Supporting Information

One-Pot Copper-Catalyzed Three-Component Reaction: a Modular Approach to Functionalized 2-Quinolones

Ah Reum Kim and Hee Nam Lim*

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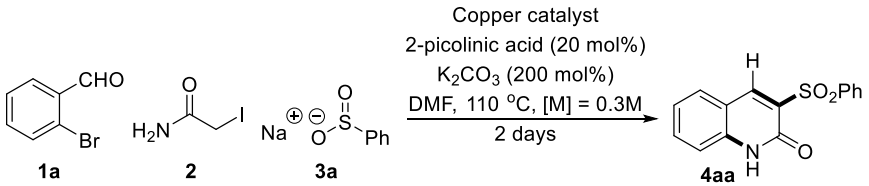
1. Preparation of starting materials

2-Bromobenzaldehydes **1a-b**, **1e-k**, **1o, 1p** and **1r** are purchased from Alfa-Aesar (AA) and Tokyo Chemical Industry (TCI) co., Ltd and **1c**[1a]**-d**[1b]**, 1l**[2a]**-m**[2b] and **1q**[3] are prepared by the known methods. The ketones **1s** and **1u** are purchased from the AA and the TCI, respectively. The ketones **1t,**[4a] **1v**[4b] and **1w**[4c] are prepared. Sodium sulfinates **2b** and **2f** are available from the TCI, and **2d**, **2e** and **2g-i** are purchased from the Fluorochem. The sodium sulfinates **2c** and **2j-n** are prepared by the known methods.[5]

2. Optimization table for the Cu-salts



1a (0.5 mmol) **2** (0.75 mmol) **3a** (0.75 mmol) **4aa**

Entry	Copper catalyst	Yield[a]
1	Cu powder (60-80nm)	55%
2	Cu(dendritic)	42%
3	Cu(25nm)	40%
4	CuI	51%
5	CuBr	42%
6	CuCl	40%
7	$Cu(OAc)_2$	46%
8	$Cu(OTf)_2$	32%
9	CuO_2	12%

[a]determined by 1H NMR using 1,3,5-trimethoxybenzene as the internal standard

[1] (a) L. R. Marcin, A. C. Good, Y.-J. Wu, D. S. Zuev, R. E. Olson and N. Wang (Bristol-Myers Squibb Co., USA), Preparation of amino acid-containing macrocycles as inhibitors of β–amyloid production, *US Patent* 20080194535, August 14, 2008; (b) B. H. Ahn, I. Y. Lee and H. N. Lim, *Org. Biomol. Chem*., 2018, **16**, 7851.

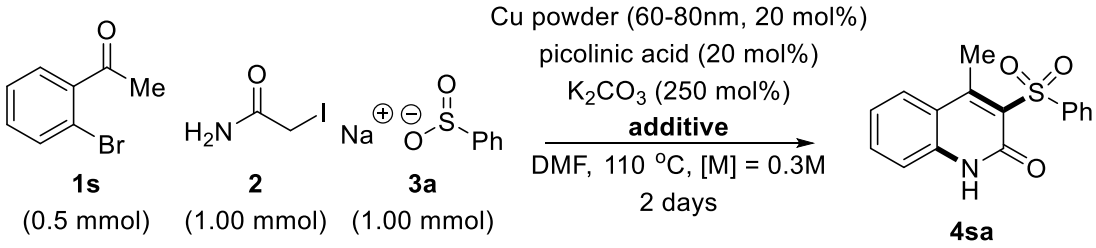
[2] (a) N. M. R. McNeil, D. J. Press, D. M. Mayder, P. Garnica, L. M. Doyle and T. G. Back, *J. Org. Chem*., 2016, **81**, 7884; (b) J. Lin, W. Zhang, N. Jiang, Z. Niu, K. Bao, L. Zhang, D. Liu, C. Pan and X. Yao, *J. Nat. Prod*., 2008, **71**, 1938.

[3] (a) S. Song, X. Sun, X. Li, Y. Yuan and N. Jiao, *Org. Lett*., 2015, **17**, 2886; (b) E. Baiceanu, K.-A. Nguyen, L. Gonzalez-Lobato, R. Nasr, H. Baubichon-Cortay, F. Loghin, M. L. Borgne, L. Chow, A. Boumendjel, M. Peuchmaur and P. Falson, *Eur. J. Med. Chem*., 2016, **122**, 408.

[4] (a) B. N. Hemric, K. Shen and Q. Wang, *J. Am. Chem. Soc*., 2016, **138**, 5813; (b) T. M. E. Dine, W. Erb, Y. Berhault, J. Rouden and J. Blanchet, *J. Org. Chem*., 2015, **80**, 4532; (c) S. L. MacNeil, M. Gray, D. G. Gusev, L. E. Briggs and V. Snieckus, *J. Org. Chem*., 2008, **73**, 9710.

[5] (a) A. U. Meyer, K. Straková, T. Slanina and B. König, *Chem. Eur. J*., 2016, **22**, 8694; (b) T. Markovic, B. N. Rocke, D. C. Blakemore, V. Mascitti and M. C. Willis, *Org. Lett*., 2017, **19**, 6033; (c) G. Bogonda, D. V. Patil, H. Y. Kim and K. Oh, *Org. Lett*., 2019, **21**, 3774.

3. Optimization tables for the ketone substrate



1s (0.5 mmol) **2** (1.00 mmol) **3a** (1.00 mmol) **4sa**

Table S1. Additive effect

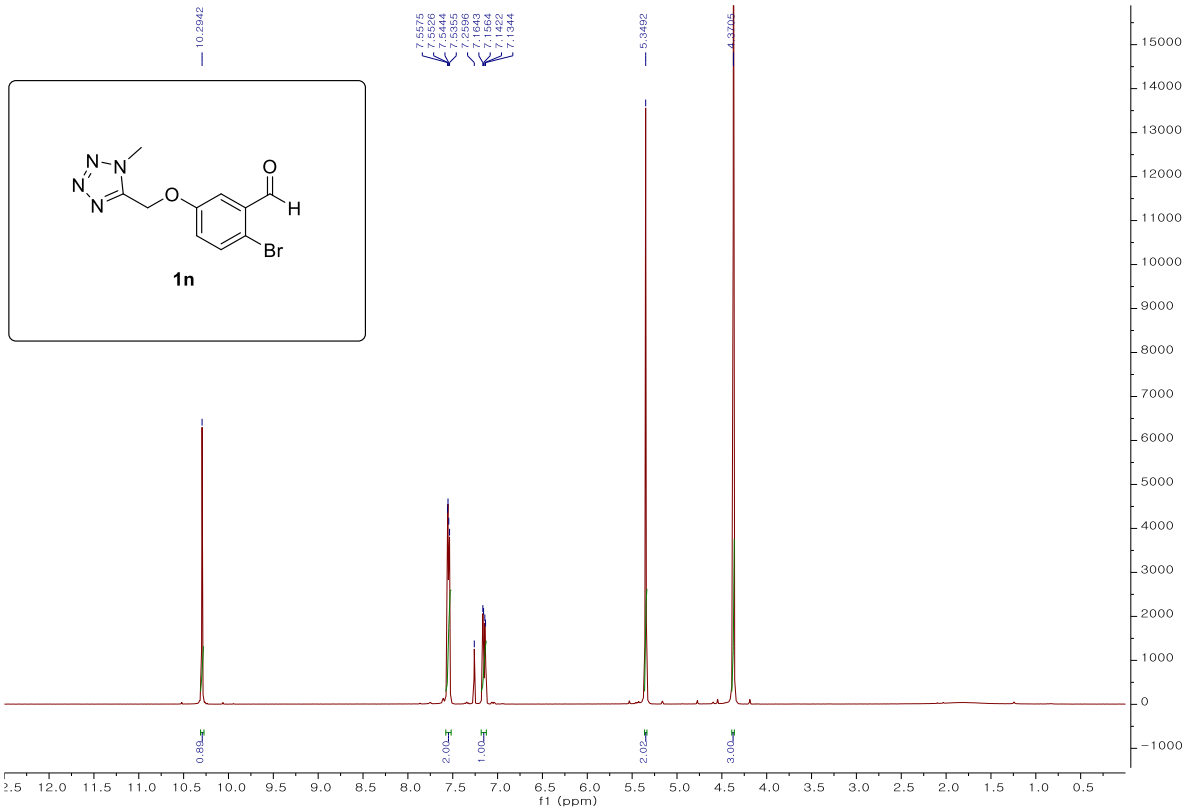
desiccant (1equiv)	*Yield*[a]
None	4%
$MgSO_4$	4%
Na_2SO_4	trace
Al_2O_3	5%
NaCl	5%
$CaCl_2$	2%
silica gel (100wt%)	trace
molecular sieve 4Å (100 wt%)	9%
CaO	trace
$Ca(OH)_2$	**20%**

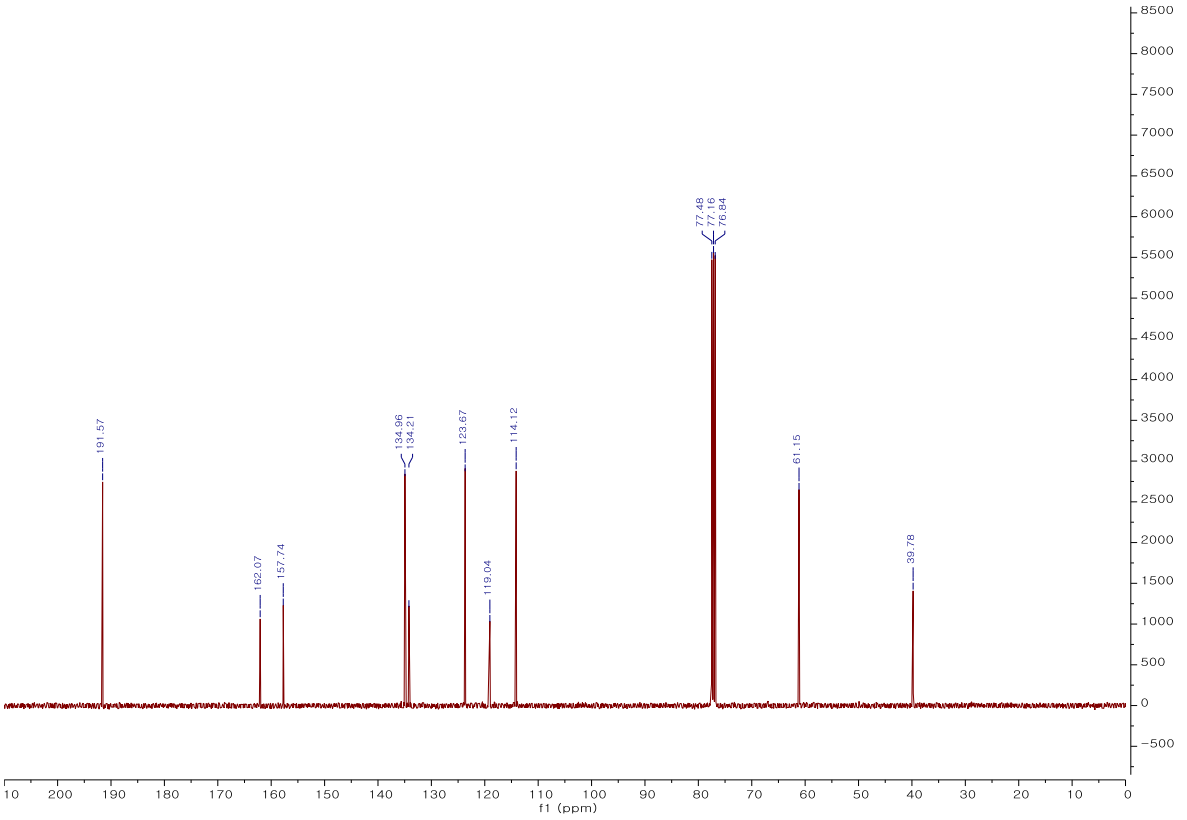
Table S2. Determination of $Ca(OH)_2$ equivalent

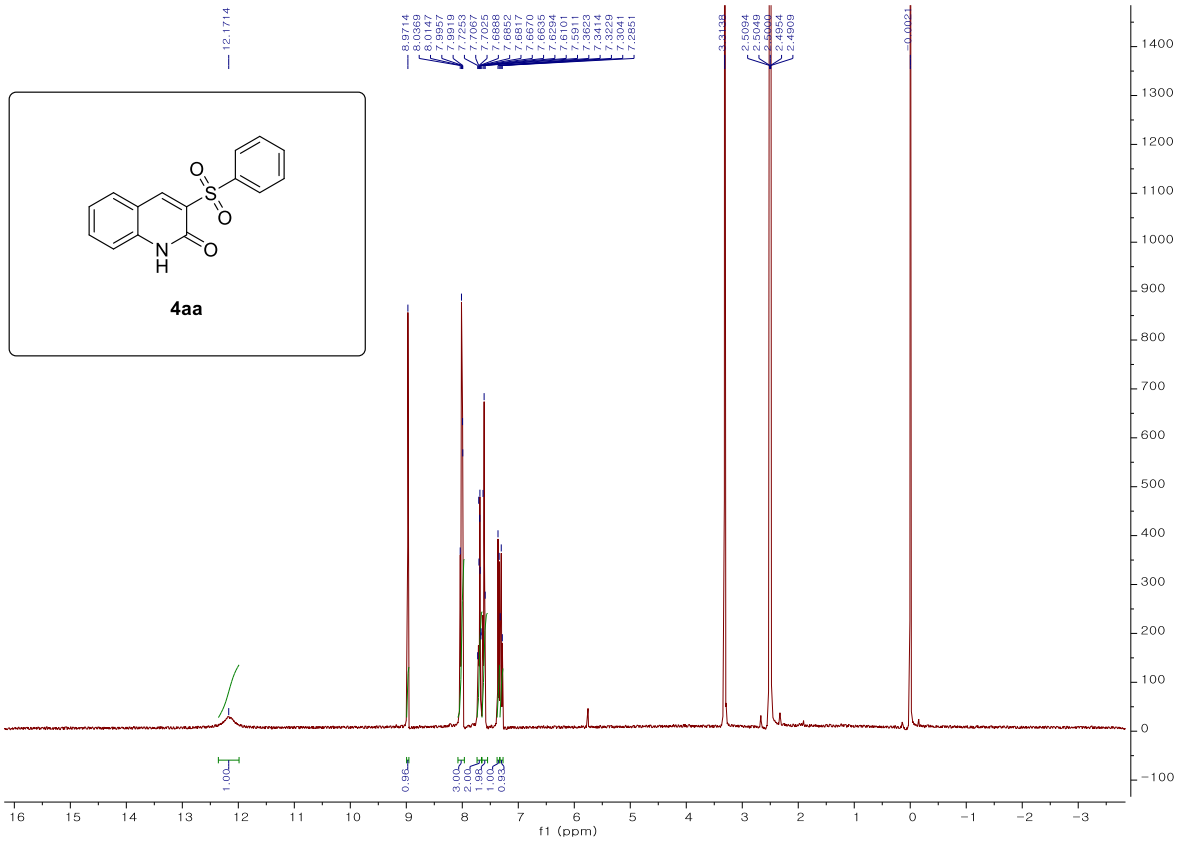
equivalent of $Ca(OH)_2$	*Yield*[a]
1.0 equiv (0.50 mmol)	20%
1.5 equiv (0.75 mmol)	29%
2.0 equiv (1.00 mmol)	56%
2.5 equiv (1.25 mmol)	**59%**
3.0 equiv (1.50 mmol)	58%

