

Supplemental material for:

Total Synthesis of Bicyclomahanimbine by Cu(II)-Promoted Photoredox Process

Shilpa Dangar, Tiyasa Roy, Suman Noskar, and Alakesh Bisai*

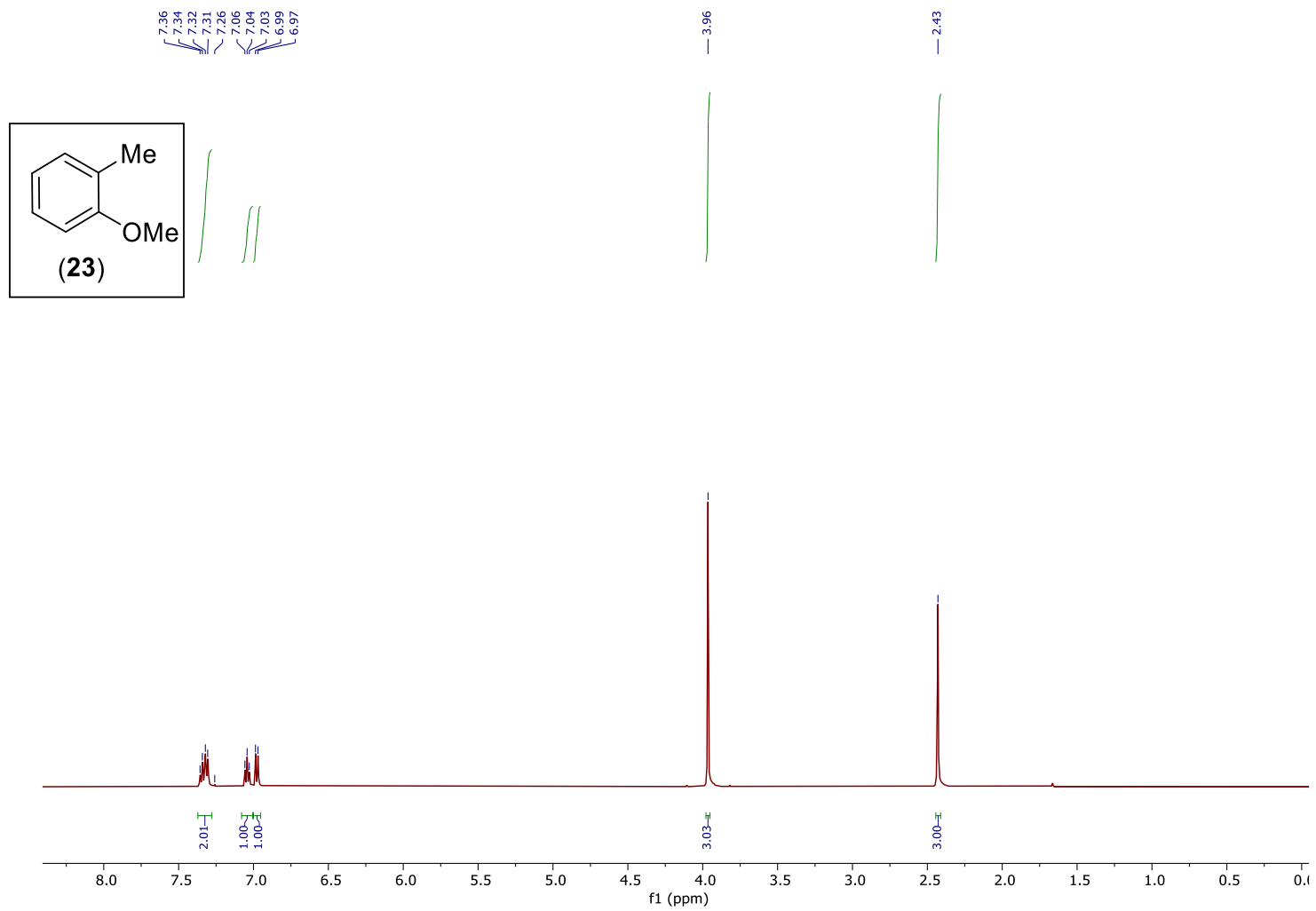
Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur Campus, Kalyani,
Nadia – 741 246, West Bengal, INDIA

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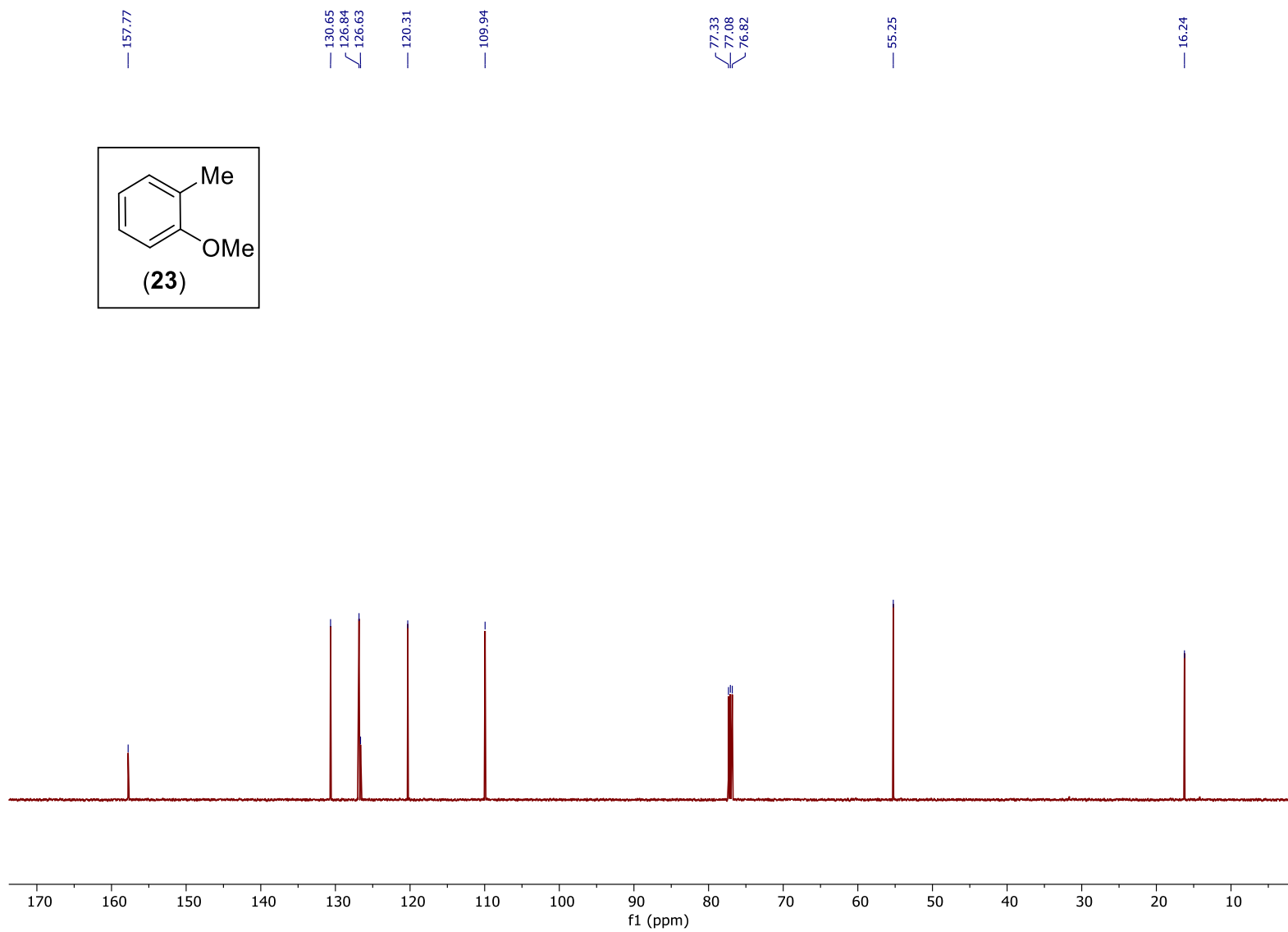
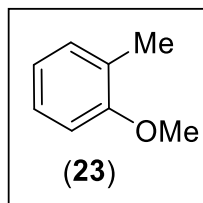
¹H-NMR, ¹³C-NMR and Spectral Traces

S02 – S44

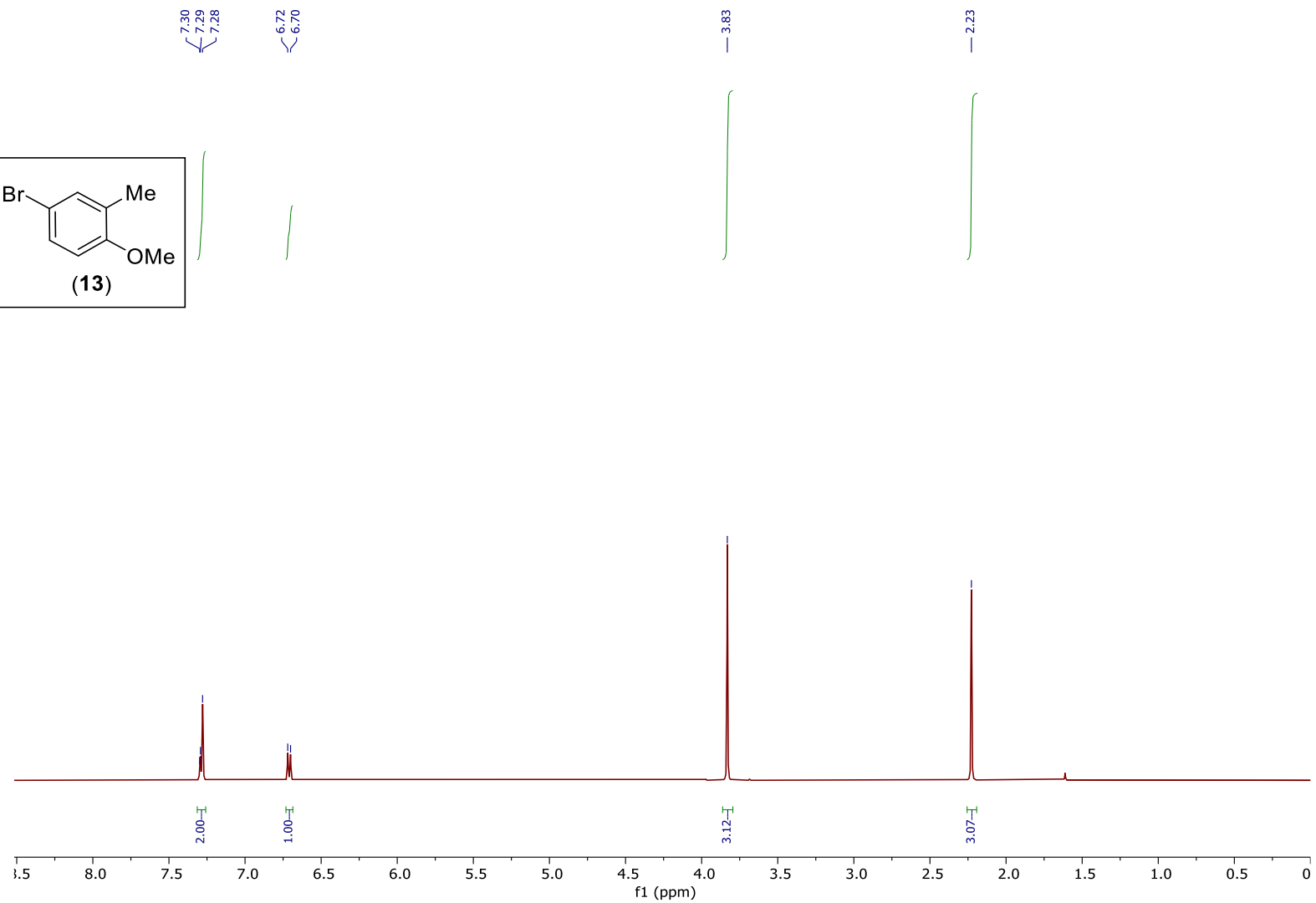
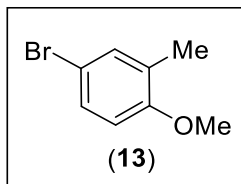
Spectral Data



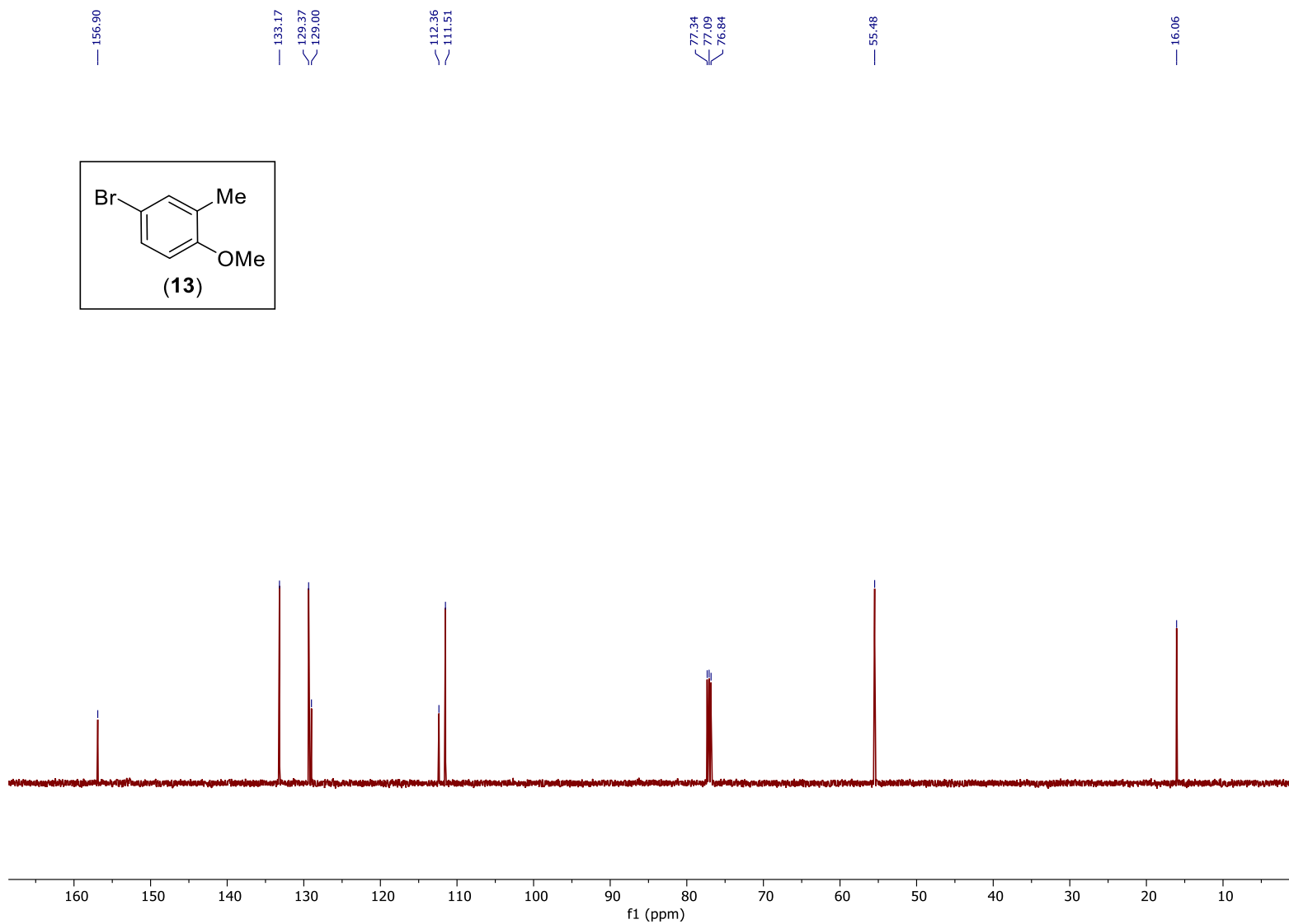
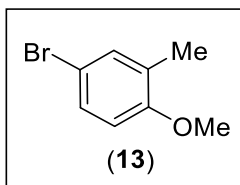
^1H NMR (500 MHz, CDCl_3) of **23**



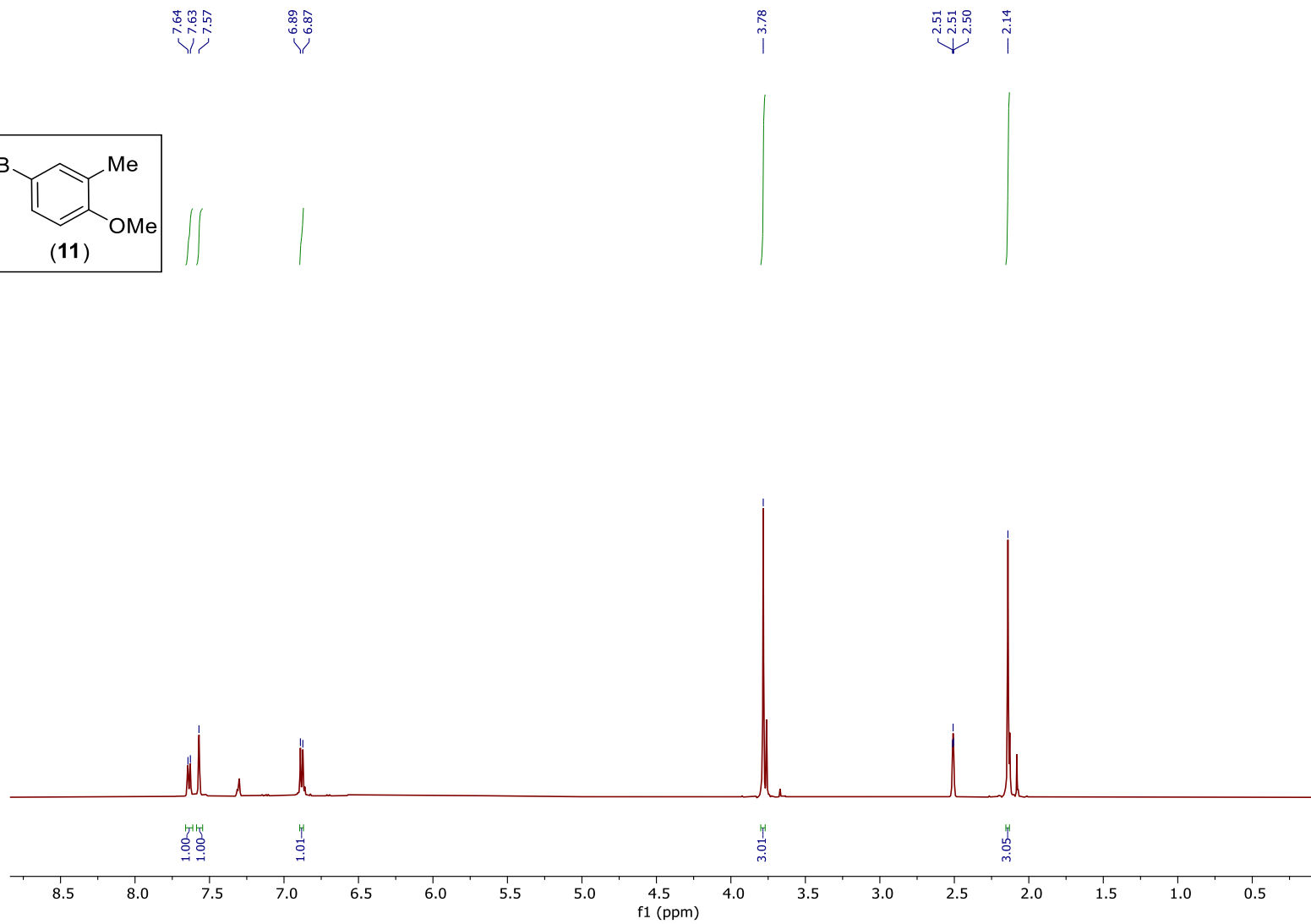
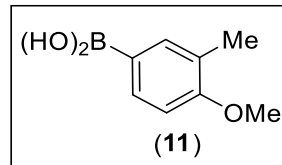
^{13}C NMR (500 MHz, CDCl_3) of **23**



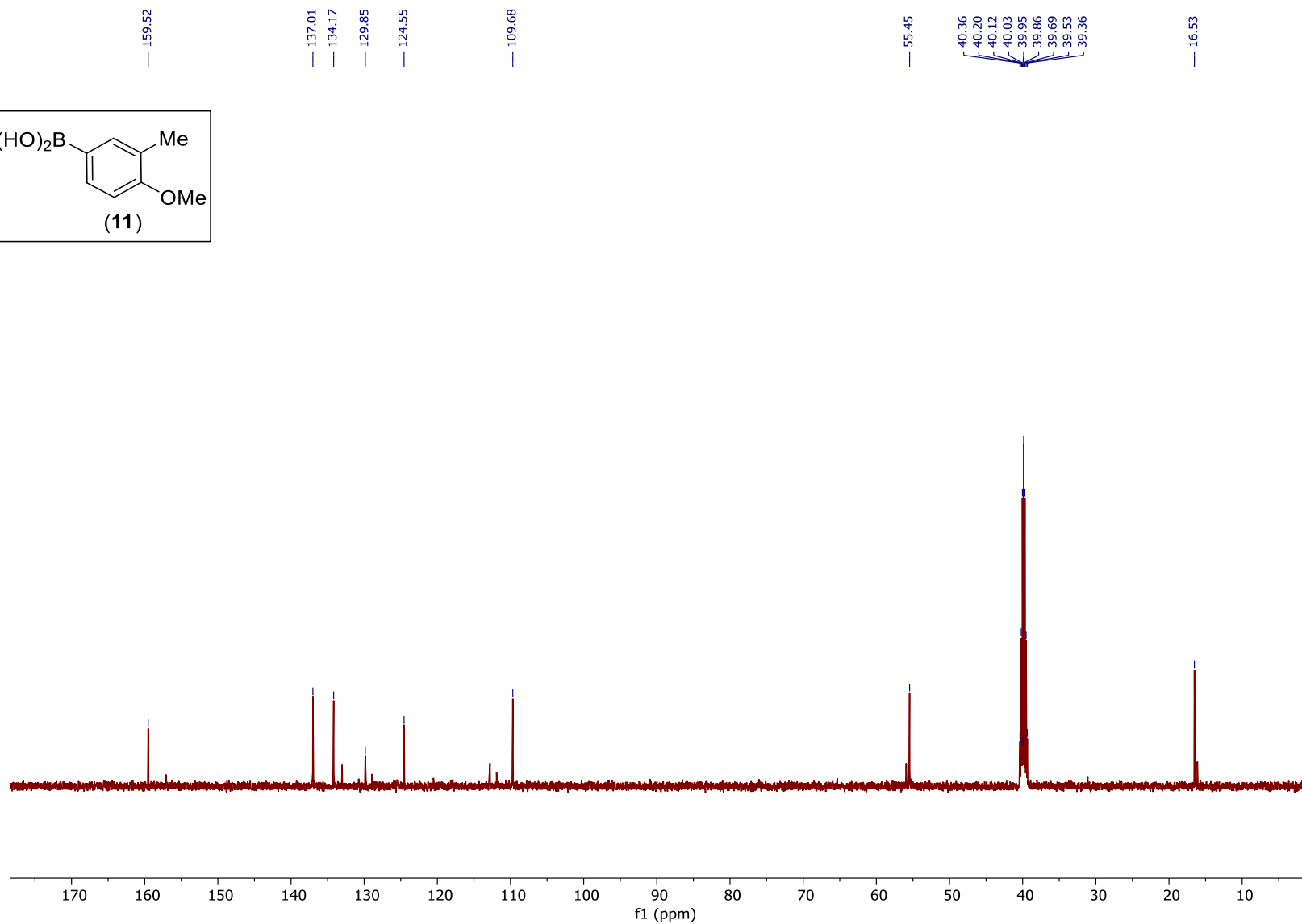
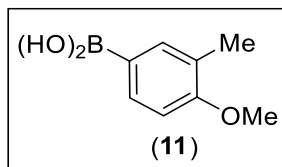
^1H NMR (500 MHz, CDCl_3) of **13**



