Supporting Information

Decarboxylative cascade cyclization of α-keto acids with 2-cyano-3-arylaniline derived acrylamides

Jia-Qi Shang,†[a] Xiang-Xiang Wang,†[a] Yangchun Xin,[b] Yi Li,[a] Bin Zhou[a] and Ya-Min Li*[a]

[a]Faculty of Life Science and Technology, Kunming University of Science and Technology, Kunming 650500, P. R. China.

[b]Katzin Diagnostic & Research PET/MR Center, Nemours/Alfred I. DuPont Hospital for Children, Wilmington, DE 19803, United States.

†These authors contributed equally.

E-mail: liym@kust.edu.cn.

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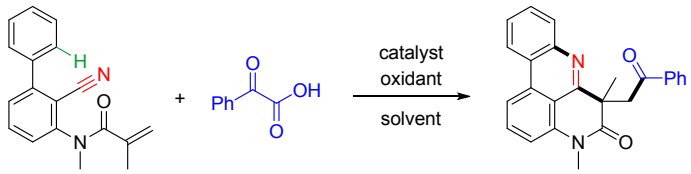
1. Reaction conditions screening



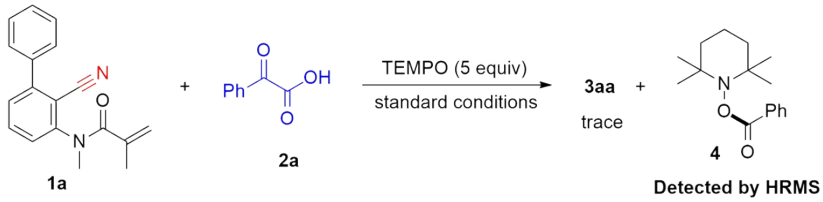
Entry[a]	**2a** (equiv)	Catalyst (mol%)	Oxidant (equiv)	Solvent (mL, v/v)	Temp (°C)	Yield[b] (%)
1	3	Ag_2CO_3 (5)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	47
2	3	AgF (5)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	33
3	3	AgOAc (5)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	28
4	3	AgOTf (5)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	46
5	3	$AgClO_4$ (5)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	47
6	3	$AgNO_3$ (5)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	52
7	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	54
8	3	Ag_2O (3)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	47
9	3	Ag_2O (10)	$(NH_4)_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	37
10	3	Ag_2O (5)	$K_2S_2O_8$ (1)	Acetone/H_2O (3, 1/1)	120	43
11	3	Ag_2O (5)	Oxone (1)	Acetone/H_2O (3, 1/1)	120	Trace
12	3	Ag_2O (5)	$Ce(SO_4)_2$ (1)	Acetone/H_2O (3, 1/1)	120	0
13	3	Ag_2O (5)	DTBP (1)	Acetone/H_2O (3, 1/1)	120	Trace
14	3	Ag_2O (5)	TBPB (1)	Acetone/H_2O (3, 1/1)	120	Trace
15	3	Ag_2O (5)	BPO (1)	Acetone/H_2O (3, 1/1)	120	11
16	3	Ag_2O (5)	DCP (1)	Acetone/H_2O (3, 1/1)	120	Trace
17	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (2)	Acetone/H_2O (3, 1/1)	120	57
18	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1)	120	61
19	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (4)	Acetone/H_2O (3, 1/1)	120	60
20	2	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1)	120	28
21	4	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1)	120	43
22	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	THF/H_2O (3, 1/1)	120	27
23	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	*i*-PrOH/H_2O (3, 1/1)	120	45
24	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	CH_3CN/H_2O (3, 1/1)	120	35
25	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Dioxane/H_2O (3, 1/1)	120	33
26	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	DMF/H_2O (3, 1/1)	120	29
27	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	DMSO/H_2O (3, 1/1)	120	Trace
28	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	DCE/H_2O (3, 1/1)	120	Trace
29	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Toluene/H_2O (3, 1/1)	120	Trace
30	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (1.5, 1/1)	120	42
31	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (4.5, 1/1)	120	38
32	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1)	90	54
33	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1)	100	61
34	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1)	110	59
35	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1)	130	47
36	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 2/1)	100	37
37	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/2)	100	Trace

38	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1.5/1)	100	48
39	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1.1)	100	61
40	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1.2)	100	58
41	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1.3)	100	66
42	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1.4)	100	58
43	3	Ag_2O (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1.5)	100	59
44	3	-	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1.3)	100	39
45	3	Ag_2O (5)	-	Acetone/H_2O (3, 1/1.3)	100	0
46	3	$AgNO_3$ (5)	$(NH_4)_2S_2O_8$ (3)	Acetone/H_2O (3, 1/1.3)	100	46

[a]Reaction conditions: **1a** (0.30 mmol), **2a**, catalyst and oxidant in solvent for 12 h under air. [b]Isolated yield of **3aa**.

2. Mechanistic studies

1) Radical-trapping experiment



Acrylamide **1a** (0.3 mmol), phenylglyoxylic acid **2a** (0.9 mmol), Ag_2O (0.015 mmol), $(NH_4)_2S_2O_8$ (0.9 mmol), TEMPO (1.5 mmol) and acetone/H_2O [3.0 mL, 1/1.3 (v/v)] were added in a sealed tube with a Teflon lined cap. The mixture was allowed to stir at 100 °C for 12 hours. After cooling down to room temperature, the mixture was under HRMS (ESI) analysis.

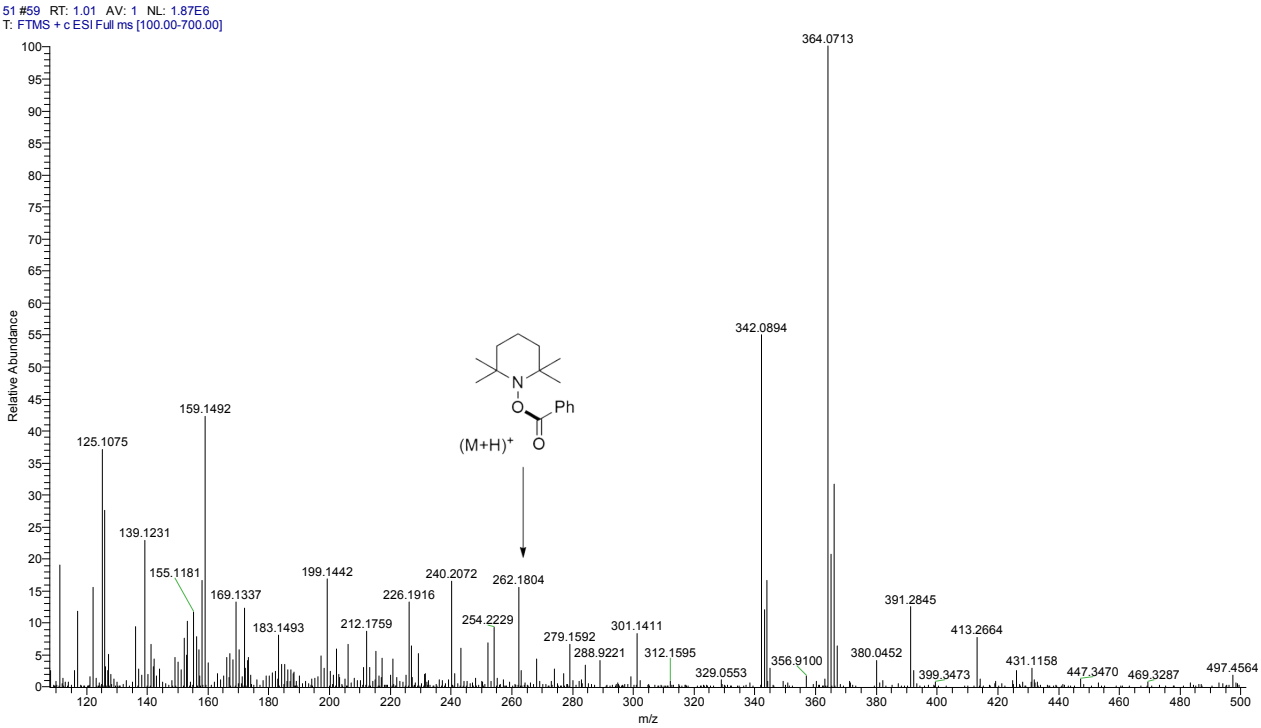
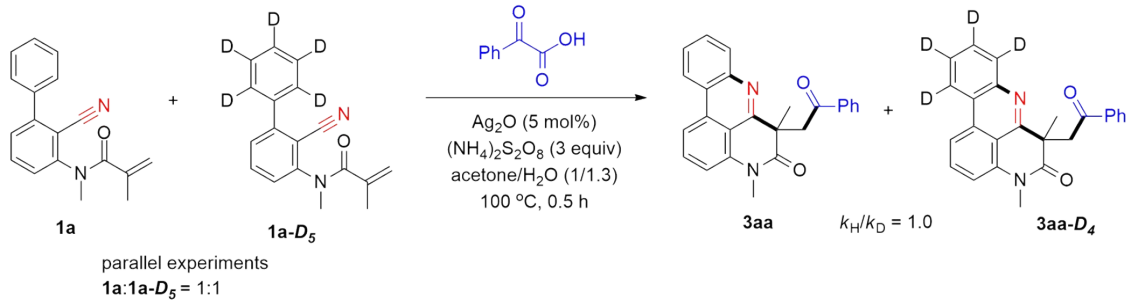


Figure S1. HRMS spectra of the reaction solution.

2) Kinetic isotope effect (KIE) experiments

a) Intermolecular KIE experiment



Acrylamide **1a** (0.3 mmol), phenylglyoxylic acid **2a** (0.9 mmol), Ag_2O (0.015 mmol), $(NH_4)_2S_2O_8$ (0.9 mmol) and acetone/H_2O [3.0 mL, 1/1.3 (v/v)] were added in a sealed tube with a Teflon lined cap. In another reaction vessel, acrylamide **1a-*D*$_5$** was used instead of **1a**. The two reactions were stirred at 100 °C for 0.5 hour. After cooling down to room temperature, the two reaction mixtures was combined, and the aqueous Na_2CO_3 (1.0 M, 10.0 mL) was added, then extracted with ethyl acetate. The organic phase was dried over anhydrous Na_2SO_4, and filtered. The filtrate was concentrated by rotary evaporation and purified by flash chromatography on silica gel with petroleum ether/ethyl acetate (6/1) as the eluent to afford the corresponding product **3aa** and **3aa-*D*$_4$** (38 mg, 17%). The products were under ^{1}H NMR analysis (Figure S2).

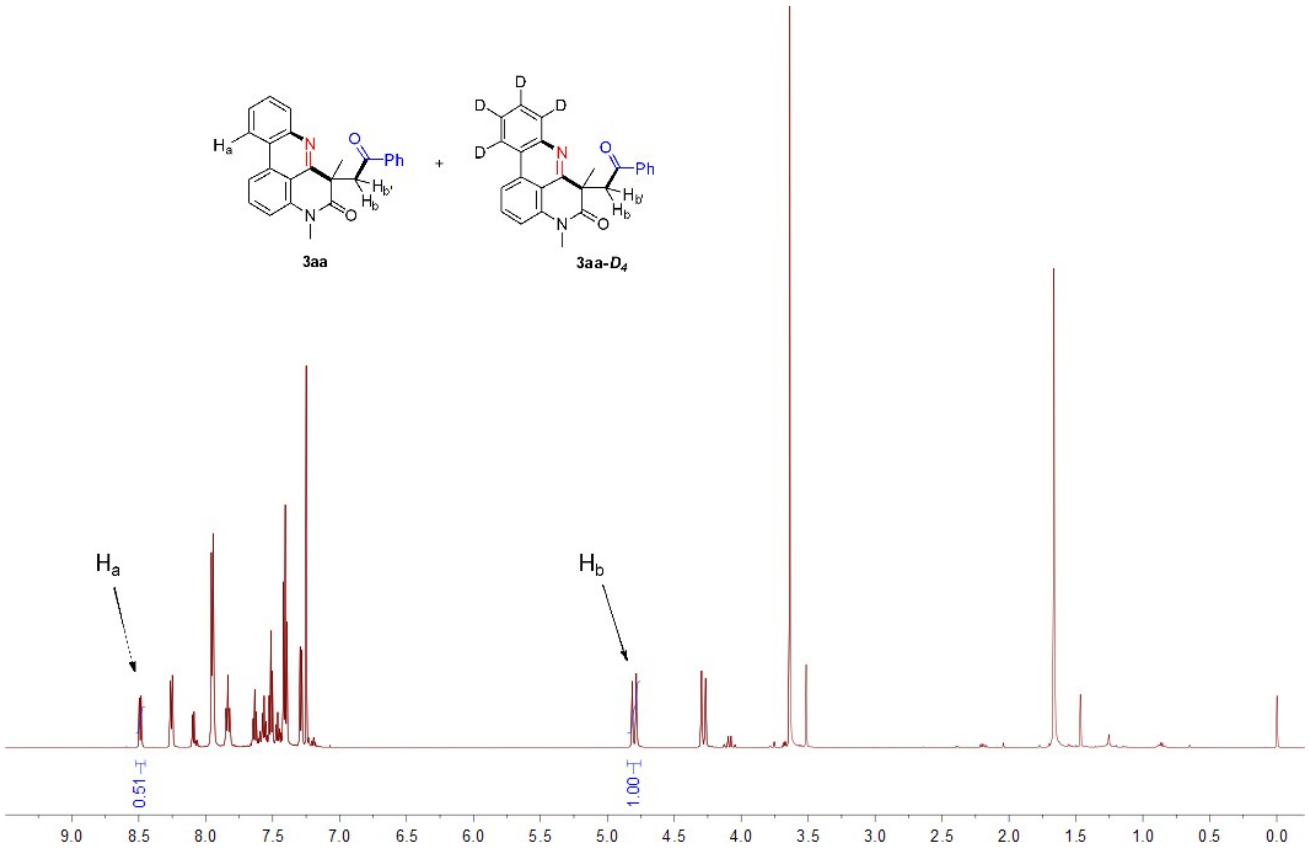
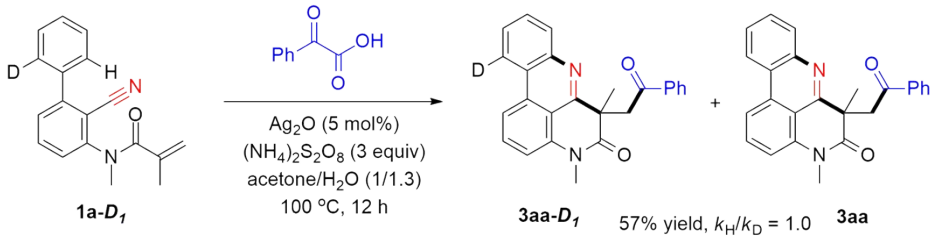


Figure S2. ^{1}H NMR spectra of the mixture of compound **3aa** and **3aa-*D*$_4$**.

b) Intramolecular KIE experiment



Acrylamide **1a-*D*$_1$** (0.3 mmol), phenylglyoxylic acid **2a** (0.9 mmol), Ag_2O (0.015 mmol), $(NH_4)_2S_2O_8$ (0.9 mmol) and acetone/H_2O [3.0 mL, 1/1.3 (v/v)] were added in a sealed tube with a Teflon lined cap. The reaction was stirred at 100 °C for 12 hours. After cooling down to room temperature, the aqueous Na_2CO_3 (1.0 M, 5.0 mL) was added, then extracted with ethyl acetate. The organic phase was dried over anhydrous Na_2SO_4, and filtered. The filtrate was concentrated by rotary evaporation and purified by flash chromatography on silica gel with petroleum ether/ethyl acetate (6/1) as the eluent to afford the corresponding product **3aa** and **3aa-*D*$_1$** (65 mg, 57%). The products were under ^{1}H NMR analysis (Figure S3).

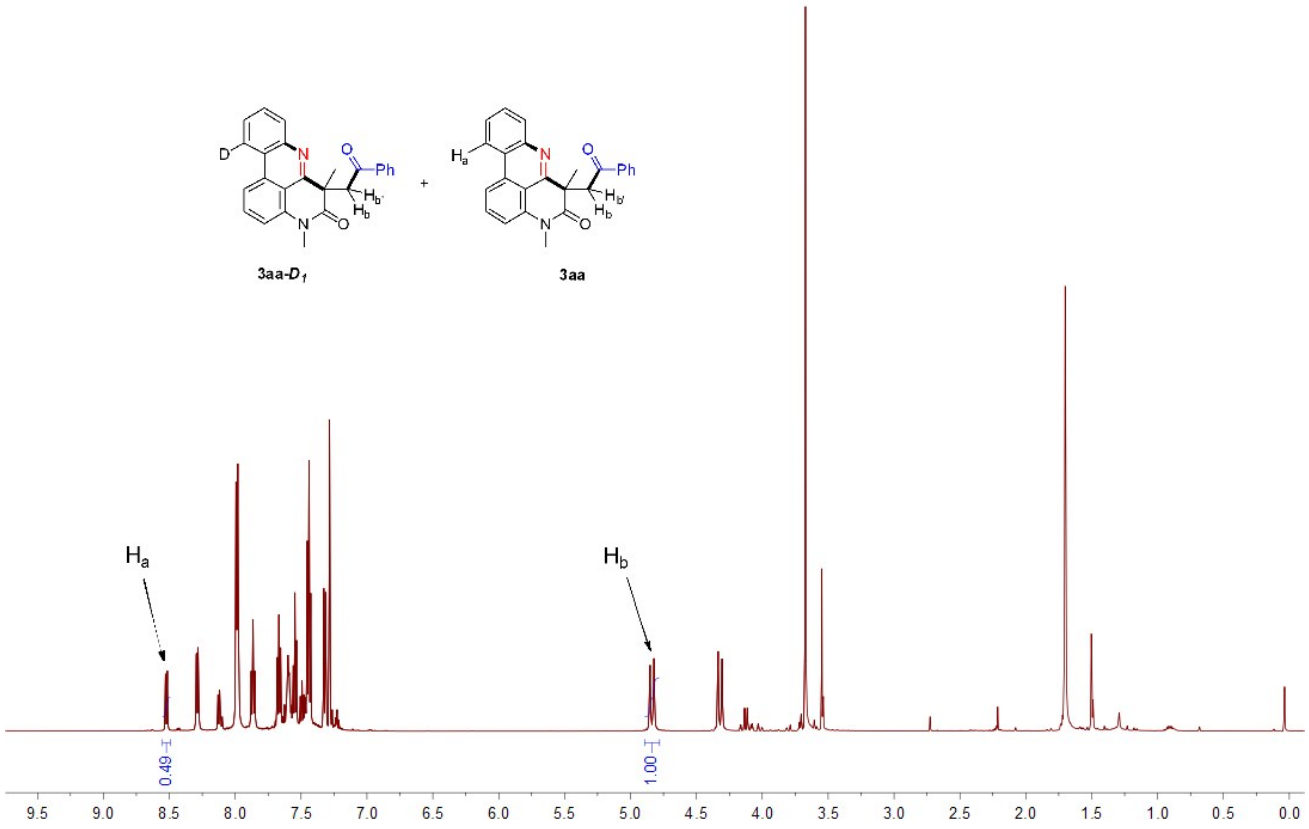
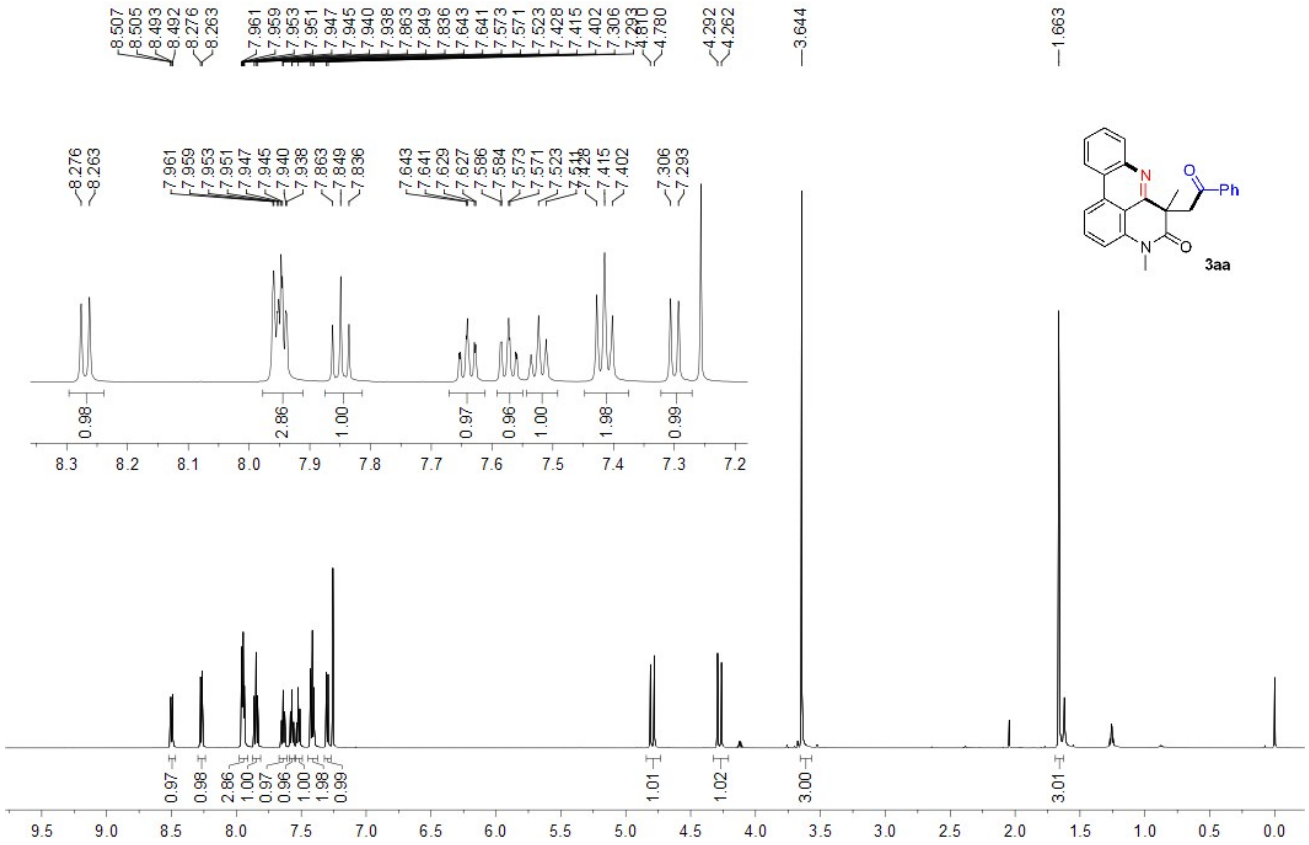
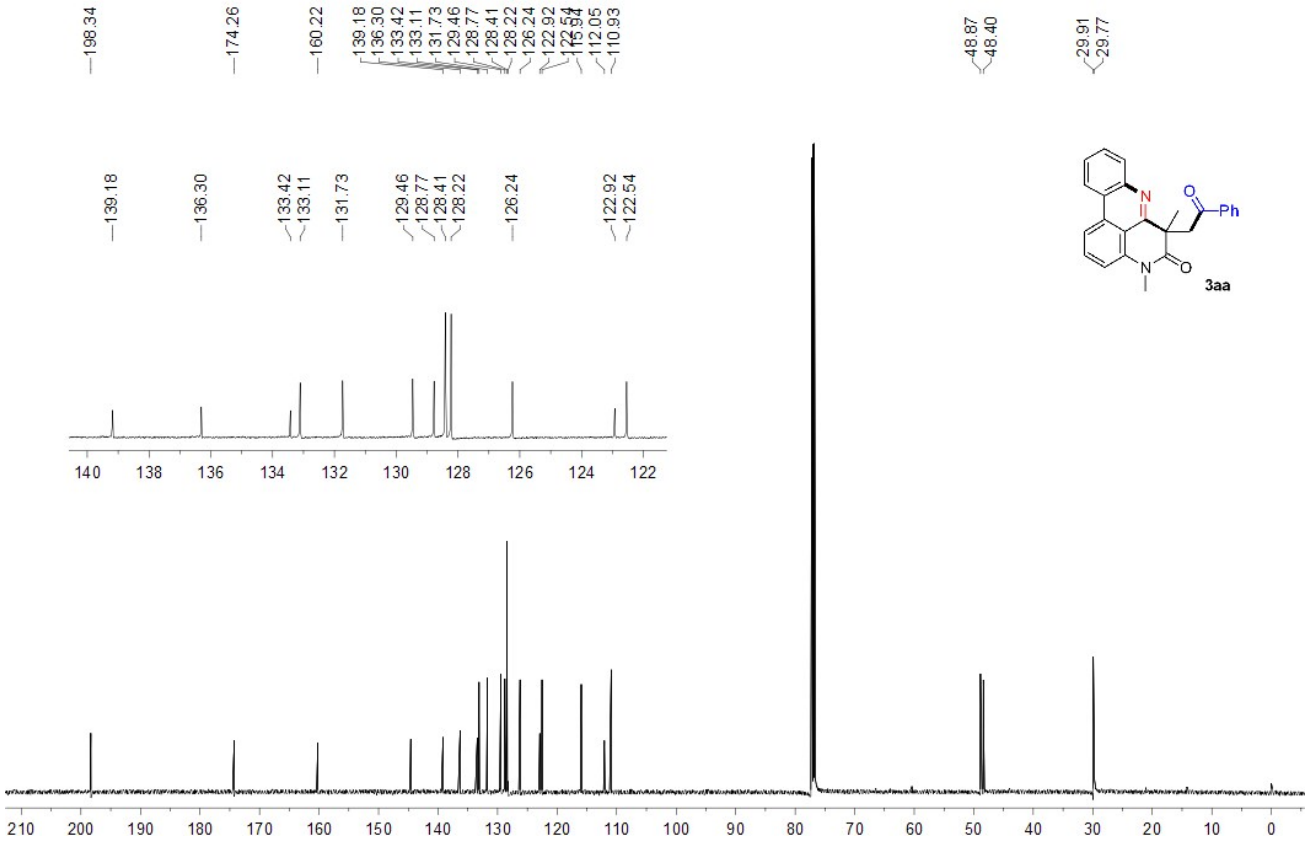
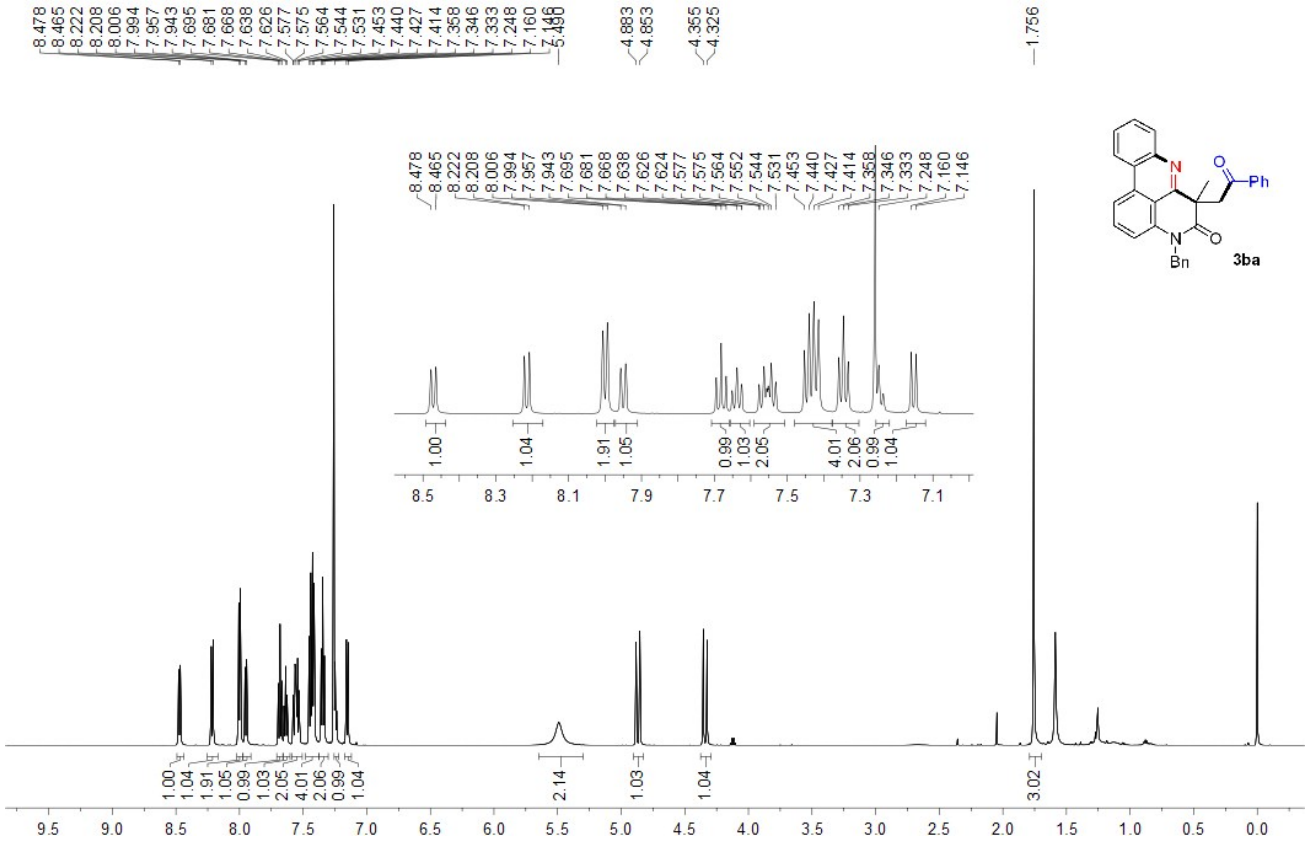


Figure S3. ^{1}H NMR spectra of the mixture of compound **3aa** and **3aa-*D*$_1$**.