[a]determined by 1H NMR using 1,3,5-trimethoxybenzene as the internal standard

3. ^{1}H-NMR, ^{13}C-NMR and ^{19}F-NMR



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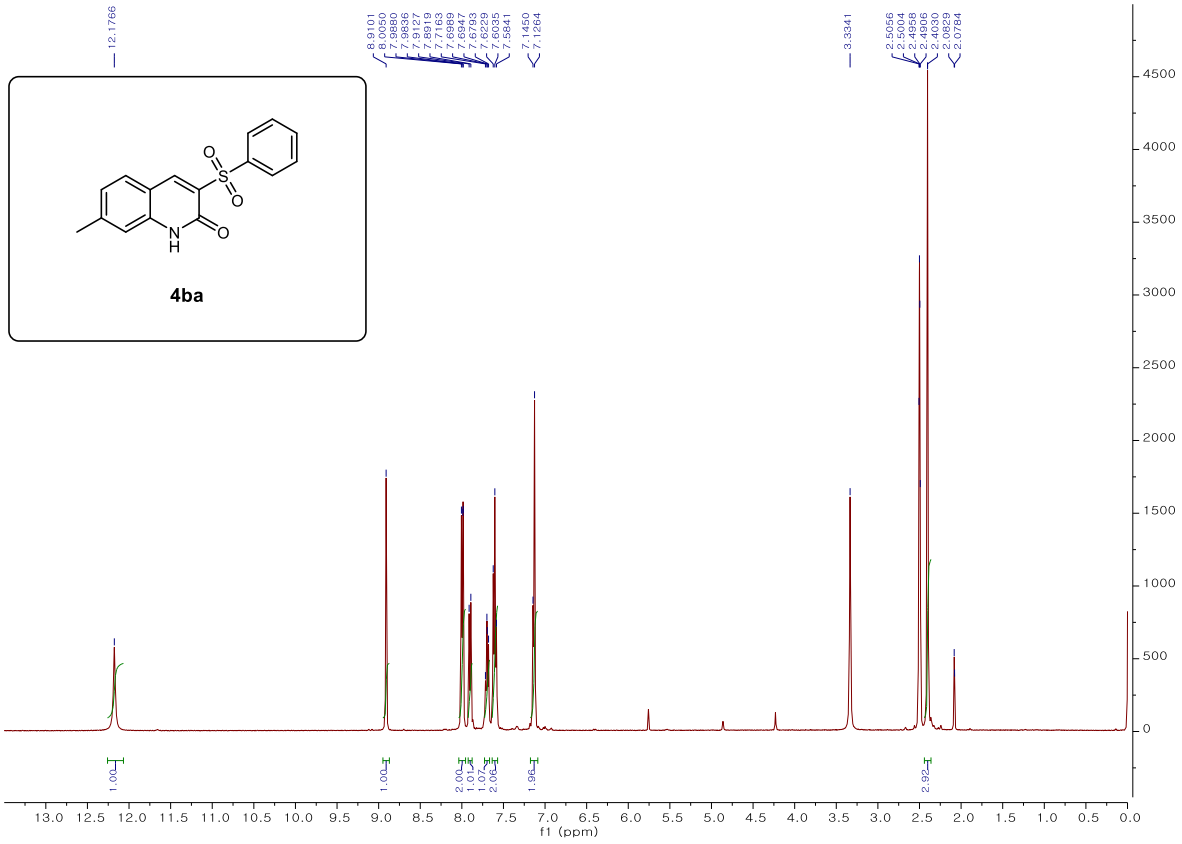
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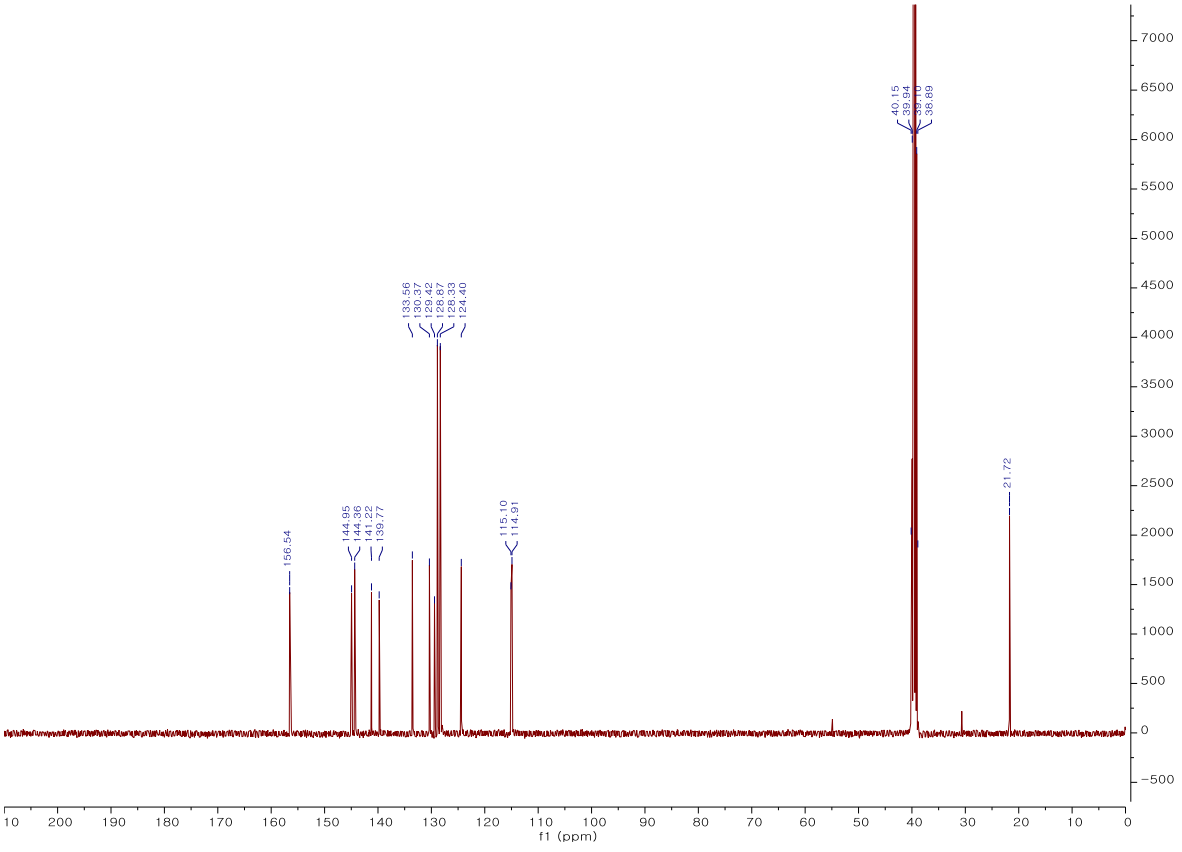
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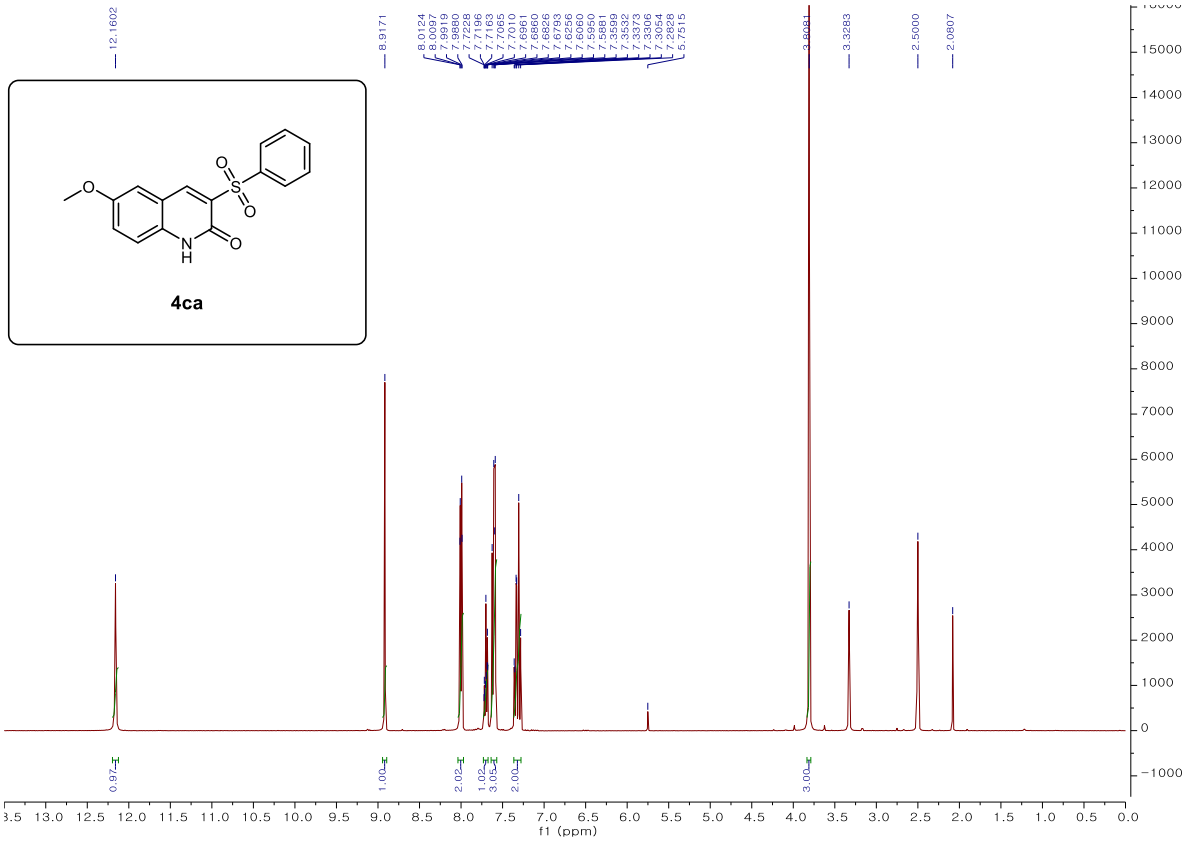
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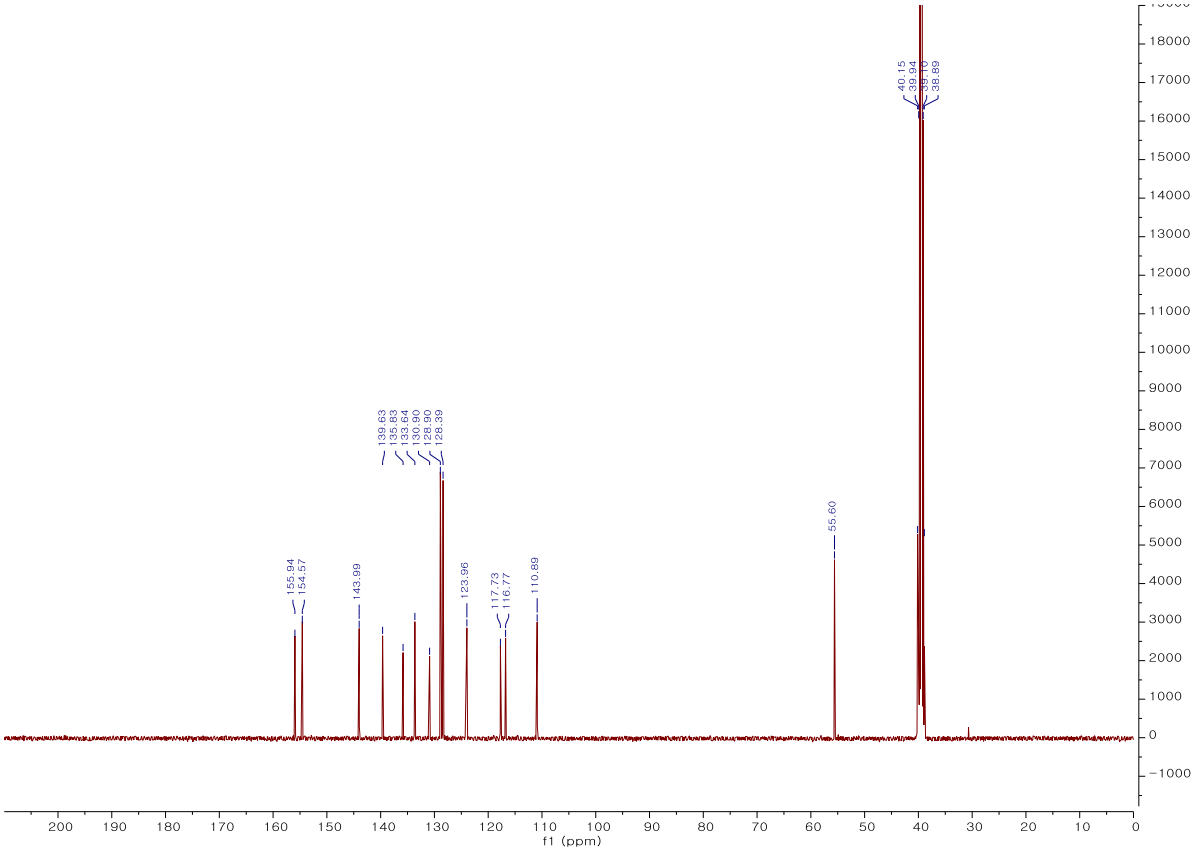
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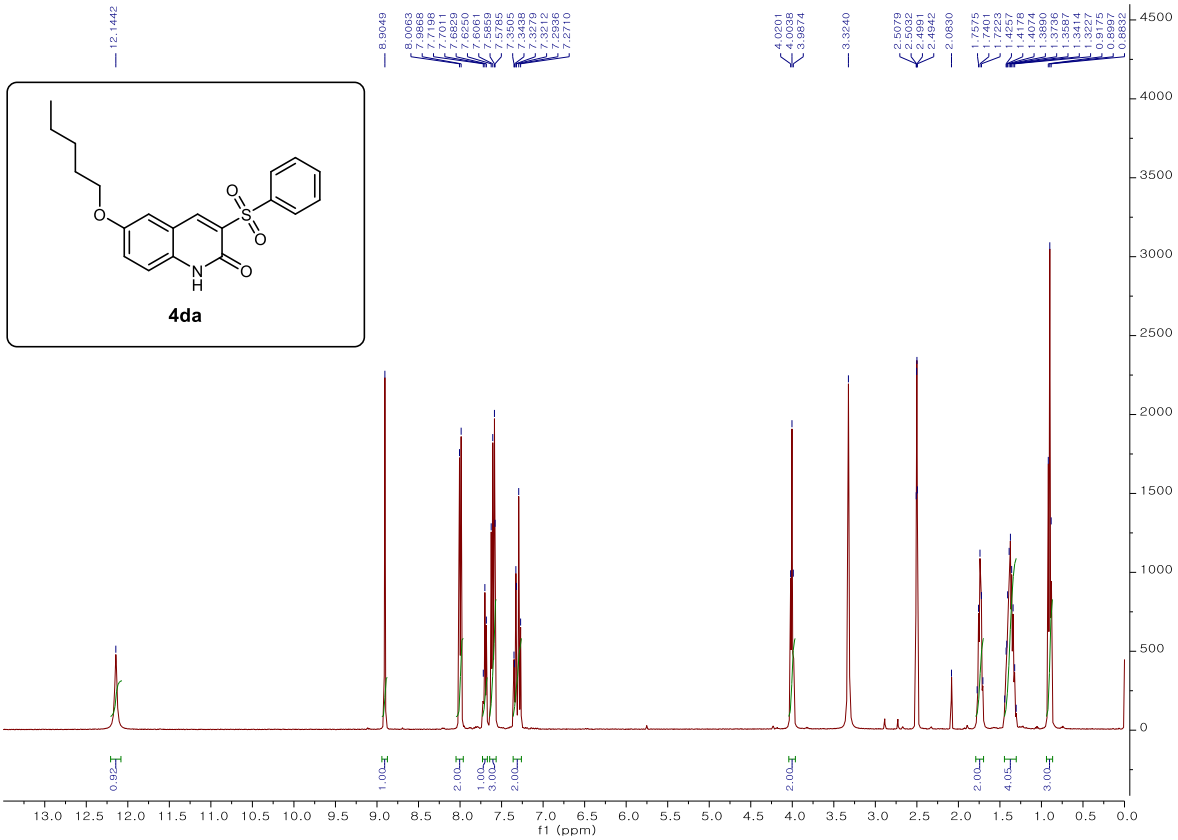
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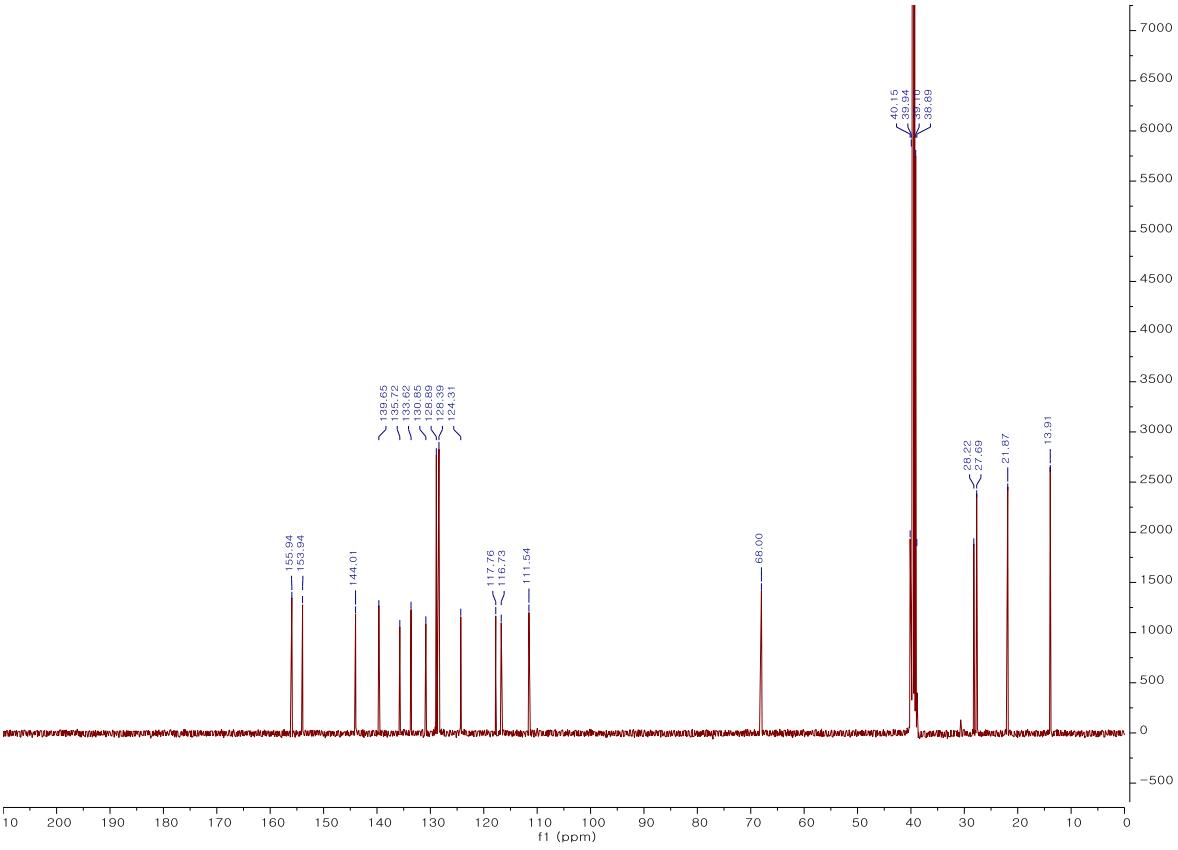
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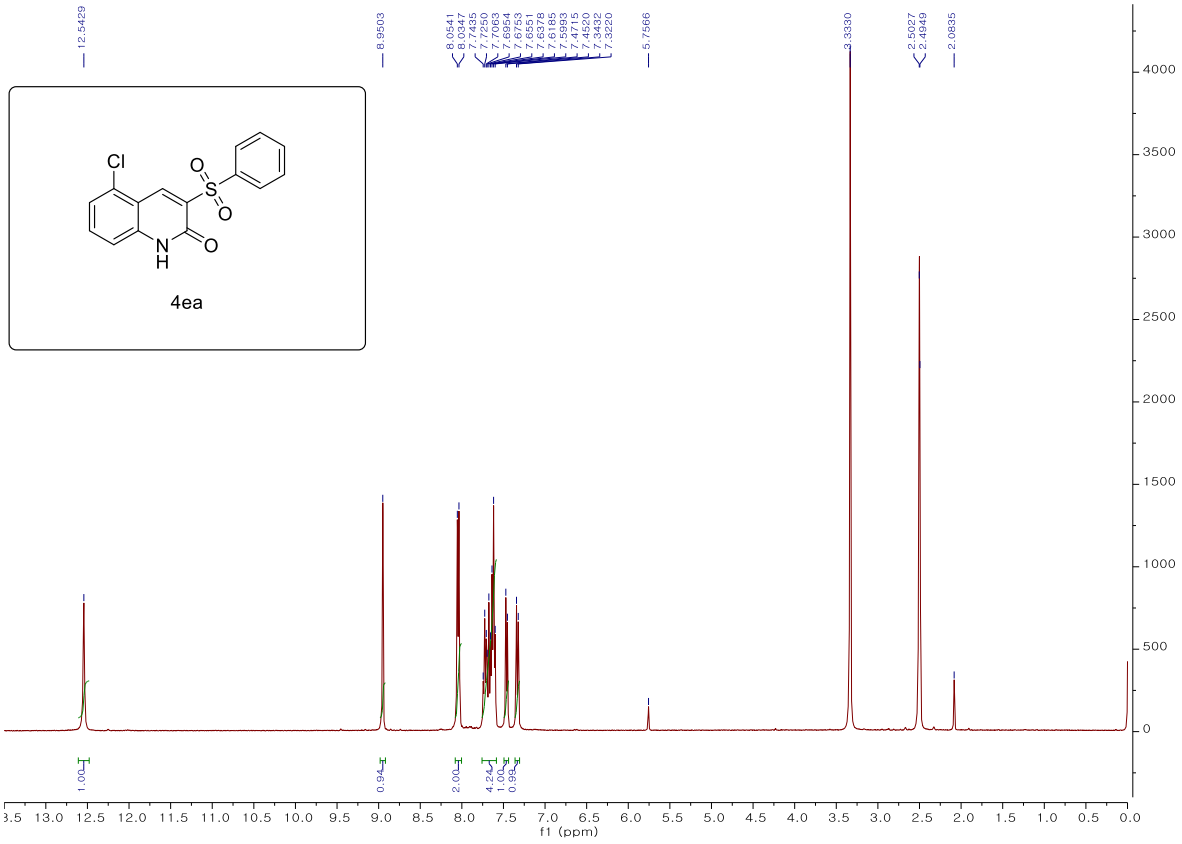
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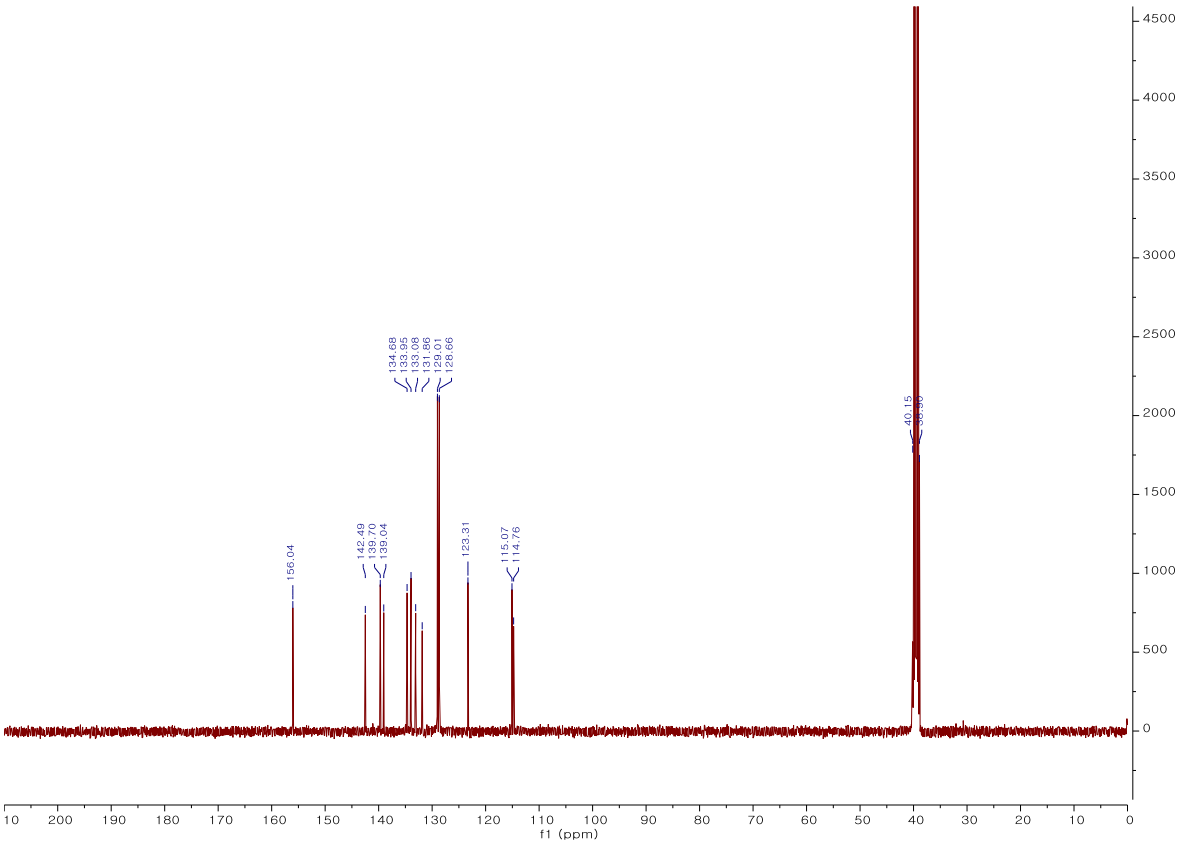
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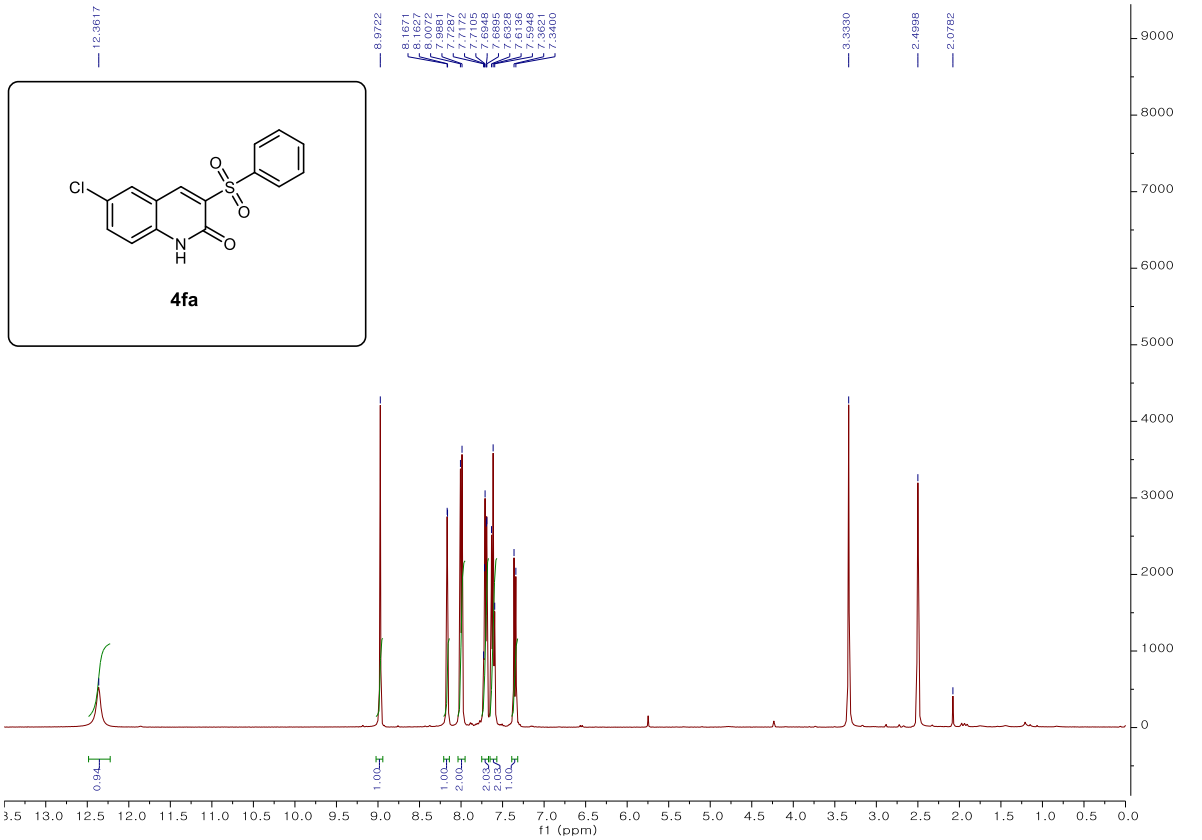
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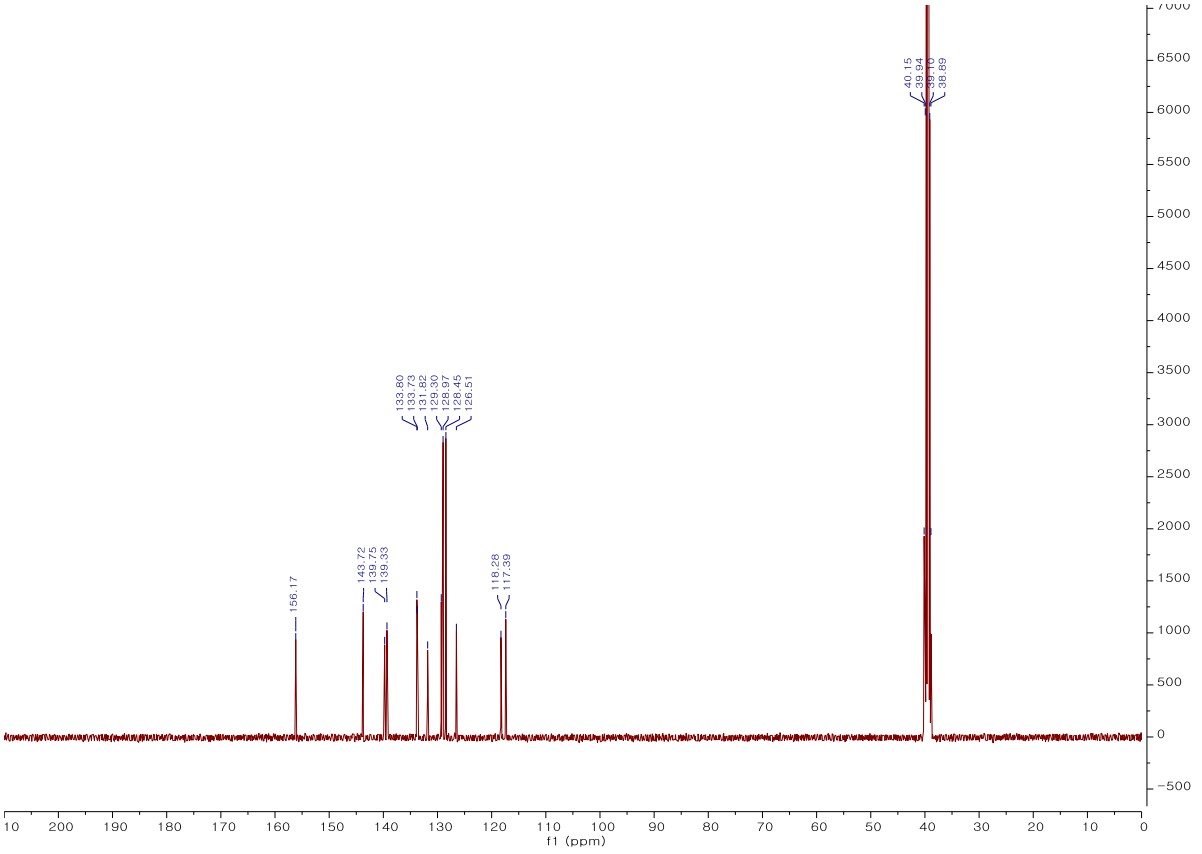
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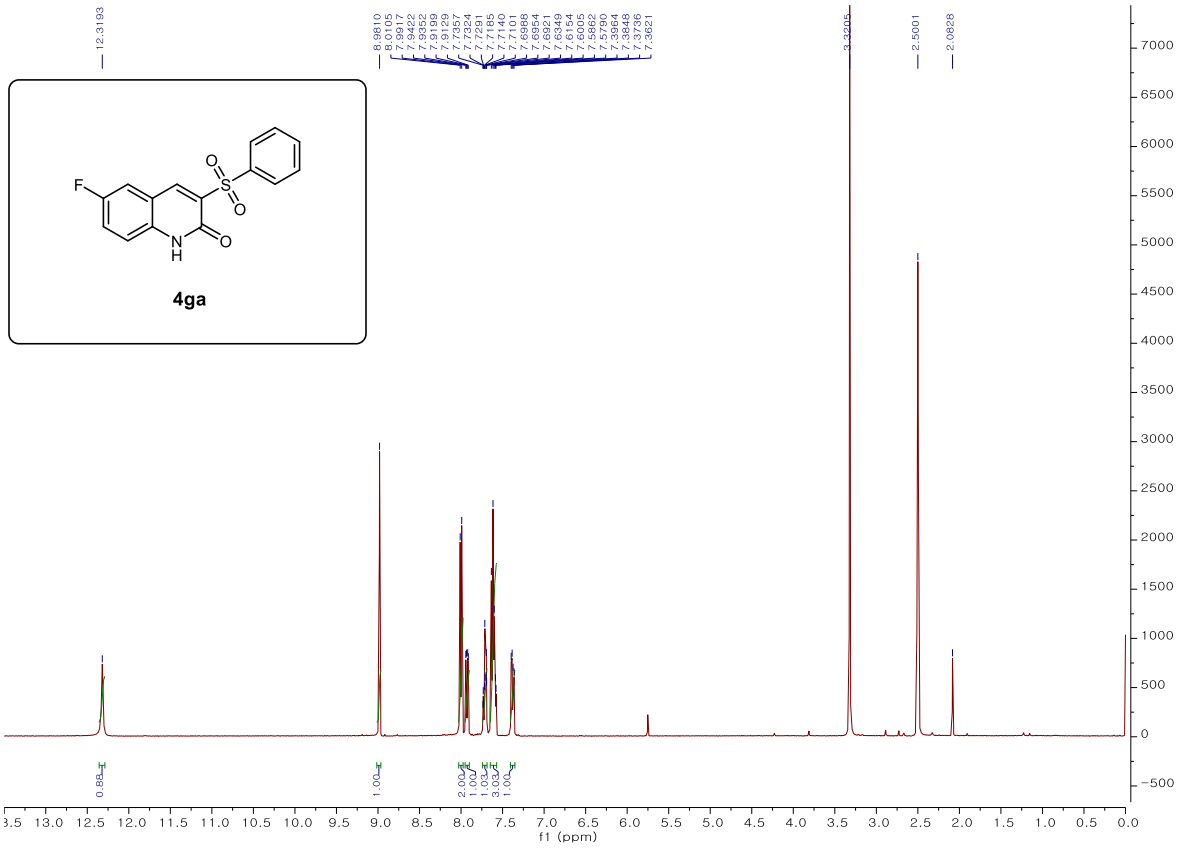
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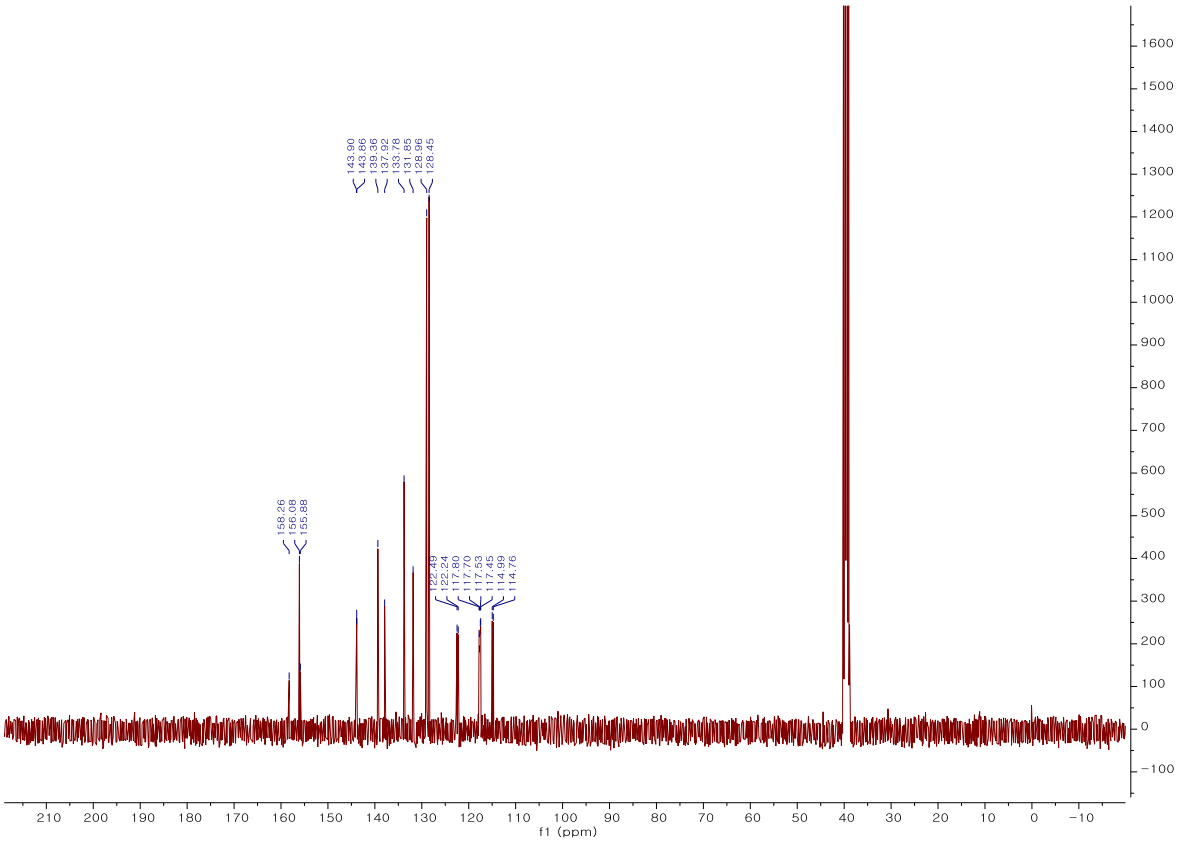
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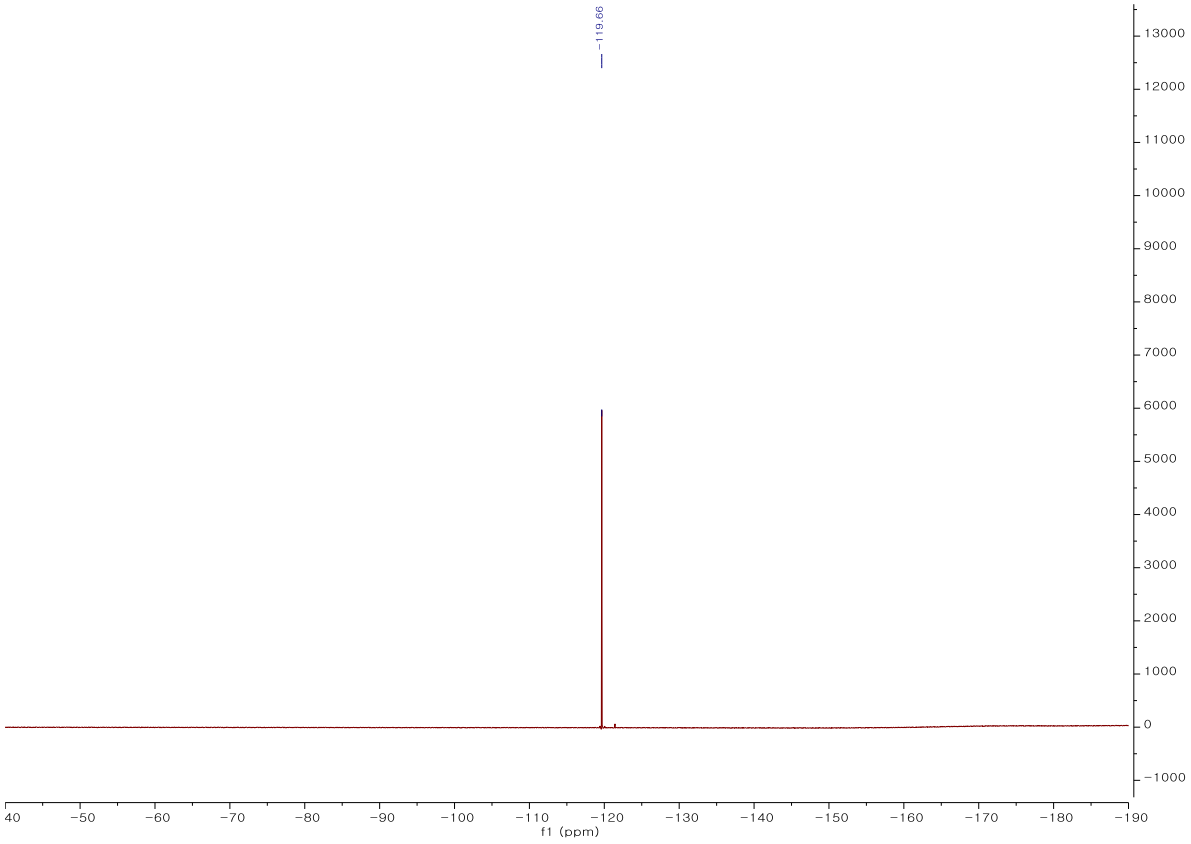
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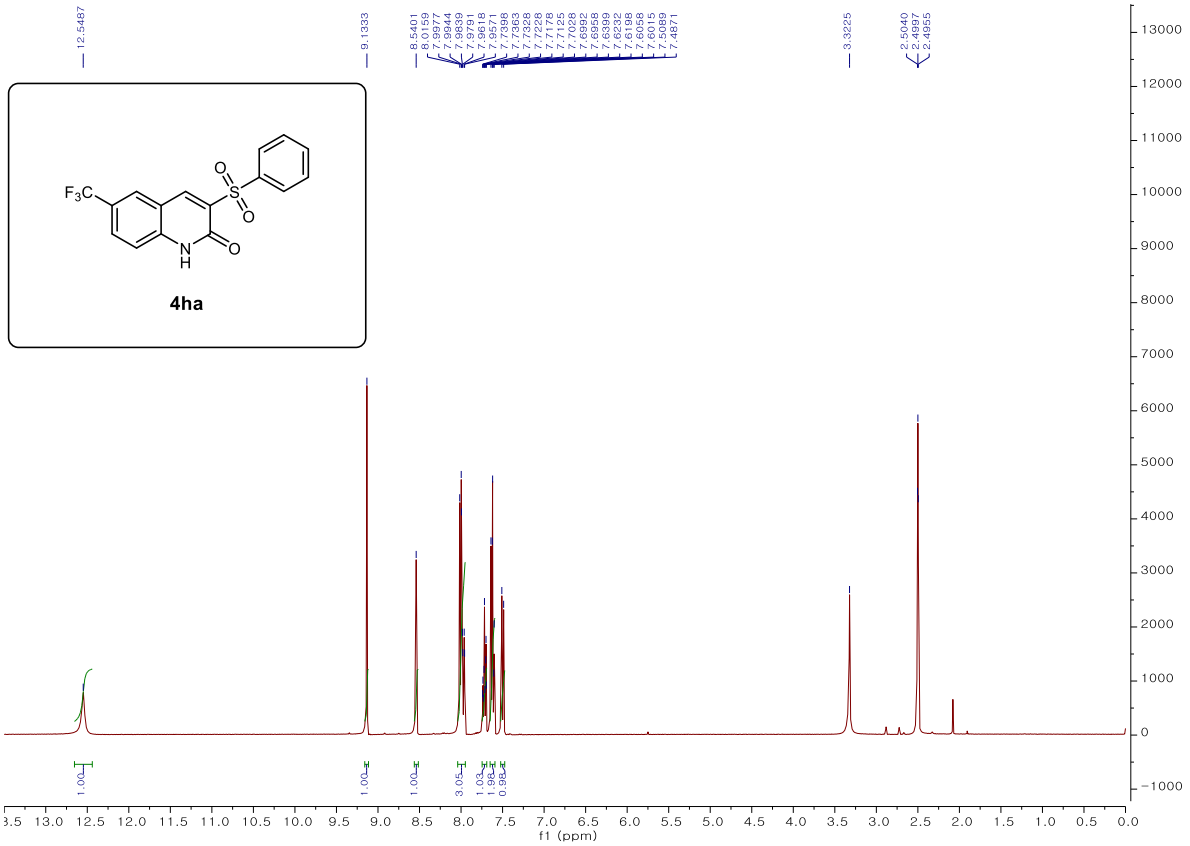
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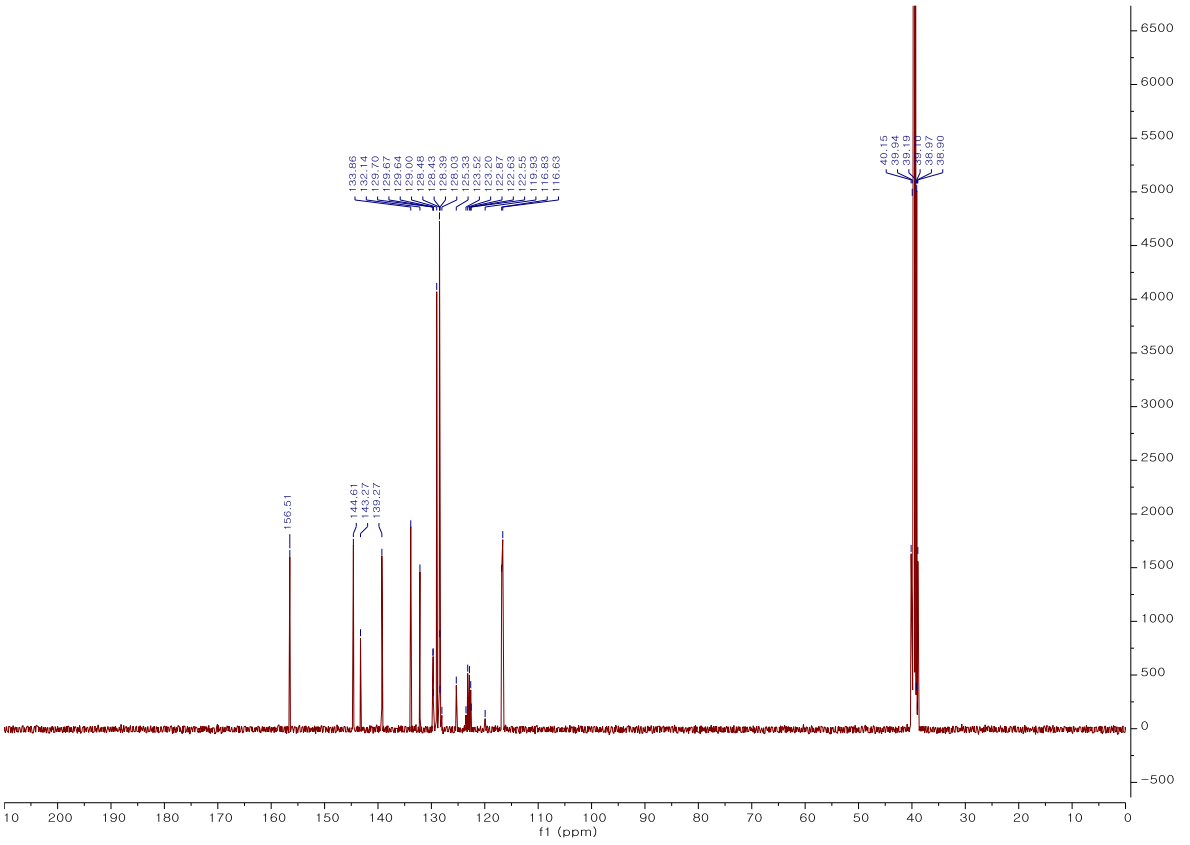
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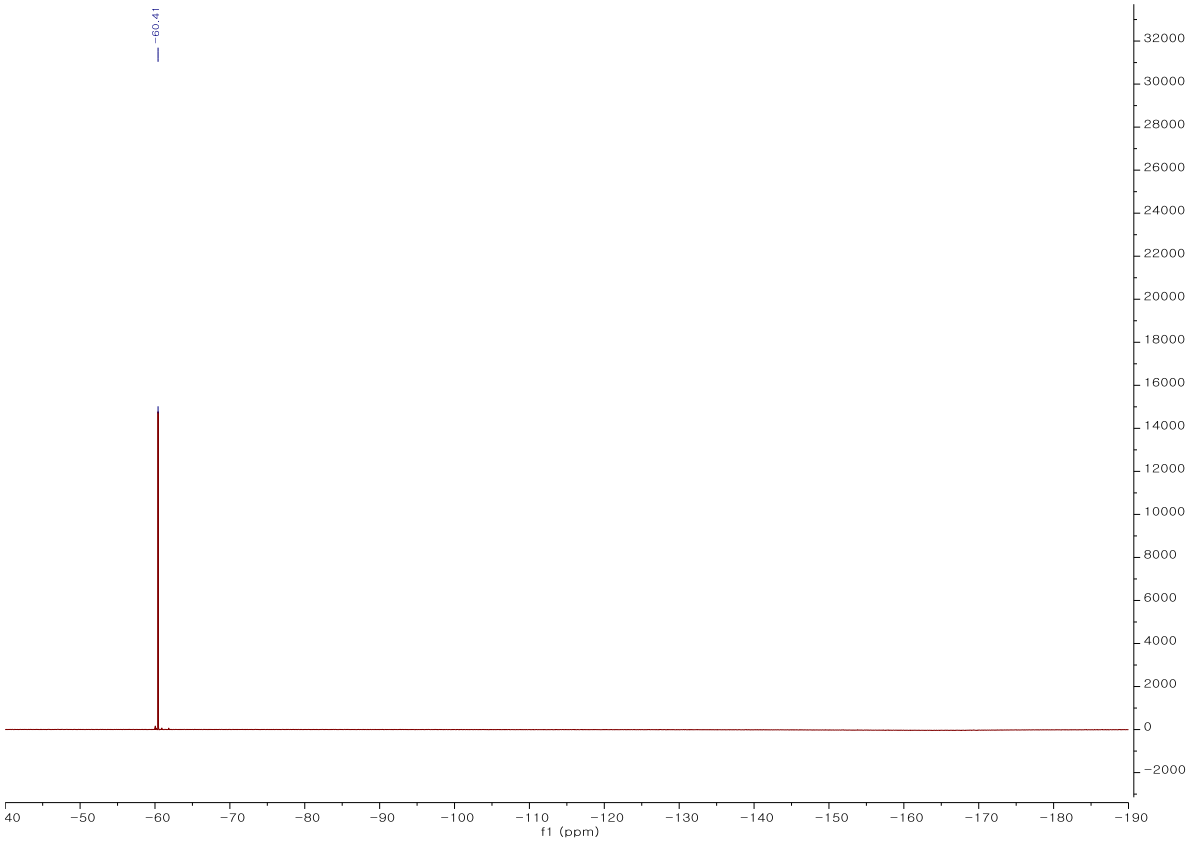
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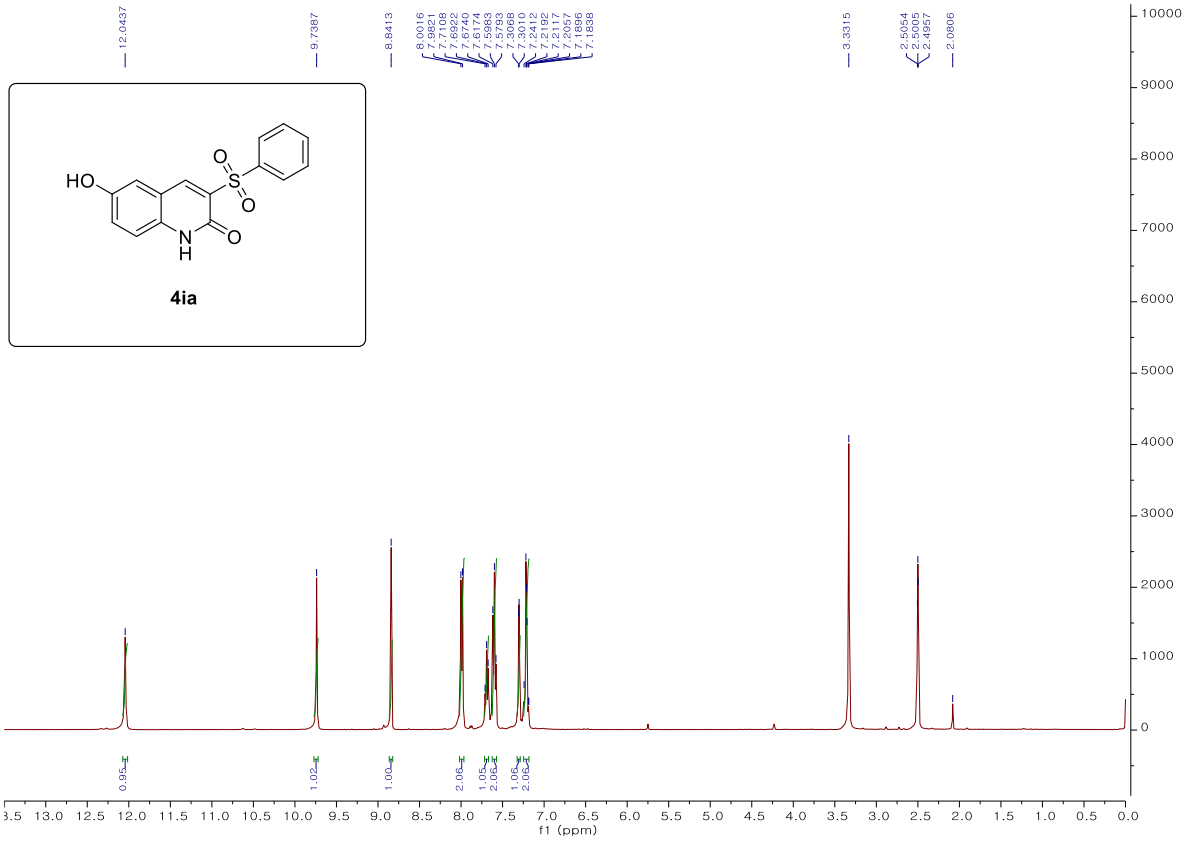
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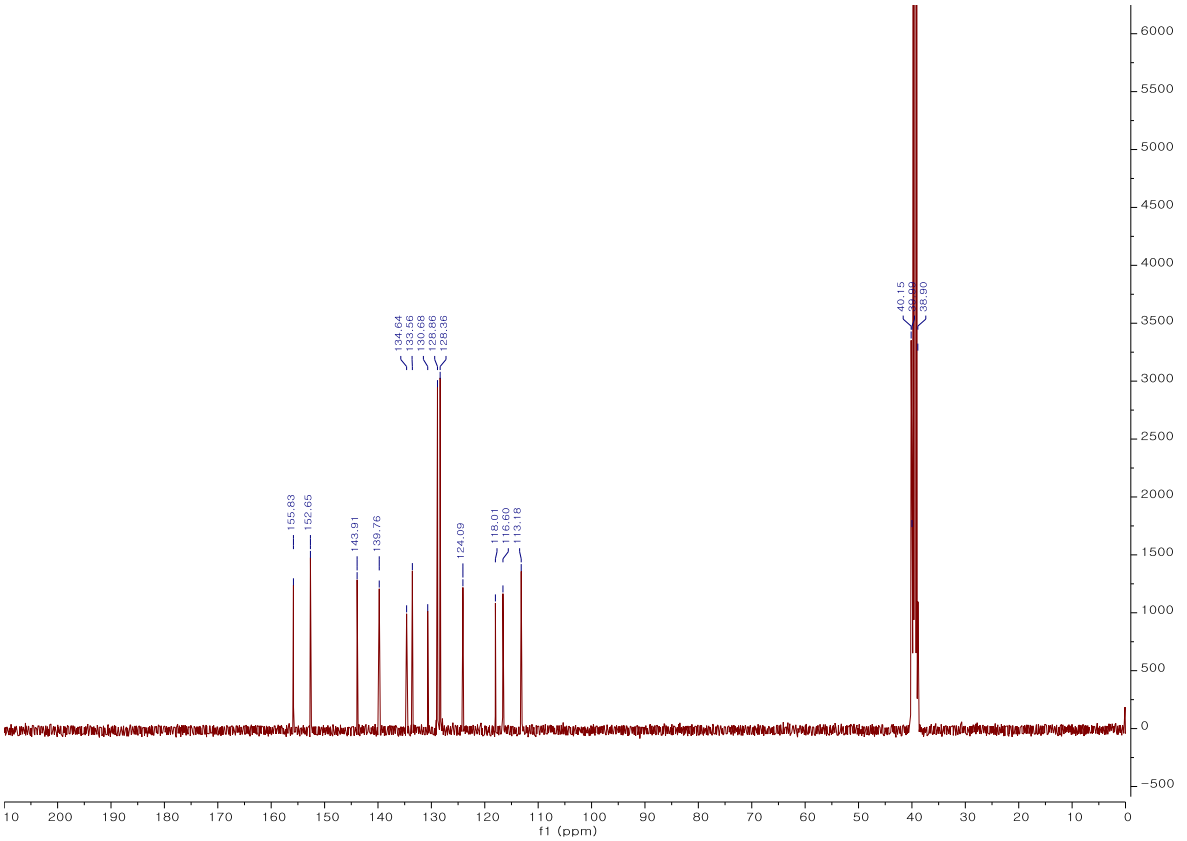
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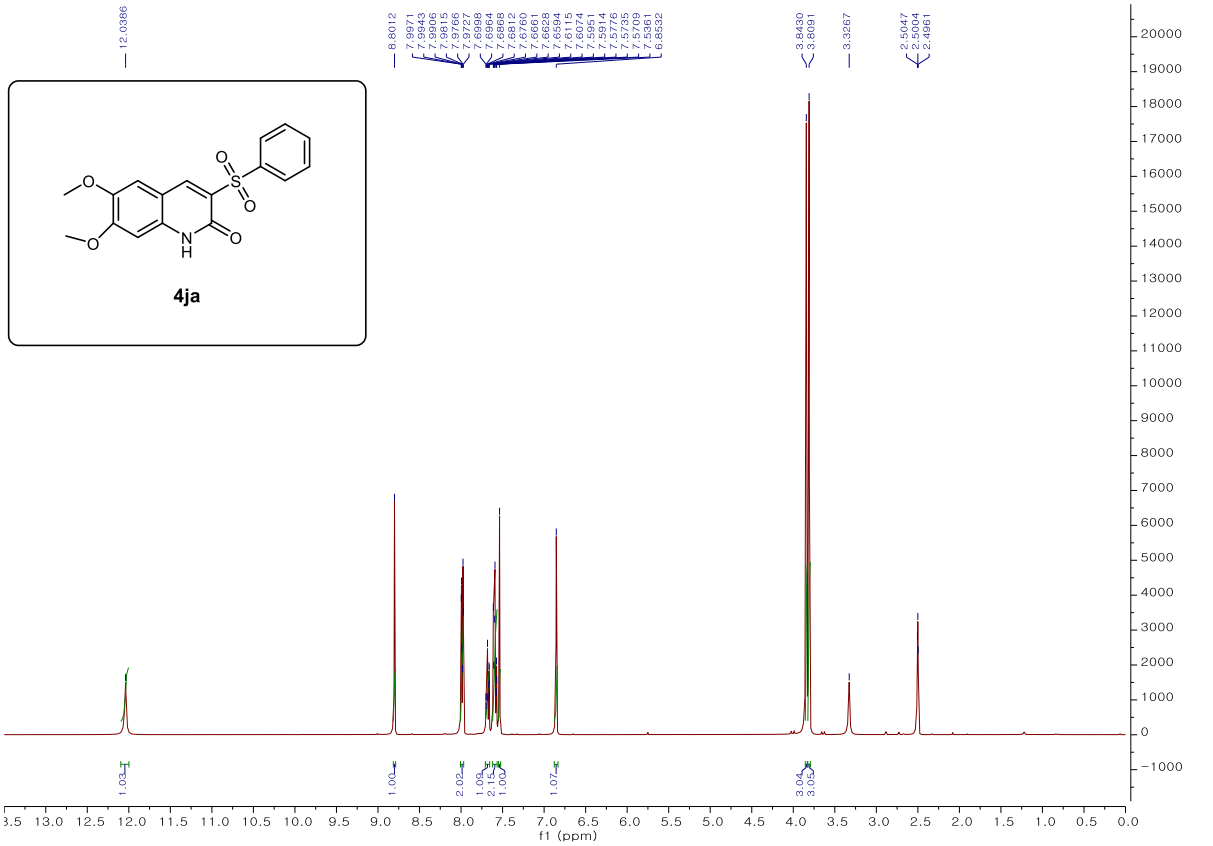
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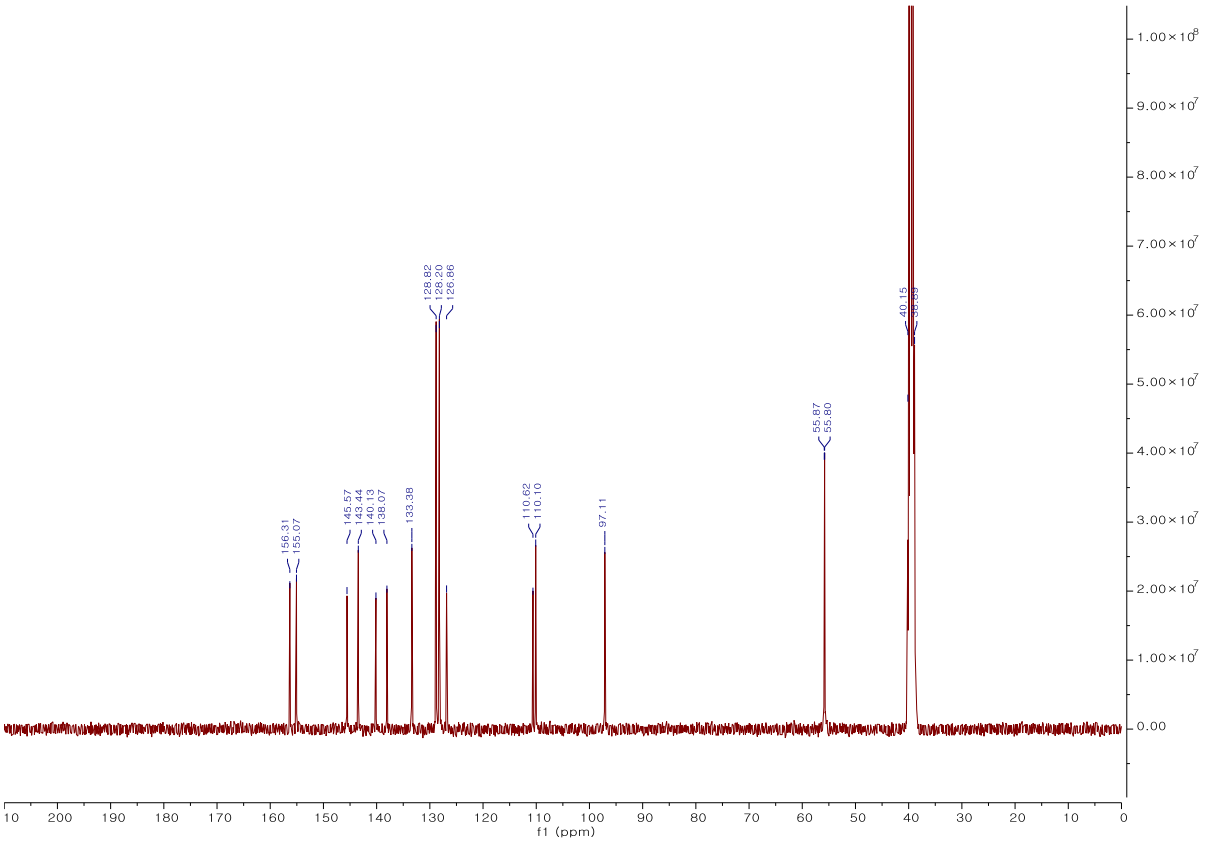
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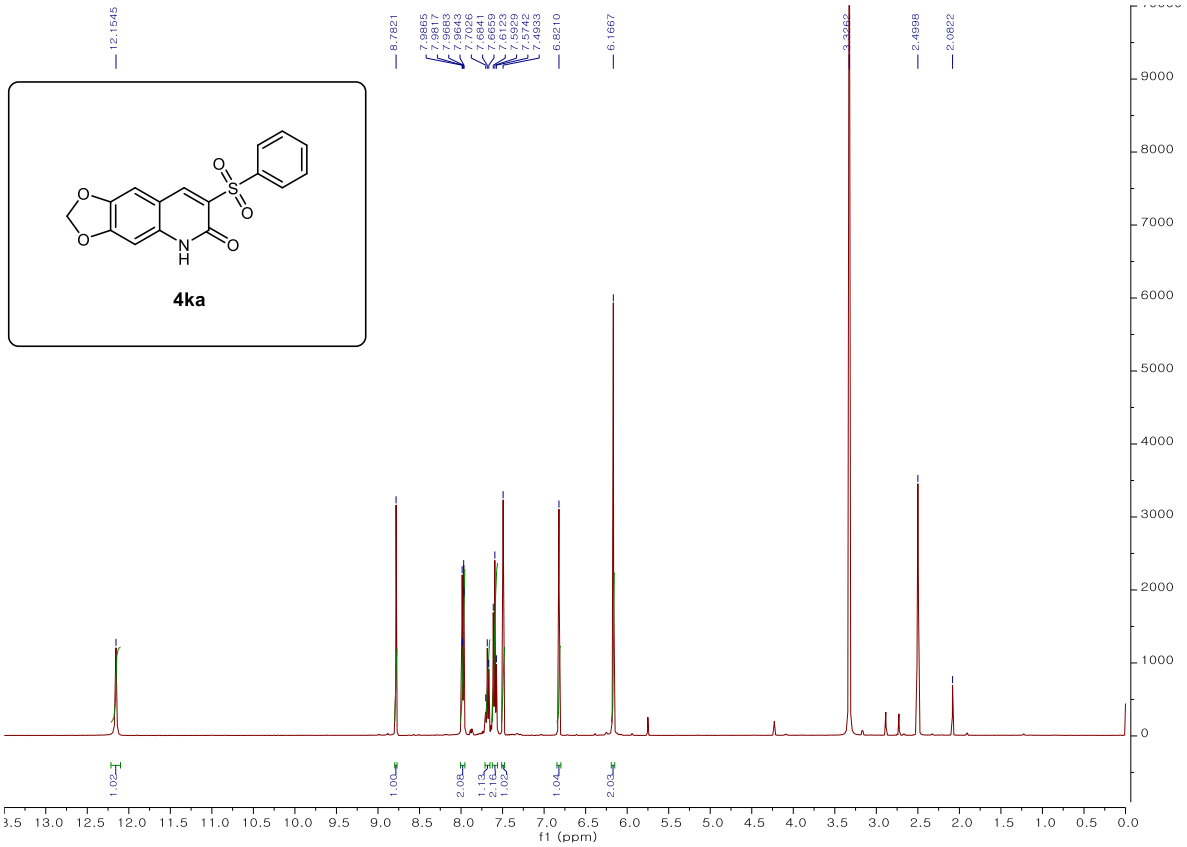
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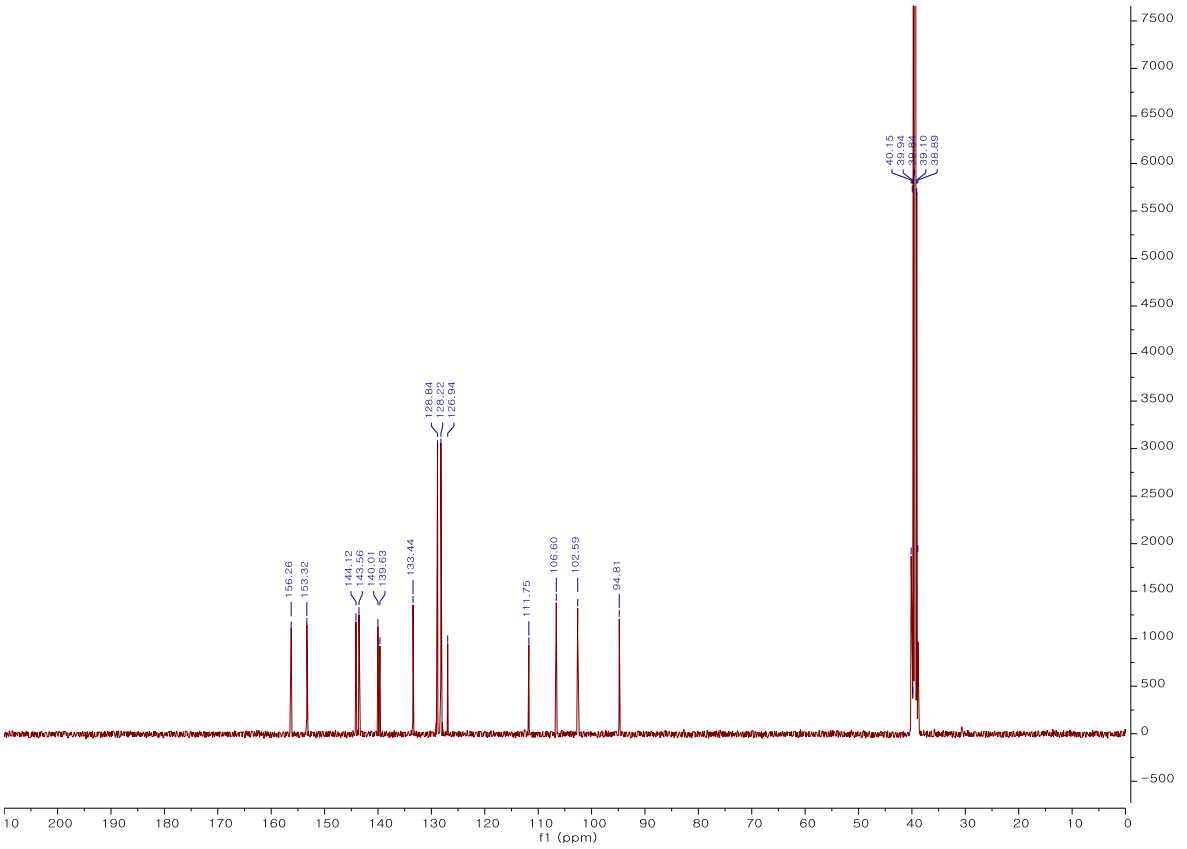
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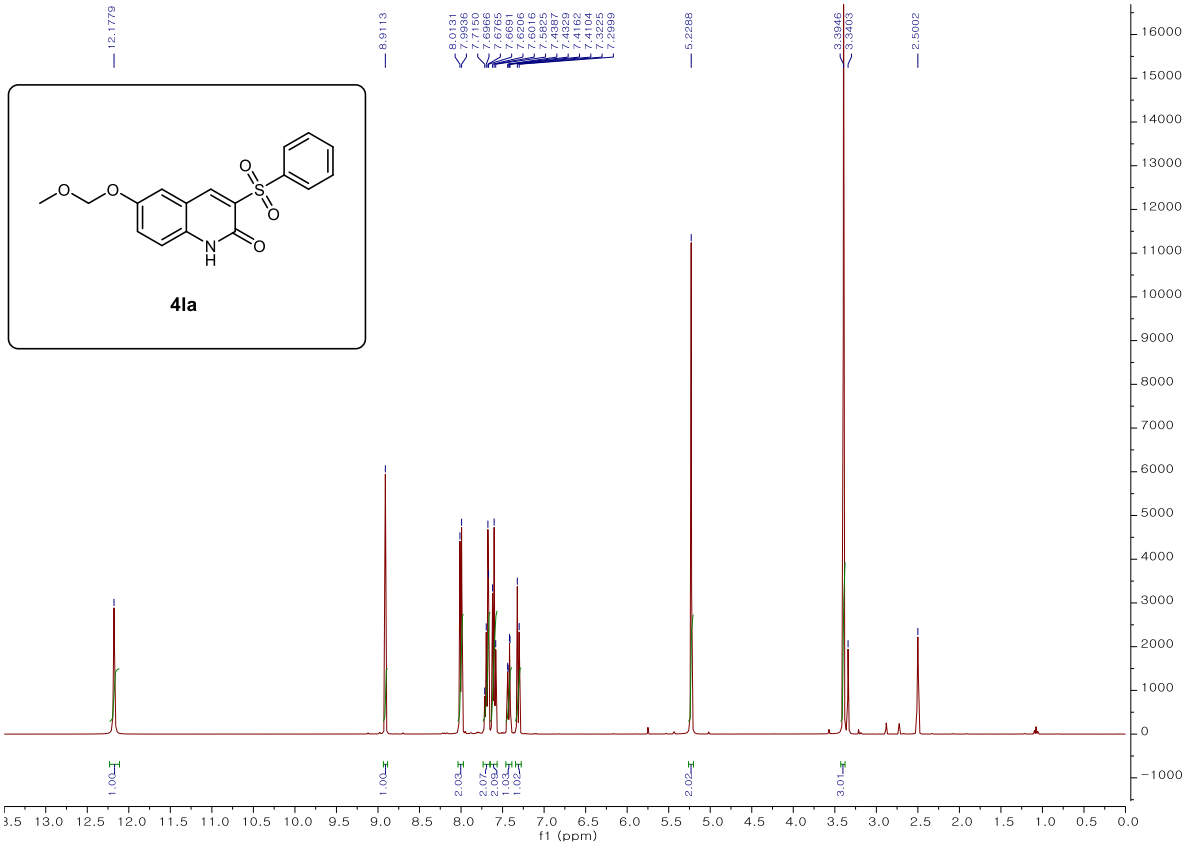
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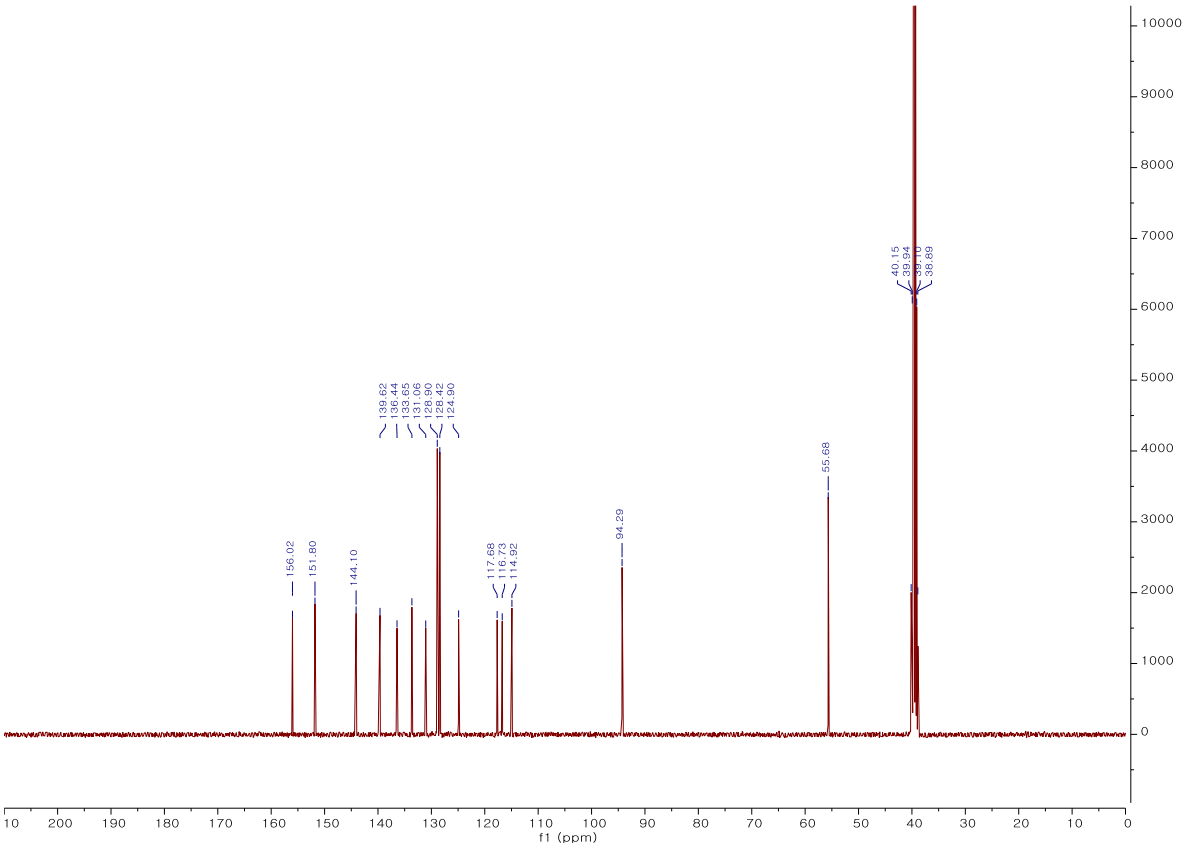
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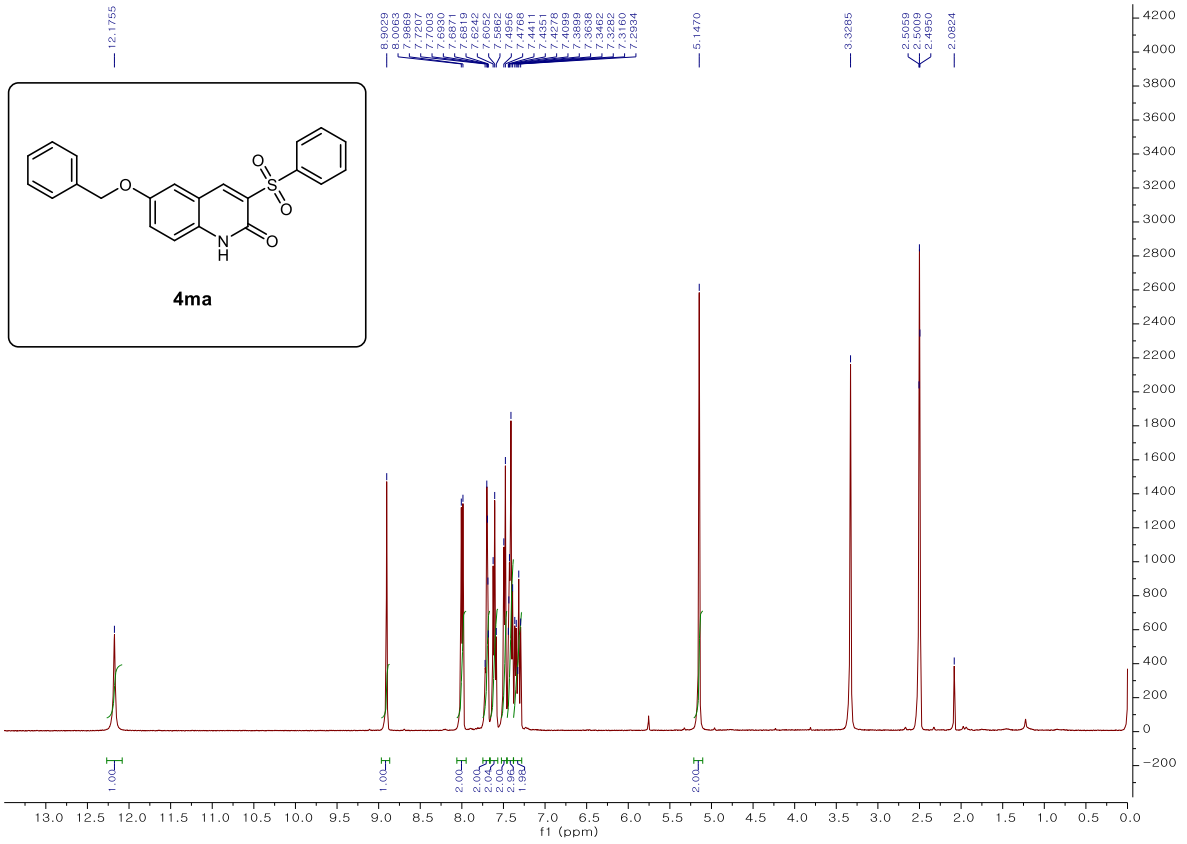
f1 (ppm)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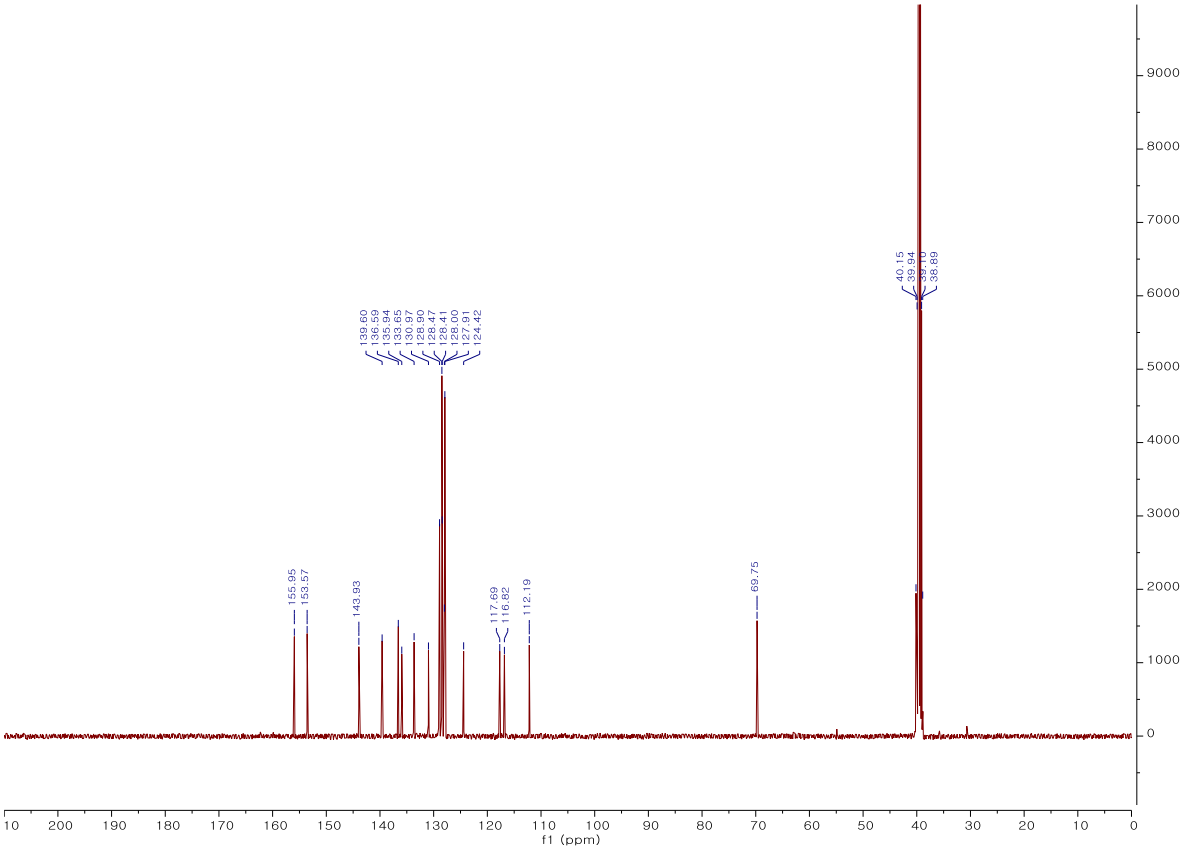
