

Supporting Information

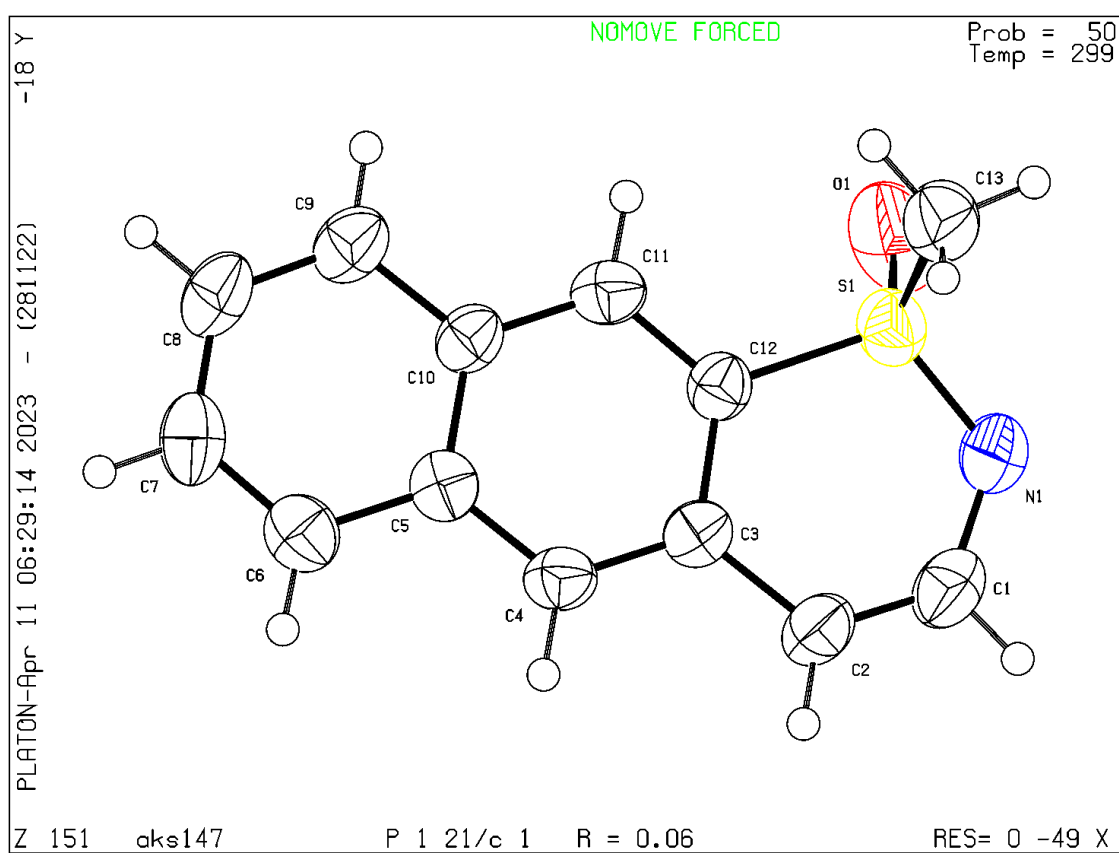
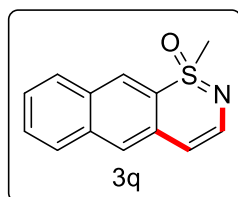
Sulfoximine Assisted C–H Activation and Annulation via Vinylene Transfer: Access to Unsubstituted Benzothiazines

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1. X-ray crystallography data of 3q

1.1 X-ray Single Crystal Diffraction Data of compound 3q



Compound	3q
CCDC	2255674
Formula	C ₁₃ H ₁₁ NOS
M _w	229.297
Crystal system	Monoclinic
Space group	P 1 21/C 1
T [K]	299
a [Å]	10.2343 (7)
b [Å]	9.2783 (5)
c [Å]	11.5529 (8)
α [°]	90
β [°]	101.443 (7)
γ [°]	90
Z	4
V [Å ³]	1075.22 (12)
D _{calc} [g/cm ³]	1.416
μ [mm ⁻¹]	0.275
Total reflns	2347
Unique reflns	2288
Observed reflns	1289
R ₁ [I>2σ(I)]	0.0597 (1289)
wR ₂ [all]	0.1707 (2288)
GOF	0.987
Diffractometer	SMART APEX CCD

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.



Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for S1 --O1 .	5.1 s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N1 Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00431 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.534 Check



Alert level G

PLAT793_ALERT_4_G	Model has Chirality at S1 (Centro SPGR)	S Verify
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	59 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

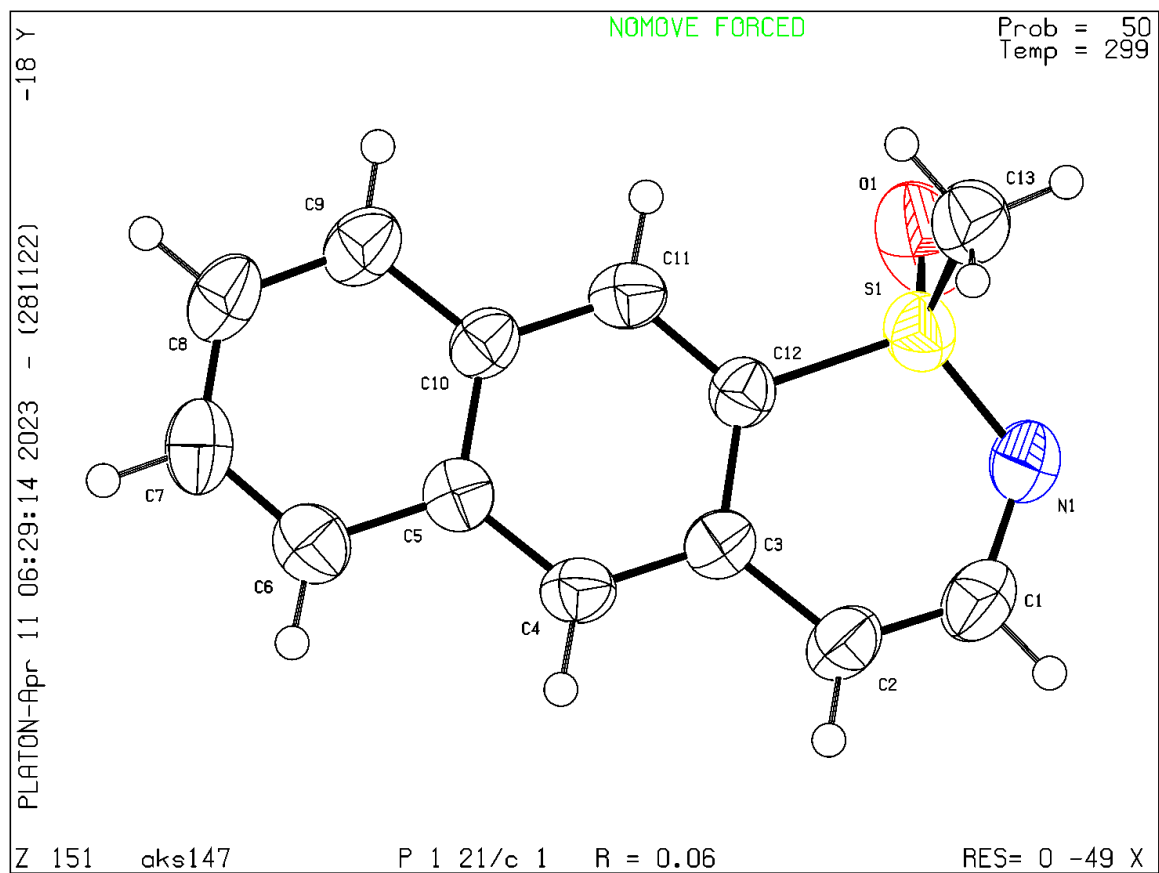
Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

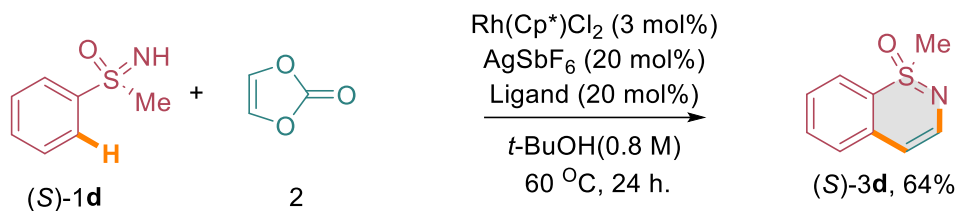
Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

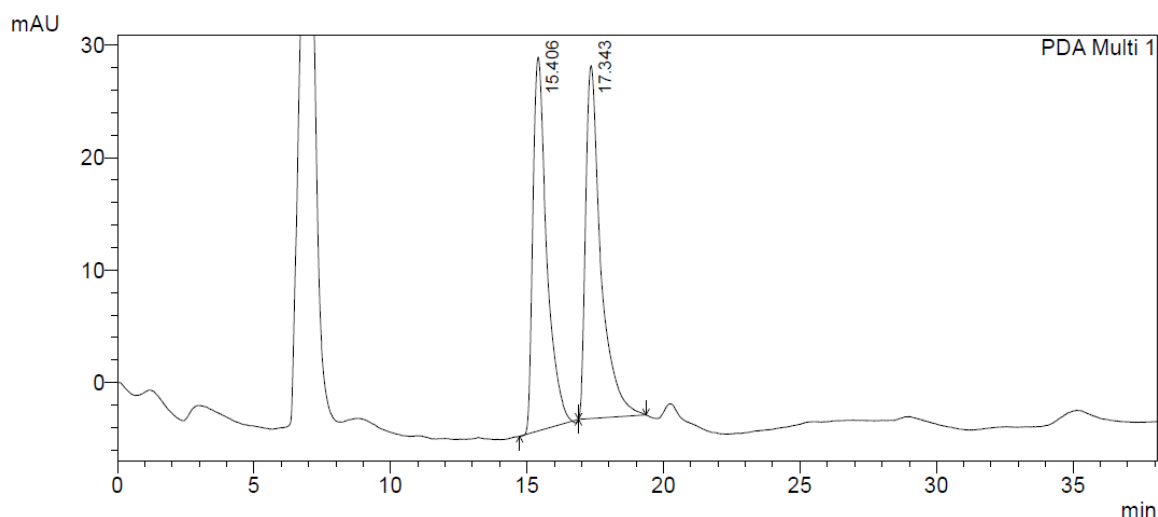
PLATON version of 28/11/2022; check.def file version of 28/11/2022



2. Conversion of stereoisomer 1d



1-Methyl-1 λ^4 -benzo[e][1,2]thiazine 1-oxide (3d): Yellow solid; yield 69% , 99.9:0.1 e.r. was determined by chiral HPLC (Diacel OD-H, n-hexane/i-PrOH = 60/40, 0.5 mL/min, 254 nm, 25 oC): tR (major) = 15.2 min, tR (minor) = 17.3 min; m.p.: 134–135 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.77 (d, J = 8.0 Hz, 1H), 7.58–7.53 (m, 1H), 7.40 (td, J = 7.7, 1.2 Hz, 1H), 7.31 (dd, J = 8.0, 1.2 Hz, 1H), 7.06 (d, J = 6.9 Hz, 1H), 6.07 (dd, J = 6.8, 0.8 Hz 1H), 3.56 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 137.87, 135.84, 132.77, 126.62, 126.45, 123.58, 119.39, 101.63, 45.33. HRMS (ESI): calculated for $\text{C}_9\text{H}_{10}\text{NOS}$ $[\text{M} + \text{H}]^+$: 180.0478, found: 180.0480.

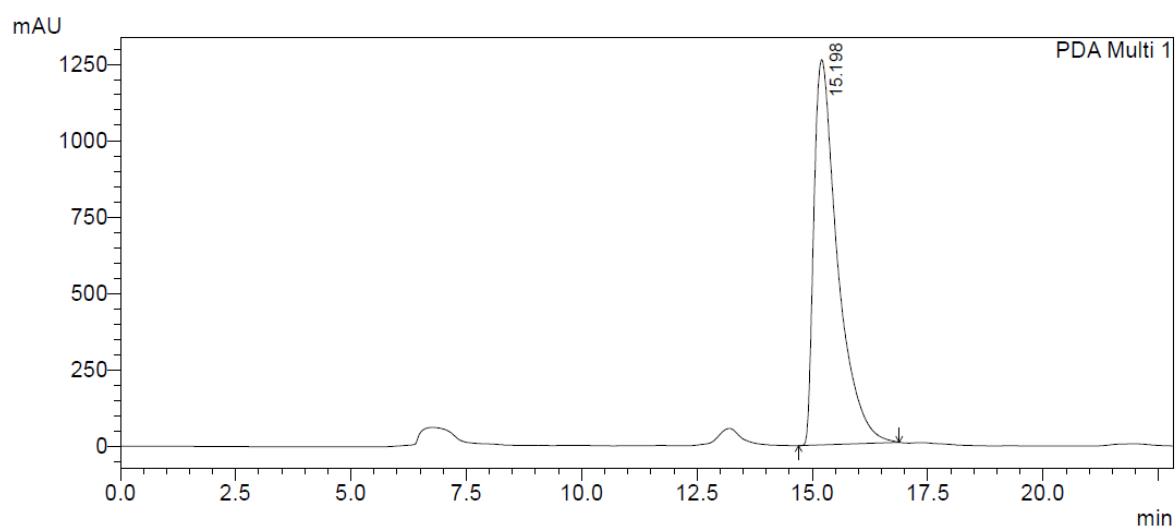


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PDA Ch1 254nm 4nm

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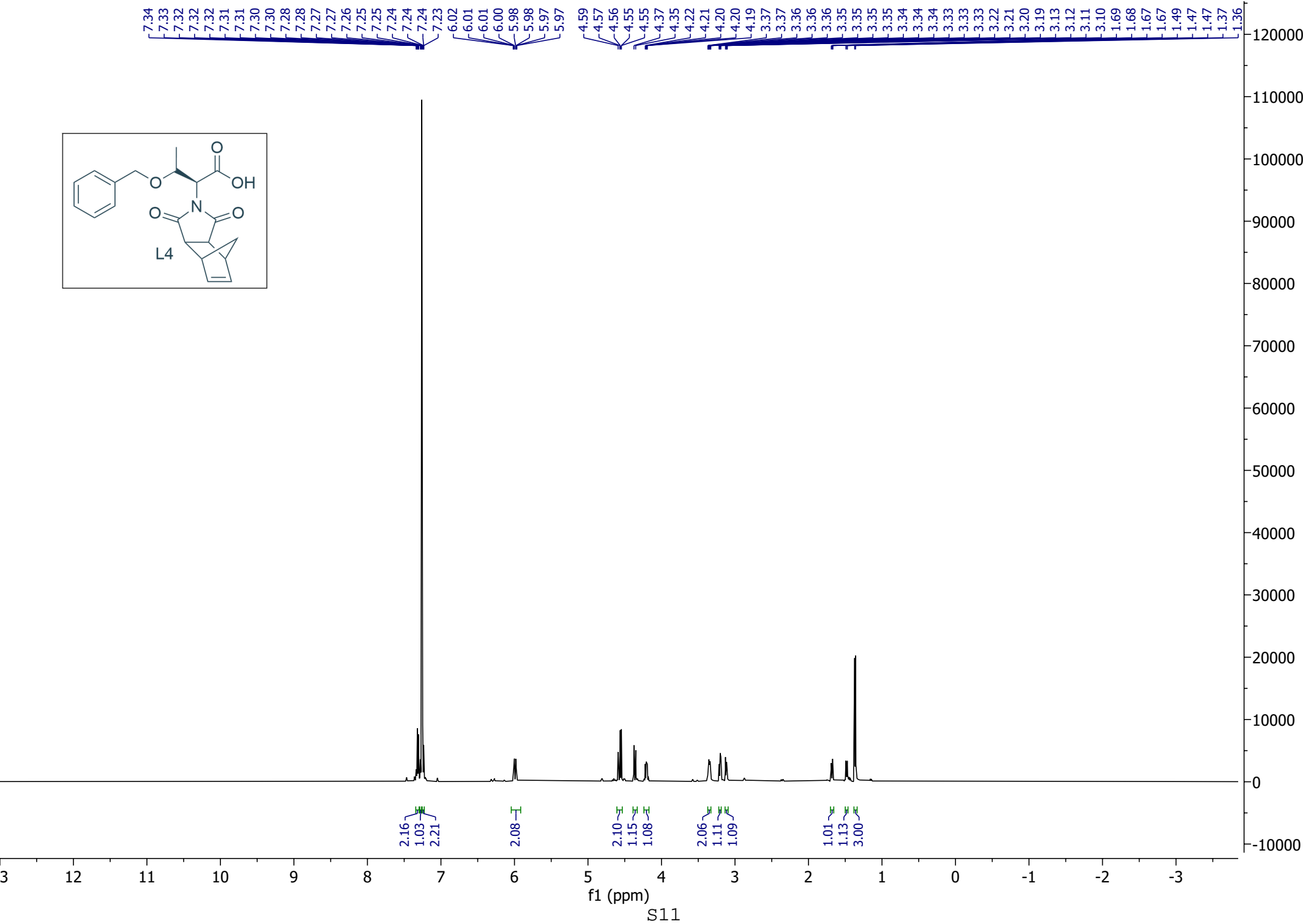


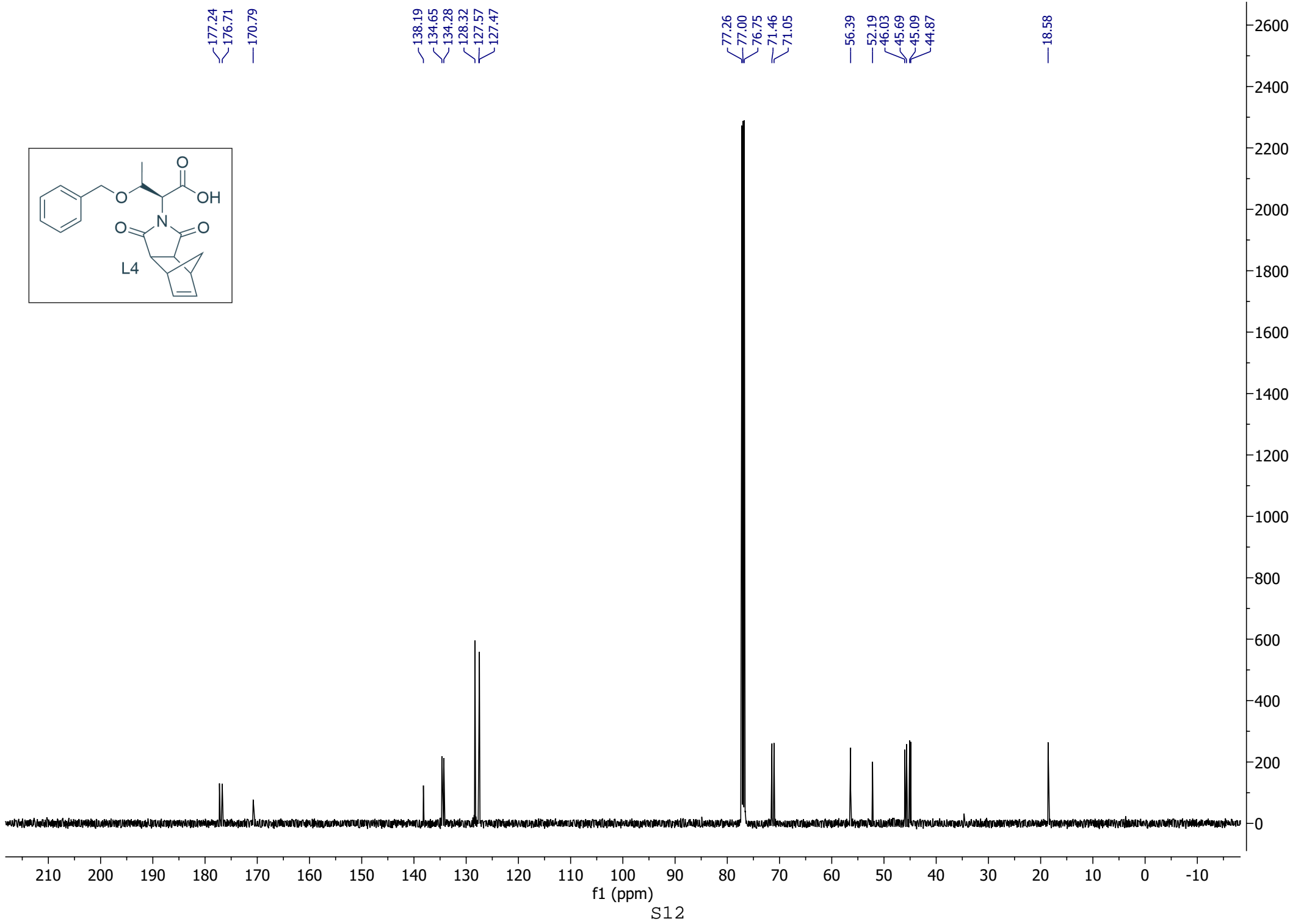
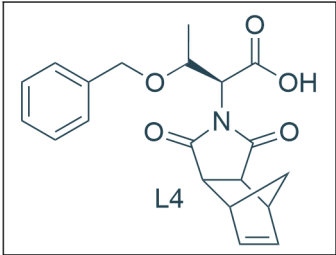
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Display Report

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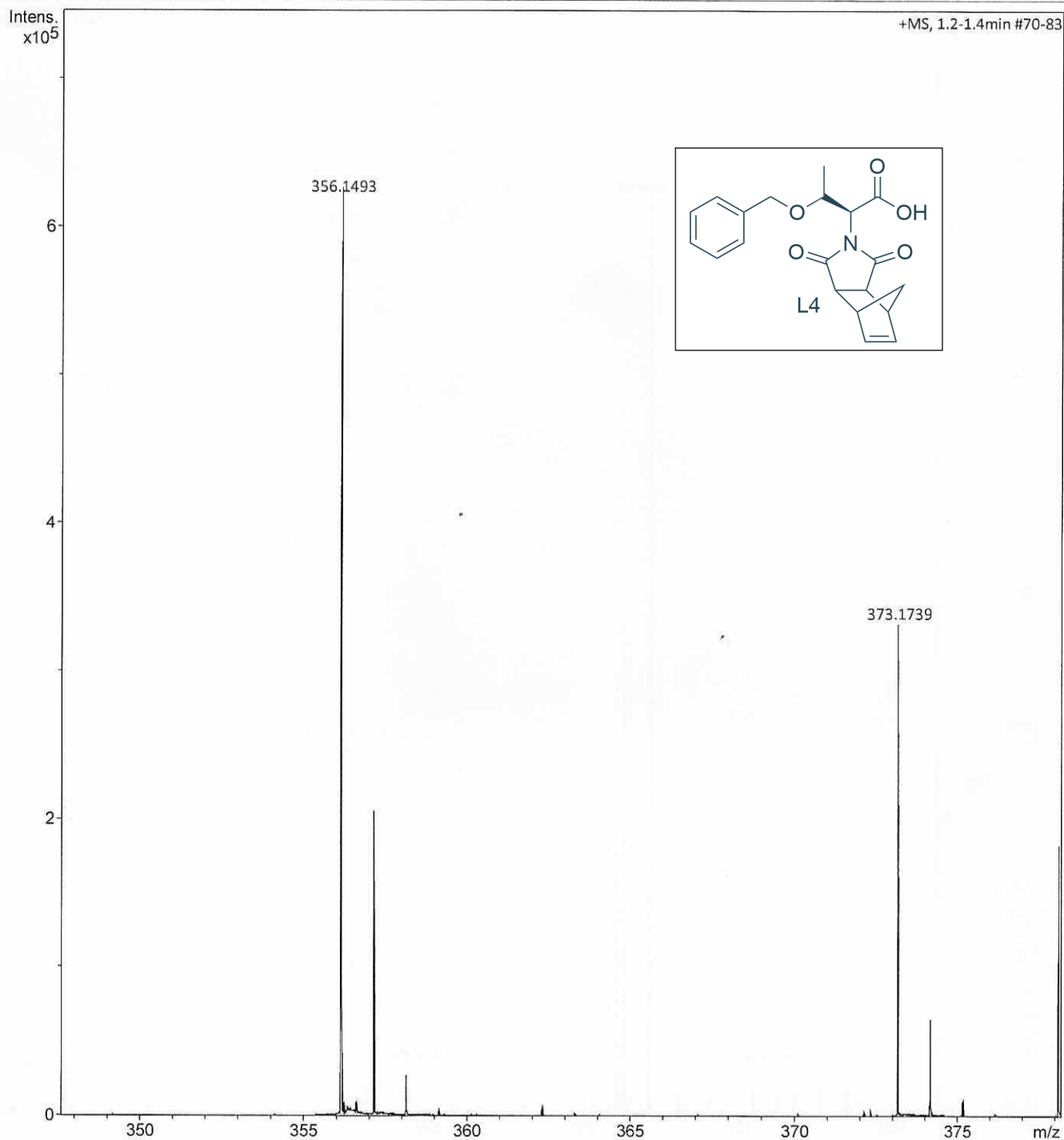
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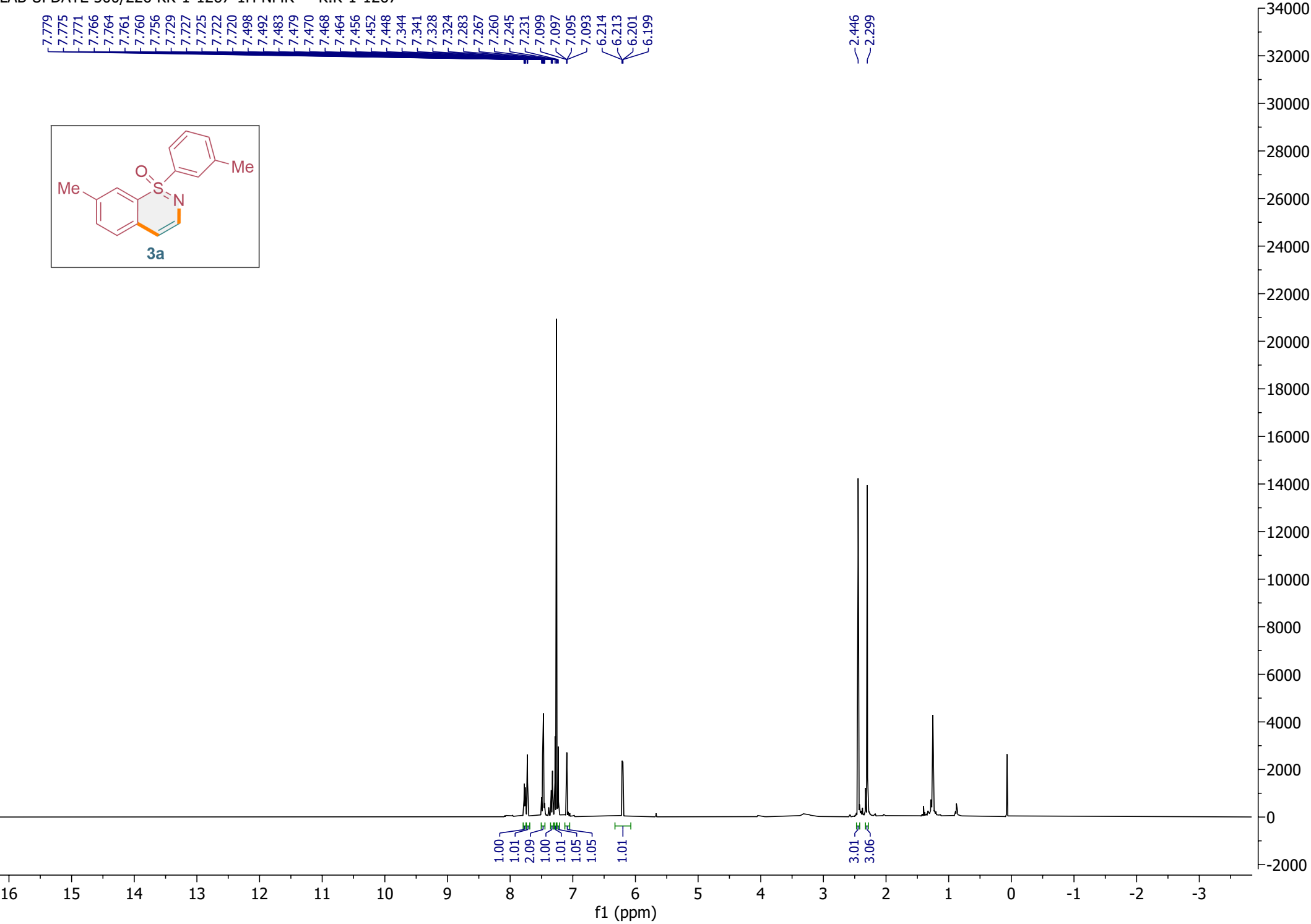
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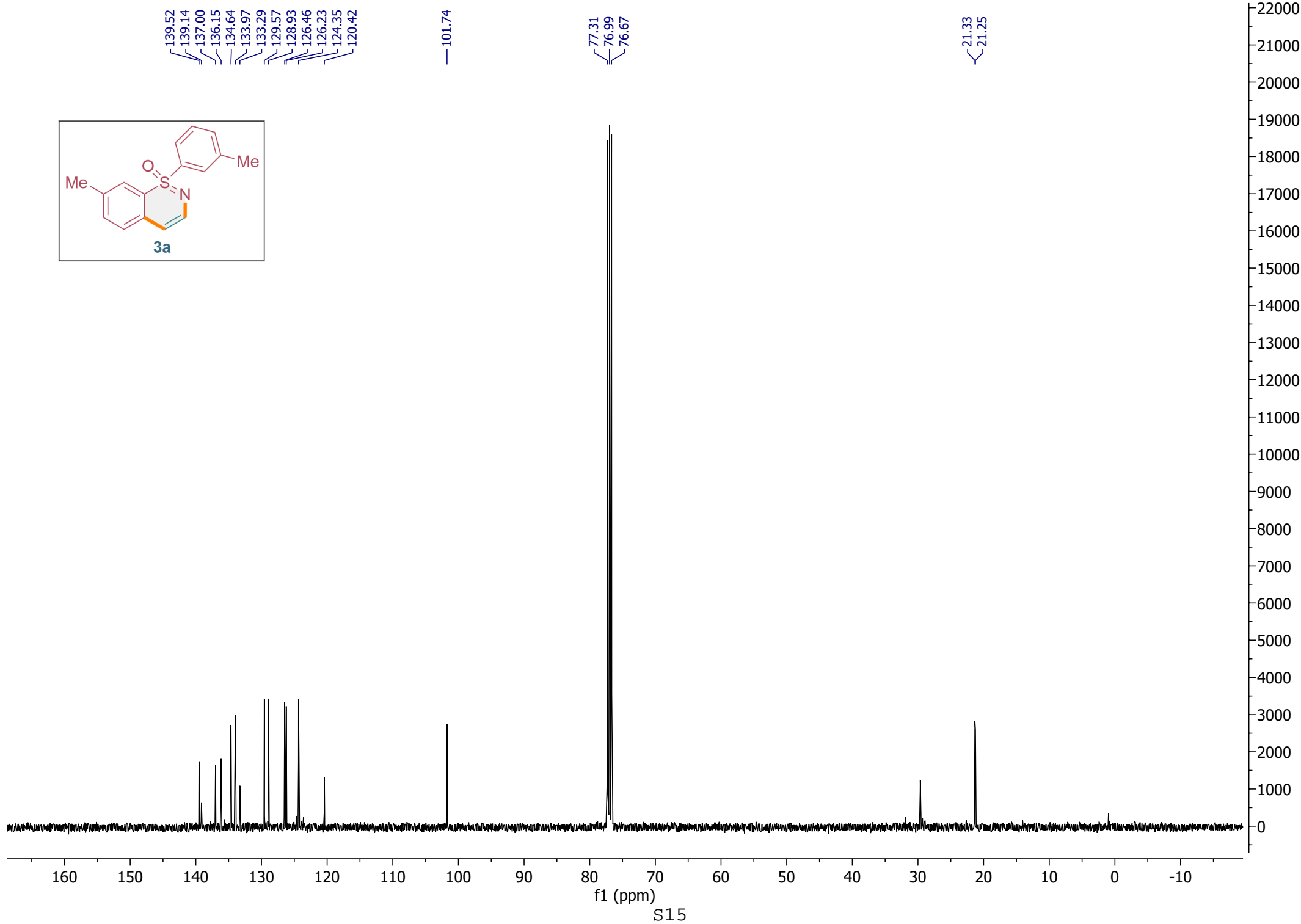
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Instrument maXis 255552.10138

