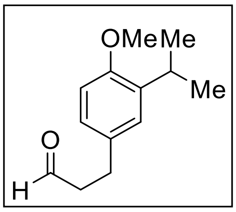
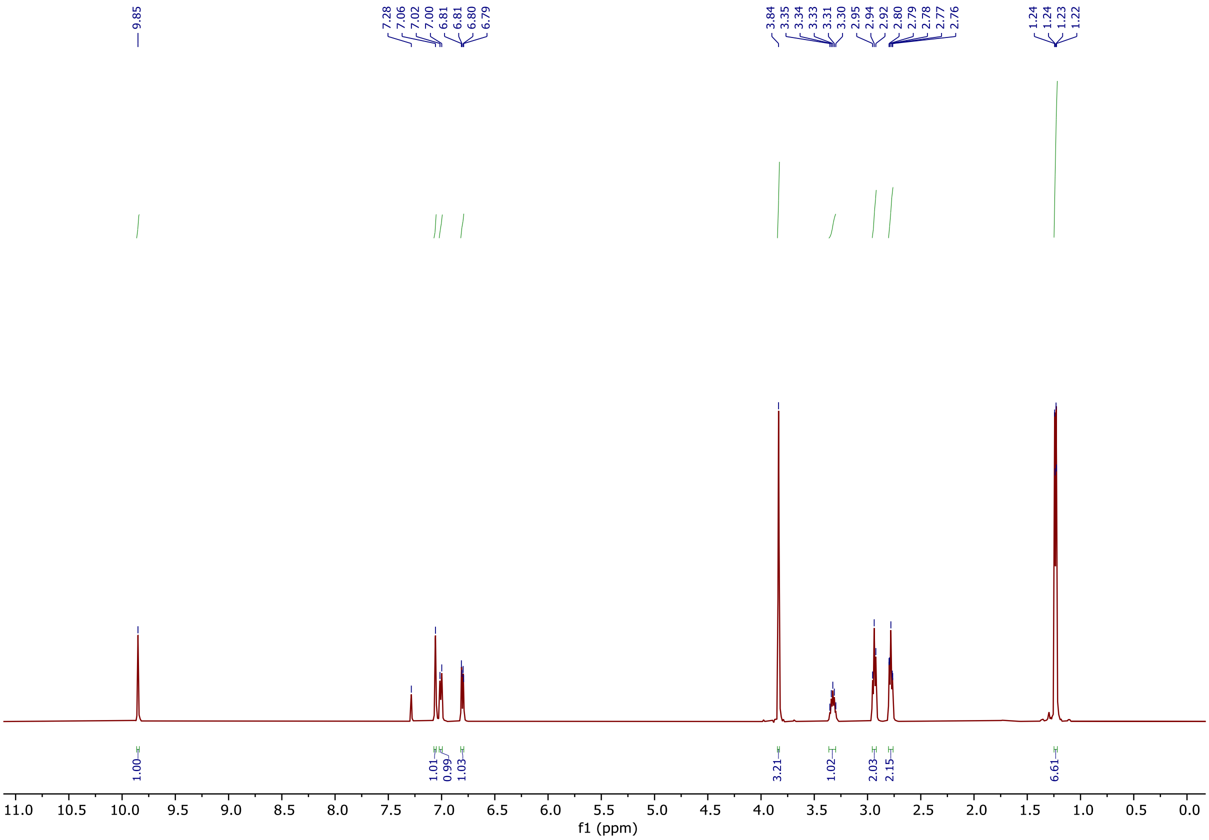
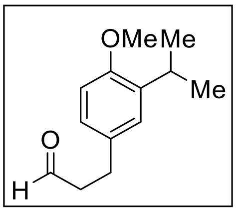
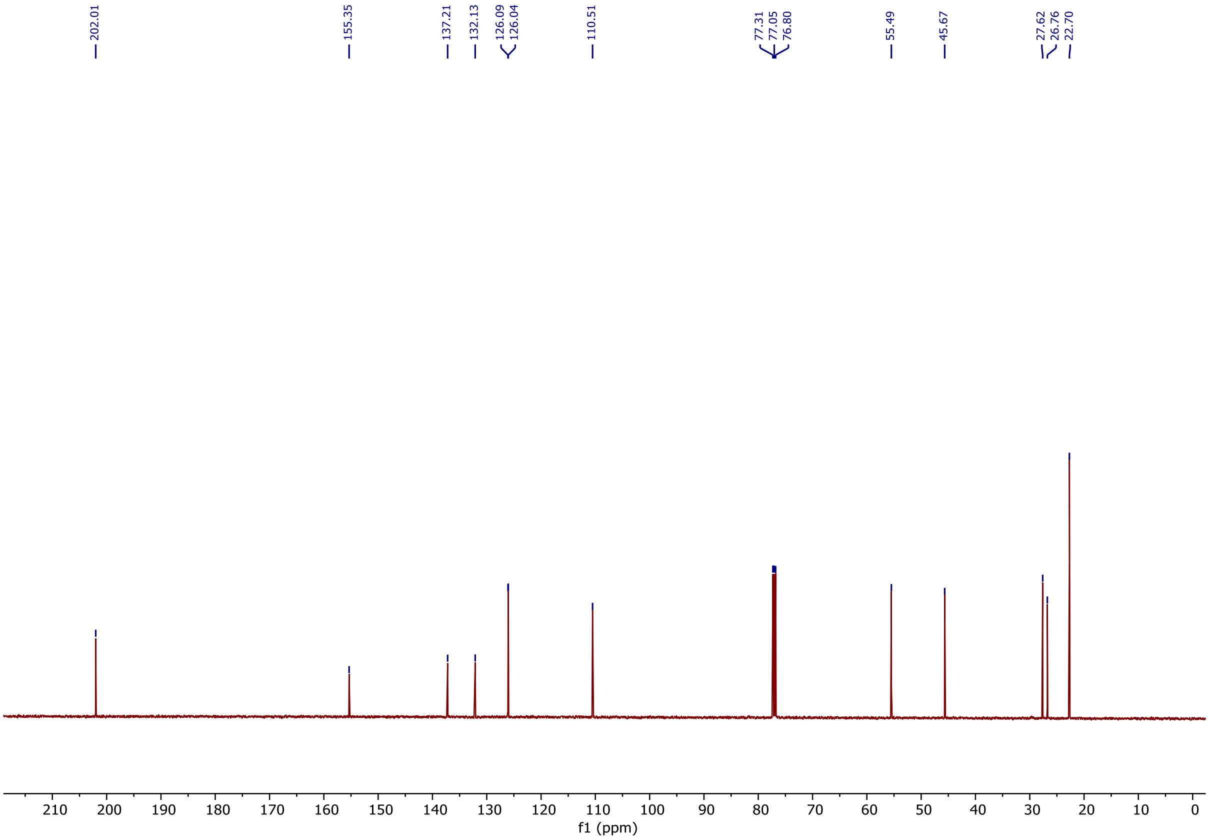
# Spectral Data



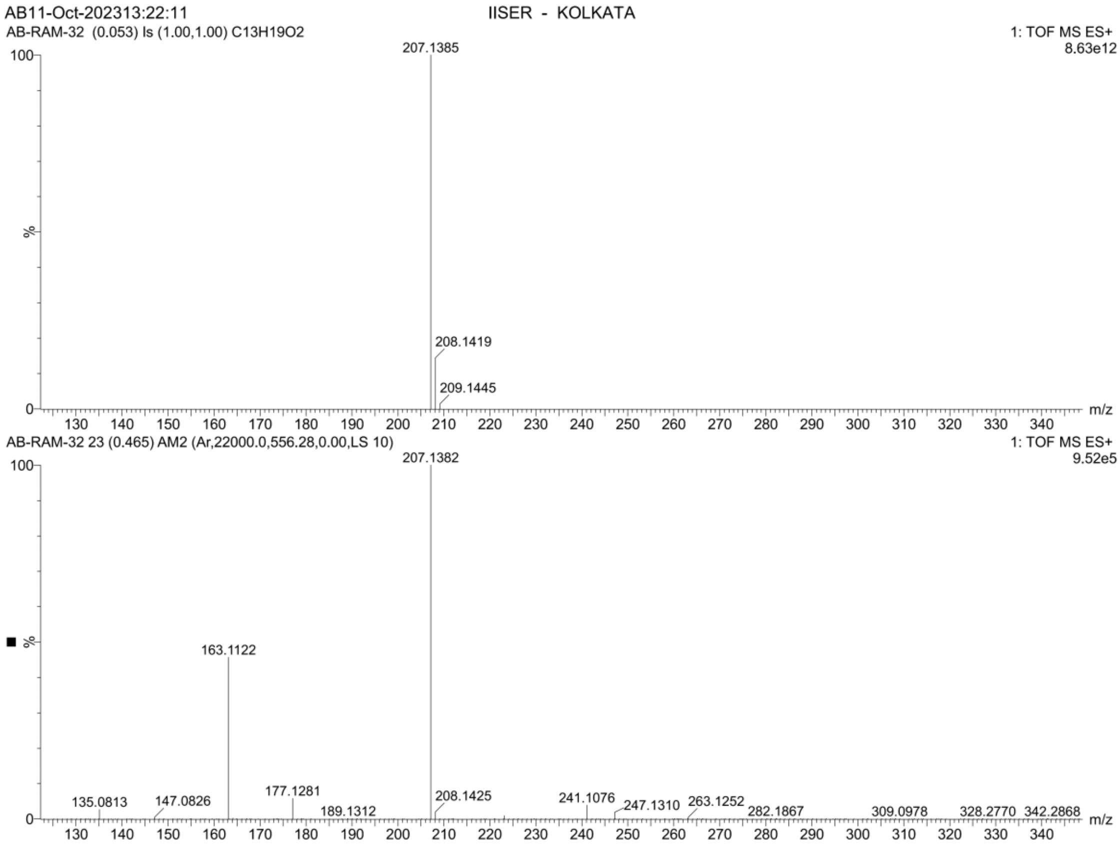



$^1$H NMR (500 MHz, $CDCl_3$) of 3-(3-isopropyl-4-methoxyphenyl)propanal

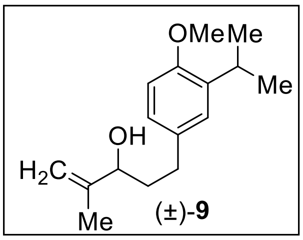


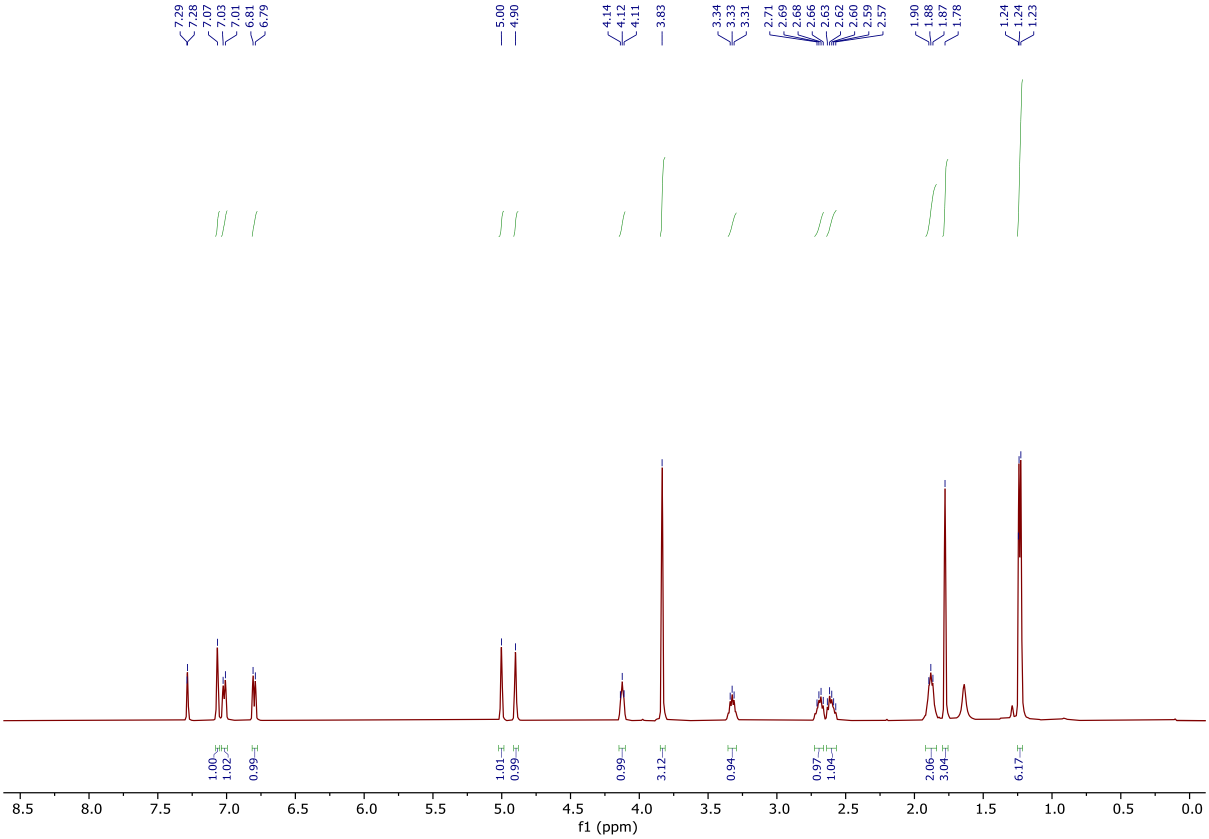




$^{13}$C NMR (126 MHz, $CDCl_3$) of 3-(3-isopropyl-4-methoxyphenyl)propanal

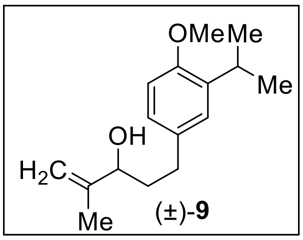


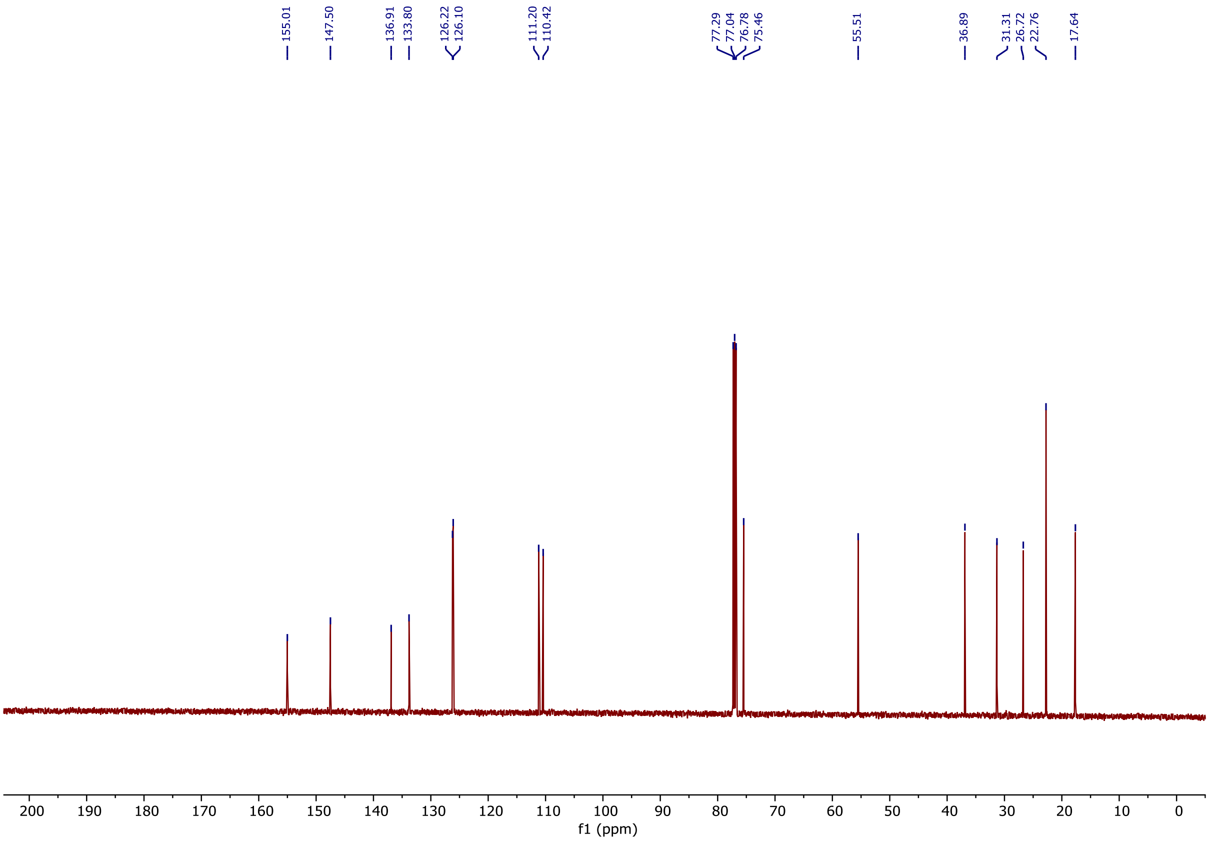

HRMS data of 3-(3-isopropyl-4-methoxyphenyl)propanal



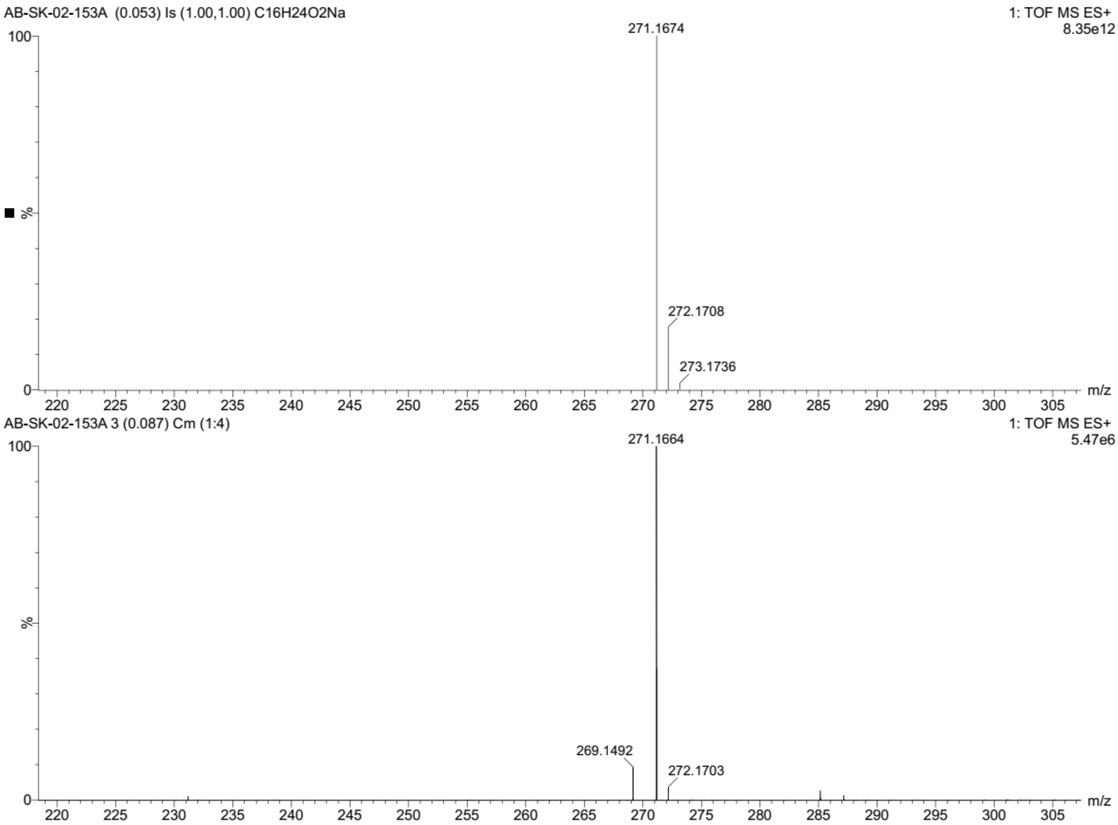


[1]H NMR (500 MHz, $CDCl_3$) of compound (±)-**9**

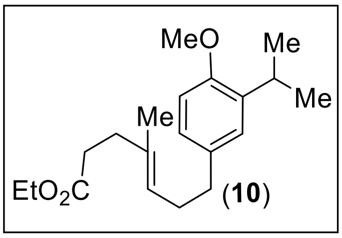


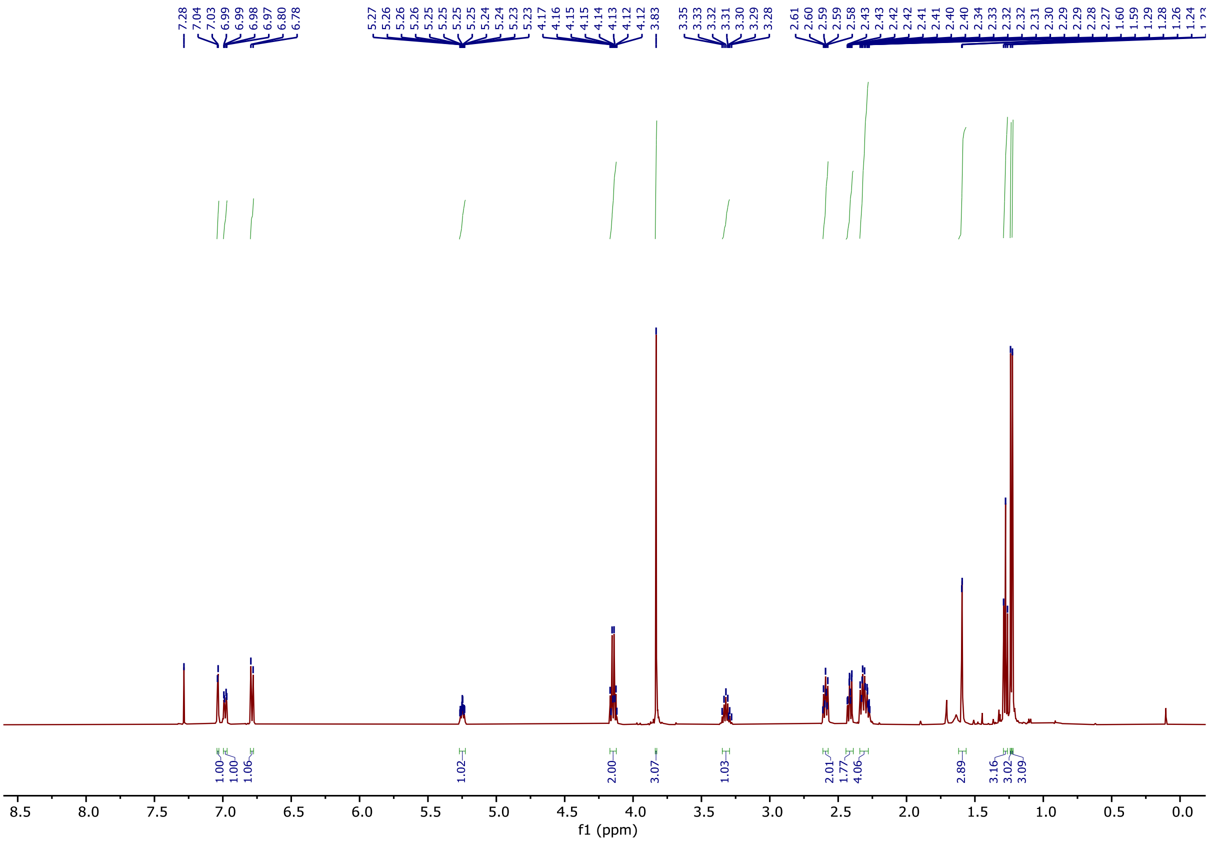

$^{13}C$ NMR (126 MHz, $CDCl_3$) of compound (±)-**9**



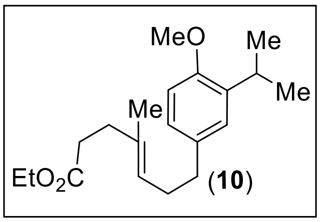

HRMS data of compound (±)-**9**

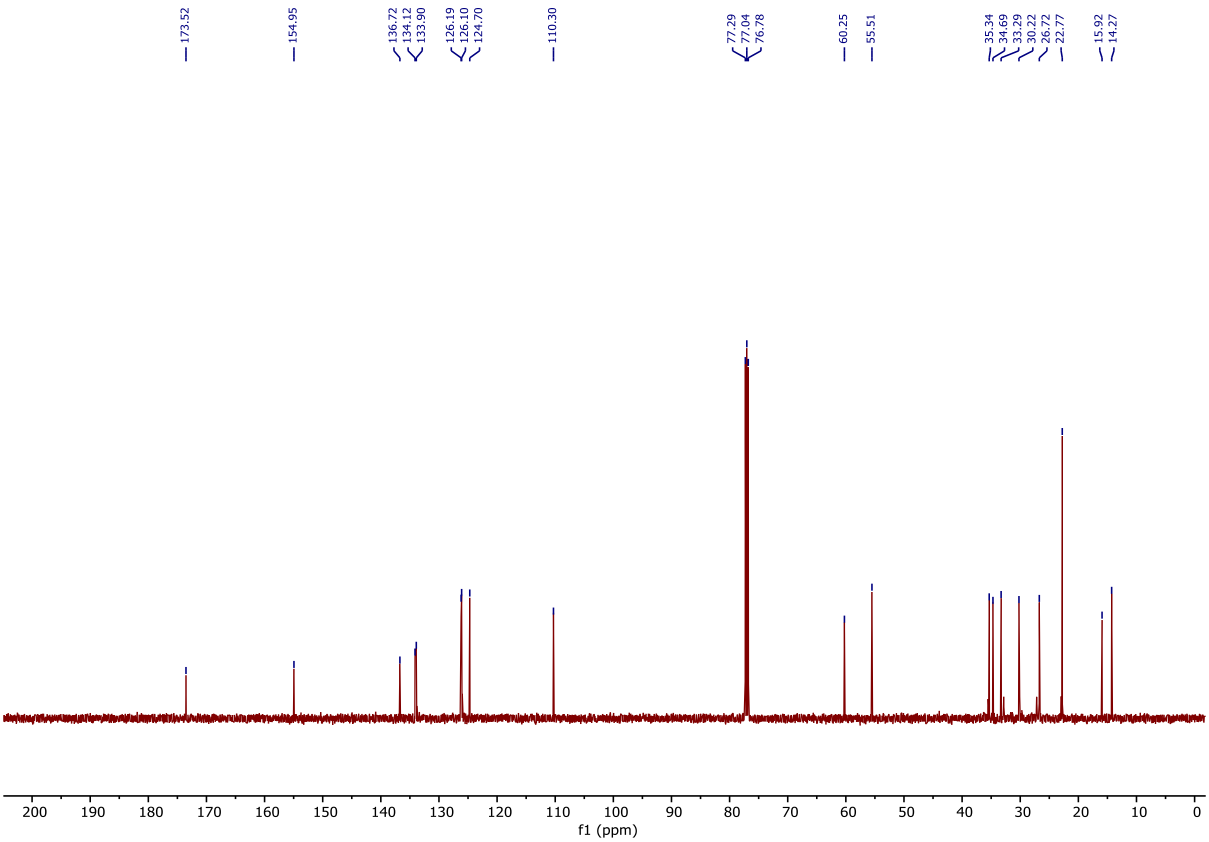


(**10**)

