

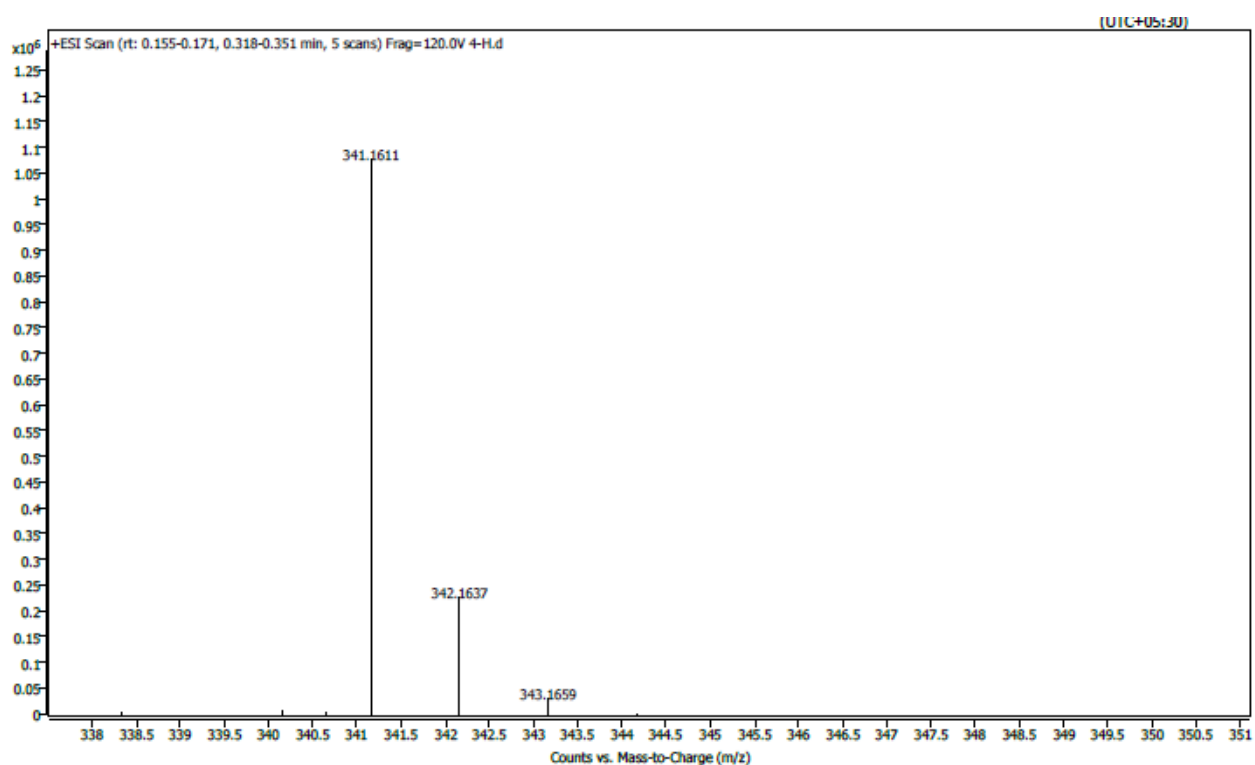
Design, Synthesis, Biological Evaluation and Molecular Docking study of novel Pyridoxine-Triazoles as Anti-Alzheimer's Agents

Tiyas Pal¹, Saipriyanka Bhimaneni², Abha Sharma^{1*} and S.J.S. Flora^{2*}

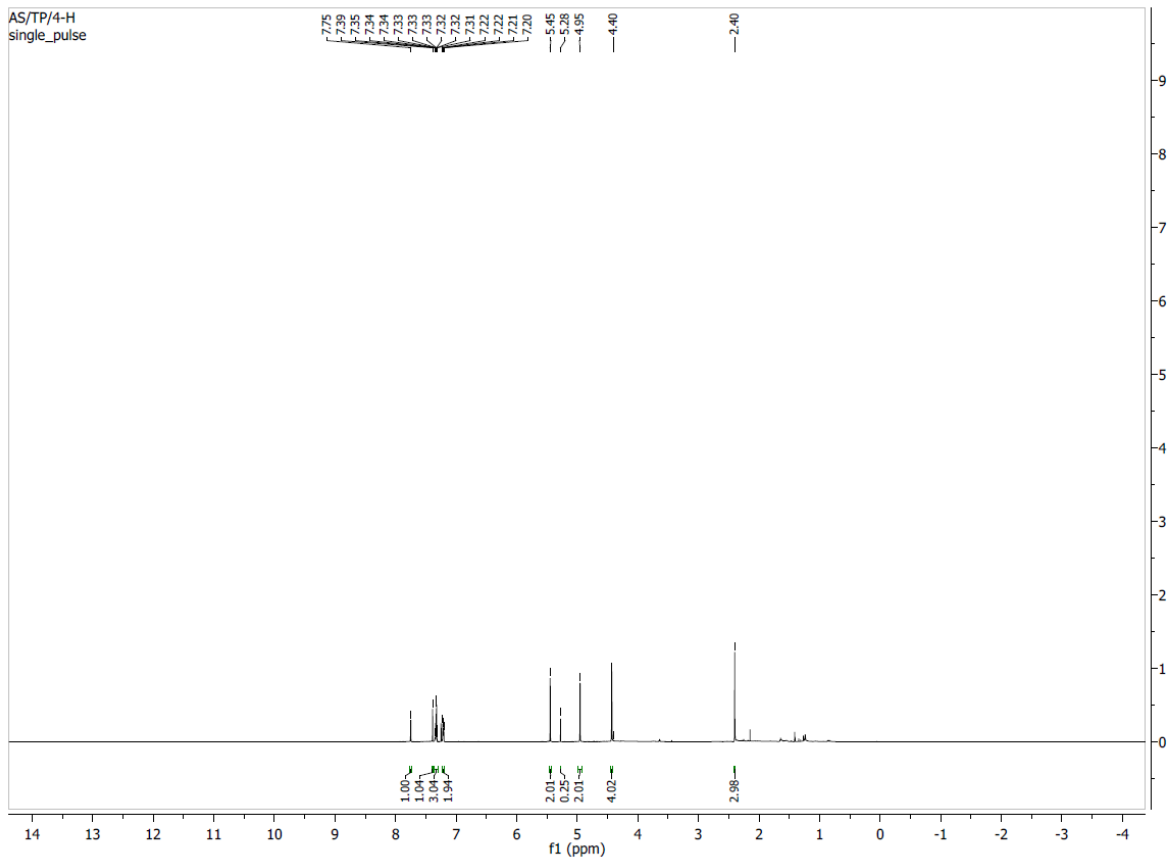
¹Department of Medicinal Chemistry and ²Pharmacology & Toxicology
National Institute of Pharmaceutical Education and Research, Raebareli, India

*E-mail: abha.sharma@niperraebareli.edu.in; sjsflora@hotmail.com

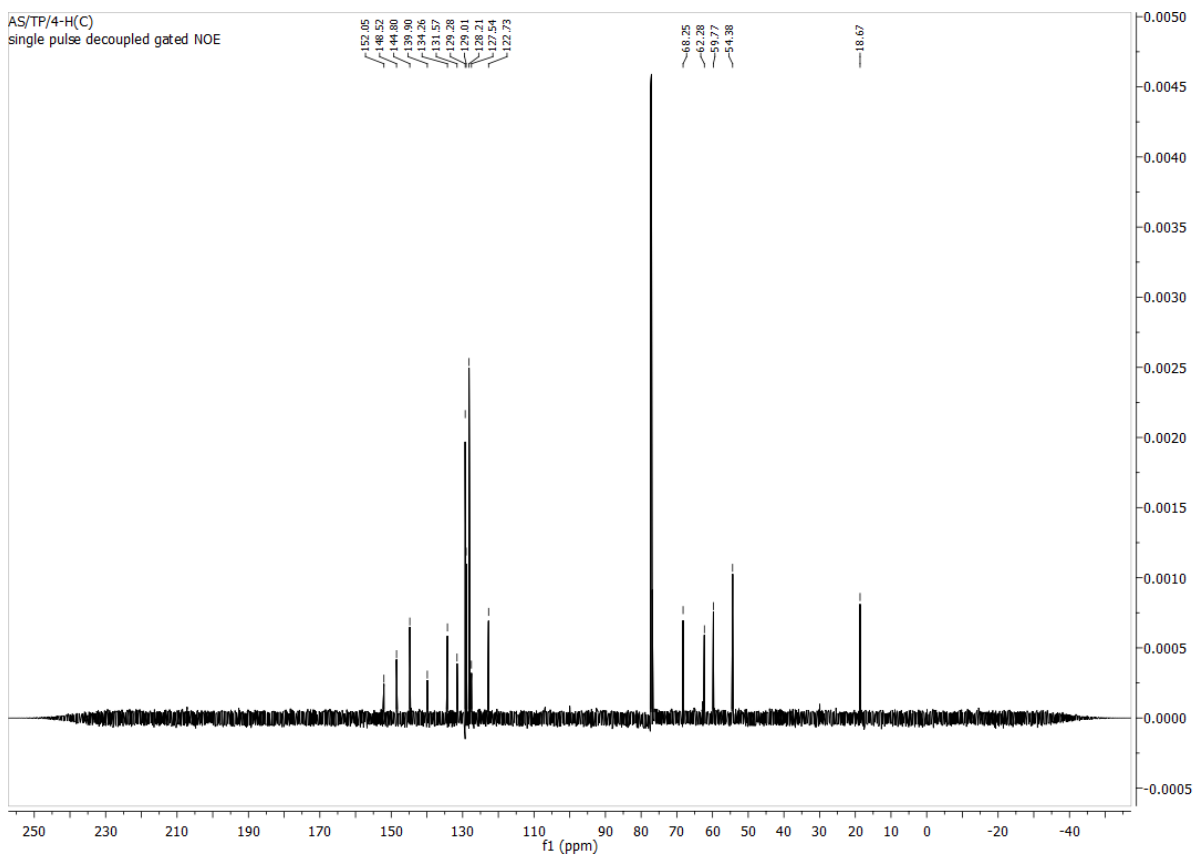
SPECTRAL DATA OF **5a**



HRMS Spectrum of **5a**



^1H NMR of 5a in CDCl_3 at 500MHz

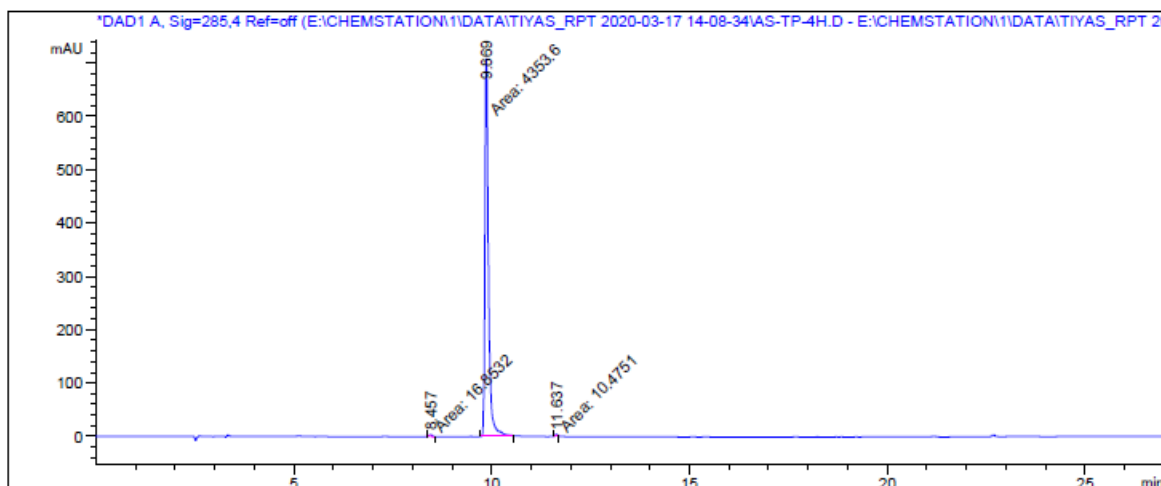


^{13}C NMR of 5a in CDCl_3 at 125MHz

HPLC Purity Data of **5a**

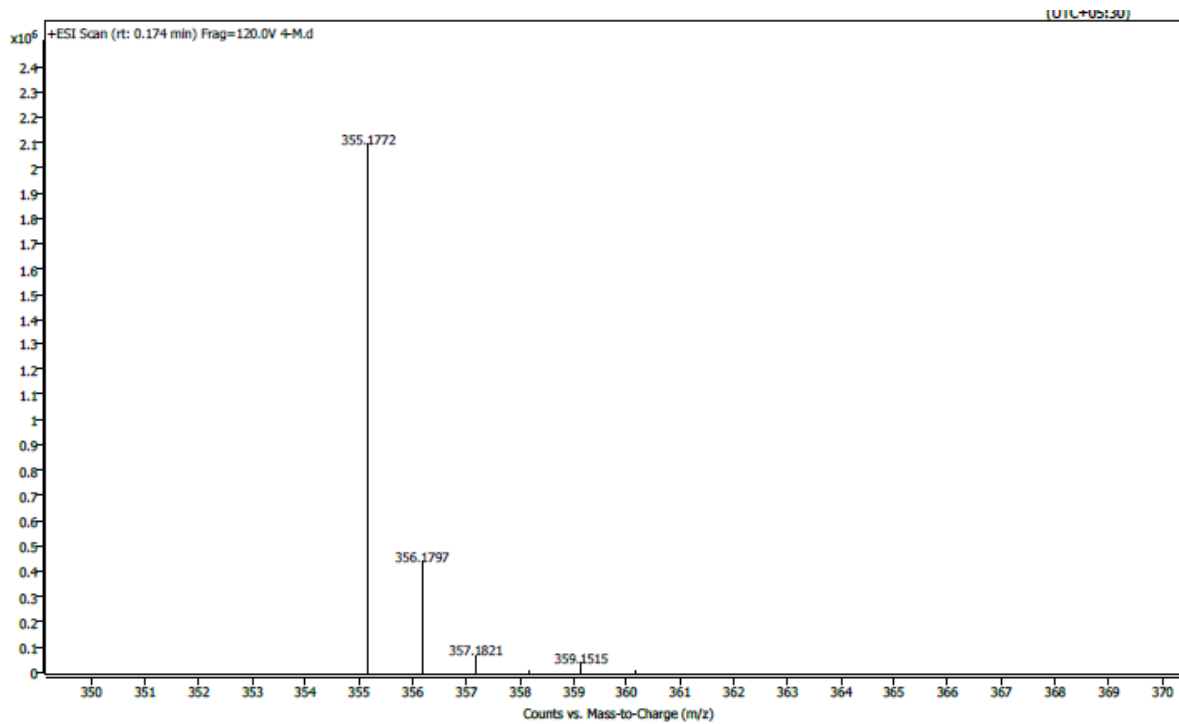
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Acq. Instrument : HPLC                      Location  : P2-C-03
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                                           Inj Volume: 10.000 µl
Acq. Method    : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 14-08-34\TIYAS_RPT.M
Last changed   : 17-03-2020 10:01:12 by SYSTEM
Analysis Method: E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed   : 23-06-2020 11:45:48 by SYSTEM
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Additional Info : Peak(s) manually integrated
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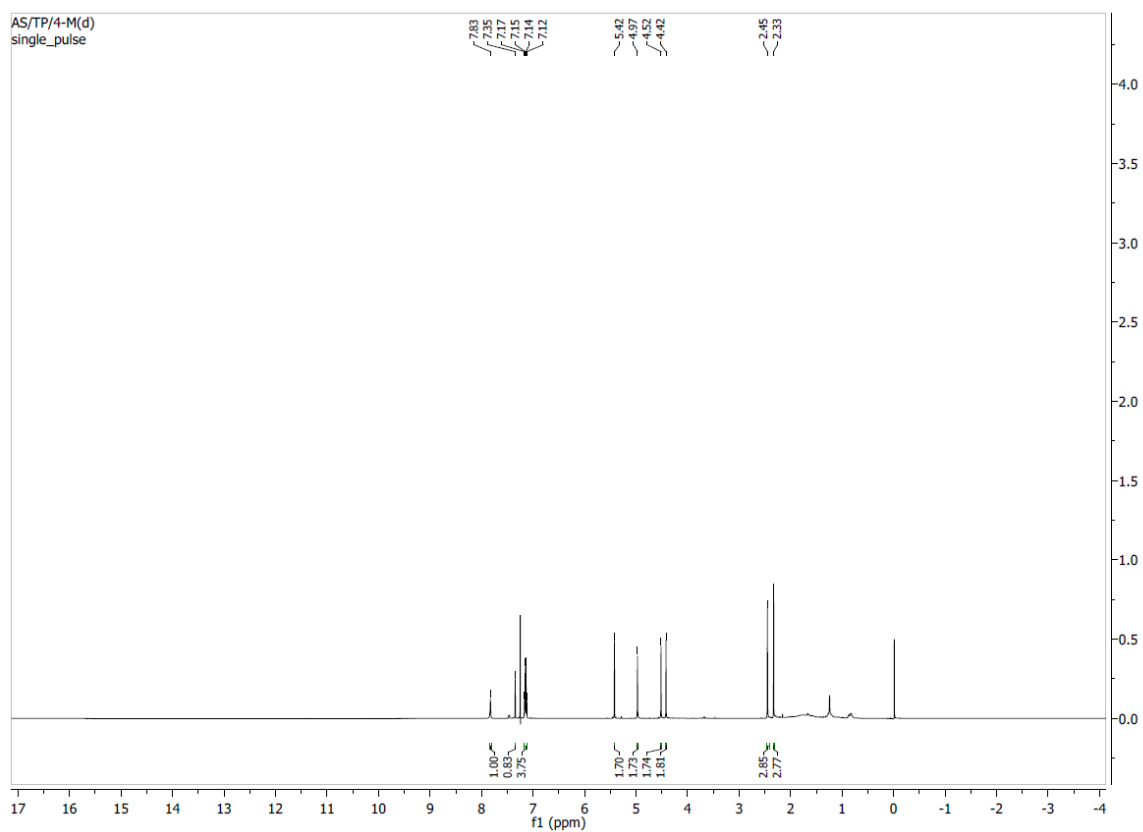


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.457	MM	0.0991	16.85318	2.83489	0.3847
2	9.869	MM	0.1025	4353.60010	708.14874	99.3762
3	11.637	MM	0.0613	10.47512	2.84878	0.2391

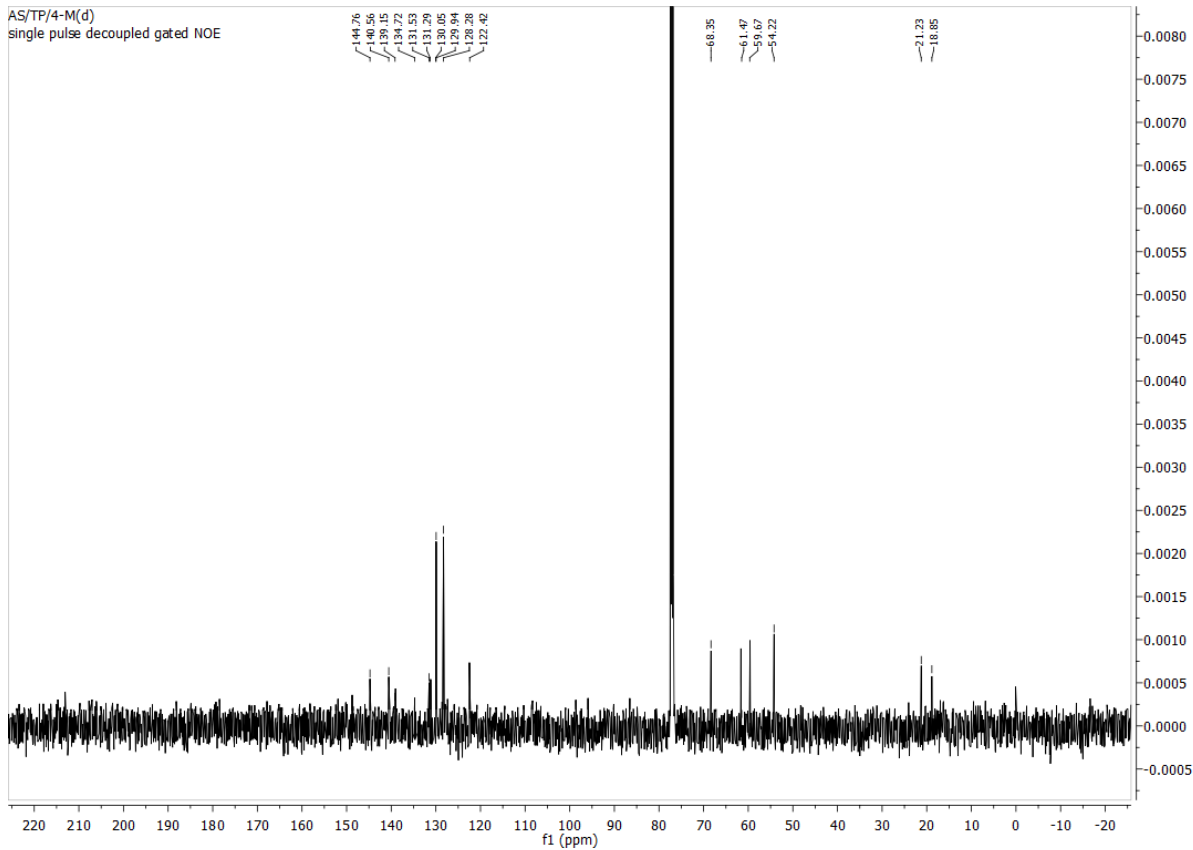
SPECTRAL DATA OF **5b**



HRMS Spectrum of **5b**



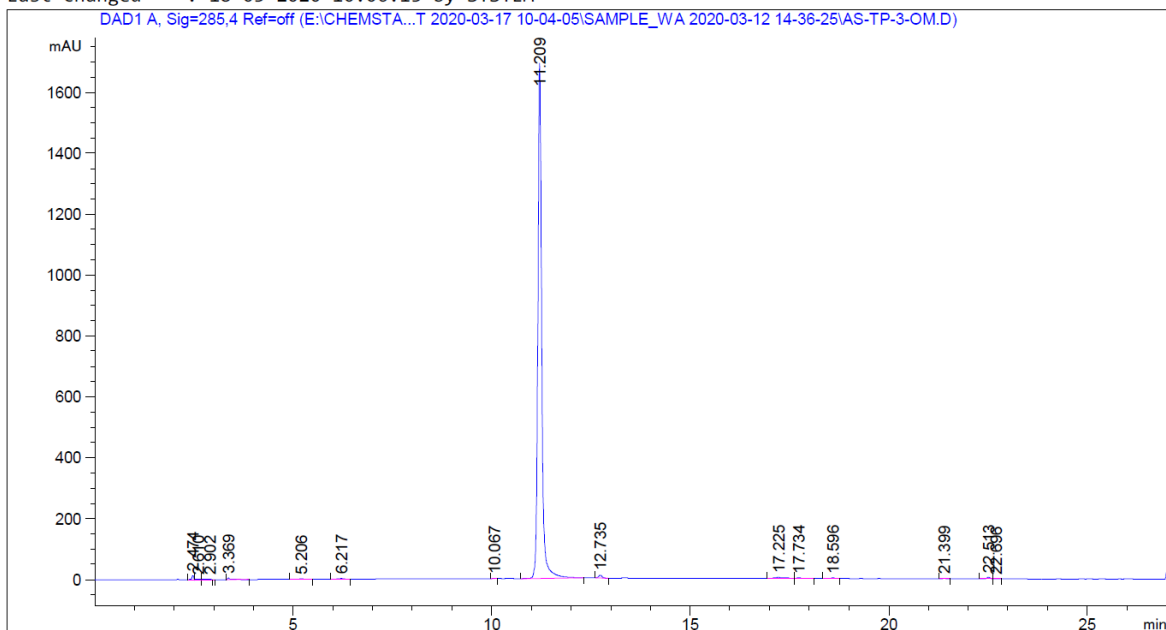
¹H NMR of **5b** in CDCl₃ at 500MHz



¹³C NMR of **5b** in CDCl₃ at 125MHz

HPLC Purity data of **5b**

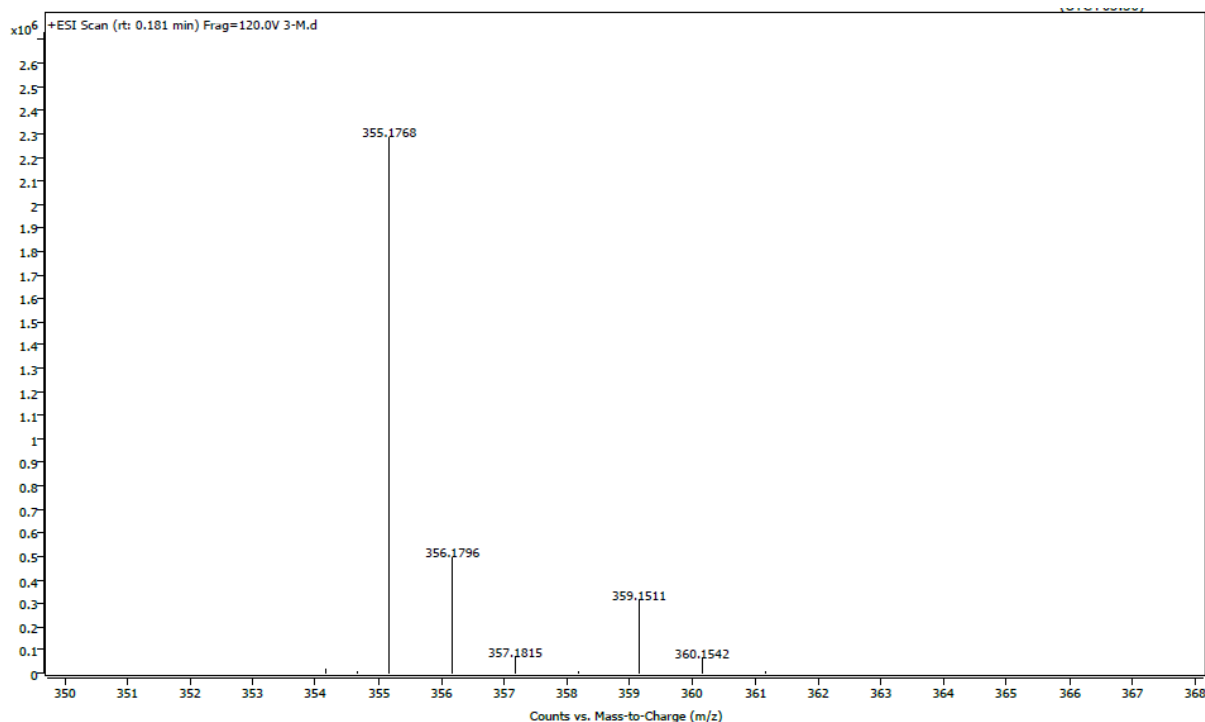
Acq. Operator : SYSTEM Seq. Line : 1
 Sample Operator : SYSTEM
 Acq. Instrument : HPLC Location : P2-D-05
 Injection Date : 12-03-2020 14:37:54 Inj : 1
 Inj Volume : 10.000 µl
 Different Inj Volume from Sample Entry! Actual Inj Volume : 20.000 µl
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 Last changed : 12-03-2020 14:21:08 by SYSTEM
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 Last changed : 18-03-2020 10:06:13 by SYSTEM



