Supporting Information for

I_2-mediated cascade reaction of 2′-bromoacetophenones with benzohydrazides/benzamides leading to quinazolino[3,2-*b*]cinnoline or tryptanthrin derivatives

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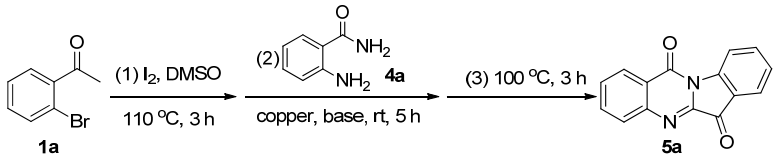
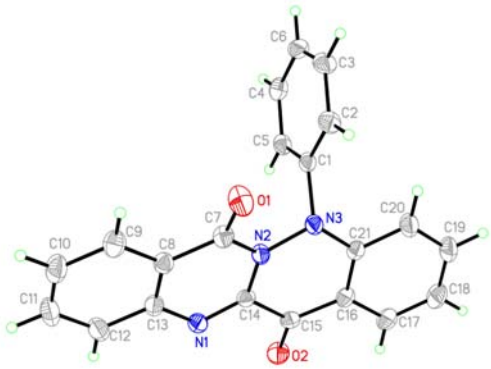
I. Table S1. Screening the Reaction Conditions for the Synthesis of 5a[a]

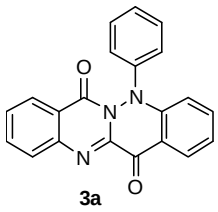


entry	I_2 (equiv.)	**1a** (equiv.)	catalyst (equiv.)	base (equiv.)	yield (%)[b]
1	1.5	1.5	–	K_2CO_3 (4.0)	nd
2	1.5	1.5	CuI (0.2)	K_2CO_3 (4.0)	60
3	1.5	1.5	CuCl (0.2)	K_2CO_3 (4.0)	63
4	1.5	1.5	CuBr (0.2)	K_2CO_3 (4.0)	71
5	1.5	1.5	CuBr (0.2)	K_3PO_4 (4.0)	64
6	1.5	1.5	CuBr (0.2)	Cs_2CO_3 (4.0)	44
7	1.5	1.5	CuBr (0.1)	K_2CO_3 (4.0)	51
8	1.5	1.5	CuBr (0.2)	K_2CO_3 (3.0)	59
9	1.0	1.0	CuBr (0.2)	K_2CO_3 (4.0)	50

[a]The reactions were run with (1) **1a**, I_2, DMSO, 110 °C, 3 h; (2) **4a** (0.4 mmol), catalyst, base, rt (5 h)~100 °C (3 h). [b]Isolated yield; nd = not detected.

II. X-ray crystal structure and data of 3a





3a

Bond precision: C-C = 0.0043 A Wavelength=0.71073

Cell: a=7.617(12) b=10.617(17) c=11.452(18)
alpha=64.336(15) beta=72.042(17) gamma=88.506(18)
Temperature: 295 K

	Calculated	Reported
Volume	788(2)	788(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C21 H13 N3 O2	C21 H13 N3 O2
Sum formula	C21 H13 N3 O2	C21 H13 N3 O2
Mr	339.34	339.34
Dx,g cm-3	1.430	1.430
Z	2	2
Mu (mm-1)	0.095	0.095
F000	352.0	352.0
F000'	352.15	
h,k,lmax	9,13,14	9,13,14
Nref	3587	3533
Tmin,Tmax	0.982,0.984	0.982,0.984
Tmin'	0.982	

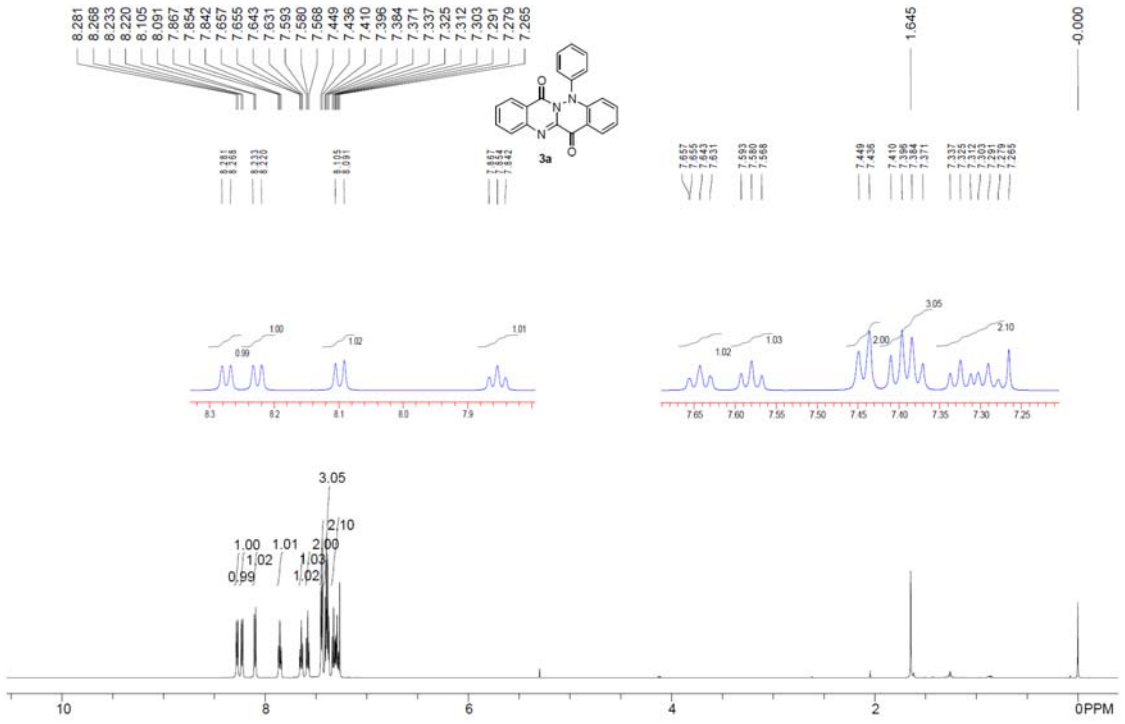
Correction method= # Reported T Limits: Tmin=0.982 Tmax=0.984
AbsCorr = MULTI-SCAN

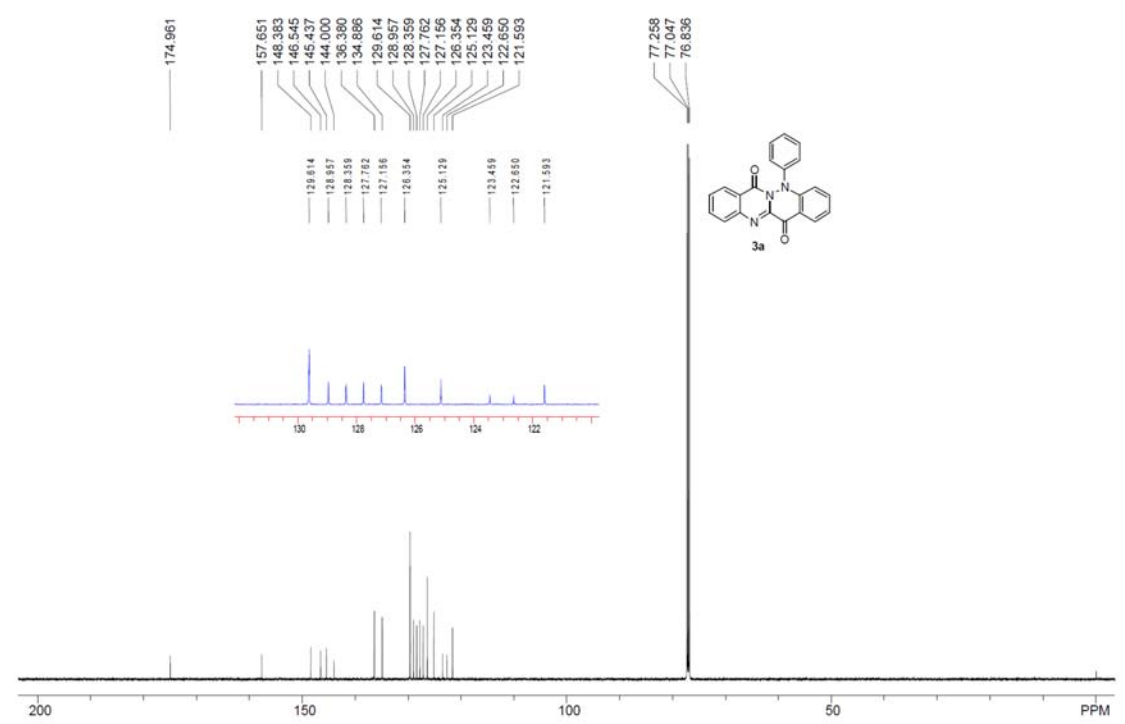
Data completeness= 0.985 Theta(max)= 27.420

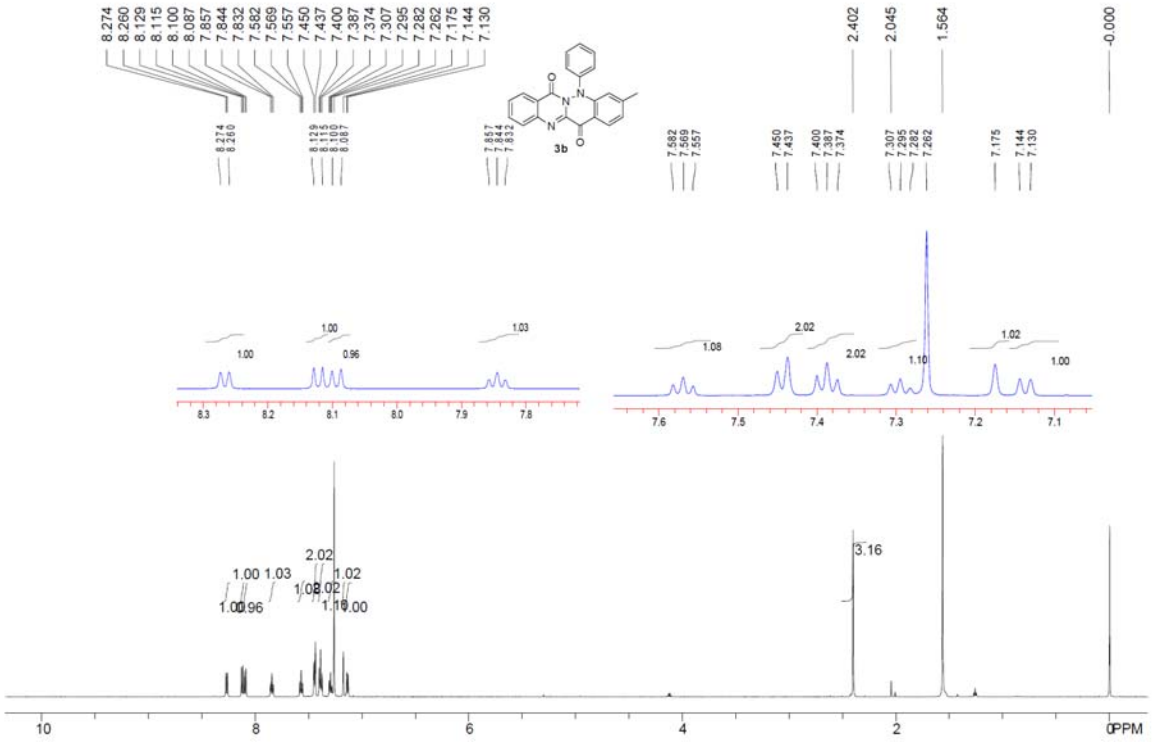
R(reflections)= 0.0682(2807) wR2(reflections)= 0.1672(3309)

