Supplementary Material

Mn-catalyzed diazidation and azidooxygenation of alkenes

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Email: yr_chen@shu.edu.cn, yuanzhen.ke@zjnu.edu.cn

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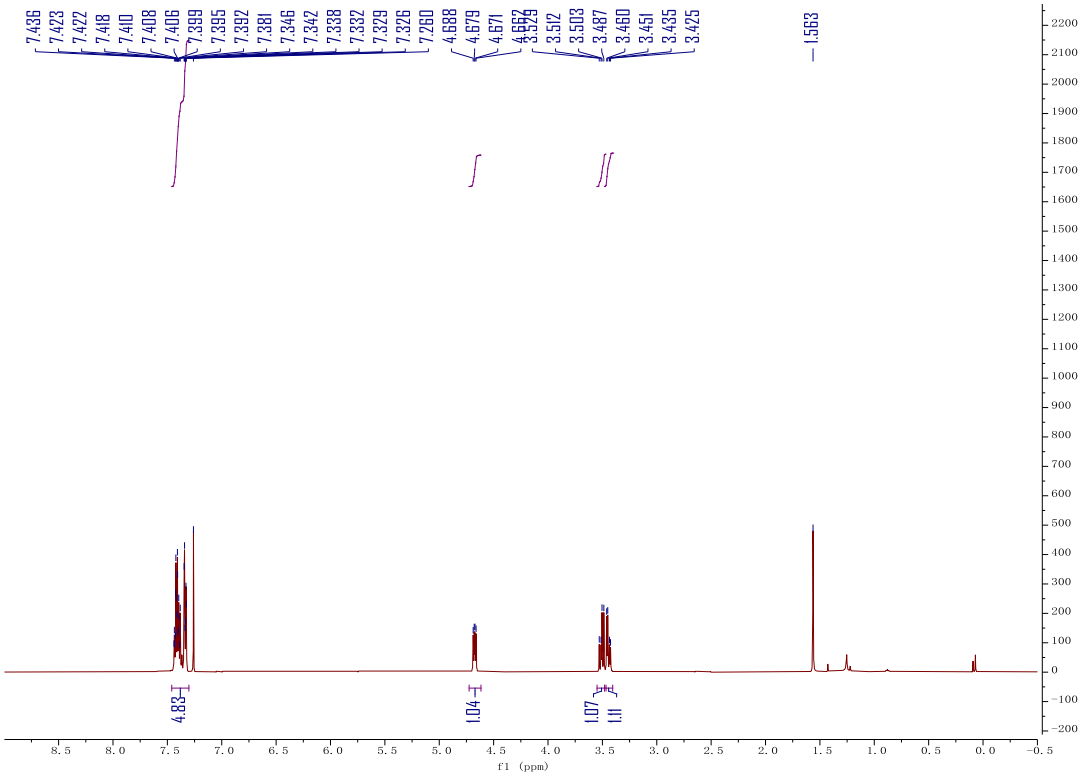
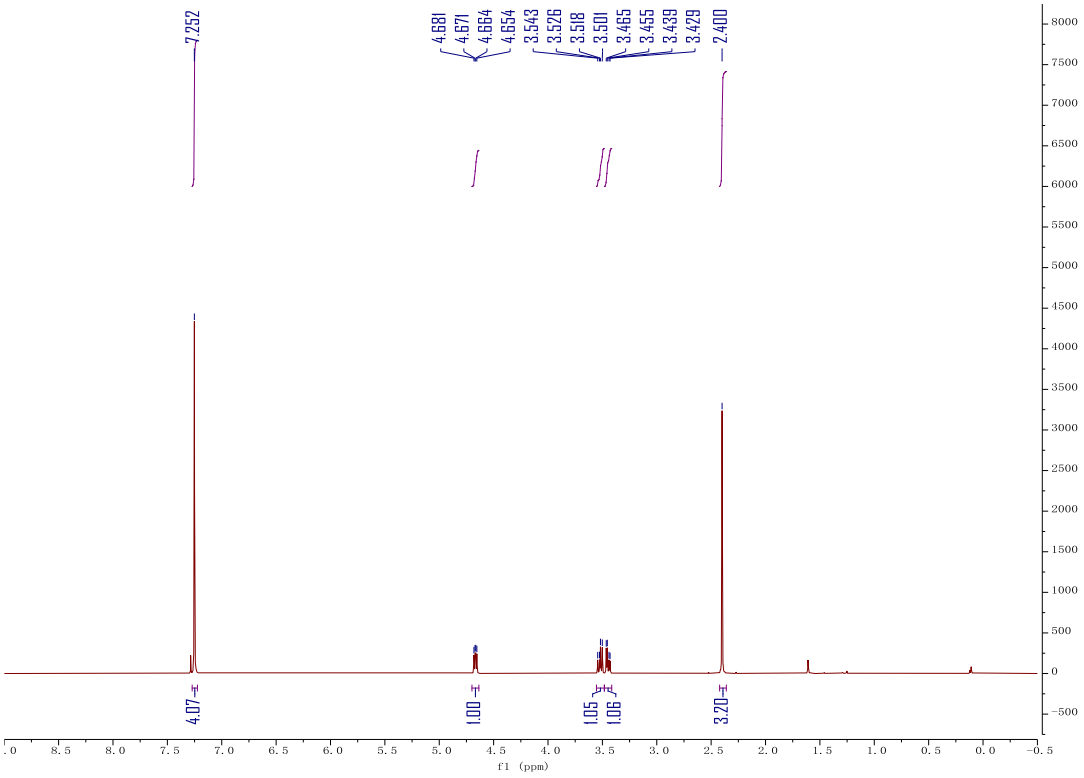
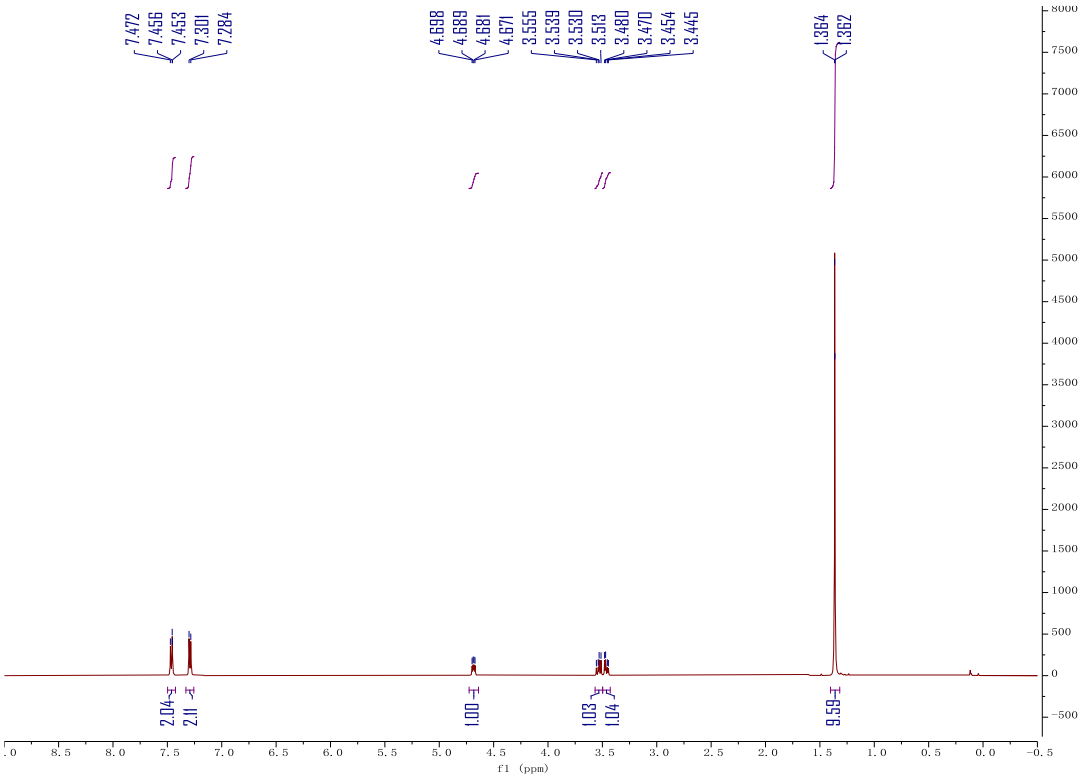
2a, ^{1}H NMR, 500 MHz, $CDCl_3$.



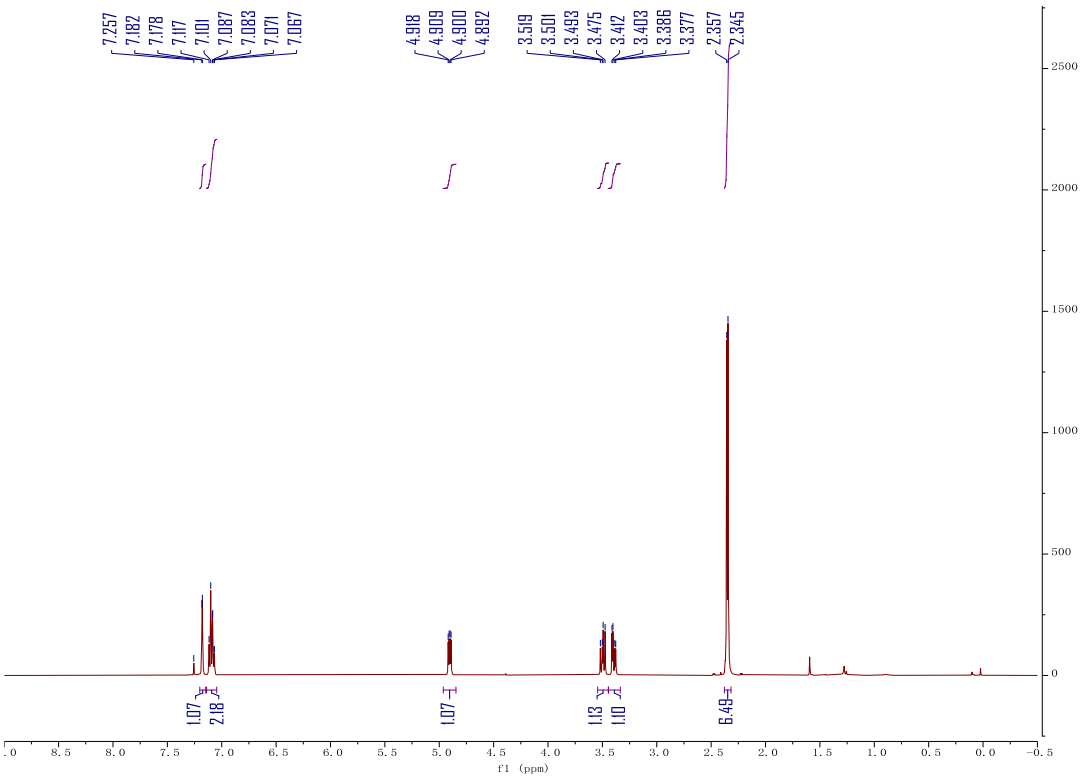
2b, ^{1}H NMR, 500 MHz, $CDCl_3$.



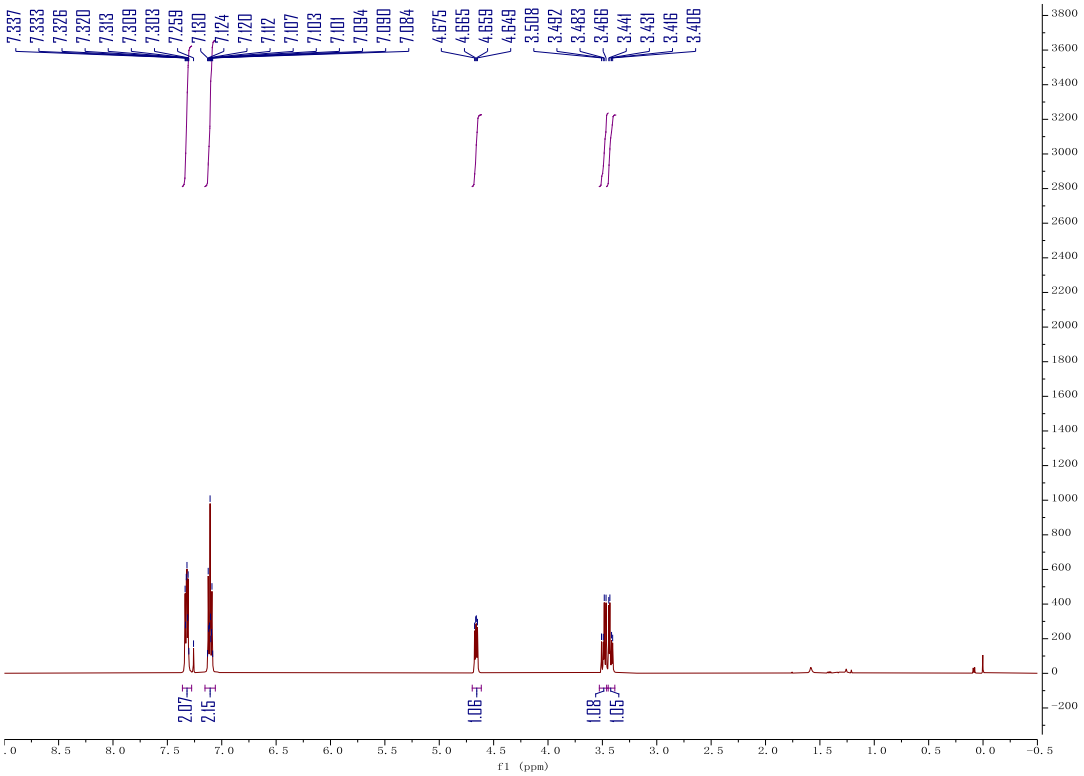
2c, ^{1}H NMR, 500 MHz, $CDCl_3$.



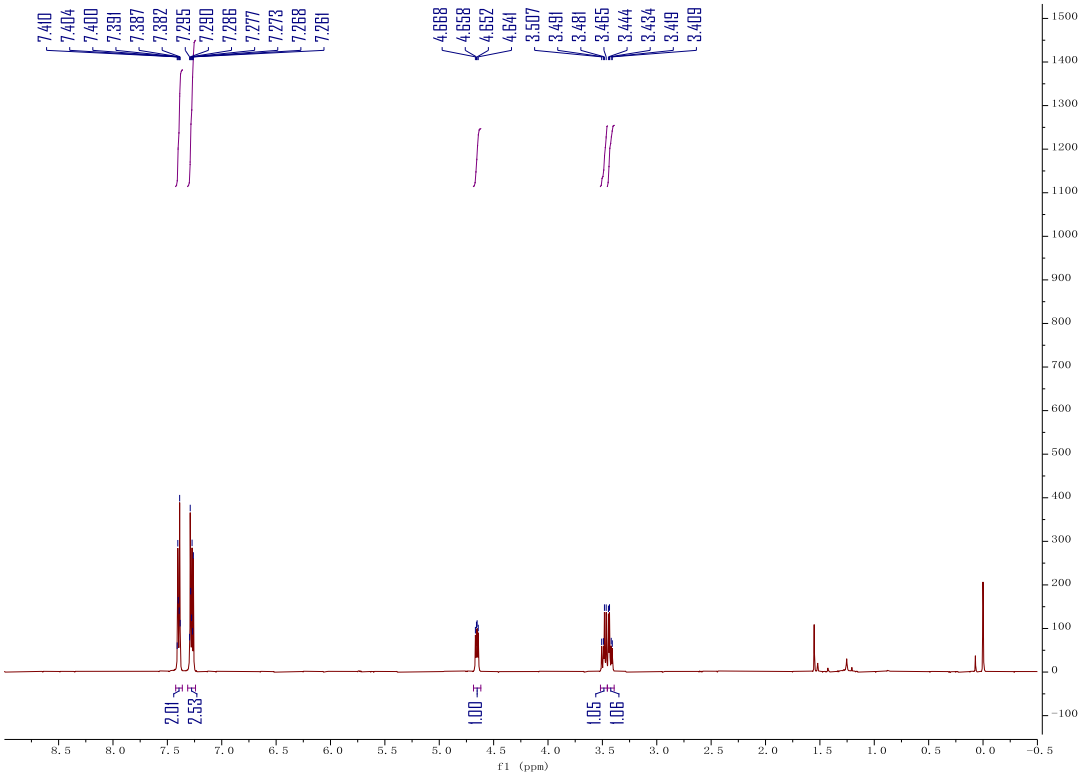
2d, ^{1}H NMR, 500 MHz, $CDCl_3$.



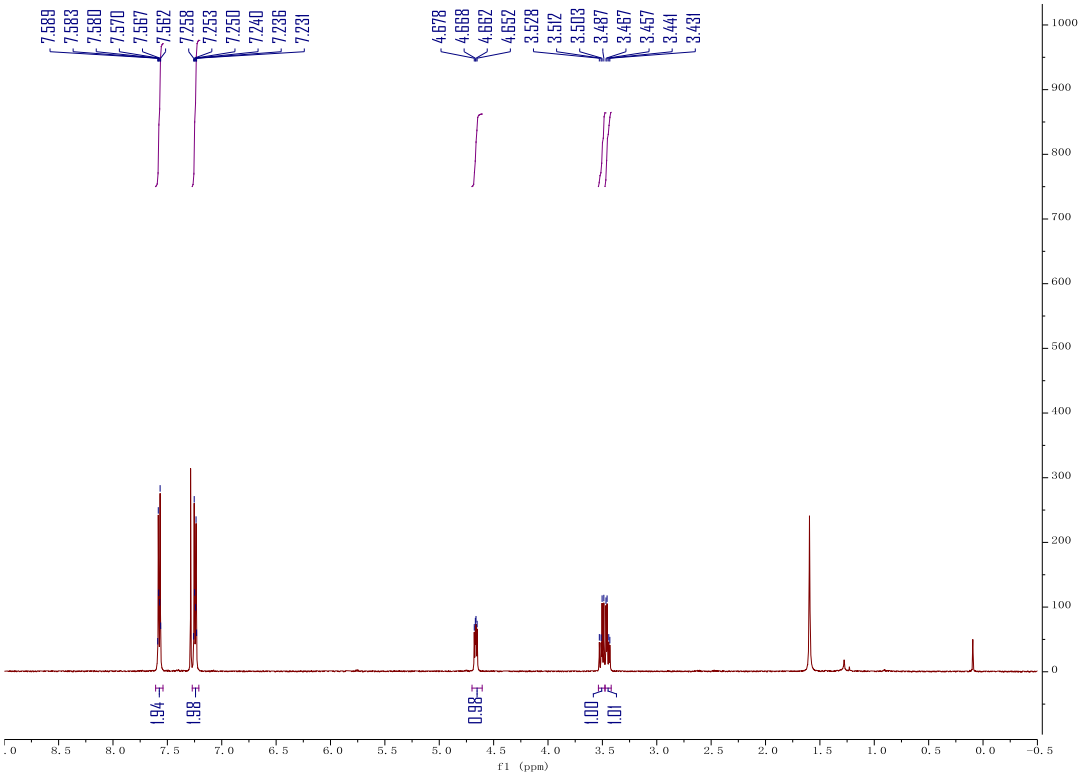
2e, ^{1}H NMR, 500 MHz, $CDCl_3$.



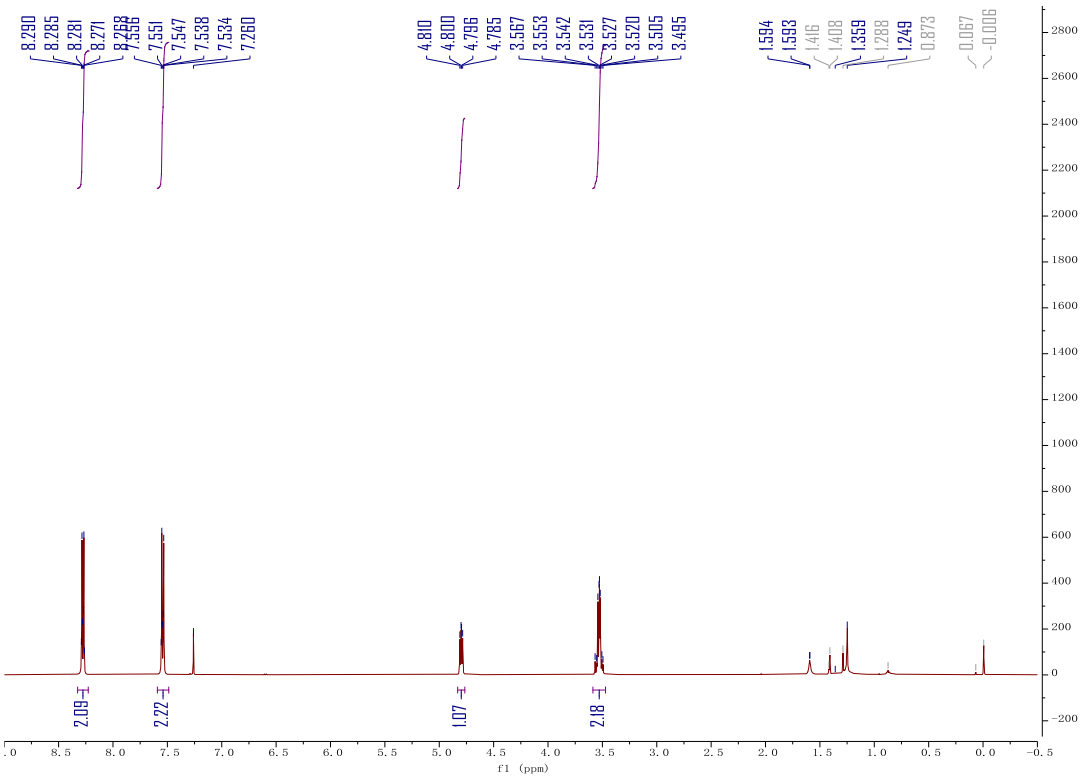
2f, ^{1}H NMR, 500 MHz, $CDCl_3$.



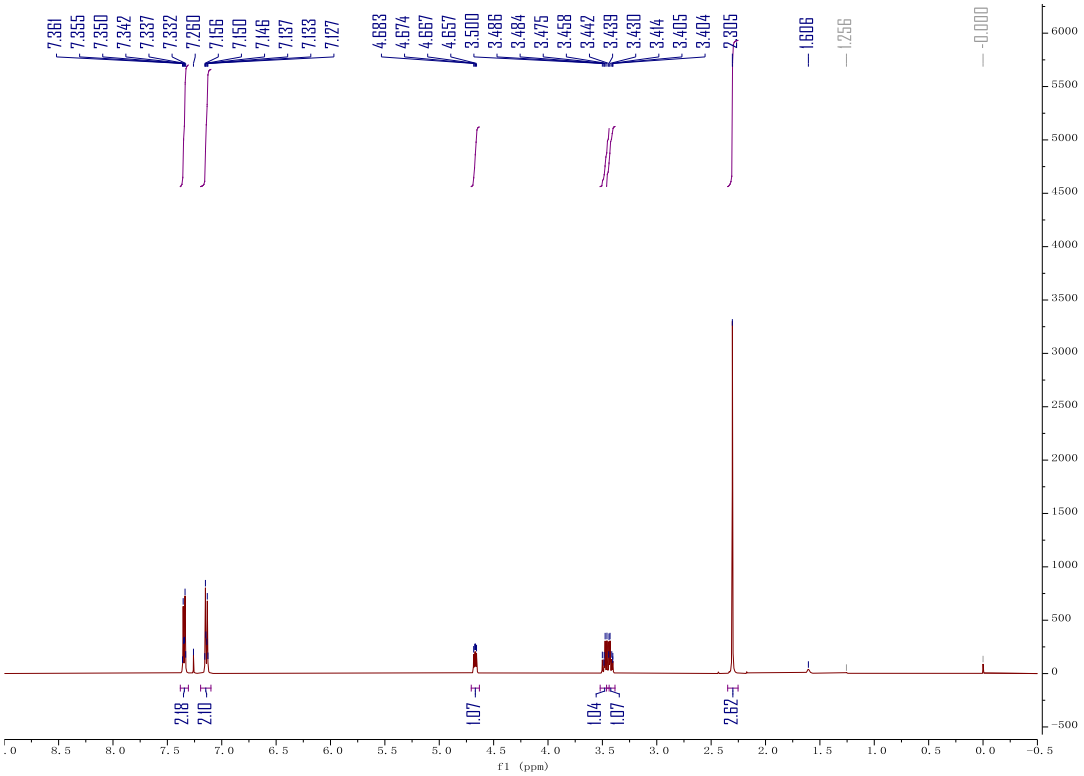
2g, ^{1}H NMR, 500 MHz, $CDCl_3$.



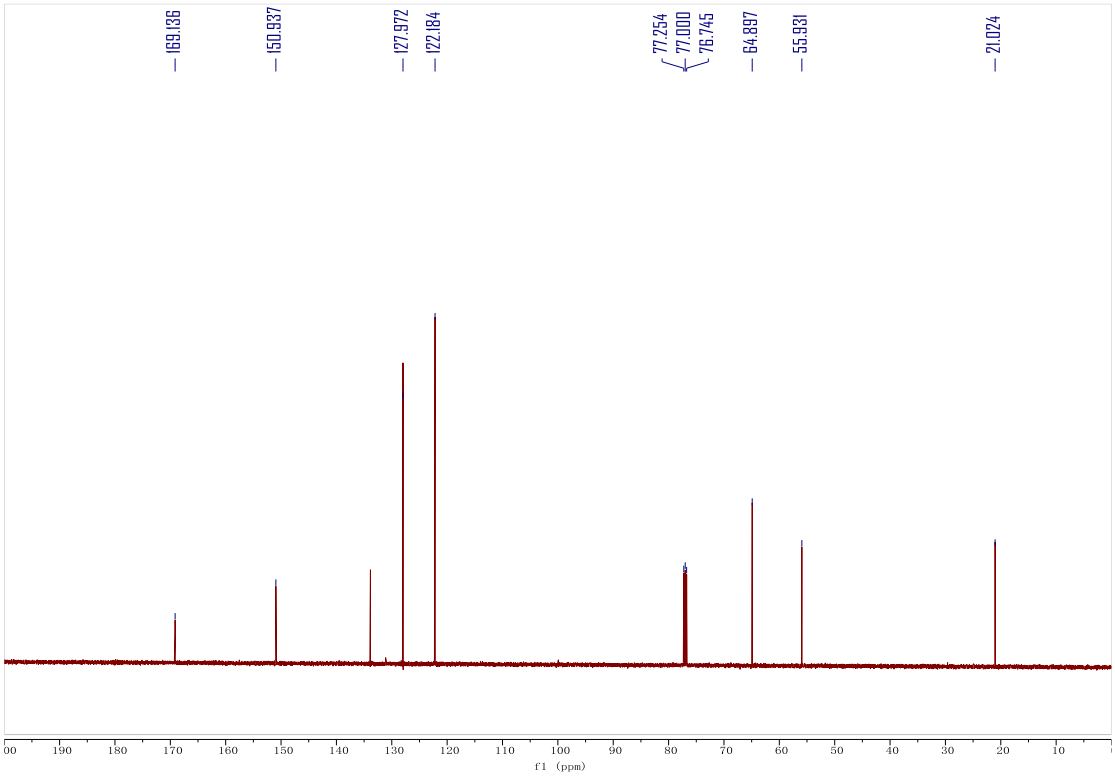
2h, ^{1}H NMR, 500 MHz, $CDCl_3$.



