

Electronic Supplementary Information

ZnCl₂ loaded TiO₂ nanomaterial: an efficient green catalyst to one-pot solvent-free synthesis of propargylamines

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Contents

- I. Fig. S1 XRD of recovered catalyst (Page No. 3)
- II. Characterization data of as-synthesized propargylamine derivatives (Page No. 4 to 9)
- III. ^1H NMR, ^{13}C NMR and HRMS spectra of propargylamine derivatives (Page No. 10 to 46)

I. Fig. S1 XRD of recovered catalyst

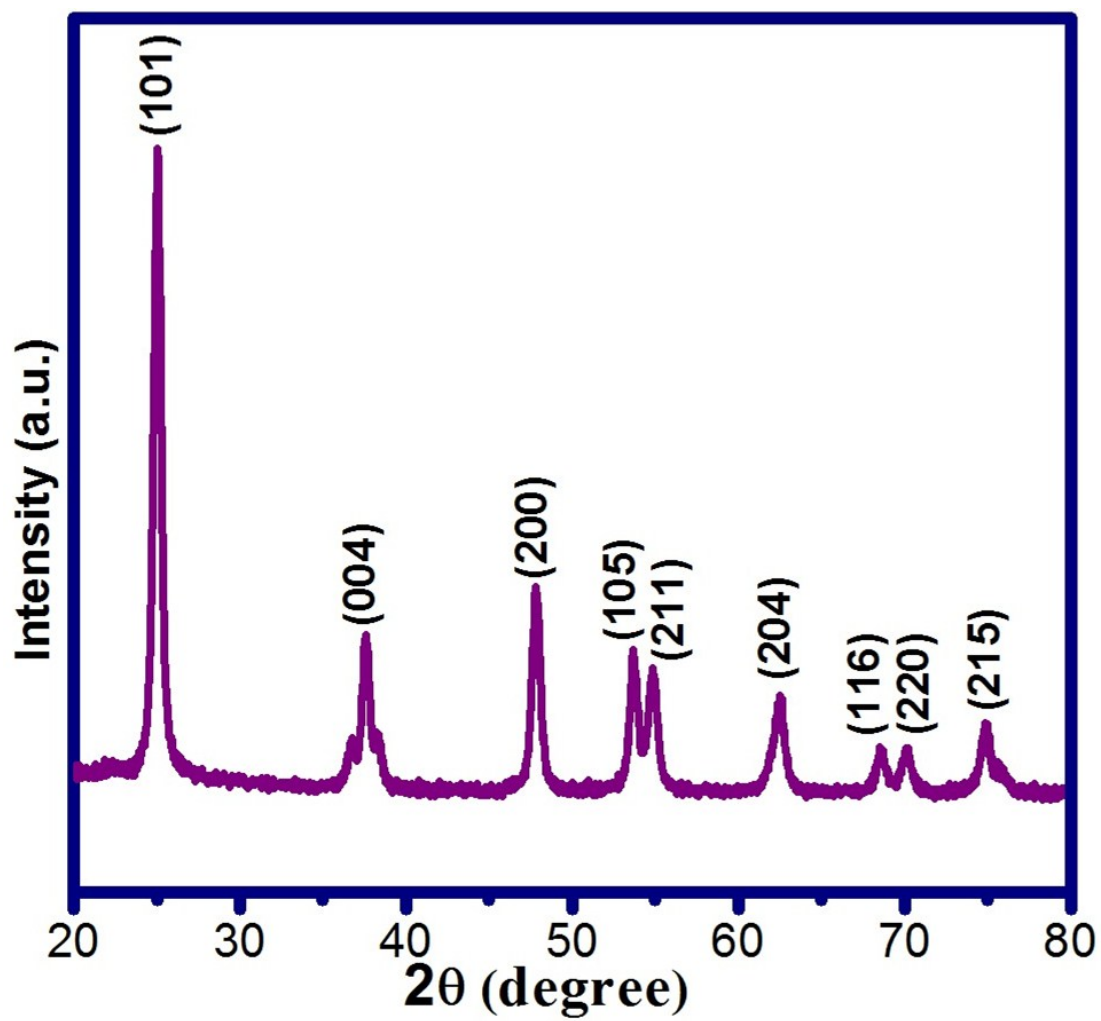
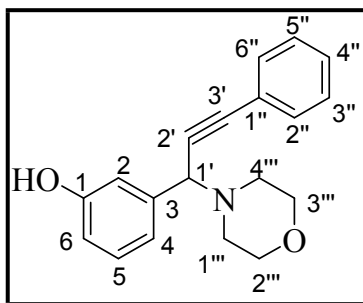


Fig. S1 XRD of recovered catalyst

II. Spectral data of as-synthesized propargylamine derivatives (Table 3, entries 1 to 12)

3-(1-morpholino-3-phenylprop-2-ynyl)phenol (Table 3, entry 1)

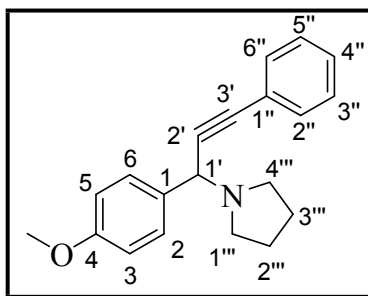


^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ = 2.47-2.56 (m, 4H, H-1''' & H-4'''), 3.60-3.63 (m, 4H, H-2''' & H-3'''), 4.86 (s, 1H, H-1'), 6.70-6.72 (m, 1H, H-2), 6.99-7.04 (m, 2H, H-4 and H-6), 7.16-7.20 (m, 1H, H-5), 7.40-7.54 (m, 5H, H-2'' to H-6''), 9.46 (s, 1H, OH);

^{13}C NMR (125 MHz, CDCl_3): δ = 49.85 (C-1''' & C-4'''), 61.91 (C-1'), 67.01 (C-2''' & C-3'''), 84.80 (C-2'), 88.52 (C-3'), 115.12 (C-2), 115.73 (C-6), 120.73 (C-4), 122.78 (C-5), 128.36 (C-3'' & C-5''), 128.39 (C-1''), 129.49 (C-4''), 131.82 (C-2'' & C-6''), 139.18 (C-3), 156.11 (C-1);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{20}\text{NO}_2$, $[\text{M}+\text{H}]$: 294.1494, found 294.1494.

1-(1-(4-methoxyphenyl)-3-phenylprop-2-ynyl)pyrrolidine (Table 3, entry 2)

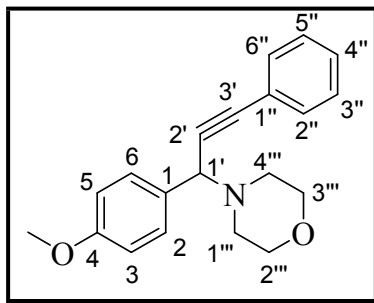


^1H NMR (500 MHz, CDCl_3): δ = 1.79-1.85 (m, 4H, H-2''' & H-3'''), 2.71-2.72 (m, 4H, H-1''' & H-4'''), 3.83 (s, 3H, OCH_3), 4.87 (s, 1H, H-1'), 6.90-6.93 (m, 2H, H-3 & H-5), 7.32-7.35 (m, 3H, ArH), 7.50-7.55 (m, 4H, ArH);

^{13}C NMR (125 MHz, CDCl_3): δ = 23.48 (C-2''' & C-3'''), 50.25 (C-1''' & C-4'''), 55.30 (C-1'), 58.51 (OCH_3), 86.74 (C-2'), 86.93 (C-3'), 113.61 (C-3 & C-5), 123.25 (C-1), 128.09 (C-1''), 128.28 (C-2 & C-6), 129.45 (C-3'' & C-5''), 131.60 (C-4''), 131.79 (C-2'' & C-6''), 159.08 (C-4);

HRMS (ESI) m/z calcd. for $\text{C}_{20}\text{H}_{22}\text{NO}$, $[\text{M}+\text{H}]$: 292.1701, found 292.1699.

4-(1-(4-methoxyphenyl)-3-phenylprop-2-ynyl)morpholine (Table 3, entry 3)

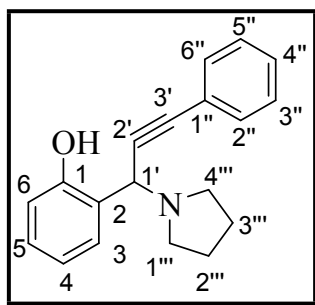


^1H NMR (500 MHz, CDCl_3): δ = 2.57-2.64 (m, 4H, H-1''' & H-4'''), 3.68-3.73 (m, 4H, H-2''' & H-3'''), 3.80 (s, 3H, OCH_3), 4.72 (s, 1H, H-1'), 6.87-6.90 (m, 2H, H-3 & H-5), 7.30-7.34 (m, 3H, ArH), 7.48-7.54 (m, 4H, ArH);

^{13}C NMR (125 MHz, CDCl_3): δ = 49.82 (C-1''' & C-4'''), 55.31 (C-1'), 61.46 (OCH_3), 67.18 (C-2''' & C-3'''), 85.39 (C-2'), 88.27 (C-3'), 113.79 (C-3 & C-5), 123.04 (C-1), 128.24 (C-1''), 128.33 (C-2 & C-6), 129.76 (C-3'' & C-5''), 129.88 (C-4''), 132.03 (C-2'' & C-6''), 159.23 (C-4);

HRMS (ESI) m/z calcd. for $\text{C}_{20}\text{H}_{22}\text{NO}_2$, $[\text{M}+\text{H}]$: 308.1650, found 308.1651.

2-(3-phenyl-1-(pyrrolidin-1-yl)prop-2-ynyl)phenol (Table 3, entry 4)

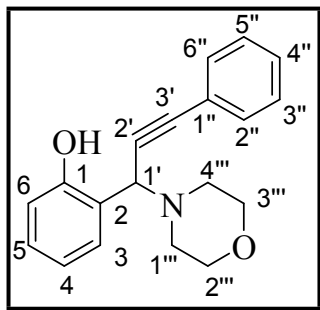


^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ = 1.74-1.79 (m, 4H, H-2''' & H-3'''), 2.63-2.75 (m, 4H, H-1''' & H-4'''), 5.32 (s, 1H, H-1'), 6.78-6.85 (m, 2H, H-4 & H-6), 7.15-7.18 (m, 1H, H-3), 7.39-7.47 (m, 4H, ArH), 7.50-7.52 (m, 2H, H-2'' & H-6'');

^{13}C NMR (125 MHz, CDCl_3): δ = 23.68 (C-2''' & C-3'''), 49.61 (C-1''' & C-4'''), 55.10 (C-1'), 85.67 (C-2'), 87.51 (C-3'), 116.18 (C-6), 119.26 (C-4), 122.50 (C-2), 123.71 (C-3), 128.58 (C-5), 129.18 (C-1''), 129.42 (C-4''), 132.04 (C-2'' & C-6''), 156.74 (C-1);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{20}\text{NO}$, $[\text{M}+\text{H}]$: 278.1544, found 278.1540.

2-(1-morpholino-3-phenylprop-2-ynyl)phenol (Table 3, entry 5)

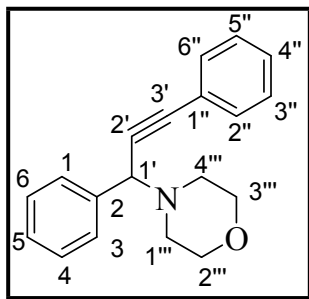


^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ = 2.56-2.66 (m, 4H, H-1''' & H-4'''), 3.63-3.66 (m, 4H, H-2''' & H-3'''), 5.22 (s, 1H, H-1'), 6.82-6.88 (m, 2H, H-4 & H-6), 7.17-7.21 (m, 1H, H-3), 7.40-7.57 (m, 6H, ArH), 10.31 (s, 1H, OH);

^{13}C NMR (125 MHz, CDCl_3): δ = 49.00 (C-1''' & C-4'''), 60.74 (C-1'), 66.90 (C-2''' & C-3'''), 81.59 (C-2'), 90.45 (C-3'), 116.53 (C-6), 119.48 (C-4), 120.57 (C-2), 122.28 (C-3), 128.67 (C-5), 128.80 (C-1'', C-3'' & C-5''), 129.80 (C-4''), 132.14 (C-2'' & C-6''), 157.03 (C-1);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{20}\text{NO}_2$, $[\text{M}+\text{H}]$: 294.1494, found 294.1492.

4-(1, 3-diphenylprop-2-ynyl)morpholine (Table 3, entry 6)

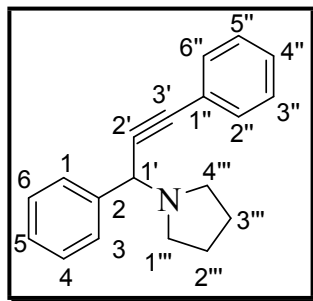


^1H NMR (500 MHz, CDCl_3): δ = 2.59-2.63 (m, 4H, H-1''' & H-4'''), 3.69-3.76 (m, 4H, H-2''' & H-3'''), 4.78 (s, 1H, H-1'), 7.28-7.38 (m, 6H, ArH), 7.49-7.53 (m, 2H, ArH), 7.62-7.63 (m, 2H, H-2'' & H-6'');

^{13}C NMR (125 MHz, CDCl_3): δ = 49.90 (C-1''' & C-4'''), 62.06 (C-1'), 67.19 (C-2''' & C-3'''), 85.07 (C-2'), 88.53 (C-3'), 123.00 (C-1), 127.94 (C-3), 128.30 (C-4 & C-6), 128.35 (C-5), 128.63 (C-3'' & C-5''), 129.94 (C-1''), 131.85 (C-2'', C-4'' & C-6''), 137.82 (C-2);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{20}\text{NO}$, $[\text{M}+\text{H}]$: 278.1544, found 278.1545.

1-(1, 3-diphenylprop-2-ynyl)pyrrolidine (Table 3, entry 7)

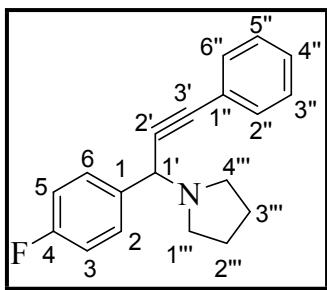


^1H NMR (500 MHz, CDCl_3): δ = 1.82-1.85 (m, 4H, H-2''' & H-3'''), 2.72-2.75 (m, 4H, H-1''' & H-4'''), 4.93 (s, 1H, H-1'), 7.31-7.40 (m, 6H, ArH), 7.51-7.53 (m, 2H, ArH), 7.63-7.65 (m, 2H, H-2'' & H-6'');

^{13}C NMR (125 MHz, CDCl_3): δ = 23.51 (C-2''' & C-3'''), 50.28 (C-1''' & C-4'''), 59.13 (C-1'), 86.66 (C-2'), 86.95 (C-3'), 123.24 (C-1), 127.62 (2 \times ArC), 128.29 (5 \times ArC), 131.81 (C-2'', C-4'' & C-6'');

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{20}\text{N}$, $[\text{M}+\text{H}]$: 262.1595, found 262.1595.

1-(1-(4-fluorophenyl)-3-phenylprop-2-ynyl)pyrrolidine (Table 3, entry 8)

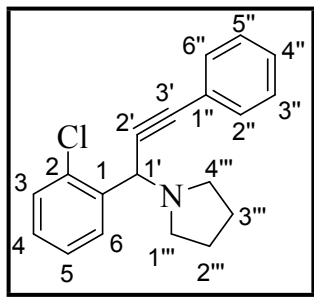


^1H NMR (500 MHz, CDCl_3): δ = 1.83-1.86 (m, 4H, H-2''' & H-3'''), 2.72-2.78 (m, 4H, H-1''' & H-4'''), 4.98(s, 1H, H-1'), 7.04-7.10 (m, 2H, H-3 & H-5), 7.34-7.36 (m, 3H, ArH), 7.51-7.53 (m, 2H, ArH), 7.60-7.63 (m, 2H, H-2'' & H-6'');

^{13}C NMR (125 MHz, CDCl_3): δ = 23.50 (C-2''' & C-3'''), 50.07 (C-1''' & C-4'''), 58.22 (C-1'), 85.96 (C-2'), 87.38 (C-3'), 115.09 (C-3 & C-5), 122.92 (1 \times ArC), 128.31 (3 \times ArC), 129.95 (2 \times ArC), 131.81 (3 \times ArC), 163.30 (C-4);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{19}\text{FN}$, $[\text{M}+\text{H}]$: 280.1501, found 280.1502.