3. Charts of compounds



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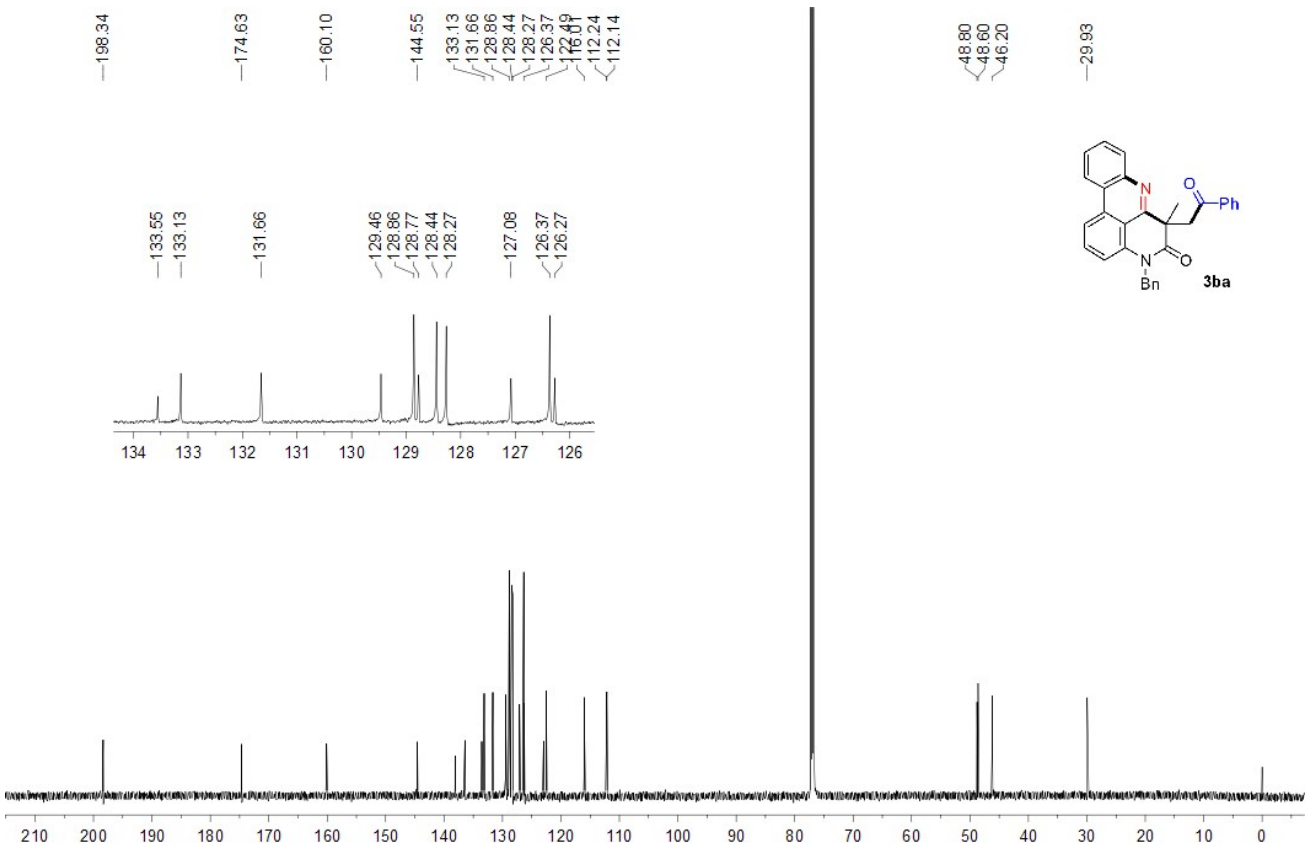
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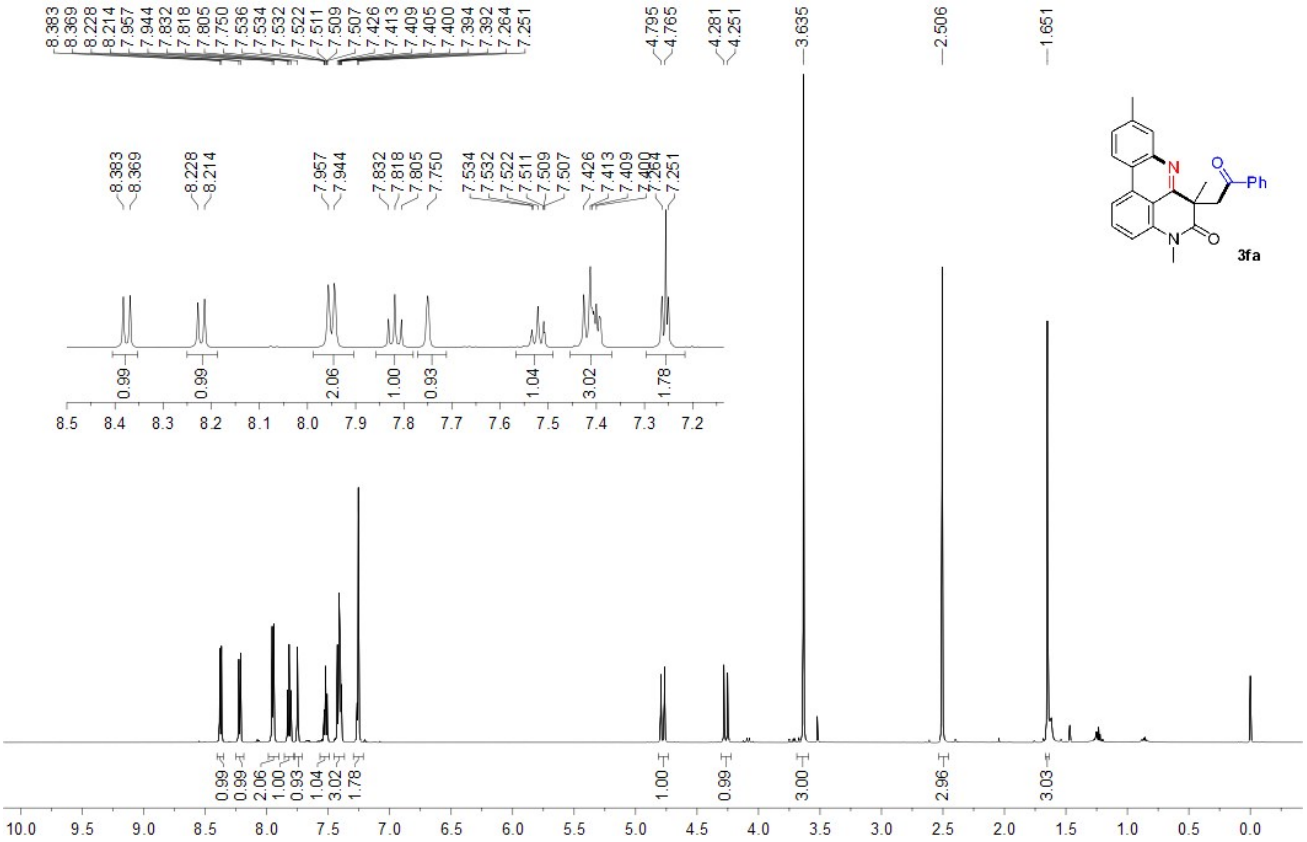
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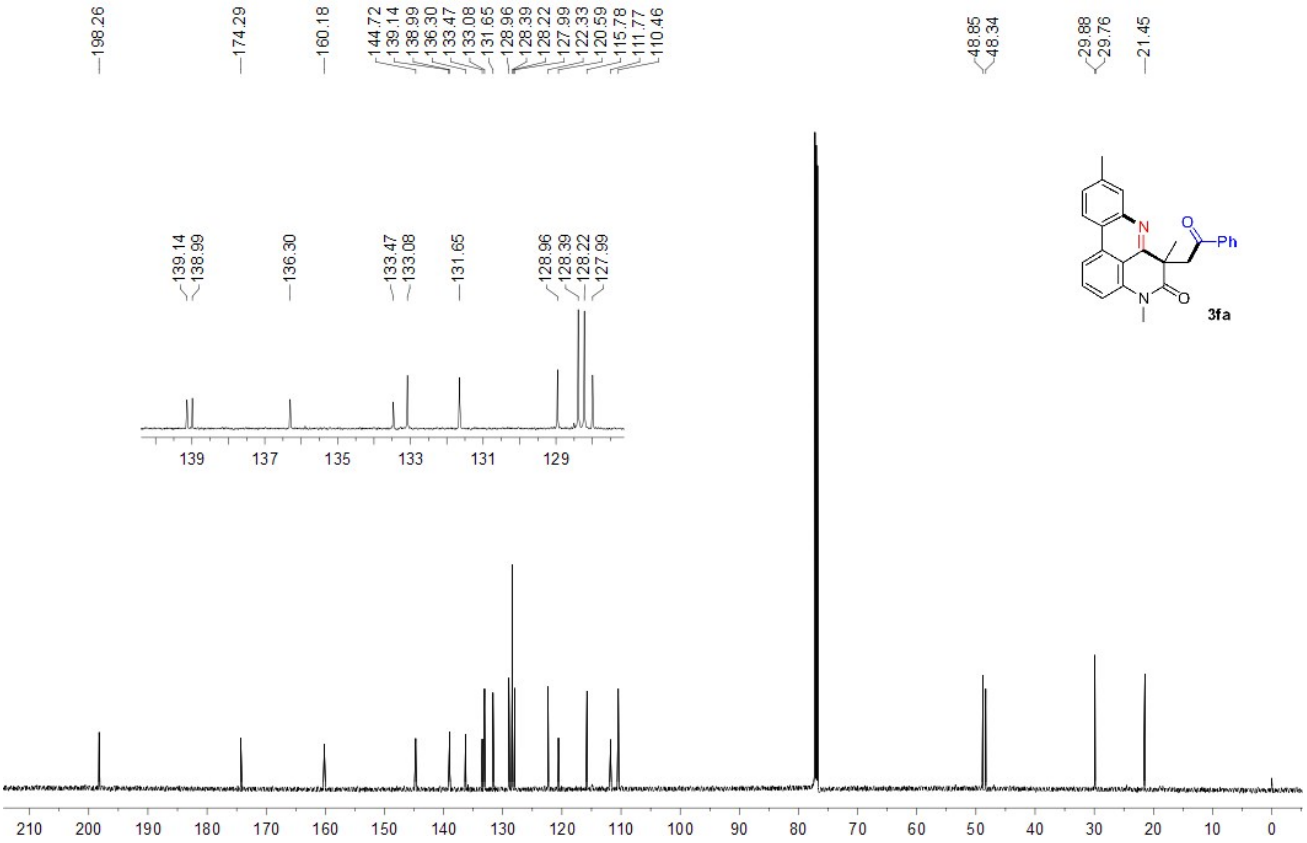
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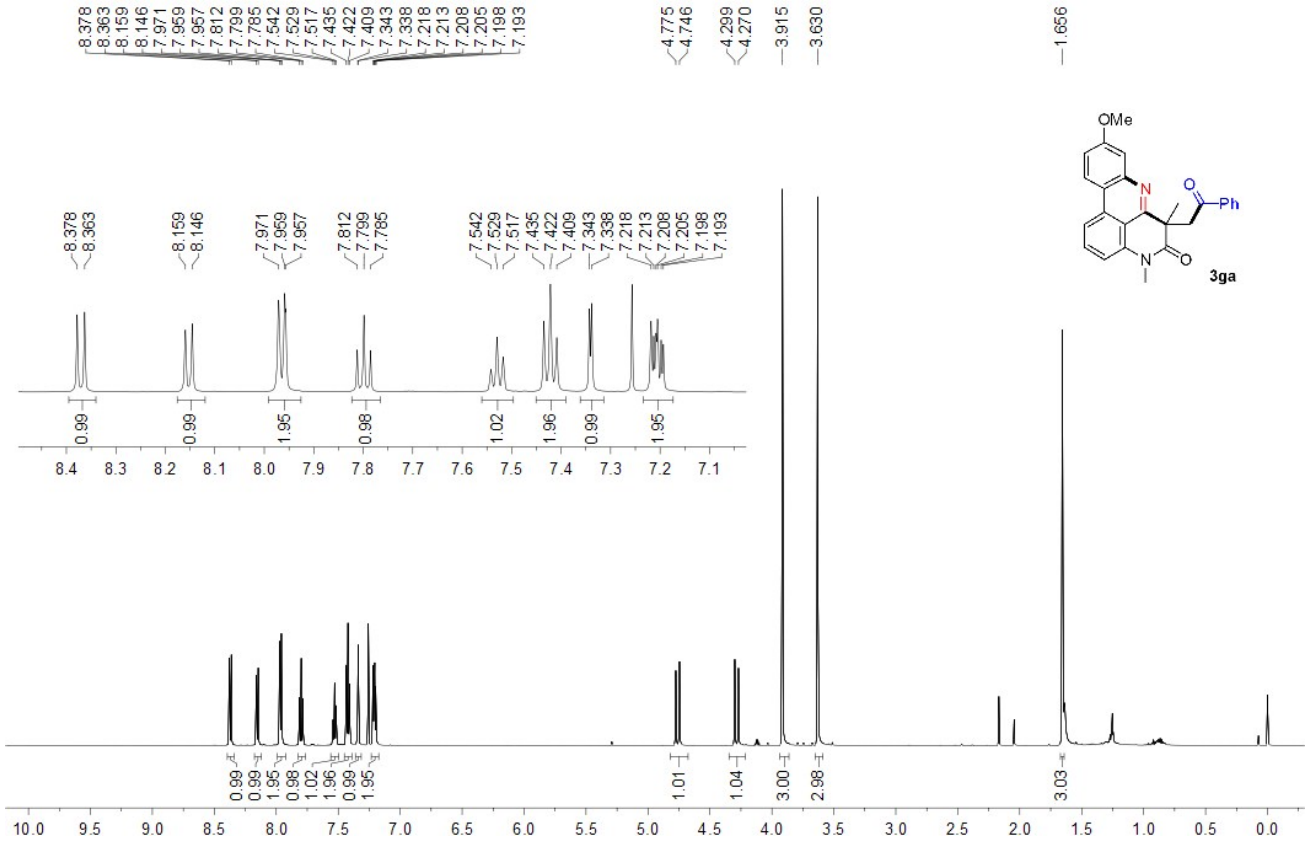
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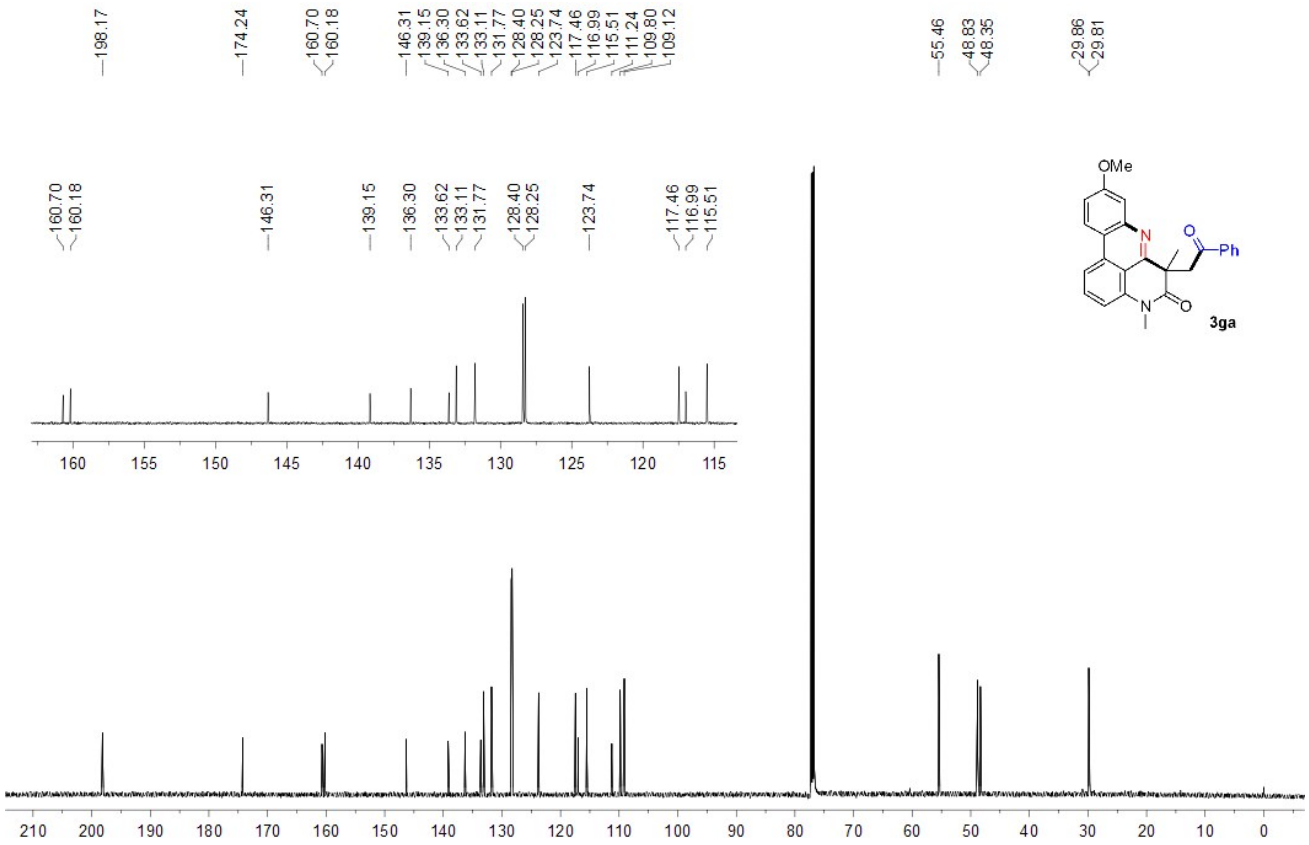
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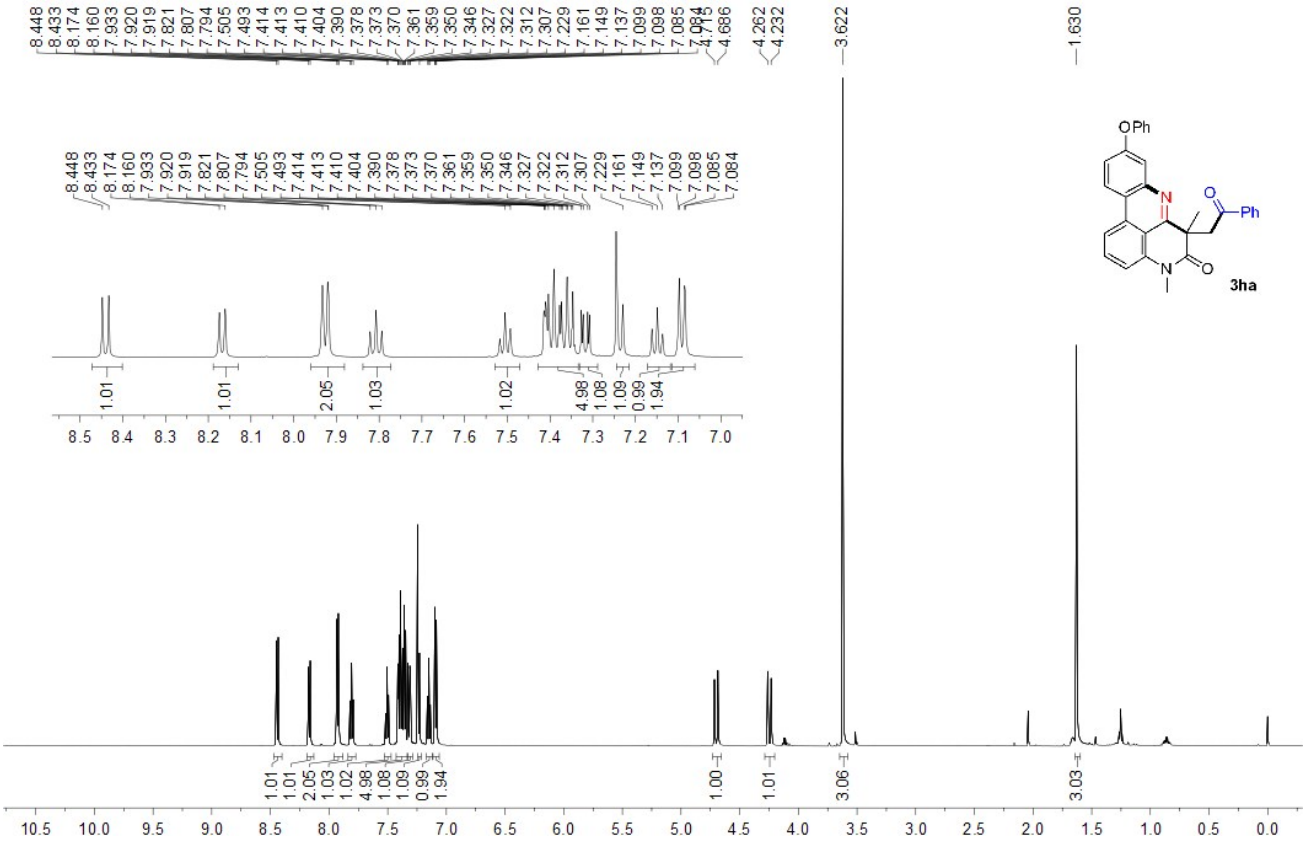
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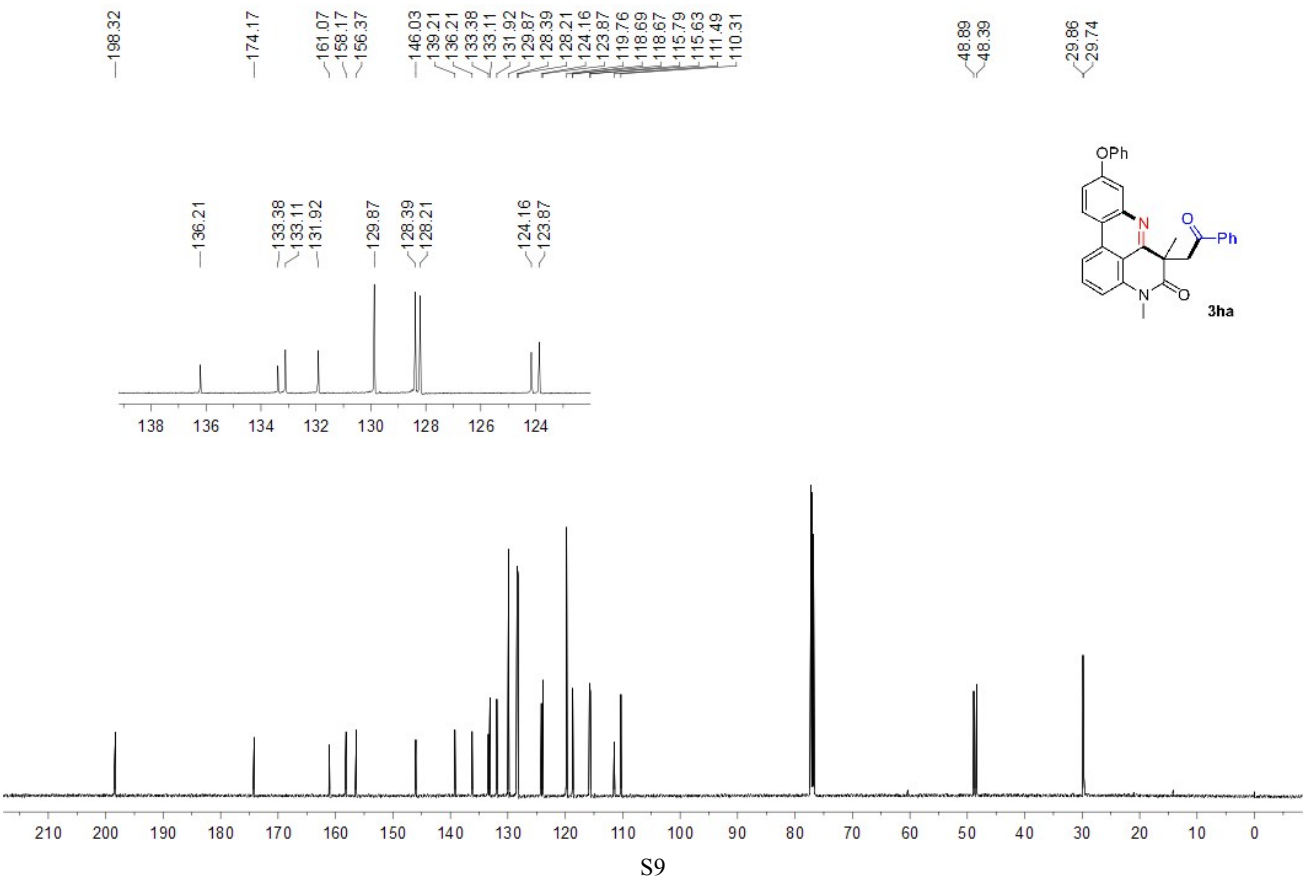
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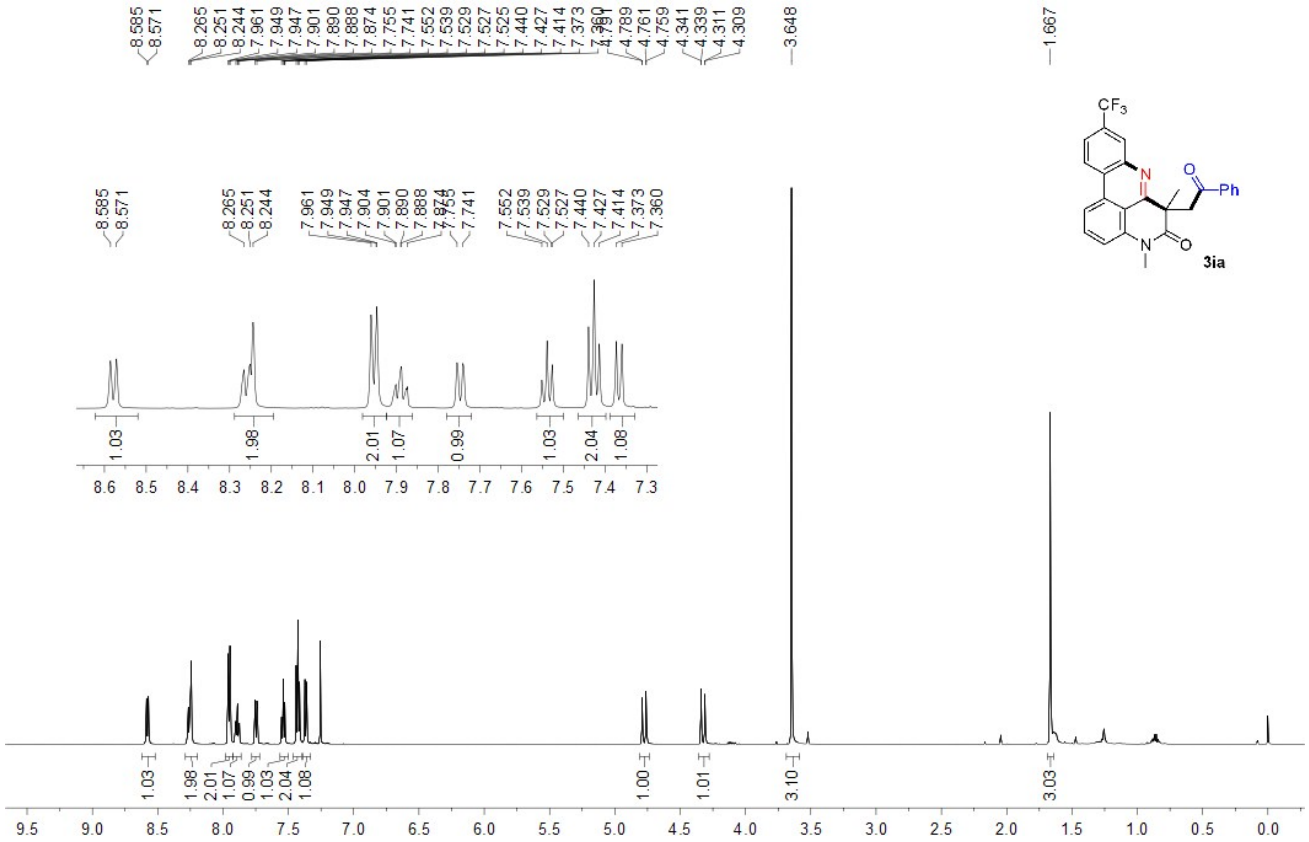