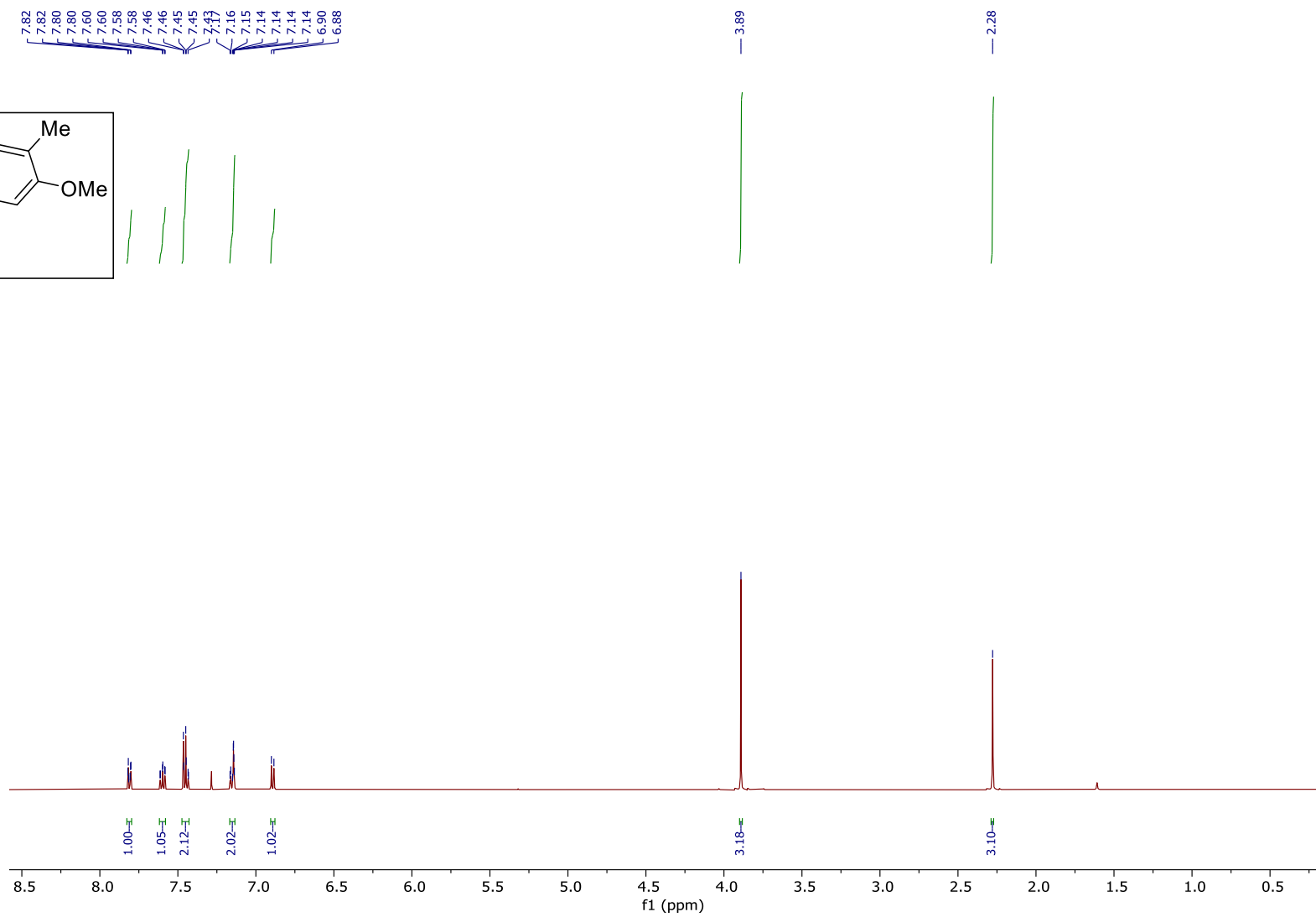
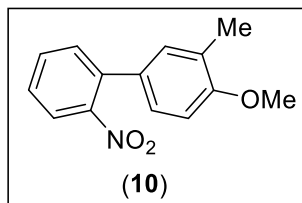
^{13}C NMR (125 MHz, CDCl_3) of **13**



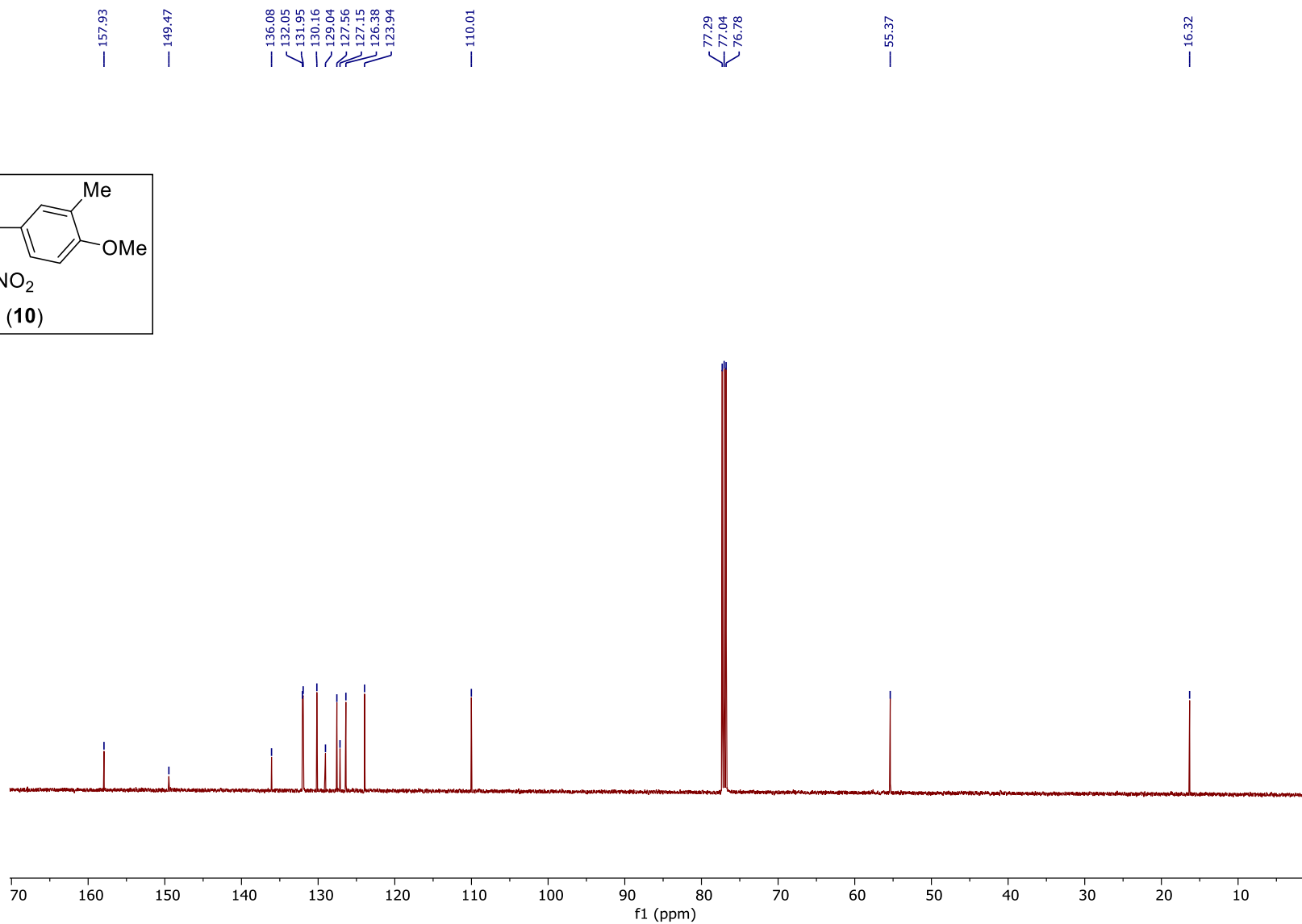
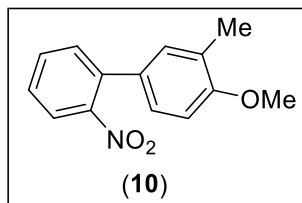
^1H NMR (500 MHz, CDCl_3) of **11**



^{13}C NMR (126 MHz, CDCl_3) of **11**



¹H NMR (500 MHz, CDCl₃) of **10**

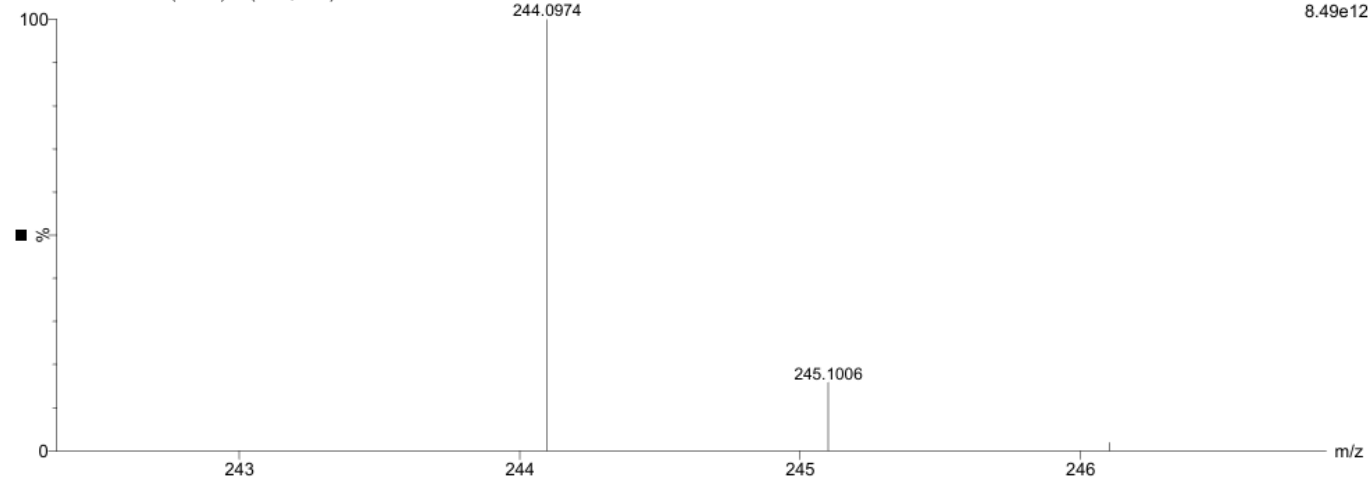


^{13}C NMR (126 MHz, CDCl_3) of **10**

AB06-May-2024 11:50:18
AB-SUM-33SUZM (0.104) Is (1.00,1.00) C₁₄H₁₄NO₃

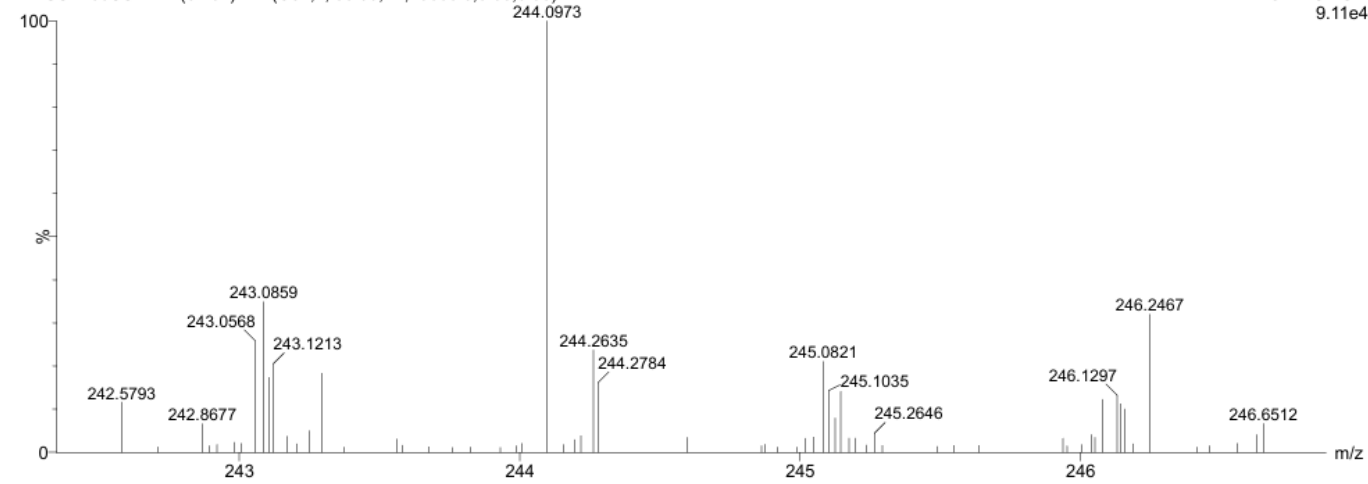
IISER - KOLKATA

1: TOF MS ES+
8.49e12

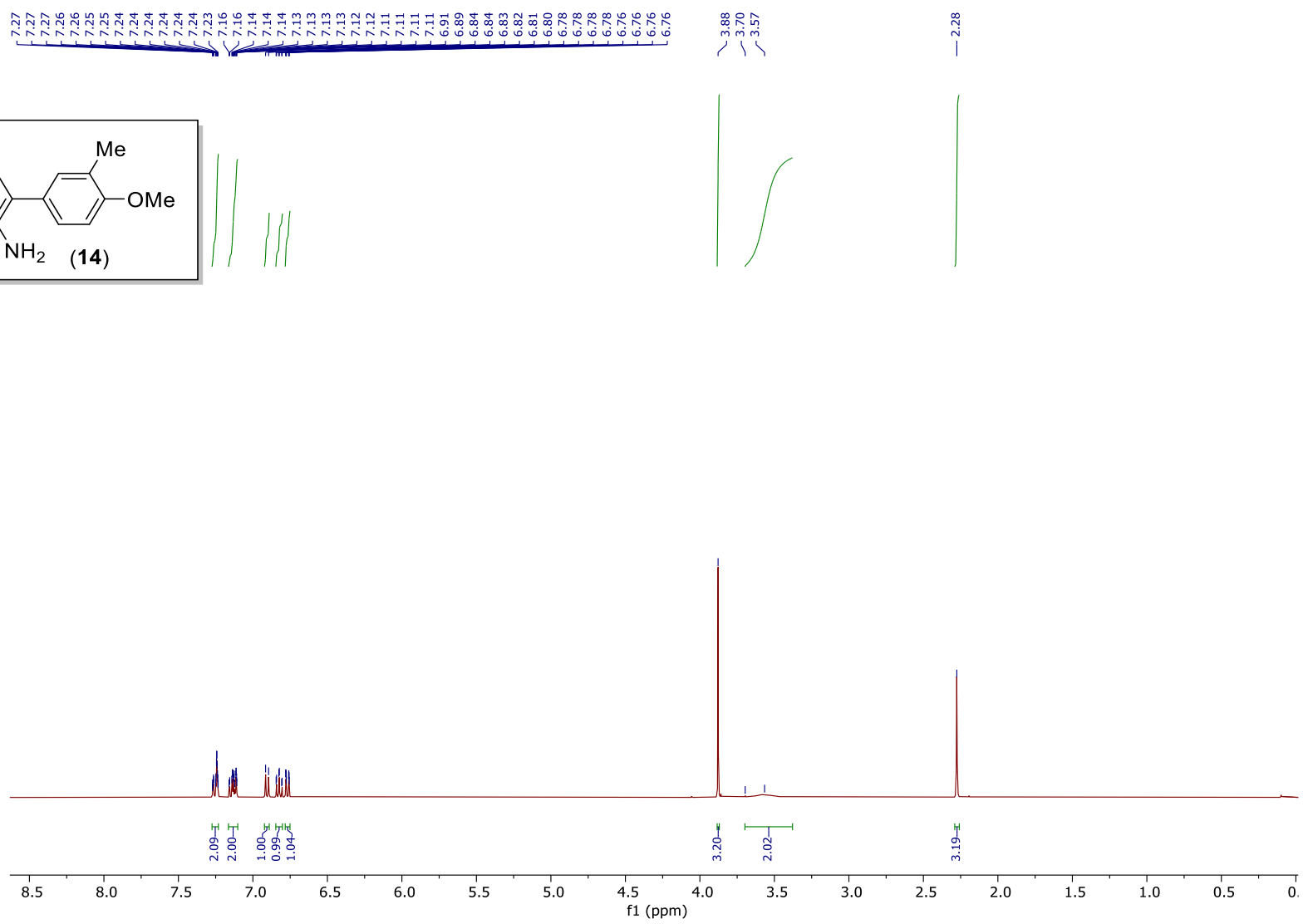
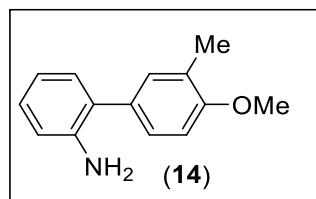


AB-SUM-33SUZM 4 (0.104) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00)

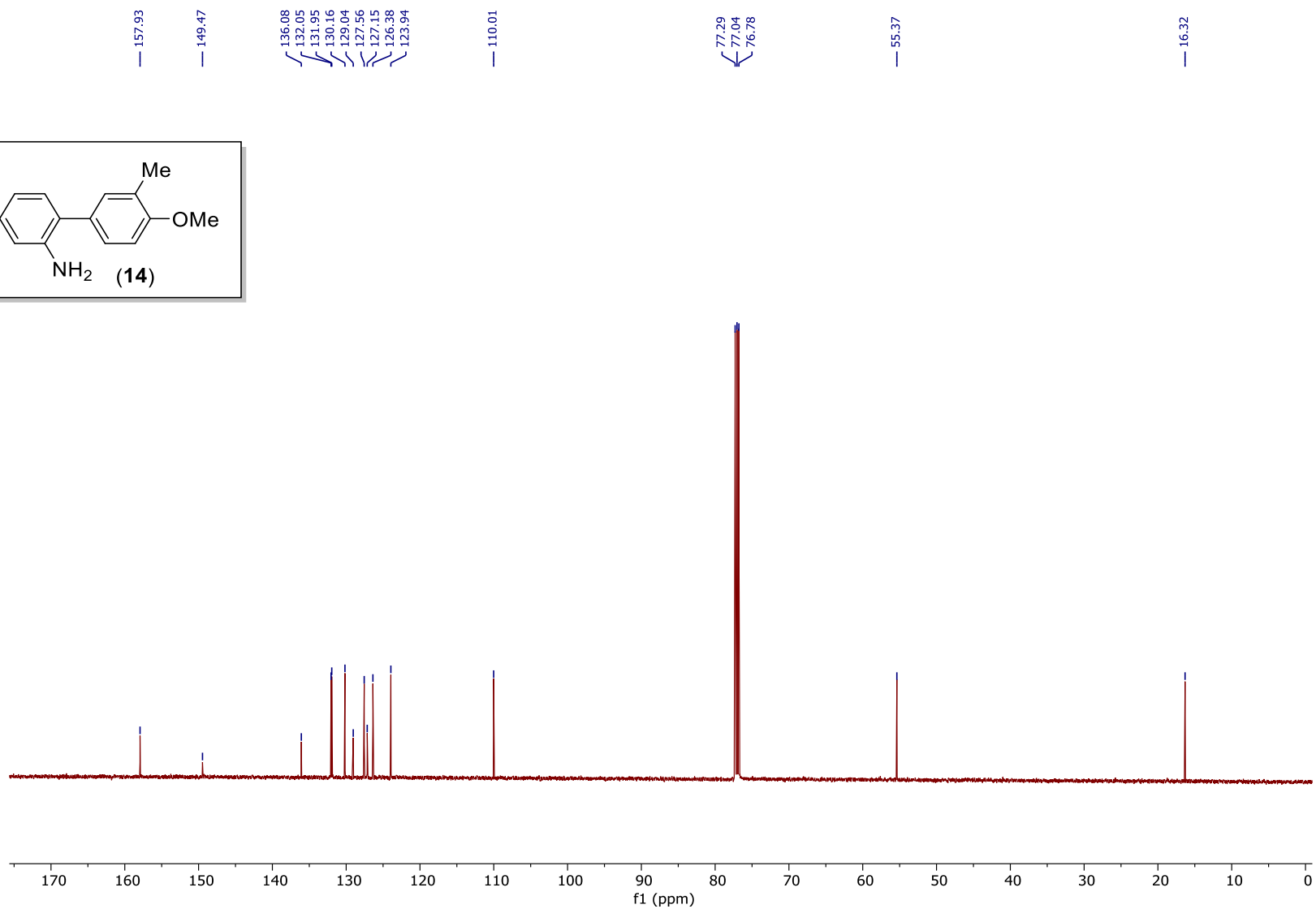
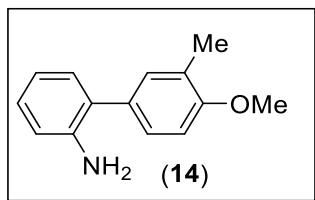
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9.11e4