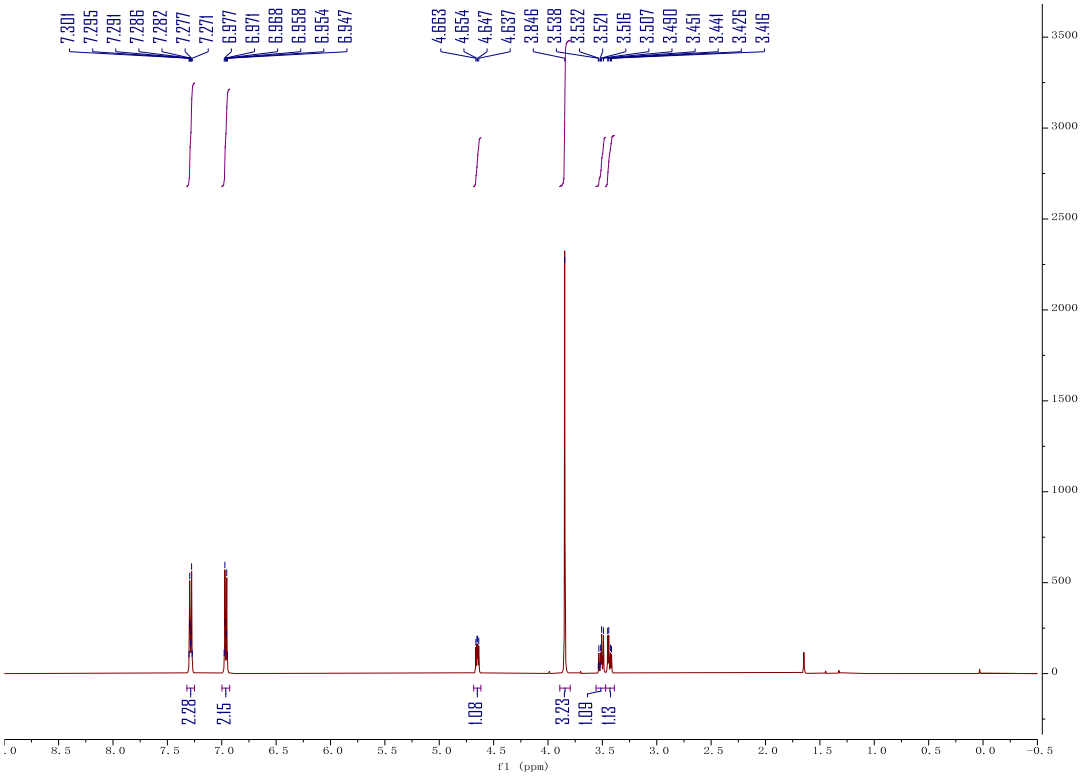
2i, ^{1}H NMR, 500 MHz, $CDCl_3$.



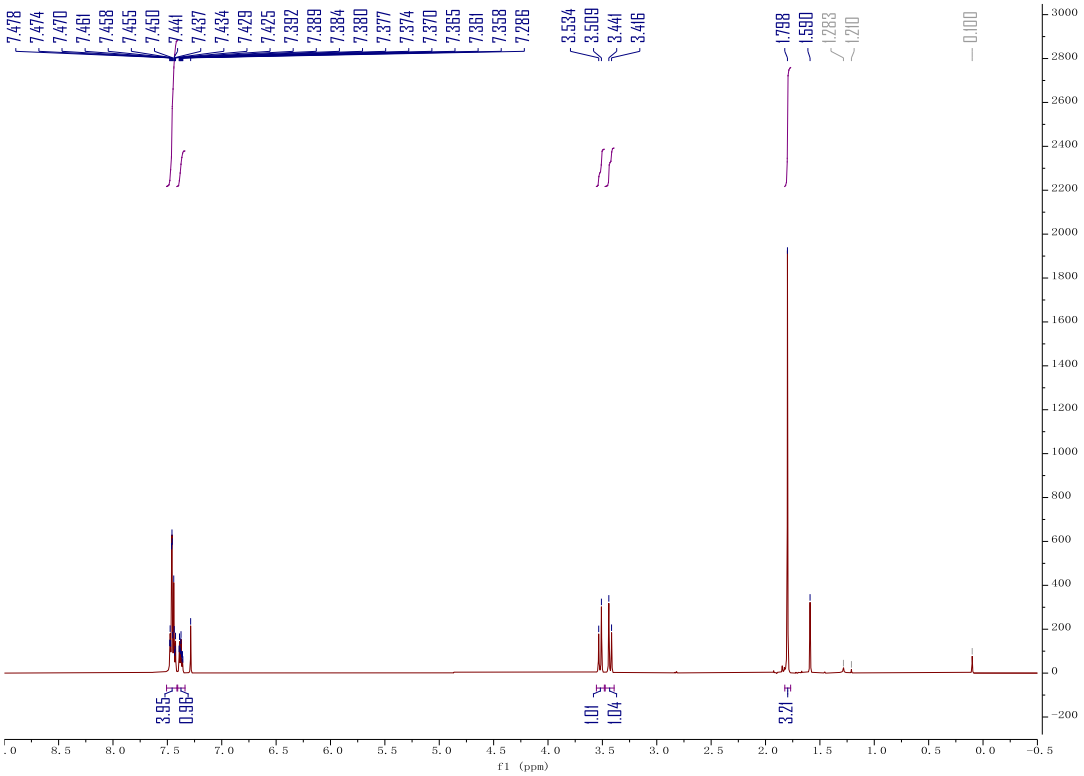
2i, ^{13}C NMR, 126 MHz, $CDCl_3$.



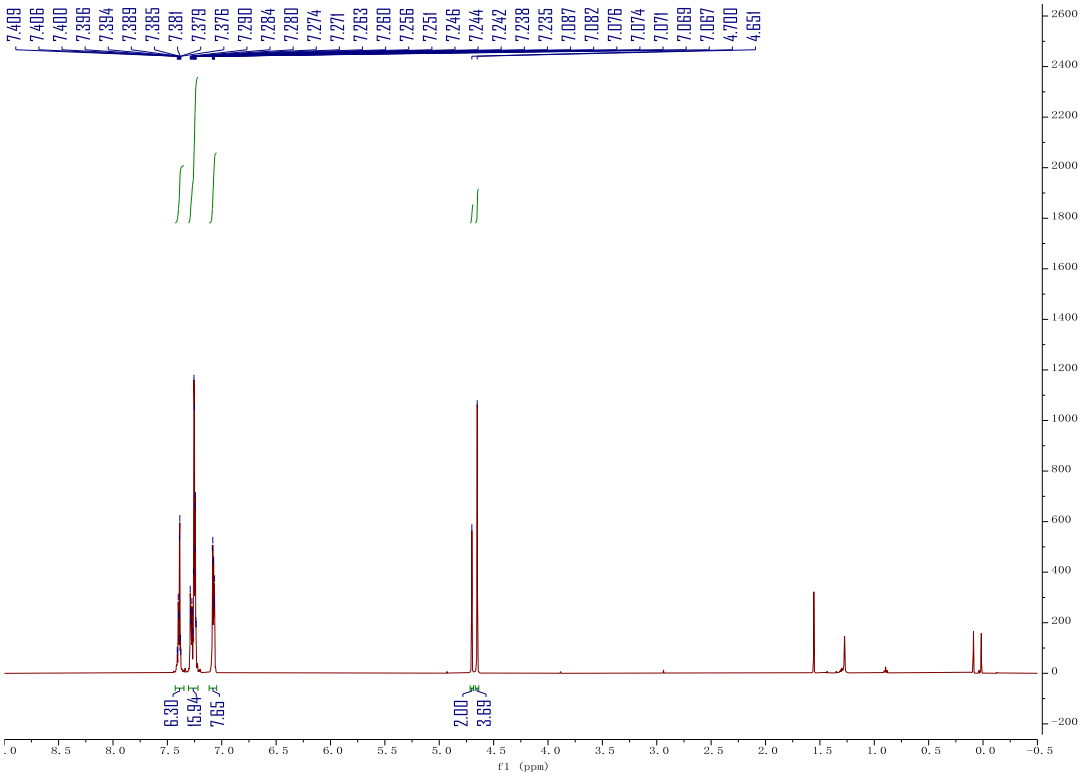
2j, ^{1}H NMR, 500 MHz, $CDCl_3$.



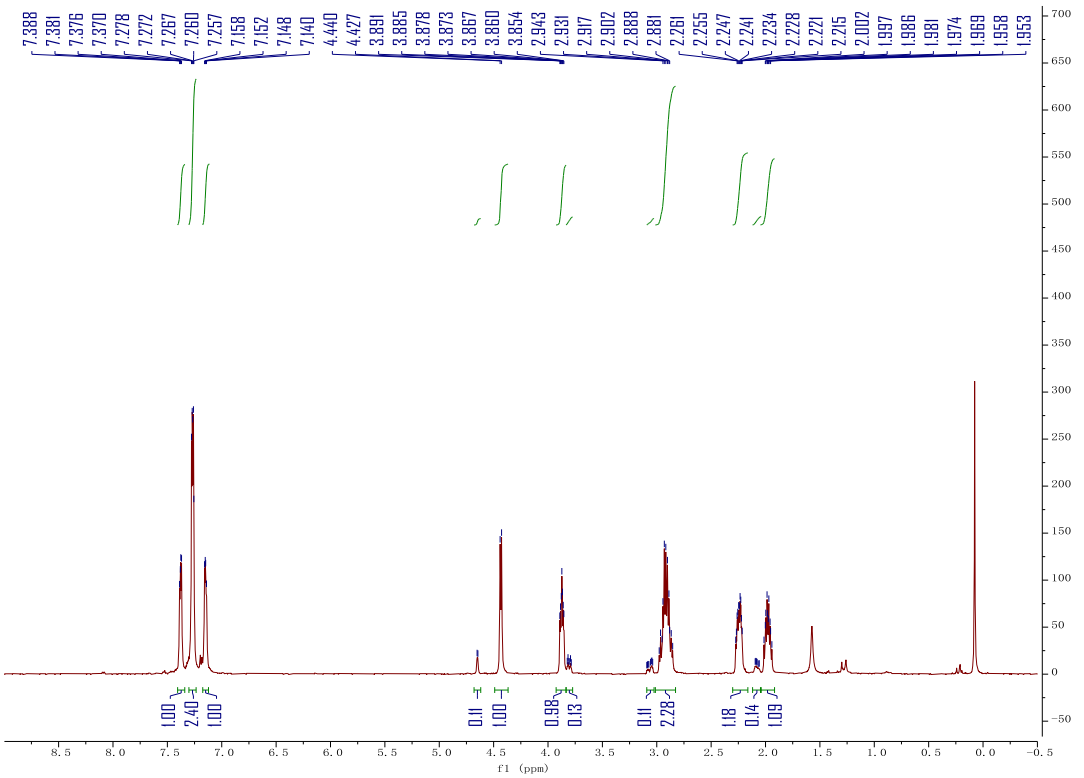
2k, ^{1}H NMR, 500 MHz, $CDCl_3$.



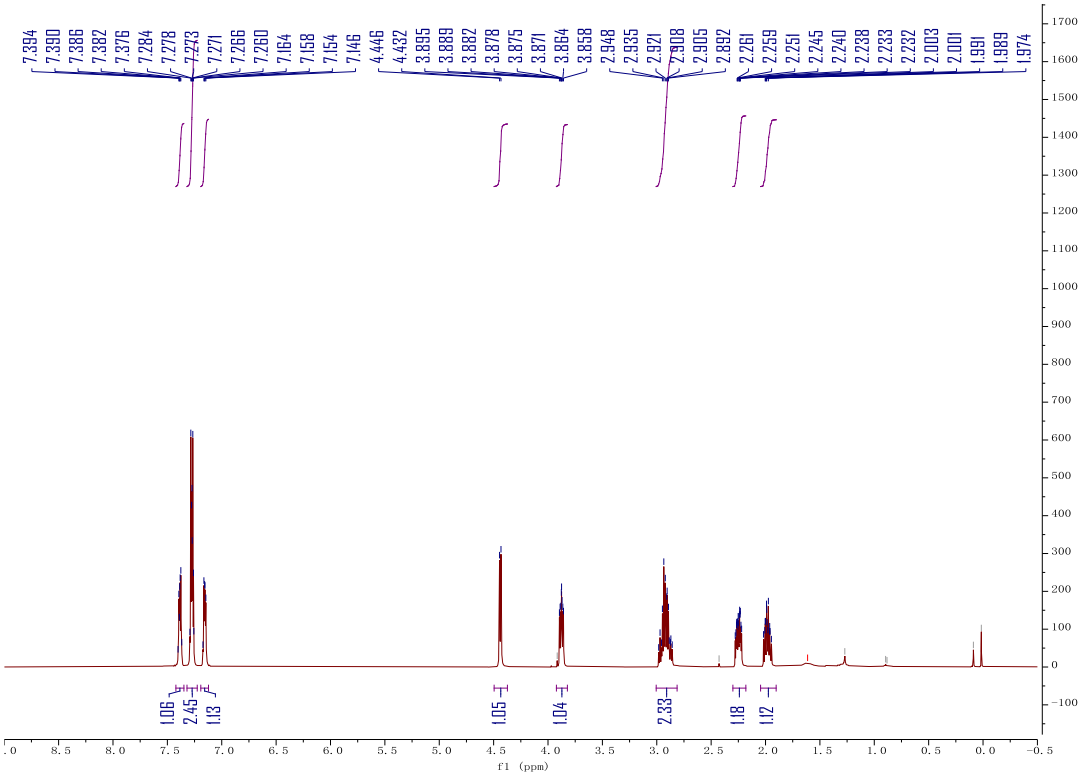
2l, ^{1}H NMR, 500 MHz, $CDCl_3$.



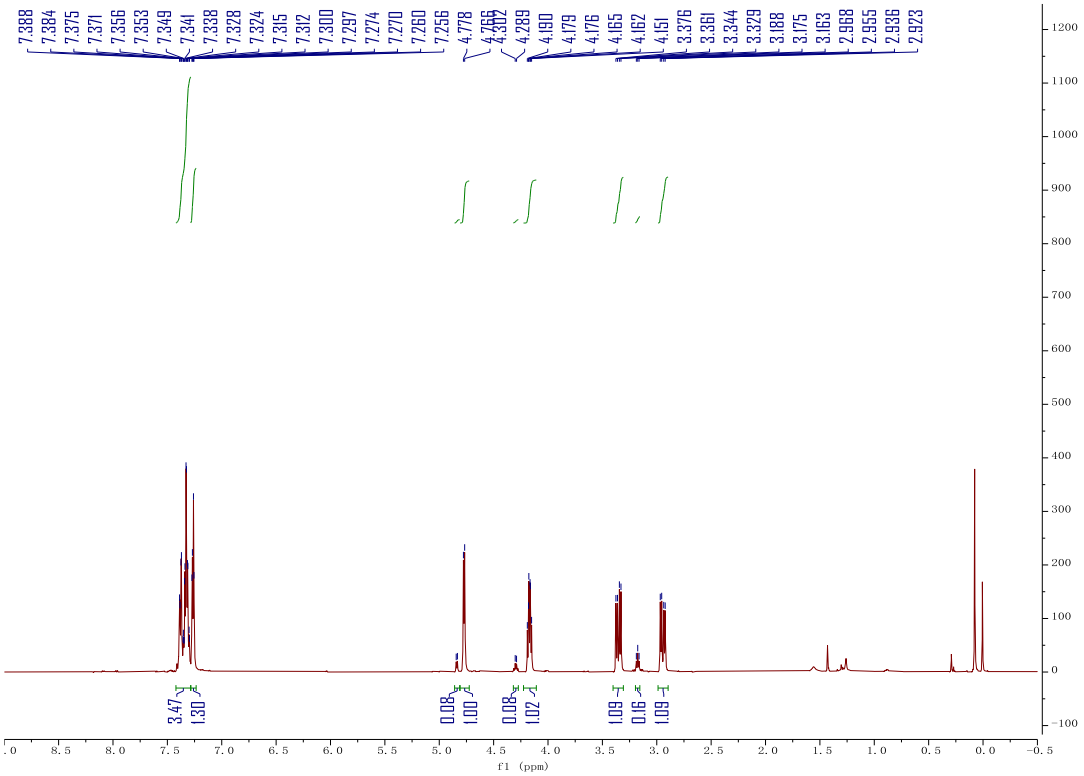
2m, ^{1}H NMR, 500 MHz, $CDCl_3$. Mixture.



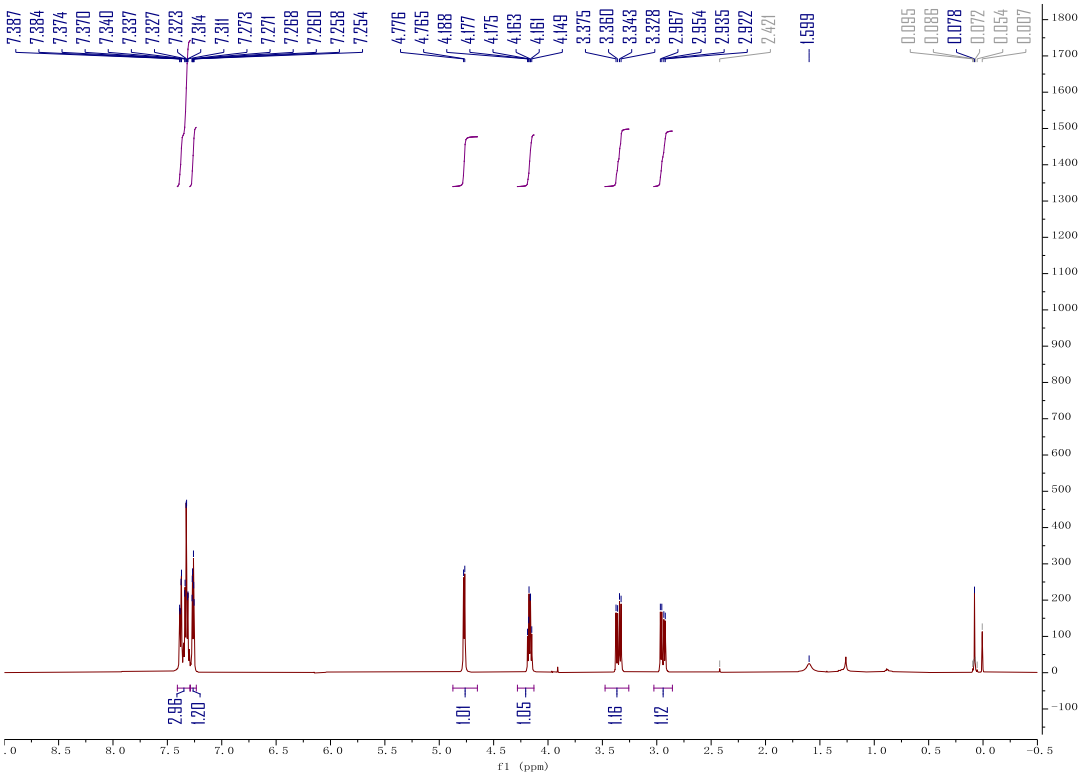
2m, ^{1}H NMR, 500 MHz, $CDCl_3$. *anti*-Isomer.



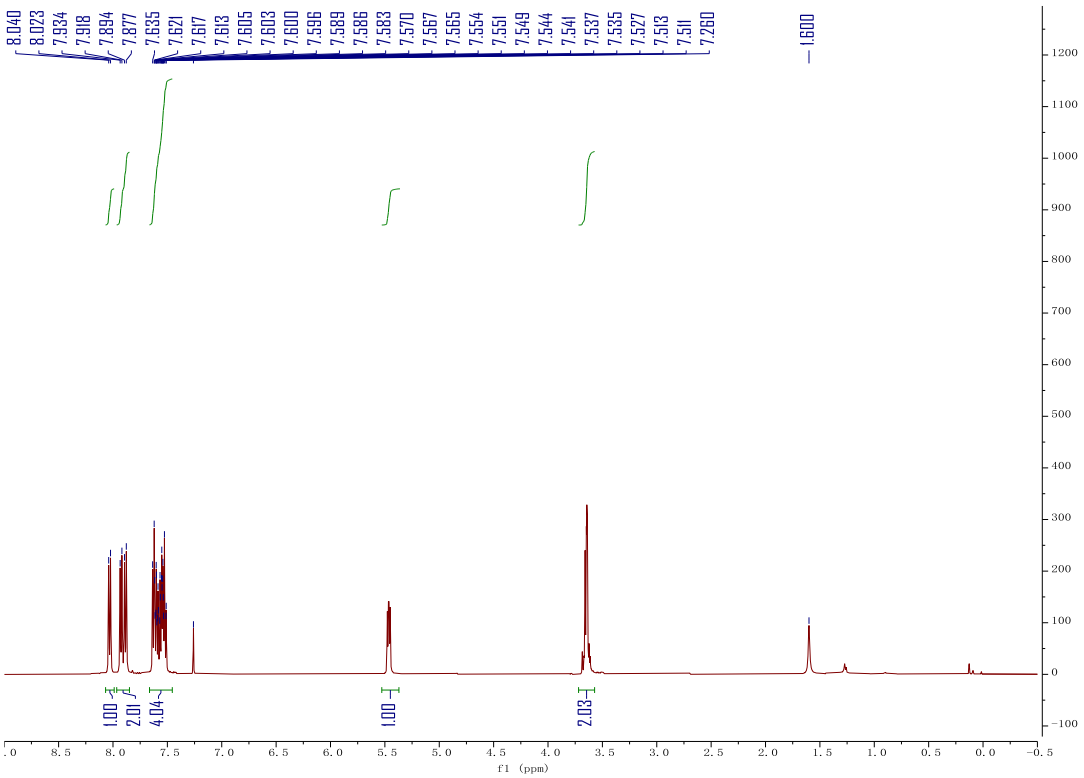
2n, ^{1}H NMR, 500 MHz, $CDCl_3$. Mixture.



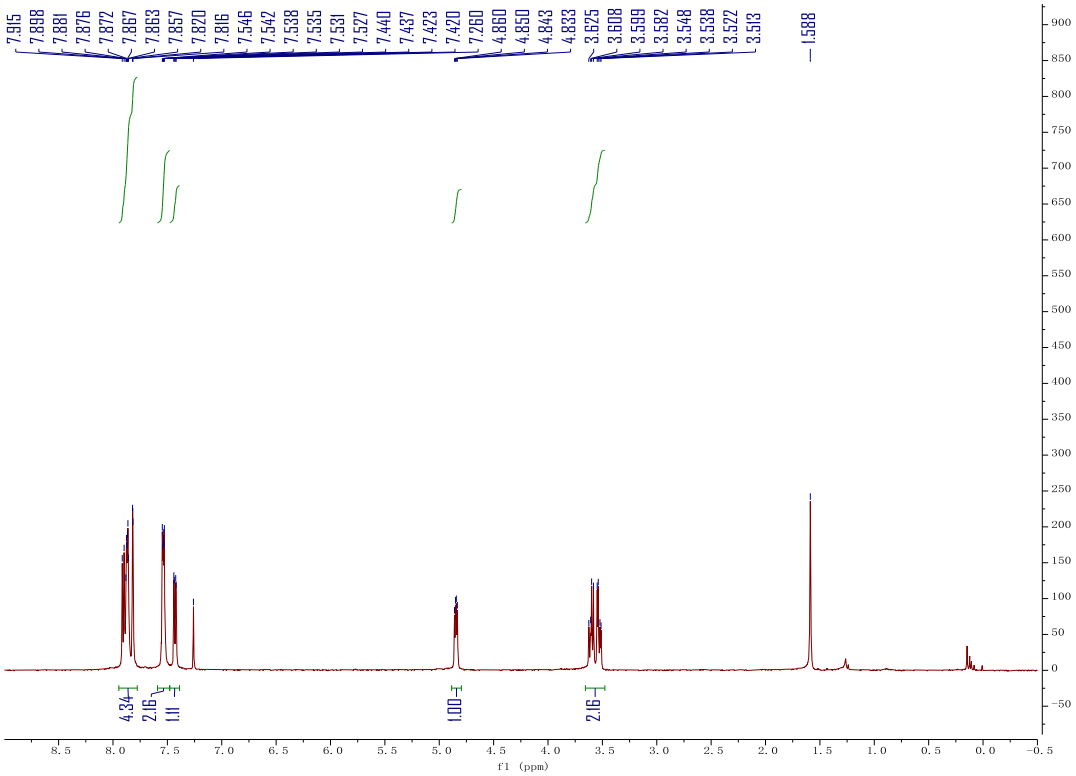
2n, ^{1}H NMR, 500 MHz, $CDCl_3$. *anti*-Isomer.



