

Supplemental material for:

**Highly Regioselective Oxidative Csp²-H Amination for
Indolosesquiterpene Alkaloids: Total Synthesis of (+)-
Dioridamycin**

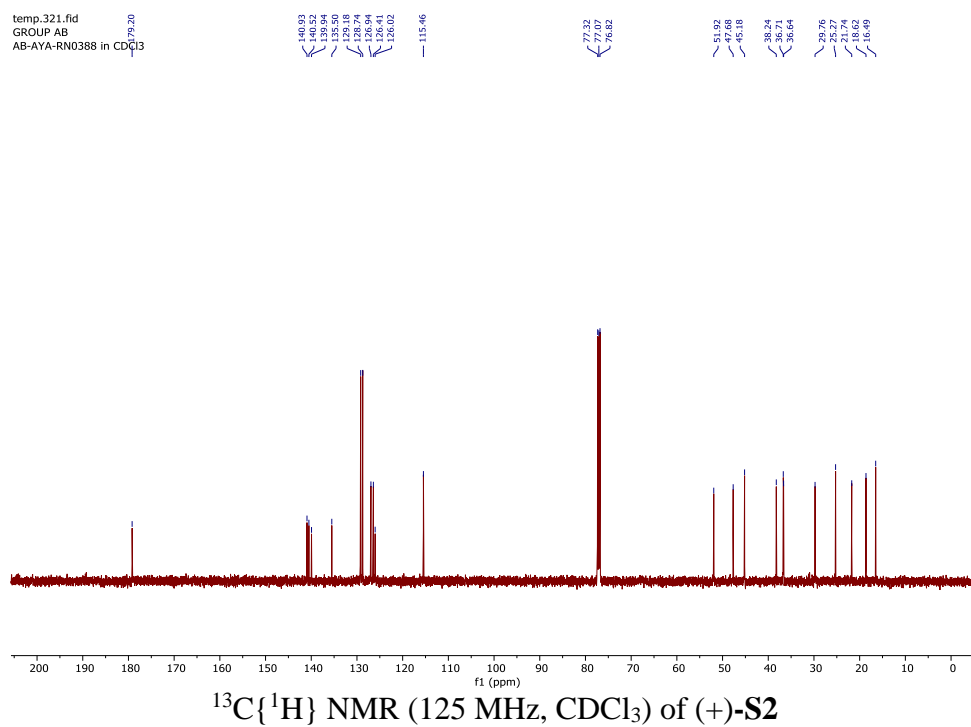
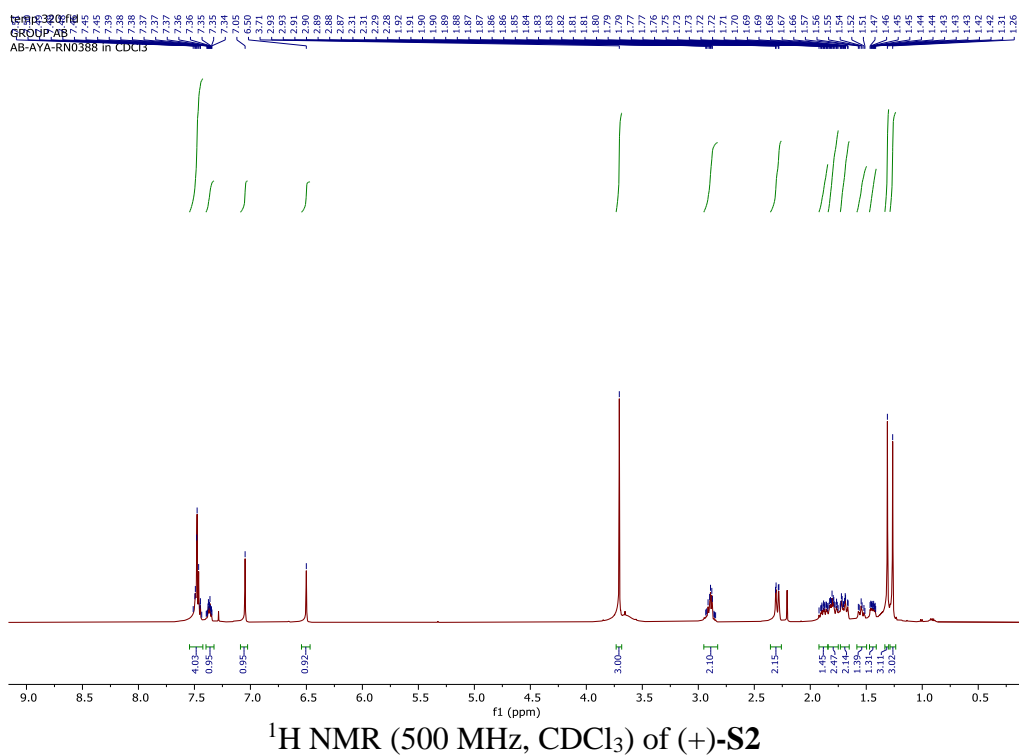
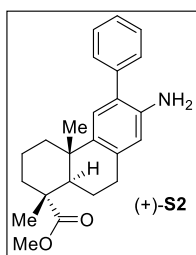
Rhituparna Nandi,^{§a} Sovan Niyogi,^{§b} Sourav Kundu,^b Ayan Mondal,^b Nanda Kishore Roy,^b
and Alakesh Bisai^{*a,b}

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Kolkata, Mohanpur, Nadia, WB - 741 246, India.

e-Mail: alakesh@iiserkol.ac.in, alakeshb@gmail.com

Spectral Traces

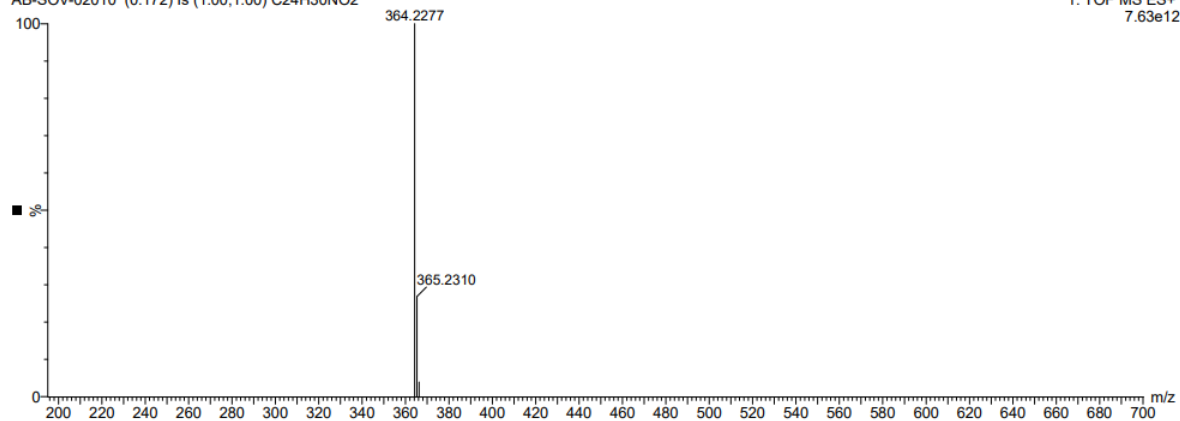


AB18-Apr-2024 13:33:02

AB-SOV-02010 (0.172) Is (1.00,1.00) C₂₄H₃₀NO₂

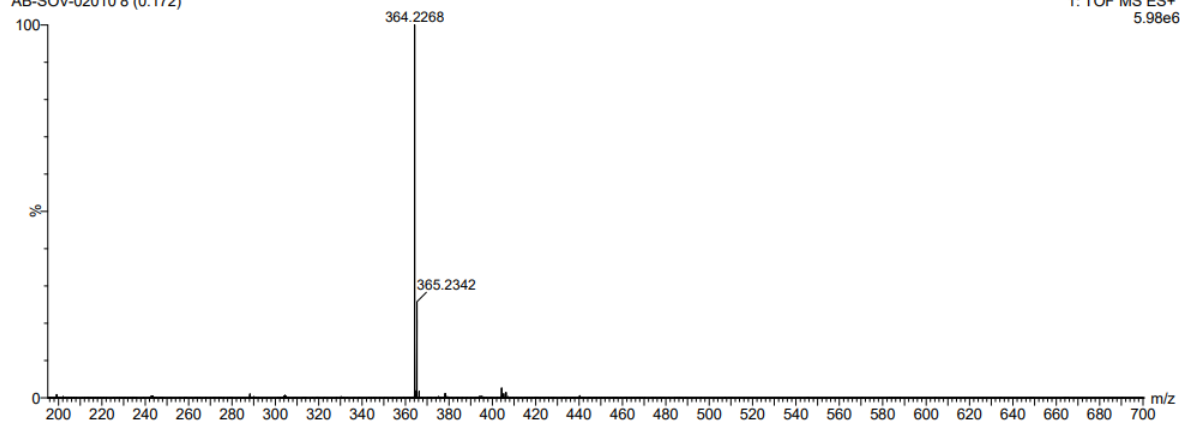
IISER - KOLKATA

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7.63e12

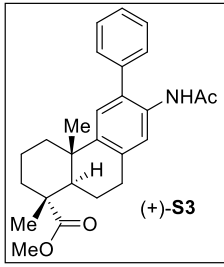


AB-SOV-02010 8 (0.172)

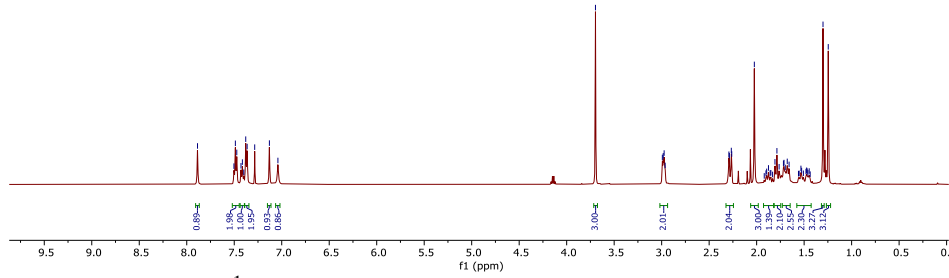
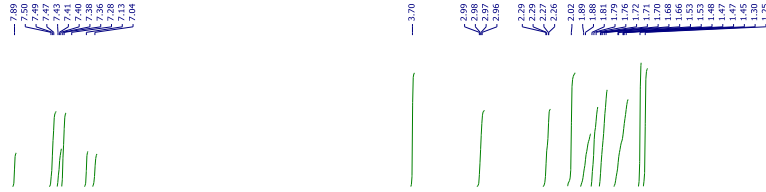
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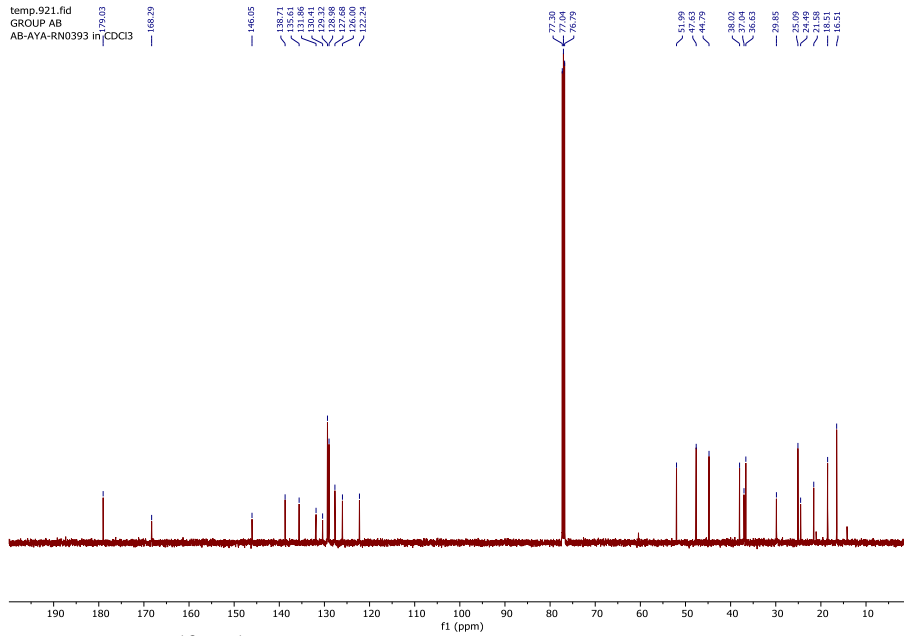
HRMS data of (+)-S2



temp.920.fid
GROUP AB
AB-AYA-RN0393 in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-S3

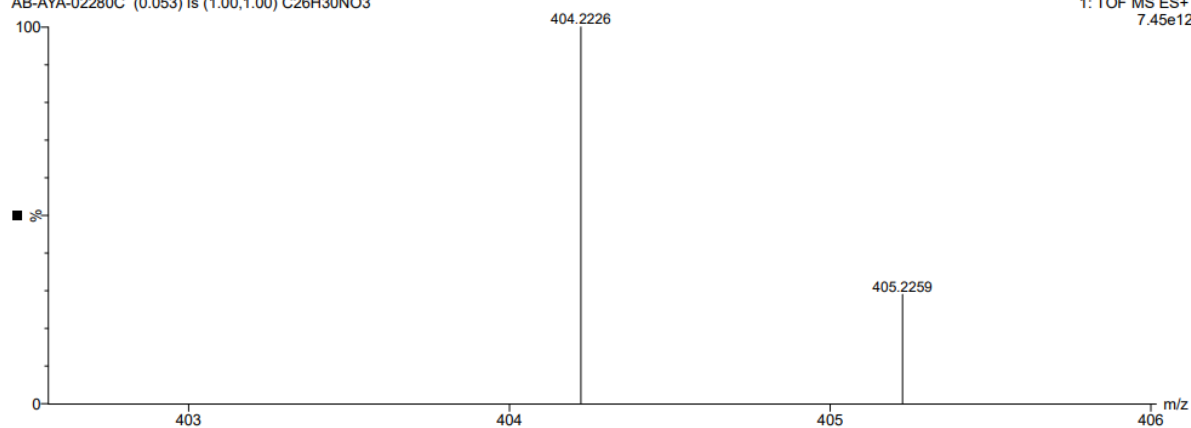


¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S3

AB26-Apr-2024 13:54:31
AB-AYA-02280C (0.053) Is (1.00,1.00) C₂₆H₃₀NO₃

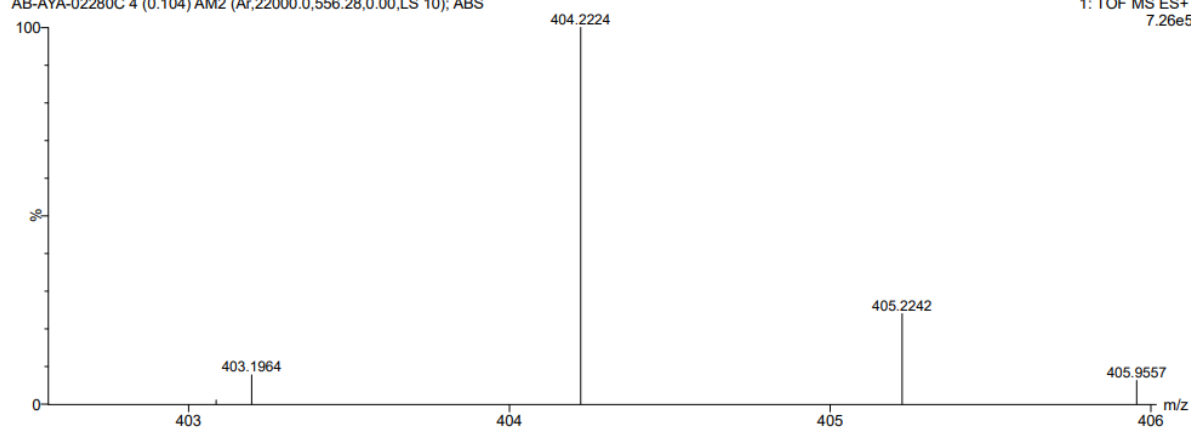
IISER - KOLKATA

1: TOF MS ES+
7.45e12

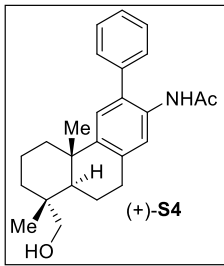


AB-AYA-02280C 4 (0.104) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

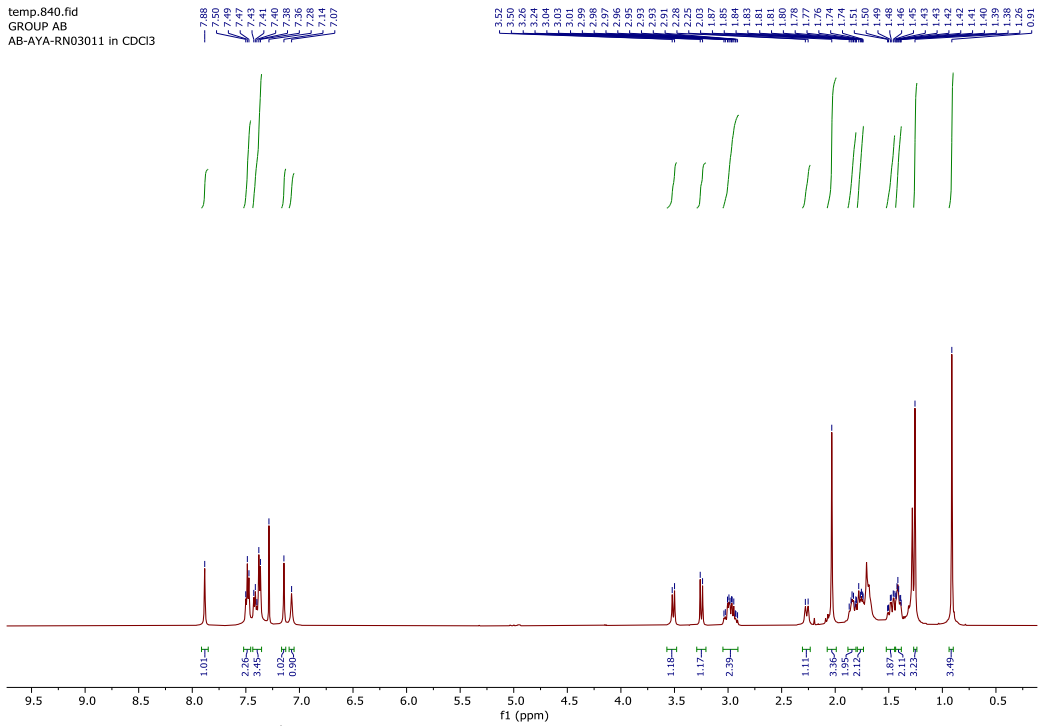
1: TOF MS ES+
7.26e5



HRMS data of (+)-S3

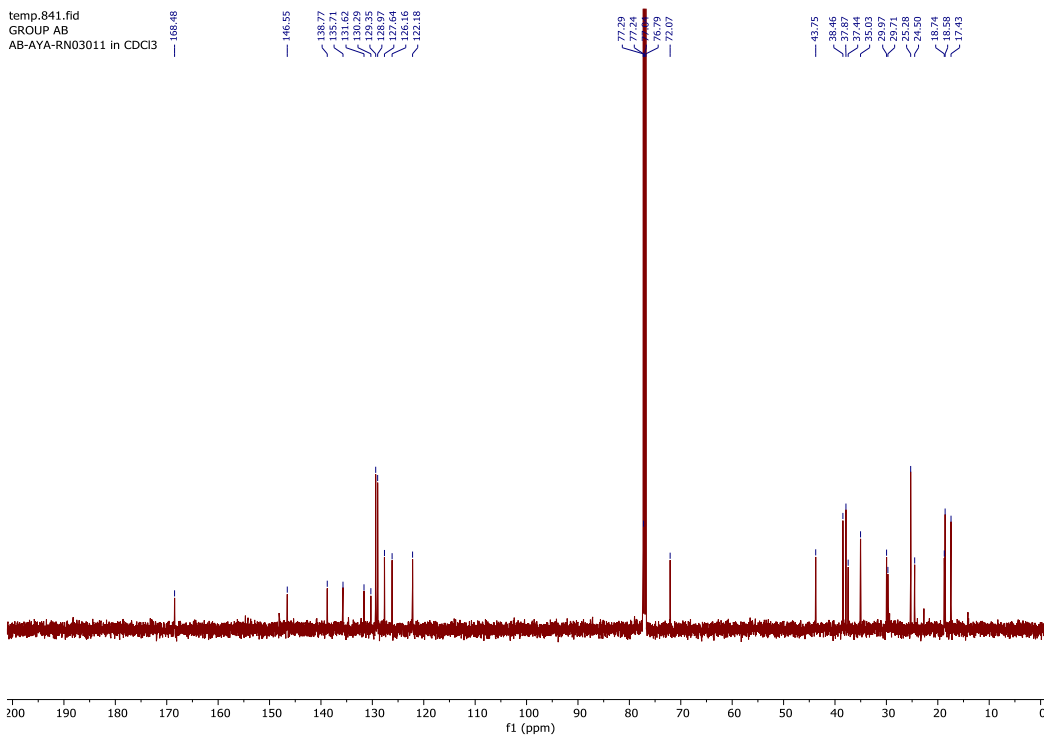


temp.840.fid
GROUP AB
AB-AYA-RN03011 in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-S4

temp.841.fid
GROUP AB
AB-AYA-RN03011 in CDCl₃



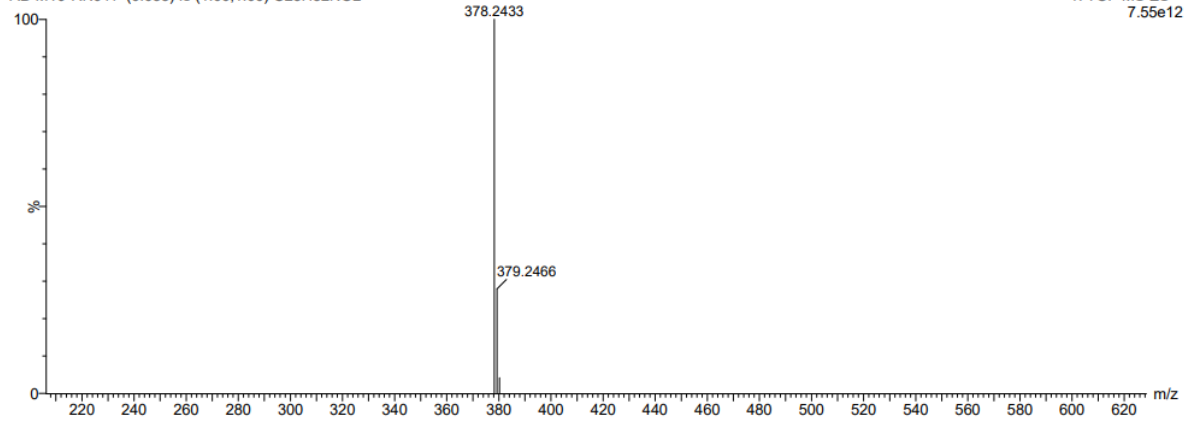
¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S4

AB02-Apr-2024 13:46:06

AB-MTJ-RN011 (0.053) Is (1.00,1.00) C25H32NO2

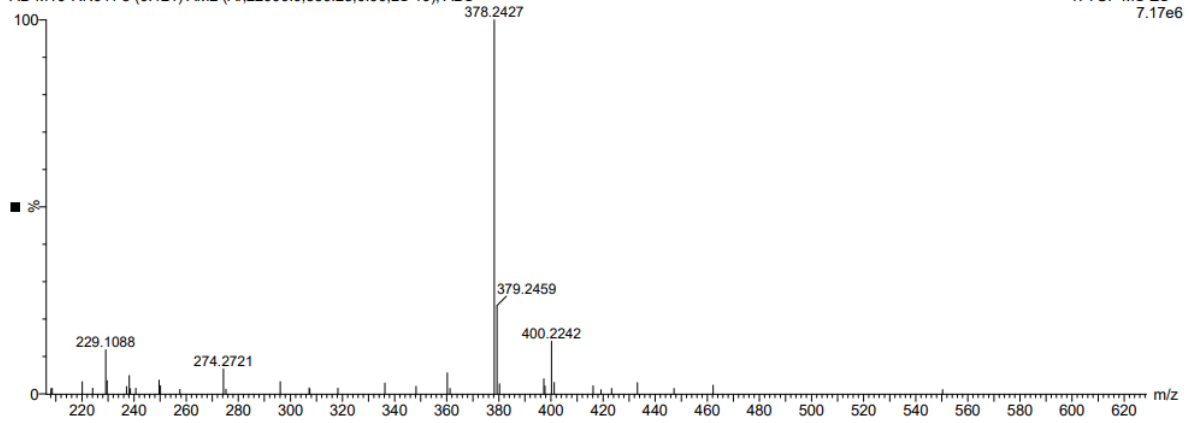
IISER - KOLKATA

1: TOF MS ES+
7.55e12

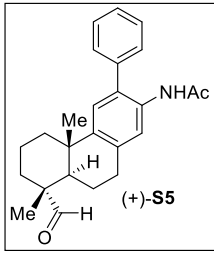


AB-MTJ-RN011 5 (0.121) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

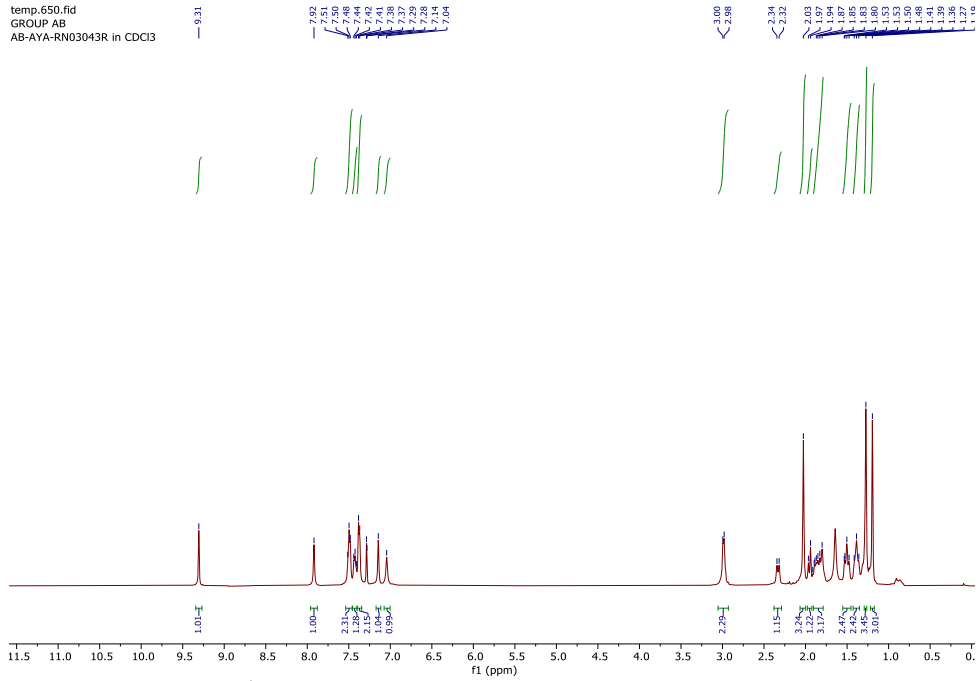
1: TOF MS ES+
7.17e6



HRMS data of (+)-S4

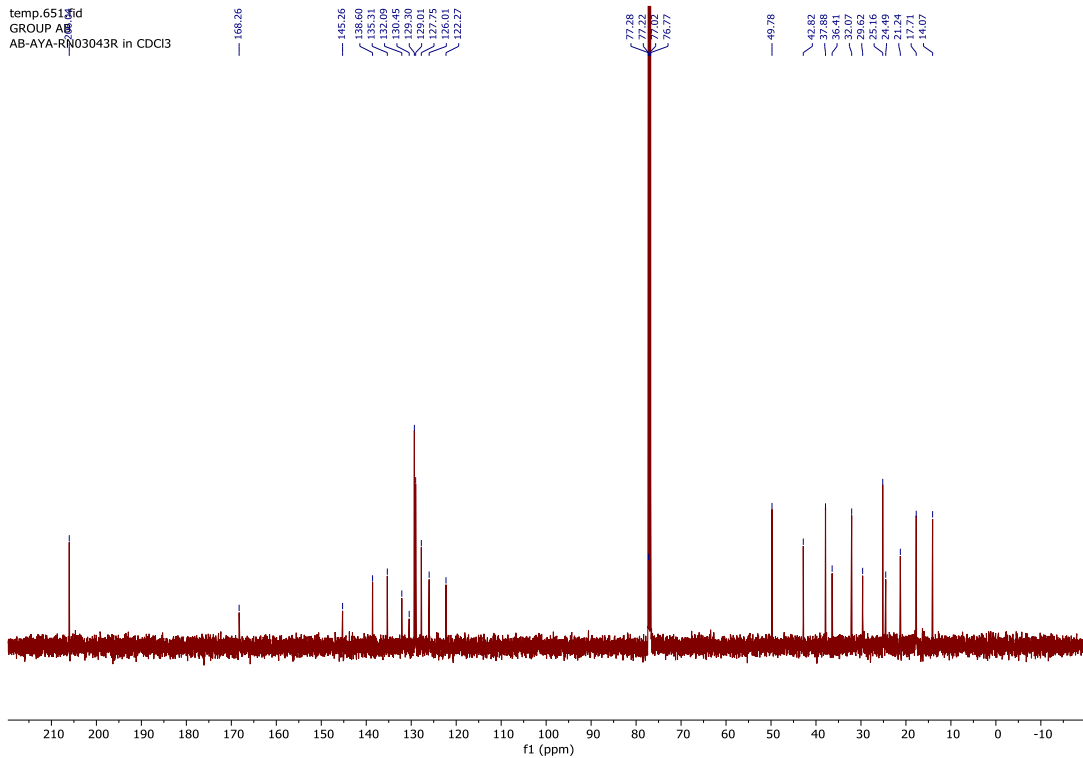


temp.650.fid
GROUP AB
AB-AYA-RN03043R in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-S5

temp.651.fid
GROUP AB
AB-AYA-RN03043R in CDCl₃



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S5

Display Report

Analysis Info

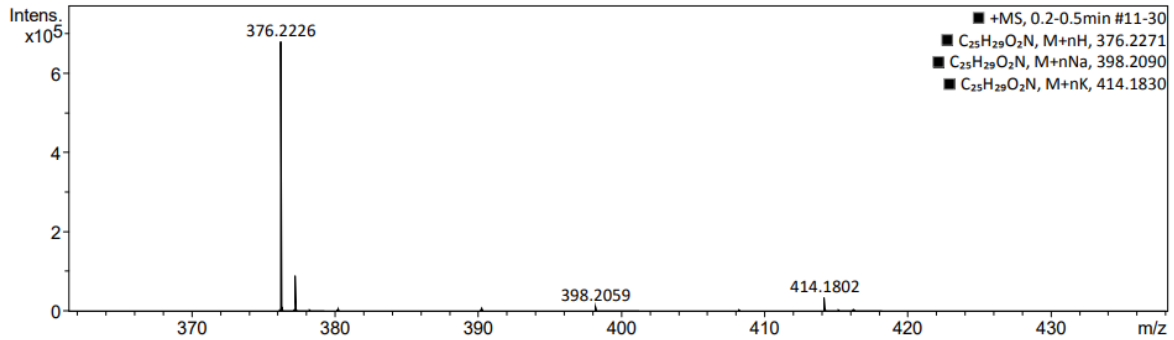
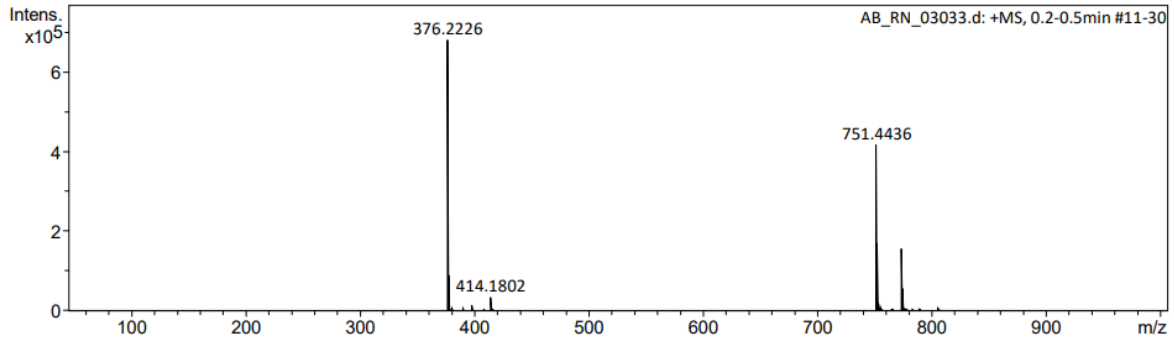
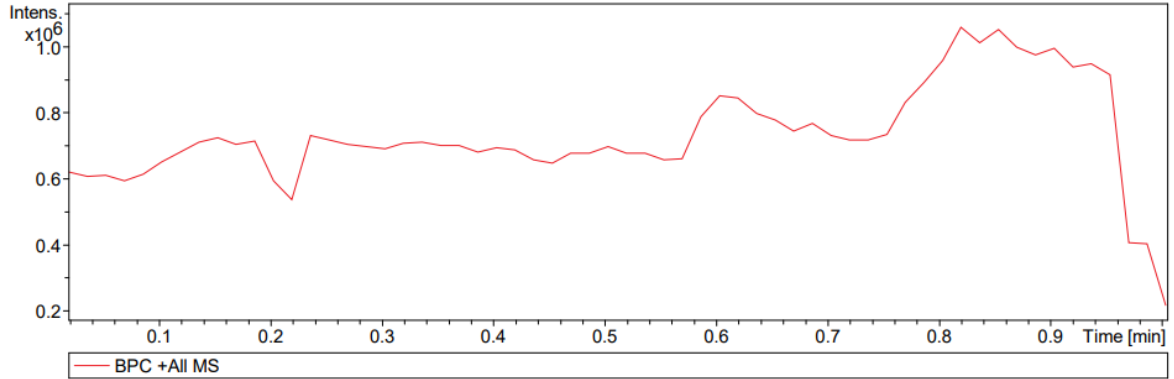
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Method Tune_pos_Standard.m
Sample Name AB_RN_03033
Comment

Acquisition Date 3/31/2022 12:57:46 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

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AB_RN_03033.d

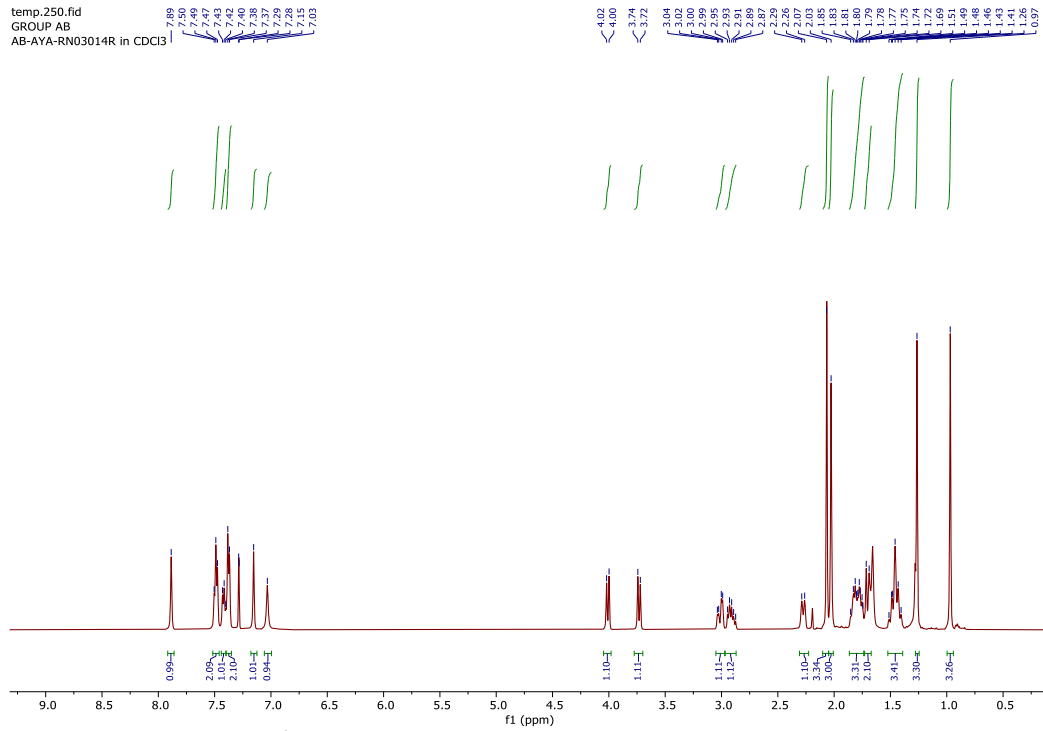
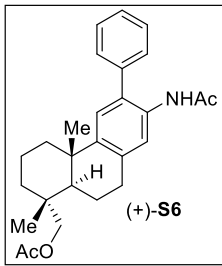
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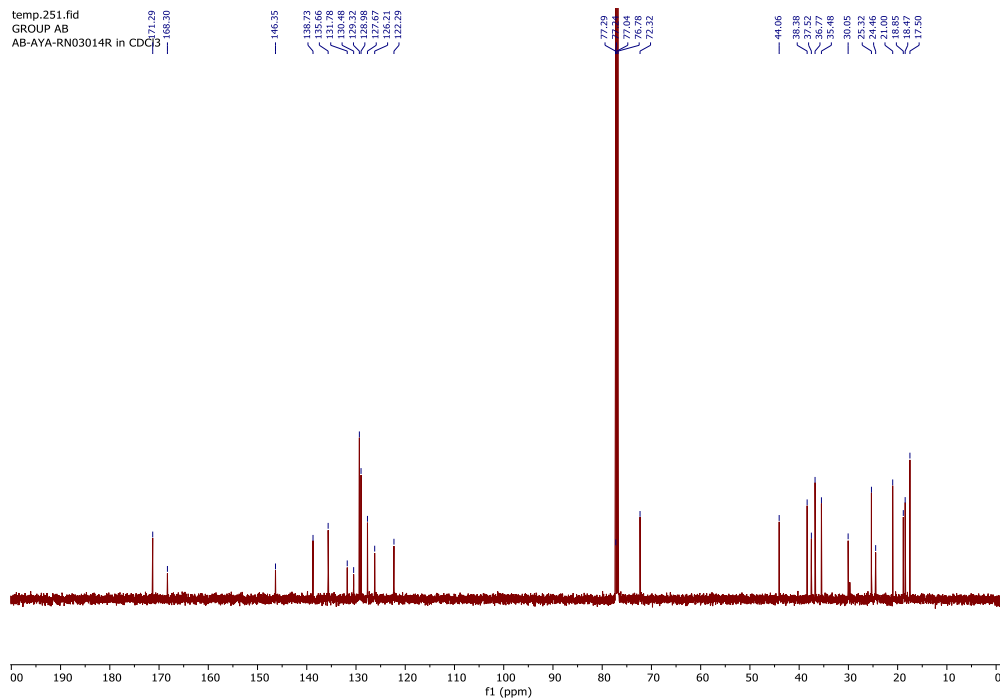
by: IISER Kolkata

Page 1 of 1

HRMS data of (+)-S5



¹H NMR (500 MHz, CDCl₃) of (+)-S6



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S6

Display Report

Analysis Info

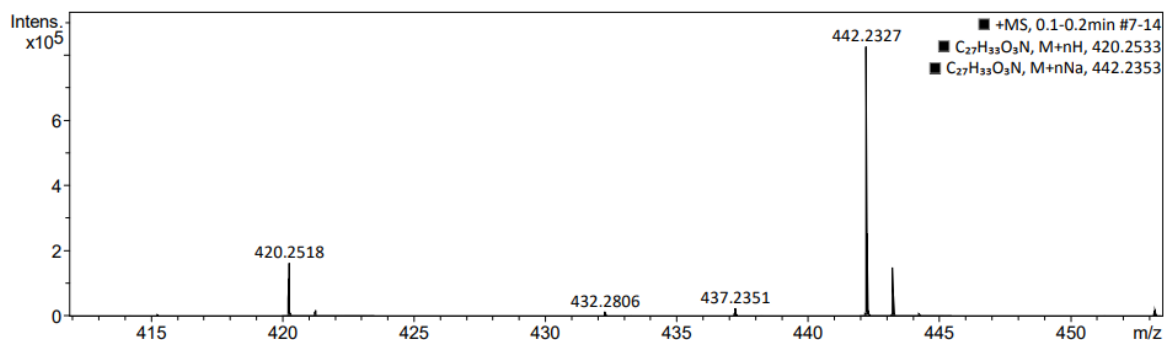
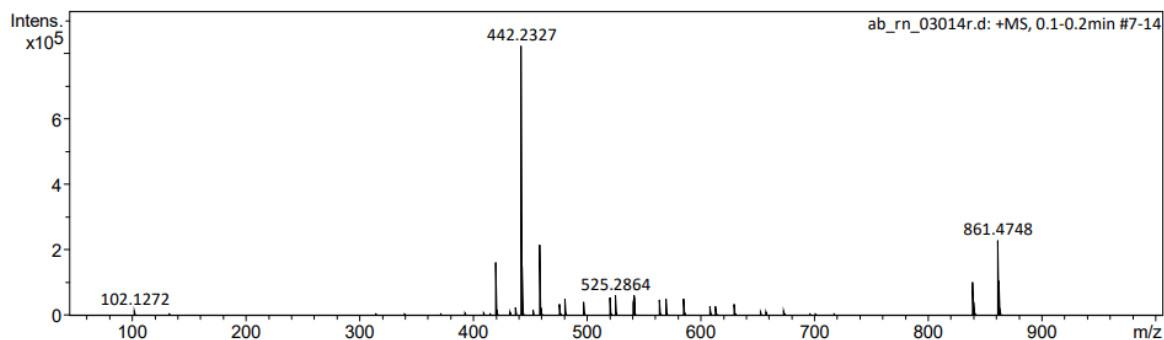
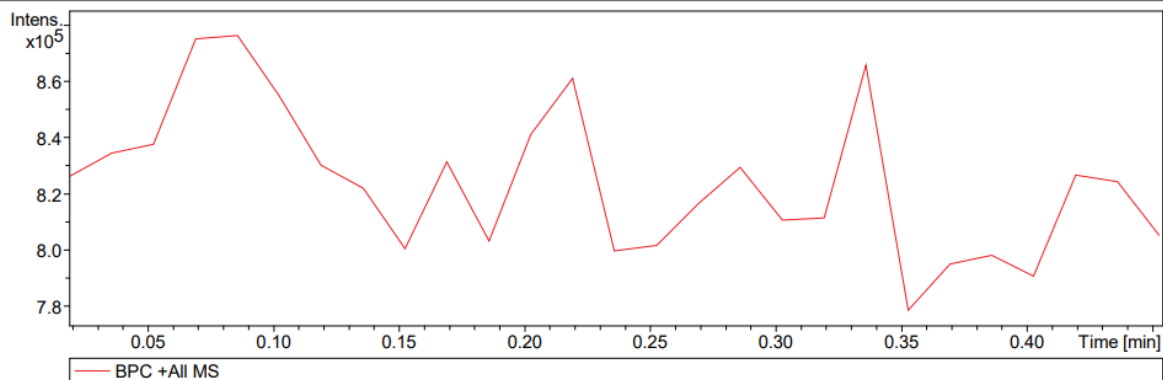
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Sample Name ab_rn_03014r
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Operator IISER Kolkata
Instrument maXis impact 8282001.00127

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ab_rn_03014r.d

Bruker Compass DataAnalysis 4.1

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by: IISER Kolkata

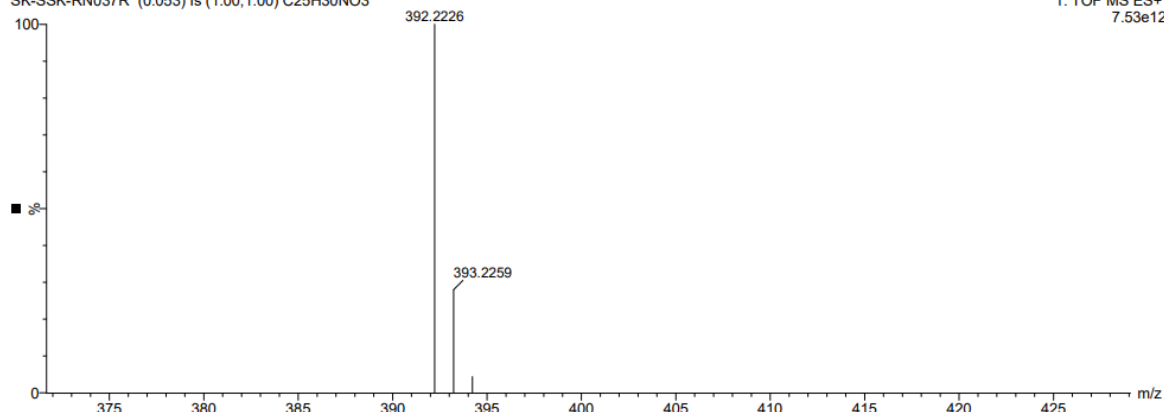
Page 1 of 1

HRMS data of (+)-S6

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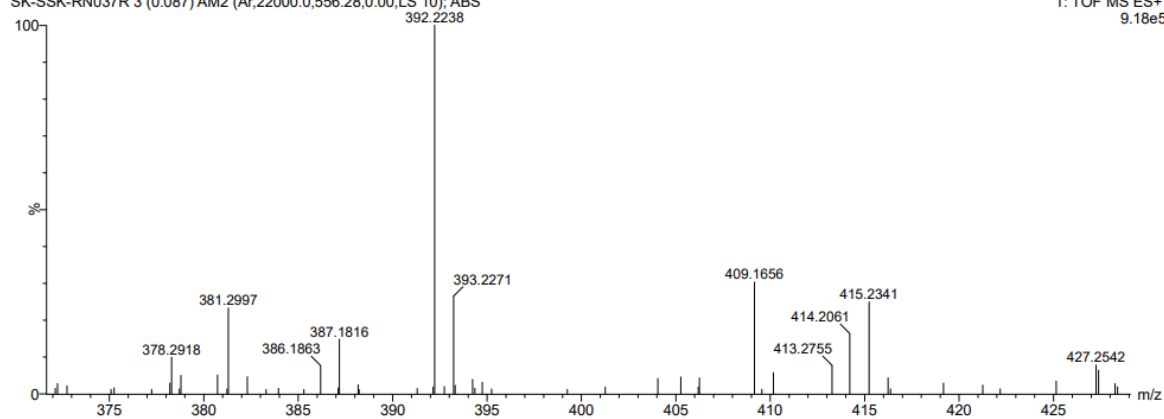
IISER - KOLKATA

1: TOF MS ES+
7.53e12

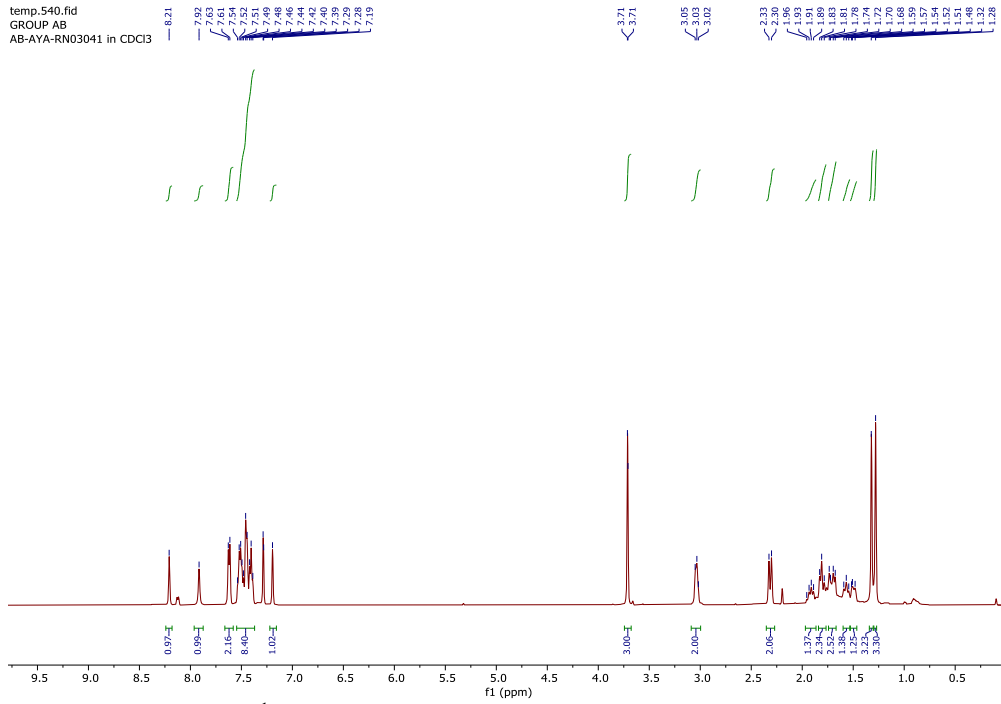
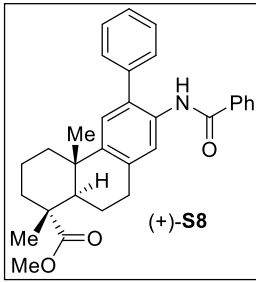


SK-SSK-RN037R 3 (0.087) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

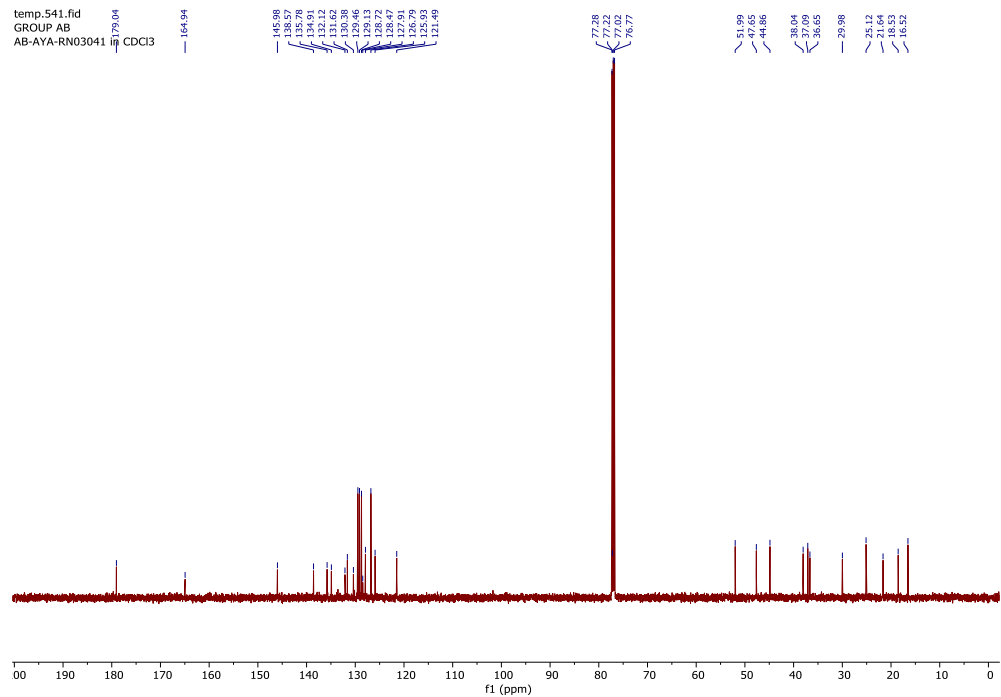
1: TOF MS ES+
9.18e5



HRMS data of (+)-S7



¹H NMR (500 MHz, CDCl₃) of (+)-S8

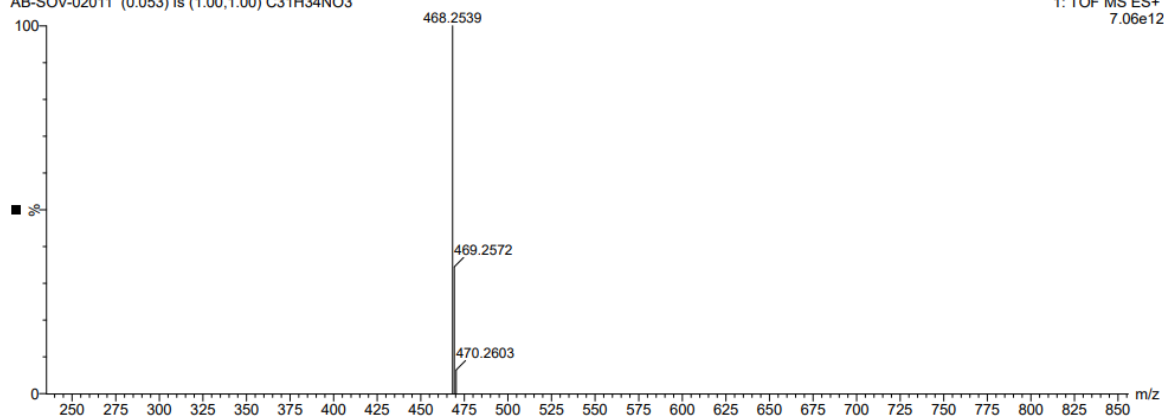


¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S8

AB18-Apr-2024 13:36:36
AB-SOV-02011 (0.053) Is (1.00,1.00) C31H34NO3

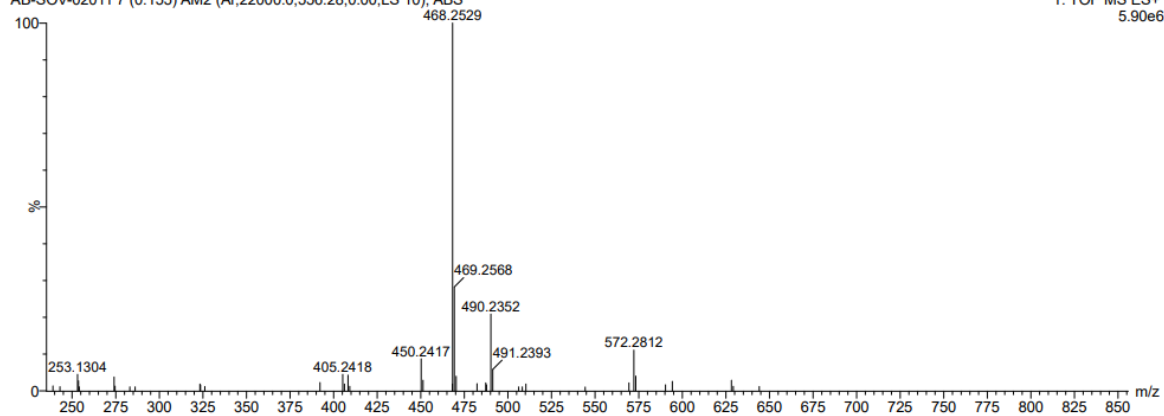
IISER - KOLKATA

1: TOF MS ES+
7.06e12

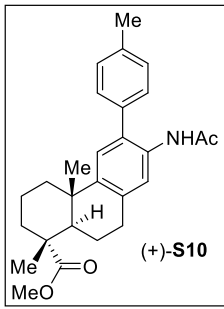


AB-SOV-02011 7 (0.155) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

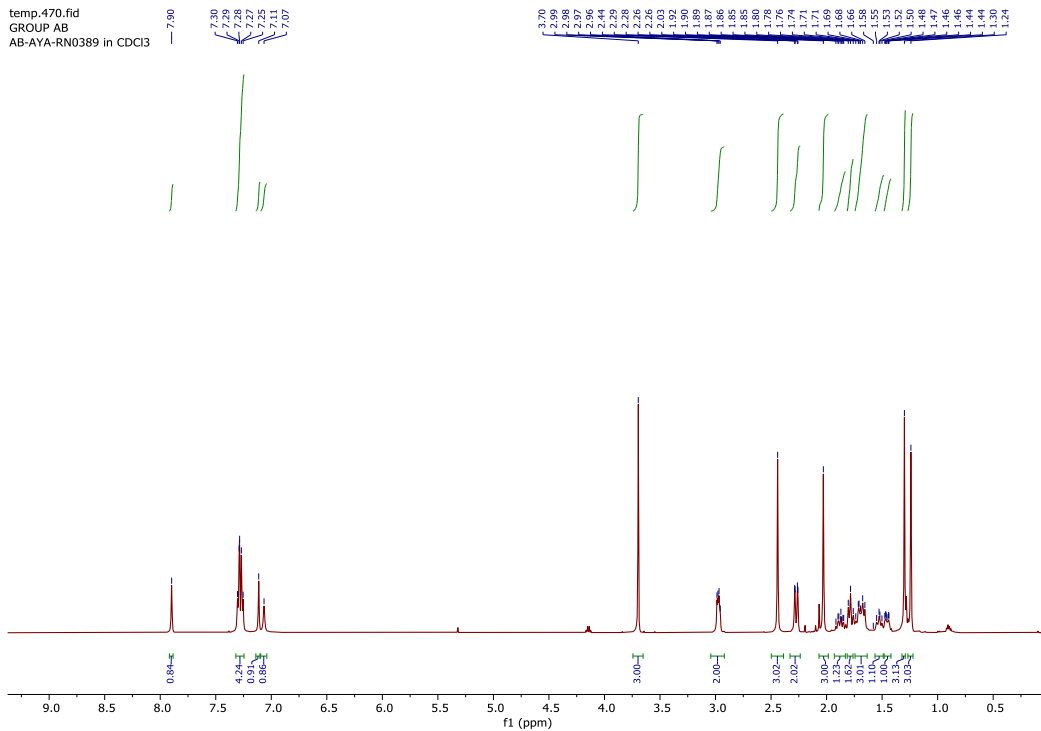
1: TOF MS ES+
5.90e6



HRMS data of (+)-**S8**

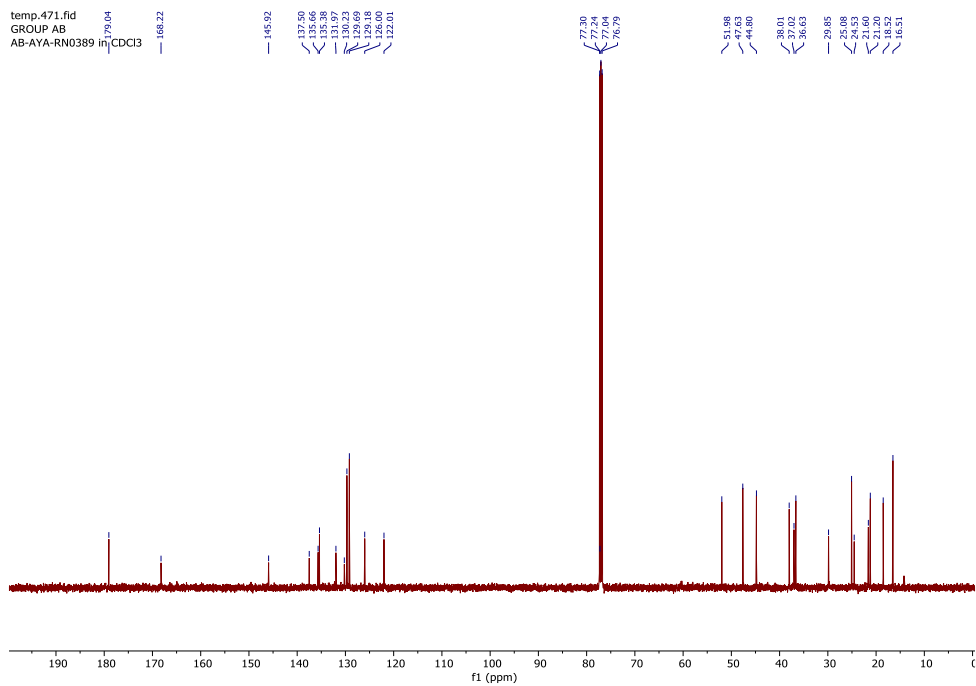


temp.470.fid
GROUP AB
AB-AYA-RN0389 in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-S10

temp.471.fid
GROUP AB
AB-AYA-RN0389 in CDCl₃



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S10

Display Report

Analysis Info

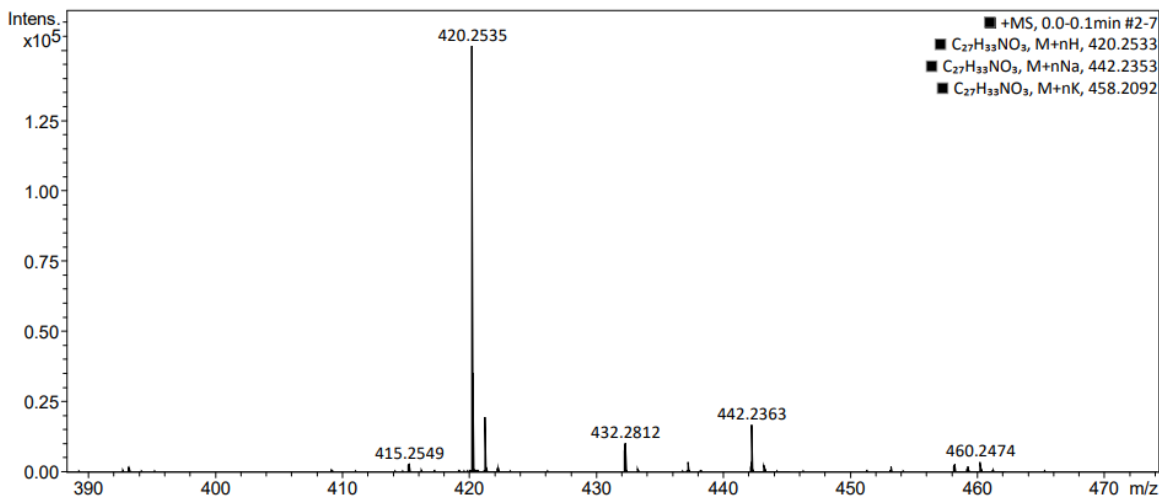
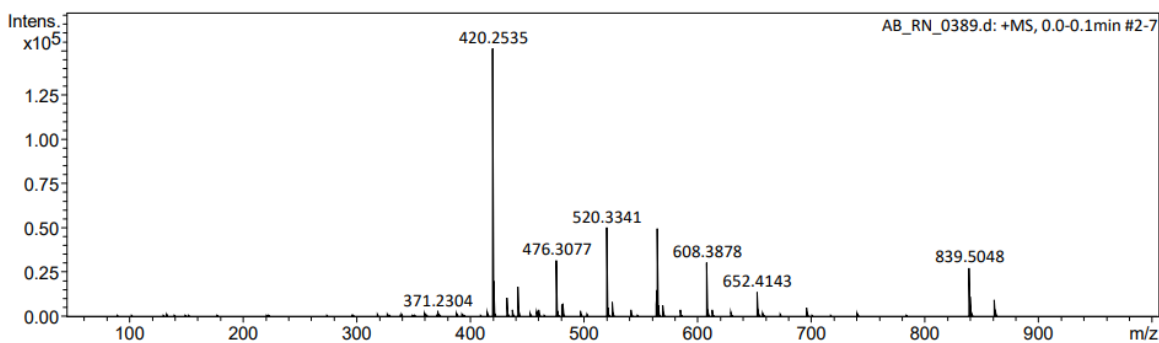
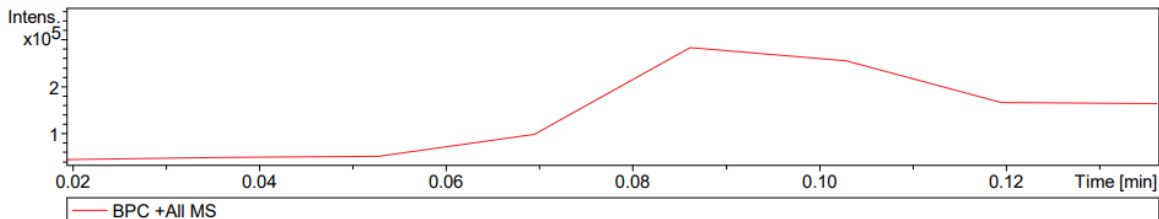
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Method Tune_pos_Standard.m
Sample Name AB_RN_0389
Comment signal dropping issue

Acquisition Date 3/16/2022 6:39:06 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

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AB_RN_0389.d

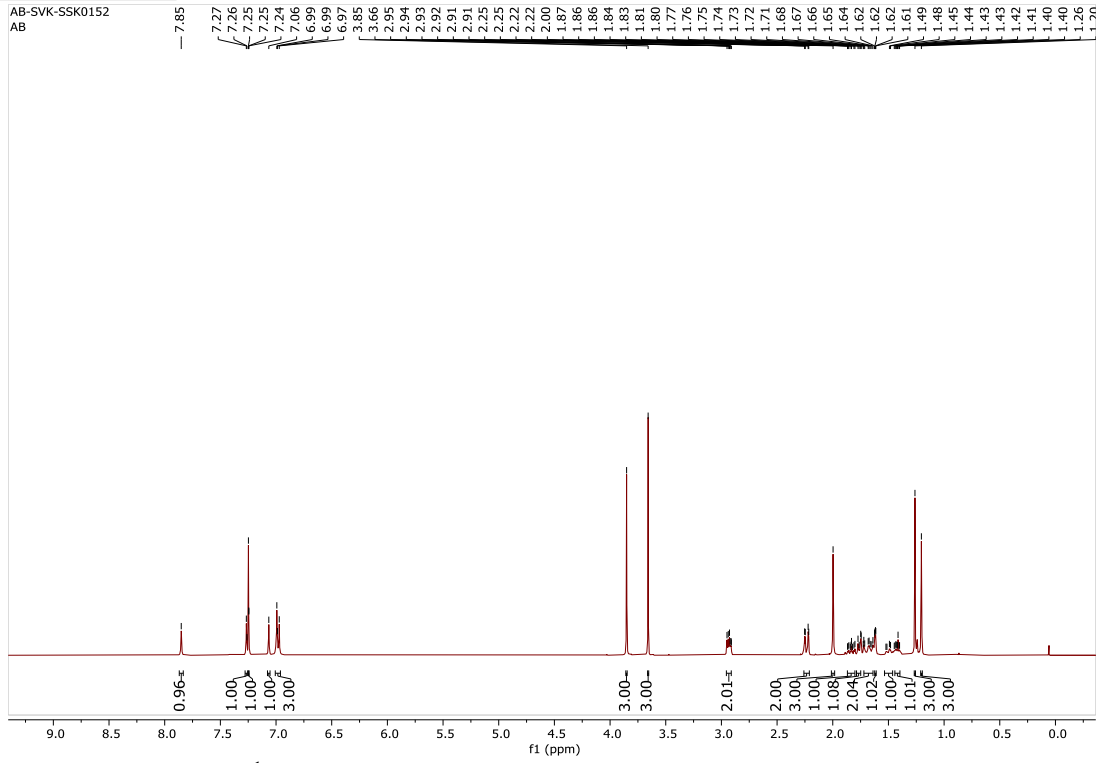
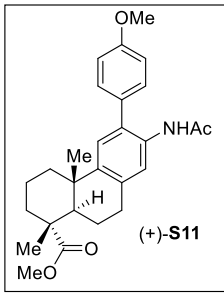
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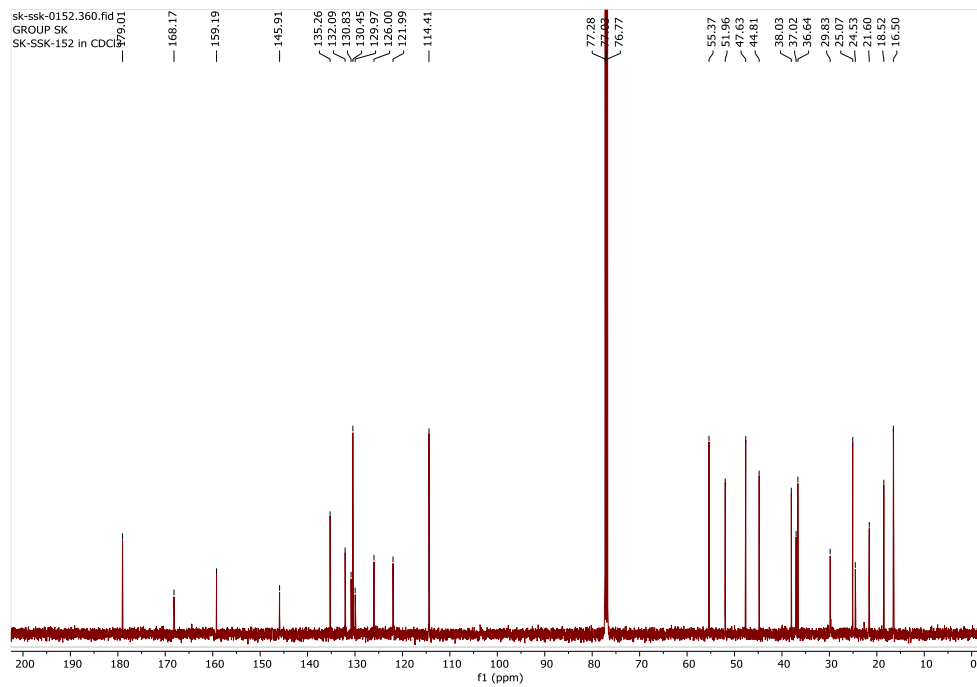
by: IISER Kolkata

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HRMS data of (+)-S10



^1H NMR (400 MHz, CDCl_3) of compound (+)-S11



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of compound (+)-S11

Display Report

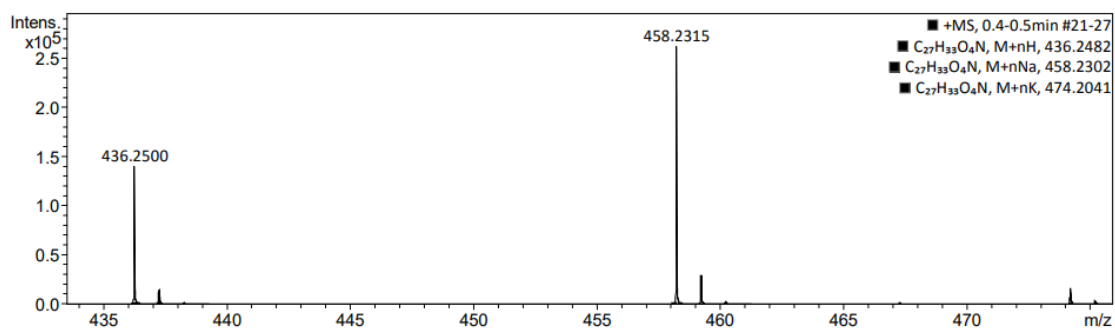
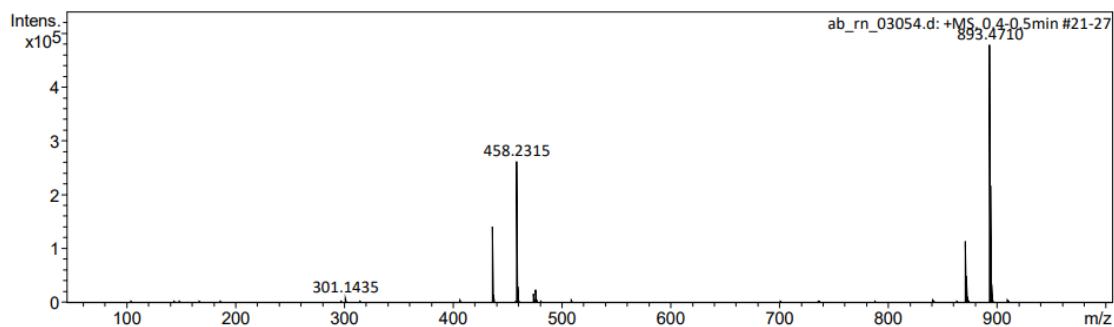
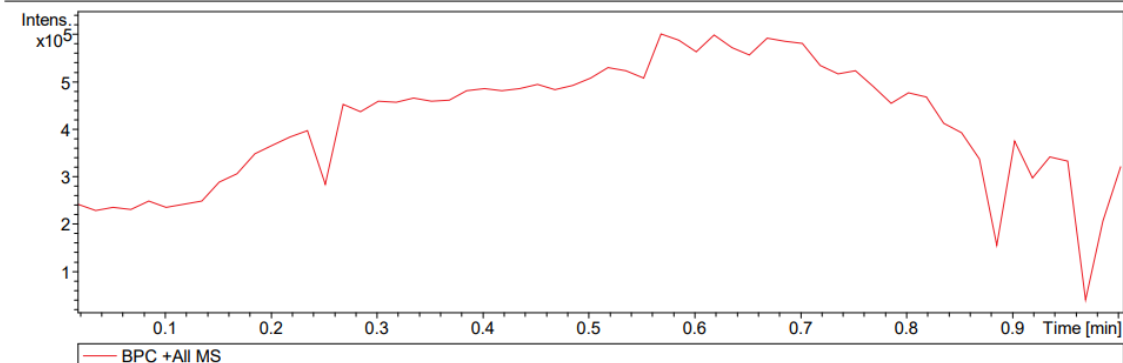
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Sample Name ab_m_03054
Comment

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Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

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ab_m_03054.d

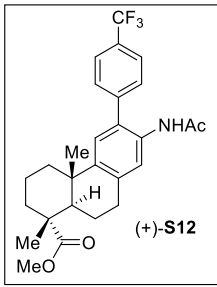
Bruker Compass DataAnalysis 4.1

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by: IISER Kolkata

Page 1 of 1

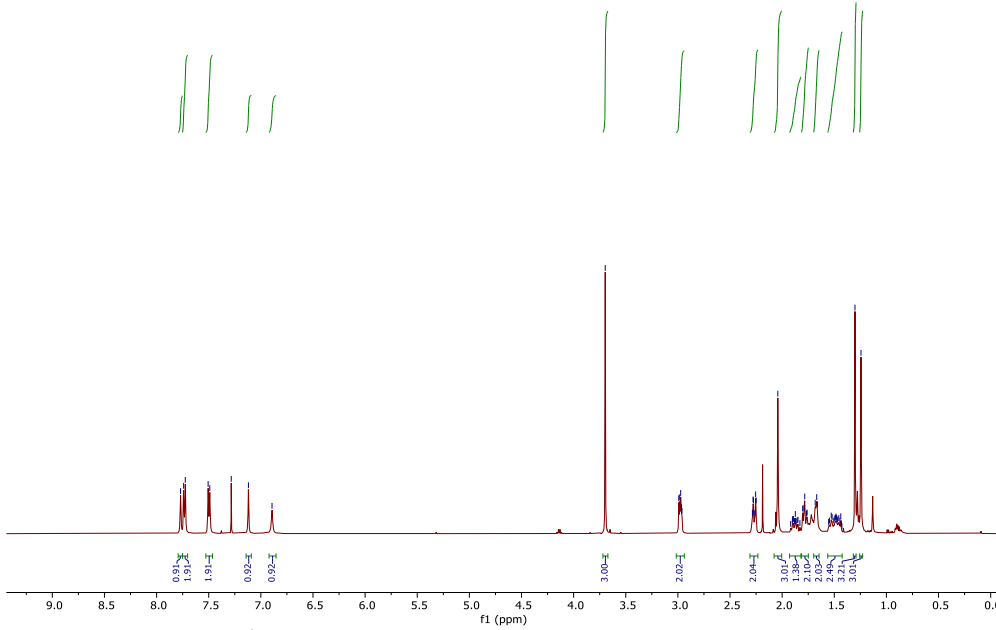
HRMS data of (+)-S11



temp.120.fid
GROUP SAB
AB-AYA-RN03032 in CDCl₃

7.74
7.72
7.51
7.49
7.12
6.89

3.93
3.79
2.98
2.97
2.96
2.29
2.28
2.27
2.26
2.25
2.24
2.04
1.92
1.90
1.89
1.88
1.87
1.86
1.85
1.84
1.83
1.80
1.79
1.78
1.77
1.76
1.69
1.67
1.66
1.55
1.54
1.53
1.52
1.51
1.50
1.49
1.48
1.47
1.46
1.45
1.44
1.43
1.42
1.24



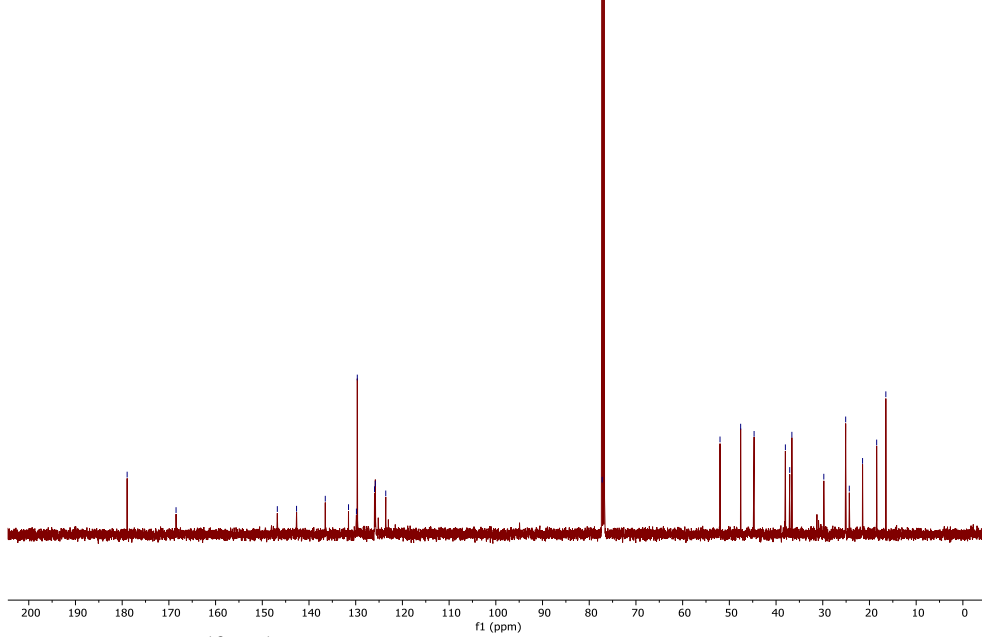
¹H NMR (500 MHz, CDCl₃) of (+)-S12

temp.121.fid
GROUP SAB
AB-AYA-RN03032 in CDCl₃

168.47
146.78
142.67
136.51
129.84
129.66
128.80
125.57

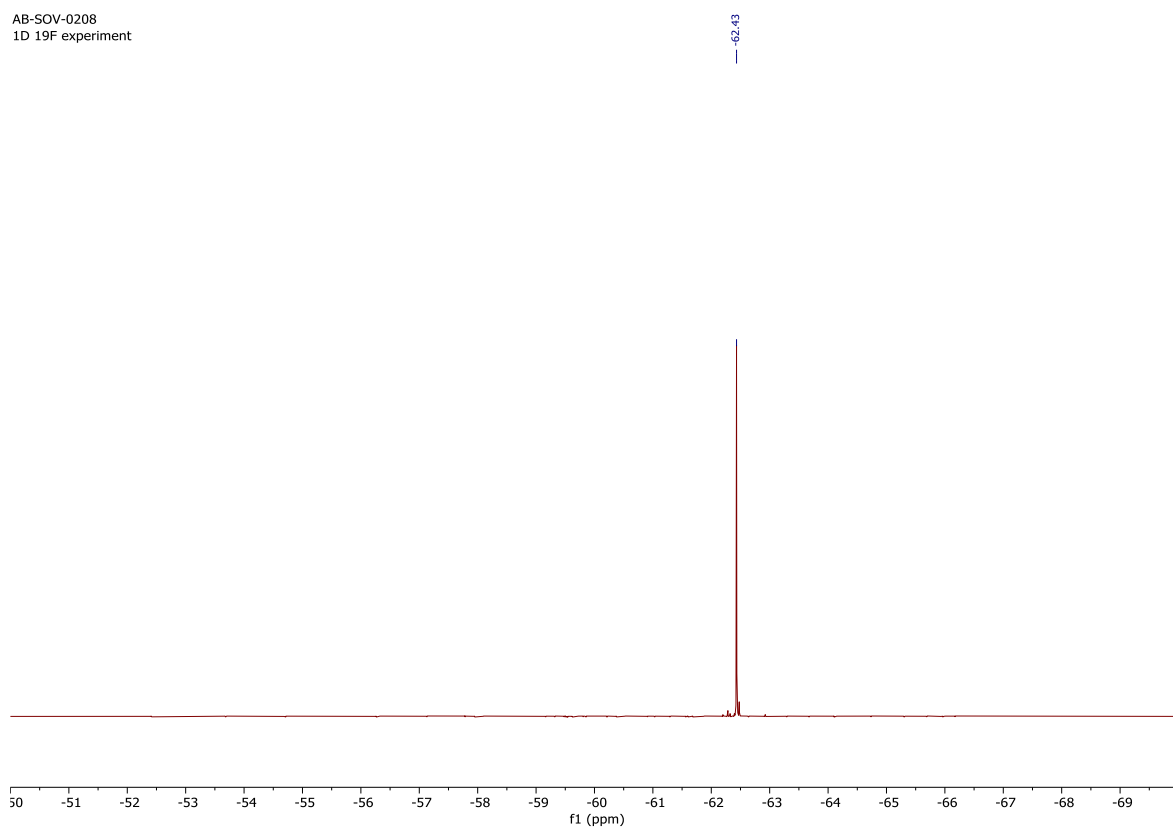
77.28
77.23
76.77

52.00
49.38
44.70
38.00
37.08
36.61
29.78
25.09
21.48
18.46
16.49



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S12

AB-SOV-0208
1D 19F experiment

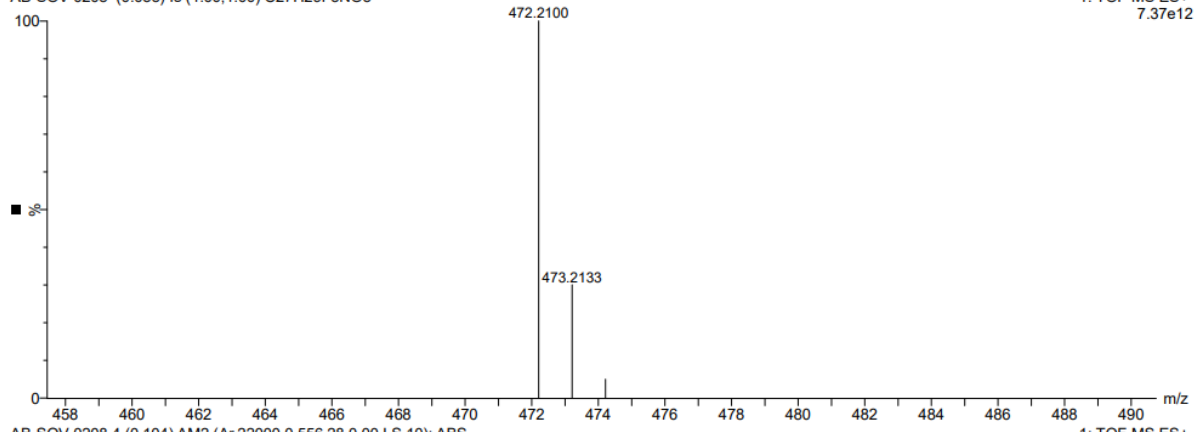


$^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) of (+)-**S12**

AB28-Mar-2024 12:42:39
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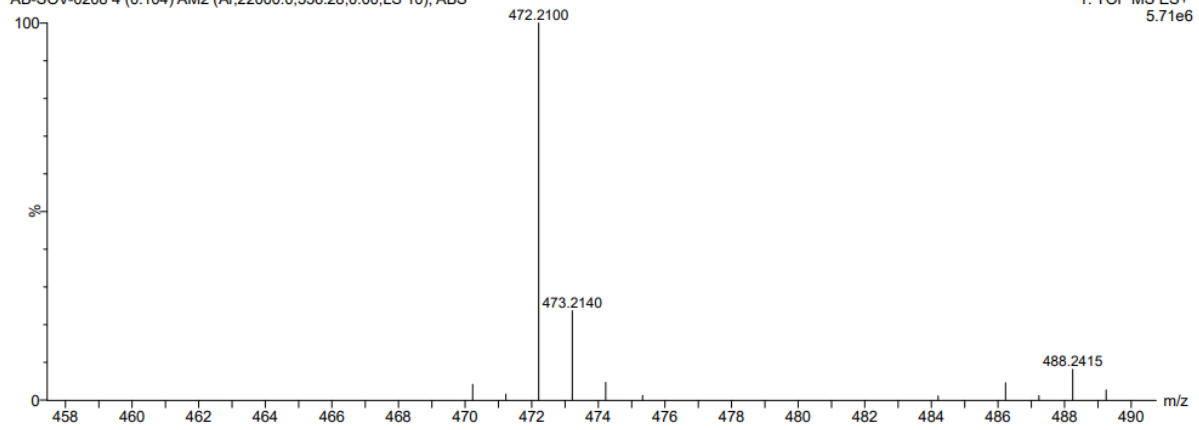
IISER - KOLKATA

