

The cycloaddition reaction of benzothiazolium ylides with α -cyanocinnamamides: the synthesis of structural analogs of inhibitors of HIV-1 post-integrational repair

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Marina B. Gottikh³, Mikhail S. Baranov^{1,4}, Andrey A. Mikhaylov^{1,4*}**

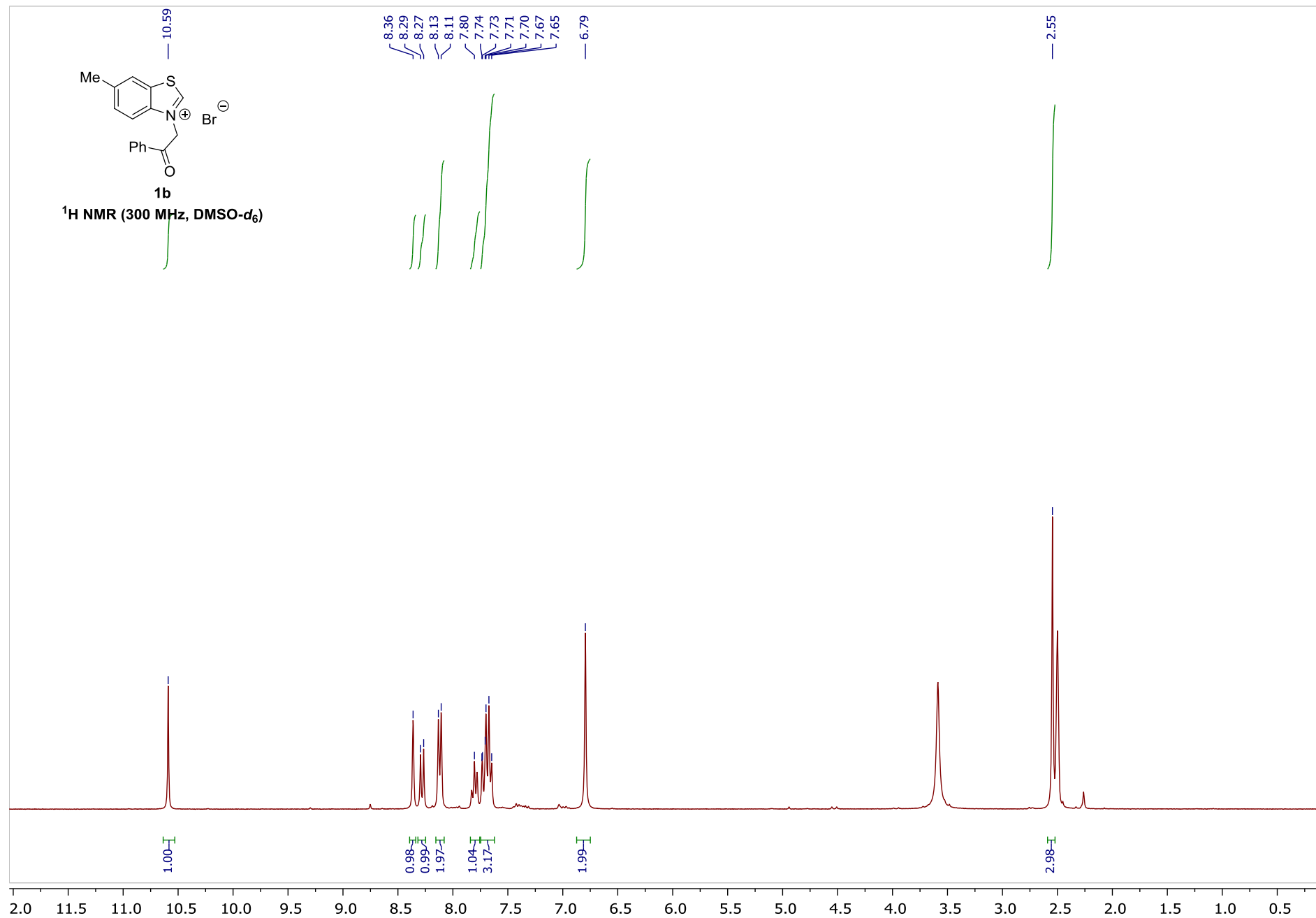
¹ *Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences,
16/10 Miklukho-Maklaya St., Moscow 117997, Russia; e-mail: mikhaylov_andrey@yahoo.com*

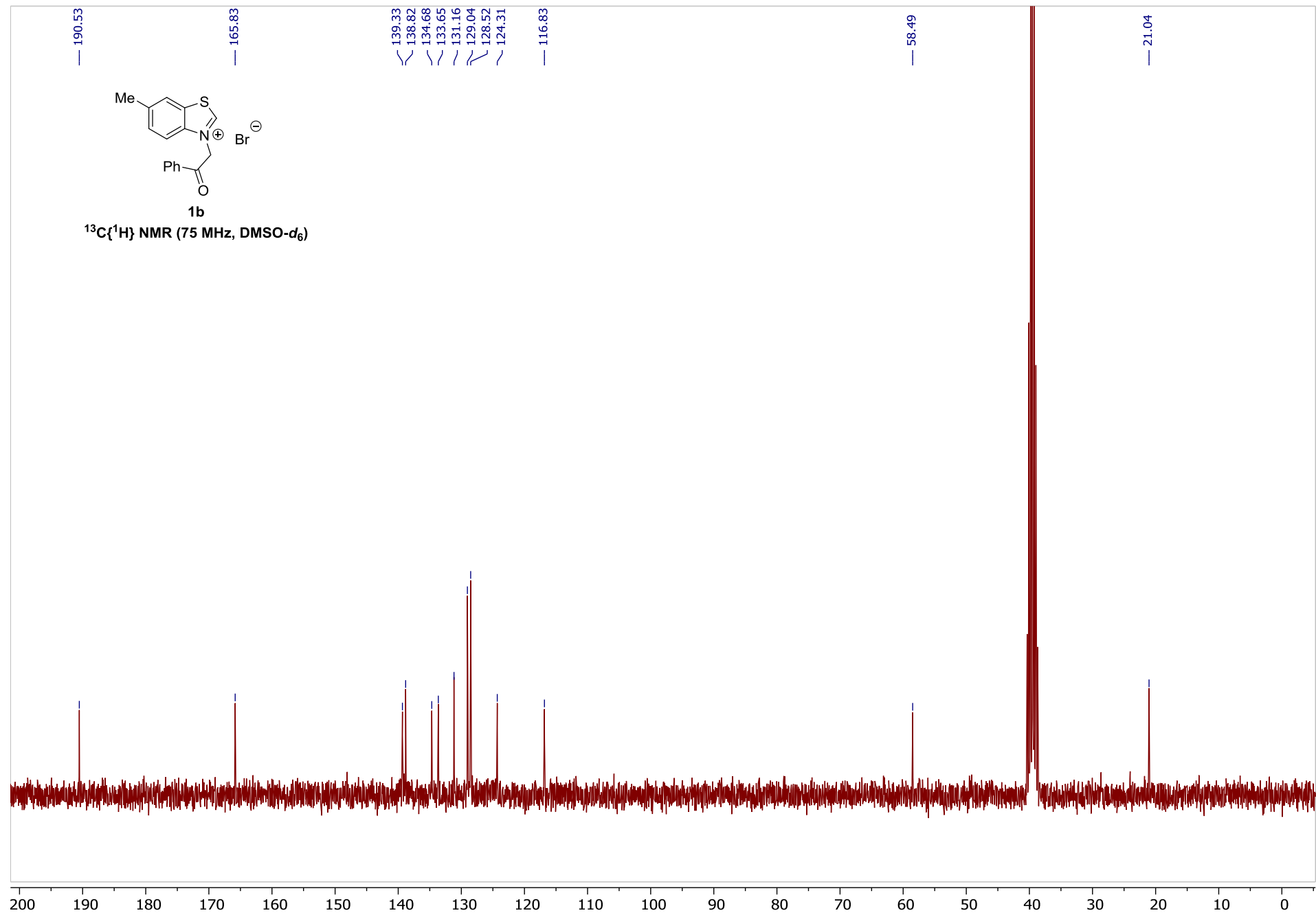
² *Lomonosov Moscow State University,
1, Build. 3 Leninskie Gory, Moscow 119992, Russia*

³ *A.N. Belozresky Institute of Physico-Chemical Biology, Moscow State University,
1, Build. 40 Leninskie Gory, Moscow 119902, Russia*

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1 Ostrovityanova St., Moscow 117997, Russia*

SUPPLEMENTARY INFORMATION





Display Report

Analysis Info

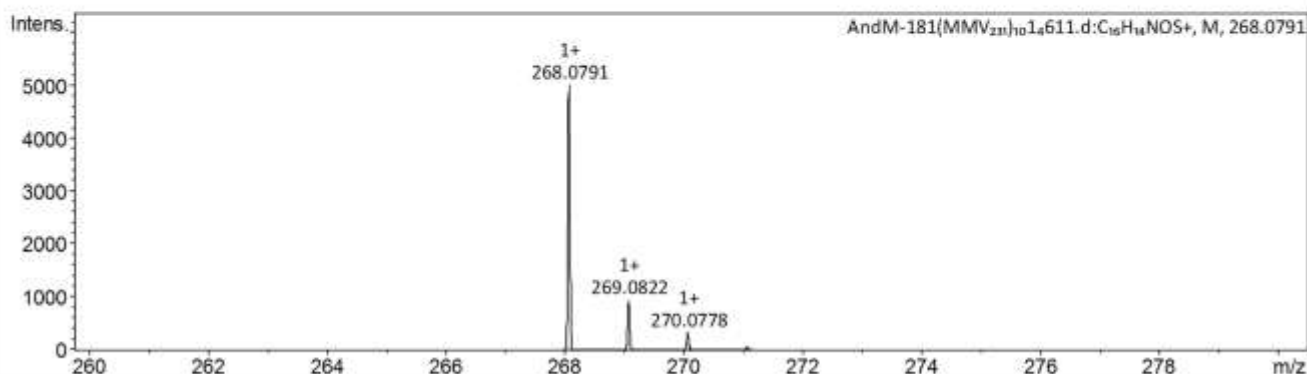
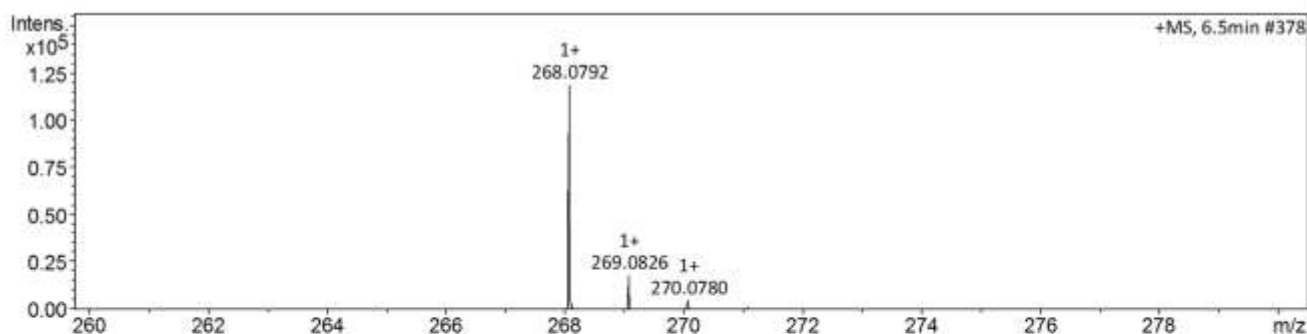
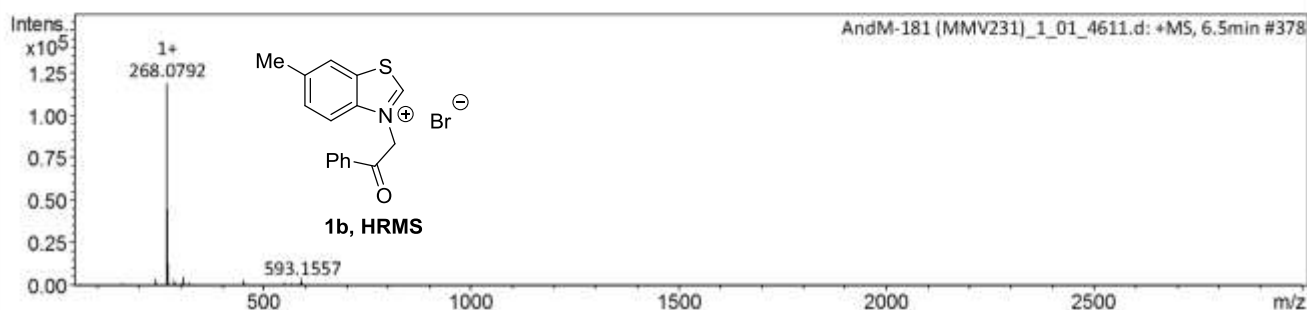
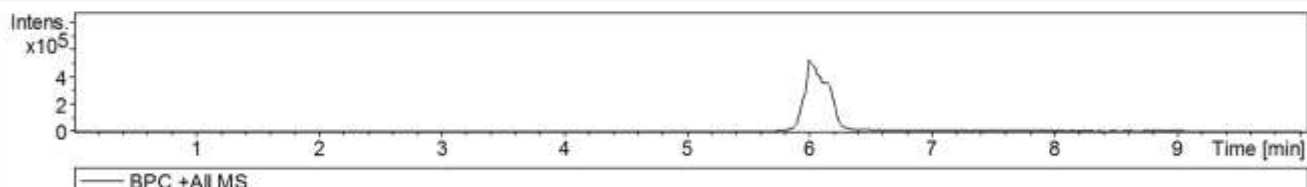
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Sample Name AndM-181 (MMV231)
Comment