HRMS data of 10



¹H NMR (400 MHz, CDCl₃) of **14**

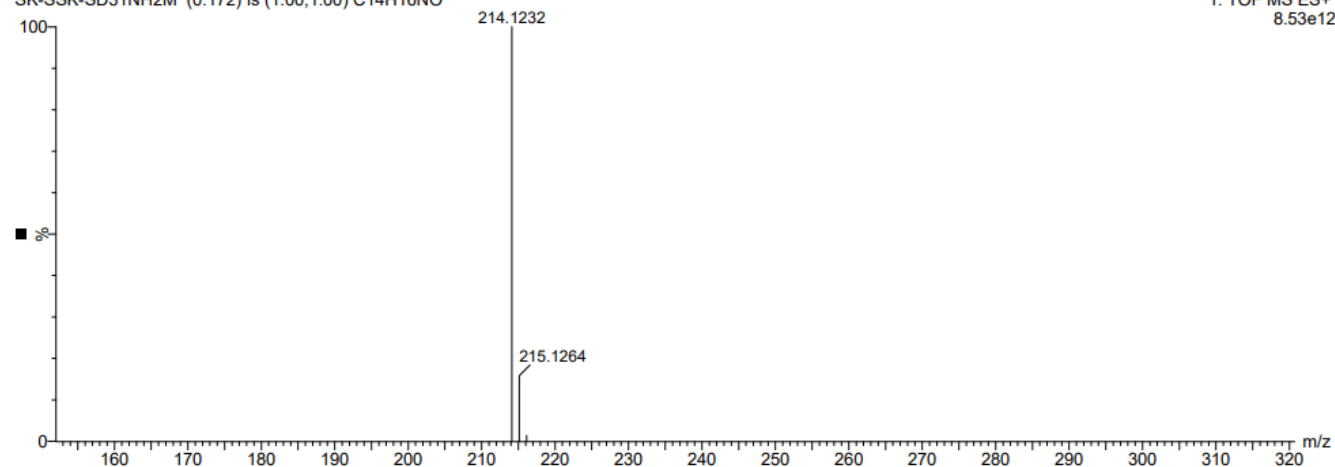


^{13}C NMR (126 MHz, CDCl_3) of **14**

SK30-Apr-2024 16:40:17
SK-SSK-SD31NH2M (0.172) Is (1.00,1.00) C14H16NO

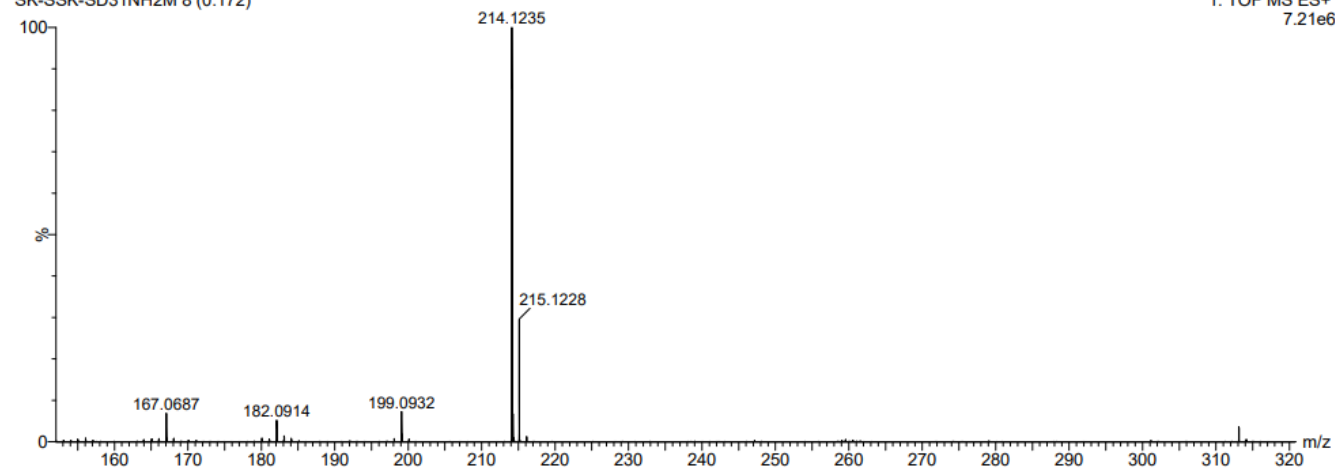
IISER - KOLKATA

1: TOF MS ES+
8.53e12

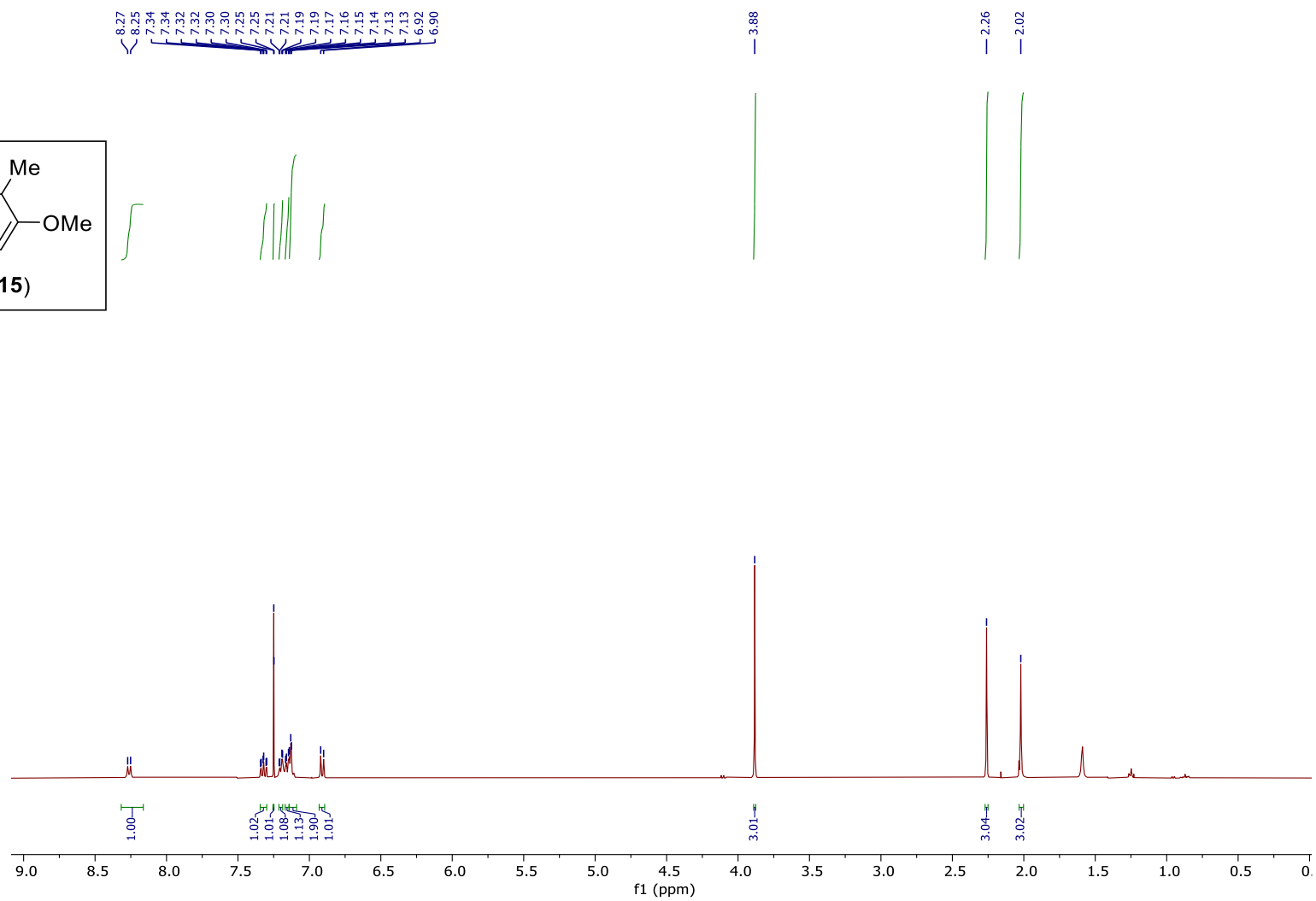
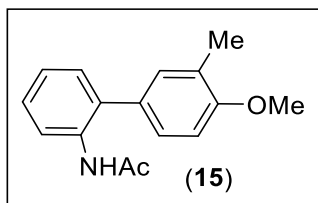


SK-SSK-SD31NH2M 8 (0.172)

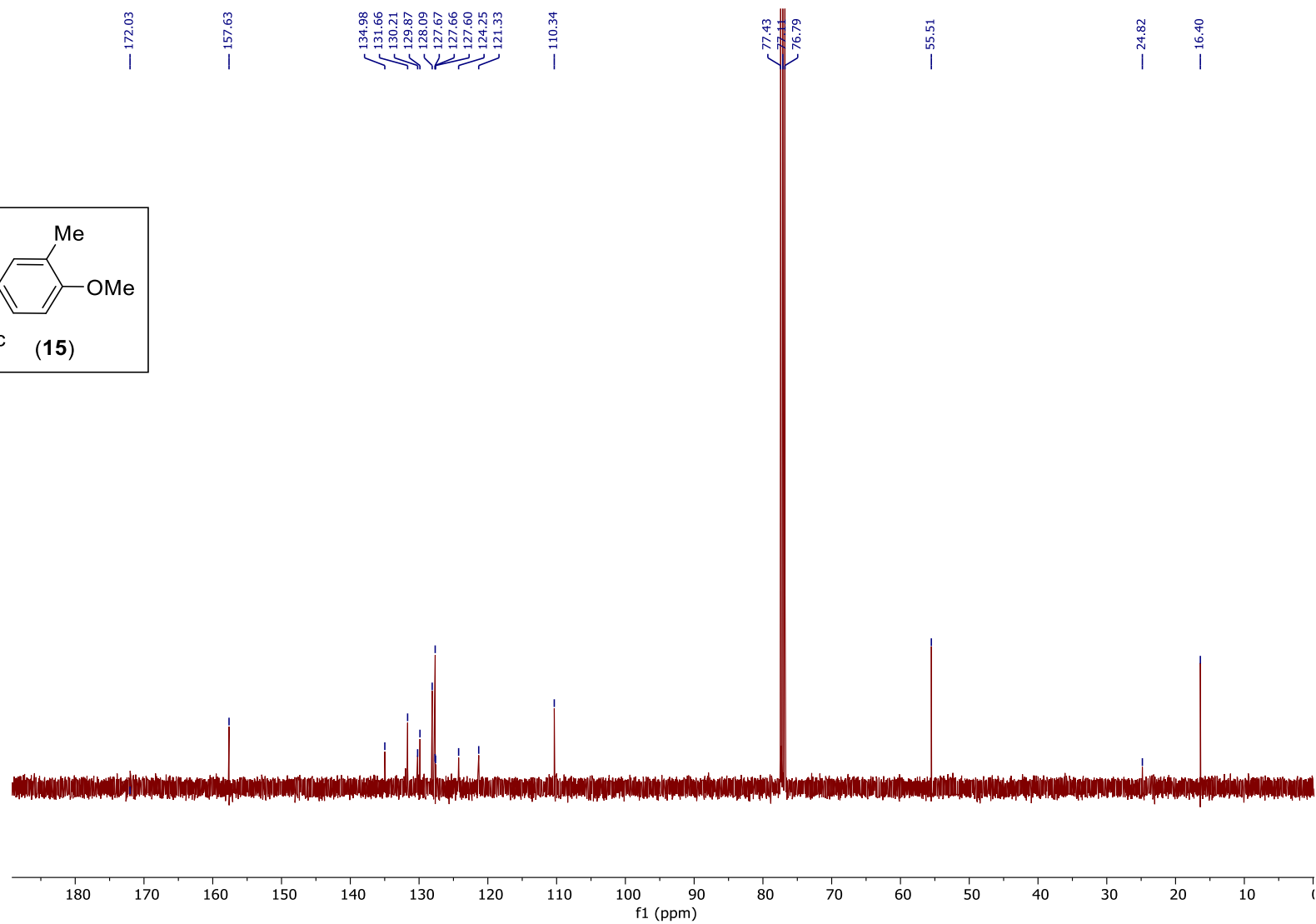
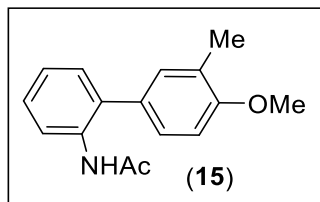
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7.21e6



HRMS data of 14



^1H NMR (400 MHz, CDCl_3) of 15

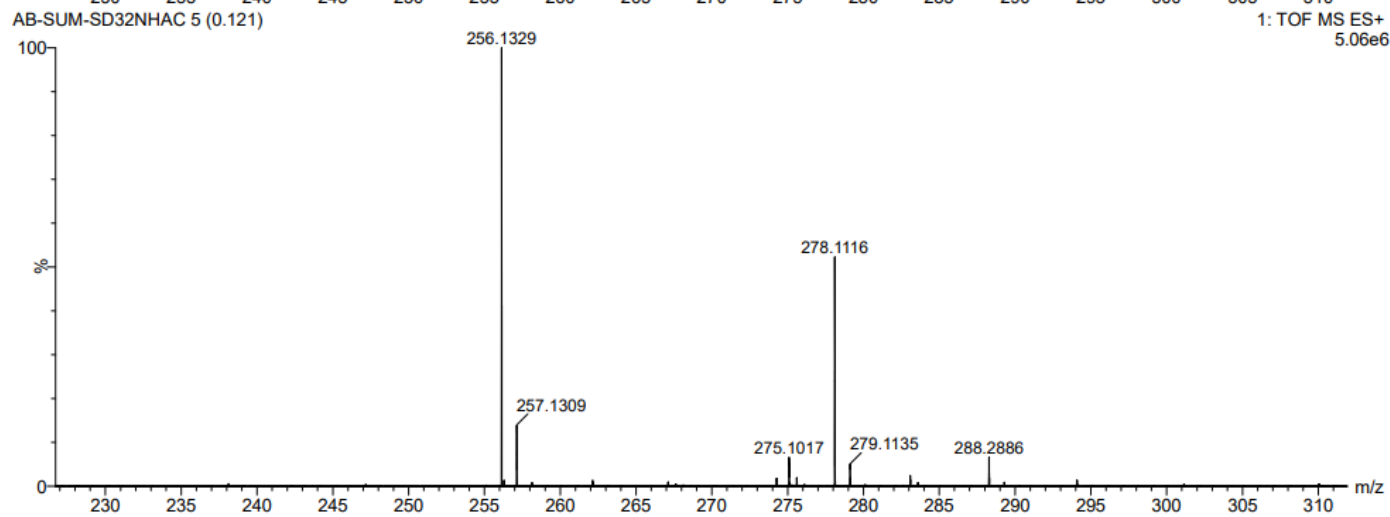
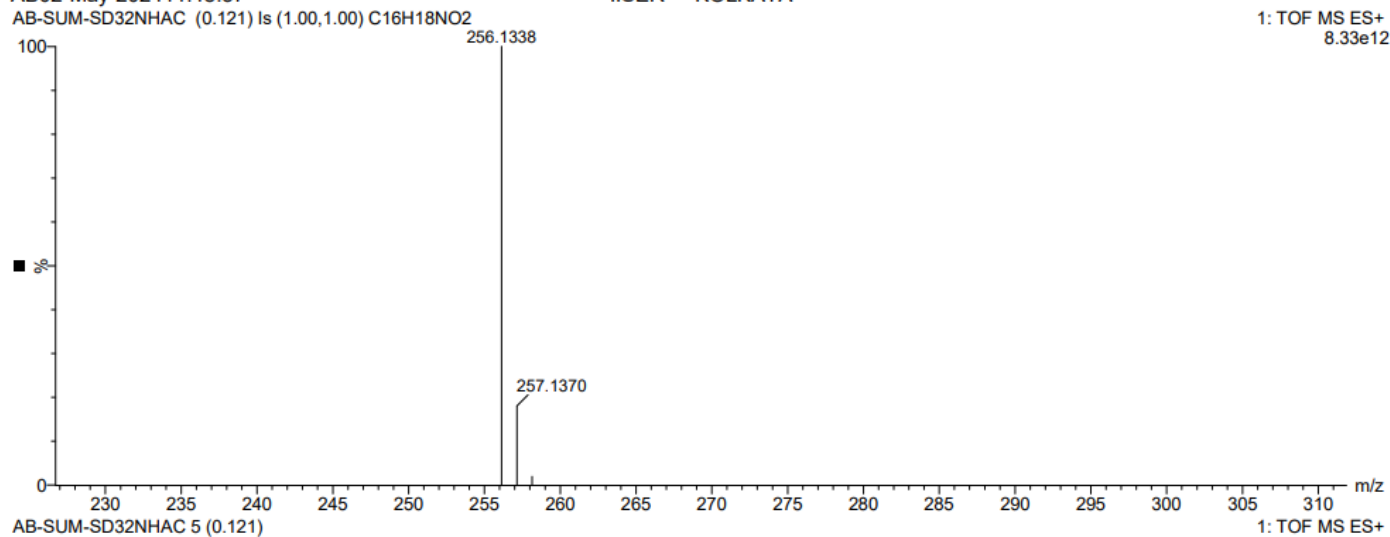


^{13}C NMR (100 MHz, CDCl_3) of **15**

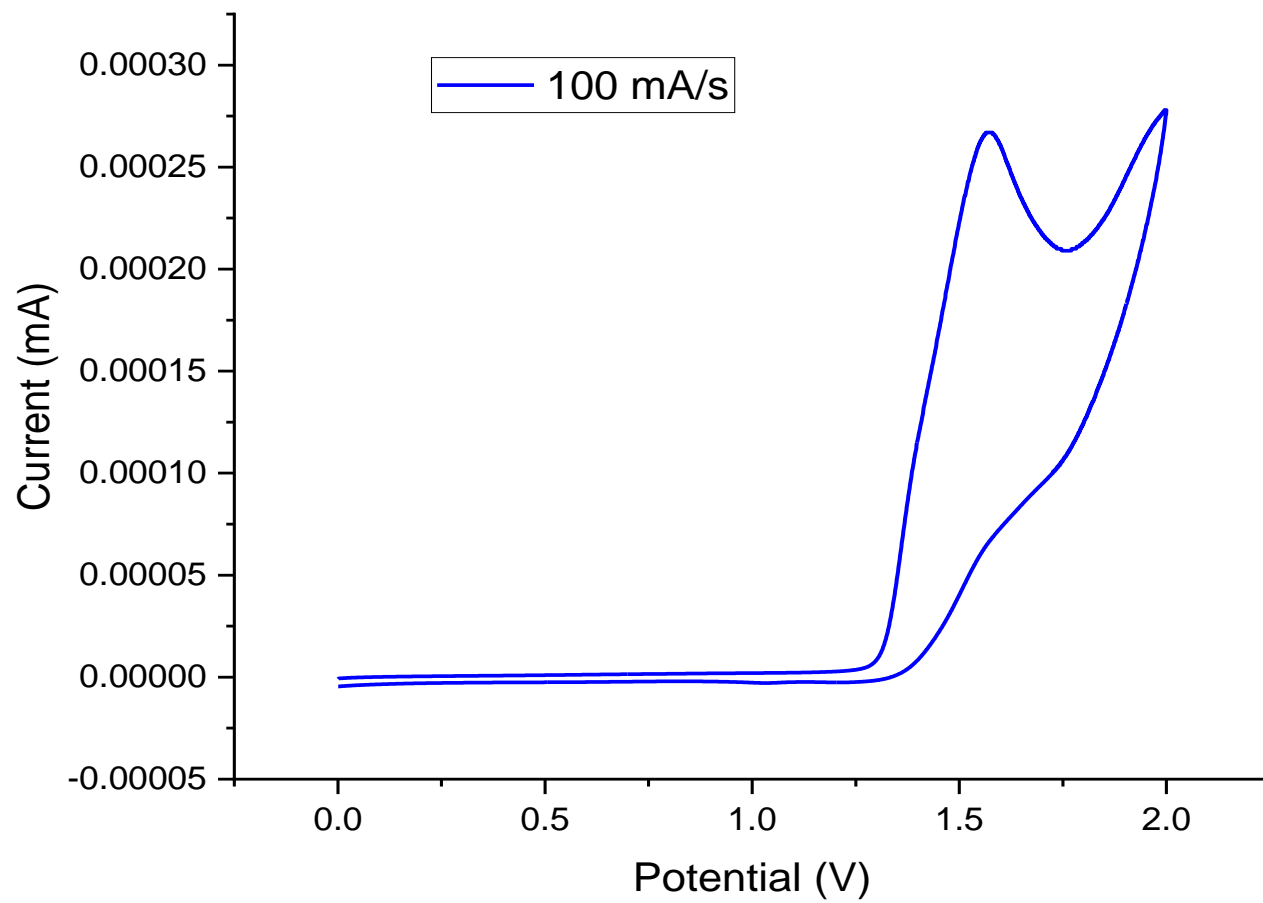
AB02-May-2024 11:48:57

IISER - KOLKATA

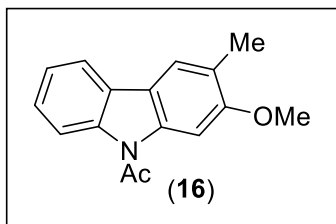
1: TOF MS ES+
8.33e12



HRMS data of 15



CV data of **15**



7.95
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7.92
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7.37
7.35
7.35
7.33
7.33
7.25