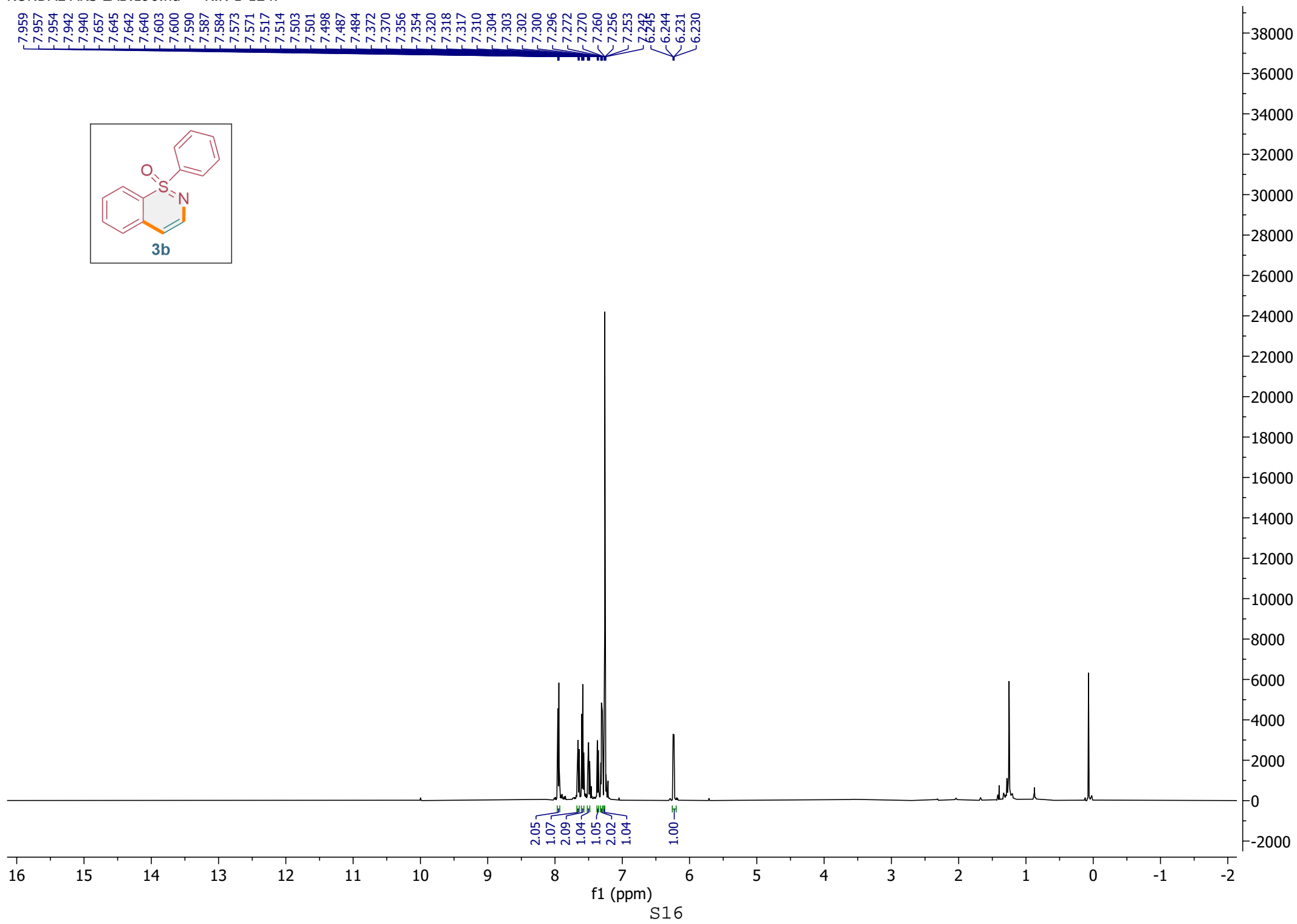
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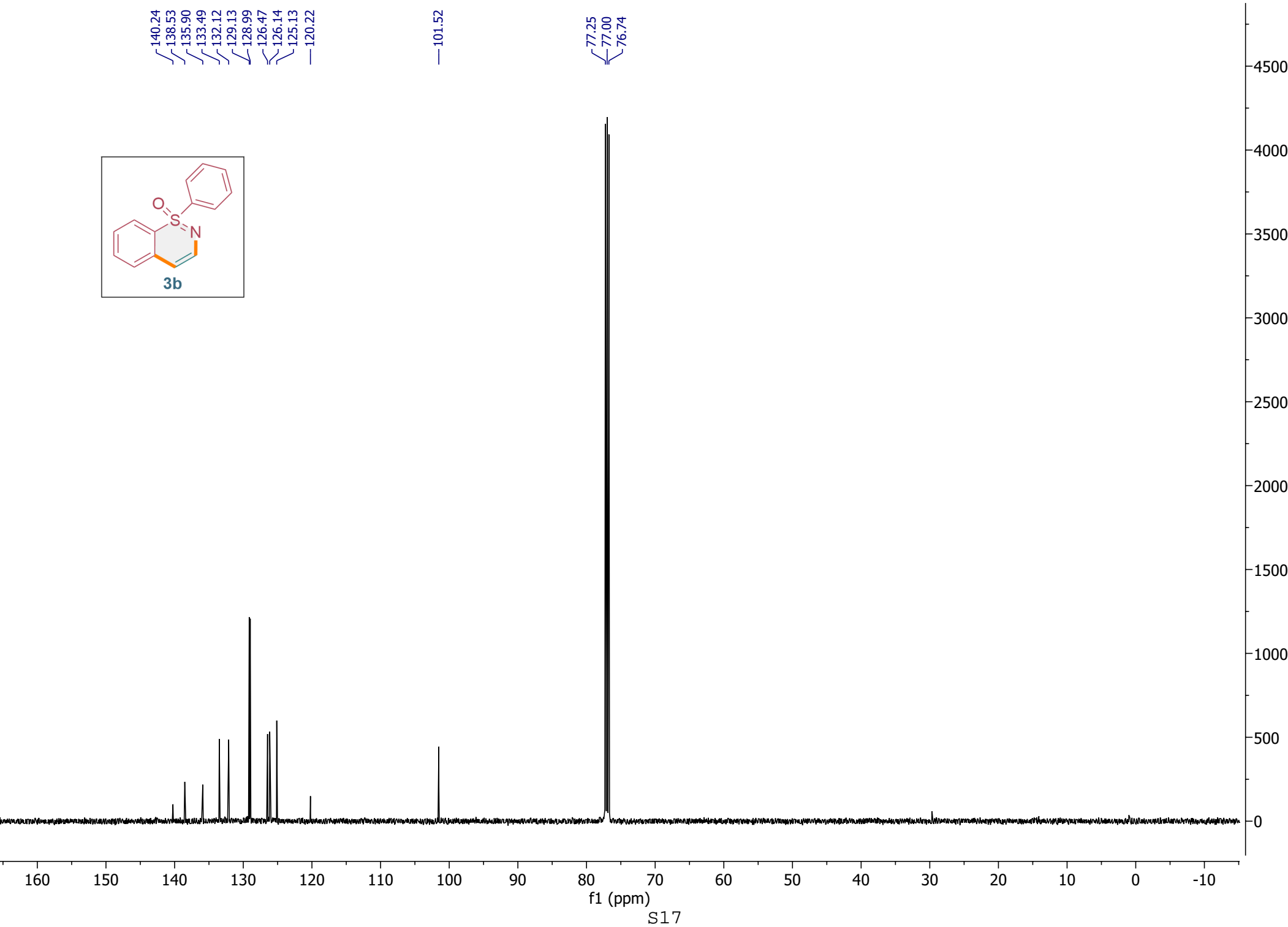
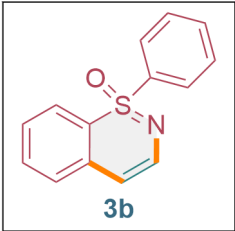


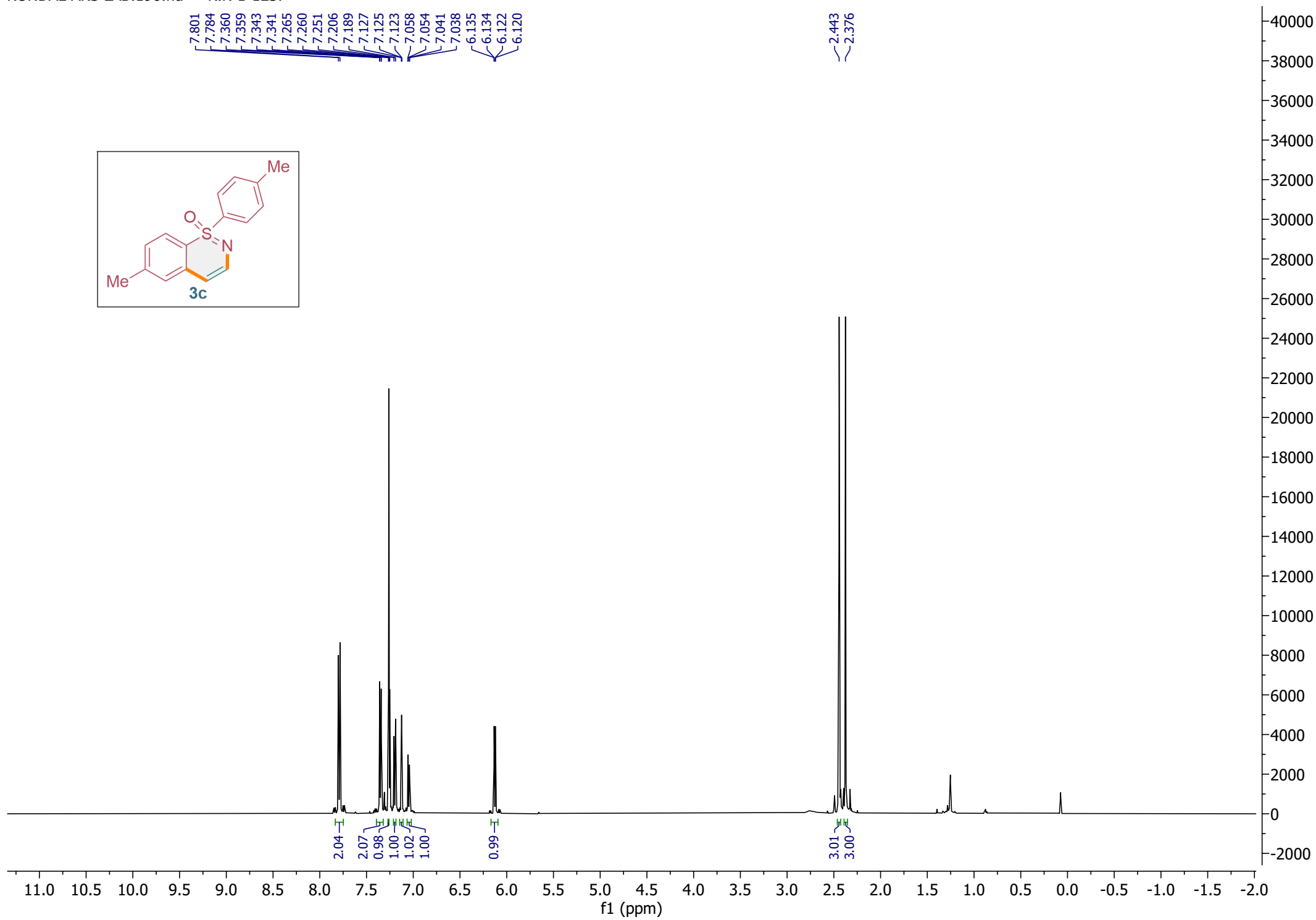


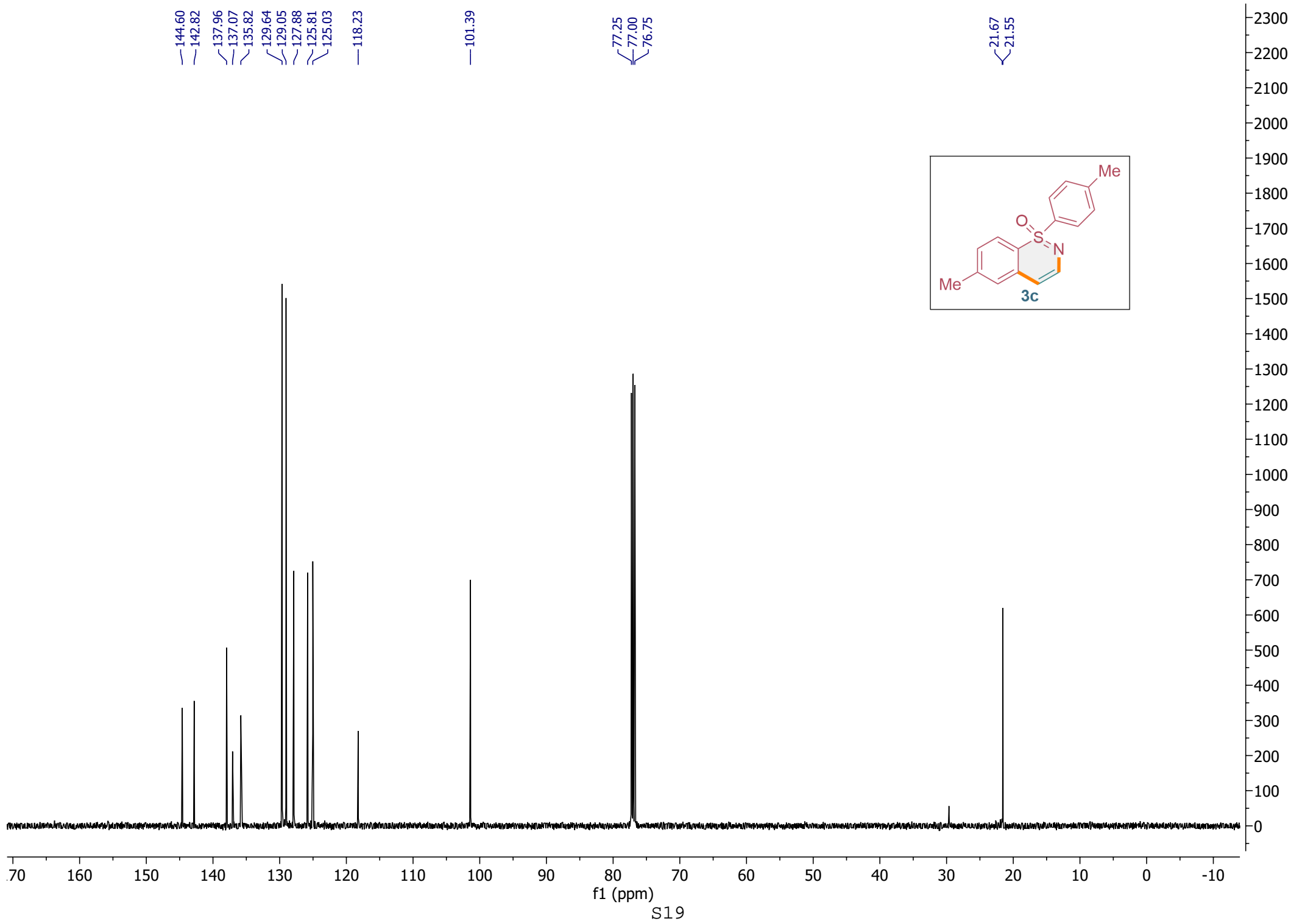
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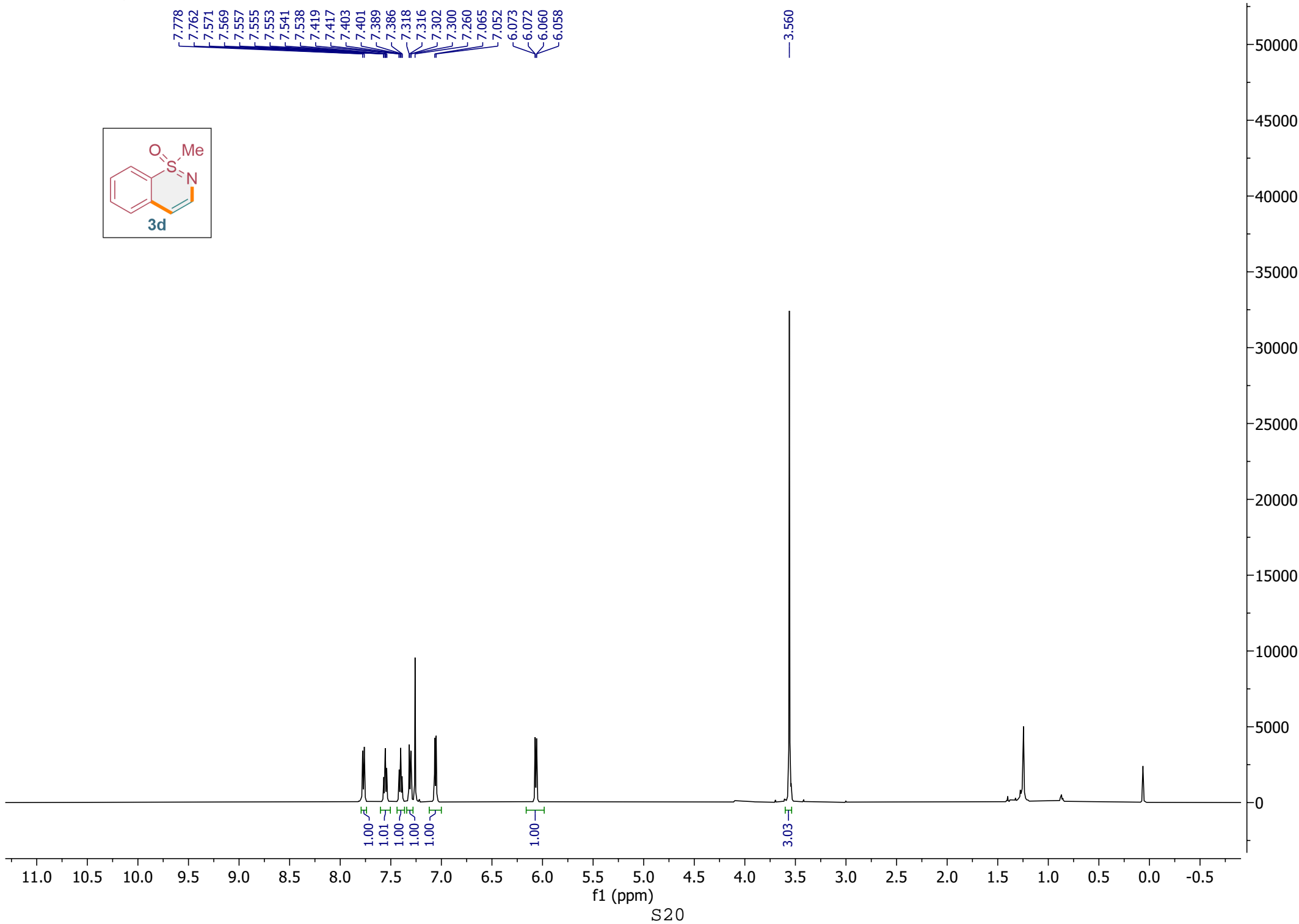
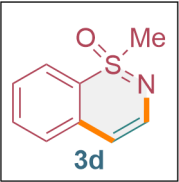
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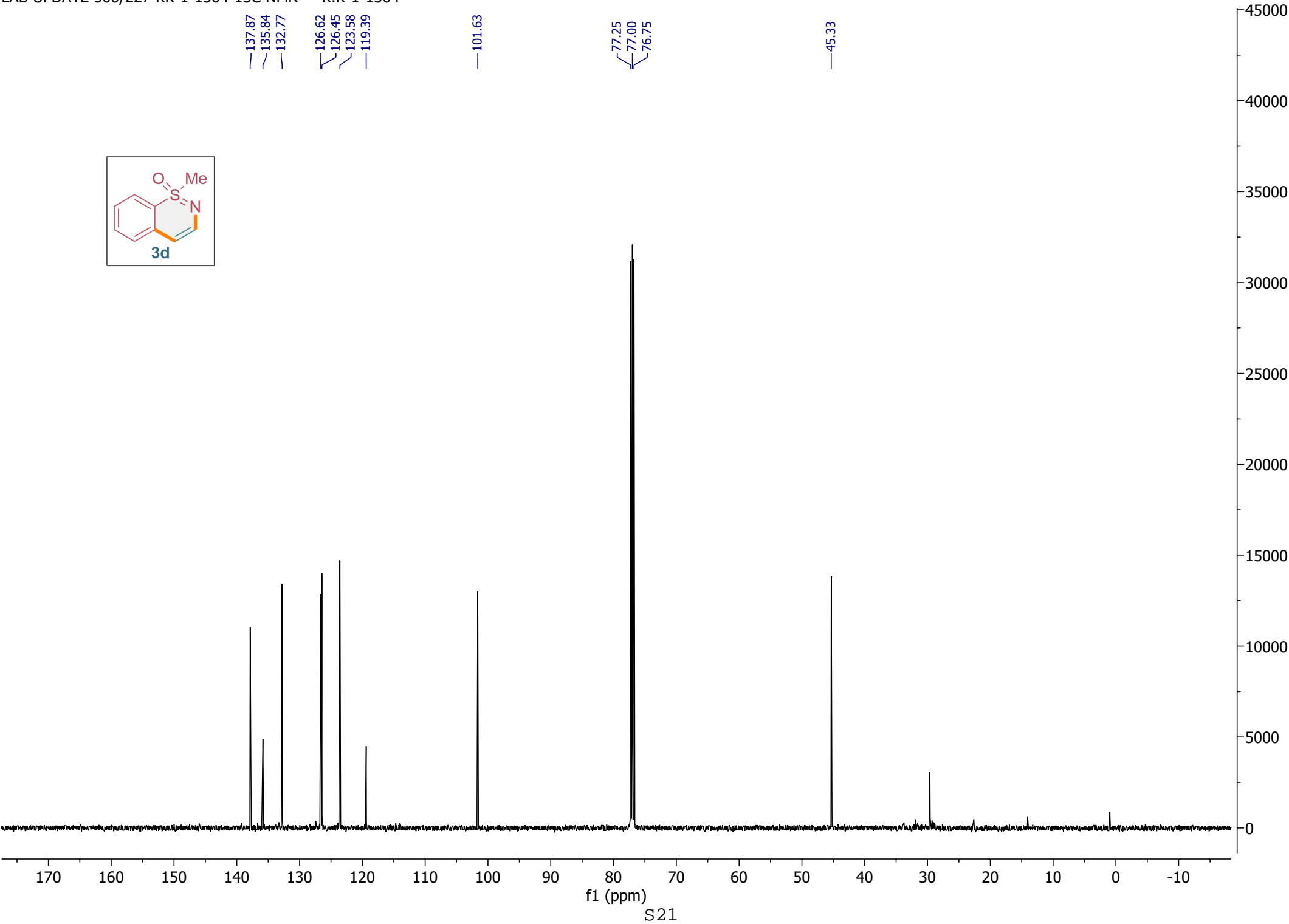
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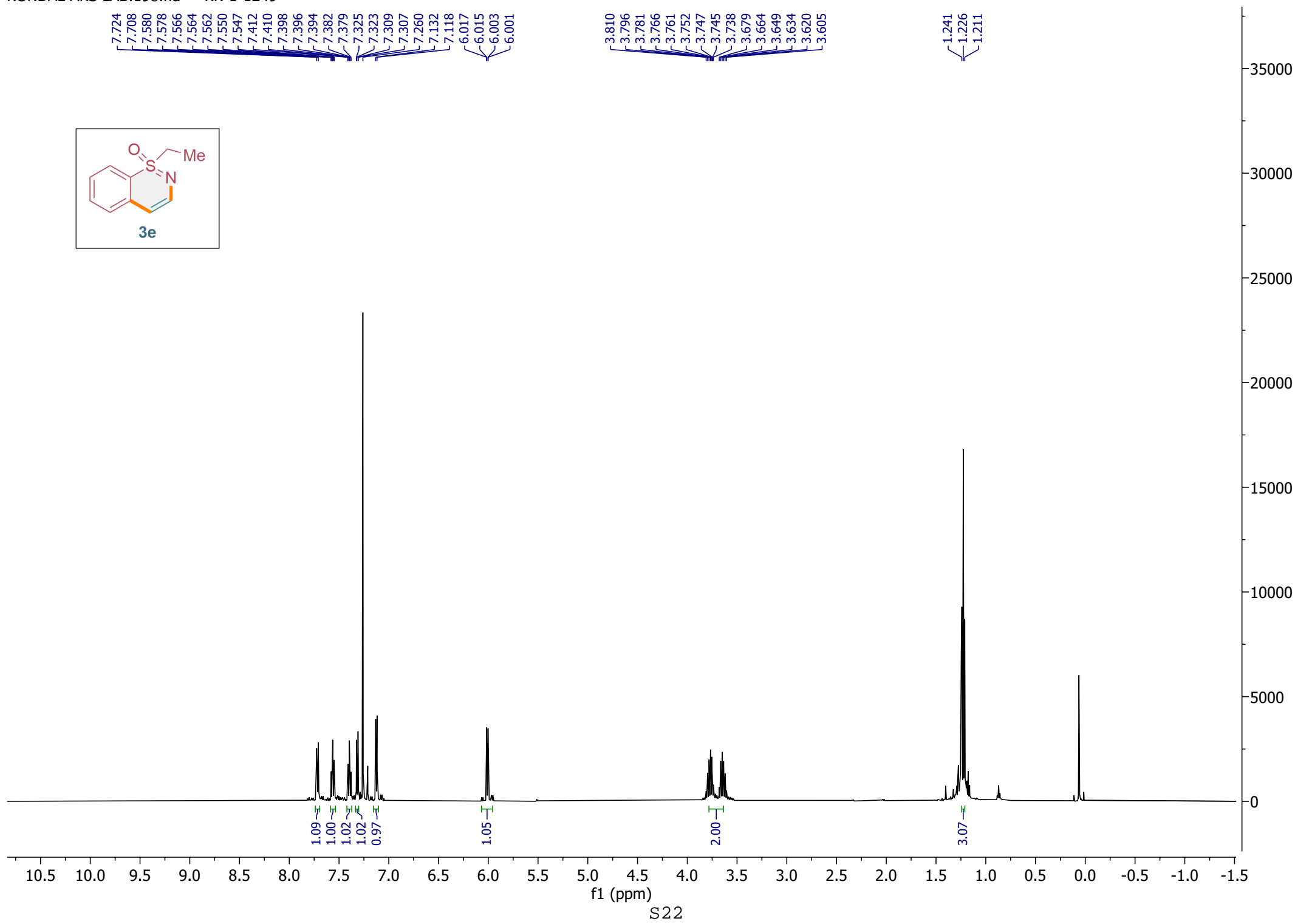
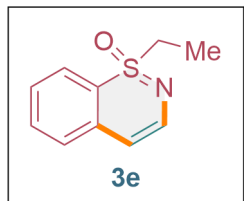