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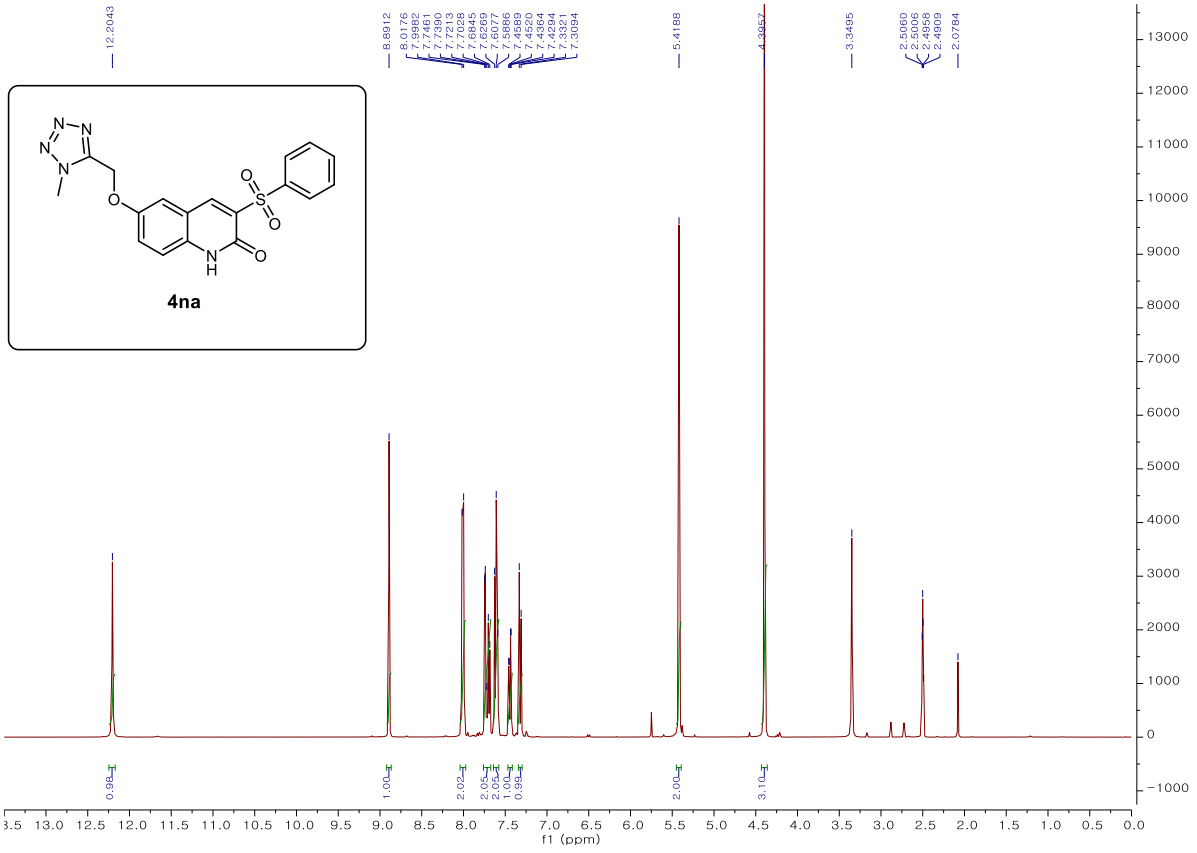
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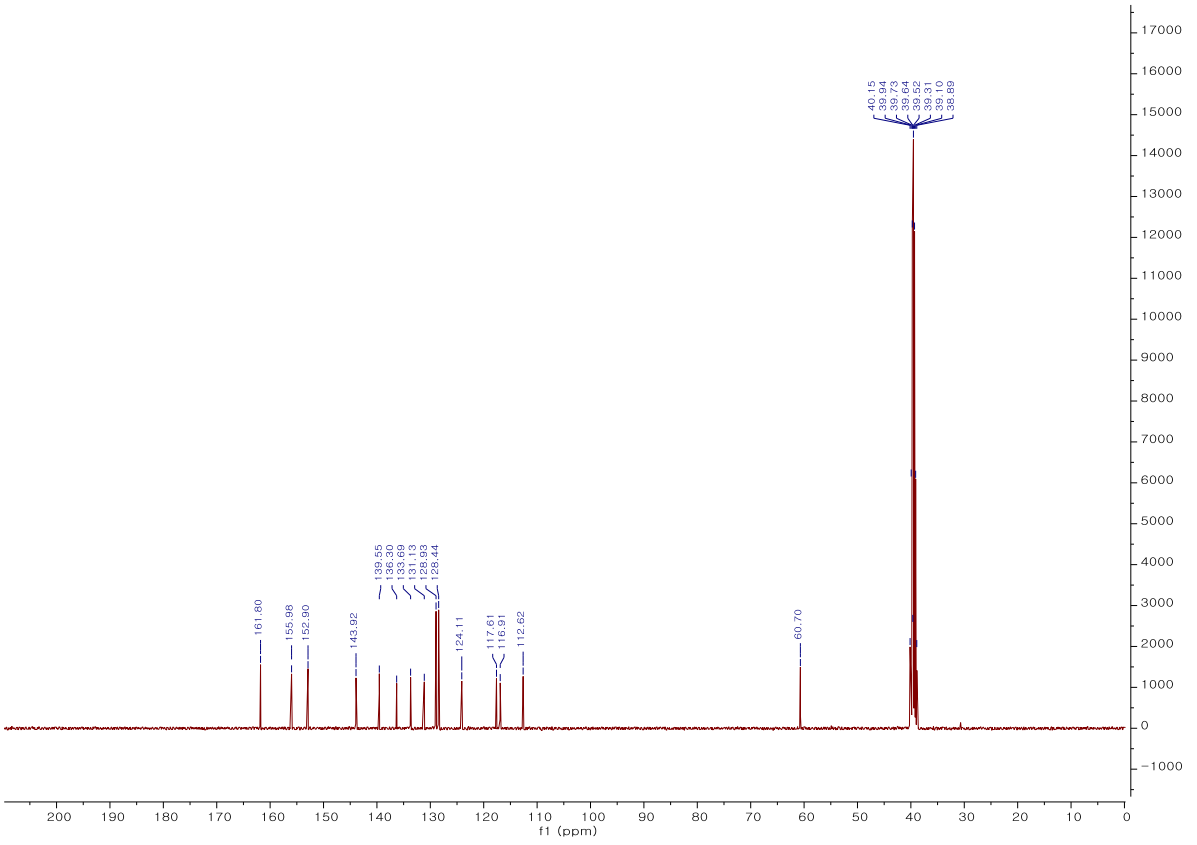
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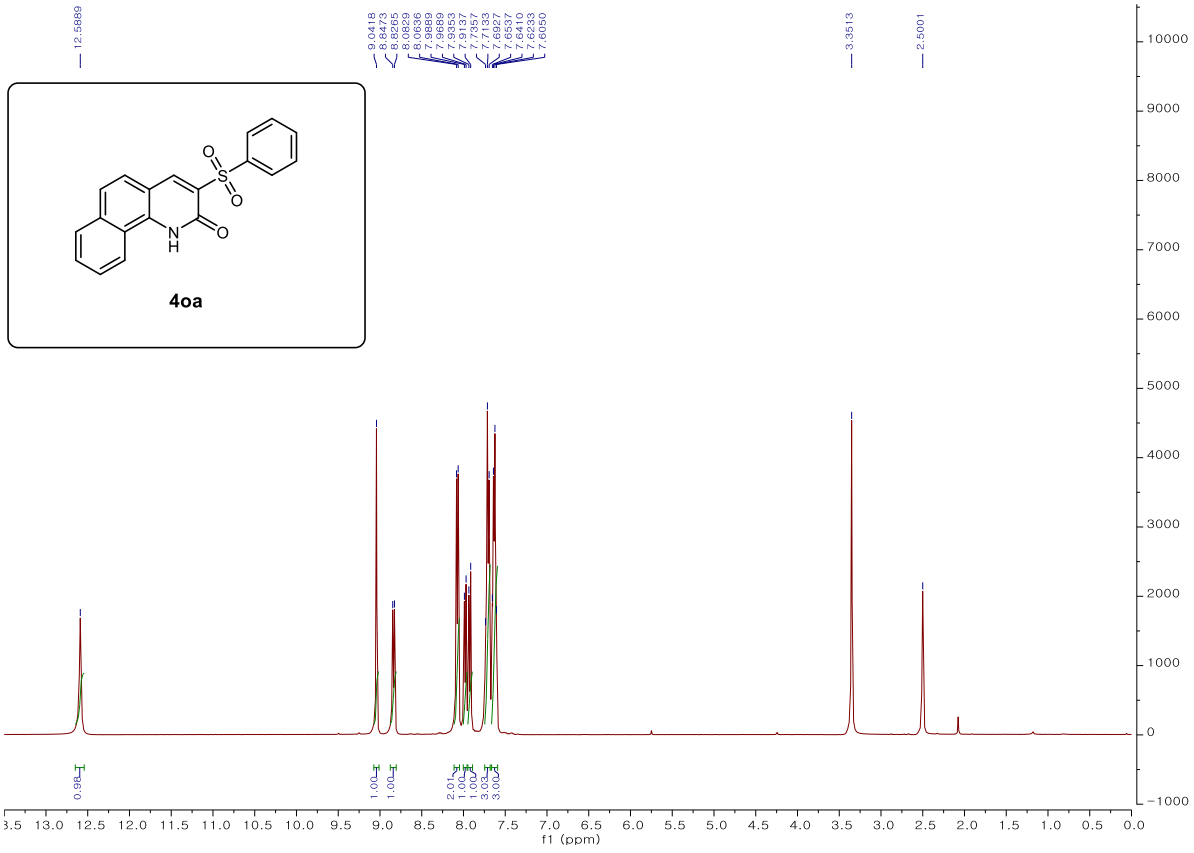
39.10
38.89
f1 (ppm)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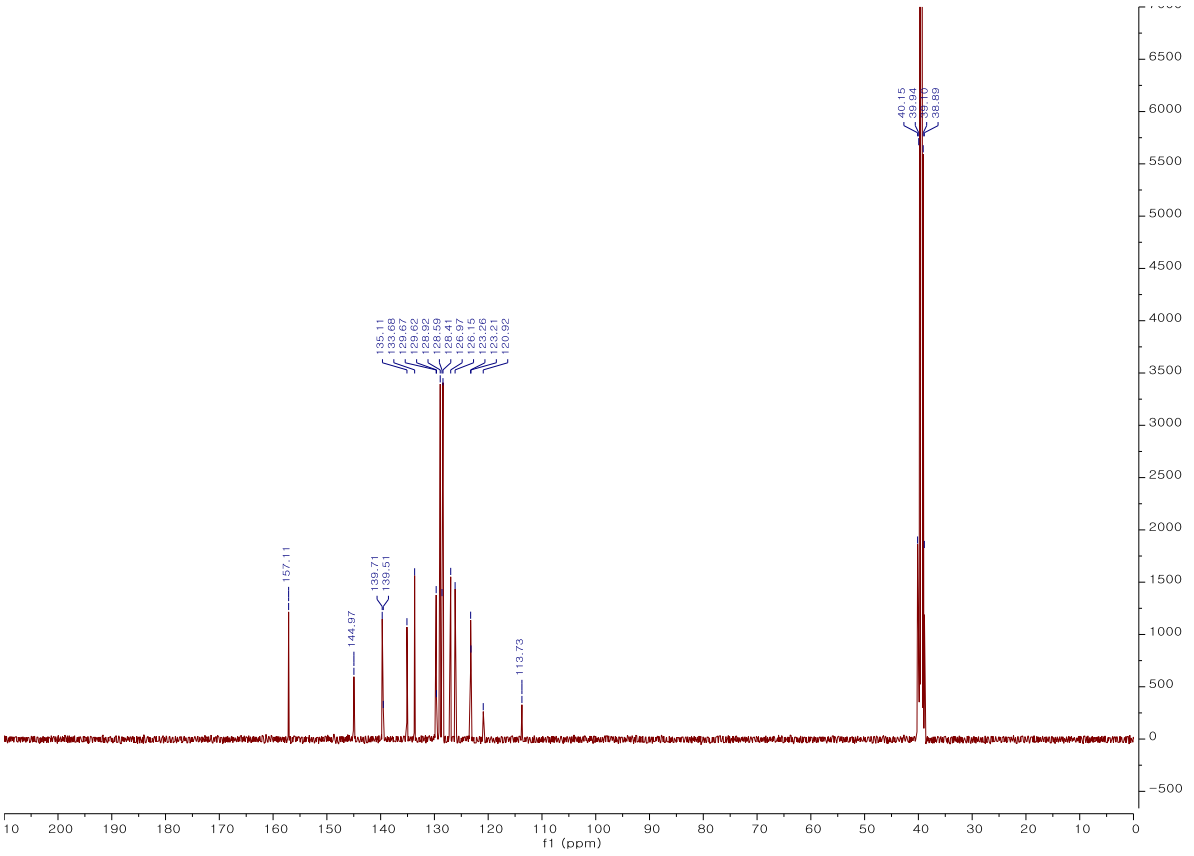
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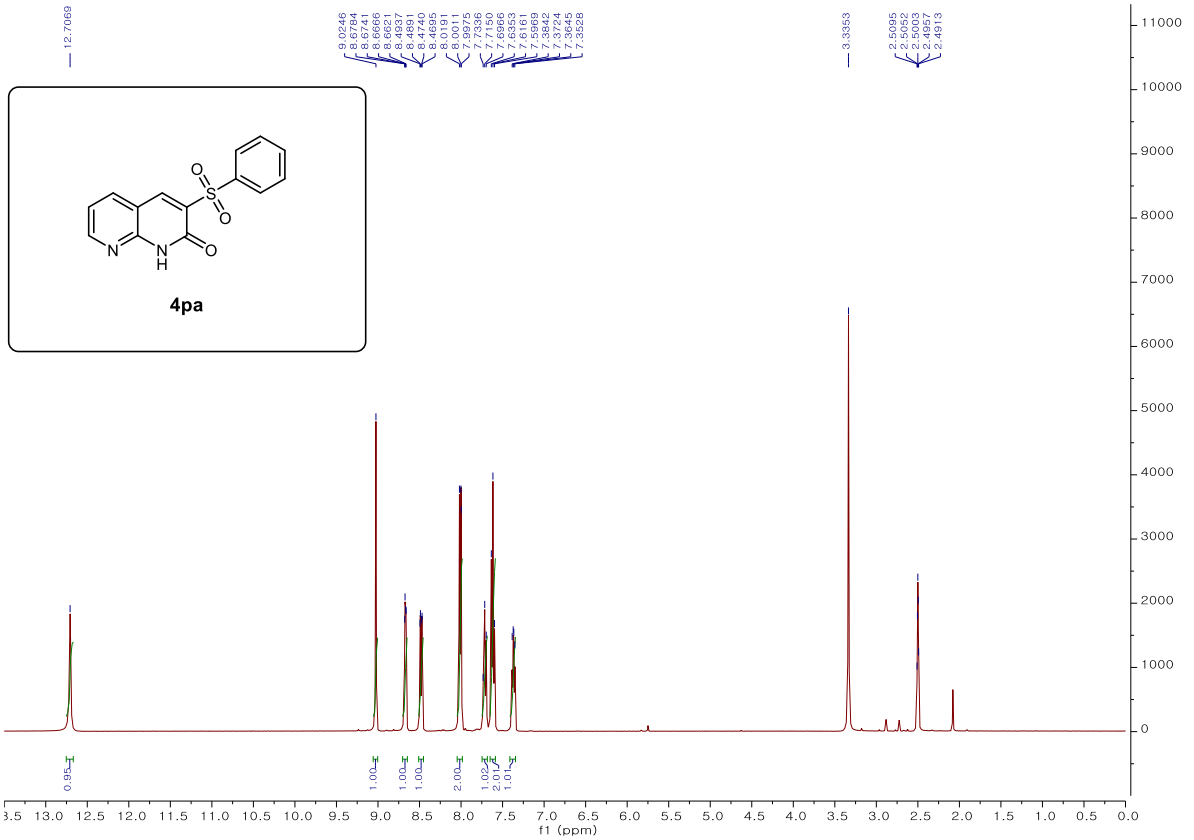
113.73
f1 (ppm)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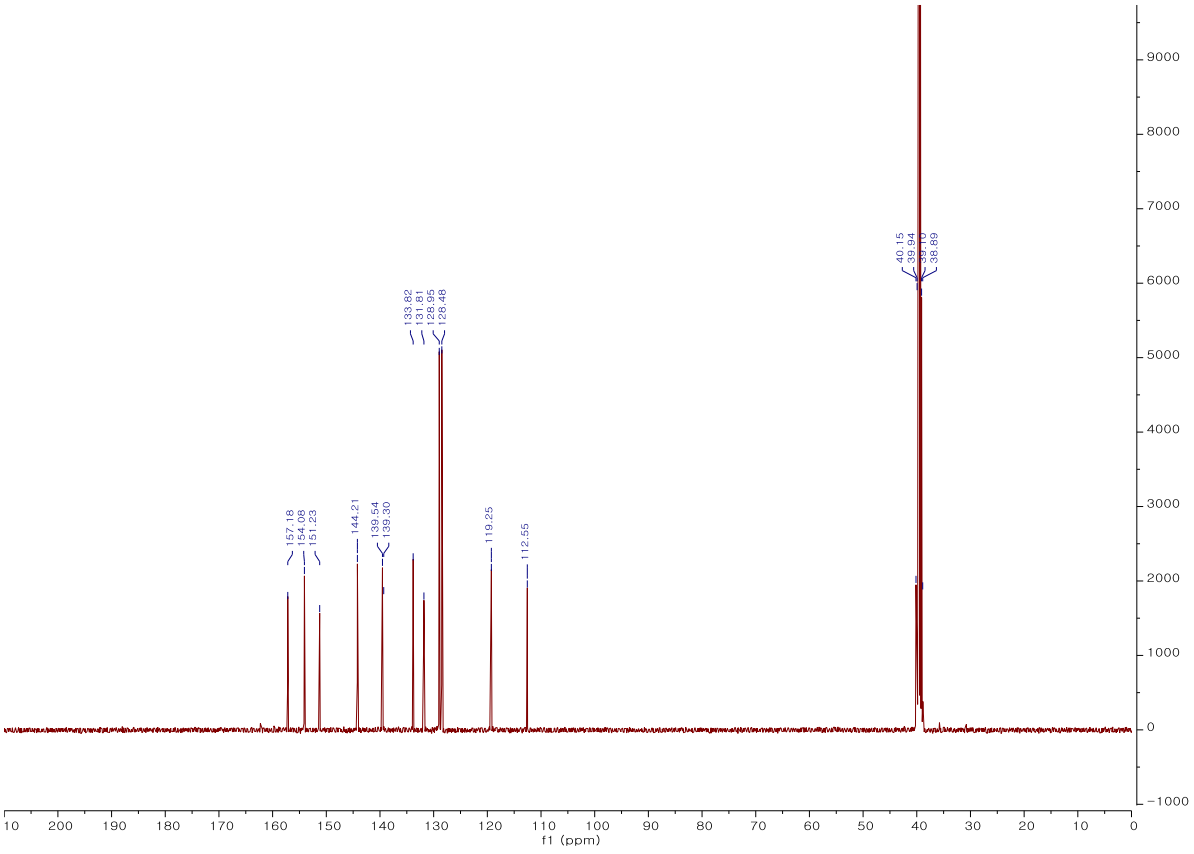
f1 (ppm)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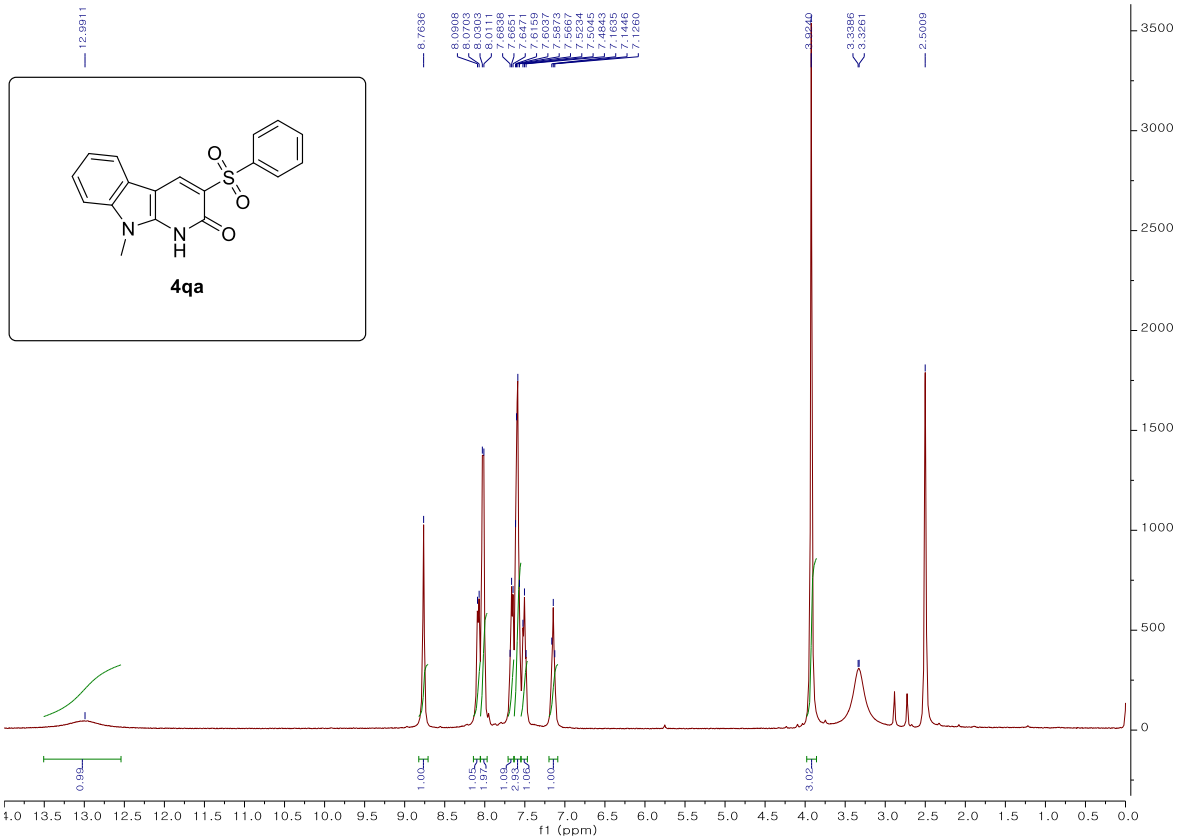
39.10
38.89
f1 (ppm)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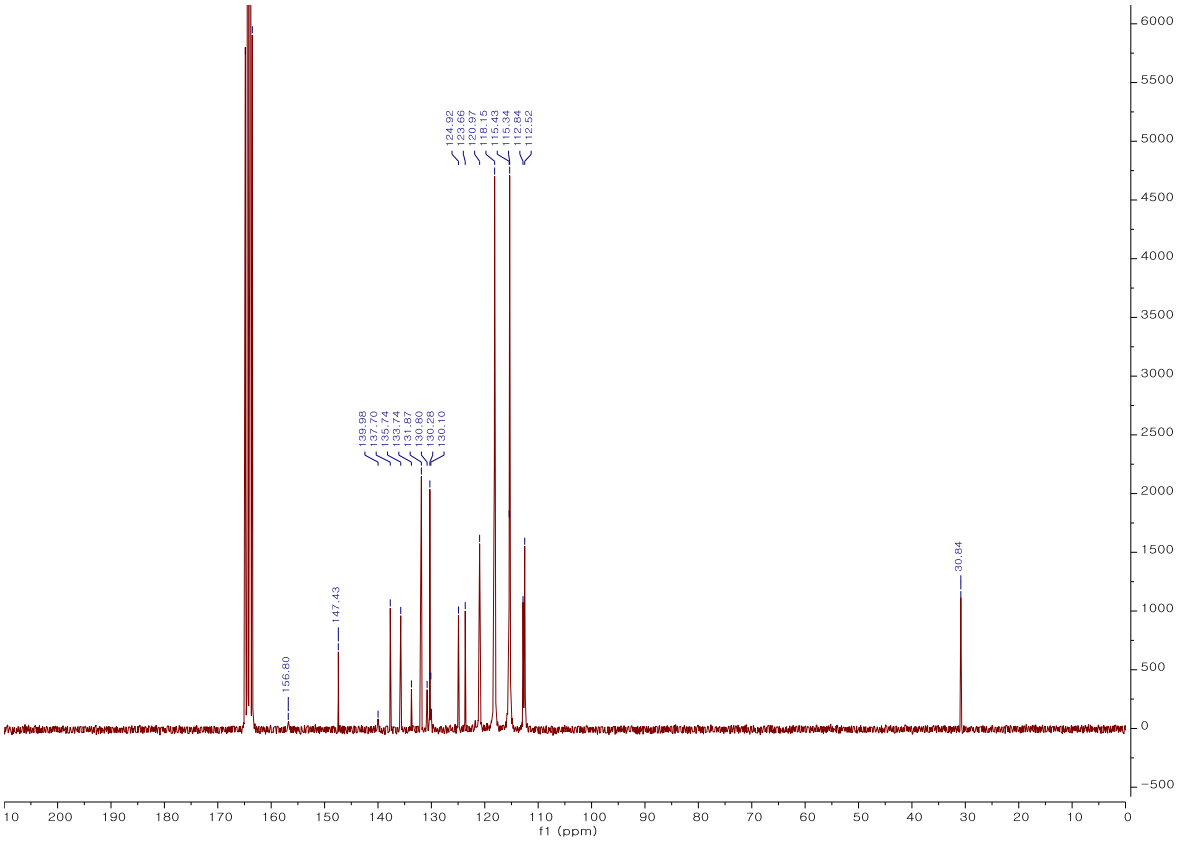
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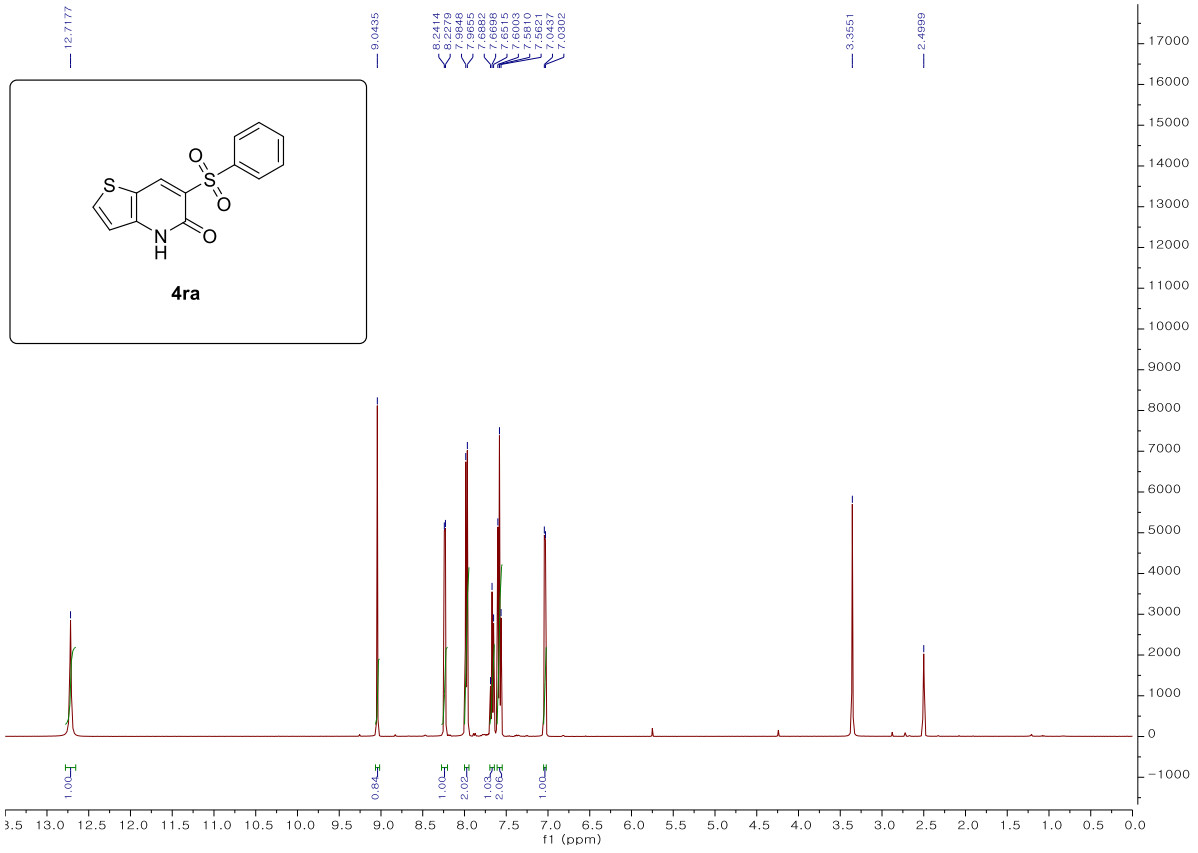
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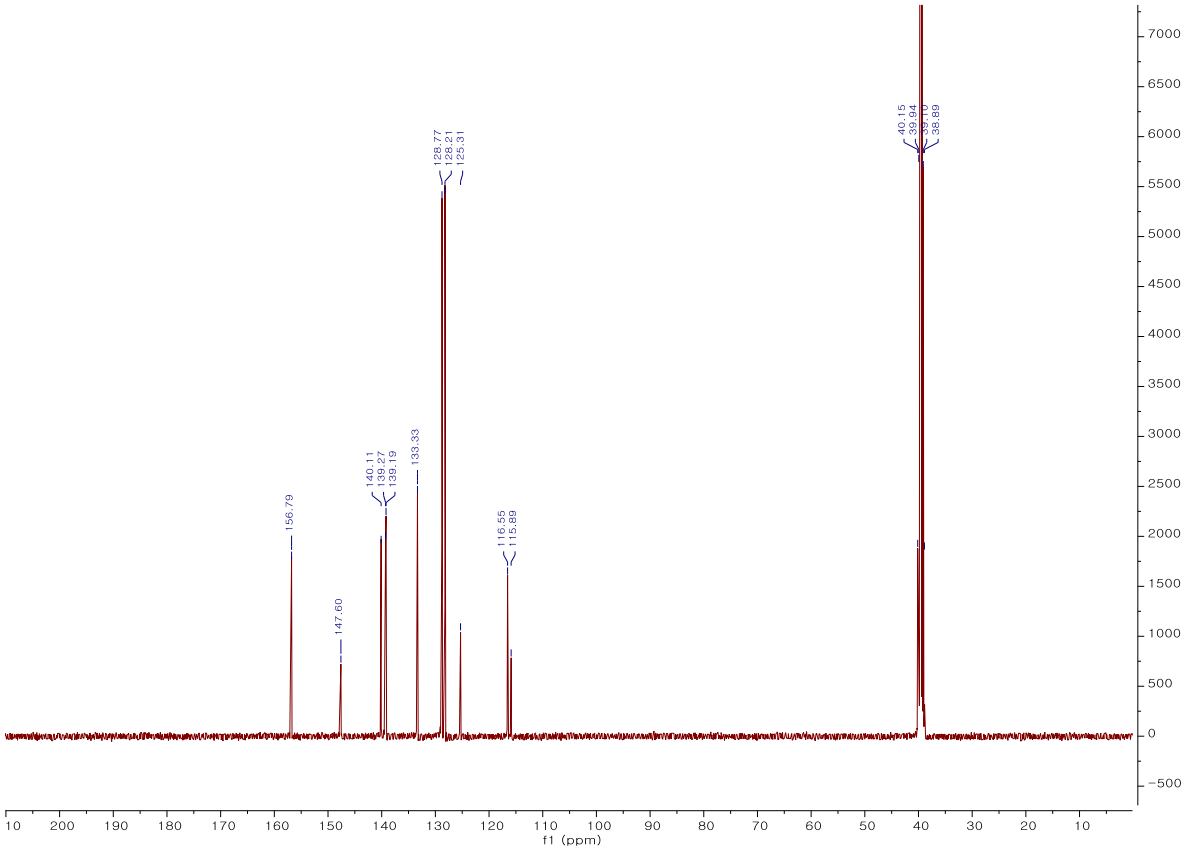
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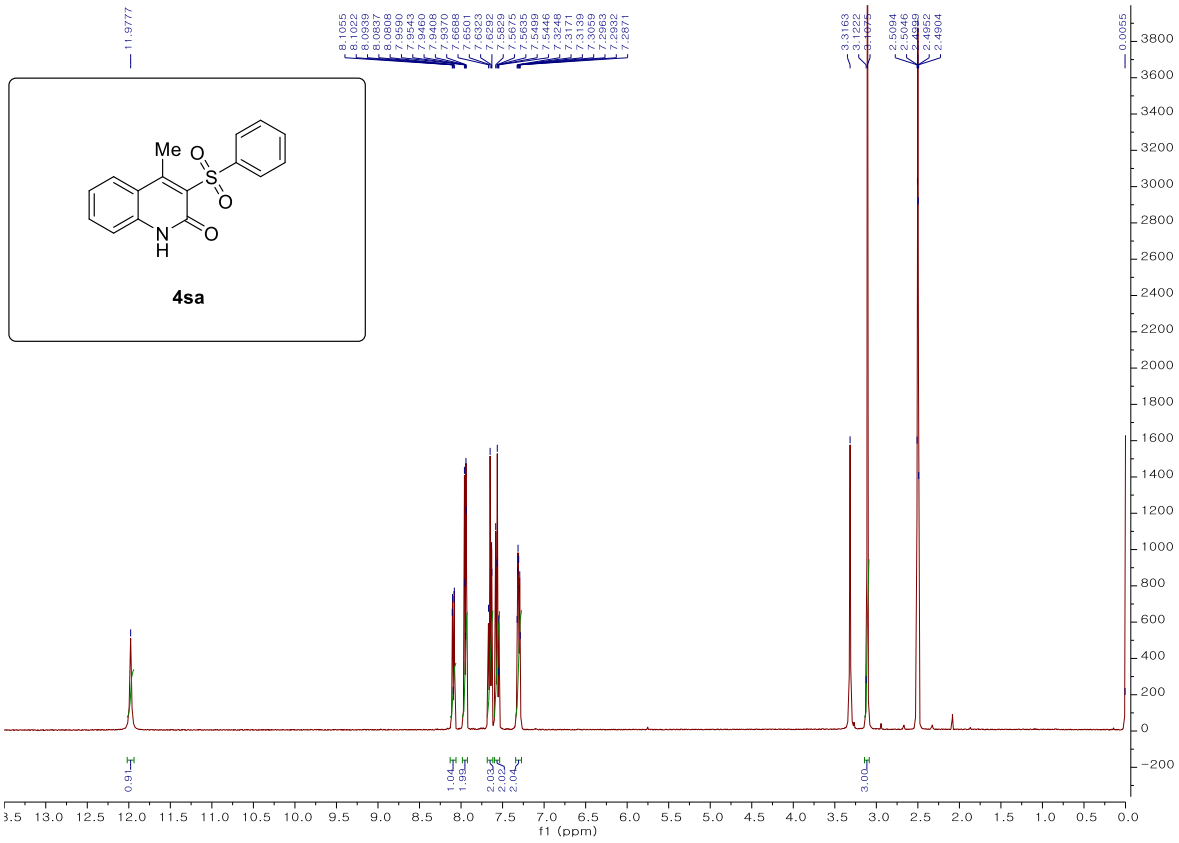
38.89
f1 (ppm)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O
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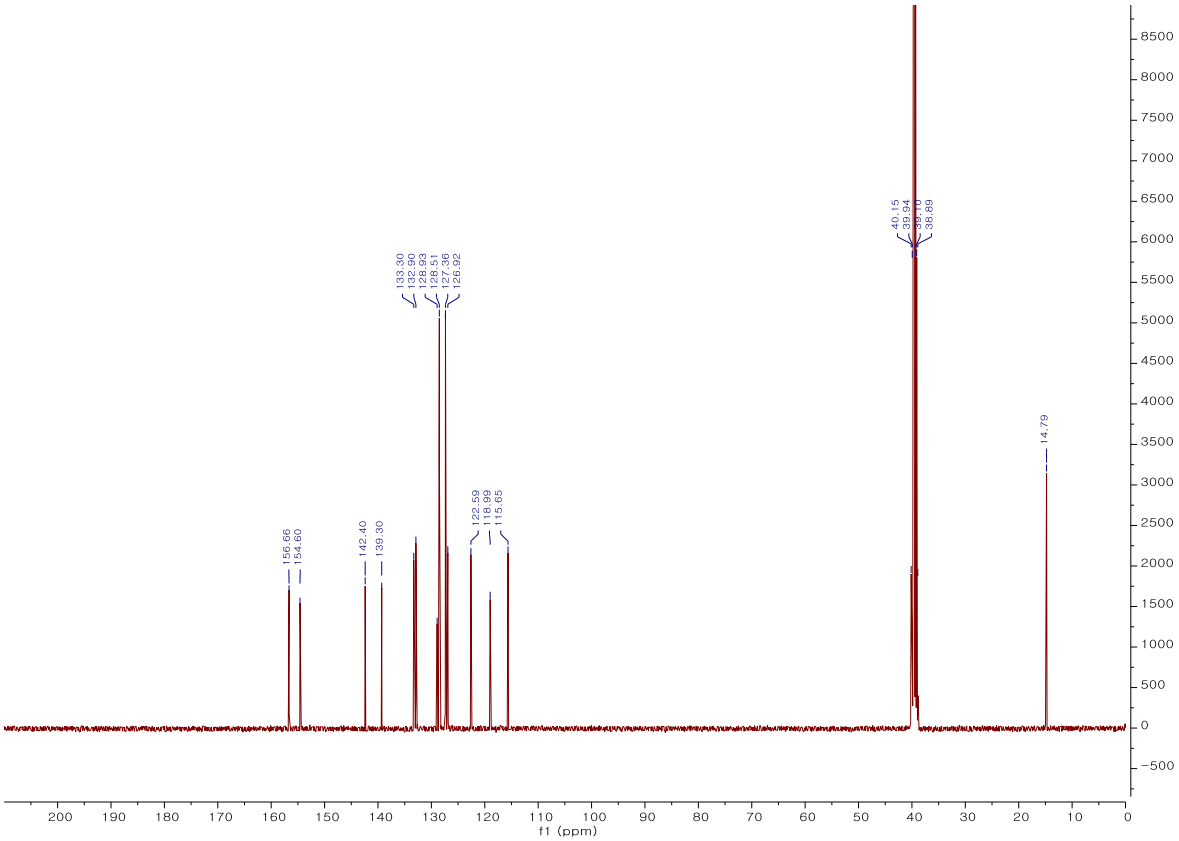
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39.94
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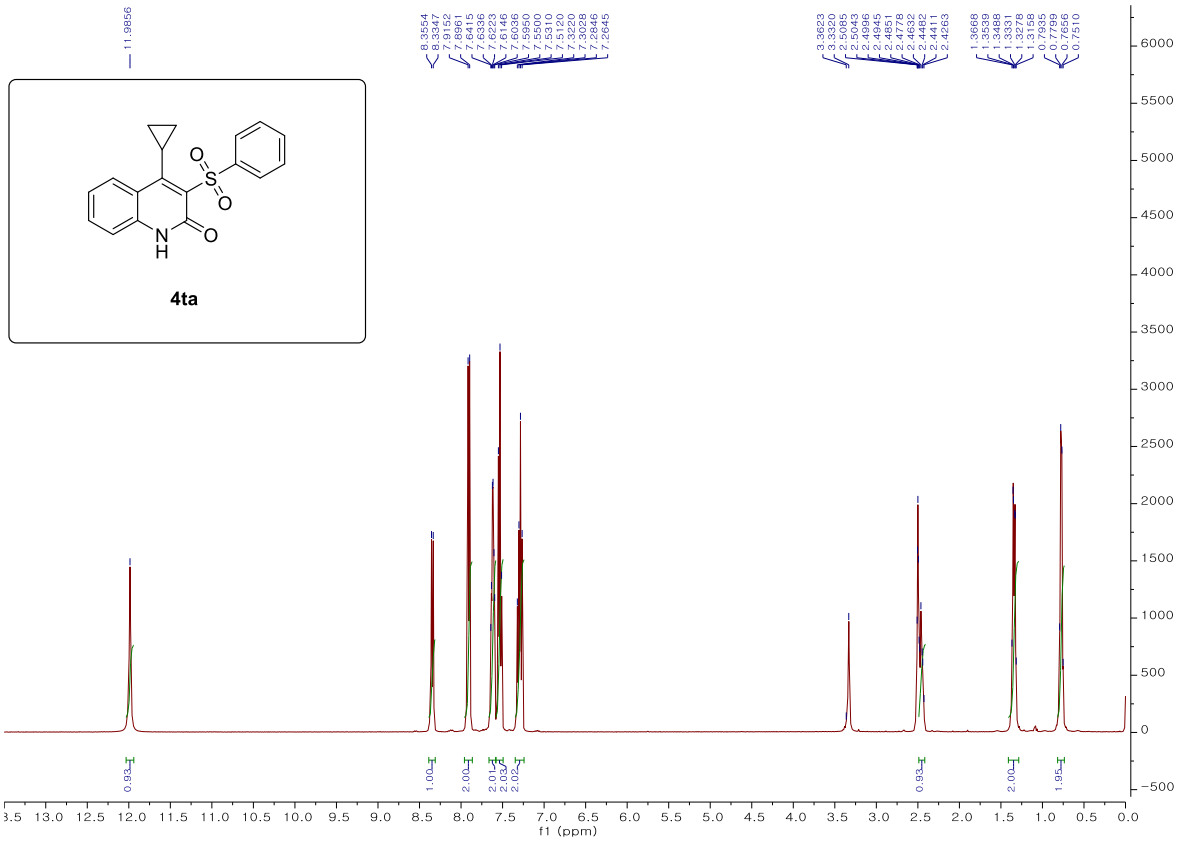
14.79
f1 (ppm)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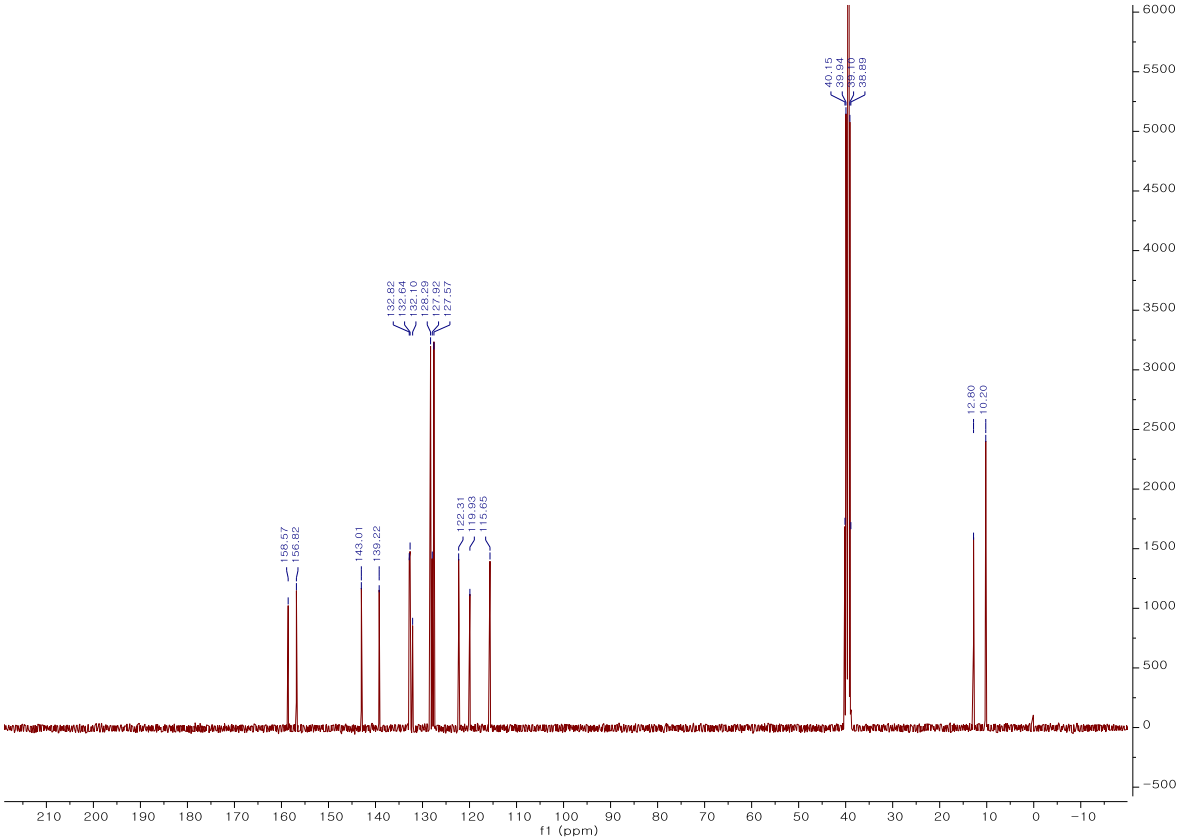
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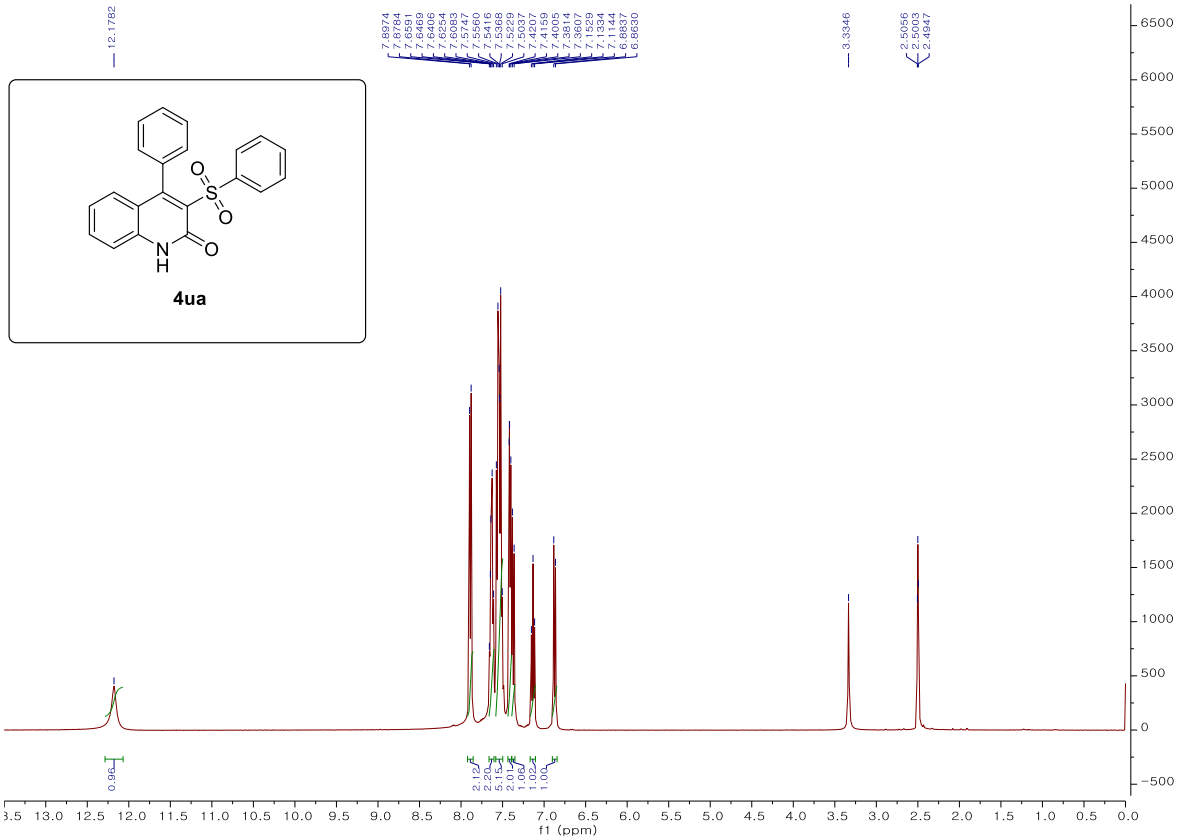
4ta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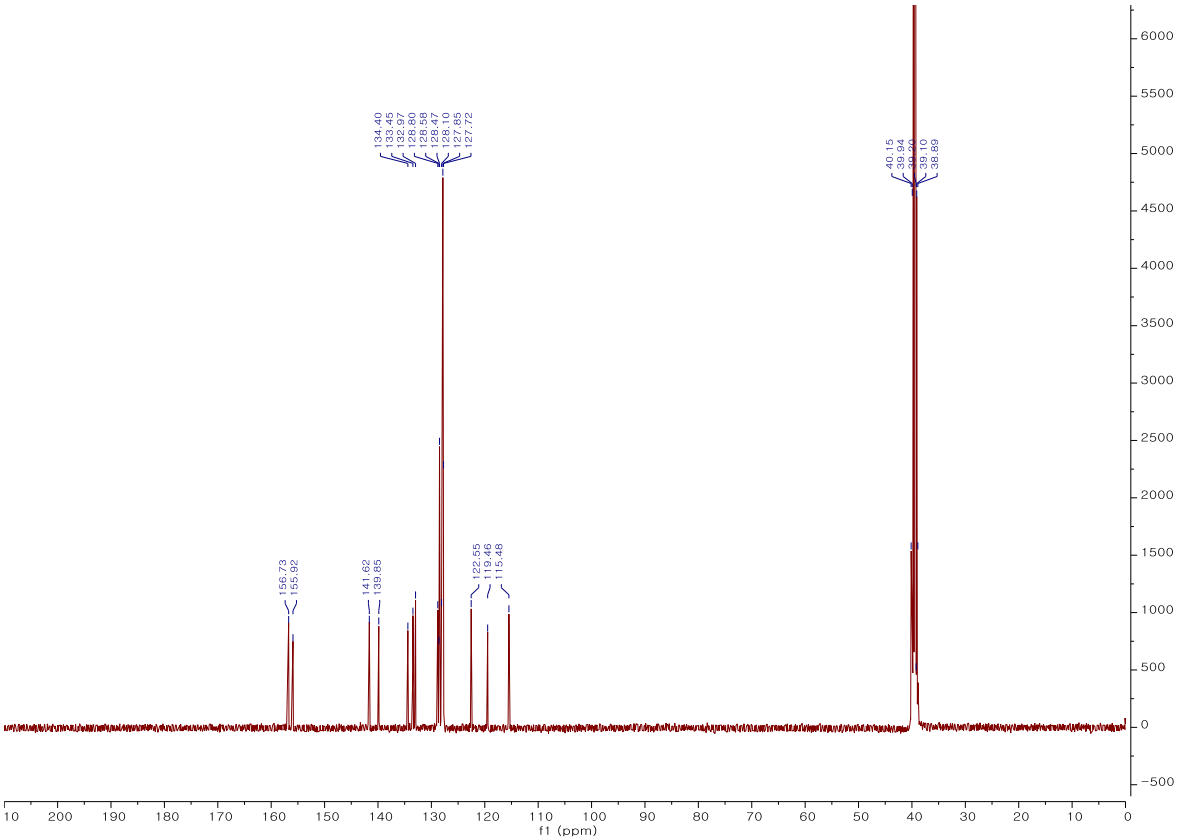
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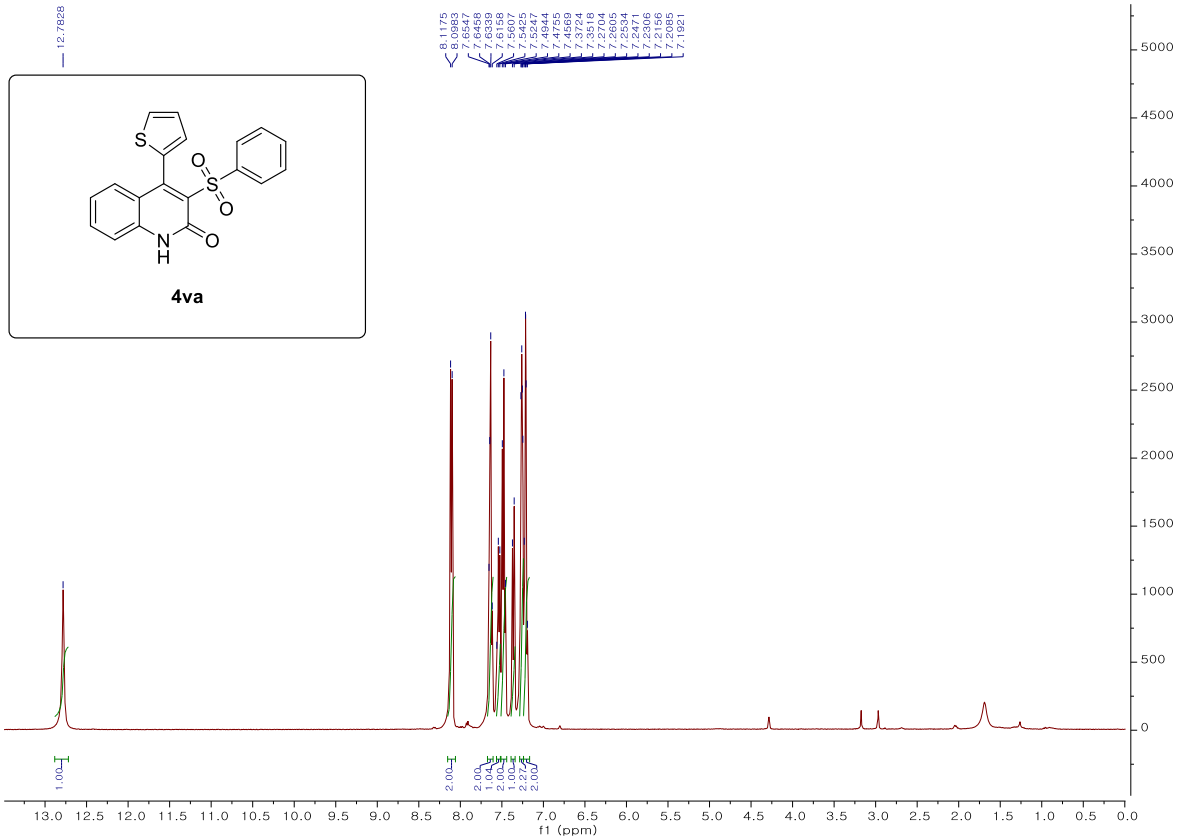
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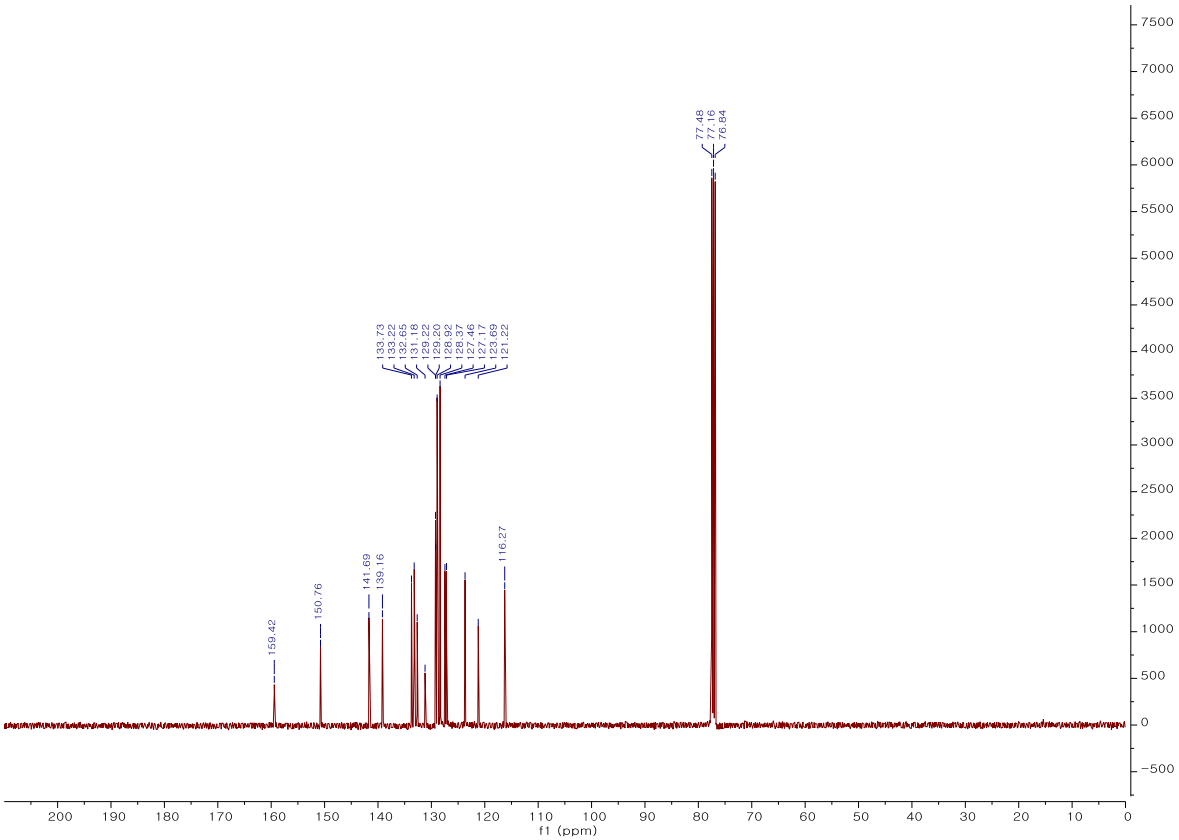
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116.27
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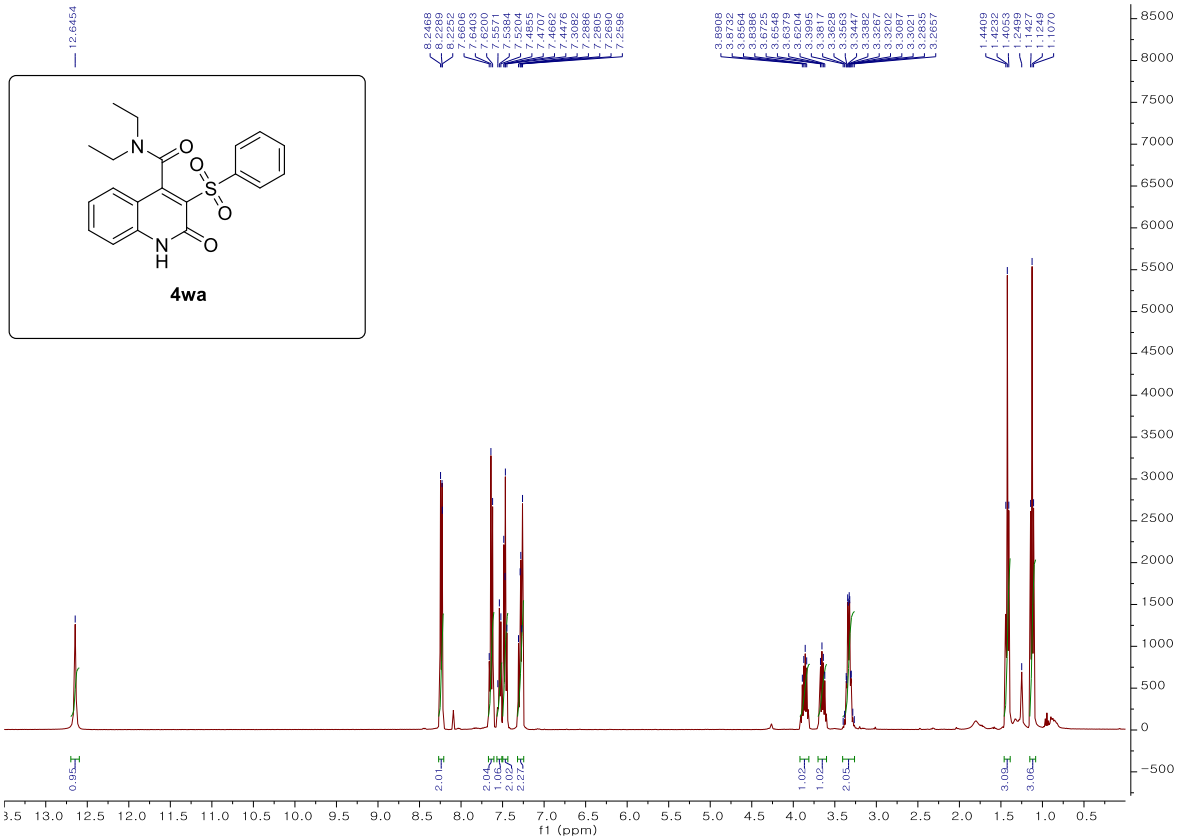
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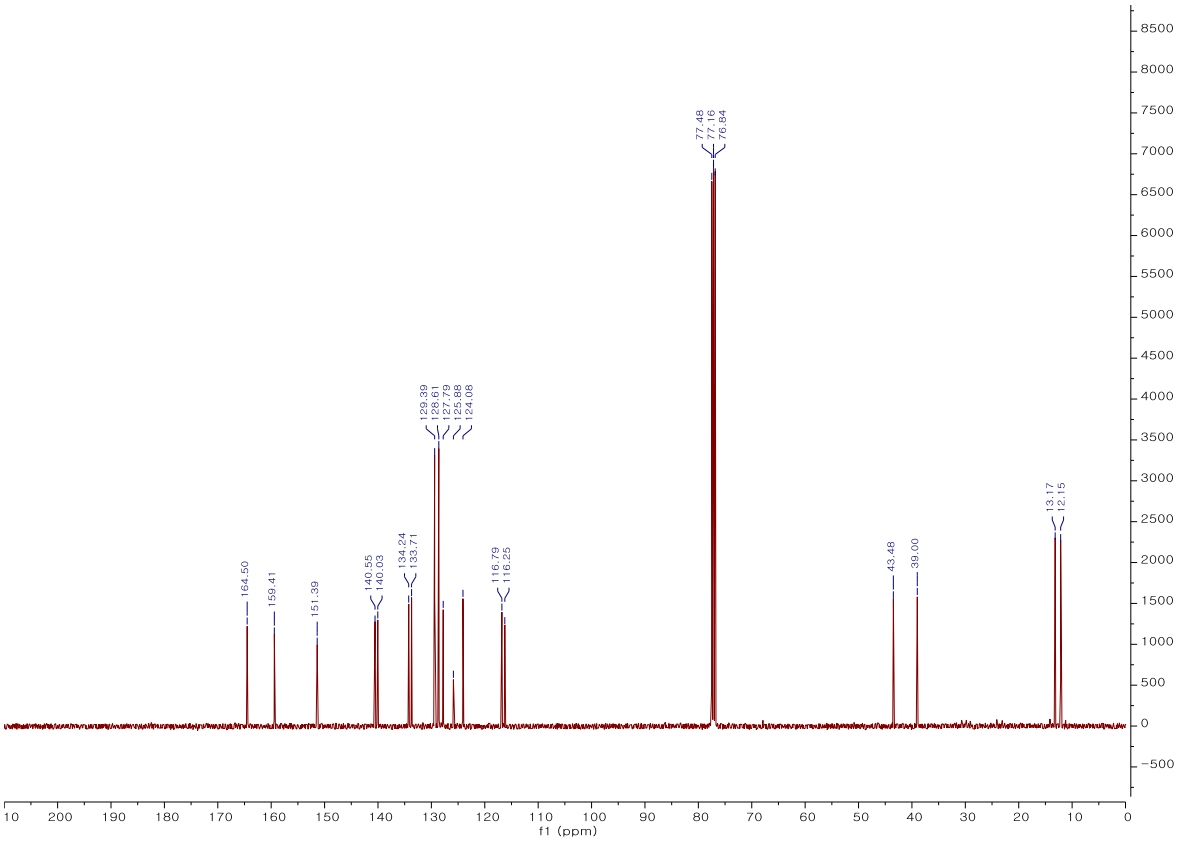
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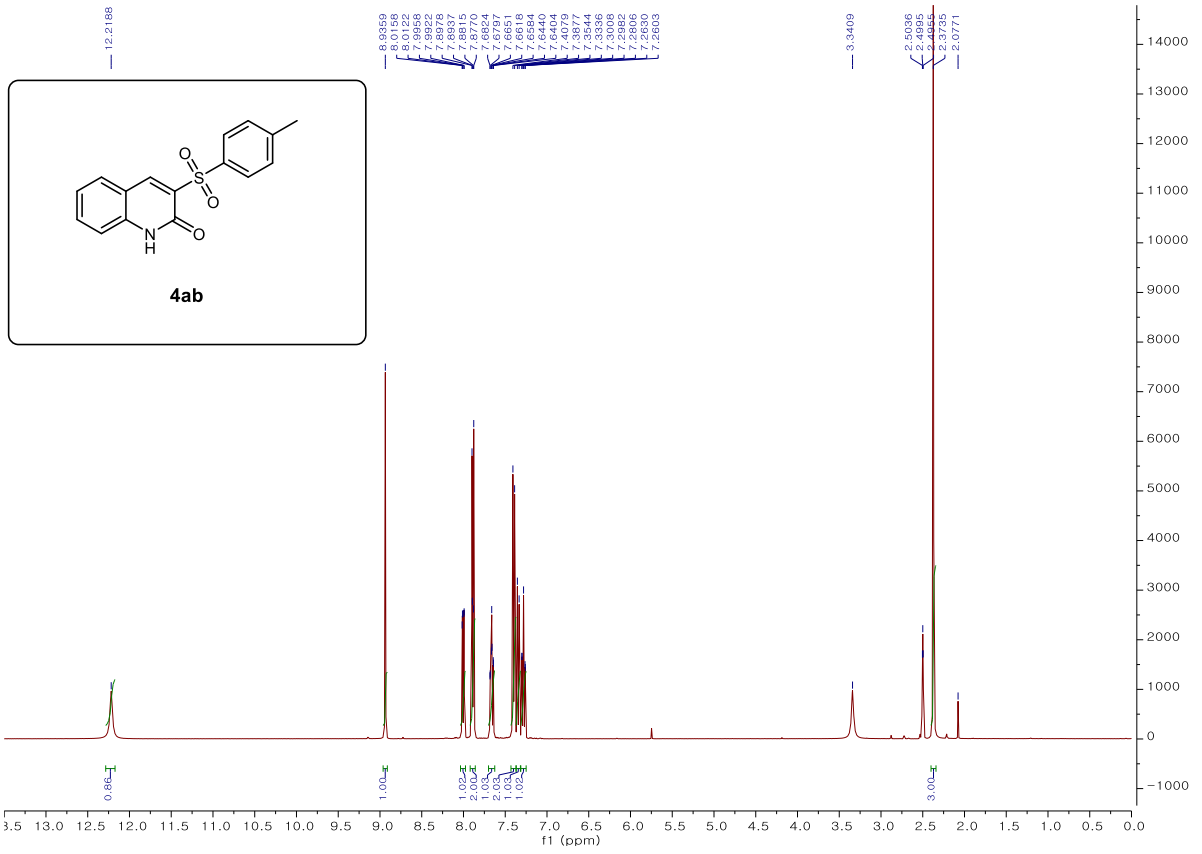
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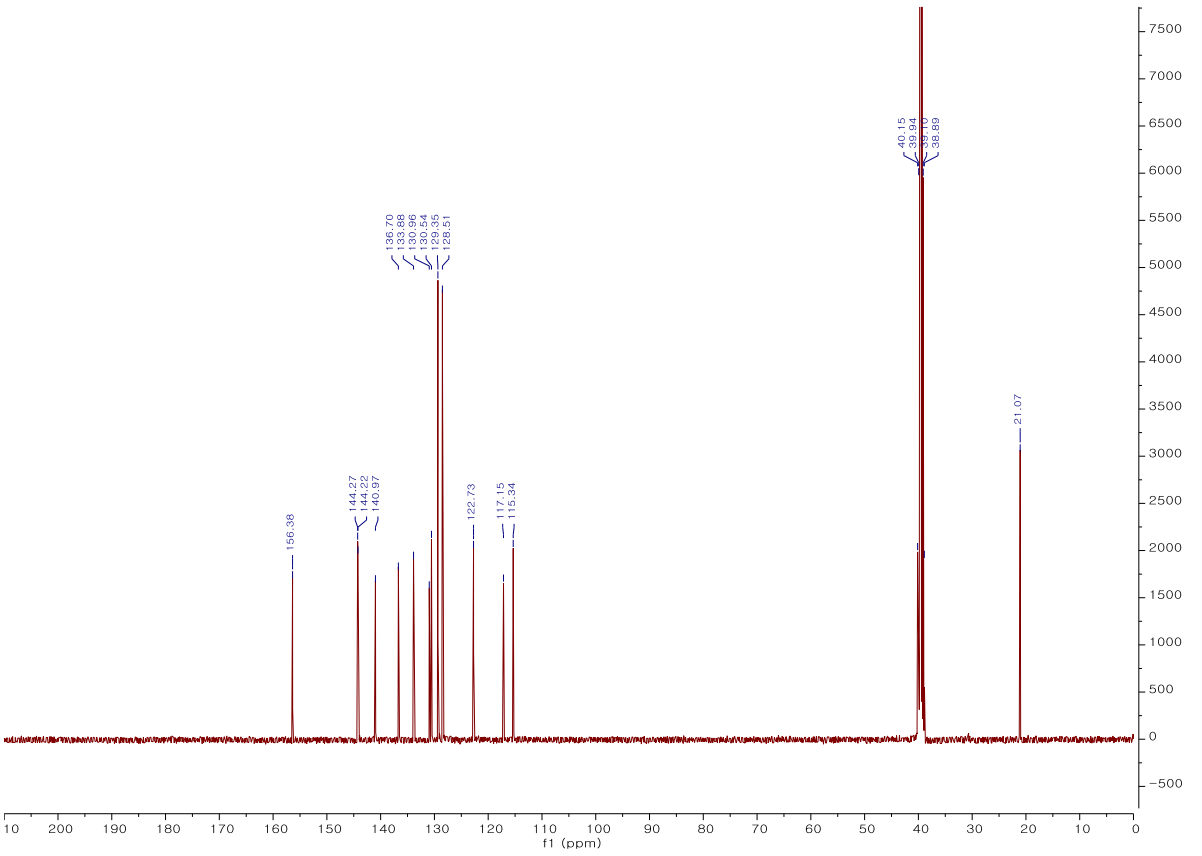
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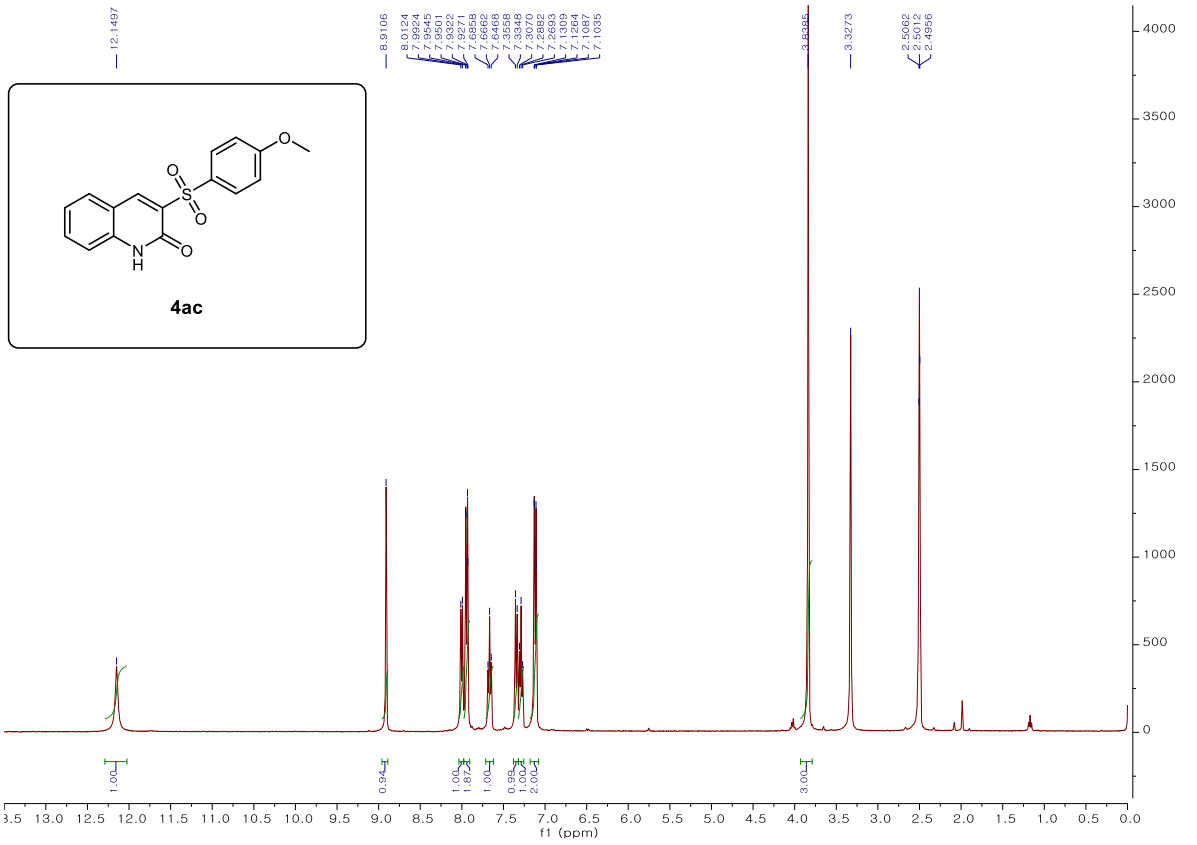
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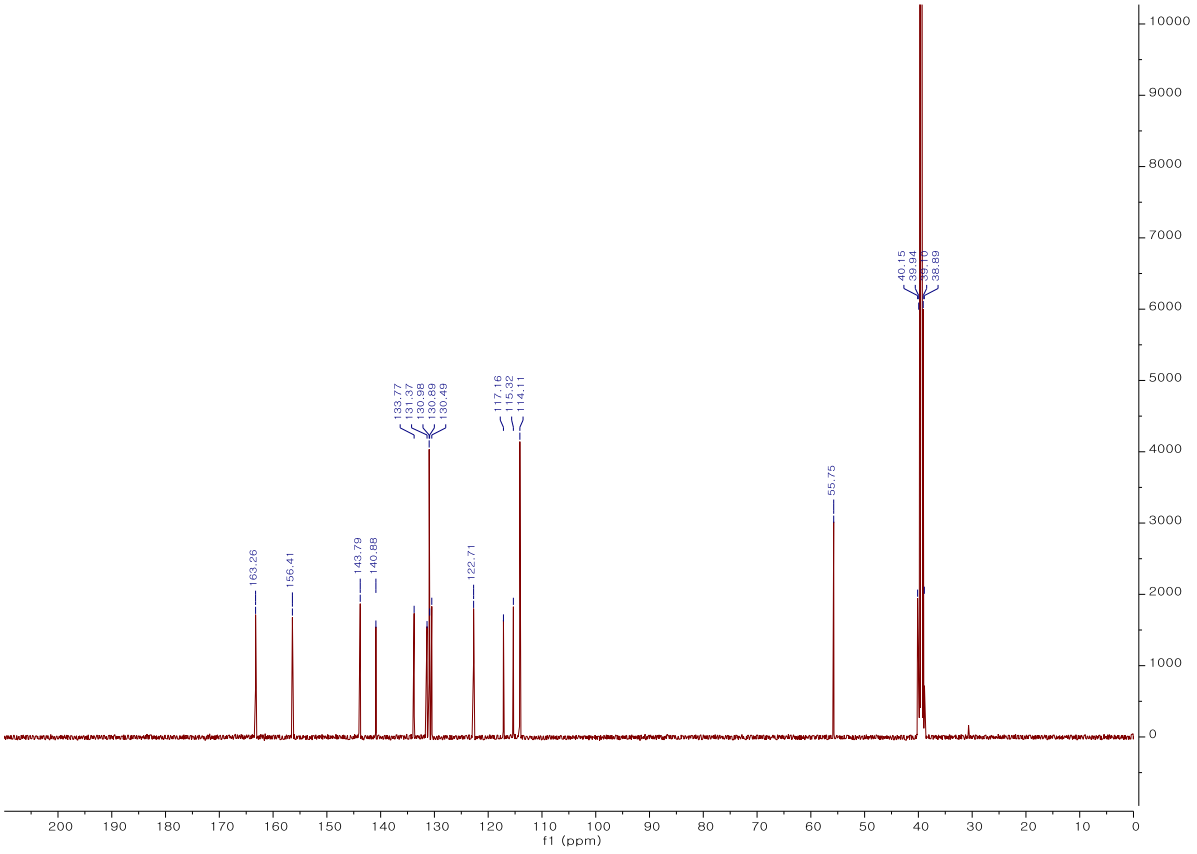
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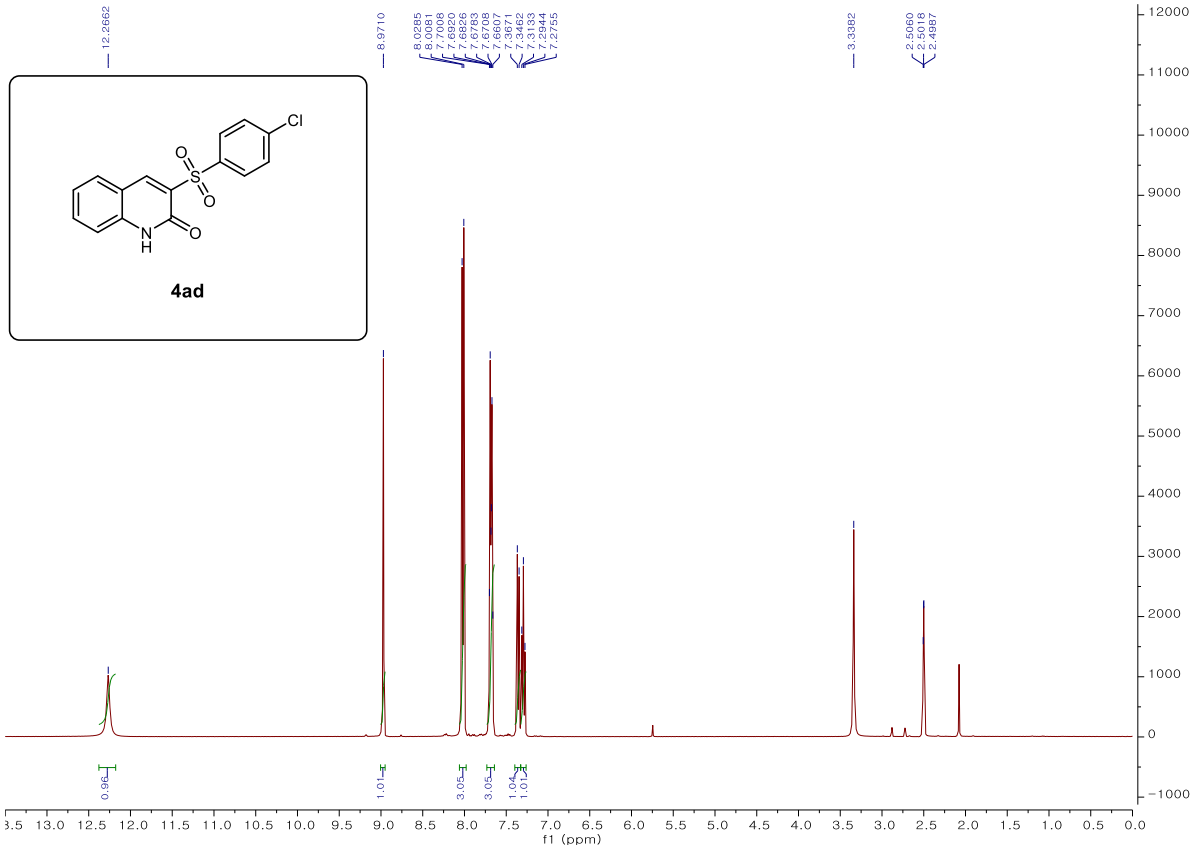
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2.4987
