

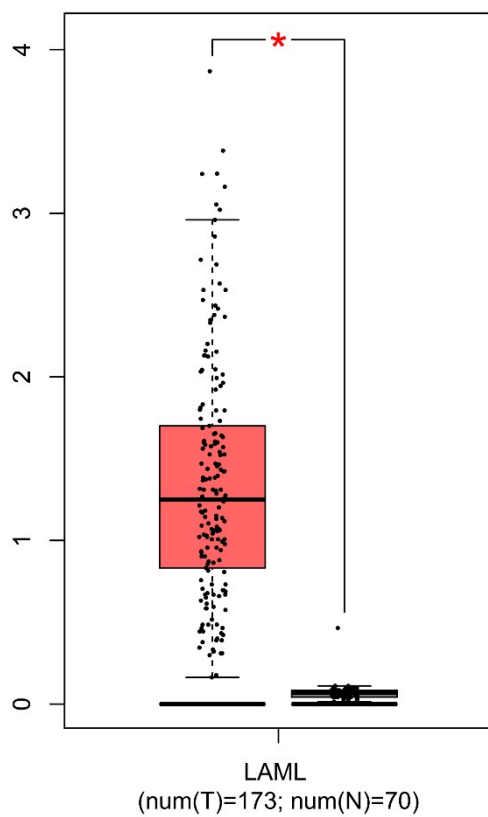
## Support Information

### Synthesis and Evaluation of Potent (Iso)ellipticine-based Inhibitors of MYLK4 Accessed via Expeditious Synthesis from Isoquinolin-5-ol

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Hsu, Shiow-Lin Pan, Hsueh-Yun Lee\*

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**Figure S1.** Expression level of MYLK4 in acute myeloid leukemia.

## HPLC spectrum of compound 1

## ==== Shimadzu LabSolutions Analysis Report ====

Sample Name : DHT-05107 (Ag 10mM ABC + NH4OH pH 8.5 60m) Data Filename  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210719-LC-60m.lcb  
 Vial # : 1-35 Injection Volume : 20 uL  
 Date Acquired : 2021/7/19 下午 06:18:28 Acquired by : System Administrator  
 Date Processed : 2021/7/19 下午 07:18:30 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

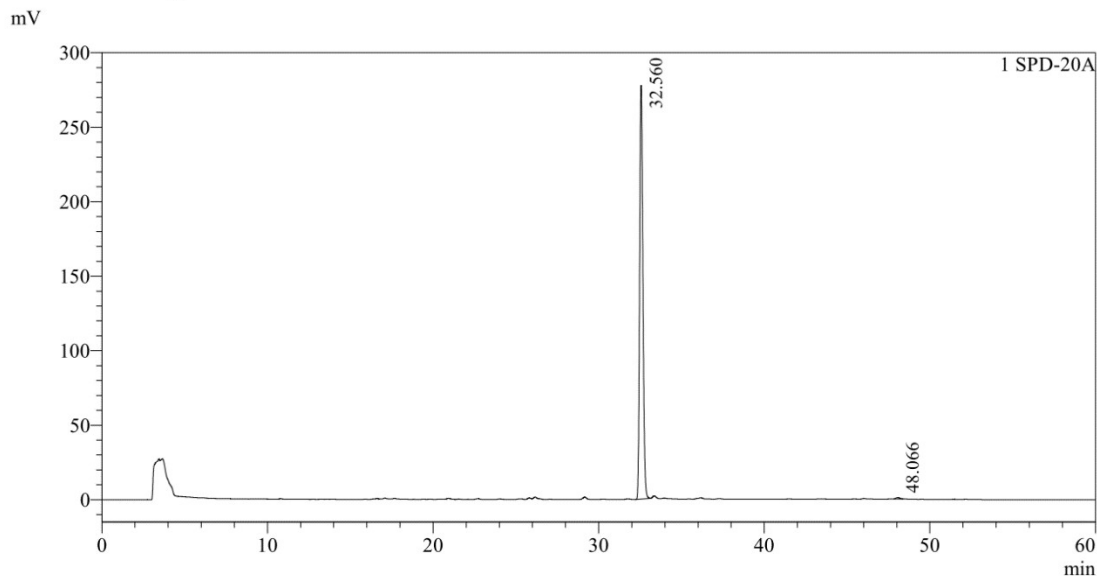
## &lt;&lt;Pump&gt;&gt;

Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;



## &lt;Peak Table&gt;

SPD-20A						
Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	32.560	3802676	277699	13.694	99.650	1.216
2	48.066	13344	884	15.099	0.350	1.185
Total		3816020	278583		100.000	

## HPLC spectrum of compound 2

## ==== Shimadzu LabSolutions Analysis Report ====

Sample Name : DHT-05538 (Ag 10mM ABC + NH4OH pH 8.5 60m) Data Filename  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210719-LC-60m.lcb  
 Vial # : 1-34 Injection Volume : 20 uL  
 Date Acquired : 2021/7/19 下午 05:18:02 Acquired by : System Administrator  
 Date Processed : 2021/7/19 下午 06:18:06 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

## &lt;&lt;Pump&gt;&gt;

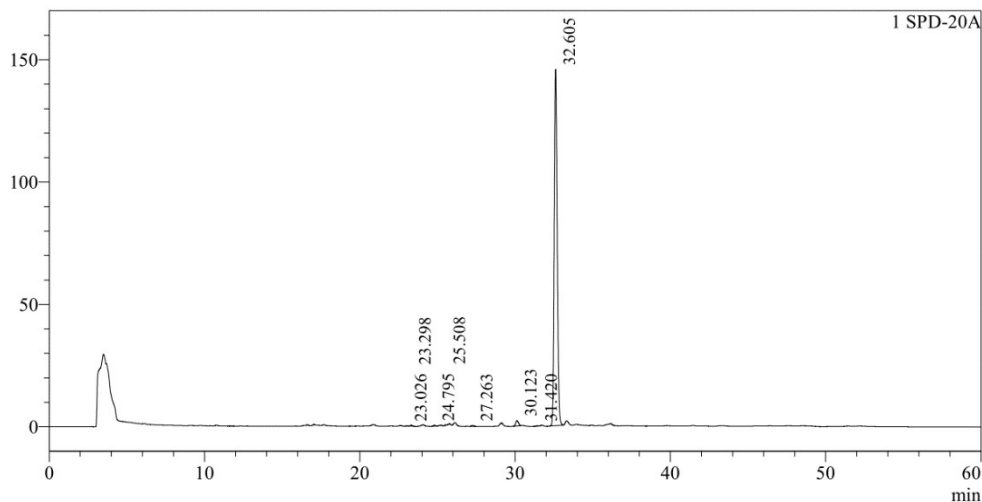
Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;

mV



## &lt;Peak Table&gt;

SPD-20A

Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	23.026	1106	148	7.493	0.056	0.977
2	23.298	3497	376	9.287	0.177	1.256
3	24.795	3460	360	9.603	0.175	1.013
4	25.508	2118	298	7.099	0.107	1.073
5	27.263	3809	383	9.956	0.192	1.153
6	30.123	26613	2180	12.209	1.345	1.114
7	31.420	1538	155	9.934	0.078	0.907
8	32.605	1937211	145497	13.314	97.871	1.155
Total		1979352	149397		100.000	

## HPLC spectrum of compound 3

## ==== Shimadzu LabSolutions Analysis Report ====

Sample Name : DHT-05540 (10mM NH<sub>4</sub>OAc+ 0.1 HCOOH 60m) Data Filename : 2  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210705-LC (10mM NH<sub>4</sub>OAc)  
 Vial # : 1-37 Injection Volume : 20 uL  
 Date Acquired : 2021/7/5 下午 08:02:31 Acquired by : System Administrator  
 Date Processed : 2021/7/5 下午 09:02:32 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

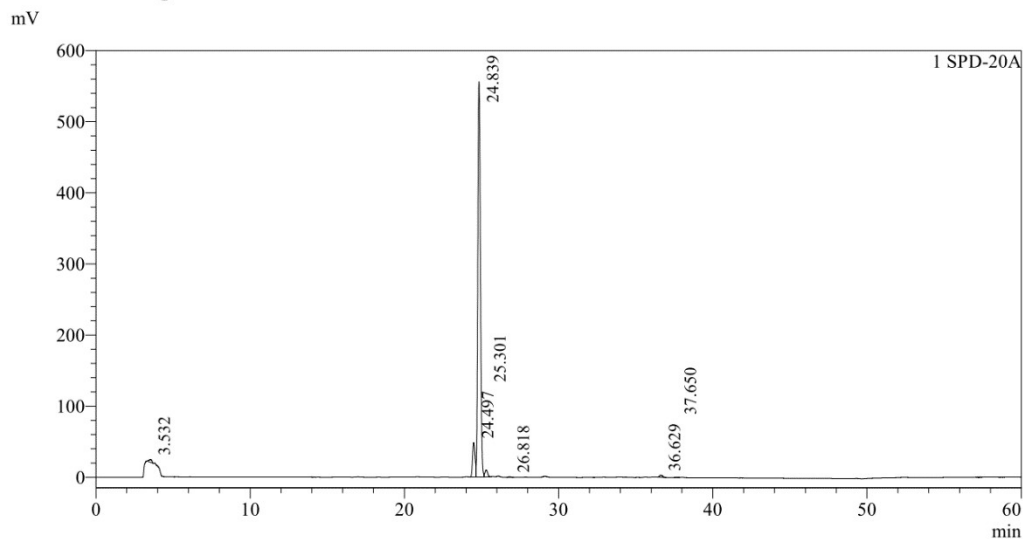
## &lt;&lt;Pump&gt;&gt;

Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;



## &lt;Peak Table&gt;

SPD-20A Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	3.532	51152	3954	12.936	0.690	0.897
2	24.497	542388	48420	11.202	7.317	--
3	24.839	6647504	556318	11.949	89.679	1.156
4	25.301	120021	10069	11.919	1.619	--
5	26.818	6398	537	11.908	0.086	1.209
6	36.629	40518	2982	13.588	0.547	1.190
7	37.650	4601	428	10.756	0.062	1.049
Total		7412582	622709		100.000	

## HPLC spectrum of compound 4

## ==== Shimadzu LabSolutions Analysis Report =====

Sample Name : DHT-05392 (10mM NH<sub>4</sub>OAc+ 0.1 HCOOH 60m) Data Filename : 2  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210705-LC (10mM NH<sub>4</sub>OAc)  
 Vial # : 1-34 Injection Volume : 20 uL  
 Date Acquired : 2021/7/5 下午 11:03:38 Acquired by : System Administrator  
 Date Processed : 2021/7/6 上午 12:03:39 Processed by : System Administrator

## &lt;&lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

## &lt;&lt;Pump&gt;&gt;

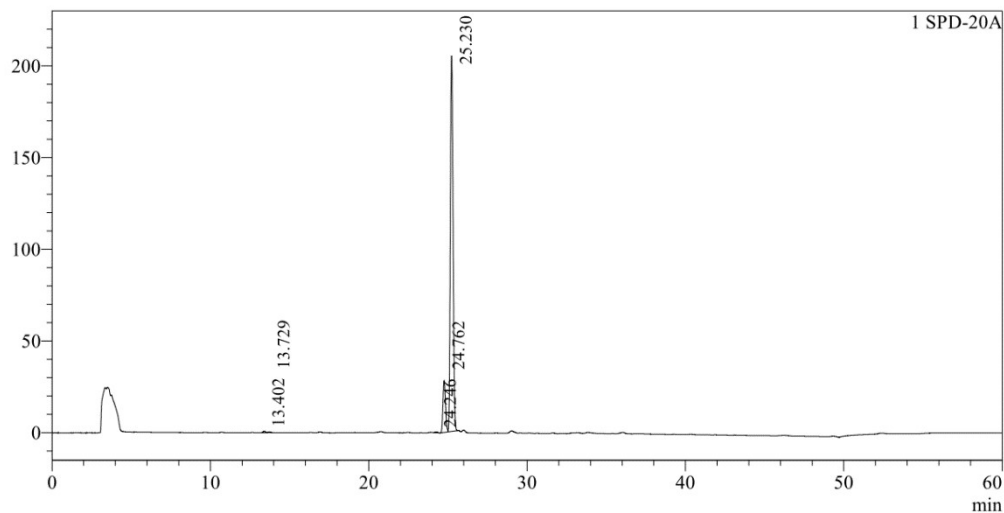
Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;

mV



## &lt;Peak Table&gt;

SPD-20A

Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	13.402	7624	773	9.869	0.278	1.046
2	13.729	3509	365	9.619	0.128	1.219
3	24.246	4863	467	10.417	0.178	1.263
4	24.762	324055	28152	11.511	11.837	1.148
5	25.230	2397636	204819	11.706	87.579	1.159
Total		2737688	234576		100.000	

## HPLC spectrum of compound 6

## ==== Shimadzu LabSolutions Analysis Report =====

Sample Name : DHT-05530 (10mM NH<sub>4</sub>OAc+ 0.1 HCOOH 60m) Data Filename : 2  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210705-LC (10mM NH<sub>4</sub>OAc)  
 Vial # : 1-35 Injection Volume : 20 uL  
 Date Acquired : 2021/7/5 下午 10:03:16 Acquired by : System Administrator  
 Date Processed : 2021/7/5 下午 11:03:17 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

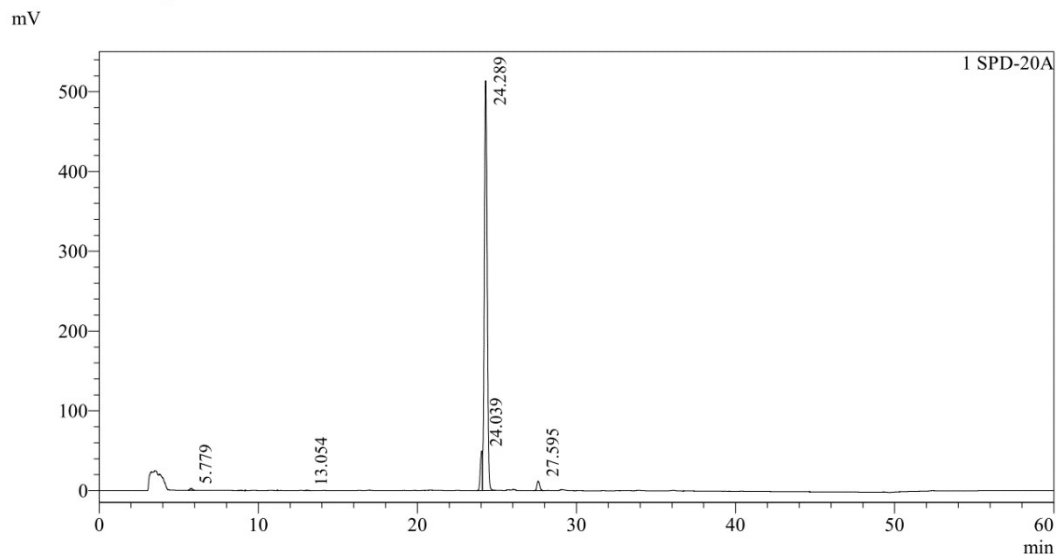
## &lt;&lt;Pump&gt;&gt;

Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;



## &lt;Peak Table&gt;

SPD-20A						
Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	5.779	23426	2352	9.959	0.340	1.082
2	13.054	4269	441	9.673	0.062	1.213
3	24.039	434390	49544	8.768	6.300	--
4	24.289	6290796	513677	12.247	91.236	--
5	27.595	142222	11865	11.986	2.063	1.164
Total		6895102	577880		100.000	

## HPLC spectrum of compound 8

## ==== Shimadzu LabSolutions Analysis Report ====

Sample Name : DHT-05-quinone (10mM NH<sub>4</sub>OAc+ 0.1 HCOOH 60m) Data Filename  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210705-LC (10mM NH<sub>4</sub>OAc)  
 Vial # : 1-38 Injection Volume : 20 uL  
 Date Acquired : 2021/7/5 下午 09:02:53 Acquired by : System Administrator  
 Date Processed : 2021/7/5 下午 10:02:54 Processed by : System Administrator

## &lt;Method&gt;

<<Data Acquisition>>  
 AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

<<Autosampler>>  
 Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

<<Oven>>  
 Oven Model : LC-2030 Oven Enable Oven : Not Used

<<Column Information>>  
 Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

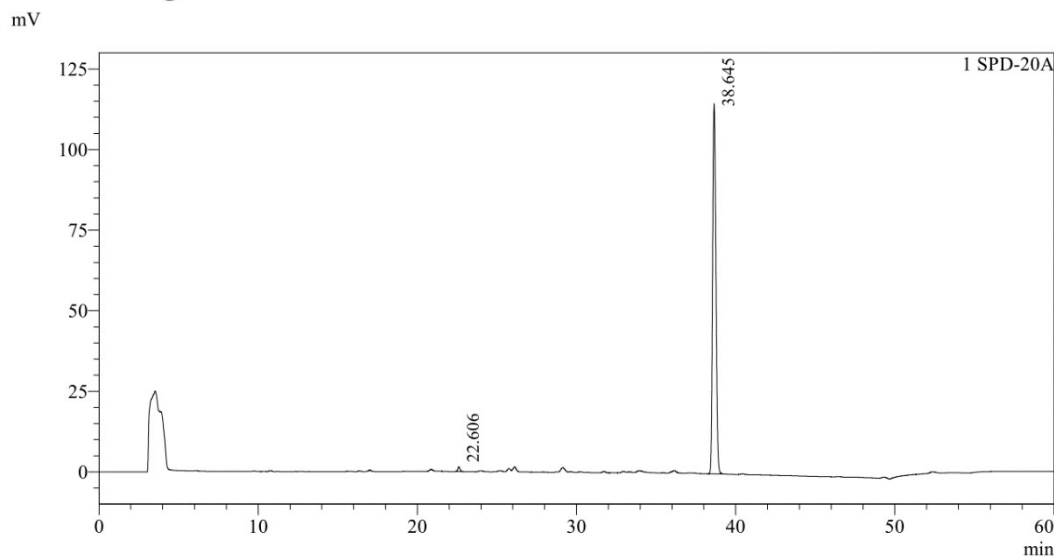
<<Mobile Phase Name>>  
 Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

<<Pump>>  
 Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

<<LC Time Program>>  

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;



## &lt;Peak Table&gt;

SPD-20A						
Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	22.606	13986	1472	9.501	0.845	1.267
2	38.645	1642058	114629	14.325	99.155	1.153
Total		1656045	116101		100.000	



## HPLC spectrum of compound 9

## ==== Shimadzu LabSolutions Analysis Report ====

Sample Name : DHT-05532 (10mM NH<sub>4</sub>OAc+ 0.1 HCOOH 60m) Data Filename : 2  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210705-LC (10mM NH<sub>4</sub>OAc)  
 Vial # : 1-36 Injection Volume : 20 uL  
 Date Acquired : 2021/7/6 上午 12:04:01 Acquired by : System Administrator  
 Date Processed : 2021/7/6 上午 01:04:04 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

## &lt;&lt;Pump&gt;&gt;

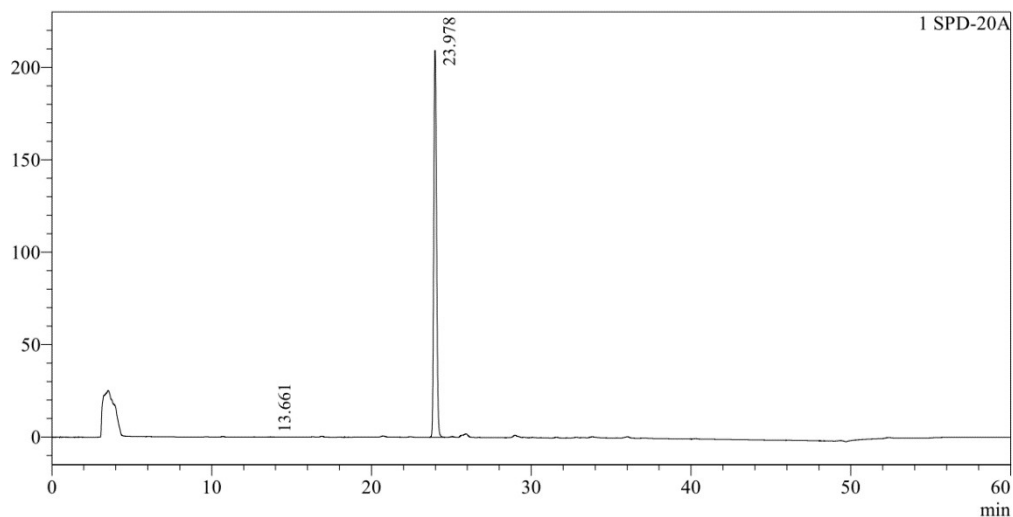
Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;

mV



## &lt;Peak Table&gt;

SPD-20A

Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	13.661	1152	108	10.622	0.047	1.400
2	23.978	2471312	209400	11.802	99.953	1.153
Total		2472463	209509		100.000	

## HPLC spectrum of compound 13

## ==== Shimadzu LabSolutions Analysis Report ====

Sample Name : DHT-05485 (Ag 10mM AmAc HCOOH pH 2.5 60m) Data Filename  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210909-LC-10m - ph 2.5.lc  
 Vial # : 1-12 Injection Volume : 20 uL  
 Date Acquired : 2021/9/10 上午 01:17:41 Acquired by : System Administrator  
 Date Processed : 2021/9/10 上午 02:17:43 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

## &lt;&lt;Pump&gt;&gt;

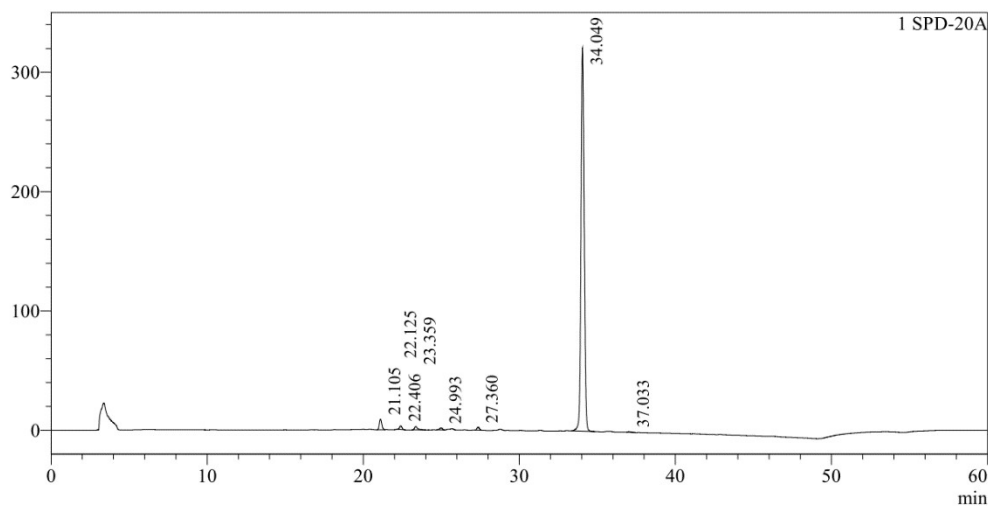
Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;

mV



## &lt;Peak Table&gt;

SPD-20A

Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	21.105	95144	8845	10.757	1.975	1.154
2	22.125	1379	174	7.941	0.029	0.891
3	22.406	32168	2918	11.023	0.668	1.141
4	23.359	41781	2965	14.090	0.867	2.083
5	24.993	22224	1669	13.313	0.461	0.872
6	27.360	28188	2575	10.947	0.585	1.156
7	34.049	4590039	321423	14.280	95.286	1.082
8	37.033	6200	461	13.464	0.129	1.420
Total		4817124	341029		100.000	

## HPLC spectrum of compound 14

## ==== Shimadzu LabSolutions Analysis Report =====

Sample Name : DHT-01125 (Ag 10mM AmAc HCOOH pH 2.5 60m) Data Filename  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210909-LC-10m - ph 2.5.lc  
 Vial # : 1-11 Injection Volume : 20 uL  
 Date Acquired : 2021/9/10 上午 12:17:17 Acquired by : System Administrator  
 Date Processed : 2021/9/10 上午 01:17:19 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

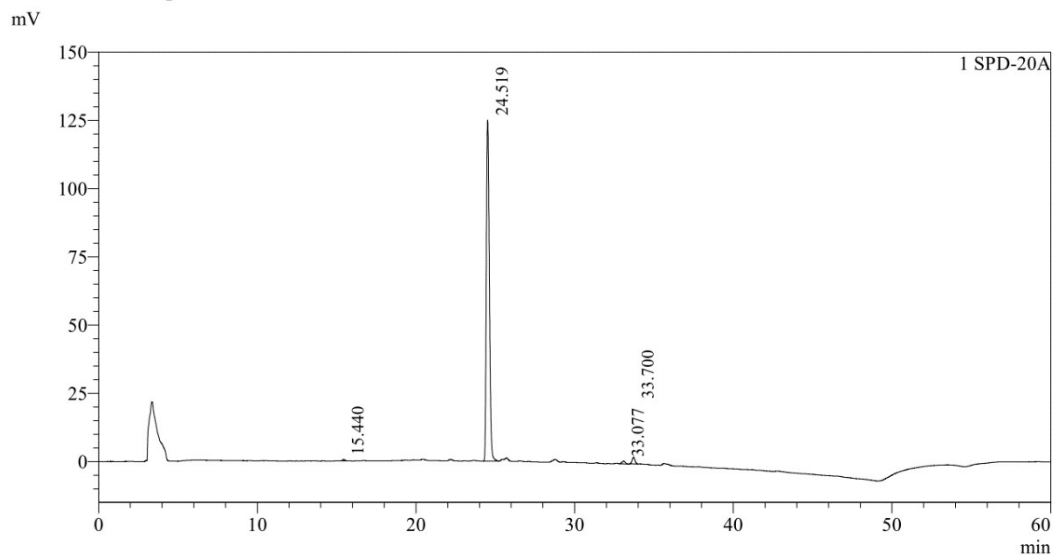
## &lt;&lt;Pump&gt;&gt;

Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

## &lt;Chromatogram&gt;



## &lt;Peak Table&gt;

SPD-20A						
Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	15.440	5312	577	9.205	0.309	1.191
2	24.519	1668033	125108	13.333	97.088	1.257
3	33.077	14435	1019	14.165	0.840	1.139
4	33.700	30284	2436	12.430	1.763	1.126
Total		1718064	129141		100.000	

## HPLC spectrum of compound 15

## ==== Shimadzu LabSolutions Analysis Report ====

Sample Name : DHT-01123 (Ag 10mM AmAc HCOOH pH 2.5 60m) Data Filename  
 Method Filename : 61-HPLC Buffer-60min.lcm Batch Filename : 20210909-LC-10m - ph 2.5.lc  
 Vial # : 1-10 Injection Volume : 20 uL  
 Date Acquired : 2021/9/9 下午 11:16:54 Acquired by : System Administrator  
 Date Processed : 2021/9/10 上午 12:16:56 Processed by : System Administrator

## &lt;Method&gt;

## &lt;&lt;Data Acquisition&gt;&gt;

AD1 Name : SPD-20A LC Stop Time : 60.00 min  
 AD1 Sampling Frequency : 2 Hz

## &lt;&lt;Autosampler&gt;&gt;

Autosampler Model : LC-2030 Autosampler  
 Enable Autosampler : Use

## &lt;&lt;Oven&gt;&gt;

Oven Model : LC-2030 Oven Enable Oven : Not Used

## &lt;&lt;Column Information&gt;&gt;

Column Name : ZORBAX Eclipse XDB-C18 Column ID : ZORBAX Eclipse XDB-C18  
 Column Length : 150 mm Inner Diameter : 4.6 mm

## &lt;&lt;Mobile Phase Name&gt;&gt;

Mobile Phase A : Acetonitrile Mobile Phase B : Water  
 Mobile Phase C : Methanol Mobile Phase D : Buffer

## &lt;&lt;Pump&gt;&gt;

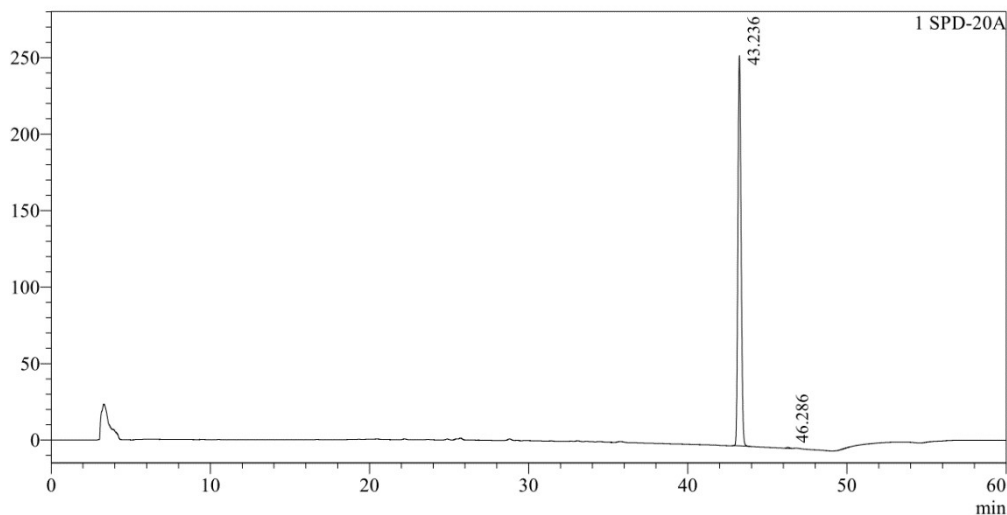
Mode : Low pressure gradient Pump A : LC-2030 Pump  
 Flow : 0.5000 mL/min B Conc. : 0.0 %  
 C Conc. : 0.0 % D Conc. : 90.0 %