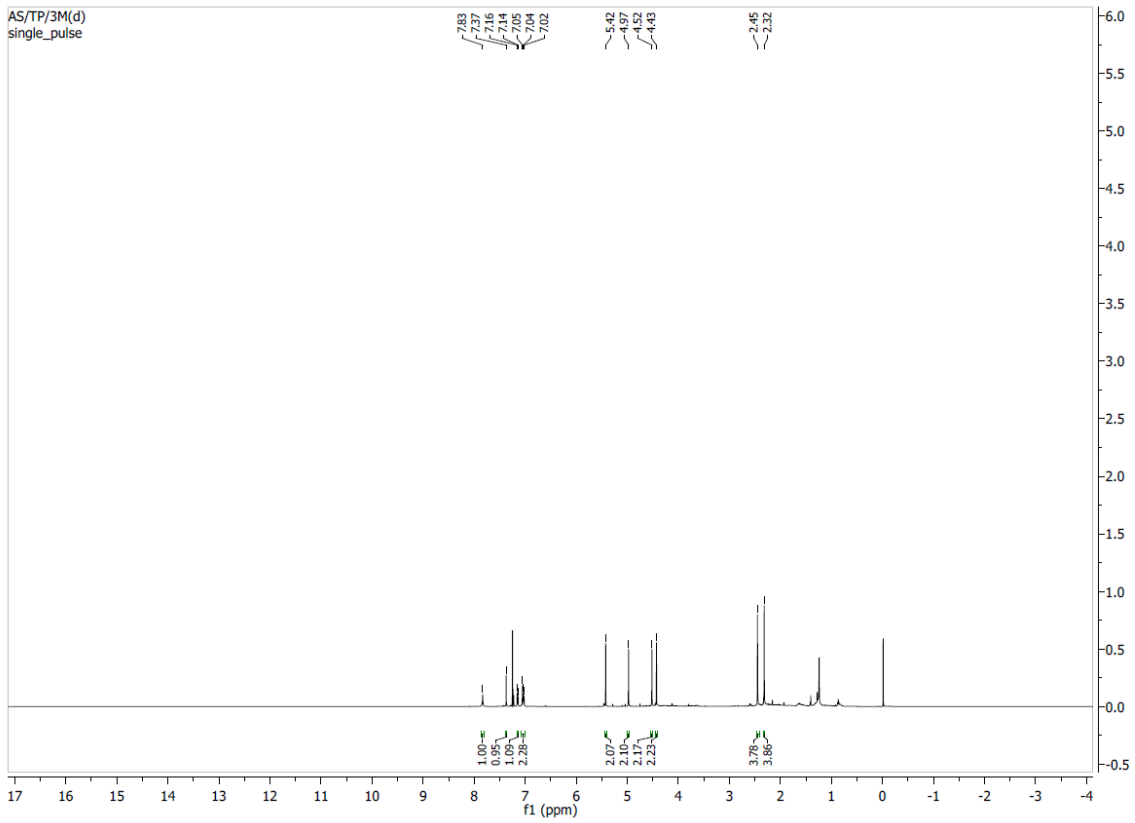
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.474	BV R	0.0466	36.14810	12.93615	0.3074
2	2.610	VV E	0.0899	9.49463	1.49859	0.0807
3	2.902	VV E	0.1211	13.31856	1.45118	0.1133
4	3.369	BB	0.0606	21.35286	5.34617	0.1816
5	5.206	BB	0.1491	10.74166	1.05181	0.0913
6	6.217	BB	0.1094	14.74261	1.92288	0.1254
7	10.067	BB	0.0787	5.77354	1.14801	0.0491
8	11.209	BB	0.1008	1.14519e4	1695.04688	97.3894
9	12.735	BB	0.0927	58.90446	9.72381	0.5009
10	17.225	BV	0.2962	59.28908	2.88012	0.5042
11	17.734	VB	0.1228	17.43097	1.97860	0.1482
12	18.596	BB	0.1025	14.70604	2.13127	0.1251
13	21.399	BB	0.1002	8.52652	1.30474	0.0725
14	22.513	BV	0.0890	29.51746	5.14132	0.2510
15	22.696	VV	0.1000	7.03197	1.05244	0.0598

Totals : 1.17589e4 1744.61395

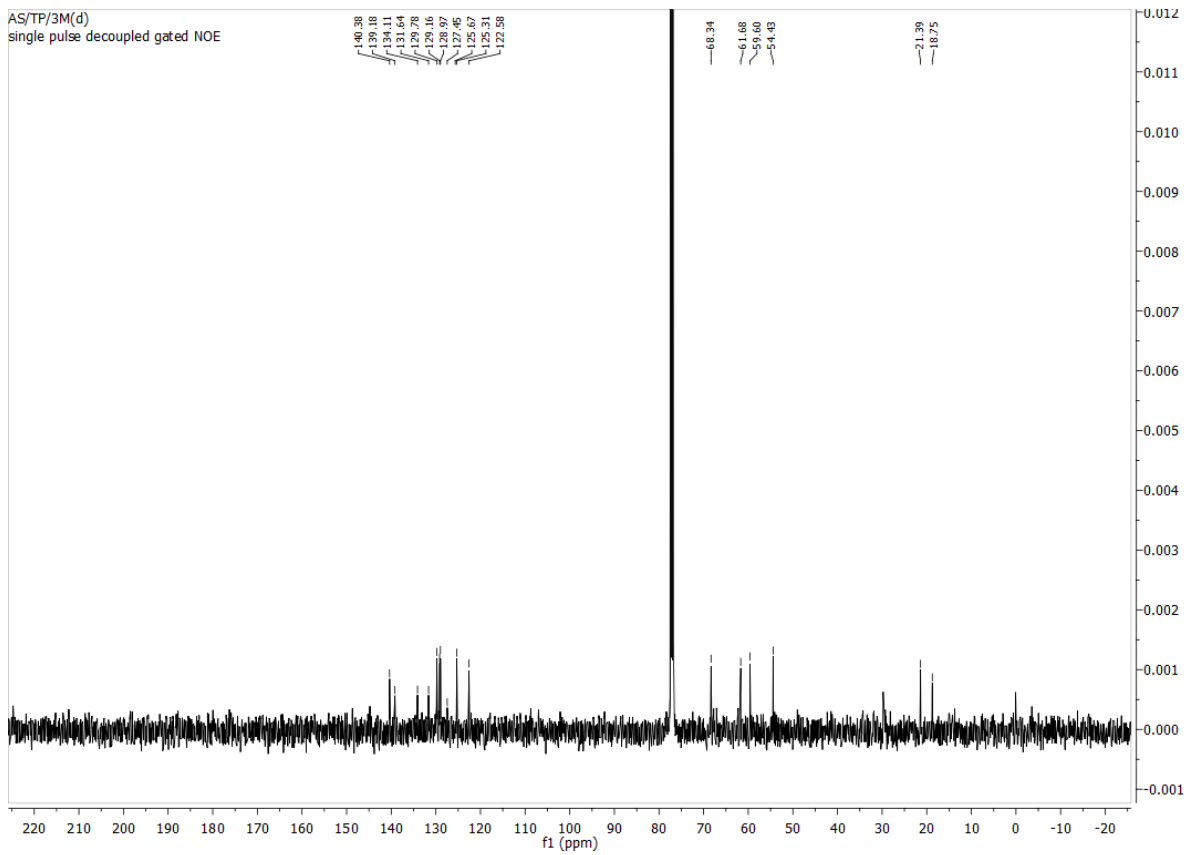
SPECTRAL DATA OF 5c



HRMS Spectrum of 5c



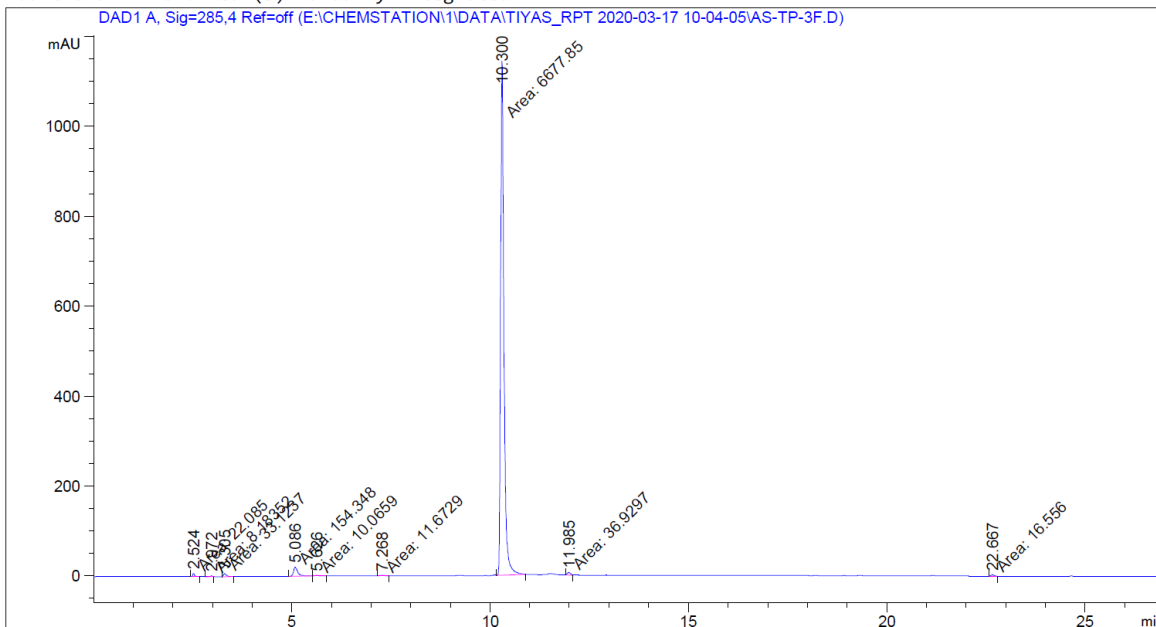
^1H NMR of **5c** in CDCl_3 at 500MHz



^{13}C NMR of **5c** in CDCl_3 at 125MHz

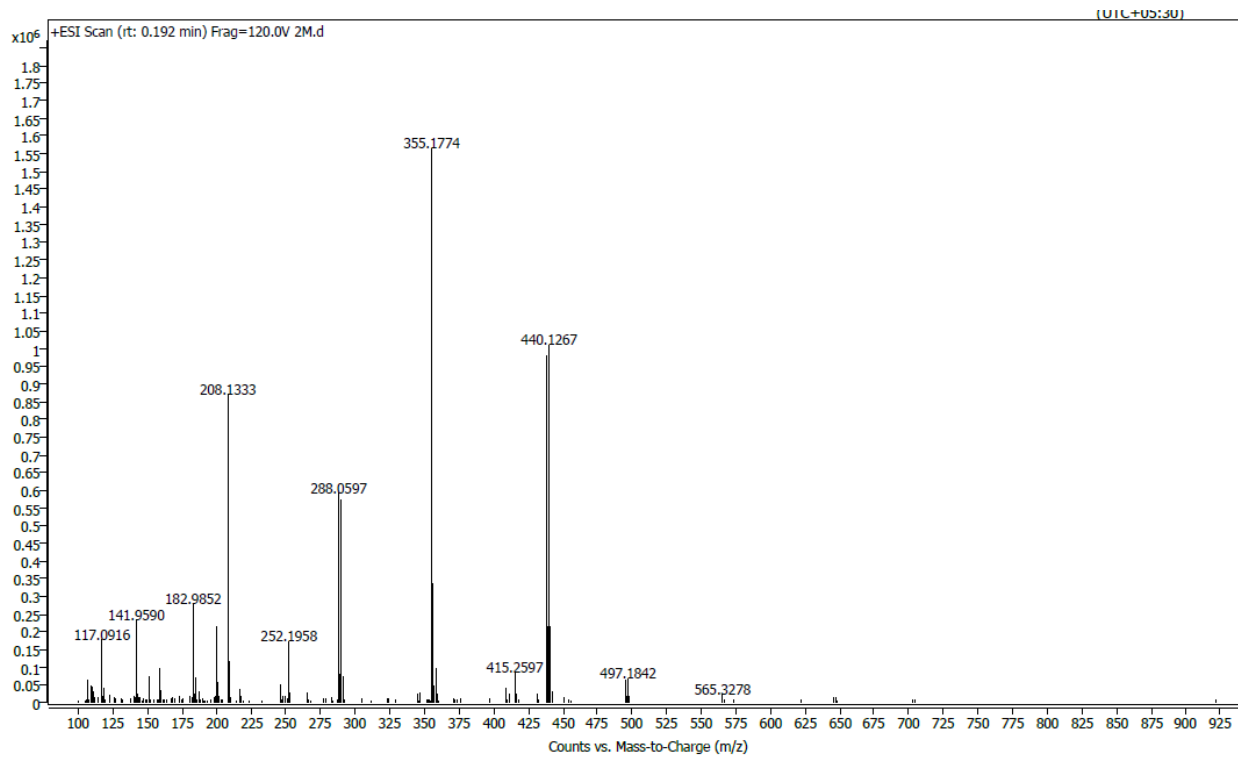
HPLC purity of **5c**

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 Sample Operator : SYSTEM
 Acq. Instrument : HPLC
 Injection Date : 17-03-2020 11:02:21
 Seq. Line : 3
 Location : P2-B-03
 Inj : 1
 Inj Volume : 10.000 µl
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 Last changed : 17-03-2020 10:01:12 by SYSTEM
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 Last changed : 18-03-2020 10:06:13 by SYSTEM
 Additional Info : Peak(s) manually integrated

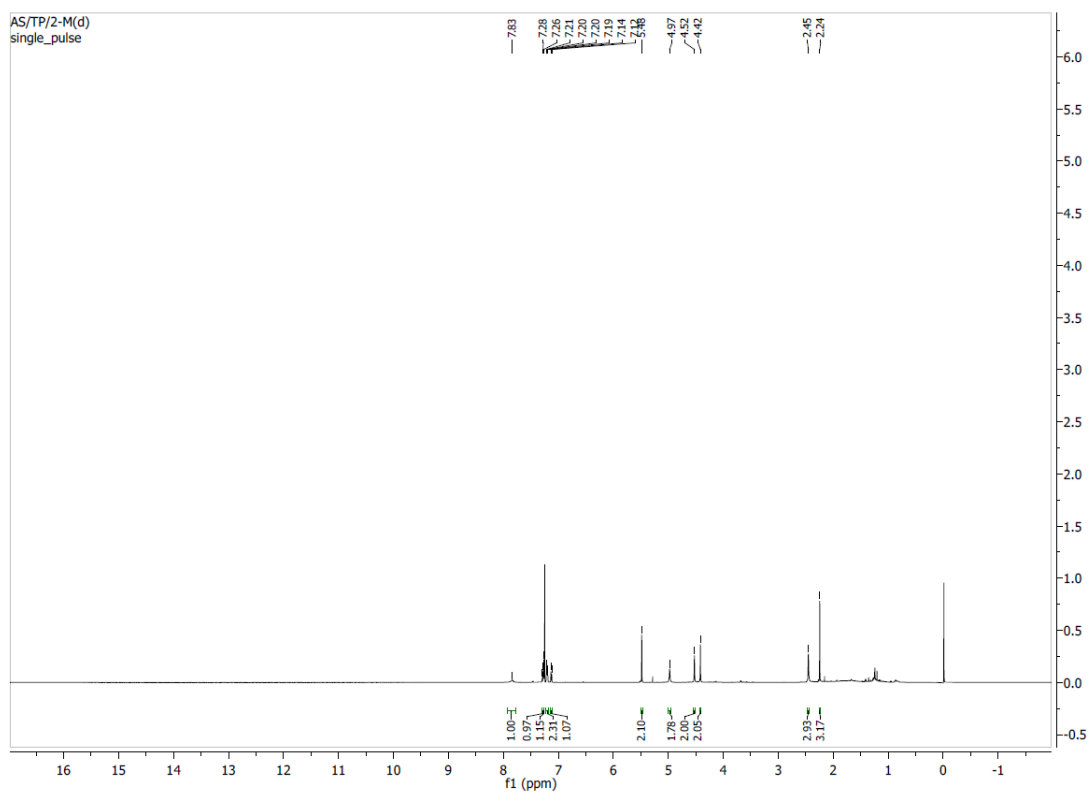


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.524	MM	0.0525	22.08498	7.01564	0.3168
2	2.972	MM	0.1079	8.18352	1.26425	0.1174
3	3.305	MM	0.0755	33.12366	7.30831	0.4752
4	5.086	MM	0.1269	154.34805	20.27901	2.2142
5	5.626	MM	0.1555	10.06588	1.07914	0.1444
6	7.268	MM	0.1465	11.67288	1.32804	0.1675
7	10.300	MM	0.0971	6677.85449	1145.75696	95.7973
8	11.985	MM	0.0984	36.92974	6.25713	0.5298
9	22.667	MM	0.0944	16.55604	2.92175	0.2375

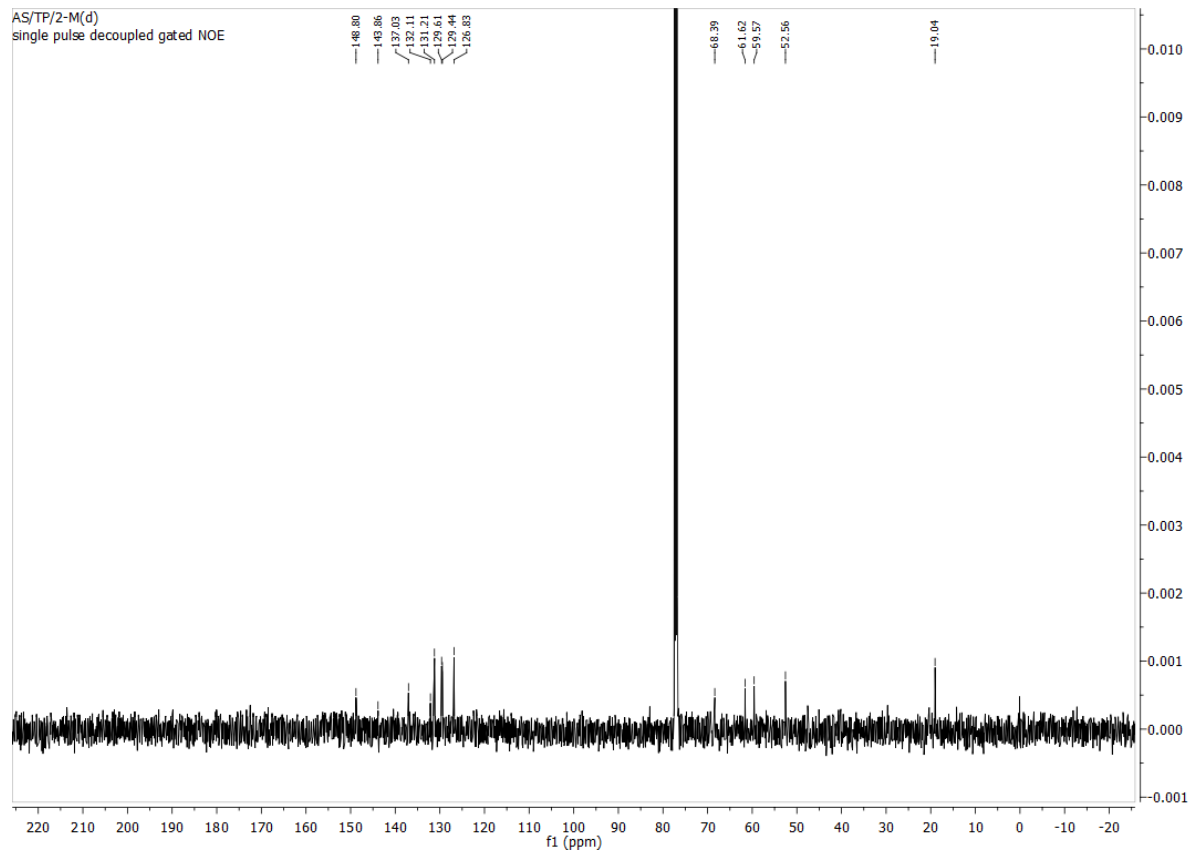
Totals : 6970.81925 1193.21024



HRMS Spectrum of **5d**



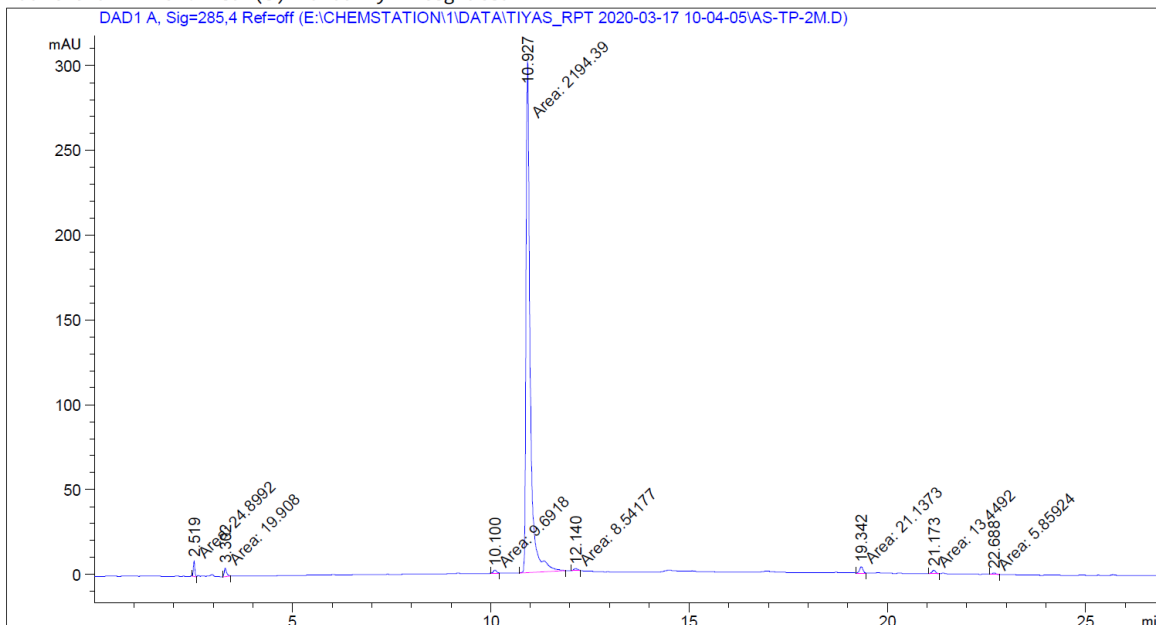
¹H NMR of **5d** in CDCl₃ at 500MHz



^{13}C NMR of **5d** in CDCl_3 at 125MHz

HPLC Purity data of **5d**

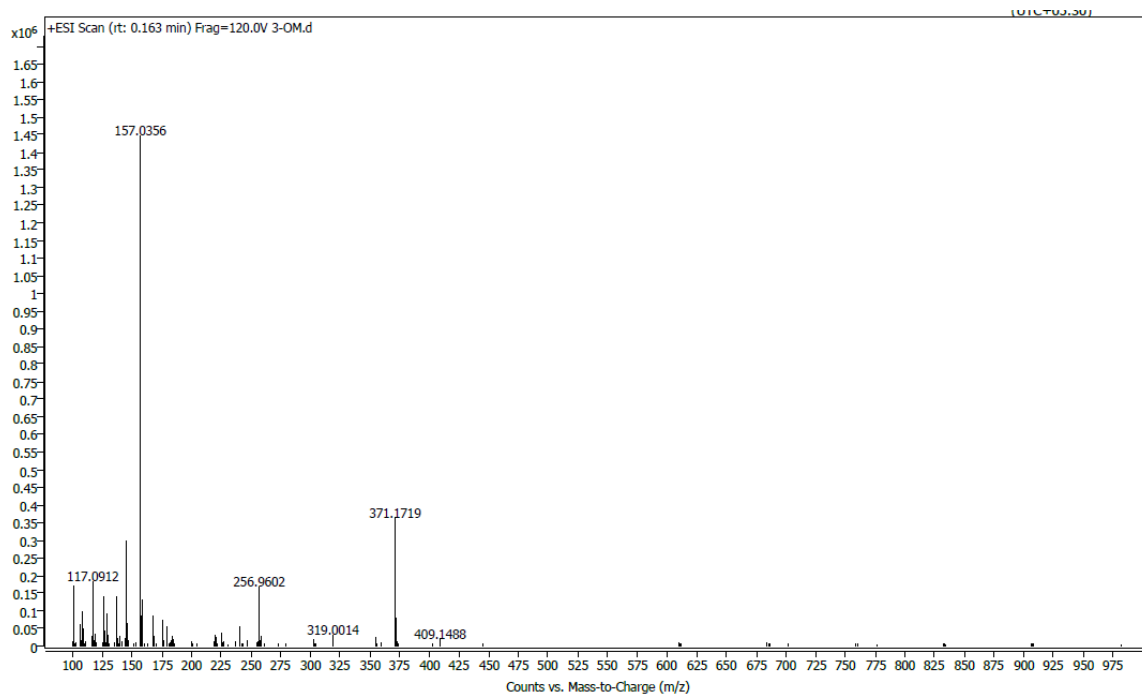
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Sample Operator : SYSTEM
Acq. Instrument : HPLC
Injection Date : 17-03-2020 13:24:49
Seq. Line : 8
Location : P2-B-08
Inj : 1
Inj Volume : 10.000 µl
Acq. Method : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 10-04-05\TIYAS_RPT.M
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Analysis Method : E:\CHEMSTATION\1\METHODS\WASH_AA_61_Min.M
Last changed : 18-03-2020 10:06:13 by SYSTEM
Additional Info : Peak(s) manually integrated



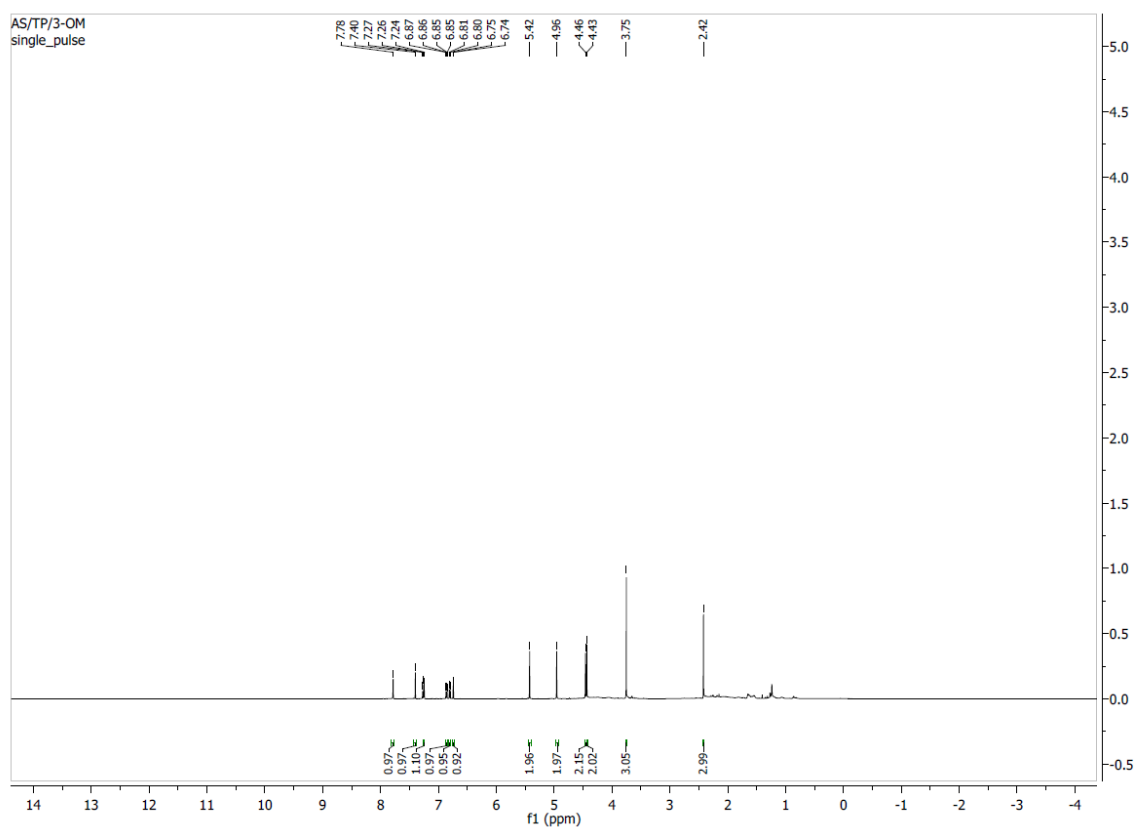
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.519	MM	0.0466	24.89920	8.89867	1.0836
2	3.302	MM	0.0655	19.90803	5.06209	0.8664
3	10.100	MM	0.0891	9.69180	1.81386	0.4218
4	10.927	MM	0.1210	2194.39136	302.31458	95.4964
5	12.140	MM	0.1177	8.54177	1.20907	0.3717
6	19.342	MM	0.0962	21.13725	3.66172	0.9199
7	21.173	MM	0.1084	13.44915	2.06748	0.5853
8	22.688	MM	0.1025	5.85924	9.52977e-1	0.2550