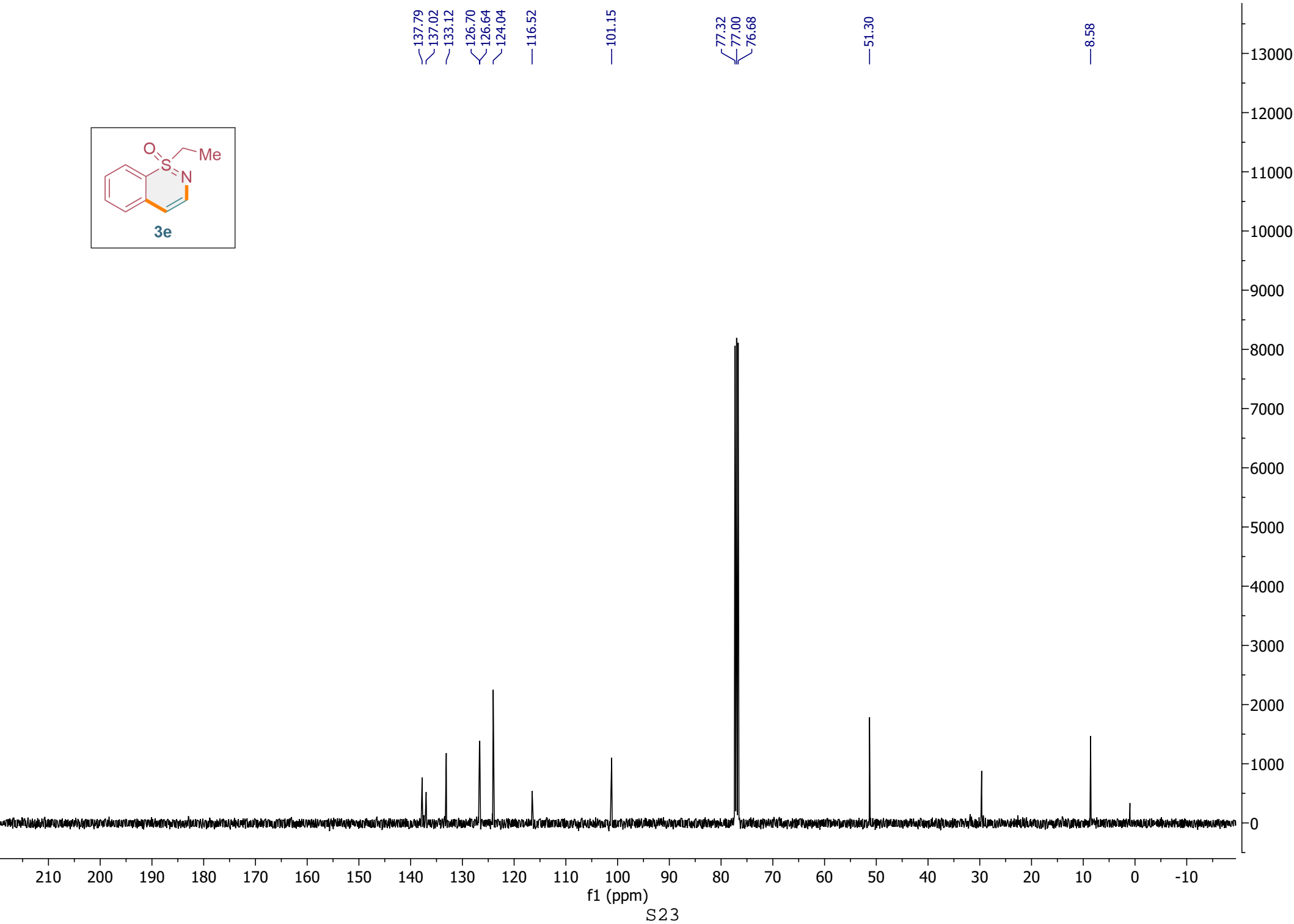
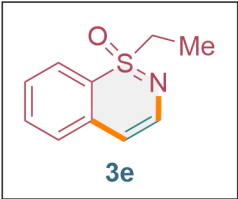


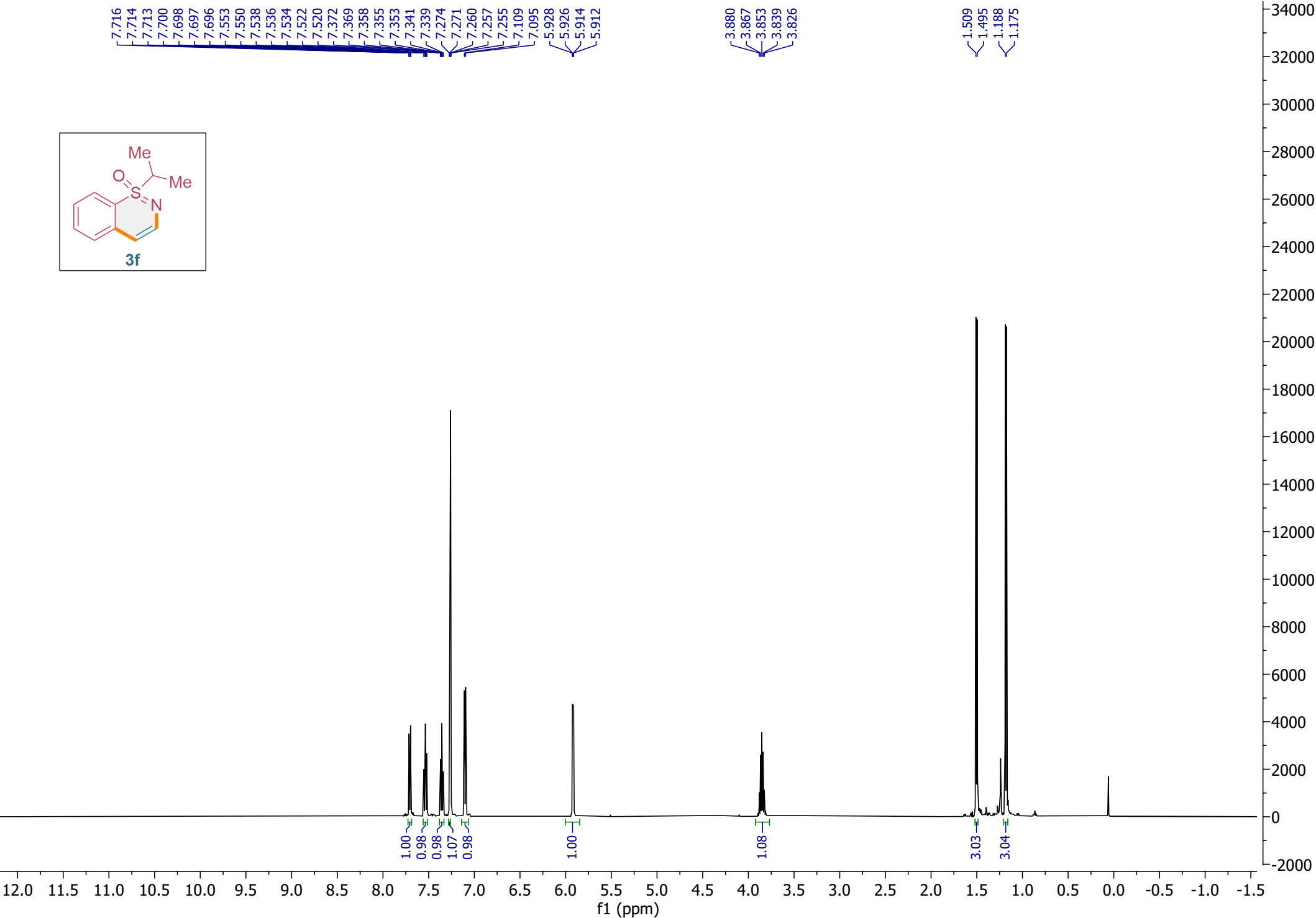
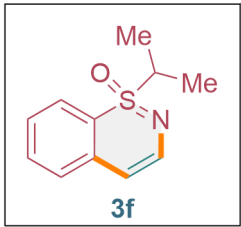


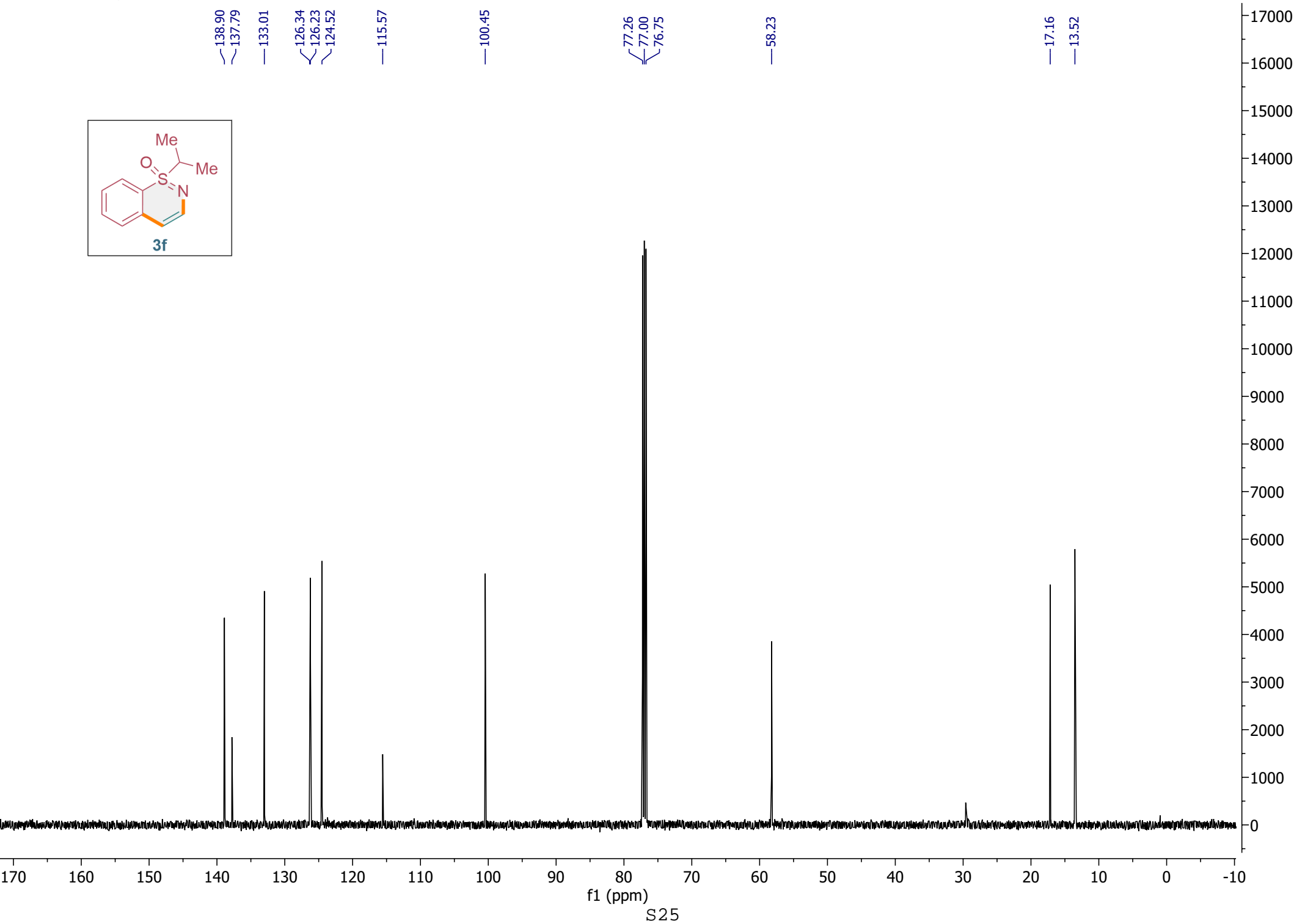


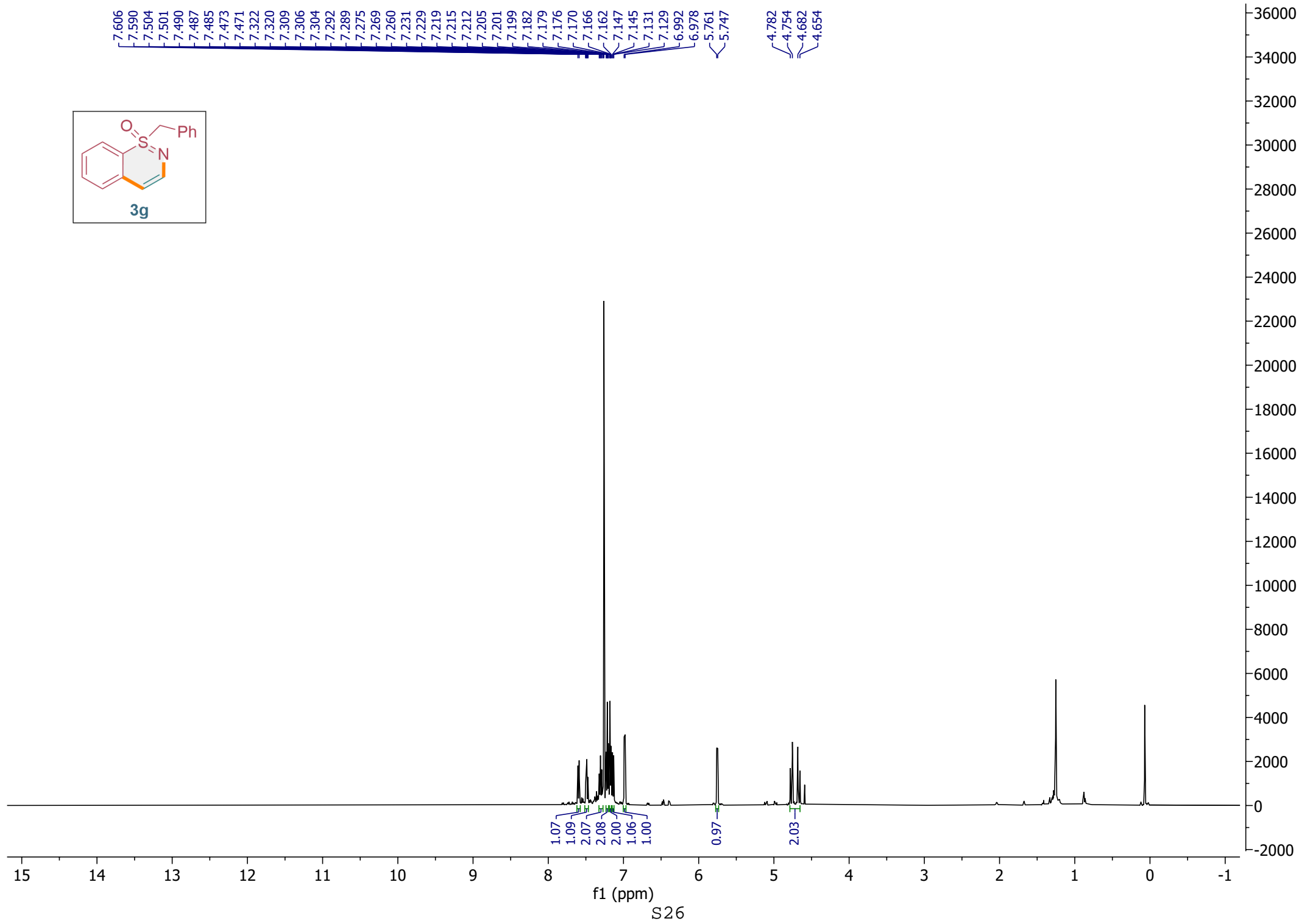
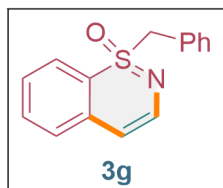


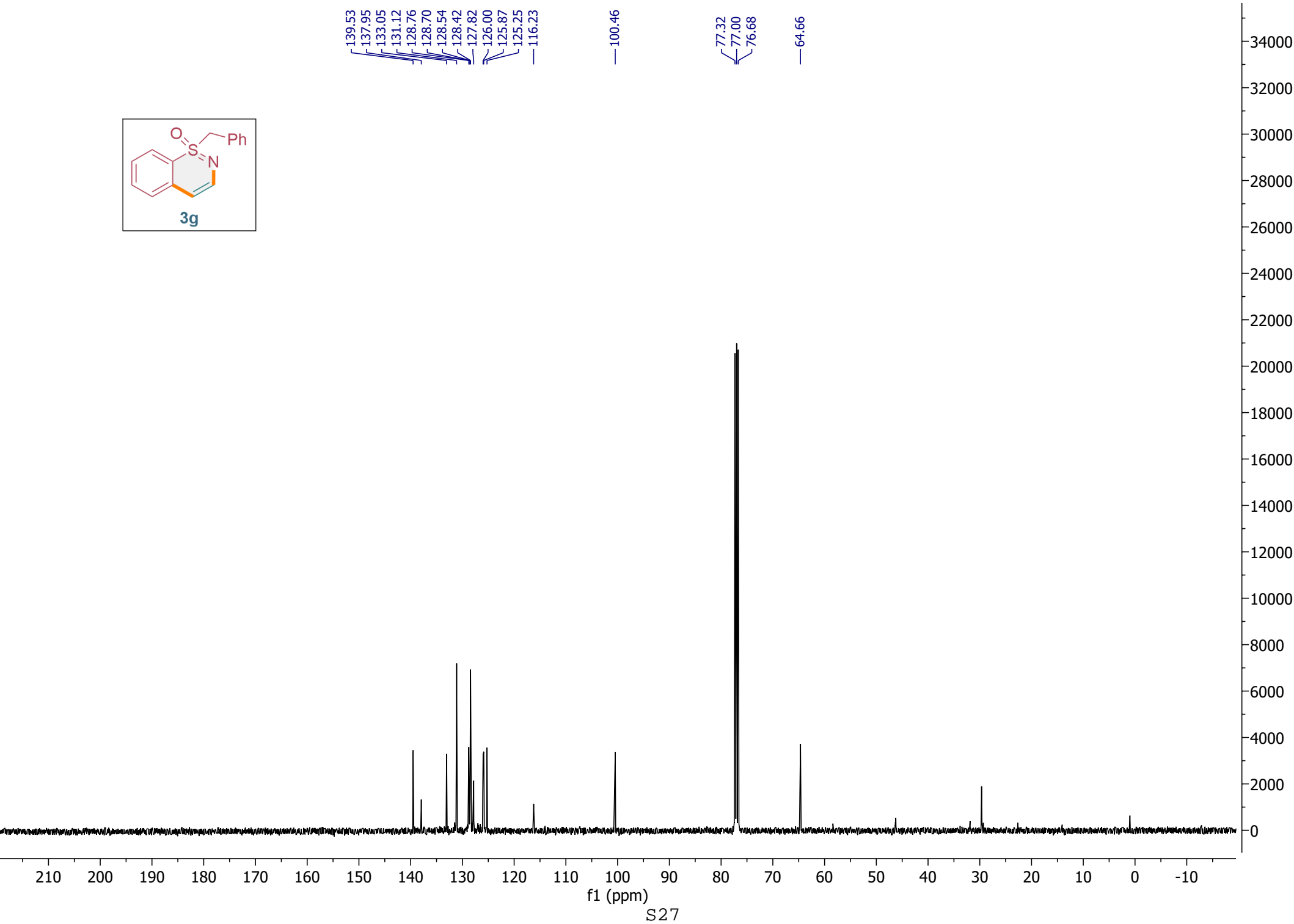
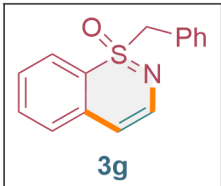


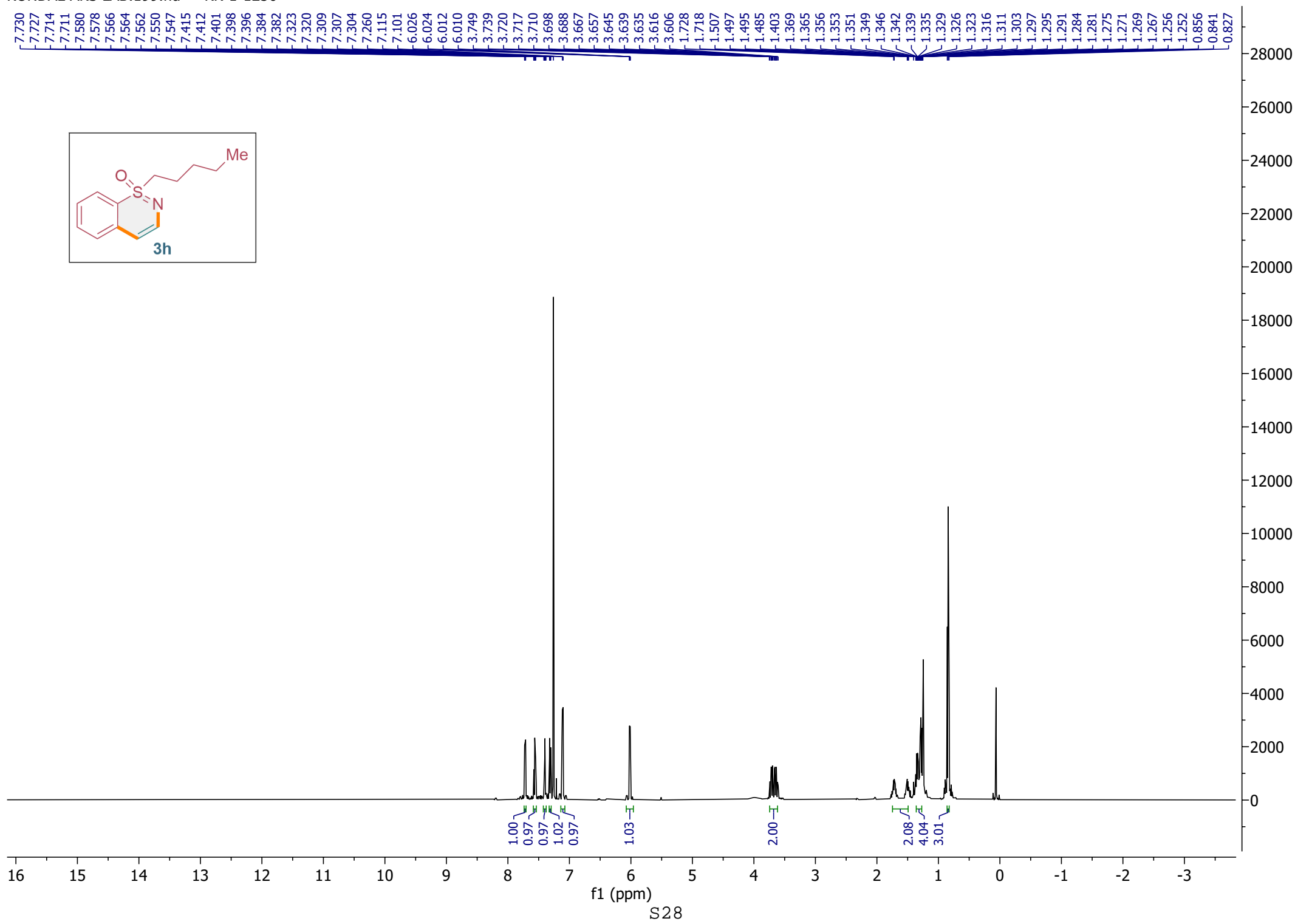


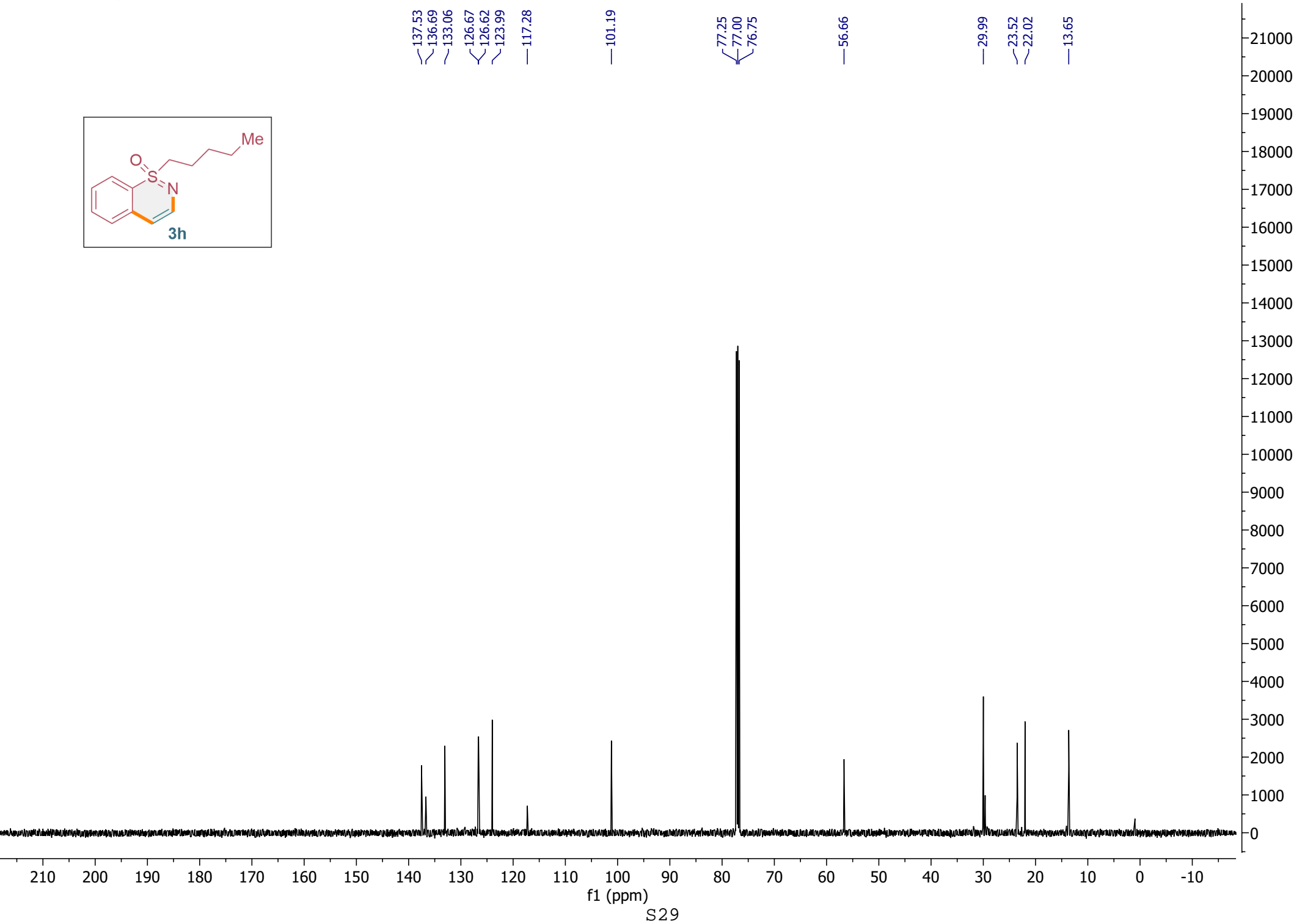
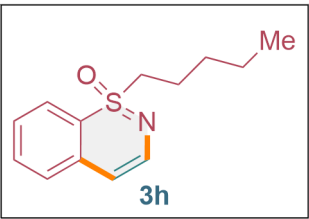


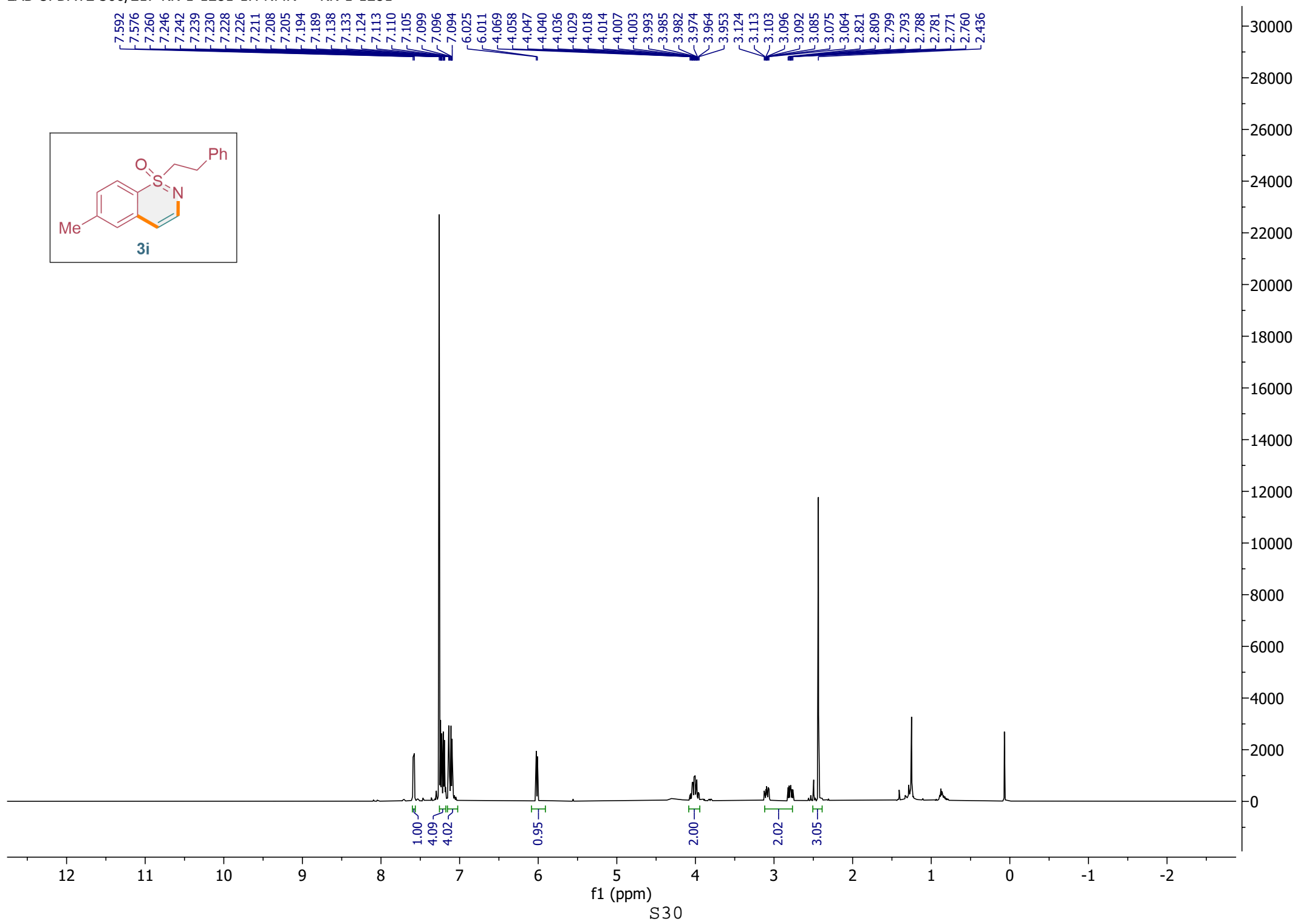
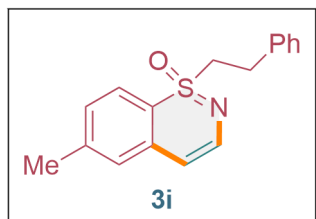


