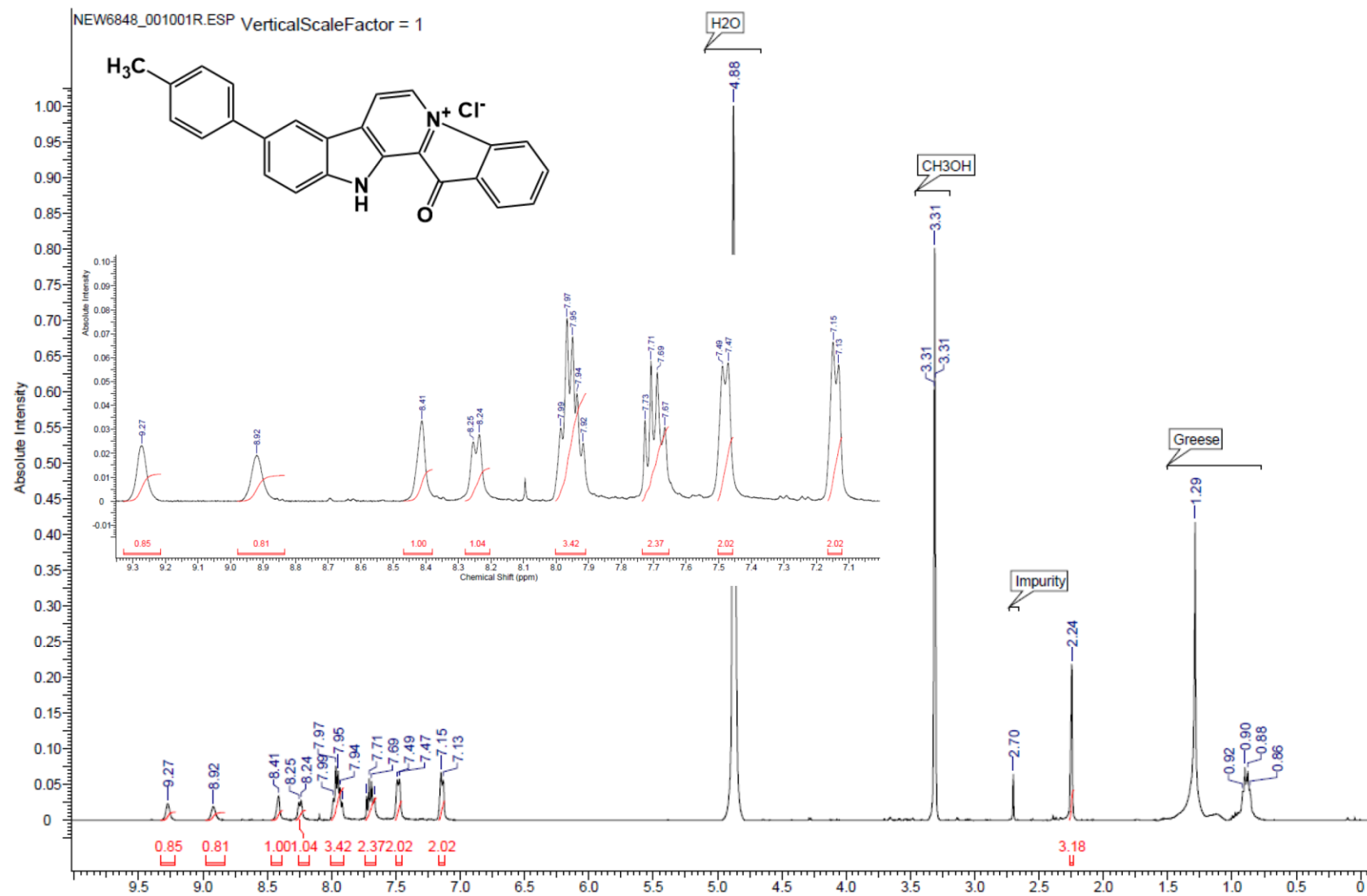
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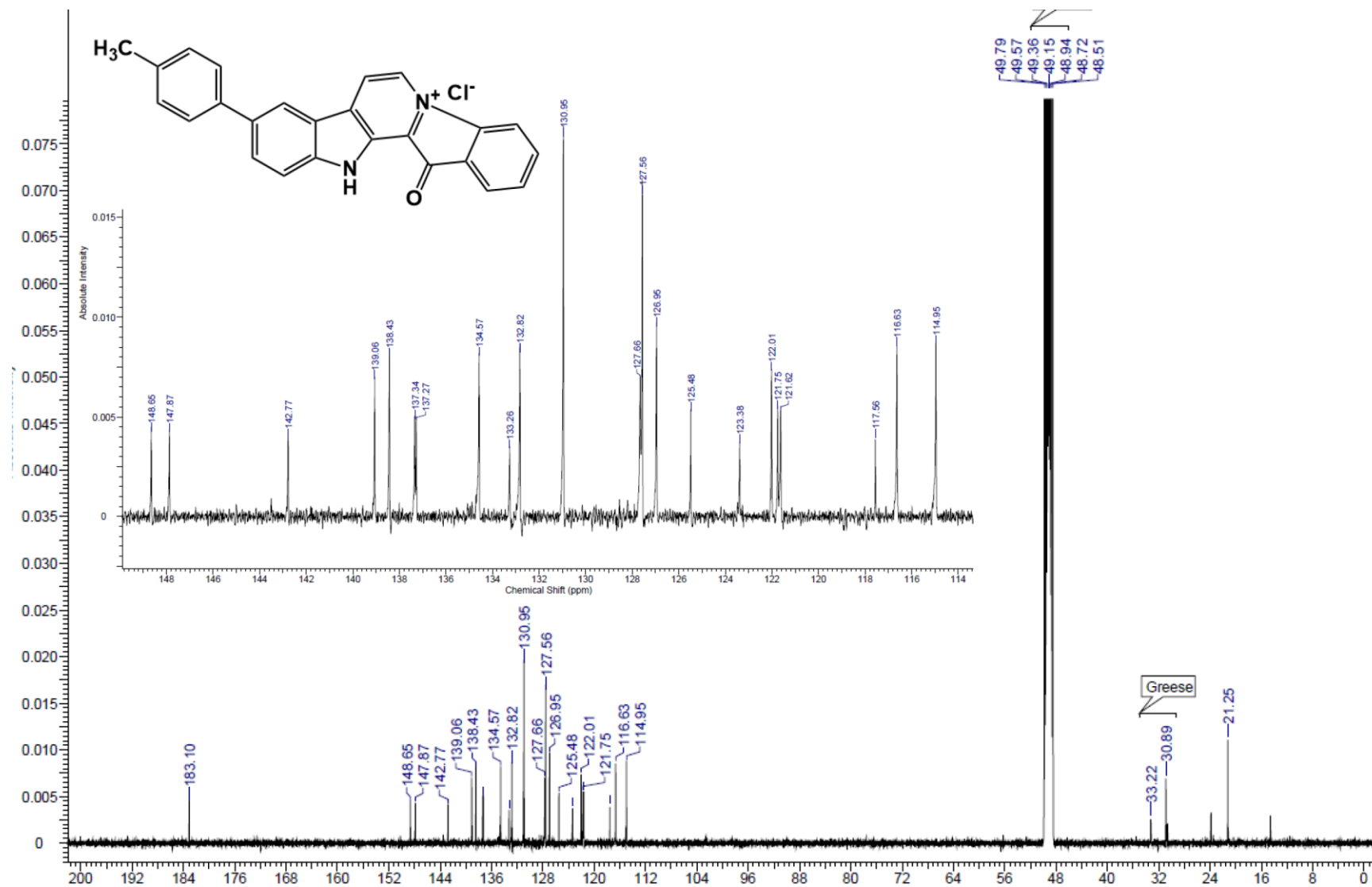
¹³C NMR spectra of compound 16



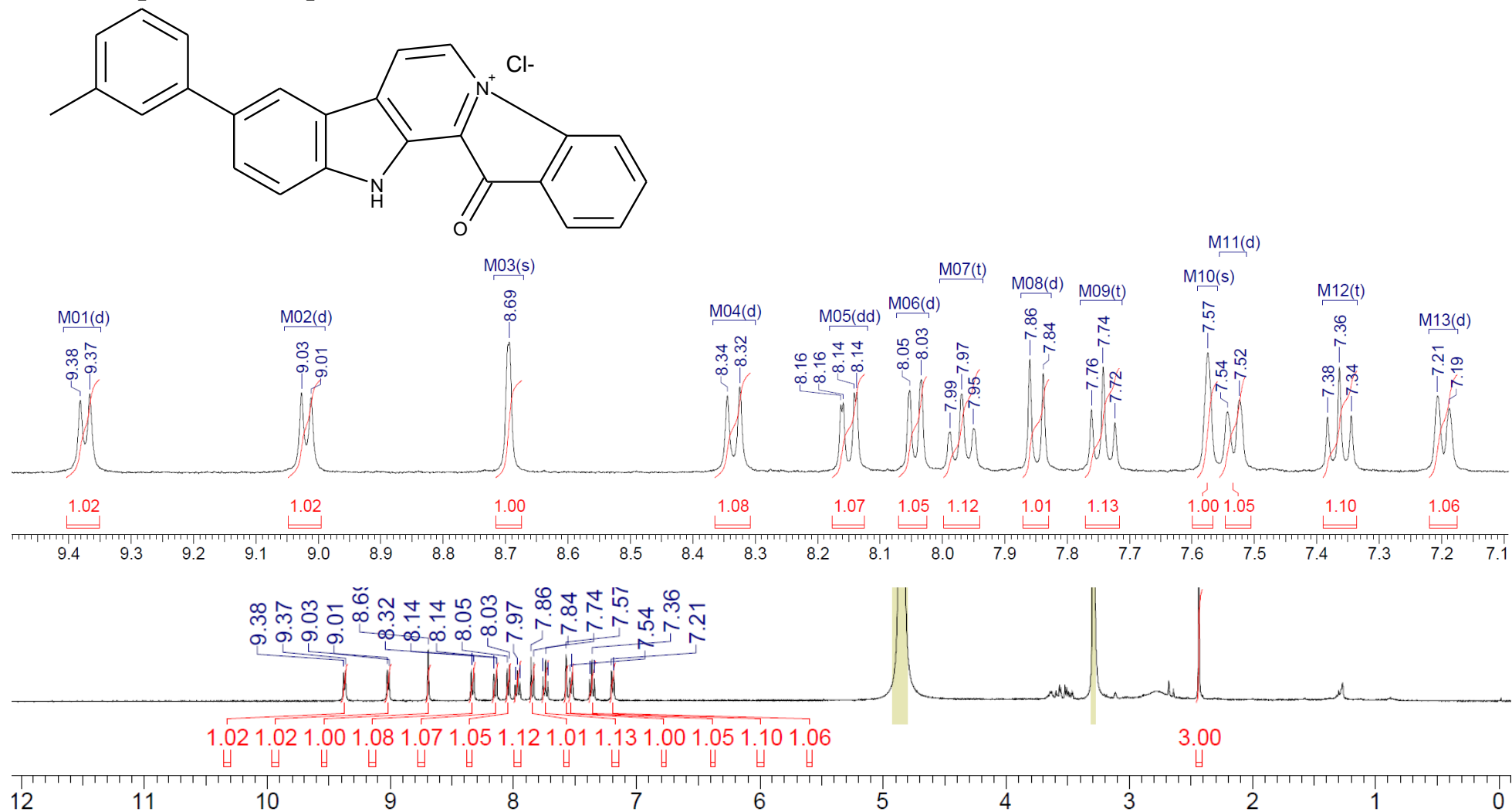