Totals : 2297.87780 325.98045

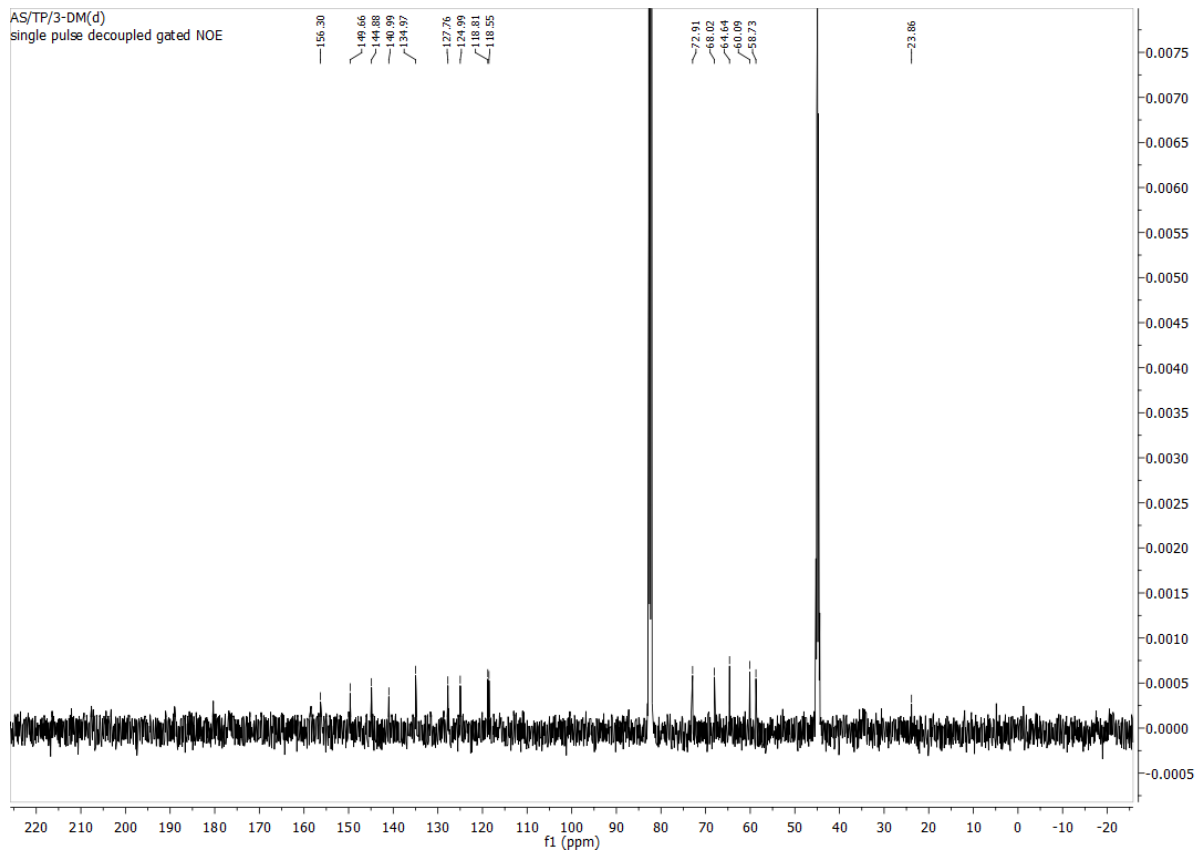
Spectral Data of 5e



HRMS Spectrum of 5e



¹H NMR of 5e in CDCl₃ at 500MHz



^{13}C NMR of **5e** in CDCl_3 and $\text{DMSO}-d_6$ at 125MHz

HPLC Purity of **5e**

Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 14-08-34\AS-TP-30M.D

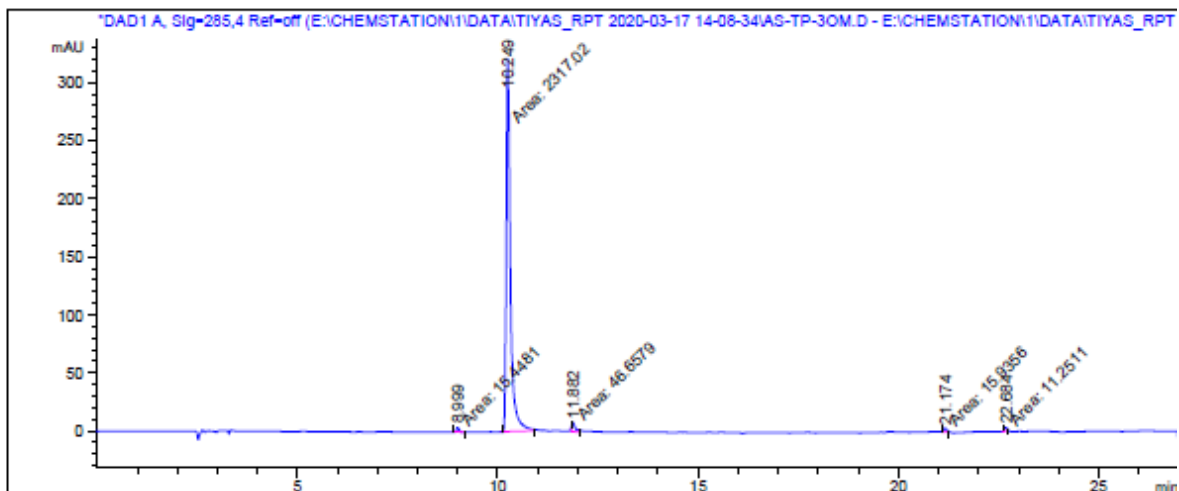
Sample Name: AS-TP-30M

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Sample Operator : SYSTEM
Acq. Instrument : HPLC                       Location  : P2-C-02
Injection Date  : 17-03-2020 16:03:55         Inj       :    1
                                                Inj Volume: 10.000 µl

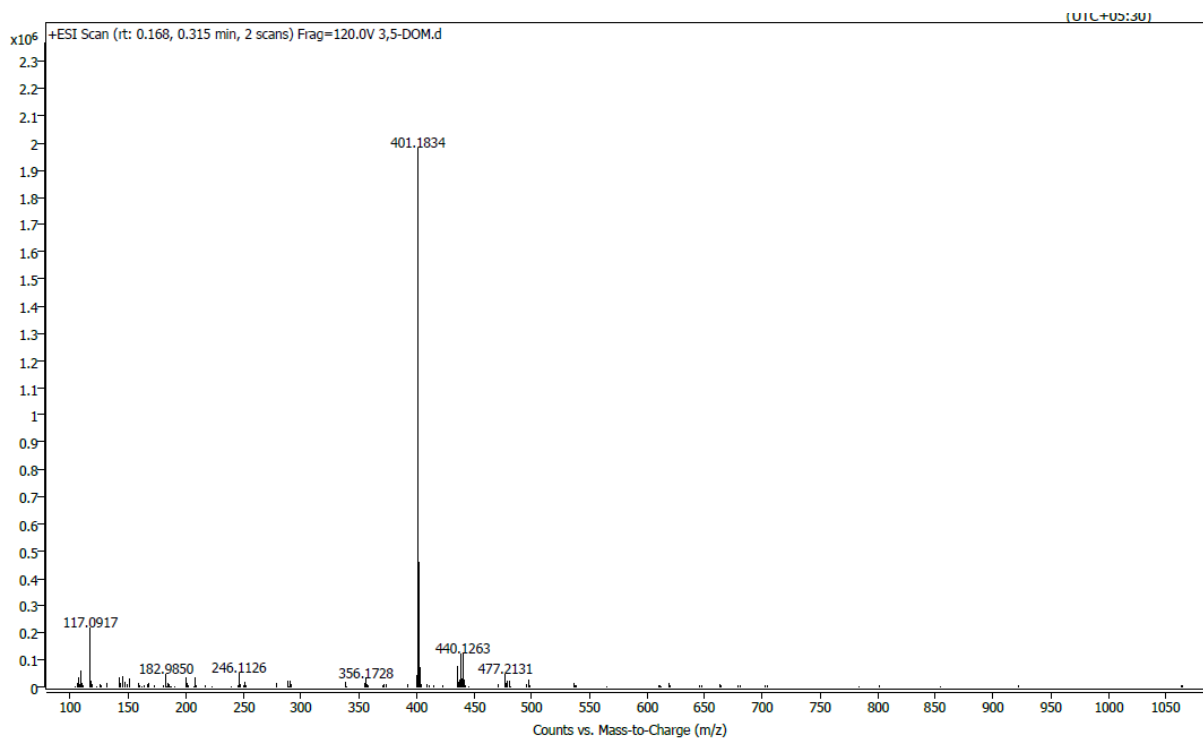
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Analysis Method : E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed   : 23-06-2020 11:45:48 by SYSTEM
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Additional Info : Peak(s) manually integrated
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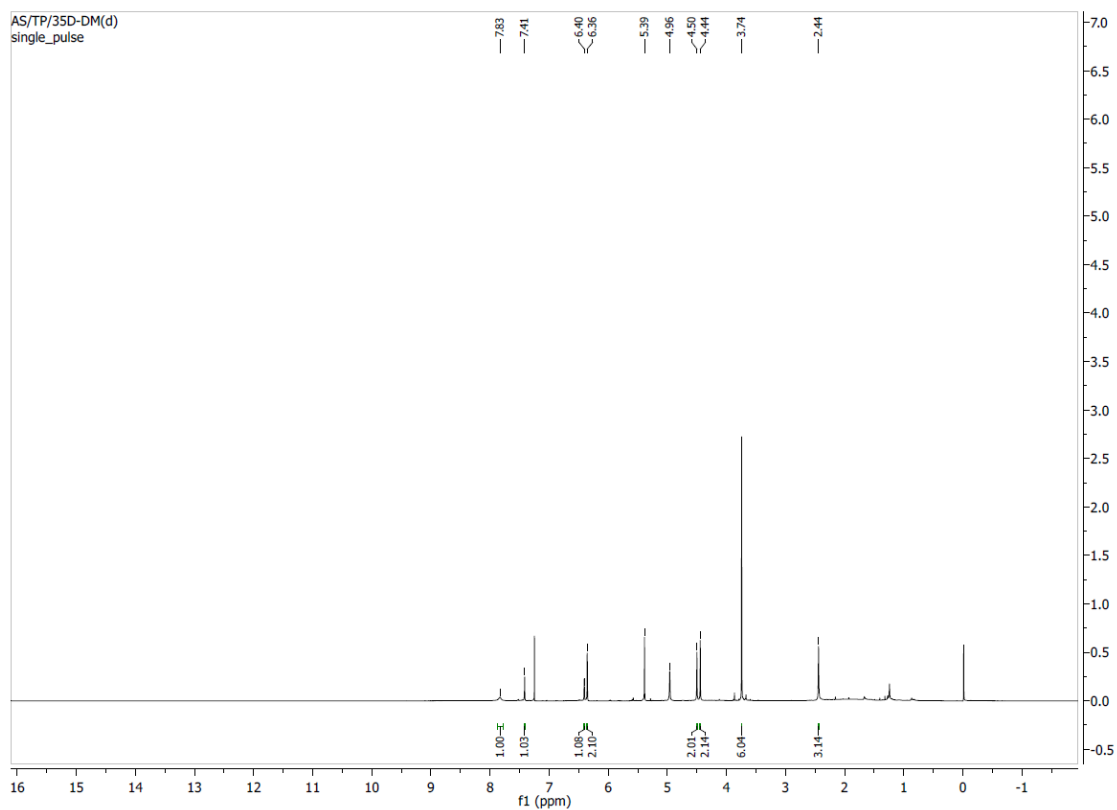


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.999	MM	0.0765	15.44812	3.36473	0.6420
2	10.249	MM	0.1201	2317.02490	321.51514	96.2892
3	11.882	MM	0.1023	46.65788	7.60121	1.9390
4	21.174	MM	0.0863	15.93561	3.07669	0.6622
5	22.684	MM	0.0660	11.25109	2.83984	0.4676

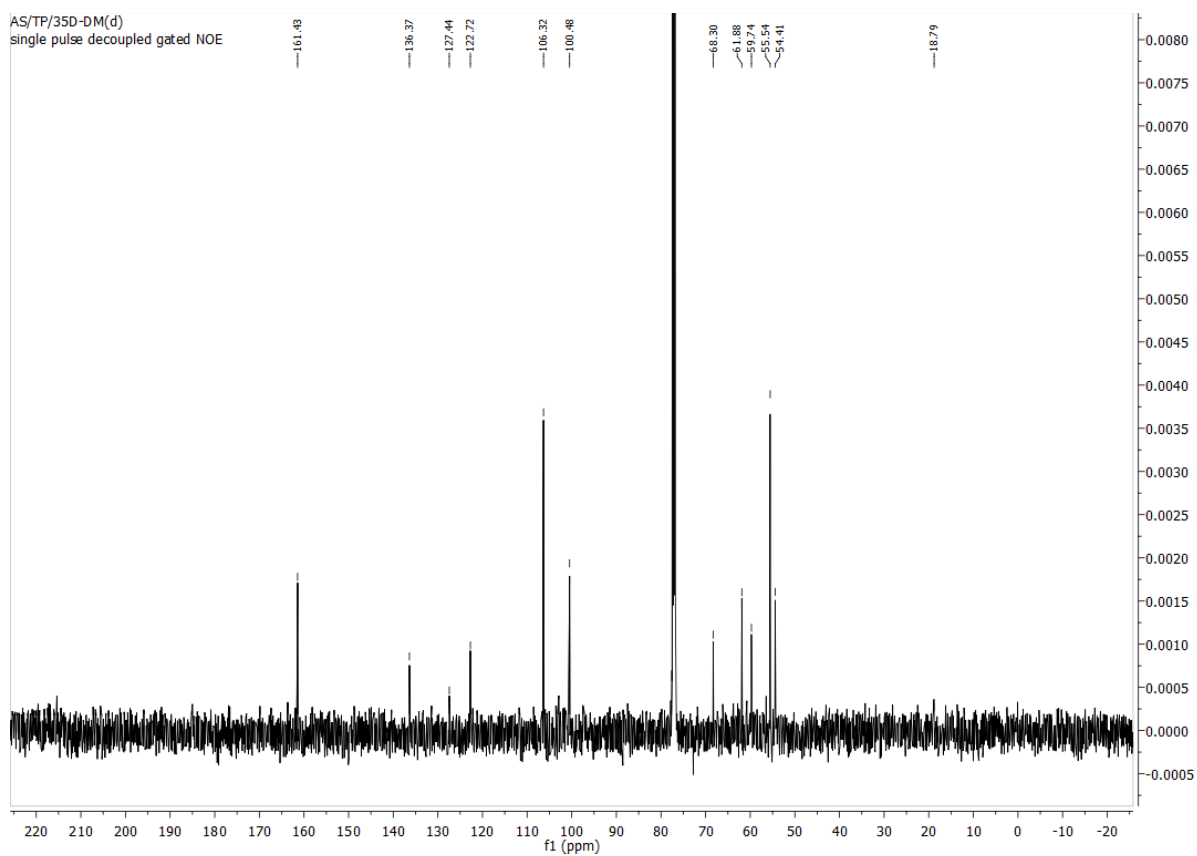
SPECTRAL DATA OF 5f



HRMS Spectrum of 5f



^1H NMR of **5f** in CDCl_3 at 500MHz

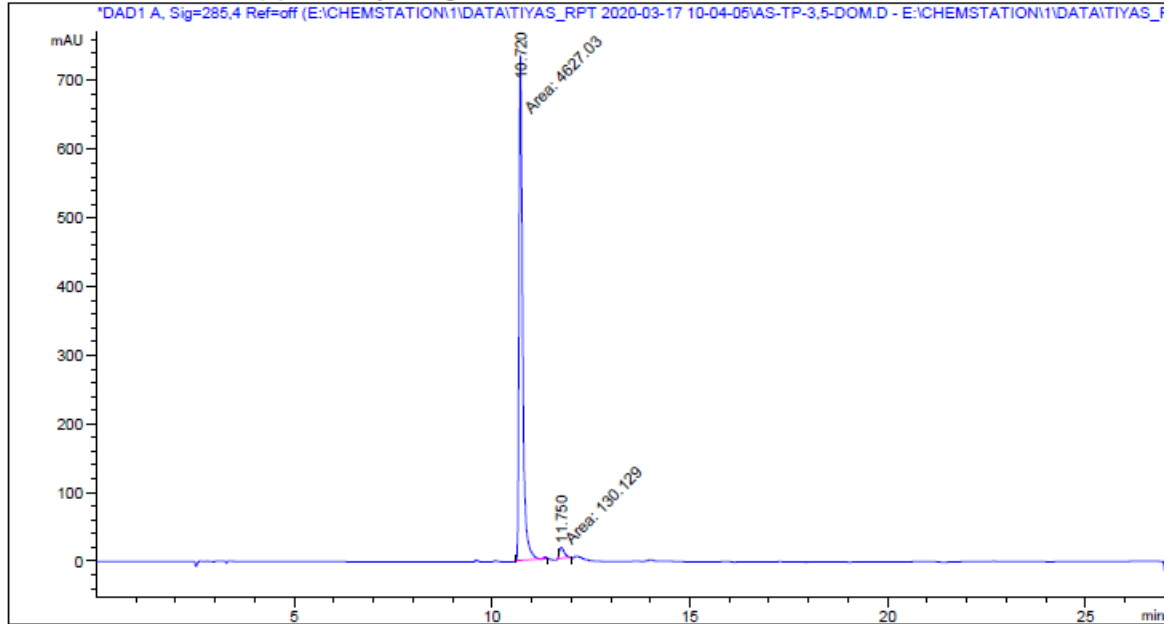


^{13}C NMR of **5f** in CDCl_3 at 500MHz

HPLC Purity Data of **5f**

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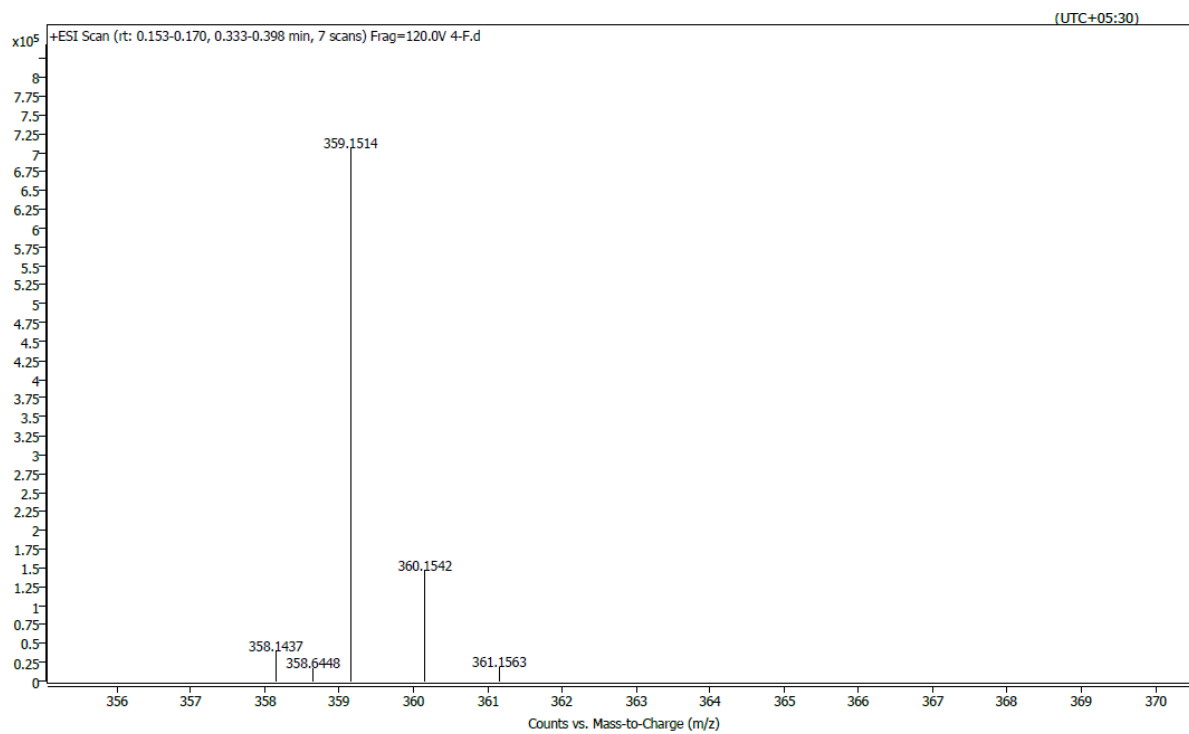
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Acq. Instrument : HPLC                      Location  : P2-B-04
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                                           Inj Volume: 10.000 µl
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Last changed    : 17-03-2020 10:01:12 by SYSTEM
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Additional Info  : Peak(s) manually integrated
  
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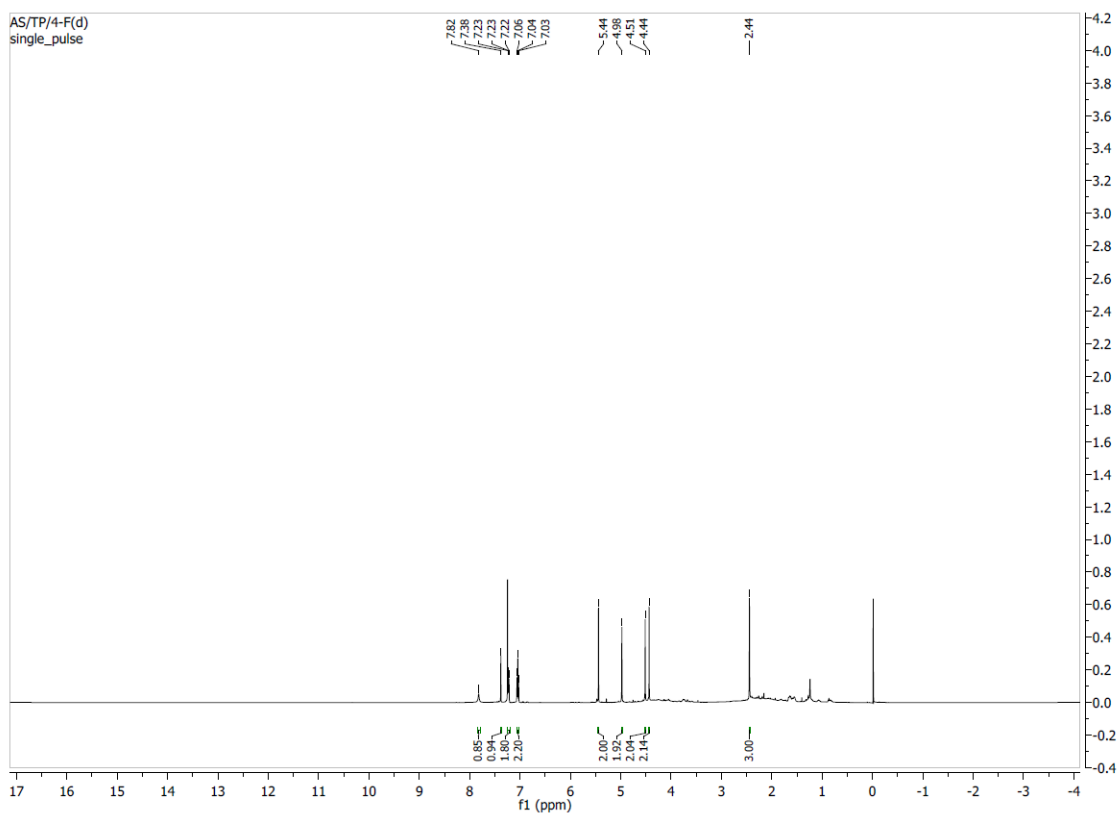
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.720	MM	0.1046	4627.03076	737.33258	97.2646
2	11.750	MM	0.1396	130.12878	15.53761	2.7354

Totals : 4757.15955 752.87019

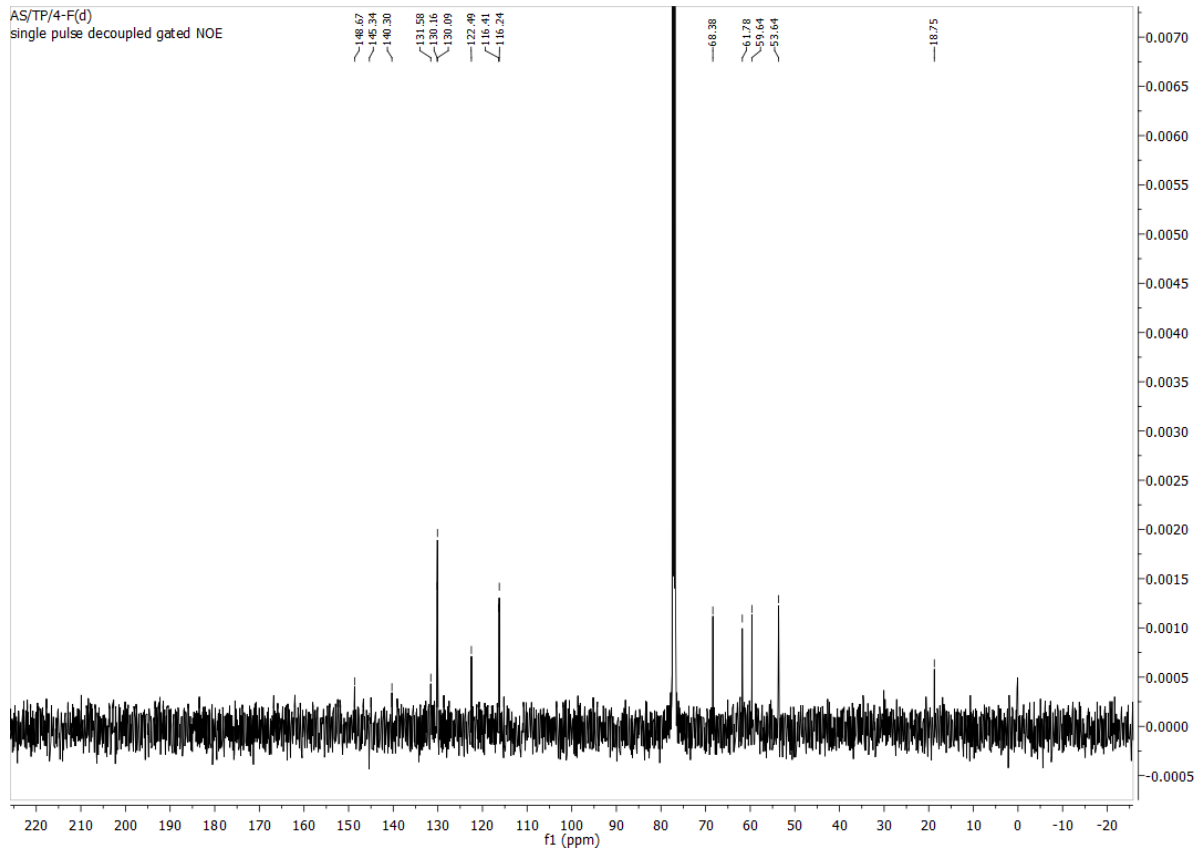
SPECTRAL DATA OF 5g



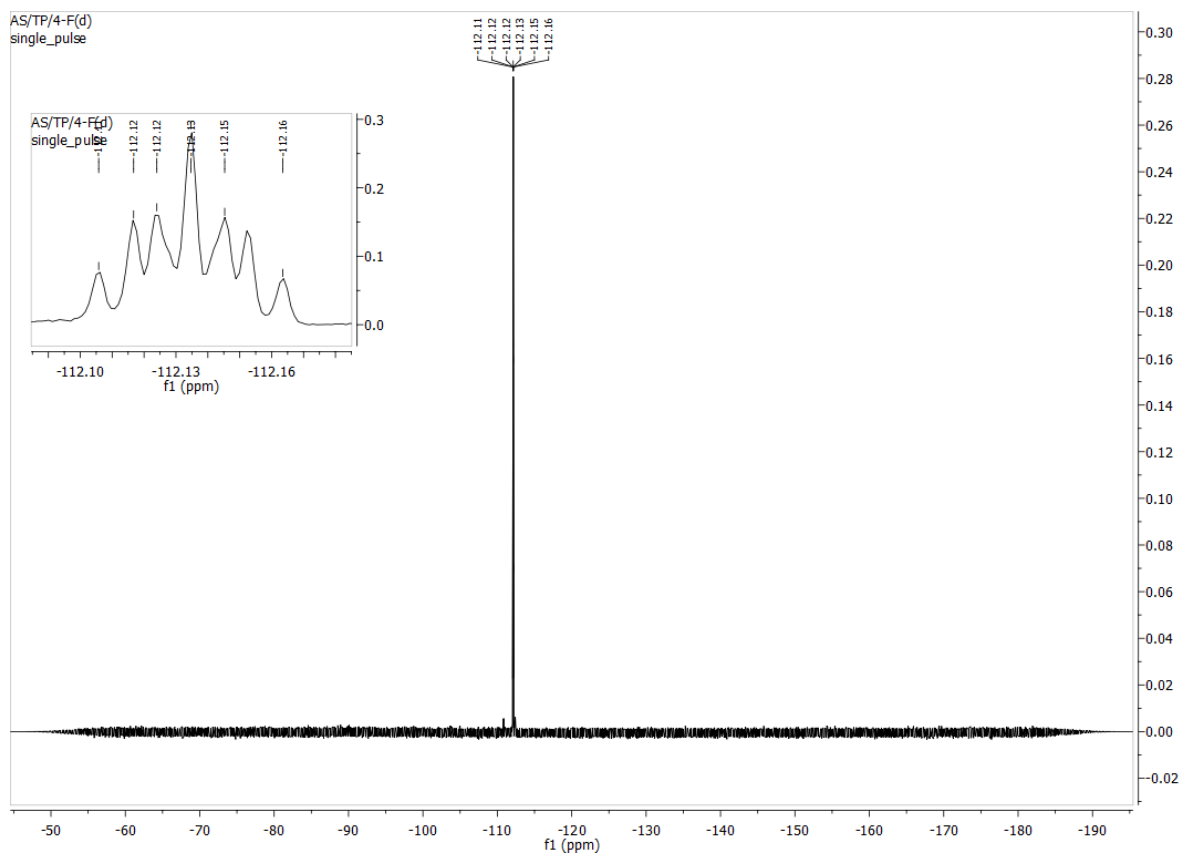
HRMS Spectrum of **5g**



¹H NMR of **5g** in CDCl₃ at 500MHz



^{13}C NMR of **5g** in CDCl_3 at 125MHz



^{19}F NMR of **5g** in CDCl_3 at 470MHz

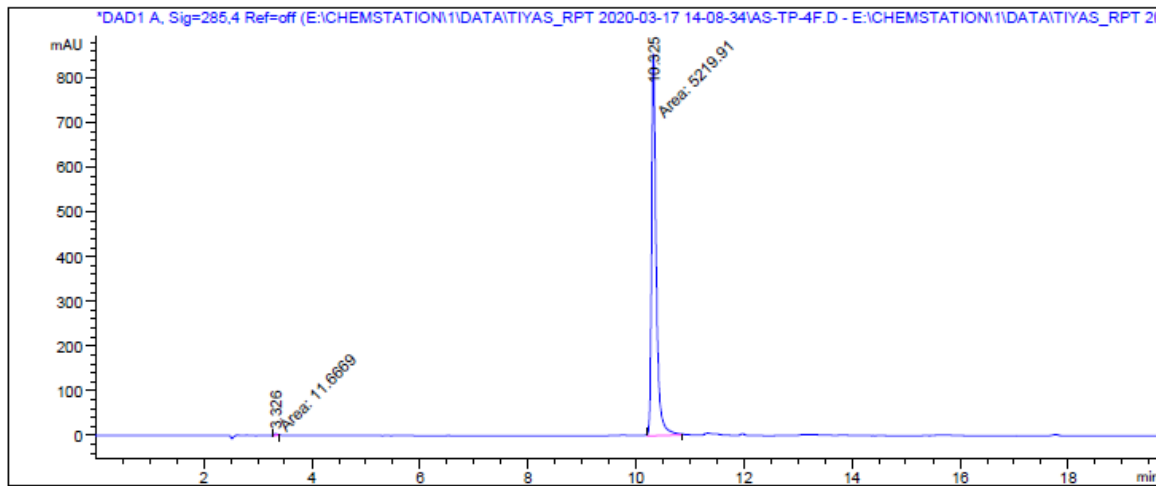
HPLC Purity Data of 5g

Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 14-08-34\AS-TP-4F.D
Sample Name: AS-TP-4F

