Supplementary Information

Chemoselective Benzylic Csp^3-H Bond Oxidation Reactions Catalyzed by $Ag^{II}(bipy)_2S_2O_8$ Complex

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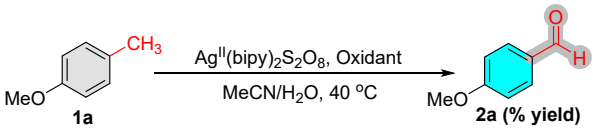
[c]School of Advanced Chemical Sciences, Shoolini University of Biotechnology and Management Sciences, Solan, HP-173229 India.

[†]Equal contribution

Table S1: Optimization study

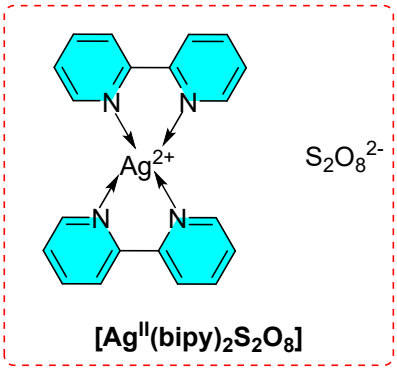


entry	R	Ag catalyst	oxidant	Solvent	time (h)	**2a (%**yield)
1	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	Oxone (3 equiv.)*	$MeCN/H_2O$	12 h	21
2	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	H_2O_2 (3 equiv.)	$MeCN/H_2O$	12 h	nd
3	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	TBHP (3 equiv.)	$MeCN/H_2O$	12 h	12
4	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	Selectfluor (3 equiv.)	$MeCN/H_2O$	0.166 h	78
5	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	$K_2S_2O_8$ (3 equiv.)	$MeCN/H_2O$	12 h	48
6	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	$NH_4S_2O_8$ (3 equiv.)	$MeCN/H_2O$	12 h	24
7	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	$Na_2S_2O_8$ (3 equiv.)	$MeCN/H_2O$	12 h	18
8	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	Selectfluor (1 equiv.)	$MeCN/H_2O$	0.5 h	56
9	*p*-OMe	$Ag^{II}(bipy)_2S_2O_8$	Selectfluor (2 equiv.)	$MeCN/H_2O$	0.333 h	62

Reaction conditions: **1a** (1 mmol), Ag catalyst (10 mol%), Selectfluor (3 equiv.), CH_3CN/H_2O (9:1, 4 mL), 40 °C, *Oxone $2KHSO_5 \cdot KHSO_4 \cdot K_2SO_4$

General procedure for the synthesis of Silver Complex:[1]

2,2'-Bipyridine (1.1 g, 7 mmol) was added to a silver nitrate solution in methanol (0.51 g, 3 mmol), and the mixture was allowed to stir for 0.5 hours at room temperature. Thereafter, methanol was evaporated using a rotary evaporator and crystalline compound was obtained. This compound was then added to cold solution of $K_2S_2O_8$ (1.1 g in 100 mL H_2O) and after some time brown coloured precipitates were observed. The precipitates were then filtered under vacuum, and upon drying brown colour compound was obtained (2.1 g).



Procedures for controlled experiments (Scheme 2)

To a stirred solution of *p*-methoxy toluene **1a** (0.8196 mmol) in CH_3CN/H_2O (9:1, 4 mL), was added (3 equiv.) of selectfluor and 10mol% of silver complex in 50 ml round bottom flask. The reaction mixture was stirred at 40 °C under Nitrogen atmosphere. After completion of the reaction as indicated by thin layer chromatography, the reaction mixture was extracted with EtOAc and water. The organic layer was dried over Na_2SO_4 and concentrated in vacuo on rotary evaporator. The crude material was purified by column chromatography using ethyl acetate/ *n*-hexane as eluent to afford the required product **2a** in 76% yield (Scheme 2, *eq. 1*).

To a 50 mL two necked round bottom flask 10mol% of silver complex was added under nitrogen atmosphere after that 4 ml of anhydrous acetonitrile (CH_3CN) was added with the

help of syringe, simultaneously we added *p*-methoxy toluene **1a** (0.8196 mmol) and (3 equiv.) of selectflour into it and place the reaction mixture on stirring at 40 ºC under nitrogen atmosphere followed by freeze thaw cycles. After completion of the reaction as indicated by thin layer chromatography, the reaction mixture was extracted with EtOAc and water. The organic layer was dried over Na_2SO_4 and concentrated in vacuo on rotary evaporator. The crude material was purified by column chromatography using ethyl acetate/ *n*-hexane as eluent to afford the required product **2a** of 46% (Scheme 2, *eq. 2*).

To a 50 mL two necked round bottom flask 10mol% of silver complex was added under argon atmosphere after that 4 mL of anhydrous tetrahydrofuran (THF) was added with the help of syringe, simultaneously we added *p*-methoxy toluene **1a** (0.8196 mmol) and (3 equiv.) of selectflour into it and place the reaction mixture on stirring at 40 ºC under argon atmosphere for 3hr followed by freeze thaw cycles. After 3 hr no new spot was observed as indicated by thin layer chromatography (Scheme 2, *eq. 3*).

To a 50 mL two necked round bottom flask 10mol% of silver complex was added under argon atmosphere after that 3.5 mL of anhydrous tetrahydrofuran (THF) was added with the help of syringe, simultaneously we added *p*-methoxy toluene **1a** (0.8196 mmol) and (3 equiv.) of selectflour into it and place the reaction mixture on stirring at 40 ºC under argon atmosphere for 3hr followed by freeze thaw cycles. After 3 hr when we check thin layer chromatography (TLC) we observe no new spot. After this, we added 0.5 mL of freeze thaw water in the reaction mixture with the help of syringe, we observe heat up of reaction. Suddenly when we check the TLC of reaction, the reaction was completed in 5 minutes. After completion of the reaction as indicated by thin layer chromatography, the reaction mixture was extracted with EtOAc and water. The organic layer was dried over Na_2SO_4 and concentrated in vacuo on rotary evaporator. The crude material was purified by column chromatography using ethyl acetate/ *n*-hexane as eluent to afford the required product **2a** of 78% (Scheme 2*, eq. 4*).

To a stirred solution of *p*-methoxy toluene **1a** (0.8196 mmol) in CH_3CN/H_2O (9:1, 4 mL), was added (3 equiv.) of selectfluor and 10mol% of silver complex after that we added (4 equiv., 6 equiv., 8 equiv. and 3 equiv.) of TEMPO as a radical scavenger. Then the reaction mixture was placed on stirring at 40 ºC under Nitrogen atmosphere. After completion of the reaction as indicated by thin layer chromatography, the reaction mixture was extracted with EtOAc and water. The organic layer was dried over Na_2SO_4 and concentrated in vacuo on

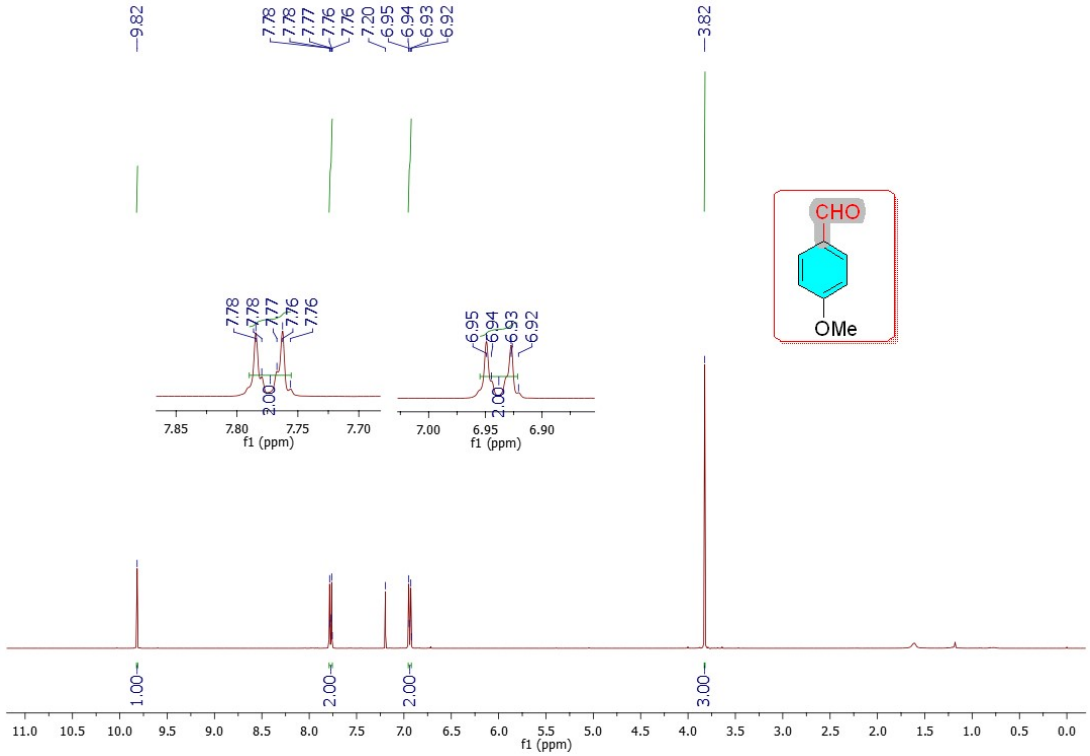
rotary evaporator. The crude material was purified by column chromatography using ethyl acetate/ *n*-hexane as eluent to afford the required product **2a** of 58%, 42%, 28%, 12% (Scheme 2, *eq. 5*).

Procedure for Isotope labelling experiment (Figure 2)

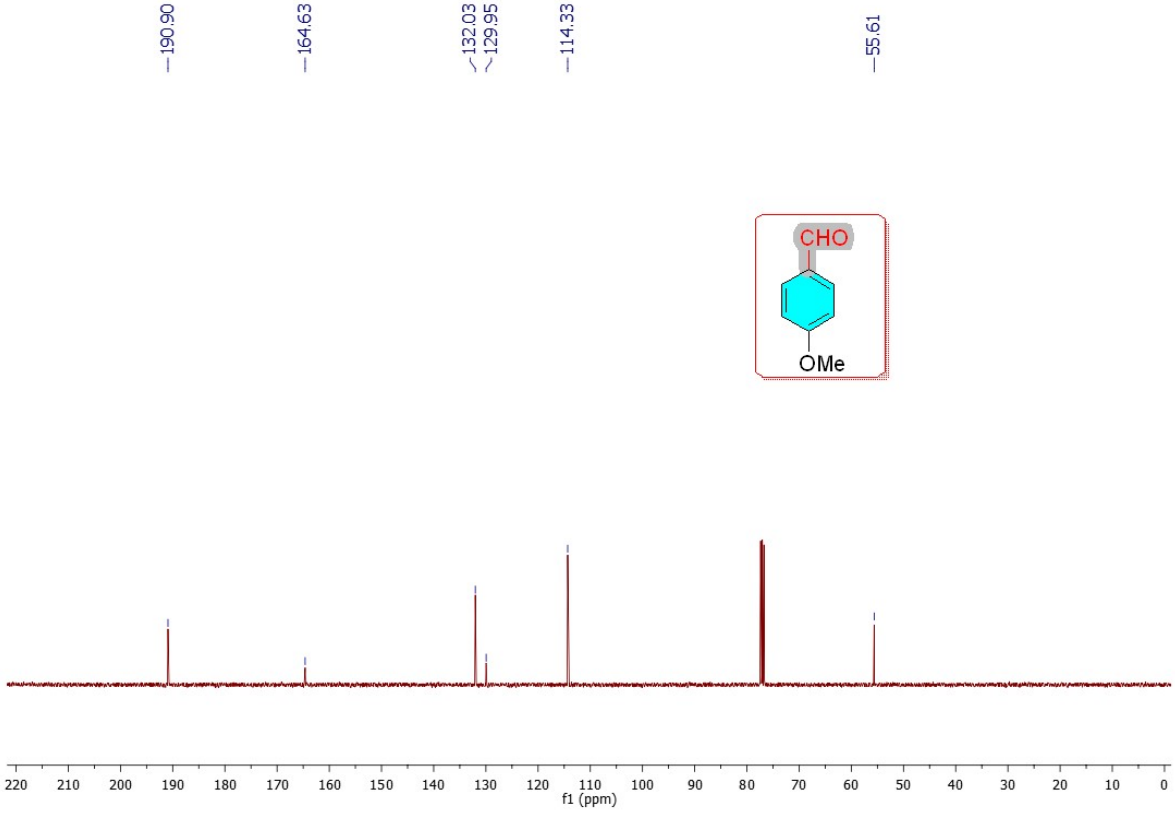
To a stirred solution of *p*-methoxy toluene **1a** (0.8196 mmol) in anhydrous CH_3CN was added (3 equiv.) of selectfluor and 10mol% of silver complex under nitrogen atmosphere after that we add 10 µl H_2O^{18}. Then the reaction was continued to stir for about 5 minutes at 40 ºC.

Spectral copies of:

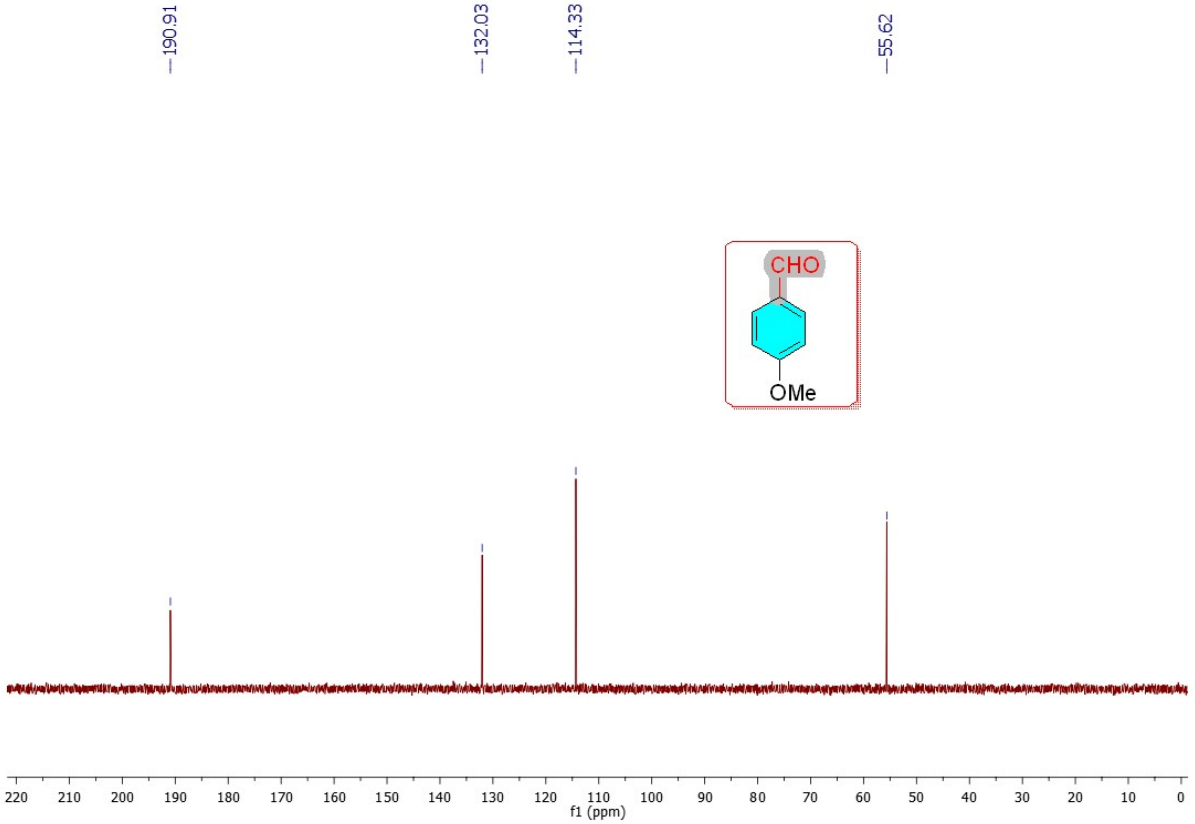
^{1}H NMR Spectra of 4-Methoxy benzaldehyde (2a)[2]



^{13}C[2] NMR Spectra of4-Methoxy benzaldehyde (2a)[2]

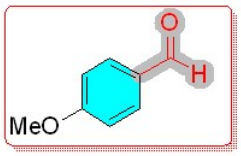


DEPT Spectra of 4-Methoxy benzaldehyde (2a)[2]



GCMS of 4-Methoxy benzaldehyde (2a)

IIIM GCMS ANALYSIS



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Molecular Weight: 136.15

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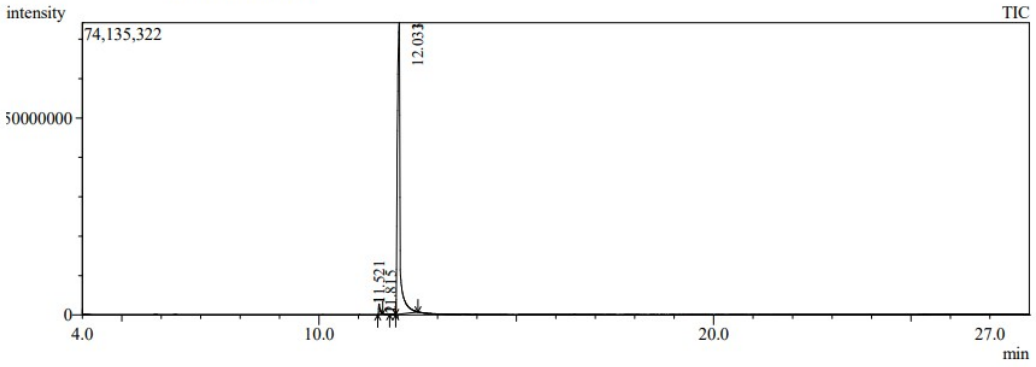

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3	12.031	357717391	98.11	73932145	96.31	83	77.05	Benzaldehyde, 4-methoxy-
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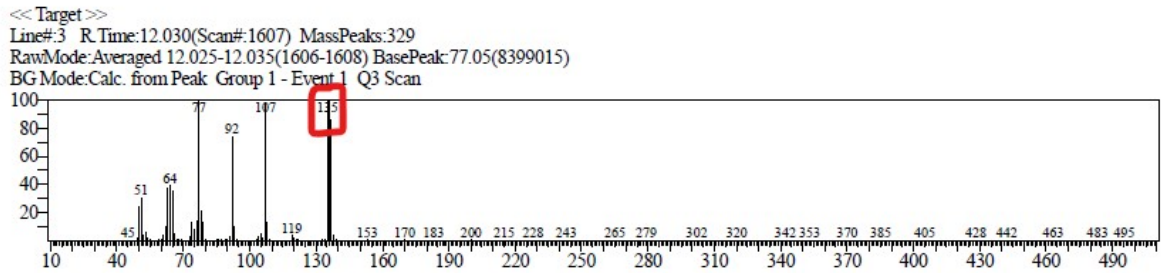
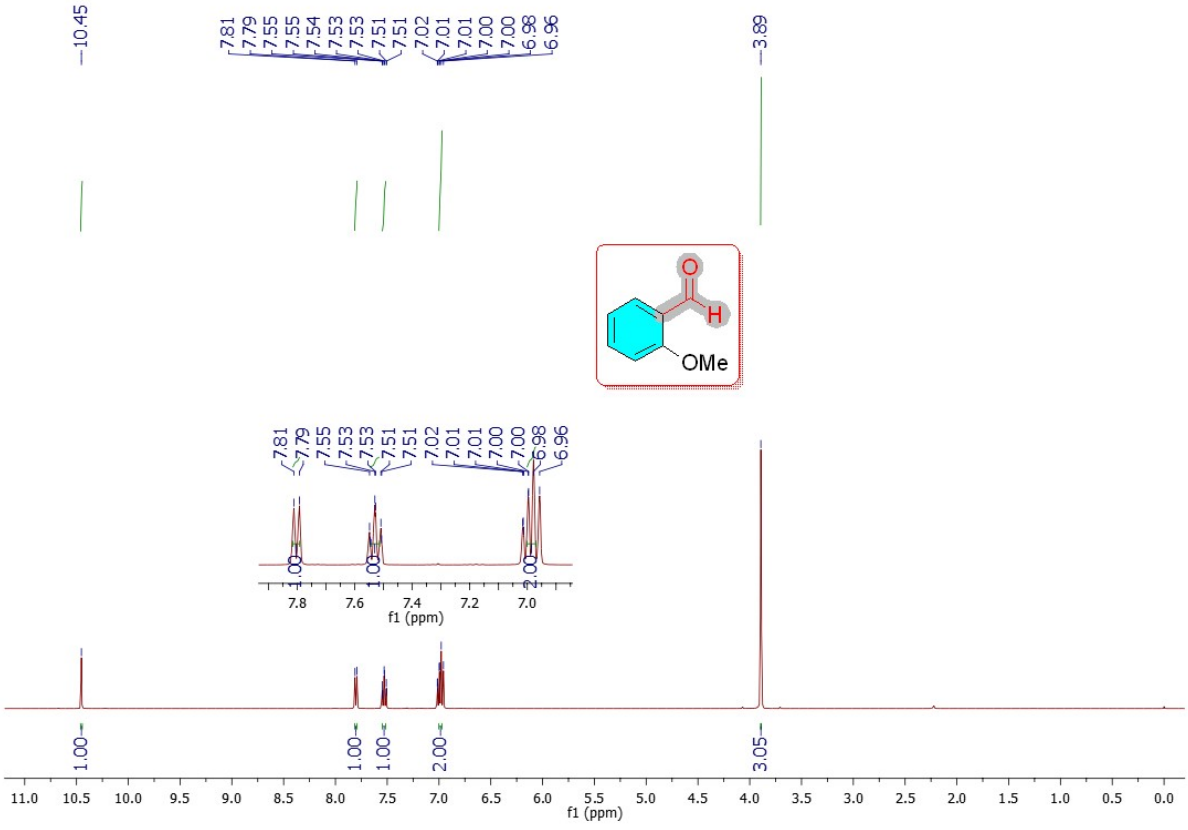
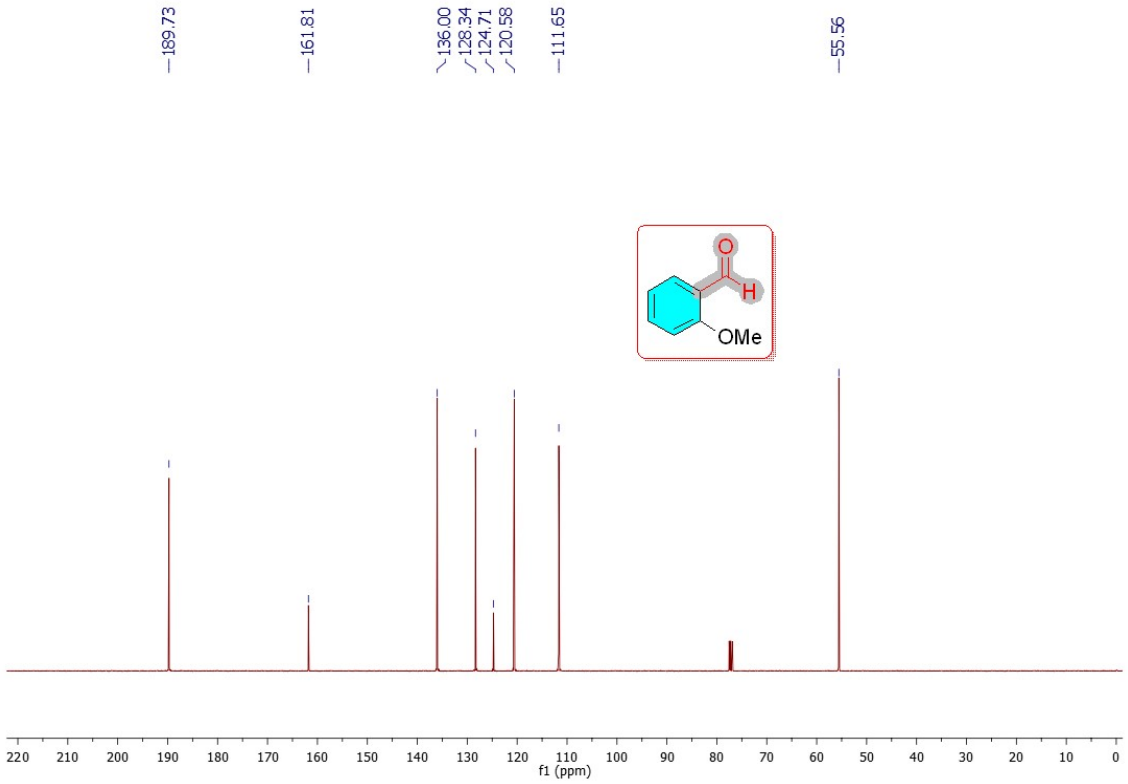


[1]HNMR Spectra of 2-Methoxy benzaldehyde (2b)[2]



$^{13}C^{2}$ NMR Spectra of 2-Methoxy benzaldehyde (2b)[2]



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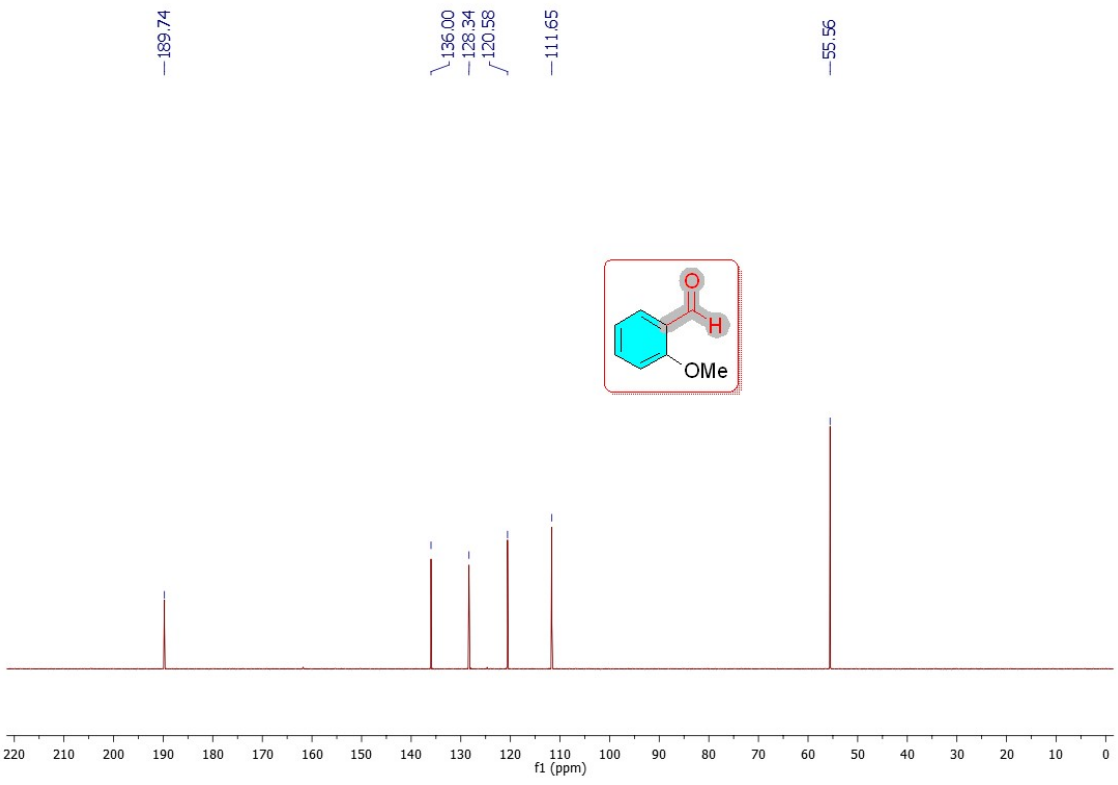

GCMS of 2-Methoxy benzaldehyde (2b)

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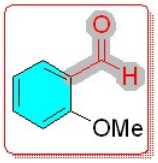
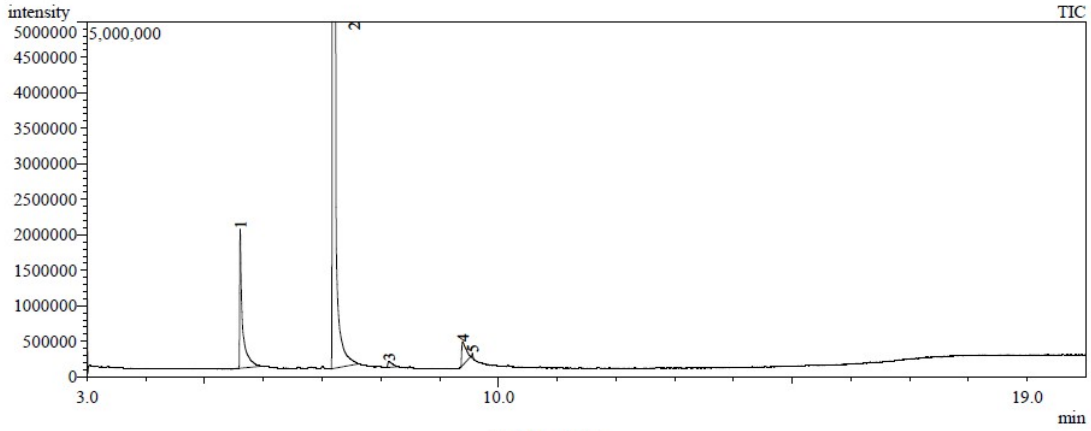


Chemical Formula: $C_8H_8O_2$
Exact Mass: 136.05



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3	8.133	443776	0.46	94	135.00	Benzoic acid, 2-methoxy-, methyl ester
4	9.393	1650466	1.70	94	105.05	Benzoic acid, 2-methoxy-
5	9.559	83451	0.09	93	191.10	2,4-Di-tert-butylphenol
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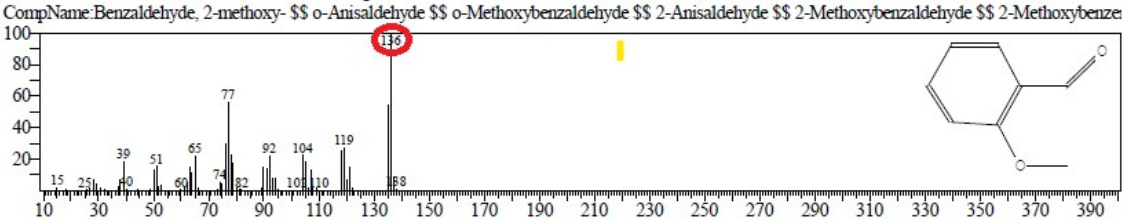
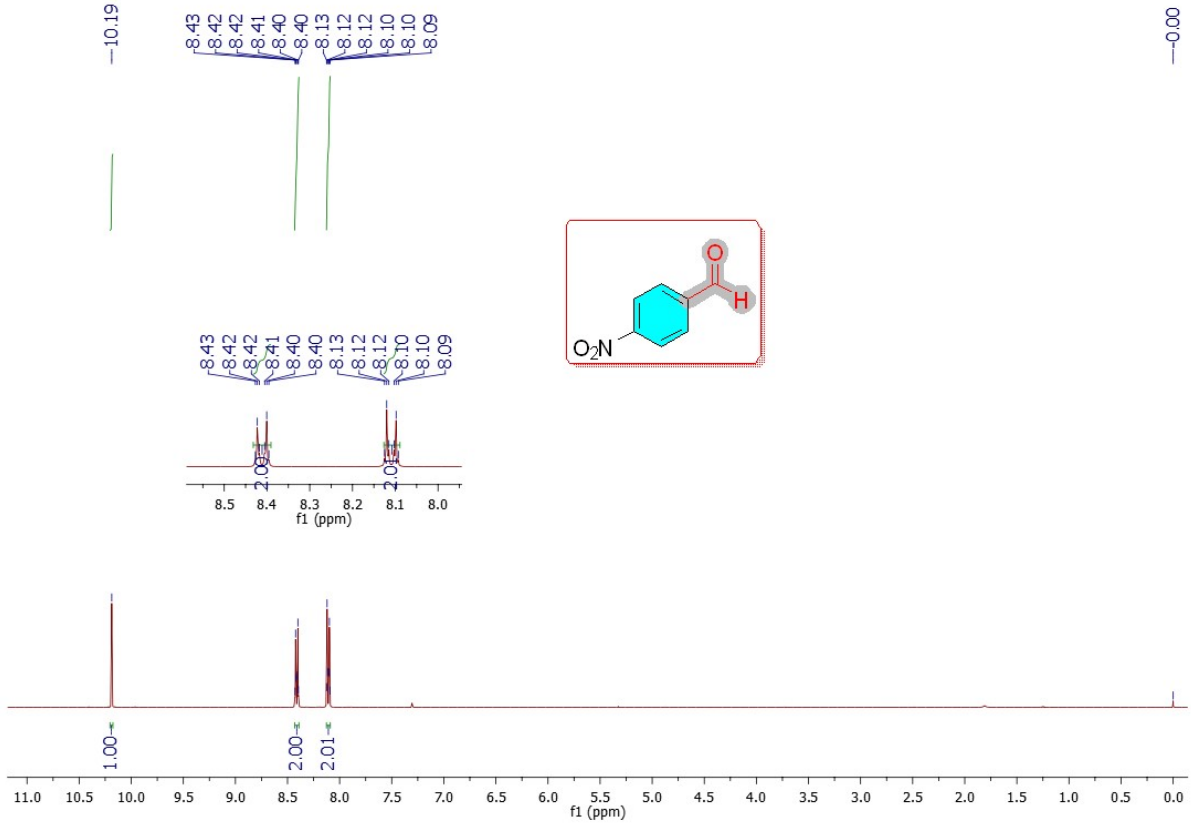
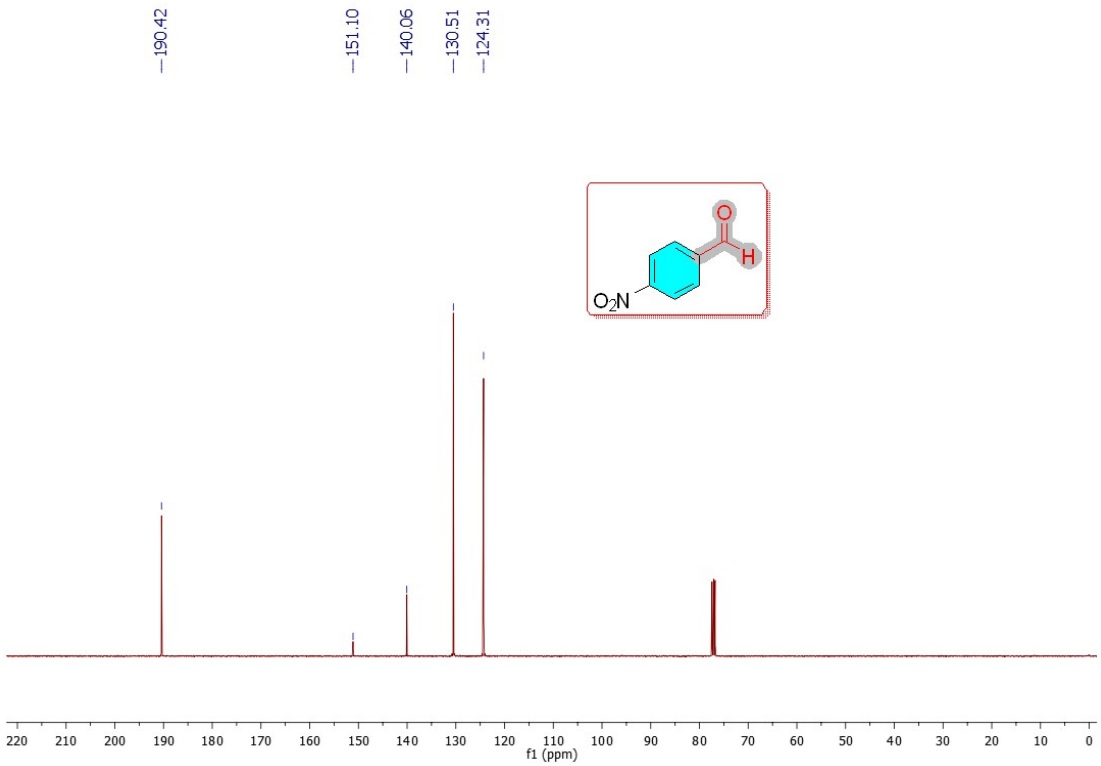


^{1}H NMR Spectra of 4-Nitro benzaldehyde (2c)[2]



^{13}C{^{1}H} NMR Spectra of 4-Nitro benzaldehyde (2c)[2]



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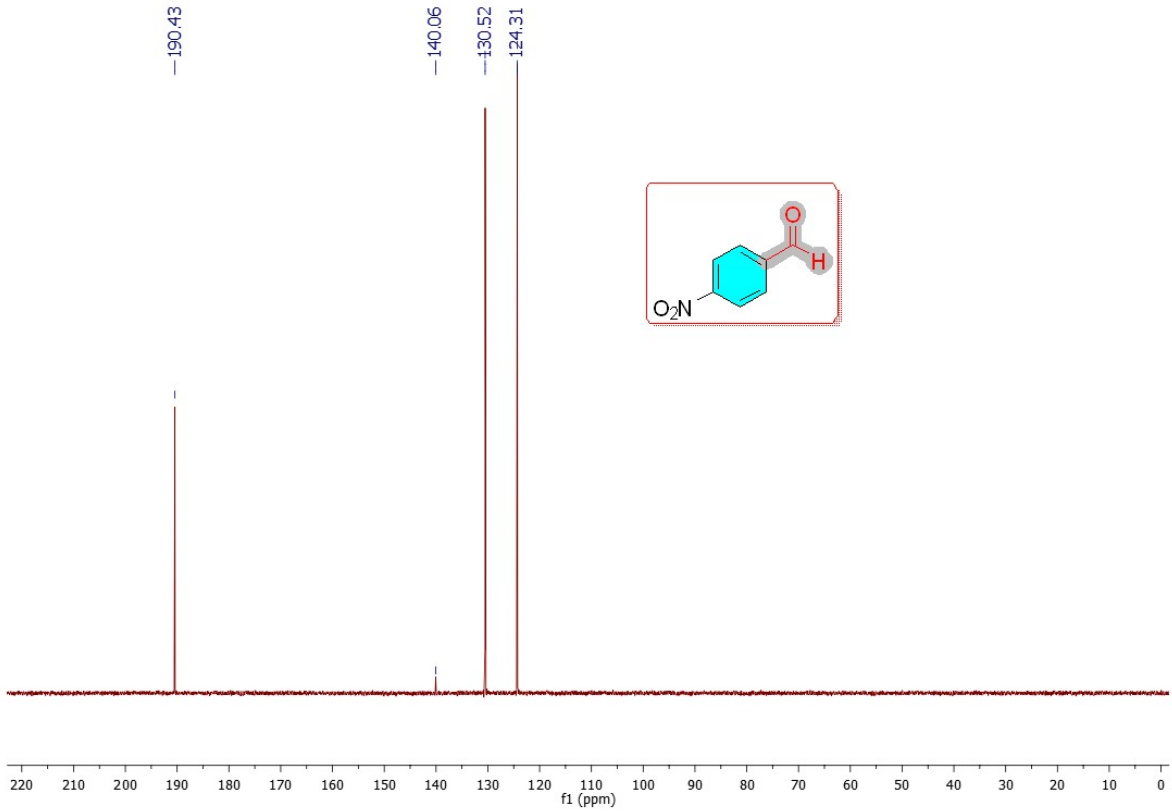

GCMS of 4-Nitro benzaldehyde (2c)

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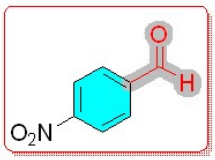

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Exact Mass: 151.03
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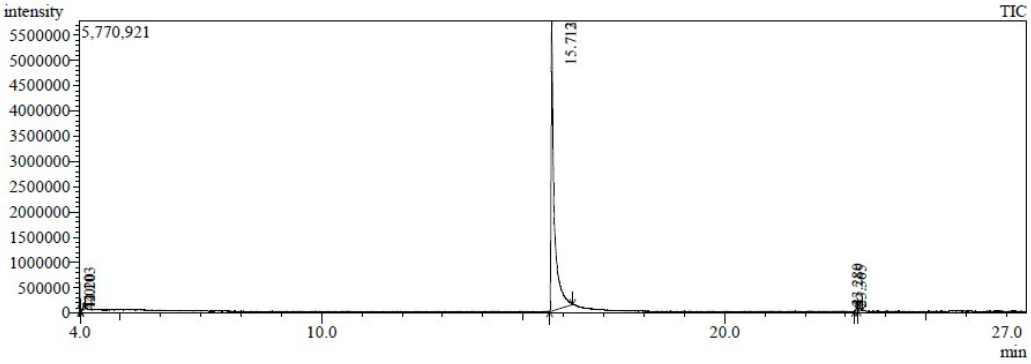

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3	15.712	31237967	97.67	5727240	95.01	96	151.05	Benzaldehyde, 4-nitro-
4	23.280	236042	0.74	79890	1.33	68	250.10	4,7-Dimethyl-3-phenylcoumarin
5	23.365	235384	0.74	50130	0.83	60	222.05	2H-Indol-2-one, 3-[(4-ethylphenyl)imino]-1,3-
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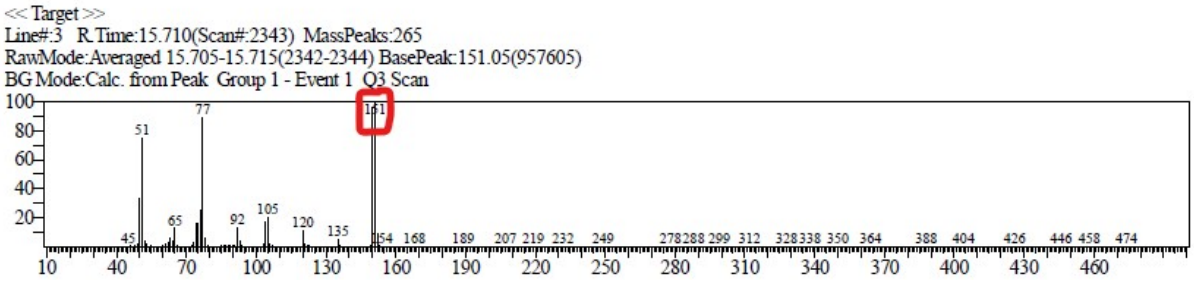
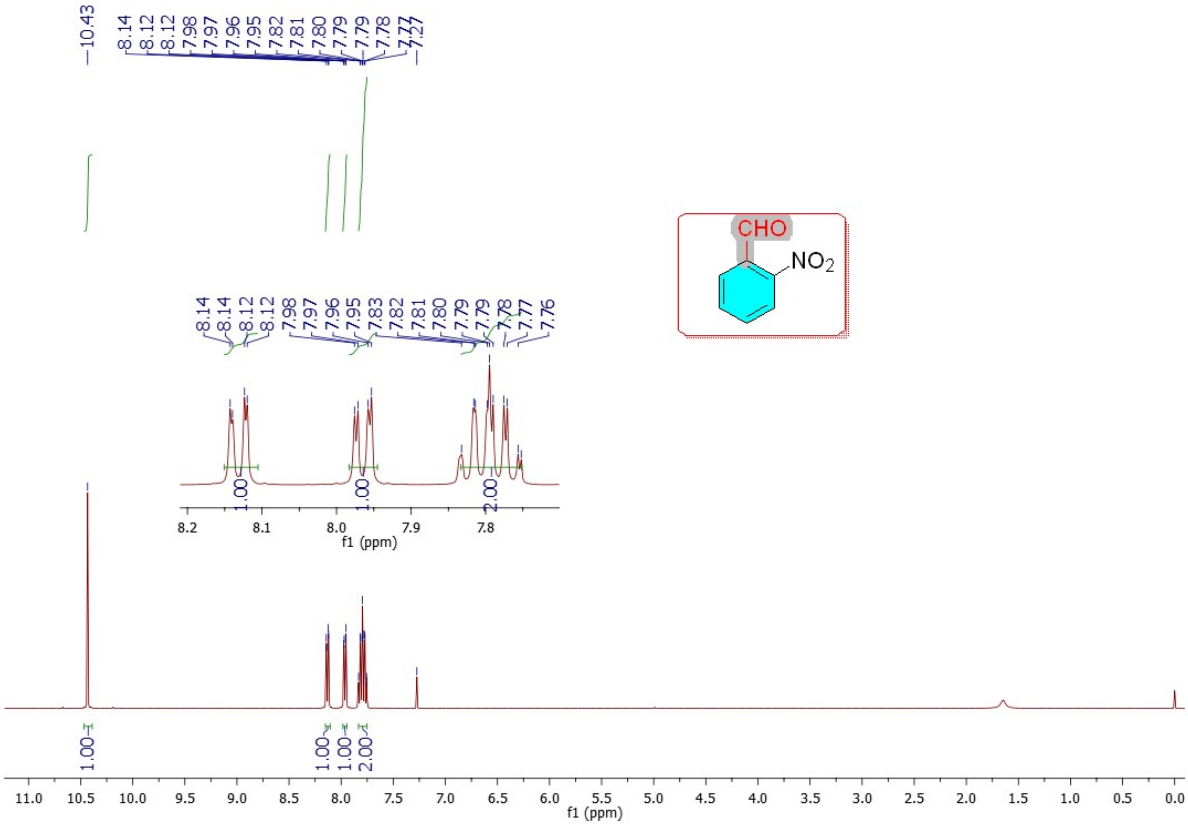
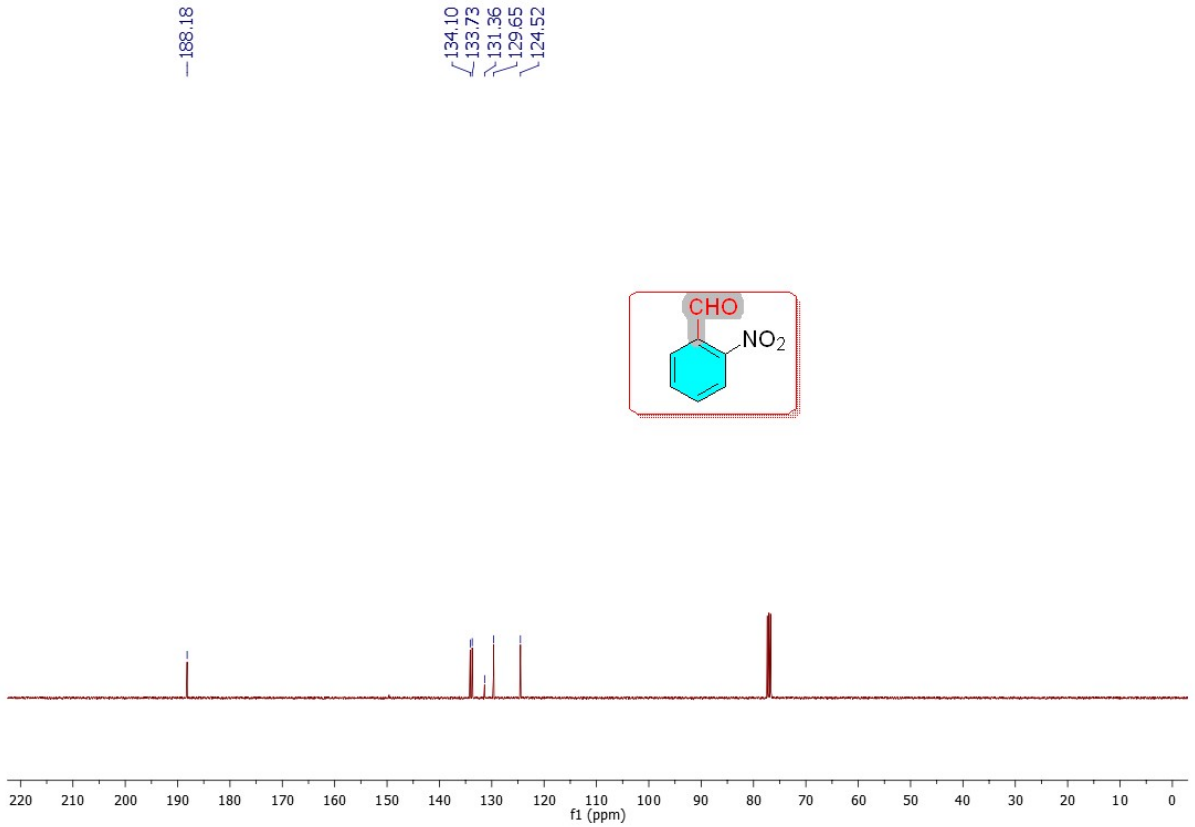


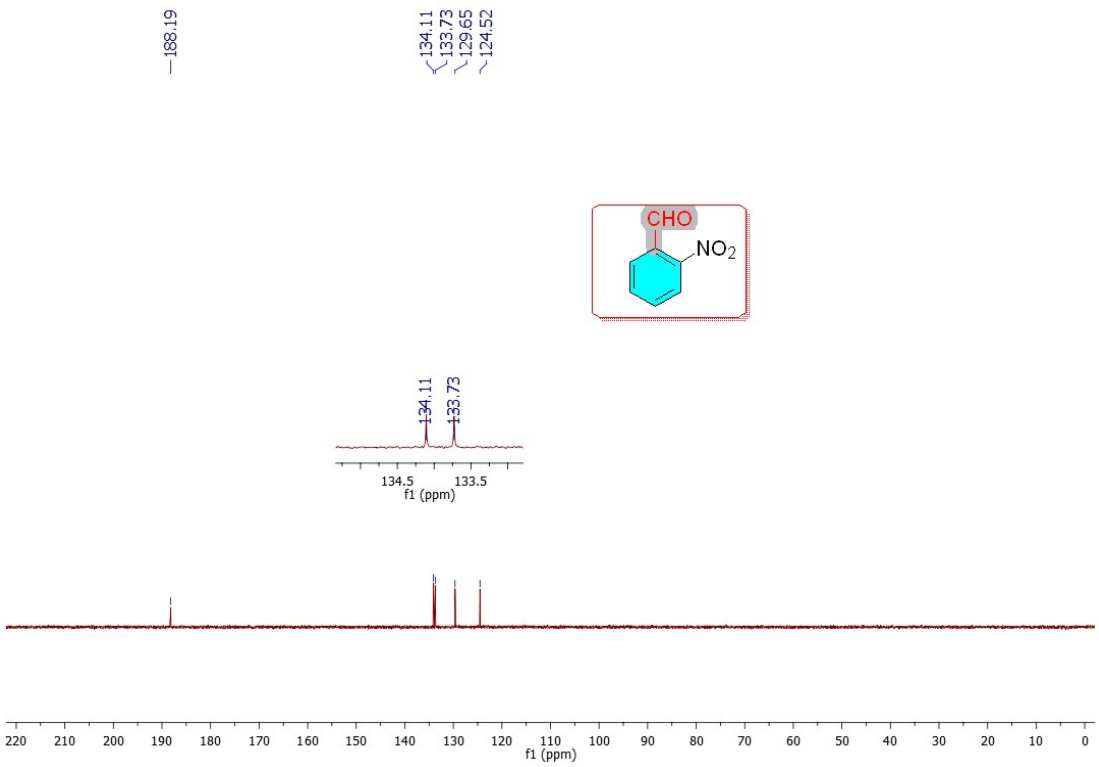
[1]H NMR Spectra of 2-Nitro benzaldehyde (2d)[2]



$^{13}C\{^{1}H\}$ NMR Spectra of 2-Nitro benzaldehyde (2d)[2]



DEPT Spectra of 2-Nitro benzaldehyde (2d)[2]



GCMS of 2-Nitro benzaldehyde (2d)

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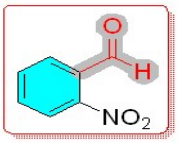

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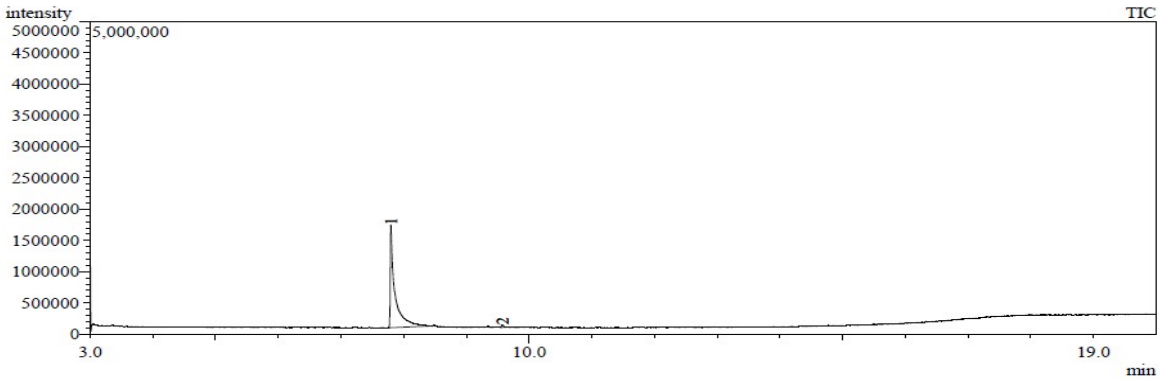
Exact Mass: 151.03



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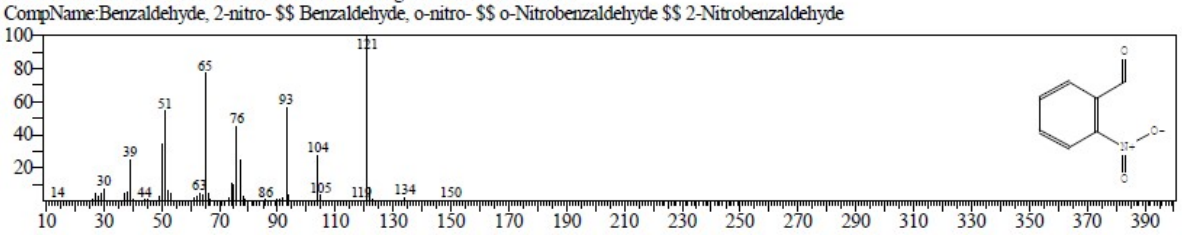
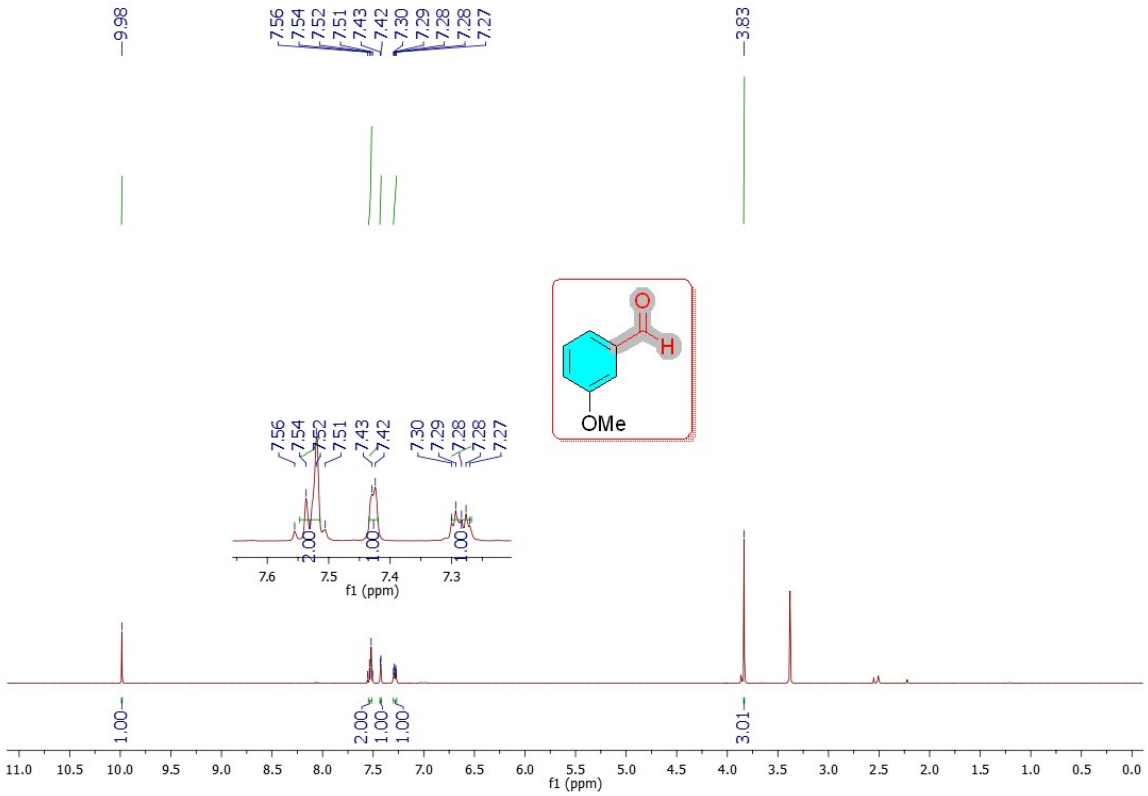
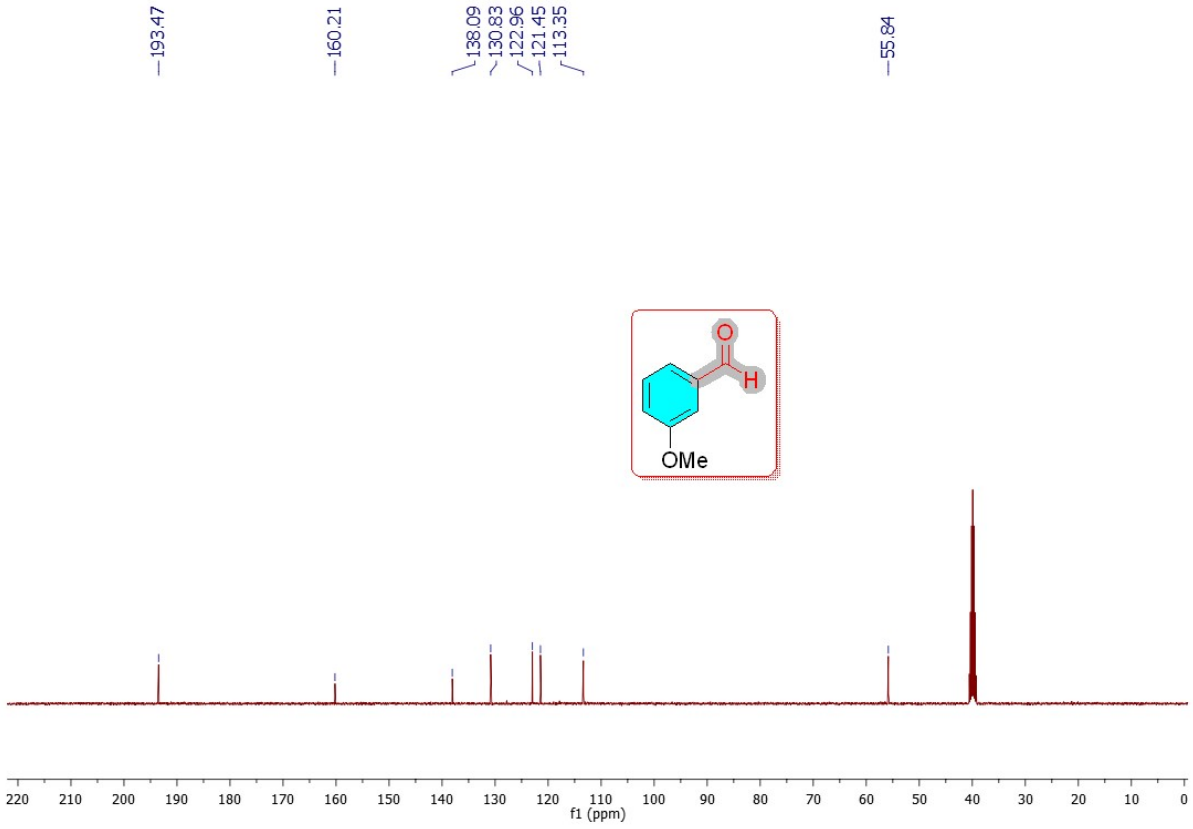


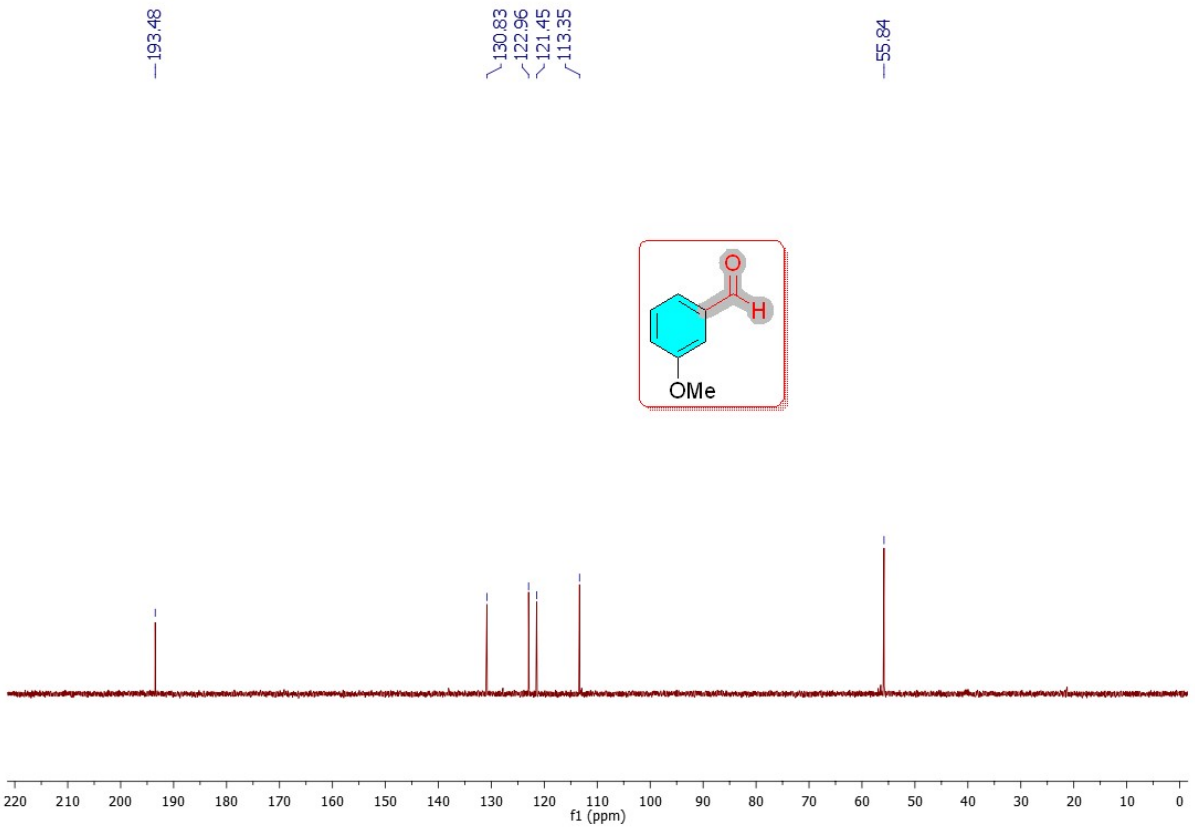
[1]HNMR Spectra of 3-Methoxy benzaldehyde (2e)[2]



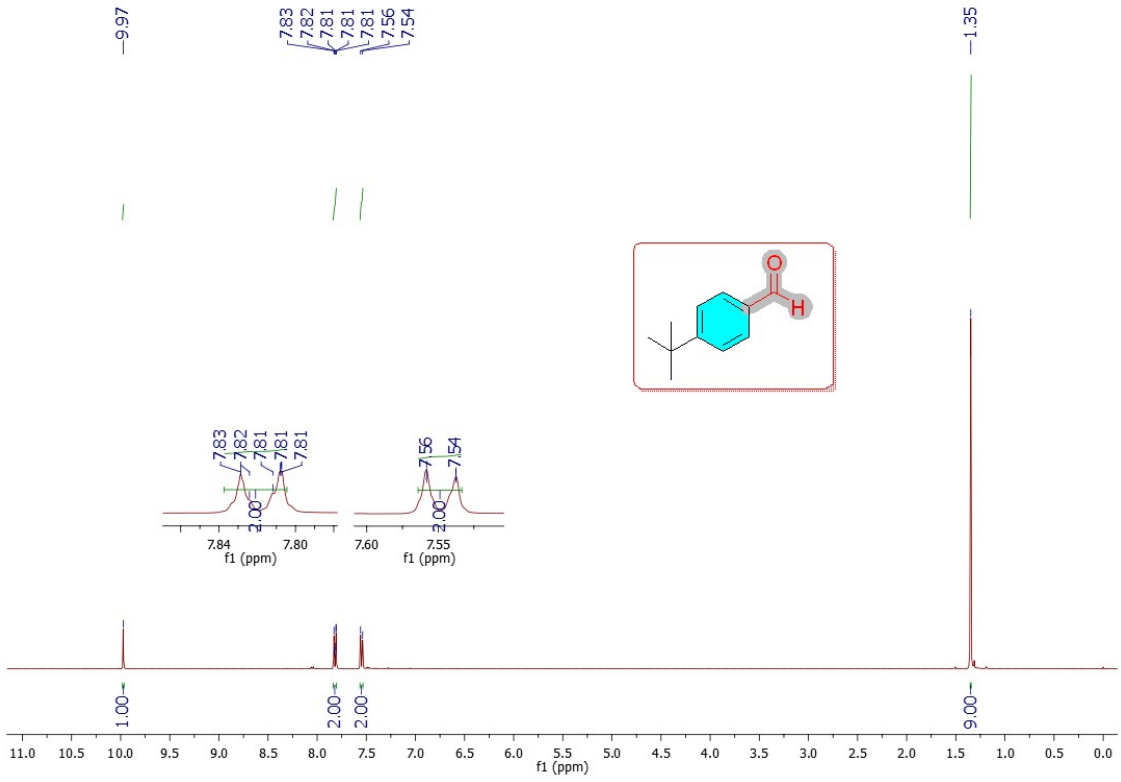
$^{13}C\{^{1}H\}$ NMR Spectra of 3-Methoxy benzaldehyde (2e)[2]