1-(1-(2-chlorophenyl)-3-phenylprop-2-ynyl)pyrrolidine (Table 3, entry 9)

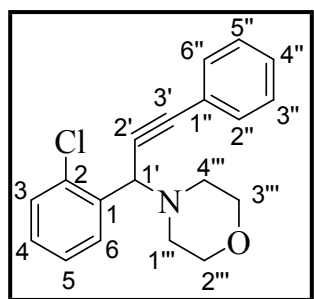


^1H NMR (500 MHz, CDCl_3): δ = 1.76-1.81 (m, 4H, H-2''' & H-3'''), 2.67-2.77 (m, 4H, H-1''' & H-4'''), 5.29 (s, 1H, H-1'), 7.23-7.27 (m, 2H, ArH), 7.29-7.32 (m, 3H, ArH), 7.36-7.38 (m, 1H, ArH), 7.44-7.48 (m, 2H, H-2'' & H-6''), 7.77-7.79 (m, 1H, H-4'');

^{13}C NMR (125 MHz, CDCl_3): δ = 22.43 (C-2''' & C-3'''), 49.34 (C-1''' & C-4'''), 54.54 (C-1'), 85.40 (C-2'), 85.44 (C-3'), 122.02 (C-5), 125.62 (C-3), 127.12 (C-1), 127.22 (C-4 & C-6), 127.77 (C-5''), 128.60 (C-3''), 129.08 (C-1''), 130.74 (C-2'' & C-6''), 132.77 (C-4''), 136.15 (C-2);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{19}\text{ClN}$, $[\text{M}+\text{H}]$: 296.1206, found 296.1210.

4-(1-(2-chlorophenyl)-3-phenylprop-2-ynyl)morpholine (Table 3, entry 10)

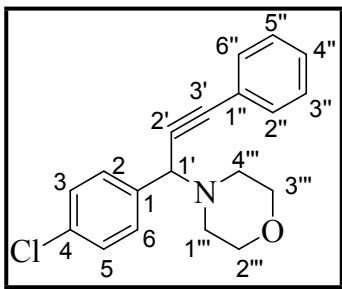


^1H NMR (500 MHz, CDCl_3): δ = 2.66-2.67 (m, 4H, H-1''' & H-4'''), 3.66-3.74 (m, 4H, H-2''' & H-3'''), 5.12 (s, 1H, H-1'), 7.23-7.29 (m, 2H, ArH), 7.31-7.33 (m, 3H, ArH), 7.39-7.41 (m, 1H, ArH), 7.47-7.50 (m, 2H, H-2'' & H-6''), 7.73-7.75 (m, 1H, H-4'');

^{13}C NMR (125 MHz, CDCl_3): δ = 49.84 (C-1''' & C-4'''), 58.94 (C-1'), 67.13 (C-2''' & C-3'''), 84.69 (C-2'), 88.36 (C-3'), 122.81 (C-5), 126.37 (C-3), 128.36 (C-4 & C-6), 128.39 (C-1), 129.16 (C-5''), 129.93 (C-3''), 130.56 (C-1''), 131.83 (C-2'' & C-6''), 134.67 (C-4''), 135.55 (C-2);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{19}\text{ClNO}$, $[\text{M}+\text{H}]$: 312.1155, found 312.1149.

4-(1-(4-chlorophenyl)-3-phenylprop-2-ynyl)morpholine (Table 3, entry 11)

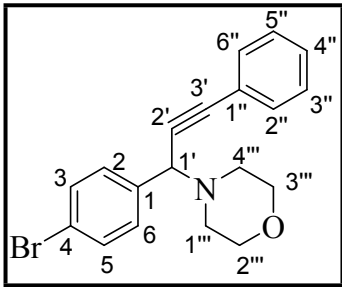


$^1\text{H NMR}$ (500 MHz, CDCl_3): δ = 2.60-2.61 (m, 4H, H-1''' & H-4'''), 3.68-3.76 (m, 4H, H-2''' & H-3'''), 4.75 (s, 1H, H-1'), 7.31-7.34 (m, 5H, ArH), 7.49-7.51 (m, 2H, ArH), 7.56-7.59 (m, 2H, H-2'' & H-6'');

$^{13}\text{C NMR}$ (125 MHz, CDCl_3): δ = 49.81 (C-1''' & C-4'''), 61.39 (C-1'), 67.13 (C-2''' & C-3'''), 84.37 (C-2'), 88.94 (C-3'), 122.73 (C-1), 128.41 (C-2, C-3, C-5 & C-6), 128.45 (C-1''), 129.92 (C-3'' & C-5''), 131.84 (C-2'' & C-6''), 133.60 (C-4''), 136.47 (C-4);

HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{19}\text{ClNO}$, $[\text{M}+\text{H}]$: 312.1155, found 312.1153.

4-(1-(4-bromophenyl)-3-phenylprop-2-ynyl)morpholine (Table 3, entry 12)



$^1\text{H NMR}$ (500 MHz, CDCl_3): δ = 2.60-2.61 (m, 4H, H-1''' & H-4'''), 3.69-3.76 (m, 4H, H-2''' & H-3'''), 4.73 (s, 1H, H-1'), 7.32-7.35 (m, 3H, ArH), 7.47-7.53 (m, 6H, ArH);

$^{13}\text{C NMR}$ (125 MHz, CDCl_3): δ = 49.81 (C-1''' & C-4'''), 61.44 (C-1'), 67.14 (C-2''' & C-3'''), 84.28 (C-2'), 88.97 (C-3'), 122.71 (C-1), 128.40 (C-3 & C-5), 128.54 (C-1''), 130.29 (C-2 & C-6), 131.38 (C-3'', C-4'' & C-5''), 131.84 (C-2'' & C-6''), 137.01 (C-4);

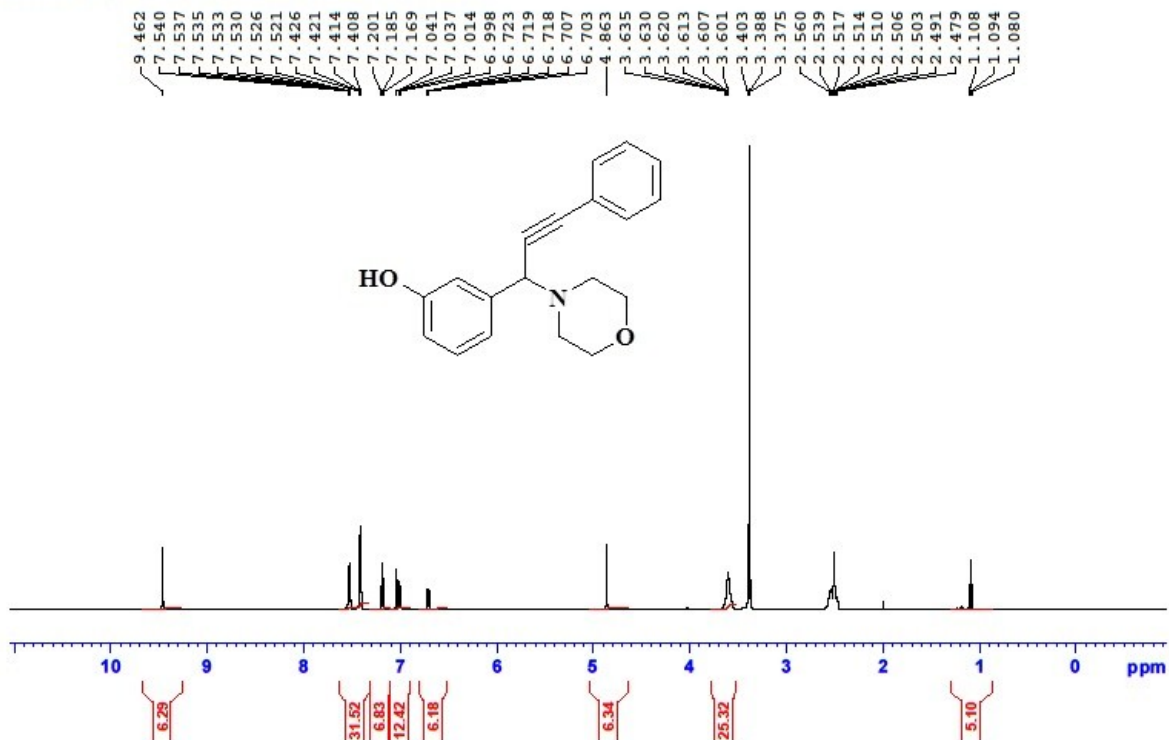
HRMS (ESI) m/z calcd. for $\text{C}_{19}\text{H}_{19}\text{BrNO}$, $[\text{M}+\text{H}]$: 356.0650, 358.0629, found 356.0653, 358.0634.

**III. ^1NMR , ^{13}C NMR and HRMS spectra of propargylamine derivatives
(Table 3, Entries 1 to 12)**

¹H NMR (Table 3, Entry 1)

DB-127

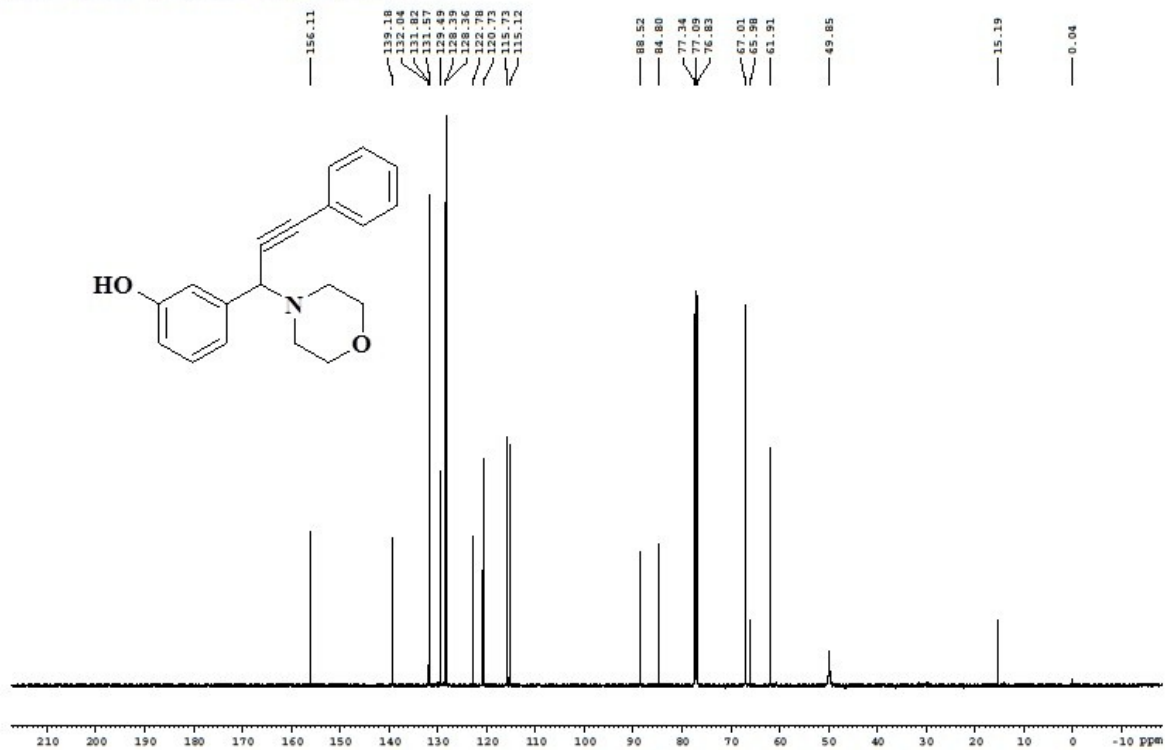
Proton_spin DMSO {E:\AWATE COLLEGE} Snehal 17



¹³C NMR (Table 3, Entry 1)

DB-127

C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 9

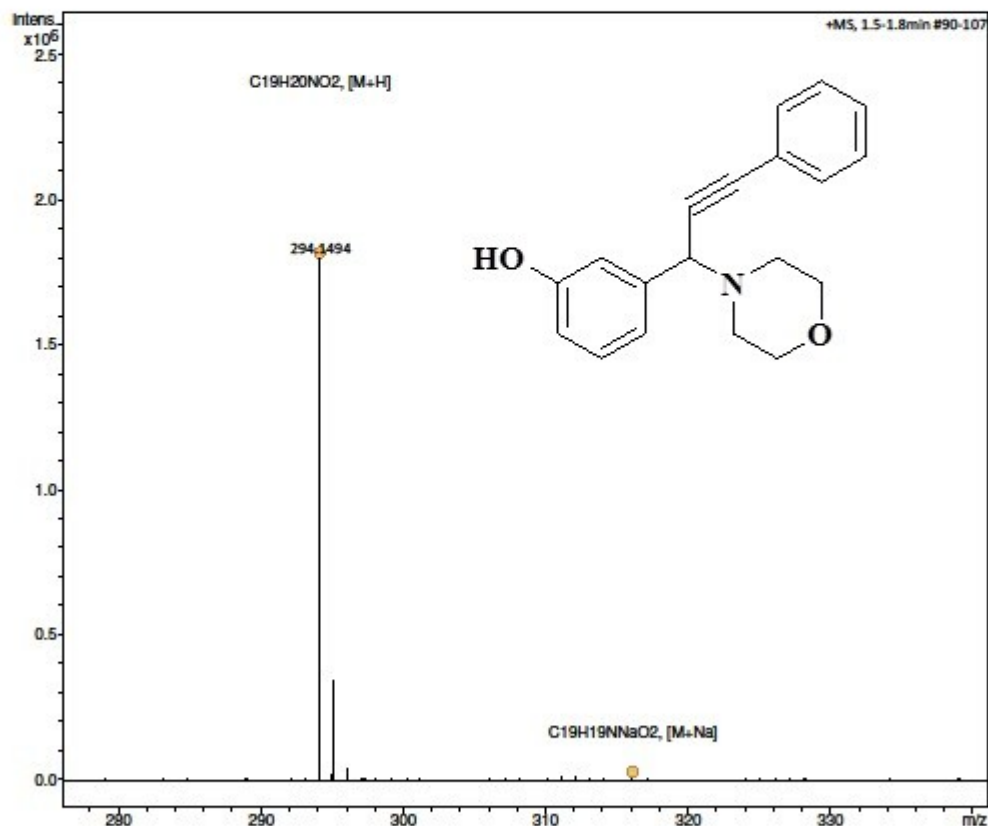


HRMS (Table 3, Entry 1)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info		Acquisition Date	10/7/2017 11:44:23 AM	
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Method	dlo-ms600mz_10min.m	Operator	CIF	
Sample Name	DB-127	Instrument	impact HD	1819696.00184
Comment				

Acquisition Parameter					
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Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
294.1494	1	C ₁₉ H ₂₀ NO ₂	294.1489	-1.9	12.7	1	100.00	10.5	even			ok	M+H
316.1310	1	C ₁₉ H ₁₉ NNaO ₂	316.1308	-0.7	9.3	1	100.00	10.5	even			ok	M+Na

DB-127_BE4_01_4439.d

Bruker Compass DataAnalysis 4.2

printed: 10/7/2017 12:01:21 PM

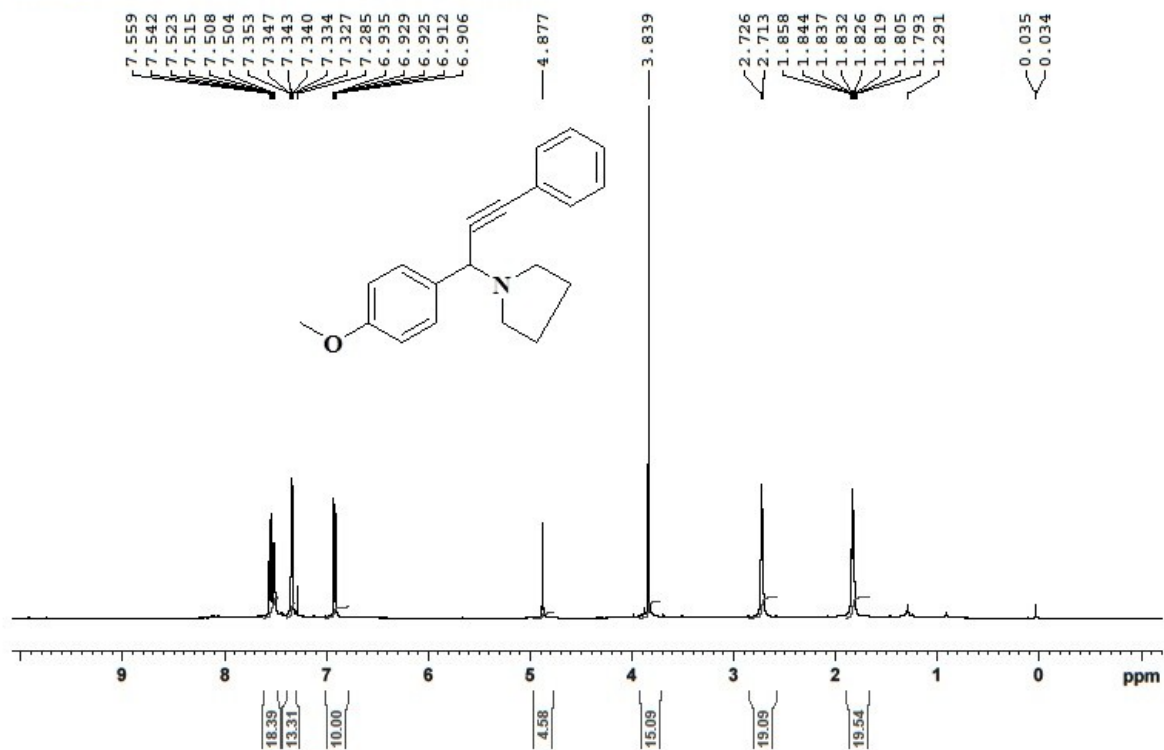
by: CIF

Page 1 of 1

¹H NMR (Table 3, Entry 2)