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Sample Operator : SYSTEM
Acq. Instrument : HPLC                      Location  : P2-C-04
Injection Date  : 17-03-2020 17:00:52       Inj       :    1
                                                Inj Volume: 10.000 µl

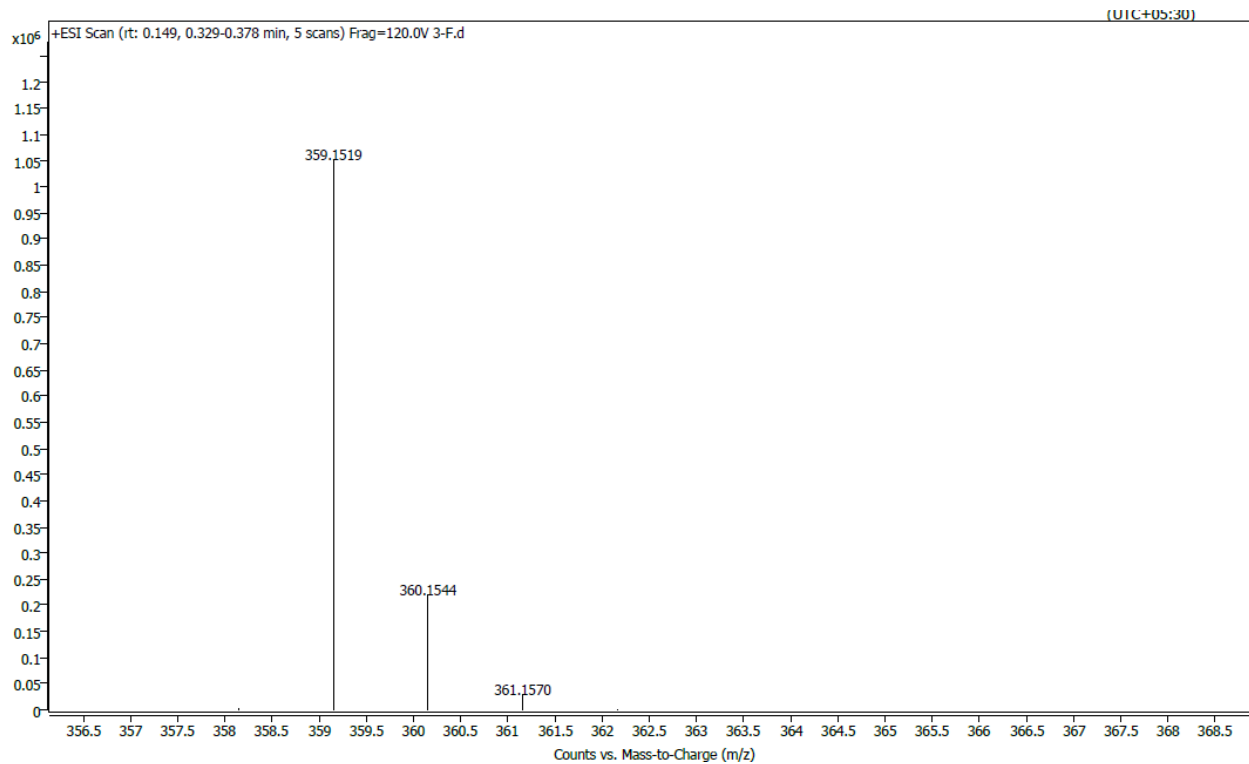
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Last changed    : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed    : 23-06-2020 11:45:48 by SYSTEM
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Additional Info : Peak(s) manually integrated
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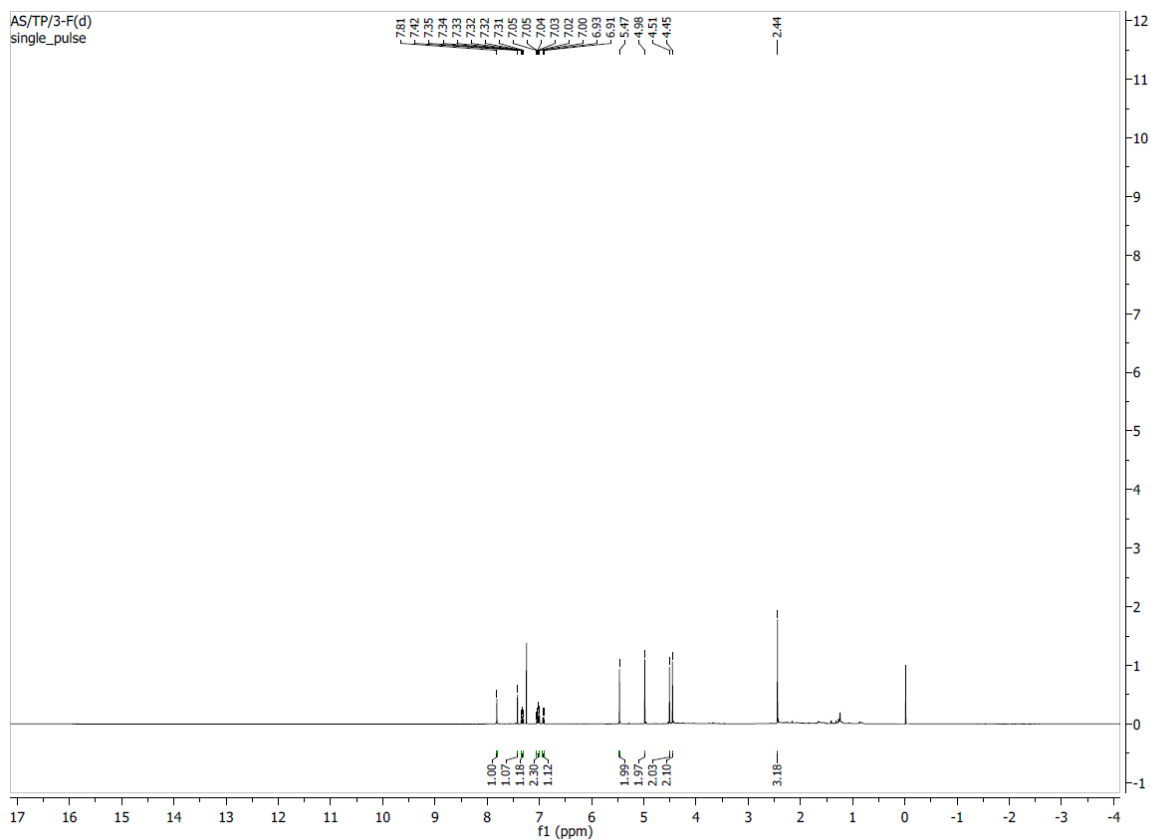


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.326	MM	0.0525	11.66694	3.70133	0.2230
2	10.325	MM	0.1016	5219.90576	856.56024	99.7770

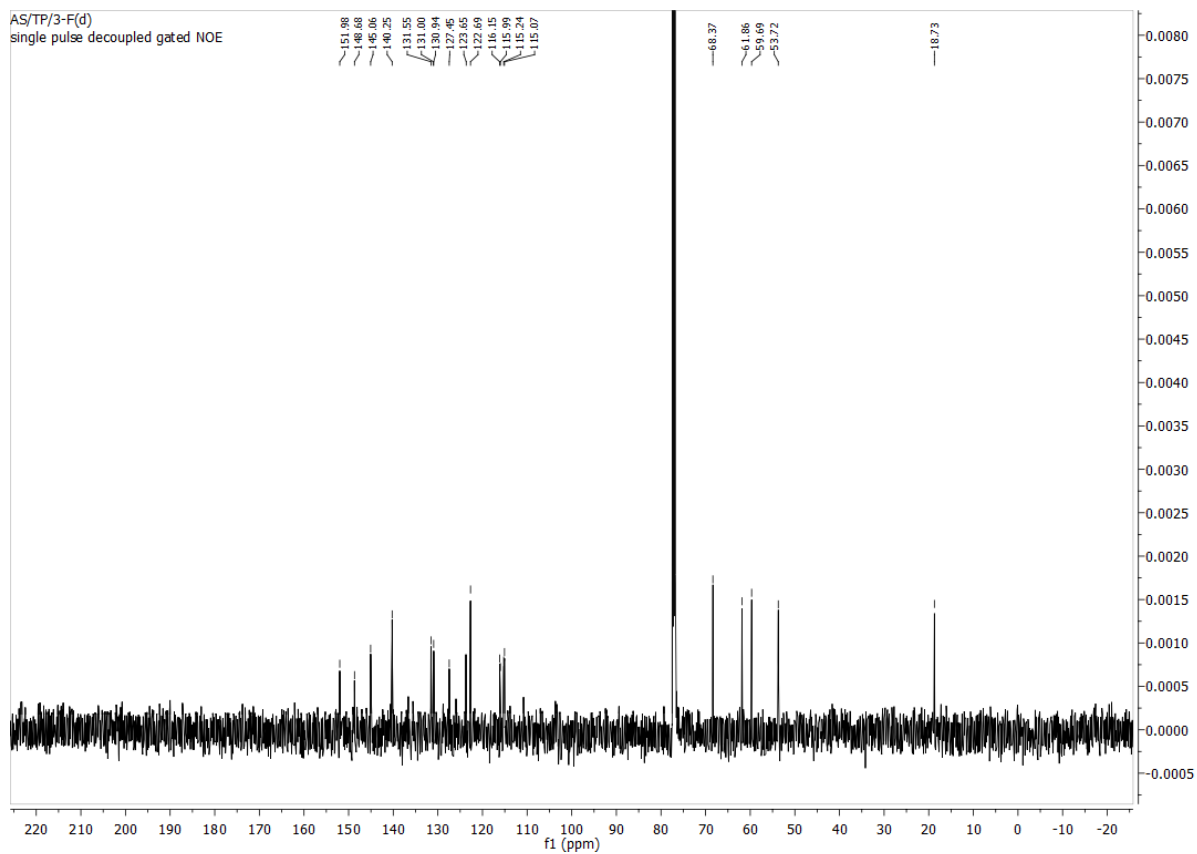
SPECTRAL DATA OF 5h



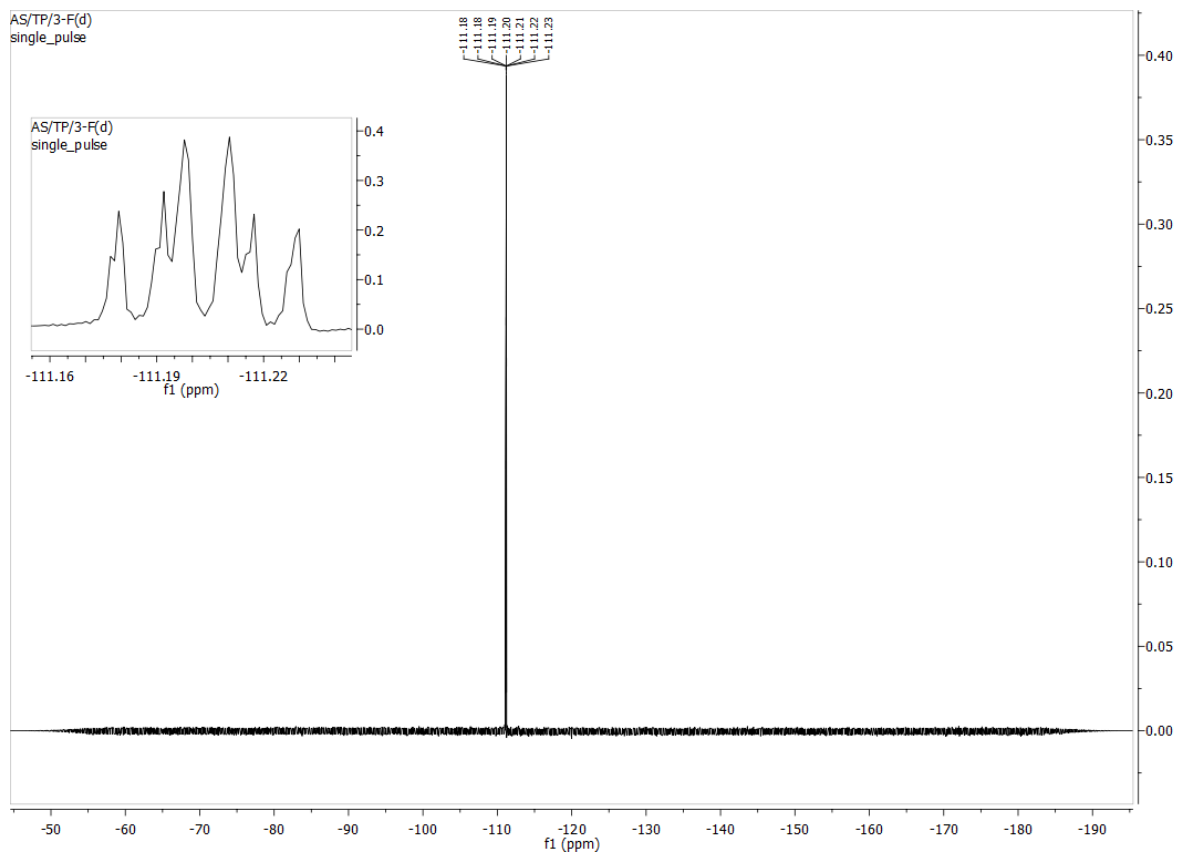
HRMS Spectrum of **5h**



¹H NMR of **5h** in CDCl₃ at 500MHz



^{13}C NMR of **5h** in CDCl_3 at 125MHz



^{19}F NMR of **5h** in CDCl_3 at 470MHz

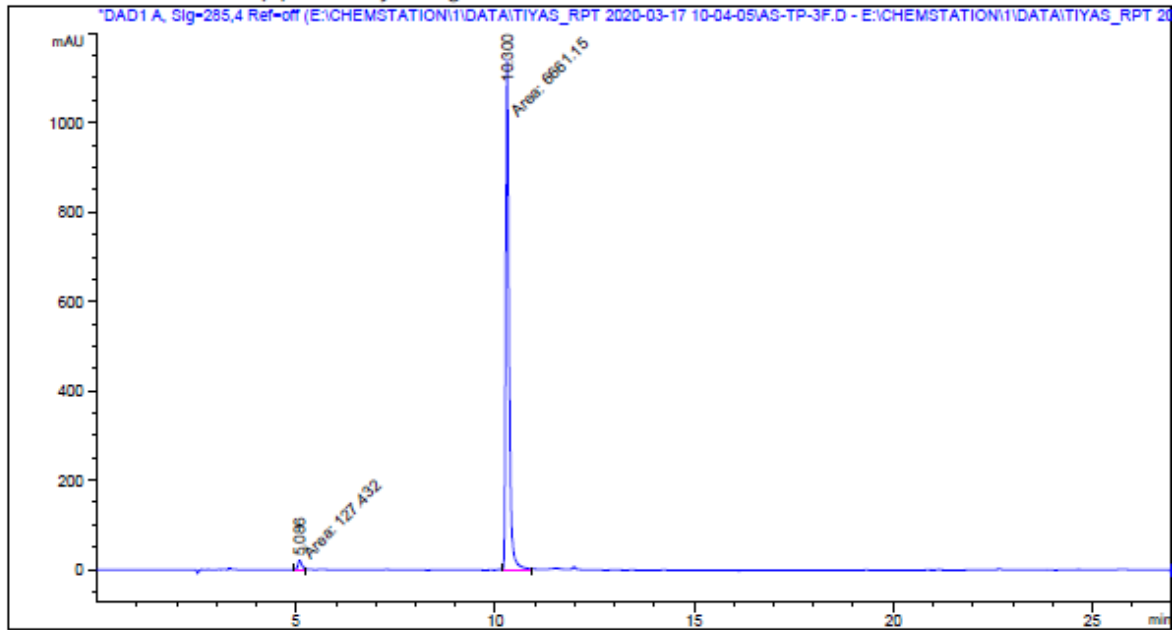
HPLC Purity Data of 5h

Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 10-04-05\AS-TP-3F.D
 Sample Name: AS-TP-3F

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Sample Operator : SYSTEM
Acq. Instrument : HPLC                      Location  : P2-B-03
Injection Date  : 17-03-2020 11:02:21        Inj       :    1
                                           Inj Volume: 10.000 µl

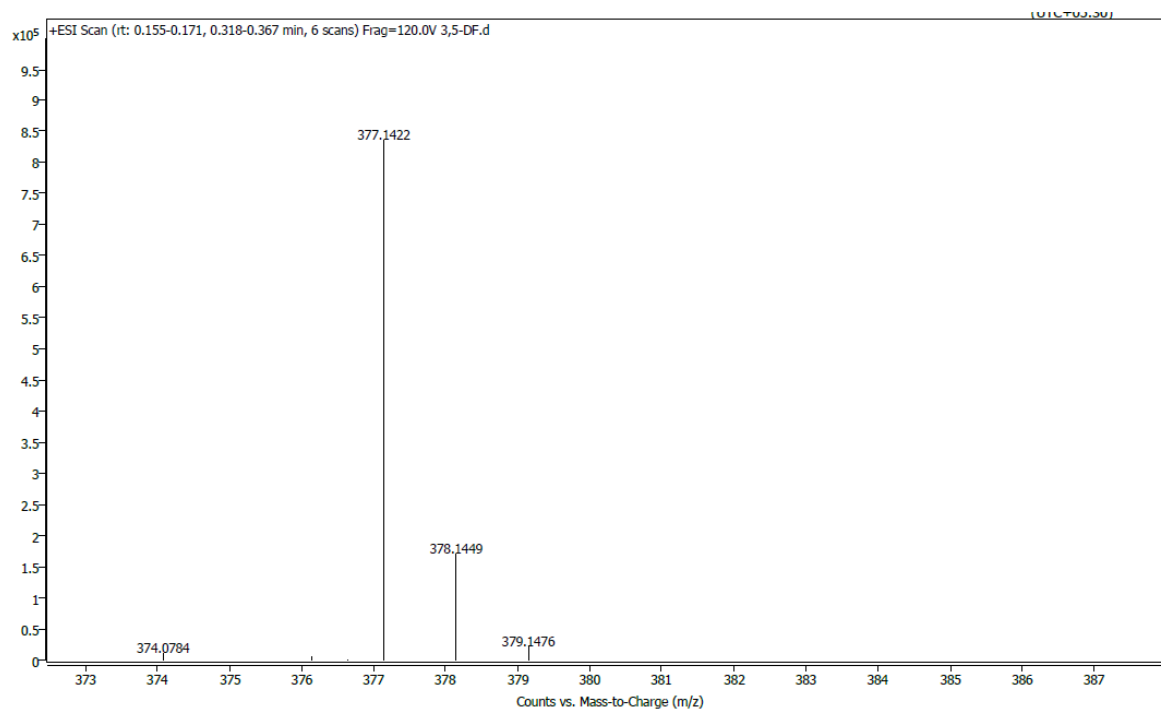
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Last changed    : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\CHEMSTATION\1\METHODS\TIYAS_RPT.M
Last changed    : 23-06-2020 12:51:16 by SYSTEM
Additional Info : Peak(s) manually integrated
  
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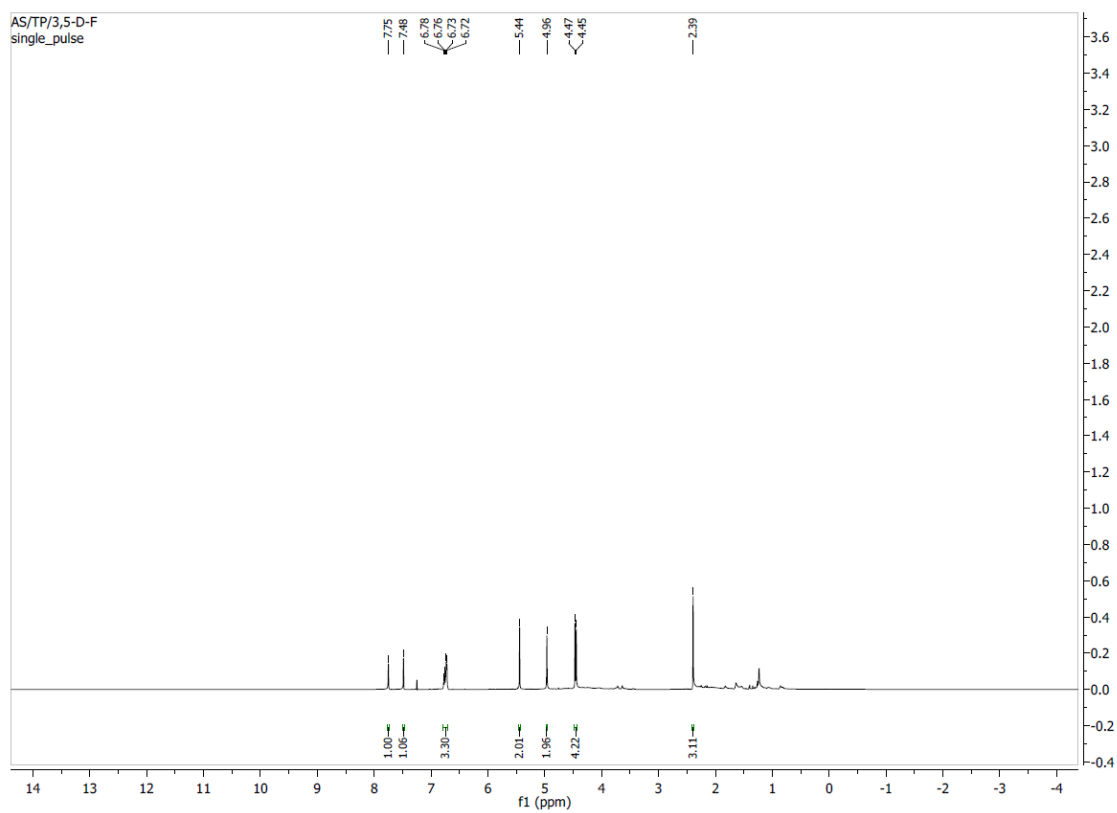
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.086	MM	0.1105	127.43169	19.22895	1.8771
2	10.300	MM	0.0970	6661.14844	1144.58276	98.1229