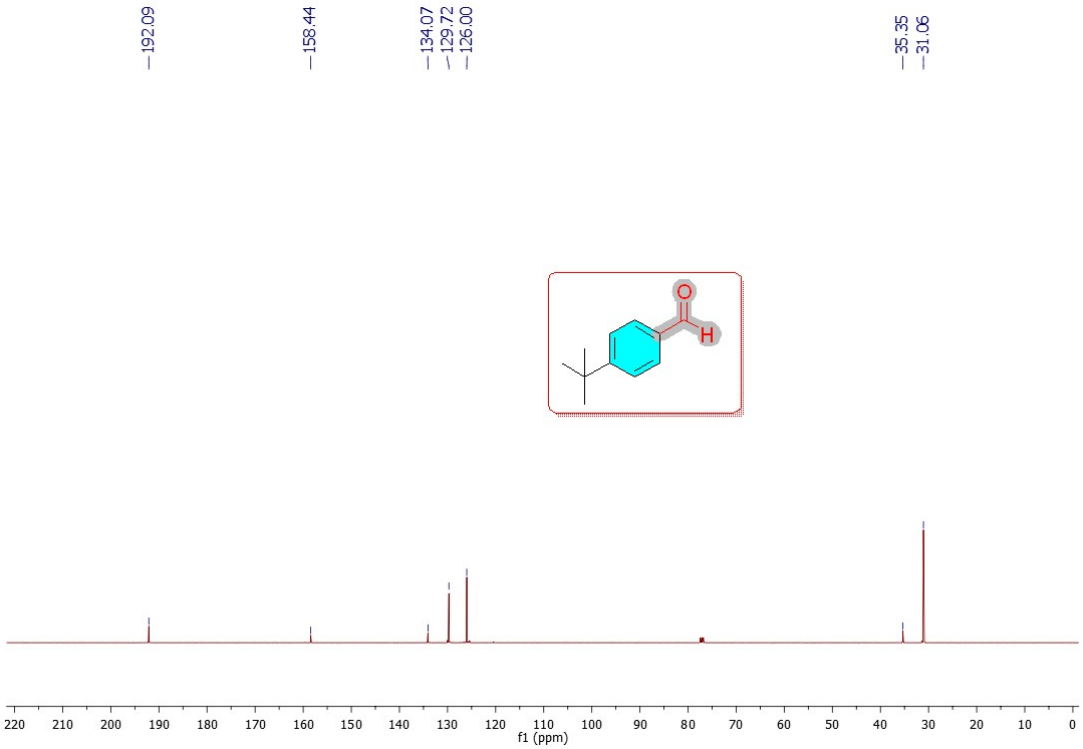
DEPT Spectra of 3-Methoxy benzaldehyde (2e)[2]



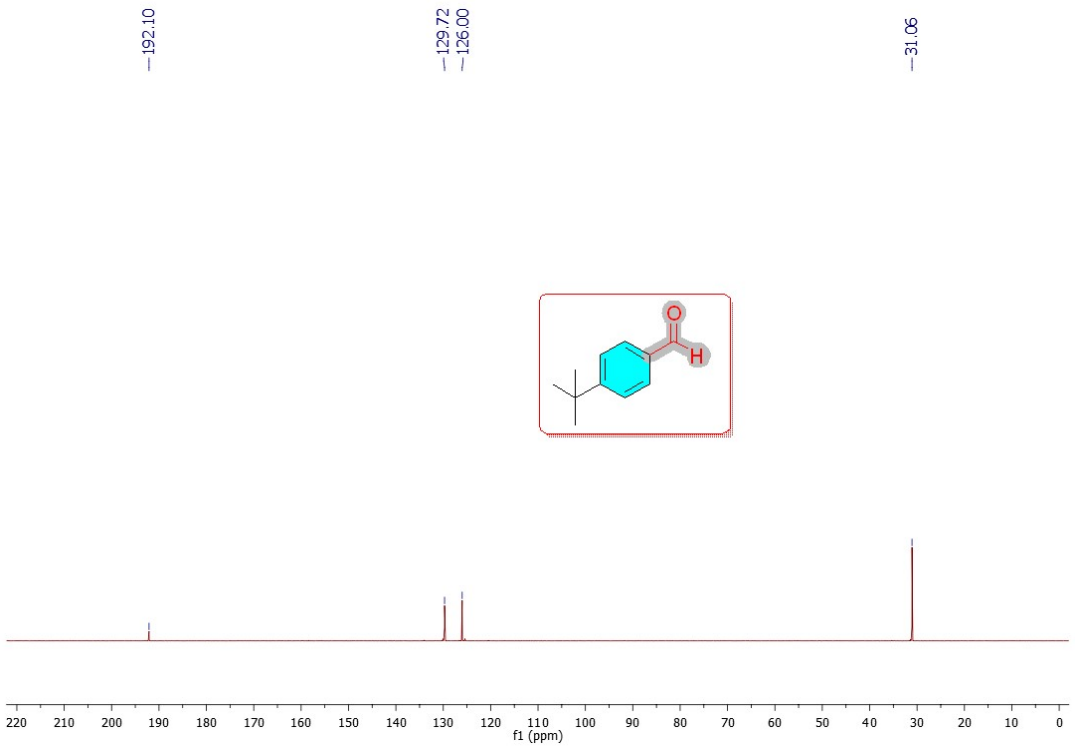
[1]HNMR Spectra of 4-(*tert*-butyl) benzaldehyde (2f)[3]



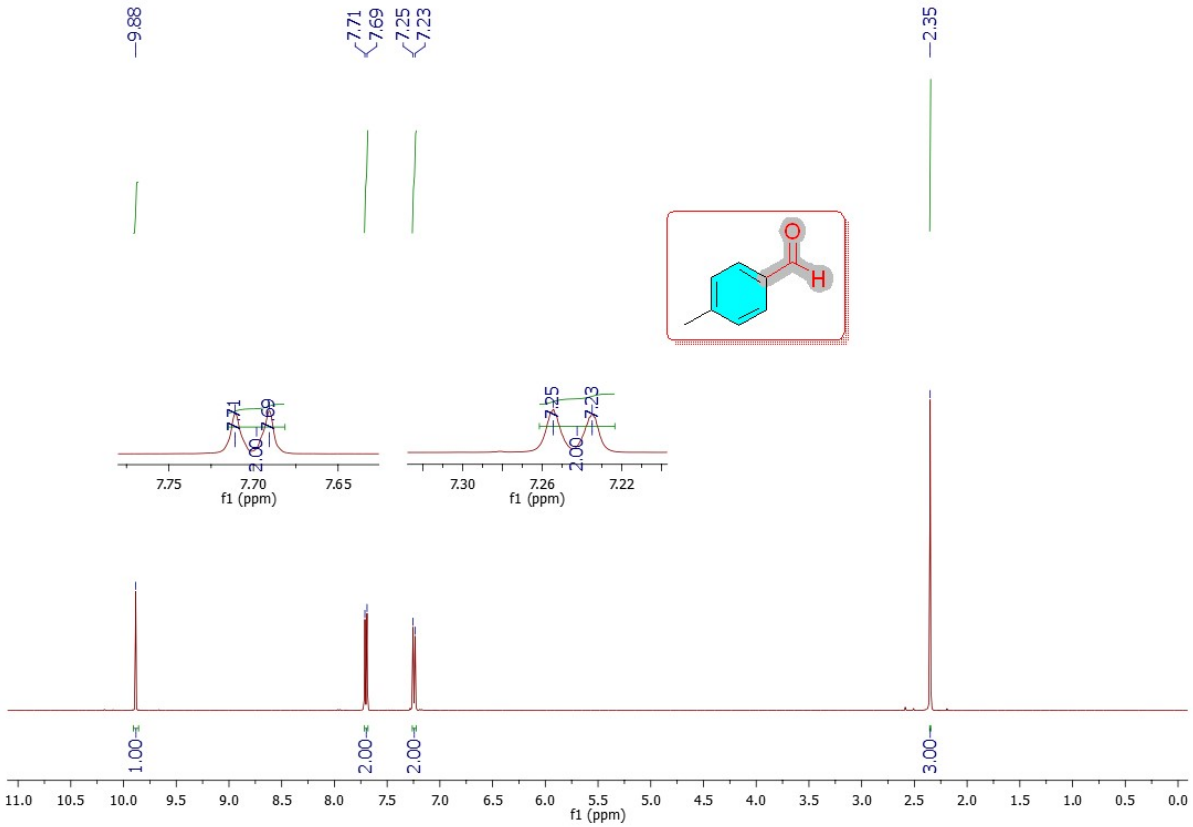
$^{13}C\{^{1}H\}$ NMR Spectra of 4-(*tert*-butyl) benzaldehyde (2f)[3]



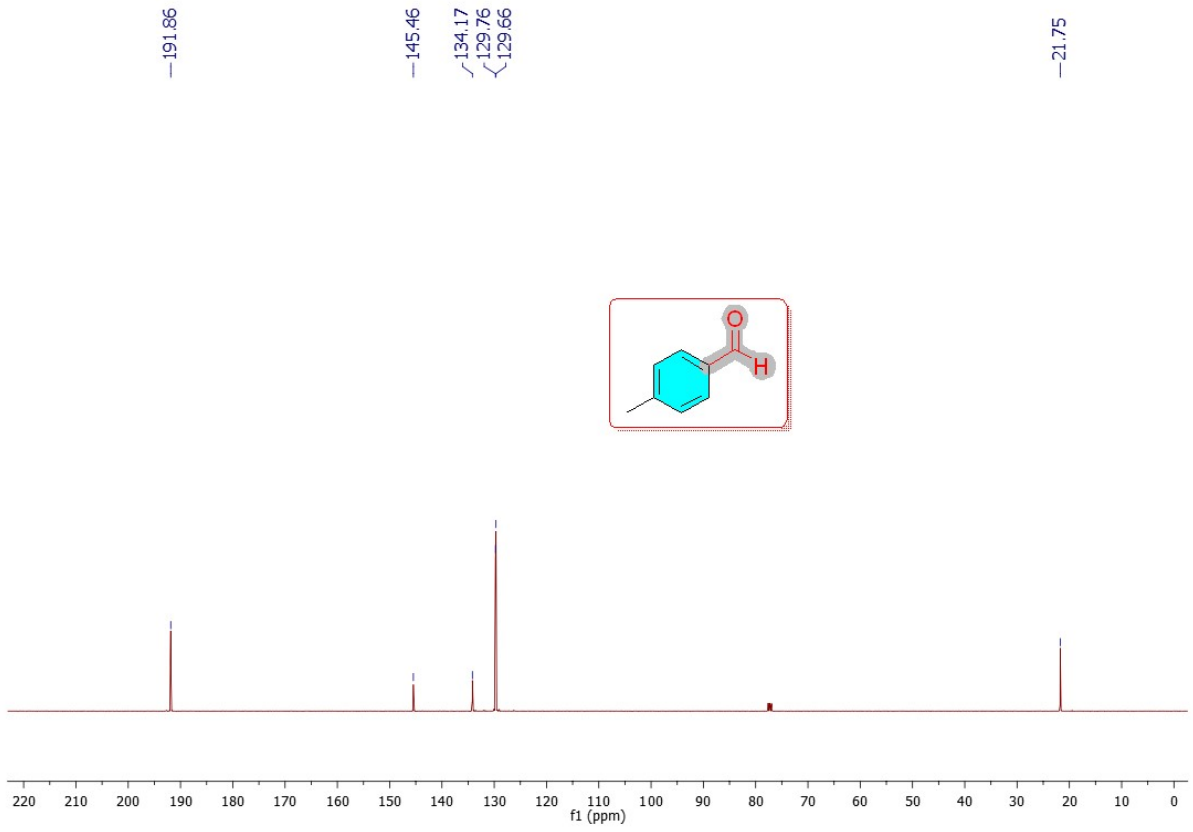
DEPT Spectra of 4-(*tert*-butyl) benzaldehyde (2f)[3]



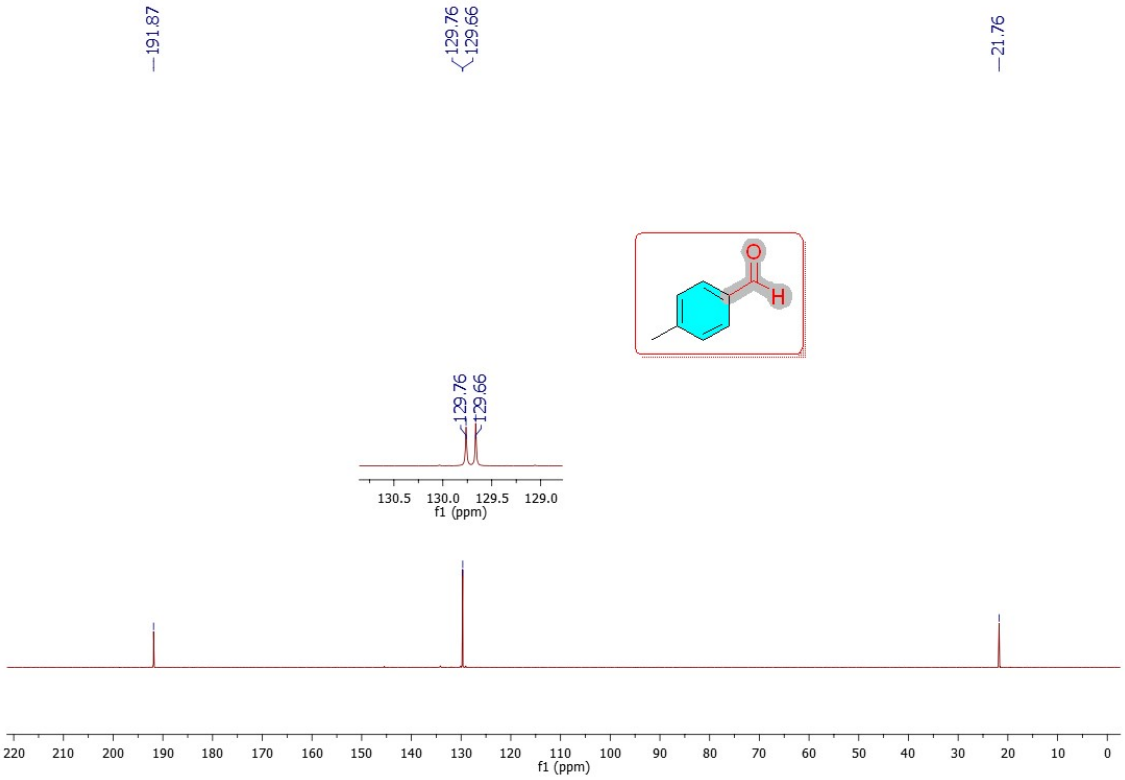
[1]HNMR Spectra of 4-Methyl benzaldehyde (2g)[4]



[13]C{[1]H} NMR Spectra of 4-Methylbenzaldehyde (2g)[4]



DEPT Spectra of 4-Methylbenzaldehyde (2g)[4]

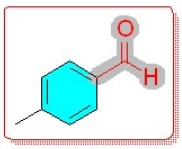


GCMS of 4-Methylbenzaldehyde (2g)

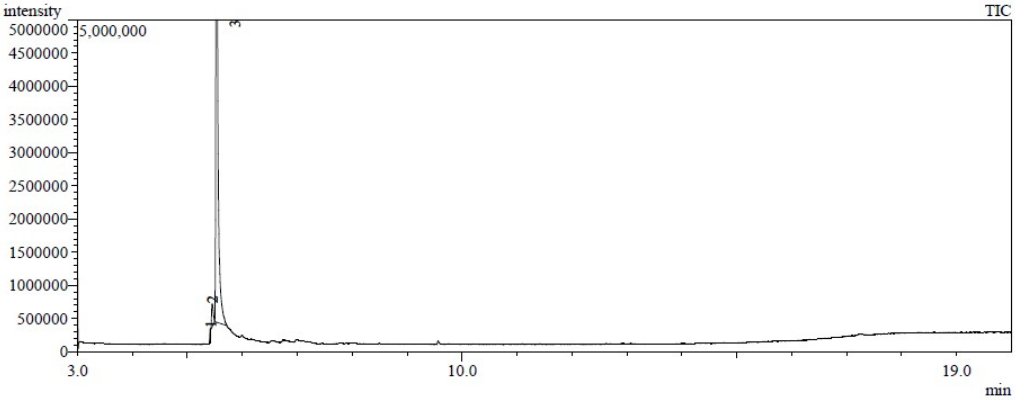
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 22-03-2023 06:20:27
Level #	: 1
Sample Name	: MZ-5
Sample ID	: MZ-5
Sample Amount	: 1
Vial #	: 25
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-45.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System.Administrator
Modified	: 22-03-2023 12:29:23

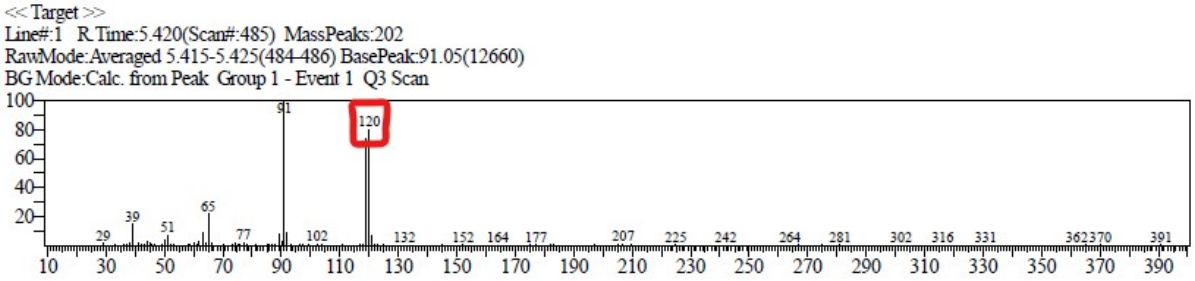


Chemical Formula: C_8H_8O
Exact Mass: 120.06

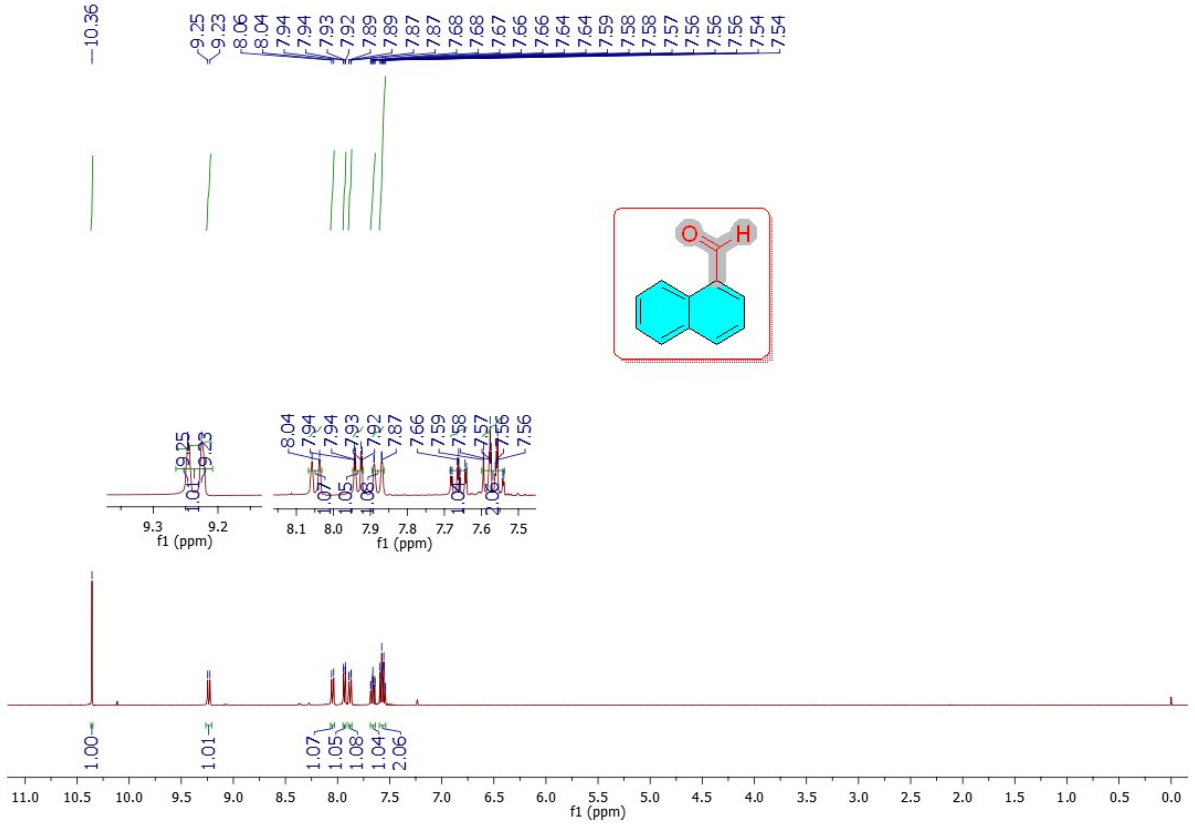


Peak Report TIC

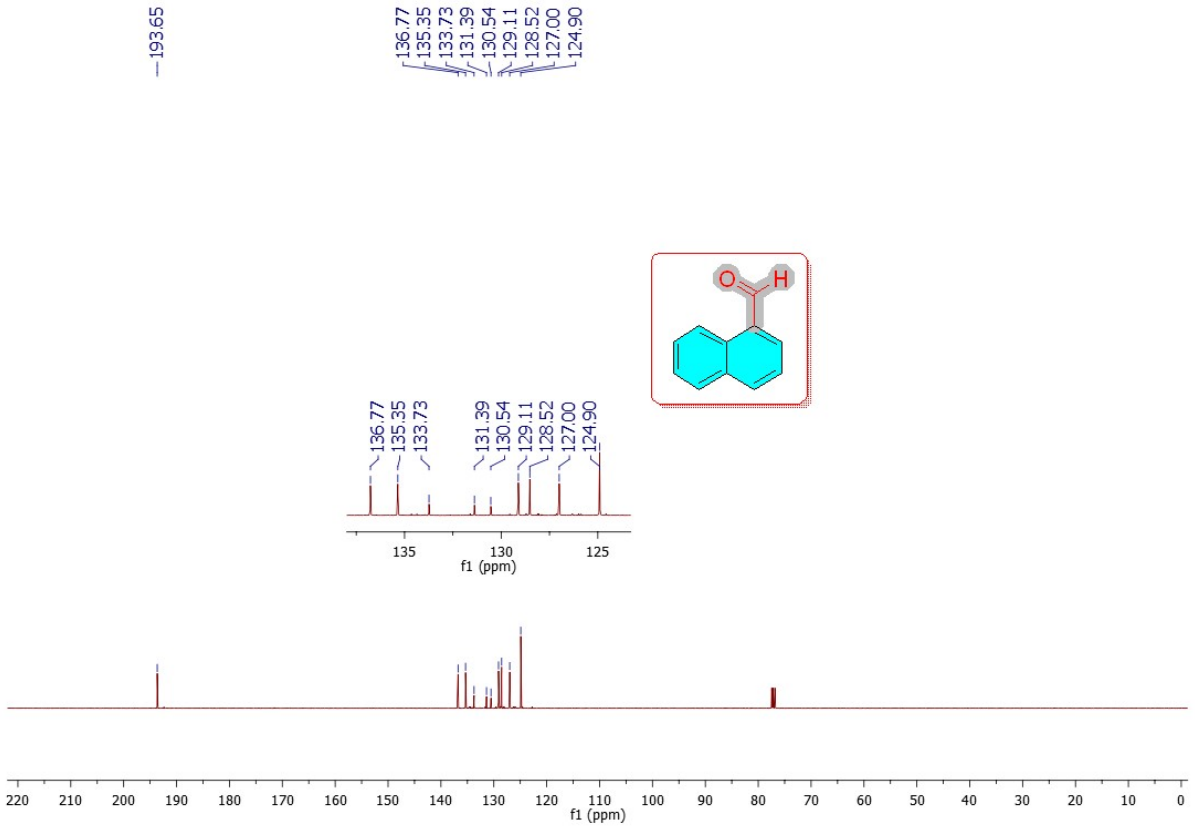
Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	5.420	242851	0.53	95	91.05	Benzaldehyde, 2-methyl-
2	5.451	815664	1.79	96	107.05	p-Cresol
3	5.533	44405604	97.67	96	119.05	Benzaldehyde, 4-methyl-
		45464119	100.00			



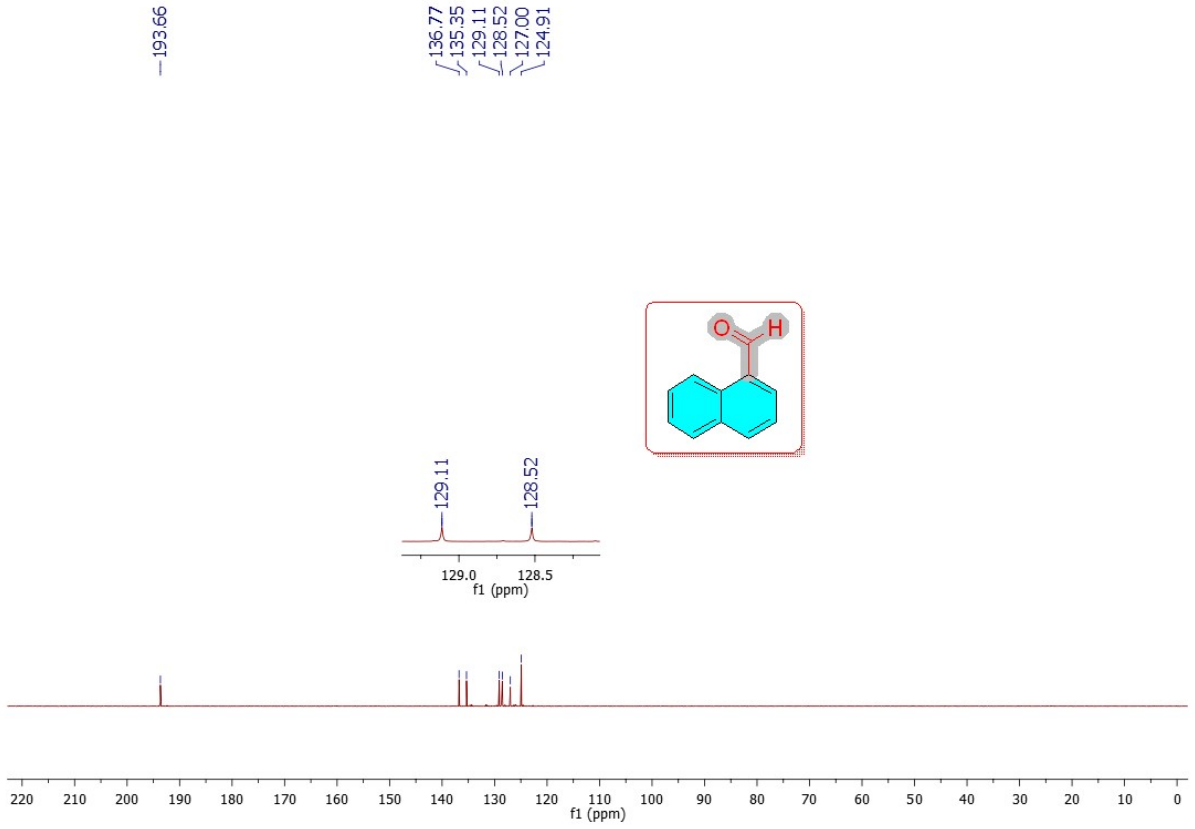
[1]HNMR Spectra of 1-Naphthaldehyde (2h)[2]



$^{13}C\{^{1}H\}$ NMR Spectra of 1-Naphthaldehyde (2h)[2]



DEPT Spectra of 1-Naphthaldehyde (2h)[2]

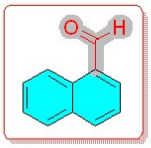


GCMS of 1-Naphthaldehyde (2h)

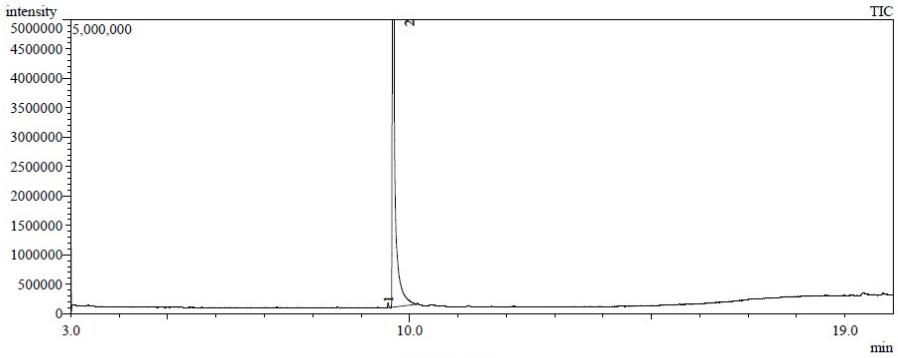
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 22-03-2023 02:25:13
Level #	: 1
Sample Name	: ZA-1
Sample ID	: ZA-1
Sample Amount	: 1
Vial #	: 16
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-36.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
EndModified by	: System Administrator
Modified	: 22-03-2023 12:22:13

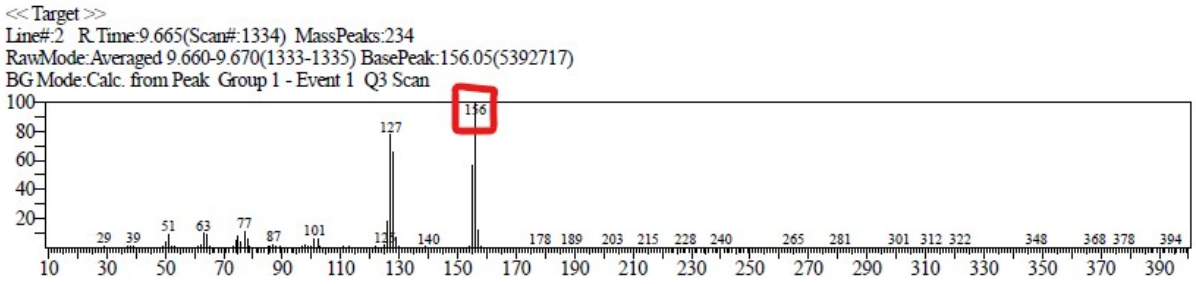


Chemical Formula: $C_{11}H_8O$
Exact Mass: 156.06

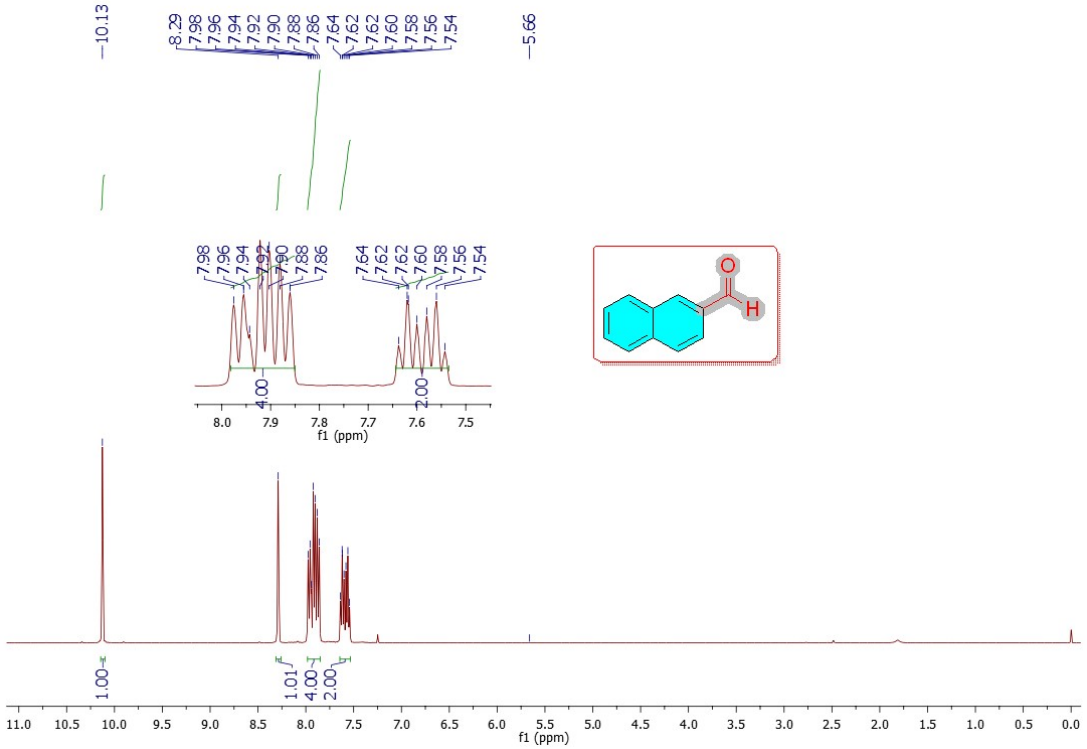


Peak Report TIC

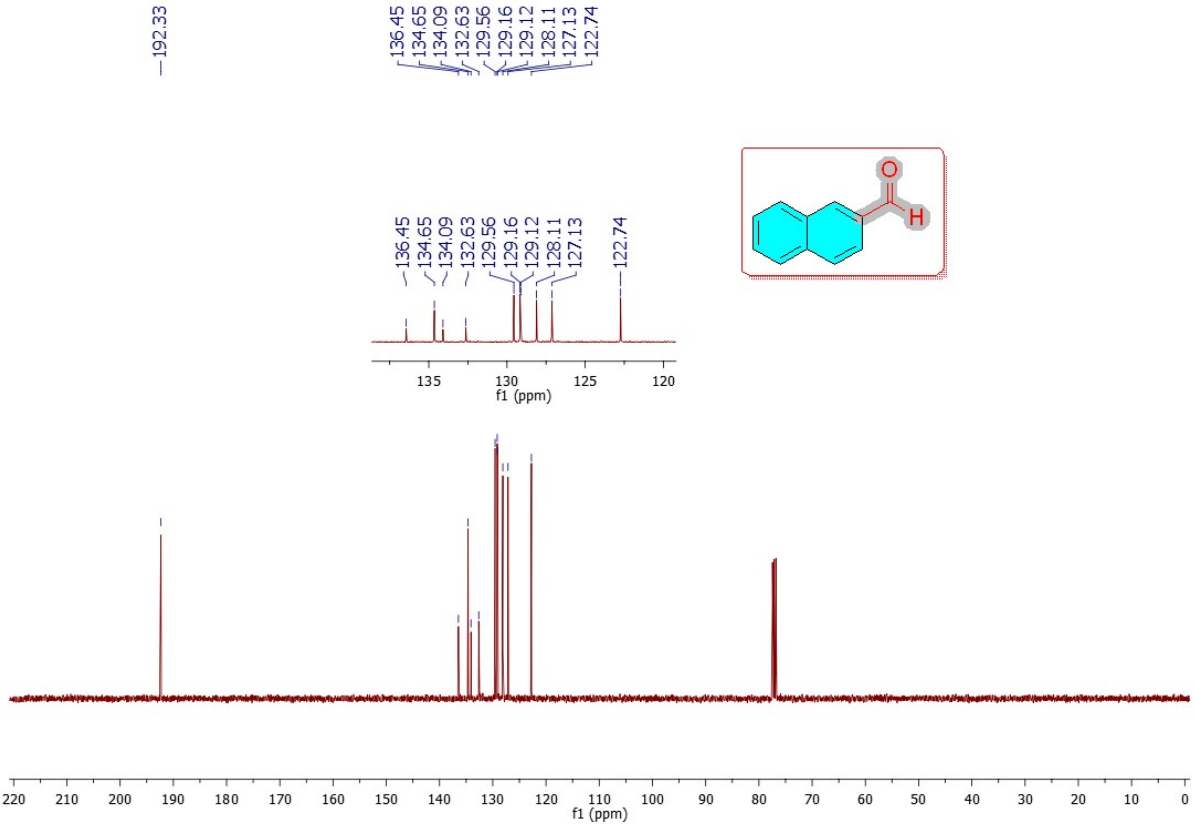
Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	9.558	115647	0.22	94	191.10	2,4-Di-tert-butylphenol
2	9.664	52761038	99.78	97	156.05	1-Naphthalenecarboxaldehyde
		52876685	100.00			



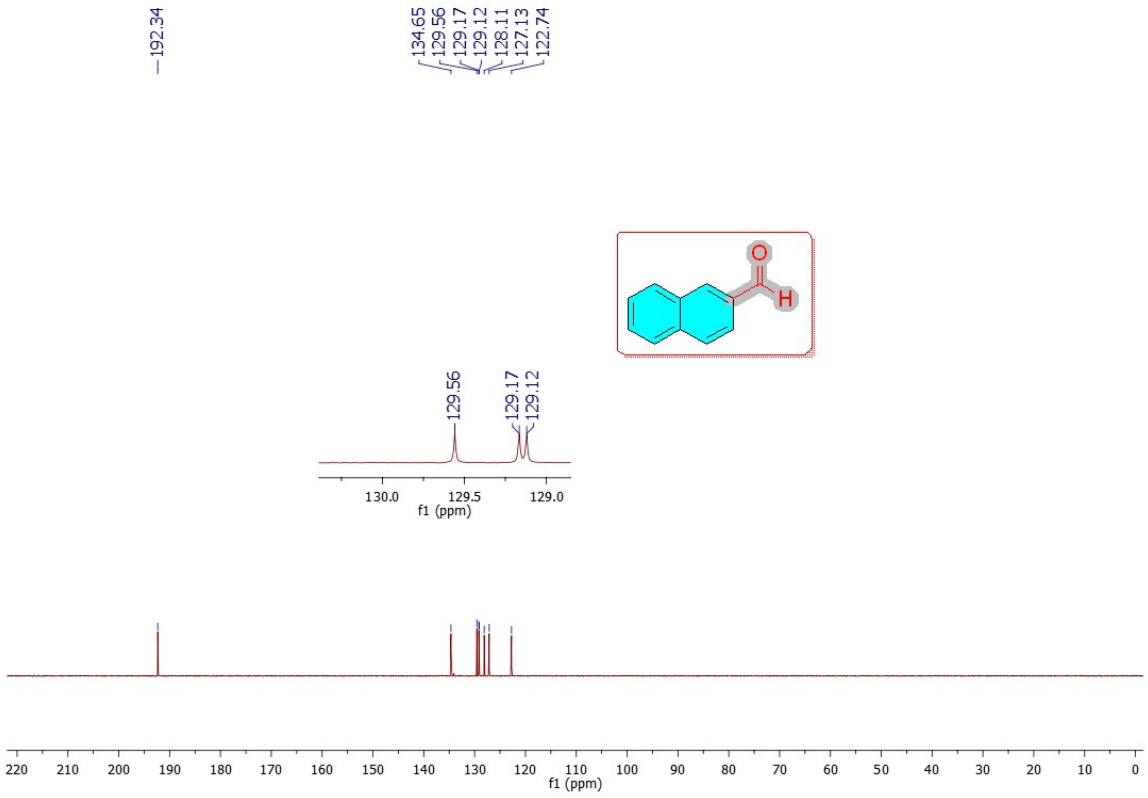
^{1}HNMR Spectra of 2-Naphthaldehyde (2i)[2]



^{13}C{^{1}H} NMR Spectra of 2-Naphthaldehyde (2i)[2]



DEPT Spectra of 2-Naphthaldehyde (2i)[2]

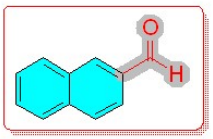


GCMS of 2-Naphthaldehyde (2i)

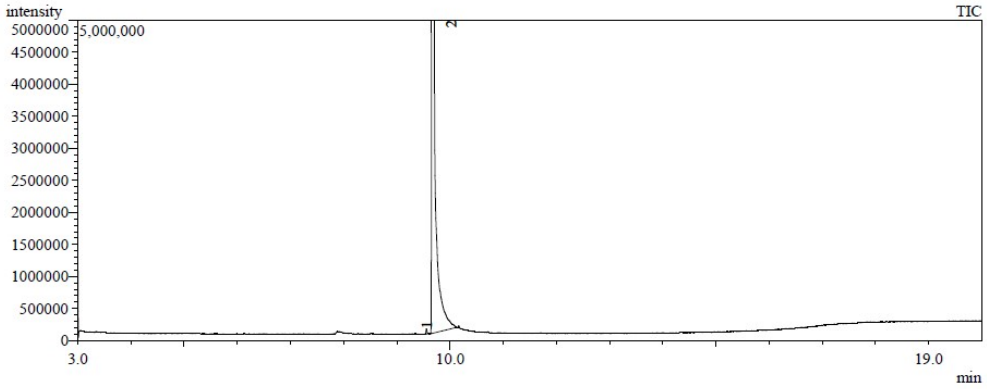
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 22-03-2023 02:51:23
Level #	: 1
Sample Name	: ZA-2
Sample ID	: ZA-2
Sample Amount	: 1
Vial #	: 17
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-37.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:22:42



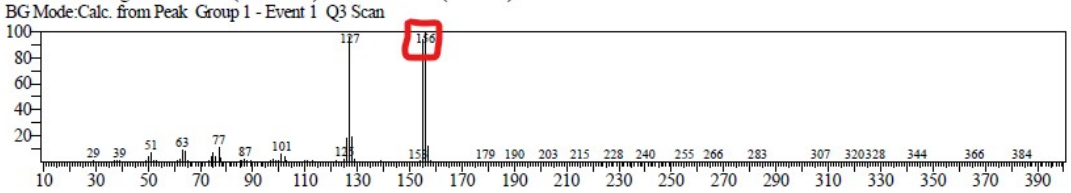
Chemical Formula: $C_{11}H_8O$
Exact Mass: 156.06



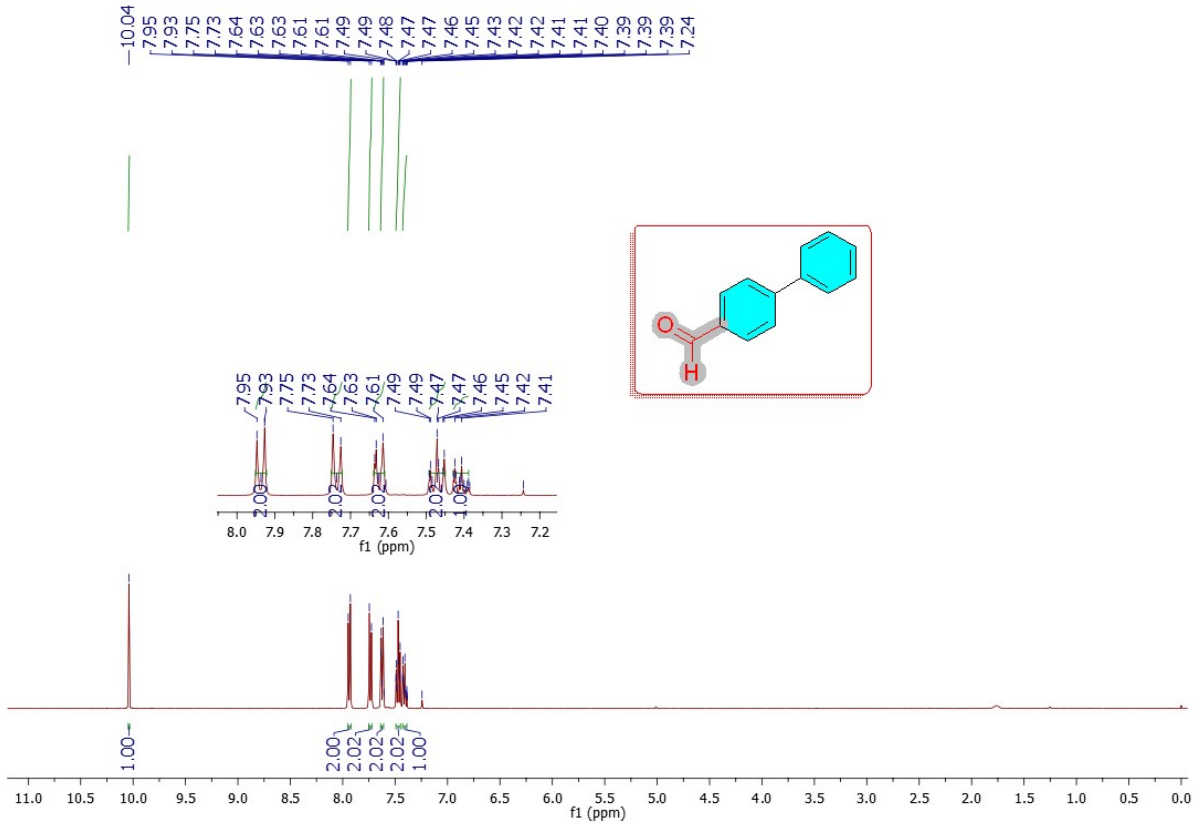
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	9.559	104866	0.13	94	191.10	2,4-Di-tert-butylphenol
2	9.688	80863644	99.87	96	156.05	2-Naphthalenecarboxaldehyde
		80968510	100.00			

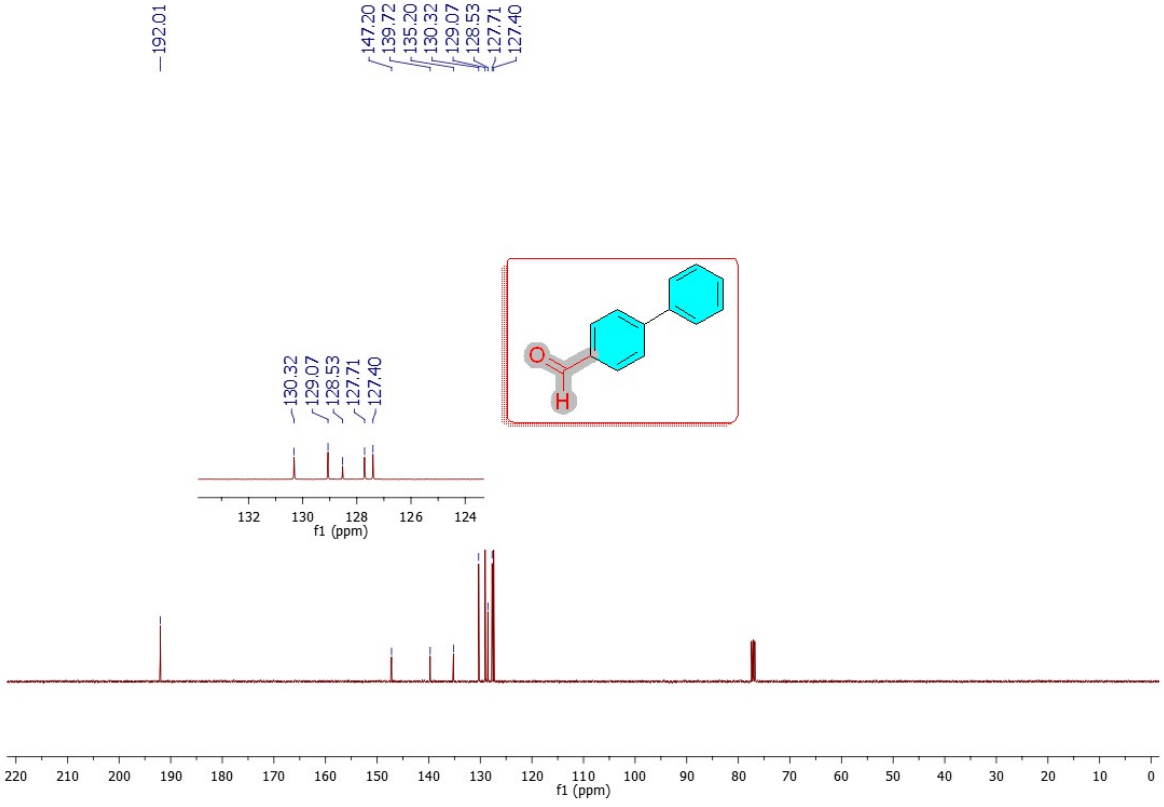
<< Target >>
Line#:2 R.Time:9.690(Scan#:1339) MassPeaks:223
RawMode:Averaged 9.685-9.695(1338-1340) BasePeak:156.05(7213445)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



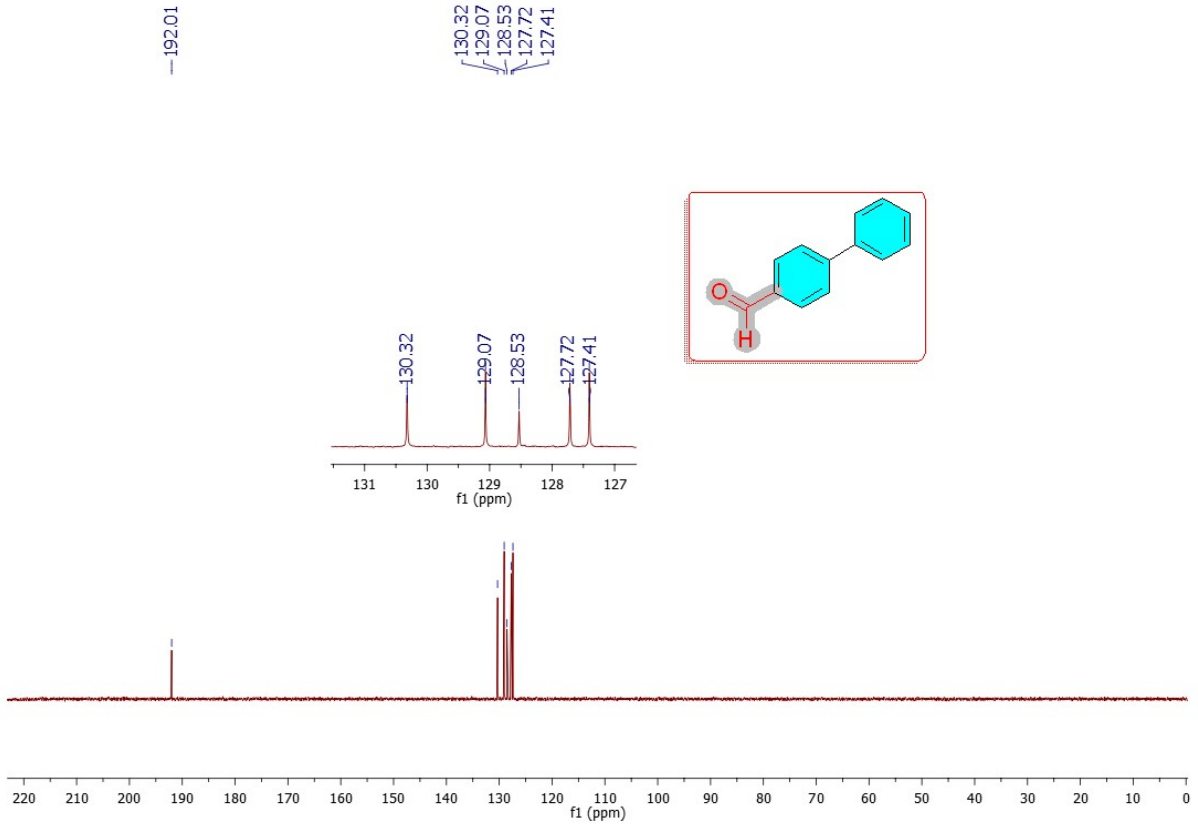
[1]HNMR Spectra of [1,1-Biphenyl]-4-carbaldehyde(2j)[2]



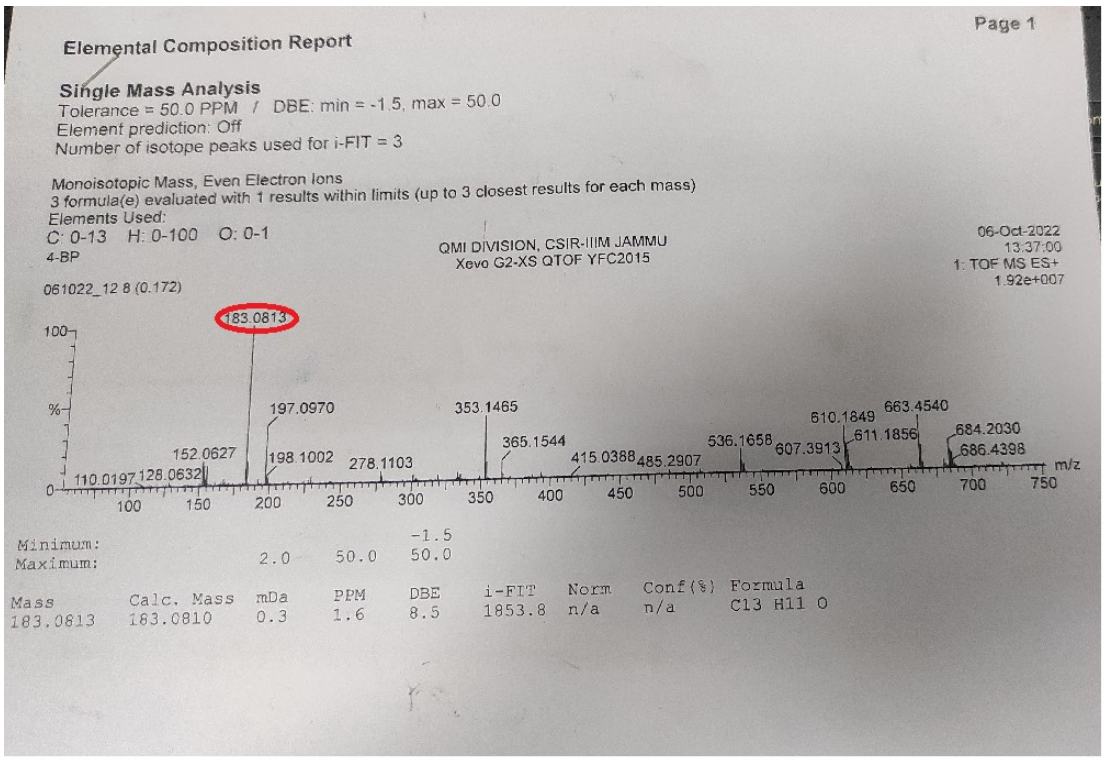
[13]C{[1]H} NMR Spectra of [1,1-Biphenyl]-4-carbaldehyde(2j)[2]



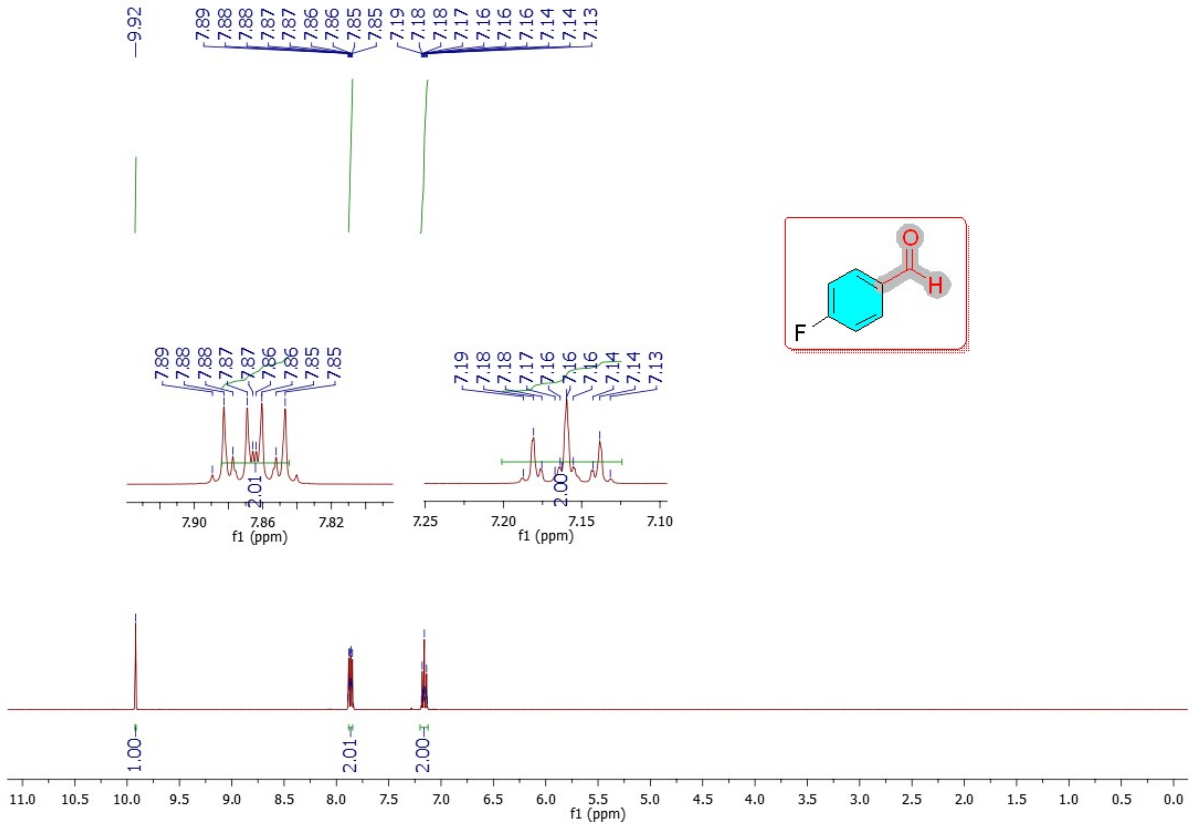
DEPT Spectra of [1,1-Biphenyl]-4-carbaldehyde(2j)[2]



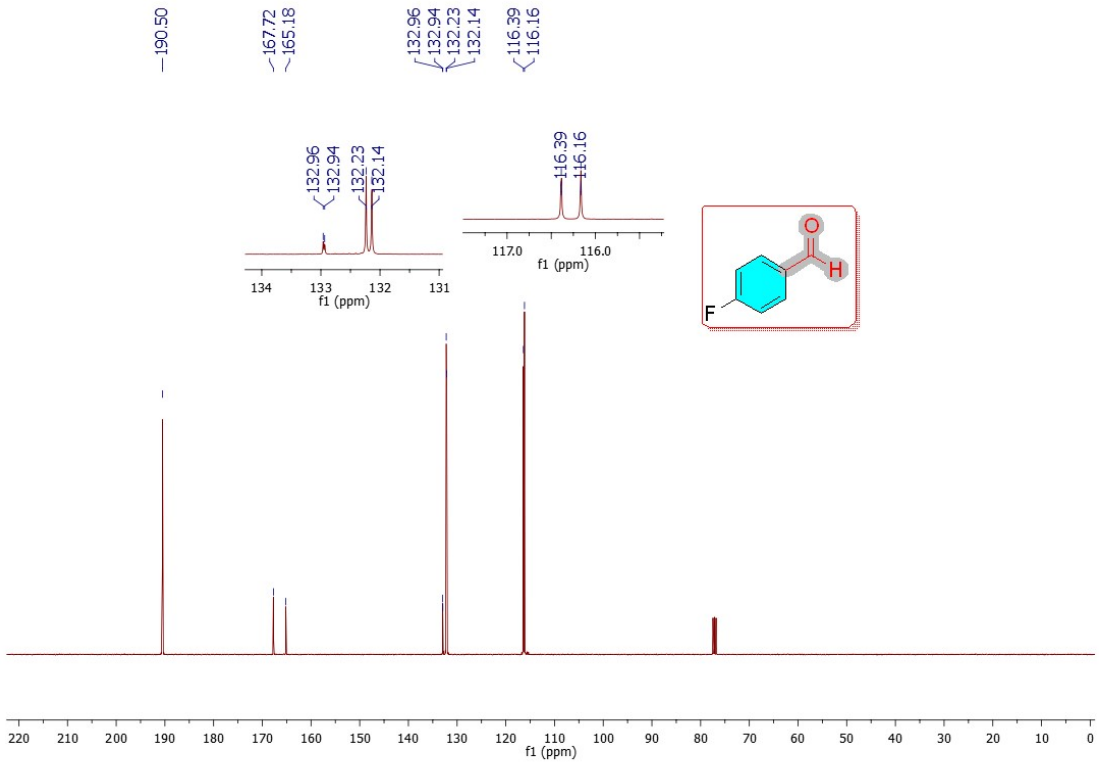
HRMS of [1,1-Biphenyl]-4-carbaldehyde(2j)



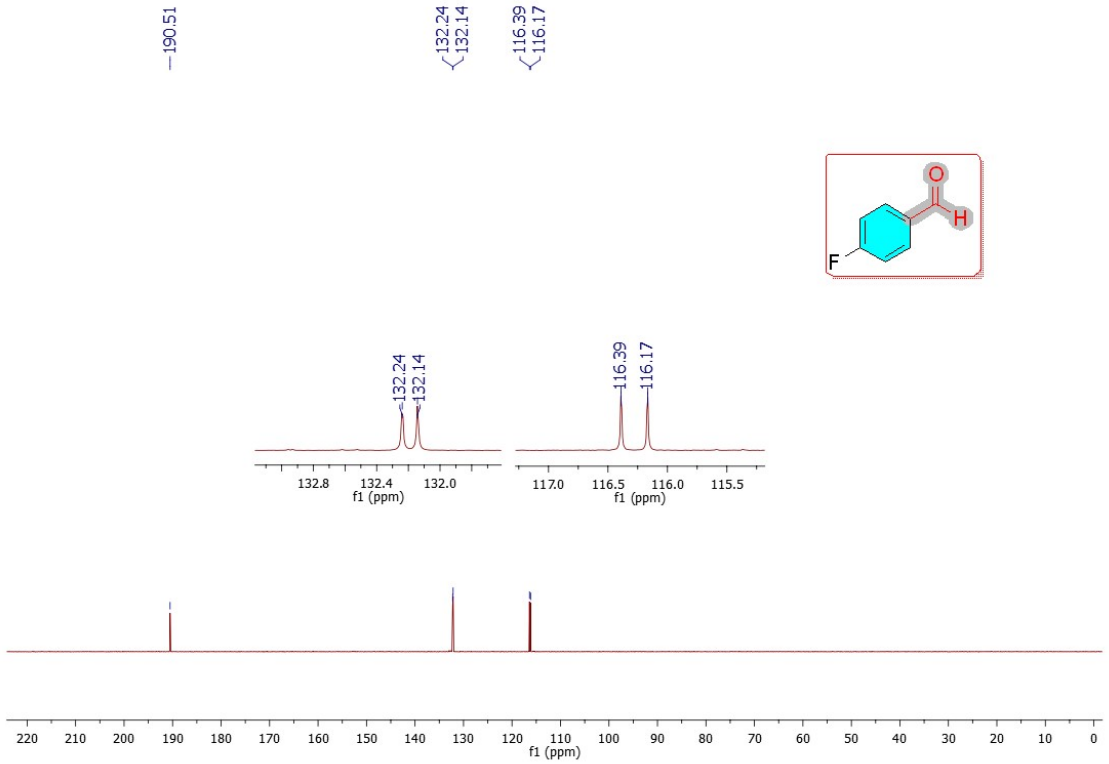
[1]HNMR Spectra of 4-Fluoro benzaldehyde (2k)[2]



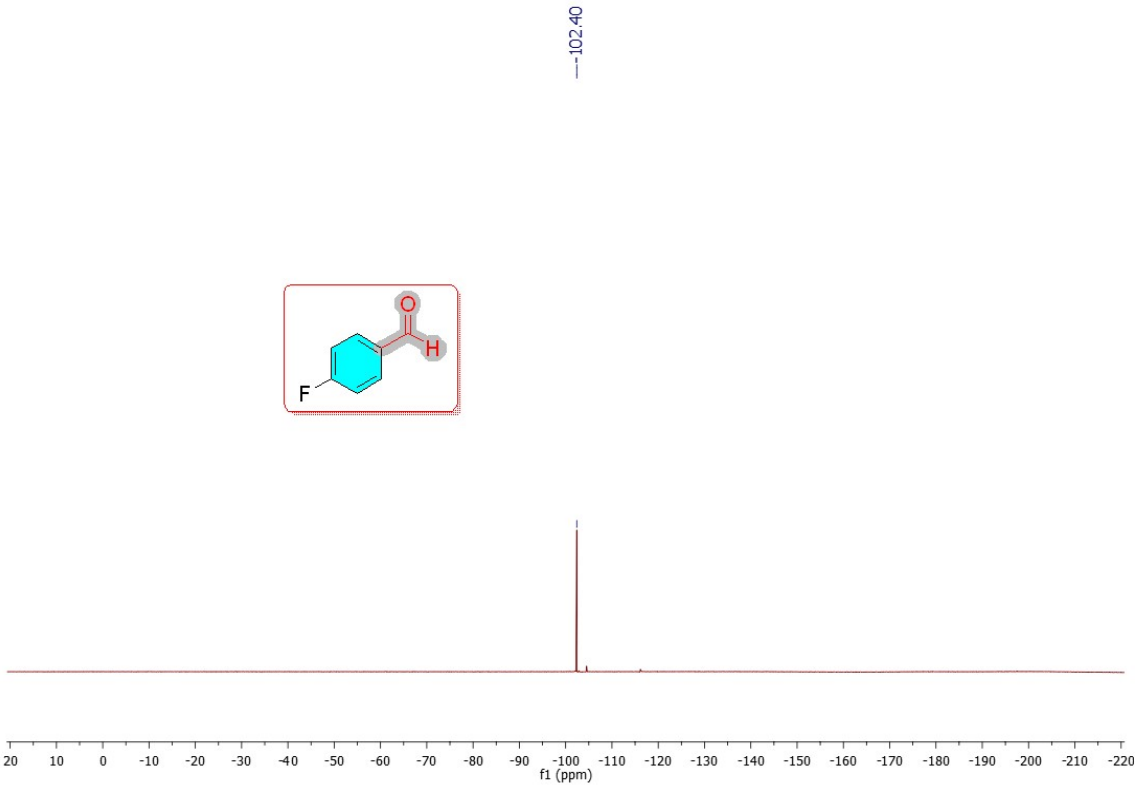
[13]C{[1]H} NMR Spectra of 4-Fluoro benzaldehyde (2k)[2]



DEPT Spectra of 4-Fluoro benzaldehyde (2k)[2]



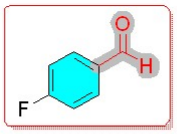
^{19}F Spectra of 4-Fluoro benzaldehyde (2k)[2]



GCMS of 4-Fluoro benzaldehyde (2k)

Qualitative Analysis Report

IIIM GCMS ANALYSIS



Chemical Formula: C_7H_5FO
Exact Mass: 124.03

Sample Information

Analyzed by	: Admin
Analyzed	: 1/27/2022 6:55:45 AM
Level #	: 1
Sample Name	: Method-12
Sample ID	:
Sample Amount	: 1
Vial #	: 10
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\JAN 2022\25.01.2022\25.01.2022 BHARTI043.qgd
Method File	: D:\GCMS METHOD\GCMS-GENERAL AMIT 1.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
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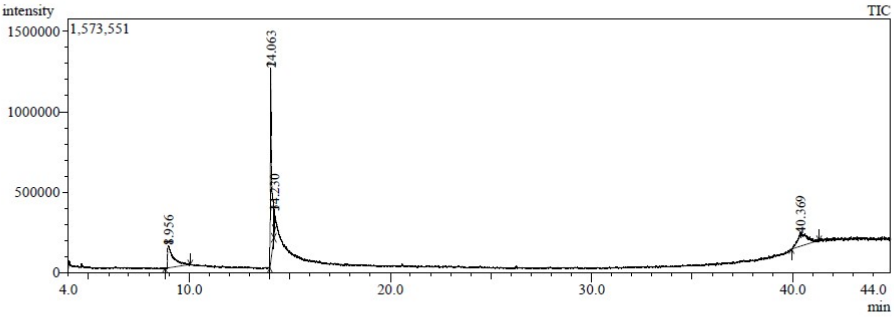
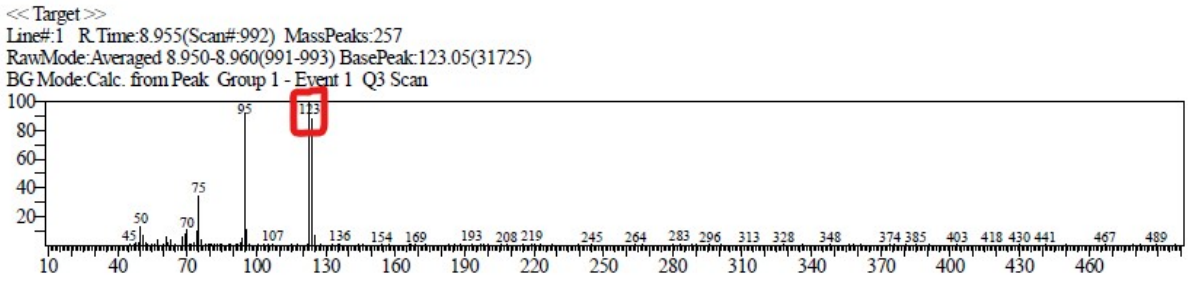
Modified	: 1/30/2022 6:50:27 PM