S = 1.053 Npar= 235

III. ^{1}H and ^{13}C NMR Spectra of Compounds 3a-3u, 5a-5k, 6, and 7



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1.00
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1.08
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2.02
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1.02
1.00
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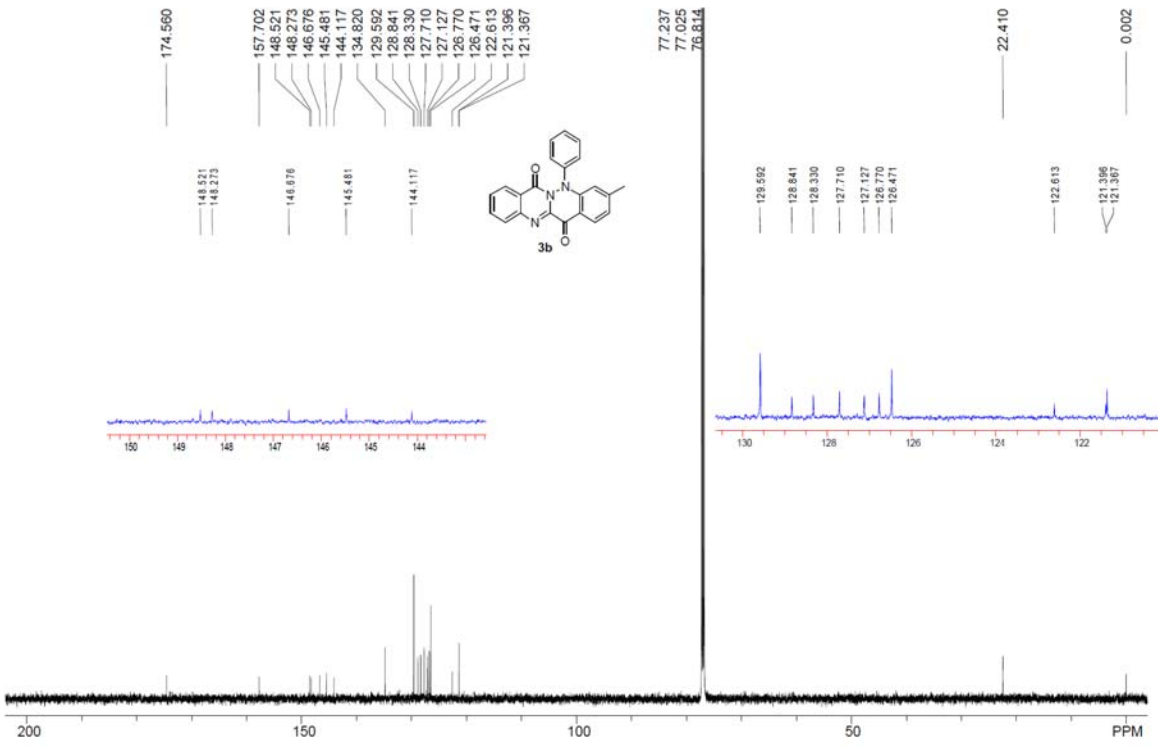
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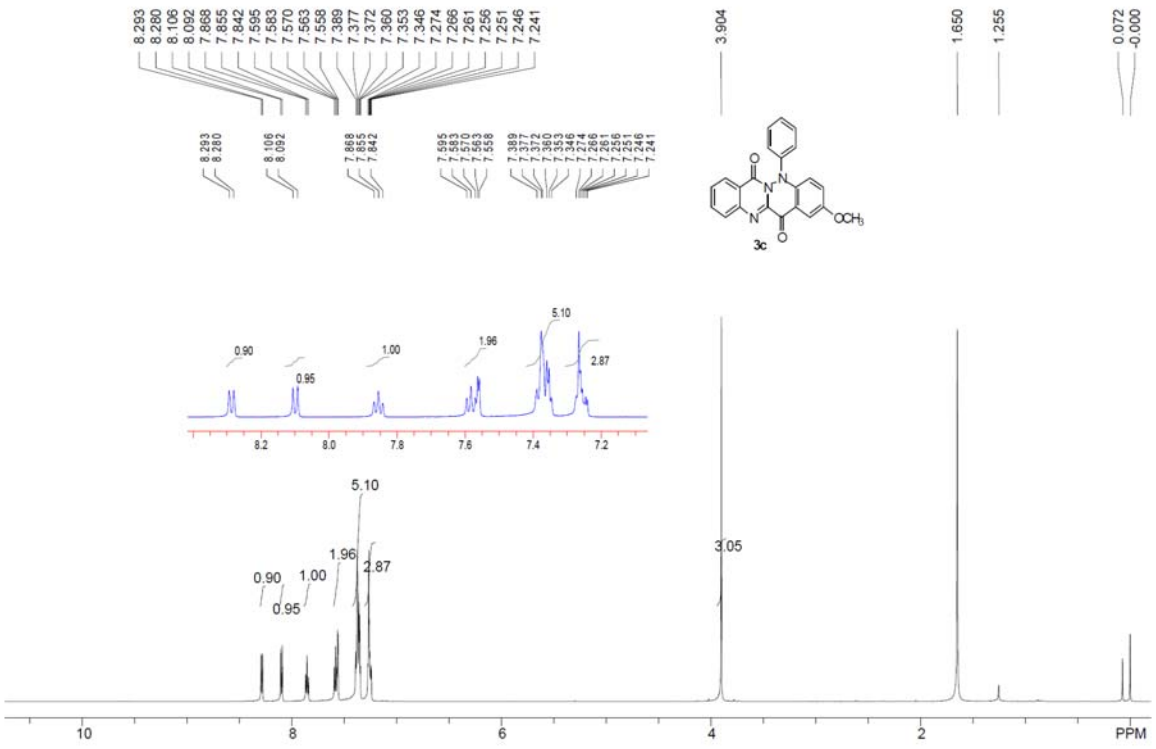
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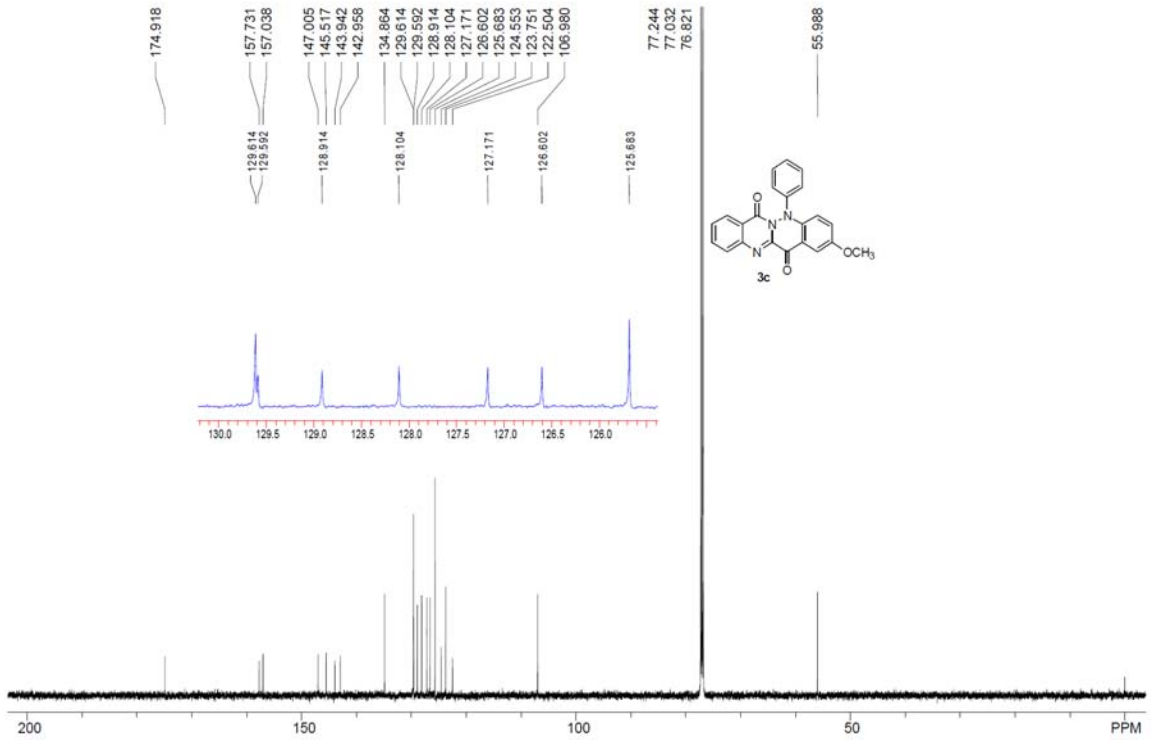