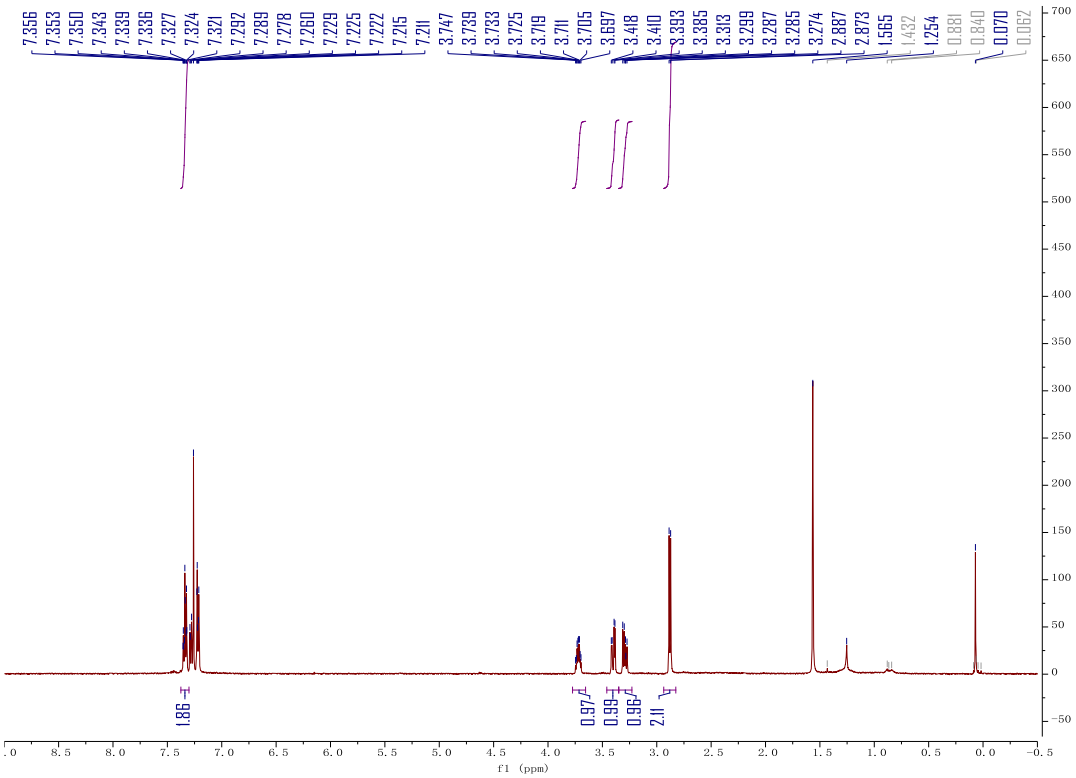
2o, ^{1}H NMR, 500 MHz, $CDCl_3$.



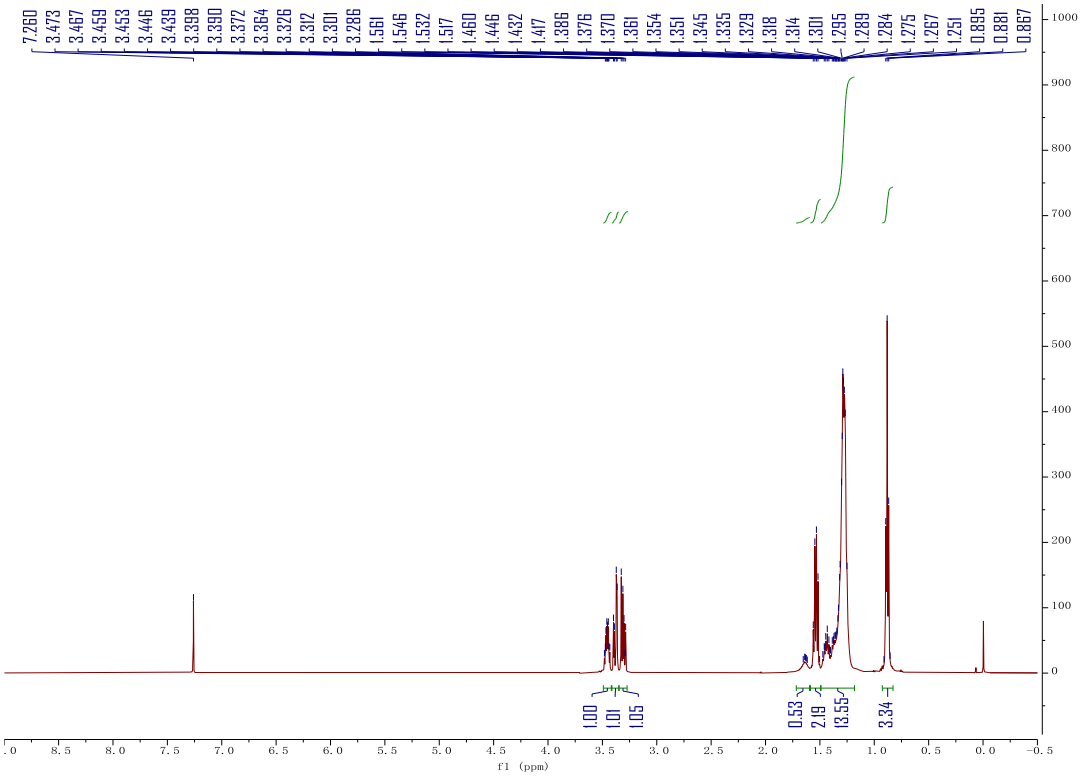
2p, ^{1}H NMR, 500 MHz, $CDCl_3$.



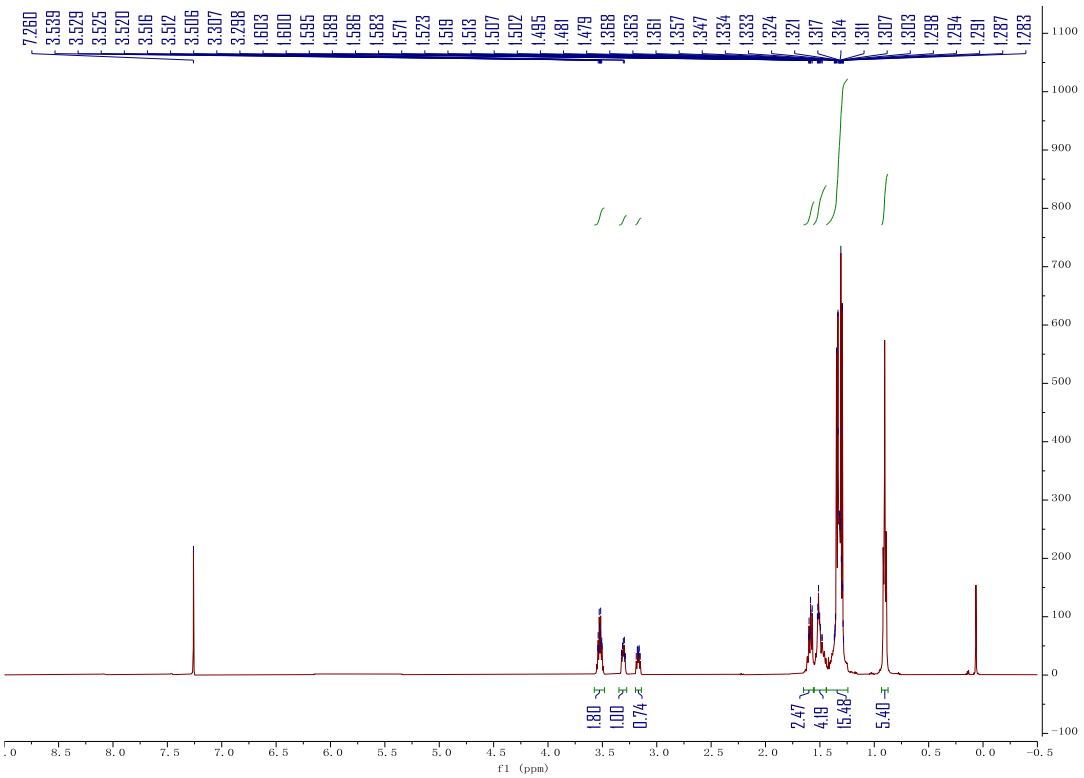
2q, ^{1}H NMR, 500 MHz, $CDCl_3$.



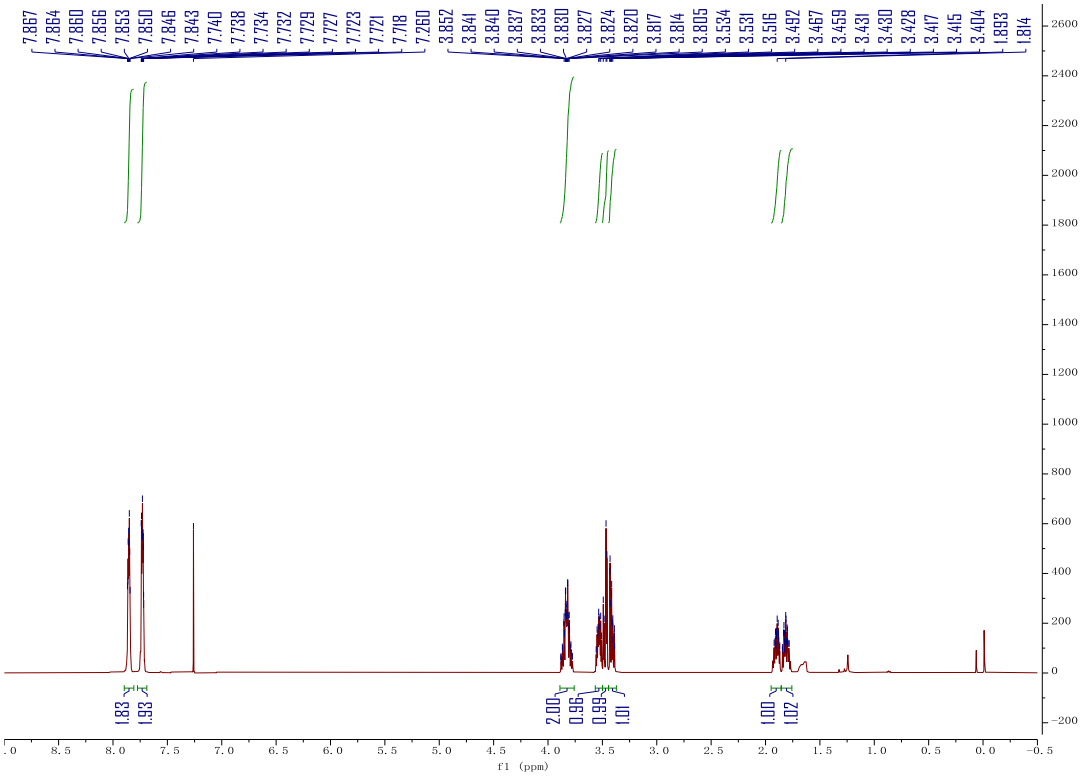
2r, ^{1}H NMR, 500 MHz, $CDCl_3$.



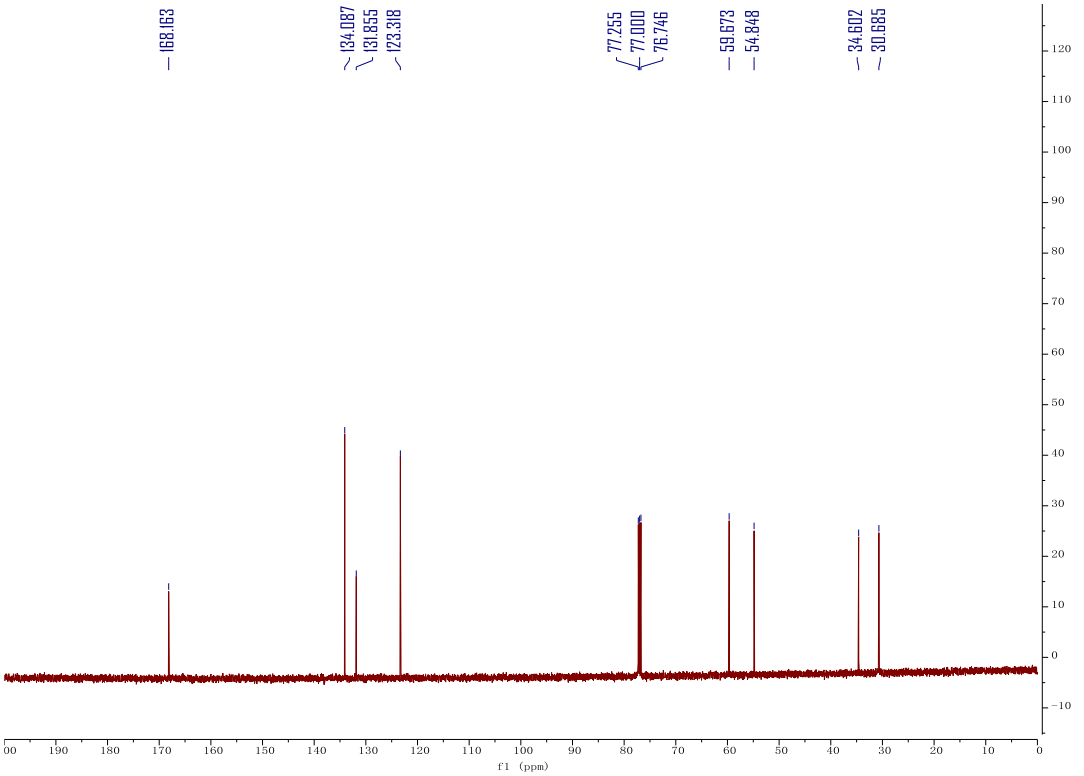
2s, ^{1}H NMR, 500 MHz, $CDCl_3$.



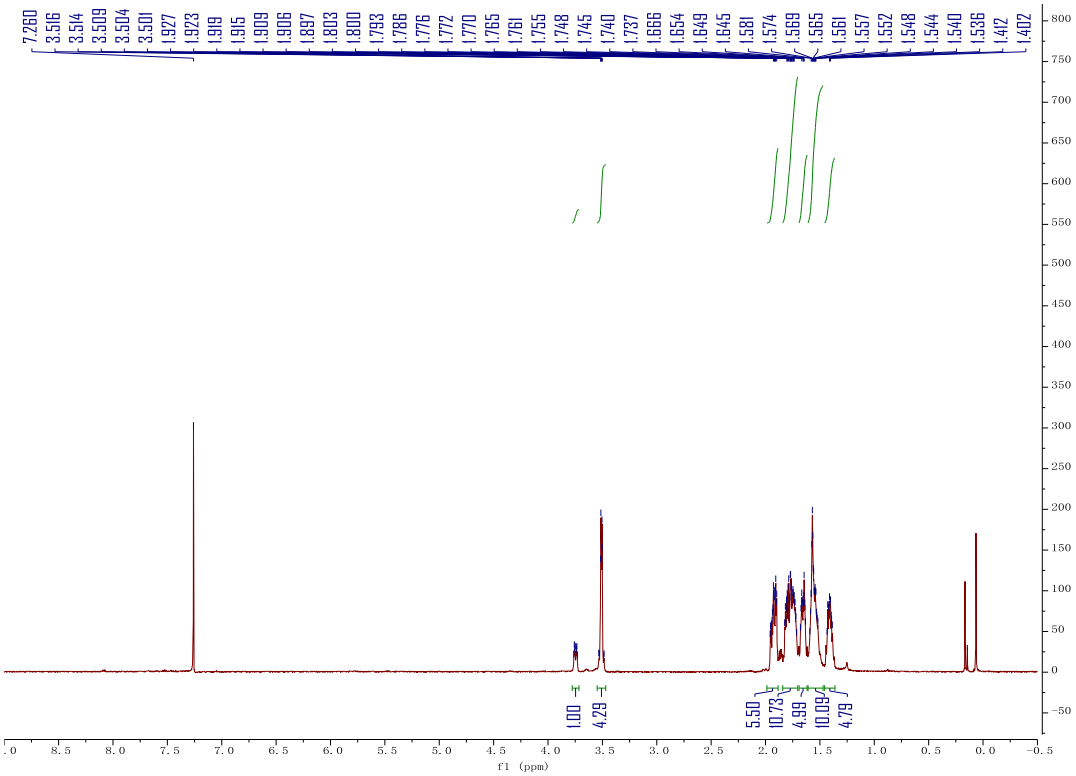
2t, ^{1}H NMR, 500 MHz, $CDCl_3$.



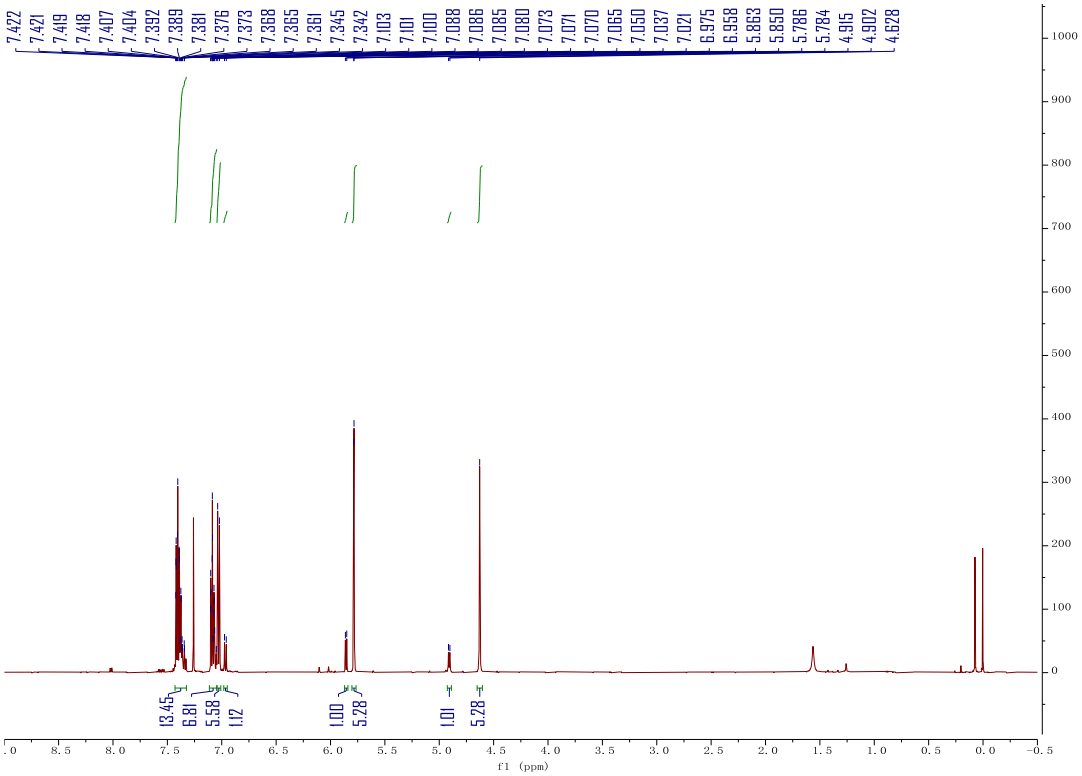
2t, ^{13}C NMR, 126 MHz, $CDCl_3$.



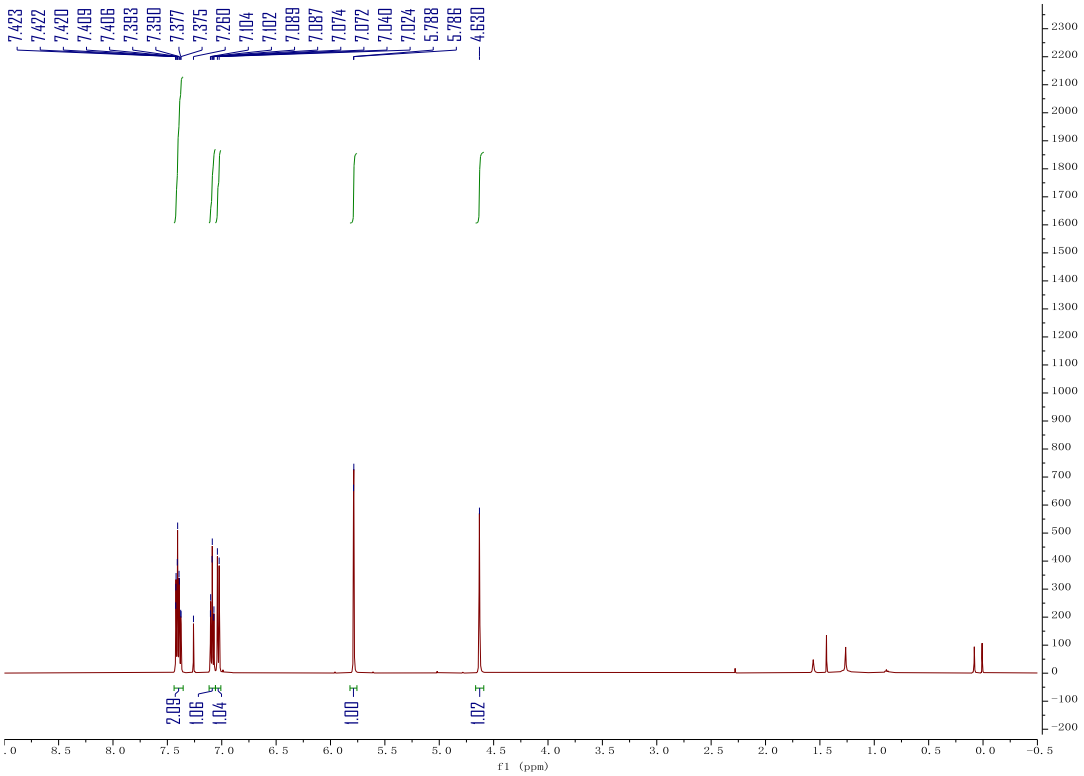
2u, ^{1}H NMR, 500 MHz, $CDCl_3$.



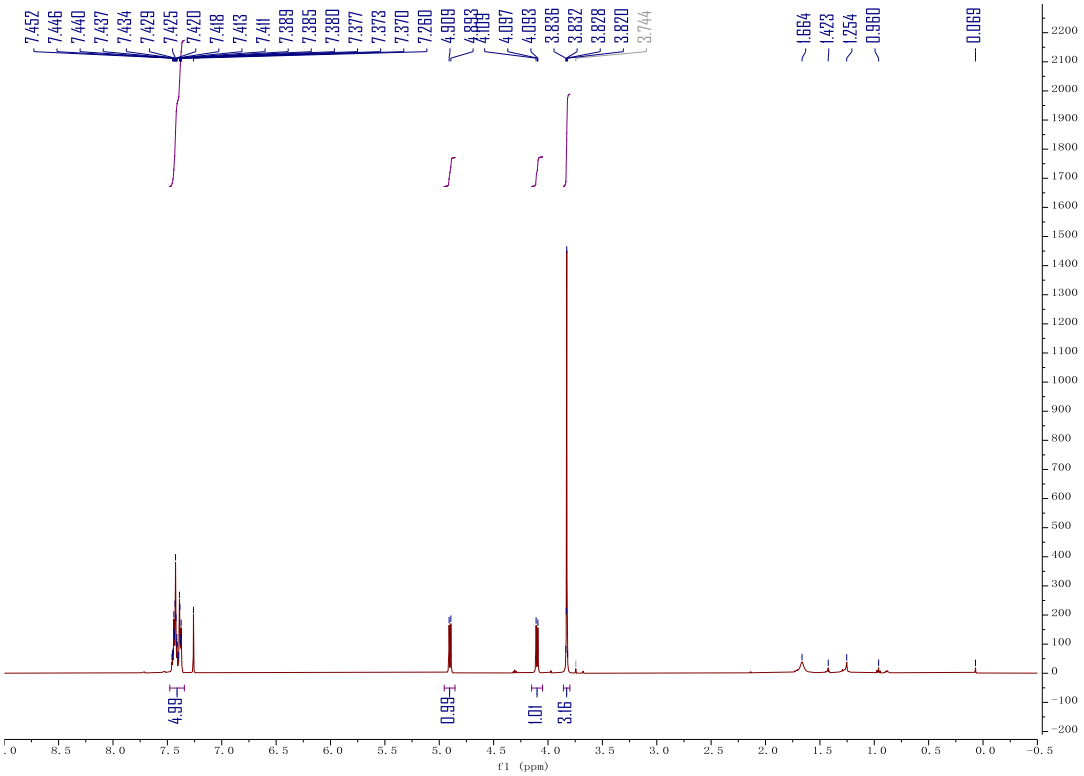
2v, ^{1}H NMR, 500 MHz, $CDCl_3$. Mixture.



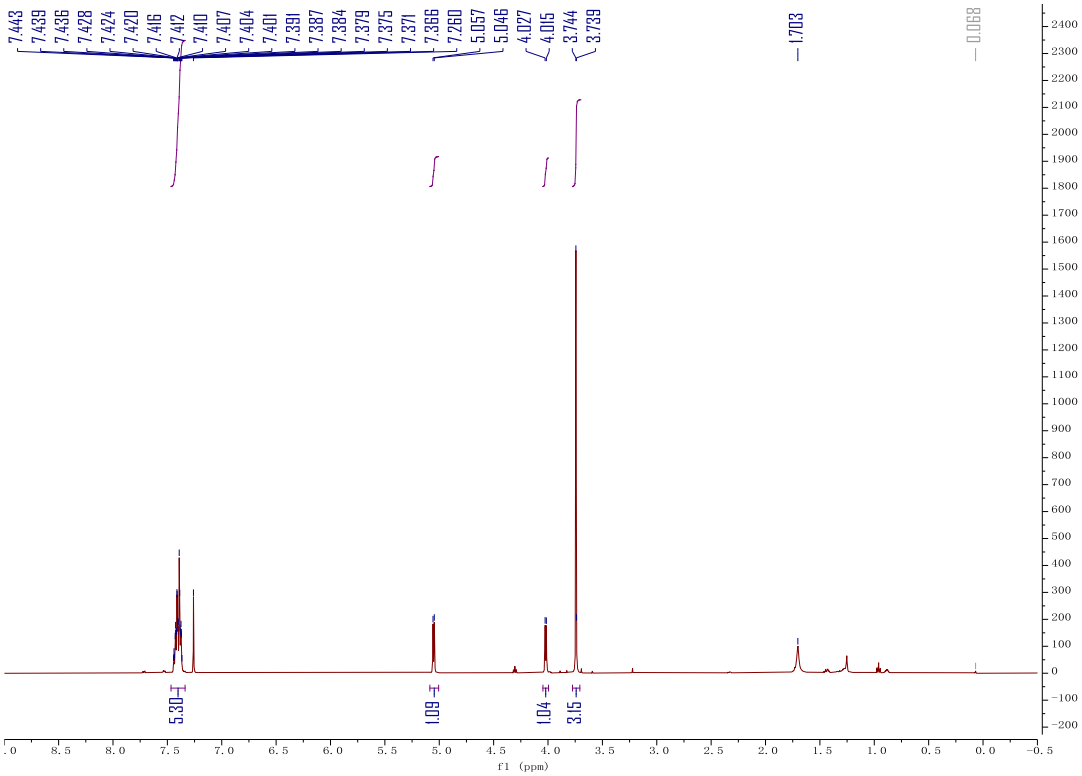
2v, ^{1}H NMR, 500 MHz, $CDCl_3$. *trans*-Isomer.