¹H NMR spectra of compound 25a



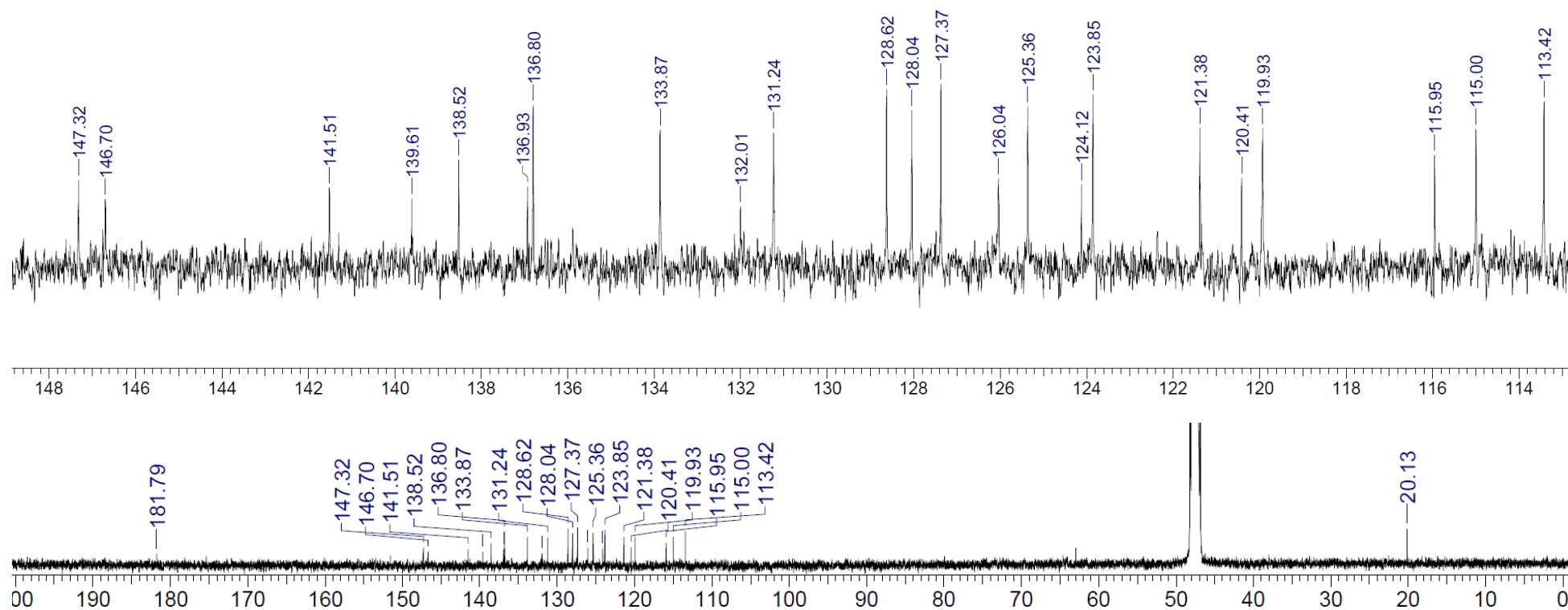
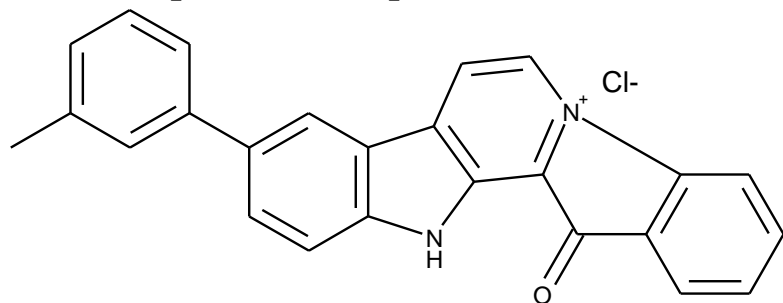
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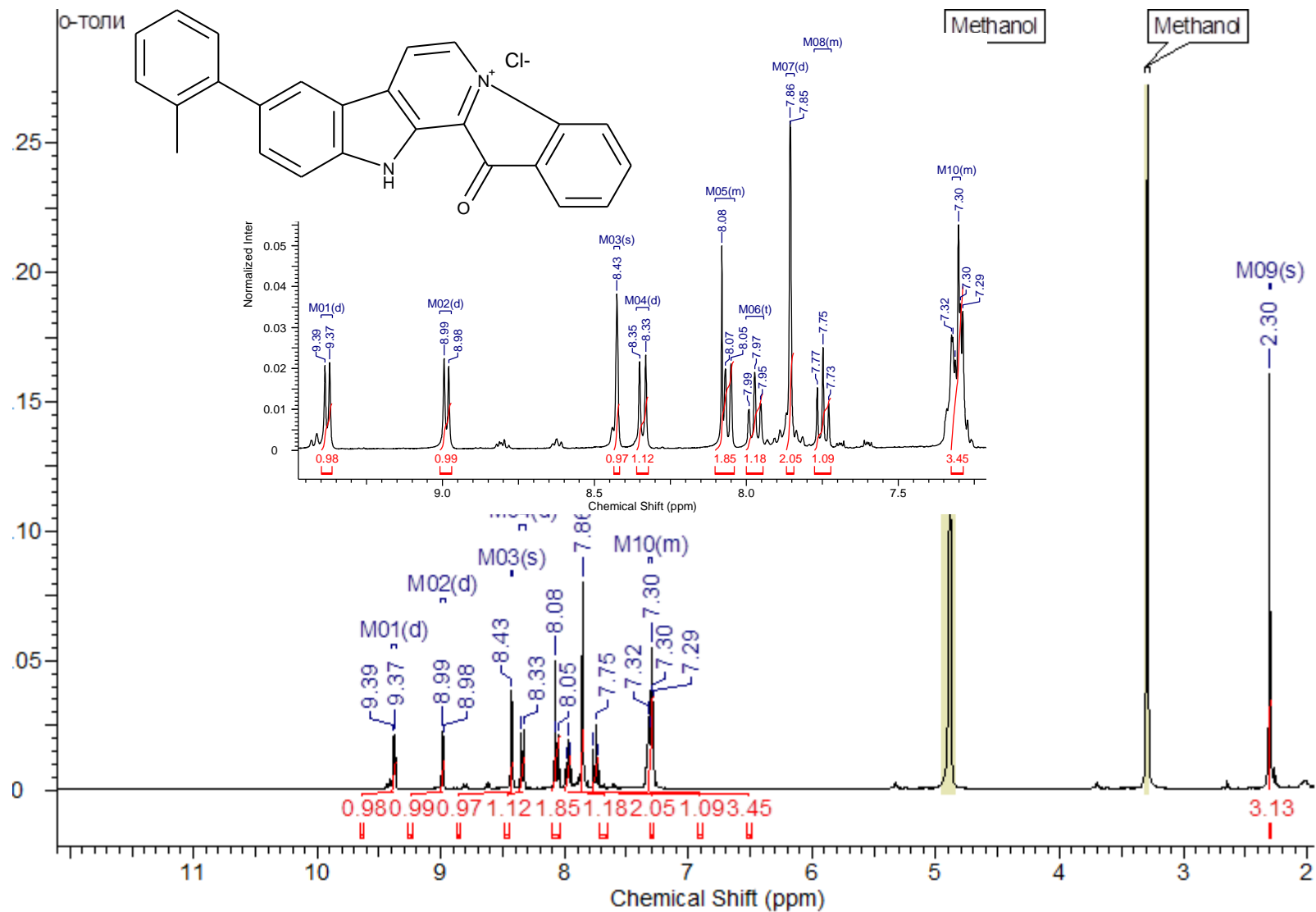