## &lt;&lt;LC Time Program&gt;&gt;

Time	Module	Command	Value	Comment
0.01	Pumps	Solvent D Conc.	90	
45.00	Pumps	Solvent D Conc.	10	
50.00	Pumps	Solvent D Conc.	90	
60.00	Pumps	Solvent D Conc.	90	
60.00	Controller	Stop		

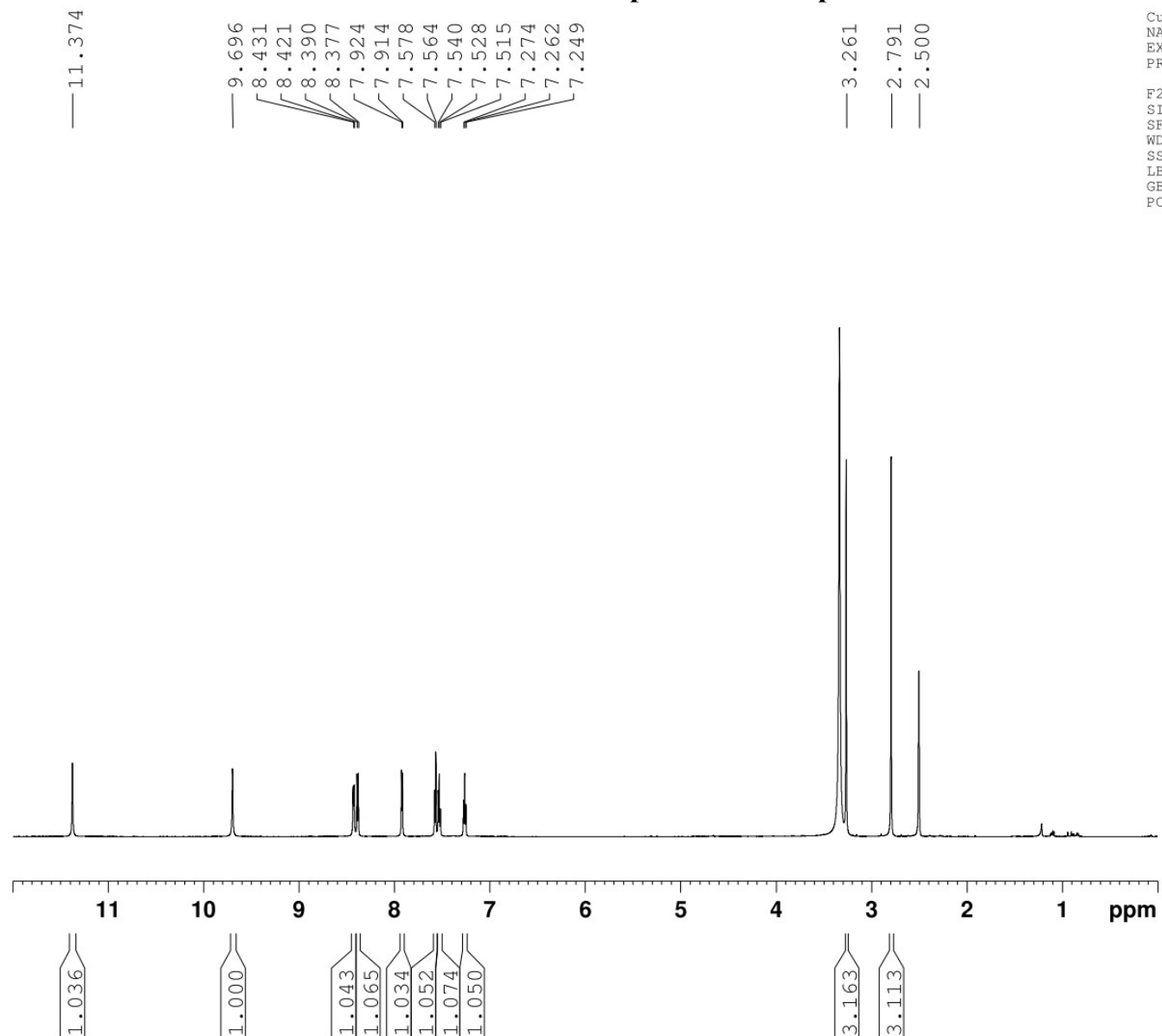
## &lt;Chromatogram&gt;

mV

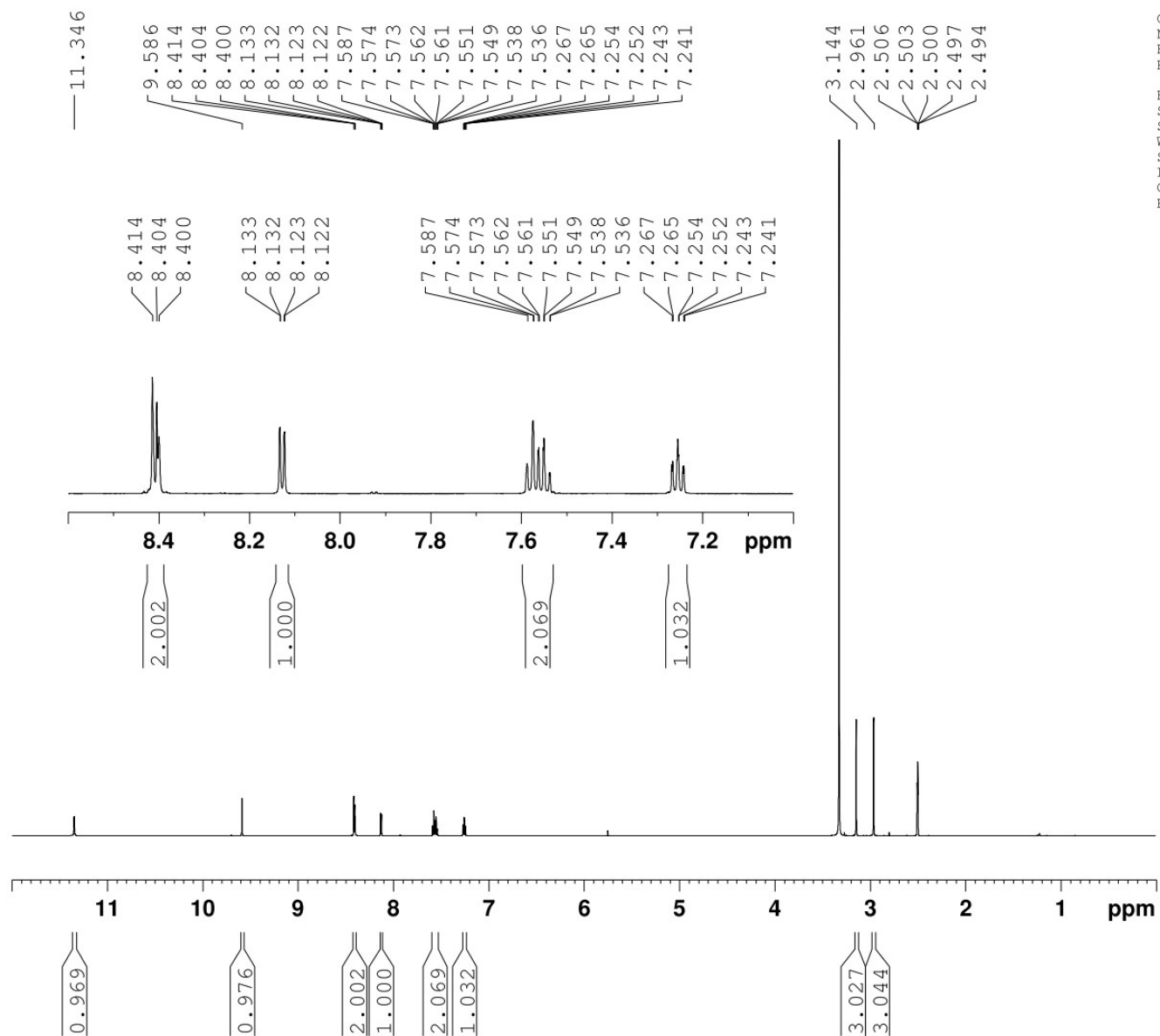


## &lt;Peak Table&gt;

SPD-20A						
Peak#	Ret. Time	Area	Height	Area/Height	Area%	Tailing Factor
1	43.236	3473308	255082	13.616	99.832	1.161
2	46.286	5841	542	10.775	0.168	1.204
Total		3479149	255624		100.000	

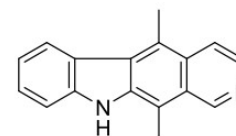
**<sup>1</sup>H Spectra for compound 1**

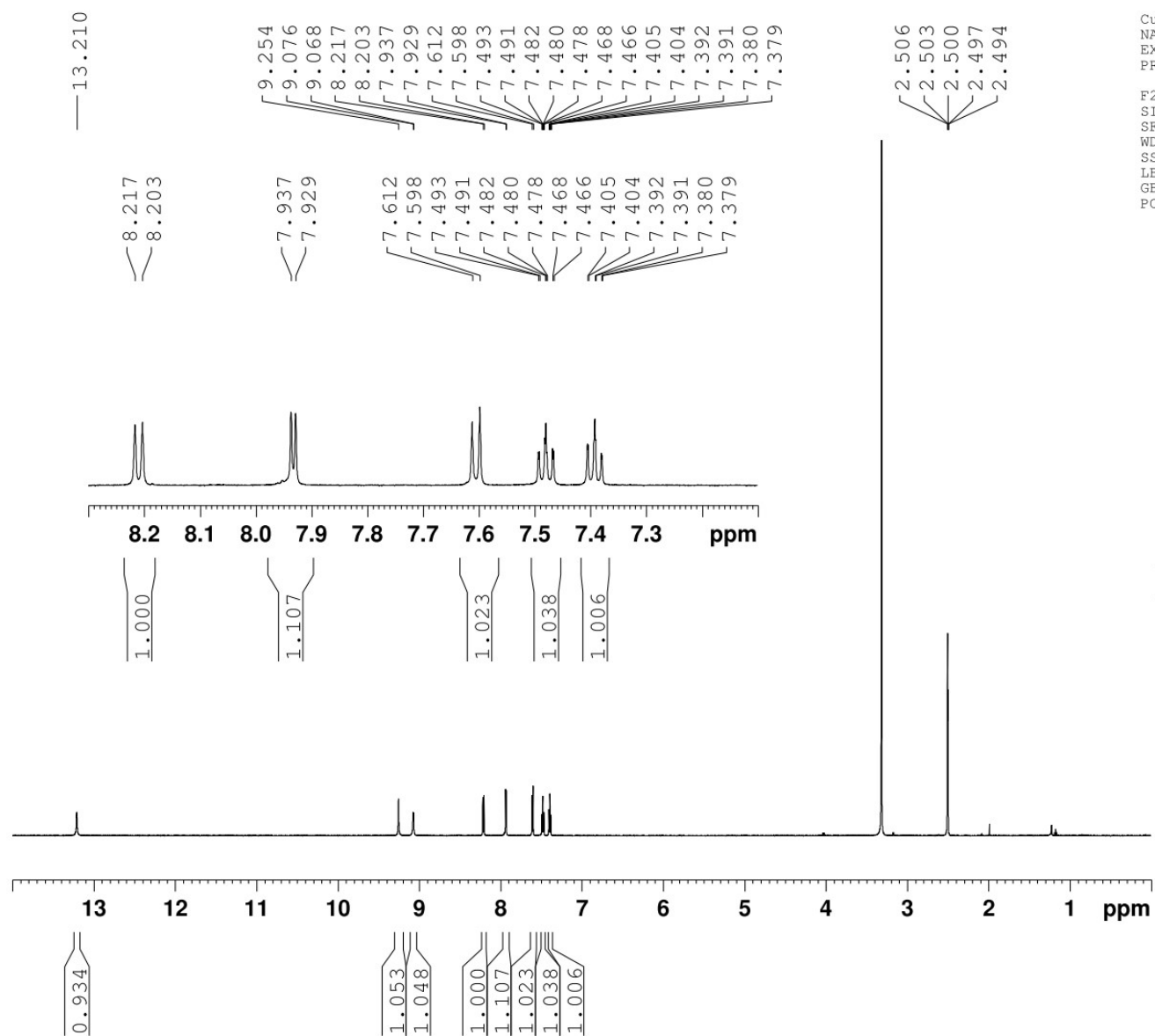
Current Data Parameters  
NAME PROTON\_20210702\_02.fid - new  
EXPNO 1  
PROCNO 1  
  
F2 - Processing parameters  
SI 65536  
SF 599.8300392 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

**<sup>1</sup>H Spectra for compound 2**

Current Data Parameters  
NAME PROTON\_20210727\_02.fid - new  
EXPNO 1  
PROCNO 1

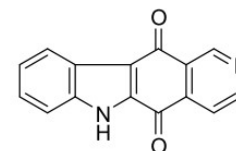
F2 - Processing parameters  
SI 65536  
SF 599.8300382 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

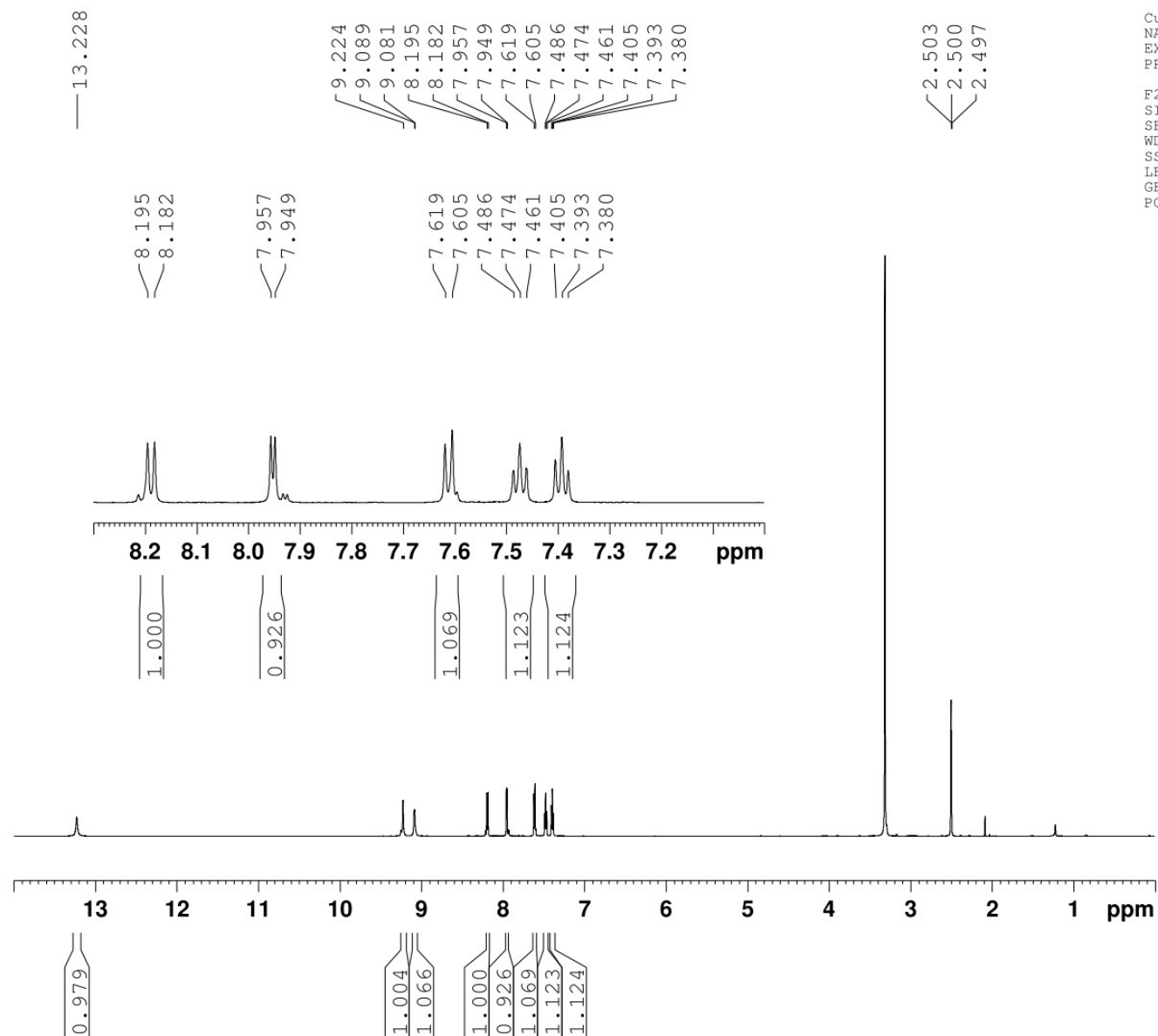


**$^1\text{H}$  Spectra for compound 3**

Current Data Parameters  
NAME PROTON\_20210629\_01.fid - new  
EXPNO 1  
PROCNO 1