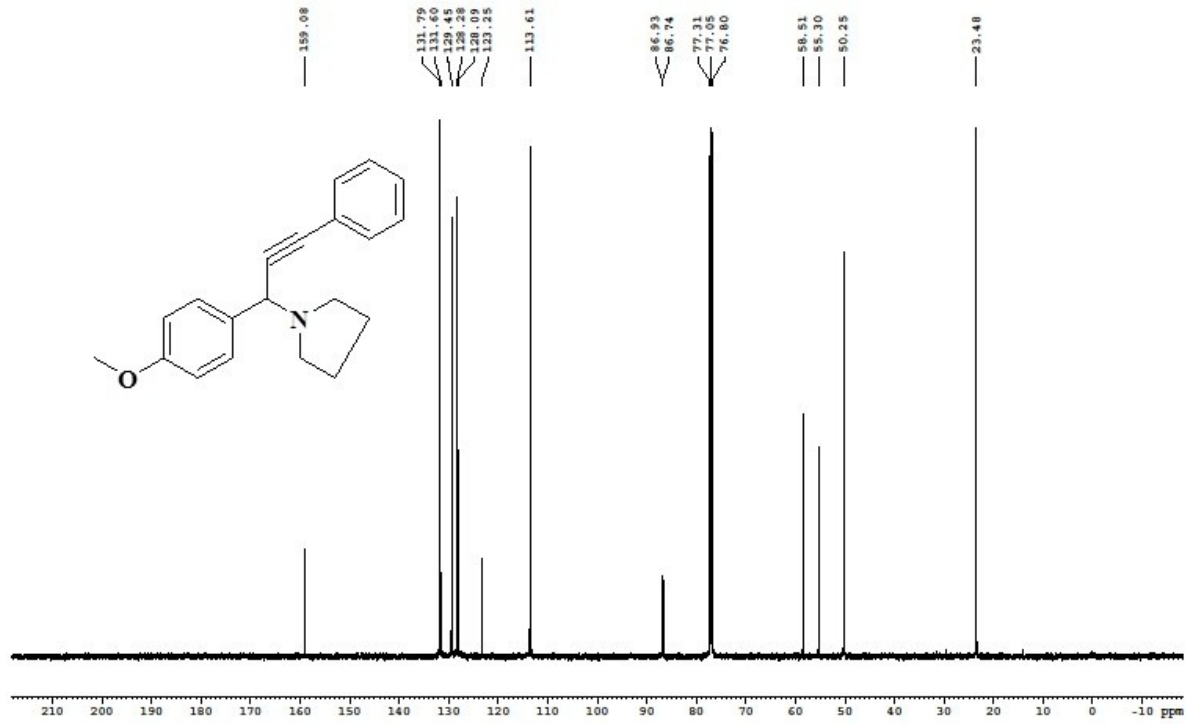
DB-123

PROTON_DepttChem CDCl₃ {D:\AWATE COLLEGE} Snehal 9



¹³C NMR (Table 3, Entry 2)

DB-123
C13CPD CDCl3 {D:\AWATE COLLEGE} Snehal 9



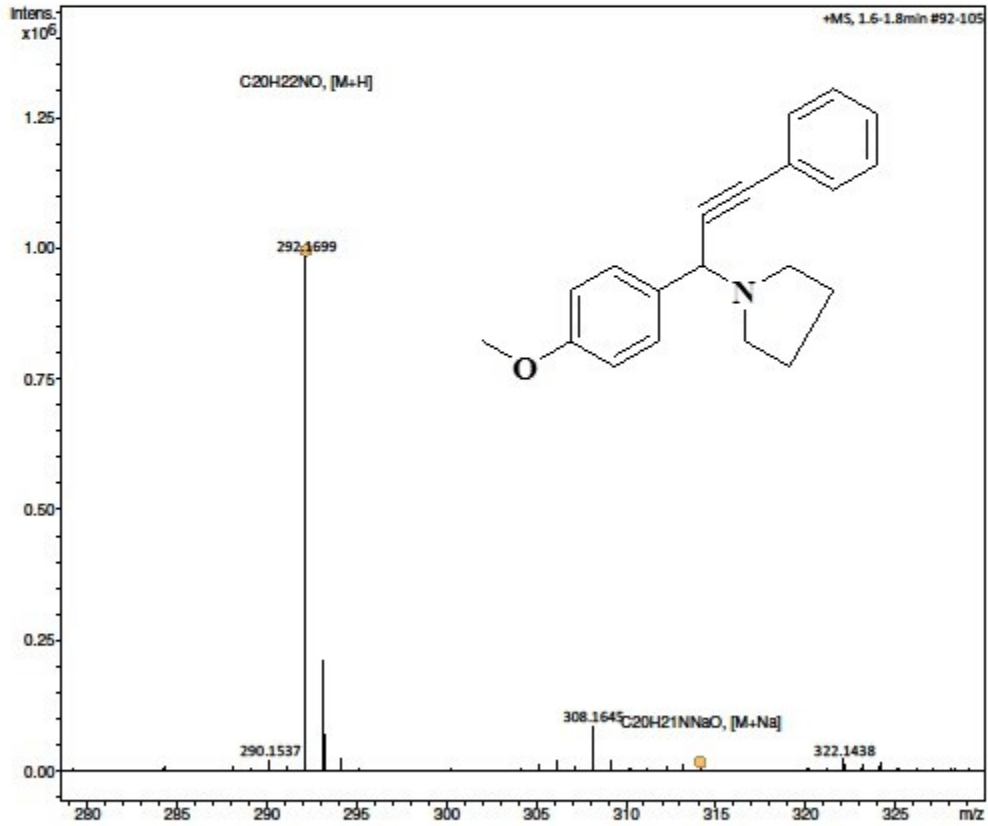
HRMS (Table 3, Entry 2)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info
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 Sample Name DB -123
 Comment
 Acquisition Date 8/10/2017 12:13:56 PM
 Operator CIF
 Instrument impact HD 1819696.00184

Acquisition Parameter

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		Set Corona	0 nA	Set APCI Heater	0 °C

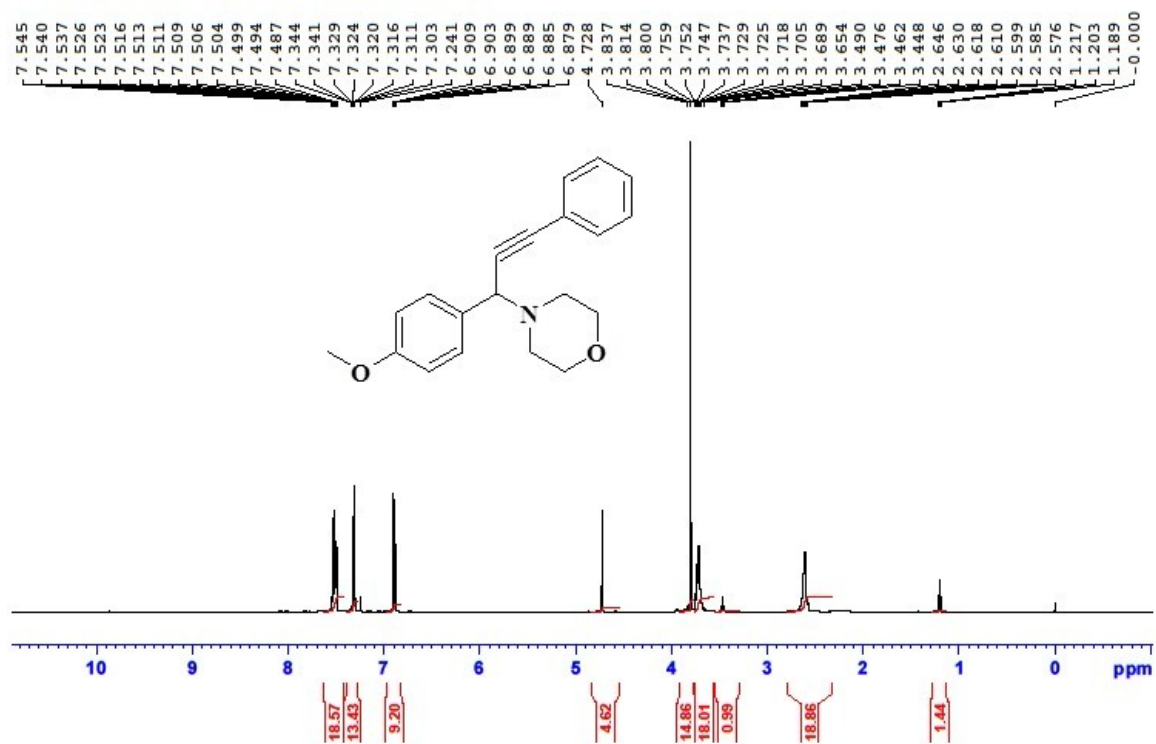


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
292.1699	1	C ₂₀ H ₂₂ NO	292.1696	-0.9	6.4	1	100.00	10.5	even		ok	M+H
314.1534	1	C ₂₀ H ₂₁ NNaO	314.1515	-6.1	90.6	1	100.00	10.5	even		ok	M+Na

¹H NMR (Table 3, Entry 3)

DB-130

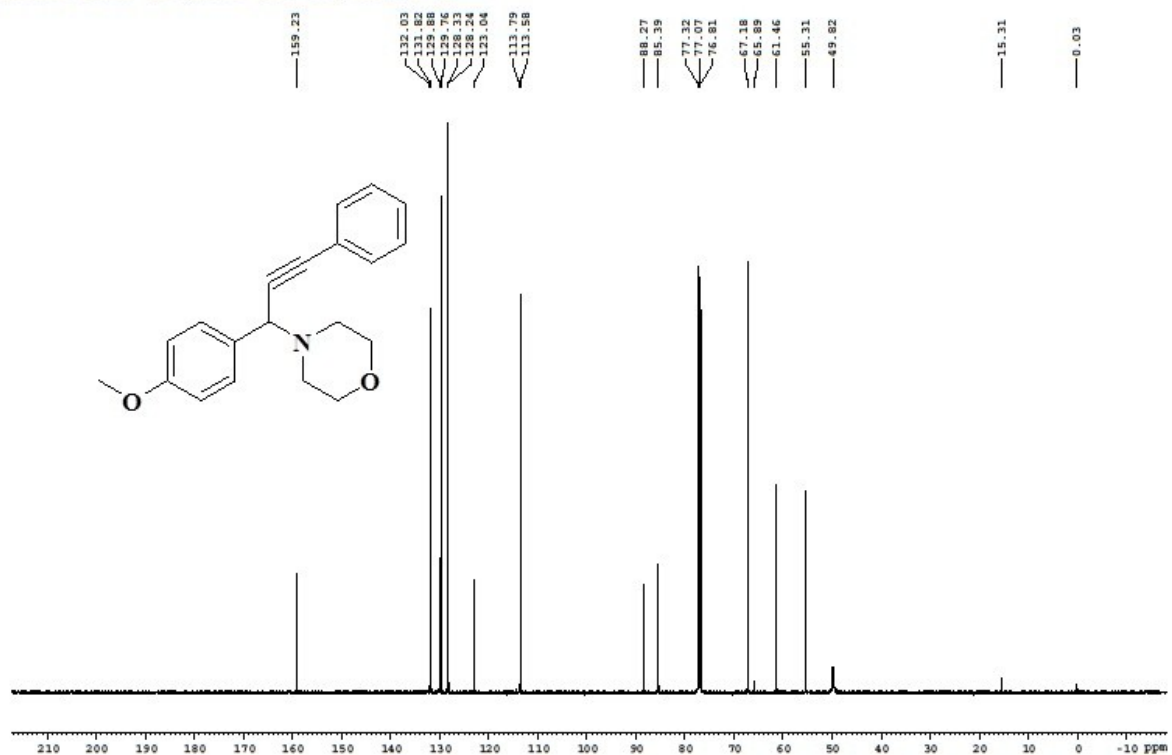
Proton_spin CDCl3 {E:\AWATE COLLEGE} Snehal 13



¹³C NMR (Table 3, Entry 3)

DB-130

C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 12

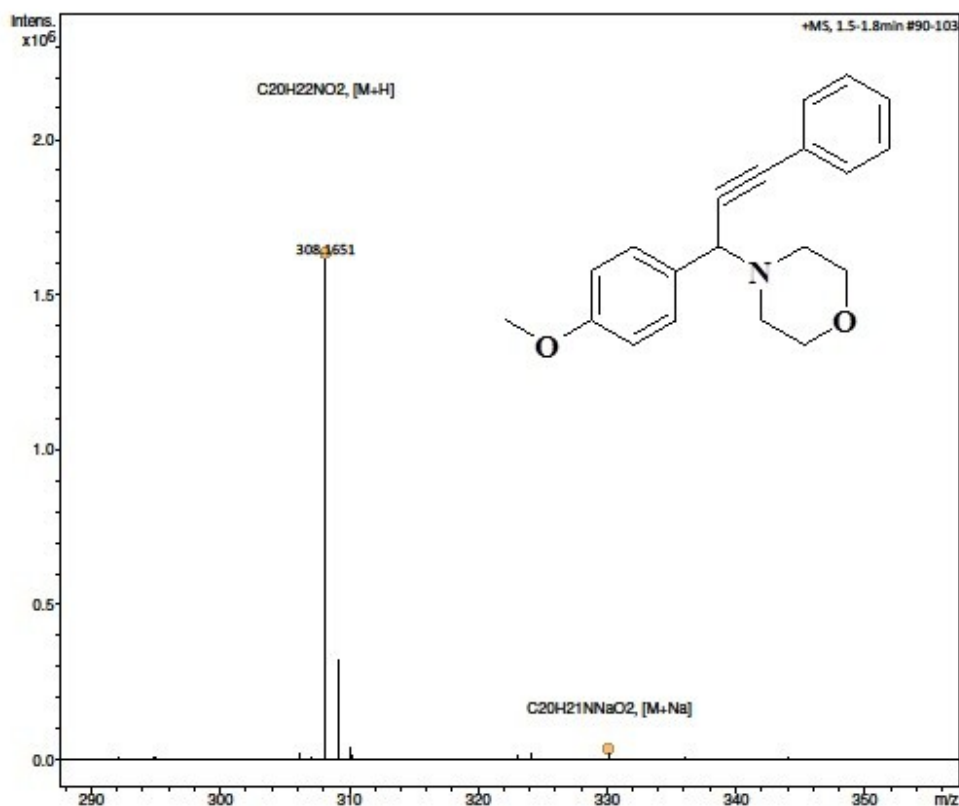


HRMS (Table 3, Entry 3)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info		Acquisition Date	10/7/2017 2:54:29 PM	
Analysis Name	D:\Data\2017\SEPTEMBER\SPPU AFFILIATED\ANNASAHEB AWATE COLLEGE MANCHARI K G KANADE\BANKAR D B\DB-130_BE7_01_4442.d			
Method	dio-ms600mz_10min.m	Operator	CIF	
Sample Name	DB-130	Instrument	impact HD	1819696.00184
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulzer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
308.1651	1	C20H22NO2	308.1645	-2.1	14.1	1	100.00	10.5	even		ok	M+H
330.1469	1	C20H21NNaO2	330.1464	-1.3	16.2	1	100.00	10.5	even		ok	M+Na