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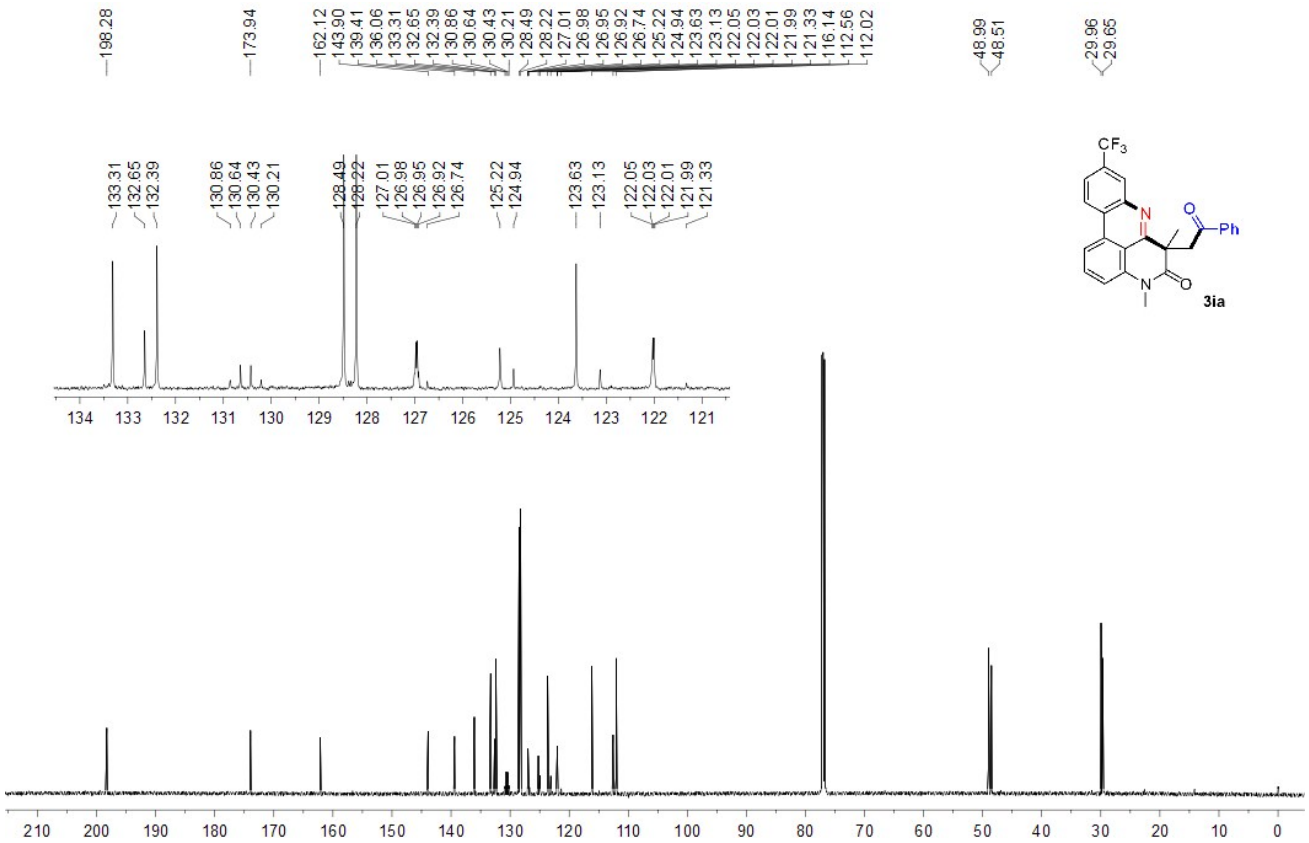
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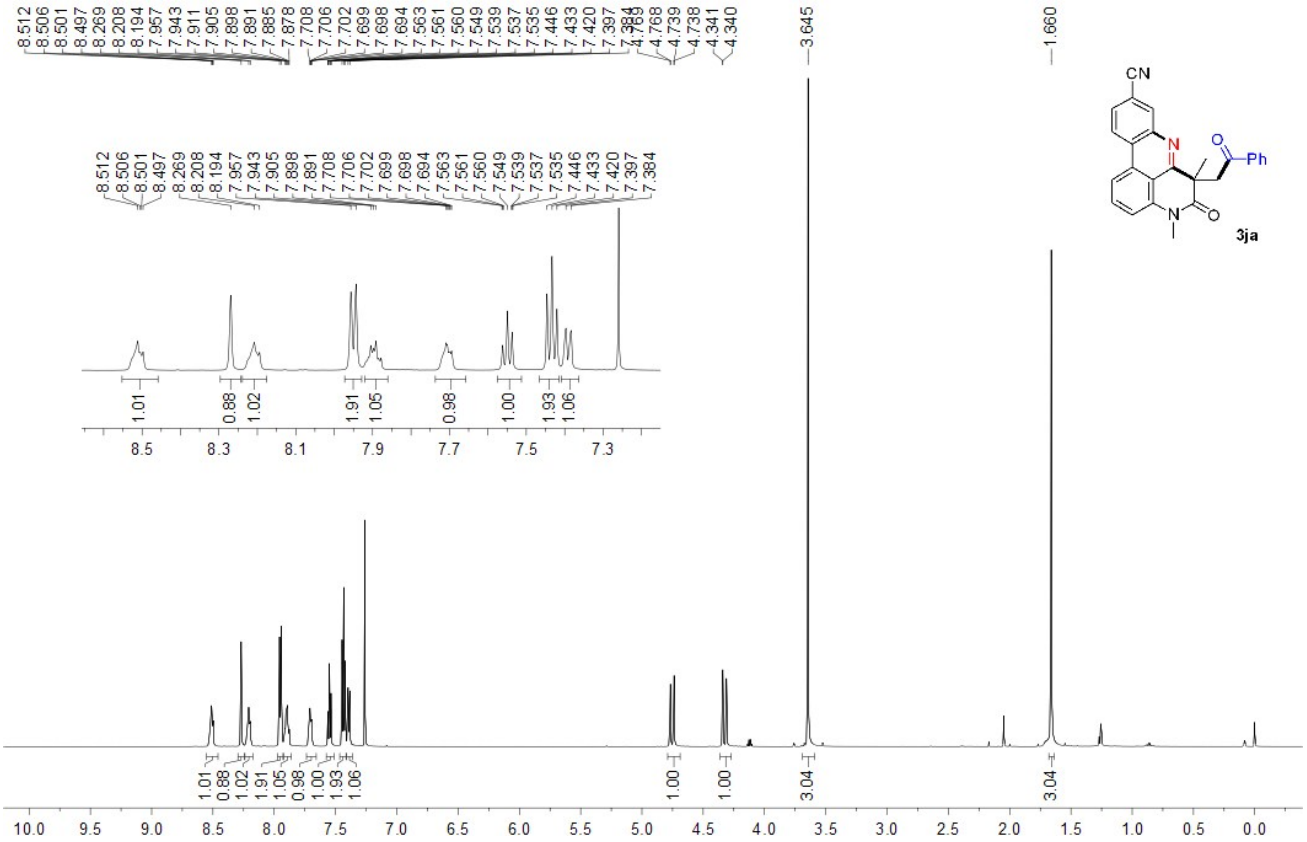
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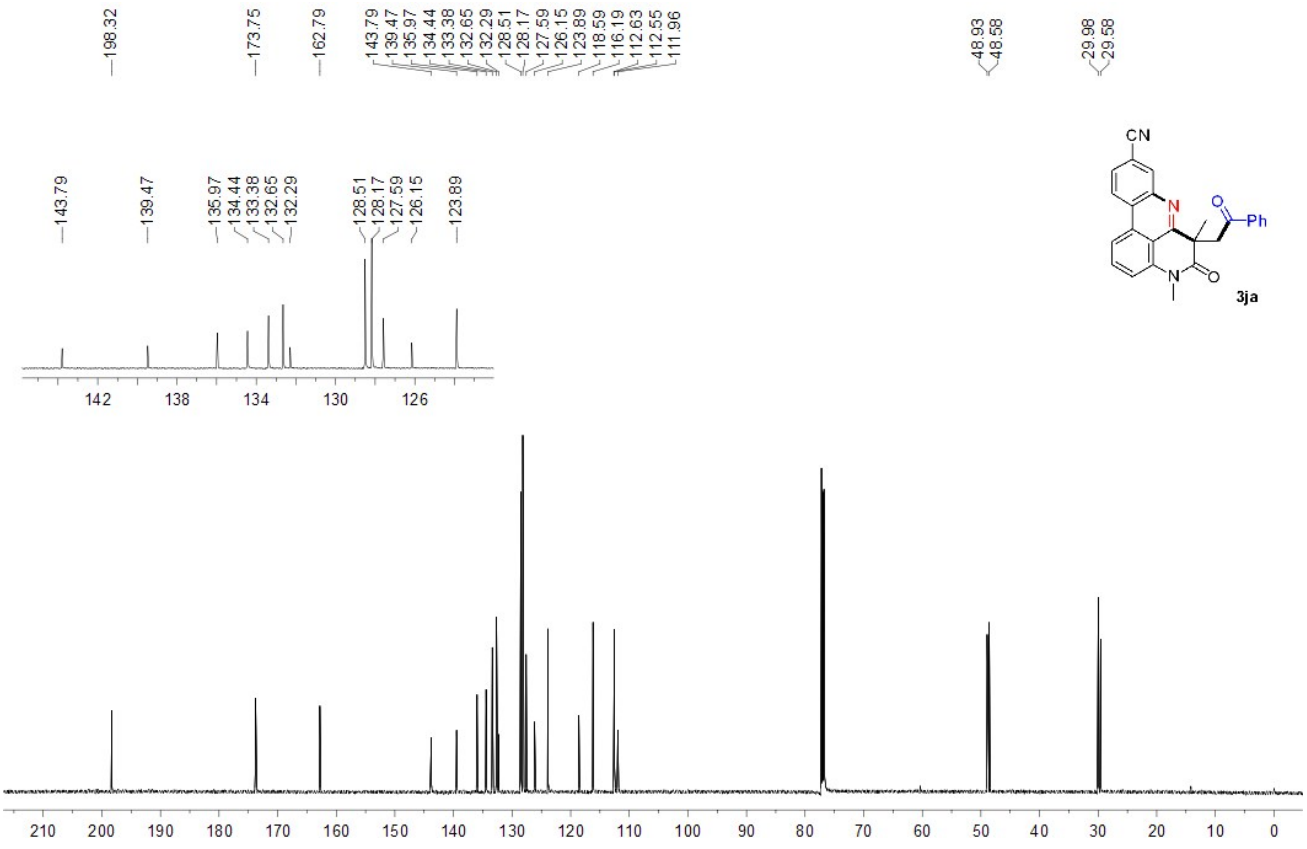
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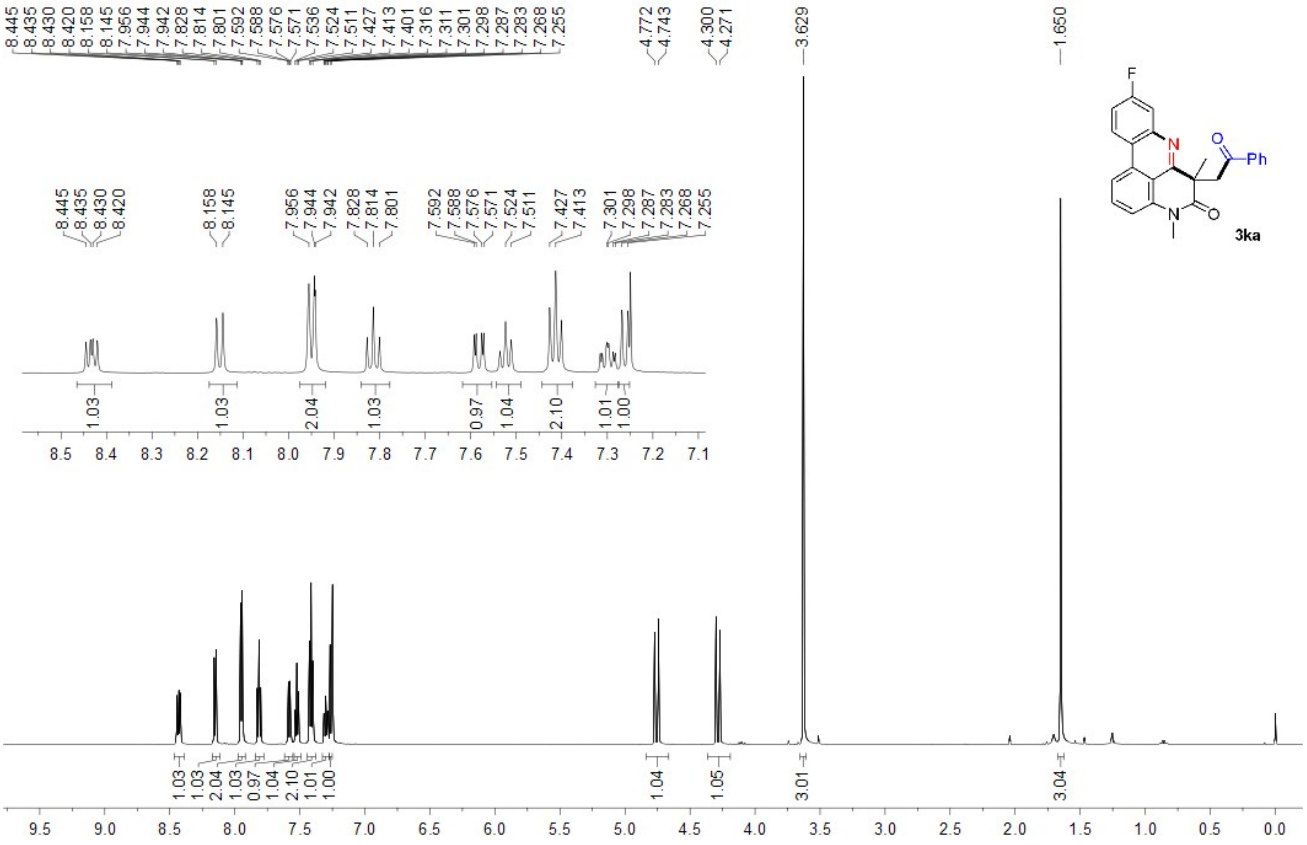
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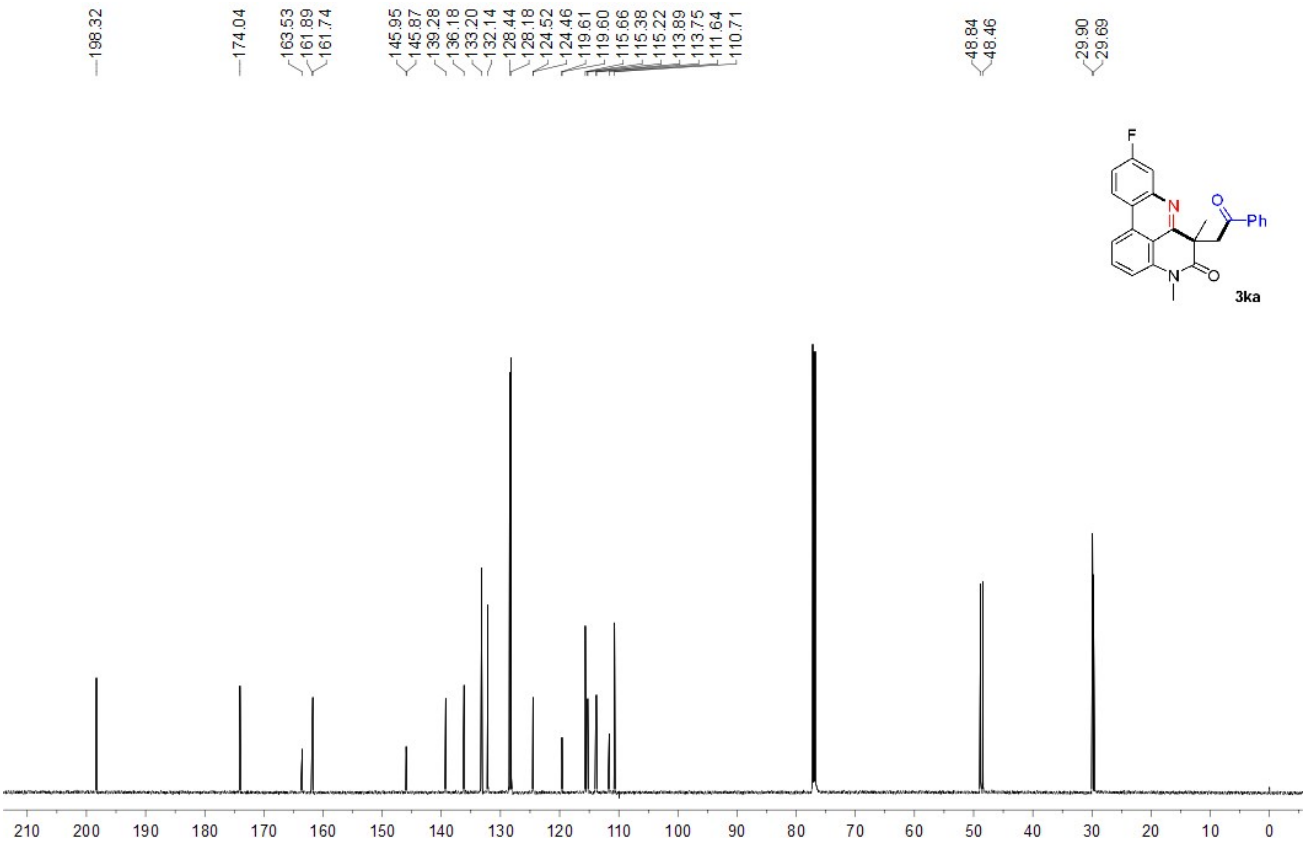
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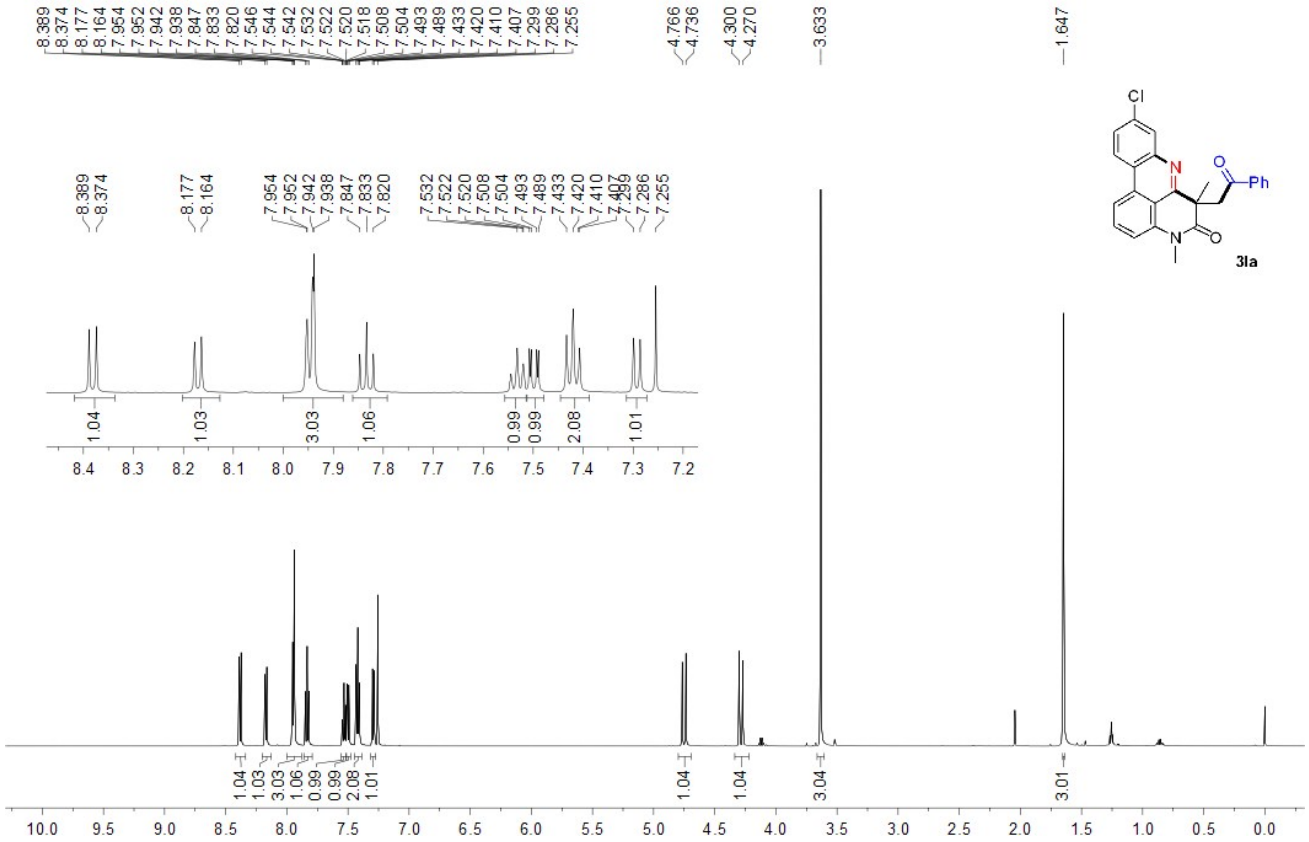
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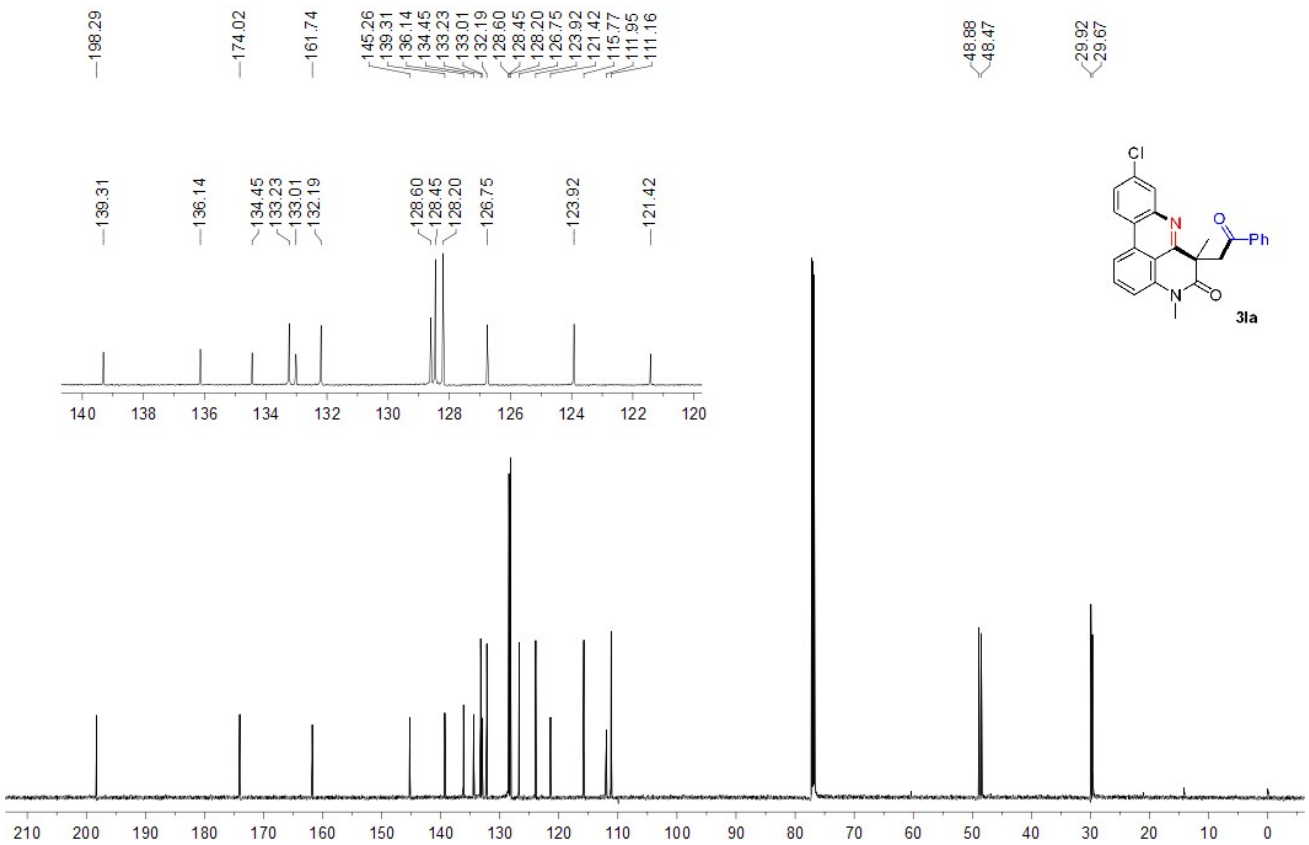
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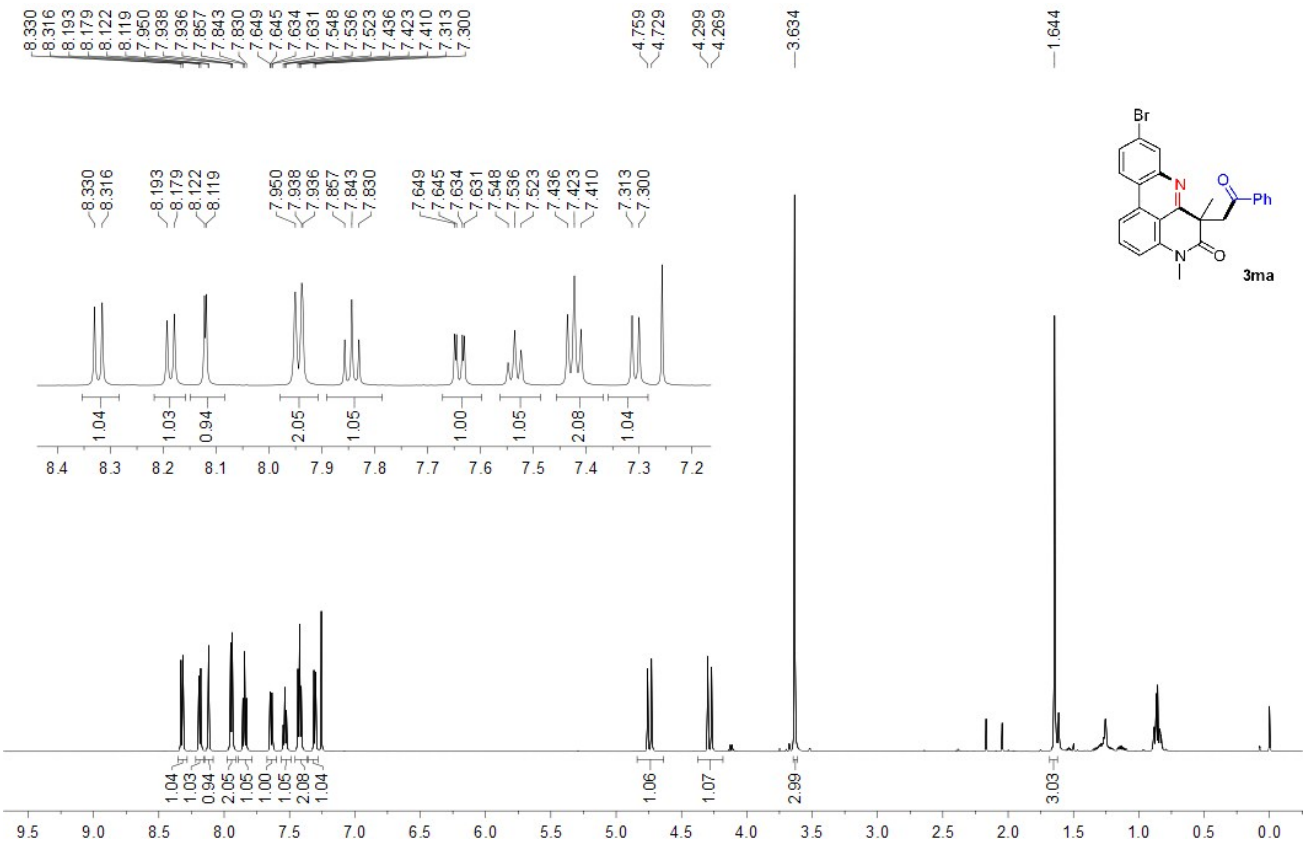