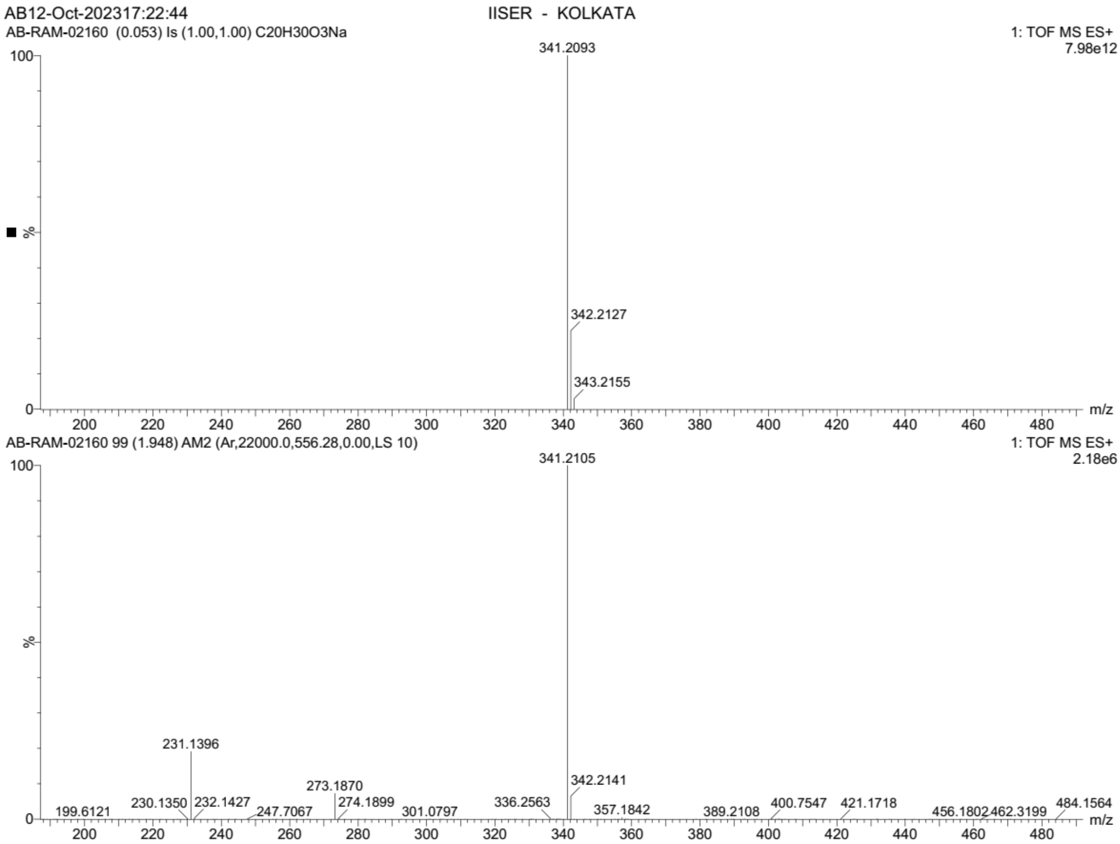


$^1$H NMR (500 MHz, $CDCl_3$) of compound **10**

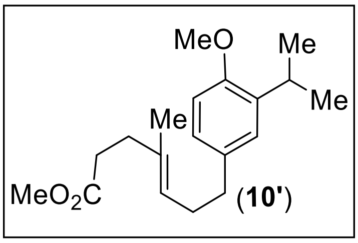


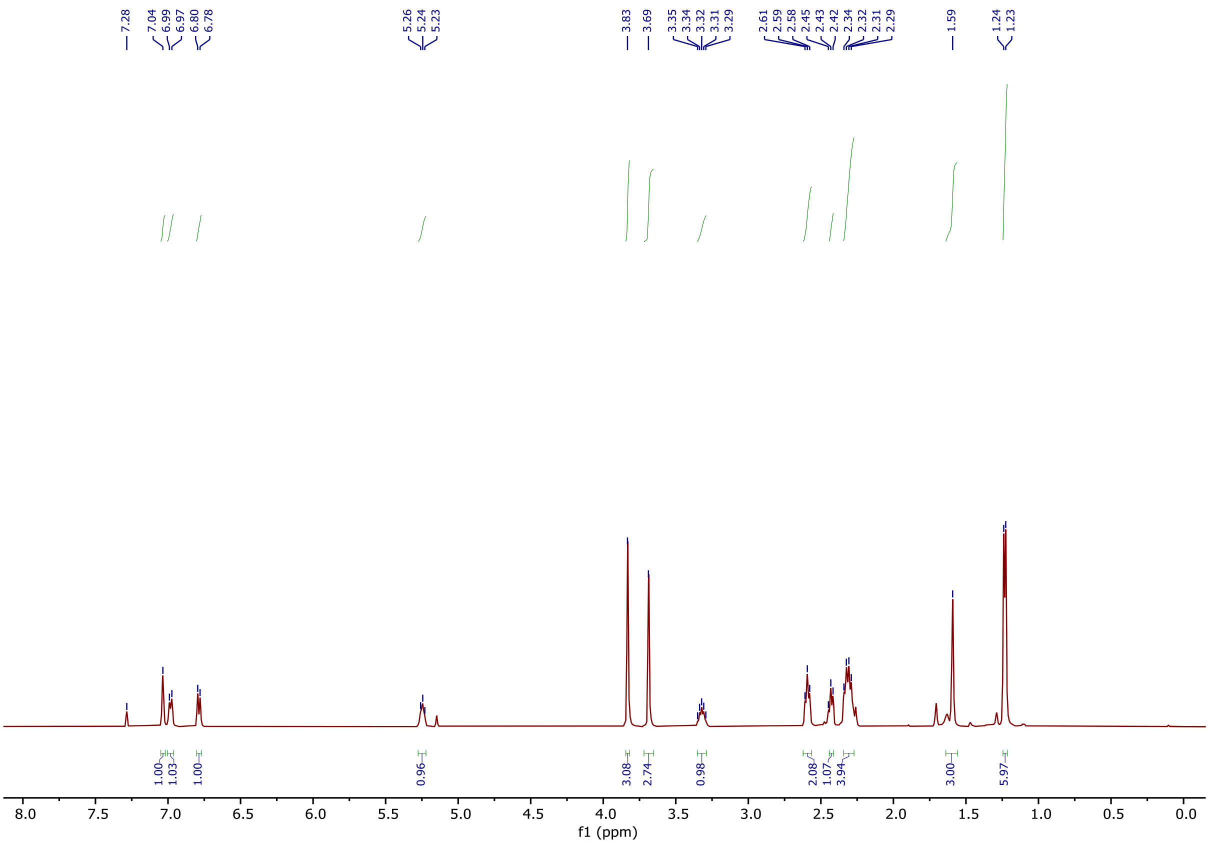




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound **10**

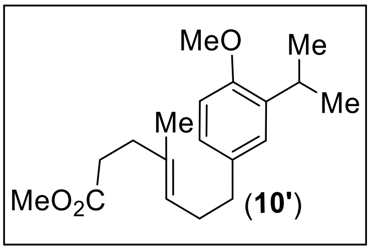


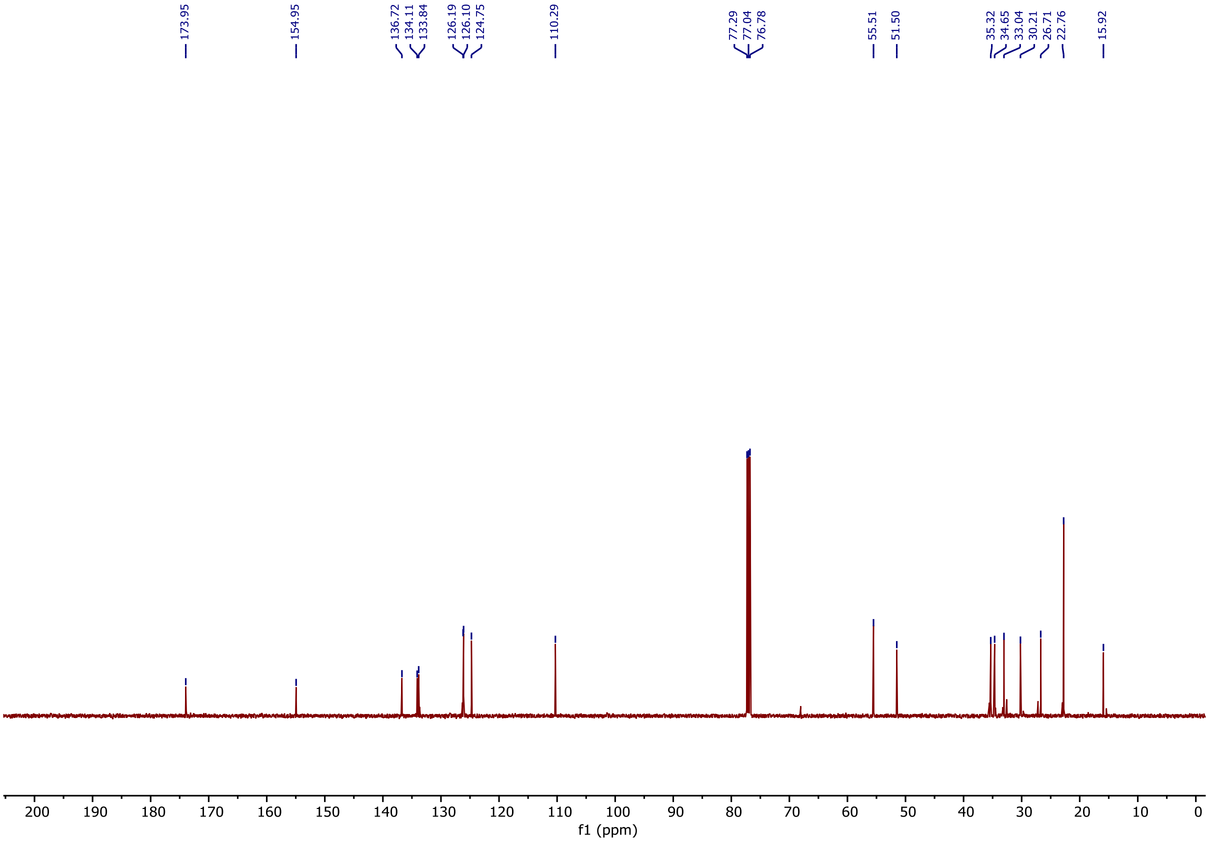

HRMS data of **10**



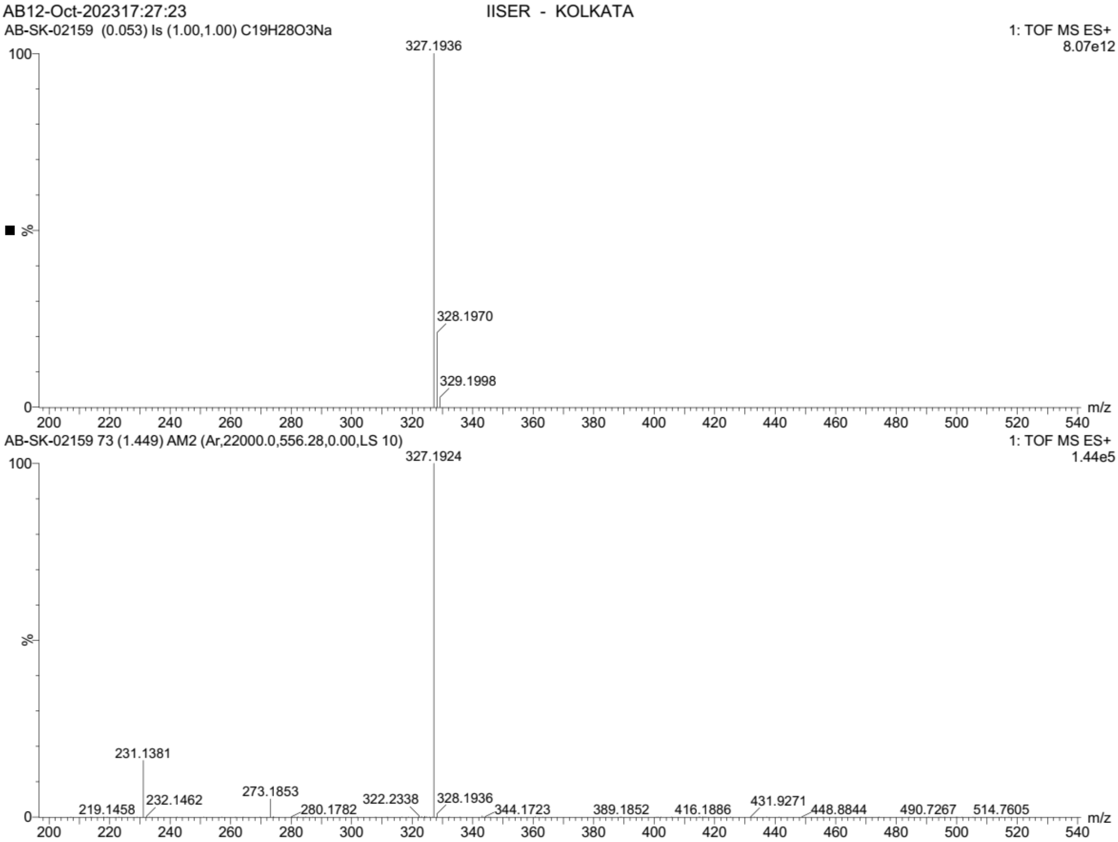



$^{1}$H NMR (500 MHz, $CDCl_3$) of compound **10’**

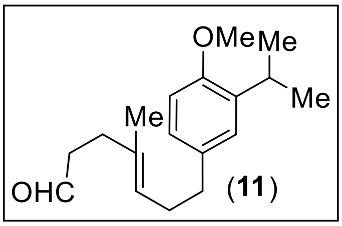


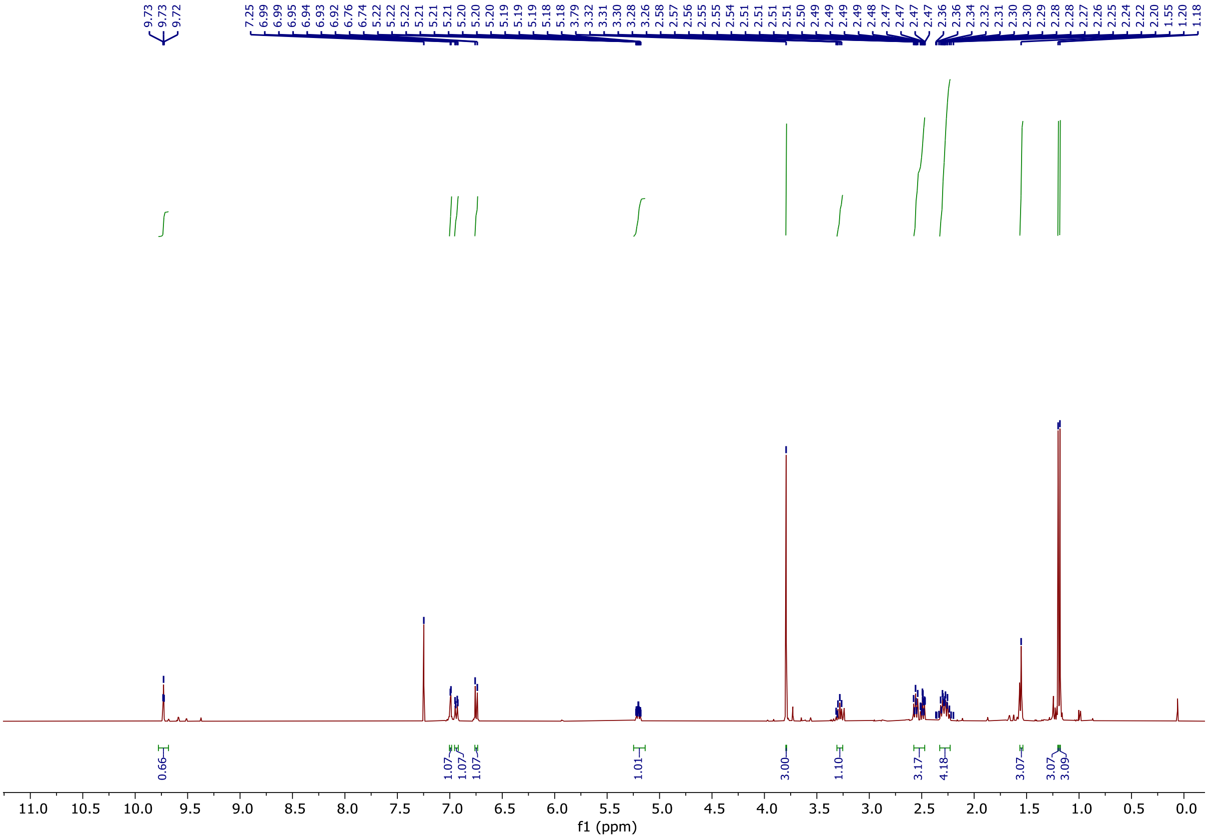




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound **10’**

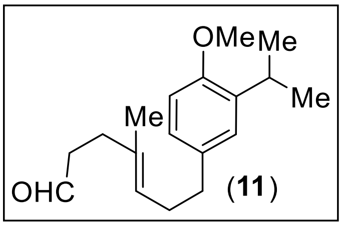


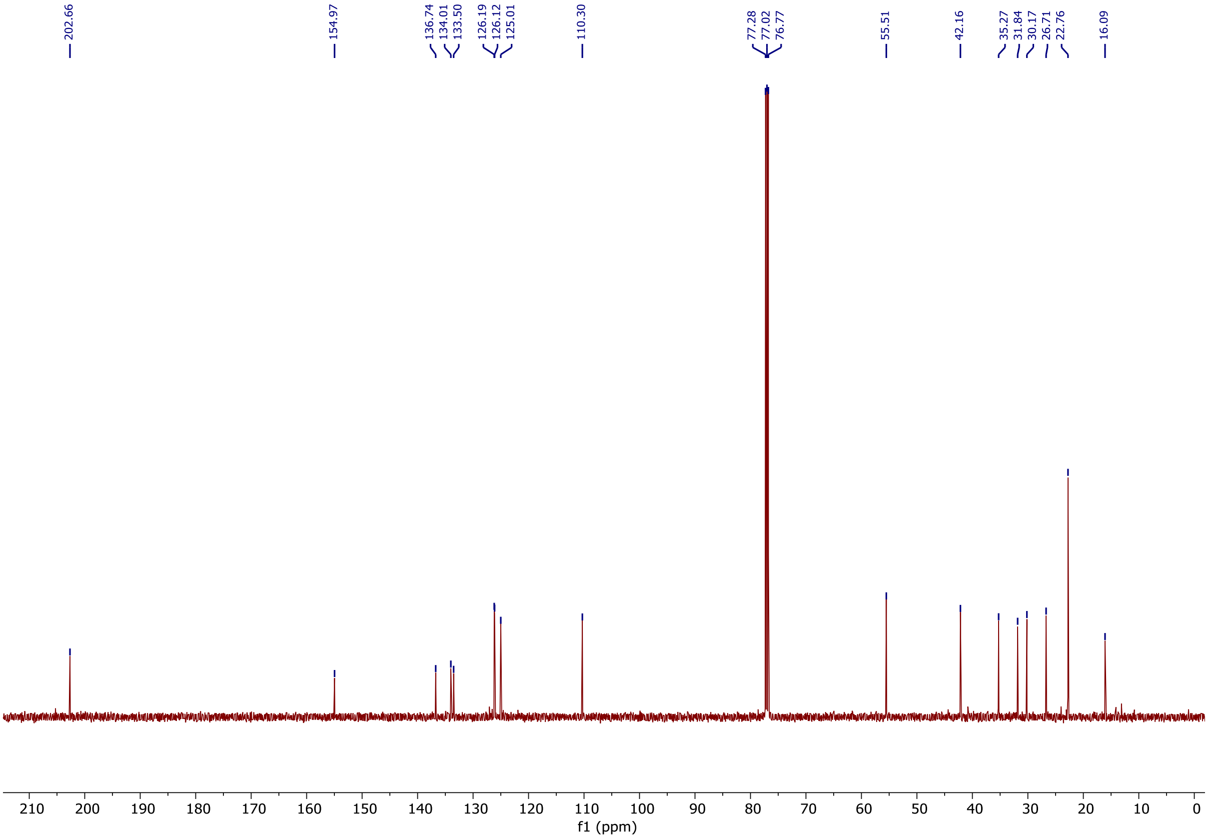

HRMS data of **10’**



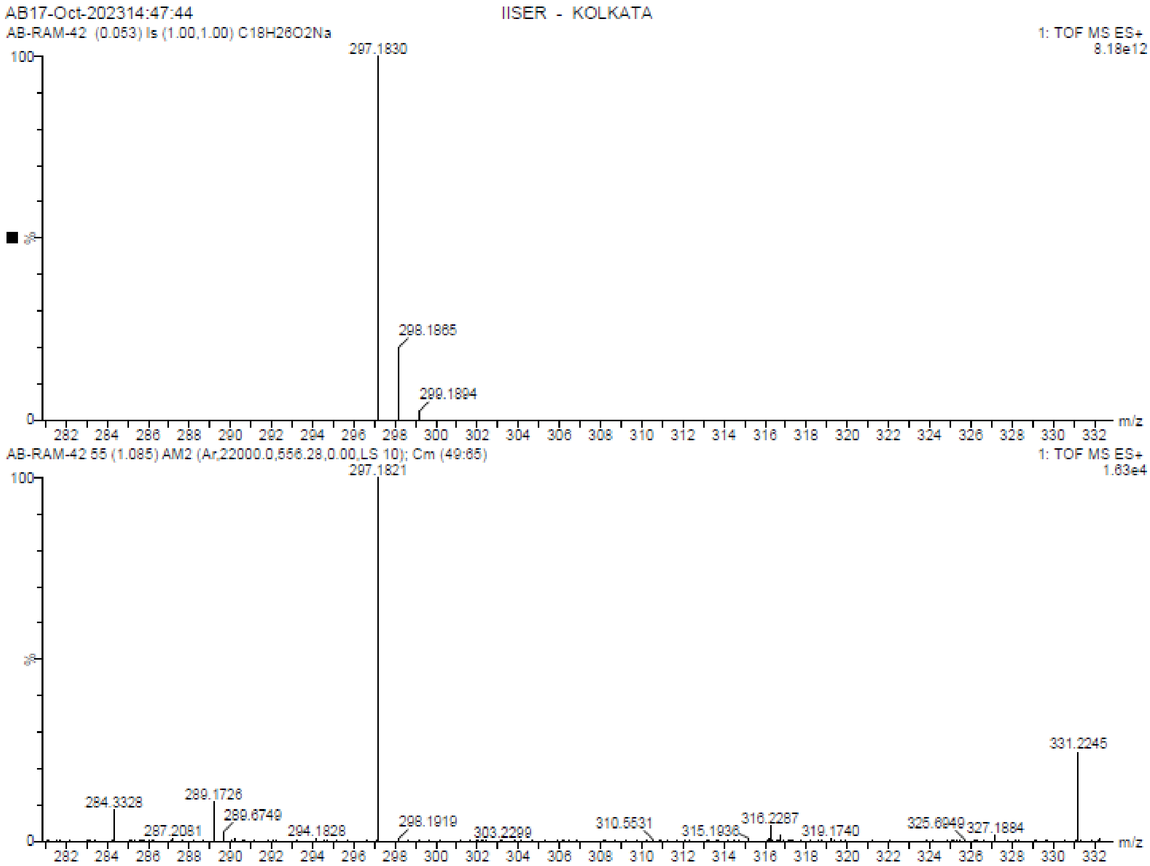




$^{1}$H NMR (400 MHz, $CDCl_3$) of **11**

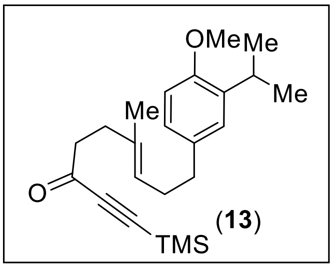


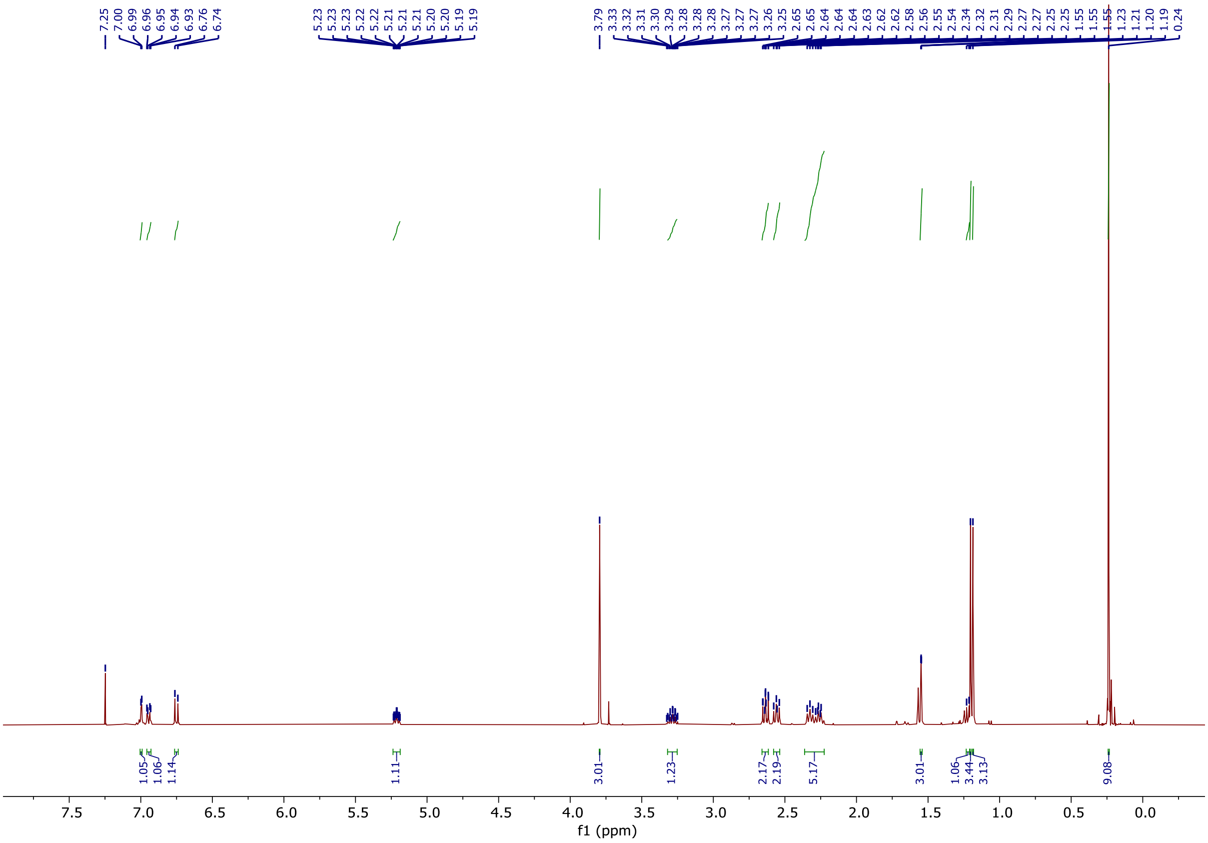



$^{13}$C NMR (126 MHz, $CDCl_3$) of **11**

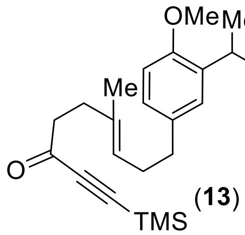



HRMS Data of **11**

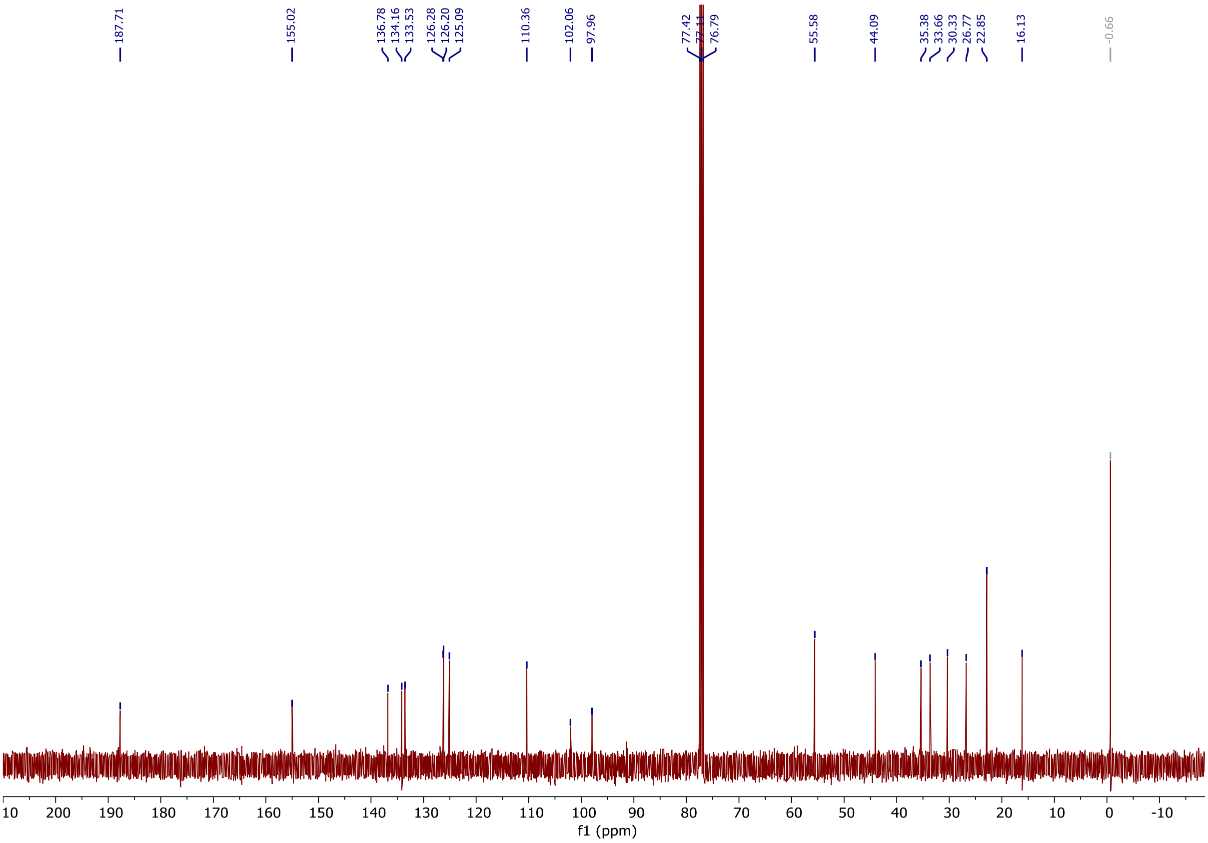




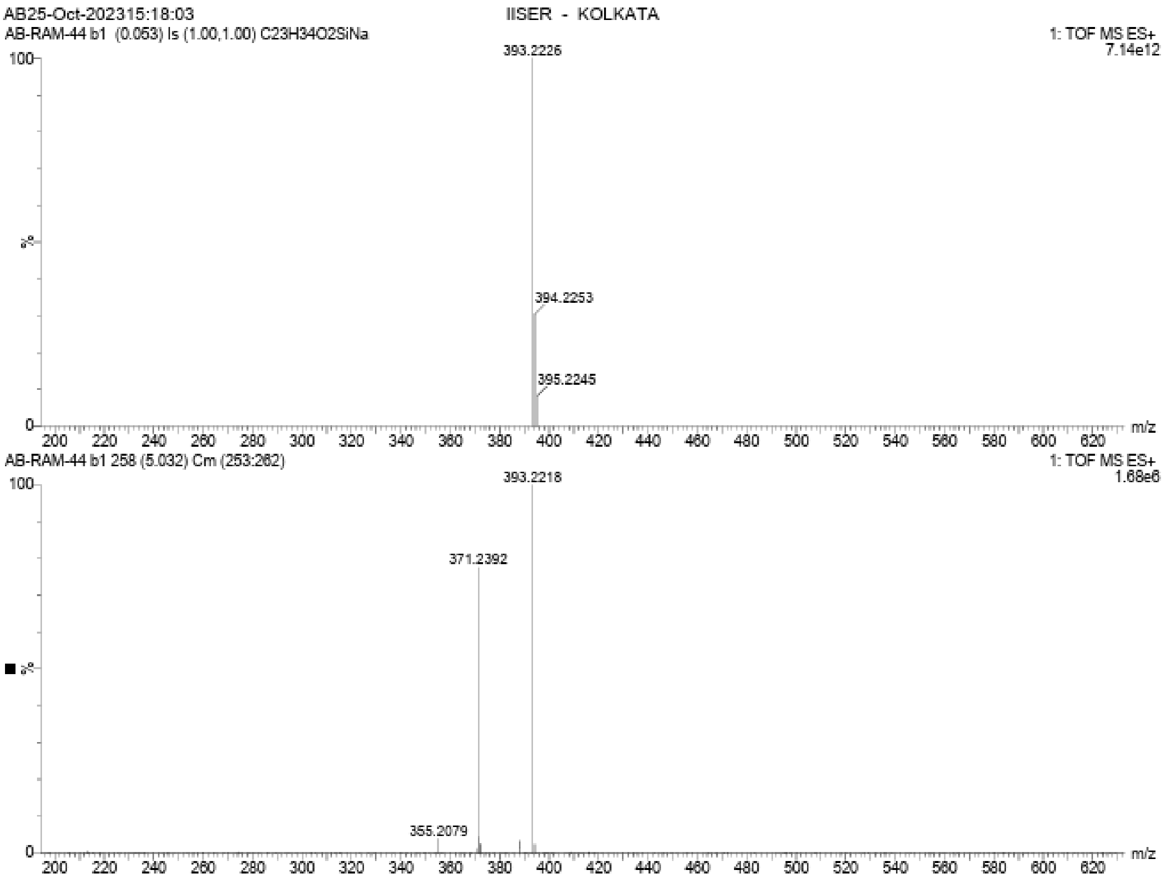
$^{1}$H NMR (400 MHz, $CDCl_3$) of **13**



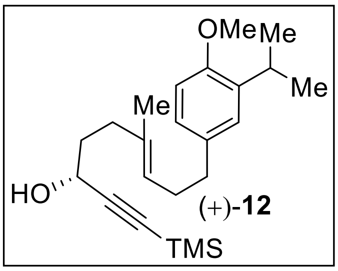

(**13**)

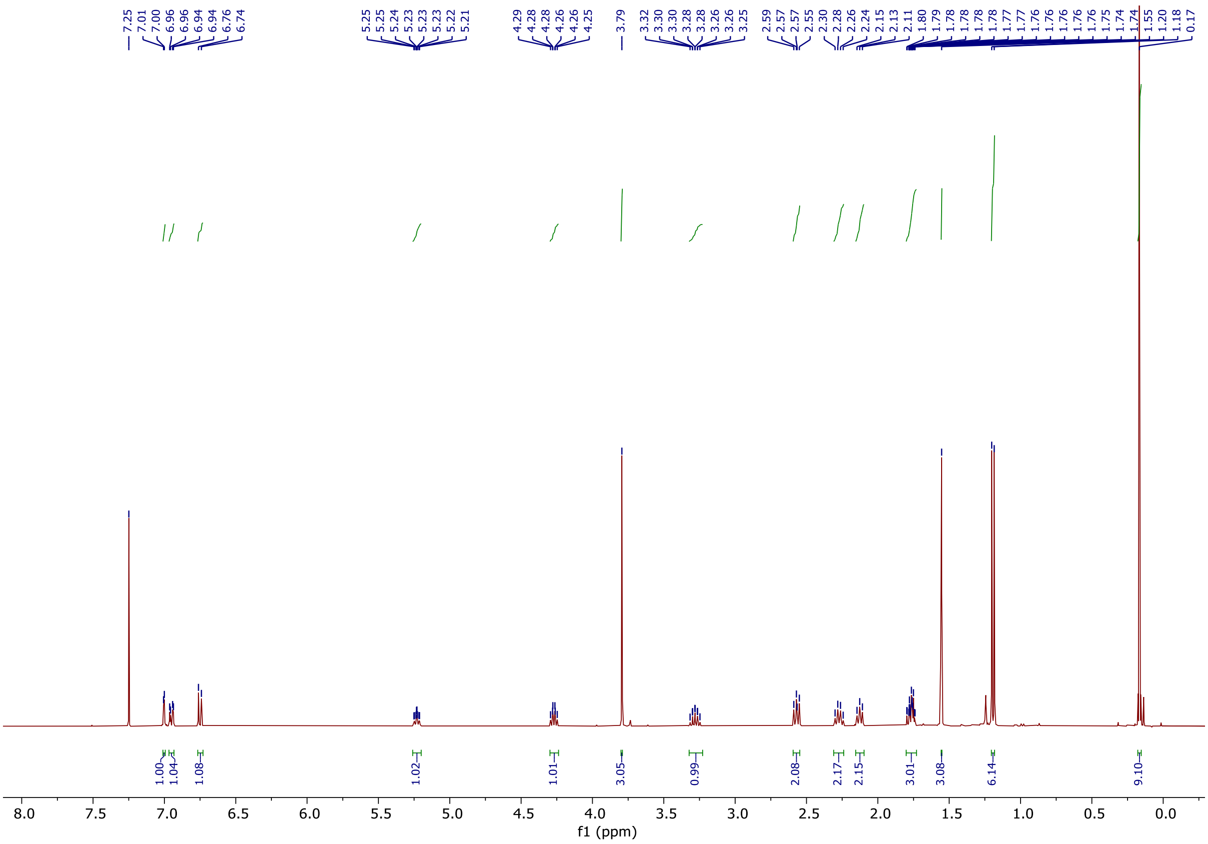



$^{13}$C NMR (101 MHz, $CDCl_3$) of **13**

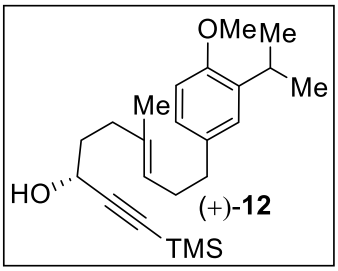



HRMS Data of **13**

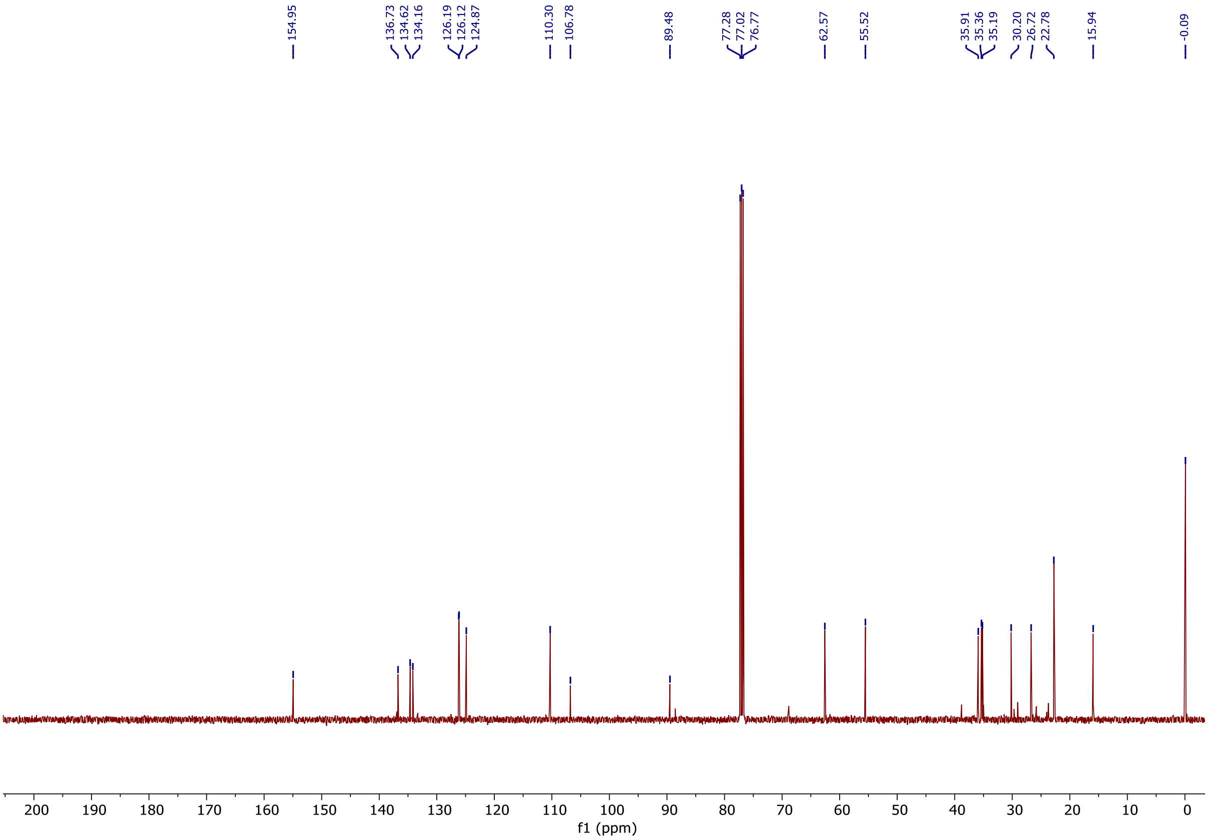


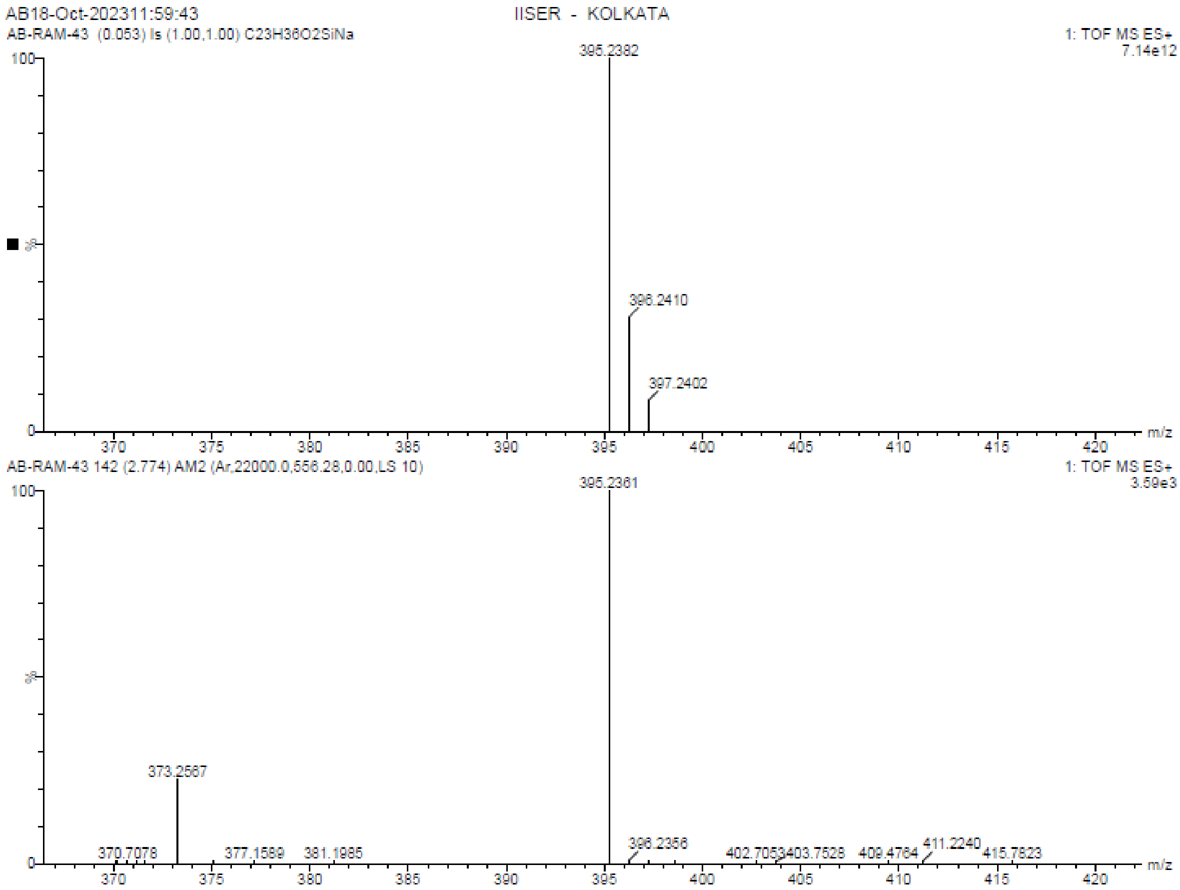
$^{1}H$ NMR (400 MHz, $CDCl_3$) of (+)-**12**



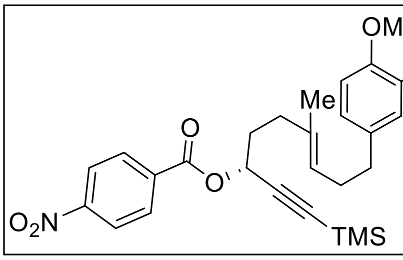
(+)-**12**

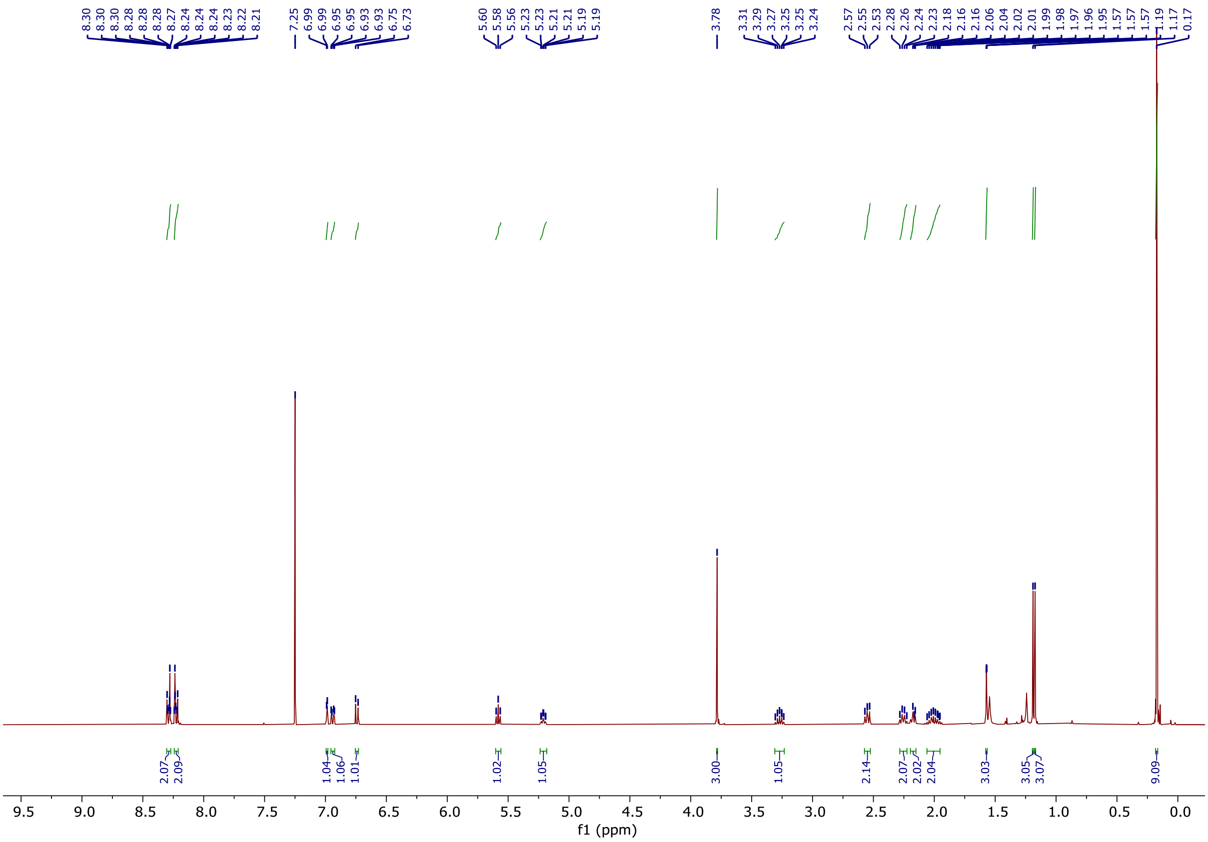



$^{13}$C NMR (126 MHz, $CDCl_3$) of (+)-**12**

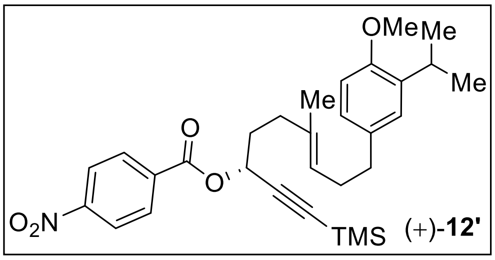


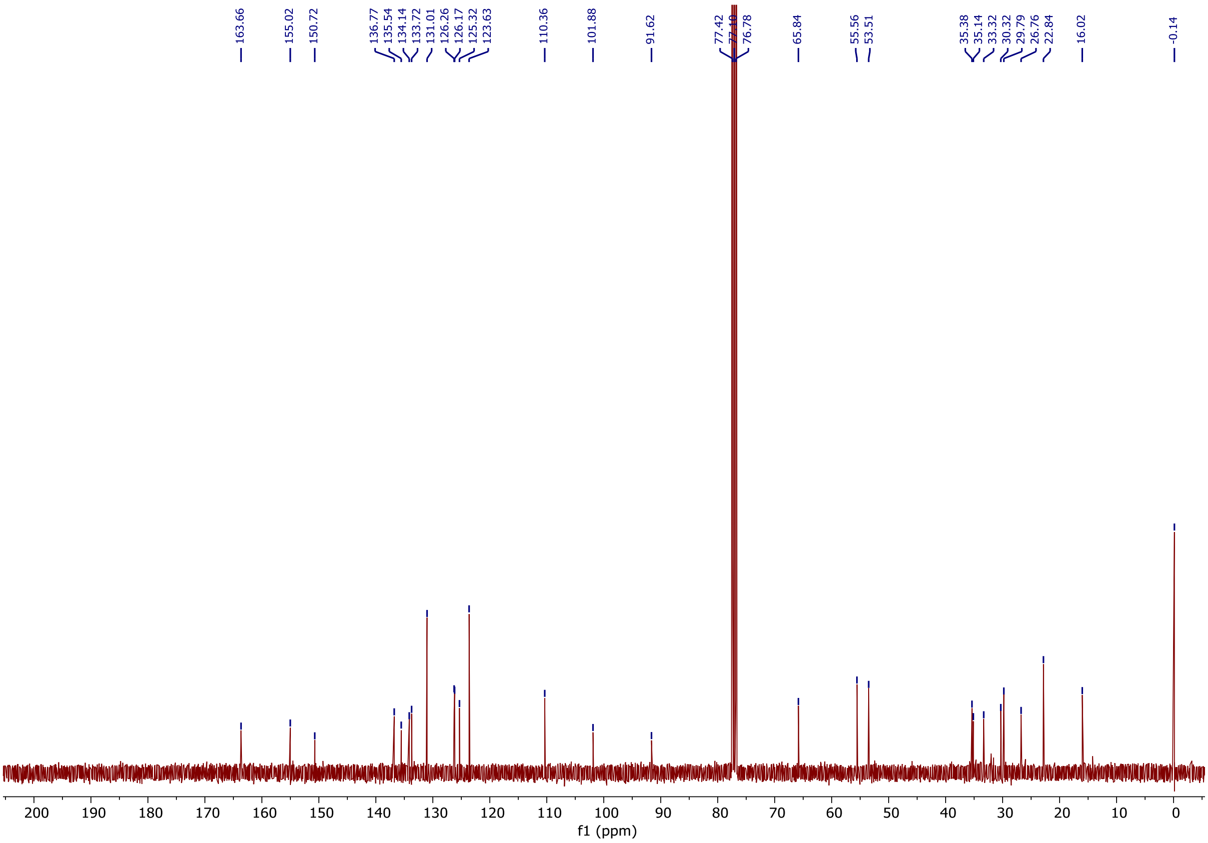

HRMS Data of (+)-**12**


(+)-**12'**

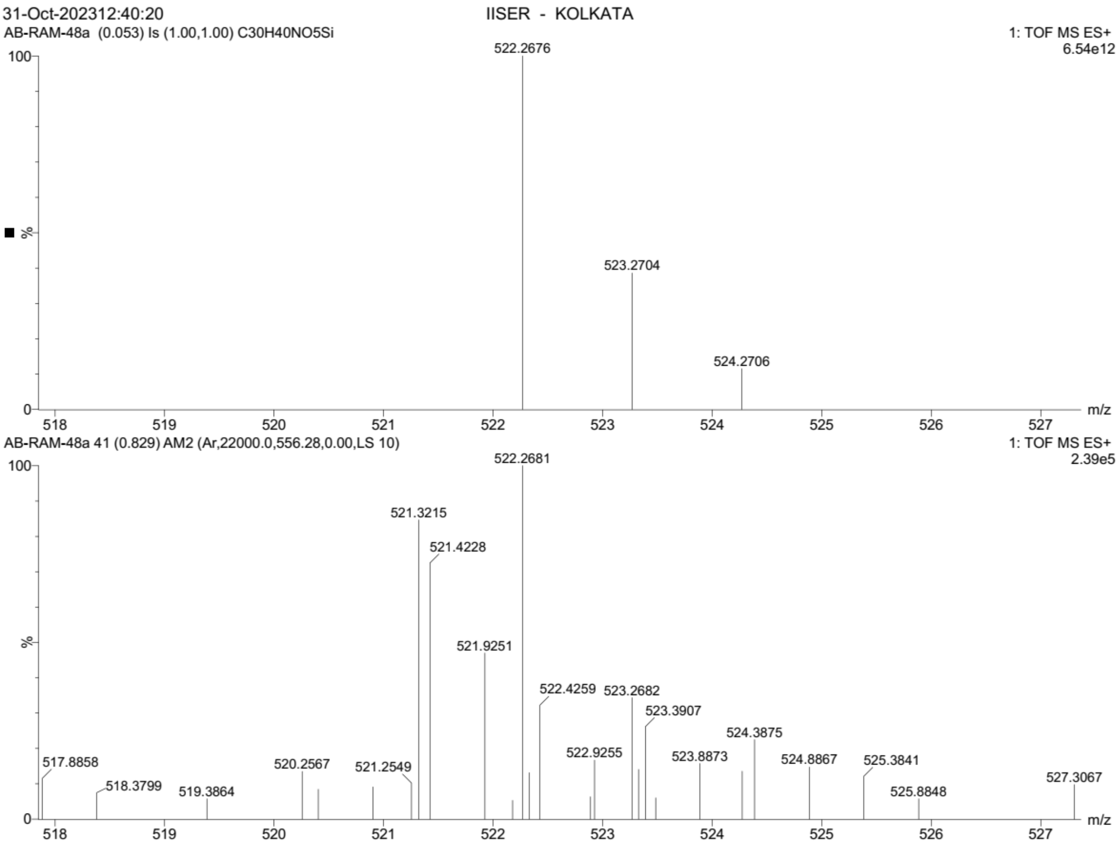


$^{1}$H NMR (400 MHz, $CDCl_3$) of (+)-**12'**



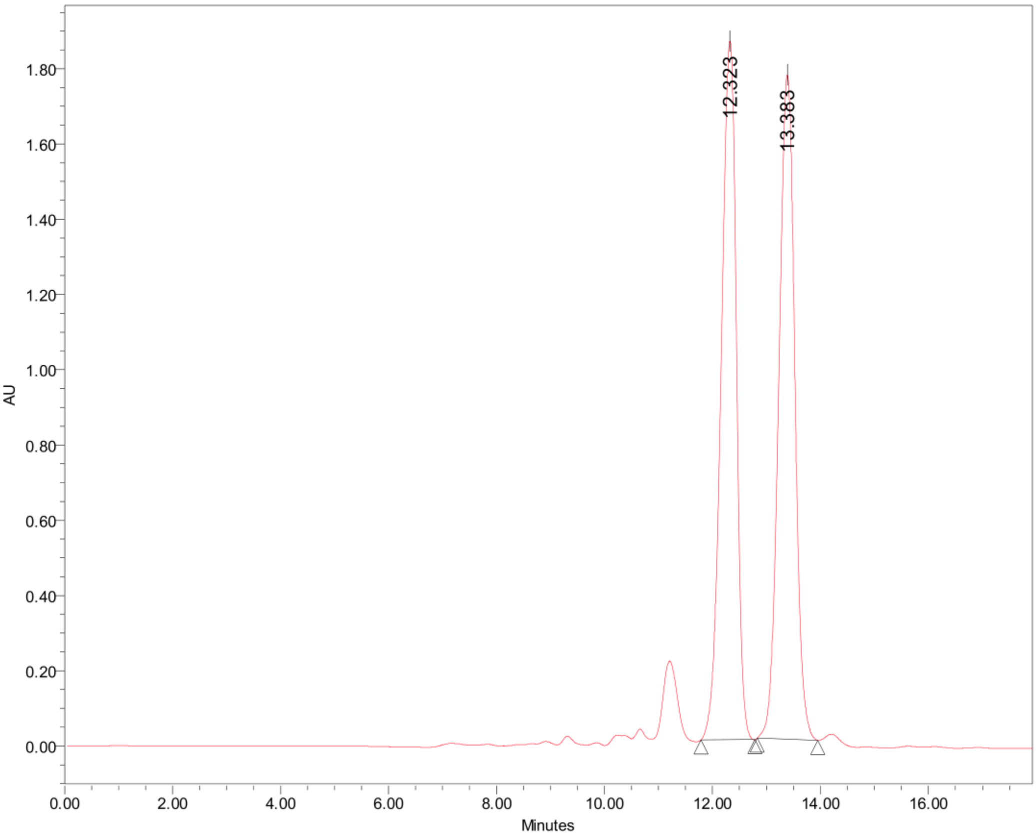

$^{13}$C NMR (101 MHz, $CDCl_3$) of (+)-**12’**




HRMS Data of (+)-**12’**

Empower 3 SOFTWARE

# Peak Summary Report



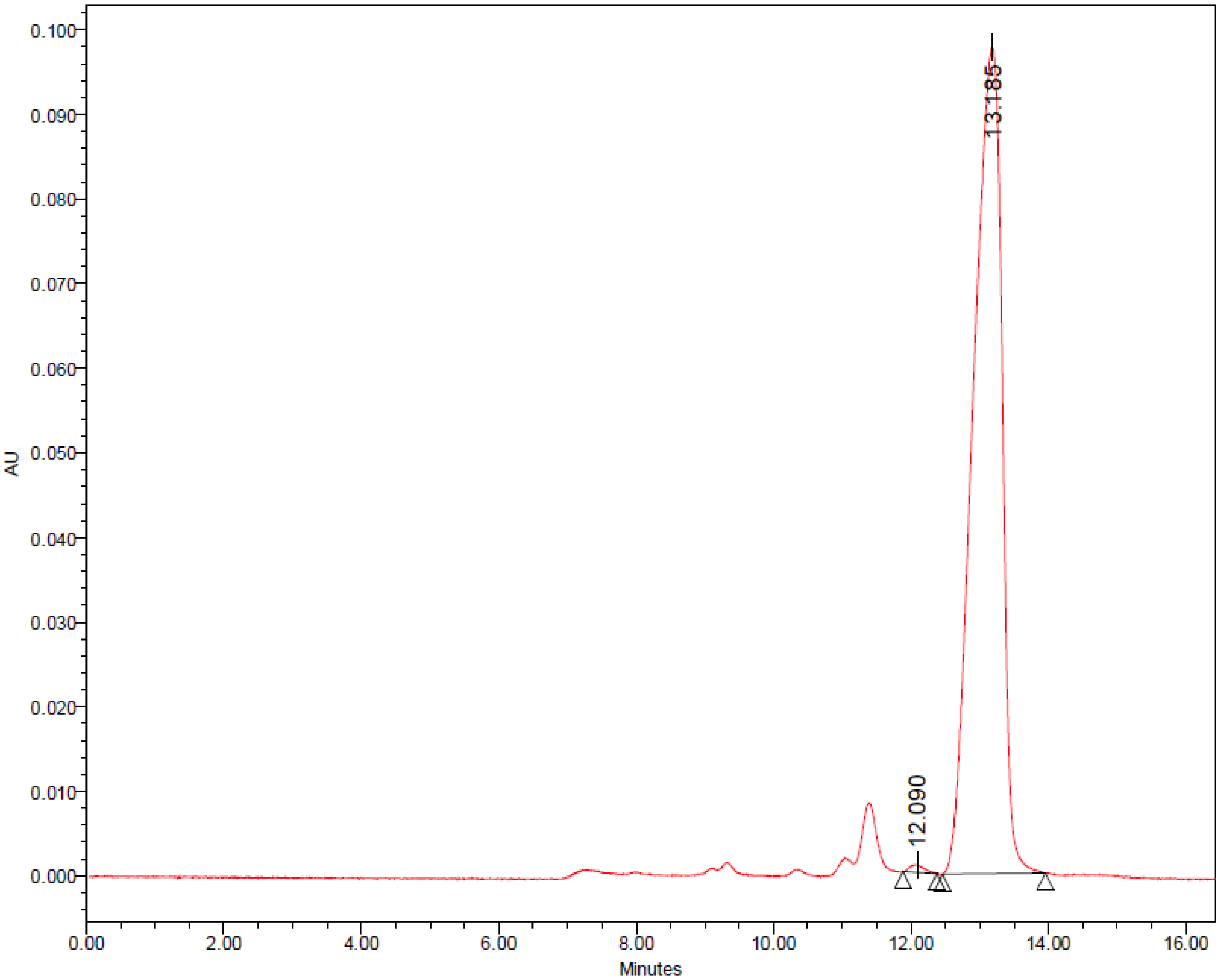

## Peak Summary with Statistics
**Name:**

| | Sample Name | Vial | Inj | Retention Time (min) | Area | % Area | Height |
|---|---|---|---|---|---|---|---|
| 1 | AB_RAM_48_RAC_AD-H_1_1 | 1 | 1 | 13.383 | 36362984 | 50.18 | 1765525 |
| 2 | AB_RAM_48_RAC_AD-H_1_1 | 1 | 1 | 12.323 | 36102165 | 49.82 | 1857250 |
| Mean | | | | 12.853 | | | |
| Std. Dev. | | | | 0.750 | | | |



HPLC Data of (±)-**12’**

# Peak Summary Report



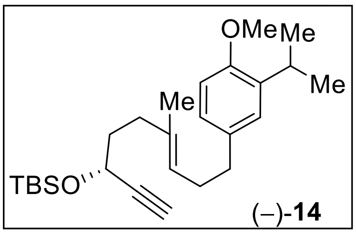

Sample Name: AB_RAM_48_RAC_AD-H_1_0P4_1; Date Acquired: 27-10-2023 21:55:11 IST; Vial: 1
Injection: 1

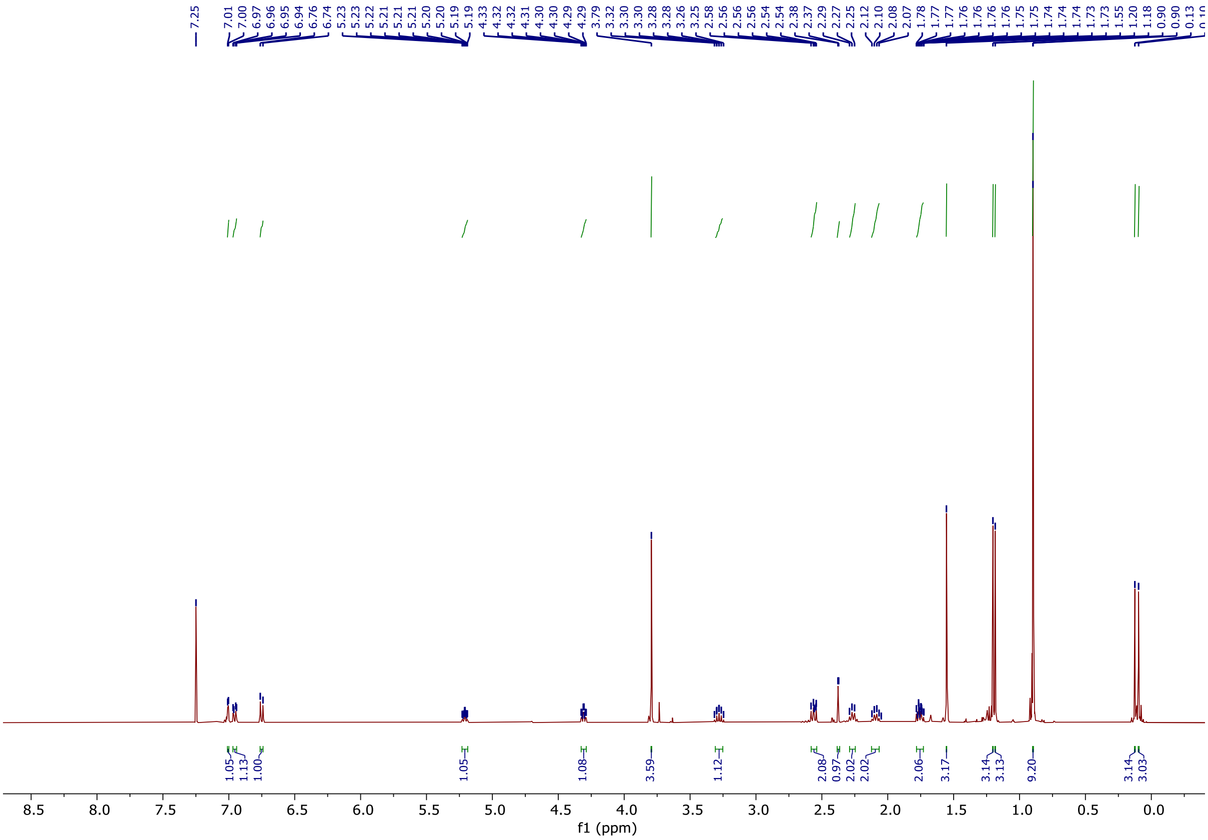
**Peak Summary with Statistics**
**Name:**

| | Sample Name | Vial | Inj | Retention Time (min) | Area | % Area | Height |
|---|---|---|---|---|---|---|---|
| 1 | AB_RAM_48_RAC_AD-H_1_0P4_1 | 1 | 1 | 13.185 | 2838946 | 99.51 | 97661 |
| 2 | AB_RAM_48_RAC_AD-H_1_0P4_1 | 1 | 1 | 12.090 | 13853 | 0.49 | 952 |
| Mean | | | | 12.638 | | | |
| Std. Dev. | | | | 0.774 | | | |

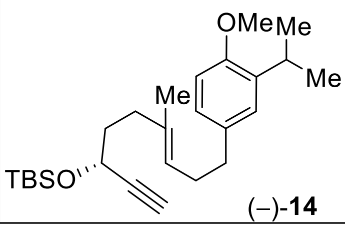


HPLC Data of (+)-**12’**

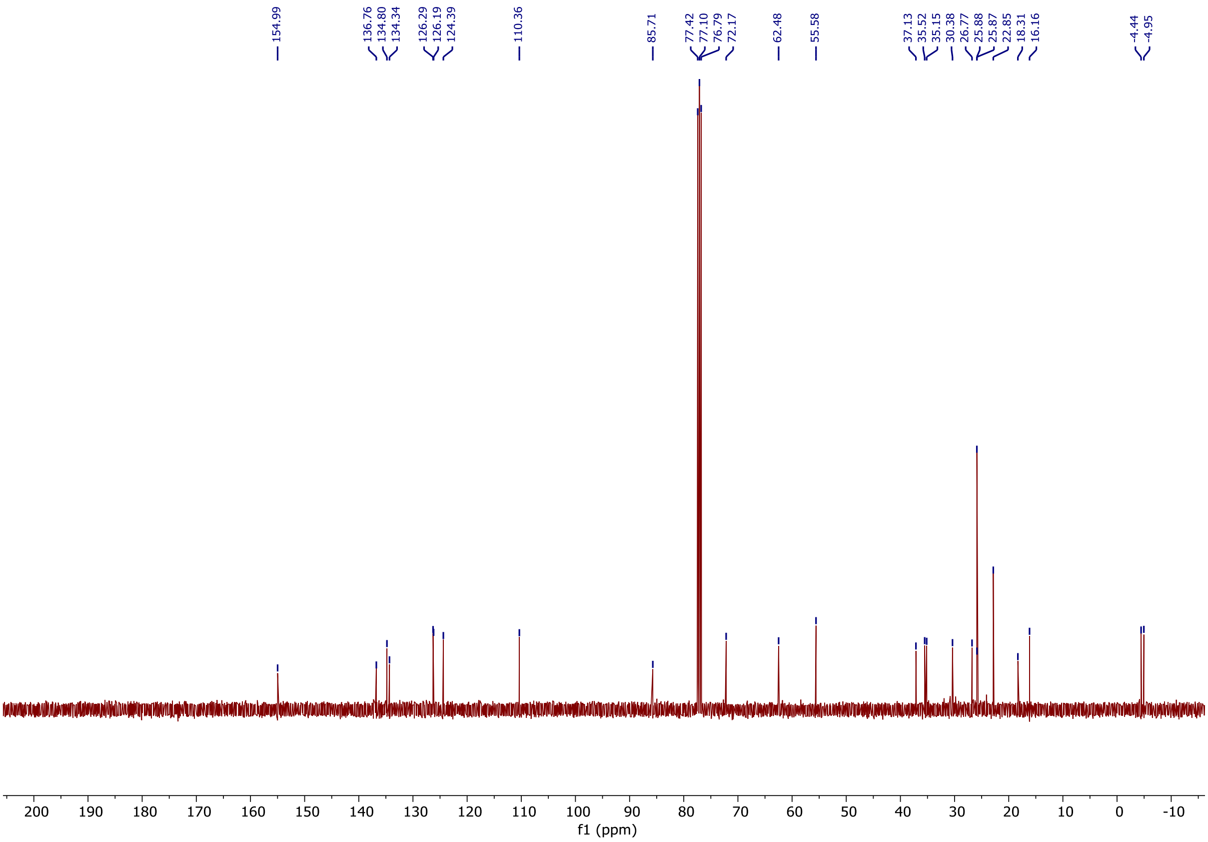


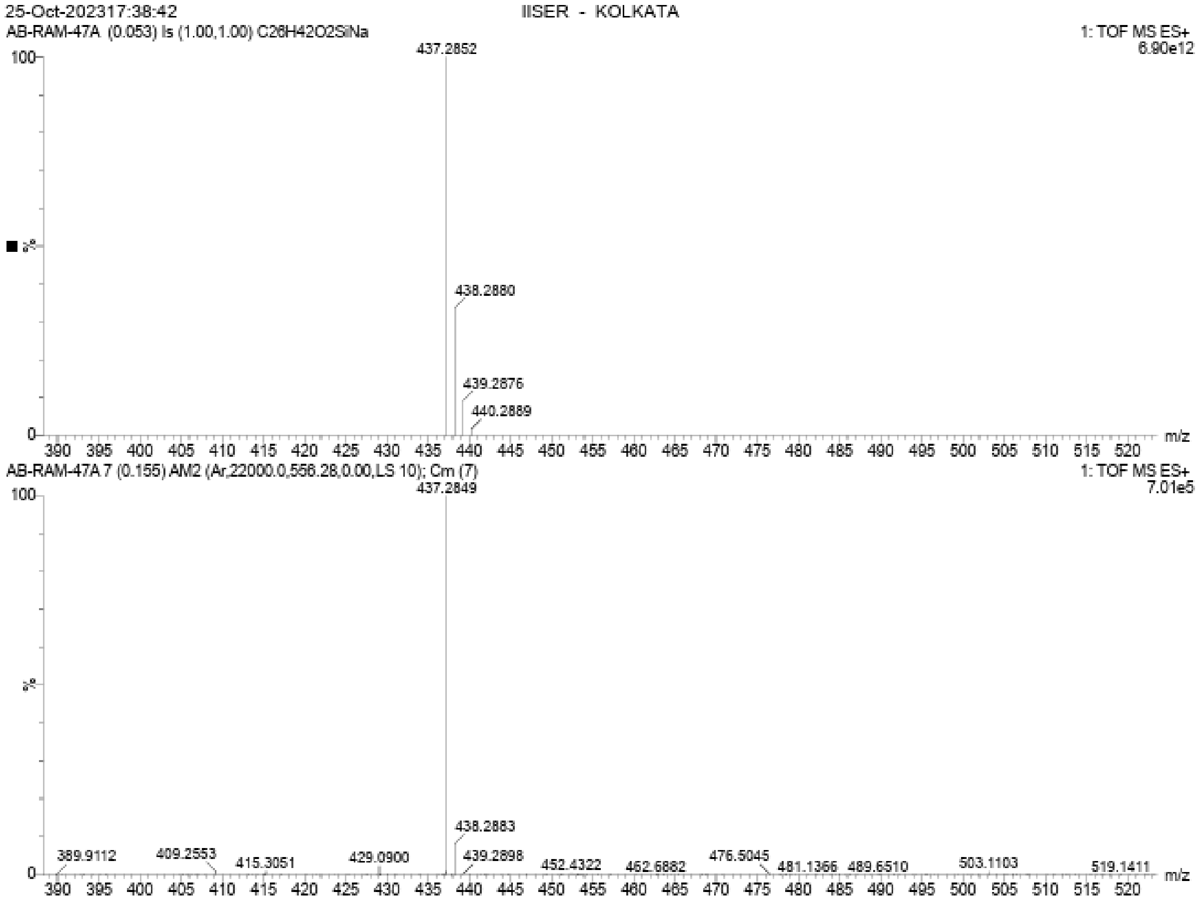
[1]H NMR (400 MHz, $CDCl_3$) of (–)-**14**