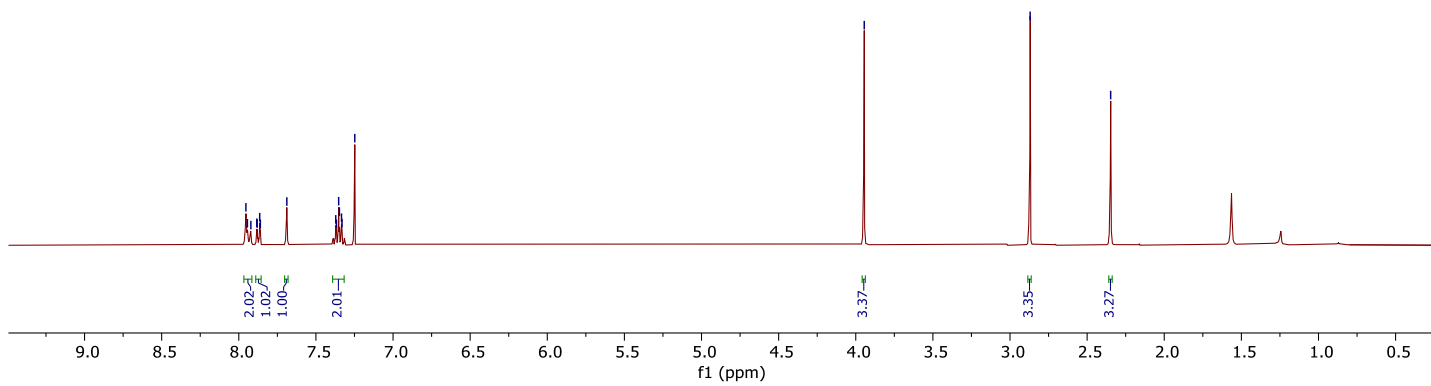
3.94



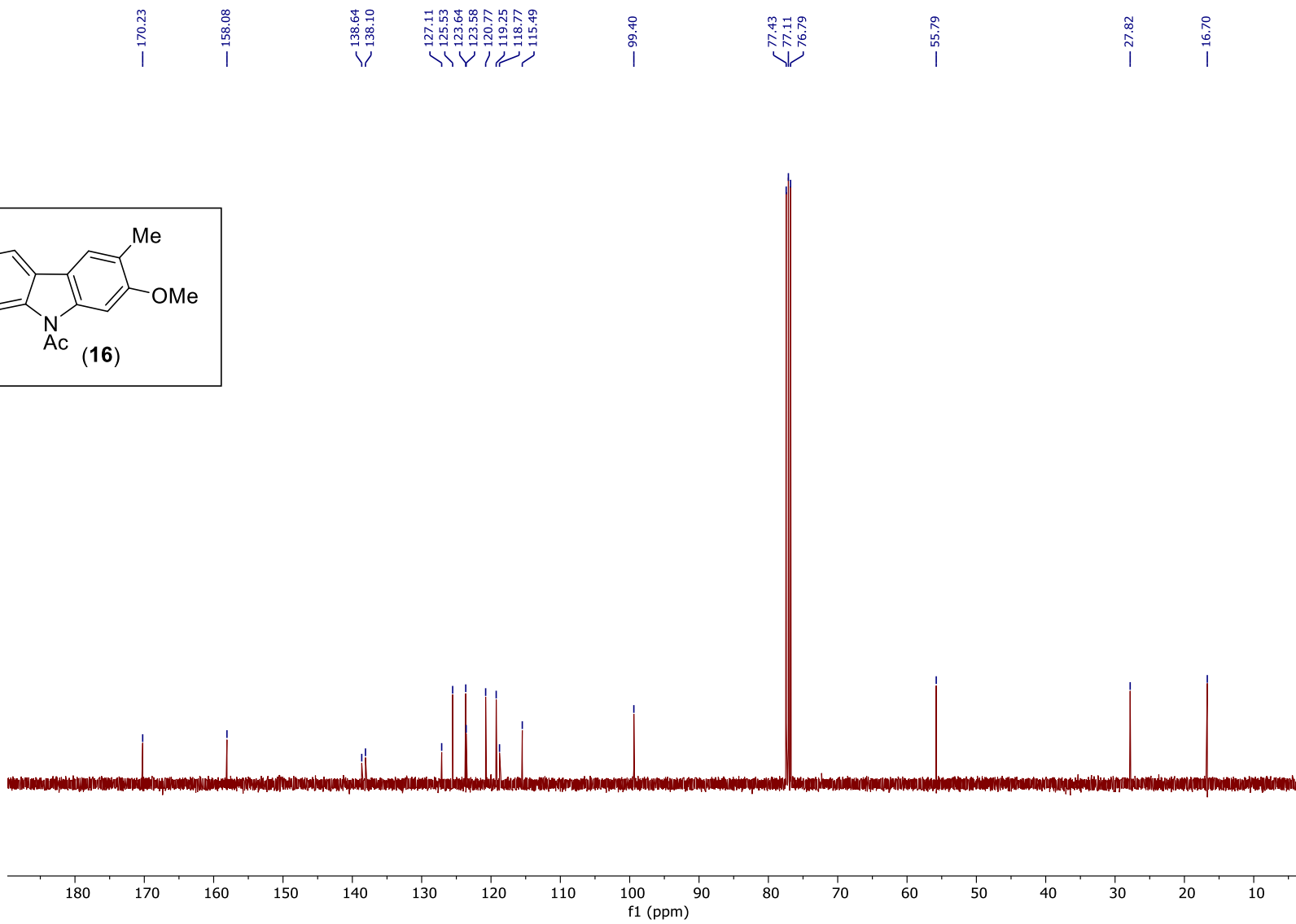
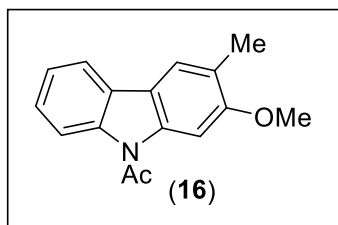
2.87



2.35



^1H NMR (400 MHz, CDCl_3) of **16**

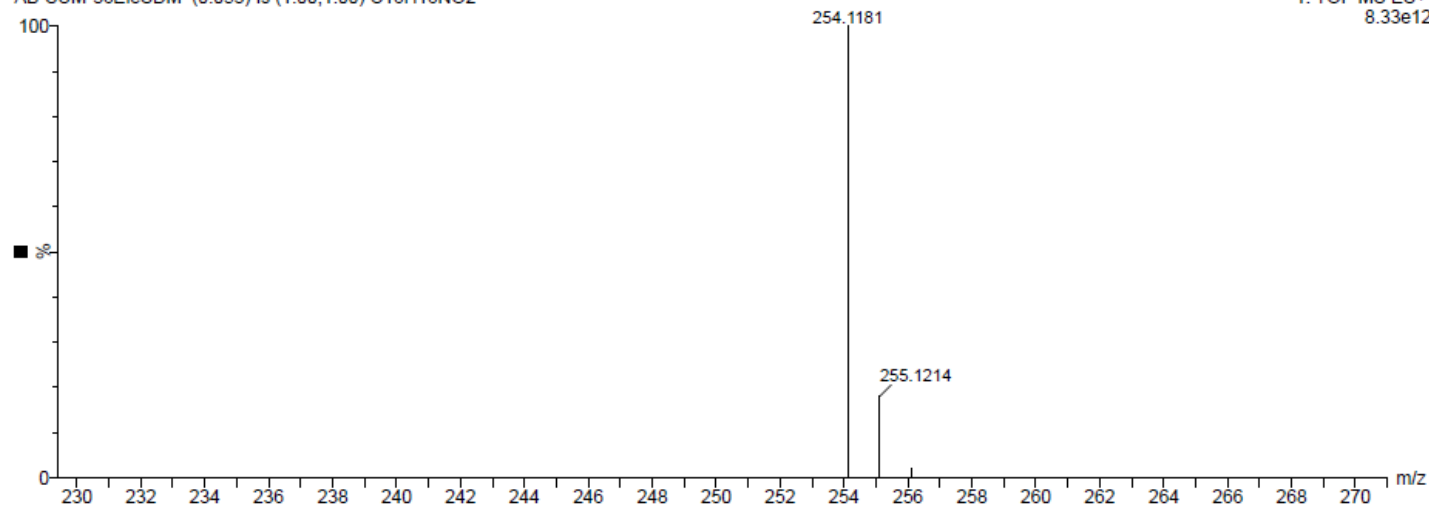


^{13}C NMR (100 MHz, CDCl_3) of **16**

AB28-Feb-2024 10:46:40
AB-SUM-36EleSDM (0.053) Is (1.00,1.00) C16H16NO2

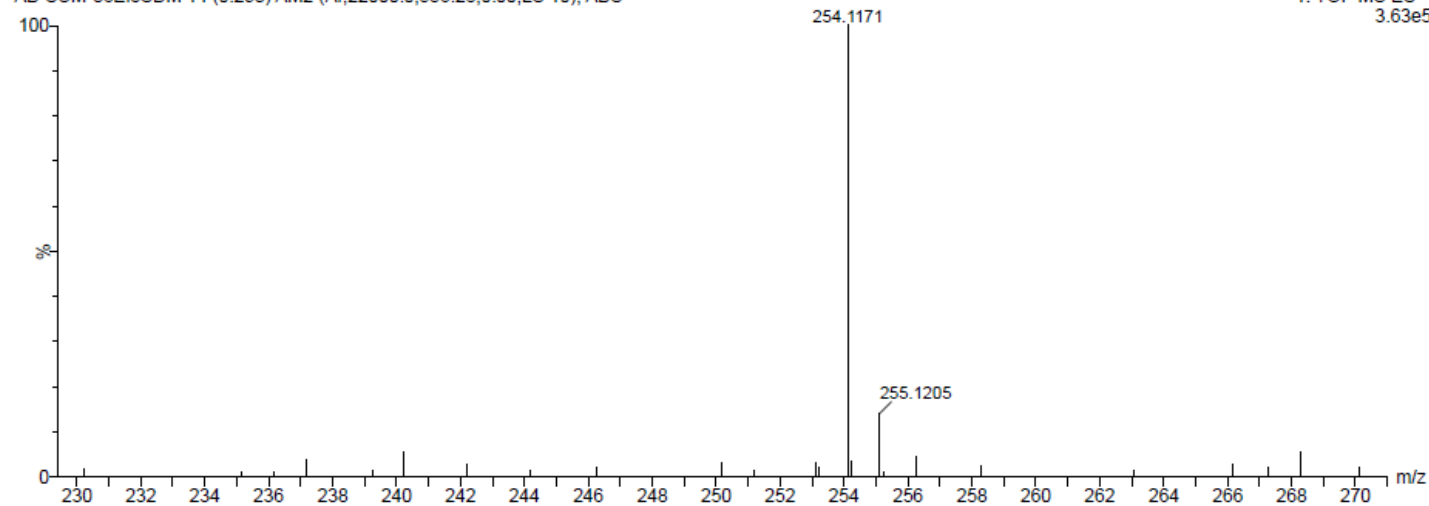
IISER - KOLKATA

1: TOF MS ES+
8.33e12

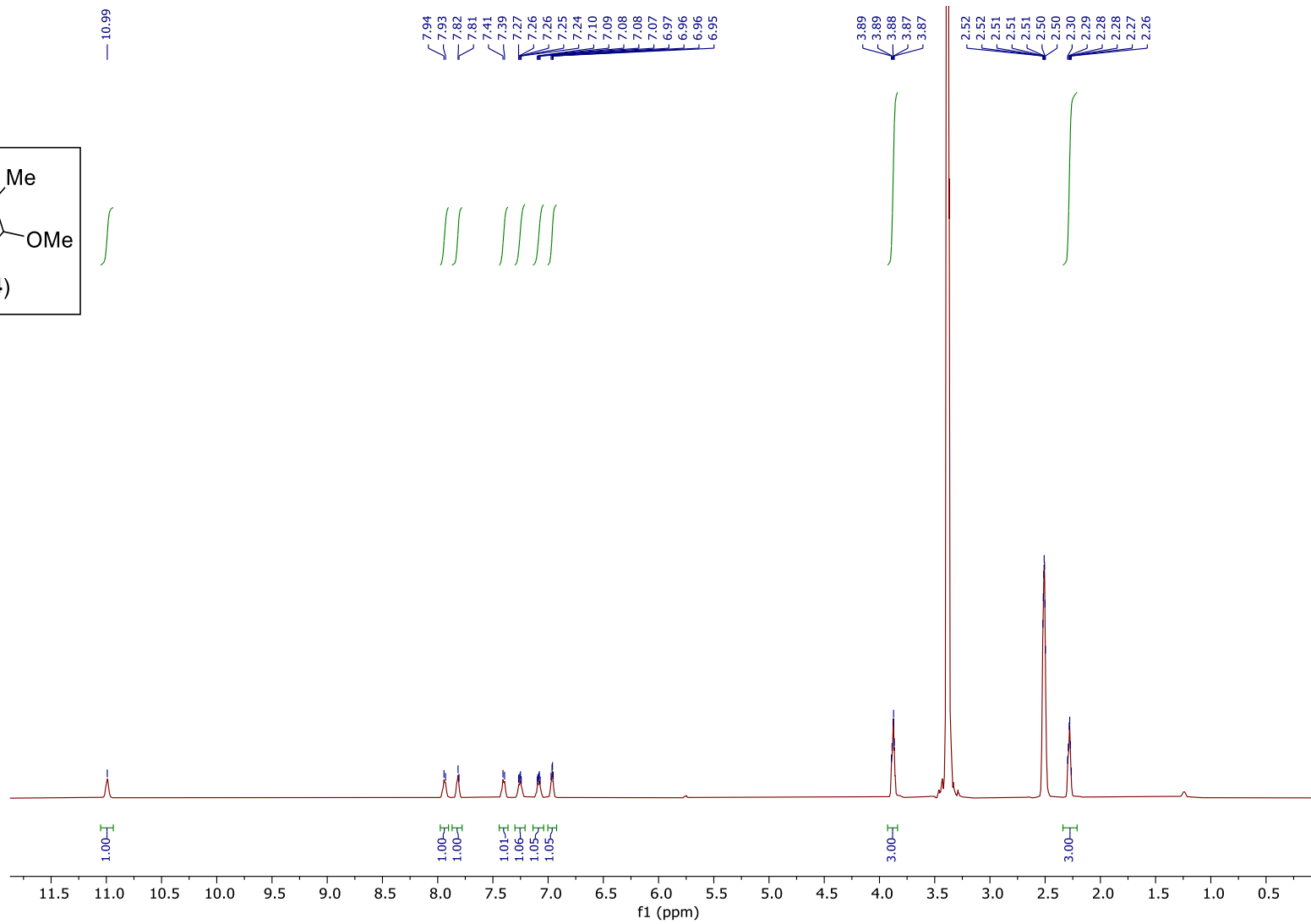
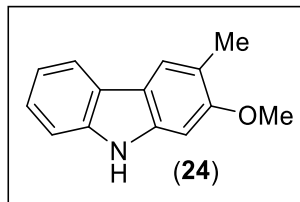


AB-SUM-36EleSDM 14 (0.293) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

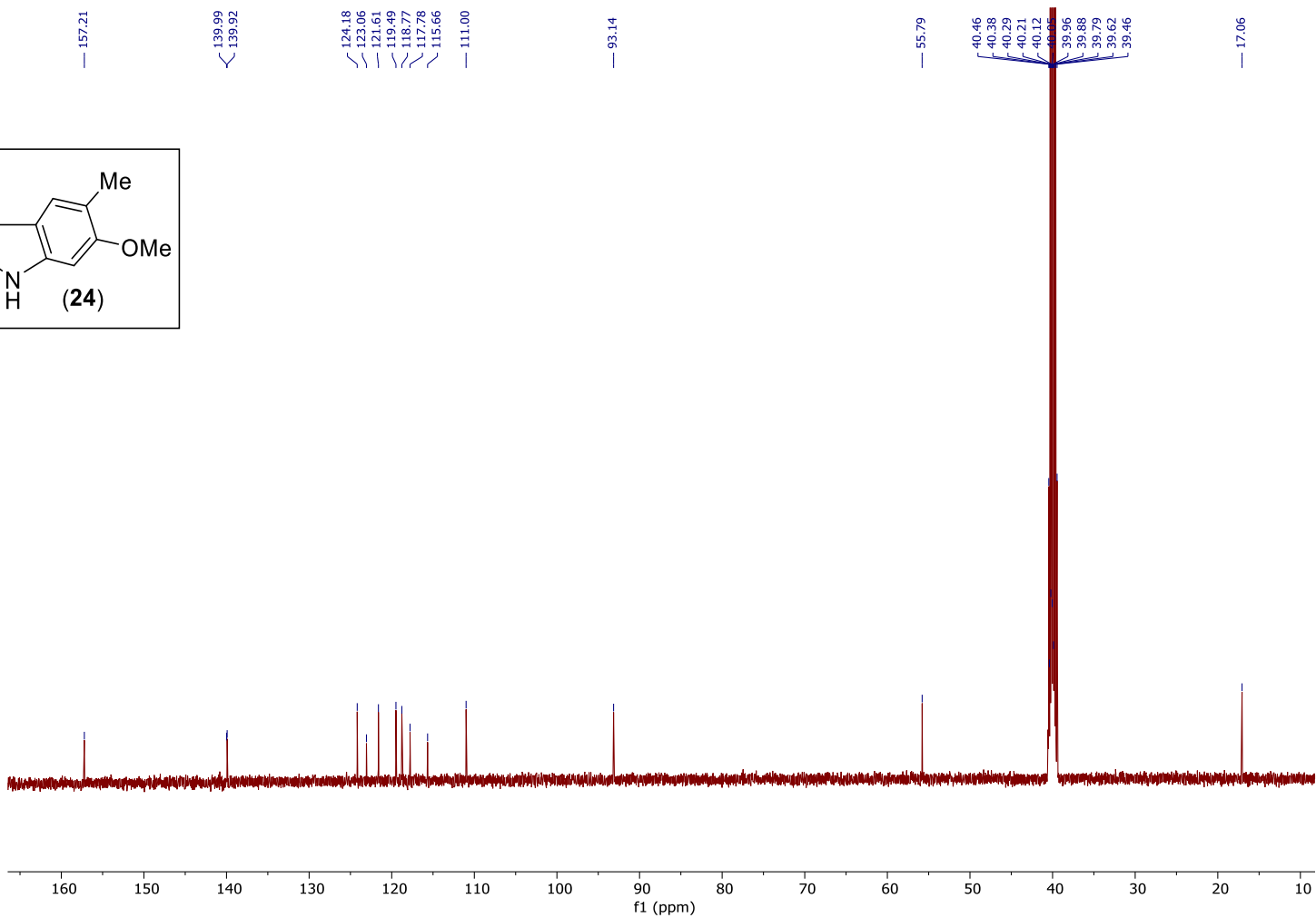
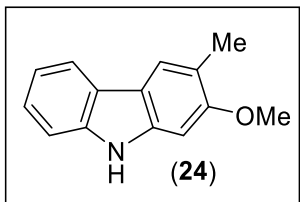
1: TOF MS ES+
3.63e5



HRMS data of 16



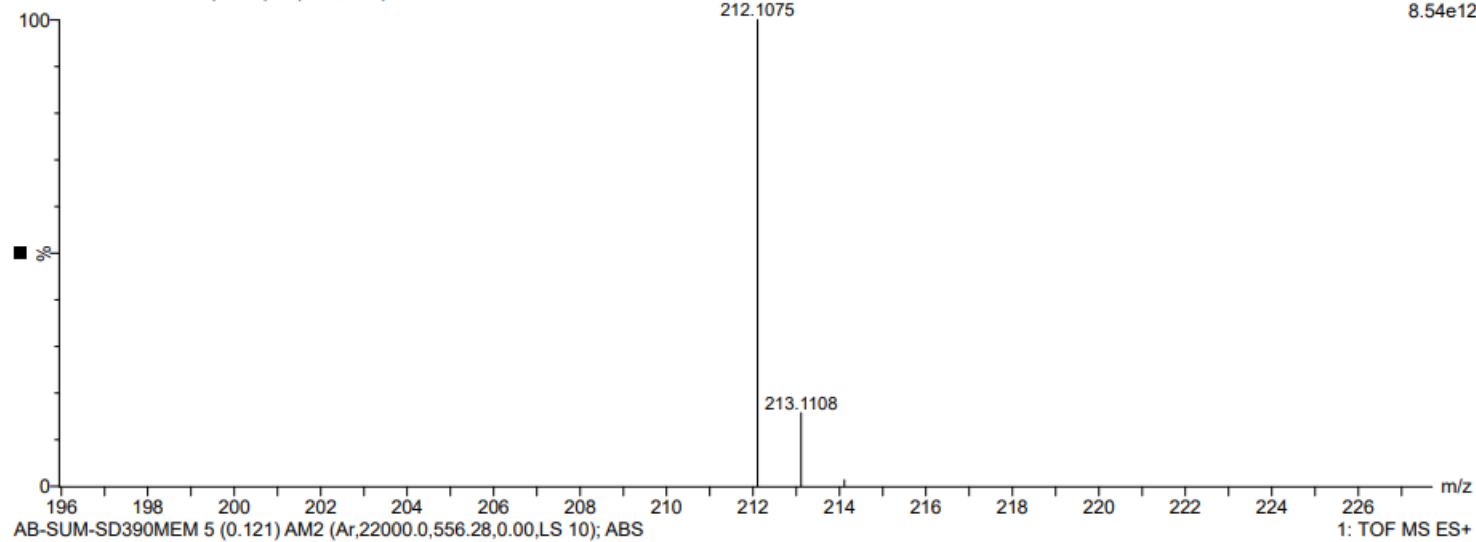
^1H NMR (500 MHz, DMSO-d_6) of **24**



AB08-May-2024 12:52:34
AB-SUM-SD390MEM (0.053) Is (1.00,1.00) C14H14NO

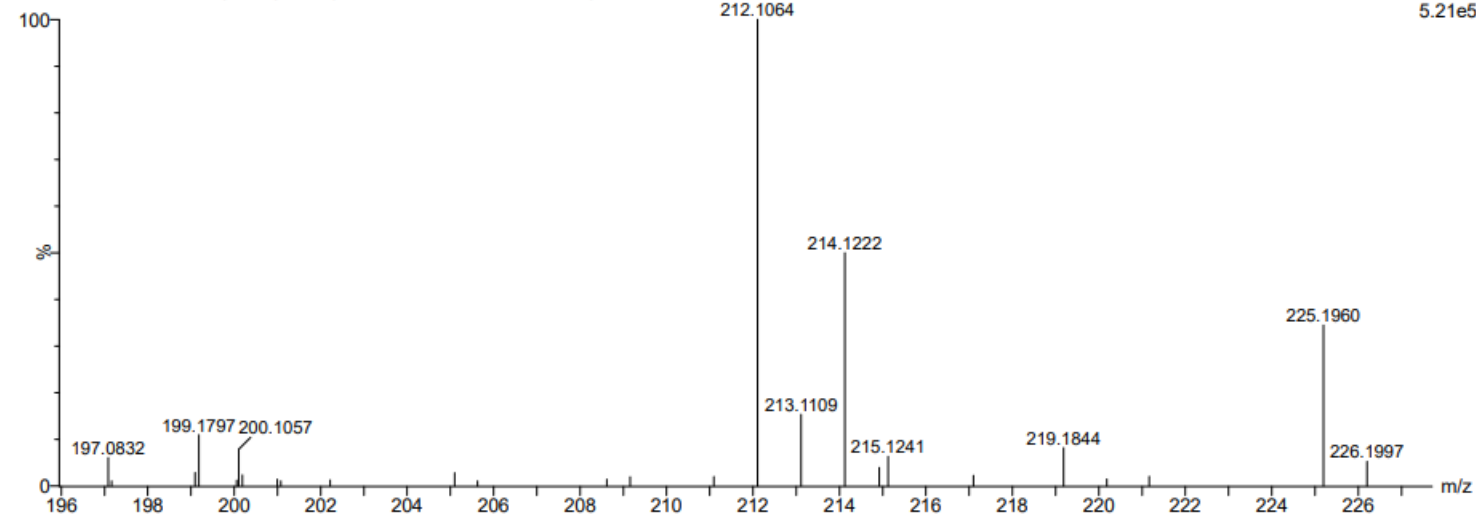
IISER - KOLKATA

1: TOF MS ES+
8.54e12

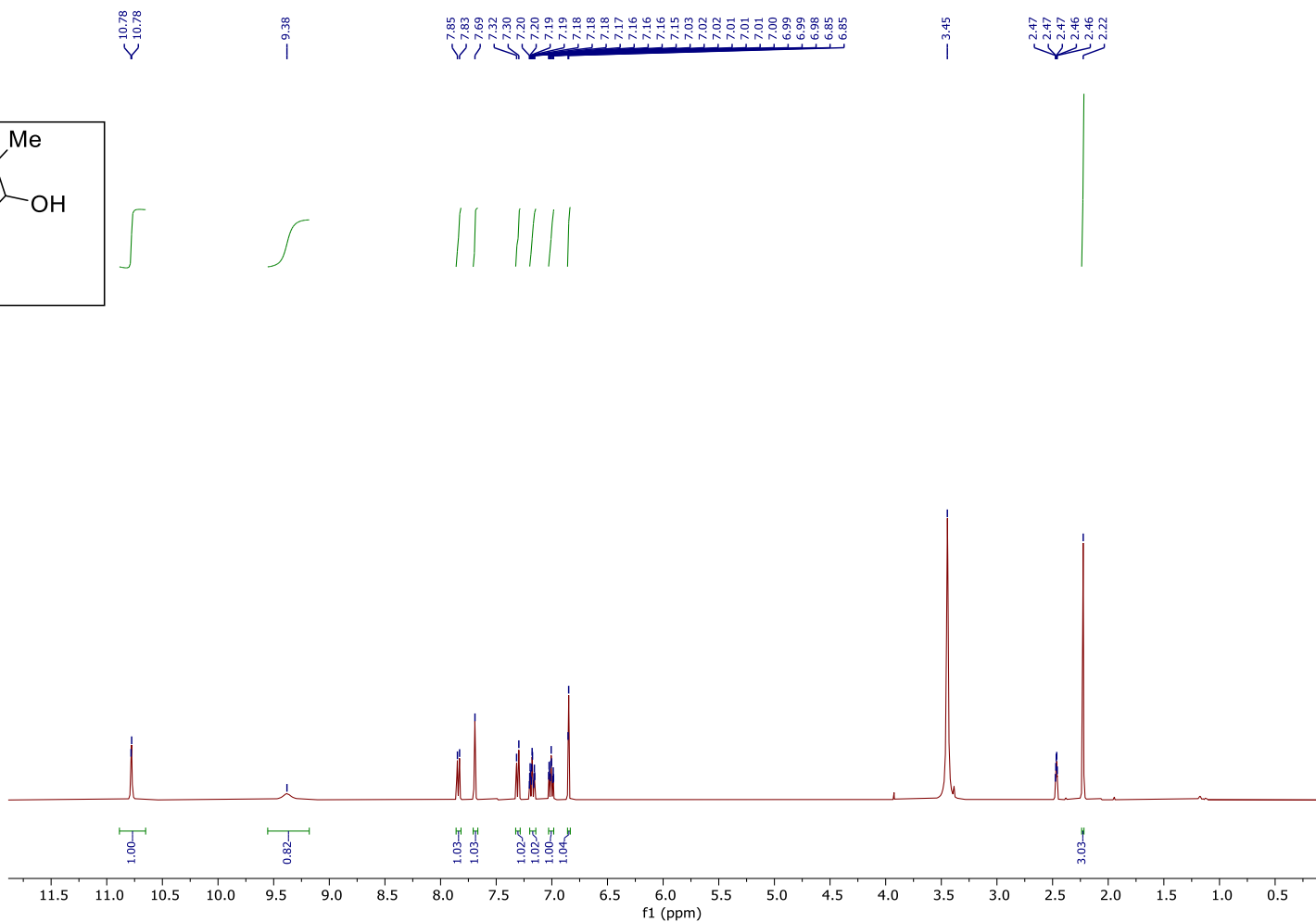
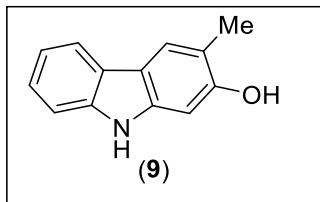