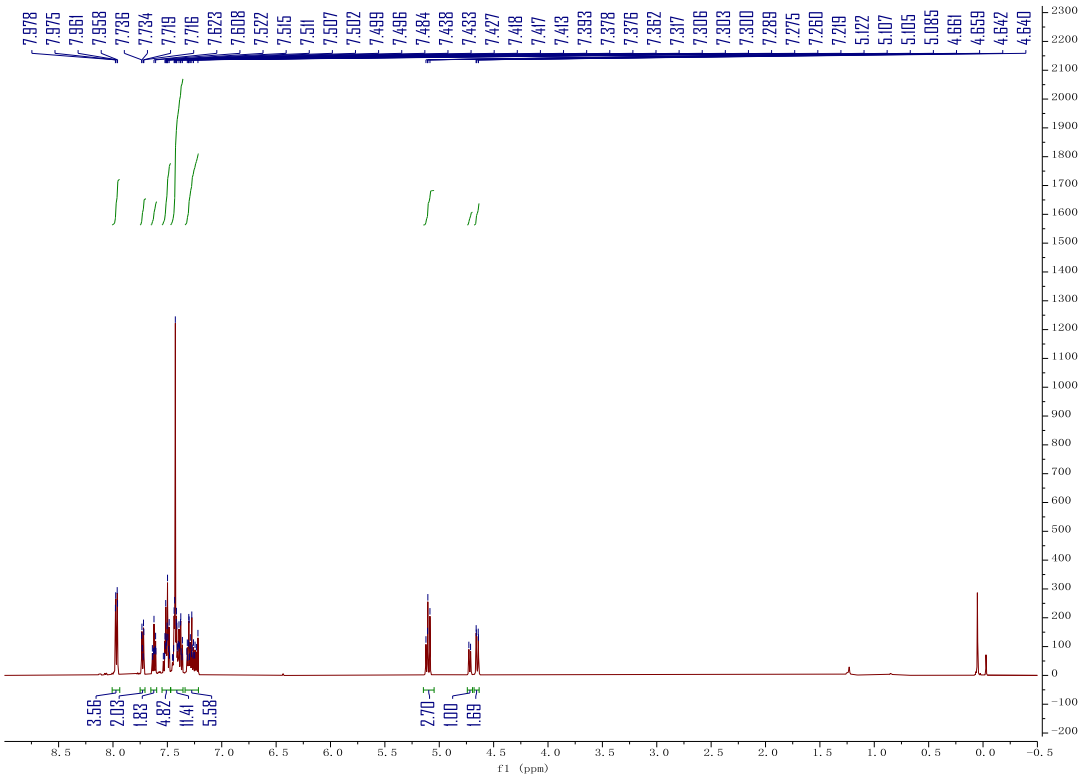
2w, ^{1}H NMR, 500 MHz, $CDCl_3$. *anti*-Isomer.



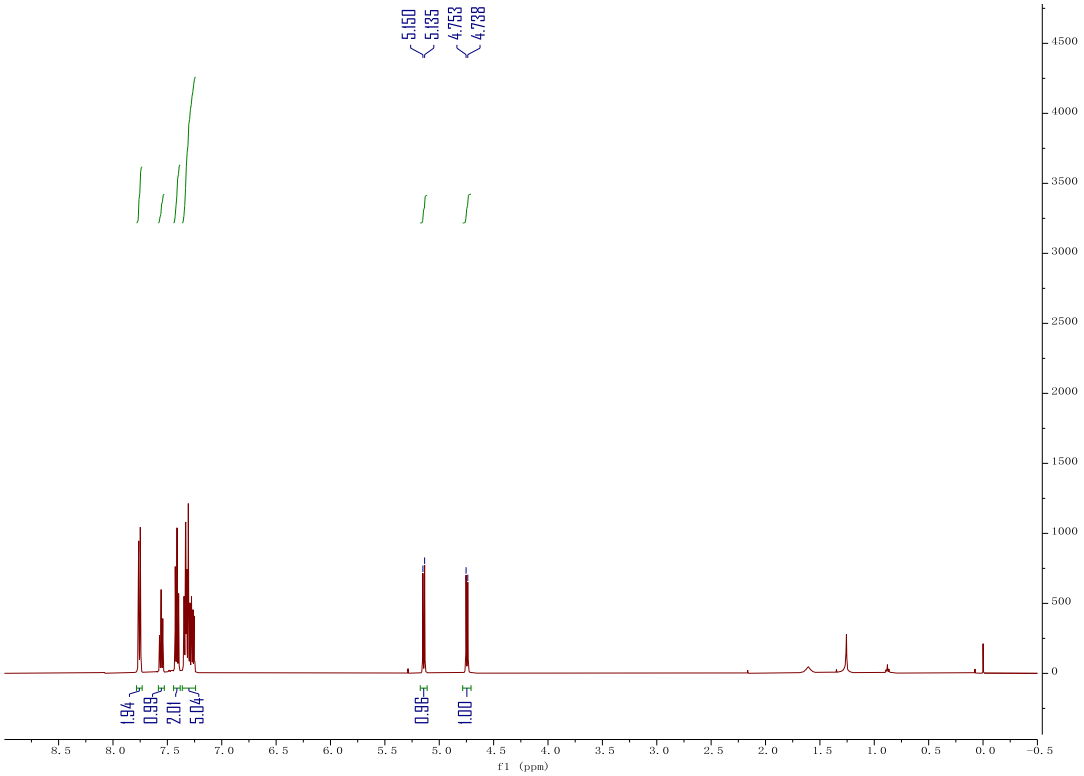
2w, ^{1}H NMR, 500 MHz, $CDCl_3$. *syn*-Isomer.



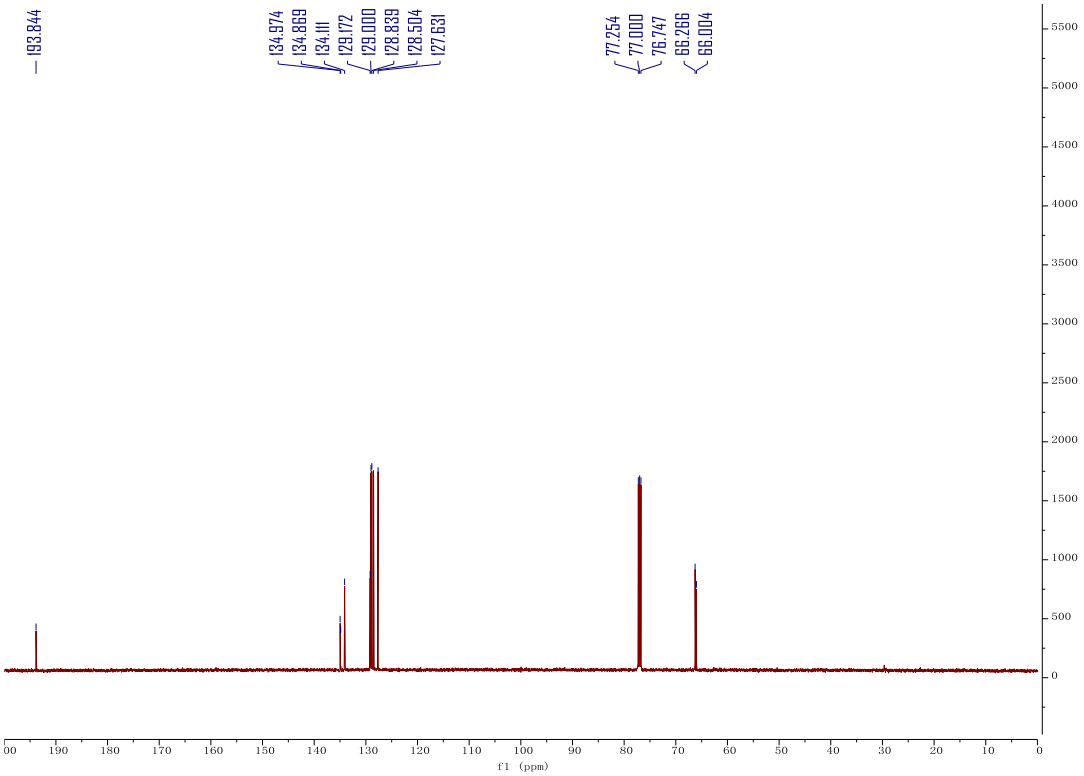
2x, ^{1}H NMR, 500 MHz, $CDCl_3$. Mixture.



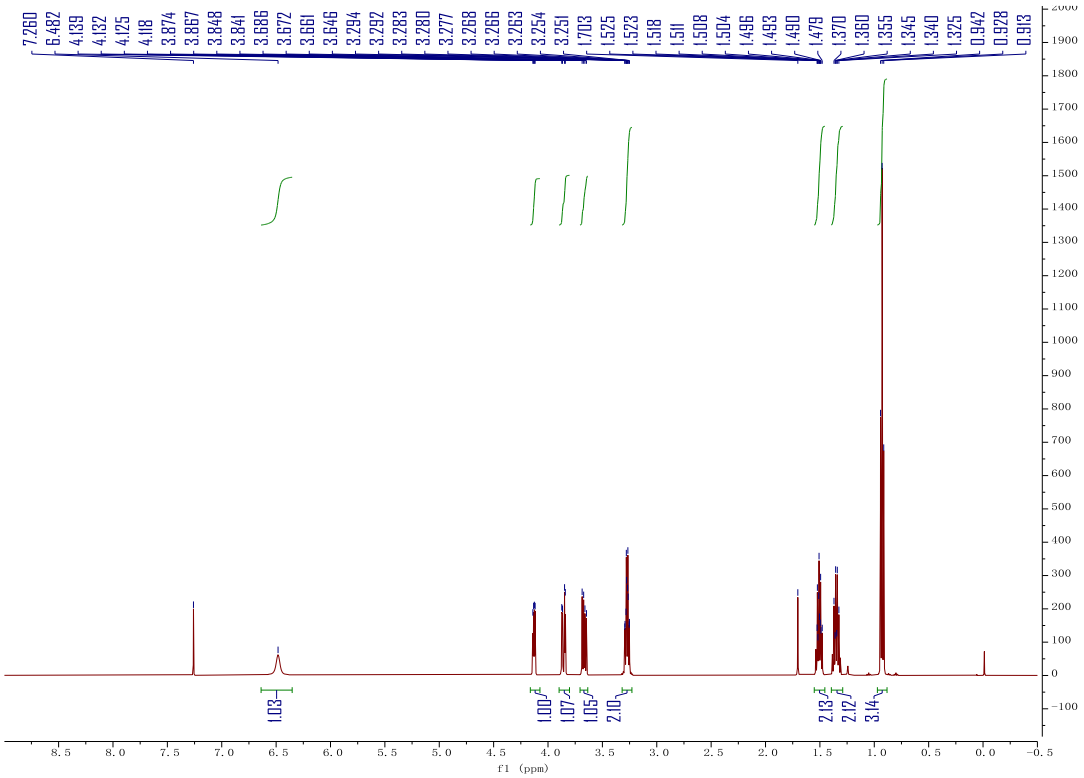
2x, ^{1}H NMR, 500 MHz, $CDCl_3$. *syn*-Isomer.



2x, ^{13}C NMR, 126 MHz, $CDCl_3$. *syn*-Isomer.



2y, ^{1}H NMR, 500 MHz, $CDCl_3$.



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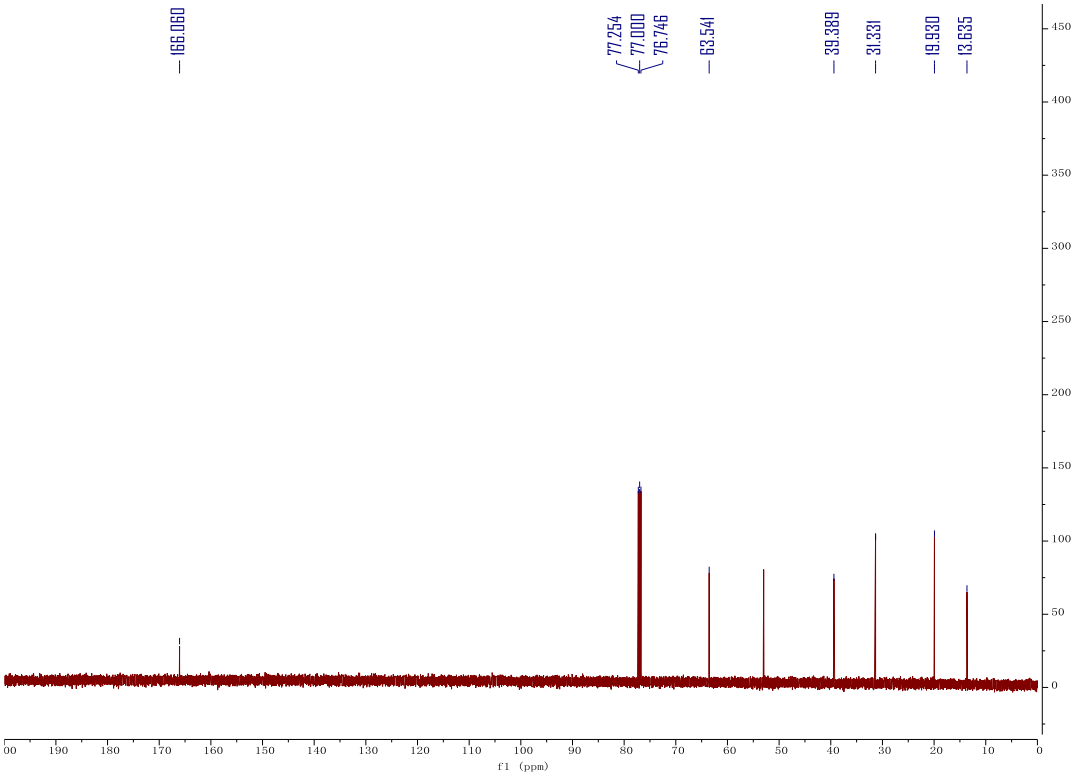
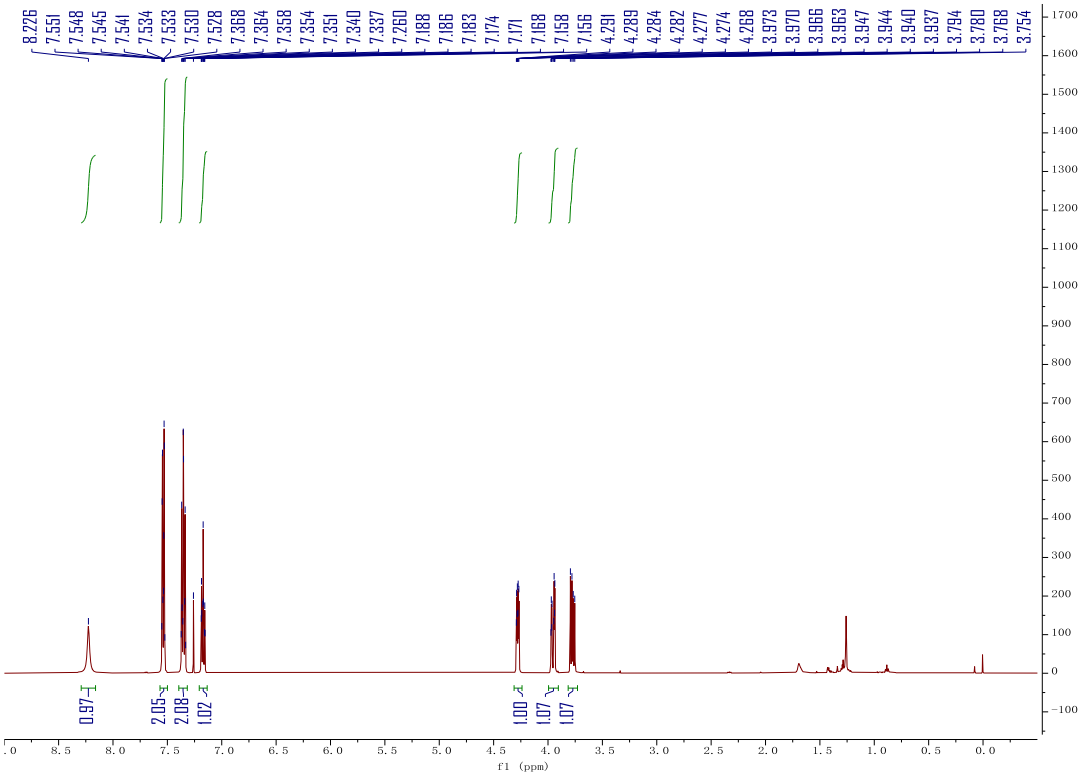
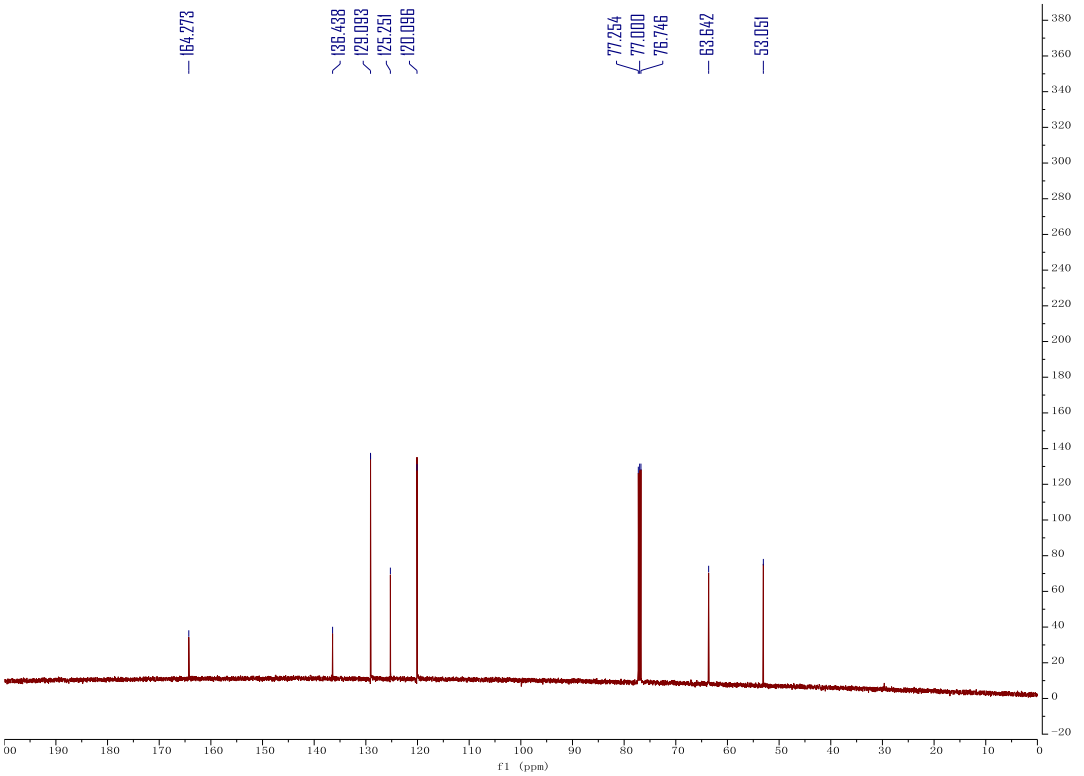


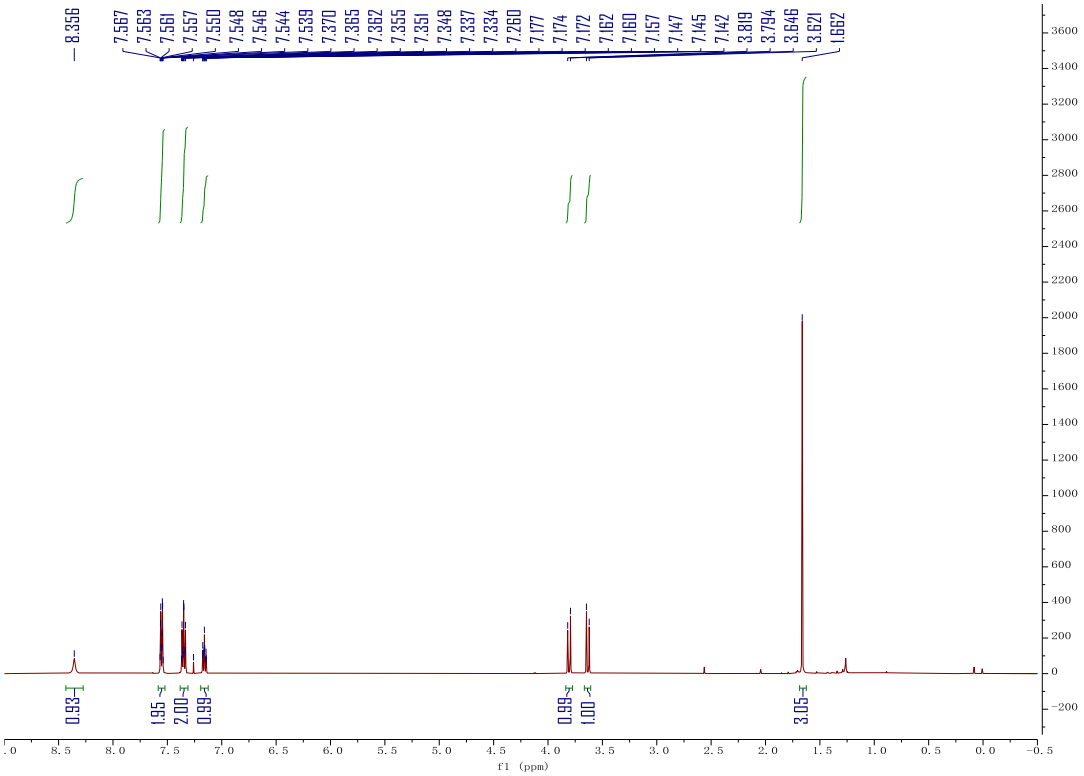
2z, ^{1}H NMR, 500 MHz, $CDCl_3$.



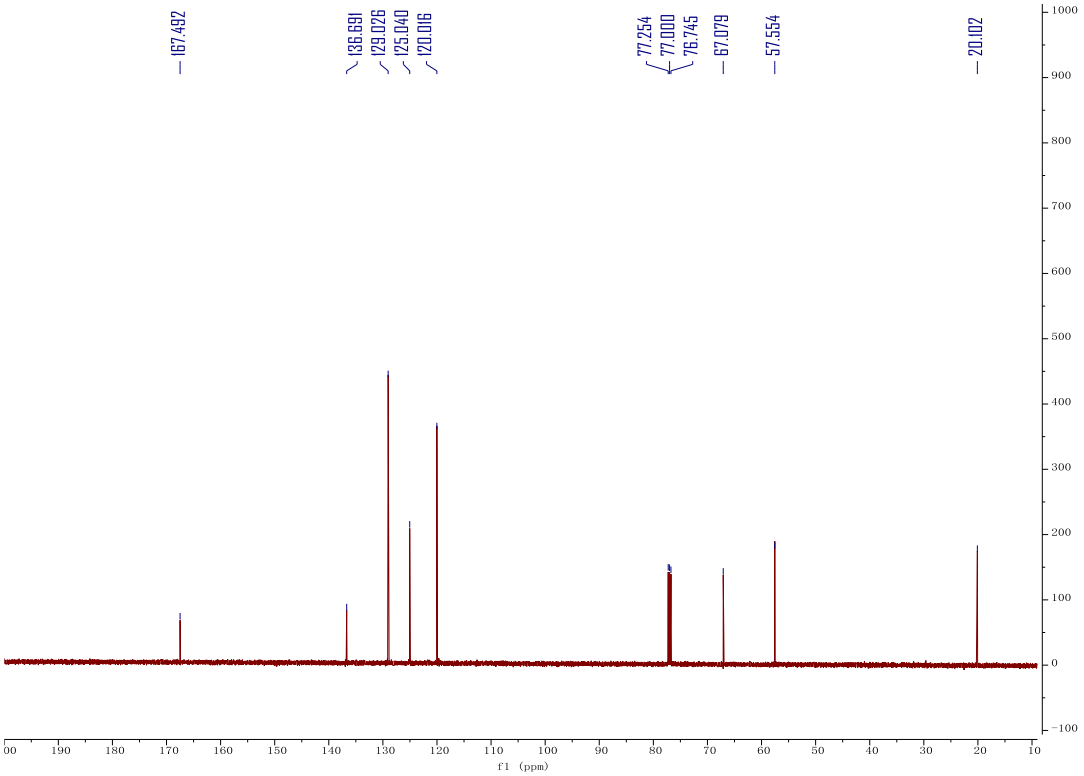
2z, ^{13}C NMR, 126 MHz, $CDCl_3$.