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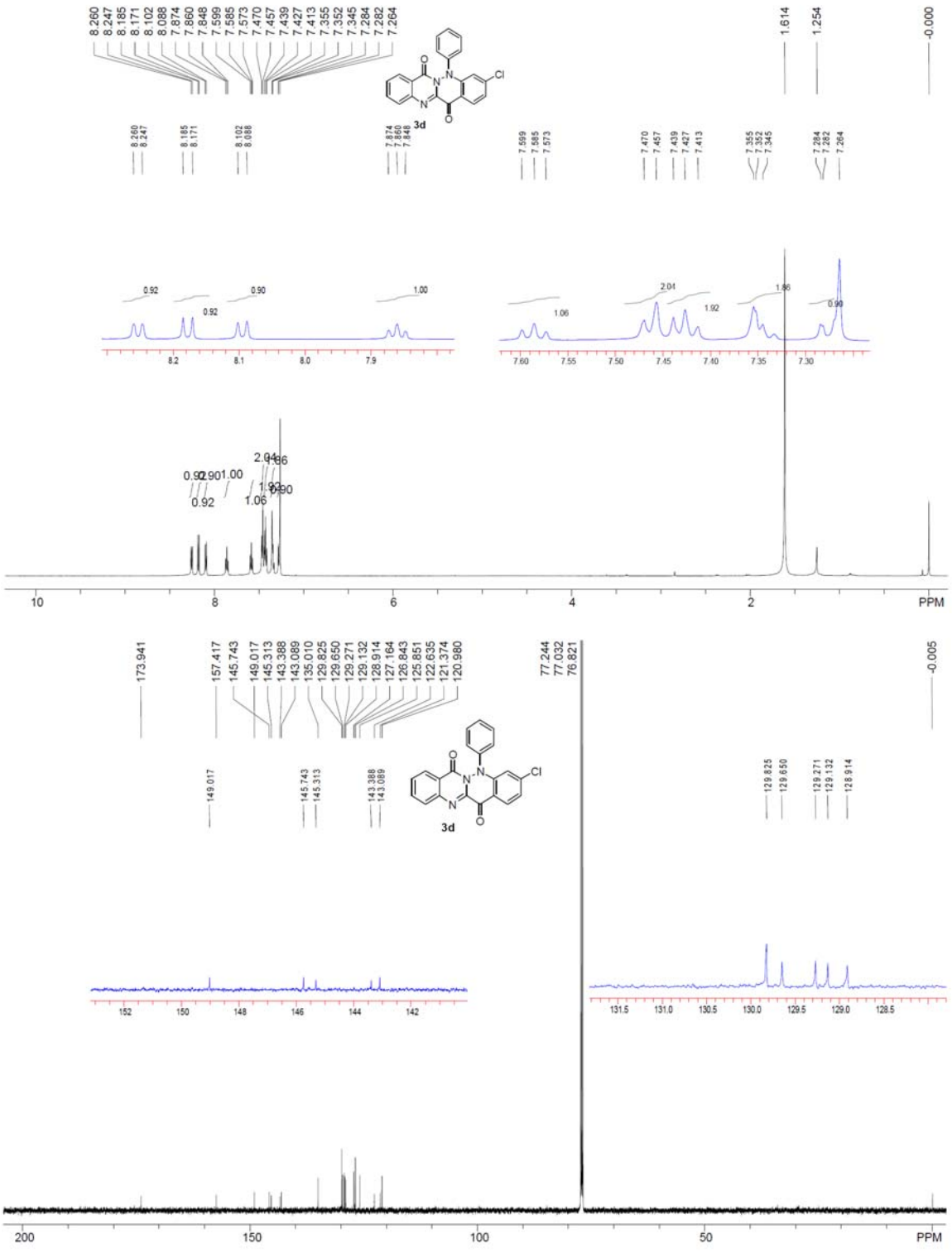
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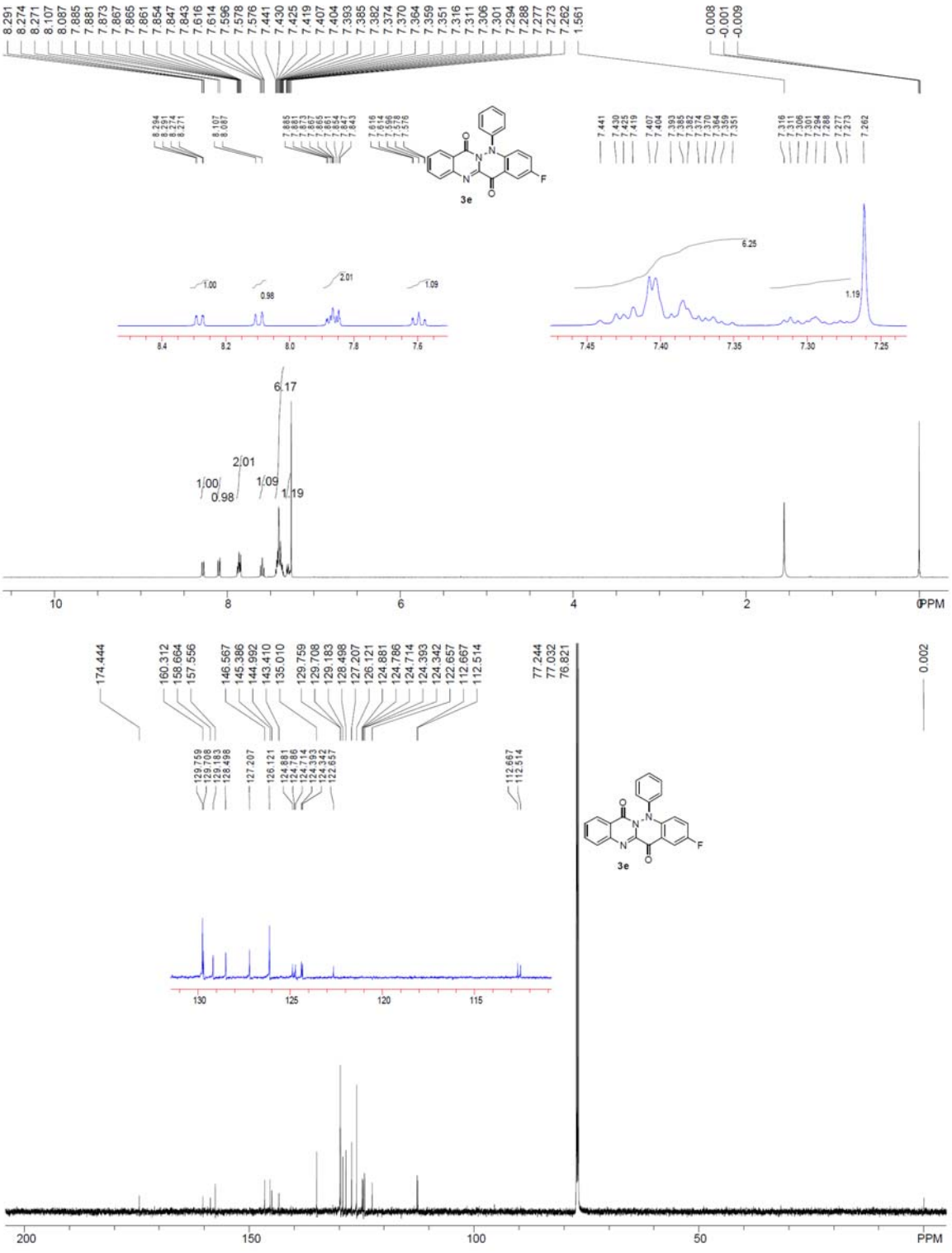
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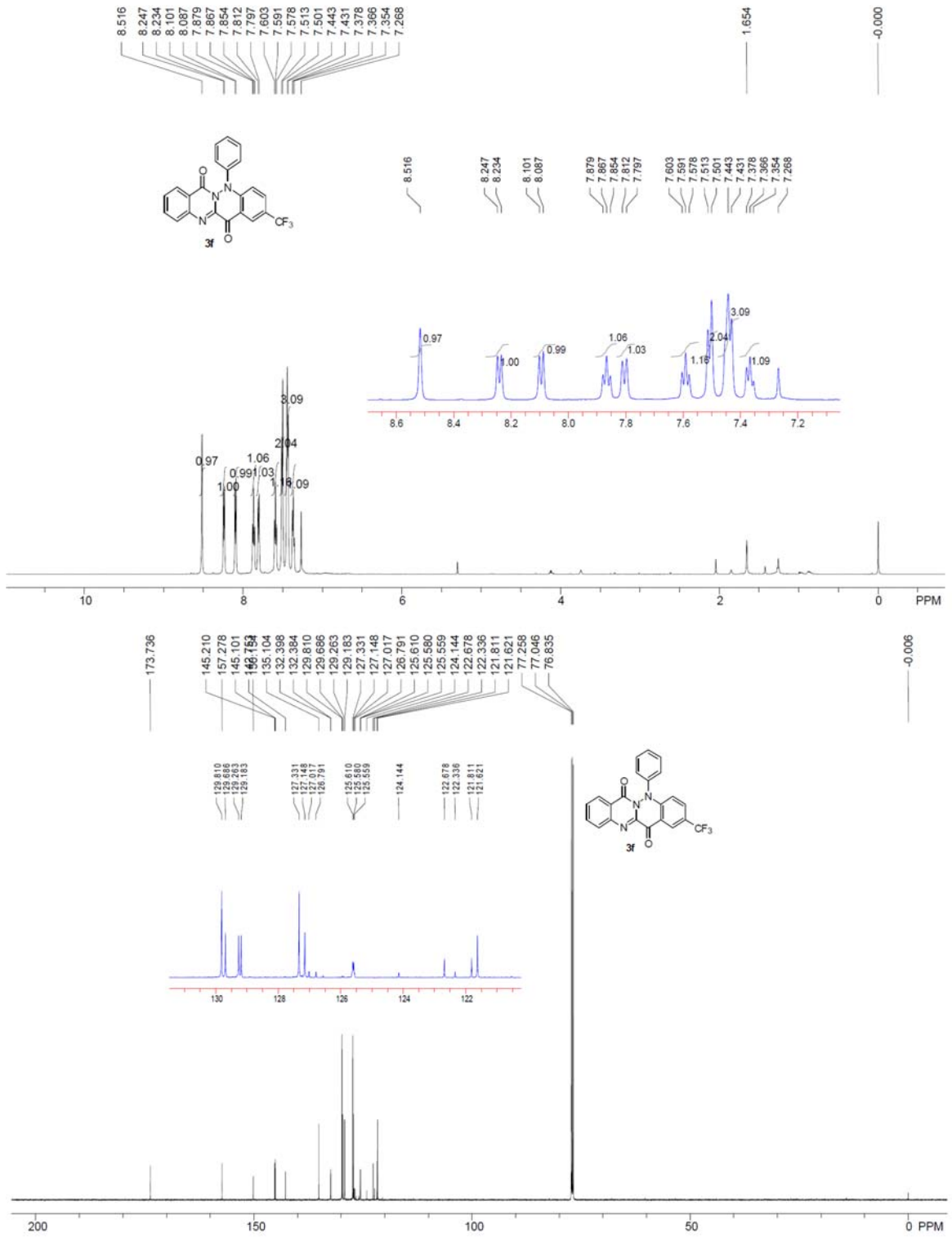
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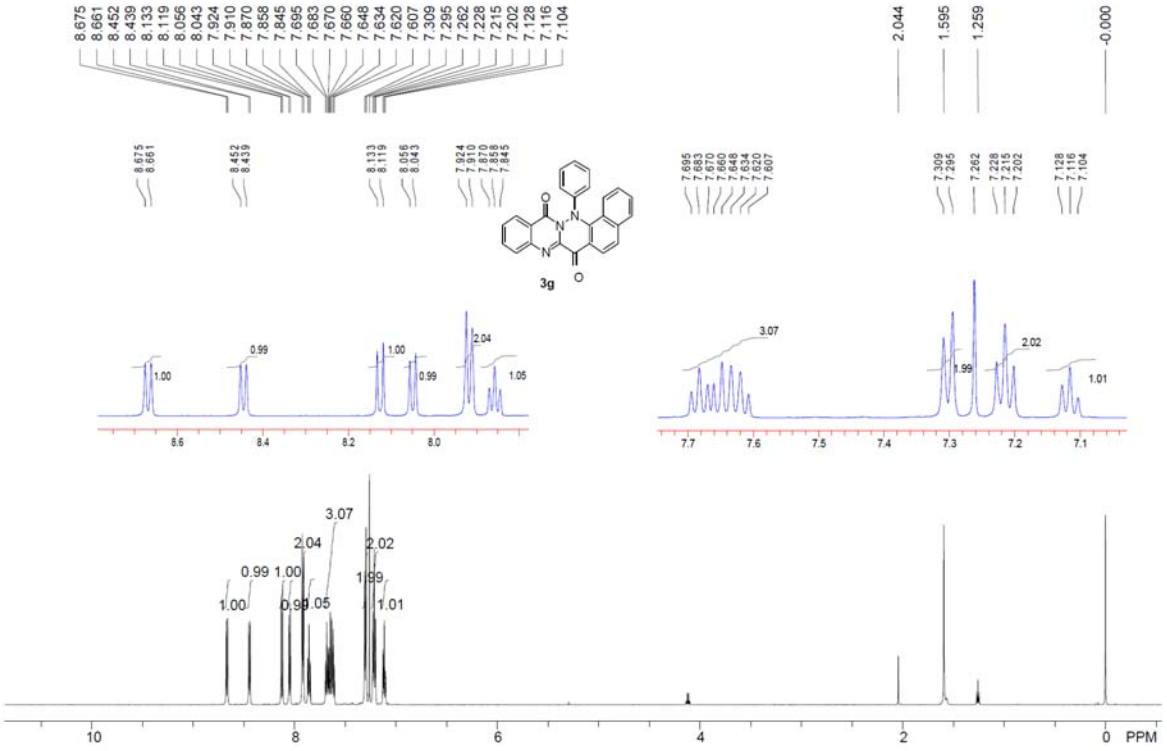
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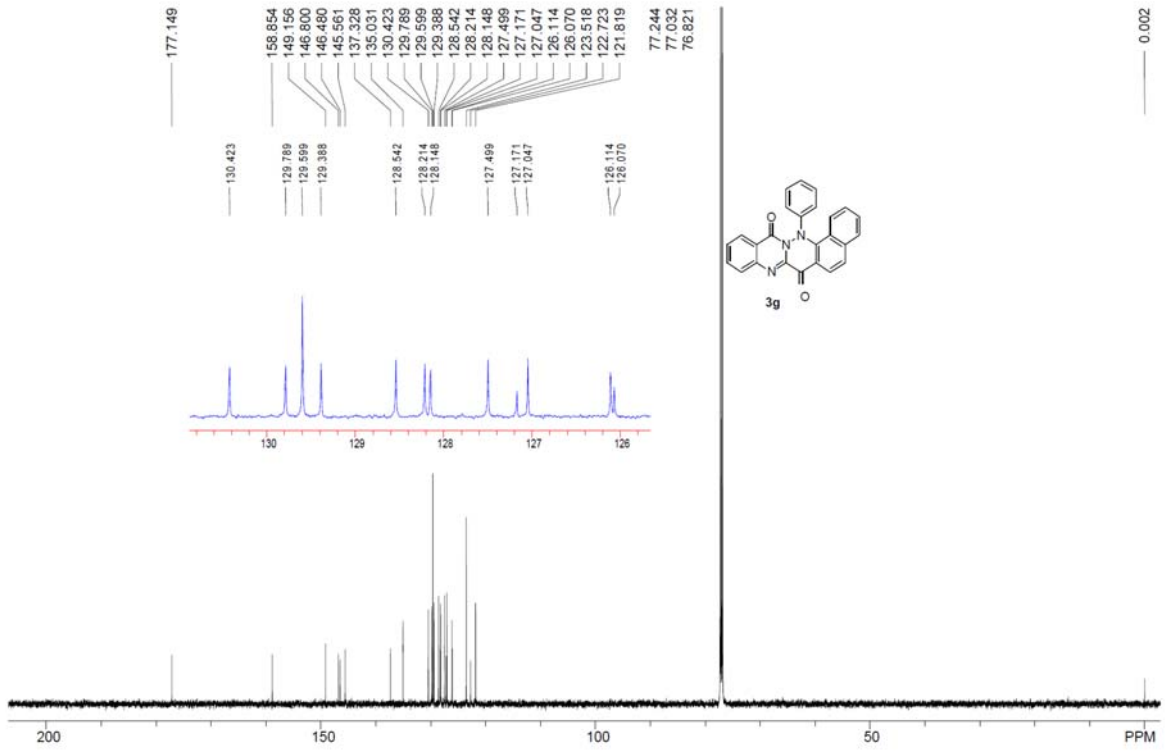
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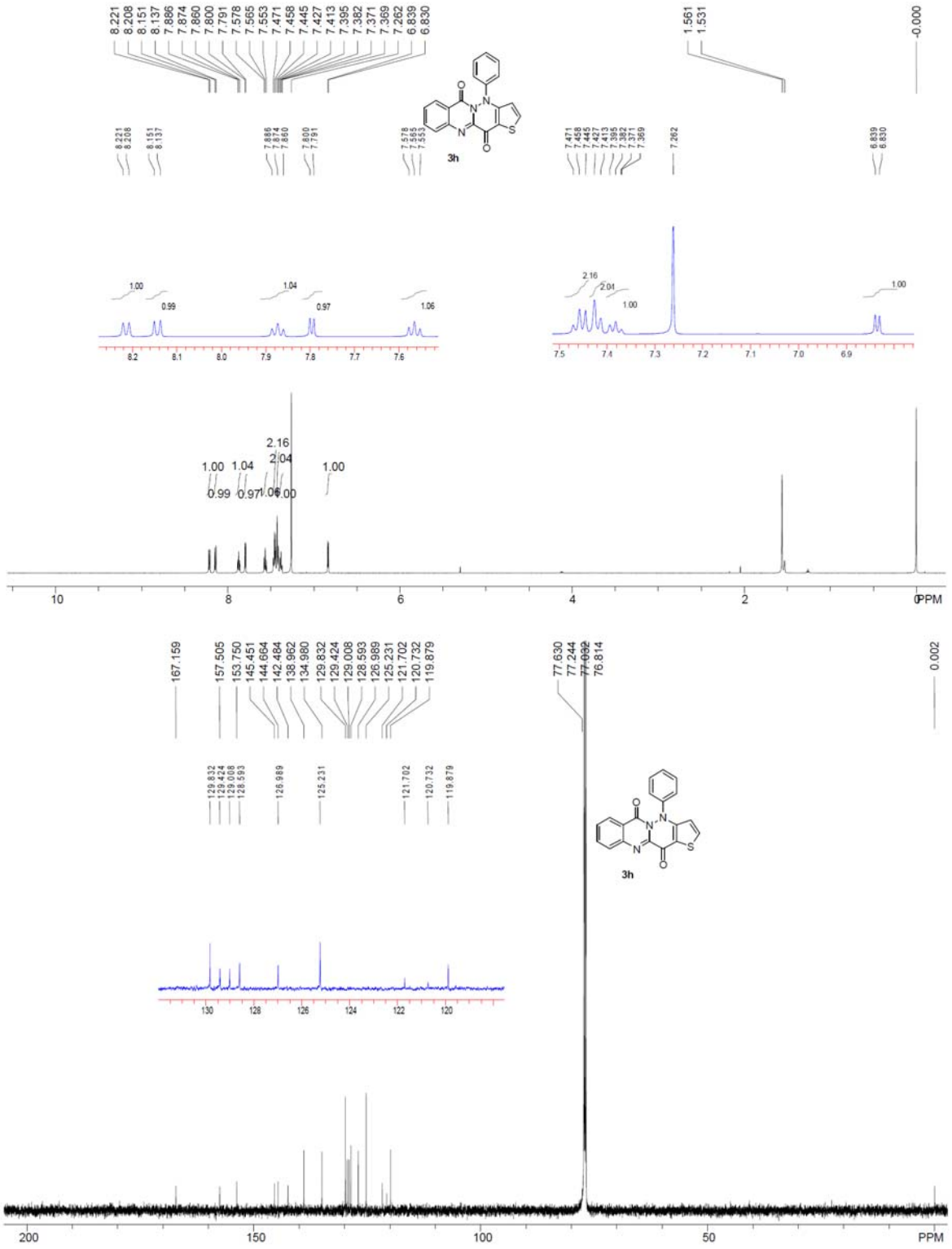