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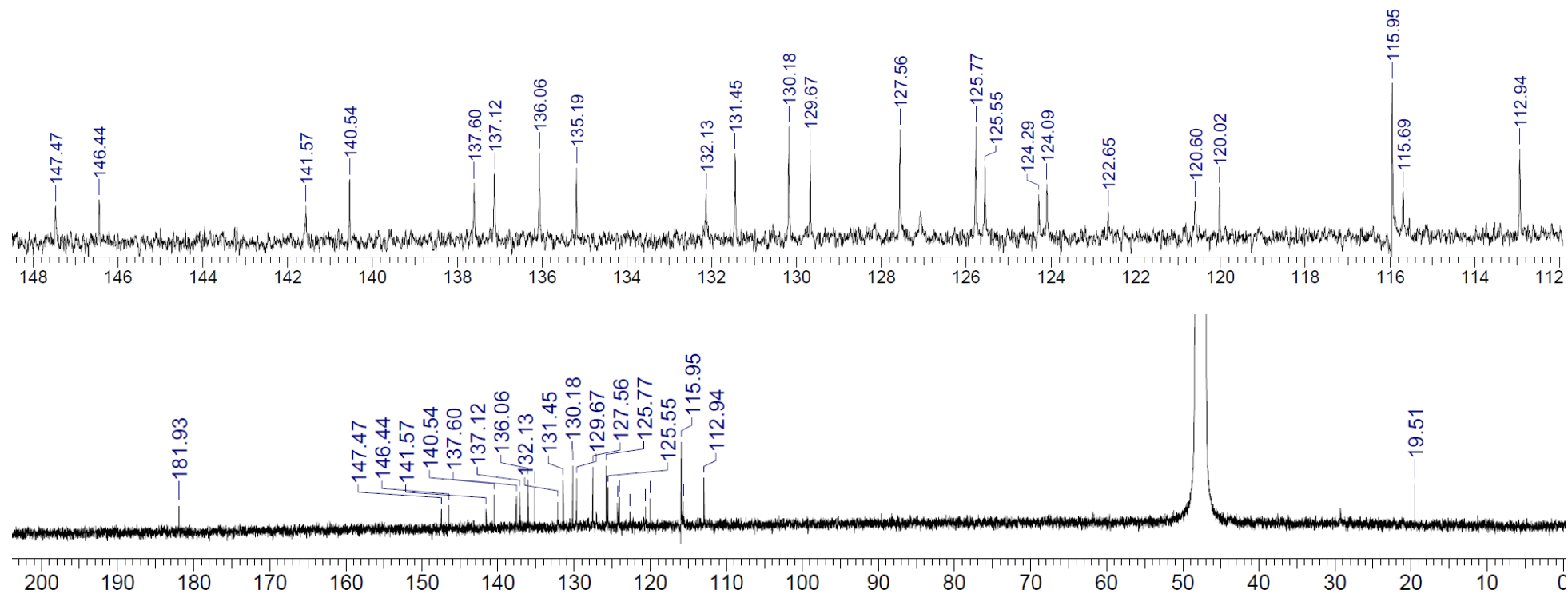
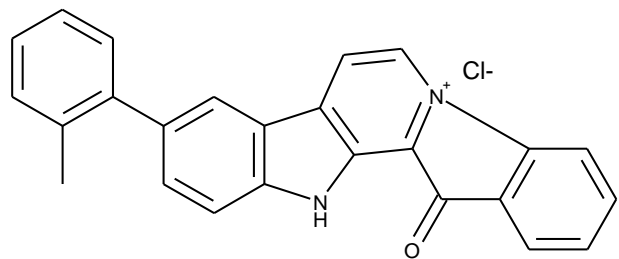
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