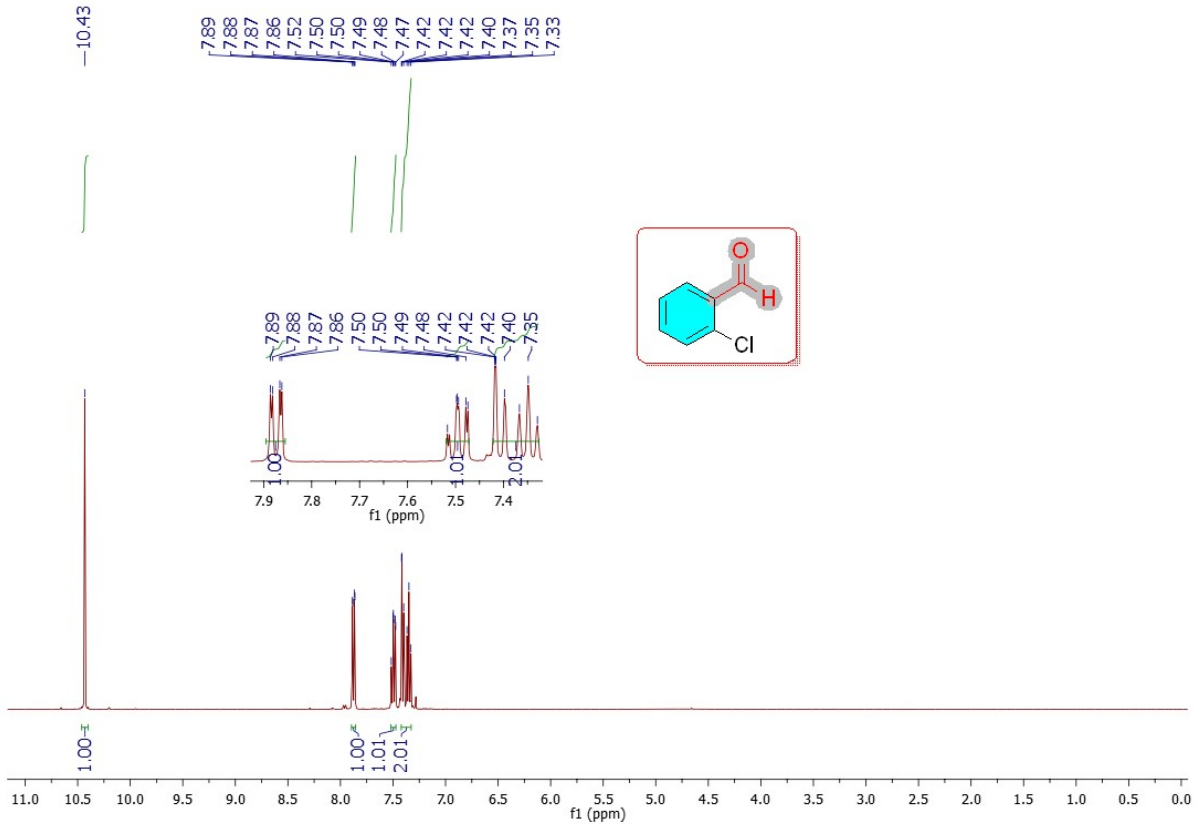


Peak Report TIC

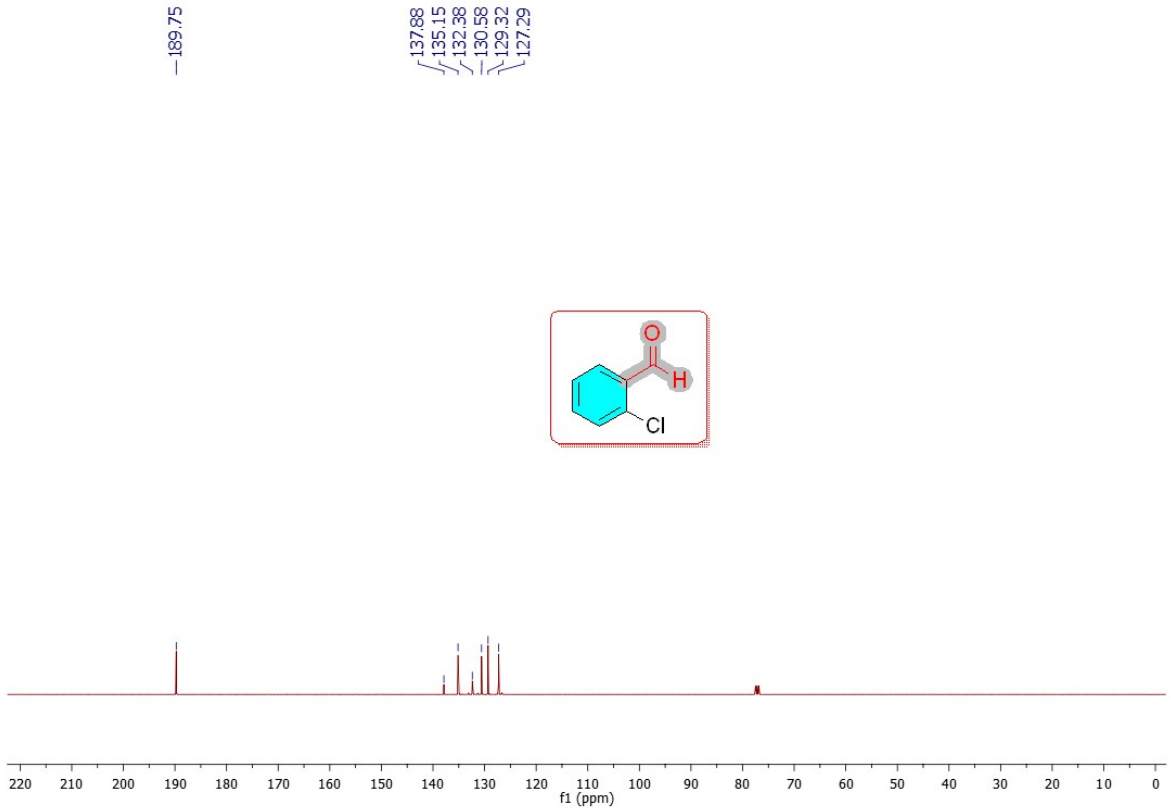
Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	8.956	2750578	24.35	138080	8.86	97	123.05	Benzaldehyde, 4-fluoro-
2	14.063	5524711	48.91	1193474	76.57	98	123.00	Benzoic acid, 4-fluoro-
3	14.230	414058	3.67	144945	9.30	56	123.00	4-Chlorophenyl 2-fluoro-3-methylbenzyl sulfo
4	40.369	2605456	23.07	82116	5.27	64	115.10	Cholest-5-ene-16,22-dione, 3,26-bis(acetyloxy
		11294803	100.00	1558615	100.00			



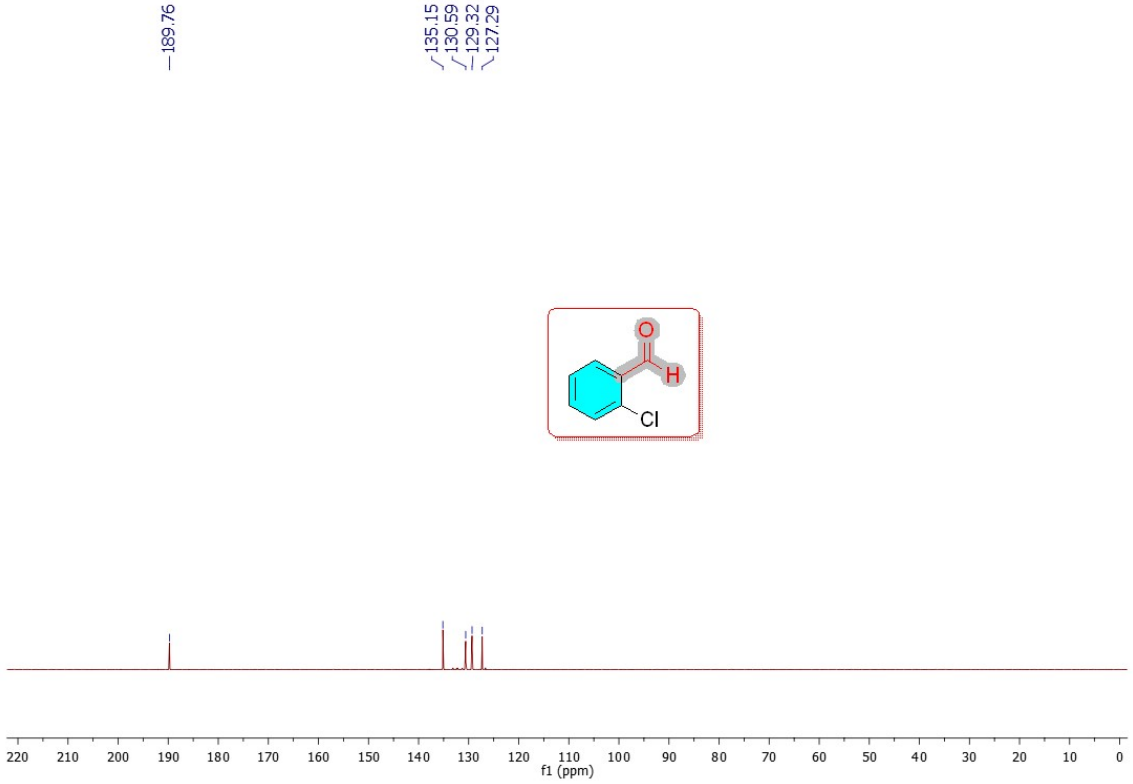
^{1}HNMR Spectra of 2-Chloro benzaldehyde (2l)[5]



^{13}C{^{1}H} NMR Spectra of 2-Chloro benzaldehyde (2l)[5]

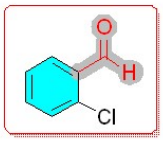


DEPT Spectra of 2-Chloro benzaldehyde (2l)[5]



GCMS of 2-Chloro benzaldehyde (2l)

IIIM GCMS ANALYSIS



Chemical Formula: C_7H_5ClO
Exact Mass: 140.00
Molecular Weight: 140.57

Sample Information

Analyzed by	: Admin
Analyzed	: 1/27/2022 10:23:00 PM
Level #	: 1
Sample Name	: Method-19
Sample ID	:
Sample Amount	: 1
Vial #	: 25
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\JAN 2022\25.01.2022\25.01.2022 BHARTI061.qgd
Method File	: D:\GCMS METHOD\GCMS-GENERAL AMIT 1.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
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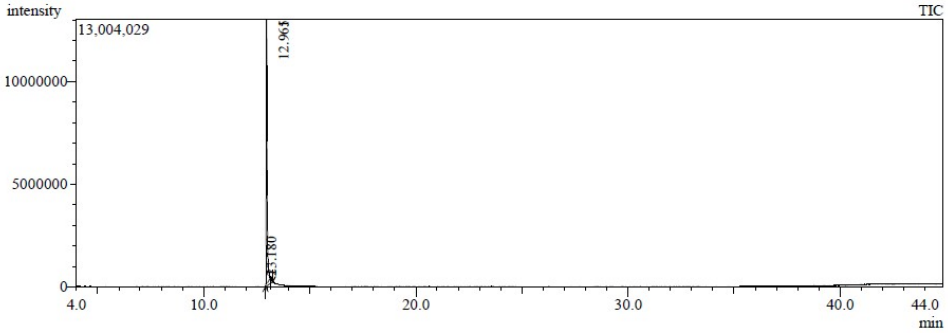
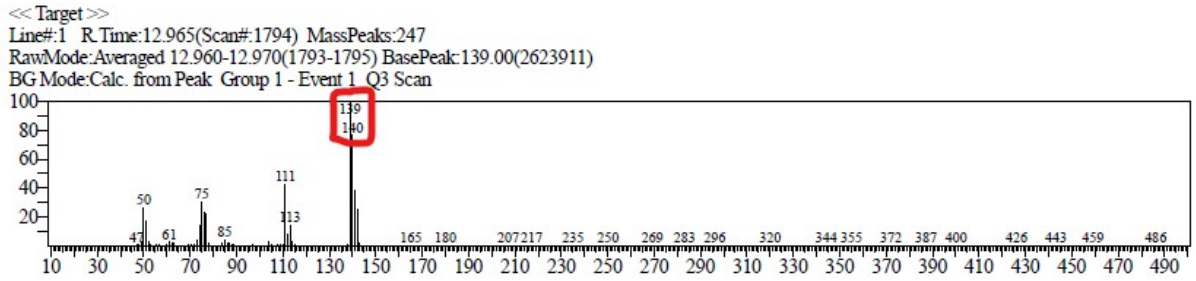
Modified	: 1/27/2022 11:07:52 PM

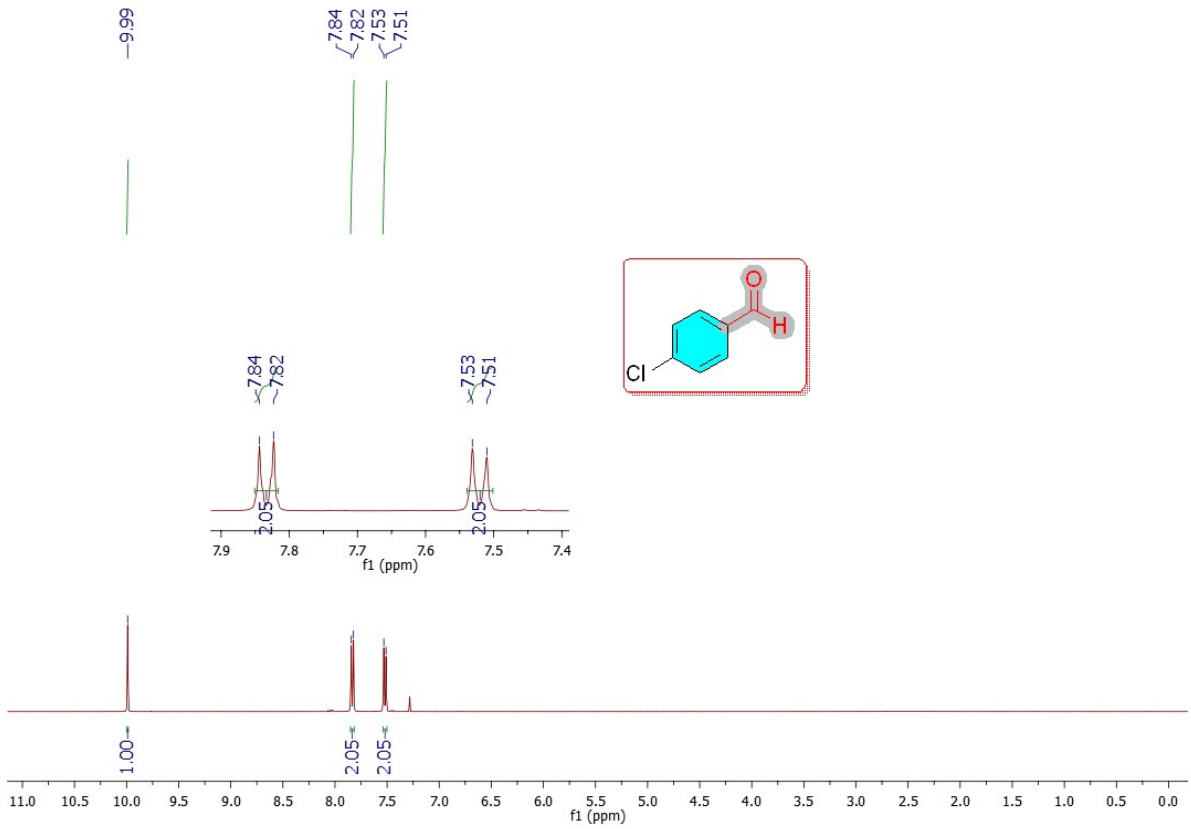


Peak Report TIC

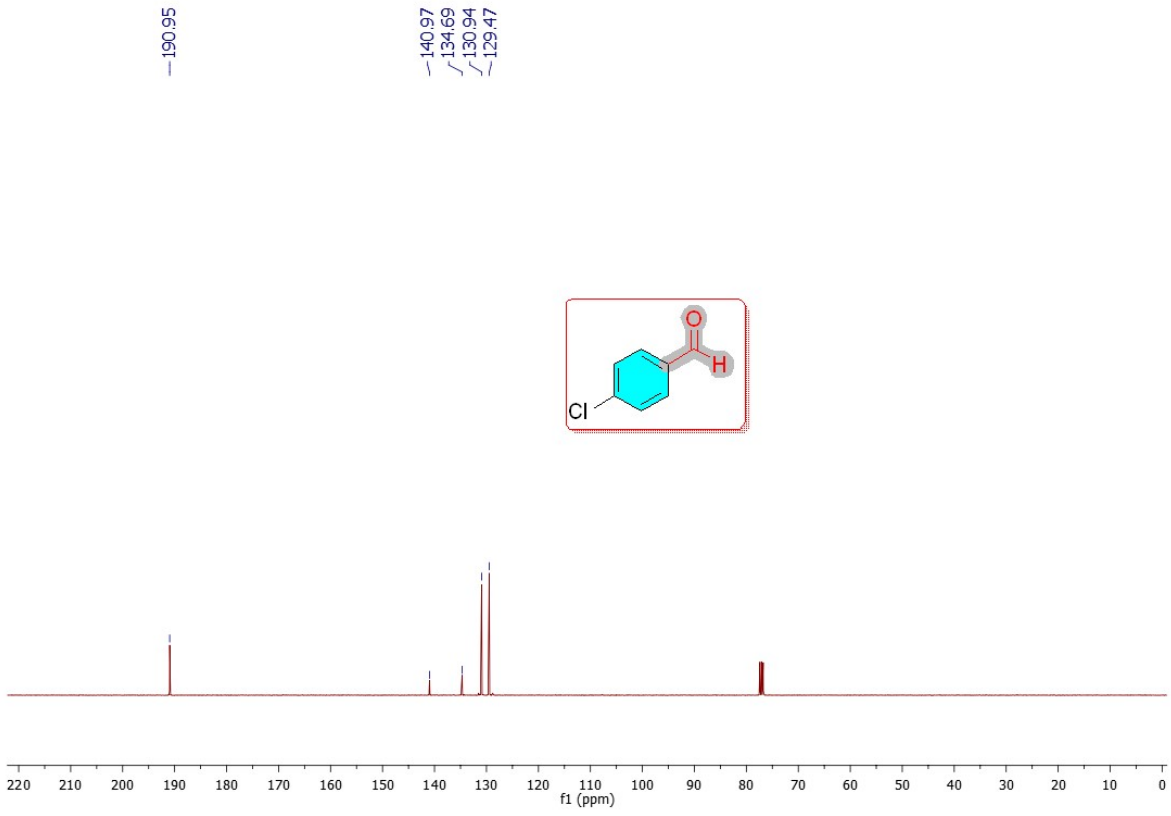
Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	12.965	39296432	99.06	12948499	98.99	99	139.00	Benzaldehyde, 2-chloro-
2	13.180	374584	0.94	132554	1.01	91	128.00	Phenol, 2-chloro-
		39671016	100.00	13081053	100.00			



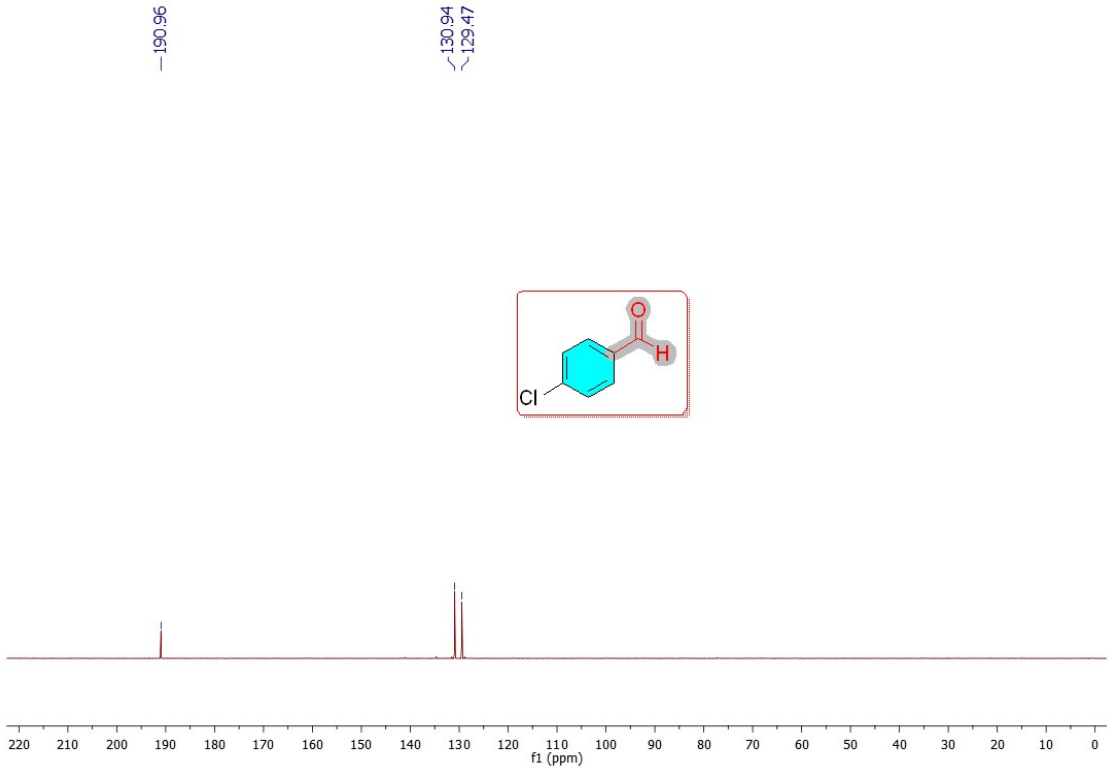
^{1}HNMR Spectra of 4-Chloro benzaldehyde (2m)[2]



^{13}C{^{1}H} NMR Spectra of 4-Chloro benzaldehyde (2m)[2]



DEPT Spectra of 4-Chloro benzaldehyde (2m)[2]

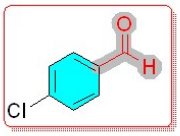


GCMS of 4-Chloro benzaldehyde (2m)

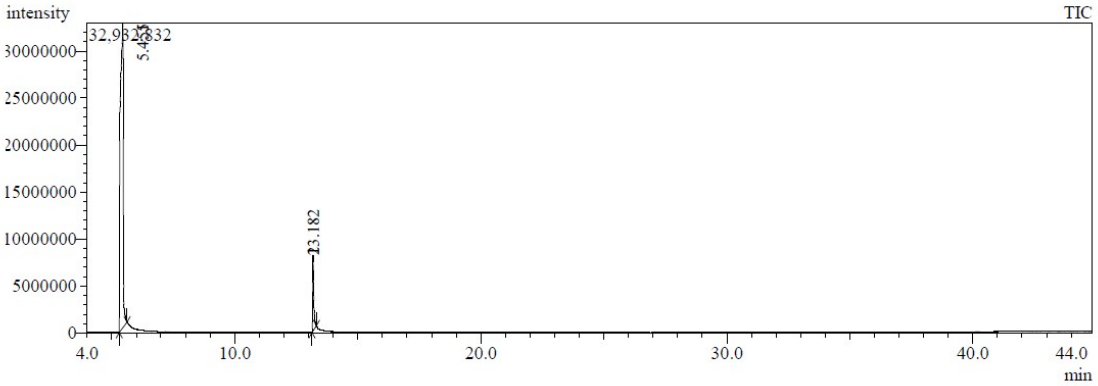
IIM GCMS ANALYSIS

Sample Information

Analyzed by	: Admin
Analyzed	: 1/27/2022 8:39:56 PM
Level #	: 1
Sample Name	: Method-23
Sample ID	:
Sample Amount	: 1
Vial #	: 23
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\JAN 2022\25.01.2022\25.01.2022 BHARTI059.qgd
Method File	: D:\GCMS METHOD\GCMS-GENERAL AMIT 1.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
$EndIf$Modified by	: Admin
Modified	: 1/27/2022 9:24:48 PM



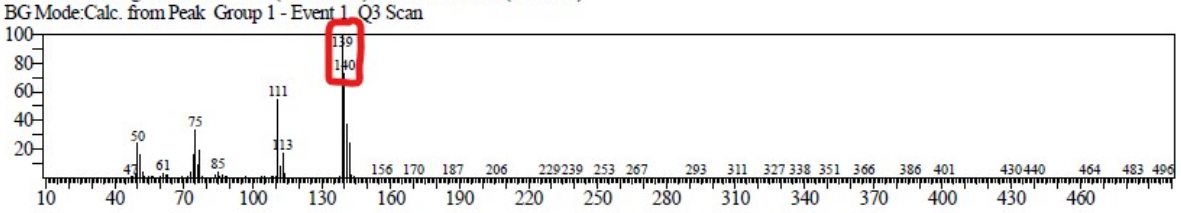
Chemical Formula: C_7H_5ClO
Exact Mass: 140.00
Molecular Weight: 140.57



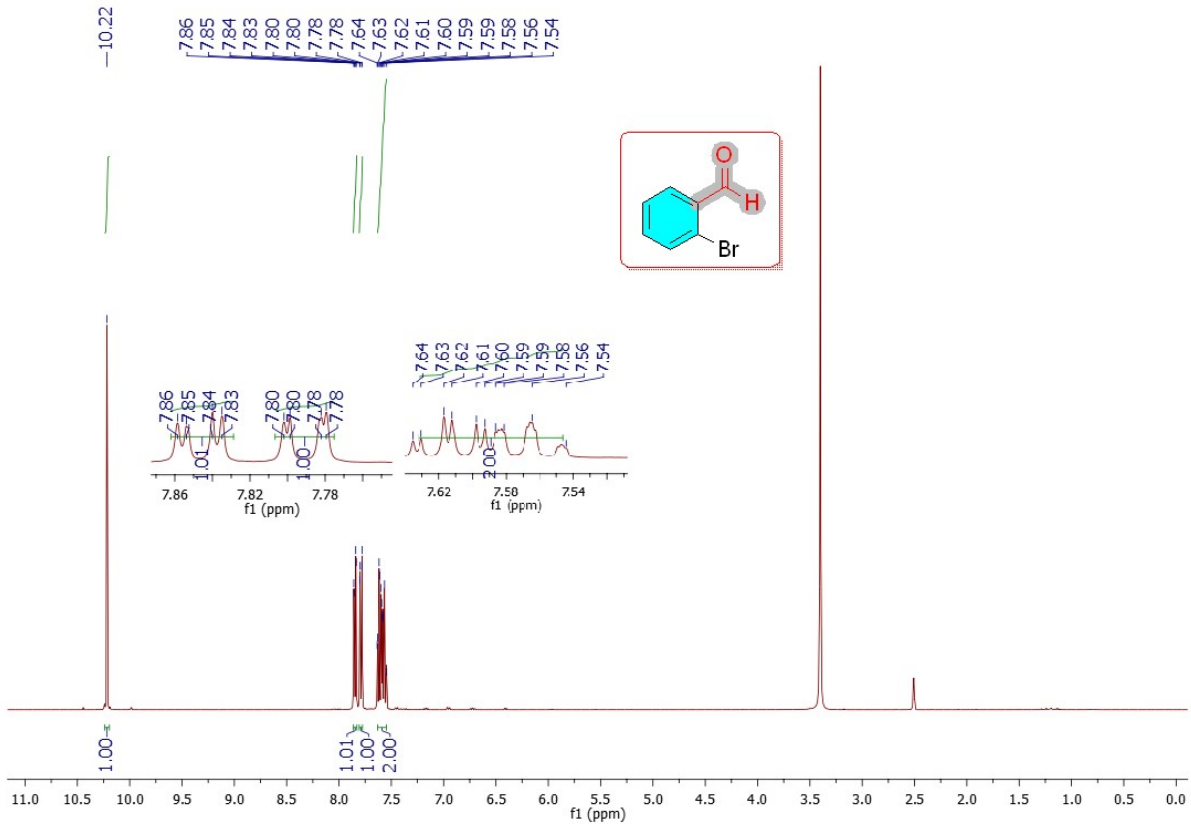
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	5.455	269012397	91.54	32382541	80.09	73	84.15	5-Aminoisoxazole
2	13.182	24867946	8.46	8048282	19.91	98	139.00	Benzaldehyde, 4-chloro-
		293880343	100.00	40430823	100.00			

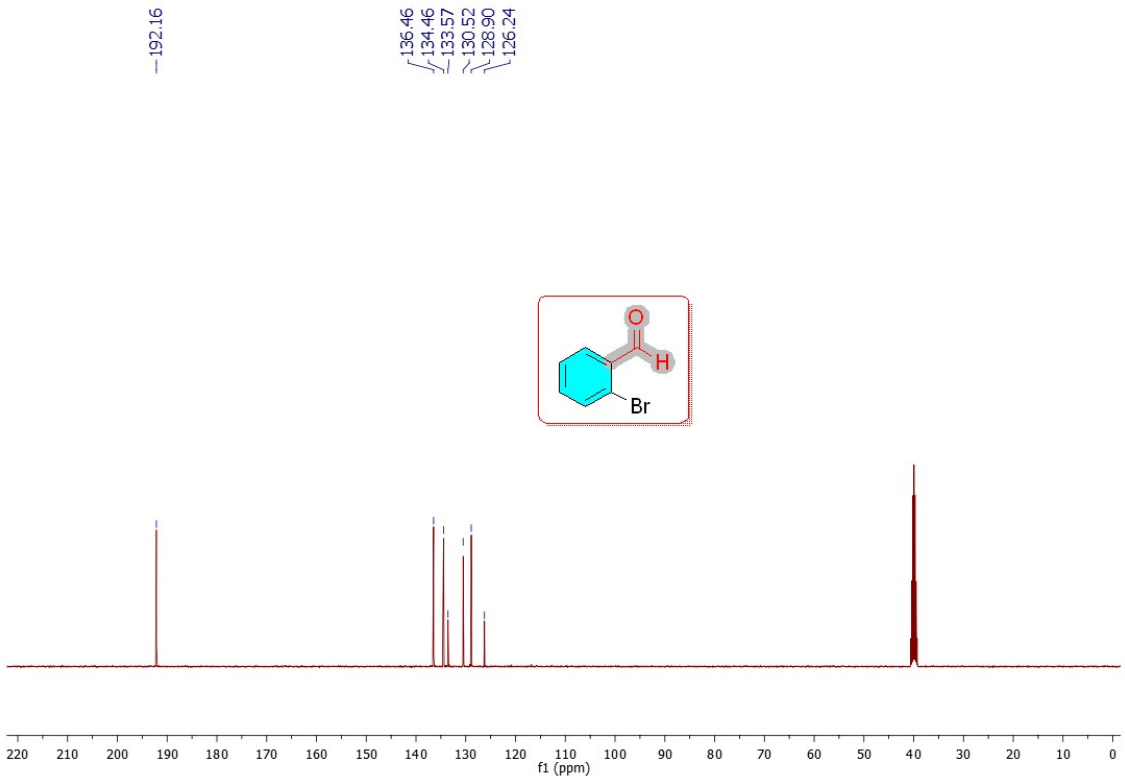
<< Target >>
Line#:2 R.Time:13.180(Scan#:1837) MassPeaks:273
RawMode:Averaged 13.175-13.185(1836-1838) BasePeak:139.00(1642747)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



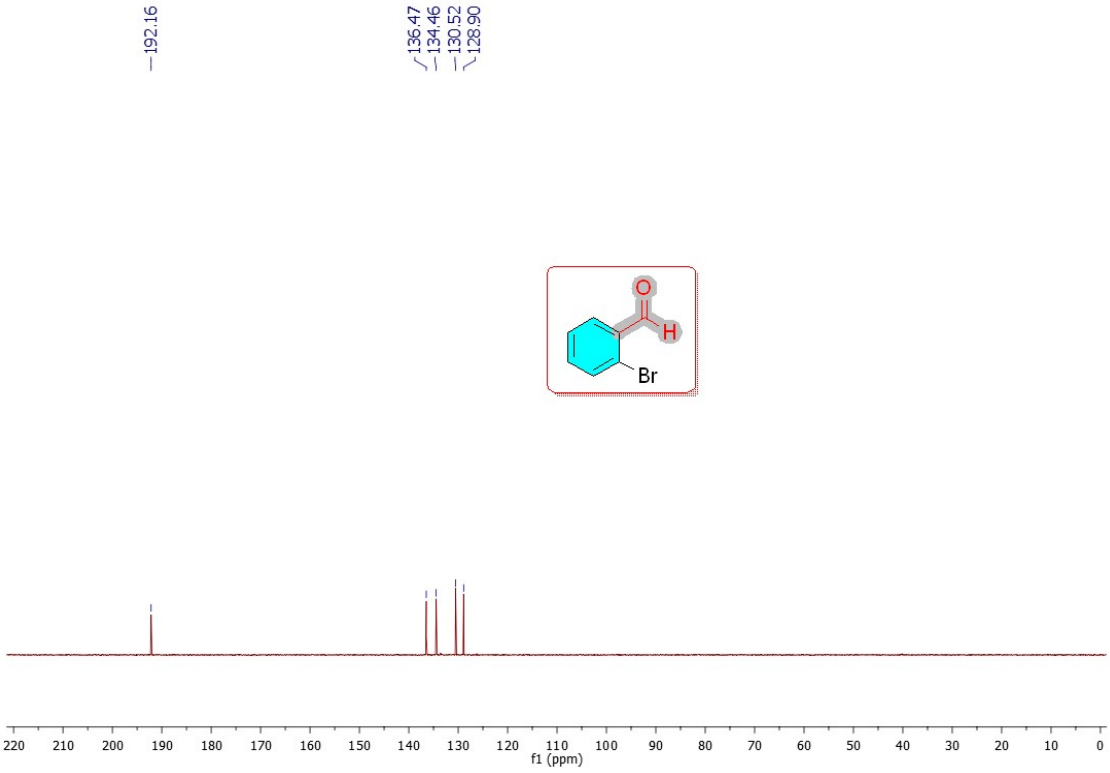
[1]HNMR Spectra of 2-Bromobenzaldehyde (2n)[2]



[13]C{[1]H} NMR Spectra of 2-Bromo benzaldehyde (2n)[2]



DEPT Spectra of 2-Bromo benzaldehyde (2n)[2]

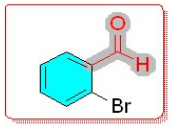


GCMS of 2-Bromo benzaldehyde (2n)

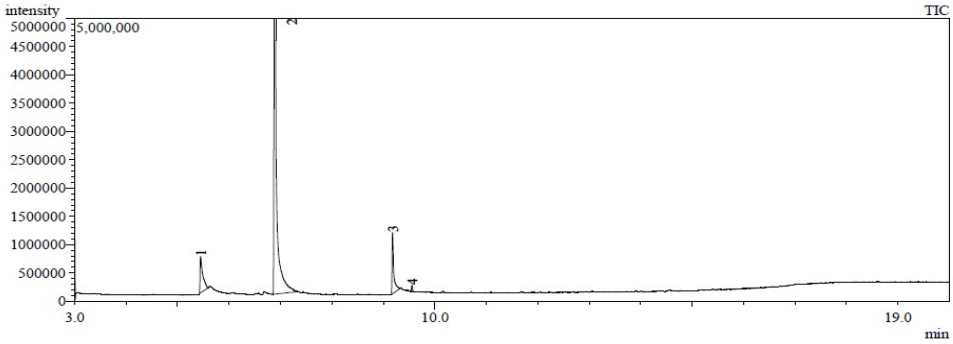
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 22-03-2023 03:43:34
Level #	: 1
Sample Name	: ZA-4
Sample ID	: ZA-4
Sample Amount	: 1
Vial #	: 19
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-39.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:25:46

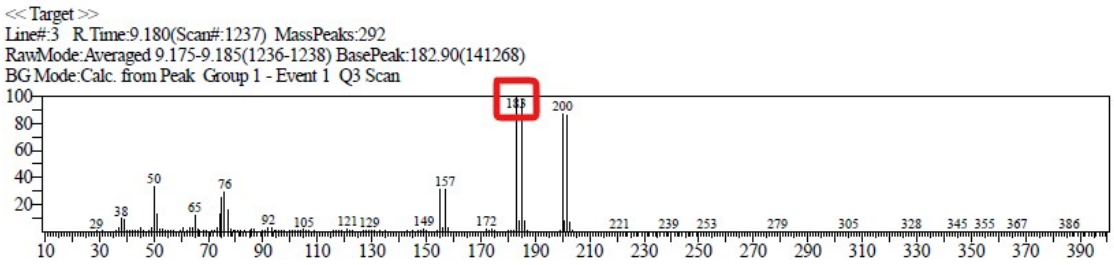


Chemical Formula: C_7H_5BrO
Exact Mass: 183.95

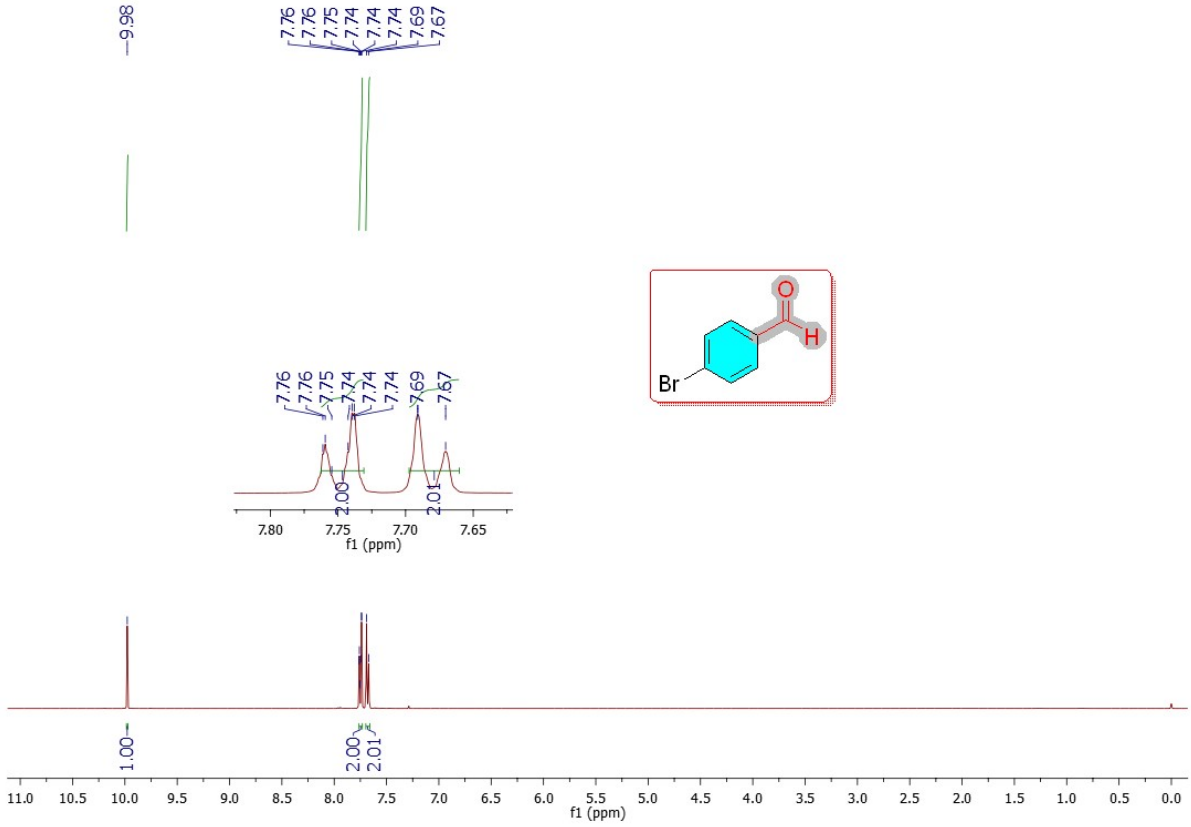


Peak Report TIC

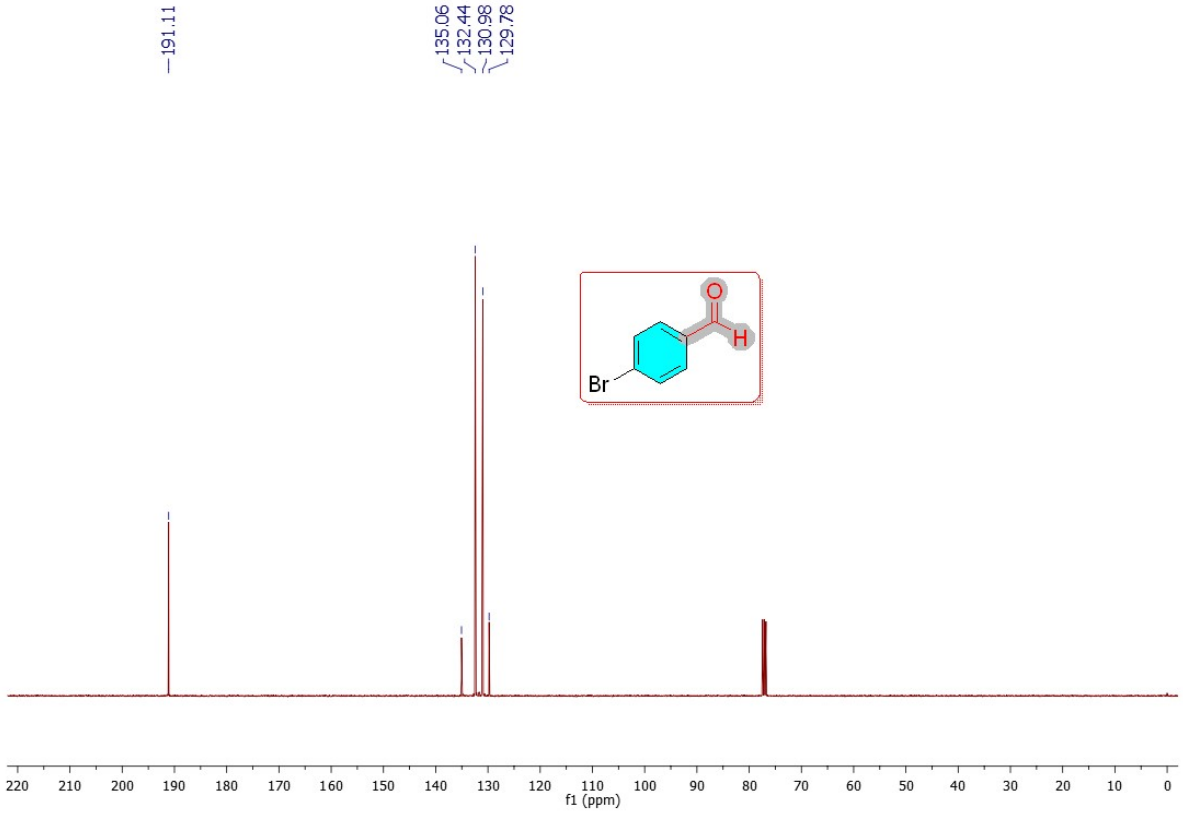
Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	5.447	2432974	5.09	96	171.90	Phenol, 2-bromo-
2	6.892	42818771	89.66	96	184.90	Benzaldehyde, 2-bromo-
3	9.180	2368506	4.96	94	182.90	Benzoic acid, 2-bromo-
4	9.555	138221	0.29	92	191.10	2,4-Di-tert-butylphenol
		47758472	100.00			



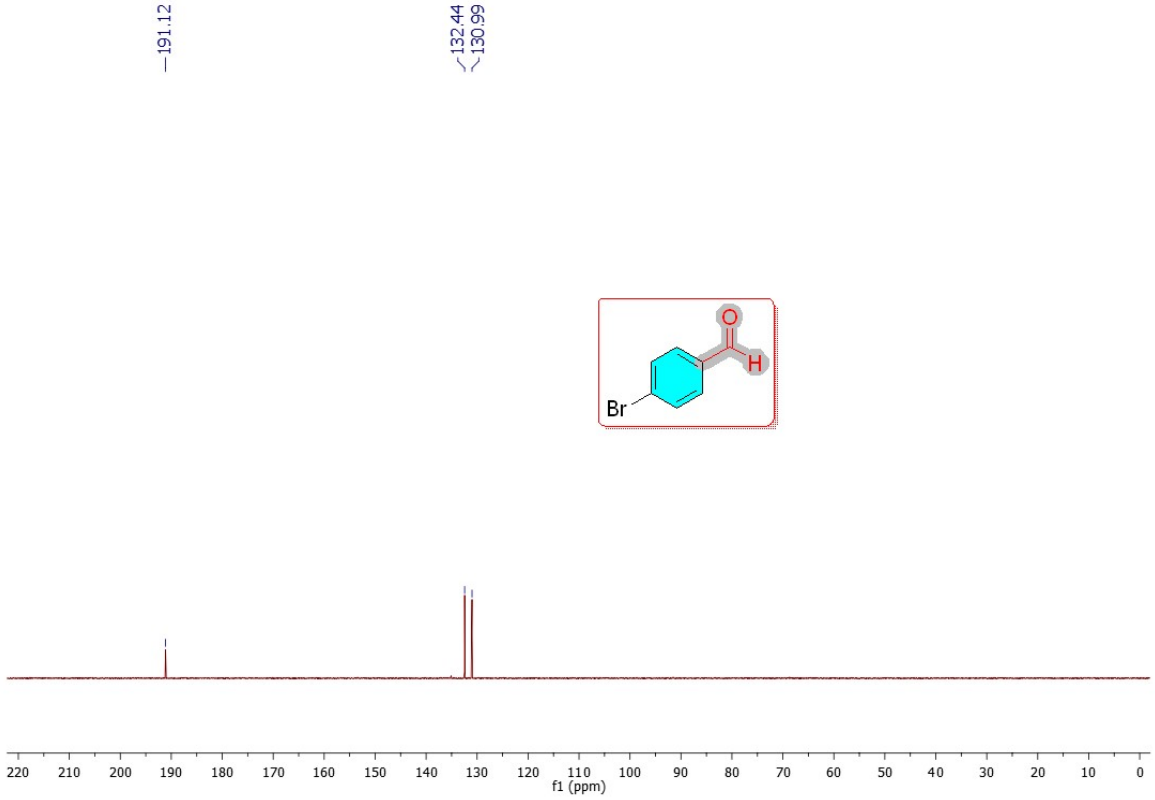
[1]HNMR Spectra of 4-Bromobenzaldehyde (2o)[2]



[13]C{[1]H} NMR Spectra of 4-Bromo benzaldehyde (2o)[2]



DEPT Spectra of 4-Bromo benzaldehyde (2o)[2]

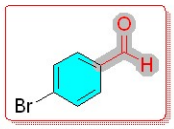


GCMS of 4-Bromo benzaldehyde (2o)

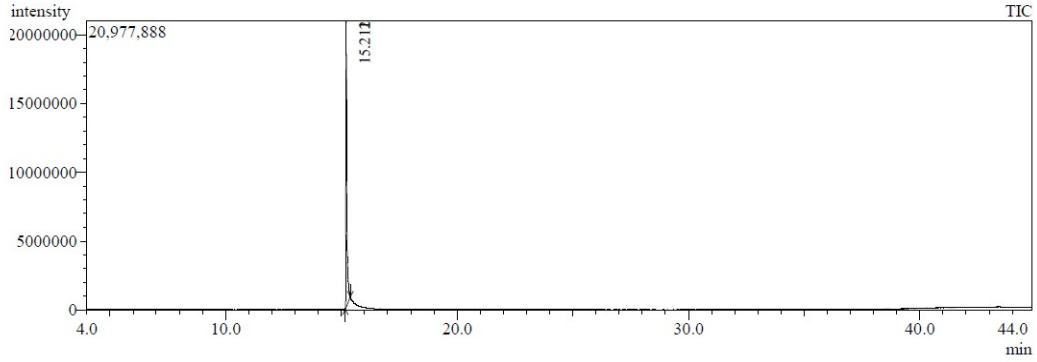
IIIM GCMS ANALYSIS

Sample Information

Analyzed by	: Admin
Analyzed	: 1/27/2022 8:38:19 AM
Level #	: 1
Sample Name	: Method-18
Sample ID	:
Sample Amount	: 1
Vial #	: 12
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\JAN 2022\25.01.2022\25.01.2022 BHARTI045.qgd
Method File	: D:\GCMS METHOD\GCMS-GENERAL AMIT 1.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
$EndIf$Modified by	: Admin
Modified	: 1/27/2022 9:23:11 AM



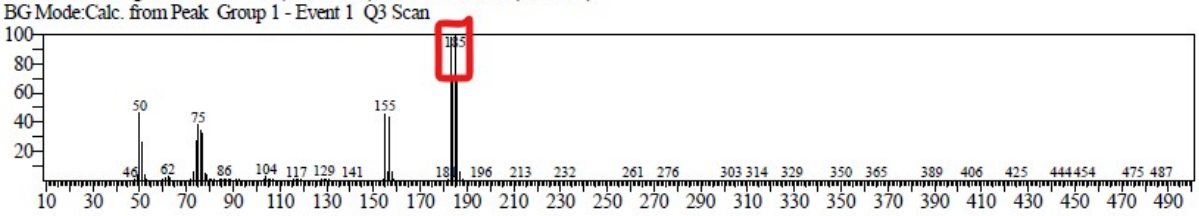
Chemical Formula: C_7H_5BrO
Exact Mass: 183.95



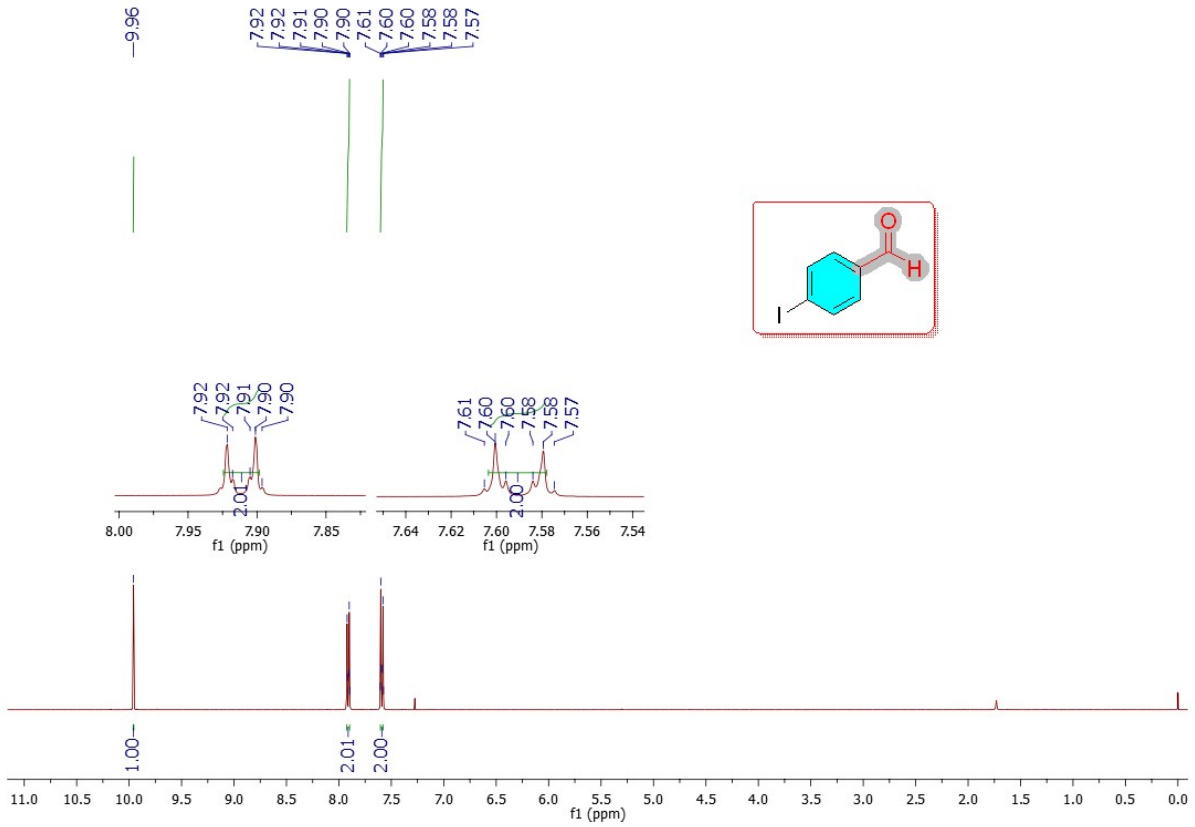
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	15.212	59071215	100.00	20762316	100.00	98	184.95	Benzaldehyde, 4-bromo-
		59071215	100.00	20762316	100.00			

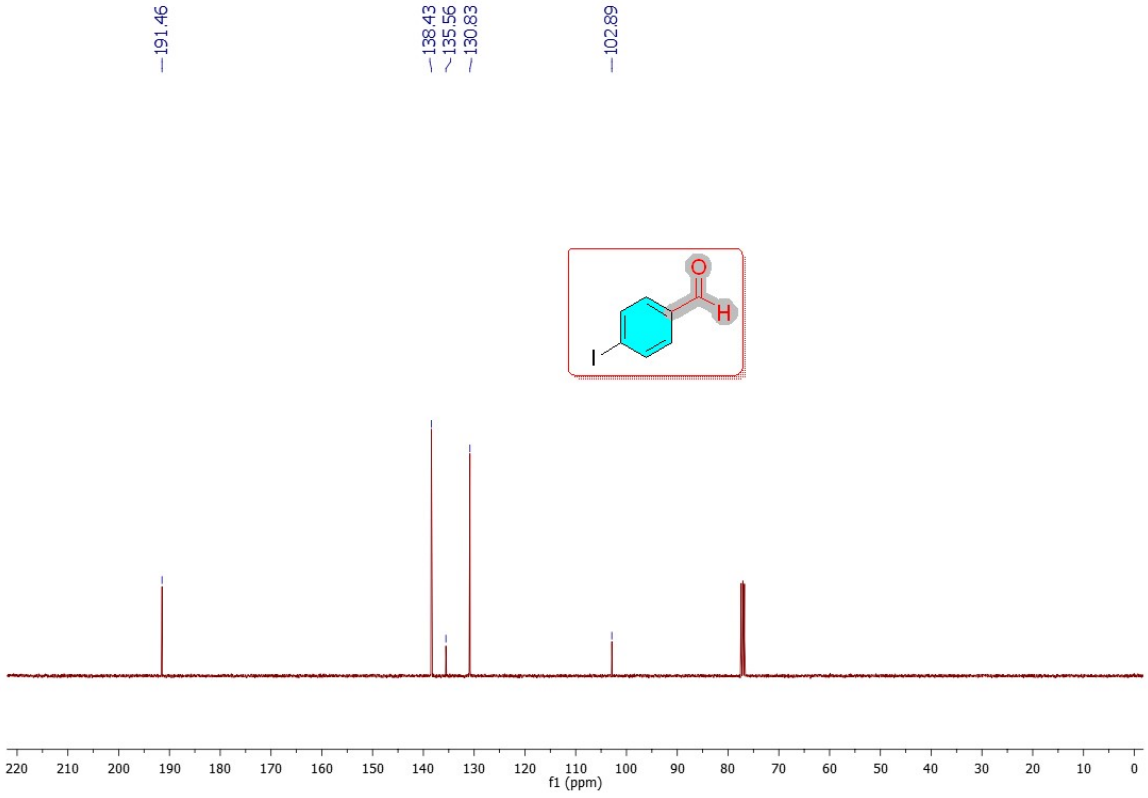
<< Target >>
Line#:1 R.Time:15.210(Scan#:2243) MassPeaks:262
RawMode:Averaged 15.205-15.215(2242-2244) BasePeak:184.95(2892016)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



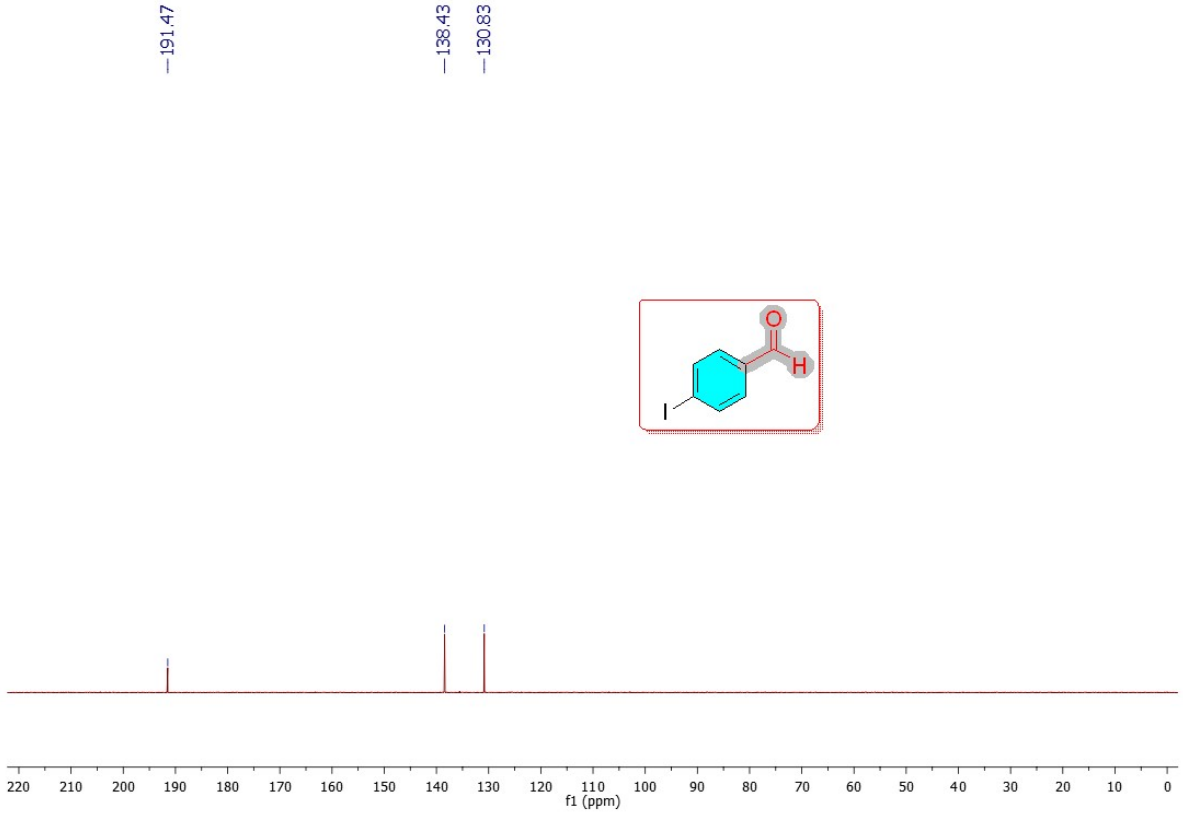
^{1}HNMR Spectra of 4-Iodo benzaldehyde (2p)[2]



^{13}C{^{1}H} NMR Spectra of 4-Iodo benzaldehyde (2p)[2]

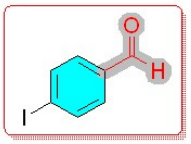


DEPT Spectra of 4-Iodo benzaldehyde (2p)[2]



GCMS Spectra of 4-Iodo benzaldehyde (2p)

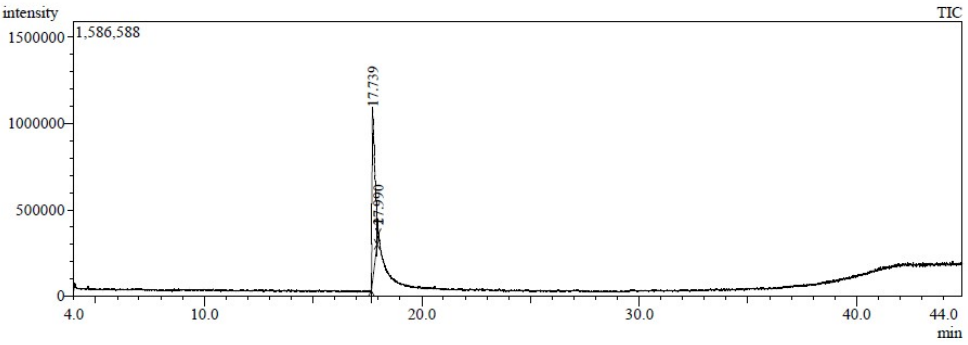
IIIM GCMS ANALYSIS



Chemical Formula: C_7H_5IO
Exact Mass: 231.94
Molecular Weight: 232.02

Sample Information

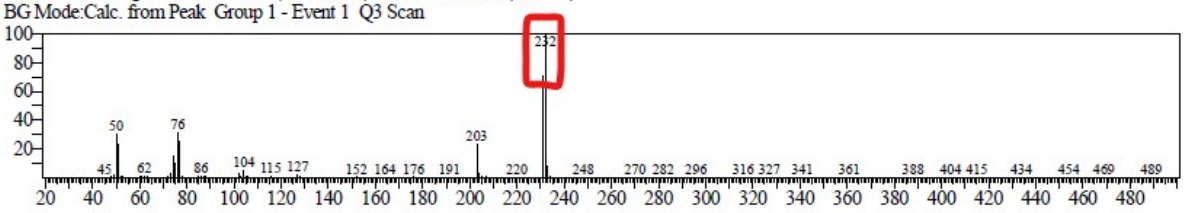
Analyzed by	: Admin
Analyzed	: 1/27/2022 12:03:37 PM
Level #	: 1
Sample Name	: I-Benzal
Sample ID	:
Sample Amount	: 1
Vial #	: 15
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\JAN 2022\25.01.2022\25.01.2022 BHARTI049.qgd
Method File	: D:\GCMS METHOD\GCMS-GENERAL AMIT 1.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
$EndIf$Modified by	: Admin
Modified	: 1/27/2022 12:48:29 PM



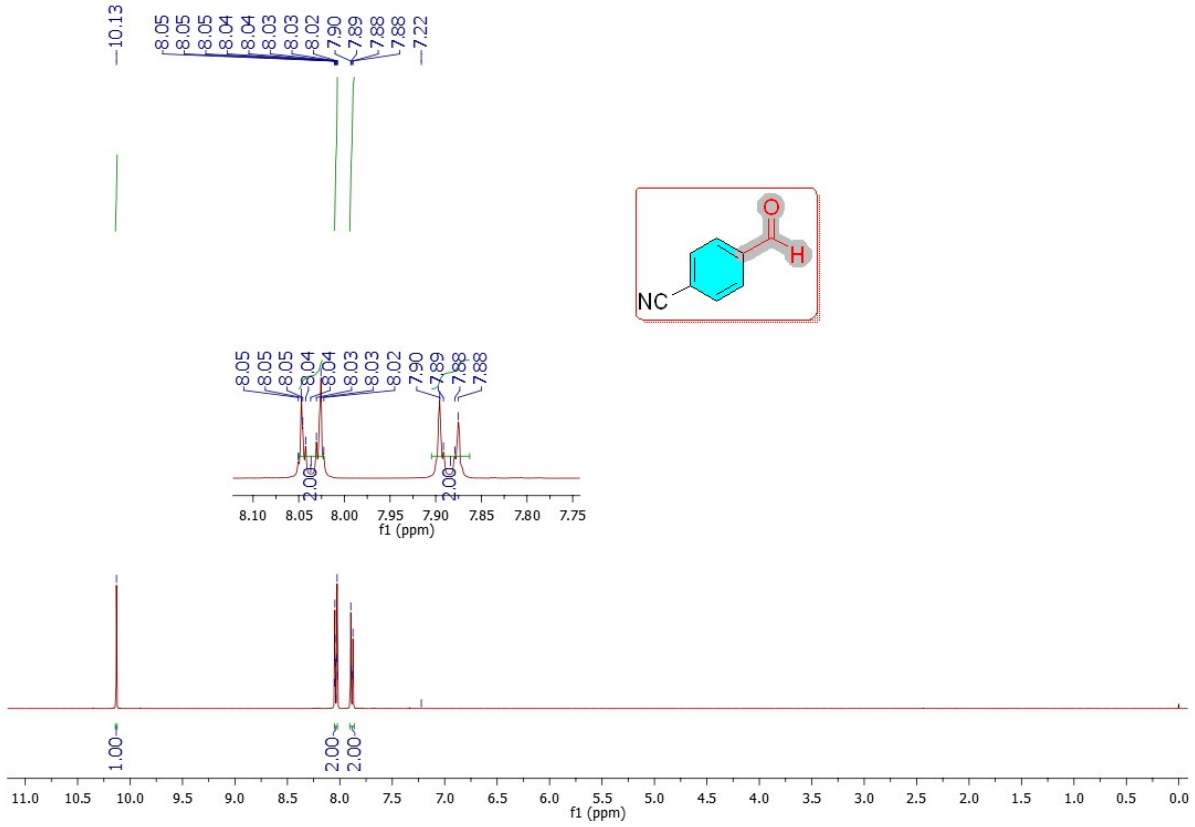
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	17.739	8746224	96.70	1010240	93.77	78	231.90	3-(4-Iodophenyl)-3-oxopropanenitrile
2	17.990	298807	3.30	67142	6.23	62	231.90	4-Pyridinamine, N-(1-naphthalenylmethyliden
		9045031	100.00	1077382	100.00			

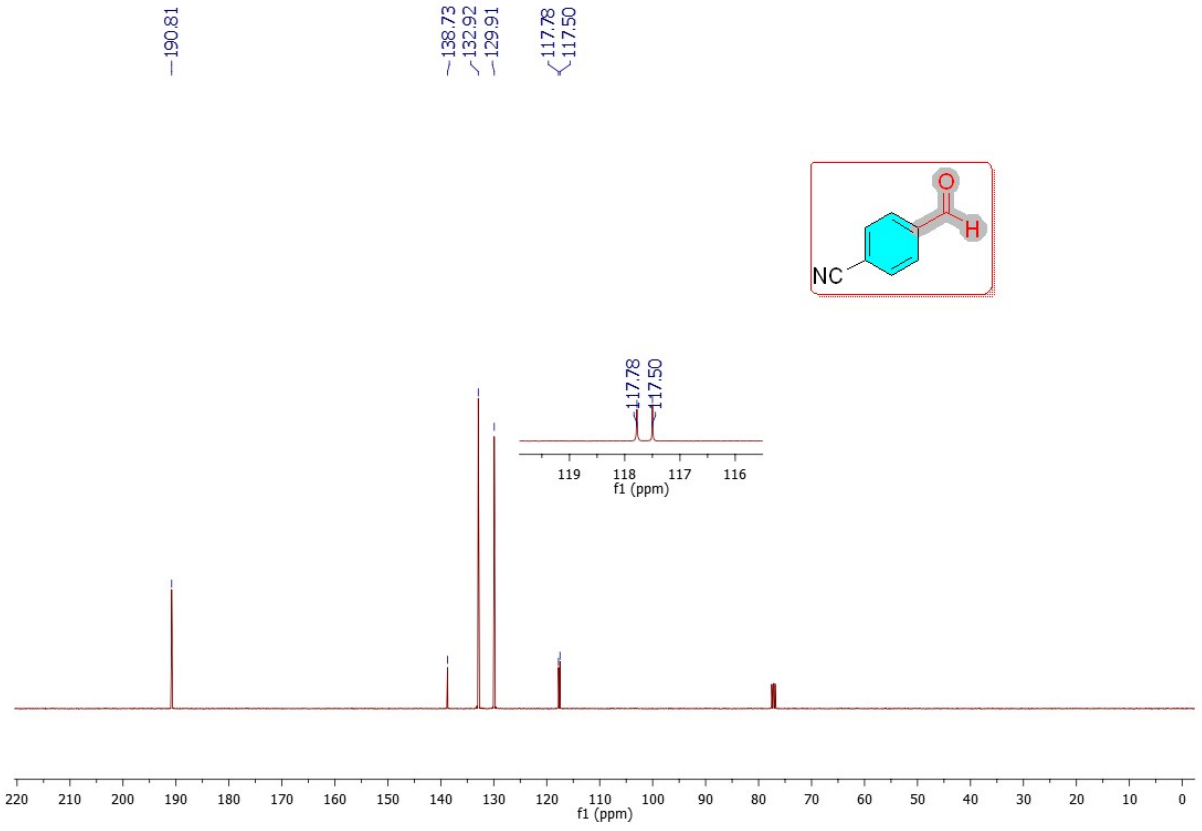
<< Target >>
Line#:1 R.Time:17.740(Scan#:2749) MassPeaks:240
RawMode:Averaged 17.735-17.745(2748-2750) BasePeak:231.90(267064)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