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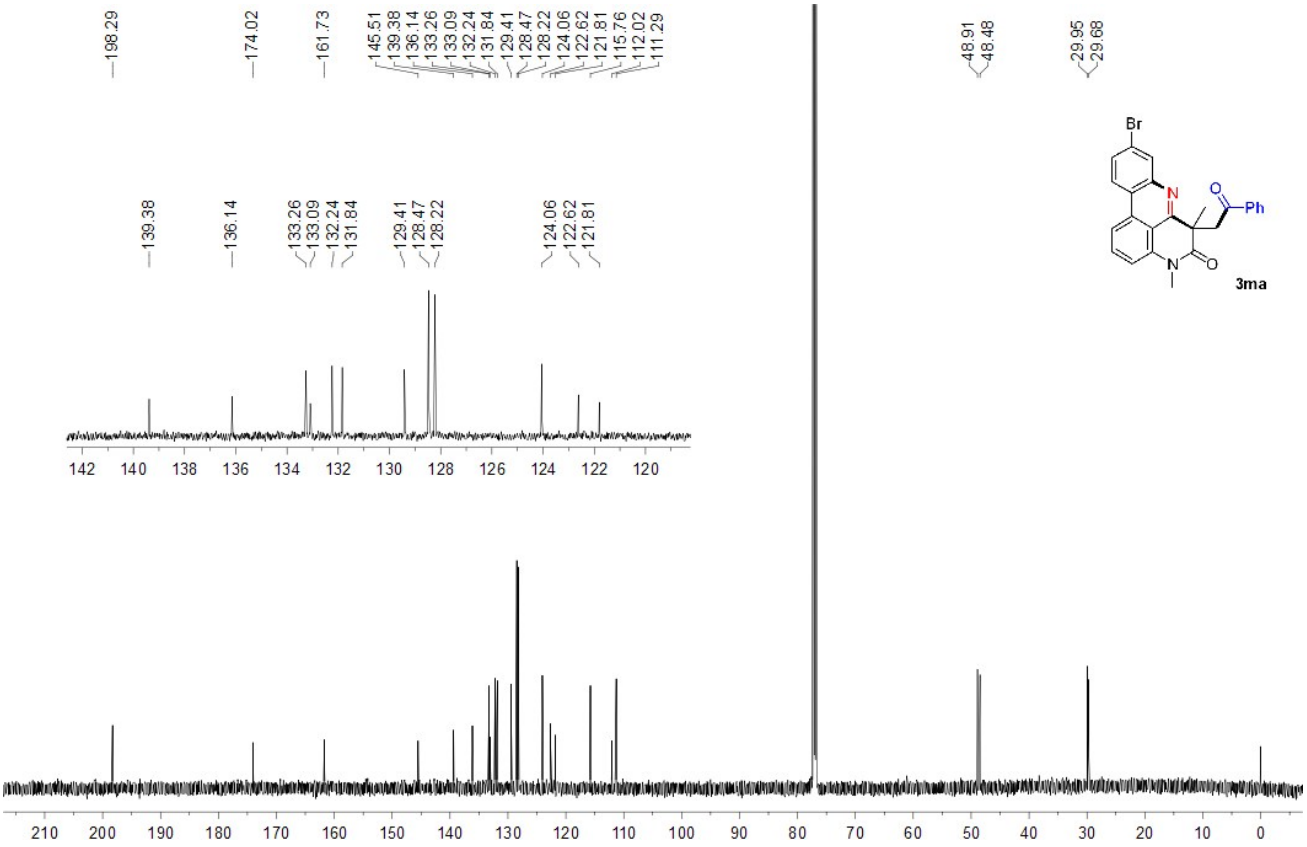
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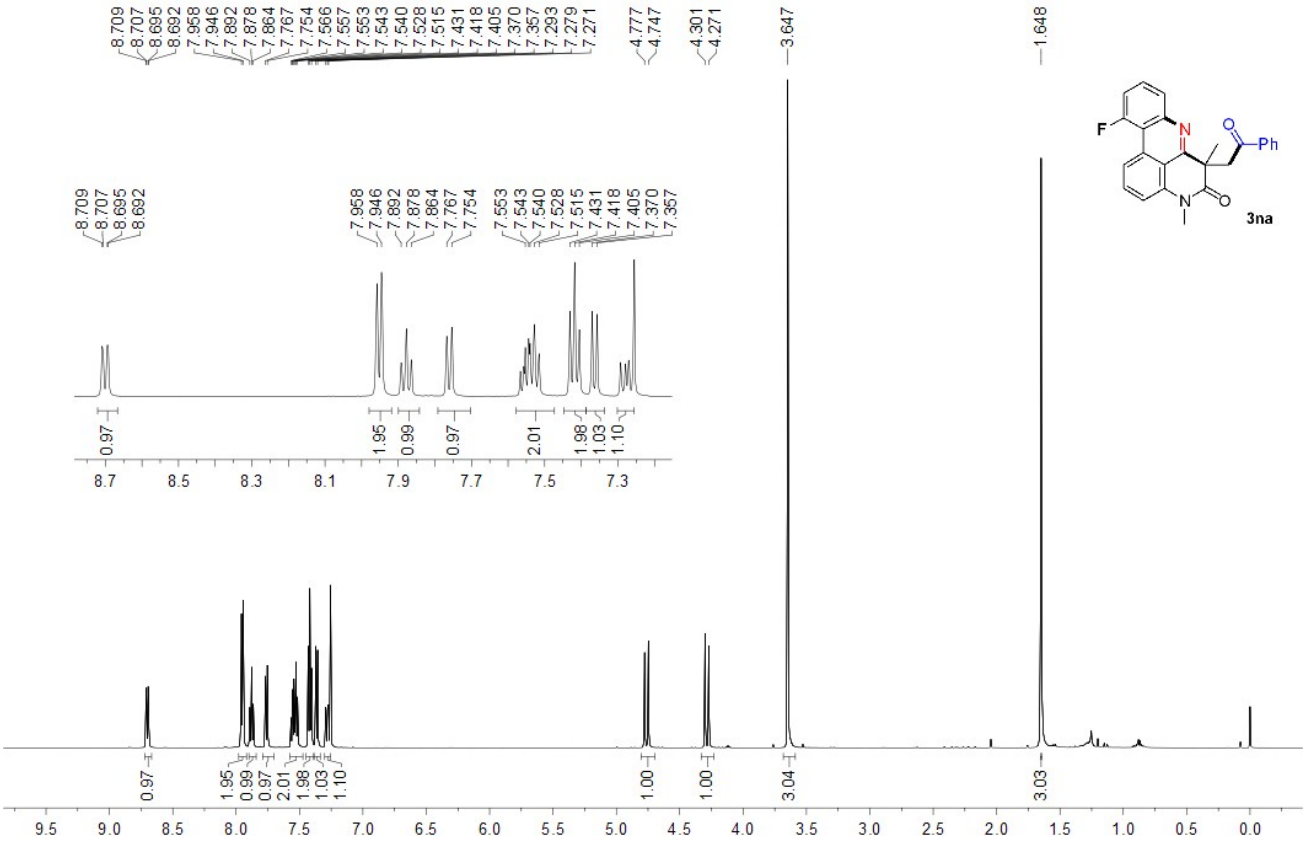
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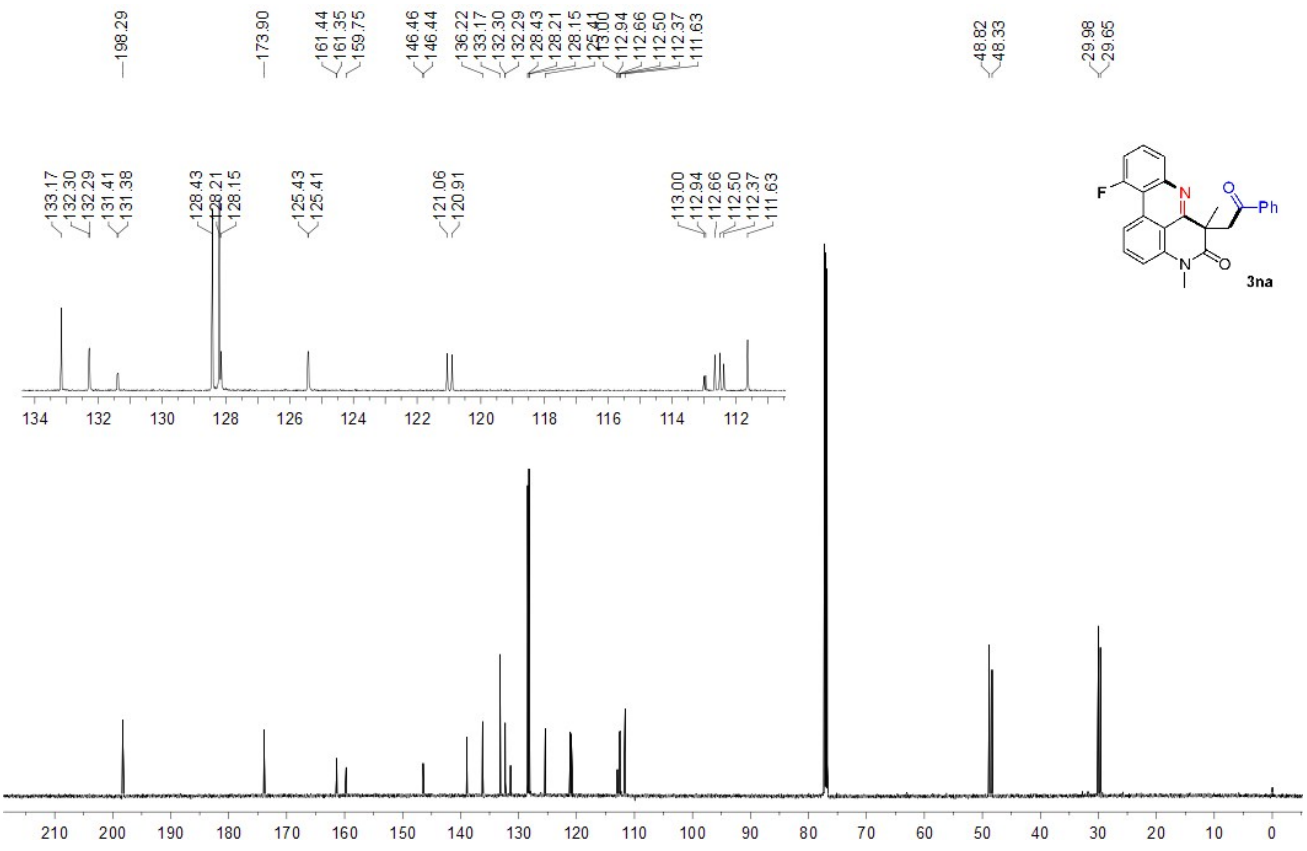
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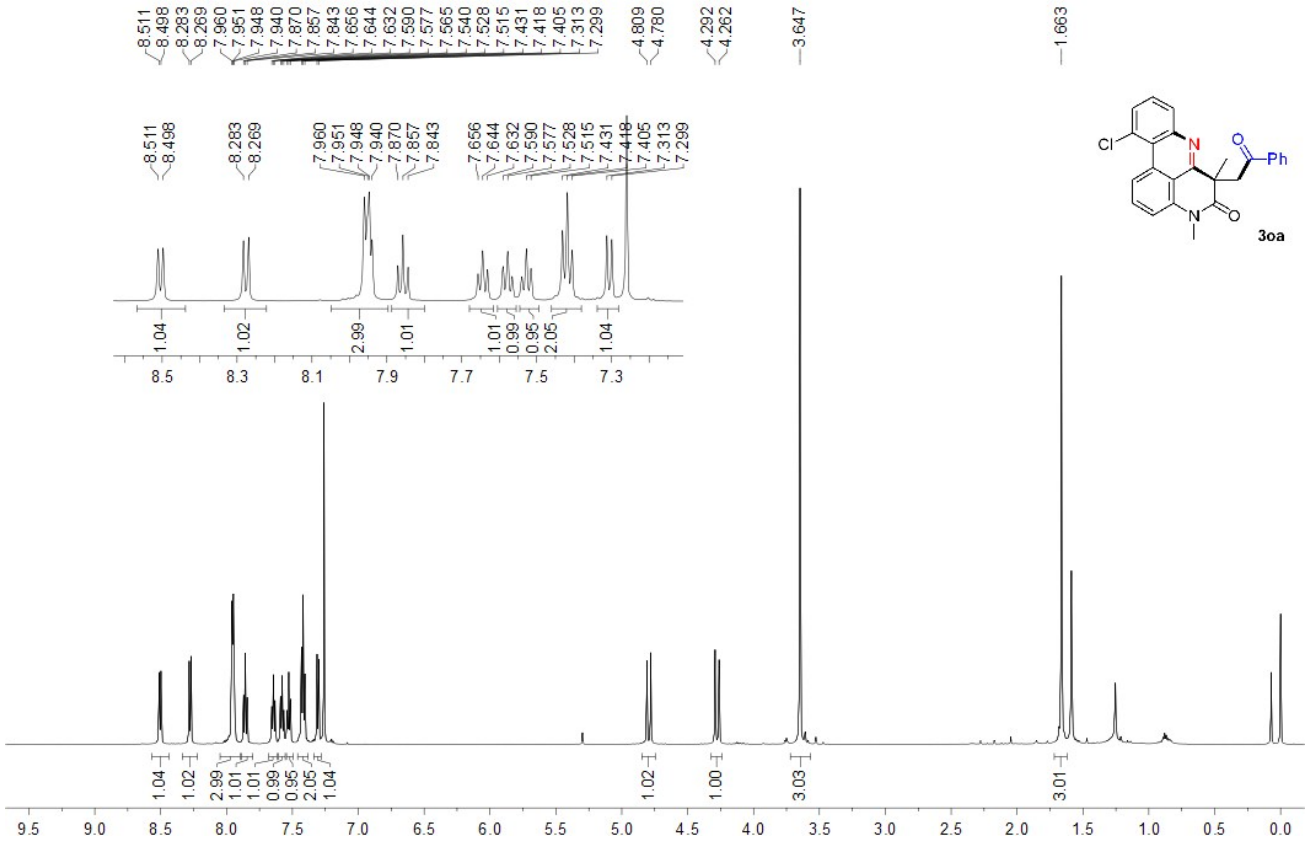
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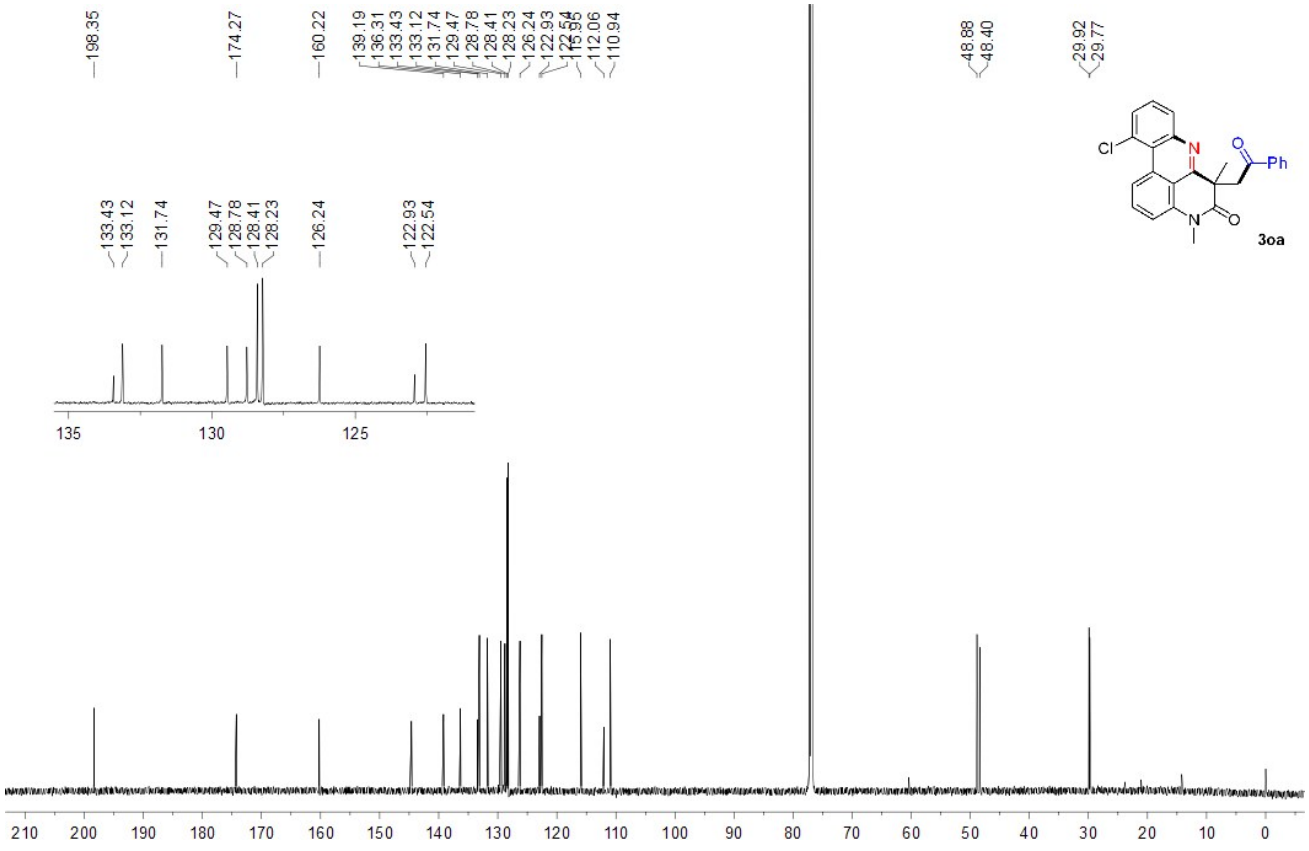
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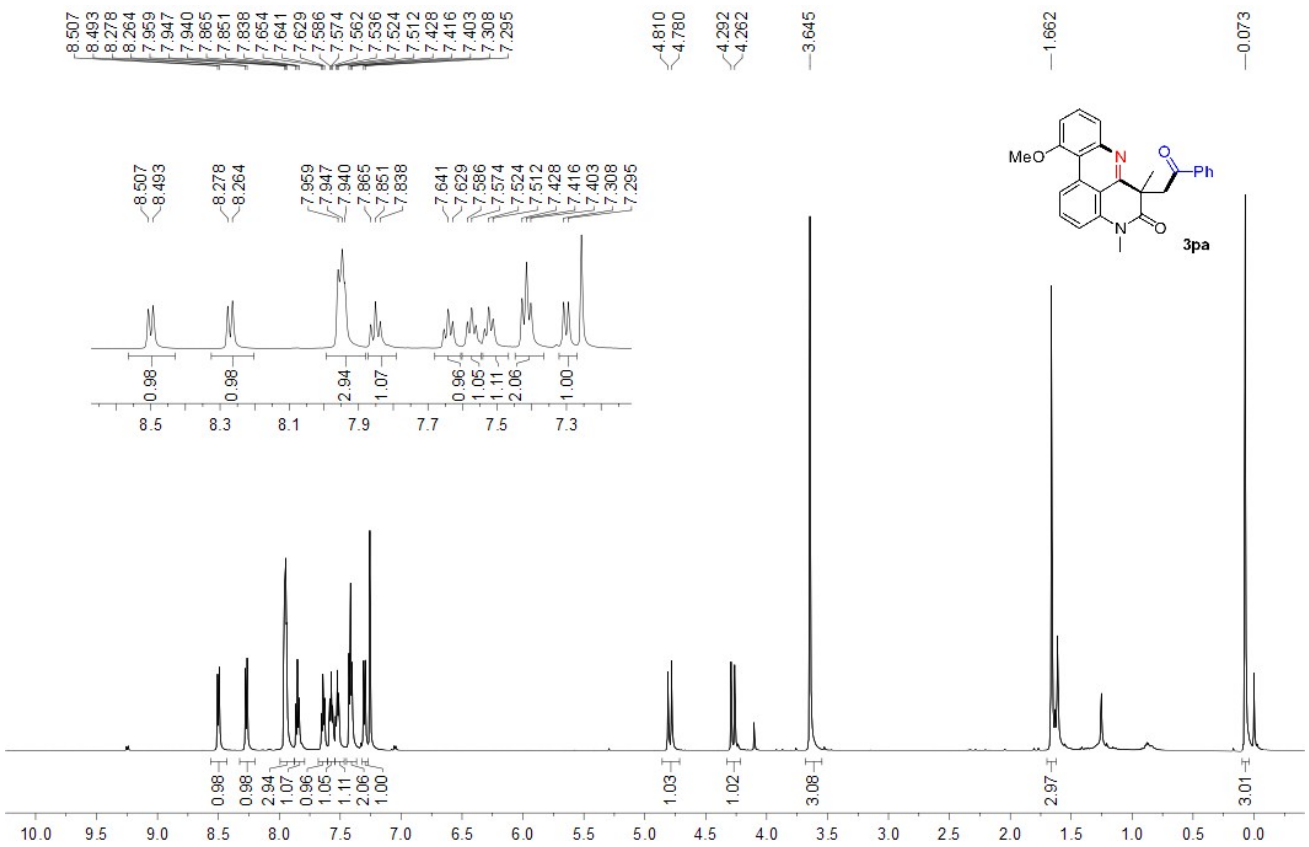
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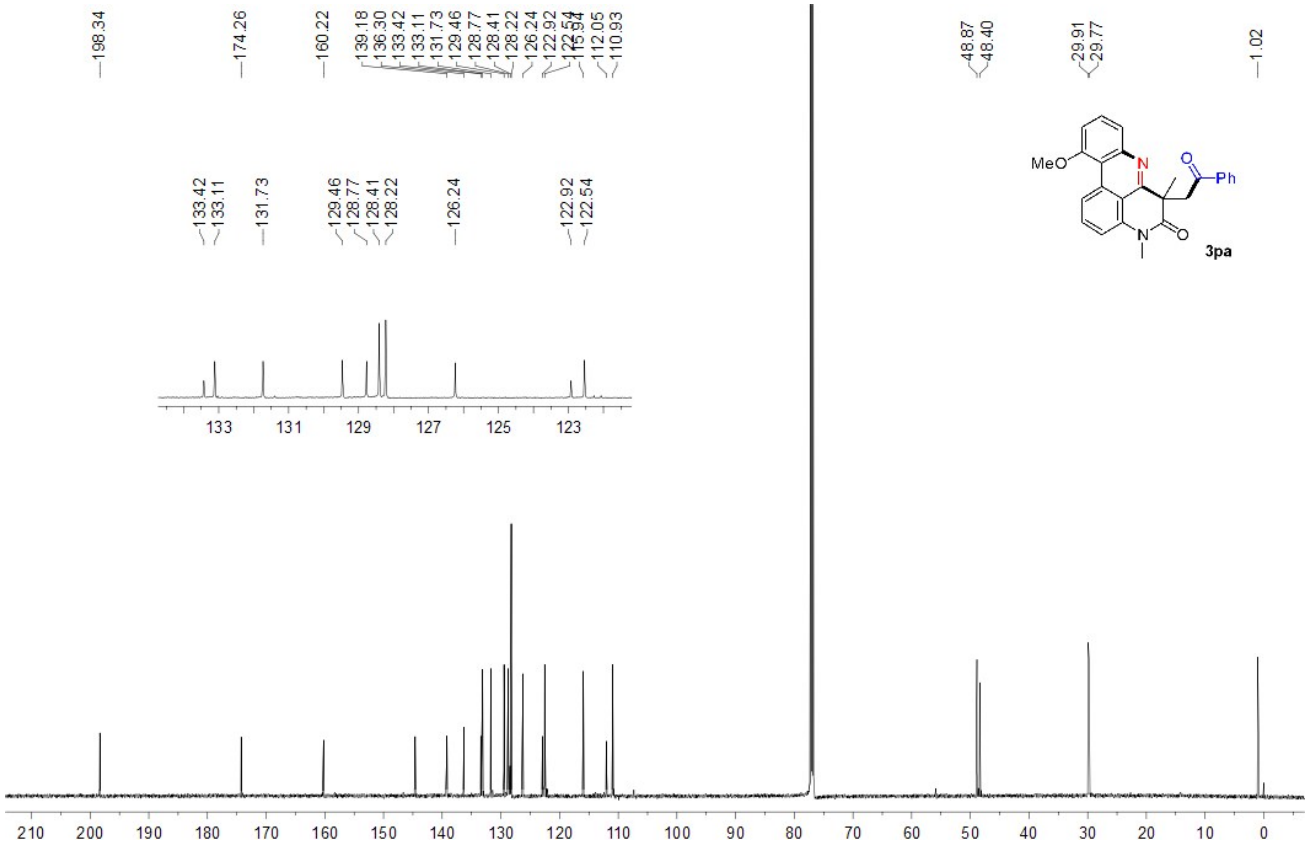
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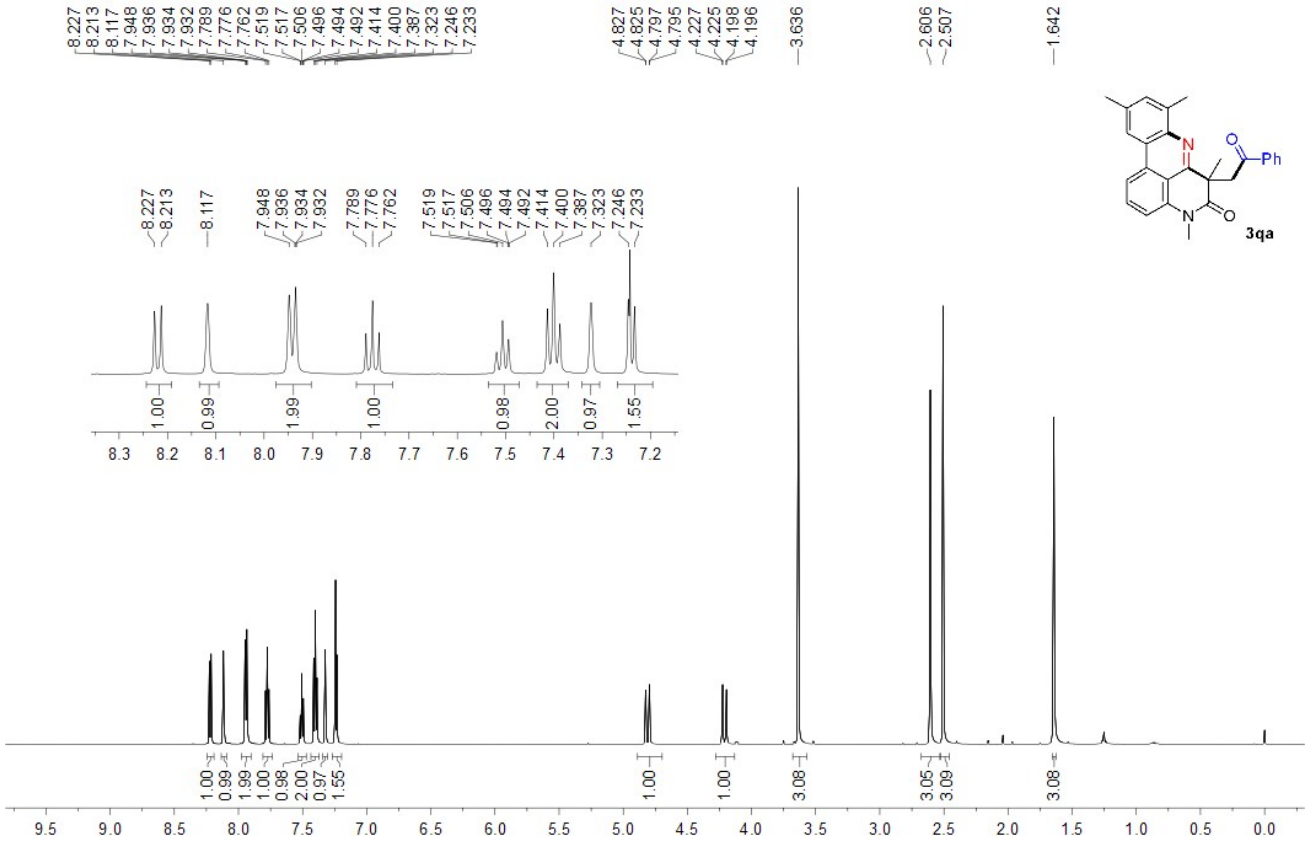
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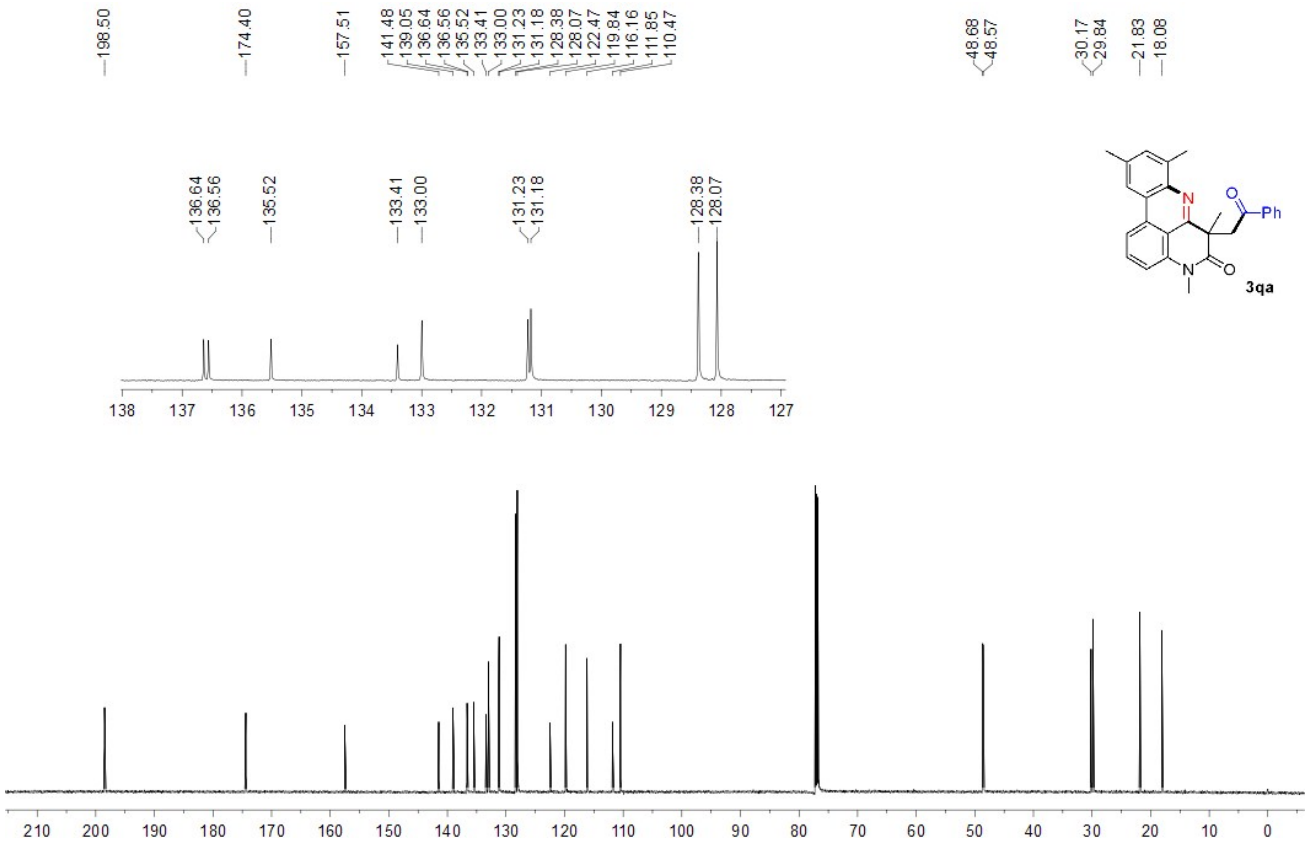