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1.01
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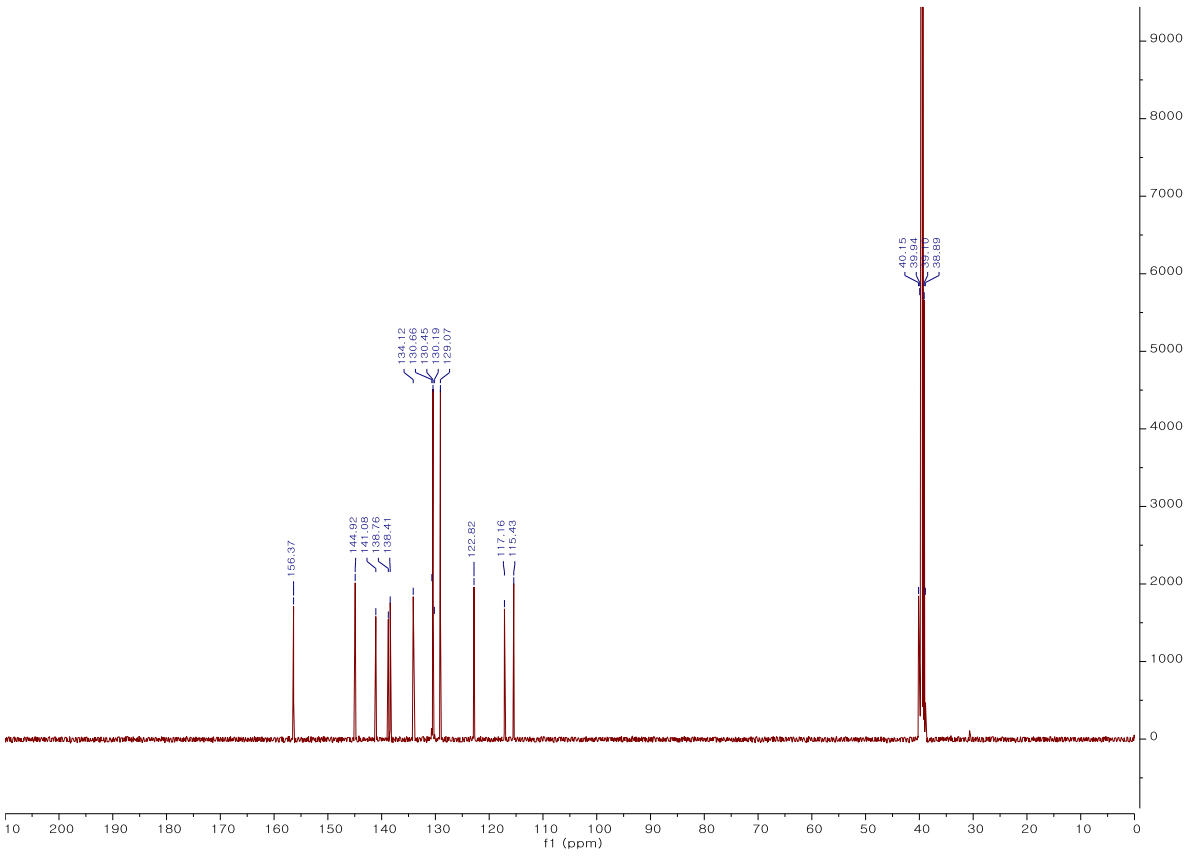
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115.43
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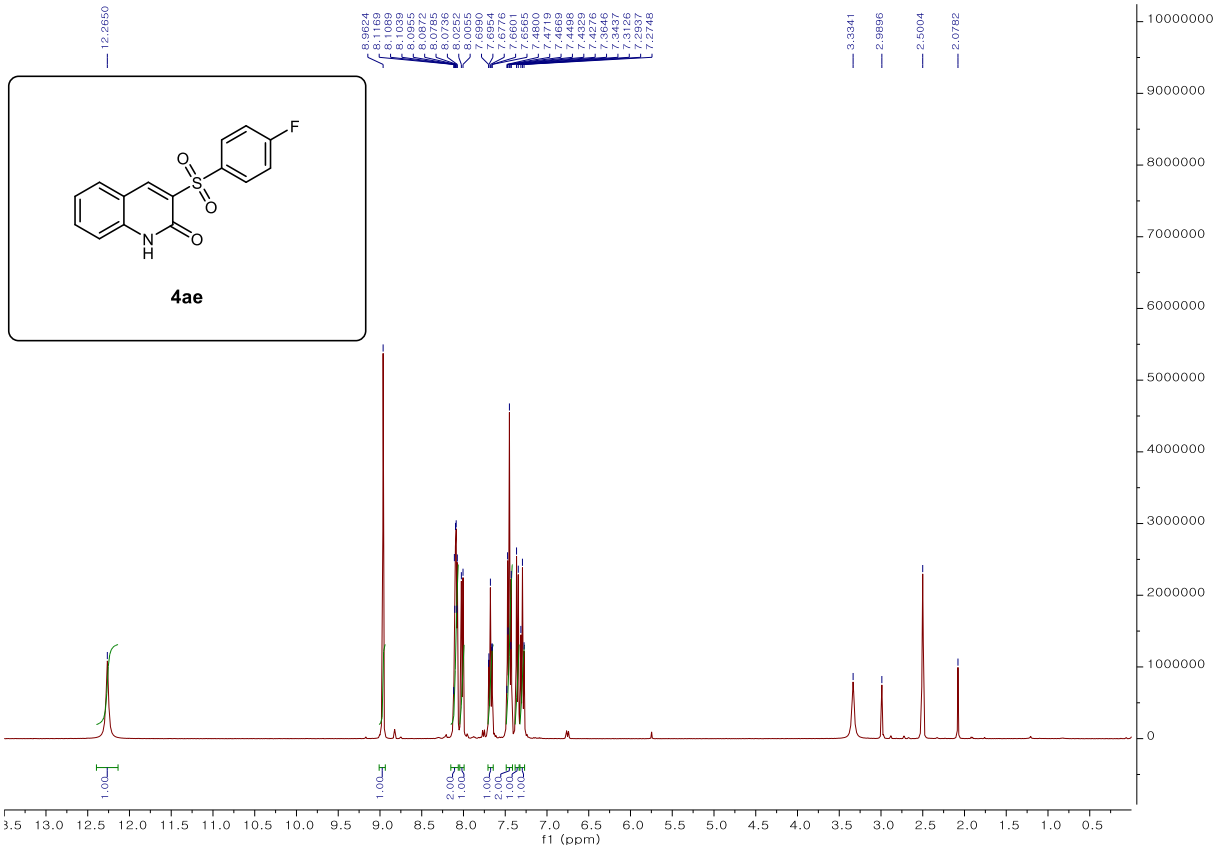
39.94
39.10
38.89
f1 (ppm)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7.2748
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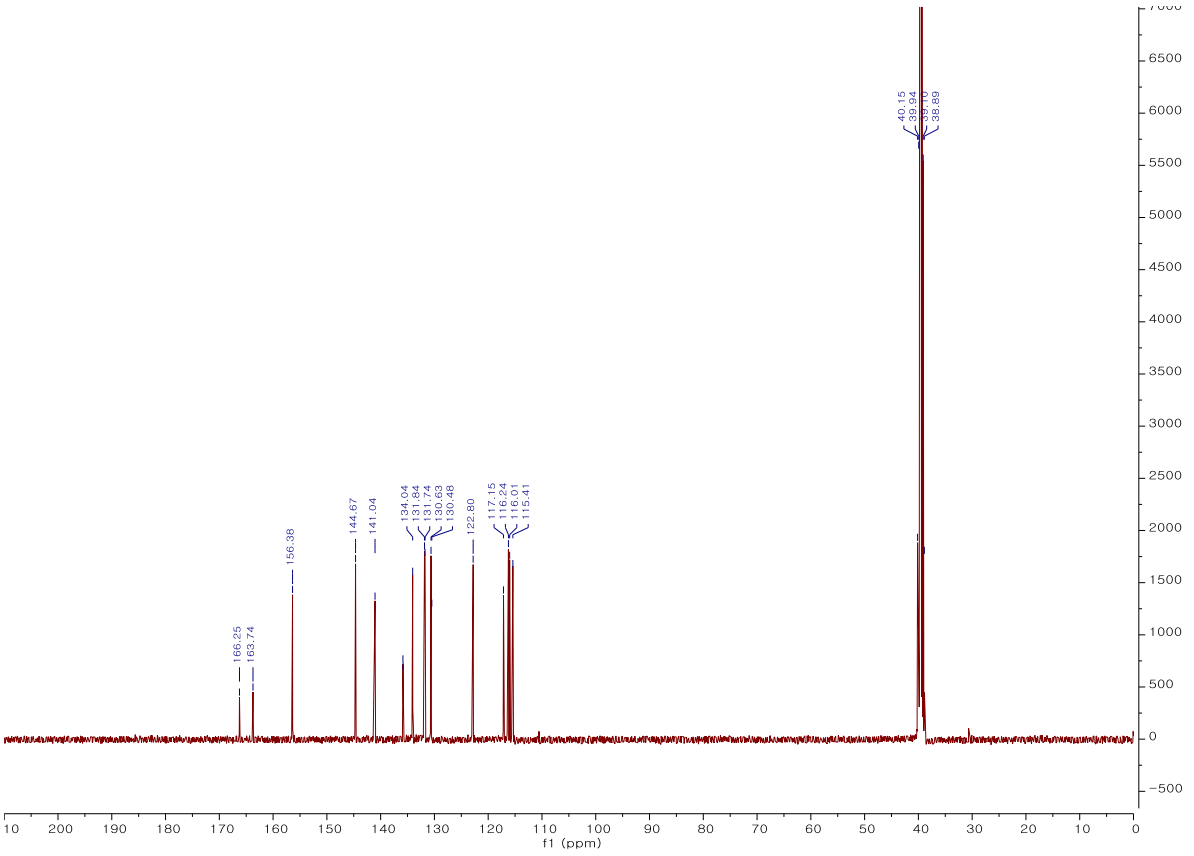
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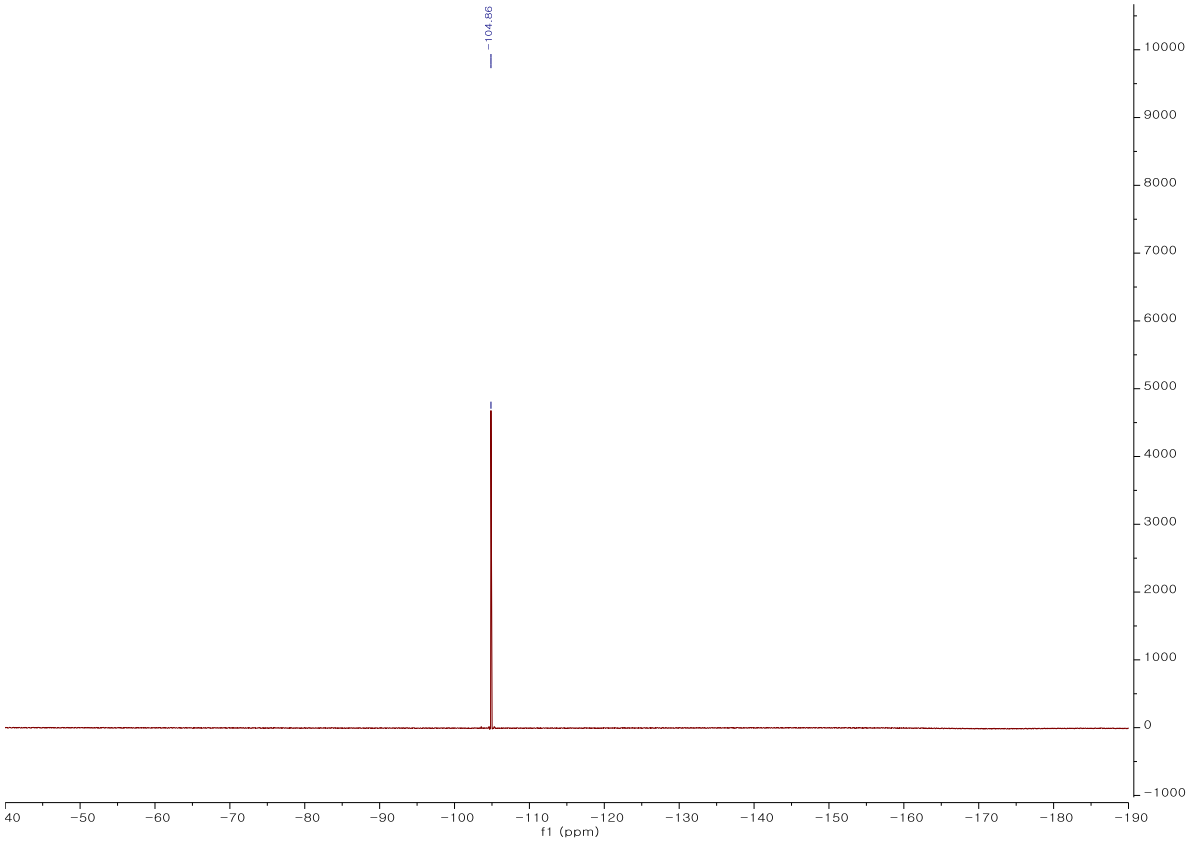
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-160
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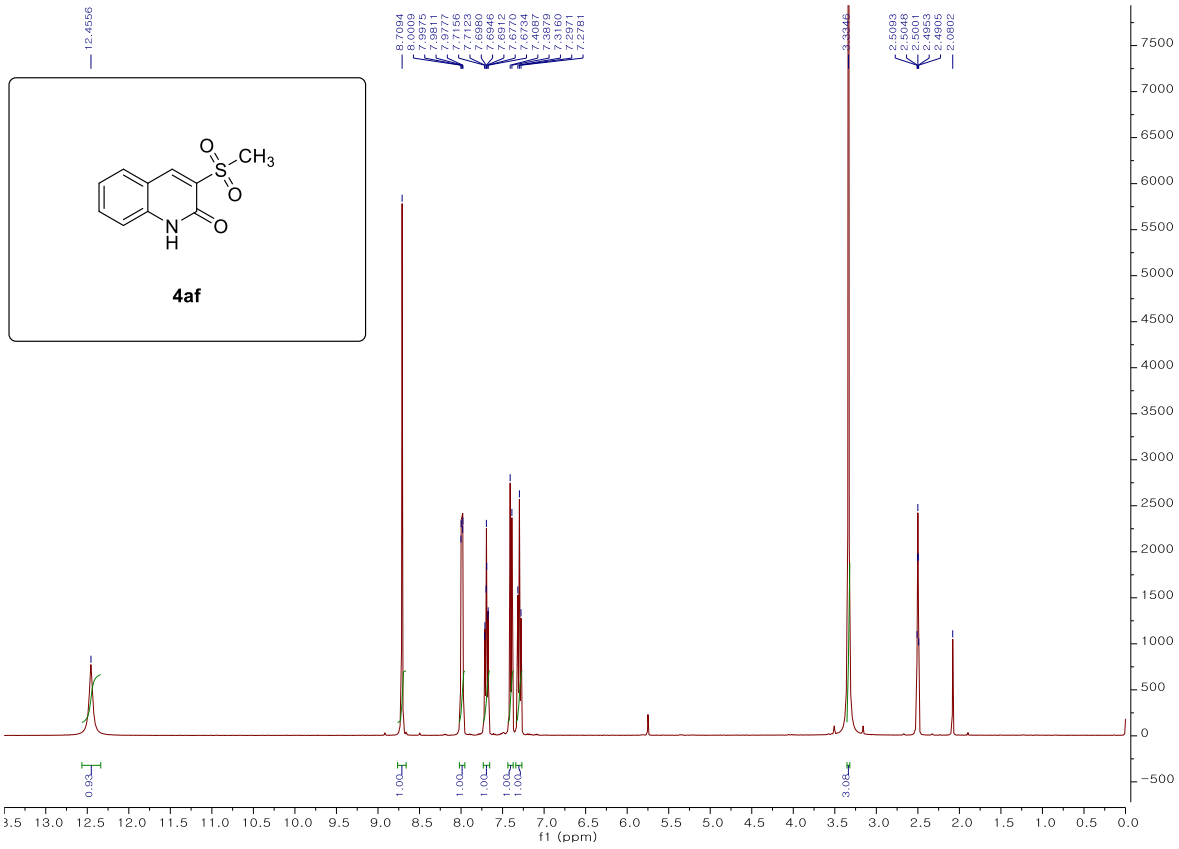
f1 (ppm)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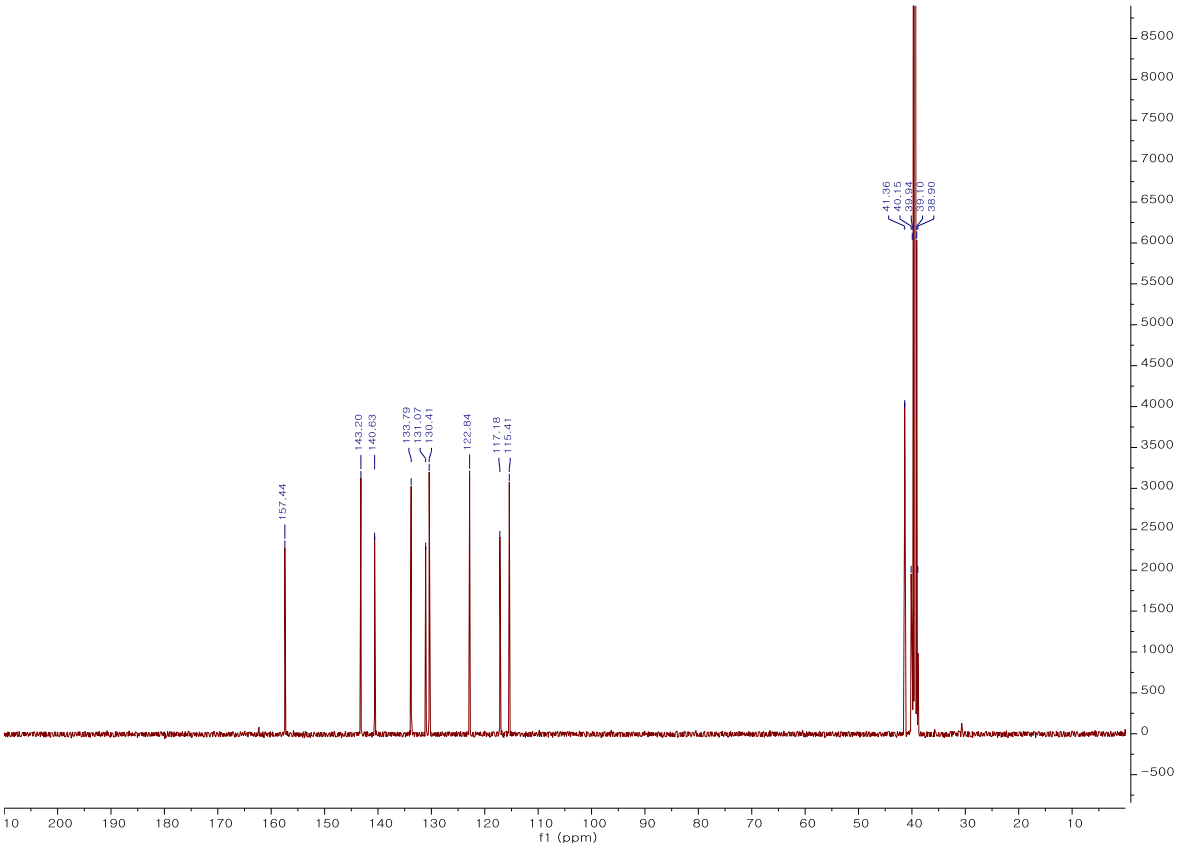
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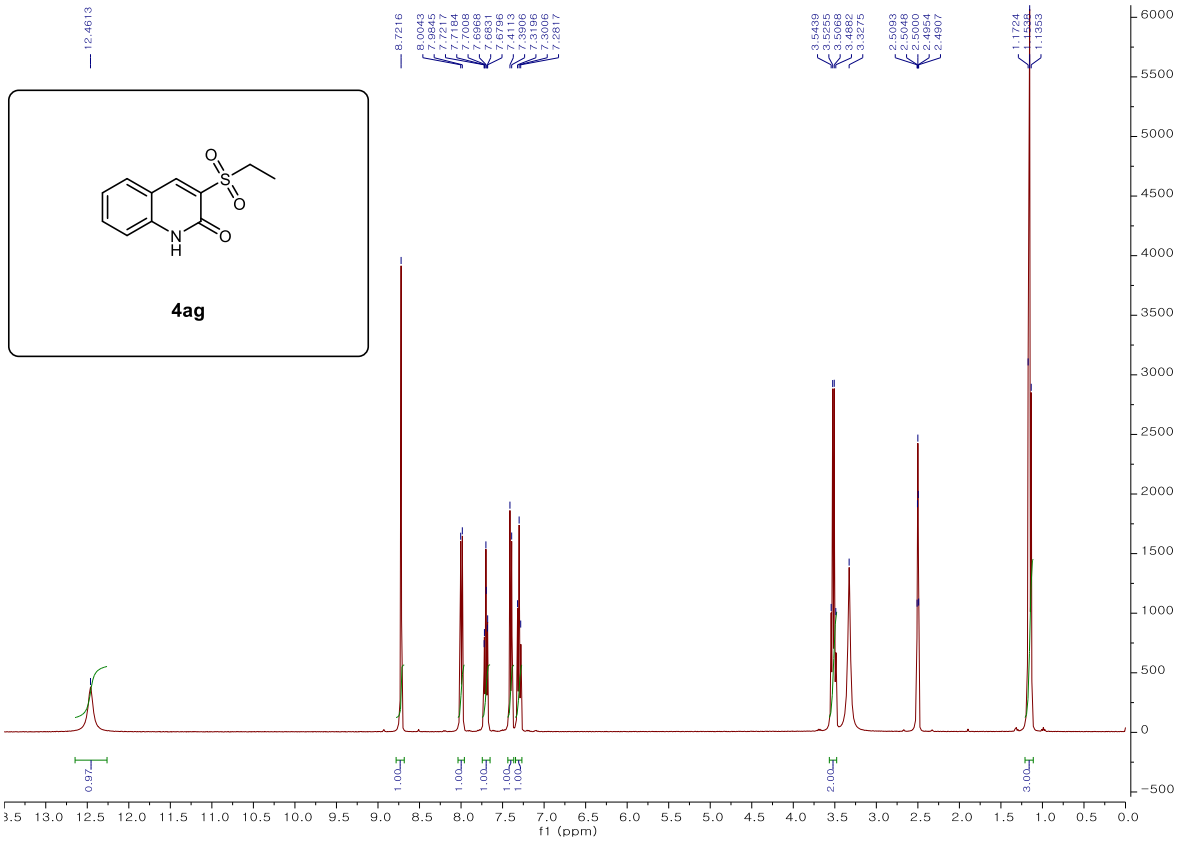
38.90
f1 (ppm)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7.3006
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3.5255
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3.3275
2.5093
2.5048
2.5000
2.4954
2.4907
1.1724
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1.00
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3.00
f1 (ppm)
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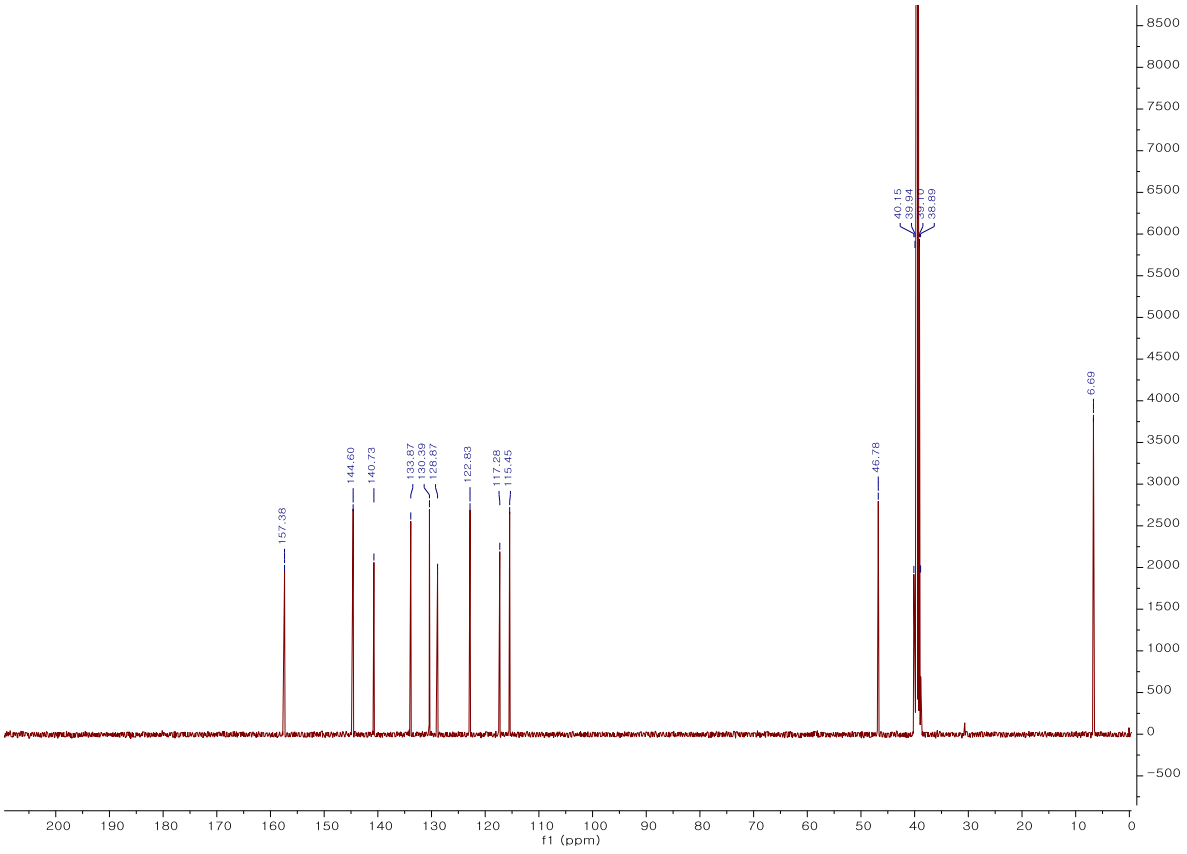
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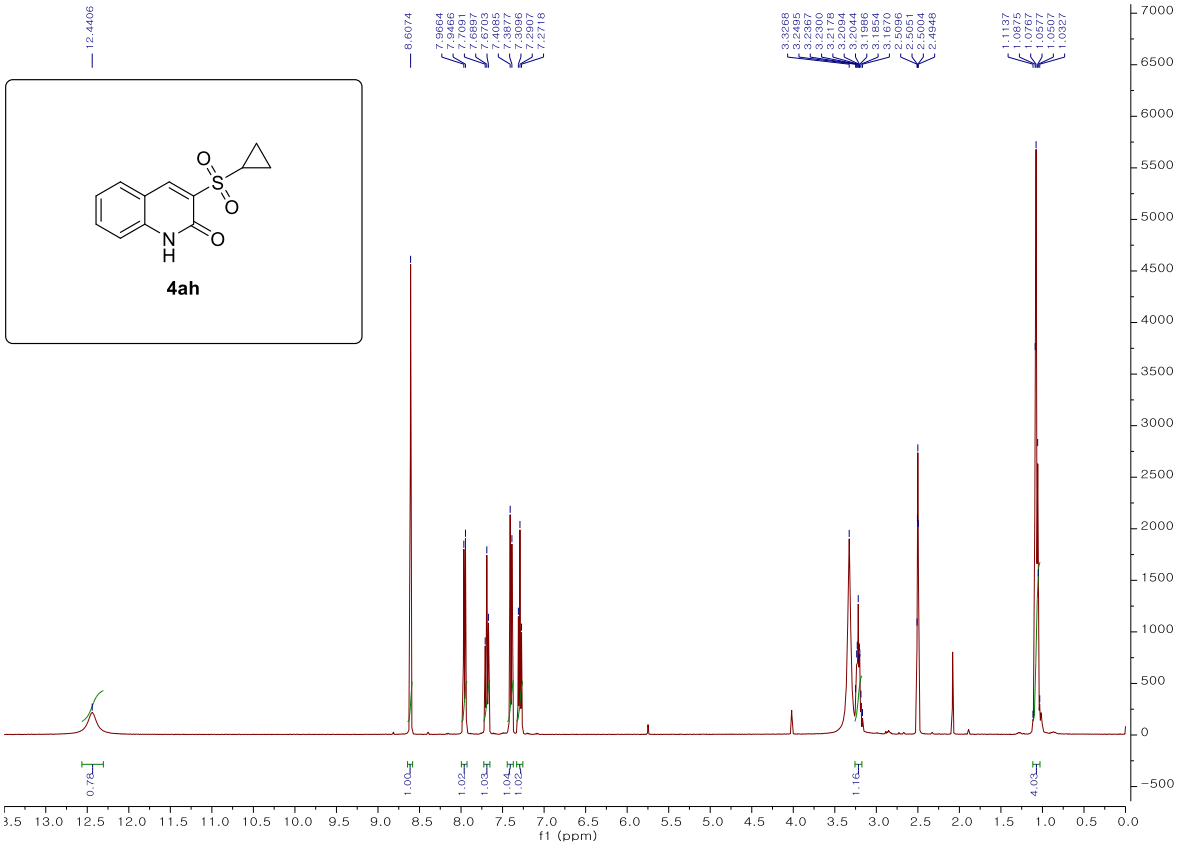
6.69
f1 (ppm)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7.2718
3.3268
3.2495
3.2367
3.2200
3.2178
3.2094
3.2044
3.1986
3.1856
3.1670
2.5096
2.5051
2.5004
2.4948
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1.0875
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f1 (ppm)
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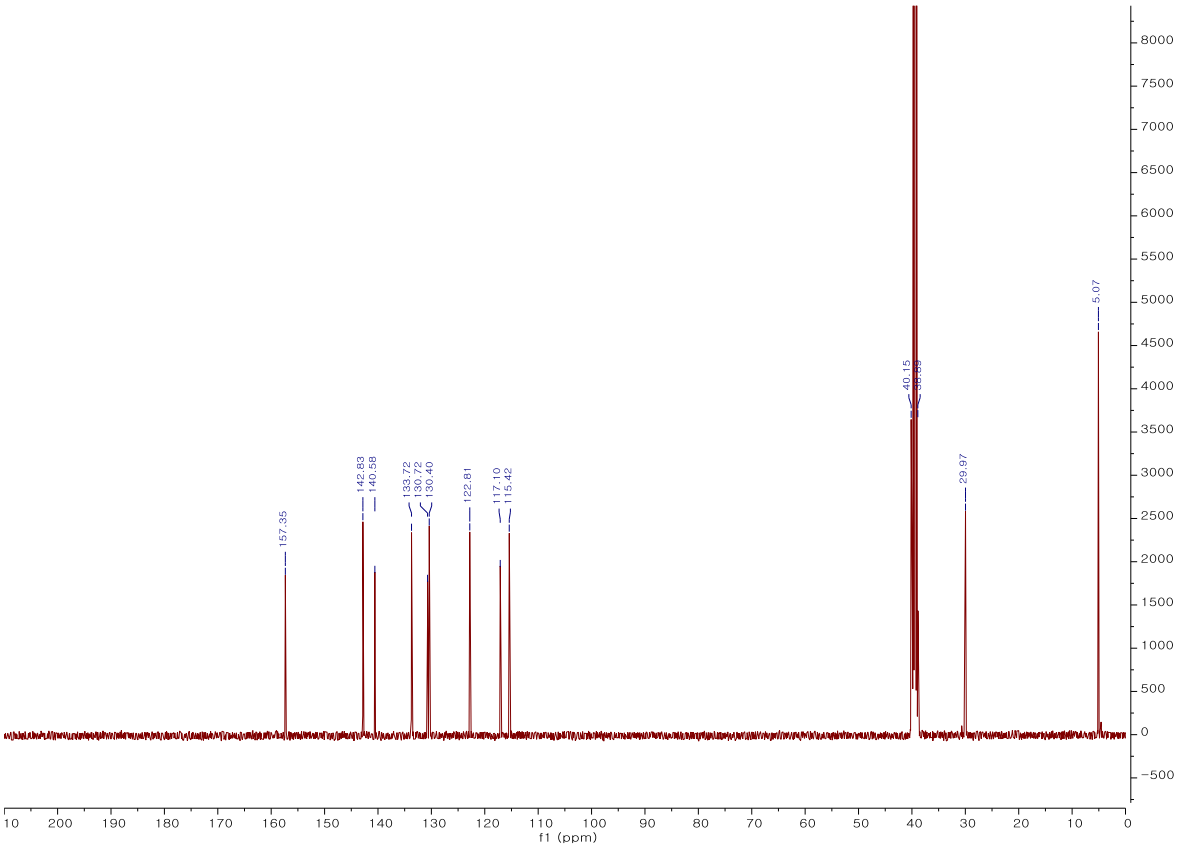
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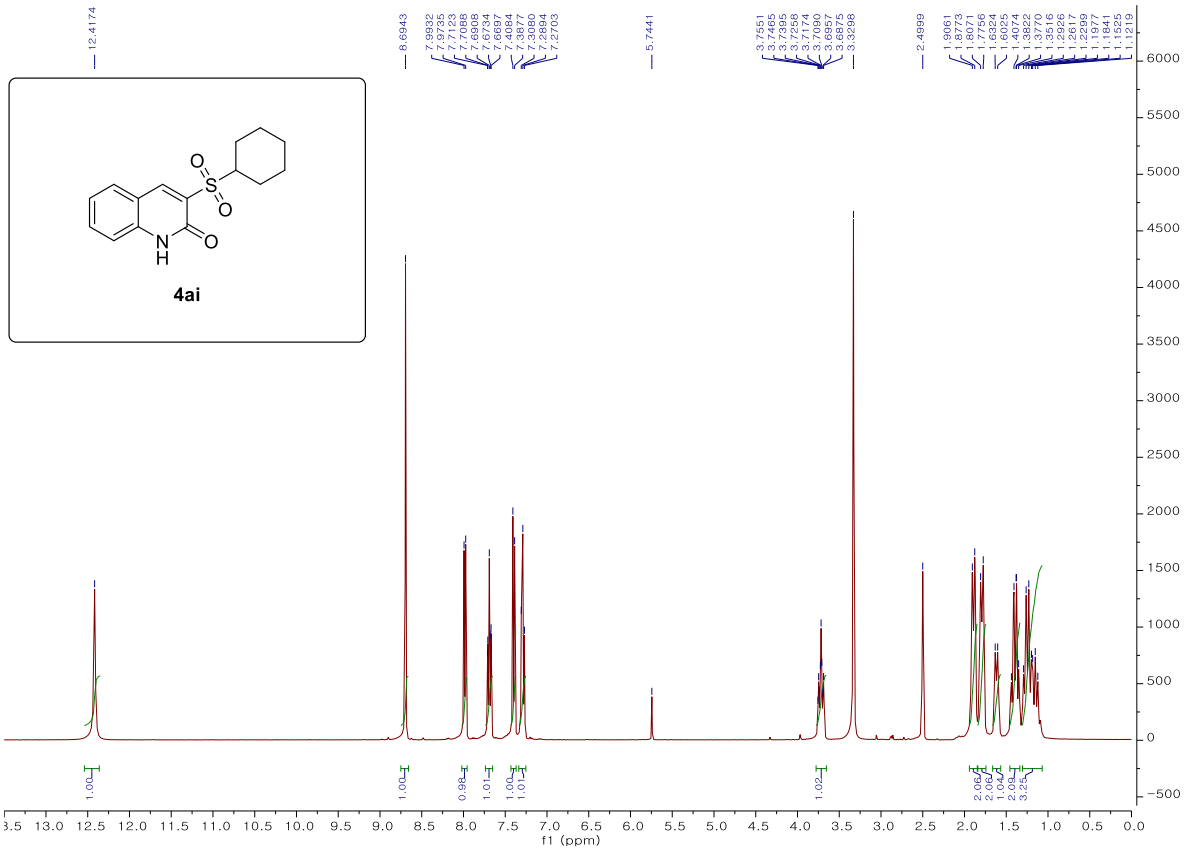
5.07
f1 (ppm)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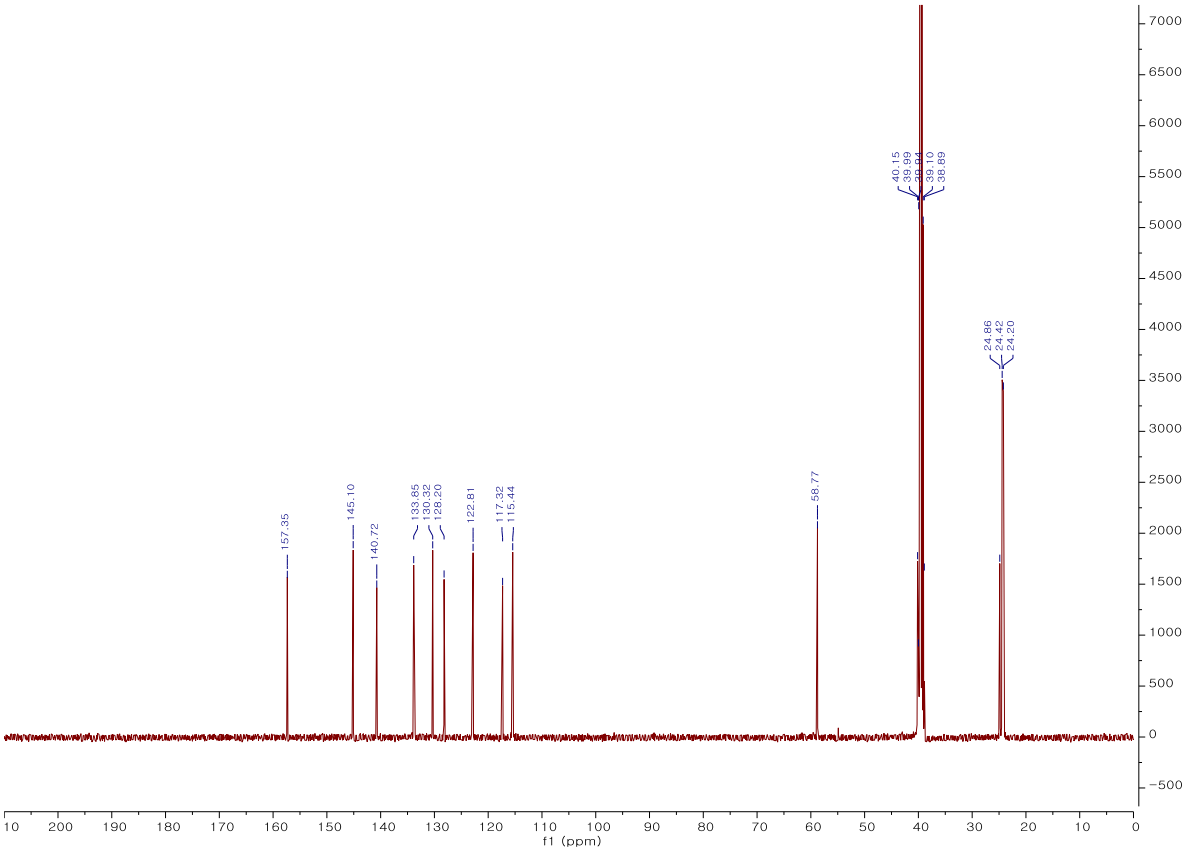
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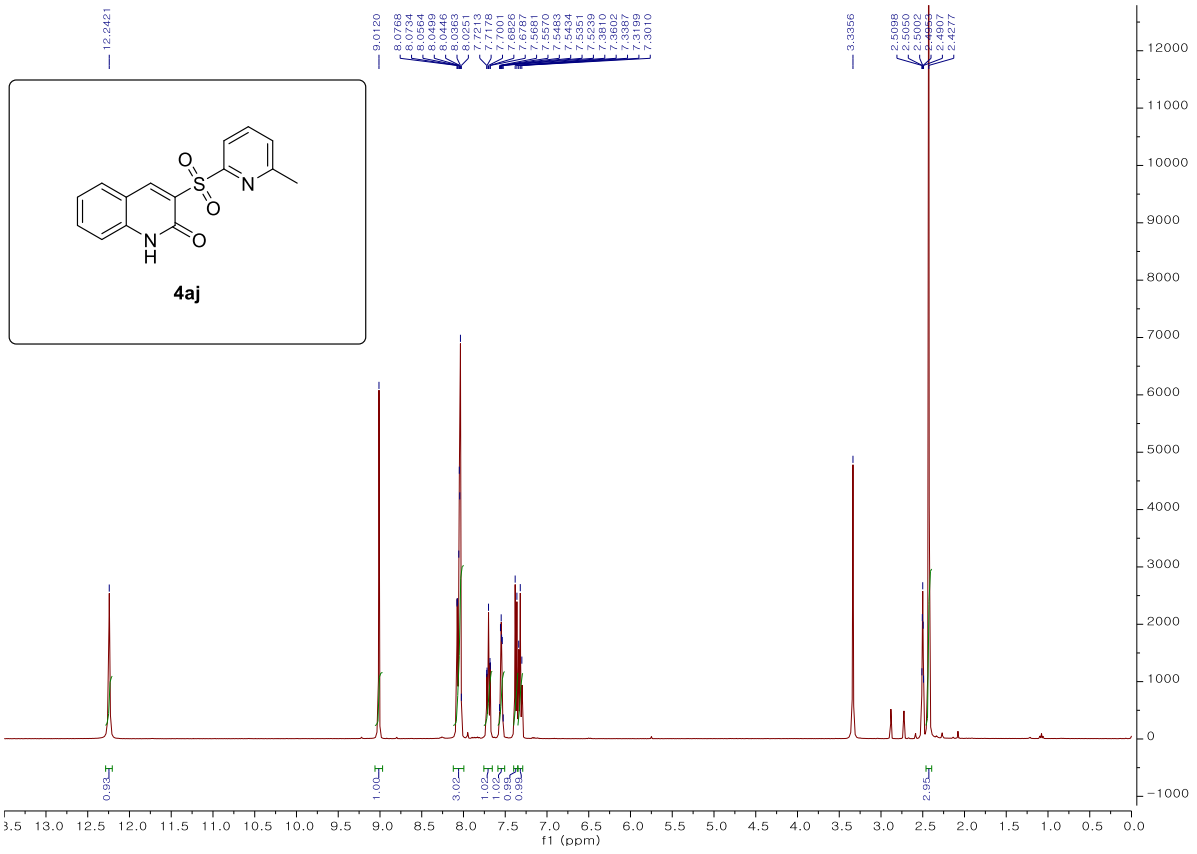
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2.4955
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f1 (ppm)
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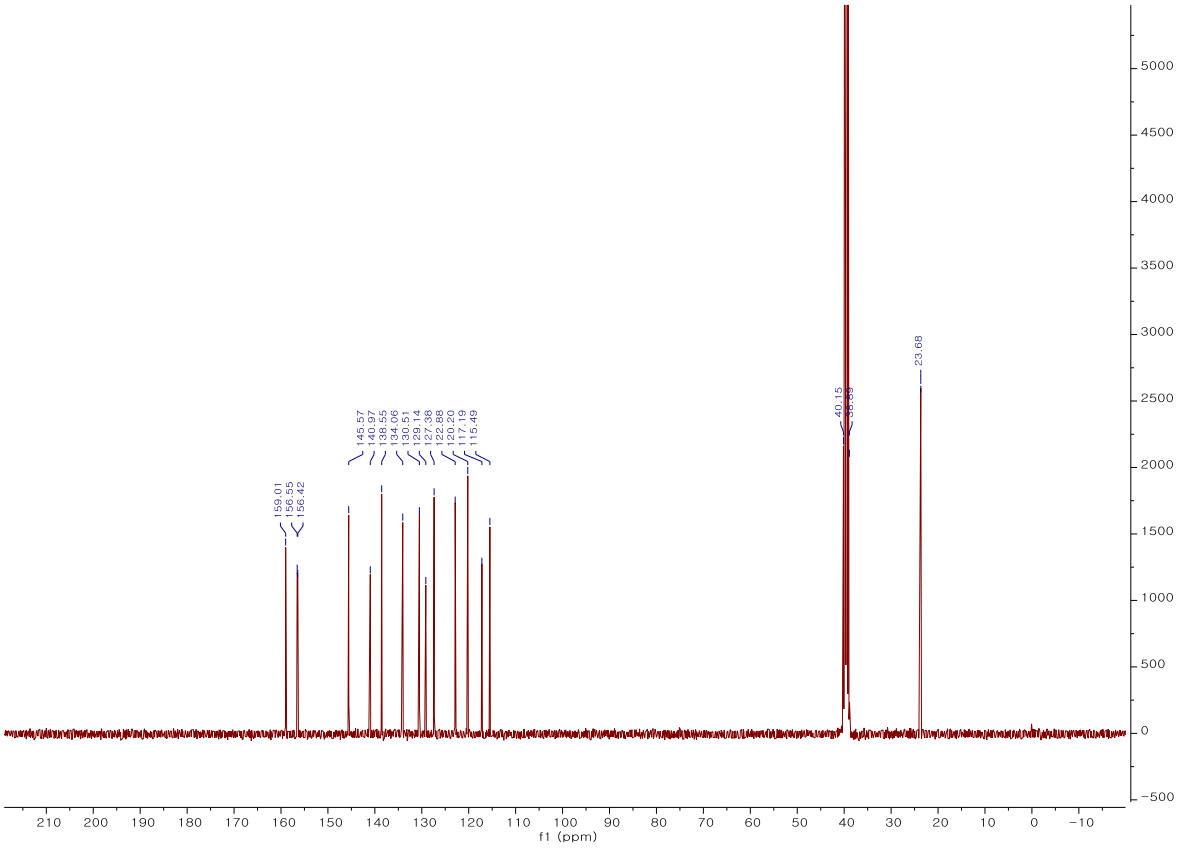
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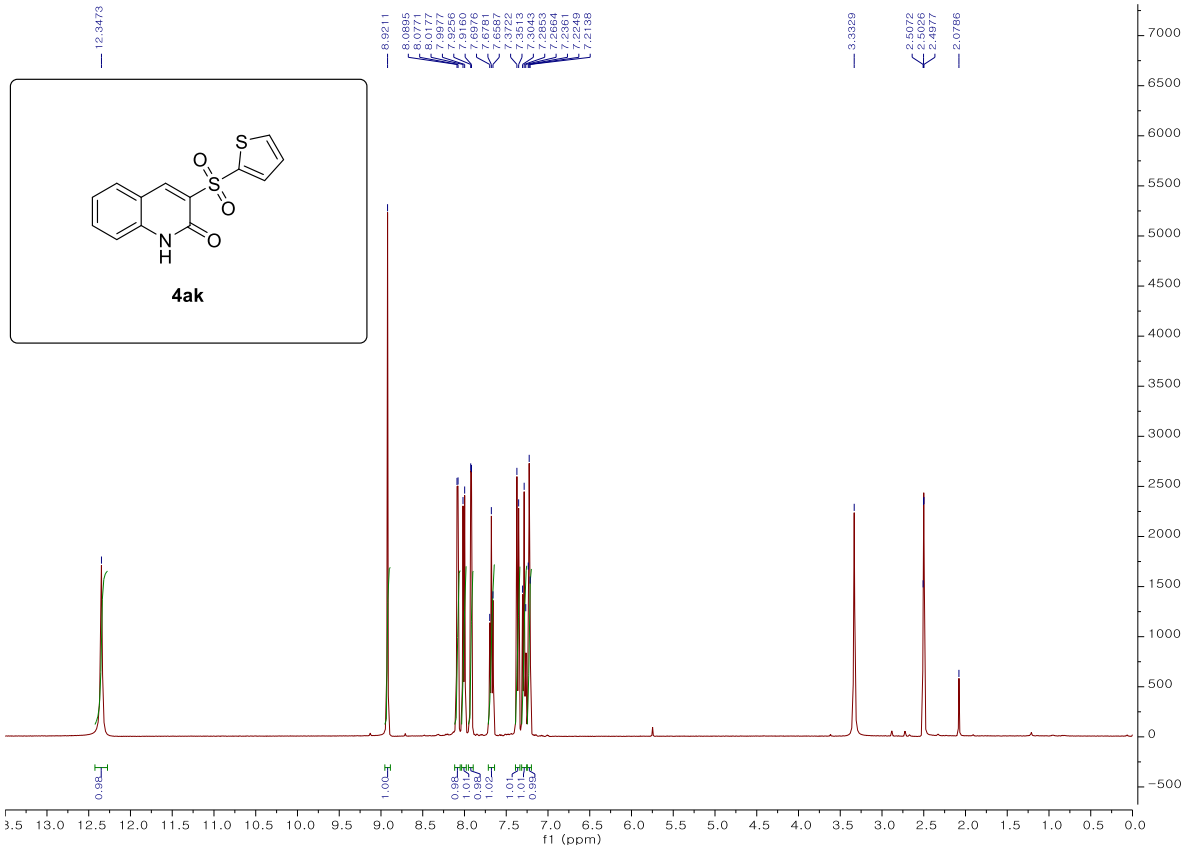
23.68
f1 (ppm)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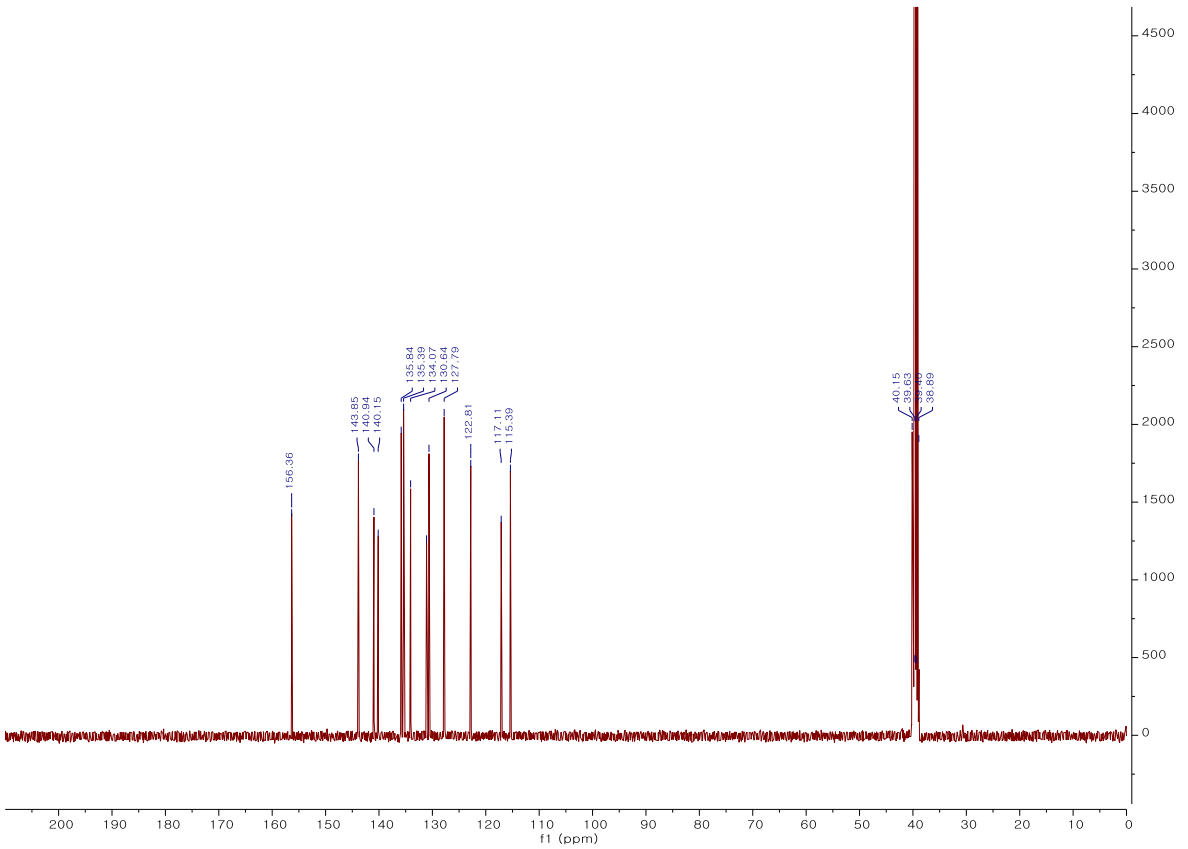