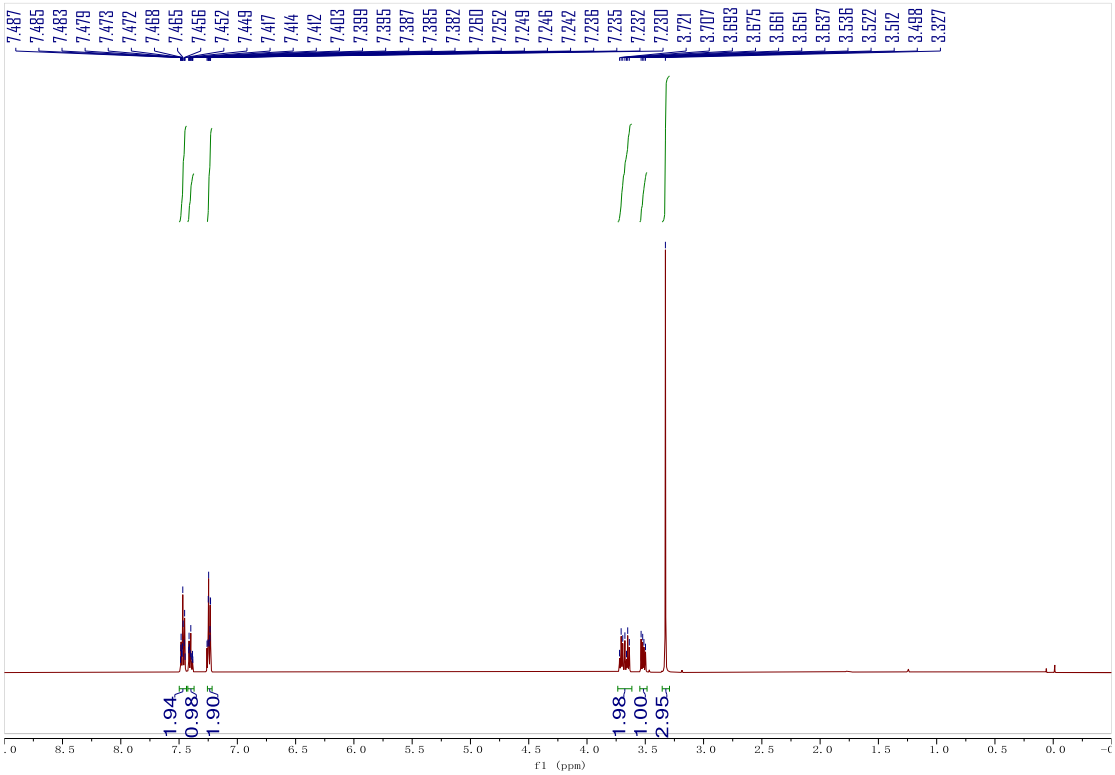
2aa, ^{1}H NMR, 500 MHz, $CDCl_3$.



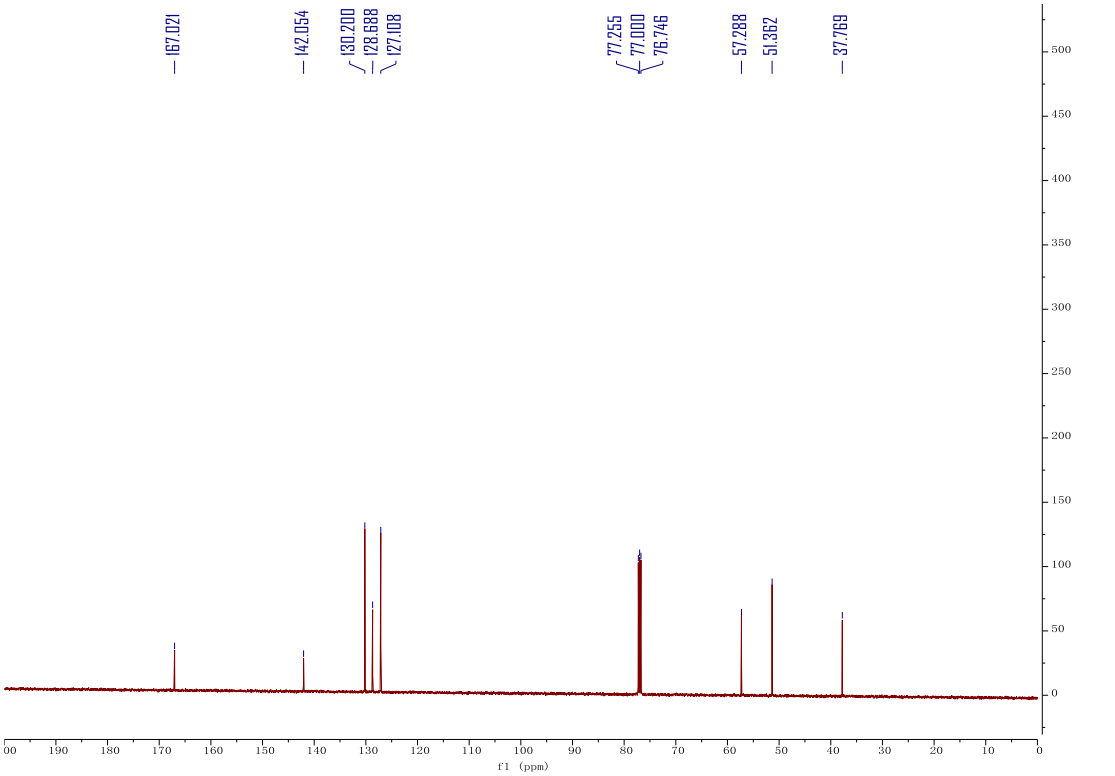
2aa, ^{13}C NMR, 126 MHz, $CDCl_3$.



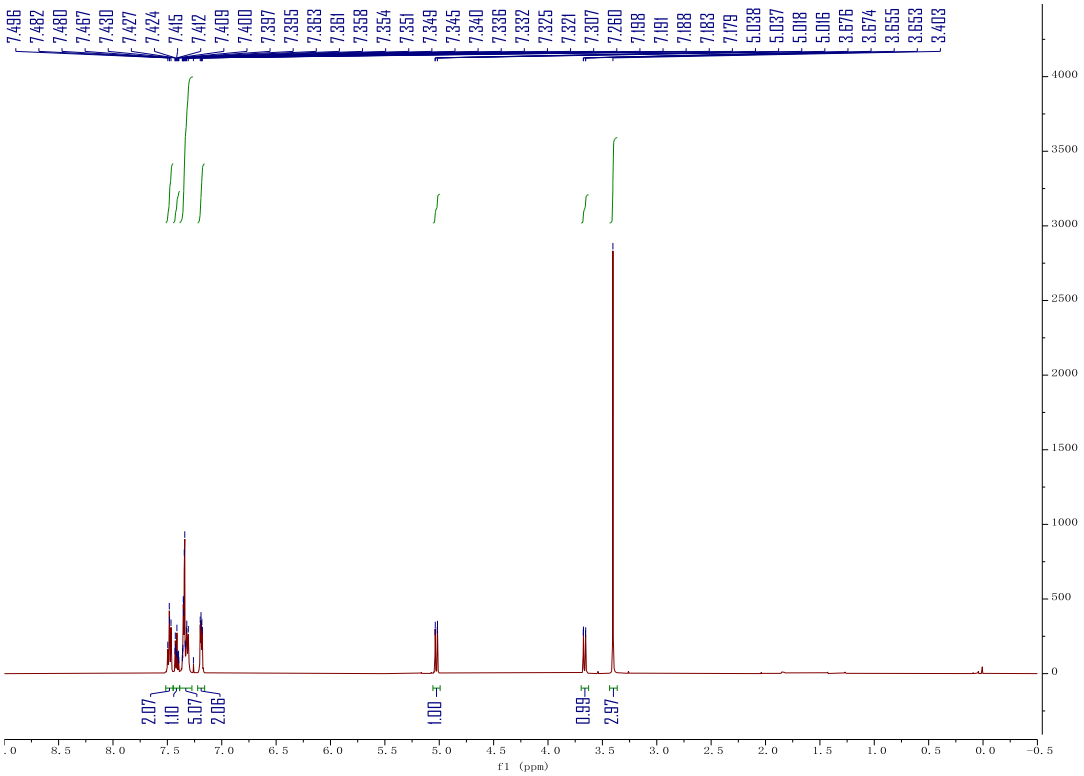
2ab, ^{1}H NMR, 500 MHz, $CDCl_3$.



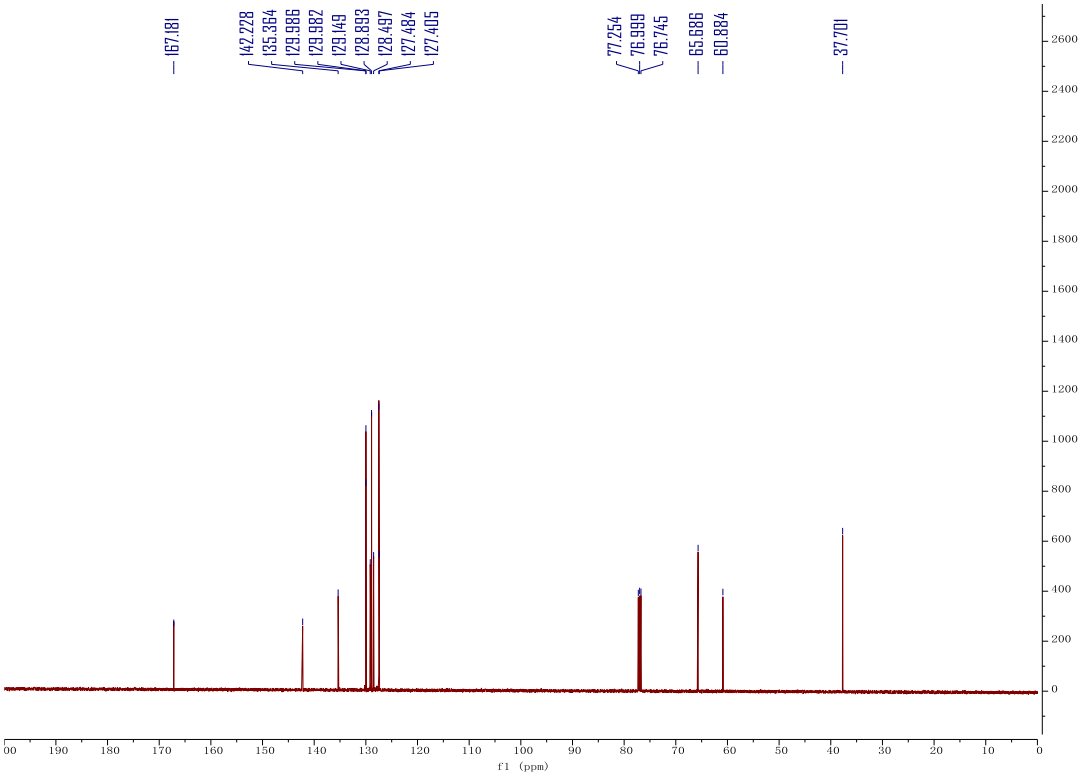
2ab, ^{13}C NMR, 126 MHz, $CDCl_3$.



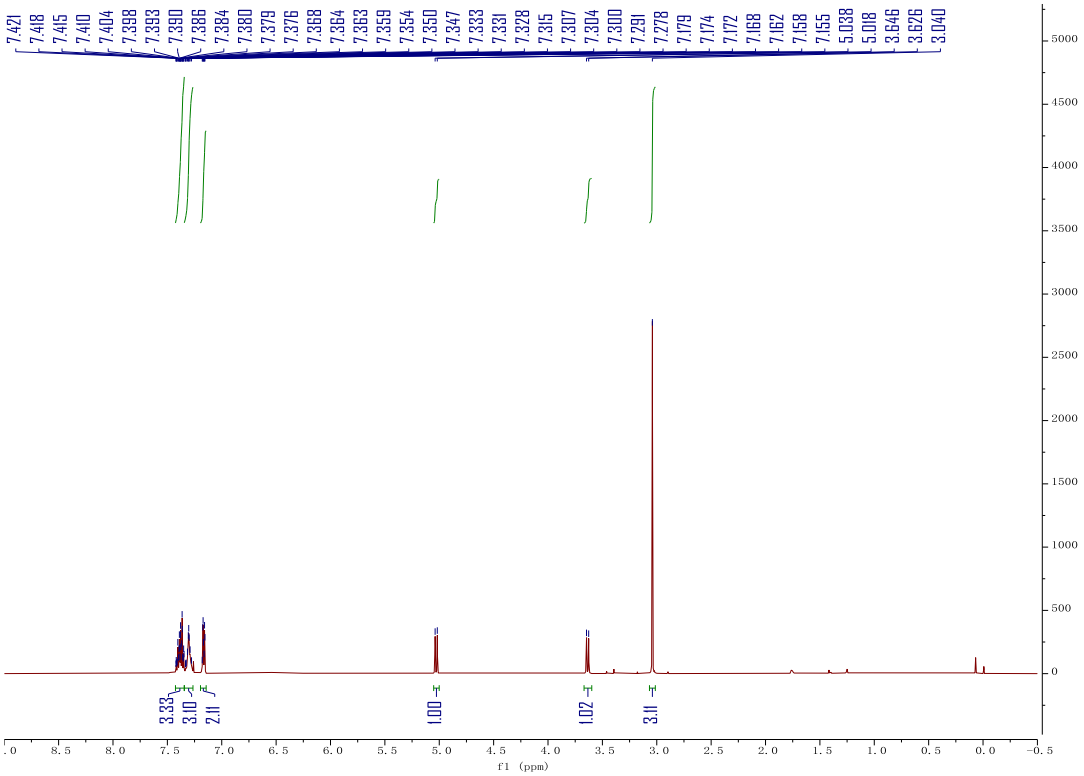
2ac, ^{1}H NMR, 500 MHz, $CDCl_3$. *anti*-Isomer.



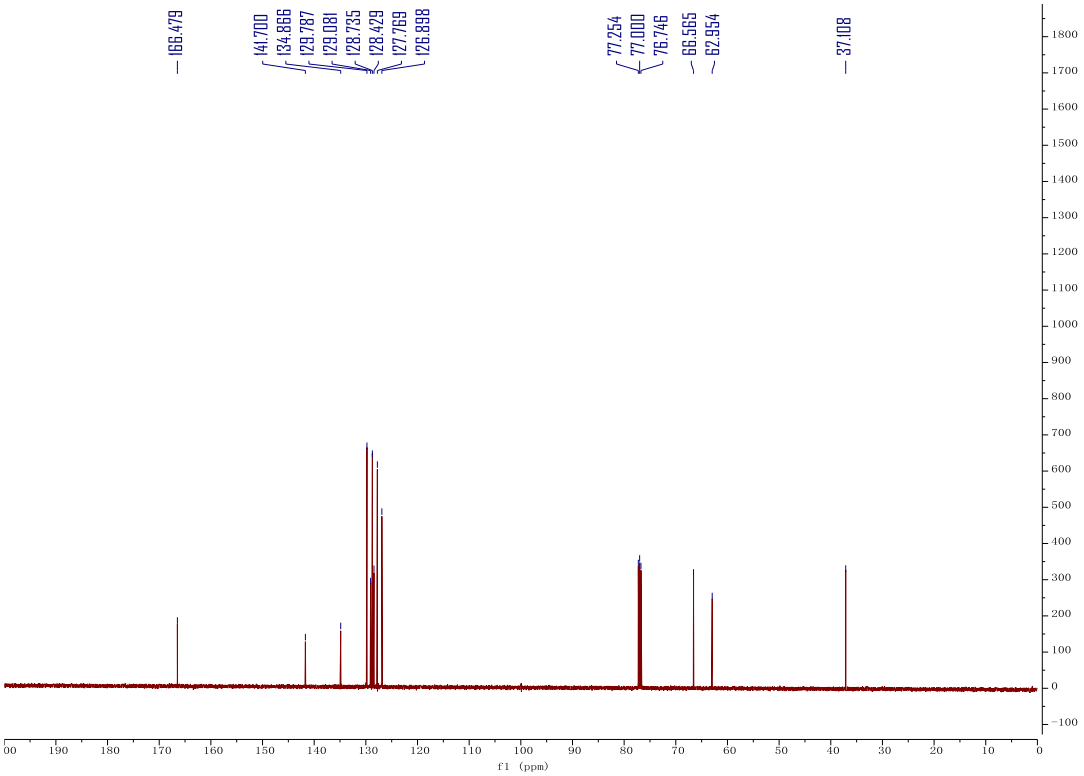
2ac, ^{13}C NMR, 126 MHz, $CDCl_3$. *anti*-Isomer.



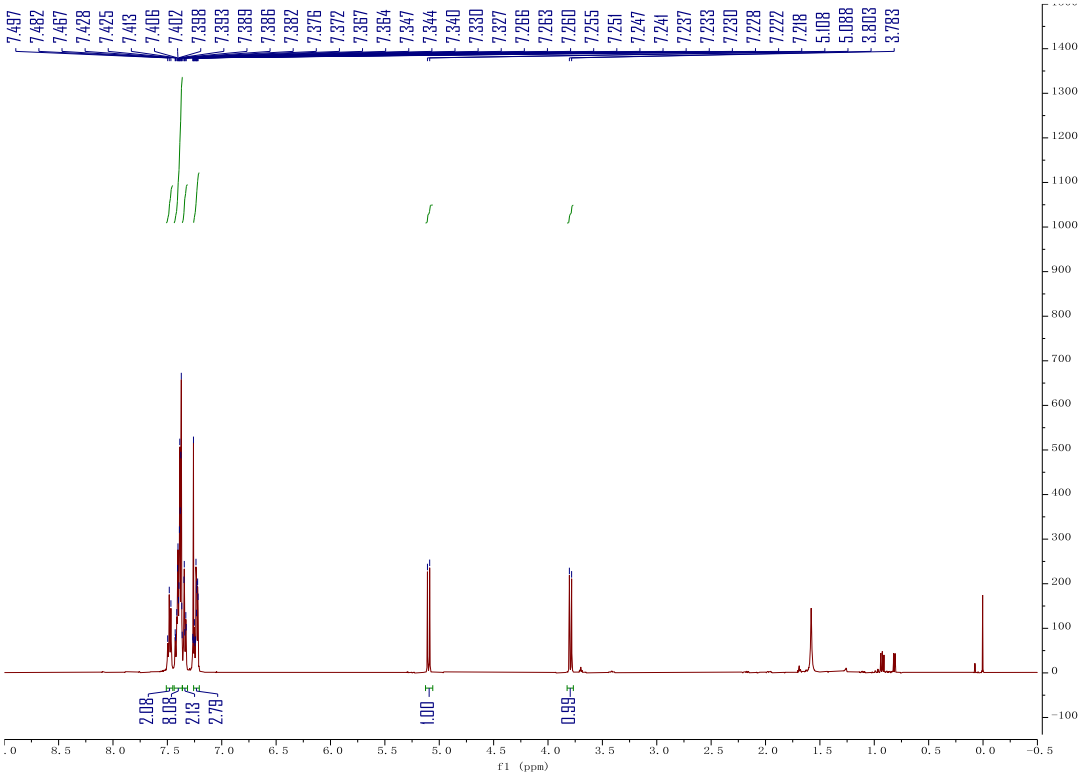
2ac, ^{1}H NMR, 500 MHz, $CDCl_3$. *syn*-Isomer.



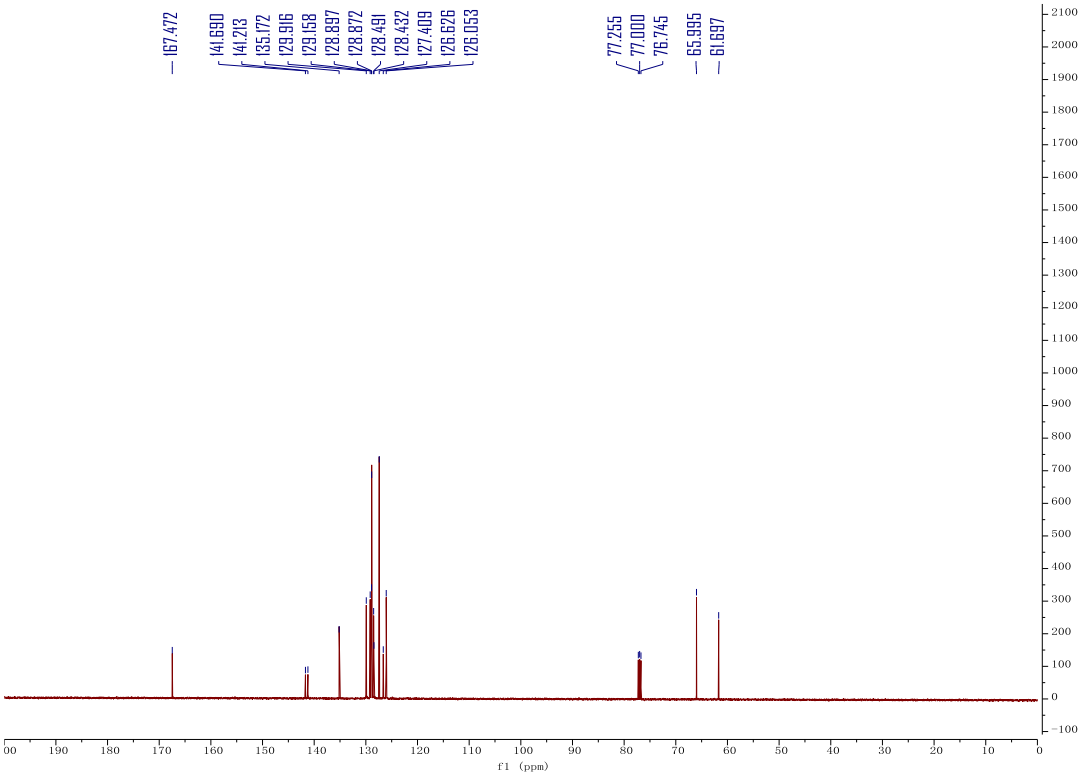
2ac, ^{13}C NMR, 126 MHz, $CDCl_3$. *syn*-Isomer.



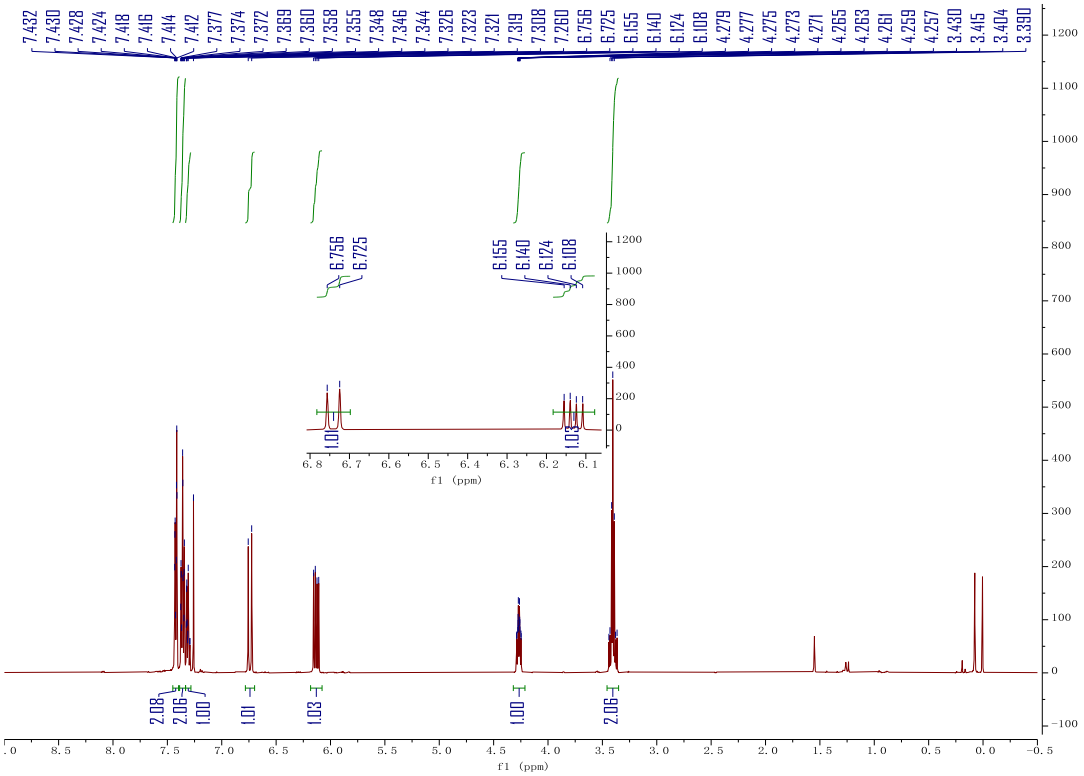
2ad, ^{1}H NMR, 500 MHz, $CDCl_3$. *anti*-Isomer.



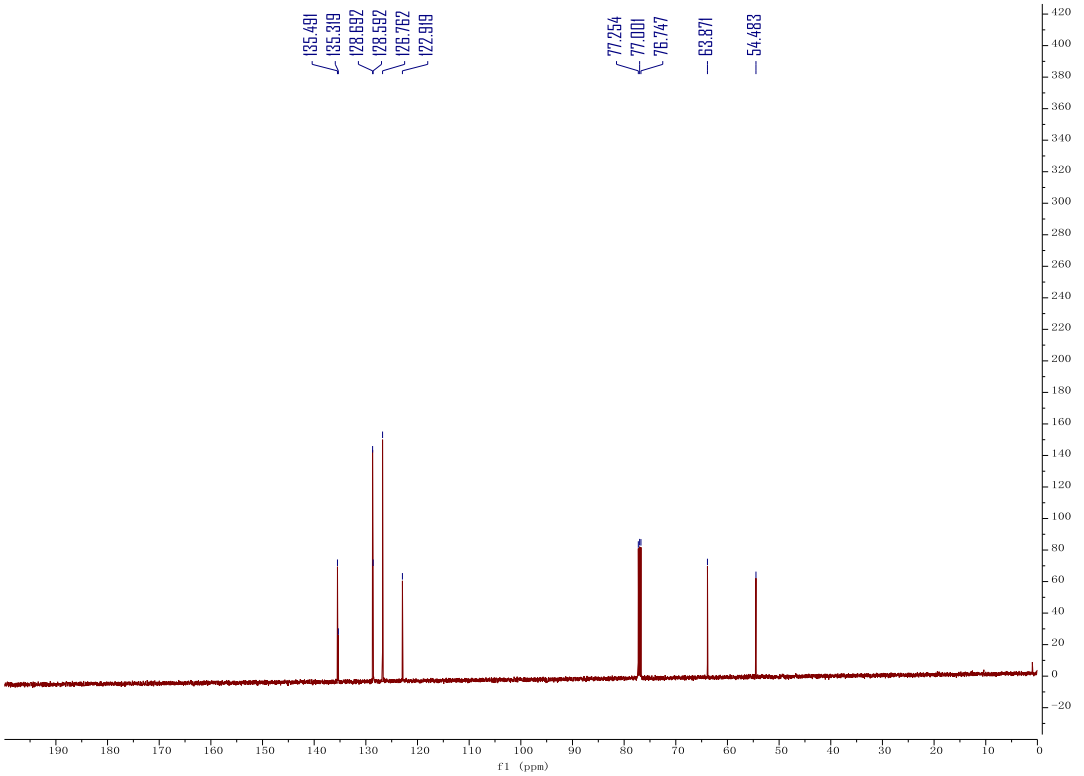
2ad, ^{13}C NMR, 126 MHz, $CDCl_3$. *anti*-Isomer.