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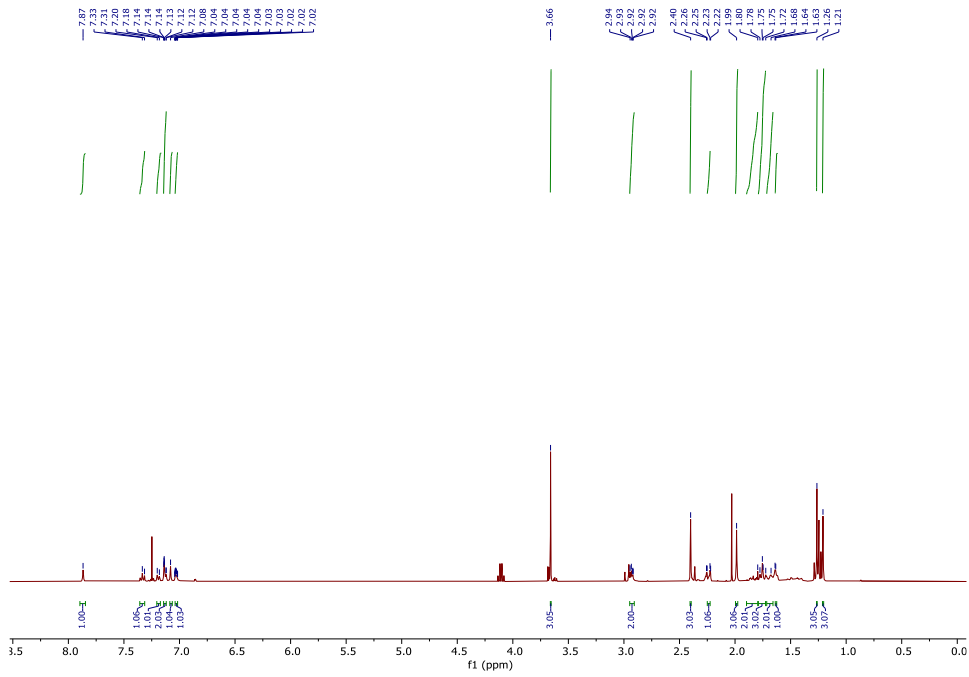
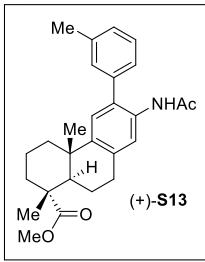


AB-SOV-0208 4 (0.104) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

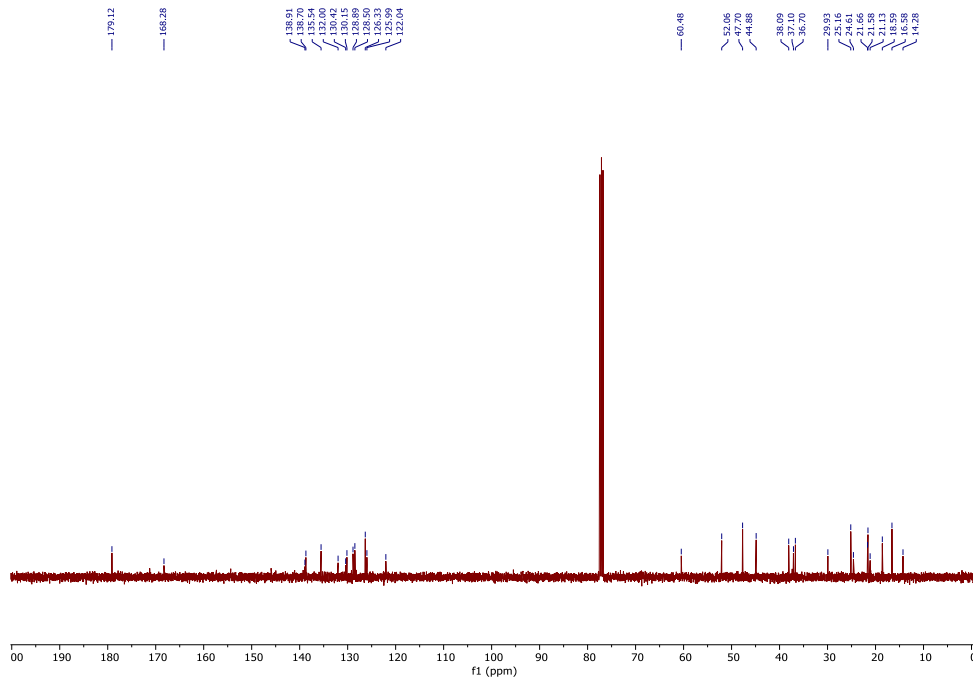
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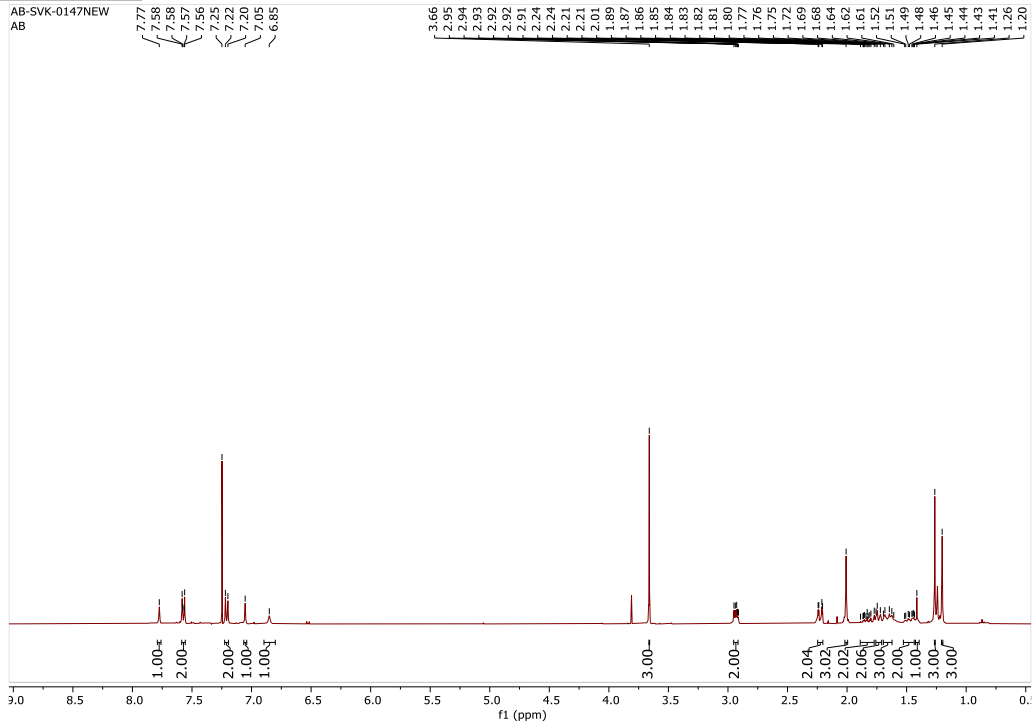
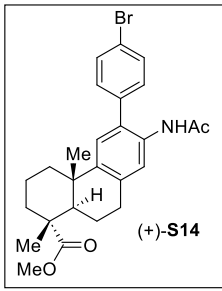
HRMS data of (+)-S12



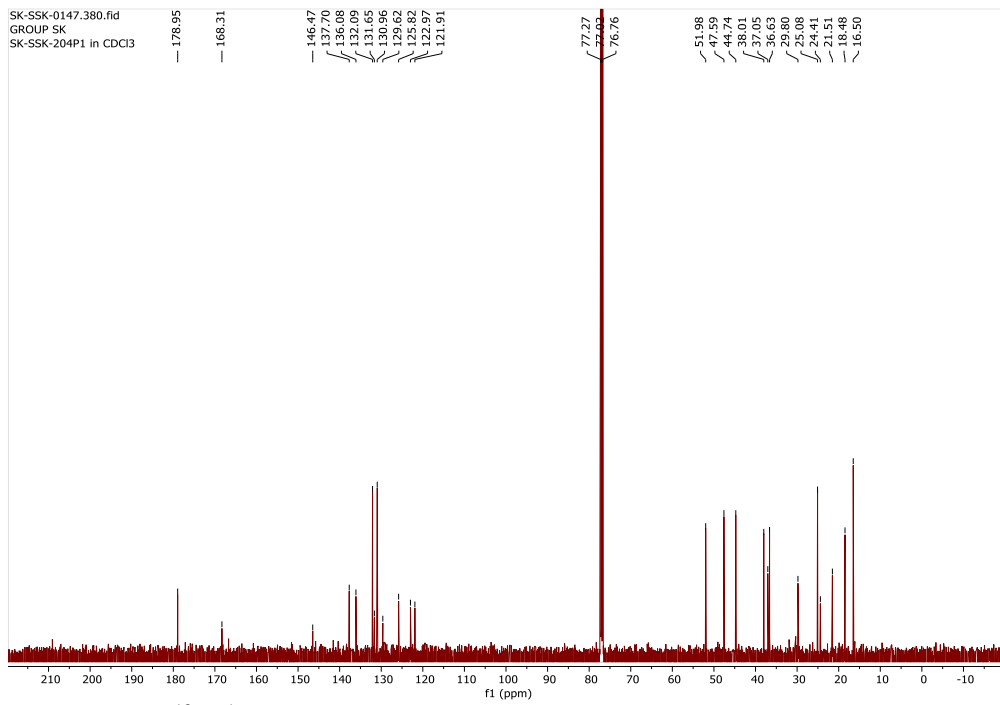
¹H NMR (400 MHz, CDCl₃) Data of (+)-S13



¹³C {¹H} NMR (101 MHz, CDCl₃) Data of (+)-S13



¹H NMR (400 MHz, CDCl₃) of compound (+)-S14

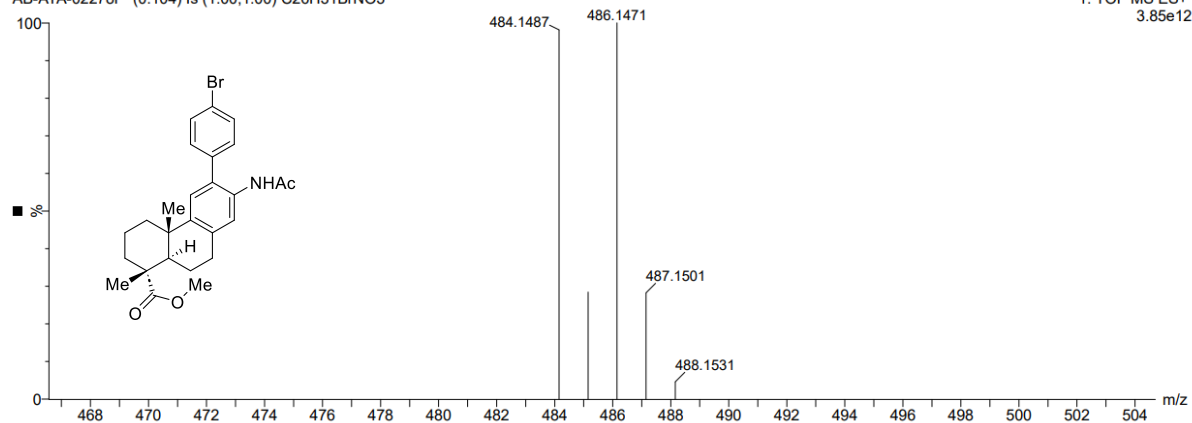


¹³C NMR (125 MHz, CDCl₃) of compound (+)-S14

AB29-Apr-2024 16:17:34
AB-AYA-02278P (0.104) Is (1.00,1.00) C₂₆H₃₁BrNO₃

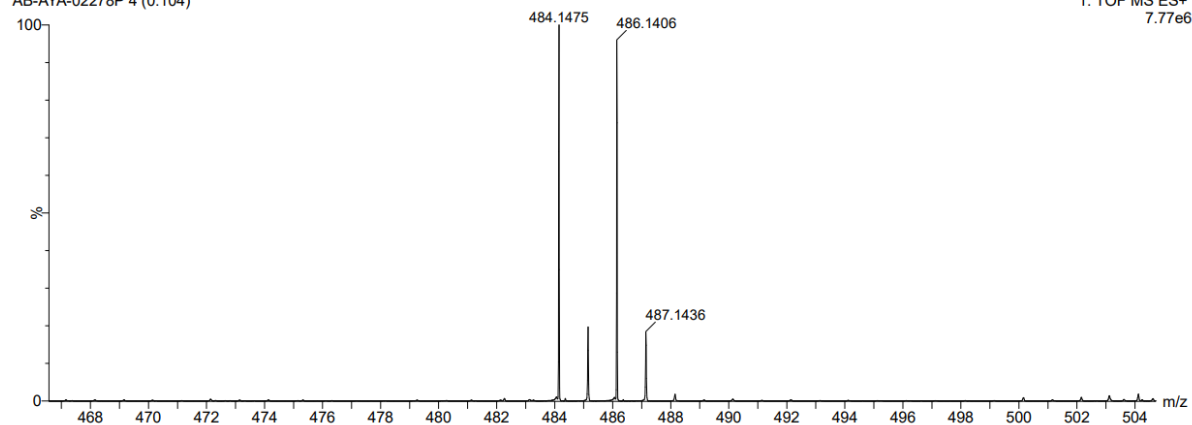
IISER - KOLKATA

1: TOF MS ES+
3.85e12

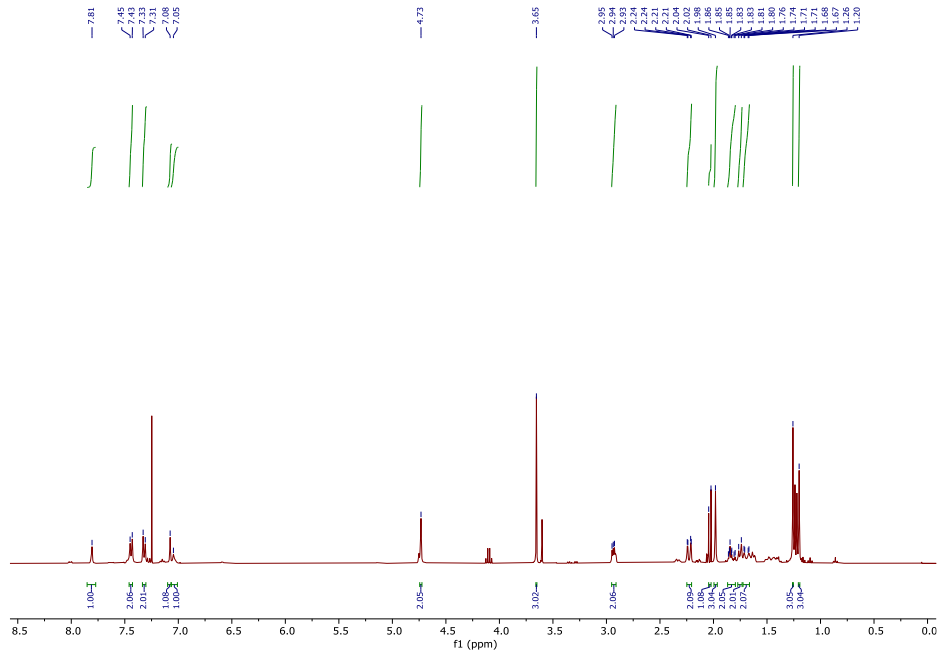
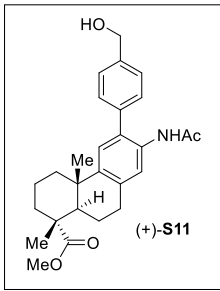


AB-AYA-02278P 4 (0.104)

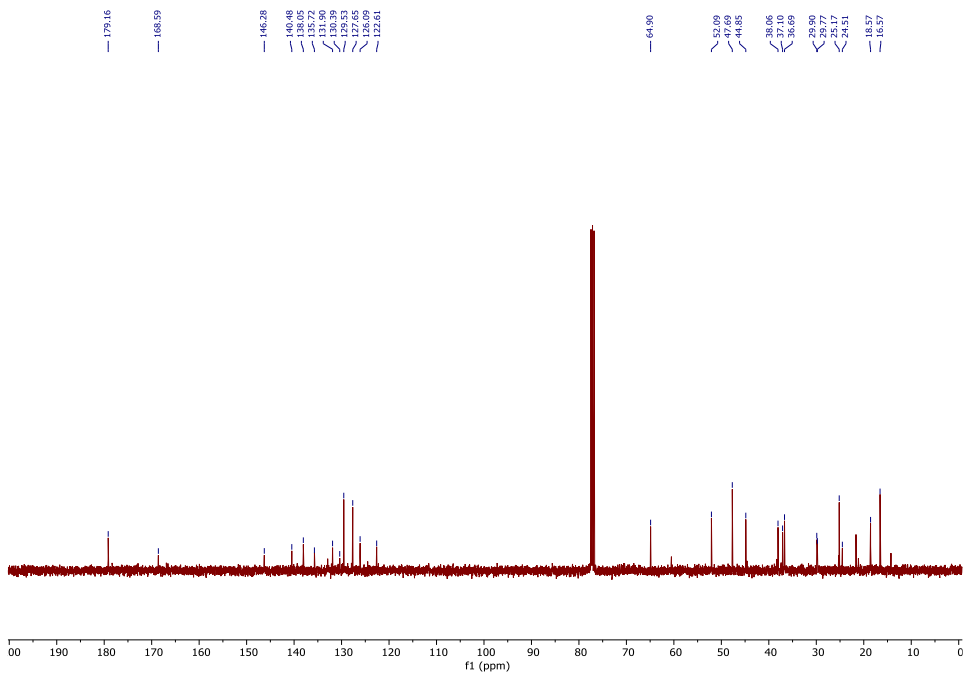
1: TOF MS ES+
7.77e6



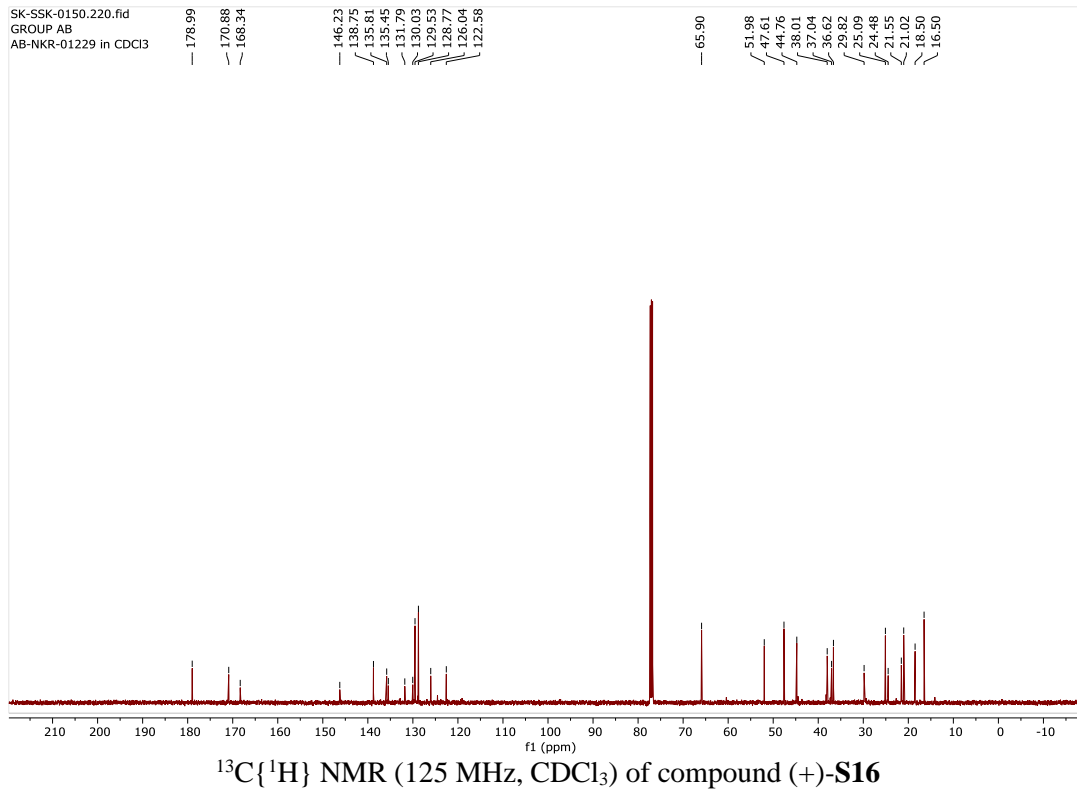
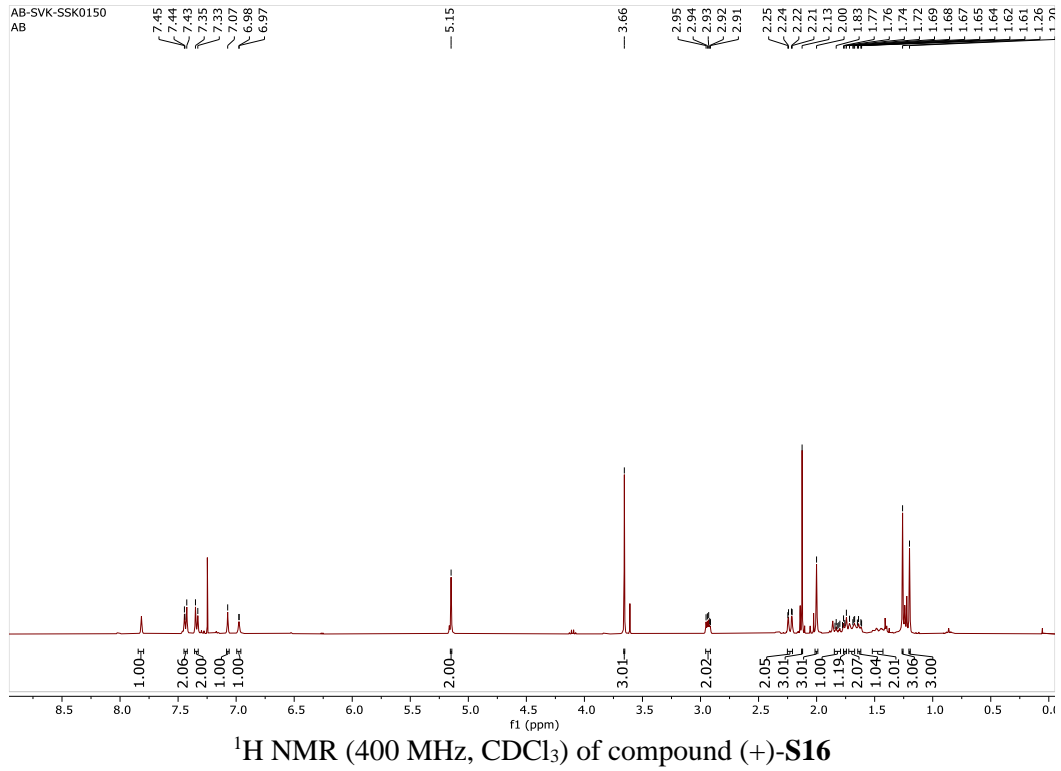
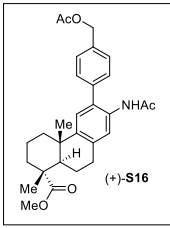
HRMS Data of (+)-S14

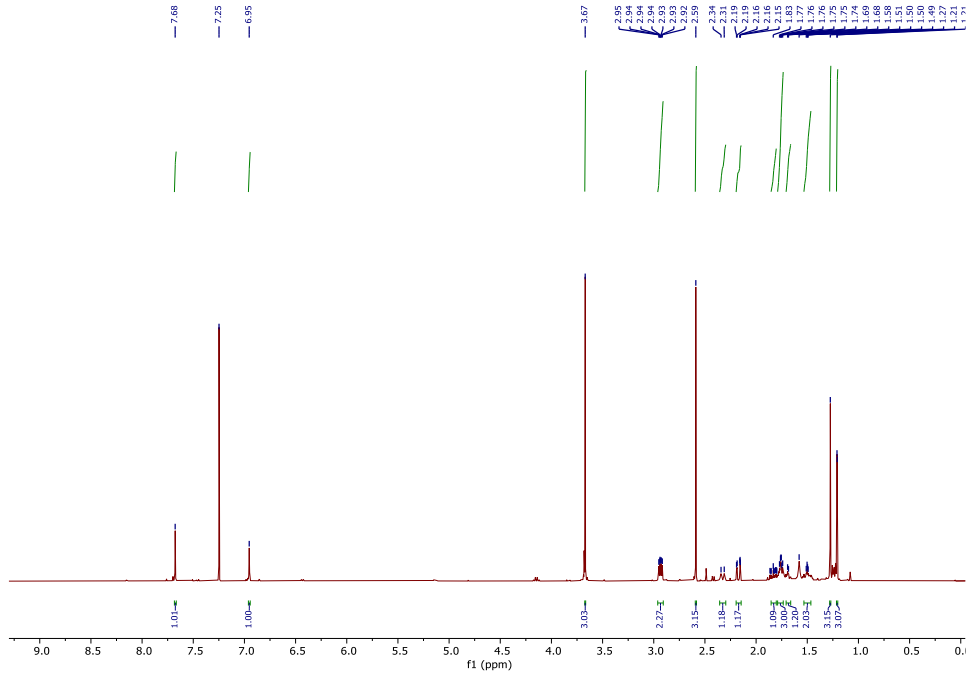
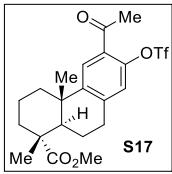


¹H NMR (400 MHz, CDCl₃) Data of (+)-S15

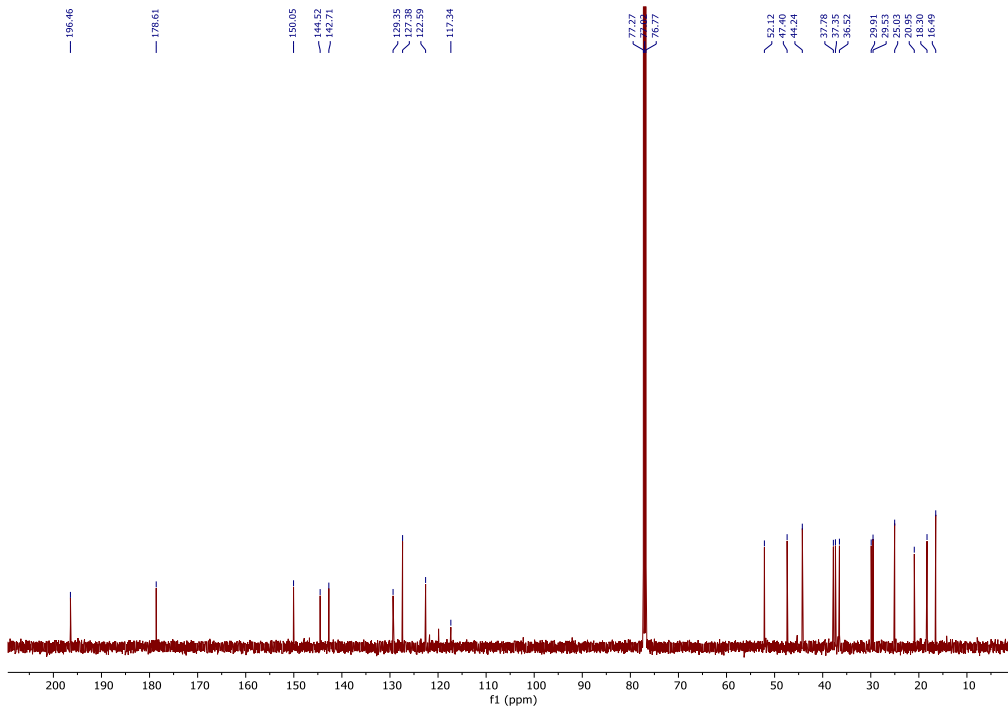


¹³C {¹H} NMR (101 MHz, CDCl₃) Data of (+)-S15





^1H NMR (500 MHz, CDCl_3) of compound **S17**

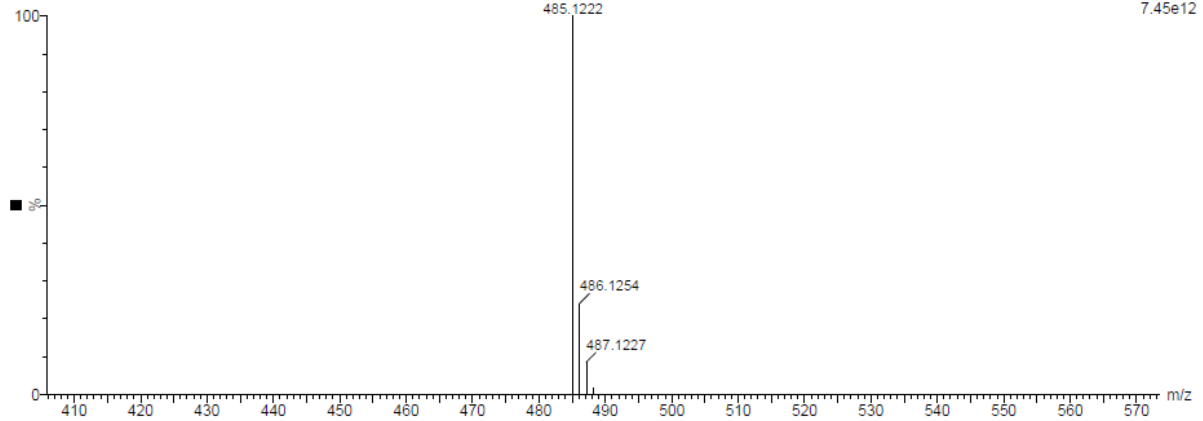


$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of compound **S17**

AB25-Apr-2024 13:23:34
AB-NKR-01036 (0.053) Is (1.00,1.00) C21H25F3O6SNa

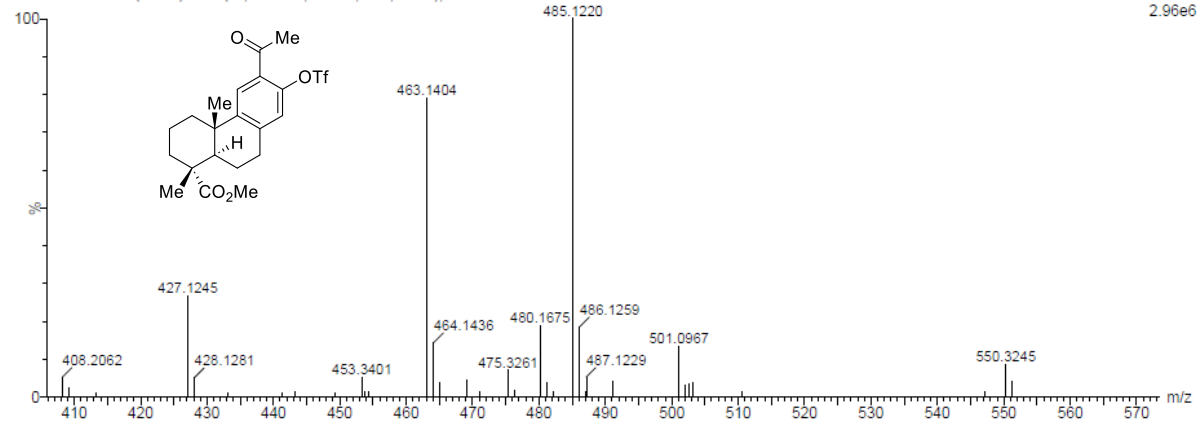
IISER - KOLKATA

1: TOF MS ES+
7.45e12

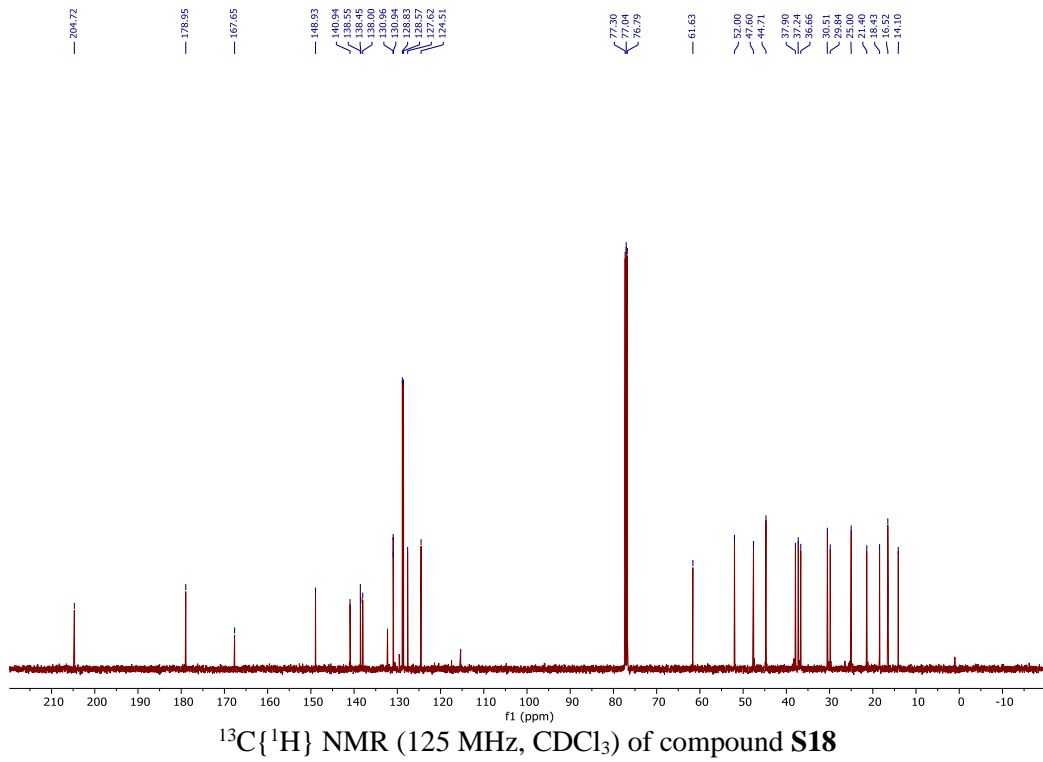
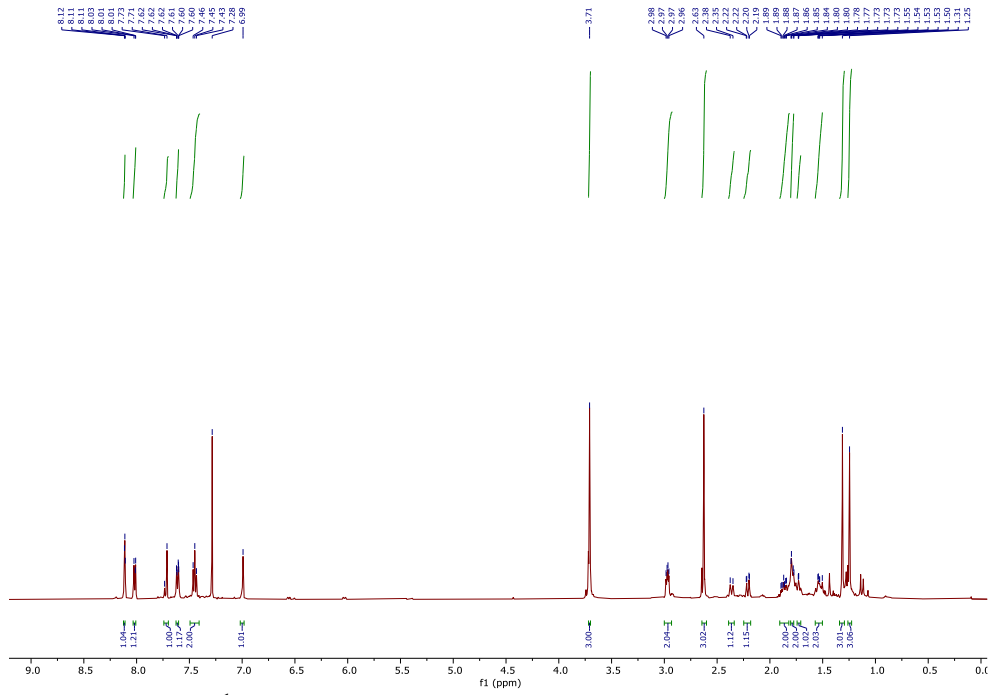
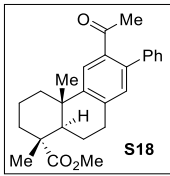


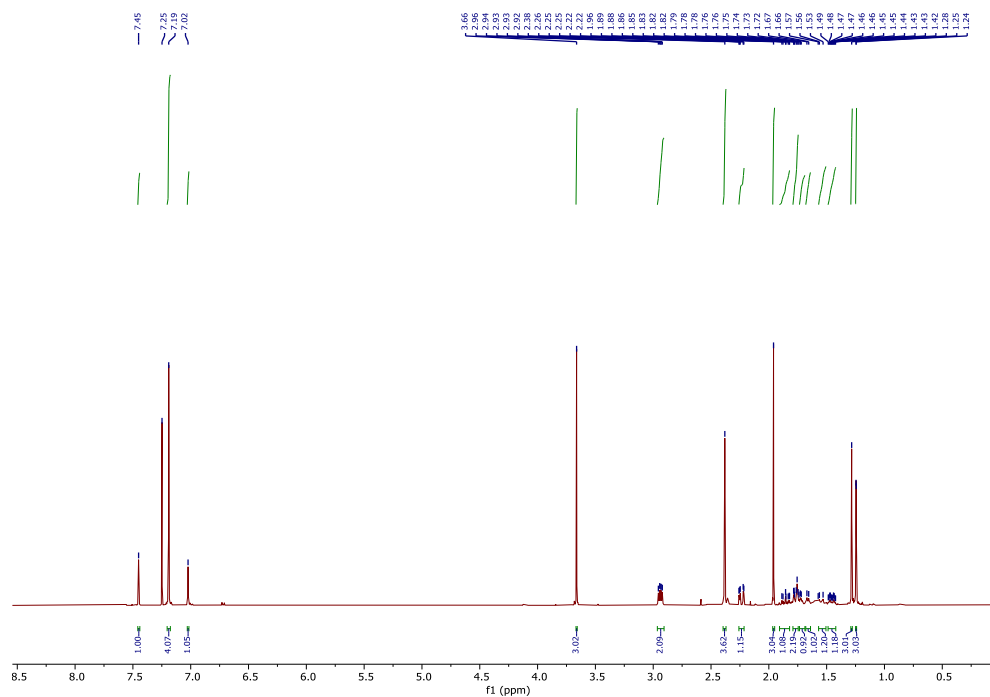
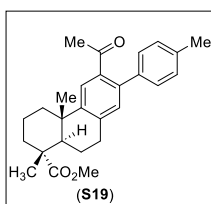
AB-NKR-01036 4 (0.104) AM2 (Ar,22000,0,556.28,0,00,LS 10); ABS

1: TOF MS ES+
2.96e6

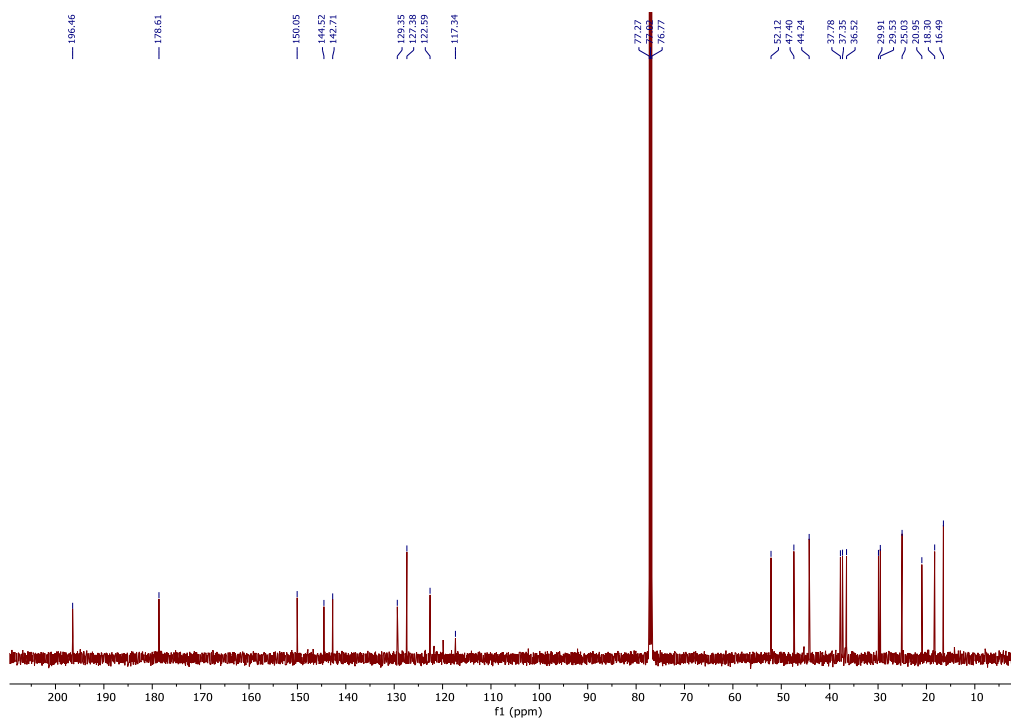


Mass data of compound S17





¹H NMR (400 MHz, CDCl₃) of compound **S19**



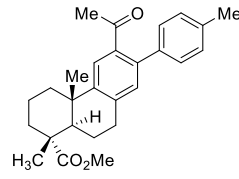
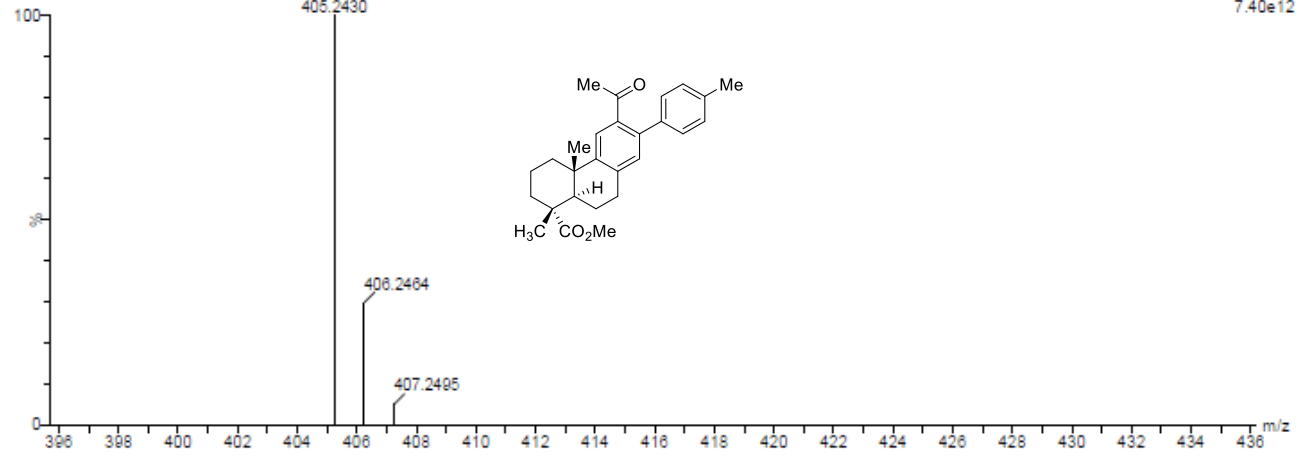
¹³C{¹H} NMR (125 MHz, CDCl₃) of compound **S19**

AB22-Apr-2024 13:13:33

IISER - KOLKATA

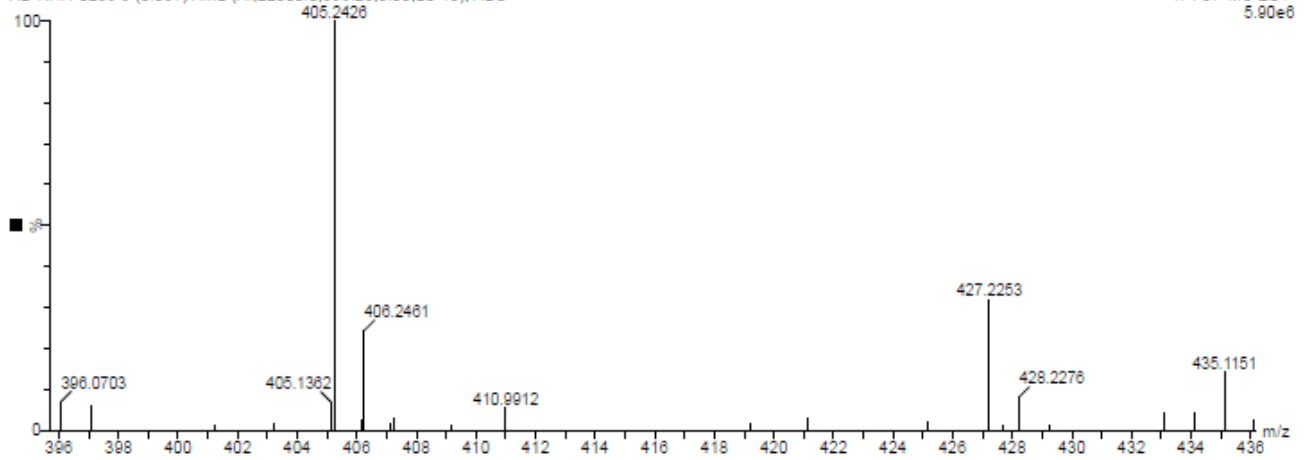
1: TOF MS ES+
7.40e12

AB-NKR-0239 (0.053) Is (1.00,1.00) C27H33O3

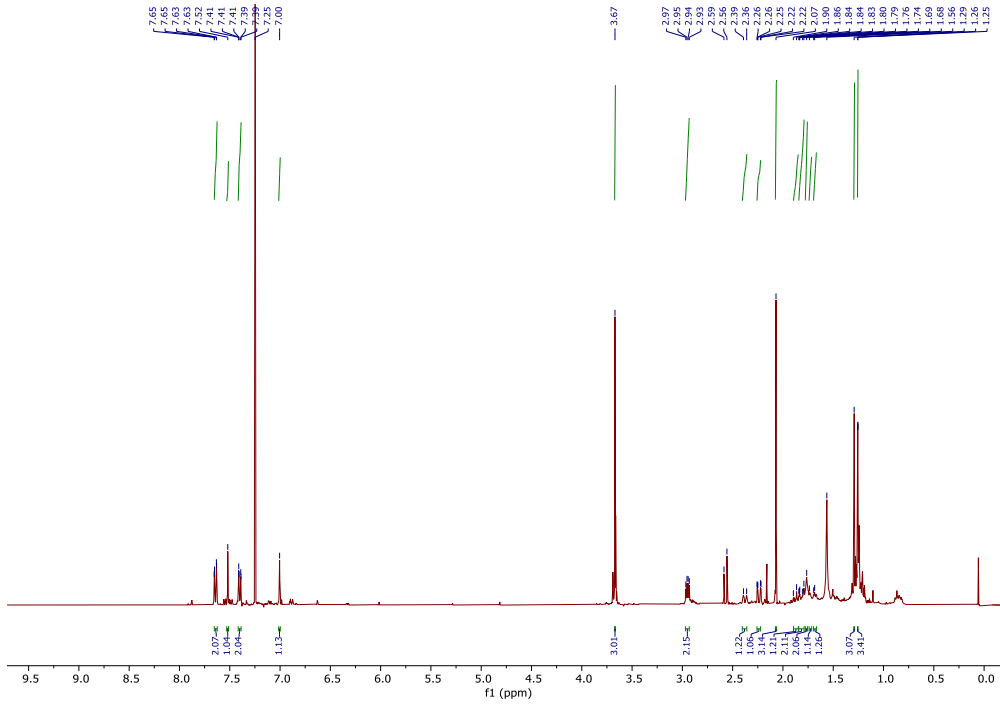
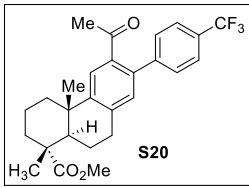


AB-NKR-0239 3 (0.087) AM2 (Ar,22000,0.556,28.0,0.0,LS 10); ABS

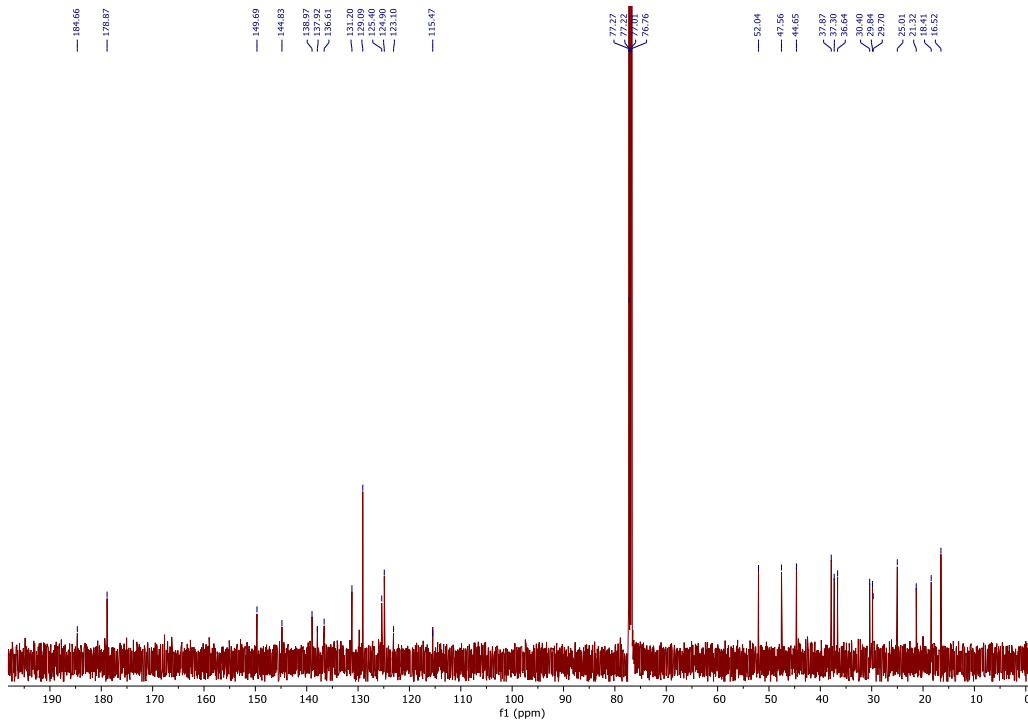
1: TOF MS ES+
5.90e6



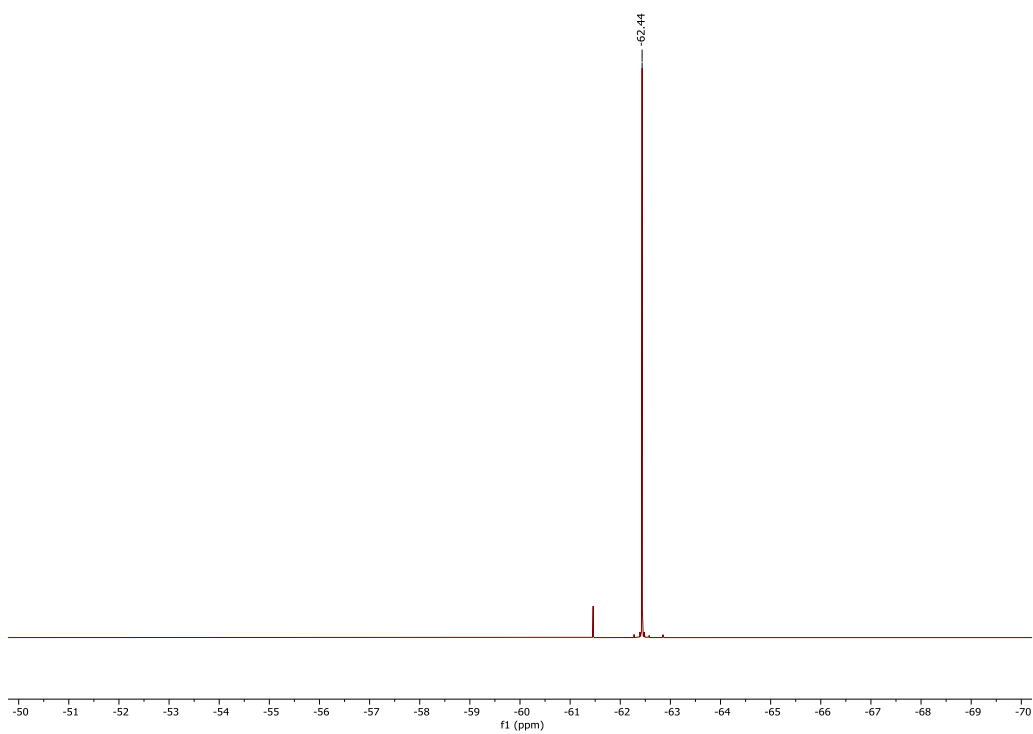
Mass spectrum of compound S19



¹H NMR (500 MHz, CDCl₃) of compound S20



¹³C{¹H} NMR (125 MHz, CDCl₃) of compound S20

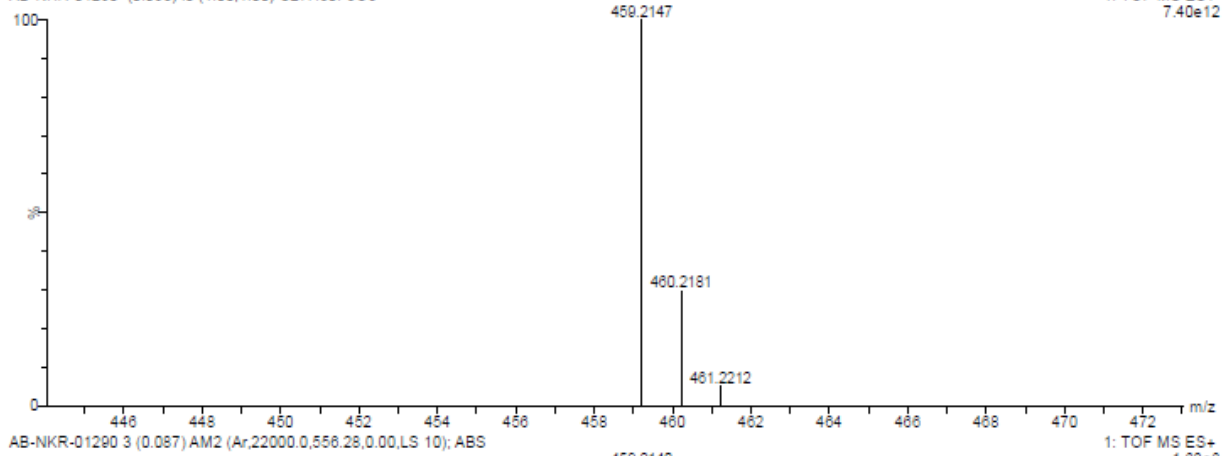


$^{19}\text{F}\{^1\text{H}\}$ NMR (471 MHz, CDCl_3) of compound **S20**

AB22-Apr-2024 13:16:48
AB-NKR-01290 (0.053) Is (1.00,1.00) C27H30F3O3

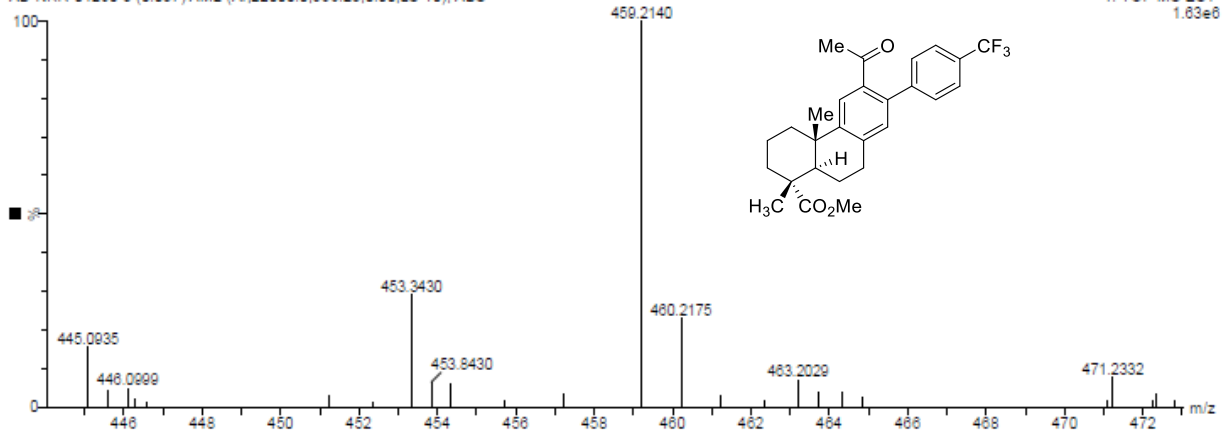
IISER - KOLKATA

1: TOF MS ES+
7.40e12

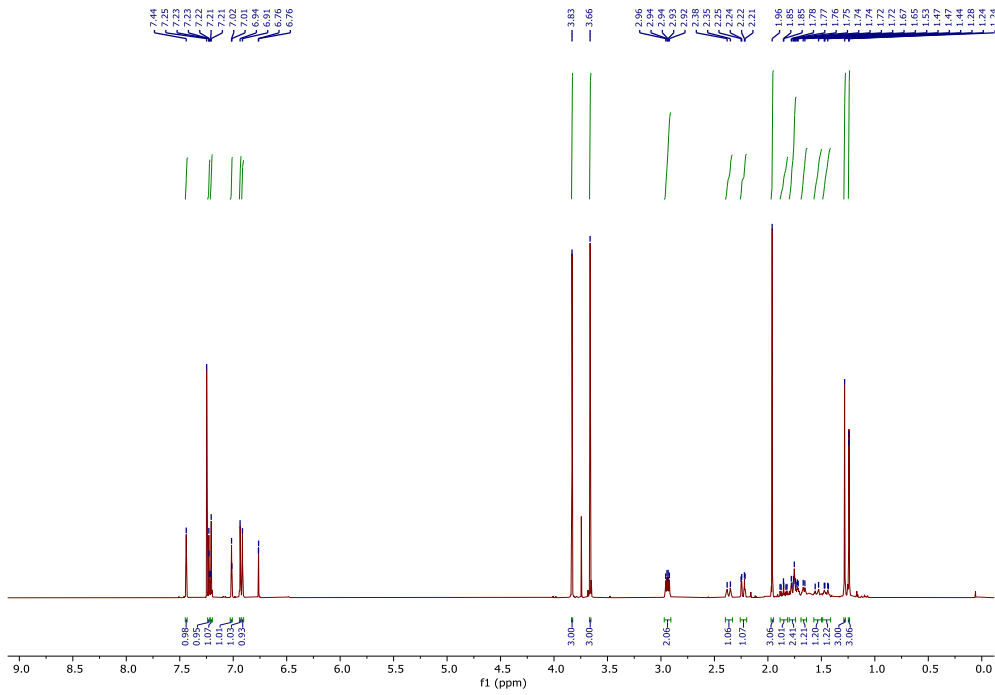
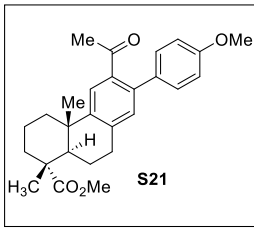


AB-NKR-01290 3 (0.087) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

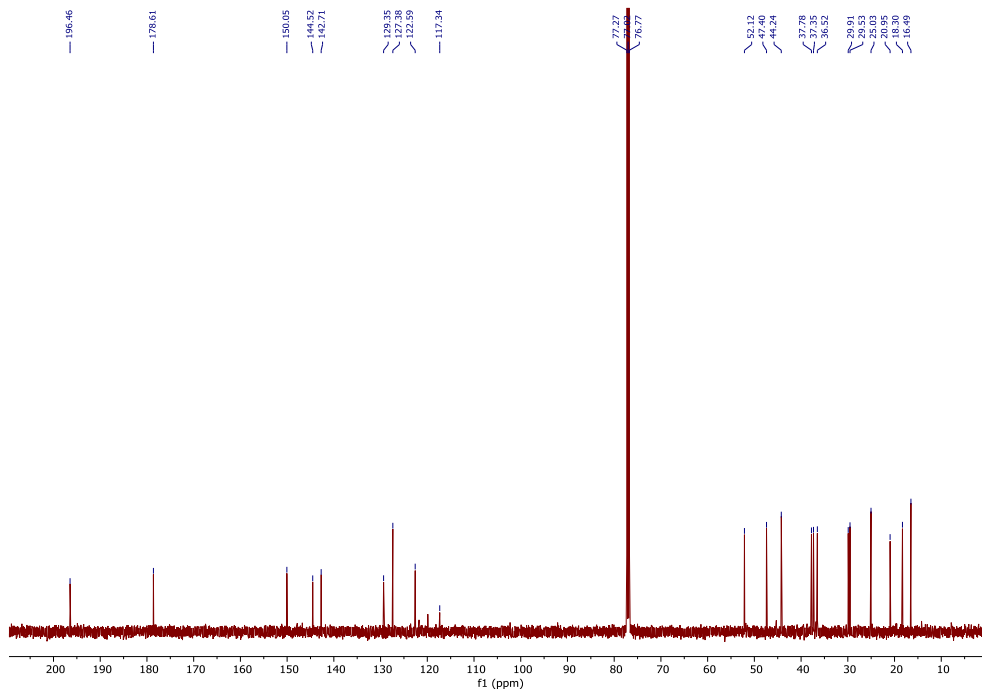
1: TOF MS ES+
1.83e6



Mass spectrum of compound S20



¹H NMR (500 MHz, CDCl₃) of compound **S21**

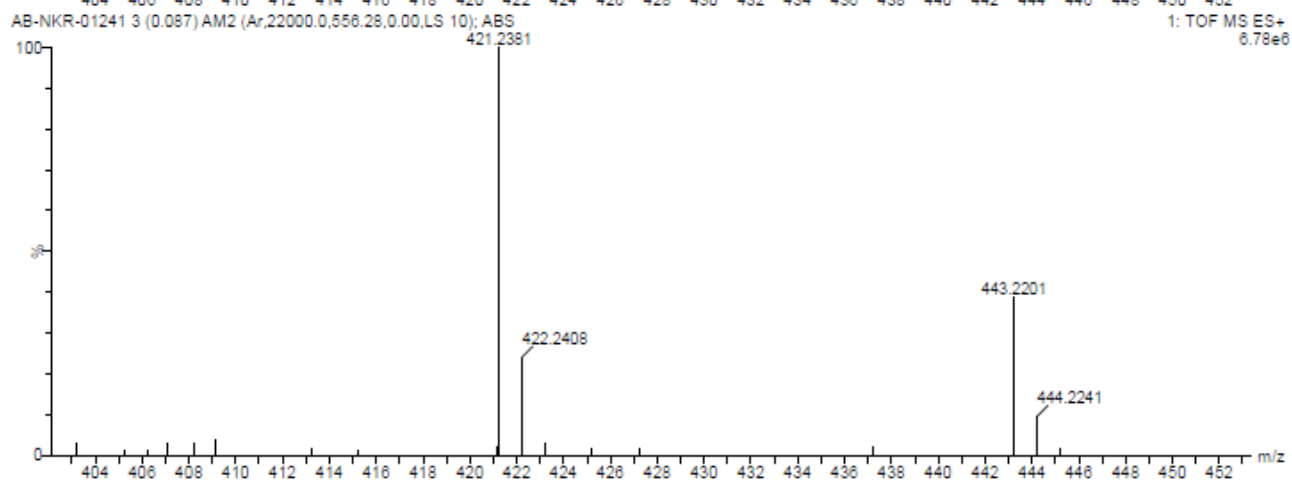
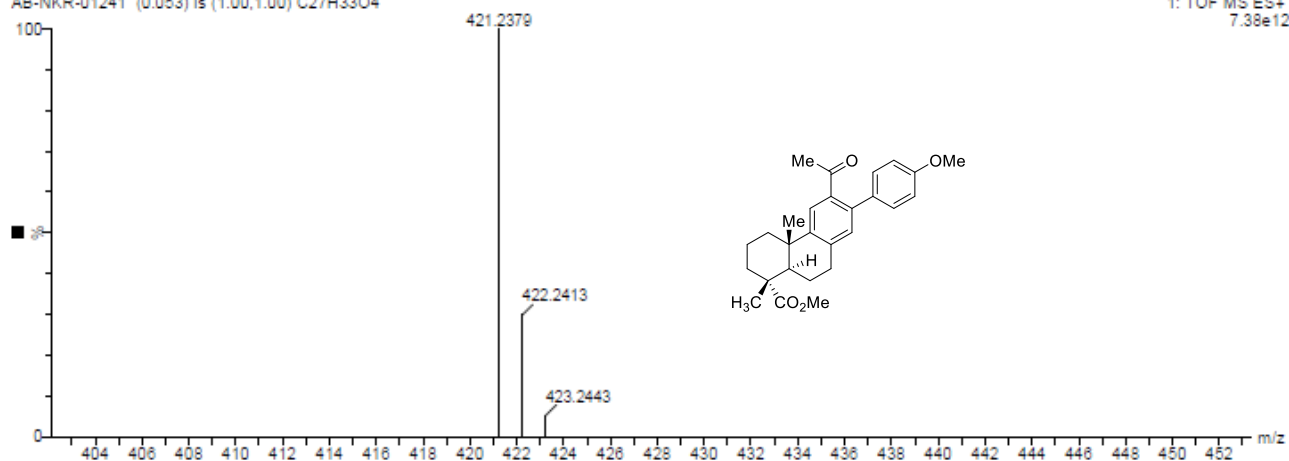


¹³C{¹H} NMR (125 MHz, CDCl₃) of compound **S21**

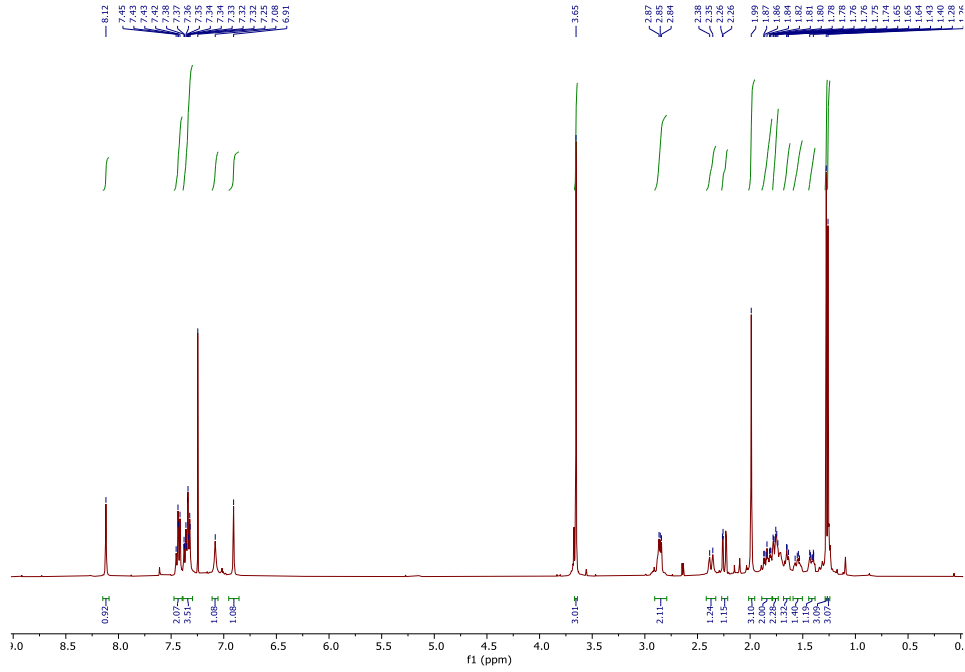
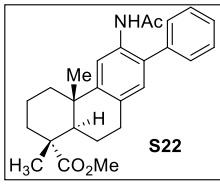
AB22-Apr-2024 12:14:42
AB-NKR-01241 (0.053) Is (1.00,1.00) C27H33O4

IISER - KOLKATA

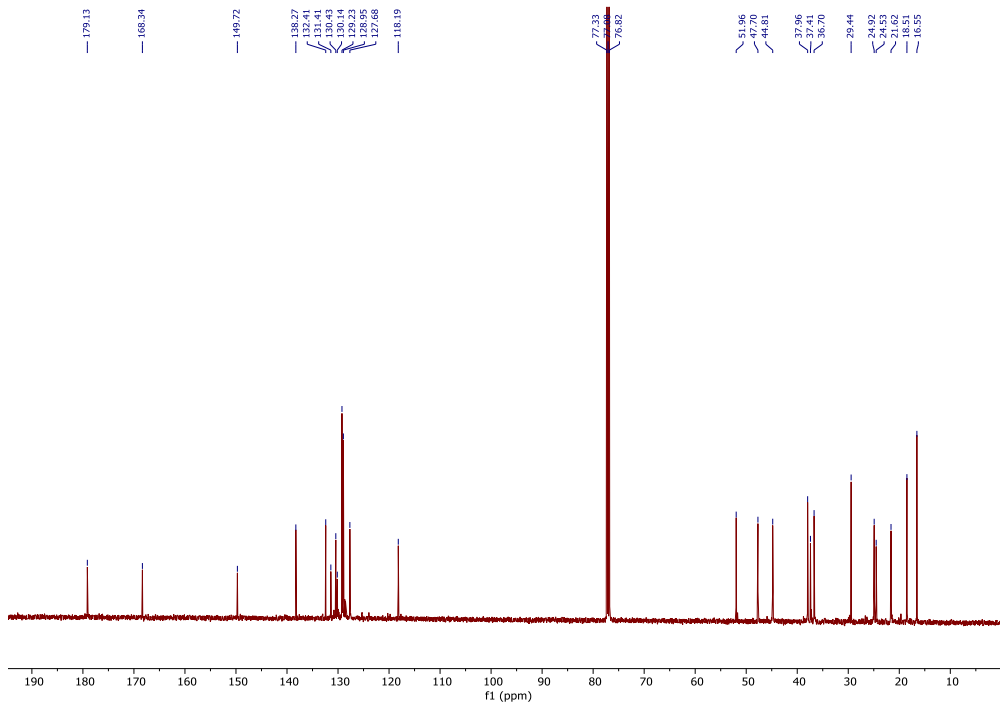
1: TOF MS ES+
7.38e12



Mass spectrum of compound S21



¹H NMR (500 MHz, CDCl₃) of compound **S22**

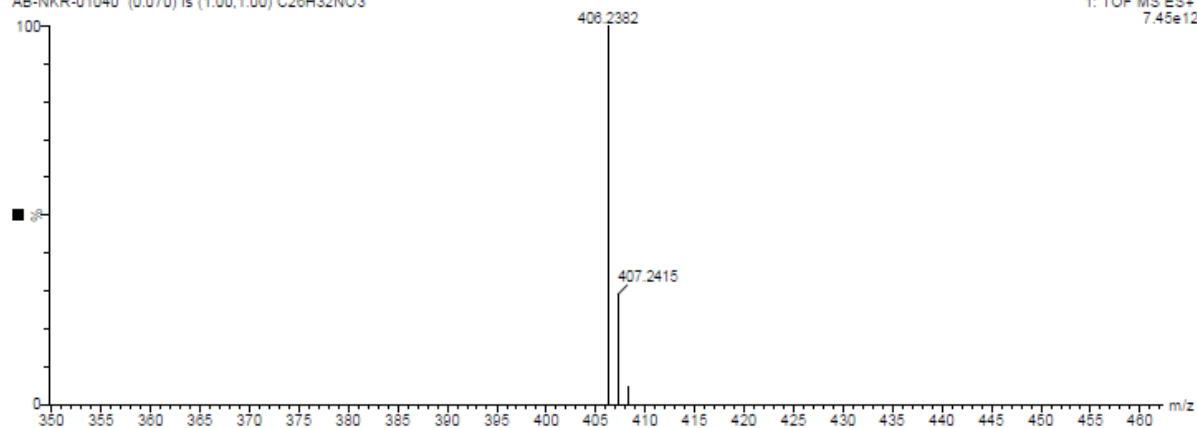


¹³C NMR (125 MHz, CDCl₃) of compound **S22**

AB28-Mar-2024 14:02:25
AB-NKR-01040 (0.070) Is (1.00,1.00) C26H32NO3

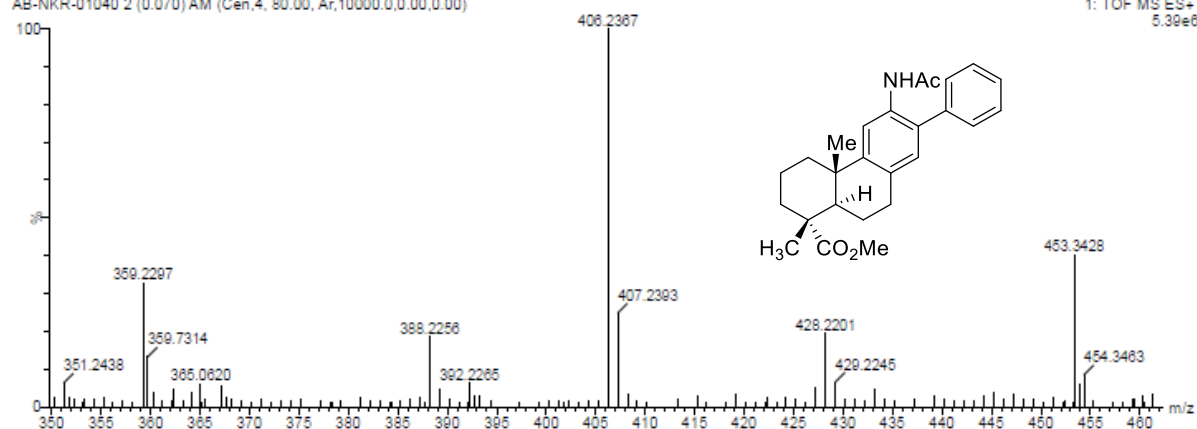
IISER - KOLKATA

1: TOF MS ES+
7.45e12

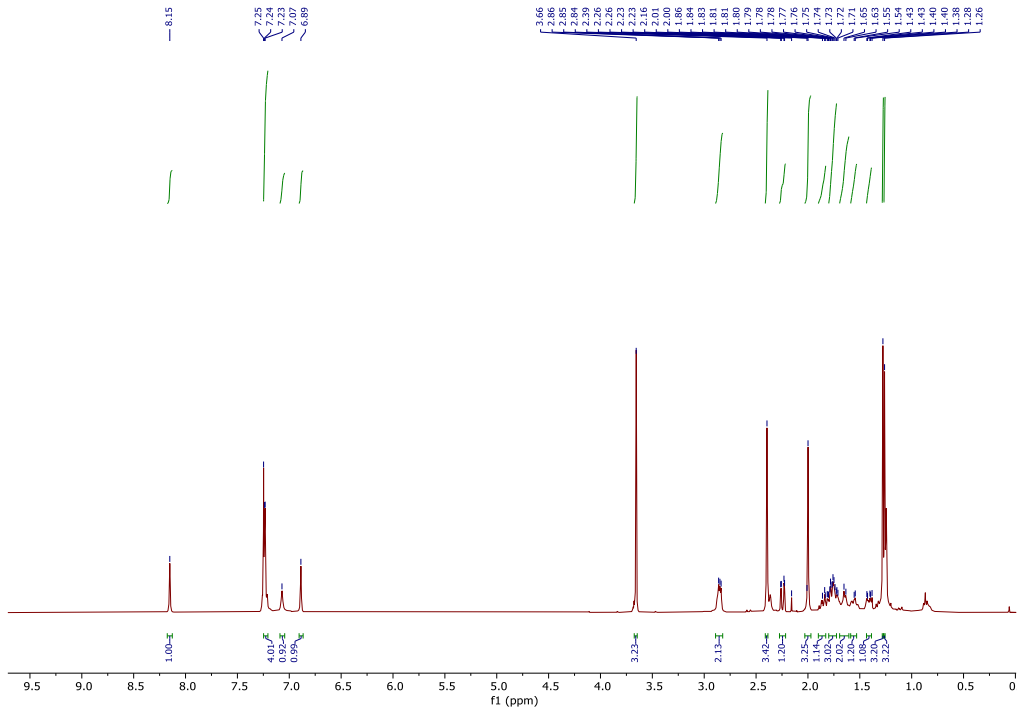
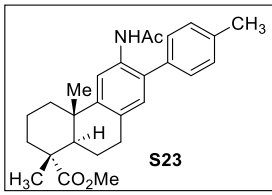


AB-NKR-01040 2 (0.070) AM (Cen,4, 80.00, Ar,100000.0,0.00,0.00)

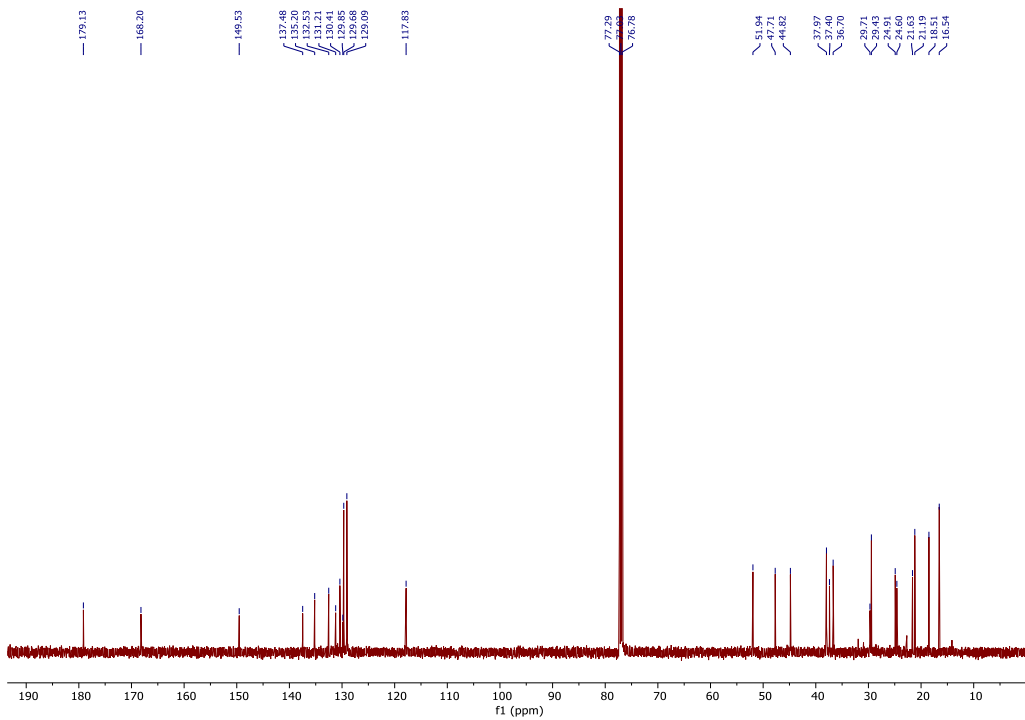
1: TOF MS ES+
5.39e6



Mass spectrum of compound S22



¹H NMR (400 MHz, CDCl₃) of compound **S23**

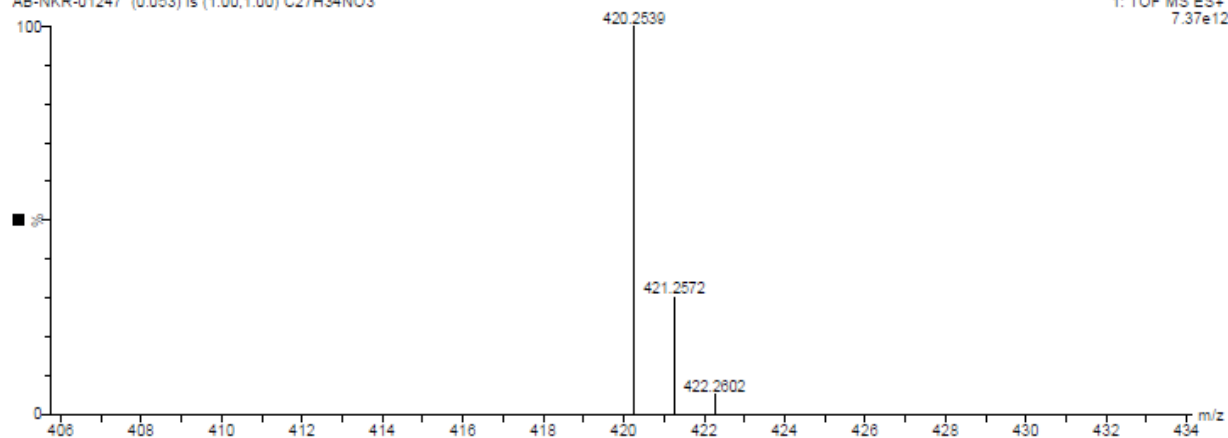


¹³C{¹H} NMR (125 MHz, CDCl₃) of compound **S23**

AB23-Apr-2024 17:07:16
AB-NKR-01247 (0.053) Is (1.00,1.00) C27H34NO3

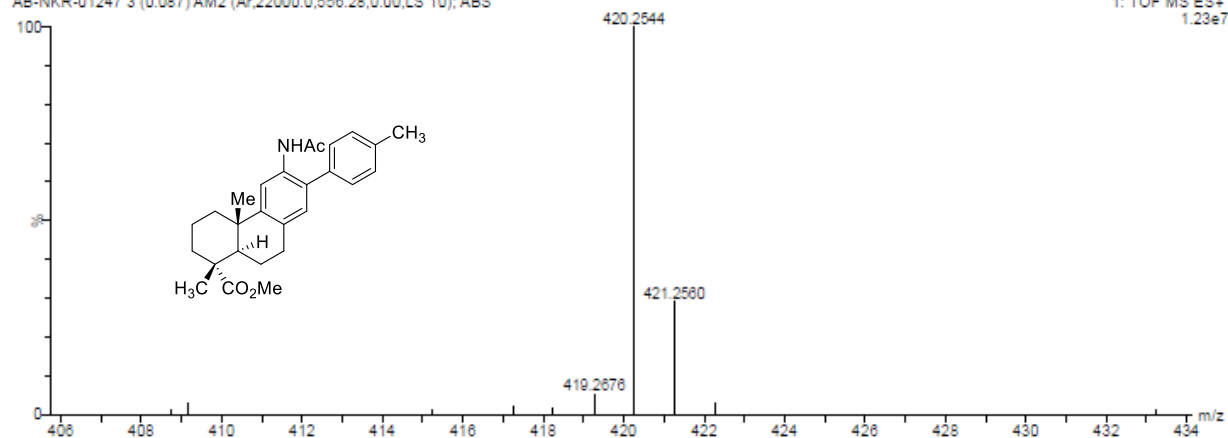
IISER - KOLKATA

1: TOF MS ES+
7.37e12

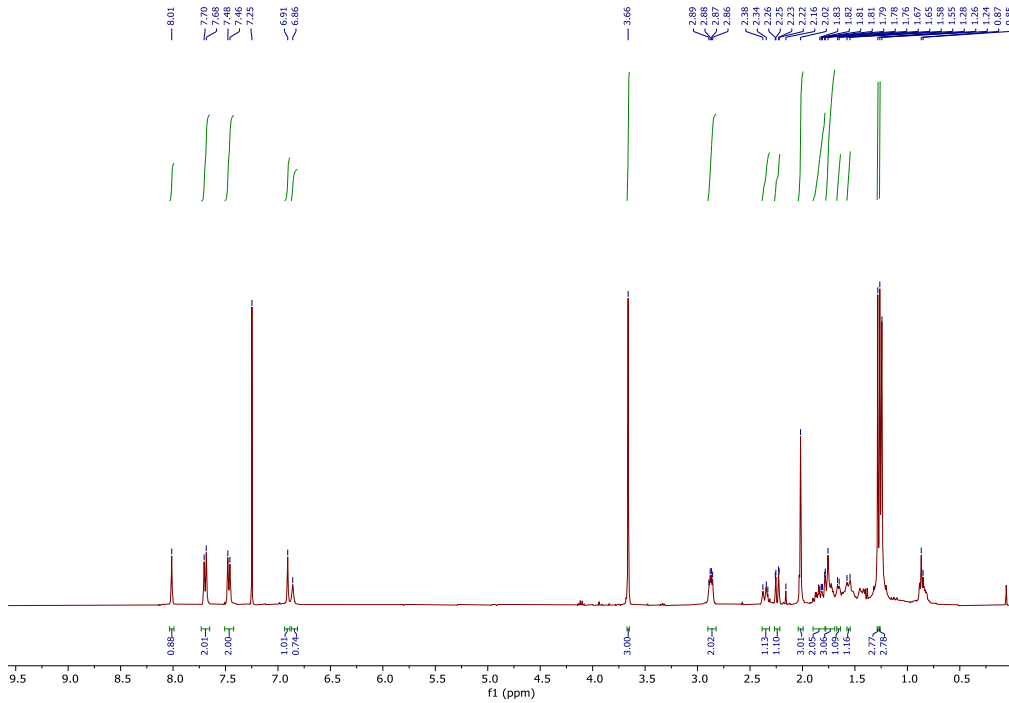
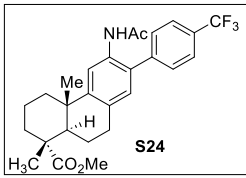