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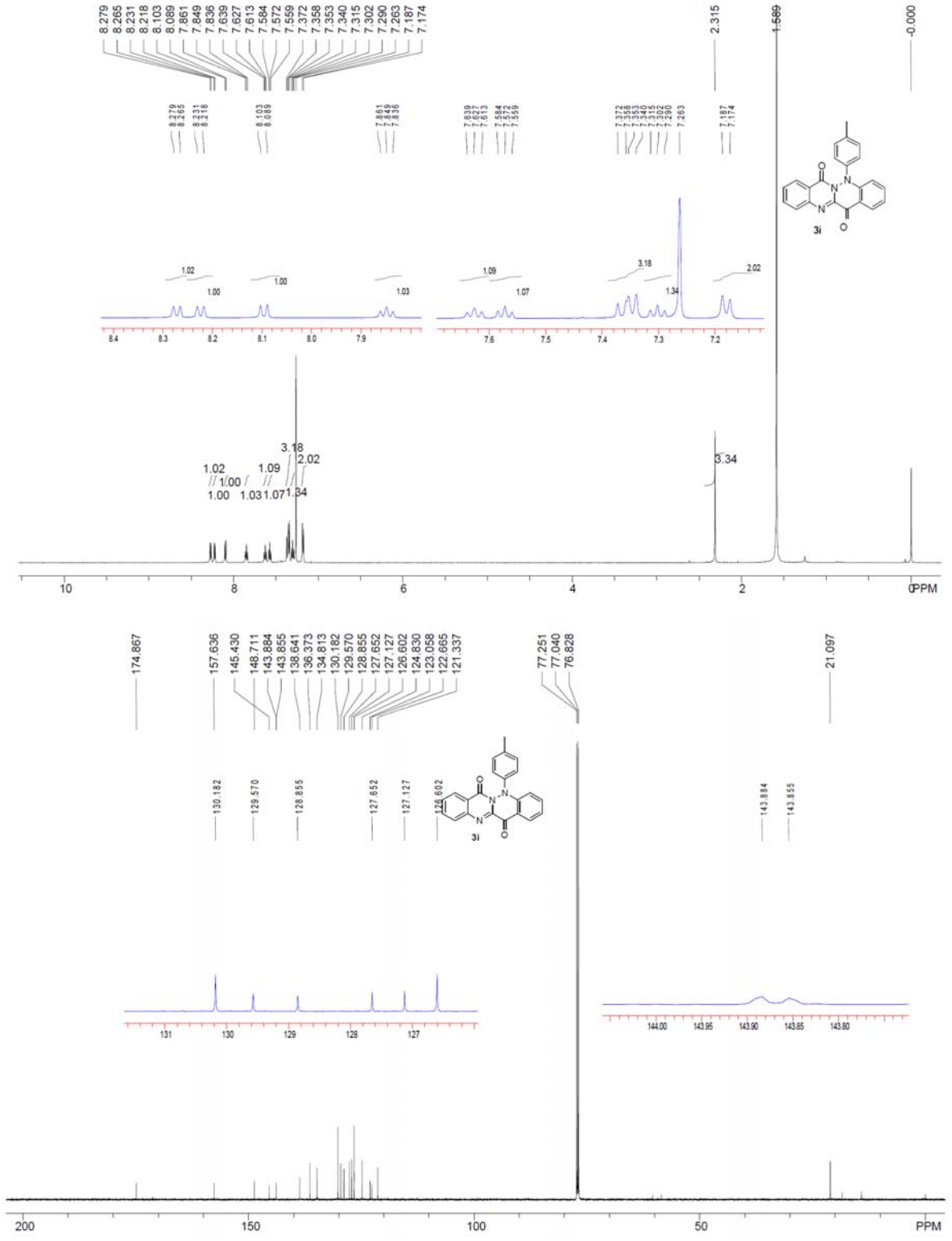
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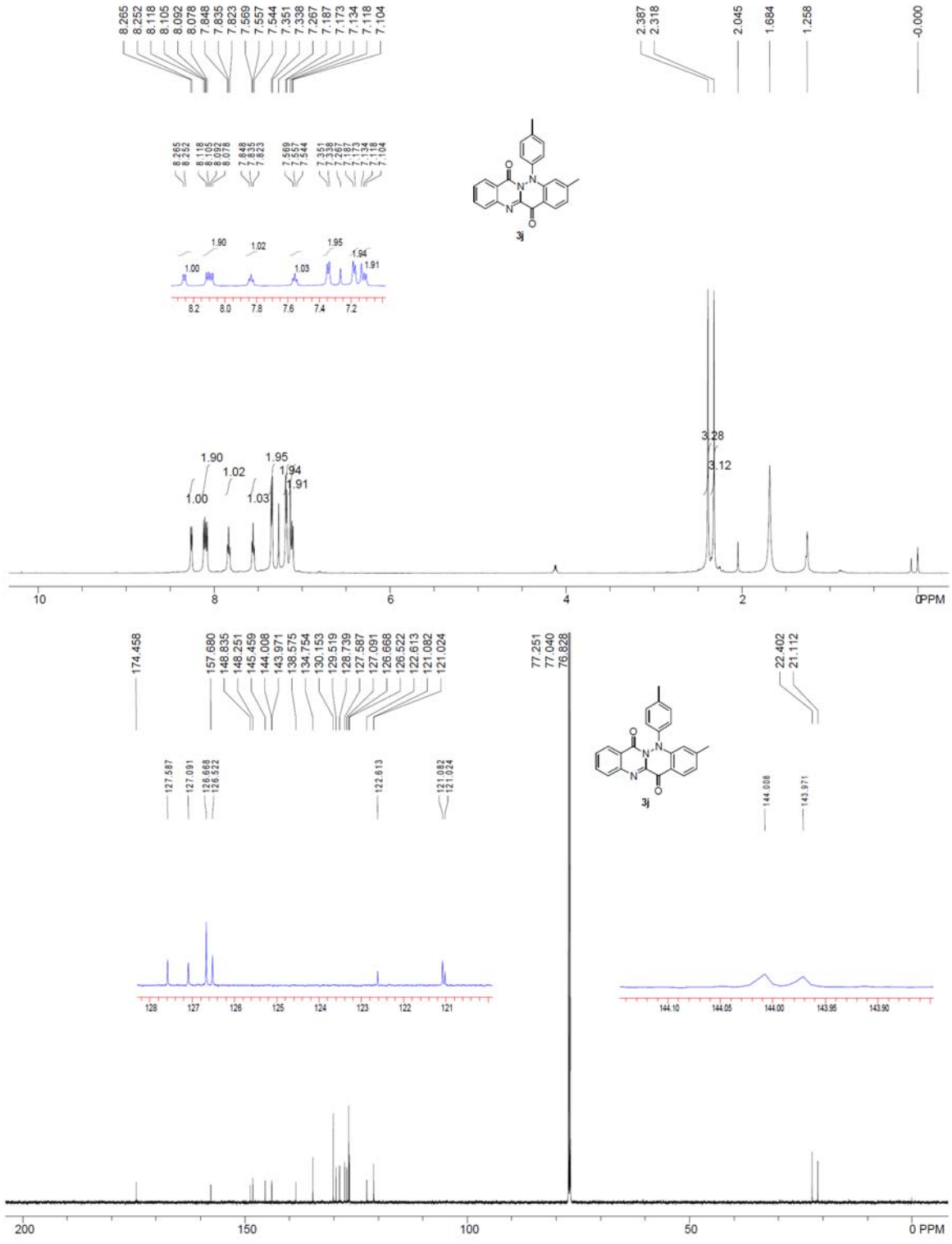
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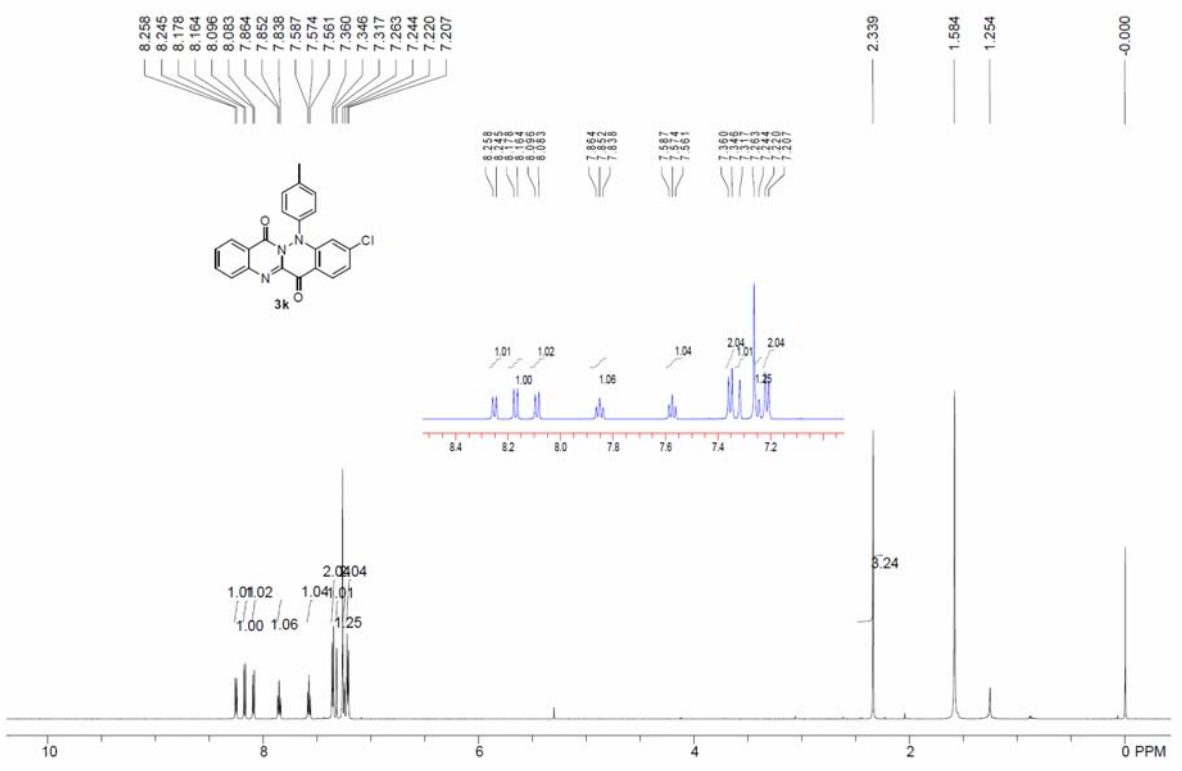
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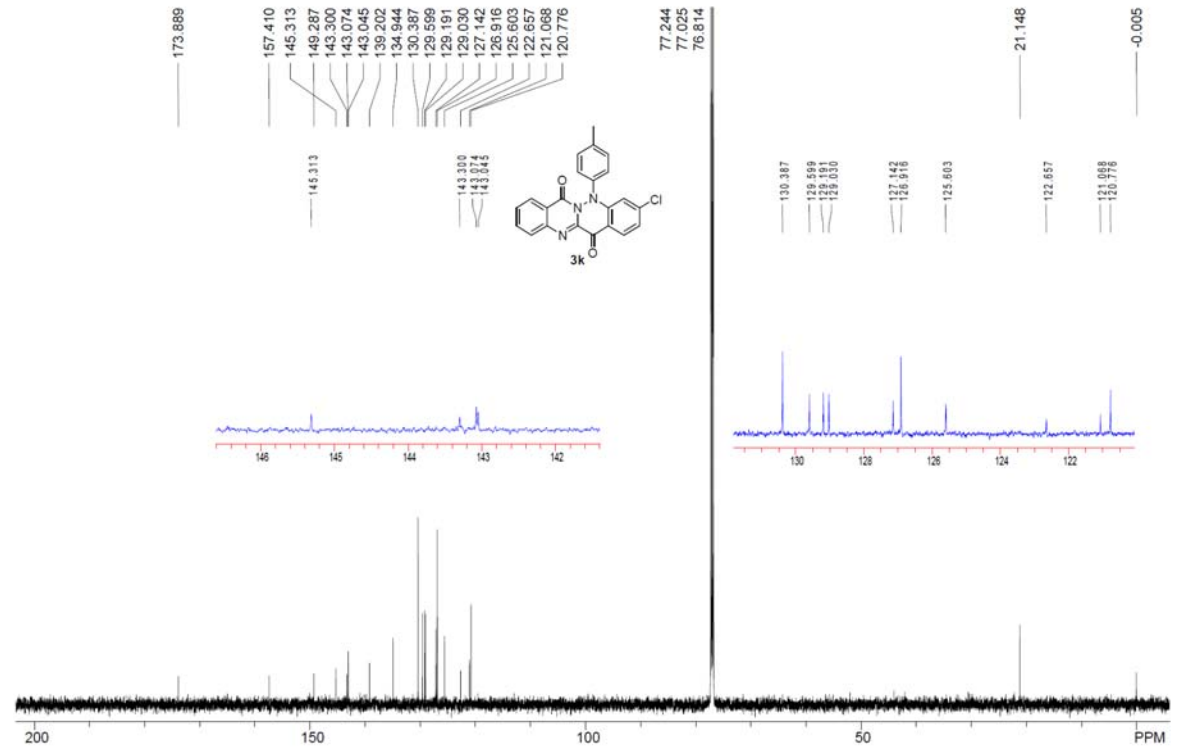
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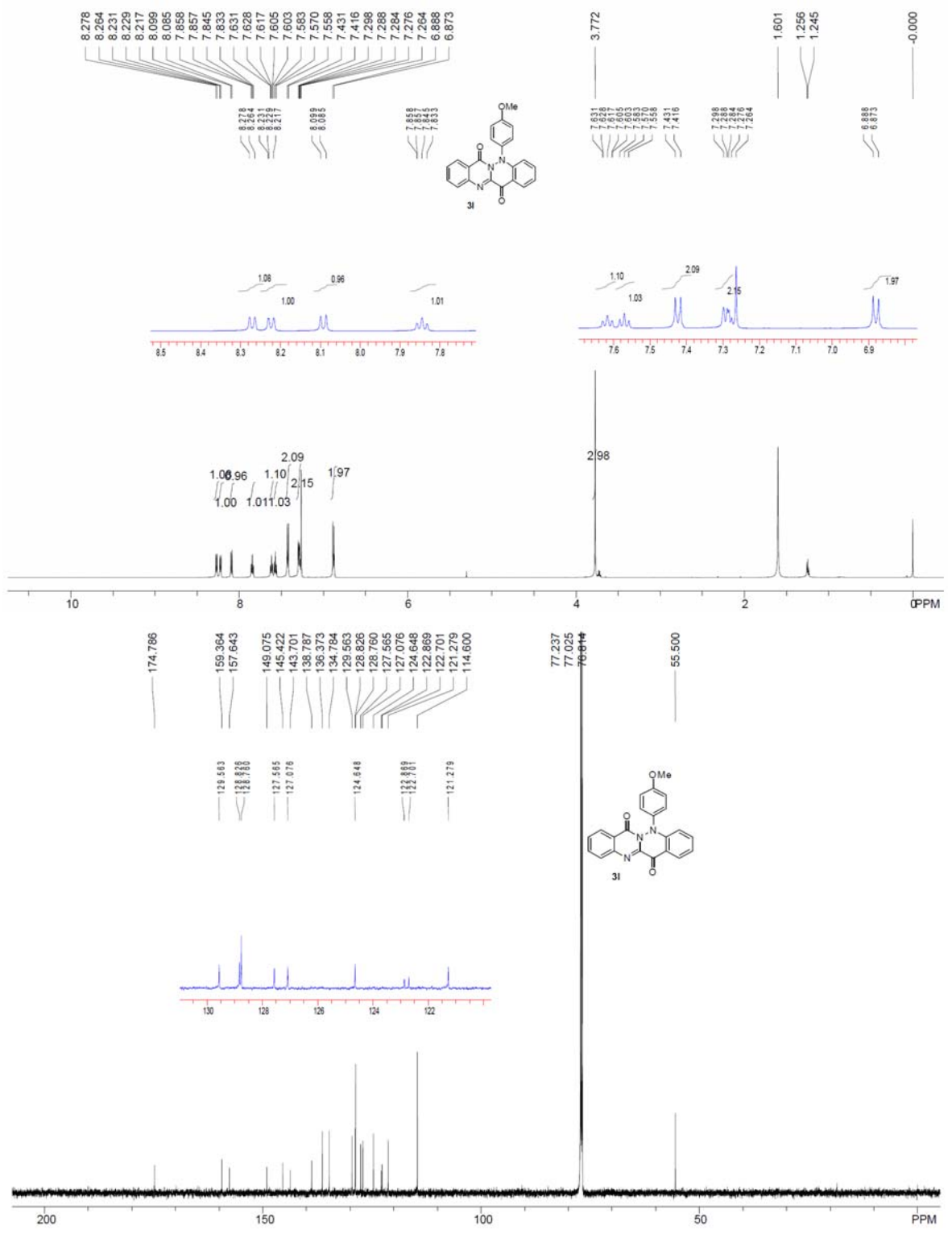
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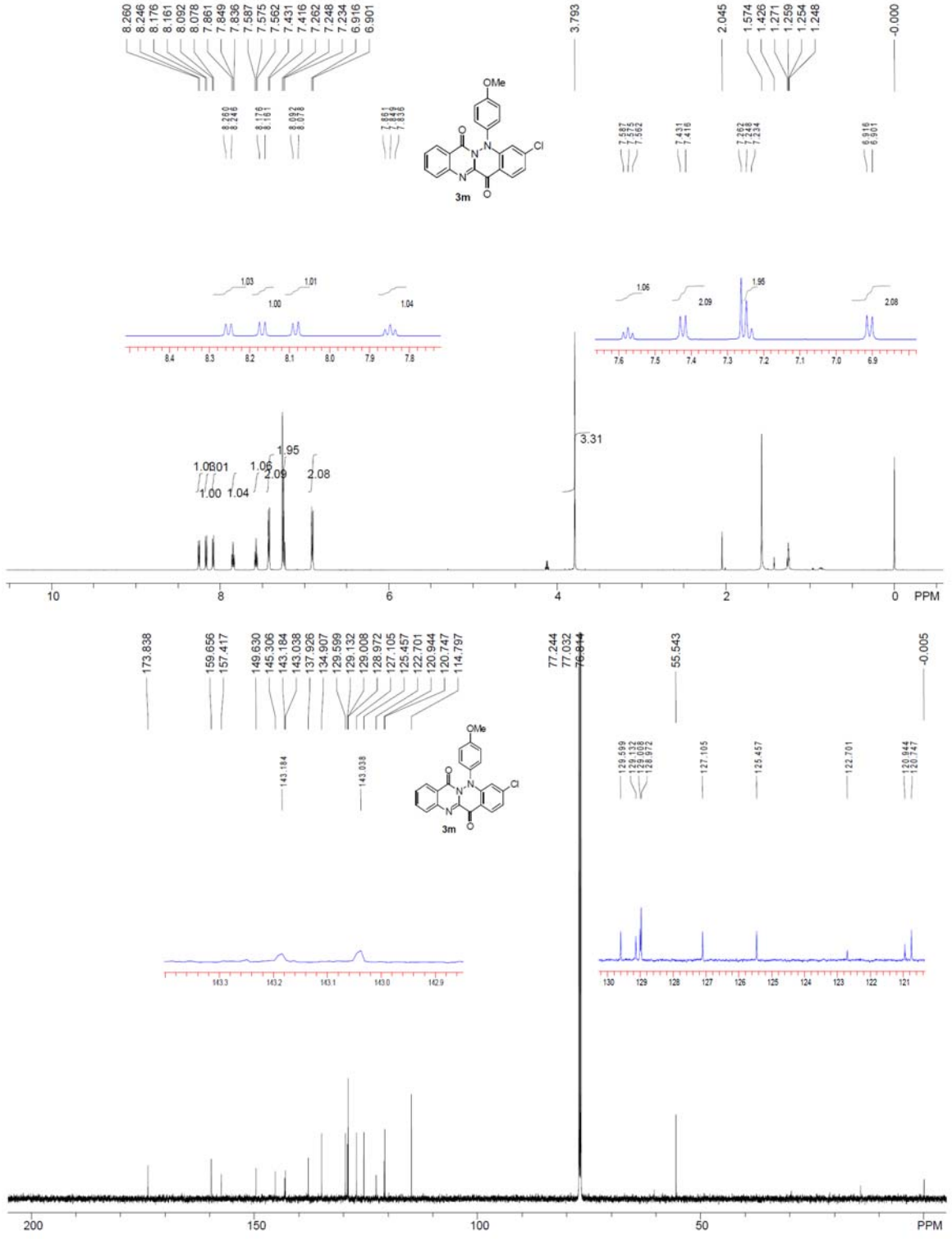
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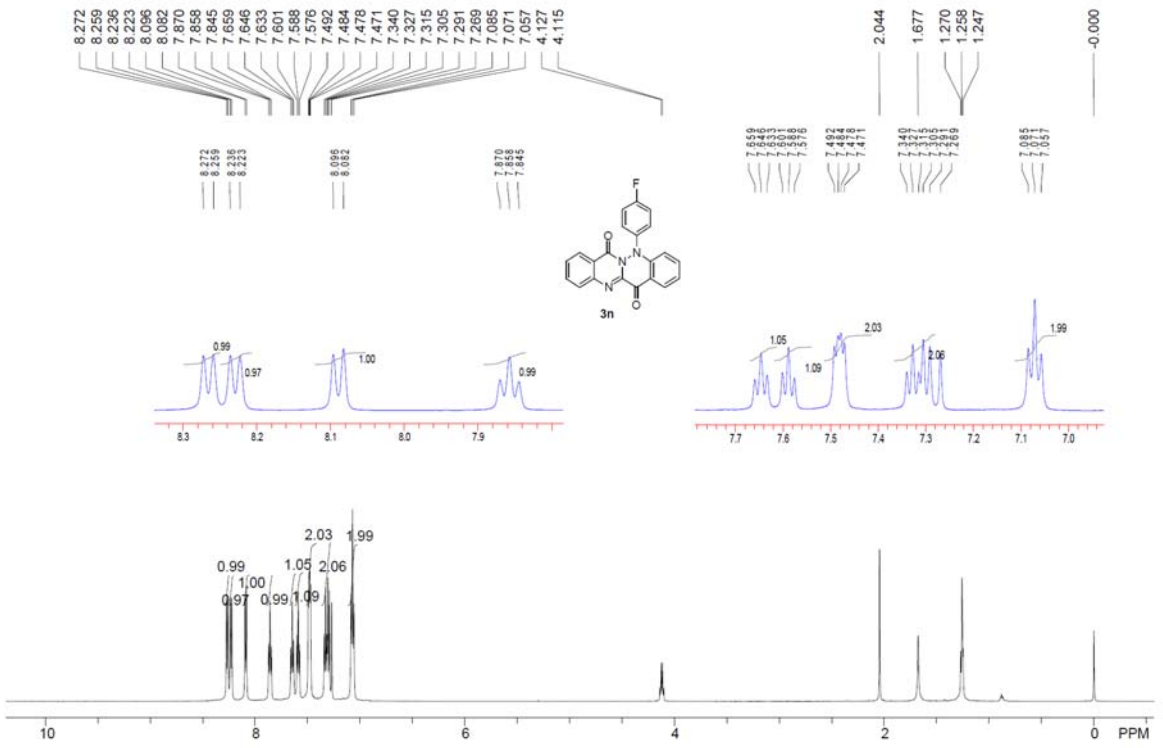