DB-130_BE7_01_4442.d

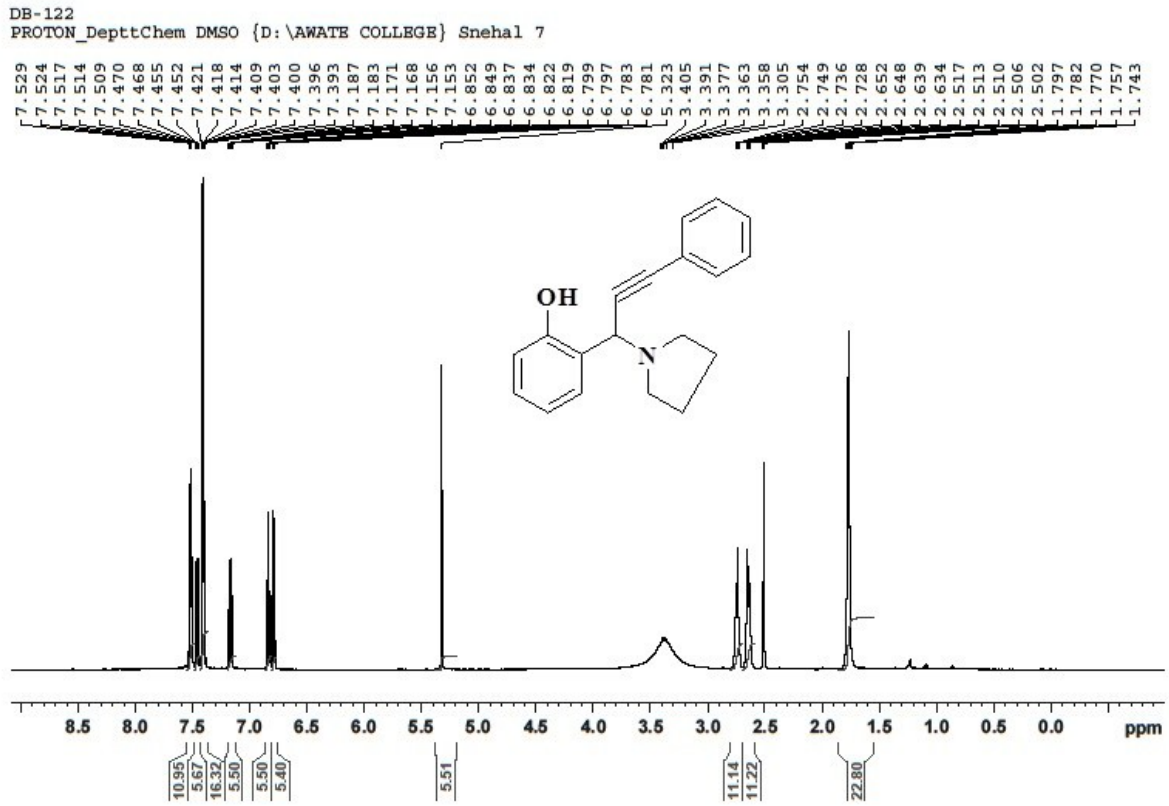
Bruker Compass DataAnalysis 4.2

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by: CIF

Page 1 of 1

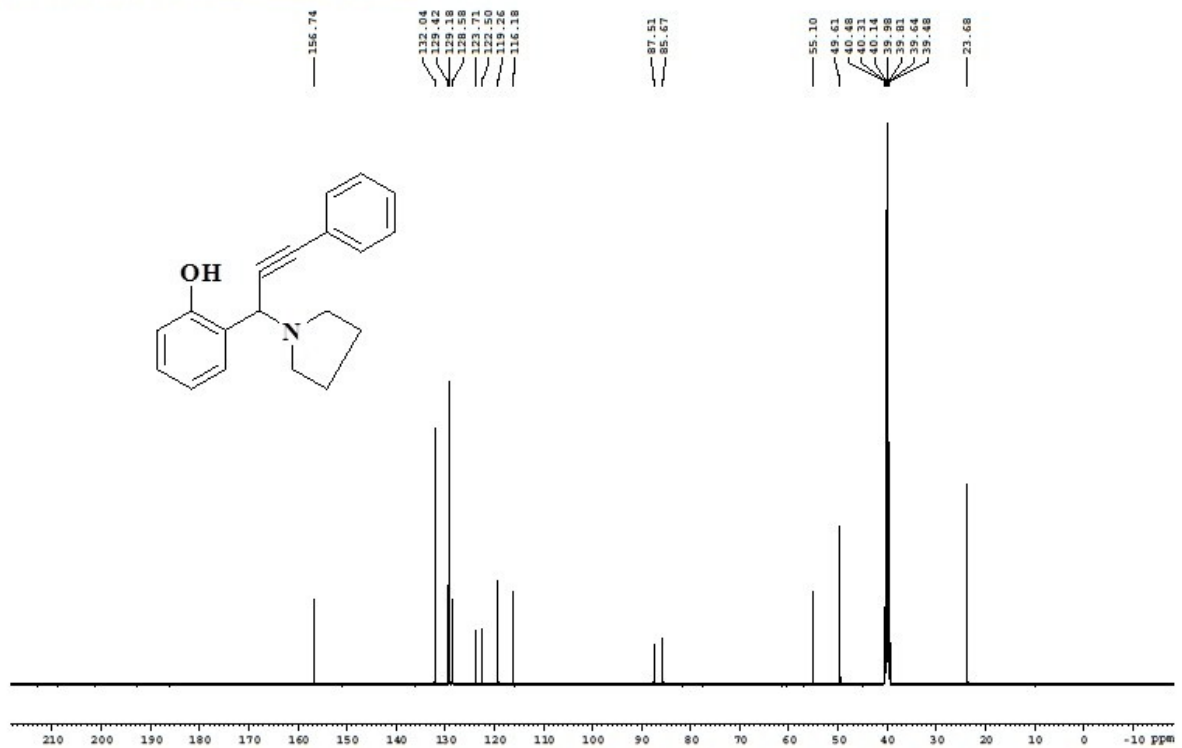
¹H NMR (Table 3, Entry 4)



¹³C NMR (Table 3, Entry 4)

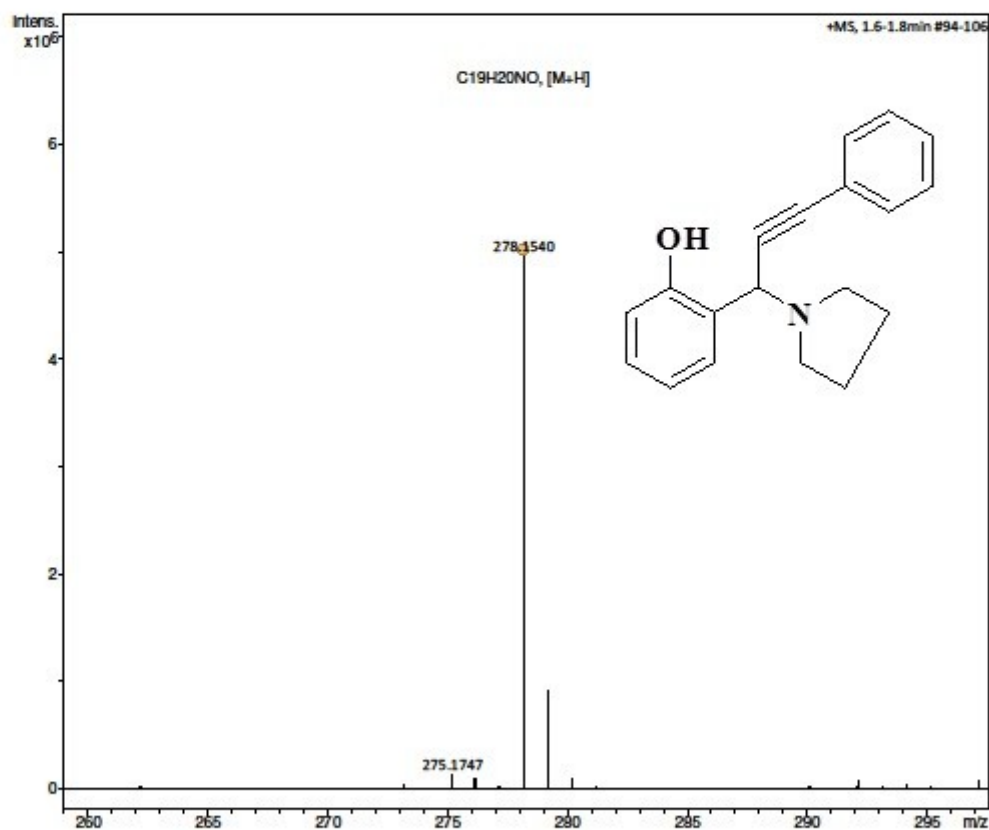
DB-122

C13CPD DMSO {D:\AWATE COLLEGE} Snehal 7



HRMS (Table 3, Entry 4)

Savitribai Phule Pune University - Central Instrumentation Facility					
Analysis Info			Acquisition Date 8/10/2017 11:58:57 AM		
Analysis Name	D:\Data\2017\JUNE\SPPU AFFILIATED\A AWATE COLLEGE, MANCHAR\KG KANADE\DB BANKAR\DB -122_BD7_01_4164.d				
Method	dlo-ms600mz_10min.m		Operator	CIF	
Sample Name	DB -122		Instrument	impact HD	1819696.00184
Comment					
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulzer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
278.1540	1	C19H20NO	278.1539	-0.0	16.1	1	100.00	10.5	even		ok	M+H

DB -122_BD7_01_4164.d

Bruker Compass DataAnalysis 4.2

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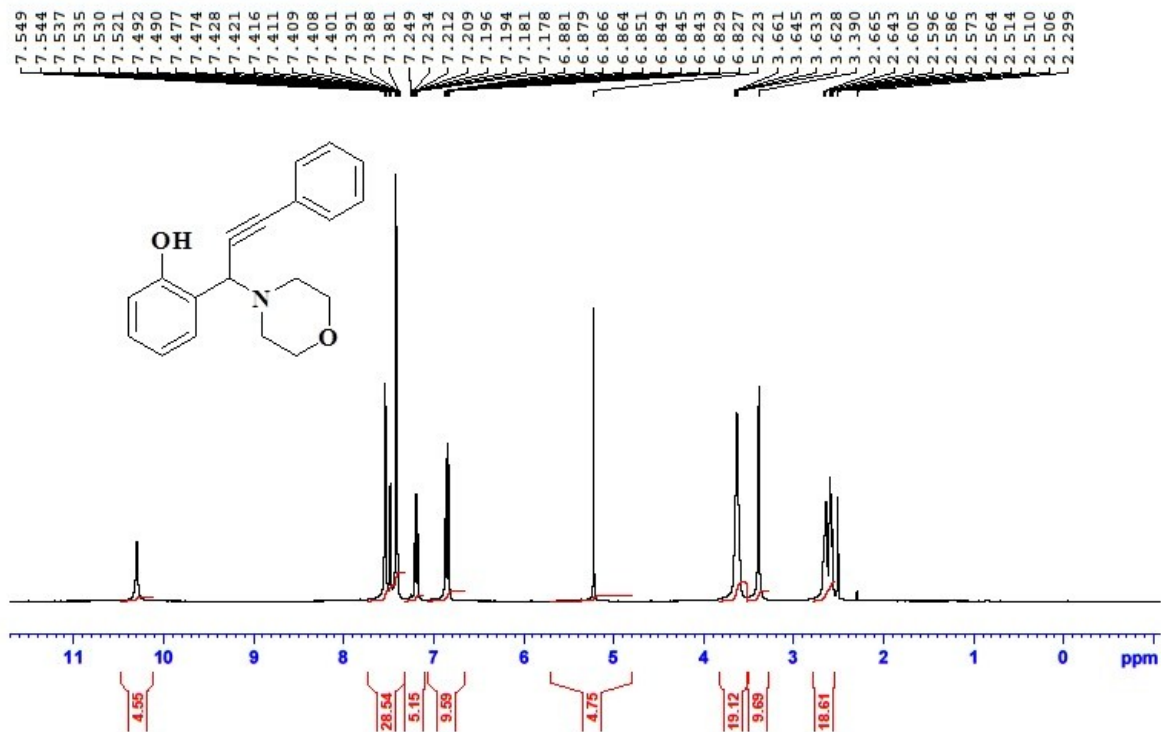
by: CIF

Page 1 of 1

¹H NMR (Table 3, Entry 5)

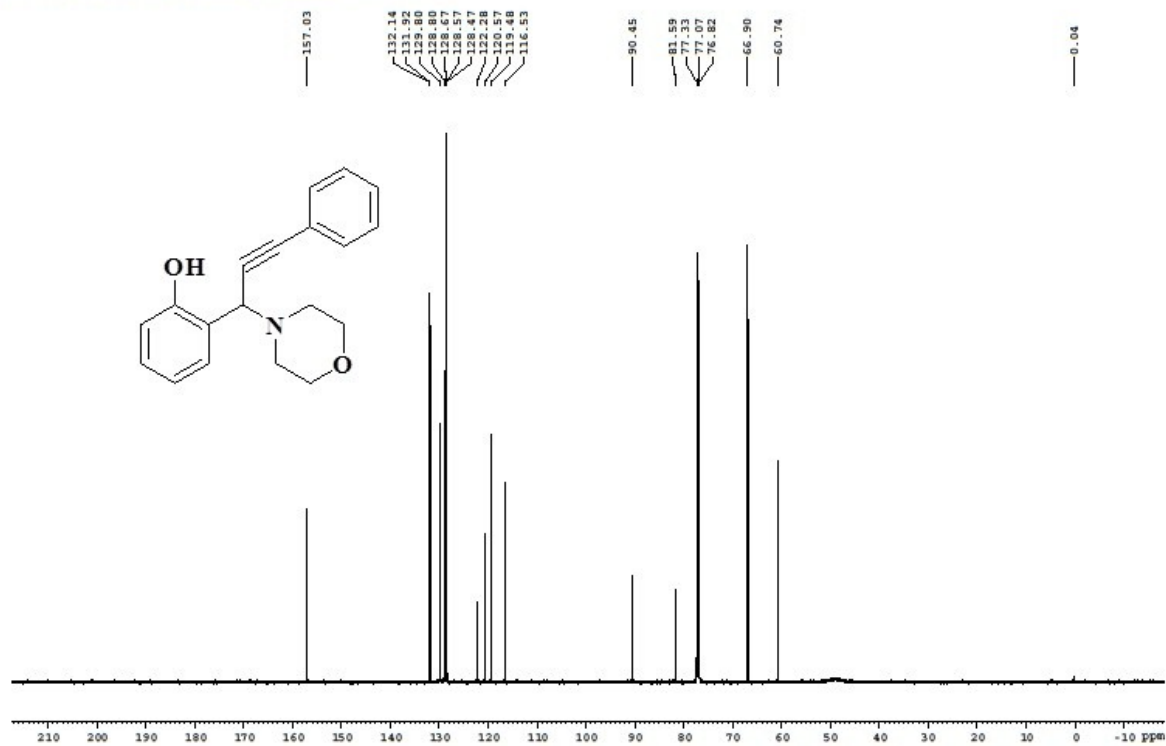
DB-128

Proton_spin DMSO {E:\AWATE COLLEGE} Snehal 18



¹³C NMR (Table 3, Entry 5)