AB-NKR-01247 3 (0.087) AM2 (Ar,22000,0,556.28,0,00,LS 10); ABS

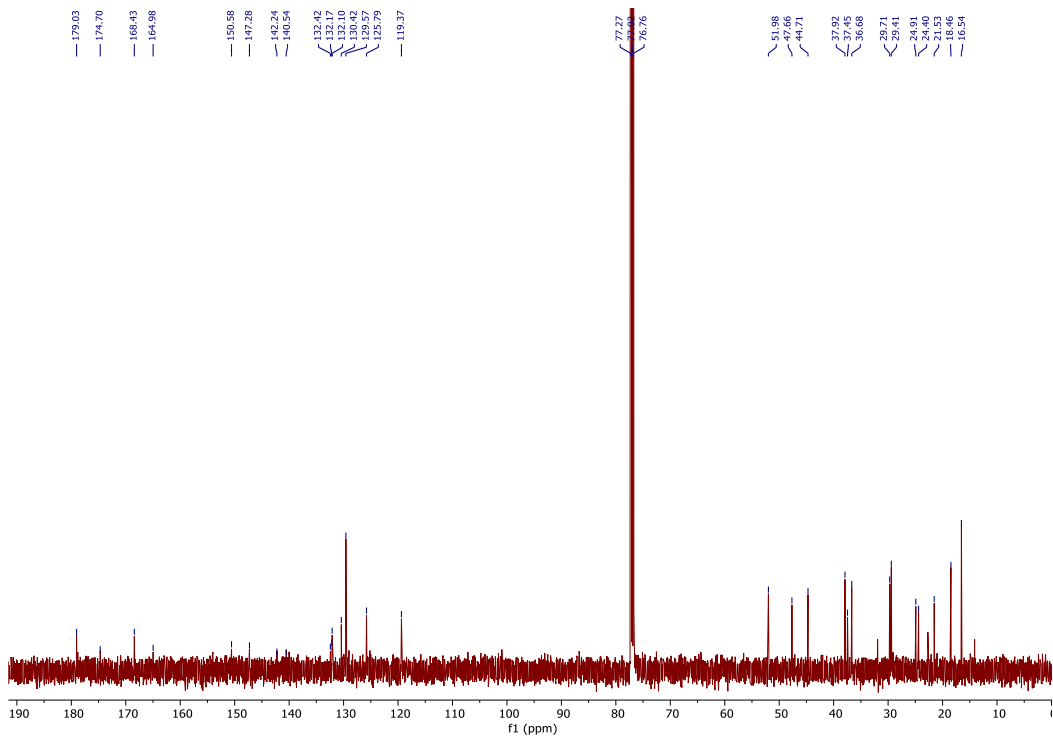
1: TOF MS ES+
1.23e7



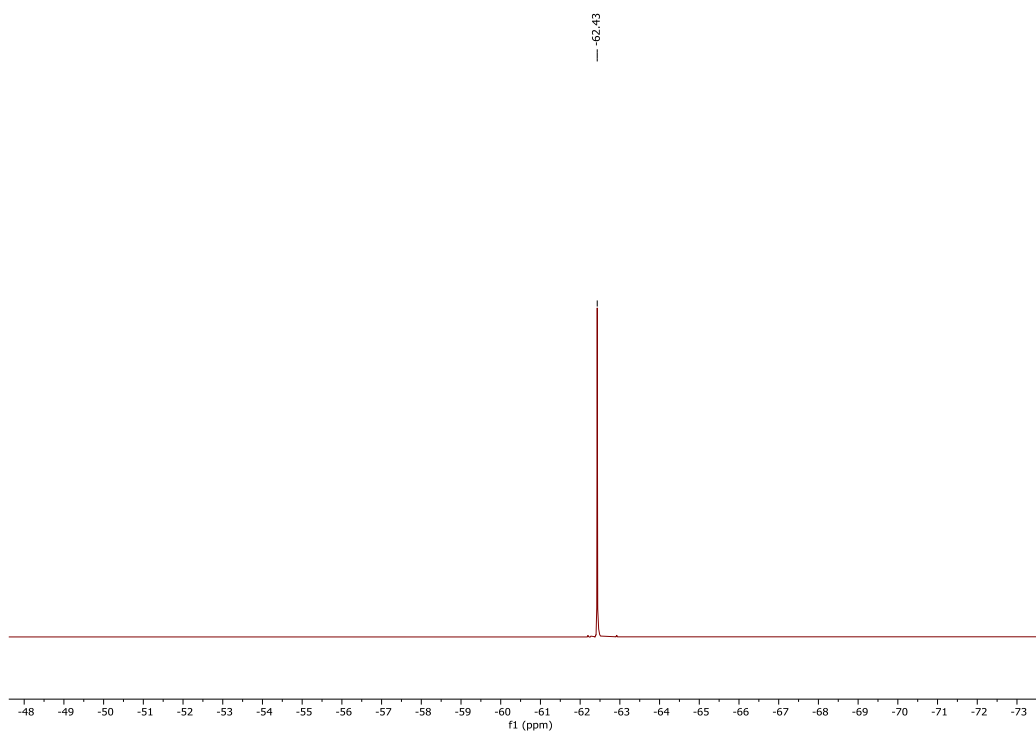
Mass data of compound S23



¹H NMR (400 MHz, CDCl₃) of compound **S24**



¹³C{¹H} NMR (125 MHz, CDCl₃) of compound **S24**

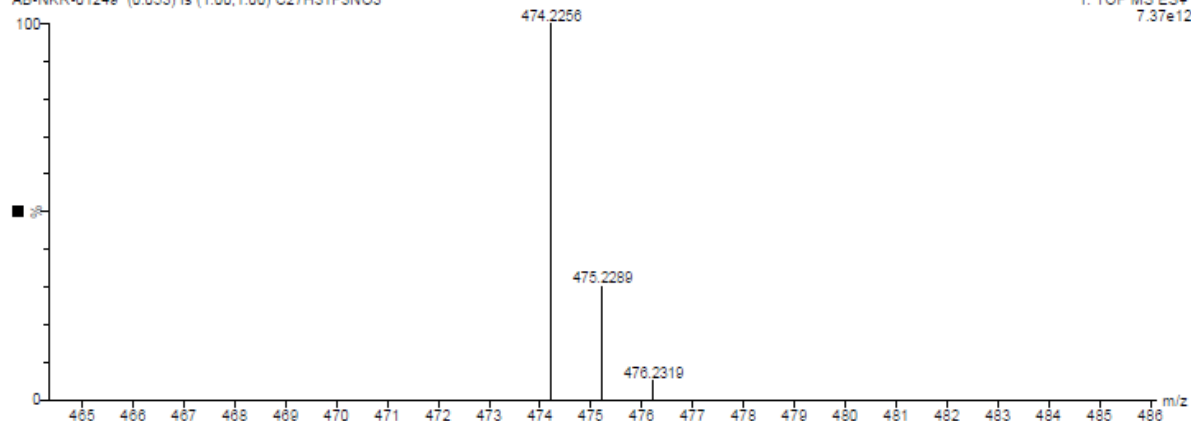


$^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) of compound **S24**

AB23-Apr-2024 17:10:24
AB-NKR-01249 (0.053) Is (1.00,1.00) C27H31F3NO3

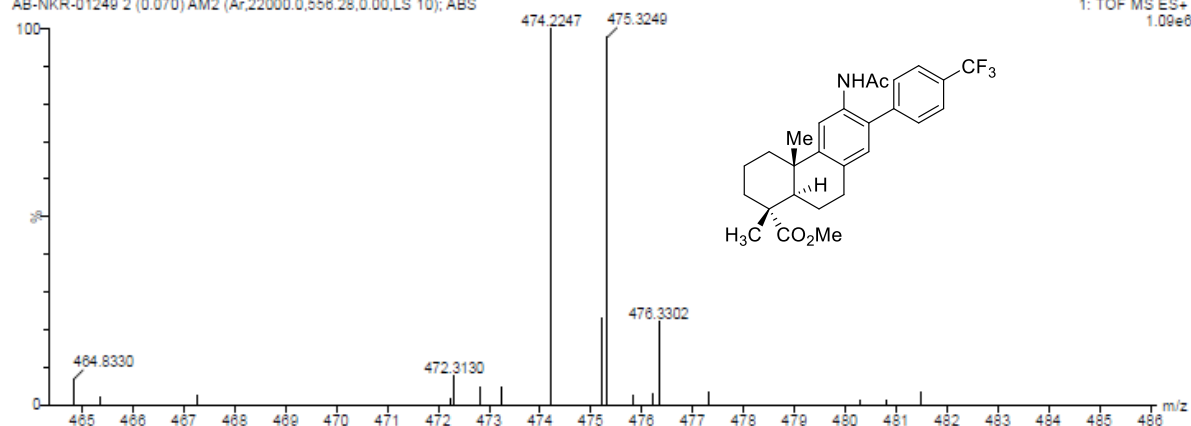
IISER - KOLKATA

1: TOF MS ES+
7.37e12

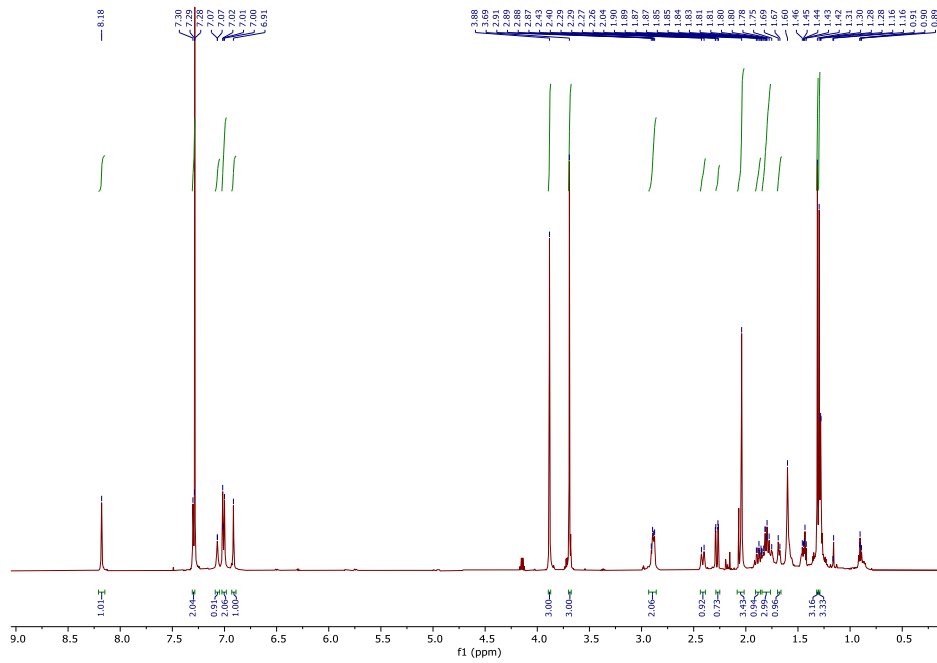
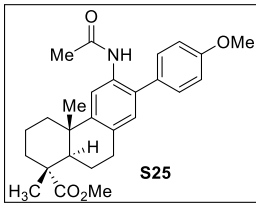


AB-NKR-01249 2 (0.070) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

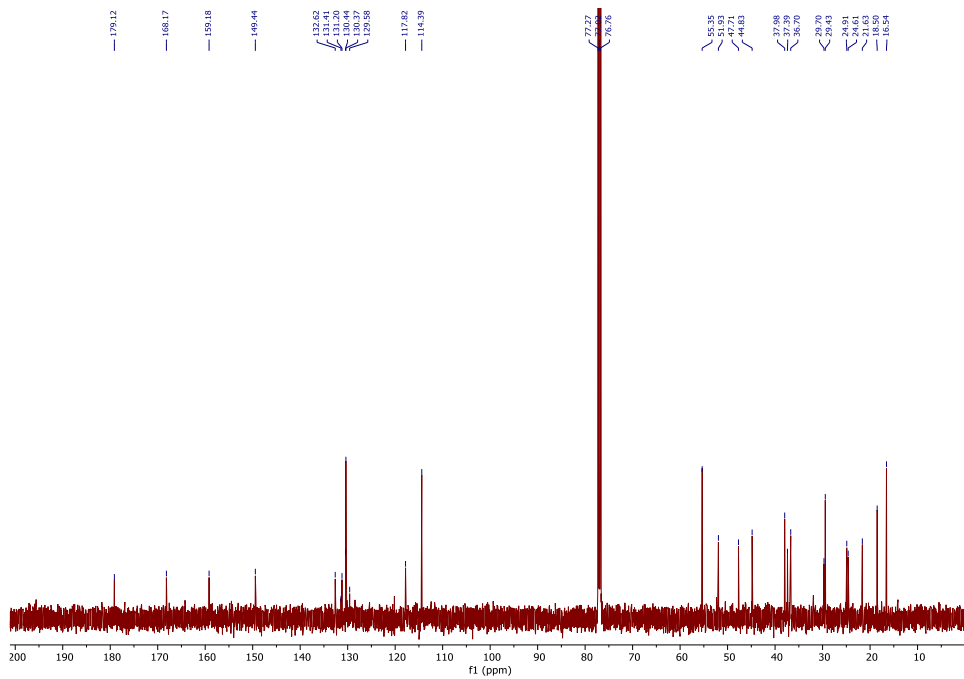
1: TOF MS ES+
1.09e8



Mass spectrum of compound S24



^1H NMR (400 MHz, CDCl_3) of compound **S25**



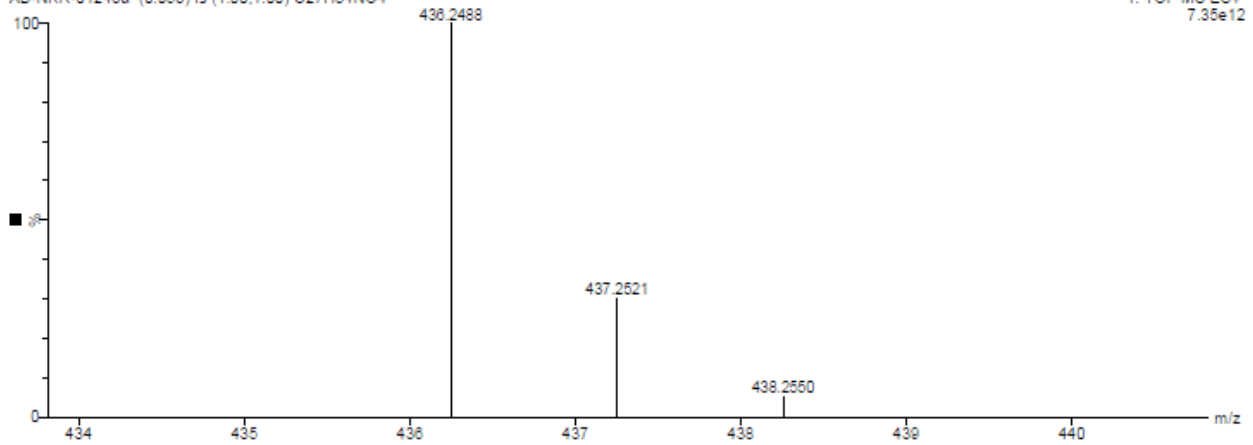
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of compound **S25**

AB24-Apr-2024 16:52:51

AB-NKR-01248a (0.053) Is (1.00,1.00) C27H34NO4

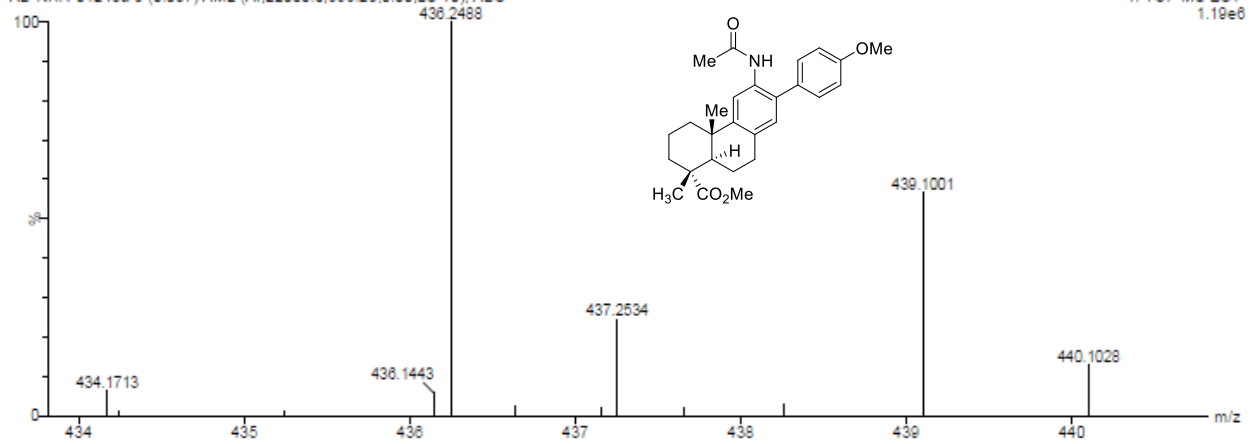
IISER - KOLKATA

1: TOF MS ES+
7.35e12

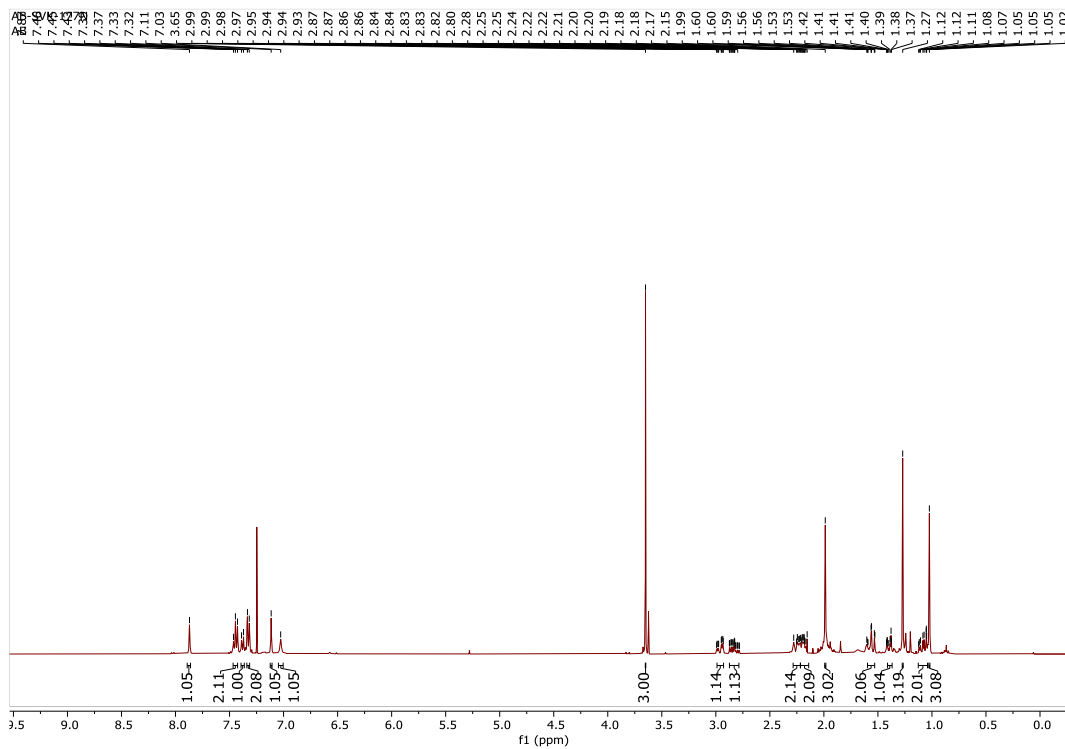
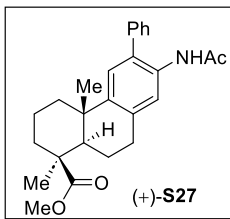


AB-NKR-01248a 3 (0.087) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

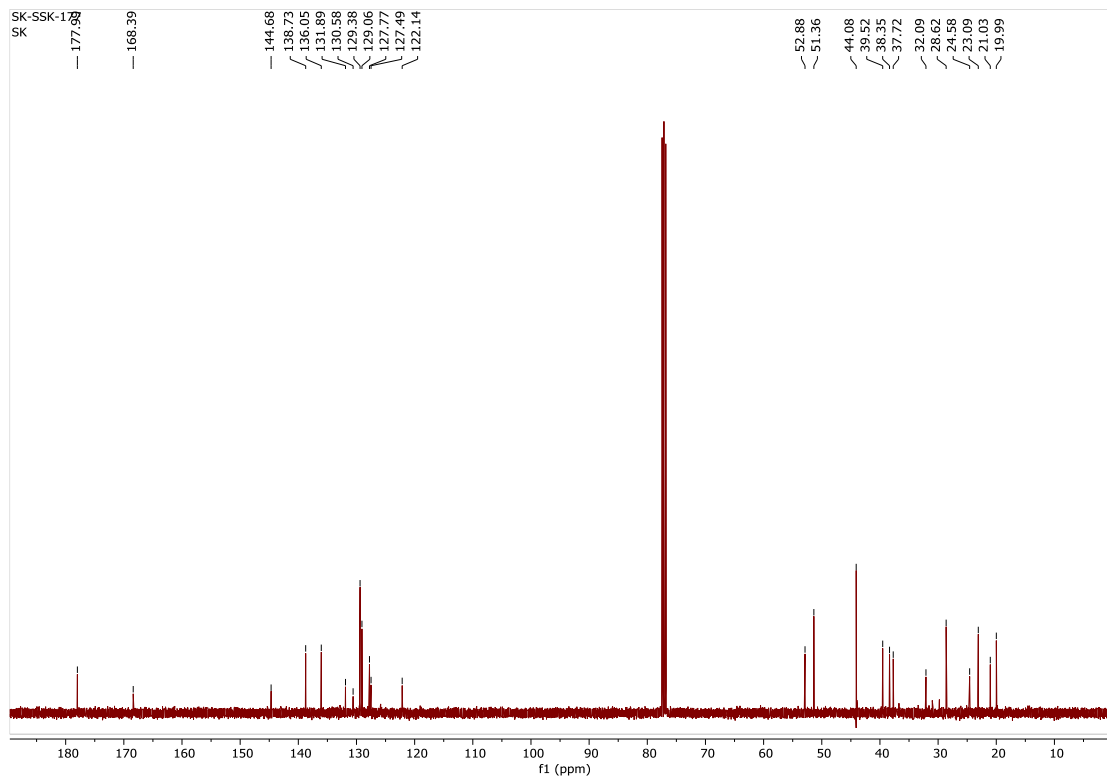
1: TOF MS ES+
1.19e6



Mass spectrum of compound S25



^1H NMR (400 MHz, CDCl_3) of compound (+)-S27



$^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) of compound (+)-S27

Display Report

Analysis Info

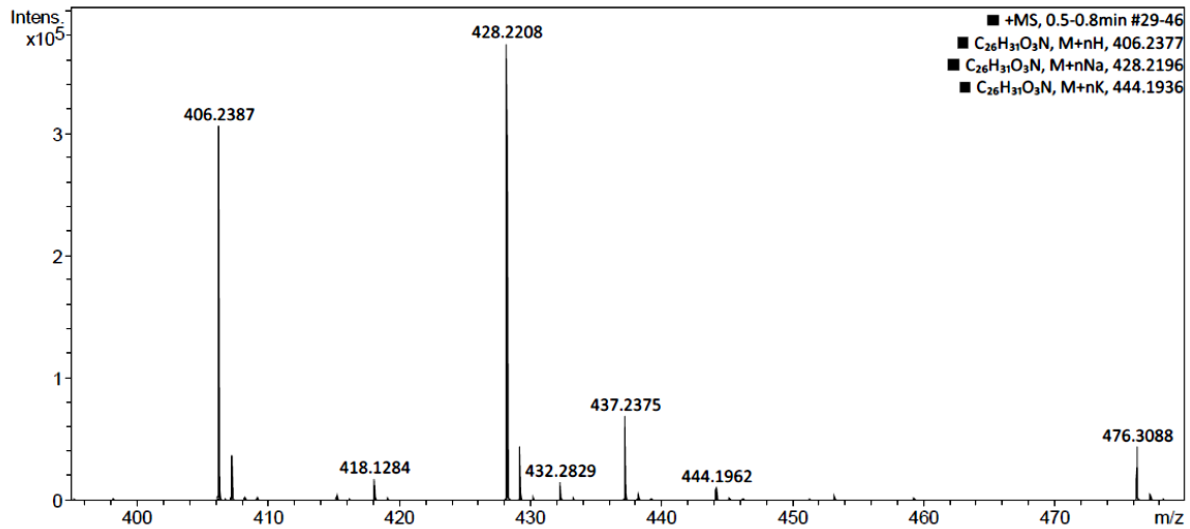
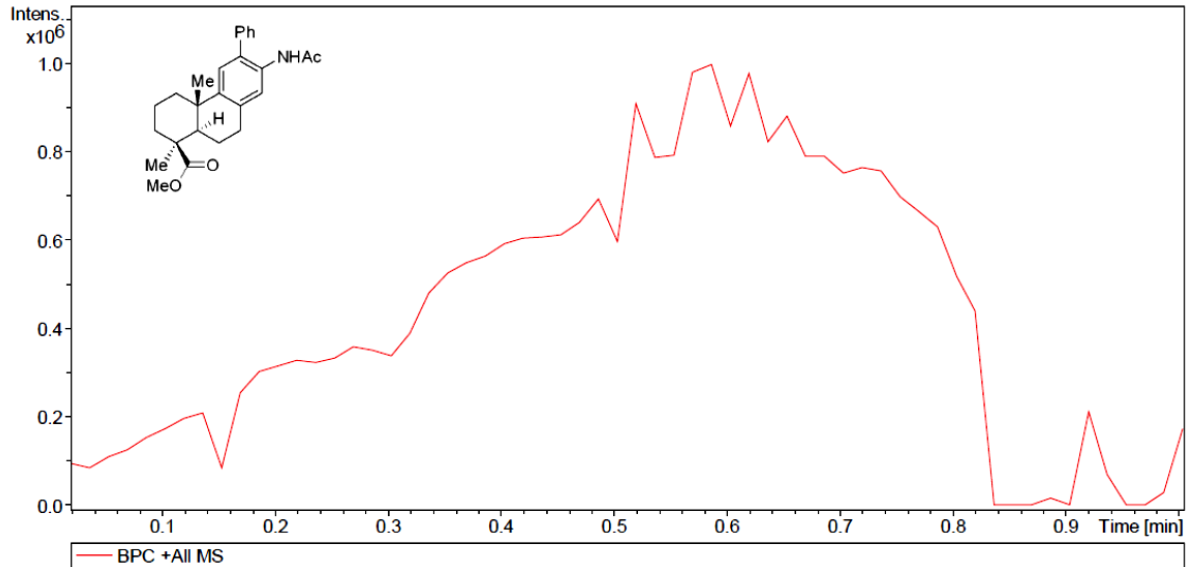
Analysis Name D:\Data\User data\2022\MAR\ab_mm_01_322.d
Method Tune_pos_Standard.m
Sample Name ab_mm_01_322
Comment signal dropping issue

Acquisition Date 3/21/2022 1:07:47 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_mm_01_322.d

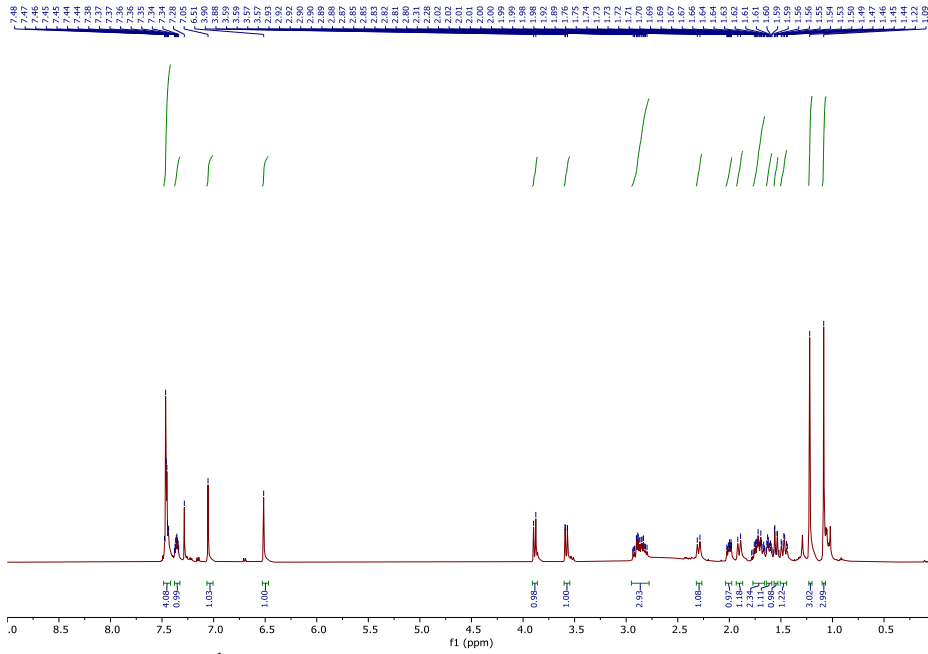
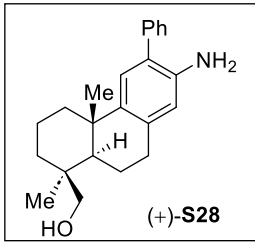
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printed: 3/21/2022 1:10:25 PM

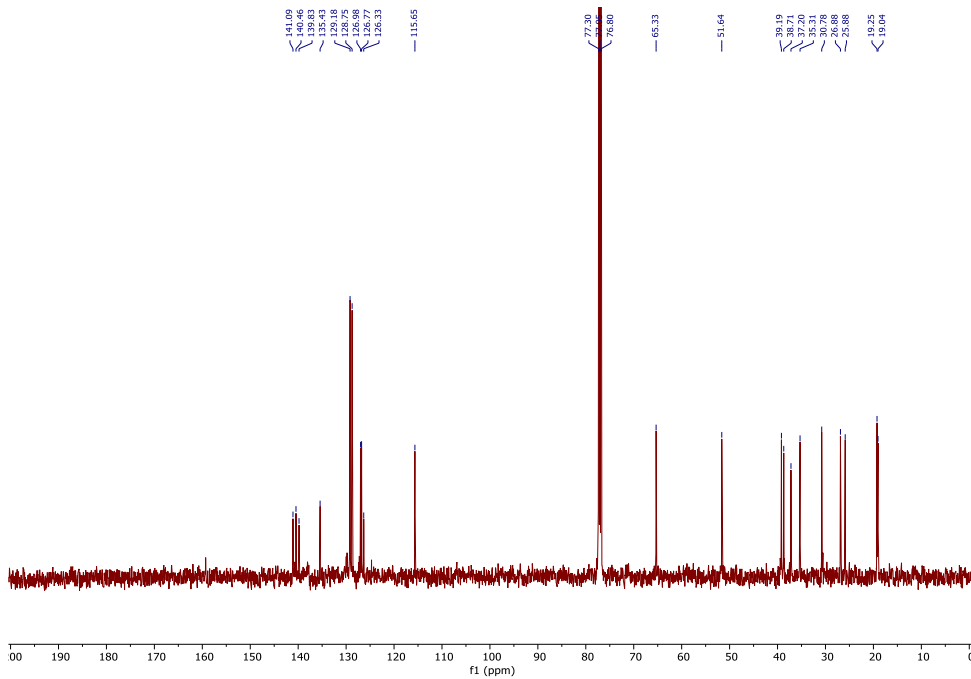
by: IISER Kolkata

Page 1 of 1

HRMS data of (+)-S27



¹H NMR (500 MHz, CDCl₃) of (+)-S28



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S28

Display Report

Analysis Info

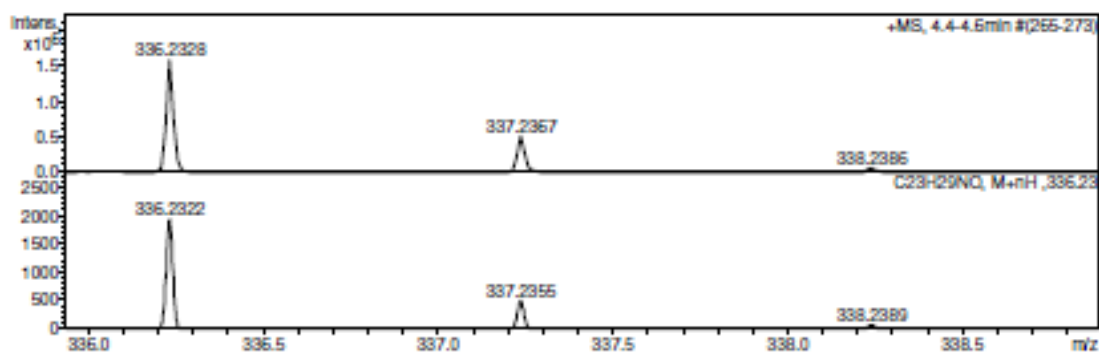
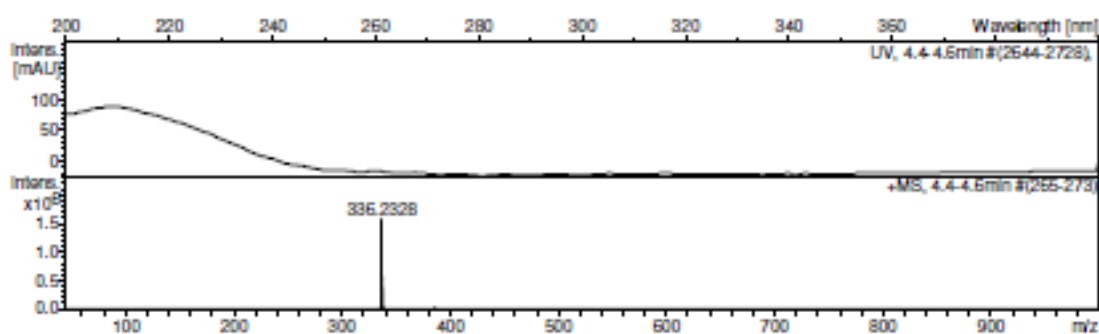
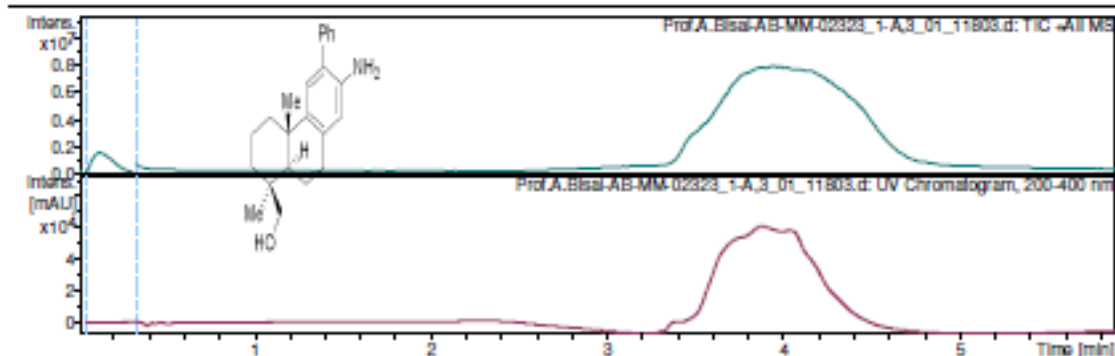
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Method	hrlcms-20 sept.m
Sample Name	Prof.A.Bisai-AB-MM-02323
Comment	

Acquisition Date 4/22/2022 12:30:09 PM

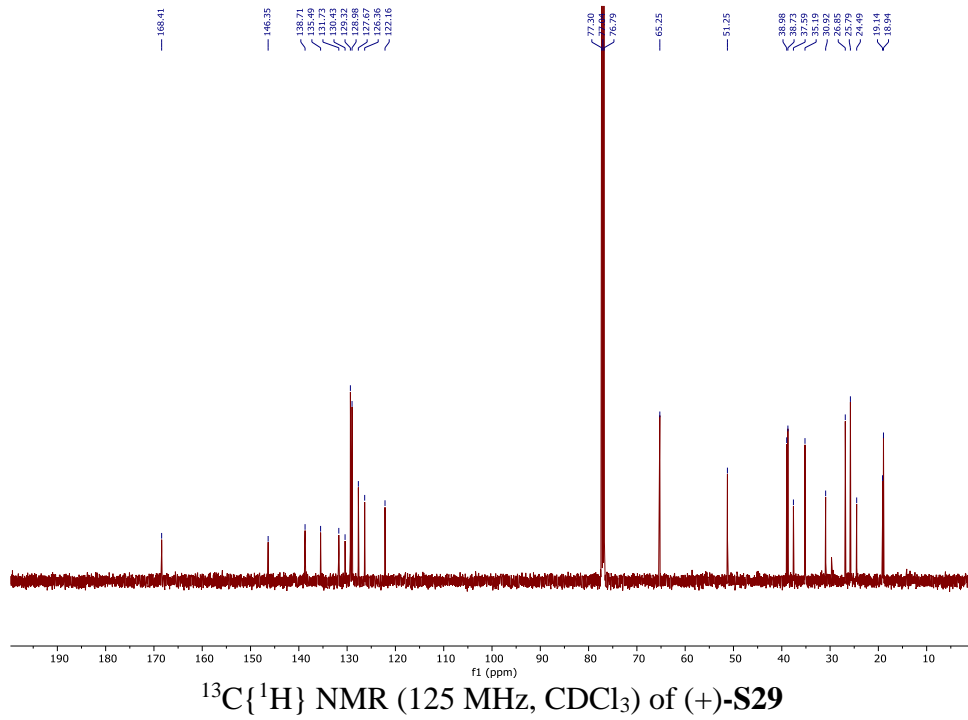
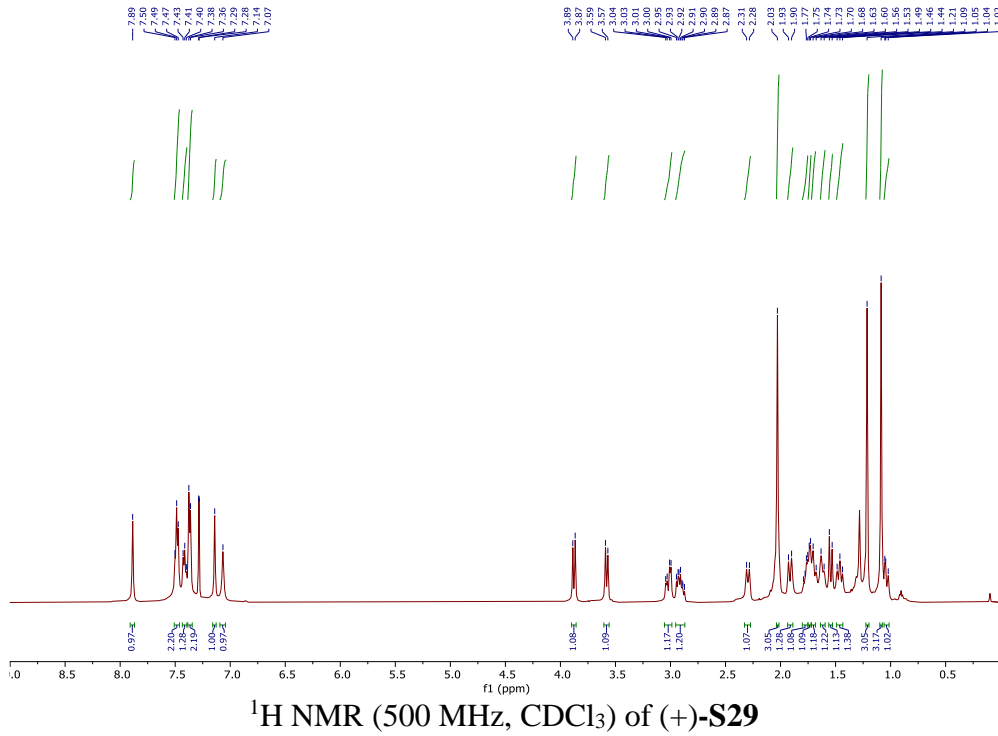
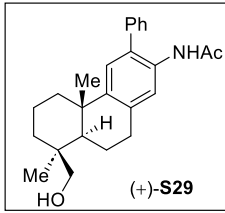
Operator RUCHI
Instrument micrOTOF-Q II 10330

Acquisition Parameter

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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



HRMS data of (+)-S28



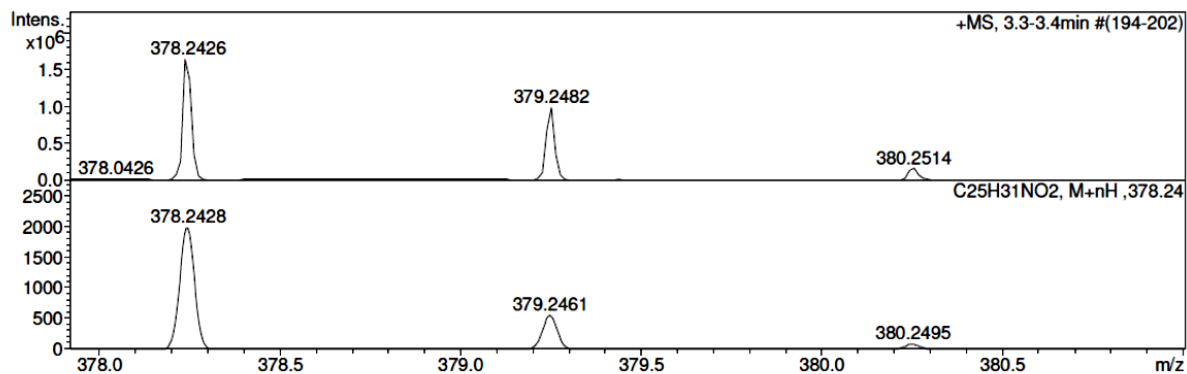
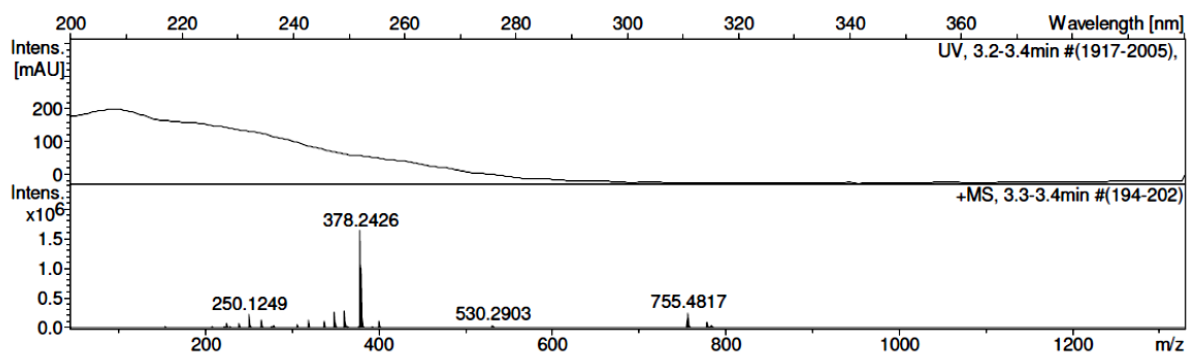
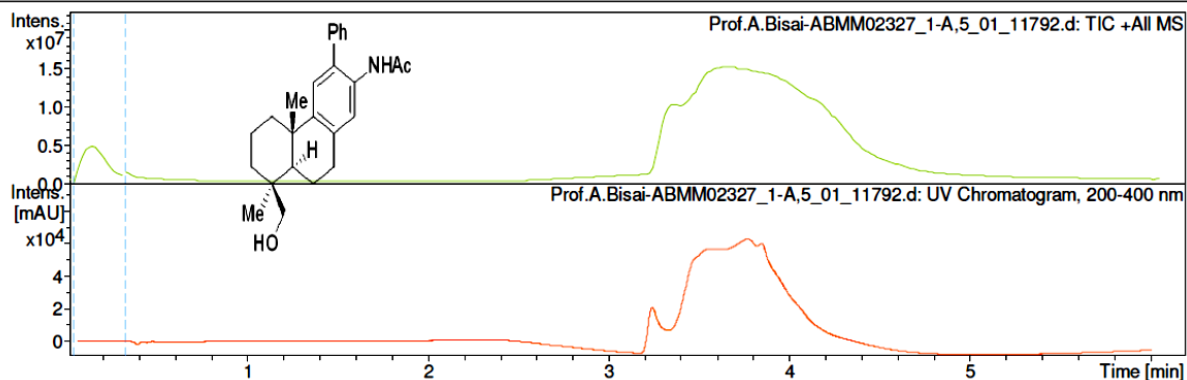
Display Report

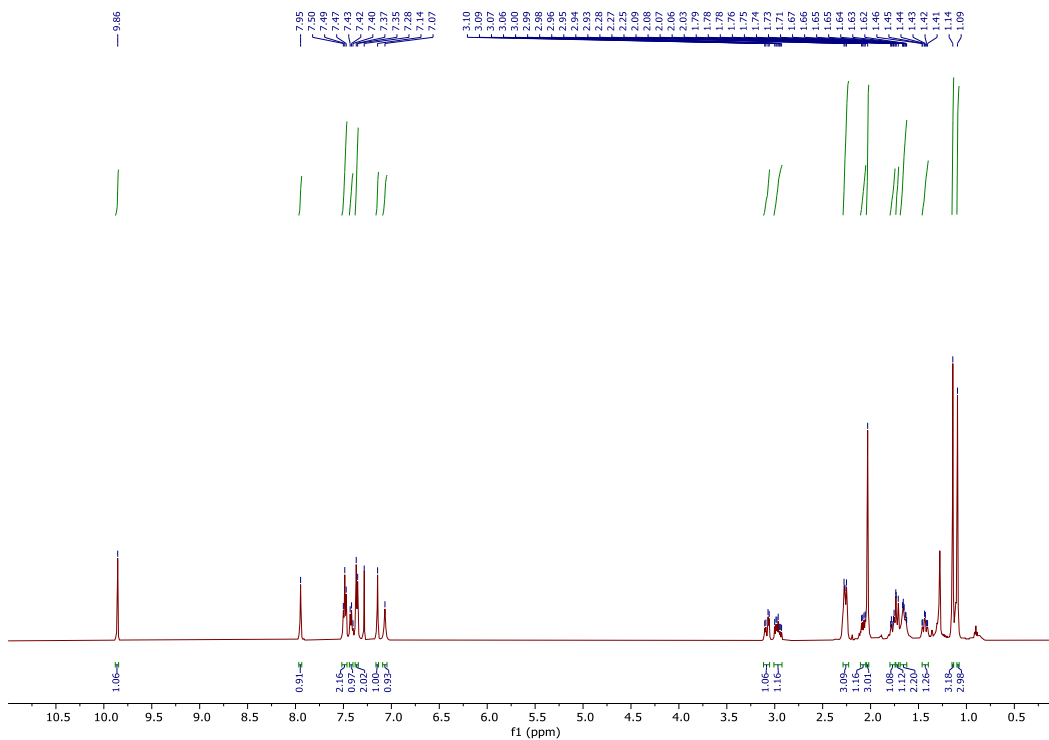
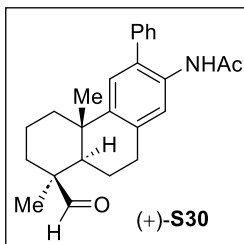
Analysis Info

Analysis Name D:\Data\NEW USER DATA 2022\April-2022\20-april\Prof.A.Bisai-ABMM02327_1-A,5_01_11792.d
Method hrlcms-20 sept.m
Sample Name Prof.A.Bisai-ABMM02327
Acquisition Date 4/20/2022 12:27:13 PM
Operator RUCHI
Instrument micrOTOF-Q II 10330
Comment

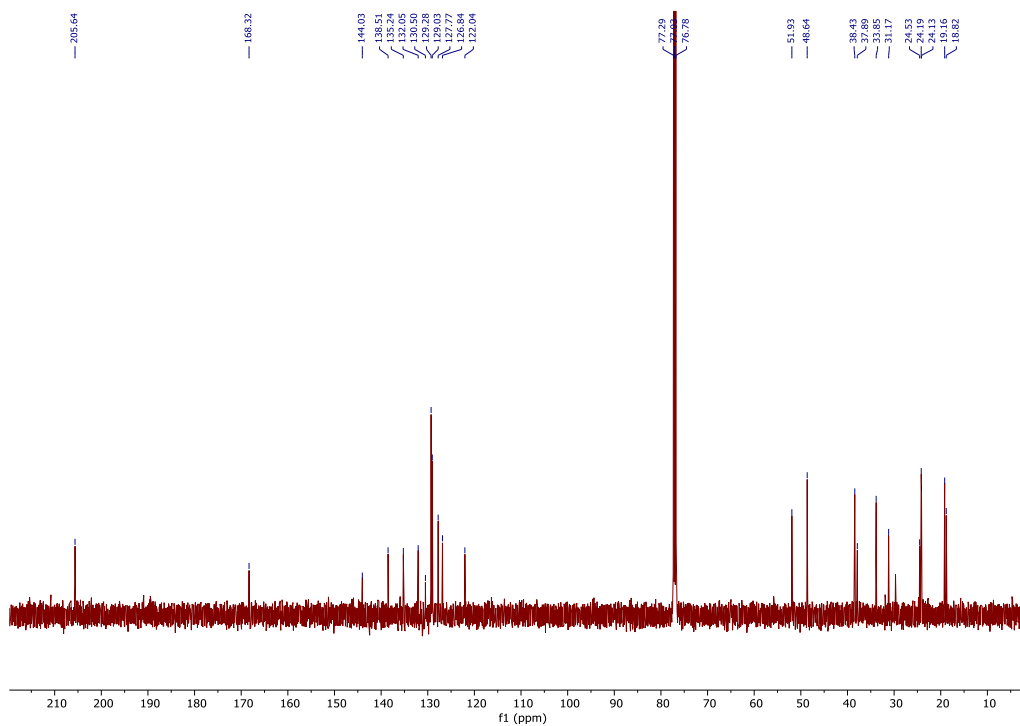
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
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Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

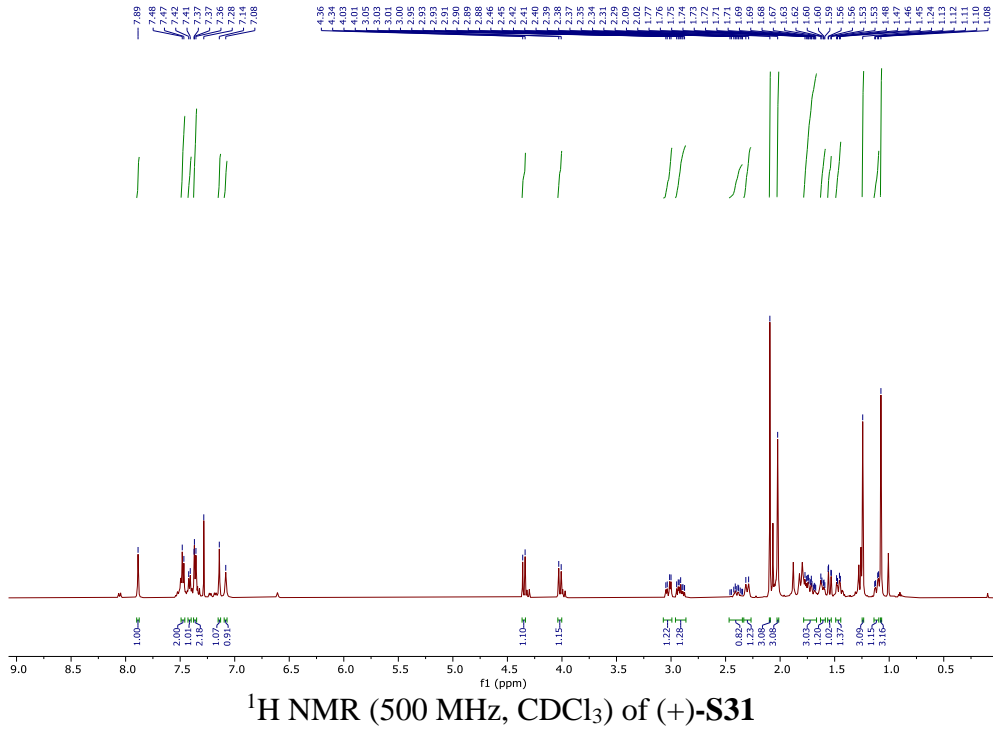
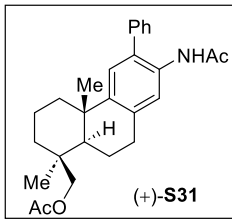




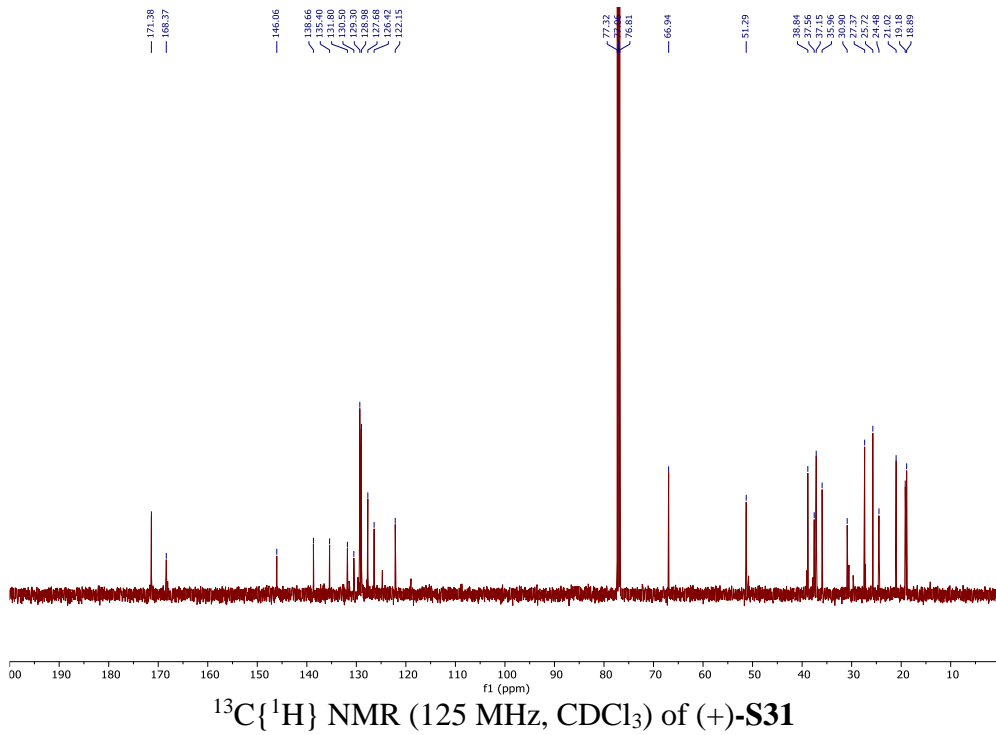
$^1\text{H NMR}$ (500 MHz, CDCl_3) of (+)-S30



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-S30



^1H NMR (500 MHz, CDCl_3) of (+)-S31



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-S31

Display Report

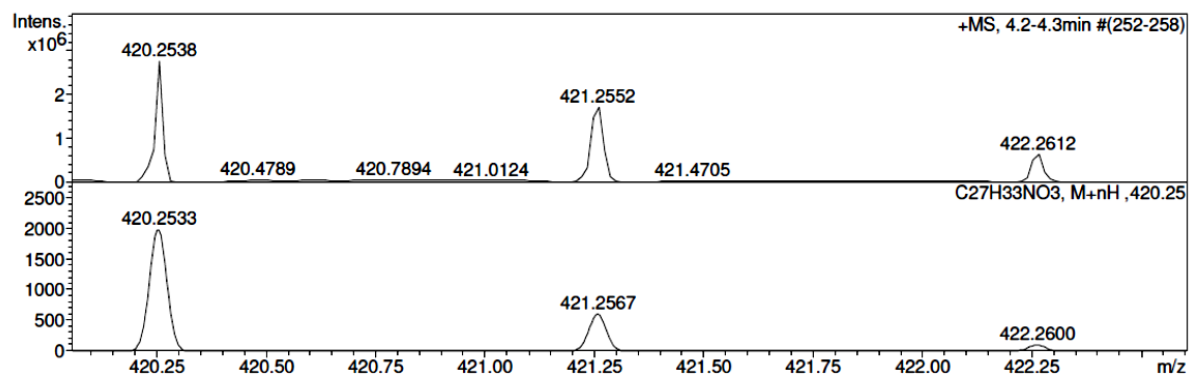
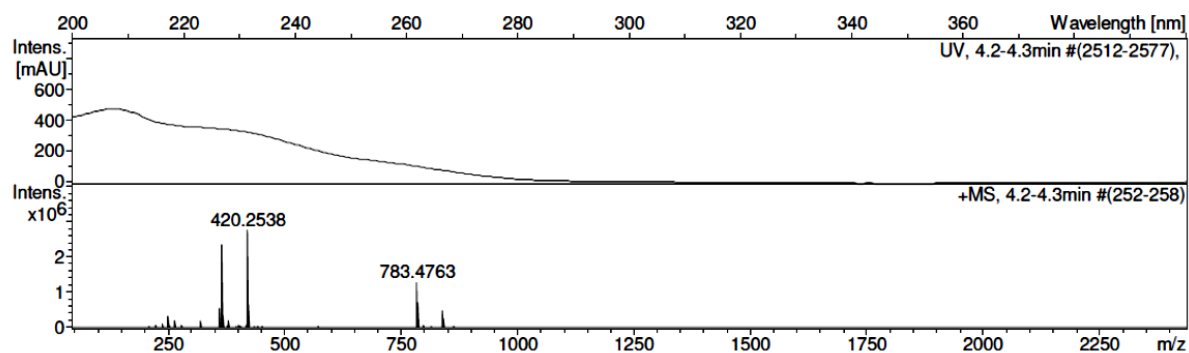
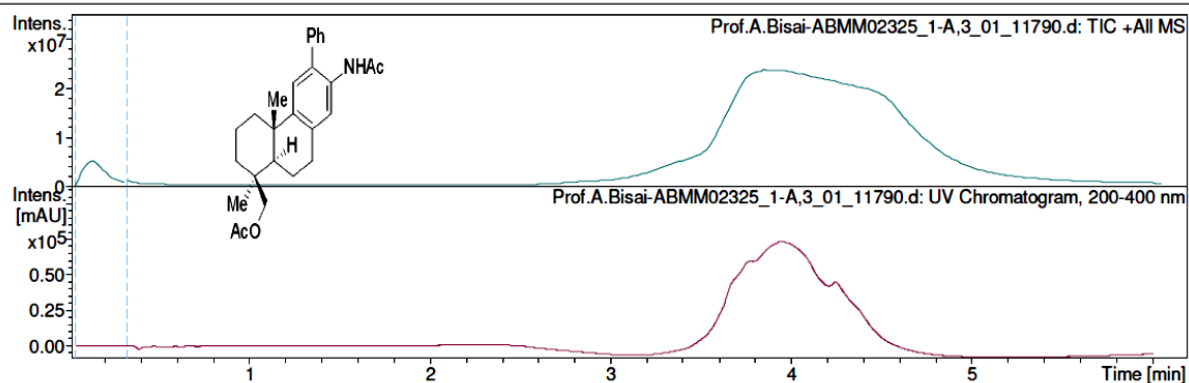
Analysis Info

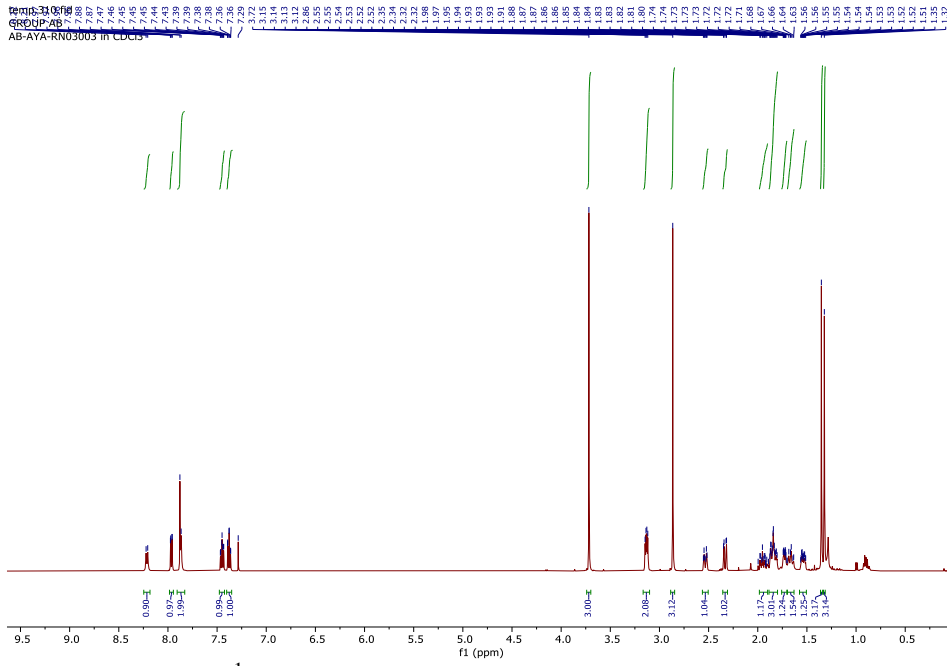
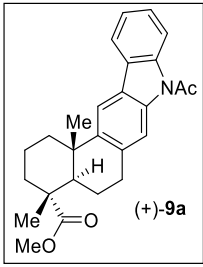
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Method hrlcms-20 sept.m
Sample Name Prof.A.Bisai-ABMM02325
Comment

Acquisition Date 4/20/2022 12:12:52 PM
Operator RUCHI
Instrument micrOTOF-Q II 10330

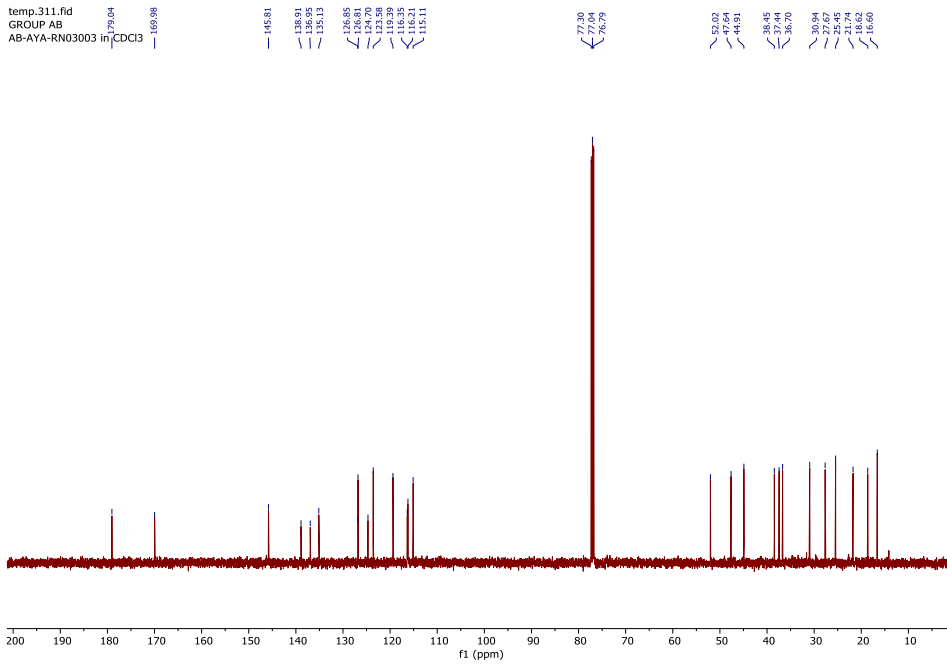
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

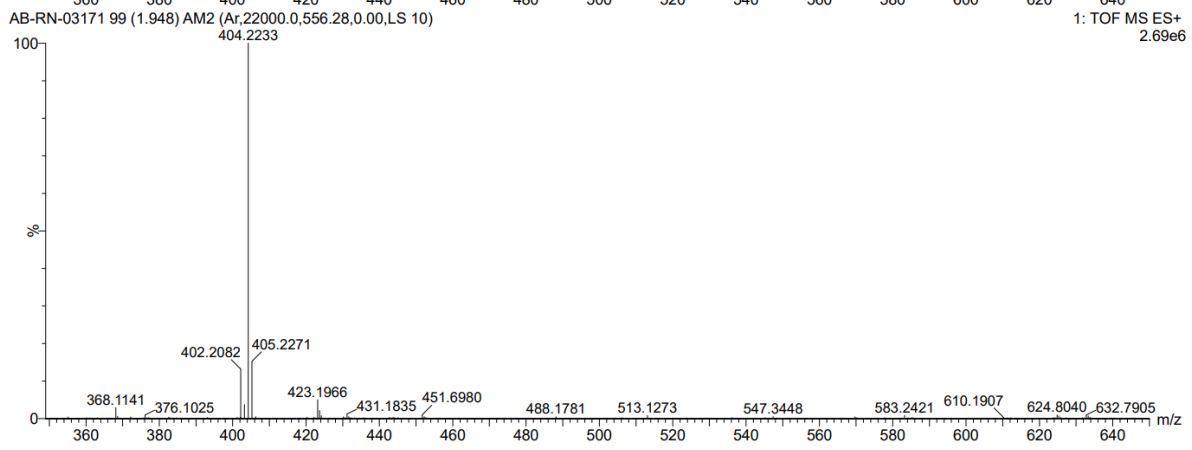
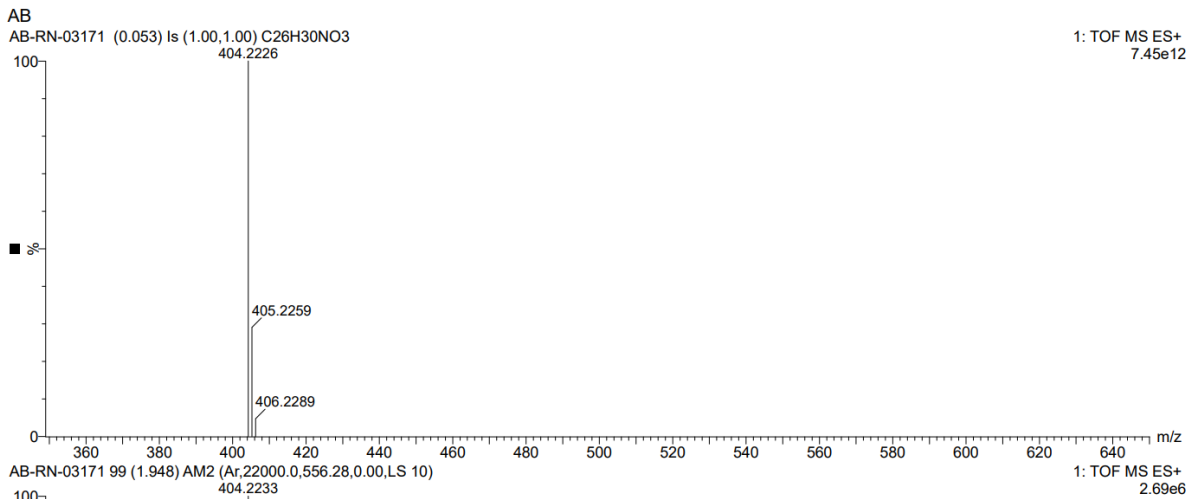




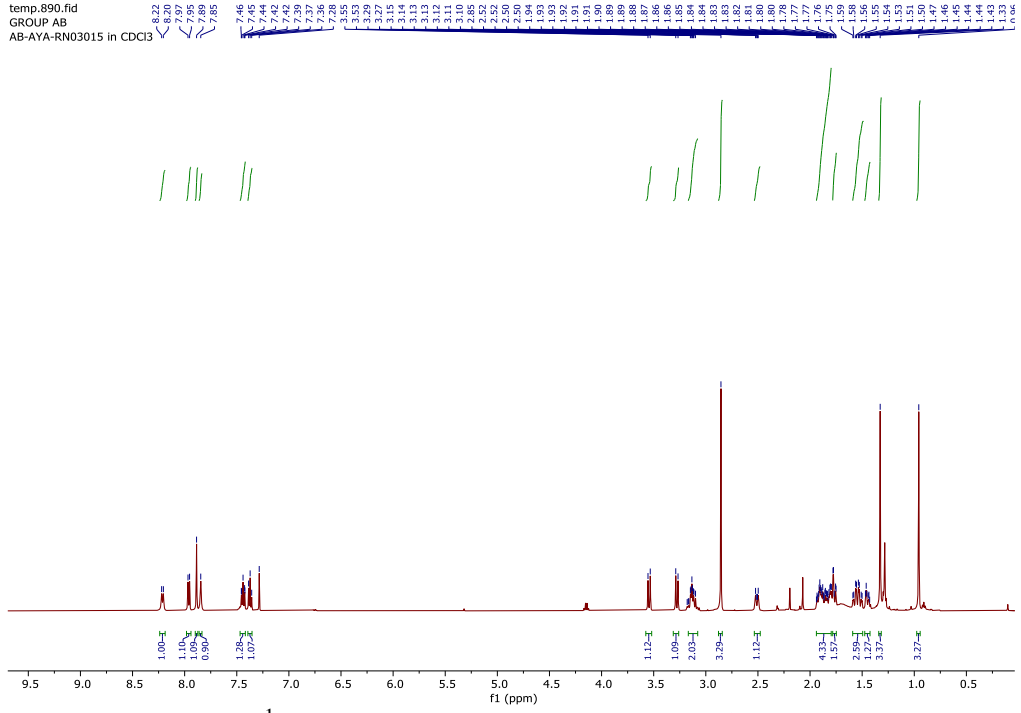
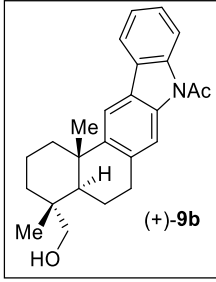
¹H NMR (500 MHz, CDCl₃) of (+)-9a



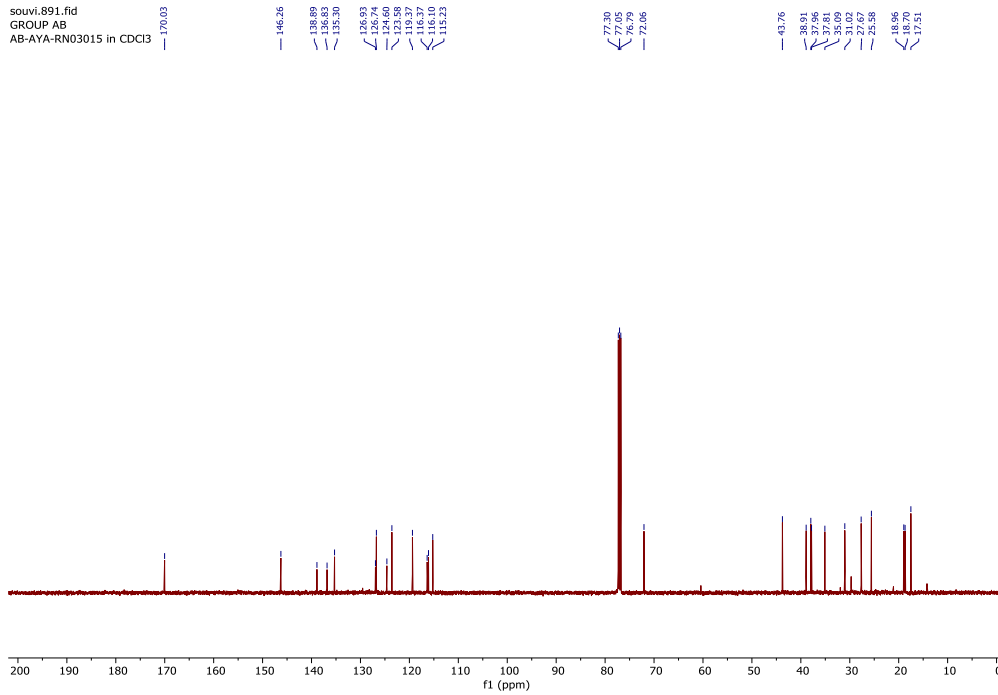
¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-9a



HRMS data of (+)-**9a**



¹H NMR (500 MHz, CDCl₃) of (+)-**9b**



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-**9b**

Display Report

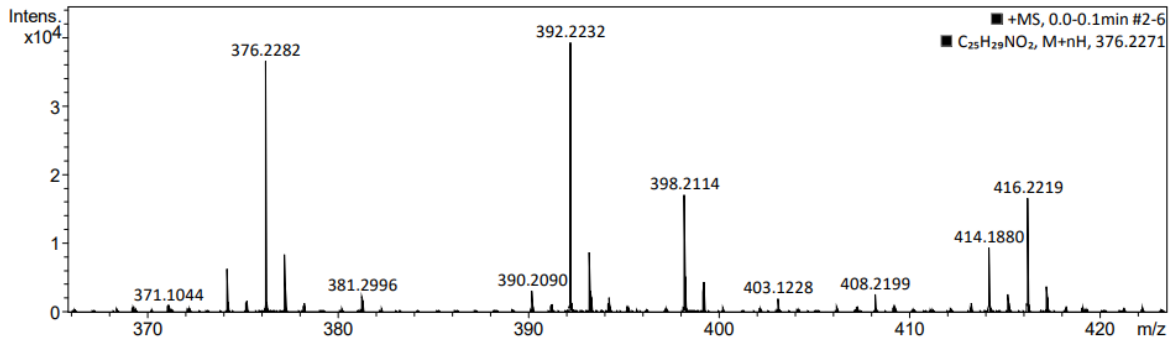
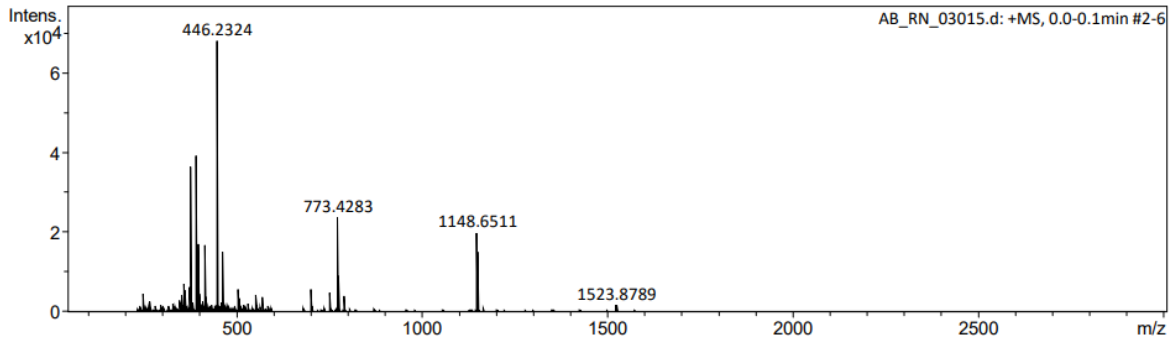
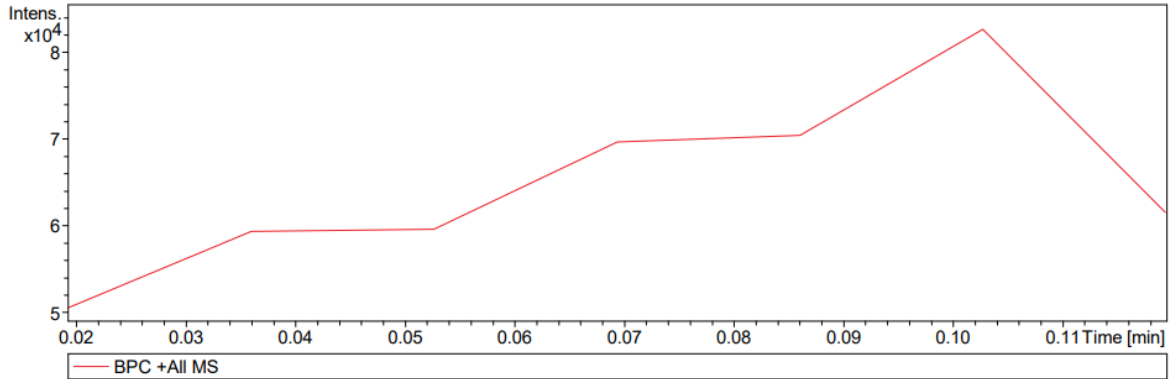
Analysis Info

Analysis Name D:\Data\User data\2022\MAR\AB_RN_03015.d
Method Tune_pos_Mid.m
Sample Name AB_RN_03015
Comment signal dropping issue

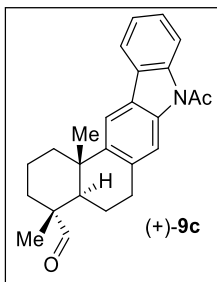
Acquisition Date 3/17/2022 7:56:10 PM
Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

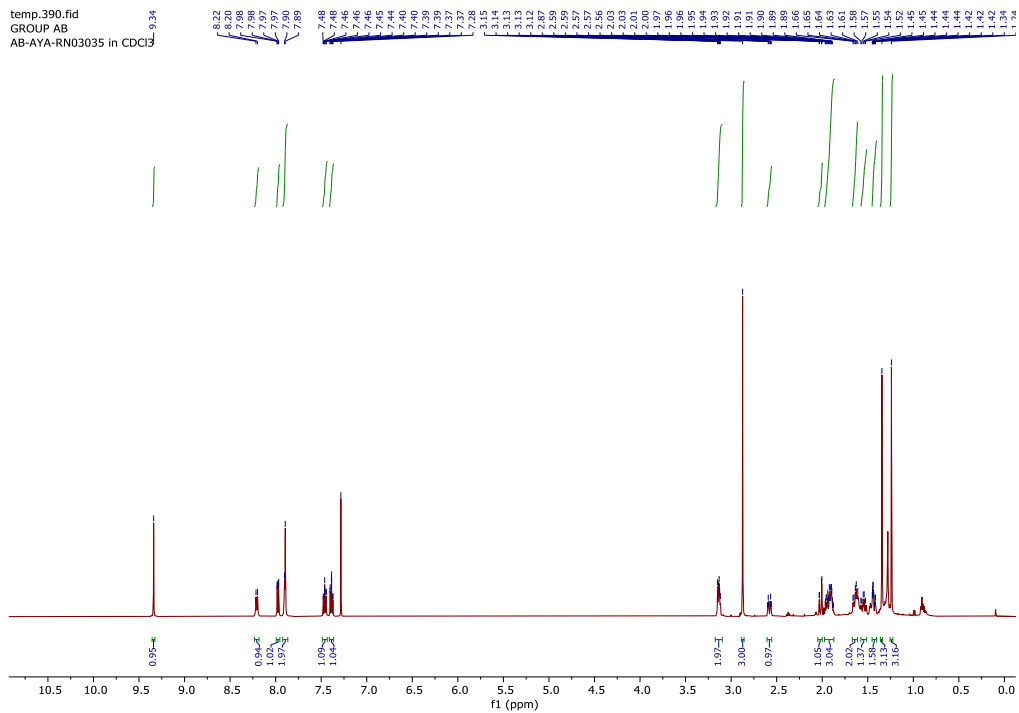
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



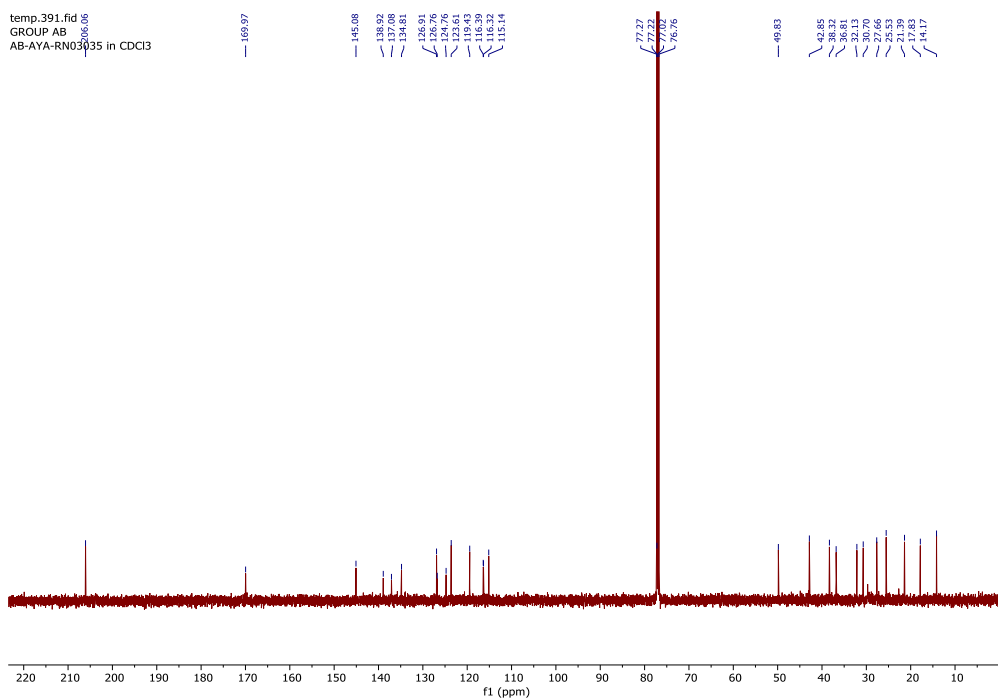
HRMS data of (+)-**9b**



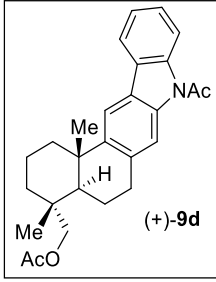
temp.390.fid
GROUP AB
AB-AYA-RN03035 in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-**9c**