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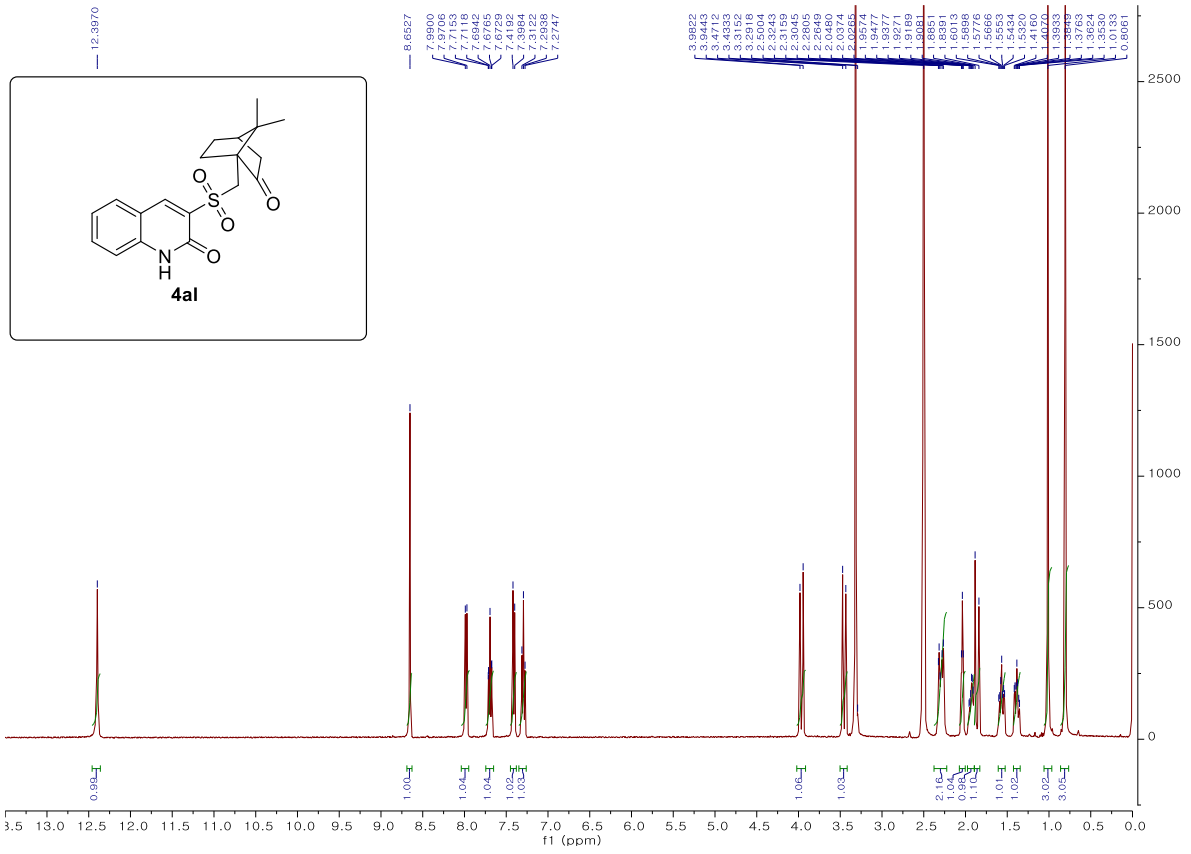
39.42
38.89
f1 (ppm)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1.02
3.02
3.06
f1 (ppm)
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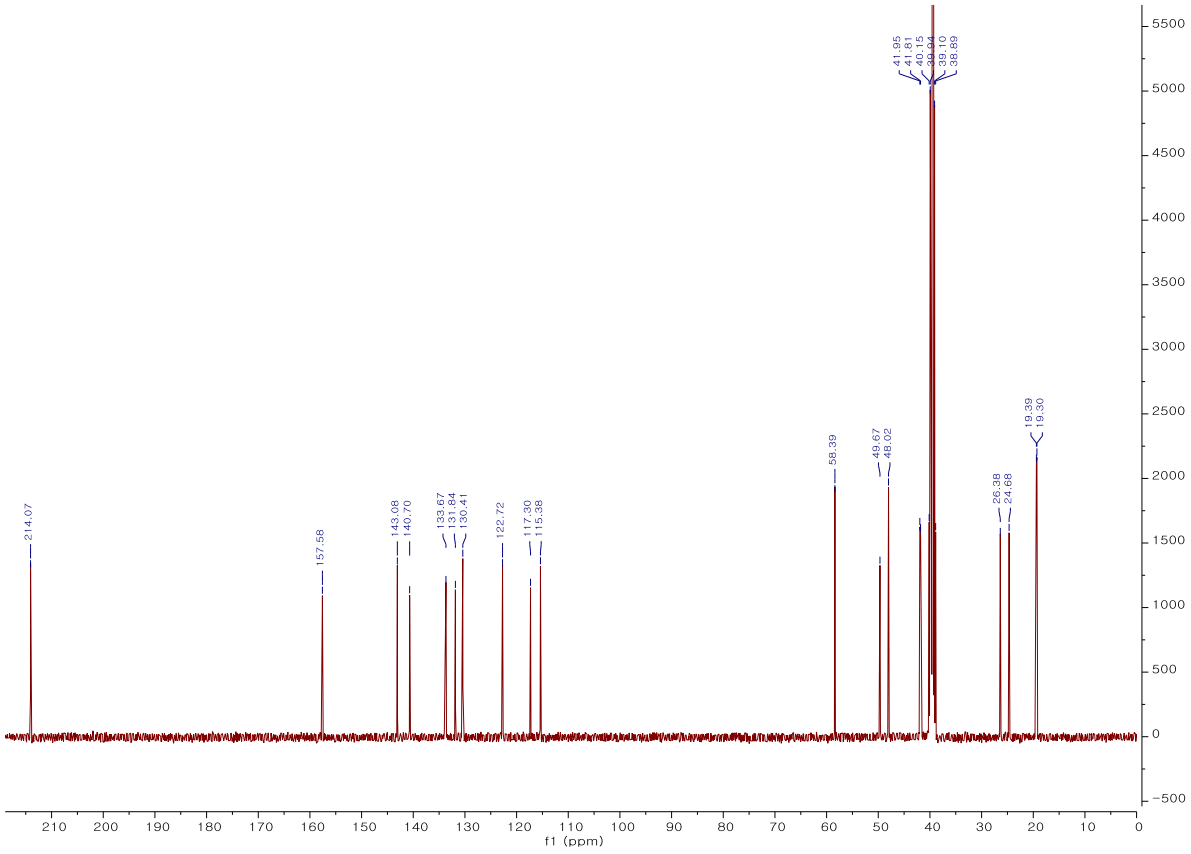
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26.38
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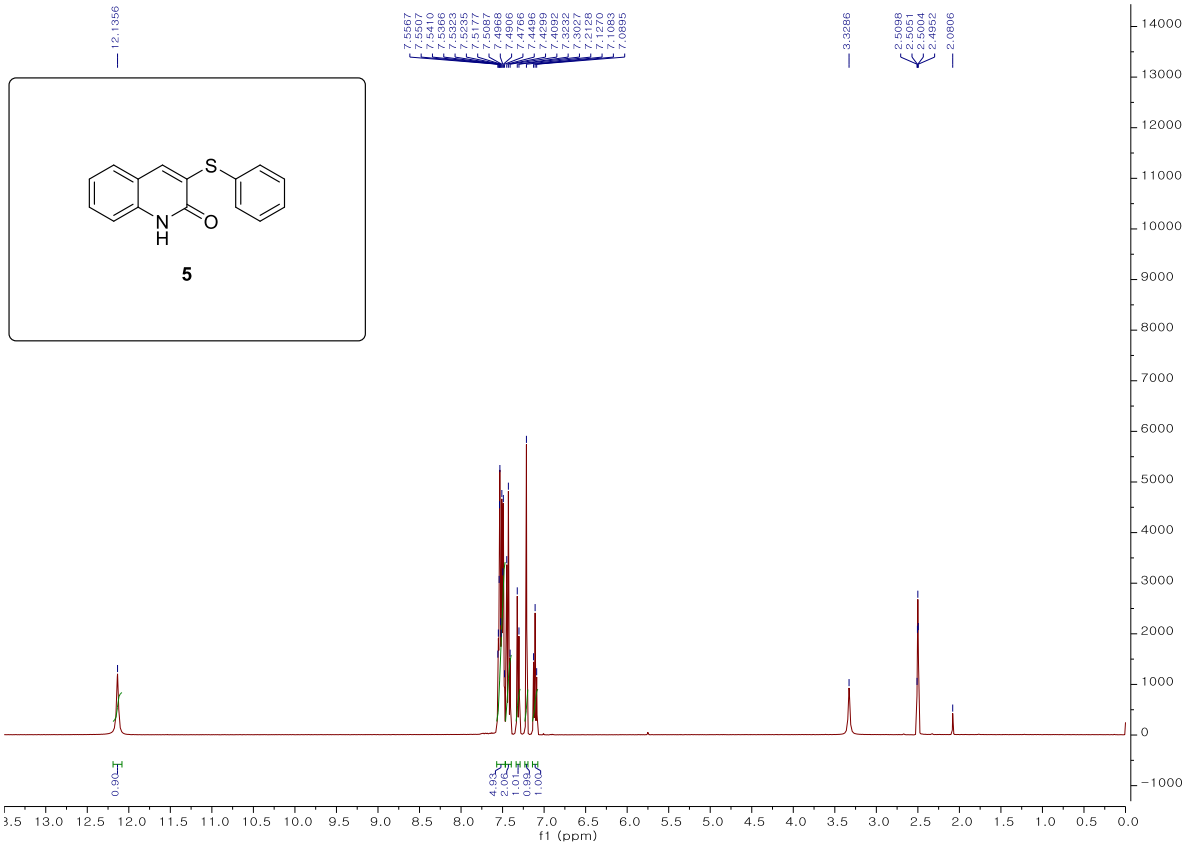
19.39
19.30
f1 (ppm)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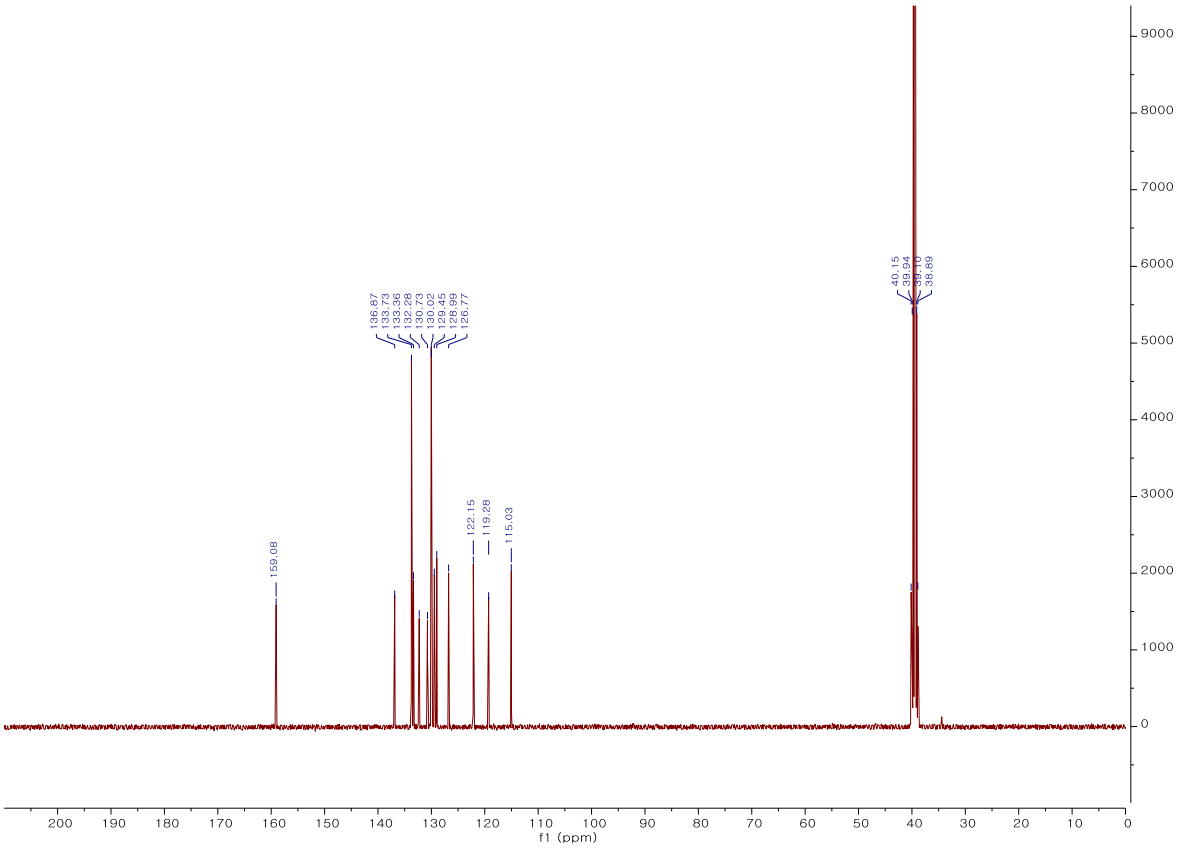
1.00
f1 (ppm)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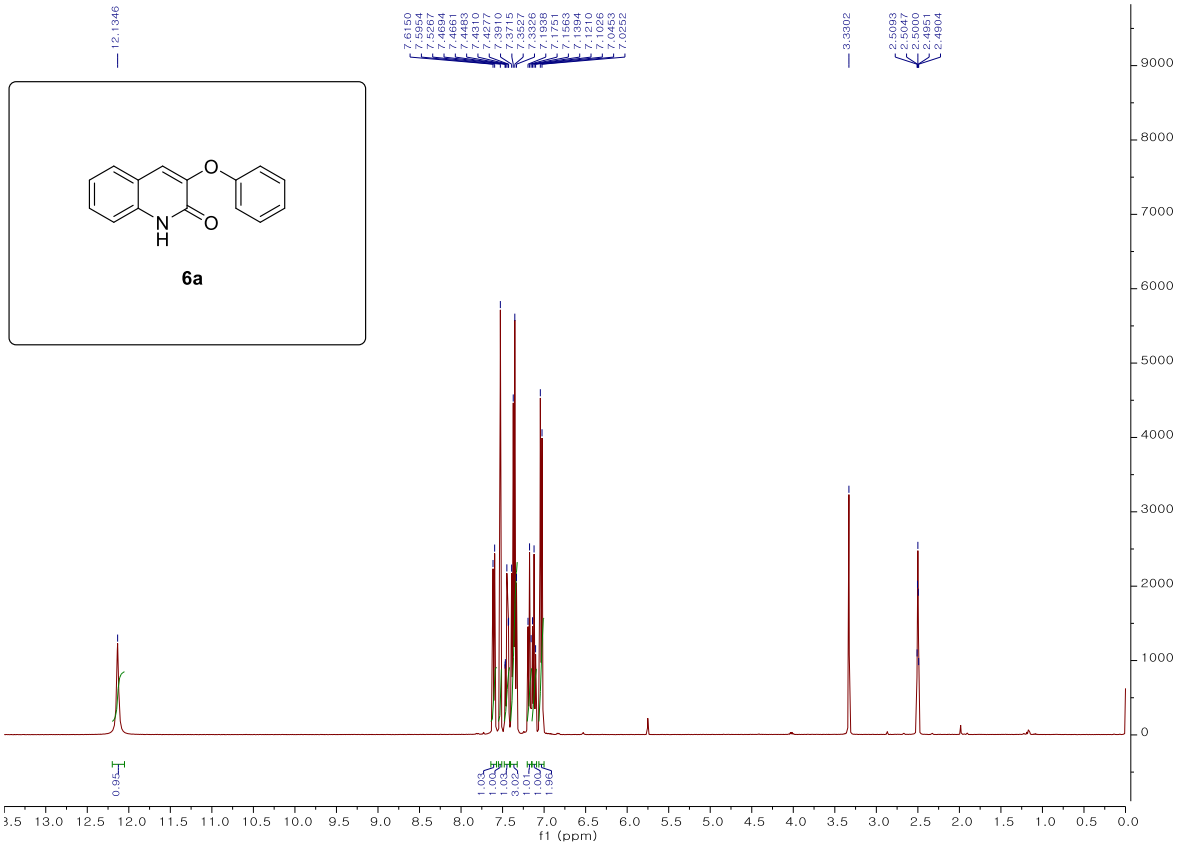
39.73
38.89
f1 (ppm)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7.1553
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7.1026
7.0453
7.0252
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H
O
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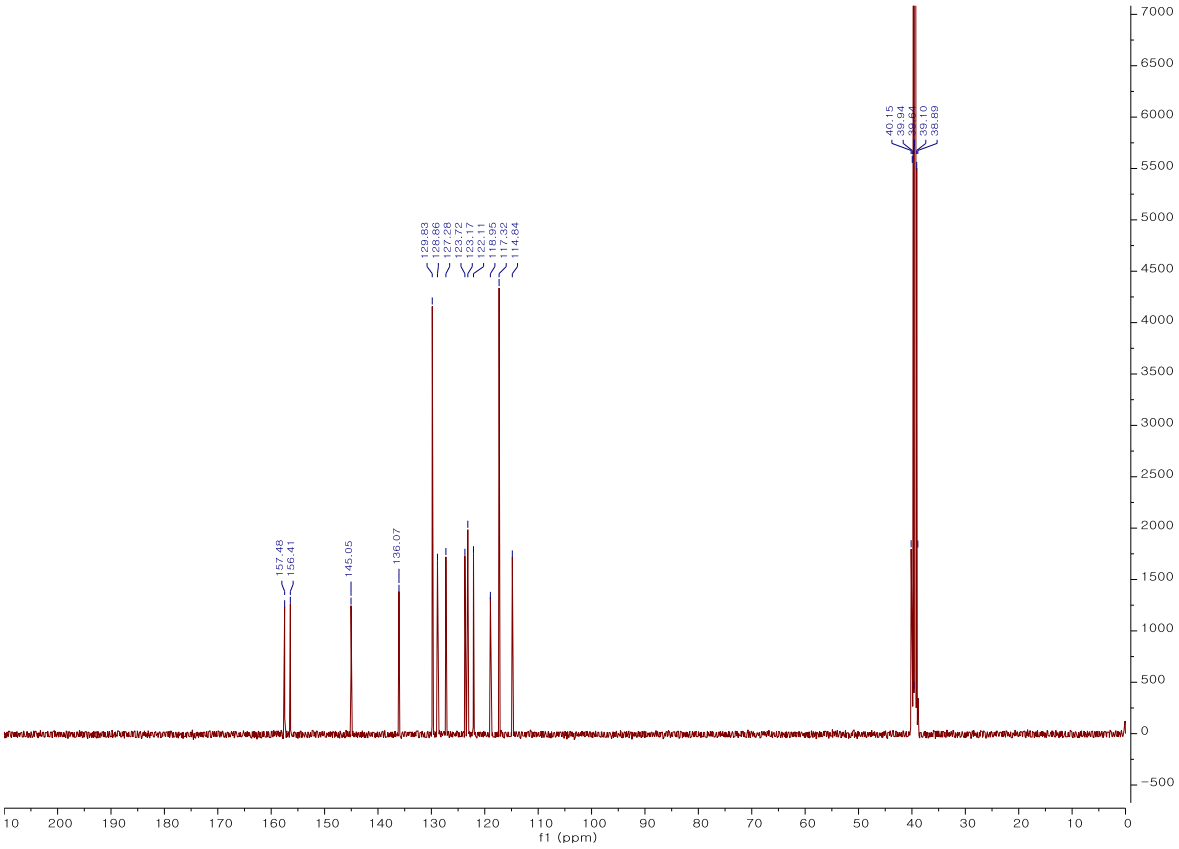
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136.07
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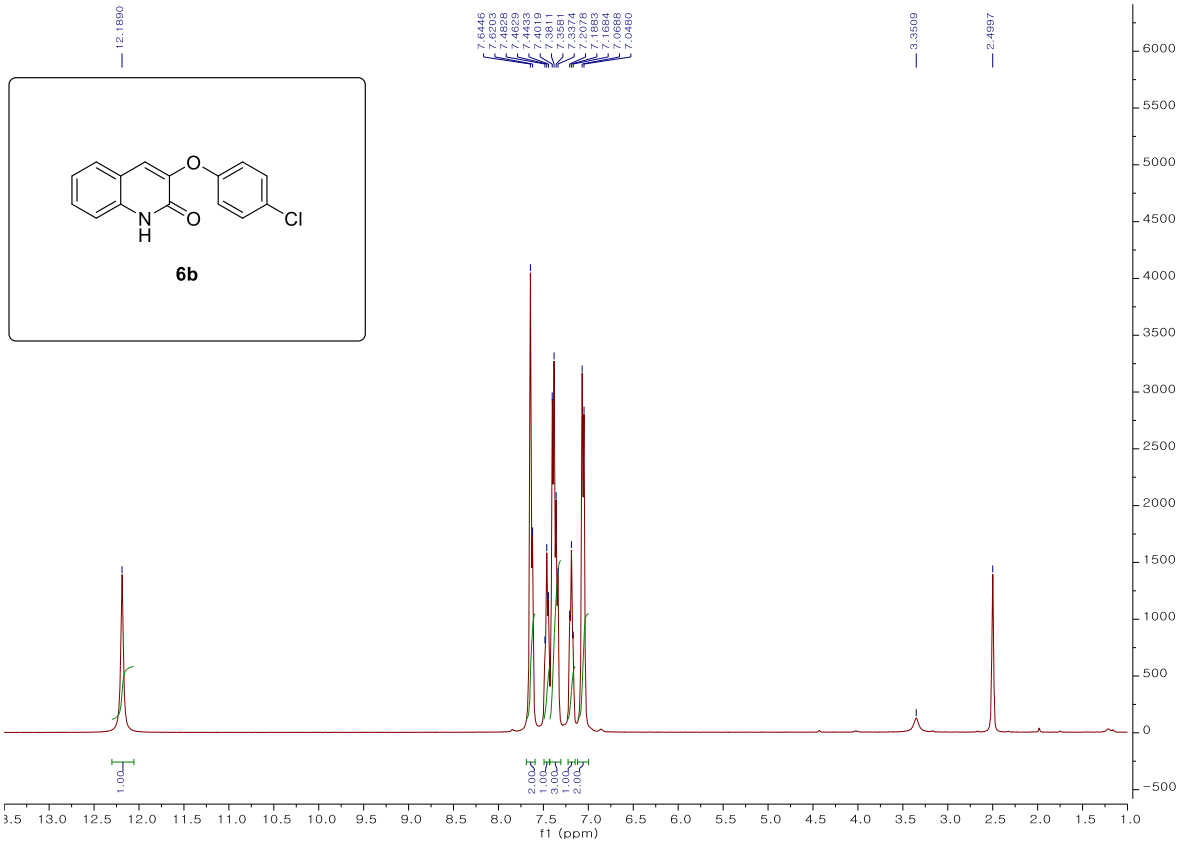
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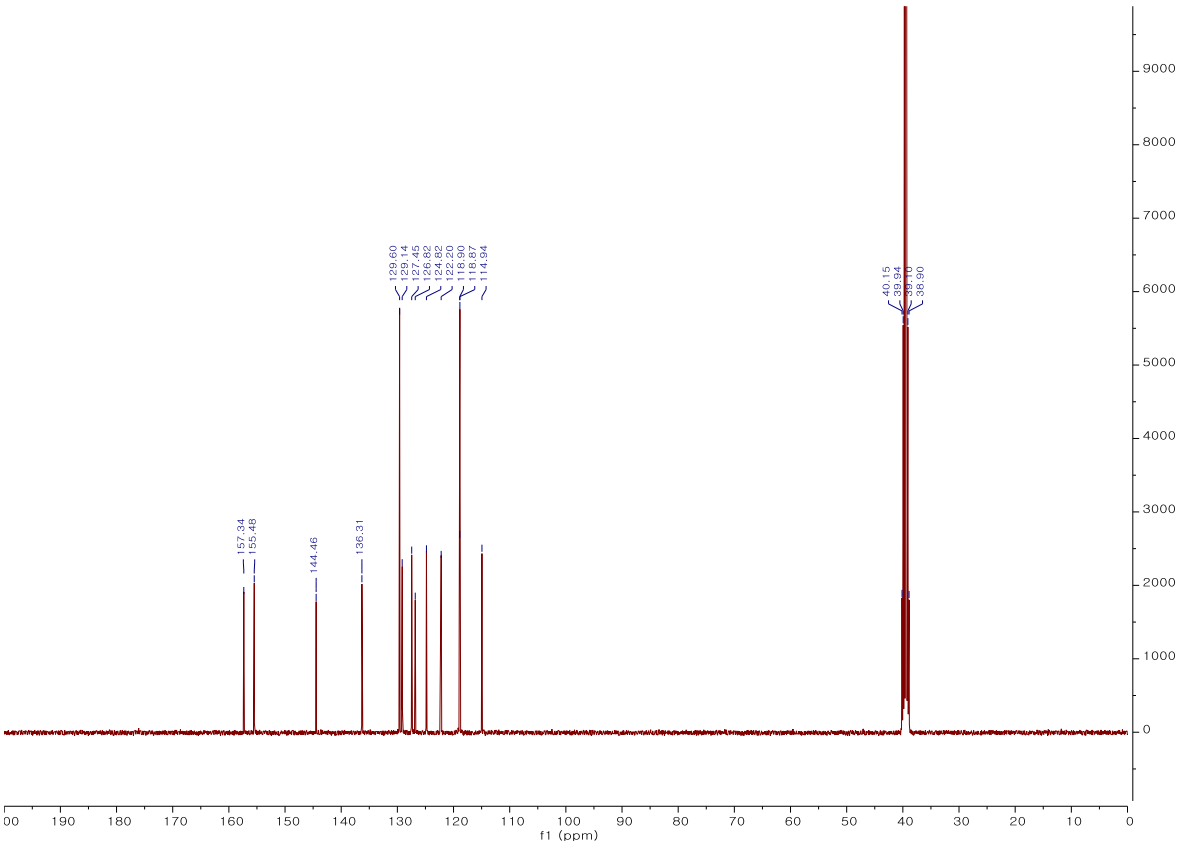
H
O
Cl
6b
f1 (ppm)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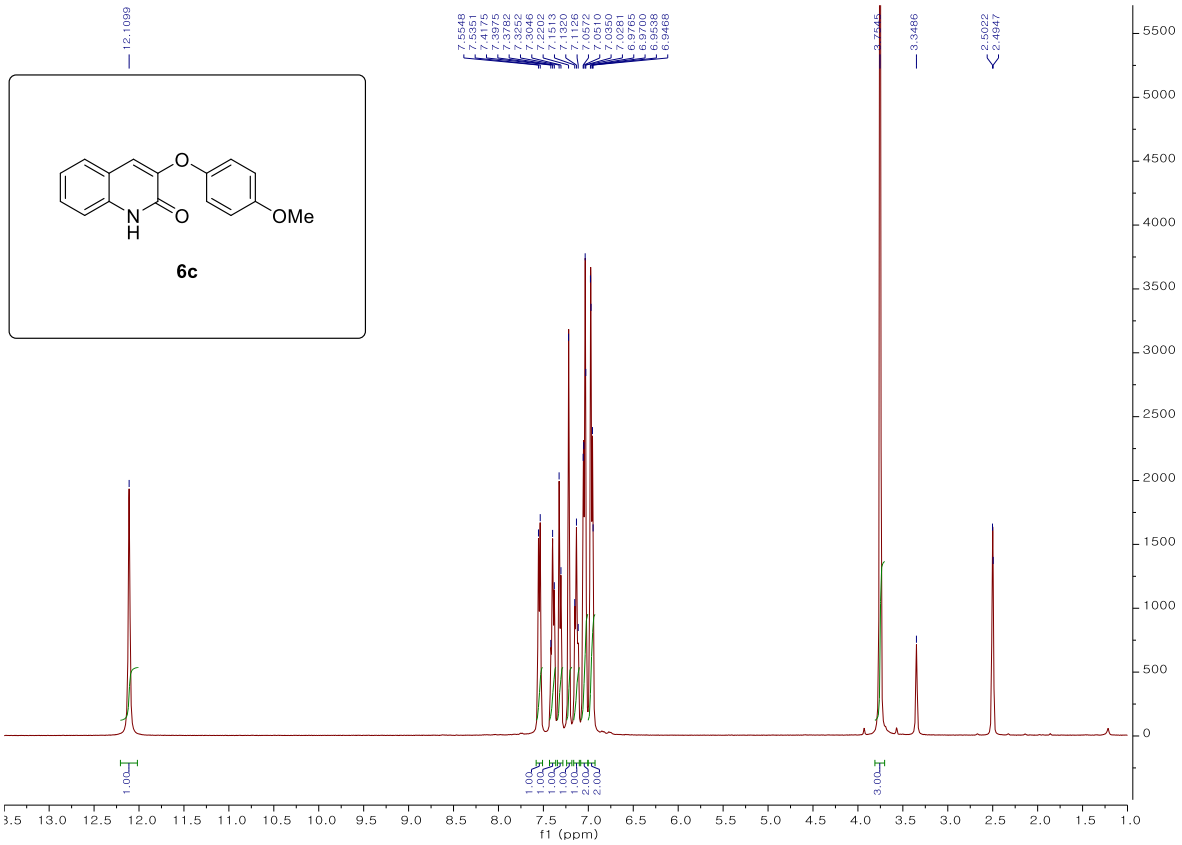
f1 (ppm)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7.0510
7.0350
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2.4947
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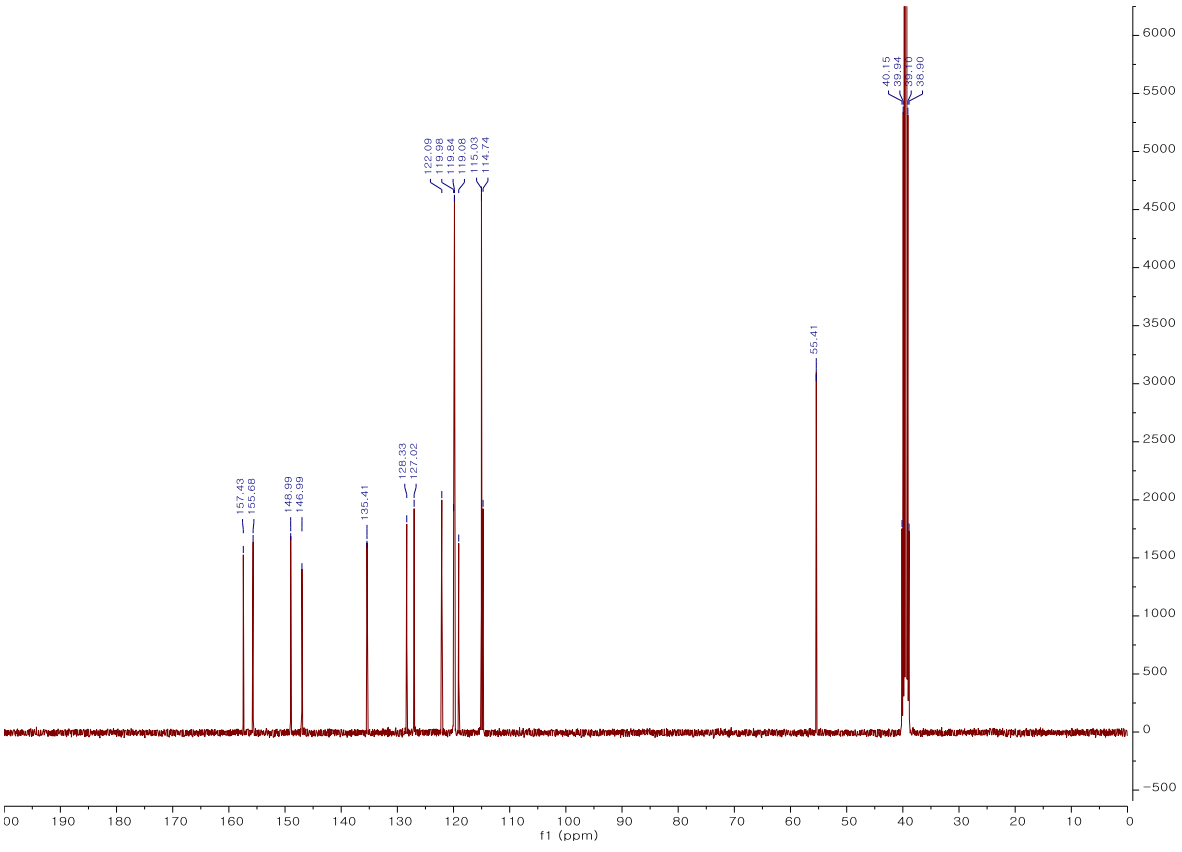
H
O
OMe
6c
f1 (ppm)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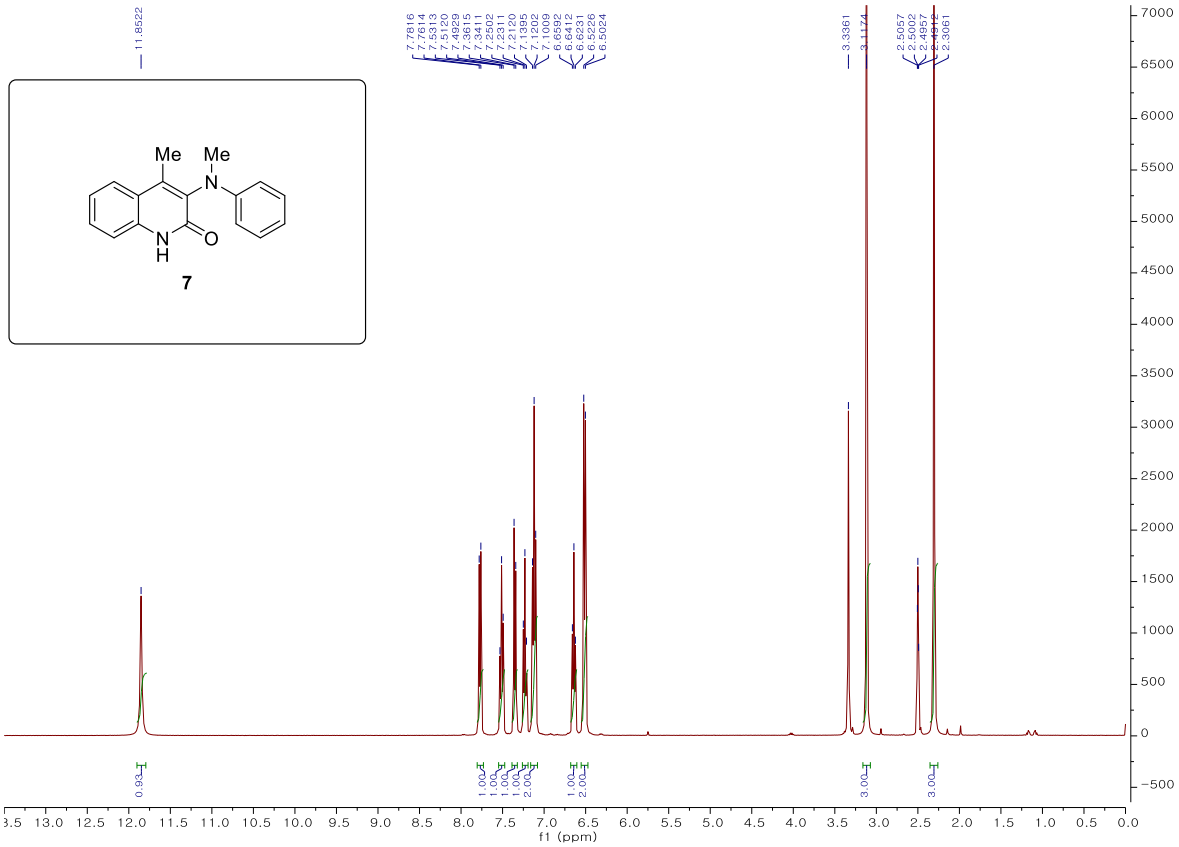
38.90
f1 (ppm)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7.1202
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3.1174
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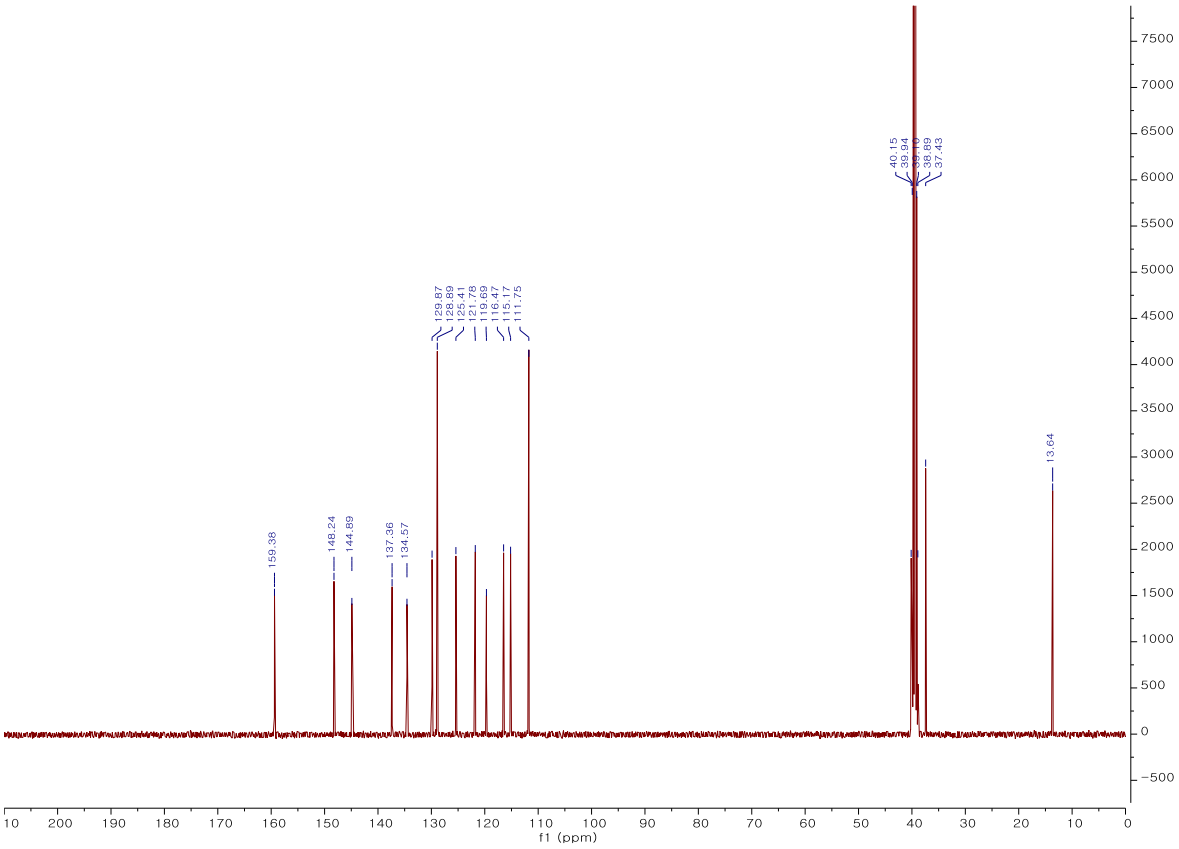
Me
N
N
H
O
7
f1 (ppm)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38.89
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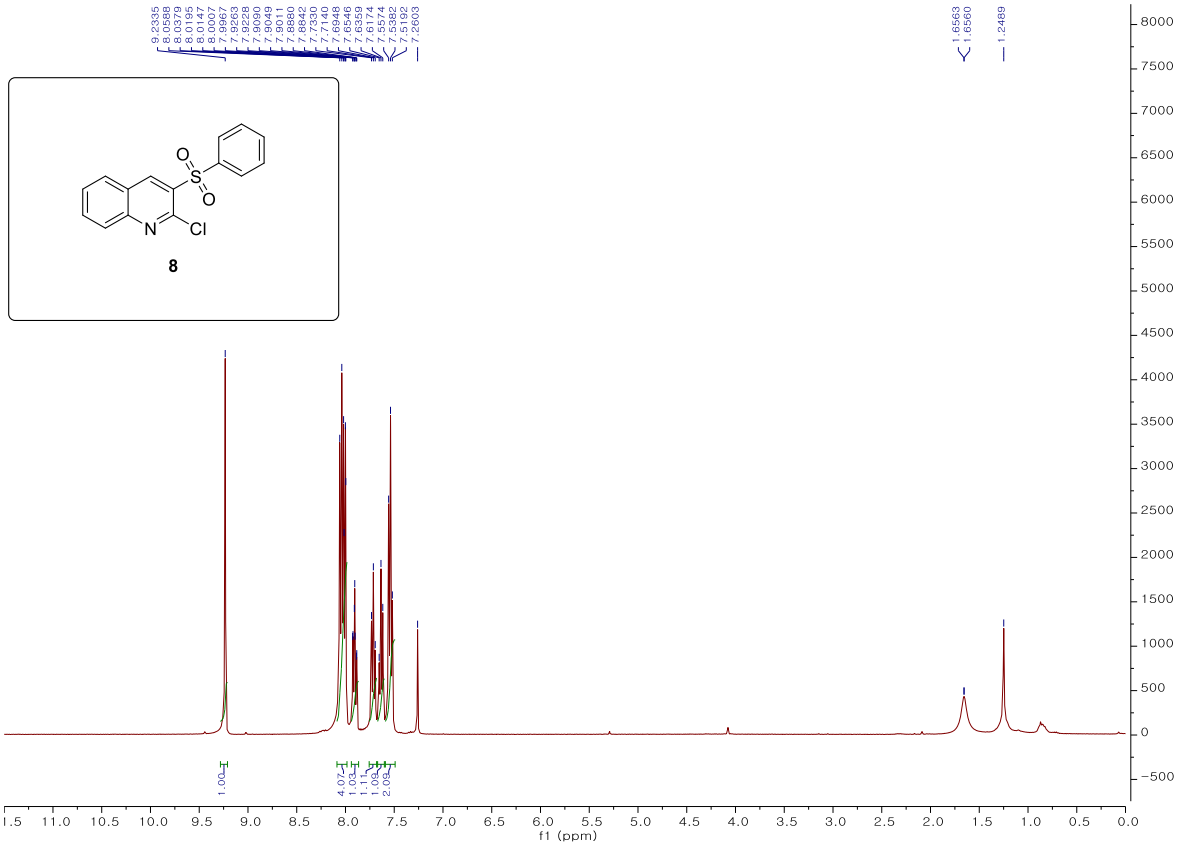
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7.5192
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2.08
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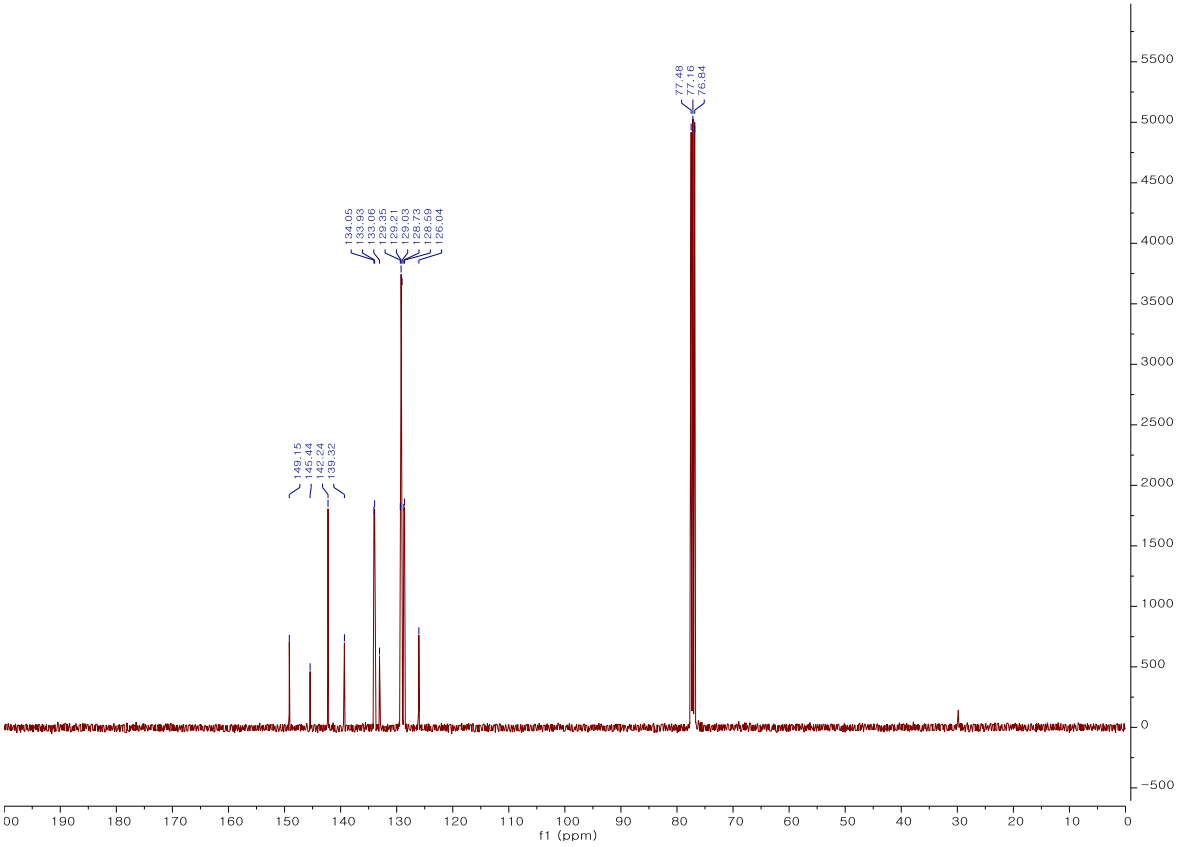
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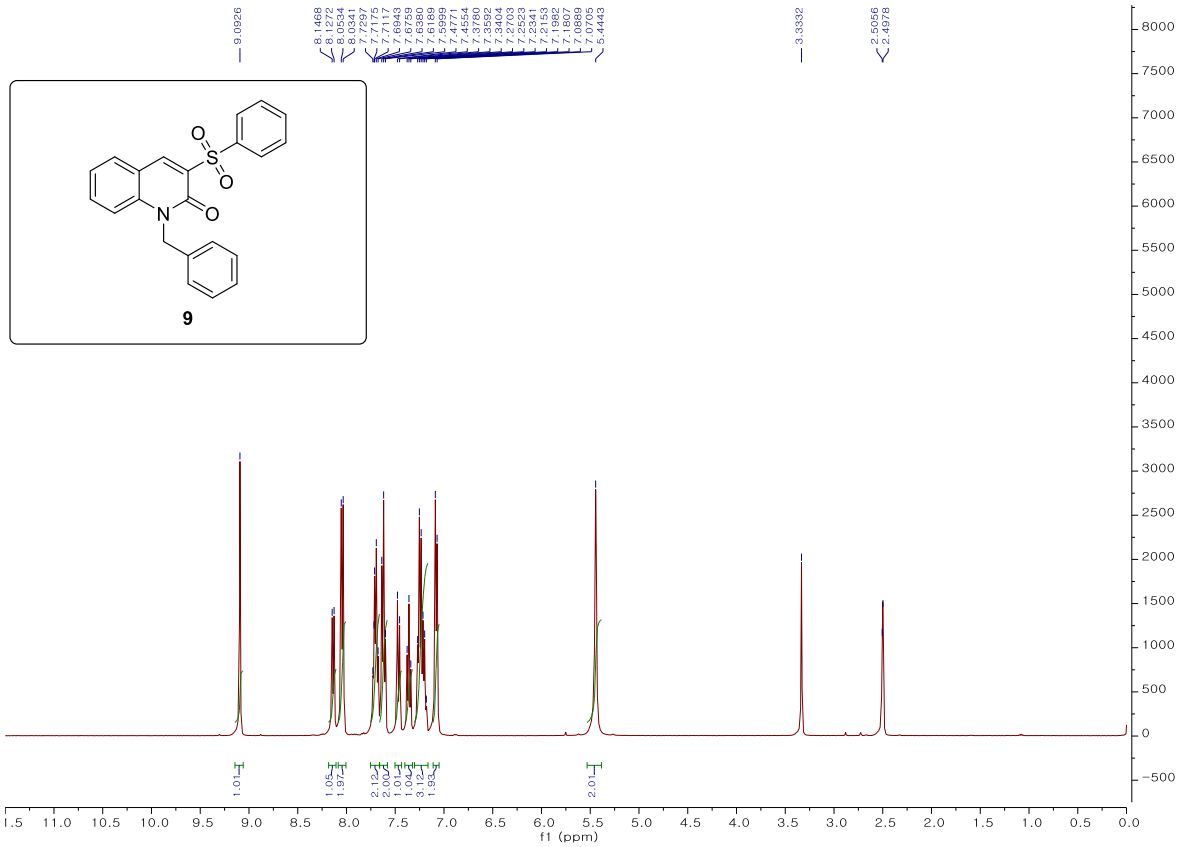
139.32
f1 (ppm)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2.01
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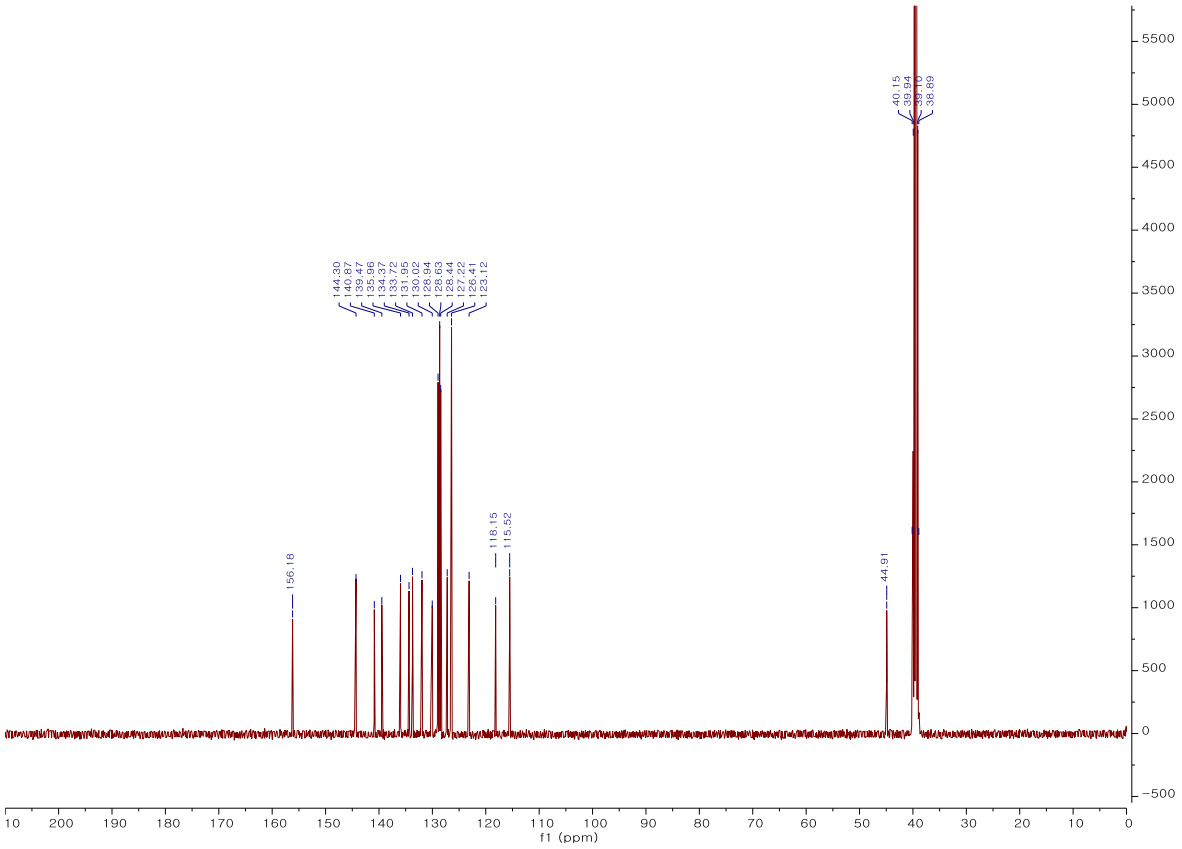
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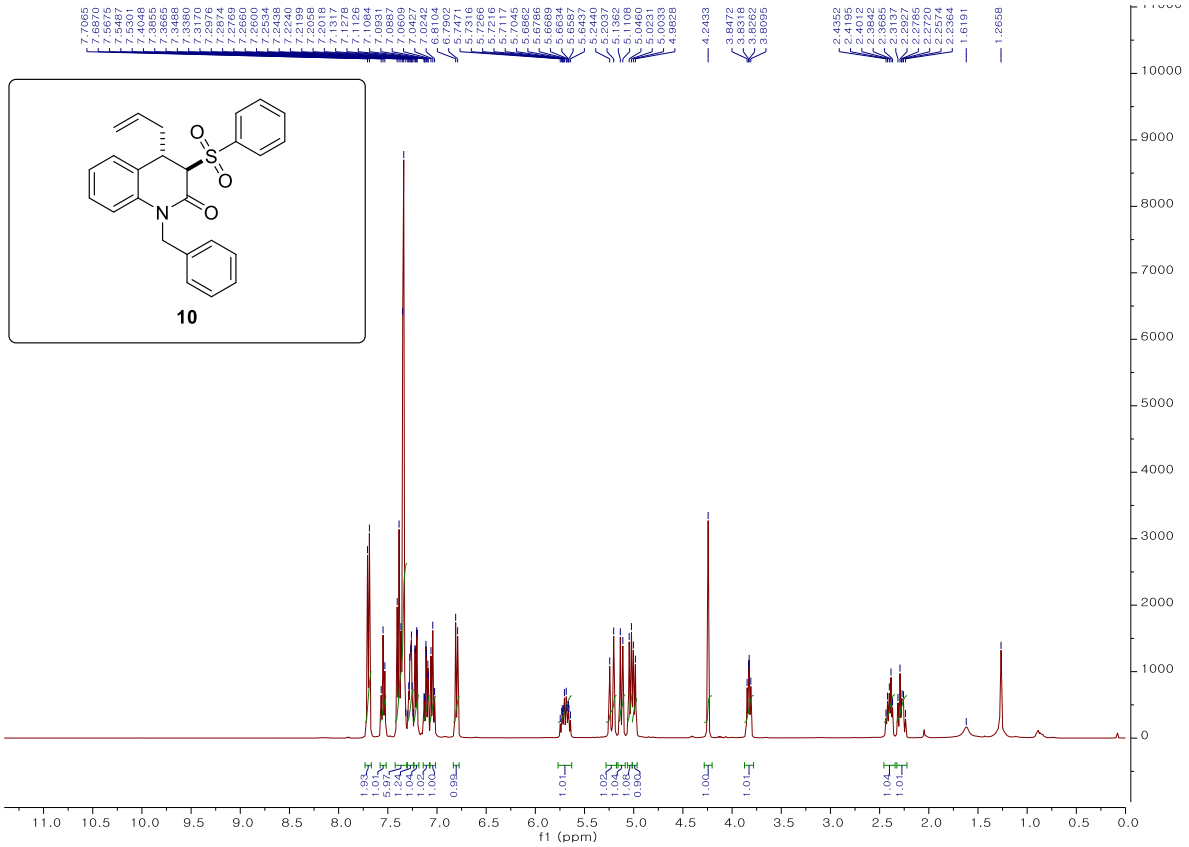
39.73
38.89
f1 (ppm)