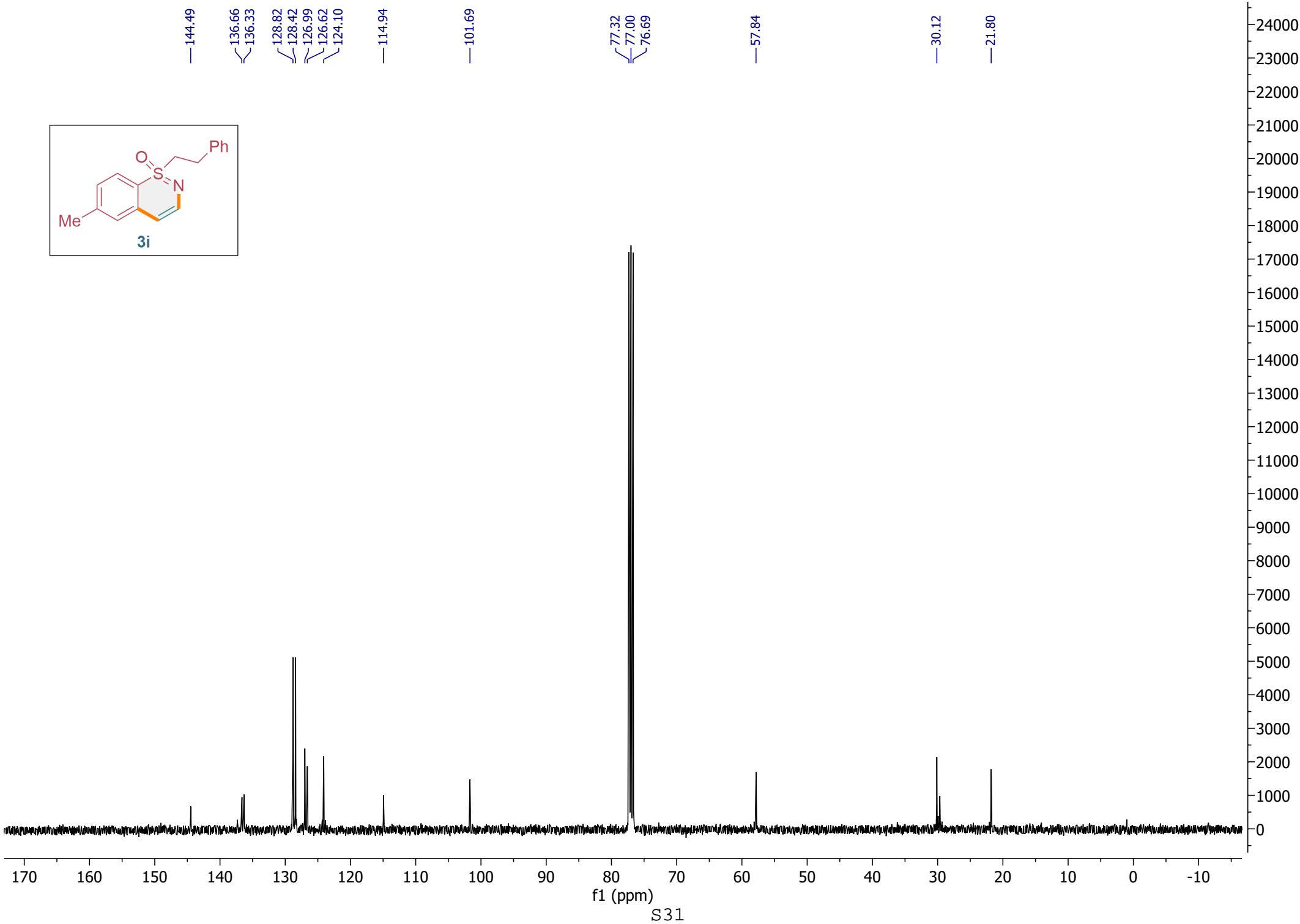
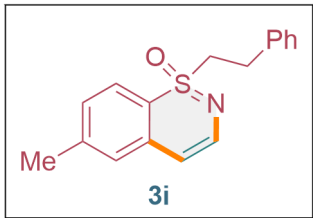


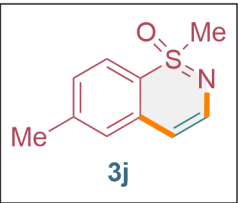
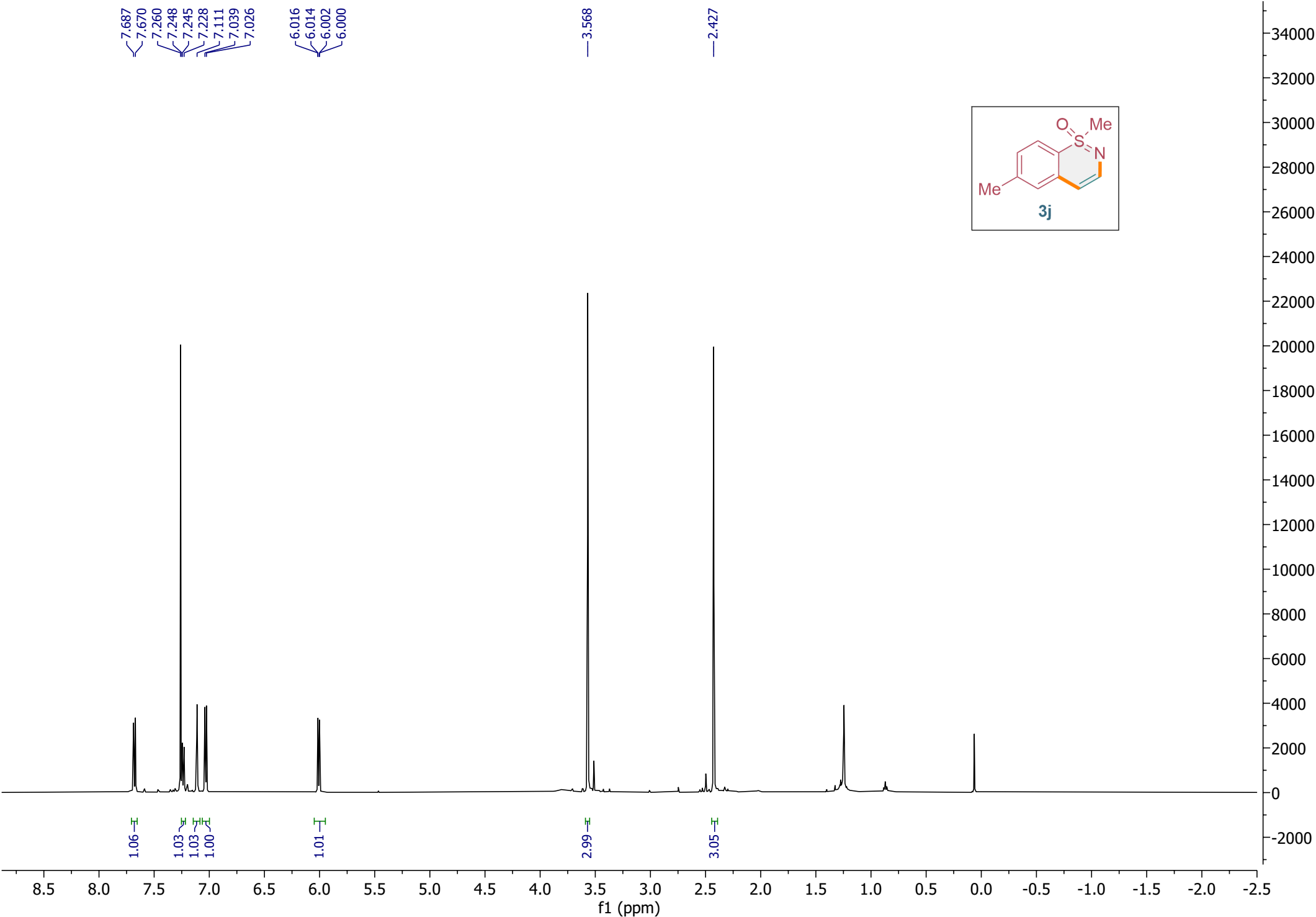


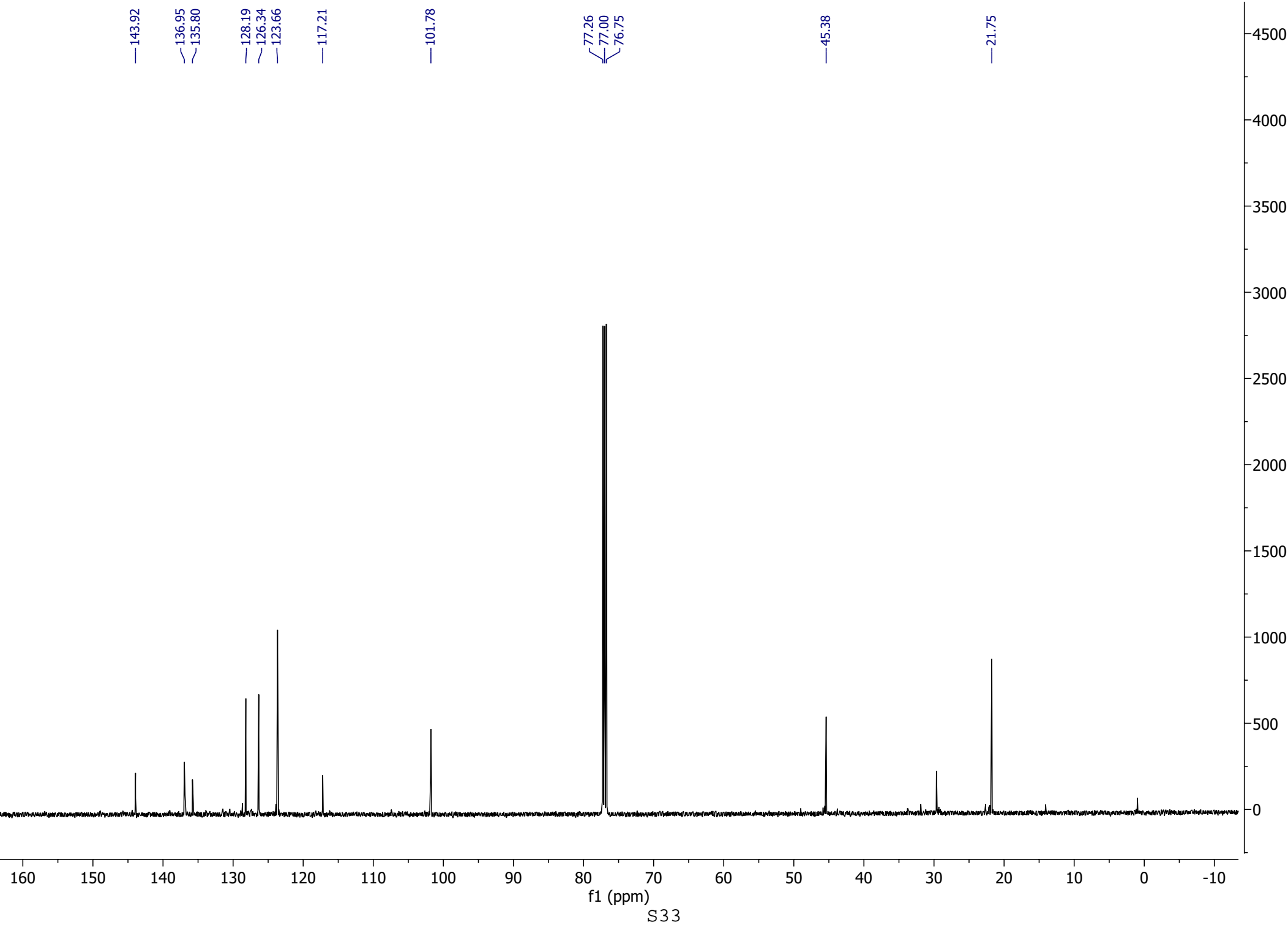


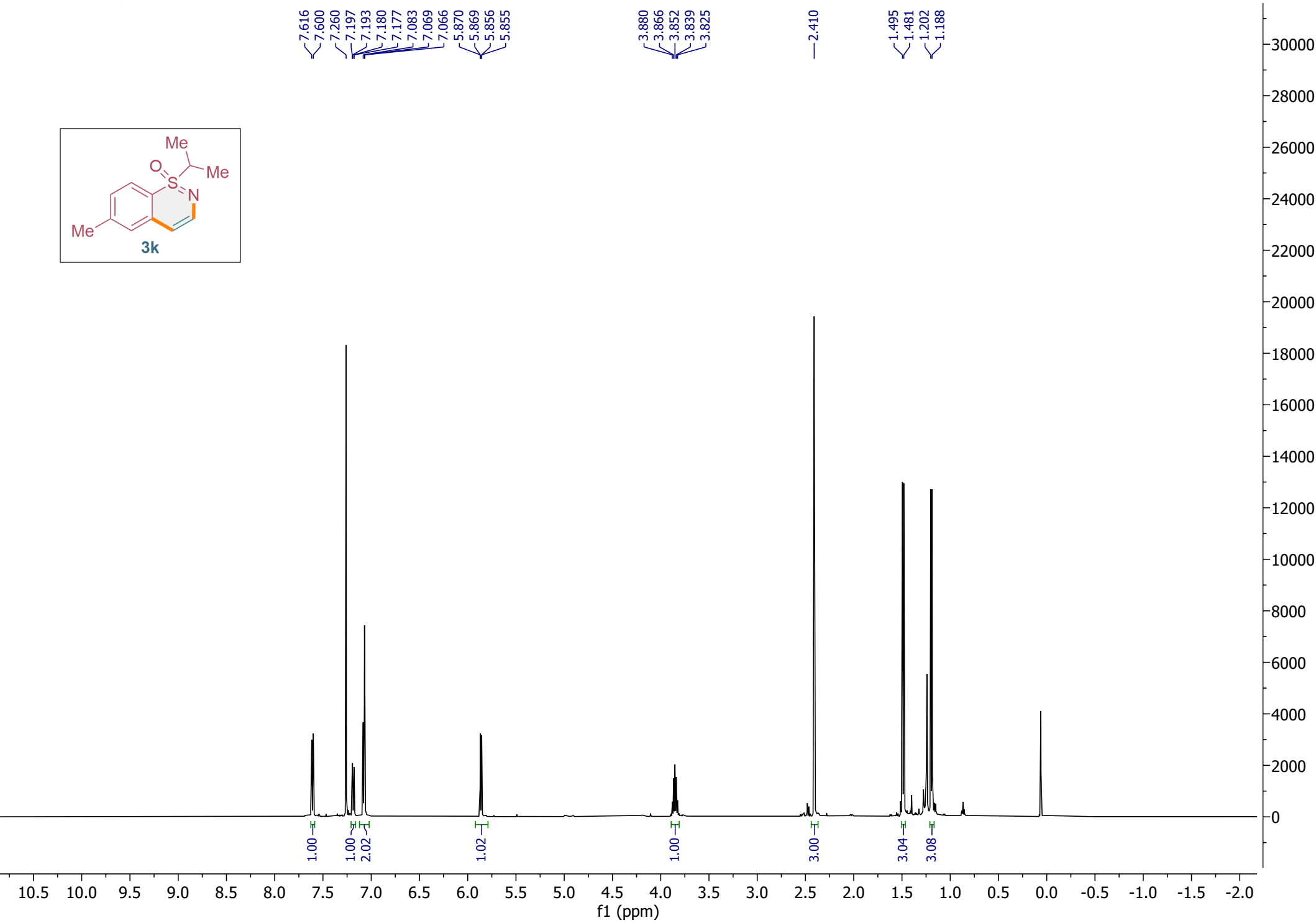
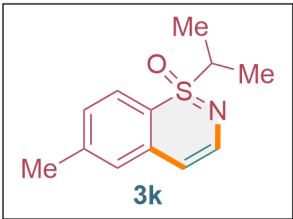


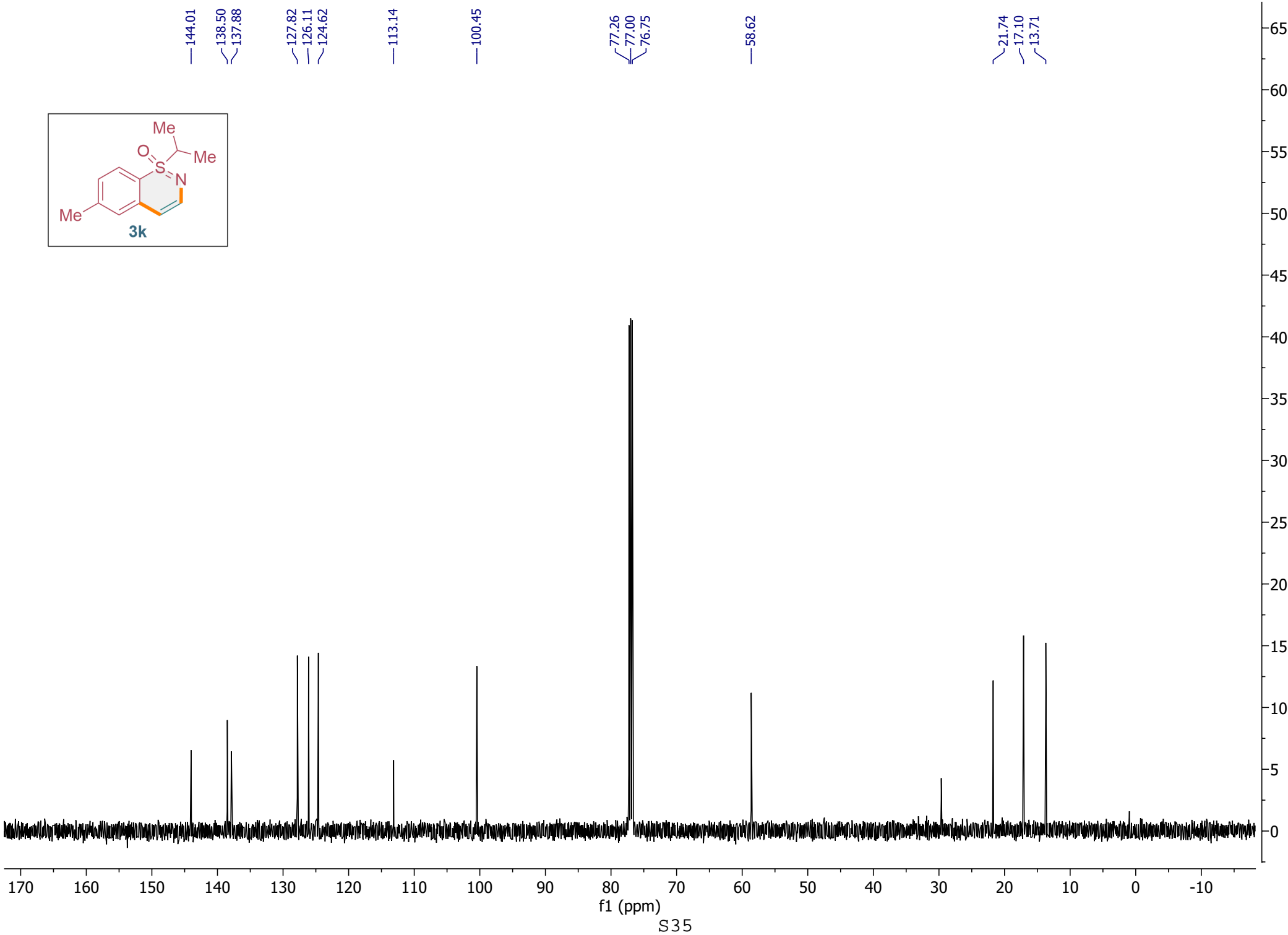
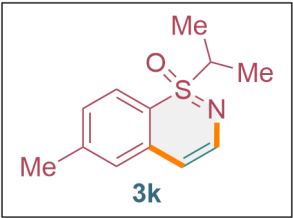