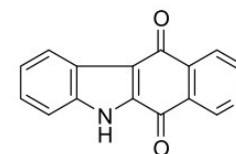
F2 - Processing parameters  
SI 65536  
SF 599.8300389 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



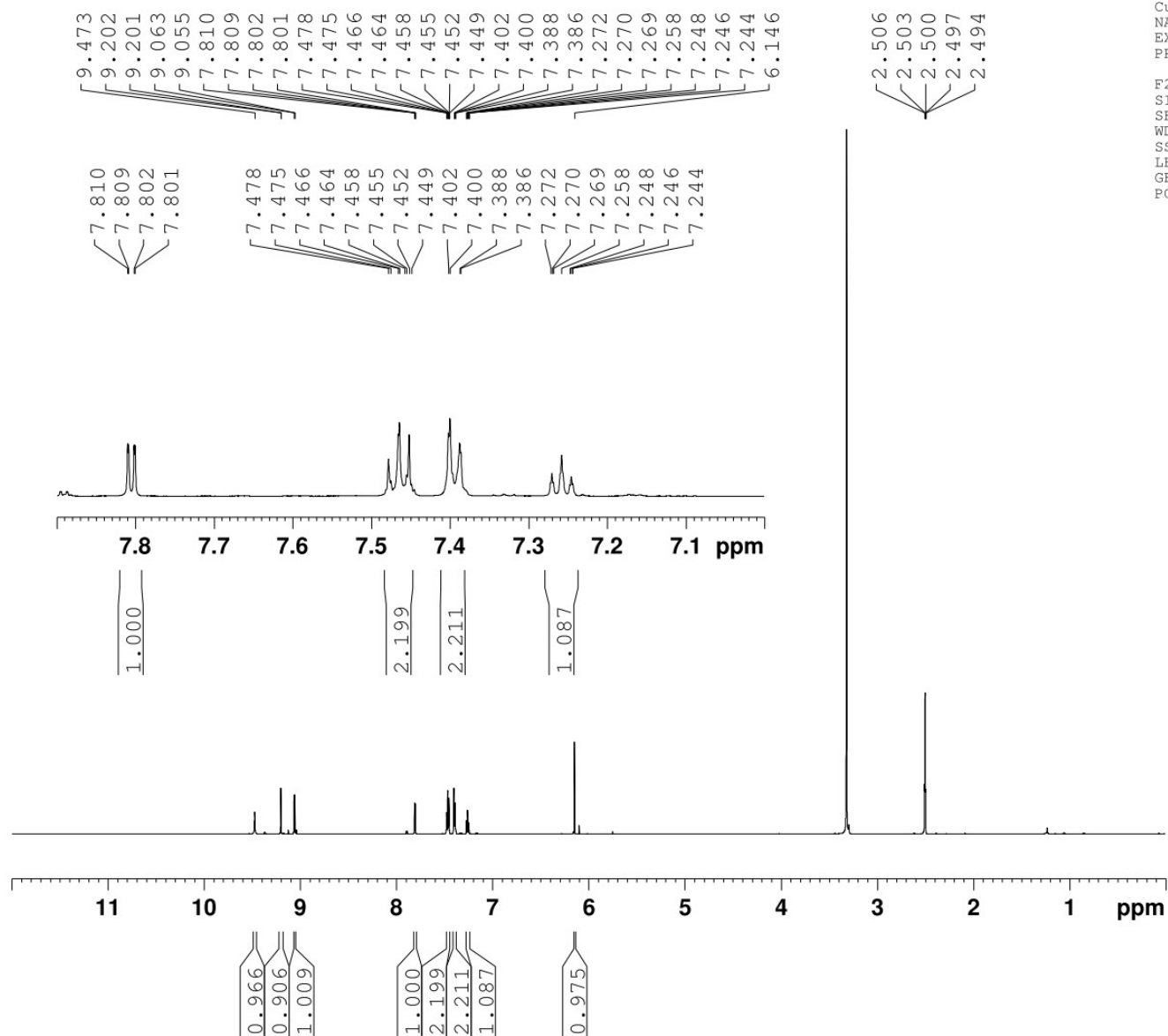
**<sup>1</sup>H Spectra for compound 4**

Current Data Parameters  
NAME PROTON\_20200605\_02.fid - new  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 599.8300380 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

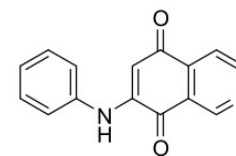




**<sup>1</sup>H Spectra for compound 6**

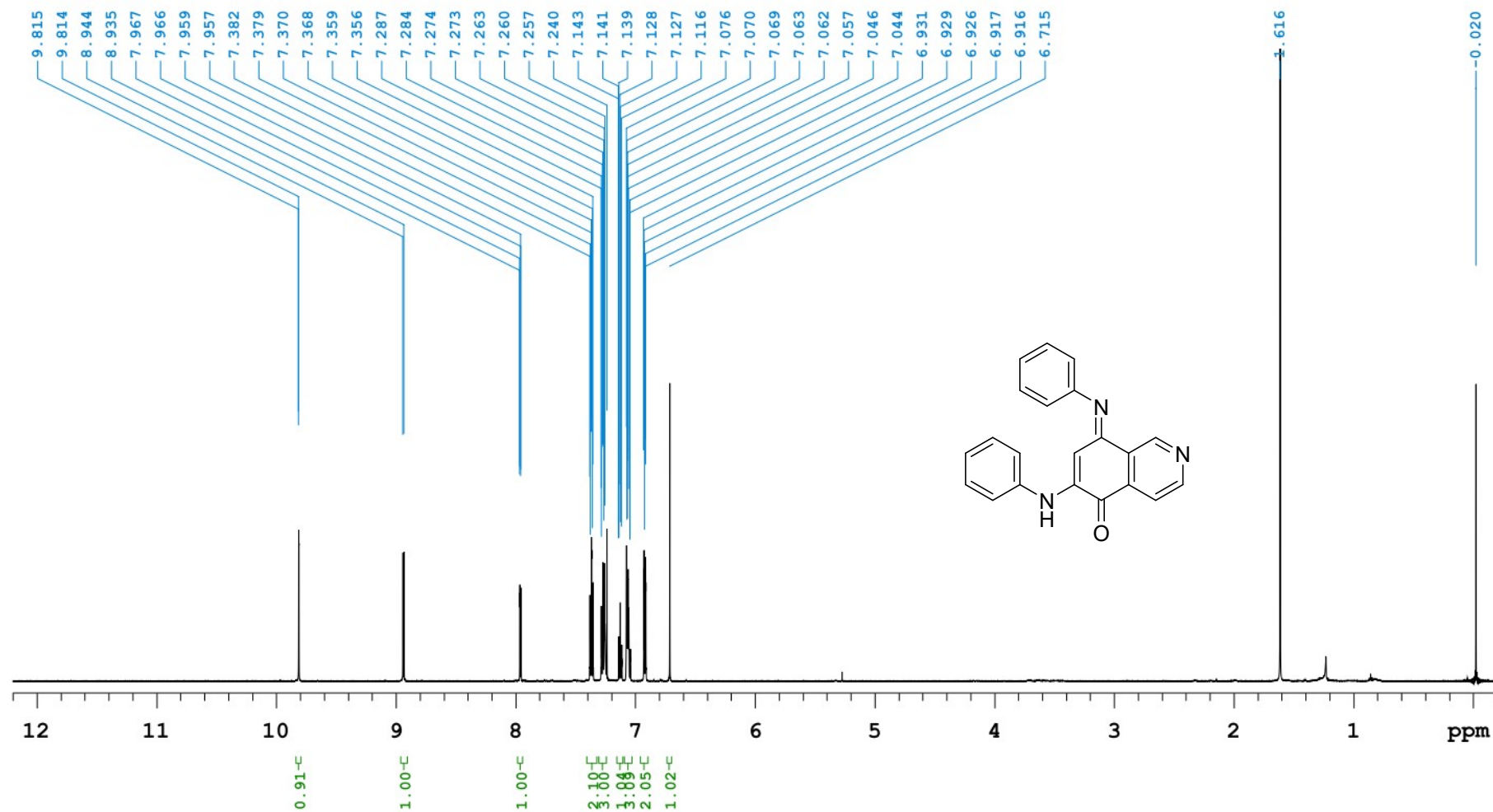
Current Data Parameters  
NAME PROTON\_20210602\_02.fid - new  
EXPNO 1  
PROCNO 1

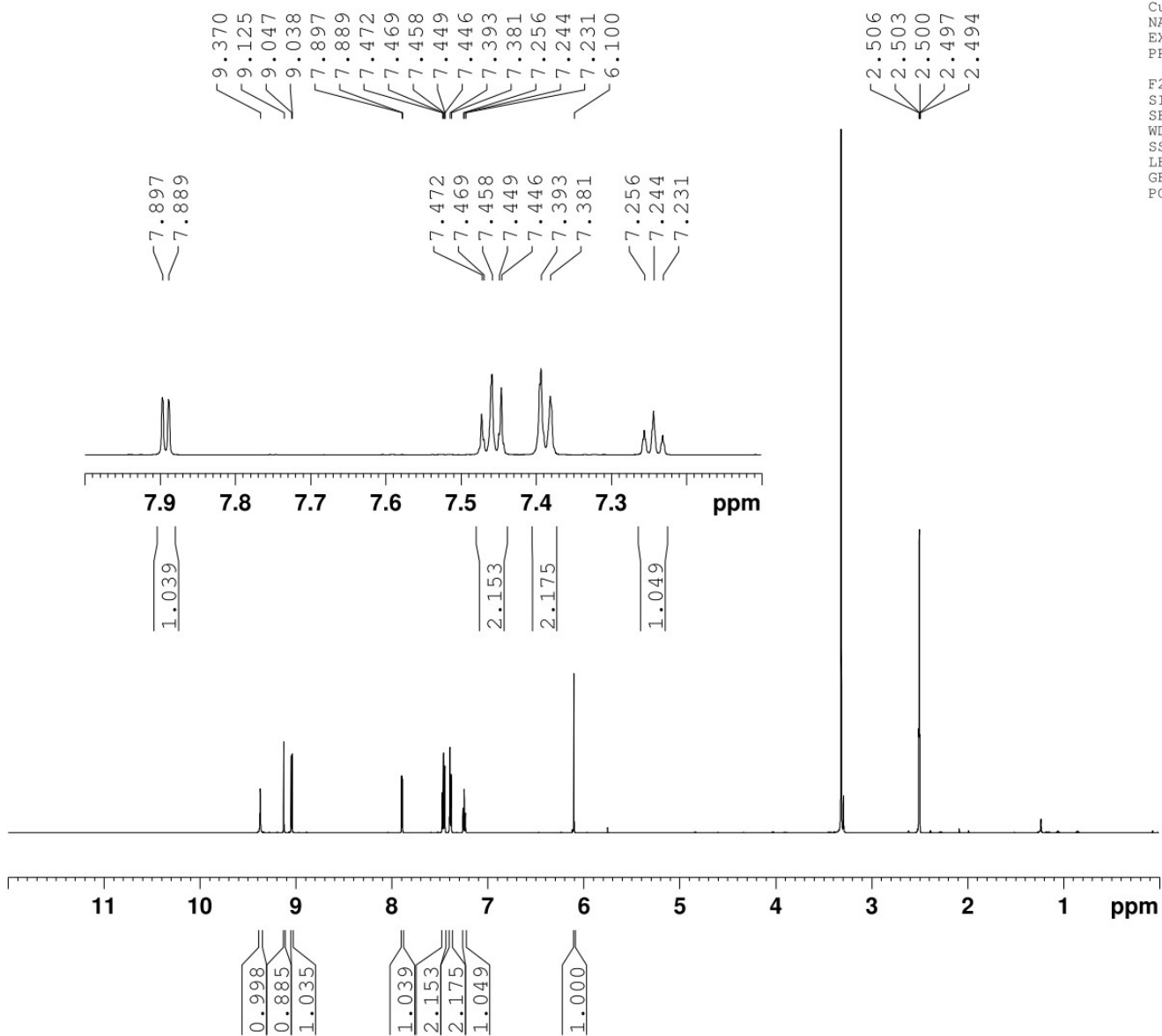
F2 - Processing parameters  
SI 65536  
SF 599.8300388 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