DB-128
C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 10



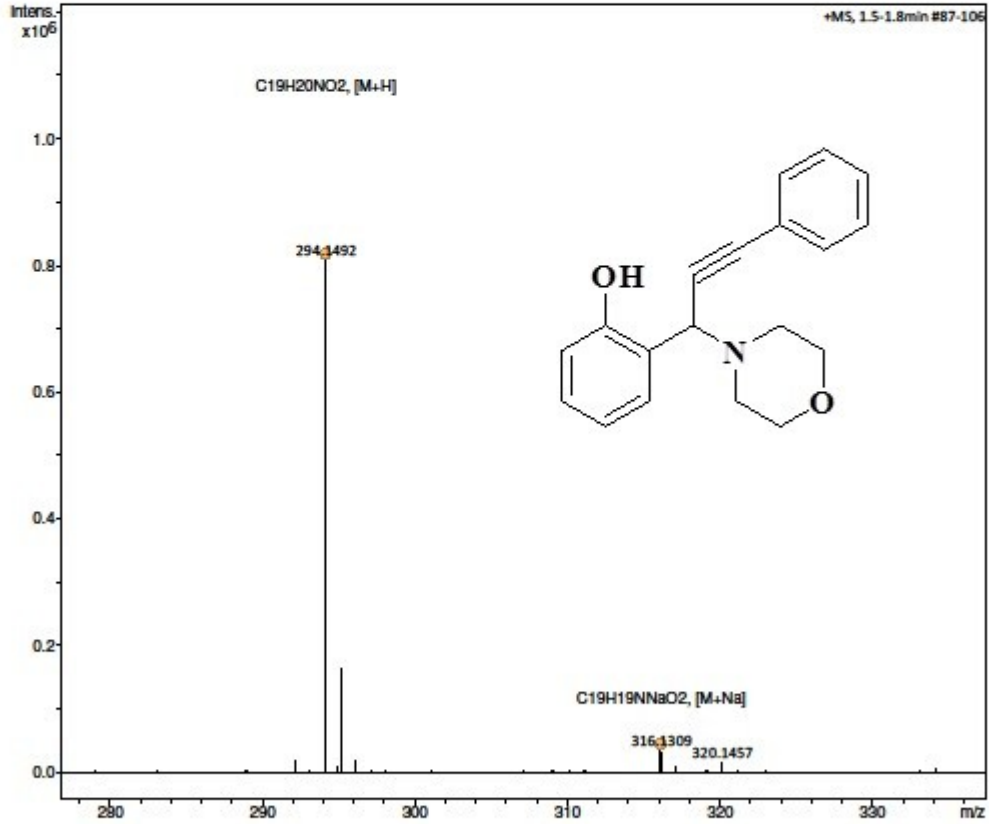
HRMS (Table 3, Entry 5)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info
 Analysis Name: D:\Data\2017\SEPTEMBER\SPPU AFFILIATED\ANNASAHEB AWATE COLLEGE MANCHAR\K G KANADE\BANKAR D B\DB-127_BE5_01_4440.d
 Method: dlc-ms600mz_10min.m
 Sample Name: DB-127
 Comment:
 Acquisition Date: 10/7/2017 2:24:14 PM
 Operator: CIF
 Instrument: impact HD
 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
294.1492	1	C ₁₉ H ₂₀ NO ₂	294.1489	-1.2	6.8	1	100.00	10.5	even		ok	M+H
316.1309	1	C ₁₉ H ₁₉ NNaO ₂	316.1308	-0.2	2.5	1	100.00	10.5	even		ok	M+Na

DB-127_BE5_01_4440.d

Bruker Compass DataAnalysis 4.2

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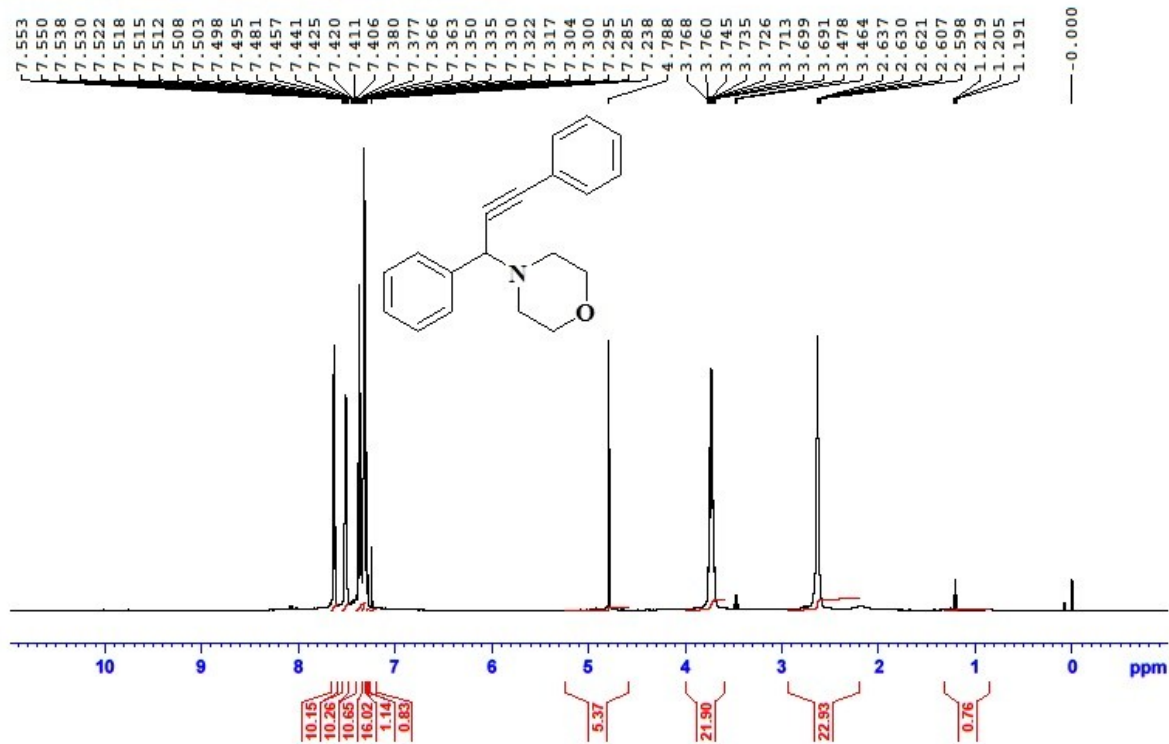
by: CIF

Page 1 of 1

¹H NMR (Table 3, Entry 6)

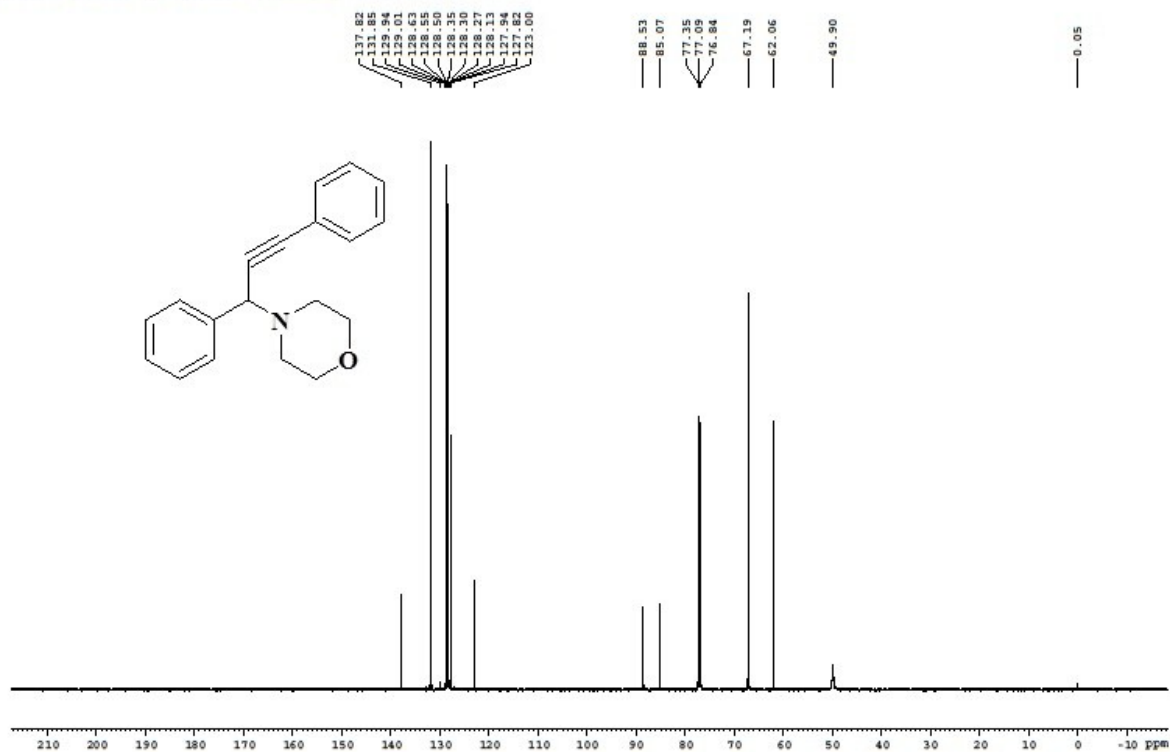
DB-132

Proton_spin CDCl3 {E:\AWATE COLLEGE} Snehal 15



¹³C NMR (Table 3, Entry 6)

DB-132
C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 14



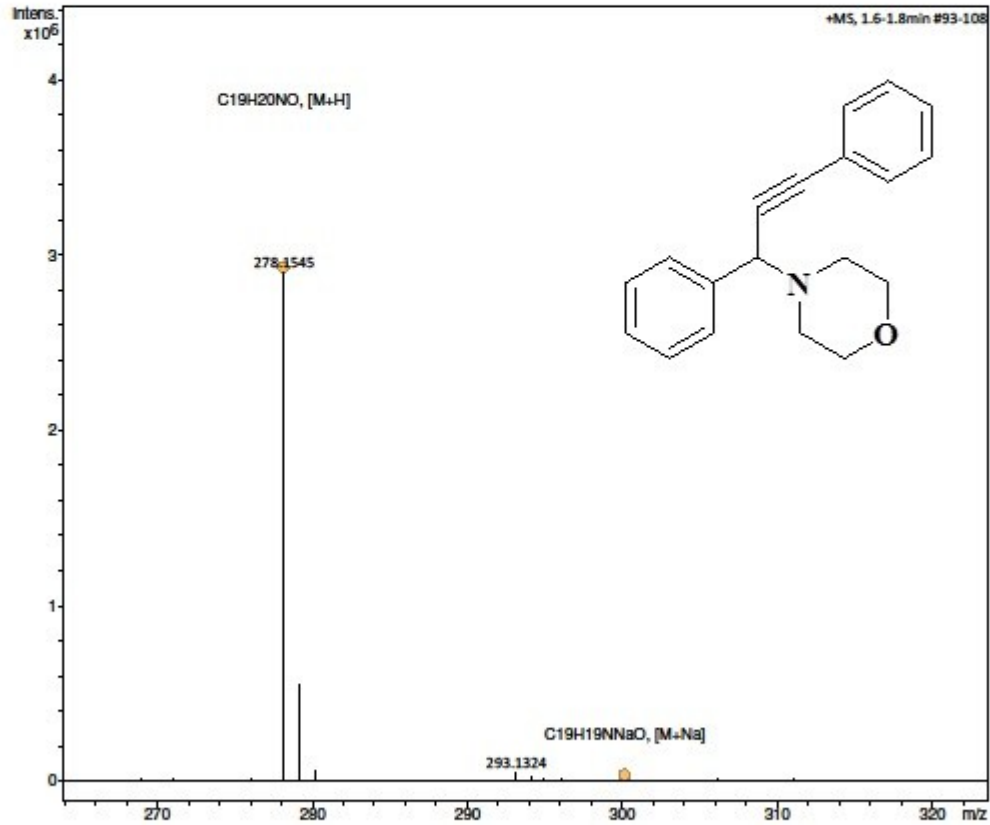
HRMS (Table 3, Entry 6)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info
 Analysis Name: D:\Data\2017\SEPTEMBER\SPPU AFFILIATED\ANNASAHEB AWATE COLLEGE MANCHAR\K G KANADE\BANKAR D B\DB-132_BD8_01_4444.d
 Method: dlc-ms600mz_10min.m
 Sample Name: DB-132
 Comment:
 Acquisition Date: 10/7/2017 3:19:15 PM
 Operator: CIF
 Instrument: impact HD
 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulzer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
278.1545	1	C19H20NO	278.1539	-2.1	14.3	1	100.00	10.5	even		ok	M+H
300.1365	1	C19H19NNaO	300.1359	-2.1	451.4	1	100.00	10.5	even		ok	M+Na

DB-132_BD8_01_4444.d

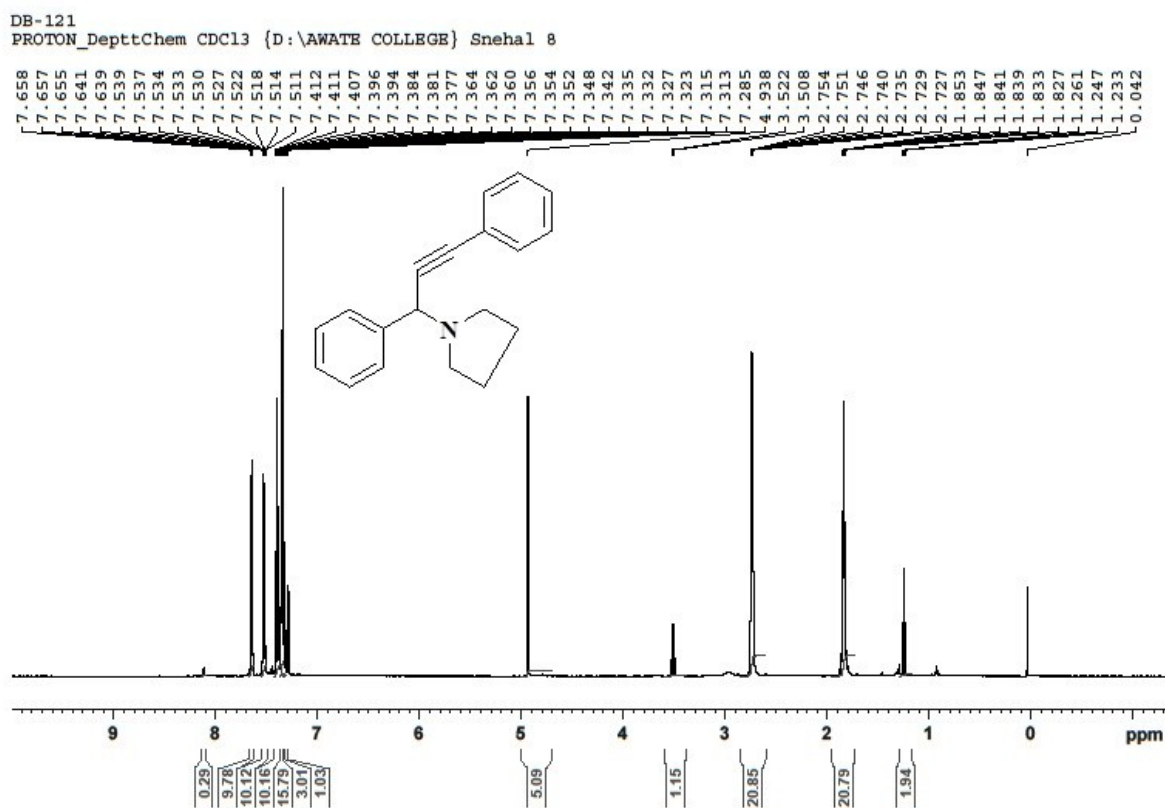
Bruker Compass DataAnalysis 4.2

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by: CIF

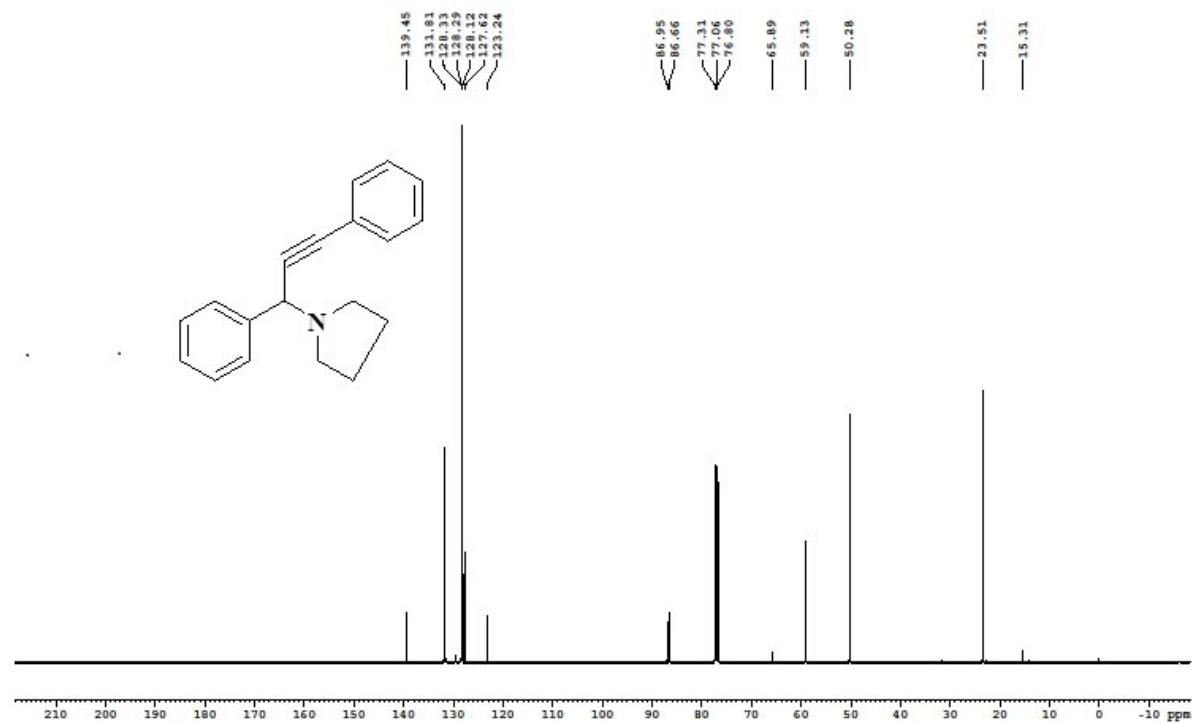
Page 1 of 1

¹H NMR (Table 3, Entry 7)