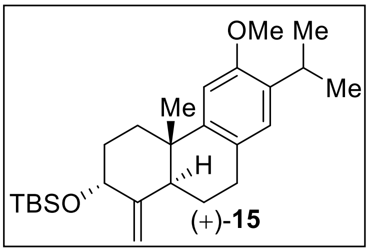

(–)-**14**

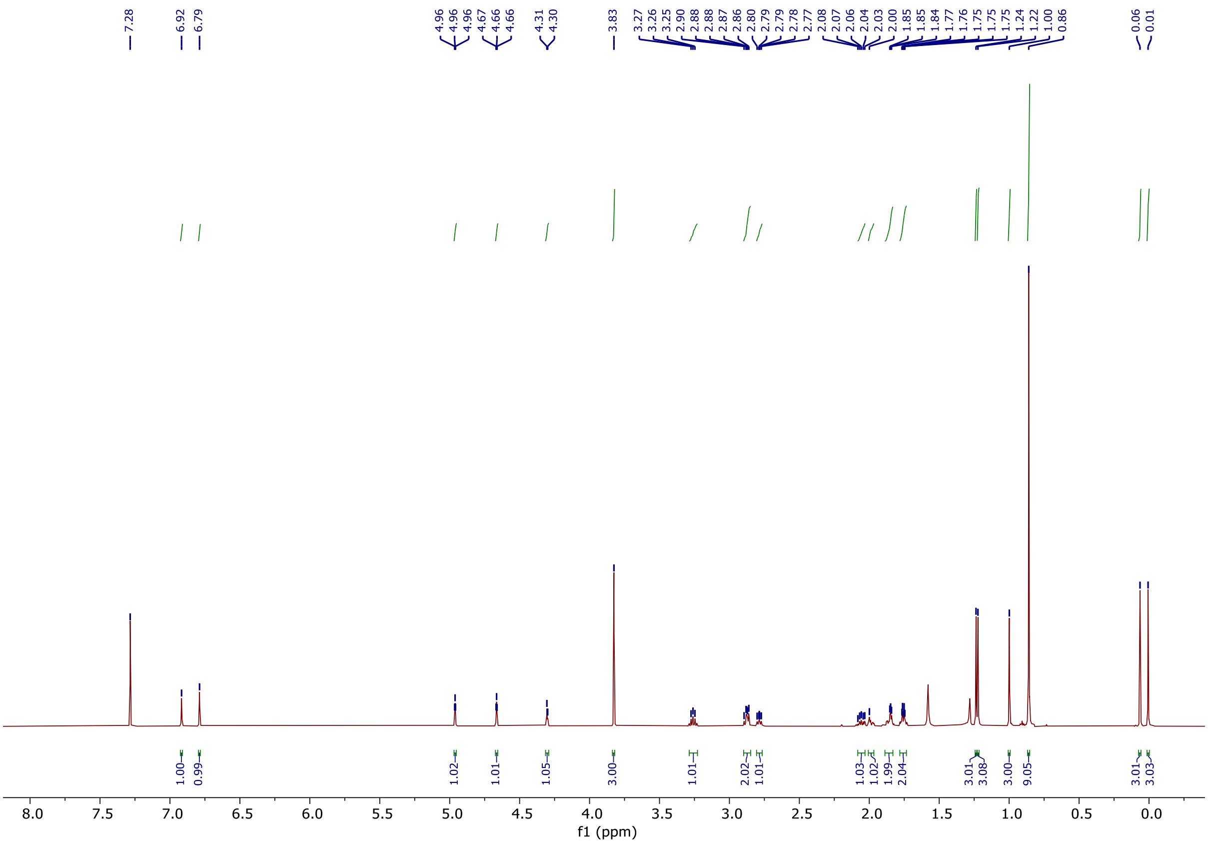



$^{13}$C NMR (101 MHz, CDCl$_3$) of (–)-**14**

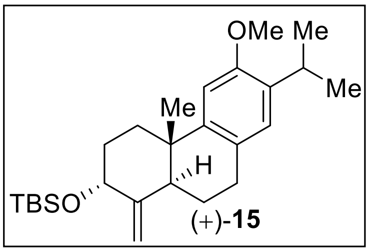


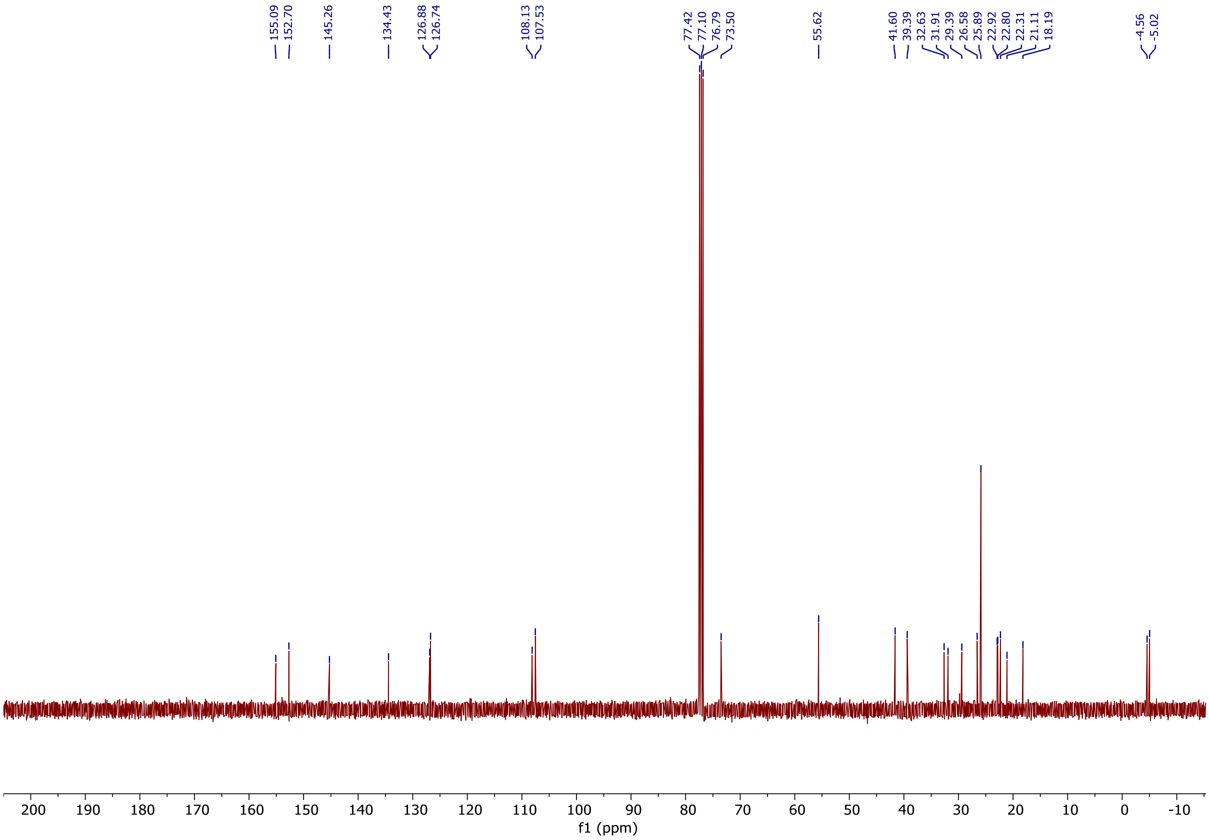

HRMS Data of (−)-**14**



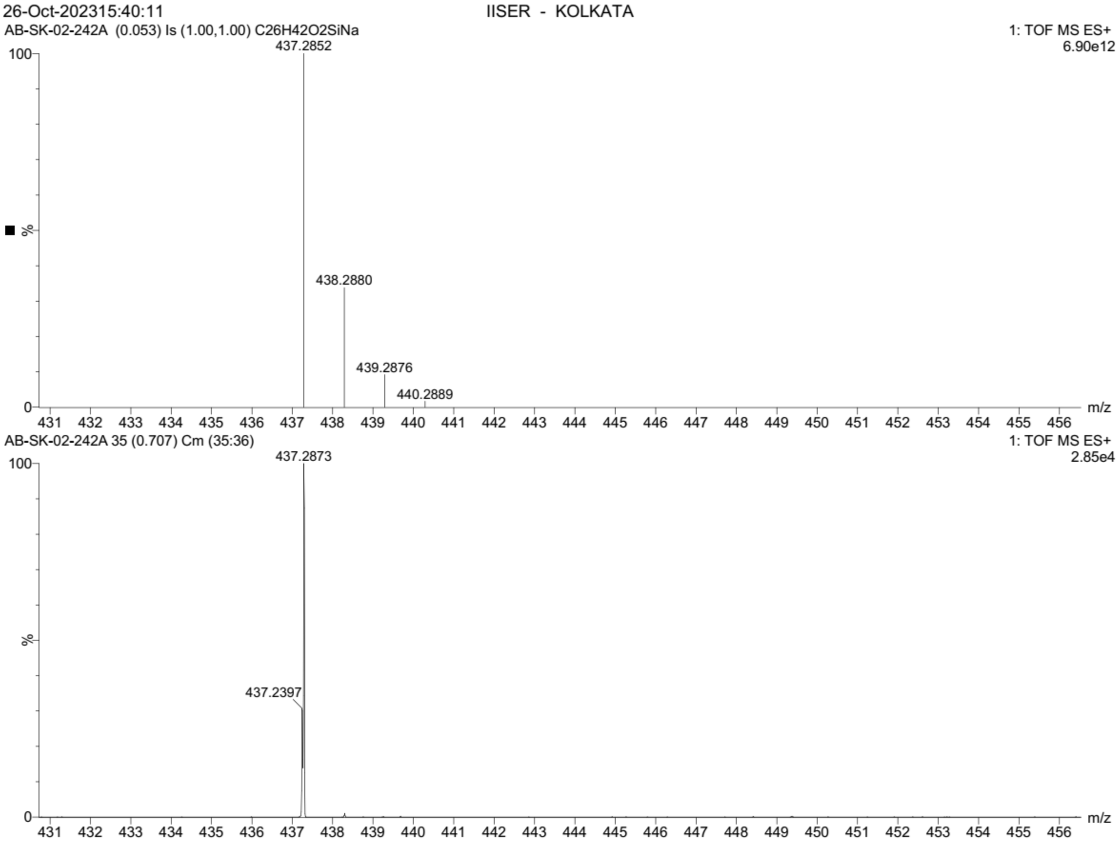


$^1$H NMR (400 MHz, $CDCl_3$) of (+)-**15**

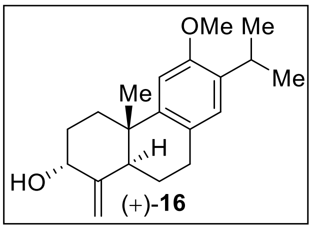


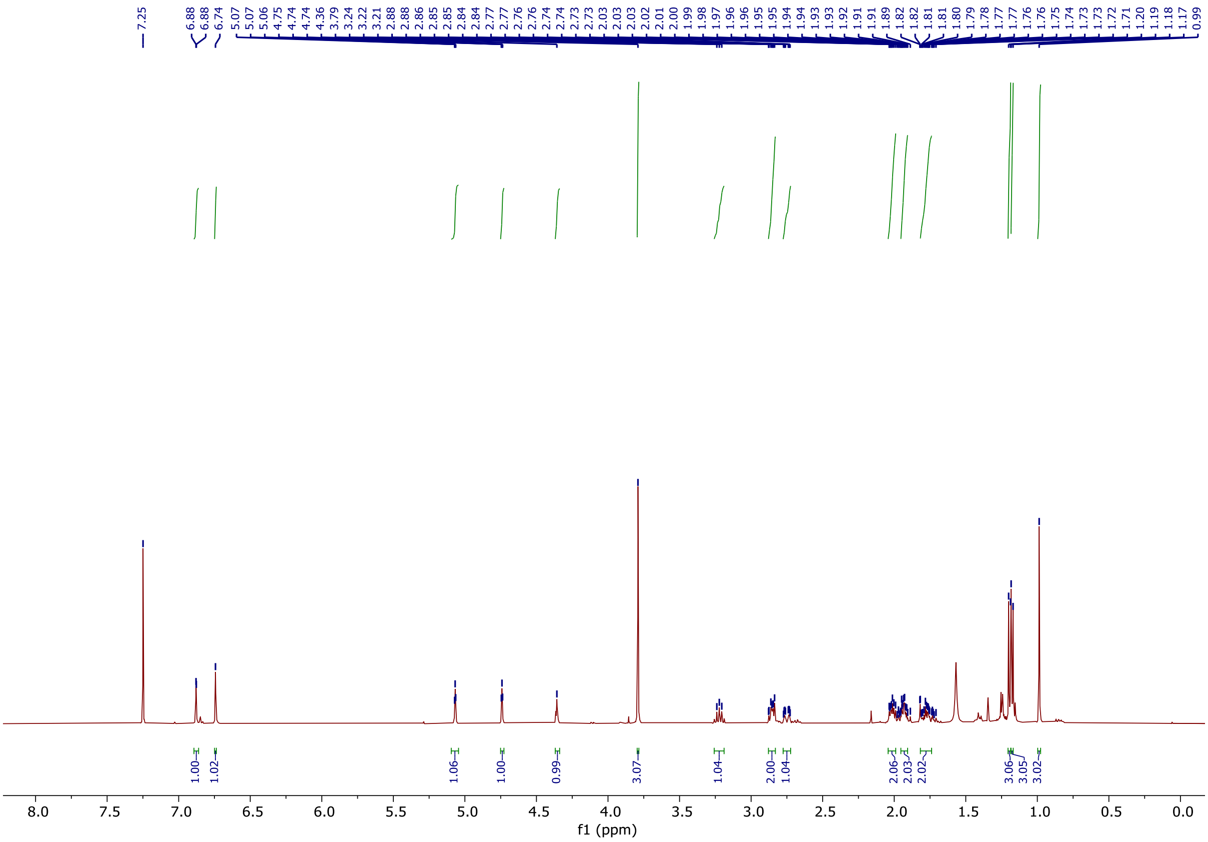



$^{13}$C NMR (101 MHz, $CDCl_3$) of (+)-**15**

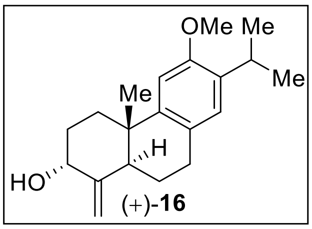


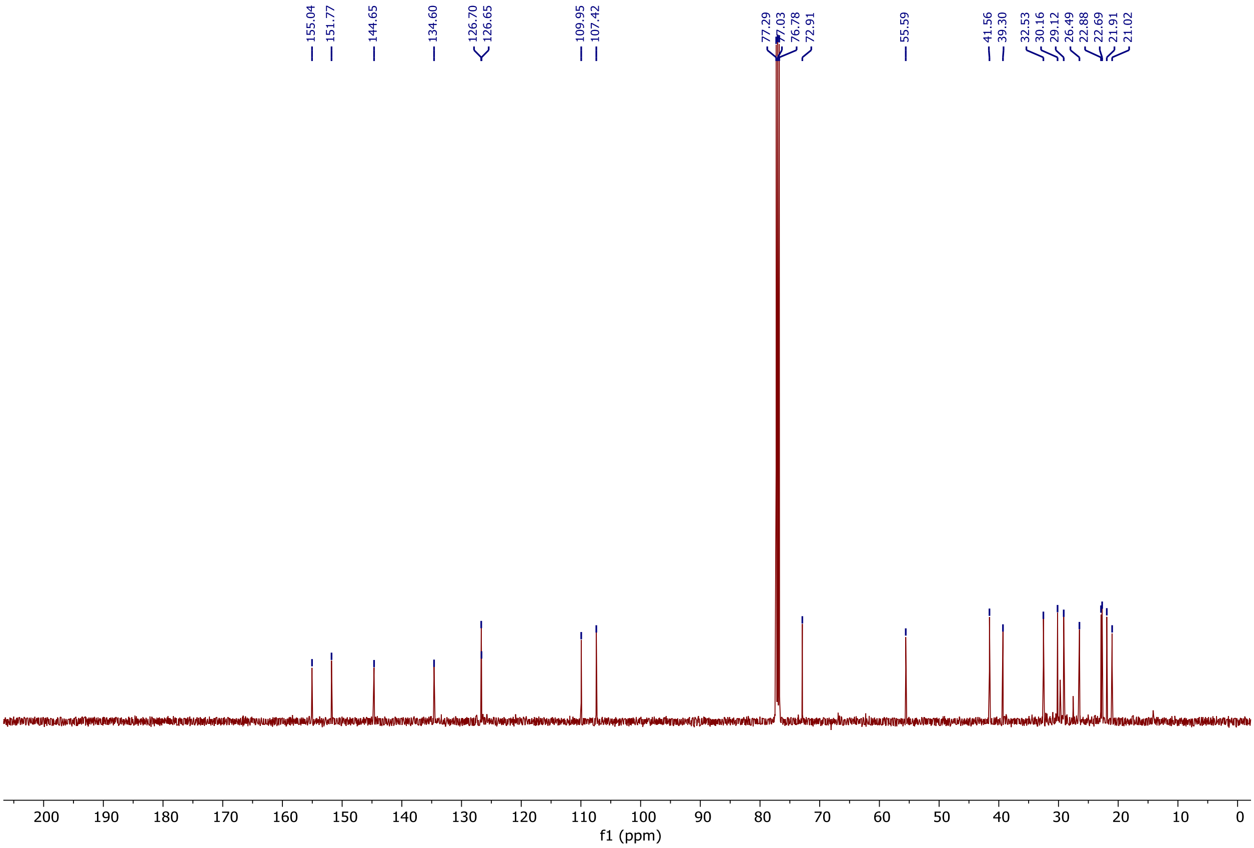

HRMS Data of (+)-**15**





$^{1}$H NMR (400 MHz, $CDCl_3$) of compound (+)-**16**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**16**

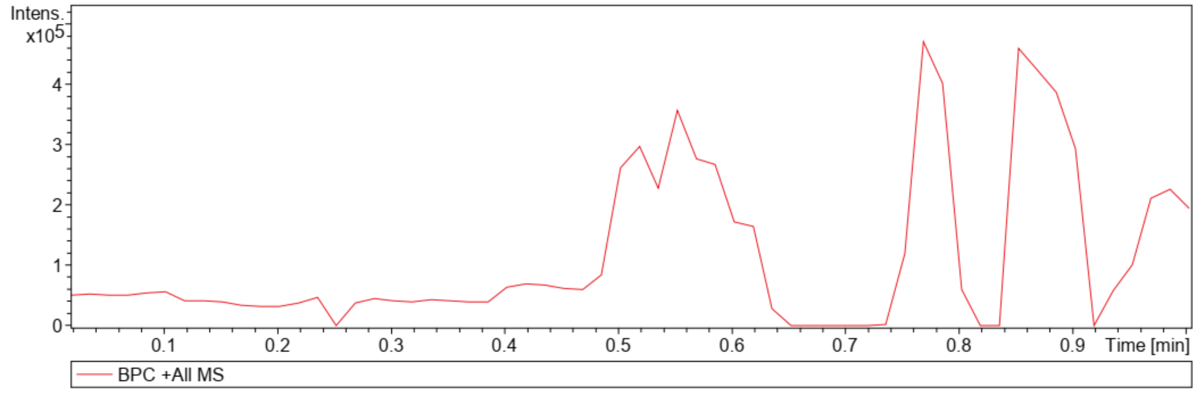
# Display Report

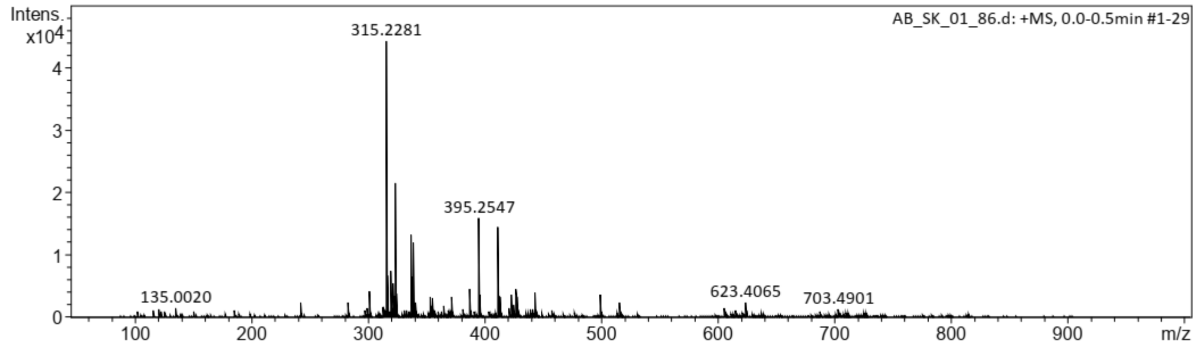
**Analysis Info**

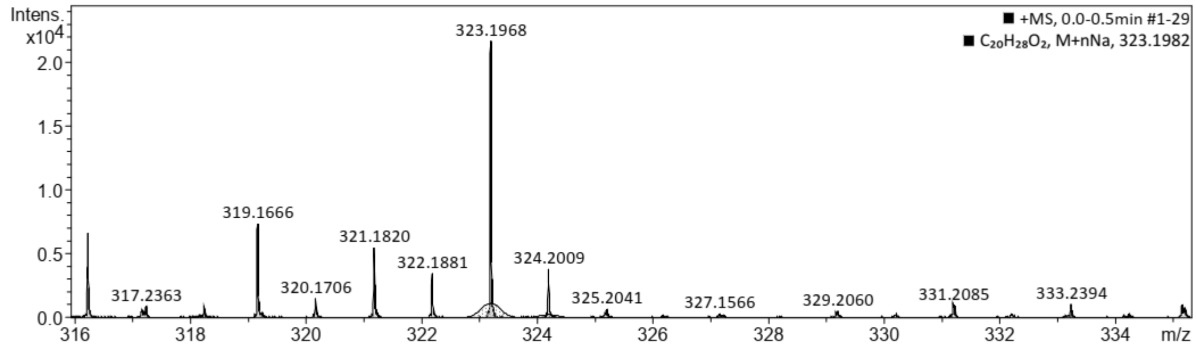
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\User data\2022\AUGUST\AB_SK_01_86.d | Acquisition Date | 8/4/2022 11:17:07 AM |
| Method | Tune_pos_Standard_July2022.m | Operator | IISER Kolkata |
| Sample Name | AB_SK_01_86 | Instrument | maXis impact 8282001.00127 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 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 | 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 |

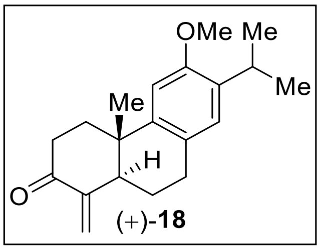


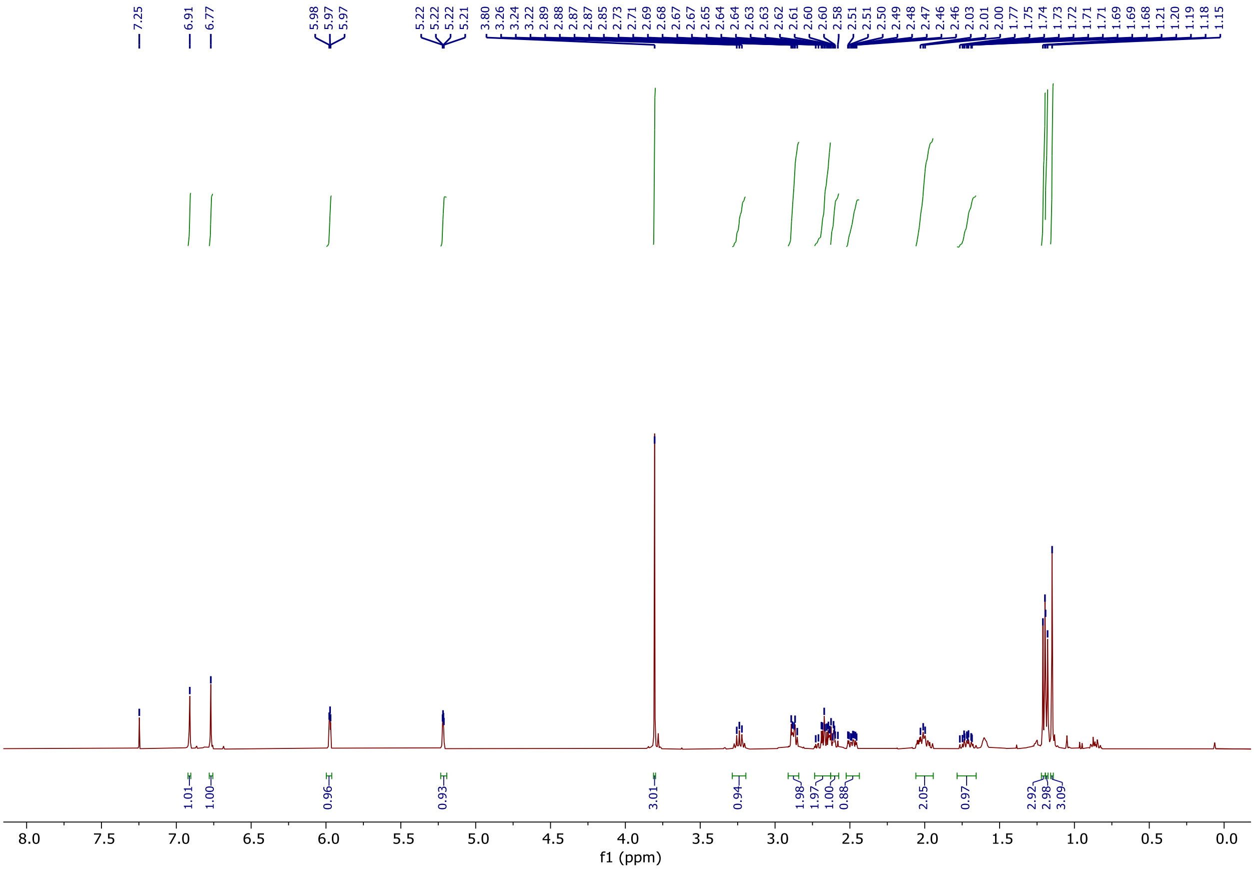



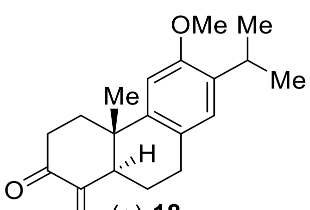



HRMS data of (+)-**16**

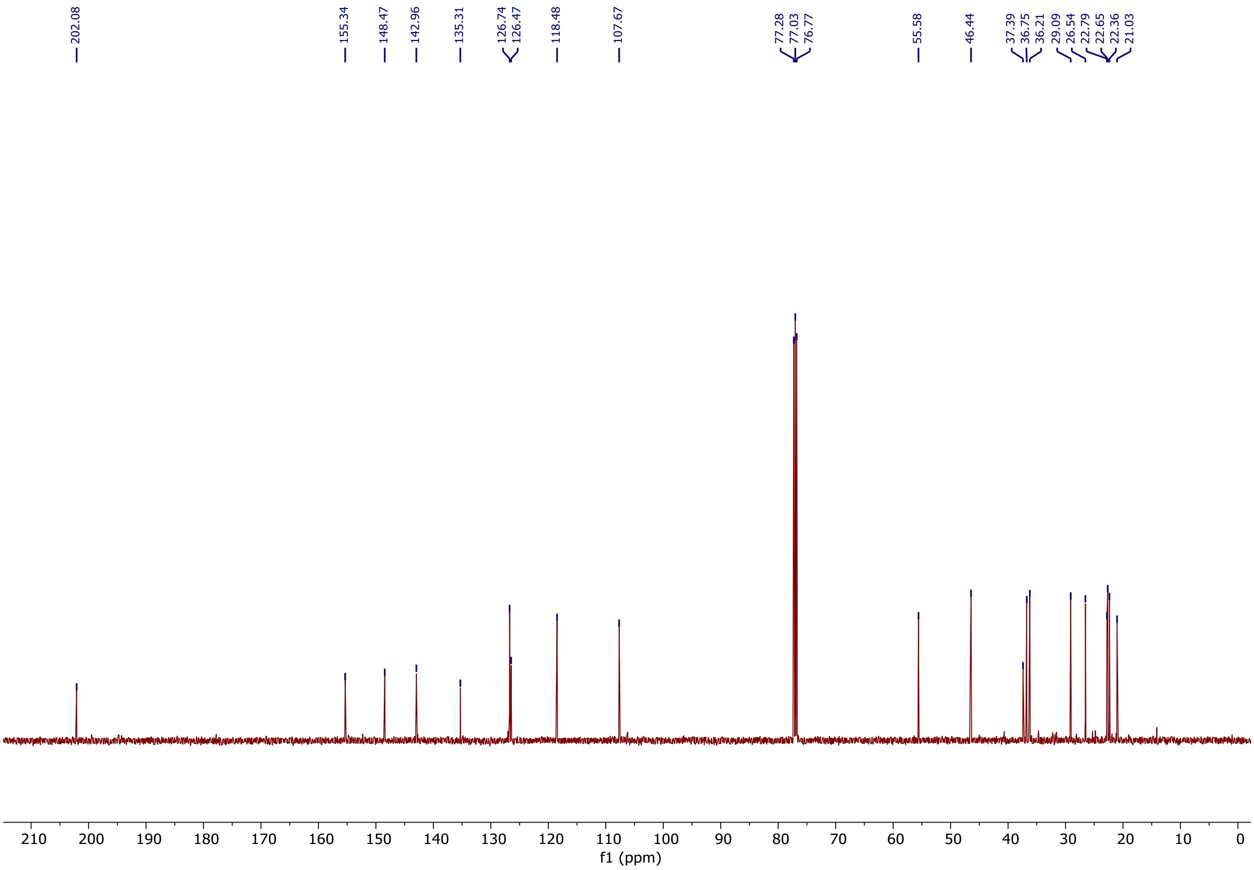




$^{1}$H NMR (500 MHz, $CDCl_3$) of compound (+)-**18**



(+)-**18**




$^{13}C$ NMR (126 MHz, $CDCl_3$) of compound (+)-**18**

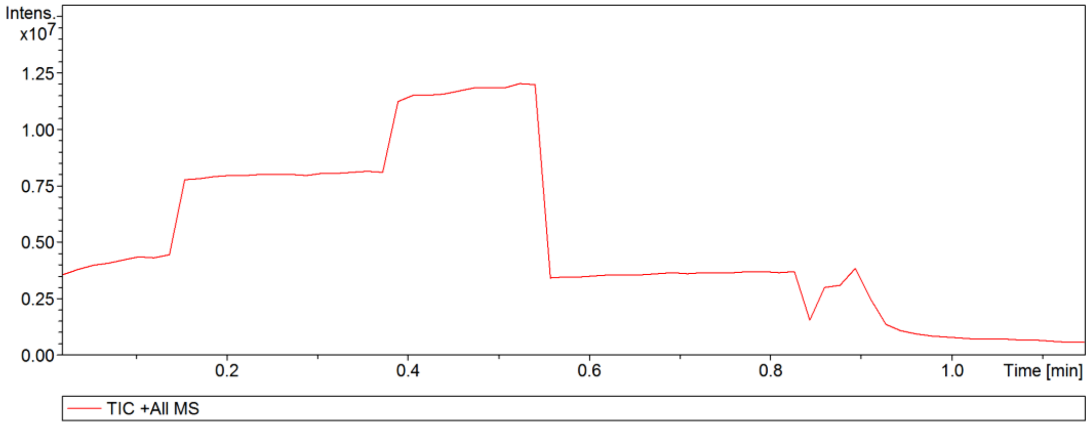
# Display Report

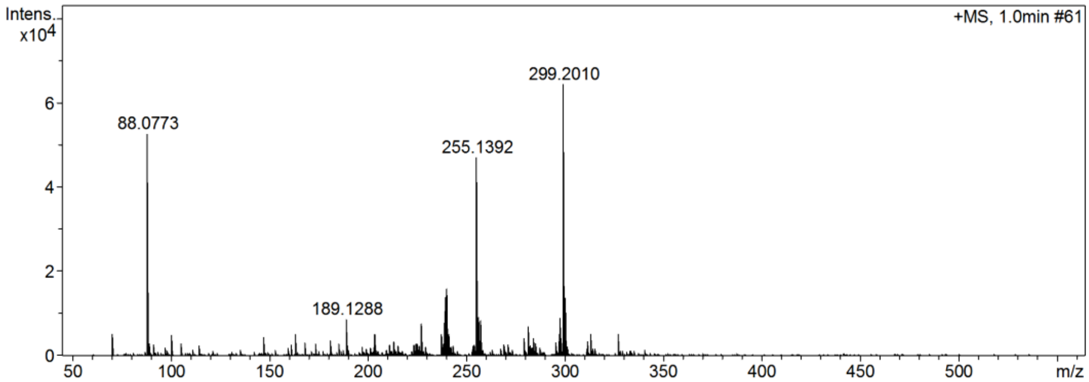
**Analysis Info**

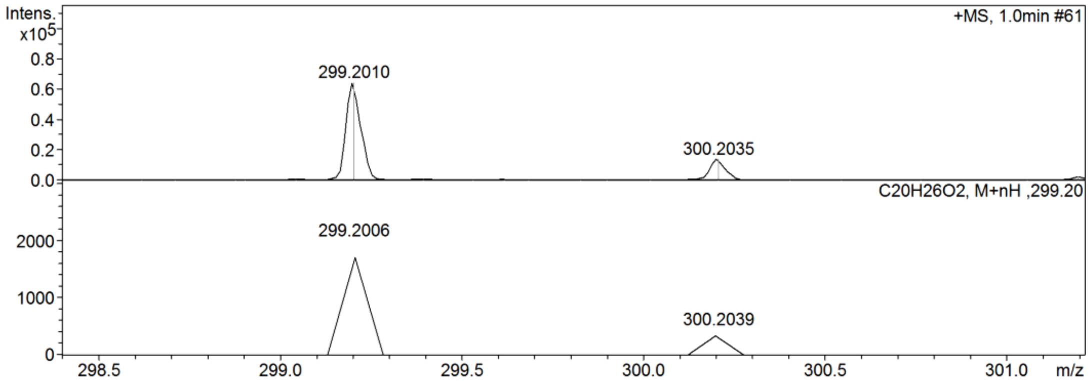
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\JUNE2022\28-06-22\Prof A Bisai-SK-01-88.d | Acquisition Date | 28-06-2022 12:03:16 |
| Method | tune mix_low.New.021117_1.m | Operator | Bruker |
| Sample Name | SK-01-88 | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 100.0 Vpp | Set Divert Valve | Source |

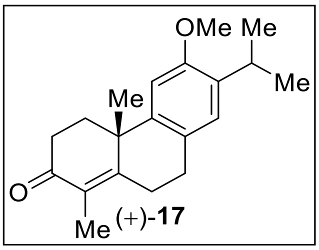


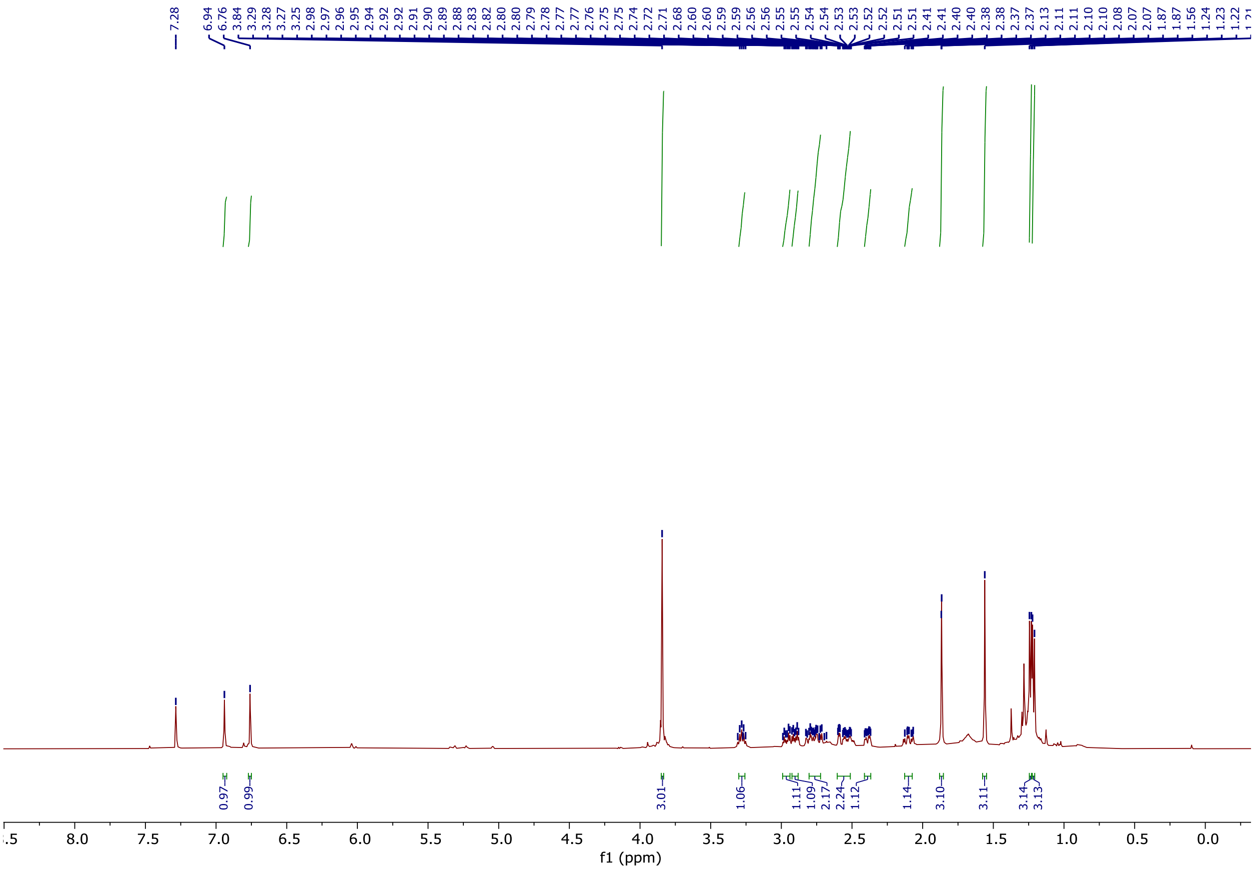



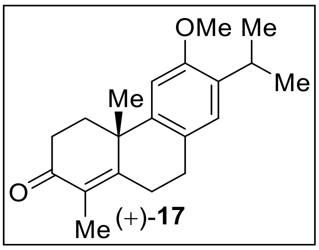


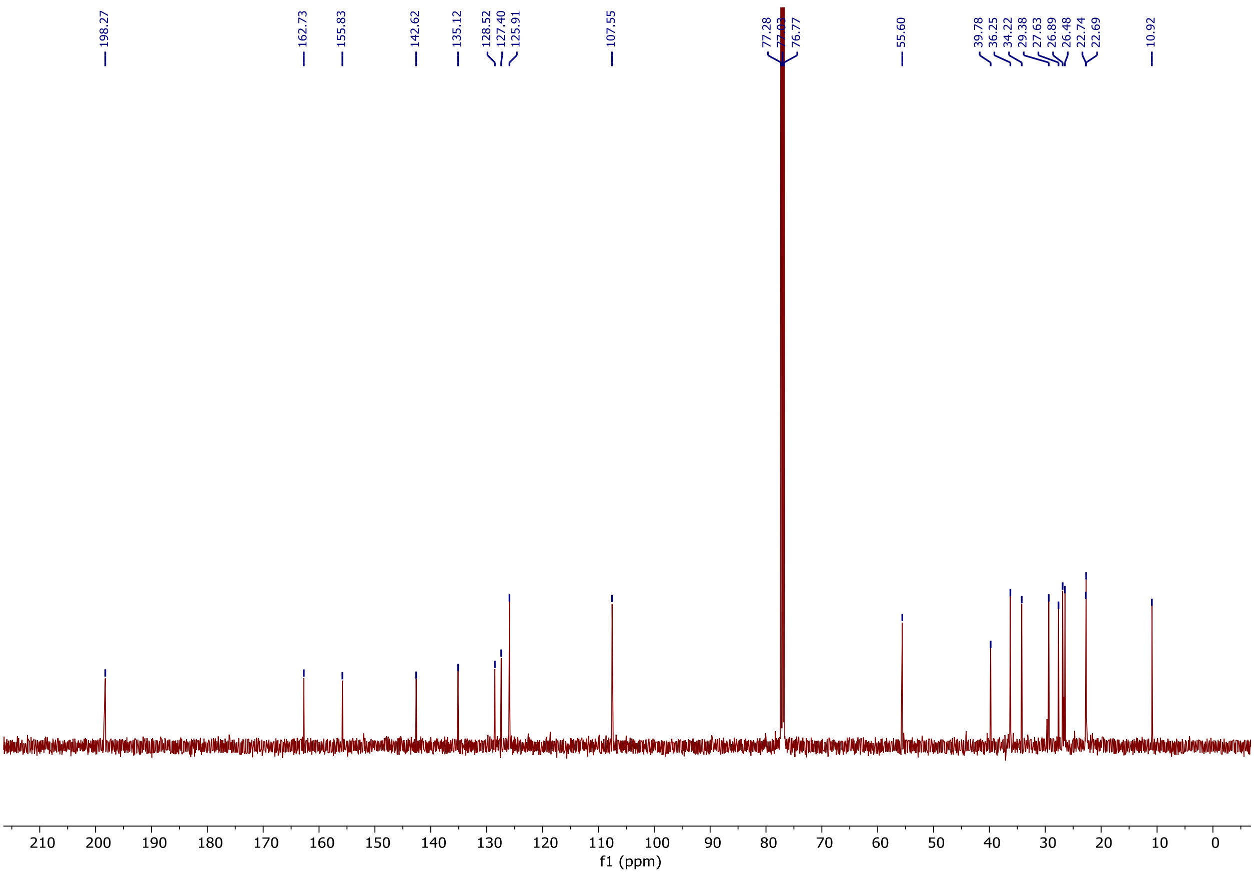

HRMS data of (+)-**18**



$^1$H NMR (500 MHz, $CDCl_3$) of compound (+)-**17**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**17**

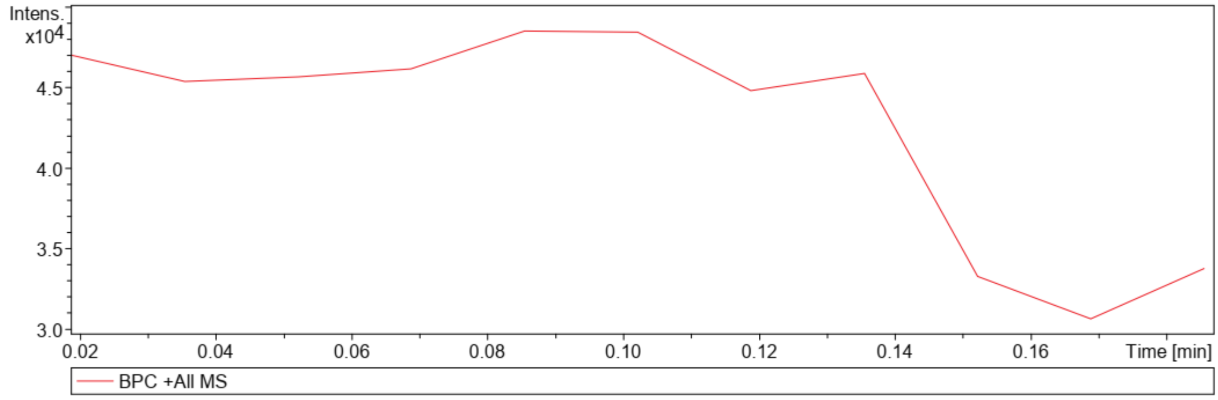
# Display Report

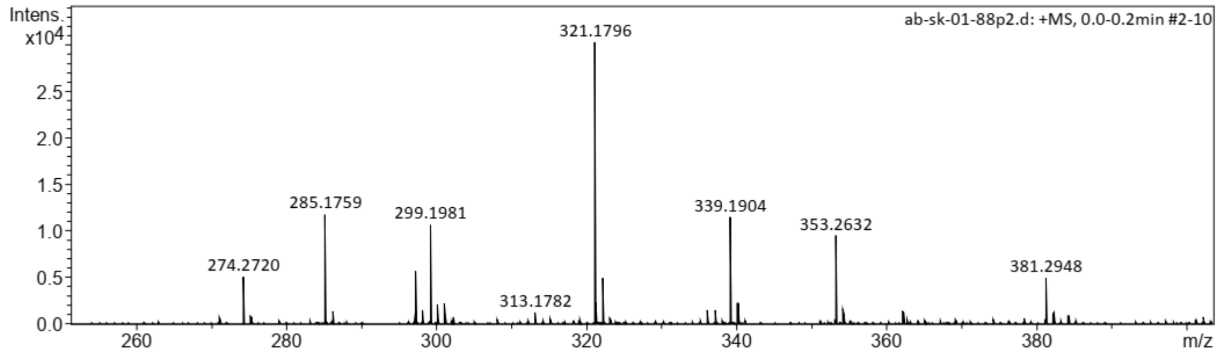
**Analysis Info**

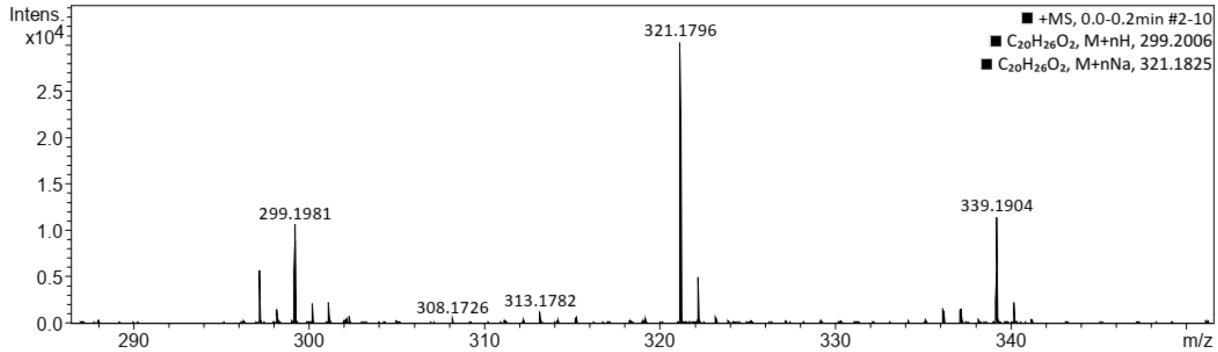
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\User data\2022\AUGUST\ab-sk-01-88p2.d | Acquisition Date | 8/12/2022 4:09:02 PM |
| Method | Tune_pos_Standard_July2022.m | Operator | IISER Kolkata |
| Sample Name | ab-sk-01-88p2 | Instrument | maXis impact 8282001.00127 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 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 | 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 |

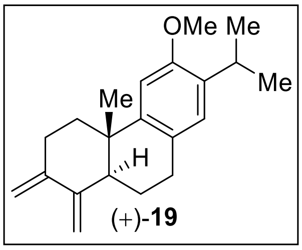


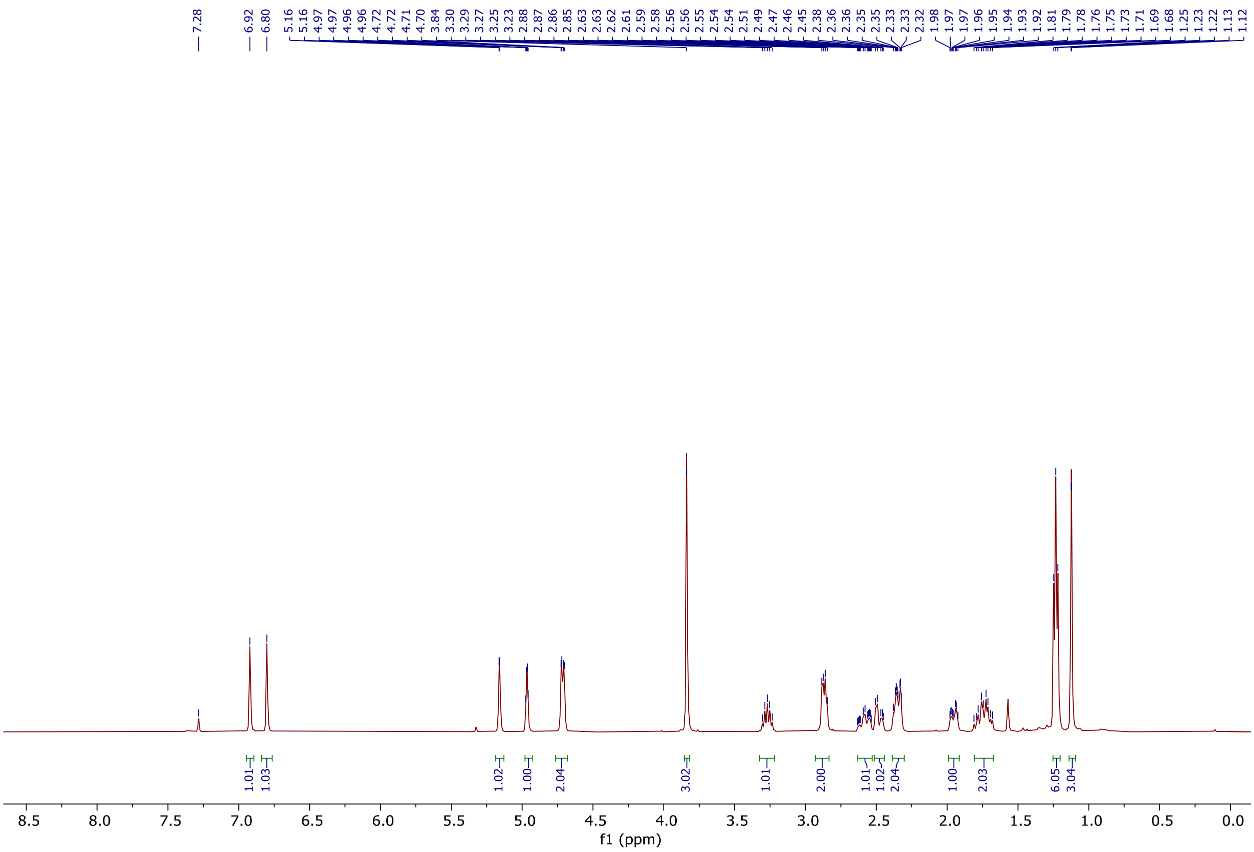



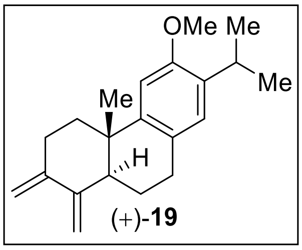



HRMS data of (+)-**17**

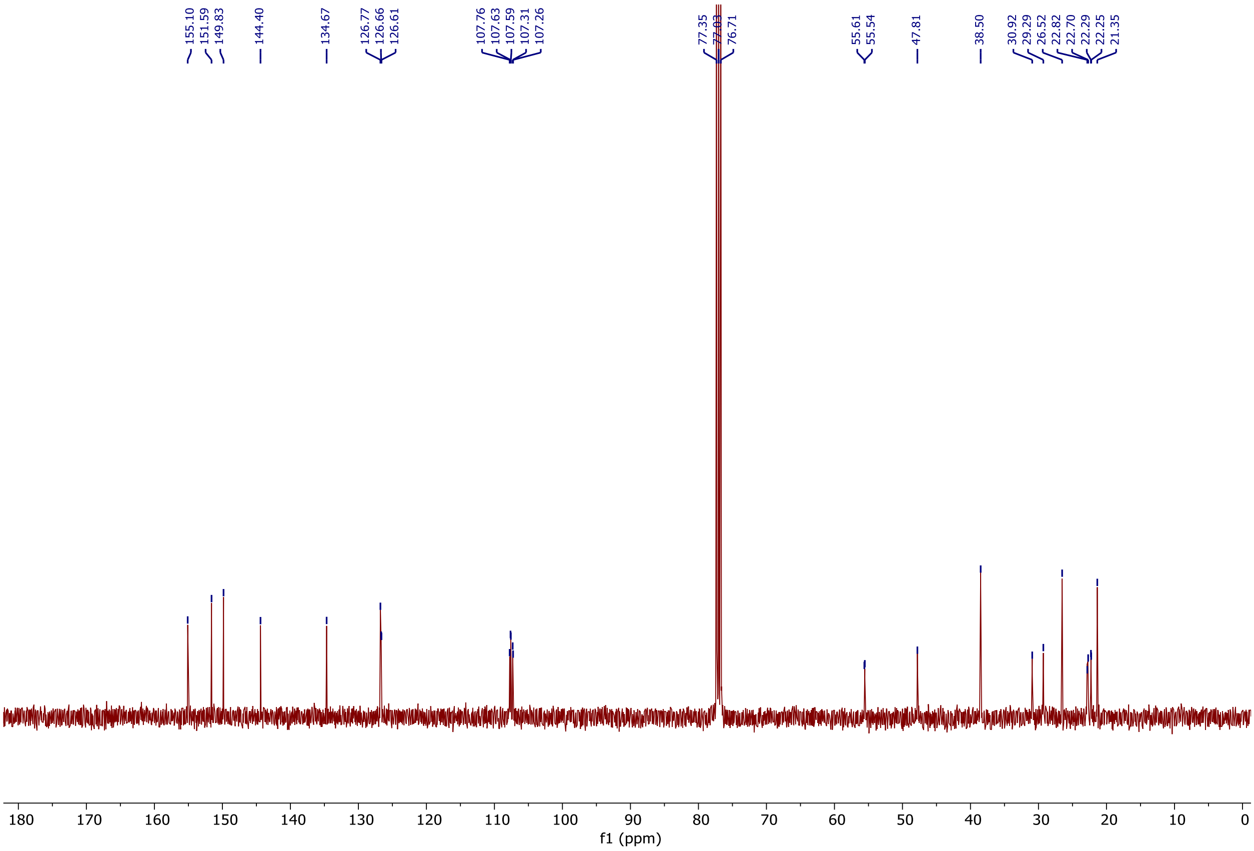



$^{1}$H NMR (400 MHz, $CDCl_3$) of compound (+)-**19**



(+)-**19**




$^{13}$C NMR (101 MHz, $CDCl_3$) of compound (+)-**19**

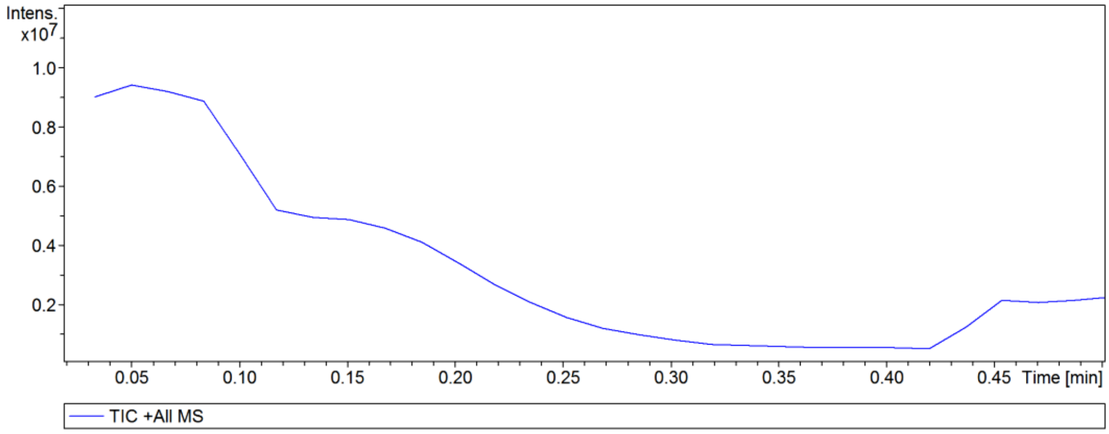
# Display Report

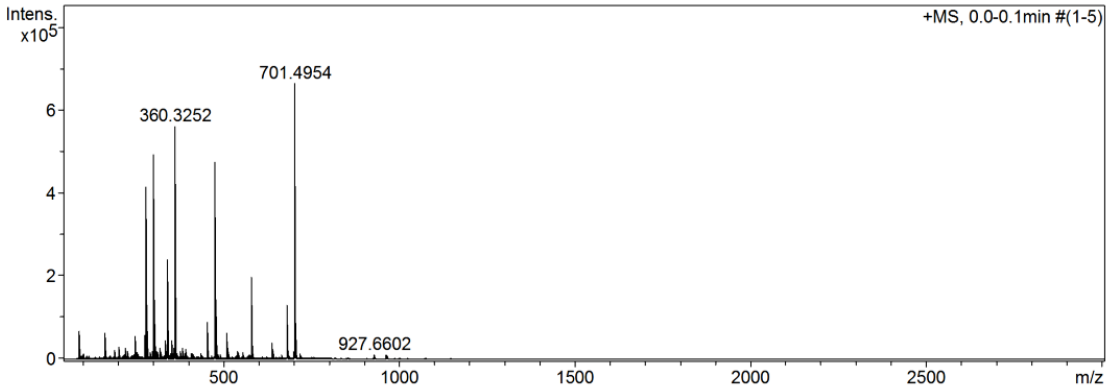
**Analysis Info**

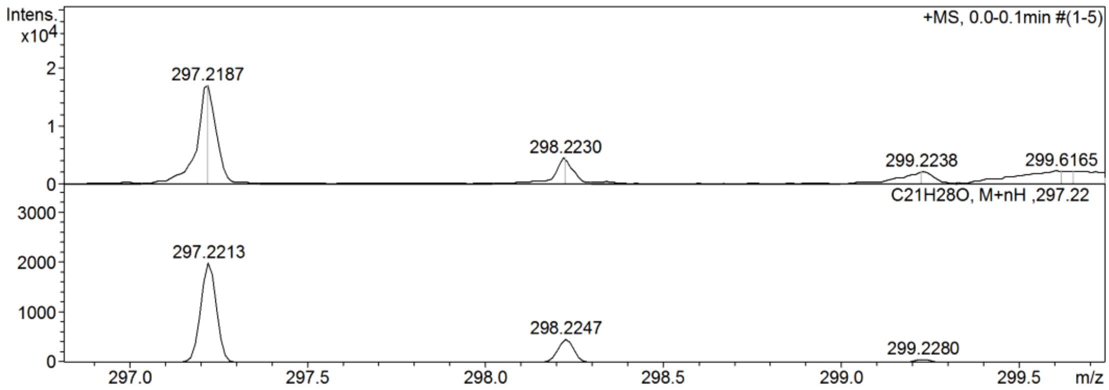
| | | | |
|---|---|---|---|
| | | Acquisition Date | 19-07-2022 14:23:57 |
| Analysis Name | D:\Data\USER DATA 2022\JULY2022\19-07-22\Dr.A.Bisai-ABSK0266.d | | |
| Method | tune mix_low.New.021117.m | Operator | Bruker |
| Sample Name | ABSK0266 | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 100.0 Vpp | Set Divert Valve | Source |