# <sup>1</sup>H Spectra for compound 9

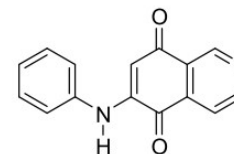
0601-DHT-quinone

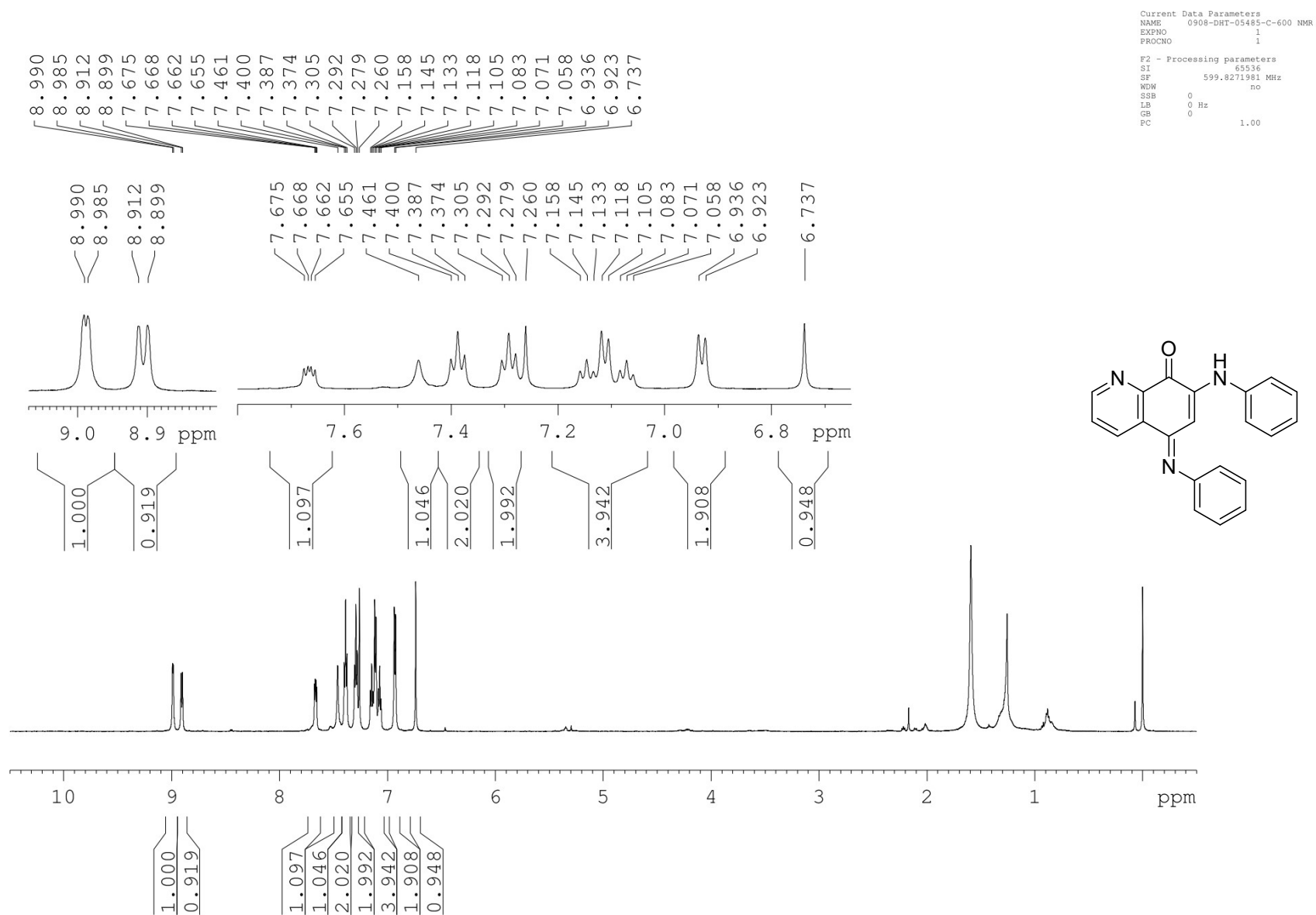
Sample Name 0601-DHT-quinone  
Date collected 2021-06-01Pulse sequence PROTON  
Solvent cdcl3Temperature 27  
Spectrometer Agilent-NMR-vnmrs600Study owner tmu  
Operator tmu

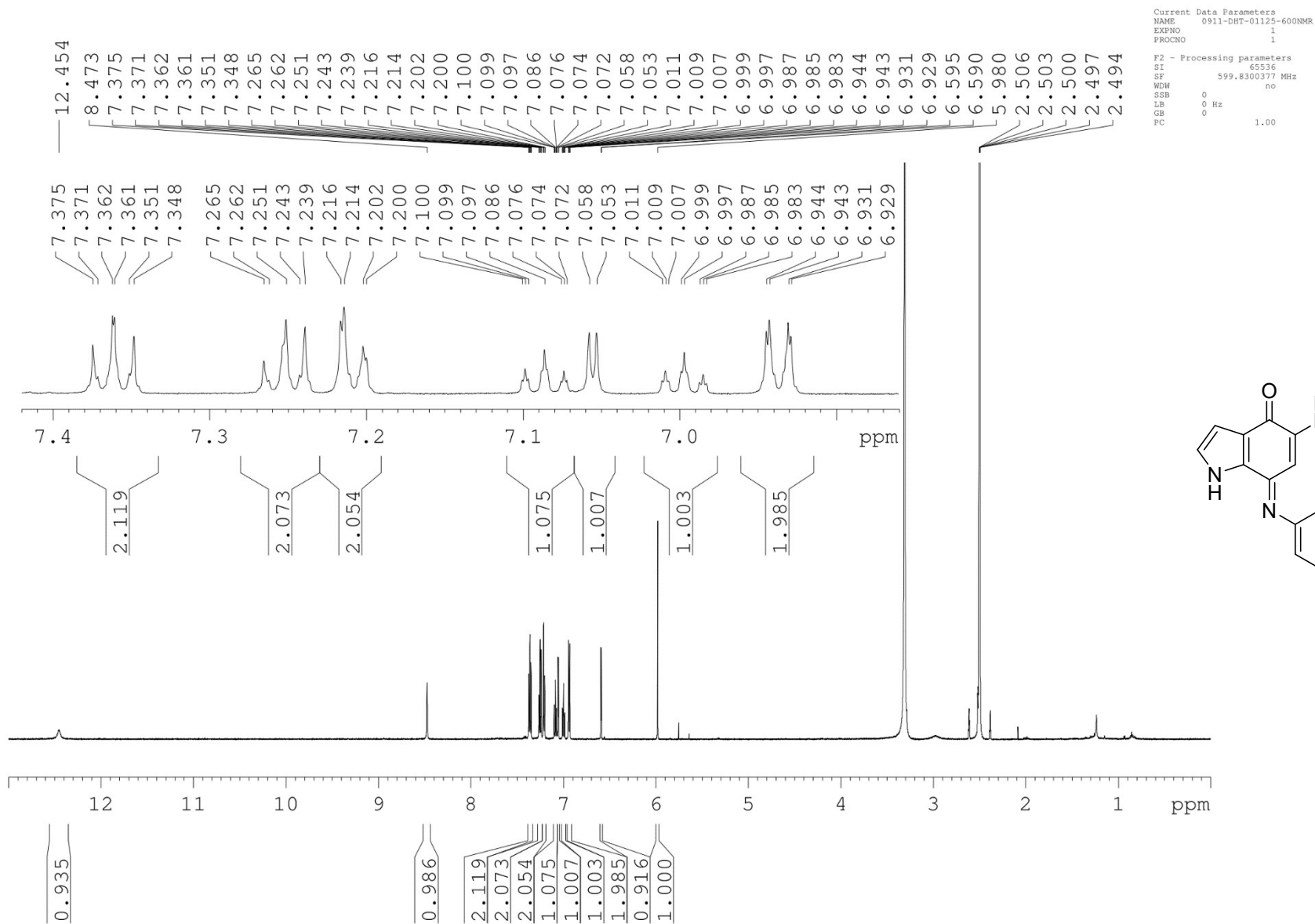
**<sup>1</sup>H Spectra for compound 9**

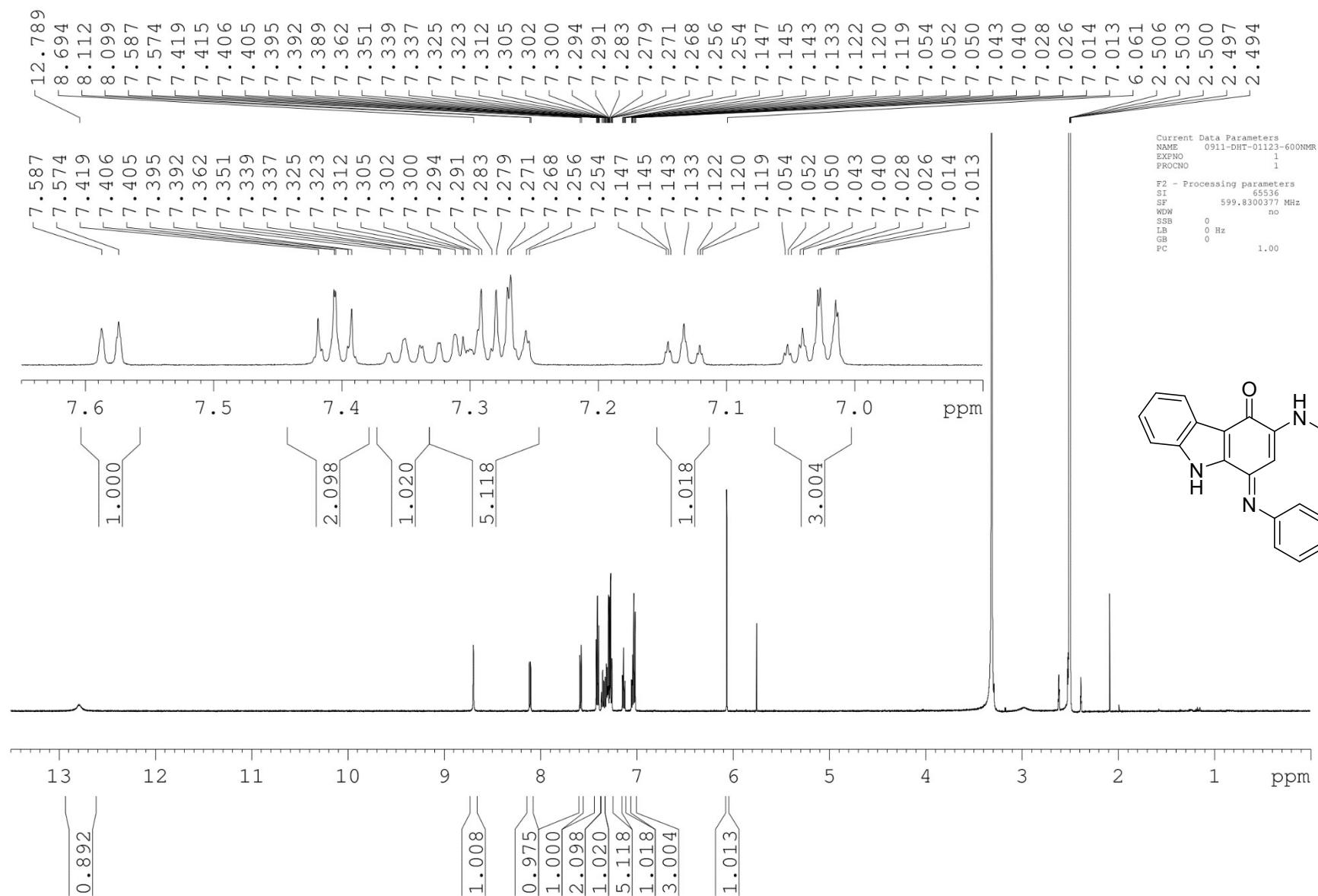
Current Data Parameters  
 NAME PROTON\_20210602\_02.fid - new  
 EXPNO 1  
 PROCNO 1

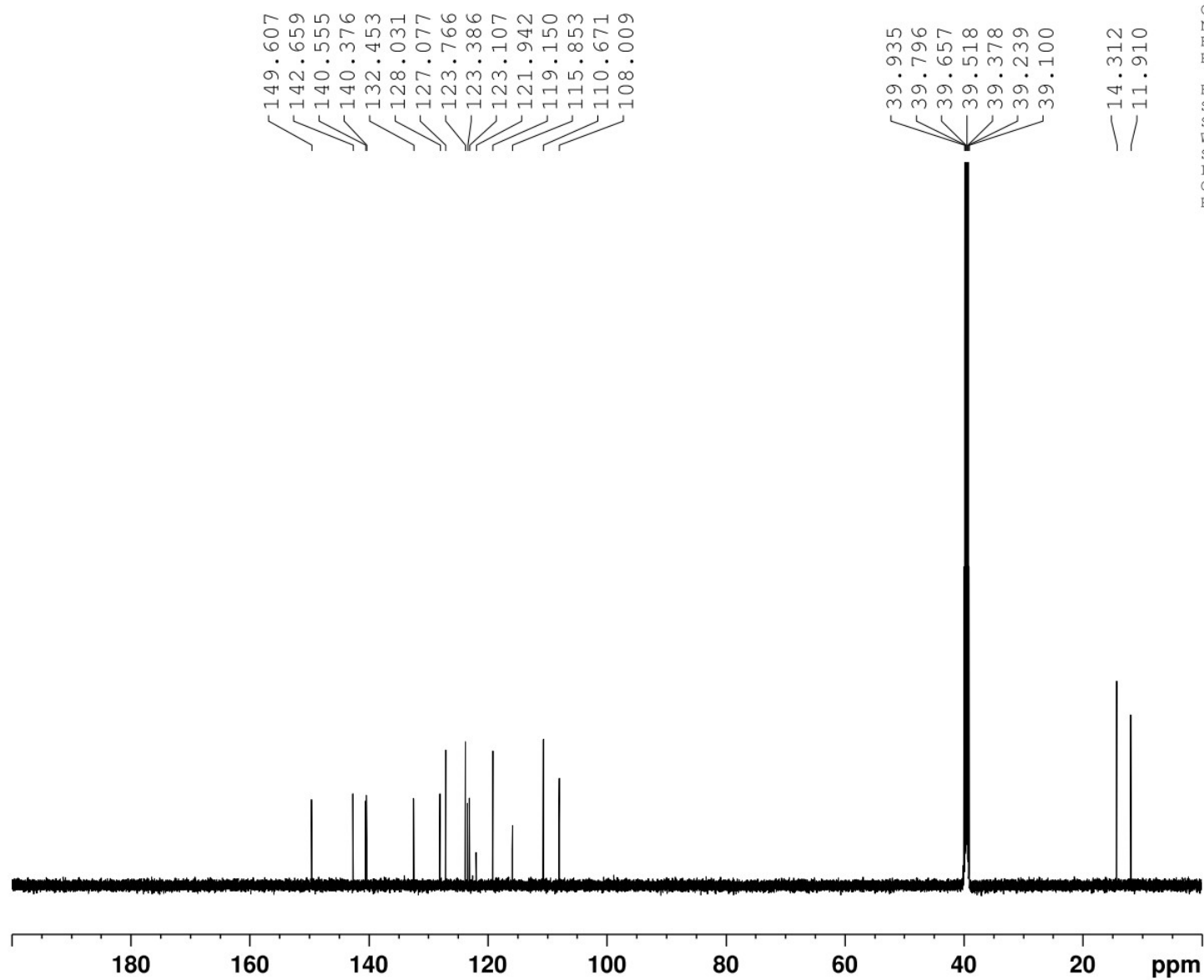
F2 - Processing parameters  
 SI 65536  
 SF 599.8300388 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00