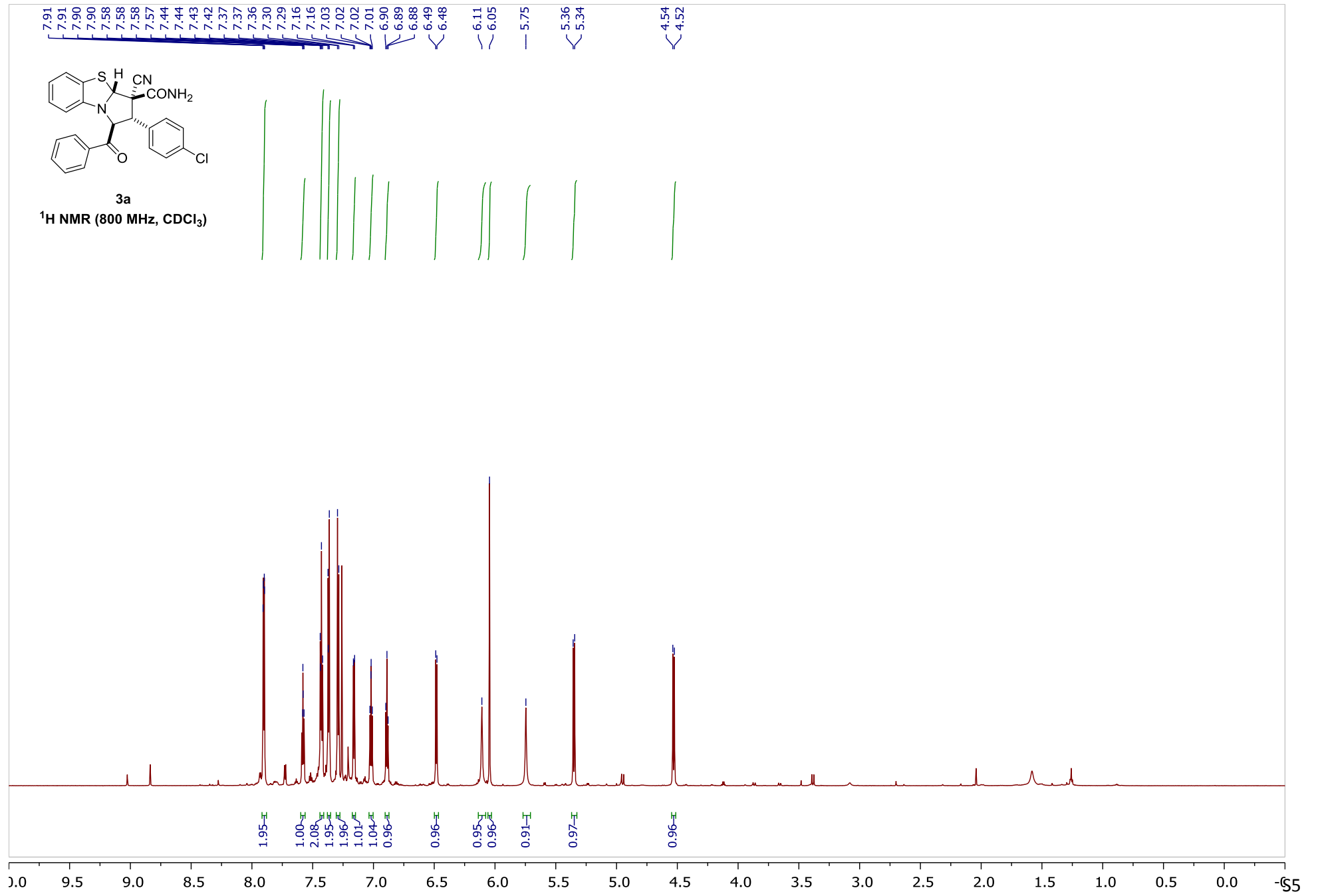
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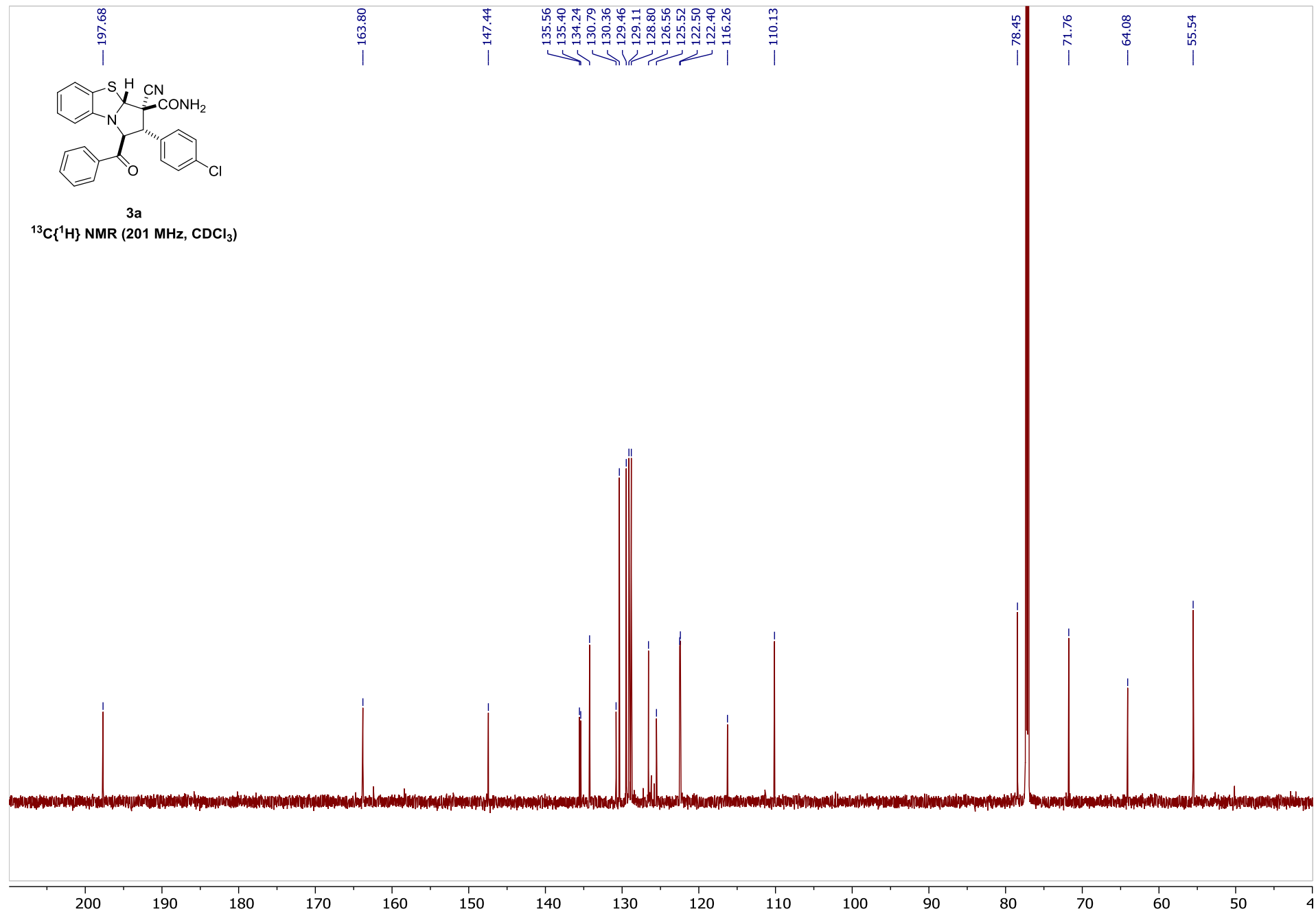
Operator BDAL@DE
Instrument compact 8255754.20088

Acquisition Parameter

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| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 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 | 3000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |







Display Report

Analysis Info

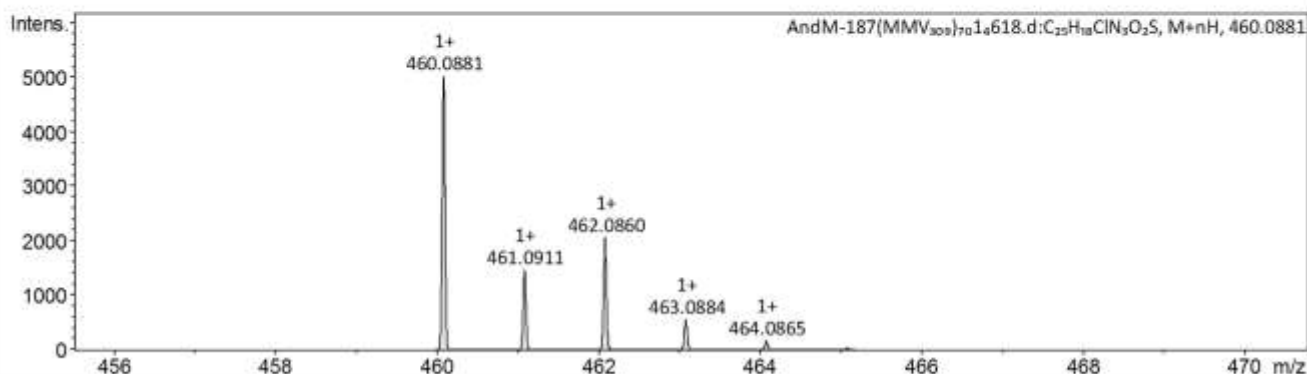
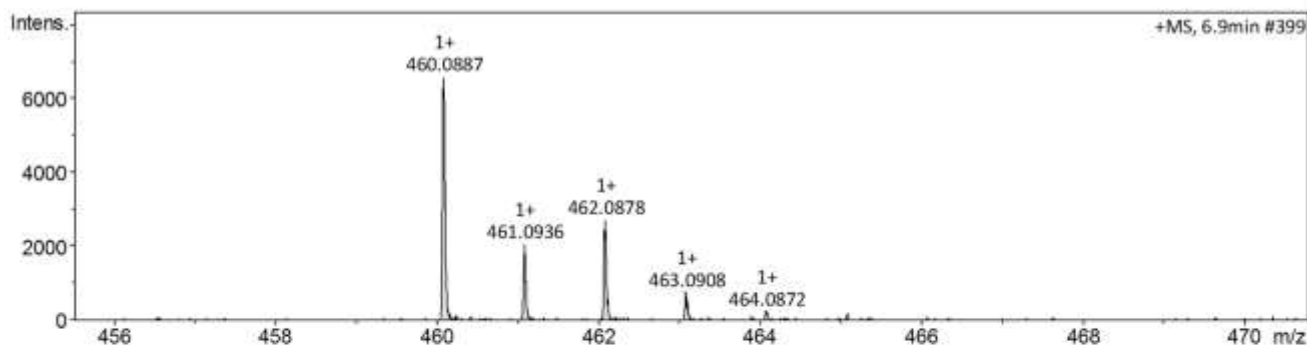
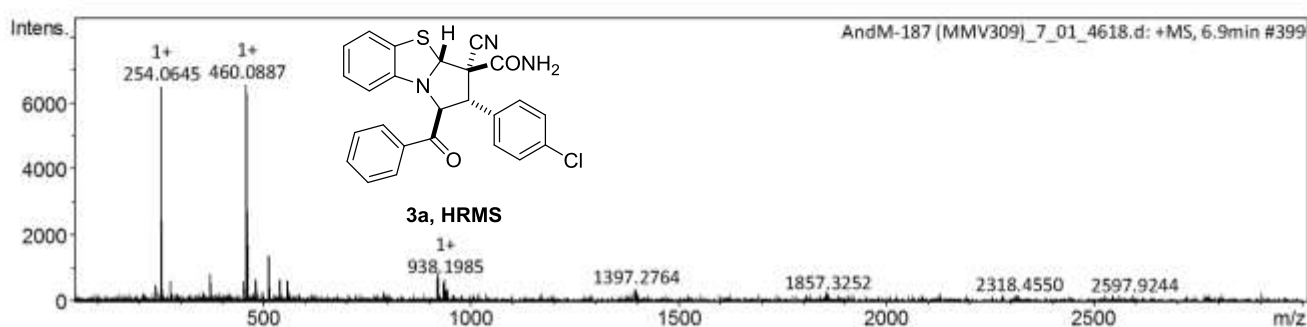
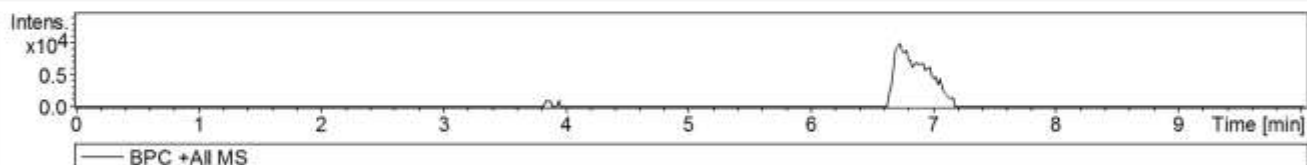
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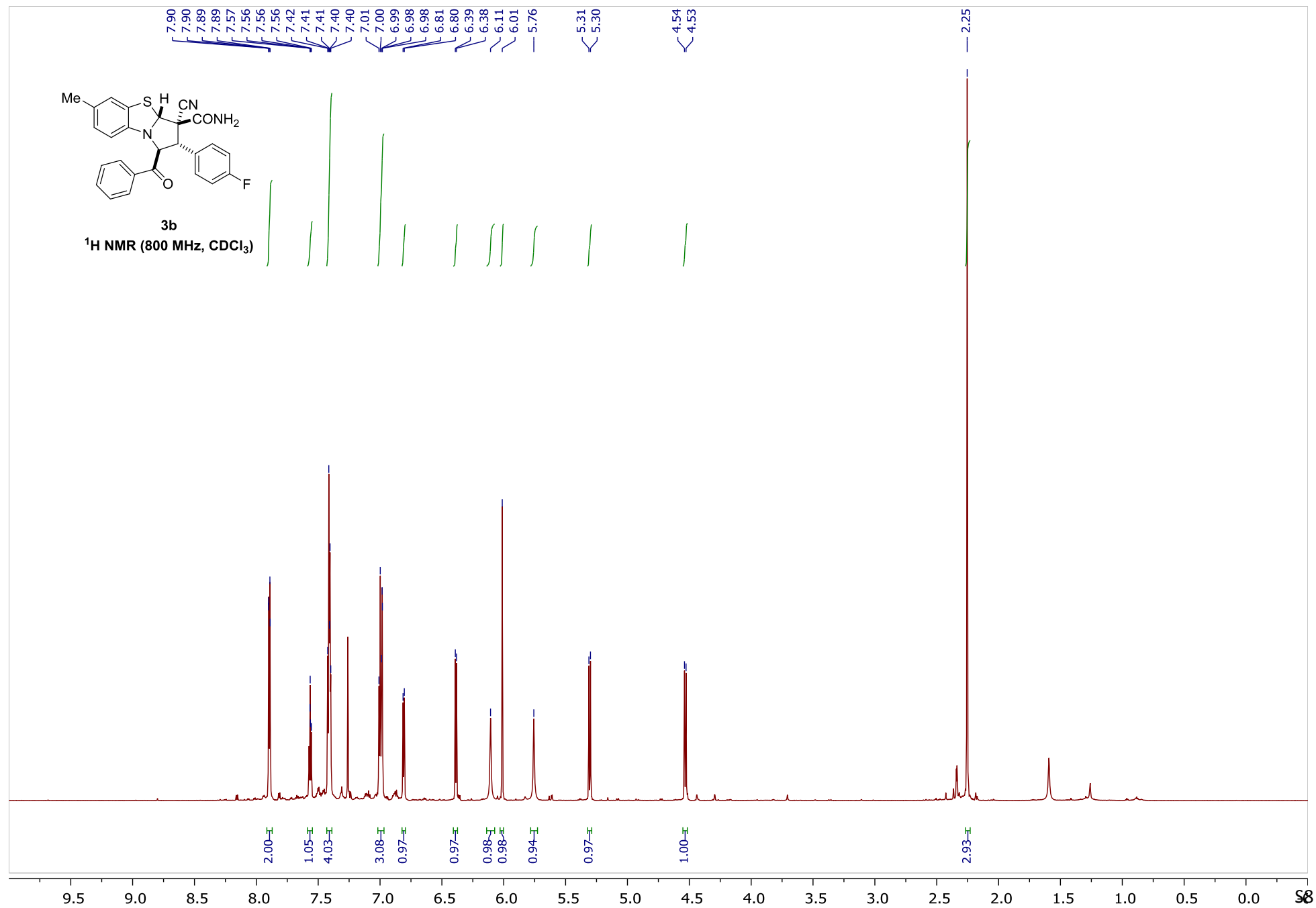
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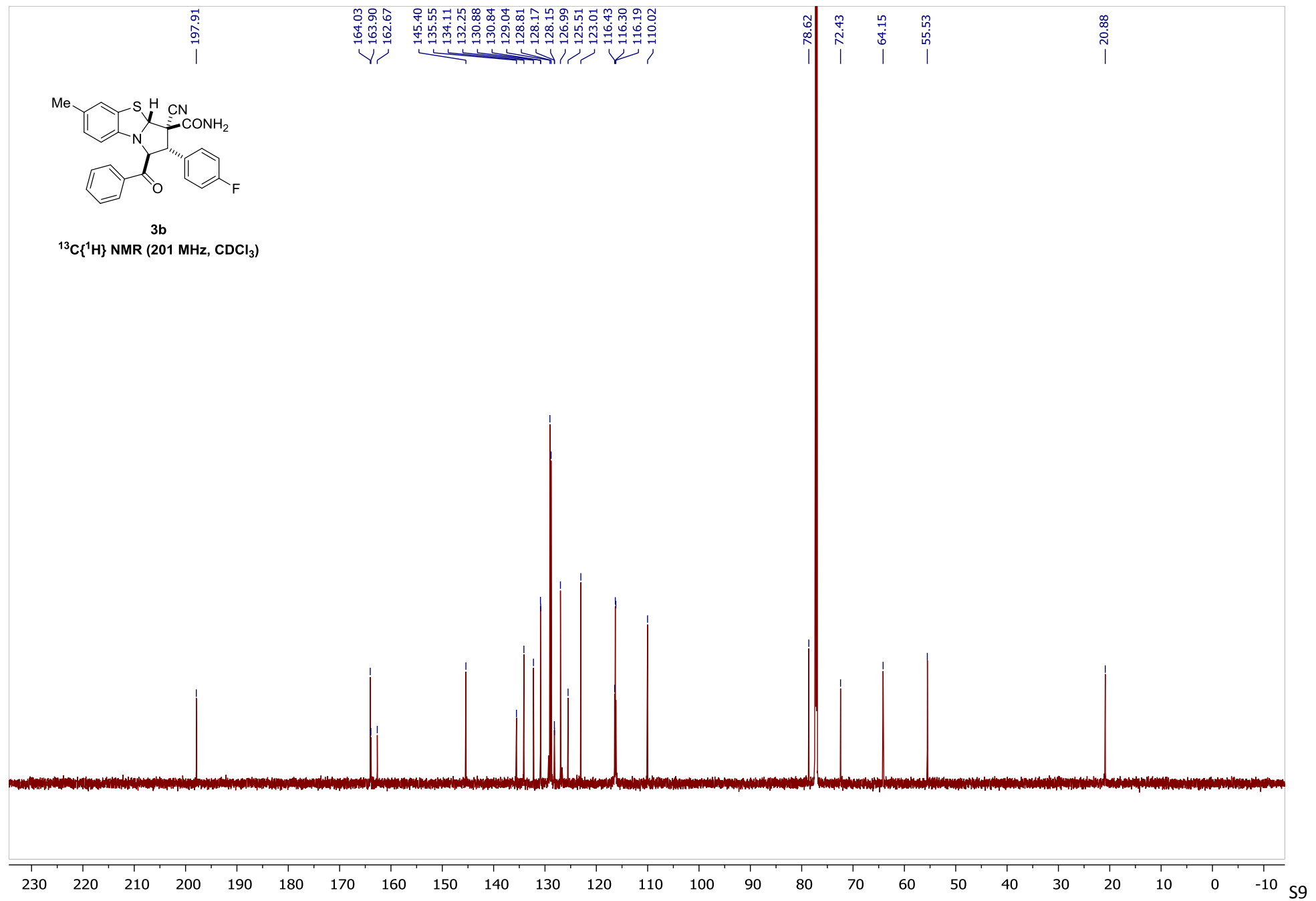
Operator BDAL@DE
Instrument compact 8255754.20088