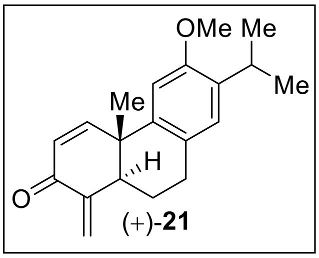


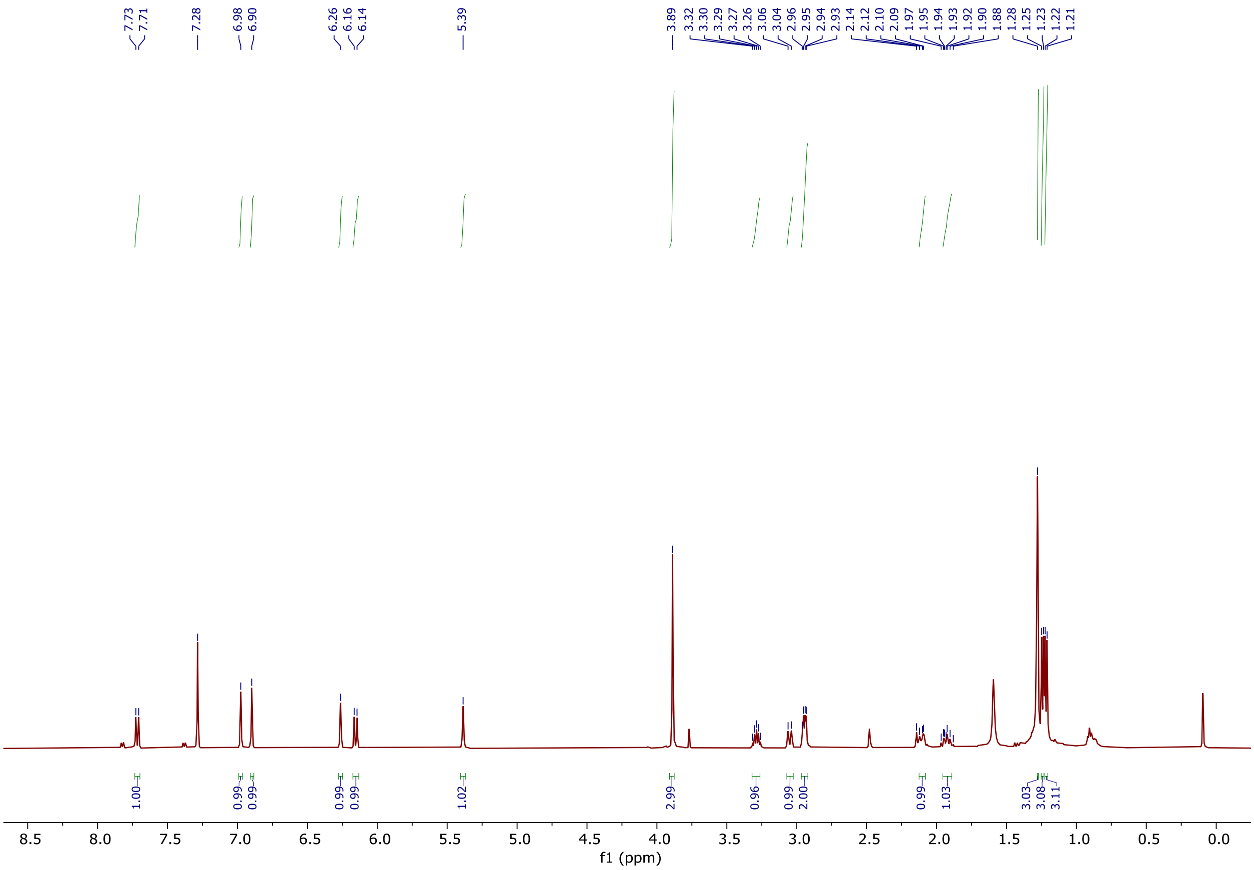



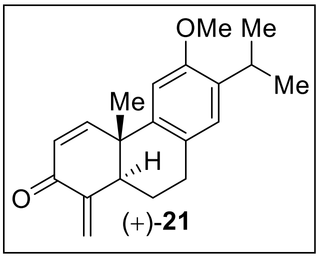


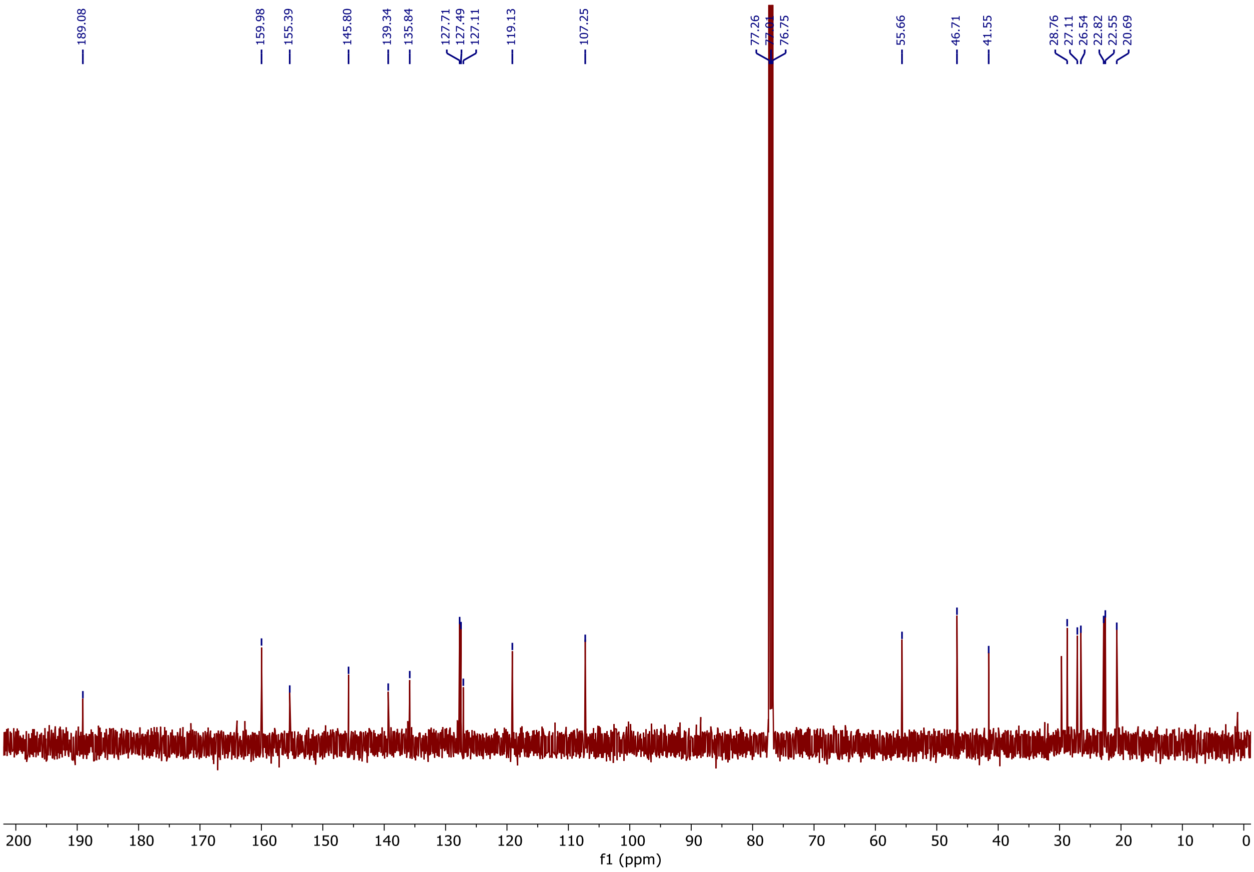

HRMS data of (+)-**19**




$^{1}$H NMR (400 MHz, $CDCl_3$) of compound (+)-**21**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**21**

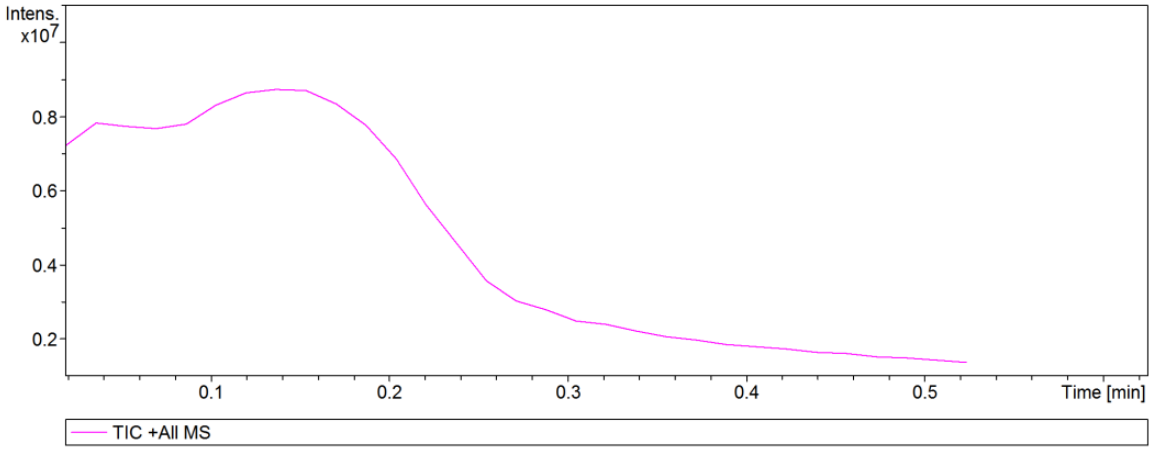
# Display Report

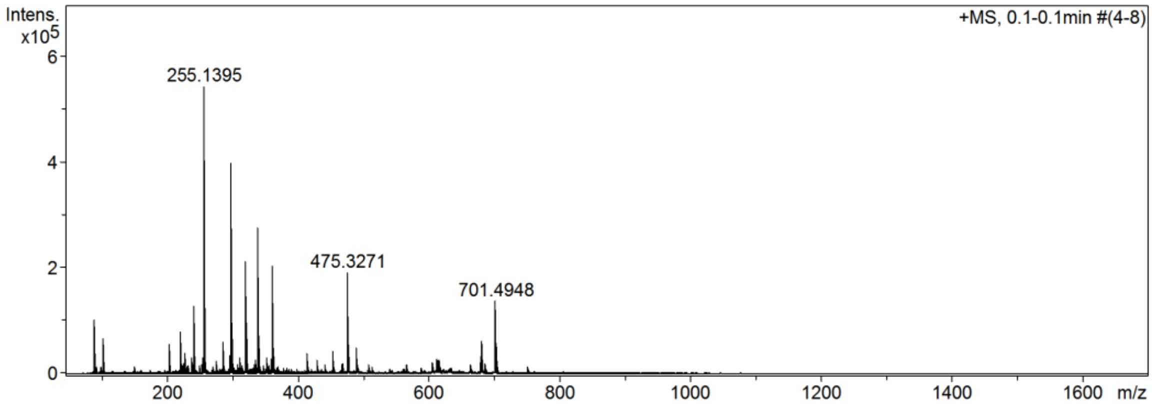
### Analysis Info

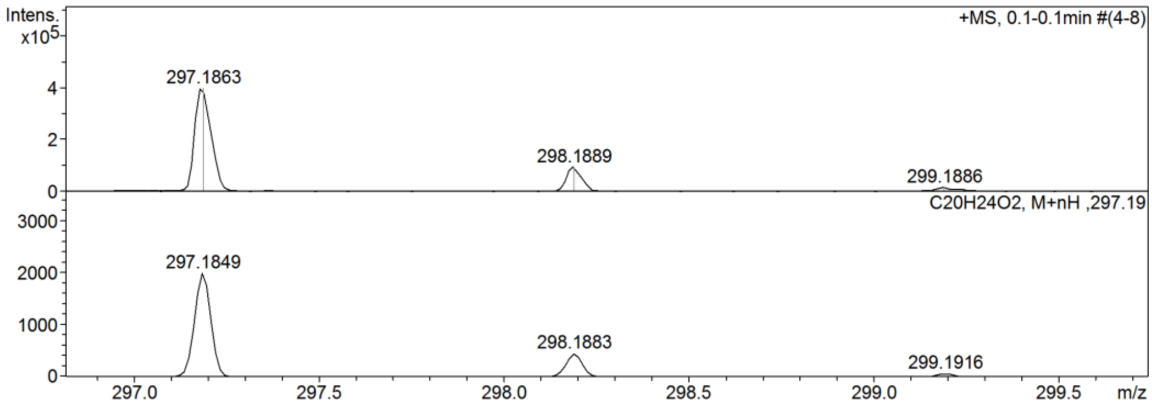
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\JULY2022\19-07-22\Dr.A.Bisai-ABSK0260.d | Acquisition Date | 19-07-2022 14:22:12 |
| Method | tune mix_low.New.021117.m | Operator | Bruker |
| Sample Name | ABSK0260 | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

### Acquisition Parameter

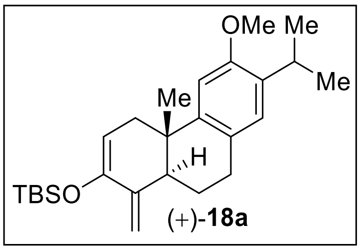
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar | | |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C | | |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min | | |
| Scan End | 3000 m/z | Set Collision Cell RF | 100.0 Vpp | Set Divert Valve | Source | | |

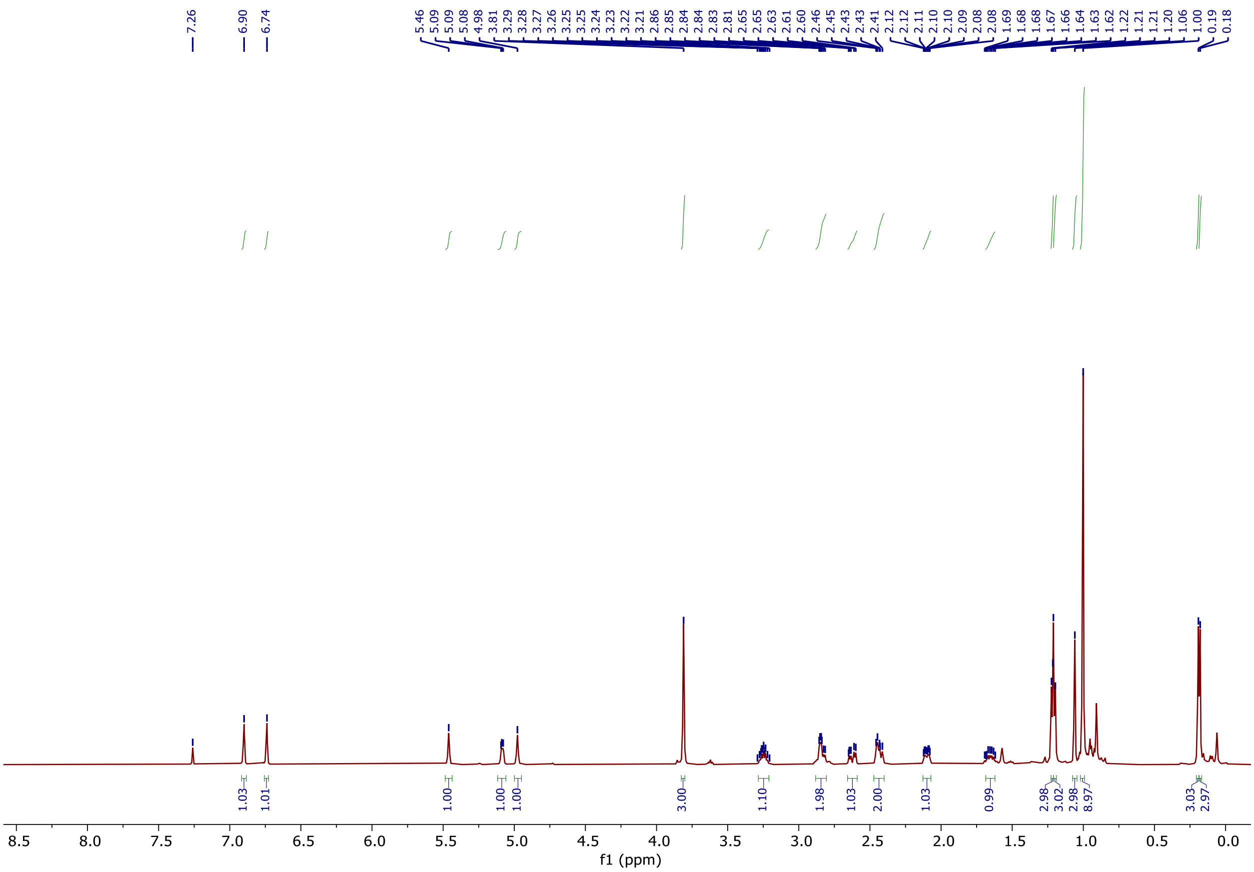


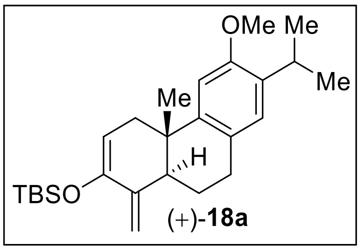



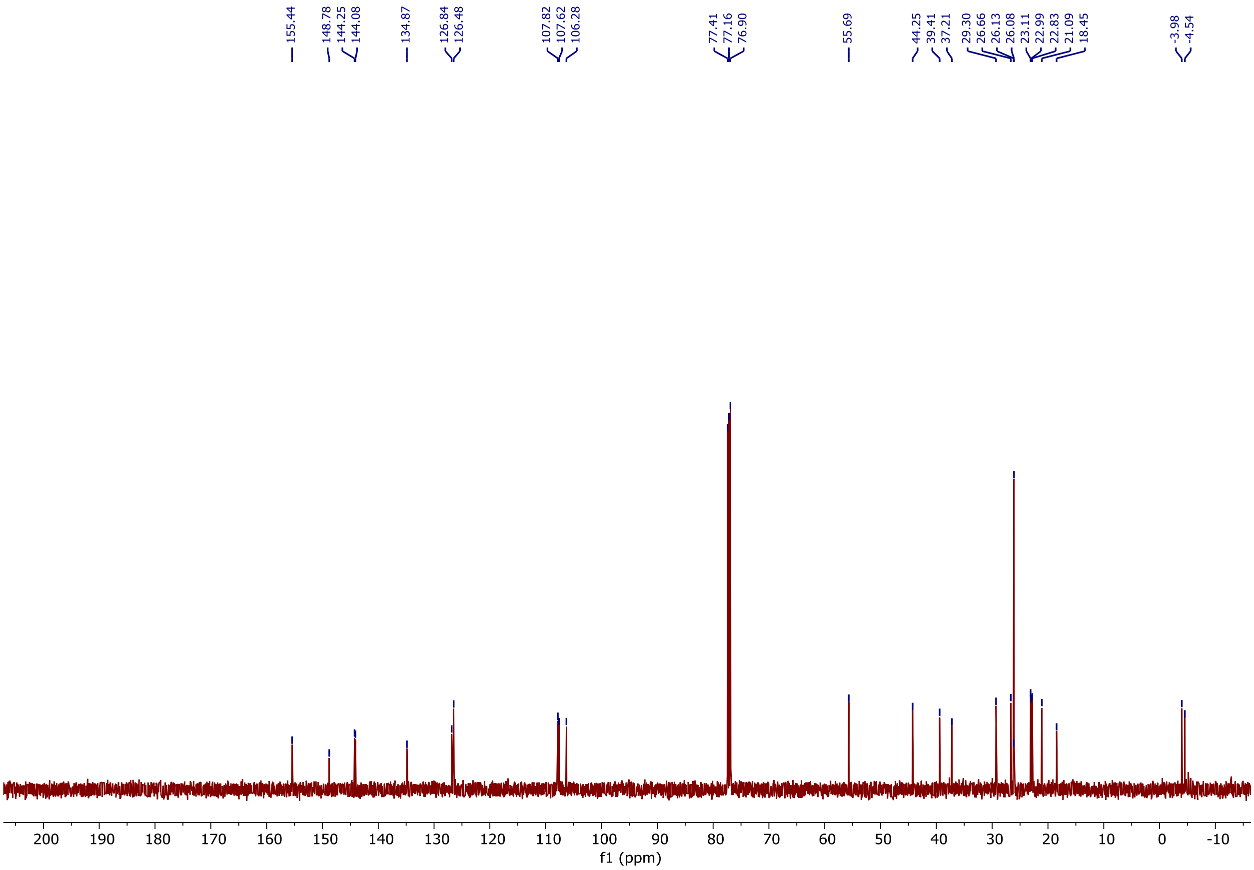

HRMS data of (+)-**21**




$^{1}$H NMR (500 MHz, $CDCl_3$) of compound (+)-**18a**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**18a**

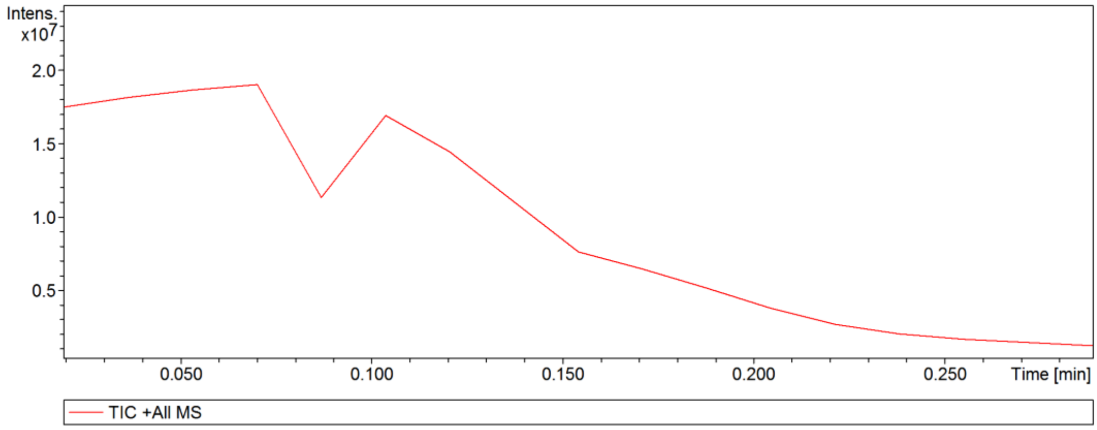
# Display Report

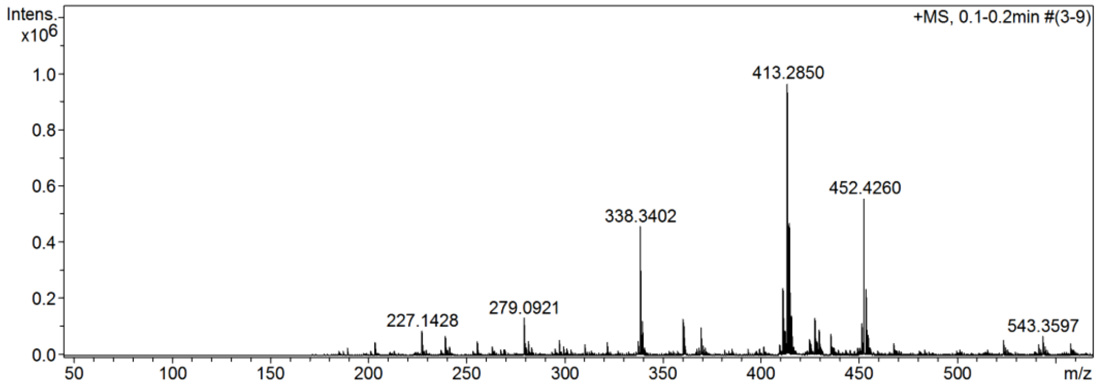
## Analysis Info

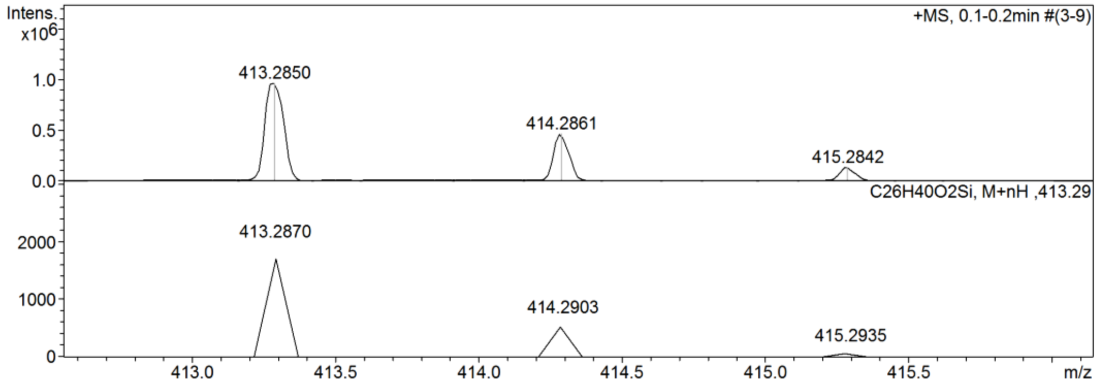
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\JUNE2022\28-06-22\Prof A Bisai-SK-02-61.d | Acquisition Date | 28-06-2022 11:15:59 |
| Method | tune mix_low.New.021117_1.m | Operator | Bruker |
| Sample Name | SK-02-61 | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

## Acquisition Parameter

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |

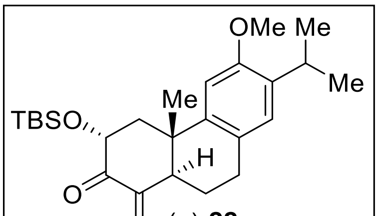


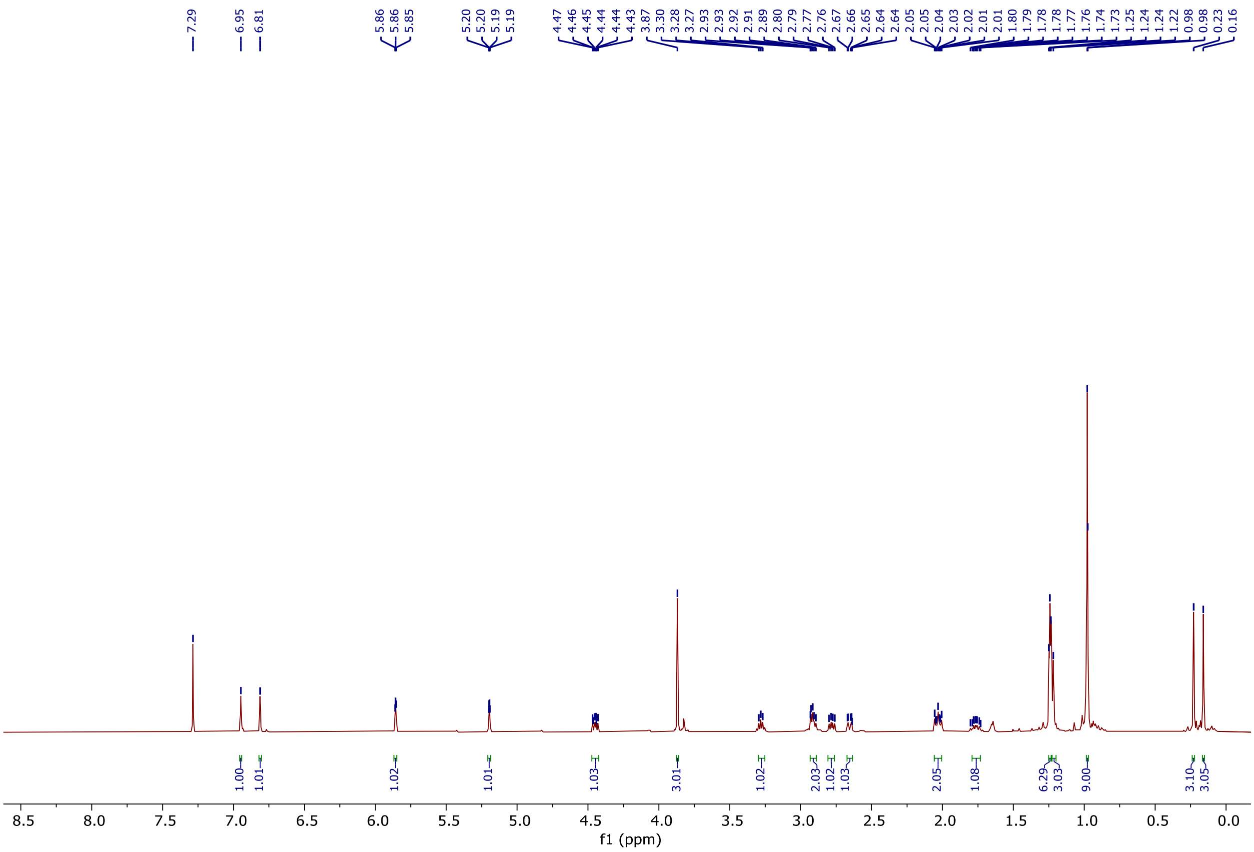





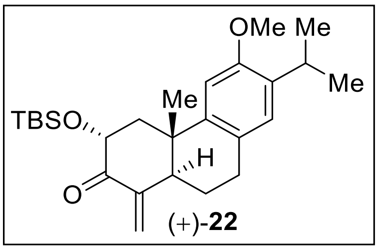

HRMS data of (+)-**18a**

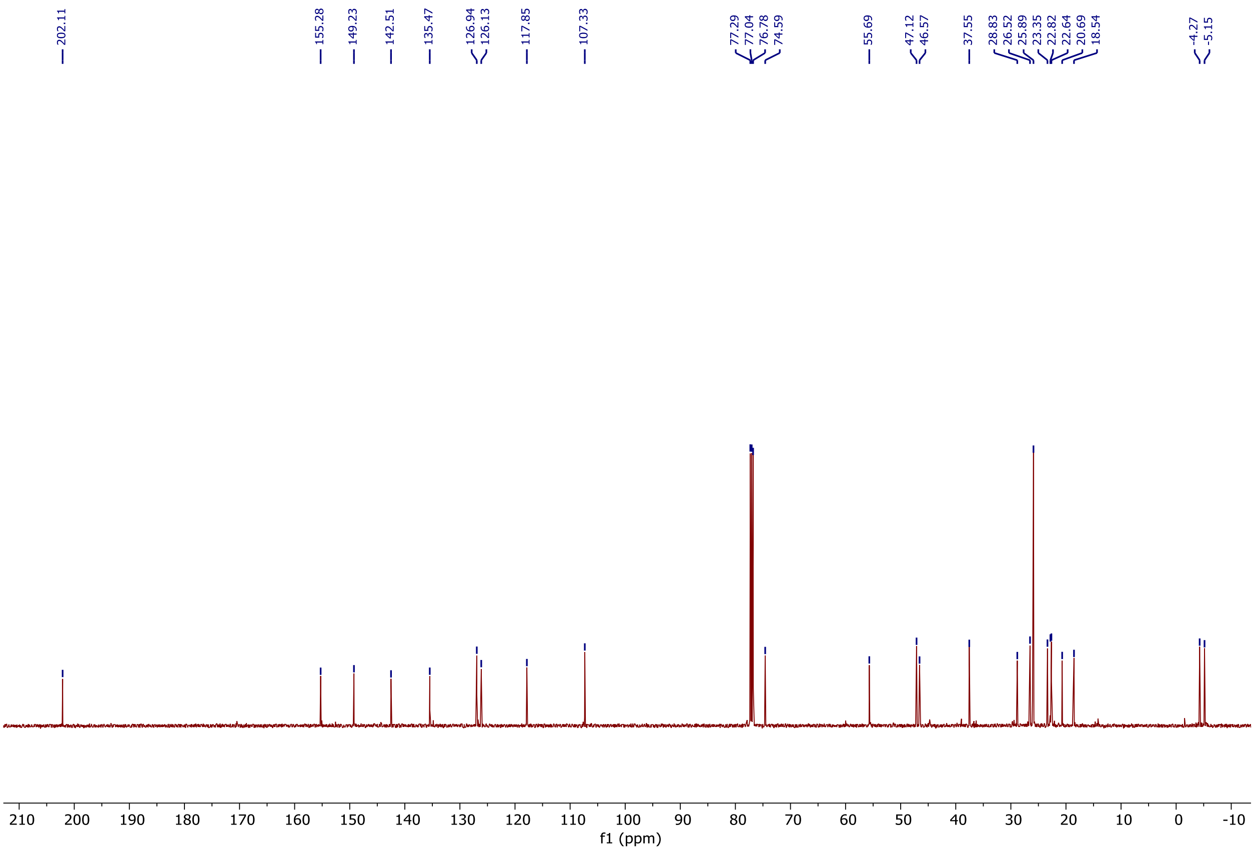


(+)-**22**



[1]H NMR (500 MHz, $CDCl_3$) of compound (+)-**22**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**22**

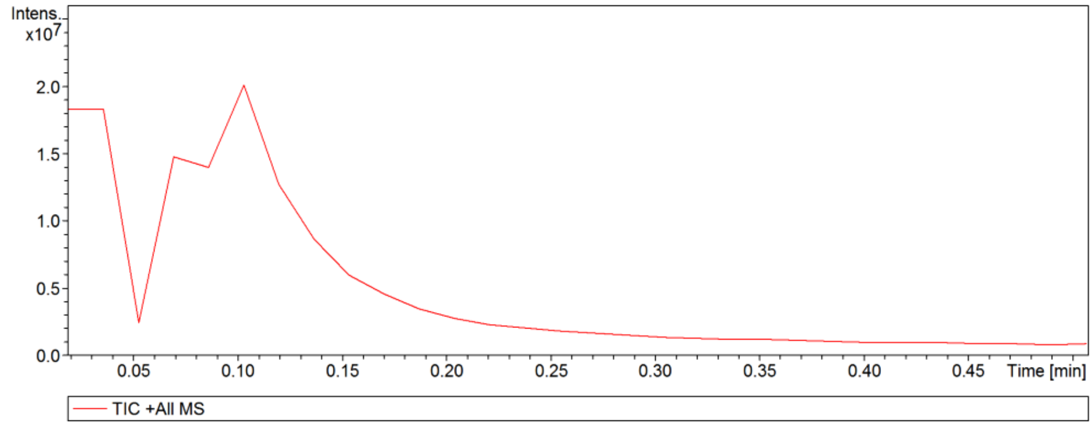
# Display Report

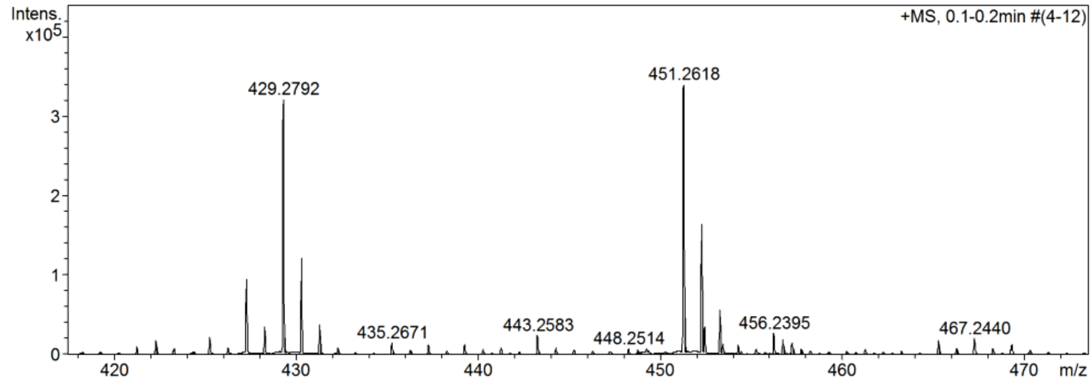
**Analysis Info**

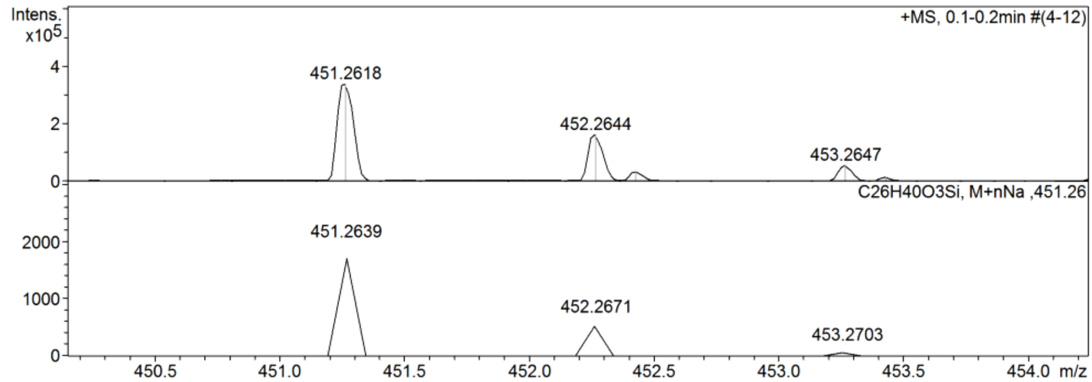
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\JUNE2022\28-06-22\Prof A Bisai-SK-02-78.d | Acquisition Date | 28-06-2022 11:23:57 |
| Method | tune mix_low.New.021117_1.m | Operator | Bruker |
| Sample Name | SK-02-78 | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 300.0 Vpp | Set Divert Valve | Source |

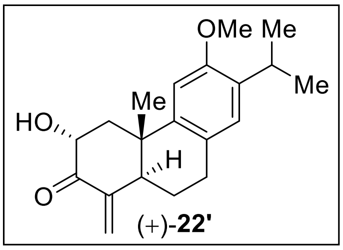


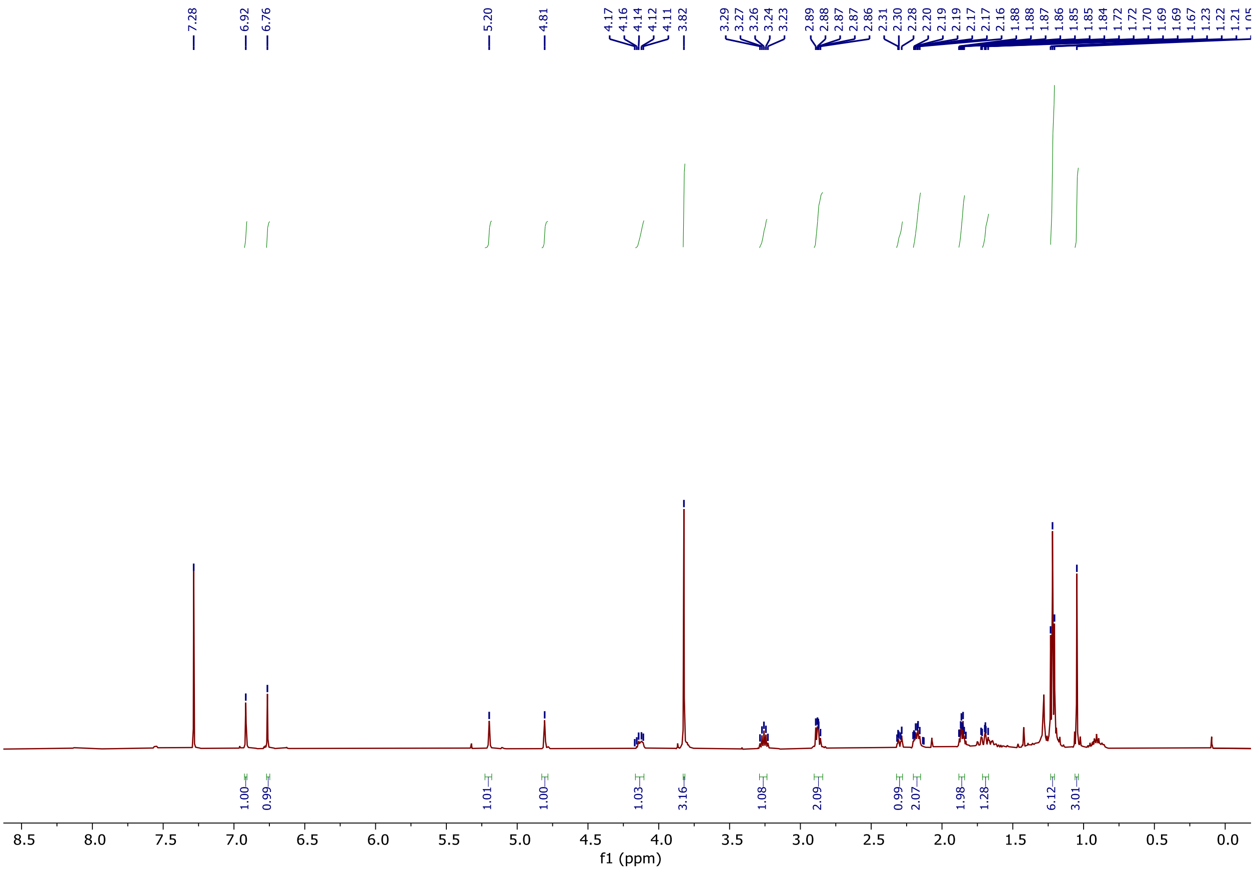



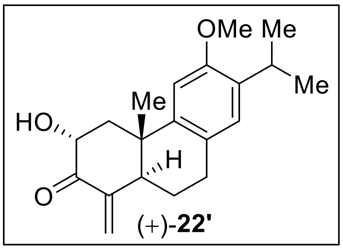


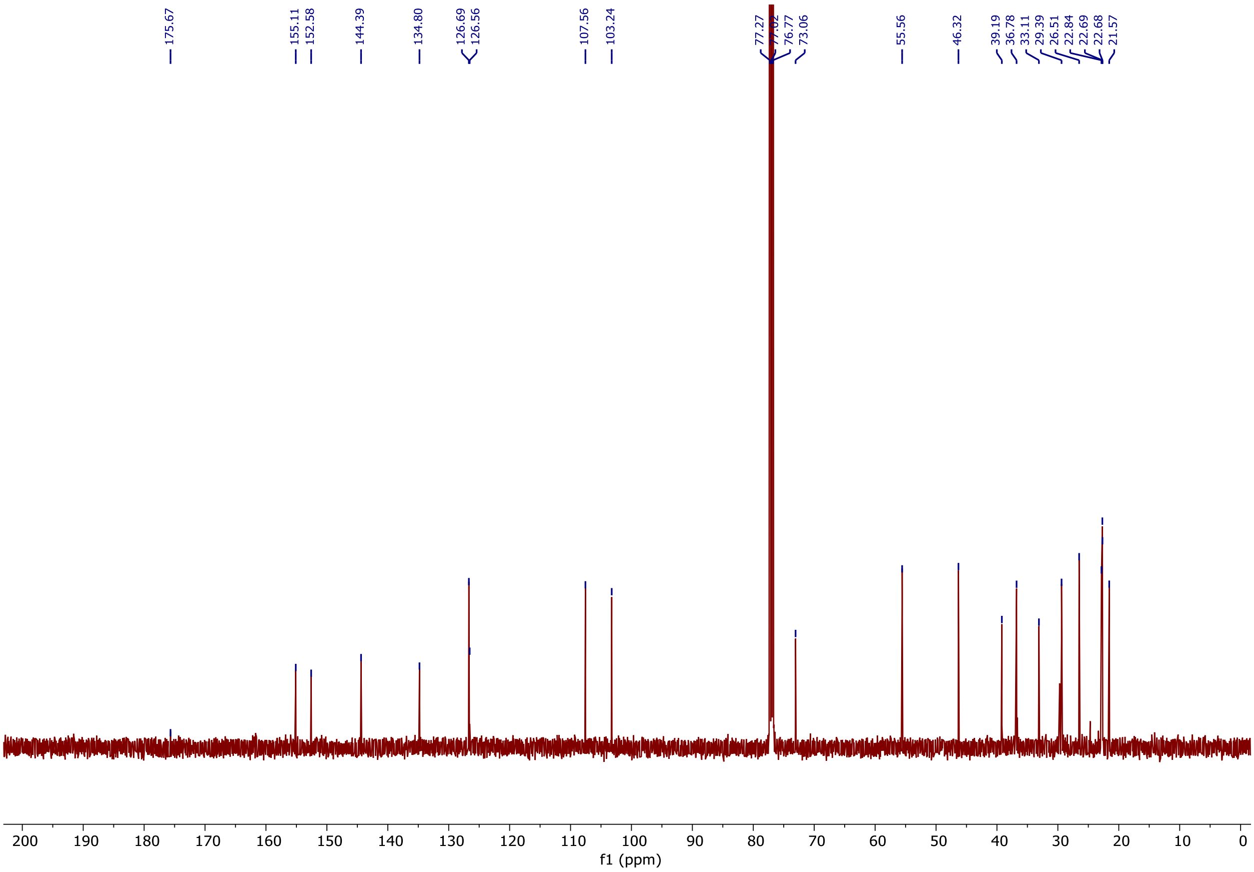

HRMS data of (+)-**22**



$^{1}$H NMR (500 MHz, $CDCl_3$) of compound (+)-**22'**






$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**22’**

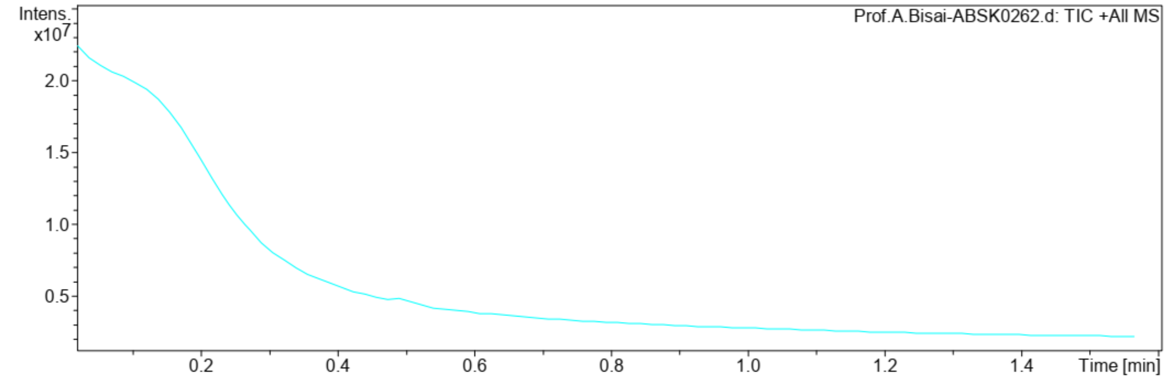
# Display Report

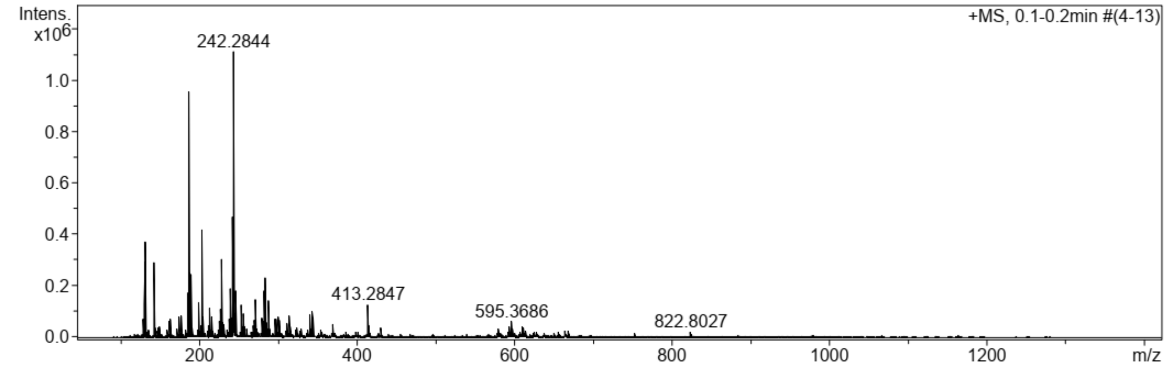
**Analysis Info**

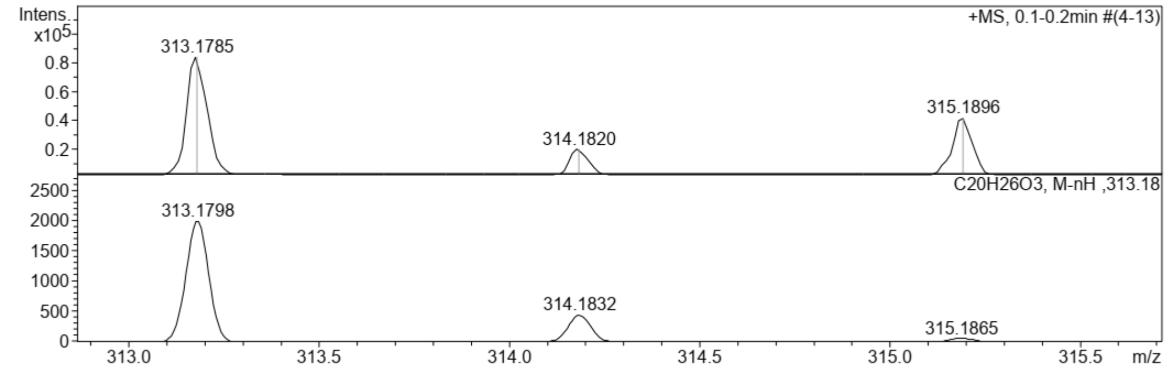
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\MAY 2022\12-05-2022\Prof.A.Bisai-ABSK0262.d | Acquisition Date | 5/12/2022 3:59:21 PM |
| Method | tune_low_APCI.m | Operator | IISER |
| Sample Name | ABSK0262 | Instrument | micrOTOF-Q II 10330 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | Multi Mode | Ion Polarity | Positive | Set Nebulizer | 2.0 Bar |
| Focus | Not active | Set Capillary | 2500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 5.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 150.0 Vpp | Set Divert Valve | Source |