AB-SUM-SD390MEM 5 (0.121) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

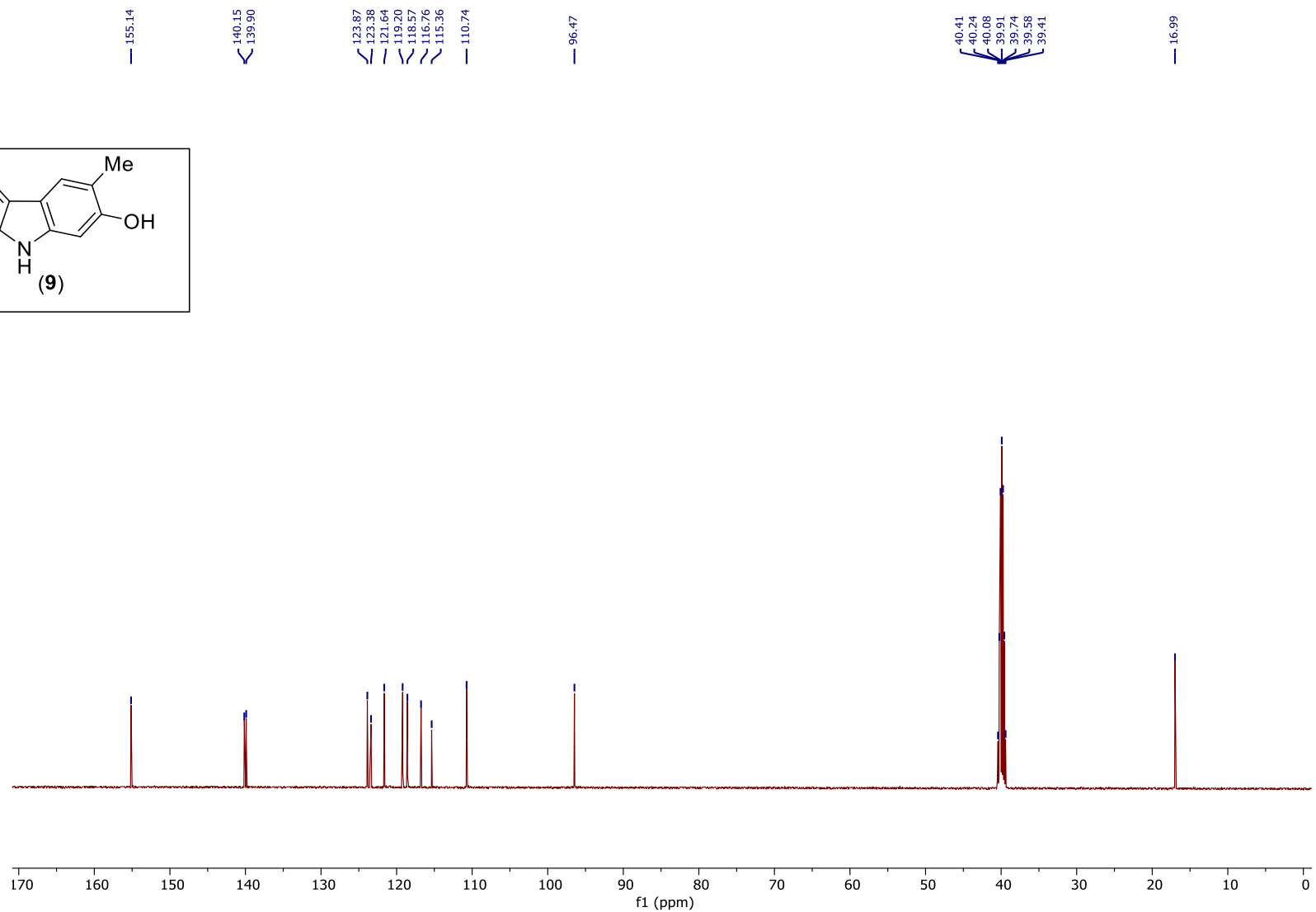
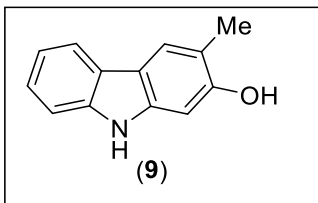
1: TOF MS ES+
5.21e5



HRMS data of 24



^1H NMR (400 MHz, DMSO-d_6) of **9**



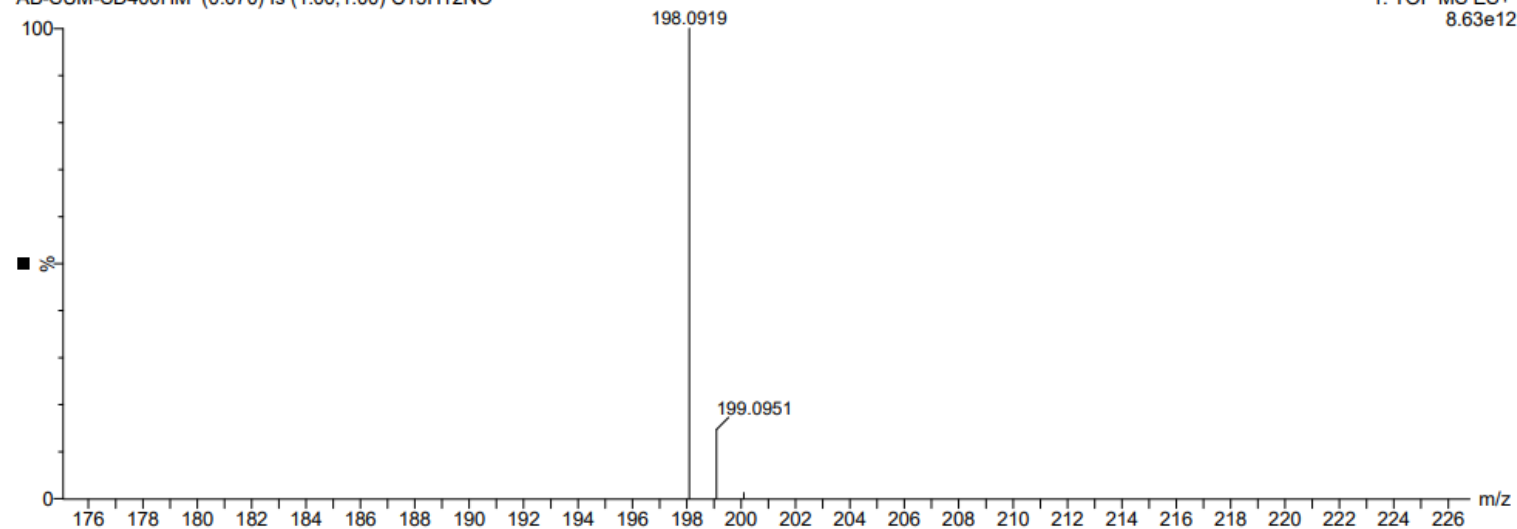
^{13}C NMR (125 MHz, DMSO- d_6) of **9**

AB06-May-2024 11:48:48

AB-SUM-SD400HM (0.070) Is (1.00,1.00) C13H12NO

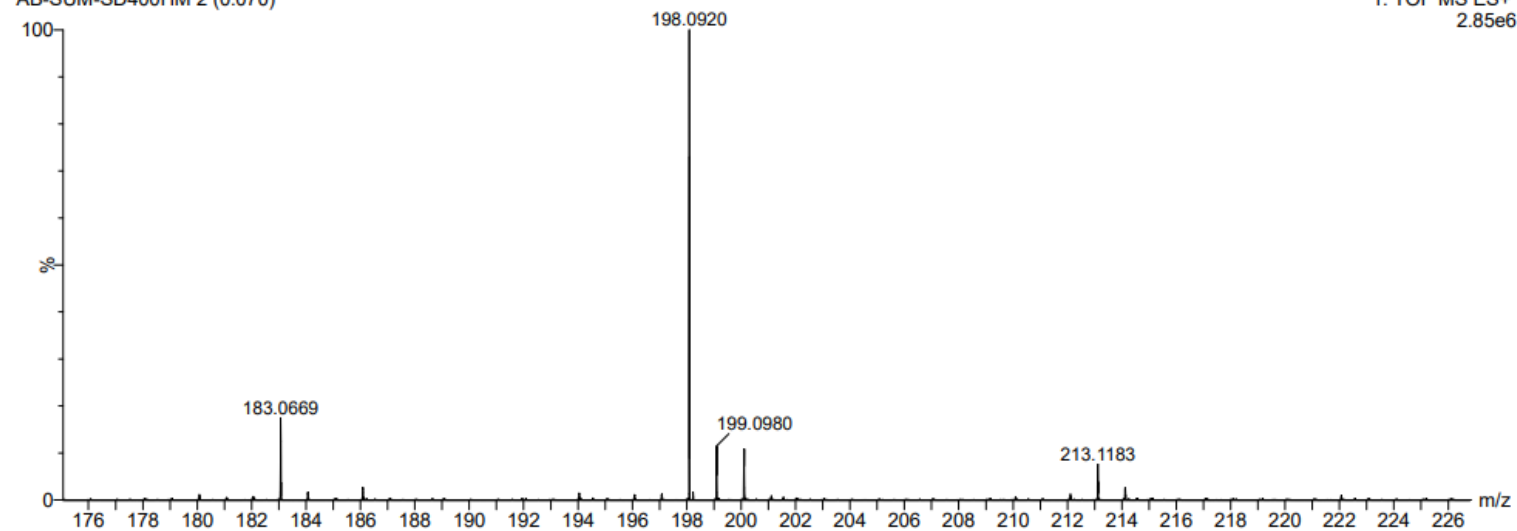
IISER - KOLKATA

1: TOF MS ES+
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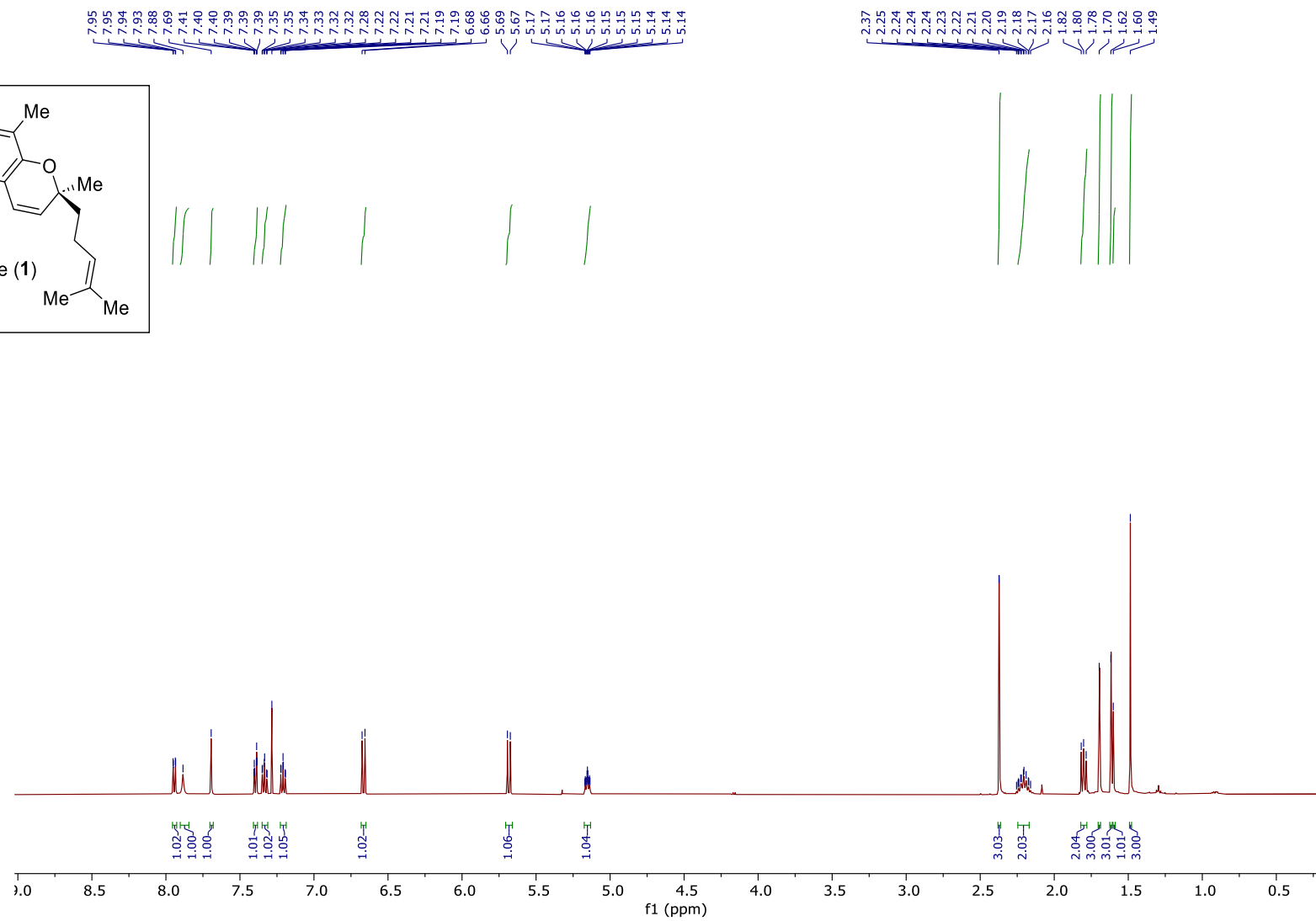
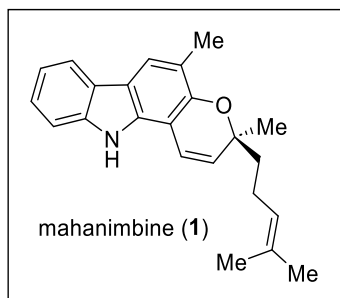


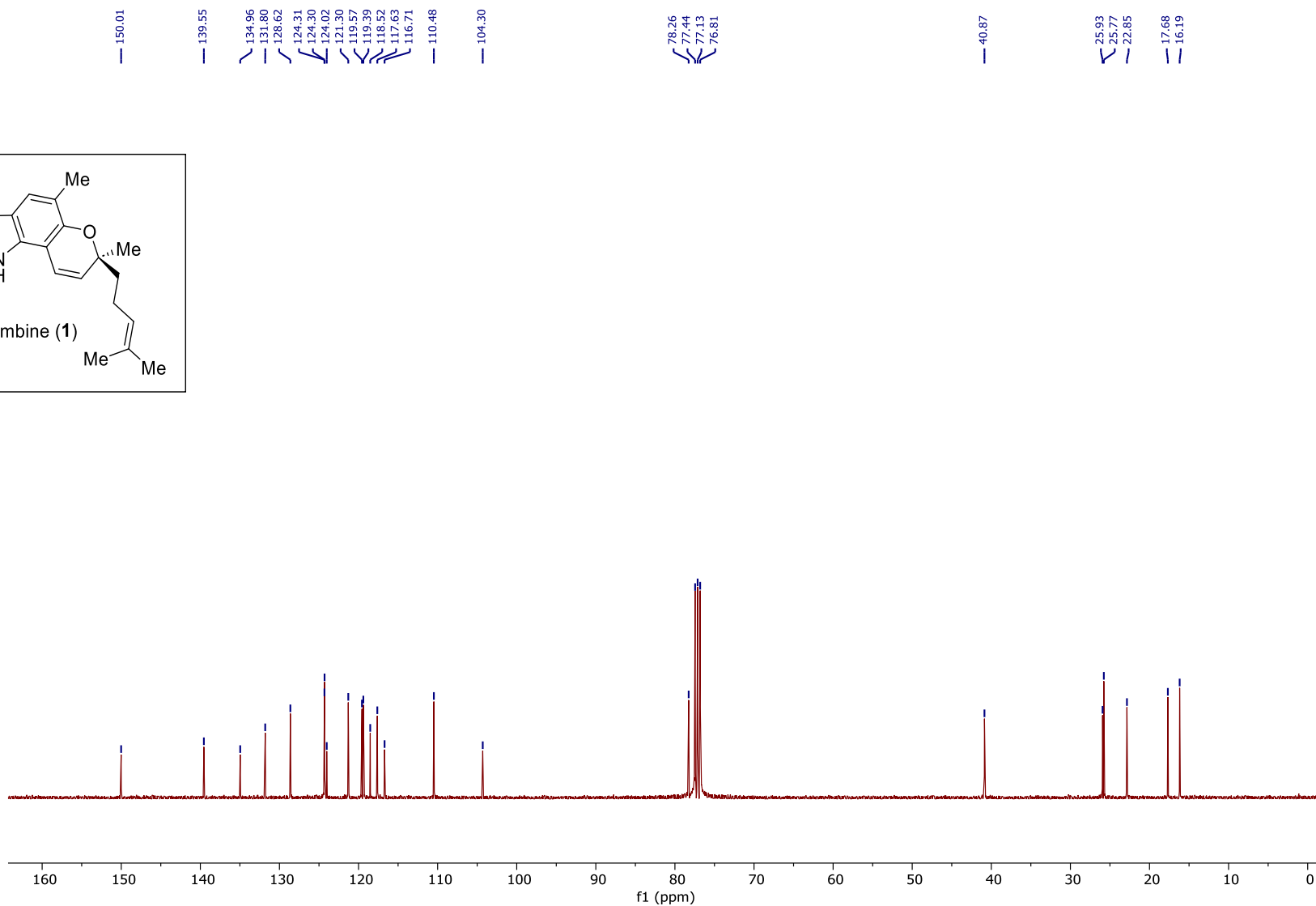
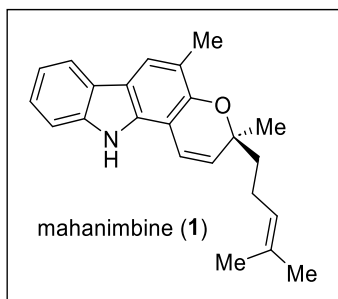
AB-SUM-SD400HM 2 (0.070)

1: TOF MS ES+
2.85e6



HRMS data of 9

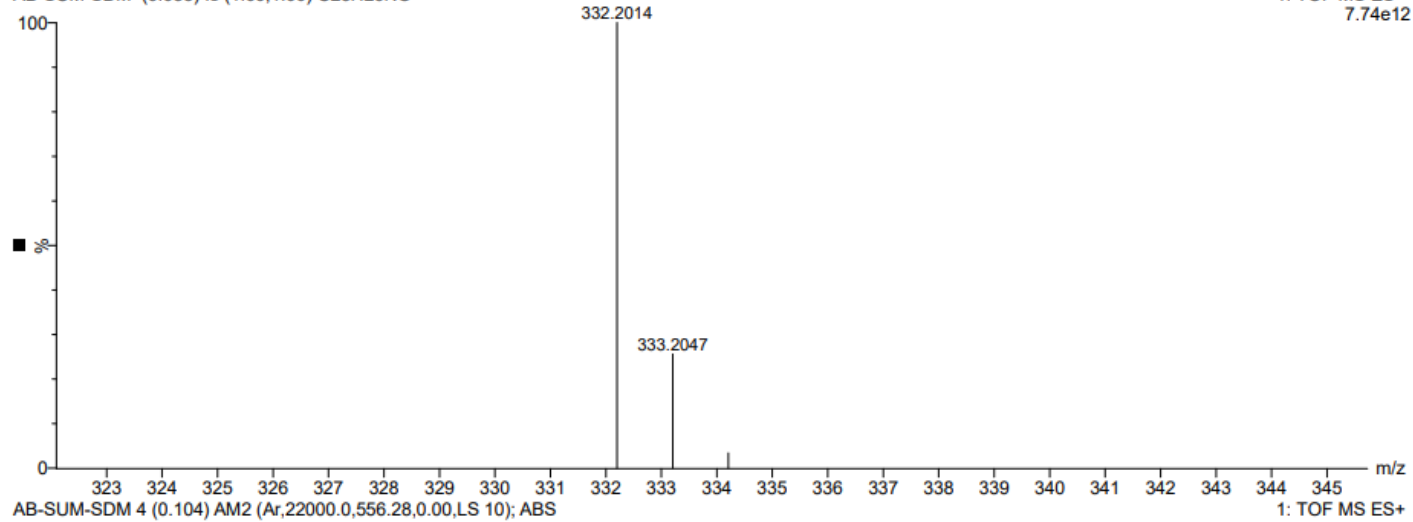




AB30-Apr-2024 11:49:17
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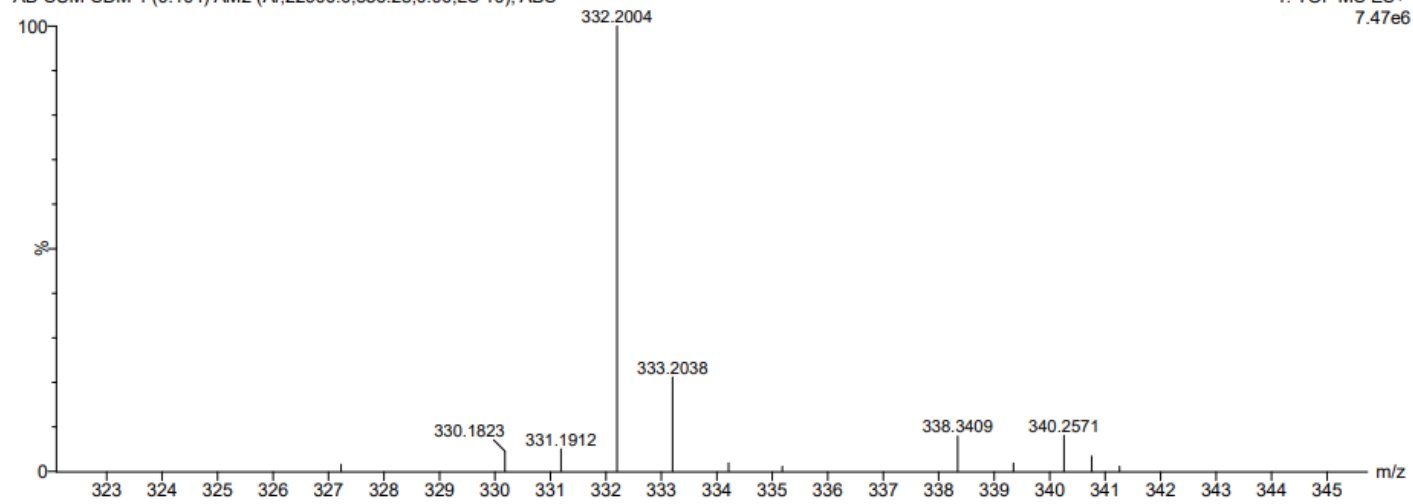
IISER - KOLKATA