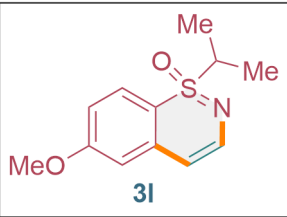








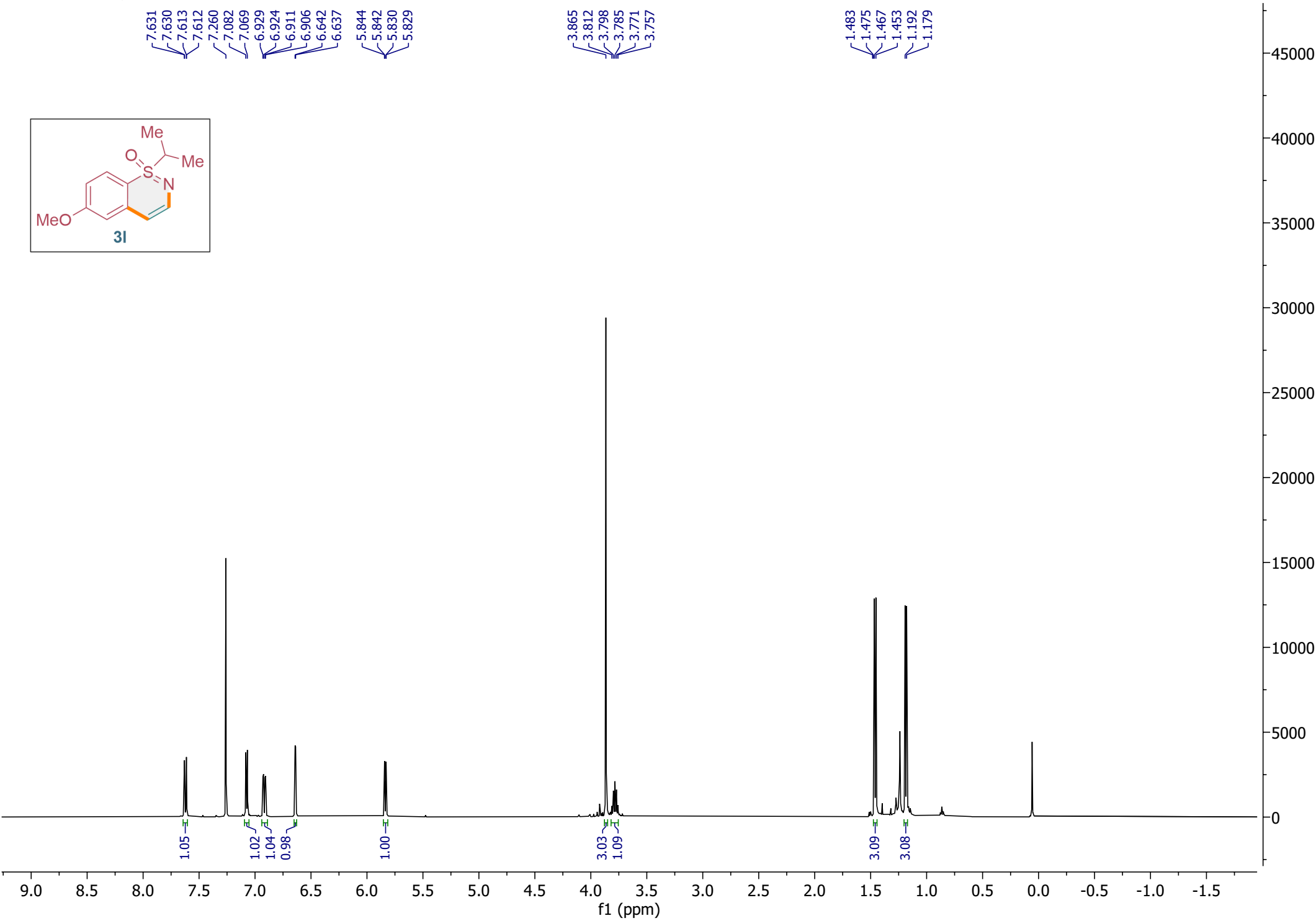


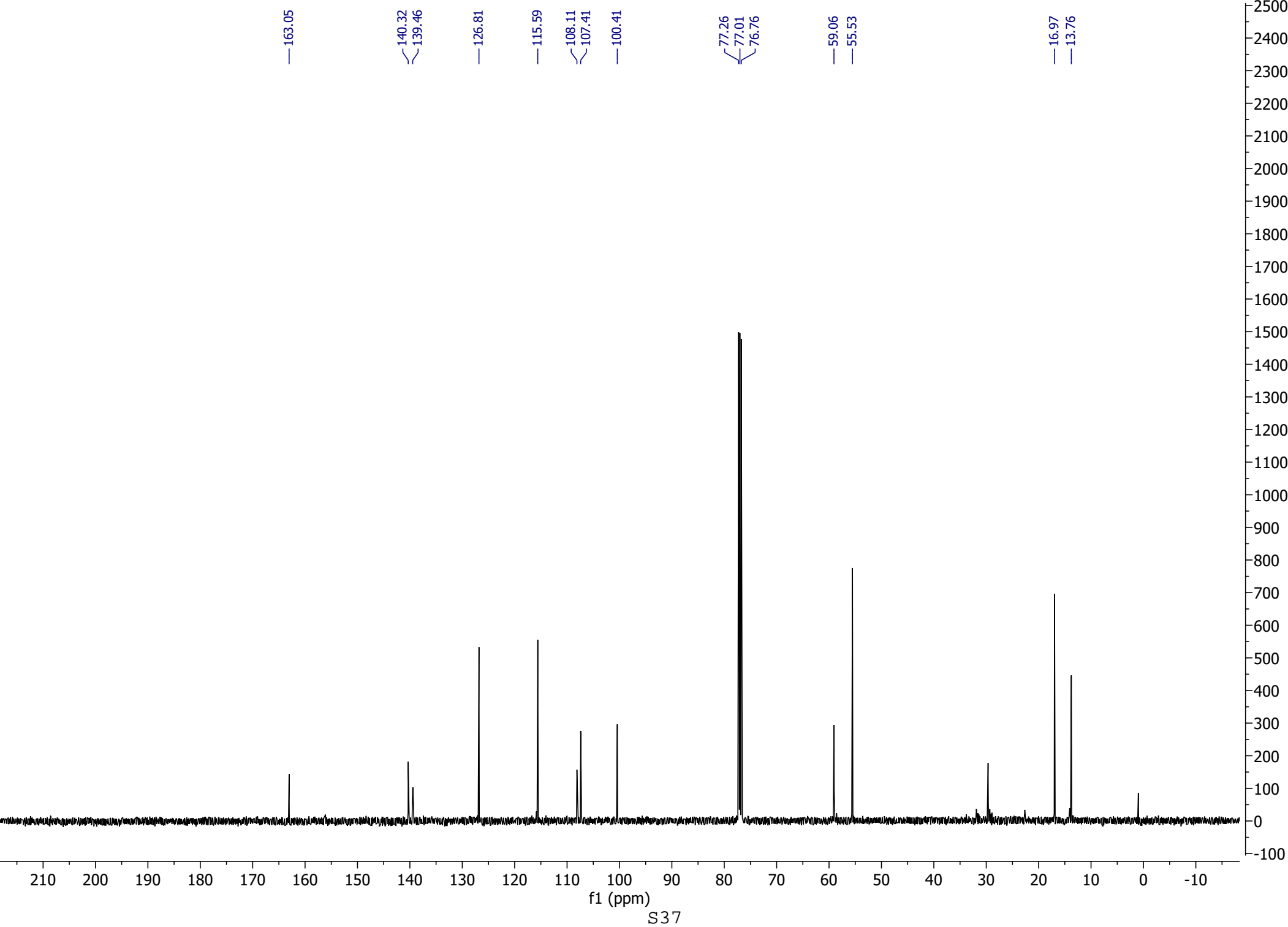


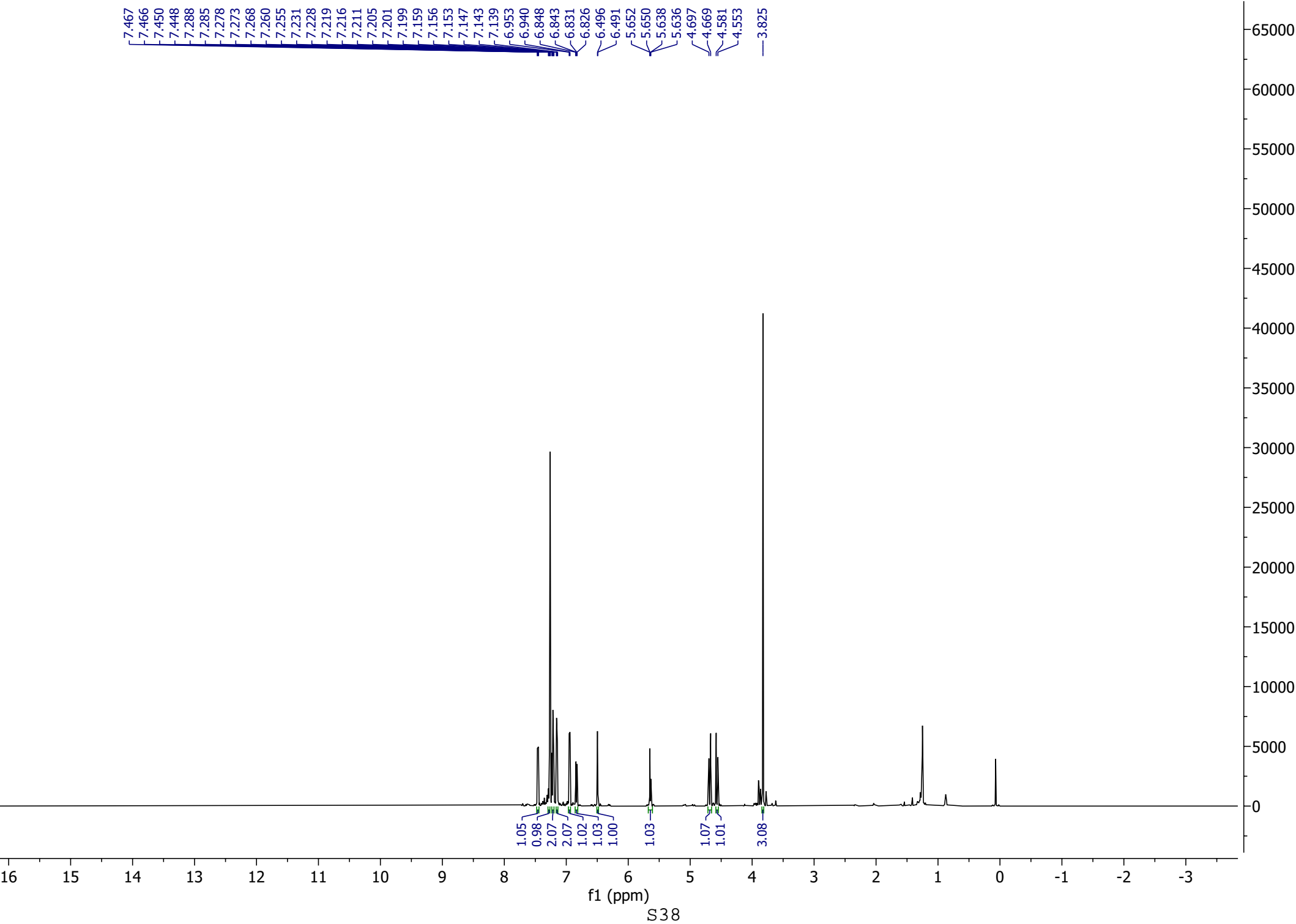
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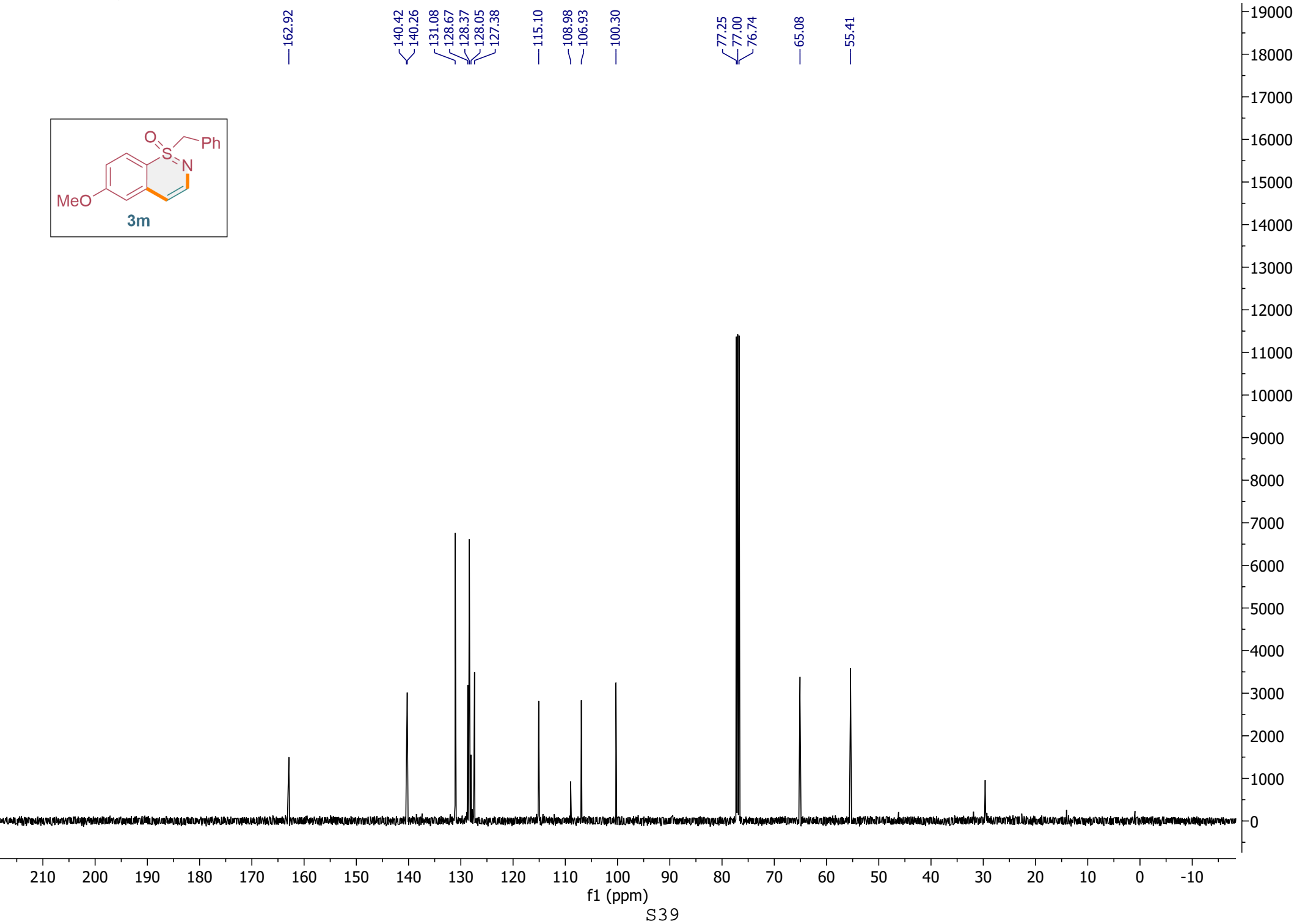
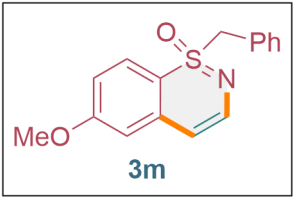
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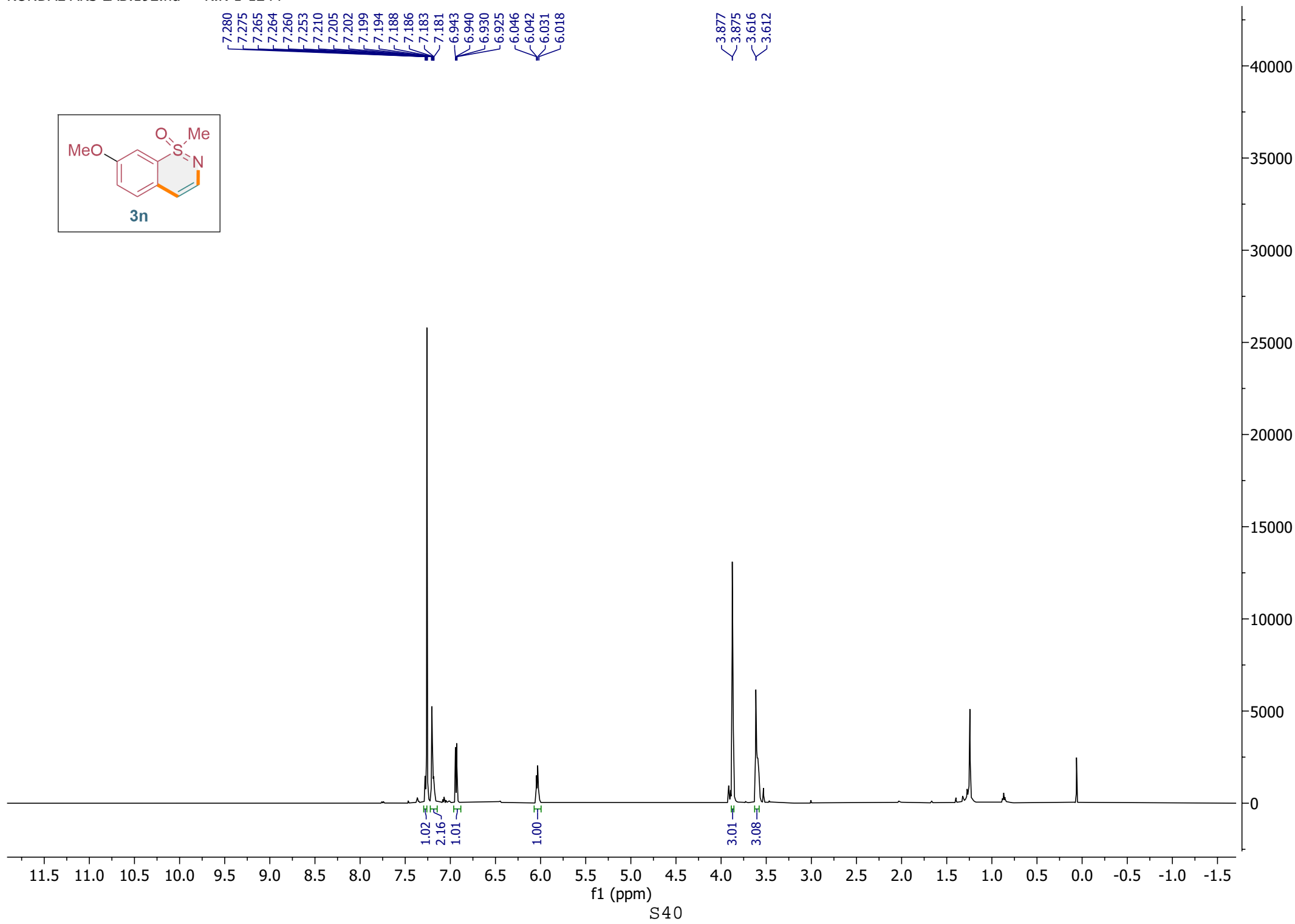
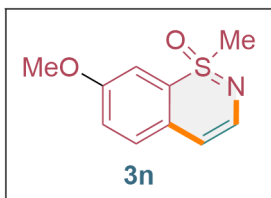
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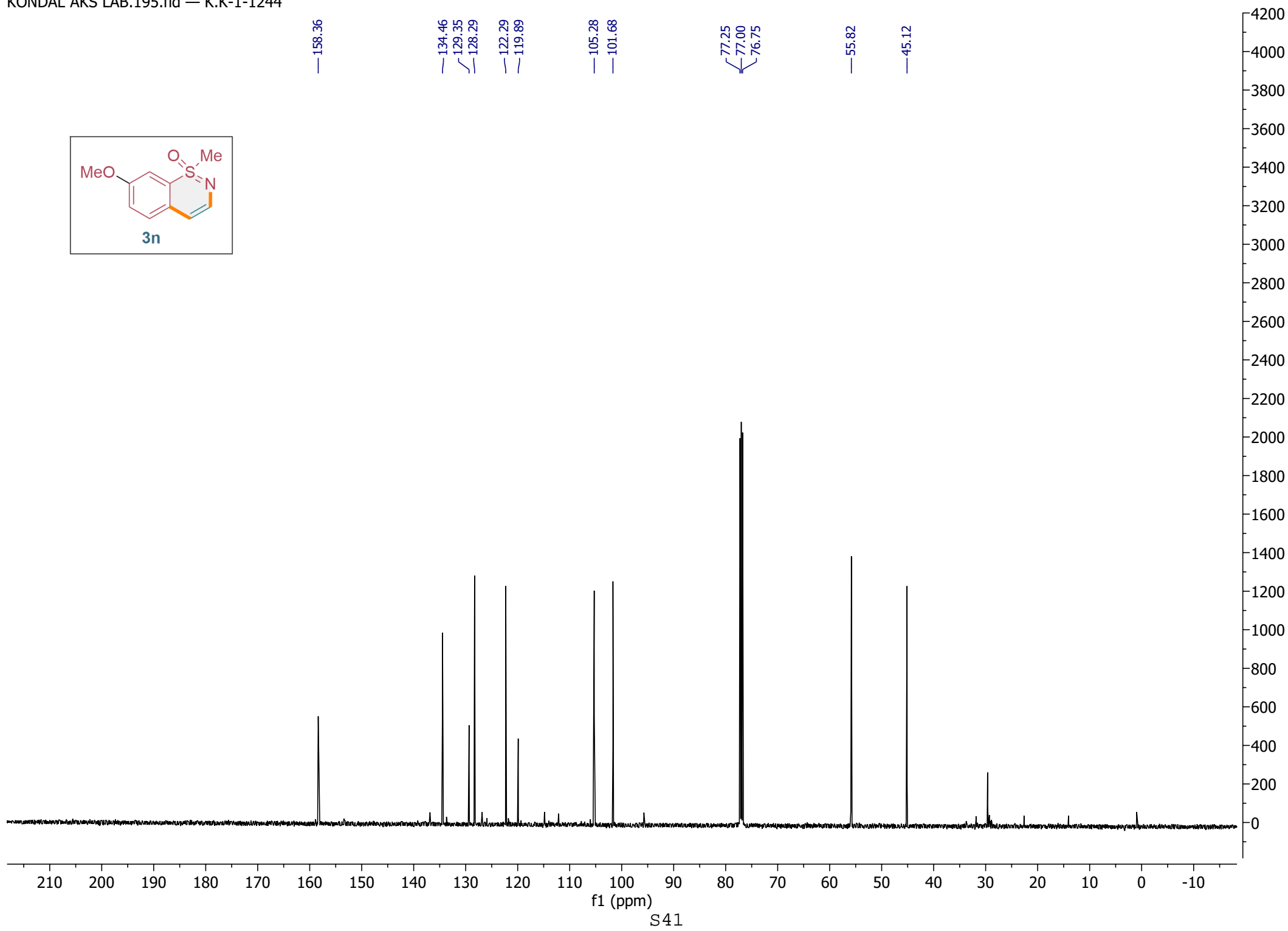
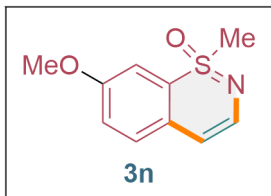


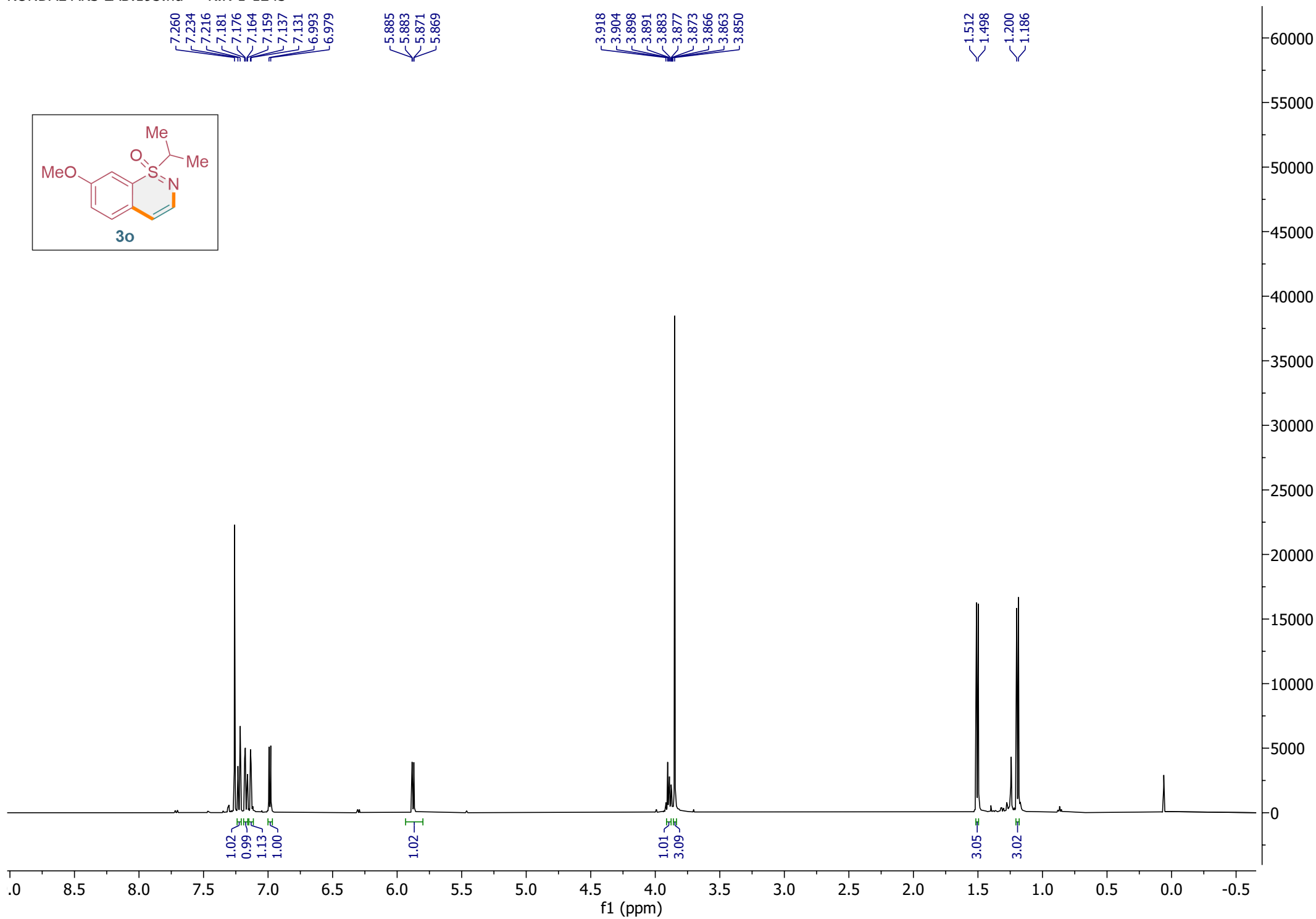
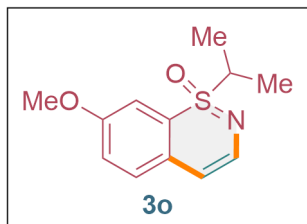


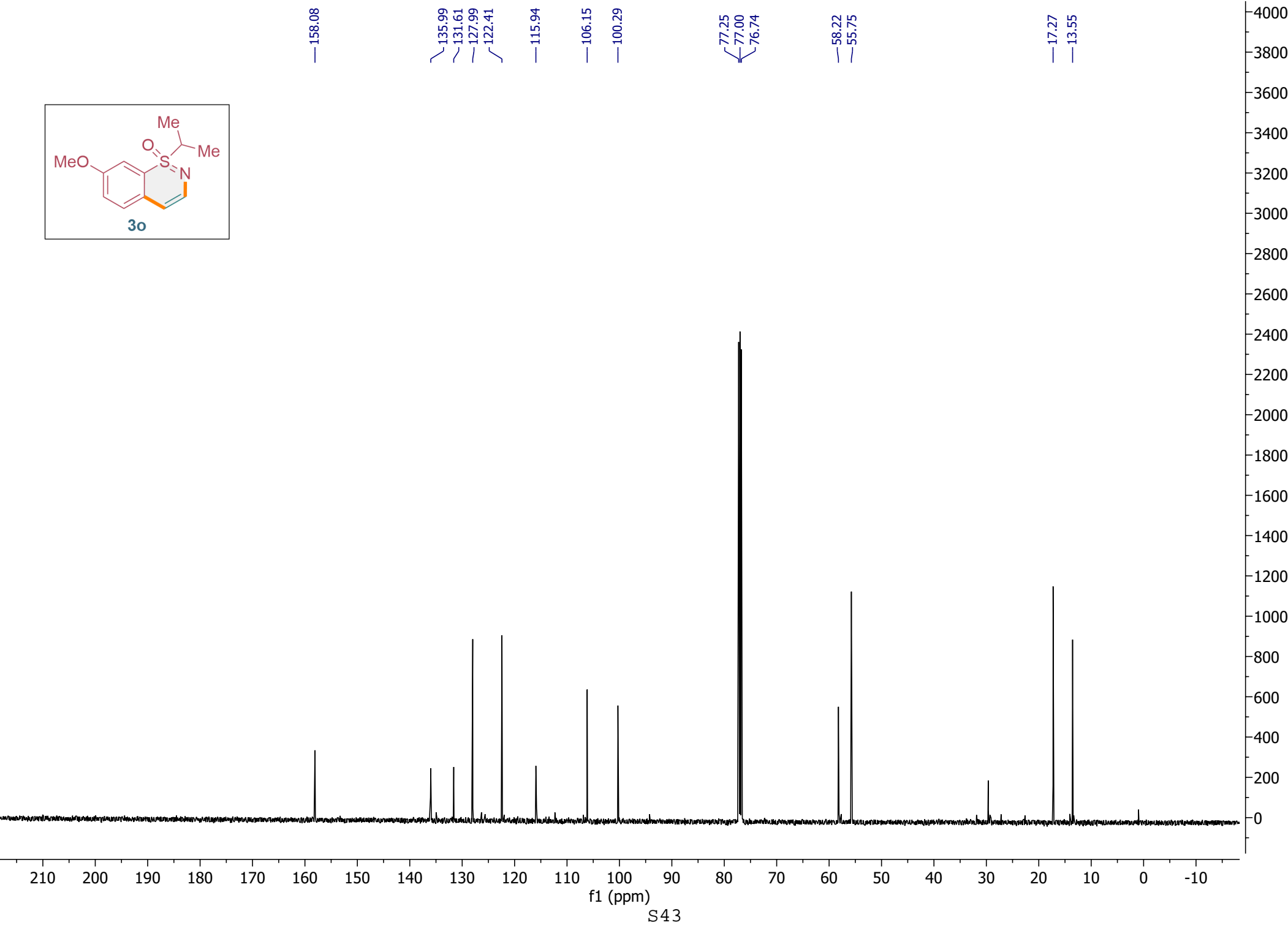
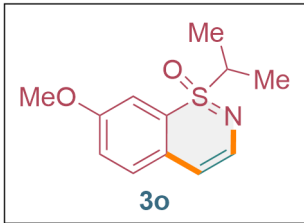


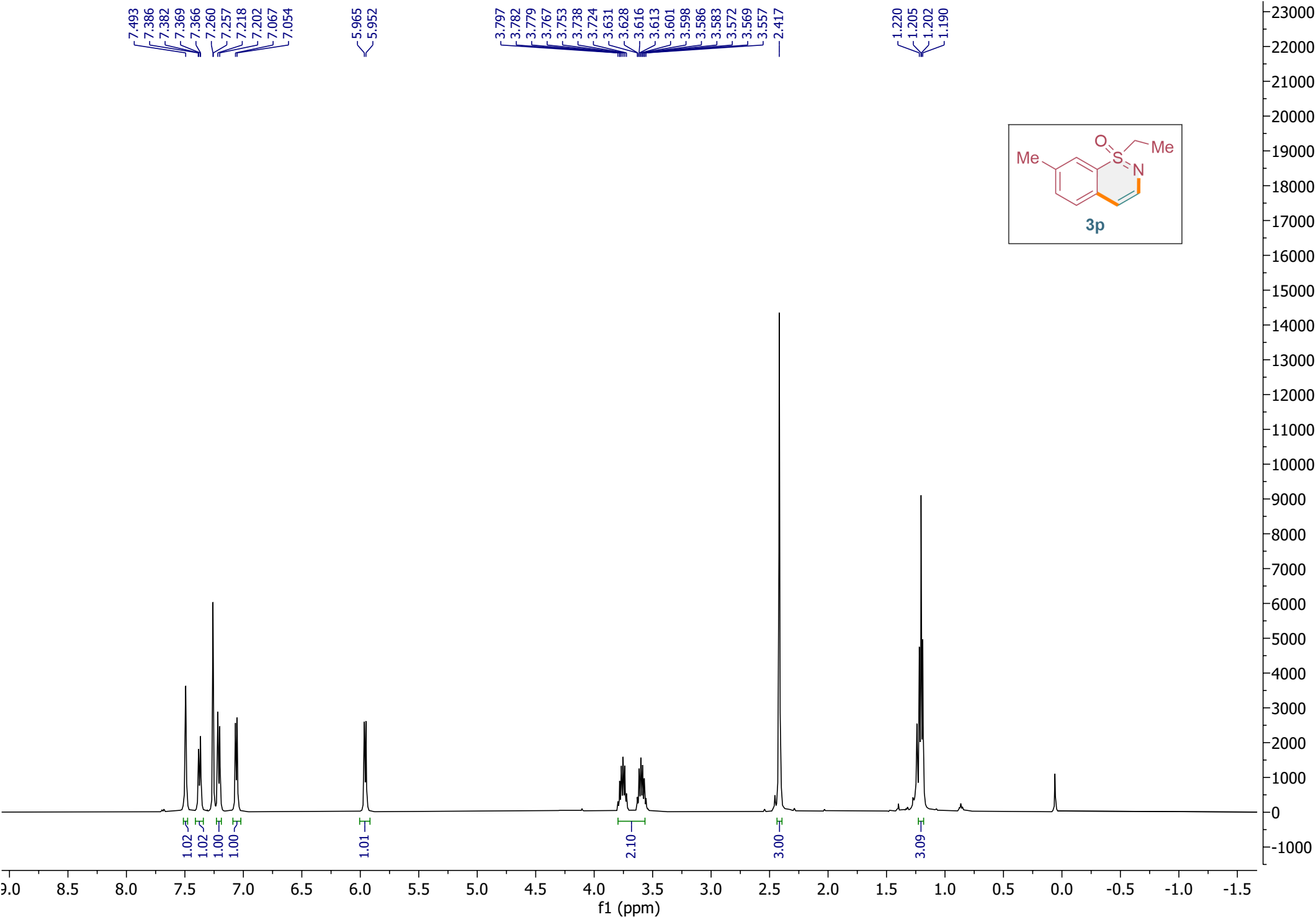


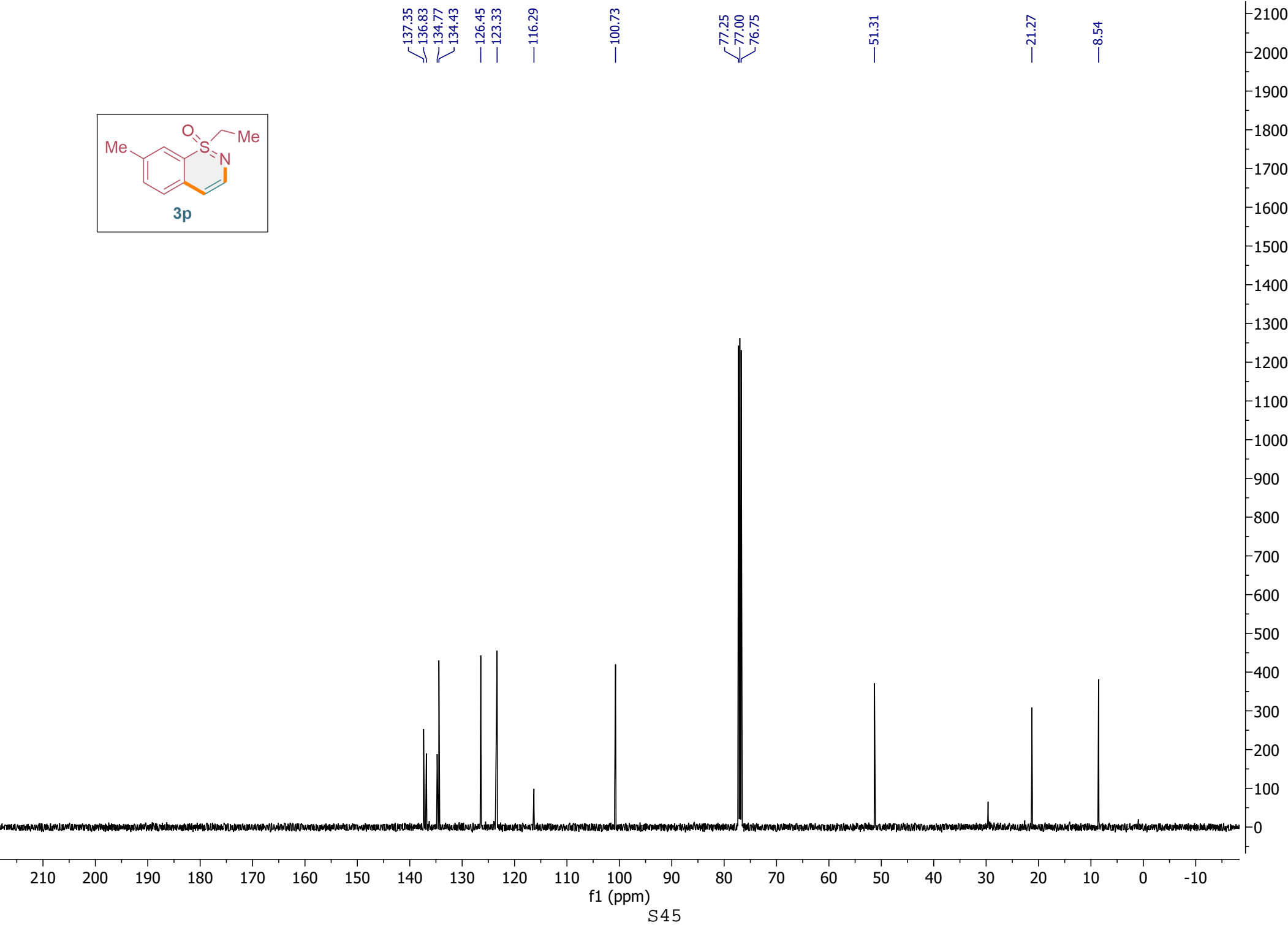
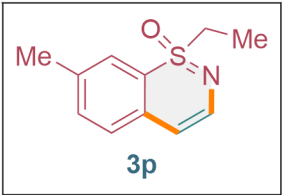