Totals : 6788.58012 1163.81171

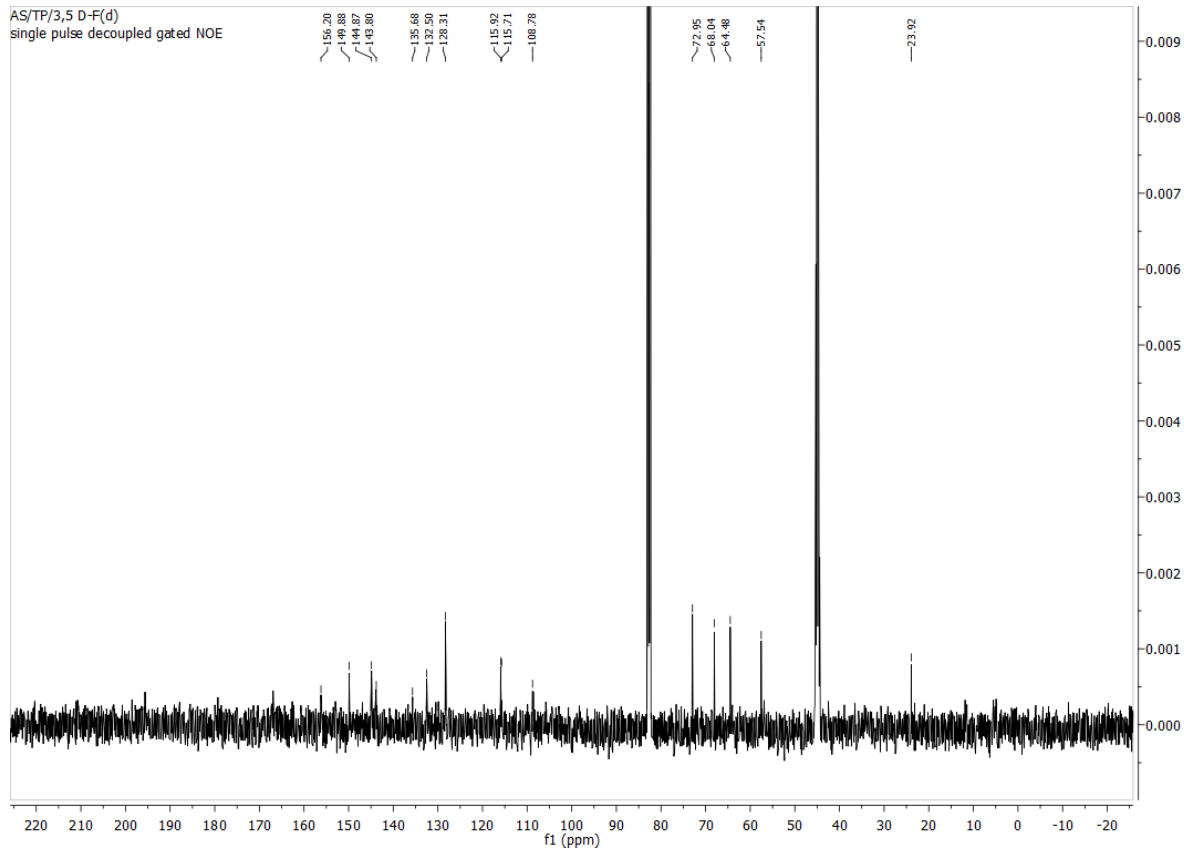
SPECTRAL DATA OF **5i**



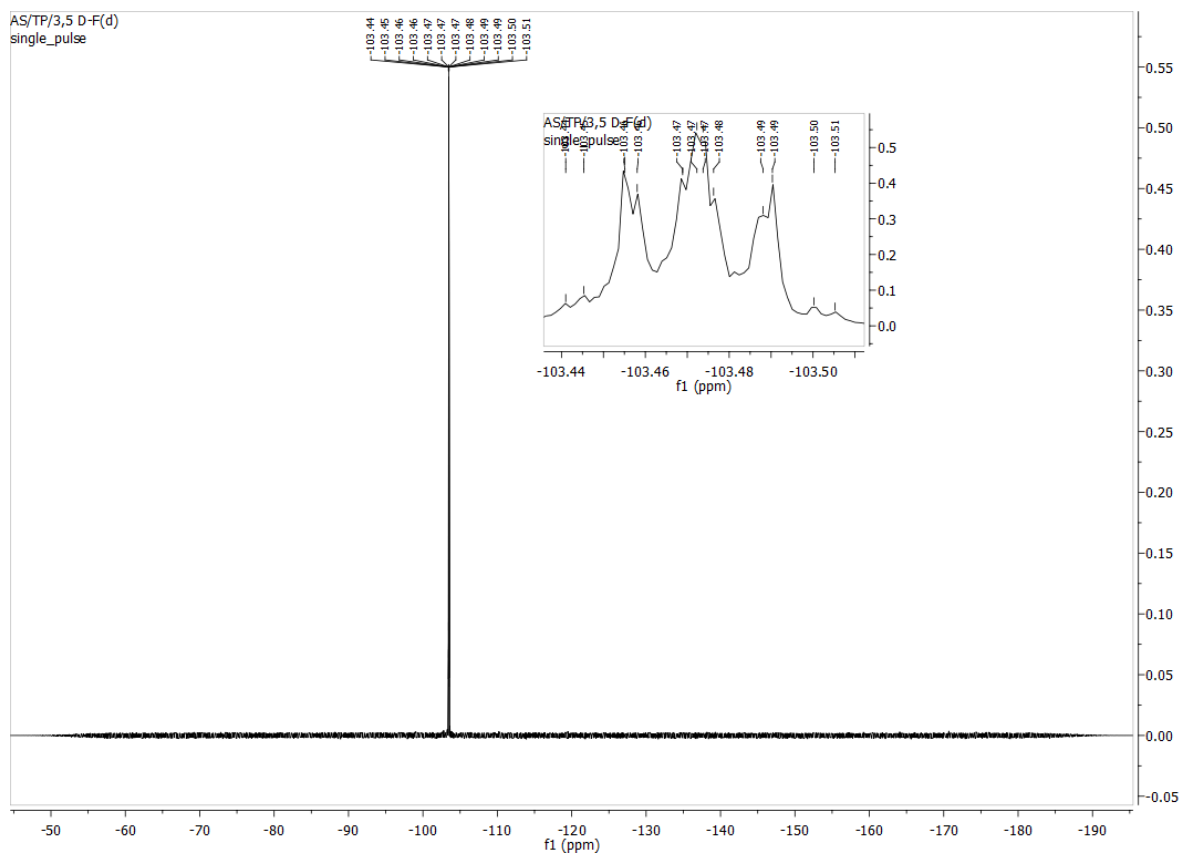
HRMS Spectrum of **5i**



¹H NMR of **5i** in CDCl₃ at 500MHz



^{13}C NMR of **5i** in CDCl_3 and $\text{DMSO}-d_6$ at 125MHz

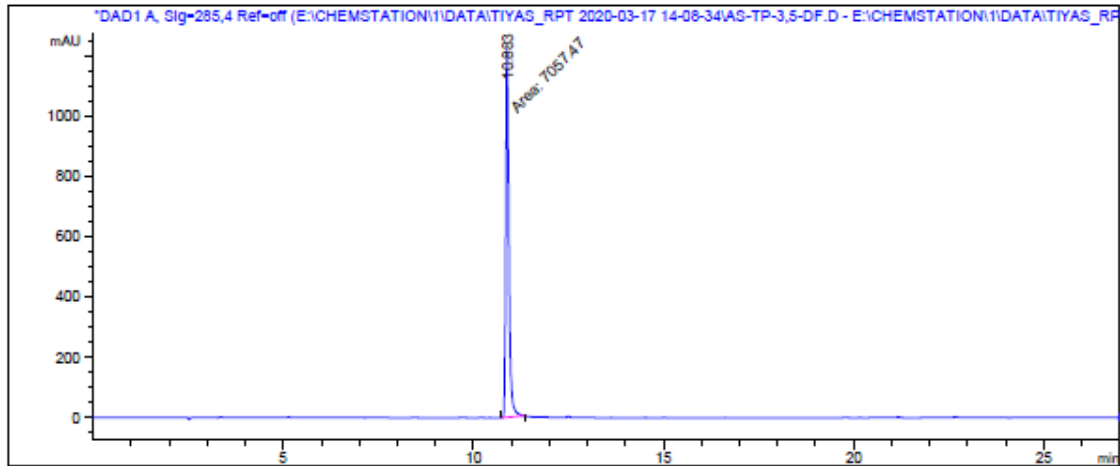


^{19}F NMR of **5i** in CDCl_3 at 470MHz

HPLC Purity Data of 5i

Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 14-08-34\AS-TP-3,5-DF.D
Sample Name: AS-TP-3,5-DF

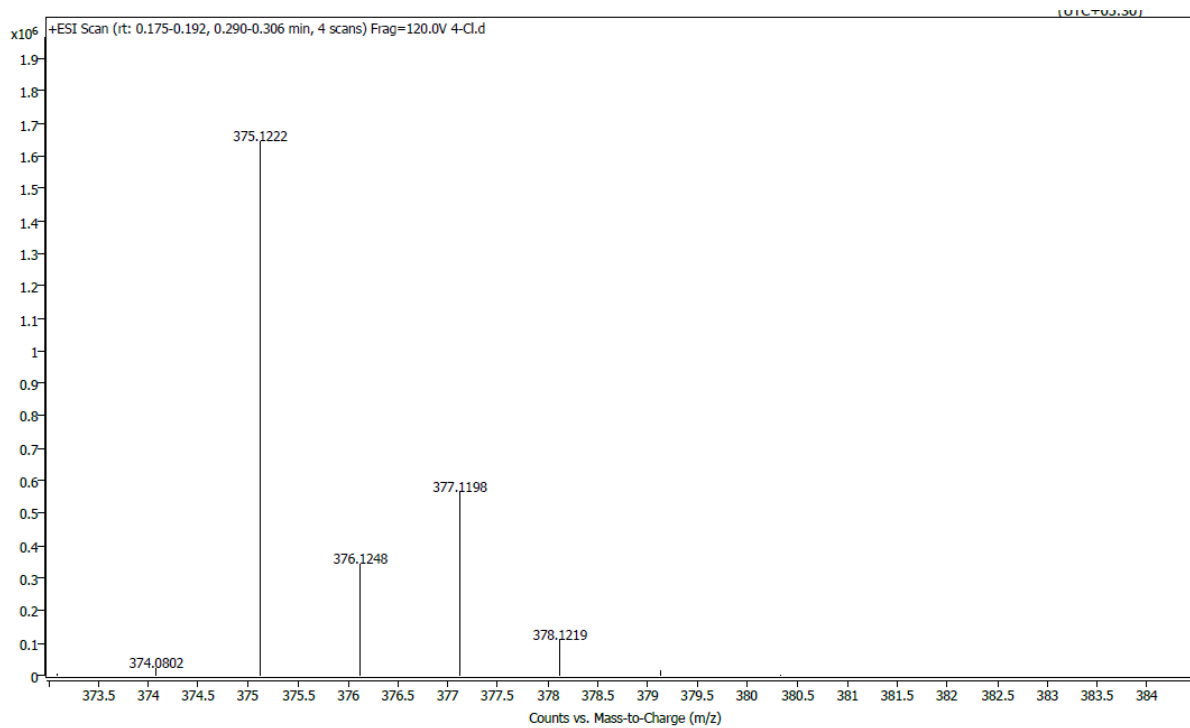
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Sample Operator : SYSTEM
Acq. Instrument : HPLC                       Location  : P2-C-01
Injection Date  : 17-03-2020 15:35:26       Inj       :    1
                                           Inj Volume: 10.000 µl
Acq. Method     : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 14-08-34\TIYAS_RPT.M
Last changed    : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed    : 23-06-2020 11:45:48 by SYSTEM
                (modified after loading)
Additional Info : Peak(s) manually integrated
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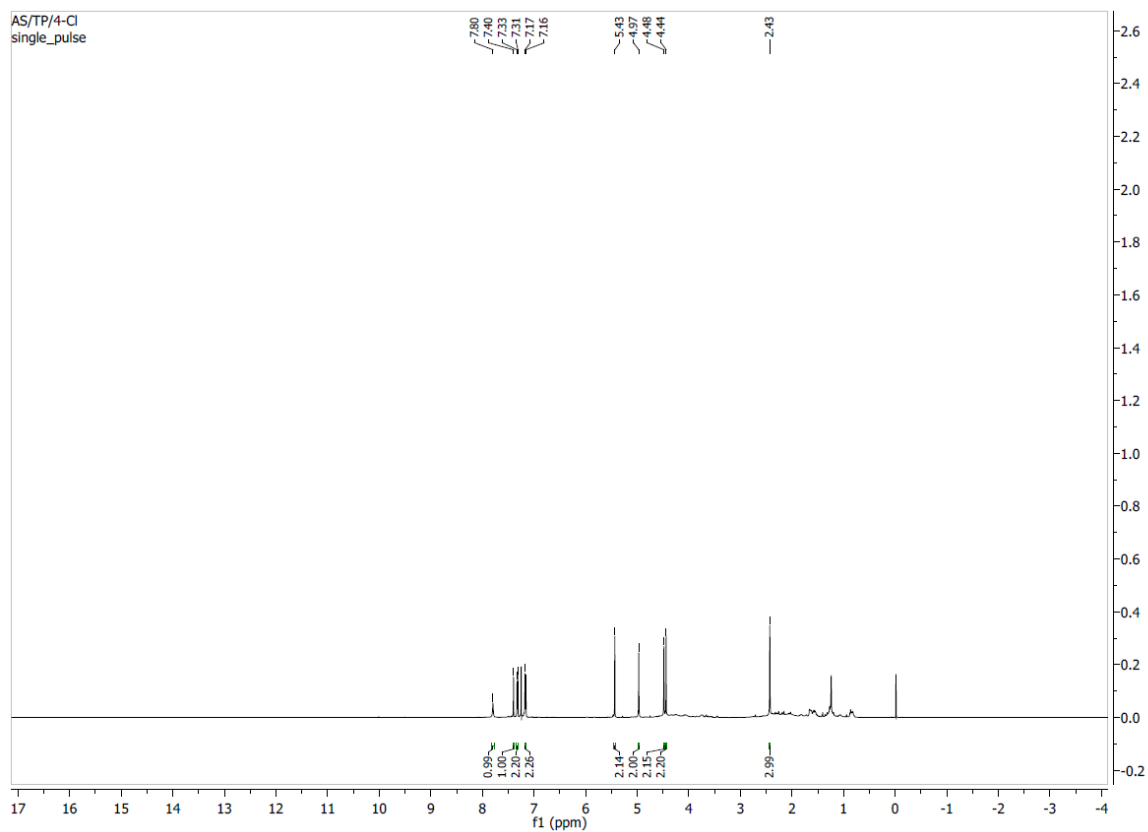
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.883	MM	0.0964	7057.46729	1220.70032	100.0000

Totals : 7057.46729 1220.70032

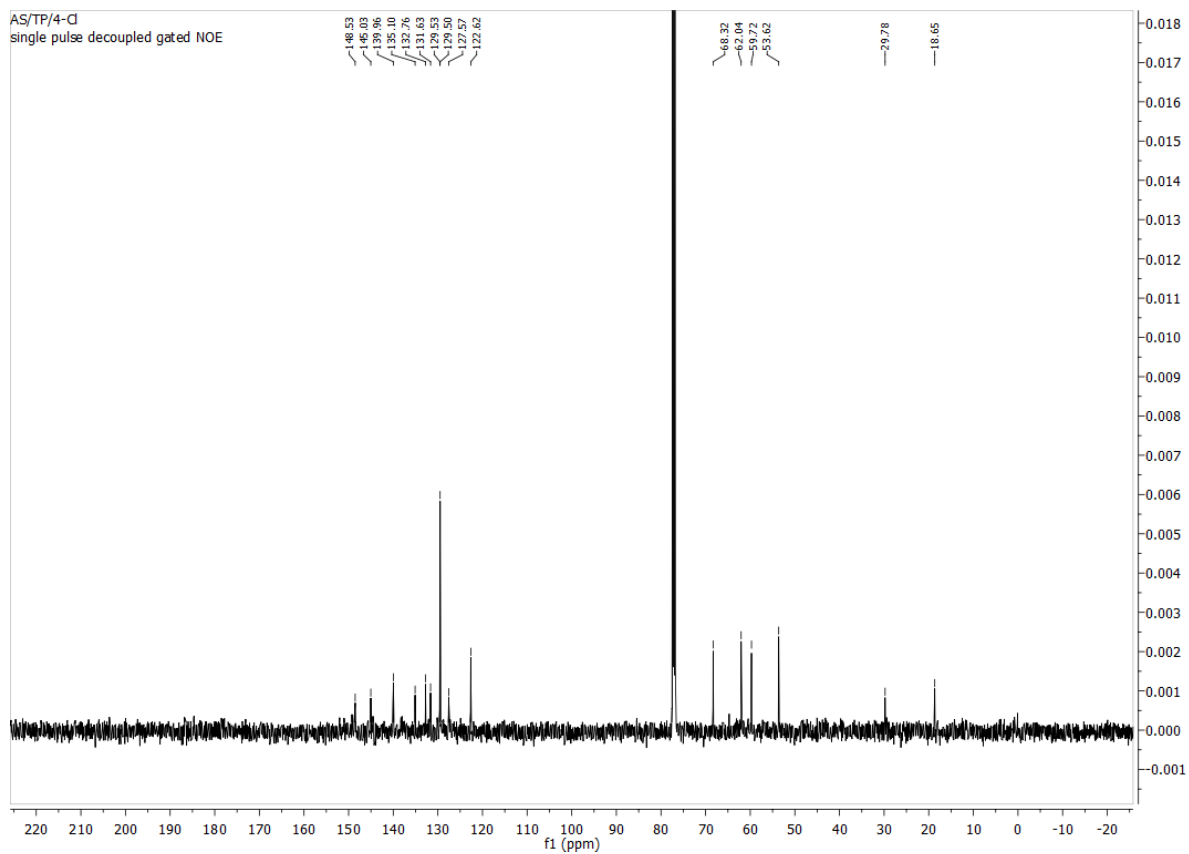
SPECTRAL DATA OF 5j



HRMS Spectrum of **5j**



¹H NMR of **5j** in CDCl₃ at 500MHz



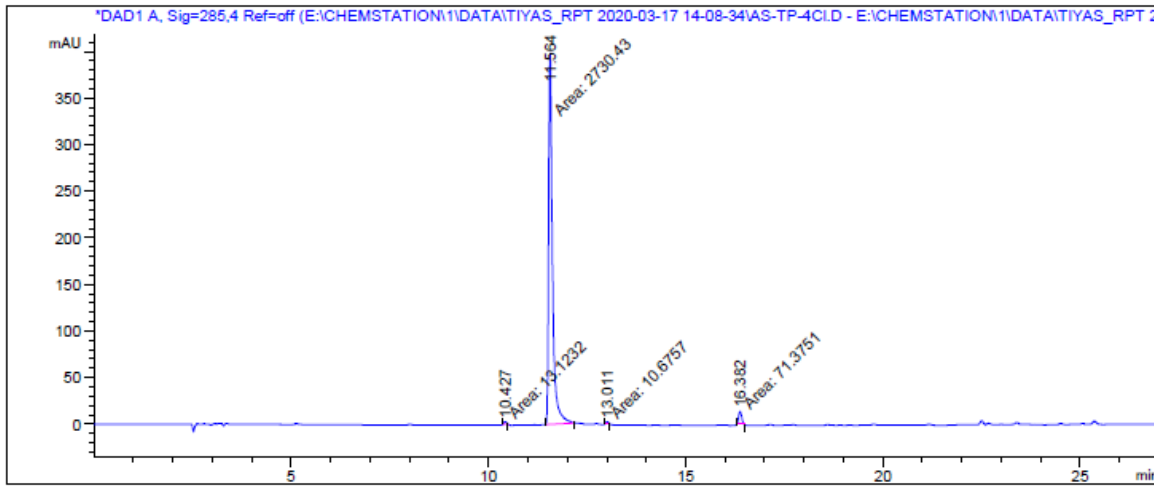
^{13}C NMR of **5j** in CDCl_3 at 125MHz

HPLC Purity Data of **5j**

Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 14-08-34\AS-TP-4C1.D
 Sample Name: AS-TP-4C1

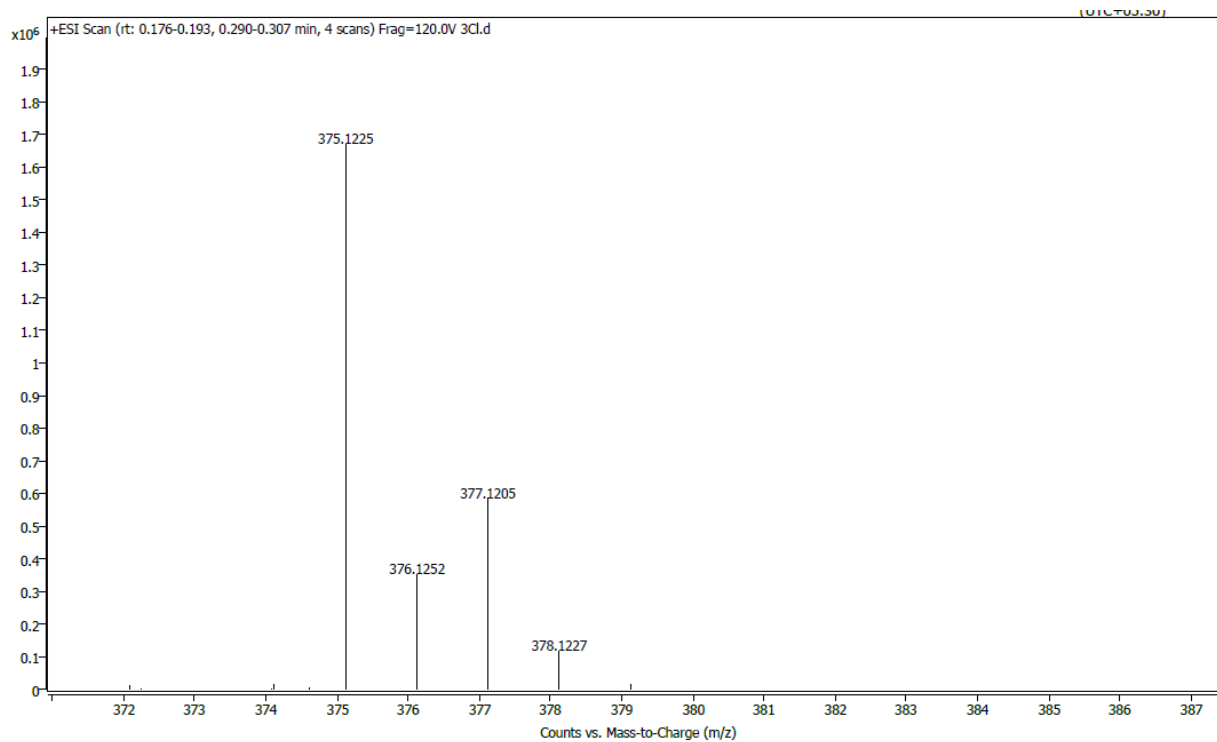
```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    3
Sample Operator : SYSTEM
Acq. Instrument : HPLC                      Location  : P2-B-11
Injection Date  : 17-03-2020 15:06:55       Inj       :    1
                                           Inj Volume: 10.000 µl
Acq. Method    : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 14-08-34\TIYAS_RPT.M
Last changed   : 17-03-2020 10:01:12 by SYSTEM
Analysis Method: E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed   : 23-06-2020 11:45:48 by SYSTEM
                (modified after loading)
Additional Info : Peak(s) manually integrated
=====
  
```

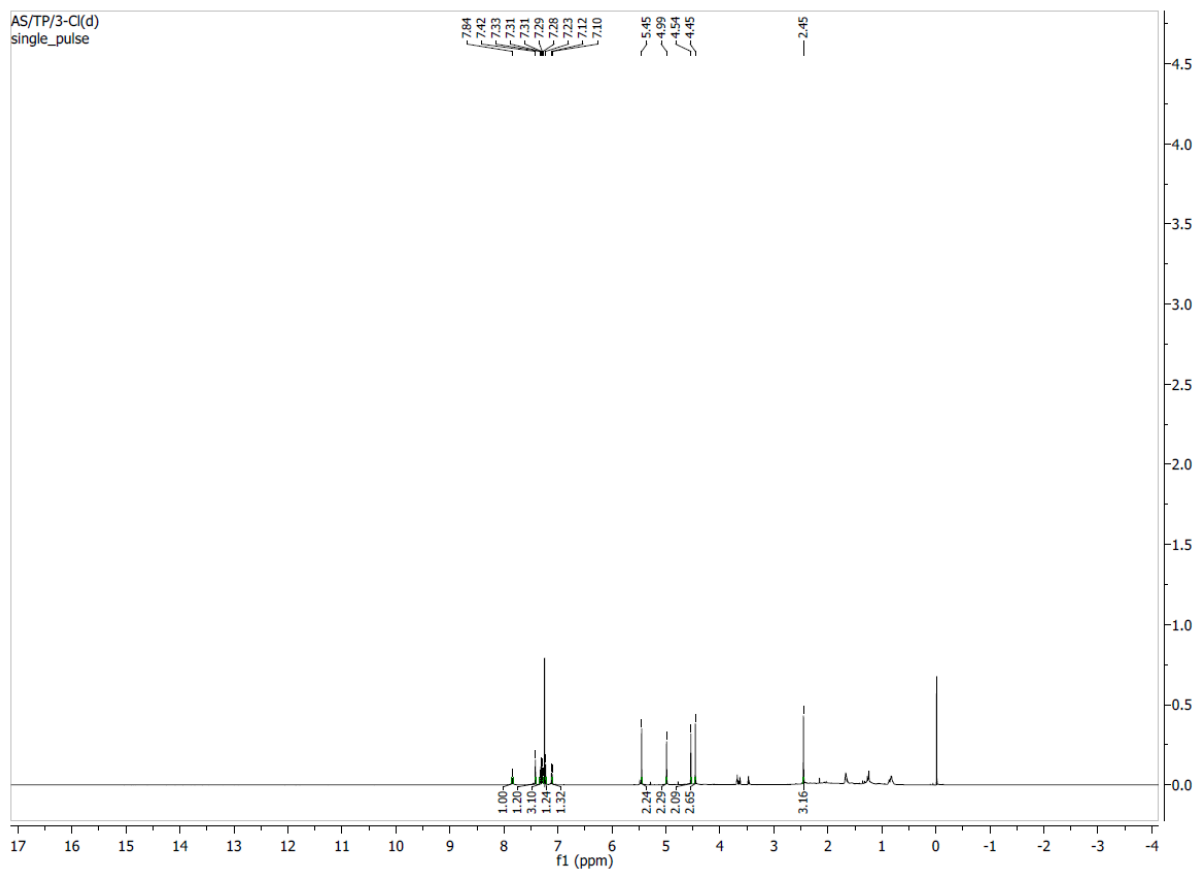


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.427	MM	0.0739	13.12324	2.95965	0.4644
2	11.564	MM	0.1136	2730.43091	400.41803	96.6317
3	13.011	MM	0.0673	10.67574	2.64308	0.3778
4	16.382	MM	0.0882	71.37511	13.49467	2.5260
Totals :				2825.60500	419.51544	

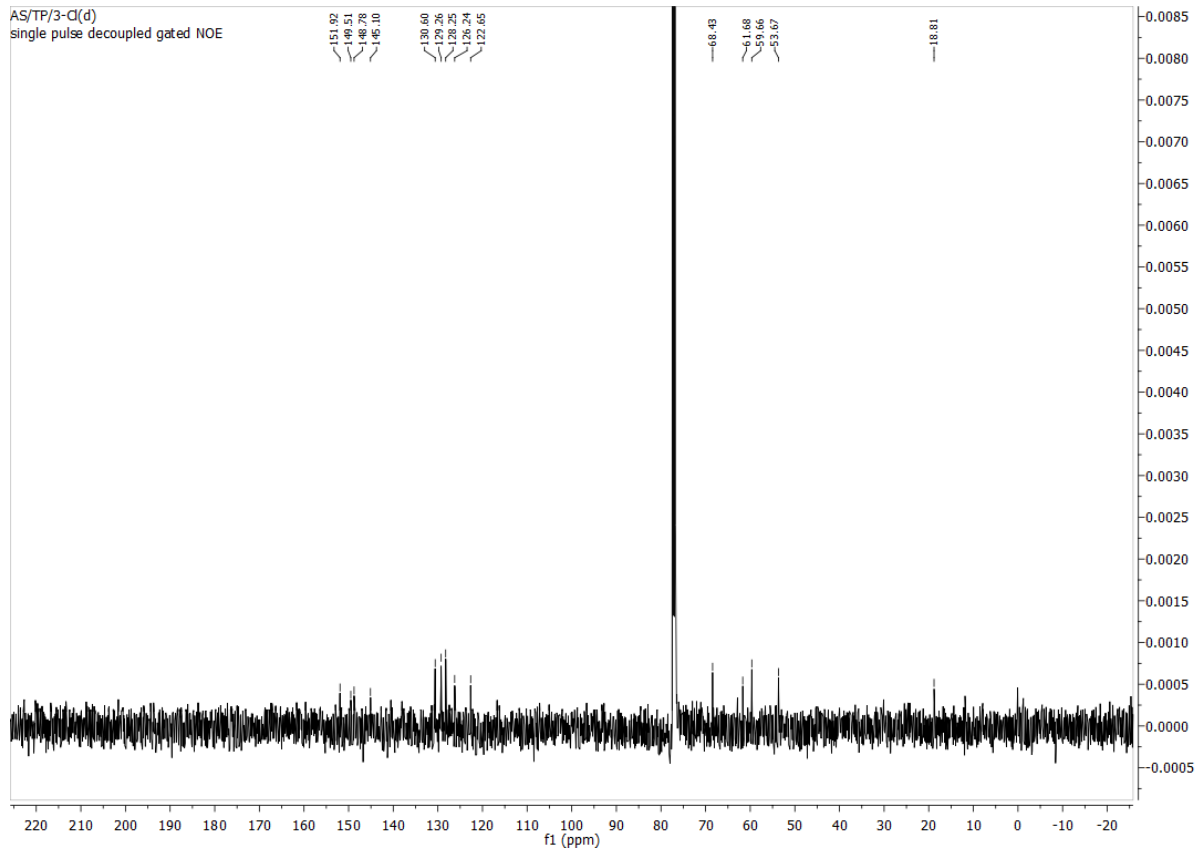
SPECTRAL DATA OF 5k



HRMS Spectrum of **5k**



¹H NMR of **5k** in CDCl₃ at 500MHz

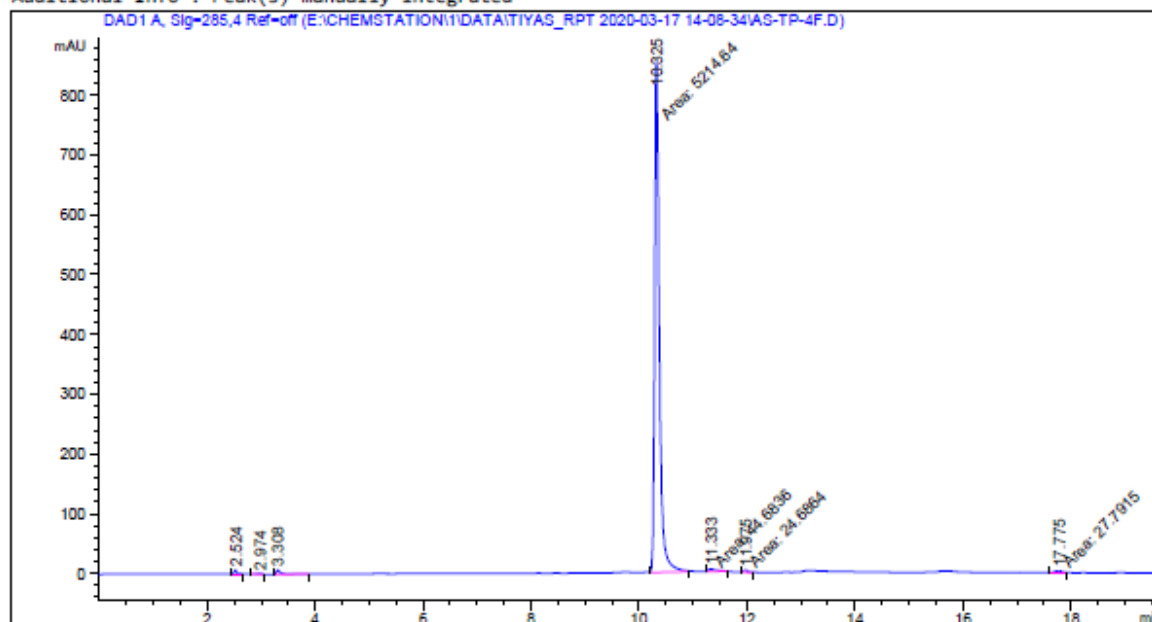


^{13}C NMR of **5k** in CDCl_3 at 125MHz

HPLC Purity Data of **5k**

```

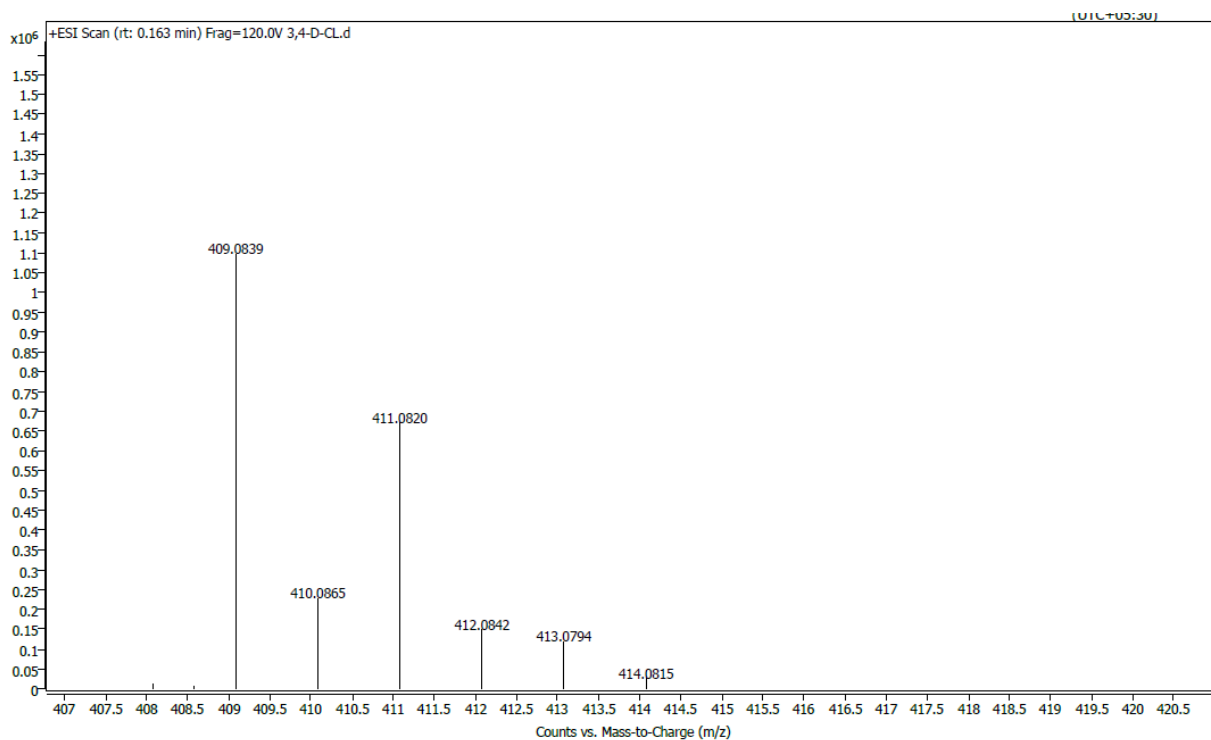
=====
Acq. Operator   : SYSTEM                      Seq. Line :    7
Sample Operator : SYSTEM
Acq. Instrument : HPLC                       Location  : P2-C-04
Injection Date  : 17-03-2020 17:00:52       Inj       :    1
                                                Inj Volume: 10.000 µl
Acq. Method     : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 14-08-34\TIYAS_RPT.M
Last changed    : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\CHEMSTATION\1\METHODS\WASH_AA_61_Min.M
Last changed    : 18-03-2020 10:06:13 by SYSTEM
Additional Info  : Peak(s) manually integrated
  