1: TOF MS ES+
7.74e12

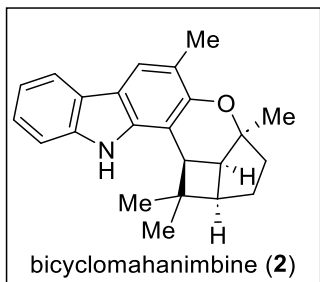


AB-SUM-SDM 4 (0.104) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+
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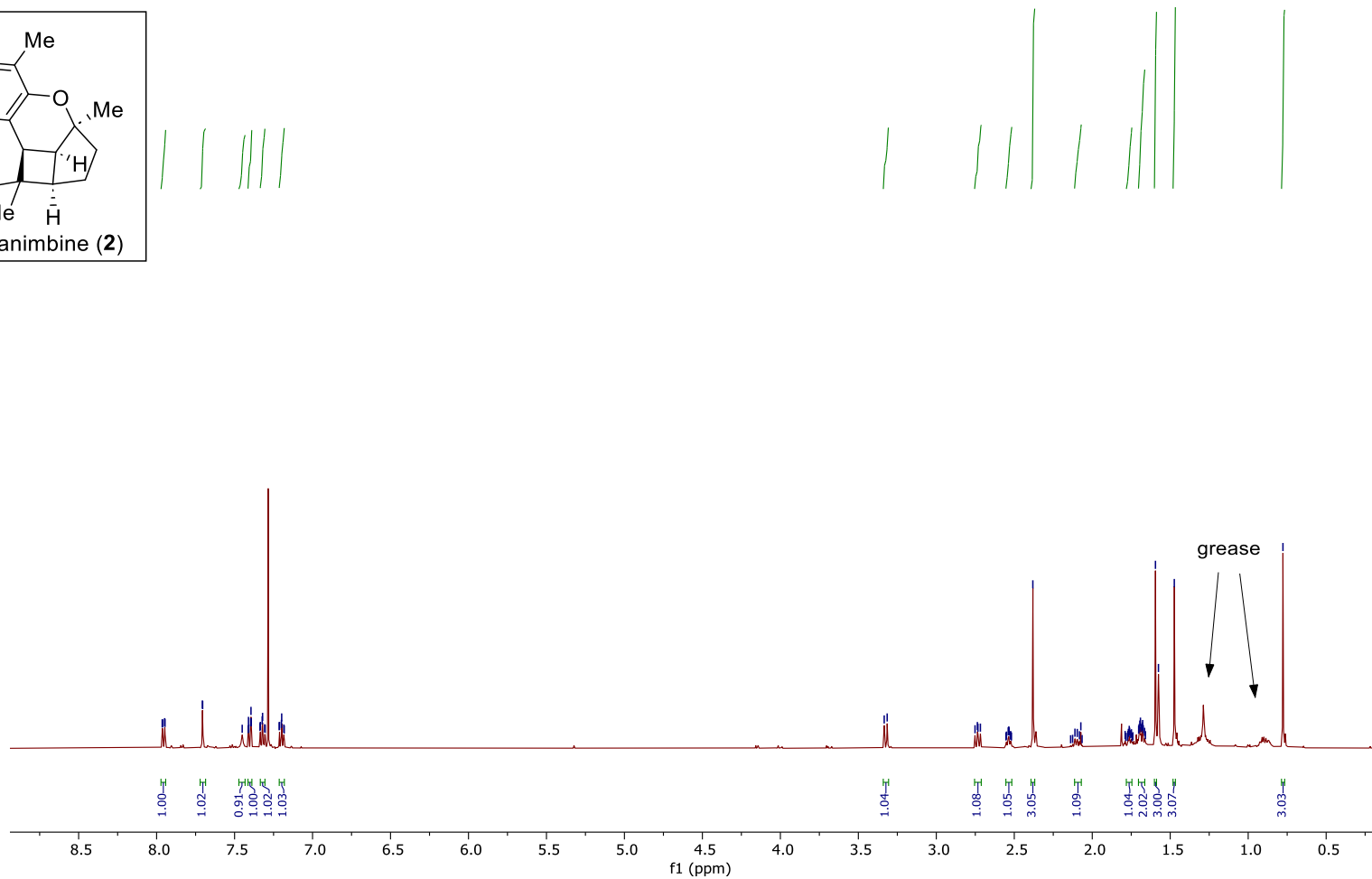


HRMS data of 1

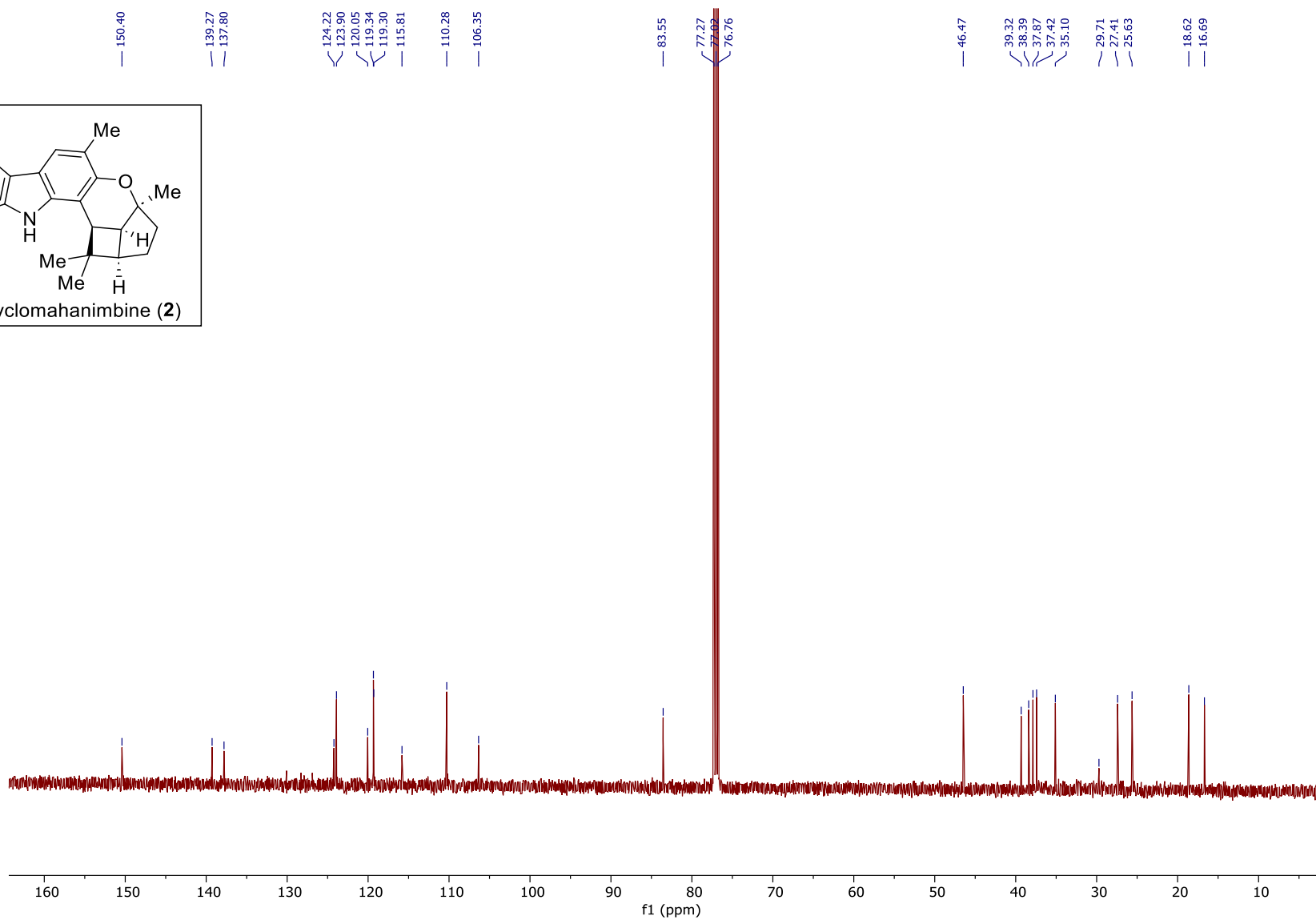
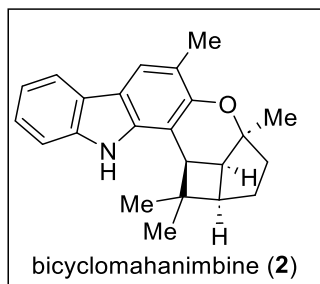


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0.78



^1H NMR (500 MHz, CDCl_3) of 2



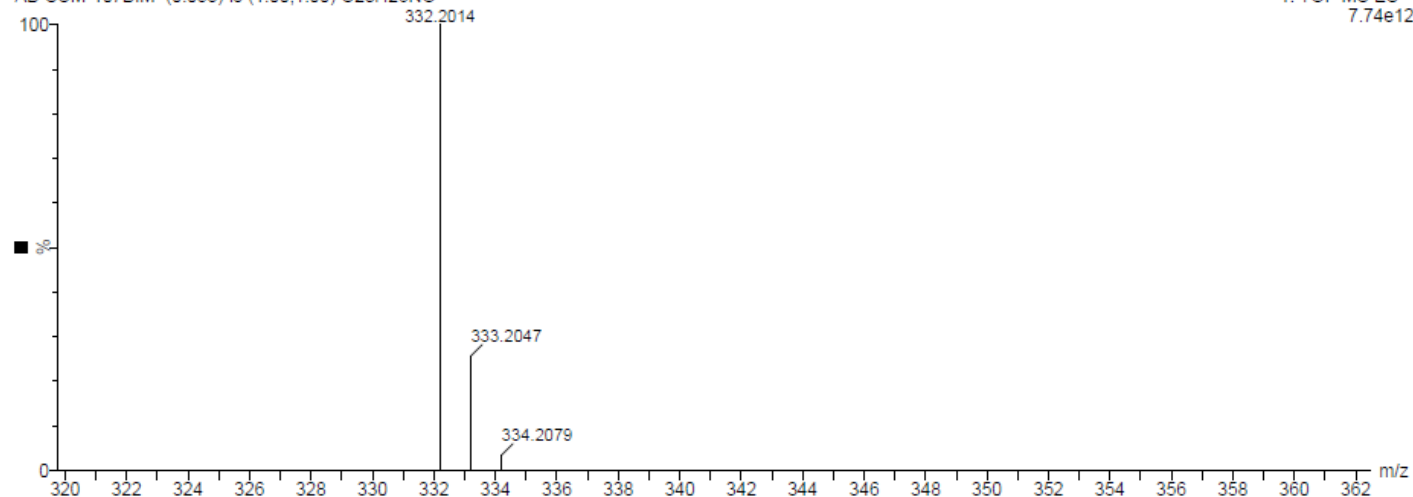
^{13}C NMR (125 MHz, CDCl_3) of **2**

AB15-Nov-2023 12:45:25

IISER - KOLKATA

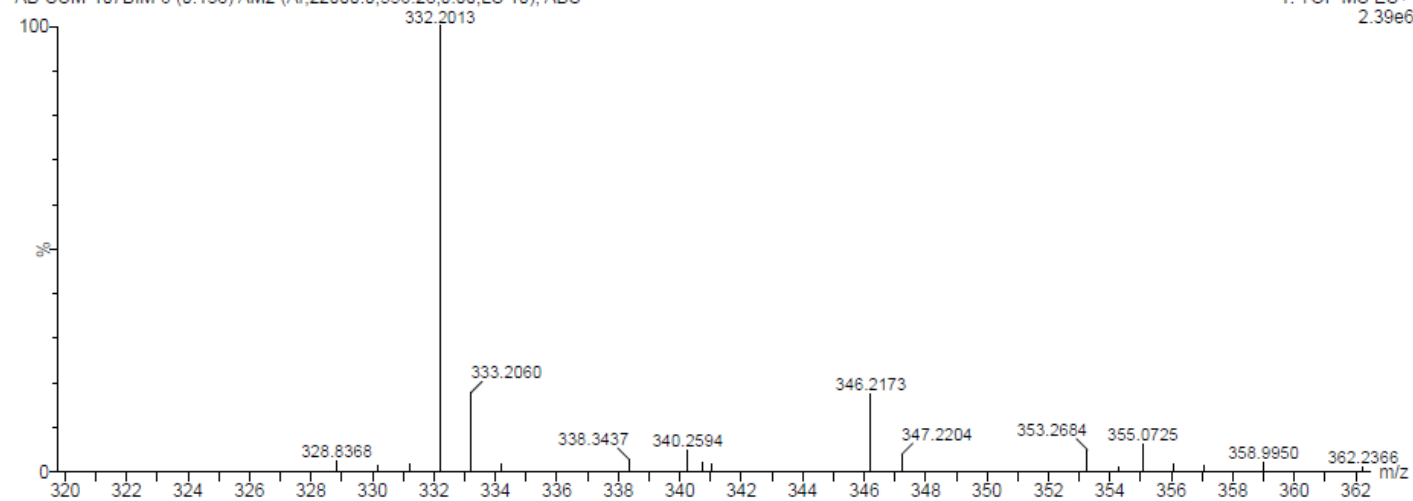
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AB-SUM-107BIM (0.053) Is (1.00,1.00) C₂₃H₂₆NO

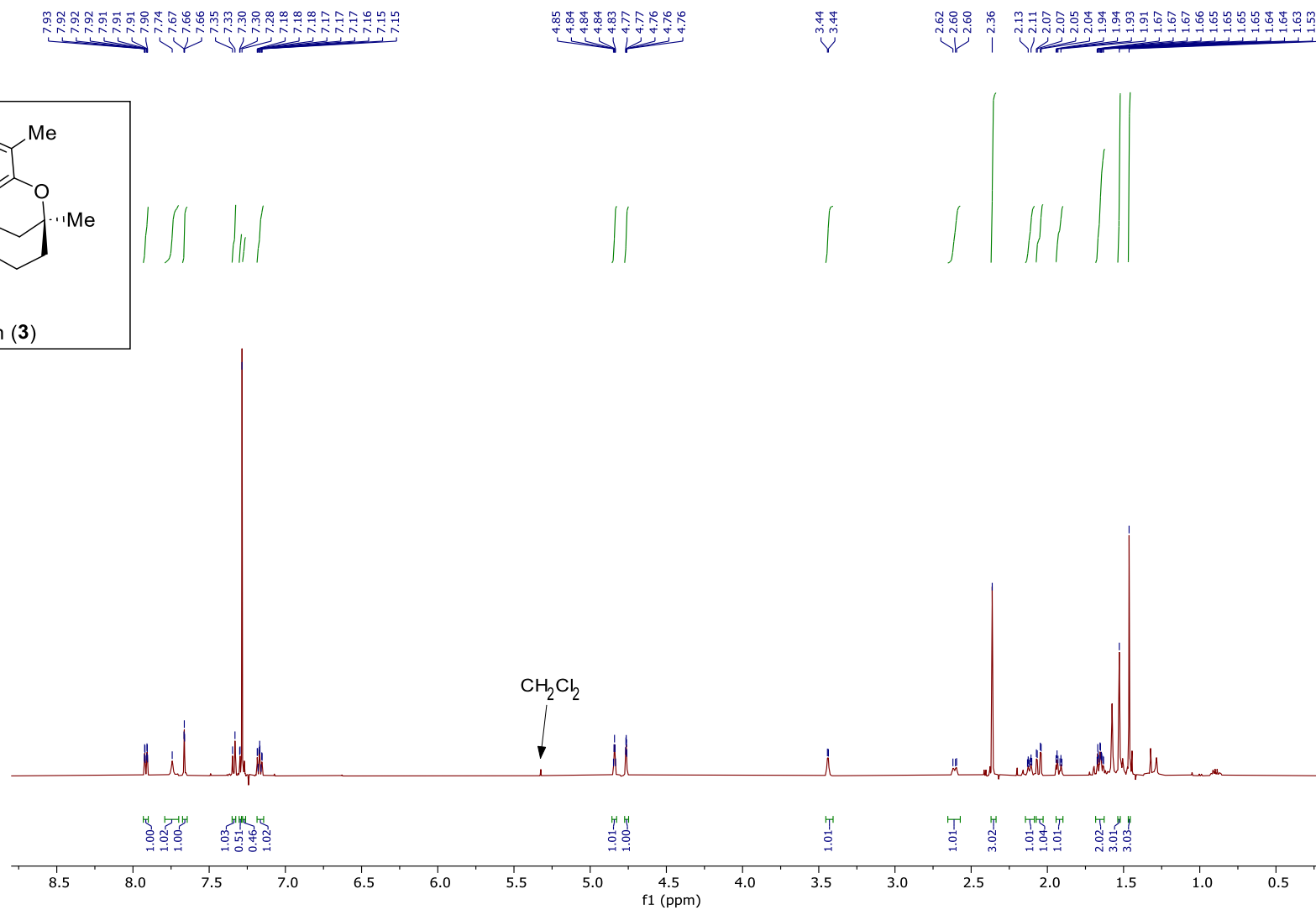
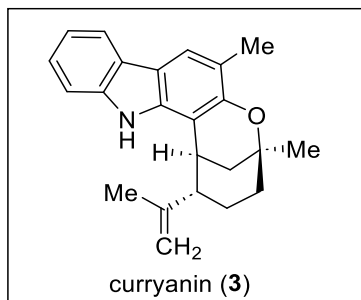


AB-SUM-107BIM 6 (0.138) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

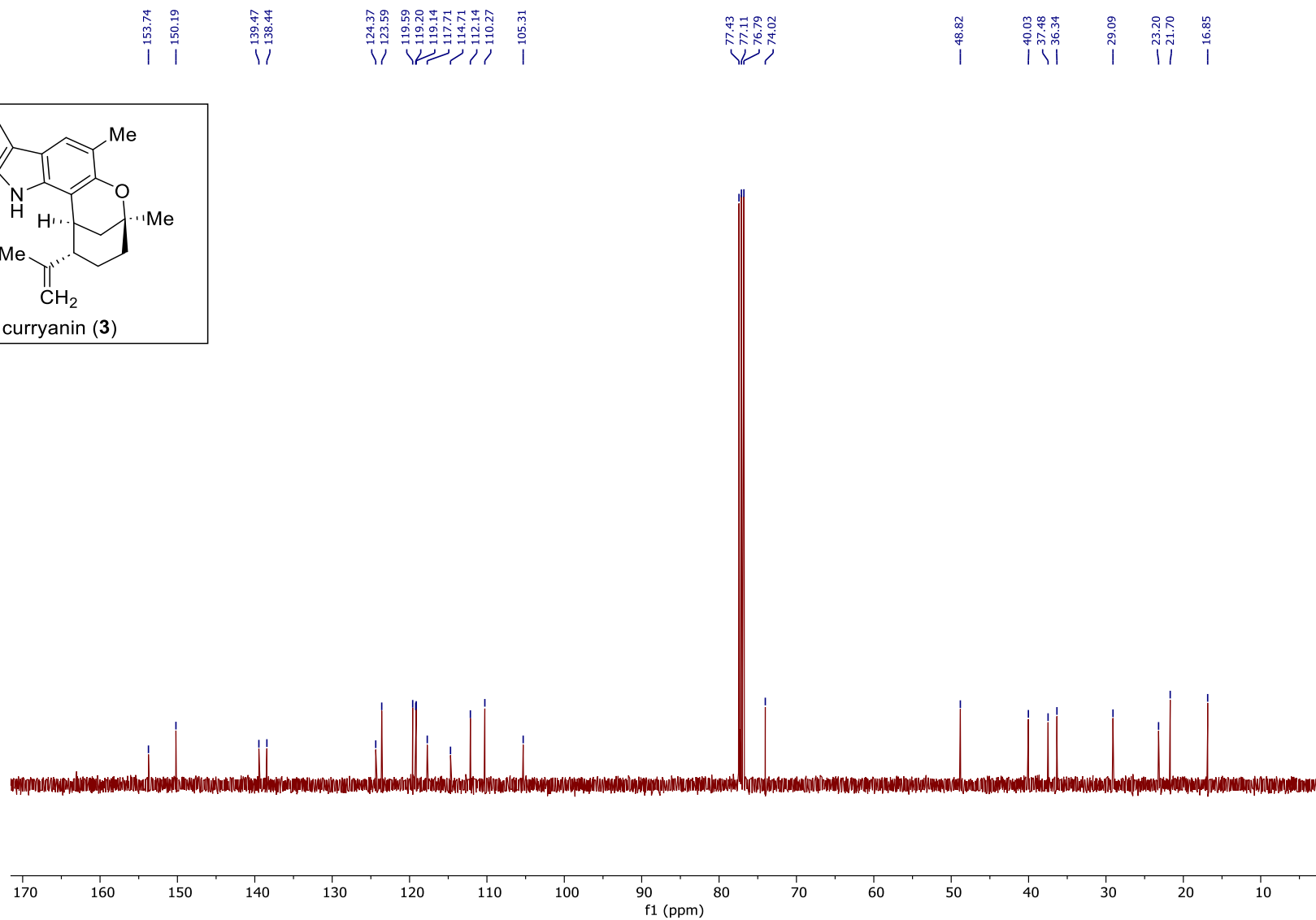
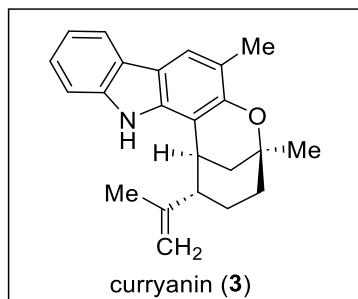
1: TOF MS ES+
2.39e6