9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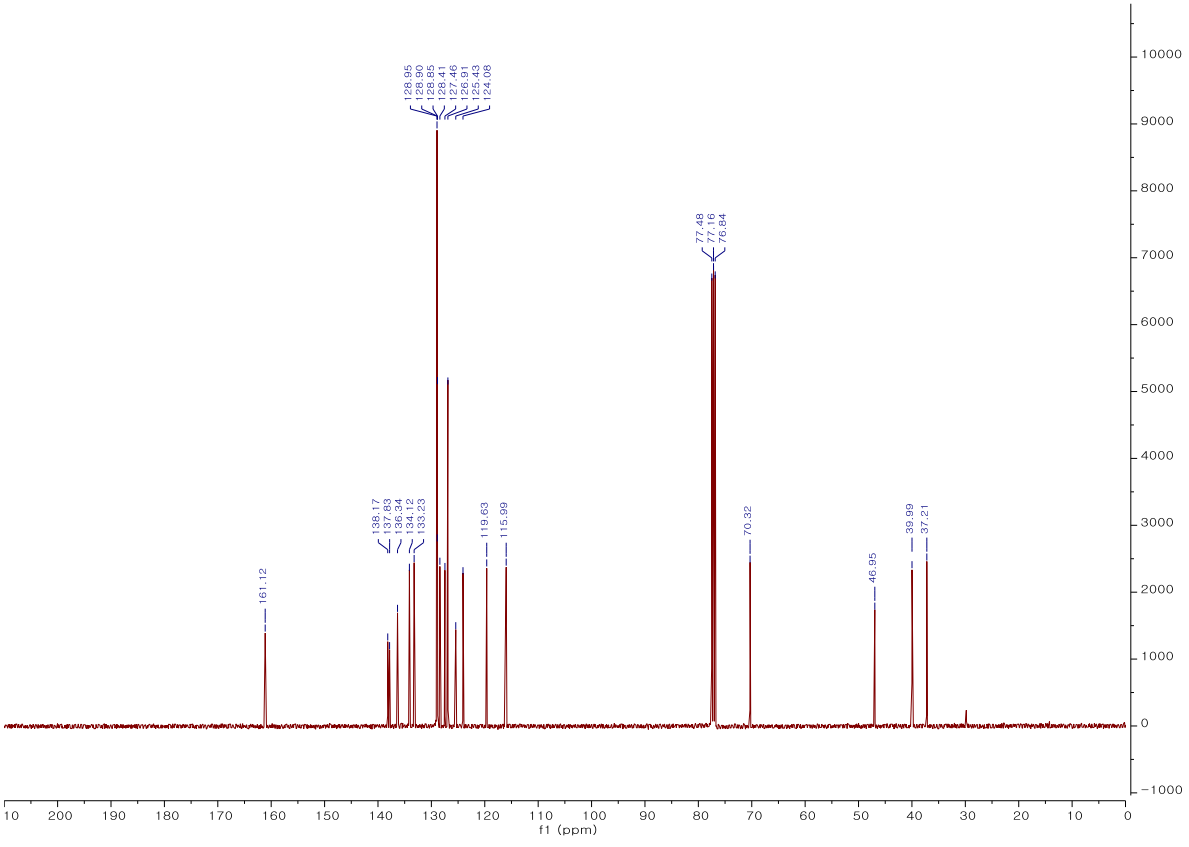
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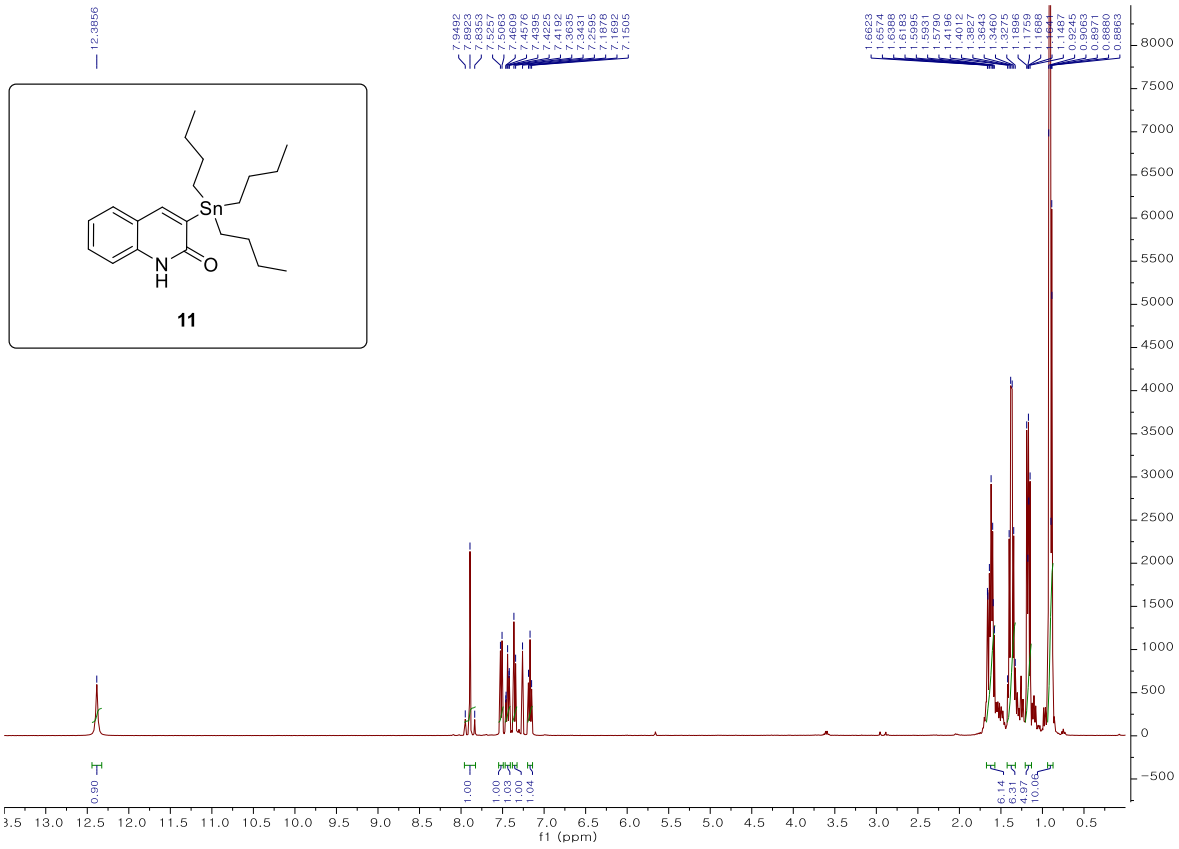
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1.04
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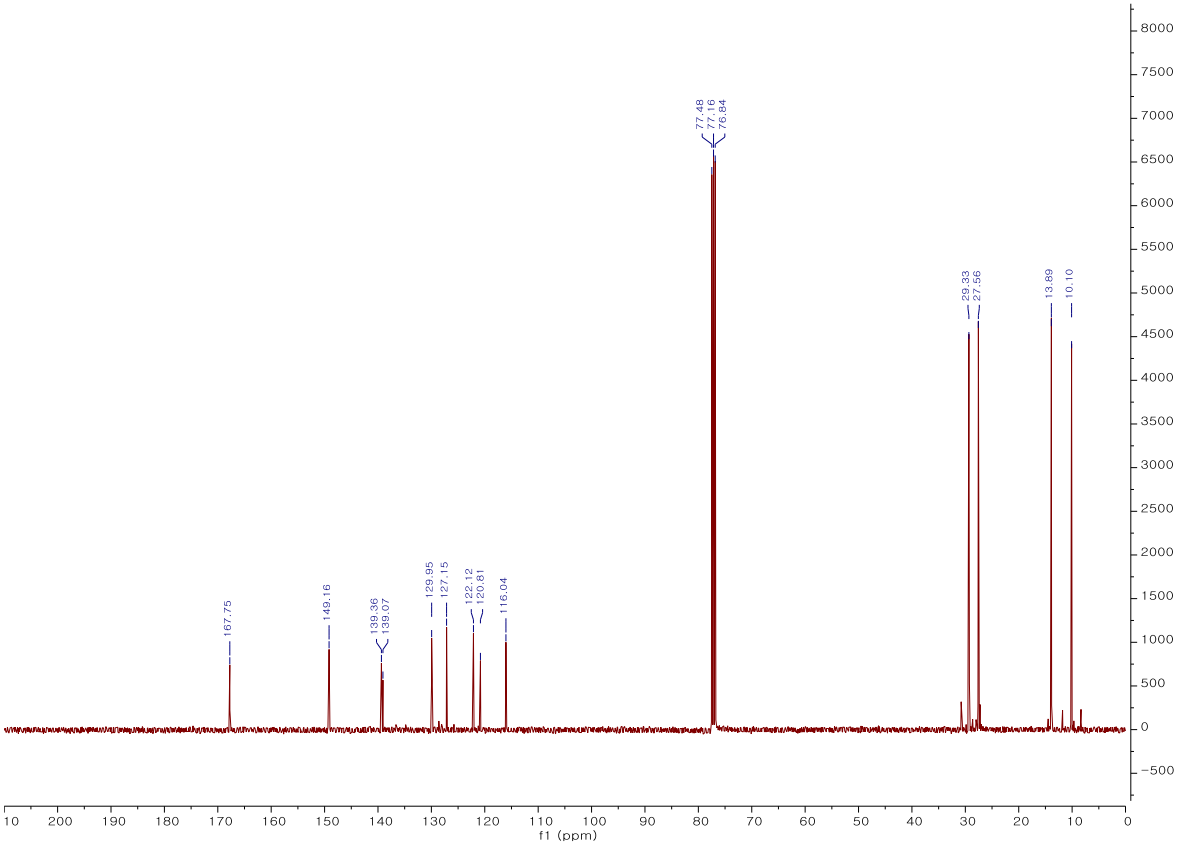
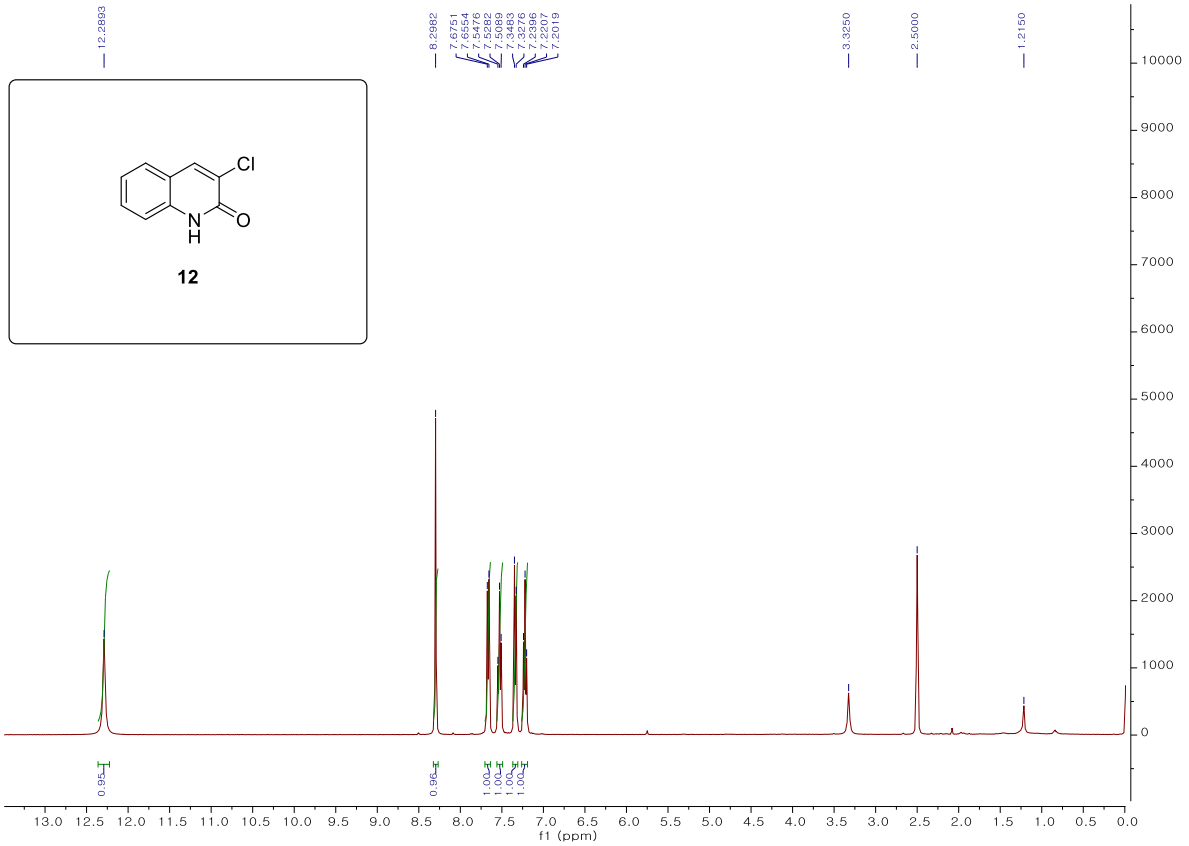
6.31
4.97
10.06
f1 (ppm)