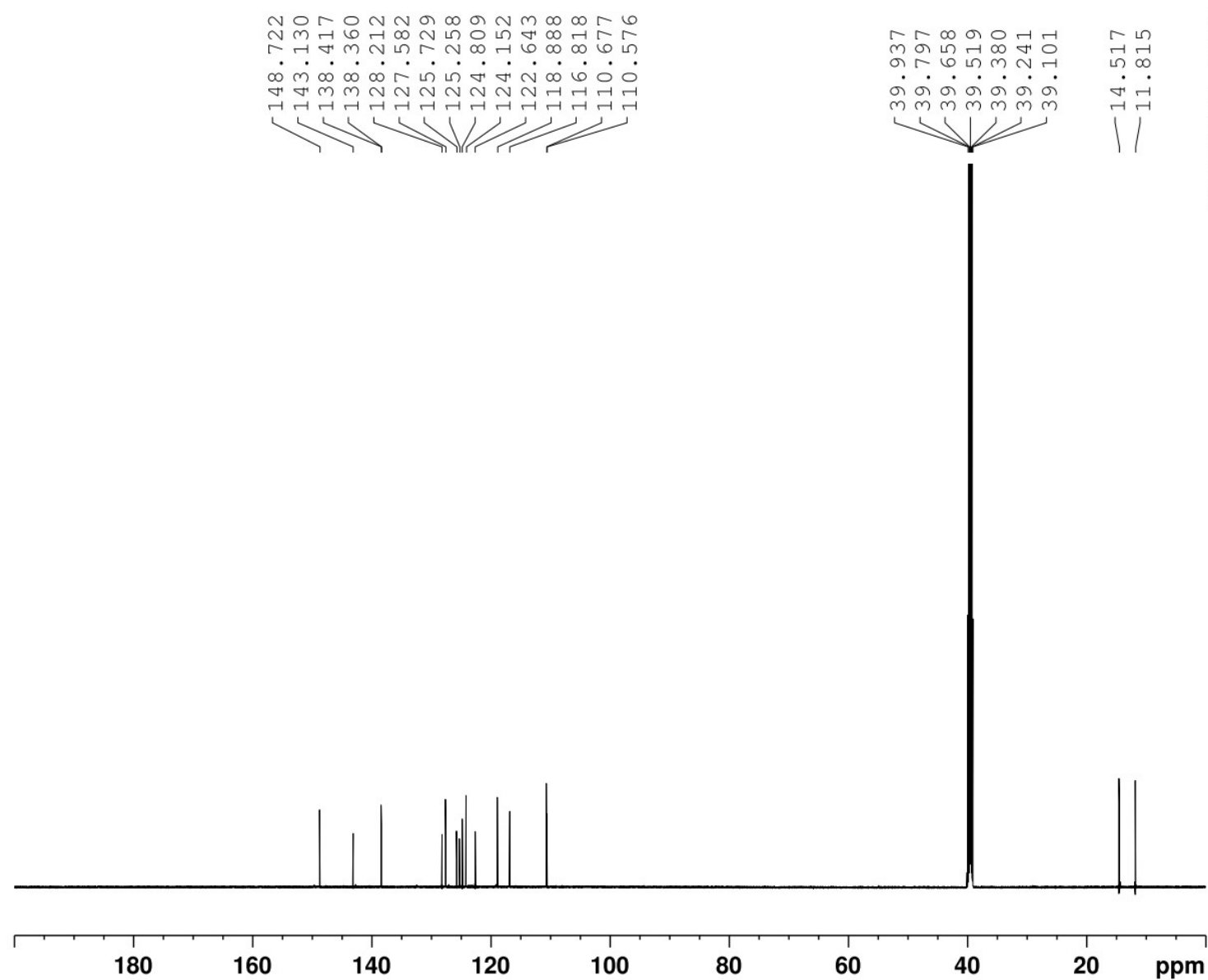
**<sup>1</sup>H Spectra for compound 13**

**<sup>1</sup>H Spectra for compound 14**

**<sup>1</sup>H Spectra for compound 15**

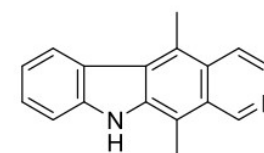
**$^{13}\text{C}$  Spectra for compound 1**

Current Data Parameters  
NAME CARBON\_20210702\_01.fid - new  
EXPNO 1  
PROCNO 1  
F2 - Processing parameters  
SI 65536  
SF 150.8296034 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

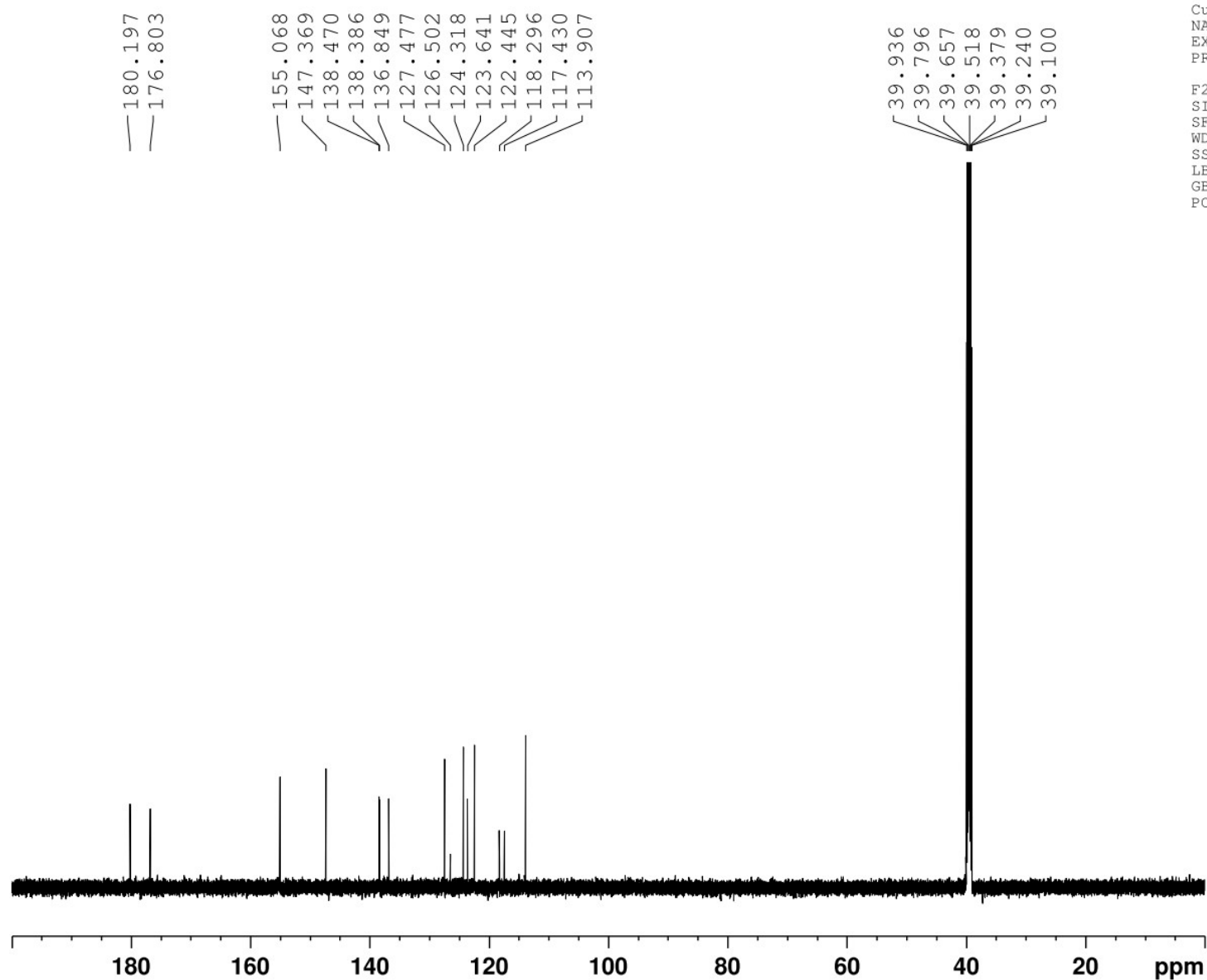
**$^{13}\text{C}$  Spectra for compound 2**

Current Data Parameters  
NAME CARBON\_20210729\_01.fid - new  
EXPNO 1  
PROCNO 1

F2 - Processing parameters  
SI 65536  
SF 150.8306883 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

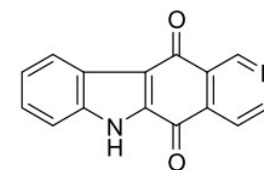


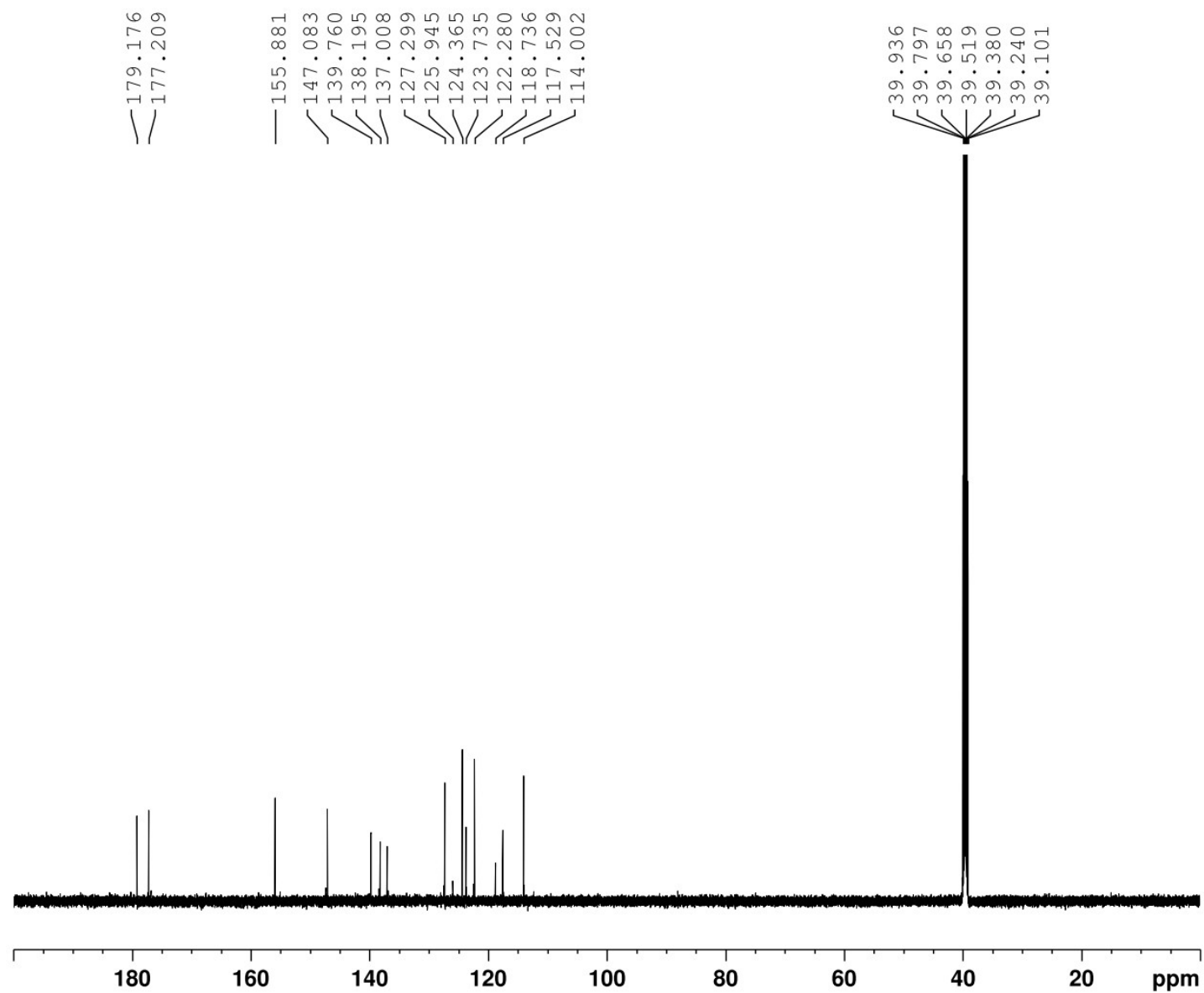


**$^{13}\text{C}$  Spectra for compound 3**

Current Data Parameters  
NAME CARBON\_20210701\_01.fid - new  
EXPNO 1  
PROCNO 1

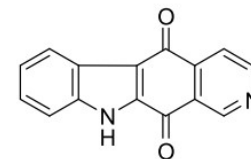
F2 - Processing parameters  
SI 65536  
SF 150.8296040 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

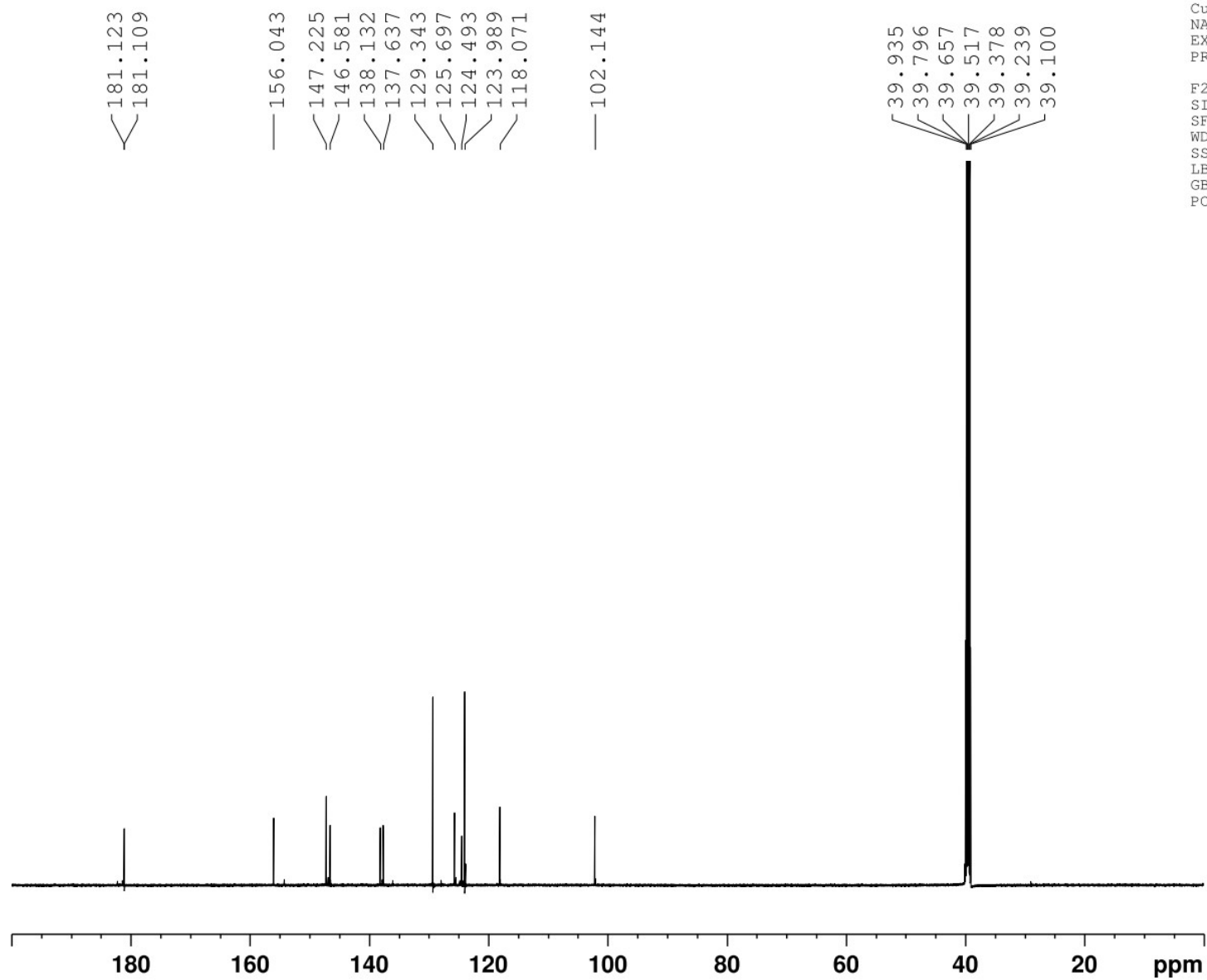


**$^{13}\text{C}$  Spectra for compound 4**

Current Data Parameters  
NAME CARBON\_20200605\_01.fid  
EXPNO 1  
PROCNO 1

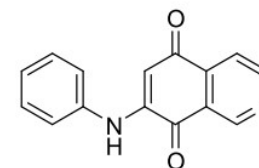
F2 - Processing parameters  
SI 65536  
SF 150.8296038 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