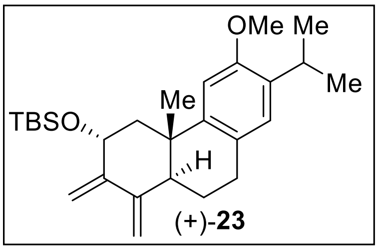


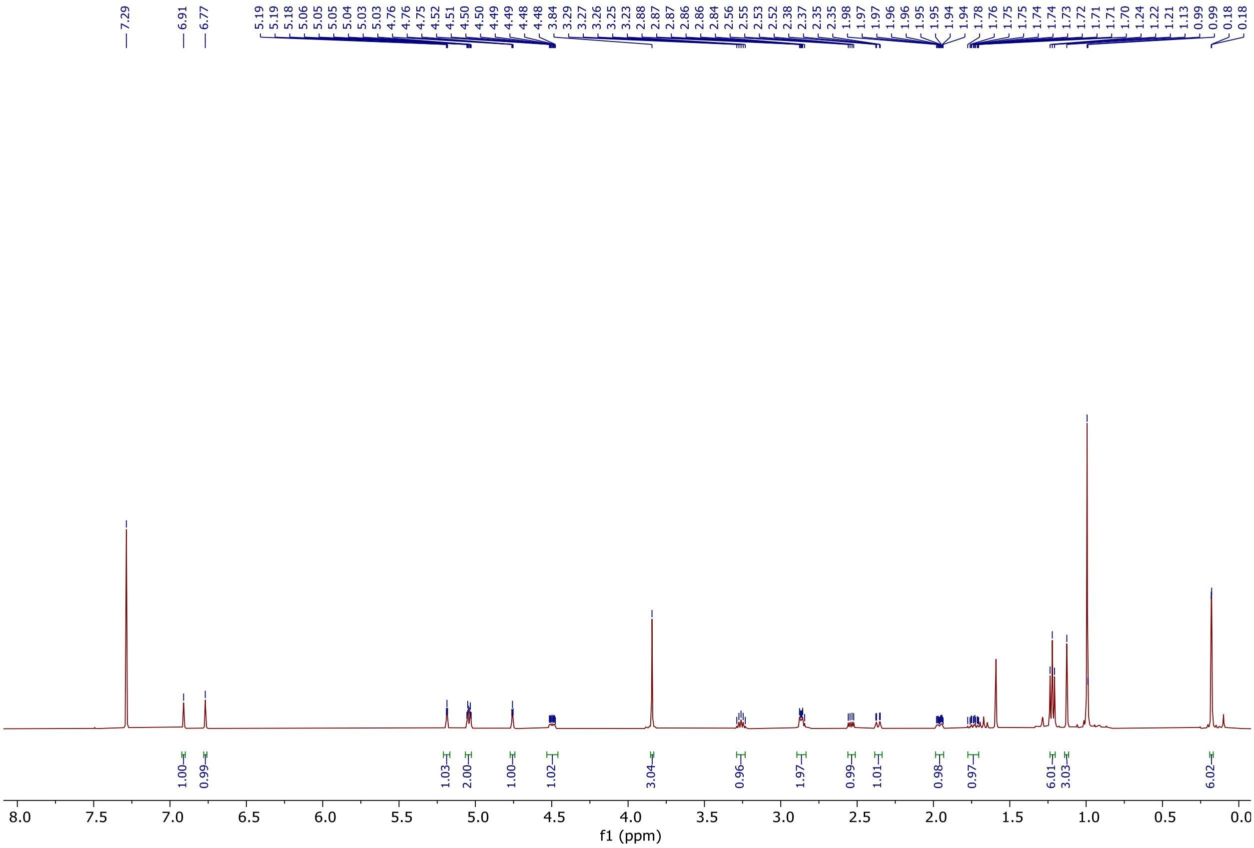



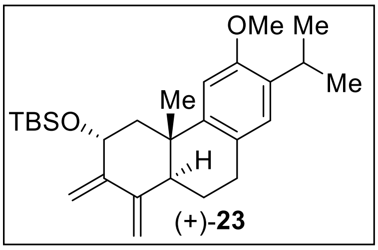


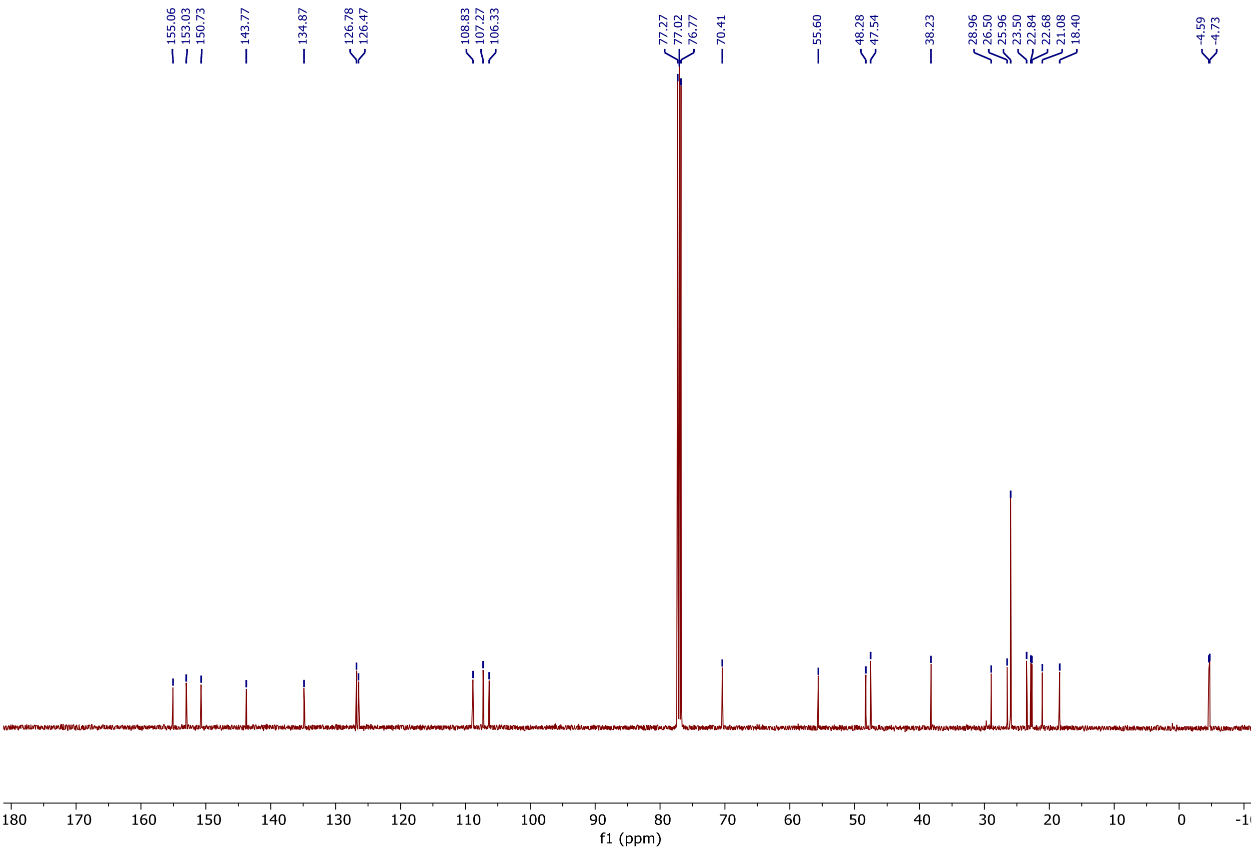

HRMS data of (+)-**22’**




$^{1}$H NMR (500 MHz, $CDCl_3$) of compound (+)-**23**




$^{13}C$ NMR (126 MHz, $CDCl_3$) of compound (+)-**23**

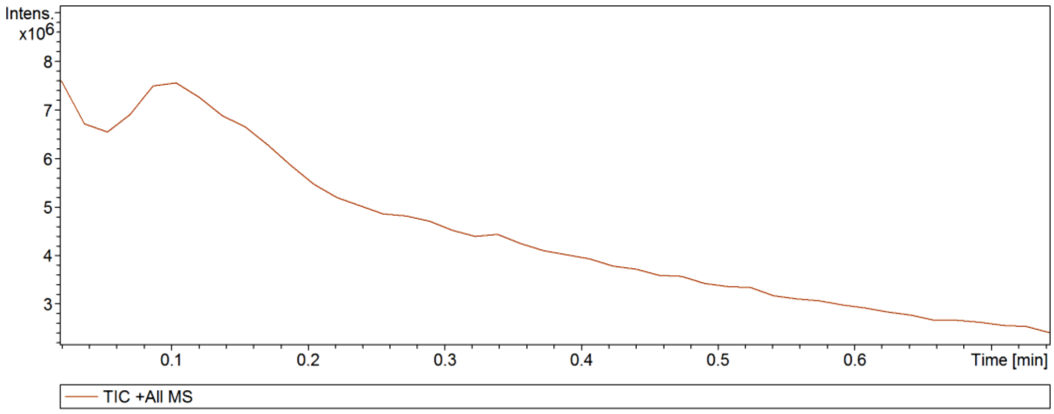
# Display Report

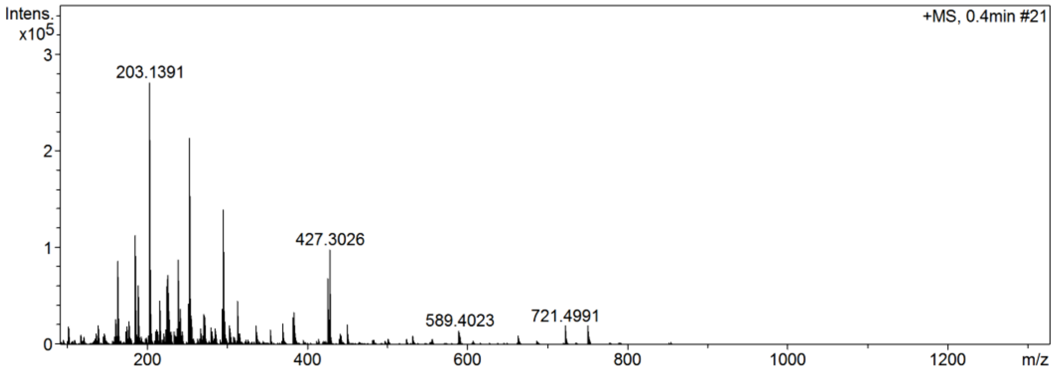
**Analysis Info**

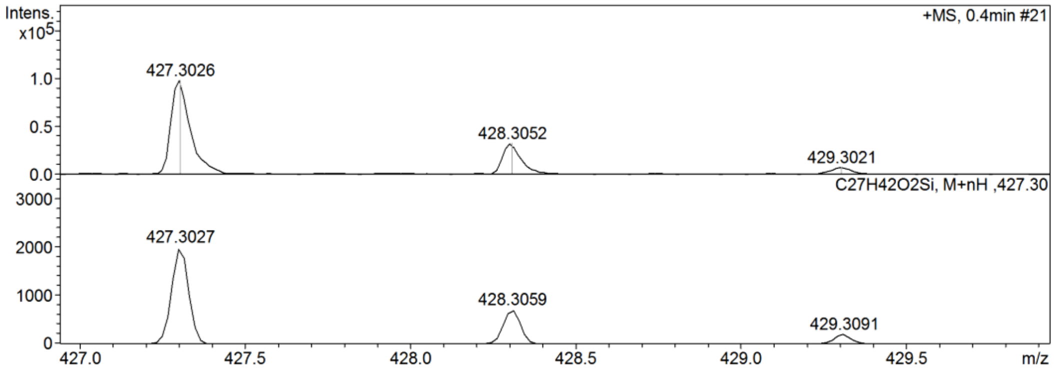
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\JULY2022\15-07-22\Dr.A.Bisai -ABSK0281-R.d | Acquisition Date | 15-07-2022 12:55:43 |
| Method | tune mix_low.New.021117.m | Operator | Bruker |
| Sample Name | ABSK0281-R | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 100.0 Vpp | Set Divert Valve | Source |

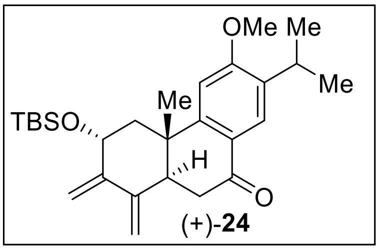


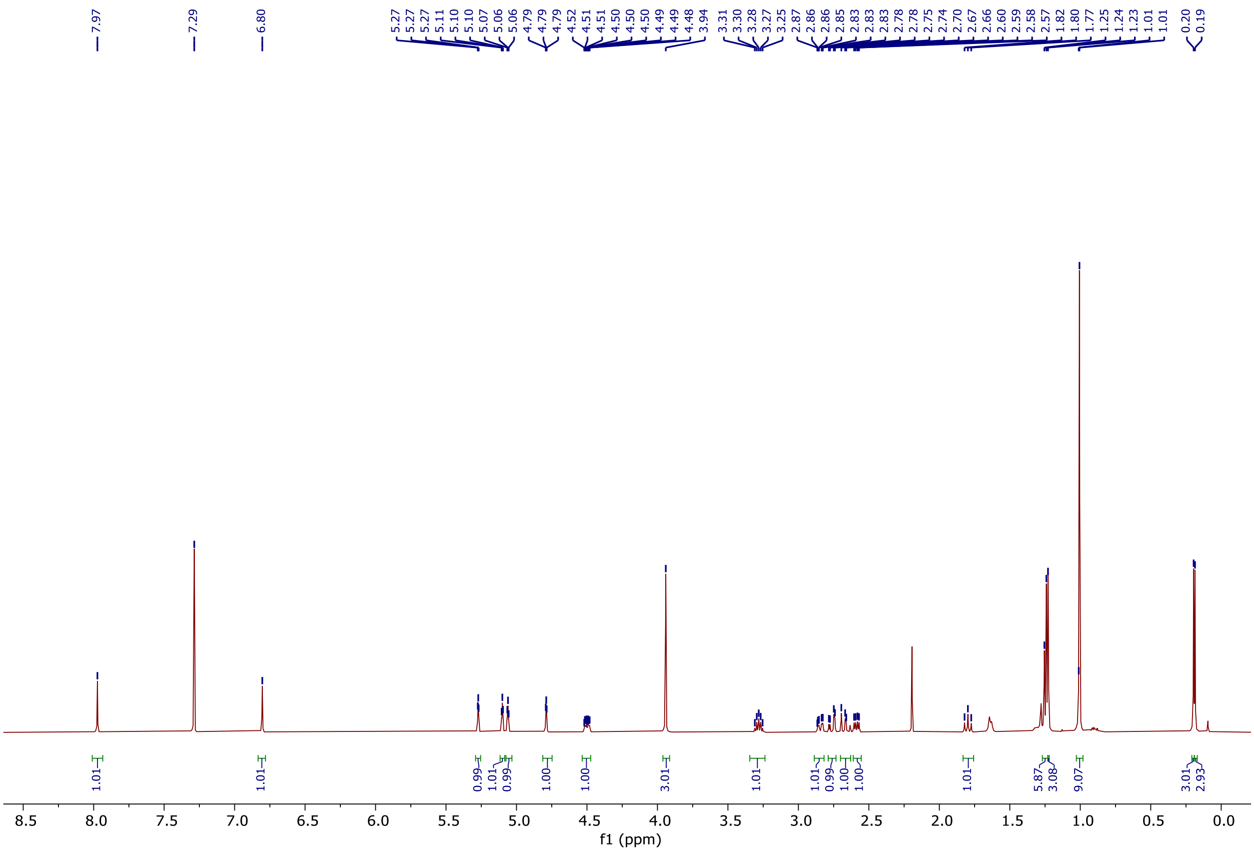



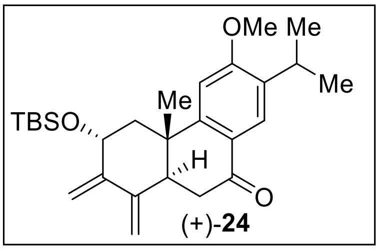


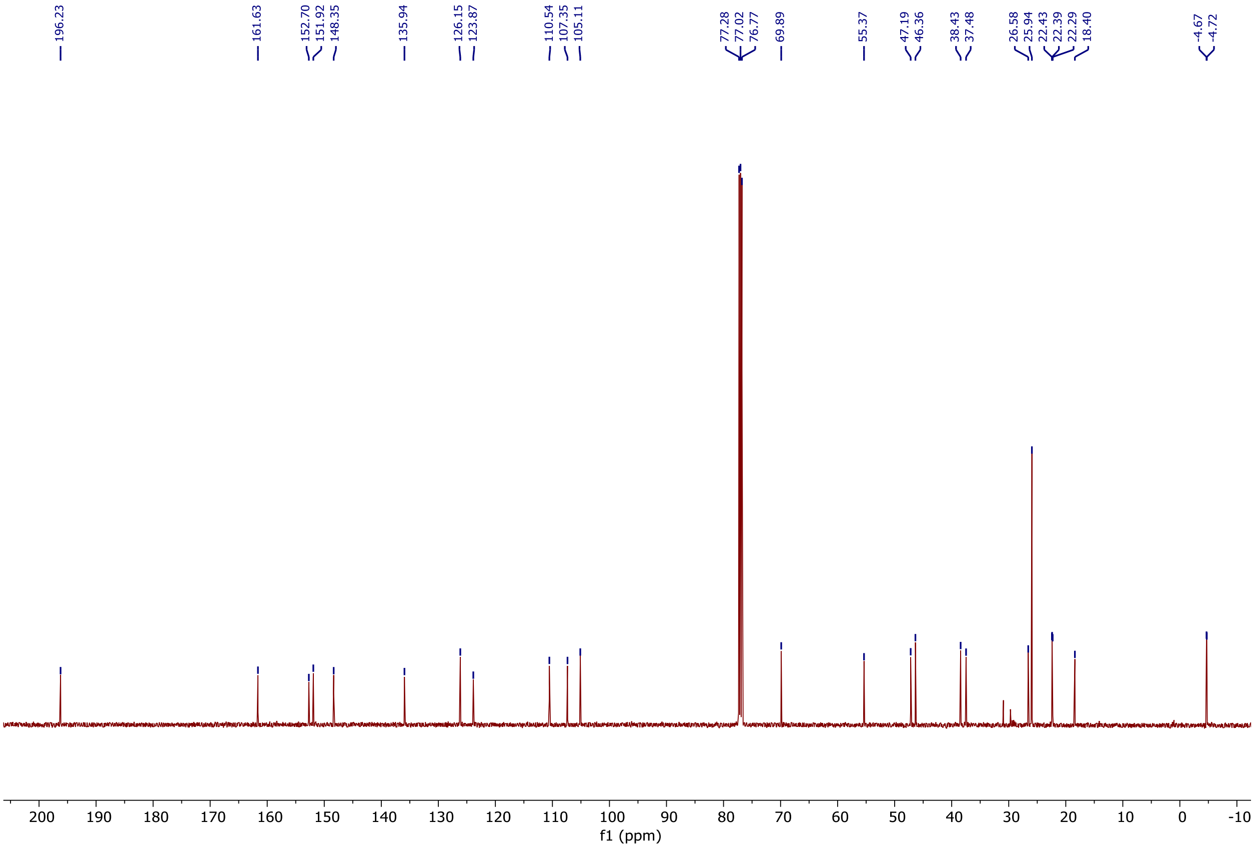

HRMS data of (+)-**23**



$^1$H NMR (500 MHz, $CDCl_3$) of compound (+)-**24**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**24**

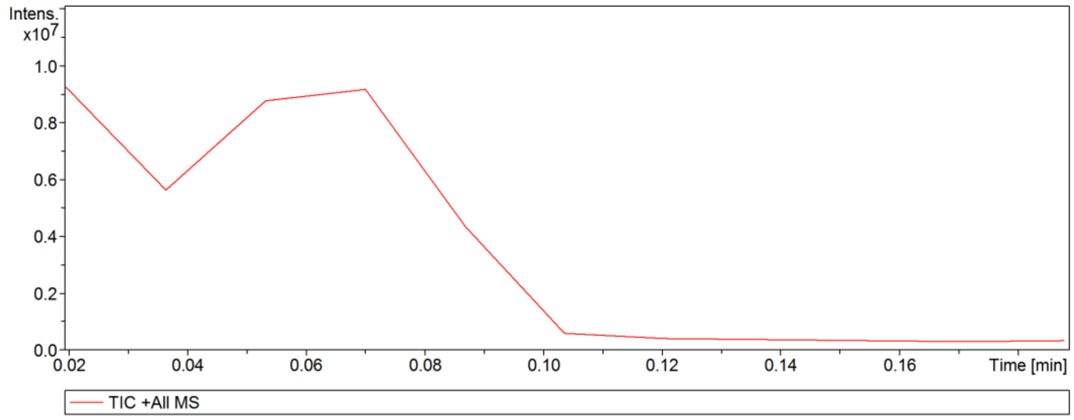
# Display Report

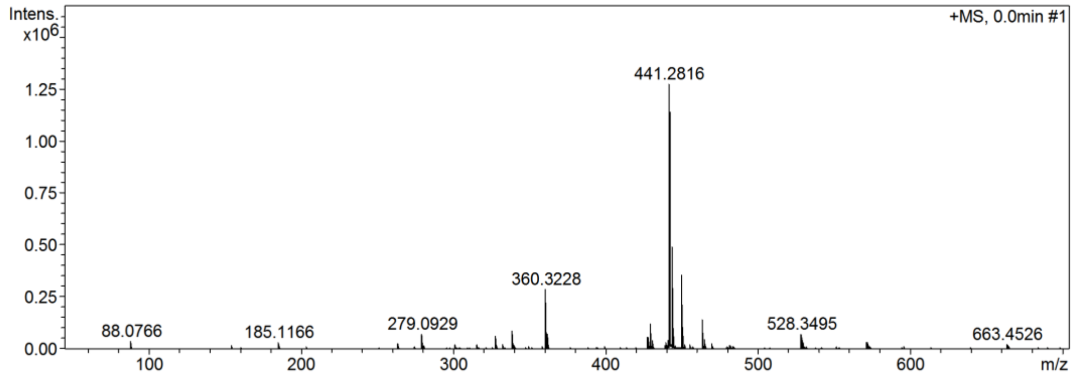
**Analysis Info**

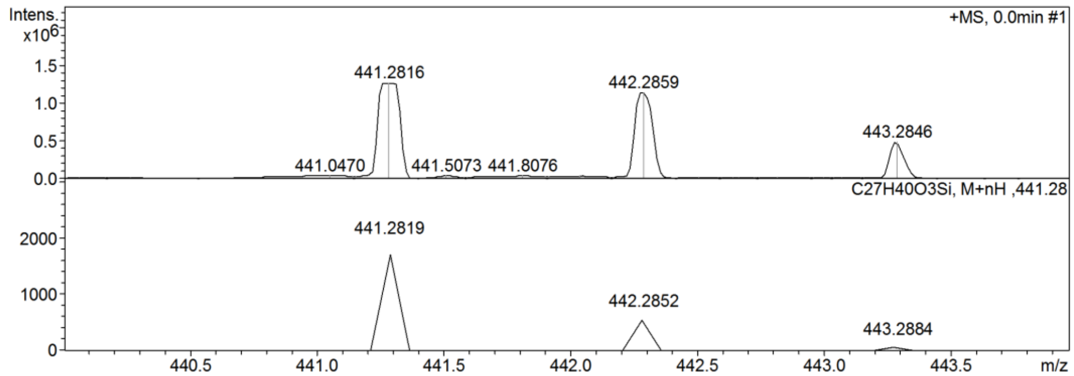
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\JUNE2022\28-06-22\Prof A Bisai-SK-02-82.d | Acquisition Date | 28-06-2022 11:55:30 |
| Method | tune mix_low.New.021117_1.m | Operator | Bruker |
| Sample Name | SK-02-82 | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 100.0 Vpp | Set Divert Valve | Source |

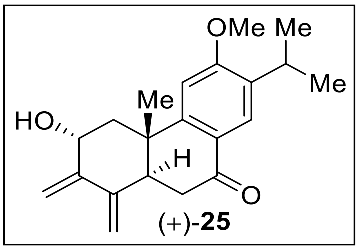


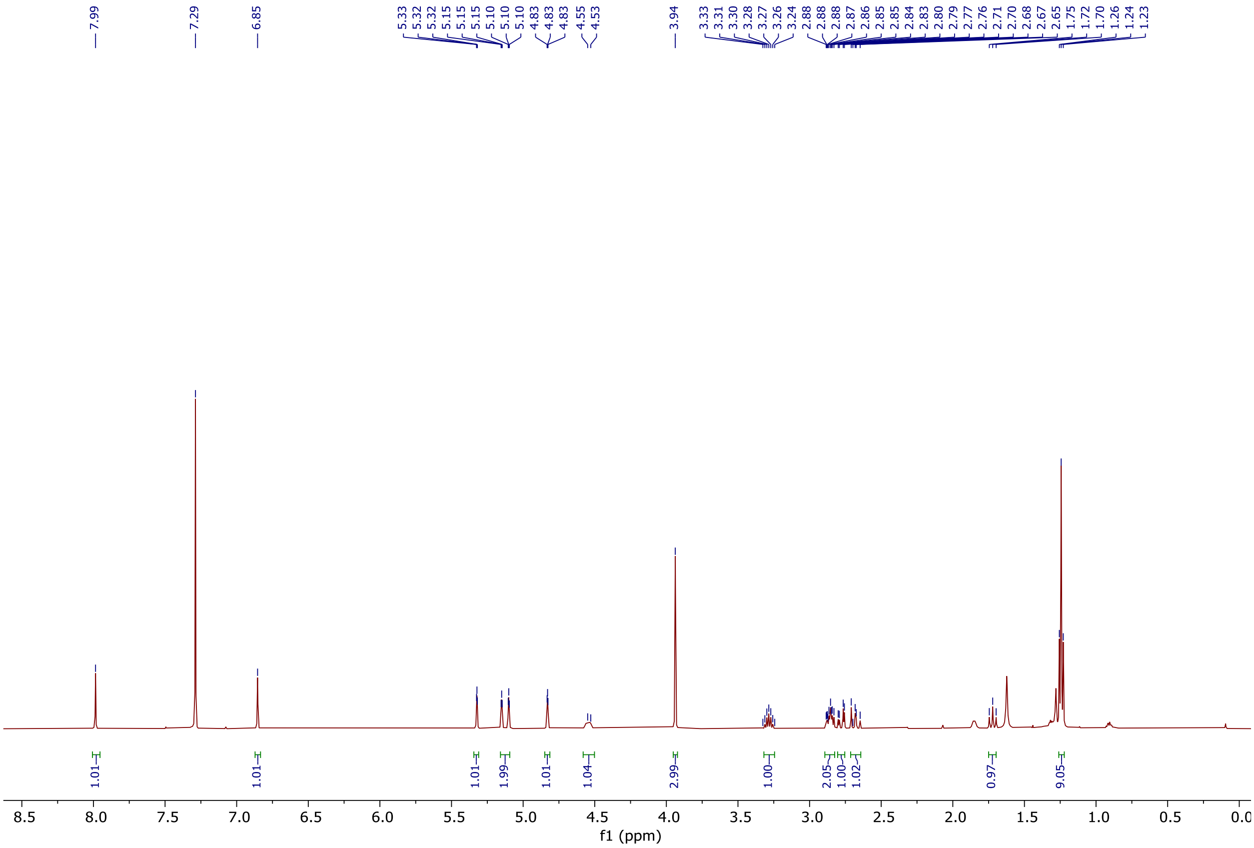



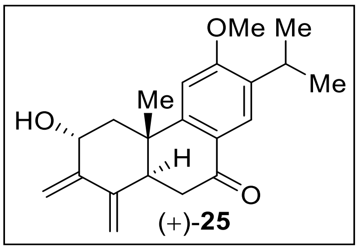


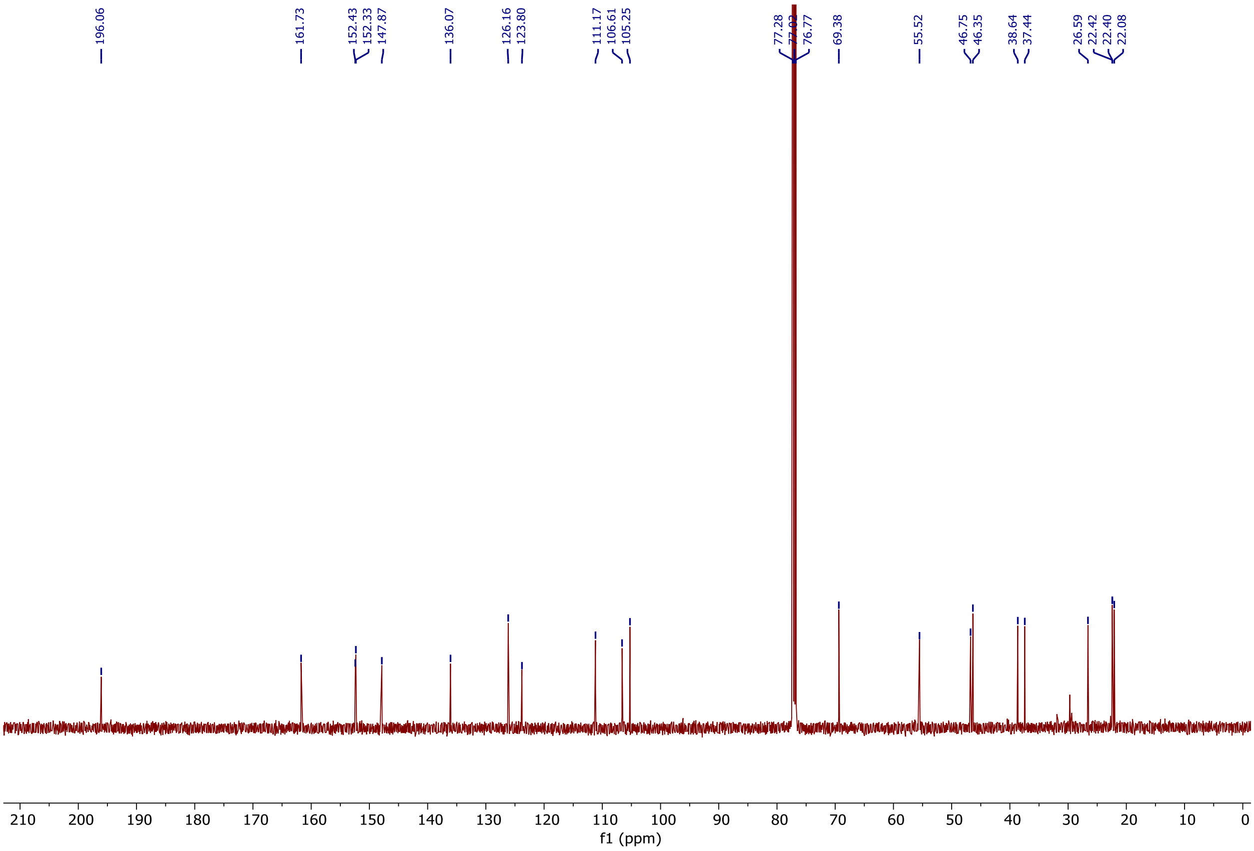

HRMS data of (+)-**24**




$^1$H NMR (500 MHz, $CDCl_3$) of compound (+)-**25**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**25**

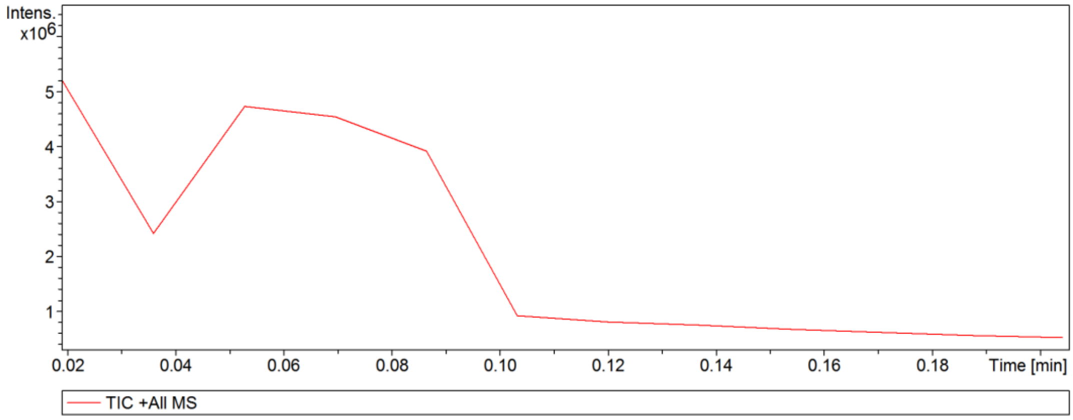
# Display Report

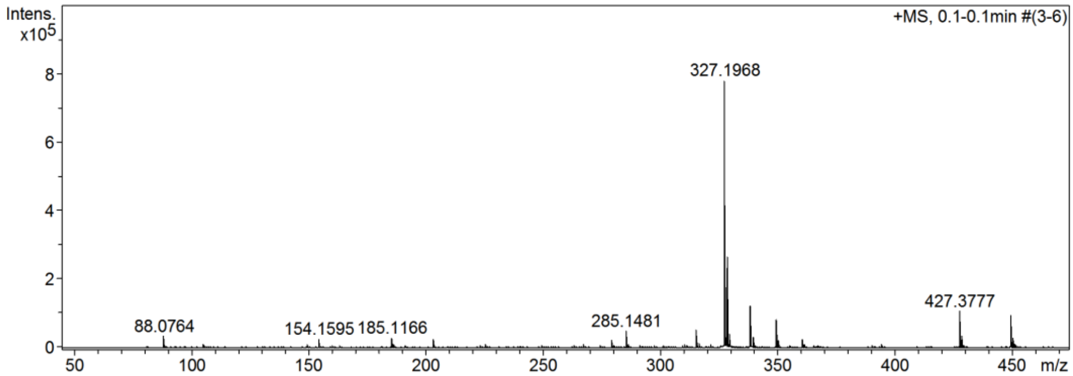
## Analysis Info

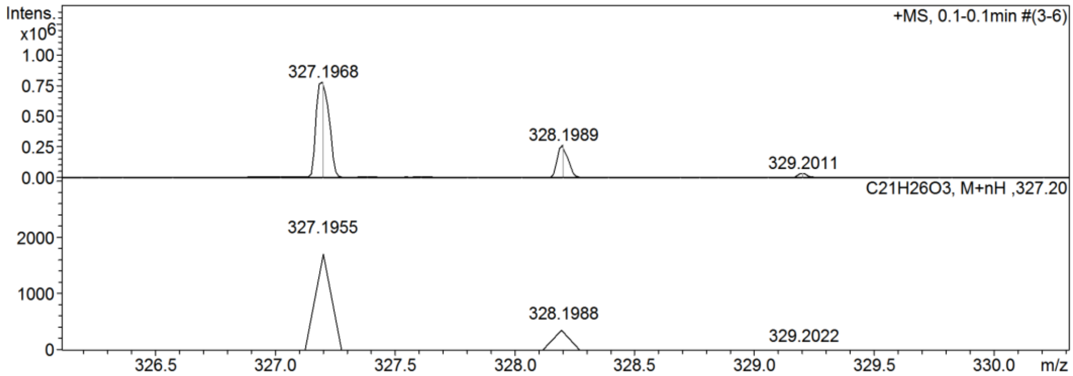
| | | | |
|---|---|---|---|
| | | Acquisition Date | 28-06-2022 11:51:44 |
| Analysis Name | D:\Data\USER DATA 2022\JUNE2022\28-06-22\Prof A Bisai-SK-02-83.d | | |
| Method | tune mix_low.New.021117_1.m | Operator | Bruker |
| Sample Name | SK-02-83 | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

## Acquisition Parameter

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 100.0 Vpp | Set Divert Valve | Source |