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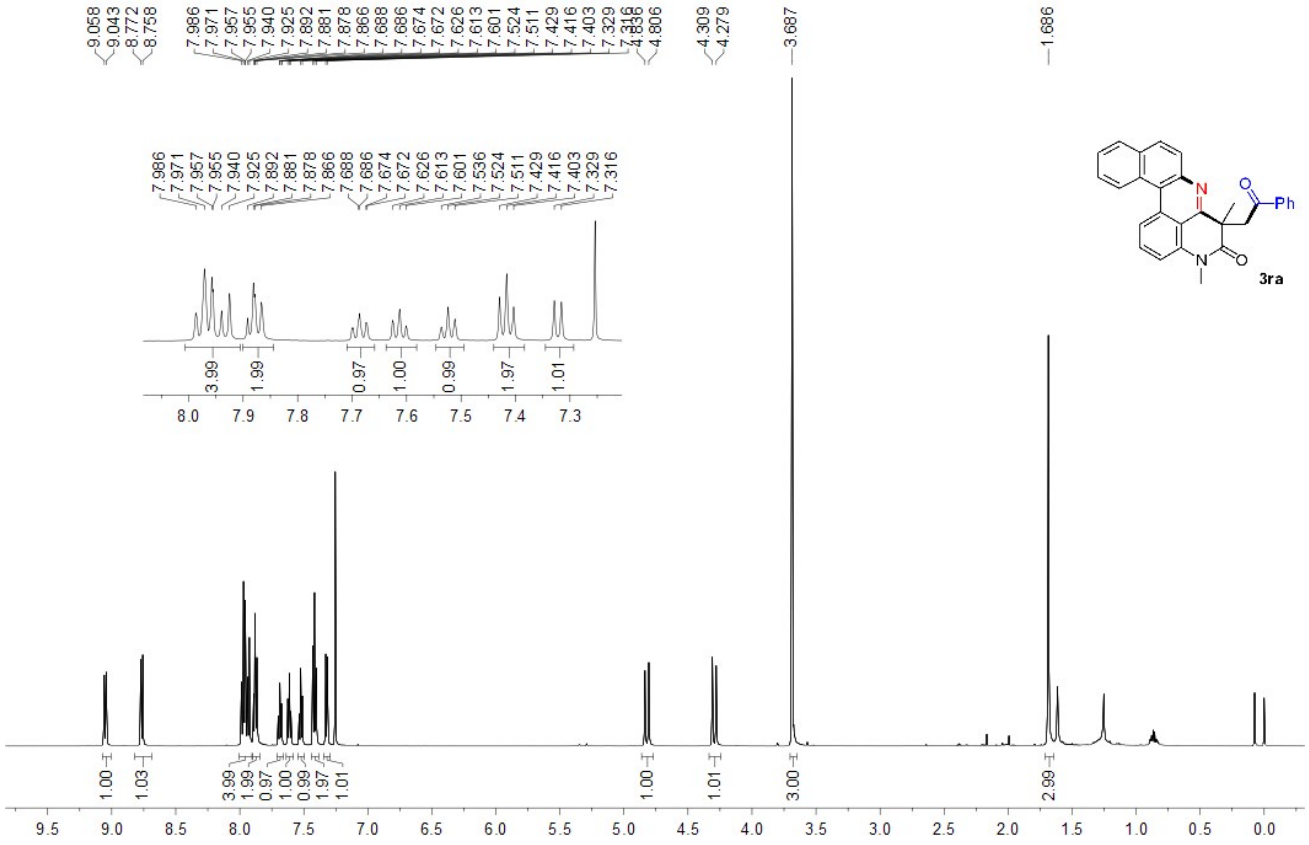
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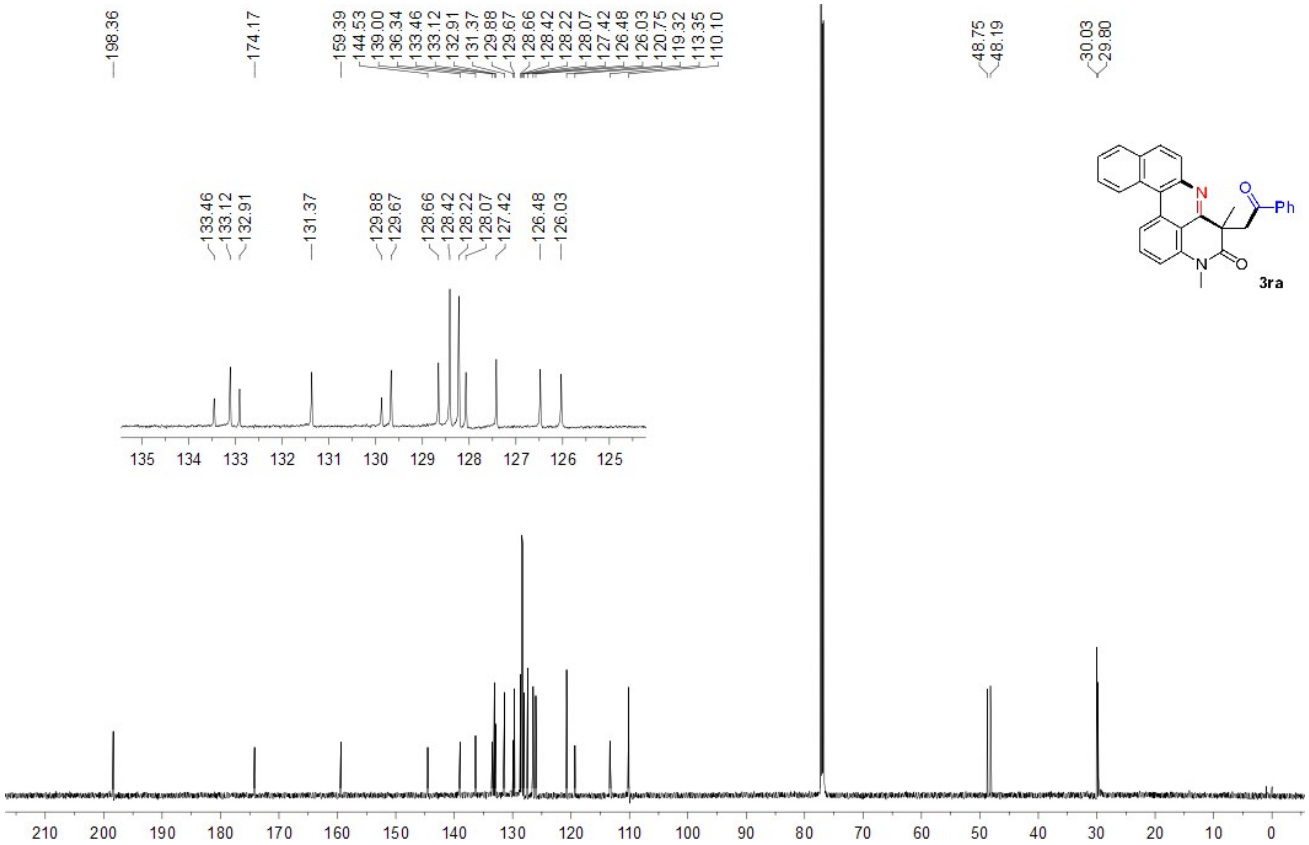
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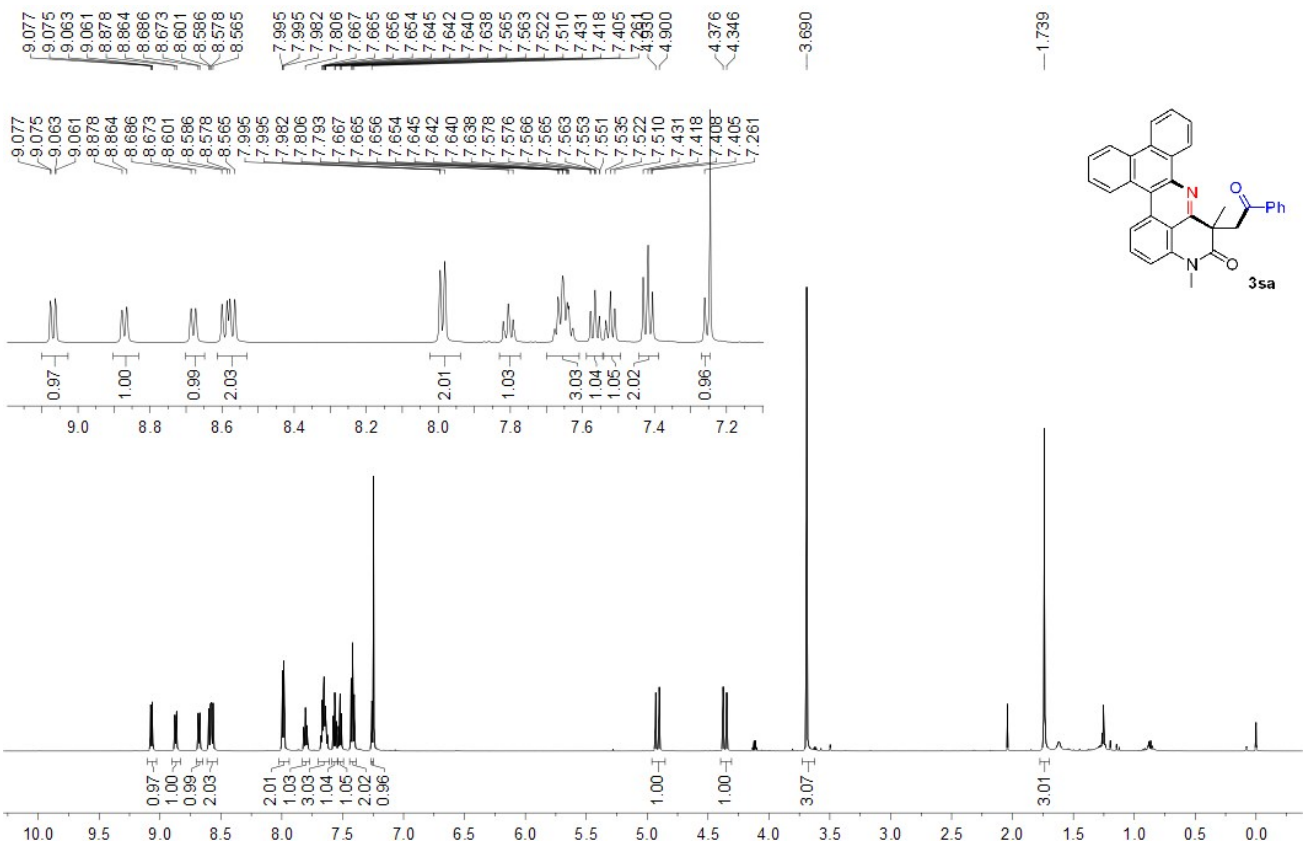
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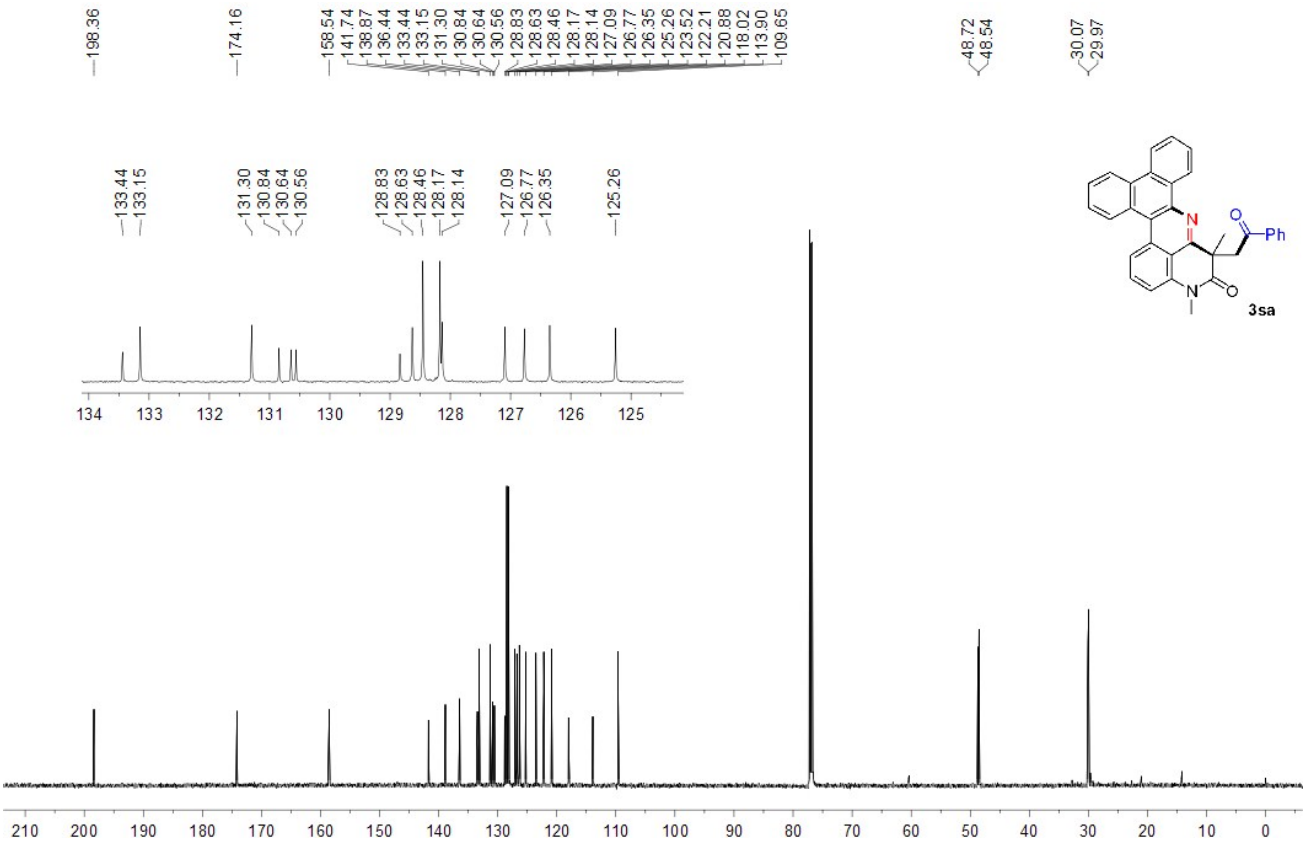
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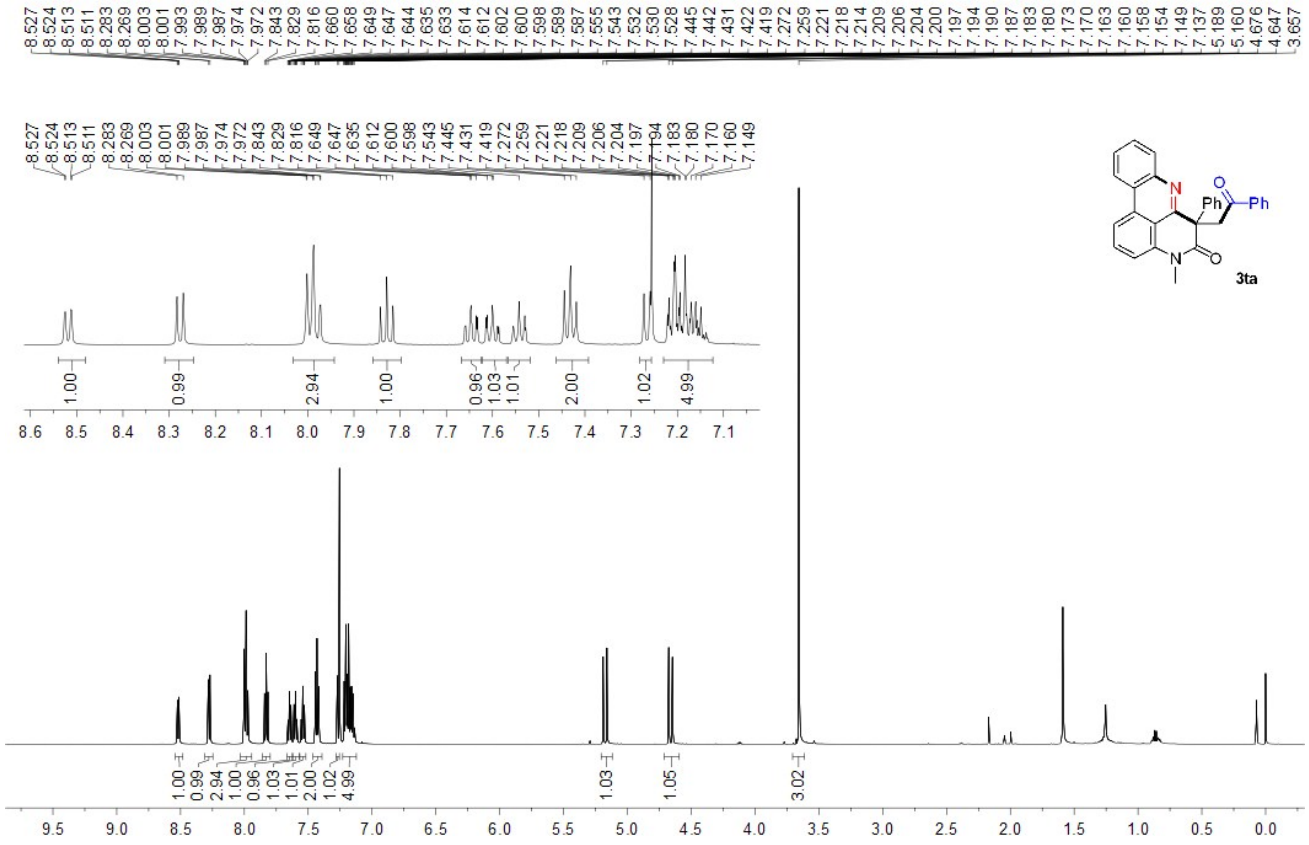
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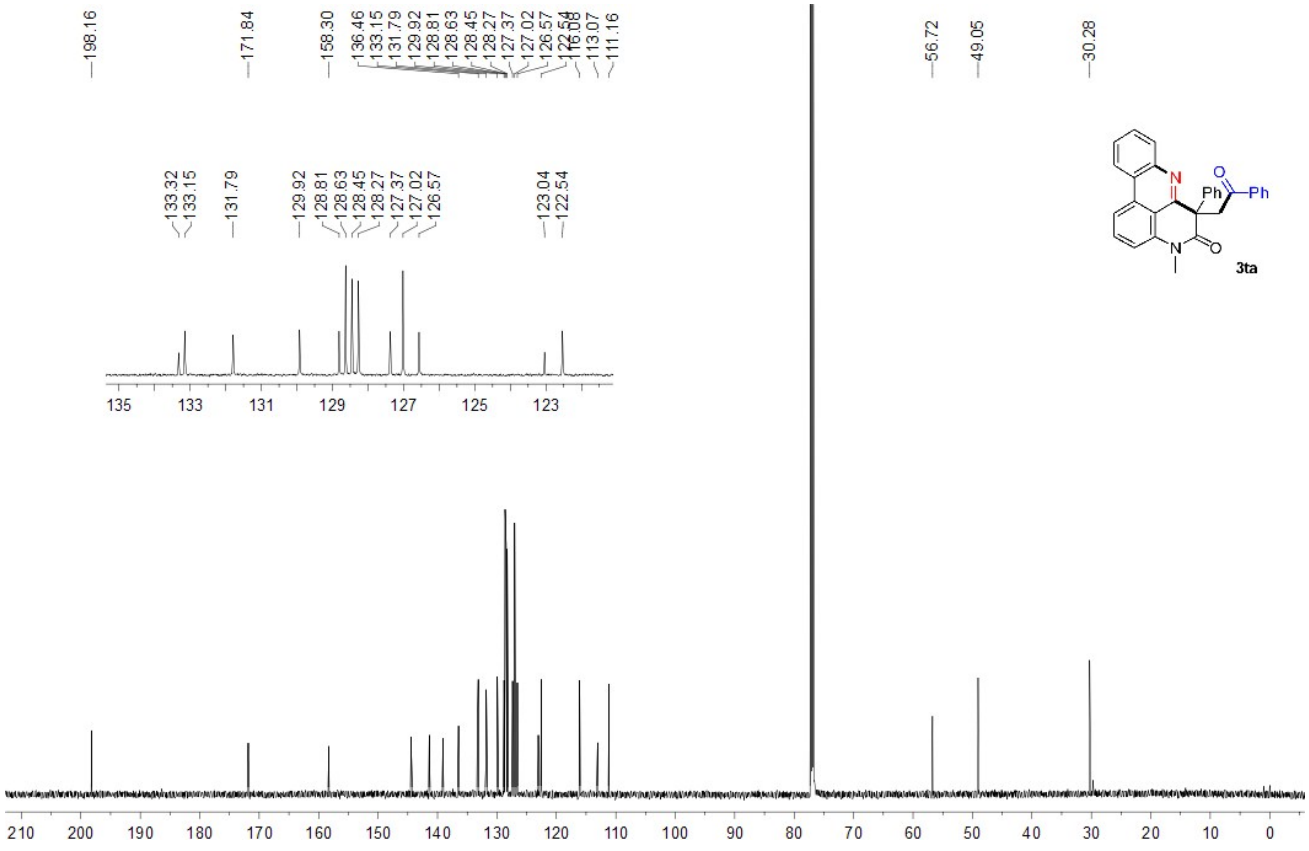
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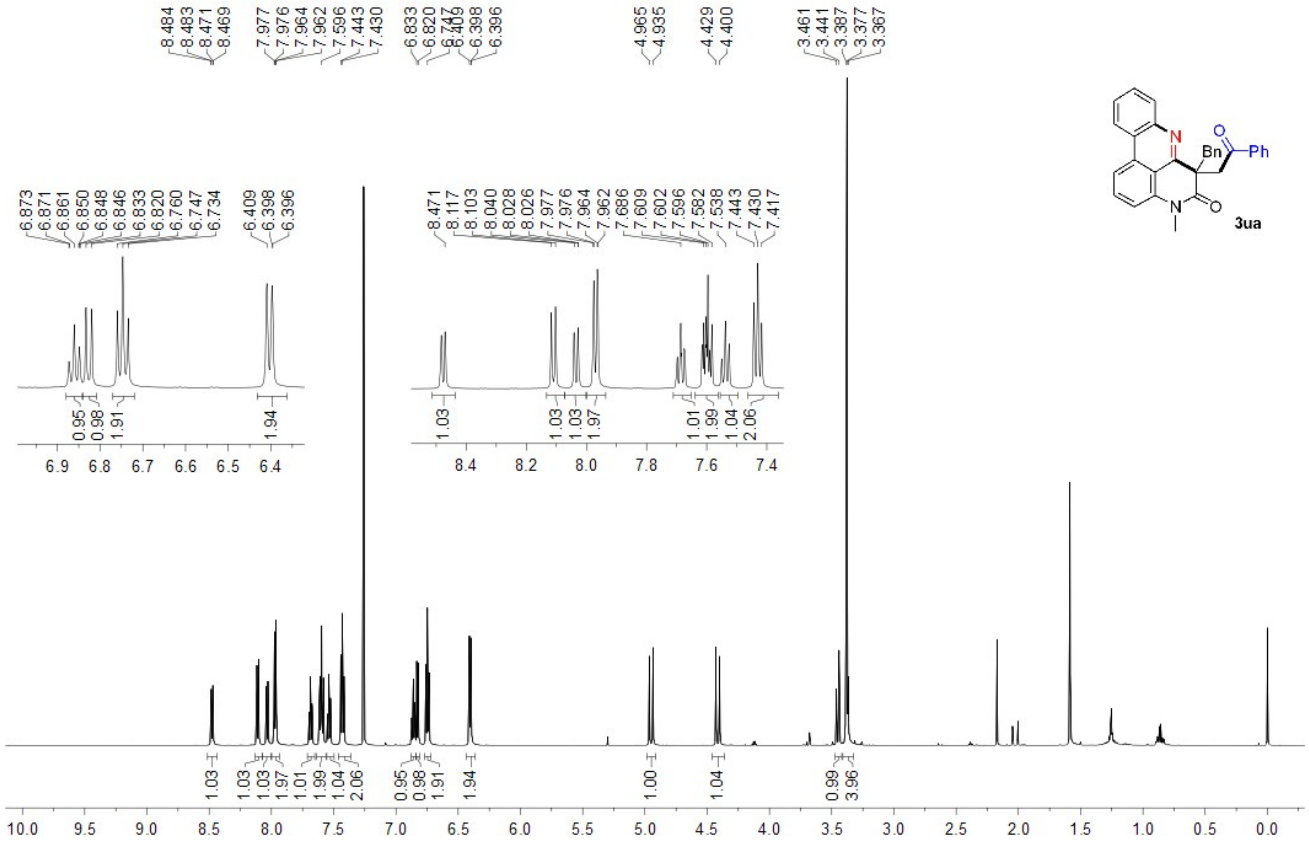
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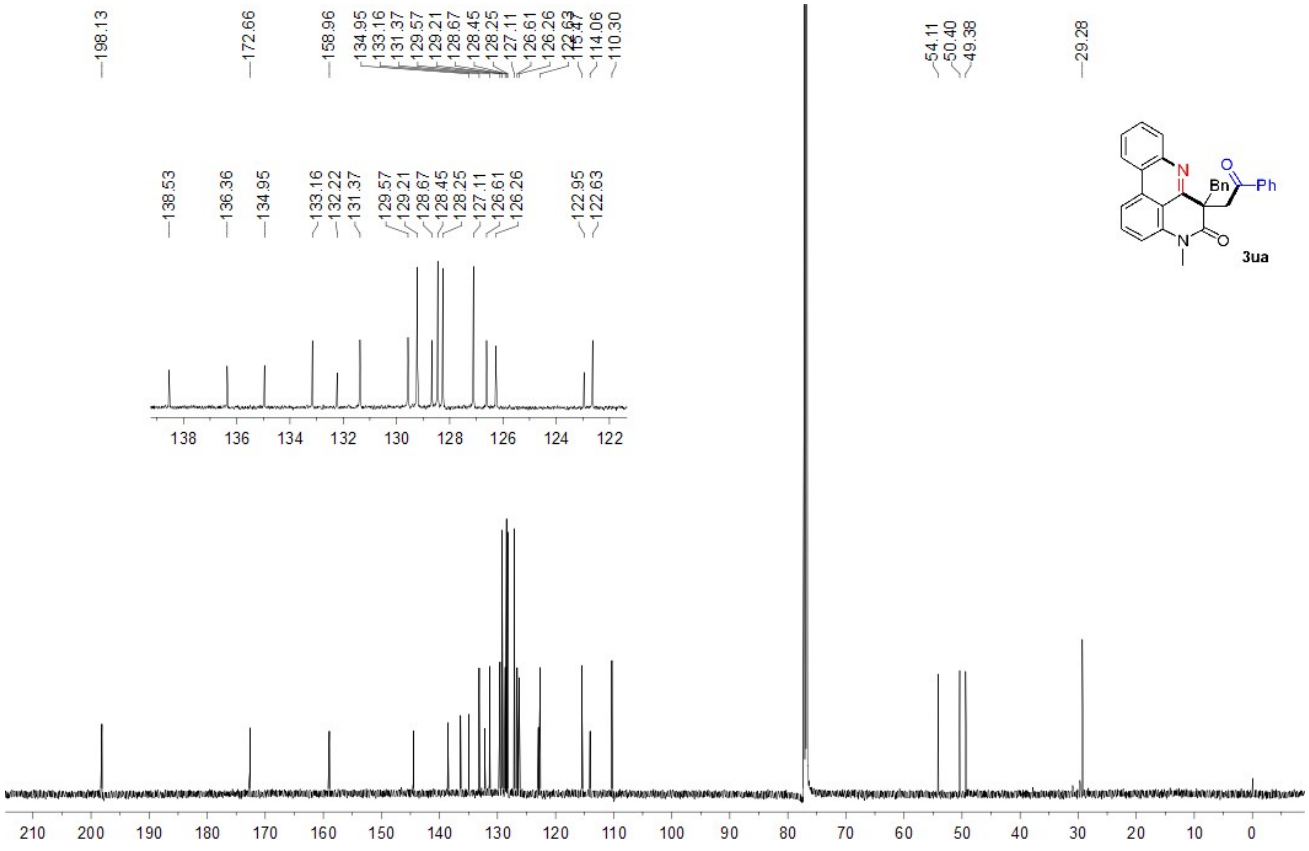