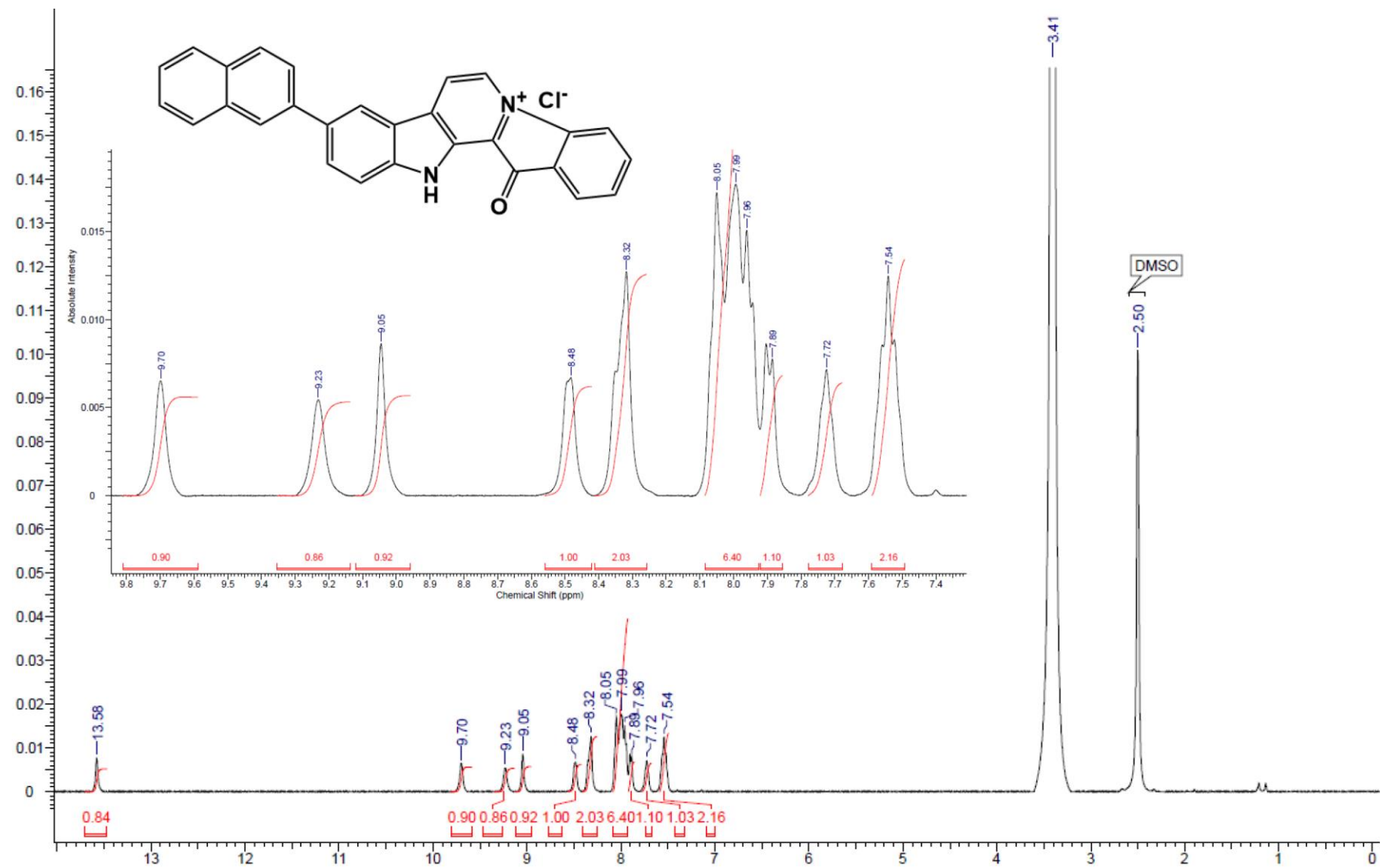
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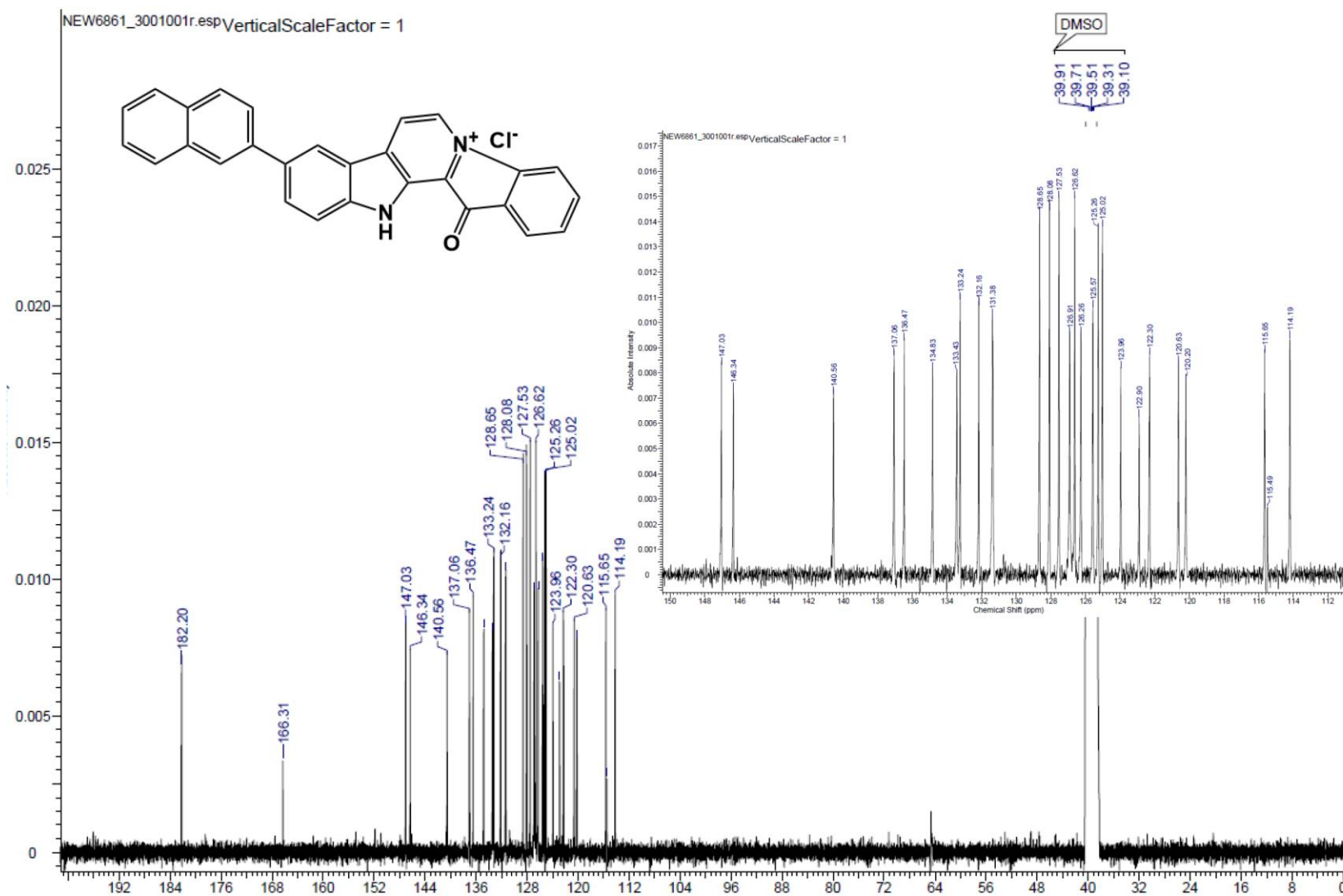
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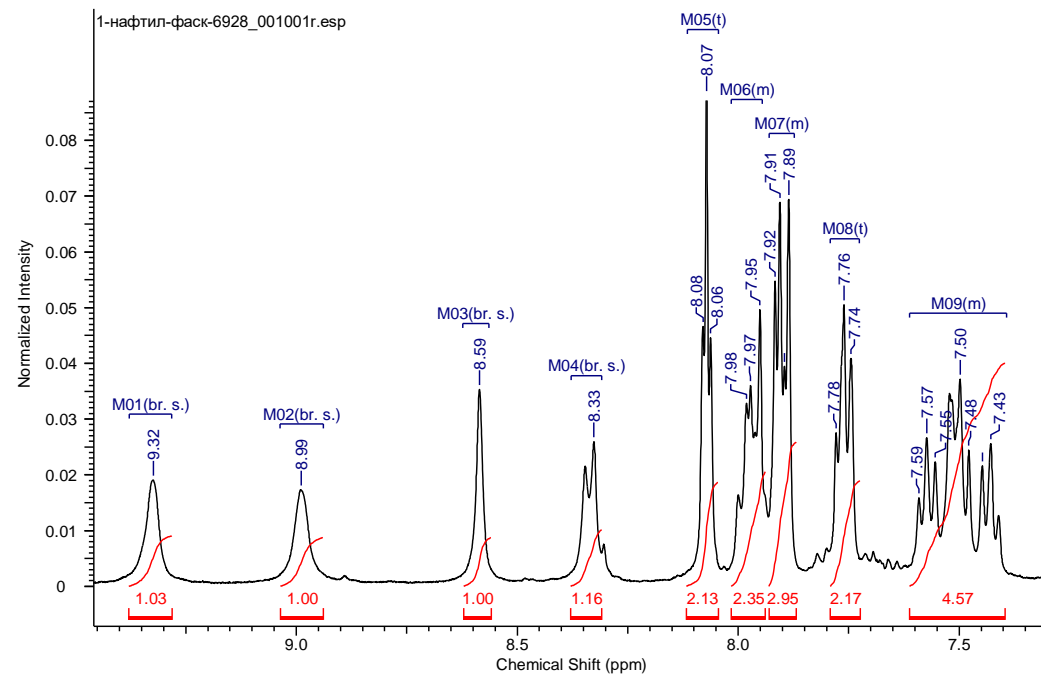