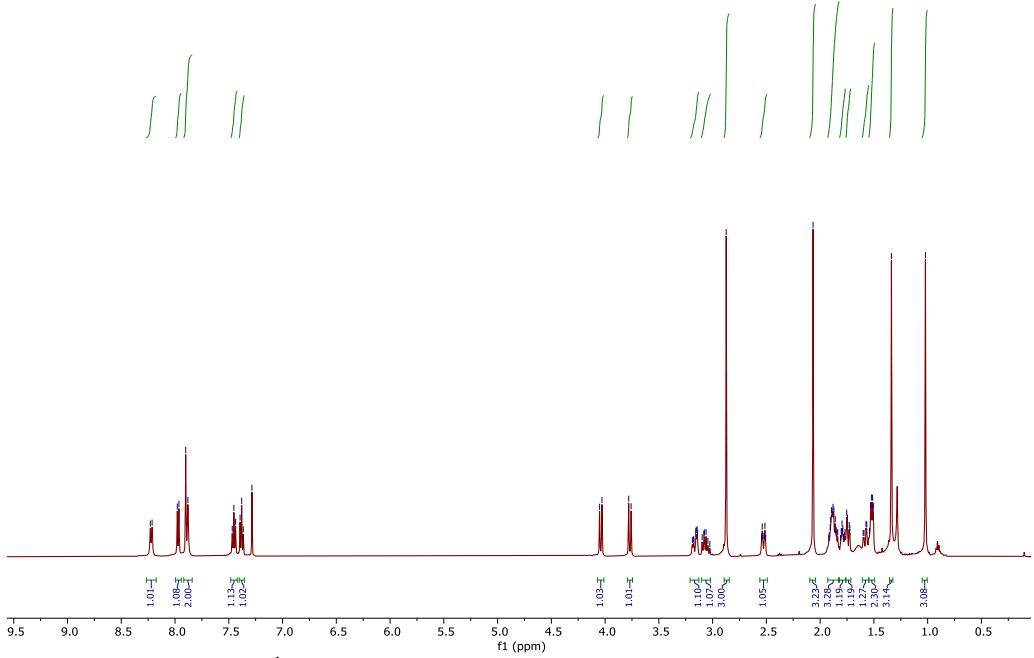
¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-**9c**



temp.910.fid
GROUP AB
AB-AYA-RN03018 in CDCl₃

8.23
8.11
7.98
7.96
7.90
7.85
7.87
7.45
7.44
7.38
7.37
7.28

4.03
3.78
3.76
3.19
3.18
3.17
3.16
3.15
3.14
3.14
3.08
3.08
3.06
3.04
3.03
2.87
2.55
2.53
2.52
2.51
2.07
1.92
1.92
1.91
1.91
1.89
1.89
1.88
1.87
1.86
1.85
1.84
1.84
1.81
1.81
1.80
1.79
1.78
1.78
1.77
1.77
1.75
1.75
1.72
1.60
1.59
1.57
1.57
1.54
1.53
1.51
1.51
1.44
1.44
1.02



¹H NMR (500 MHz, CDCl₃) of (+)-9d

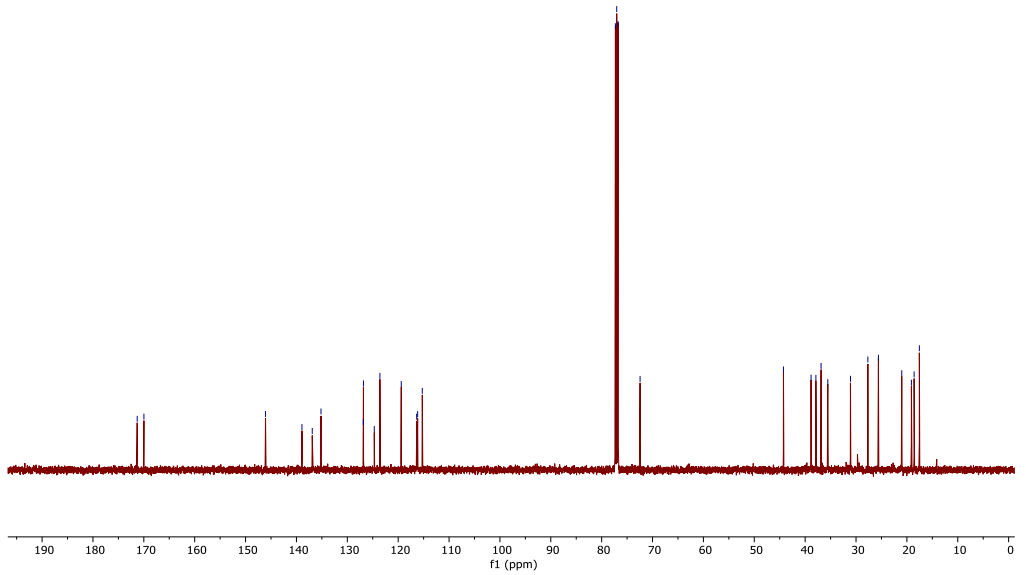
temp.911.fid
GROUP AB
AB-AYA-RN03018 in CDCl₃

171.30
169.26

146.08
138.92
136.89
135.18
126.86
124.70
124.69
119.90
116.37
116.17
115.26

77.30
77.29
77.25

44.27
38.84
37.89
36.87
31.09
27.67
25.60
19.11
18.58
17.55



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-9d

Display Report

Analysis Info

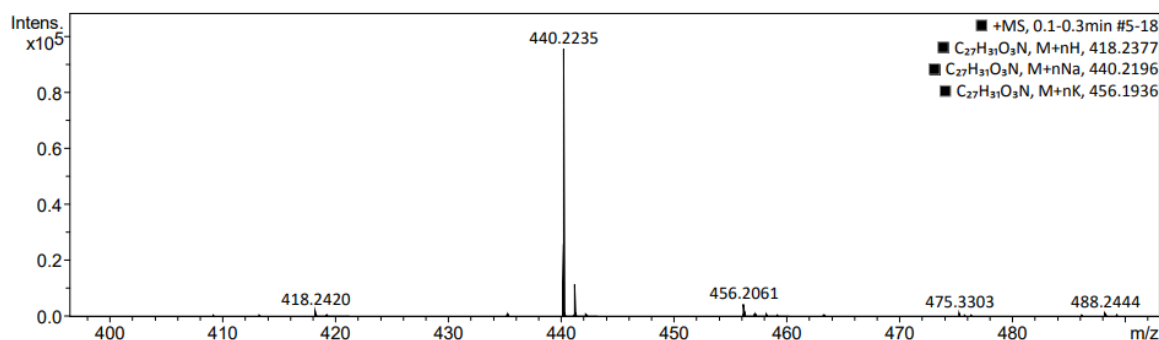
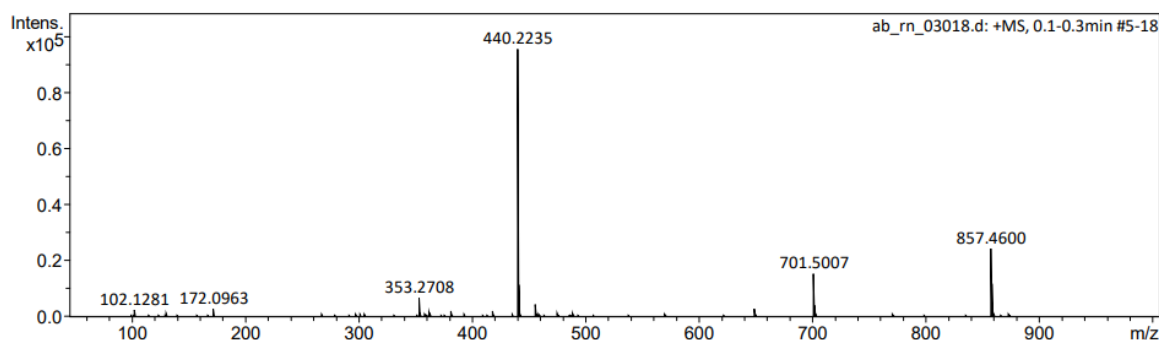
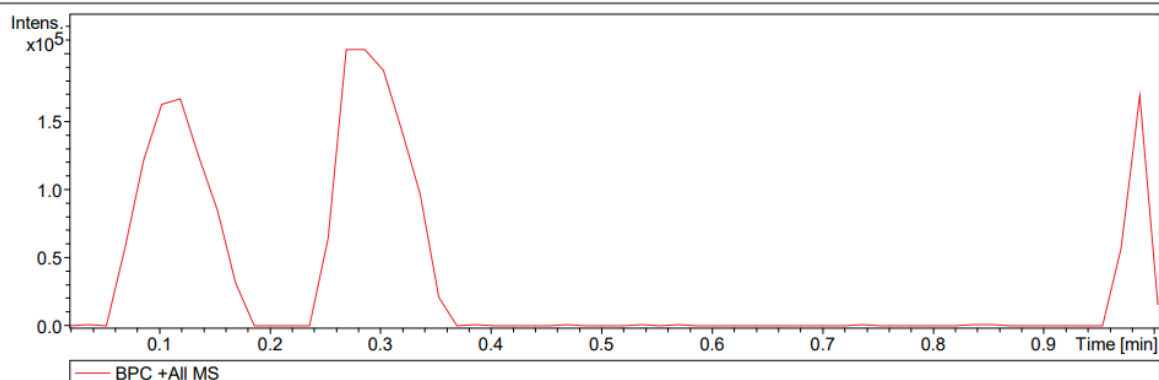
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Method Tune_pos_Standard.m
Sample Name ab_m_03018
Comment signal dropping issue

Acquisition Date 3/21/2022 11:56:58 AM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_m_03018.d

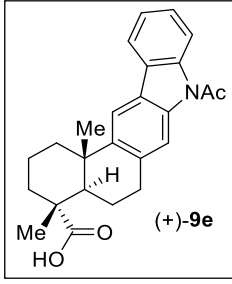
Bruker Compass DataAnalysis 4.1

printed: 3/21/2022 12:05:16 PM

by: IISER Kolkata

Page 1 of 1

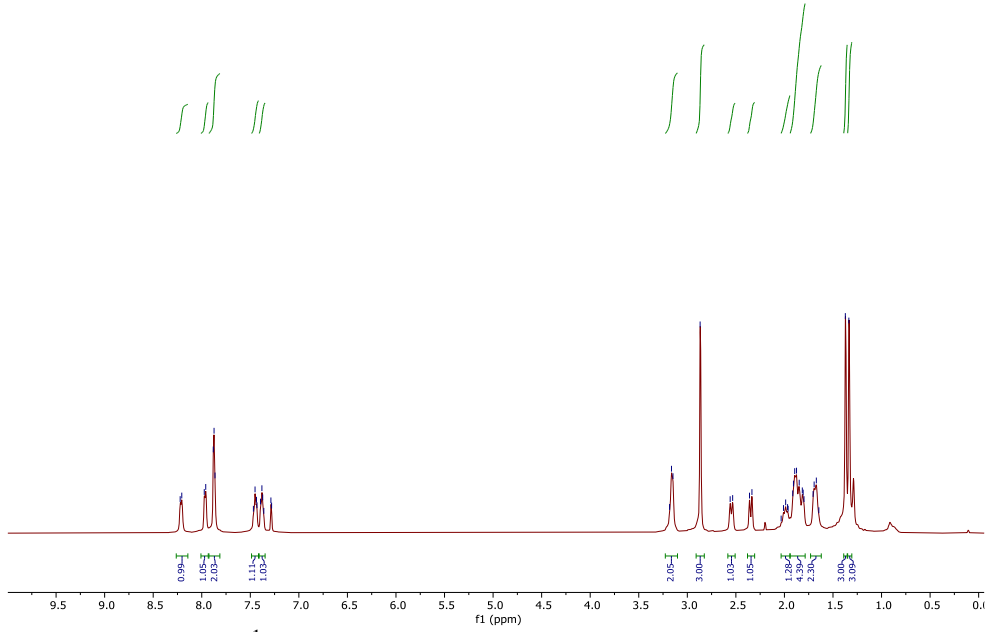
HRMS data of (+)-**9d**



temp.740.fid
GROUP AB
AB-AYA-RN03040R in CDCl₃

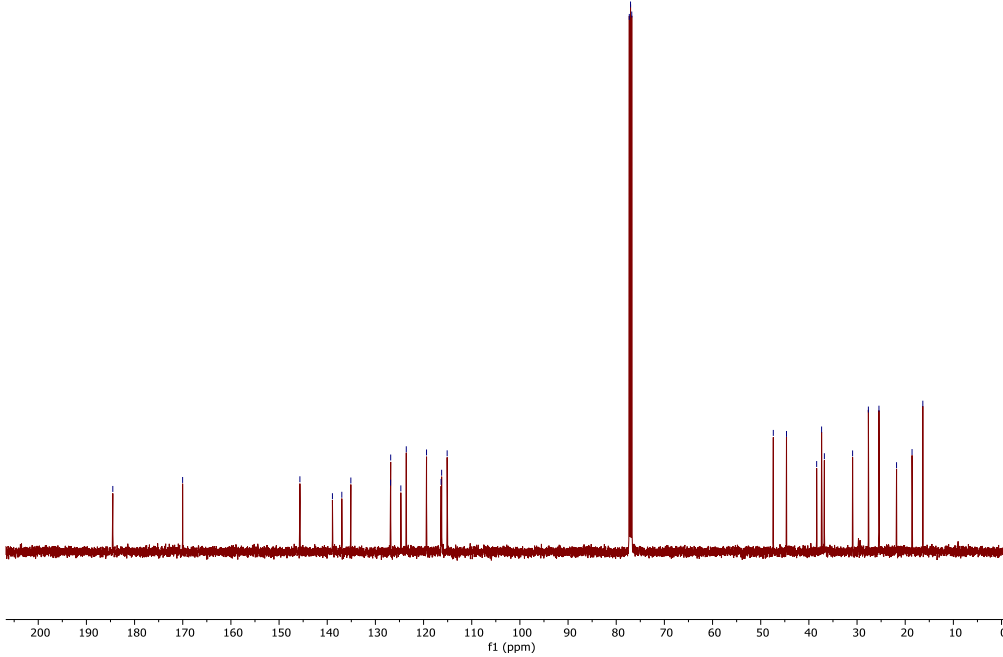
8.22
7.97
7.97
7.88
7.87
7.66
7.67
7.45
7.44
7.40
7.38
7.36
7.29
7.28

3.18
3.15
2.87
2.56
2.56
2.36
2.33
2.33
2.01
1.99
1.97
1.91
1.91
1.88
1.85
1.81
1.80
1.70
1.67
1.65
1.34



temp.741.fid
GROUP AB
AB-AYA-RN03040R in CDCl₃

170.03
145.68
138.92
136.97
135.10
126.85
126.82
126.66
123.72
119.39
116.36
115.40
77.28
77.03
76.78
47.38
44.65
38.39
37.36
36.78
30.03
27.64
25.45
18.90
15.34



Display Report

Analysis Info

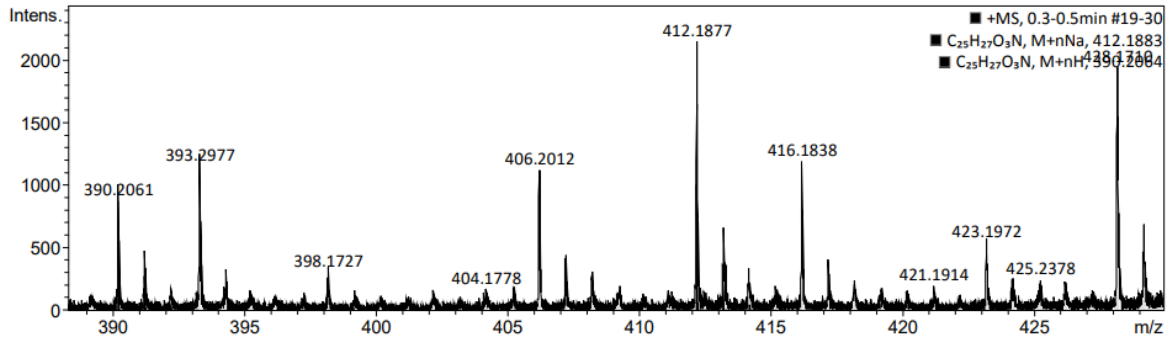
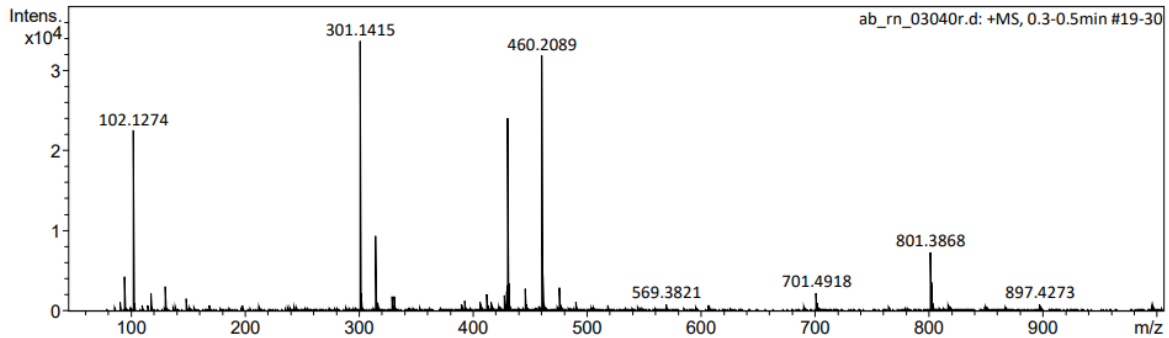
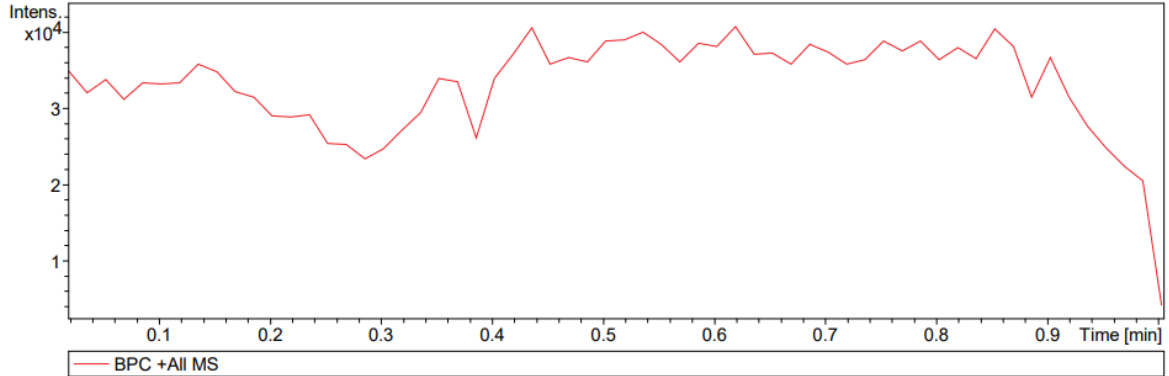
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Method Tune_pos_Standard.m
Sample Name AB_RN_03040r
Comment

Acquisition Date 4/18/2022 12:59:53 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_rn_03040r.d

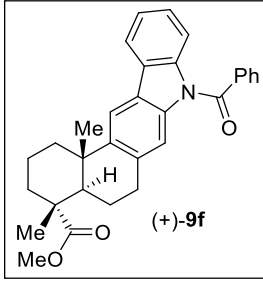
Bruker Compass DataAnalysis 4.1

printed: 4/18/2022 1:02:34 PM

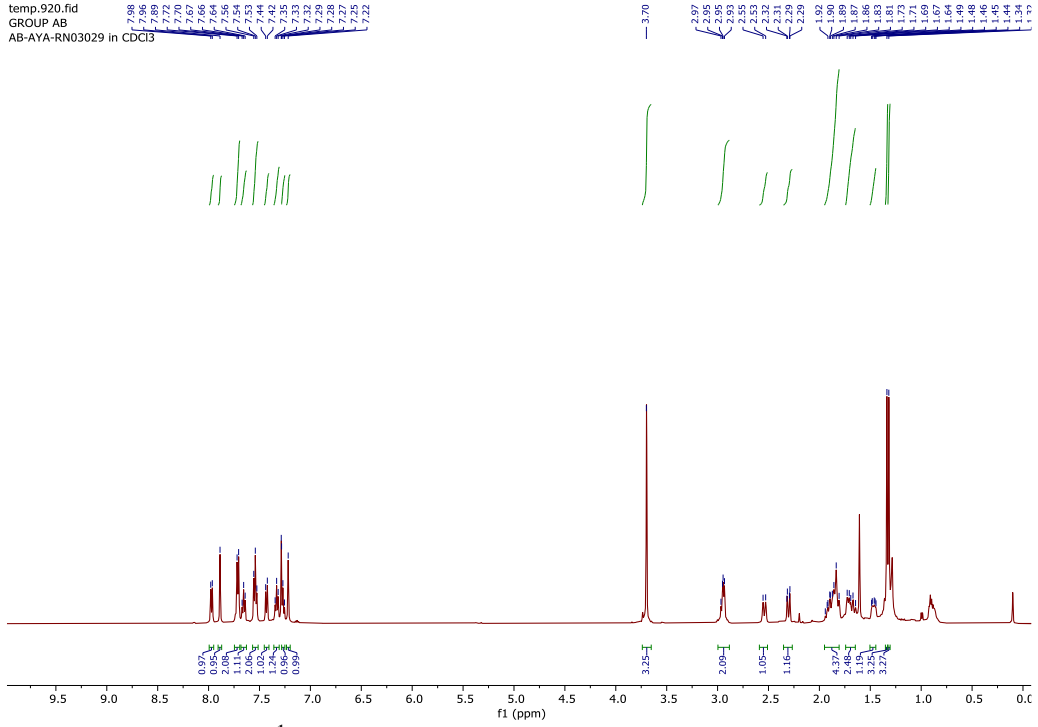
by: IISER Kolkata

Page 1 of 1

HRMS data of (+)-**9e**

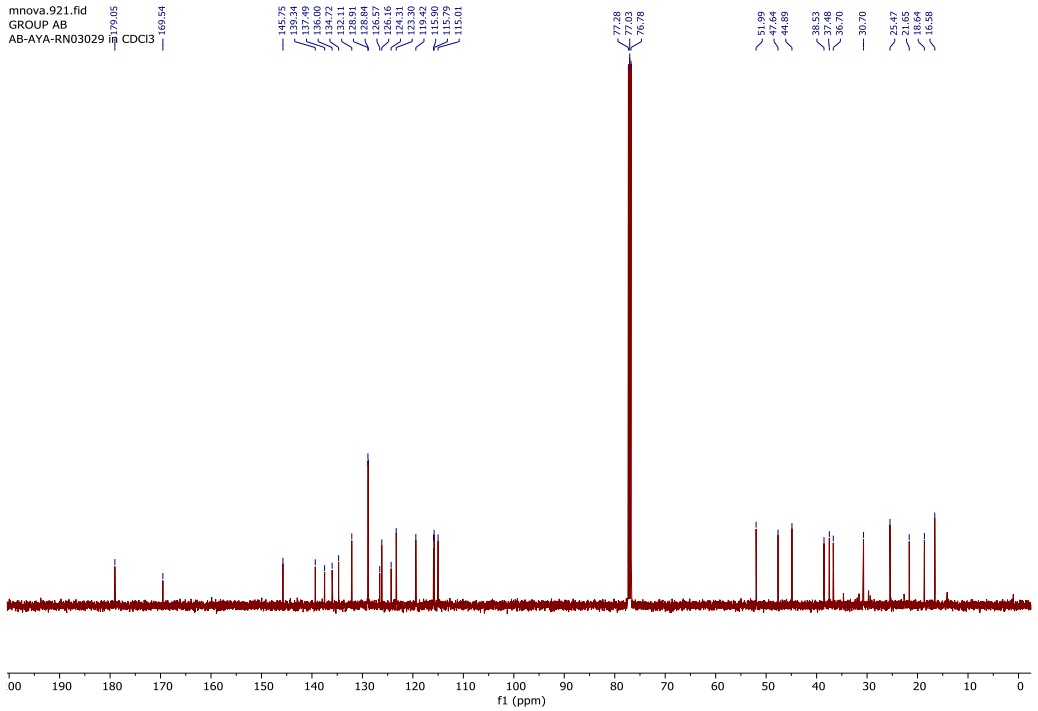


temp.920.fid
GROUP AB
AB-AYA-RN03029 in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-**9f**

mnova.921.fid
GROUP AB
AB-AYA-RN03029 in CDCl₃



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-**9f**

Display Report

Analysis Info

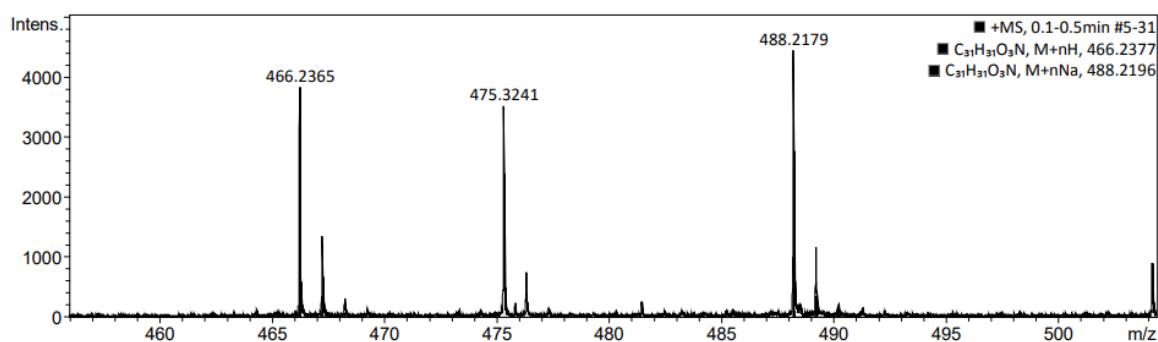
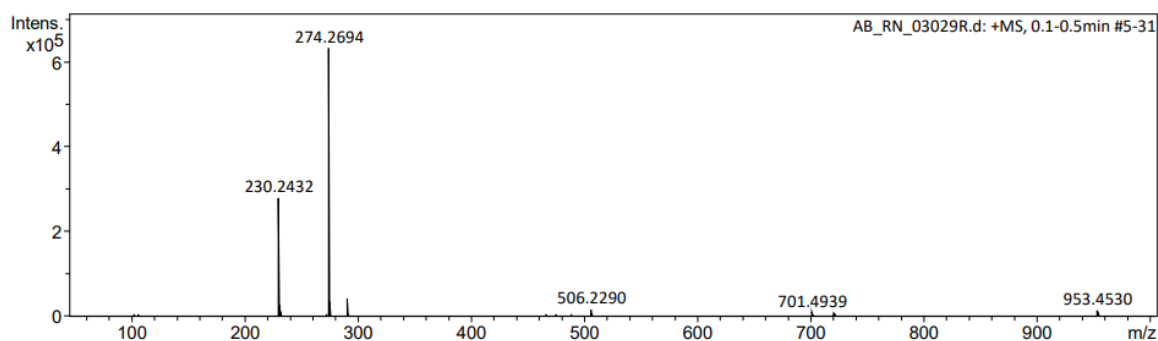
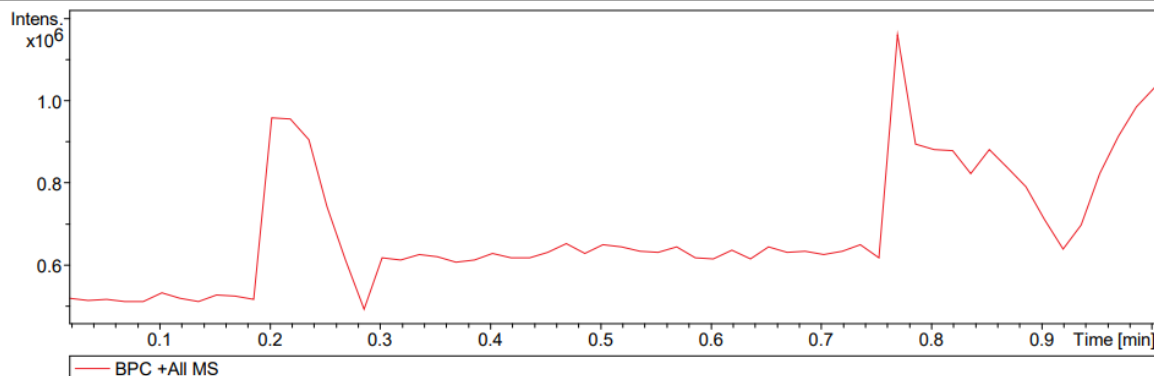
Analysis Name D:\Data\User data\2022\MAR\AB_RN_03029R.d
Method Tune_pos_Standard.m
Sample Name ab_m_03029R
Comment

Acquisition Date 3/31/2022 12:30:12 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



AB_RN_03029R.d

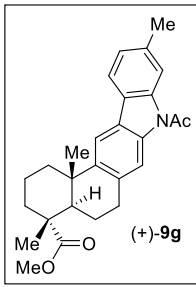
Bruker Compass DataAnalysis 4.1

printed: 3/31/2022 12:34:35 PM

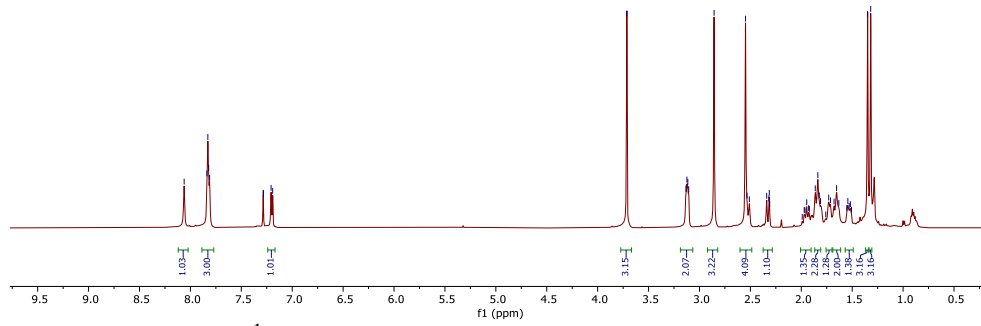
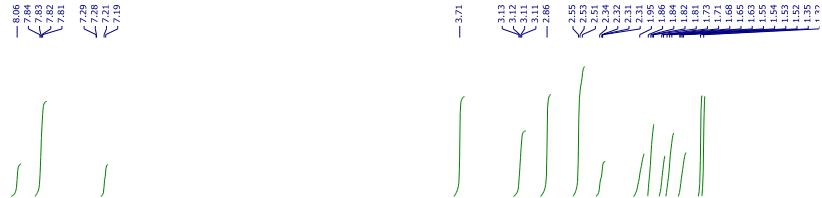
by: IISER Kolkata

Page 1 of 1

HRMS data of (+)-**9f**

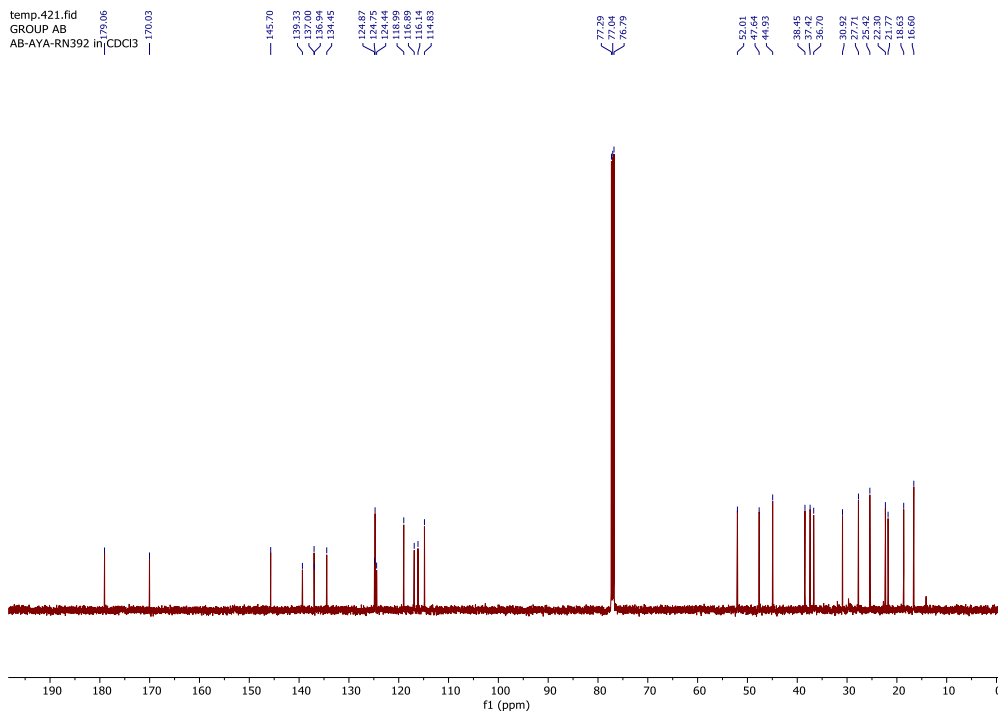


temp.420.fid
GROUP AB
AB-AYA-RN392 in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-**9g**

temp.421.fid
GROUP AB
AB-AYA-RN392 in CDCl₃



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-**9g**

Display Report

Analysis Info

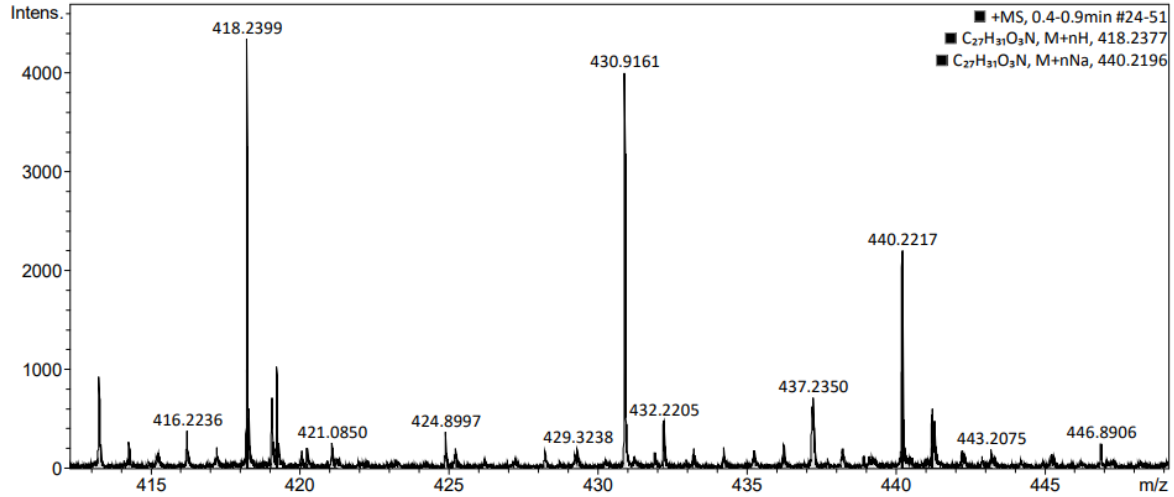
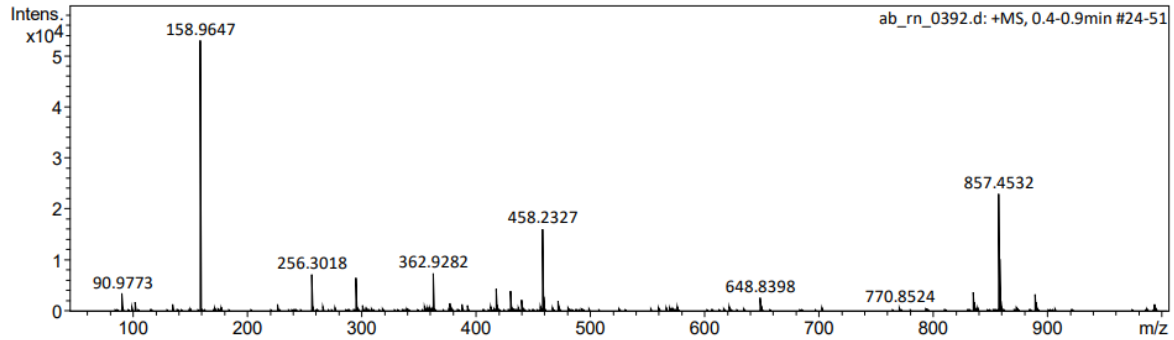
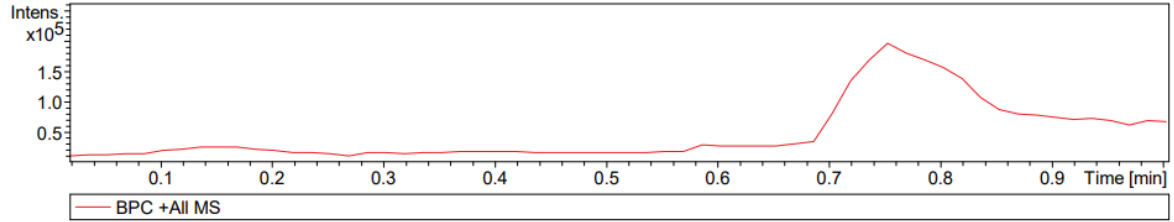
Analysis Name D:\Data\User data\2022\MAR\lab_m_0392.d
Method Tune_pos_Standard.m
Sample Name ab_m_0392
Comment signal dropping issue

Acquisition Date 3/16/2022 11:30:47 AM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_m_0392.d

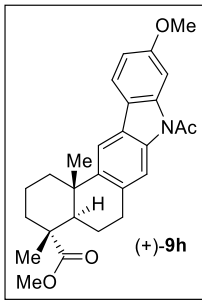
Bruker Compass DataAnalysis 4.1

printed: 3/16/2022 11:35:34 AM

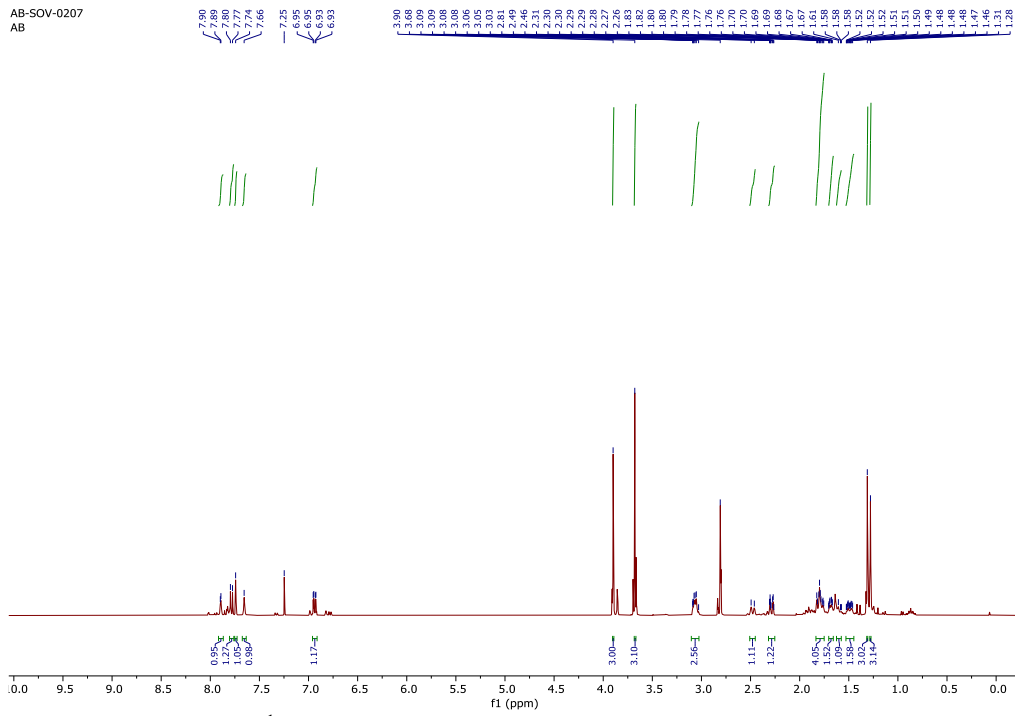
by: IISER Kolkata

Page 1 of 1

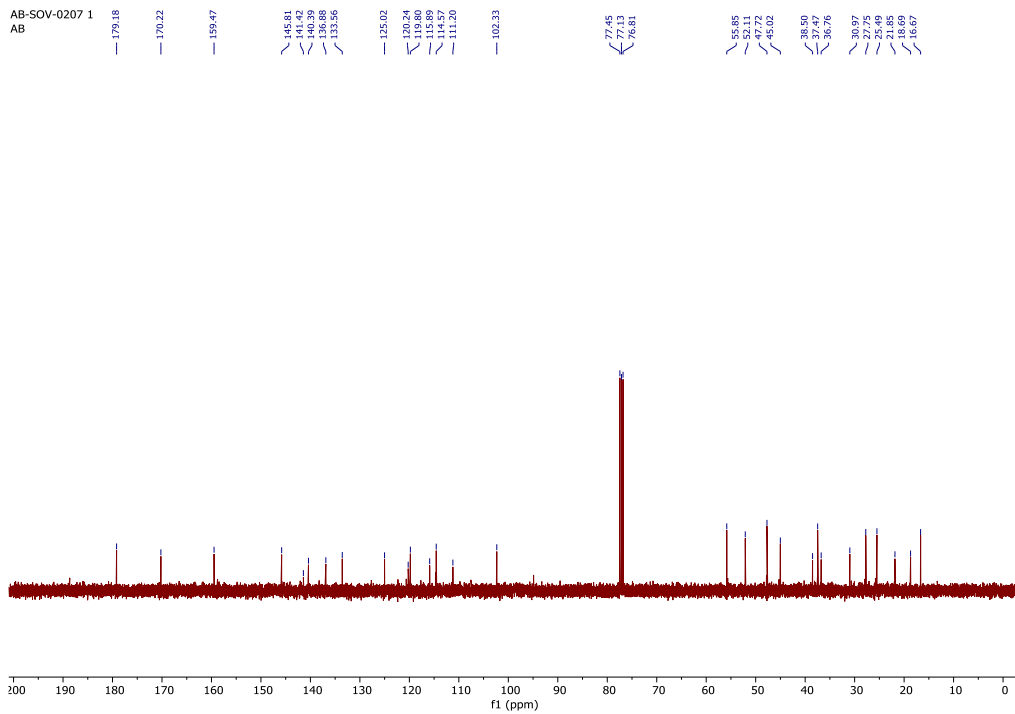
HRMS data of (+)-**9g**



AB-SOV-0207
AB



AB-SOV-0207 1
AB

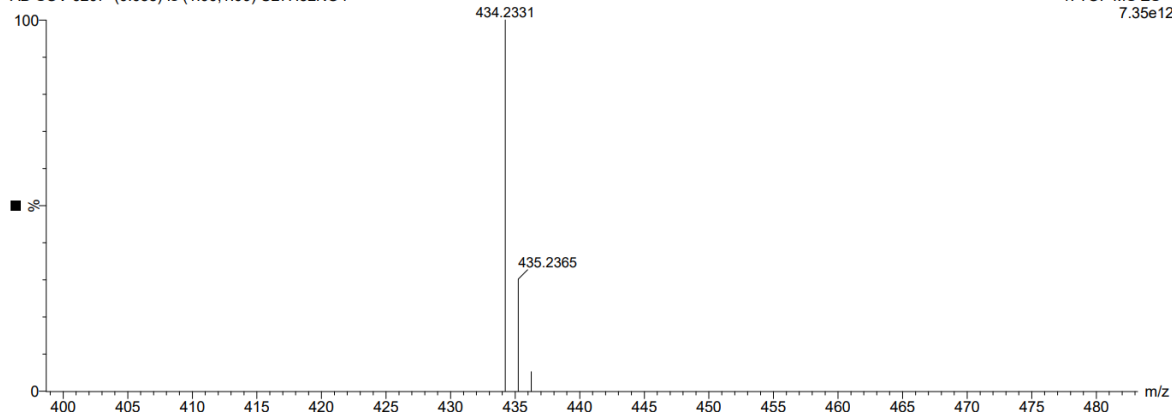


AB28-Mar-2024 12:41:02

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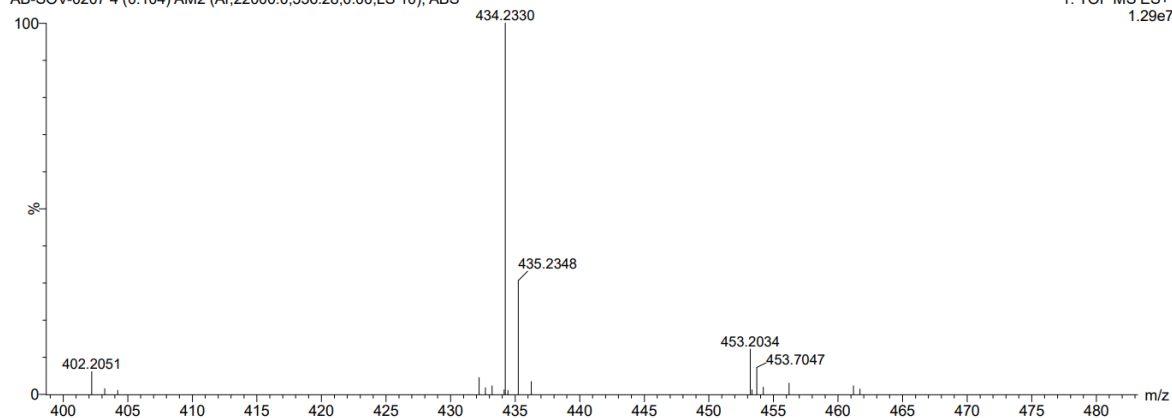
IISER - KOLKATA

1: TOF MS ES+
7.35e12

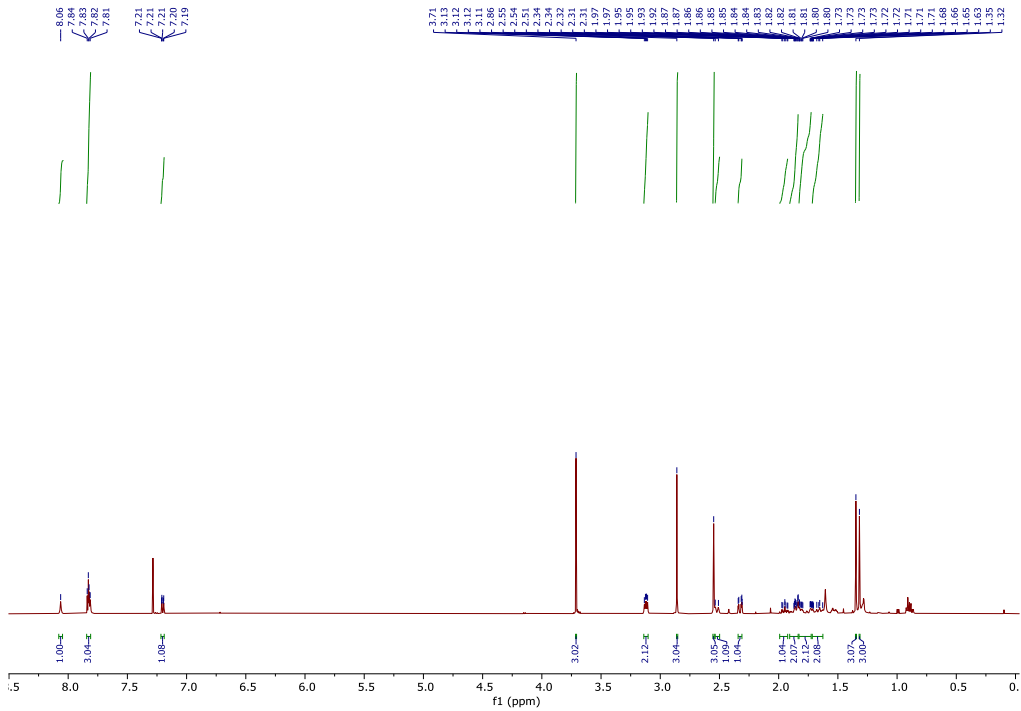
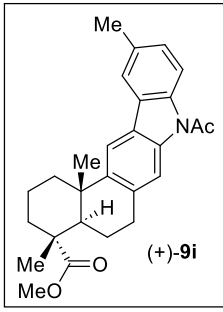


AB-SOV-0207 4 (0.104) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

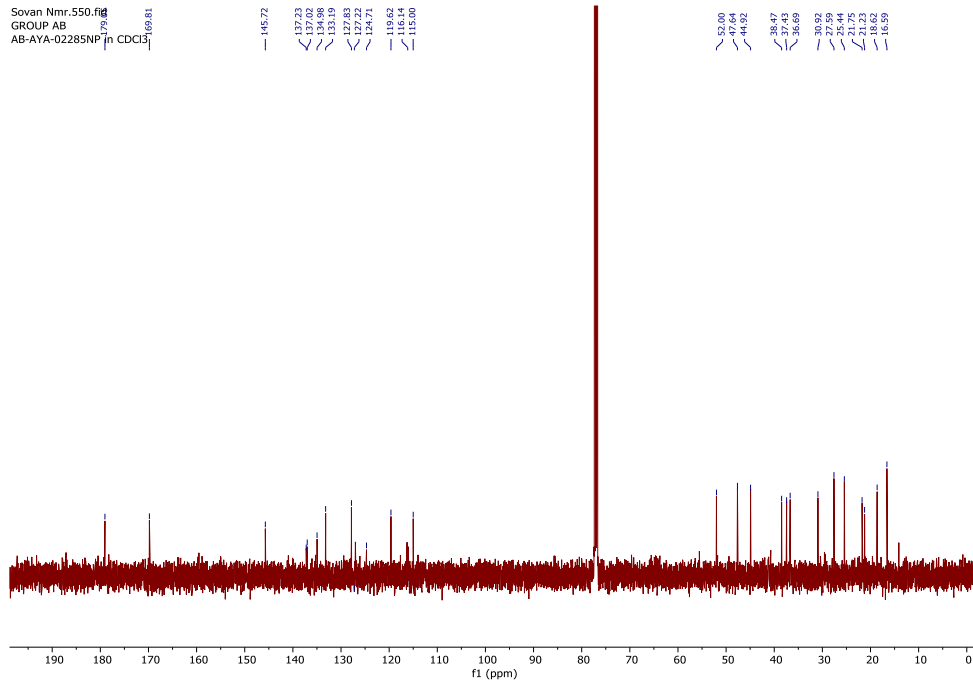
1: TOF MS ES+
1.29e7



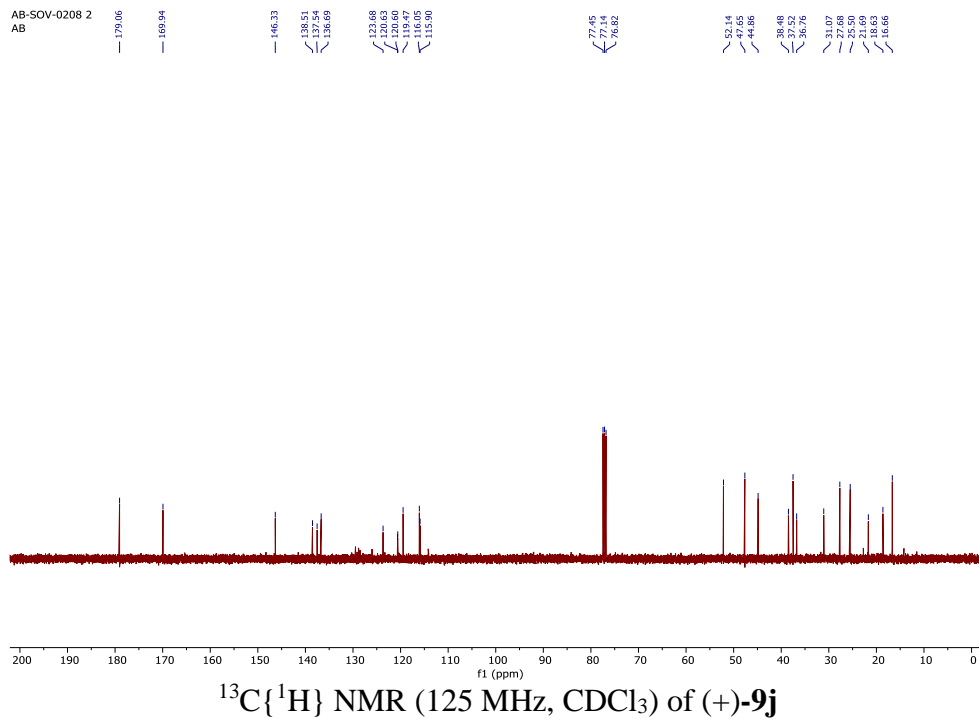
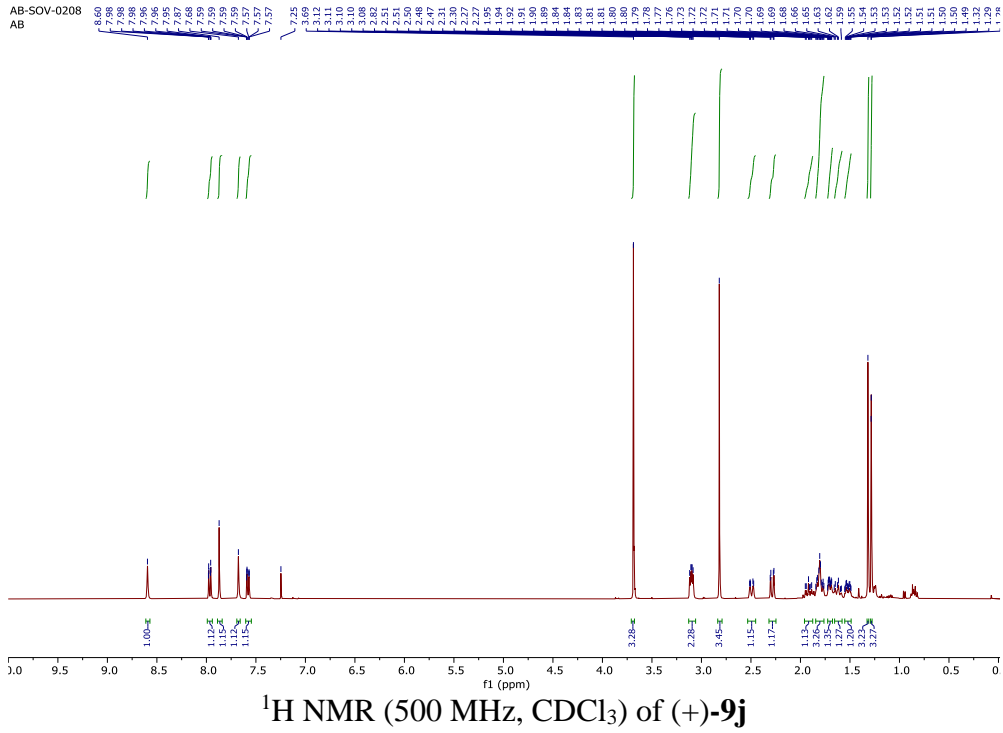
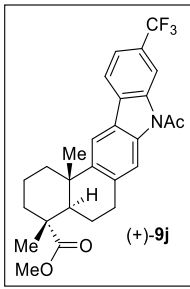
HRMS data of (+)-**9h**



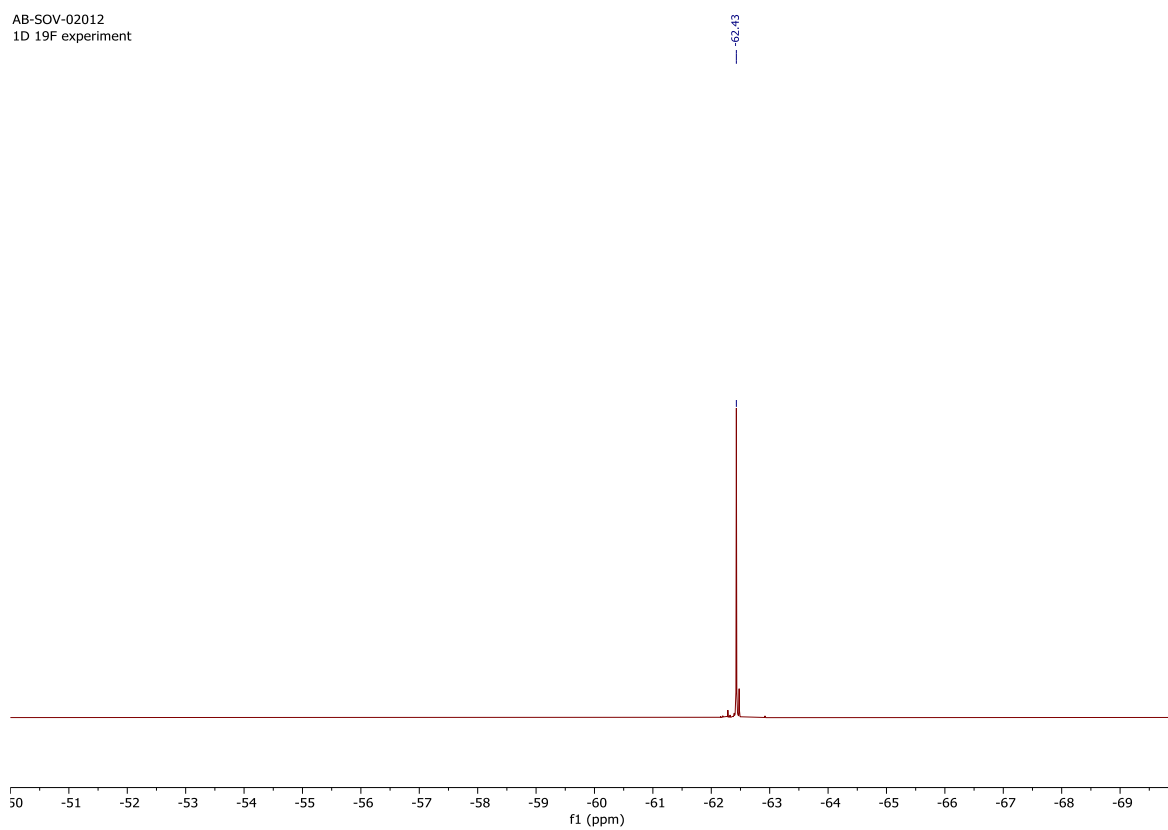
$^1\text{H NMR}$ (500 MHz, CDCl_3) Data of (+)-9i



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-9i



AB-SOV-02012
1D 19F experiment

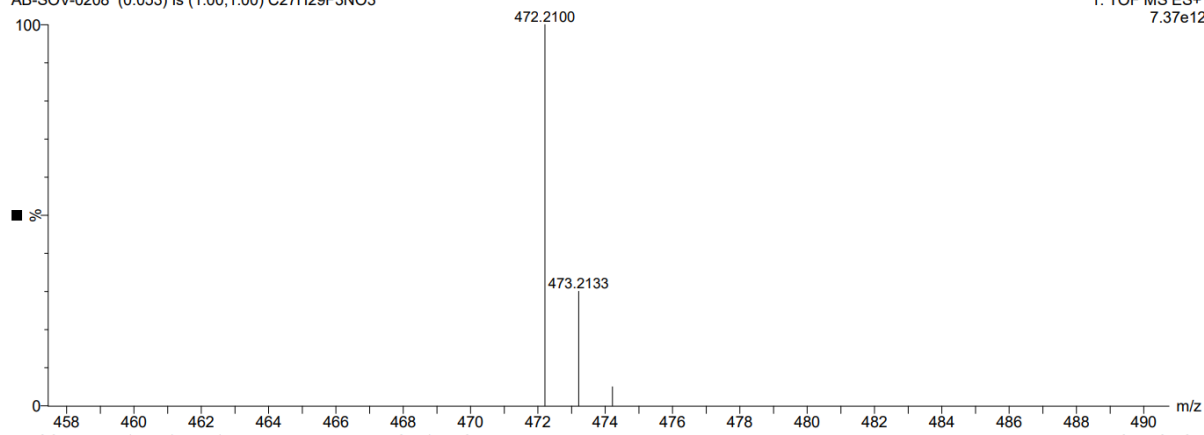


$^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) of compound (+)-**9j**

AB28-Mar-2024 12:42:39
AB-SOV-0208 (0.053) Is (1.00,1.00) C27H29F3NO3

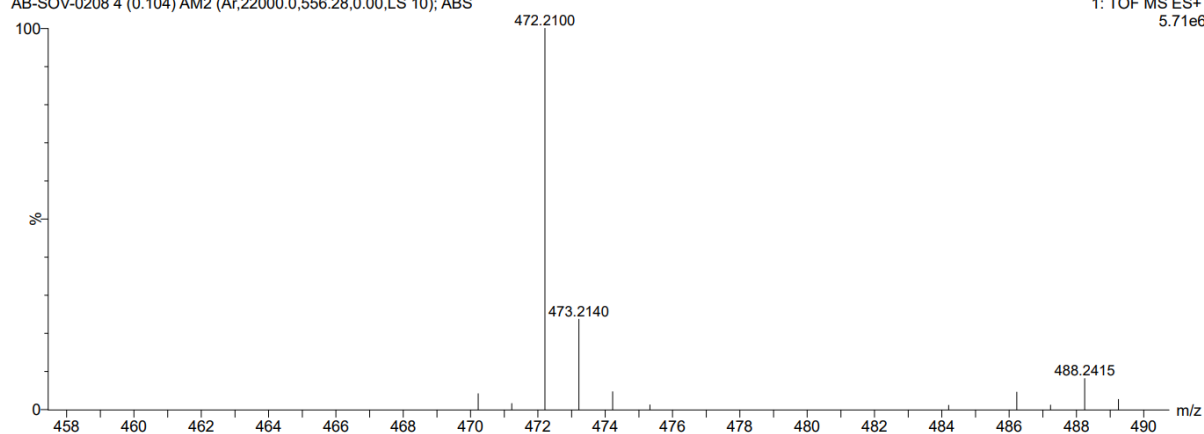
IISER - KOLKATA

1: TOF MS ES+
7.37e12

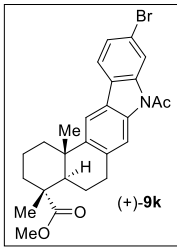


AB-SOV-0208 4 (0.104) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

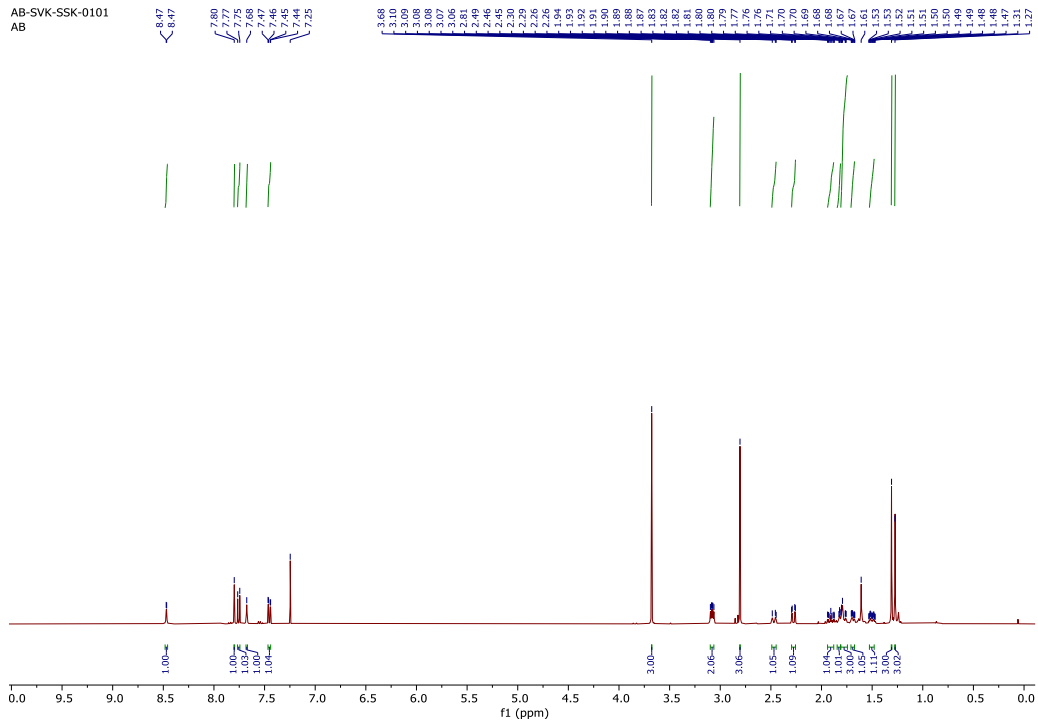
1: TOF MS ES+
5.71e6



HRMS data of (+)-**9j**

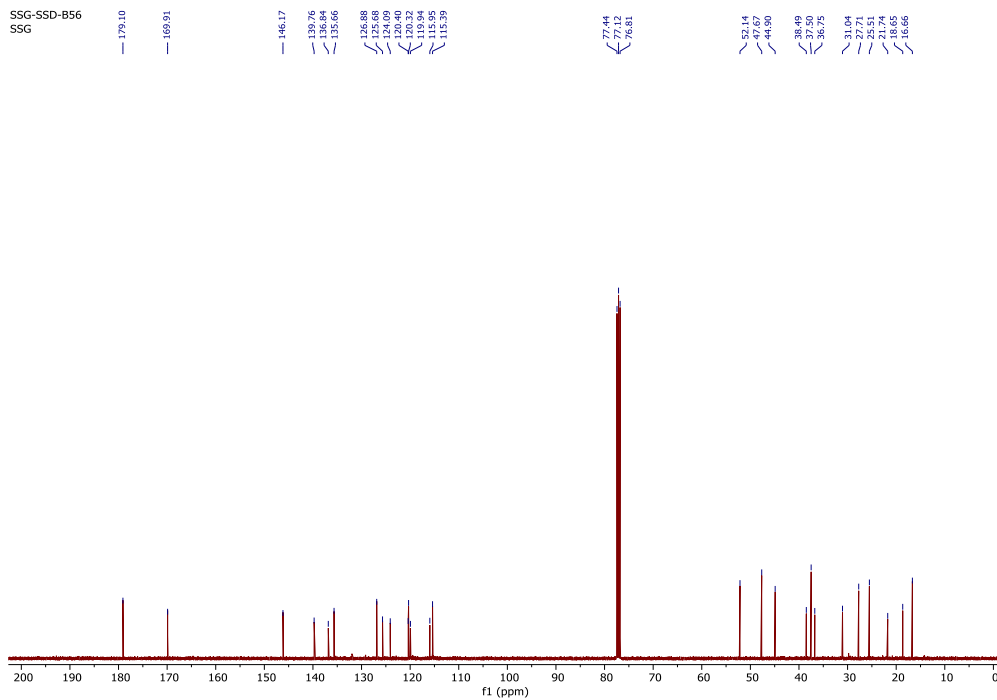


AB-SVK-SSK-0101
AB

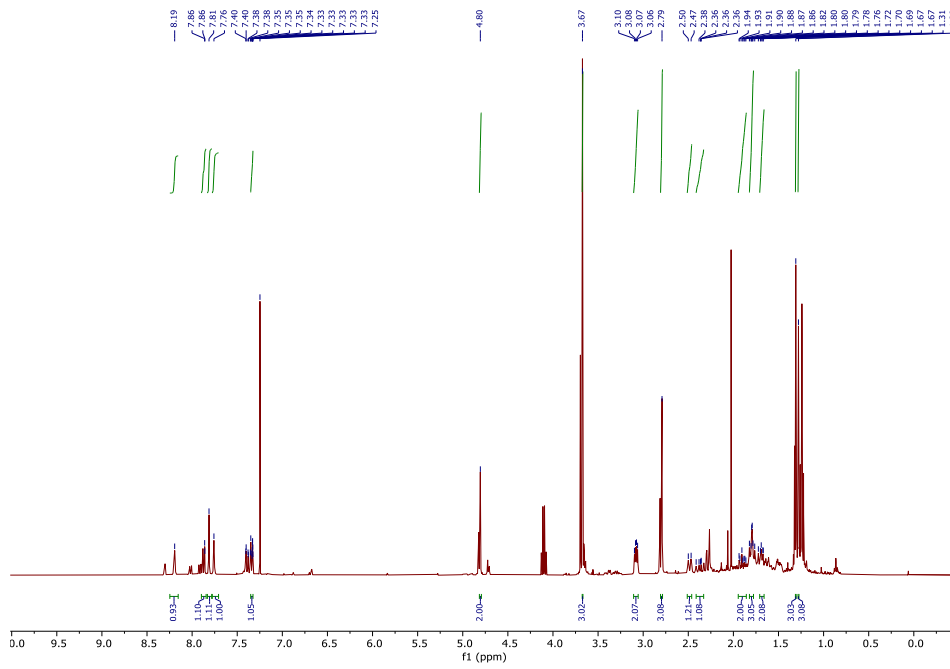
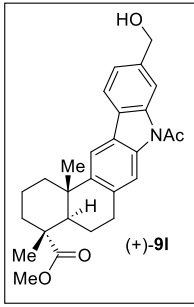


¹H NMR (500 MHz, CDCl₃) data of (+)-**9k**

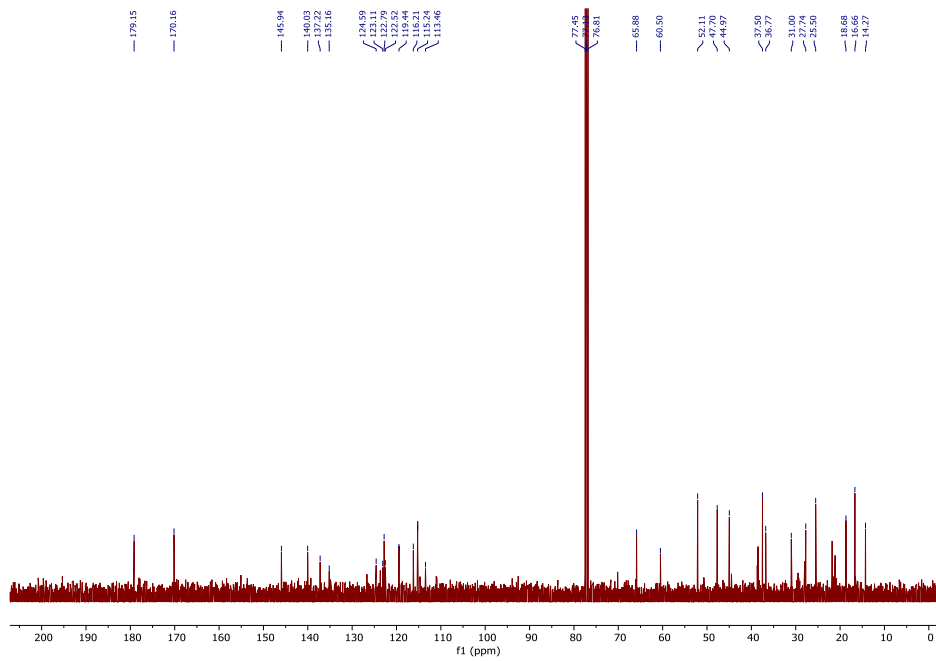
SSG-SSD-B56
SSG



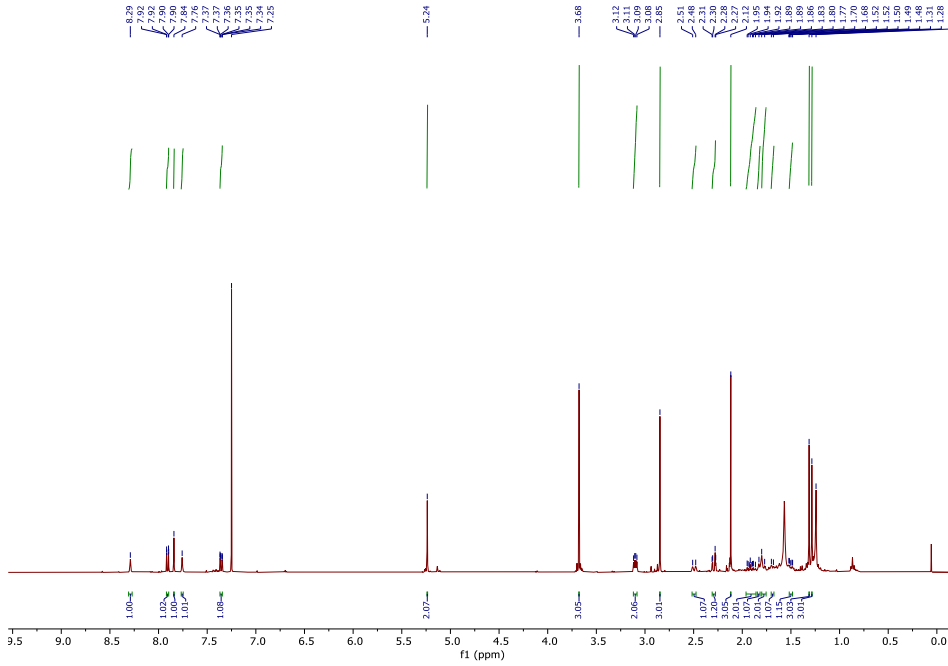
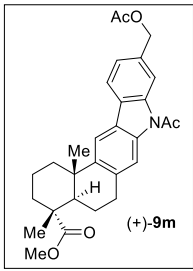
¹³C{¹H} NMR (126 MHz, CDCl₃) data of (+)-**9k**



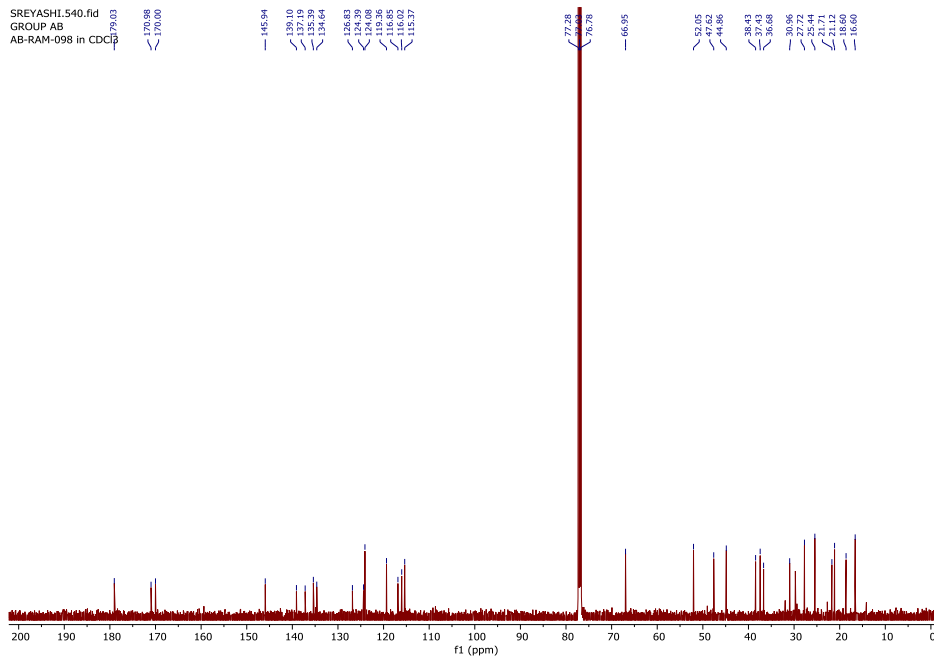
¹H NMR (500 MHz, CDCl₃) data of (+)-91



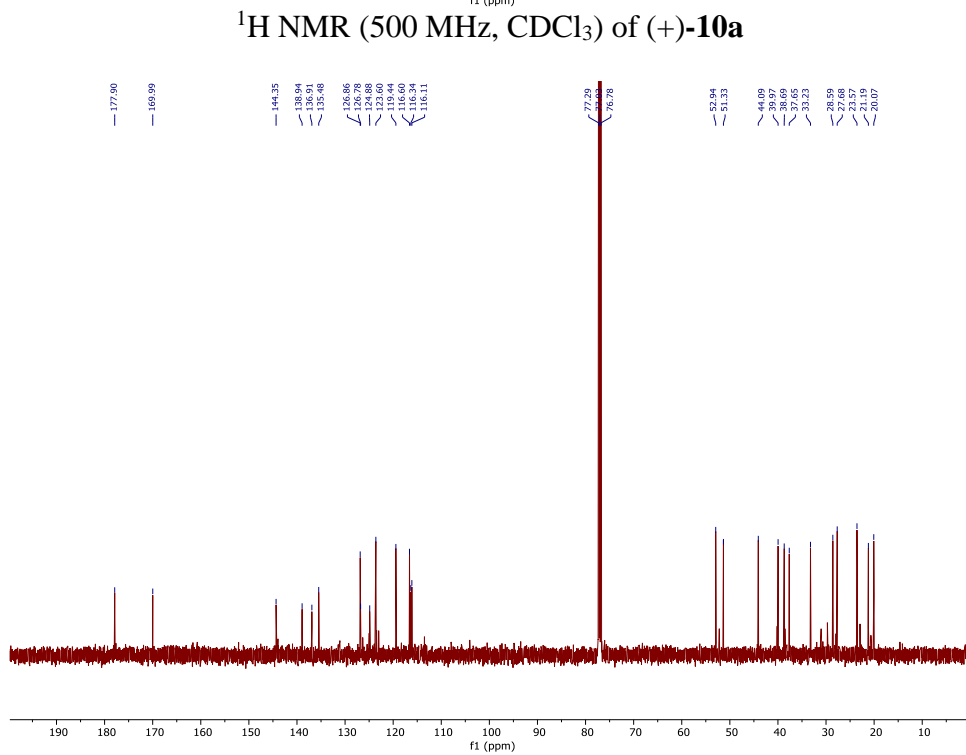
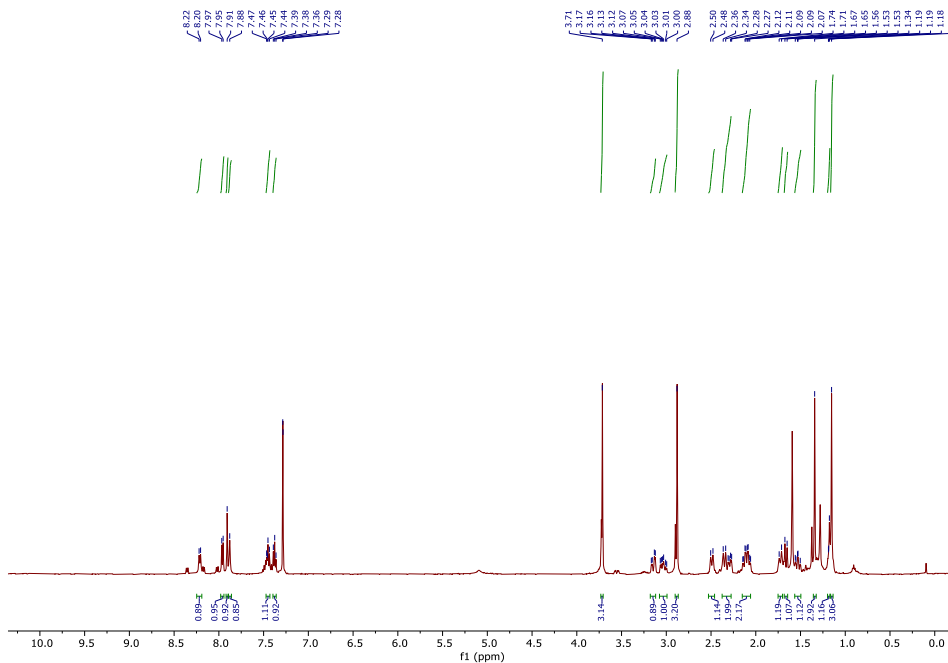
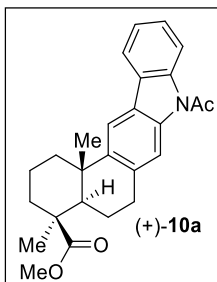
¹³C{¹H} NMR (126 MHz, CDCl₃) data of (+)-91



¹H NMR (500 MHz, CDCl₃) data of (+)-9m



¹³C{¹H} NMR (126 MHz, CDCl₃) data of (+)-9m



Display Report

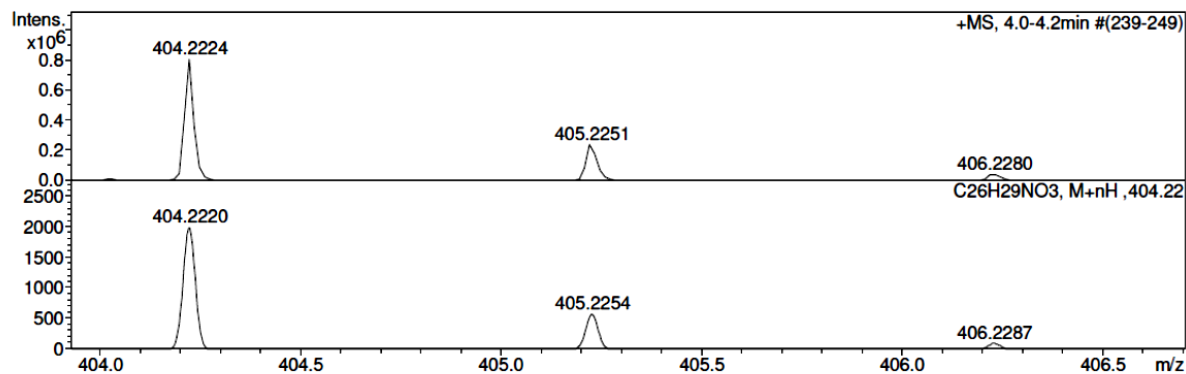
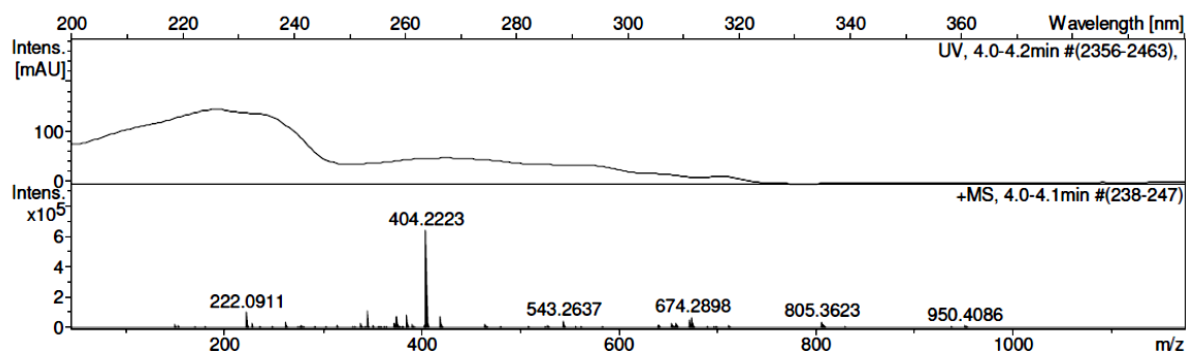
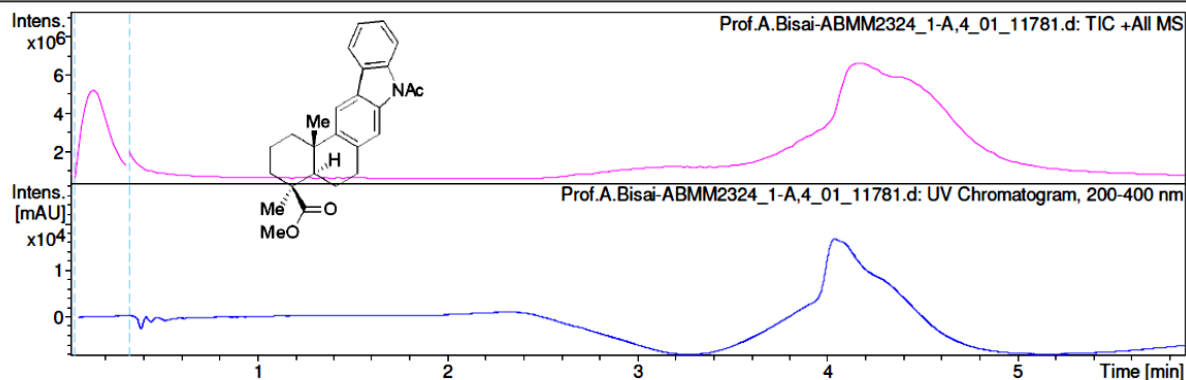
Analysis Info