77.48
77.16
76.84
167.75
149.16
139.36
139.07
129.95
127.15
122.12
120.81
116.04
29.33
27.56
13.89
10.10
f1 (ppm)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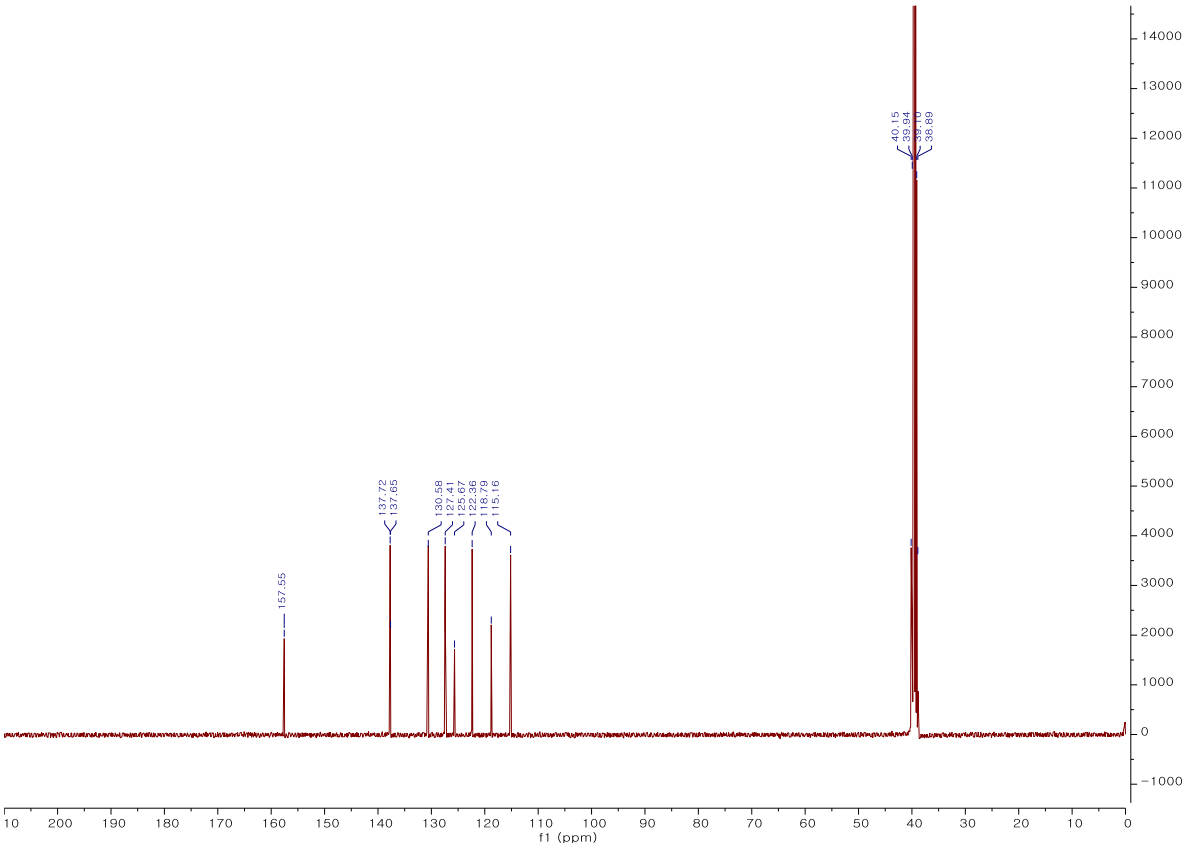
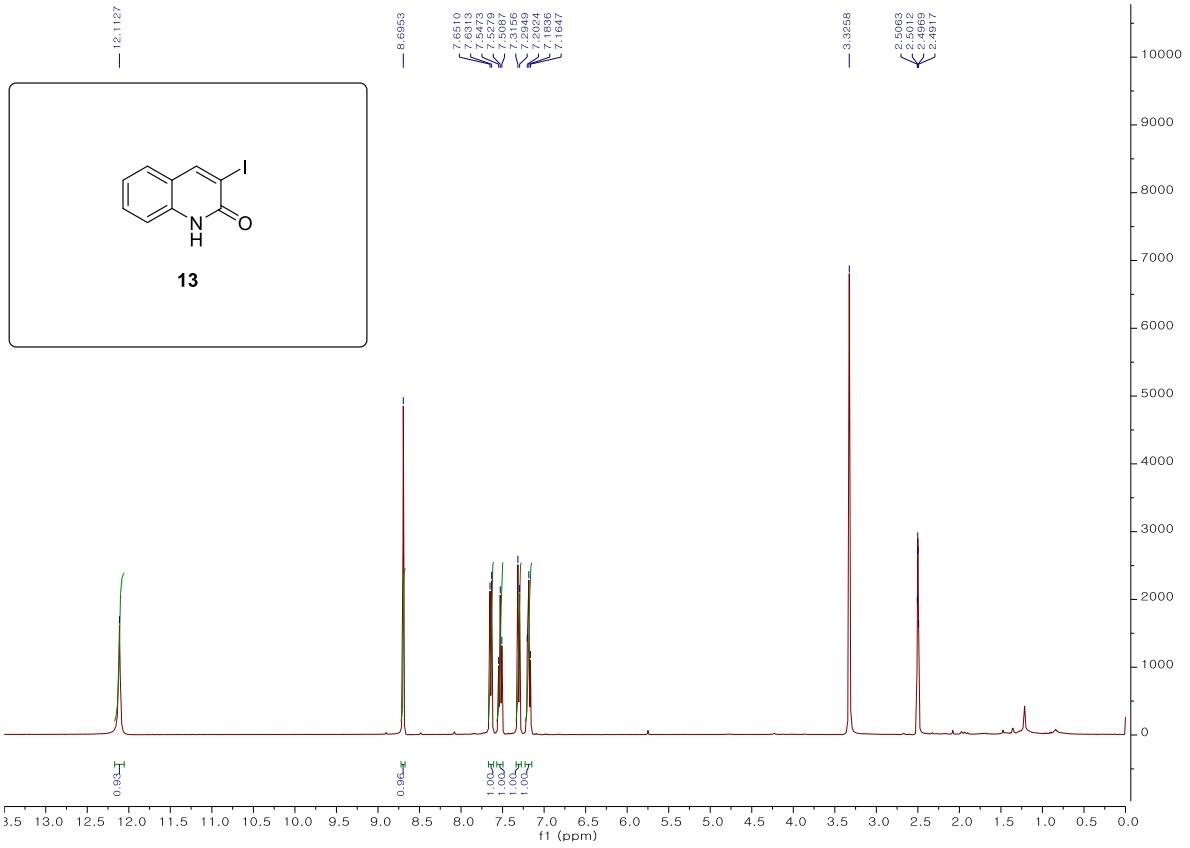
8.2982
7.6751
7.6554
7.5476
7.5282
7.3089
7.2883
7.2483
7.3276
7.2396
7.2207
7.2019
3.3250
2.5000
1.2150
Cl
N
H
O
12
f1 (ppm)