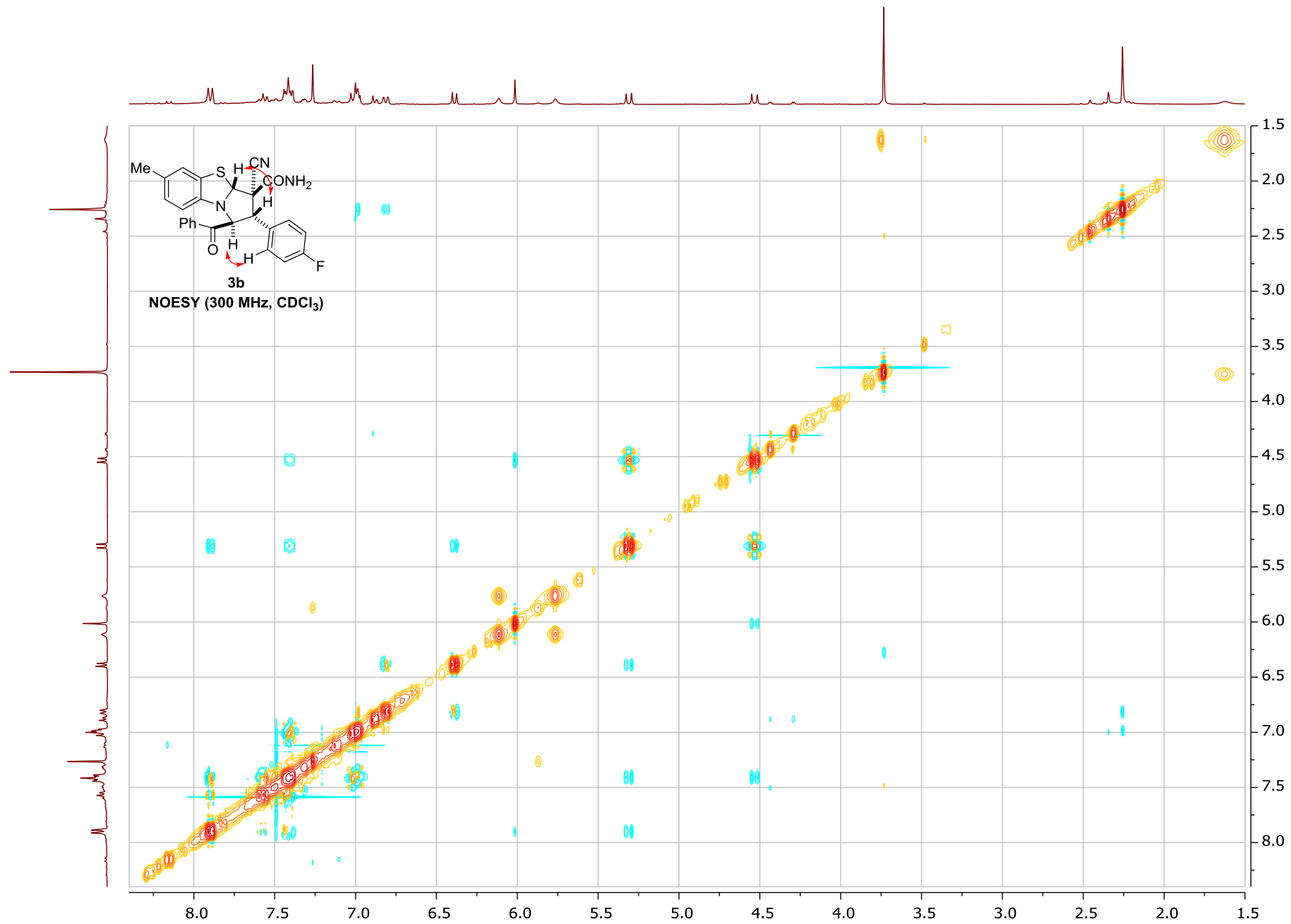
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| Focus | Active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |









Sample Name: MMV183

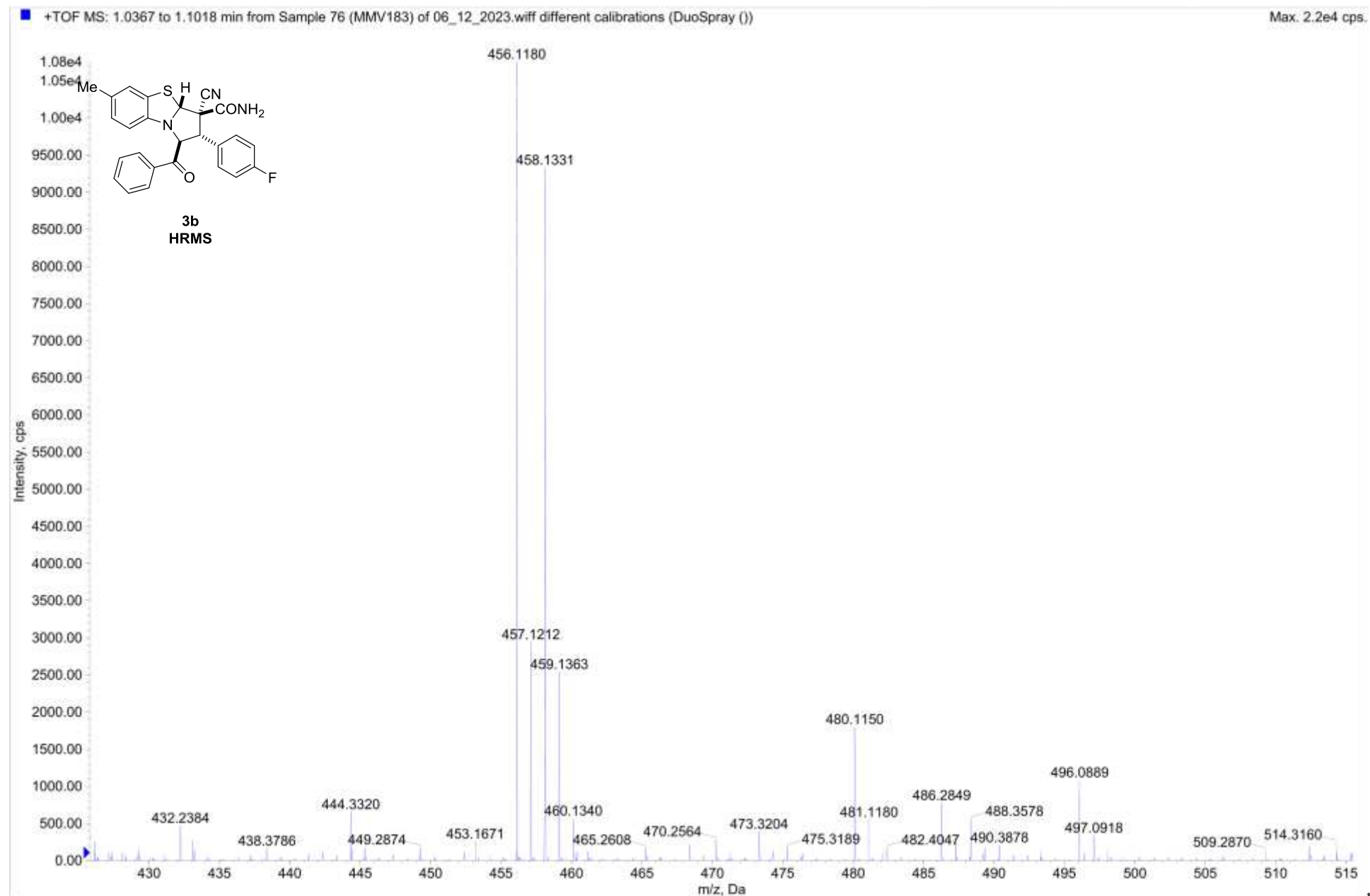
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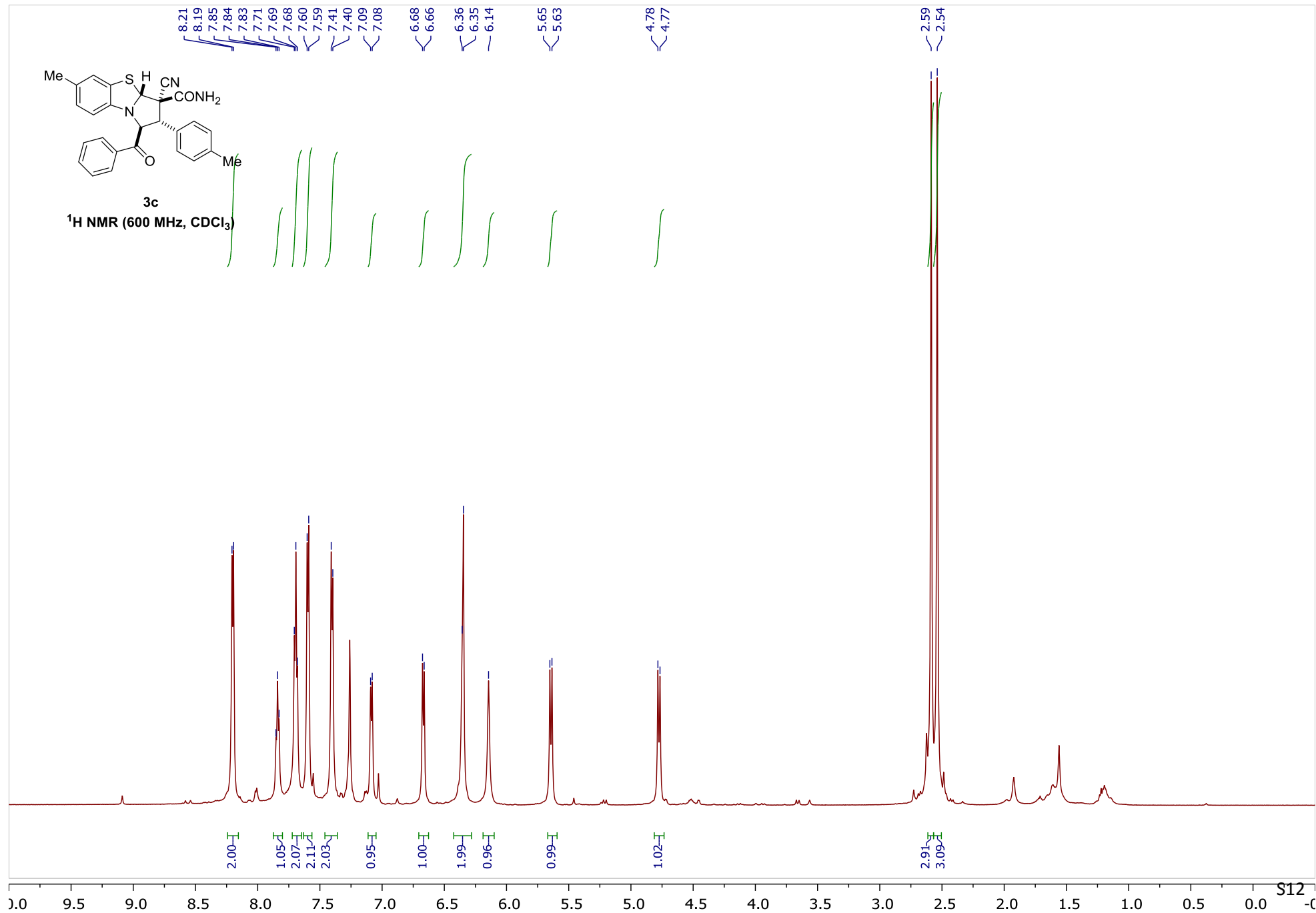
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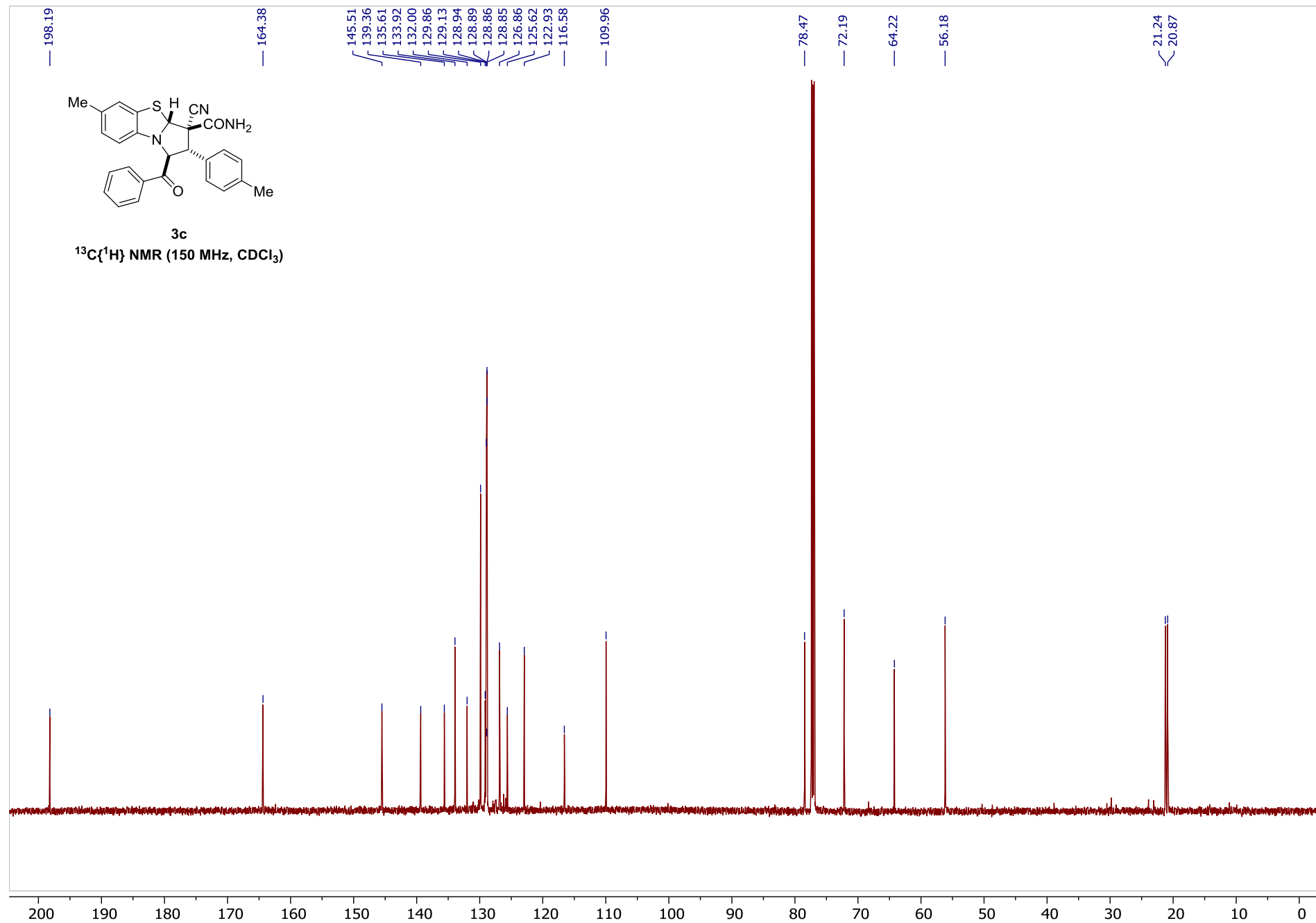
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*5600 TripleTOF Service Report