HRMS data of 2



¹H NMR (500 MHz, CDCl₃) of 3

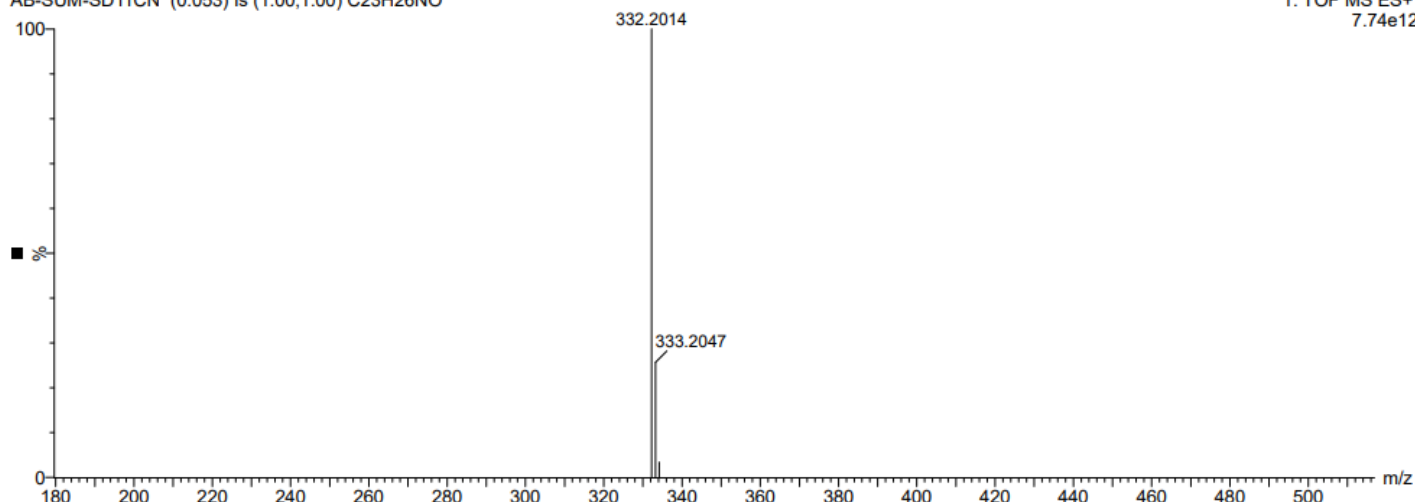


¹³C NMR (100 MHz, CDCl₃) of 3

AB04-Mar-2024 11:55:45
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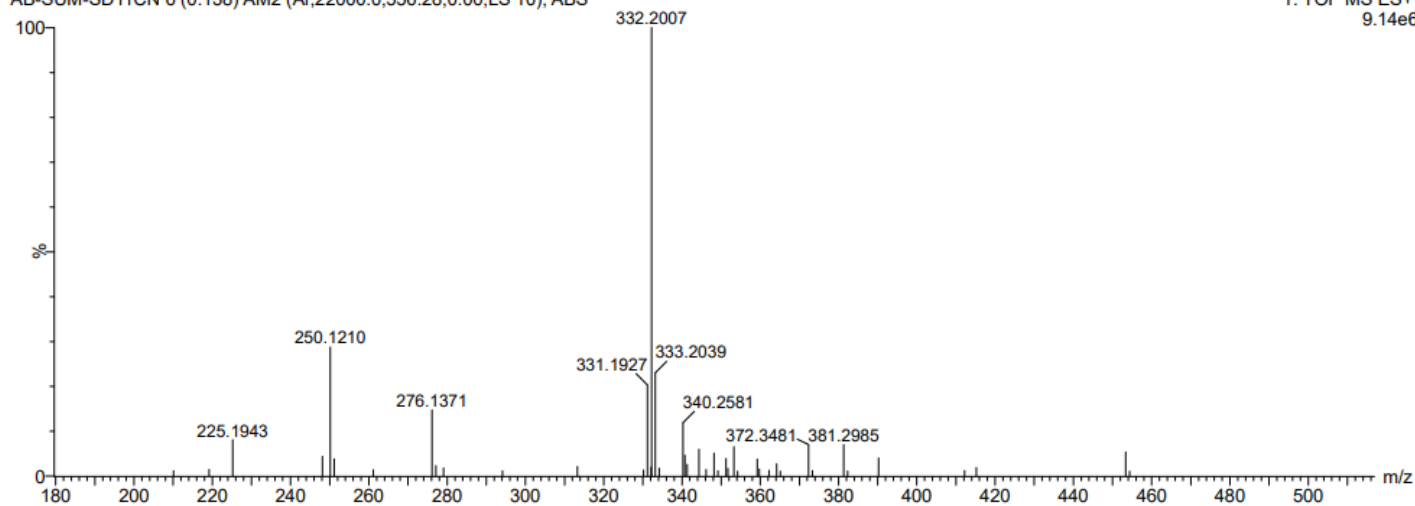
IISER - KOLKATA

1: TOF MS ES+
7.74e12

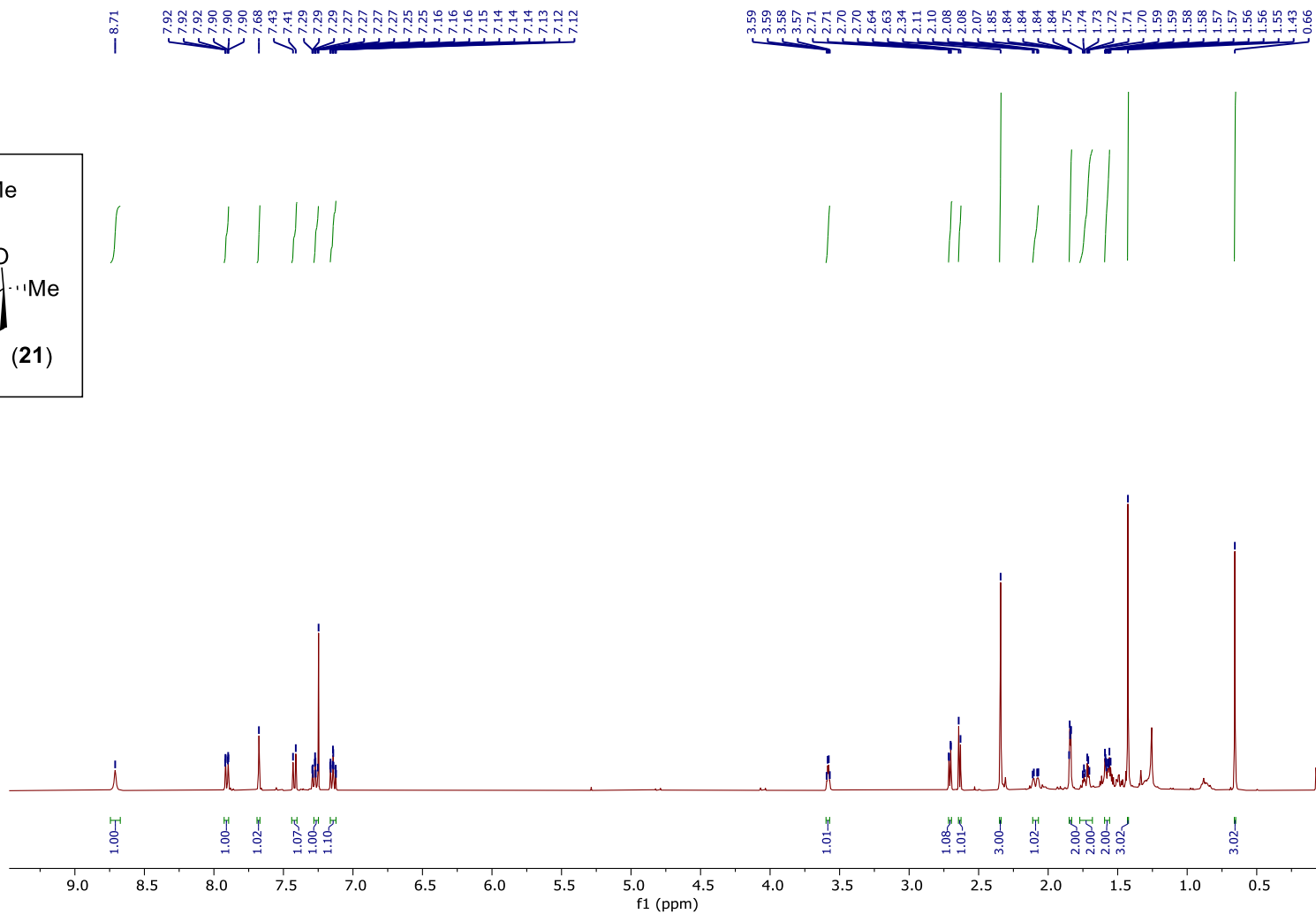
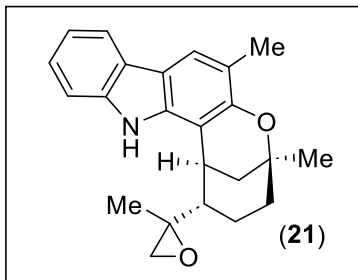


AB-SUM-SD11CN 6 (0.138) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

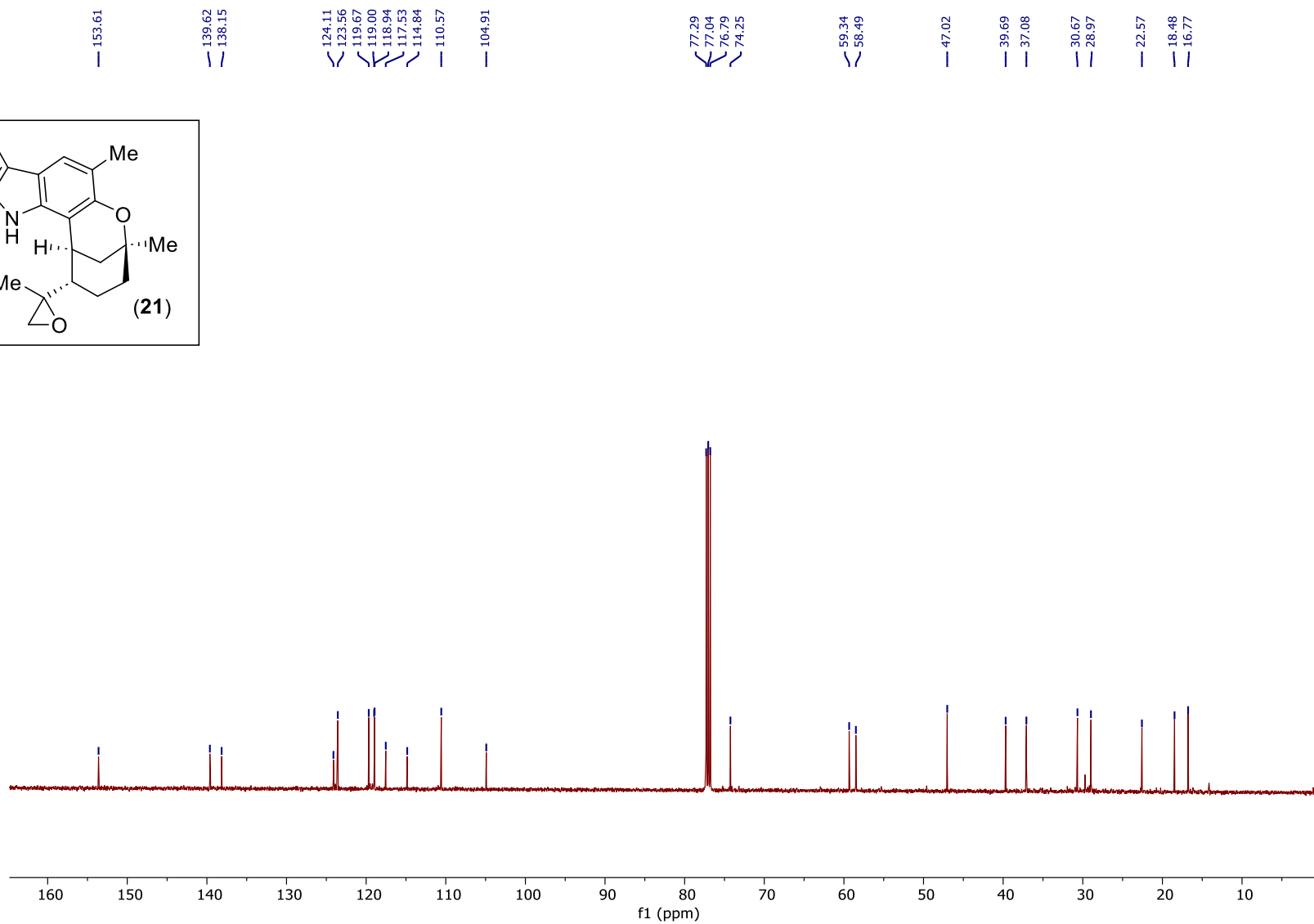
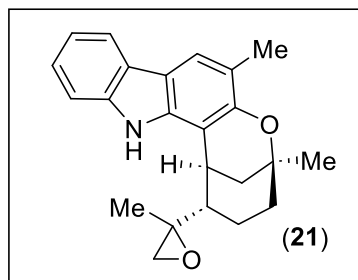
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9.14e6



HRMS data of 3



^1H NMR (500 MHz, CDCl_3) of **21**



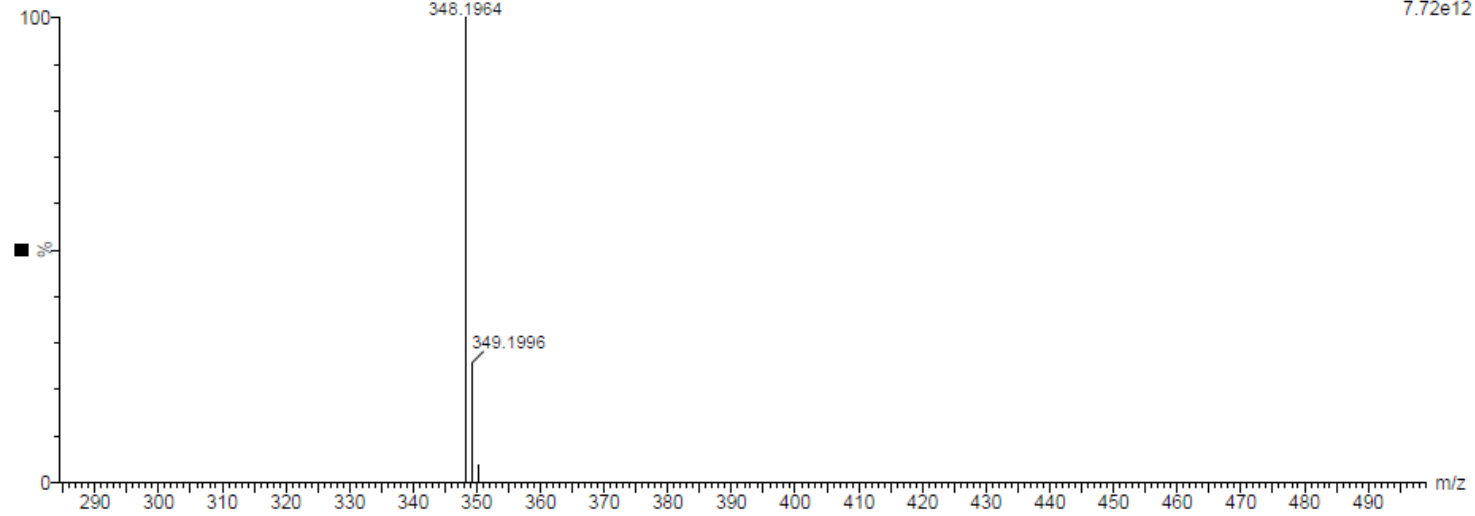
^{13}C NMR (125 MHz, CDCl_3) of **21**

AB16-Apr-2024 12:28:10

IISER - KOLKATA

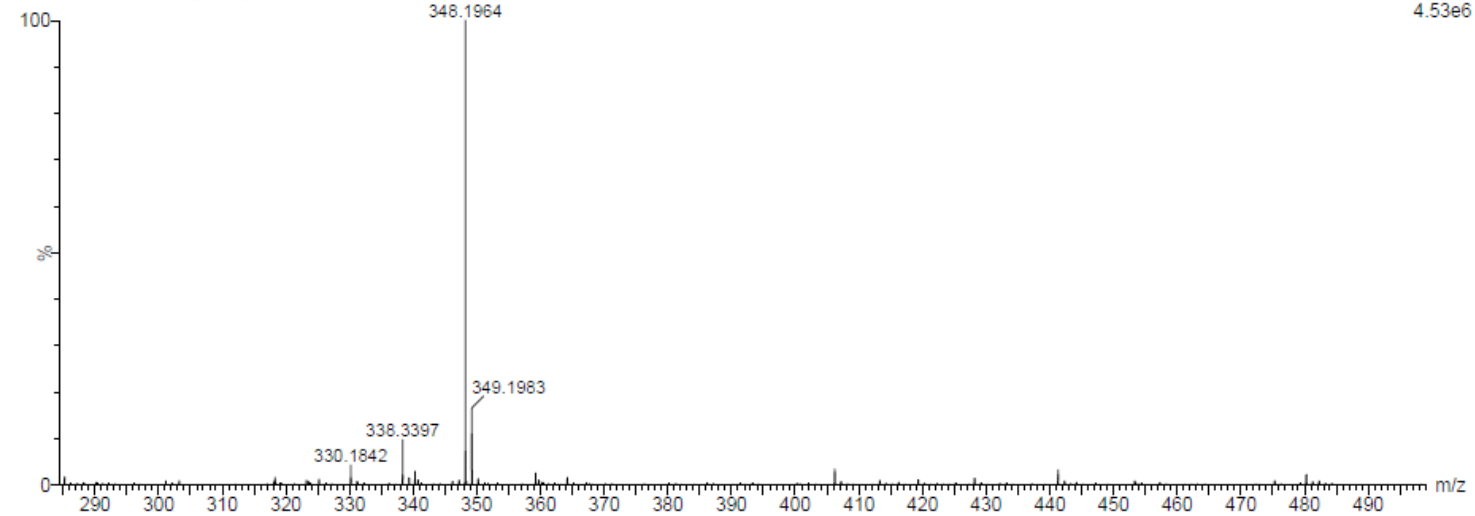
1: TOF MS ES+
7.72e12

AB-SUM-SD EPM (0.104) Is (1.00,1.00) C₂₃H₂₆NO₂

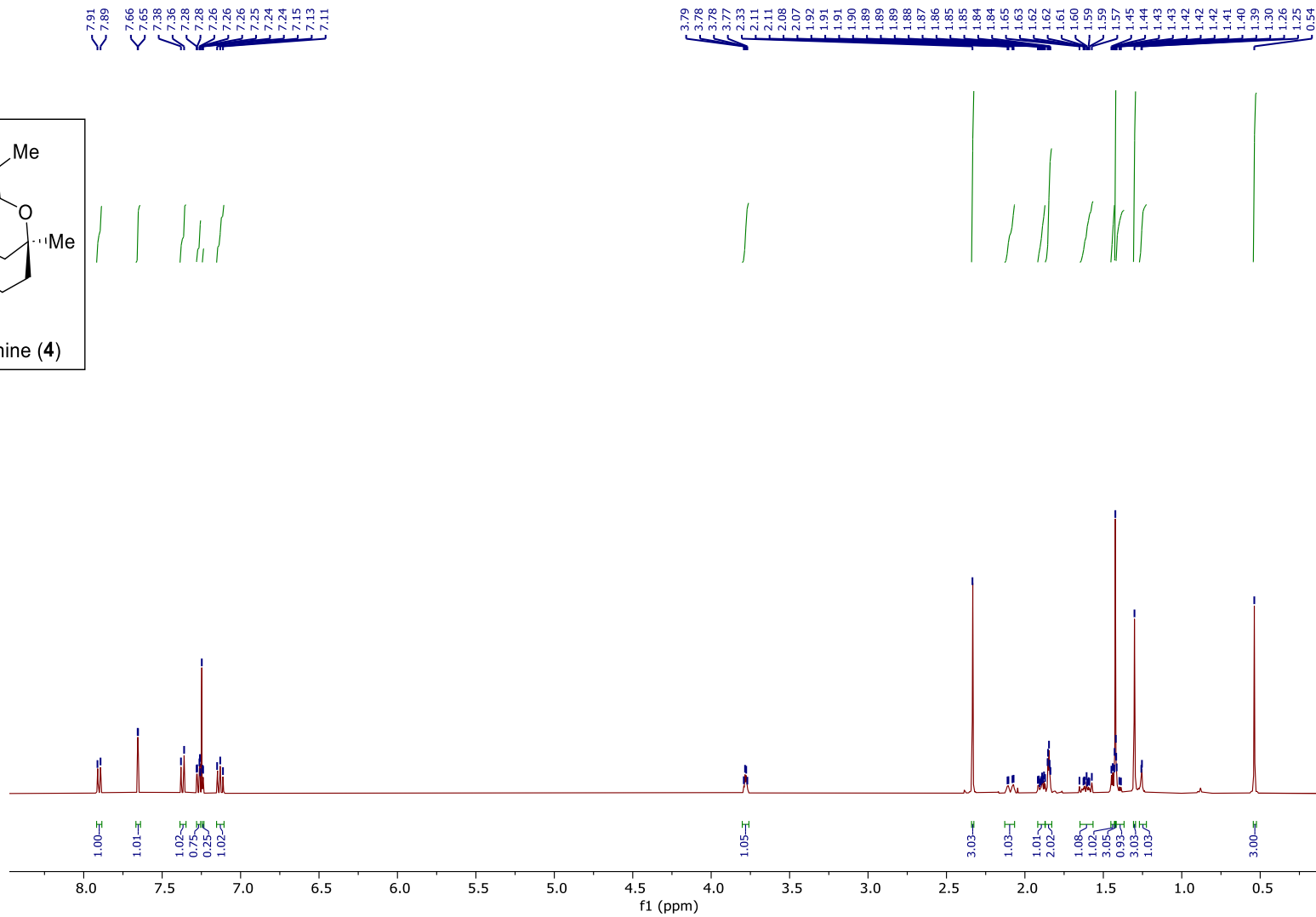
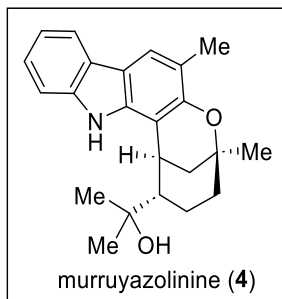


AB-SUM-SD EPM 4 (0.104)