**$^{13}\text{C}$  Spectra for compound 6**

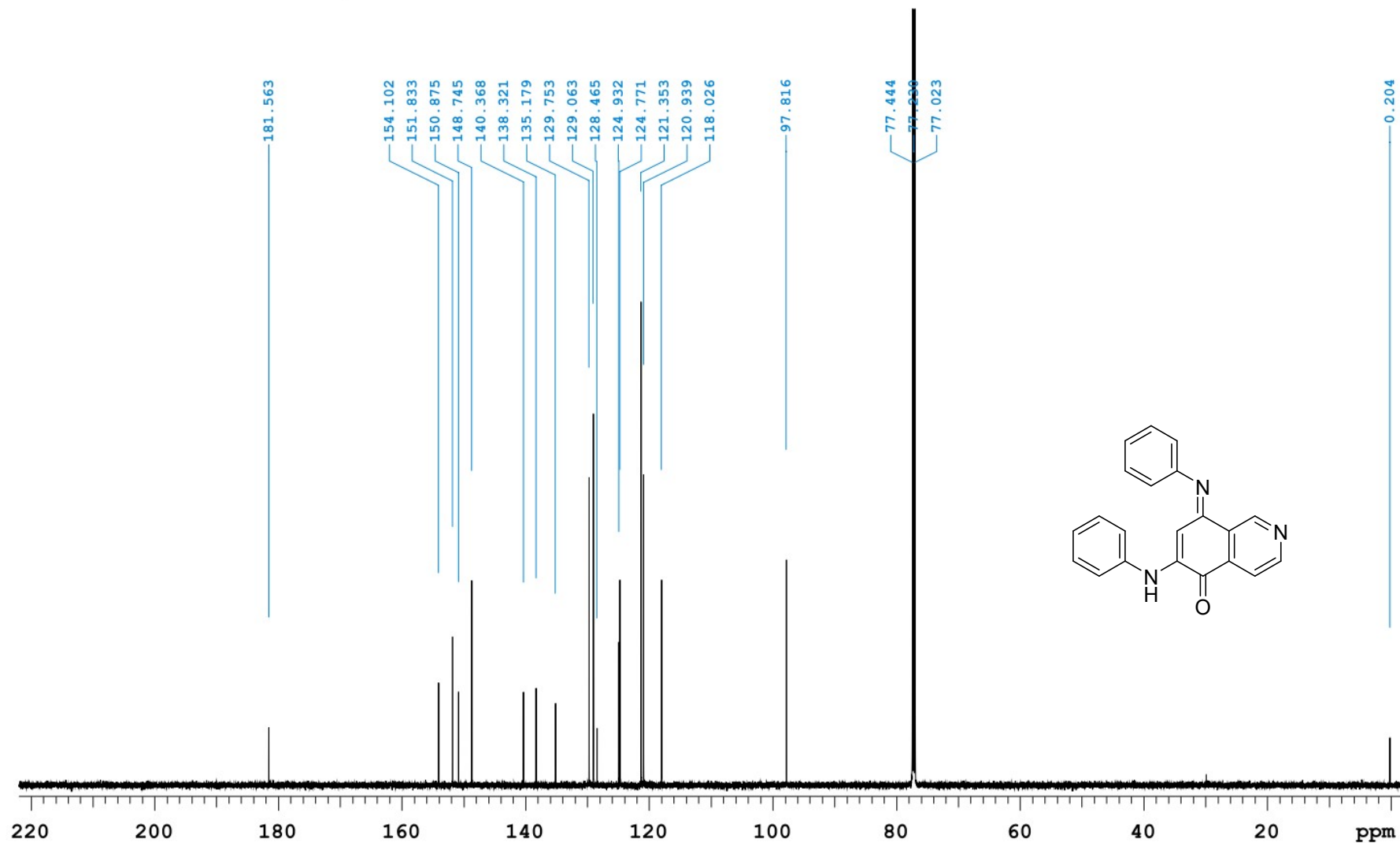
Current Data Parameters  
NAME CARBON\_20210603\_01.fid - new  
EXPNO 1  
PROCNO 1

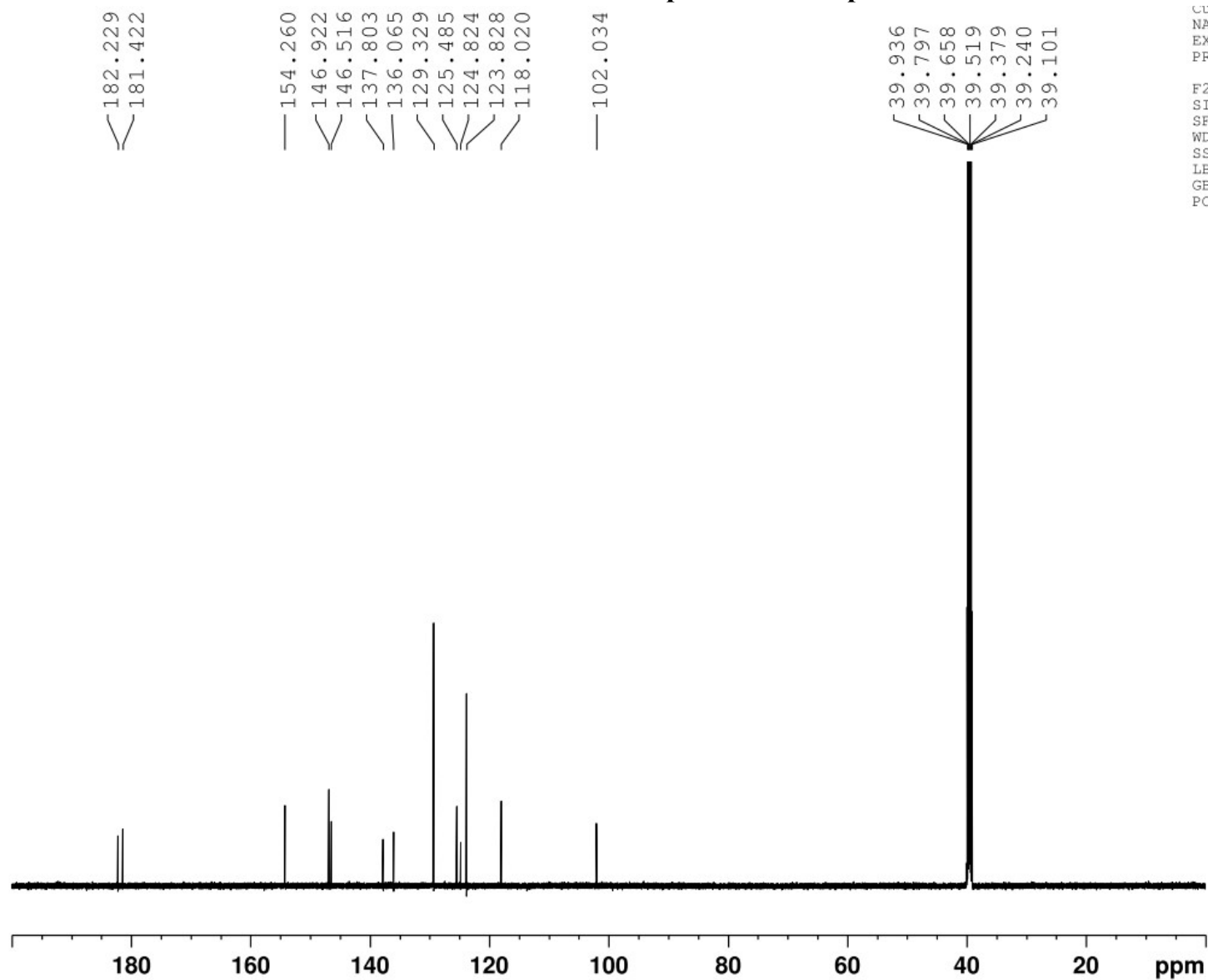
F2 - Processing parameters  
SI 65536  
SF 150.8296036 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



**$^{13}\text{C}$  Spectra for compound 8**

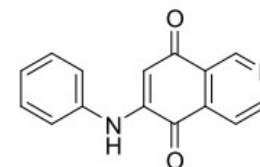
0601-DHT-quinone

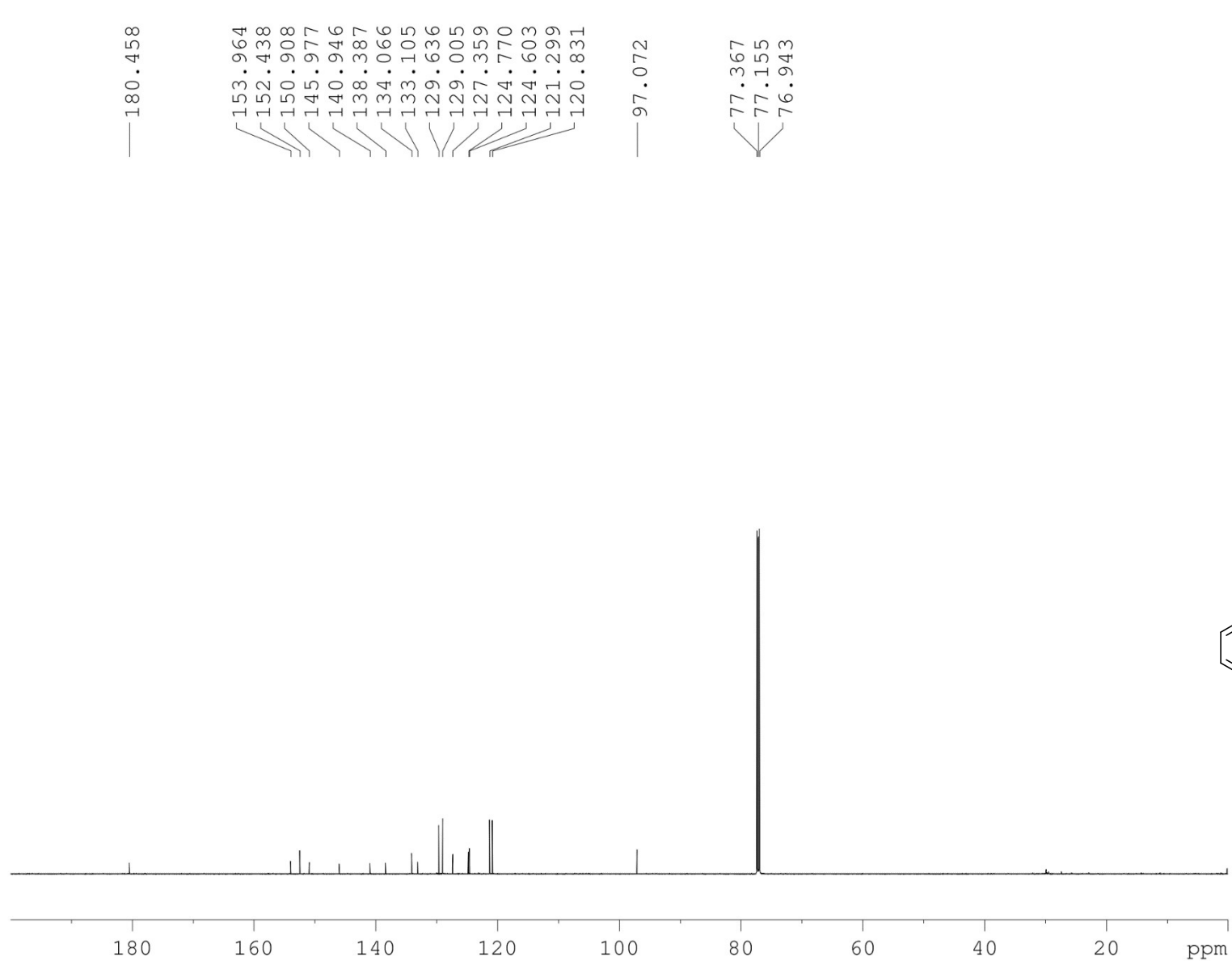
Sample Name **0601-DHT-quinone**  
Date collected **2021-06-01**Pulse sequence **CARBON**  
Solvent **cdcl3**Temperature **27**  
Spectrometer **Agilent-NMR-vnmrs600**Study owner **tmu**  
Operator **tmu**

**$^{13}\text{C}$  Spectra for compound 9**

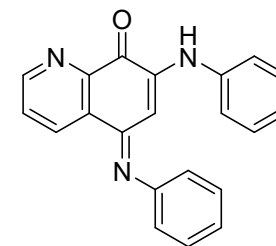
Current Data Parameters  
NAME CARBON\_20210602\_01.fid - new  
EXPNO 1  
PROCNO 1