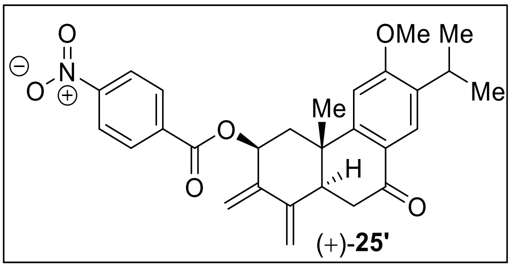


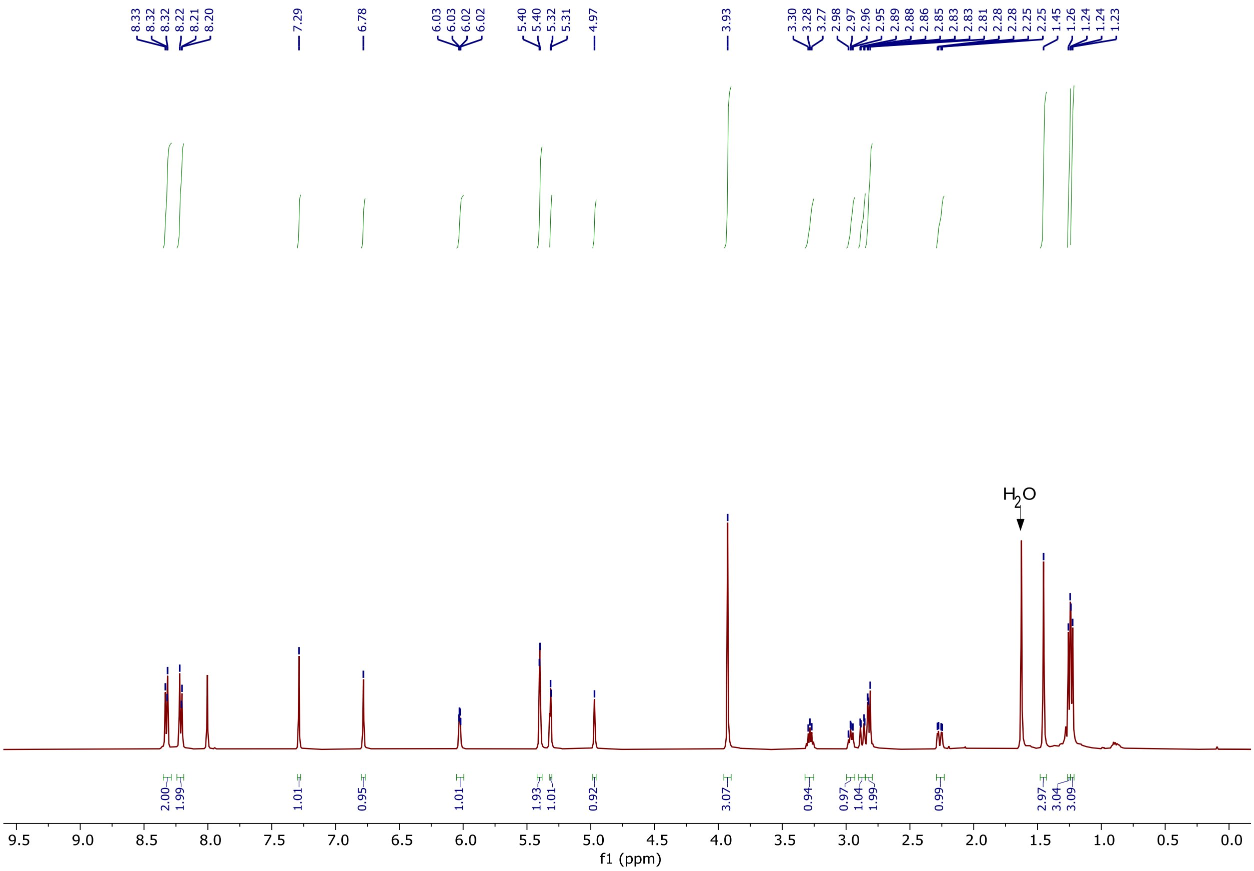



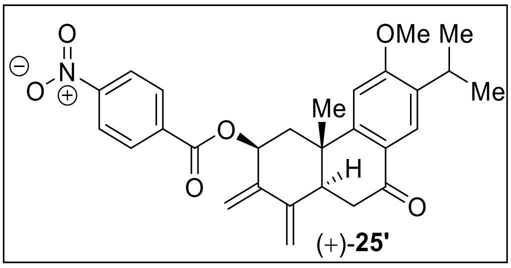


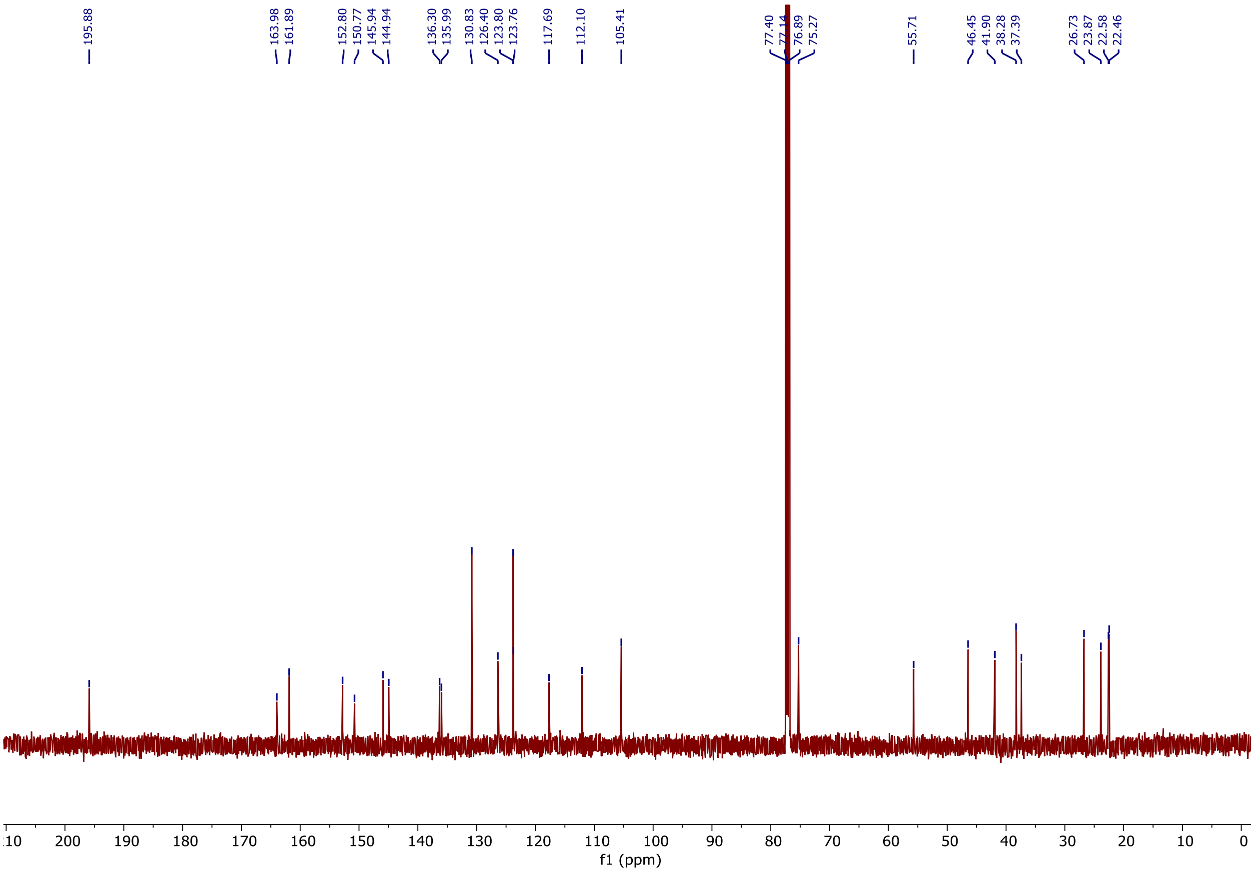

HRMS data of (+)-**25**



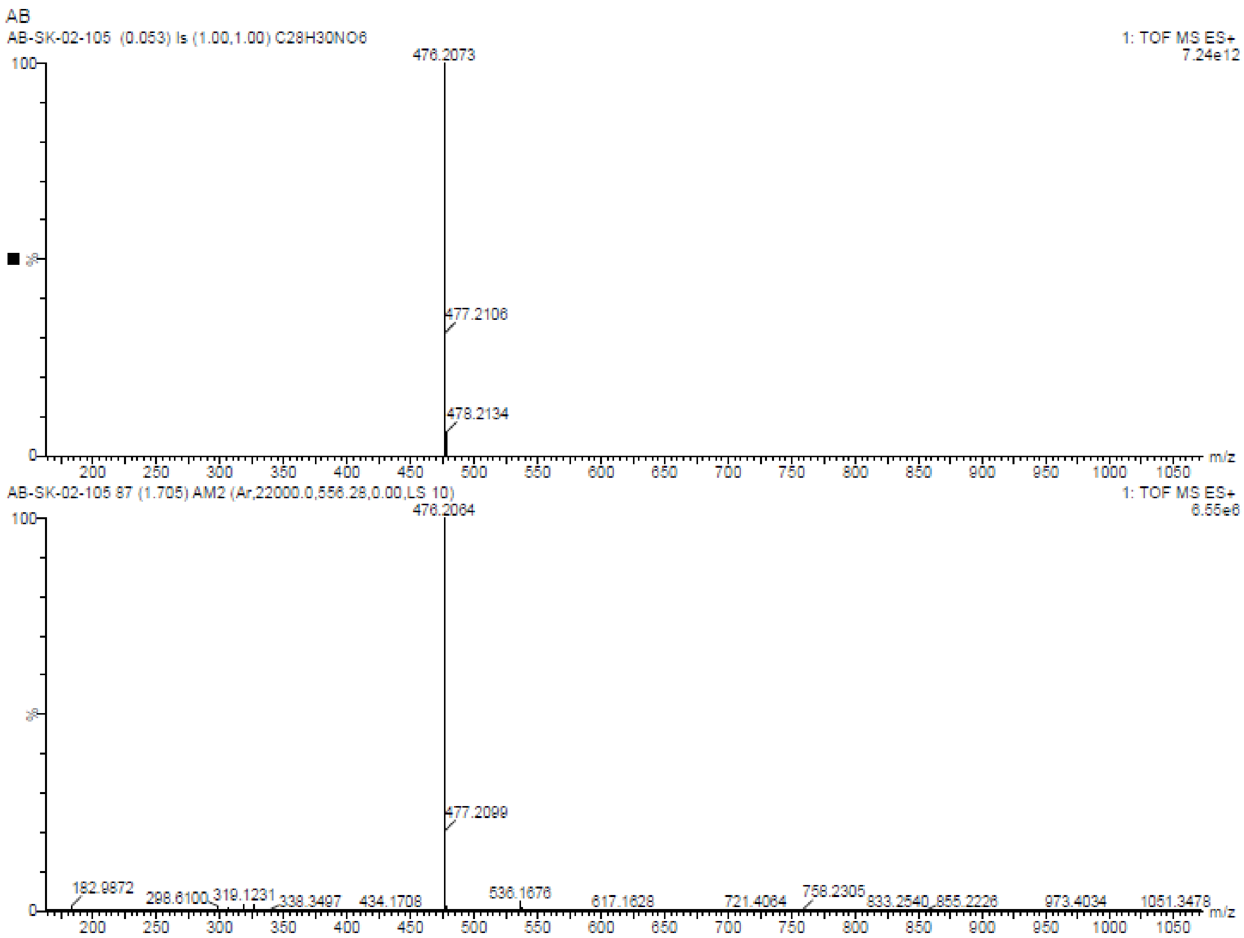


[1]H NMR (500 MHz, $CDCl_3$) of compound (+)-**25’**

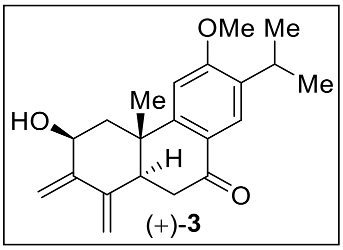


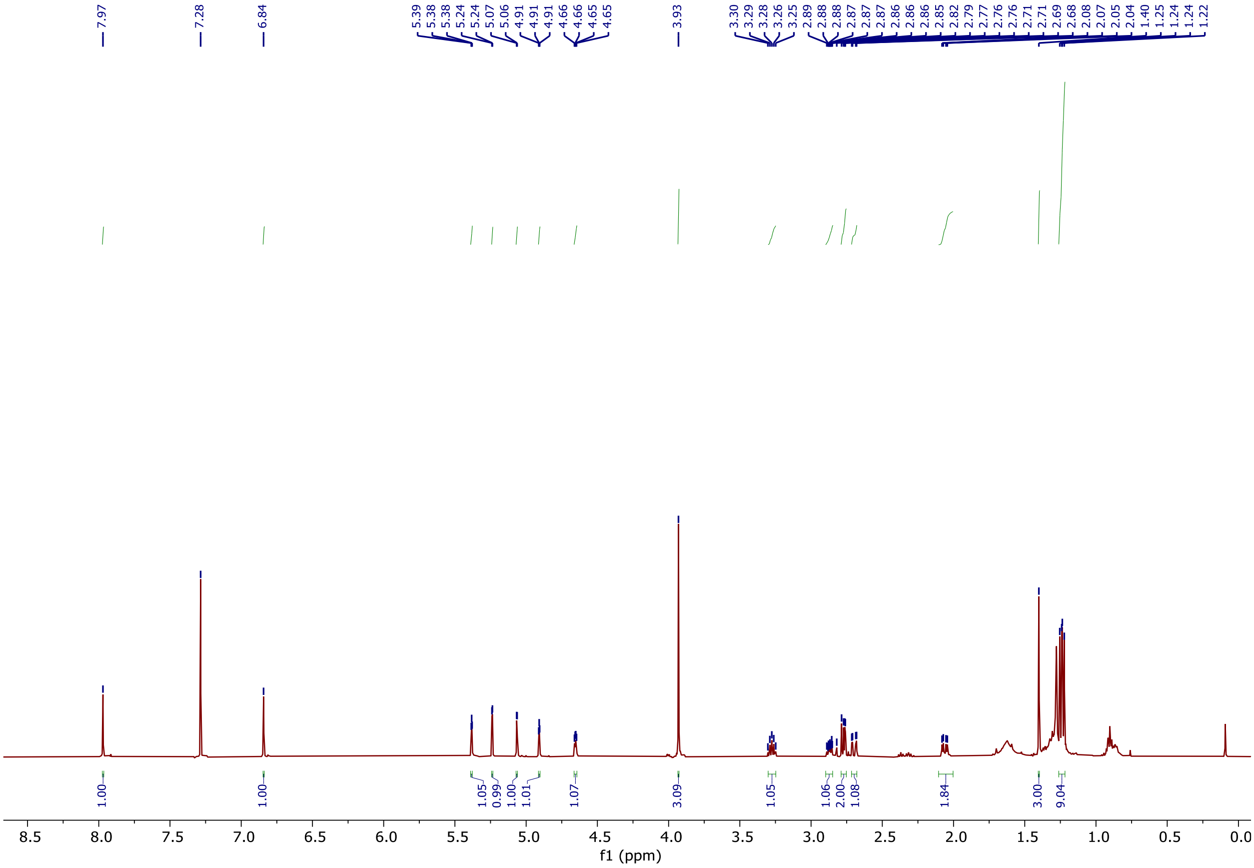




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**25'**

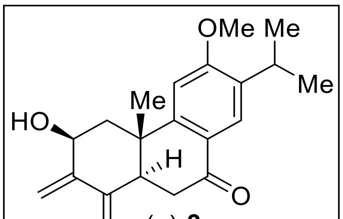


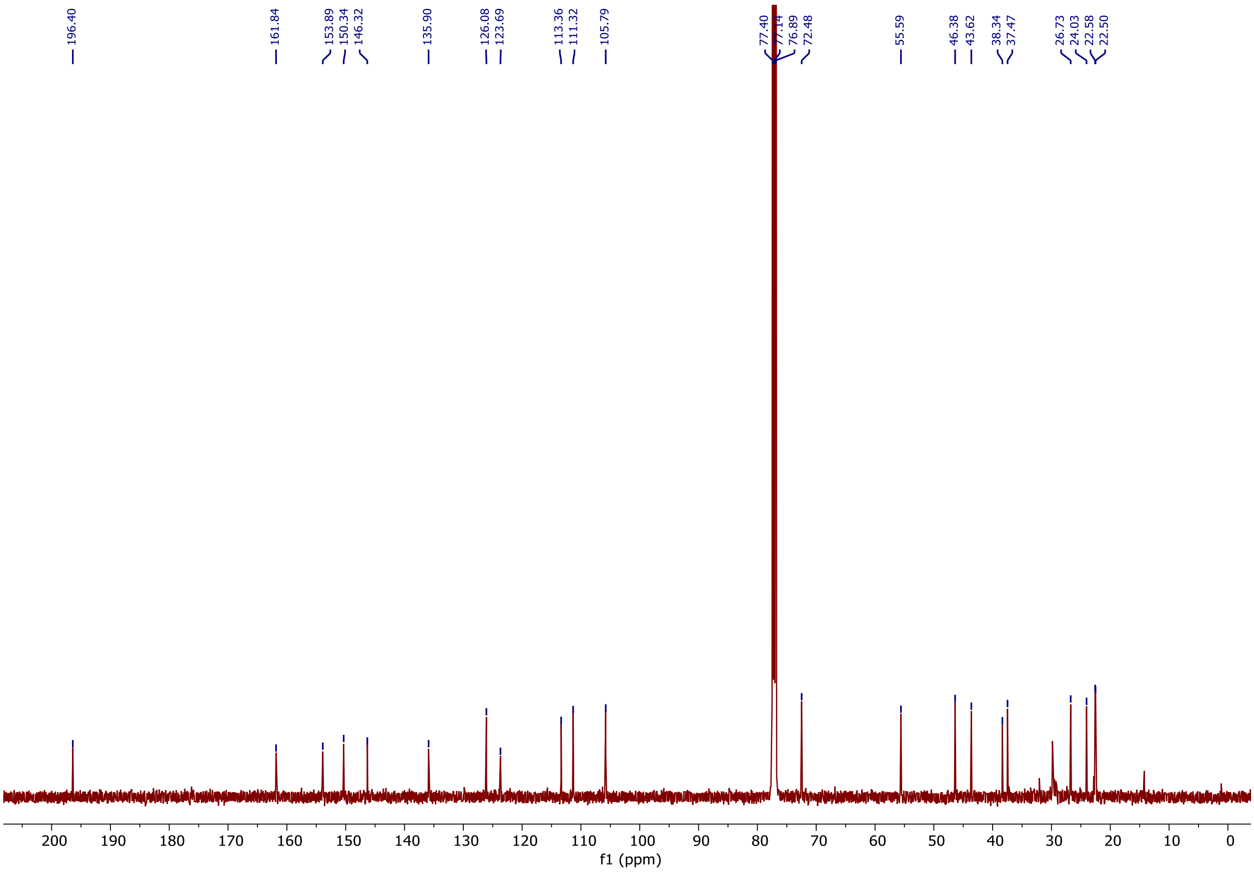

HRMS data of (+)-**25’**



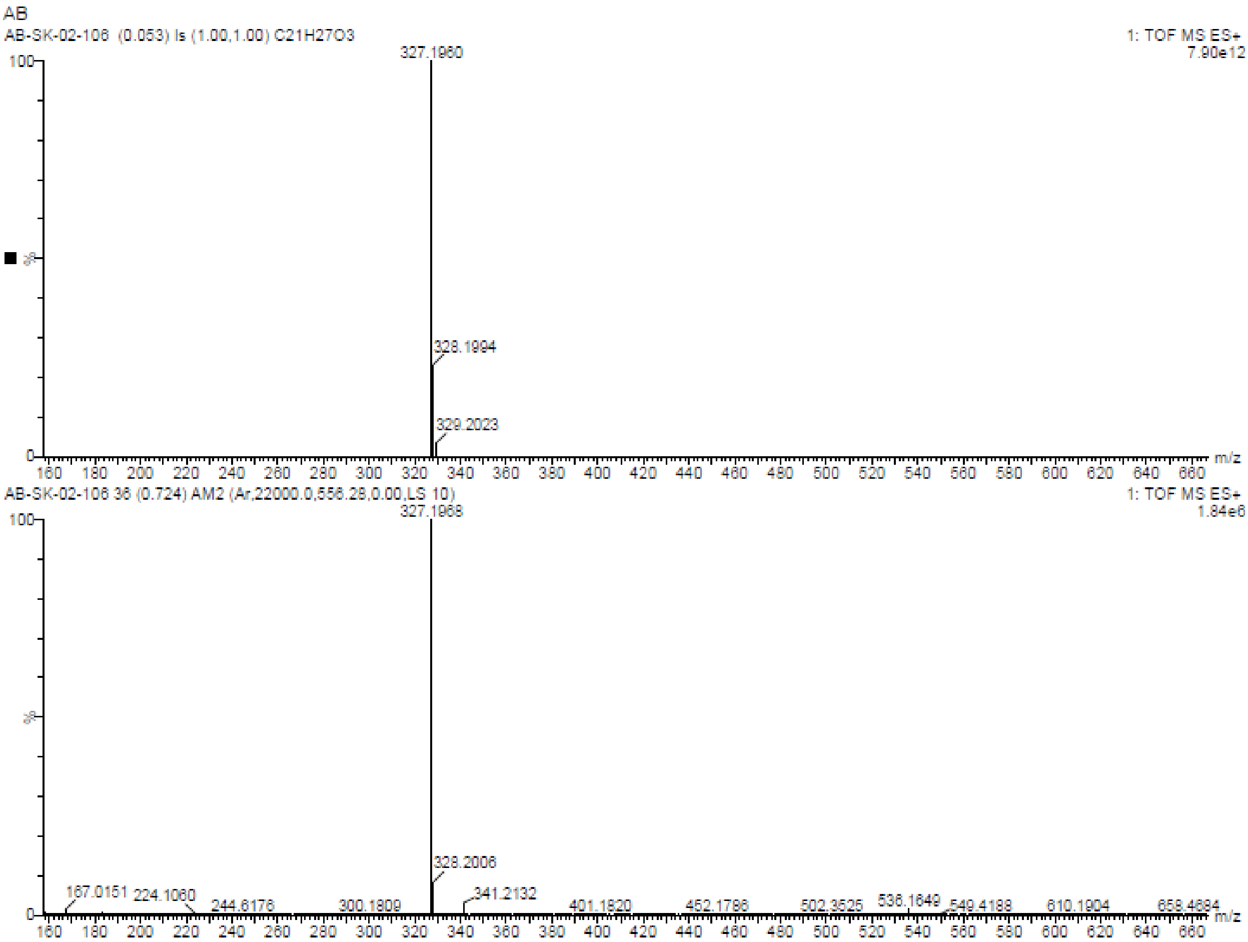


$^{1}$H NMR (500 MHz, $CDCl_3$) of compound (+)-**3**

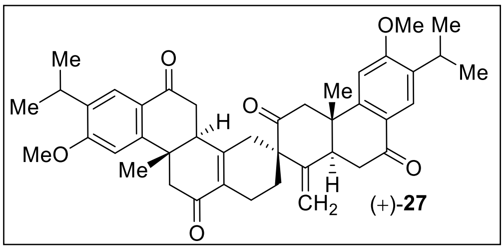

(+)-**3**

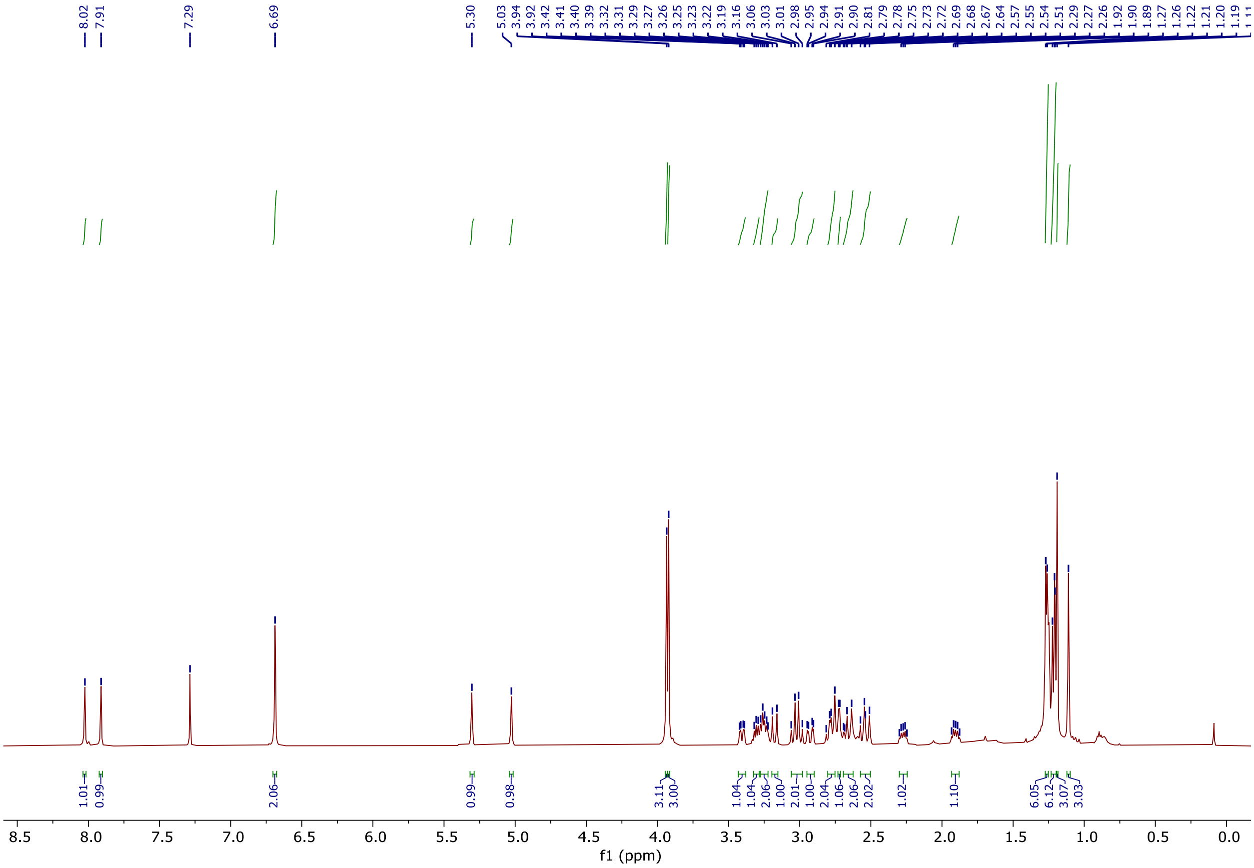



$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**3**

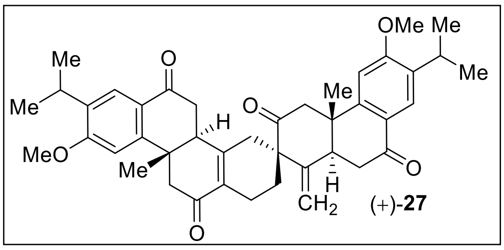


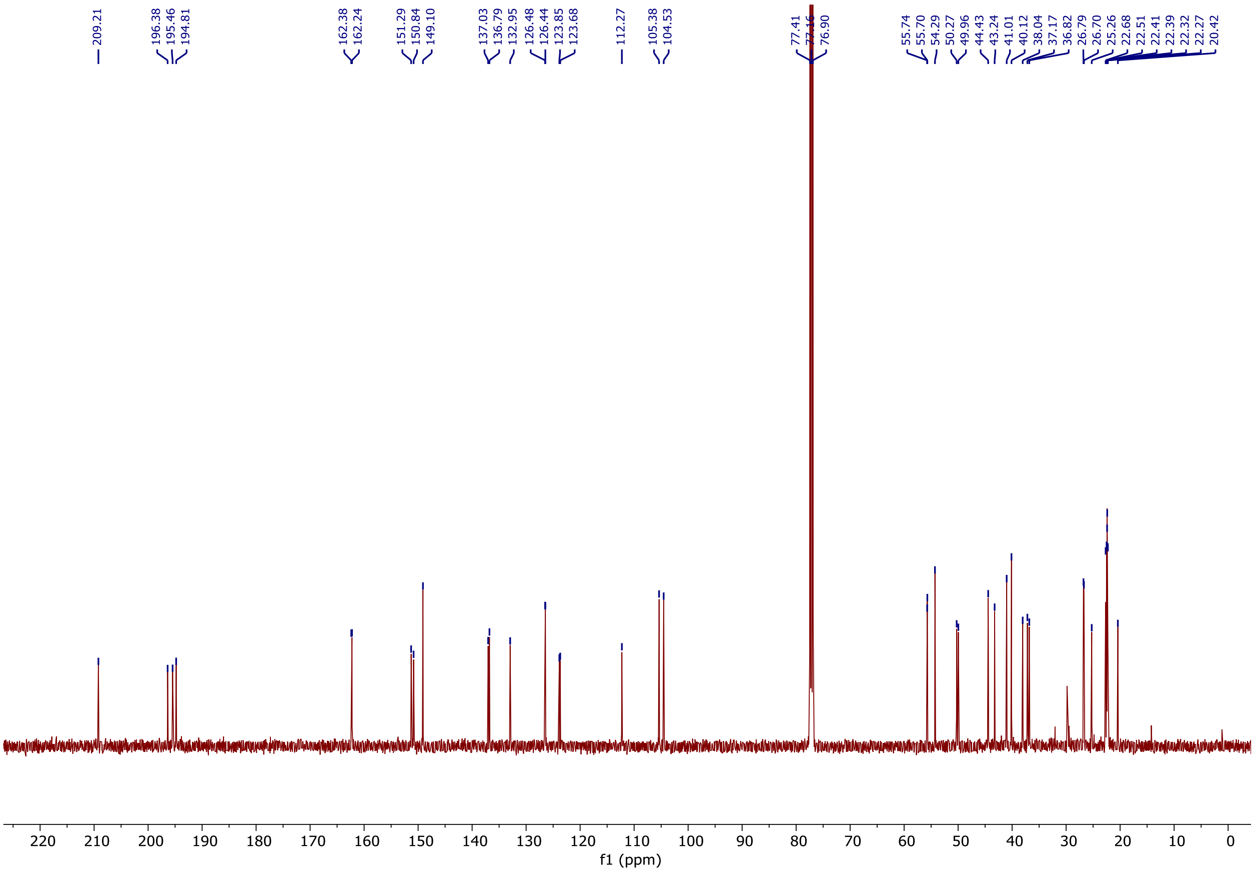

HRMS data of (+)-**3**





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




$^{13}C$ NMR (126 MHz, $CDCl_3$) of compound (+)-**27**

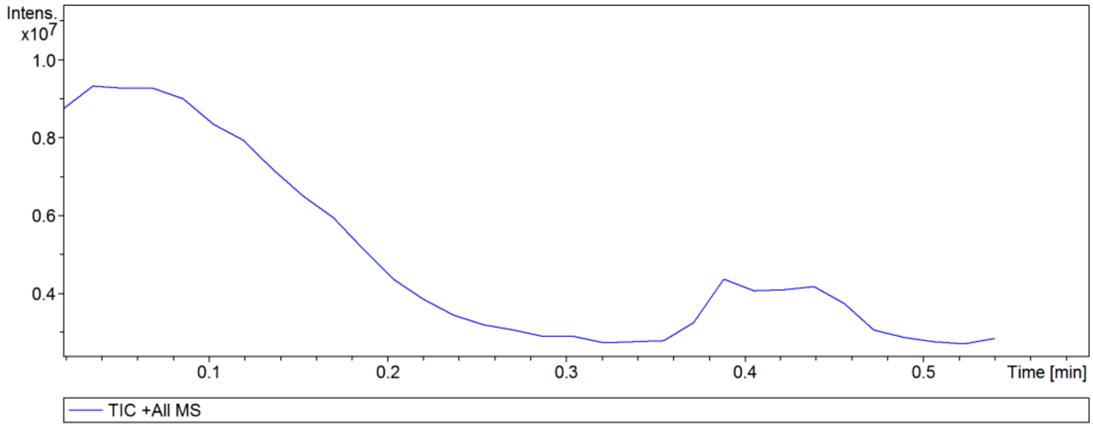
# Display Report

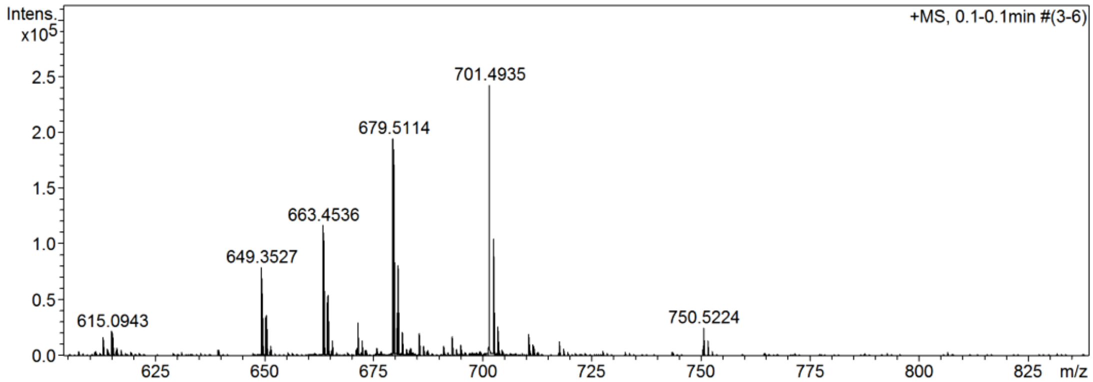
**Analysis Info**

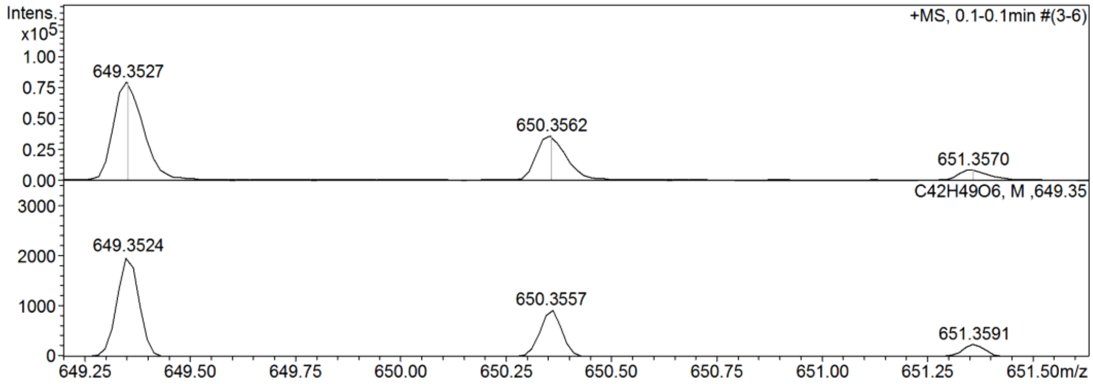
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\USER DATA 2022\JULY2022\05-07-22\Dr.A.Bisai-ABSK0284SP.d | Acquisition Date | 05-07-2022 16:11:23 |
| Method | tune mix_low.New.021117.m | Operator | Bruker |
| Sample Name | ABSK0284SP | Instrument | micrOTOF-Q 10330 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Not active | Set Capillary | 4600 V | Set Dry Heater | 180 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 3000 m/z | Set Collision Cell RF | 100.0 Vpp | Set Divert Valve | Source |

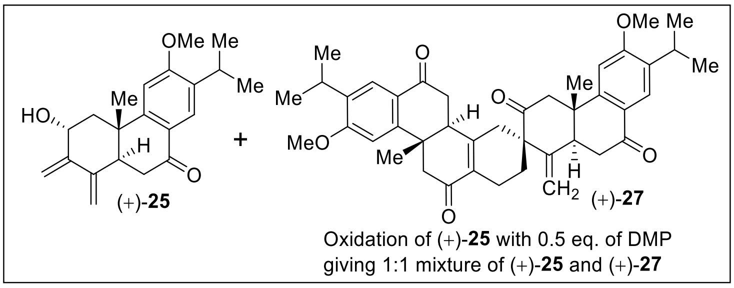


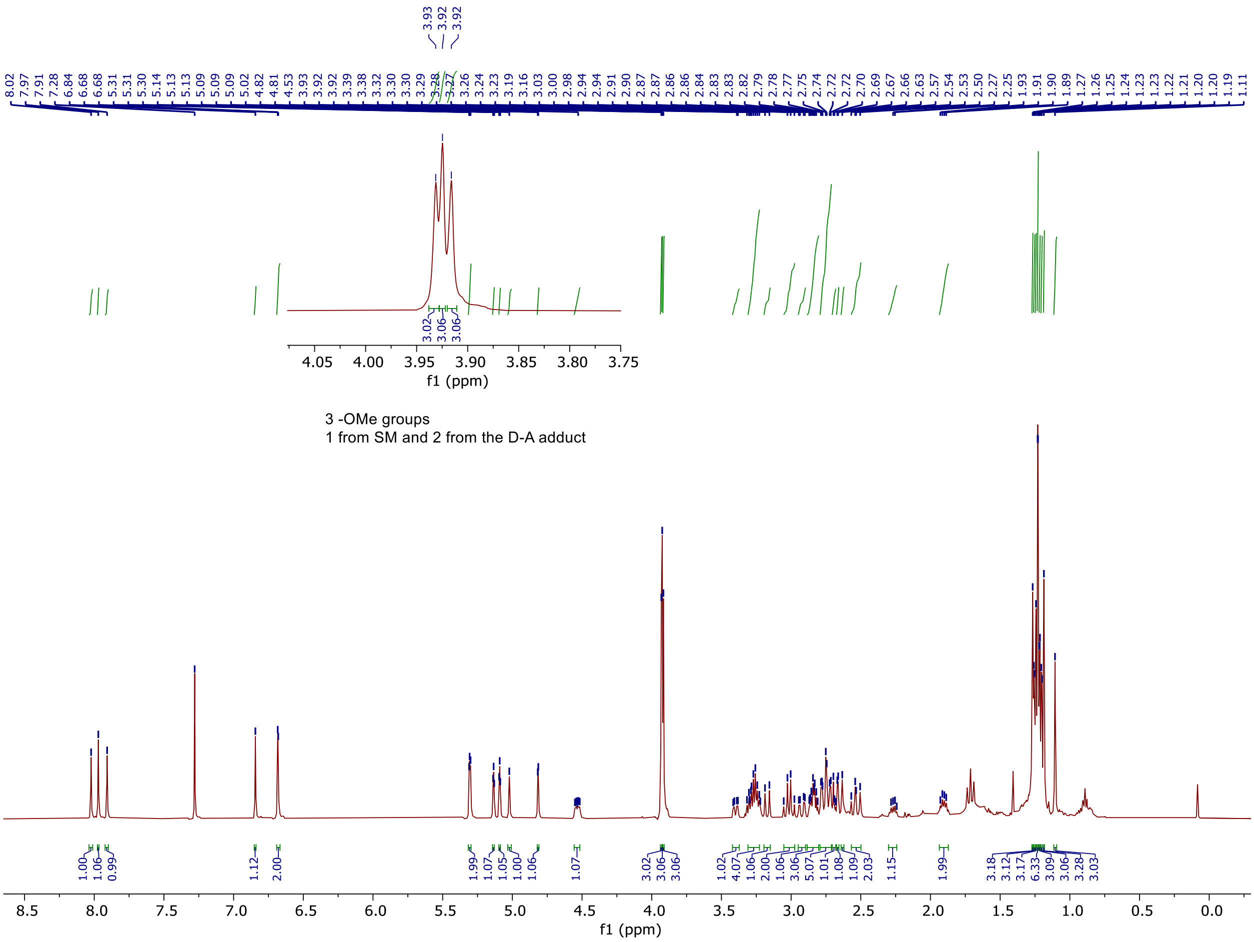



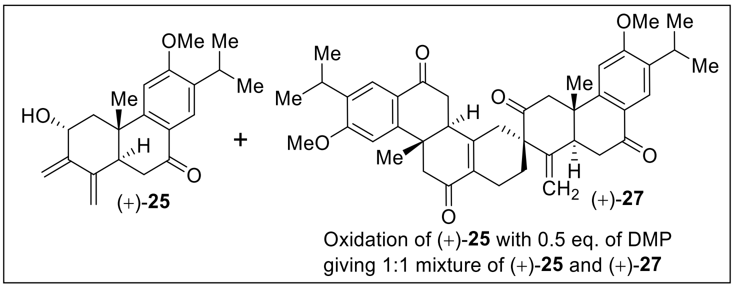


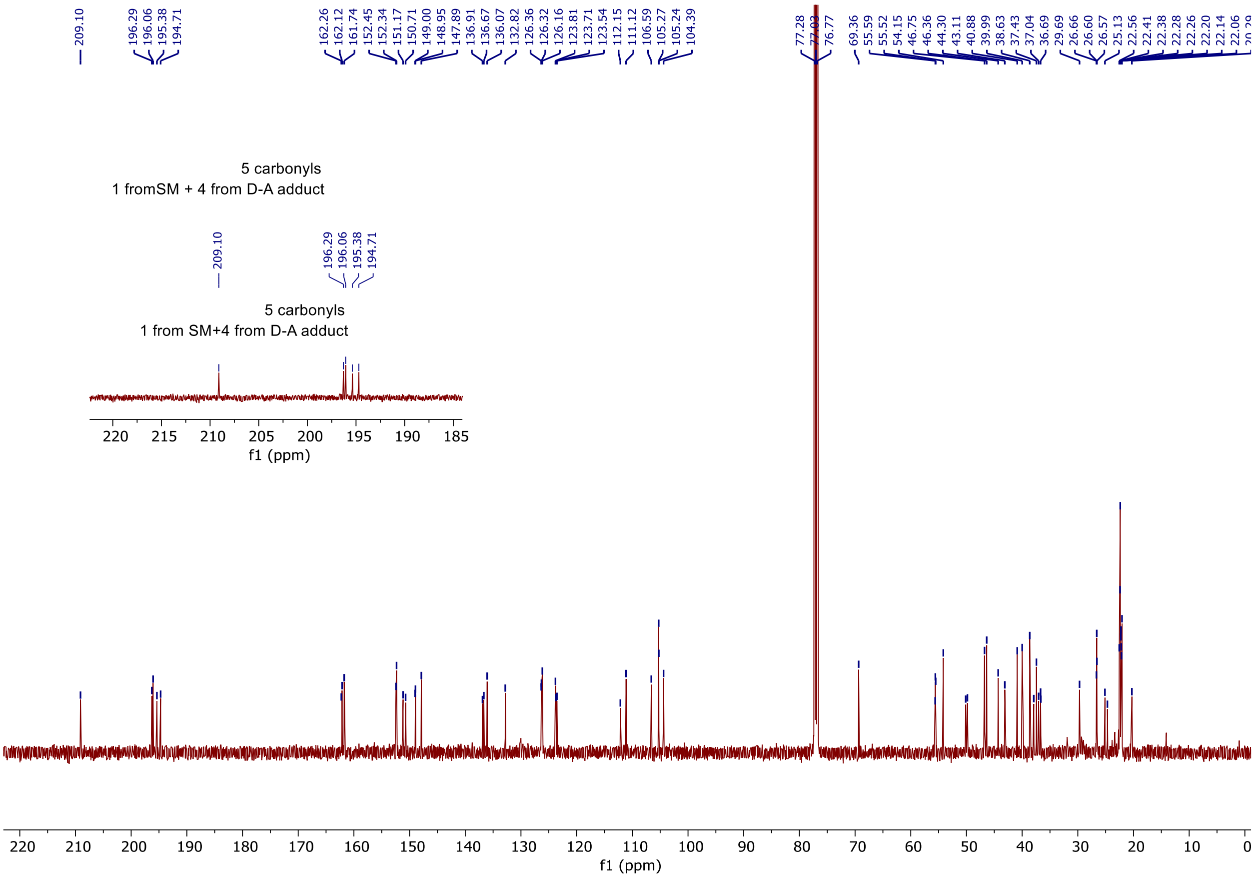

HRMS data of (+)-**27**



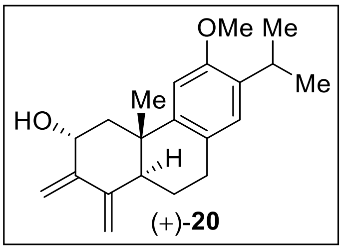



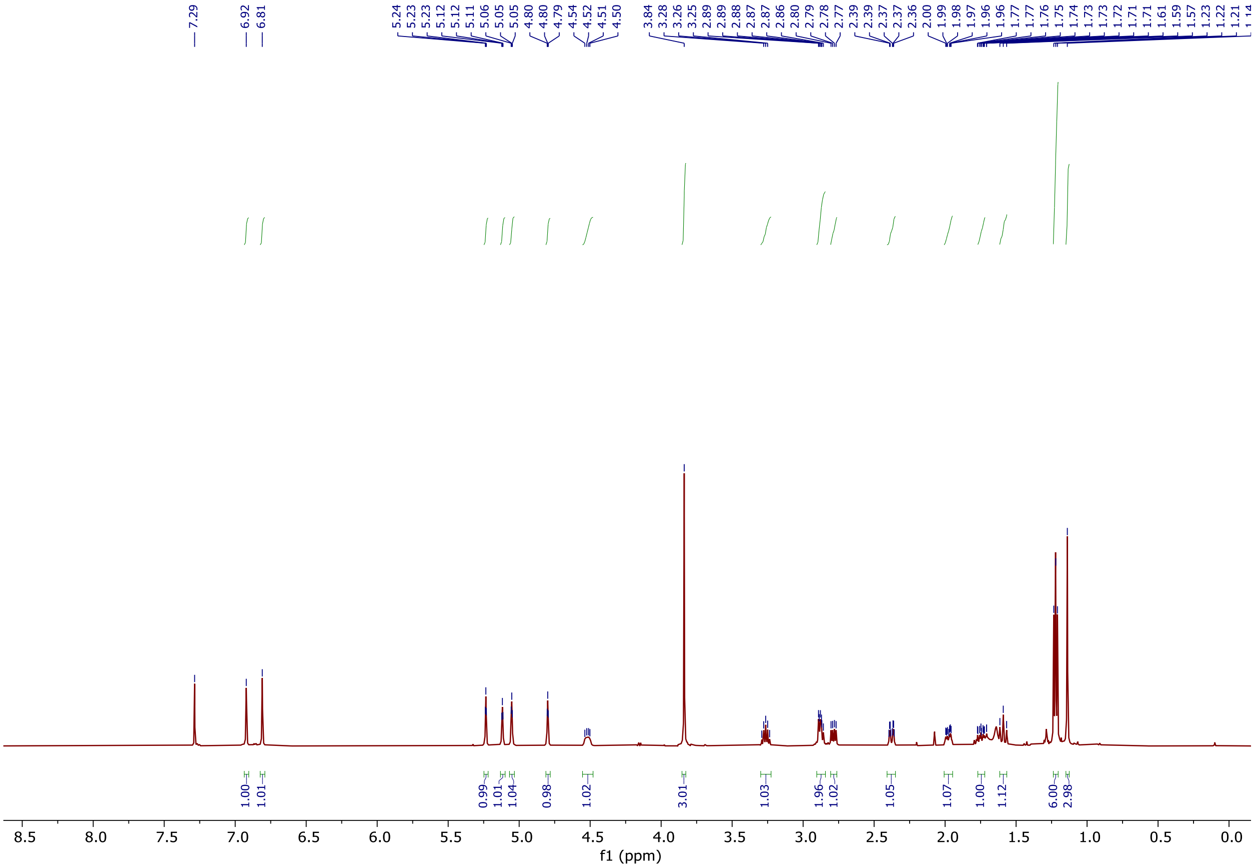

$^1$H NMR (500 MHz, $CDCl_3$) of 1:1 mixture of (+)-**25** and (+)-**27**



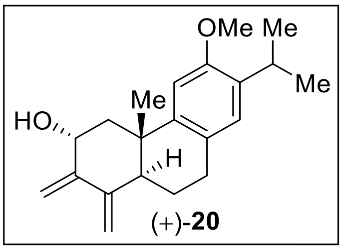



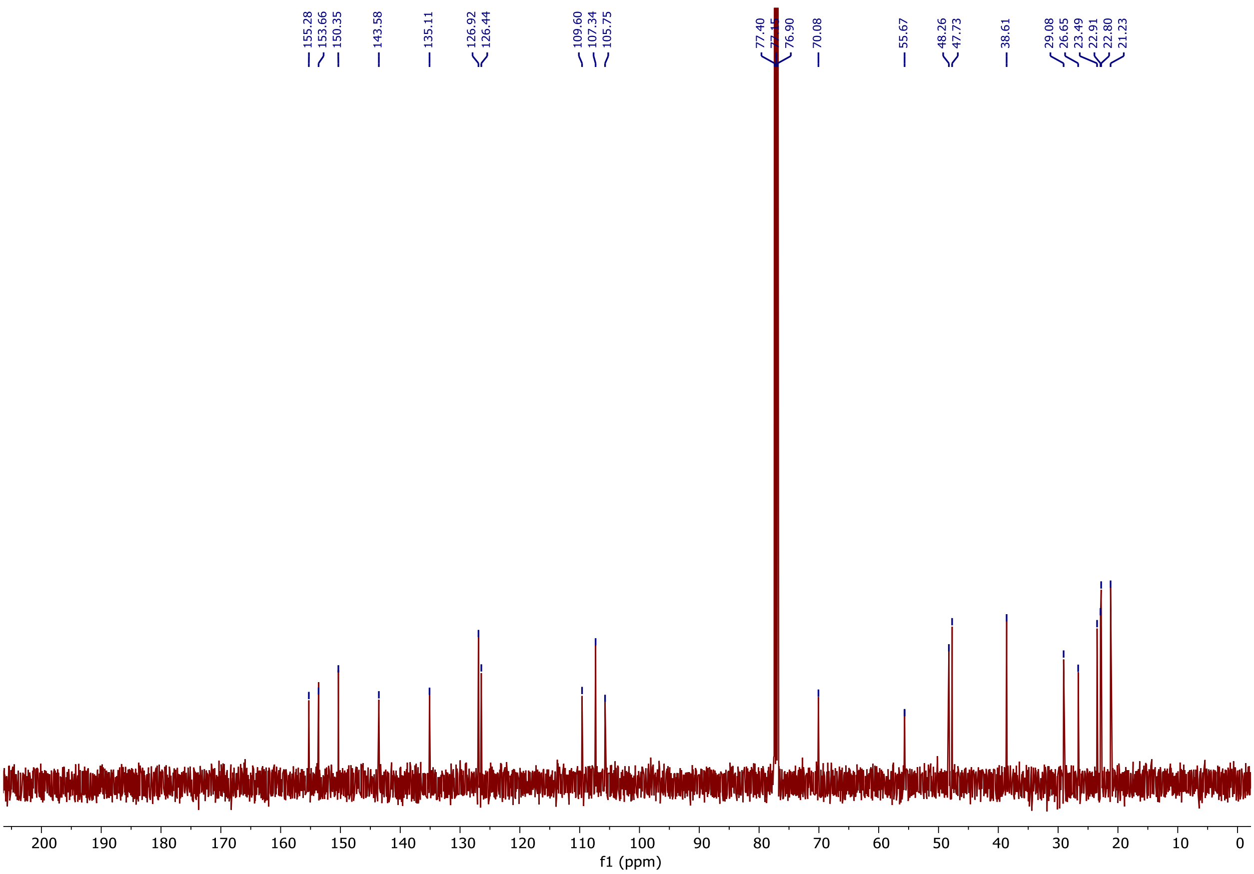

$^{13}$C NMR (126 MHz, $CDCl_3$) of 1:1 mixture of (+)-**25** and (+)-**27**




$^{1}H$ NMR (500 MHz, $CDCl_3$) of compound (+)-**20**





$^{13}C$ NMR (126 MHz, $CDCl_3$) of compound (+)-**20**

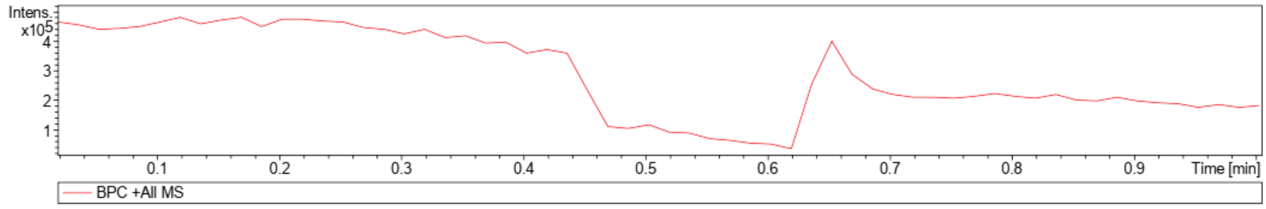
## Display Report

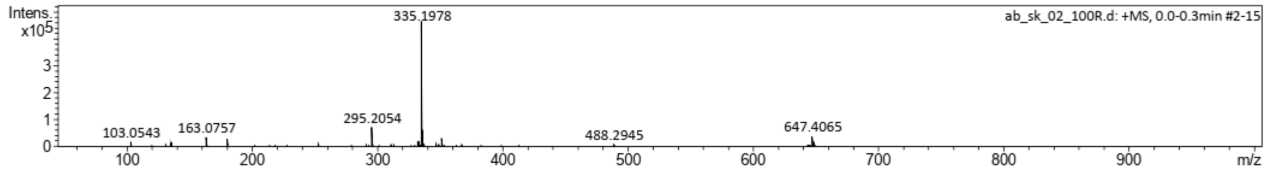
**Analysis Info**

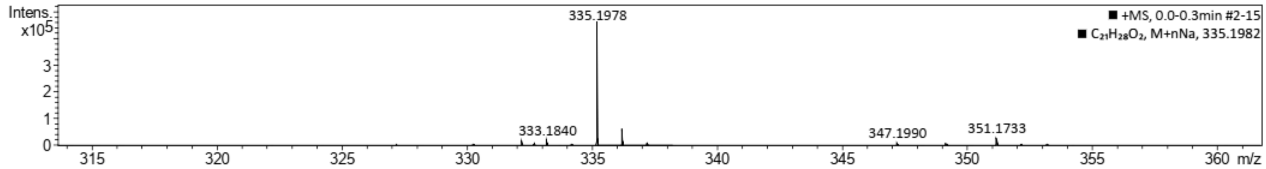
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\User data\2022\OCT\ab_sk_02_100R.d | Acquisition Date | 10/10/2022 11:29:49 AM |
| Method | Tune_pos_Standard_July2022.m | Operator | IISER Kolkata |
| Sample Name | ab_sk_02_100R | Instrument | maXis impact 8282001.00127 |
| Comment | | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 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 | 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 |

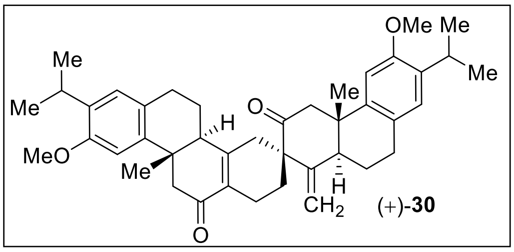


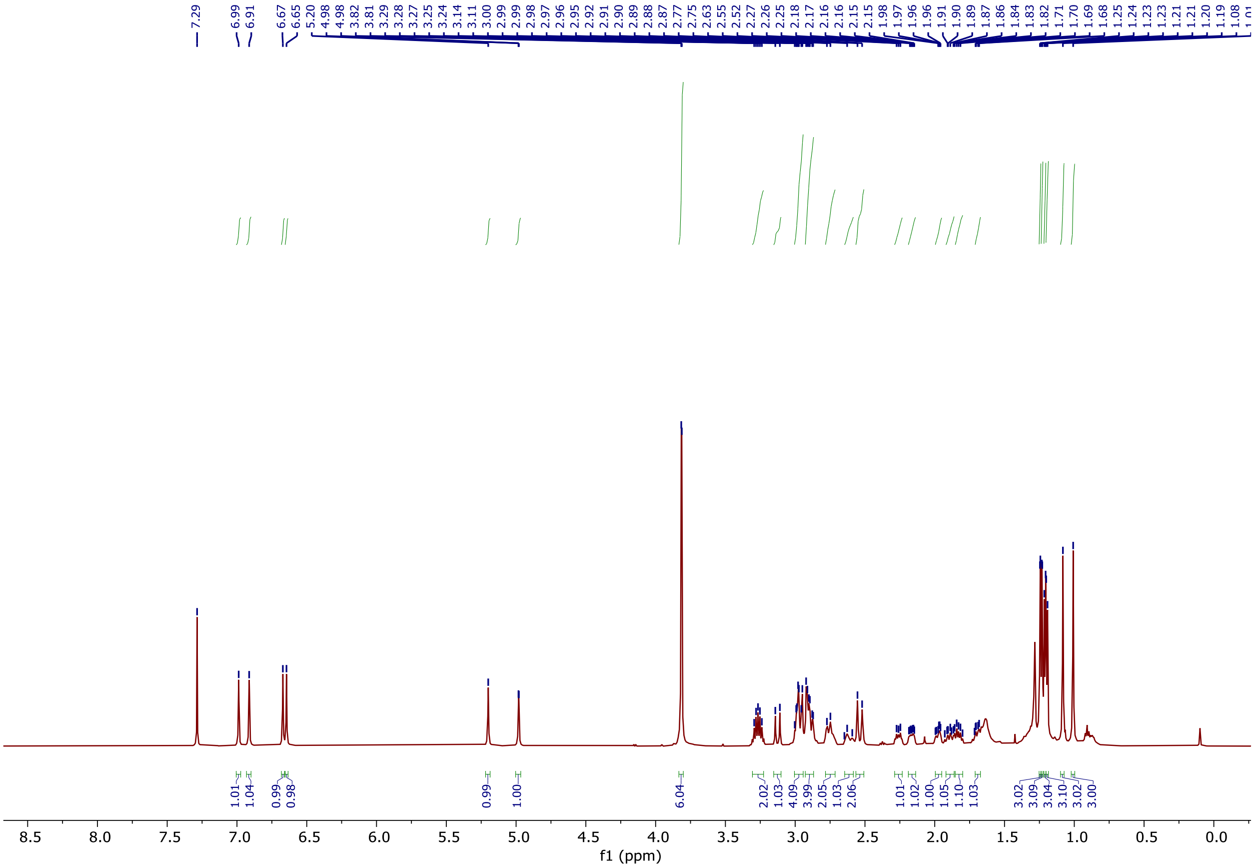



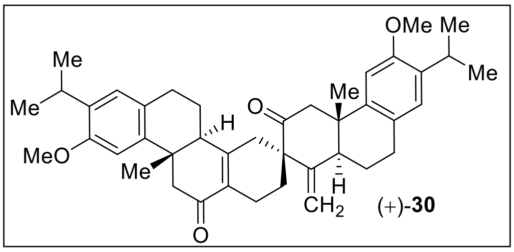


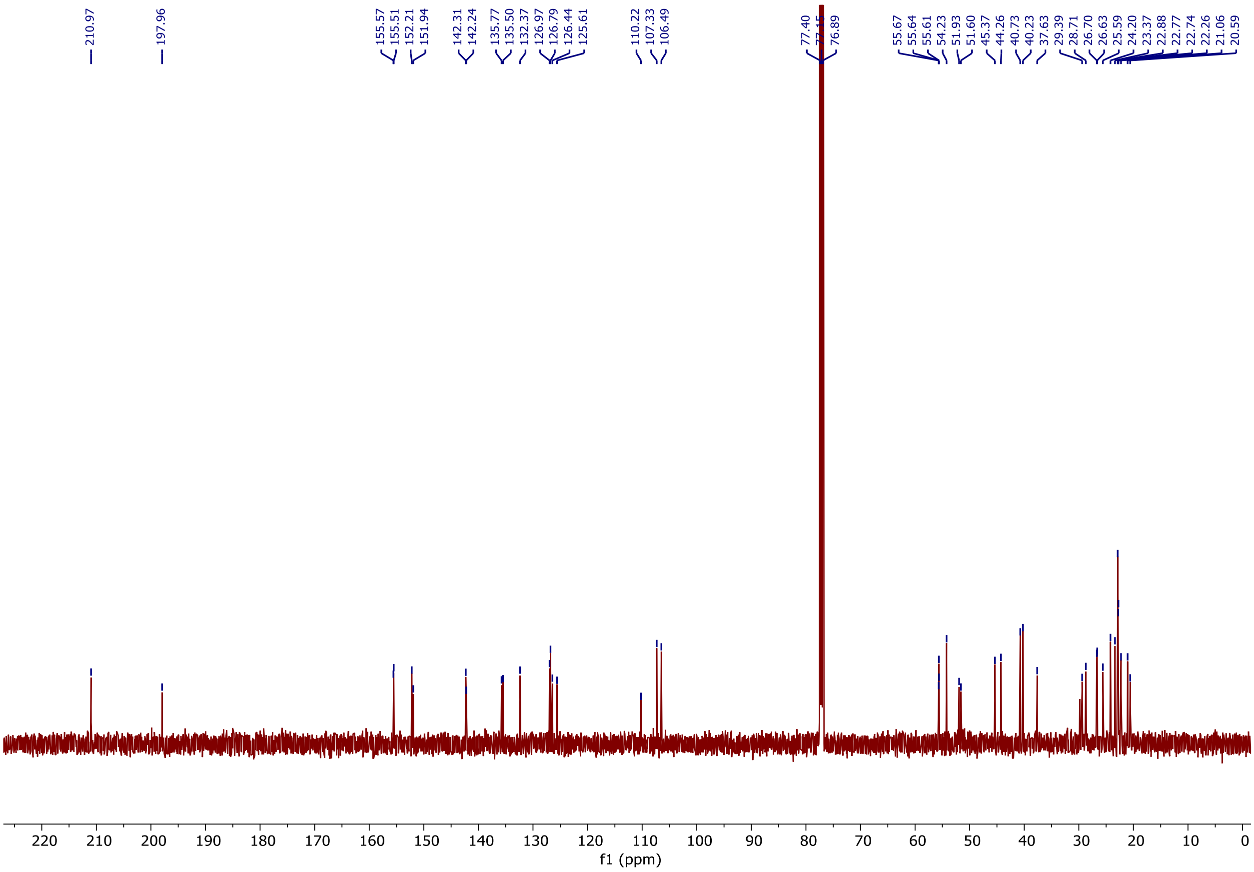

HRMS data of (+)-**20**



$^{1}$H NMR (500 MHz, $CDCl_3$) of compound (+)-**30**



$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**30**

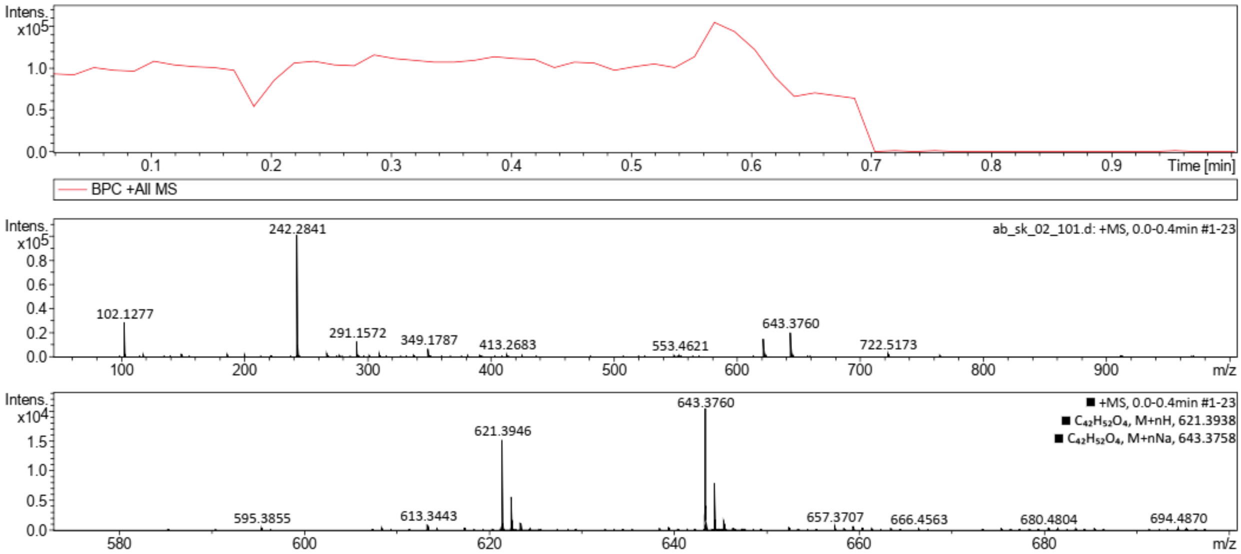
# Display Report

**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\User data\2022\SEPT\ab_sk_02_101.d | Acquisition Date | 10/10/2022 10:58:45 AM |
| Method | Tune_pos_Standard_July2022.m | Operator | IISER Kolkata |
| Sample Name | ab_sk_02_101 | Instrument | maXis impact 8282001.00127 |
| Comment | | | |

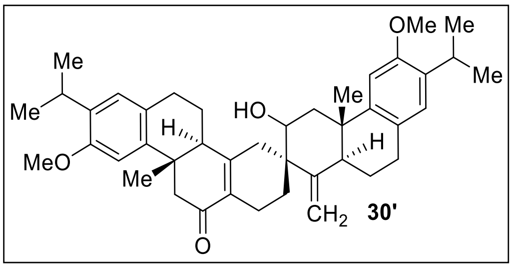
**Acquisition Parameter**

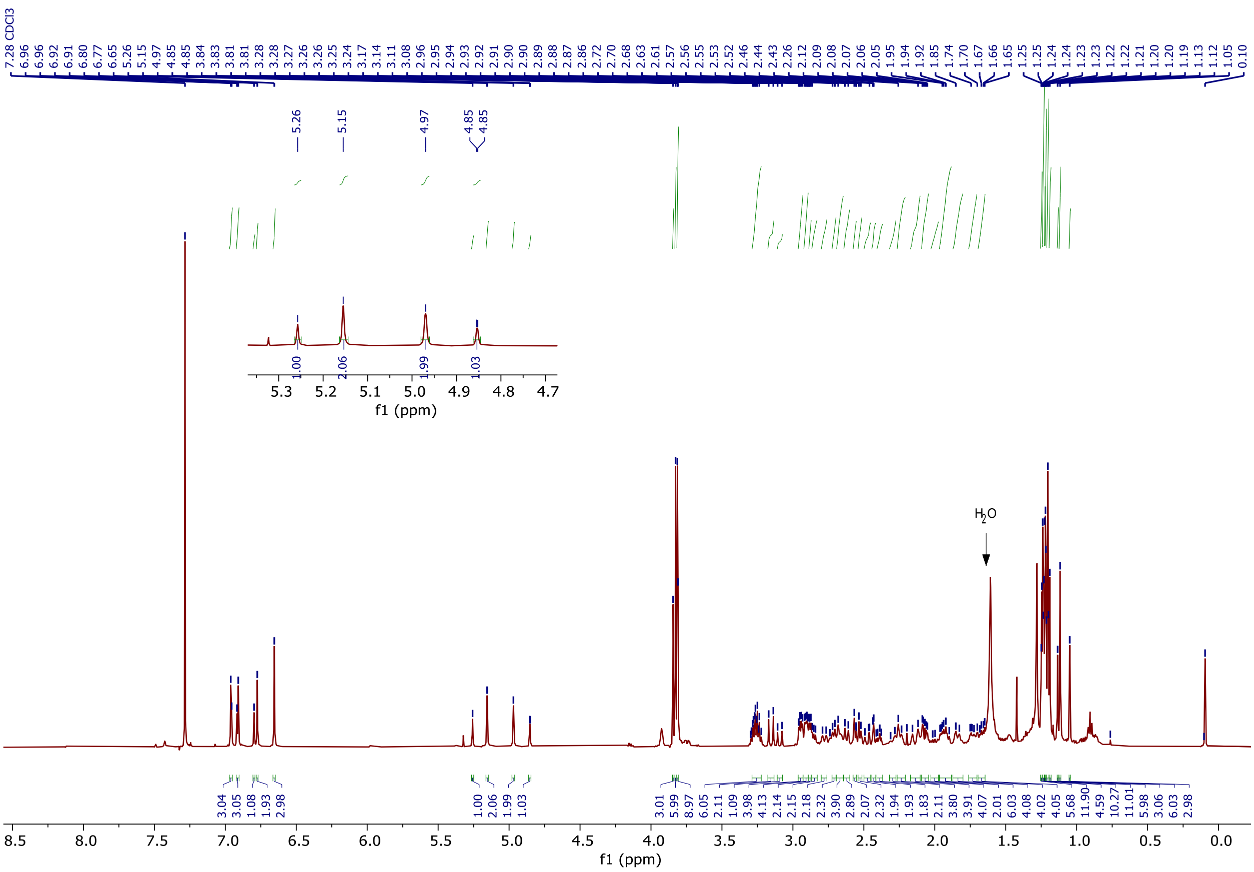
| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4500 V | Set Dry Heater | 200 °C |
| Scan Begin | 50 m/z | Set End Plate Offset | -500 V | Set Dry Gas | 4.0 l/min |
| Scan End | 1000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |



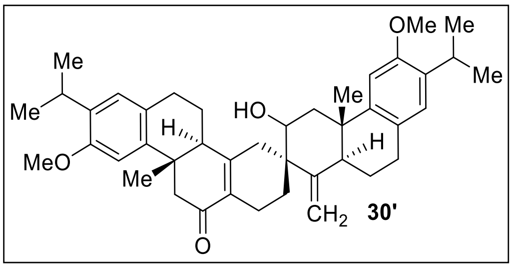


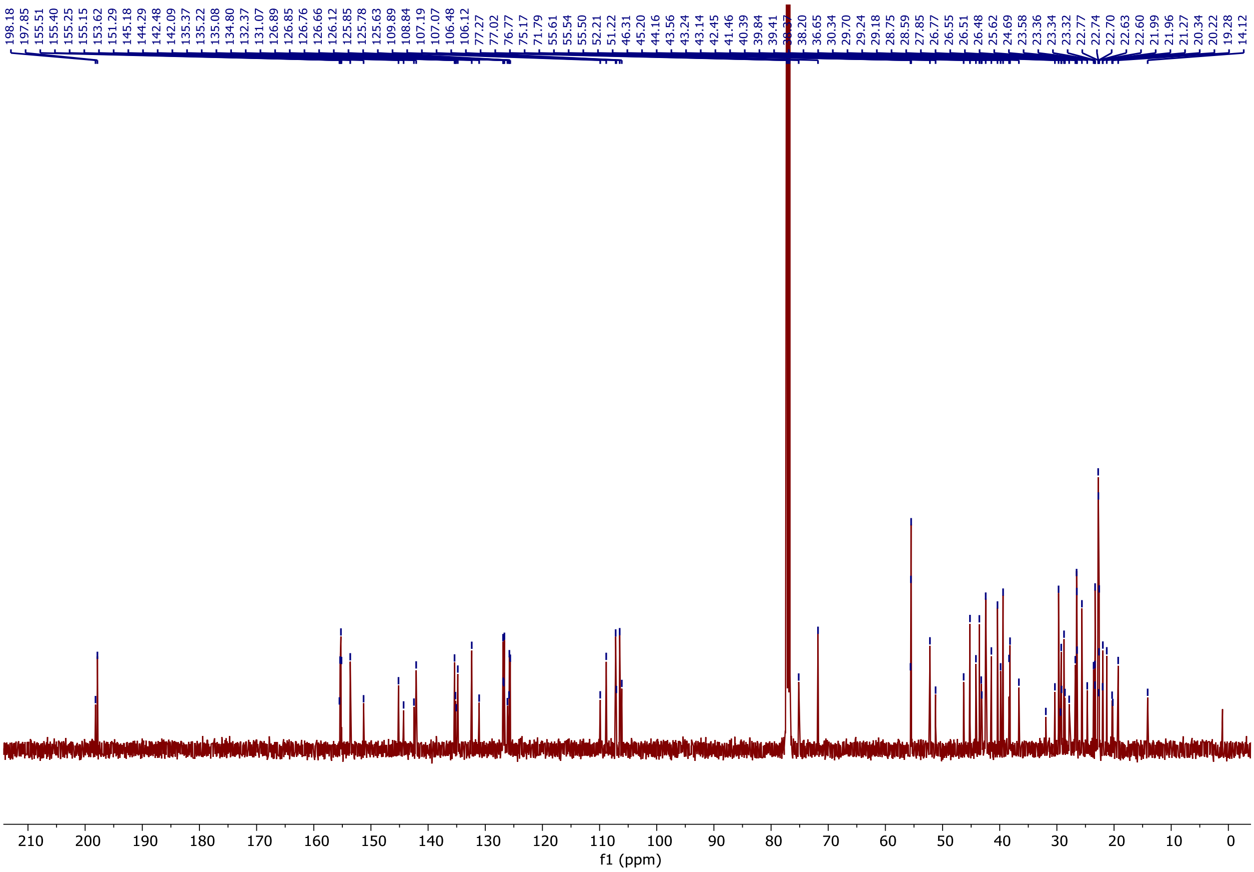

HRMS data of (+)-**30**



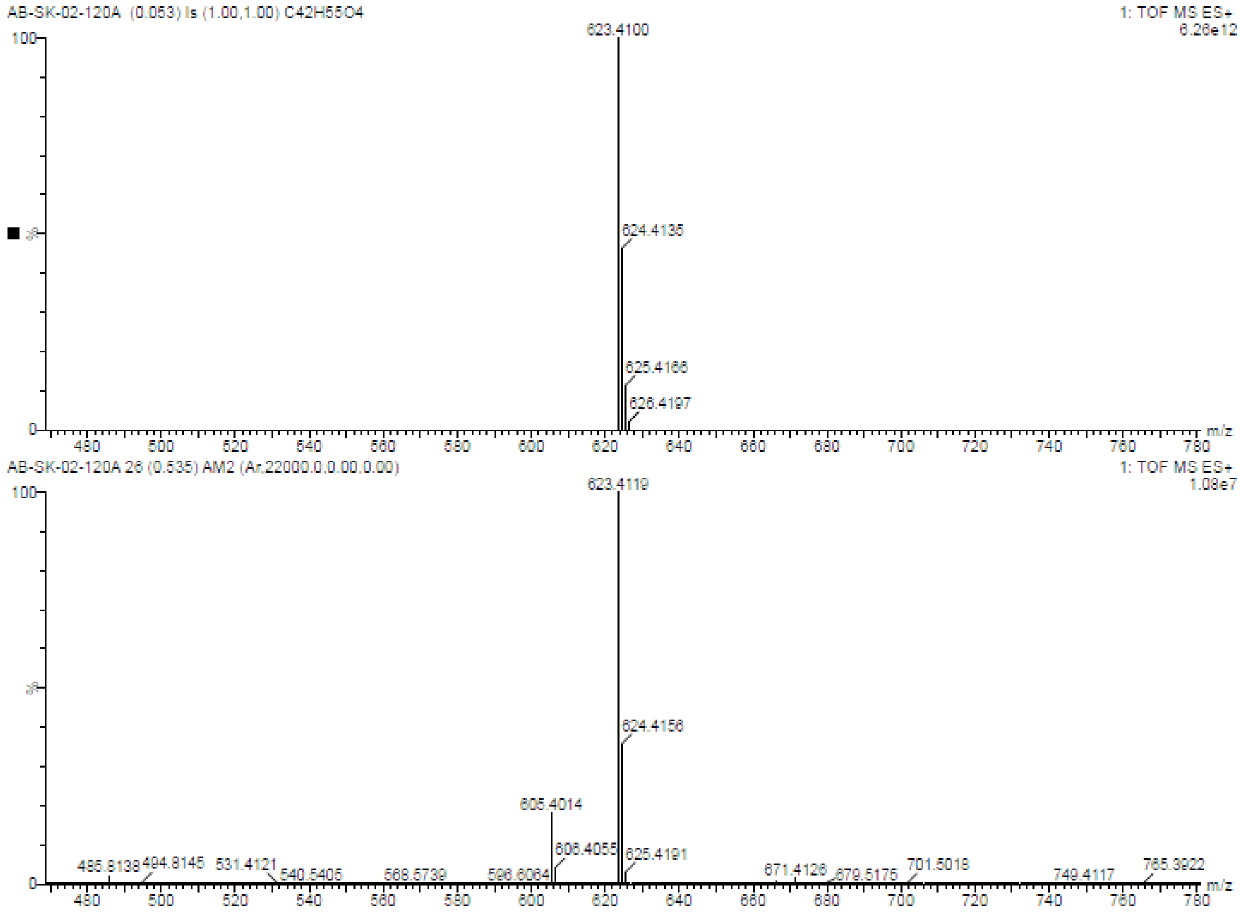



$^{1}$H NMR (500 MHz, $CDCl_3$) inseparable (2:1) diasteromeric mixture of **30'**

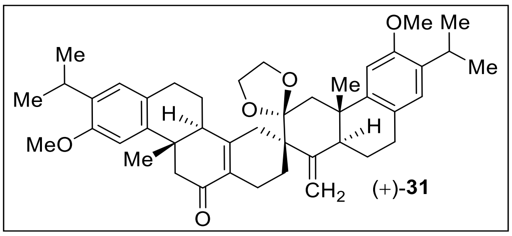


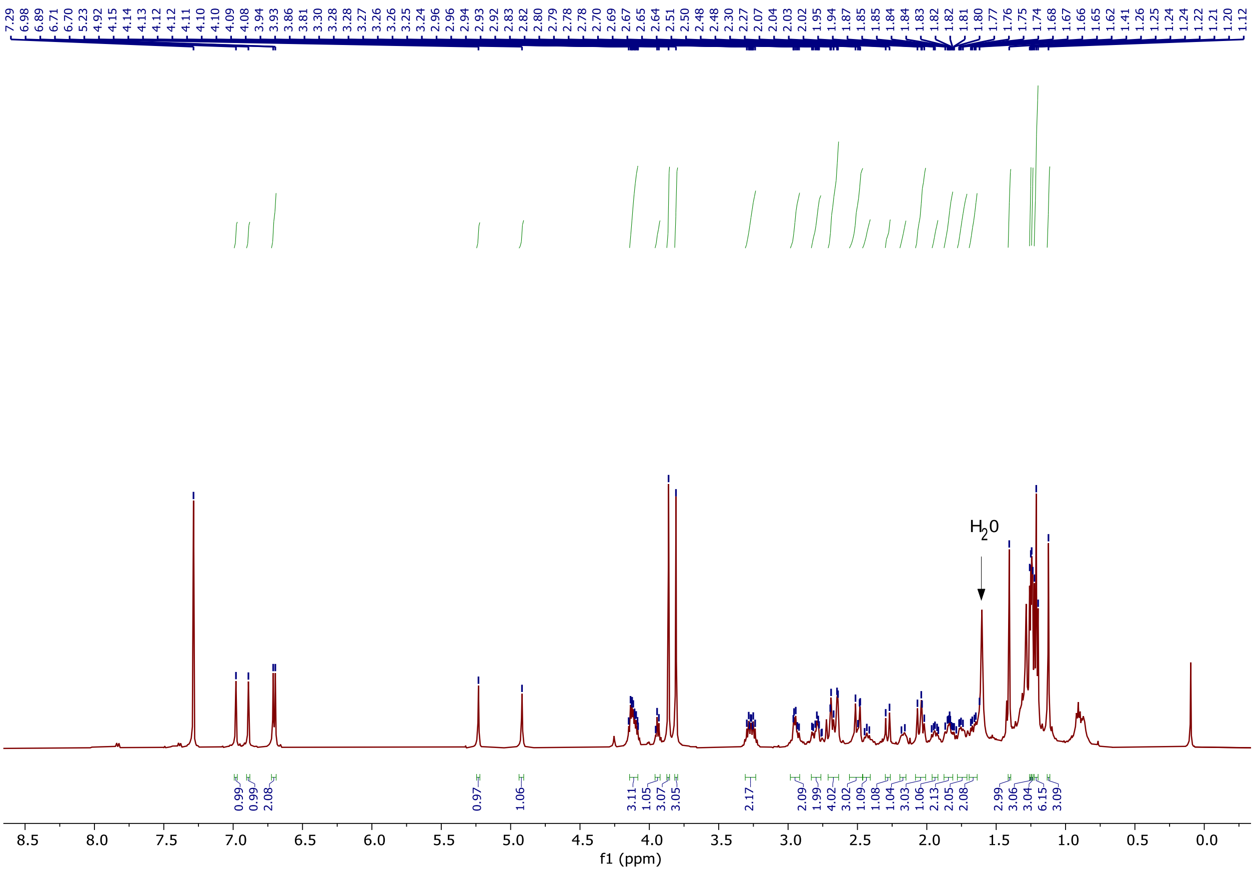


$^{13}C$ NMR (126 MHz, $CDCl_3$) inseparable (2:1) diasteromeric mixture of **30'**

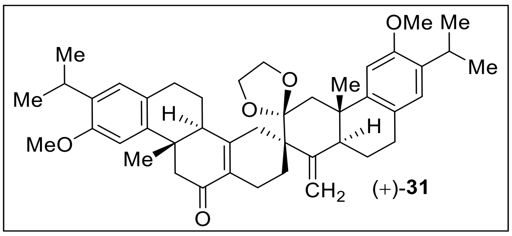


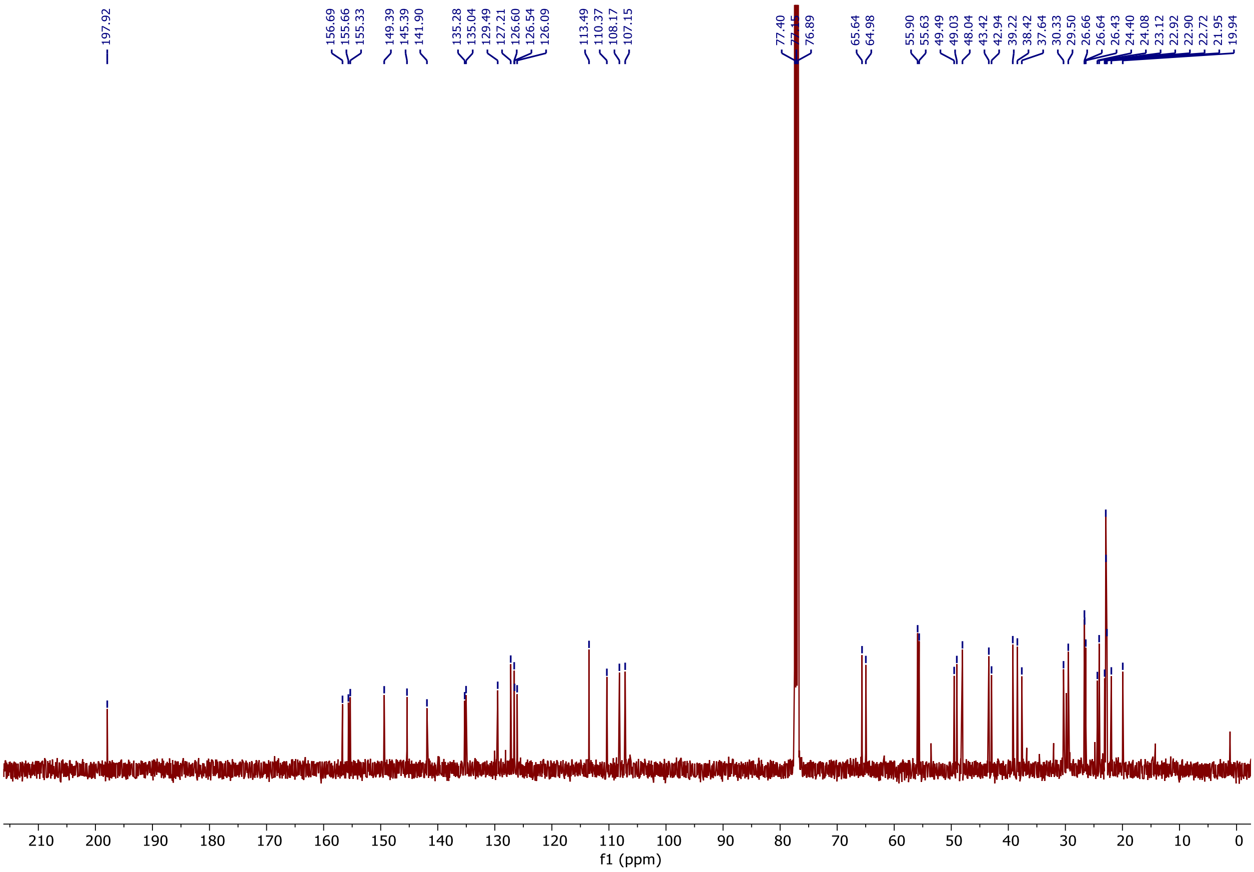

HRMS data of **30’**



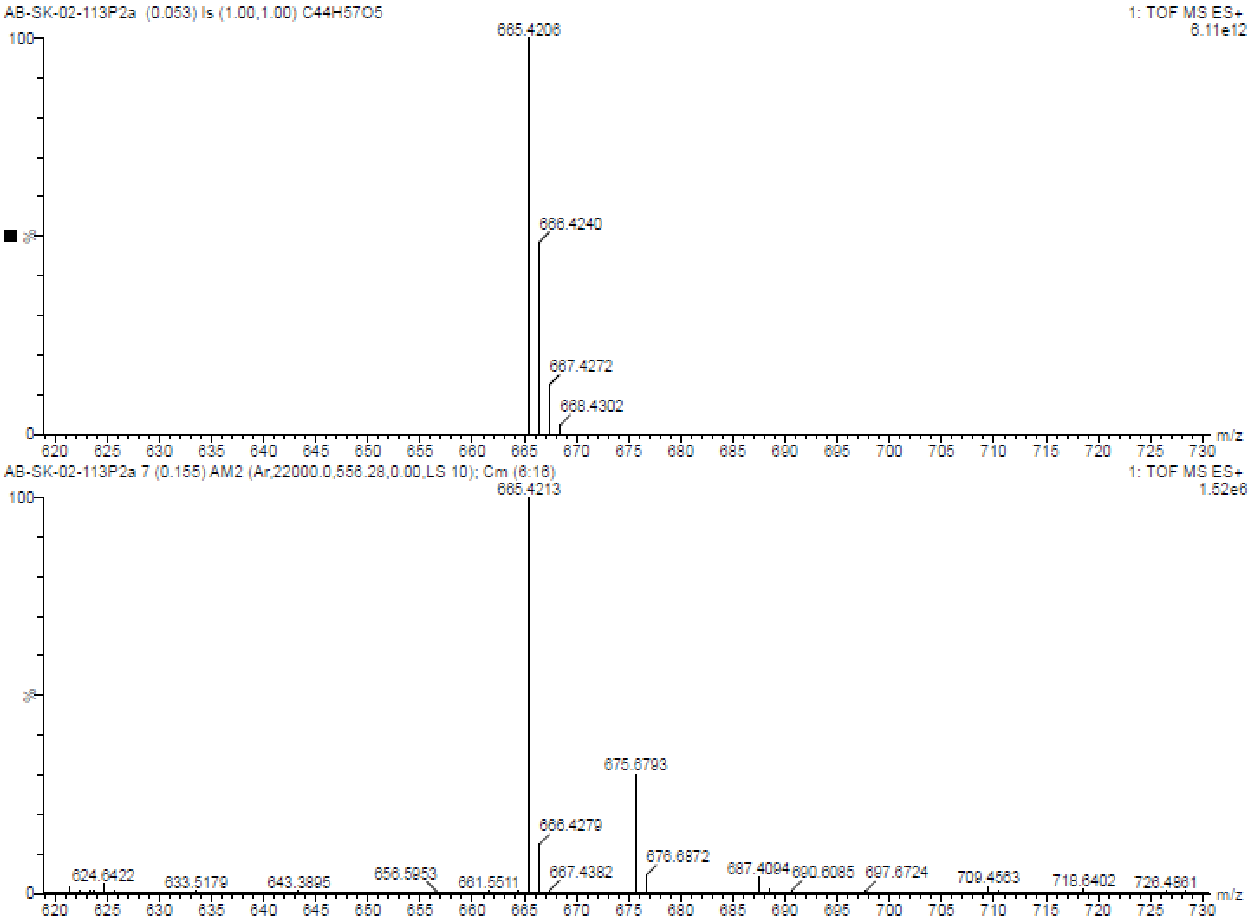


$^{1}H$ NMR (500 MHz, $CDCl_3$) of compound (+)-**31**

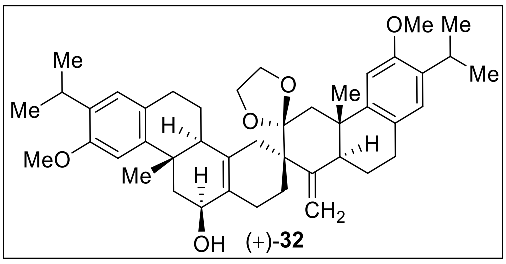


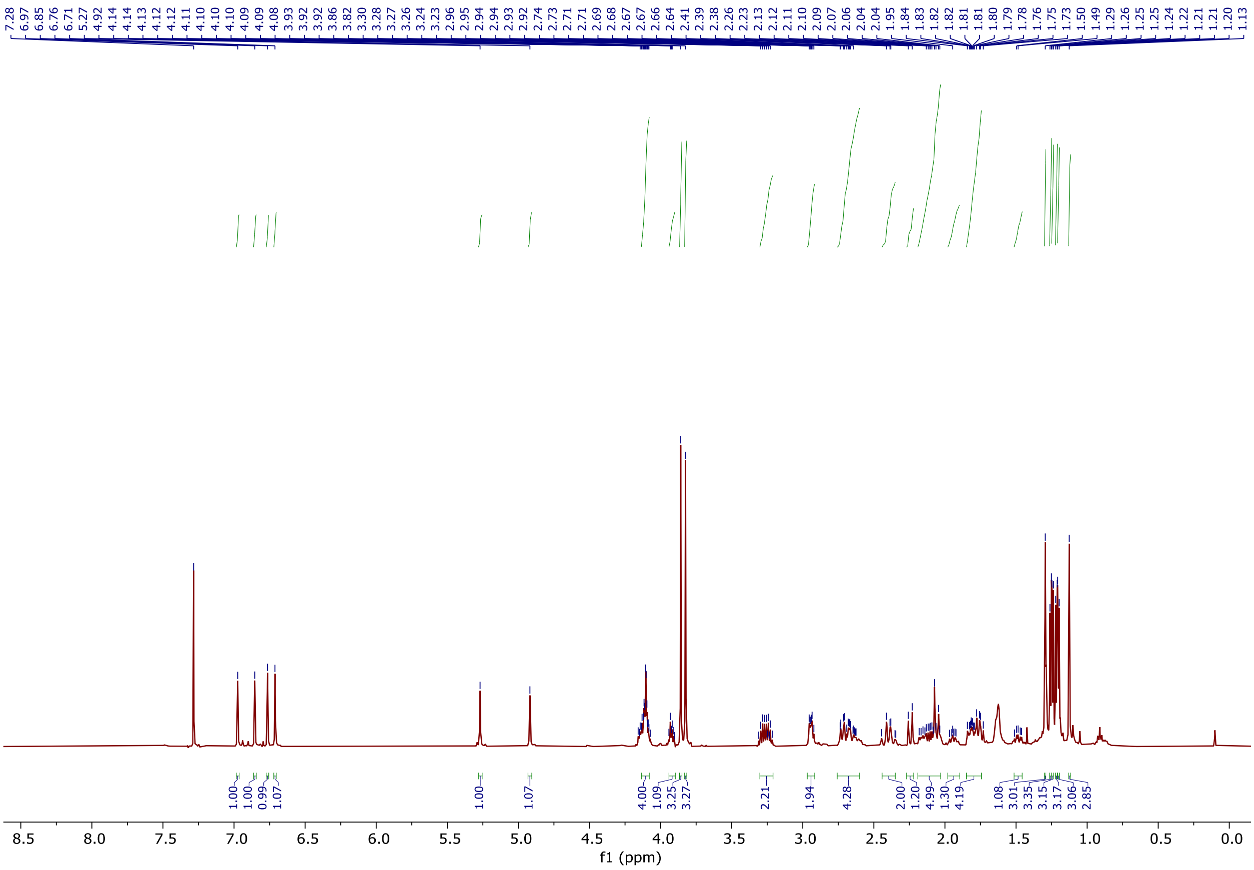


$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**31**

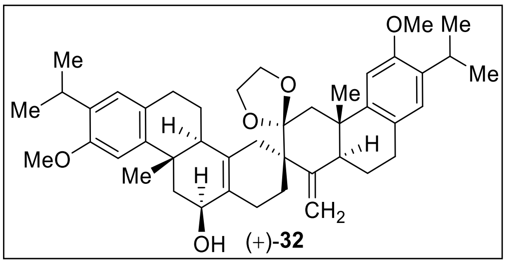


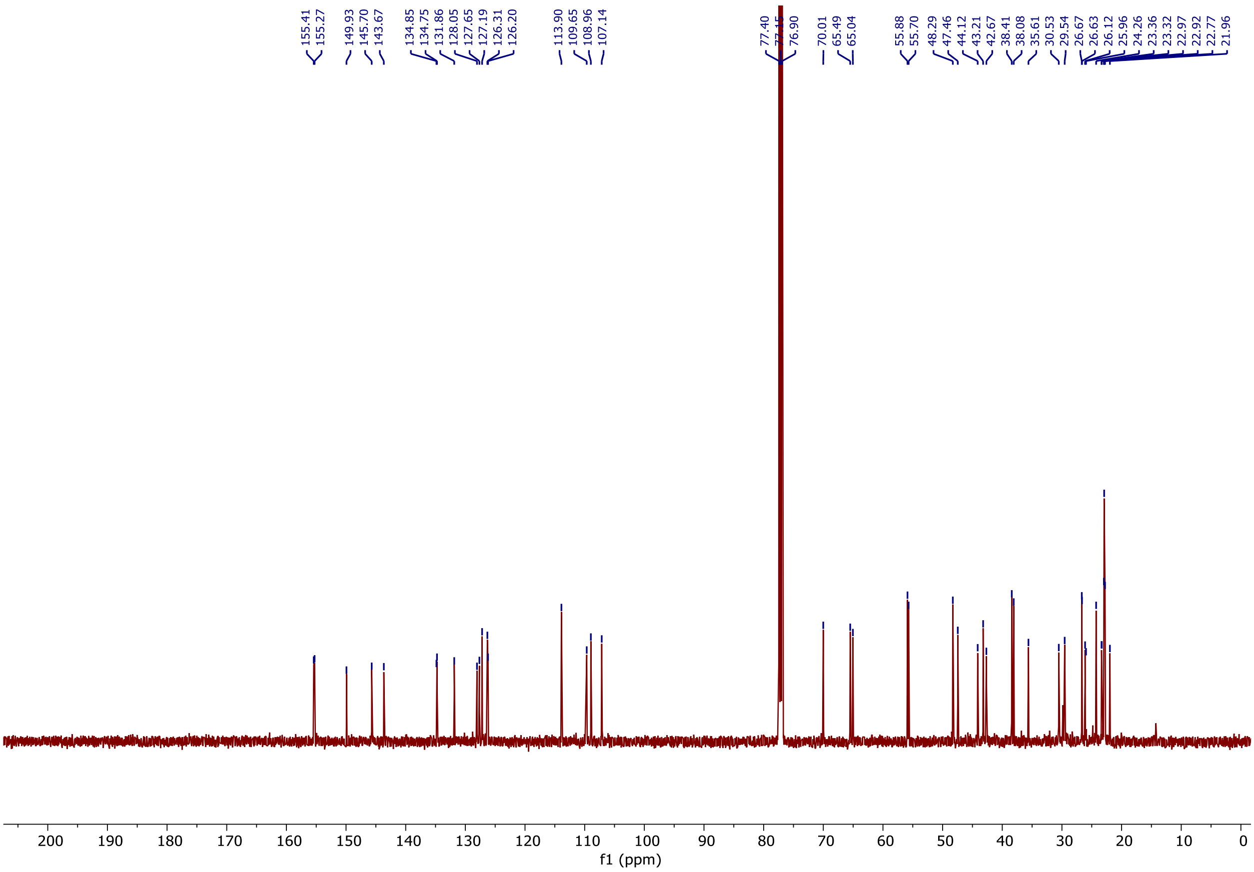

HRMS data of (+)-**31**



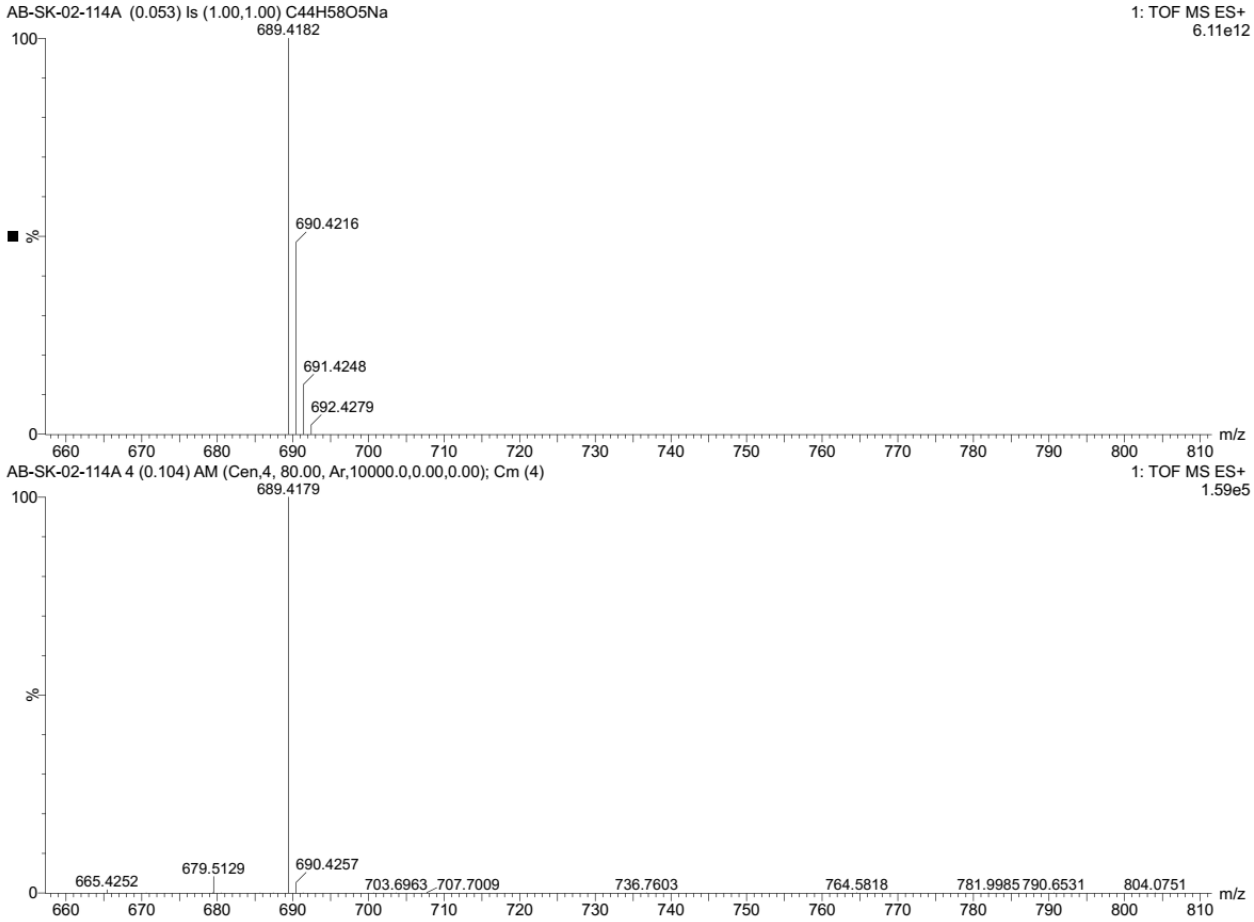


$^{1}$H NMR (500 MHz, $CDCl_3$) of compound (+)-**32**

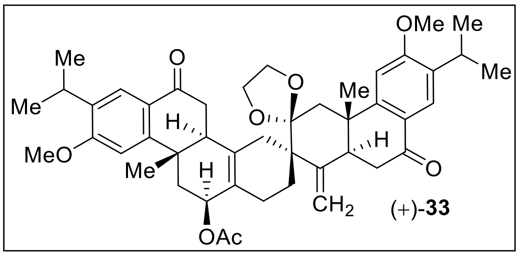


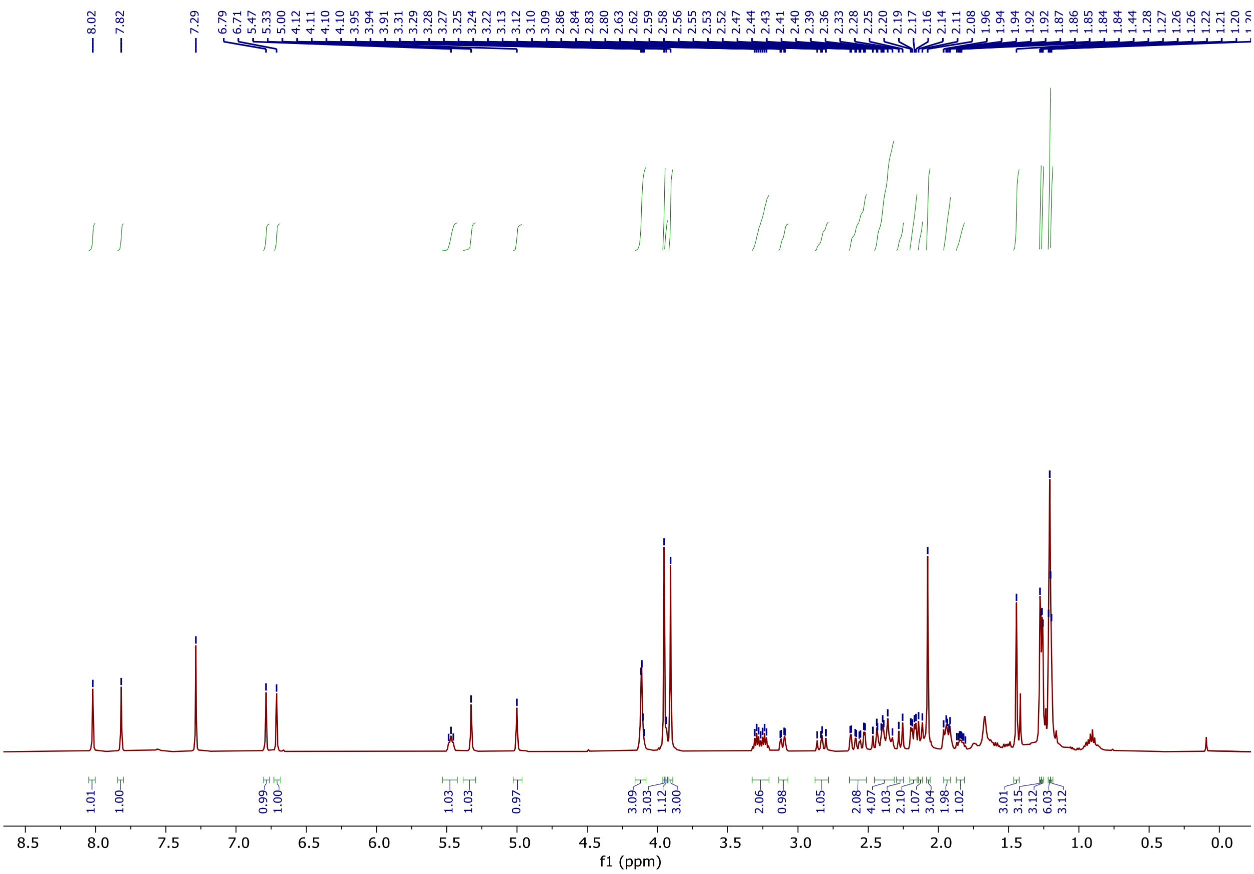


$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**32**

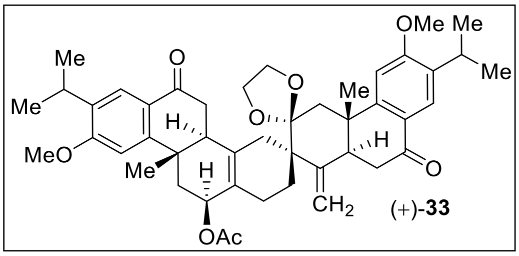


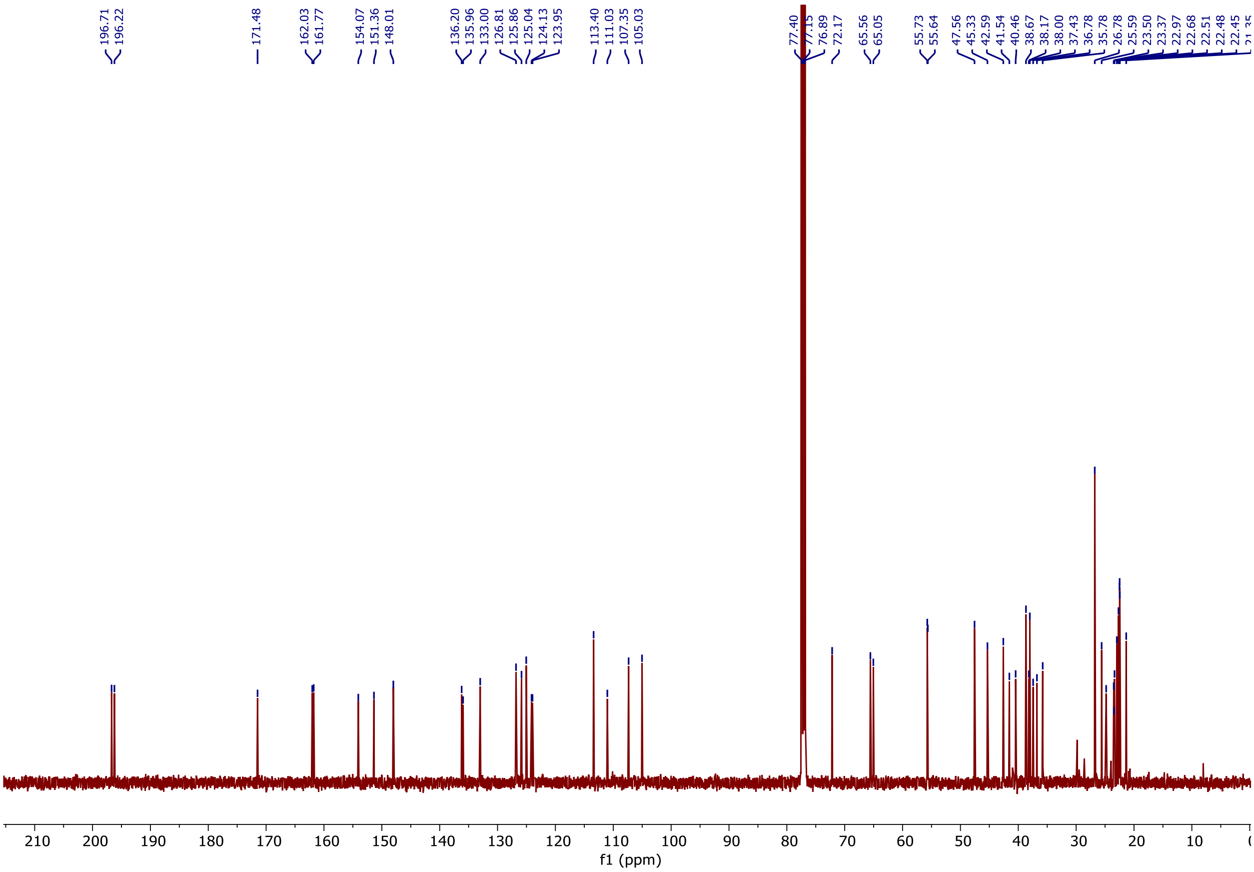

HRMS data of (+)-**32**





[1]H NMR (500 MHz, $CDCl_3$) of compound (+)-**33**




$^{13}$C NMR (126 MHz, $CDCl_3$) of compound (+)-**33**

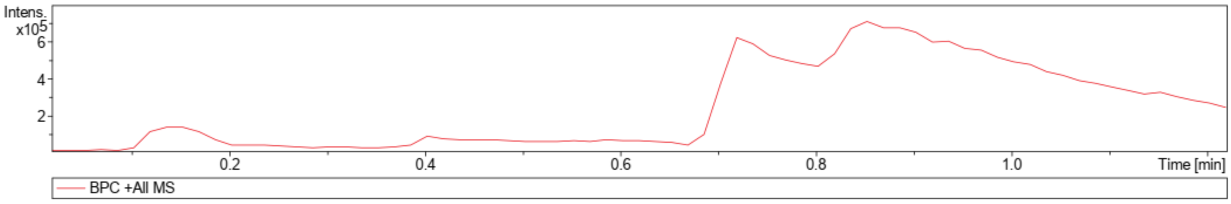
# Display Report

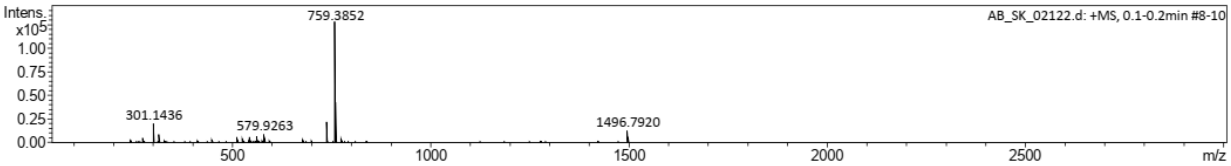
**Analysis Info**

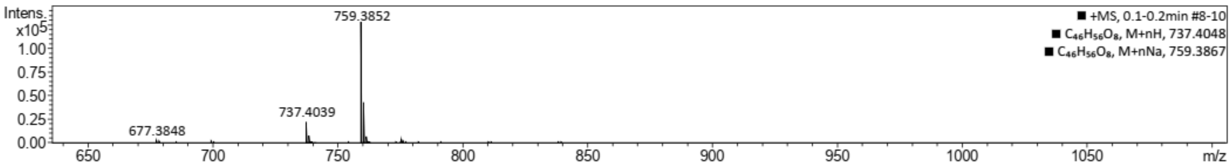
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\User data\2022\NOV\AB_SK_02122.d | Acquisition Date | 11/17/2022 11:06:11 AM |
| Method | Tune_pos_Mid_July.m | Operator | IISER Kolkata |
| Sample Name | AB_SK_02122 | Instrument | maXis impact 8282001.00127 |
| Comment | | | |

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

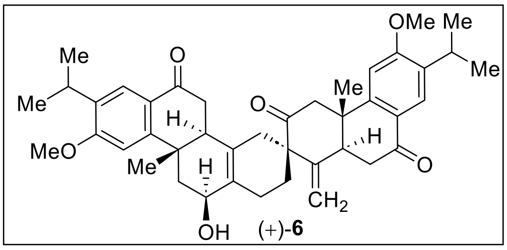


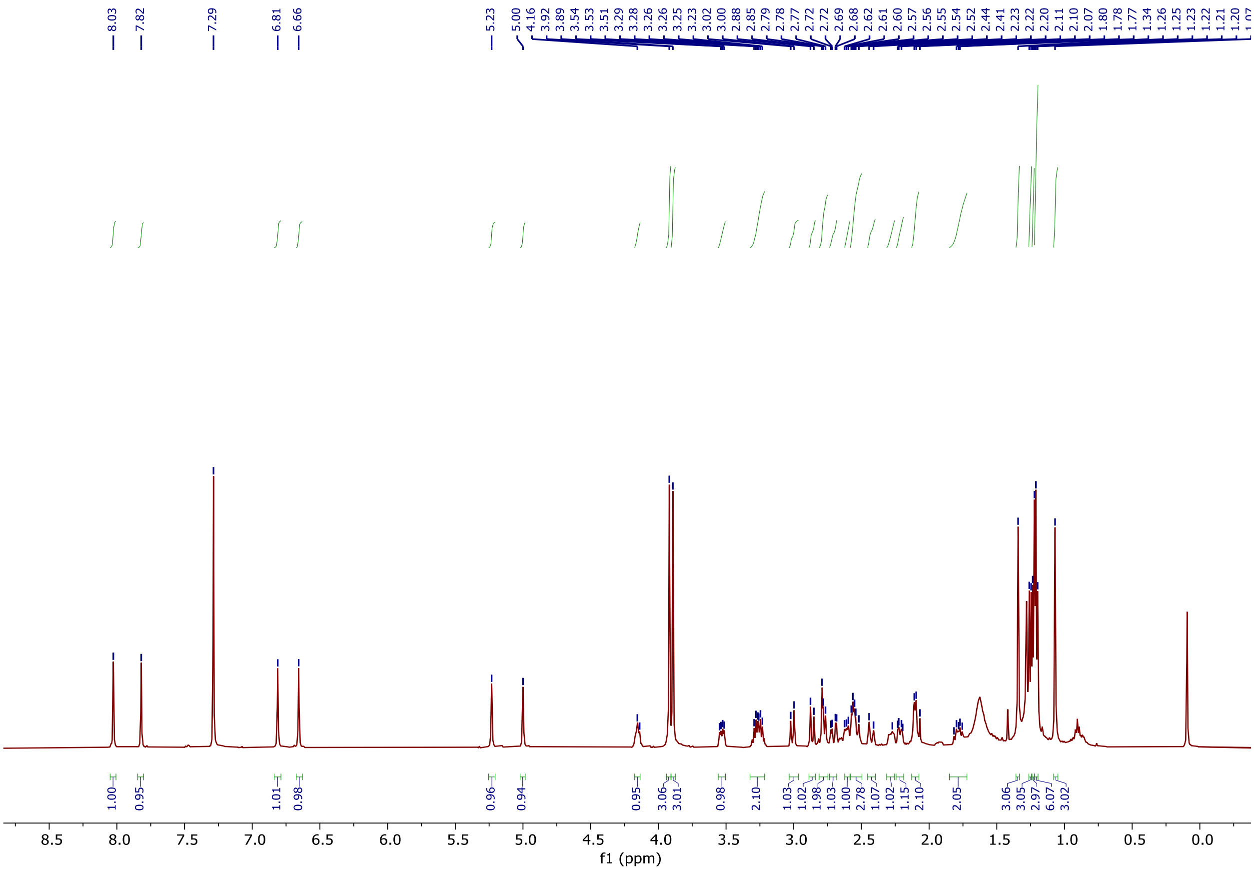



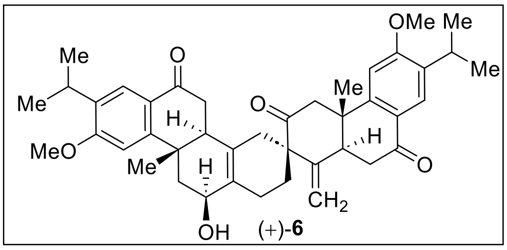


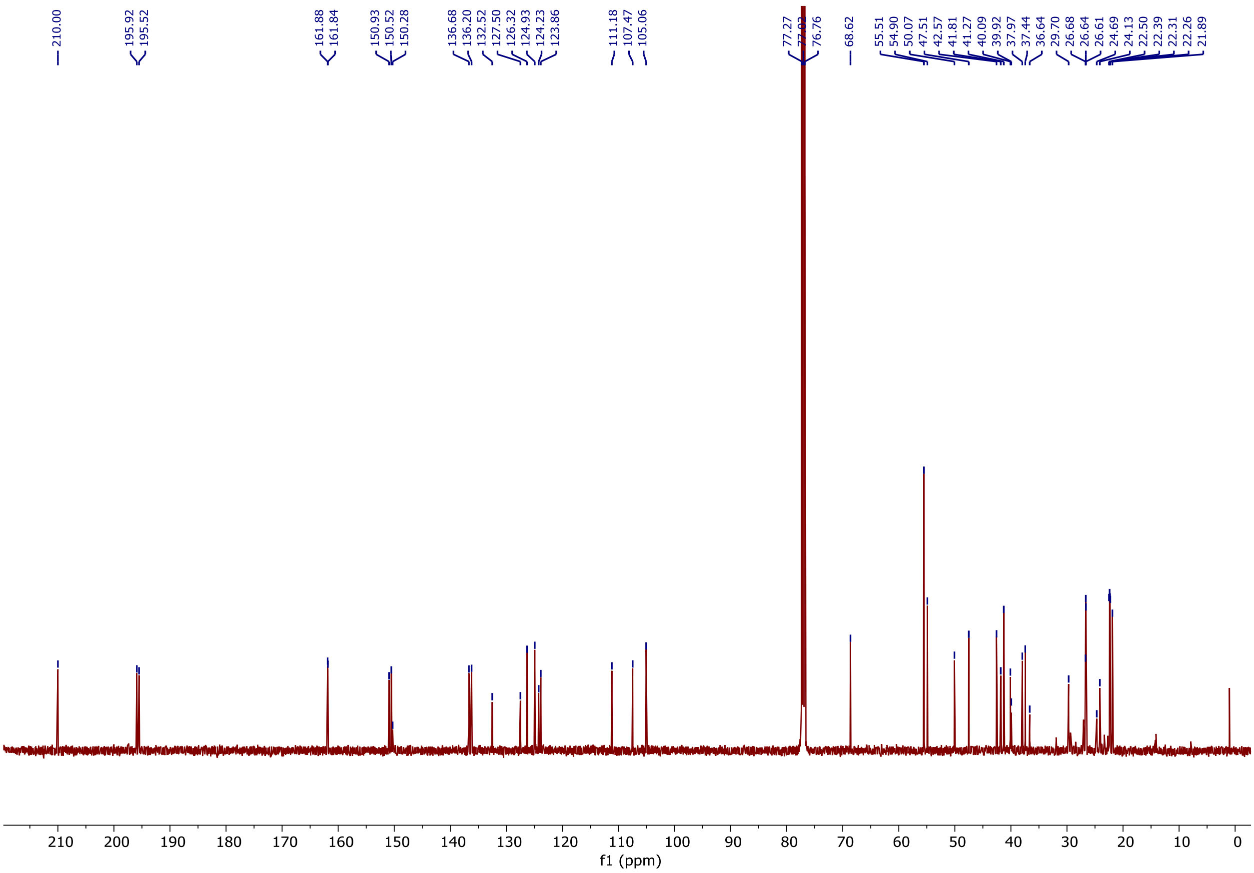

HRMS data of (+)-**33**



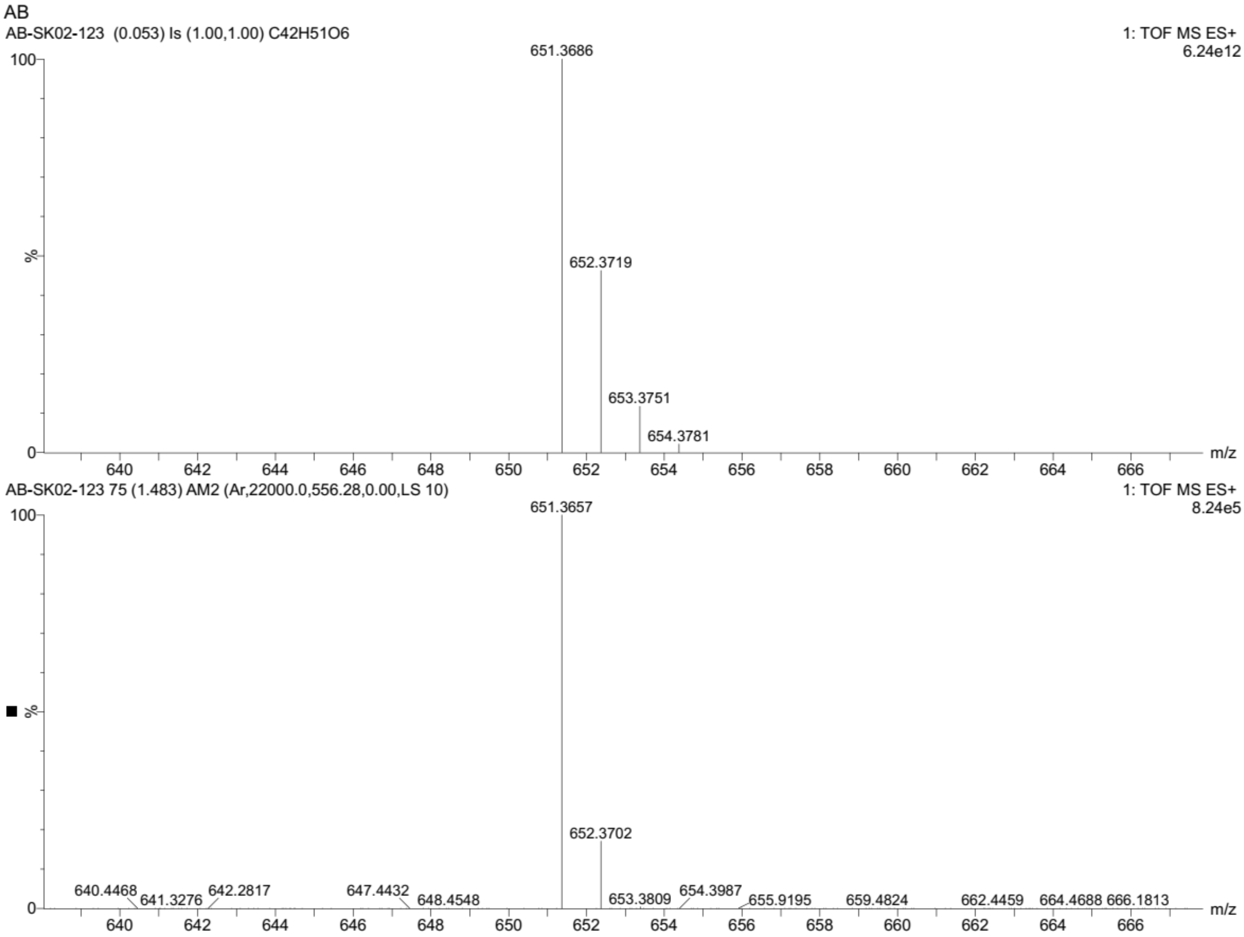

$^1$H NMR (500 MHz, $CDCl_3$) of compound (+)-**6**



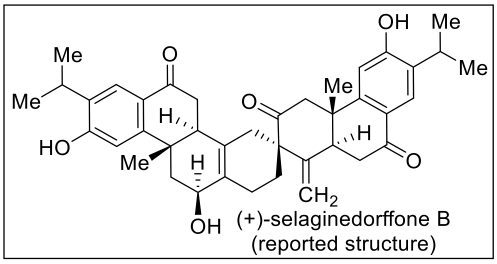



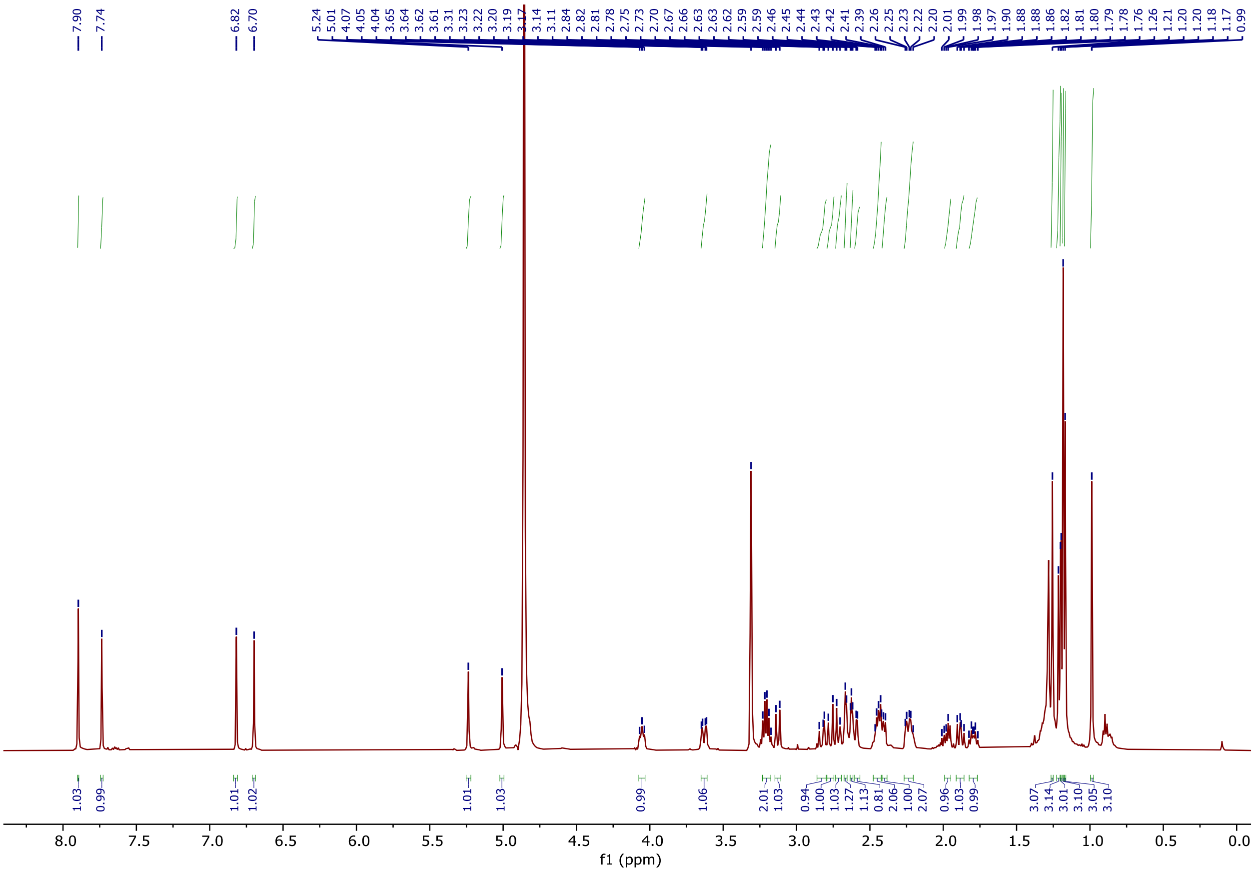
$^{13}C$ NMR (126 MHz, $CDCl_3$) of compound (+)-**6**

.