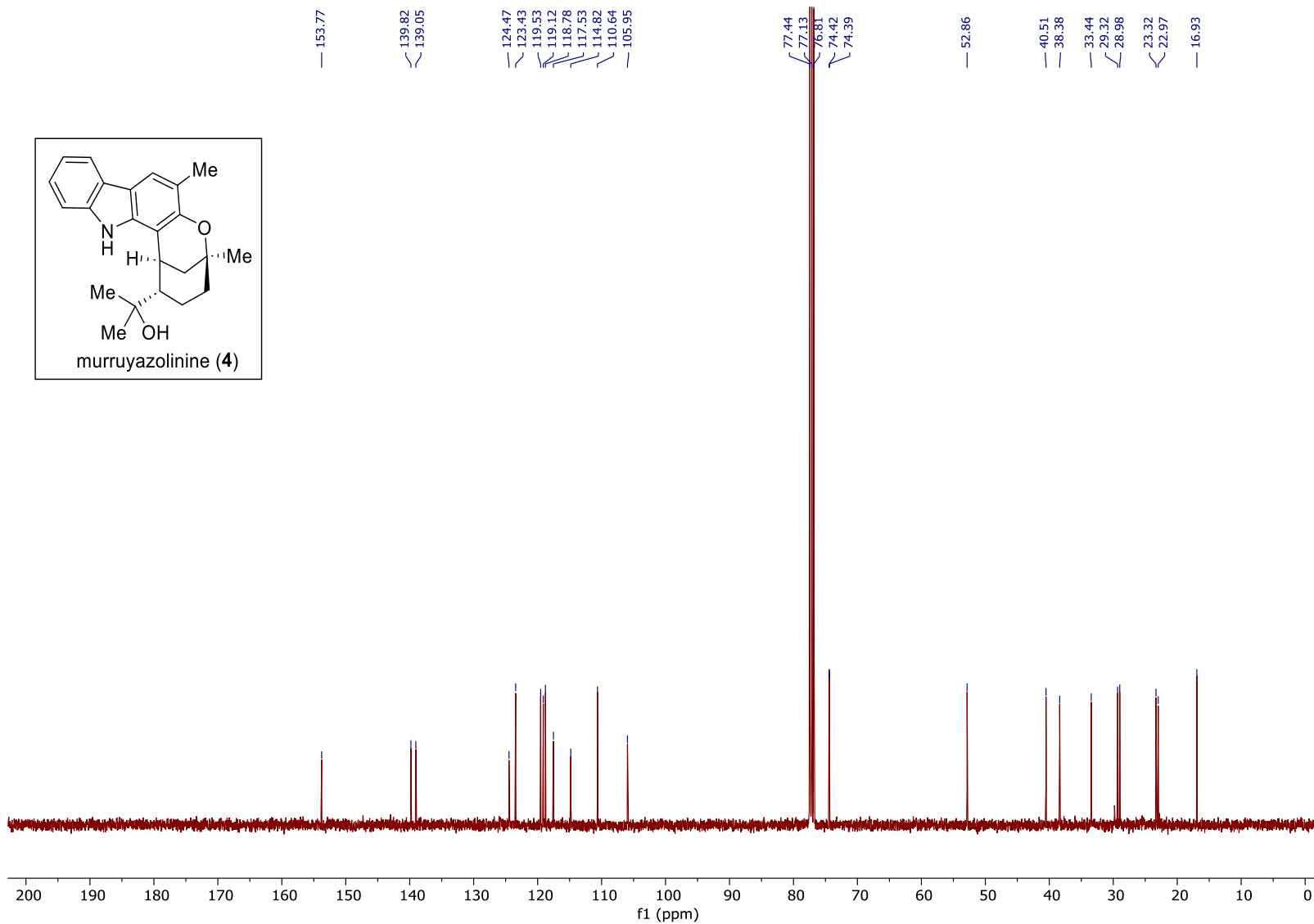
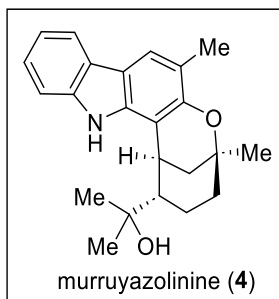
1: TOF MS ES+
4.53e6



HRMS data of 21



¹H NMR (400 MHz, CDCl₃) of 4



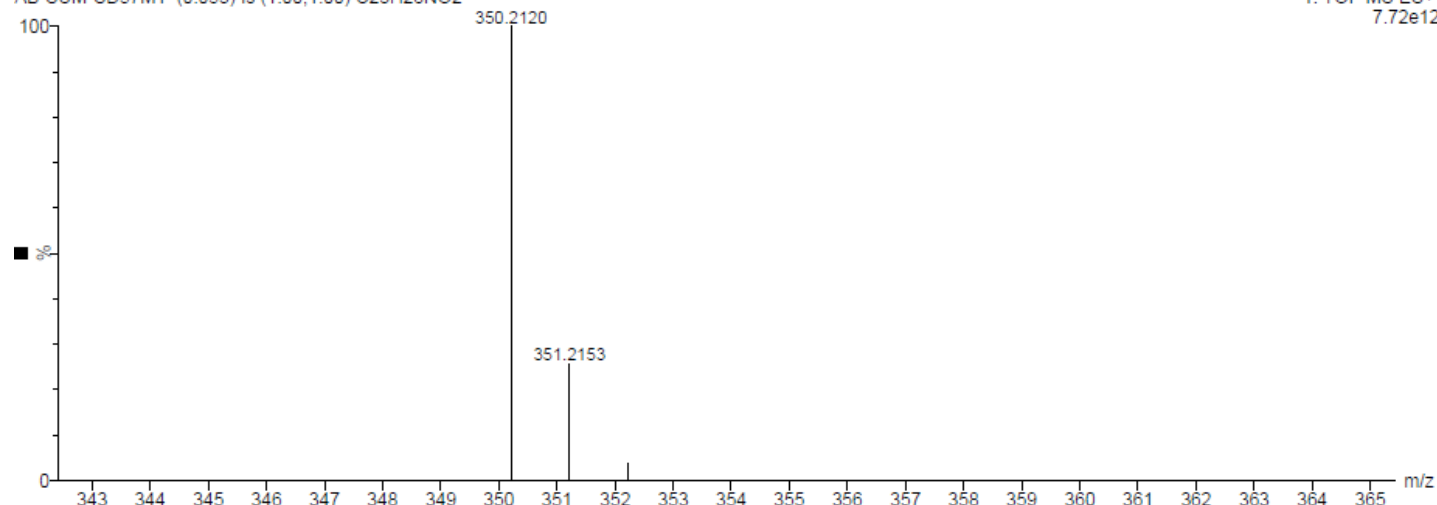
^{13}C NMR (100 MHz, CDCl_3) of 4

AB10-Apr-2024 14:57:34

IISER - KOLKATA

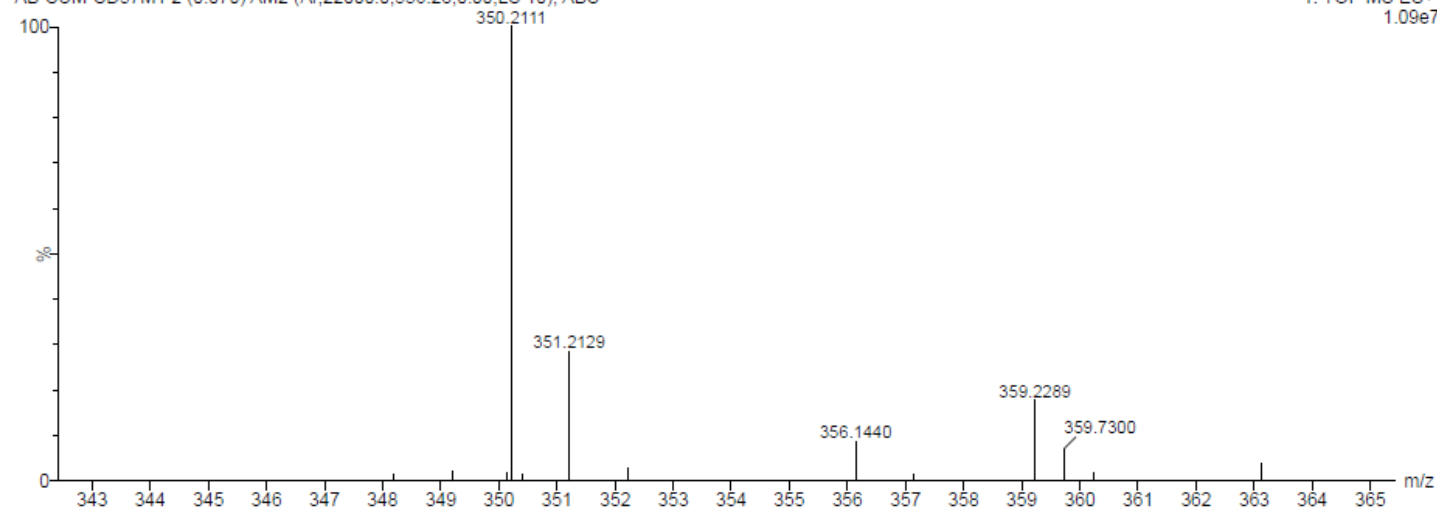
1: TOF MS ES+
7.72e12

AB-SUM-SD57M1 (0.053) Is (1.00,1.00) C₂₃H₂₈NO₂

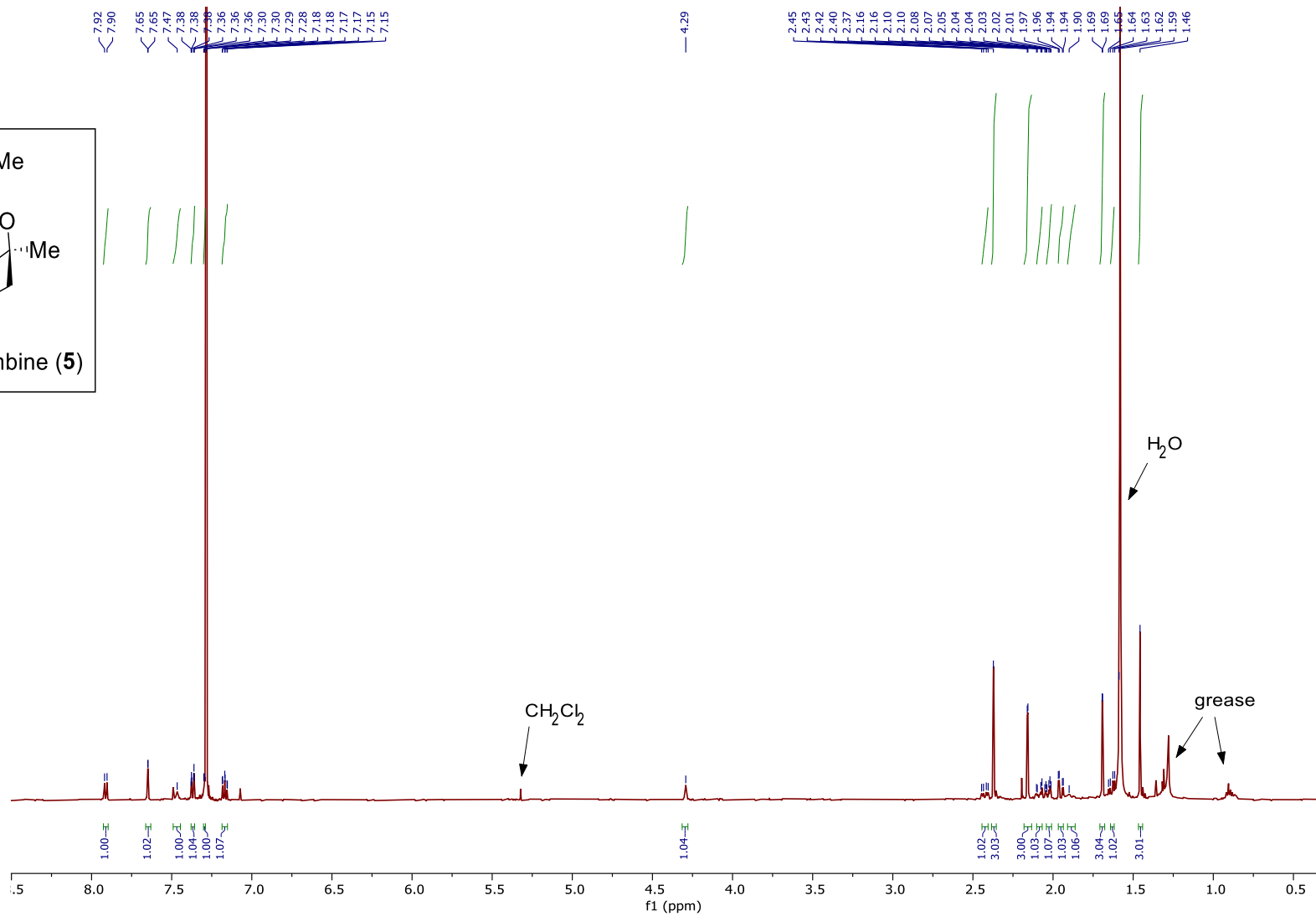
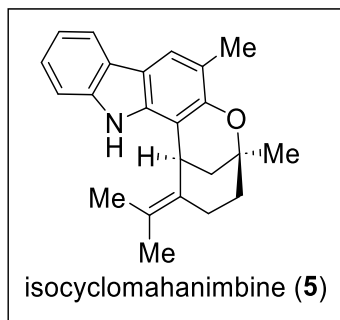


AB-SUM-SD57M1 2 (0.070) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

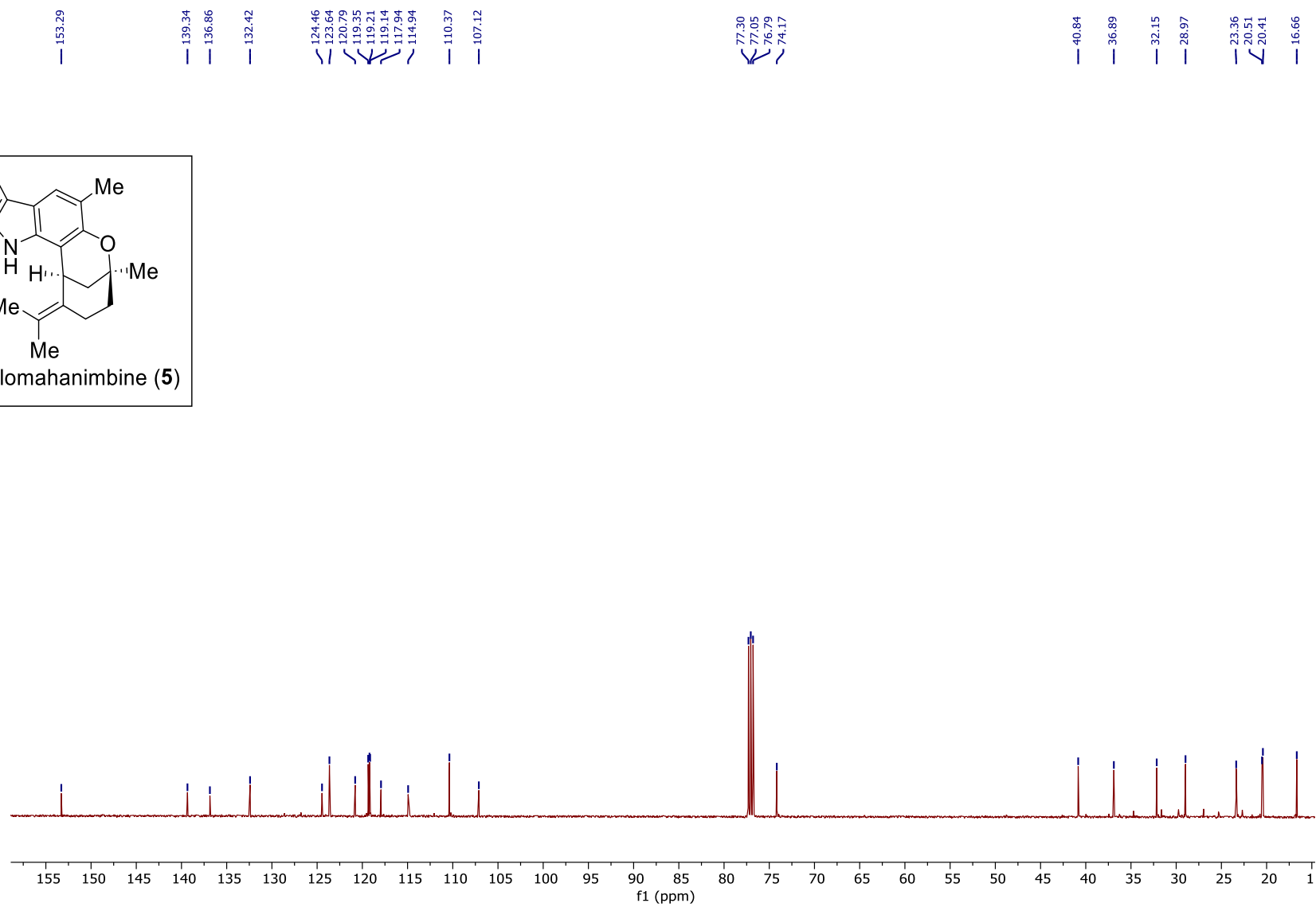
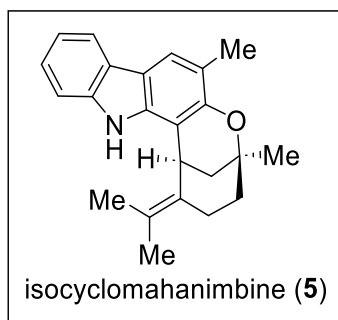
1: TOF MS ES+
1.09e7



HRMS data of 4



¹H NMR (500 MHz, CDCl₃) of 5

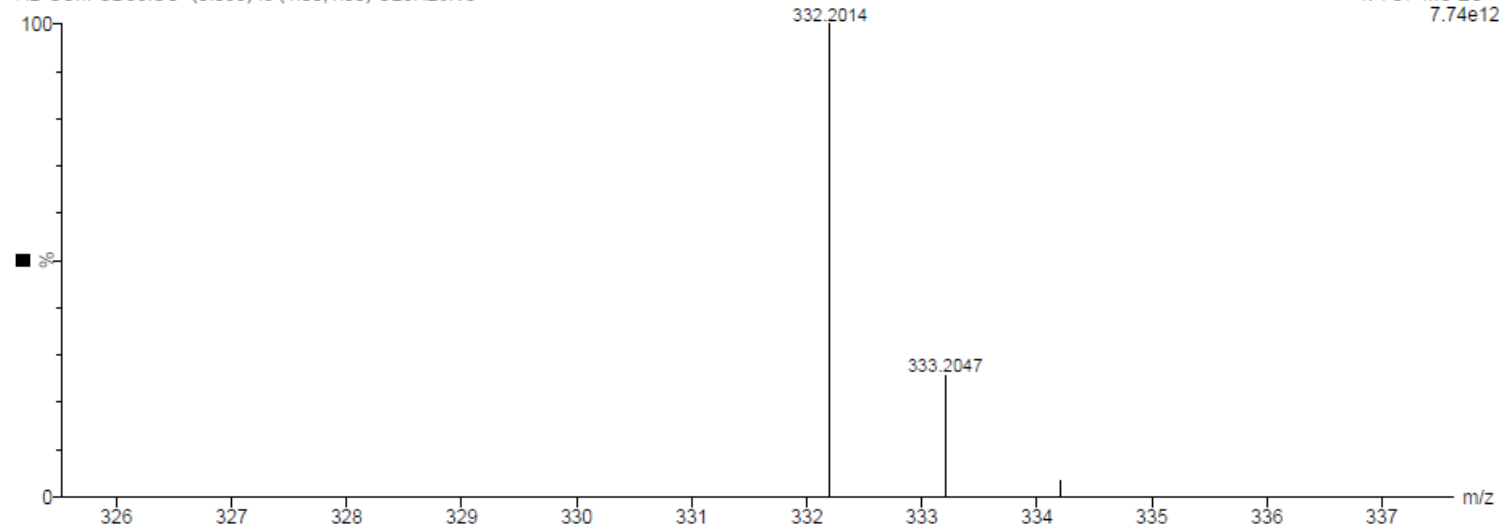


^{13}C NMR (100 MHz, CDCl_3) of **5**

AB25-Apr-2024 13:17:27
AB-SUM-SD58ISO (0.053) Is (1.00,1.00) C23H26NO

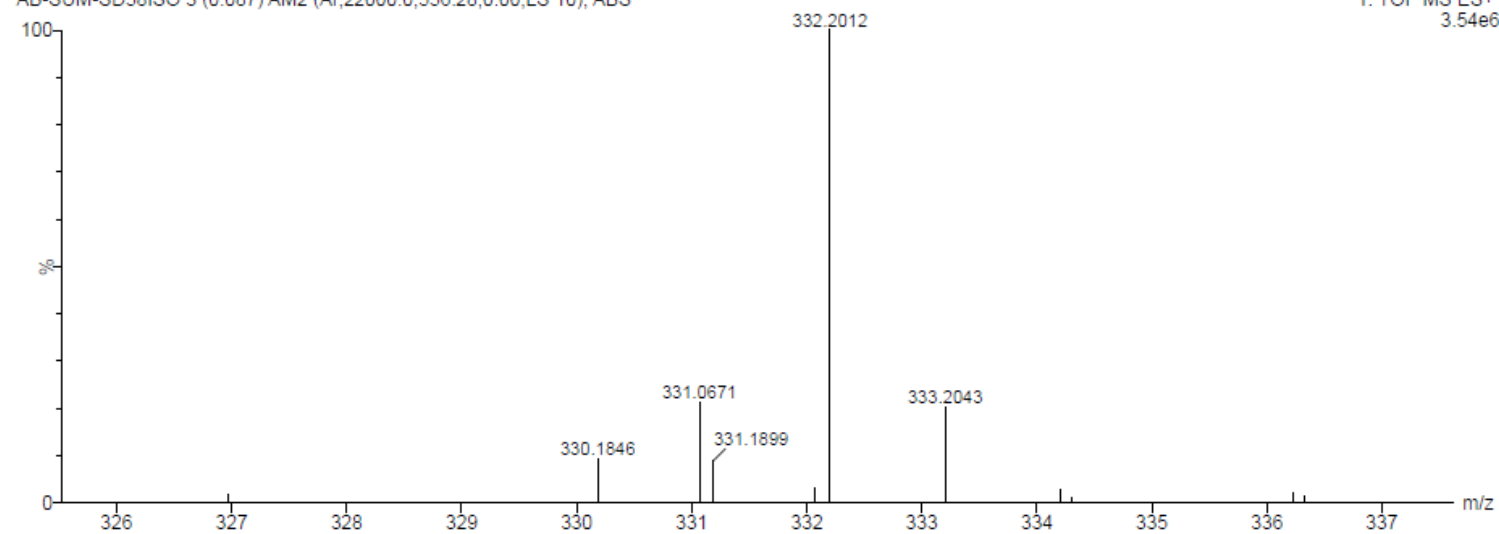
IISER - KOLKATA

1: TOF MS ES+
7.74e12



AB-SUM-SD58ISO 3 (0.087) AM2 (Ar,22000,0,556.28,0,00,LS 10); ABS

1: TOF MS ES+
3.54e6



HRMS data of 5