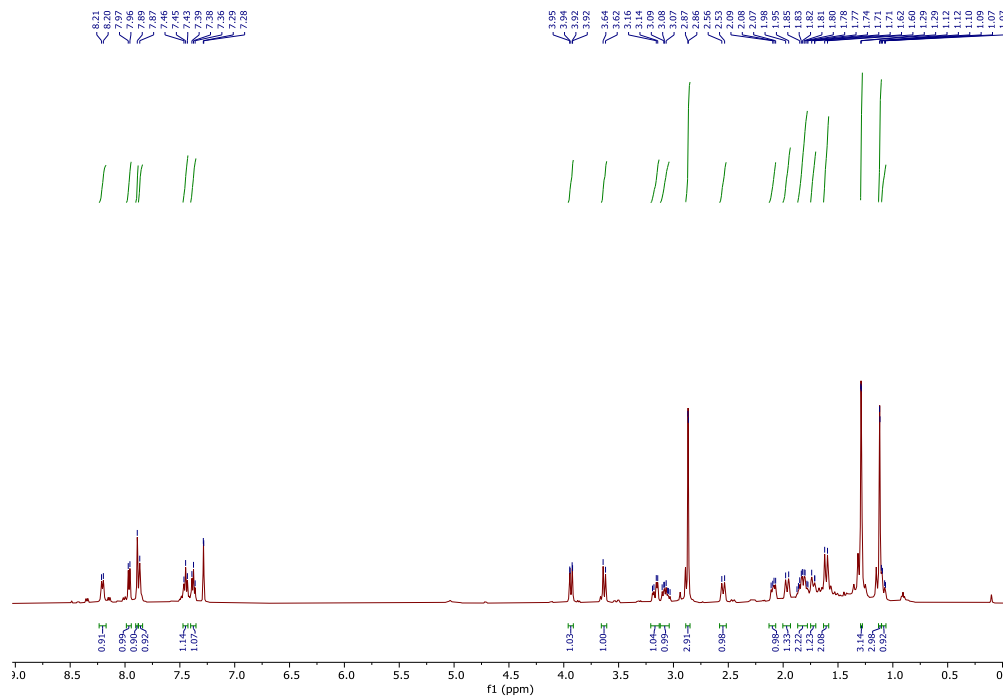
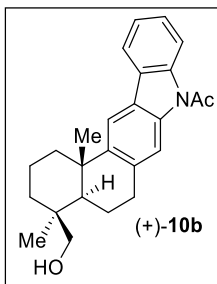
Analysis Name D:\Data\NEW USER DATA 2022\April-2022\19-april\Prof.A.Bisai-ABMM2324_1-A,4_01_11781.d
Method hrlcms-20 sept.m
Sample Name Prof.A.Bisai-ABMM2324
Comment

Acquisition Date 4/19/2022 4:37:06 PM
Operator RUCHI
Instrument micrOTOF-Q II 10330

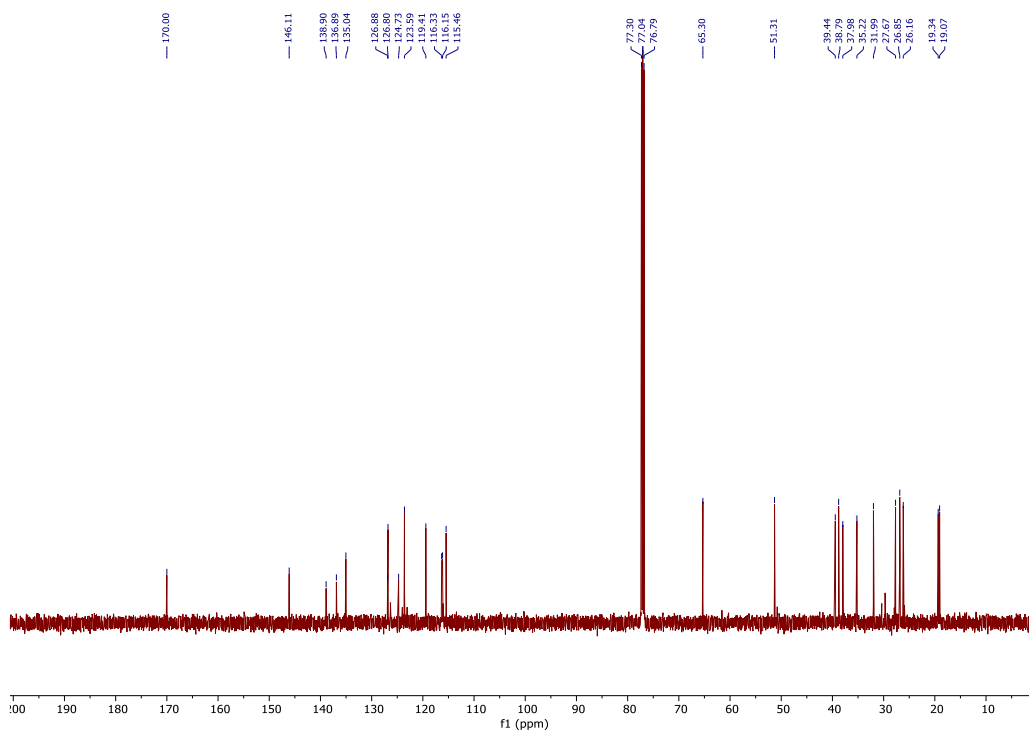
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste





^1H NMR (500 MHz, CDCl_3) of (+)-10b

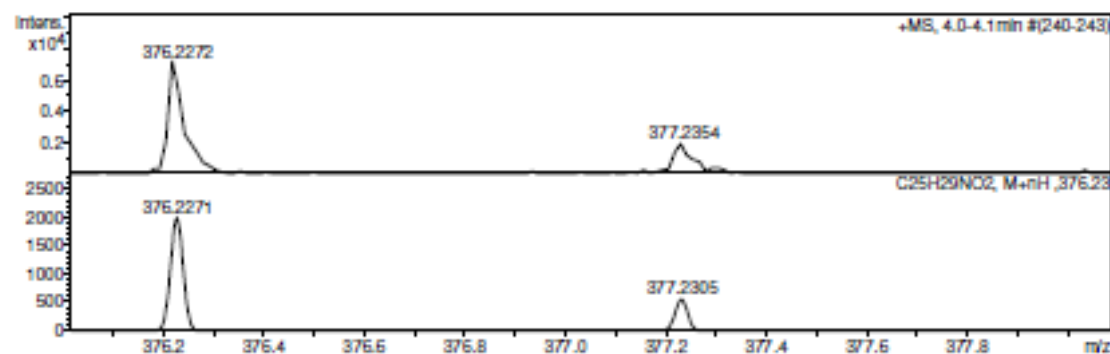
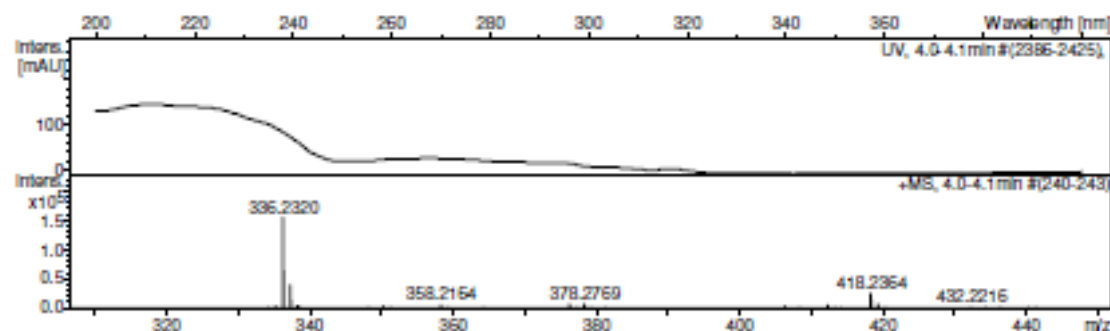
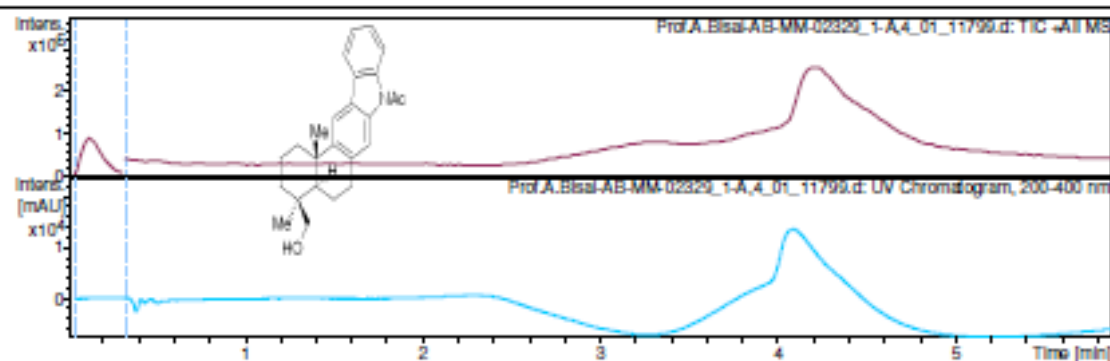


$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-10b

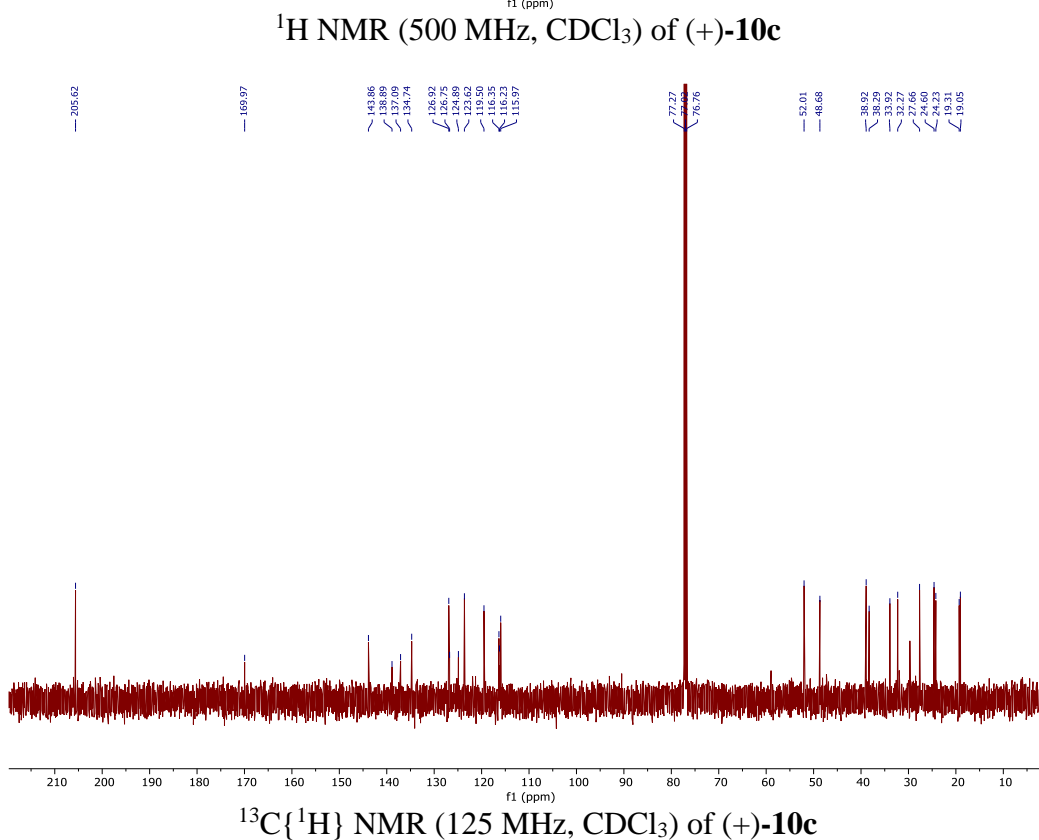
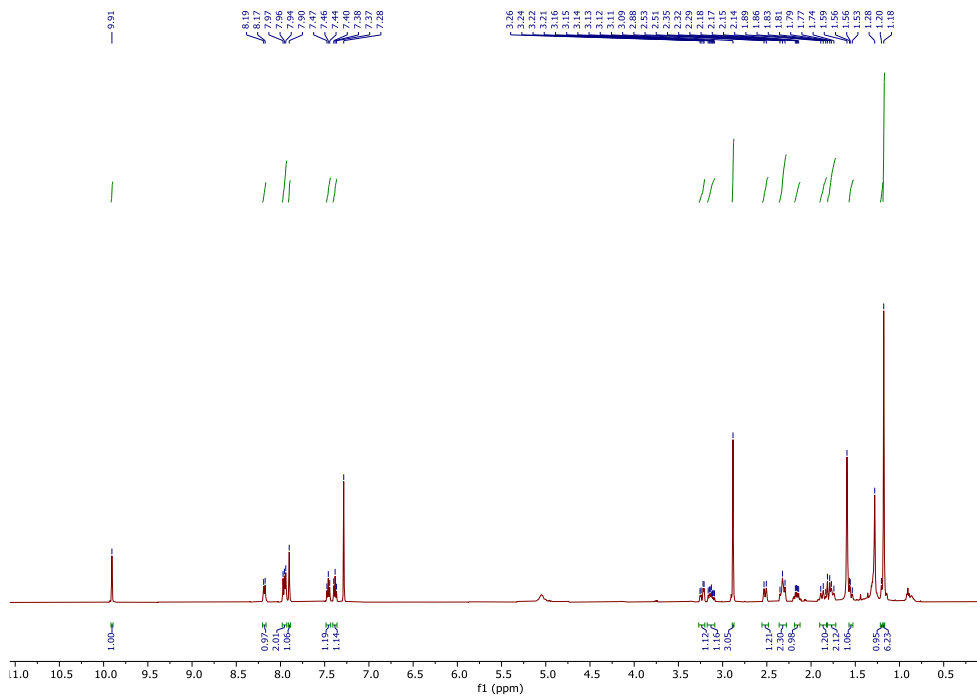
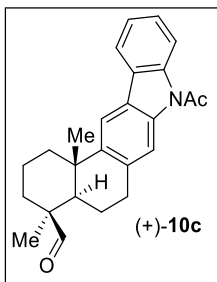
Display Report

Analysis Info	D:\Data\NEW_USER_DATA_2022\April-2022\22-April\Prof.A.Bisai-AB-MM-02329_1-A_4_01_11799.d	Acquisition Date	4/22/2022 12:01:24 PM
Method	hrlcms-20 sept.m	Operator	RUCHI
Sample Name	Prof.A.Bisai-AB-MM-02329	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter					
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Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste



HRMS data of (+)-10b



Display Report

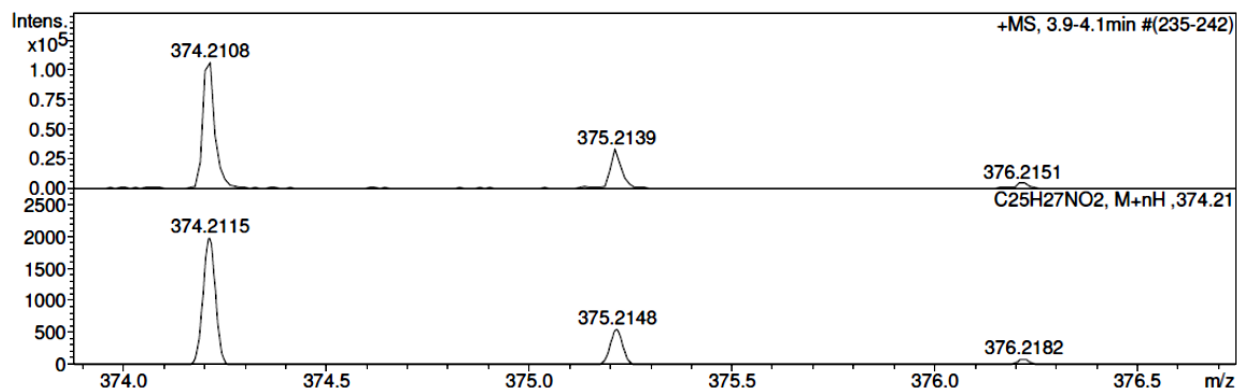
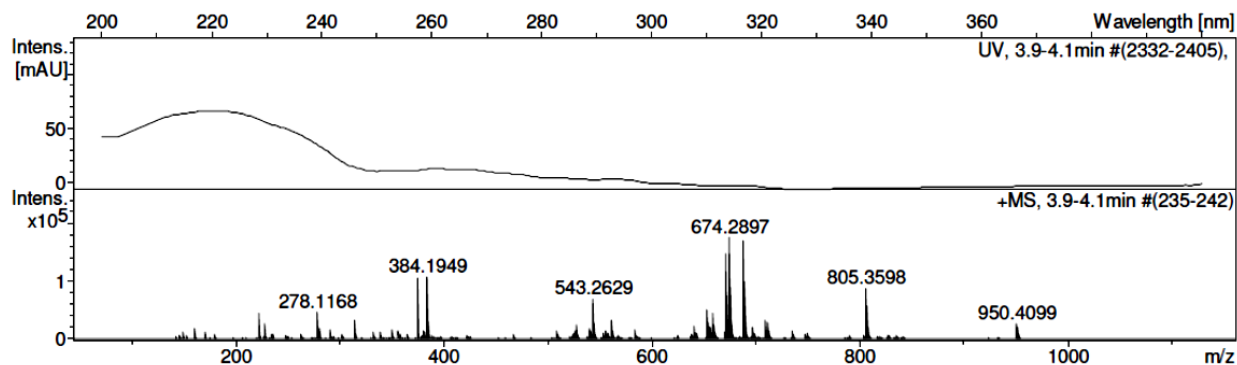
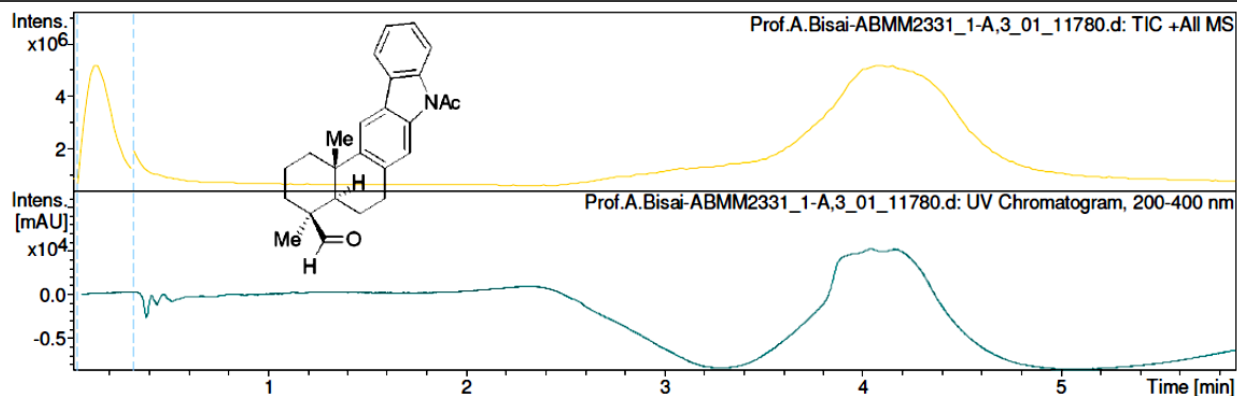
Analysis Info

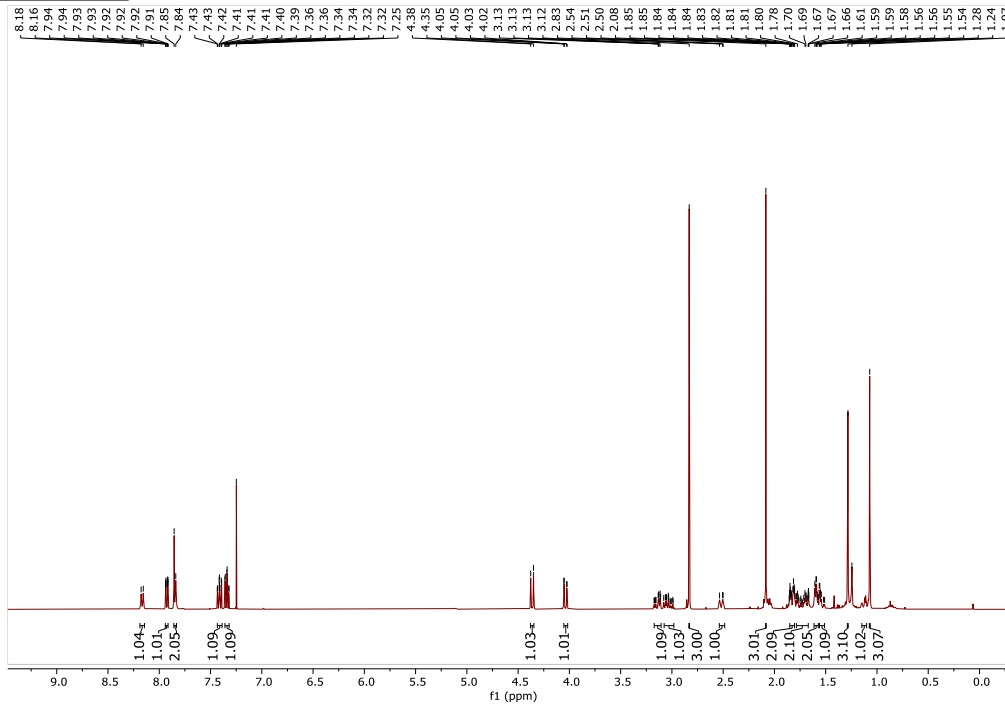
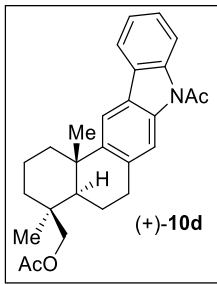
Analysis Name D:\Data\NEW USER DATA 2022\April-2022\19-april\Prof.A.Bisai-ABMM2331_1-A,3_01_11780.d
Method hrlcms-20 sept.m
Sample Name Prof.A.Bisai-ABMM2331
Comment

Acquisition Date 4/19/2022 4:29:57 PM
Operator RUCHI
Instrument microTOF-Q II 10330

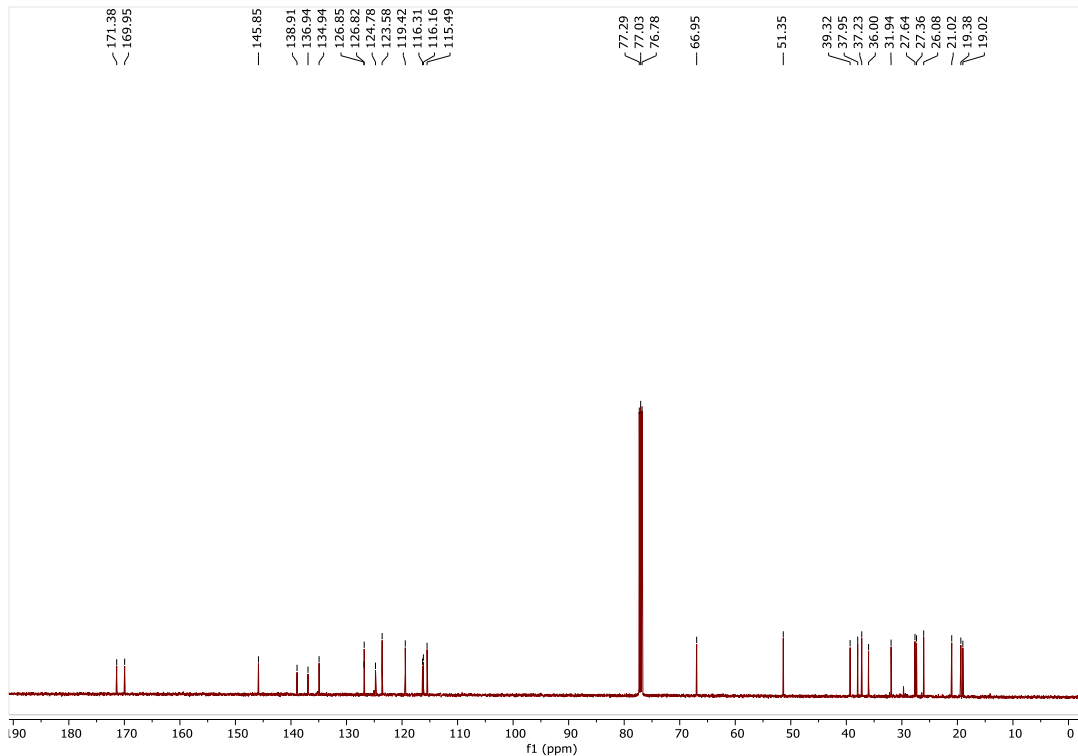
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.2 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

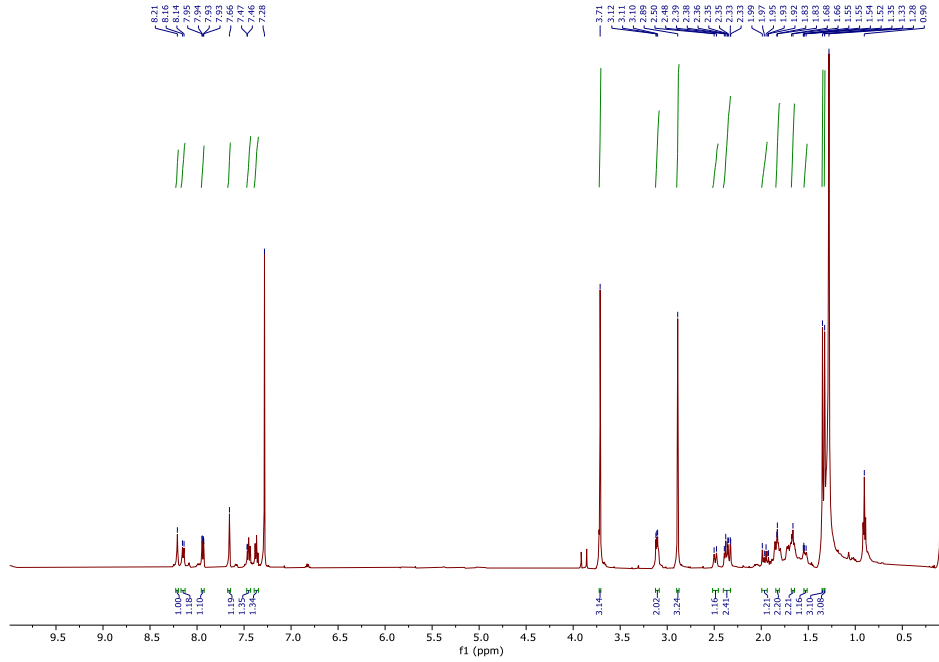
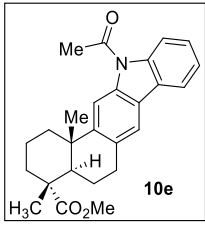




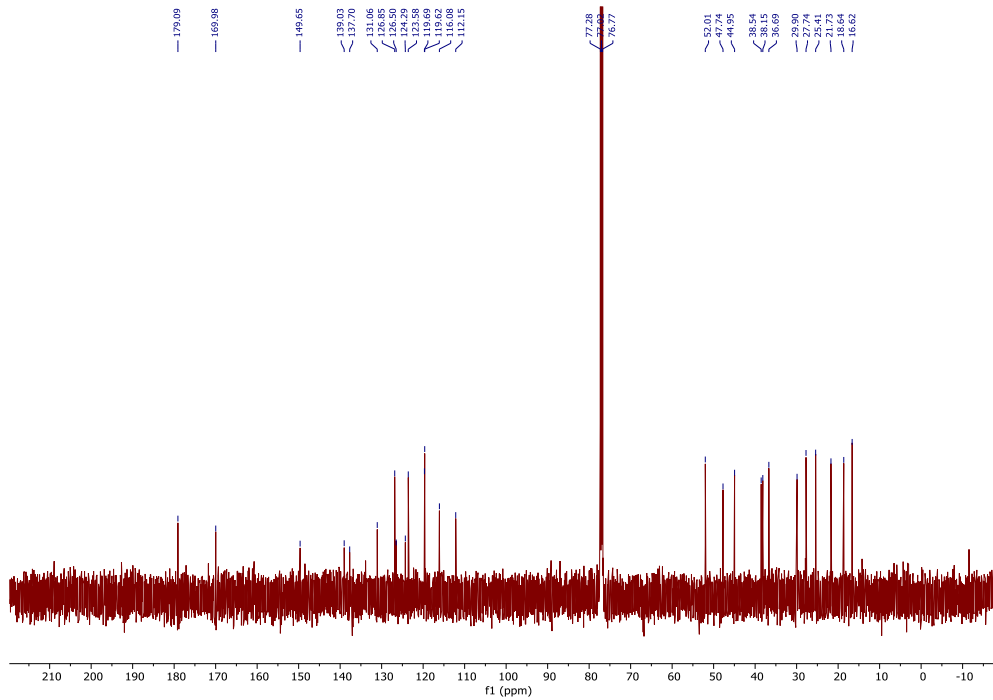
^1H NMR (400 MHz, CDCl_3) of compound (+)-10d



$^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CDCl_3) of compound (+)-10d



¹H NMR (500 MHz, CDCl₃) of compound **10e**

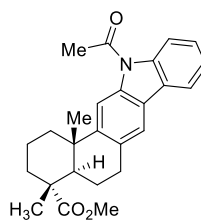
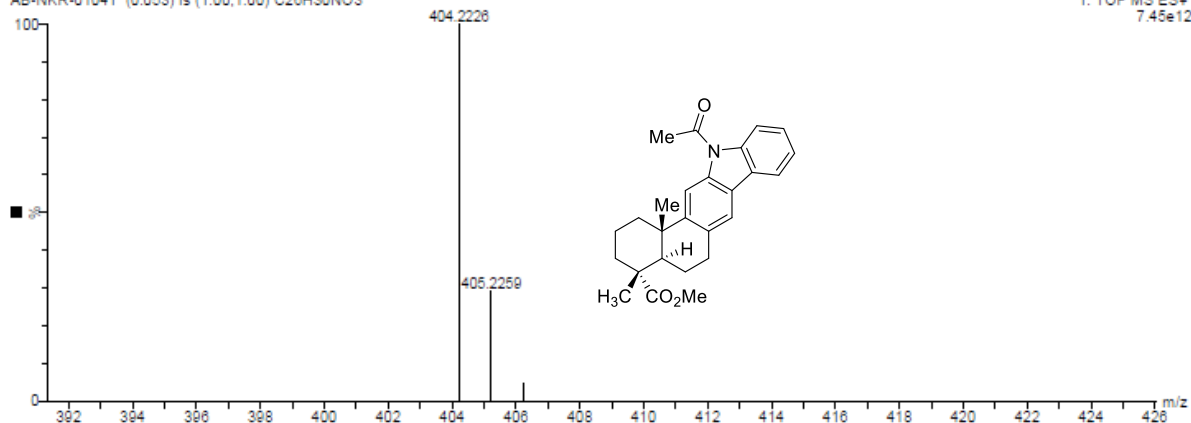


¹³C NMR (125 MHz, CDCl₃) of compound **10e**

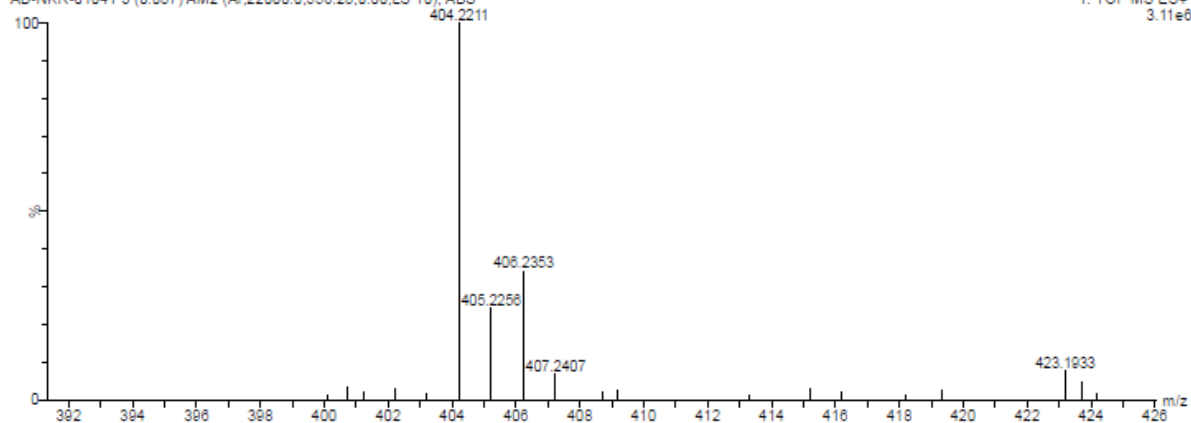
AB02-Apr-2024 13:43:06
AB-NKR-01041 (0.053) Is (1.00,1.00) C₂₆H₃₀NO₃

IISER - KOLKATA

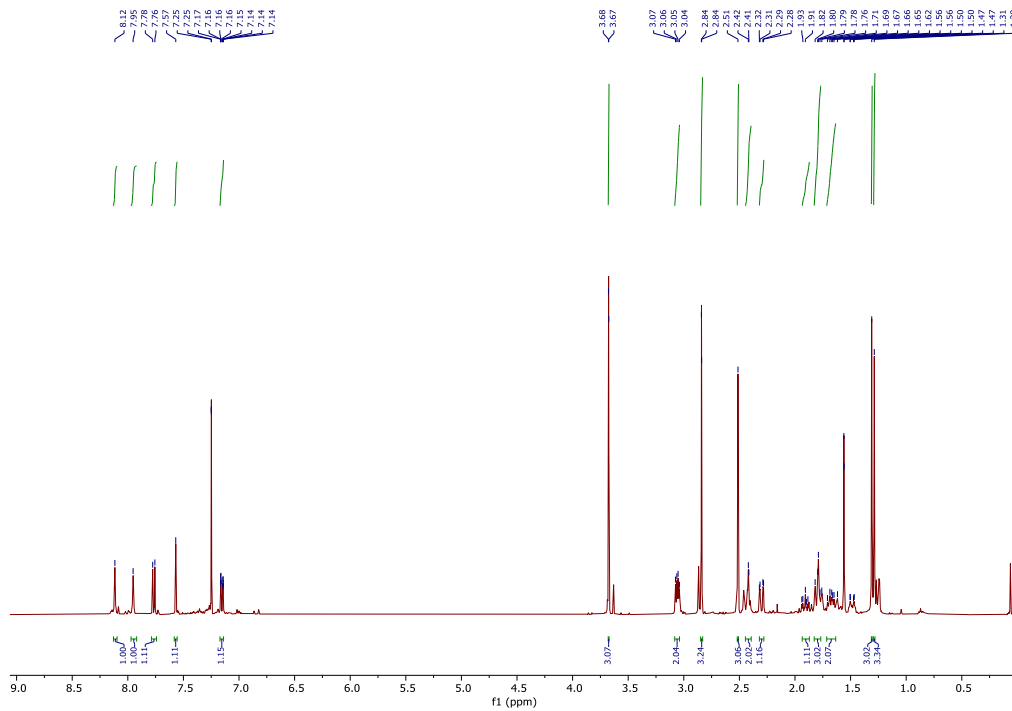
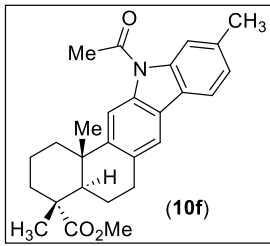
1: TOF MS ES+
7.45e12



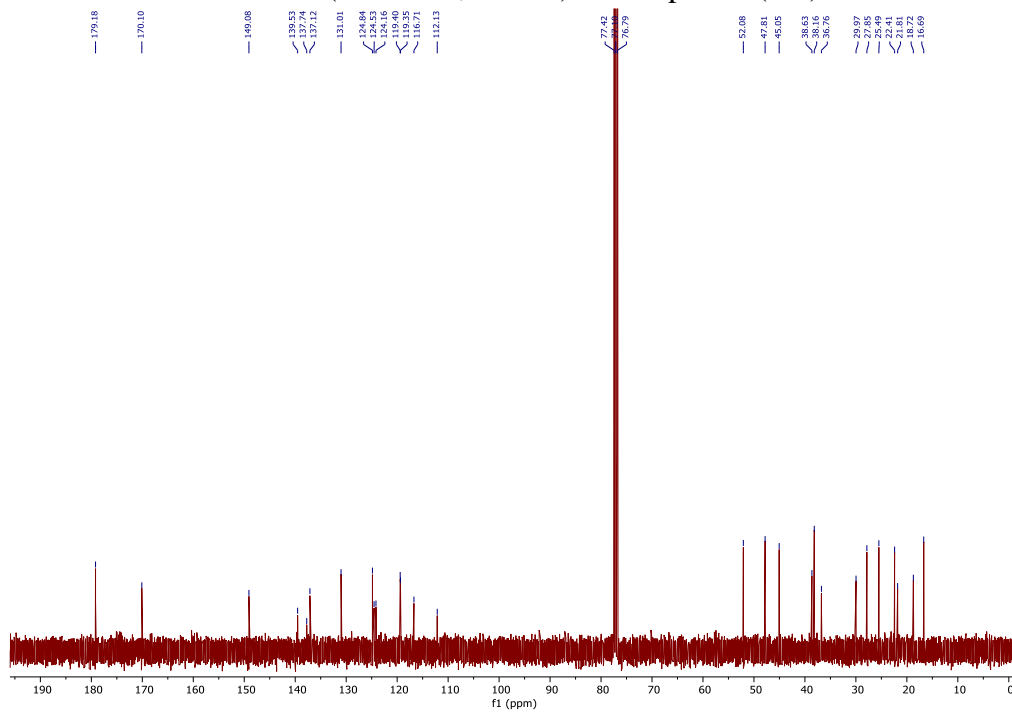
AB-NKR-01041 3 (0.087) AM2 (Ar,22000,0,556,28,0,00,LS 10); ABS
404.2211
1: TOF MS ES+
3.11e8



Mass data of compound 10e



¹H NMR (500 MHz, CDCl₃) of compound (10f)



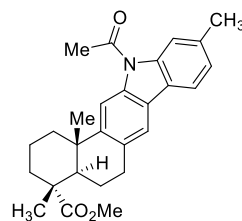
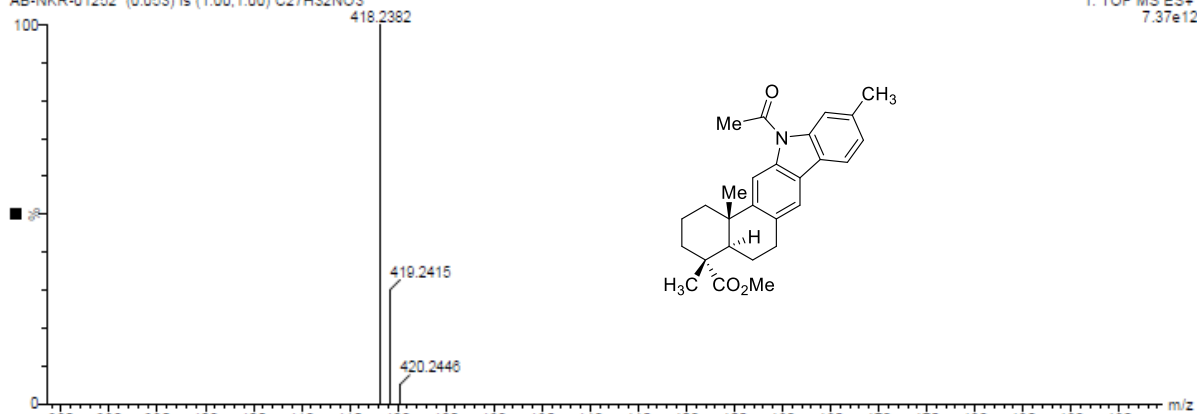
¹³C{¹H} NMR (125 MHz, CDCl₃) of compound (10f)

AB29-Apr-2024 14:39:02

IISER - KOLKATA

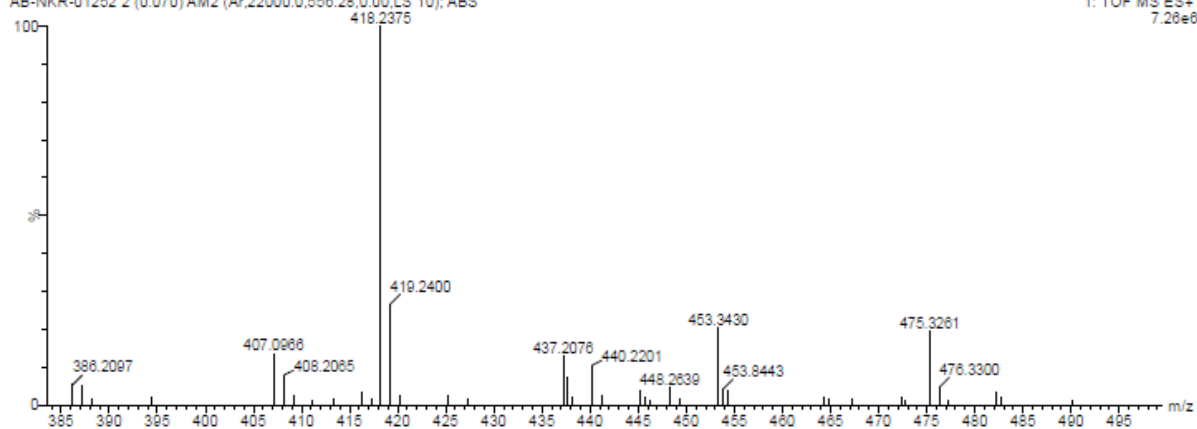
1: TOF MS ES+
7.37e12

AB-NKR-01262 (0.053) Is (1.00,1.00) C₂₇H₃₂NO₃

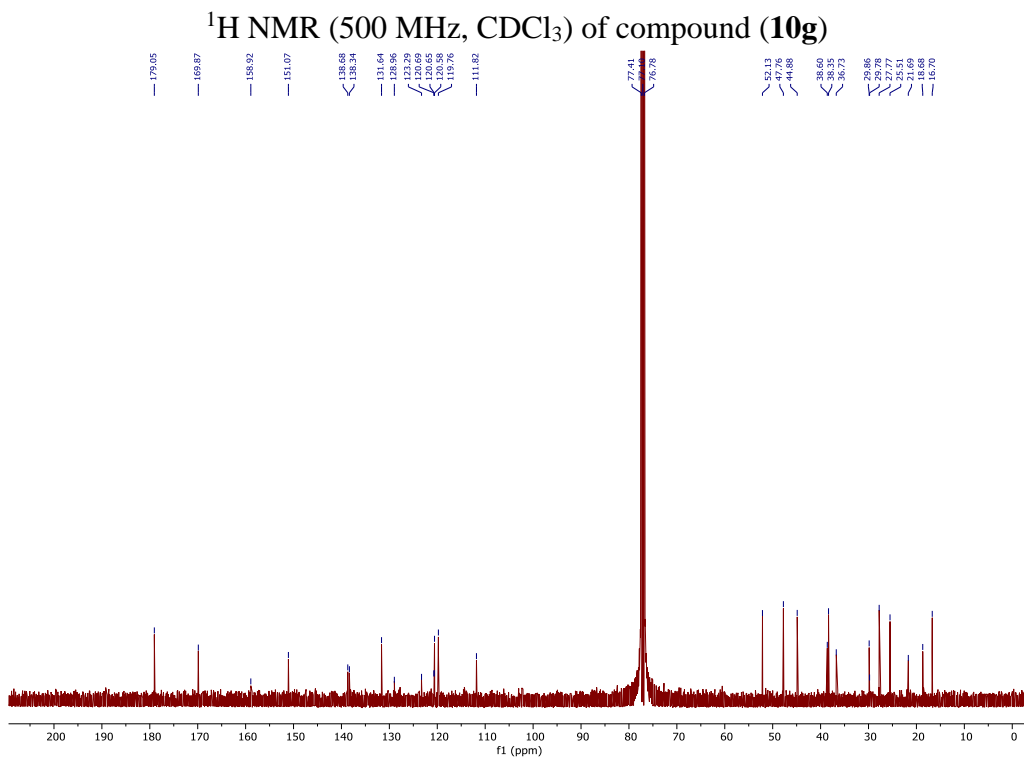
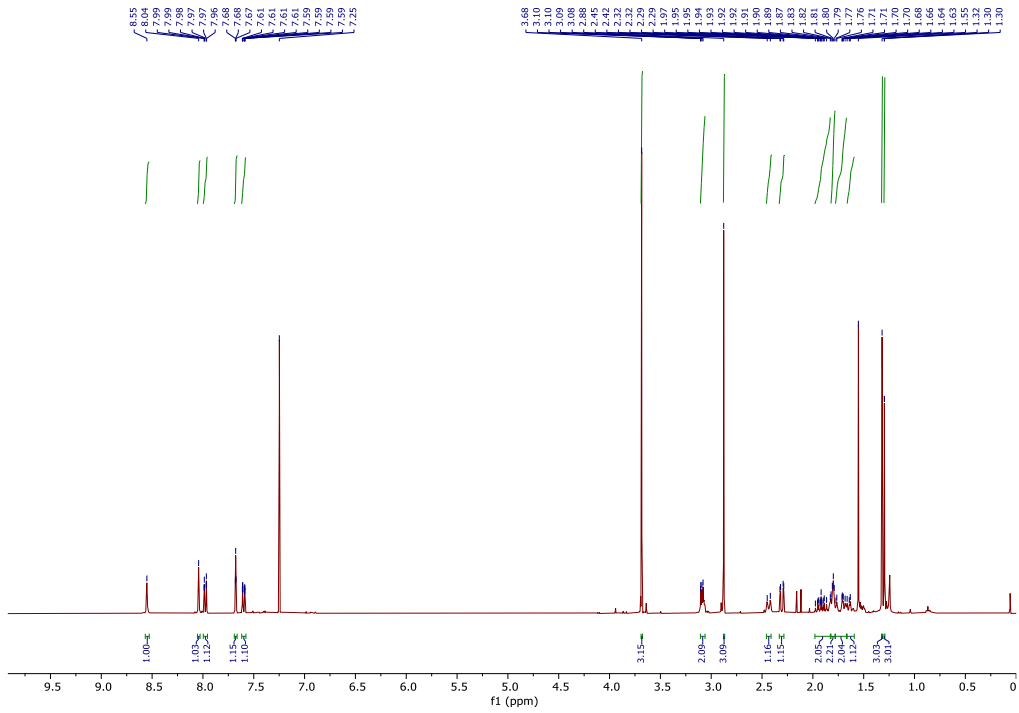
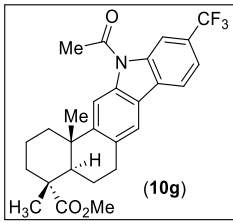


AB-NKR-01262 2 (0.070) AM2 (Ar.22000,0.556,28,0,00,LS 10); ABS

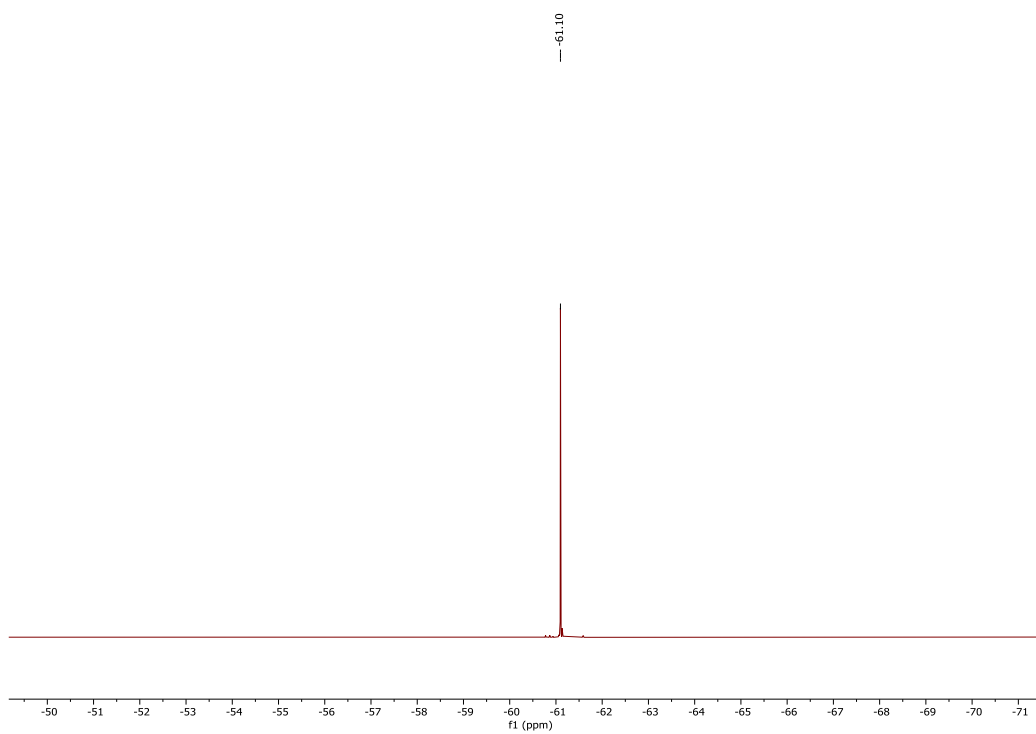
1: TOF MS ES+
7.28e8



Mass data of compound **10f**



¹³C{¹H} NMR (125 MHz, CDCl₃) of compound (10g)



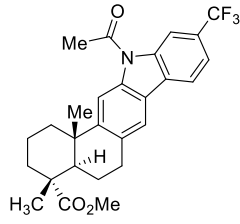
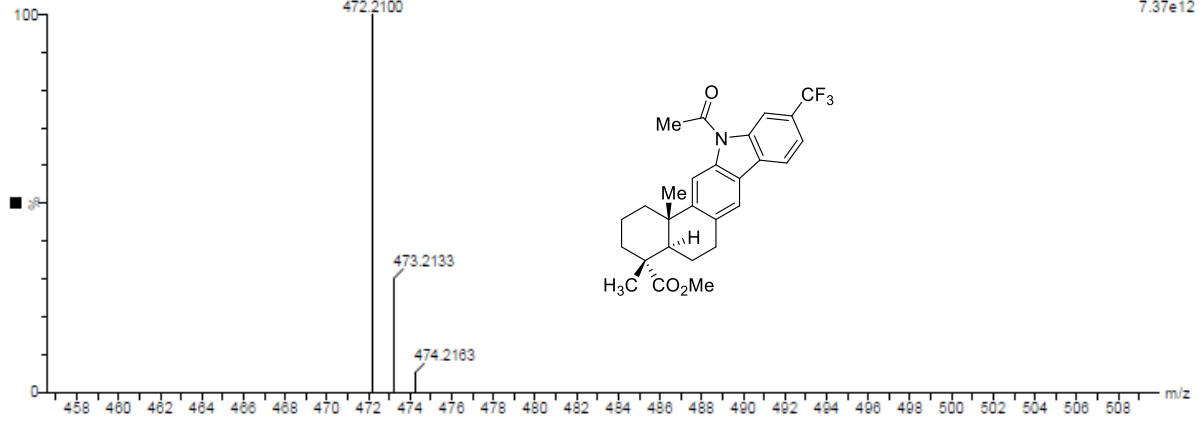
$^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) of compound **10g**

AB29-Apr-2024 14:37:25

IISER - KOLKATA

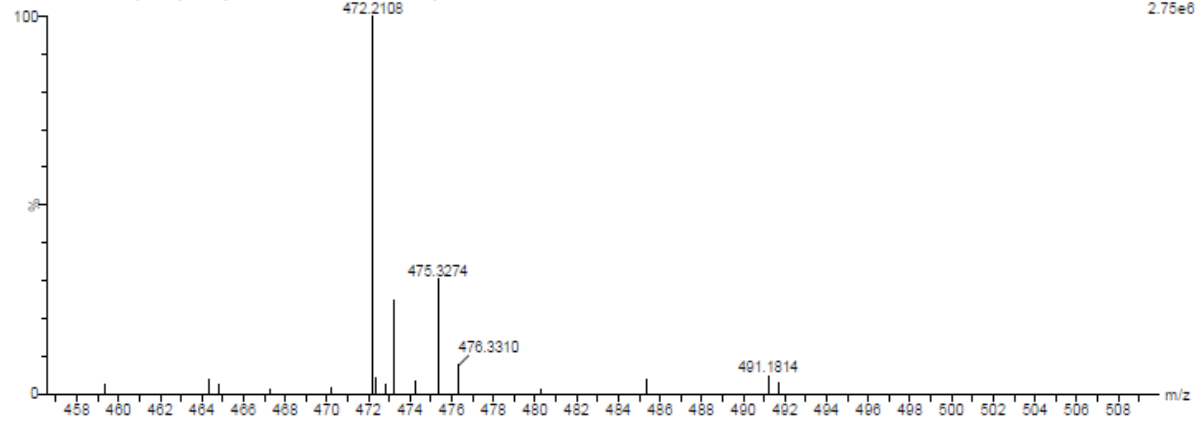
1: TOF MS ES+
7.37e12

AB-NKR-01251 (0.053) Is (1.00,1.00) C₂₇H₂₉F₃NO₃

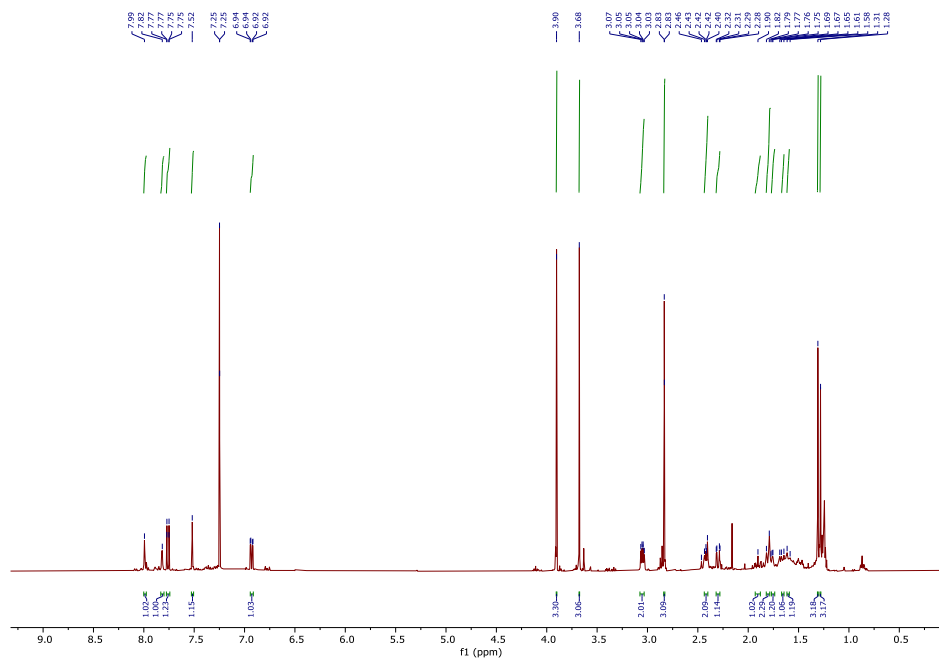
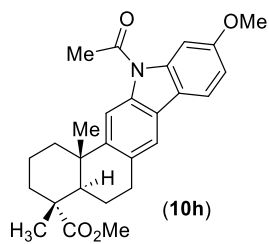


AB-NKR-01251 2 (0.070) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

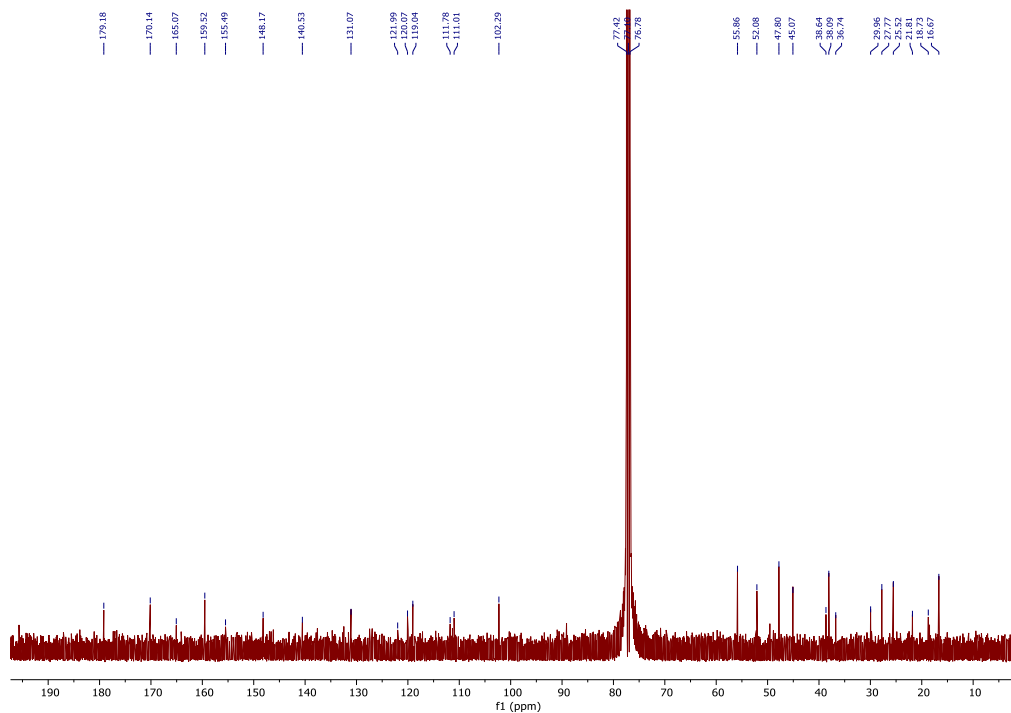
1: TOF MS ES+
2.75e8



Mass data of compound (10g)



¹H NMR (500 MHz, CDCl₃) of compound (10h)



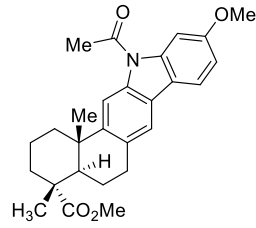
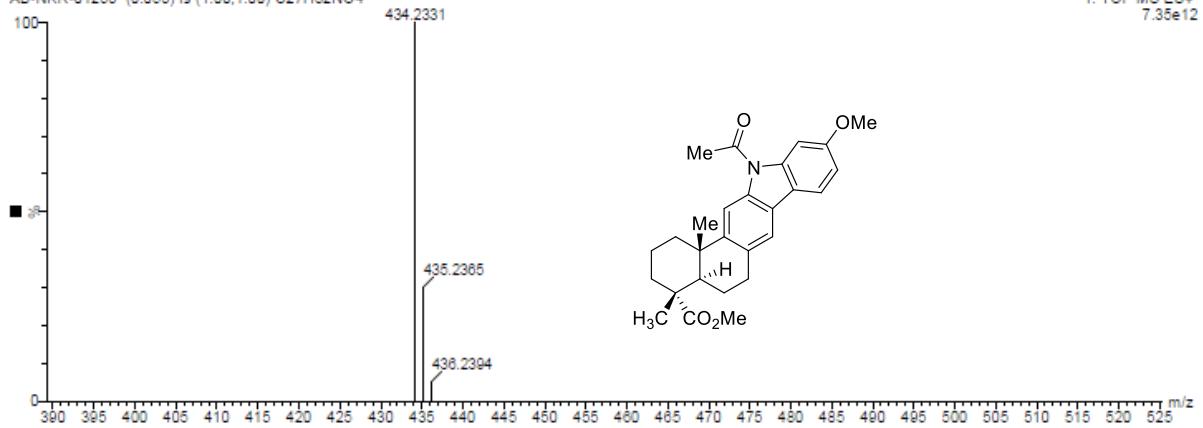
¹³C{¹H} NMR (125 MHz, CDCl₃) of compound (10h)

AB29-Apr-2024 14:40:39

IISER - KOLKATA

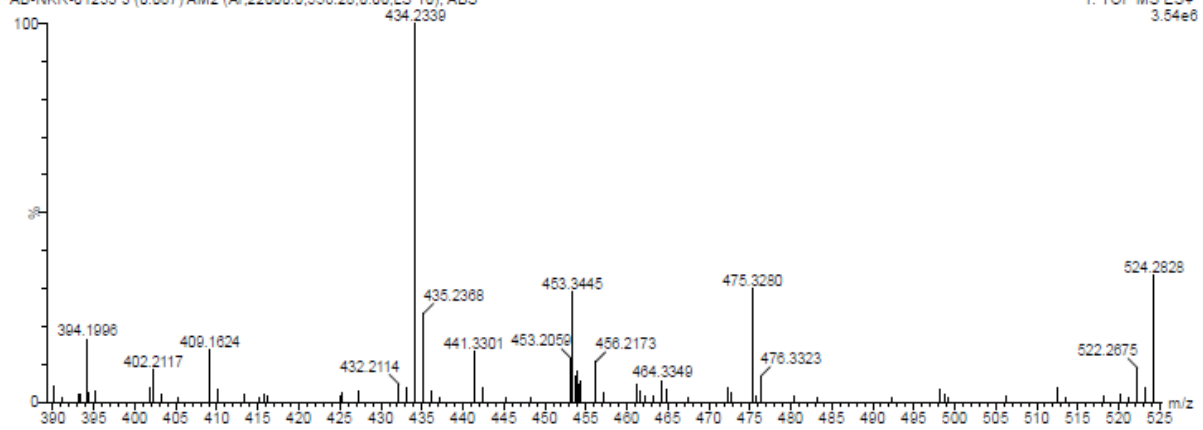
1: TOF MS ES+
7.35e12

AB-NKR-01253 (0.053) Is (1.00,1.00) C₂₇H₃₂NO₄

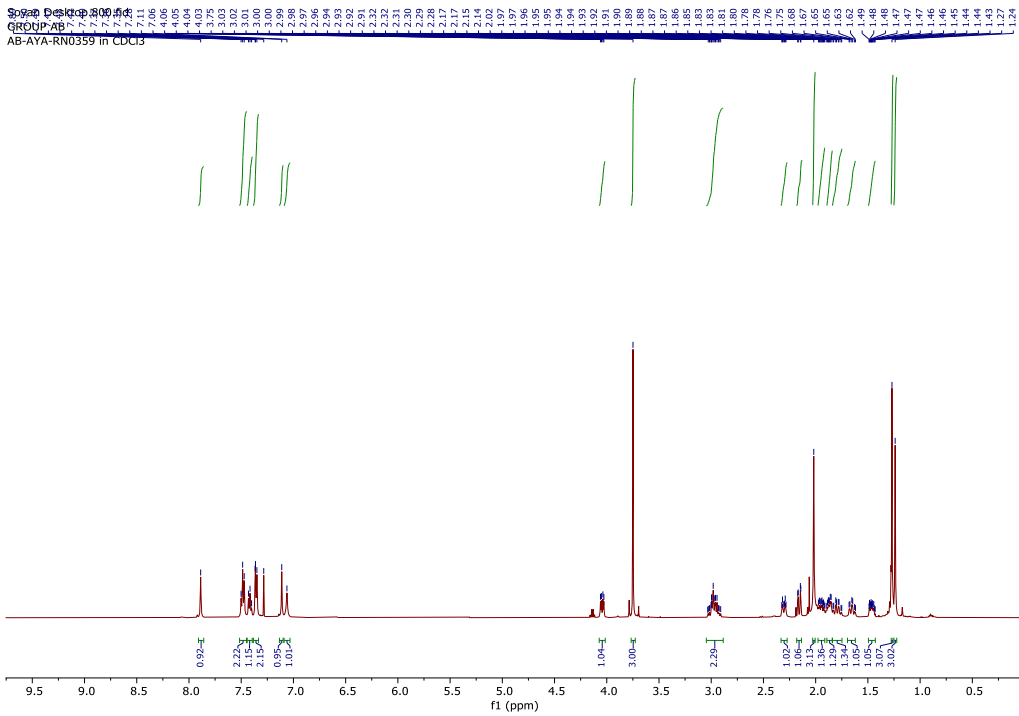
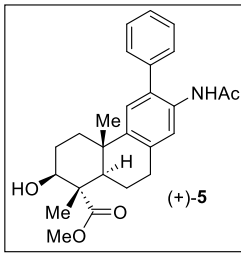


AB-NKR-01253 3 (0.087) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

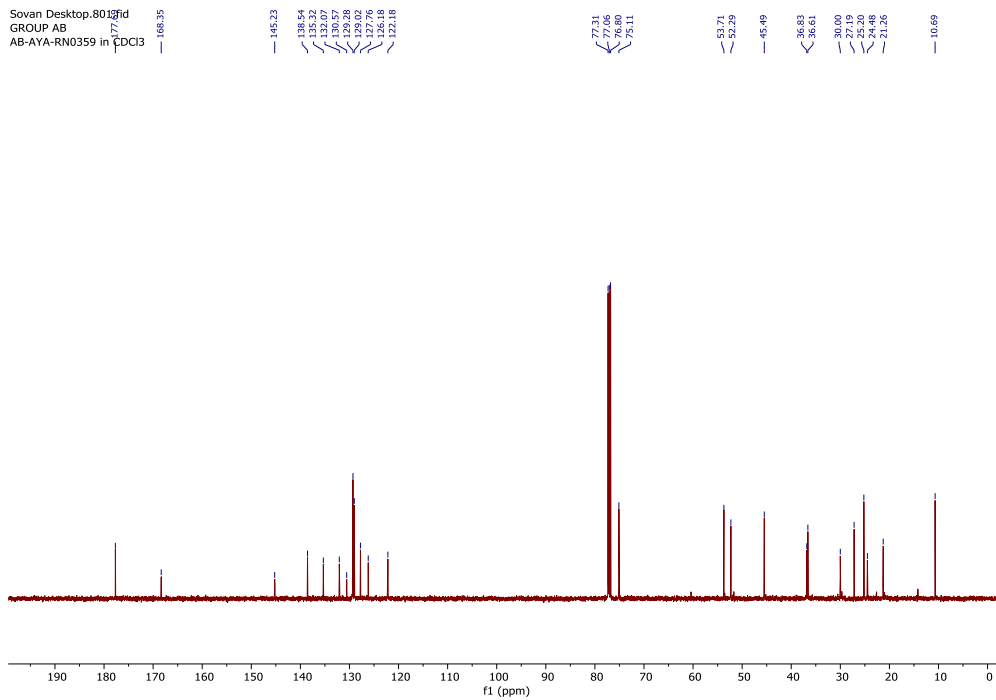
1: TOF MS ES+
3.54e8



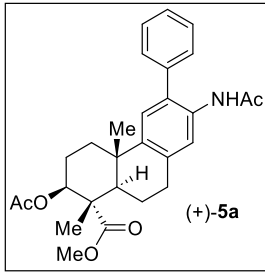
Mass data of compound (**10h**)



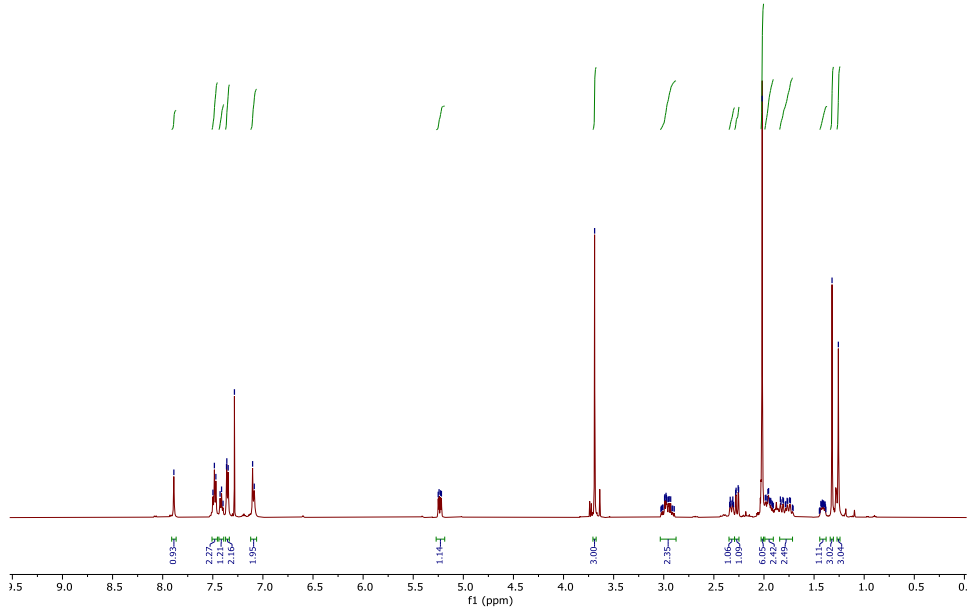
¹H NMR (500 MHz, CDCl₃) of (+)-5



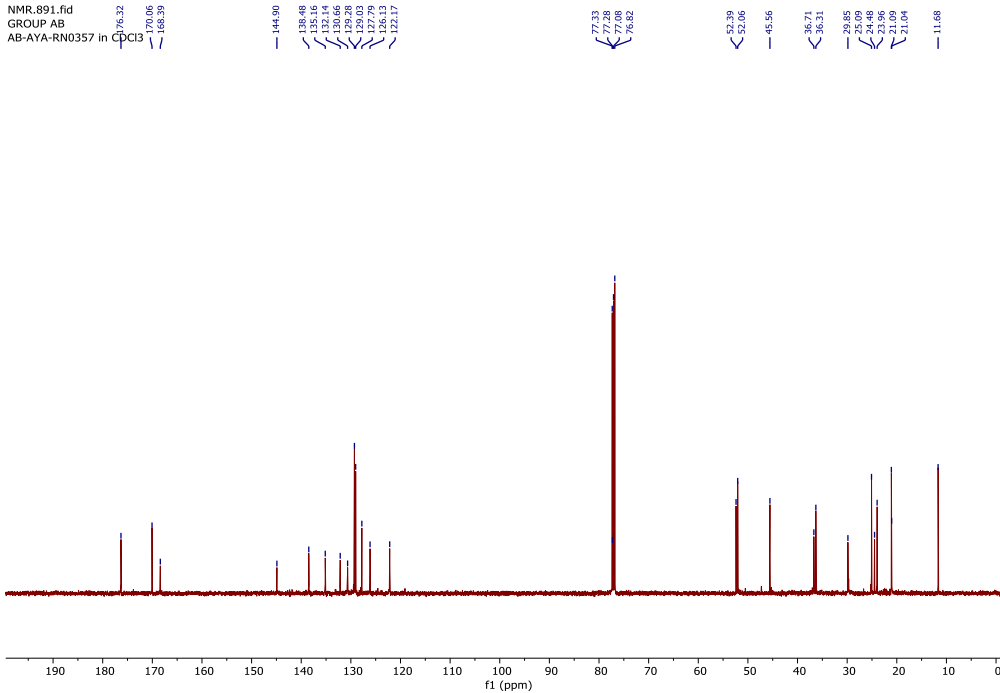
¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-5



NMR_891.fid
 GROUP AB
 AB-AYA-RN0357 in CDCl₃



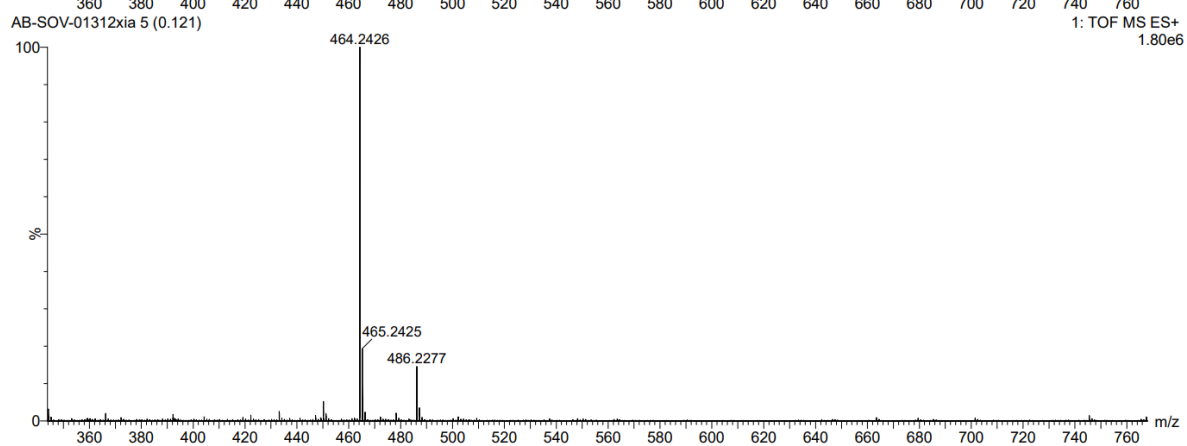
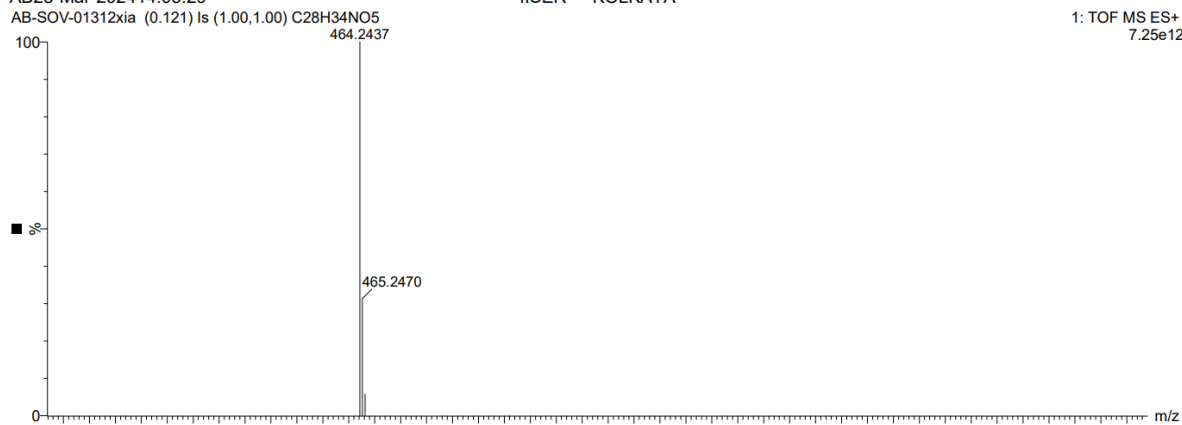
NMR_891.fid
 GROUP AB
 AB-AYA-RN0357 in CDCl₃



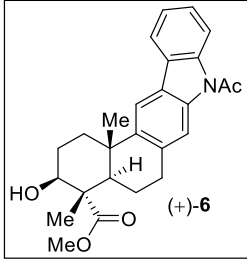
AB28-Mar-2024 14:05:29

IISER - KOLKATA

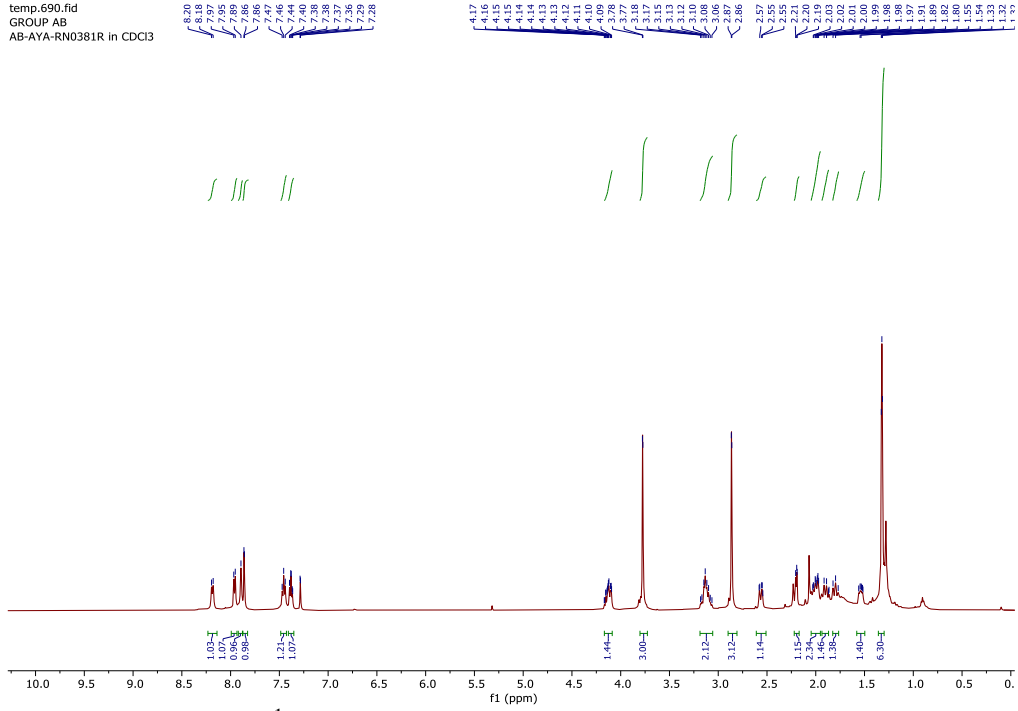
1: TOF MS ES+
7.25e12



HRMS data of (+)-**5a**

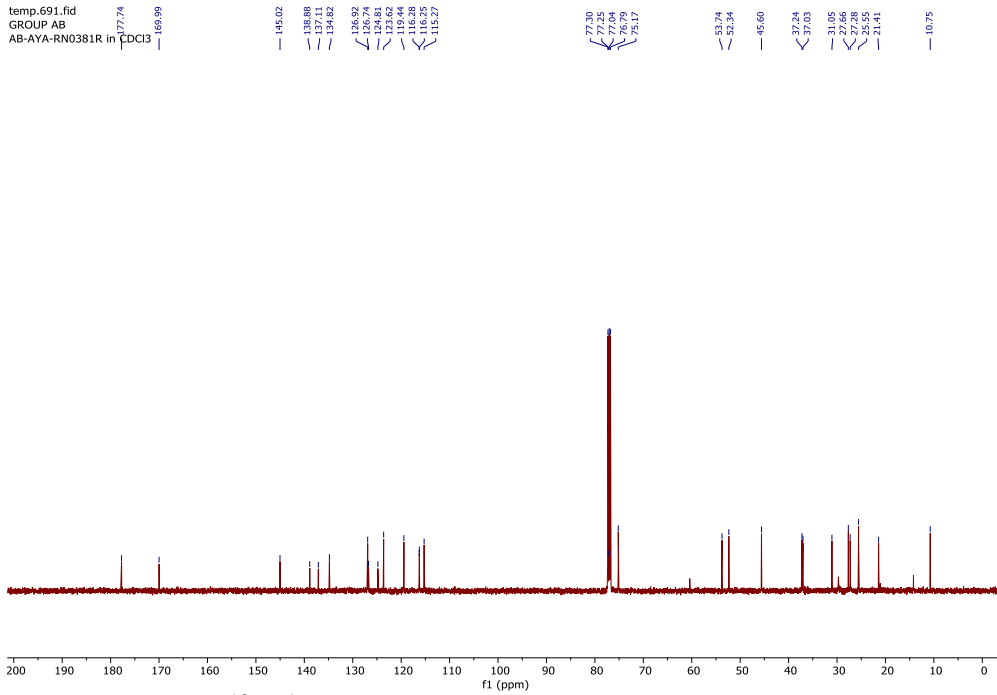


temp.690.fid
GROUP AB
AB-AYA-RN0381R in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-6

temp.691.fid
GROUP AB
AB-AYA-RN0381R in CDCl₃



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-6

Display Report

Analysis Info

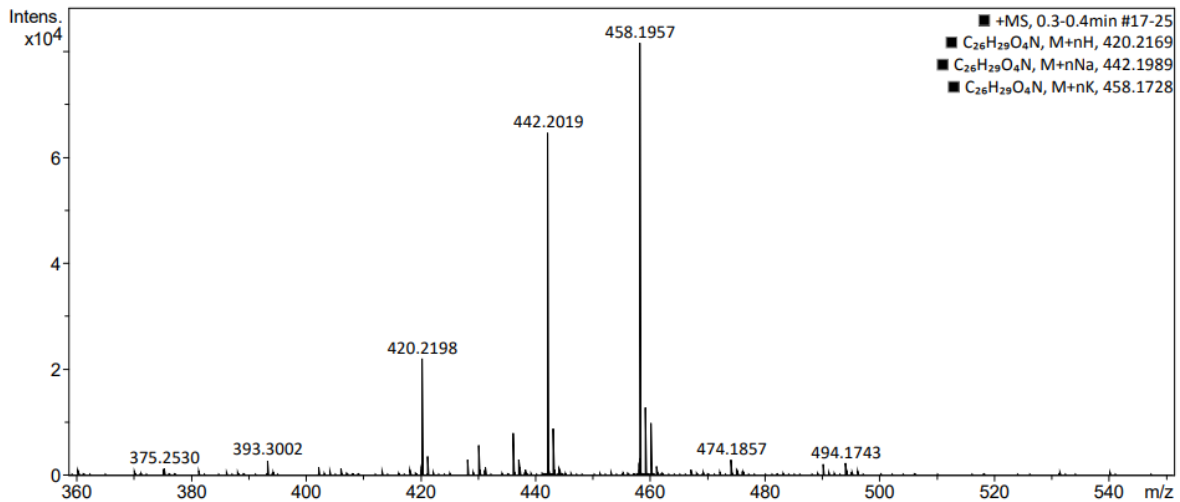
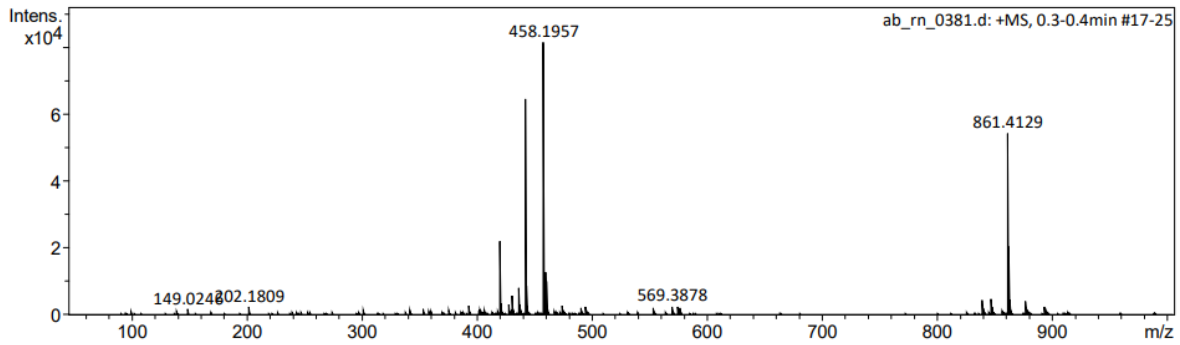
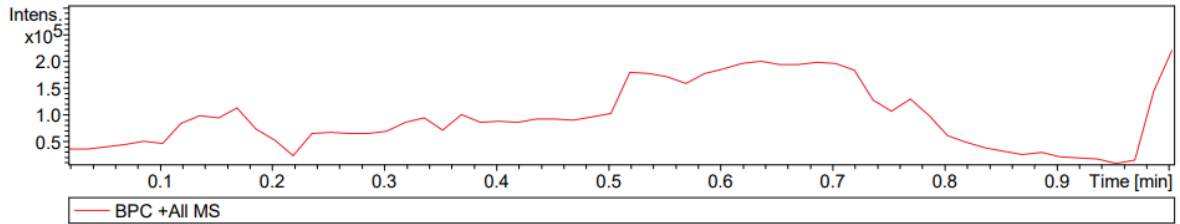
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Method Tune_pos_Standard.m
Sample Name ab_rn_0381
Comment signal dropping issue

Acquisition Date 3/7/2022 11:57:33 AM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_rn_0381.d