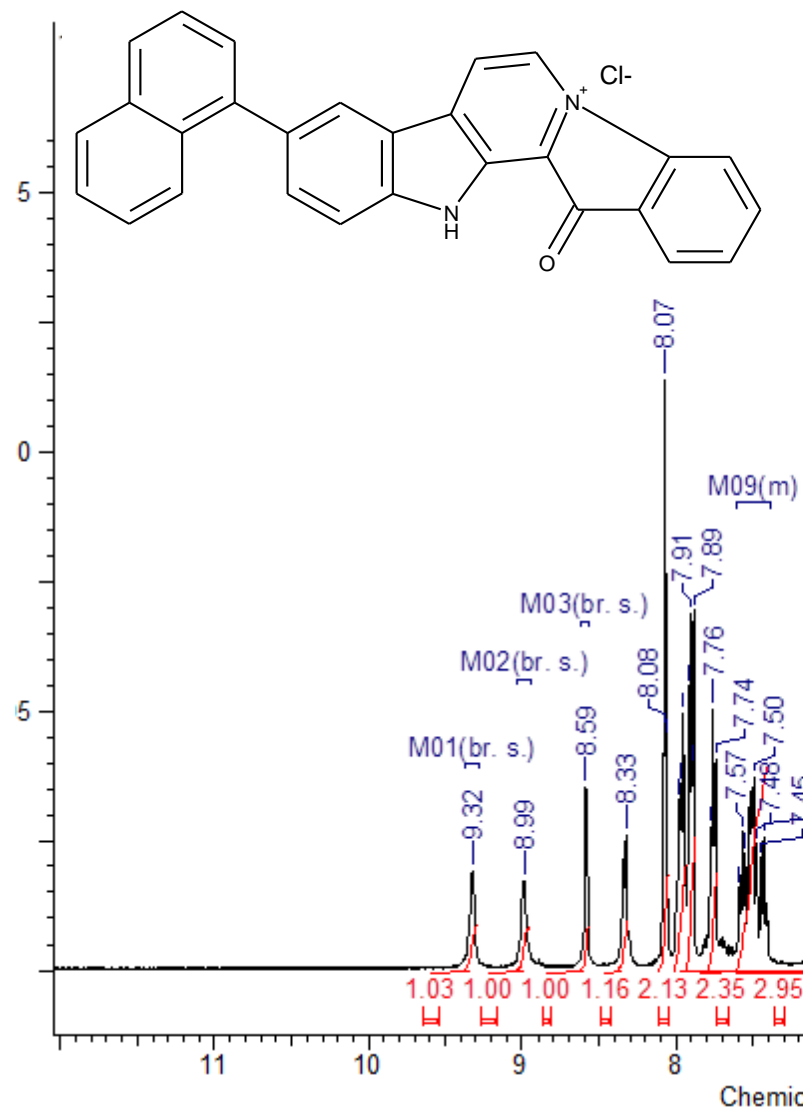
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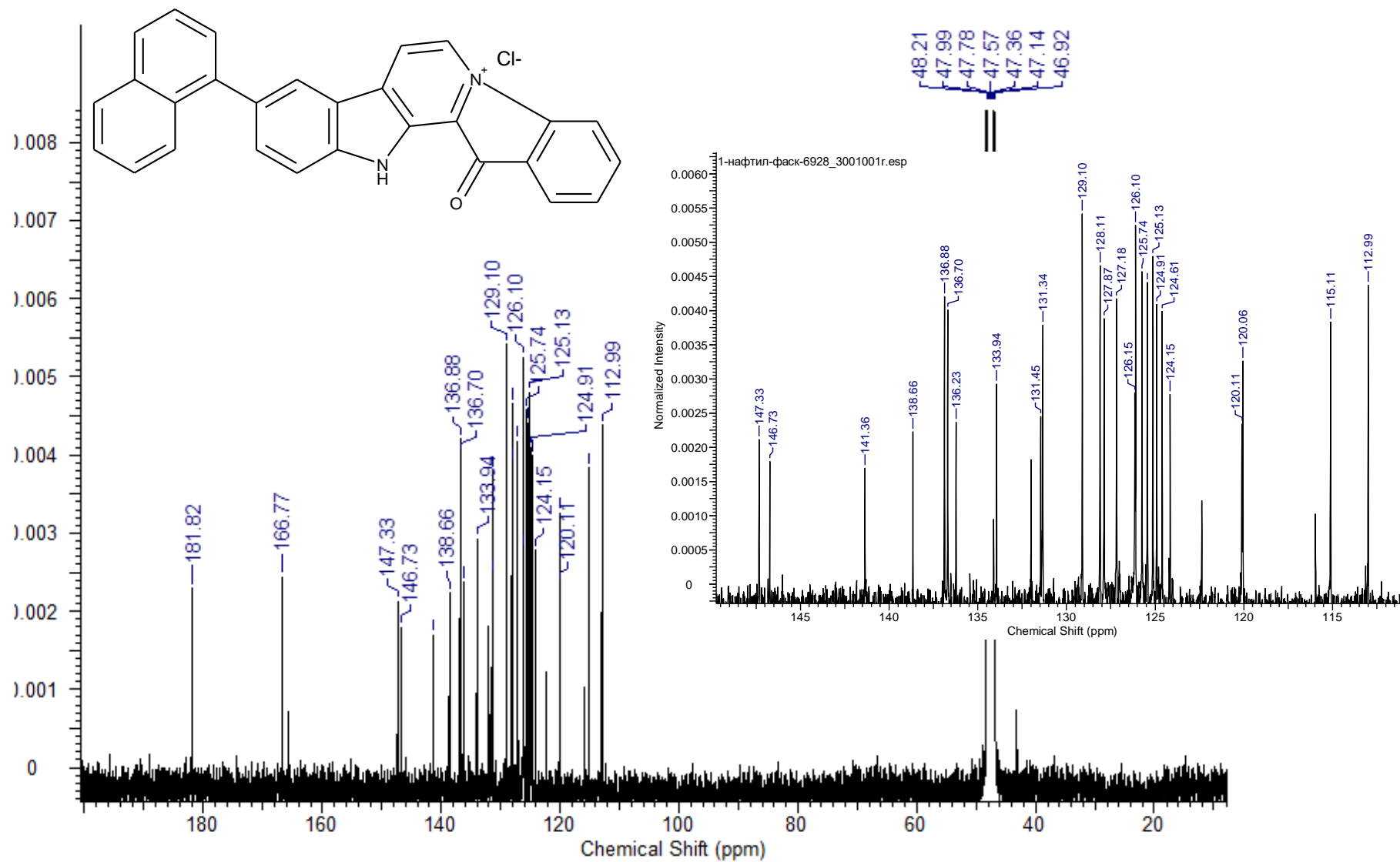
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