```



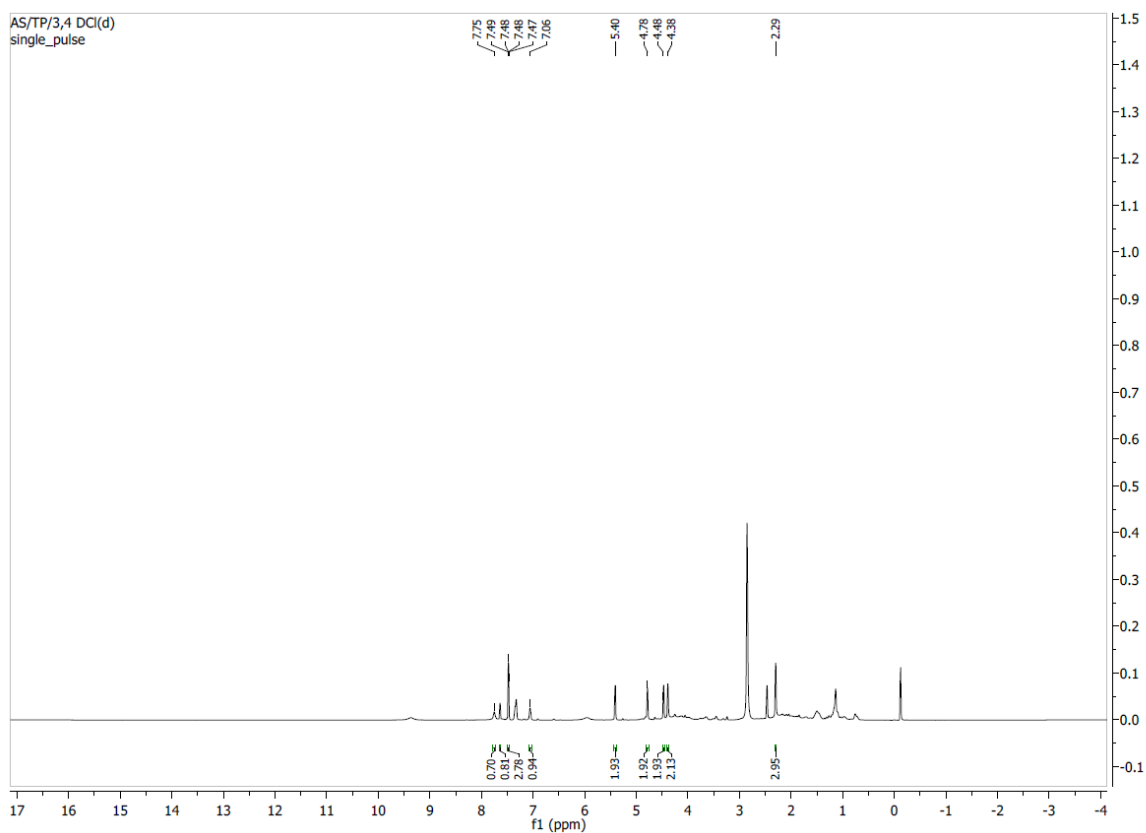
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.524	BV R	0.0527	23.56682	7.09809	0.4377
2	2.974	BB	0.0865	7.85408	1.29955	0.1459
3	3.308	BB	0.0783	40.85798	7.41770	0.7589
4	10.325	MM	0.1015	5214.64063	856.06323	96.8529
5	11.333	MM	0.1868	44.68361	3.98615	0.8299
6	11.975	MM	0.1035	24.68643	3.97545	0.4585
7	17.775	MM	0.1364	27.79146	3.39607	0.5162

Totals : 5384.08101 883.23625

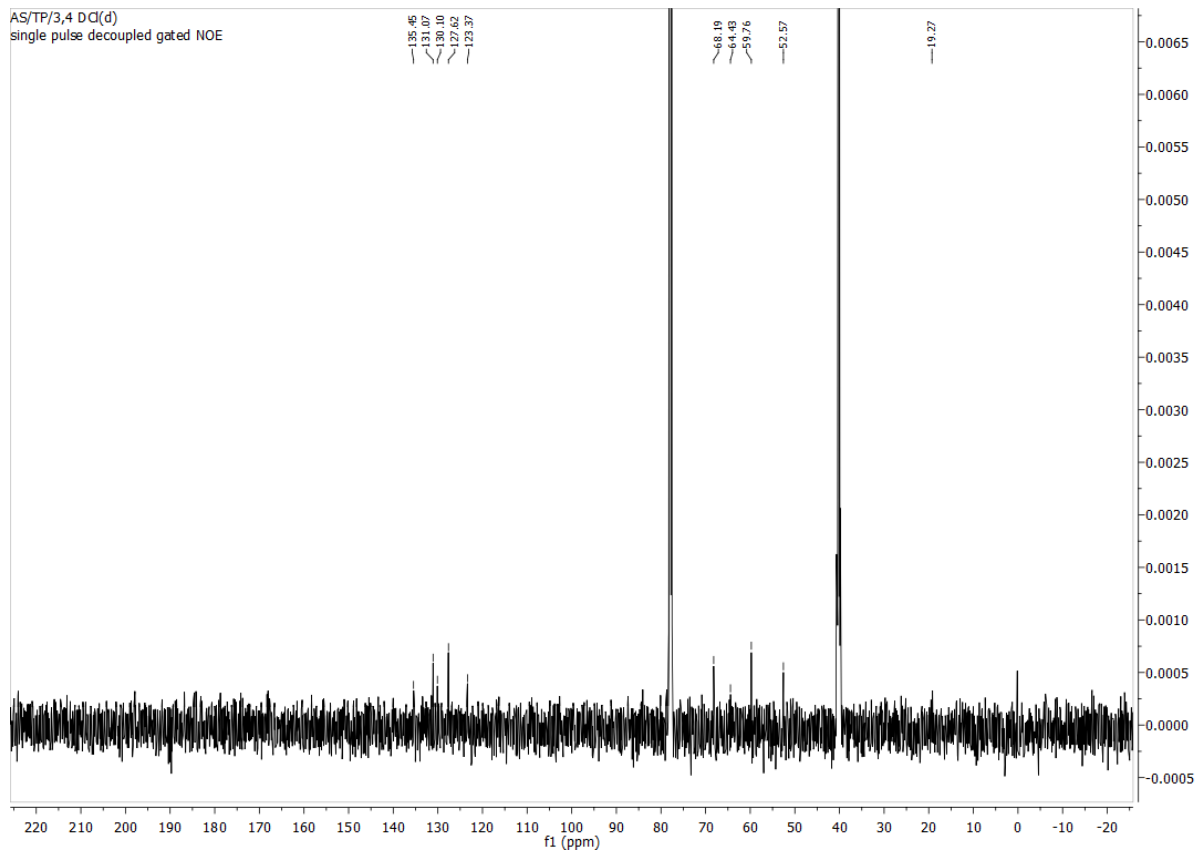
SPECTRAL DATA OF **51**



HRMS Spectrum of **51**



¹H NMR of **51** in CDCl₃ and DMSO-*d*₆ at 500MHz



^{13}C NMR of **5I** in CDCl_3 and $\text{DMSO}-d_6$ at 125MHz

HPLC Purity Data of **5I**

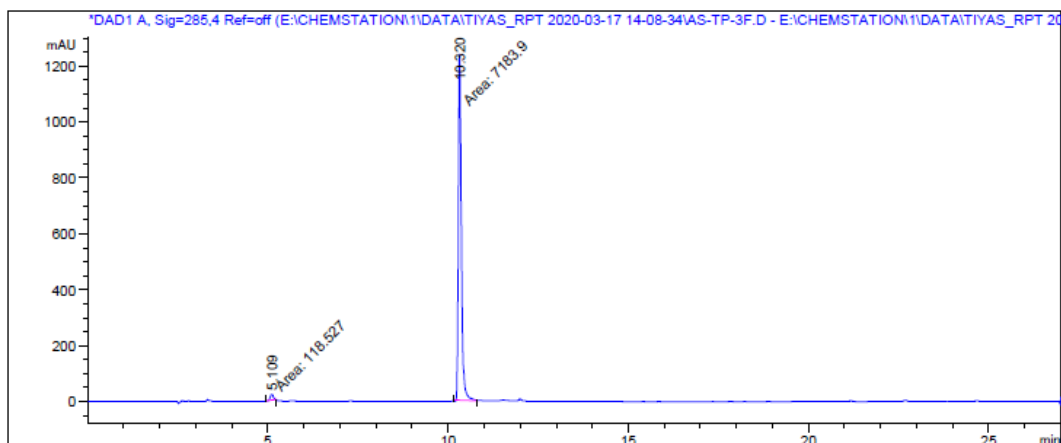
Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 14-08-34\AS-TP-3F.D

Sample Name: AS-TP-3F

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    1
Sample Operator : SYSTEM
Acq. Instrument : HPLC                       Location  : P2-B-09
Injection Date  : 17-03-2020 14:09:56        Inj       :    1
                                           Inj Volume: 10.000 µl
Acq. Method    : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 14-08-34\TIYAS_RPT.M
Last changed   : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed   : 23-06-2020 11:45:48 by SYSTEM
                (modified after loading)
  
```

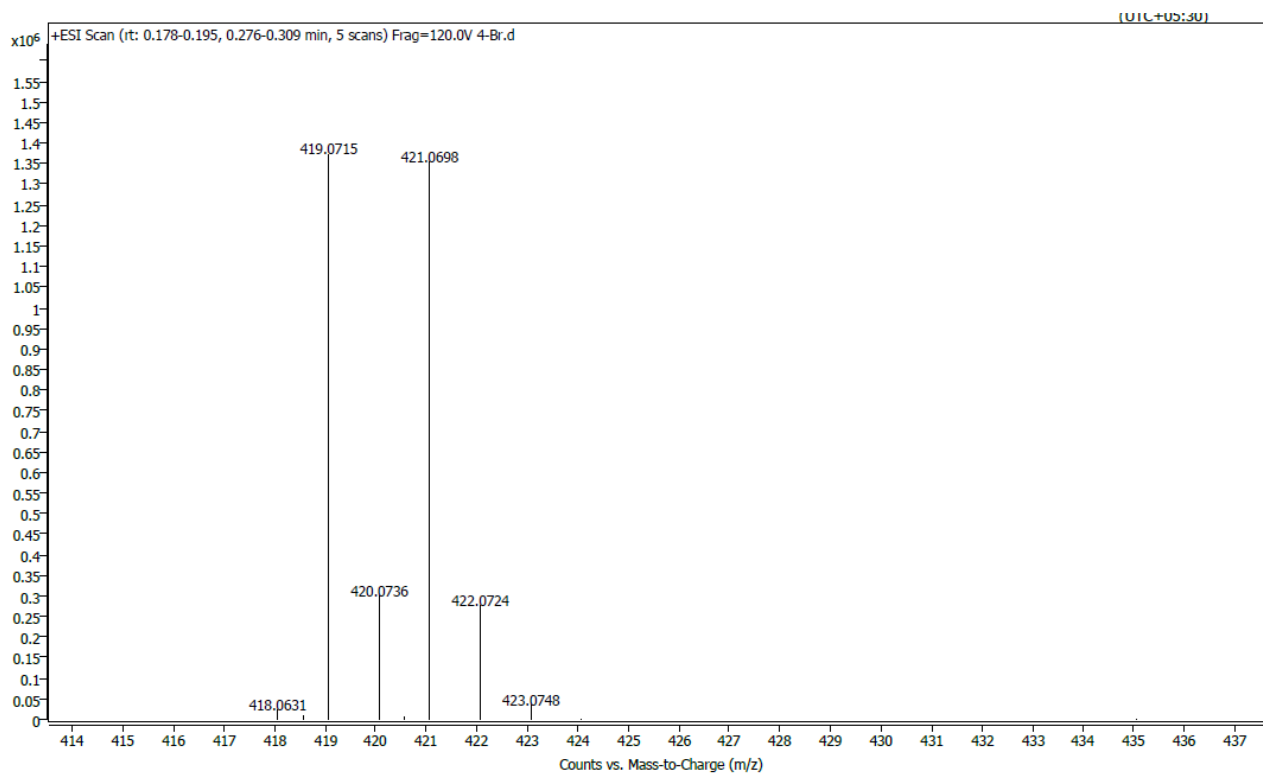
Additional Info : Peak(s) manually integrated



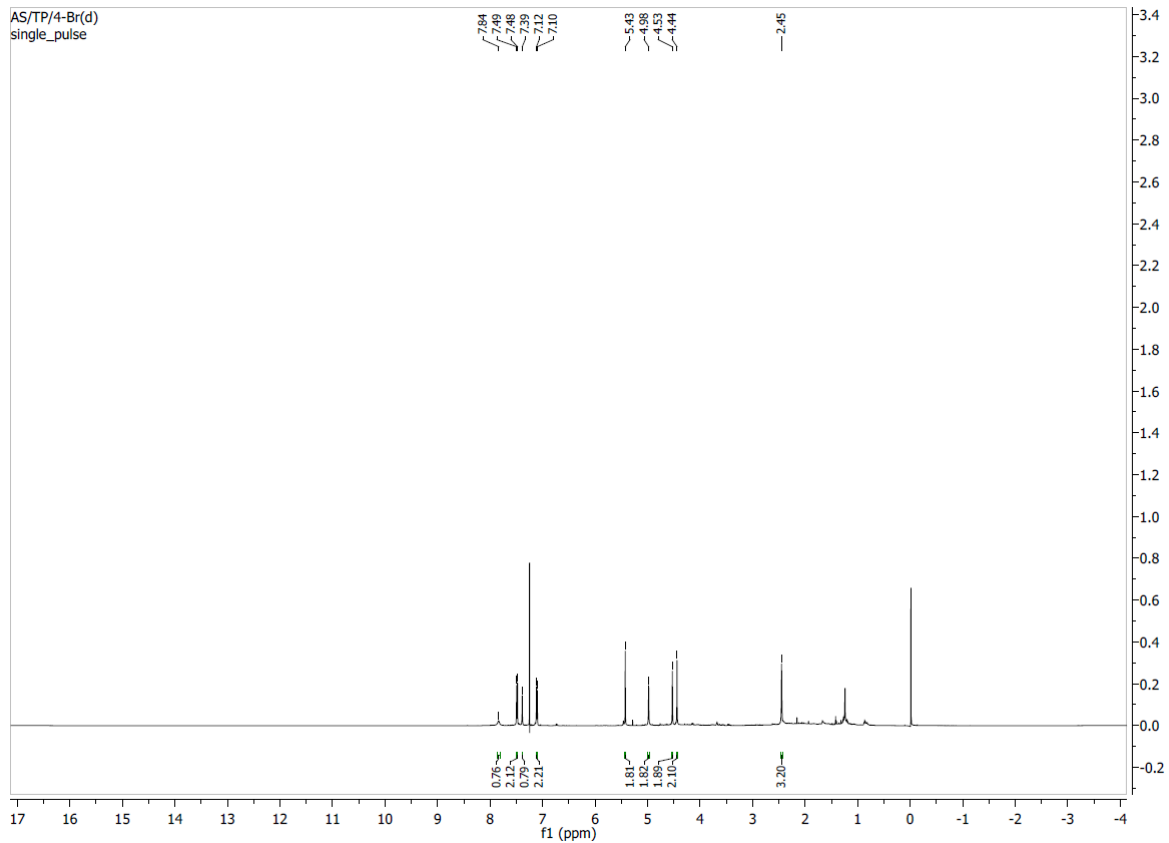
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.109	MM	0.0968	118.52690	20.41121	1.6231
2	10.320	MM	0.0965	7183.89844	1240.68188	98.3769

Totals : 7302.42534 1261.09309

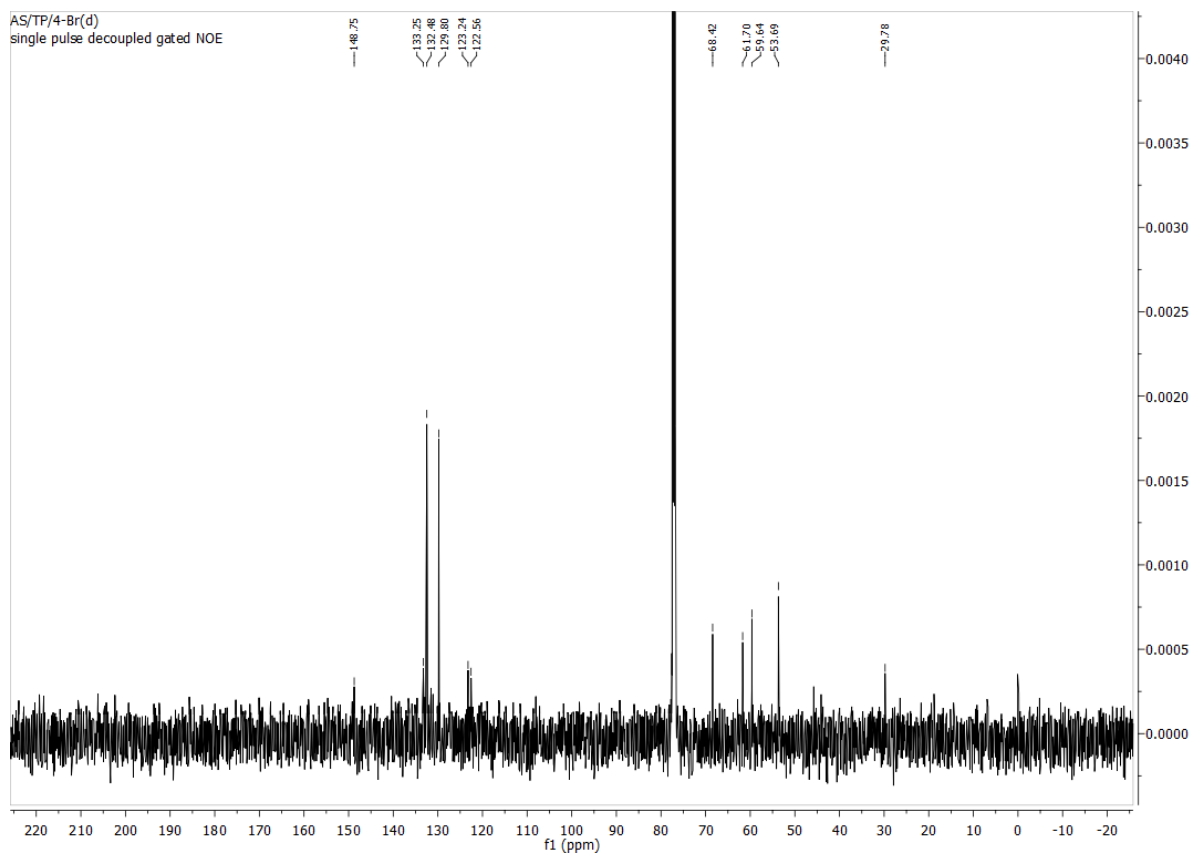
SPECTRAL DATA OF 5m



HRMS Spectrum of 5m



^1H NMR of **5m** in CDCl_3 at 500MHz

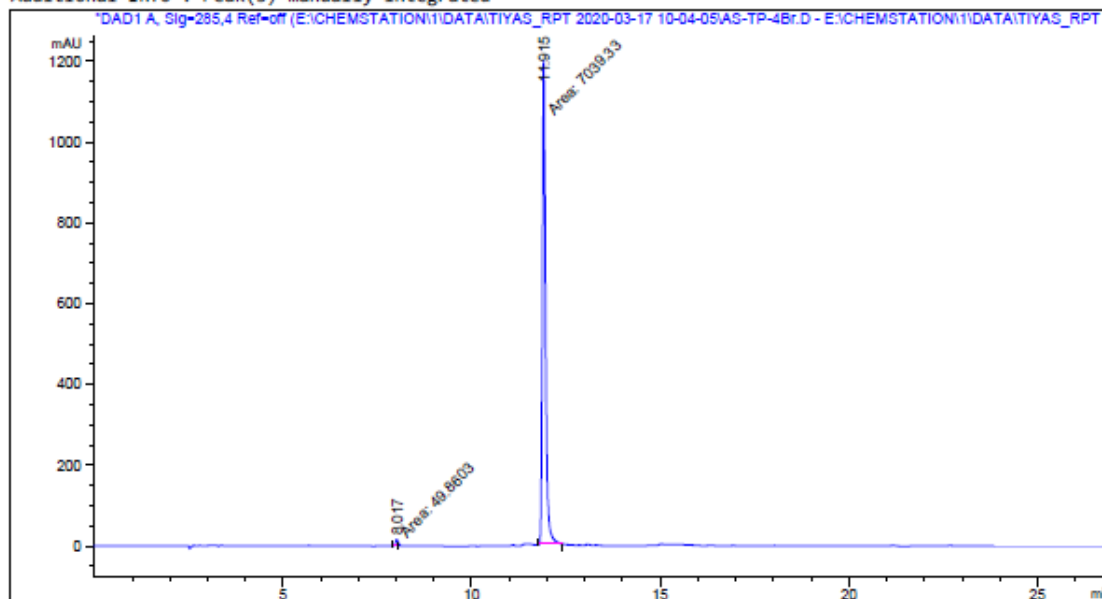


¹³C NMR of **5m** in CDCl₃ at 125MHz

HPLC Purity Data of **5m**

Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 10-04-05\AS-TP-4Br.D
Sample Name: AS-TP-4Br

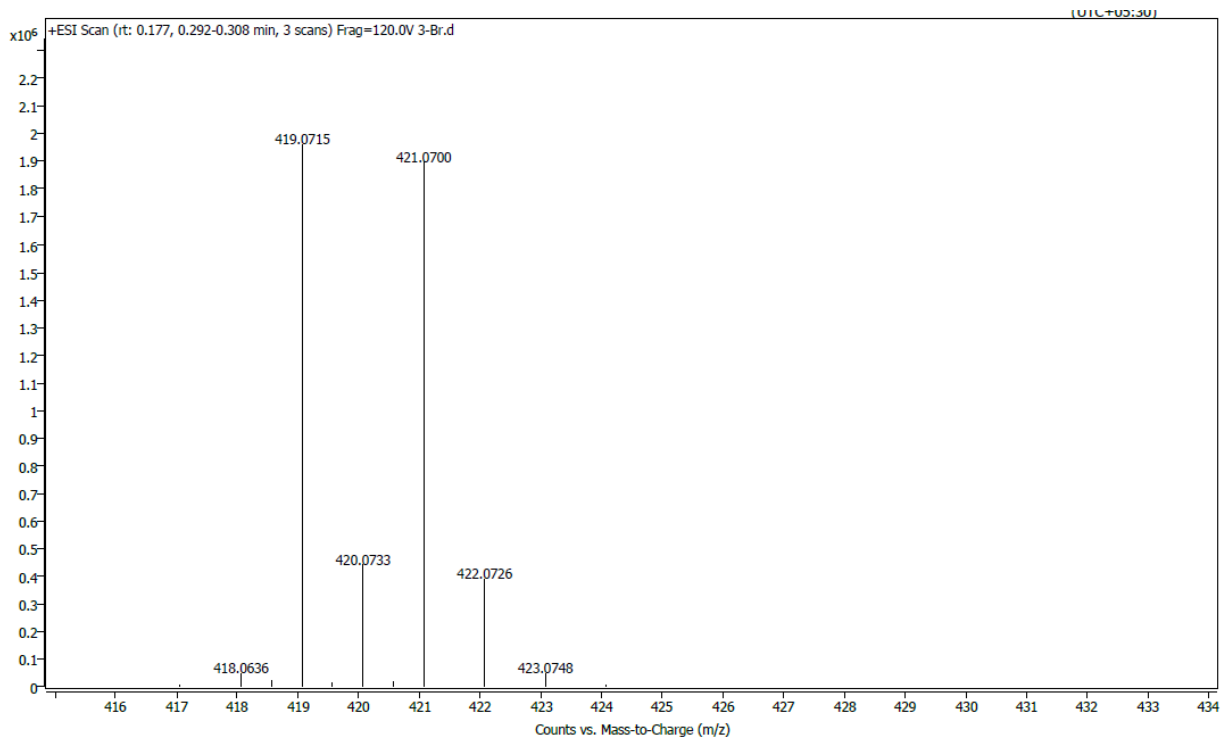
```
=====
Acq. Operator   : SYSTEM                      Seq. Line :    5
Sample Operator : SYSTEM
Acq. Instrument : HPLC                       Location  : P2-B-05
Injection Date  : 17-03-2020 11:59:20        Inj       :    1
                                                Inj Volume: 10.000 µl
Acq. Method    : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 10-04-05\TIYAS_RPT.M
Last changed   : 17-03-2020 10:01:12 by SYSTEM
Analysis Method: E:\CHEMSTATION\1\METHODS\TIYAS_RPT.M
Last changed   : 23-06-2020 12:51:16 by SYSTEM
Additional Info : Peak(s) manually integrated
```



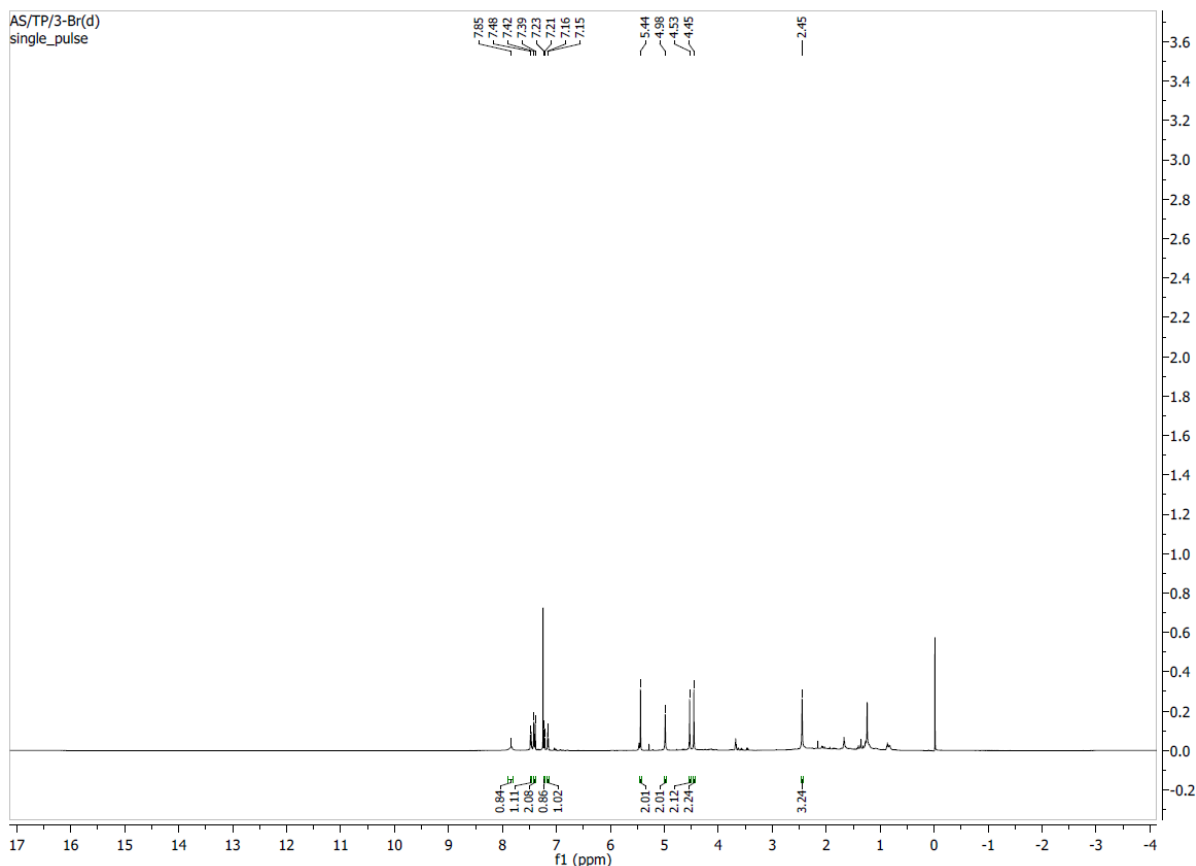
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.017	MM	0.0634	49.86025	13.11576	0.7033
2	11.915	MM	0.0977	7039.33203	1200.87622	99.2967

Totals : 7089.19228 1213.99198

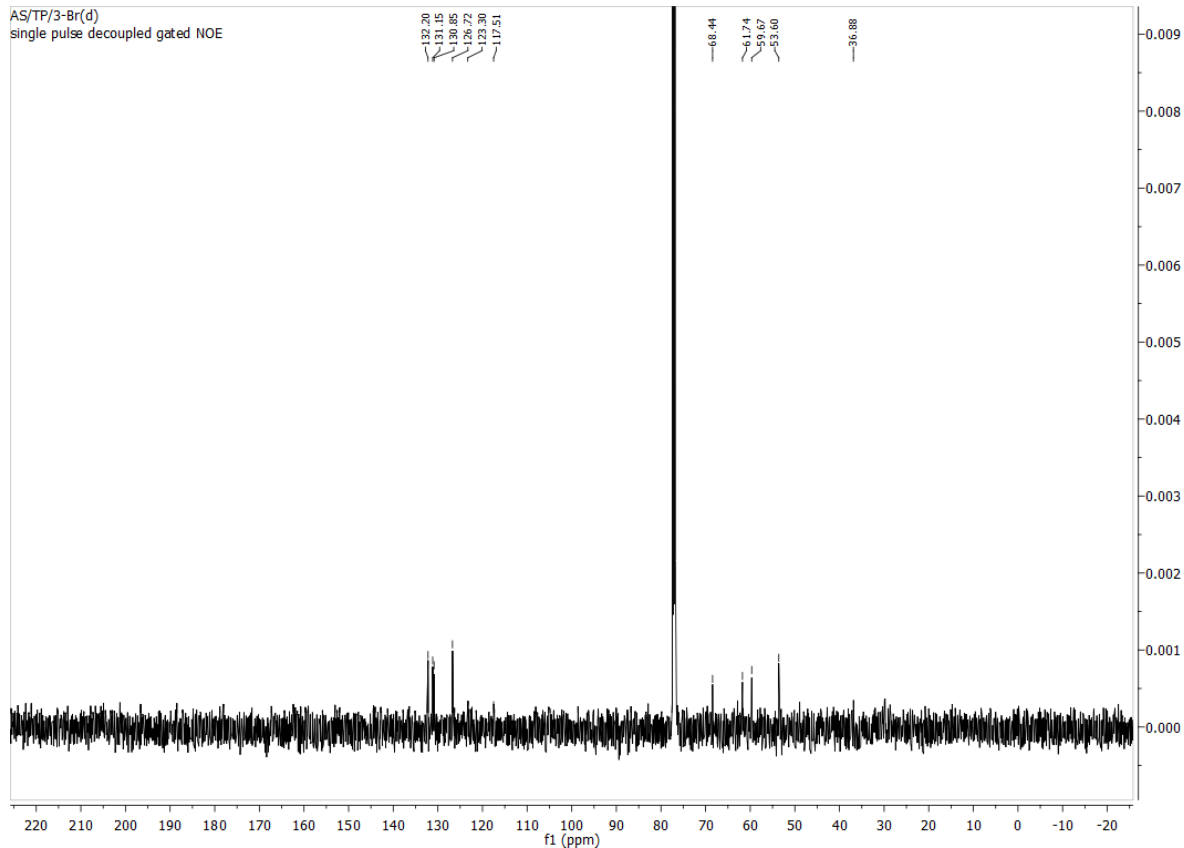
SPECTRAL DATA OF **5n**



HRMS Spectrum of **5n**



¹H NMR of **5n** in CDCl₃ at 500MHz



^{13}C NMR of **5n** in CDCl_3 at 125MHz

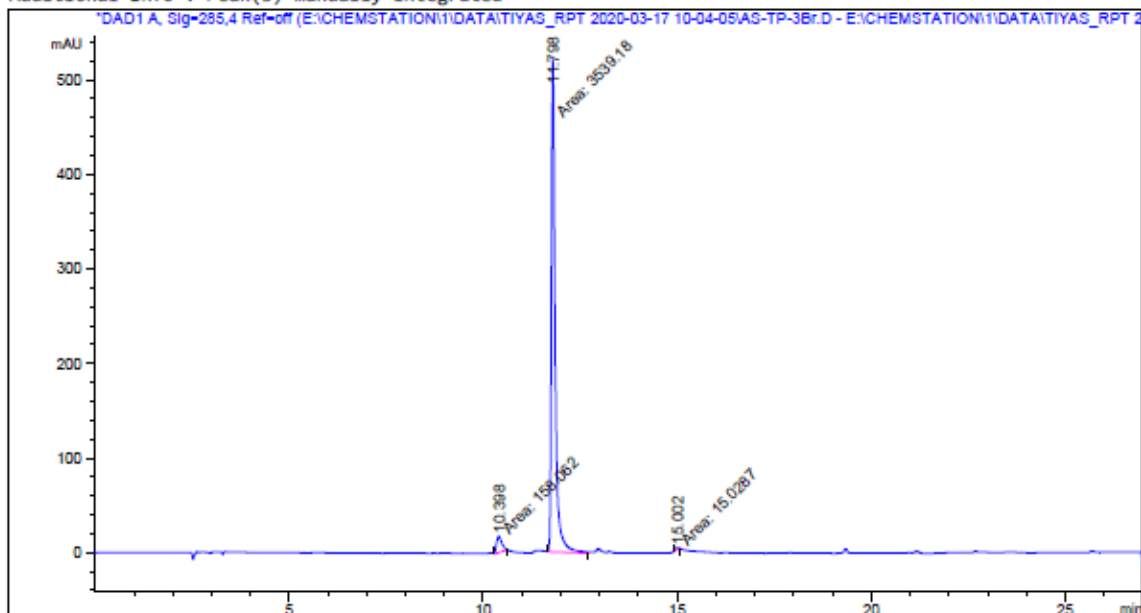
HPLC Purity Data of **5n**

Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 10-04-05\AS-TP-3Br.D
Sample Name: AS-TP-3Br

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    6
Sample Operator : SYSTEM
Acq. Instrument : HPLC                      Location  : P2-B-06
Injection Date  : 17-03-2020 12:27:49        Inj       :    1
                                           Inj Volume: 10.000 µl

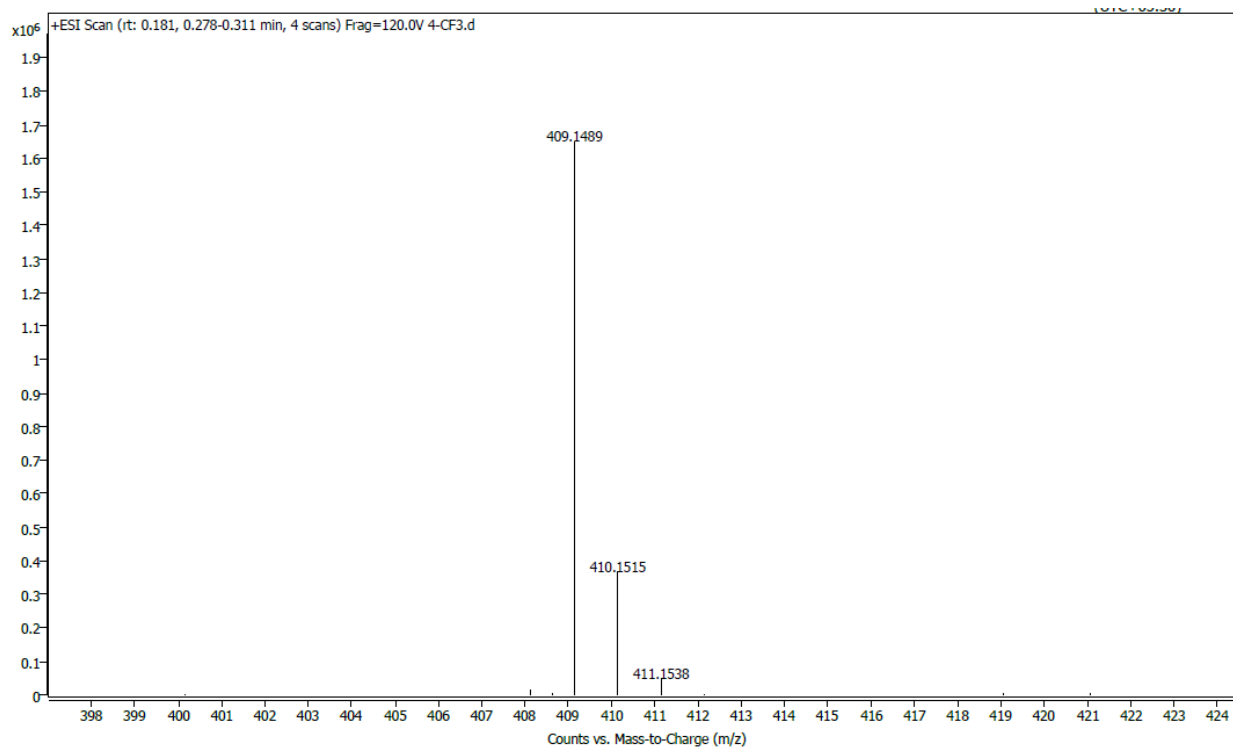
Acq. Method    : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 10-04-05\TIYAS_RPT.M
Last changed   : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\CHEMSTATION\1\METHODS\TIYAS_RPT.M
Last changed   : 23-06-2020 12:51:16 by SYSTEM
Additional Info : Peak(s) manually integrated
  