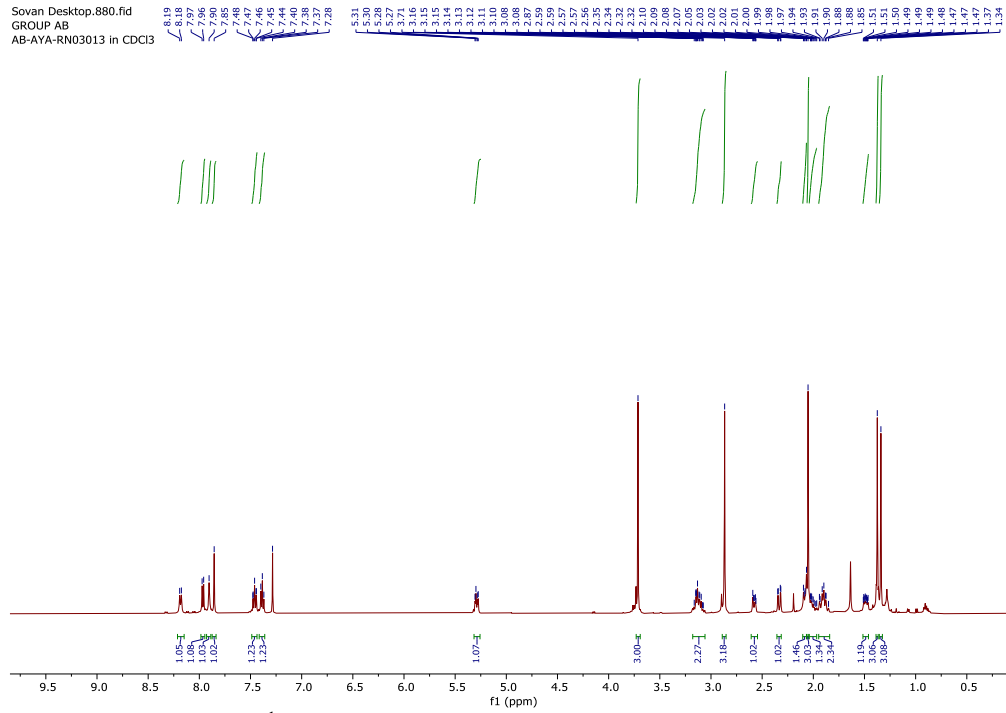
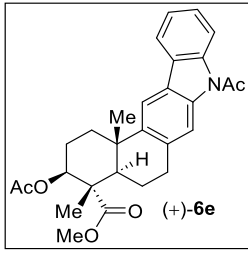
Bruker Compass DataAnalysis 4.1

printed: 3/7/2022 11:59:59 AM

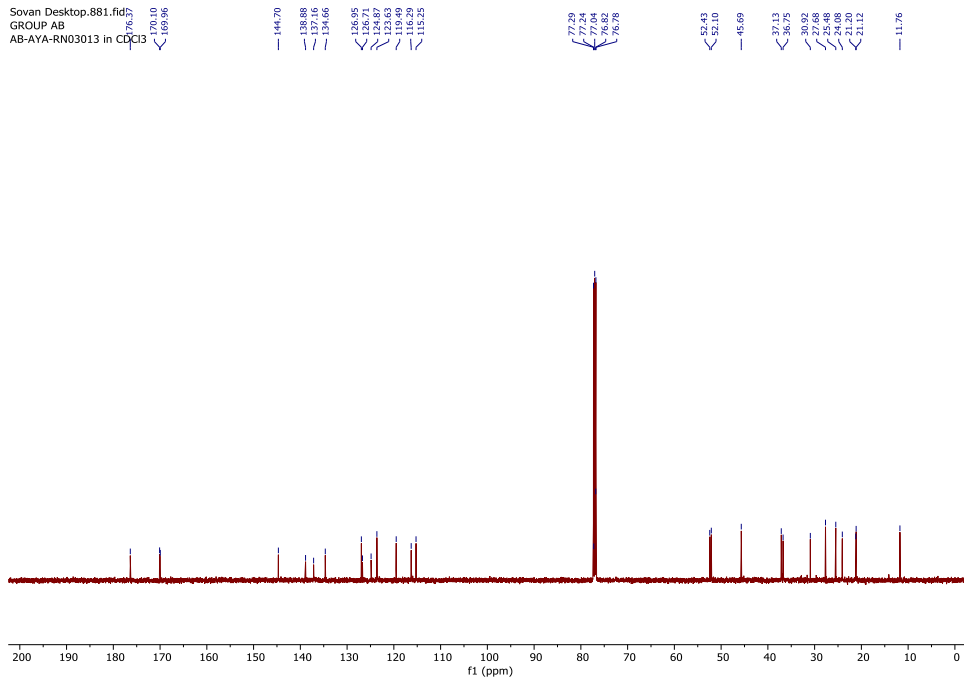
by: IISER Kolkata

Page 1 of 1

HRMS data of (+)-6



¹H NMR (500 MHz, CDCl₃) of (+)-6e

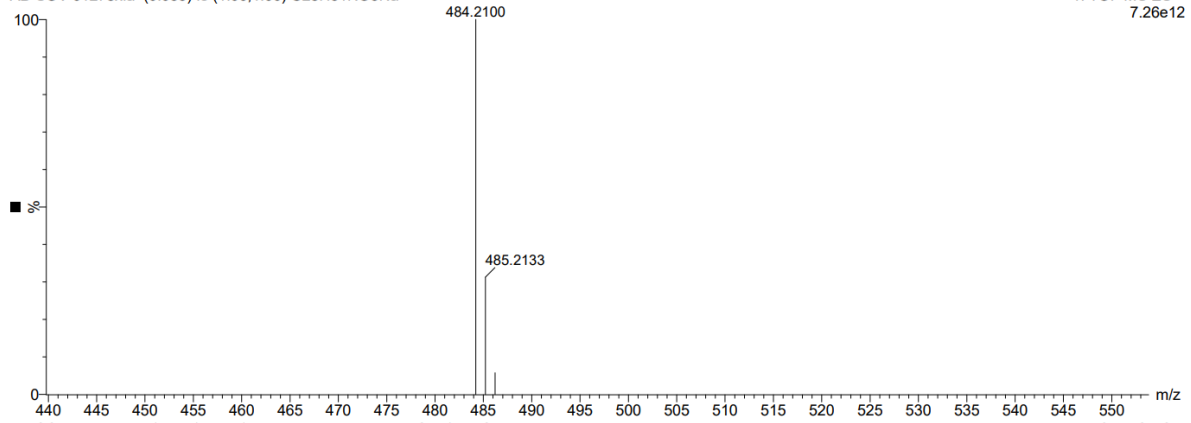


¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-6e

AB28-Mar-2024 14:04:00
AB-SOV-01278xia (0.053) Is (1.00,1.00) C28H31NO5Na

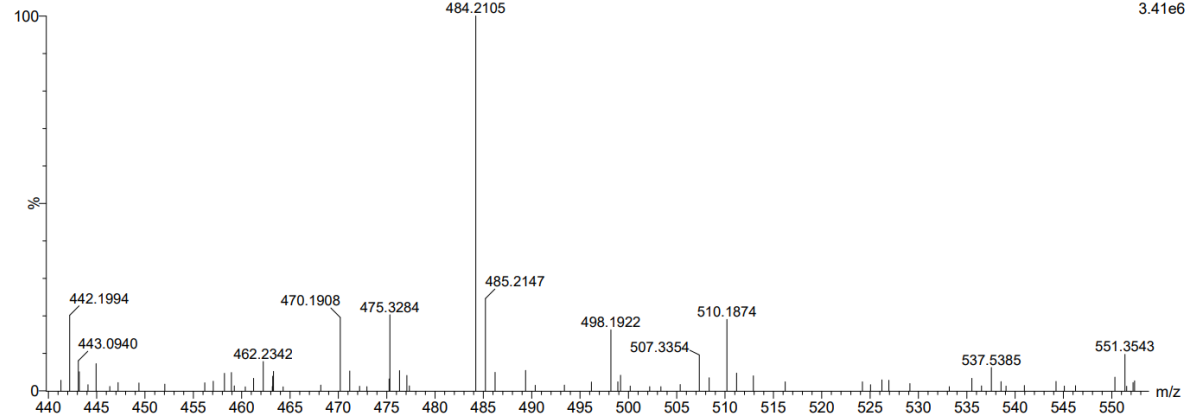
IISER - KOLKATA

1: TOF MS ES+
7.26e12

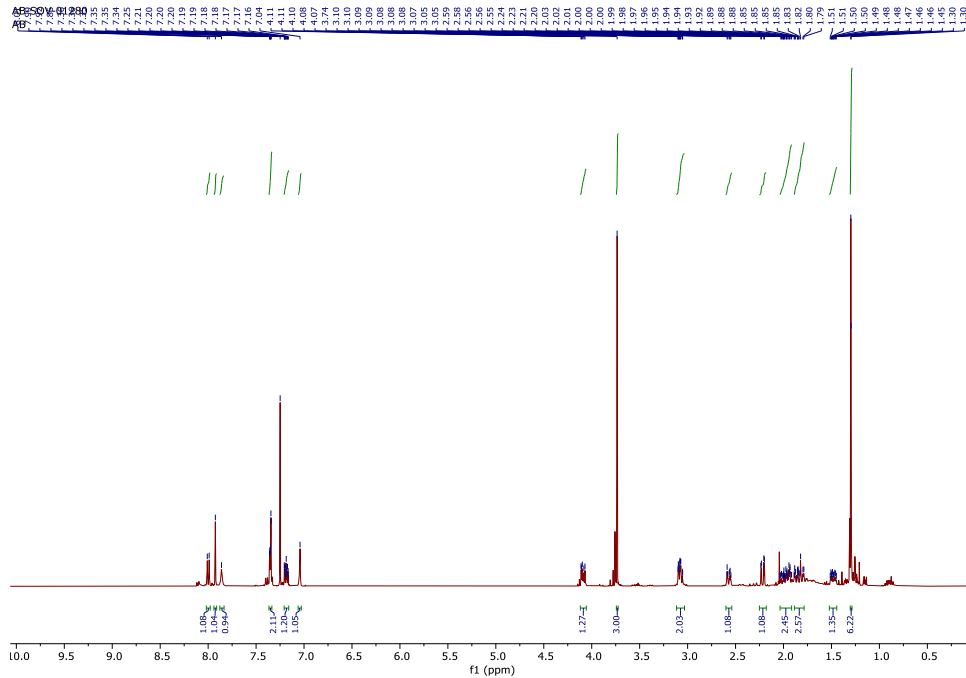
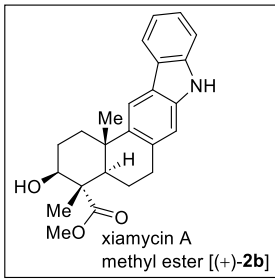


AB-SOV-01278xia 3 (0.087) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

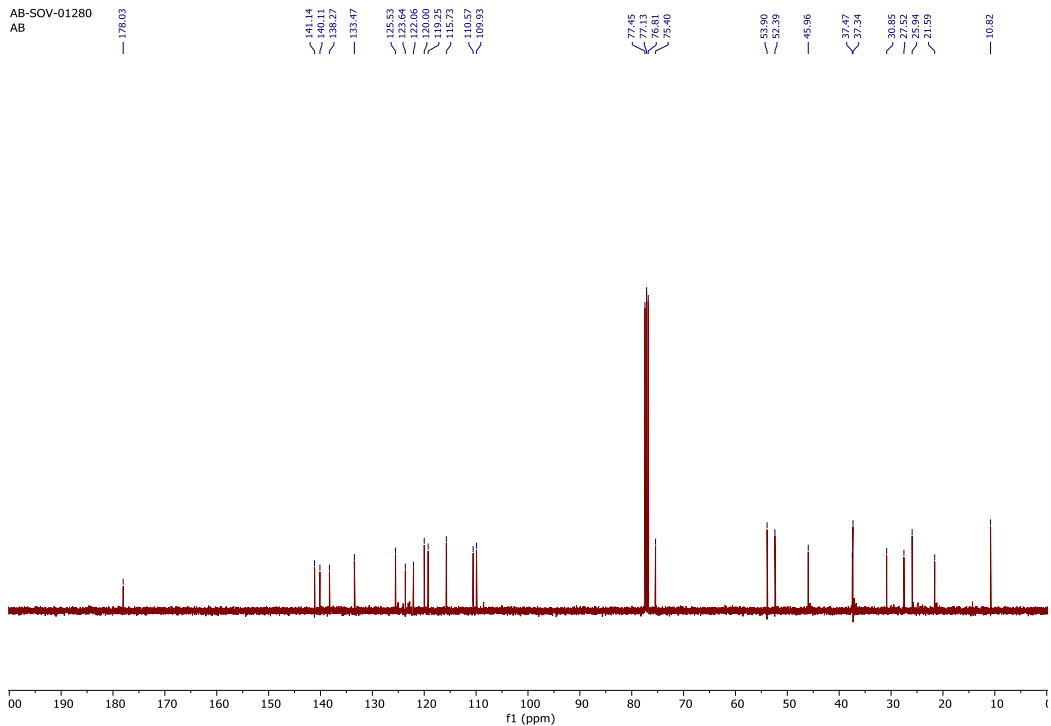
1: TOF MS ES+
3.41e6



HRMS data of (+)-6e



^1H NMR (500 MHz, CDCl_3) of xiamycin A methylester (+)-2b



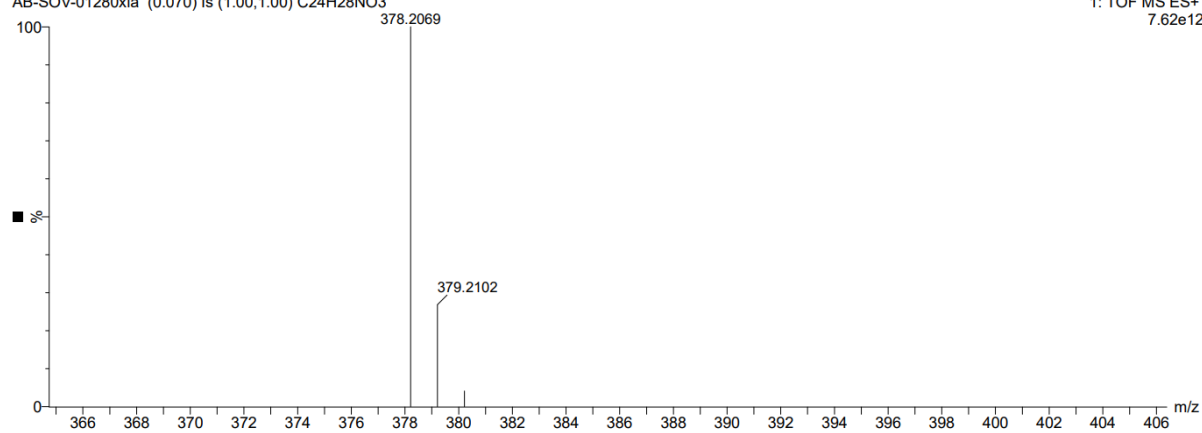
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of xiamycin A methylester (+)-2b

AB28-Mar-2024 12:33:35

IISER - KOLKATA

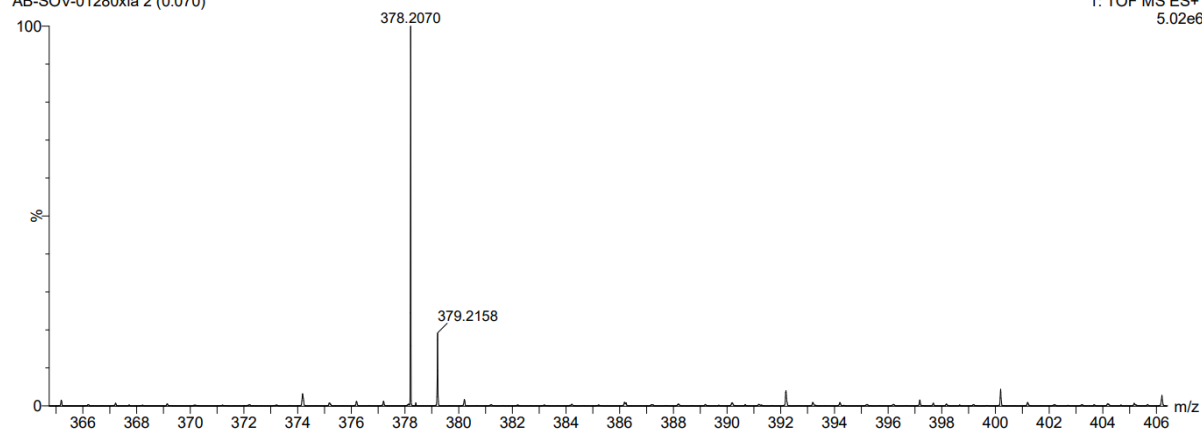
1: TOF MS ES+
7.62e12

AB-SOV-01280xia (0.070) Is (1.00,1.00) C₂₄H₂₈NO₃

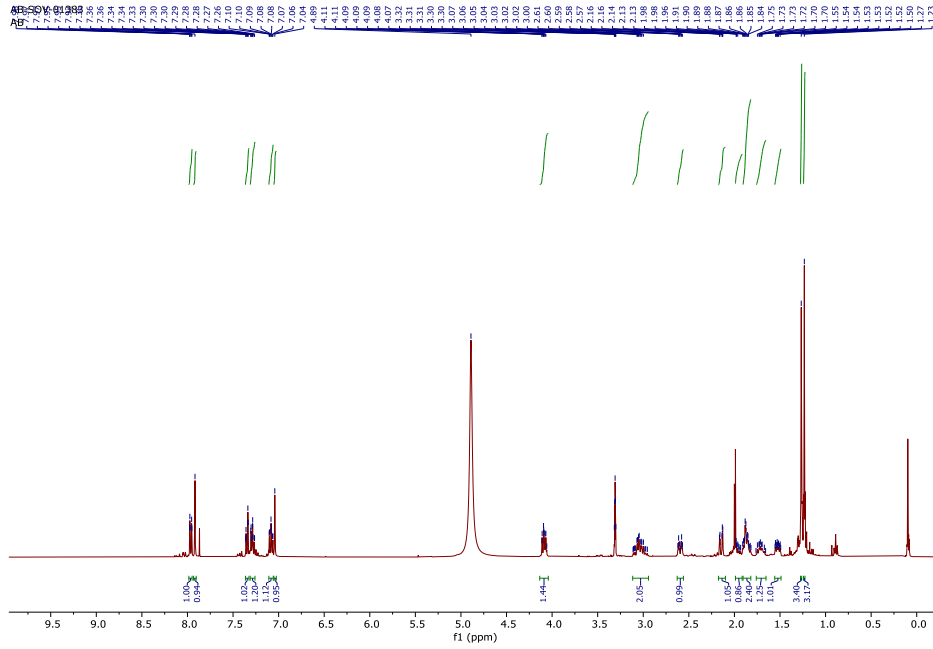
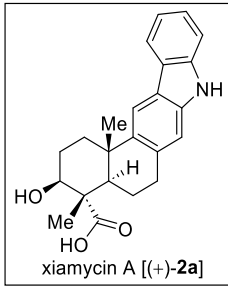


AB-SOV-01280xia 2 (0.070)

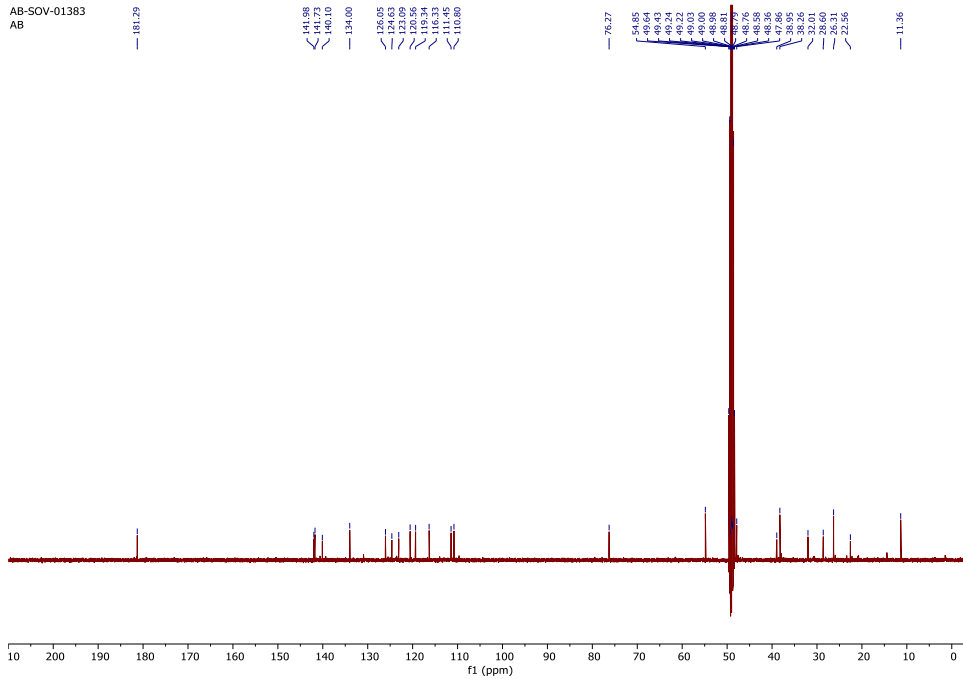
1: TOF MS ES+
5.02e6



HRMS data of xiamycin A methylester (+)-**2b**



¹H NMR (400 MHz, CD₃OD) of xiamycin A [(+)-2a]



¹³C {¹H} NMR (100 MHz, CD₃OD) of xiamycin A [(+)-2a]

Display Report

Analysis Info

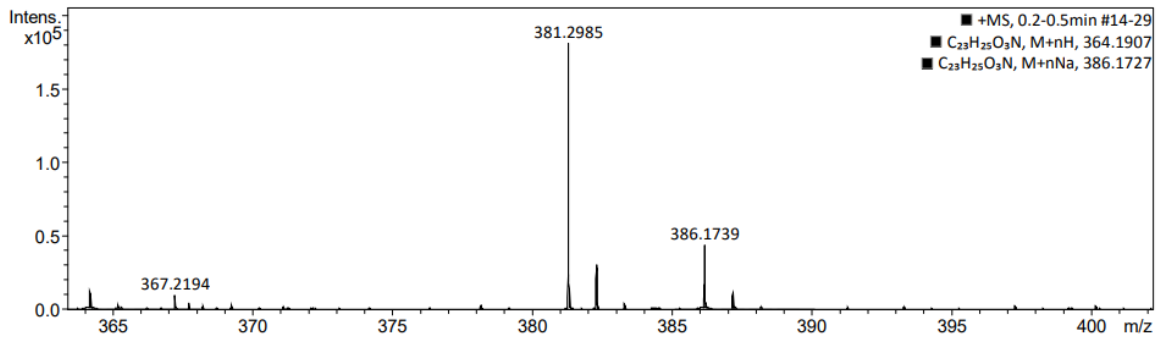
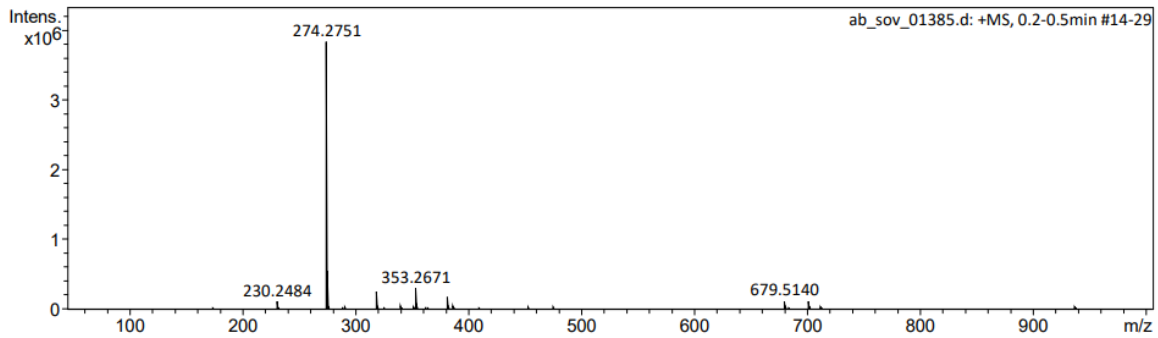
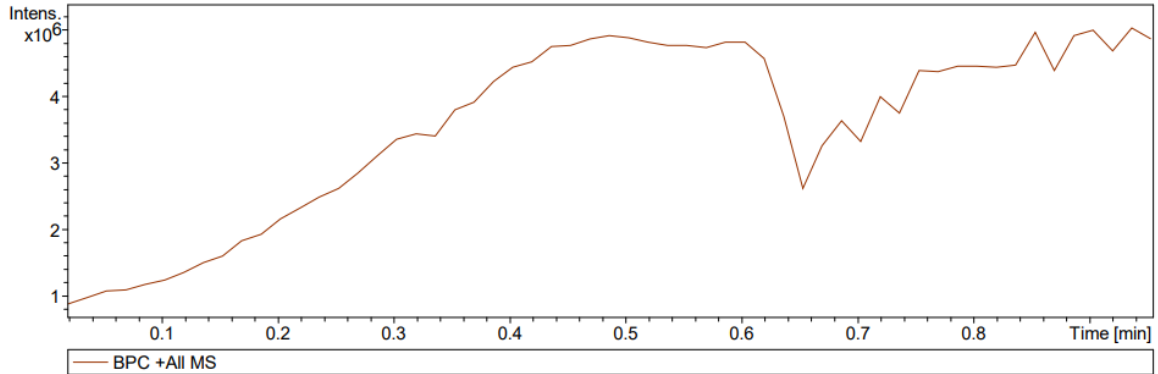
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Method Tune_pos_Standard_JAN2024.new.m
Sample Name ab_sov_01385
Comment

Acquisition Date 1/16/2024 12:58:35 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

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ab_sov_01385.d

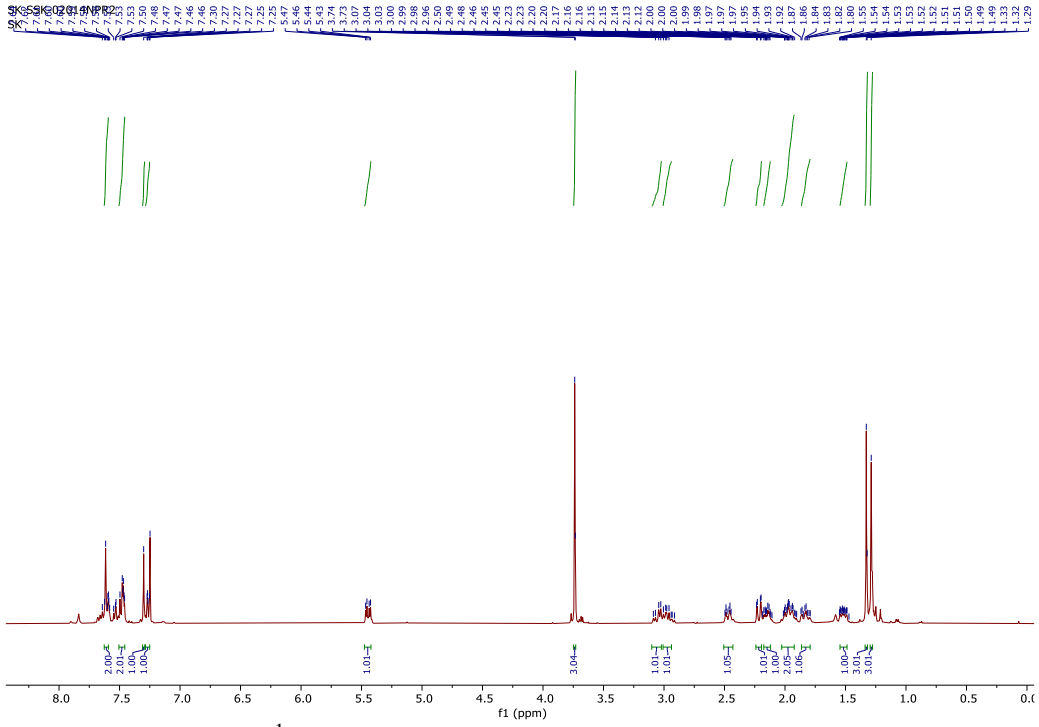
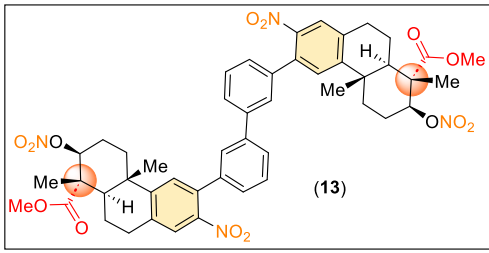
Bruker Compass DataAnalysis 4.1

printed: 1/16/2024 1:02:11 PM

by: IISER Kolkata

Page 1 of 1

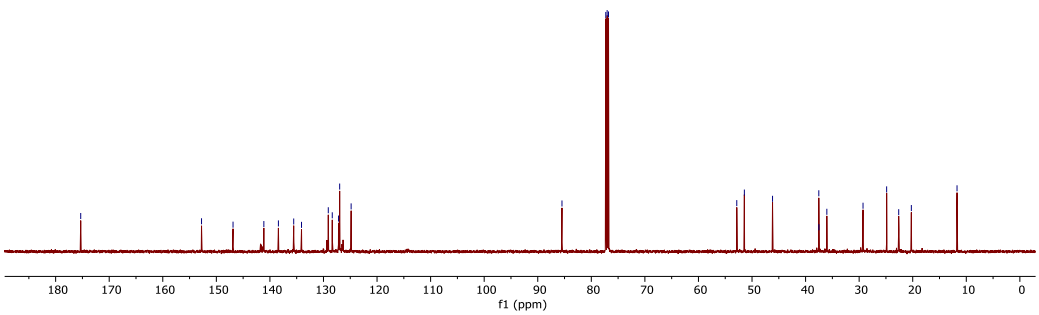
HRMS data of xiamycin A [(+)-2a]



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

Sovan Nmr. 410.fid
GROUP AB
AB-SOV-02014NPR2 in CDCl_3

152.76
146.88
141.13
138.41
135.56
134.10
128.36
127.19
126.98
124.84
85.48
77.30
77.04
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37.23
36.93
32.78
24.87
22.62
20.26
11.73

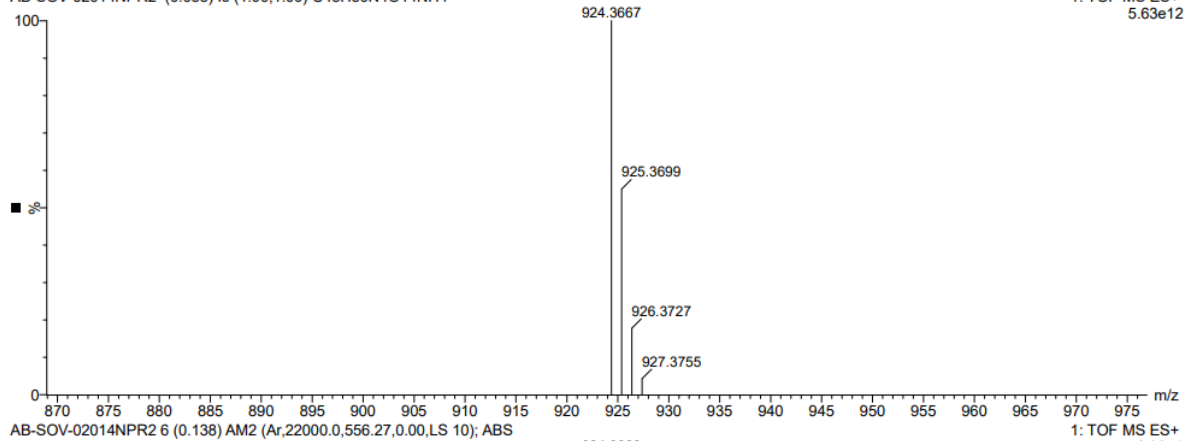


$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-13

AB29-Apr-2024 15:44:16
AB-SOV-02014NPR2 (0.053) Is (1.00,1.00) C₄₈H₅₀N₄O₁₄NH₄

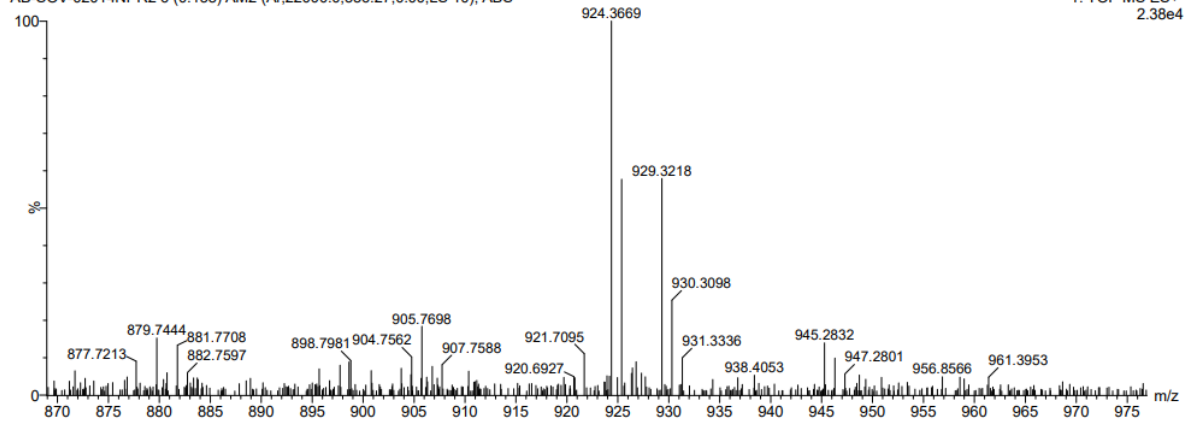
IISER - KOLKATA

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5.63e12

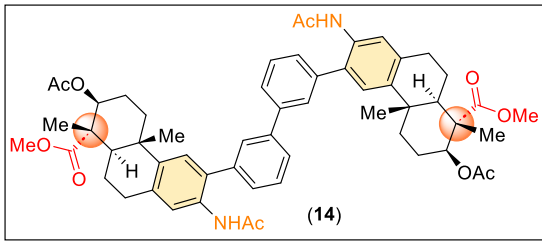


AB-SOV-02014NPR2 6 (0.138) AM2 (Ar,22000.0,556.27,0.00,LS 10); ABS

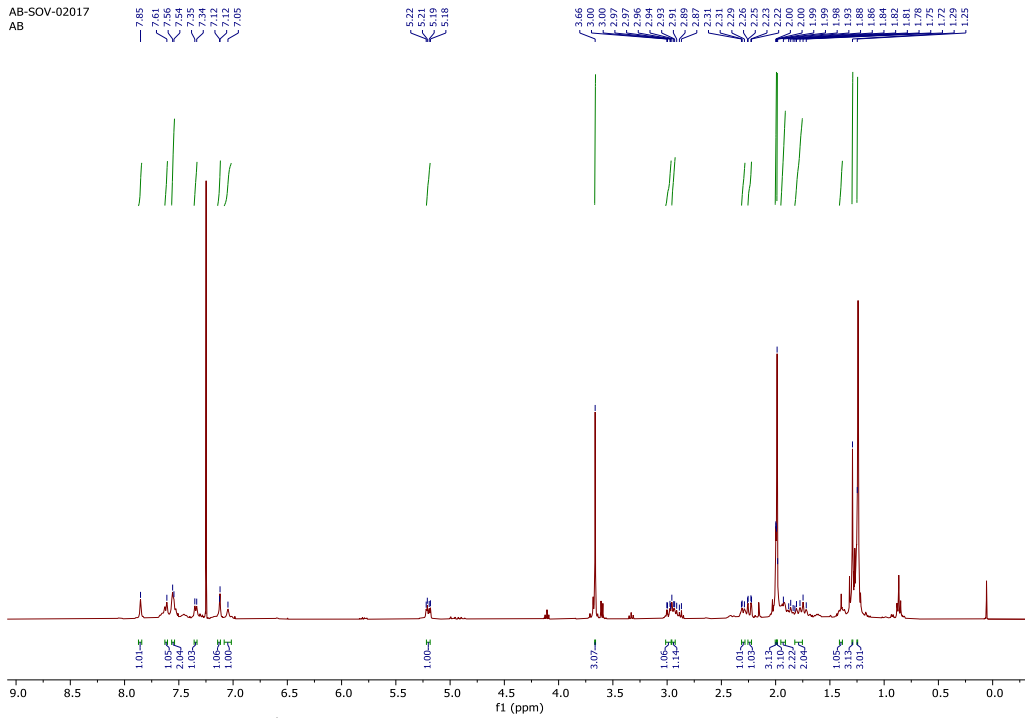
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2.38e4



HRMS data of (+)-**13**

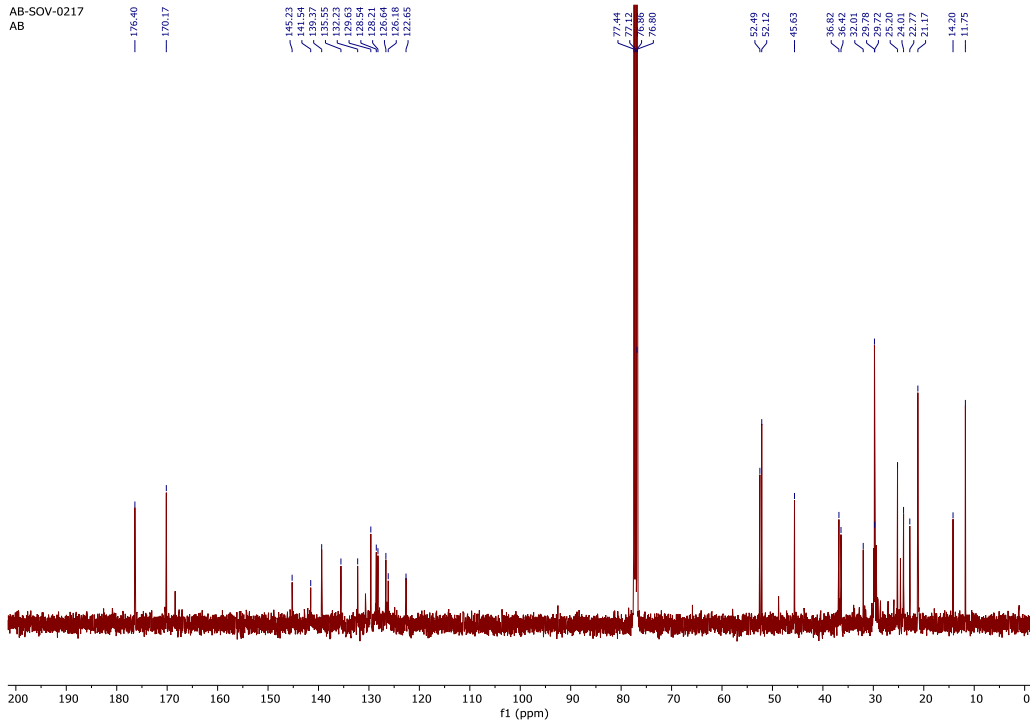


AB-SOV-02017
AB



^1H NMR (500 MHz, CDCl_3) of (+)-14

AB-SOV-0217
AB

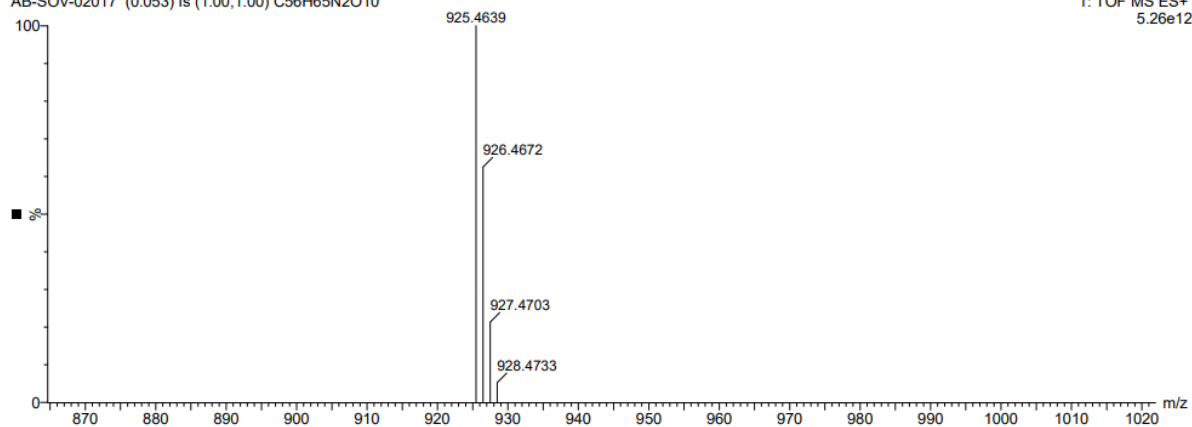


$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-14

AB22-Apr-2024 13:10:19
AB-SOV-02017 (0.053) Is (1.00,1.00) C56H65N2O10

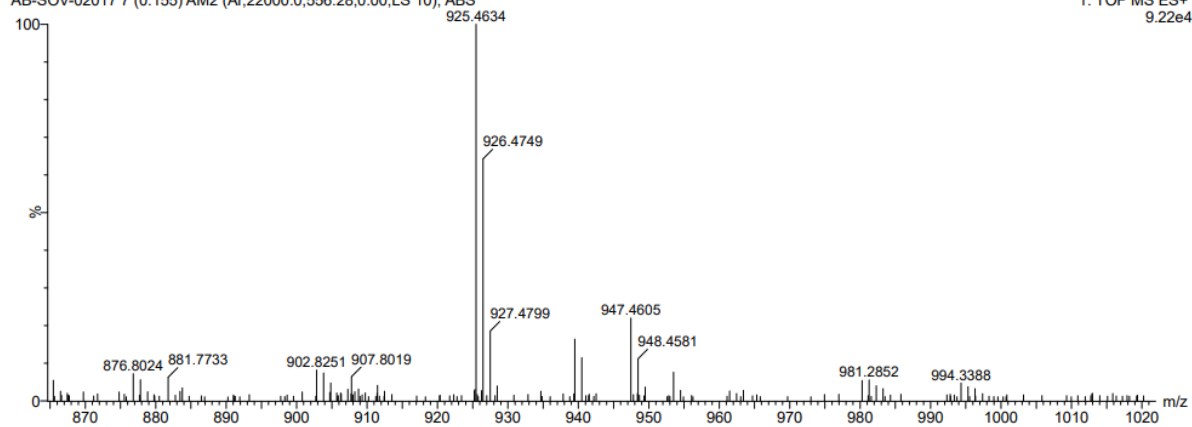
IISER - KOLKATA

1: TOF MS ES+
5.26e12

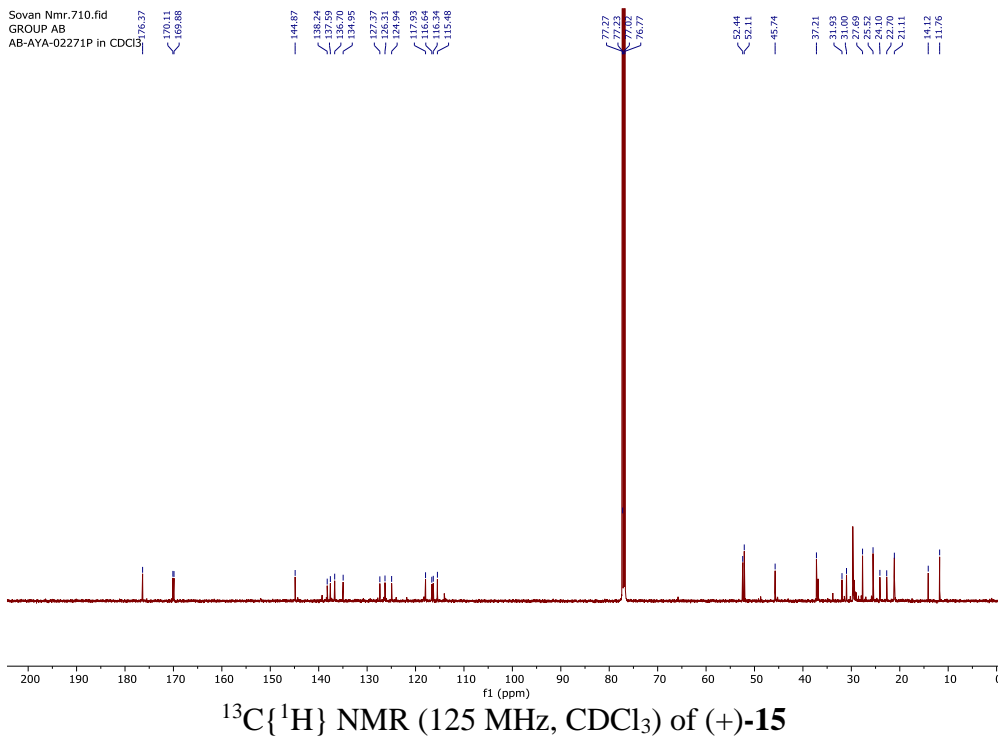
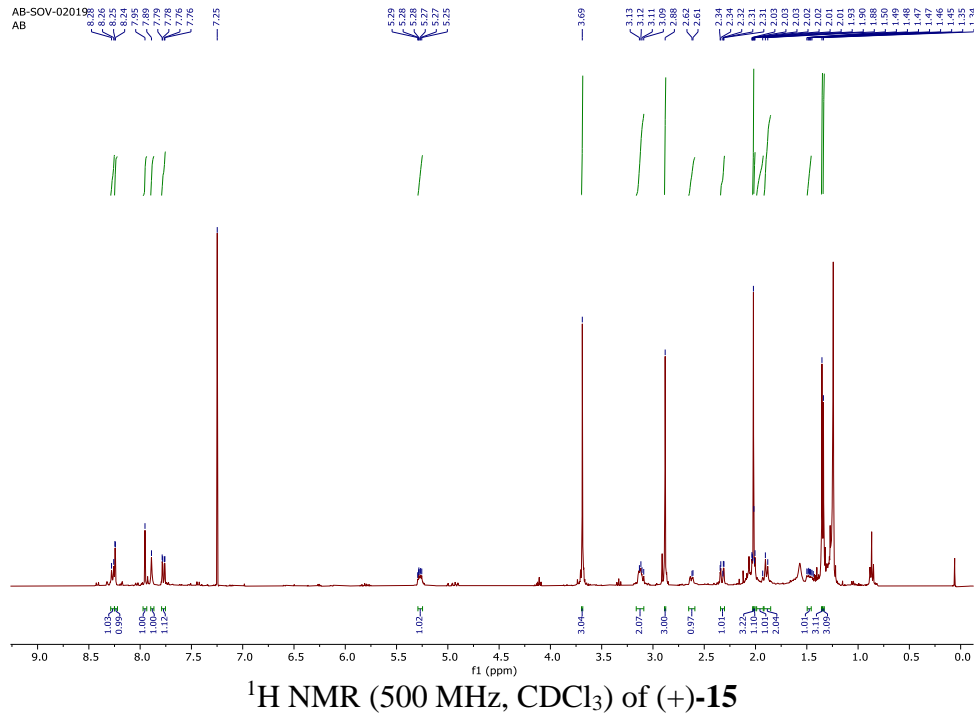
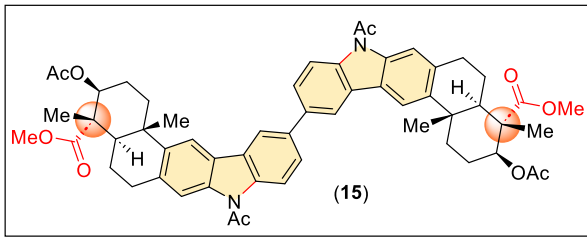


AB-SOV-02017 7 (0.155) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+
9.22e4



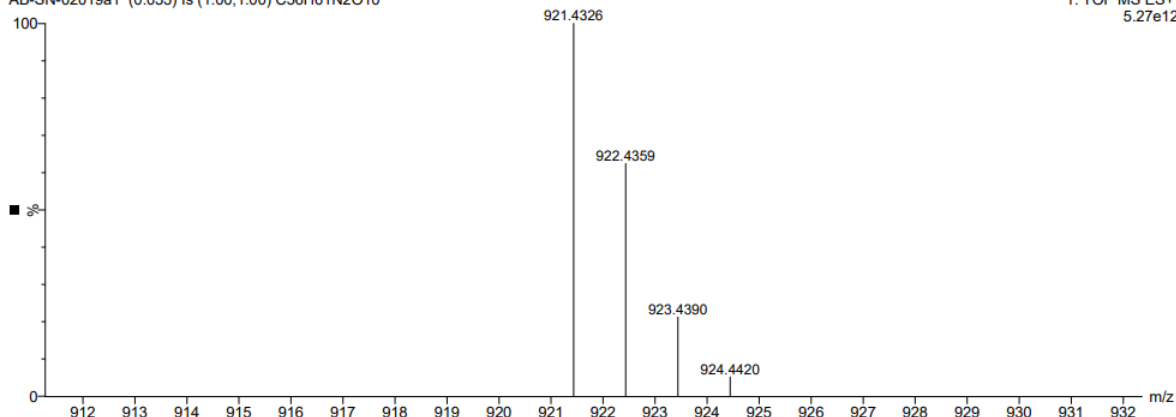
HRMS data of (+)-14



SKD24-Apr-202416:31:54
AB-SN-02019a1 (0.053) Is (1.00,1.00) C₅₆H₆₁N₂O₁₀

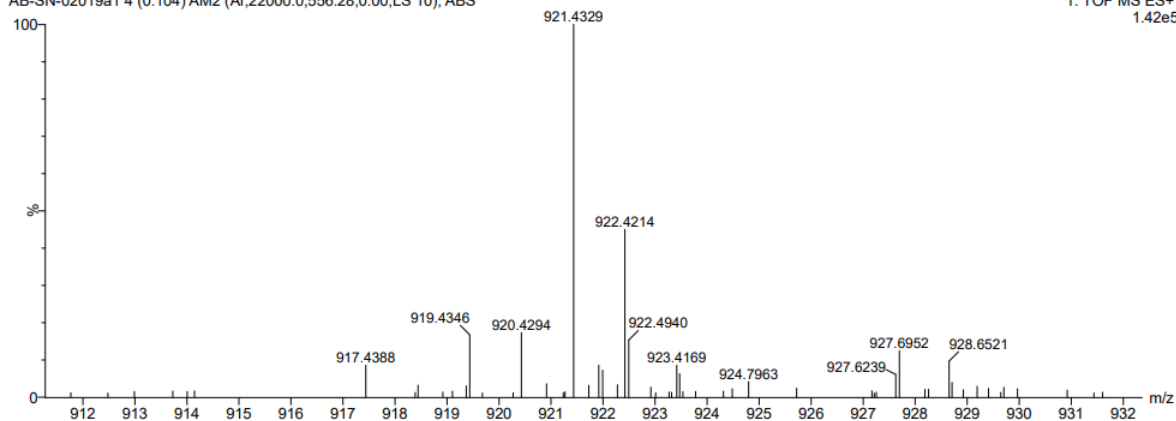
IISER - KOLKATA

1: TOF MS ES+
5.27e12

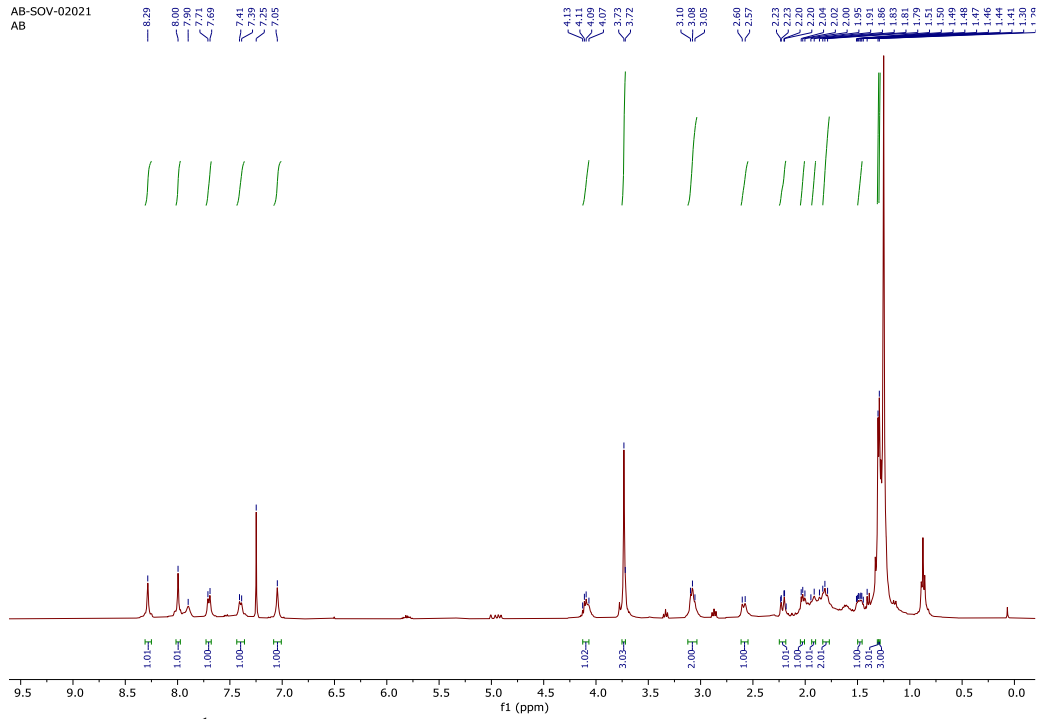
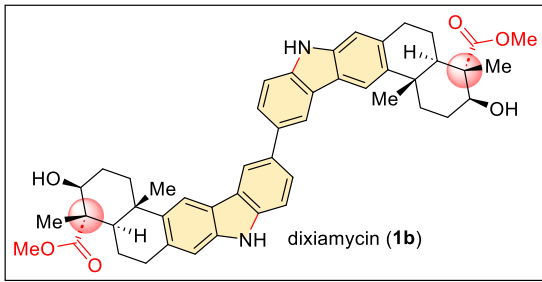


AB-SN-02019a1 4 (0.104) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

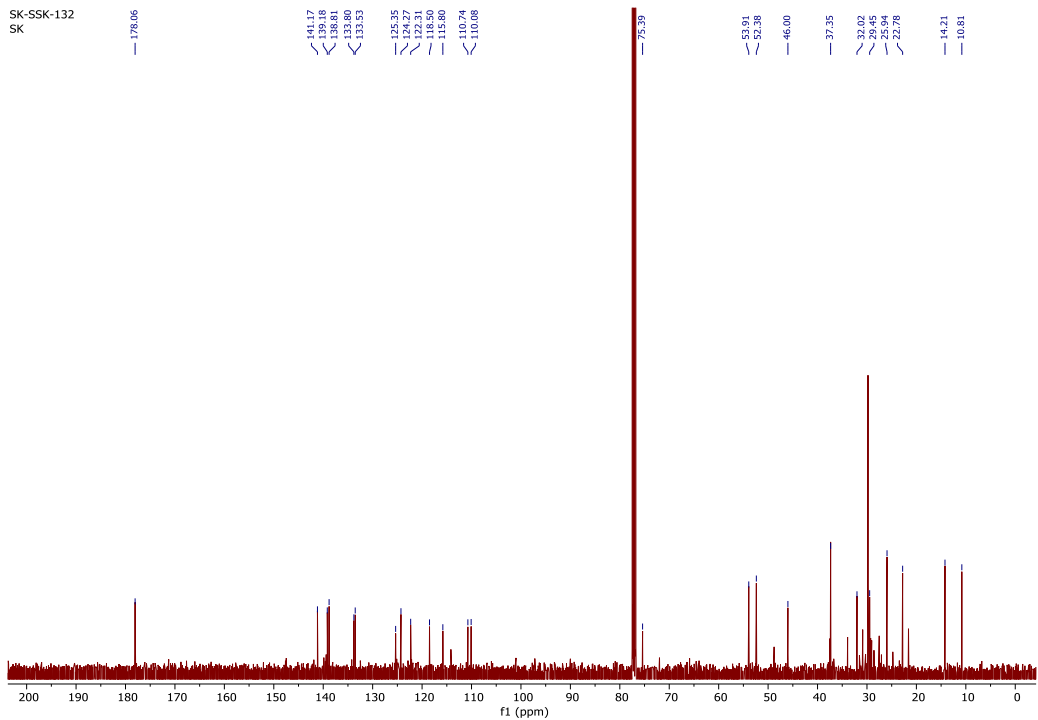
1: TOF MS ES+
1.42e5



HRMS data of (+)-15



¹H NMR (400 MHz, CDCl₃) of Compound (+)-1b



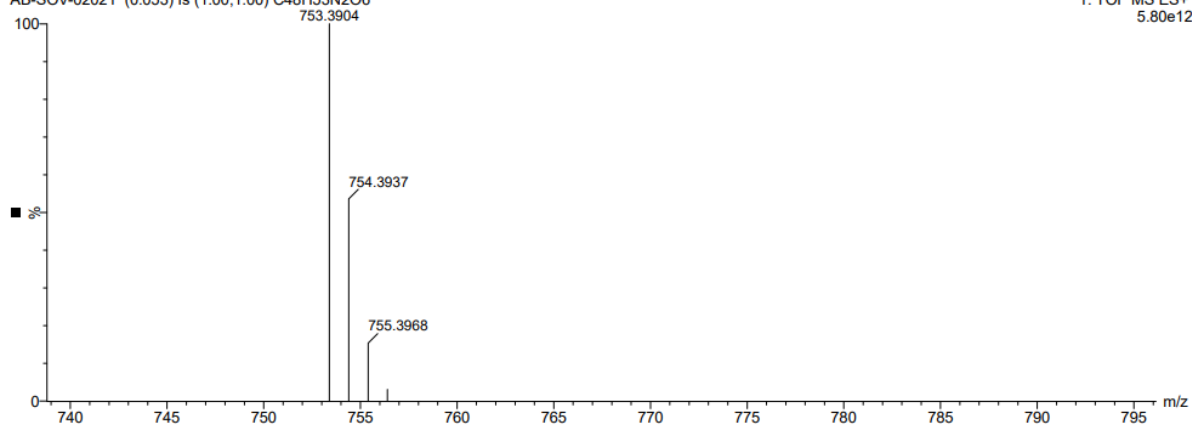
¹³C{¹H} NMR (125 MHz, CDCl₃) of compound (+)-1b

AB29-Apr-2024 15:45:48

AB-SOV-02021 (0.053) Is (1.00,1.00) C₄₈H₅₃N₂O₆

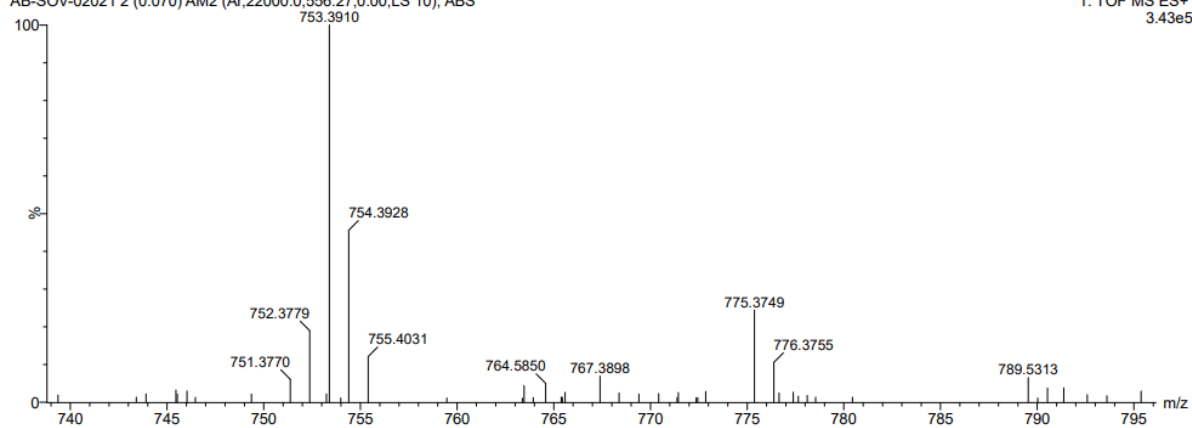
IISER - KOLKATA

1: TOF MS ES+
5.80e12

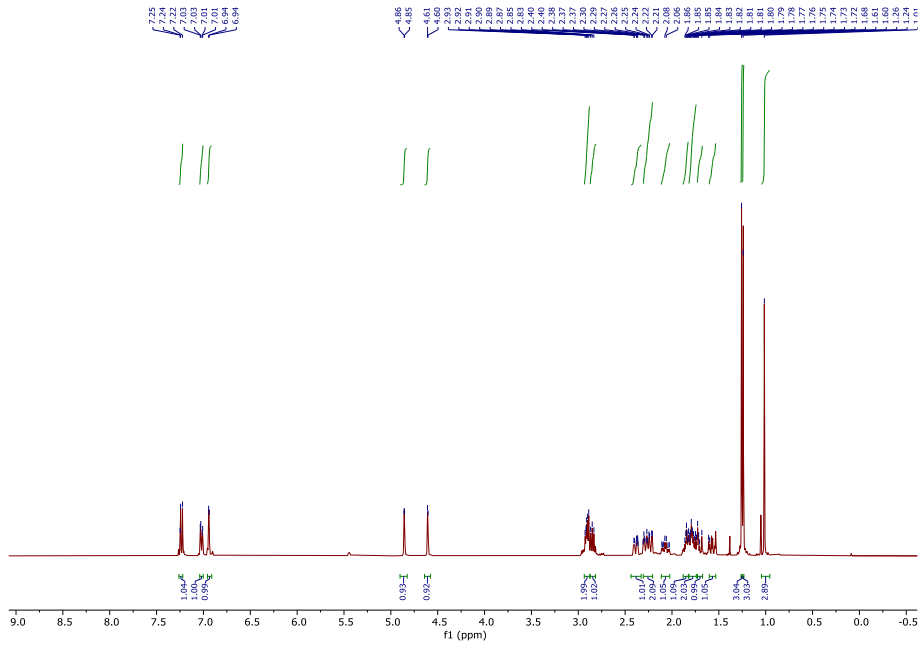
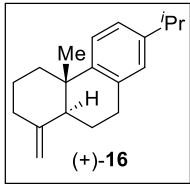


AB-SOV-02021 2 (0.070) AM2 (Ar,22000.0,556.27,0.00,LS 10); ABS

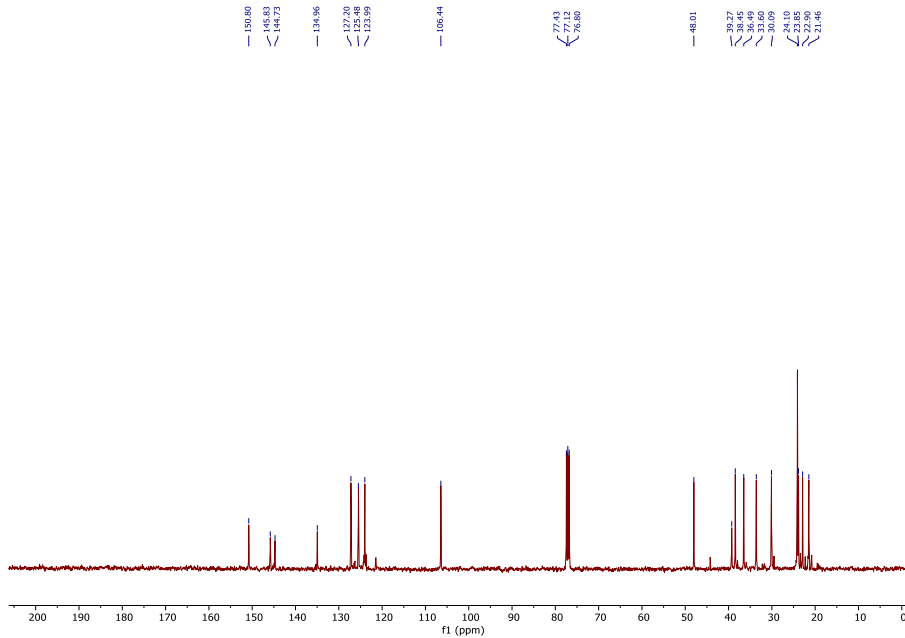
1: TOF MS ES+
3.43e5



HRMS data of (+)-**1b**



^1H NMR (400 MHz, CDCl_3) of compound (+)-16



$^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) of compound (+)-16

Display Report

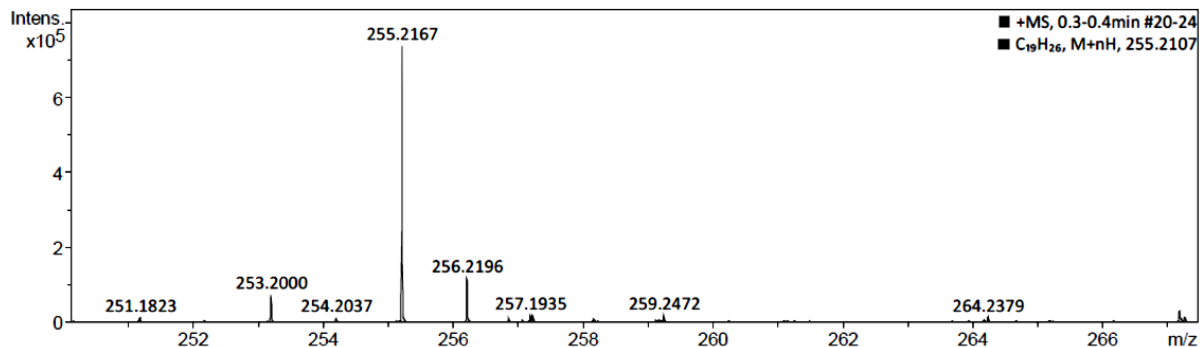
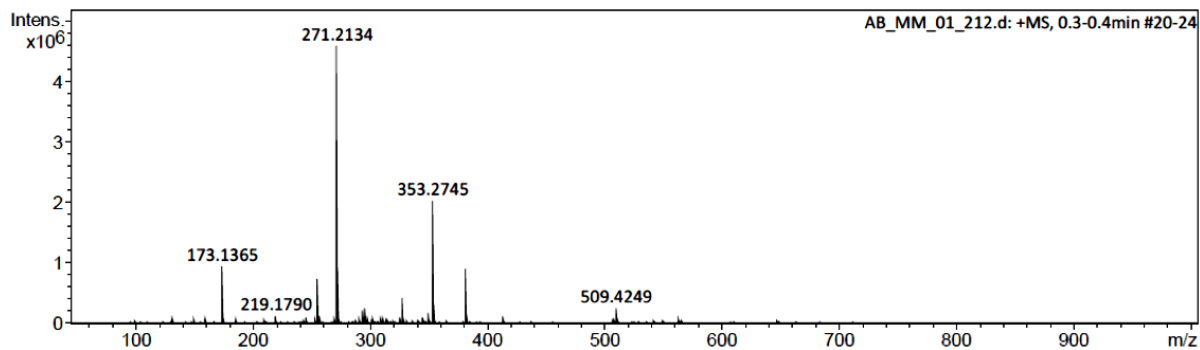
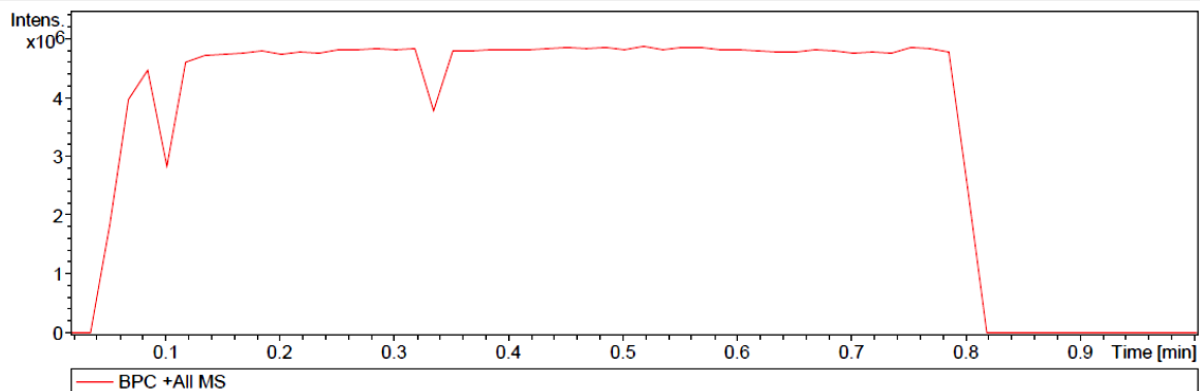
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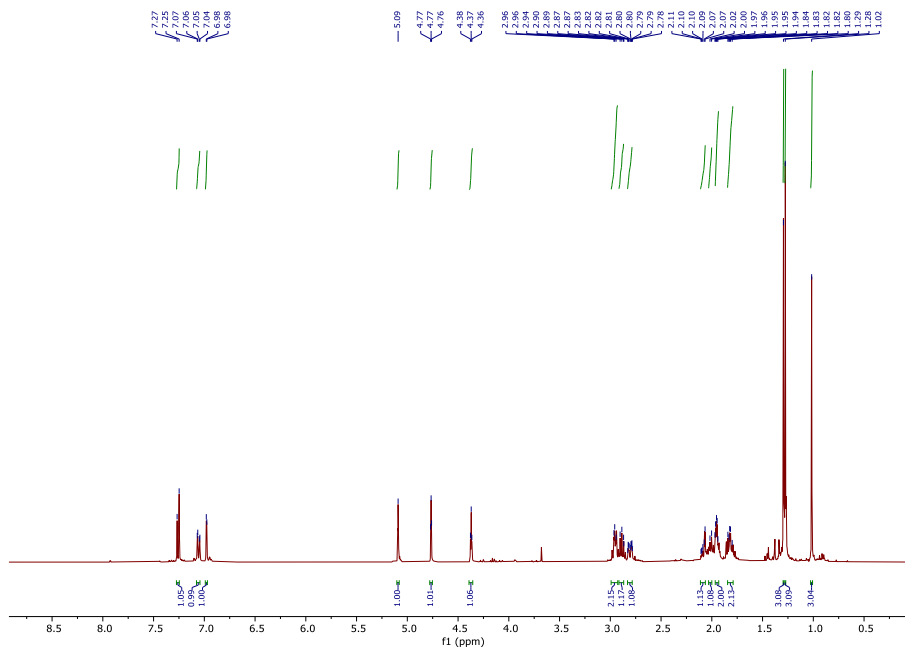
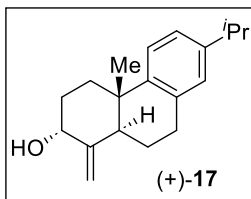
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Method Tune_pos_Standard.m
Sample Name AB_MM_01_212
Comment

Acquisition Date 12/14/2021 3:02:21 PM
Operator IISER Kolkata
Instrument maXis impact 8282001.00127

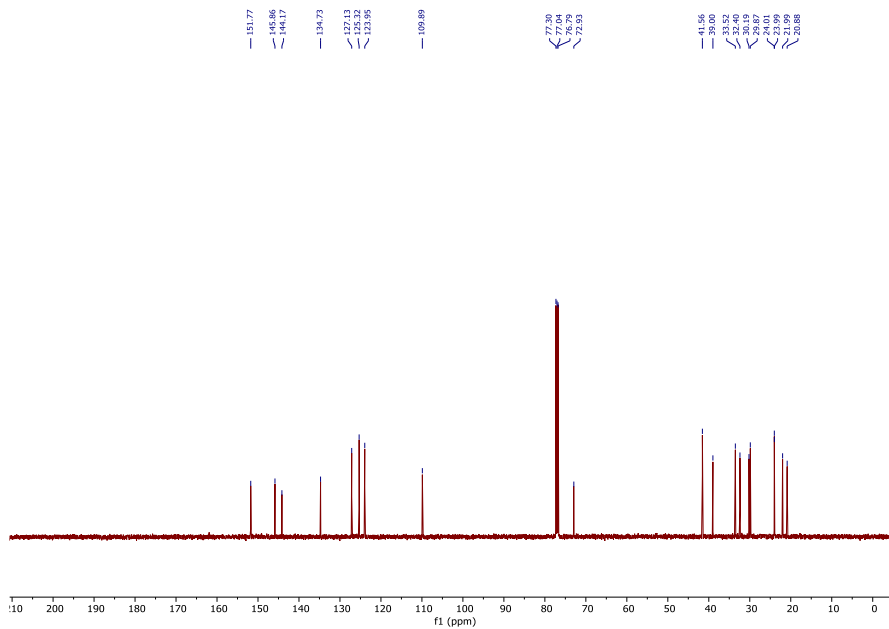
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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





^1H NMR (400 MHz, CDCl_3) of compound (+)-17



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of compound (+)-17

Display Report

Analysis Info

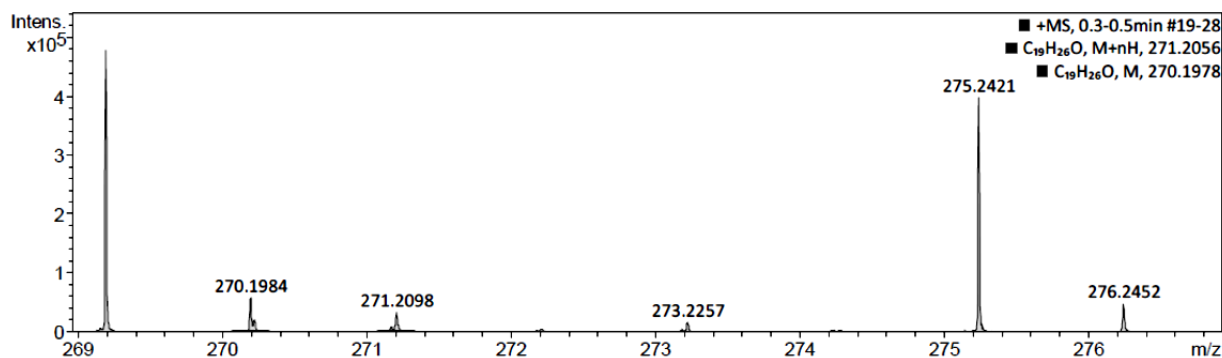
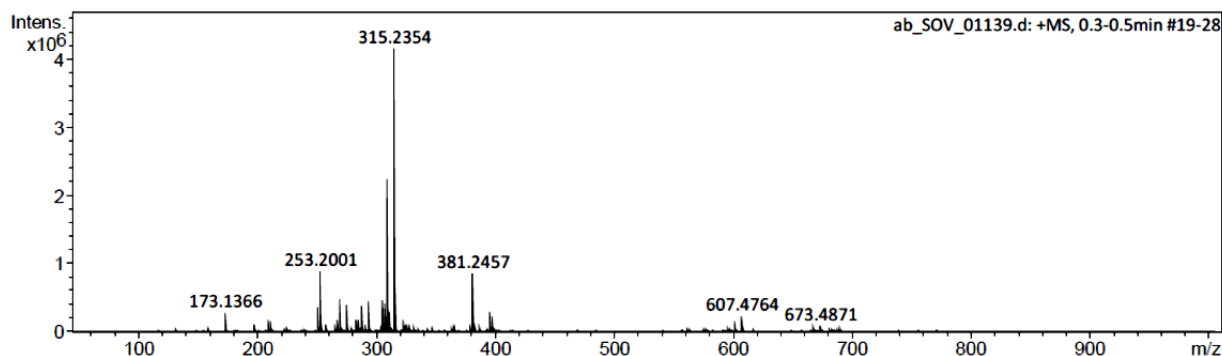
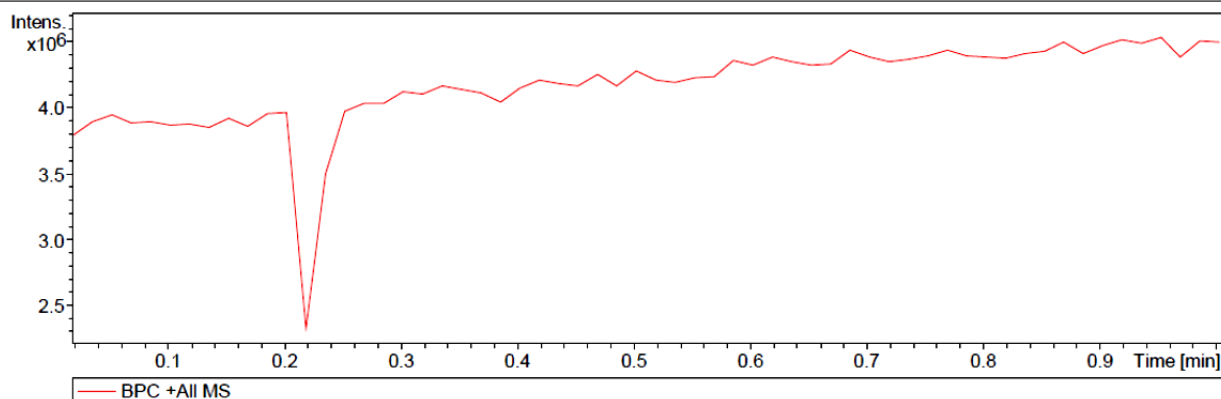
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Method Tune_pos_Standard.m
Sample Name ab_SOV_01139
Comment

Acquisition Date 12/14/2021 11:26:04 AM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
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Display Report

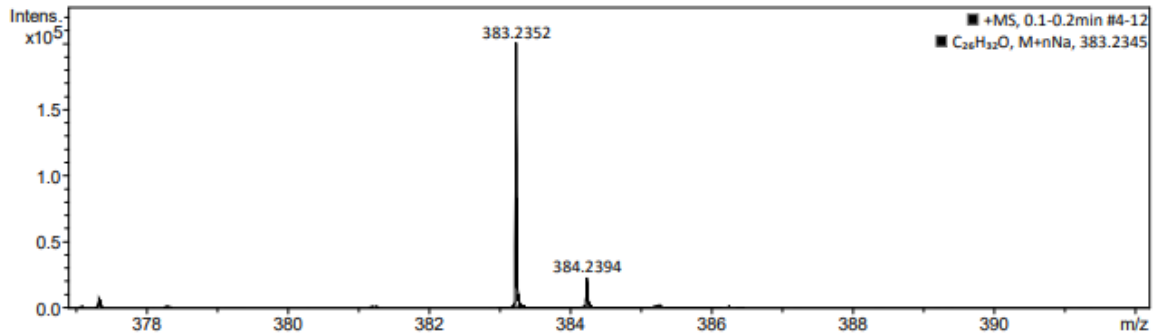
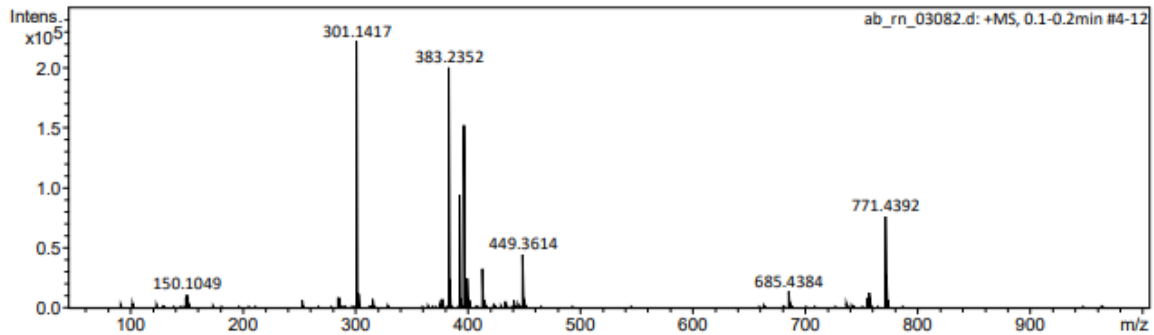
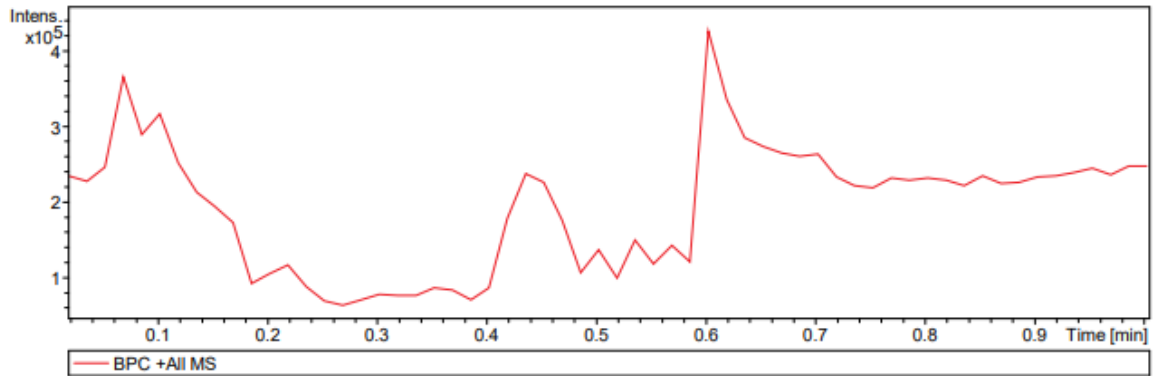
Analysis Info

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Method Tune_pos_Standard.m
Sample Name ab_m_03082
Comment

Acquisition Date 5/12/2022 12:01:20 PM
Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_m_03082.d