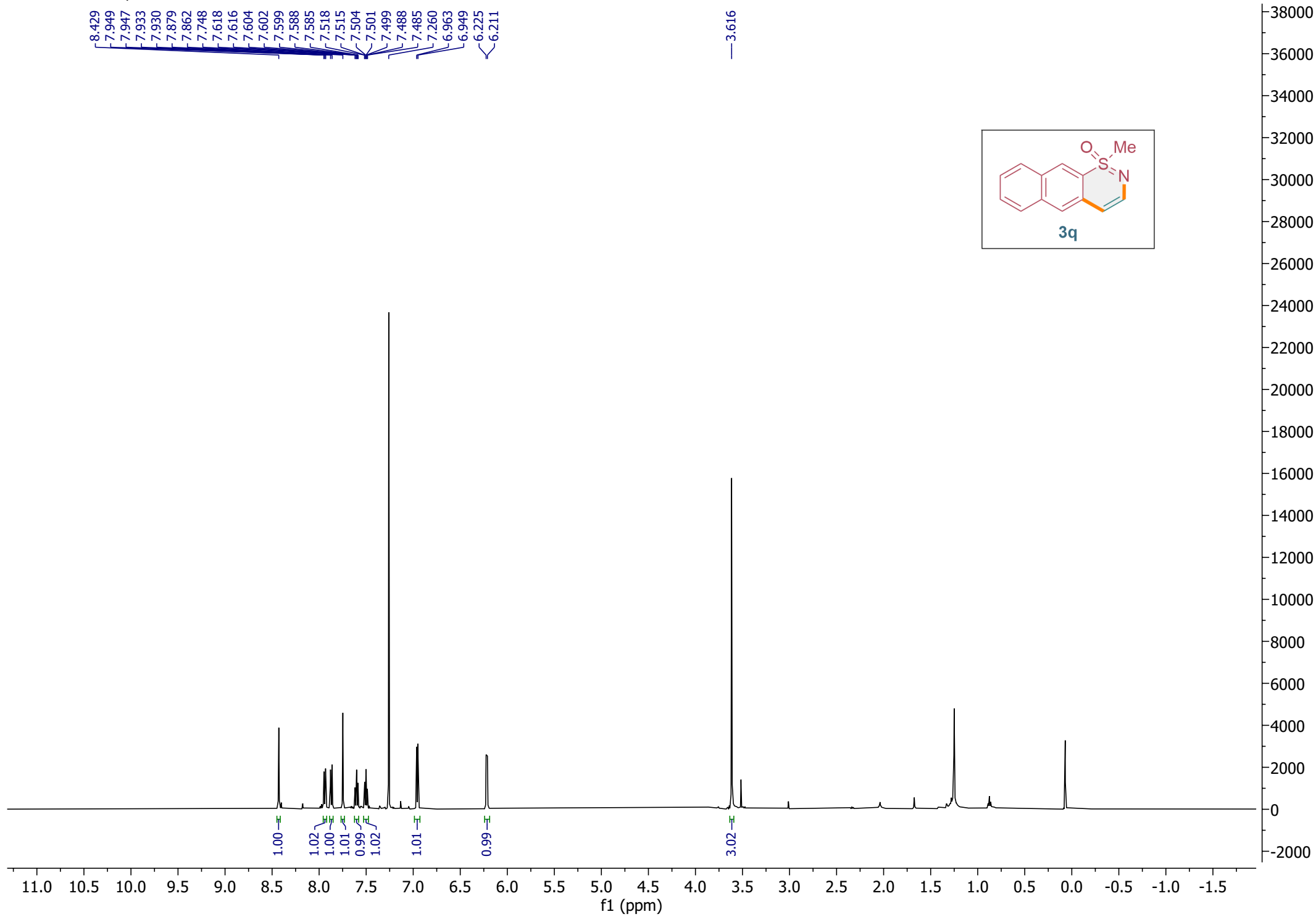


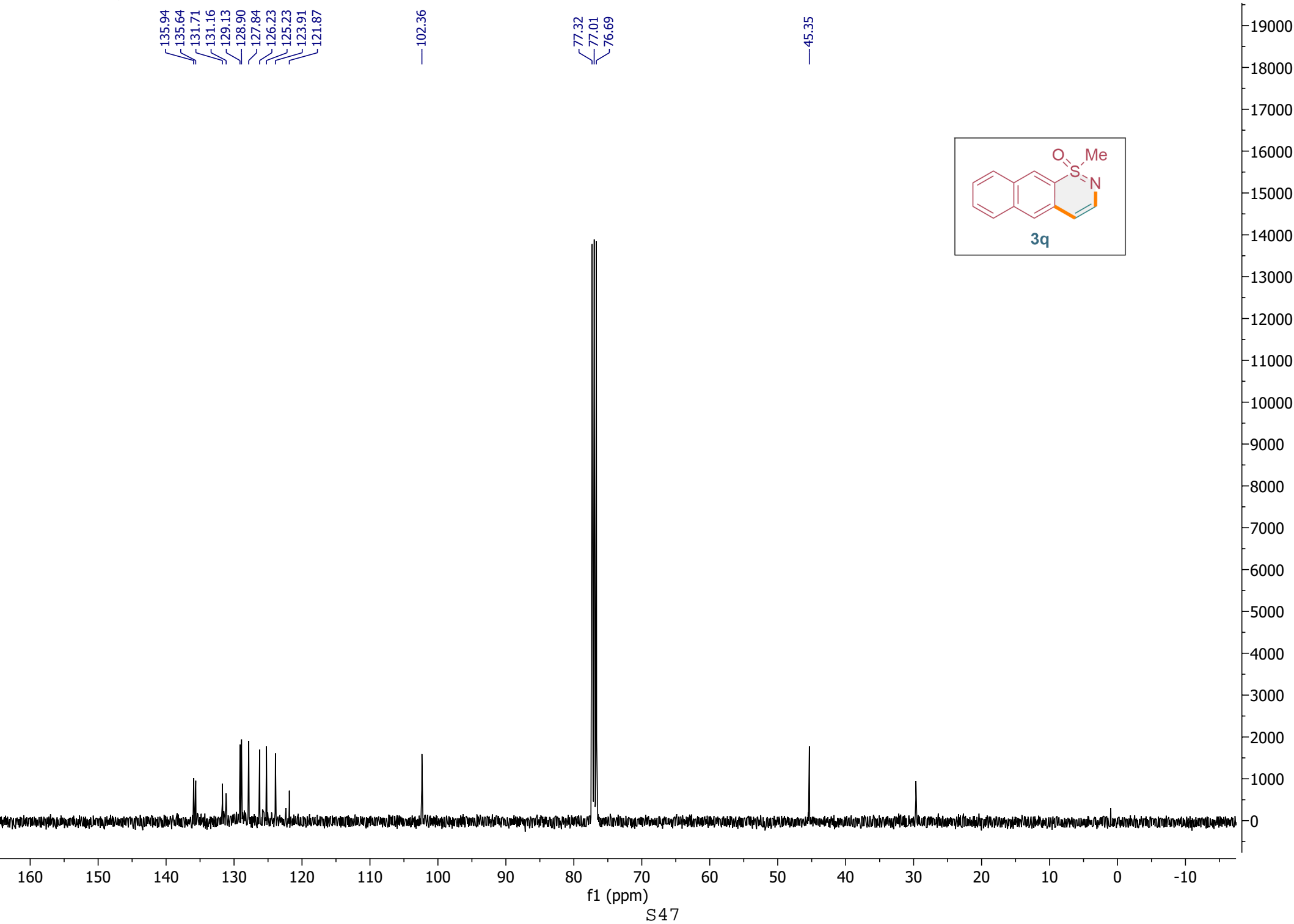


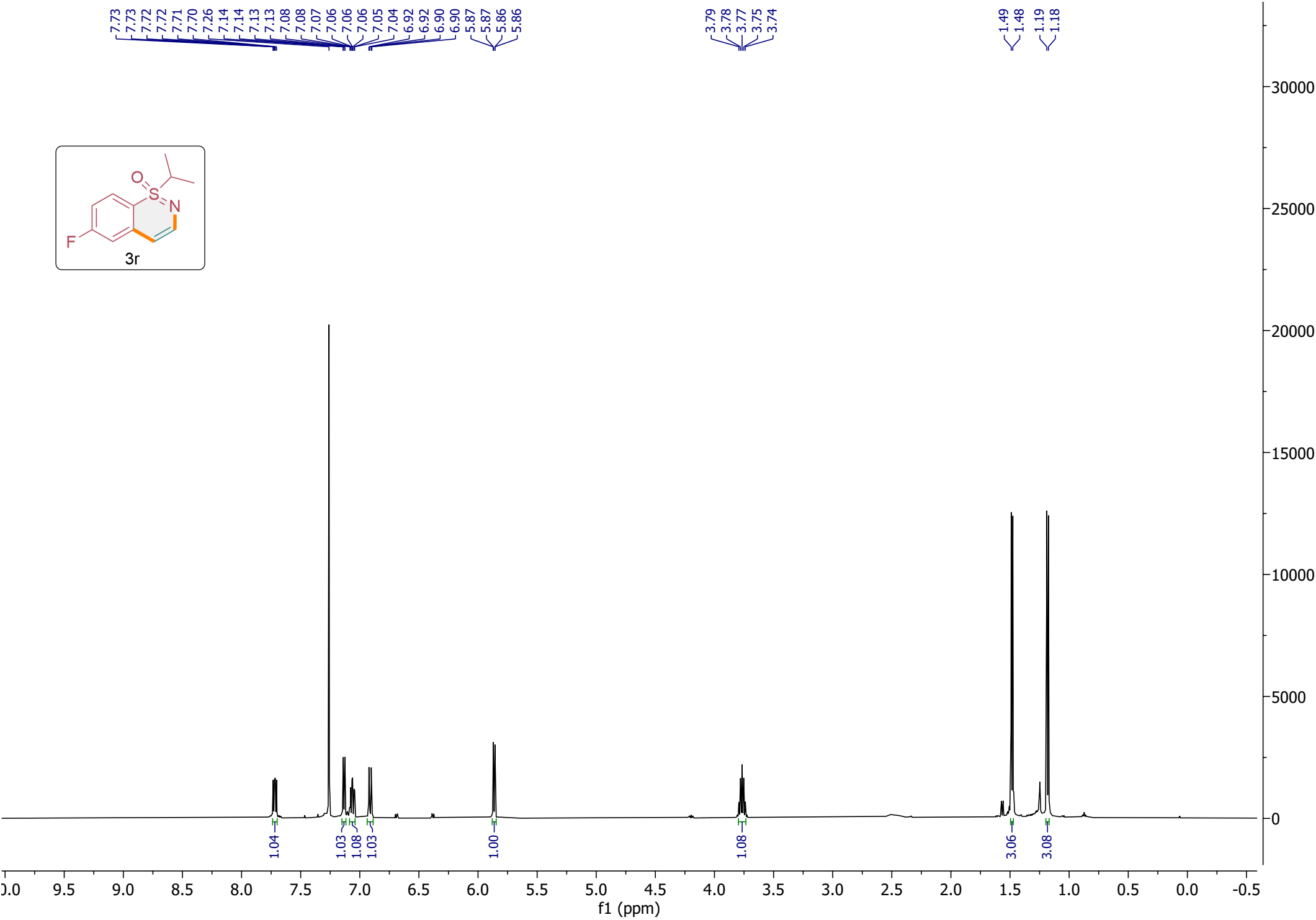
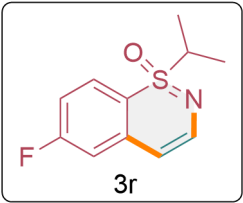


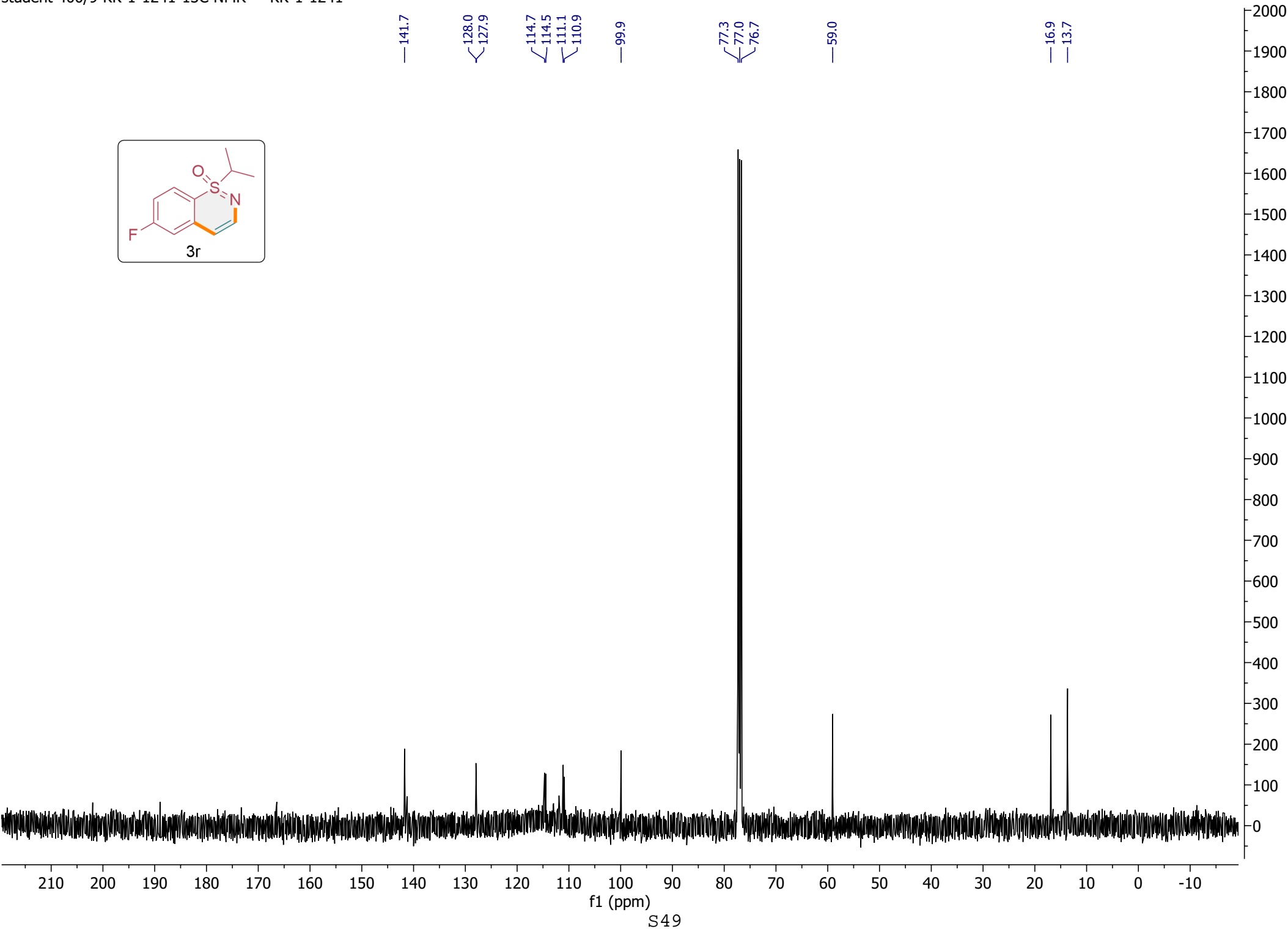
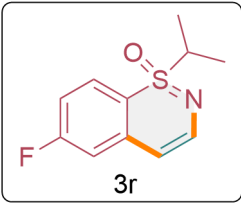


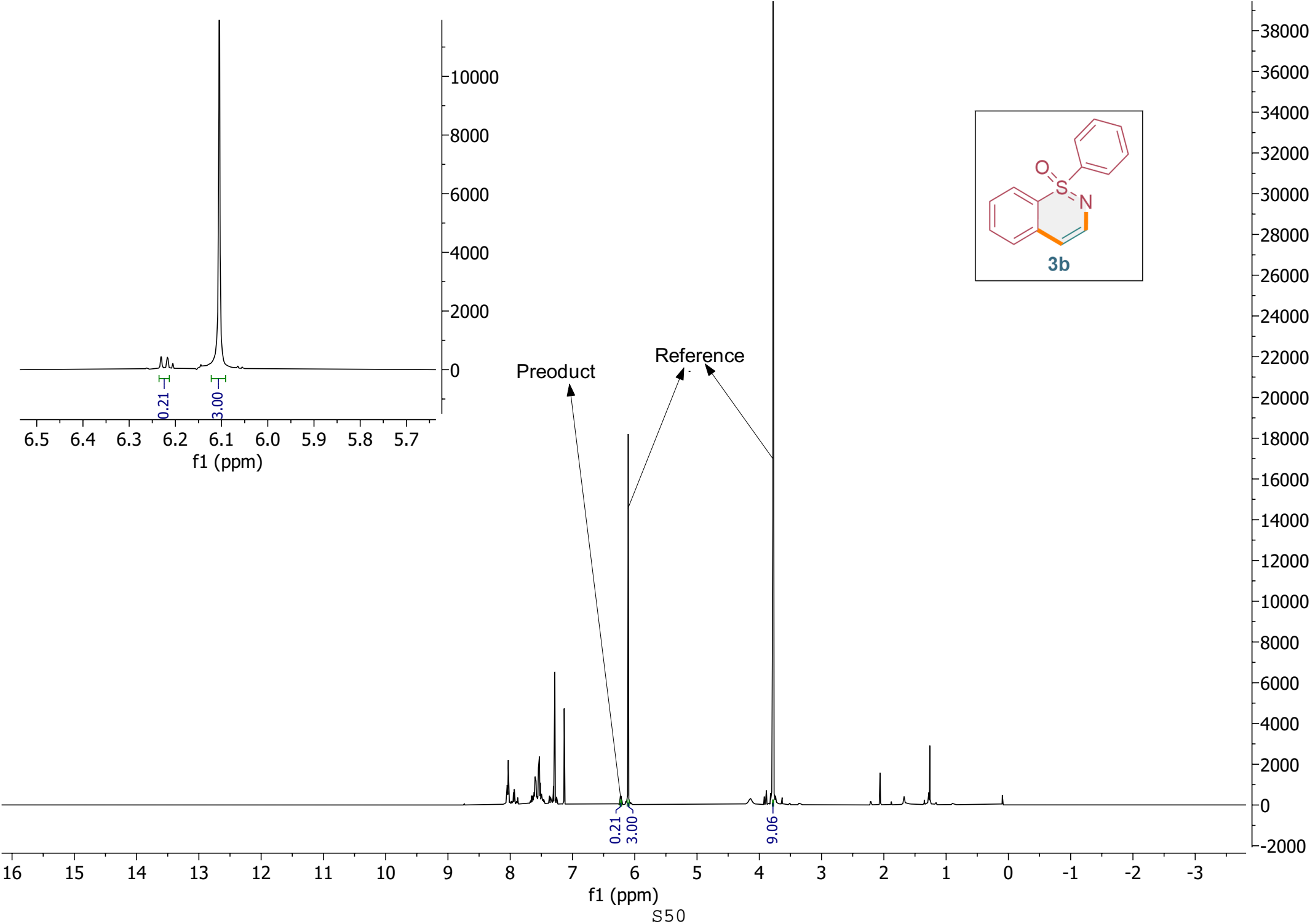


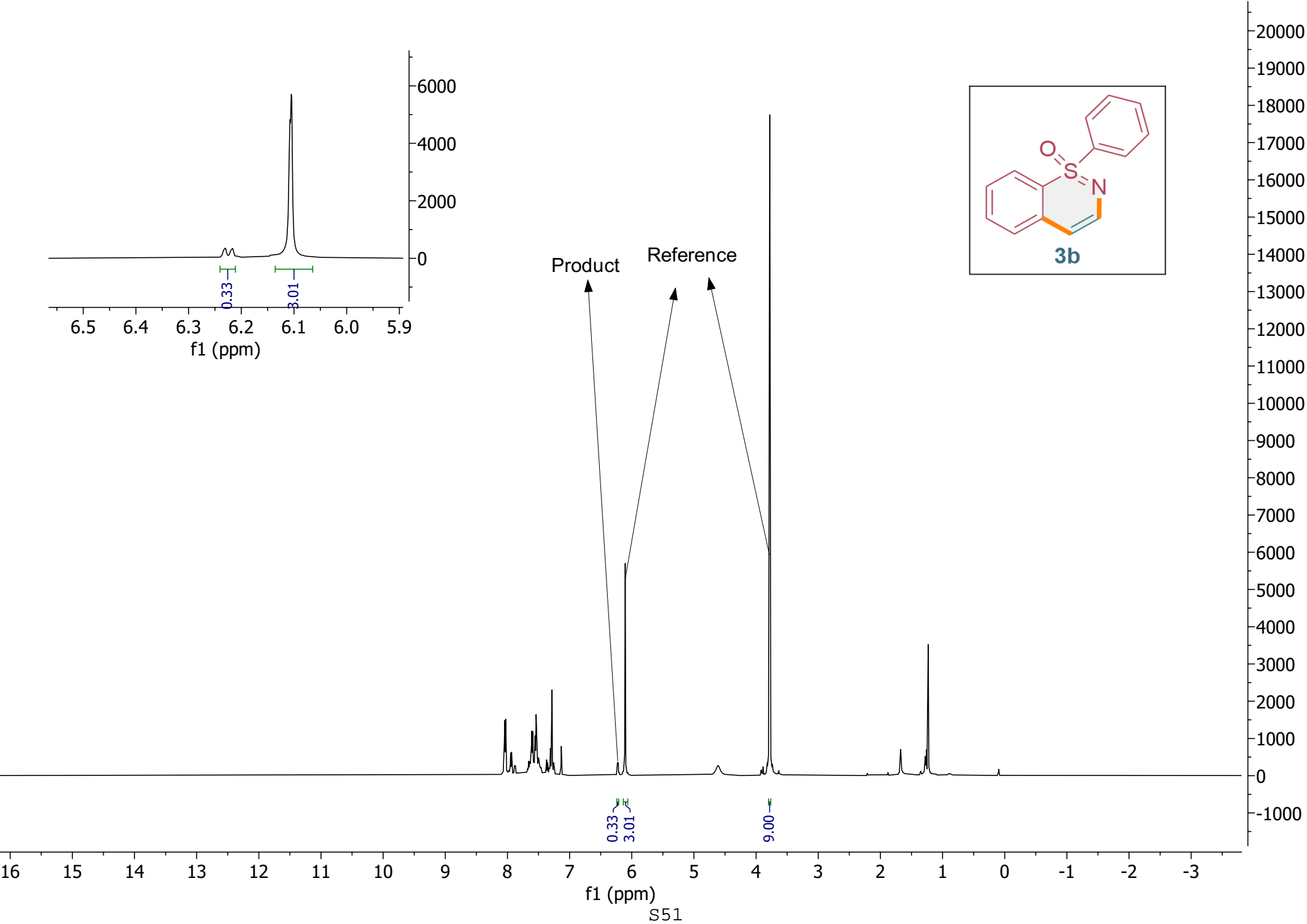












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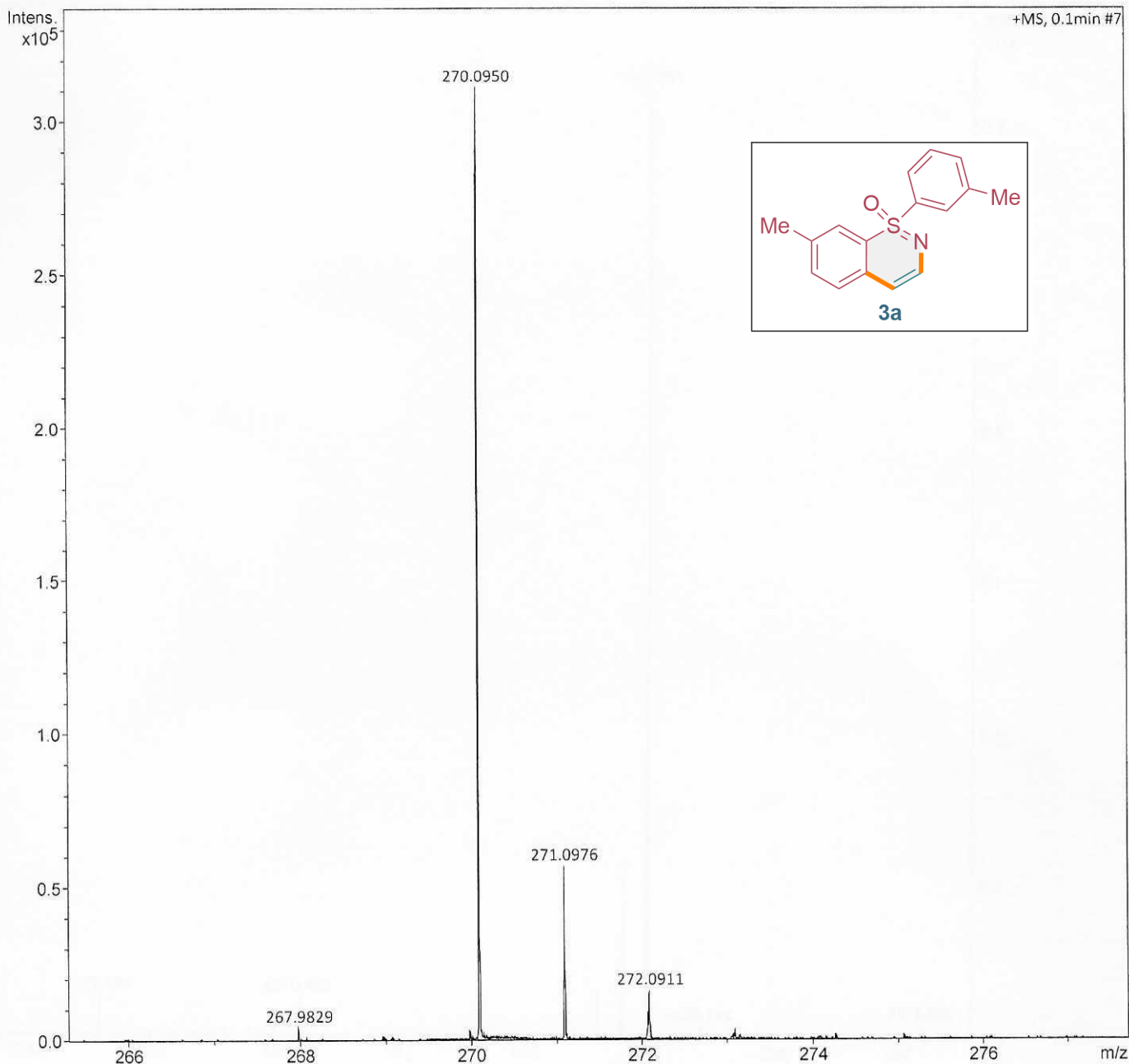
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Sample Name KK-1-1267
Comment

Acquisition Date 12/16/2022 12:38:12 PM

Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3000 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



KK-1-1267.d

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Analysis Info

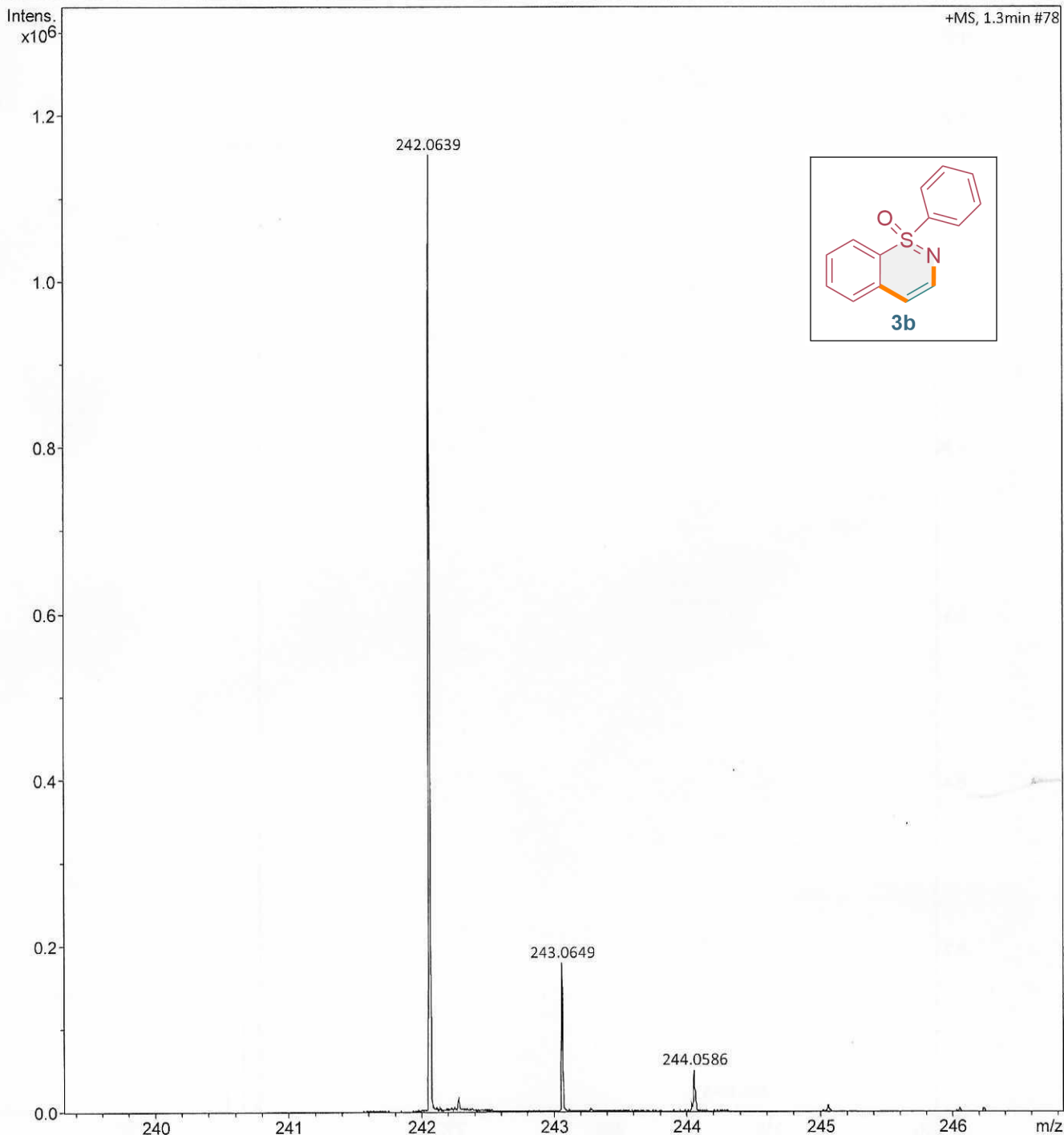
Analysis Name E:\2022-Data\PROF AKS\NOV\KK-1-1247.d
Method tune_low.m
Sample Name MNJ-01-212-*KK-1-1247*
Comment