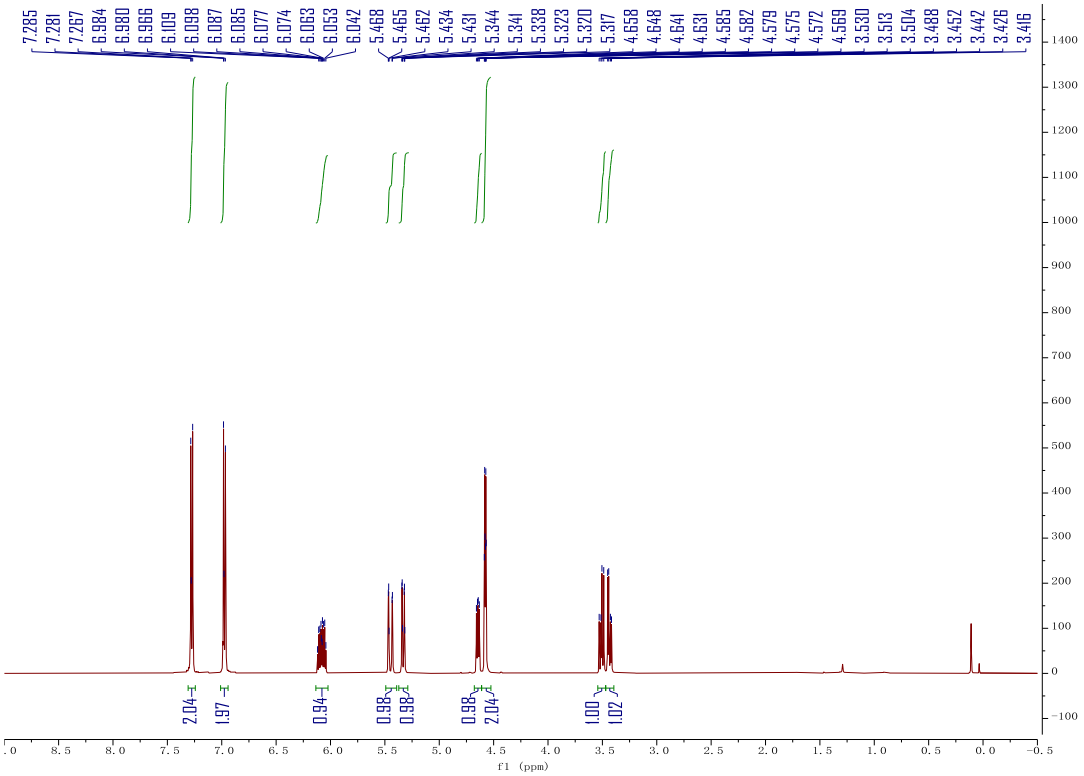
2ae, ^{1}H NMR, 500 MHz, $CDCl_3$.



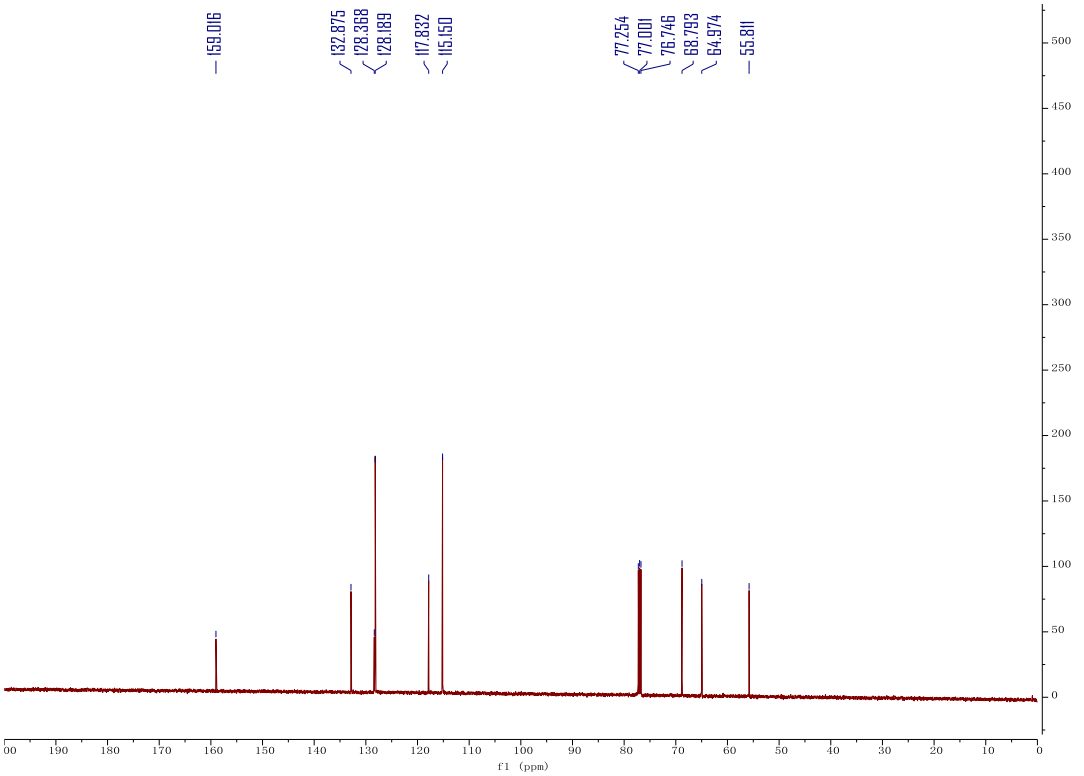
2ae, ^{13}C NMR, 126 MHz, $CDCl_3$.



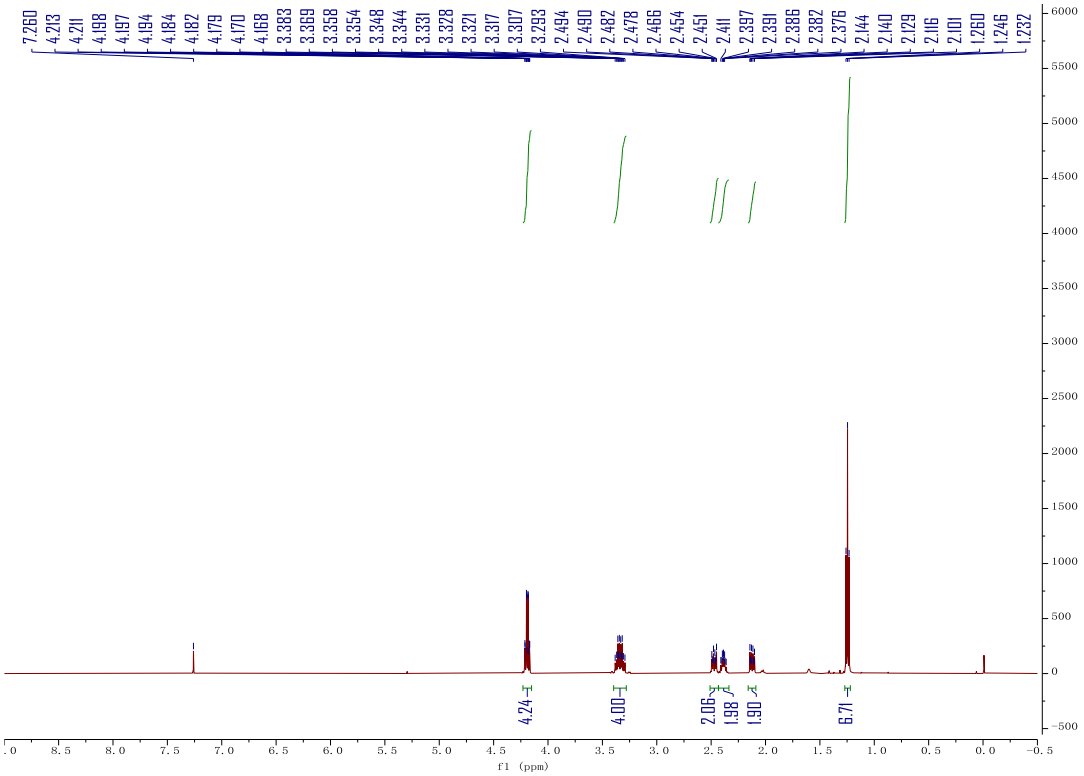
2af, ^{1}H NMR, 500 MHz, $CDCl_3$.



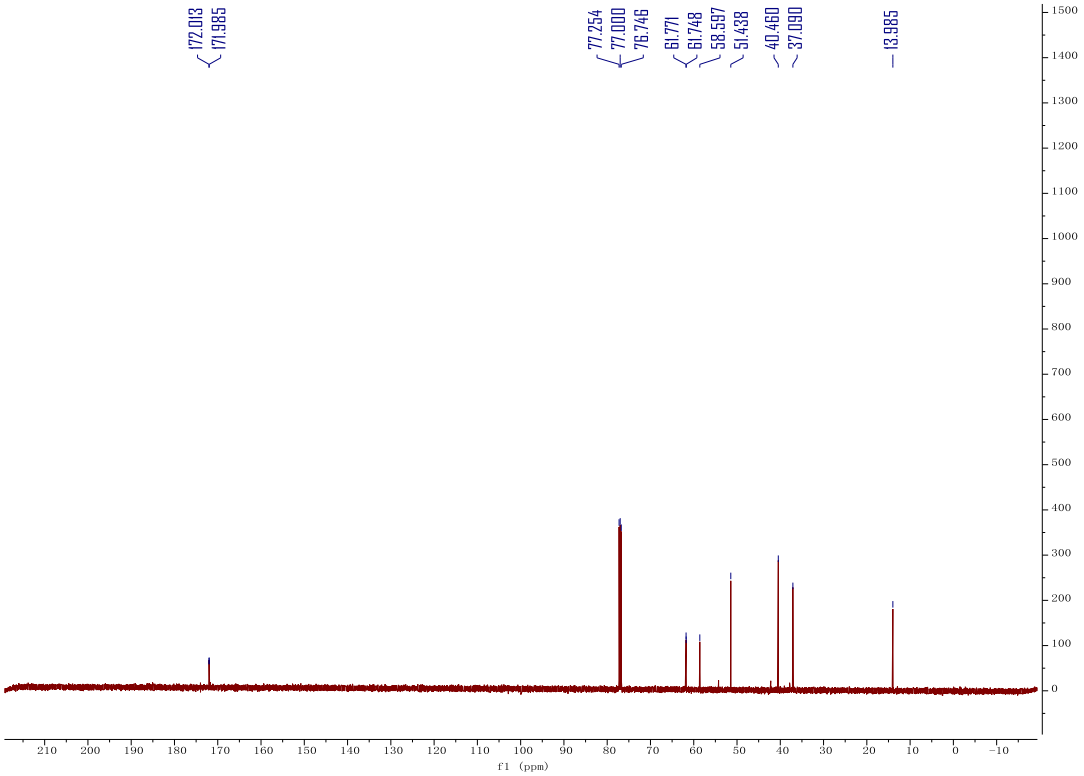
2af, ^{13}C NMR, 126 MHz, $CDCl_3$.



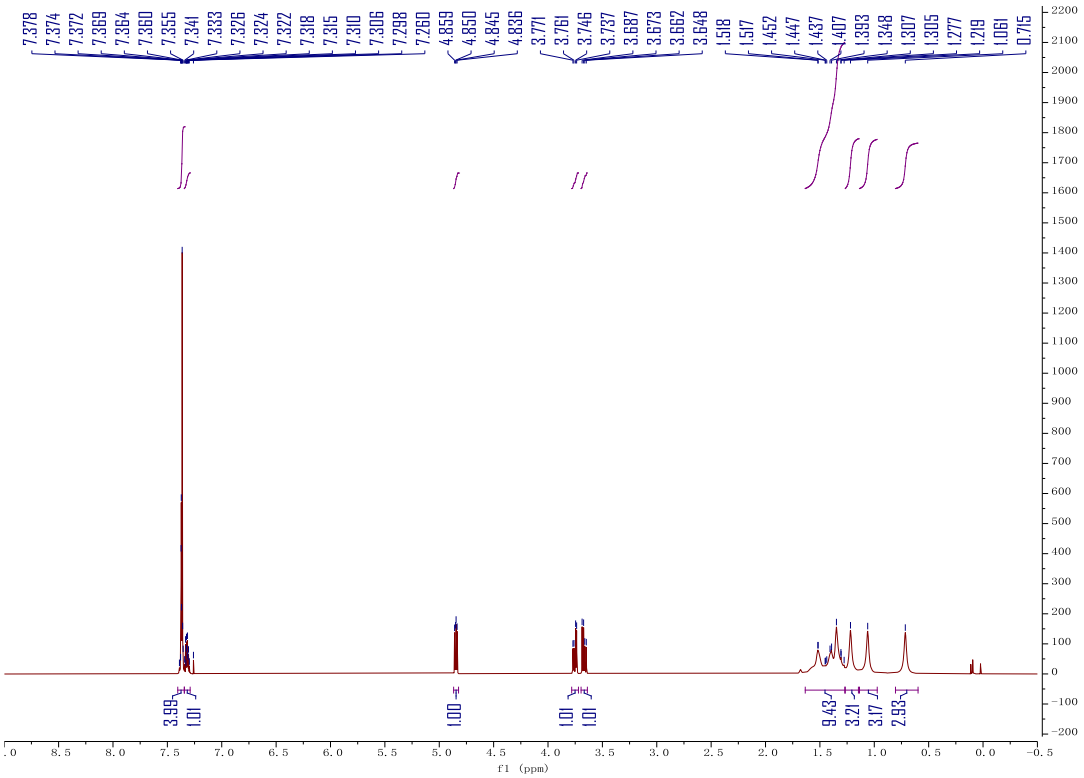
4, ^{1}H NMR, 500 MHz, $CDCl_3$.



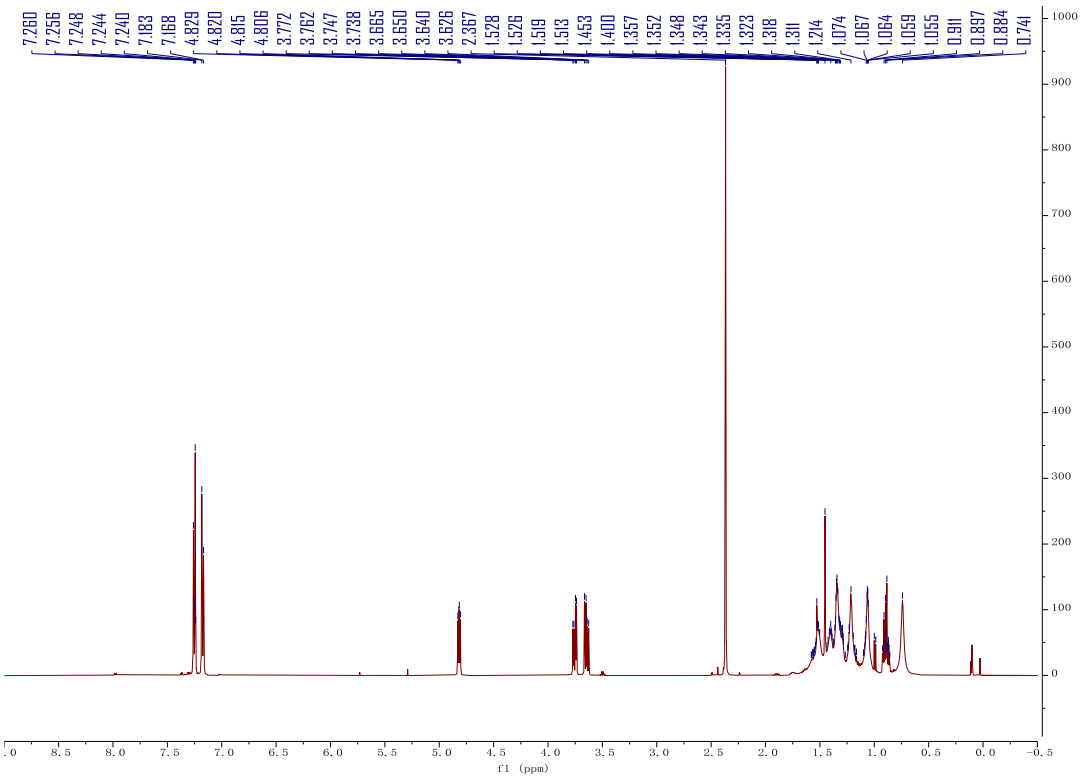
4, ^{13}C NMR, 126 MHz, $CDCl_3$.



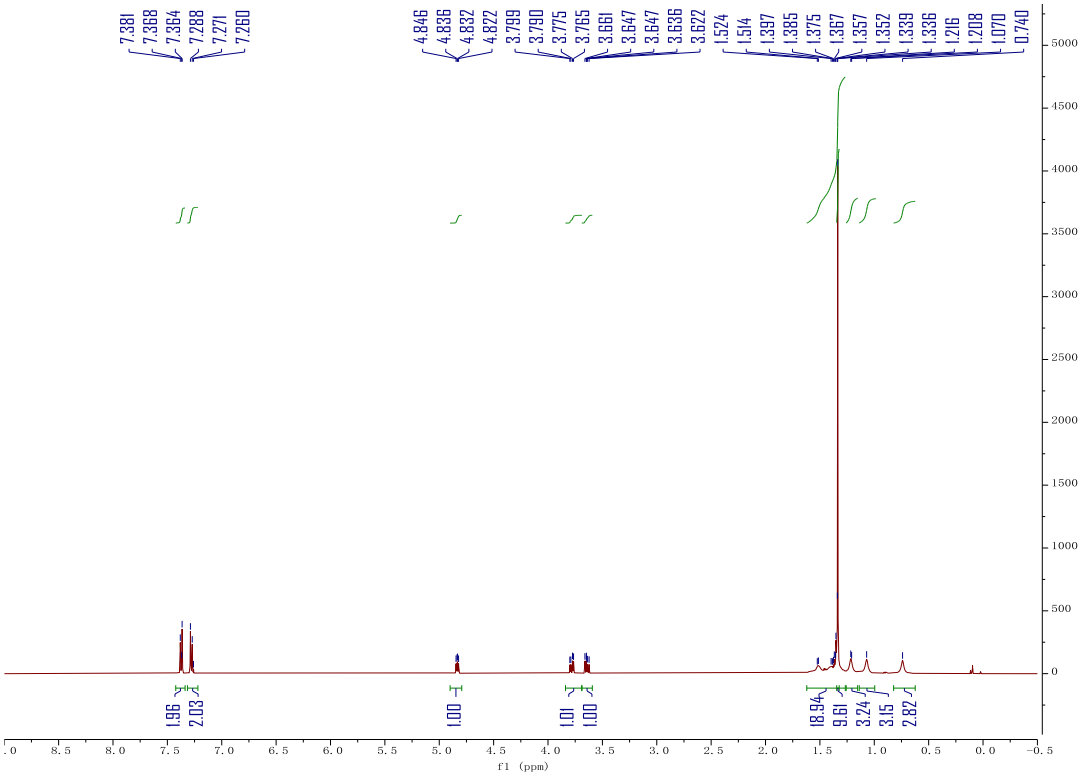
5a, ^{1}H NMR, 500 MHz, $CDCl_3$.



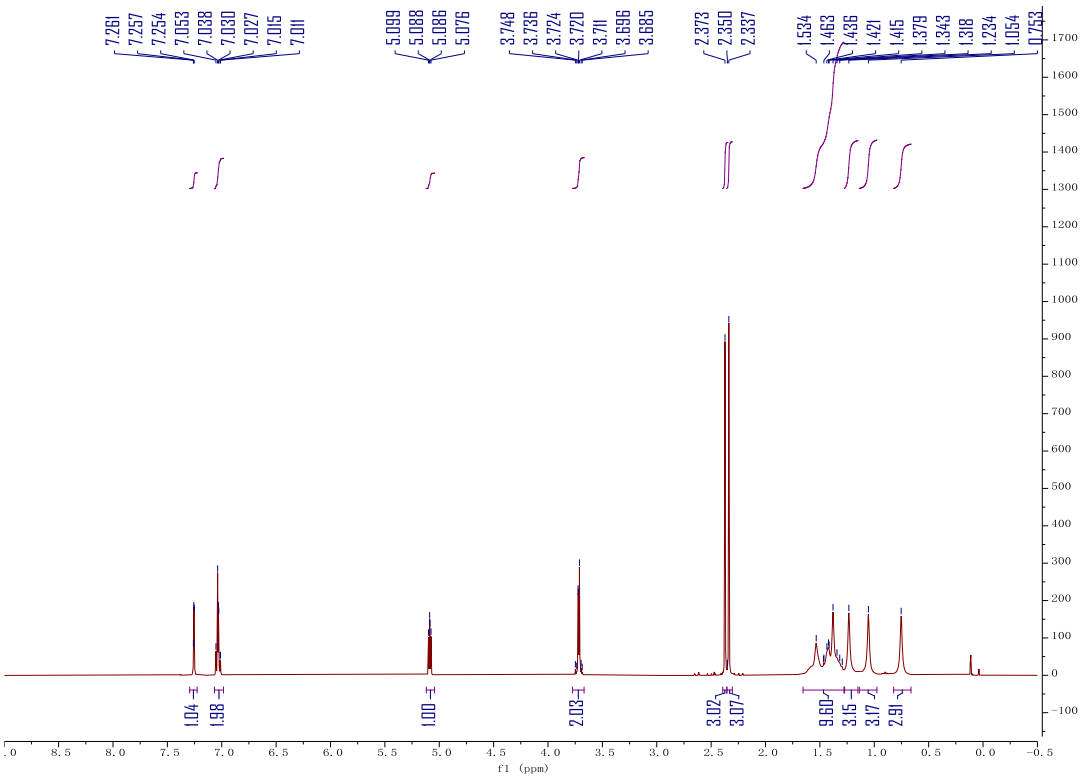
5b, ^{1}H NMR, 500 MHz, $CDCl_3$.



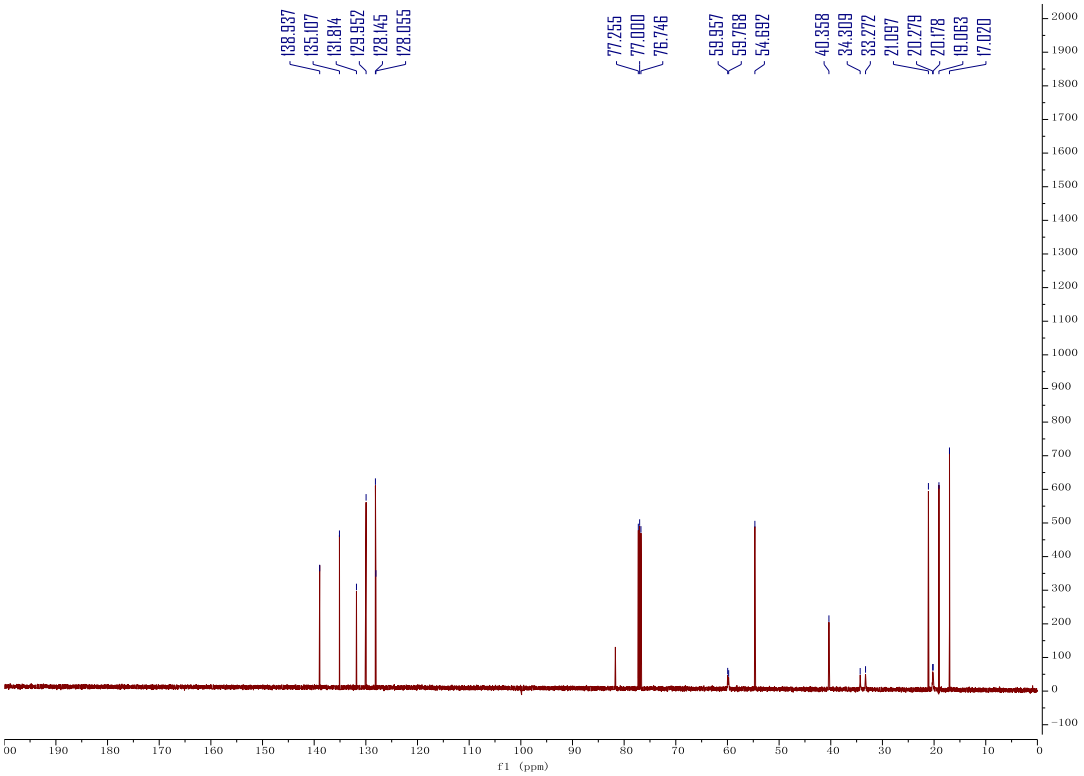
5c, ^{1}H NMR, 500 MHz, $CDCl_3$.



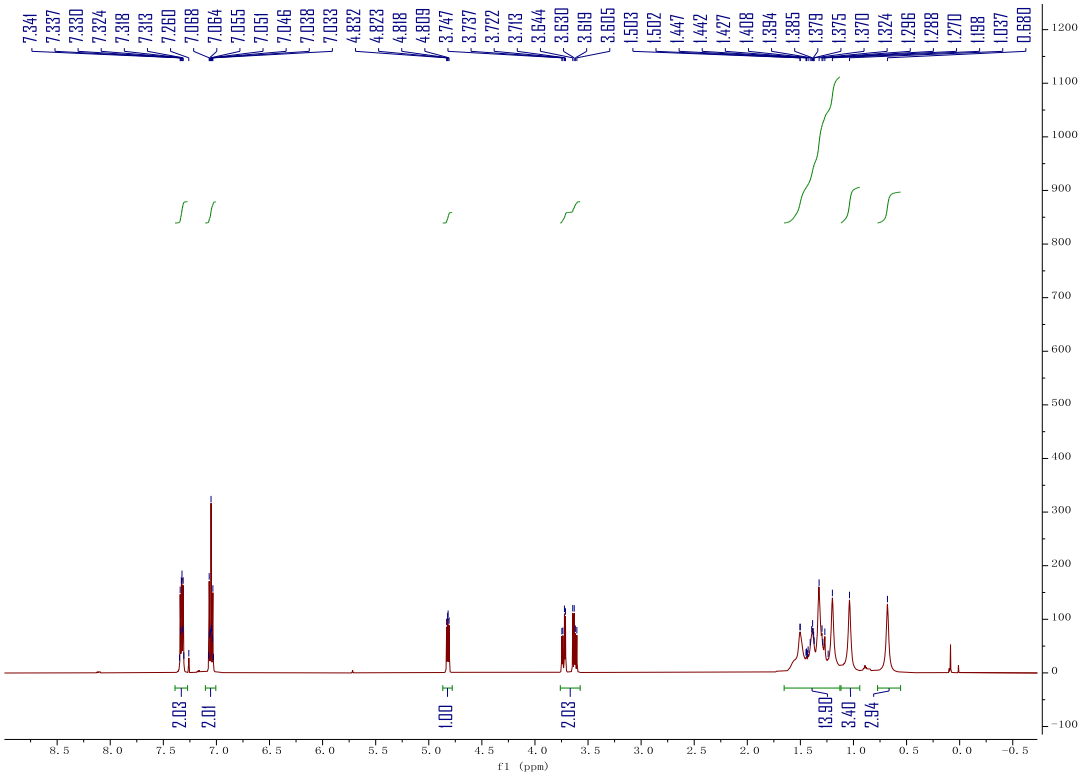
5d, ^{1}H NMR, 500 MHz, $CDCl_3$.