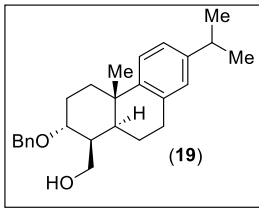
Bruker Compass DataAnalysis 4.1

printed: 5/12/2022 12:05:14 PM

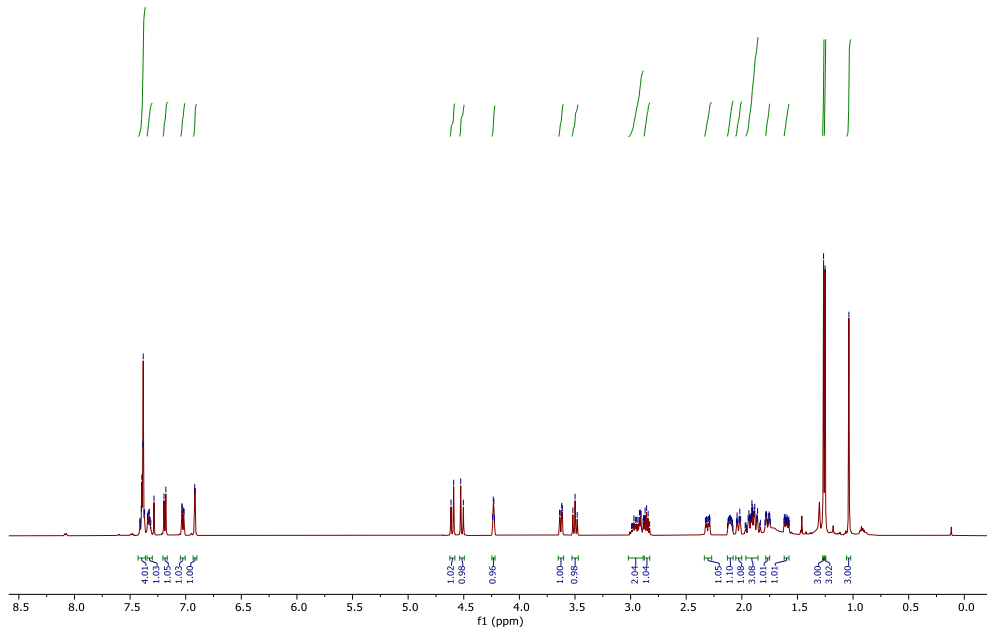
by: IISER Kolkata

Page 1 of 1

HRMS data for (+)-18

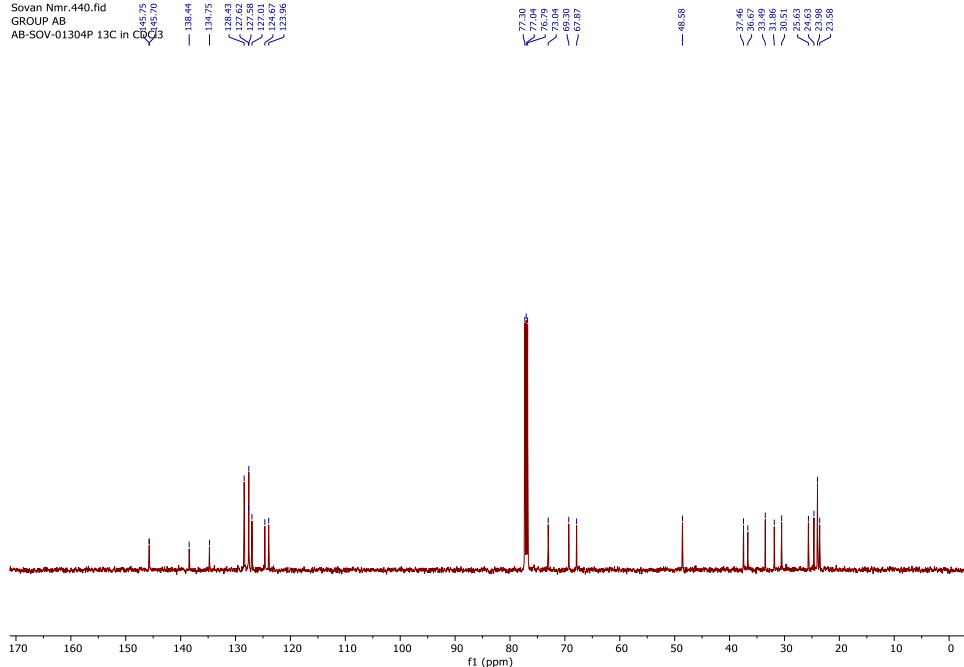


Sovan Nmr-440.fid
GROUP AB
AB-SOV-01304P 1H in CDCl3



¹H NMR (400 MHz, CDCl₃) of (+)-**19**

Sovan Nmr-440.fid
GROUP AB
AB-SOV-01304P 13C in CDCl3



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-**19**

Display Report

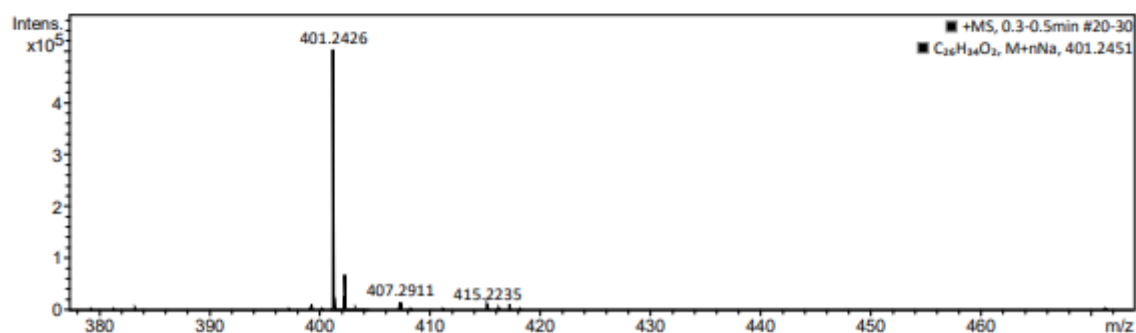
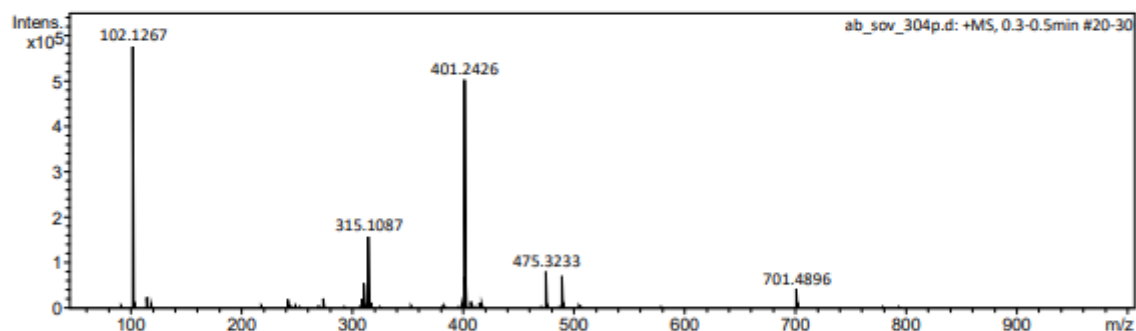
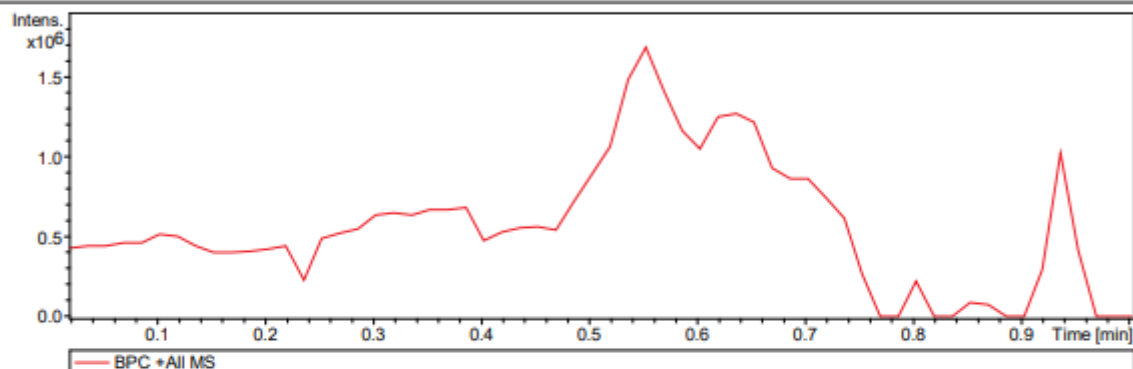
Analysis Info

Analysis Name D:\Data\User data\2022\MAY\lab_sov_304p.d
Method Tune_pos_Standard.m
Sample Name ab_sov_304p
Comment

Acquisition Date 5/23/2022 1:18:48 PM
Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_sov_304p.d

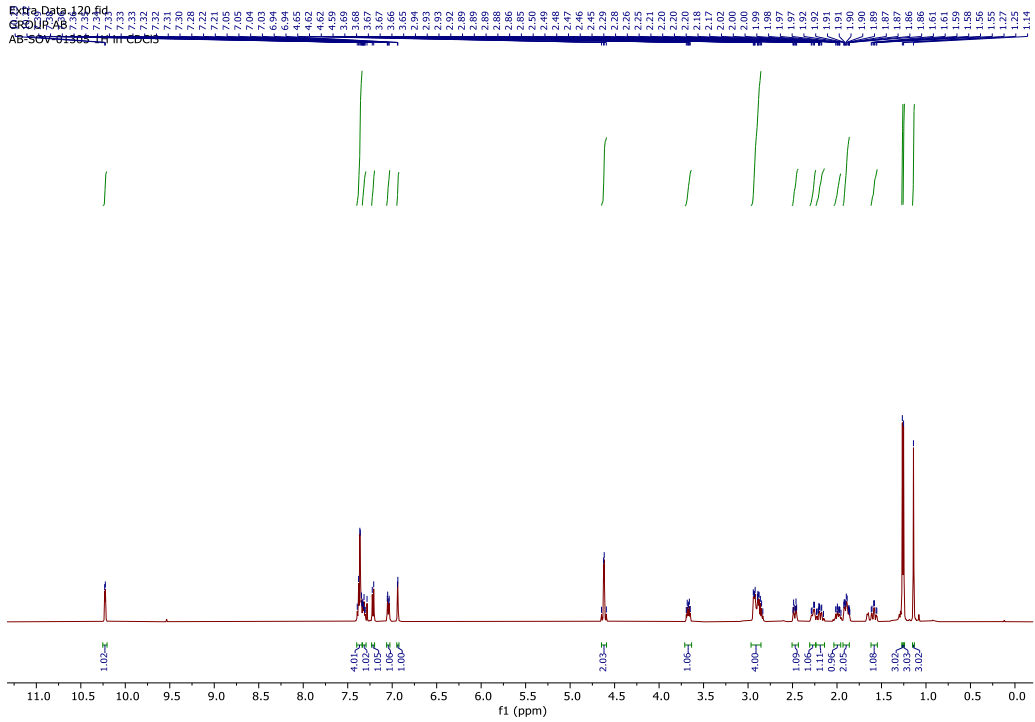
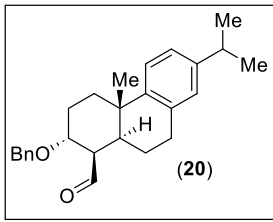
Bruker Compass DataAnalysis 4.1

printed: 5/23/2022 1:20:55 PM

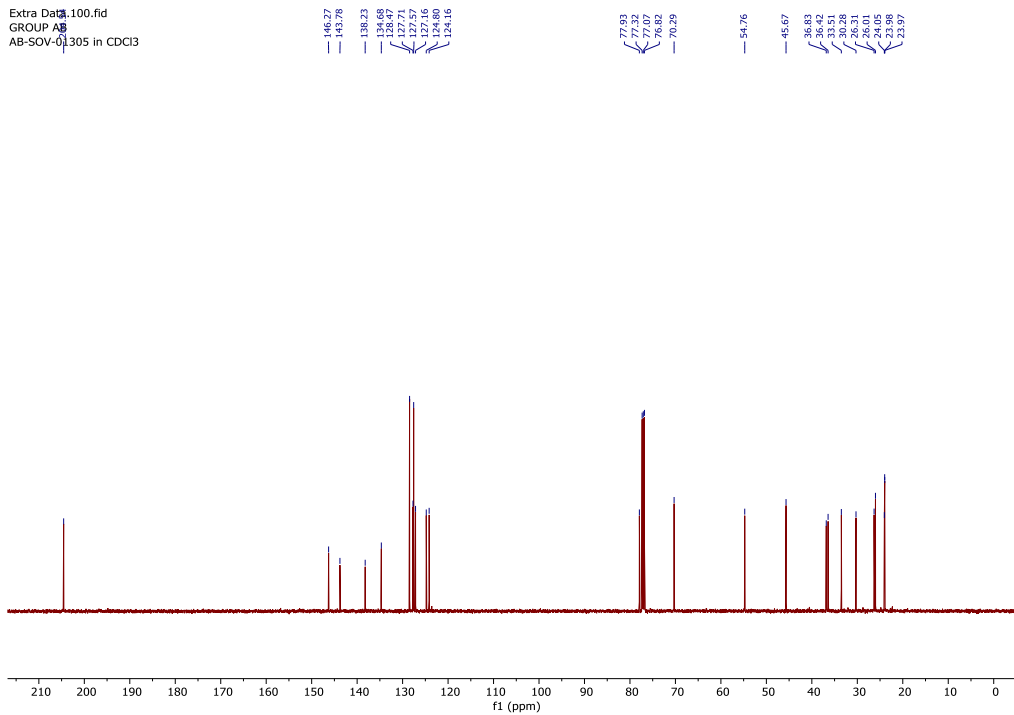
by: IISER Kolkata

Page 1 of 1

HRMS data for (+)-19



Extra Data: 100.fid
 GROUP AB
 AB-SOV-01305 in CDCl₃



Display Report

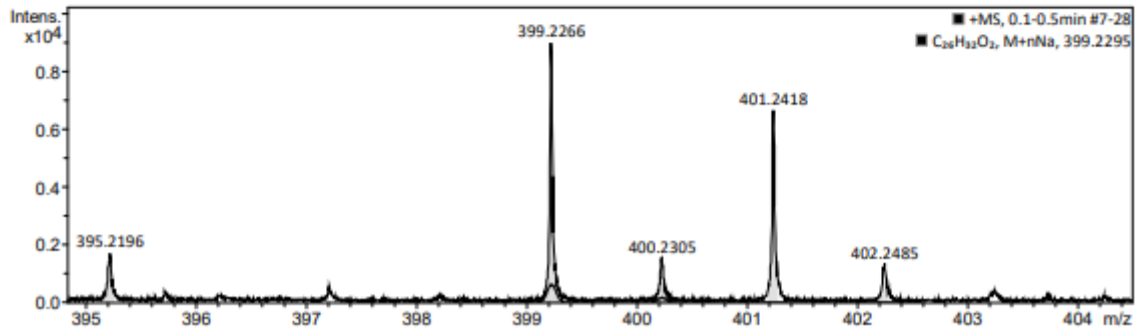
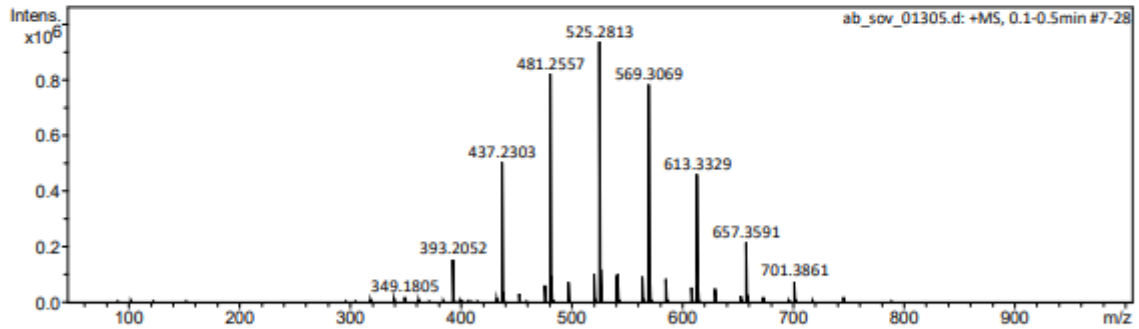
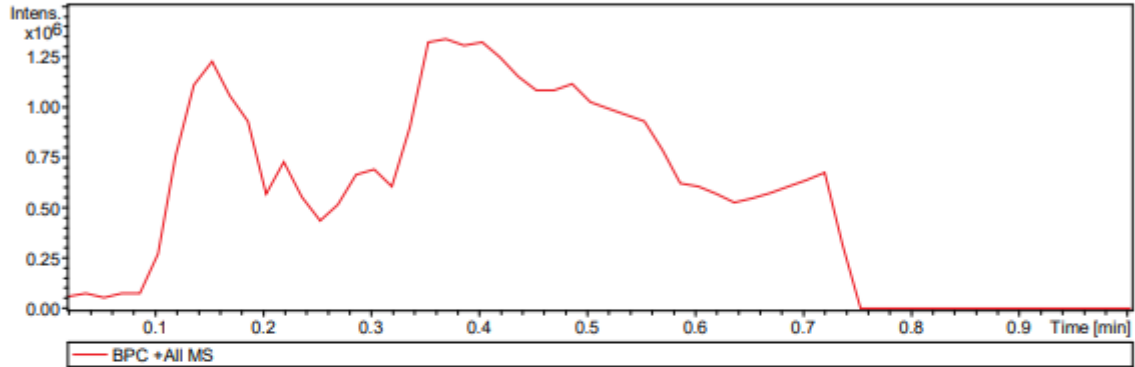
Analysis Info

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Method Tune_pos_Standard.m
Sample Name ab_sov_01305
Comment

Acquisition Date 5/24/2022 12:50:45 PM
Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulzer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_sov_01305.d

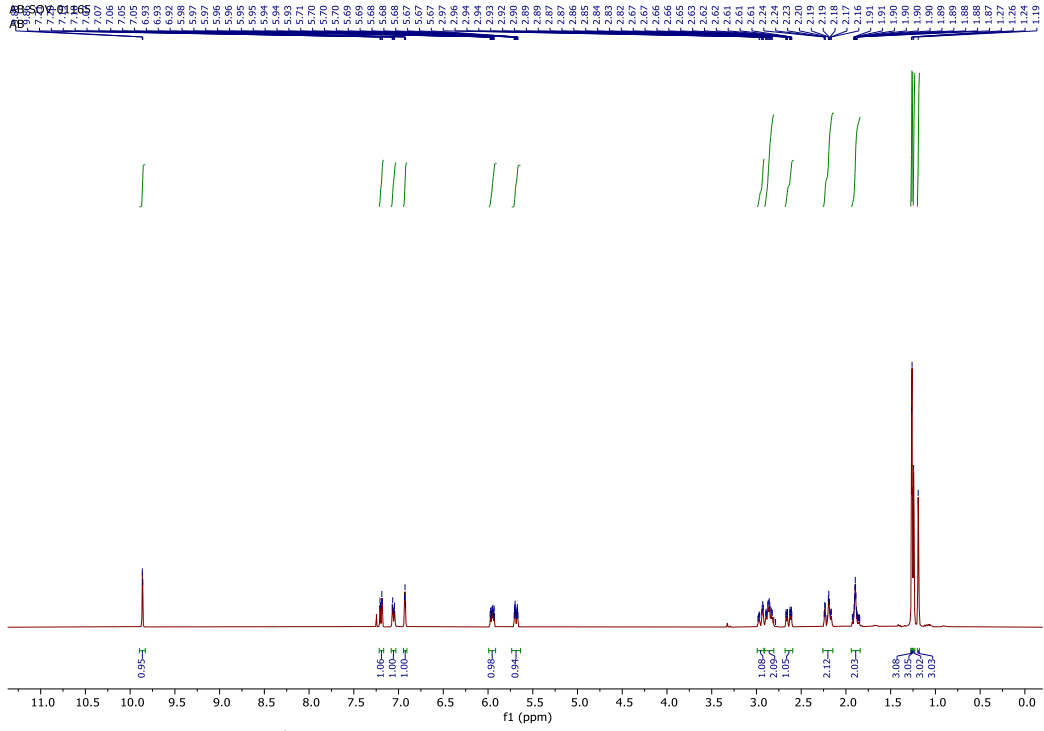
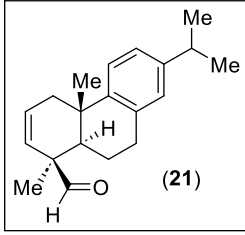
Bruker Compass DataAnalysis 4.1

printed: 5/24/2022 1:02:18 PM

by: IISER Kolkata

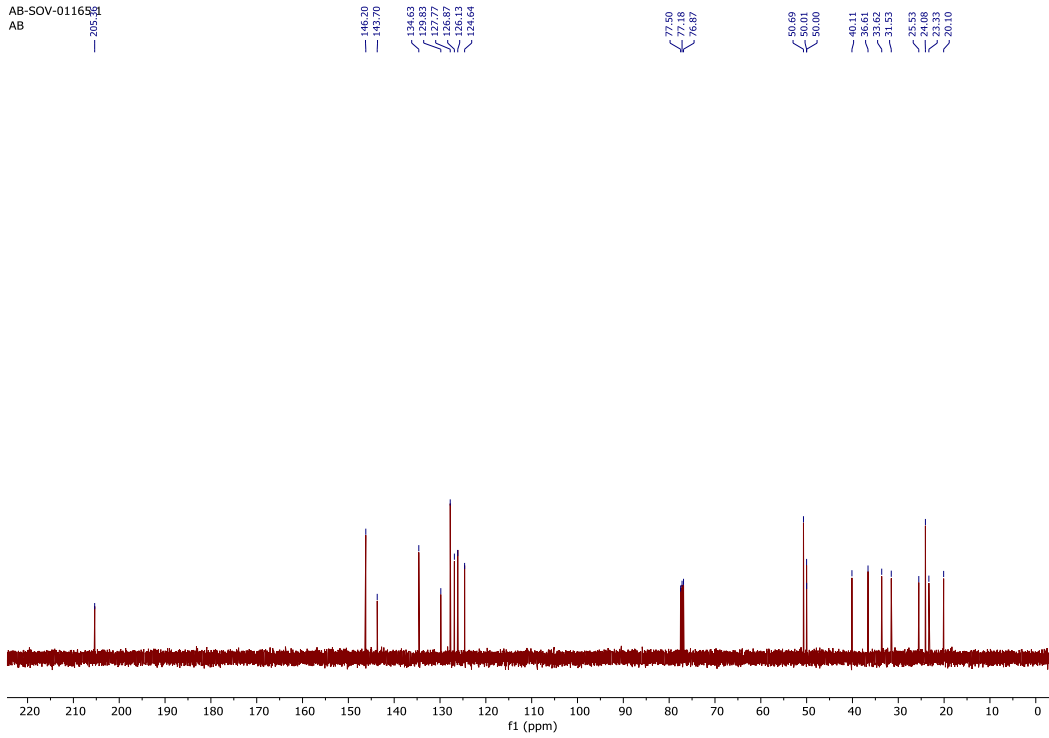
Page 1 of 1

HRMS data for (+)-20



^1H NMR (400 MHz, CDCl_3) of (+)-21

AB-SOV-011659
AB



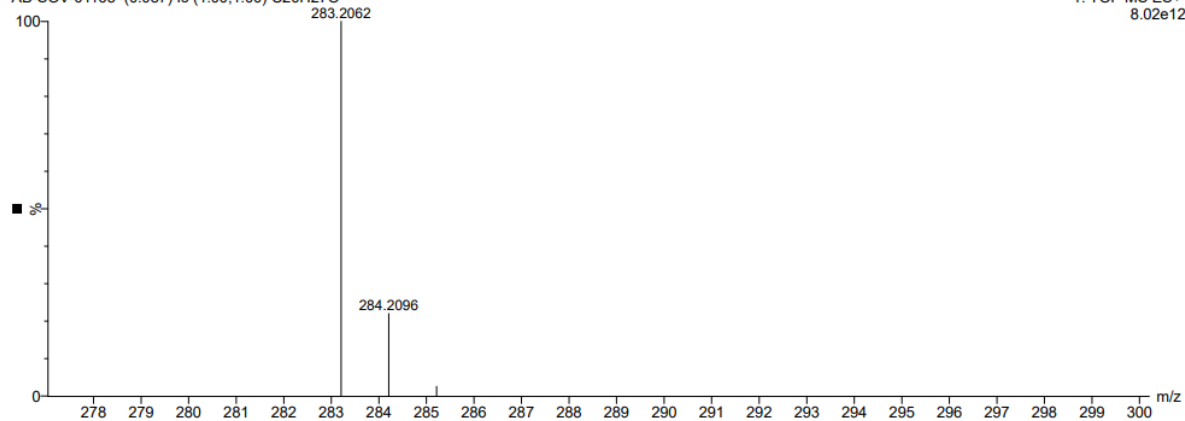
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-21

AB29-Apr-2024 11:52:50

IISER - KOLKATA

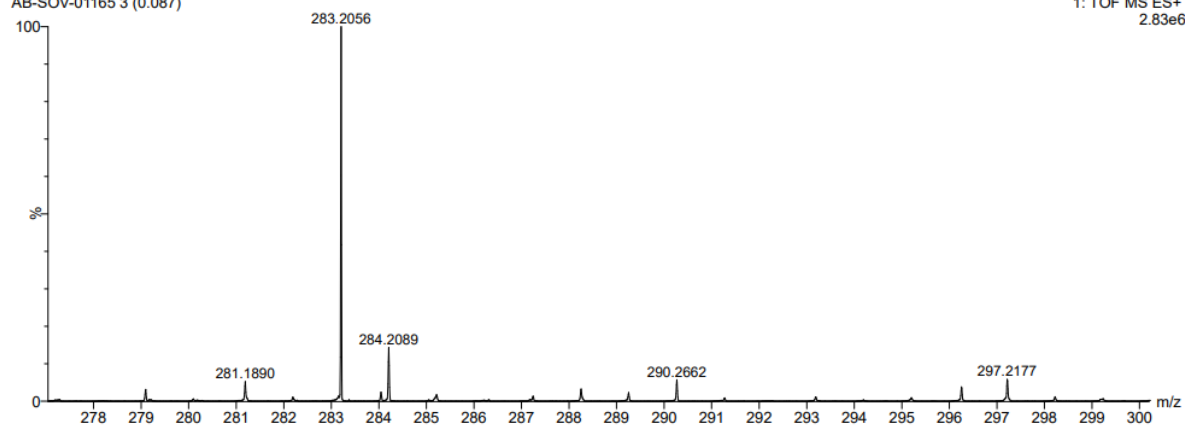
1: TOF MS ES+
8.02e12

AB-SOV-01165 (0.087) Is (1.00,1.00) C₂₀H₂₇O

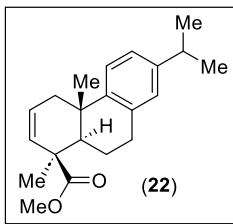


AB-SOV-01165 3 (0.087)

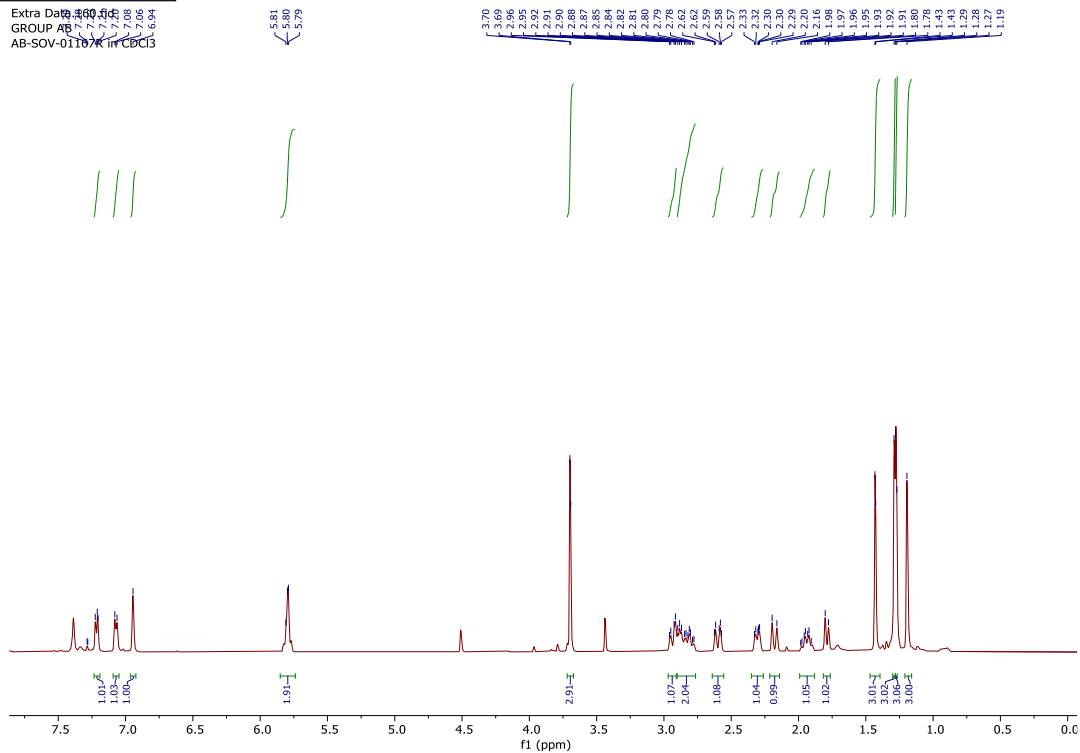
1: TOF MS ES+
2.83e6



HRMS data for (+)-**21**

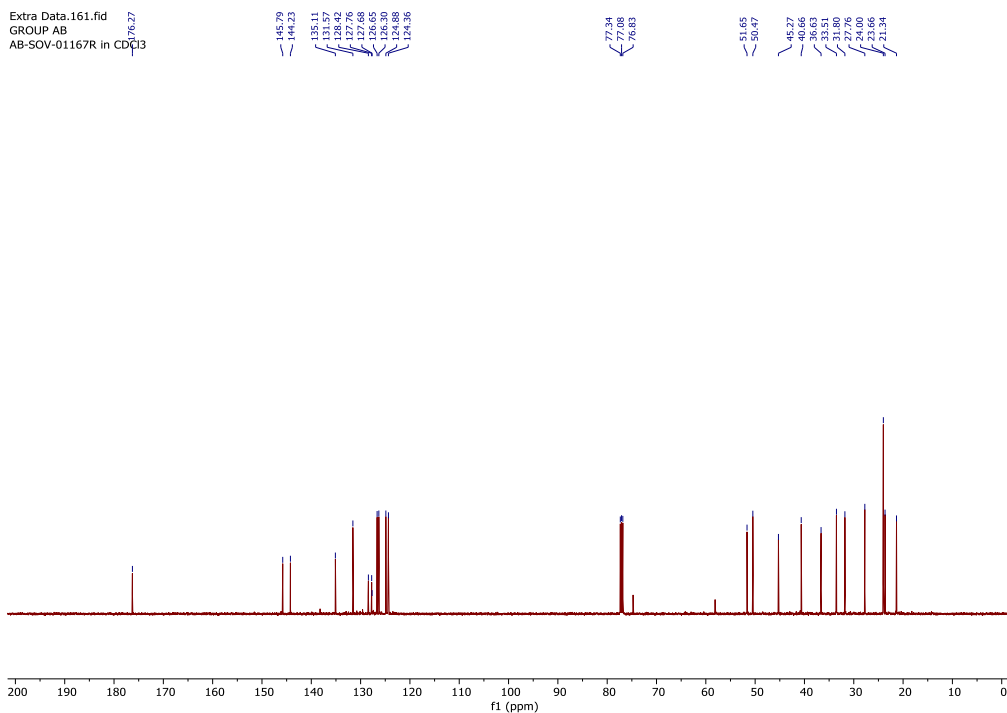


Extra Data: 161.fid
 GROUP AB
 AB-SOV-01167R in CDCl₃



¹H NMR (400 MHz, CDCl₃) of (+)-22

Extra Data: 161.fid
 GROUP AB
 AB-SOV-01167R in CDCl₃

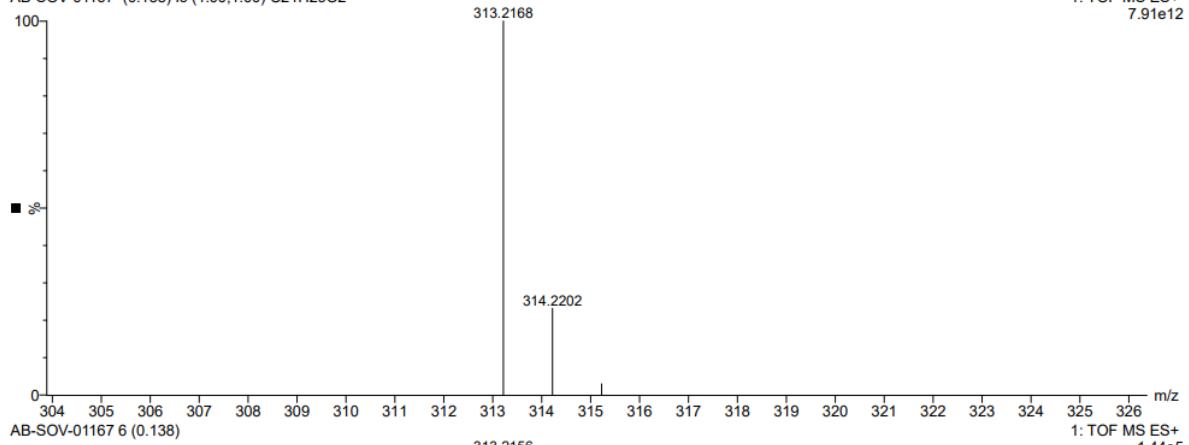


¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-22

AB29-Apr-2024 11:54:47
AB-SOV-01167 (0.138) Is (1.00,1.00) C₂₁H₂₉O₂

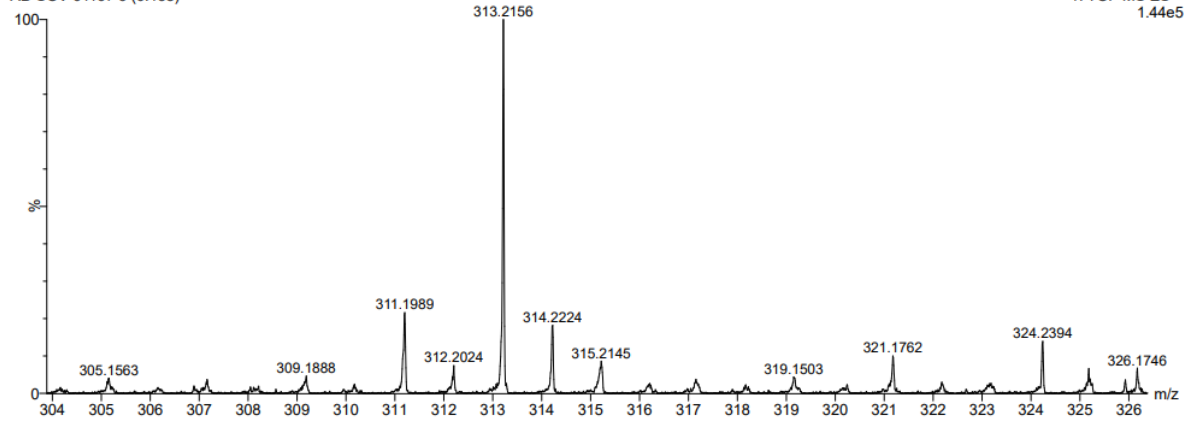
IISER - KOLKATA

1: TOF MS ES+
7.91e12

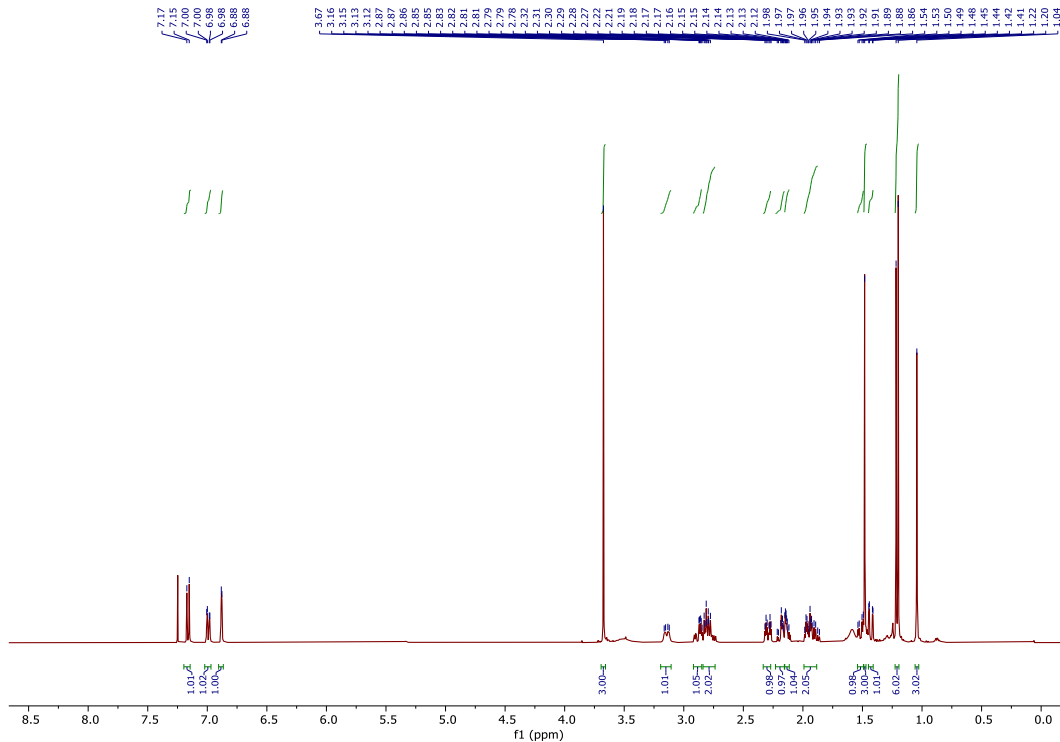
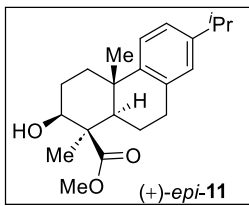


AB-SOV-01167 6 (0.138)

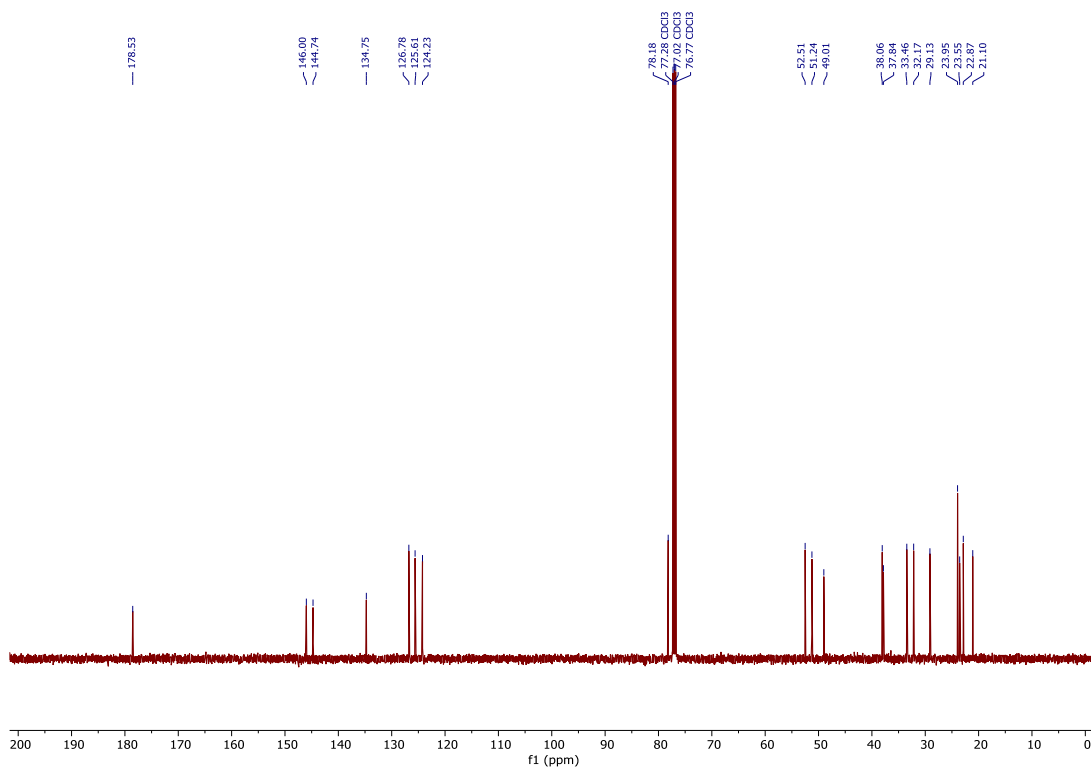
1: TOF MS ES+
1.44e5



HRMS data for (+)-**22**



^1H NMR (400 MHz, CDCl_3) of (+)-epi-11



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-epi-11

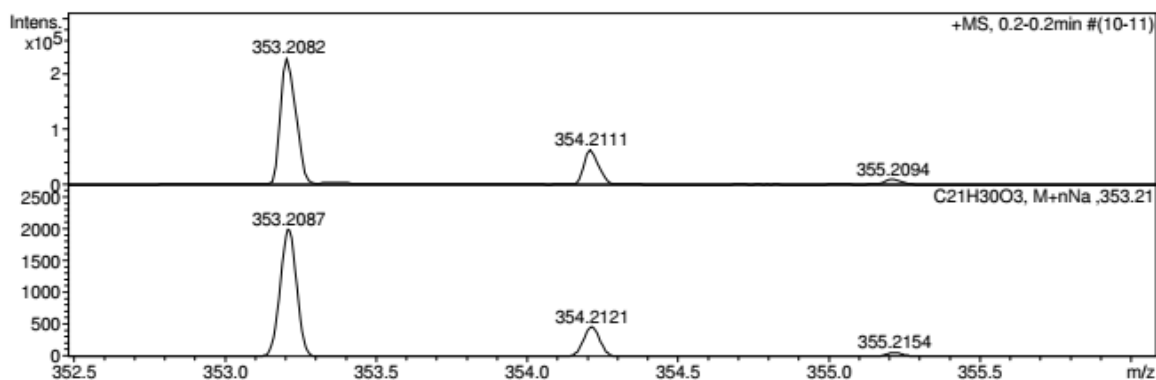
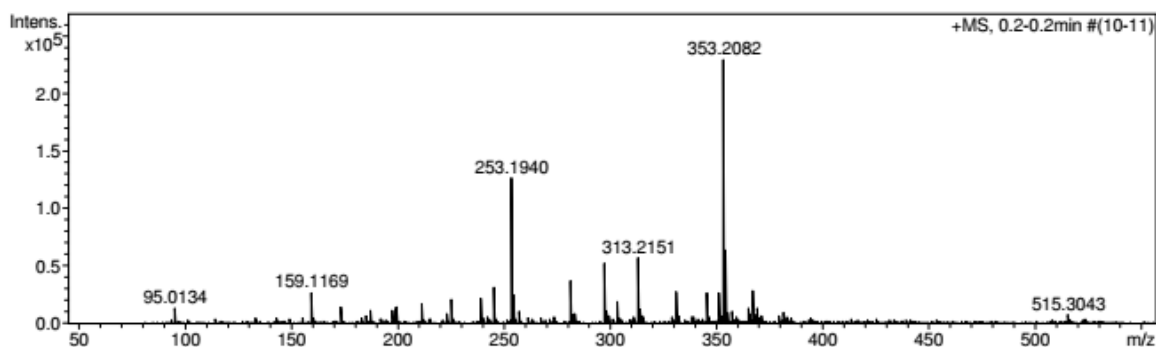
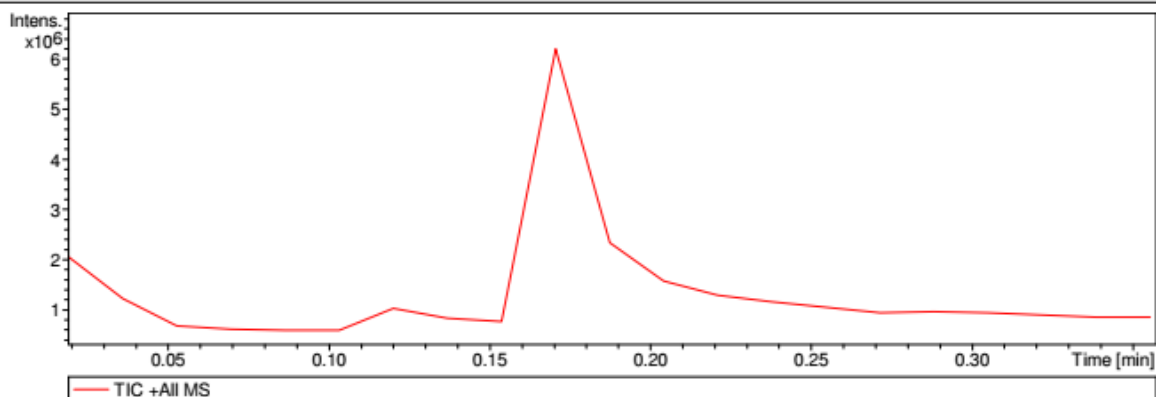
Display Report

Analysis Info

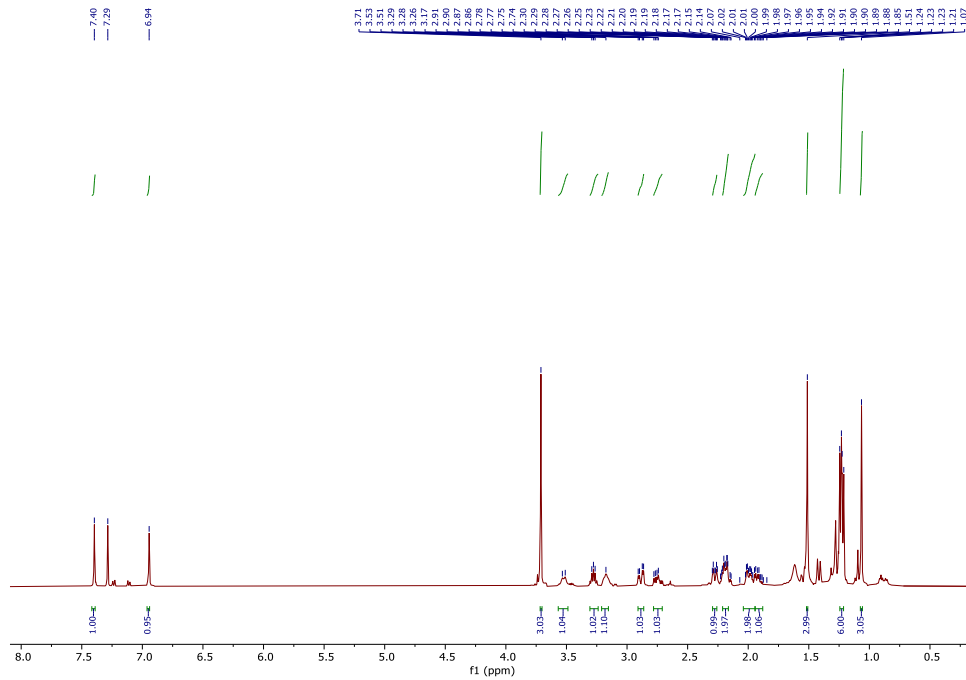
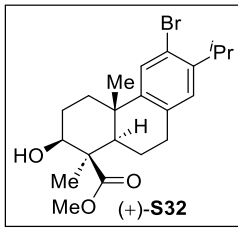
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Method tune mix_low.New.021117.m Operator RUCHI
Sample Name ABKS04174P1 Instrument micrOTOF-Q II 10330
Comment

Acquisition Parameter

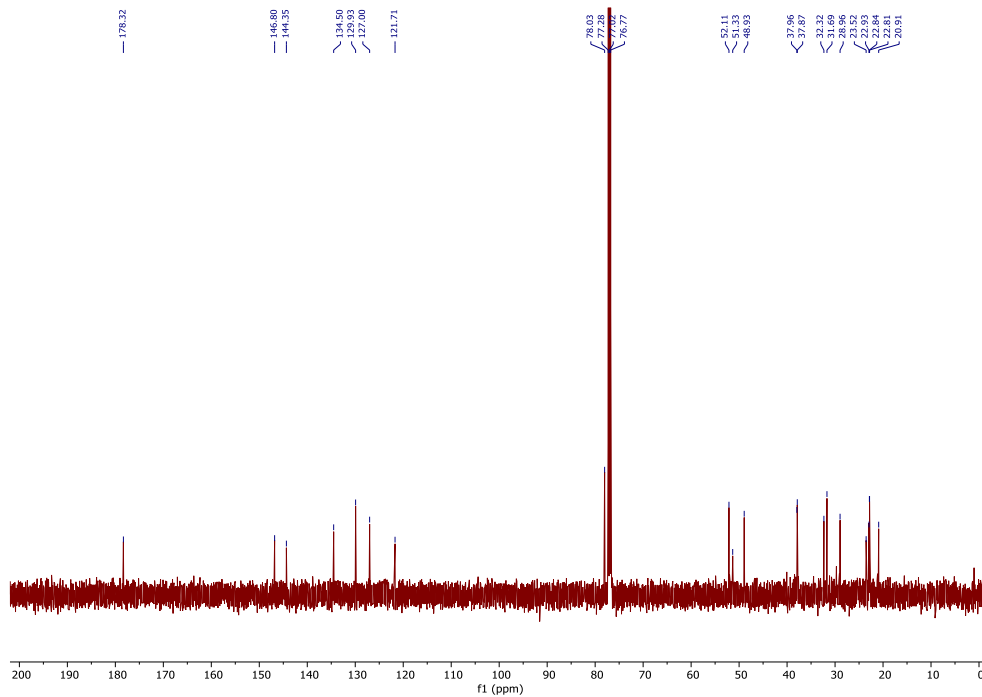
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Scan End	3000 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste



HRMS data for (+)-*epi*-11



^1H NMR (500 MHz, CDCl_3) of (+)-S32



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-S32

Display Report

Analysis Info

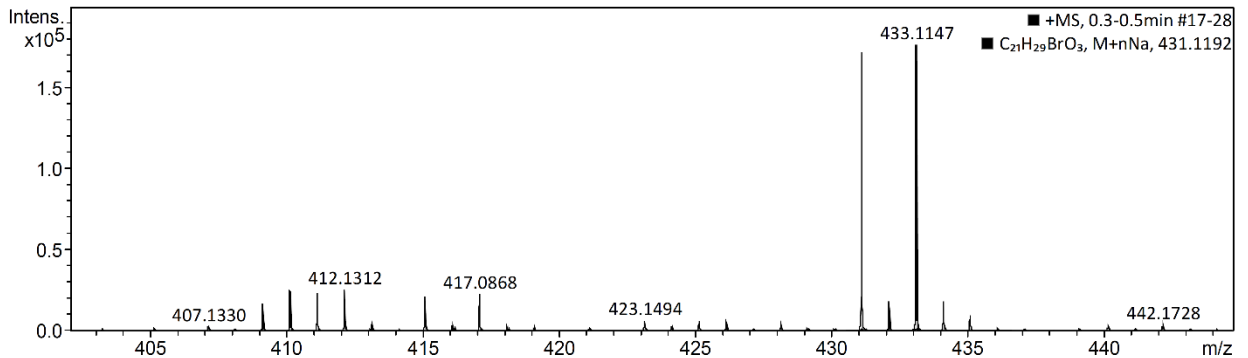
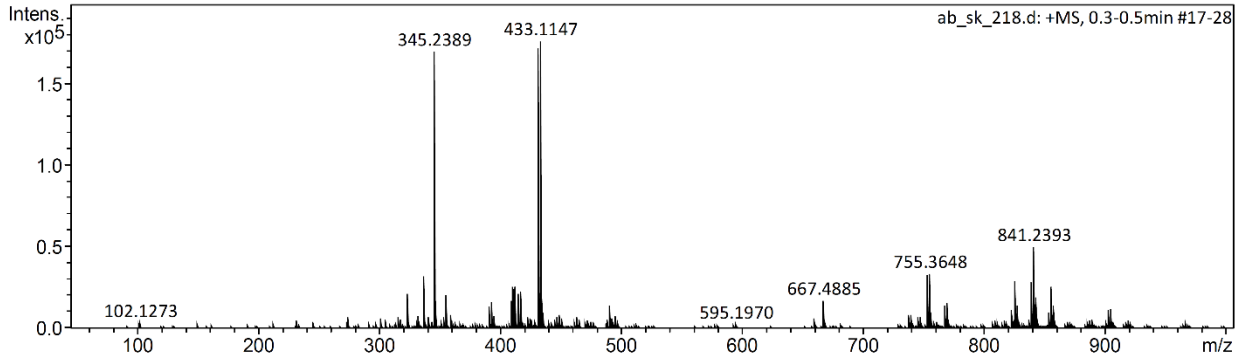
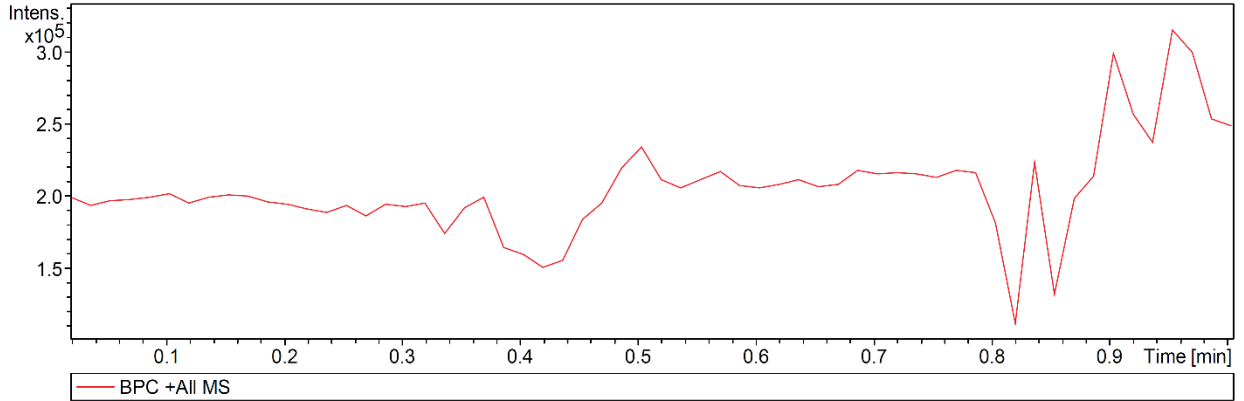
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Method Tune_pos_Standard.m
Sample Name ab_sk_218
Comment

Acquisition Date 1/24/2022 11:20:03 AM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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ab_sk_218.d

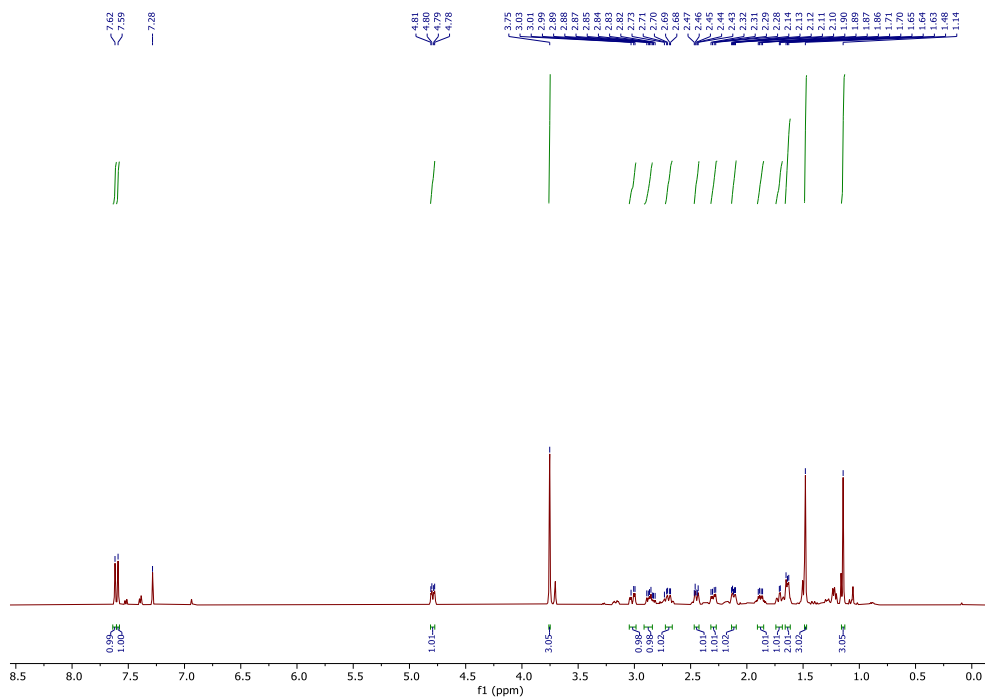
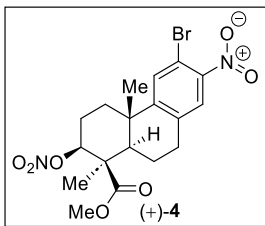
Bruker Compass DataAnalysis 4.1

printed: 1/24/2022 11:23:39 AM

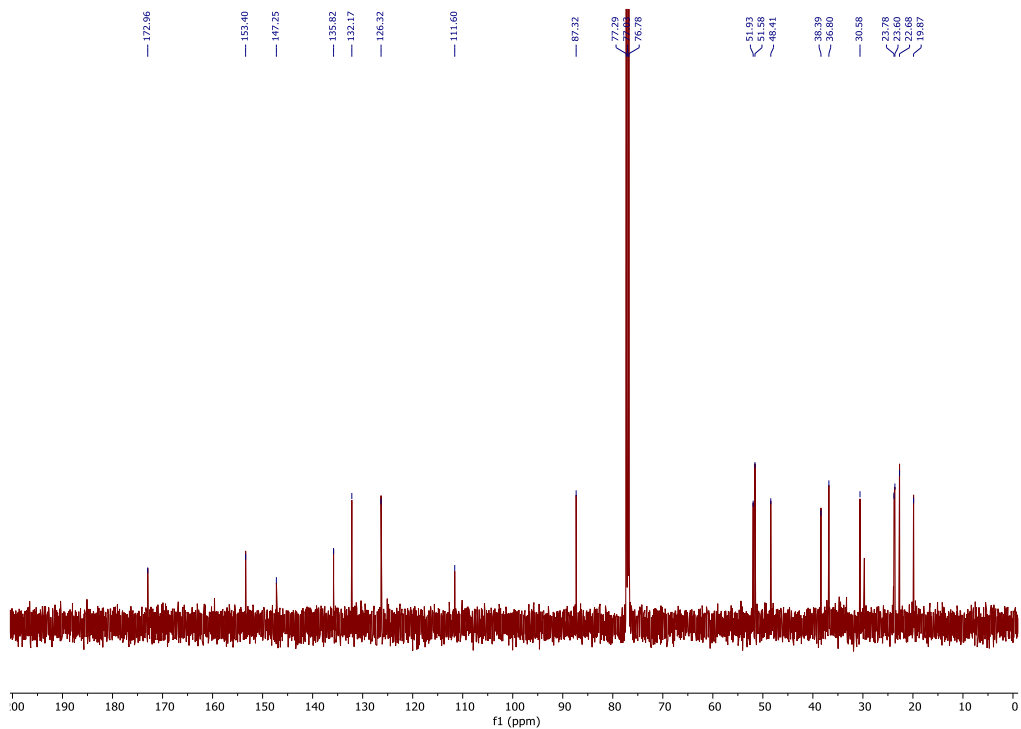
by: IISER Kolkata

Page 1 of 1

HRMS data of (+)-S32



¹H NMR (500 MHz, CDCl₃) of (+)-4



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-4

Display Report

Analysis Info

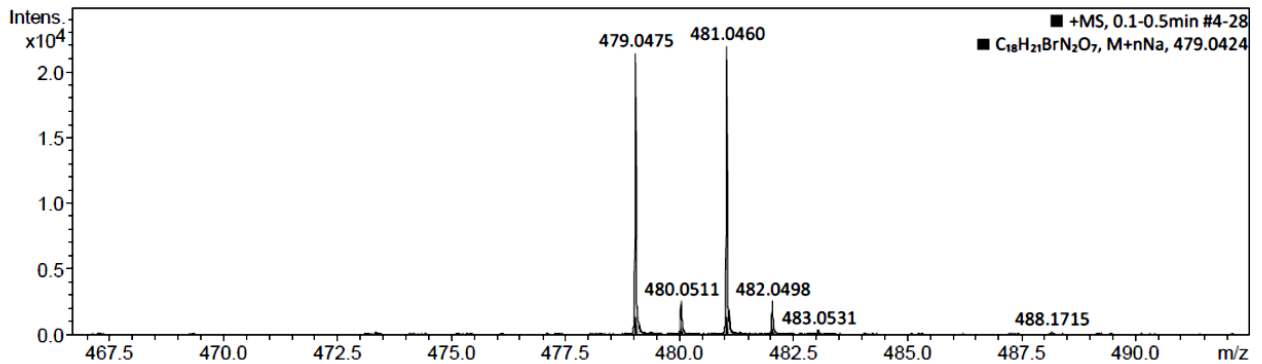
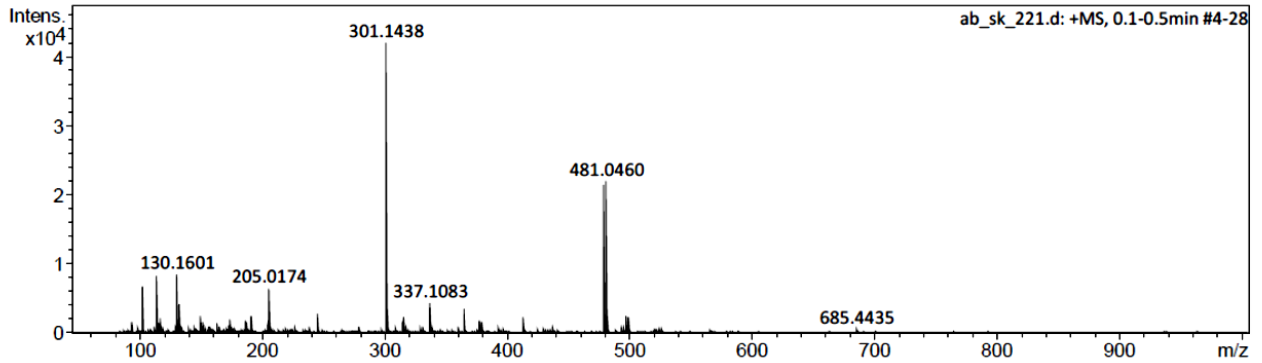
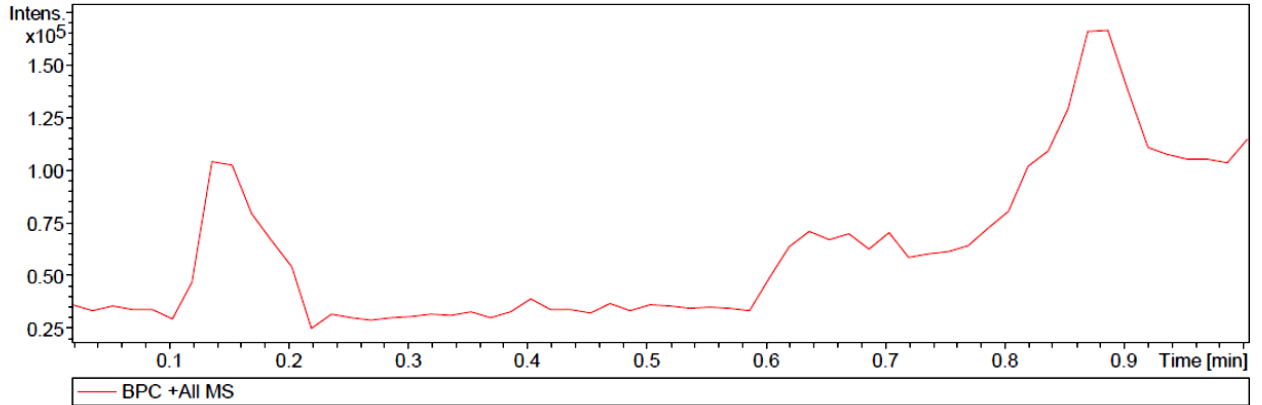
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Method Tune_pos_Standard.m
Sample Name ab_sk_221
Comment

Acquisition Date 2/14/2022 11:43:29 AM

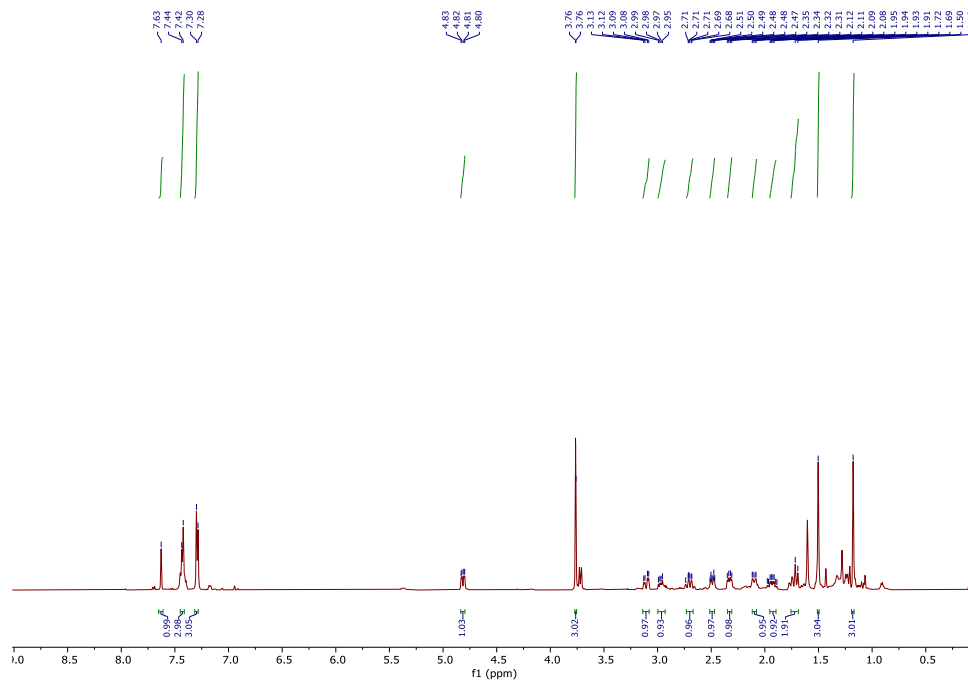
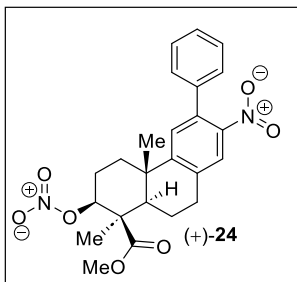
Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

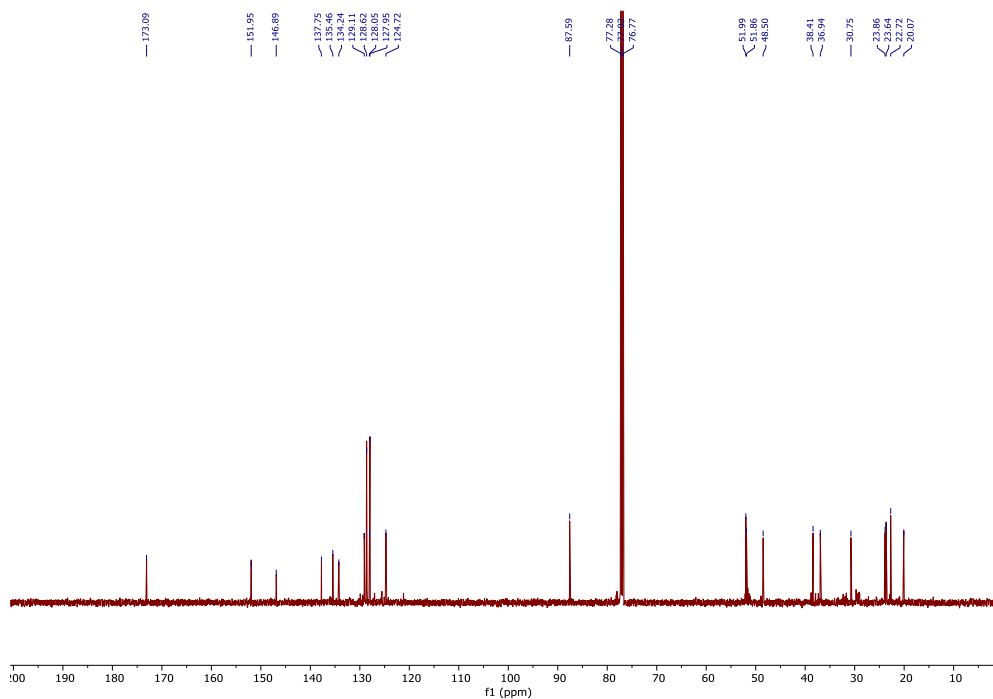
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		Set Corona	0 nA	Set APCI Heater	0 °C



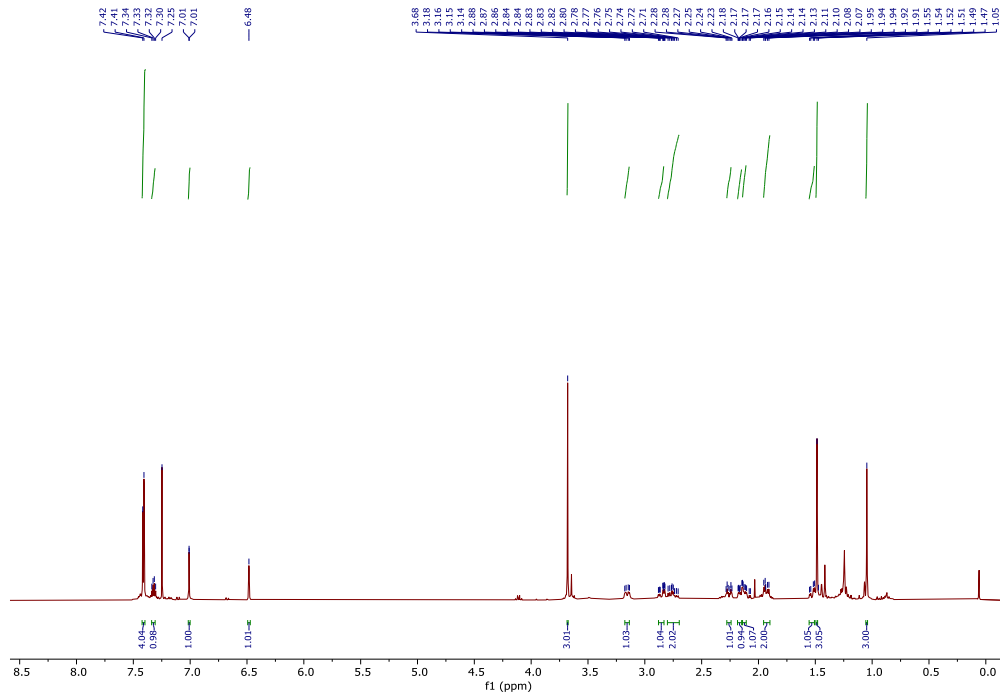
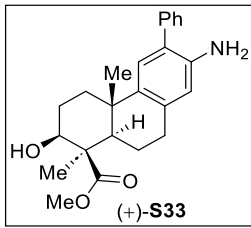
HRMS data of (+)-4



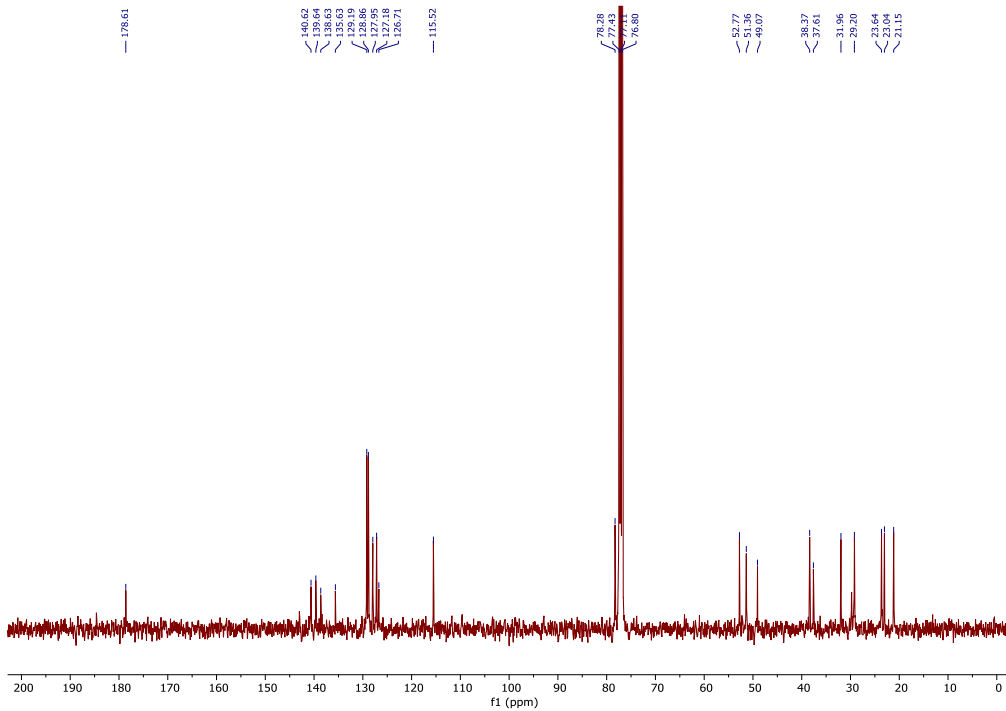
¹H NMR (500 MHz, CDCl₃) of (+)-24



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-24



¹H NMR (500 MHz, CDCl₃) of (+)-S33



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-S33

Display Report

Analysis Info

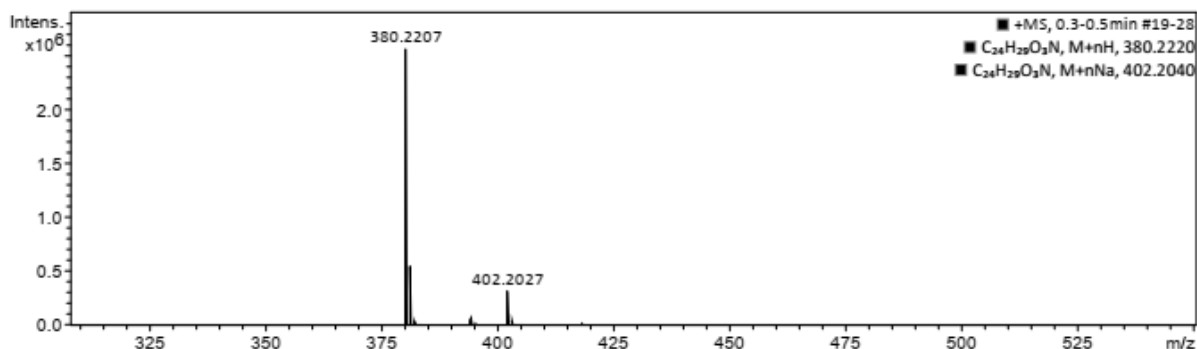
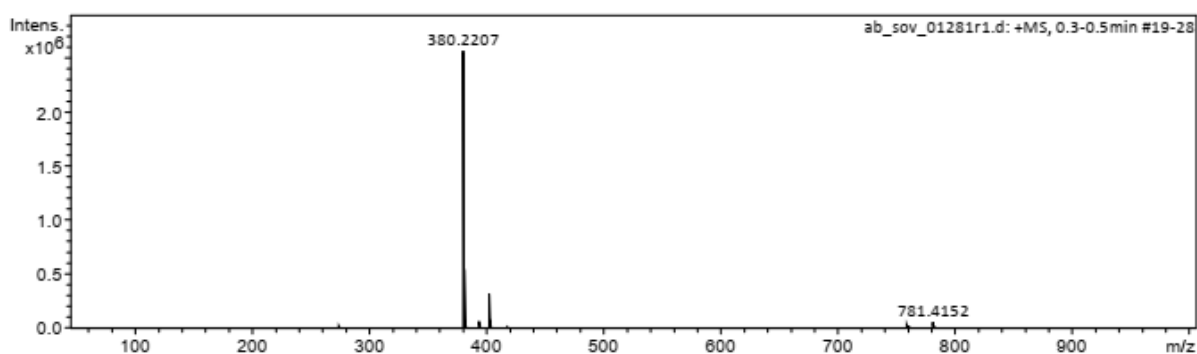
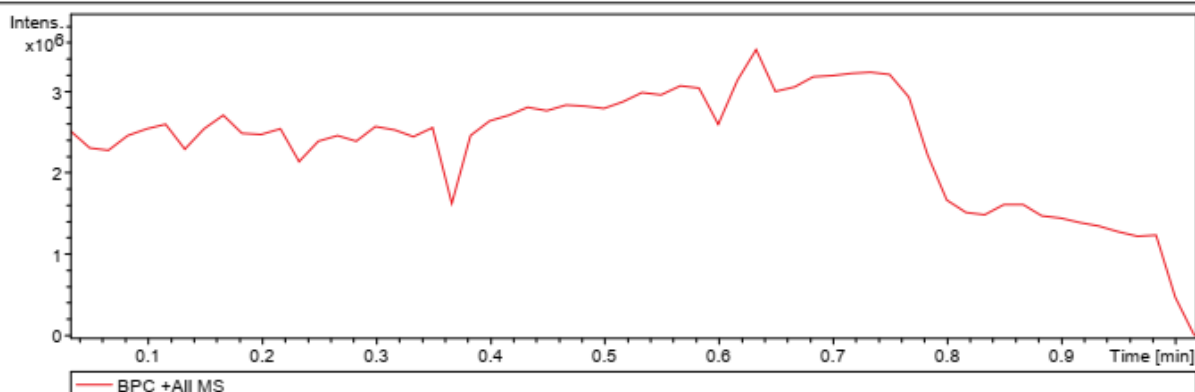
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Method Tune_pos_Standard.m
Sample Name AB_SOV_01281R1
Comment

Acquisition Date 1/24/2022 11:31:54 AM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
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Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_sov_01281r1.d

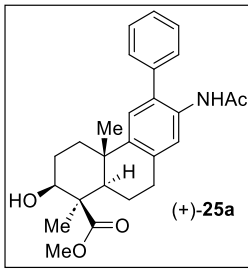
Bruker Compass DataAnalysis 4.1

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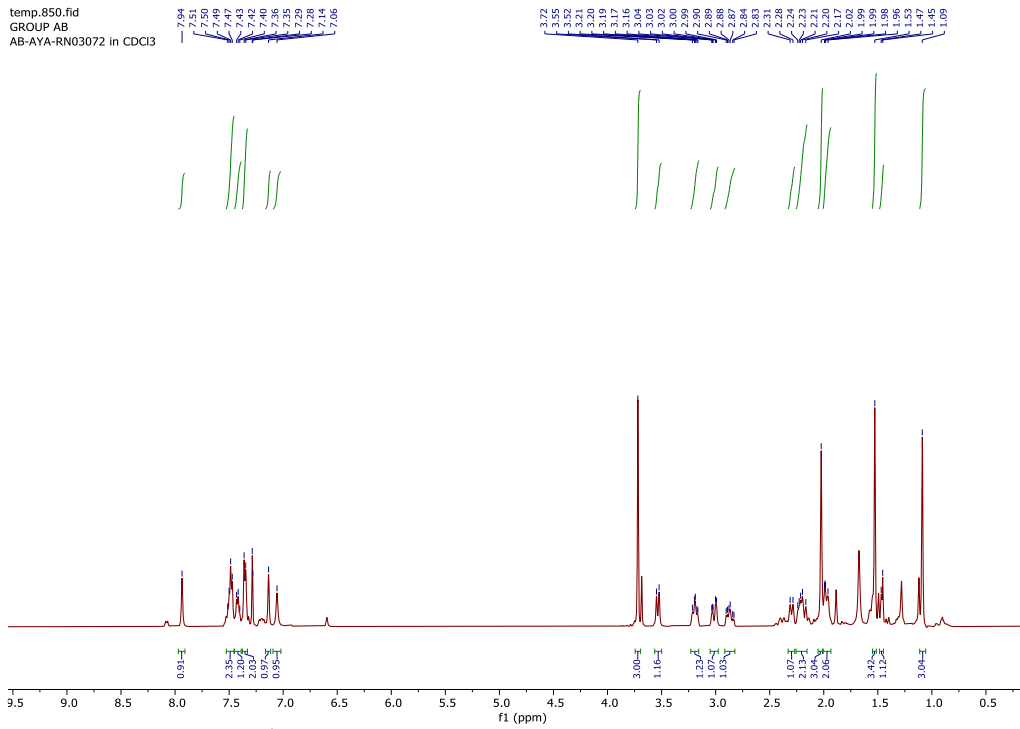
by: IISER Kolkata

Page 1 of 1

HRMS data of (+)-S33

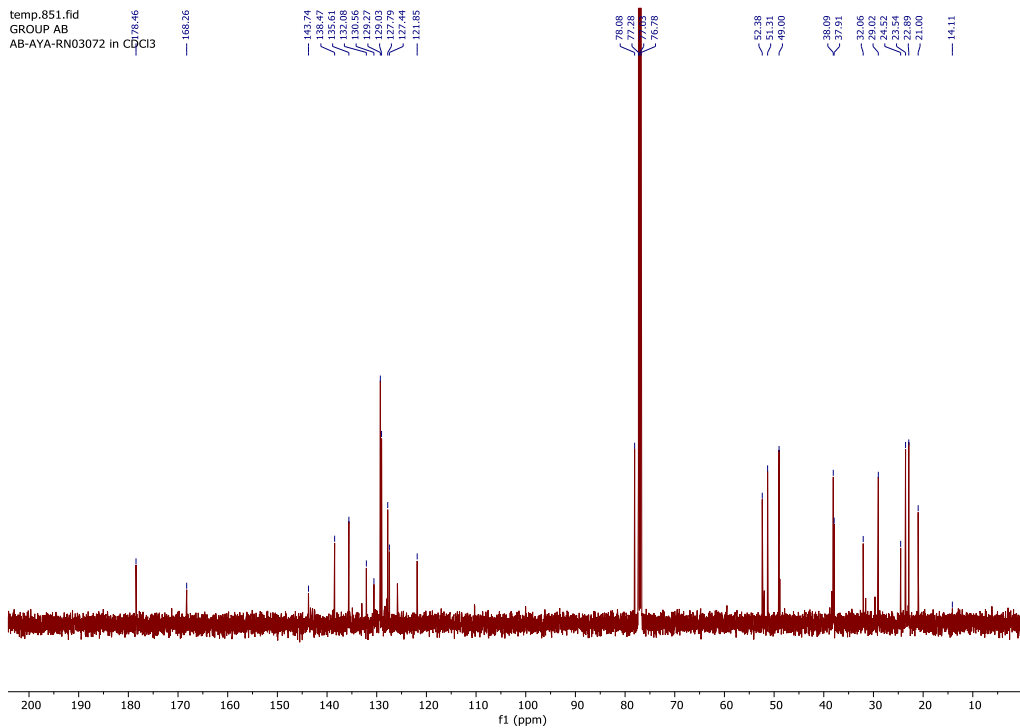


temp.850.fid
GROUP AB
AB-AYA-RN03072 in CDCl₃



¹H NMR (500 MHz, CDCl₃) of (+)-25a

temp.851.fid
GROUP AB
AB-AYA-RN03072 in CDCl₃



¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-25a

Display Report

Analysis Info

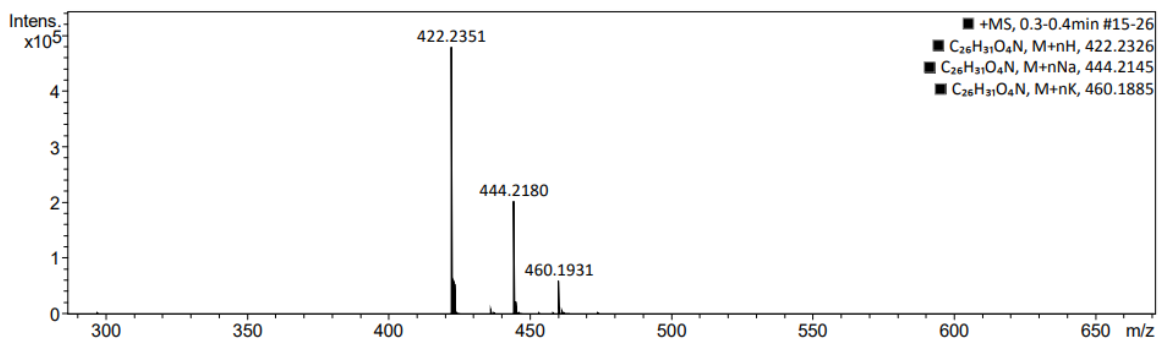
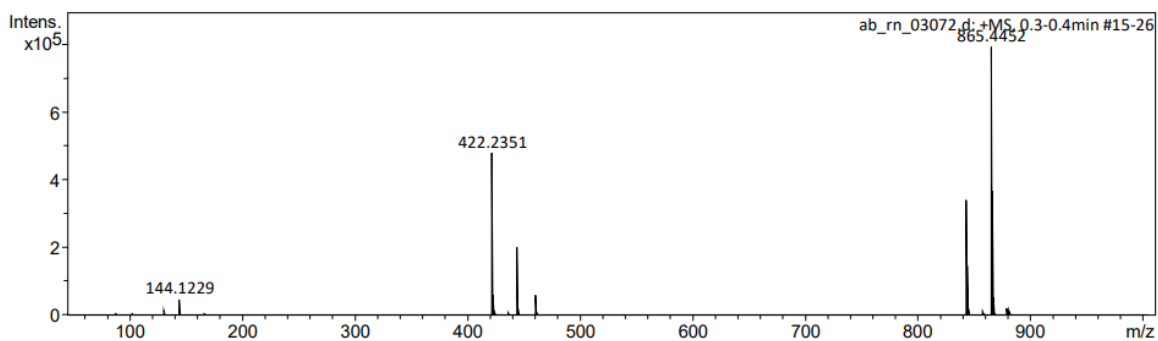
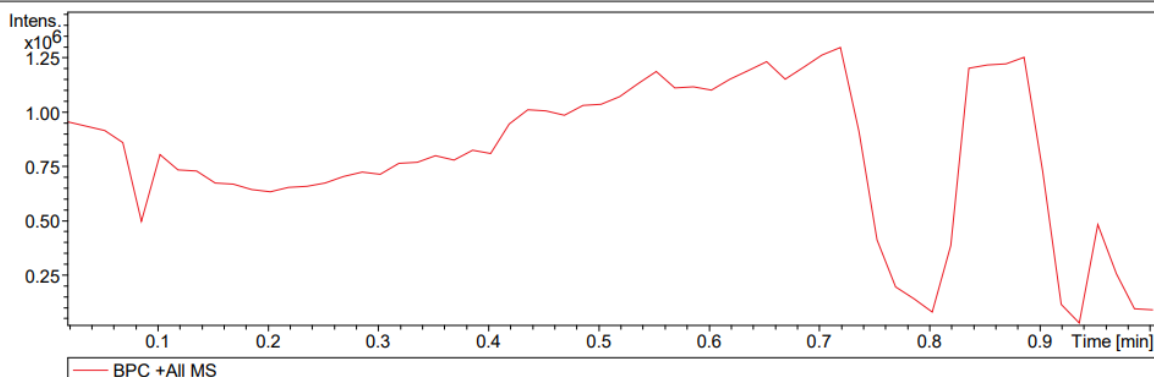
Analysis Name D:\Data\User data\2022\APRIL\ab_rn_03072.d
Method Tune_pos_Standard.m
Sample Name ab_rn_03072
Comment