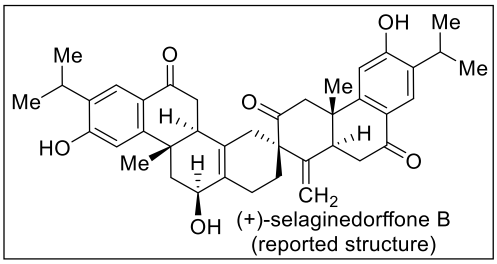


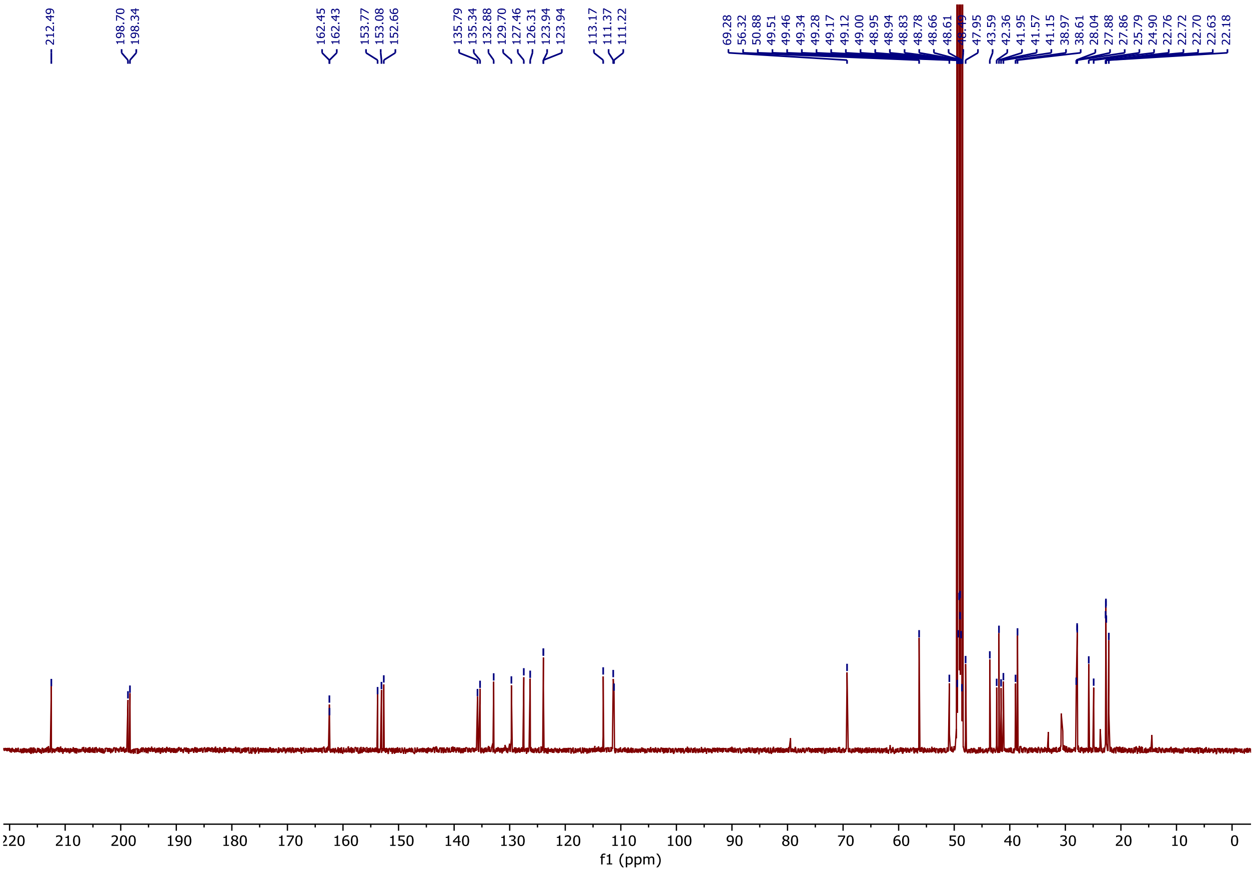

HRMS data of (+)-**6**



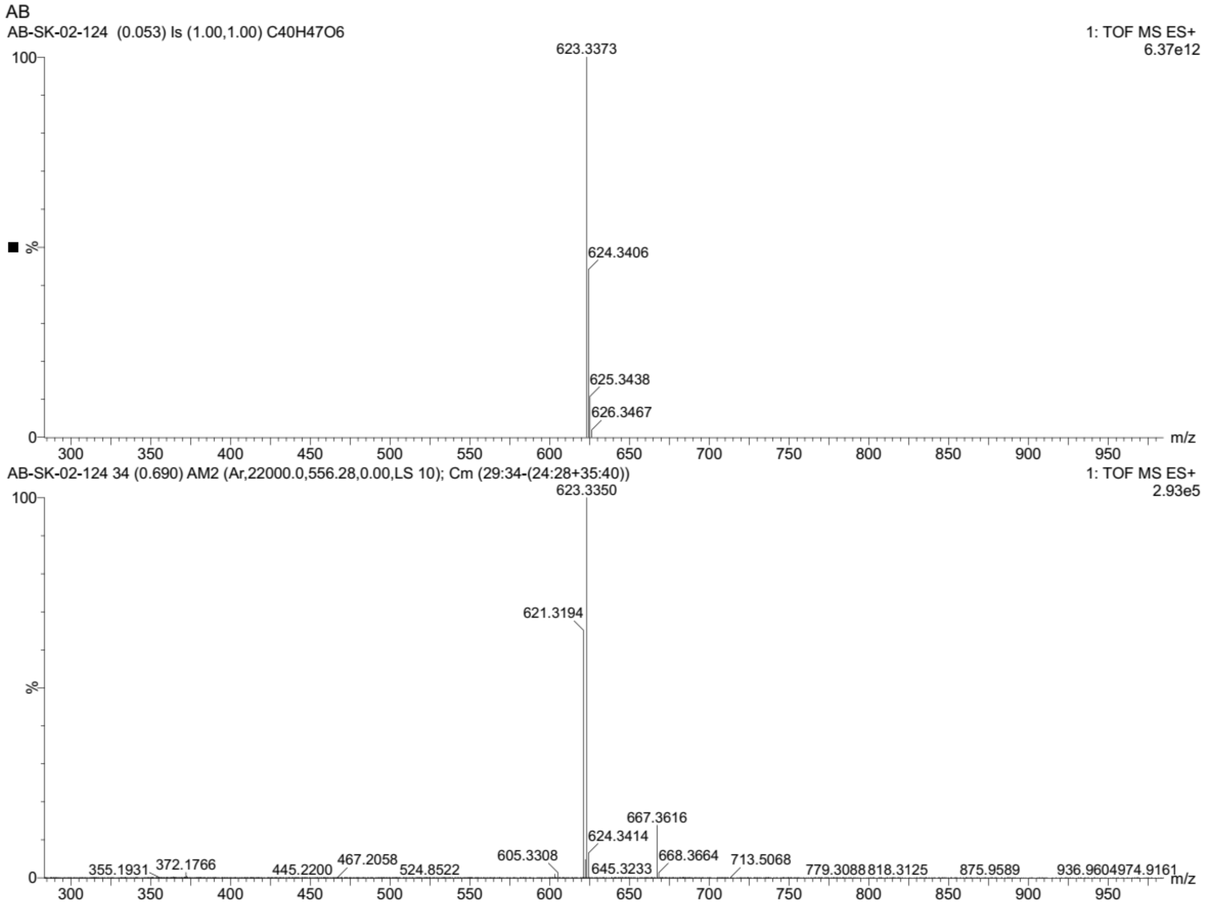



$^1$H NMR (500 MHz, $CD_3OD$) of compound (+)-**2**

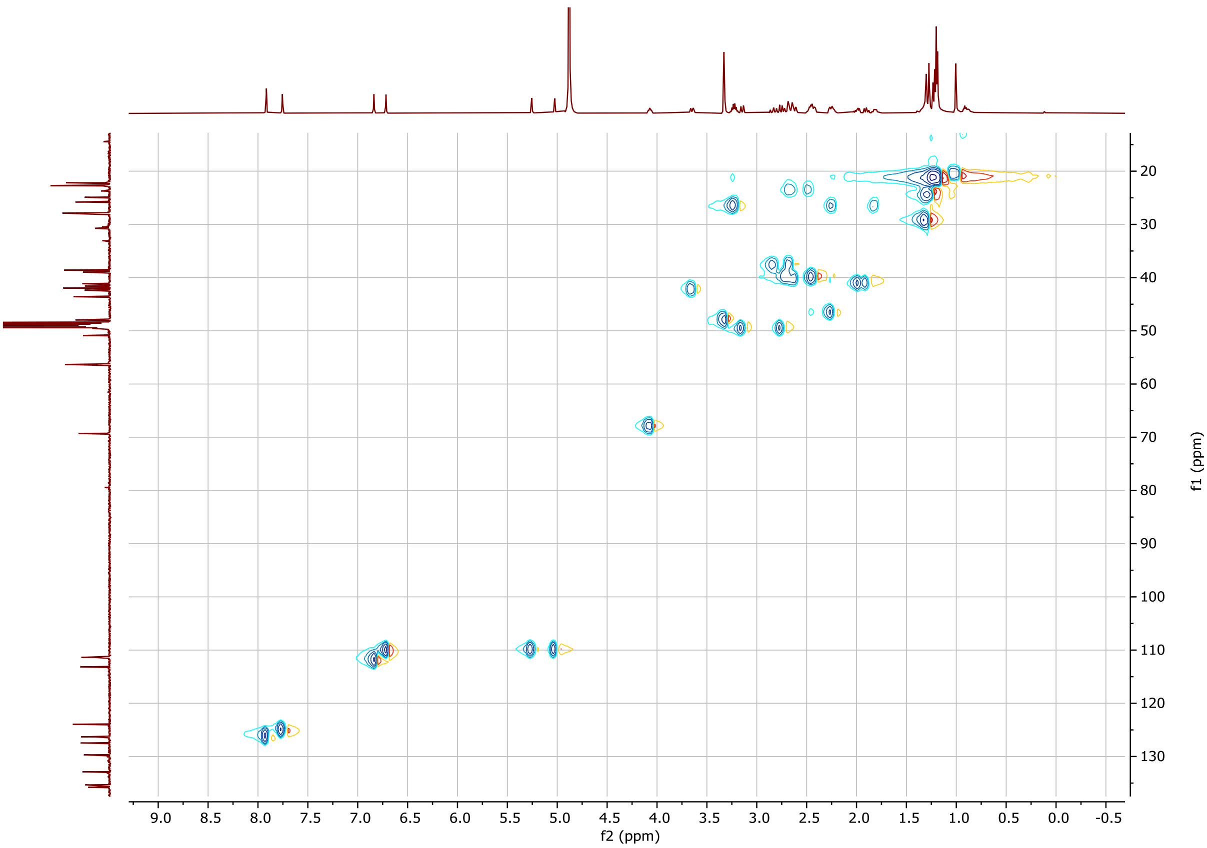


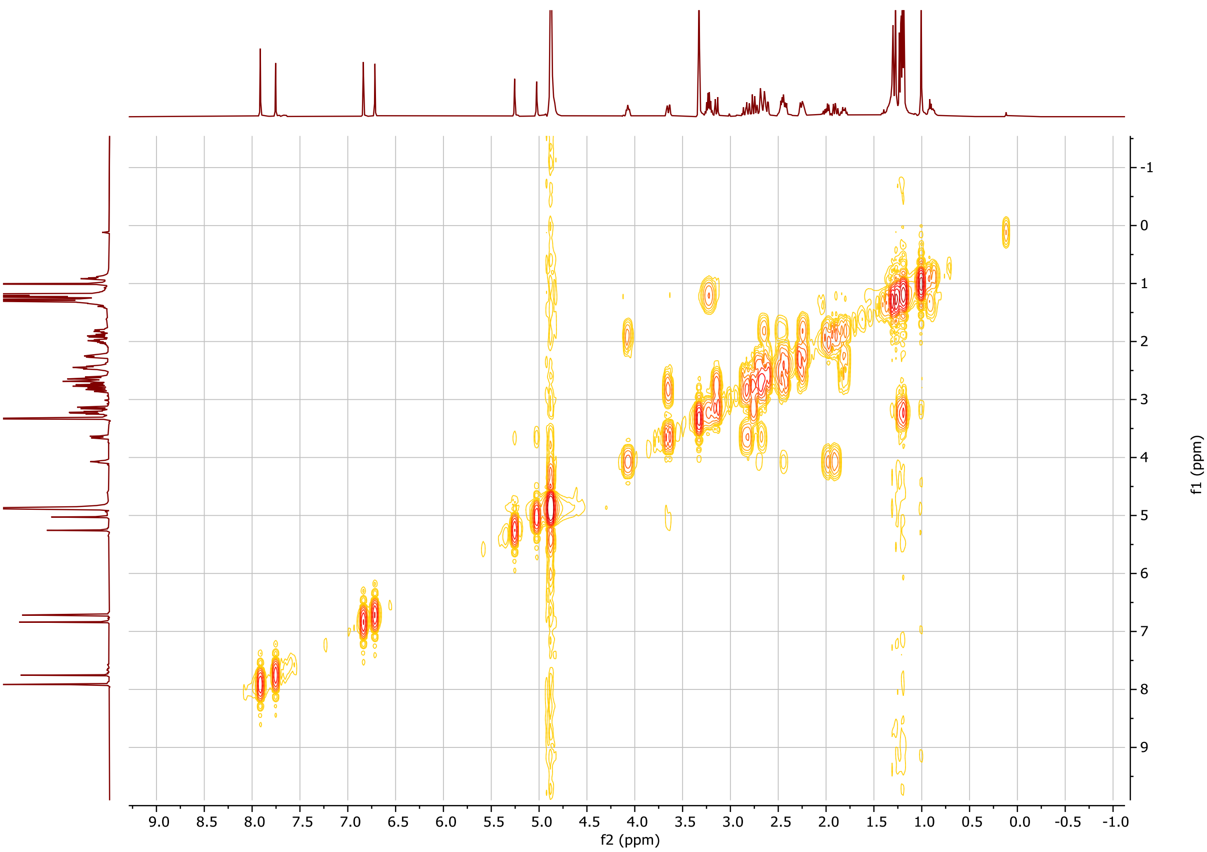
$^{13}$C NMR (126 MHz, $CD_3OD$) of compound (+)-**2**



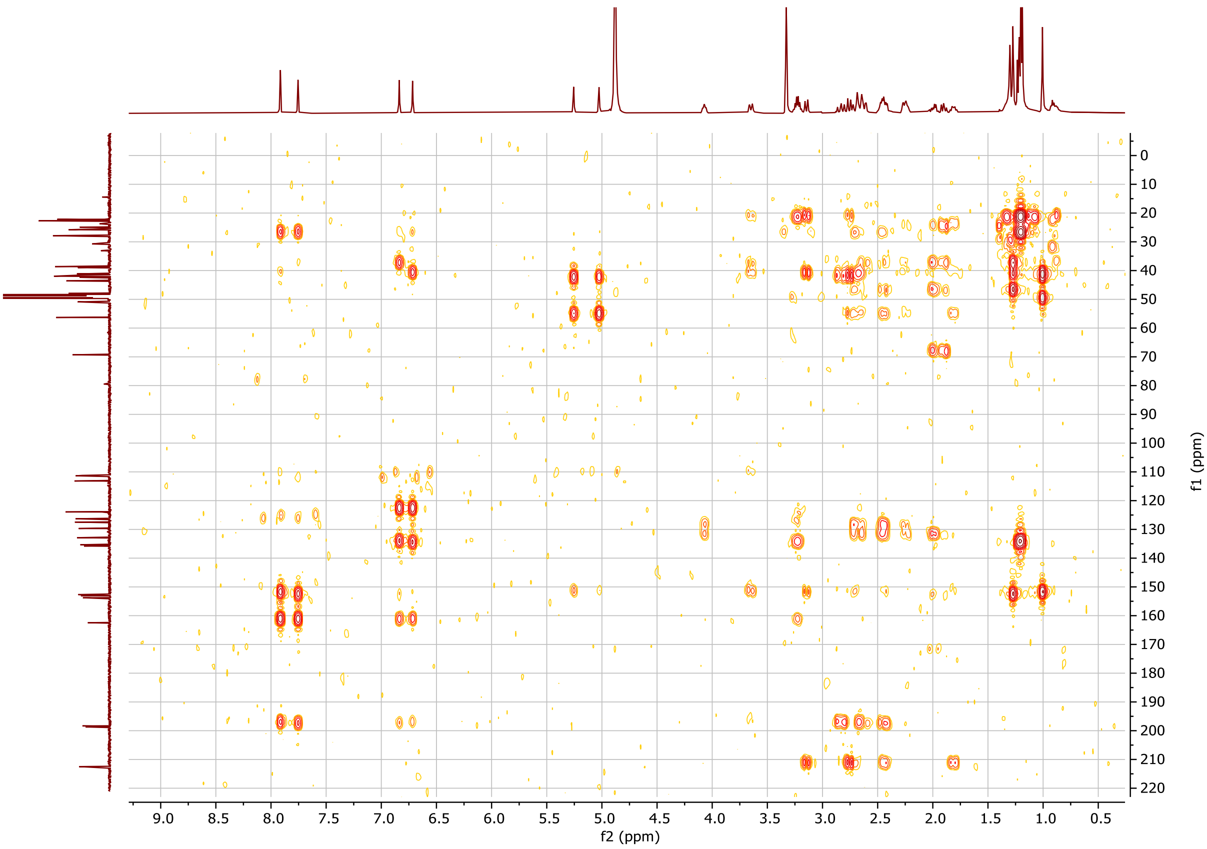

HRMS data of (+)-**2**



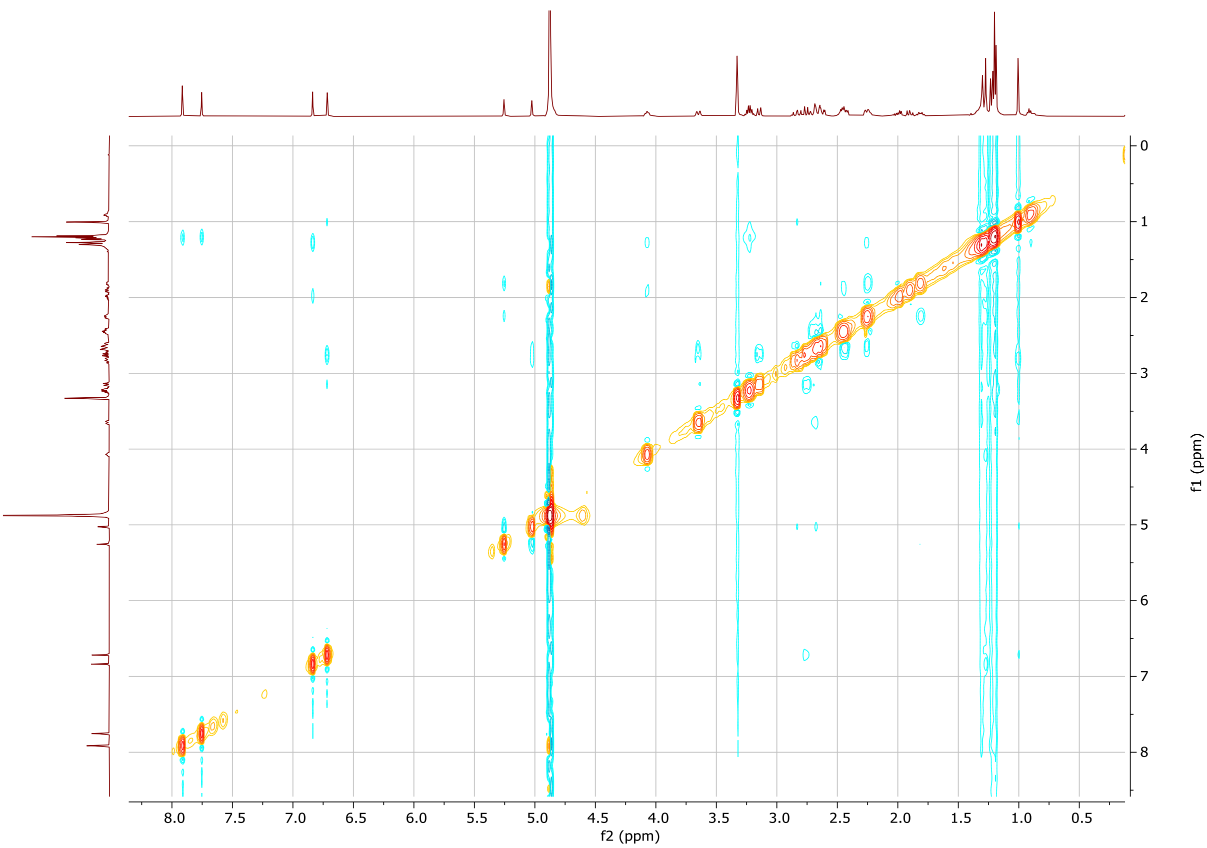

HSQC spectrum of (+)-**2**



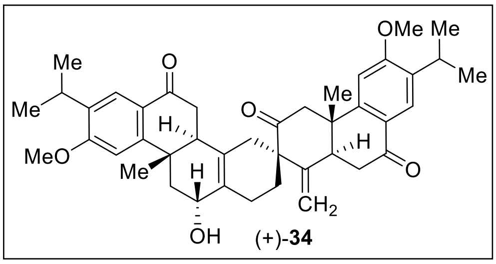

$^{1}$H-$^{1}$H COSY spectrum of (+)-**2**

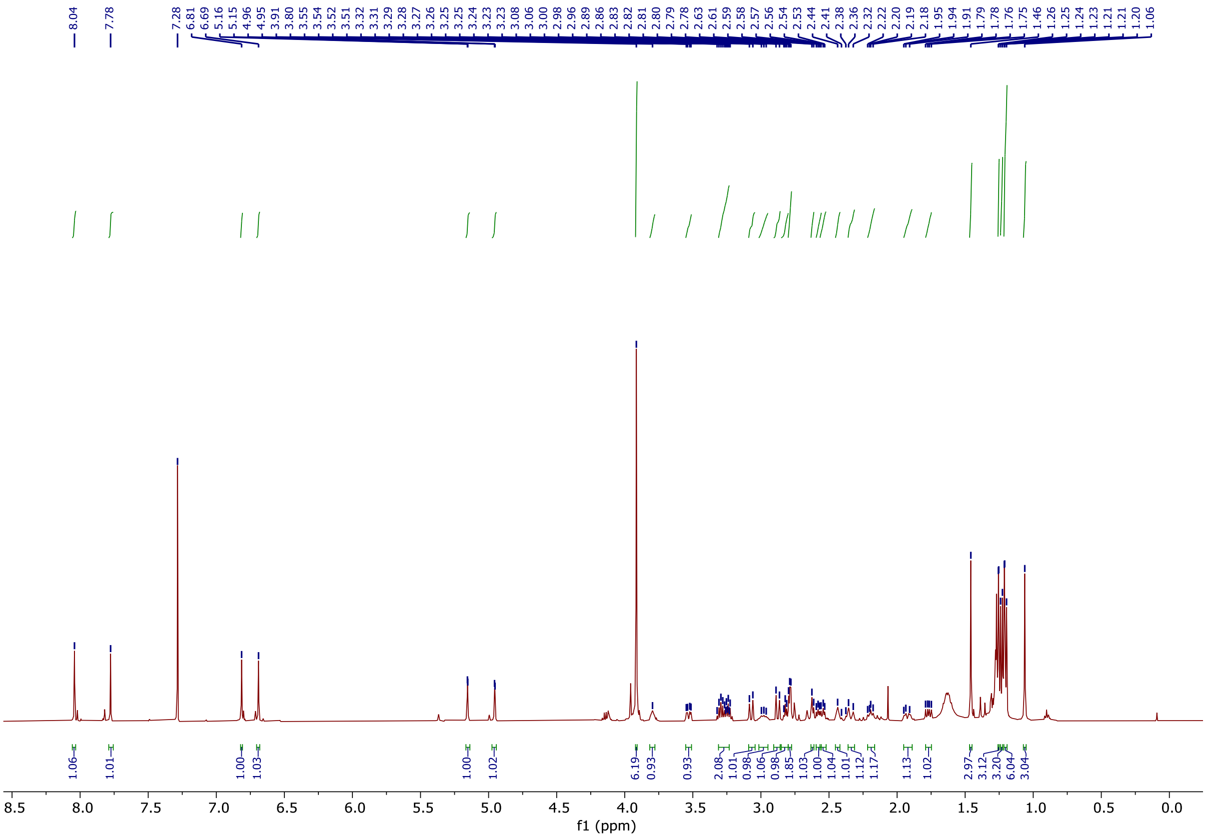



HMBC spectrum of (+)-**2**

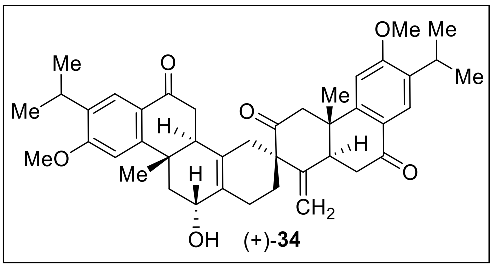


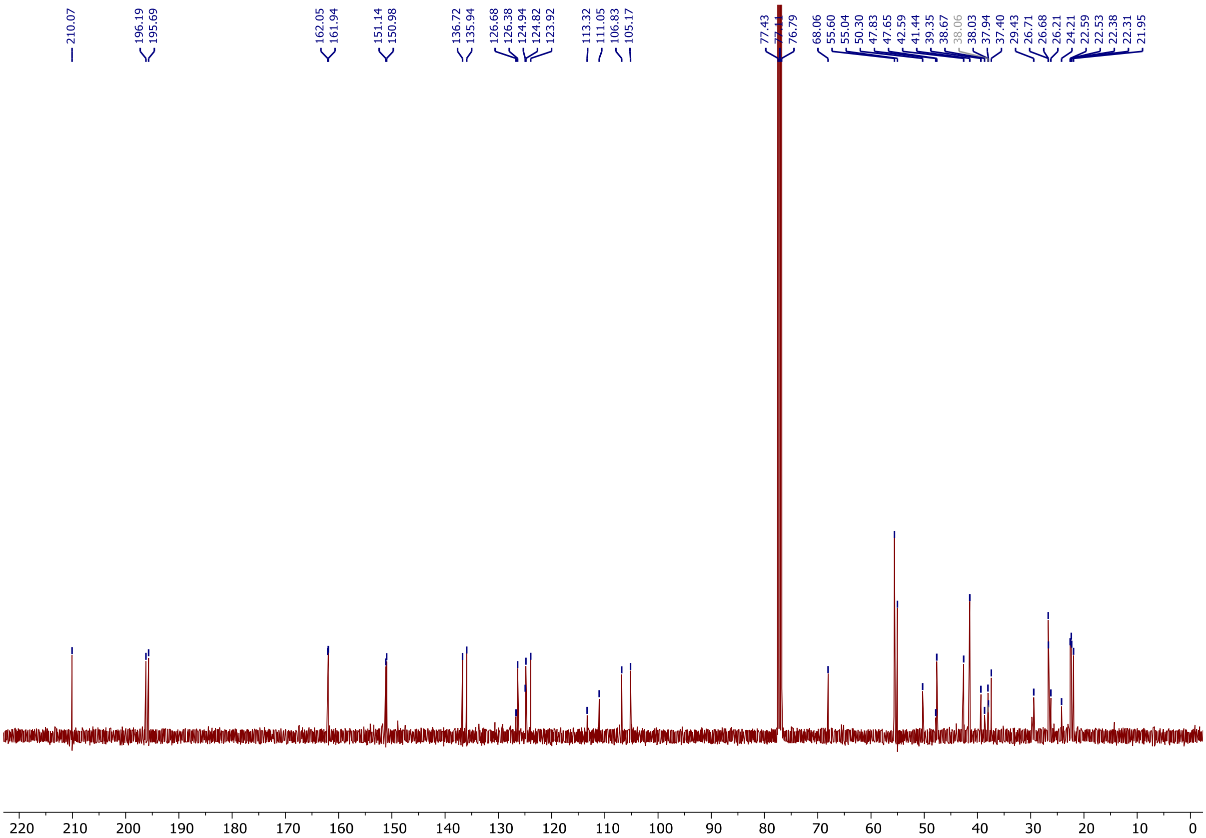

NOESY spectrum of (+)-**2**



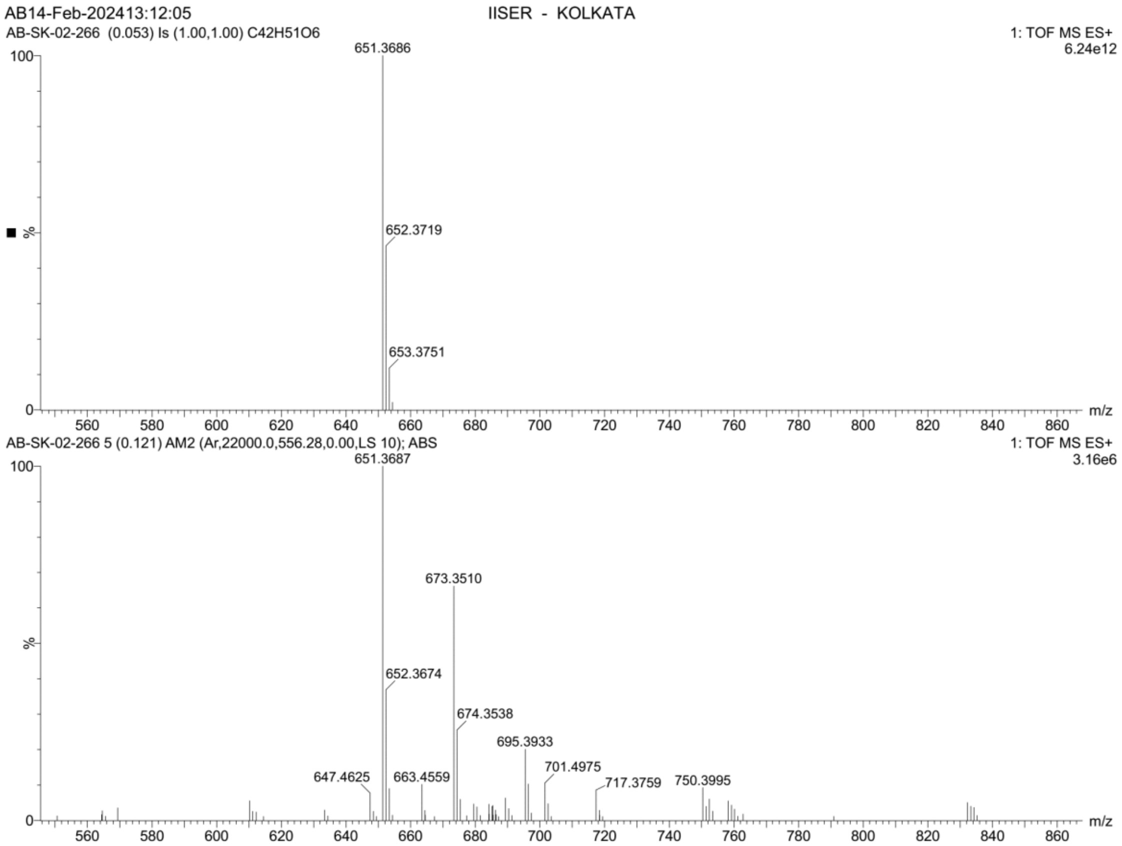



$^{1}$H NMR (500 MHz, $CD_3OD$) of compound (+)-**34**

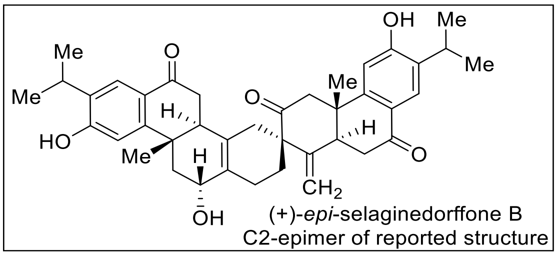


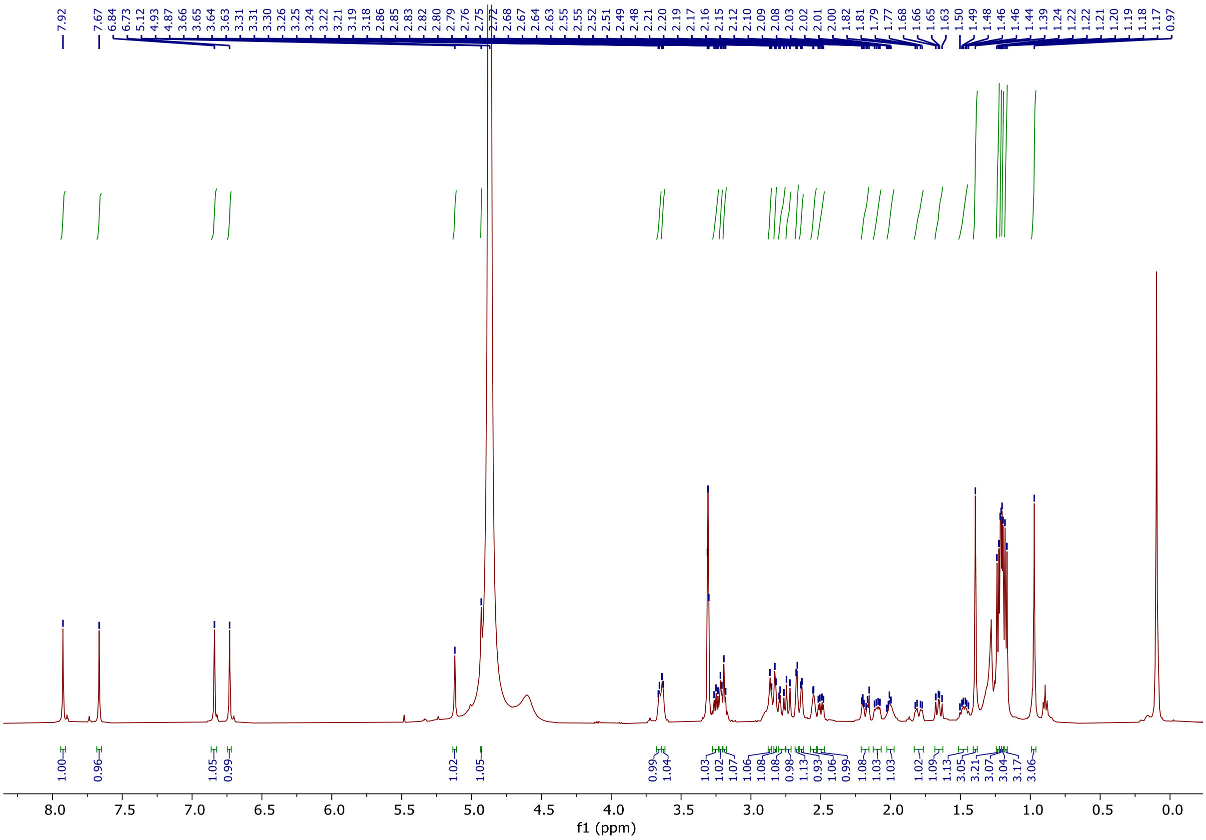



$^{13}$C NMR (101 MHz, $CD_3OD$) of compound (+)-**34**

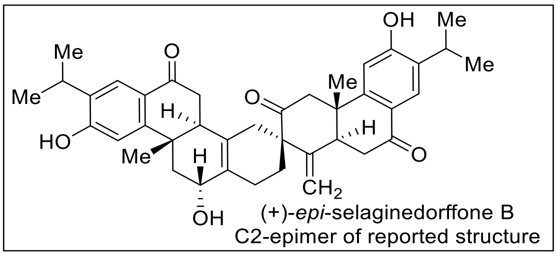


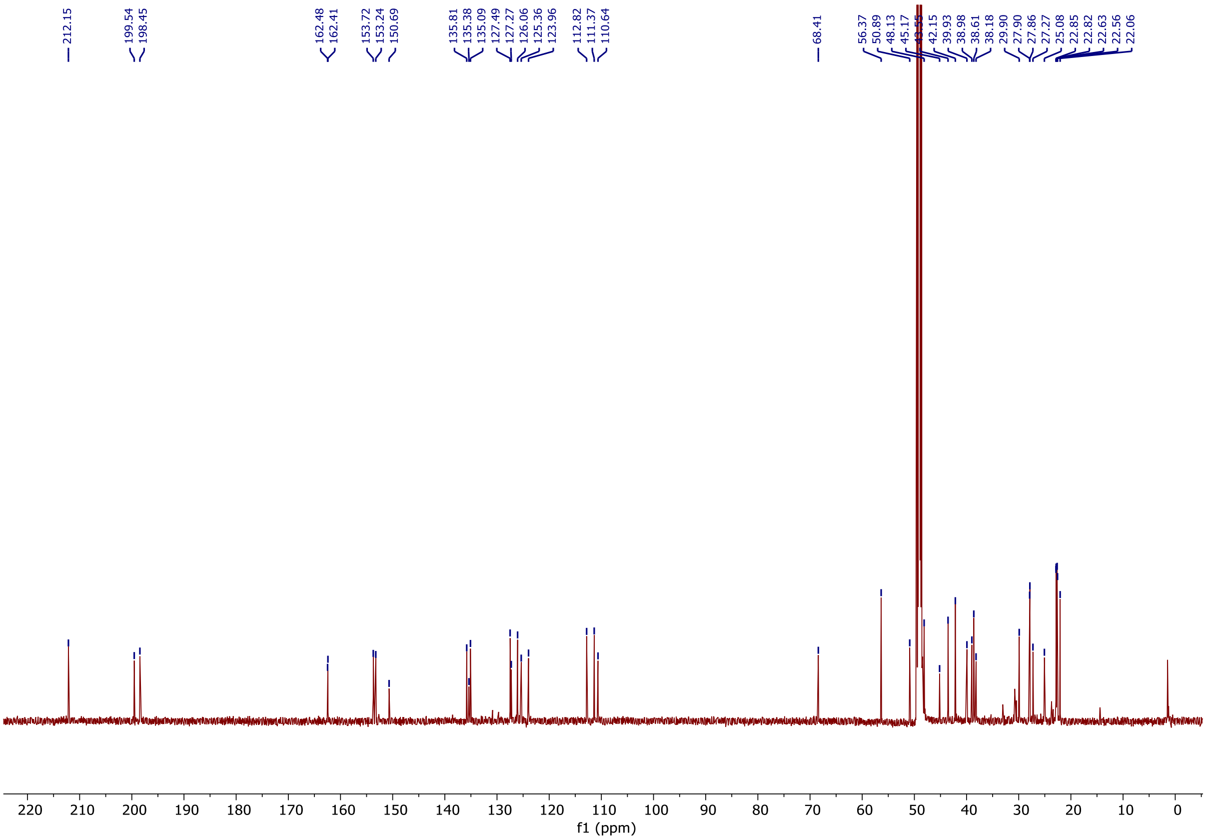

HRMS data of (+)-**34**



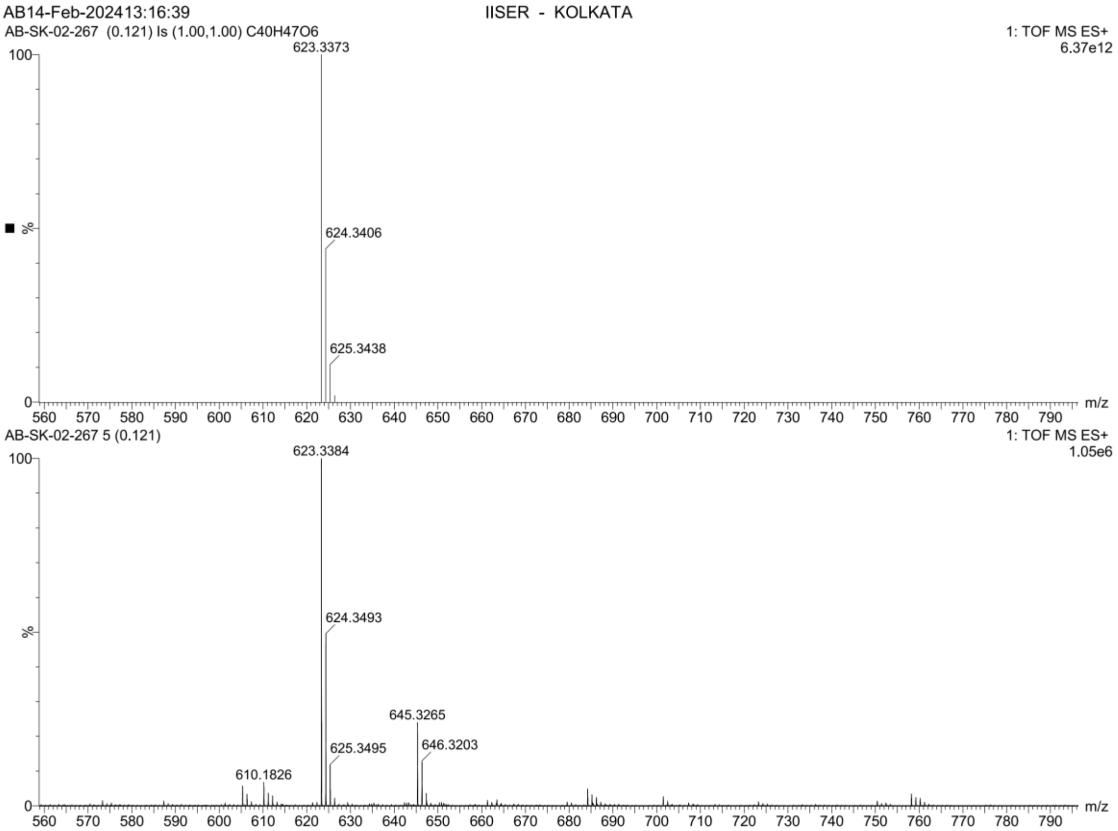



$^{1}$H NMR (500 MHz, $CD_3OD$) of compound (+)-***epi*-2**



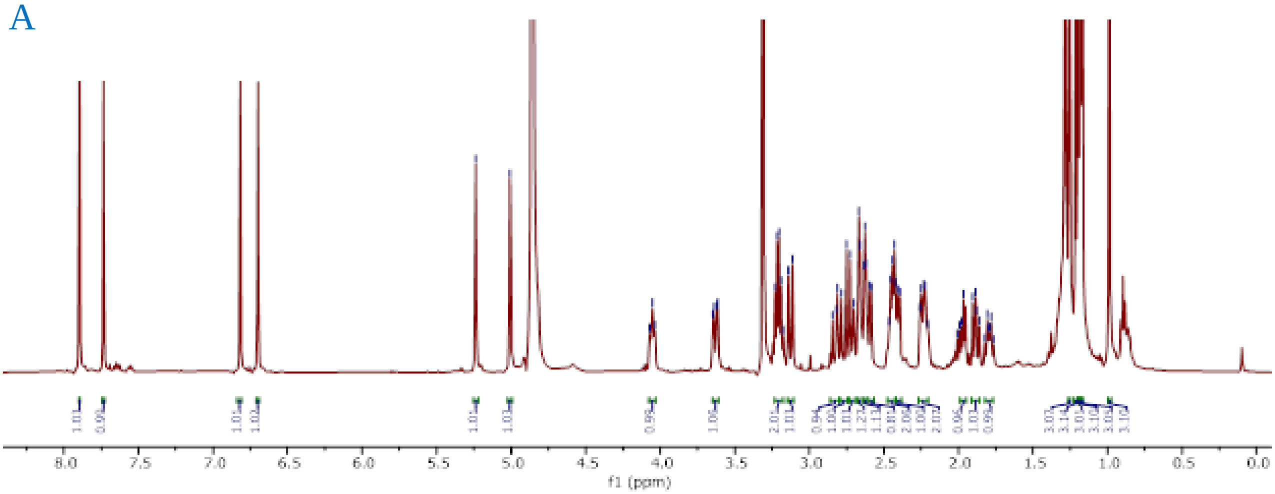




$^{13}C$ NMR (126 MHz, $CD_3OD$) of compound (+)-***epi*-2**

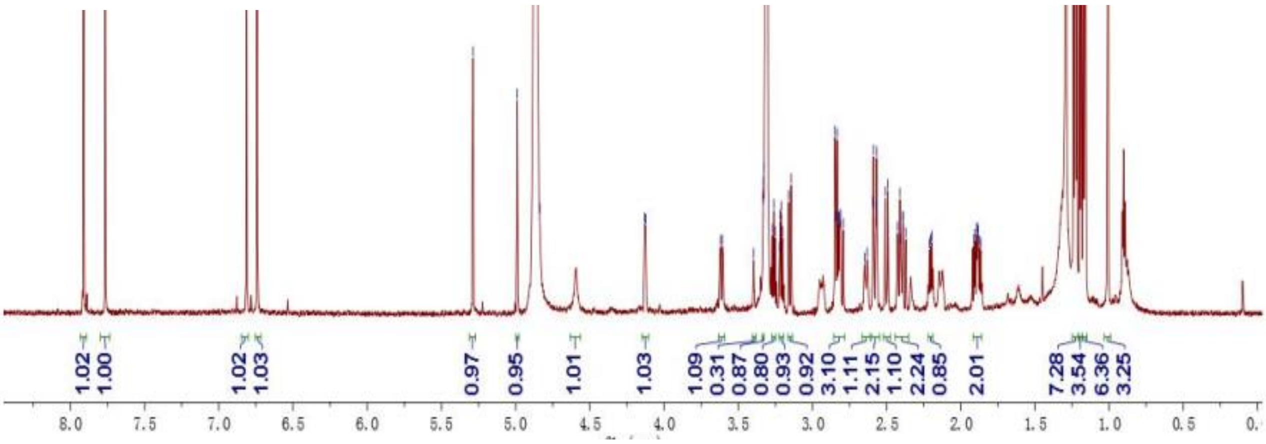



HRMS data of (+)***-epi*-2**

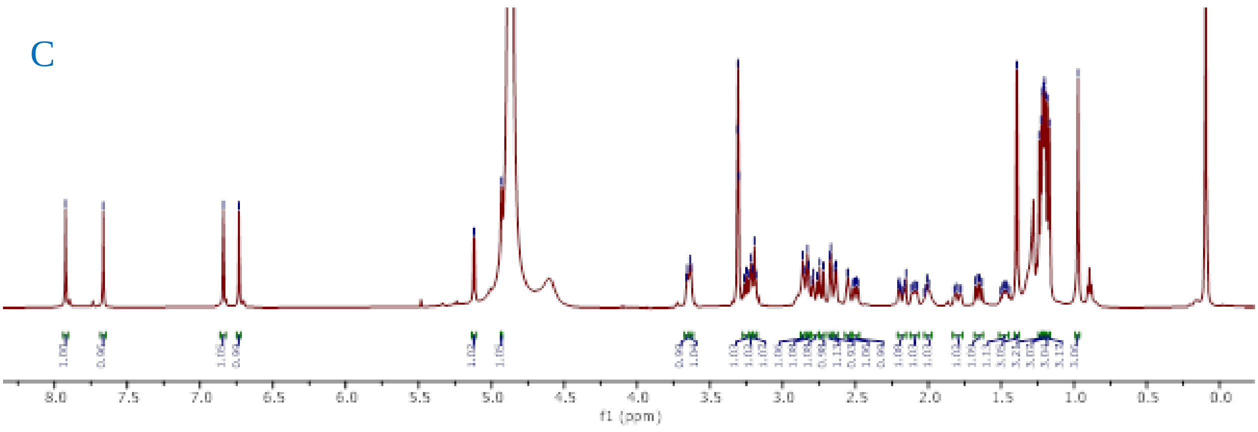
A



B



C



A. [1]H-NMR of reported structure of (+)-selaginedorffone B
B. [1]H-NMR by Long et al. (Isolation)
C. [1]H-NMR of reported structure of (+)-*epi*-selaginedorffone B