```



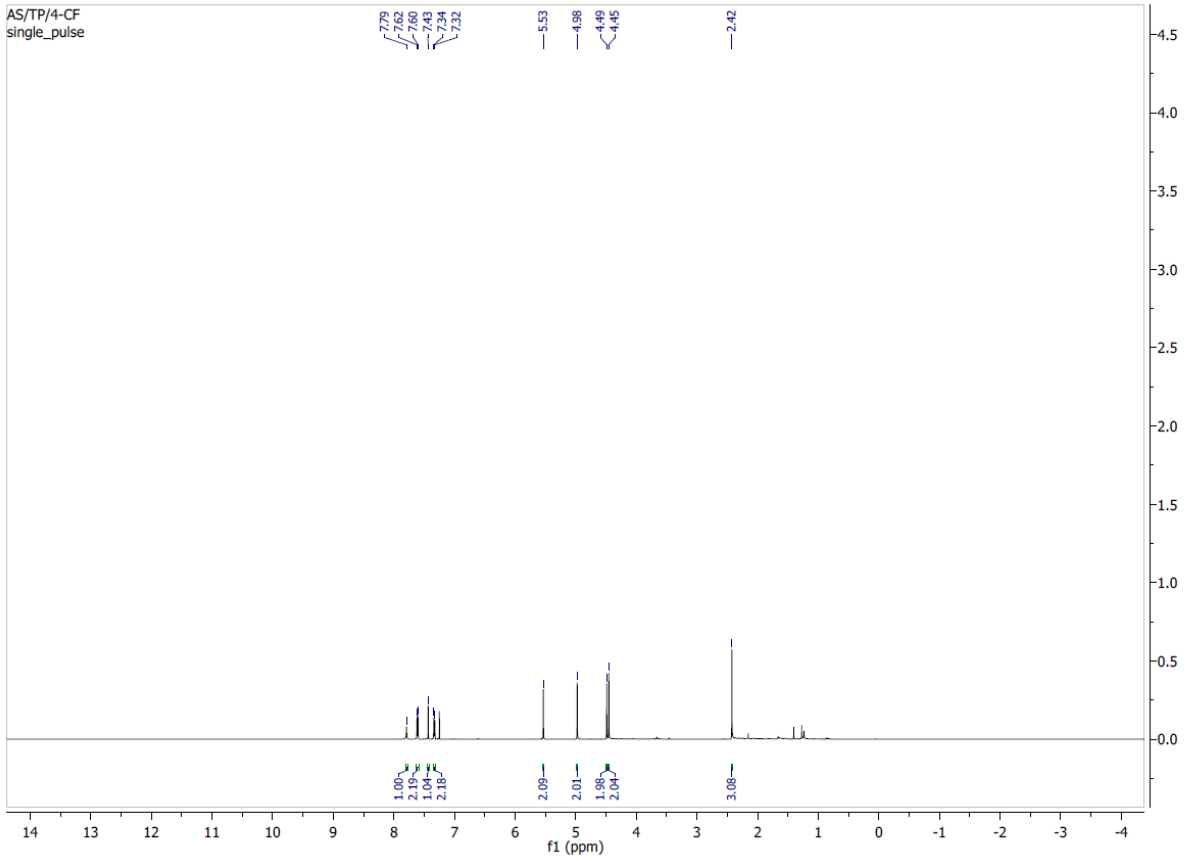
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.398	MM	0.1536	158.06219	17.14530	4.2578
2	11.798	MM	0.1130	3539.17969	521.87903	95.3373
3	15.002	MM	0.1190	15.02869	2.10459	0.4048

Totals : 3712.27057 541.12892

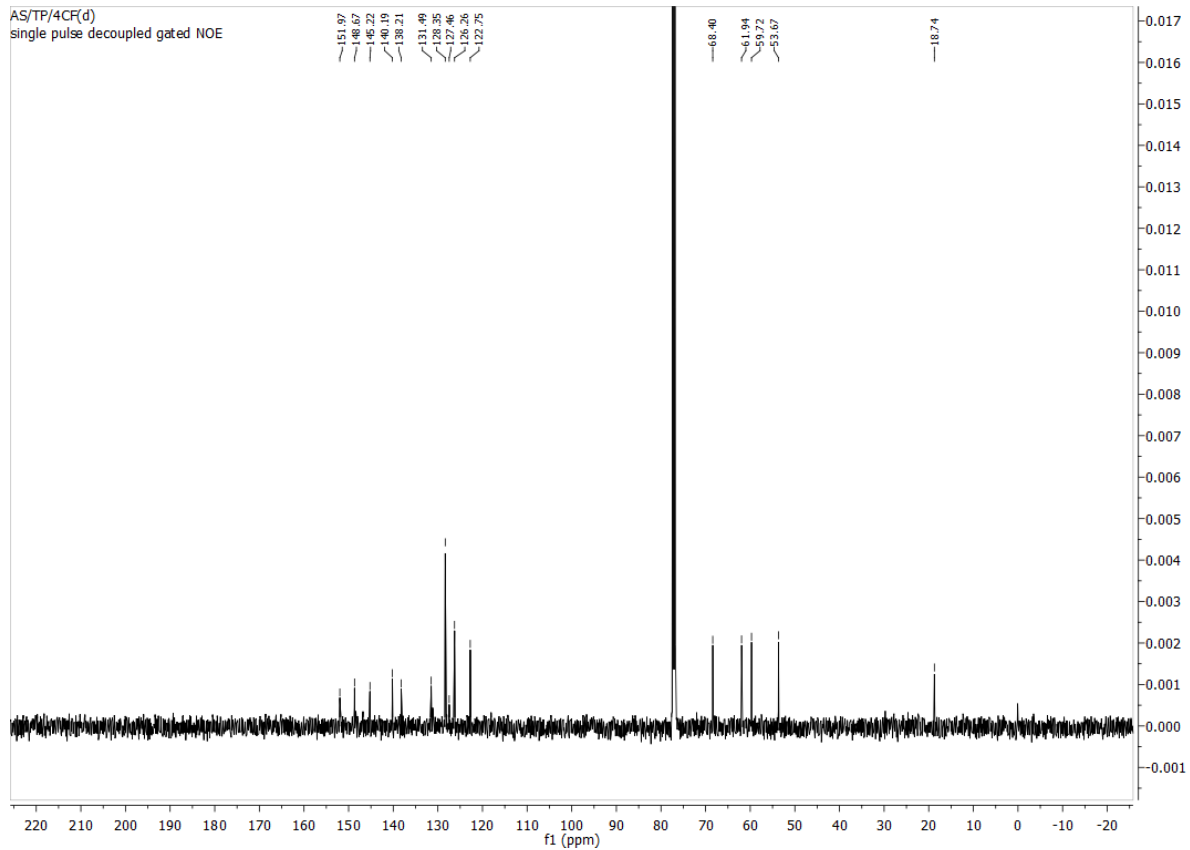
SPECTRAL DATA OF 5o



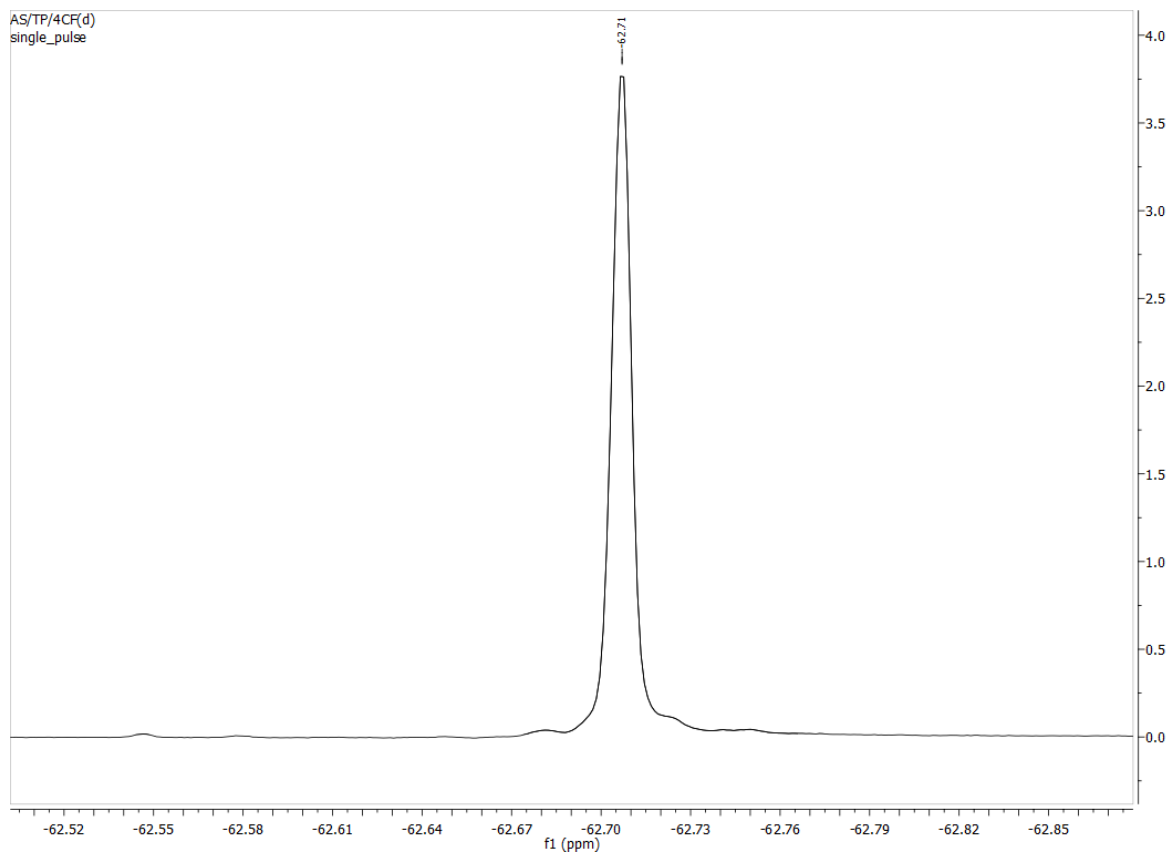
HRMS Spectrum of 5o



^1H NMR of **5o** in CDCl_3 at 500MHz



^{13}C NMR of **5o** in CDCl_3 at 125MHz



^{19}F NMR of **5o** in CDCl_3 at 470MHz

HPLC Purity Data of 5o

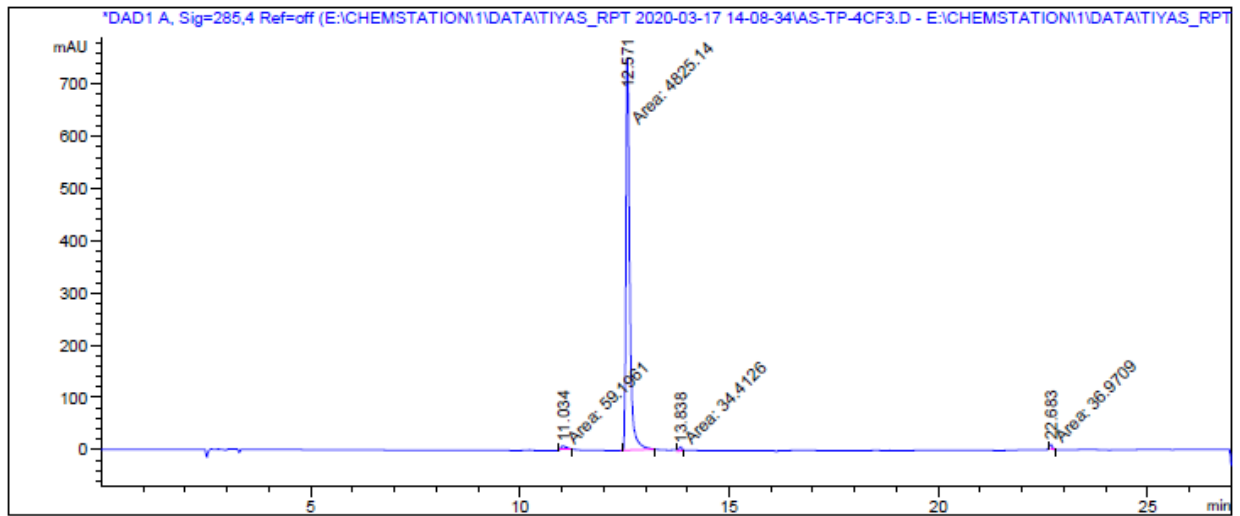
Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 14-08-34\AS-TP-4CF3.D
 Sample Name: AS-TP-4CF3

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    2
Sample Operator : SYSTEM
Acq. Instrument : HPLC                      Location  : P2-B-10
Injection Date  : 17-03-2020 14:38:25       Inj       :    1
                                           Inj Volume: 10.000 µl

Acq. Method     : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 14-08-34\TIYAS_RPT.M
Last changed    : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed    : 23-06-2020 11:45:48 by SYSTEM
                 (modified after loading)