Acquisition Date 4/21/2022 1:01:41 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_rn_03072.d

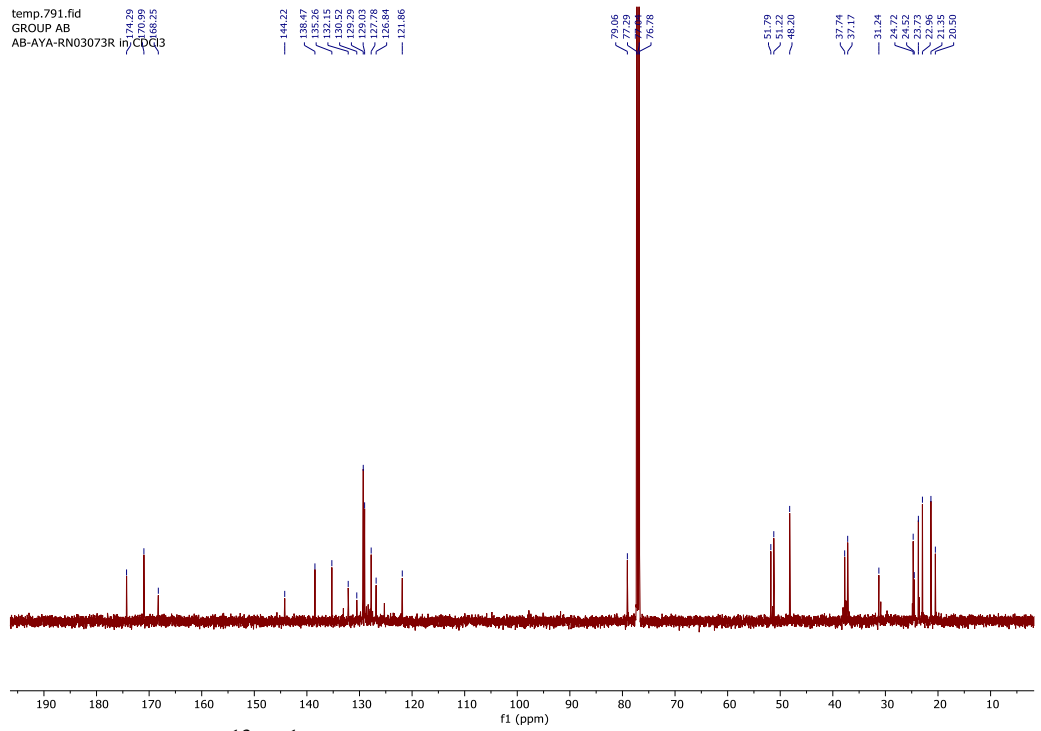
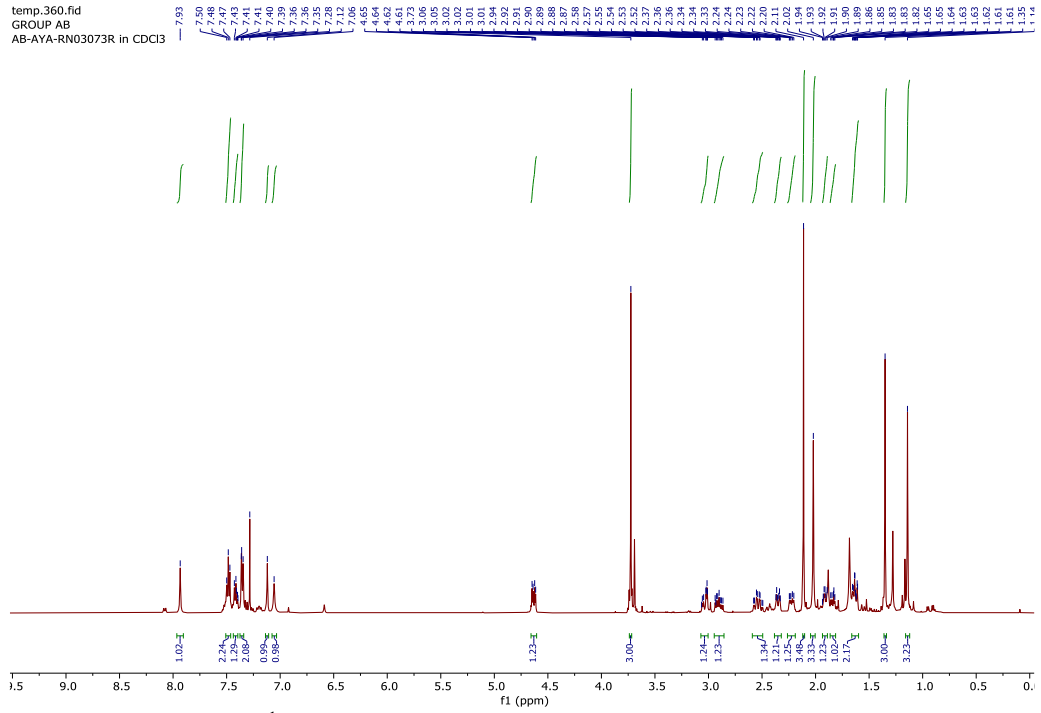
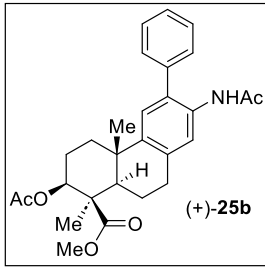
Bruker Compass DataAnalysis 4.1

printed: 4/21/2022 1:03:53 PM

by: IISER Kolkata

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HRMS data of (+)-25a

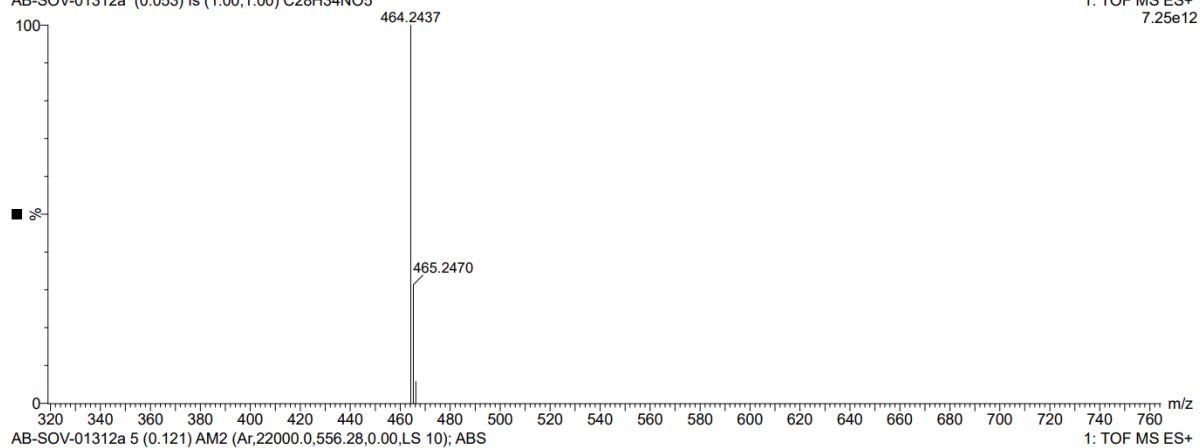


AB27-Mar-2024 12:50:32

IISER - KOLKATA

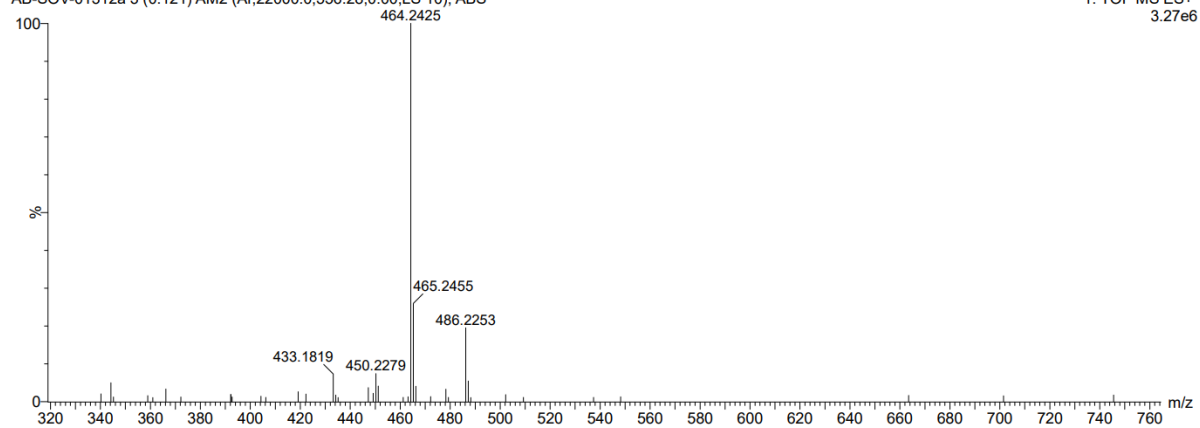
AB-SOV-01312a (0.053) Is (1.00,1.00) C₂₈H₃₄NO₅

1: TOF MS ES+
7.25e12

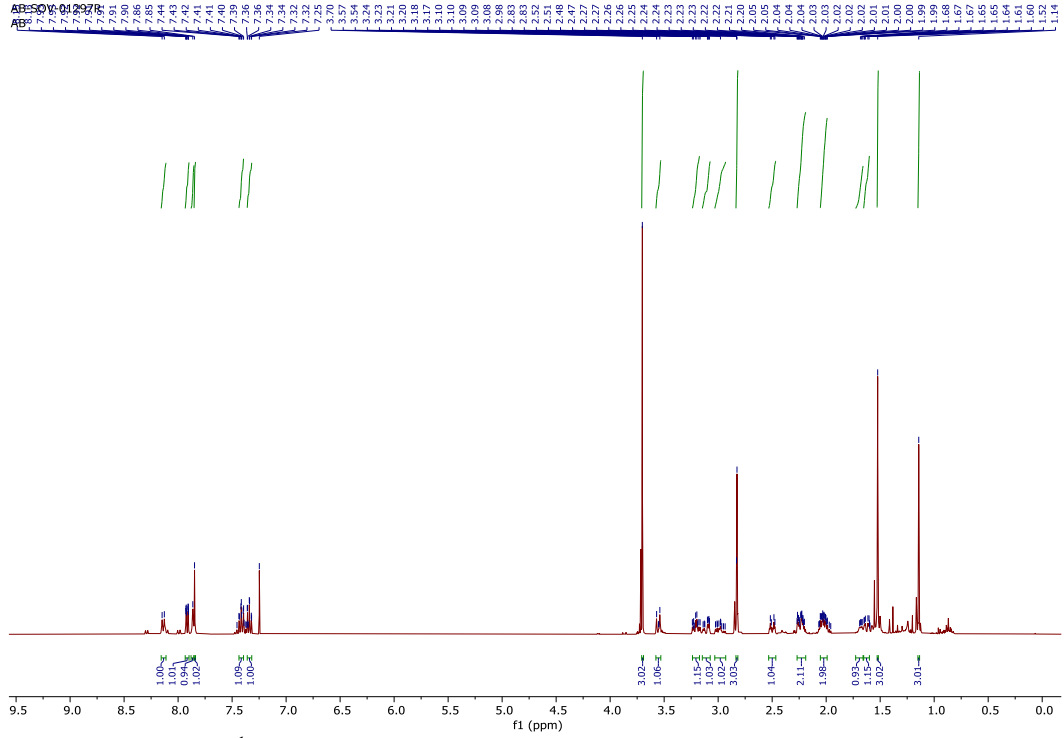
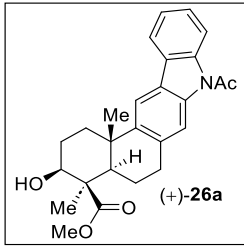


AB-SOV-01312a 5 (0.121) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+
3.27e6



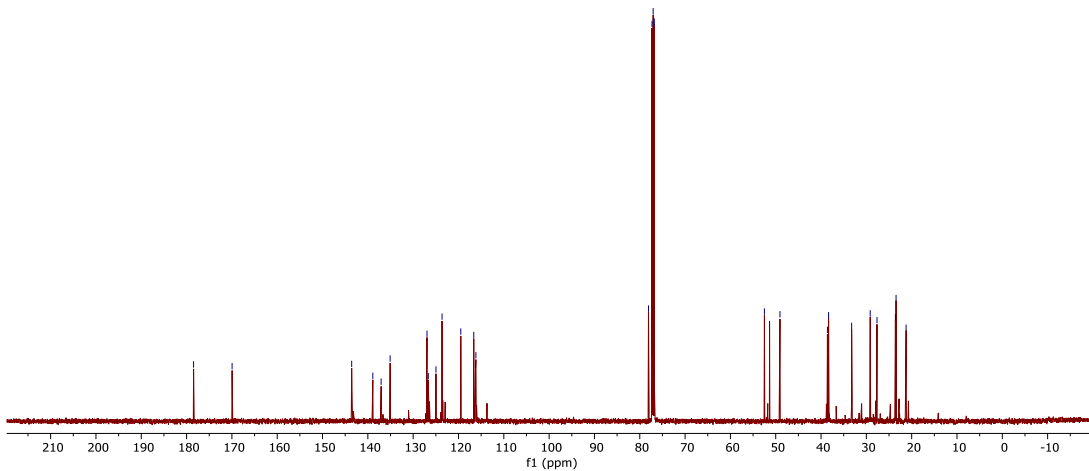
HRMS data of (+)-**25b**



^1H NMR (500 MHz, CDCl_3) of compound (+)-26a

Dioridamycin NMR.240.fid
GROUP AB
AB-AOV-01267R in CDCl_3

178.46
169.96
143.57
138.90
137.07
135.08
126.95
126.66
124.98
123.63
119.69
116.25
116.16
76.08
77.05
76.79
52.49
49.07
36.59
33.74
29.15
27.65
23.48
21.23



$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of compound (+)-26a

Display Report

Analysis Info

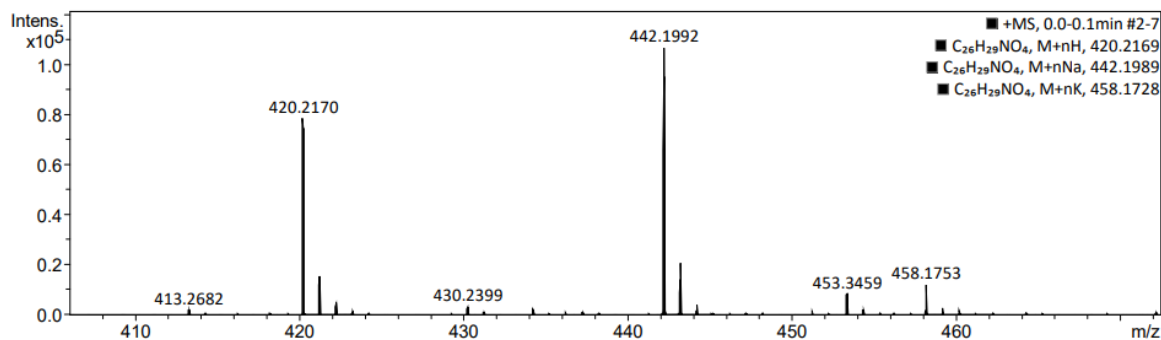
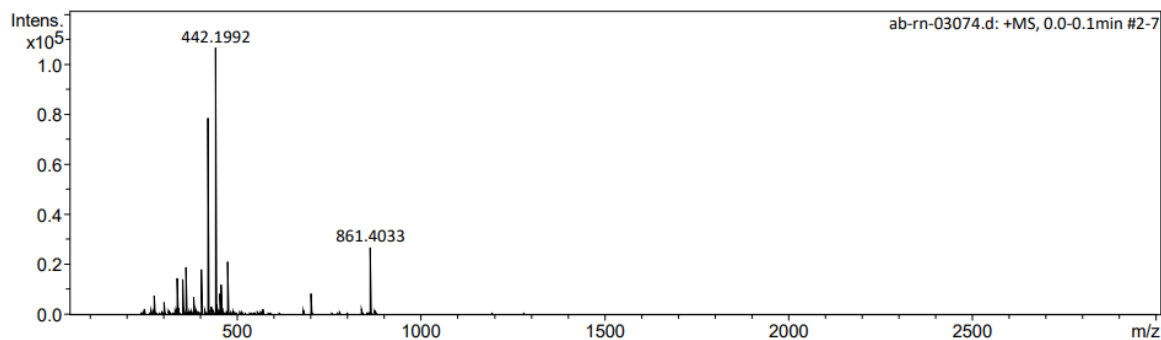
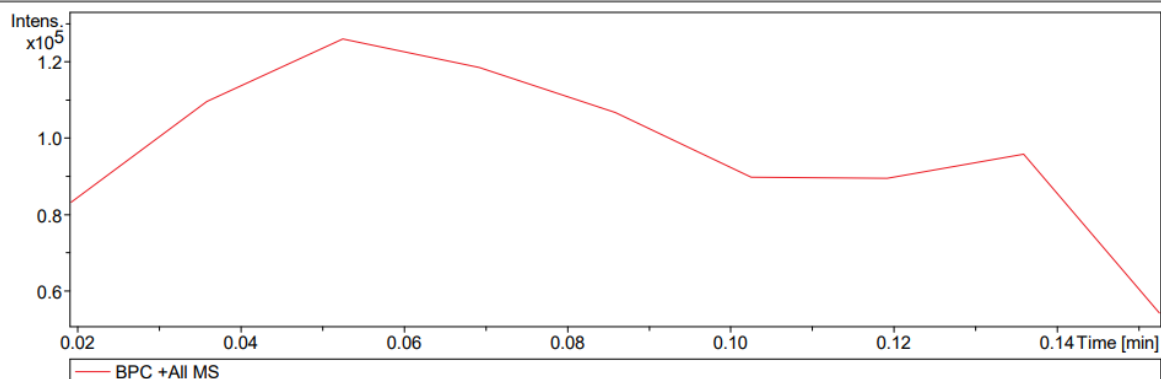
Analysis Name D:\Data\User data\2022\APRIL\ab-rn-03074.d
Method Tune_pos_Mid.m
Sample Name ab-rn-03074
Comment

Acquisition Date 4/22/2022 11:14:44 AM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °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



ab-rn-03074.d

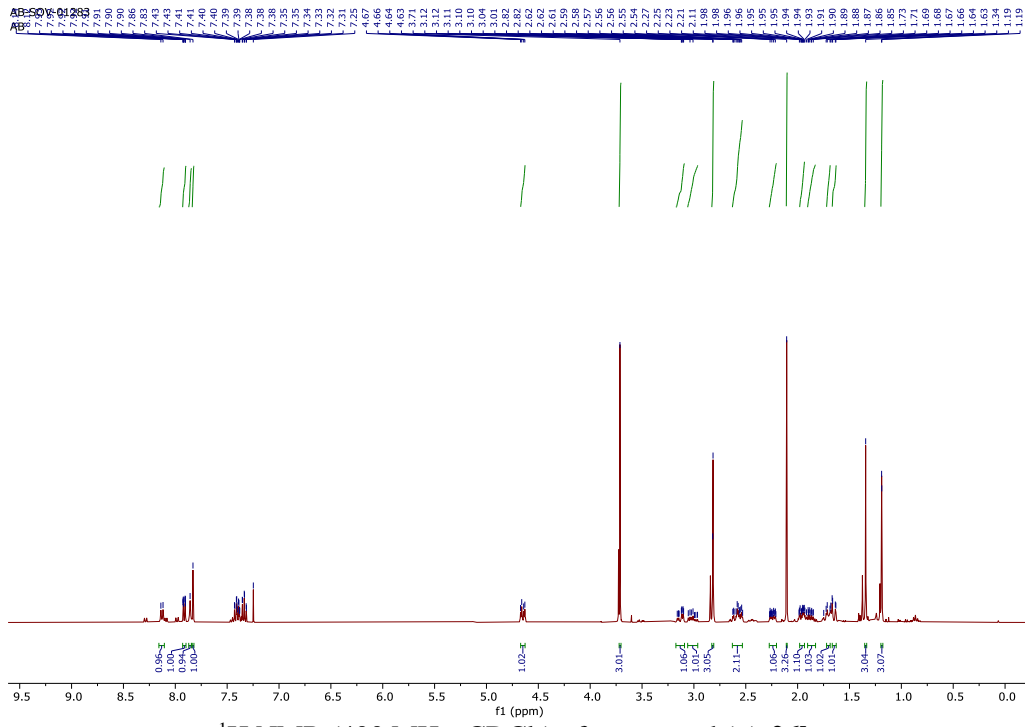
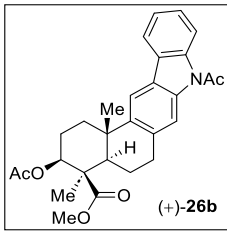
Bruker Compass DataAnalysis 4.1

printed: 4/22/2022 11:17:37 AM

by: IISER Kolkata

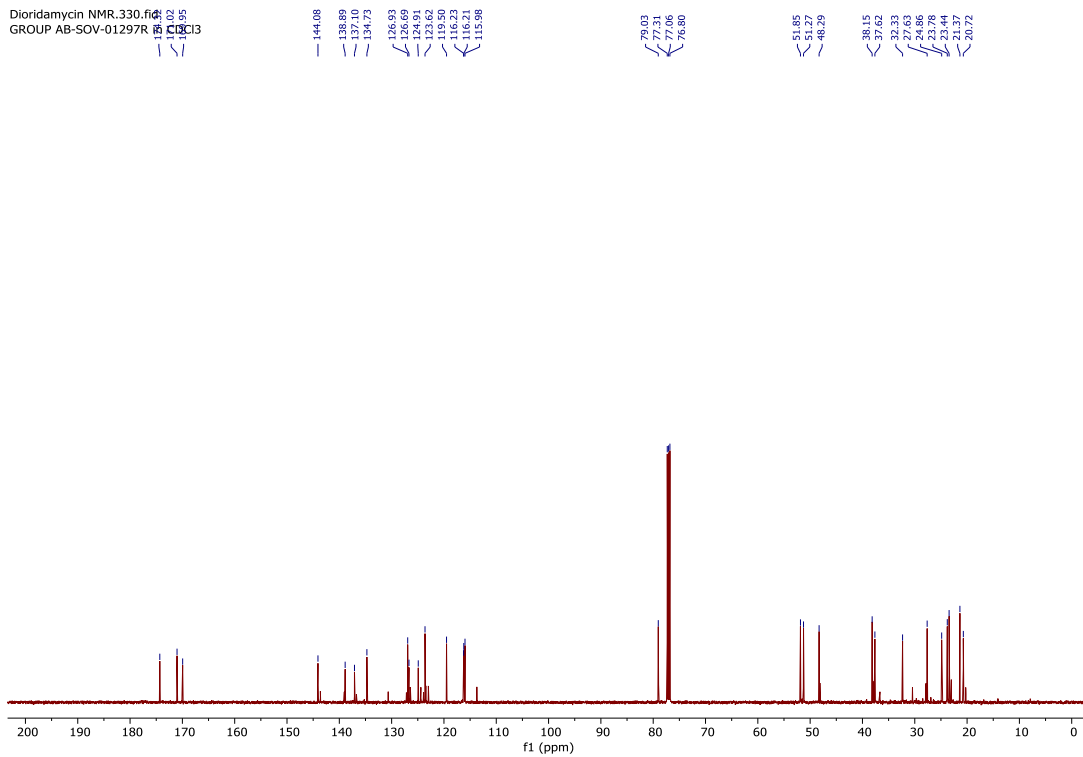
Page 1 of 1

HRMS data of (+)-26a



¹H NMR (400 MHz, CDCl₃) of compound (+)-26b

Dioridamycin NMR.330.fid
GROUP AB-SOV-01297R-5
CDCl₃



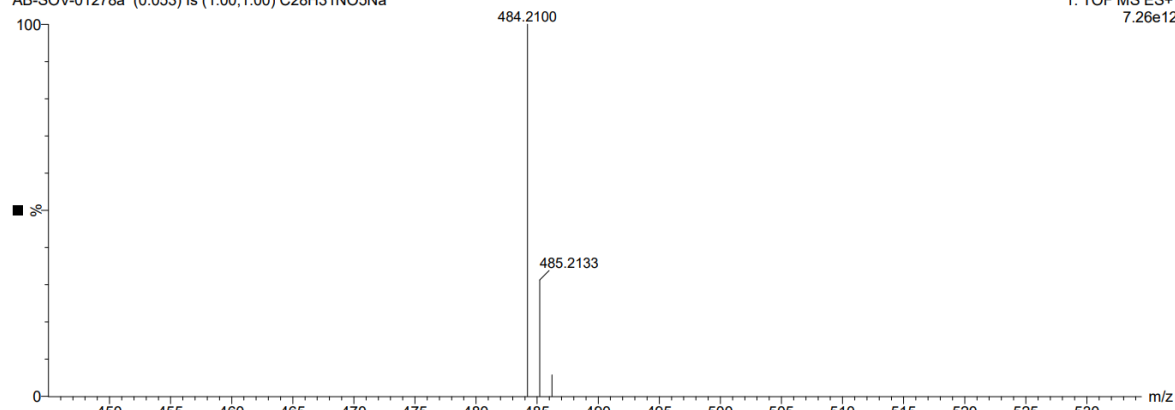
¹³C{¹H} NMR (125 MHz, CDCl₃) of compound (+)-26b

AB27-Mar-2024 12:48:55

AB-SOV-01278a (0.053) ls (1.00,1.00) C28H31NO5Na

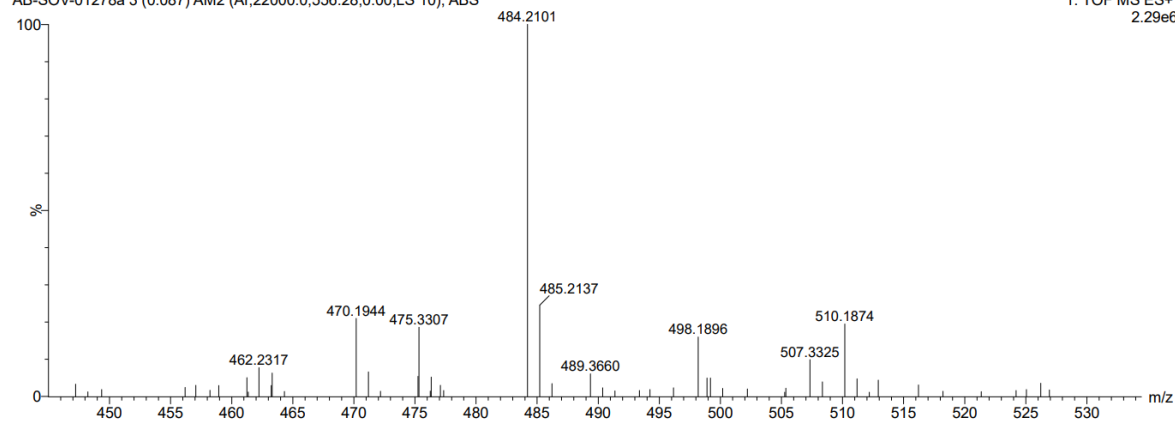
IISER - KOLKATA

1: TOF MS ES+
7.26e12

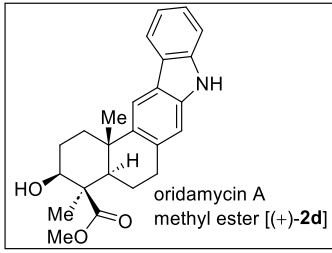


AB-SOV-01278a 3 (0.087) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

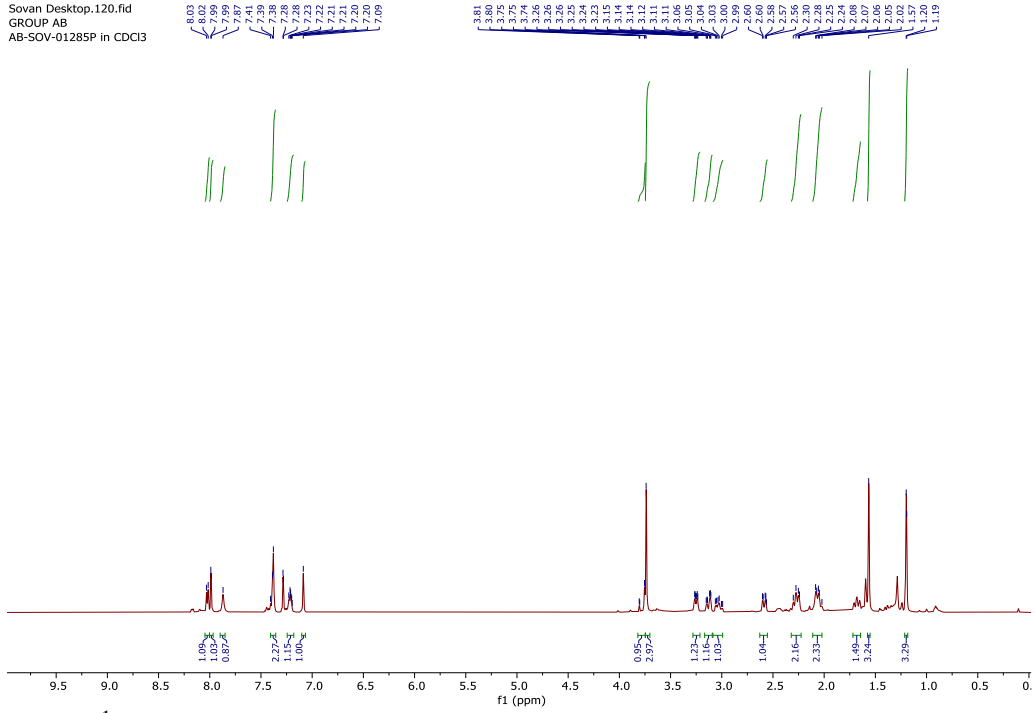
1: TOF MS ES+
2.29e6



HRMS data of (+)-26b

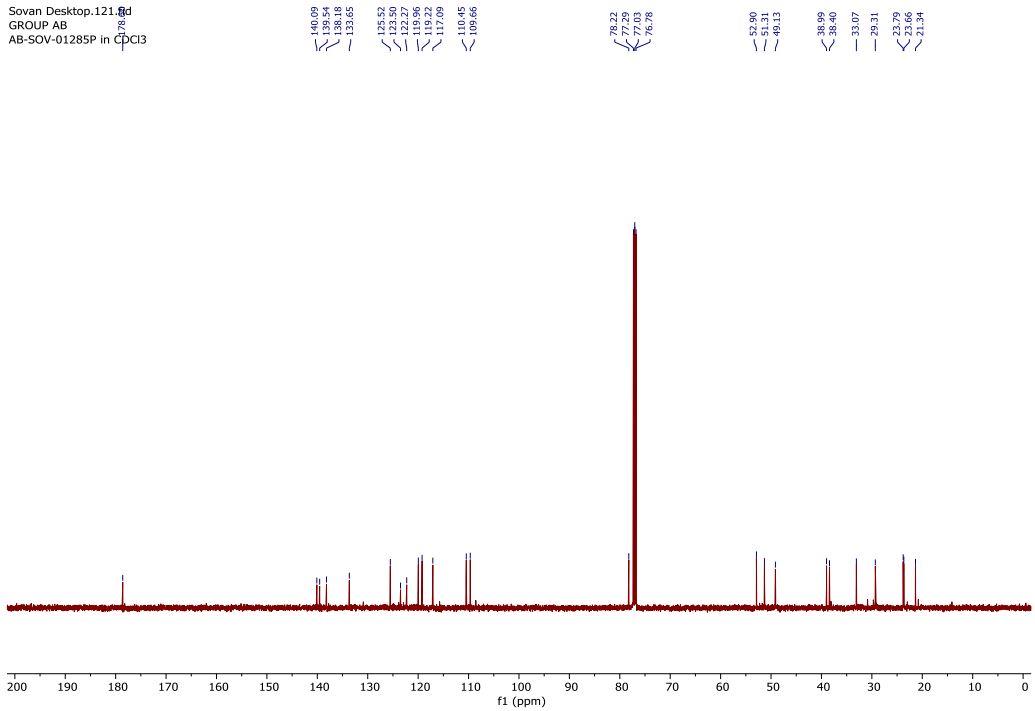


Sovan Desktop.120.fid
GROUP AB
AB-SOV-01285P in CDCl₃



¹H NMR (500 MHz, CDCl₃) of oridamycin A methylester (+)-2d

Sovan Desktop.121.fid
GROUP AB
AB-SOV-01285P in CDCl₃



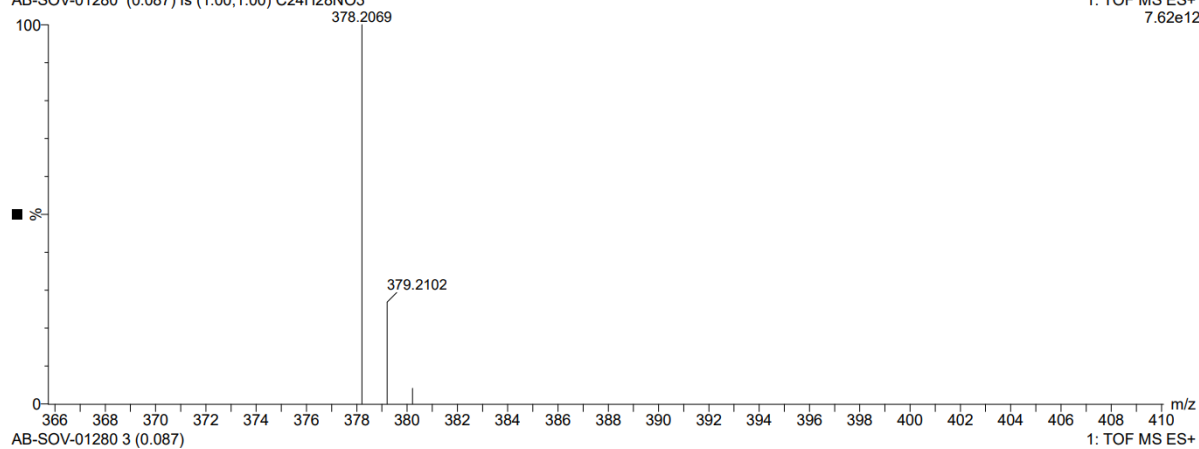
¹³C{¹H} NMR (125 MHz, CDCl₃) of oridamycin A methylester (+)-2d

AB28-Mar-2024 12:31:16

IISER - KOLKATA

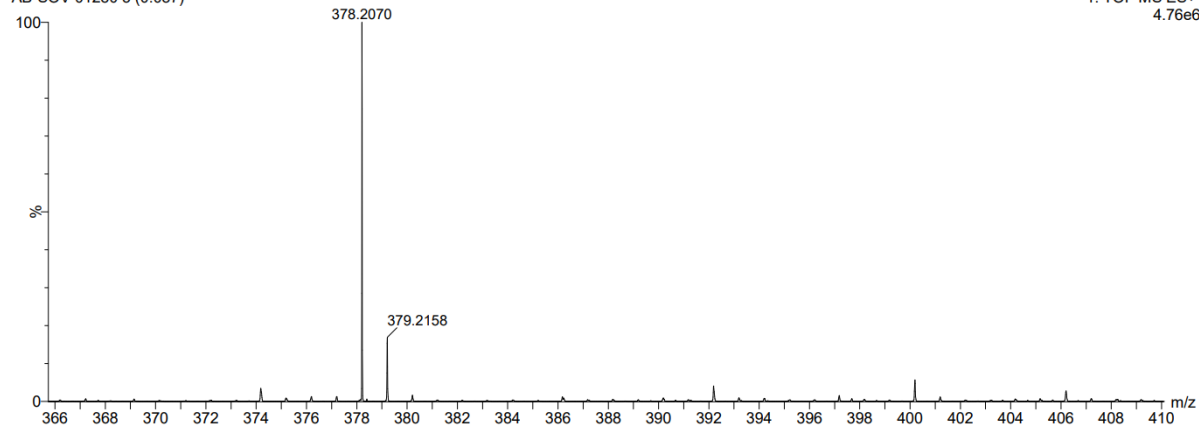
AB-SOV-01280 (0.087) Is (1.00,1.00) C₂₄H₂₈NO₃

1: TOF MS ES+
7.62e12

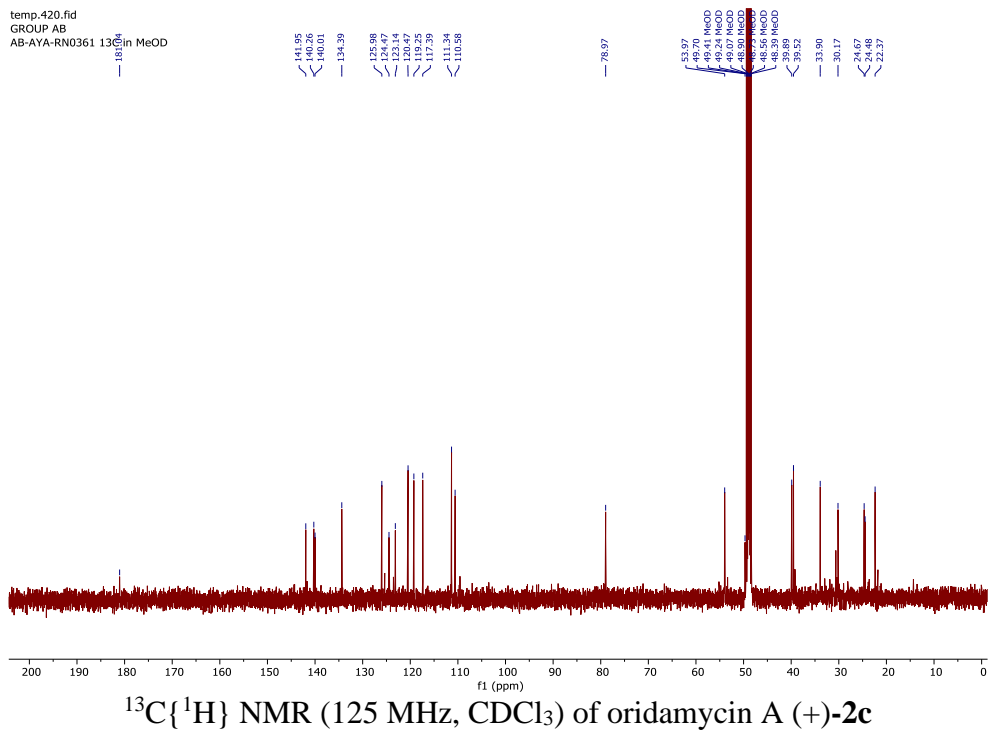
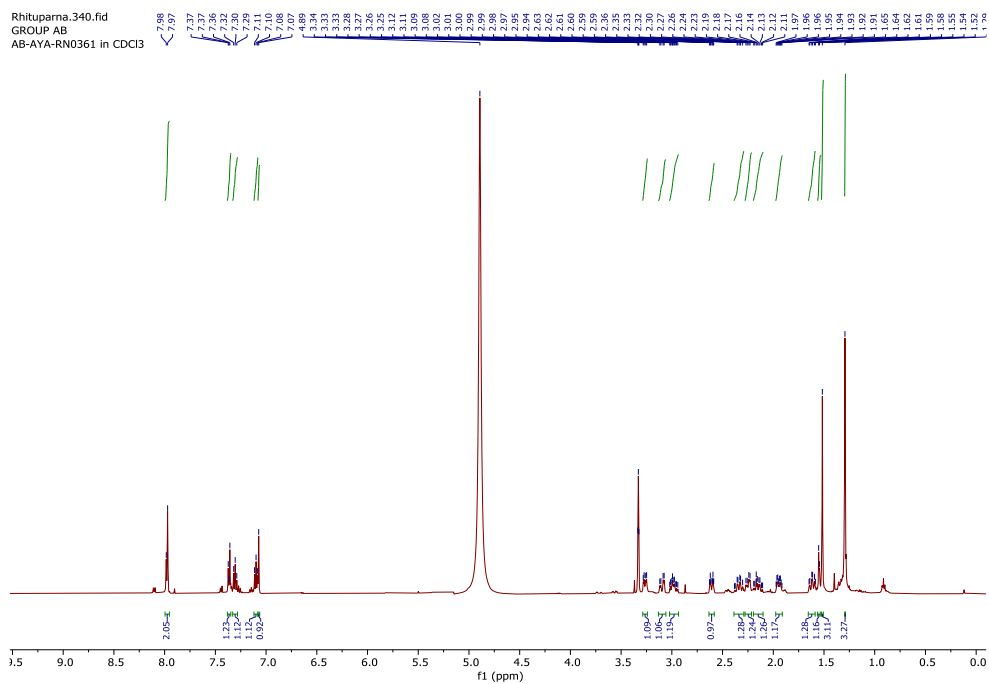
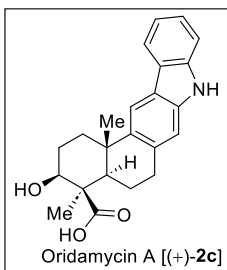


AB-SOV-01280 3 (0.087)

1: TOF MS ES+
4.76e6



HRMS data of oridamycin A methylester (+)-**2d**



Display Report

Analysis Info

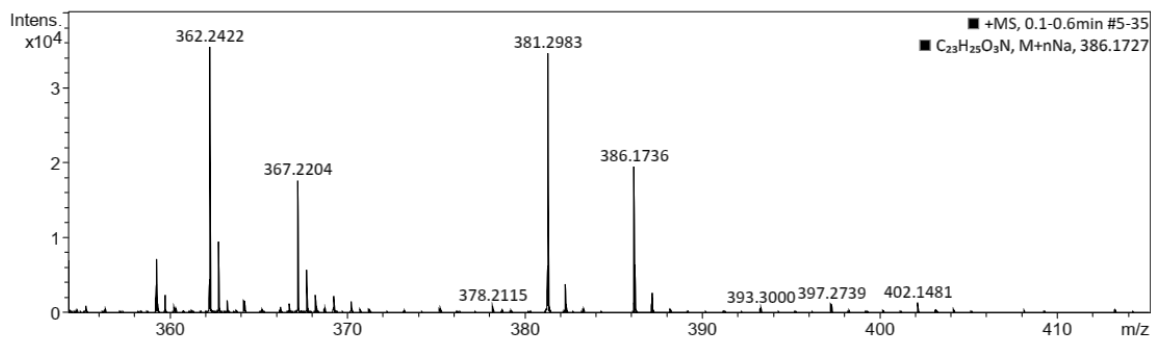
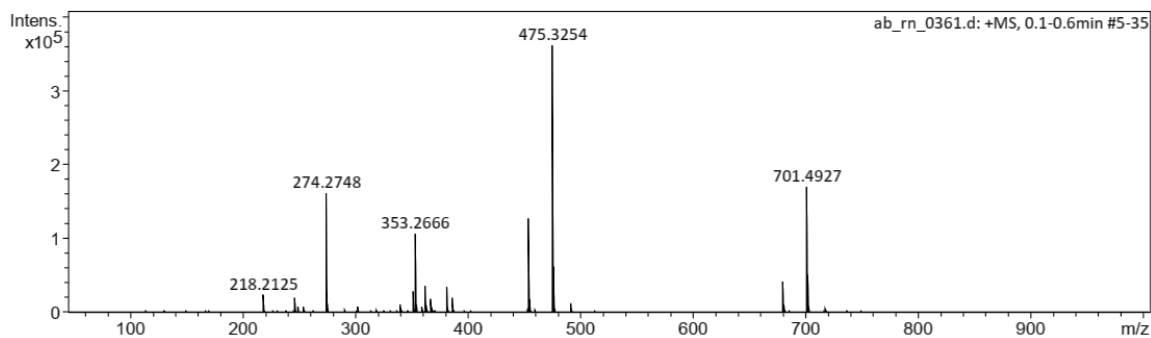
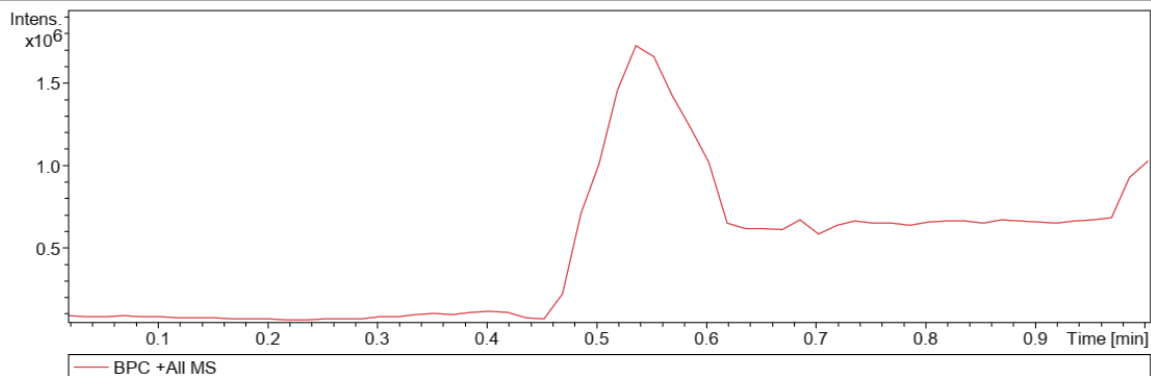
Analysis Name D:\Data\User data\2022\FEB\lab_rn_0361.d
Method Tune_pos_Standard.m
Sample Name ab_rn_0361
Comment

Acquisition Date 2/9/2022 12:29:14 PM

Operator IISER Kolkata
Instrument maXis impact 8282001.00127

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Focus	Active	Set Capillary	3400 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



ab_rn_0361.d

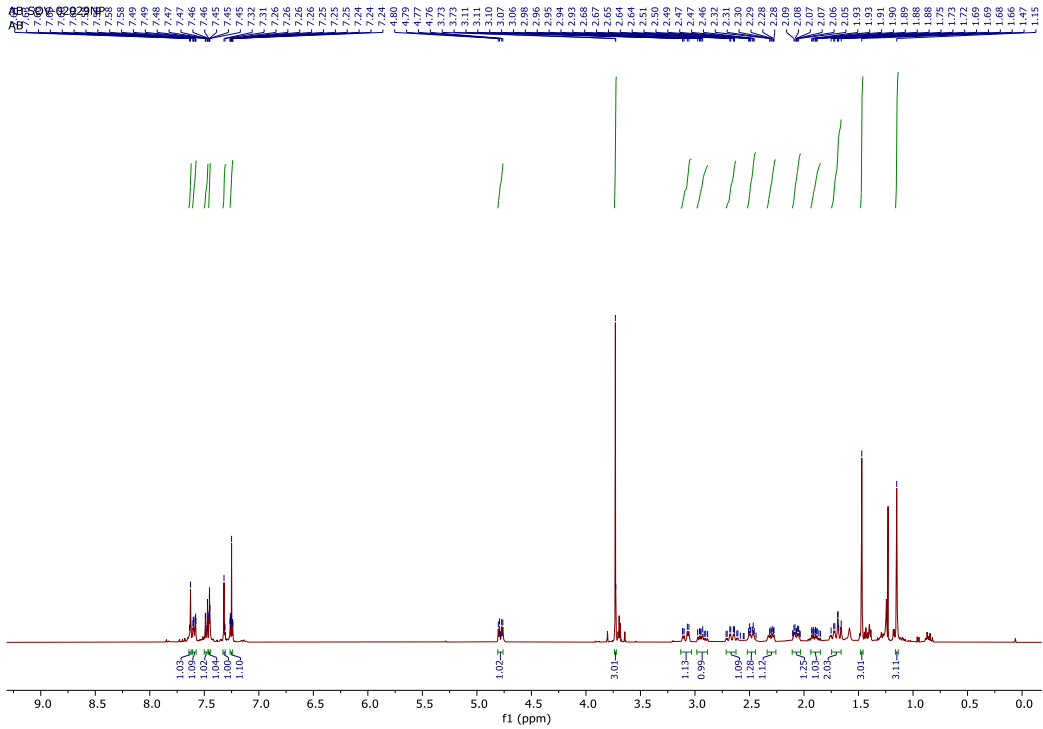
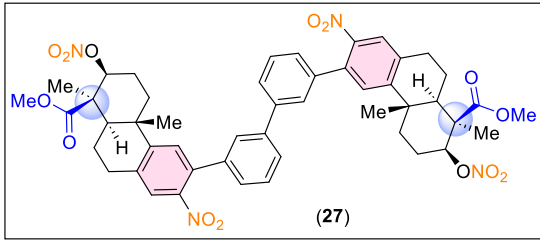
Bruker Compass DataAnalysis 4.1

printed: 2/9/2022 12:32:21 PM

by: IISER Kolkata

Page 1 of 1

HRMS data of oridamycin A (+)-**2c**



^1H NMR (500 MHz, CDCl_3) of (+)-27

Dioridamycin NMR.410.fid
GROUP AB
AB-SOV-02029 in CDCl_3

173.10

152.14

146.03

141.14

138.36

135.69

132.84

129.19

128.10

127.16

126.83

124.82

87.60

77.59

77.24

77.04

76.78

51.97

51.88

48.50

38.45

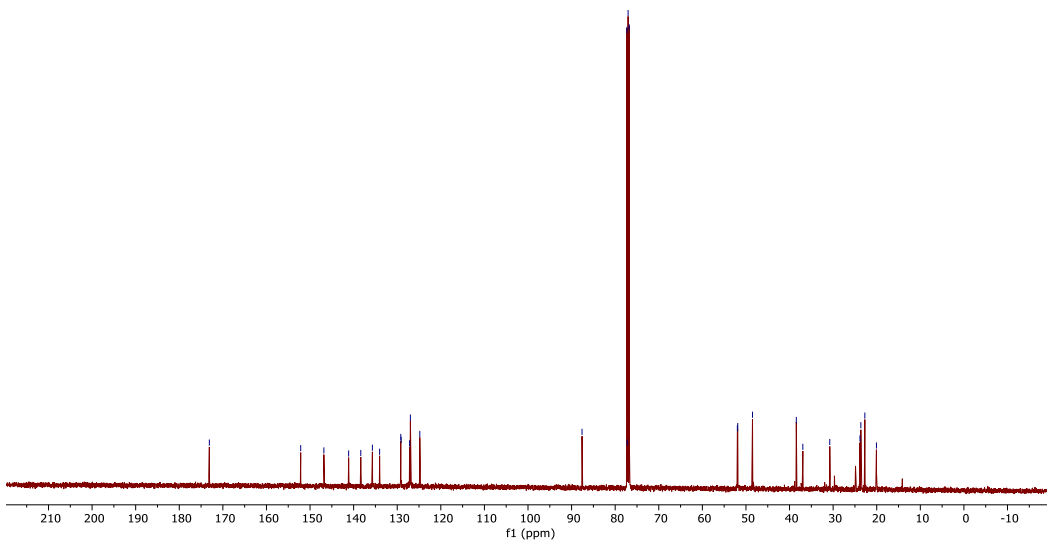
36.95

30.77

23.84

22.73

20.07

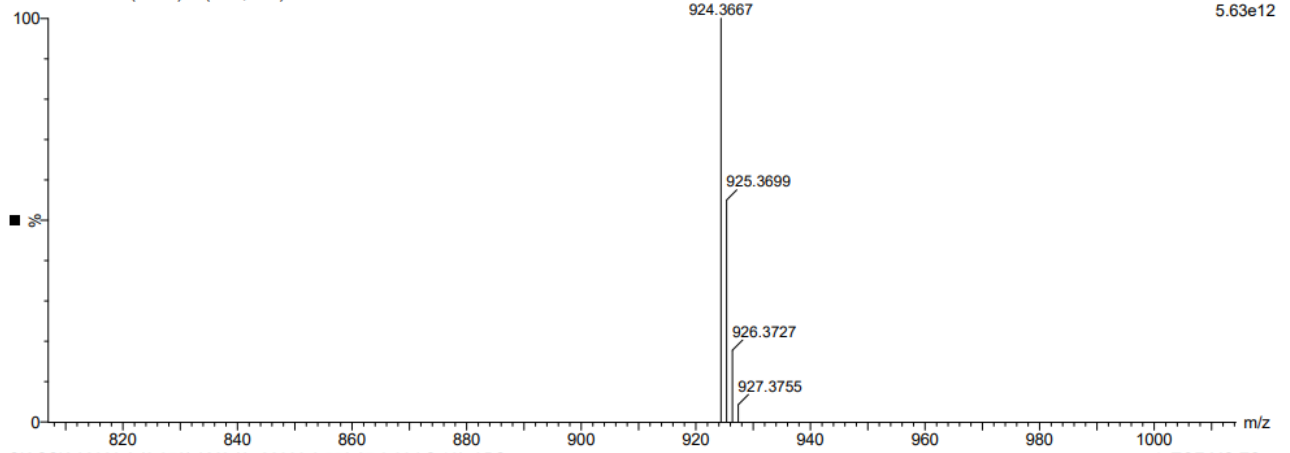


$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-27

SK02-Aug-2024 14:02:42
SK-SSK-02029 (0.053) Is (1.00,1.00) C48H50N4O14NH4

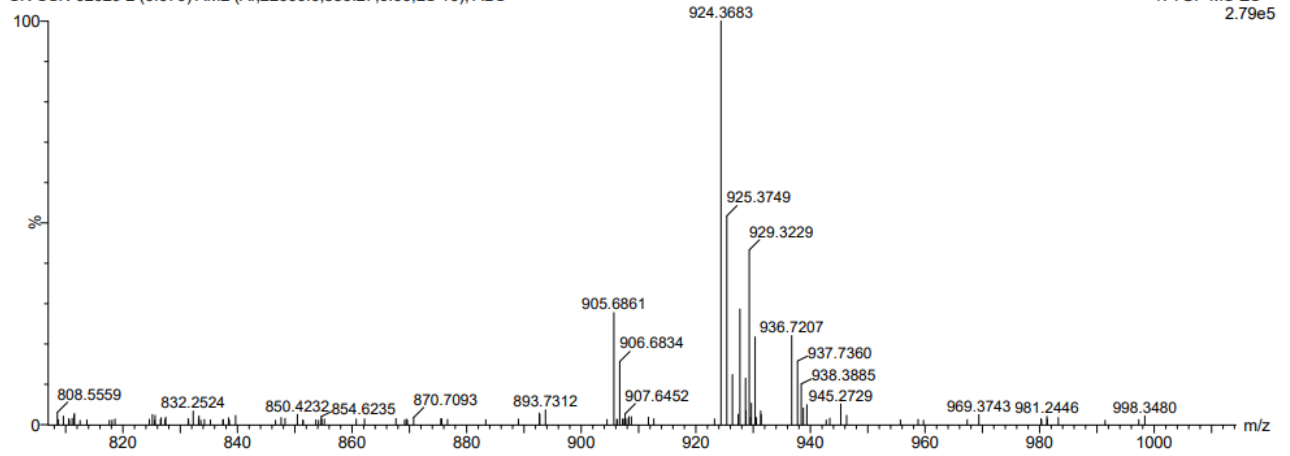
IISER - KOLKATA

1: TOF MS ES+
5.63e12

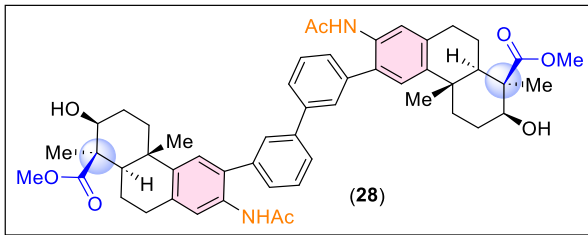


SK-SSK-02029 2 (0.070) AM2 (Ar,22000.0,556.27,0.00,LS 10); ABS

1: TOF MS ES+
2.79e5



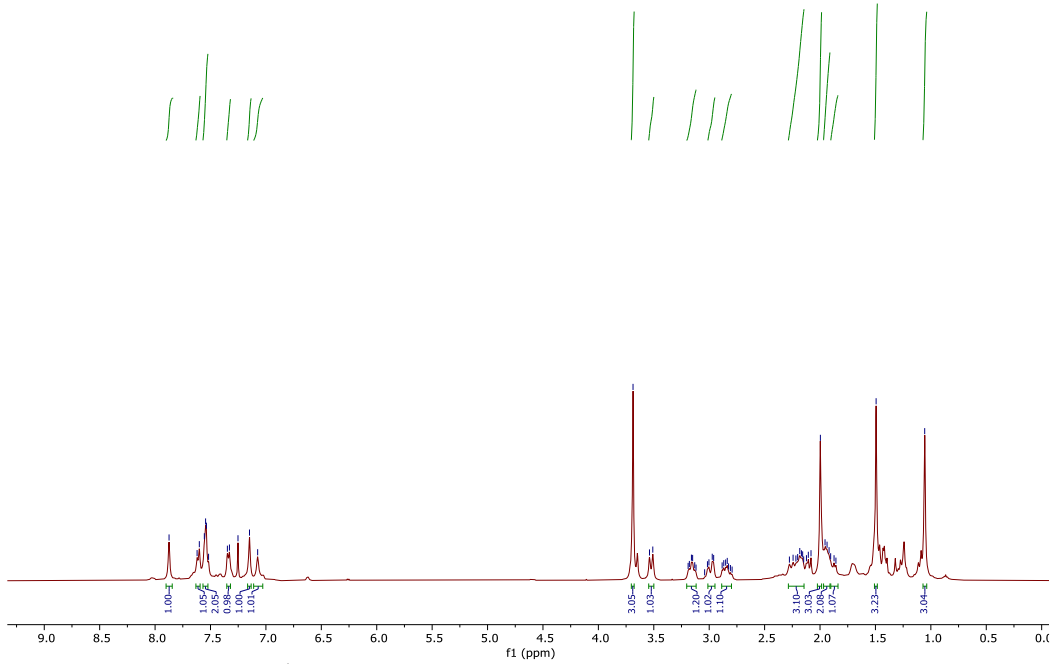
HRMS data of (+)-27



AB-SOV-02031
AB

7.87
7.60
7.56
7.54
7.54
7.52
7.35
7.33
7.15
7.07

3.69
3.64
3.51
3.19
3.18
3.15
3.13
3.12
3.07
3.00
2.96
2.88
2.87
2.85
2.83
2.81
2.79
2.74
2.22
2.20
2.17
2.15
2.11
2.08
2.00
1.94
1.92
1.90
1.86
1.49
1.06



AB-DGJ-004
AB

178.56

168.47

144.11
144.55
139.33
136.00
132.10
129.62
128.52
128.20
126.65
122.47

78.12
77.46
76.83

52.40

51.68

49.03

38.18

38.01

32.14

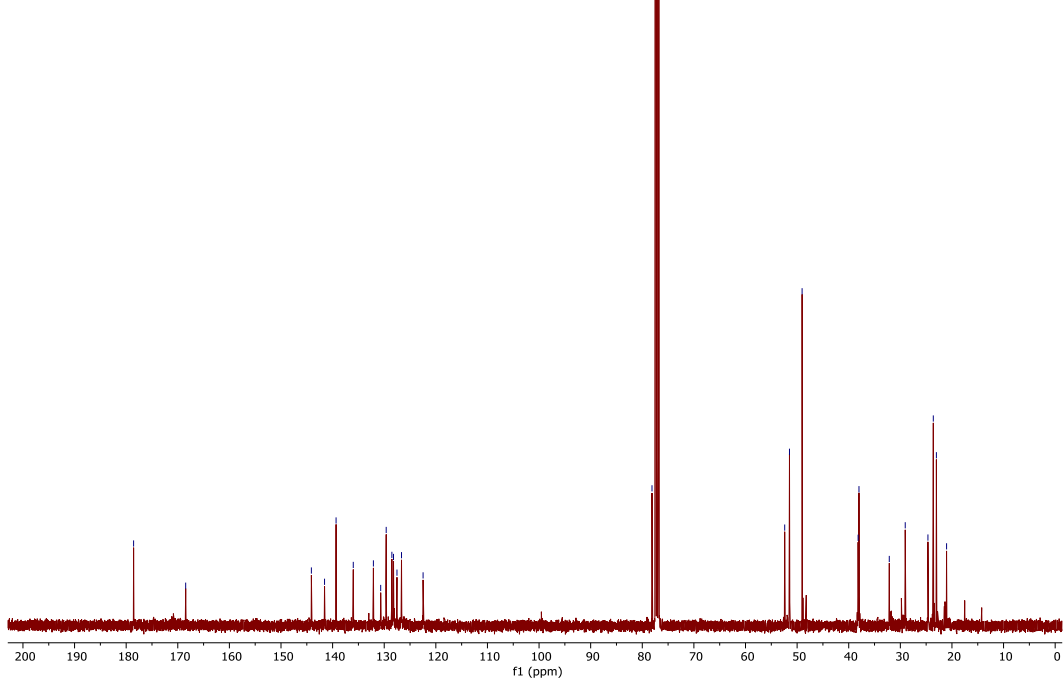
29.05

24.65

23.61

23.01

21.04



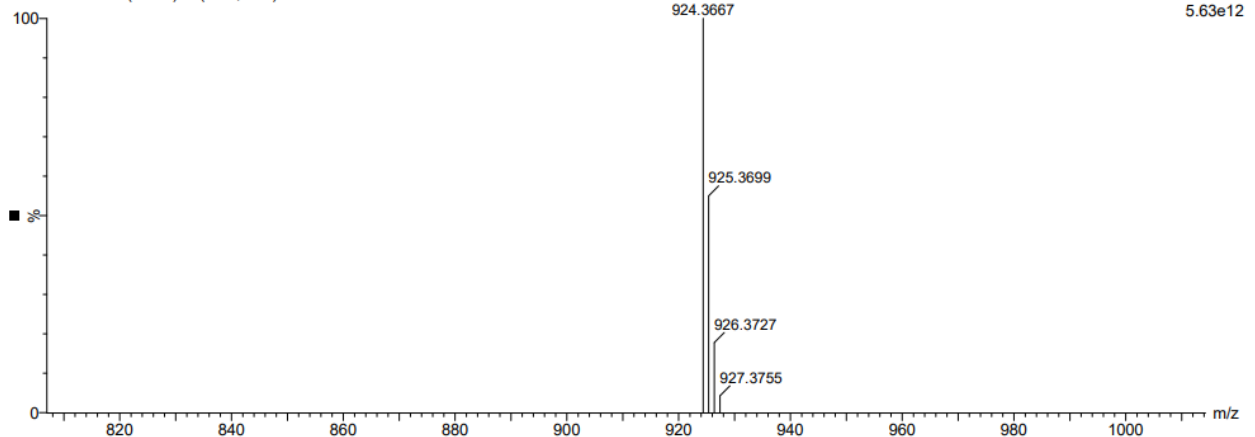
$^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) of (+)-28

SK02-Aug-2024 14:02:42

SK-SSK-02029 (0.053) Is (1.00,1.00) C48H50N4O14NH4

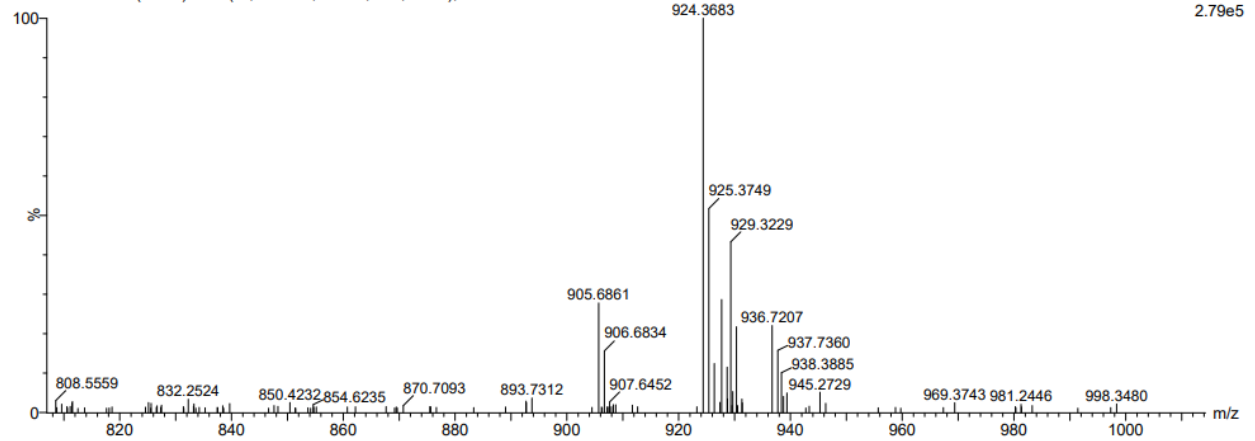
IISER - KOLKATA

1: TOF MS ES+
5.63e12

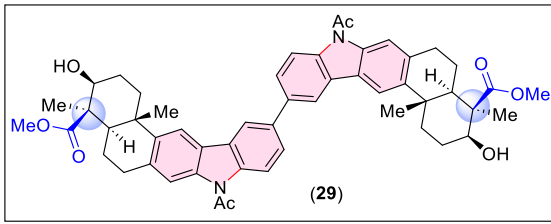


SK-SSK-02029 2 (0.070) AM2 (Ar,22000.0,556.27,0.00,LS 10); ABS

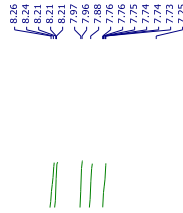
1: TOF MS ES+
2.79e5



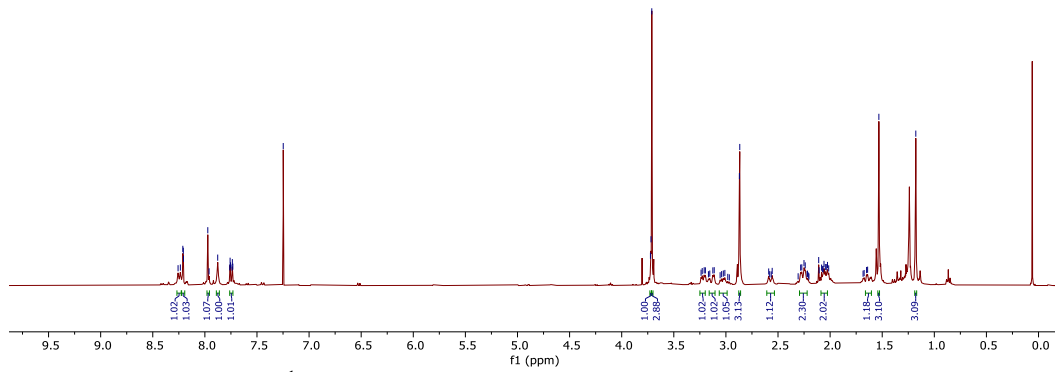
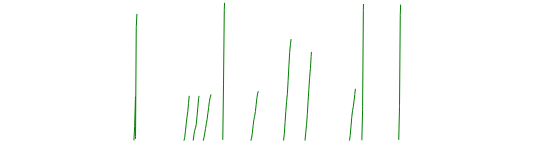
HRMS data of (+)-28



AB-SOV-02032 1
AB



3.72
3.72
3.71
3.24
3.24
3.21
3.20
3.17
3.13
3.13
3.06
3.04
3.02
3.01
2.99
2.87
2.87
2.59
2.58
2.56
2.27
2.27
2.25
2.24
2.24
2.22
2.11
2.11
2.07
2.07
2.06
2.06
2.03
2.03
2.01
1.67
1.65
1.64
1.64
1.14



¹H NMR (500 MHz, CDCl₃) of (+)-29

AB-SOV-02032 1
AB

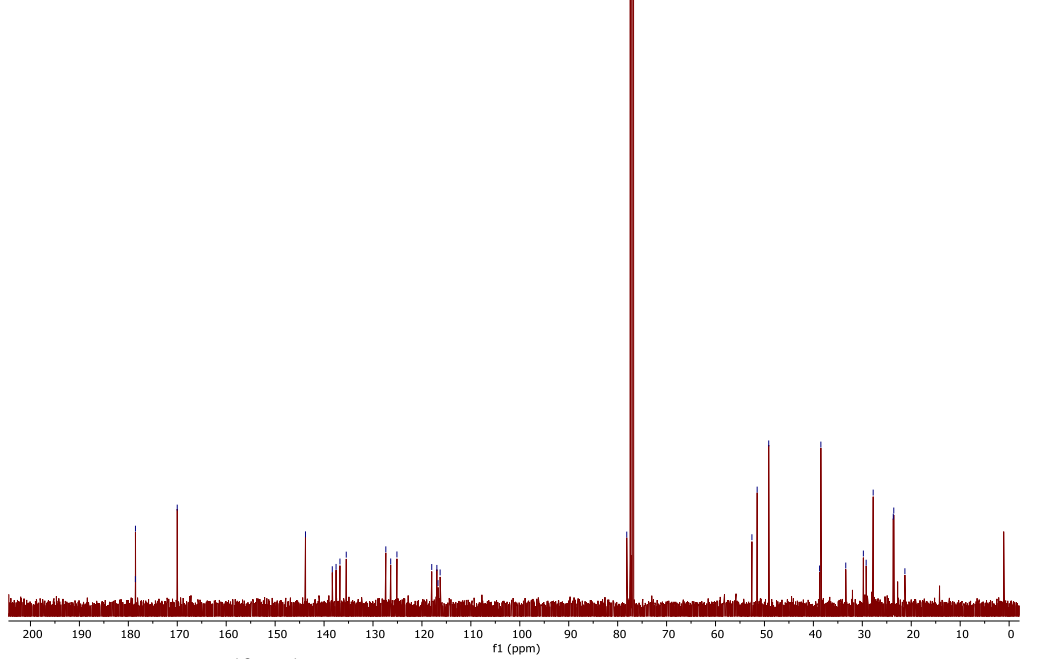
178.56
178.54
170.01

143.80
138.32
137.55
136.75
135.46
127.38
126.38
124.41
118.00
116.95
116.72
116.28

78.54
77.44
76.80

52.56
51.49
49.13

38.73
38.47
33.38
29.79
27.78
23.67
23.36
21.30

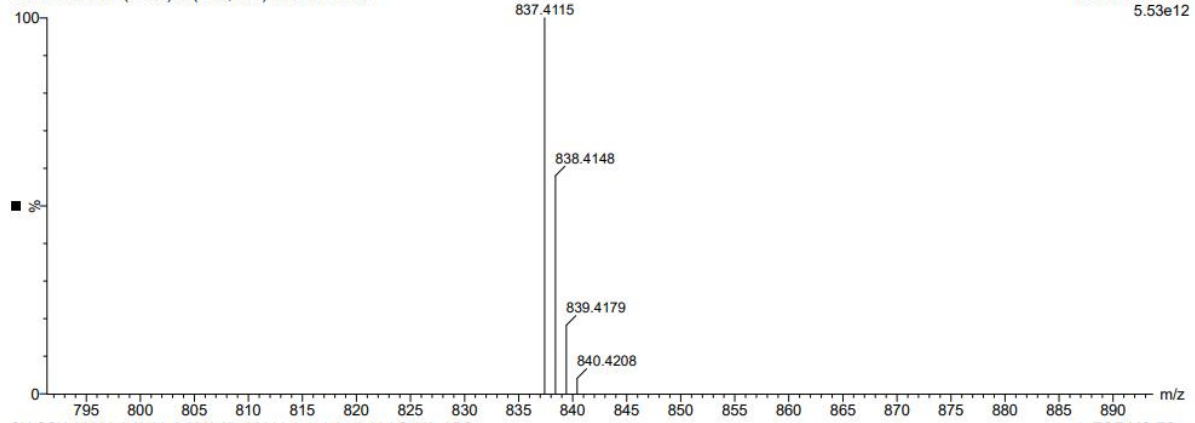


¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-29

SK22-Jul-2024 15:42:15
SK-SSK-02032 (0.053) Is (1.00,1.00) C52H57N2O8

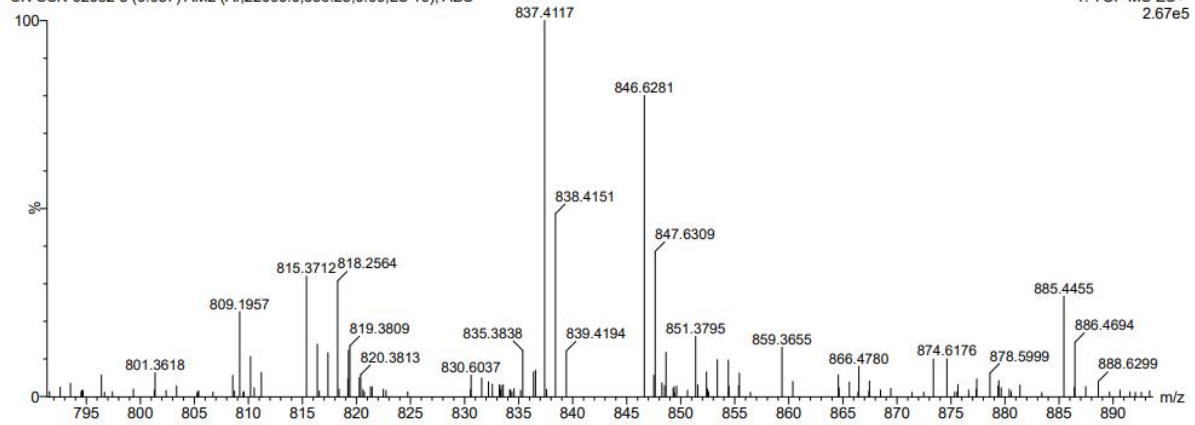
IISER - KOLKATA

1: TOF MS ES+
5.53e12

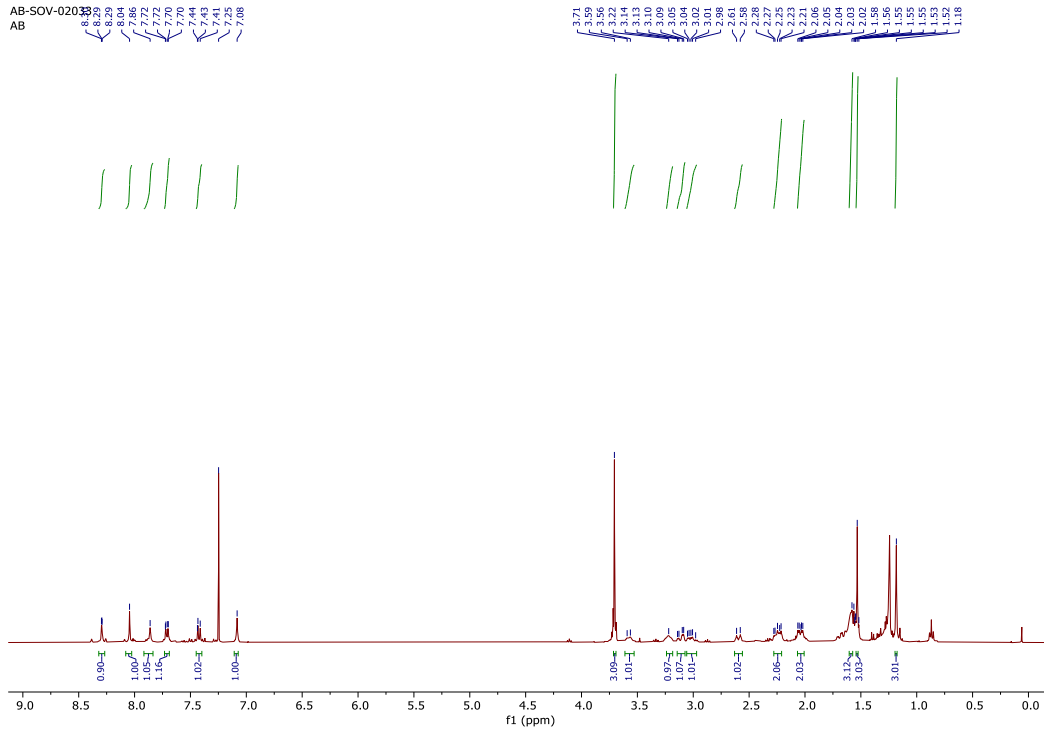
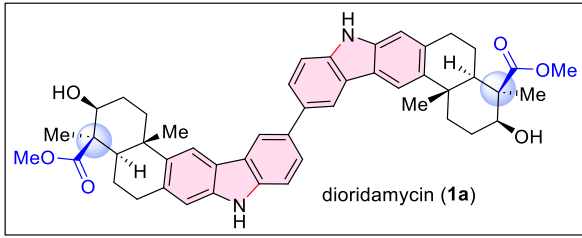


SK-SSK-02032 3 (0.087) AM2 (Ar,22000.0,556.25,0.00,LS 10); ABS

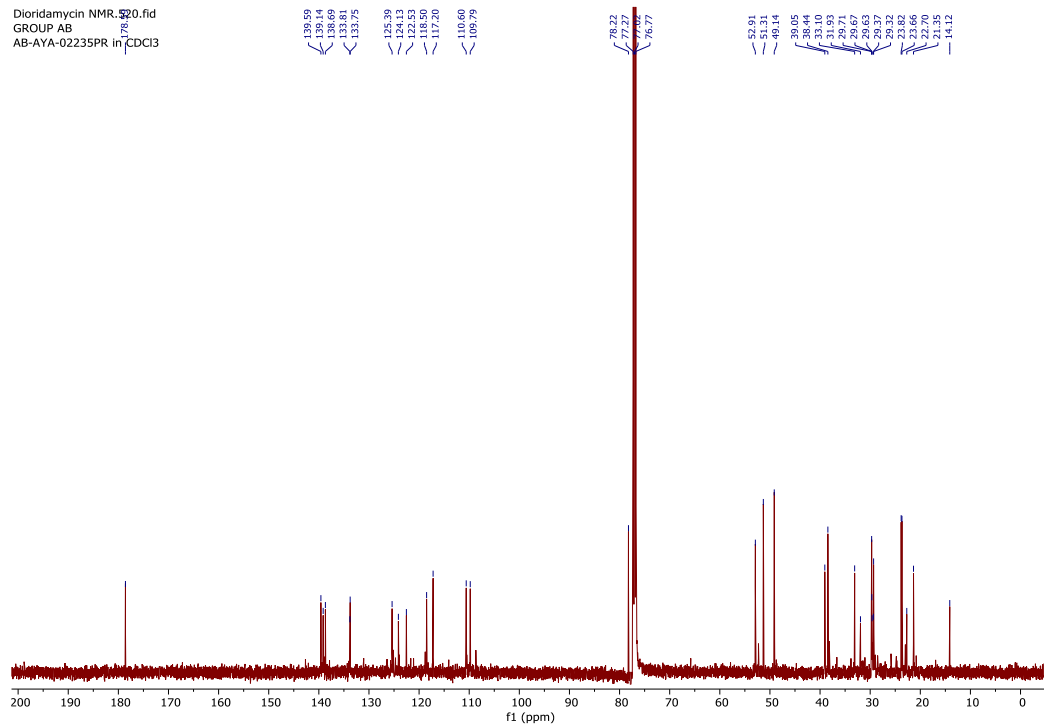
1: TOF MS ES+
2.67e5



HRMS data of (+)-**29**



¹H NMR (500 MHz, CDCl₃) of (+)-1a

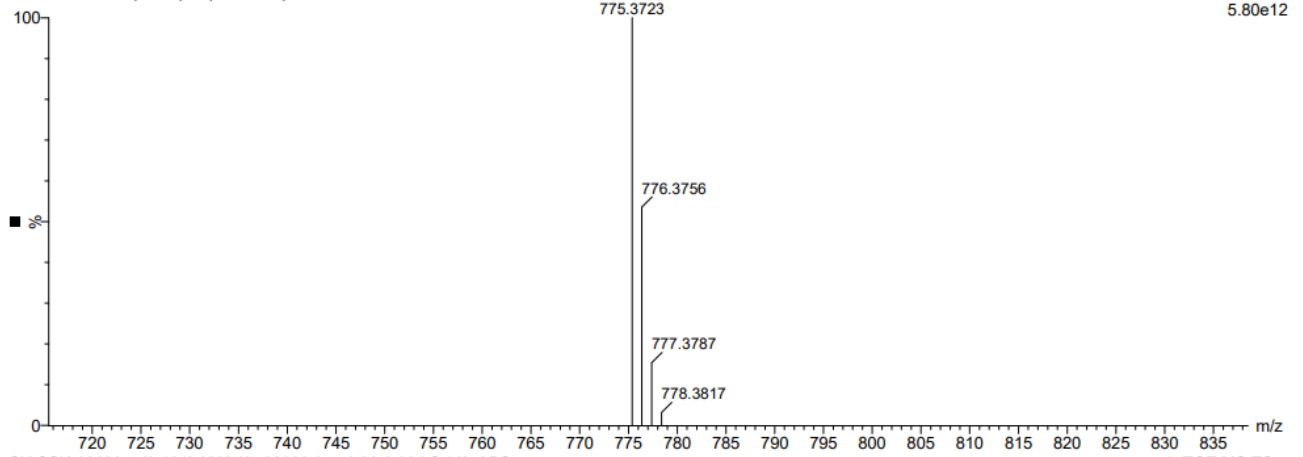


¹³C{¹H} NMR (125 MHz, CDCl₃) of (+)-1a

SK22-Jul-2024 15:40:42
SK-SSK-02033 (0.053) Is (1.00,1.00) C₄₈H₅₂N₂O₆Na

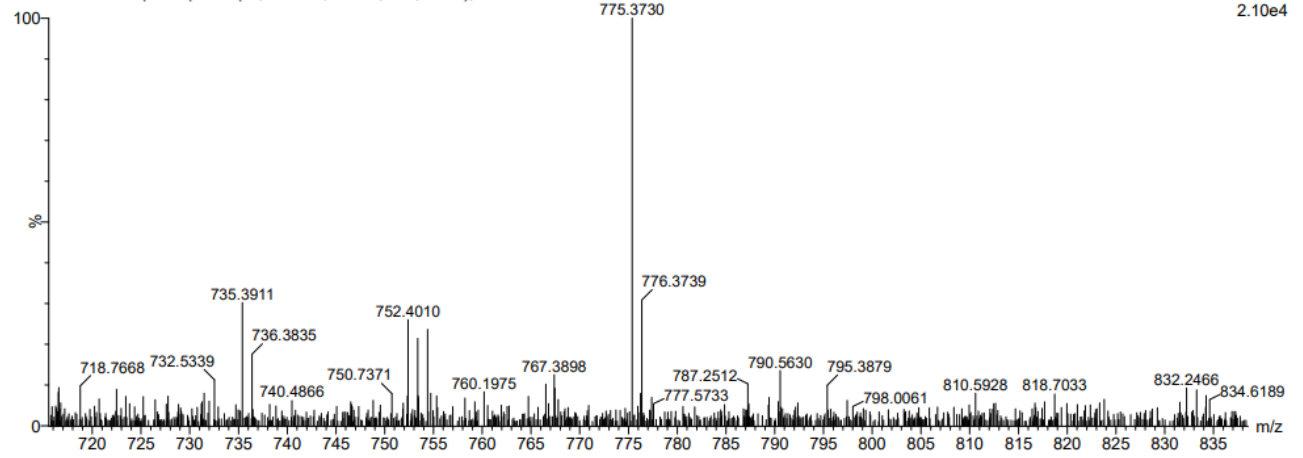
IISER - KOLKATA

1: TOF MS ES+
5.80e12



SK-SSK-02033 5 (0.121) AM2 (Ar,22000.0,556.28,0.00,LS 10); ABS

1: TOF MS ES+
2.10e4



HRMS data of (+)-**1a**