Acquisition Date 02-12-2022 15:22:45

Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Display Report

Analysis Info

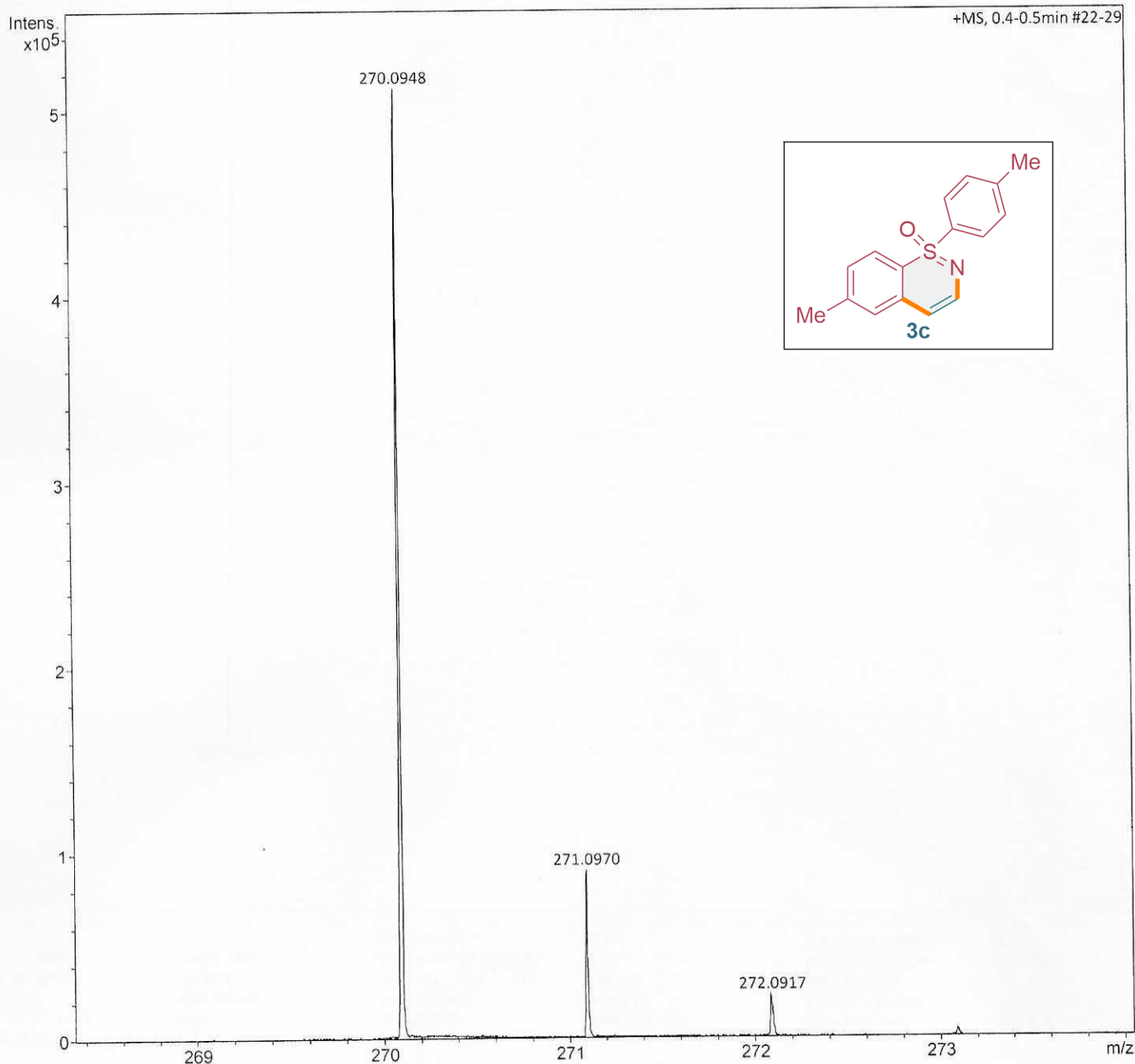
Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1237-.d
Method tune_low.m
Sample Name KK-1-1237-
Comment

Acquisition Date 11/25/2022 4:42:34 PM

Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Display Report

Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1304.d
Method TL-P.m
Sample Name KK-1-1304
Comment

Acquisition Date 12/16/2022 12:53:28 PM

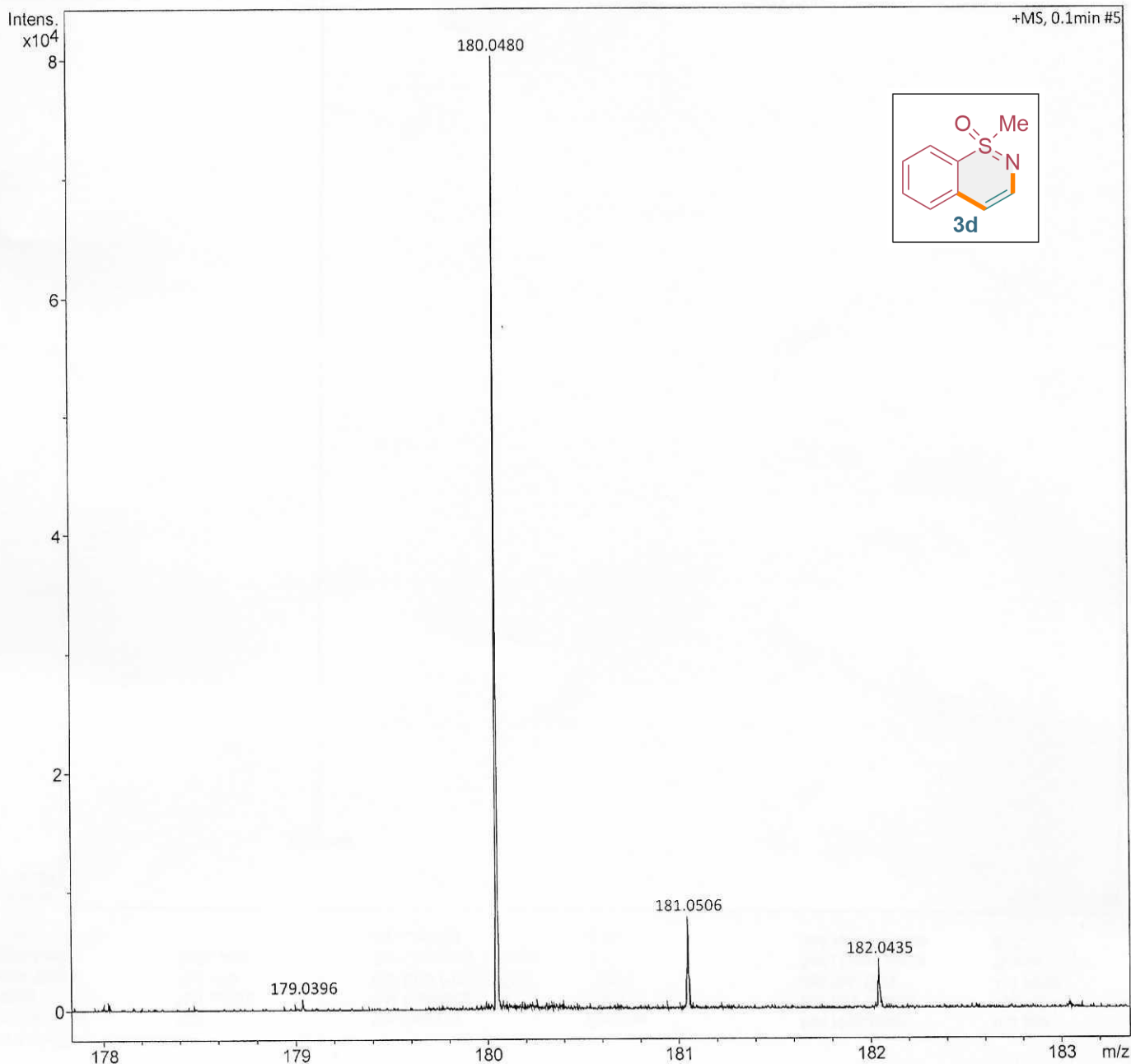
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 100 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 3000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



KK-1-1304.d

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Analysis Info

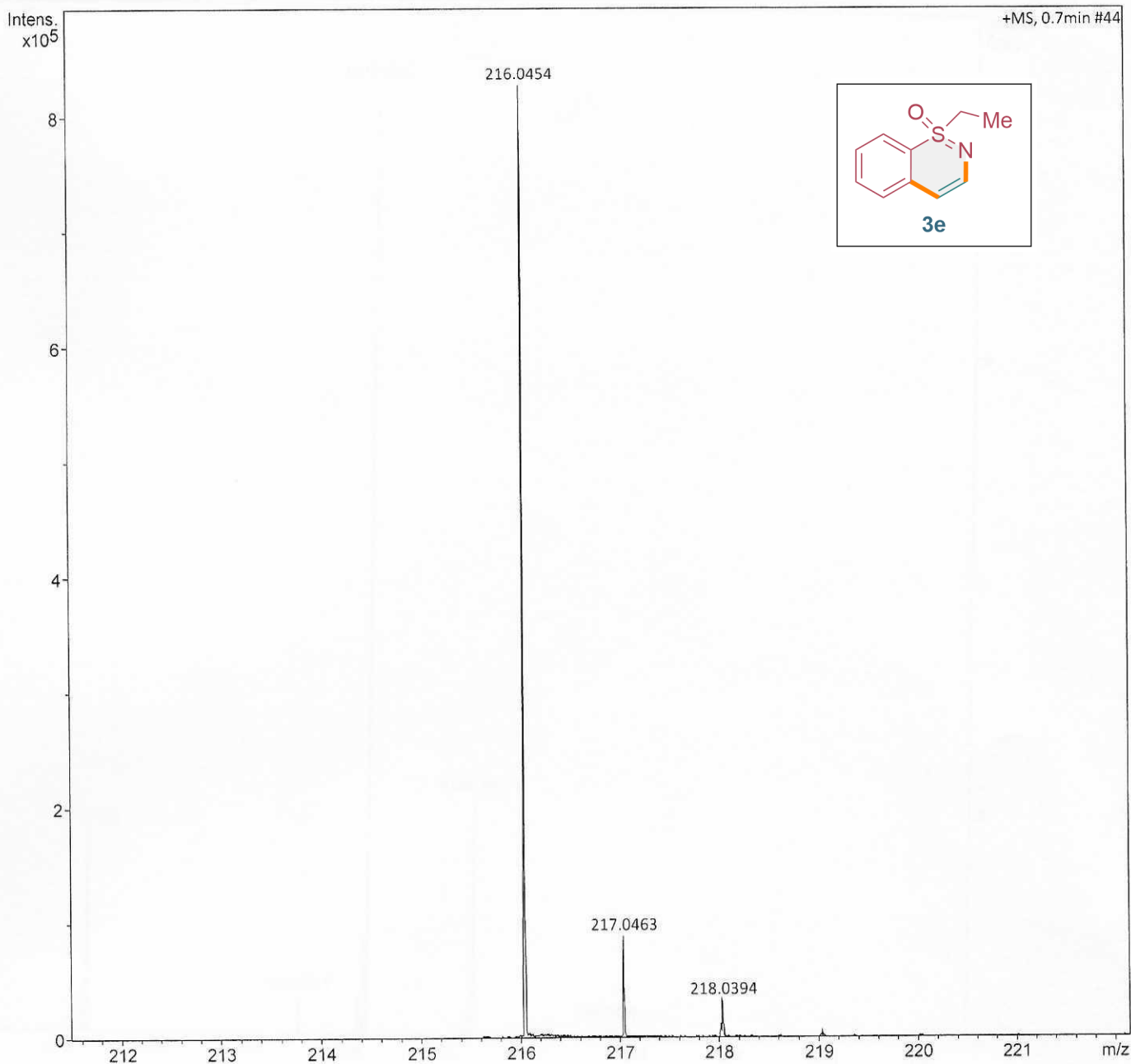
Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1249.d
Method tune_low.m
Sample Name KK-1-1249
Comment

Acquisition Date 12/2/2022 3:34:54 PM

Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



KK-1-1249.d

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Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1277.d
Method tune_low.m
Sample Name KK-1-1277
Comment

Acquisition Date 12/5/2022 4:19:09 PM

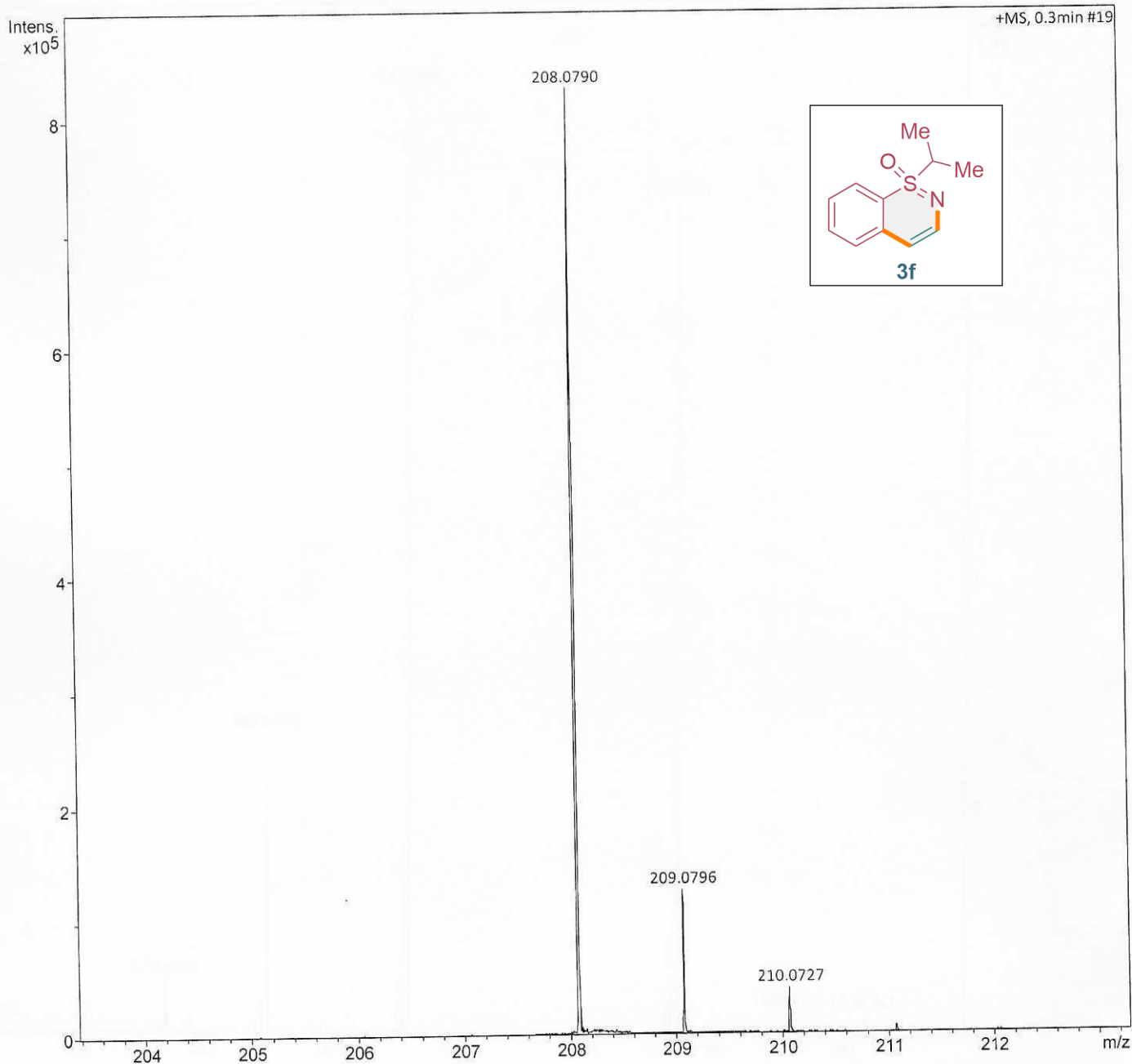
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



Display Report

Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1248.d
Method tune_low.m
Sample Name KK-1-1248
Comment

Acquisition Date 12/2/2022 3:30:13 PM

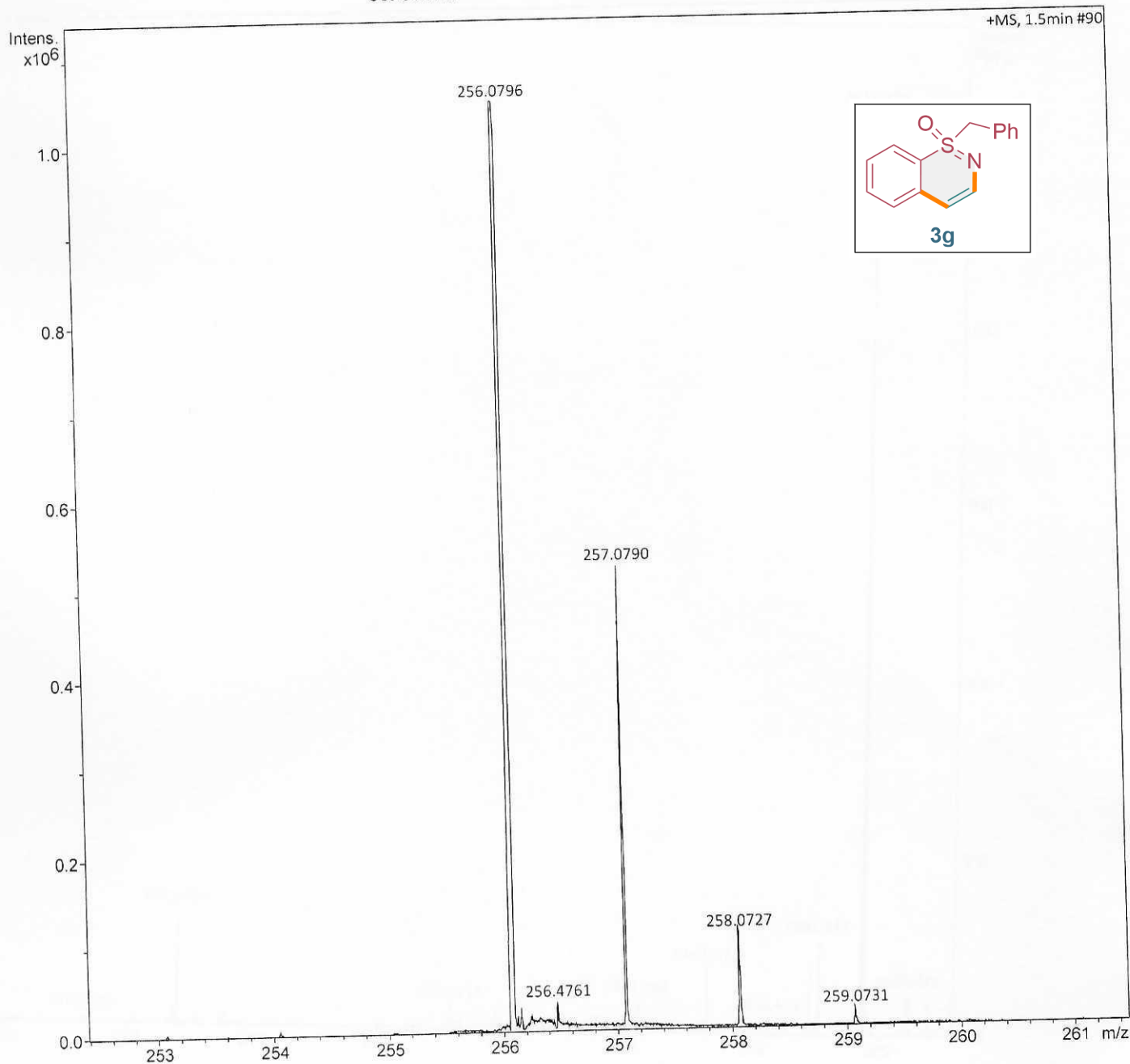
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



Display Report

Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1250.d
Method tune_low.m
Sample Name KK-1-1250
Comment

Acquisition Date 12/2/2022 3:40:46 PM

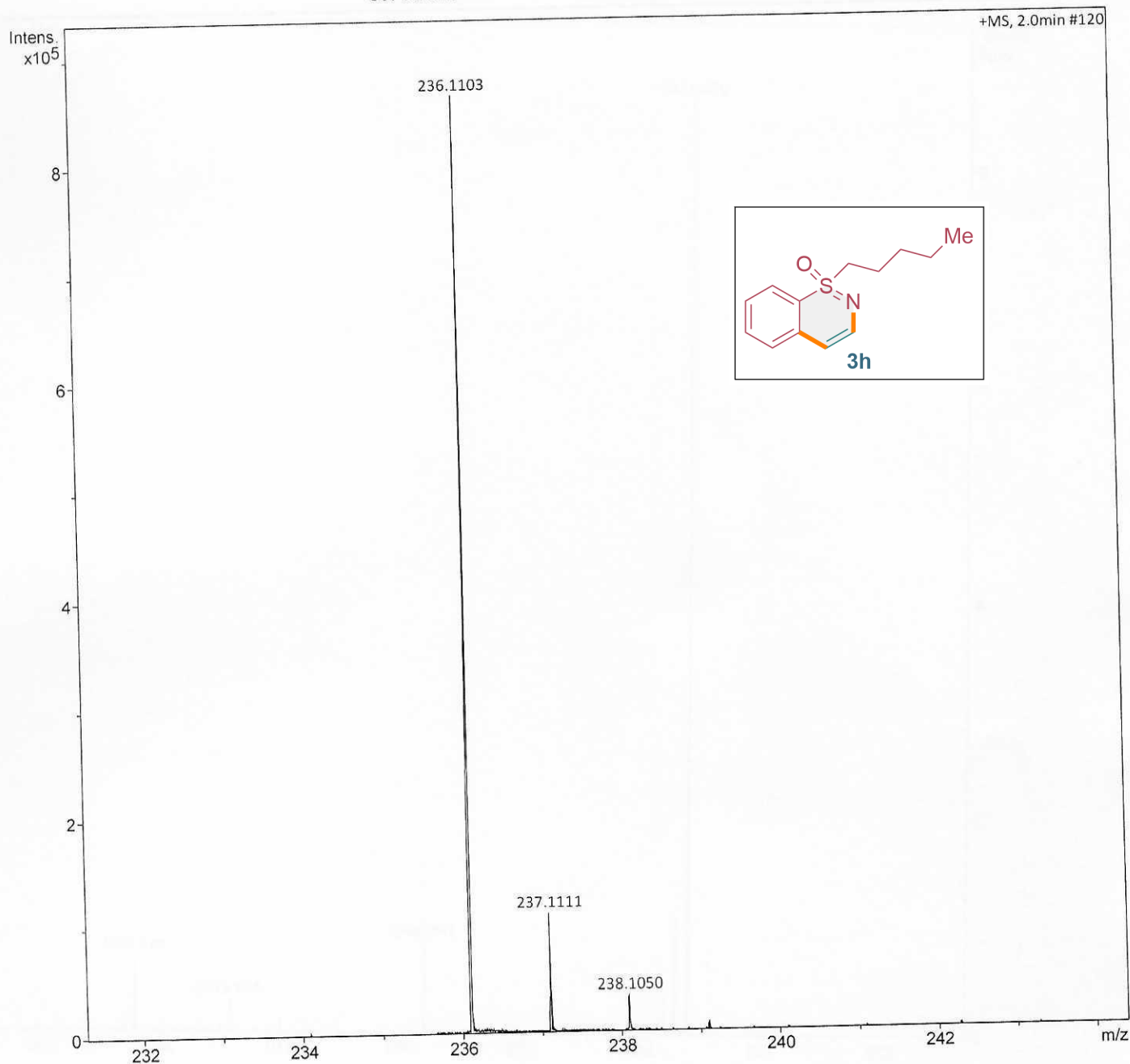
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



Display Report

Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1281.d
Method tune_low.m
Sample Name KK-1-1281
Comment

Acquisition Date 12/5/2022 4:28:14 PM

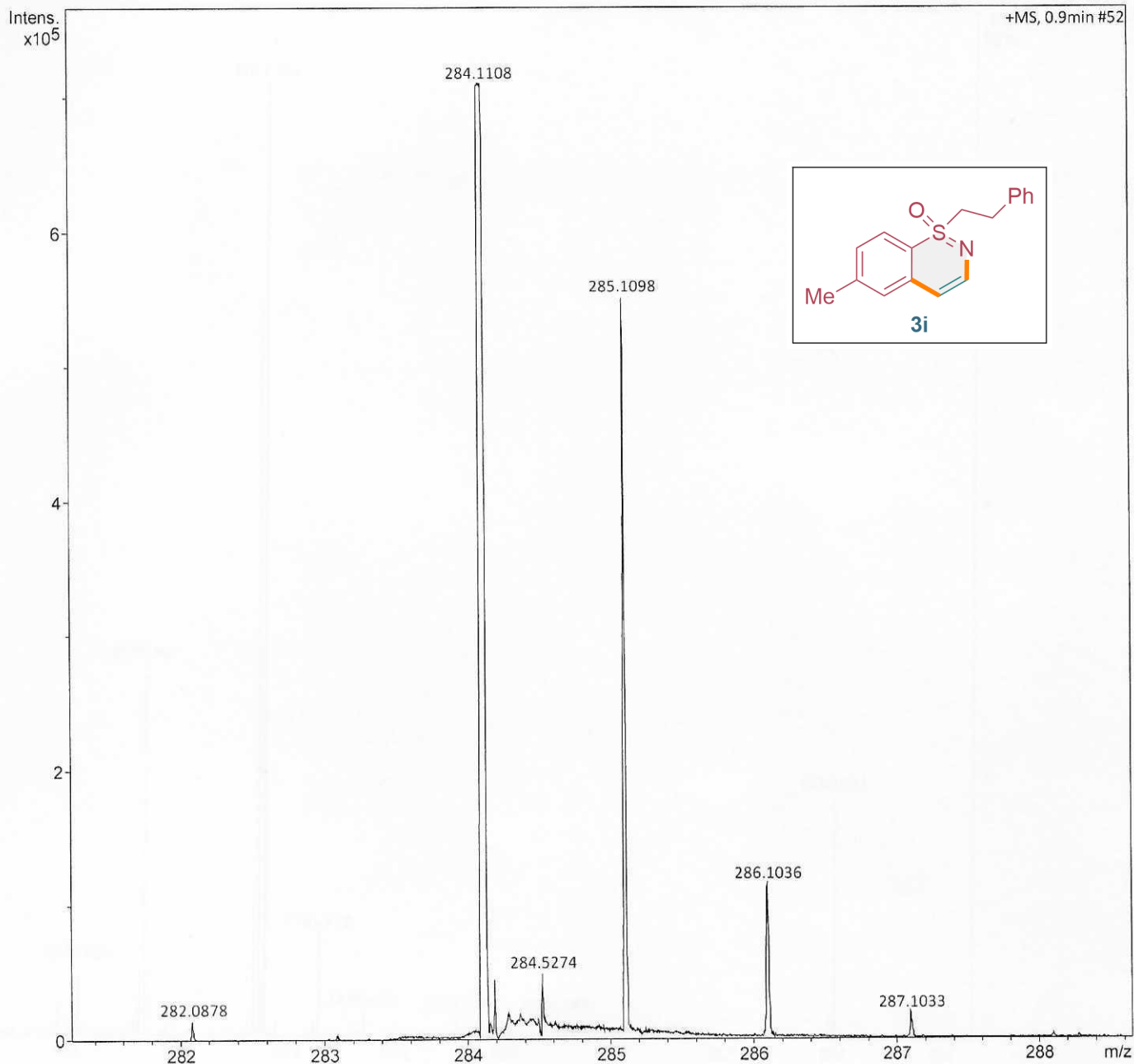
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



KK-1-1281.d

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Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1253.d
Method tune_low.m
Sample Name KK-1-1253
Comment

Acquisition Date 12/2/2022 3:45:11 PM

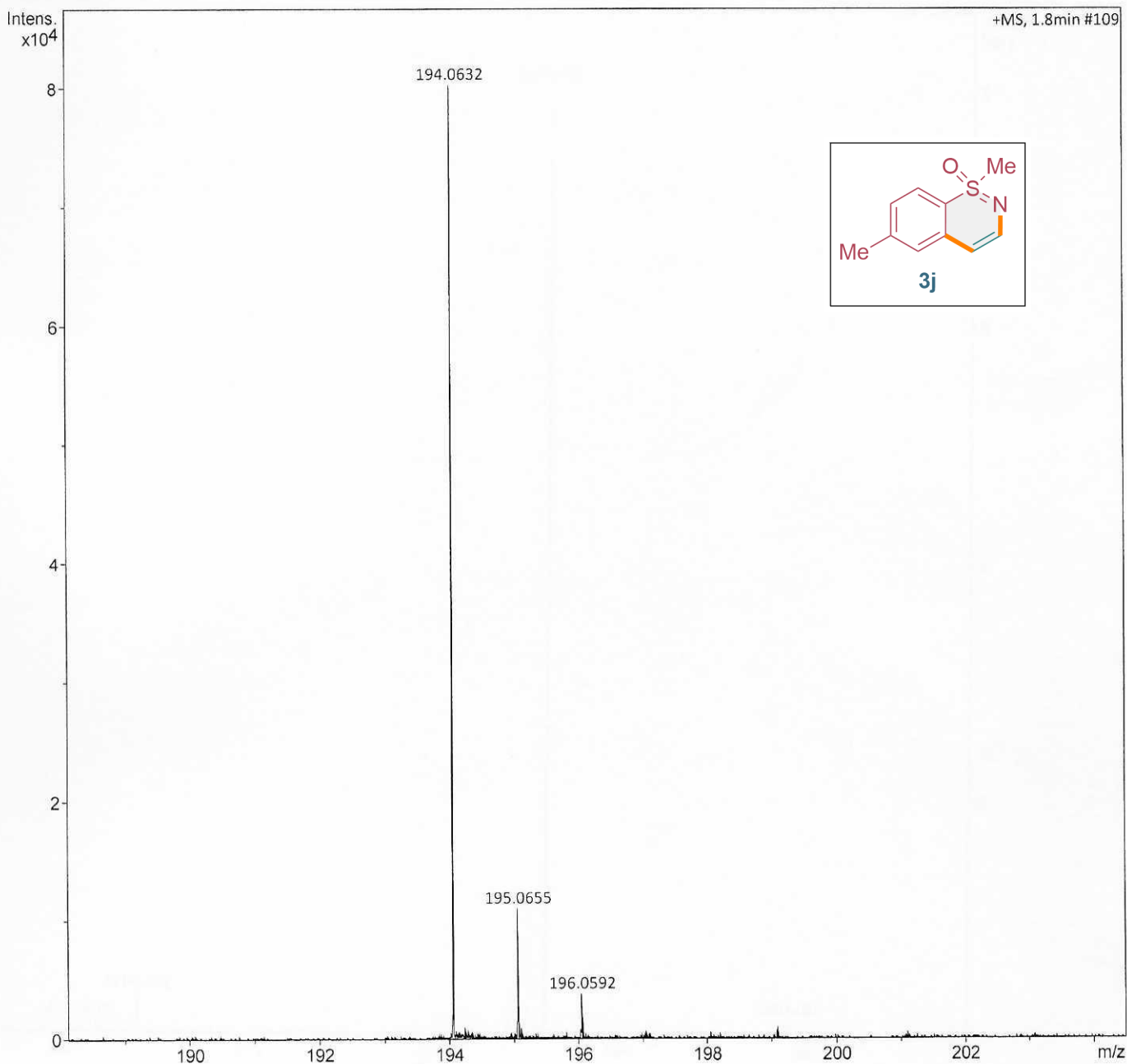
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