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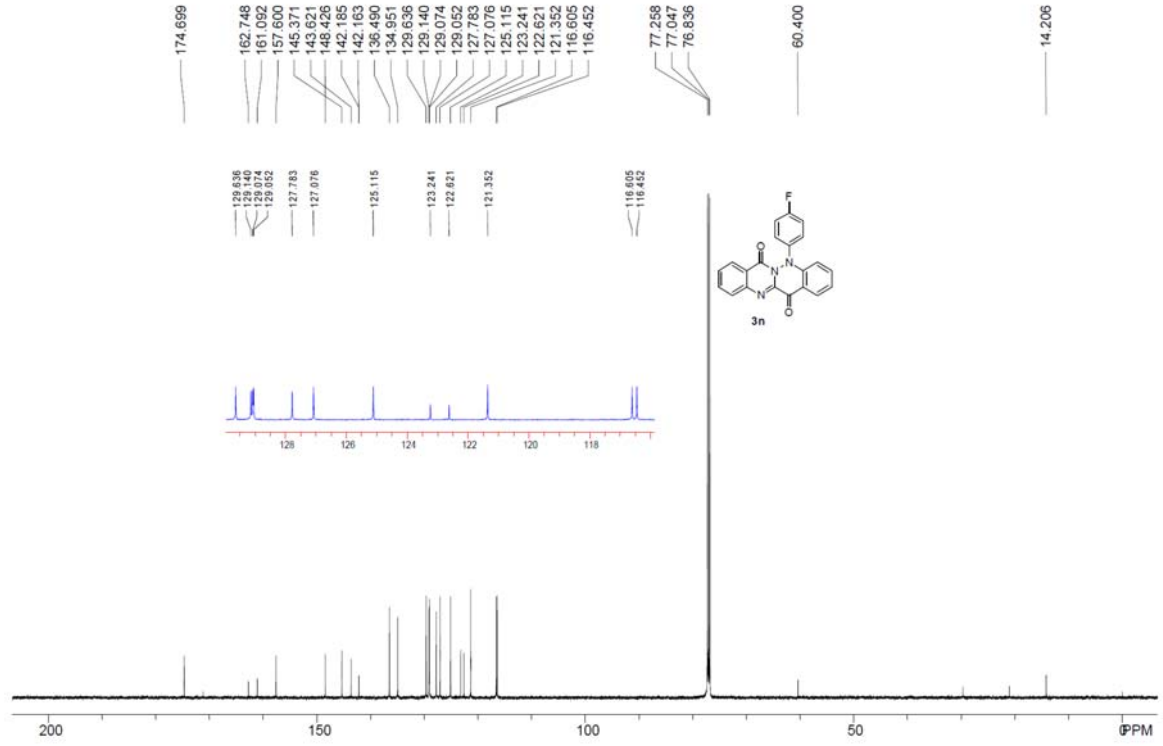
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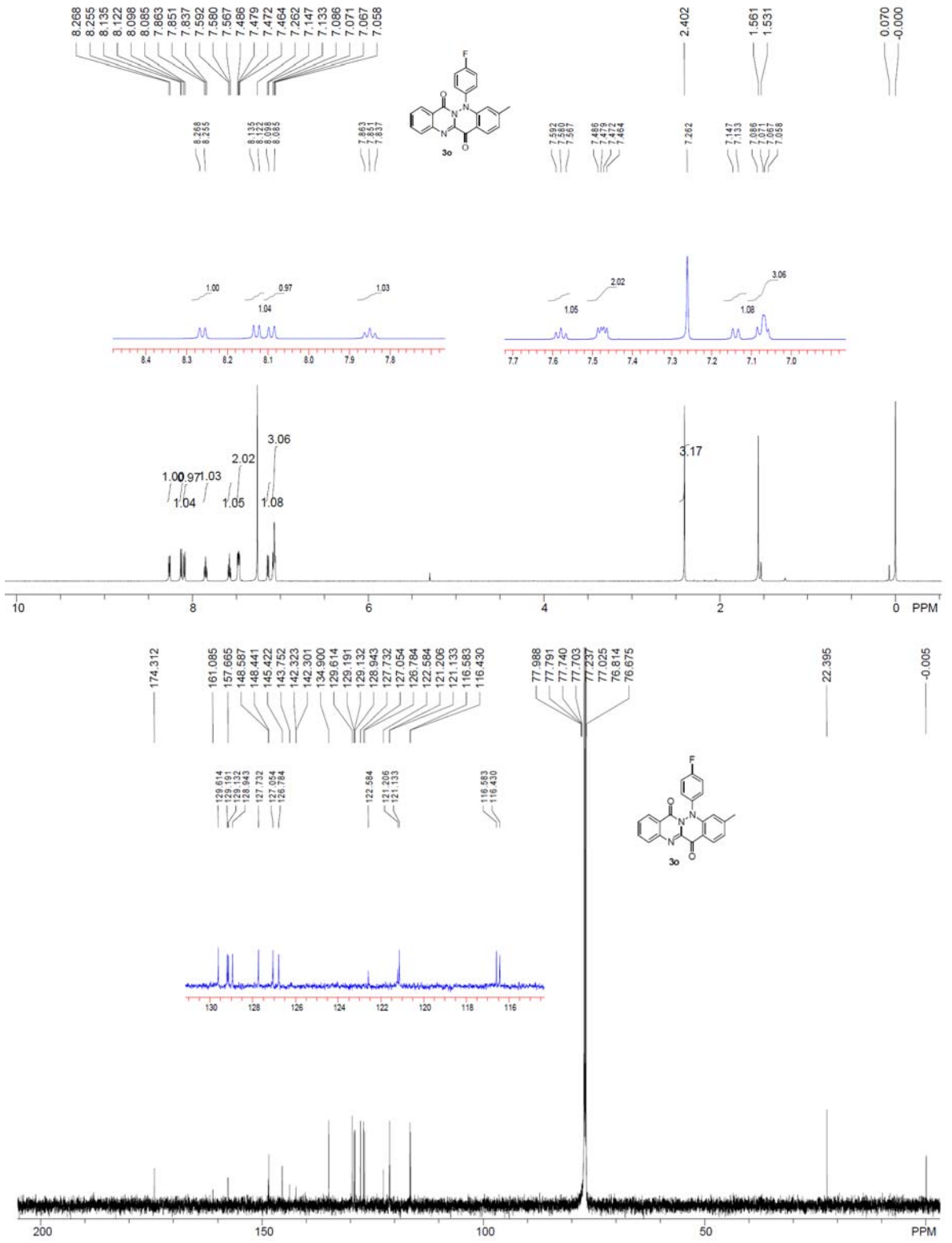
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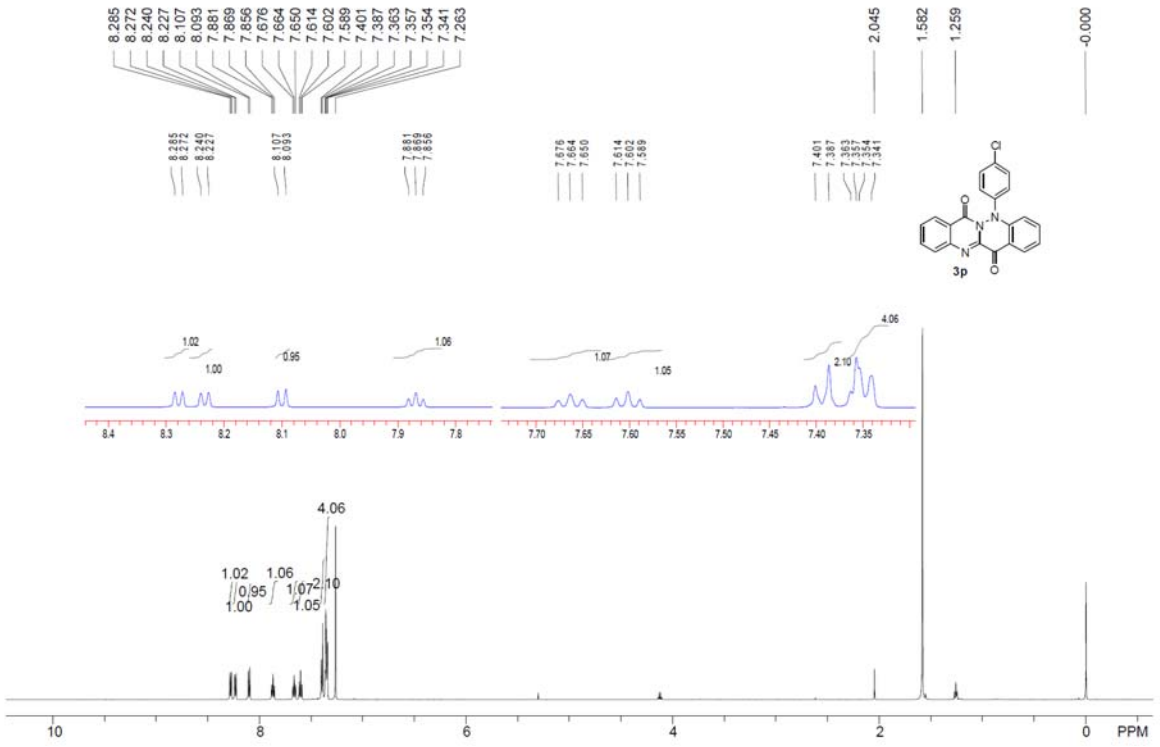
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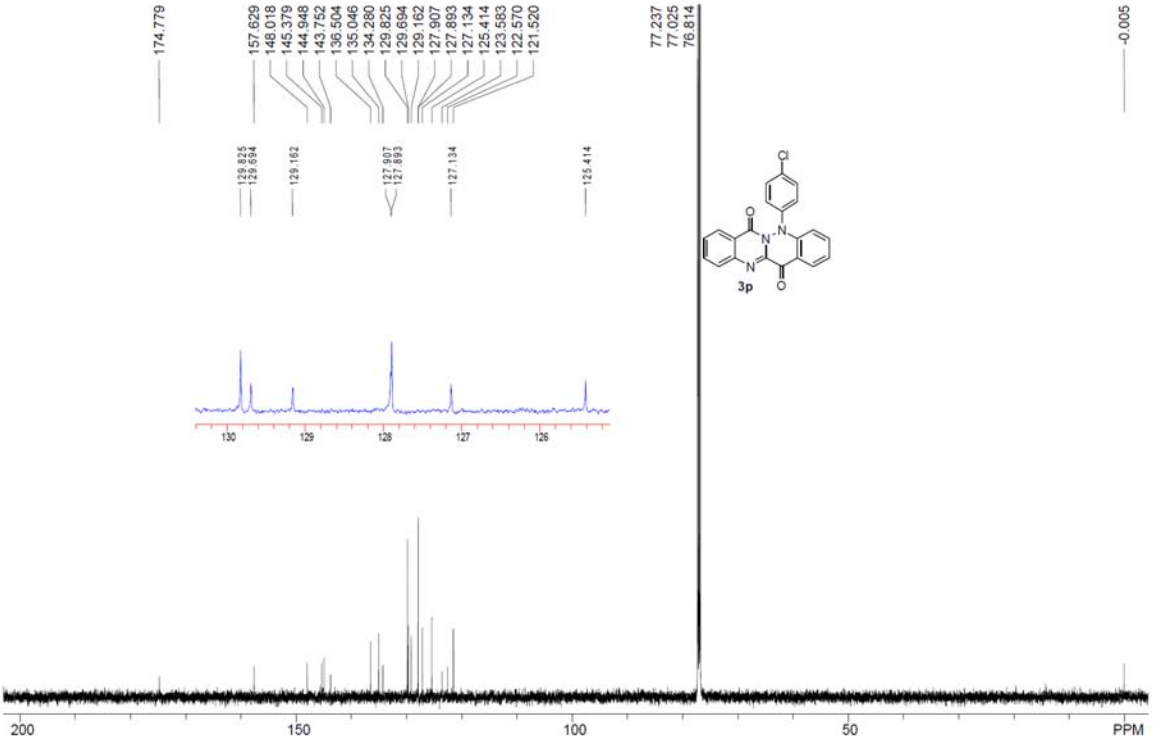
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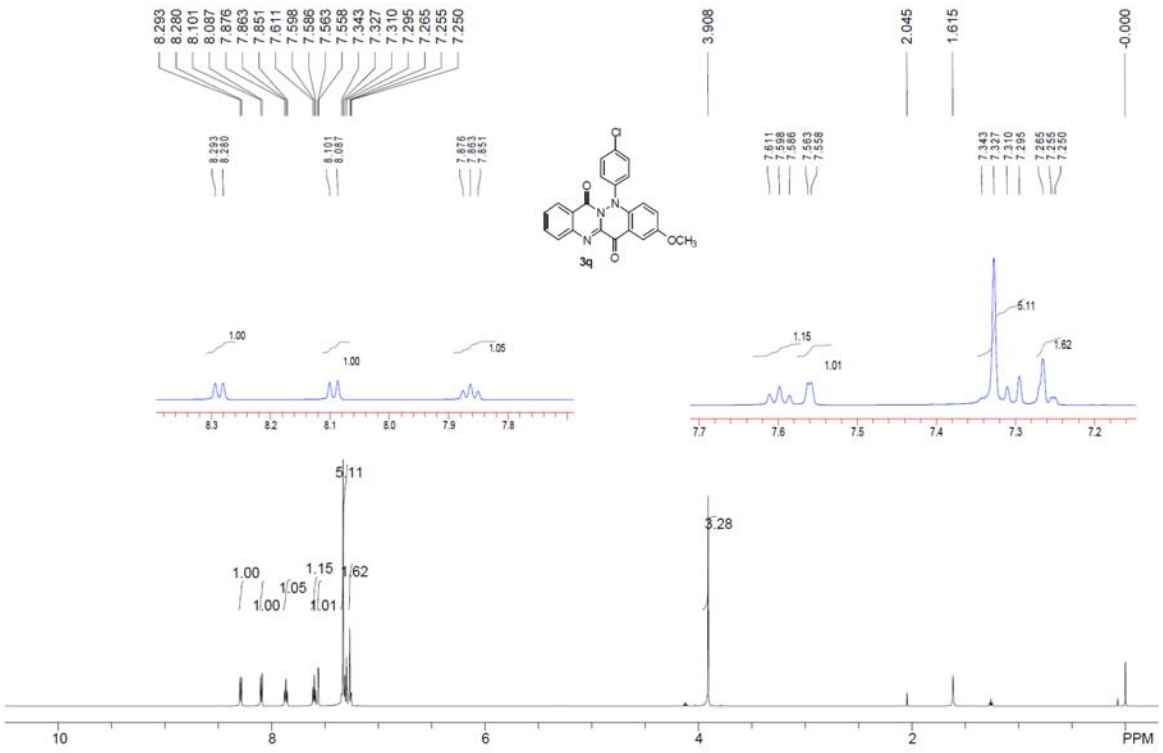
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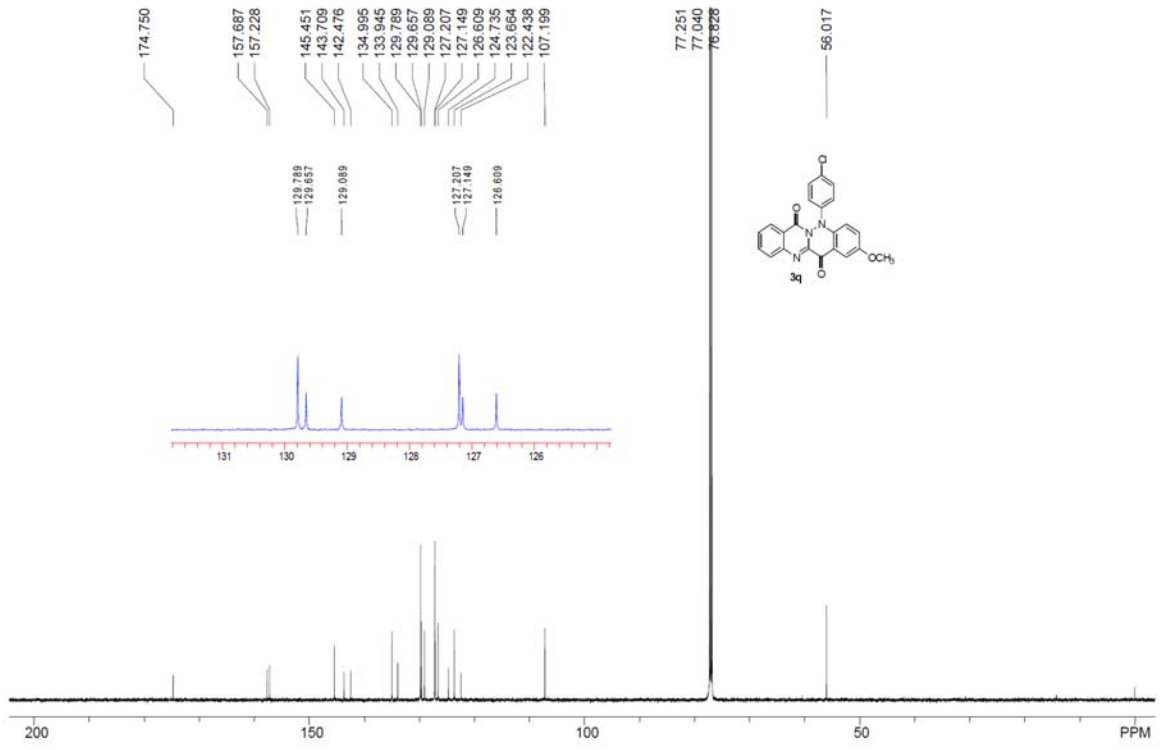