40.15
39.94
39.73
38.89
157.55
137.72
137.65
130.58
127.41
125.67
122.36
118.78
115.16
f1 (ppm)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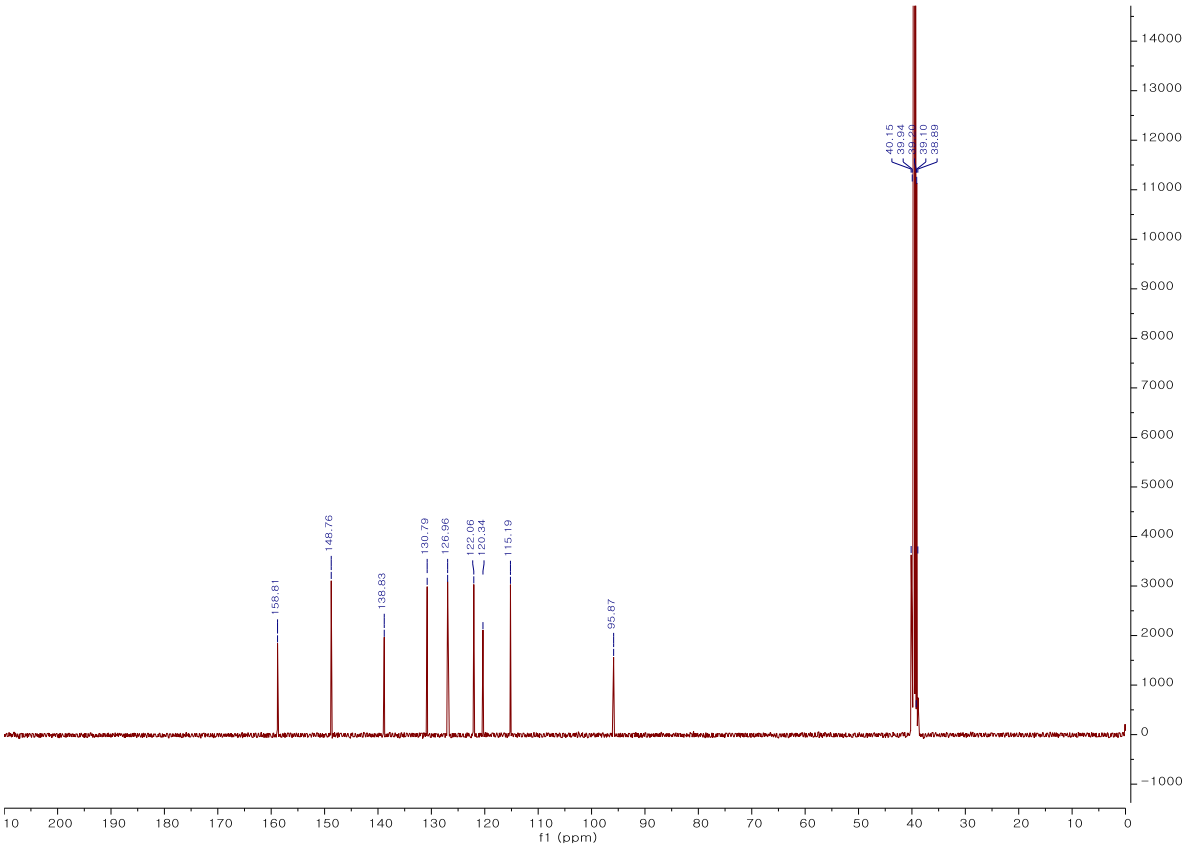
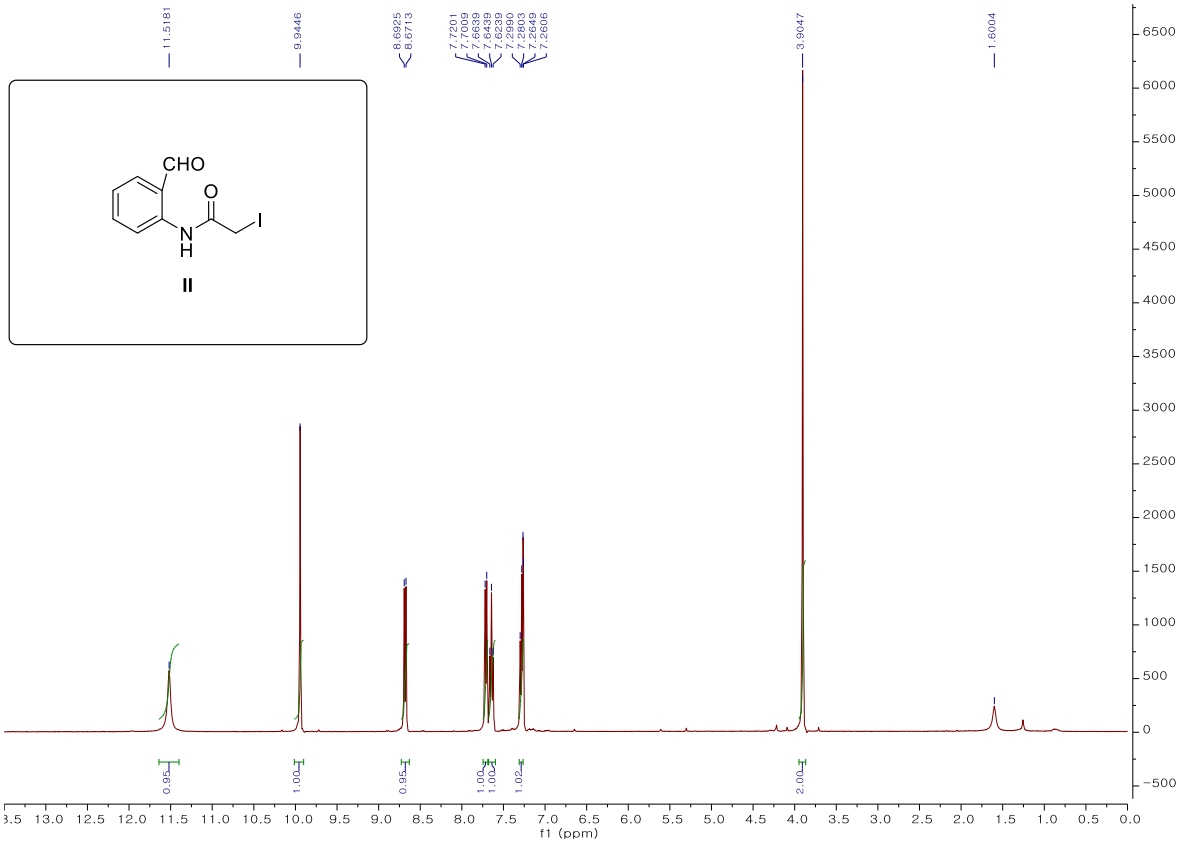
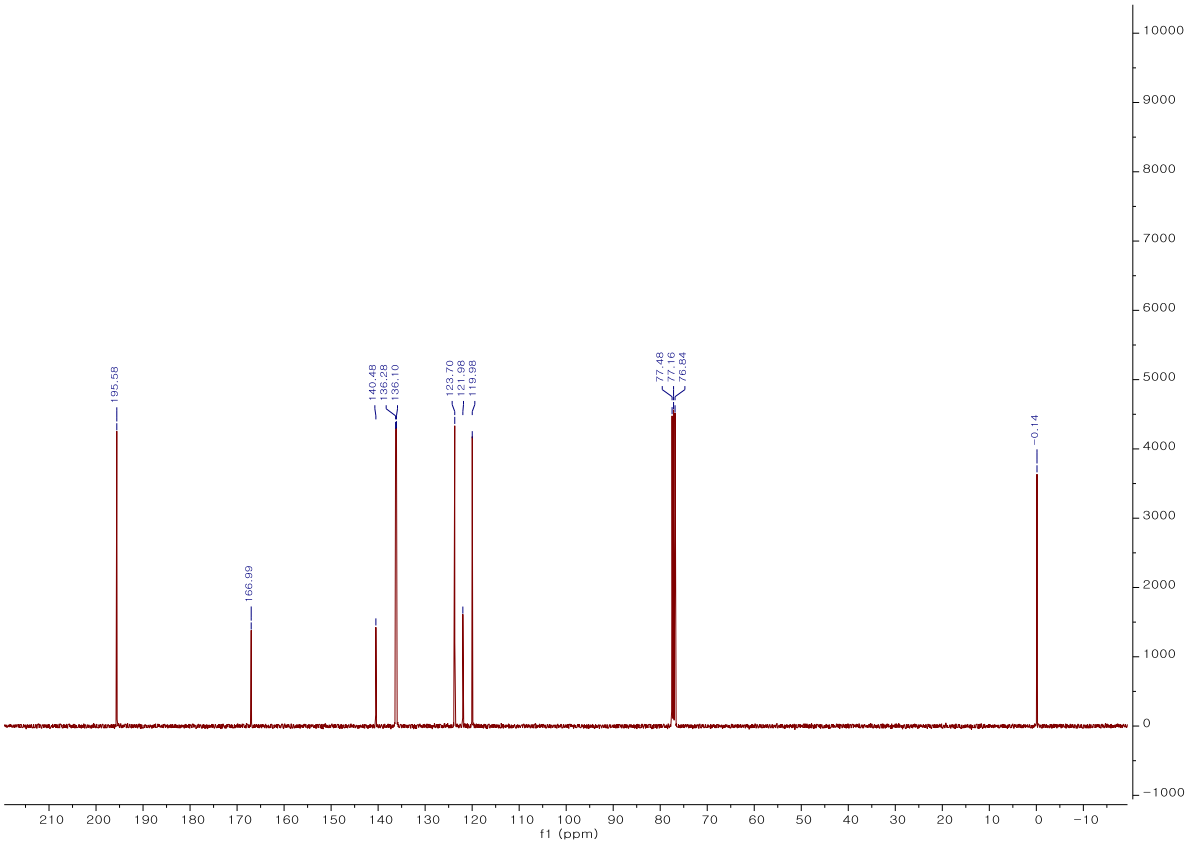
7.6510
7.6313
7.5473
7.5279
7.5087
7.3156
7.2964
7.2024
7.1836
7.1647
3.3258
2.5063
2.5012
2.4969
2.4917
I
N
H
O
13
f1 (ppm)


158.81
148.76
138.83
130.79
126.96
122.06
120.34
115.19
95.87
40.15
39.94
39.20
39.10
38.89
f1 (ppm)


11.5181
9.9446
8.6925
8.6713
7.7201
7.7009
7.6639
7.6439
7.6089
7.2980
7.2803
7.2649
7.2606
3.9047
1.6004
CHO
O
N
H
I
II
f1 (ppm)


195.58
166.99
140.48
136.28
136.10
123.70
121.98
119.98
77.48
77.16
76.84
-0.14
f1 (ppm)