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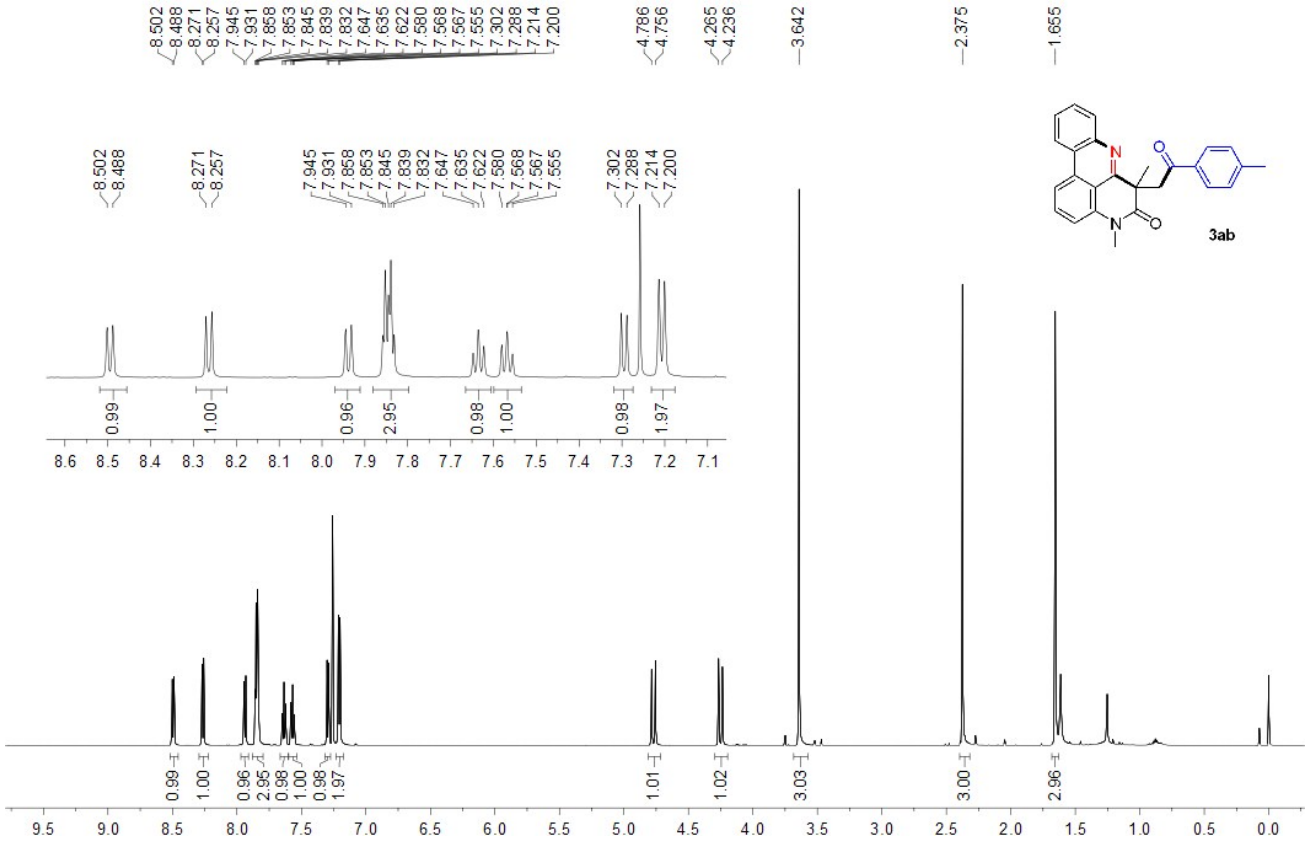
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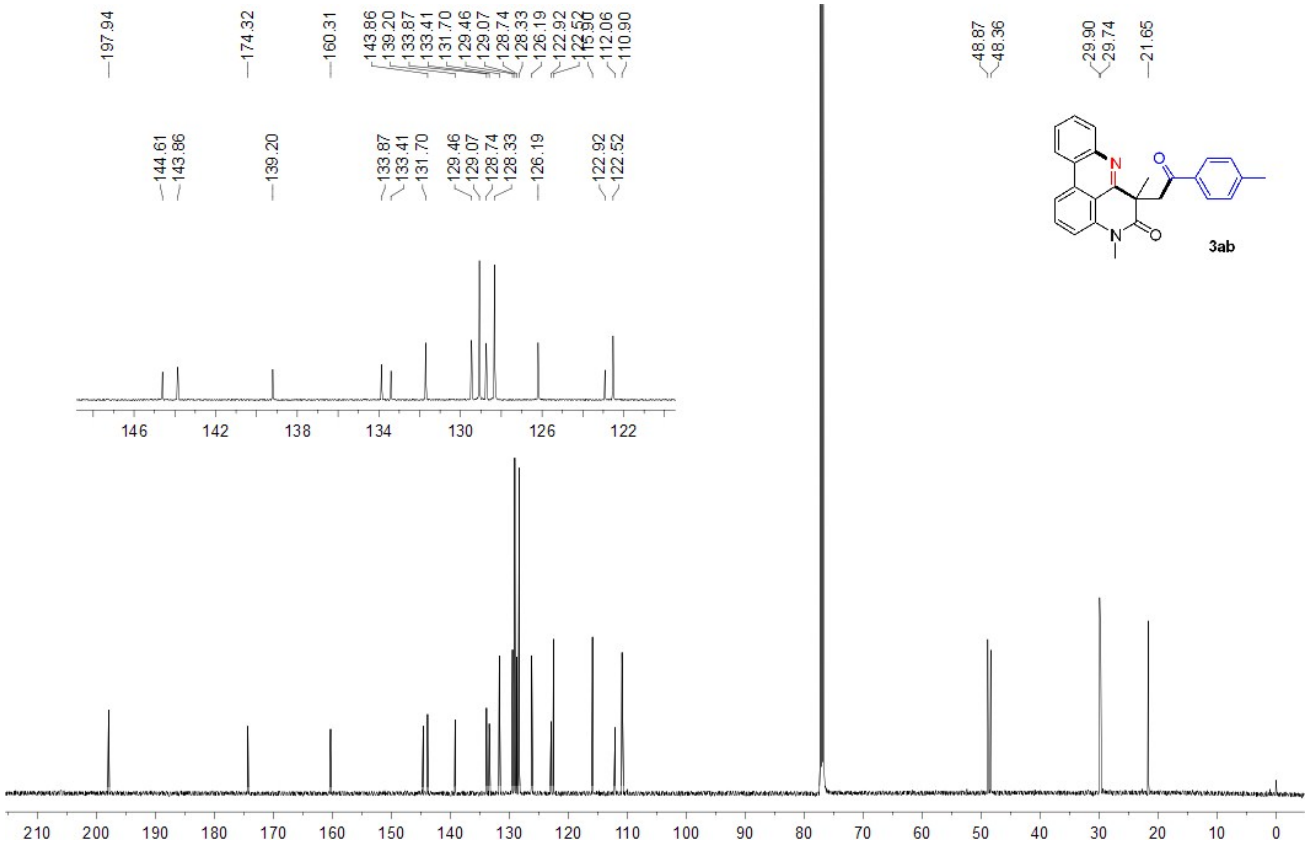
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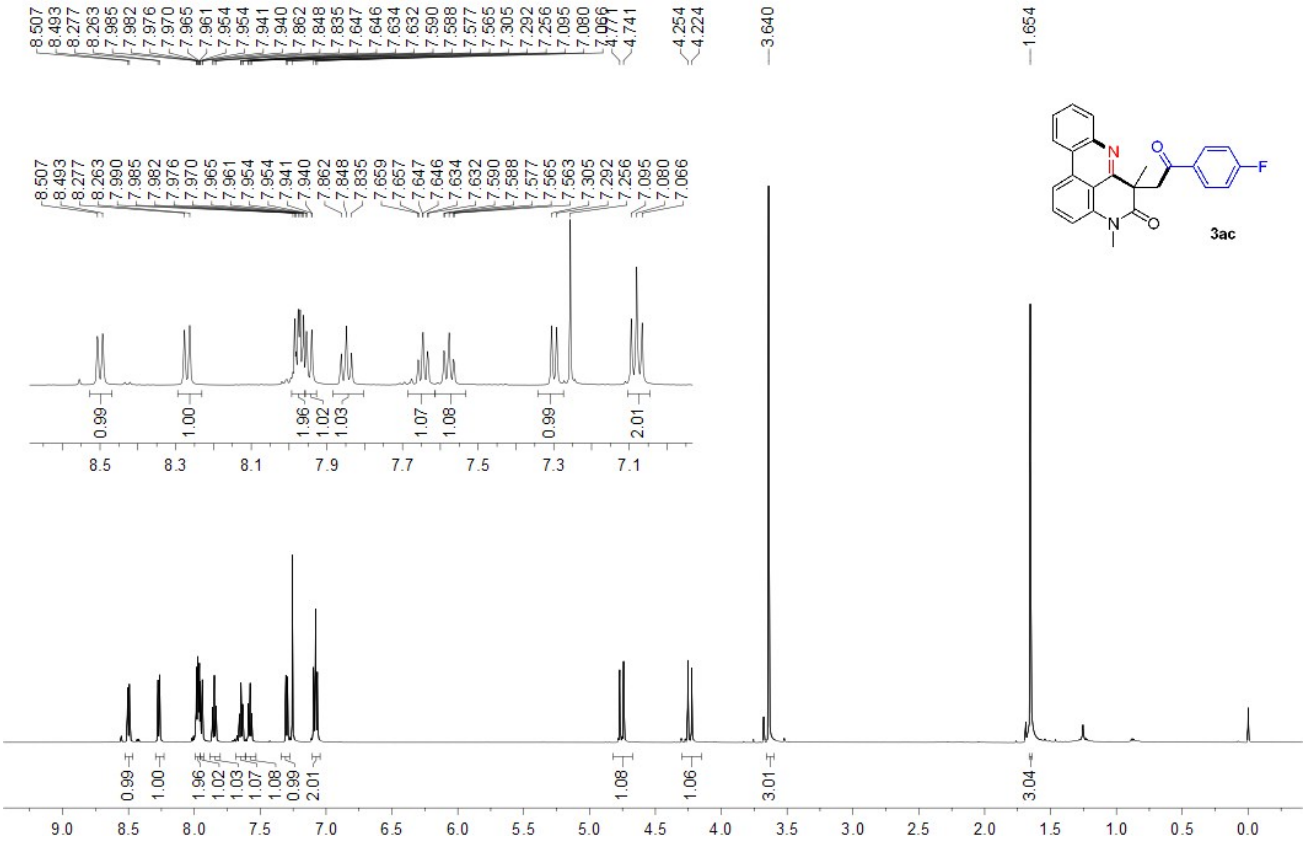
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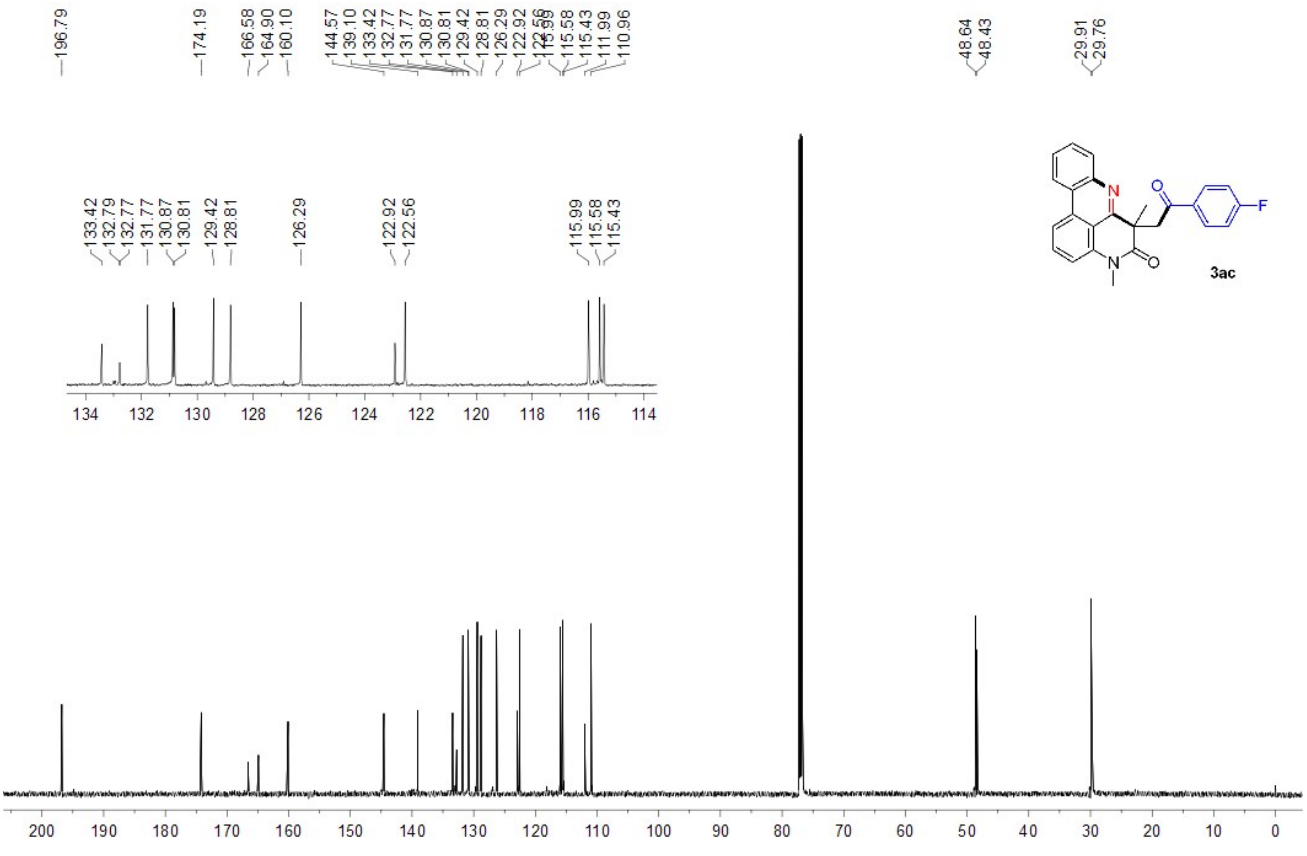
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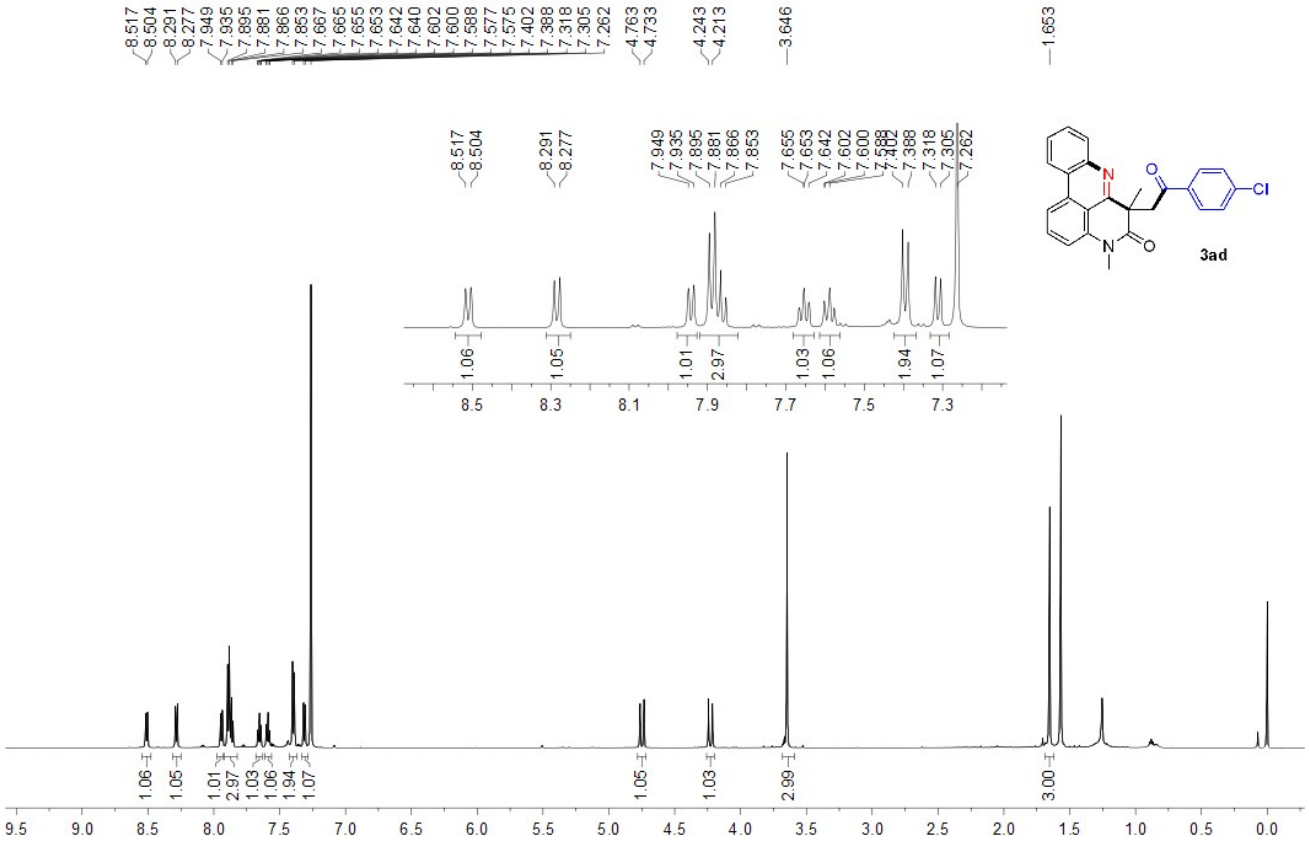
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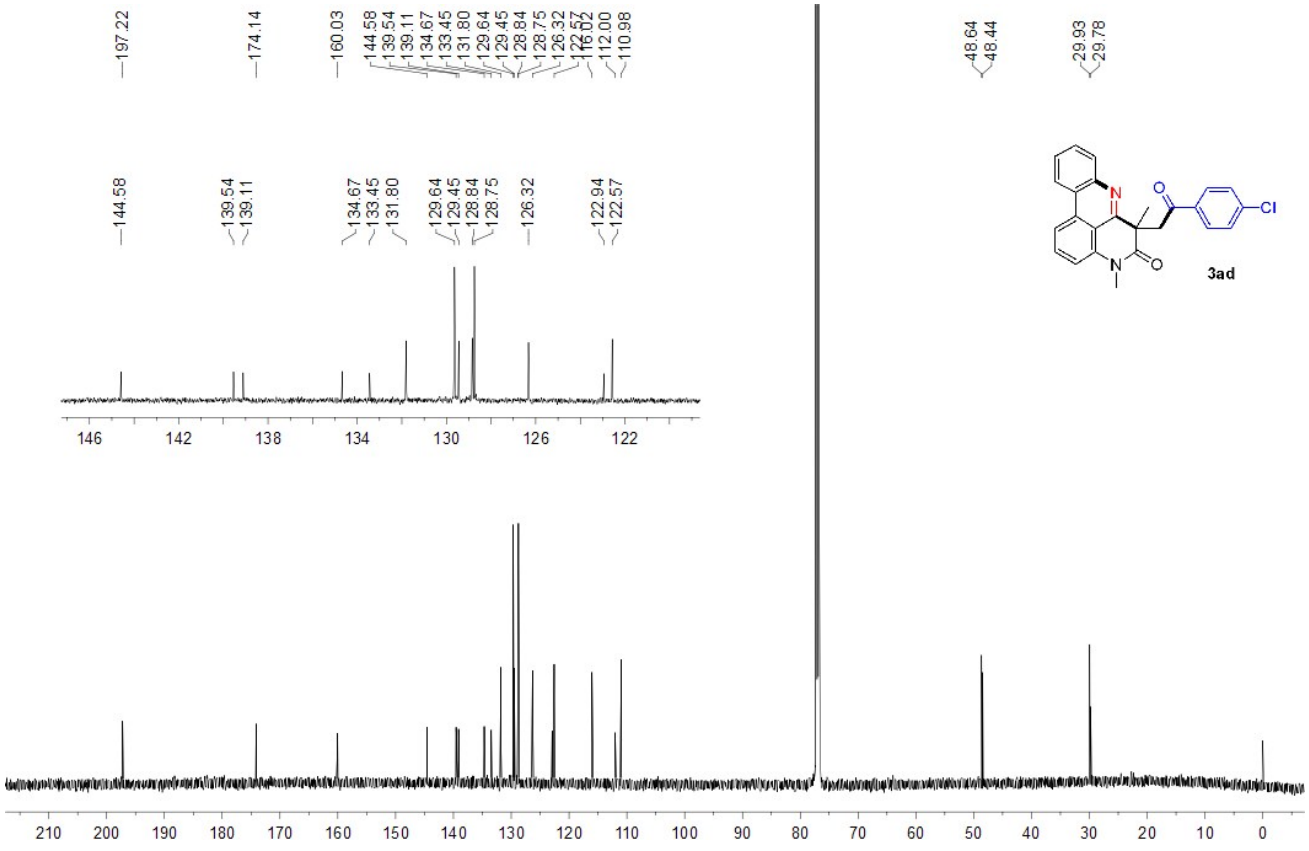
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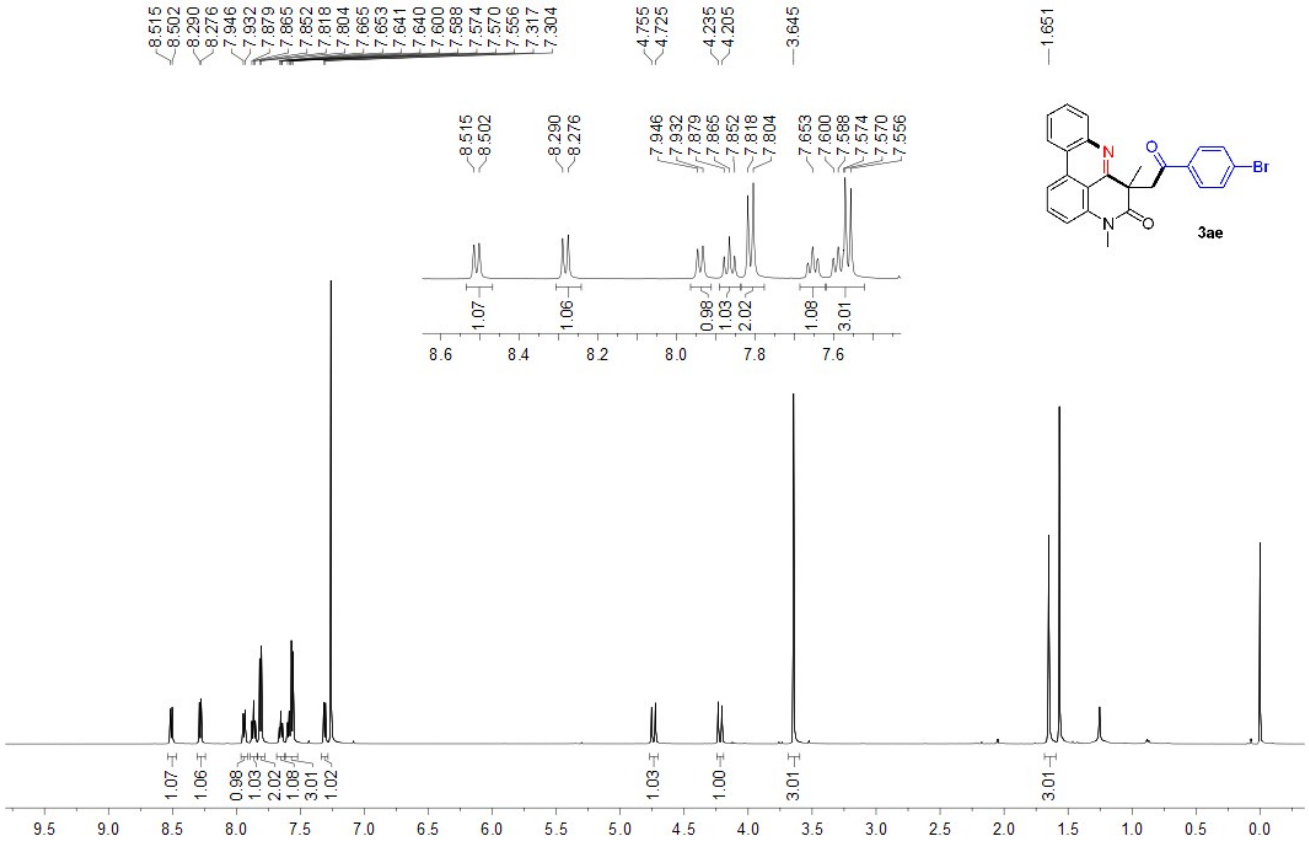
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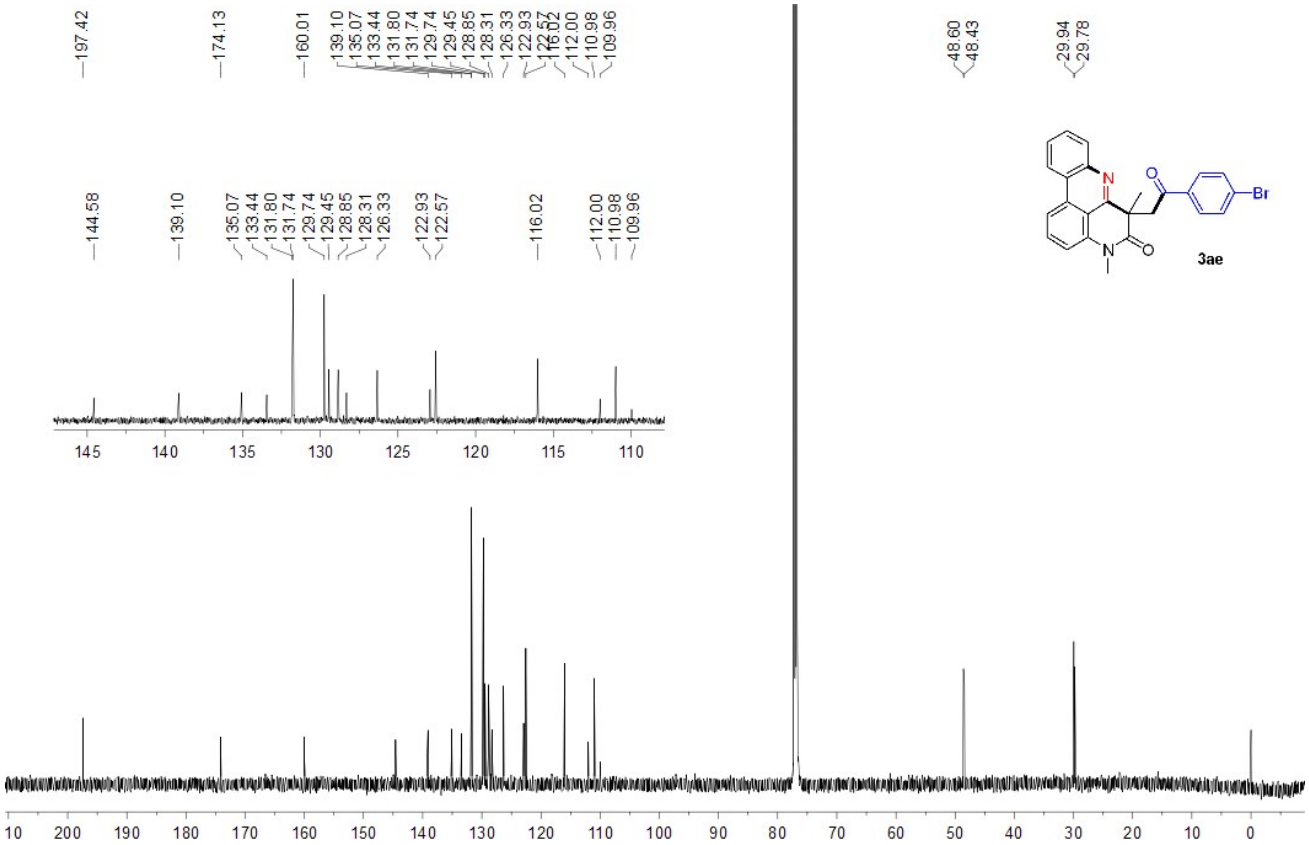