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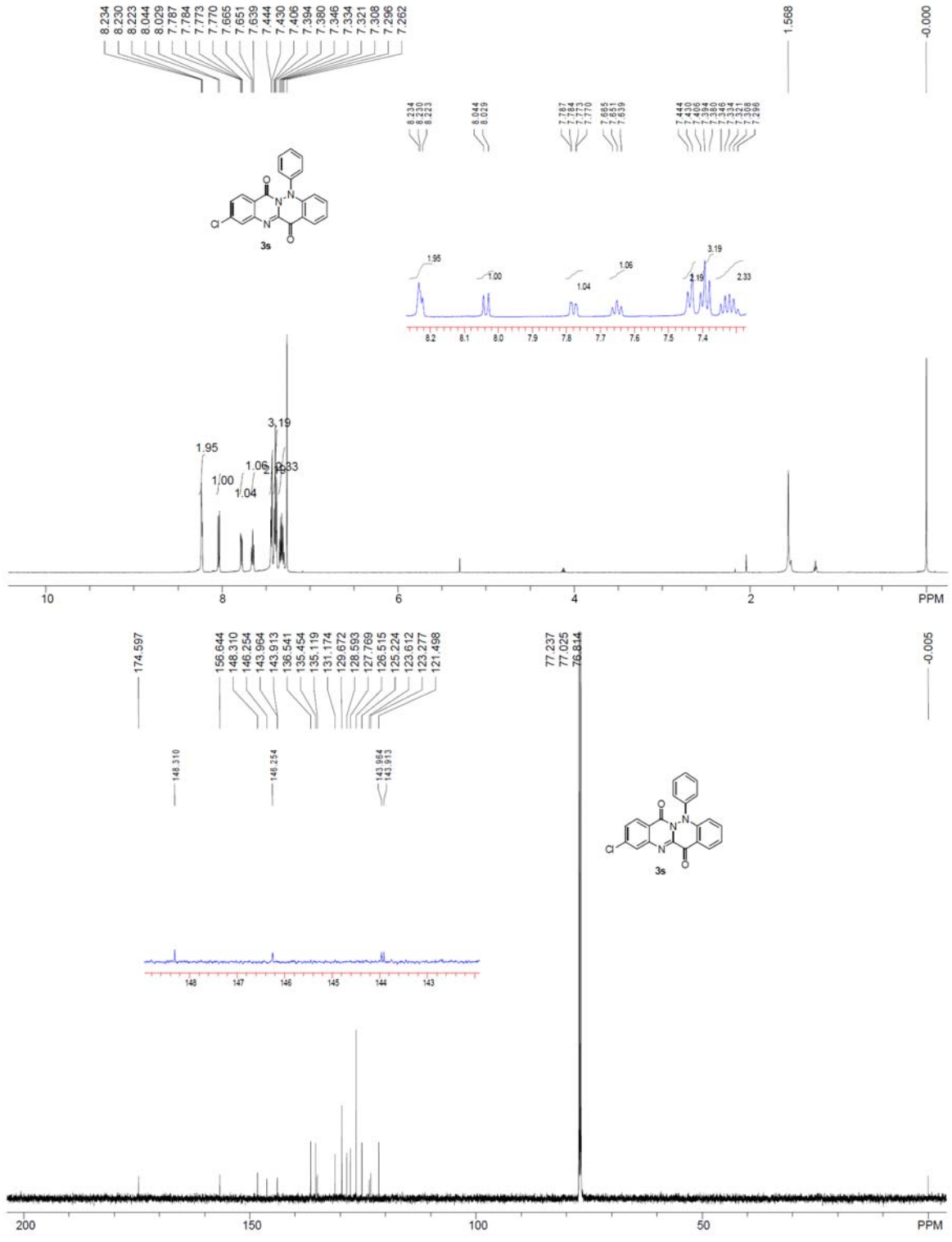
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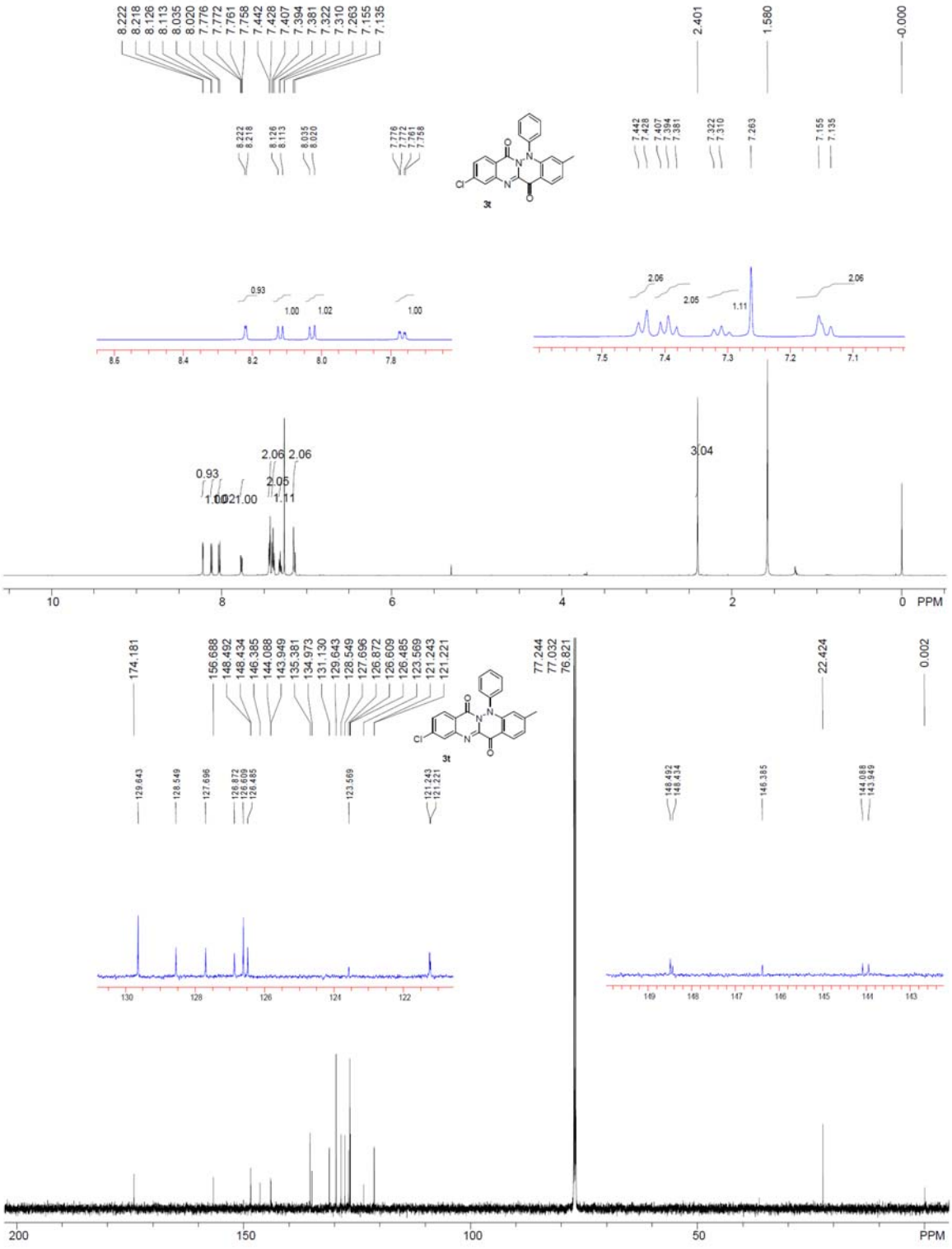
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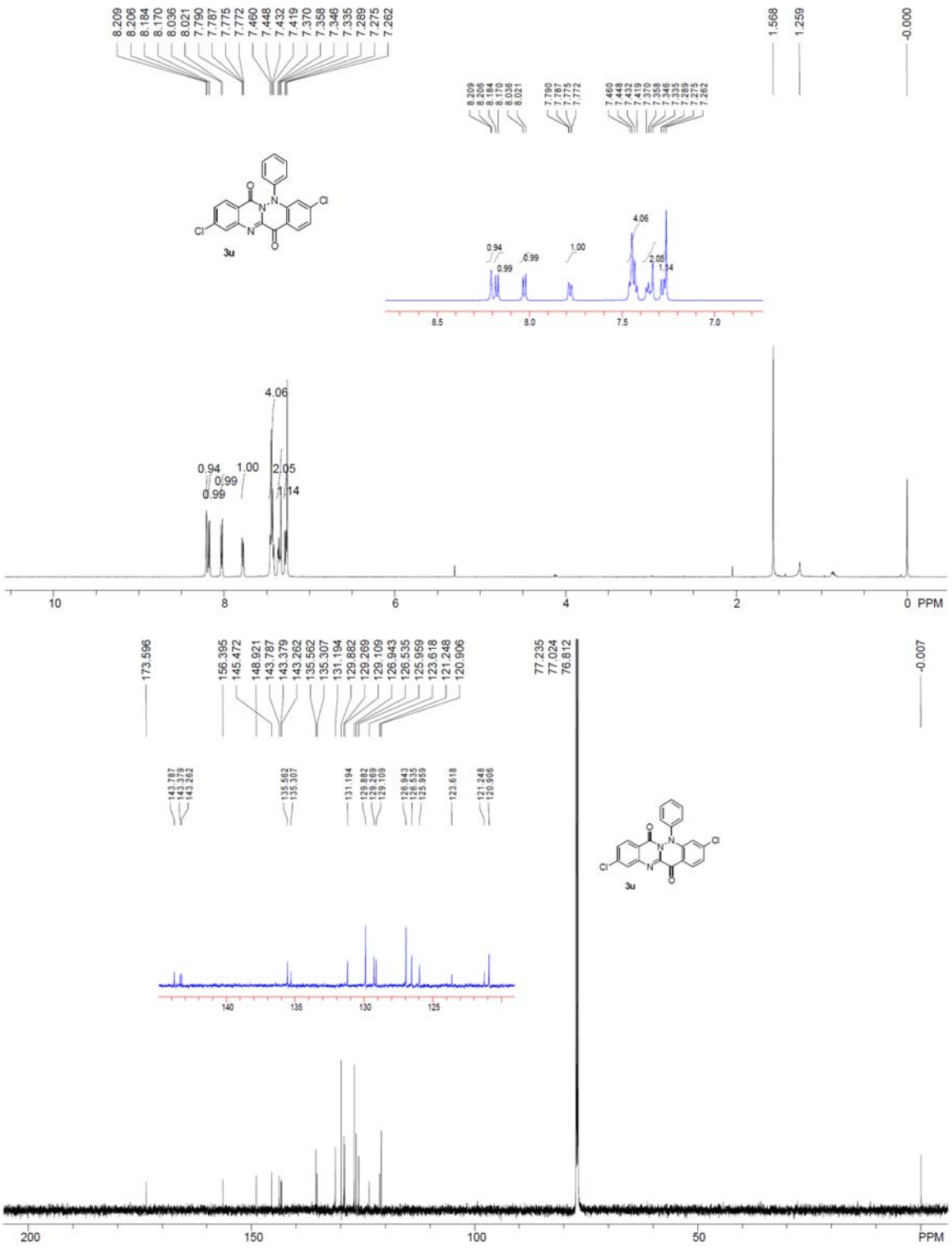
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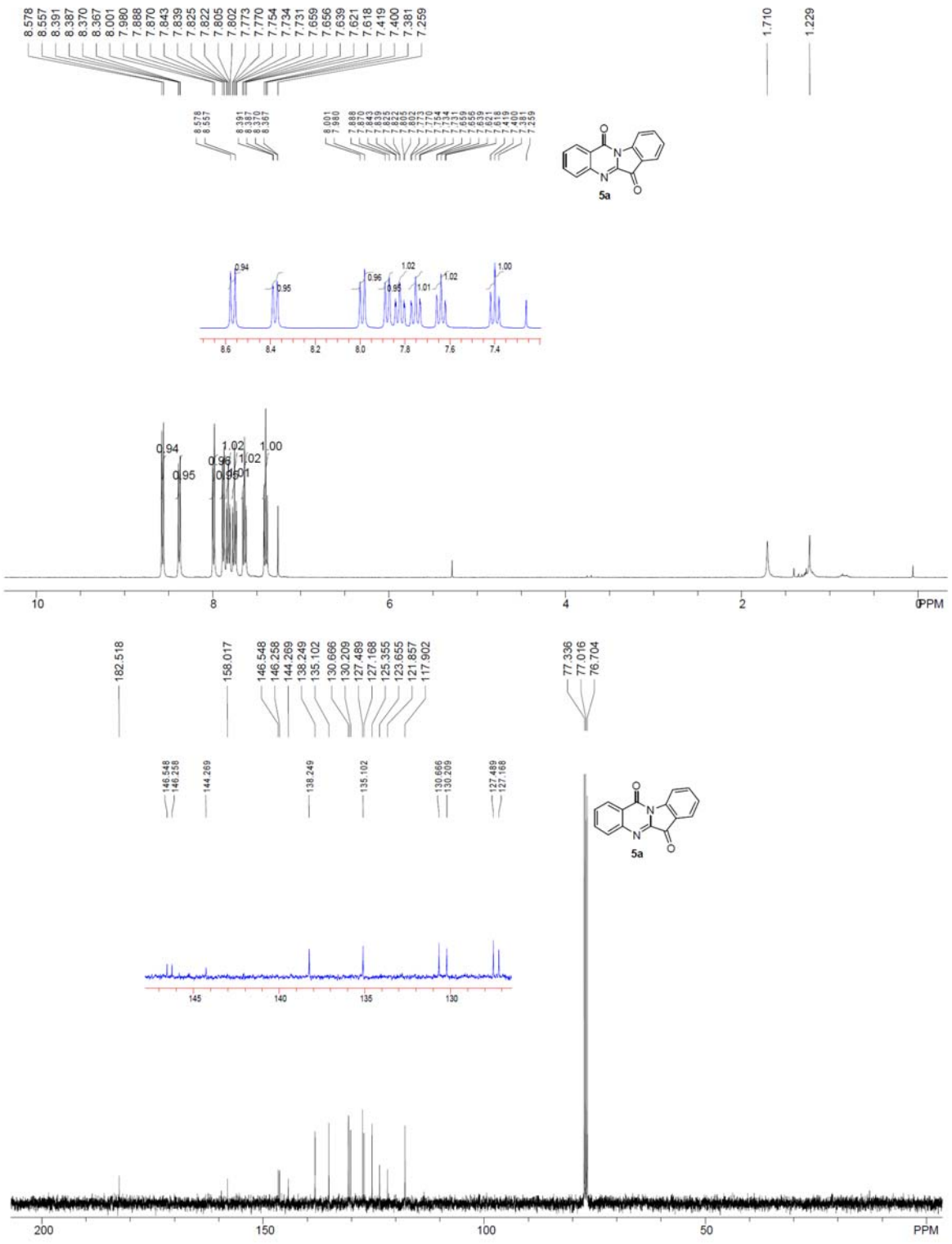
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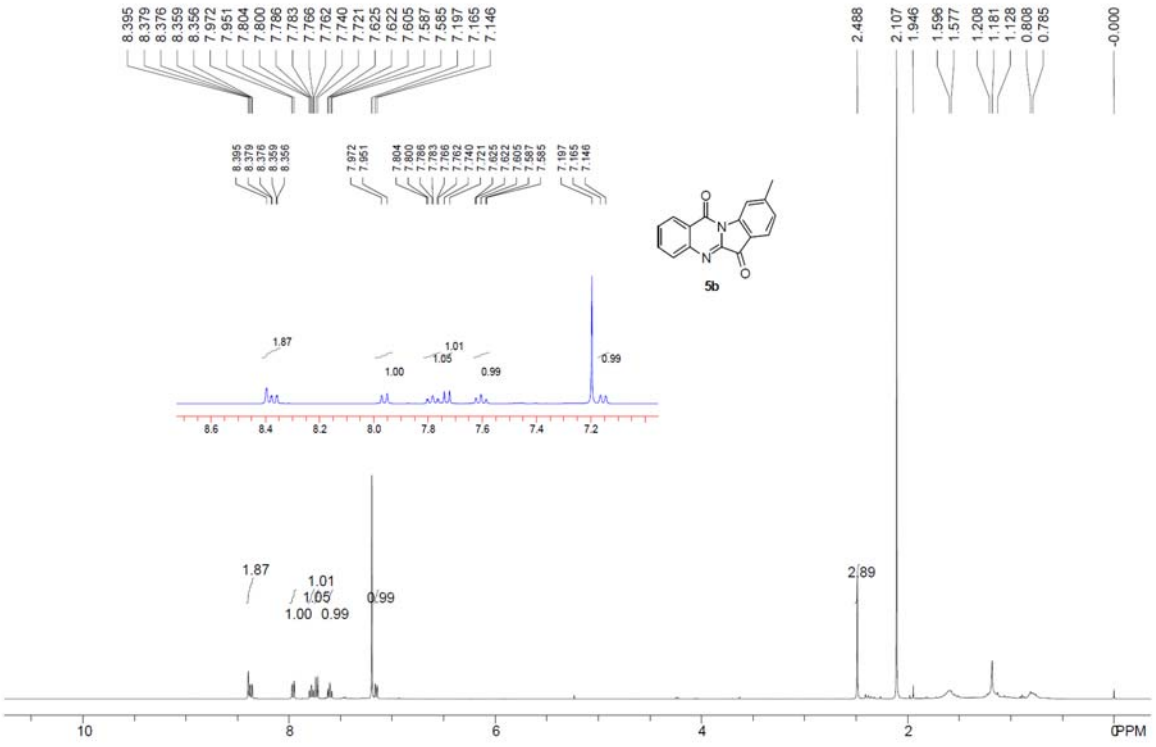
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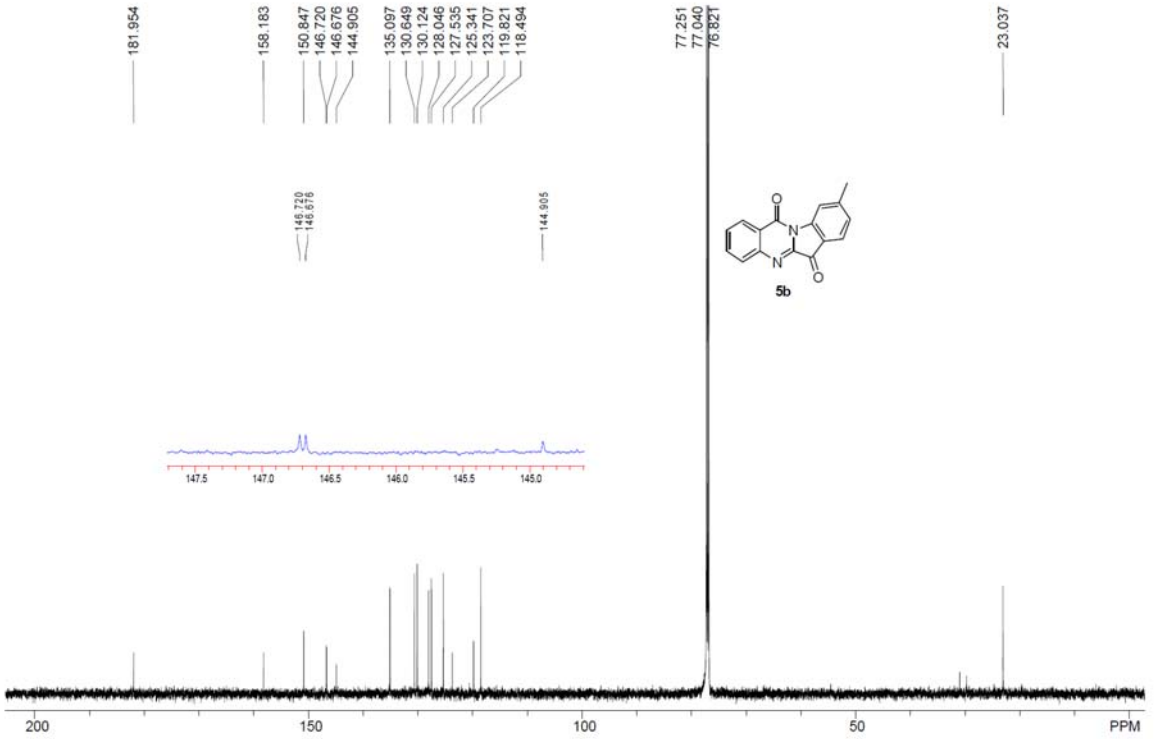
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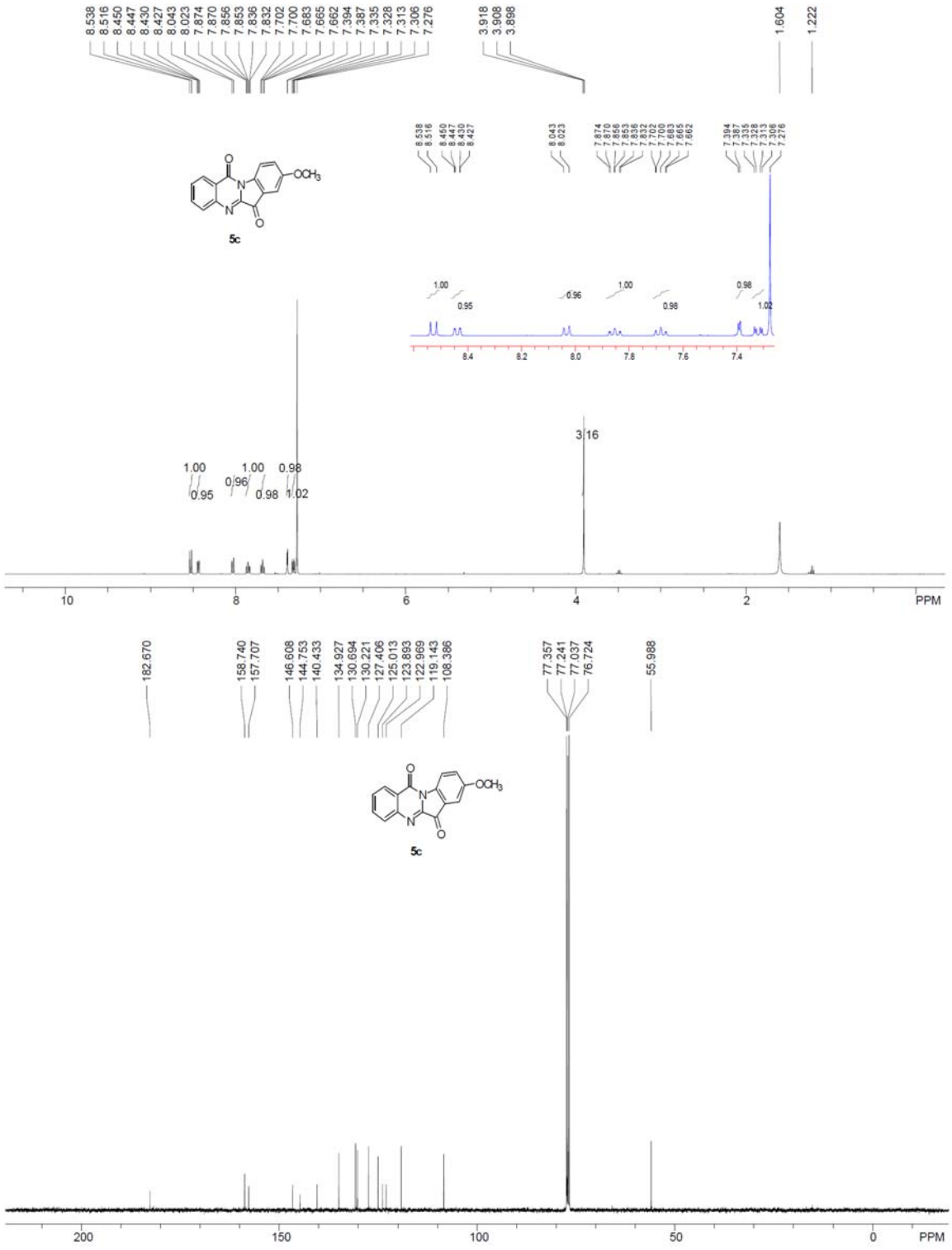