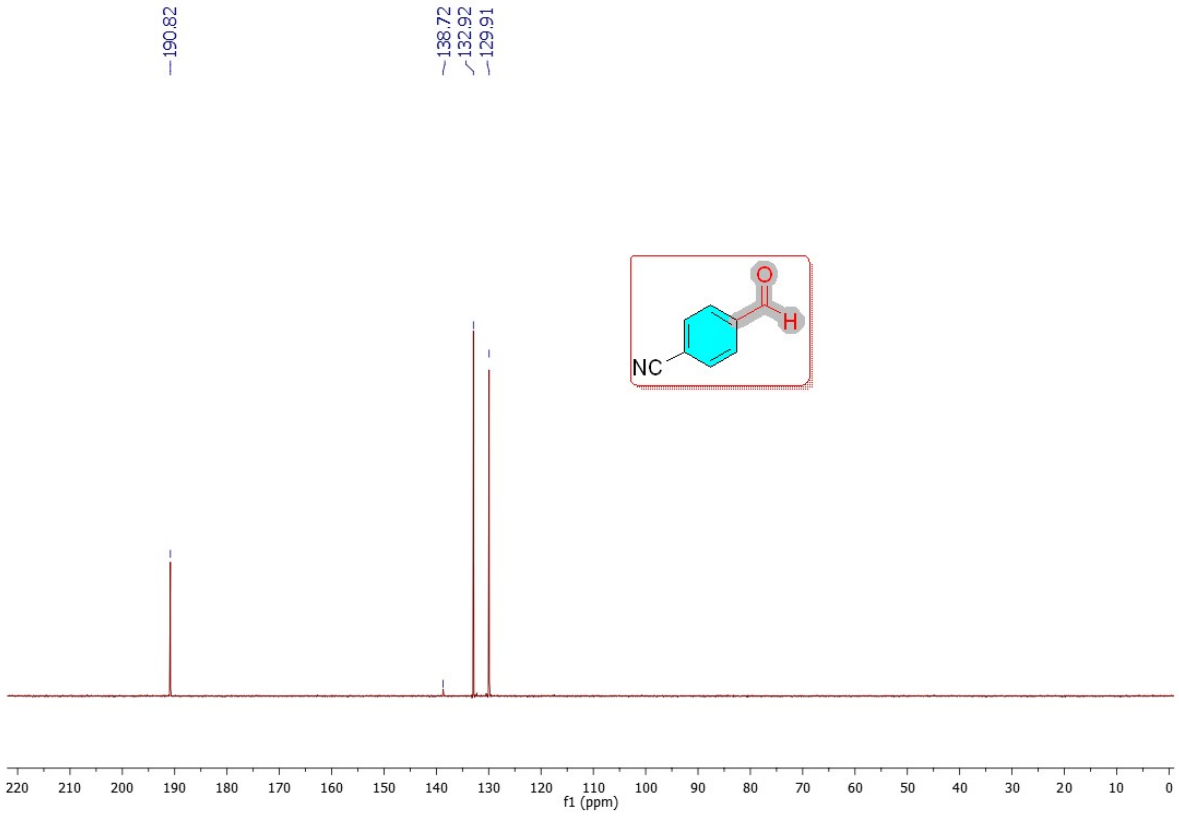
^{1}HNMR Spectra of 4-Formylbenzonitrile (2q)[2]



^{13}C{^{1}H} NMR Spectra of 4-Formylbenzonitrile (2q)[2]

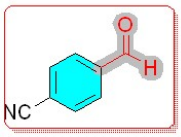


DEPT Spectra of 4-Formylbenzonitrile (2q)[2]



GCMS of 4-Formylbenzonitrile (2q)

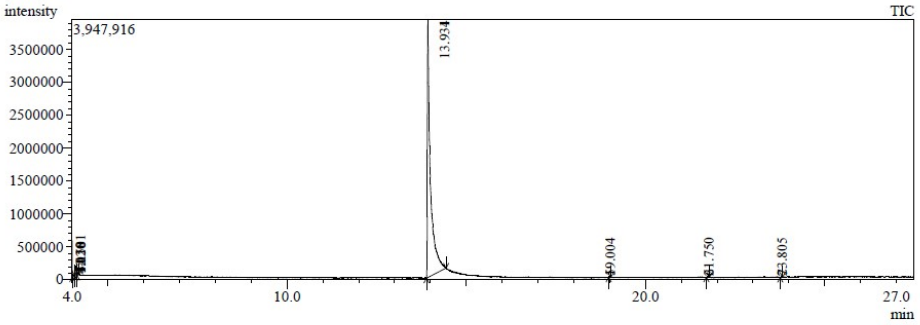
IIIM GCMS ANALYSIS



Chemical Formula: C_8H_5NO
Exact Mass: 131.04
Molecular Weight: 131.13

Sample Information

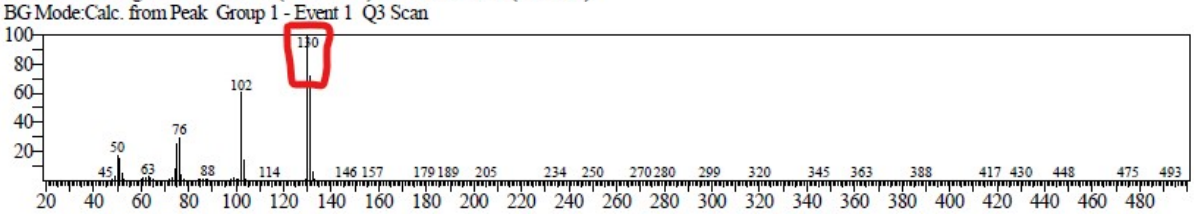
Analyzed by	: Admin
Analyzed	: 2/17/2022 1:21:19 AM
Level #	: 1
Sample Name	: method-30
Sample ID	:
Sample Amount	: 1
Vial #	: 11
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\FEB 2022\16.02.2022\16.02.2022 BHARTI039.qgd
Method File	: D:\GCMS METHOD\GC MS METHOD PP SIR.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
$EndIf$Modified by	: Admin
Modified	: 2/18/2022 12:18:15 PM



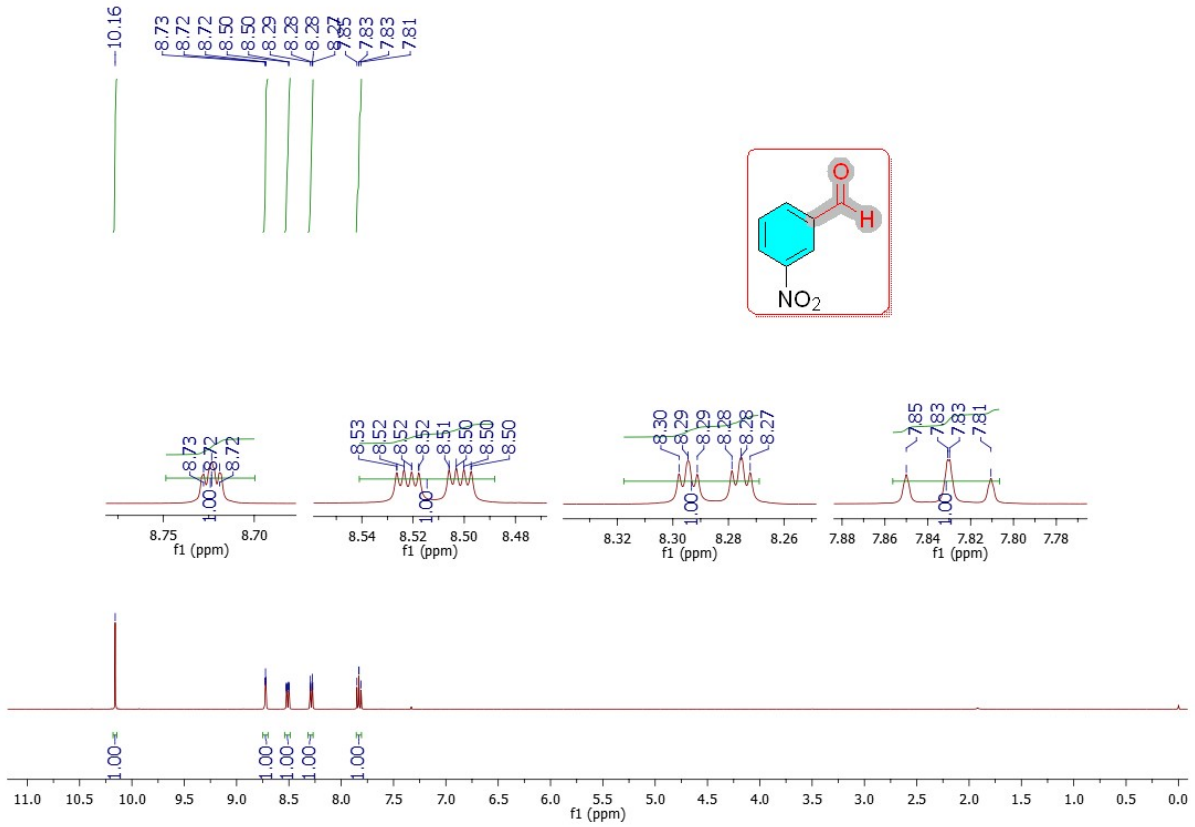
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	4.020	92801	0.40	39131	0.93	71	48.00	Phosphine, methyl-
2	4.101	266365	1.14	142291	3.40	96	57.00	Propanoic acid, ethyl ester
3	4.158	58863	0.25	32028	0.77	82	60.95	n-Propyl acetate
4	13.931	22866131	97.75	3912683	93.48	97	130.05	Benzonitrile, 4-formyl-
5	19.004	32586	0.14	20516	0.49	80	73.05	Cycloheptasiloxane, tetradecamethyl-
6	21.750	46792	0.20	23680	0.57	76	355.10	Cyclooctasiloxane, hexadecamethyl-
7	23.805	29327	0.13	15119	0.36	67	73.00	Cyclononasiloxane, octadecamethyl-
		23392865	100.00	4185448	100.00			

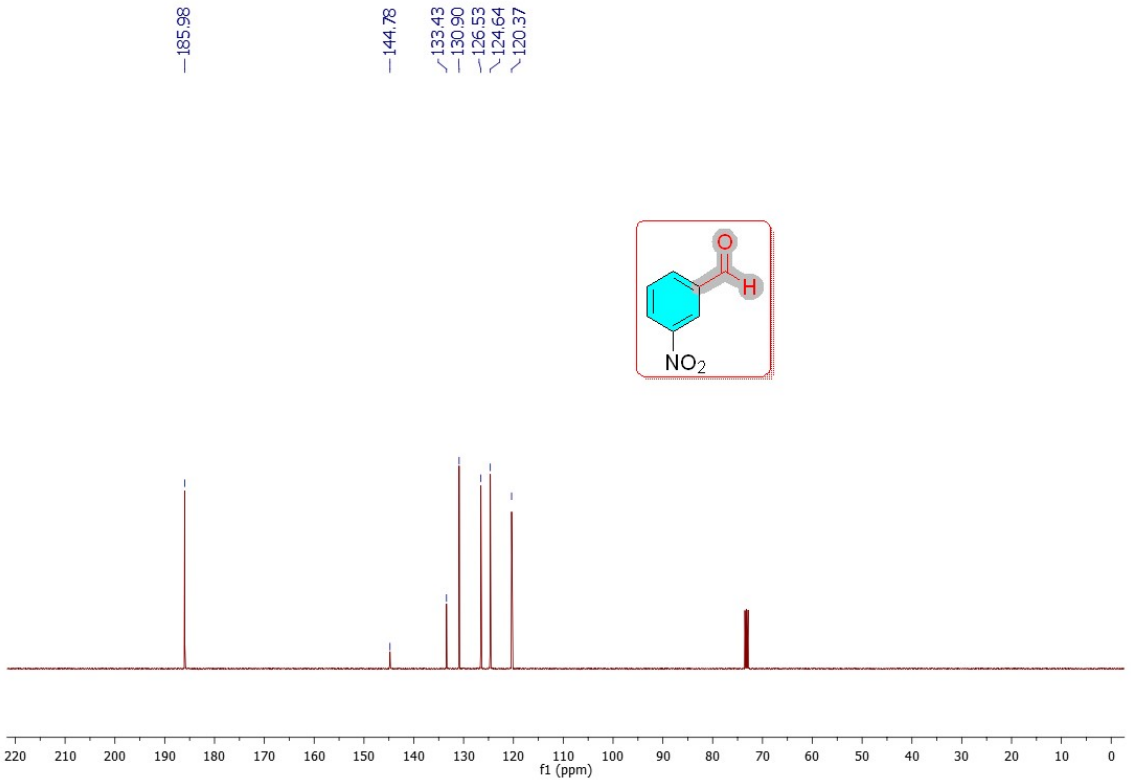
<< Target >>
Line#:4 R.Time:13.930(Scan#:1987) MassPeaks:270
RawMode:Averaged 13.925-13.935(1986-1988) BasePeak:130.05(1001335)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



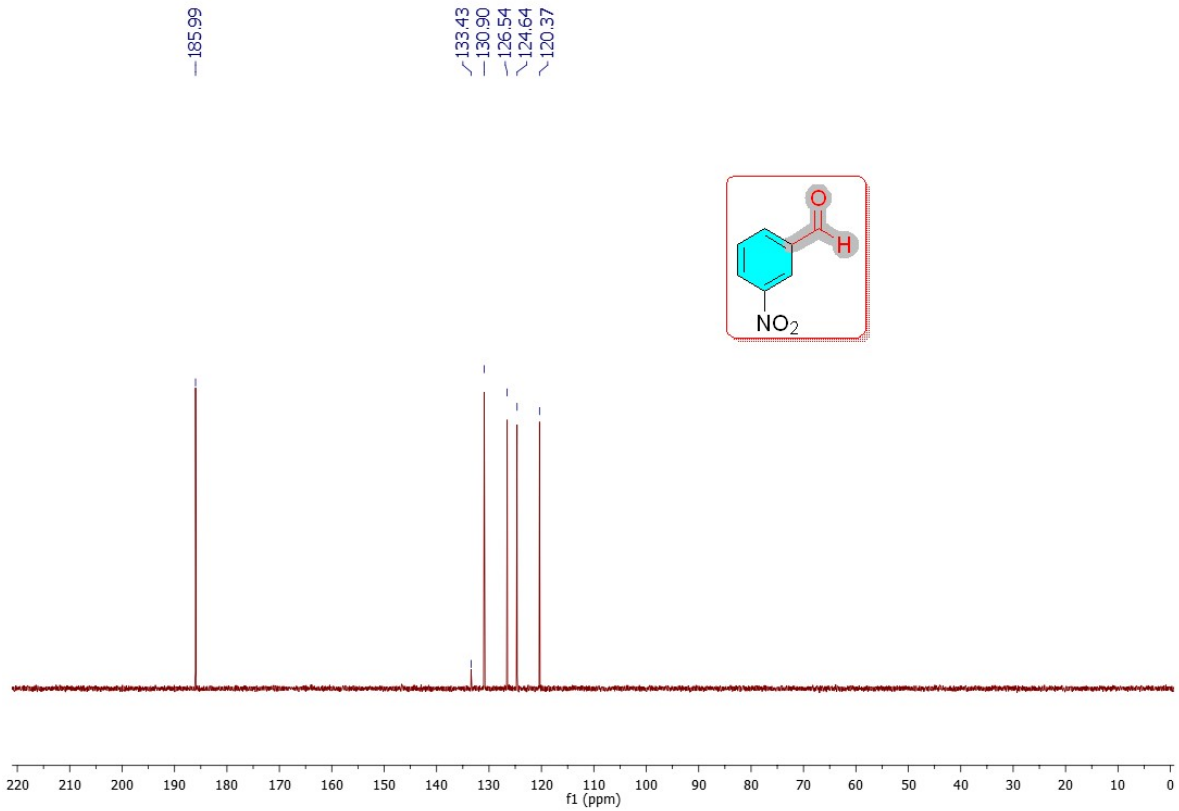
^{1}HNMR Spectra of 3-Nitro benzaldehyde (2r)[3]



^{13}C{^{1}H} NMR Spectra of 3-Nitro benzaldehyde (2r)[3]



DEPT Spectra of 3-Nitro benzaldehyde (2r)[3]

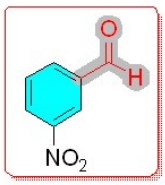


GCMS of 3-Nitro benzaldehyde (2r)

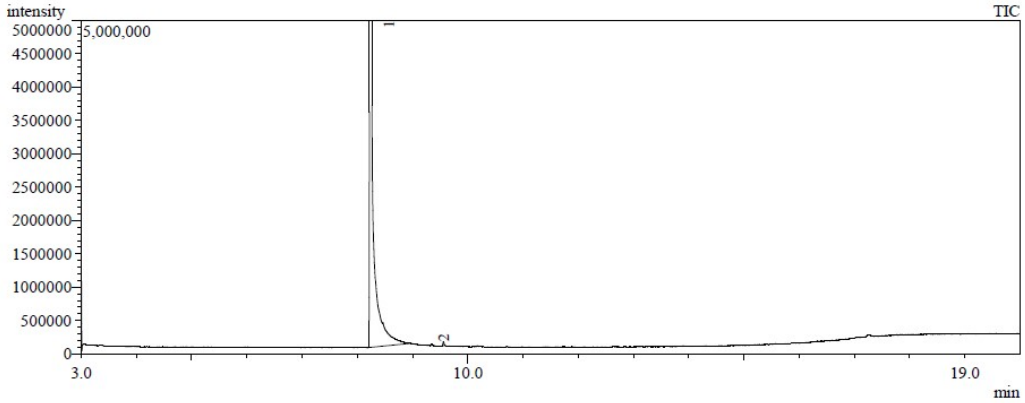
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 22-03-2023 00:14:32
Level #	: 1
Sample Name	: RG-1
Sample ID	: RG-1
Sample Amount	: 1
Vial #	: 11
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-31.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:16:19



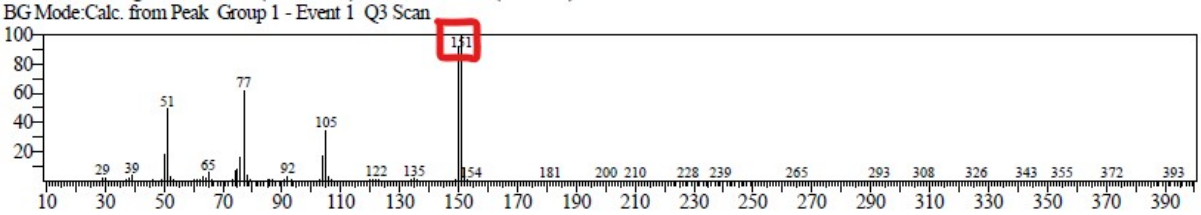
Chemical Formula: $C_7H_5NO_3$
Exact Mass: 151.03



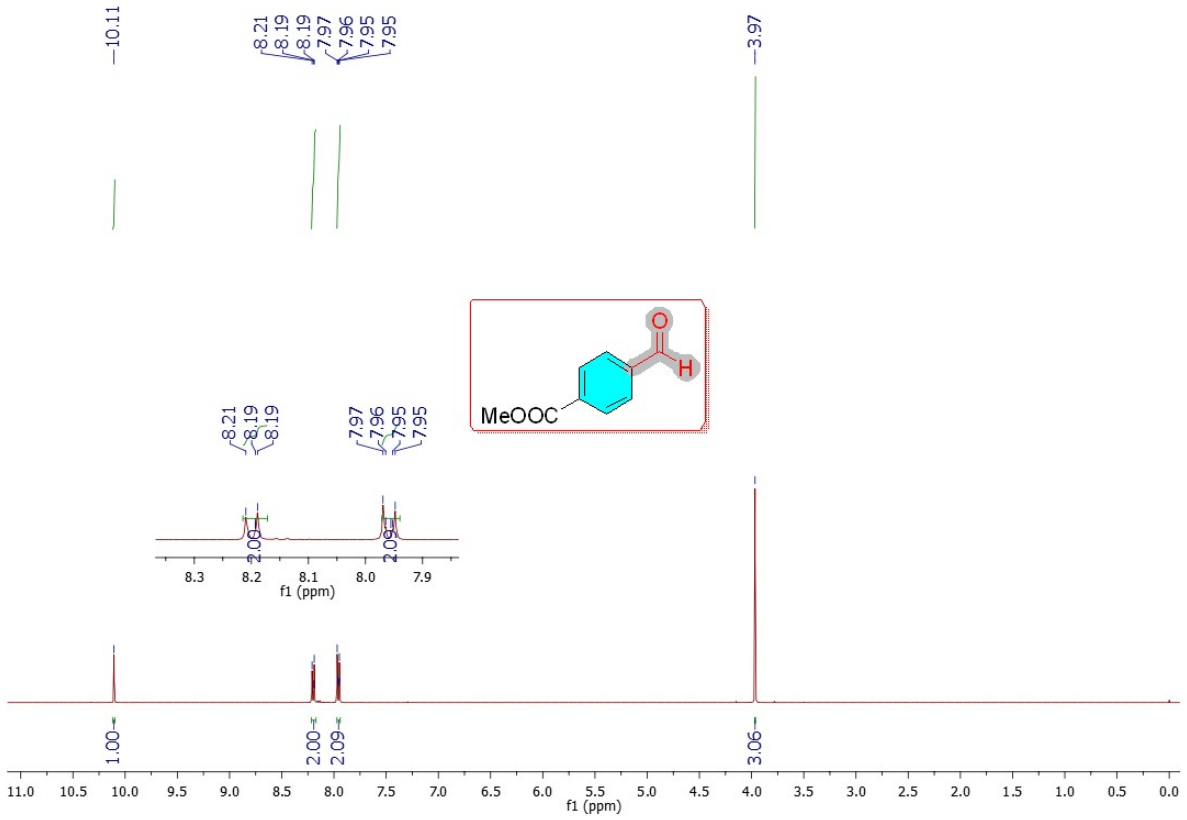
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	8.245	50467567	99.83	97	151.00	Benzaldehyde, 3-nitro-
2	9.561	85106	0.17	92	191.10	2,4-Di-tert-butylphenol
		50552673	100.00			

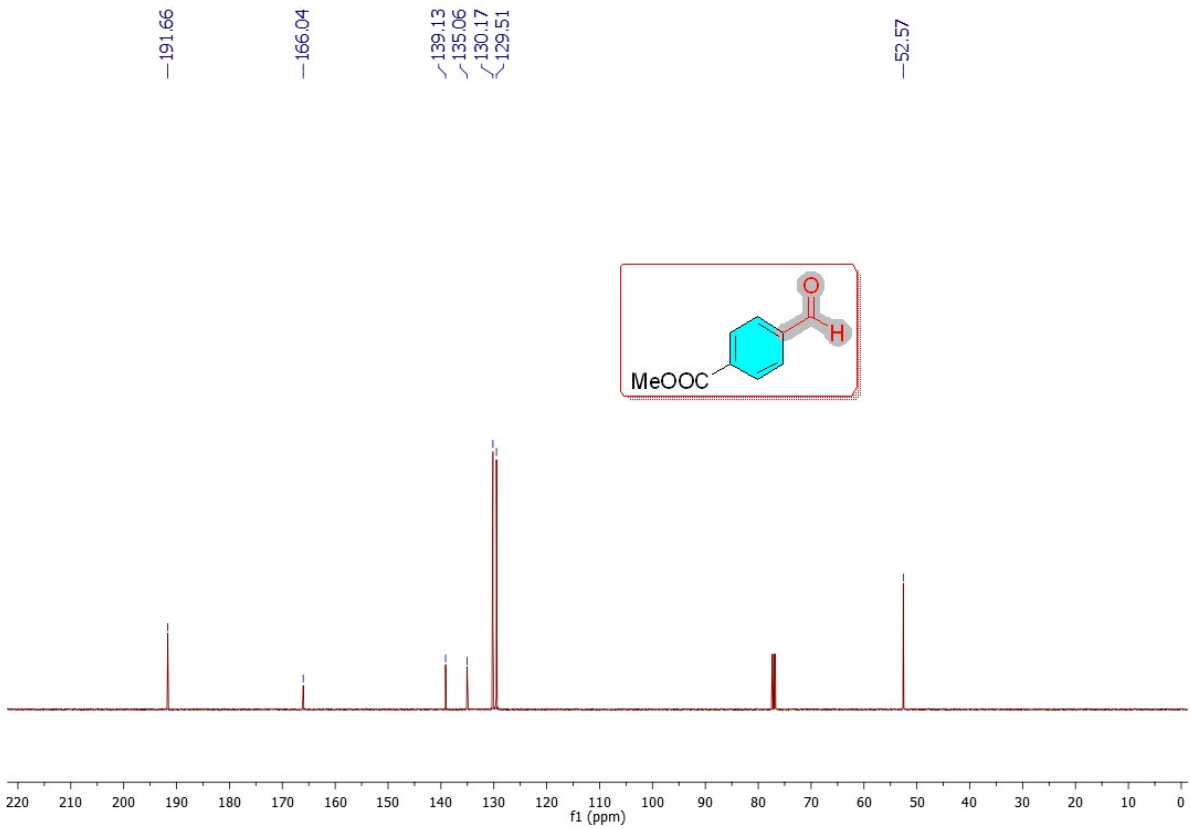
<< Target >>
Line#:1 R.Time:8.245(Scan#:1050) MassPeaks:241
RawMode:Averaged 8.240-8.250(1049-1051) BasePeak:151.00(4275355)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



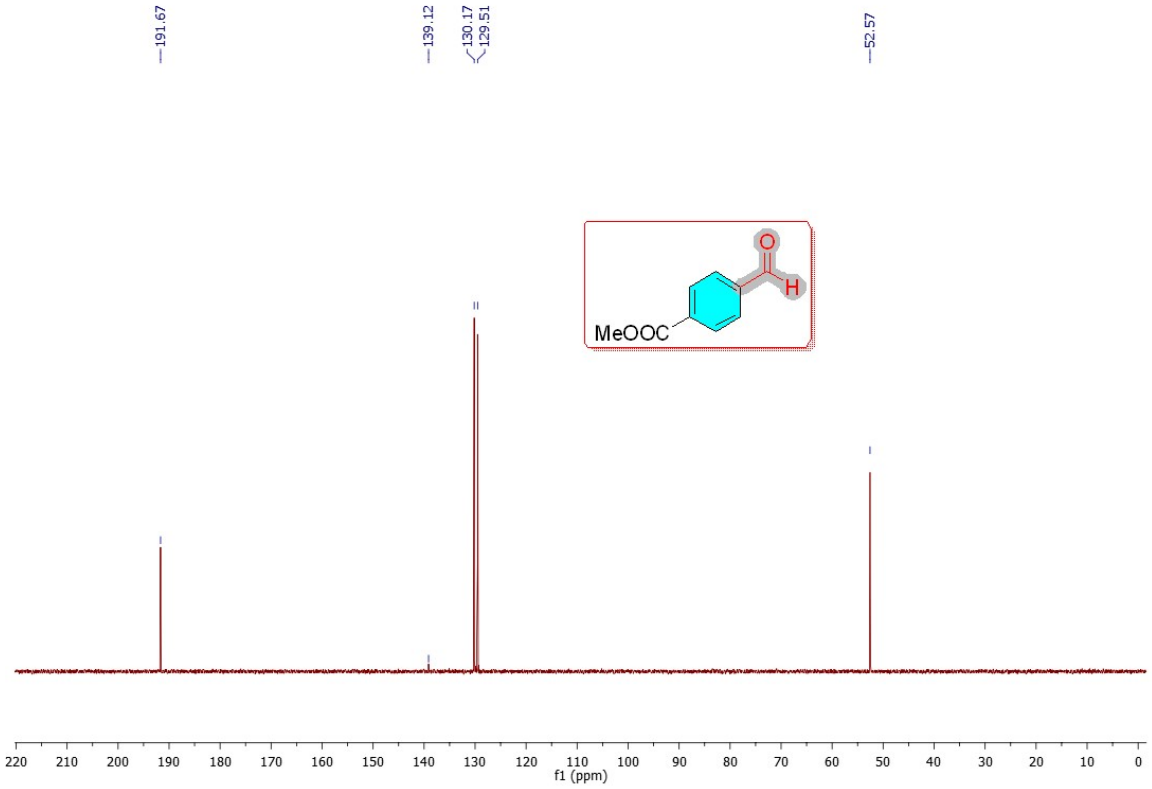
^{1}H NMR Spectra of Methyl 4-formylbenzoate (2s)[2]



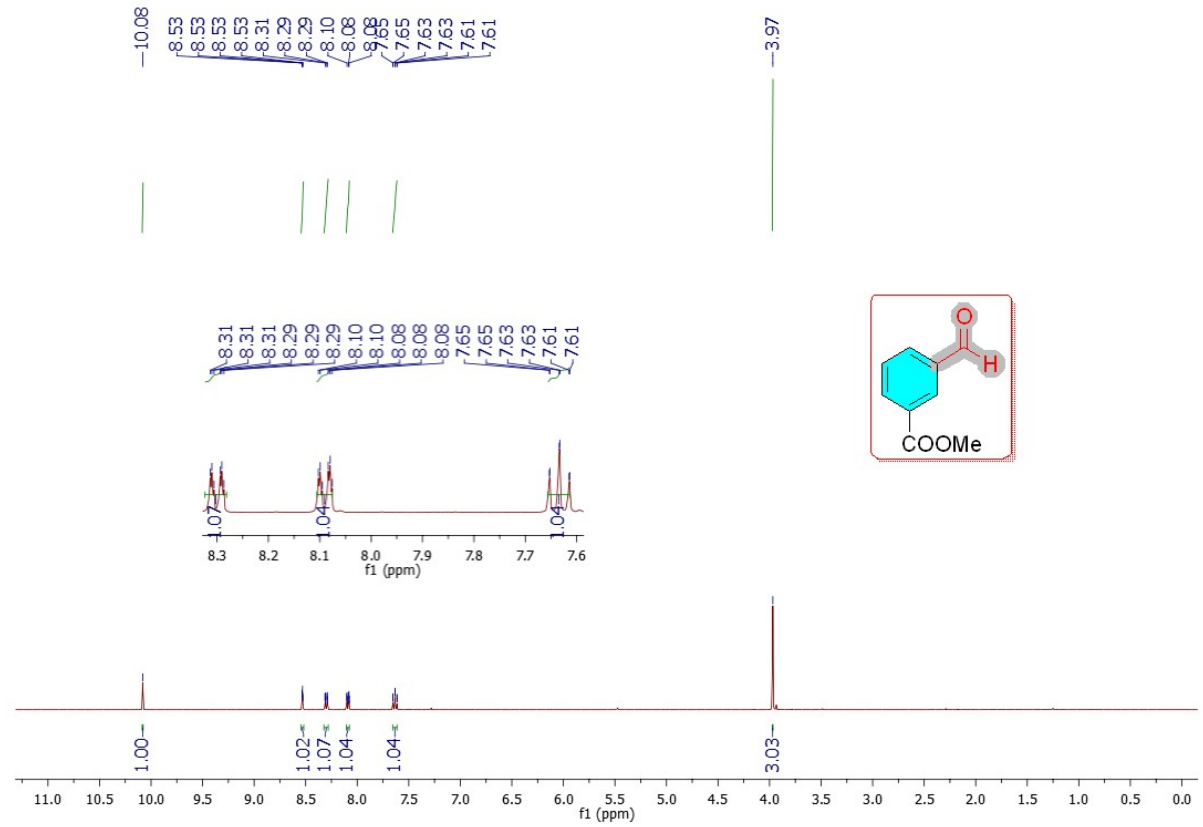
^{13}C{^{1}H} NMR Spectra of Methyl 4-formylbenzoate (2s)[2]



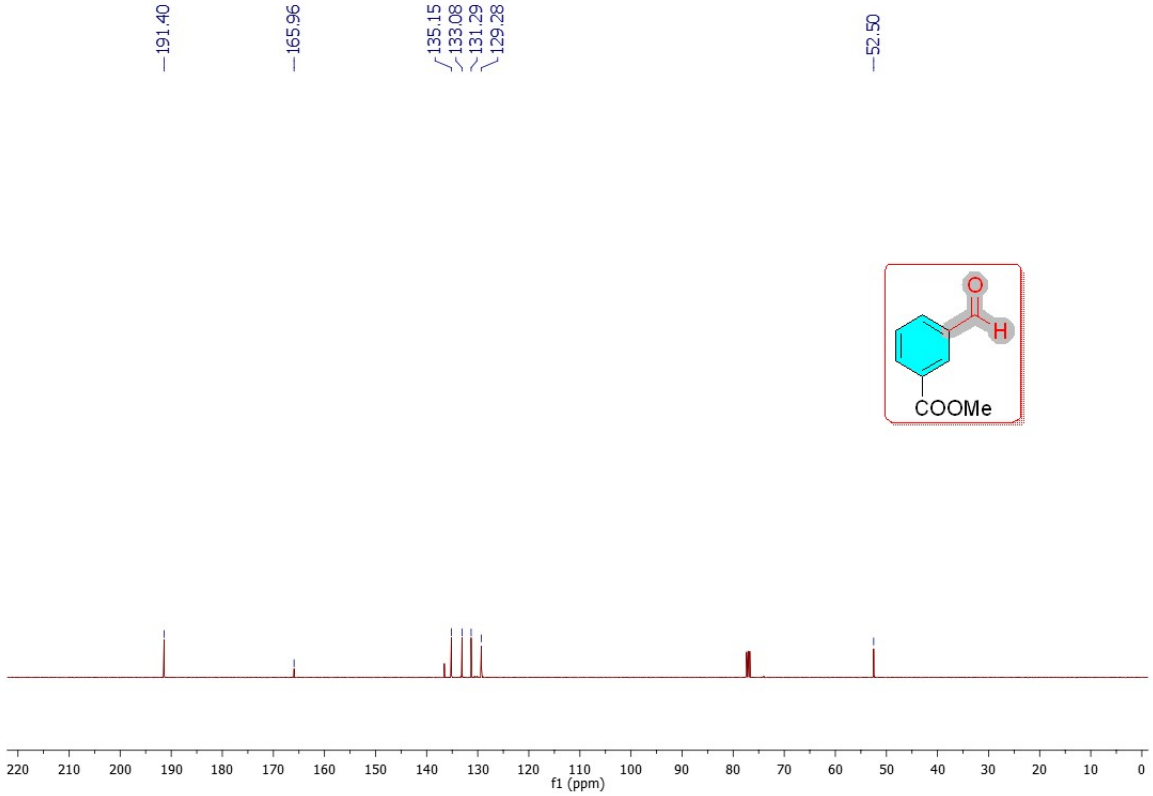
DEPT Spectra of Methyl 4-formylbenzoate (2s)[2]



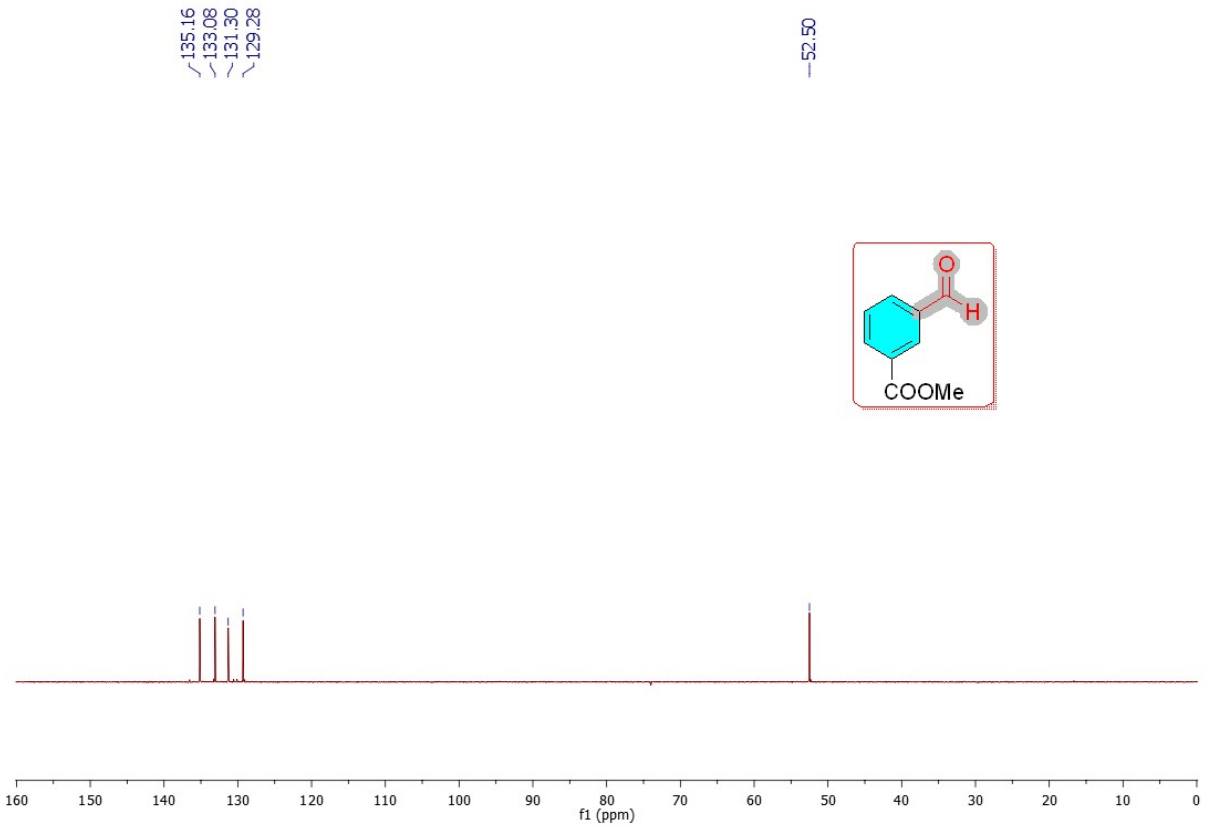
^{1}HNMR Spectra of Methyl 3-formylbenzoate (2t)[3]



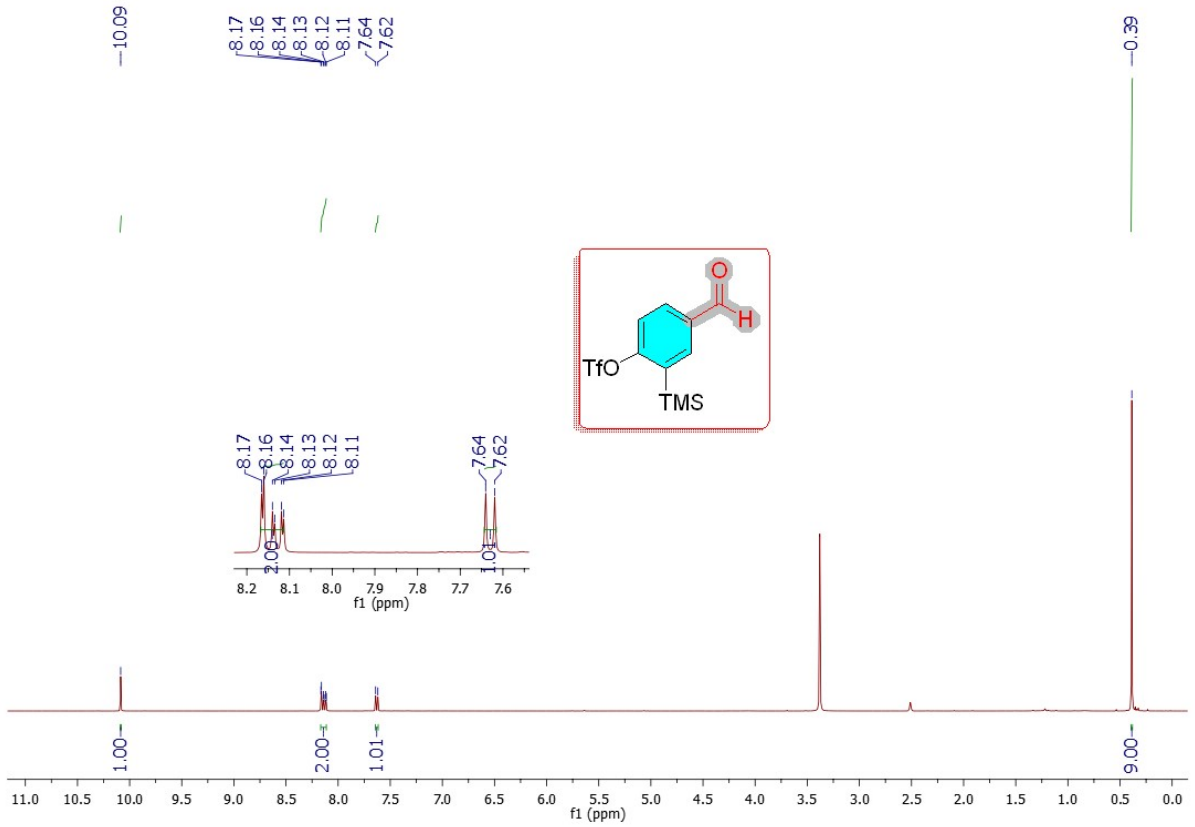
$^{13}C\{^{1}H\}$ NMR Spectra of Methyl 3-formylbenzoate (2t)[3]



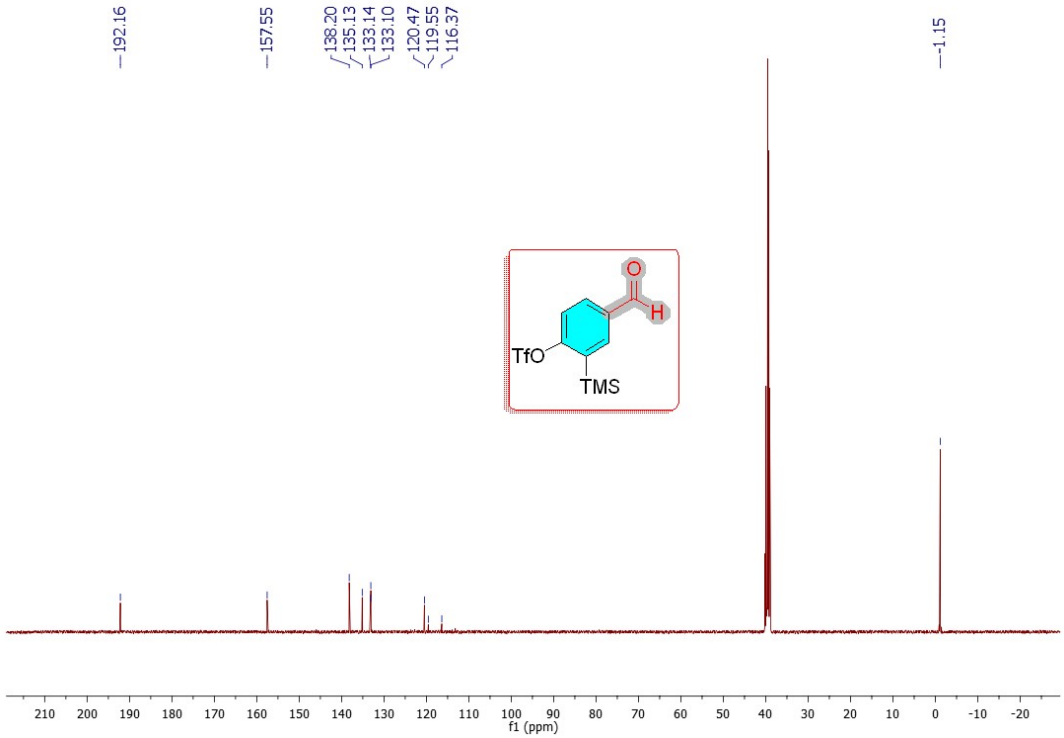
DEPT Spectra of Methyl 3-formylbenzoate (2t)[3]



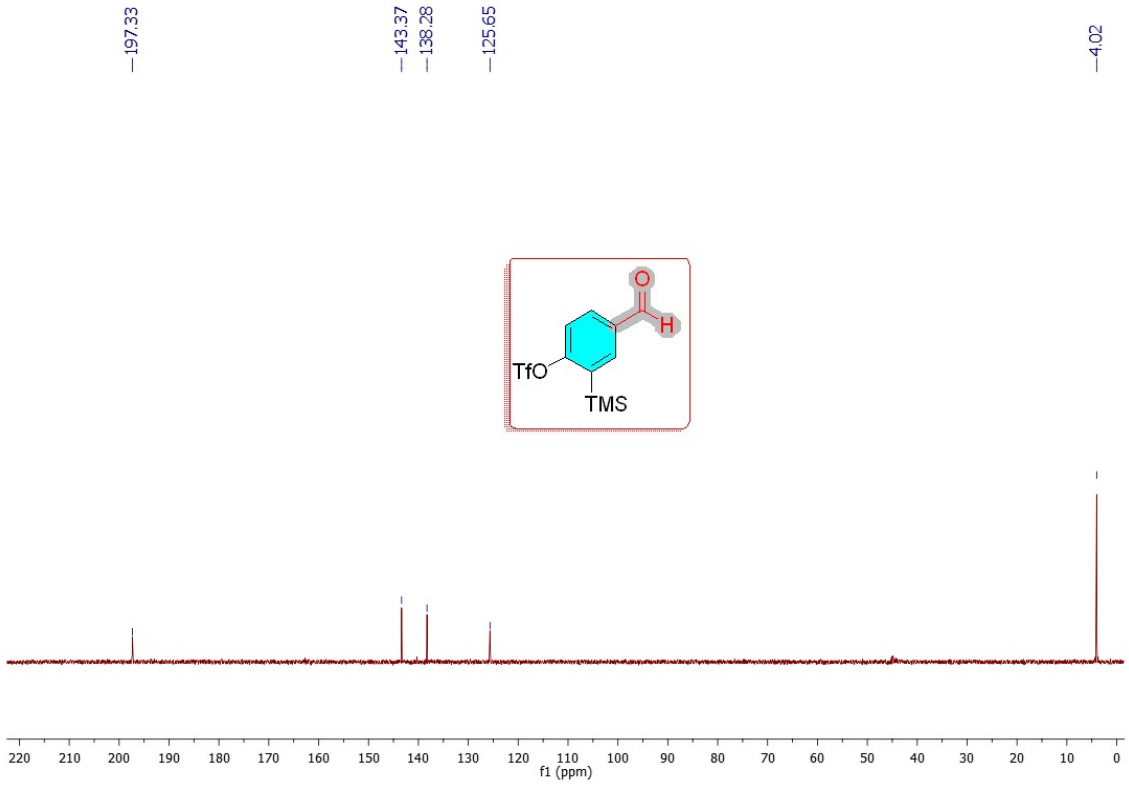
[1]HNMR Spectra of 4-formyl-2-(trimethylsilyl) phenyltrifluoromethanesulfonate(2u)



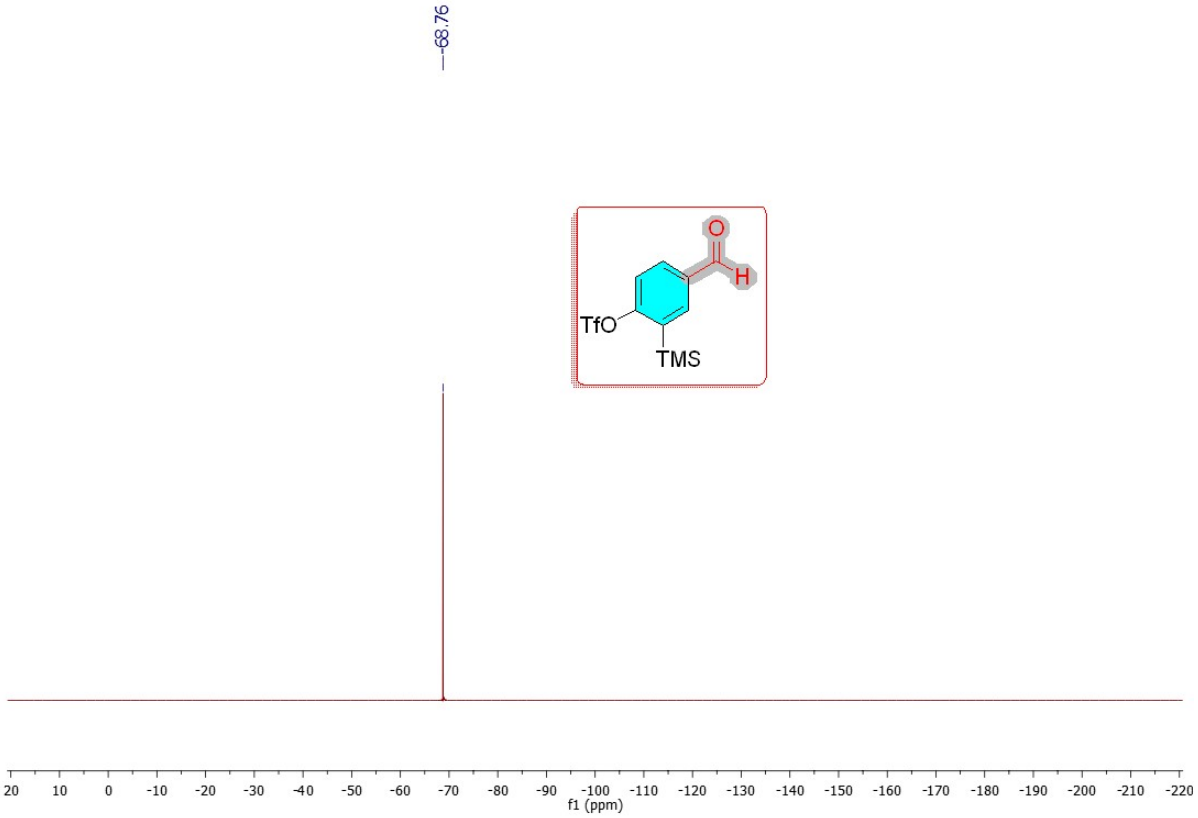
[13]C{[1]H} NMR Spectra of 4-formyl-2-(trimethylsilyl) phenyltrifluoromethanesulfonate(2u)



DEPT Spectra of 4-formyl-2-(trimethylsilyl) phenyltrifluoromethanesulfonate(2u)



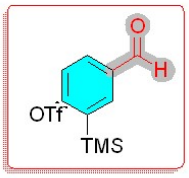
^{19}F Spectra of 4-formyl-2-(trimethylsilyl) phenyltrifluoromethanesulfonate(2u)



GCMS of 4-formyl-2-(trimethylsilyl) phenyltrifluoromethanesulfonate(2u)

CSIR-IIIM GCMS ANALYSIS REPORT

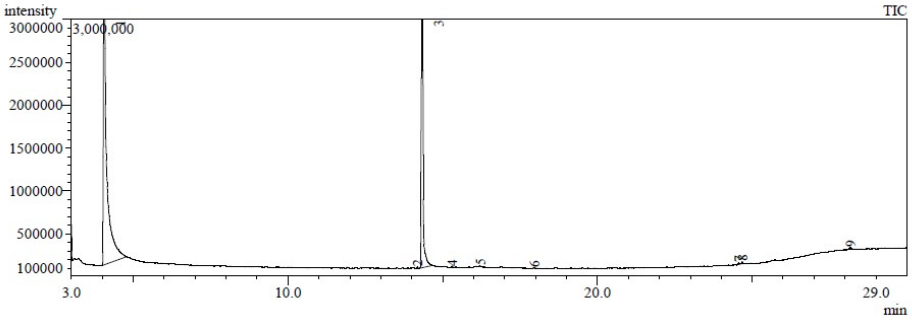
Chemical Formula: $C_{10}H_{14}OSi$
Exact Mass: 178.08



Chemical Formula: CF_3O_3S
Exact Mass: 148.95

Sample Information

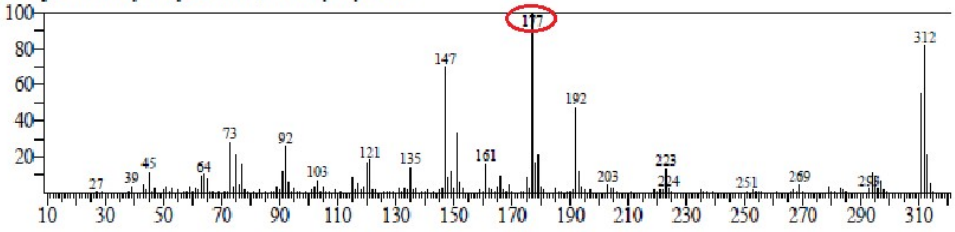
Analyzed by	: System Administrator
Analyzed	: 28-12-2022 18:38:07
Level #	: 1
Sample Name	: PPS-46
Sample ID	: PPS-46
Sample Amount	: 1
Vial #	: 21
Injection Volume	: 1.00
Data File	: D:\GCMS DATA\LIQUID\Dec 2022\28.12.2022_09.qgd
Method File	: D:\GCMS METHOD\GCMS_LIQ_1_5ms.qgm
Tuning File	: C:\GCMSsolution\System\Tune1\14122022_F1_Col_N.qgt
$EndIf$Modified by	: System Administrator
Modified	: 29-12-2022 09:55:06



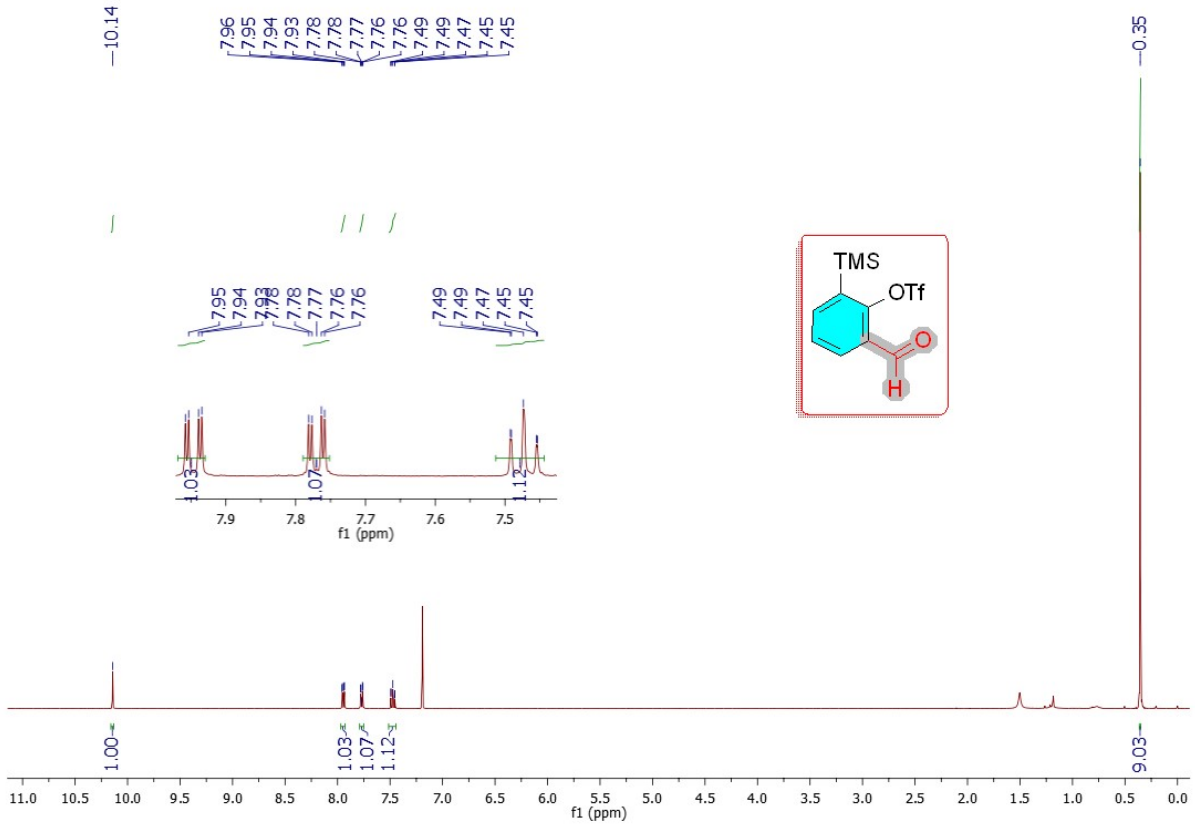
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	4.058	36052270	50.68	69	66.00	Thiazolidine-2,4-dione, 5-(bicyclo[2.2.1]hept-5-en-2-yl)methylene-
2	14.180	30182	0.04	78	281.00	Cycloheptasiloxane, tetradecamethyl-
3	14.335	34823567	48.95	64	311.00	1,2,4-benzenetricarboxylic acid, 3,5-dinitro-, trimethyl ester
4	15.301	33947	0.05	0	163.05	
5	16.203	21507	0.03	80	355.05	Cyclooctasiloxane, hexadecamethyl-
6	17.953	22525	0.03	71	73.05	Heptasiloxane, hexadecamethyl-
7	24.572	51572	0.07	71	149.10	Bis(2-ethylhexyl) phthalate
8	24.679	61228	0.09	78	325.00	N,N-Bis(salicylidene)ethylenediiminocobalt (II)
9	28.175	46432	0.07	64	355.05	Heptasiloxane, hexadecamethyl-
		71143230	100.00			

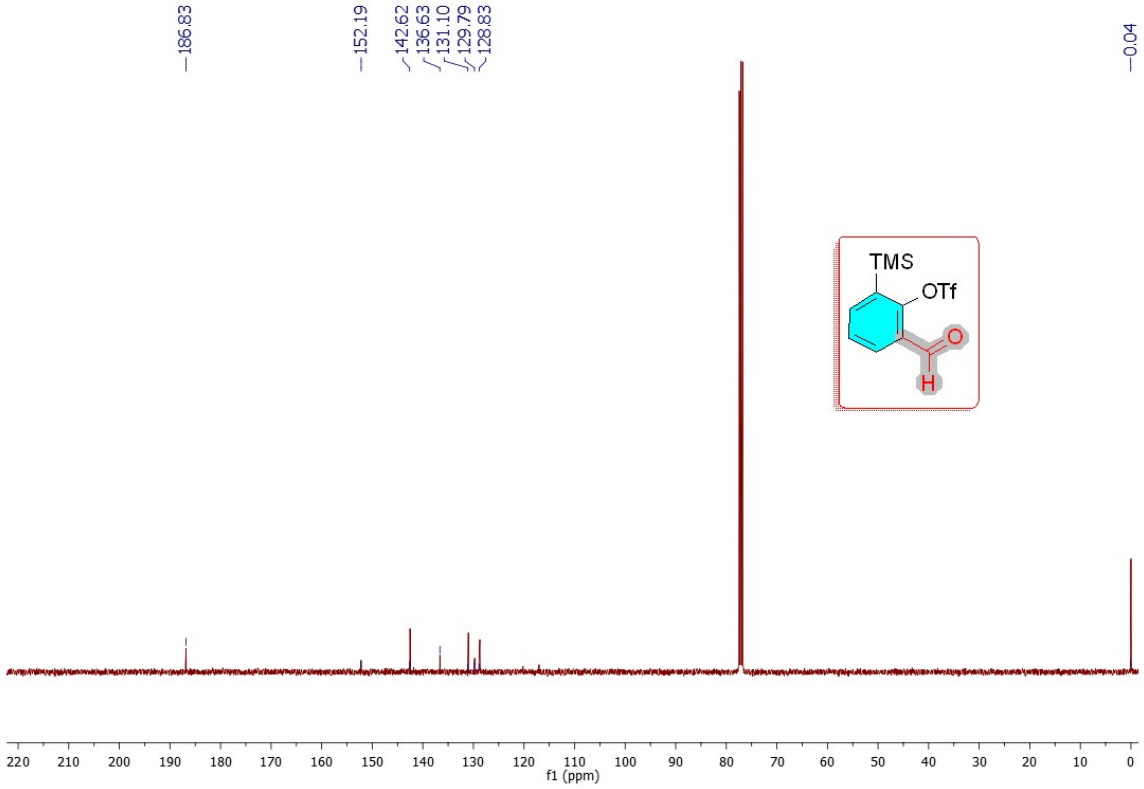
Hit#:2 Entry:155785 Library:NIST17M1.lib
SI:60 Formula:C18H20O3Si CAS:0-00-0 MolWeight:312 RetIndex:2259
CompName:3'-Hydroxyflavanone, trimethylsilyl ether



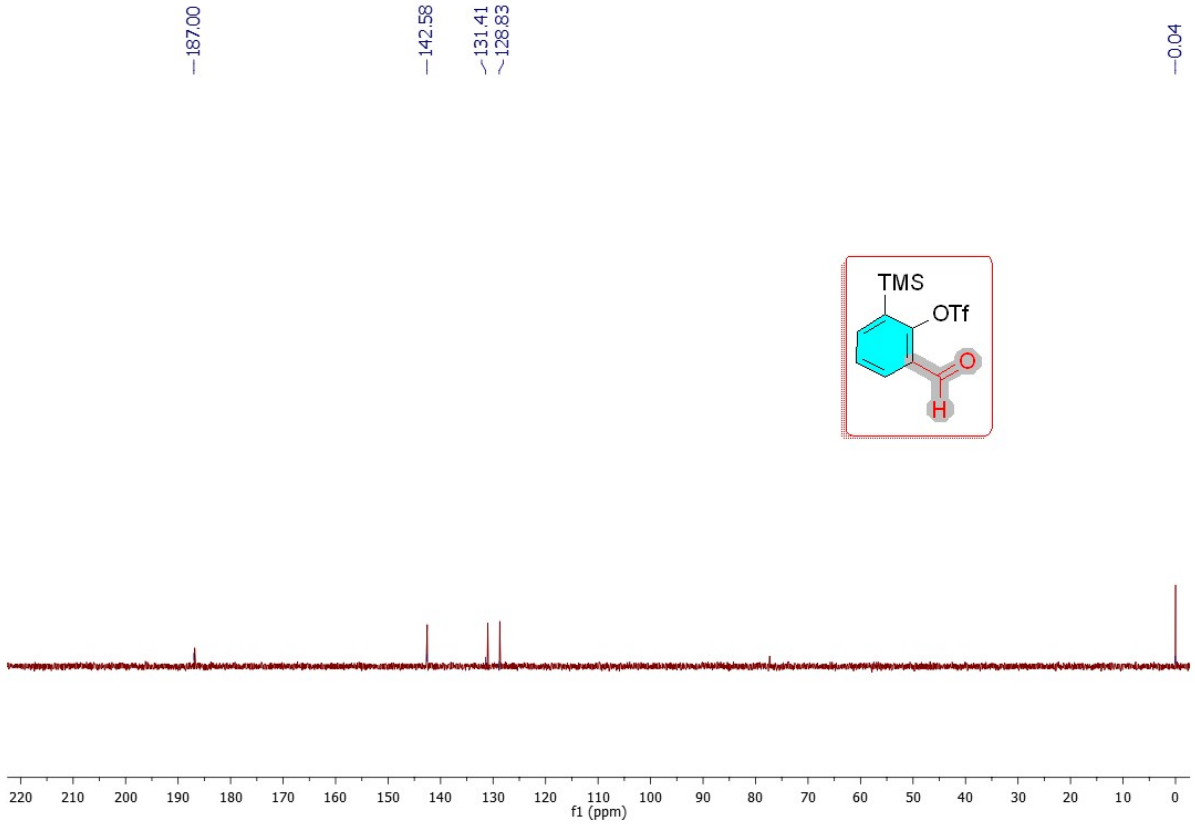
[1]HNMR Spectra of 4-formyl-2-(trimethylsilyl) phenyltrifluoromethanesulfonate(2v)



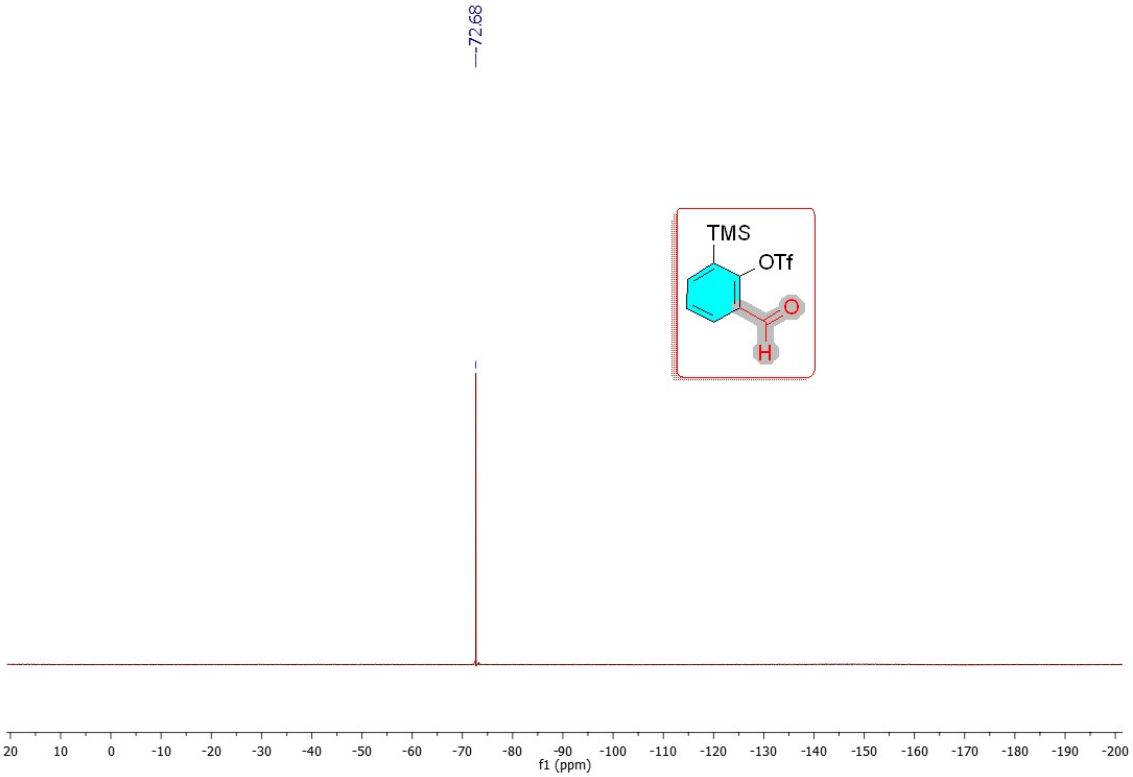
[13]C{[1]H} NMR Spectra of 2-formyl-5-(trimethylsilyl) phenyltrifluoromethanesulfonate (2v)