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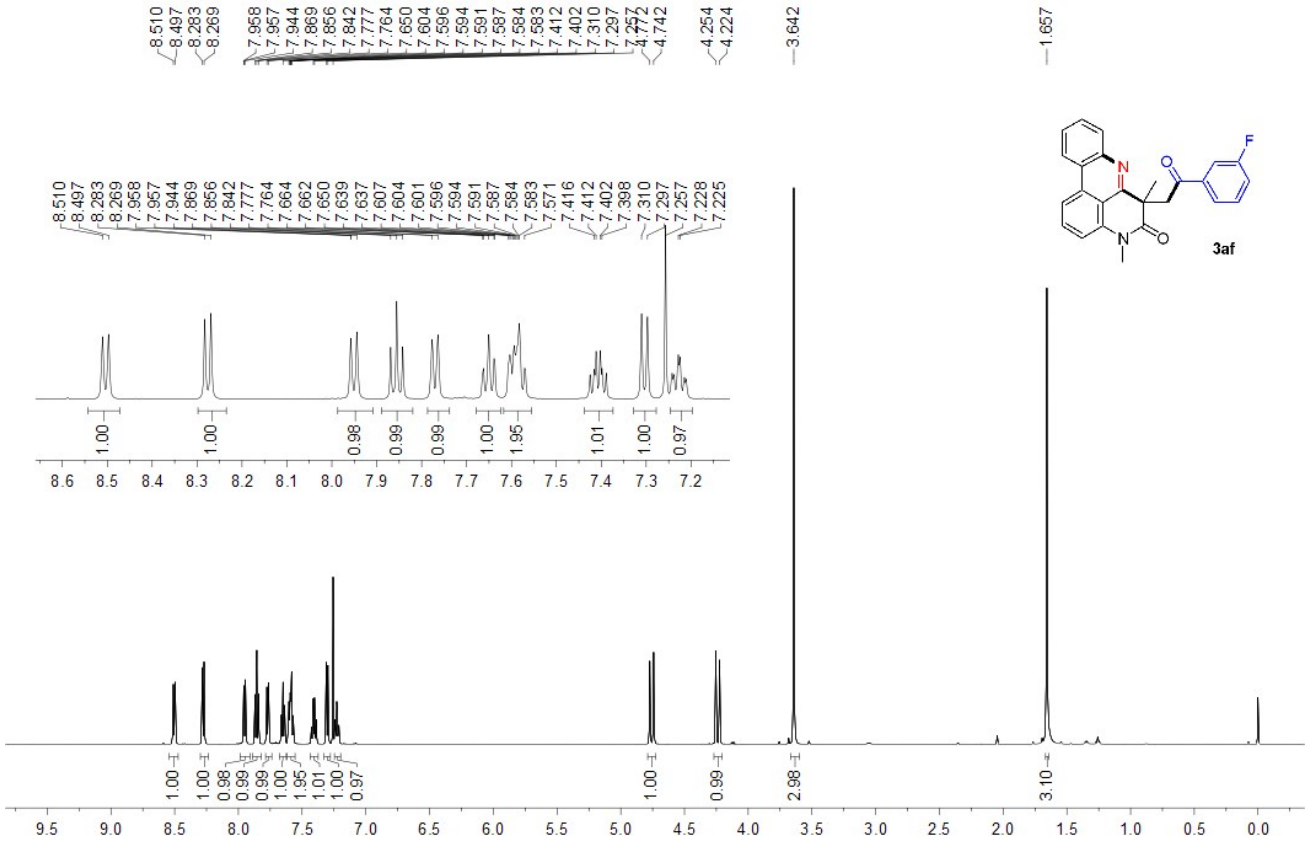
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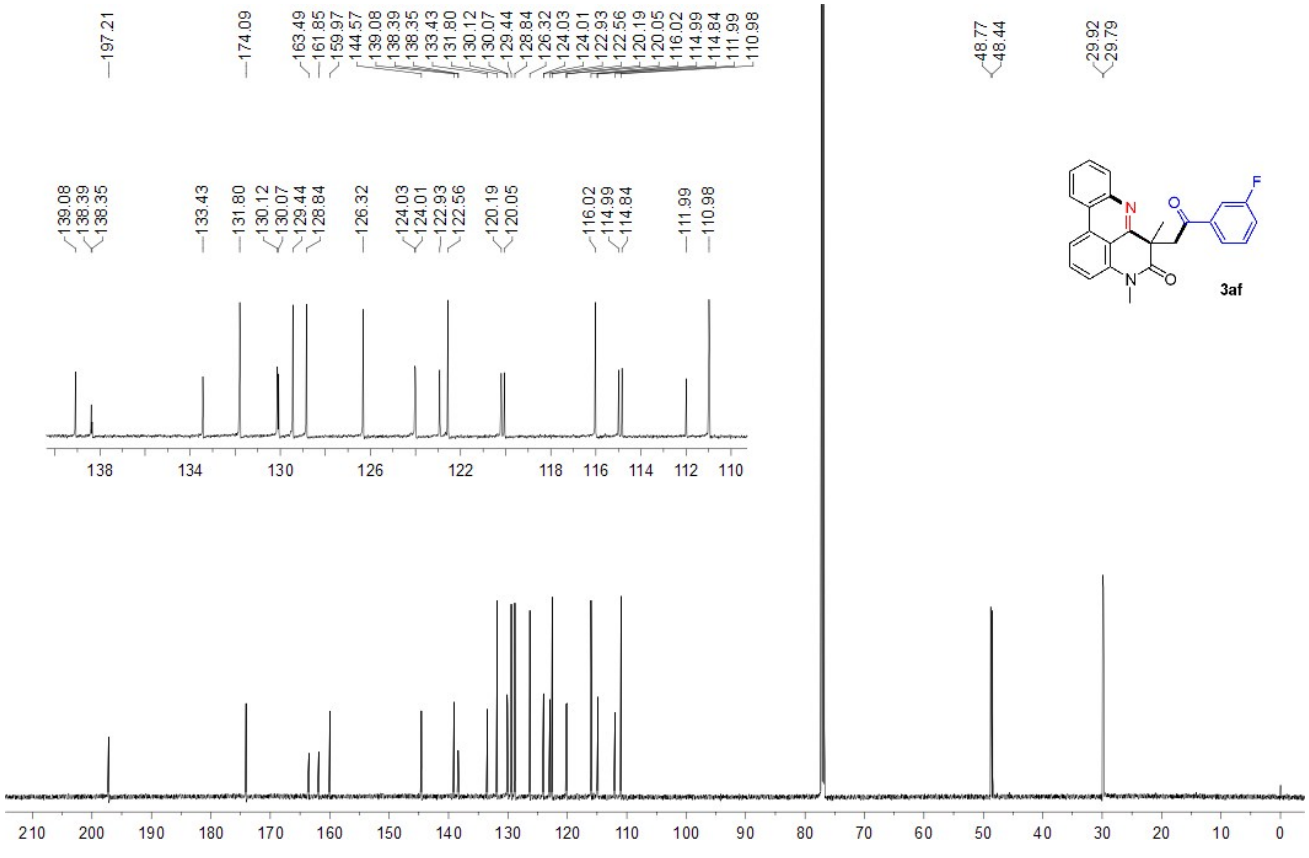
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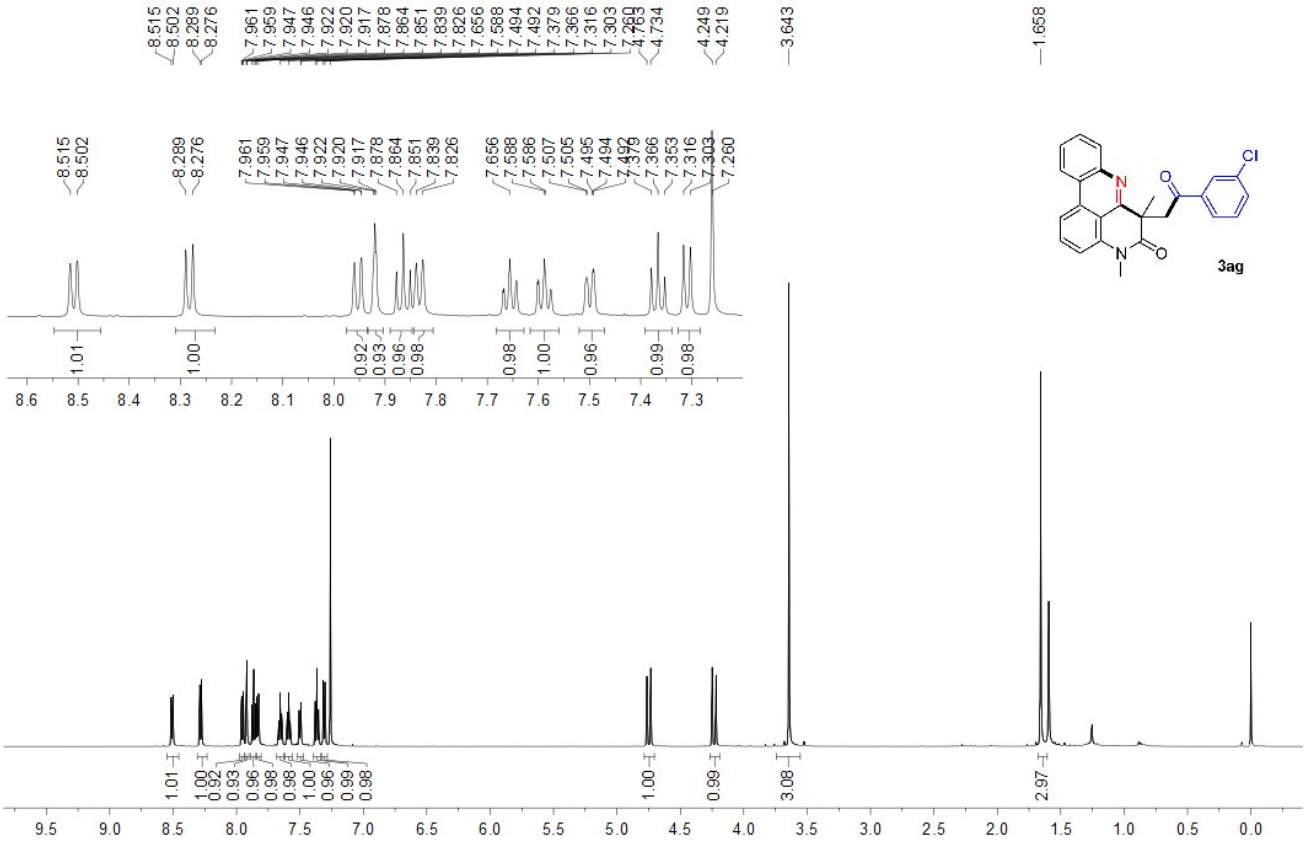
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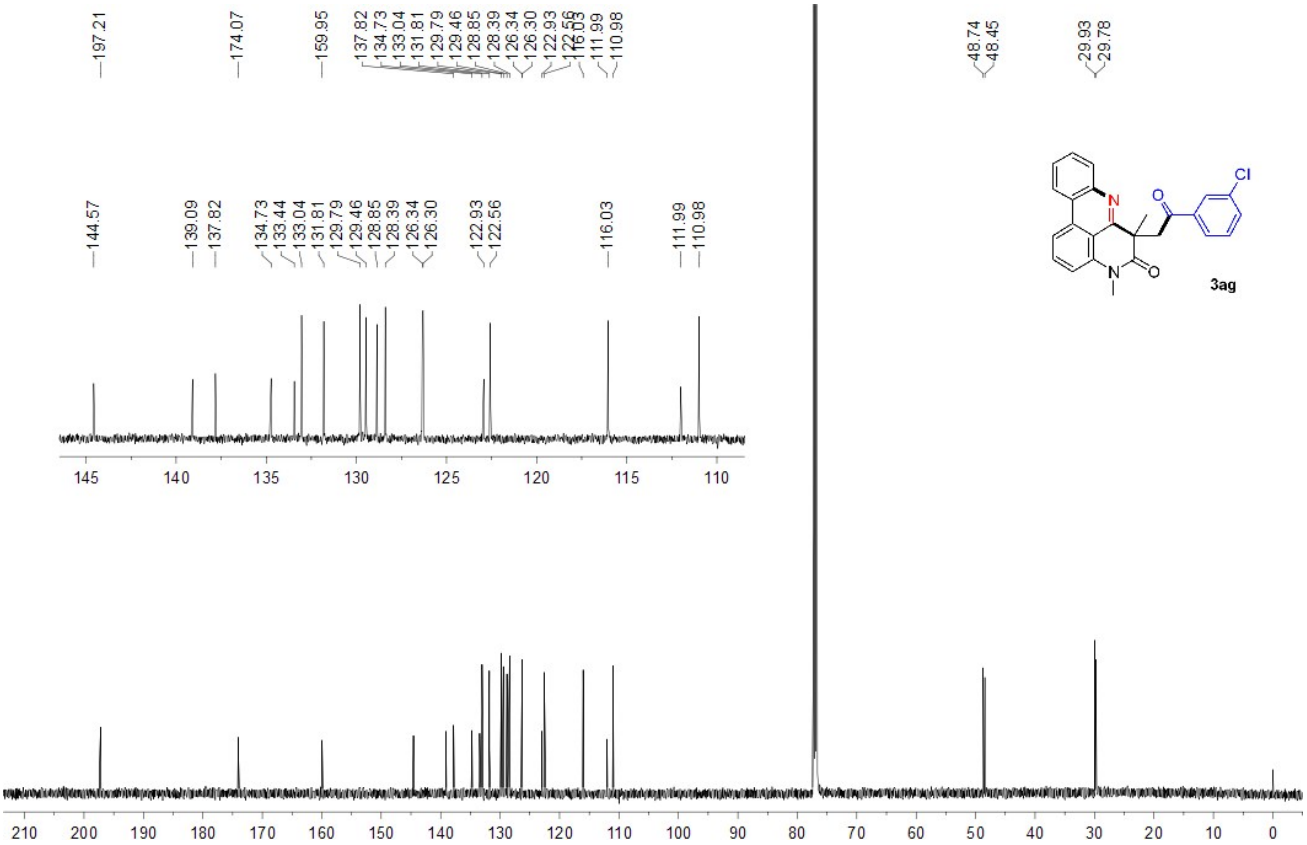
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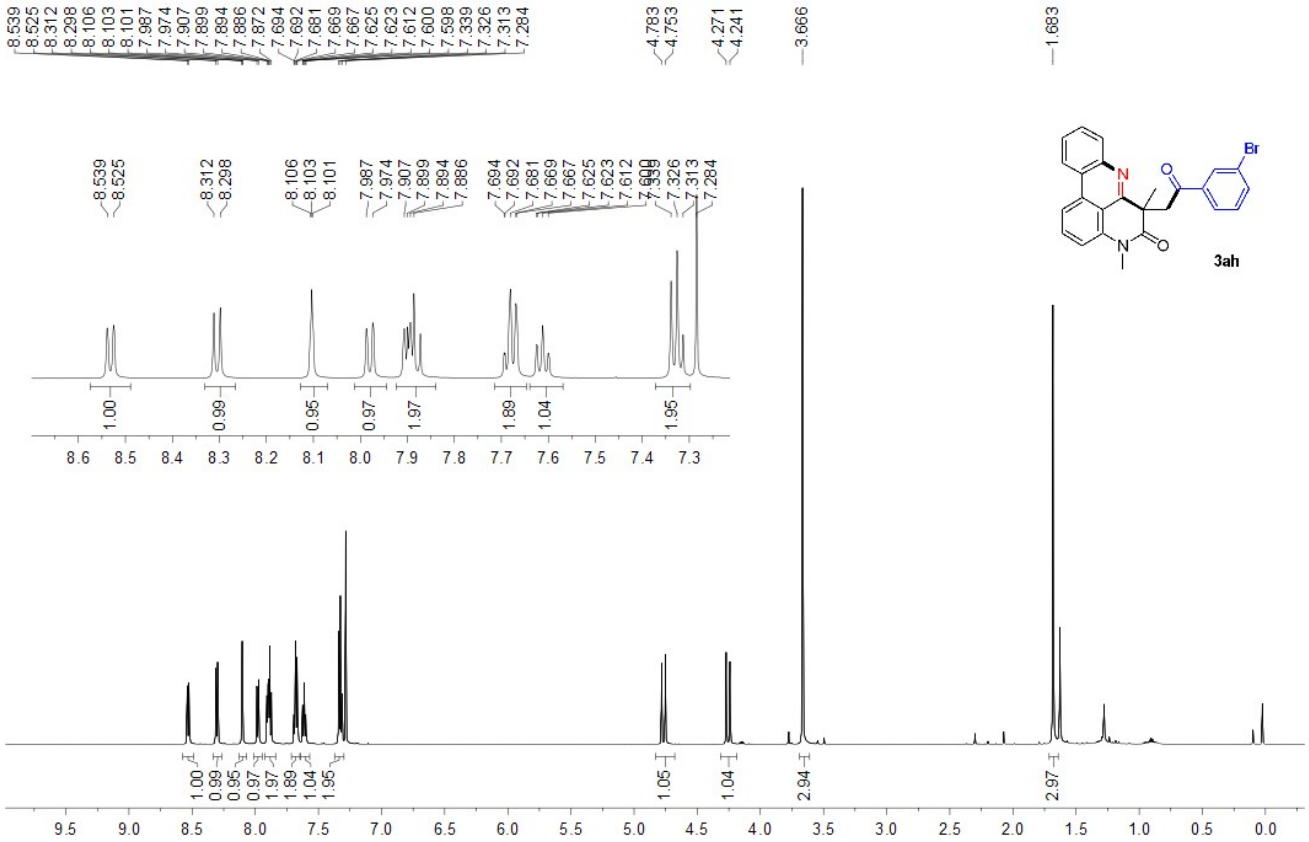
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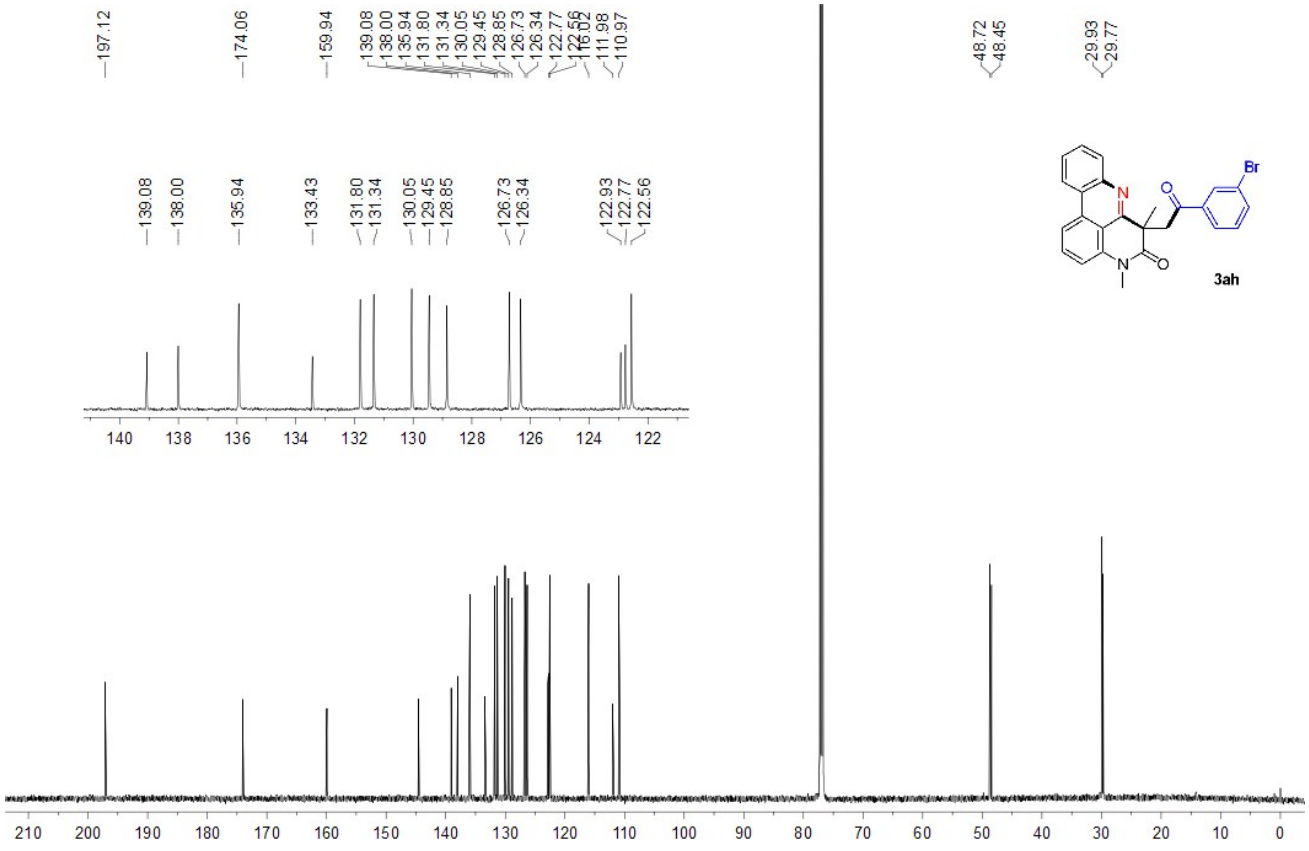
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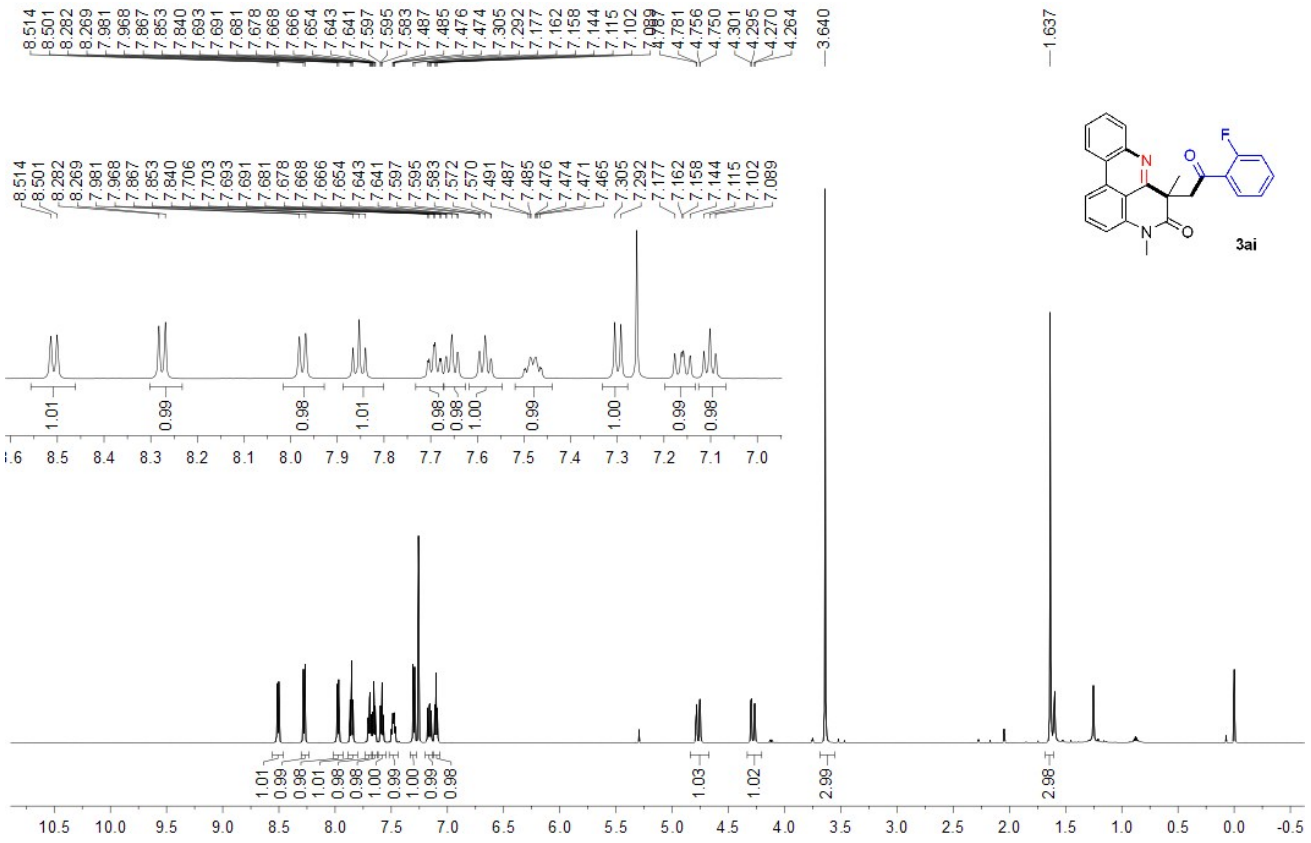
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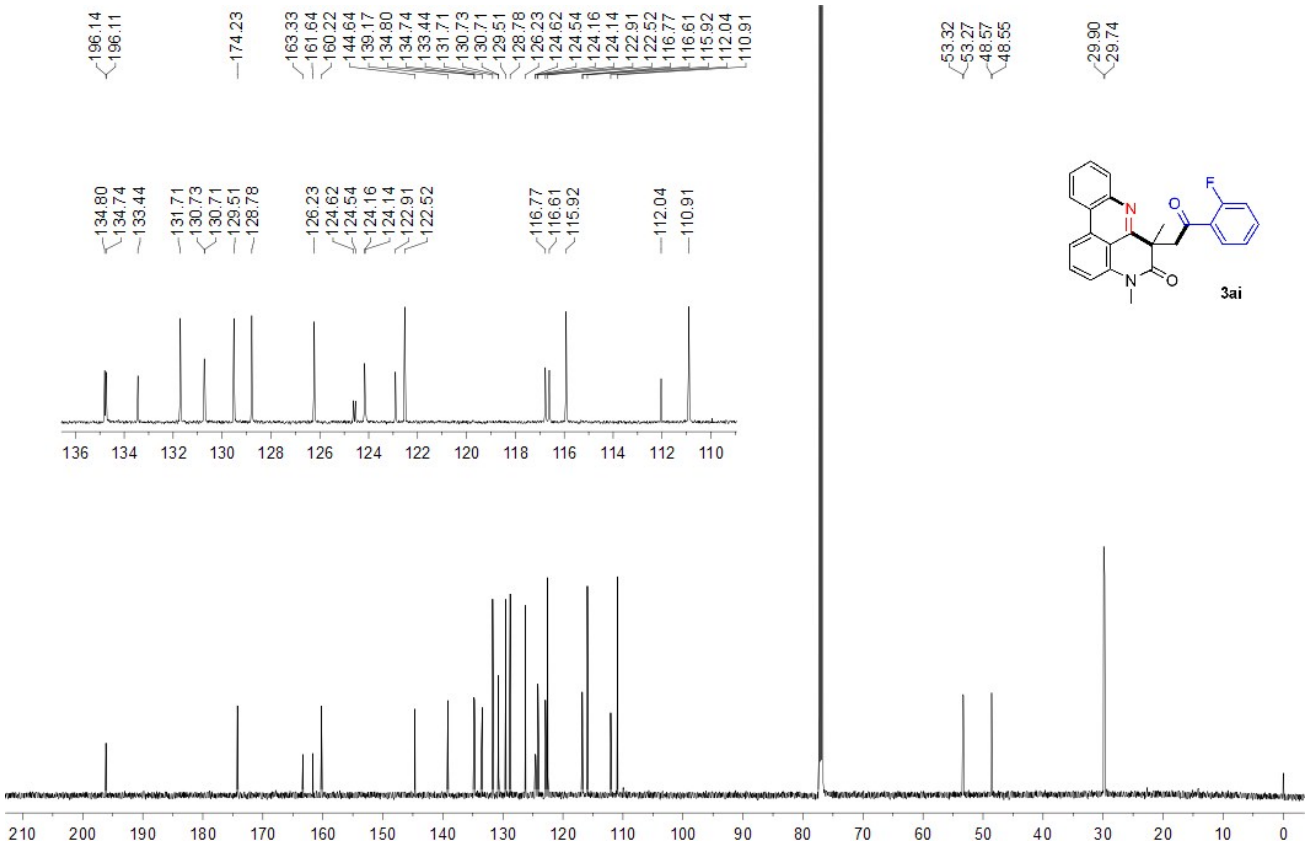