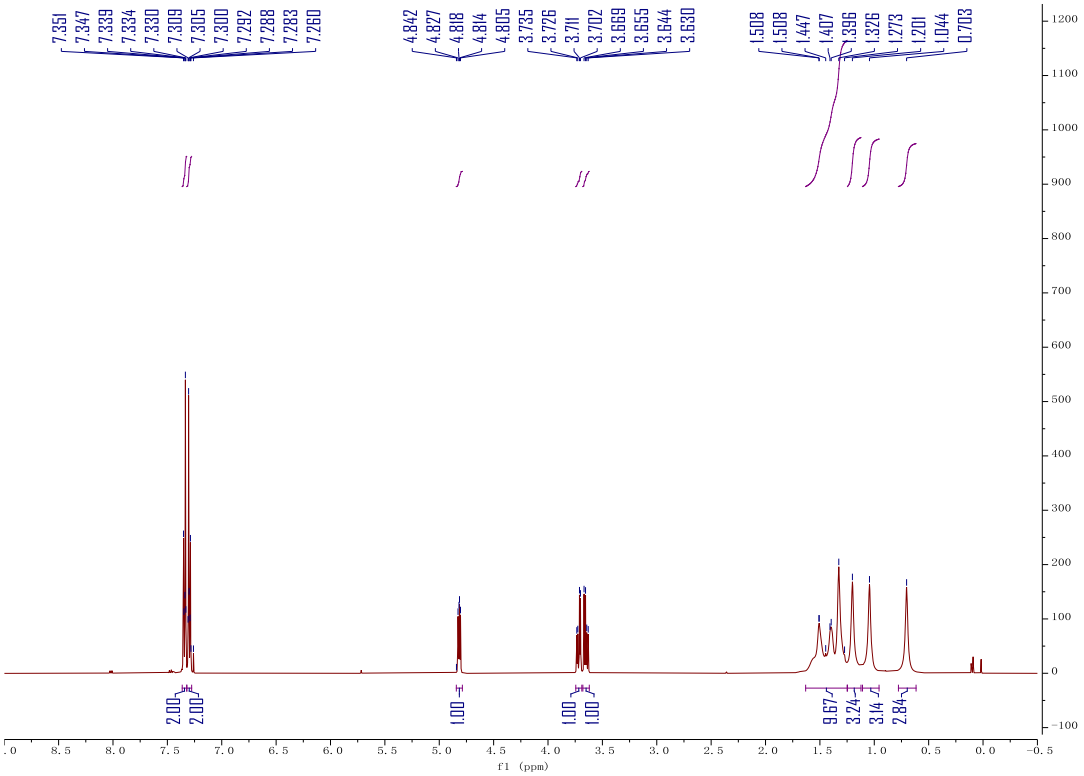
5d, ^{13}C NMR, 126 MHz, $CDCl_3$.



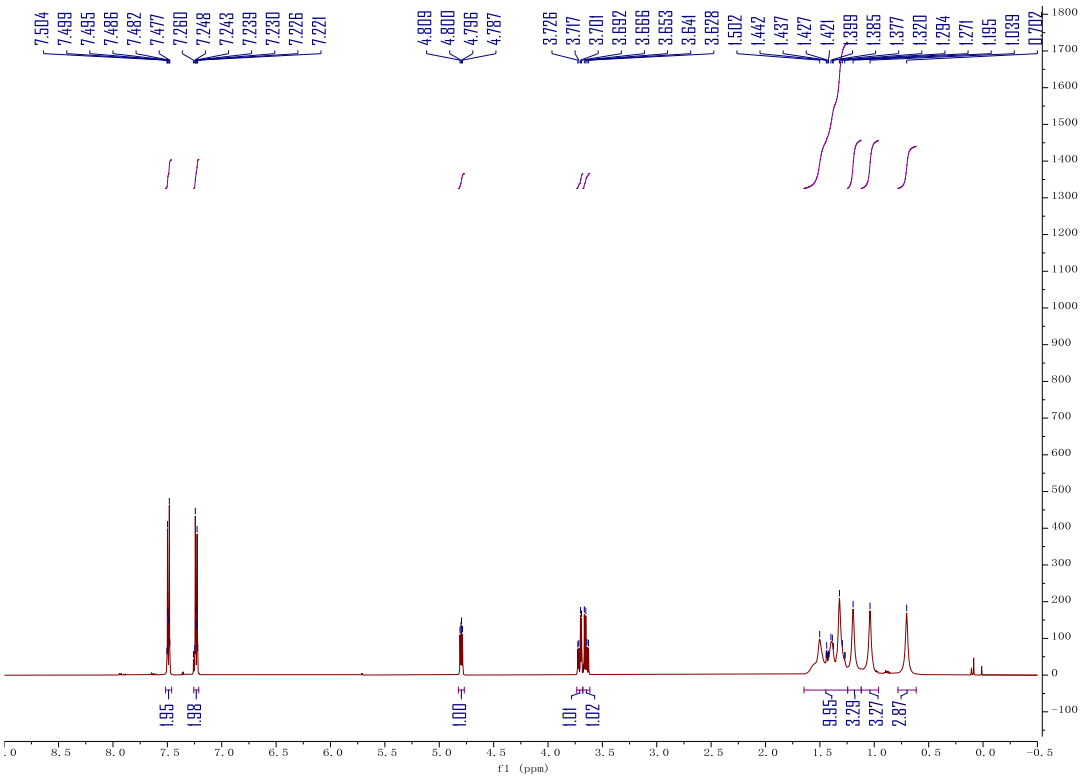
5e, ^{1}H NMR, 500 MHz, $CDCl_3$.



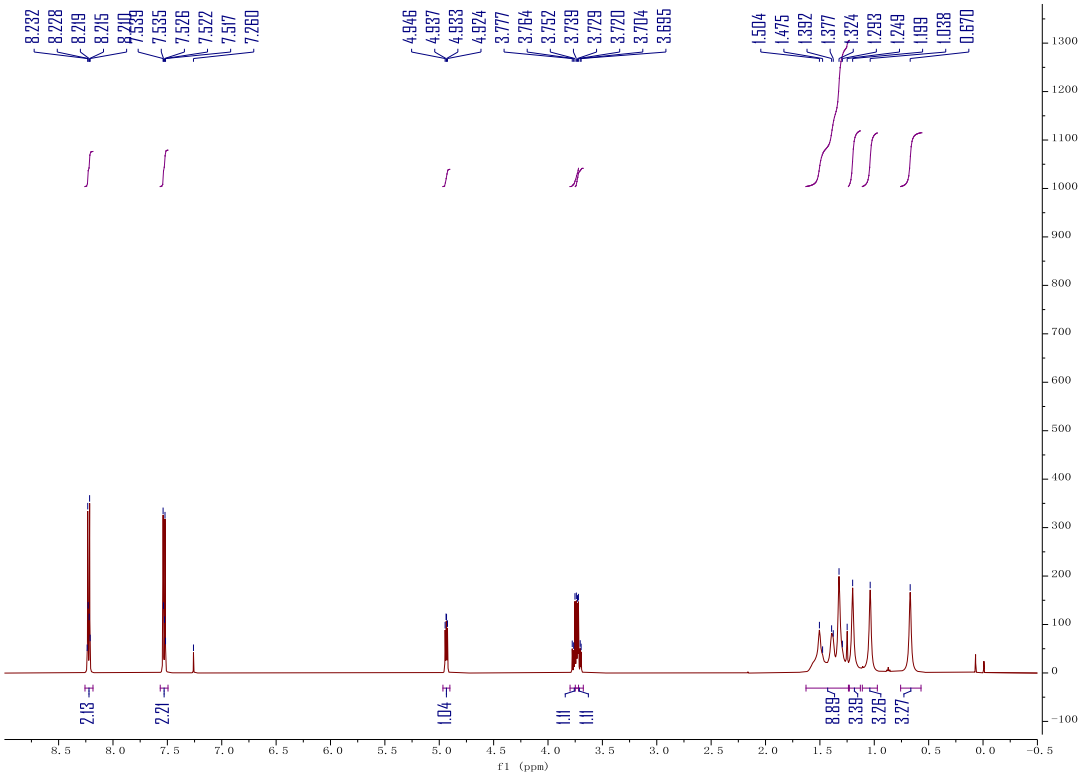
5f, ^{1}H NMR, 500 MHz, $CDCl_3$.



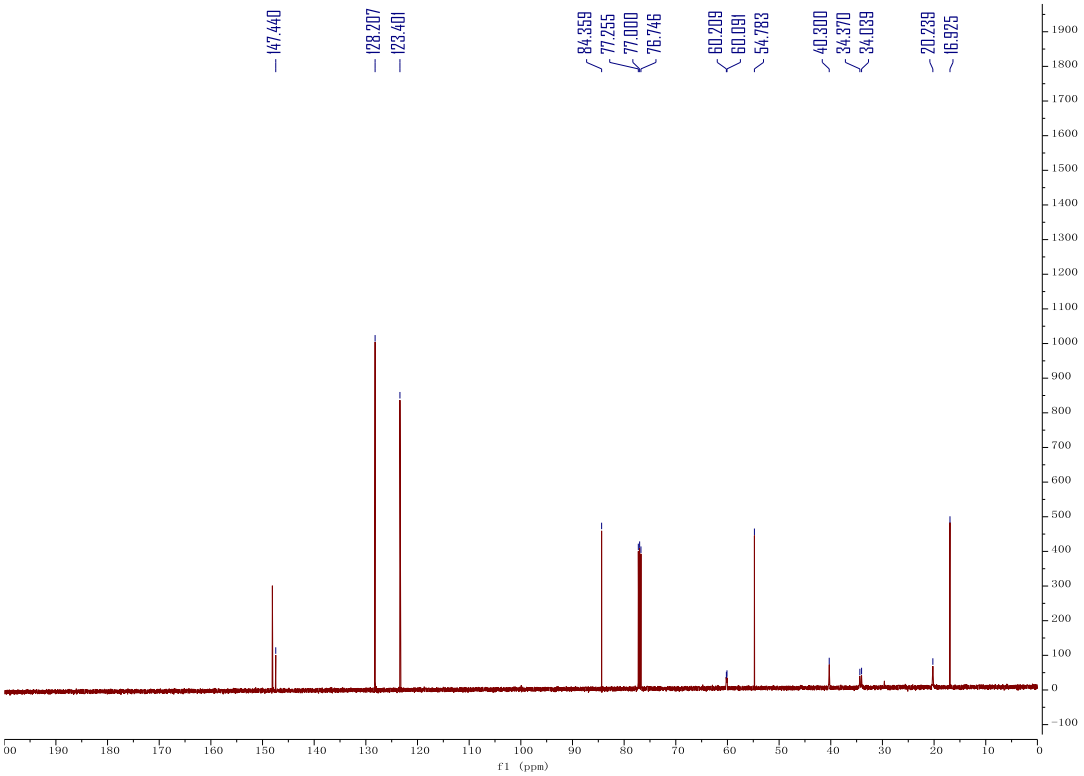
5g, ^{1}H NMR, 500 MHz, $CDCl_3$.



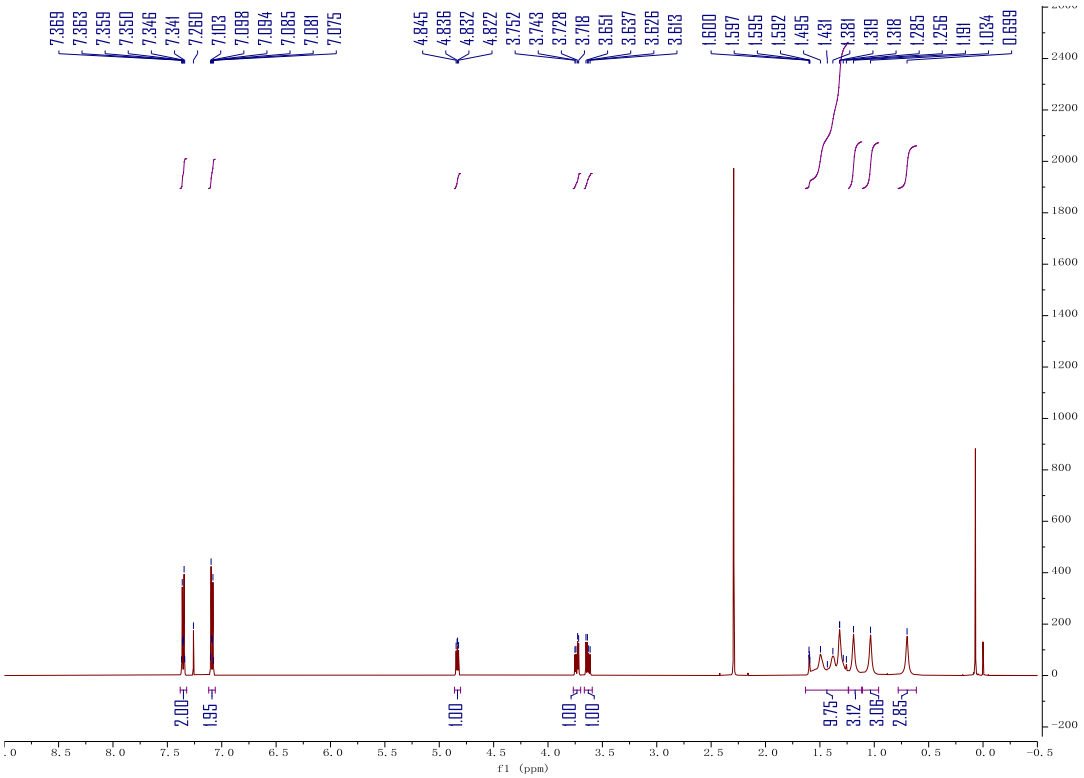
5h, ^{1}H NMR, 500 MHz, $CDCl_3$.



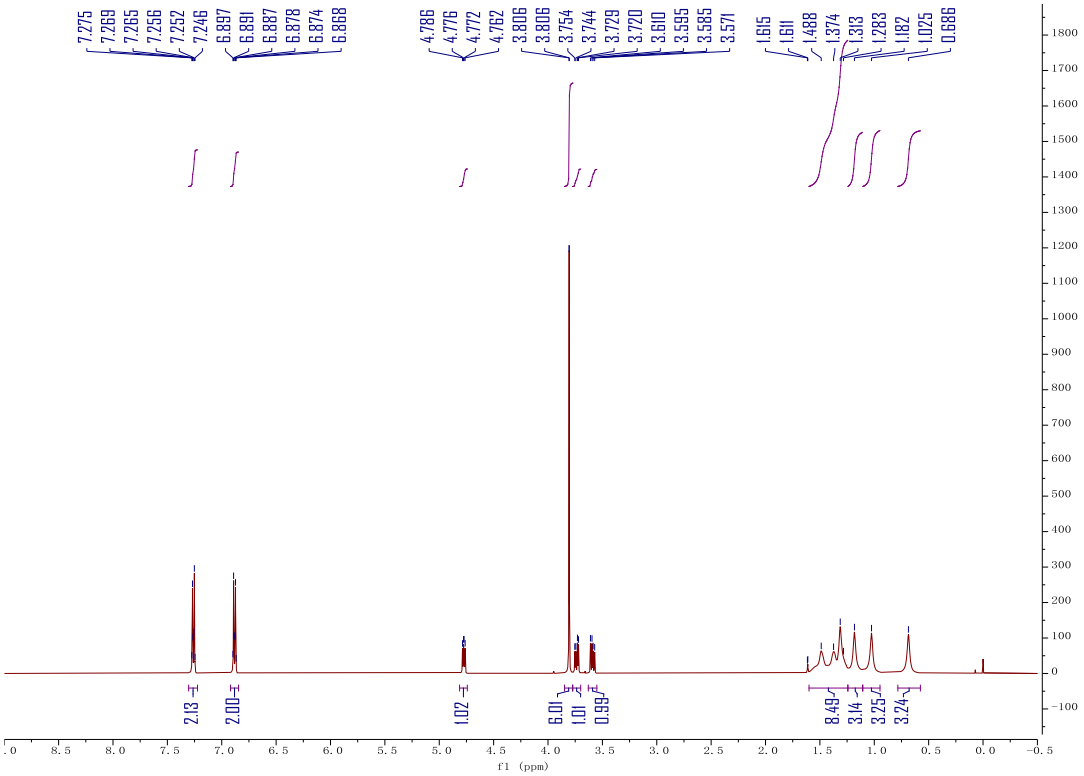
5h, ^{13}C NMR, 126 MHz, $CDCl_3$.



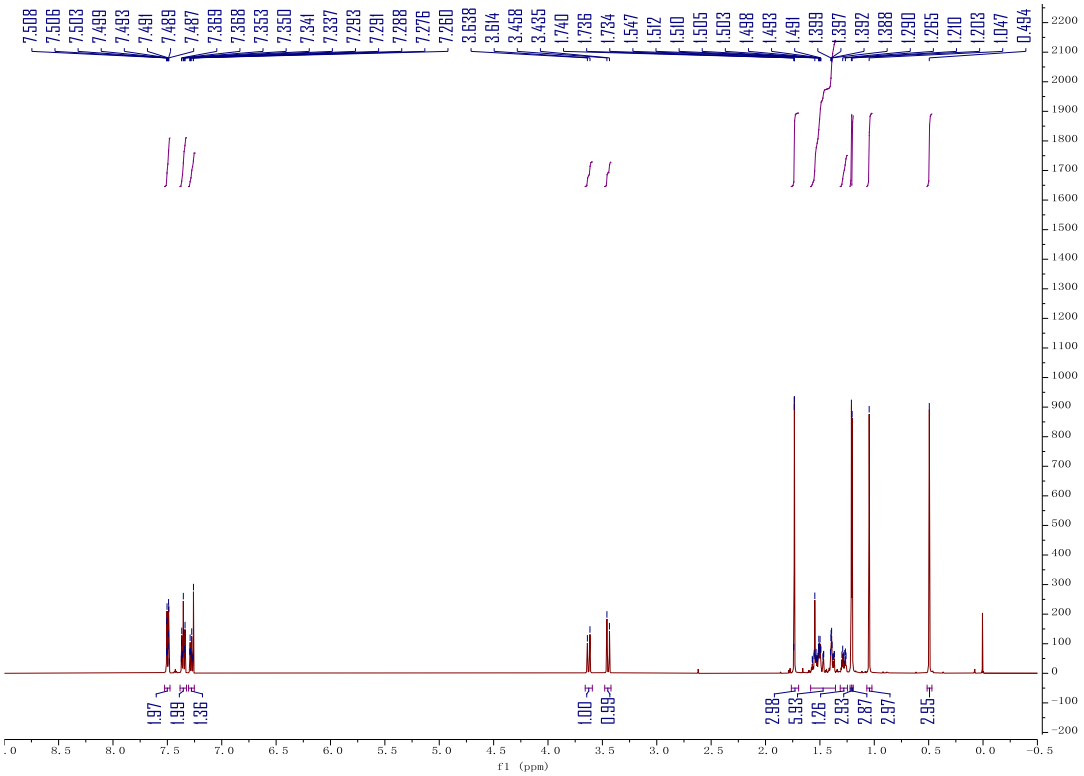
5i, ^{1}H NMR, 500 MHz, $CDCl_3$.



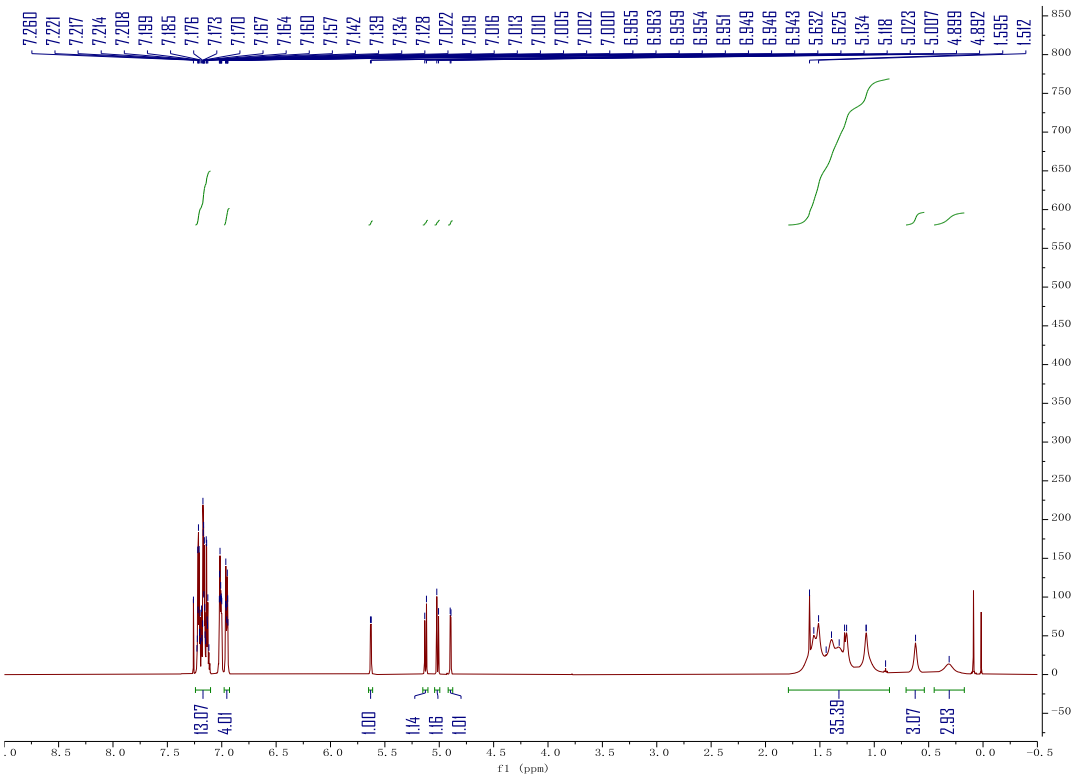
5j, ^{1}H NMR, 500 MHz, $CDCl_3$.



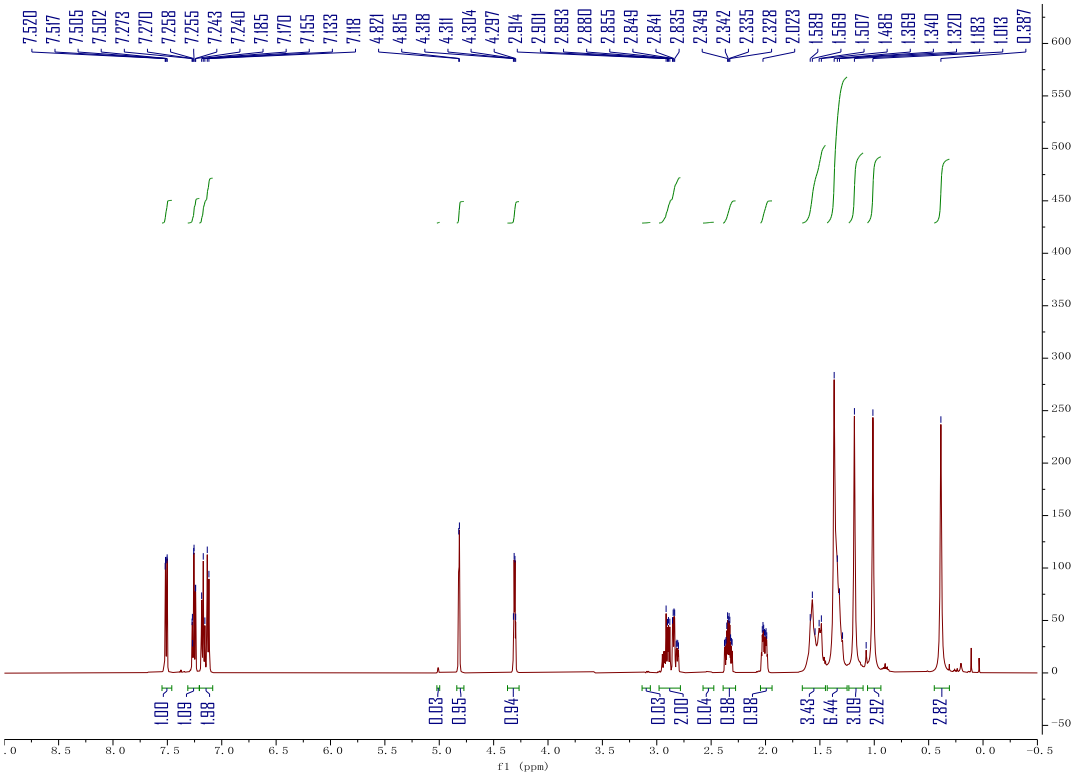
5k, ^{1}H NMR, 500 MHz, $CDCl_3$.