Acq. Date: Wednesday, December 06, 2023







Display Report

Analysis Info

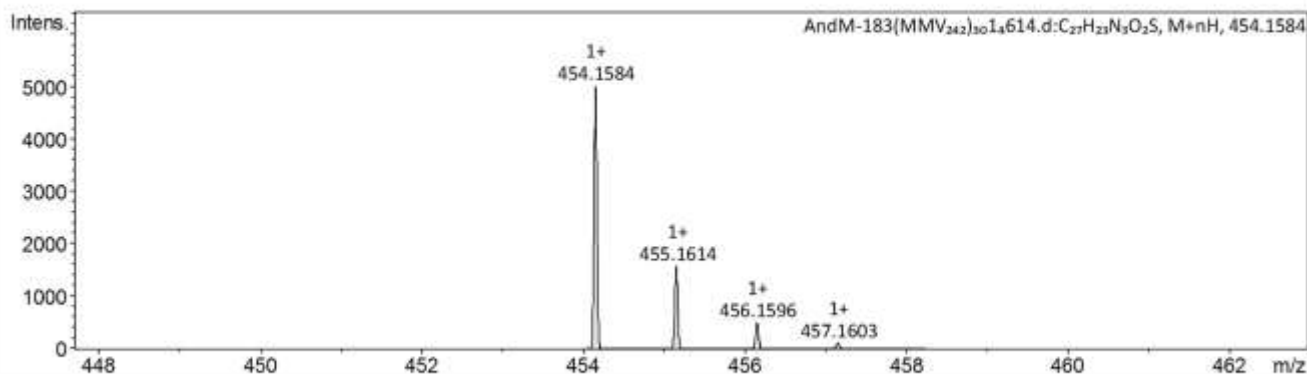
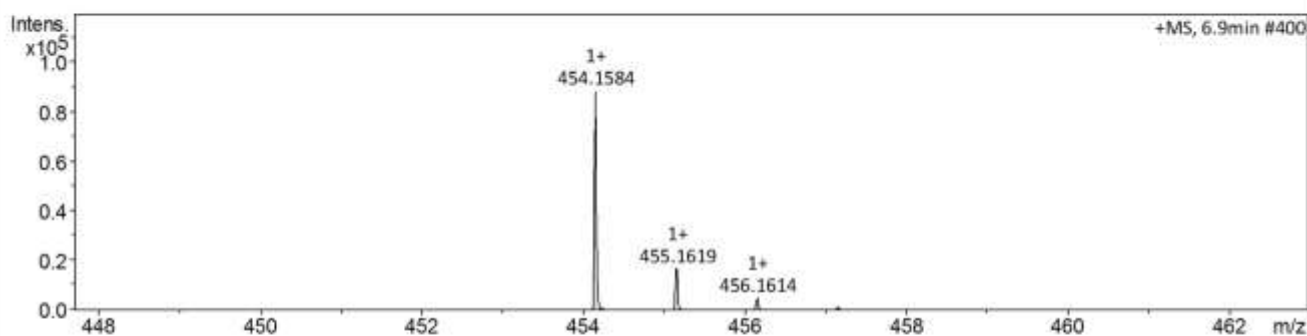
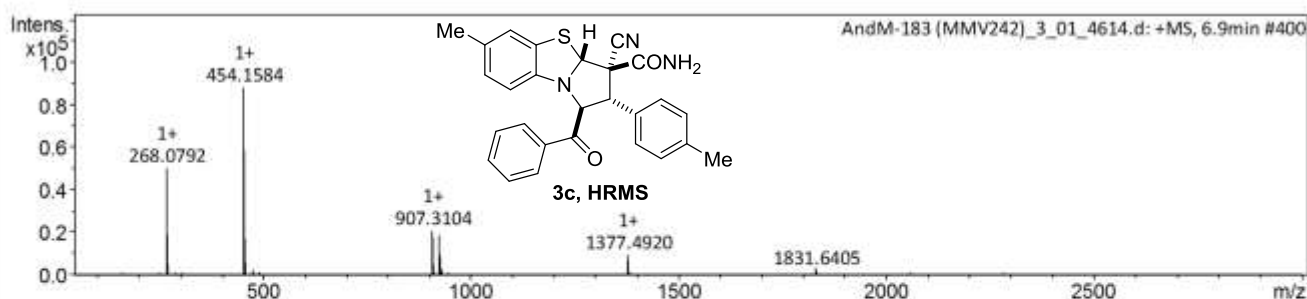
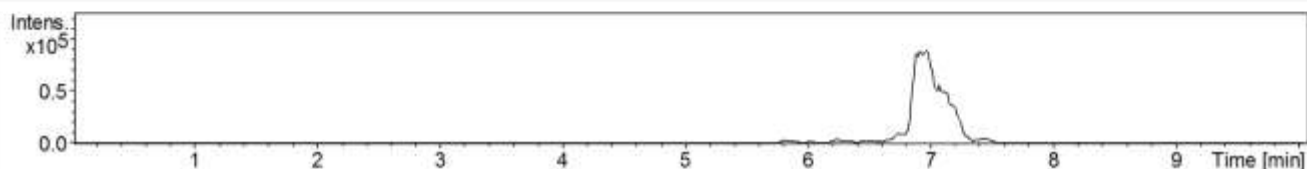
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Sample Name AndM-183 (MMV242)
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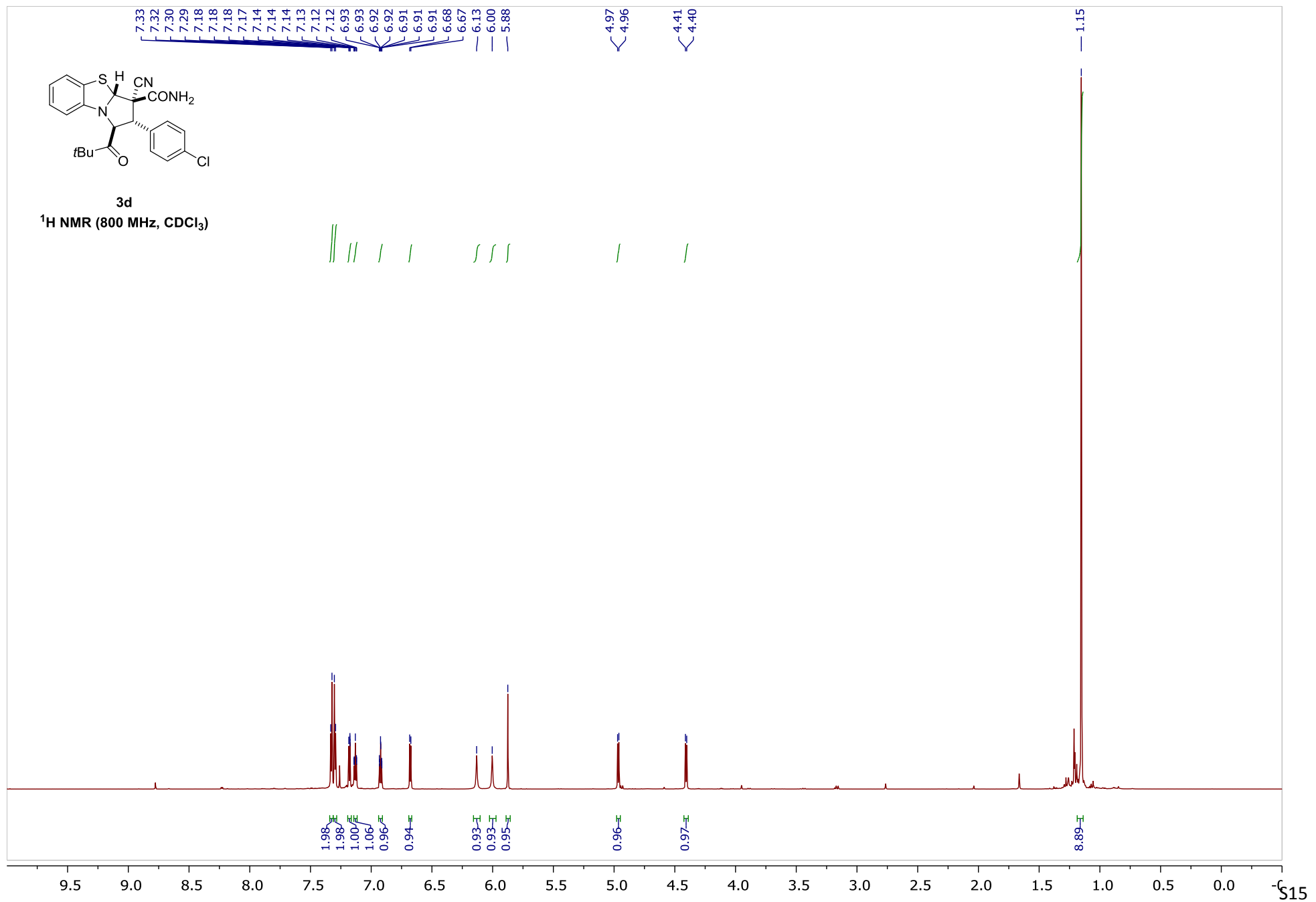
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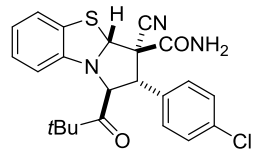
Operator BDAL@DE
Instrument compact 8255754.20088

Acquisition Parameter

| | | | | | |
|-------------|----------|----------------------|----------|------------------|-----------|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 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 | 3000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |

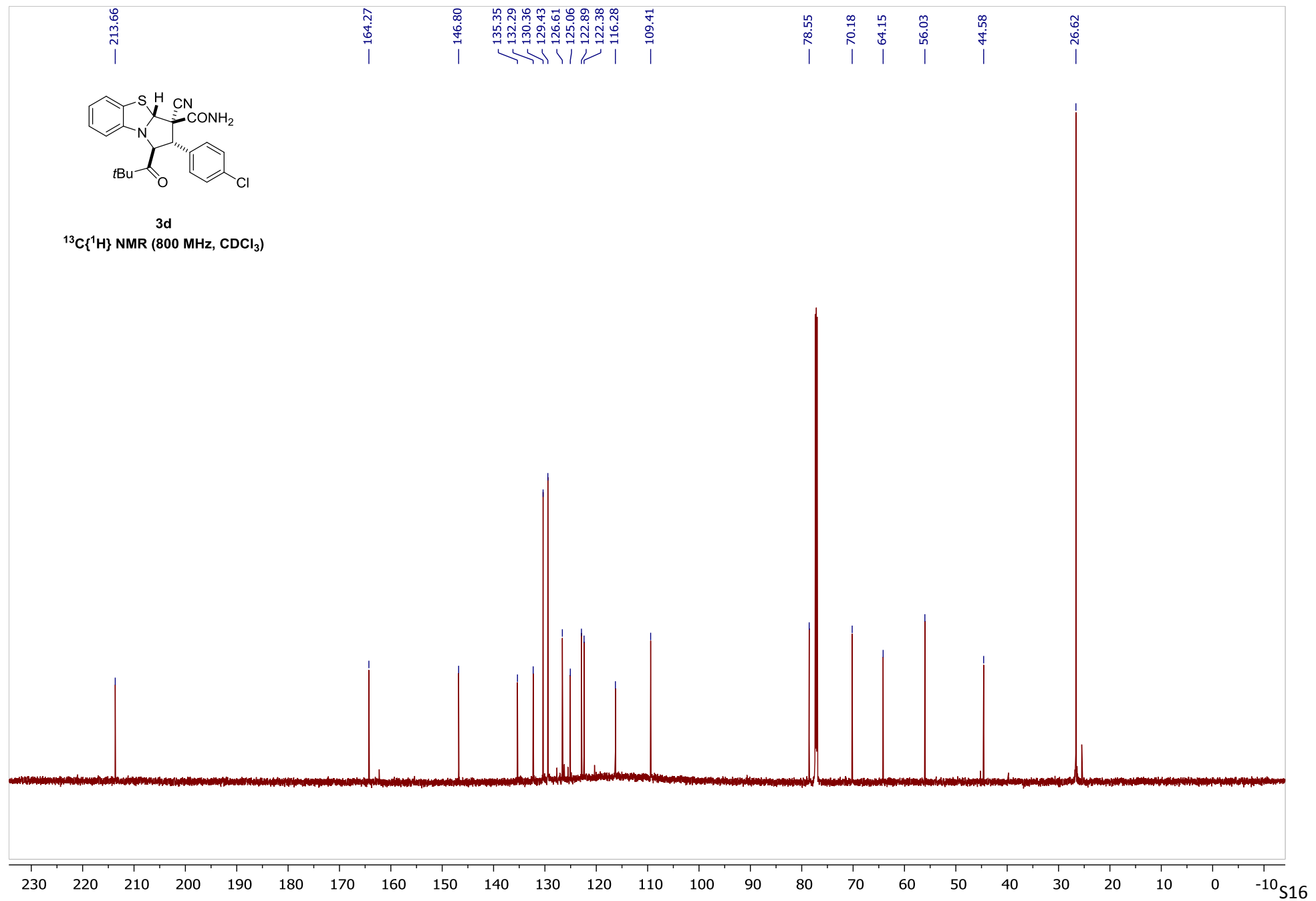






3d

$^{13}\text{C}\{^1\text{H}\}$ NMR (800 MHz, CDCl_3)



Display Report

Analysis Info

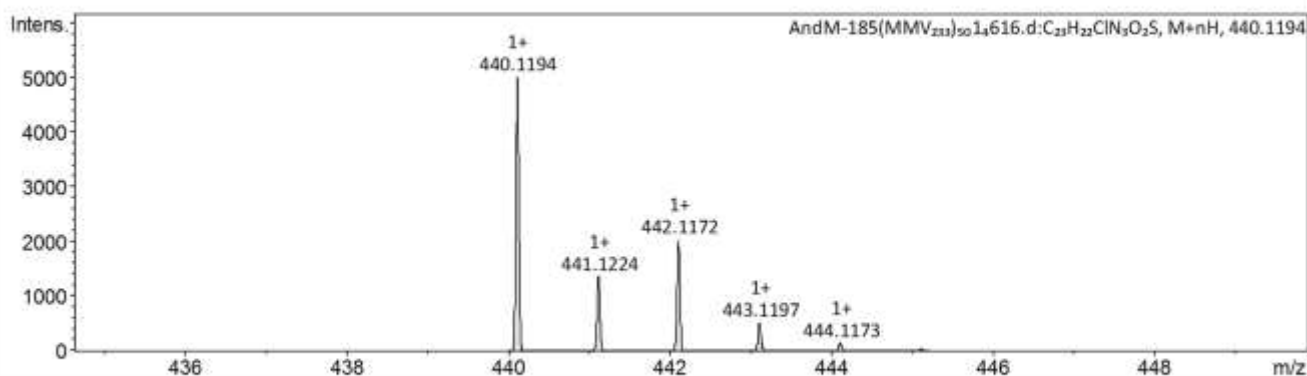
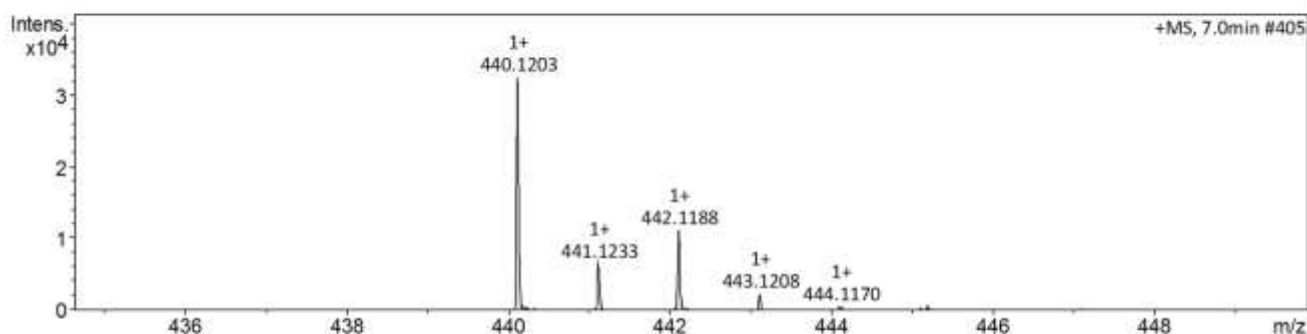
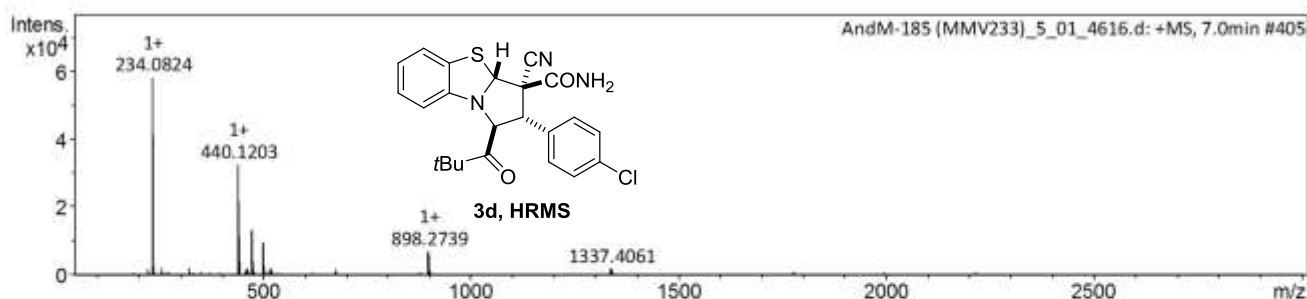
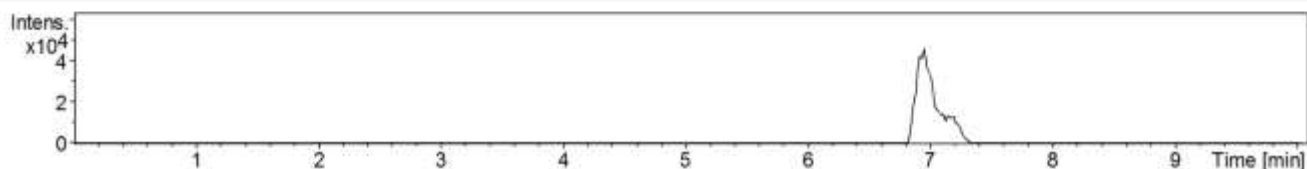
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Sample Name AndM-185 (MMV233)
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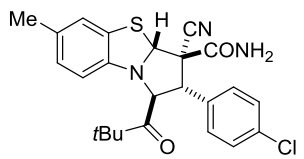
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Operator BDAL@DE
Instrument compact 8255754.20088