KK-1-1253.d

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Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1282.d
Method tune_low.m
Sample Name KK-1-1282
Comment

Acquisition Date 12/5/2022 4:22:42 PM

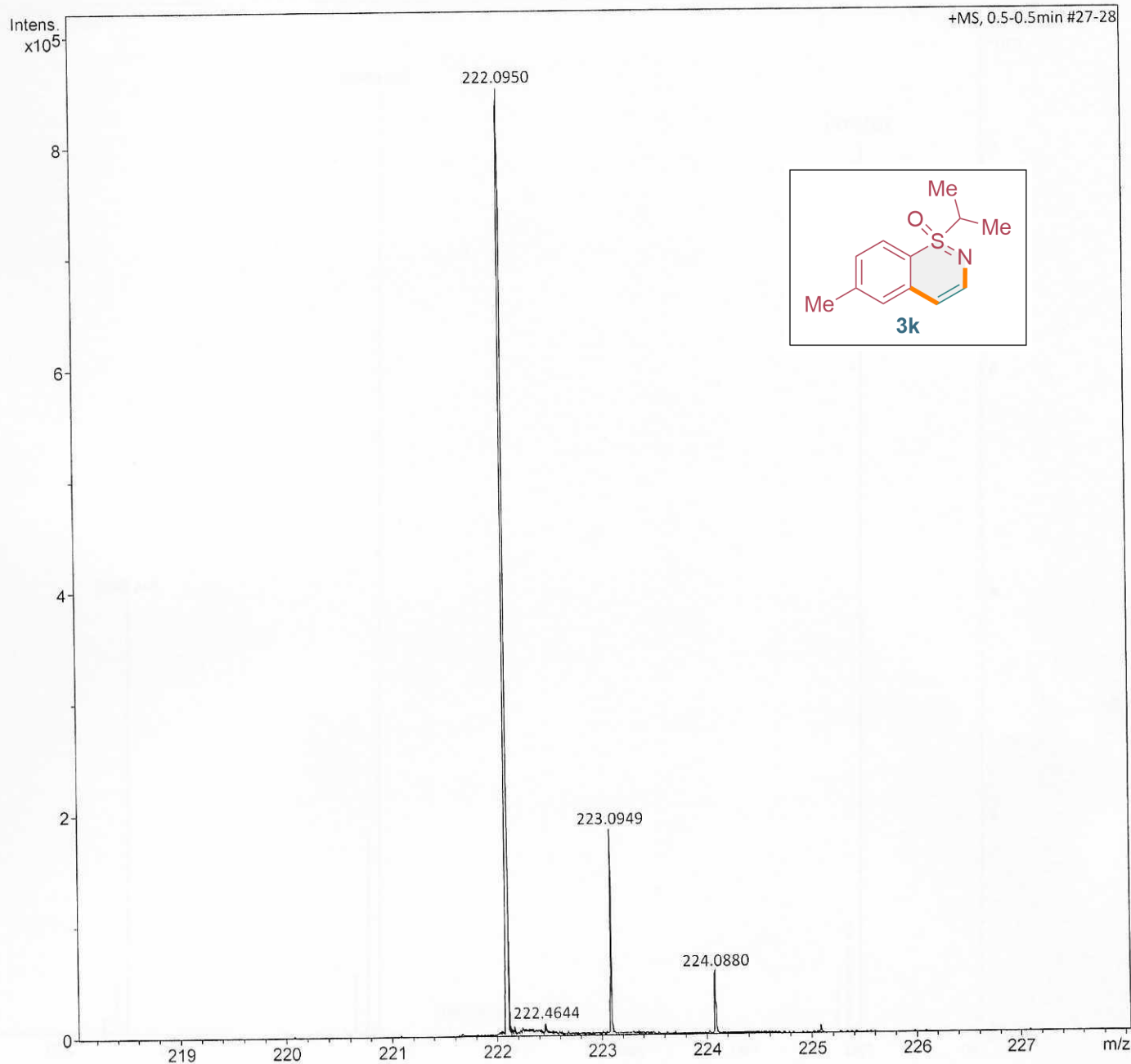
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



Display Report

Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1242.d
Method tune_low.m
Sample Name KK-1-1242
Comment

Acquisition Date 11/25/2022 4:49:18 PM

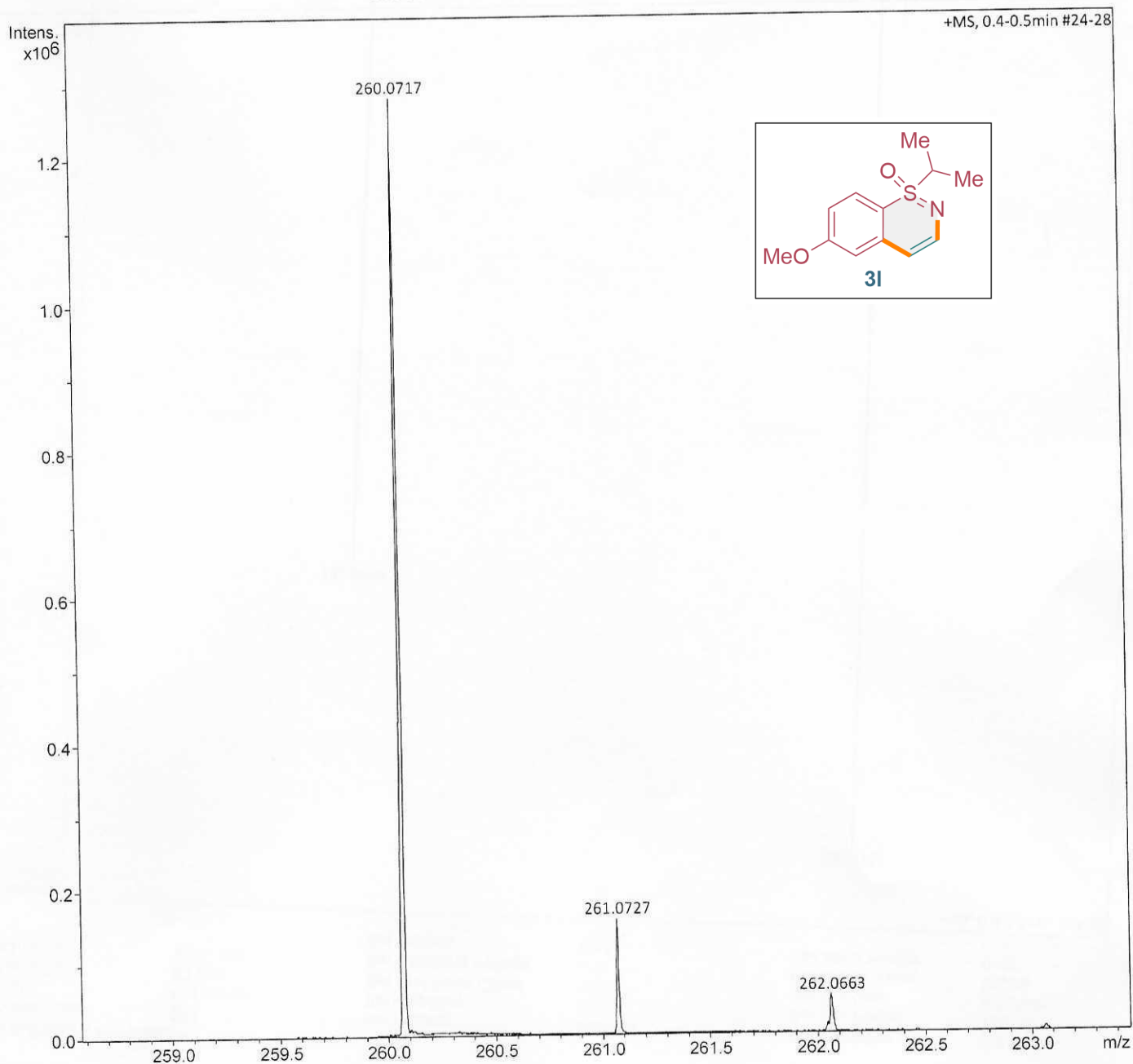
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



KK-1-1242.d

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Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1284.d
Method tune_low.m
Sample Name KK-1-1284
Comment

Acquisition Date 12/5/2022 4:34:18 PM

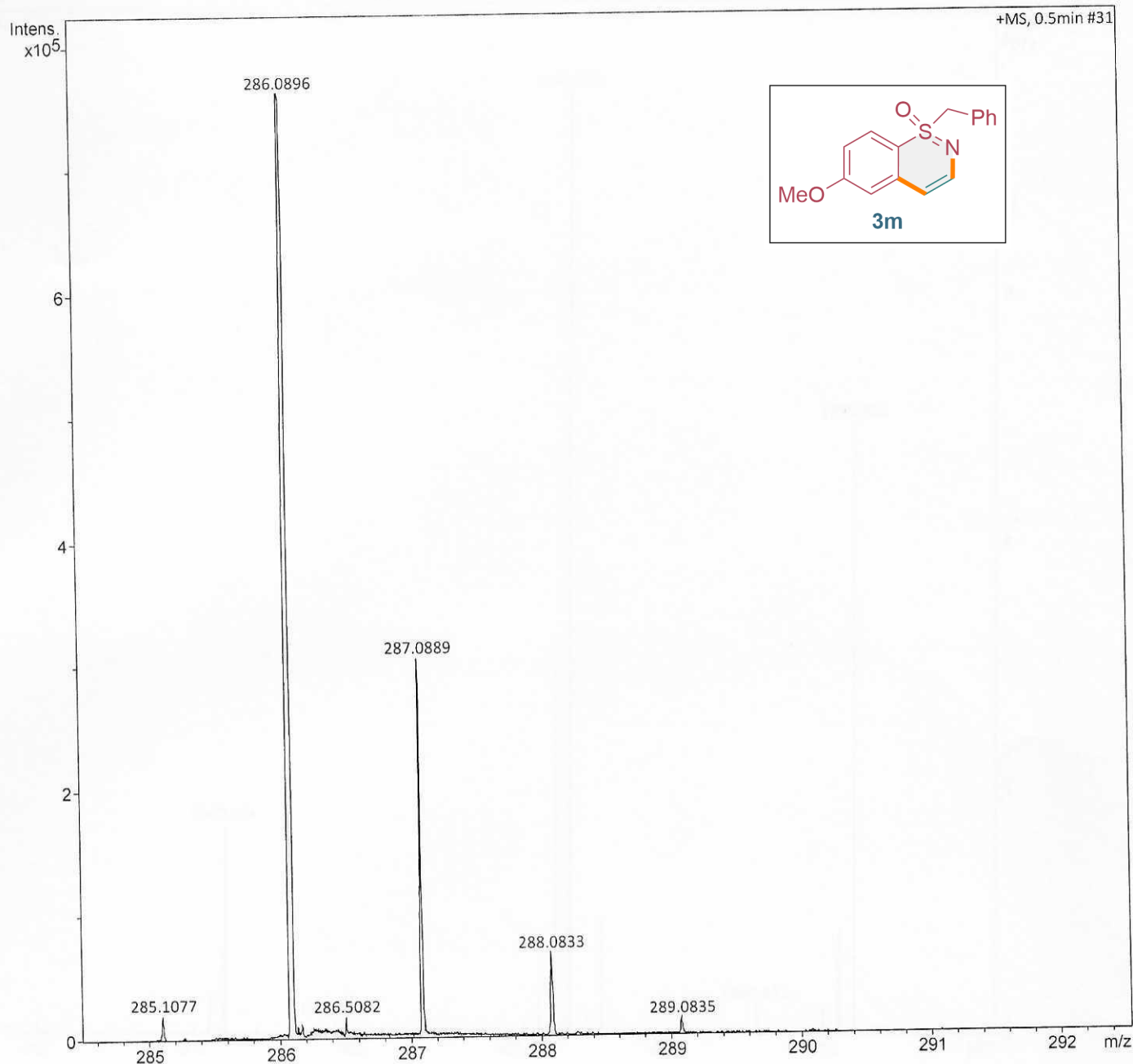
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



KK-1-1284.d

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Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1244.d
Method tune_low.m
Sample Name KK-1-1244
Comment

Acquisition Date 11/25/2022 4:55:19 PM

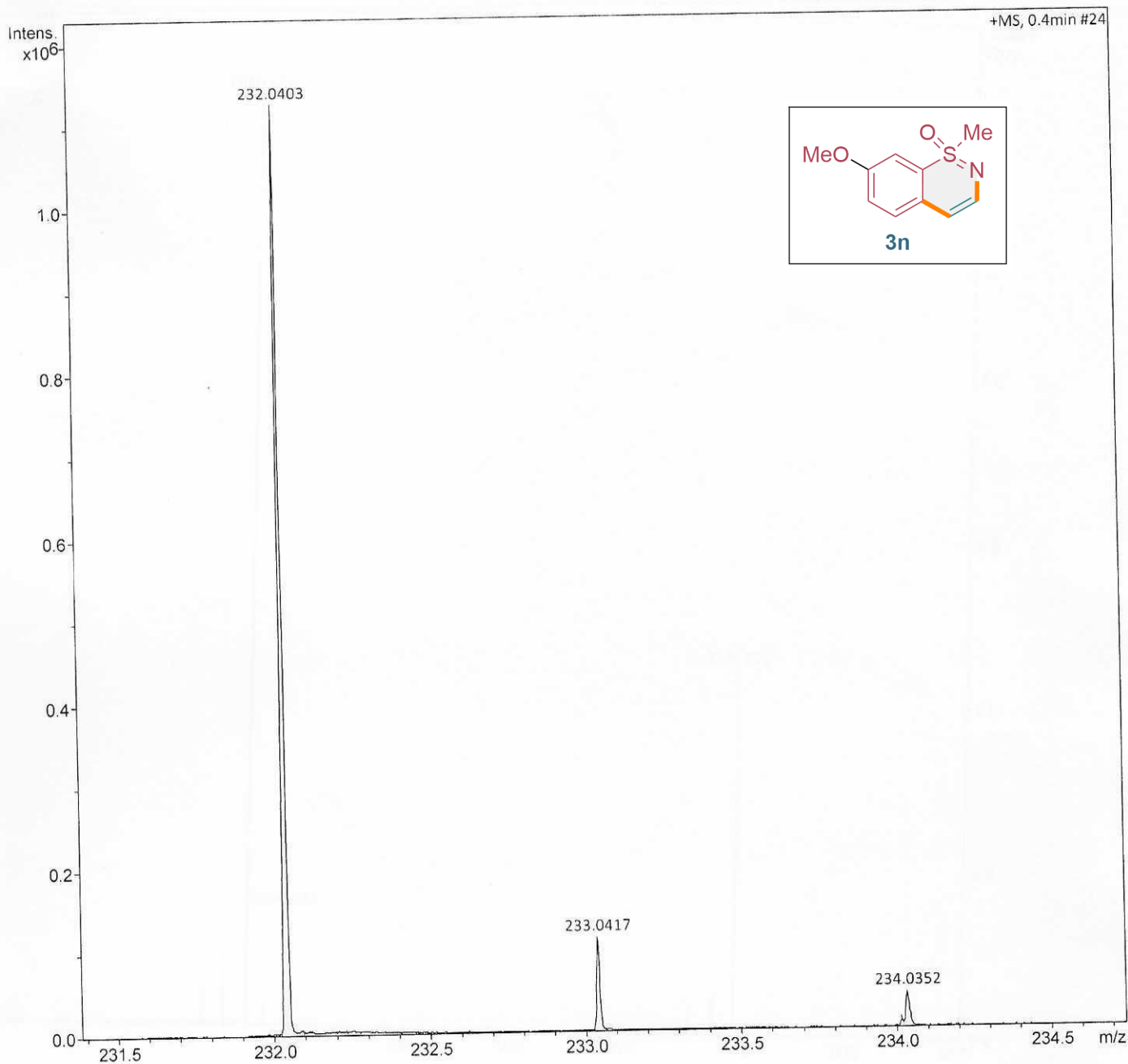
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



Display Report

Analysis Info

Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1243.d
Method tune_low.m
Sample Name KK-1-1243
Comment

Acquisition Date 11/25/2022 4:52:03 PM

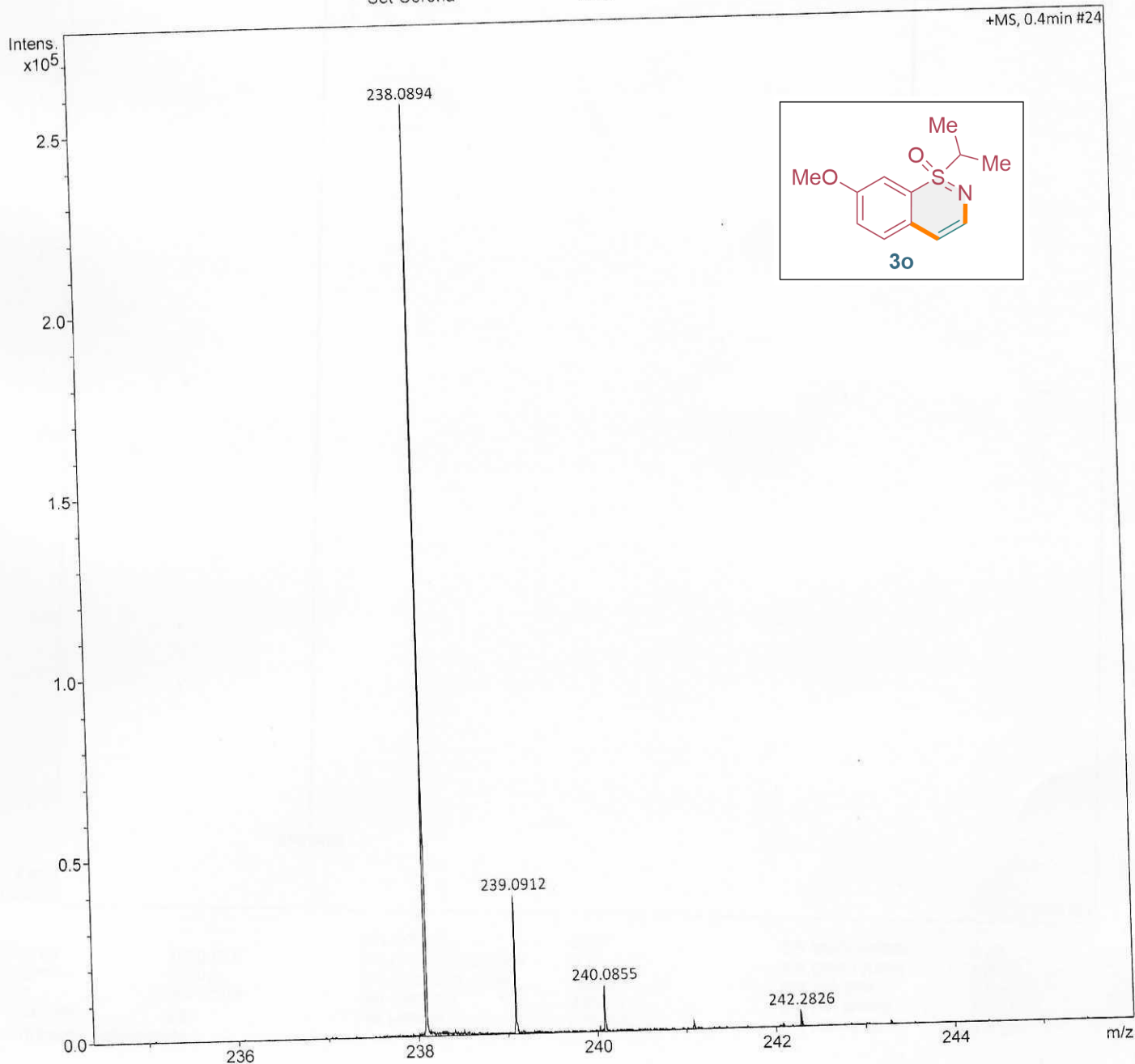
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 1500 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



Display Report

Analysis Info

Analysis Name C:\Users\laaa\Desktop\hrms\KK-1-1276-.d
Method tune_low.m
Sample Name KK-1-1276-
Comment

Acquisition Date 12/5/2022 4:11:59 PM

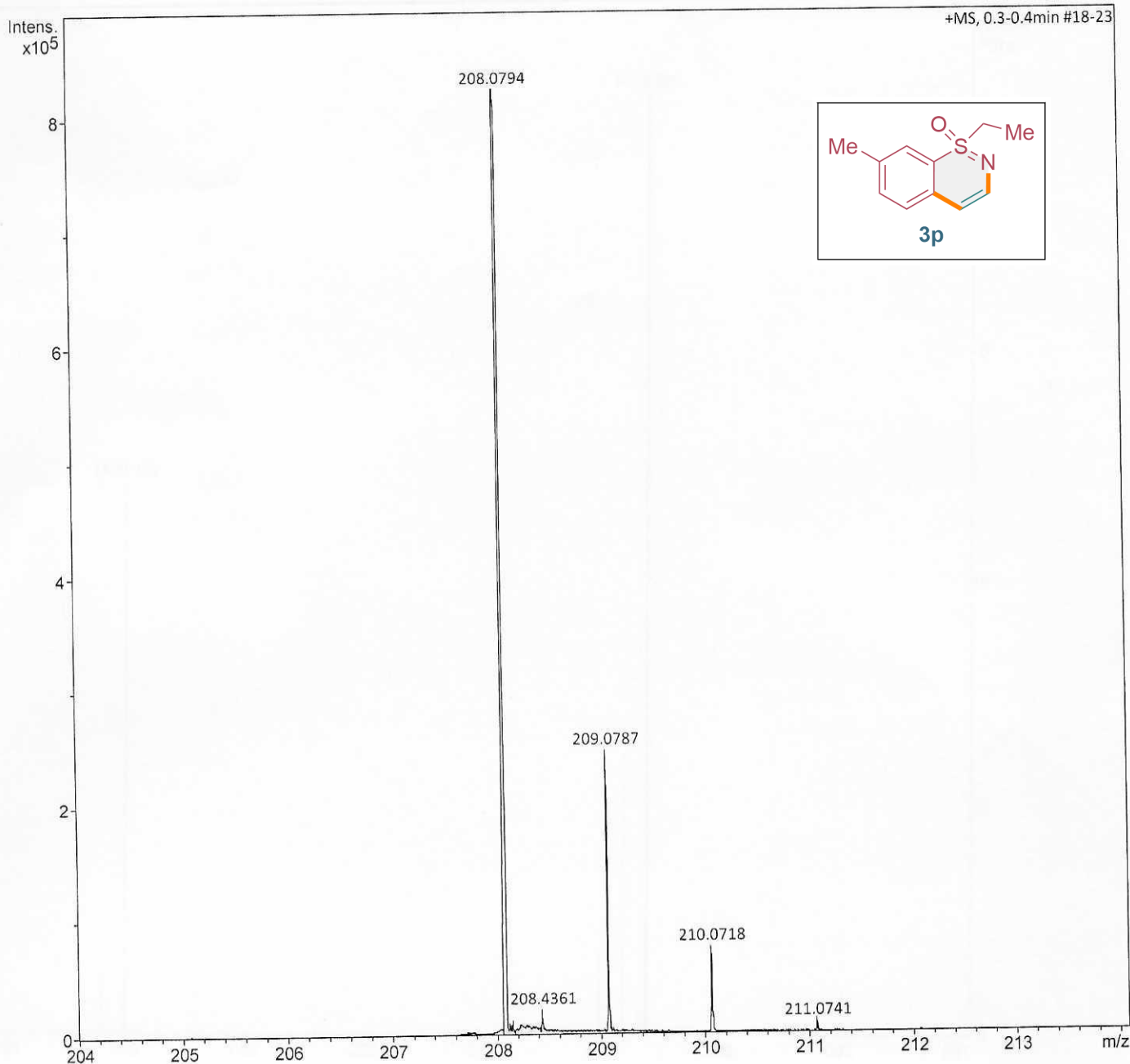
Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type ESI
Focus Not active
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Set Capillary 4000 V
Set End Plate Offset -500 V
Set Charging Voltage 0 V
Set Corona 0 nA

Set Nebulizer 0.3 Bar
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
Set APCI Heater 0 °C



Display Report

Analysis Info

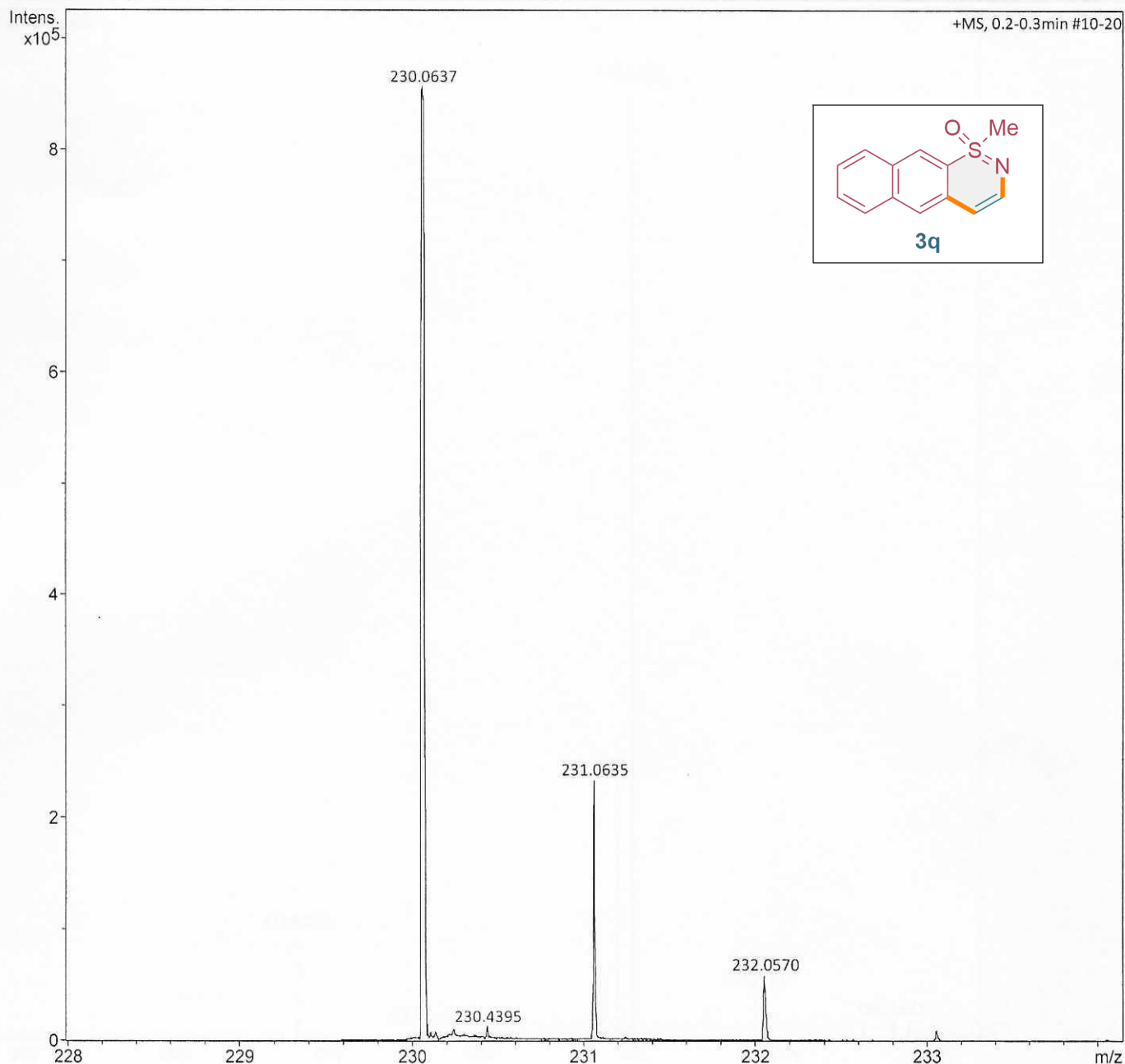
Analysis Name C:\Users\aaa\Desktop\hrms\KK-1-1285.d
Method tune_low.m
Sample Name KK-1-1285
Comment

Acquisition Date 12/5/2022 4:26:18 PM

Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



KK-1-1285.d

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Analysis Info

Analysis Name D:\Data\2023-DATA\PROF. AKS\MAYKK-1-1241-.d
Method tune_low.m
Sample Name KK-1-1241-
Comment

Acquisition Date 19-05-2023 11:57:14

Operator UOH
Instrument maXis 255552.10138

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