DEPT Spectra of 2-formyl-5-(trimethylsilyl) phenyltrifluoromethanesulfonate (2v)



^{19}F Spectra of 2-formyl-5-(trimethylsilyl) phenyltrifluoromethanesulfonate (2u)

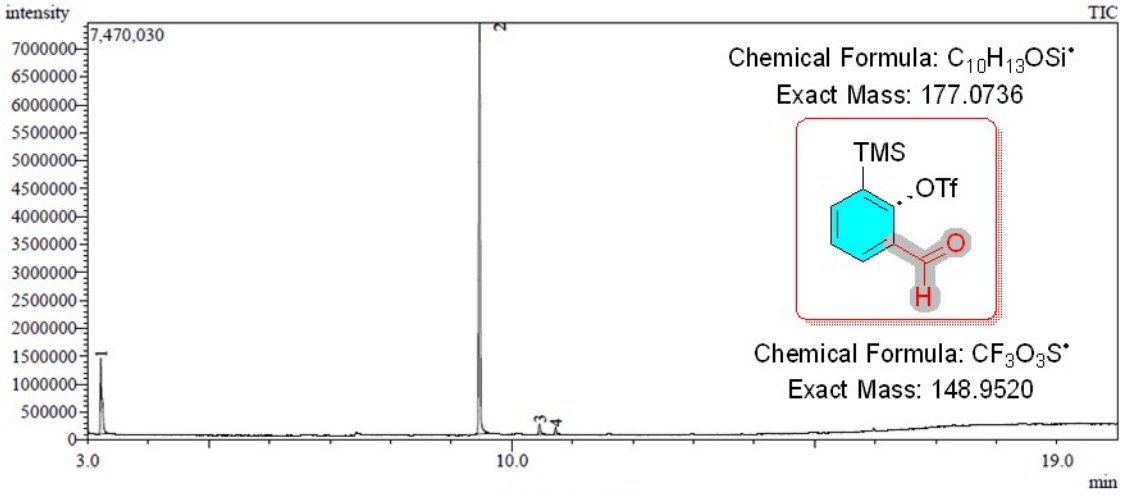


GCMS of 2-formyl-5-(trimethylsilyl) phenyltrifluoromethanesulfonate (2u)

CSIR-INDIAN INSTITUTE OF INTEGRATIVE MEDICINE
Quality Management and Instrumentation Division
GCMS ANALYSIS REPORT

Sample Information

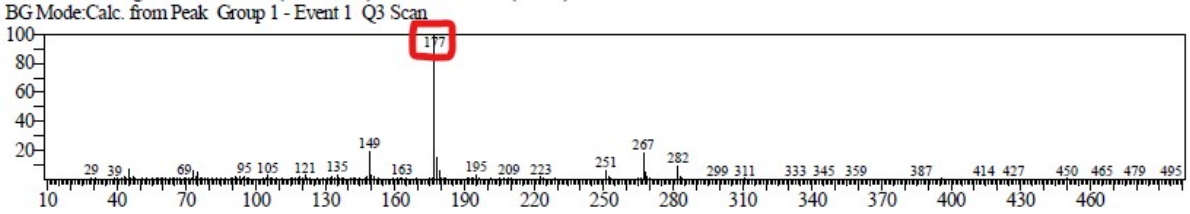
Analyzed by	: System Administrator
Analyzed	: 05-02-2024 13:36:06
Level #	: 1
Sample Name	: PPS-312
Sample ID	: PPS-312
Sample Amount	: 1
Vial #	: 2
Injection Volume	: 1.00
Data File	: D:\GCMS-2024\DATA\FEB-2024\05.02.2024-2.qgd
Method File	: D:\GCMS-2024\METHODS\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2024\TUNNING\03.01.2024-LIQ-5MS.qgt
$EndIf$Modified by	: System Administrator
Modified	: 05-02-2024 14:59:05



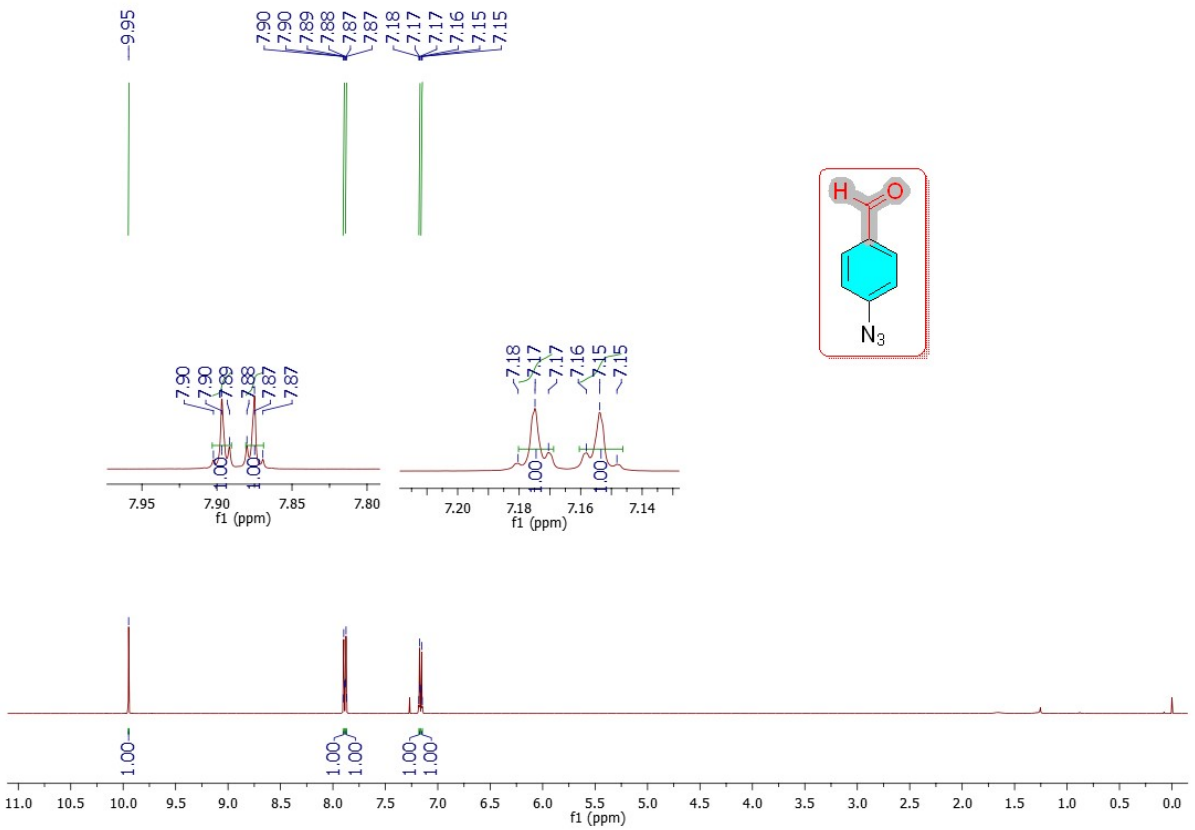
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Name
1	3.221	2665718	18.79	96	1-Butanol, 3-methyl-, acetate
2	9.469	10929128	77.02	0	
3	10.459	332760	2.35	75	Isophthalic acid, ethyl 2-isopropylphenyl ester
4	10.722	261951	1.85	78	Silane, dimethyl(4-acetylphenoxy)butoxy-
		14189557	100.00		

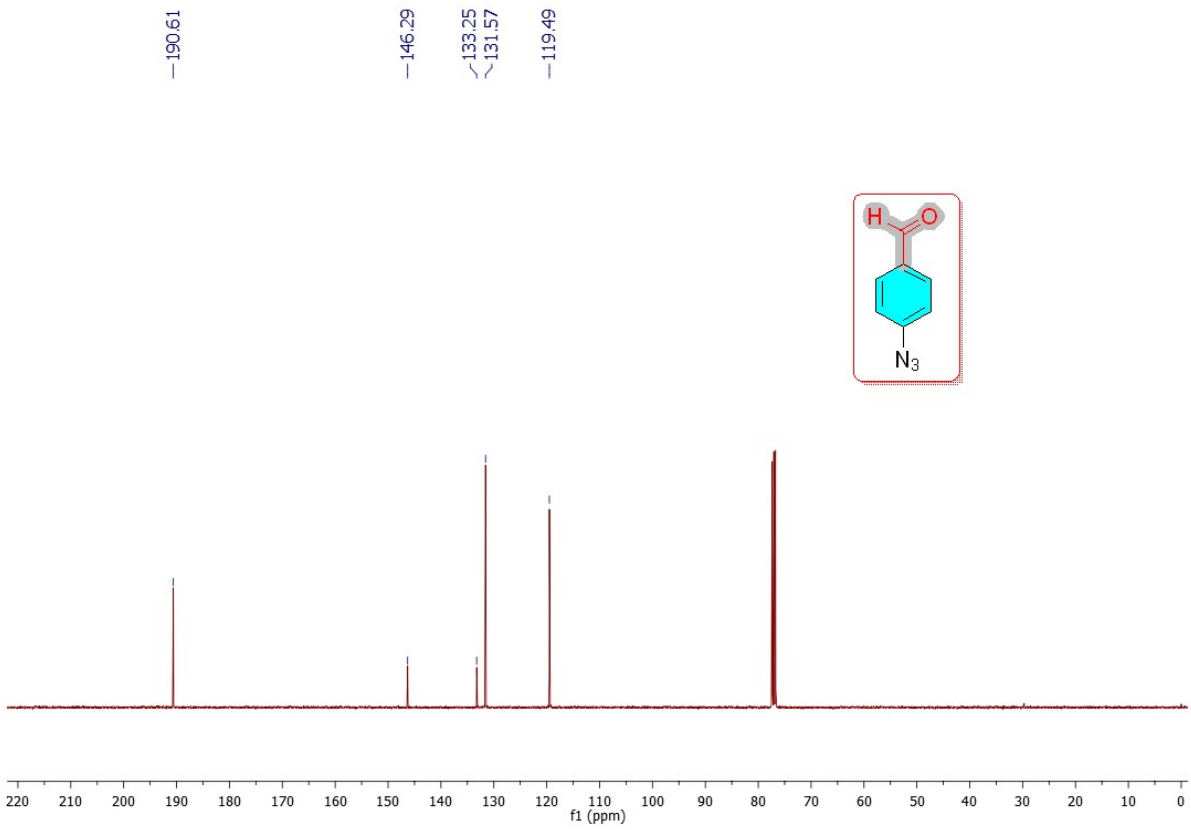
<< Target >>
Line#:3 R.Time:10.460(Scan#:1493) MassPeaks:307
RawMode:Averaged 10.455-10.465(1492-1494) BasePeak:177.05(67507)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



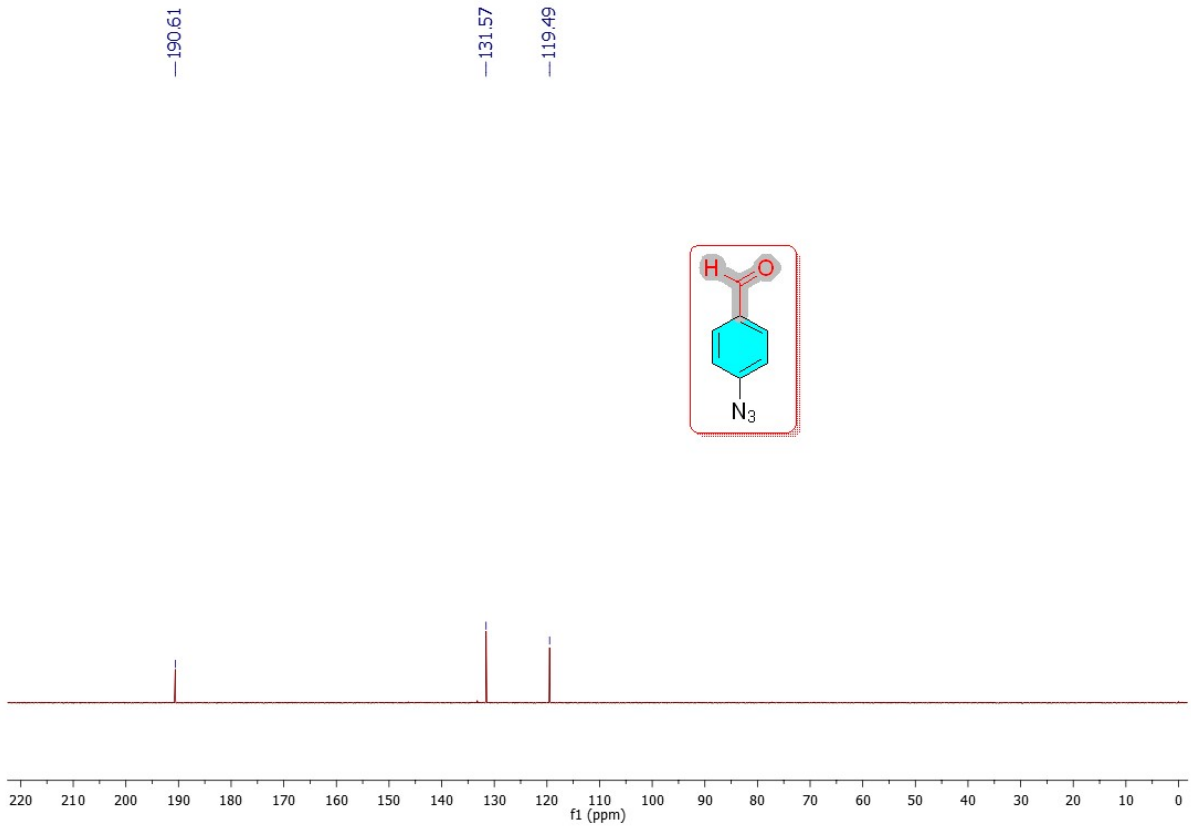
^{1}HNMR Spectra of 4-Azidobenzaldehyde (2w)[6]



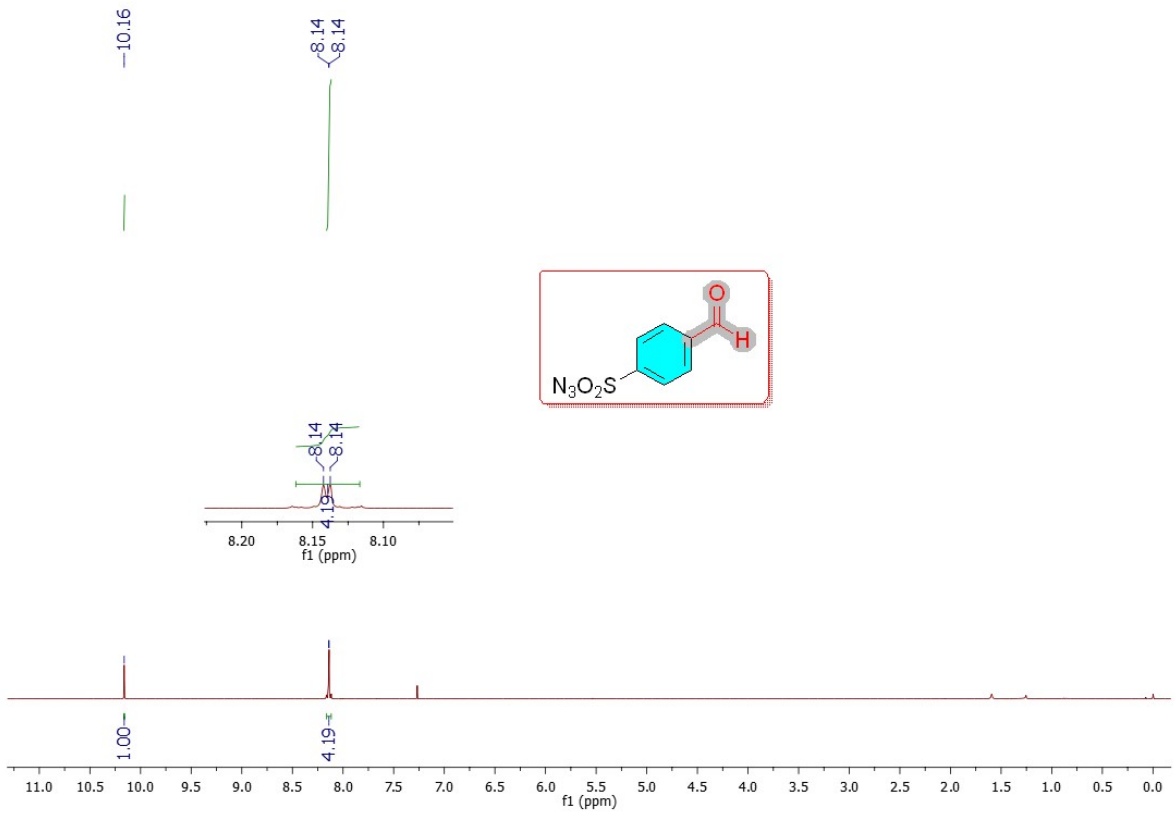
^{13}C{^{1}H} NMR Spectra of 4-Azidobenzaldehyde (2w)[6]



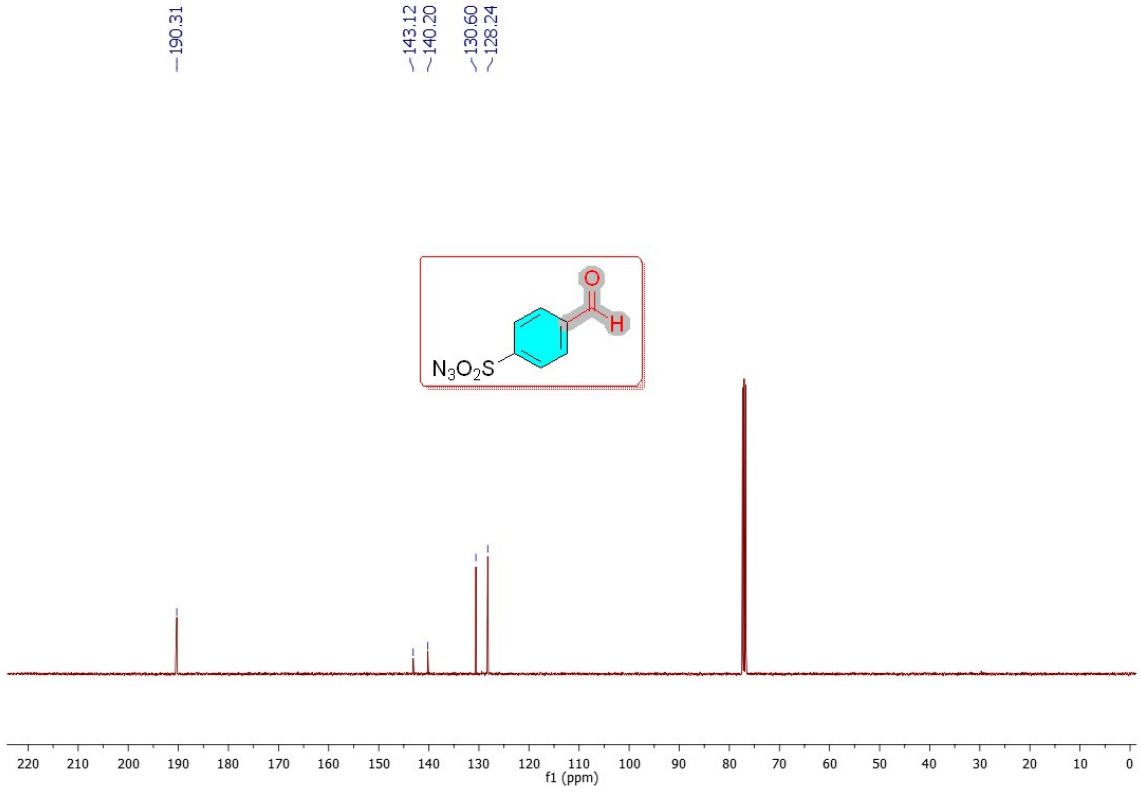
DEPT Spectra of 4-Azidobenzaldehyde (2w)[6]



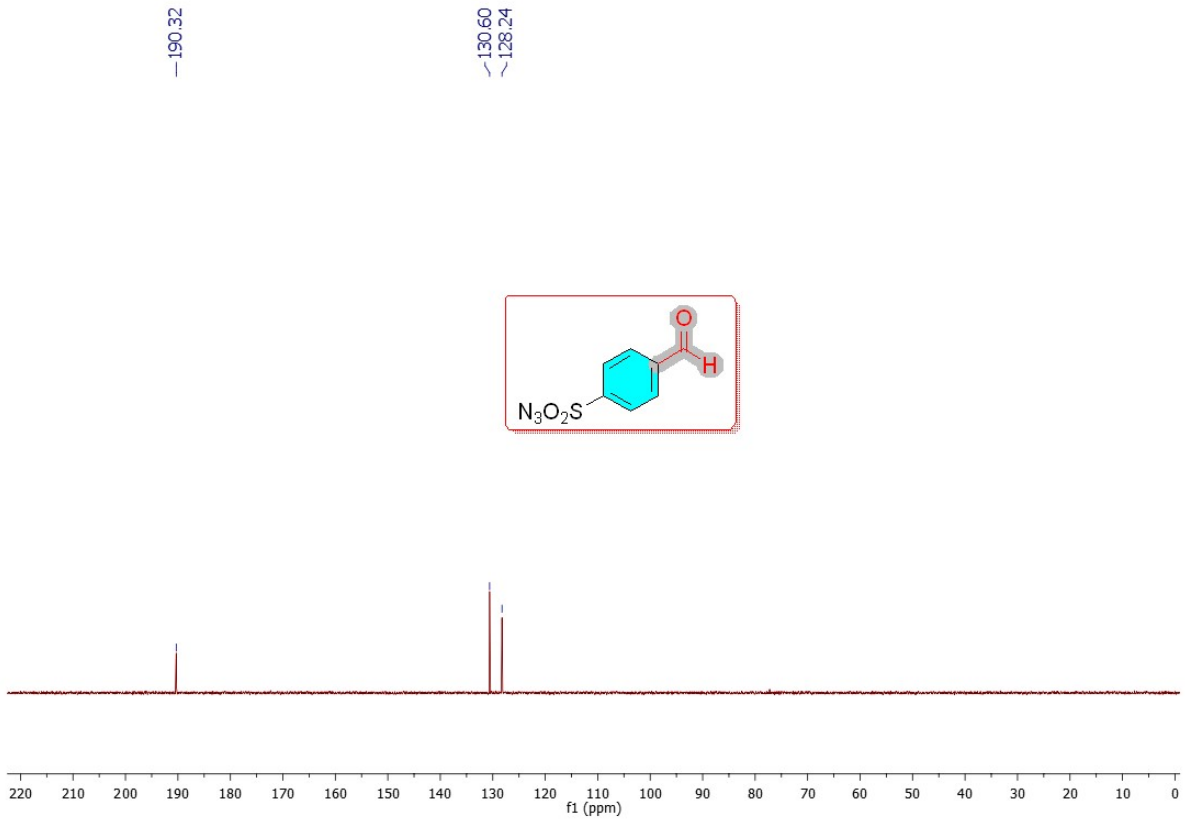
[1]HNMR Spectra of 4-Formylbenzenesulfonyl azide (2x)



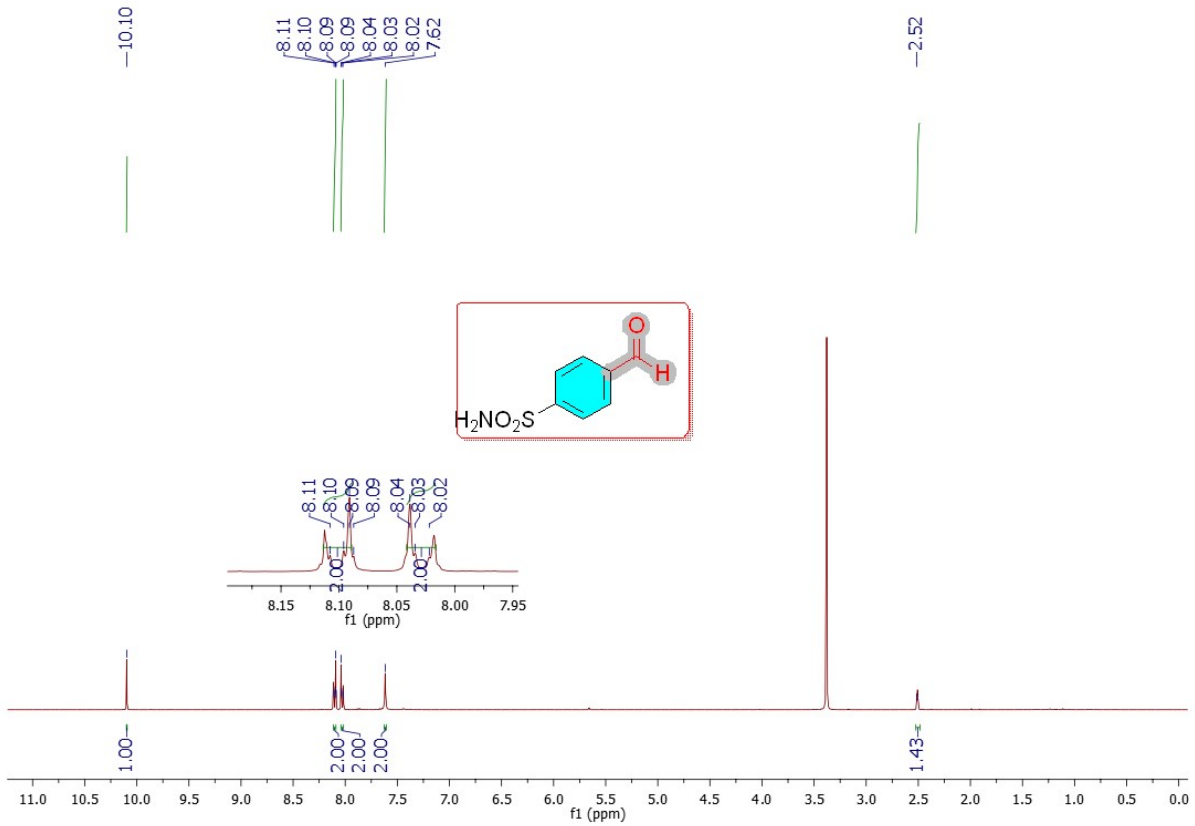
$^{13}C\{^{1}H\}$ NMR Spectra of 4-Formylbenzenesulfonyl azide (2x)



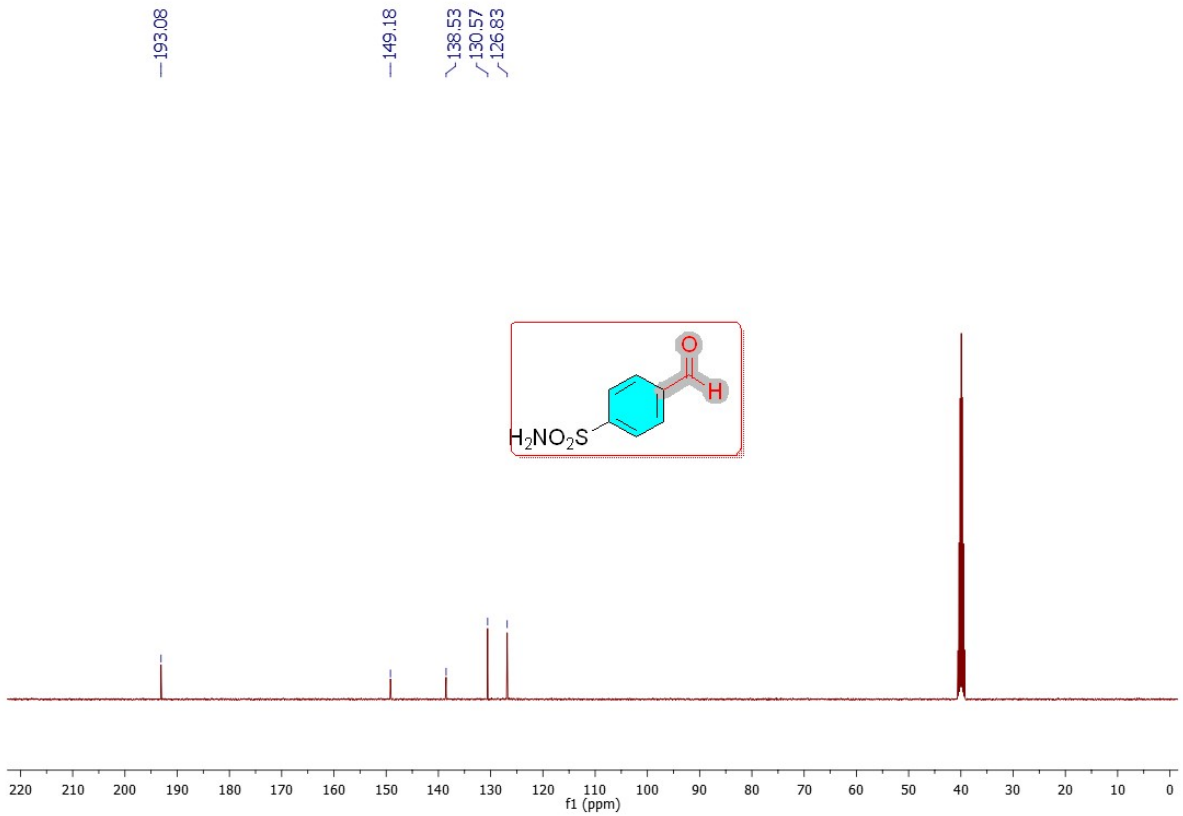
DEPT Spectra of 4-Formylbenzenesulfonyl azide (2x)



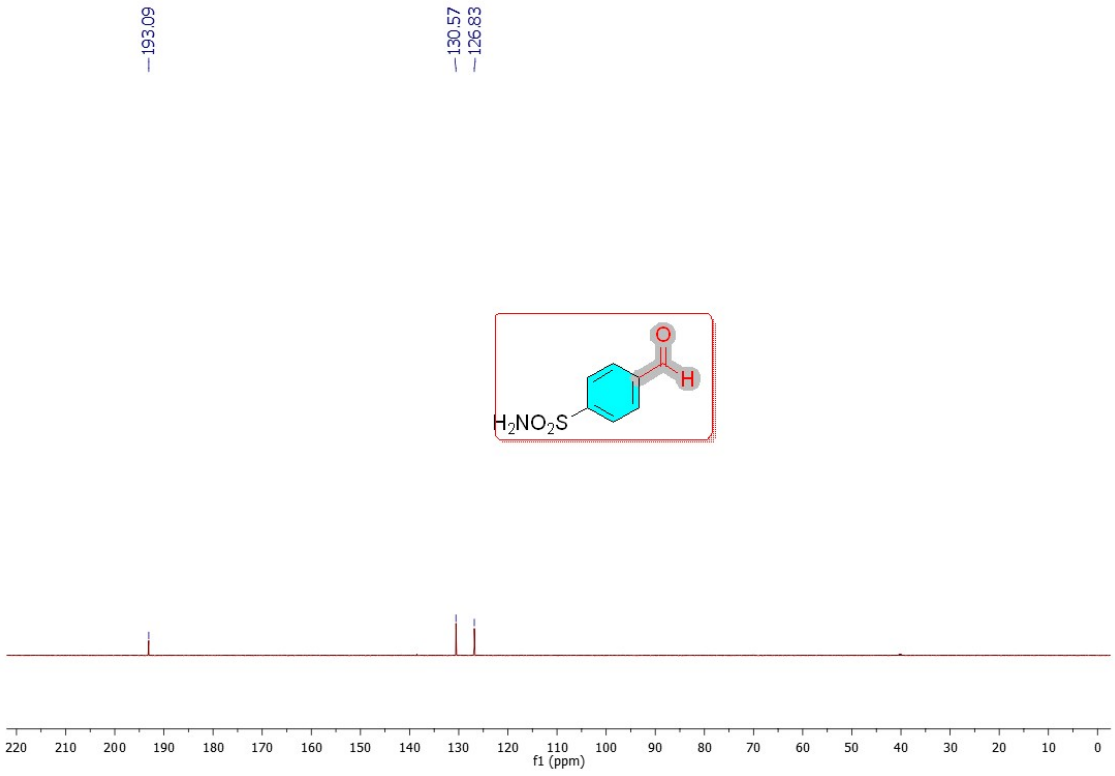
[1]HNMR Spectra of 4-Formylbenzenesulfonamide (2y)[7]



[13]C{[1]H} NMR Spectra of 4-Formylbenzenesulfonamide (2y)[7]



DEPT Spectra of 4-Formylbenzenesulfonamide (2y)[7]

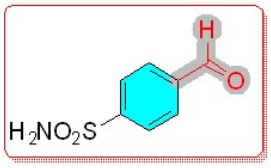


GCMS of 4-Formylbenzenesulfonamide (2y)

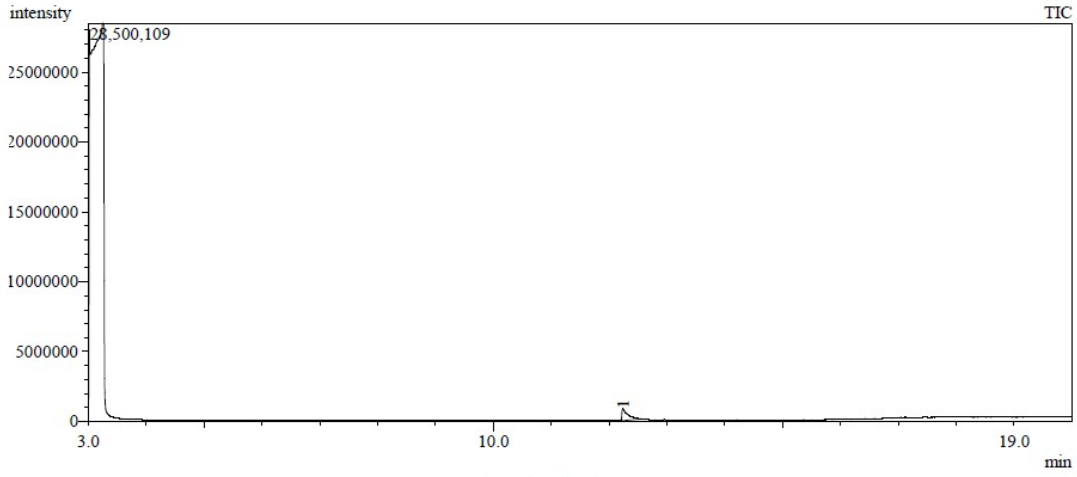
CSIR-INDIAN INSTITUTE OF INTEGRATIVE MEDICINE
Quality Management and Instrumentation Division
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 23-01-2024 12:04:28
Level #	: 1
Sample Name	: S-AMIDE
Sample ID	: S-AMIDE
Sample Amount	: 1
Vial #	: 4
Injection Volume	: 1.00
Data File	: D:\GCMS-2024\DATA\JAN-2024\23.01.2024-04.qgd
Method File	: D:\GCMS-2024\METHODS\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2024\TUNNING\03.01.2024-LIQ-5MS.qgt
$EndIf$Modified by	: System Administrator
Modified	: 23-01-2024 14:59:41



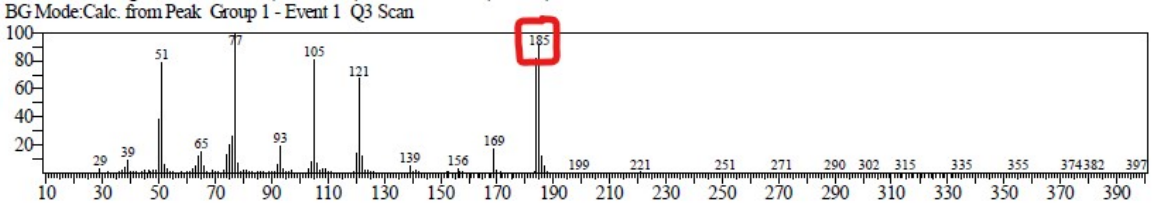
Chemical Formula: $C_7H_7NO_3S$
Exact Mass: 185.0147
Molecular Weight: 185.1970



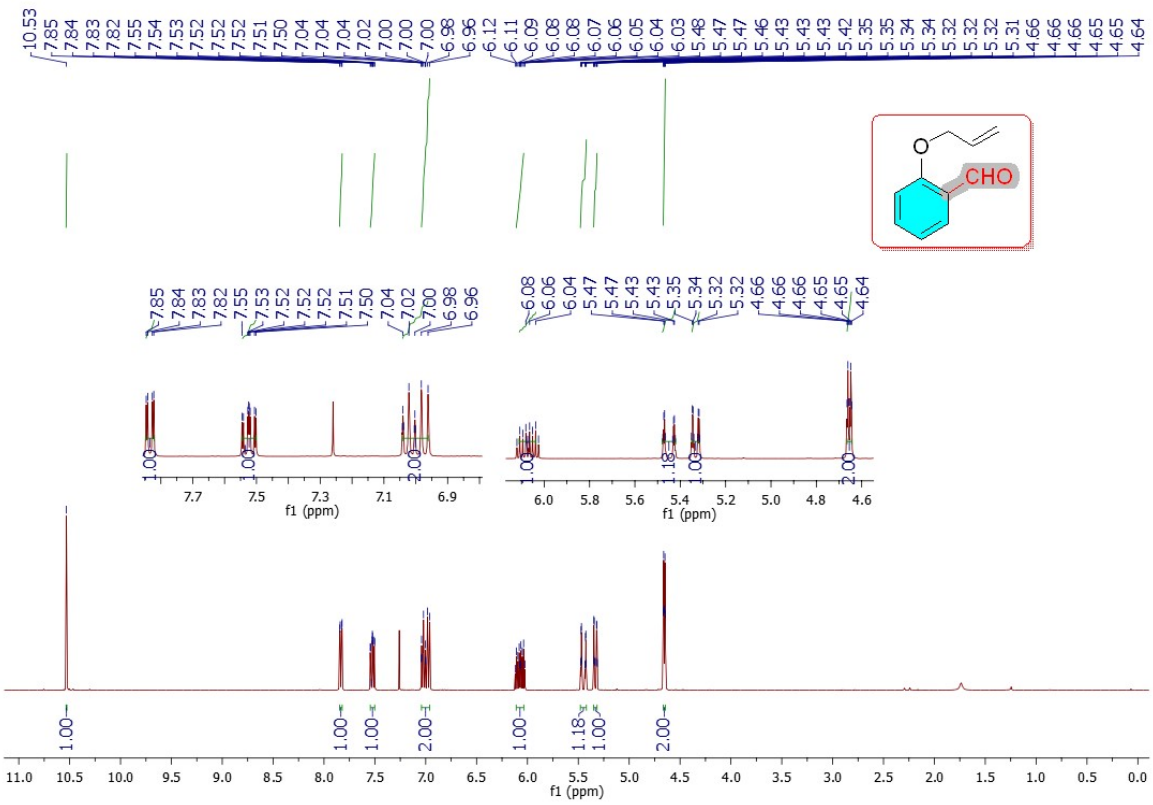
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Name
1	12.237	6237221	100.00	72	Benzamide
		6237221	100.00		

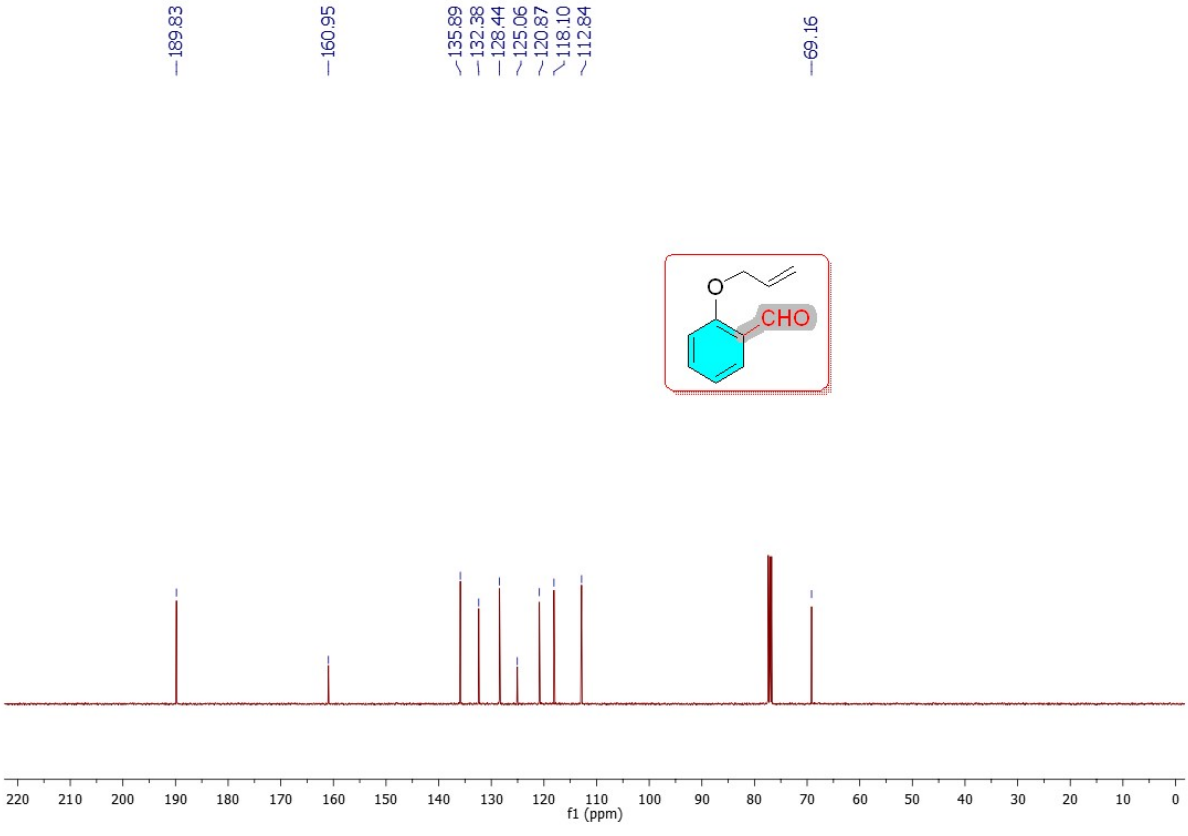
<< Target >>
Line#:1 R.Time:12.235(Scan#:1848) MassPeaks:255
RawMode:Averaged 12.230-12.240(1847-1849) BasePeak:77.05(101883)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



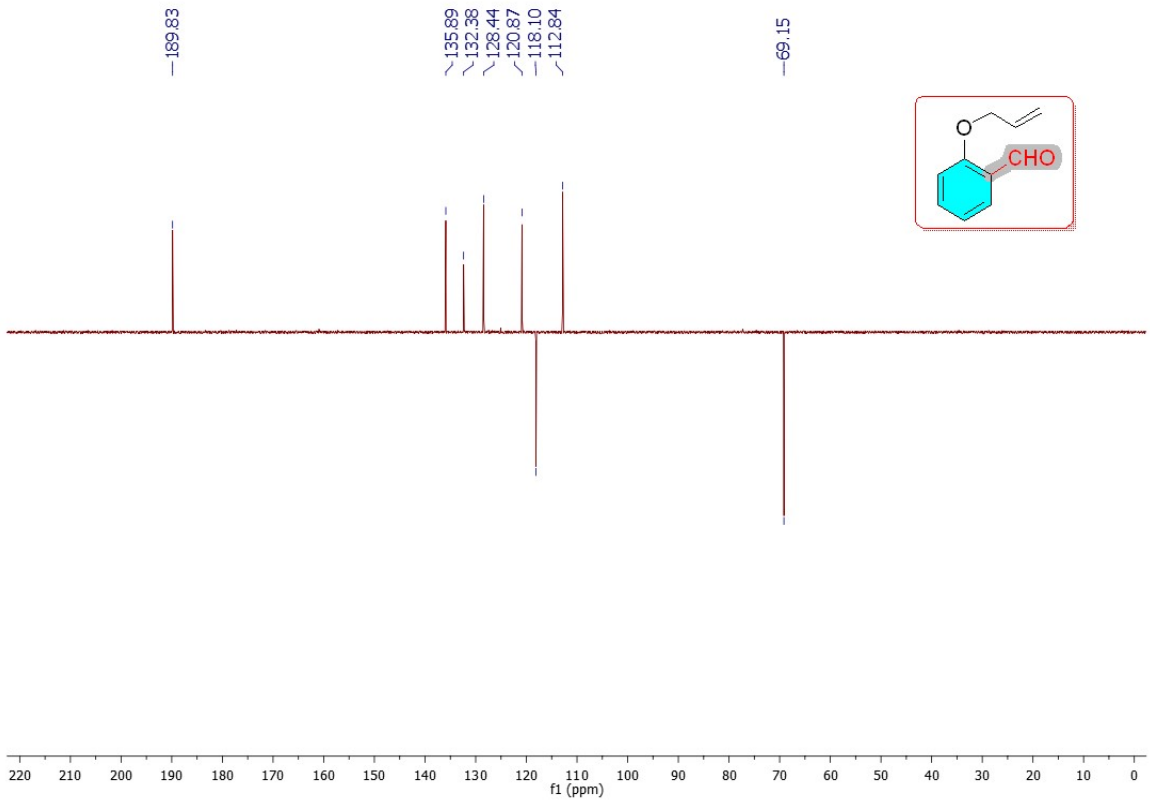
[1]HNMR Spectra of 2-(allyloxy) benzaldehyde (2z)[8]



$^{13}C\{^{1}H\}$ NMR Spectra of 2-(allyloxy) benzaldehyde (2z)[8]



DEPT Spectra of 2-(allyloxy) benzaldehyde (2z)[8]

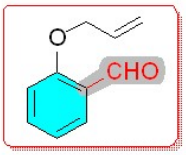


GCMS of 2-(allyloxy) benzaldehyde (2z)

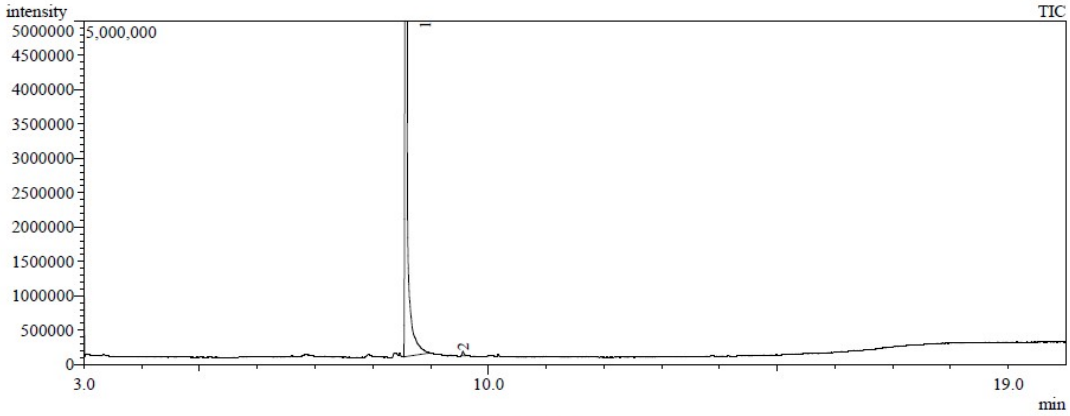
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 21-03-2023 21:11:51
Level #	: 1
Sample Name	: RD-4
Sample ID	: RD-4
Sample Amount	: 1
Vial #	: 4
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-24.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:09:28



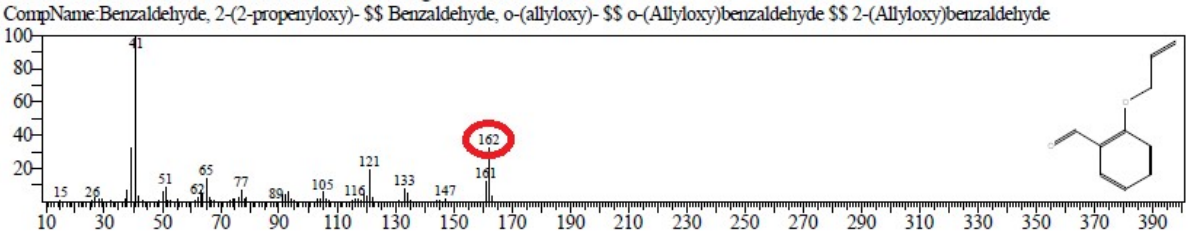
Chemical Formula: $C_{10}H_{10}O_2$
Exact Mass: 162.07



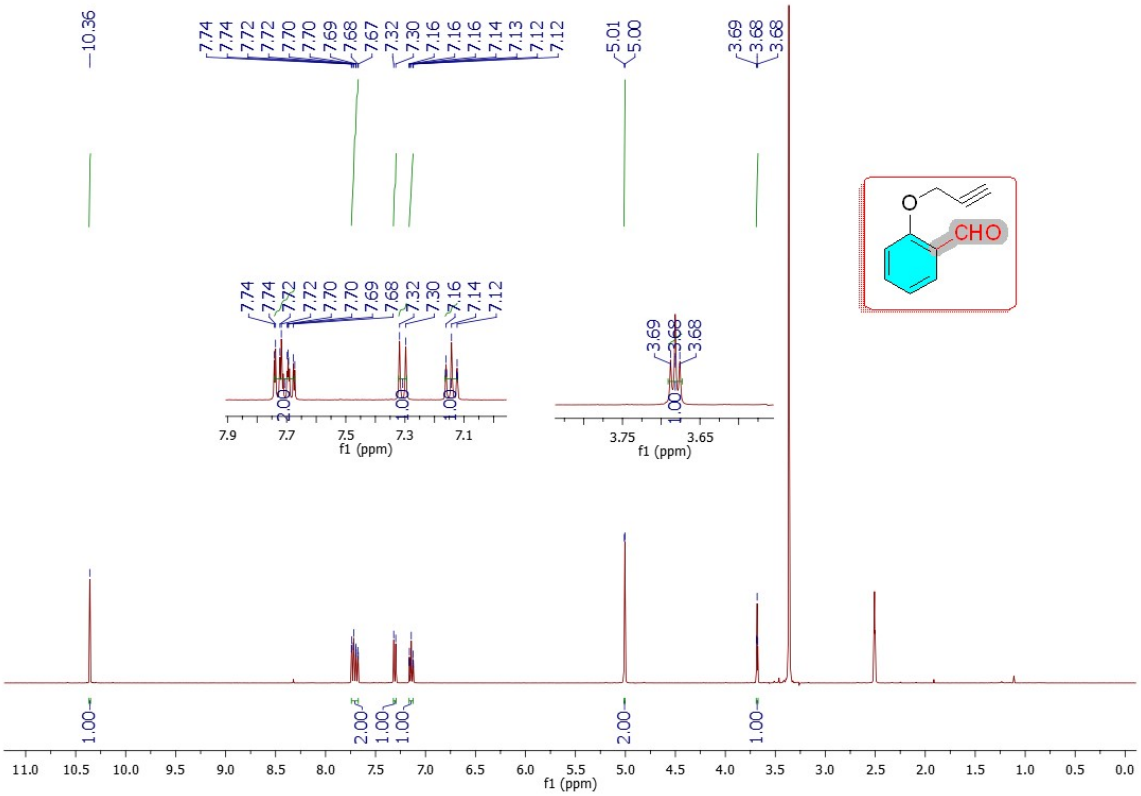
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	8.574	40325233	99.66	80	41.05	Benzaldehyde, 2-(2-propenyloxy)-
2	9.561	137051	0.34	92	191.10	2,4-Di-tert-butylphenol
		40462284	100.00			

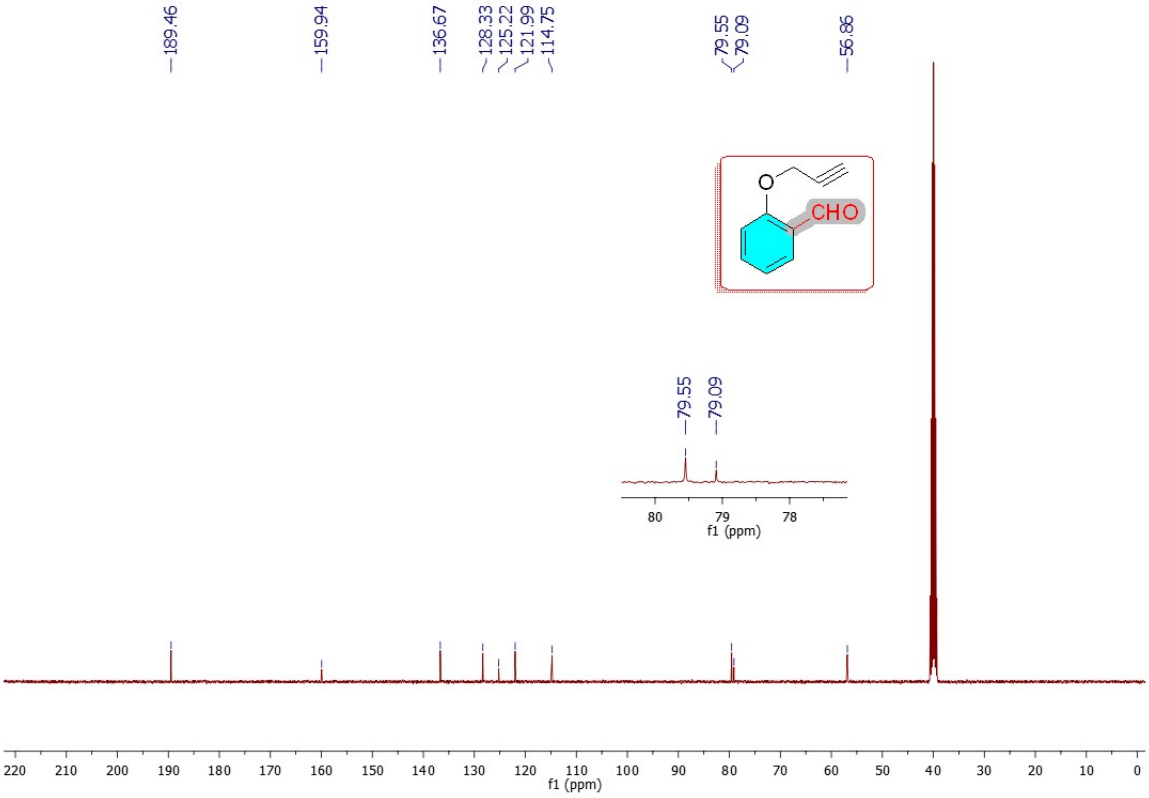
Hit#:1 Entry:22920 Library:NIST17M1.lib
SI:80 Formula:C10H10O2 CAS:28752-82-1 MolWeight:162 RetIndex:1360
CompName:Benzaldehyde, 2-(2-propenyloxy)- $$ Benzaldehyde, o-(allyloxy)- $$ o-(Allyloxy)benzaldehyde $$ 2-(Allyloxy)benzaldehyde



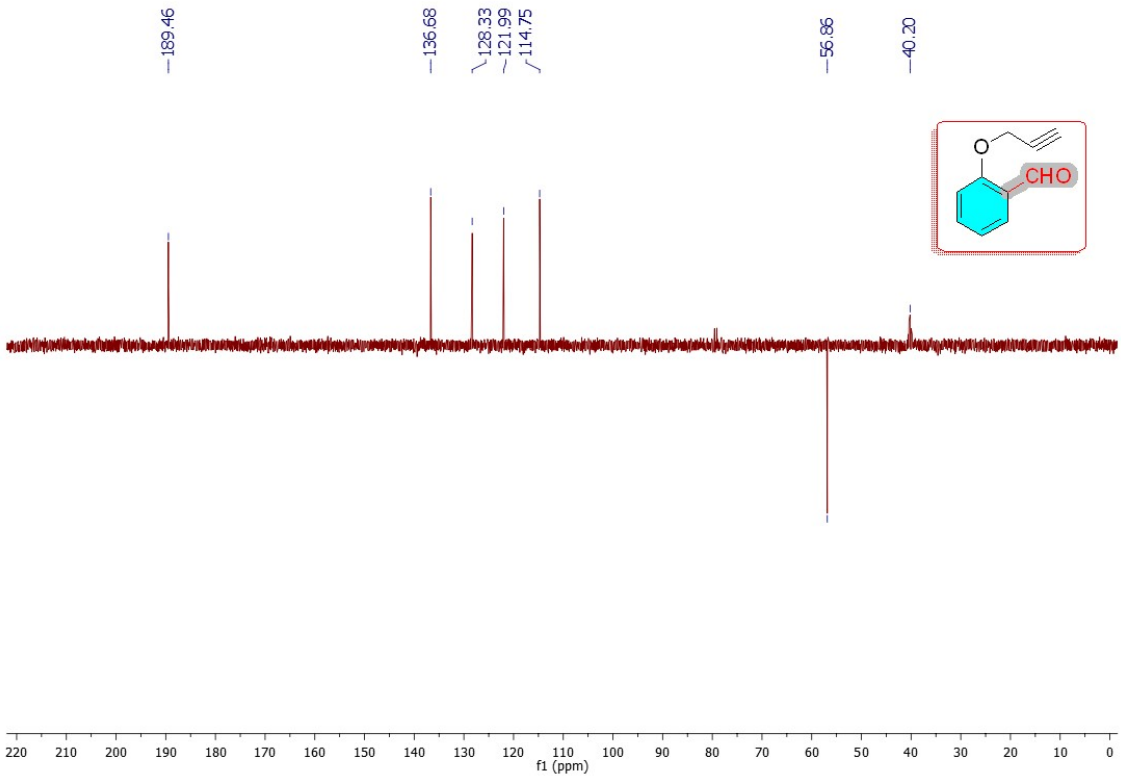
[1]HNMR Spectra of 2-(prop-2-yn-1-yloxy) benzaldehyde (2aa)[8]



$^{13}C\{^{1}H\}$ NMR Spectra of 2-(prop-2-yn-1-yloxy) benzaldehyde (2aa)[8]



DEPT Spectra of 2-(prop-2-yn-1-yloxy) benzaldehyde (2aa)[8]

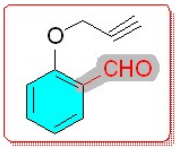


GCMS of 2-(prop-2-yn-1-yloxy) benzaldehyde (2aa)

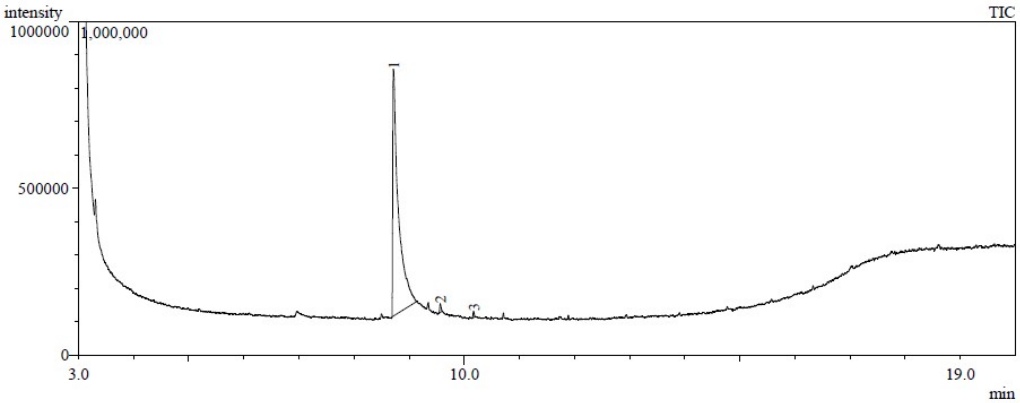
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 21-03-2023 21:37:58
Level #	: 1
Sample Name	: RD-5
Sample ID	: RD-5
Sample Amount	: 1
Vial #	: 5
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-25.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:11:01



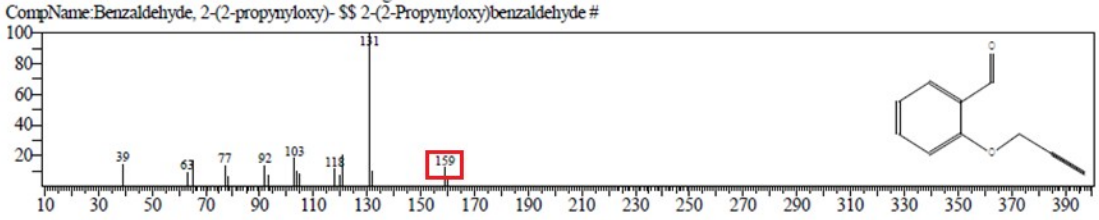
Chemical Formula: $C_{10}H_8O_2$
Exact Mass: 160.05



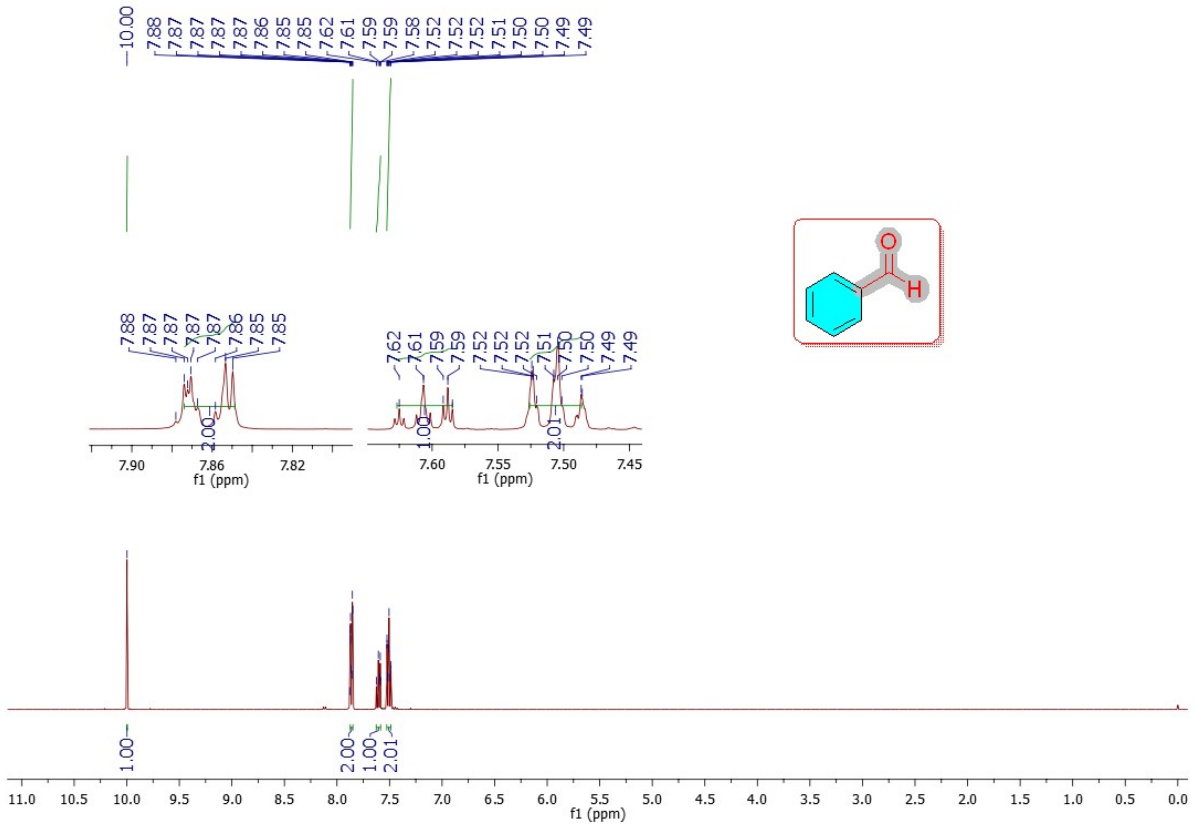
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	8.717	5207453	98.60	86	131.05	Benzaldehyde, 2-(2-propynyloxy)-
2	9.566	41518	0.79	88	191.10	2,4-Di-tert-butylphenol
3	10.169	32260	0.61	89	83.10	1-Heptadecene

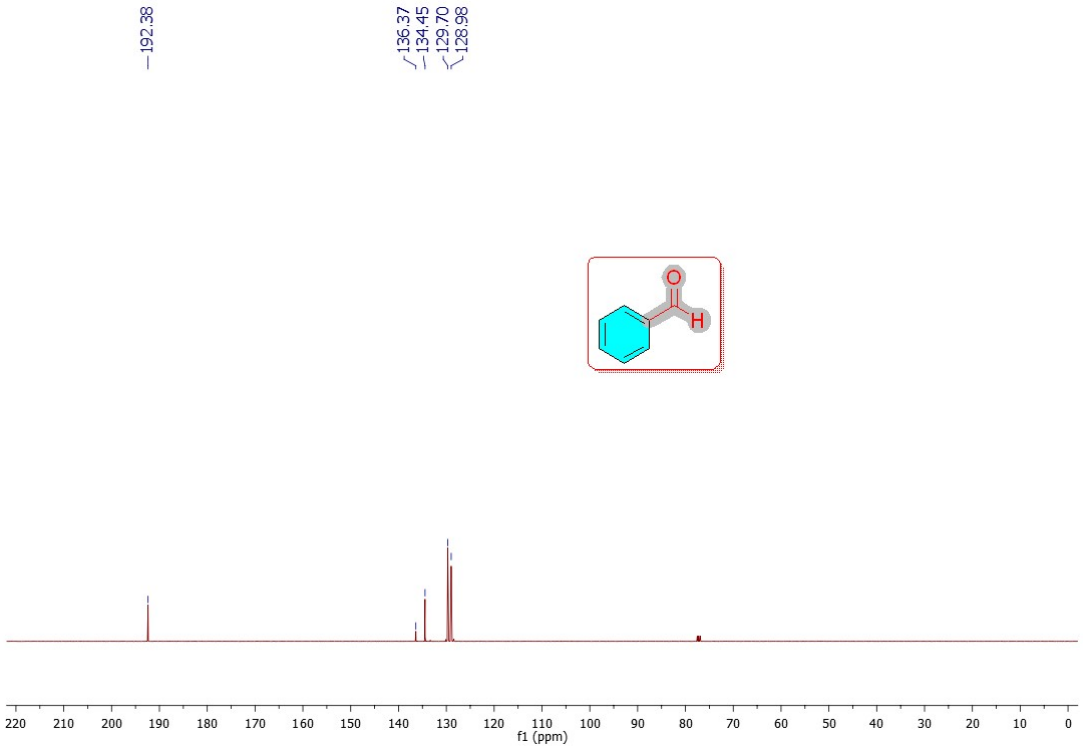
Hit#:1 Entry:21987 Library:NIST17M1.lib
SI:86 Formula:C10H8O2 CAS:29978-83-4 MolWeight:160 RetIndex:1368
CompName:Benzaldehyde, 2-(2-propynyloxy)- $$ 2-(2-Propynyloxy)benzaldehyde #