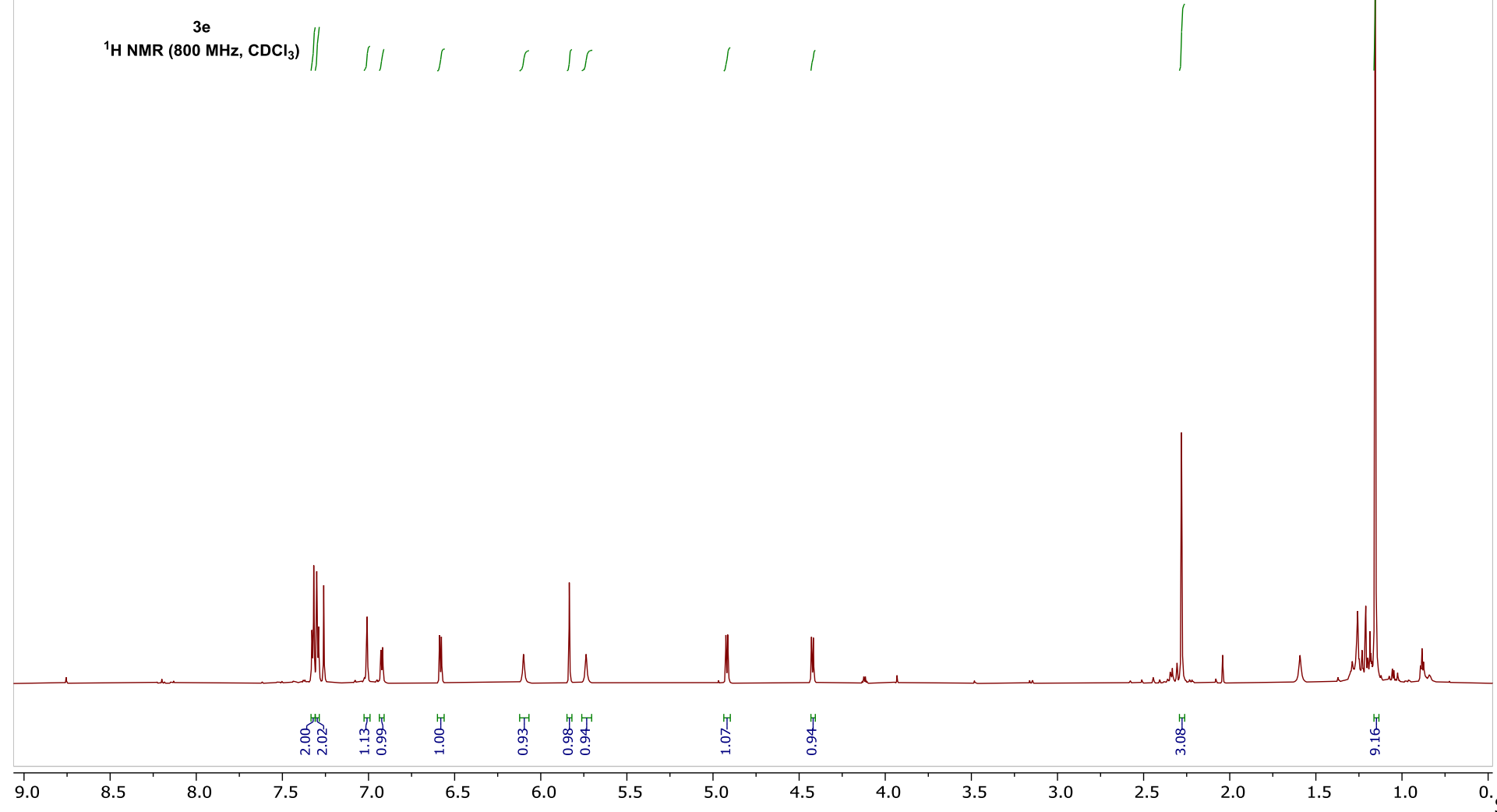
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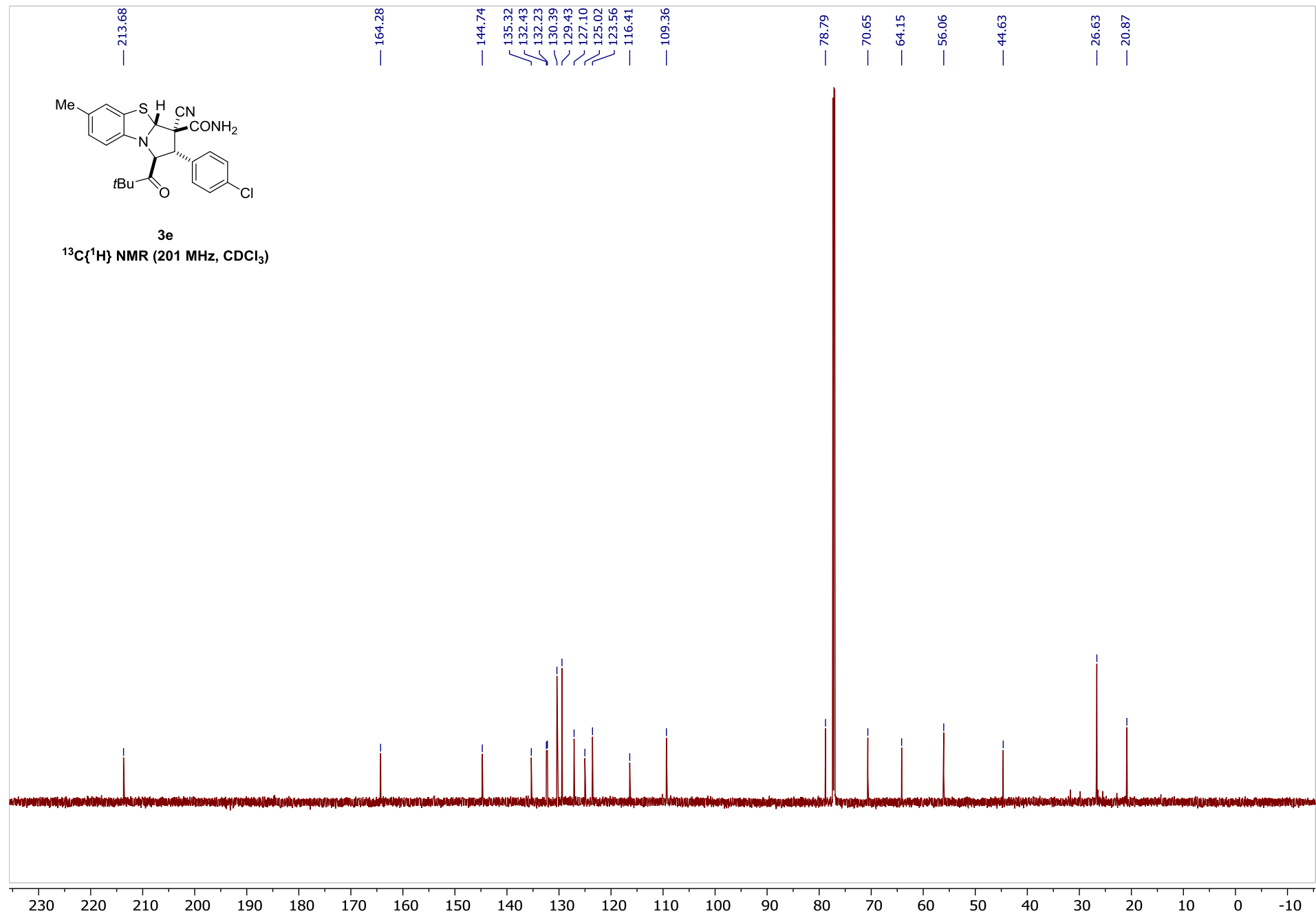
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| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |





3e
¹H NMR (800 MHz, CDCl₃)





Display Report

Analysis Info

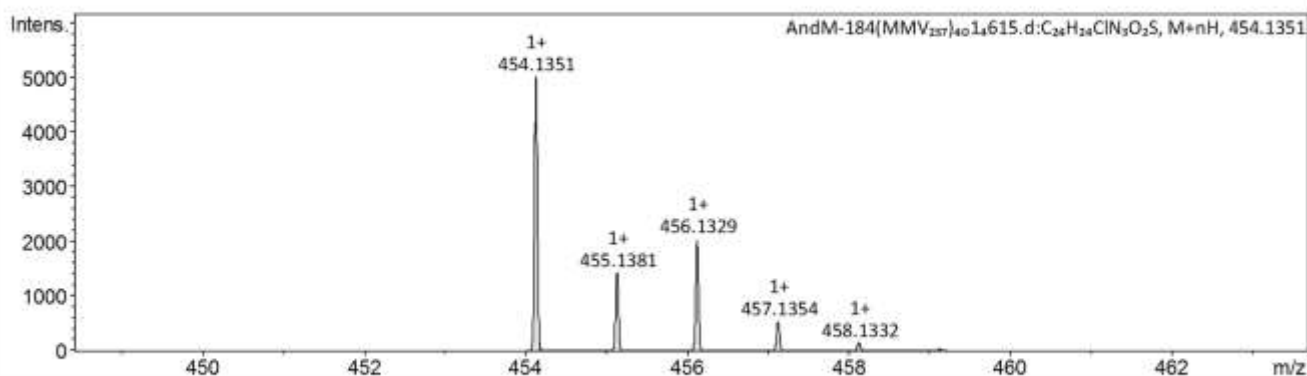
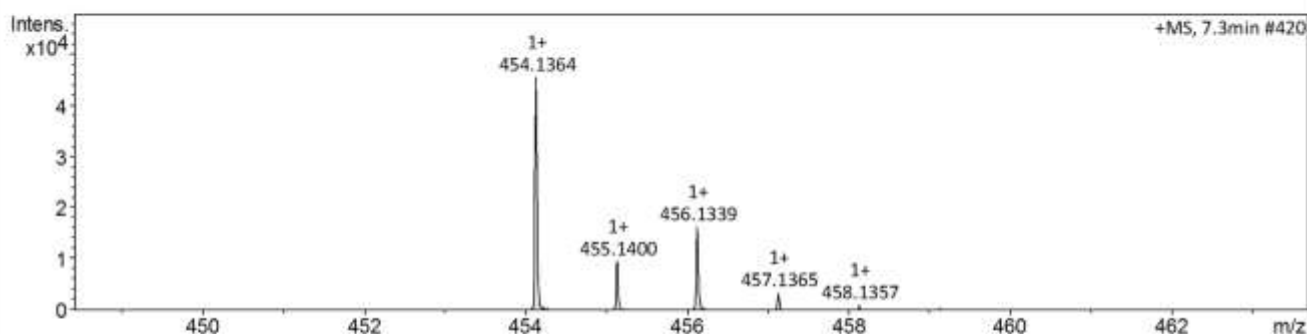
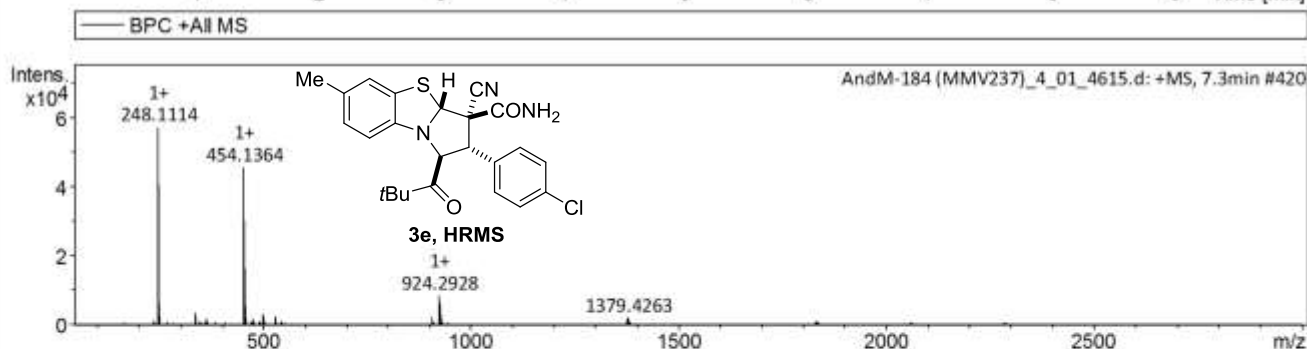
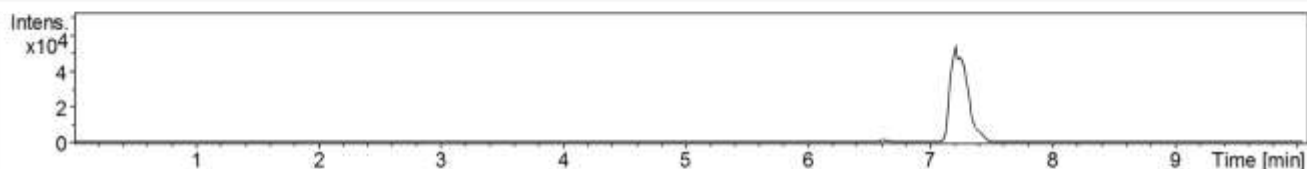
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Method la_2.2_small2.m
Sample Name AndM-184 (MMV237)
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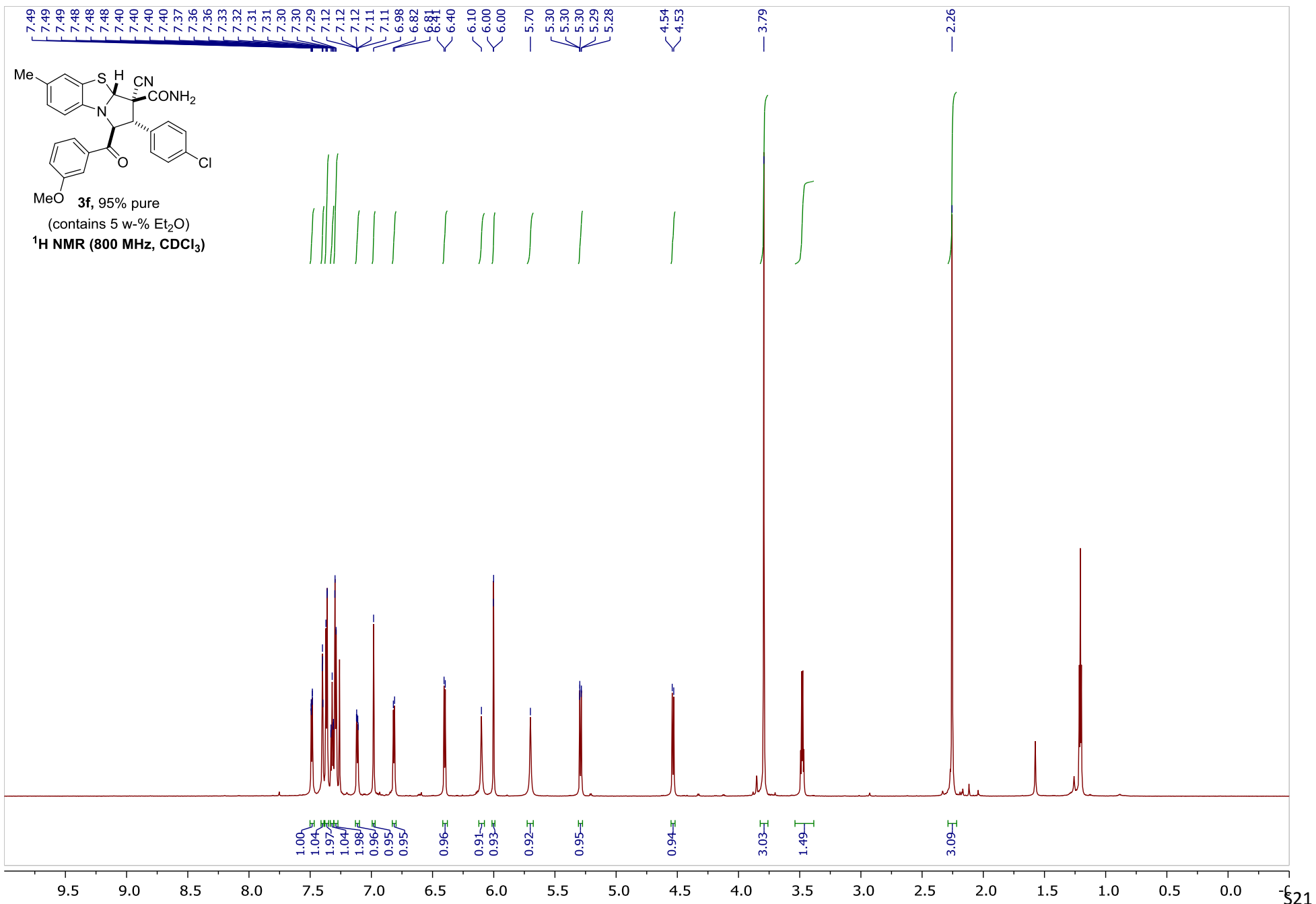
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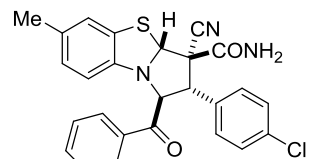
Operator BDAL@DE
Instrument compact 8255754.20088