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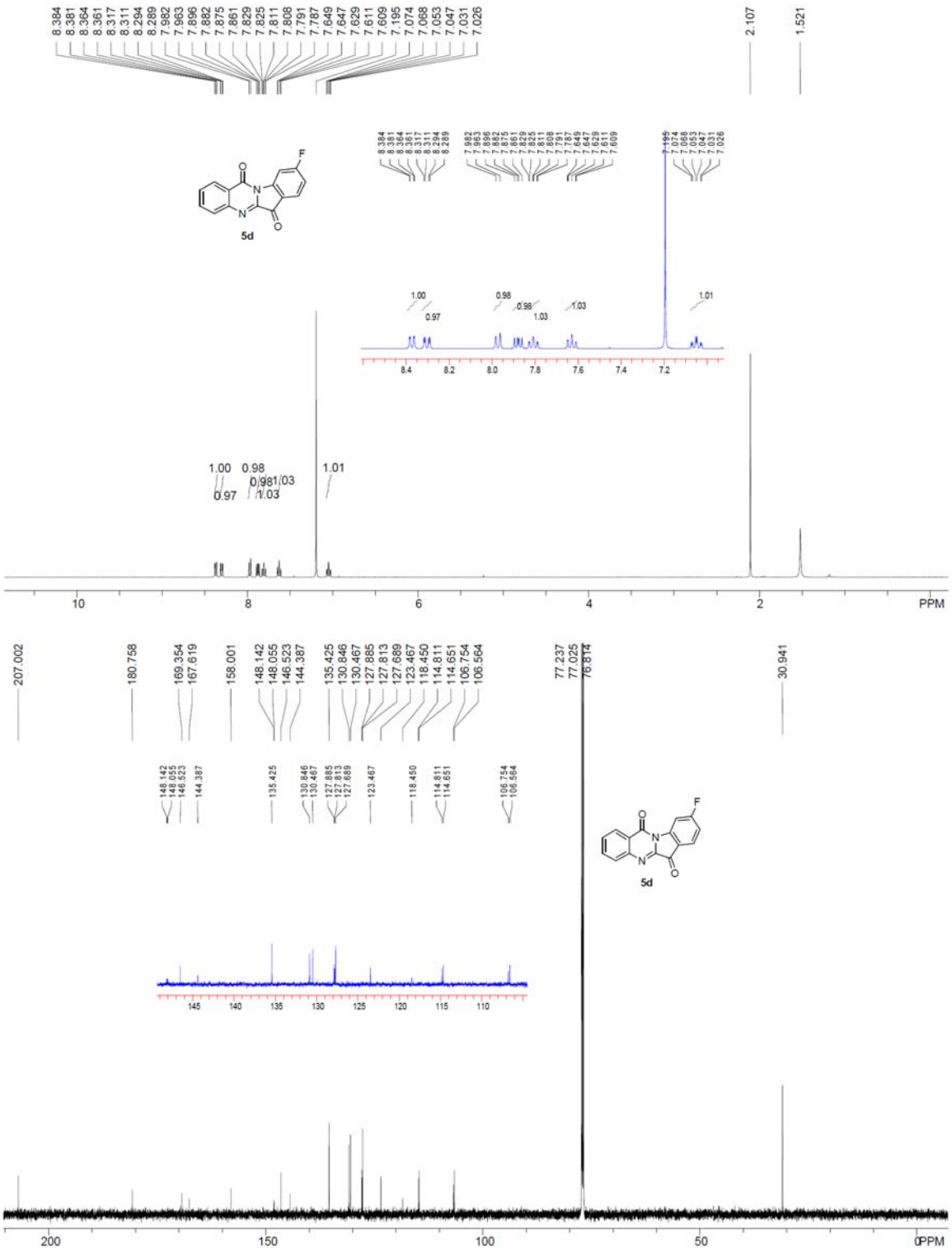
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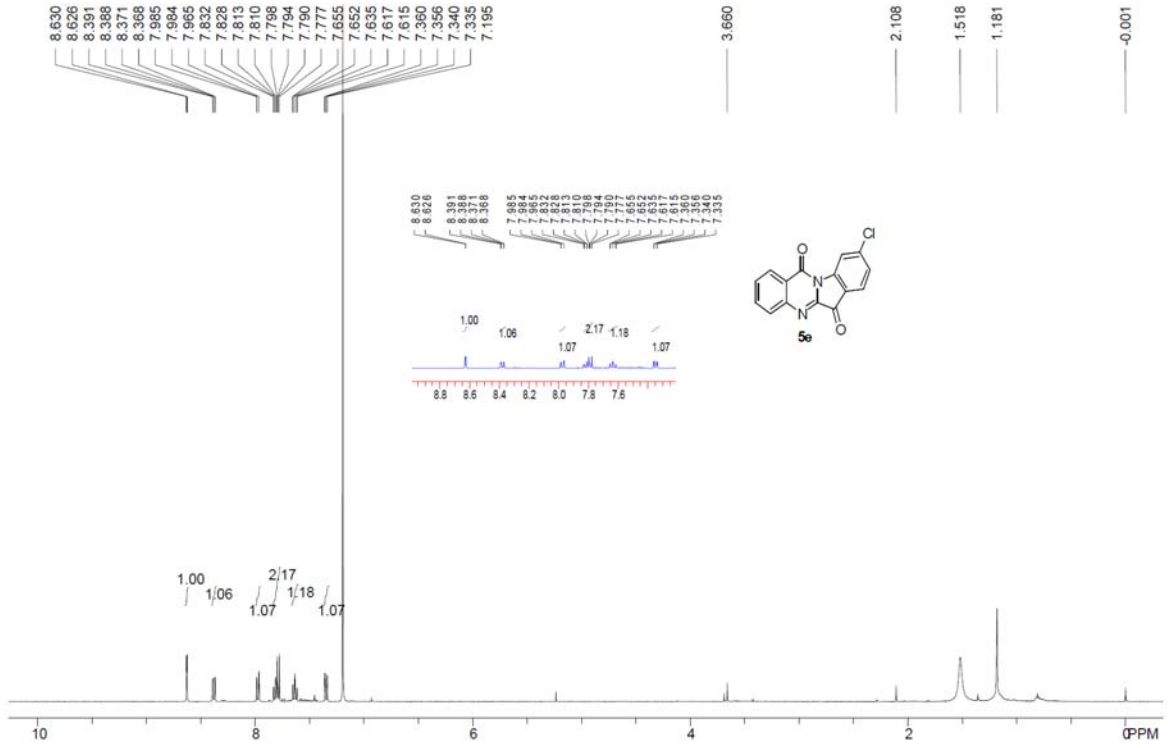
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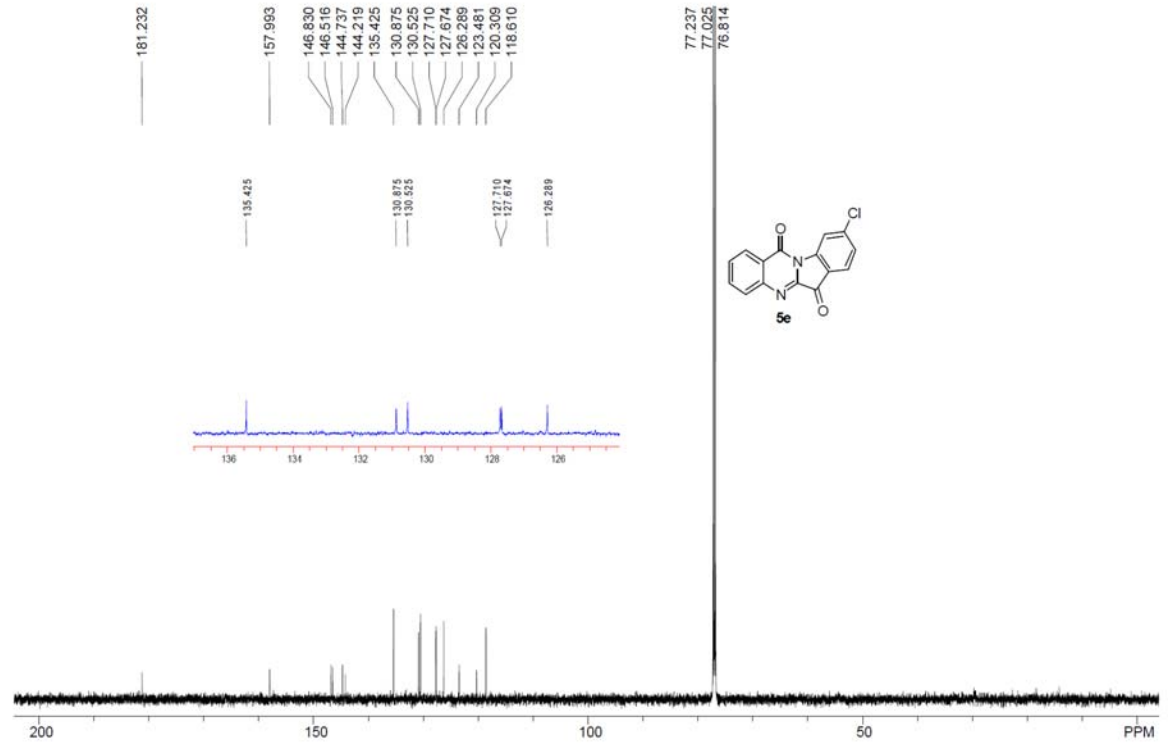
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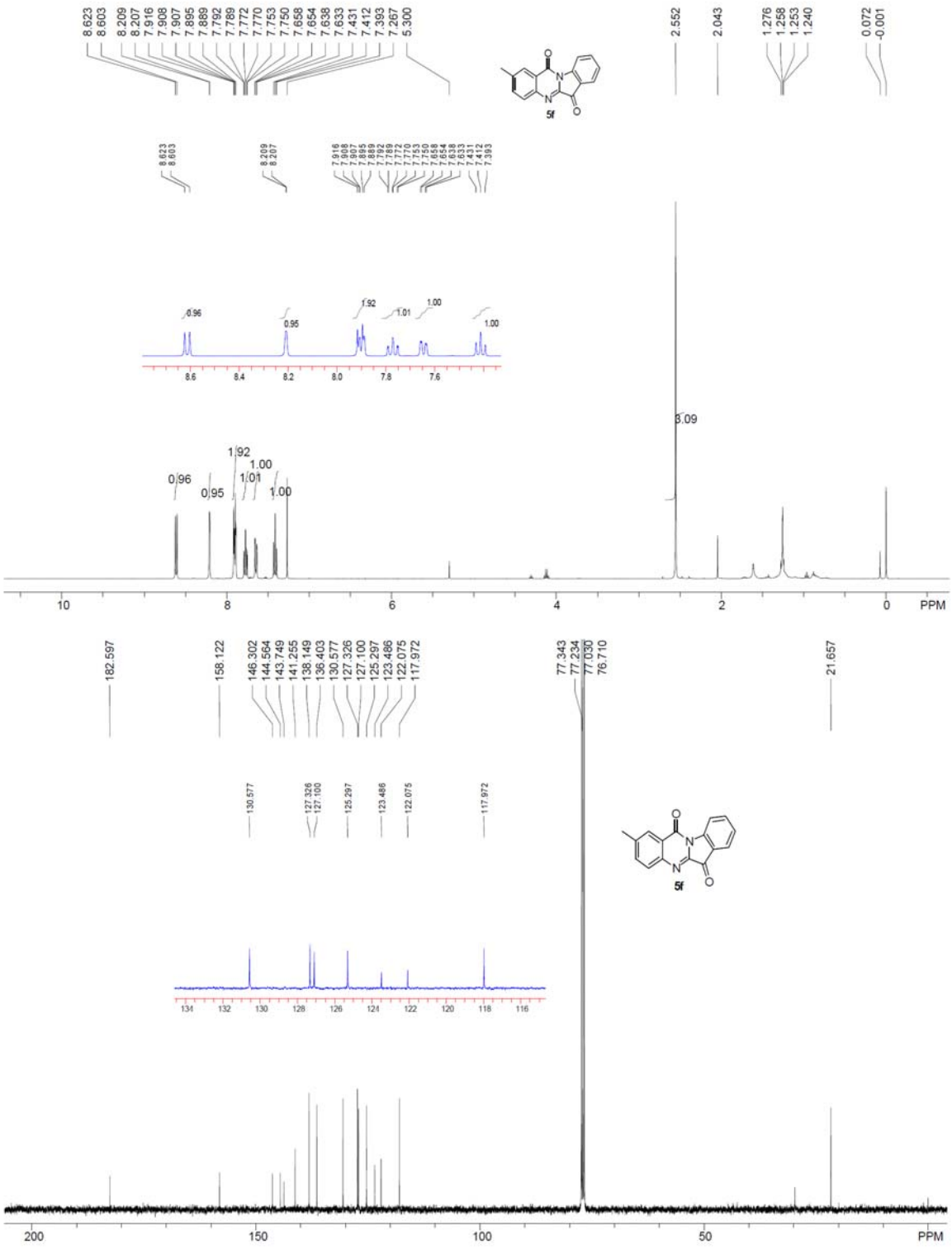
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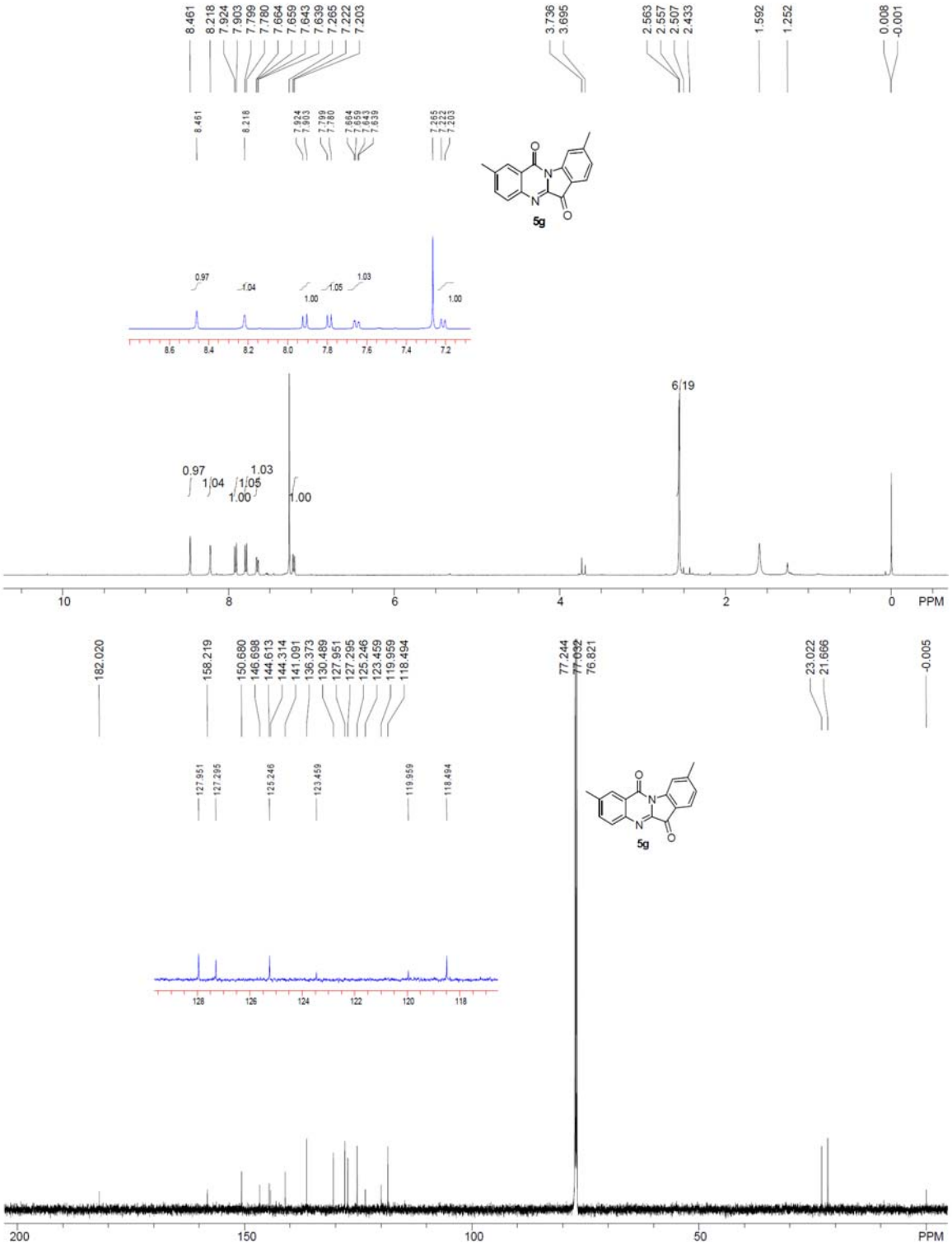
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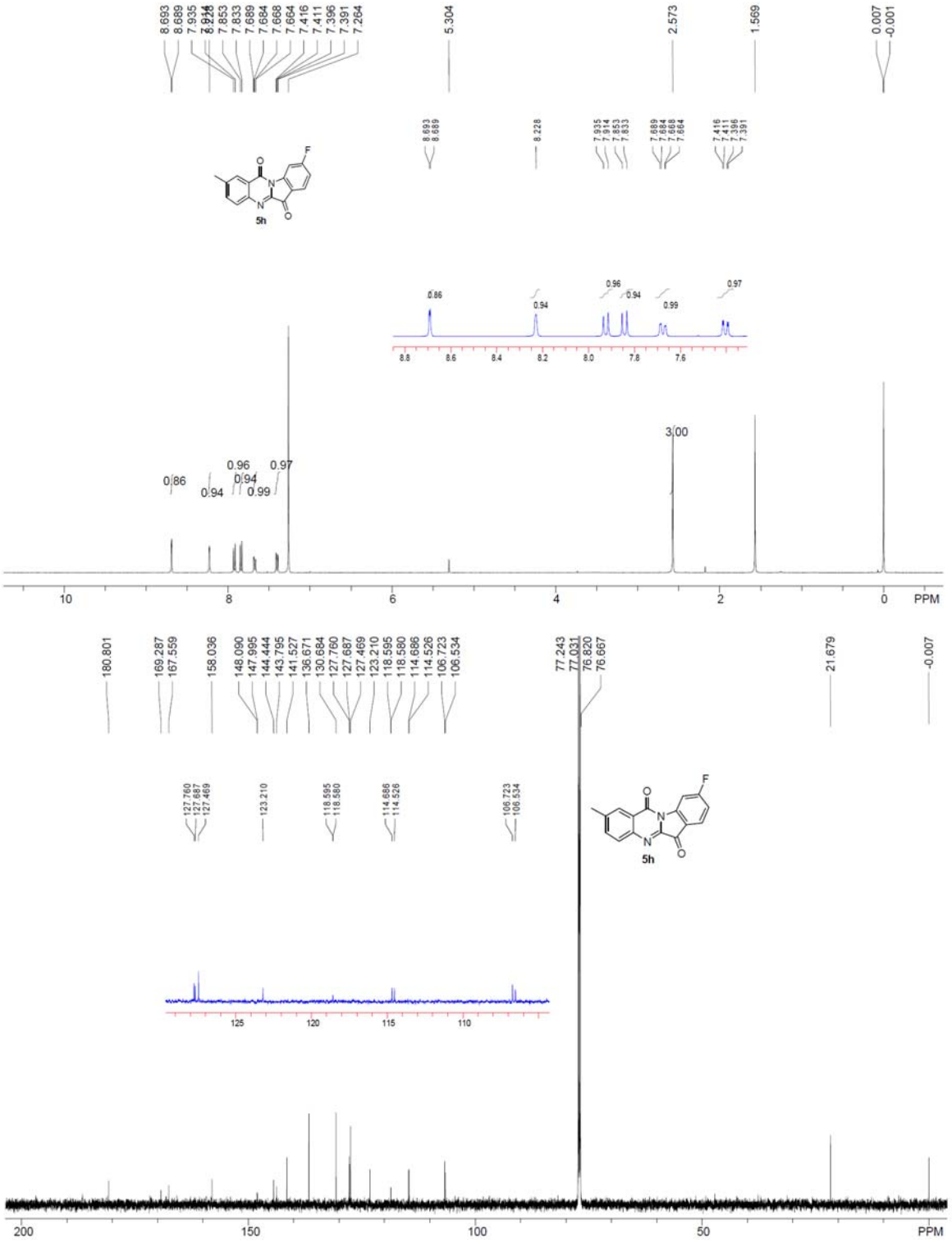