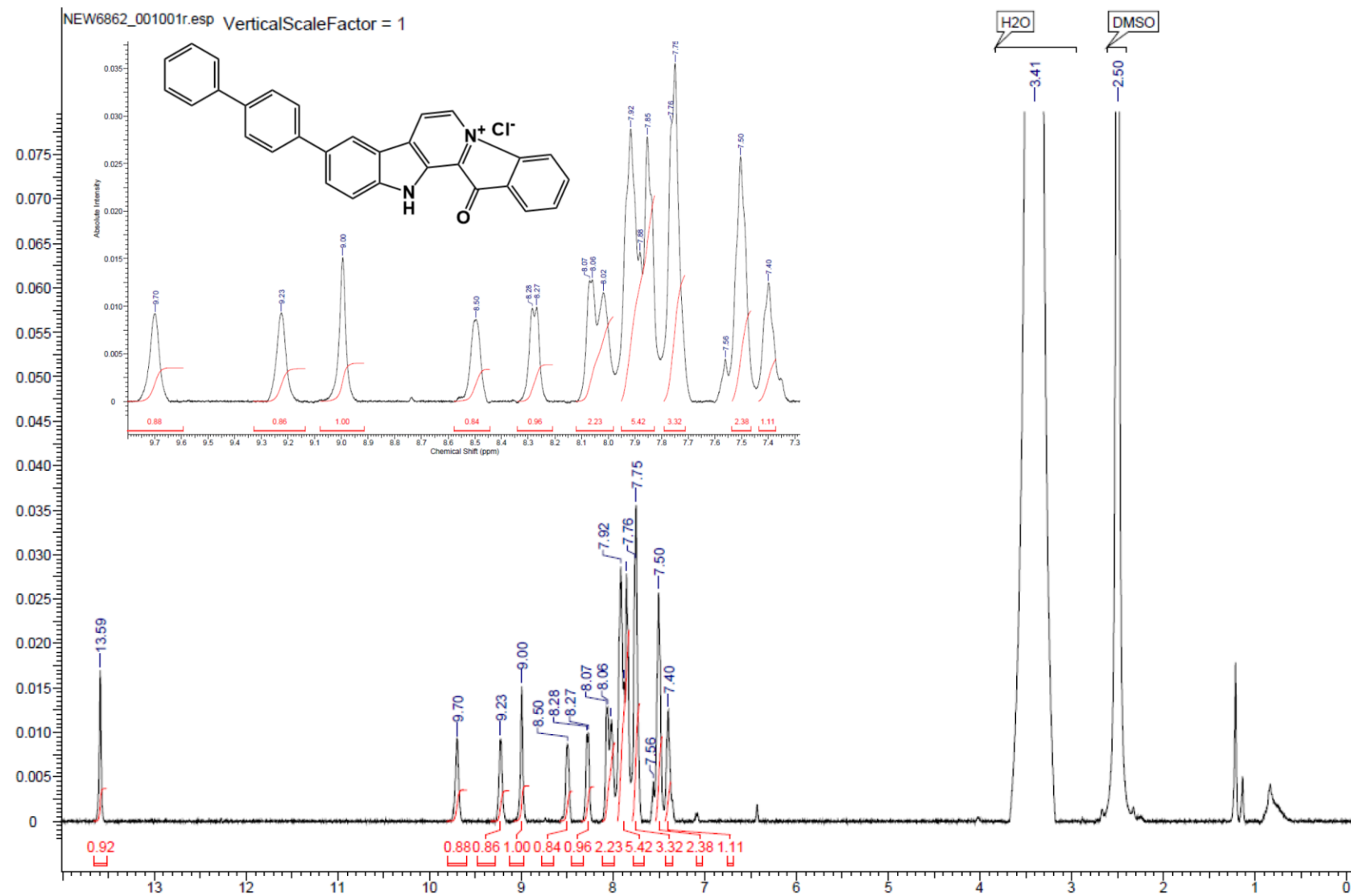
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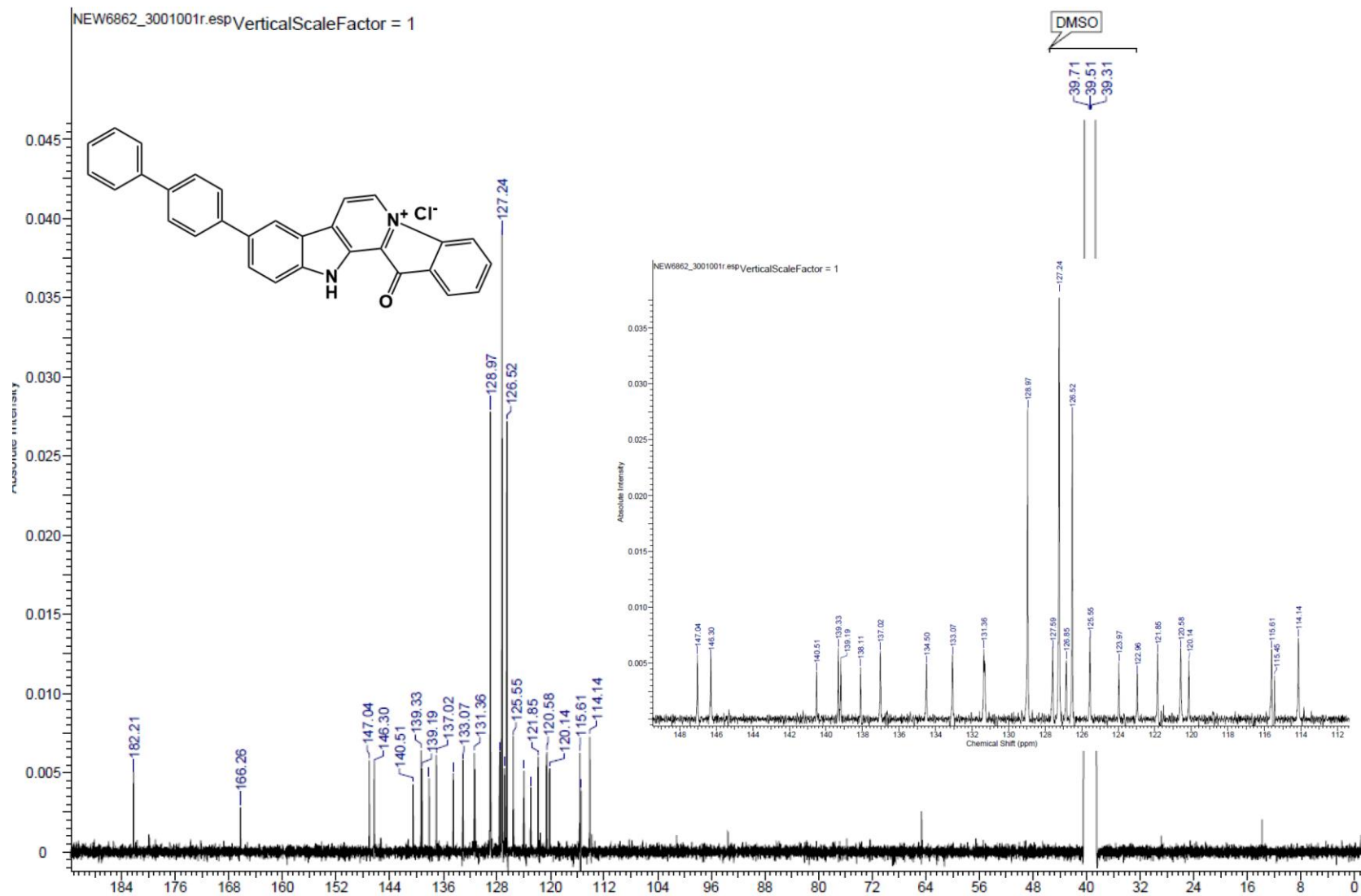
¹³C NMR spectra of compound 25e



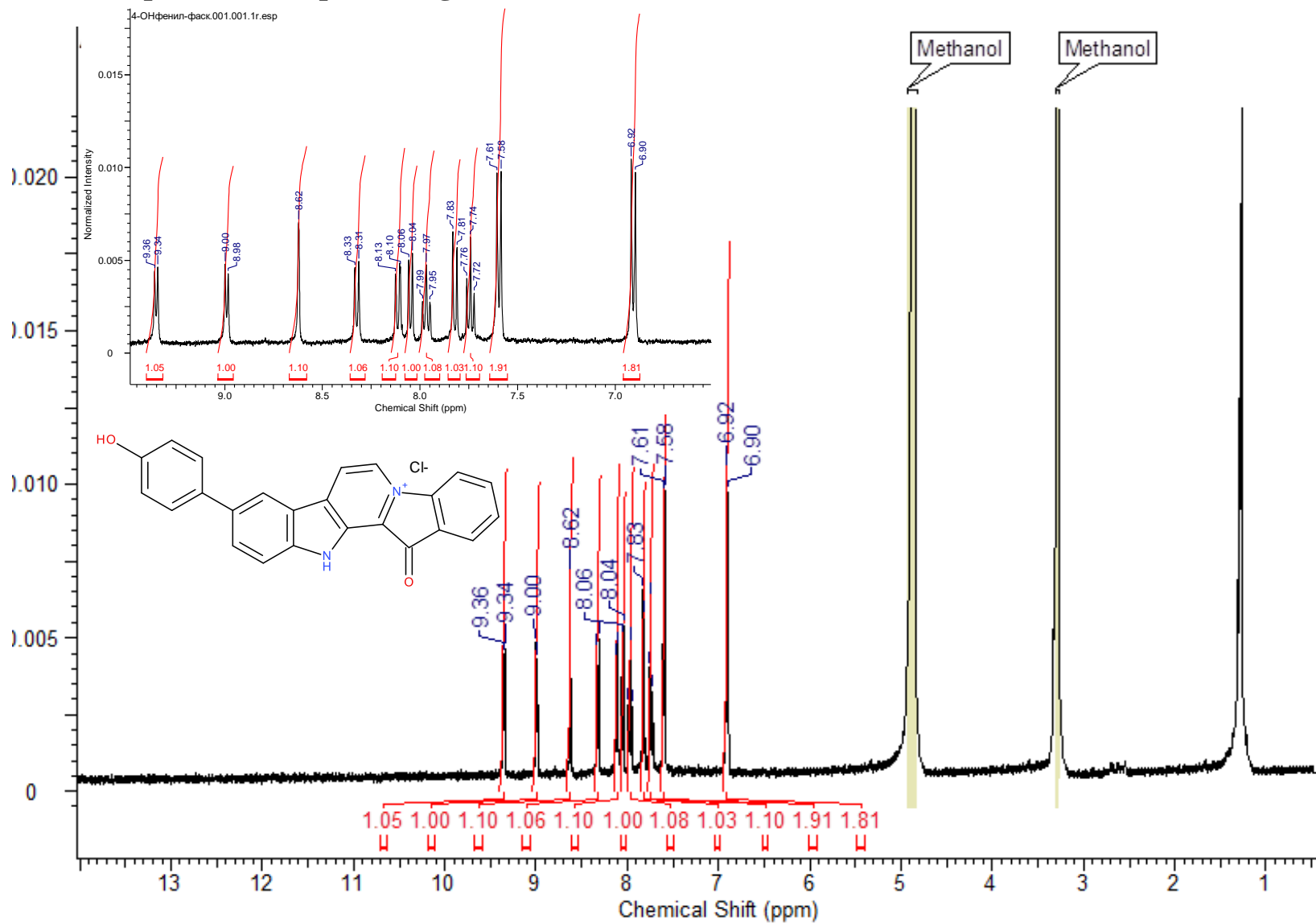