¹³C NMR (Table 3, Entry 7)

DB-121
C13CPD CDC13 {D:\AWATE COLLEGE} Snehal 8



HRMS (Table 3, Entry 7)

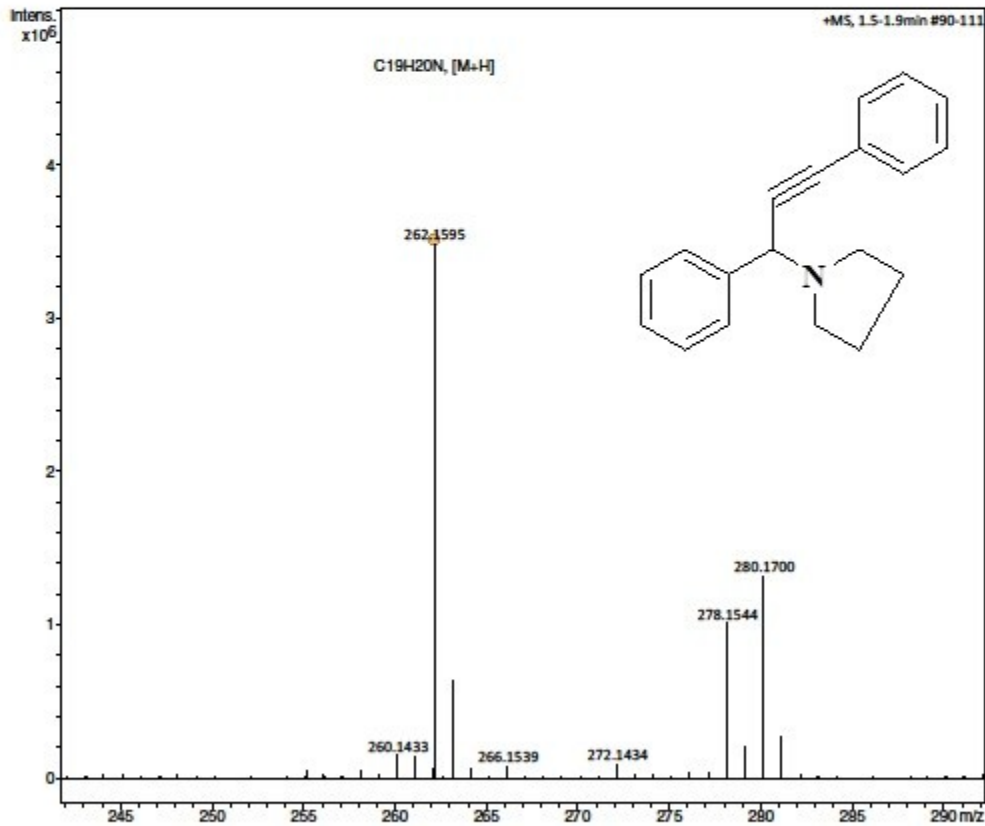
Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info
 Analysis Name D:\Data\2017\JUNE\SPPU AFFILIATED\A AWATE COLLEGE, MANCHAR\KG KANADE\DB BANKAR\DB -121_BD6_01_4163.d
 Method dlo-ms600mz_10min.m
 Sample Name DB -121
 Comment

Acquisition Date 8/10/2017 11:33:18 AM
 Operator CIF
 Instrument impact HD 1819696.00184

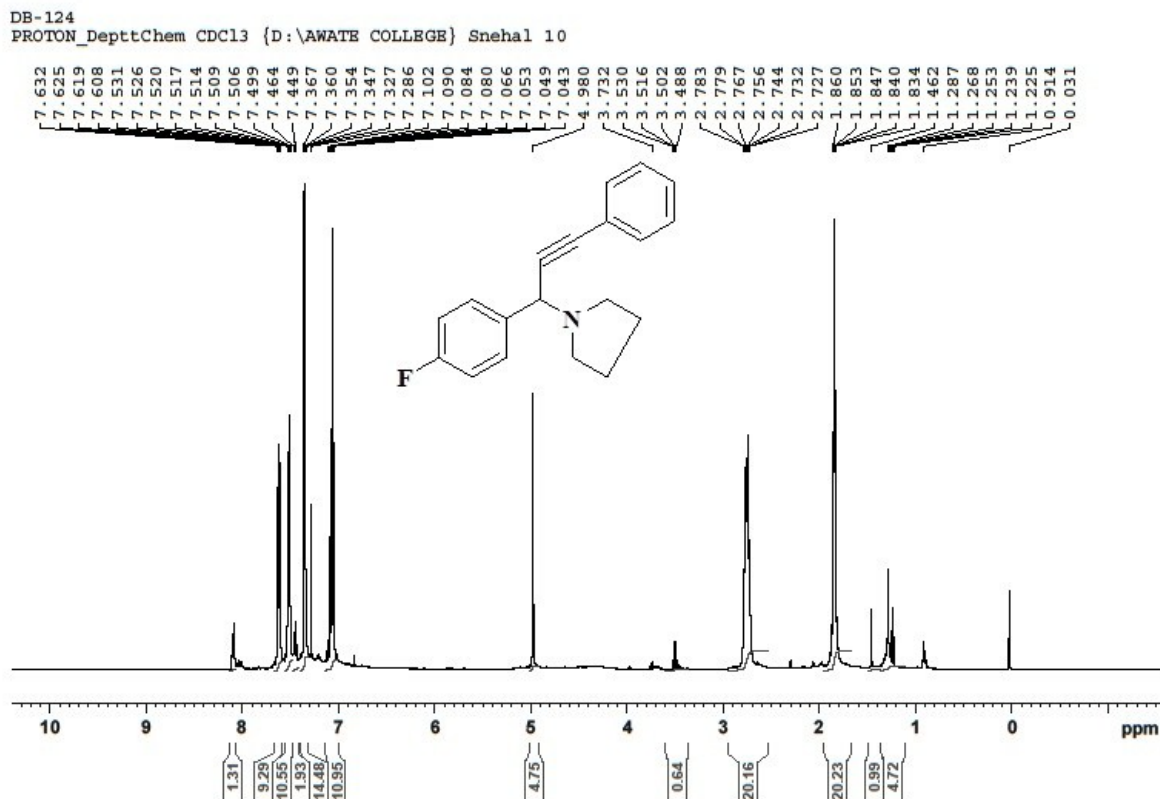
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



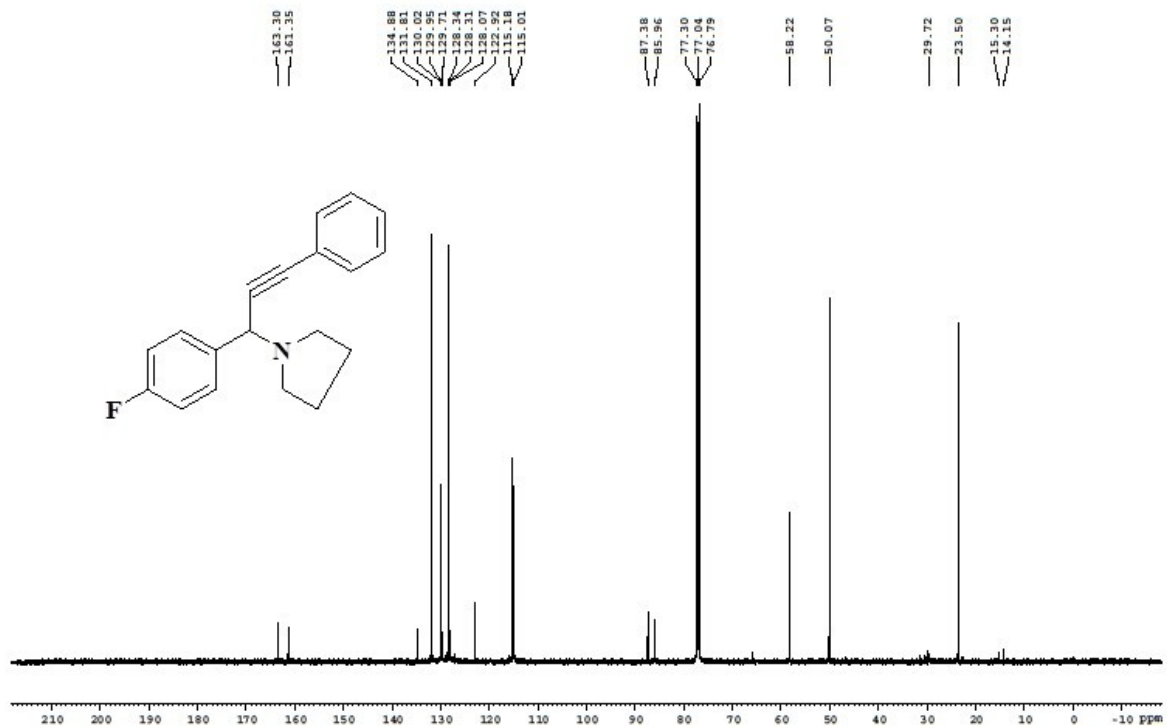
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
262.1595	1	C ₁₉ H ₂₀ N	262.1590	-1.7	17.0	1	100.00	10.5	even		ok

¹H NMR (Table 3, Entry 8)



¹³C NMR (Table 3, Entry 8)

DB-124
C13CPD CDC13 {D:\AWATE COLLEGE} Snehal 10



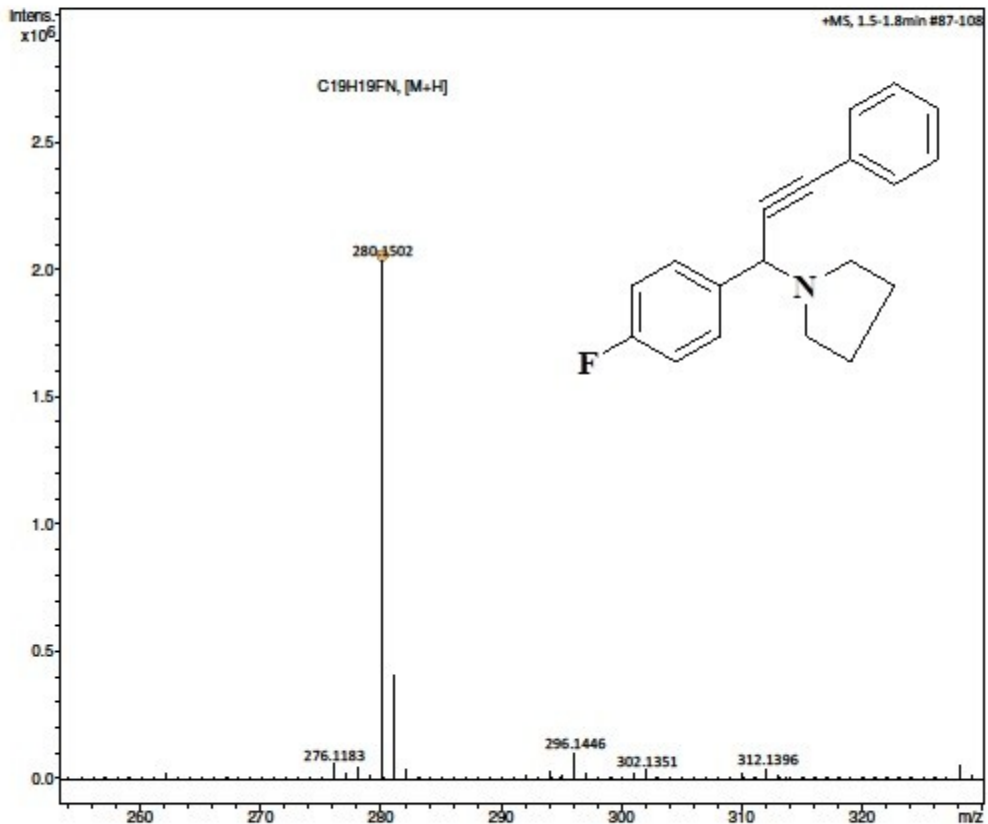
HRMS (Table 3, Entry 8)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info
 Analysis Name: D:\Data\2017\JUNE\SPPU AFFILIATED\A AWATE COLLEGE, MANCHAR\KG KANADE\DB BANKAR\DB -124_BE1_01_4166.d
 Method: dlc-ms600mz_10min.m
 Sample Name: DB -124
 Comment:
 Acquisition Date: 8/10/2017 12:28:47 PM
 Operator: CIF
 Instrument: impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

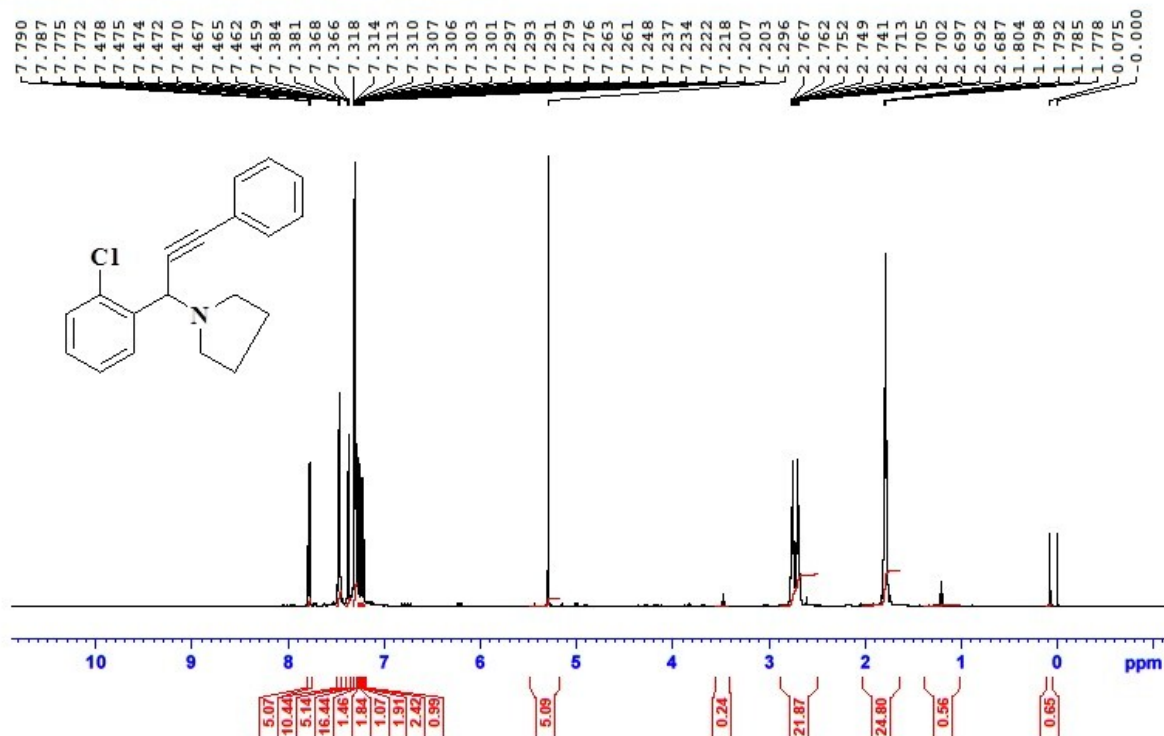


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	#	mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
280.1502	1	C ₁₉ H ₁₉ N	280.1496	-2.2	7.7	1	100.00	10.5	even			ok	M+H

¹H NMR (Table 3, Entry 9)