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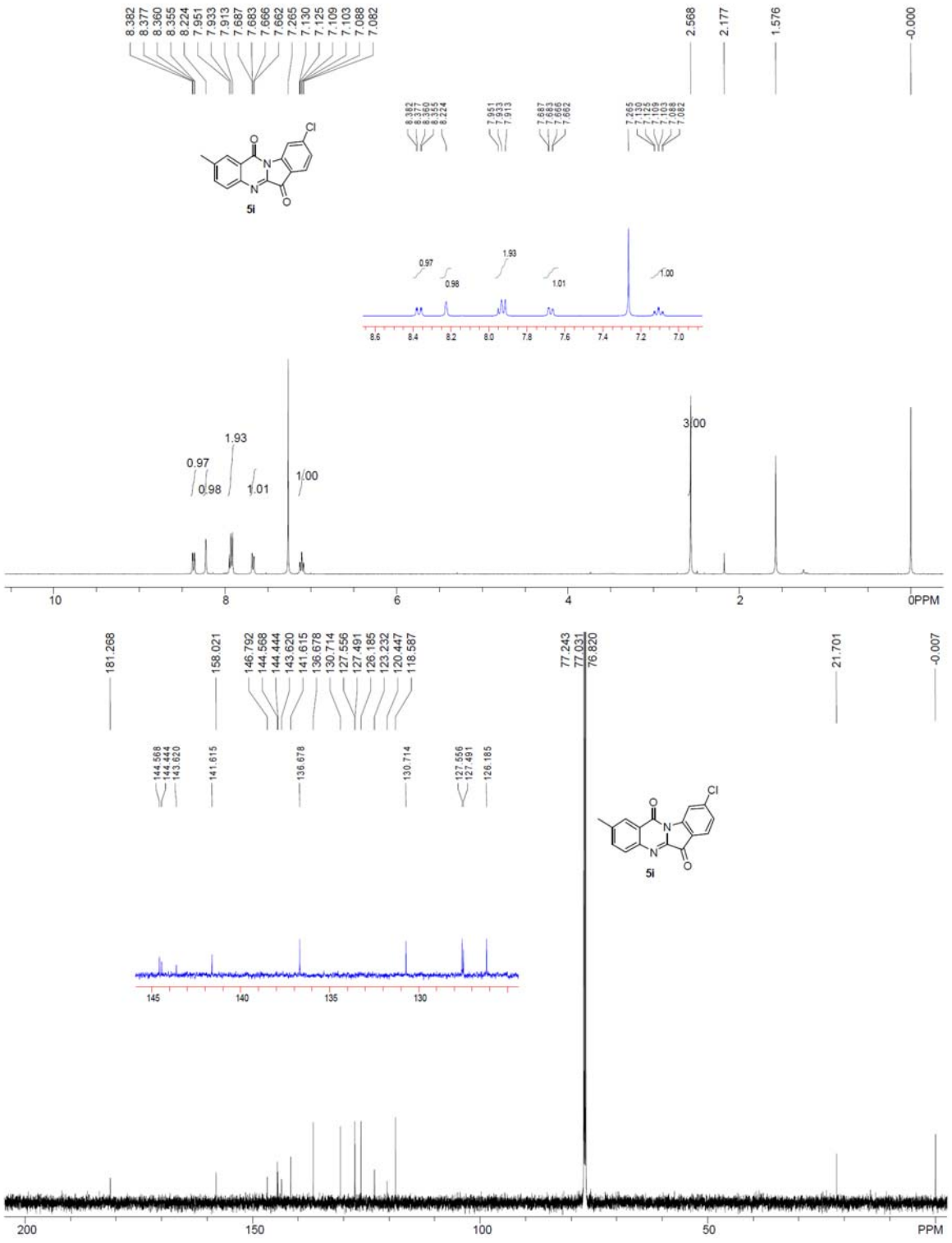
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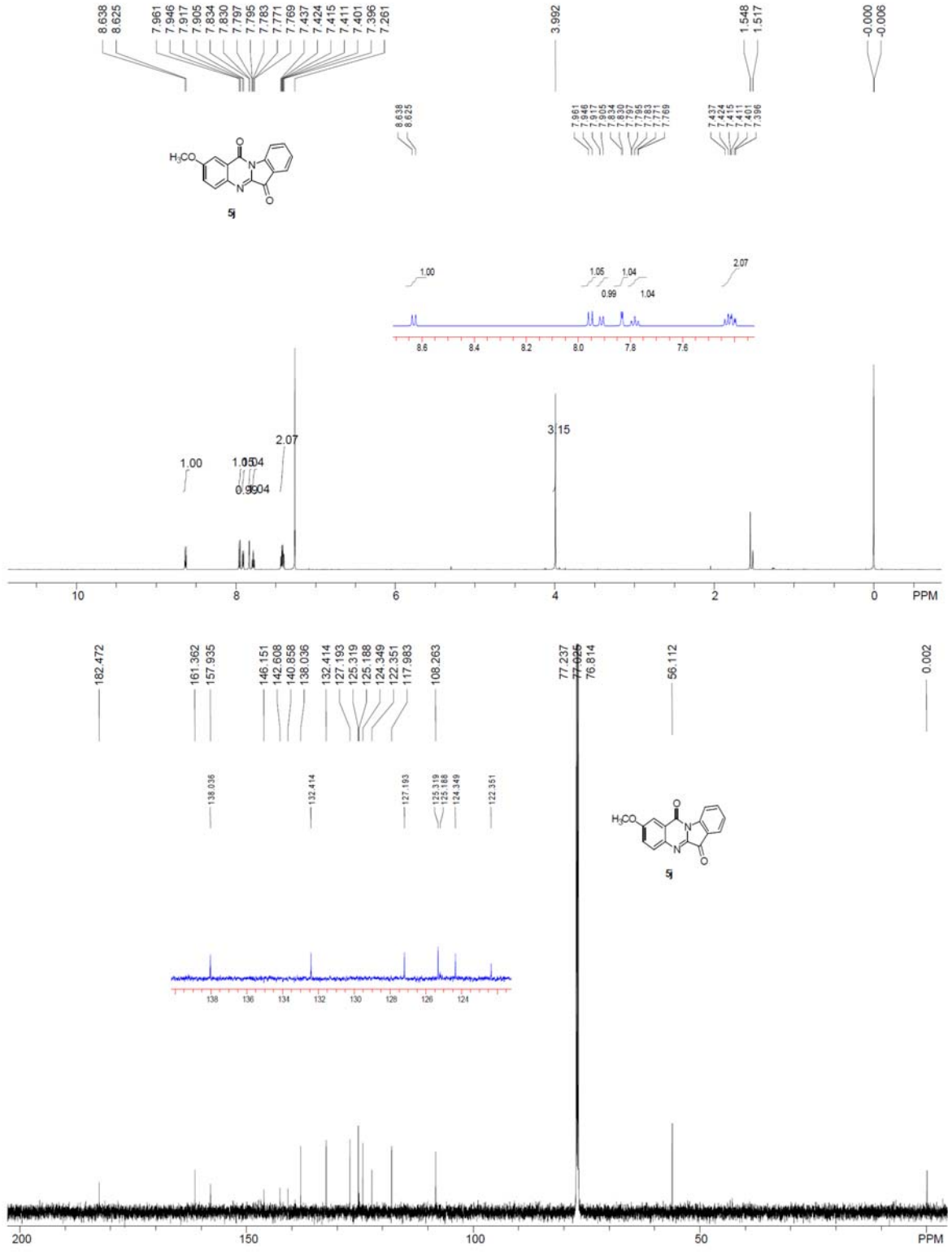
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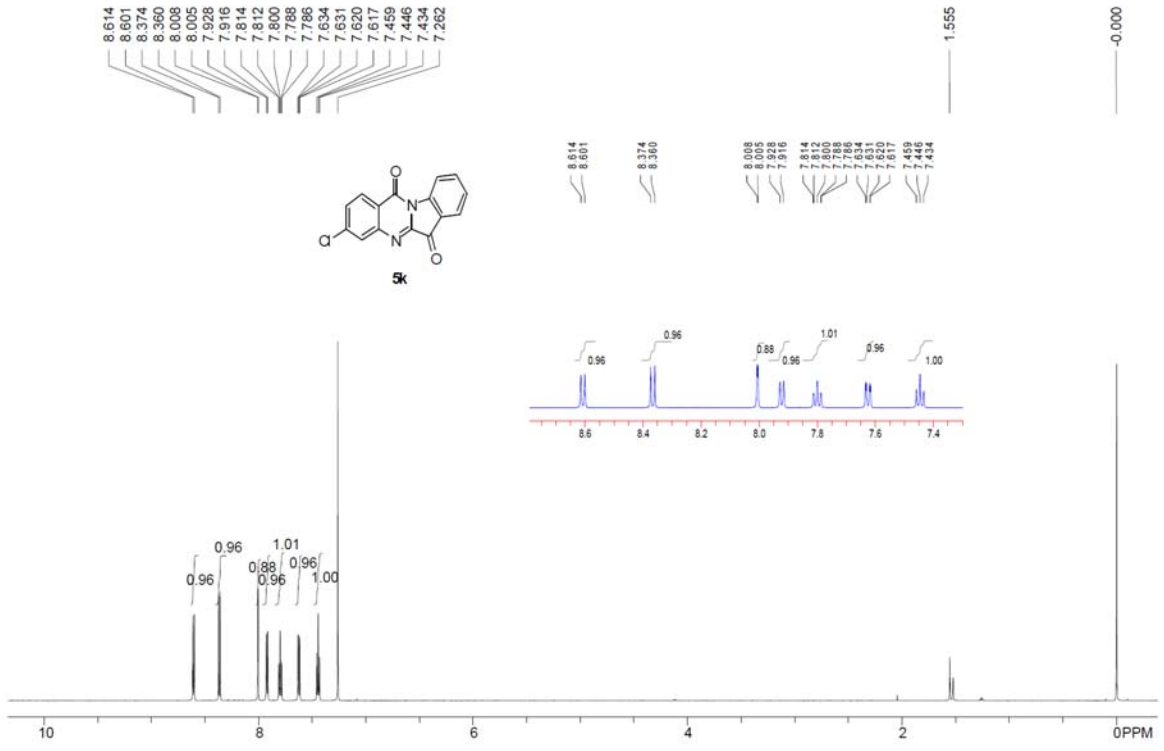
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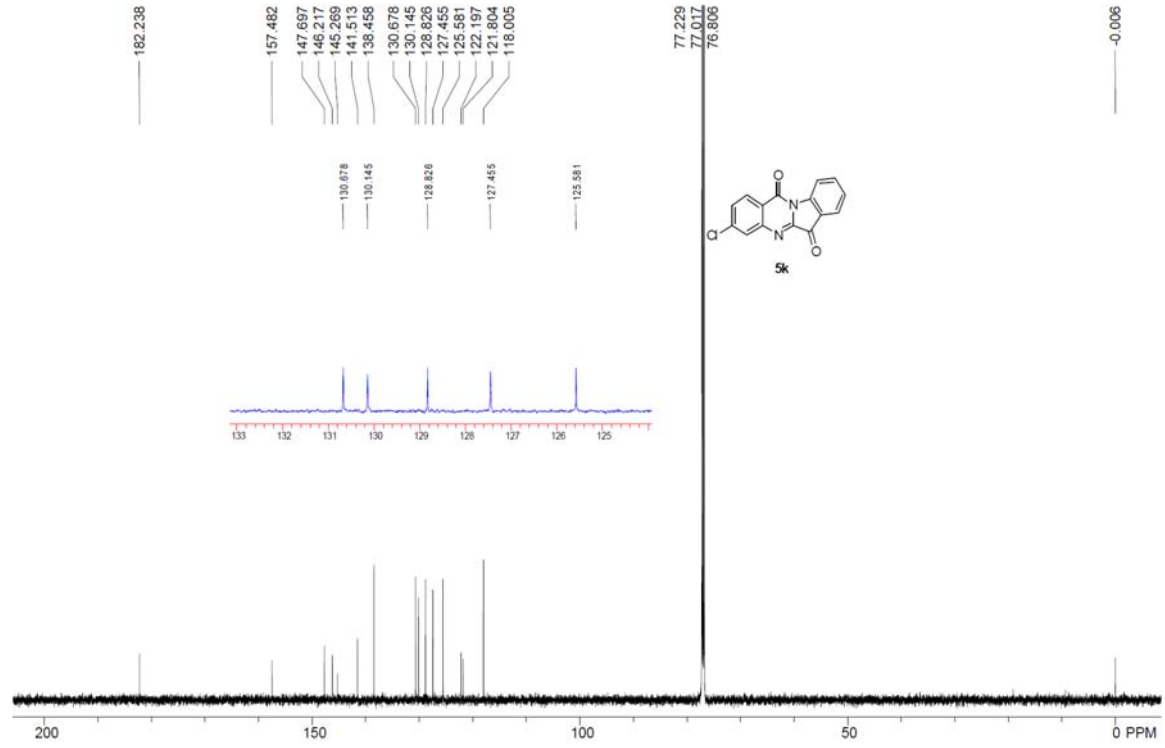
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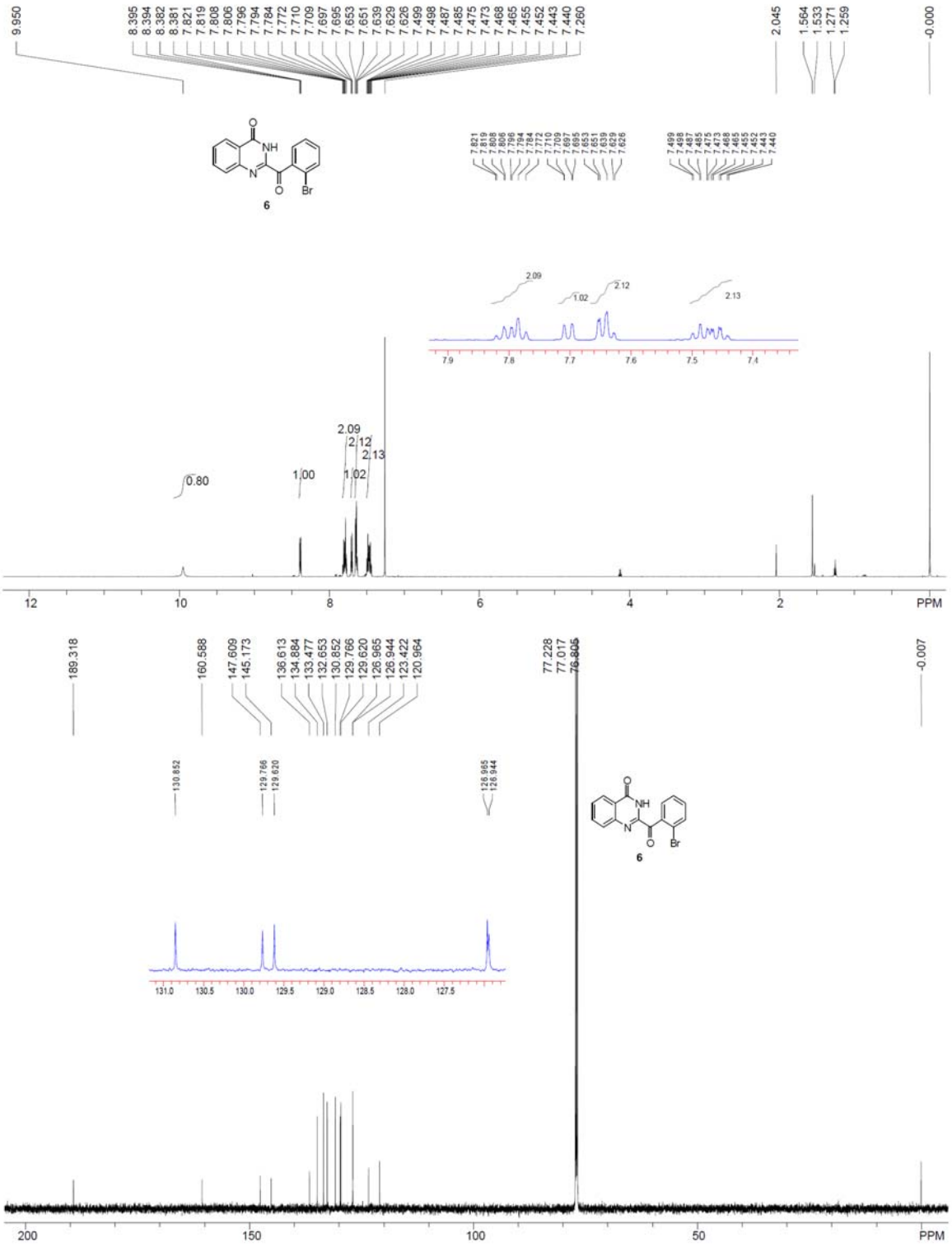
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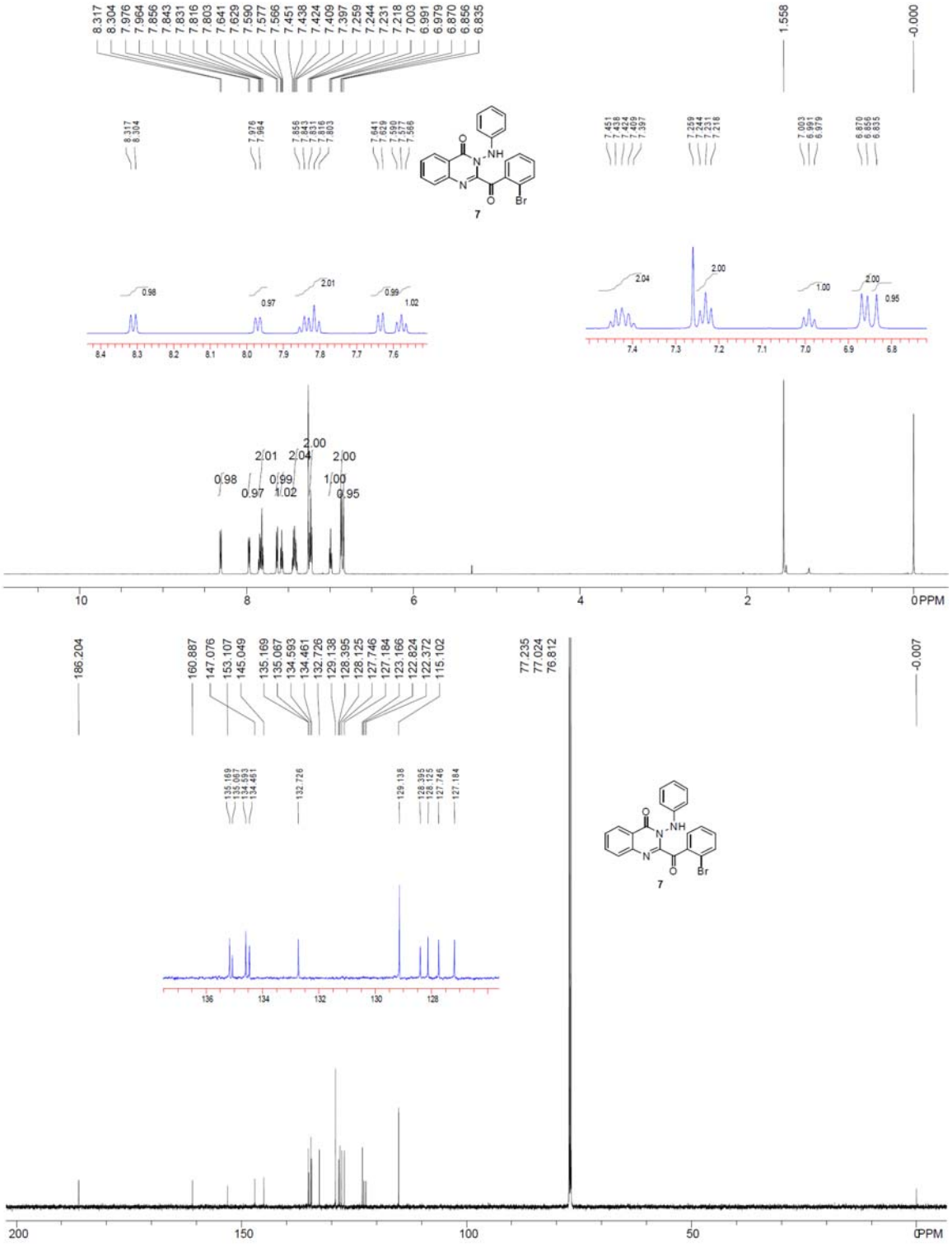
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