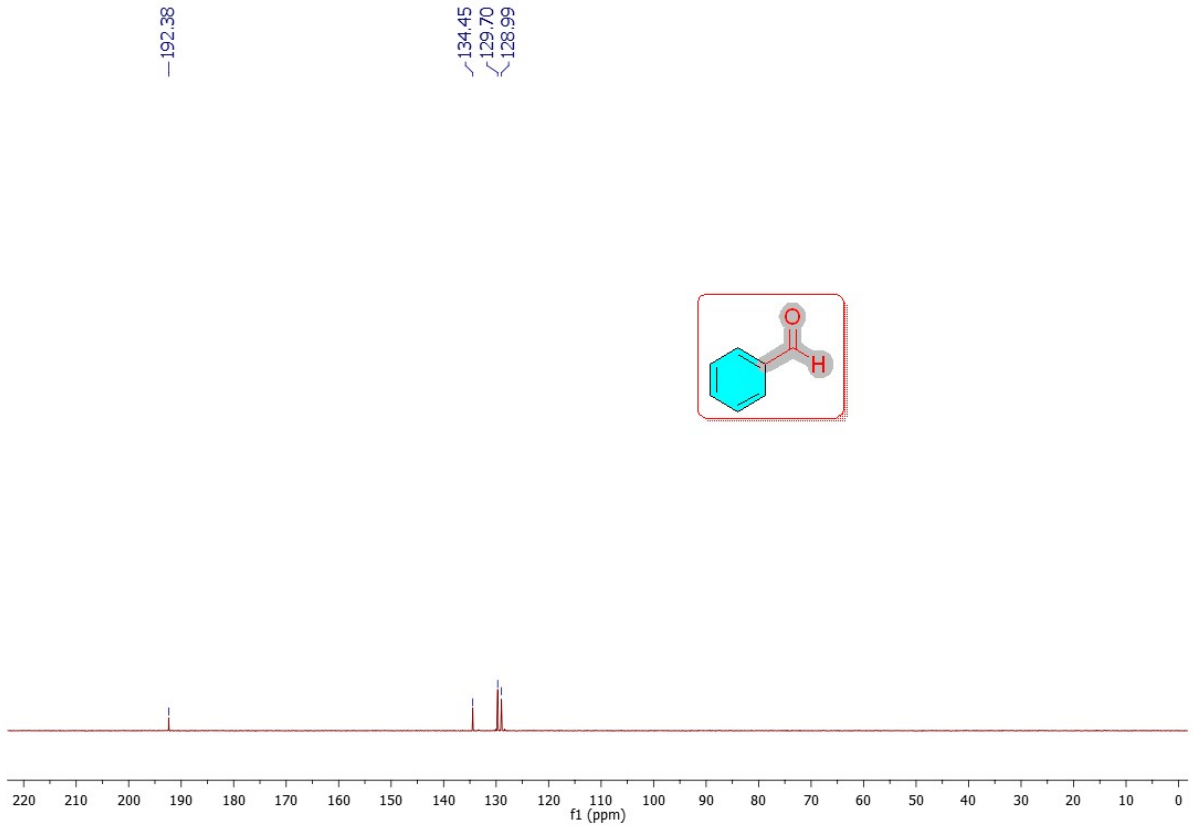
^{1}HNMR Spectra of Benzaldehyde (2ab)[2]



^{13}C{^{1}H} NMR Spectra of Benzaldehyde (2ab)[2]



DEPT Spectra of Benzaldehyde (2ab)[2]

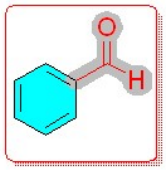


GCMS of Benzaldehyde (2ab)

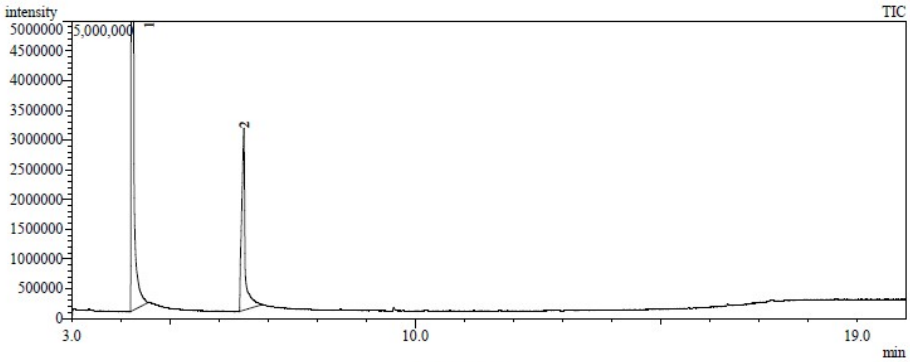
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 22-03-2023 04:35:53
Level #	: 1
Sample Name	: MZ-1
Sample ID	: MZ-1
Sample Amount	: 1
Vial #	: 21
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-41.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:26:56



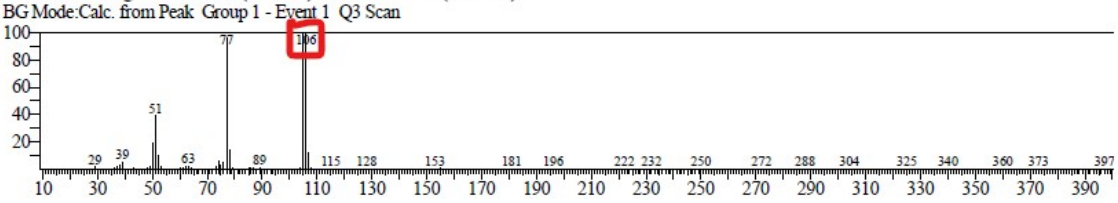
Chemical Formula: C_7H_6O
Exact Mass: 106.04



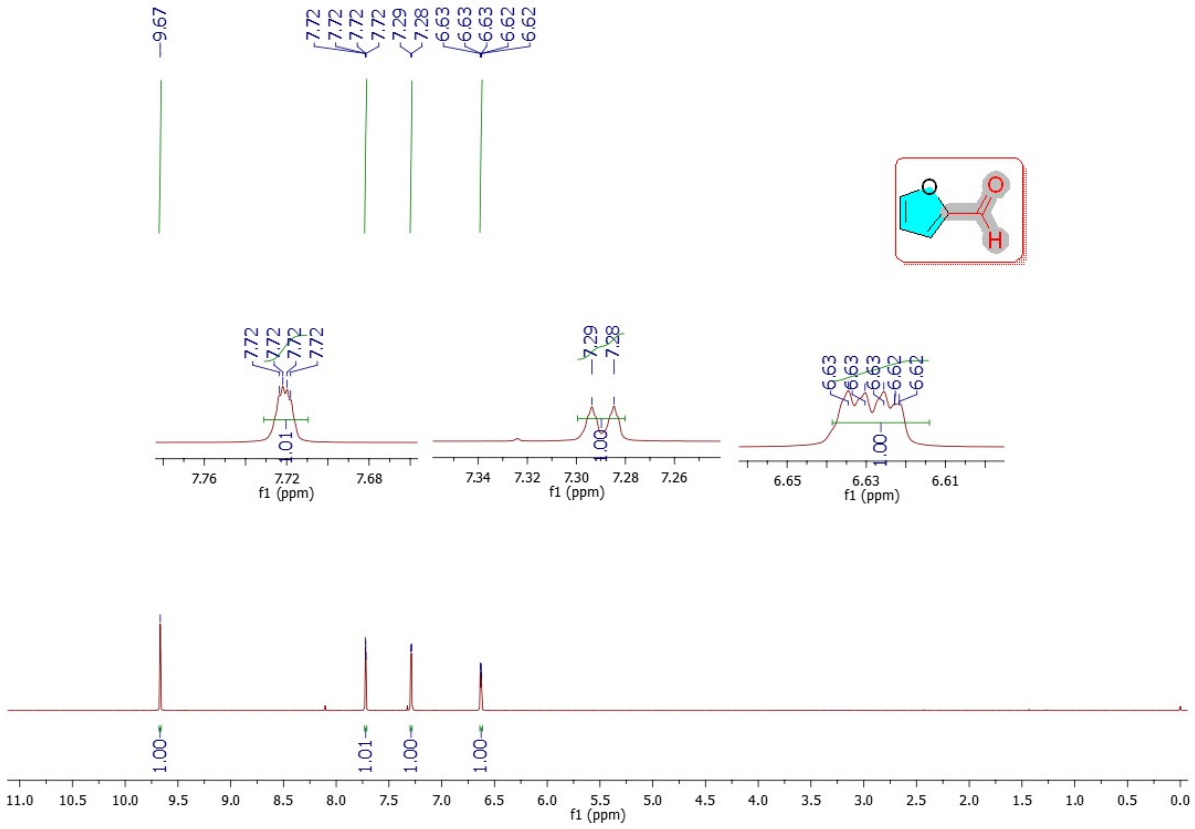
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	4.247	92452147	86.00	98	106.05	Benzaldehyde
2	6.513	15048198	14.00	97	105.00	Benzoic acid
		107500345	100.00			

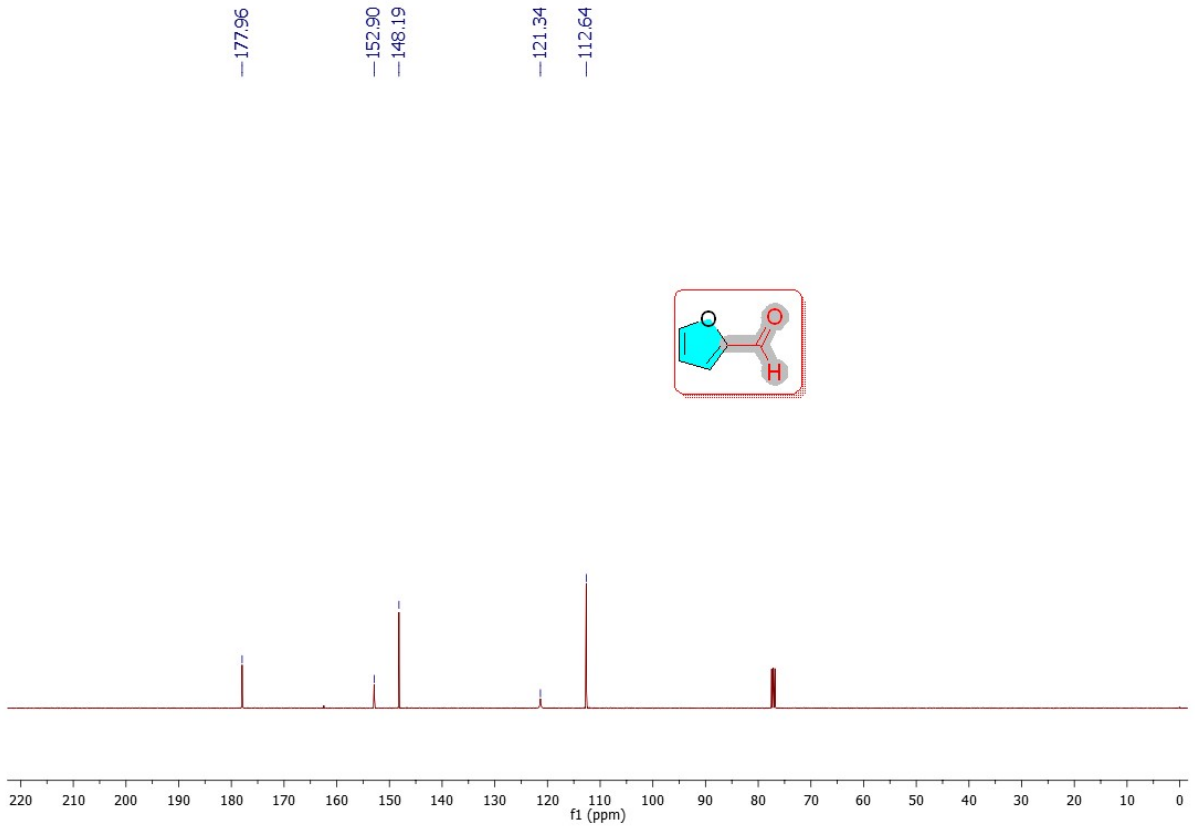
<< Target >>
Line#:1 R.Time:4.245(Scan#:250) MassPeaks:205
RawMode:Averaged 4.240-4.250(249-251) BasePeak:106.05(8199413)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



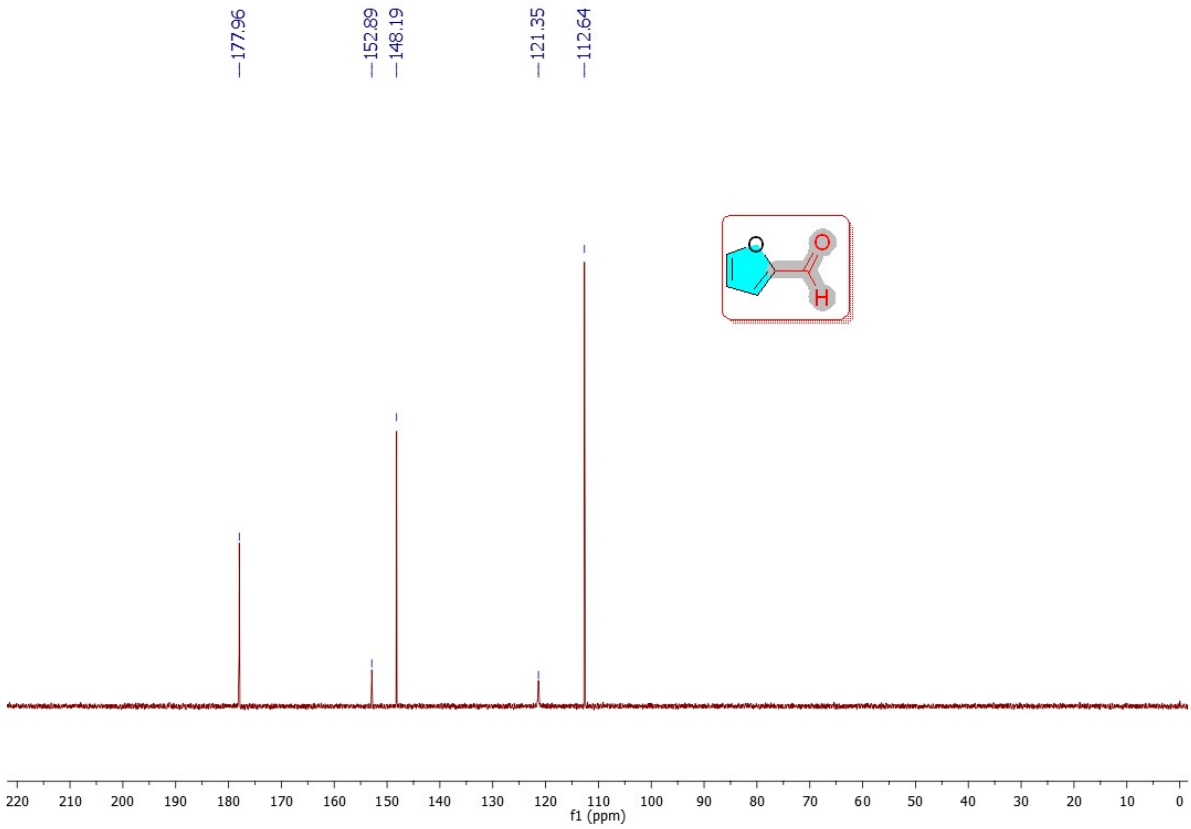
^{1}H NMR Spectra of Furan-2-carbaldehyde (2ac)[2]



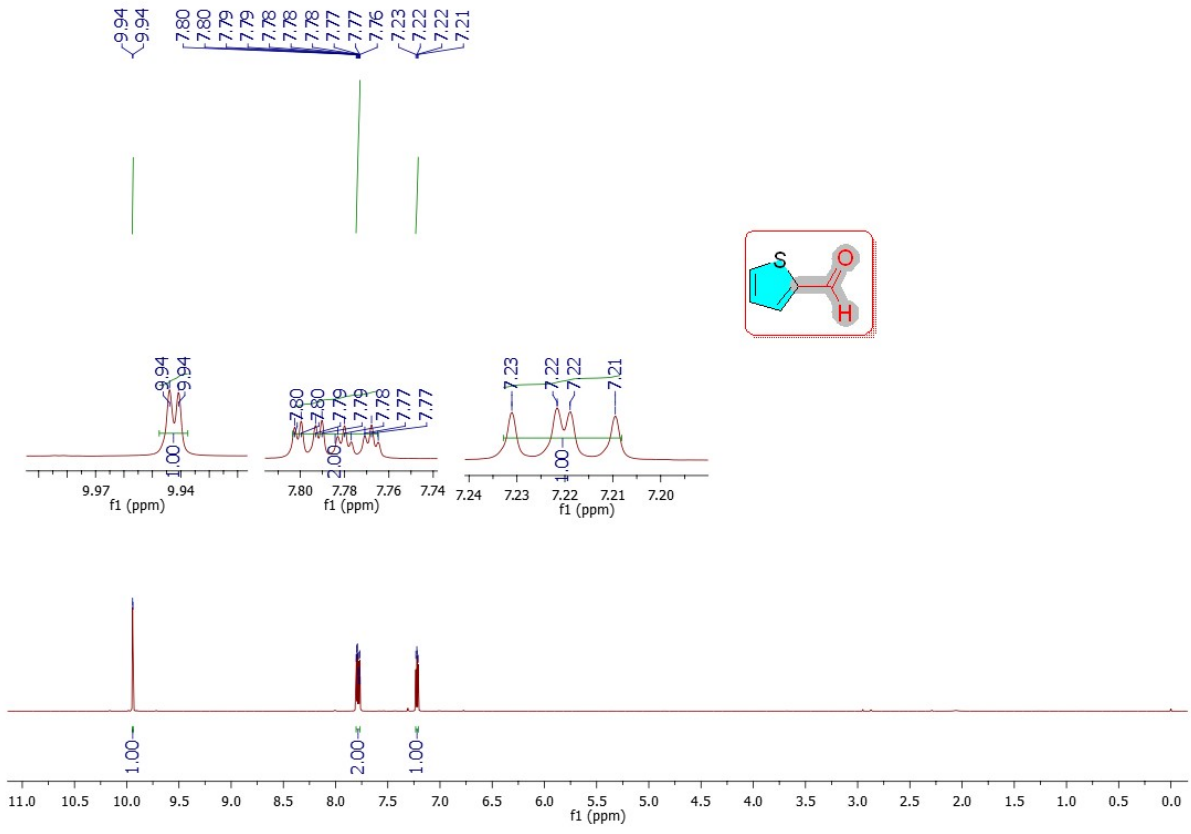
^{13}C{^{1}H} NMR Spectra of Furan-2-carbaldehyde (2ac)[2]



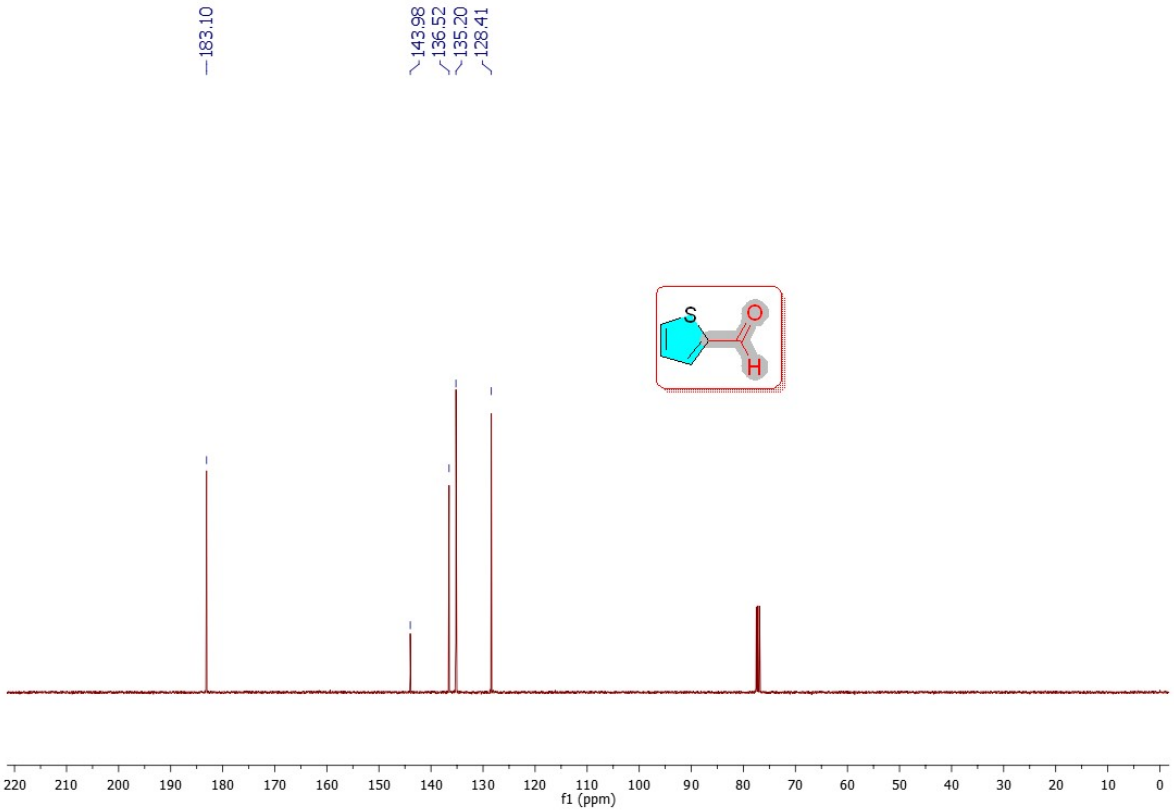
DEPT Spectra of Furan-2-carbaldehyde (2ac)[2]



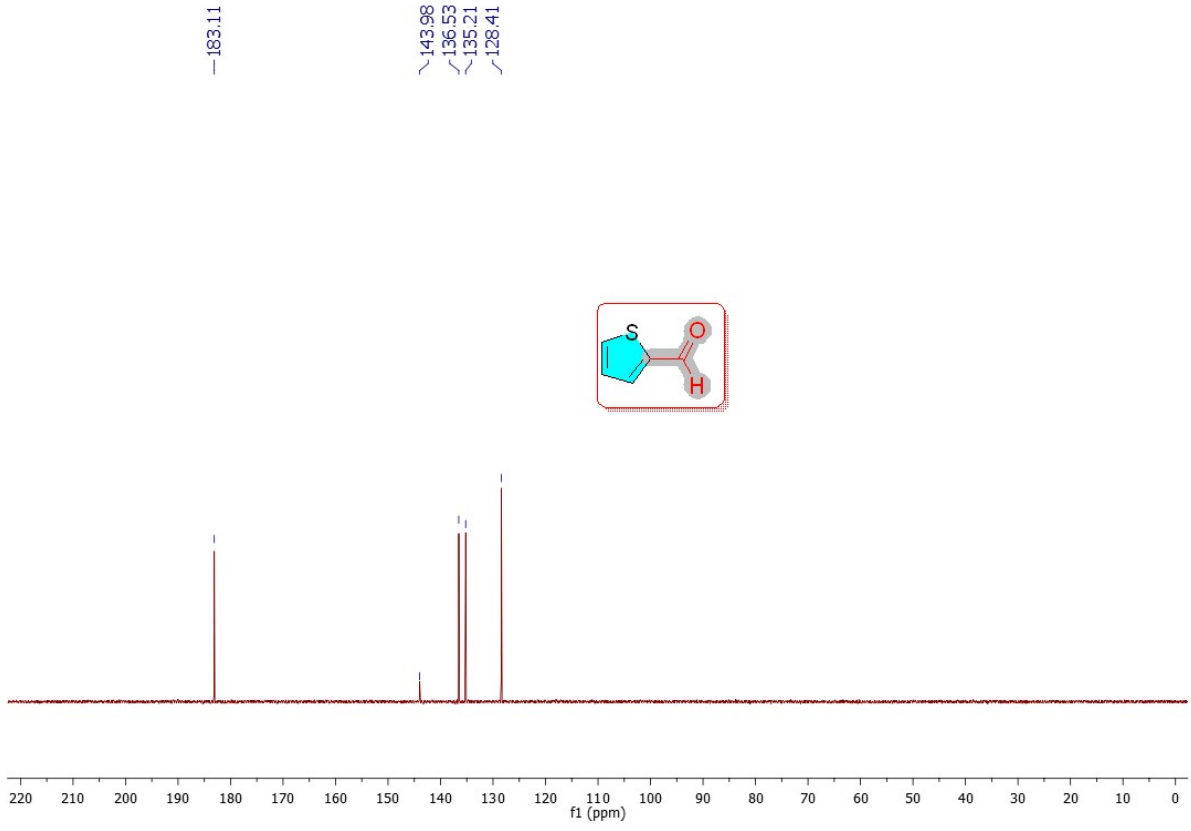
^{1}H NMR Spectra of Thiophene-2-carbaldehyde (2ad)[9]



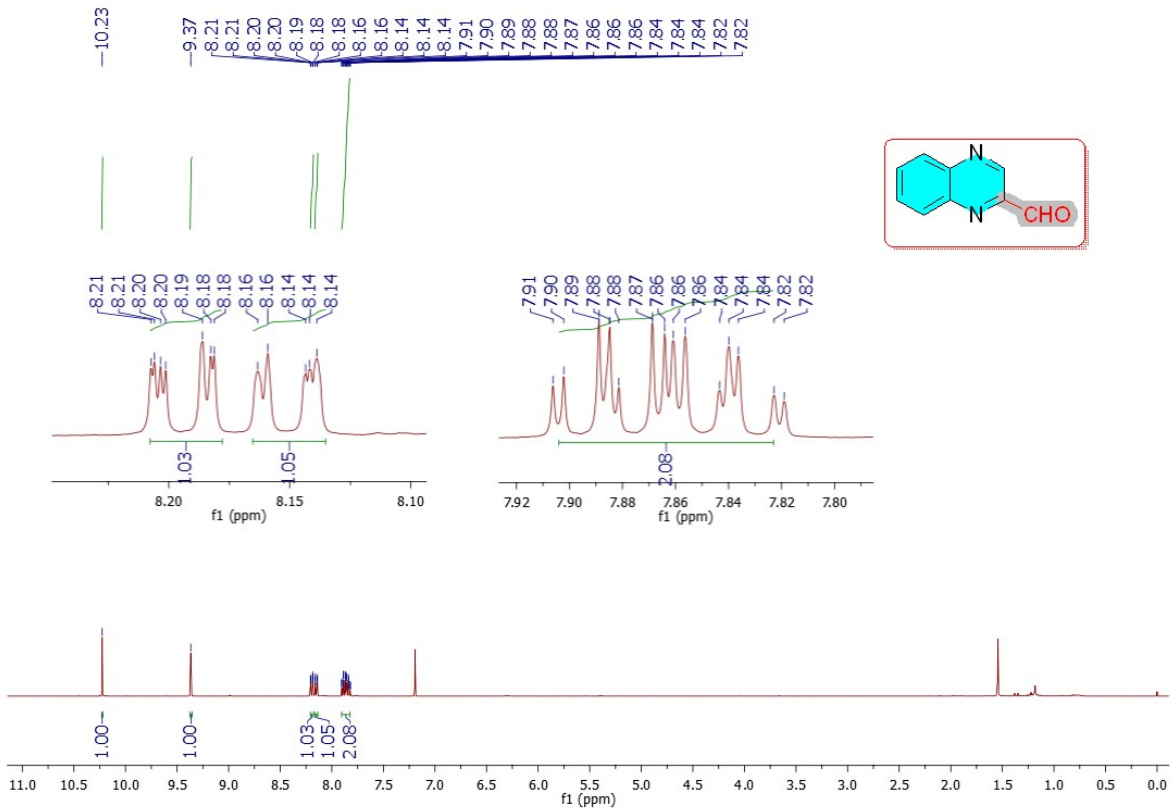
$^{13}C\{^{1}H\}$ NMR Spectra of Thiophene-2-carbaldehyde (2ad)[9]



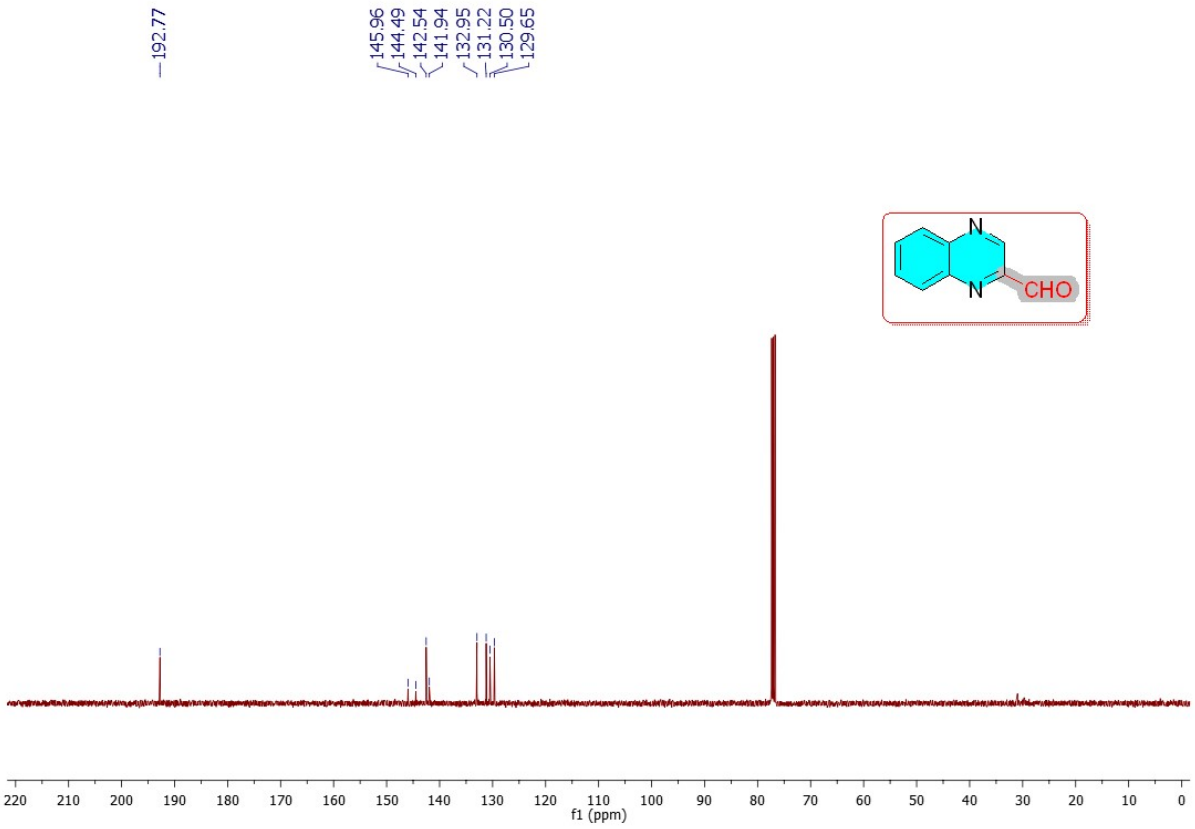
DEPT Spectra of Thiophene-2-carbaldehyde (2ad)[9]



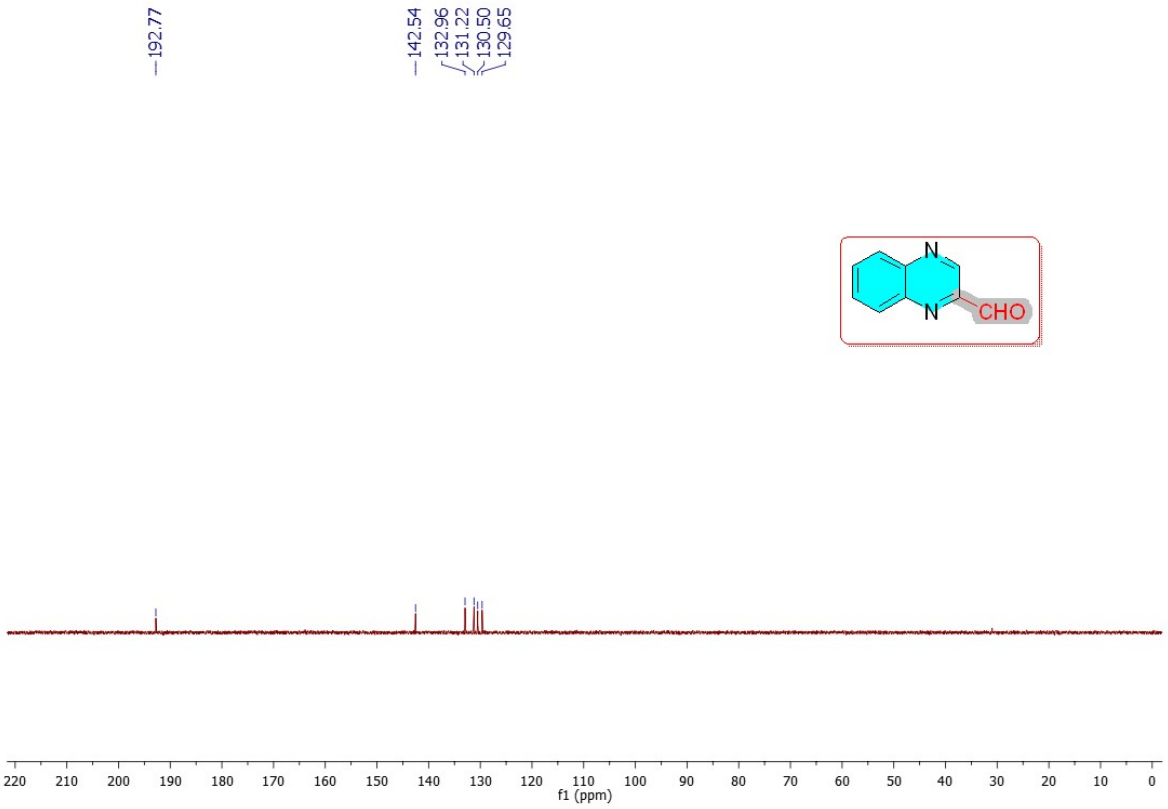
[1]HNMR Spectra of Quinoxaline-2-carbaldehyde (2aj)



[13]C{[1]H} NMR Spectra of Quinoxaline-2-carbaldehyde (2aj)



DEPT Spectra of Quinoxaline-2-carbaldehyde (2aj)

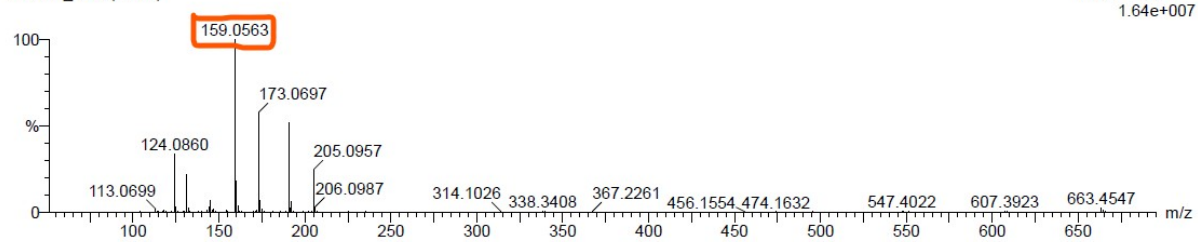


HRMS of Quinoxaline-2-carbaldehyde (2aj)

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

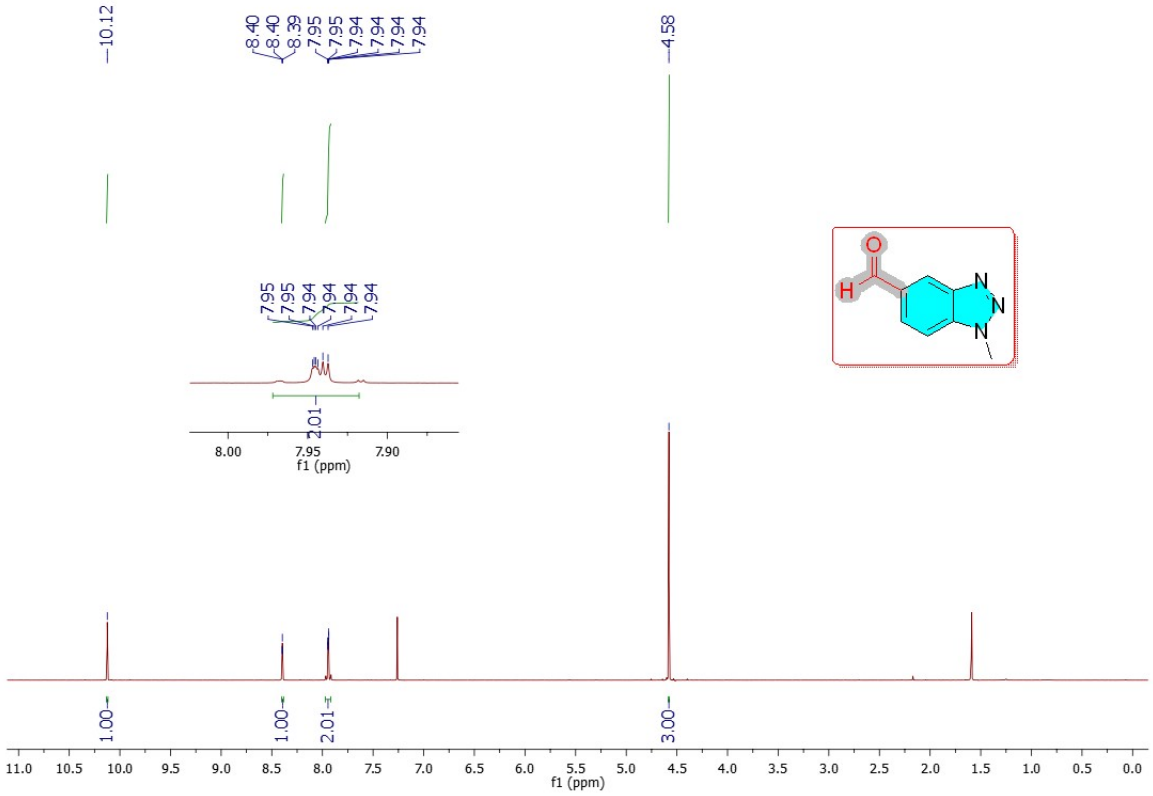
Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-9 H: 0-100 N: 0-2 O: 0-1

PPS-352(1)
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
30-May-2024
13:37:14
300524_02 6 (0.138)
1: TOF MS AP+
1.64e+007

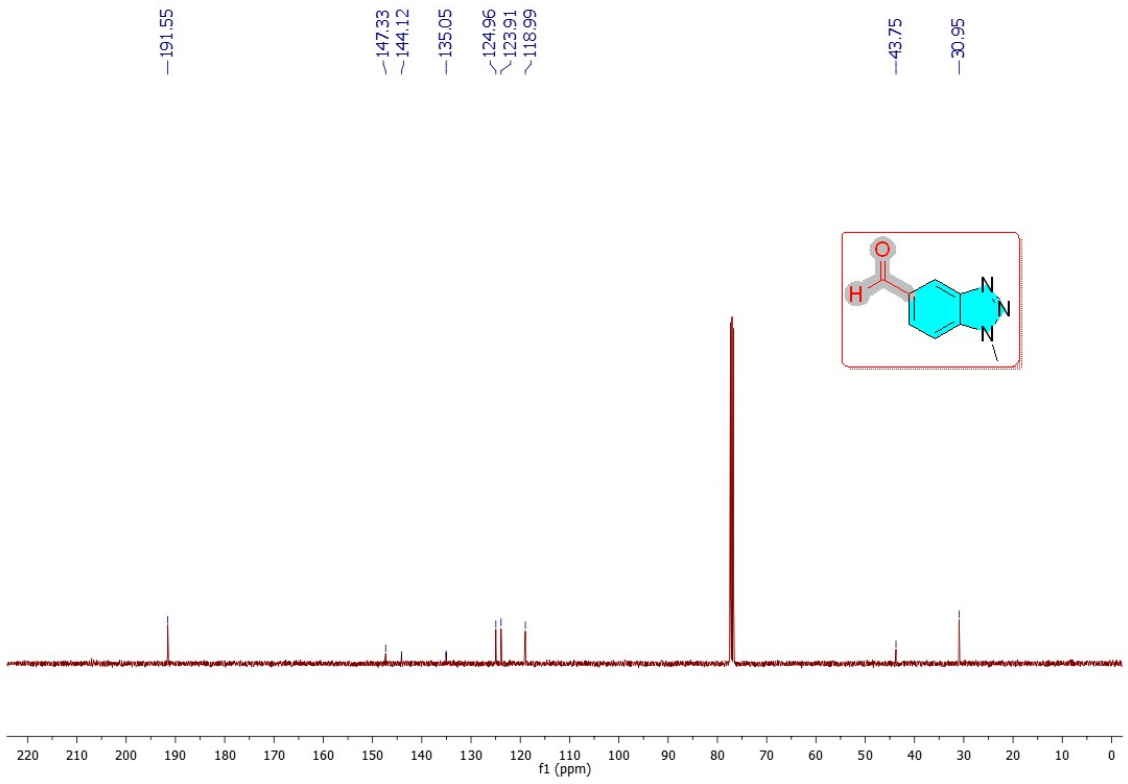


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
159.0563	159.0558	0.5	3.1	7.5	1809.2	n/a	n/a	C9 H7 N2 O

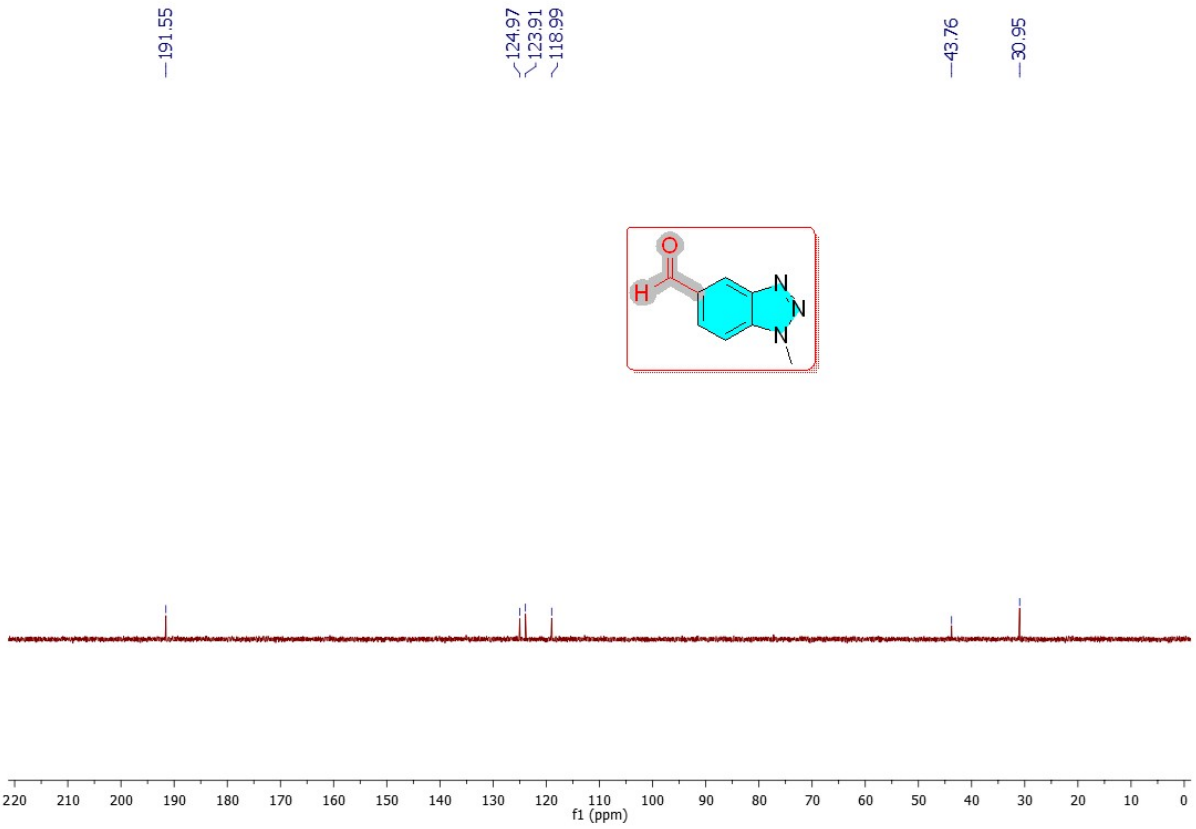
[1]HNMR Spectra of 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carbaldehyde (2ak)



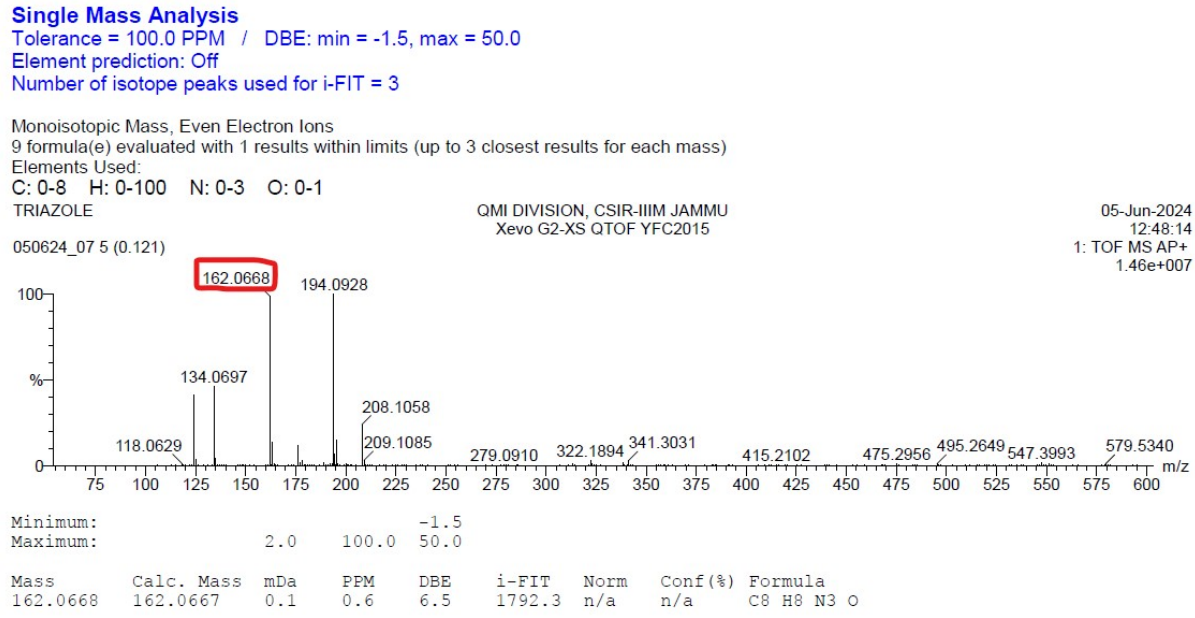
[13]C{[1]H} NMR Spectra of 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carbaldehyde (2ak)



DEPT Spectra of 1-methyl-1*H*-benzo[*d*][1,2,3]triazole-5-carbaldehyde (2ak)

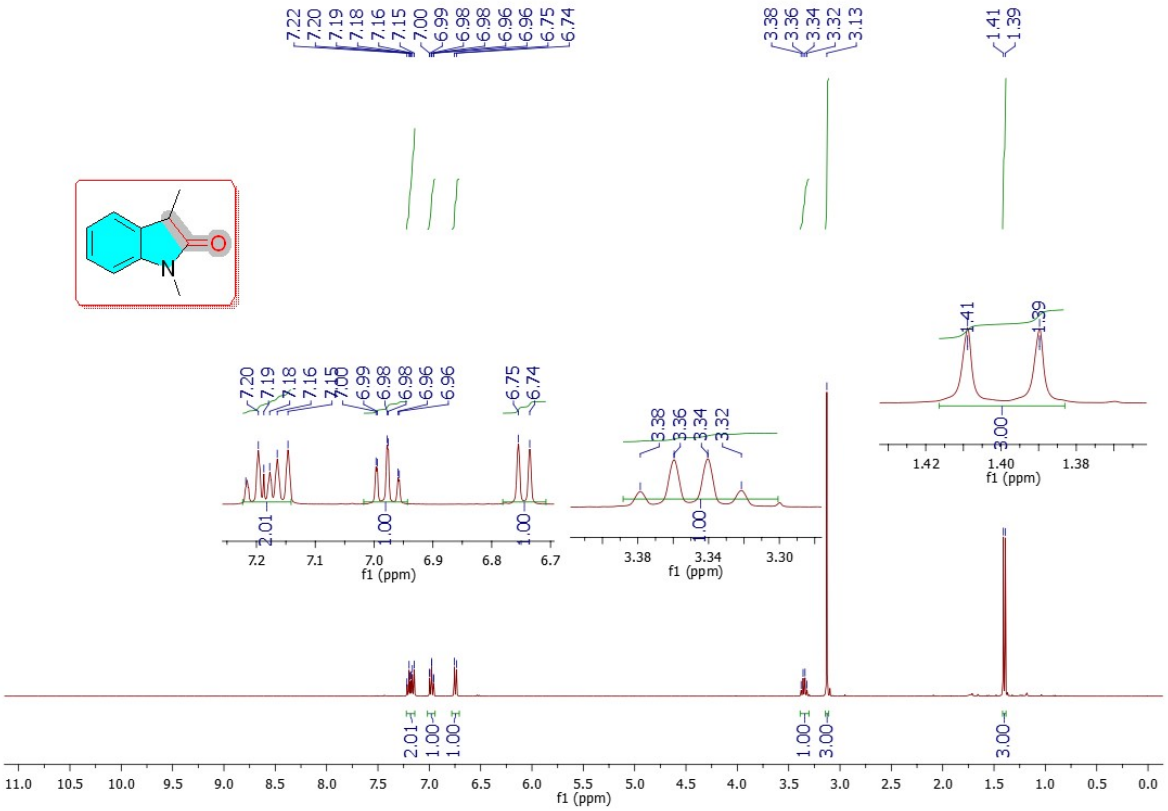


HRMS of 1-methyl-1*H*-benzo[d][1,2,3]triazole-5-carbaldehyde (2ak)

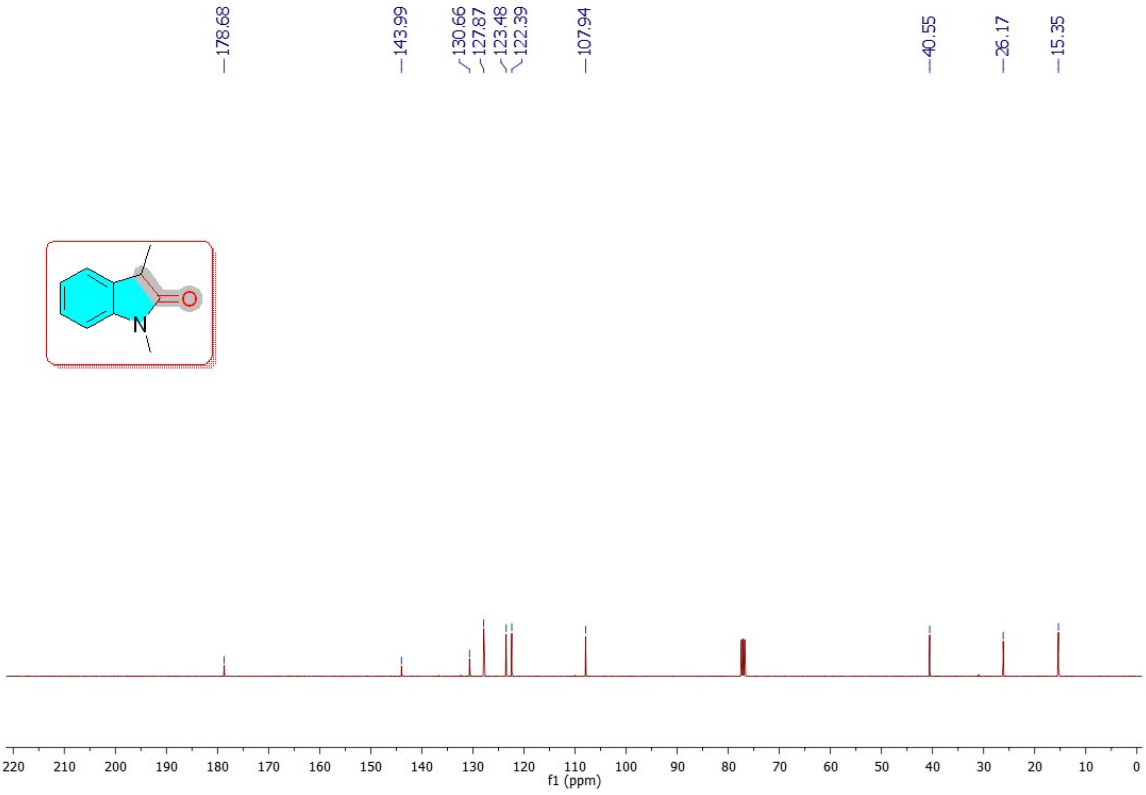


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
162.0668	162.0667	0.1	0.6	6.5	1792.3	n/a	n/a	C8 H8 N3 O

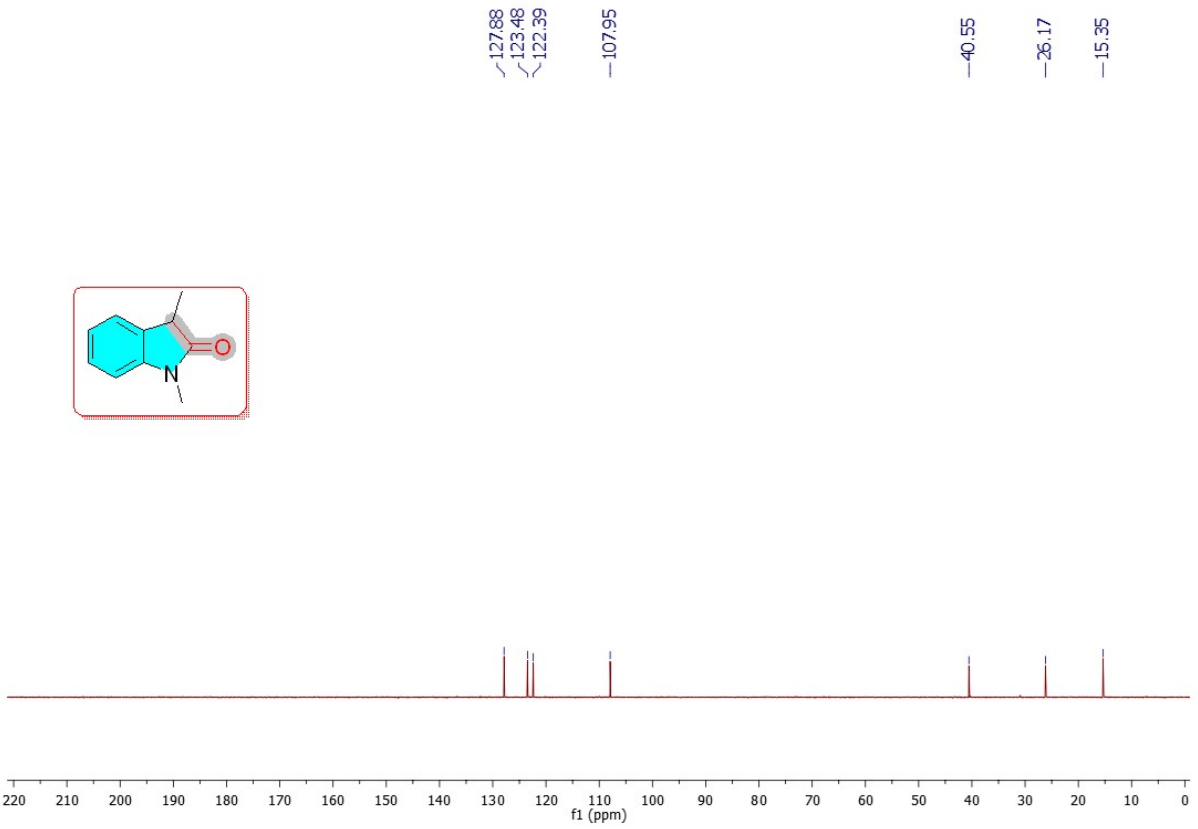
^{1}HNMR Spectra of 1,3-dimethylindolin-2-one (2al)[10]



^{13}C{^{1}H} NMR Spectra of 1,3-dimethylindolin-2-one (2al)[10]



DEPT Spectra of 1,3-dimethylindolin-2-one (2al)[10]

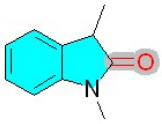


GCMS of 1,3-dimethylindolin-2-one (2al)

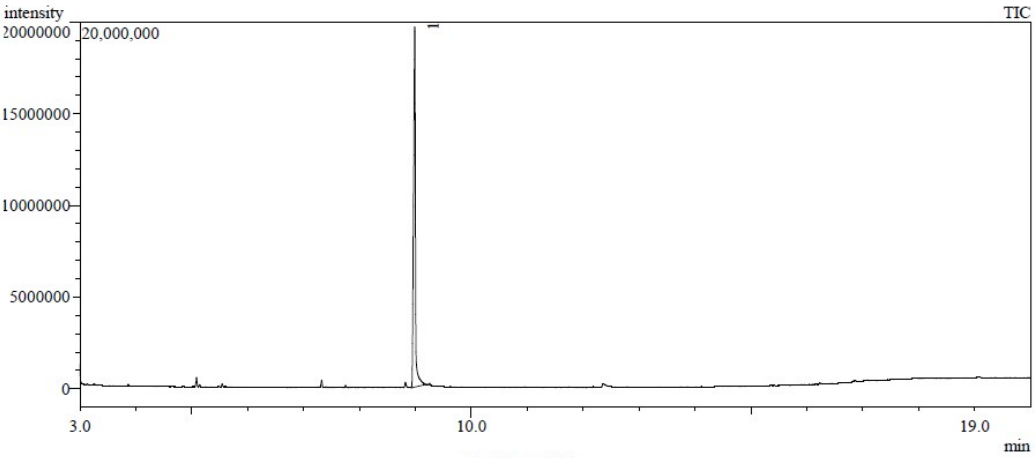
CSIR-INDIAN INSTITUTE OF INTEGRATIVE MEDICINE
Quality Management and Instrumentation Division
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 05-06-2024 11:09:49
Level #	: 1
Sample Name	: PPS-375
Sample ID	: PPS-375
Sample Amount	: 1
Vial #	: 2
Injection Volume	: 3.00
Data File	: D:\GCMS-2024\DATA\MAY-2024\05.06.2024-02.qgd
Method File	: D:\GCMS-2024\METHODS\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2024\TUNNING\03.01.2024-LIQ-5MS.qgt
$EndIf$Modified by	: System Administrator
Modified	: 05-06-2024 12:01:06



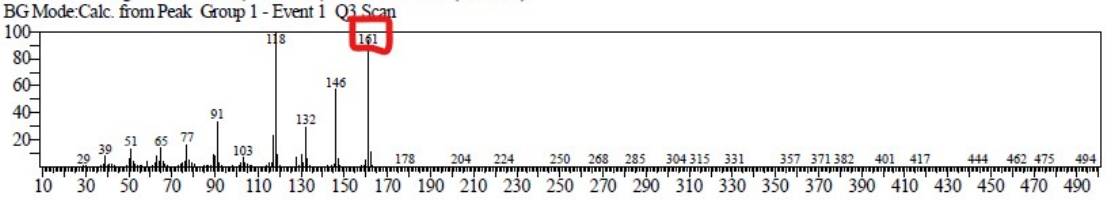
Chemical Formula: $C_{10}H_{11}NO$
Exact Mass: 161.0841



Peak Report TIC

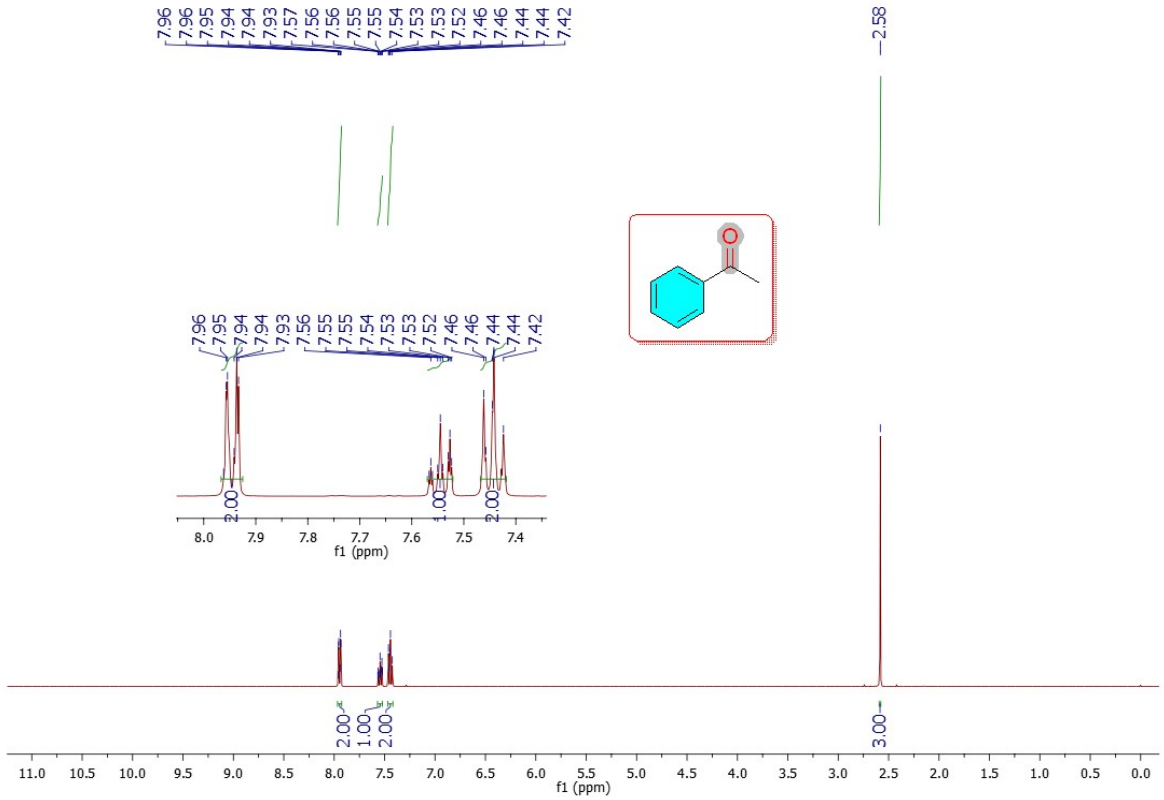
Peak#	R.Time	Area	Area%	Similarity	Name
1	8.987	46057957	100.00	96	2-Indolinone, N,O-dimethyl-
		46057957	100.00		

Library
<< Target >>
Line#:1 R.Time:8.985(Scan#:1198) MassPeaks:254
RawMode:Averaged 8.980-8.990(1197-1199) BasePeak:118.05(3522739)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan

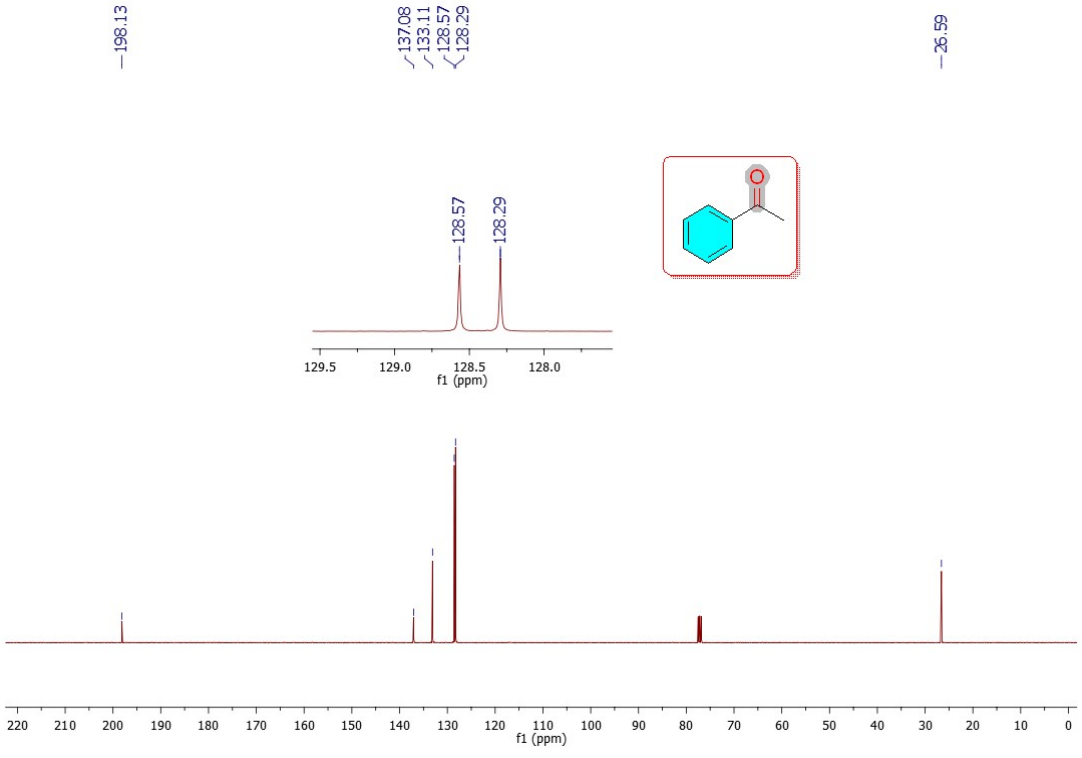


Spectral copies:

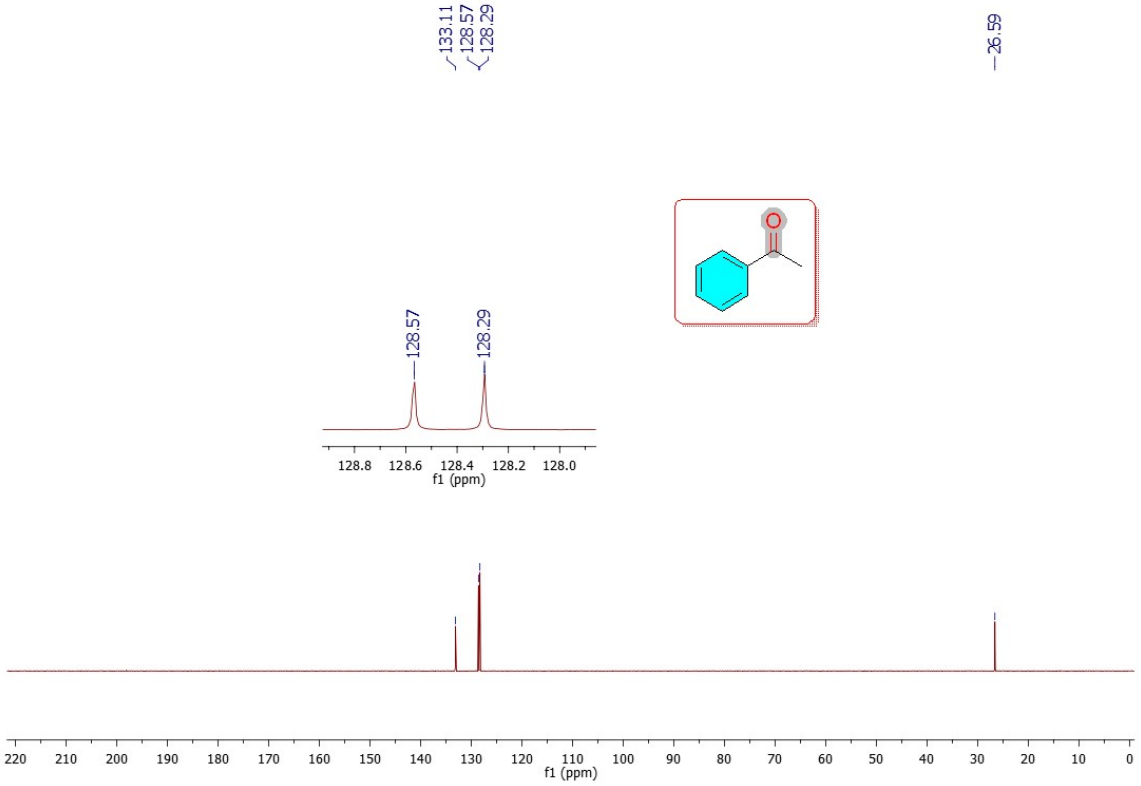
^{1}HNMR Spectra of Acetophenone (4a)[11]