DB-126

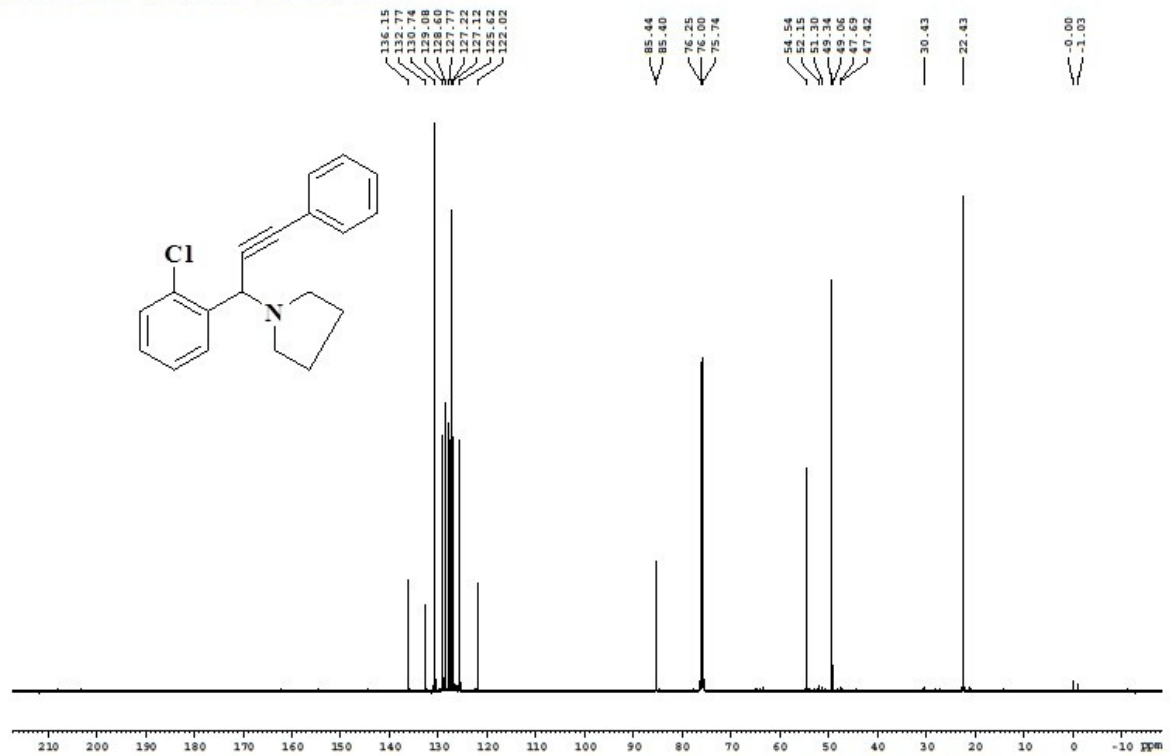
Proton_spin CDCl3 {E:\AWATE COLLEGE} Snehal 11



¹³C NMR (Table 3, Entry 9)

DB-126

C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 8



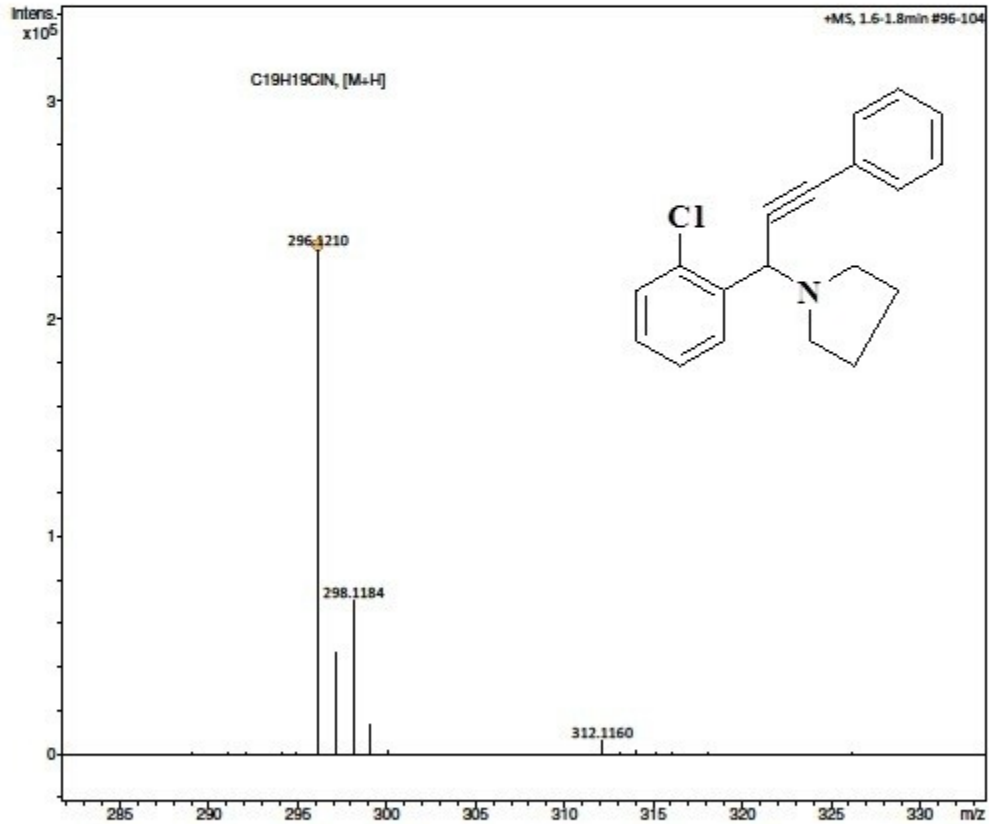
HRMS (Table 3, Entry 9)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info
 Analysis Name: D:\Data\2017\SEPTEMBER\SPPU AFFILIATED\ANNASAHEB AWATE COLLEGE MANCHARK G
 KANADE\BANKAR D B\DB-126_BD3_01_4438.d
 Method: dlc-ms350mz_10min_90b.m
 Sample Name: DB-126
 Comment:
 Acquisition Date: 10/7/2017 11:27:30 AM
 Operator: CIF
 Instrument: impact HD 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
296.1210	1	C ₁₉ H ₁₉ ClN	296.1201	-3.4	19.6	1	100.00	10.5	even		ok	M+H

DB-126_BD3_01_4438.d

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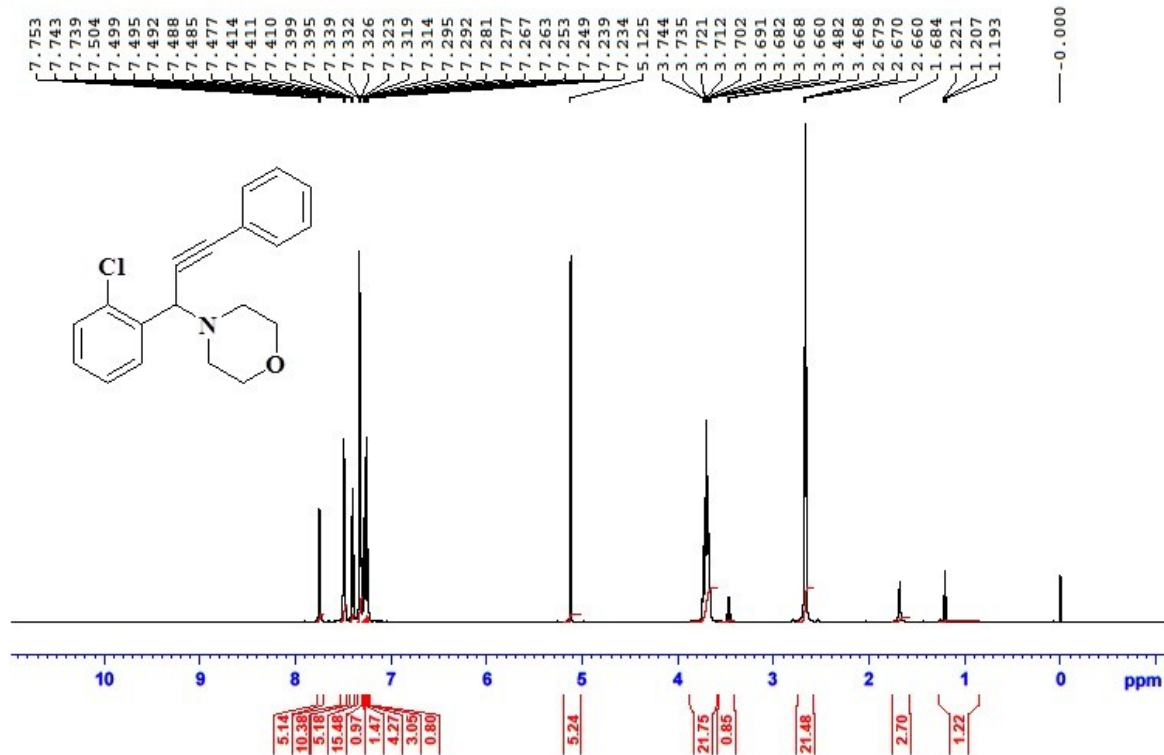
by: CIF

Page 1 of 1

¹H NMR (Table 3, Entry 10)

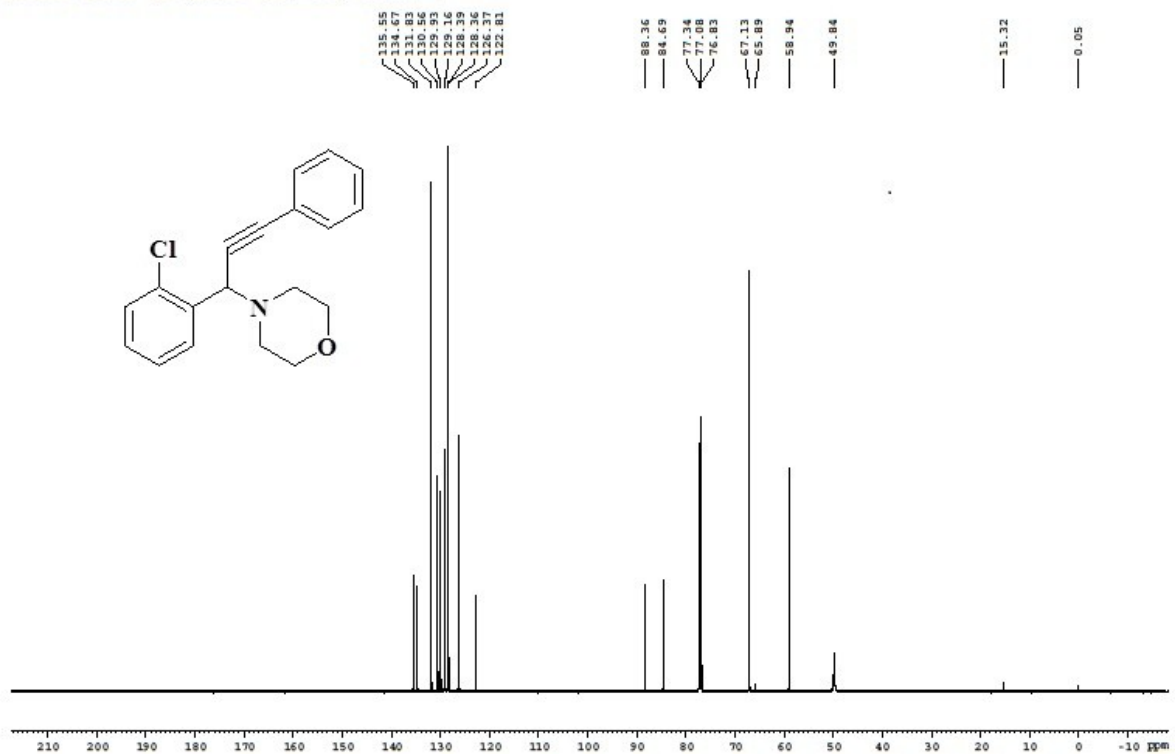
DB-125

Proton_spin CDCl3 {E:\AWATE COLLEGE} Snehal 10



¹³C NMR (Table 3, Entry 10)

DB-125
C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 7



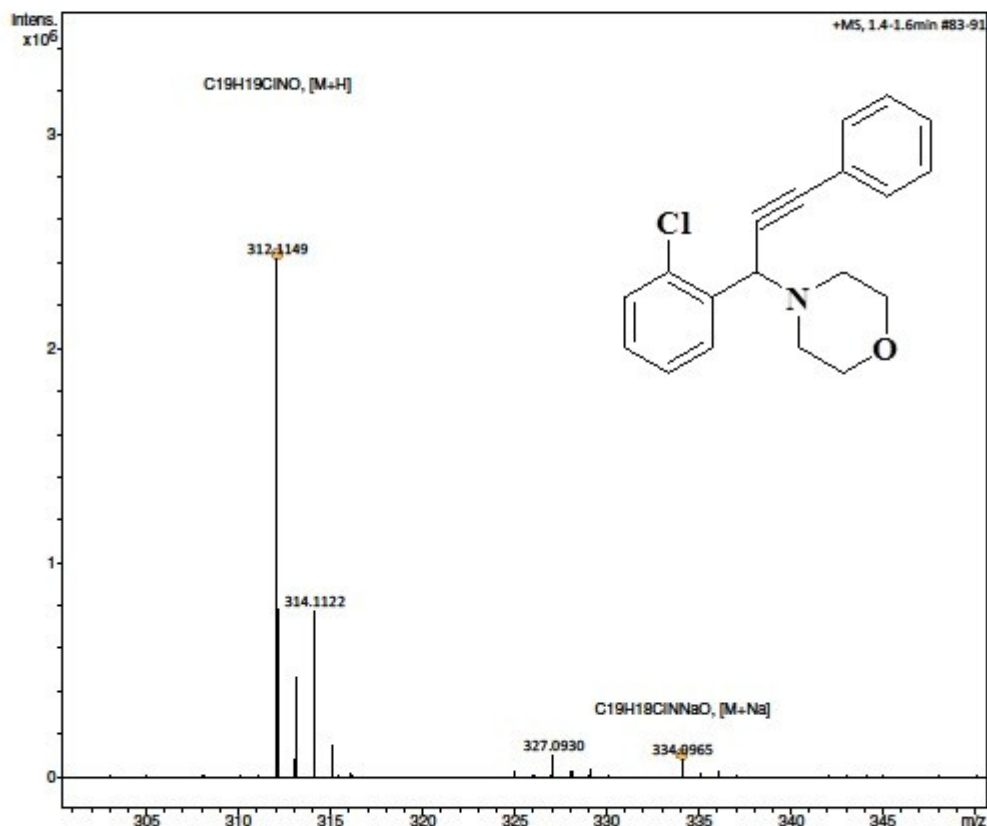
HRMS (Table 3, Entry 10)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info
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 KANADE\BANKAR D B\DB-125_BA6_01_4394.d
 Method: dlc-ms600mz_10min.m
 Sample Name: DB-125
 Comment:
 Acquisition Date: 9/27/2017 3:23:41 PM
 Operator: CIF
 Instrument: impact HD
 1819696.00184

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
312.1149	1	C ₁₉ H ₁₉ ClNO	312.1150	0.1	14.5	1	100.00	10.5	even		ok	M+H
334.0965	1	C ₁₉ H ₁₈ ClNNaO	334.0969	1.4	5.8	1	100.00	10.5	even		ok	M+Na