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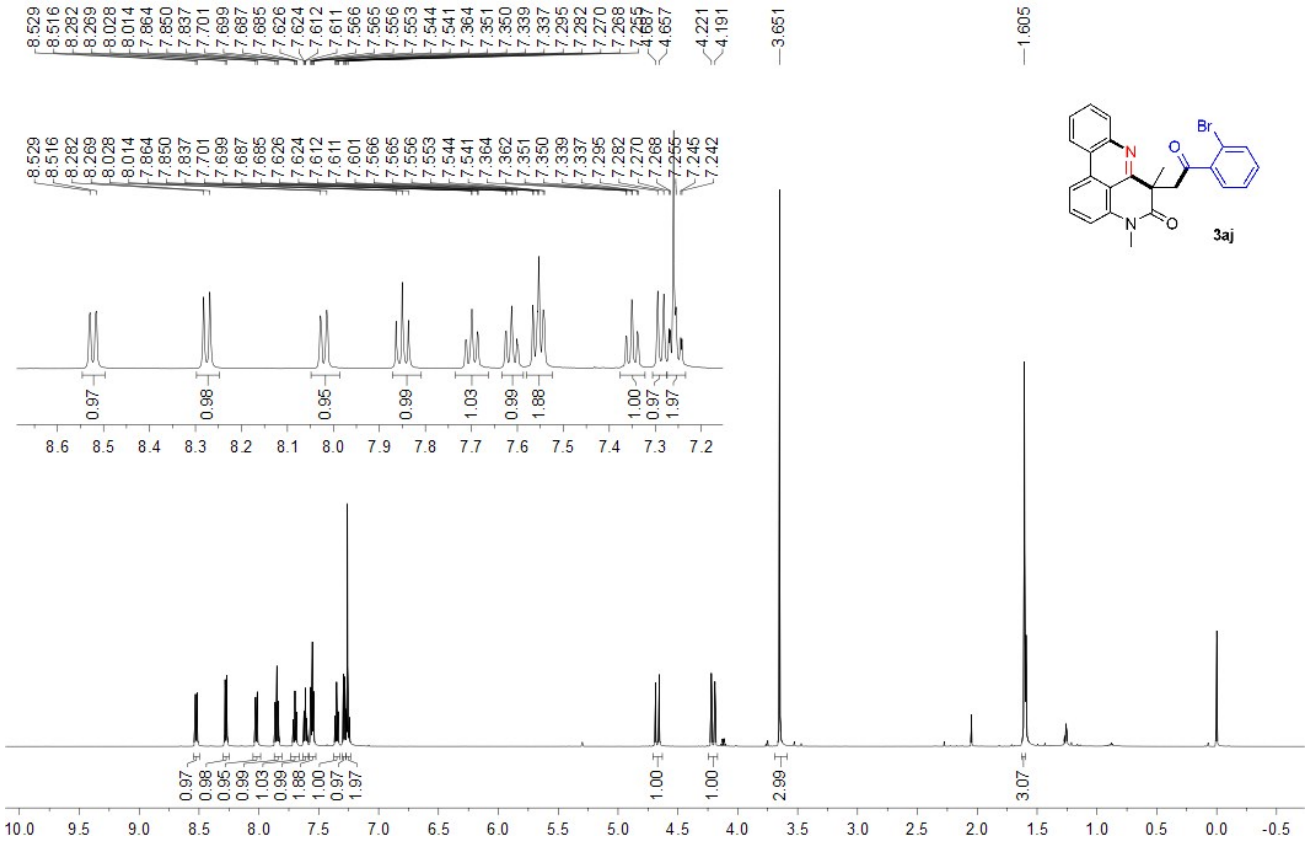
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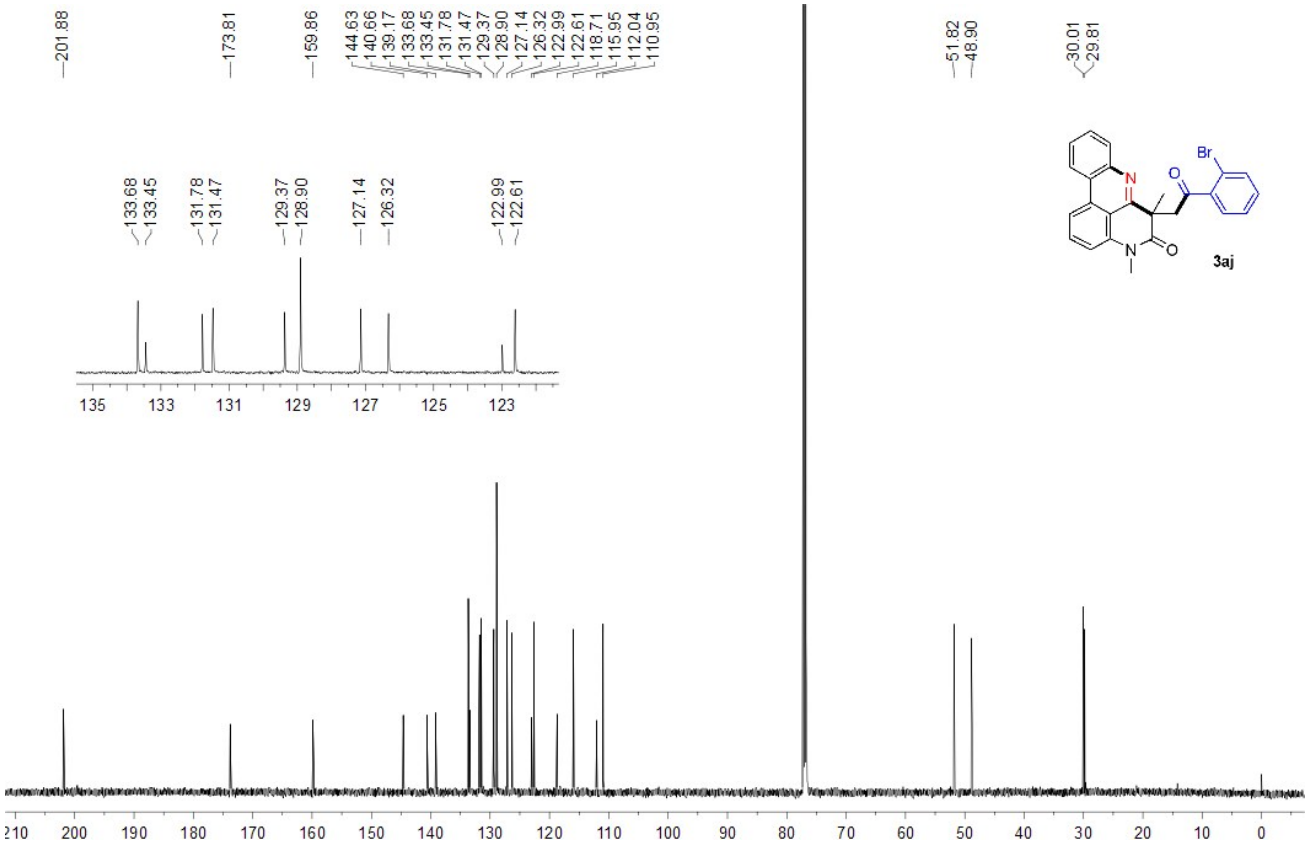
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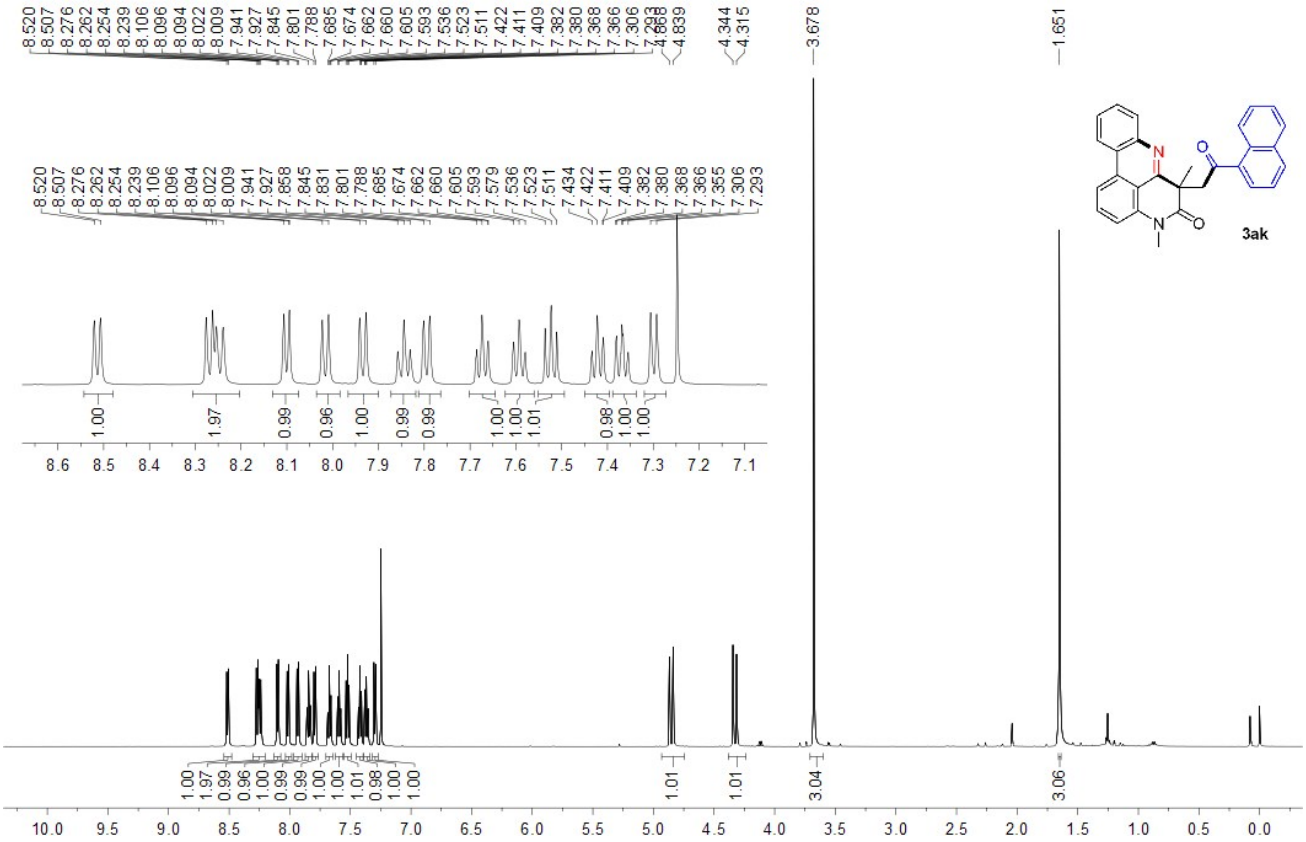
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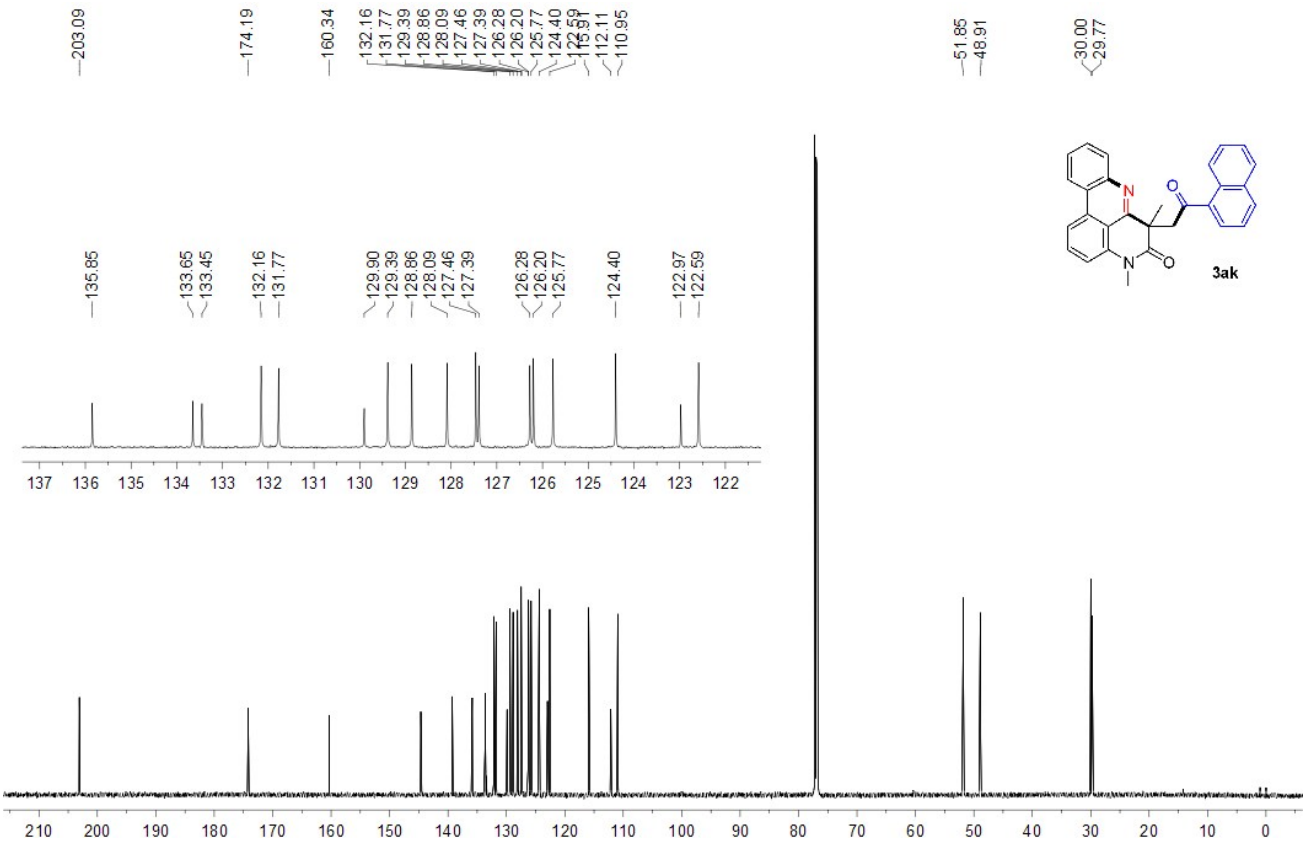
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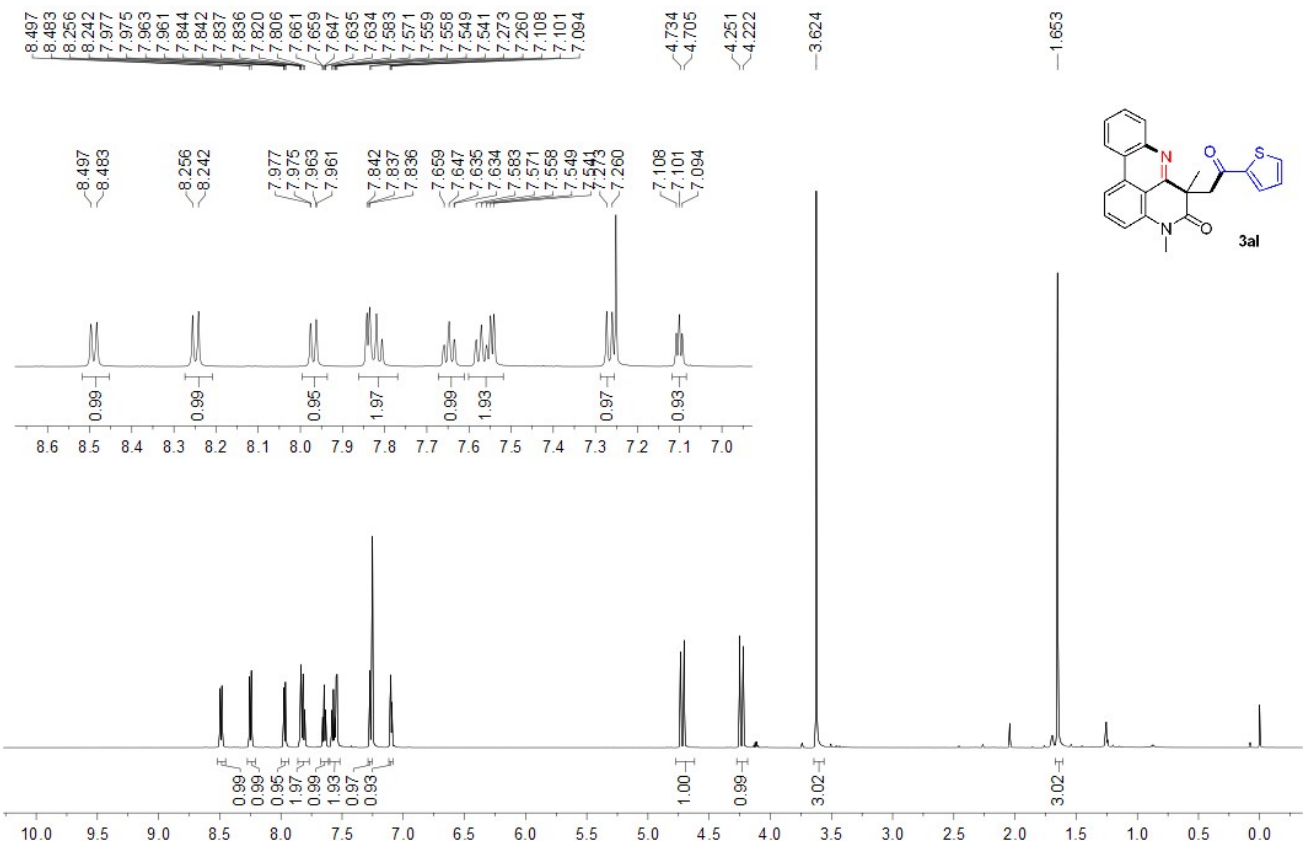
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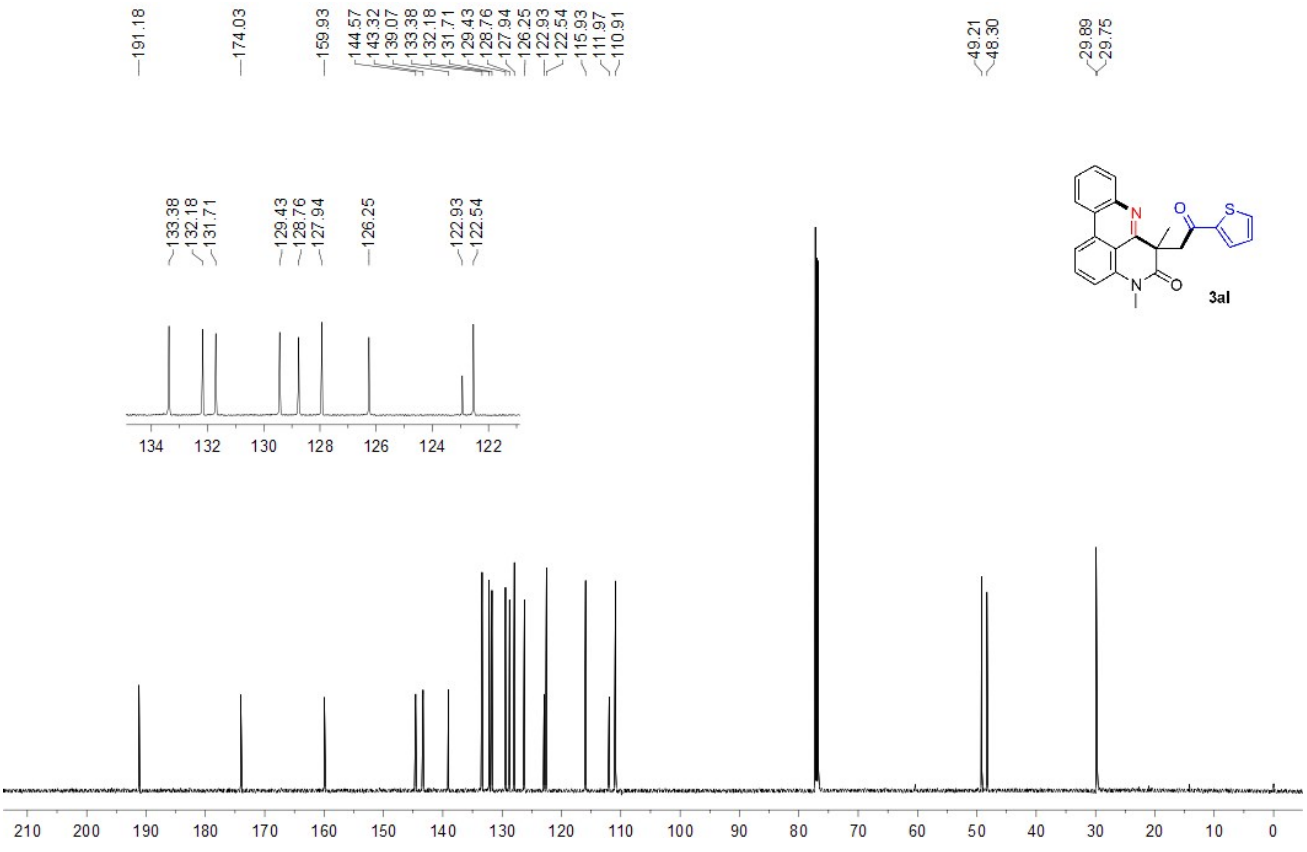
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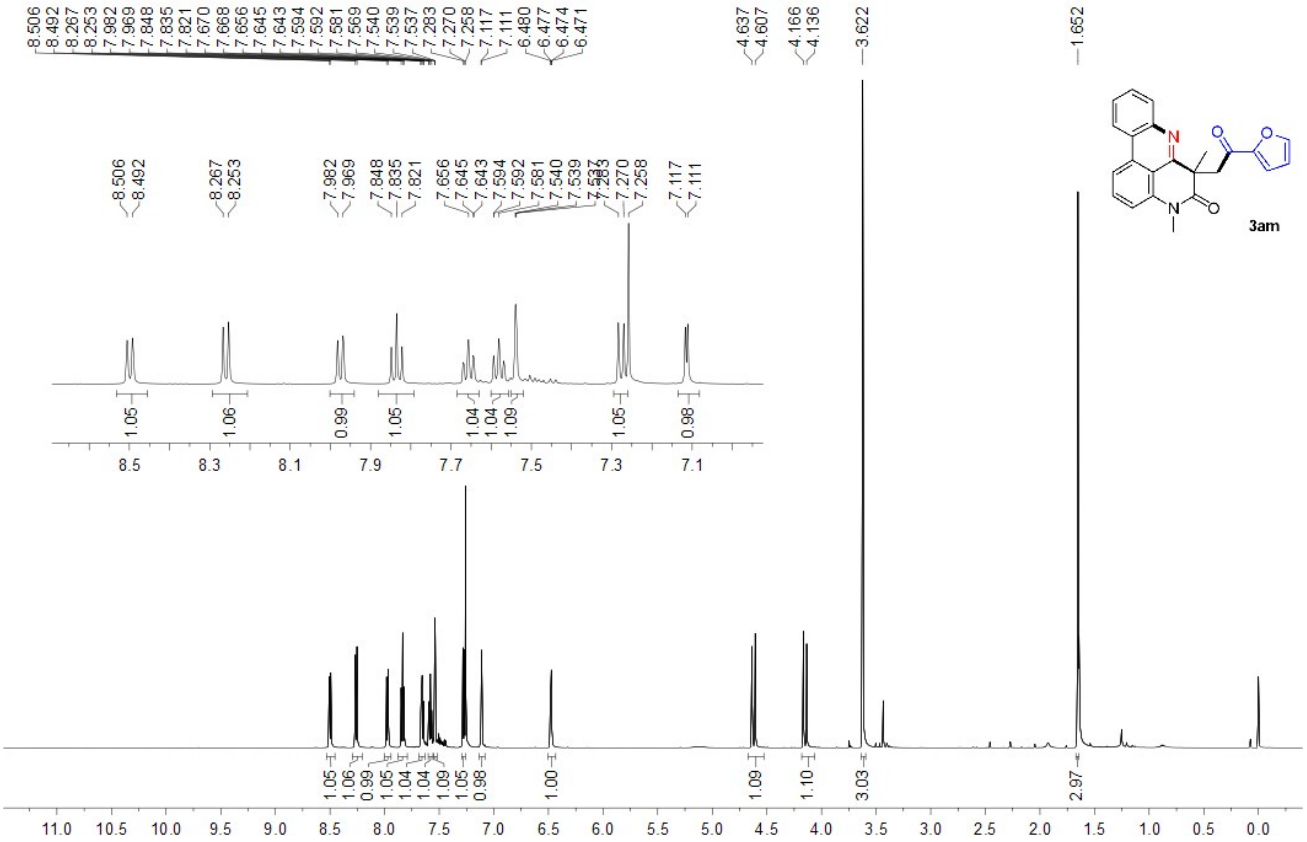
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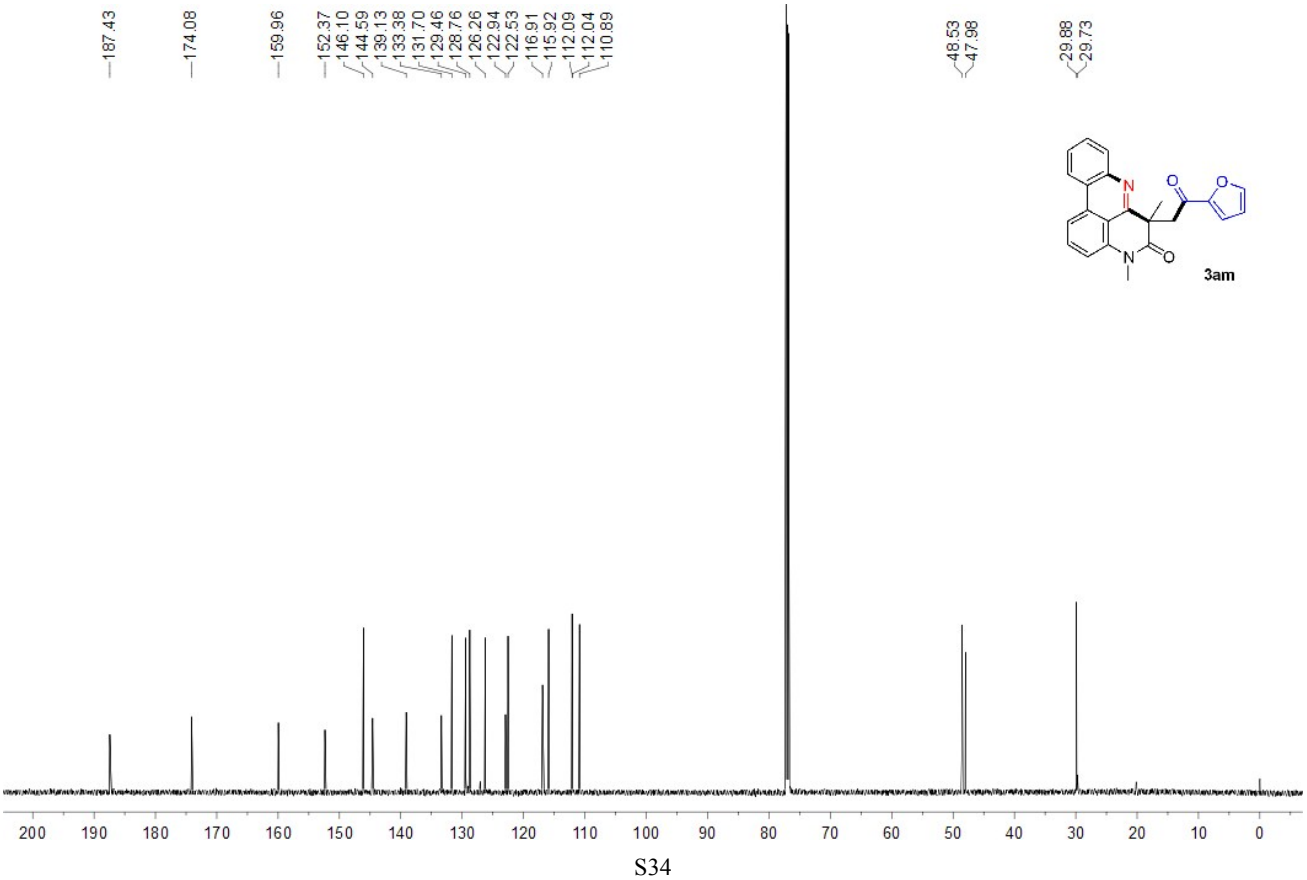
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