^{13}C{^{1}H} NMR Spectra of Acetophenone (4a)[11]



DEPT Spectra of Acetophenone (4a)[11]

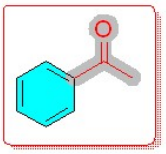


GCMS of Acetophenone (4a)

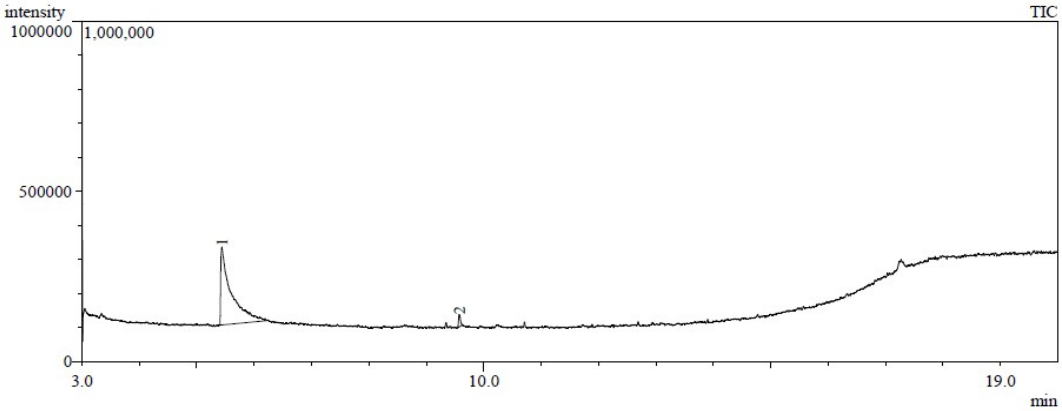
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 21-03-2023 22:04:09
Level #	: 1
Sample Name	: RA-1
Sample ID	: RA-1
Sample Amount	: 1
Vial #	: 6
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-26.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:12:00



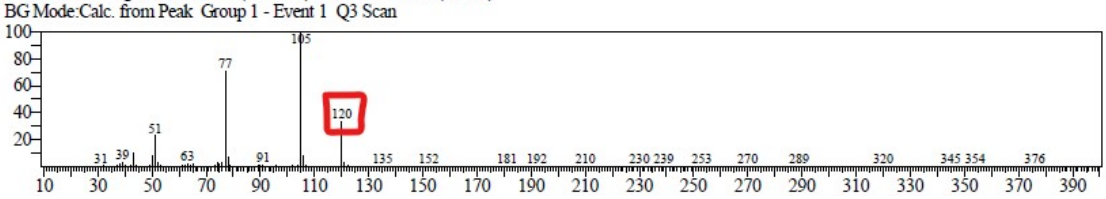
Chemical Formula: C_8H_8O
Exact Mass: 120.06



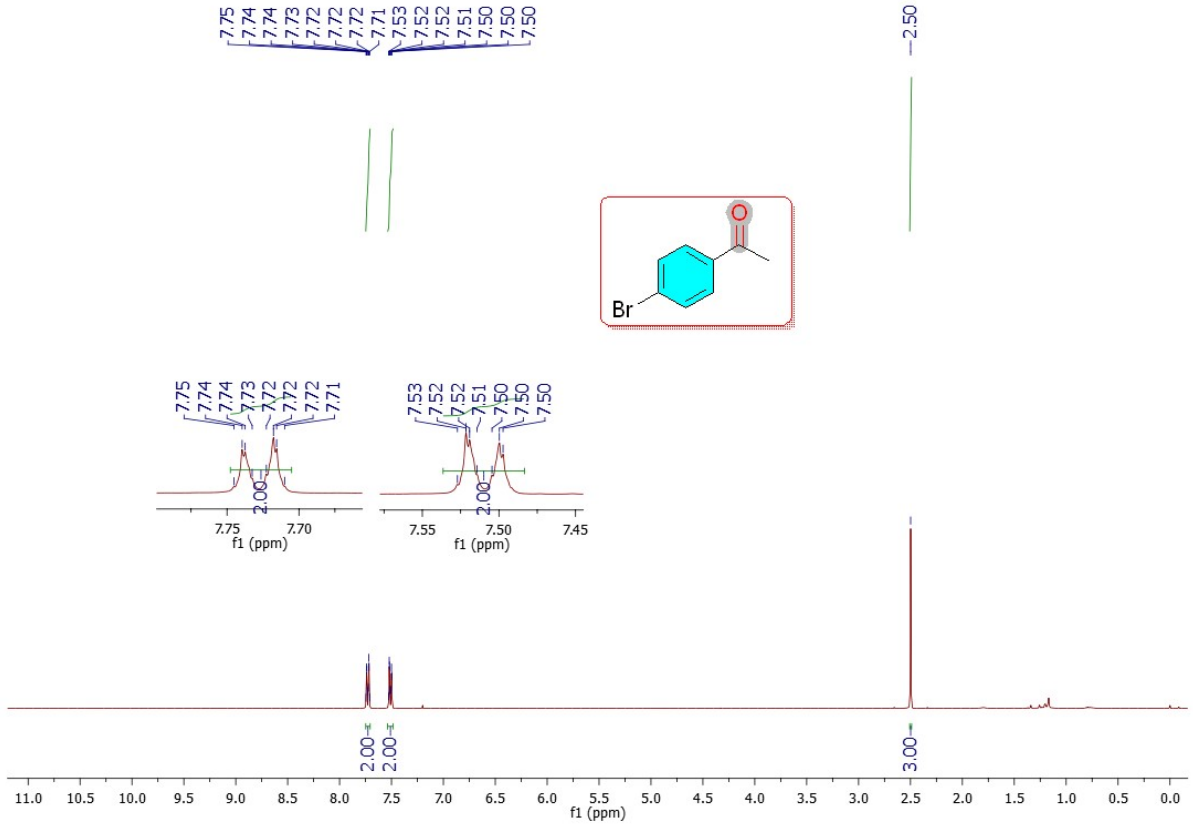
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	5.436	2896668	97.35	98	105.00	Acetophenone
2	9.575	78803	2.65	93	191.10	2,4-Di-tert-butylphenol
		2975471	100.00			

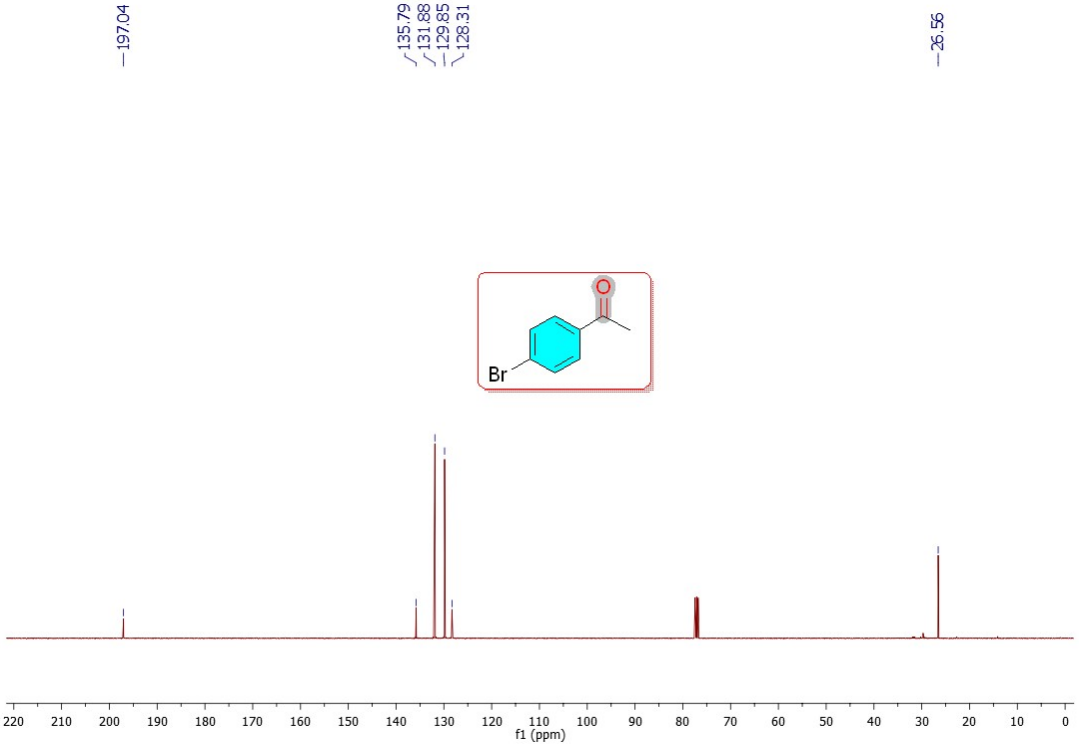
<< Target >>
Line#:1 R.Time:5.435(Scan#:488) MassPeaks:190
RawMode:Averaged 5.430-5.440(487-489) BasePeak:105.00(78674)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



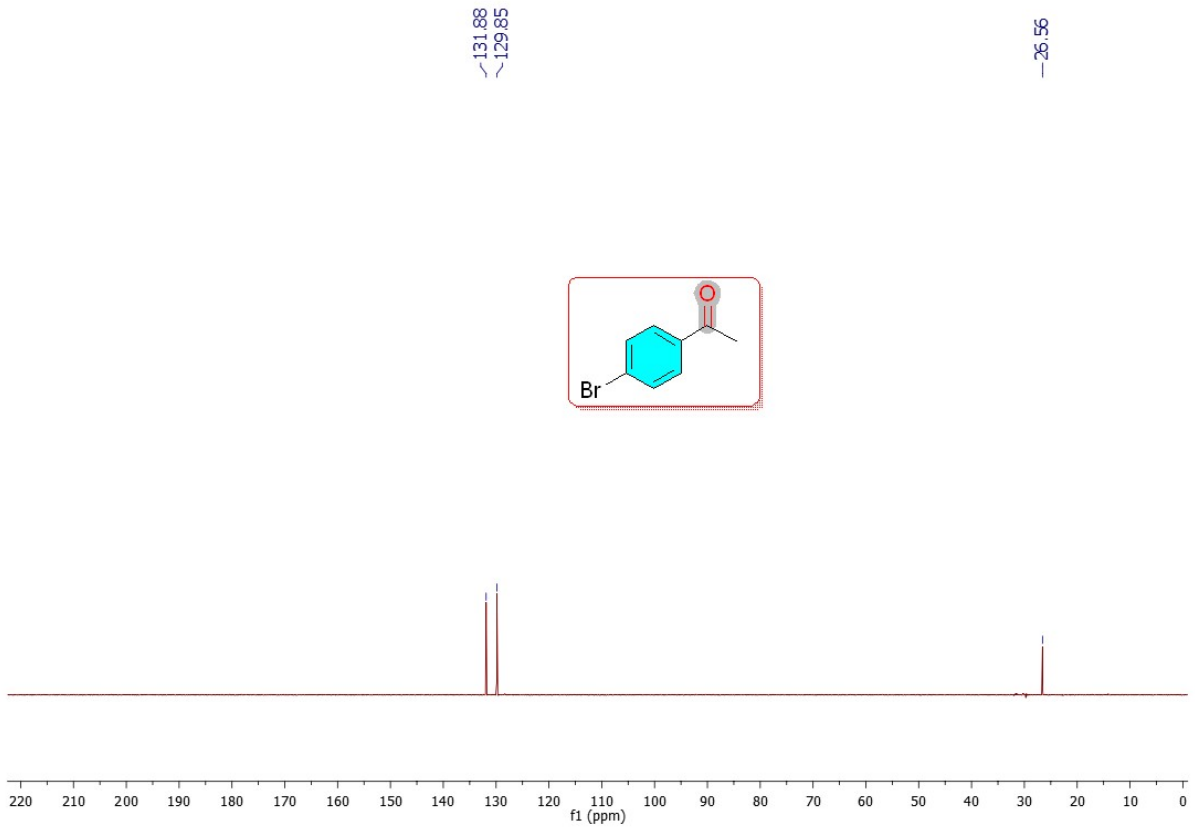
[1]HNMR Spectra of 4- Bromoacetophenone (4b)[11]



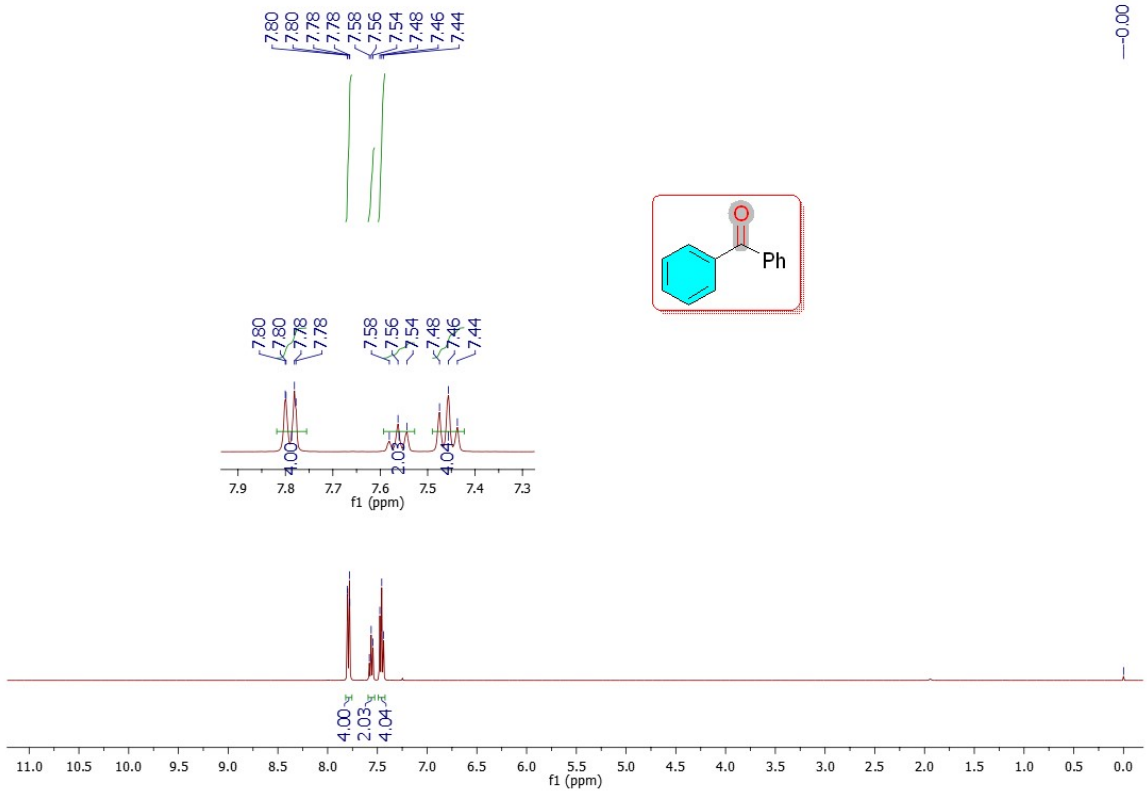
[13]C{[1]H} NMR Spectra of 4- Bromoacetophenone (4b)[11]



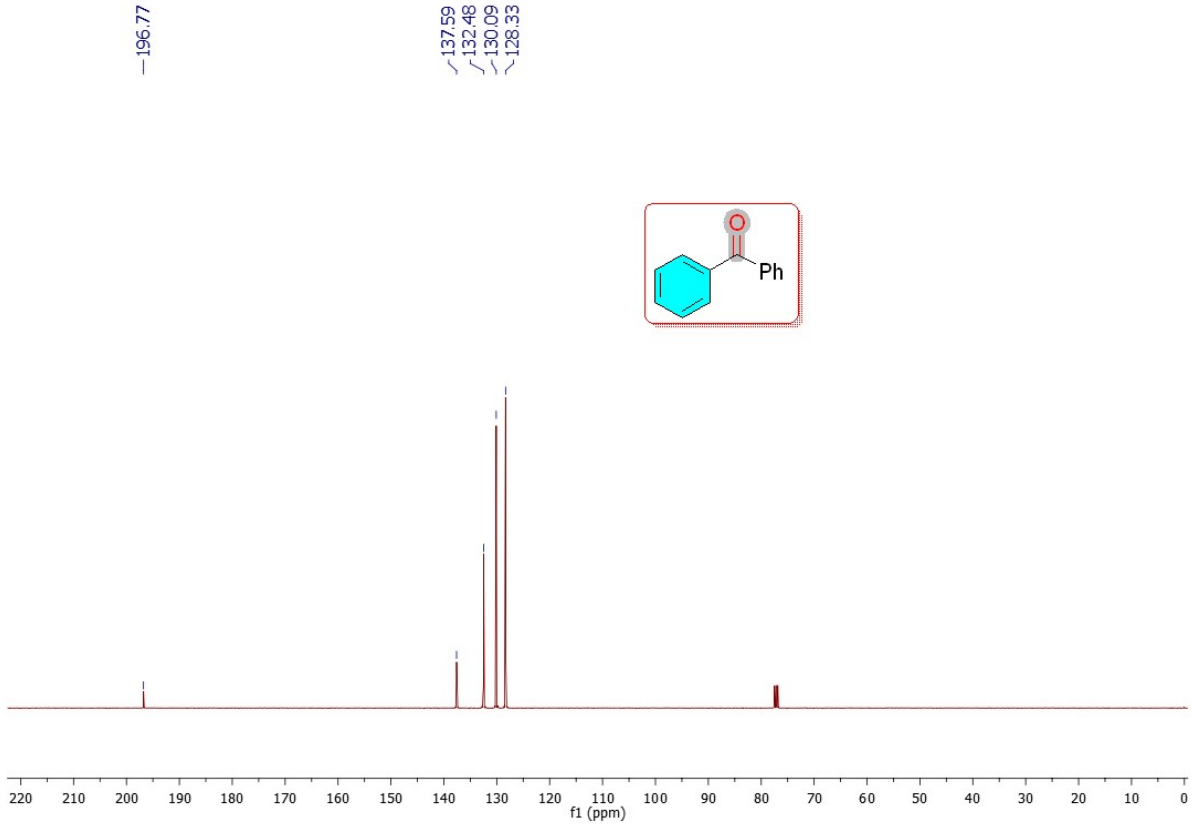
DEPT Spectra of 4- Bromoacetophenone (4b)[11]



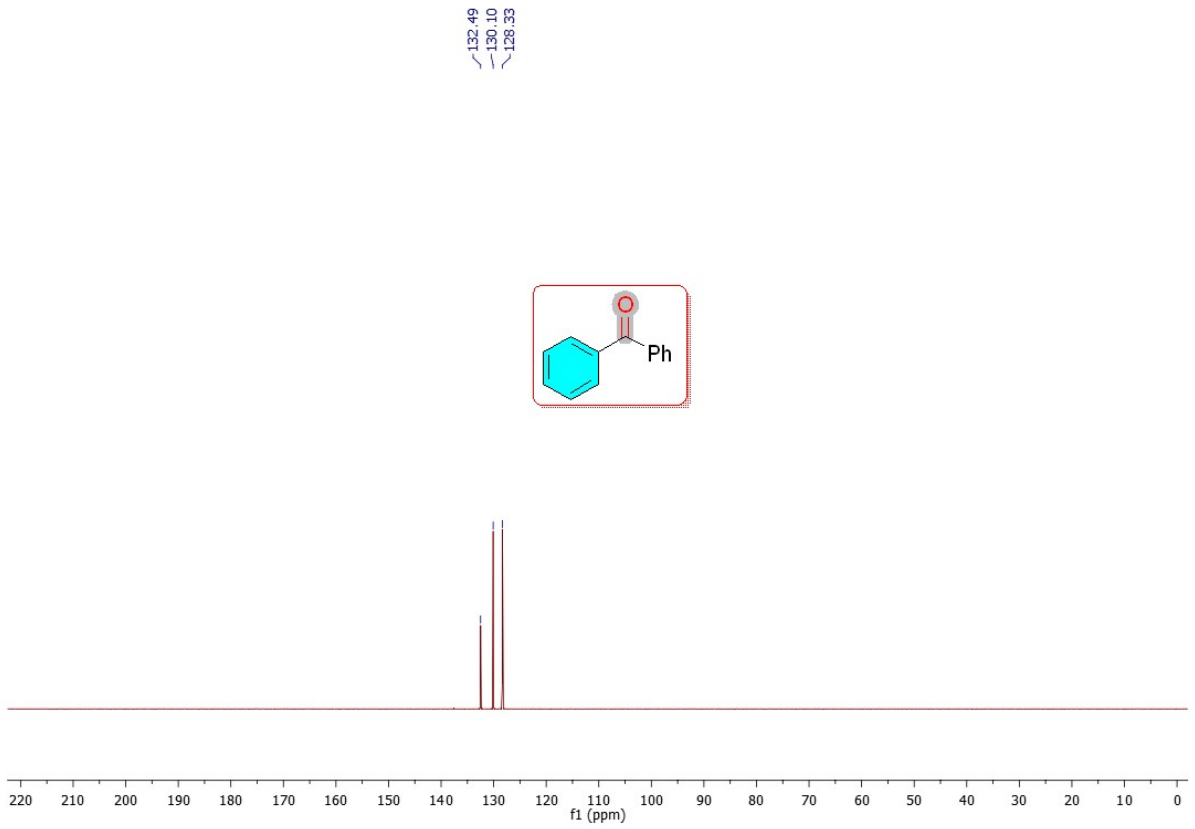
[1]HNMR Spectra of Benzophenone (4c)[2]



$^{13}C\{^{1}H\}$ NMR Spectra of Benzophenone (4c)[2]

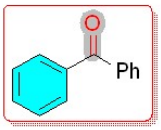


DEPT Spectra of Benzophenone (4c)[2]



GCMS of Benzophenone (4c)

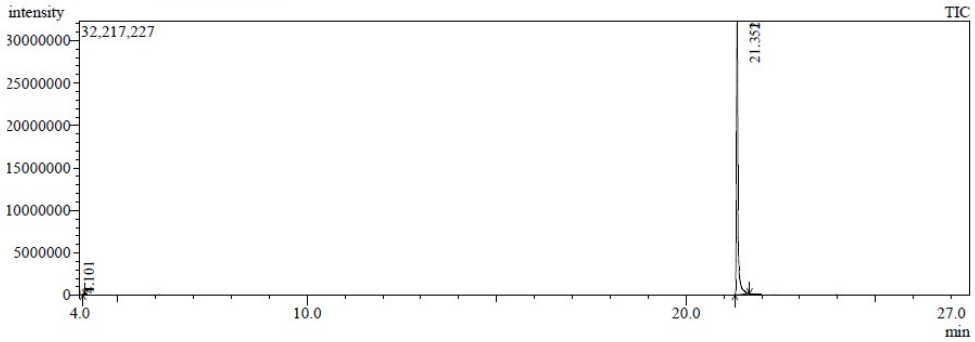
IIIM GCMS ANALYSIS



Chemical Formula: $C_{13}H_{10}O$
Exact Mass: 182.07
Molecular Weight: 182.22

Sample Information

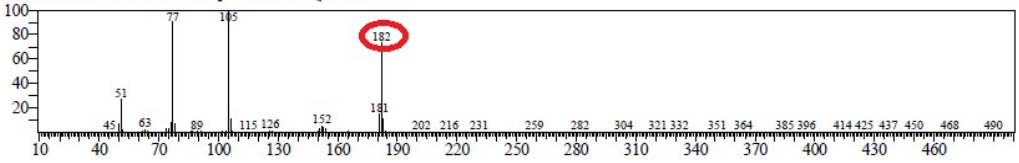
Analyzed by	: Admin
Analyzed	: 2/17/2022 12:11:19 AM
Level #	: 1
Sample Name	: Method-38
Sample ID	:
Sample Amount	: 1
Vial #	: 9
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\FEB 2022\16.02.2022\16.02.2022 BHARTI037.qgd
Method File	: D:\GCMS METHOD\GC MS METHOD PP SIR.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
$EndIf$Modified by	: Admin
Modified	: 2/18/2022 12:15:14 PM



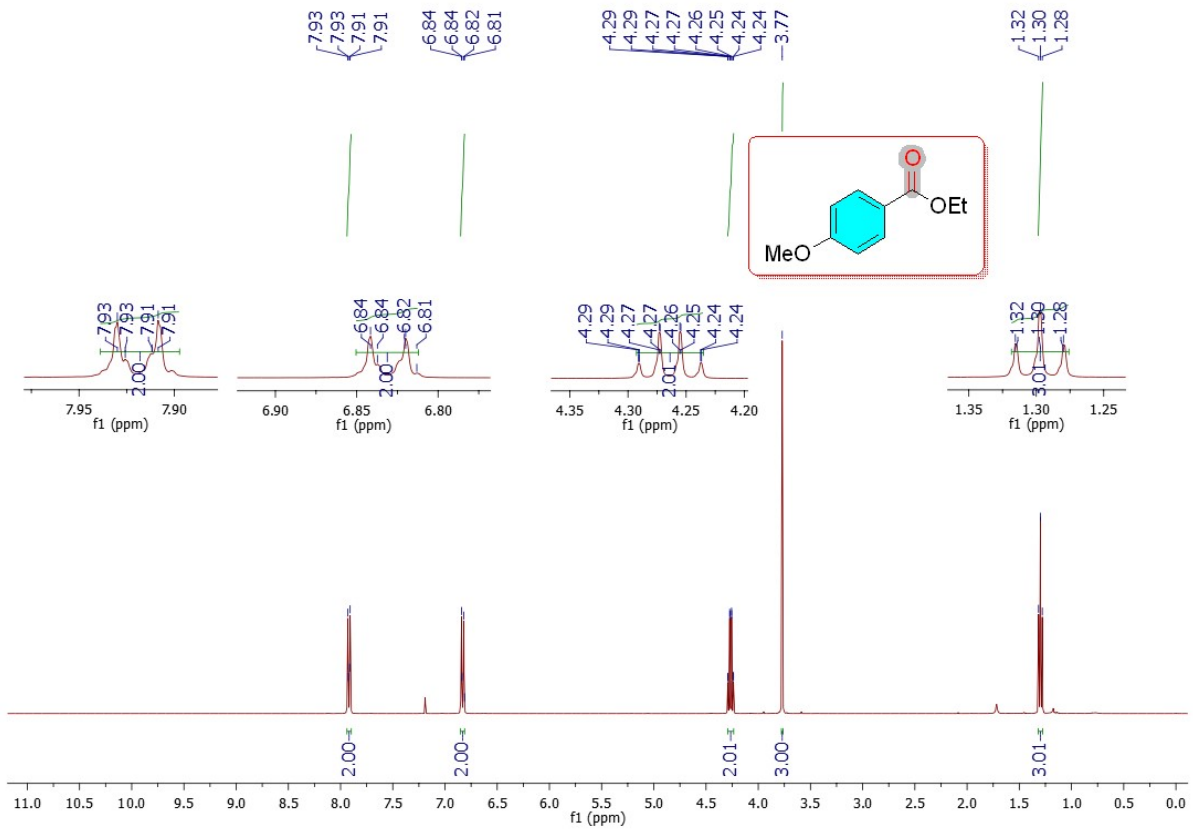
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	4.101	191871	0.22	124488	0.39	96	57.00	Propanoic acid, ethyl ester
2	21.351	88265248	99.78	32155421	99.61	93	105.05	Benzophenone
		88457119	100.00	32279909	100.00			

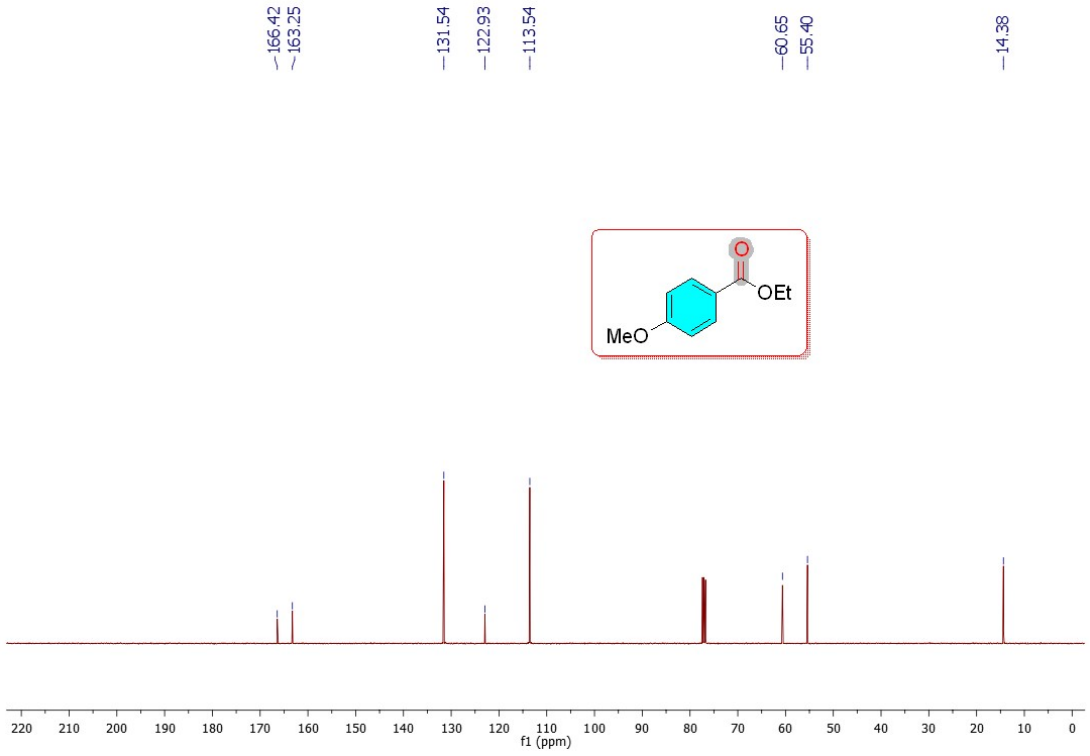
<< Target >>
Line#:2 R.Time:21.350(Scan#:3471) MassPeaks:272
RawMode:Averaged 21.345-21.355(3470-3472) BasePeak:105.05(8145535)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



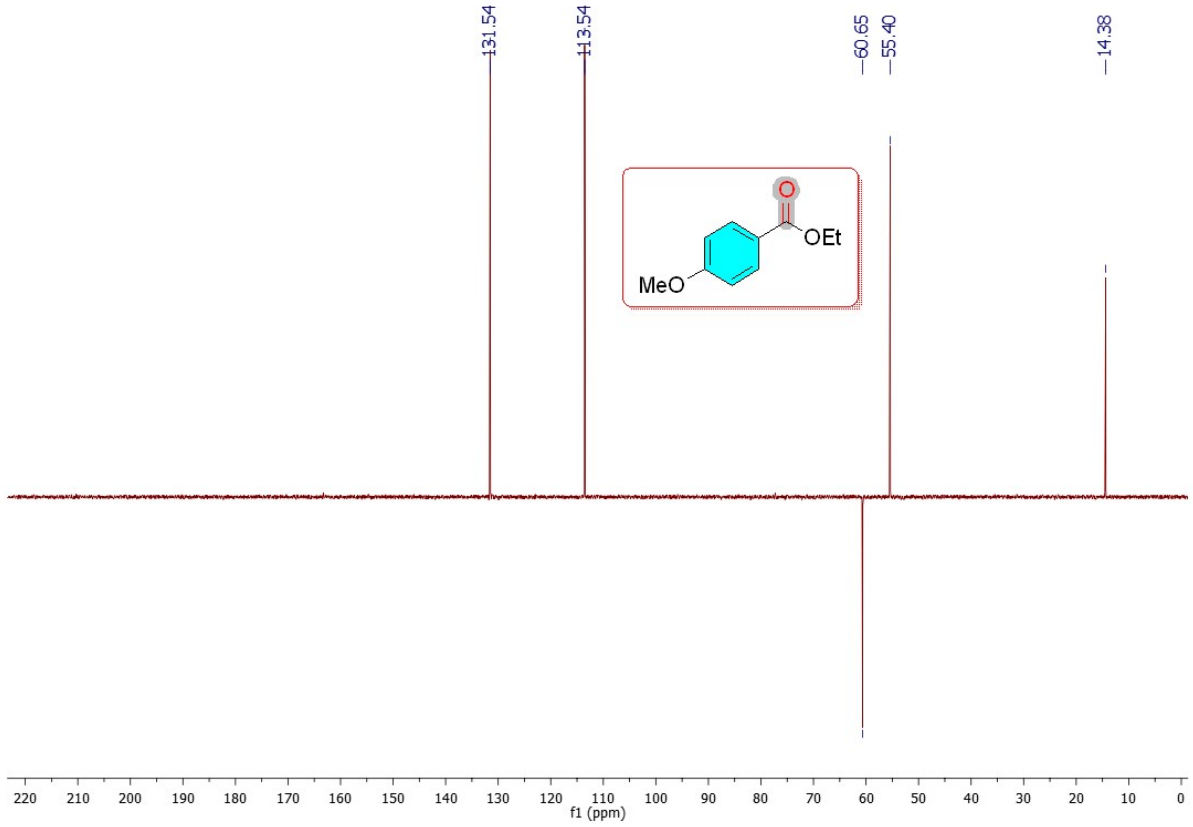
^{1}HNMR Spectra of Ethyl-4-methoxy benzoate (4d)[12]



^{13}C{^{1}H} NMR Spectra of Ethyl-4-methoxy benzoate (4d)[12]



DEPT Spectra of Ethyl-4-methoxy benzoate (4d)[12]

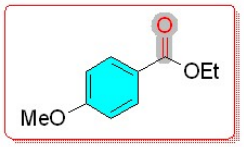


GCMS of Ethyl-4-methoxy benzoate (4d)

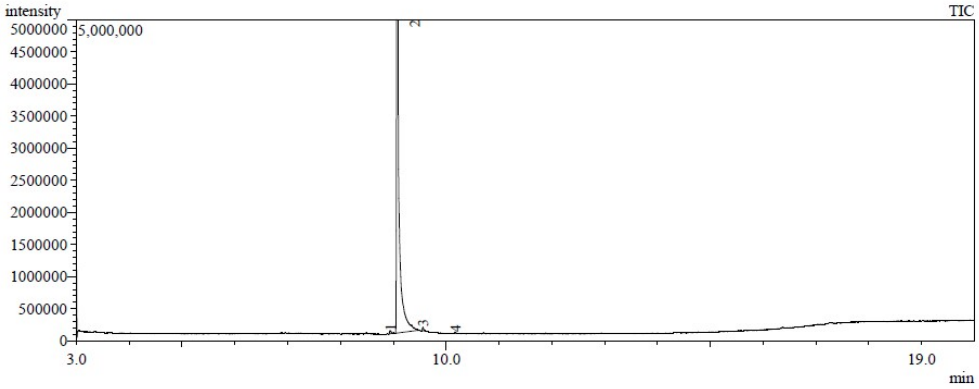
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 21-03-2023 22:56:22
Level #	: 1
Sample Name	: RA-3
Sample ID	: RA-3
Sample Amount	: 1
Vial #	: 8
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-28.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:14:06



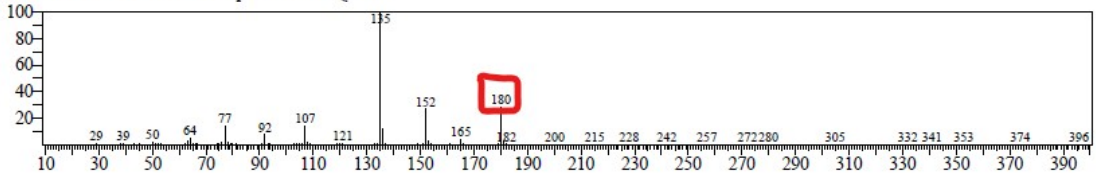
Chemical Formula: $C_{10}H_{12}O_3$
Exact Mass: 180.08



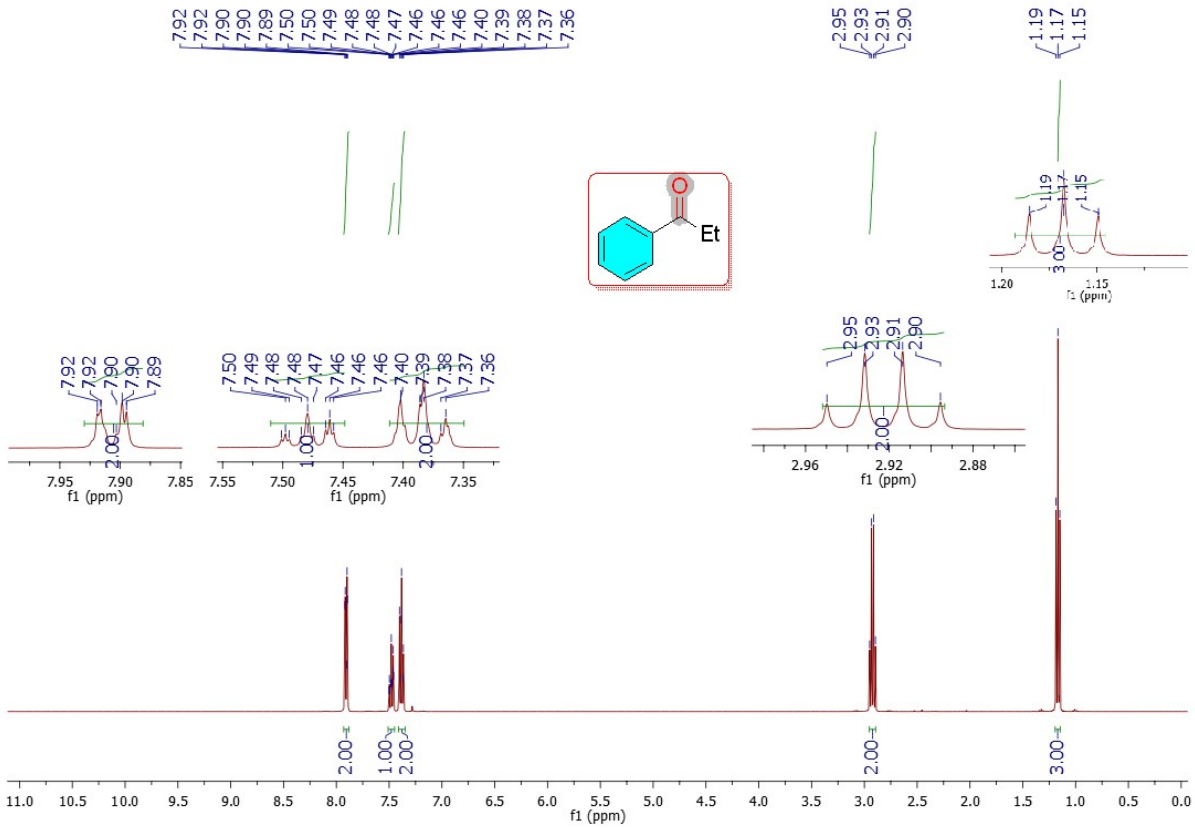
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	8.940	86642	0.25	81	135.00	4-Methoxybenzoic acid, 2,4,5-trichlorophenyl ester
2	9.075	34808525	99.42	96	135.05	Benzoic acid, 4-methoxy-, ethyl ester
3	9.562	82314	0.24	92	191.10	2,4-Di-tert-butylphenol
4	10.171	32564	0.09	91	57.05	n-Nonadecanol-1
		35010045	100.00			

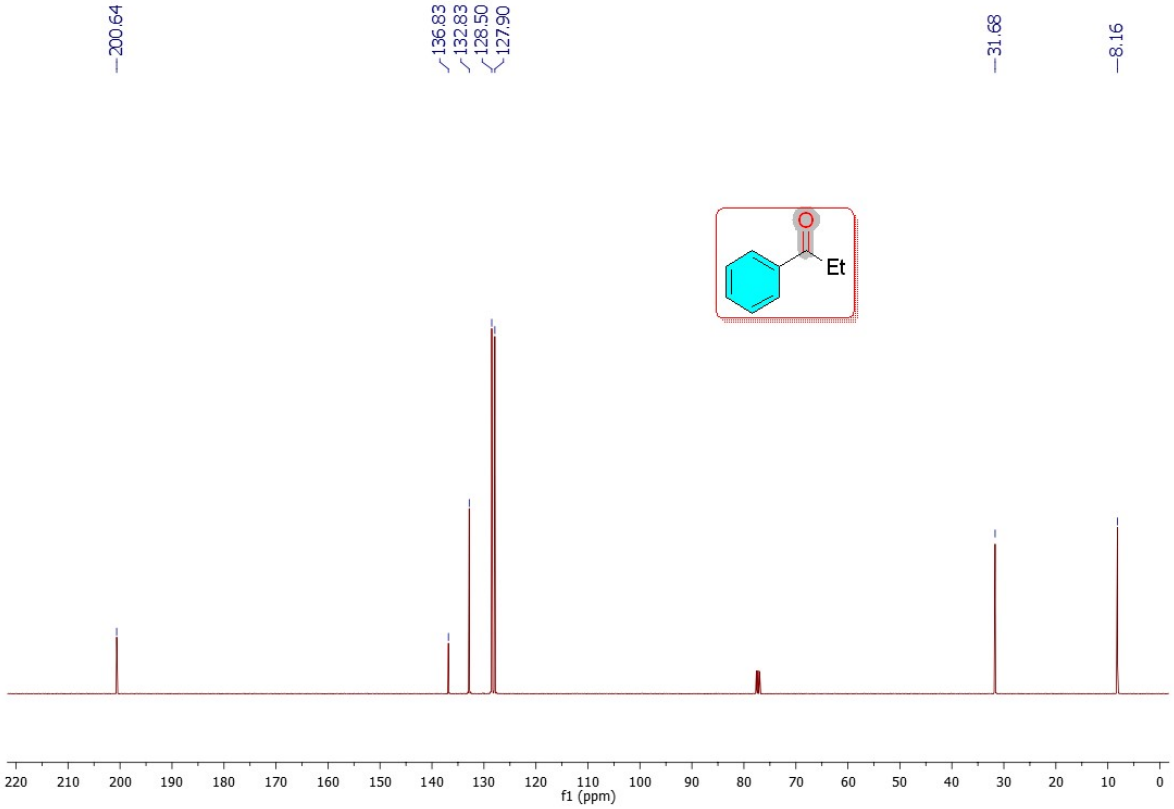
<< Target >>
Line#:2 R.Time:9.075(Scan#:1216) MassPeaks:251
RawMode:Averaged 9.070-9.080(1215-1217) BasePeak:135.05(6911432)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



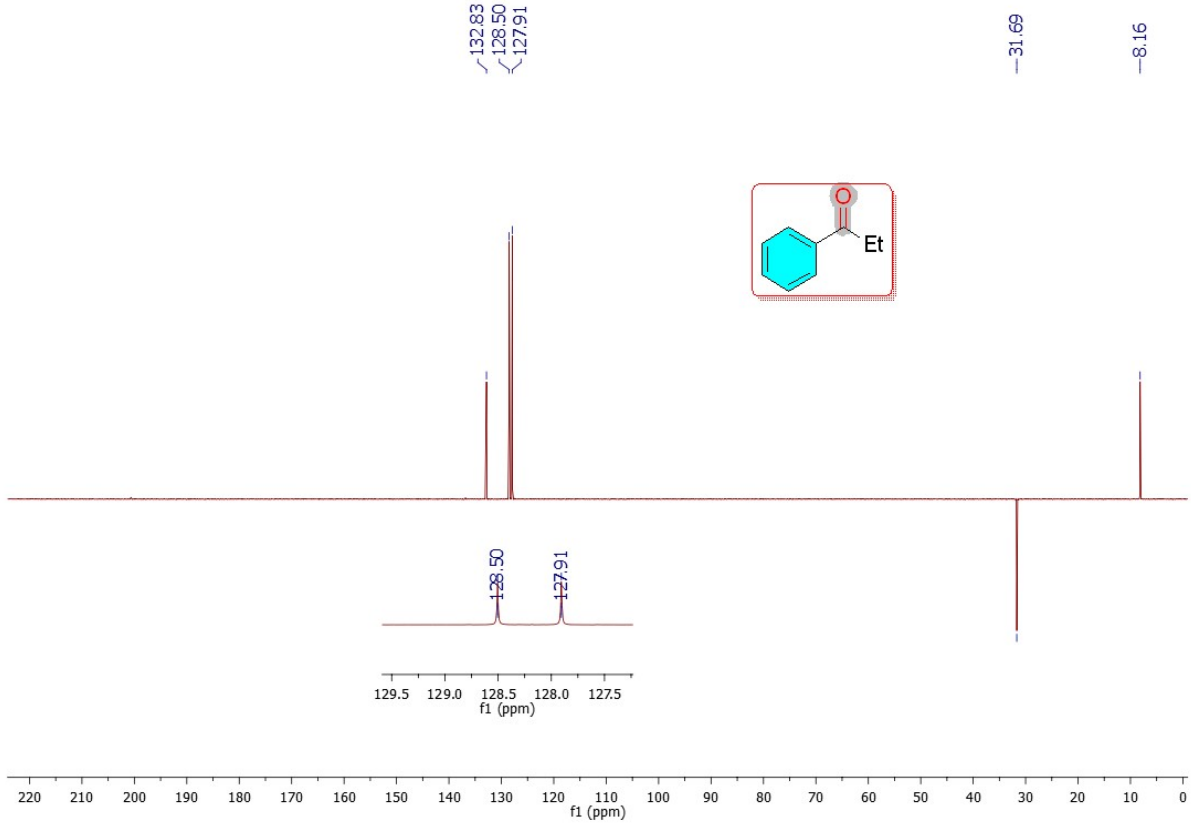
^{1}HNMR Spectra of Propiophenone (4e)[13]



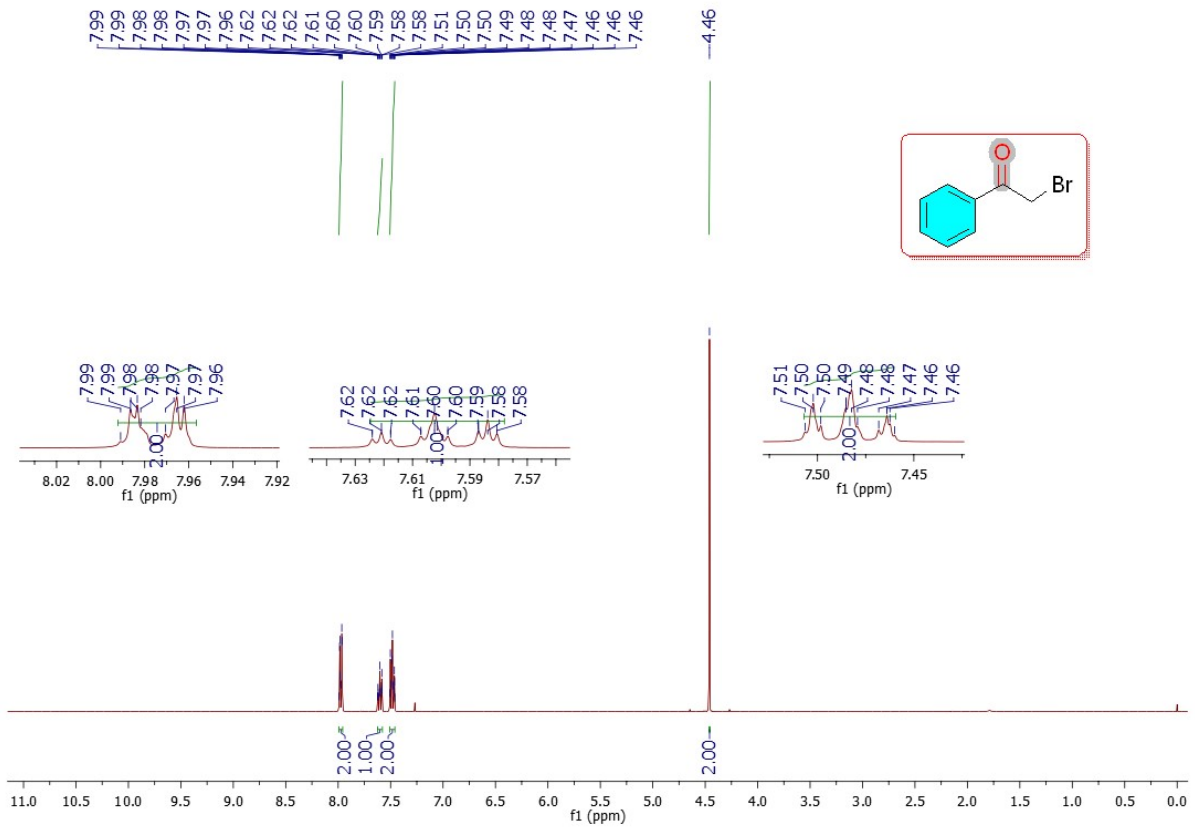
$^{13}C\{^{1}H\}$ NMR Spectra of Propiophenone (4e)[13]



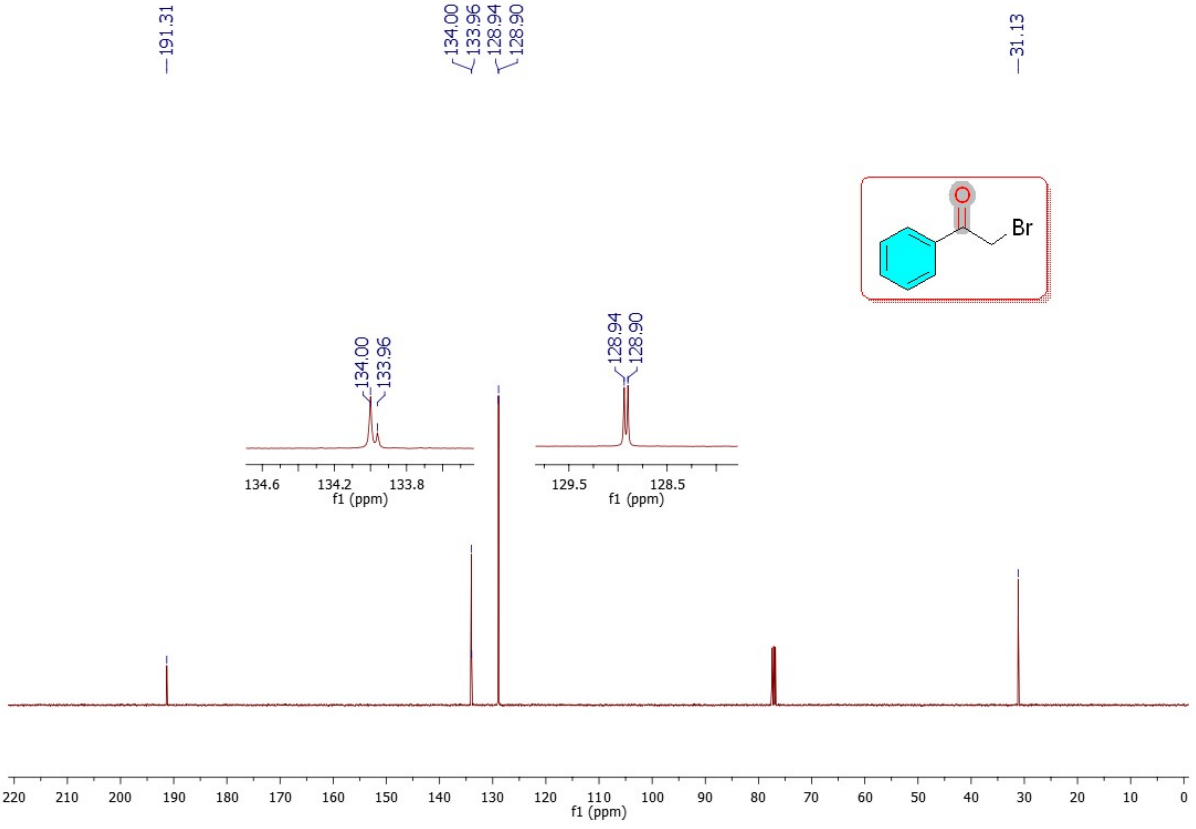
DEPT Spectra of Propiophenone (4e)[13]



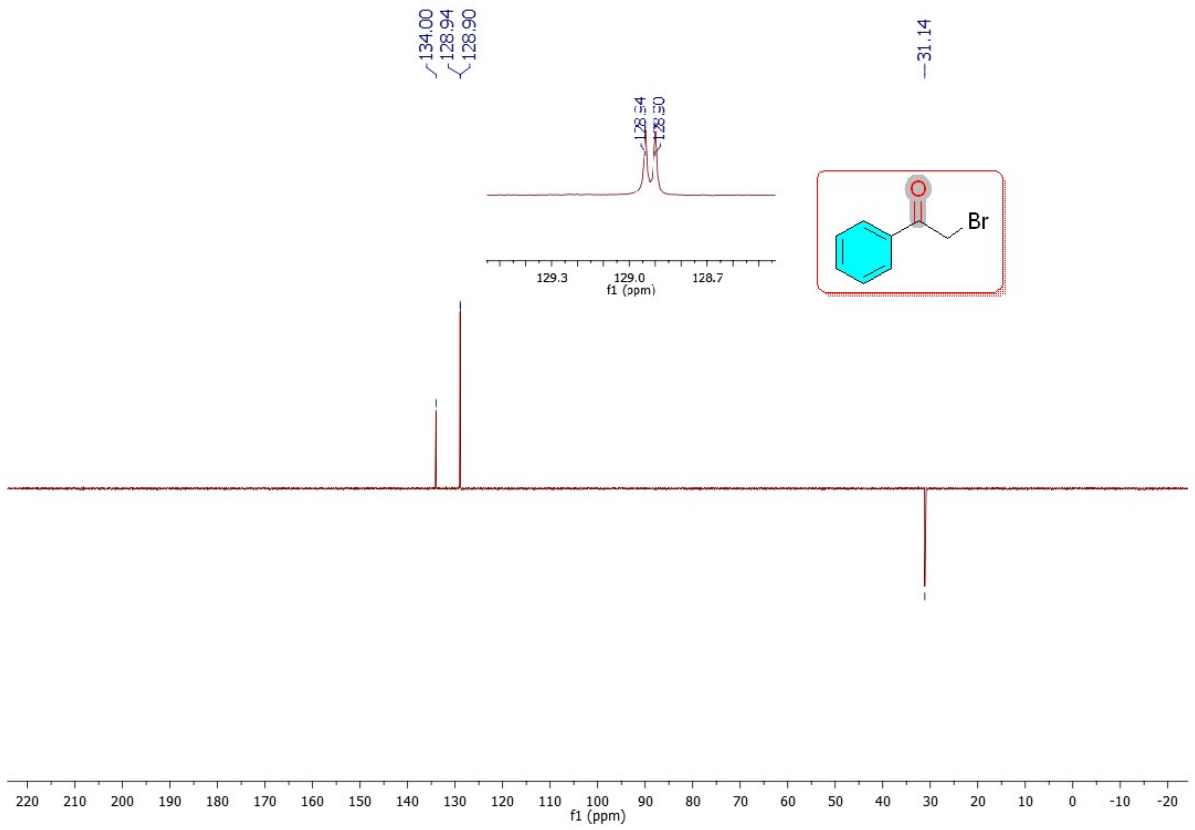
^{1}HNMR Spectra of 2-Bromo-1-phenylethan-1-one (4f)[14]



$^{13}C\{^{1}H\}$ NMR Spectra of 2-Bromo-1-phenylethan-1-one (4f)[14]



DEPT Spectra of 2-Bromo-1-phenylethan-1-one (4f)[14]

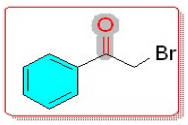


GCMS of 2-Bromo-1-phenylethan-1-one (4f)

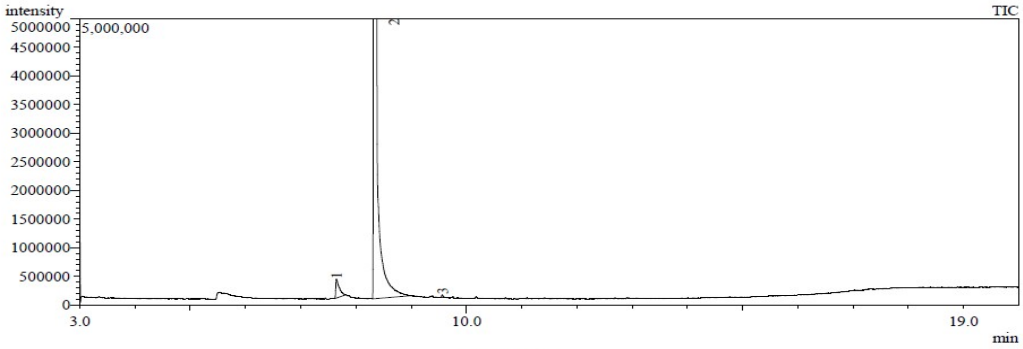
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 21-03-2023 23:48:34
Level #	: 1
Sample Name	: RA-5
Sample ID	: RA-5
Sample Amount	: 1
Vial #	: 10
Injection Volume	: 0.50
Data File	: D:\GCMS-2023\Data\Mar-2023\21.03.2023-30.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\06.Mar.2023_Liquid.qgt
$EndIf$Modified by	: System Administrator
Modified	: 22-03-2023 12:15:39



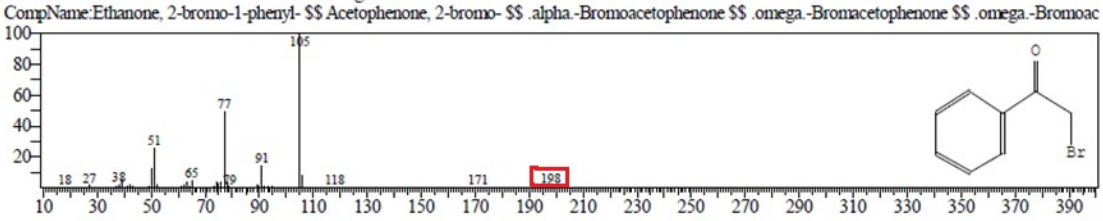
Chemical Formula: C_8H_7BrO
Exact Mass: 197.97



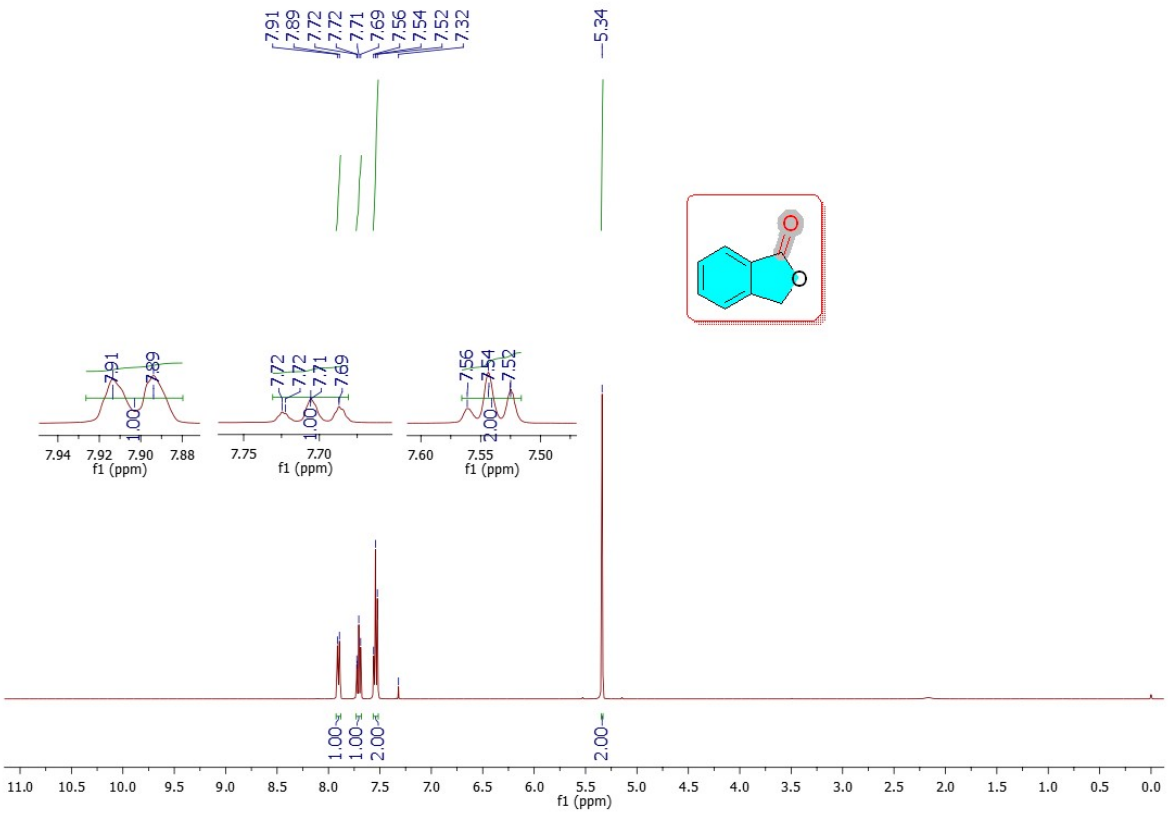
Peak Report TIC

Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	7.645	1491815	1.73	98	105.00	Acetophenone, 2-chloro-
2	8.363	84514720	98.19	94	105.15	Ethanone, 2-bromo-1-phenyl-
3	9.564	63928	0.07	91	191.10	2,4-Di-tert-butylphenol
		86070463	100.00			

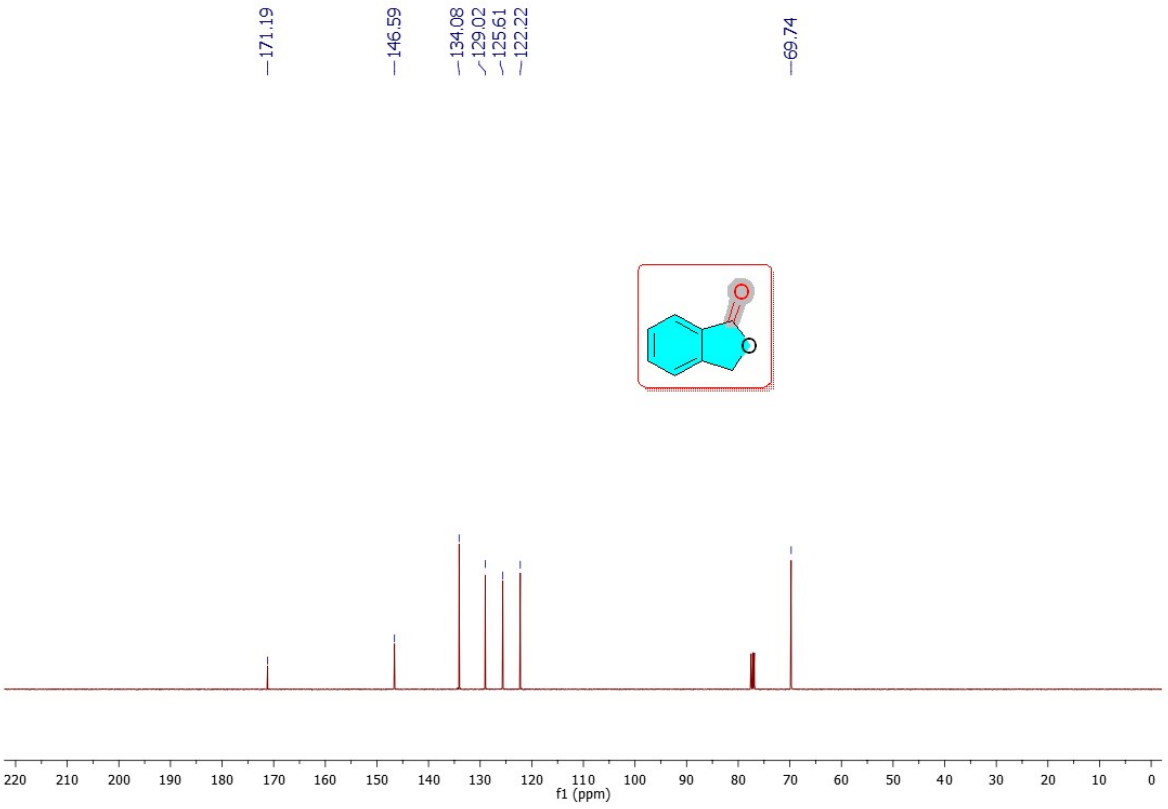
Hit#:1 Entry:47463 Library:NIST17M1.lib
SI:94 Formula:C8H7BrO CAS:70-11-1 MolWeight:198 RetIndex:1325
CompName:Ethanone, 2-bromo-1-phenyl- $$ Acetophenone, 2-bromo- $$ .alpha.-Bromoacetophenone $$ .omega.-Bromacetophenone $$ .omega.-Bromoac



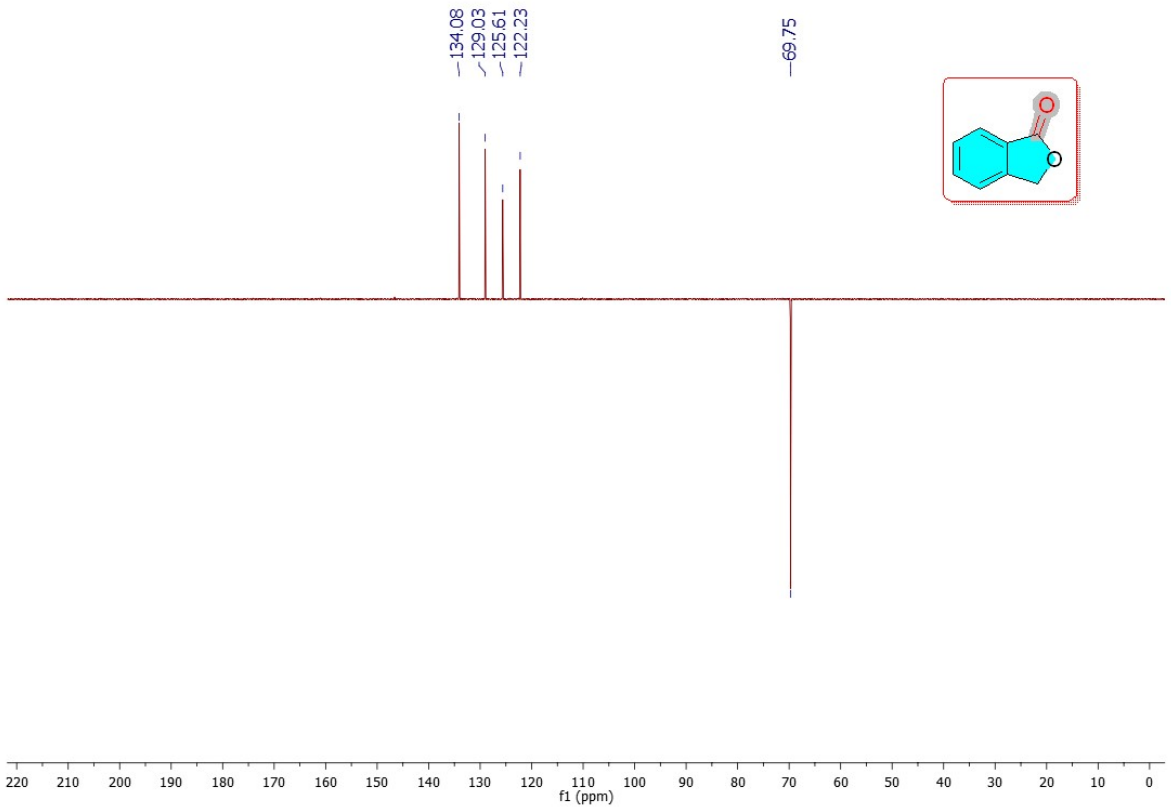
[1]HNMR Spectra of Isobenzofuran-1(3H)-one (4g)[15]