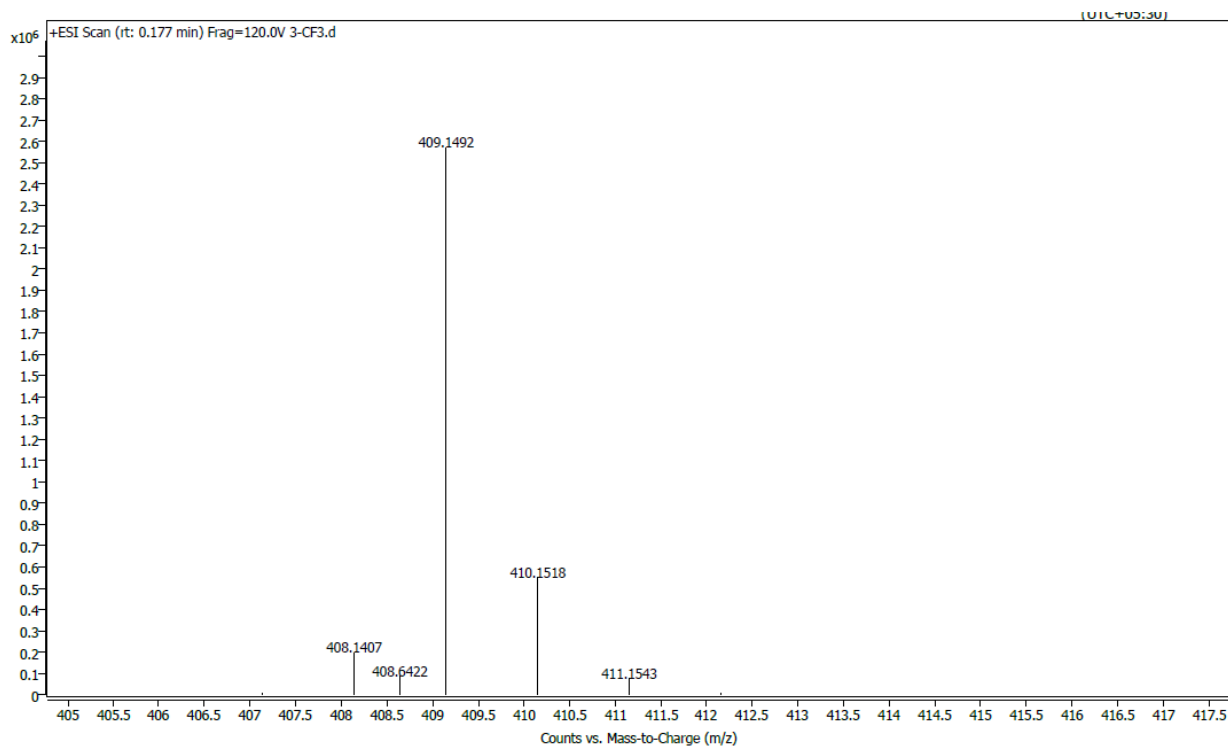
Additional Info : Peak(s) manually integrated
=====
  
```



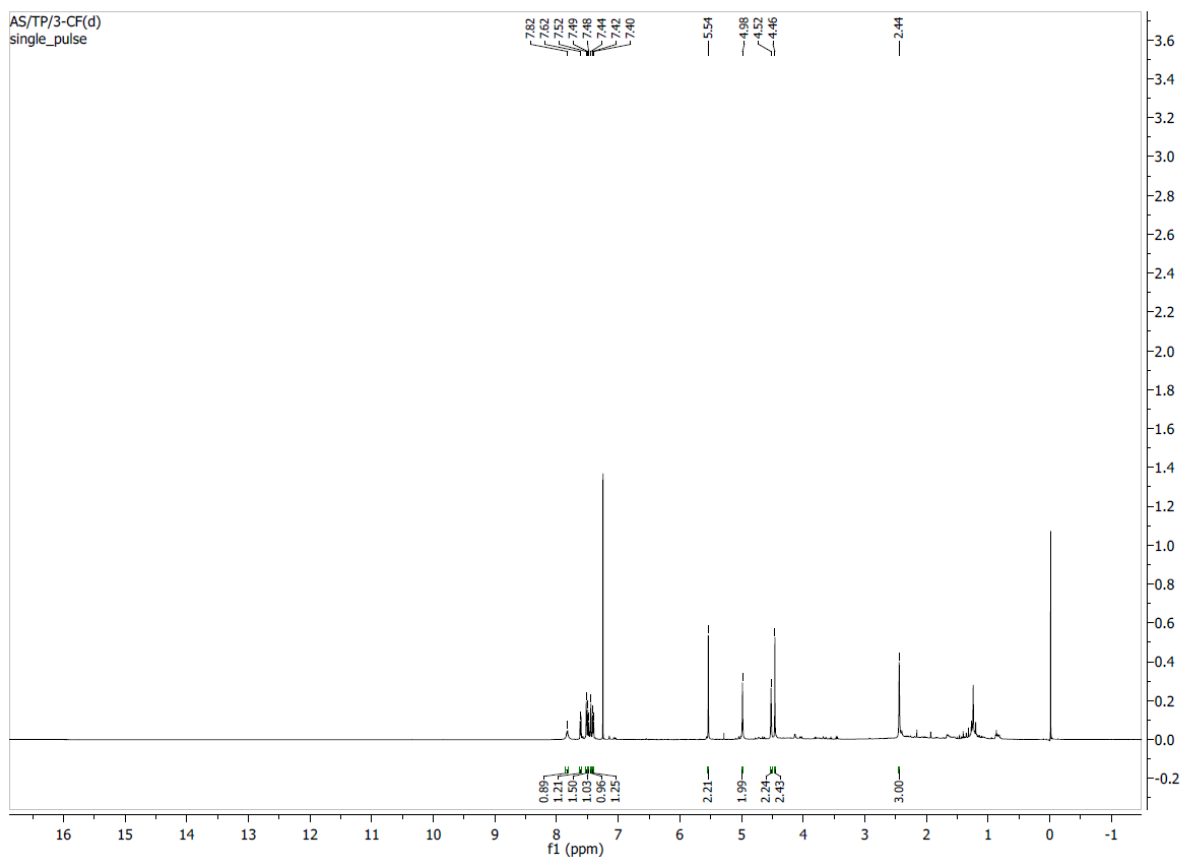
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.034	MM	0.1571	59.19608	6.28135	1.1945
2	12.571	MM	0.1067	4825.13770	753.77130	97.3651
3	13.838	MM	0.0903	34.41263	6.35487	0.6944
4	22.683	MM	0.0753	36.97089	8.17996	0.7460

Totals : 4955.71730 774.58748

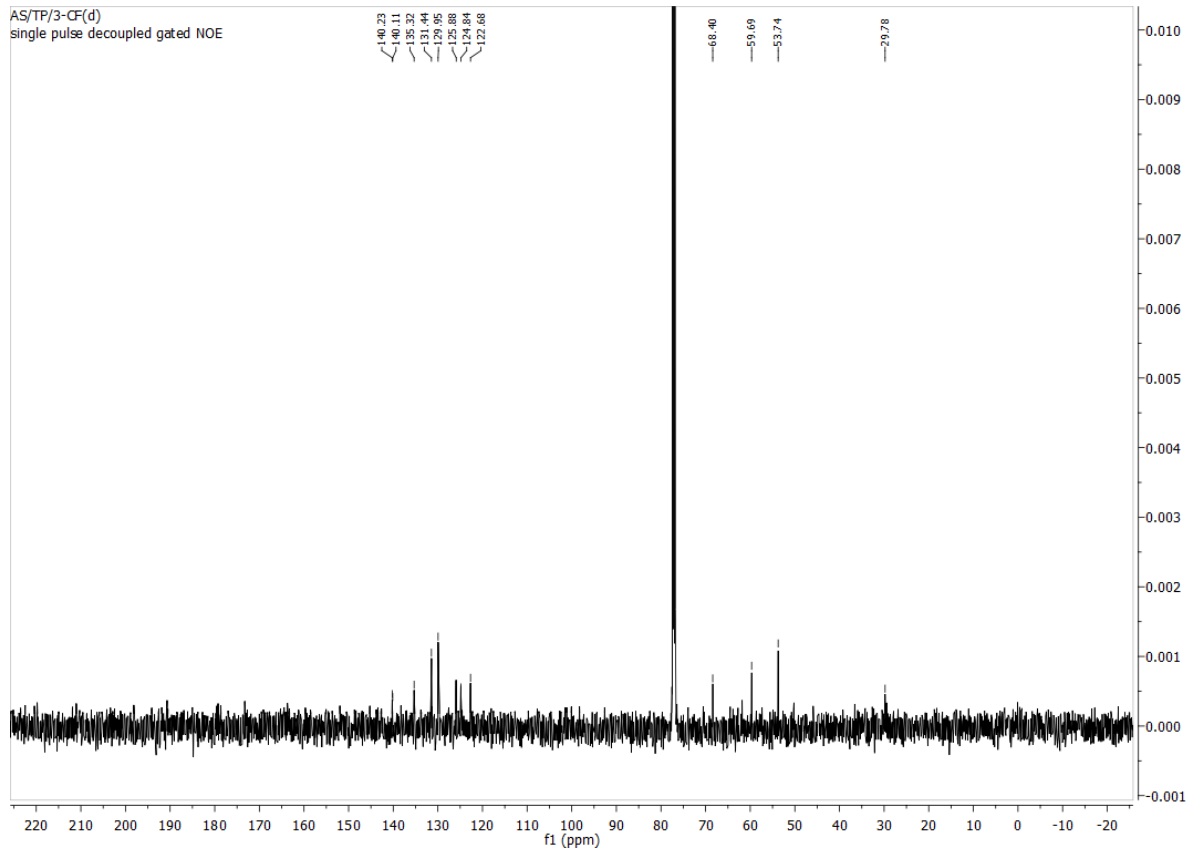
SPECTRAL DATA OF 5p



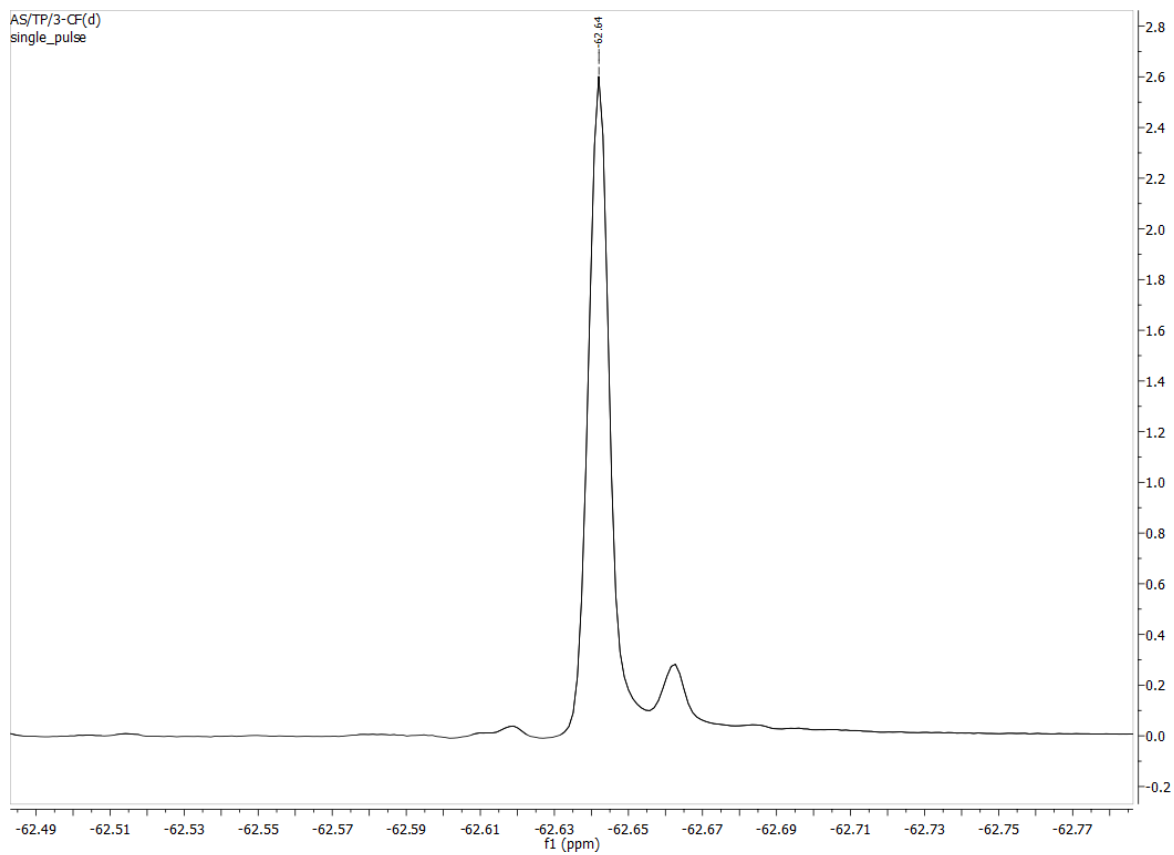
HRMS Spectrum of 5p



¹H NMR of 5p in CDCl₃ at 500MHz



^{13}C NMR of **5p** in CDCl_3 at 125MHz



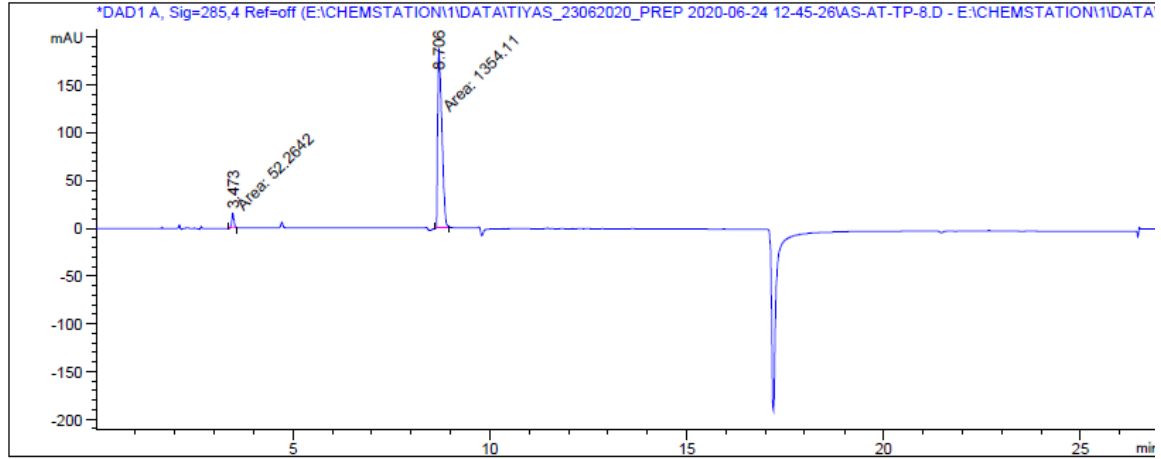
^{19}F NMR of **5p** in CDCl_3 at 470MHz

HPLC Purity Data of **5p**

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    1
Sample Operator : SYSTEM
Acq. Instrument : HPLC                      Location  : P2-D-03
Injection Date  : 24-06-2020 12:46:28       Inj       :    1
                                           Inj Volume: 10.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 4.000 µl
Acq. Method     : E:\Chemstation\1\Data\TIYAS_23062020_PREP 2020-06-24 12-45-26\TIYAS_RPT.M
Last changed    : 23-06-2020 12:51:16 by SYSTEM
Analysis Method : E:\CHEMSTATION\1\METHODS\AshimaFA_C-18_PREP.M
Last changed    : 23-06-2020 15:02:47 by SYSTEM
Sample Info     : AS-AT-TP-8
  
```

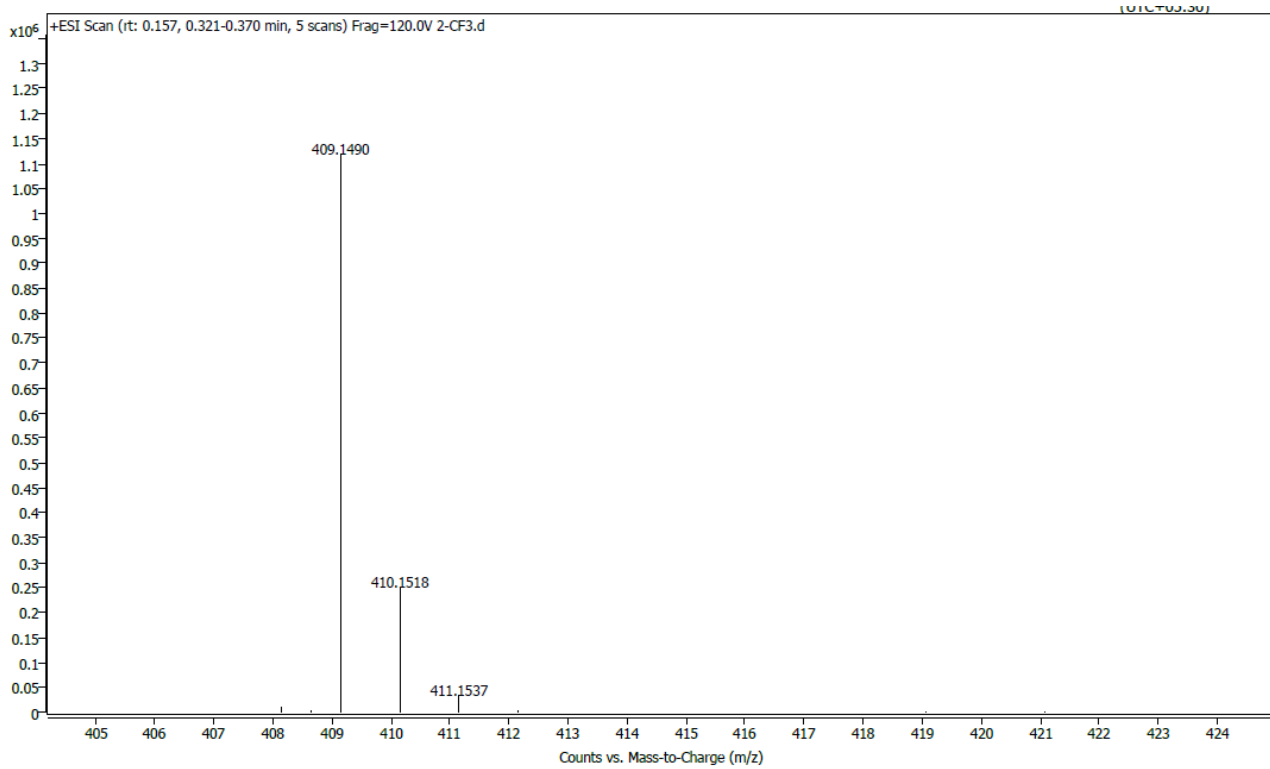
Additional Info : Peak(s) manually integrated



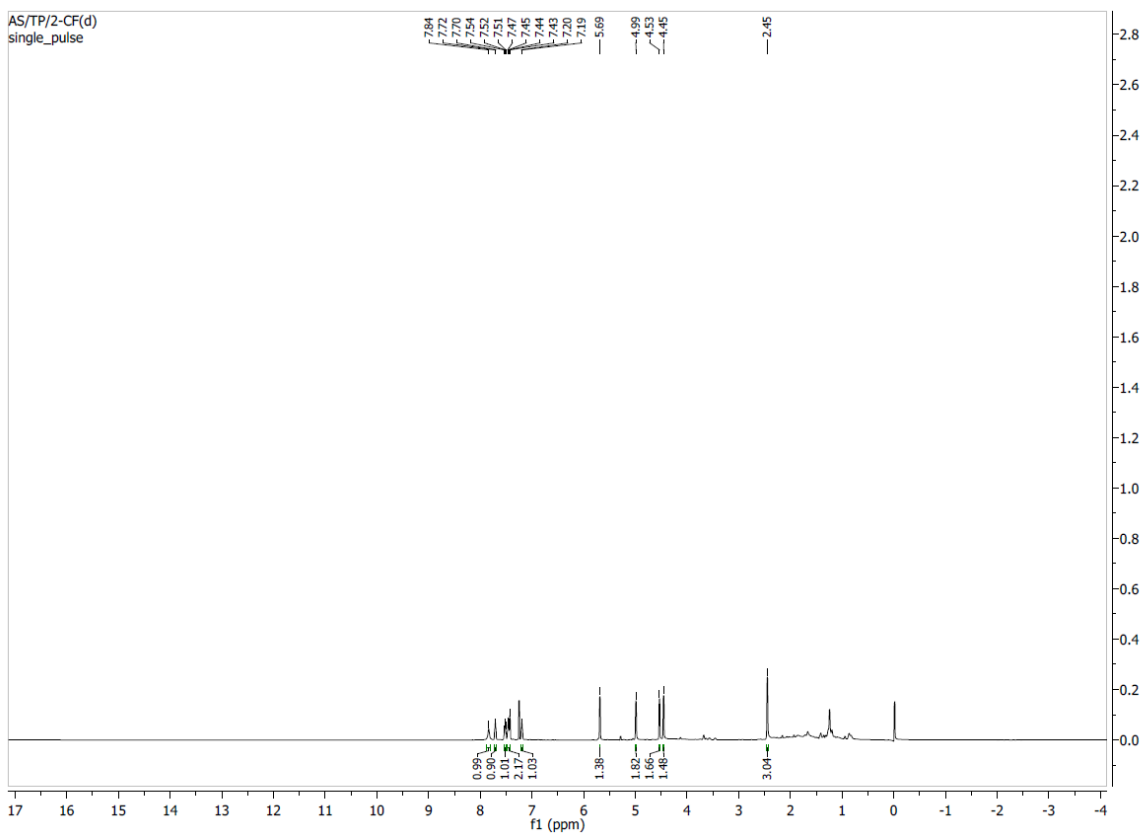
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.473	MM	0.0593	52.26423	14.68460	3.7162
2	8.706	MM	0.1199	1354.10974	188.24948	96.2838

Totals : 1406.37397 202.93408

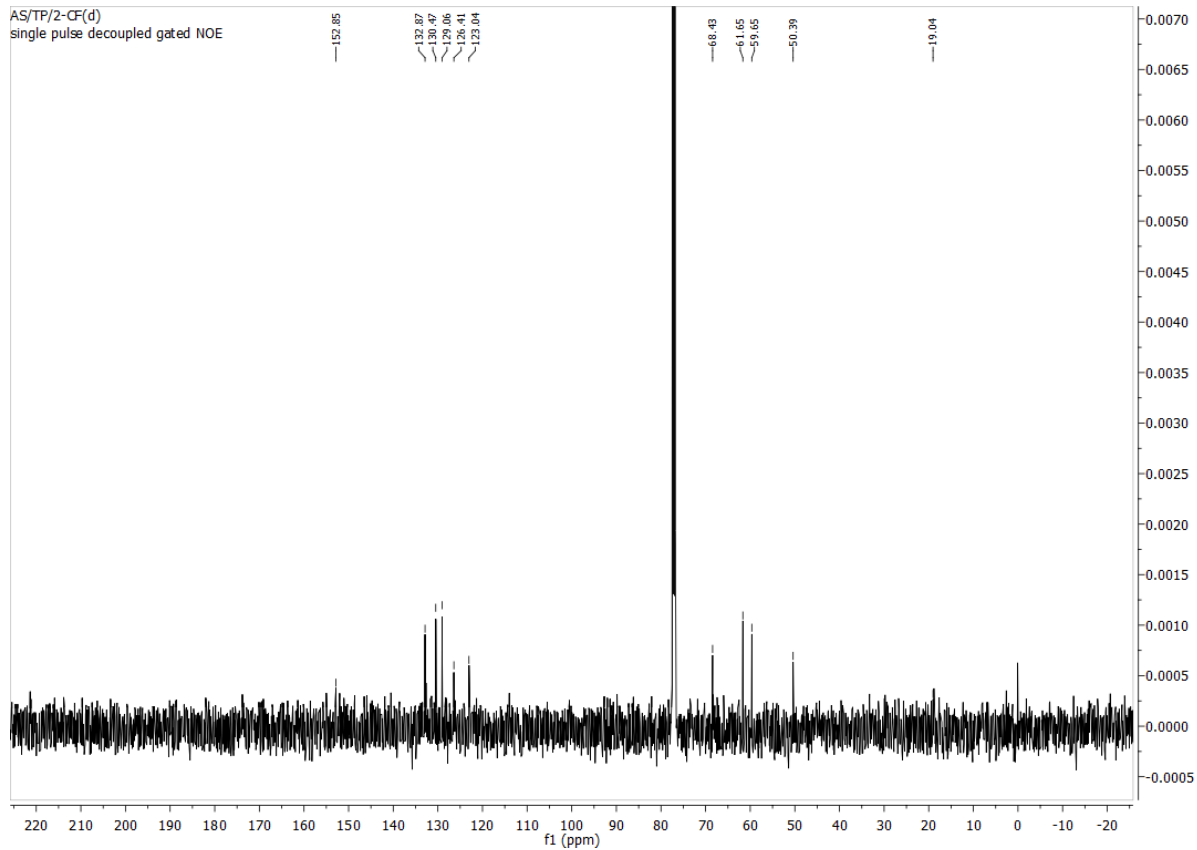
SPECTRAL DATA OF 5q



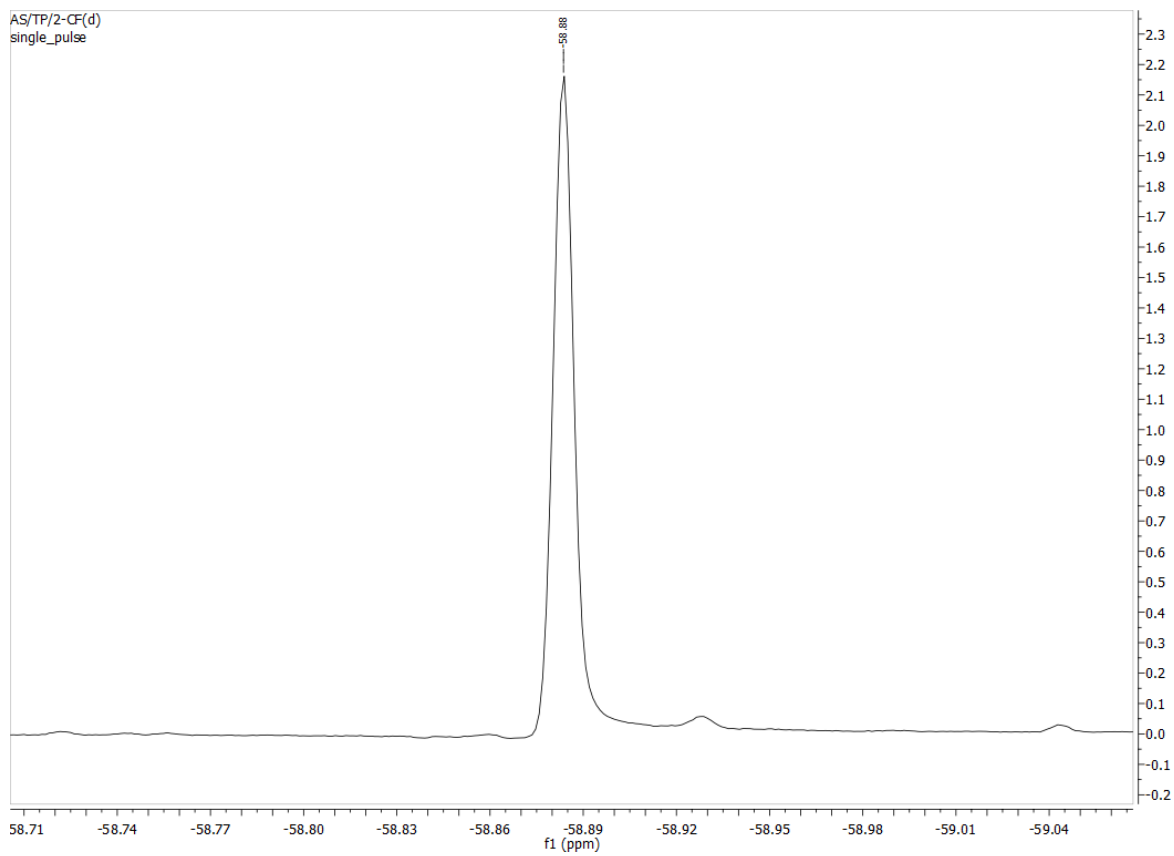
HRMS Spectrum of **5q**



¹H NMR of **5q** in CDCl₃ at 500MHz



^{13}C NMR of **5q** in CDCl_3 at 125MHz



^{19}F NMR of **5q** in CDCl_3 at 470MHz

HPLC Purity Data of 5q

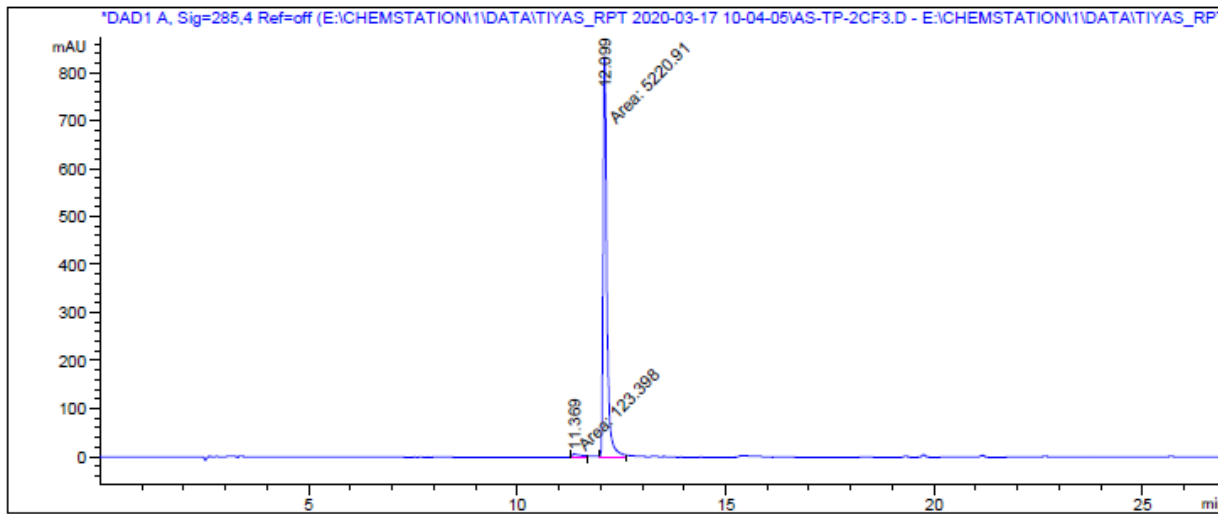
Data File E:\CHEMSTATION\1\DATA\TIYAS_RPT 2020-03-17 10-04-05\AS-TP-2CF3.D
 Sample Name: AS-TP-2CF3

```

=====
Acq. Operator   : SYSTEM                      Seq. Line :    2
Sample Operator : SYSTEM
Acq. Instrument : HPLC                      Location  : P2-B-02
Injection Date  : 17-03-2020 10:33:53        Inj       :    1
                                           Inj Volume: 10.000 µl

Acq. Method     : E:\Chemstation\1\Data\TIYAS_RPT 2020-03-17 10-04-05\TIYAS_RPT.M
Last changed    : 17-03-2020 10:01:12 by SYSTEM
Analysis Method : E:\Chemstation\1\Methods\AshimaFA_C-18_PREP.M
Last changed    : 23-06-2020 11:45:48 by SYSTEM
                 (modified after loading)

Additional Info : Peak(s) manually integrated
=====
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.369	MM	0.2720	123.39763	7.56185	2.3090
2	12.099	MM	0.1041	5220.90869	836.01648	97.6910

Totals : 5344.30632 843.57833

Metal Chelation UV spectrum of Compounds 5c, 5d, 5h, 5i, 5n, 5q against Fe, Cu, Zn, Al.