DB-125_BA6_01_4394.d

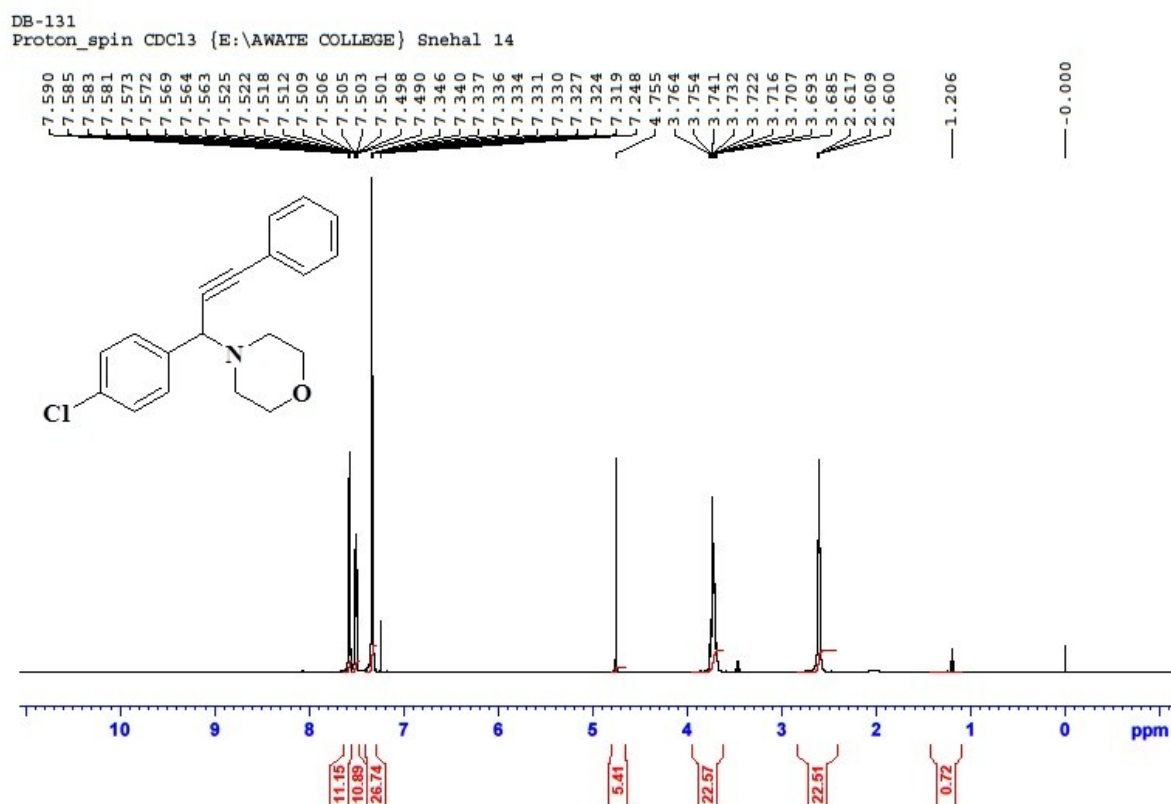
Bruker Compass DataAnalysis 4.2

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by: CIF

Page 1 of 1

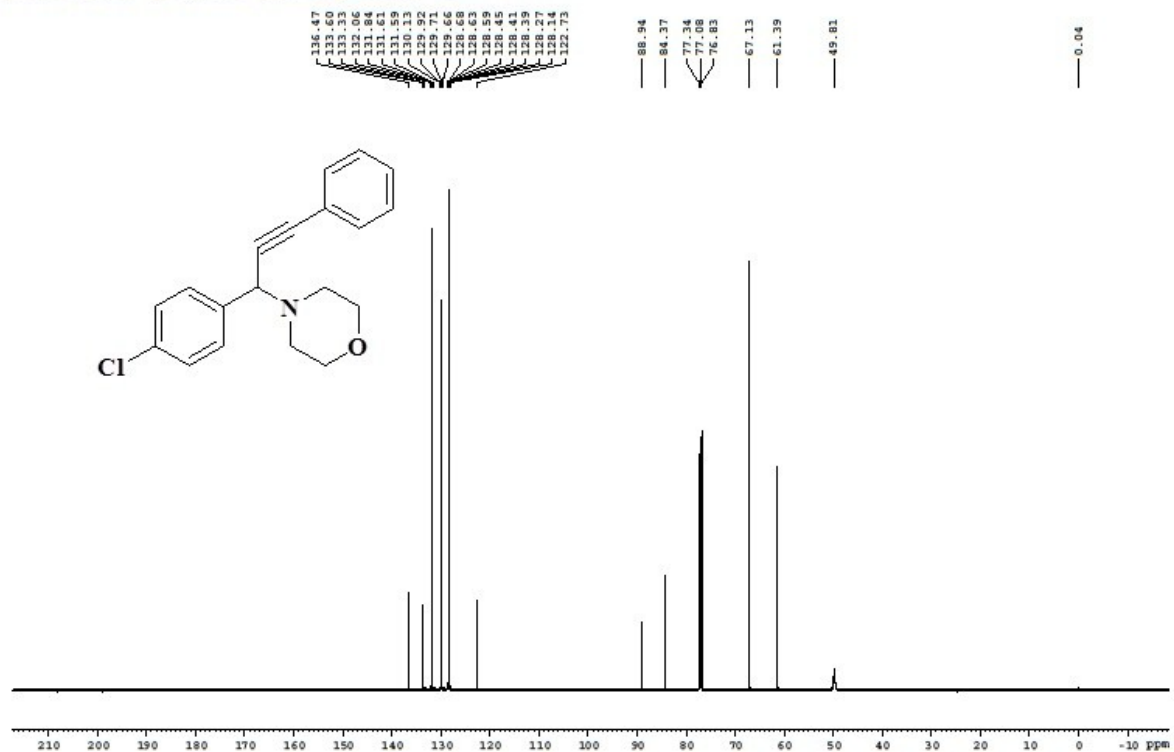
¹H NMR (Table 3, Entry 11)



¹³C NMR (Table 3, Entry 11)

DB-131

C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 13

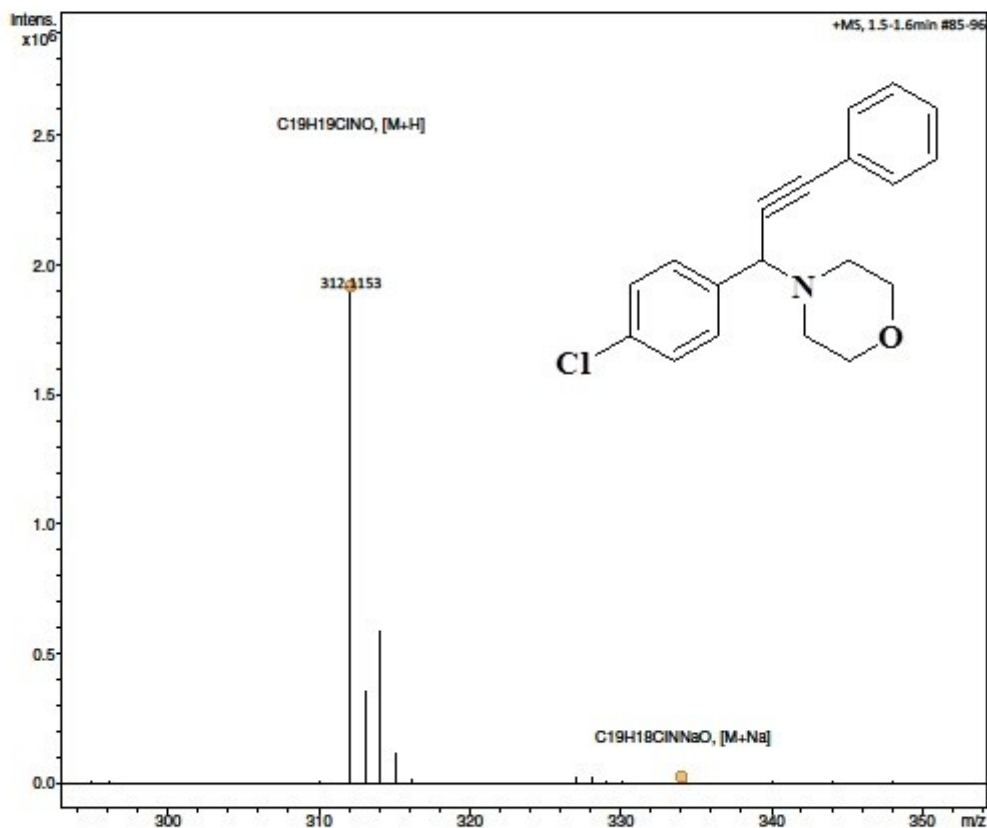


HRMS (Table 3, Entry 11)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info		Acquisition Date	10/7/2017 3:06:01 PM	
Analysis Name	D:\Data\2017\SEPTEMBER\SPPU AFFILIATED\MANASAHEB AWATE COLLEGE MANCHARK G			
	KANADE\BANKAR D B\DB-131_BE8_01_4443.d			
Method	dlo-ms600mz_10min.m	Operator	CIF	
Sample Name	DB-131	Instrument	impact HD	1819696.00184
Comment				

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulzer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
312.1153	1	C19H19ClNO	312.1150	-1.1	20.7	1	100.00	10.5	even		ok	M+H
334.0973	1	C19H18ClNNaO	334.0969	-1.1	188.1	1	100.00	10.5	even		ok	M+Na

DB-131_BE8_01_4443.d

Bruker Compass DataAnalysis 4.2

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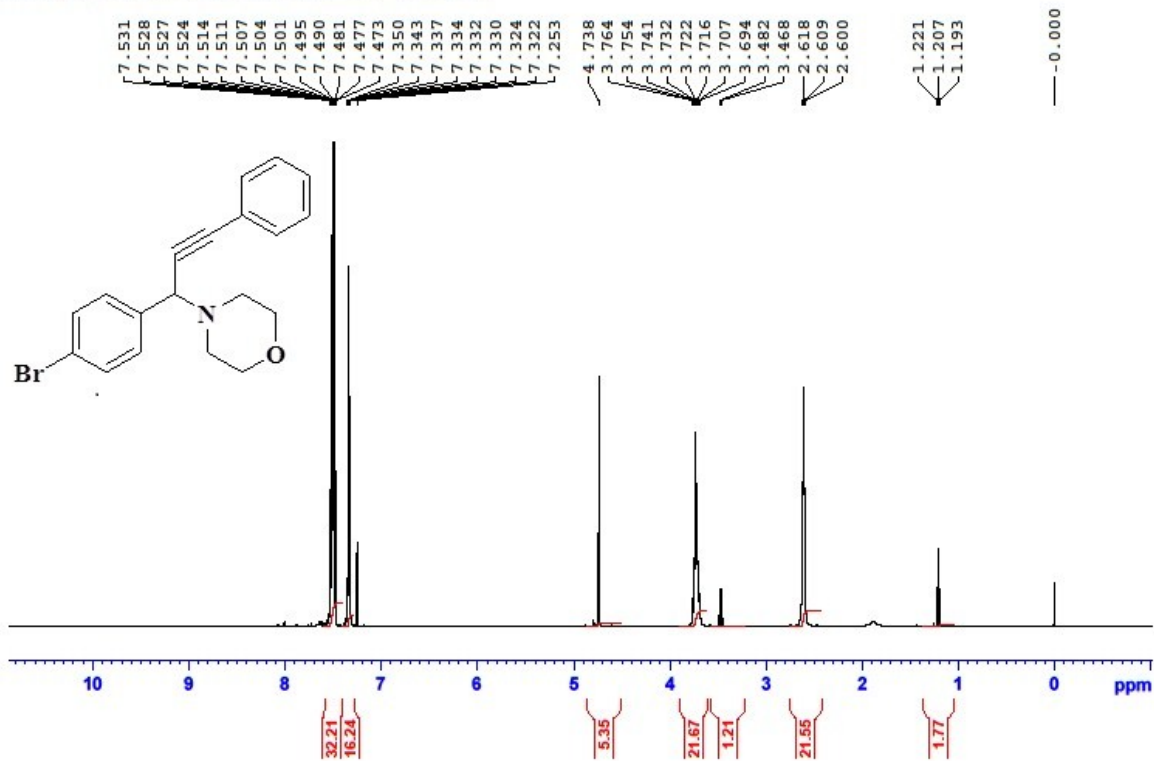
by: CIF

Page 1 of 1

¹H NMR (Table 3, Entry 12)

DB-129

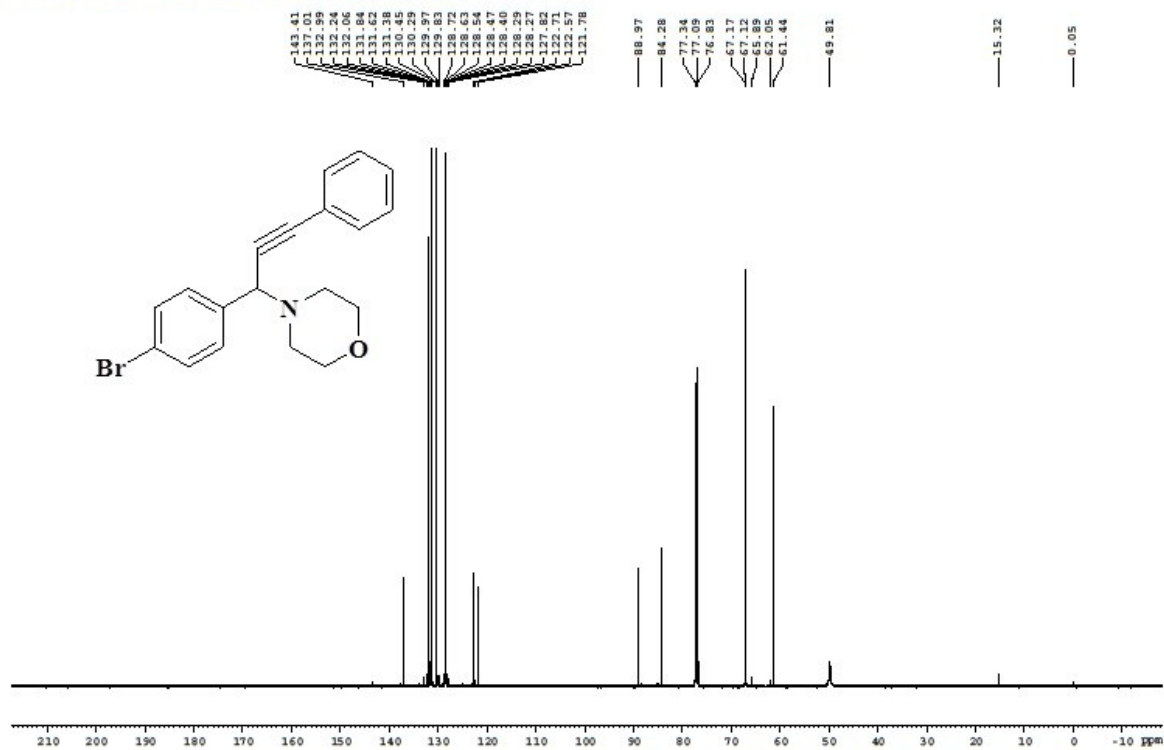
Proton_spin CDCl3 {E:\AWATE COLLEGE} Snehal 12



¹³C NMR (Table 3, Entry 12)

DB-129

C13CPD CDC13 {E:\AWATE COLLEGE} Snehal 11

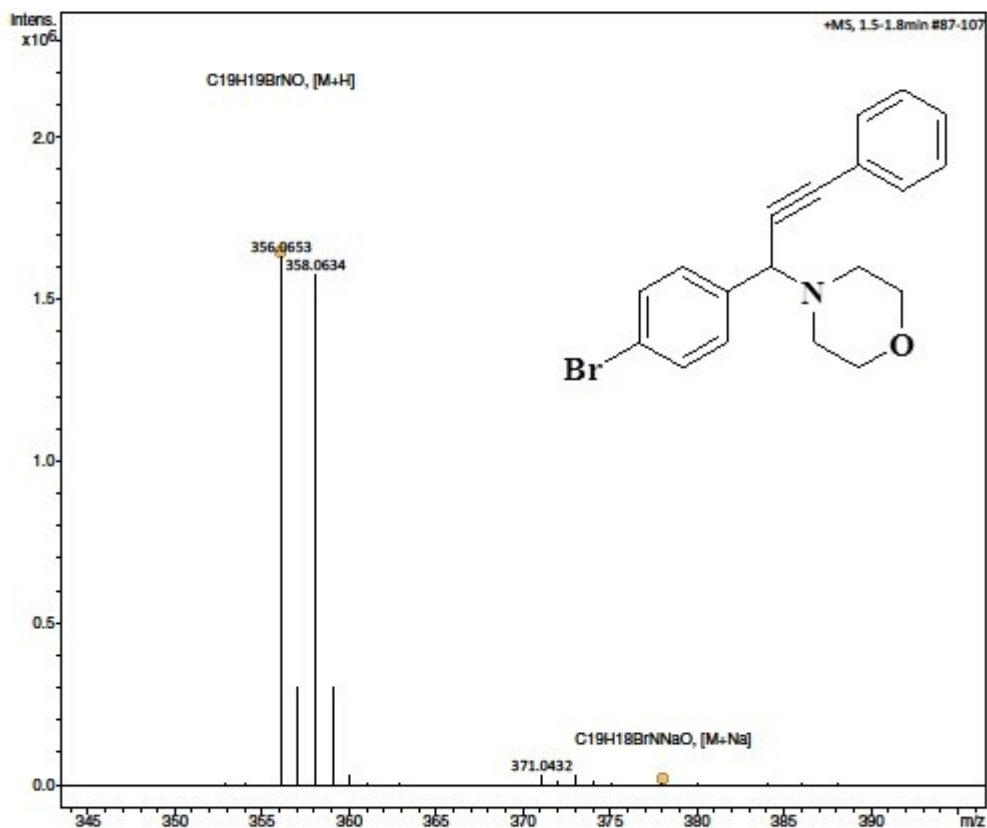


HRMS (Table 3, Entry 12)

Savitribai Phule Pune University - Central Instrumentation Facility

Analysis Info	Acquisition Date 10/7/2017 2:37:19 PM	
Analysis Name	D:\Data\2017\SEPTEMBER\SPPU AFFILIATED\ANNASAHEB AWATE COLLEGE MANCHAR\K G KANADE\BANKAR D B\DB-129_BE6_01_4441.d	
Method	dlc-ms600mz_10min.m	Operator CIF
Sample Name	DB-129	Instrument impact HD 1819696.00184
Comment		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule	Adduct
356.0653	1	C ₁₉ H ₁₉ BrNO	356.0645	-2.3	20.8	1	100.00	10.5	even		ok	M+H
378.0470	1	C ₁₉ H ₁₈ BrNNaO	378.0464	-1.5	54.0	1	100.00	10.5	even		ok	M+Na

DB-129 BE6_01_4441.d

Bruker Compass DataAnalysis 4.2

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by: CIF

Page 1 of 1