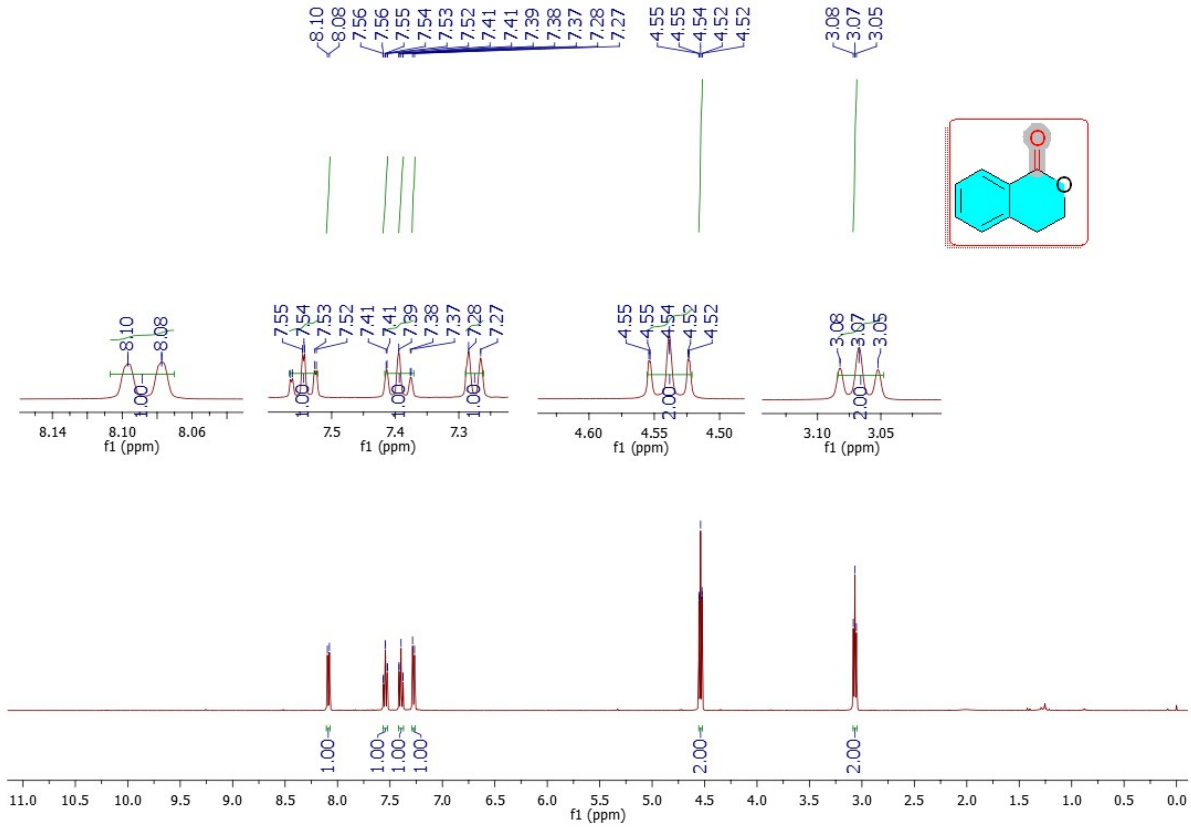
$^{13}C\{^{1}H\}$ NMR Spectra of Isobenzofuran-1(3H)-one (4g)[15]



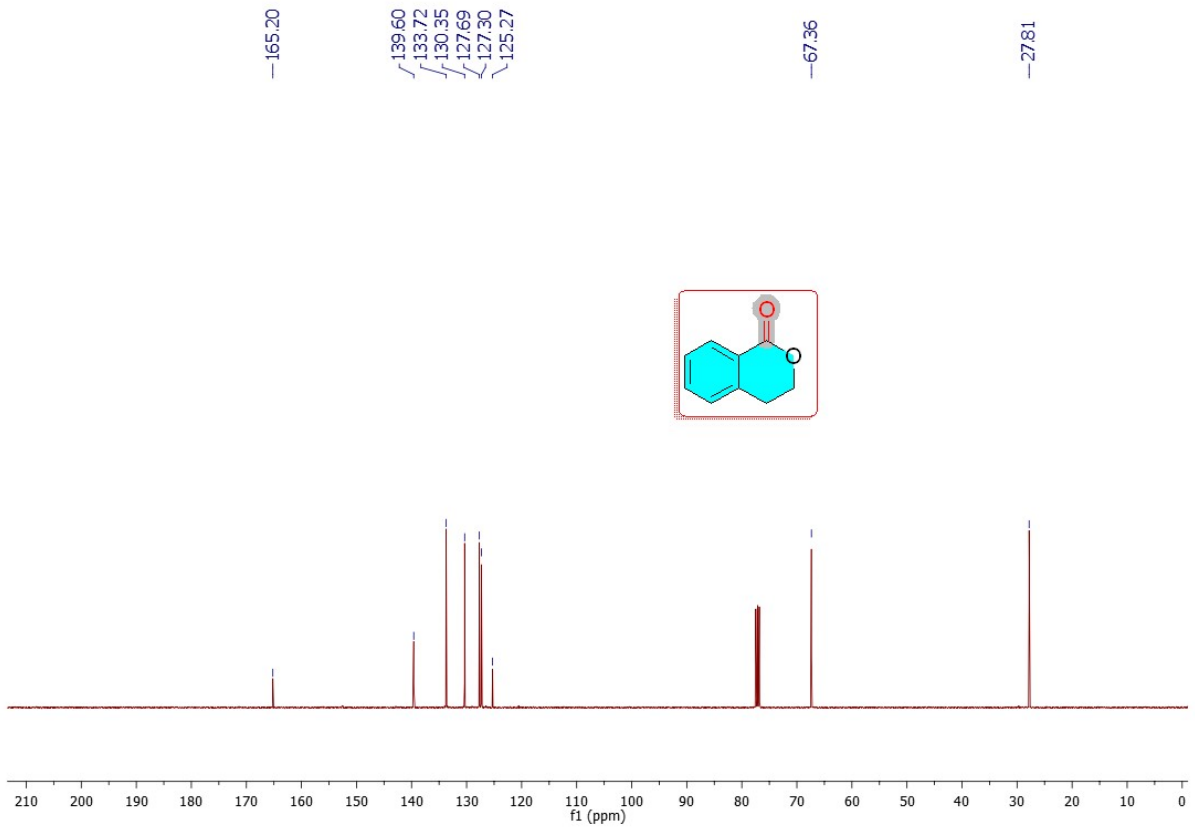
DEPT Spectra of Isobenzofuran-1(3H)-one (4g)[15]



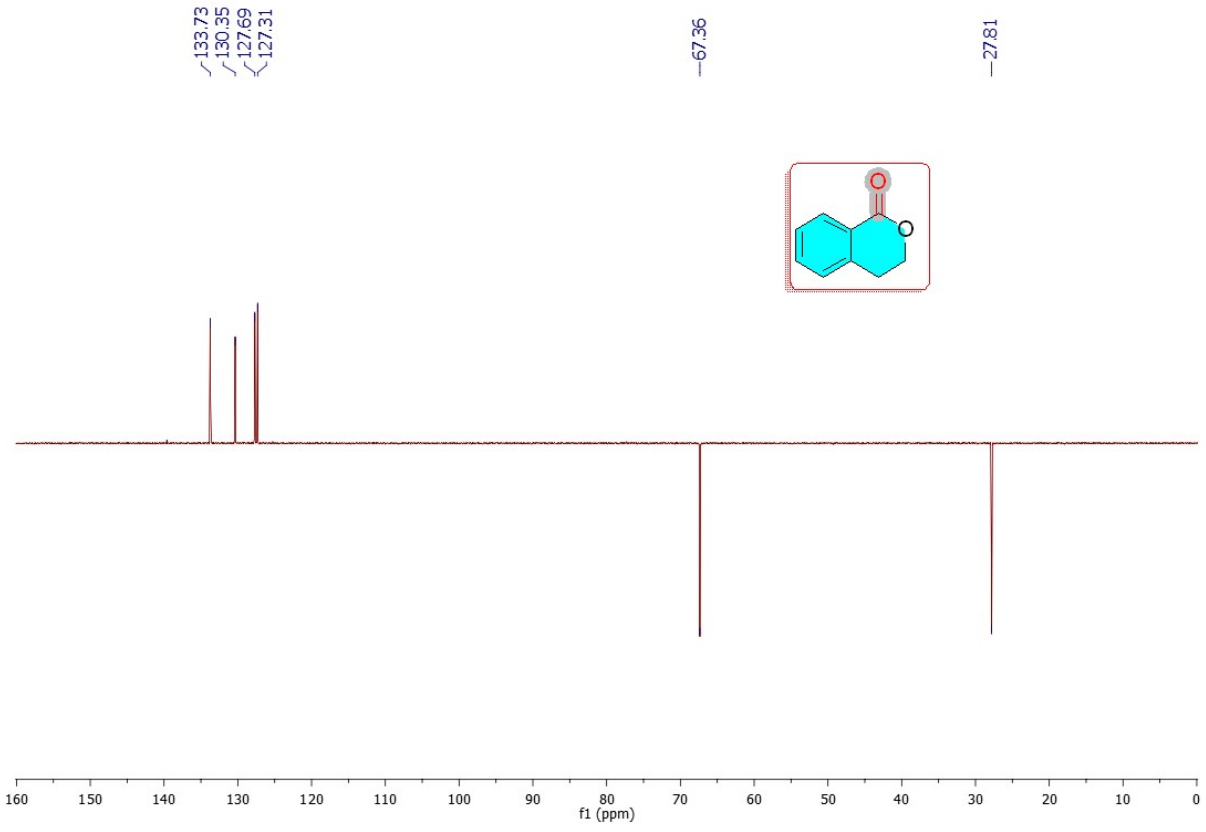
^{1}HNMR Spectra of Isochroman-1-one (4h)[11]



^{13}C{^{1}H} NMR Spectra of Isochroman-1-one (4h)[11]



DEPT Spectra of Isochroman-1-one (4h)[11]

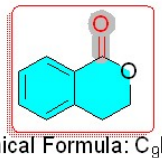


GCMS of Isochroman-1-one (4h)

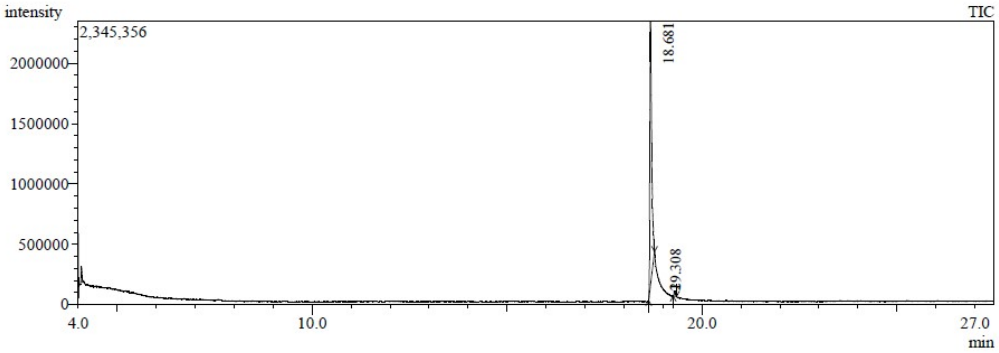
IIIM GCMS ANALYSIS

Sample Information

Analyzed by	: Admin
Analyzed	: 3/8/2022 1:36:16 PM
Level #	: 1
Sample Name	: ISO-2
Sample ID	:
Sample Amount	: 1
Vial #	: 5
Injection Volume	: 0.50
Data File	: D:\GCMS DATA\LIQUID\MARCH 2022\08.03.2022\08.03.2022 BHARTI006.qgd
Method File	: D:\GCMS METHOD\GC MS METHOD PP SIR.qgm
Tuning File	: D:\Tuning\Tuning-NM-F1 18.01.2022.qgt
$EndIf$Modified by	: Admin
Modified	: 3/8/2022 2:36:15 PM



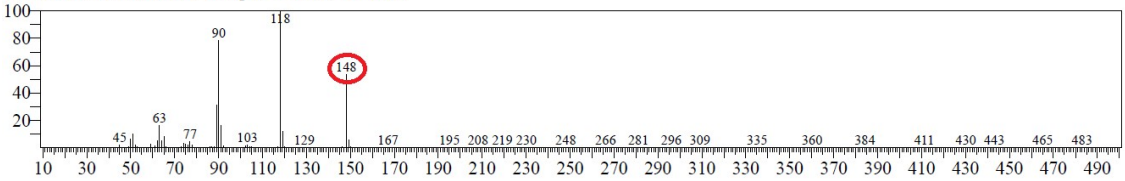
Chemical Formula: $C_9H_8O_2$
Exact Mass: 148.05
Molecular Weight: 148.16



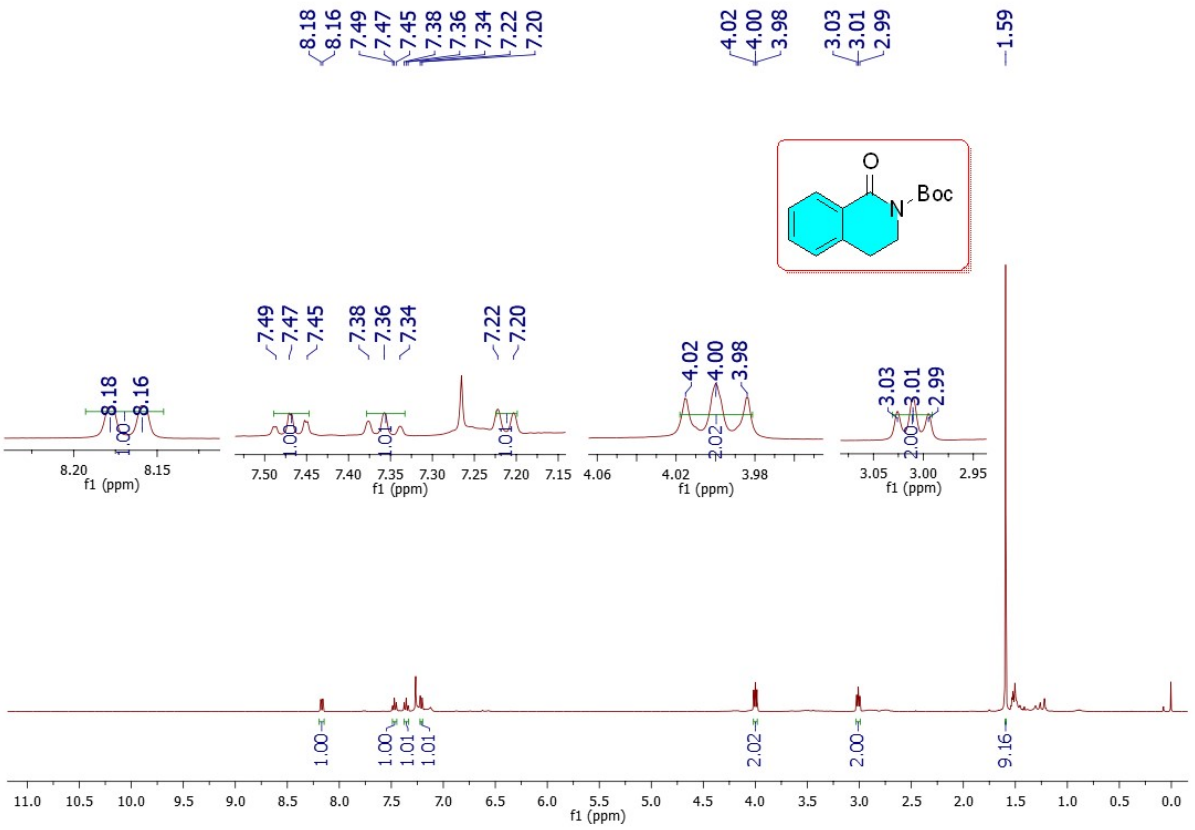
Peak Report TIC

Peak#	R.Time	Area	Area%	Height	Height%	Similarity	Base m/z	Name
1	18.681	7511297	98.71	2186163	98.10	83	118.05	Oxazolidin-4-one, 5-benzylideno-2-thione-
2	19.308	98221	1.29	42239	1.90	90	191.15	Phenol, 3,5-bis(1,1-dimethylethyl)-
		7609518	100.00	2228402	100.00			

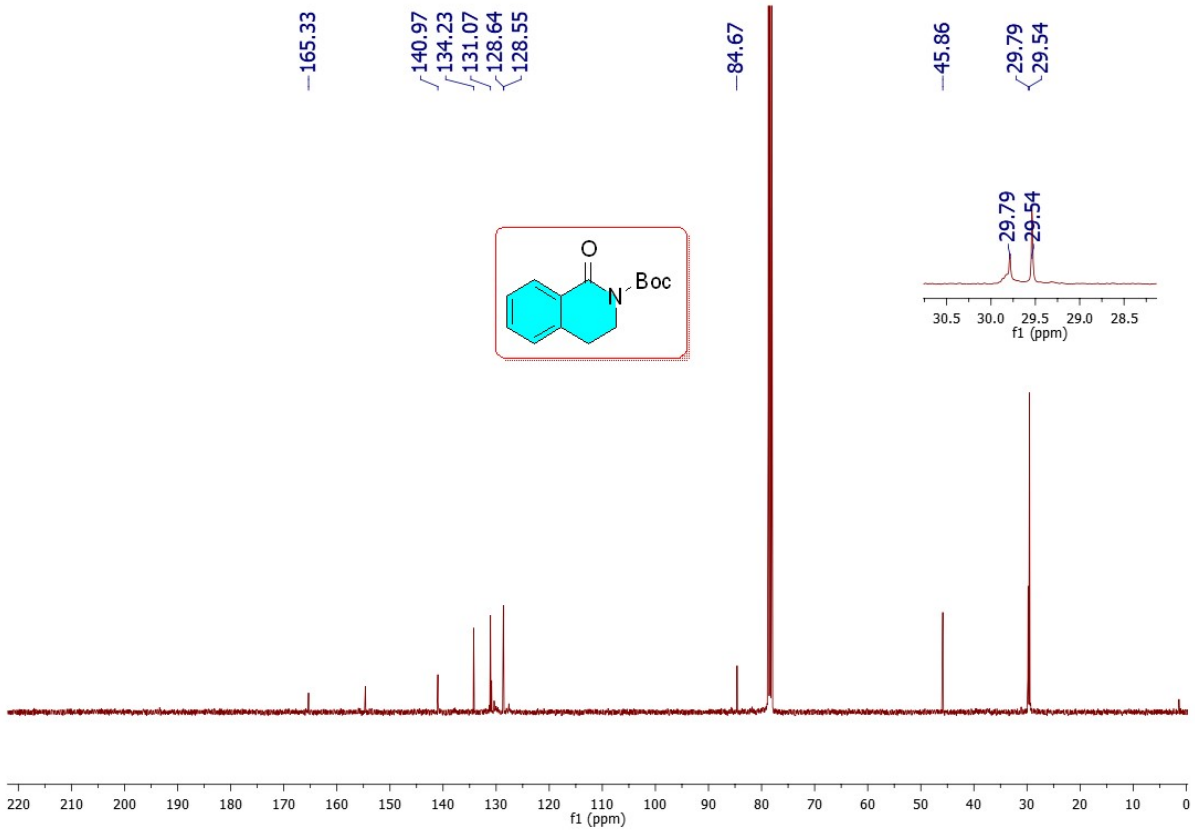
Line#:1 R.Time:18.680(Scan#:2937) MassPeaks:229
RawMode:Averaged 18.675-18.685(2936-2938) BasePeak:118.05(560644)
BG Mode:Calc. from Peak Group 1 - Event 1 Q3 Scan



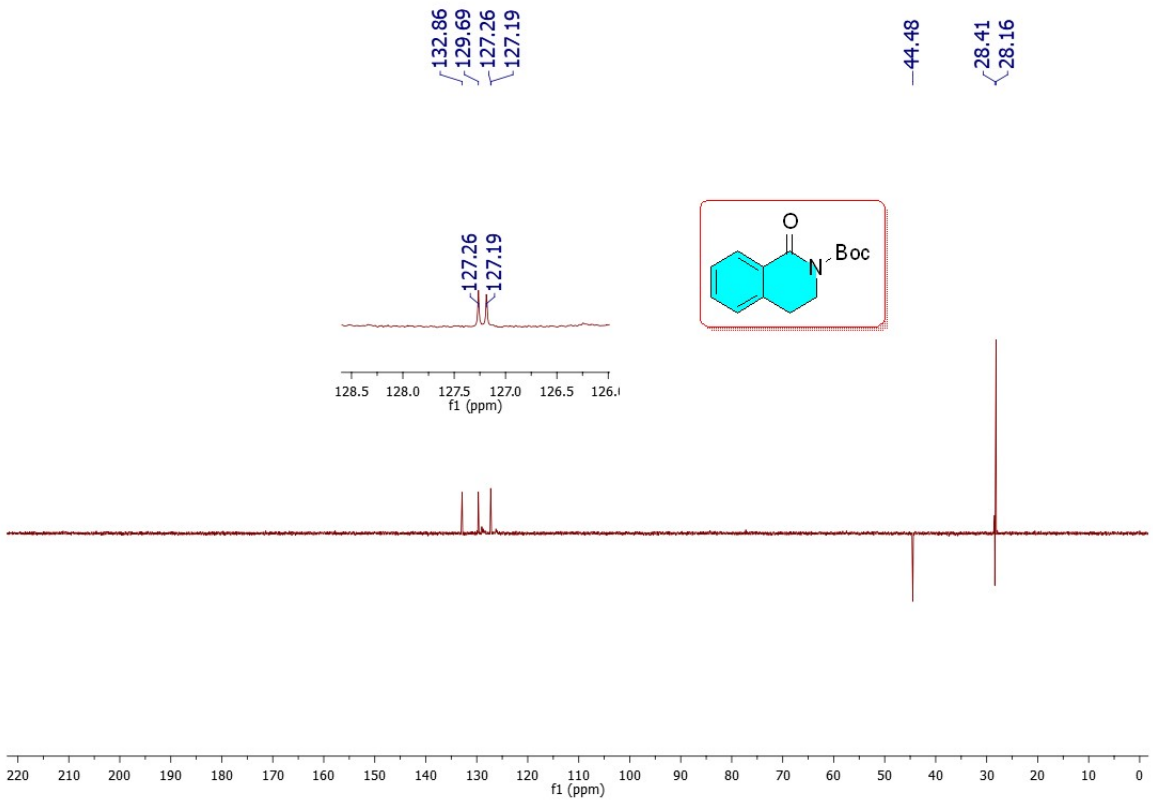
^{1}HNMR Spectra of *tert* 1-oxo-3,4-dihydroisoquinoline-2(1H)-carboxylate (4i)[16]



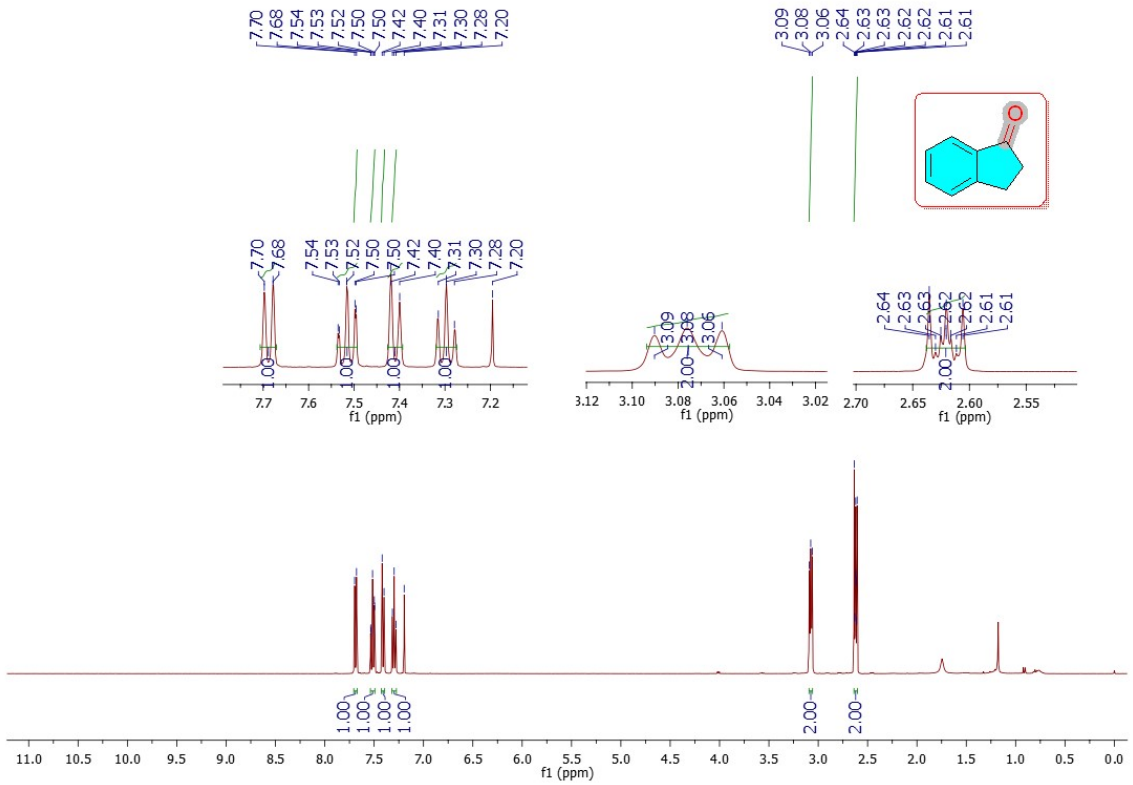
$^{13}C\{^{1}H\}$ NMR Spectra of *tert* 1-oxo-3,4-dihydroisoquinoline-2(1H)-carboxylate (4i)[16]



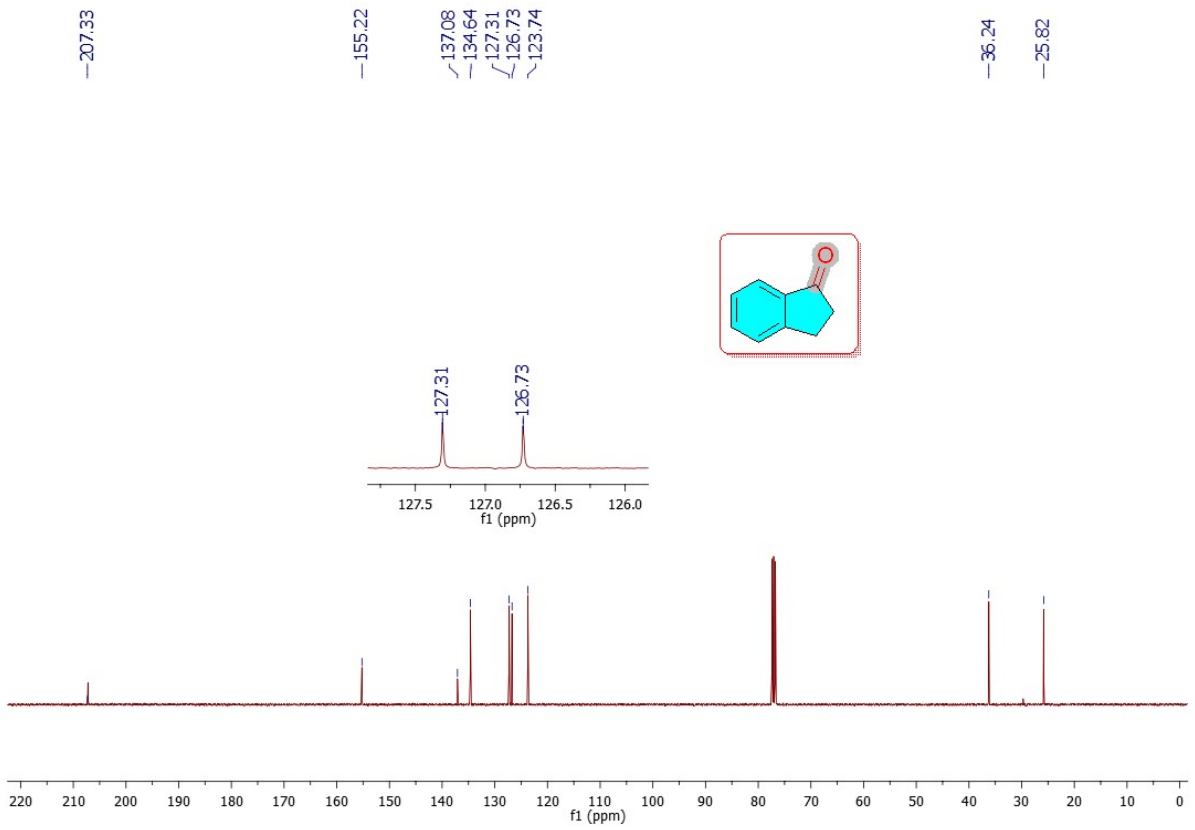
DEPT Spectra of *tert* 1-oxo-3,4-dihydroisoquinoline-2(1H)-carboxylate (4i)[16]



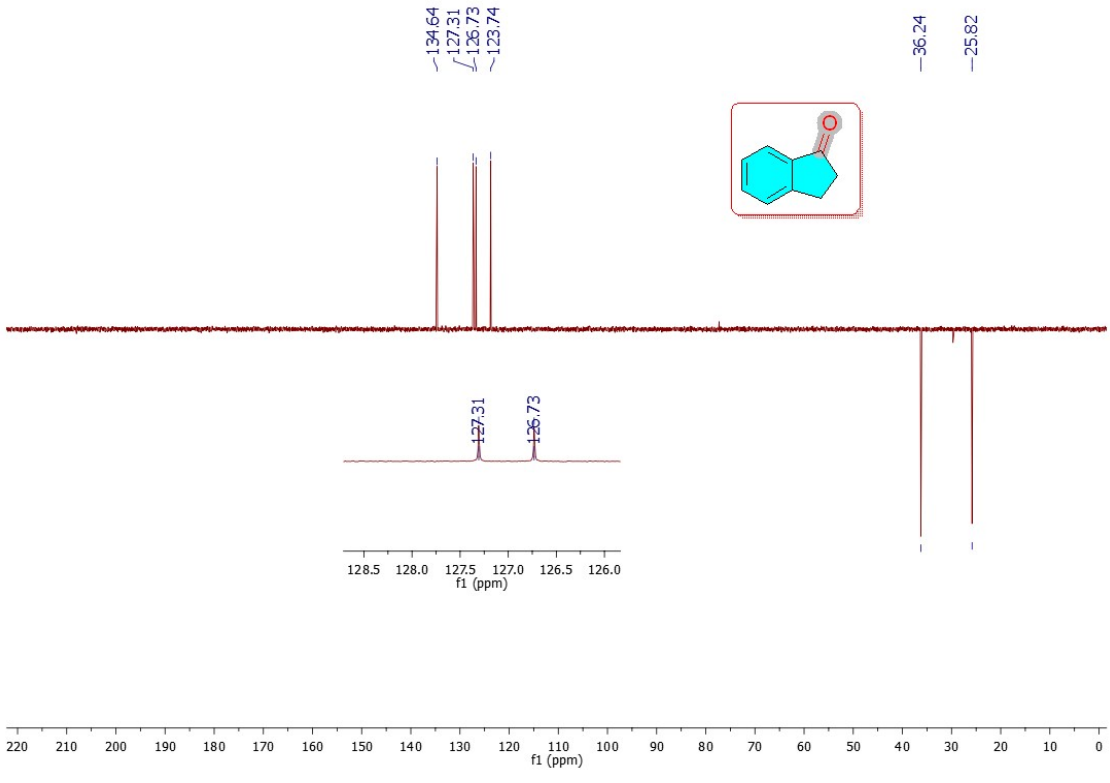
[1]HNMR Spectra of 2,3-dihydro-1*H*-inden-1-one (4j)[11]



[13]C{[1]H} NMR Spectra of 2,3-dihydro-1*H*-inden-1-one (4j)[11]



DEPT Spectra of 2,3-dihydro-1*H*-inden-1-one (4j)[11]

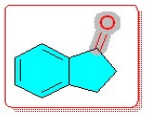


GCMS of 2,3-dihydro-1*H*-inden-1-one (4j)

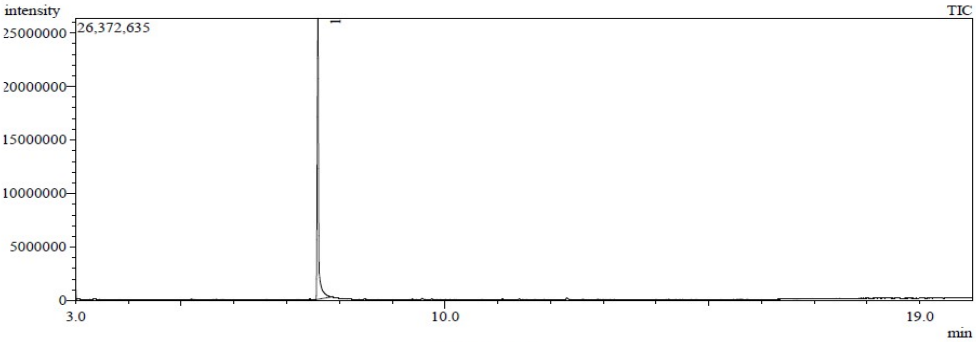
GCMS ANALYSIS REPORT

Sample Information

Analyzed by	: System Administrator
Analyzed	: 04-04-2023 01:06:40
Level #	: 1
Sample Name	: IND
Sample ID	: IND
Sample Amount	: 1
Vial #	: 23
Injection Volume	: 1.00
Data File	: D:\GCMS-2023\Data\Apr-2023\03.04.2023-25.qgd
Method File	: D:\GCMS-2023\Method\GCMS_LIQ_1_5ms_01.qgm
Tuning File	: D:\GCMS-2023\Tuning\31.Mar.2023_HS.qgt
$EndIf$Modified by	: System Administrator
Modified	: 04-04-2023 01:26:41



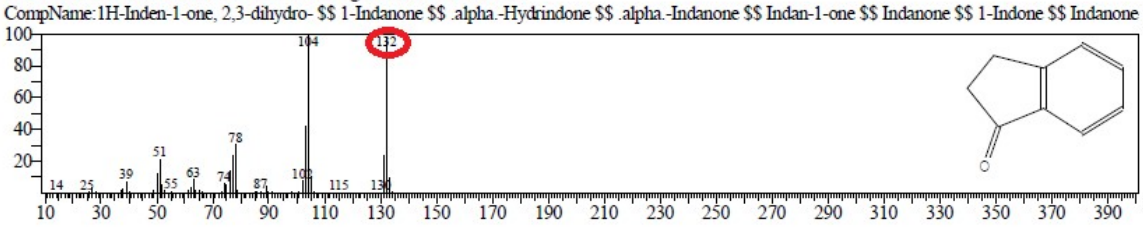
Chemical Formula: C_9H_8O
Exact Mass: 132.06



Peak Report TIC

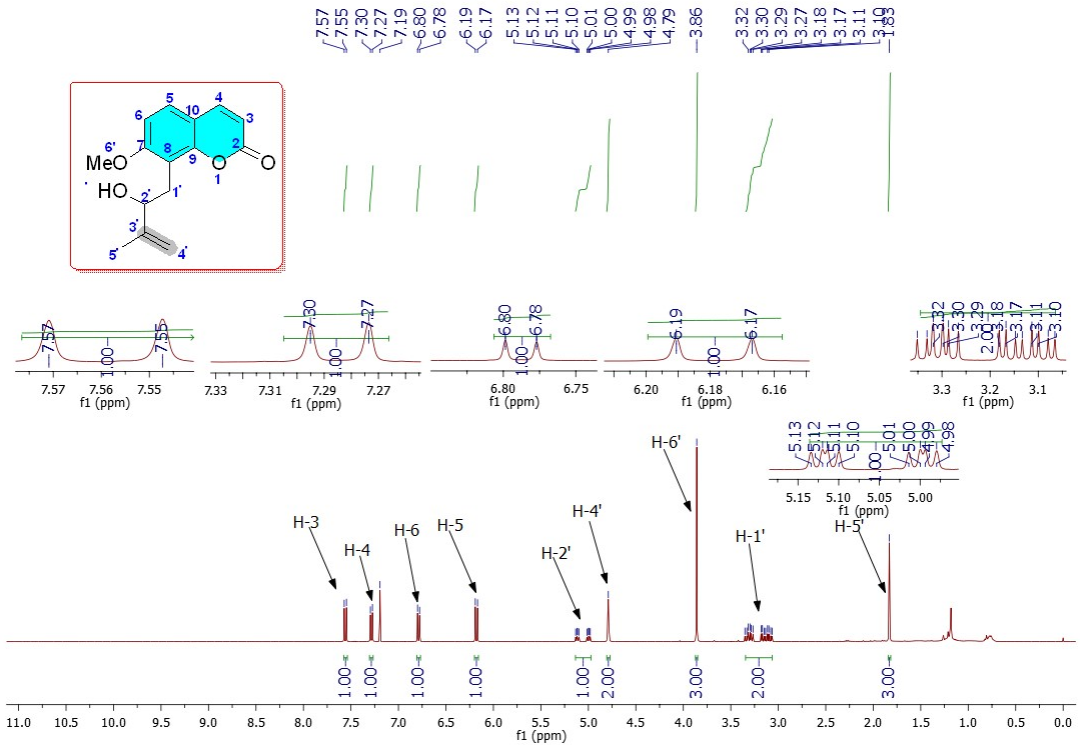
Peak#	R.Time	Area	Area%	Similarity	Base m/z	Name
1	7.592	53691408	100.00	96	132.10	1H-Inden-1-one, 2,3-dihydro-
		53691408	100.00			

Hit#:1 Entry:9059 Library:NIST17M1.lib
SI:96 Formula:C9H8O CAS:83-33-0 MolWeight:132 RetIndex:1218
CompName:1H-Inden-1-one, 2,3-dihydro- $$ 1-Indanone $$ .alpha.-Hydrindone $$ .alpha.-Indanone $$ Indan-1-one $$ Indanone $$ 1-Indone $$ Indanone

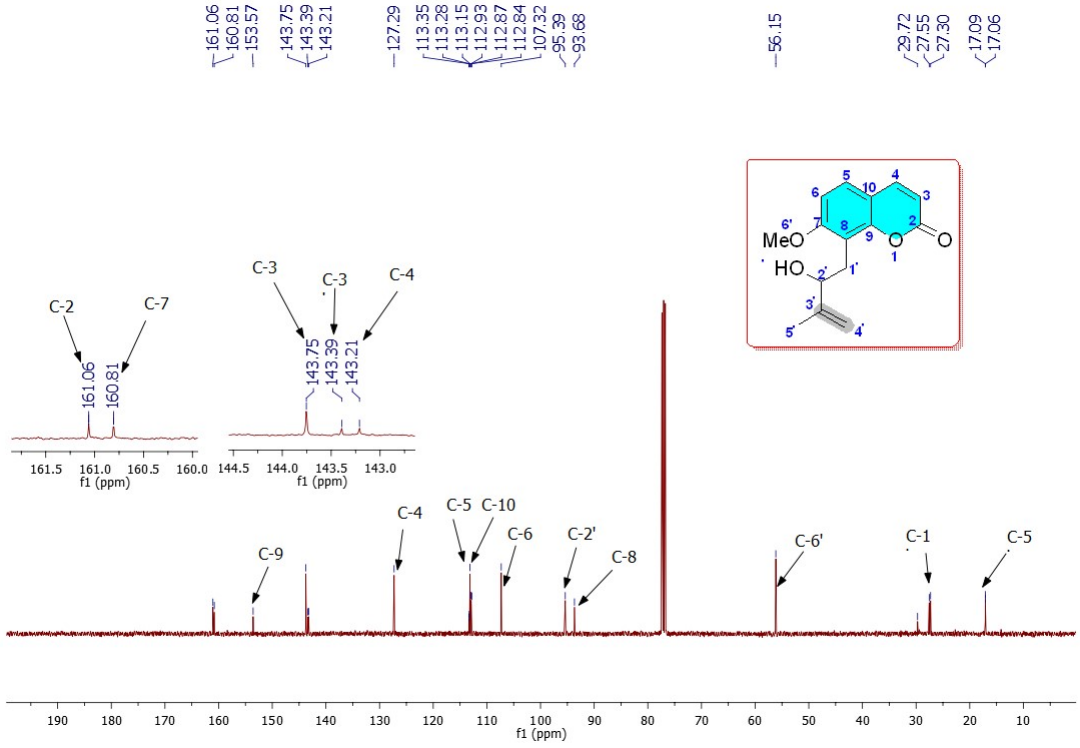


Spectral Copies:

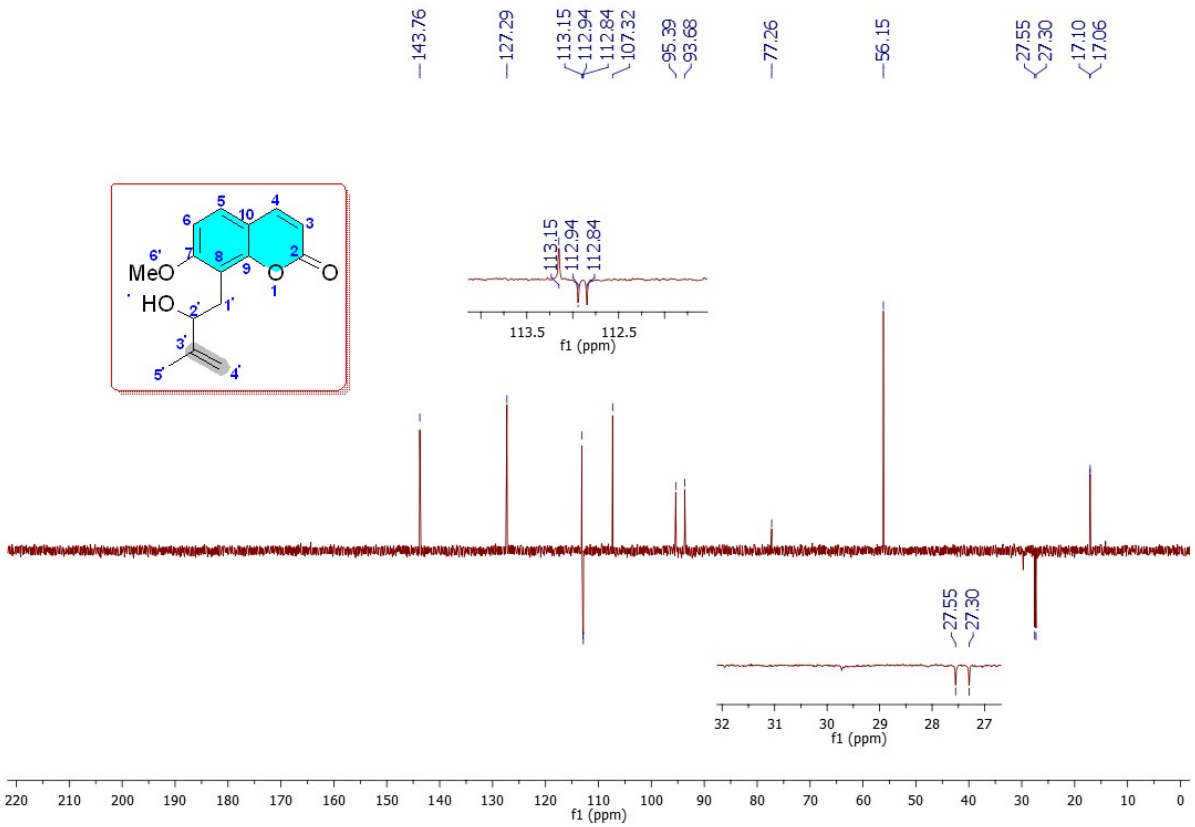
[1]HNMR Spectra of 8-(4-hydroxy-3-methylbut-2-en-1-yl)-7-methoxy-2*H*-chromen-2-one (8a)



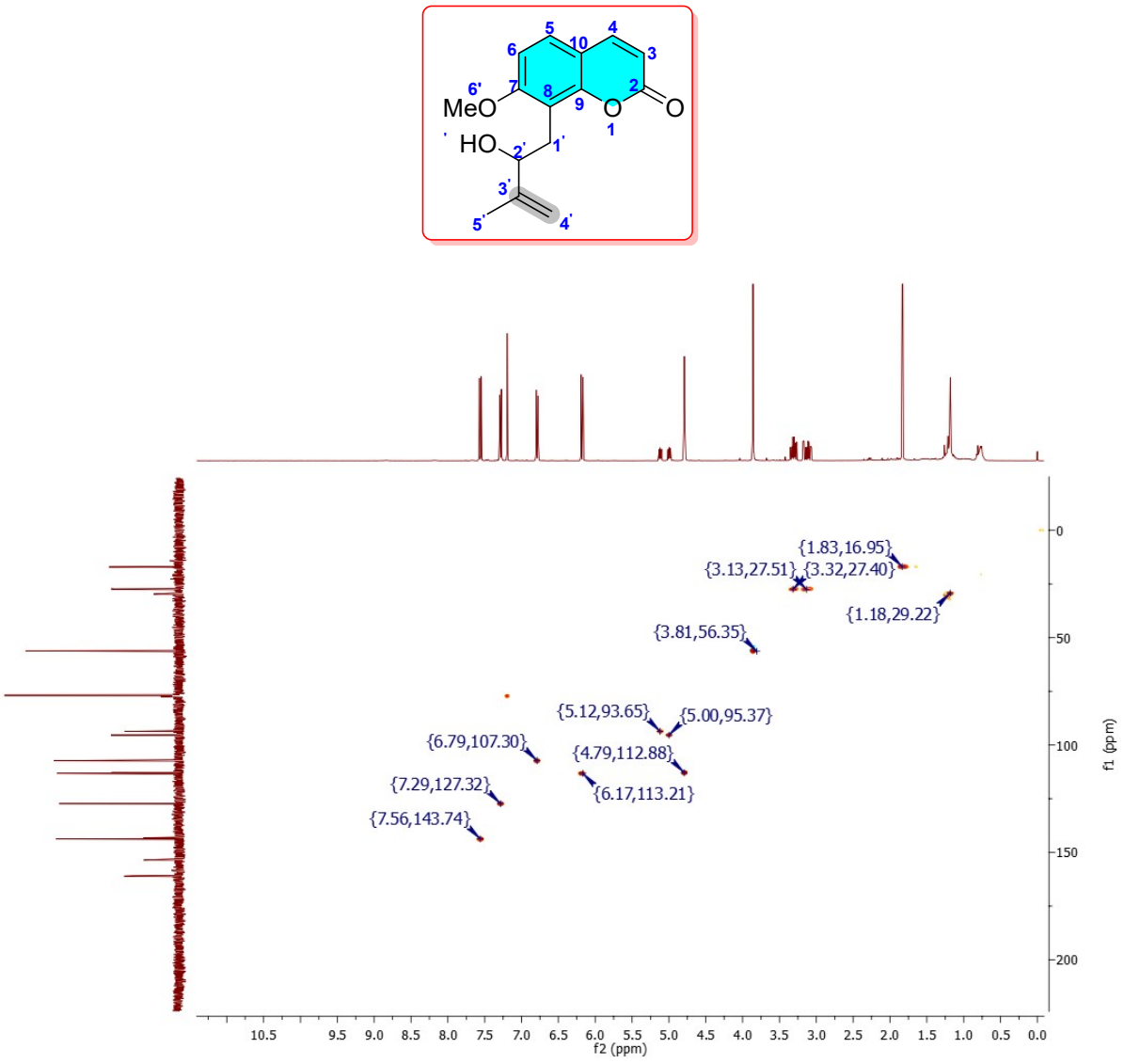
[13]C{[1]H} NMR Spectra of 8-(4-hydroxy-3-methylbut-2-en-1-yl)-7-methoxy-2*H*-chromen-2-one (8a)



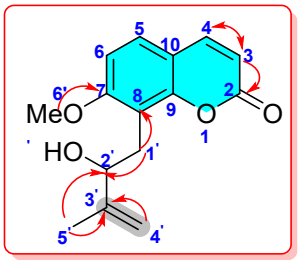
DEPT Spectra of 8-(4-hydroxy-3-methylbut-2-en-1-yl)-7-methoxy-2*H*-chromen-2-one (8a)

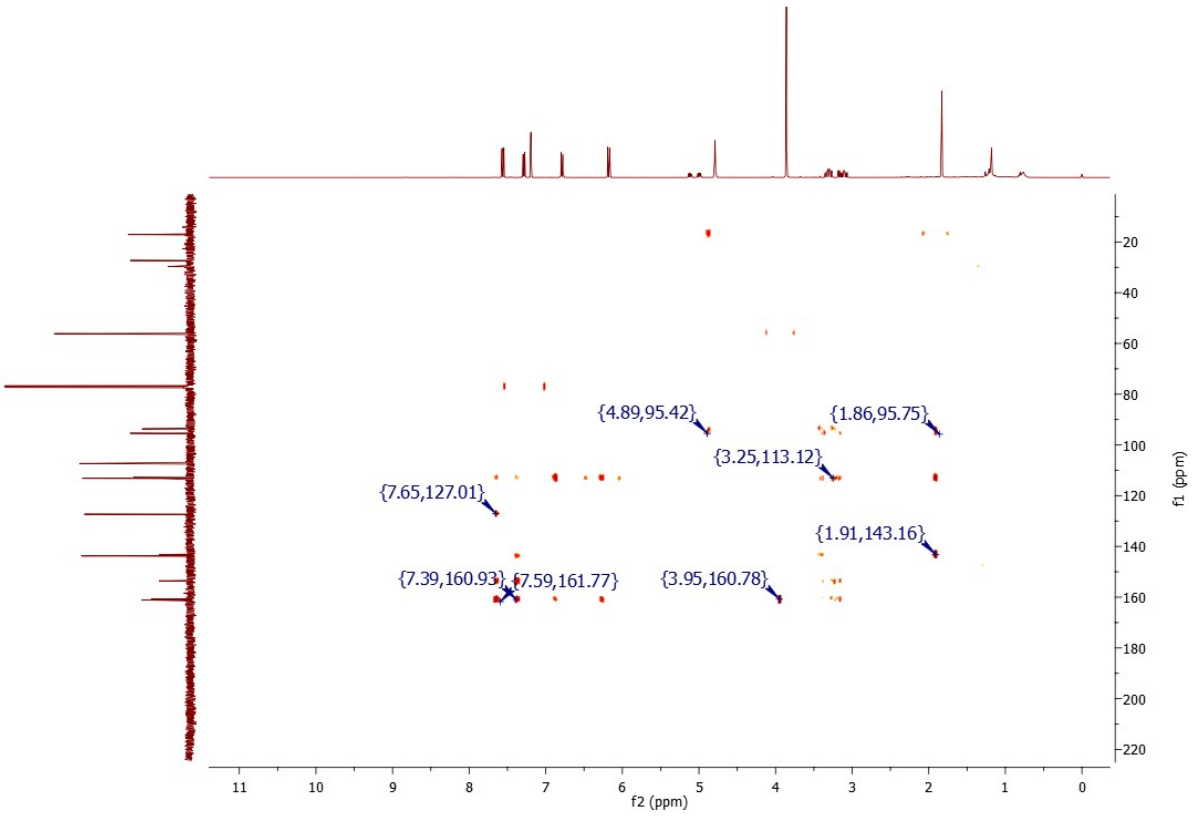


HSQC correlation in 8-(4-hydroxy-3-methylbut-2-en-1-yl)-7-methoxy-2*H*-chromen-2-one (8a)

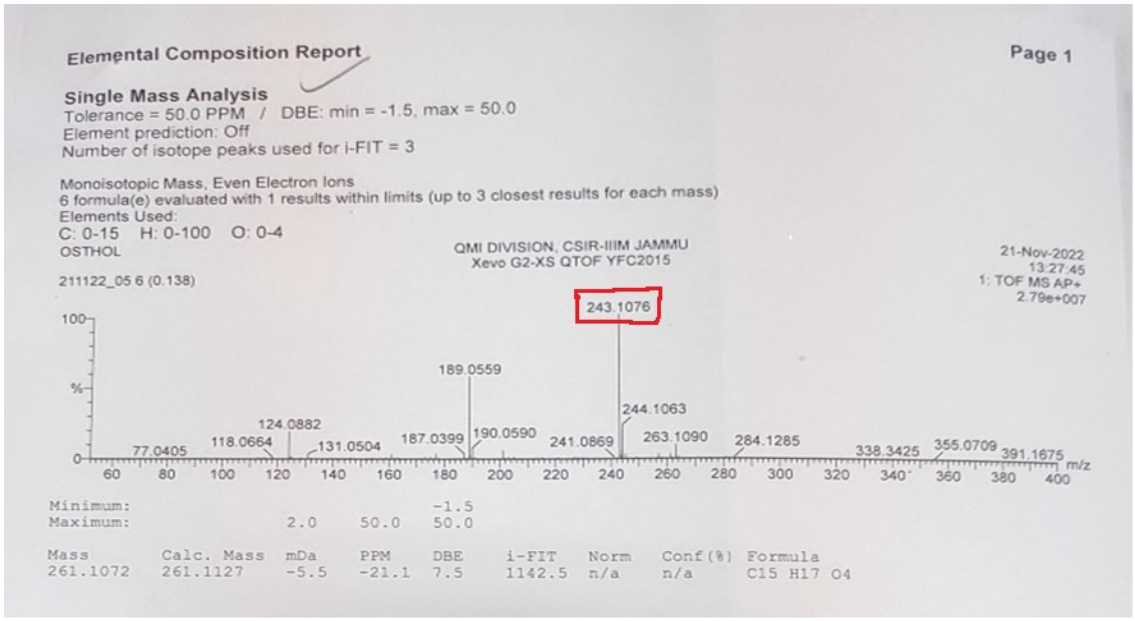


HMBC correlations in 8-(4-hydroxy-3-methylbut-2-en-1-yl)-7-methoxy-2*H*-chromen-2-one (8a)

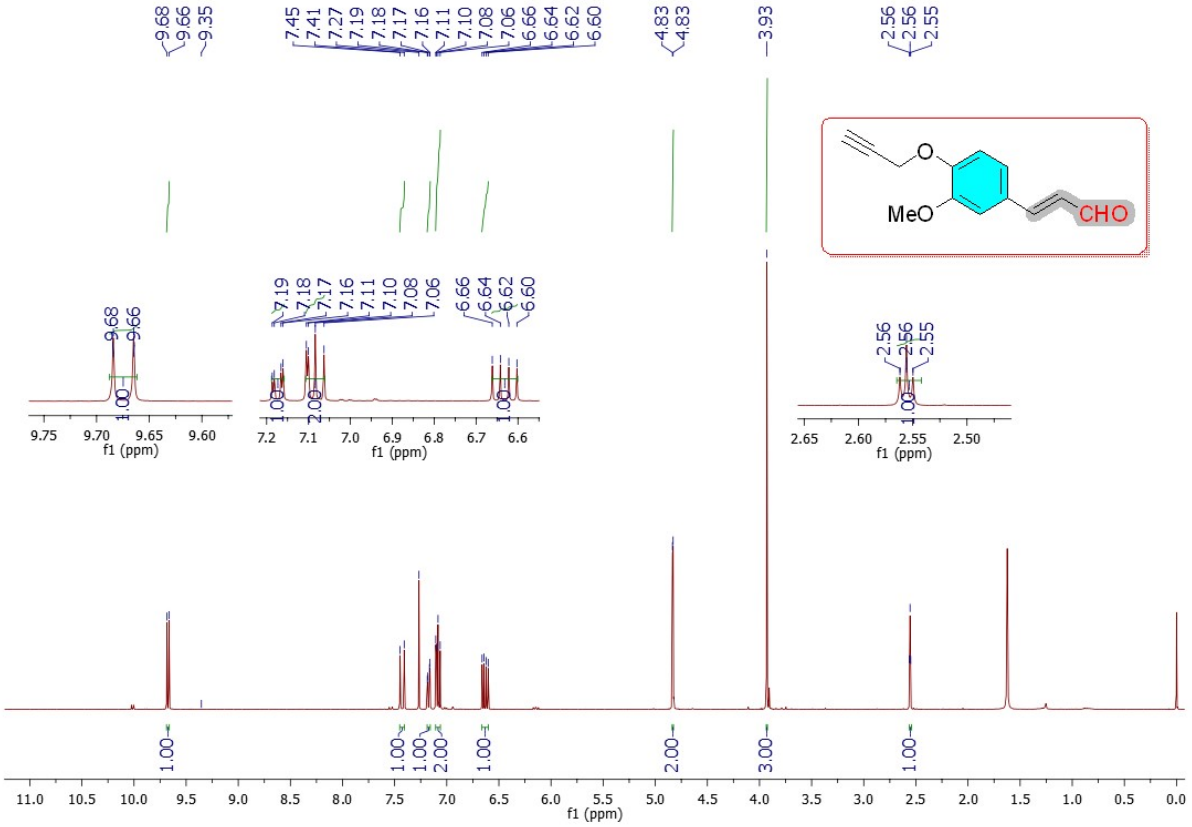




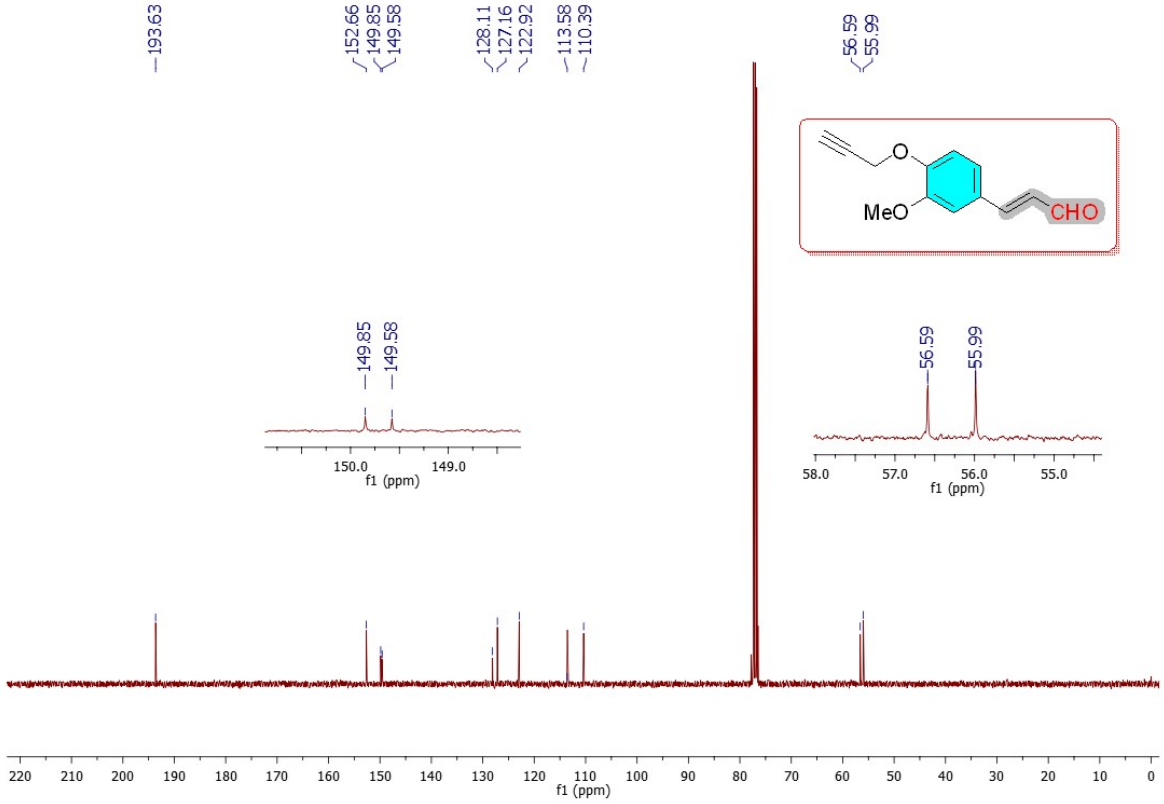
HRMS of 8-(4-hydroxy-3-methylbut-2-en-1-yl)-7-methoxy-2H-chromen-2-one (8a)



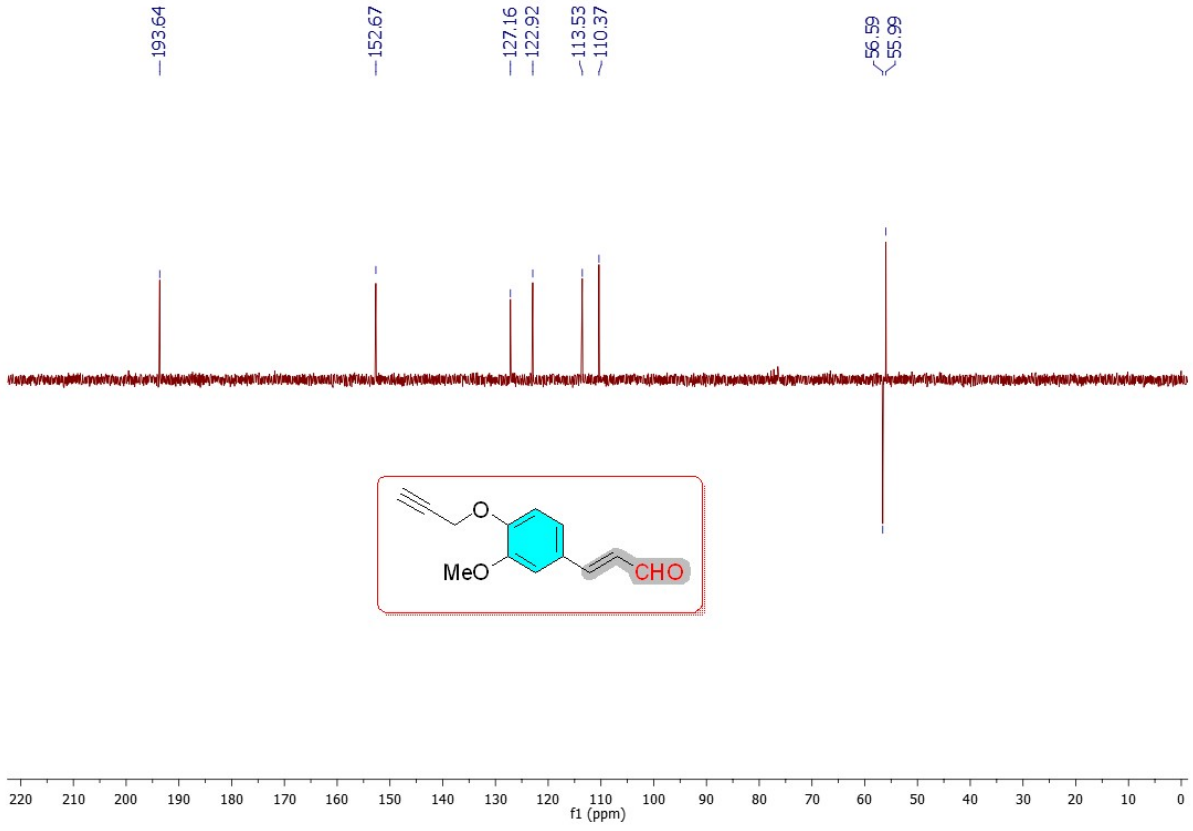
[1]HNMR Spectra of 3-(3-methoxy-4-(prop-2-yn-1-yloxy) phenyl) acrylaldehyde (10a)



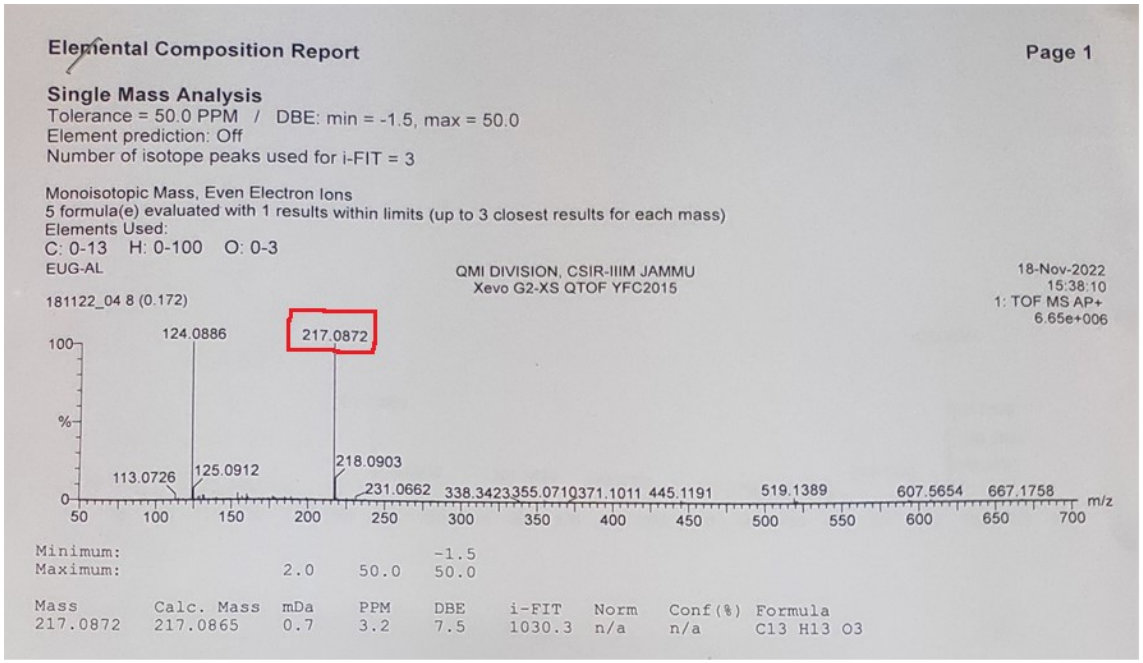
$^{13}C\{^{1}H\}$ NMR Spectra of3-(3-methoxy-4-(prop-2-yn-1-yloxy) phenyl) acrylaldehyde (10a)



DEPT Spectra of 3-(3-methoxy-4-(prop-2-yn-1-yloxy) phenyl) acrylaldehyde (10a)



HRMS of 3-(3-methoxy-4-(prop-2-yn-1-yloxy) phenyl) acrylaldehyde (10a)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 O: 0-3

EUG-AL

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

18-Nov-2022
15:38:10
1: TOF MS AP+
6.65e+006

181122_04 8 (0.172)

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
217.0872	217.0865	0.7	3.2	7.5	1030.3	n/a	n/a	C13 H13 O3

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