Acquisition Parameter

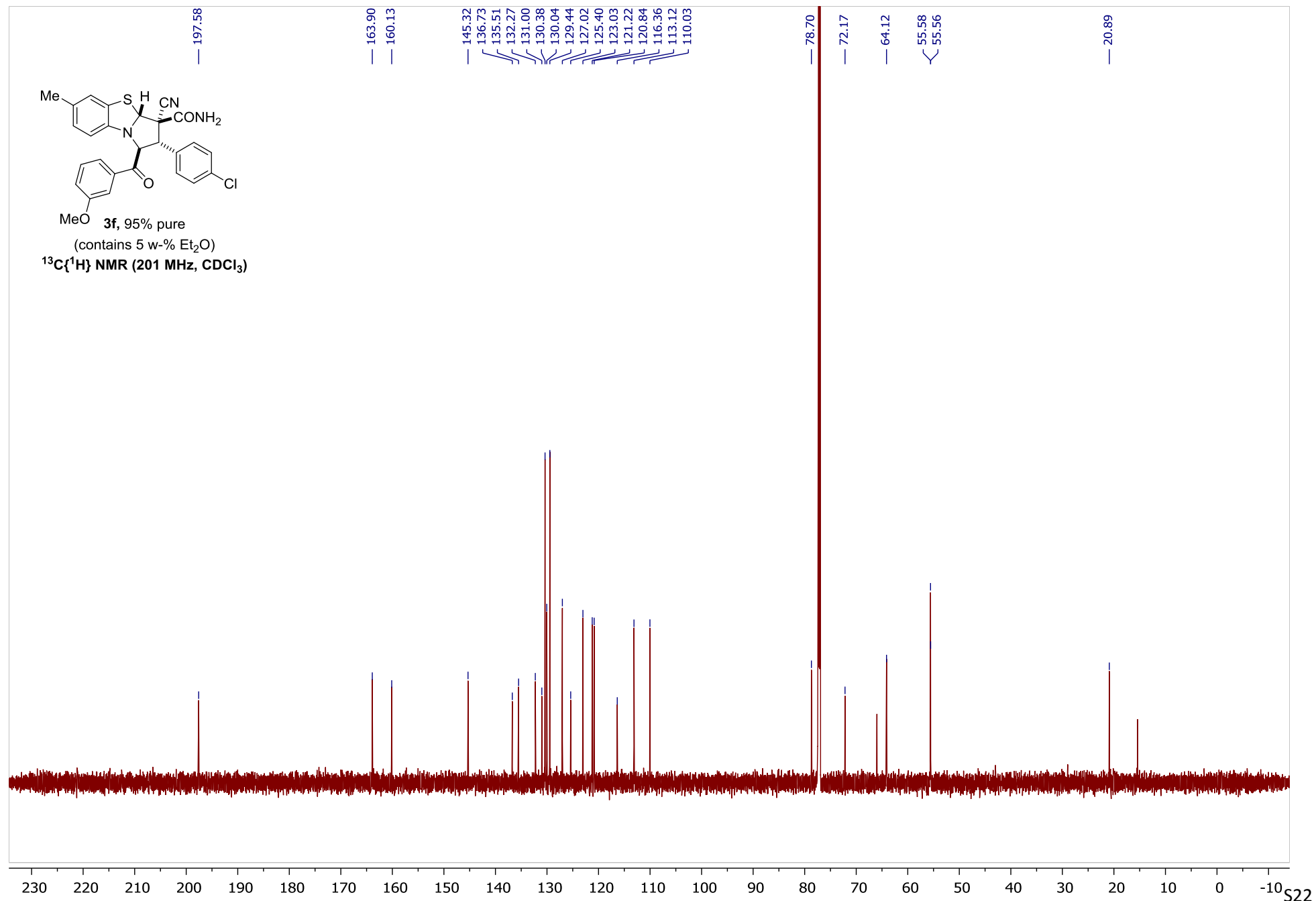
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| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |







3f, 95% pure
(contains 5 w-% Et₂O)
¹³C{¹H} NMR (201 MHz, CDCl₃)



Display Report

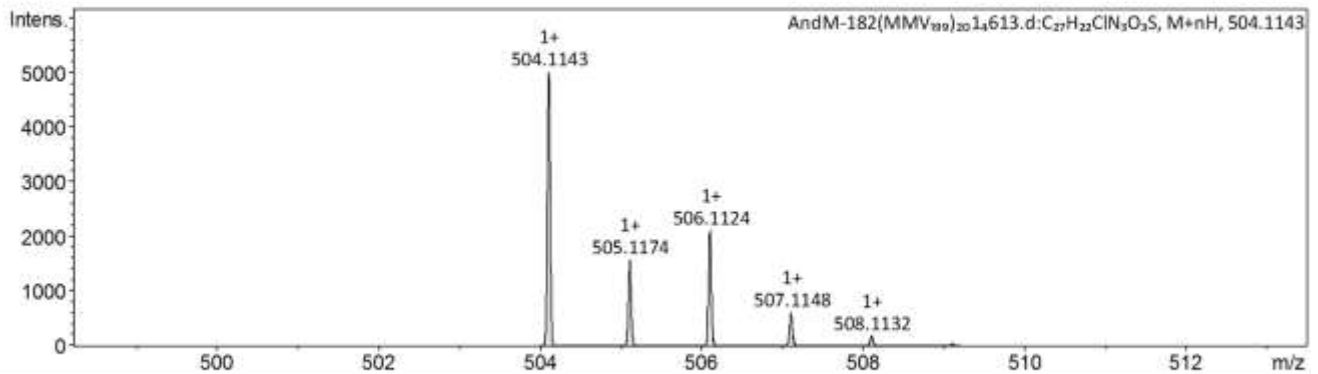
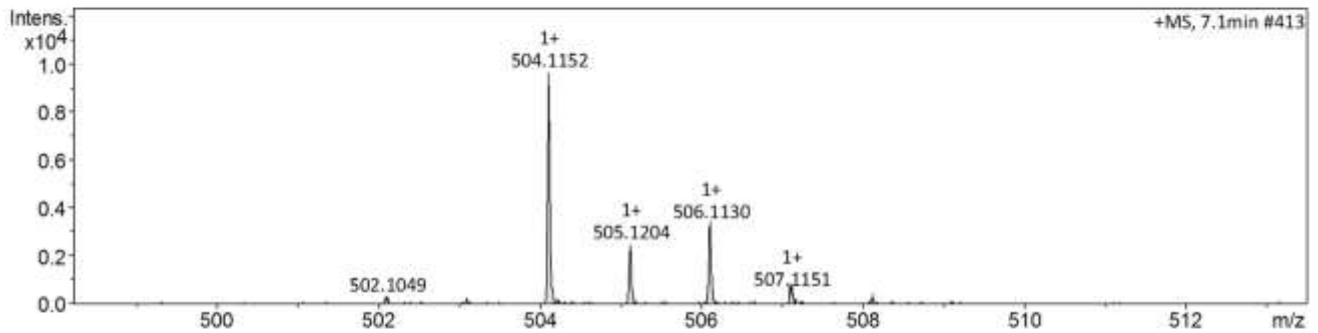
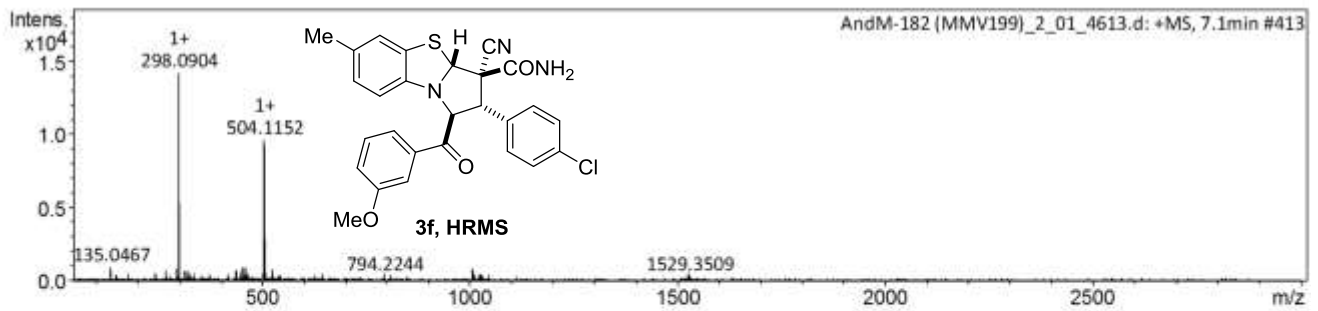
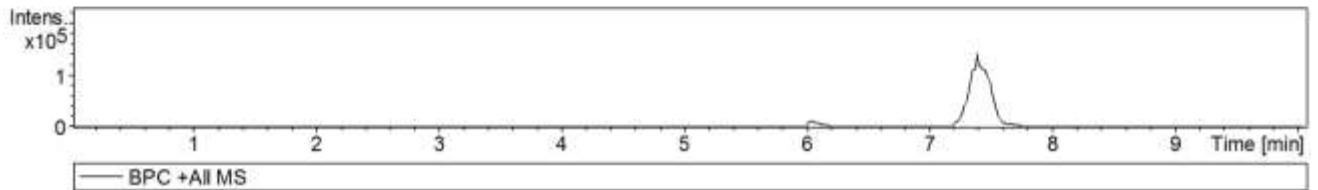
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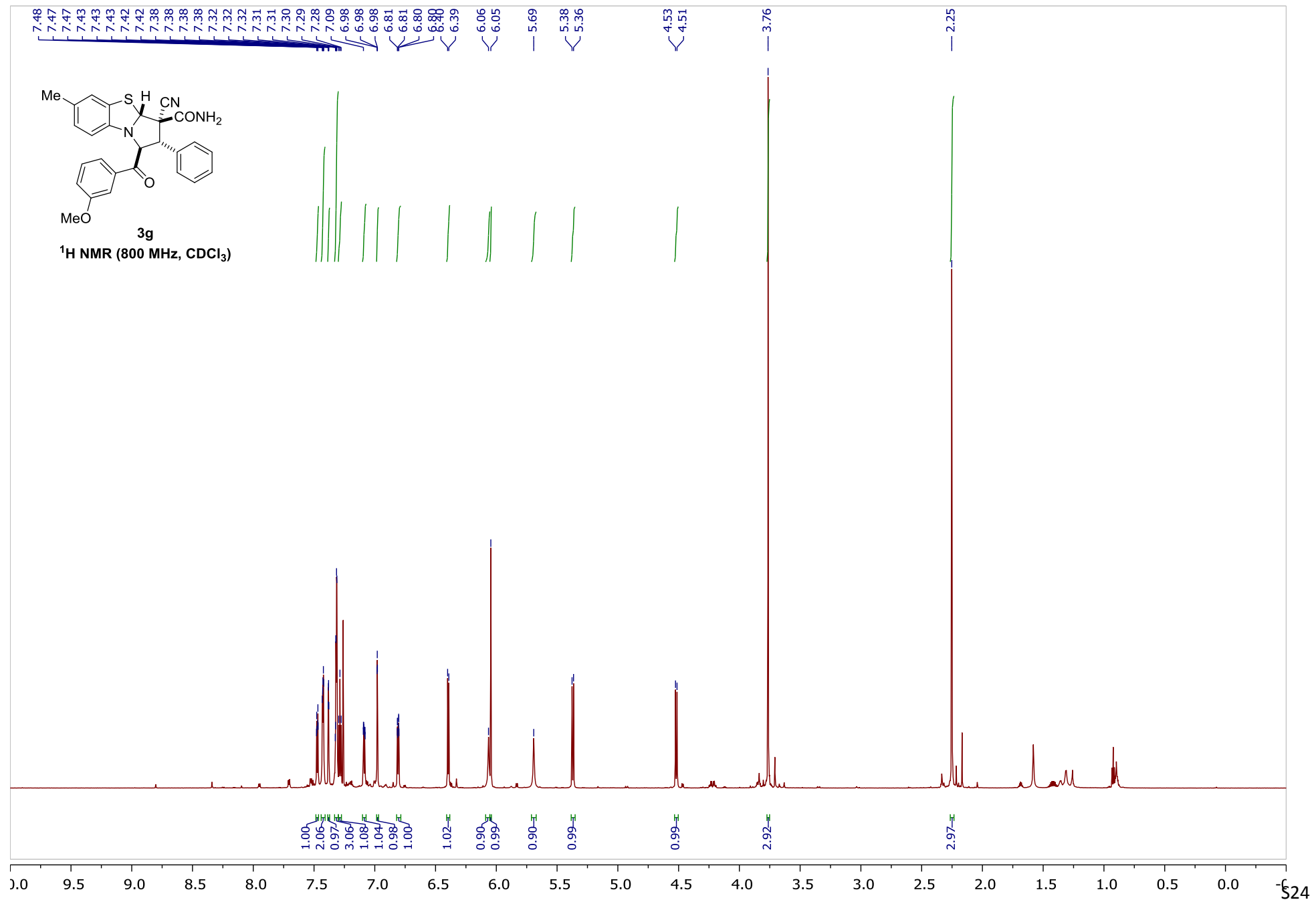
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Sample Name AndM-182 (MMV199)
Comment

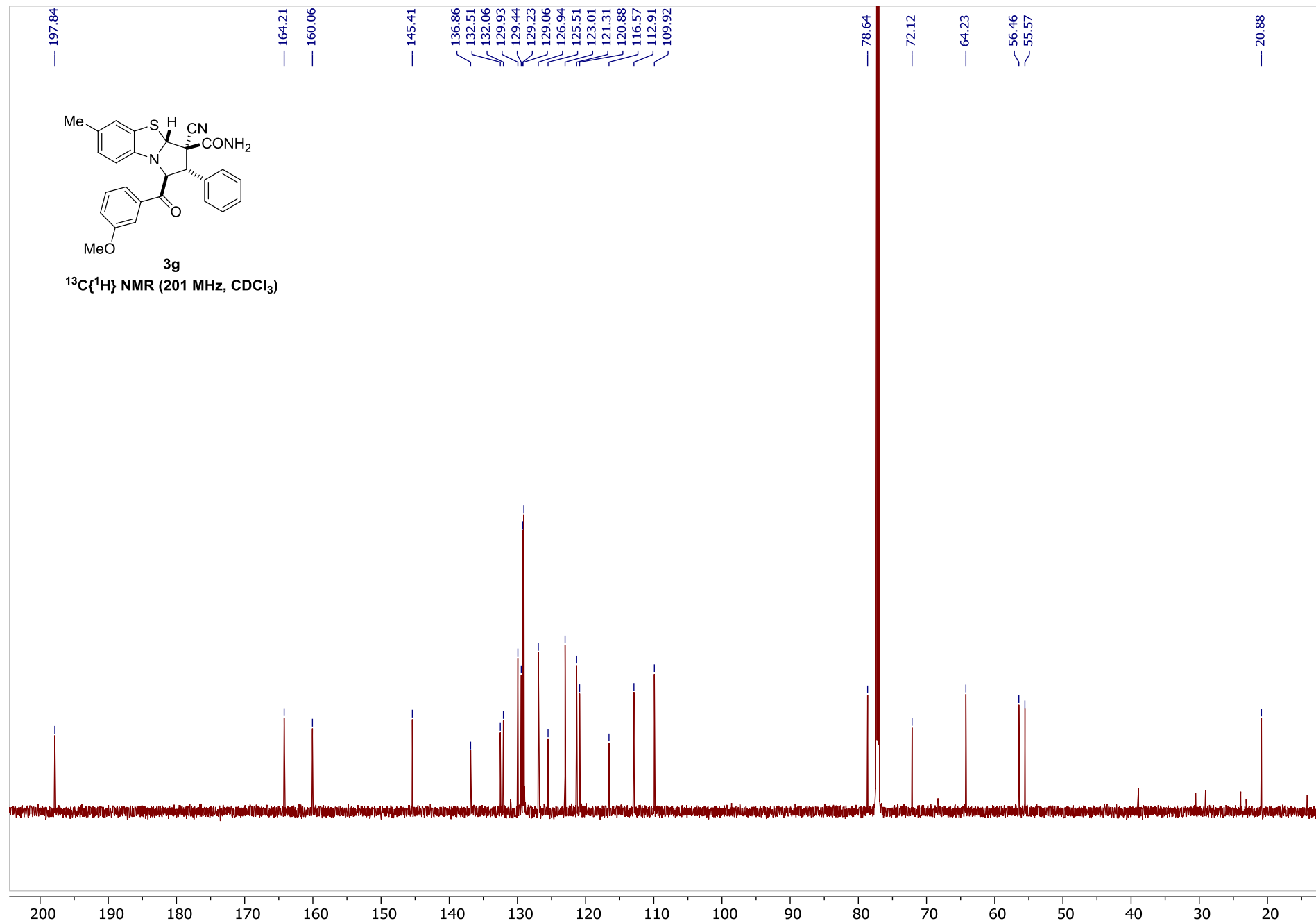
Acquisition Date 8/14/2024 8:02:20 PM
Operator BDAL@DE
Instrument compact 8255754.20088

Acquisition Parameter

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| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 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 | 3000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
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Sample Name: MMV181