¹H NMR spectra of compound 25f



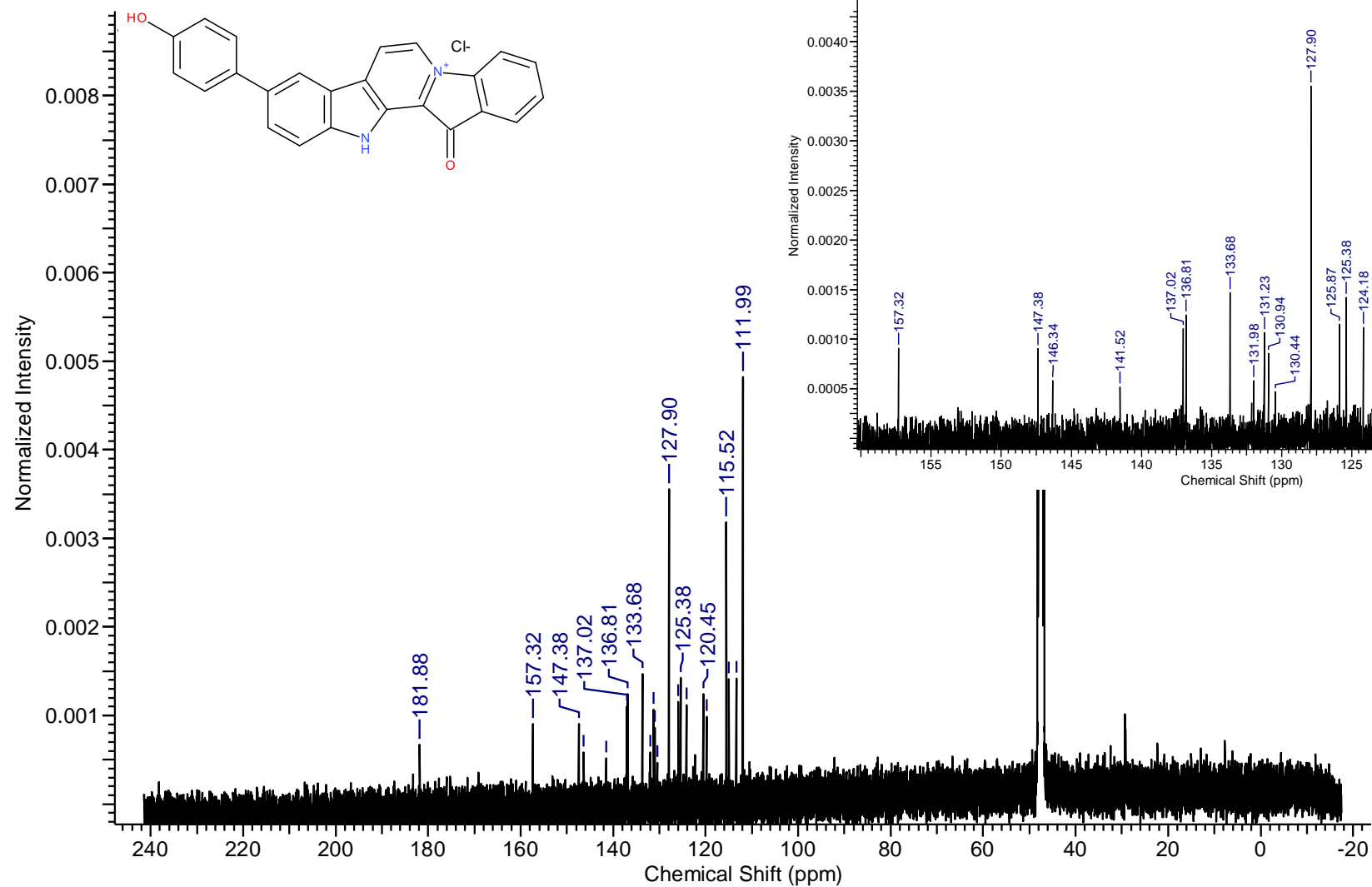
¹³C NMR spectra of compound 25f



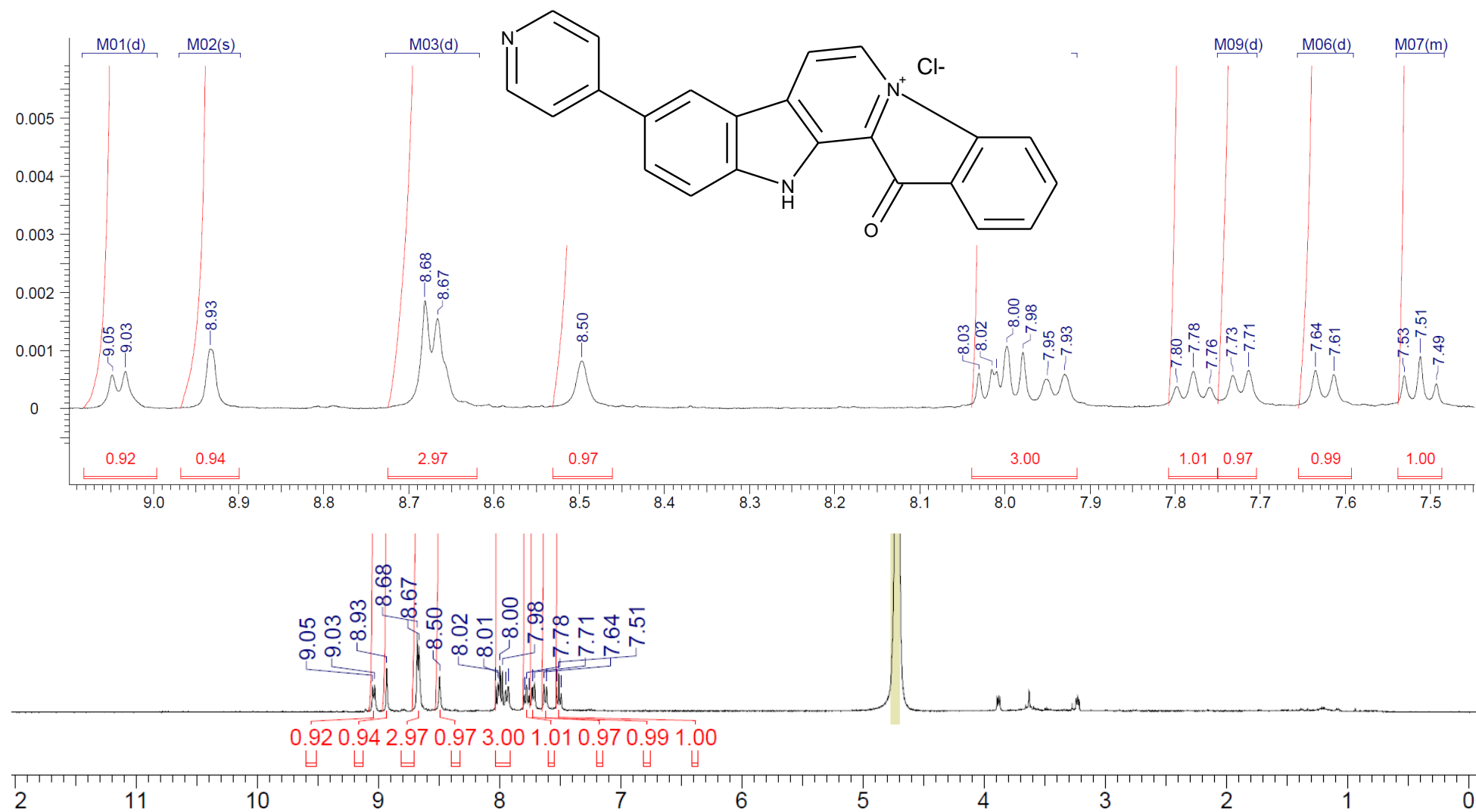
¹H NMR spectra of compound 25g