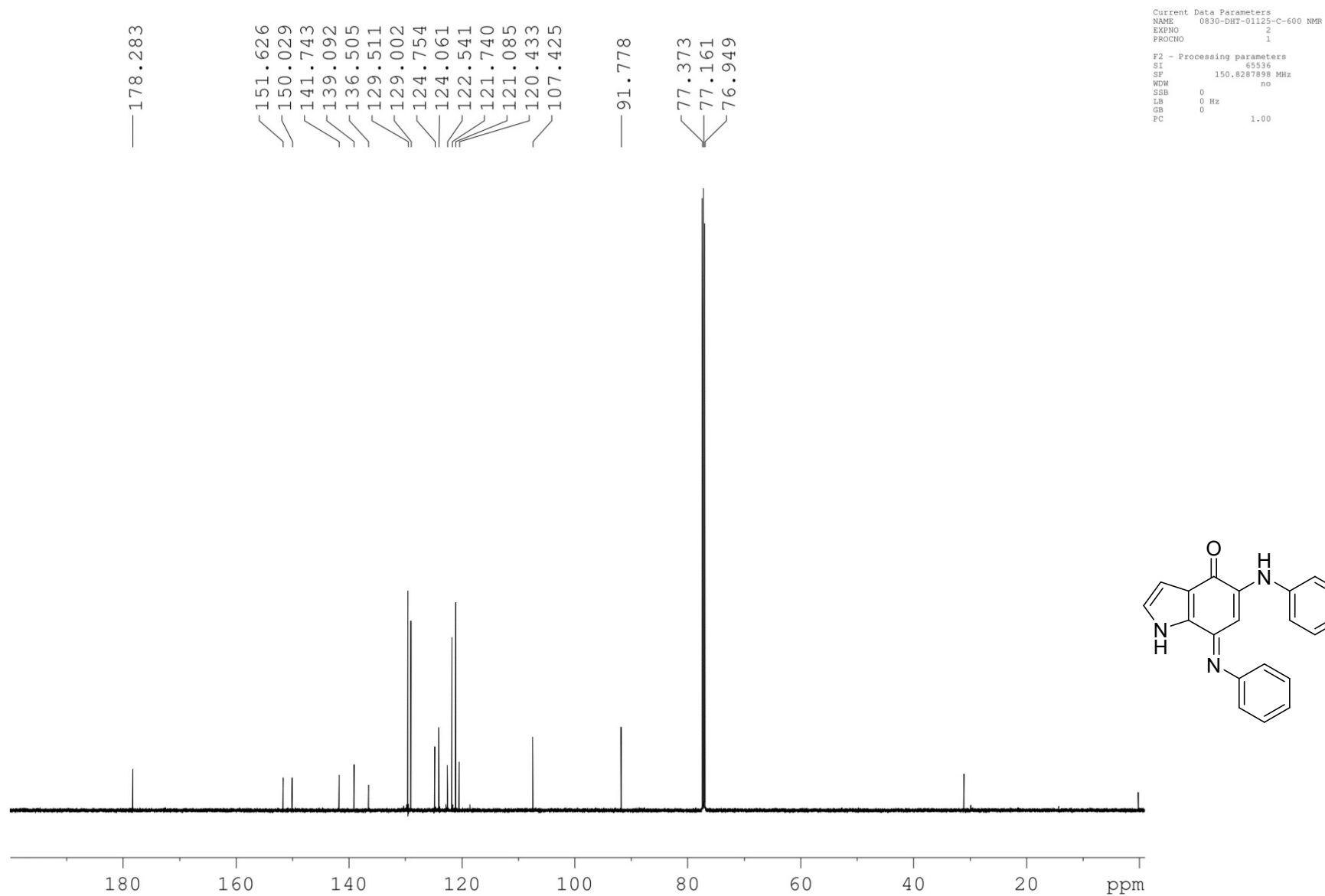
F2 - Processing parameters  
SI 65536  
SF 150.8296037 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

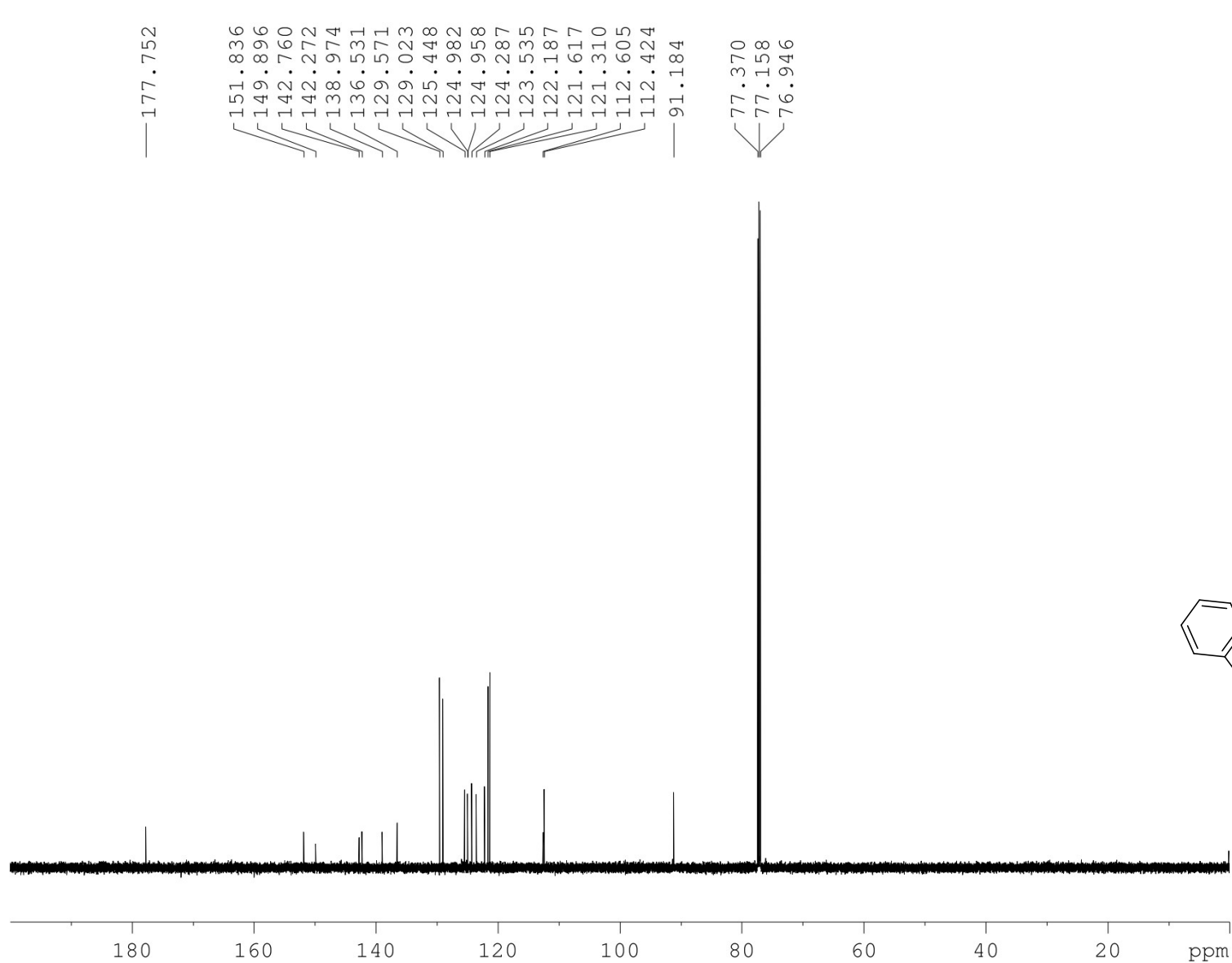


**$^{13}\text{C}$  Spectra for compound 13**

Current Data Parameters  
NAME 0908-DHT-05485-C-600 NMR  
EXPNO 2  
PROCNO 1  
F2 - Processing parameters  
SI 65536  
SF 150.8287899 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

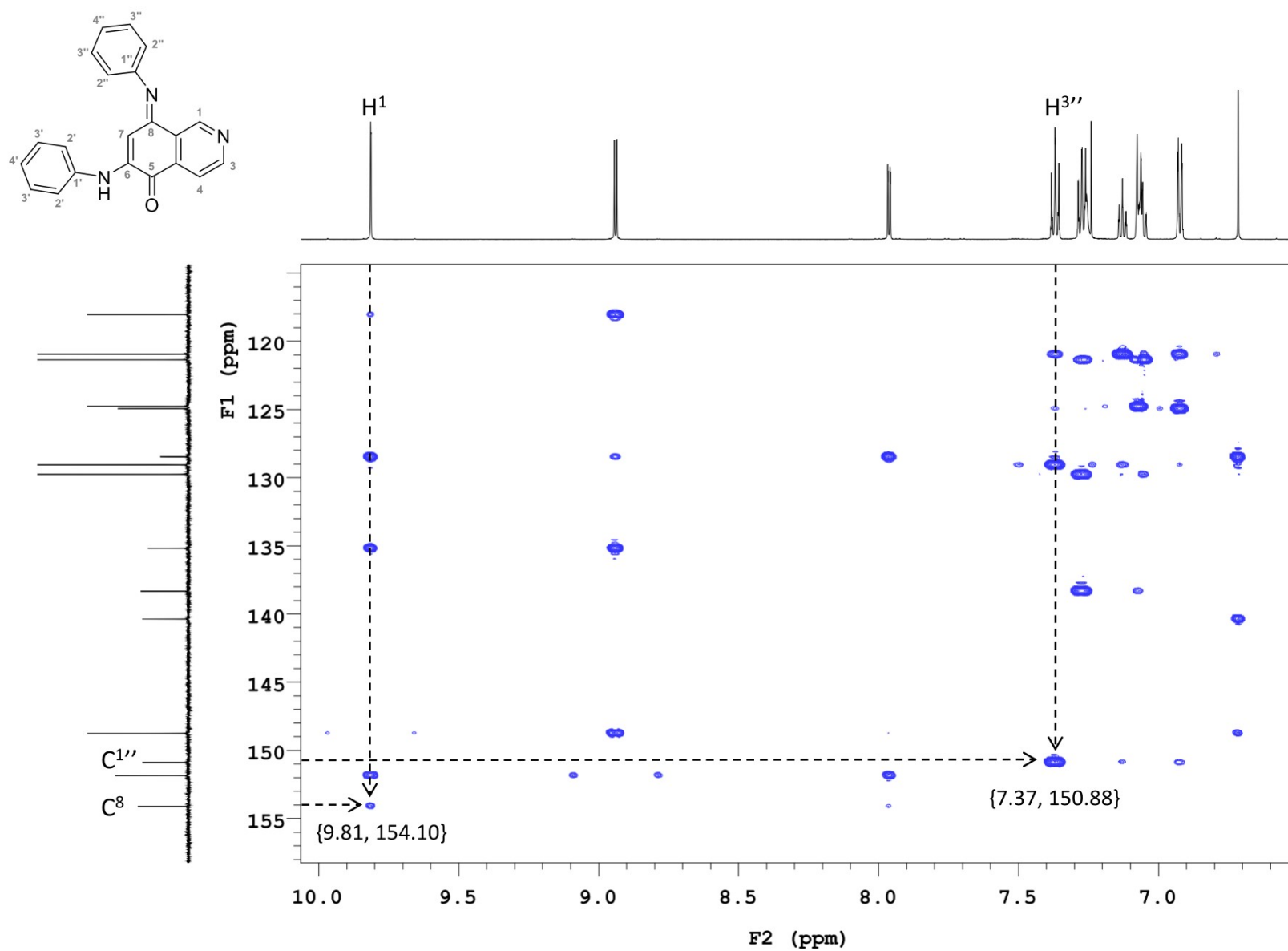


**$^{13}\text{C}$  Spectra for compound 14**

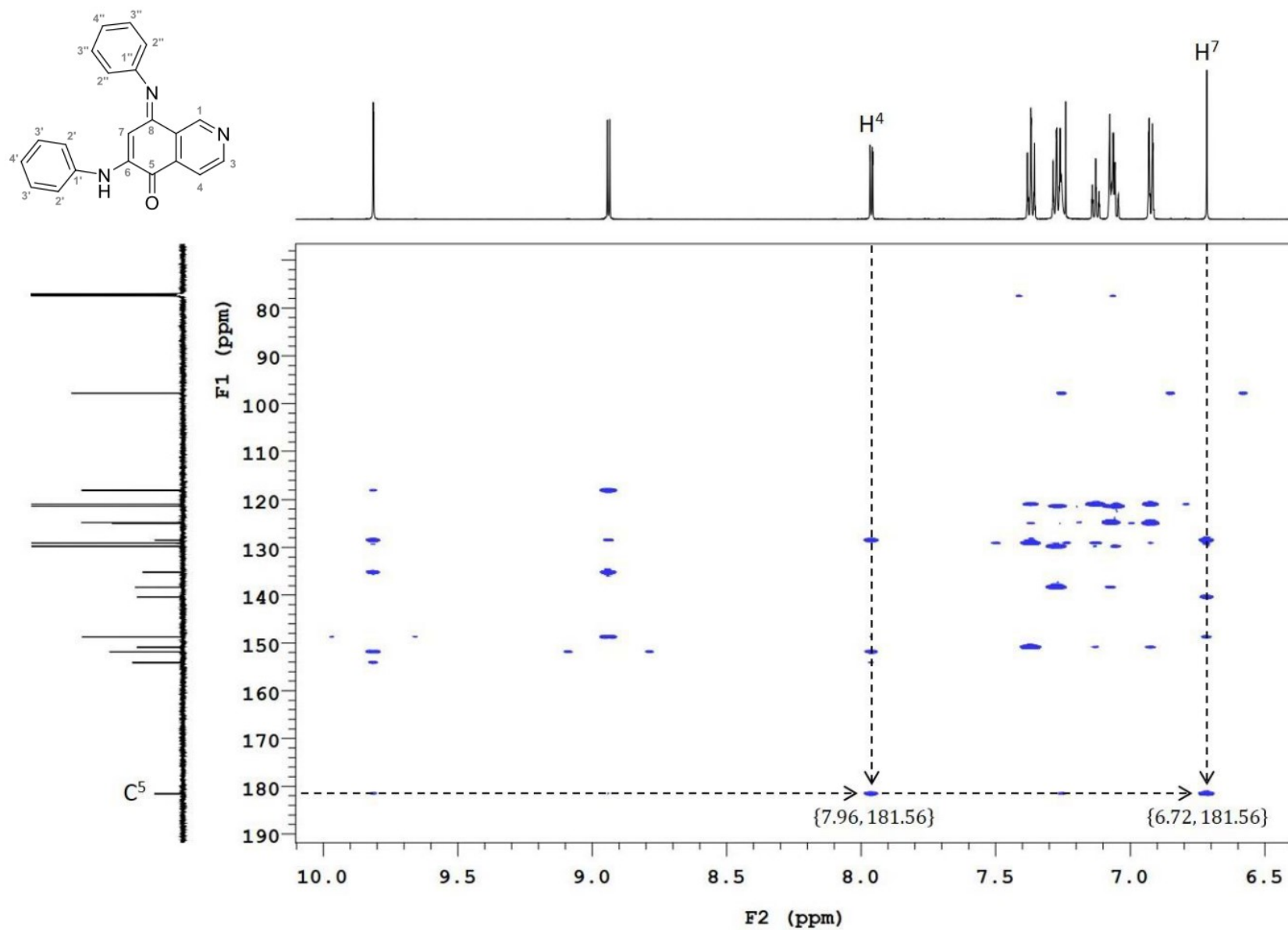
**$^{13}\text{C}$  Spectra for compound 15**



## HMBC Spectra for compound 8



## HMBC Spectra for compound 8



## NOESY Spectra for compound 8