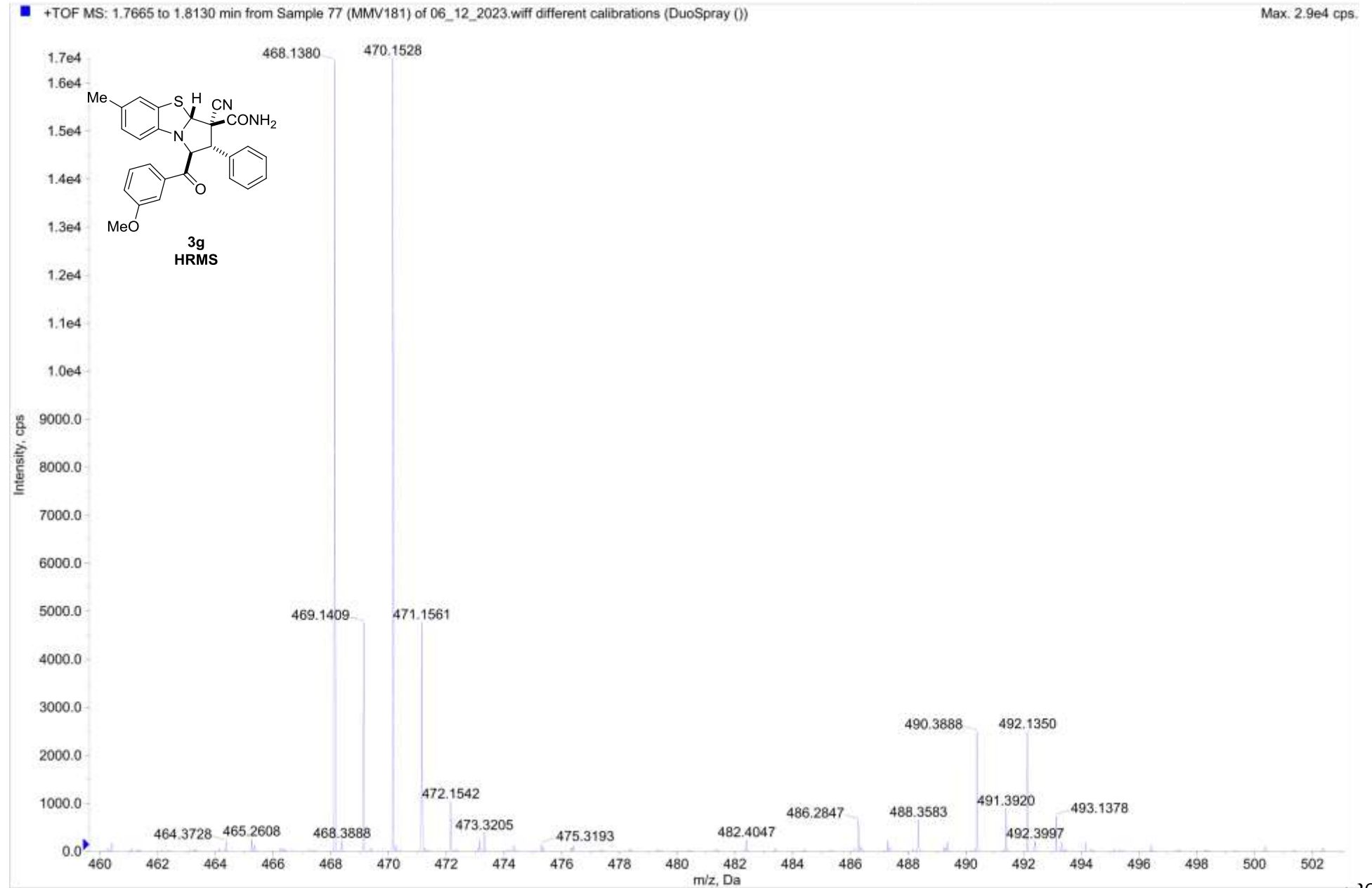
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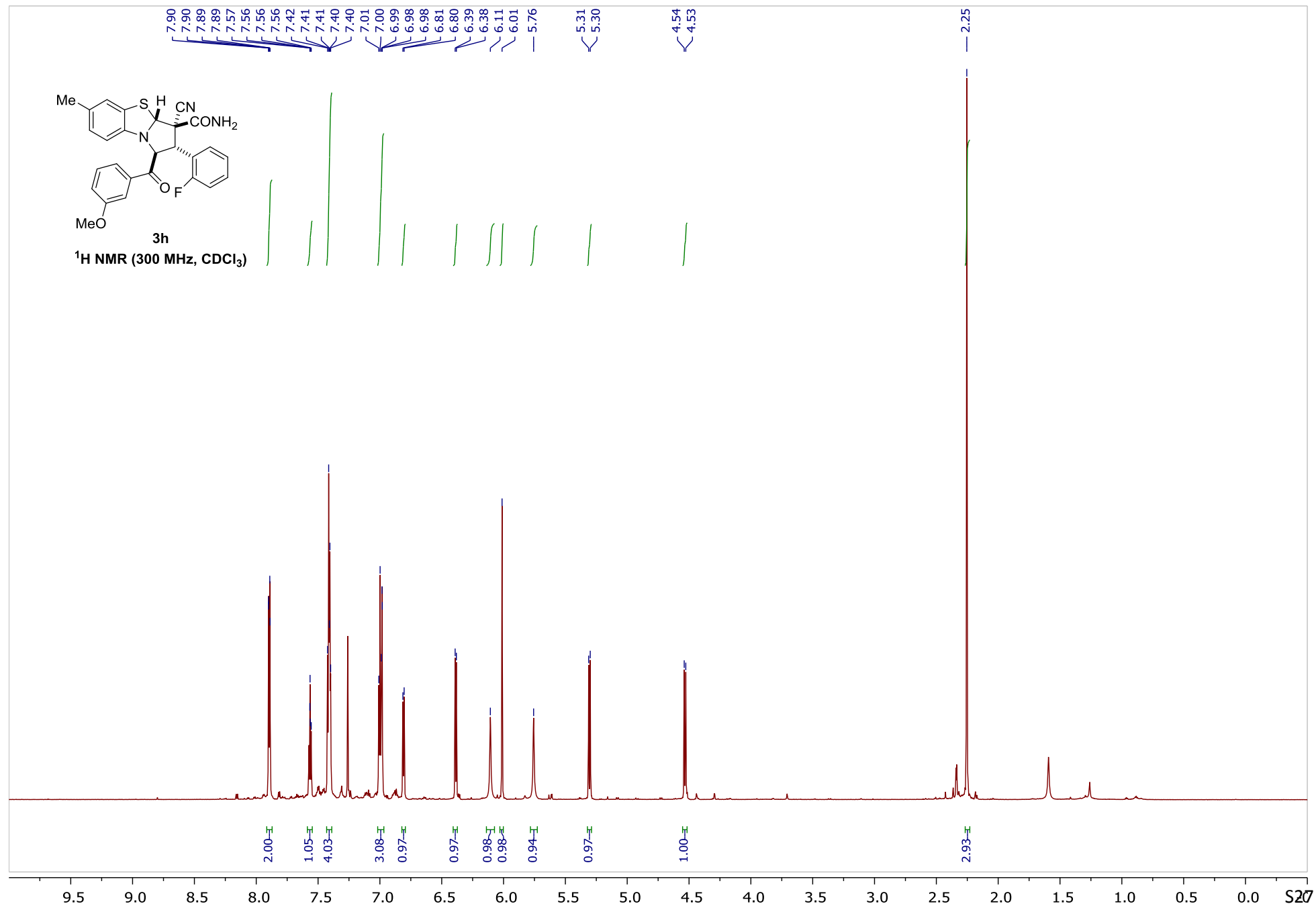
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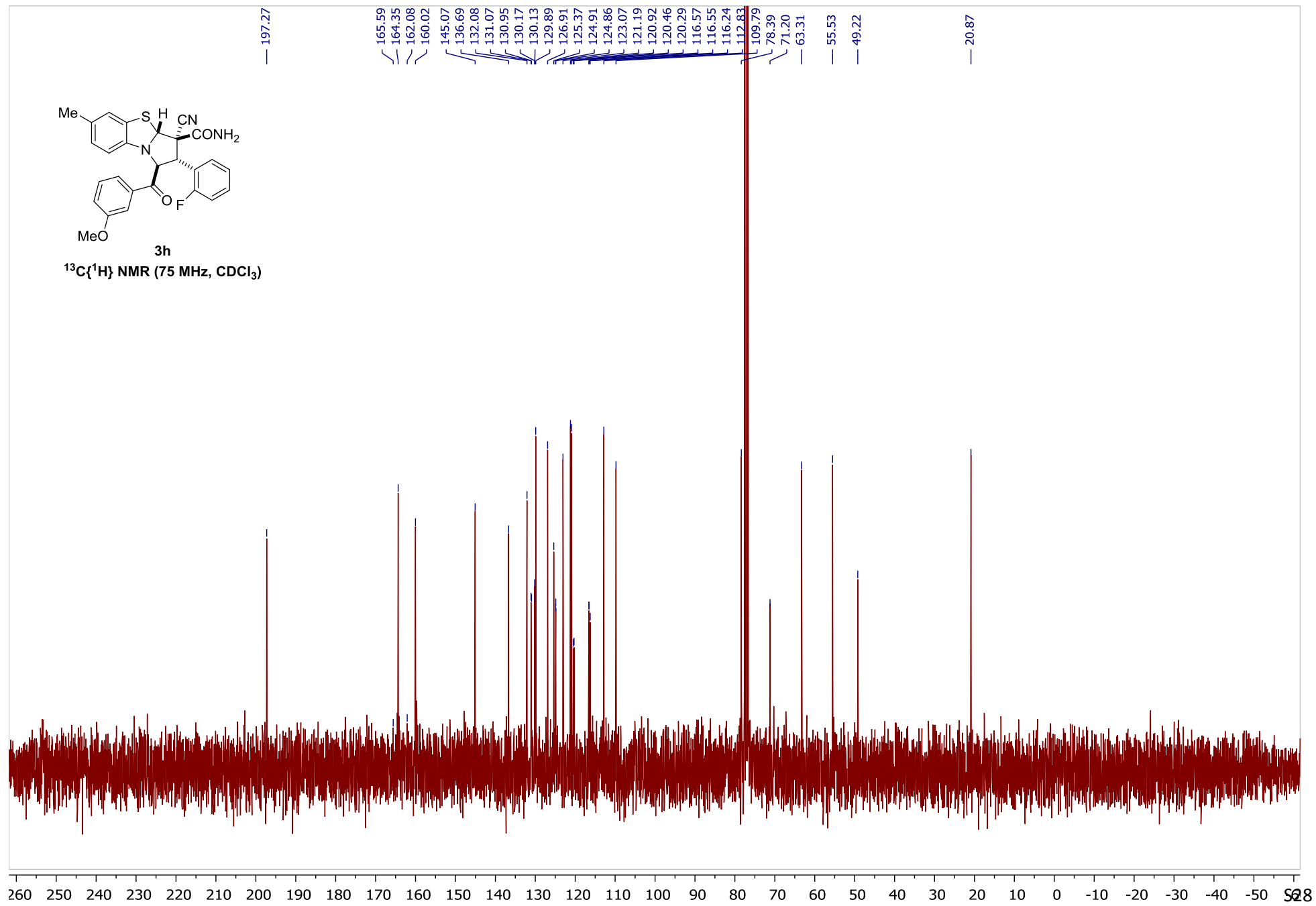
Acq. File: 06_12_2023.wiff

*5600 TripleTOF Service Report

Acq. Date: Wednesday, December 06, 2023







Sample Name: MMV187

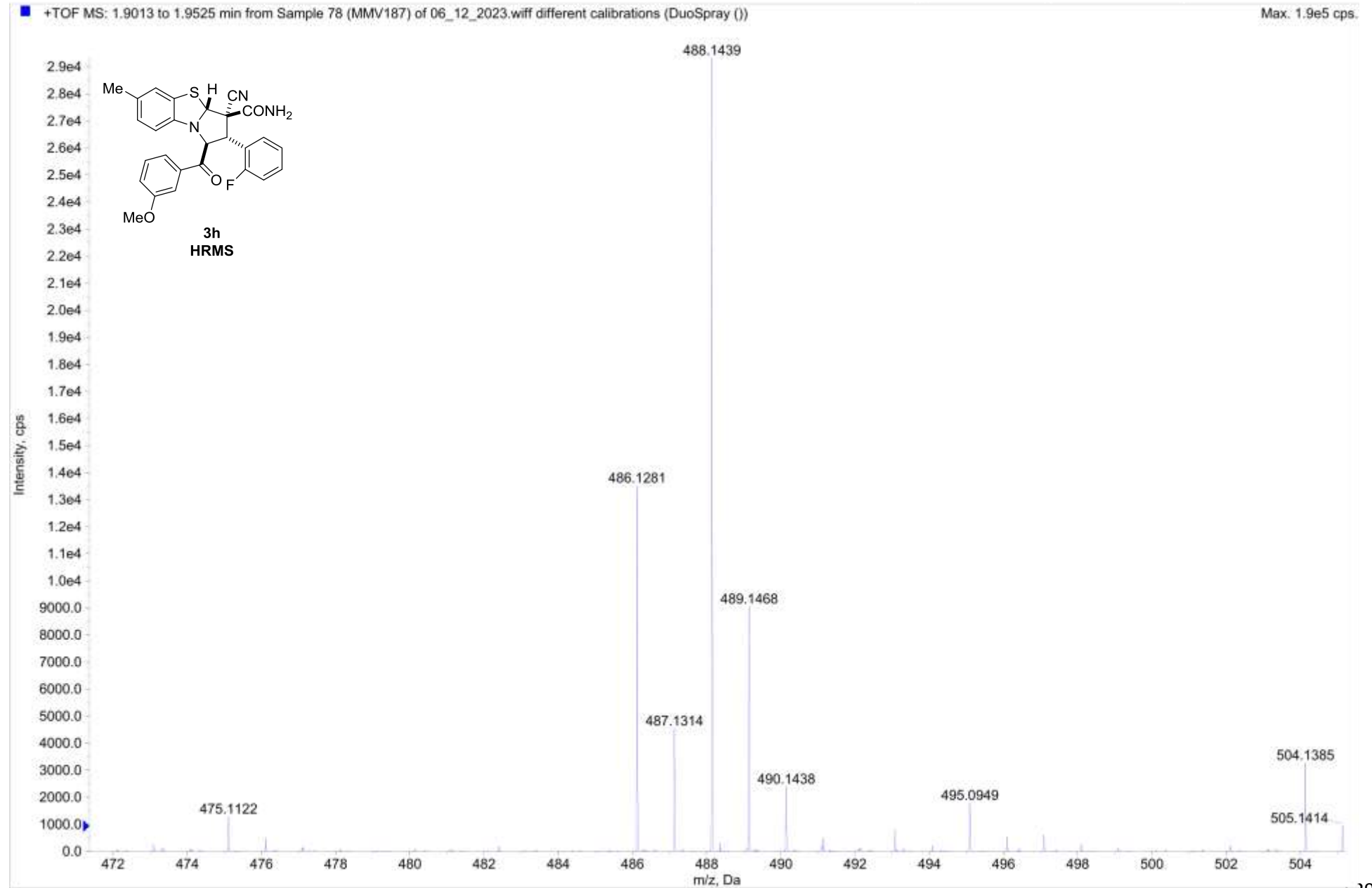
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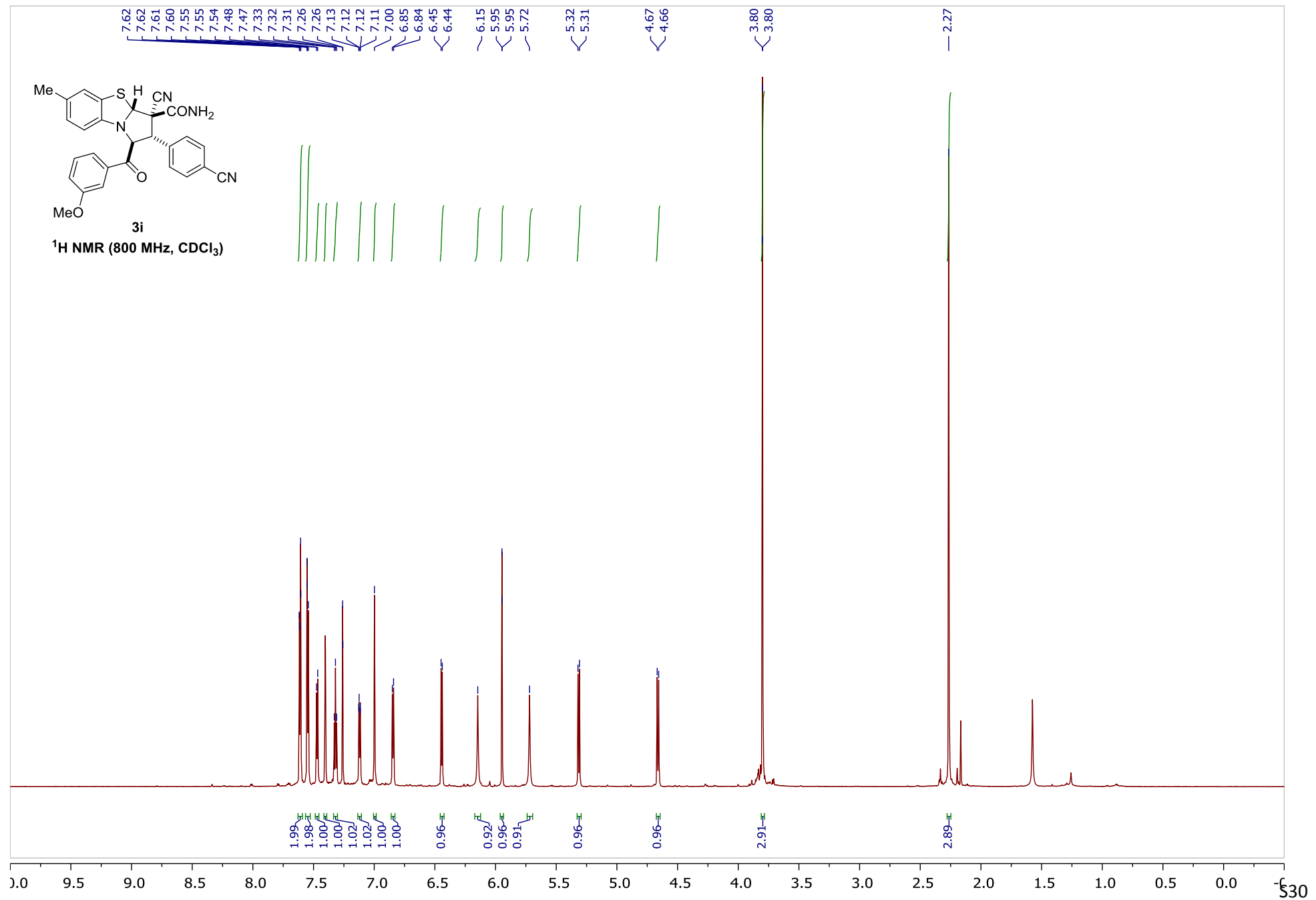
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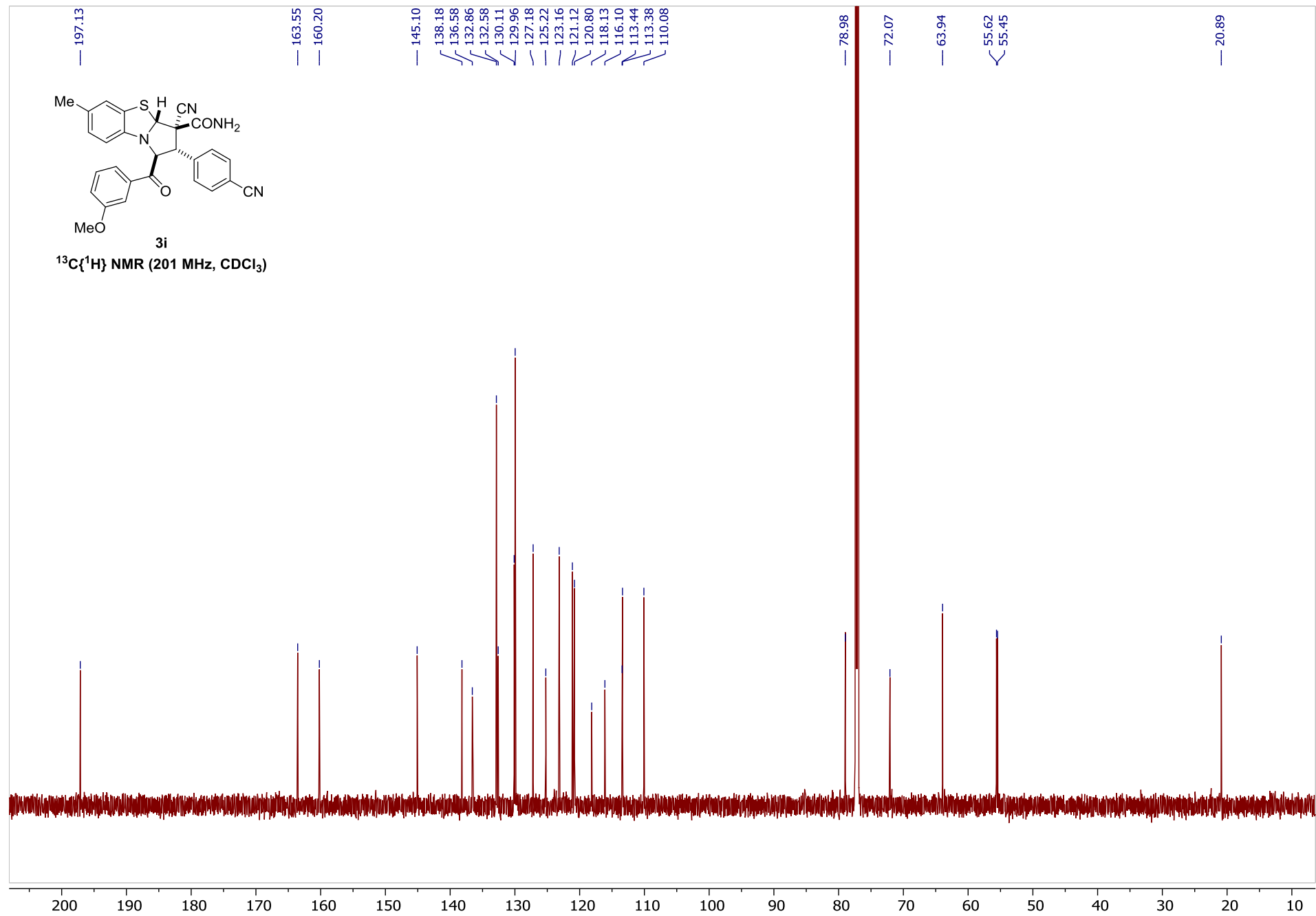
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*5600 TripleTOF Service Report