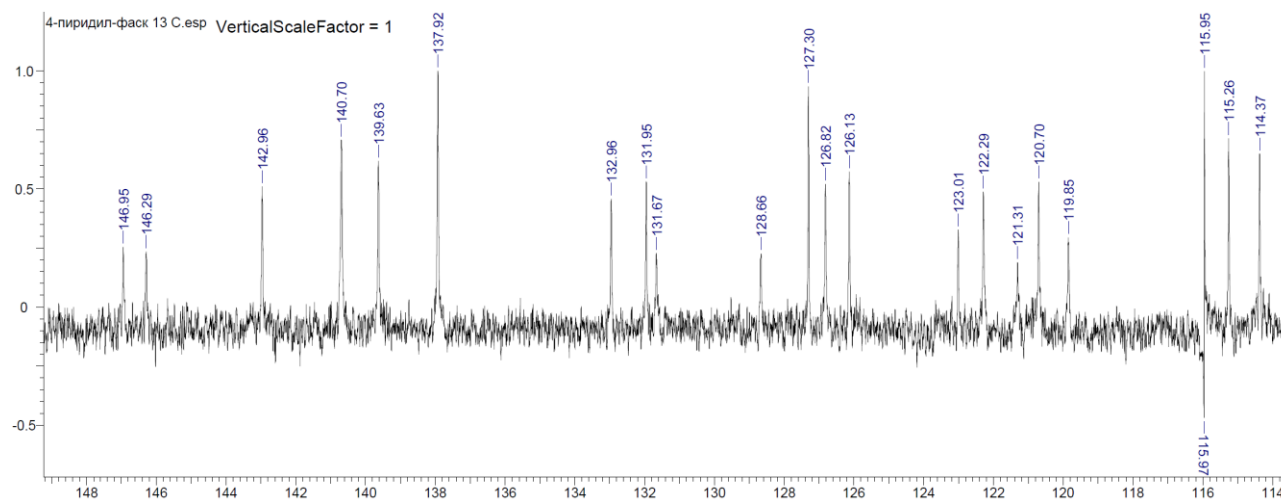
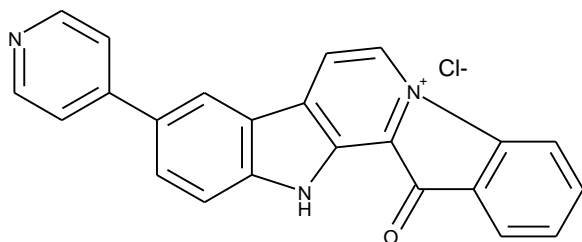
¹³C NMR spectra of compound 25g



¹H NMR spectra of compound 25h



¹³C NMR spectra of compound 25h



VerticalScaleFactor = 1