Acq. Date: Wednesday, December 06, 2023







Sample Name: MMV182

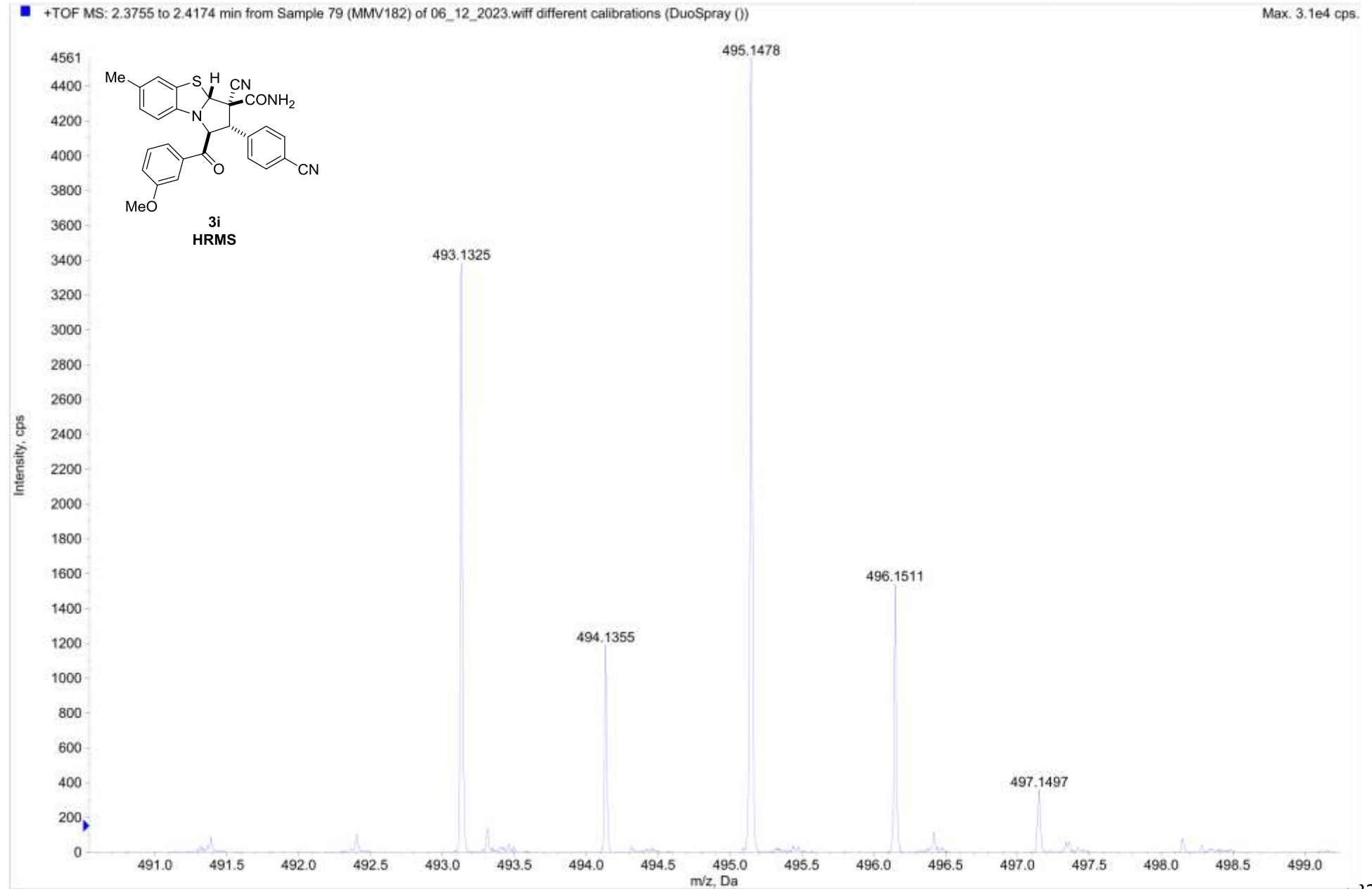
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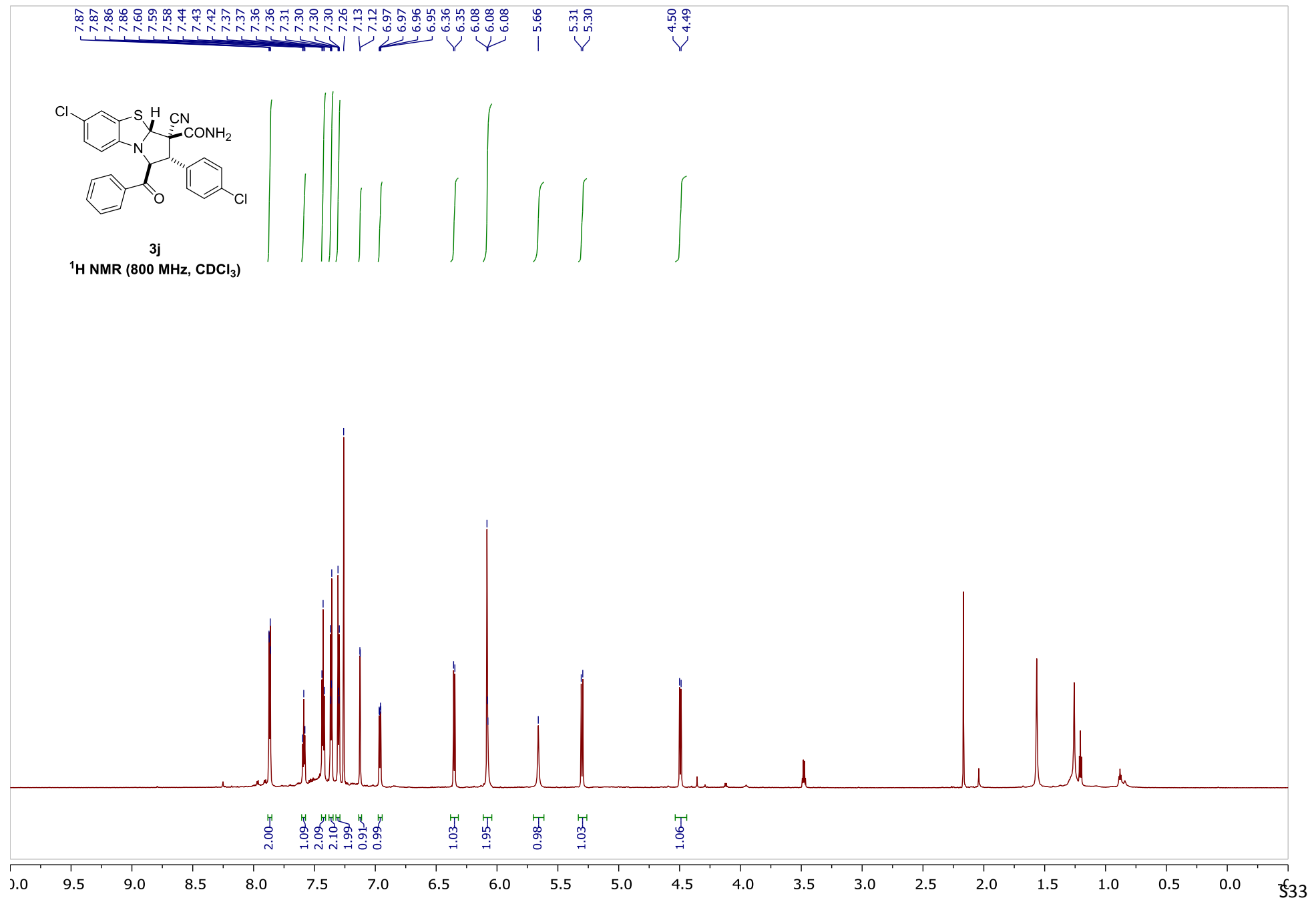
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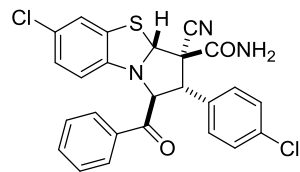
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*5600 TripleTOF Service Report

Acq. Date: Wednesday, December 06, 2023

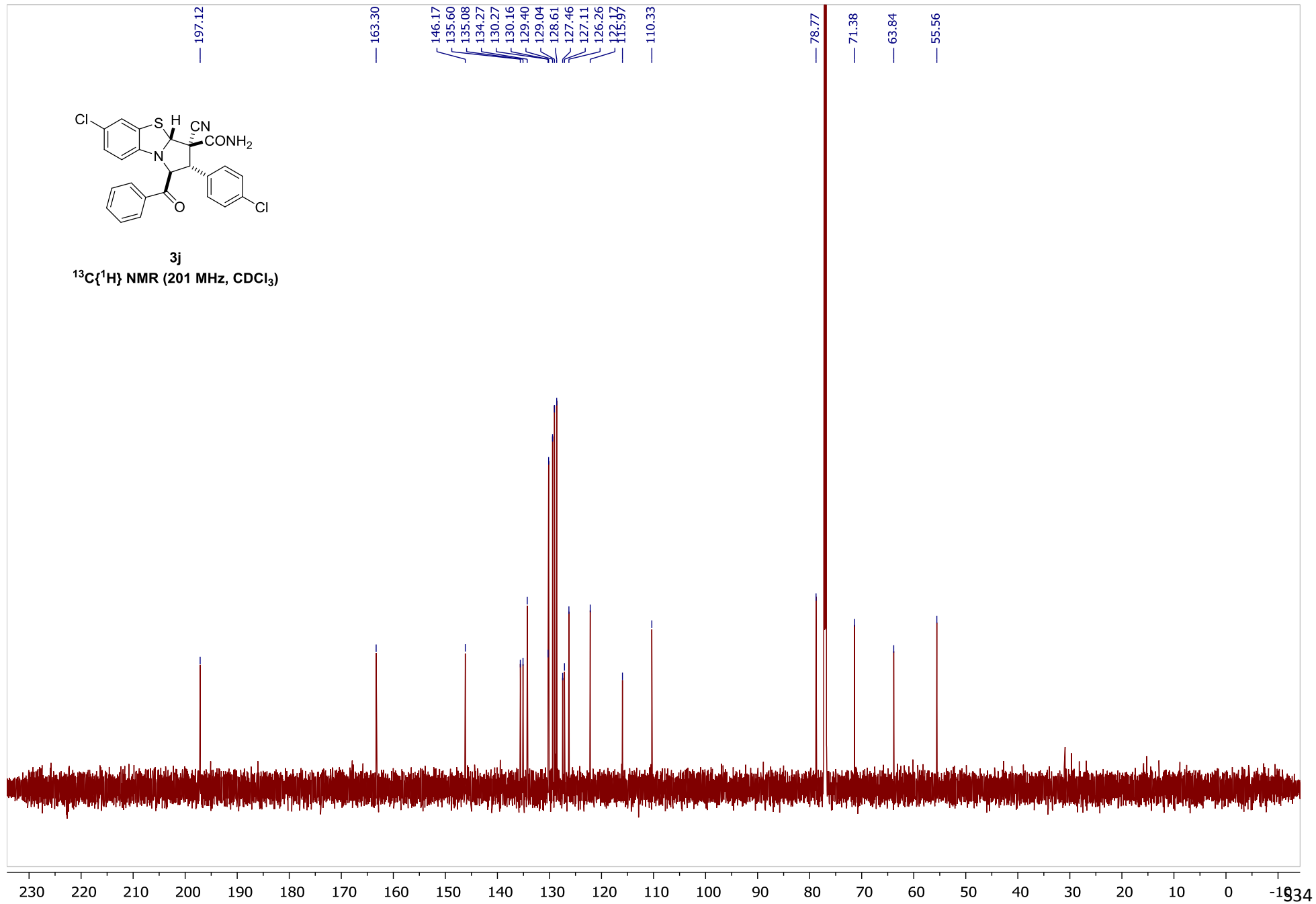






3j

$^{13}\text{C}\{^1\text{H}\}$ NMR (201 MHz, CDCl_3)



Display Report

Analysis Info

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Method la_2.2_small2.m
Sample Name AndM-186 (MMV275)
Comment

Acquisition Date 8/14/2024 8:48:37 PM
Operator BDAL@DE
Instrument compact 8255754.20088

Acquisition Parameter

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| Focus | Active | Set Capillary | 4500 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 | 3000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |