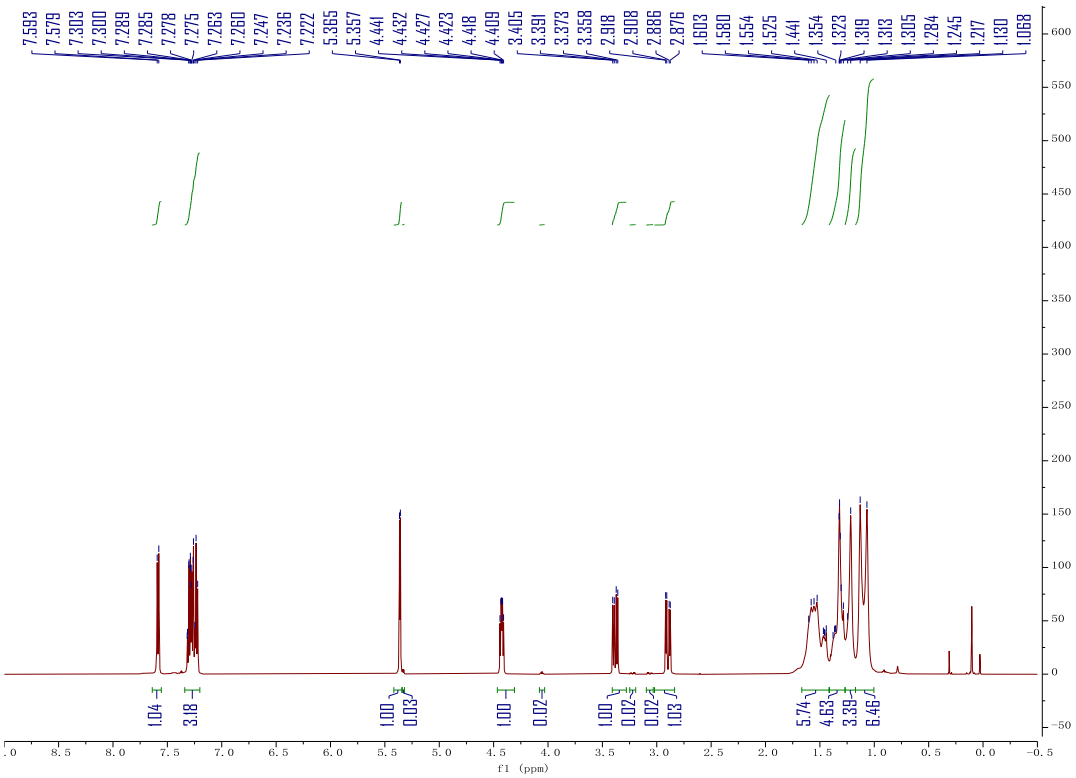
5l, ^{1}H NMR, 500 MHz, $CDCl_3$.



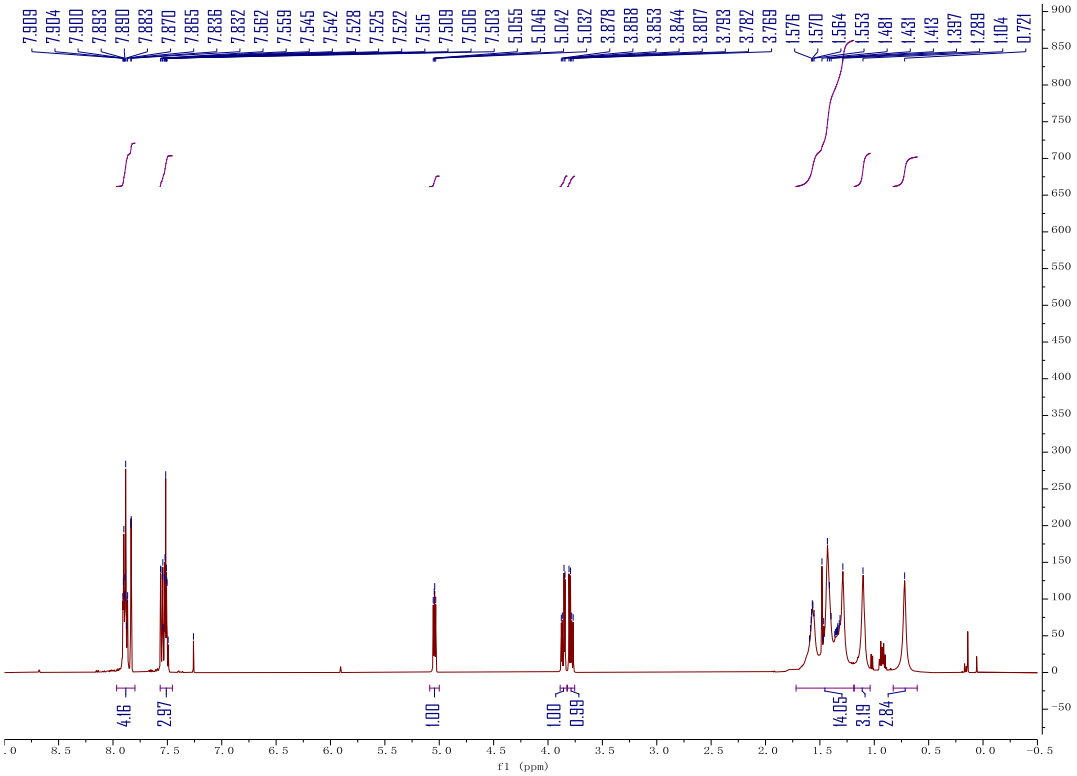
5m, ^{1}H NMR, 500 MHz, $CDCl_3$.



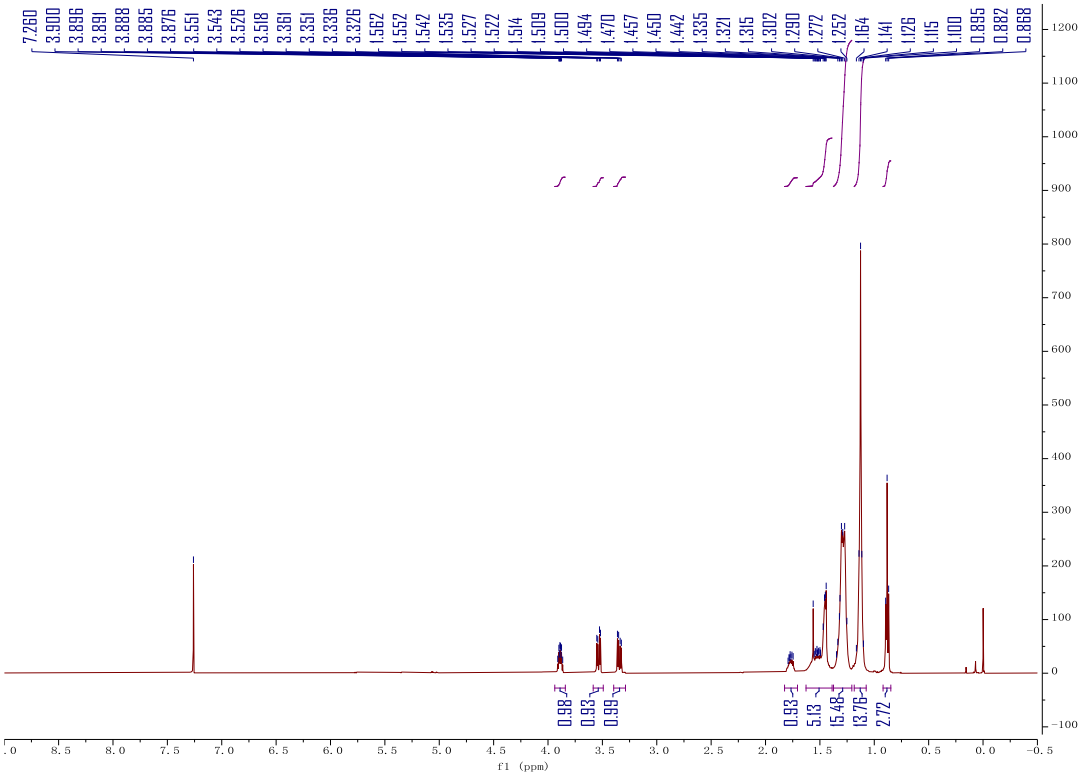
5n, ^{1}H NMR, 500 MHz, $CDCl_3$.



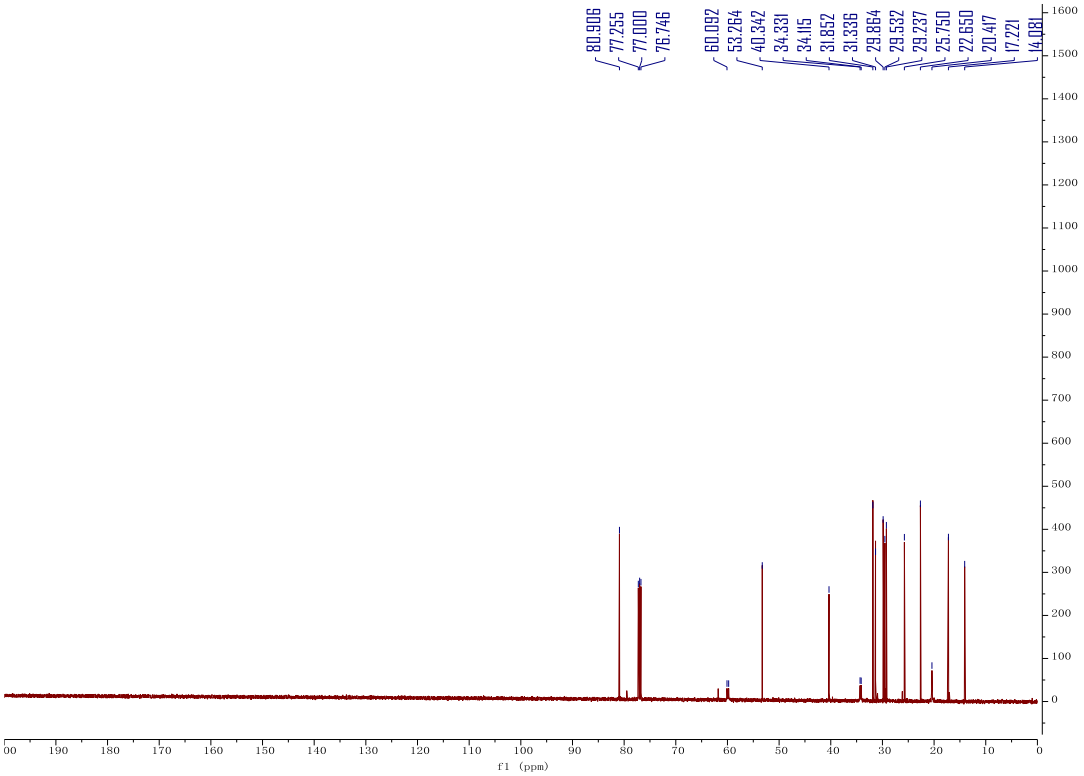
5o, ^{1}H NMR, 500 MHz, $CDCl_3$.



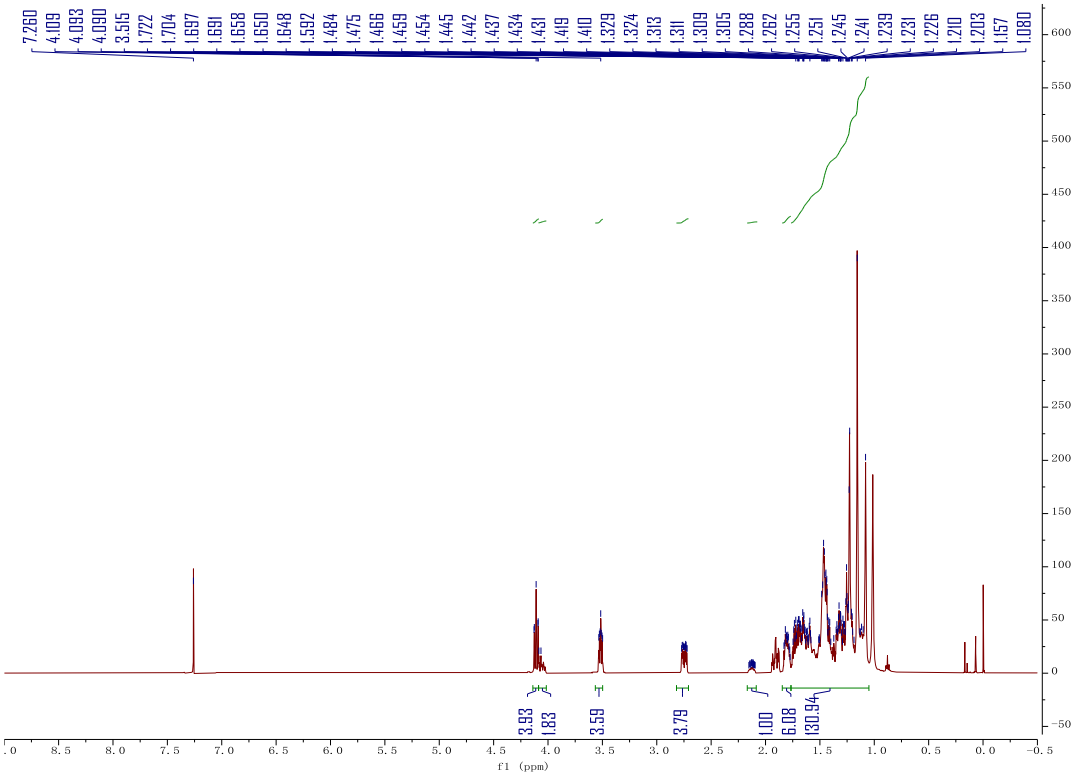
5p, ^{1}H NMR, 500 MHz, $CDCl_3$.



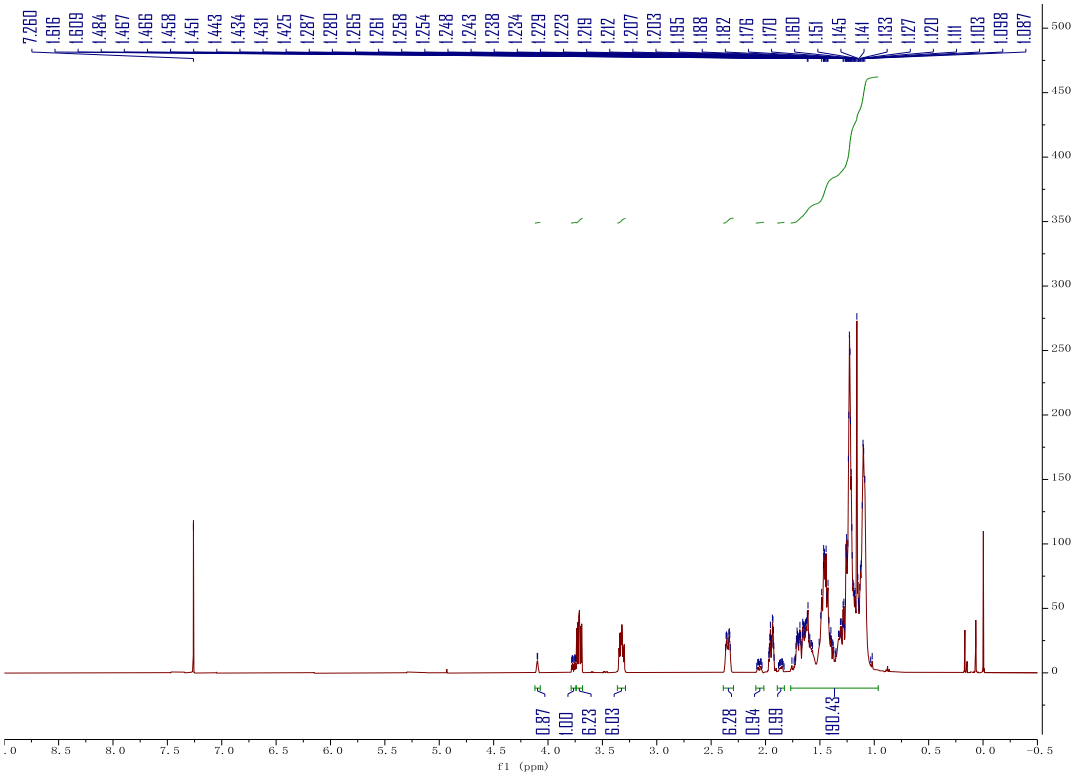
5p, ^{13}C NMR, 126 MHz, $CDCl_3$.



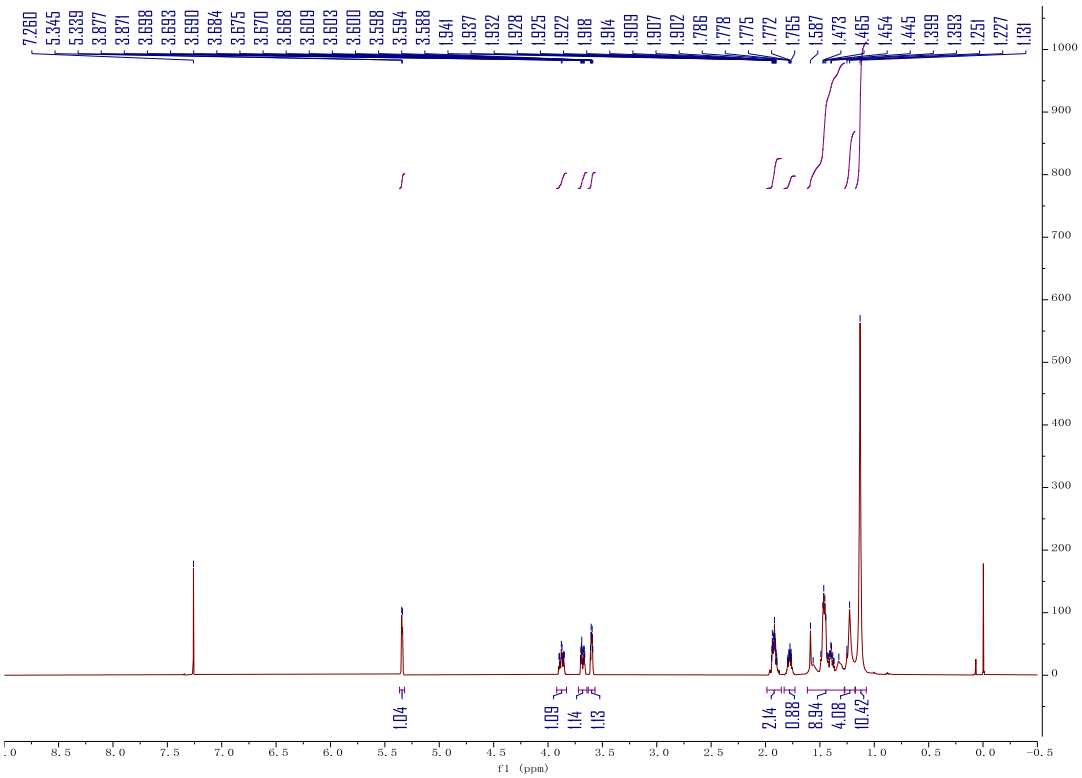
5q, ^{1}H NMR, 500 MHz, $CDCl_3$.



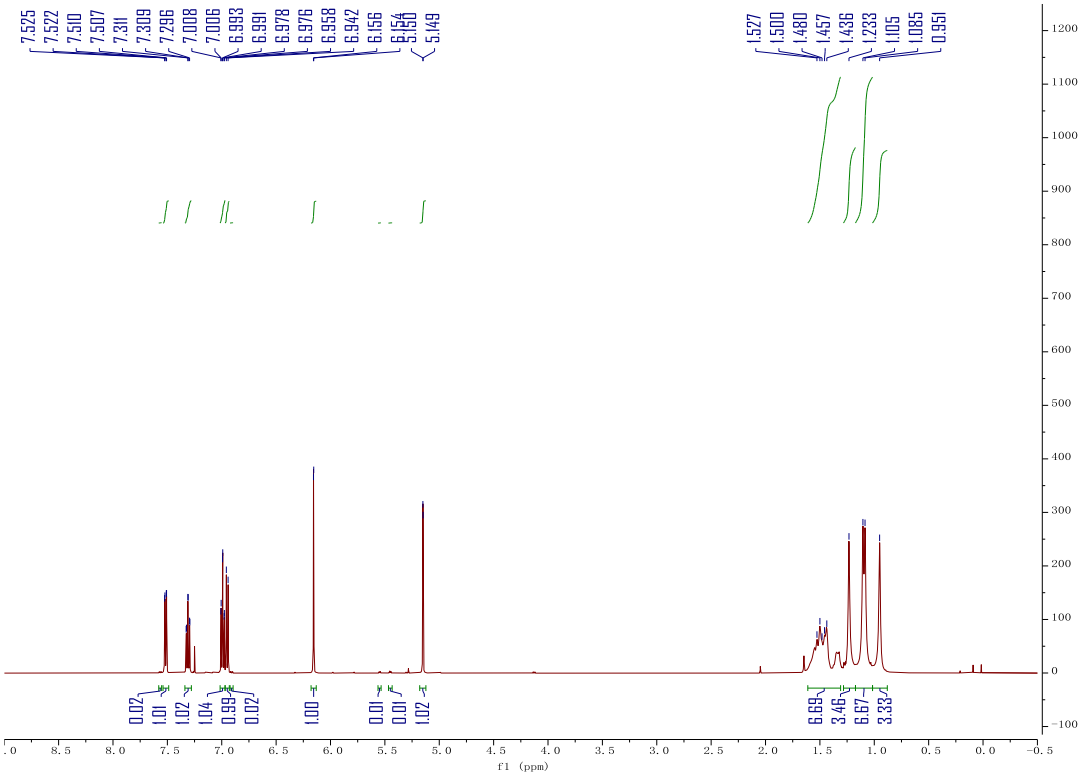
5r, ^{1}H NMR, 500 MHz, $CDCl_3$.



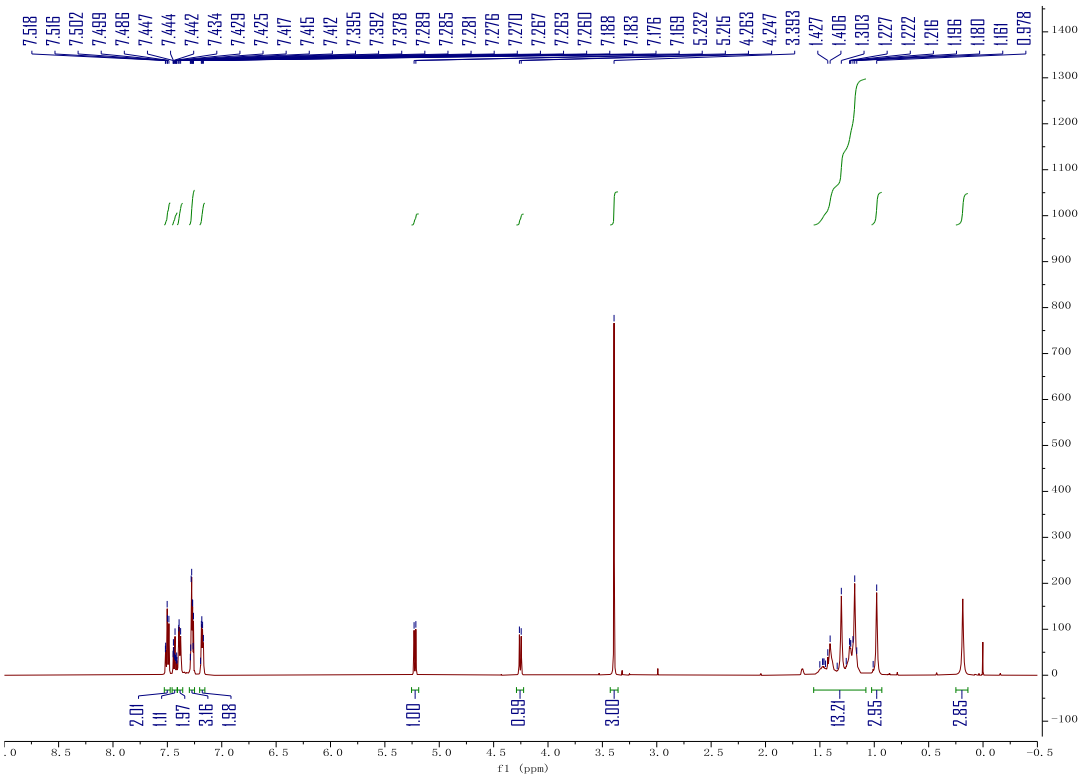
5s, ^{1}H NMR, 500 MHz, $CDCl_3$.



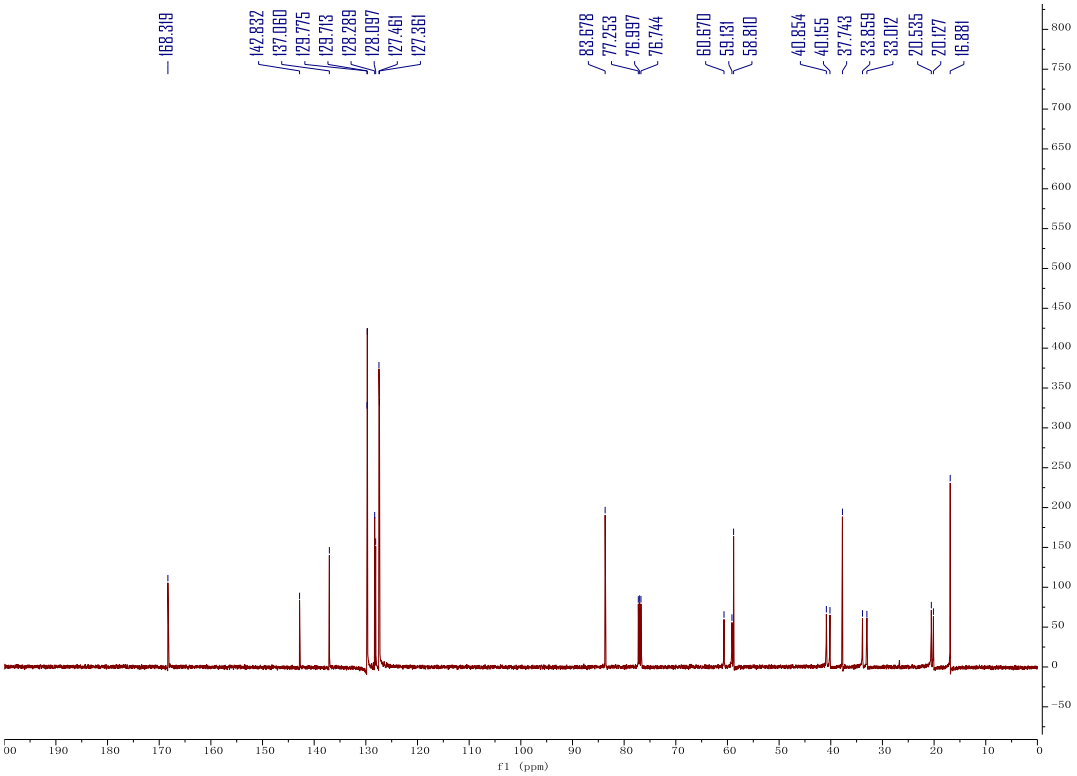
5t, ^{1}H NMR, 500 MHz, $CDCl_3$.



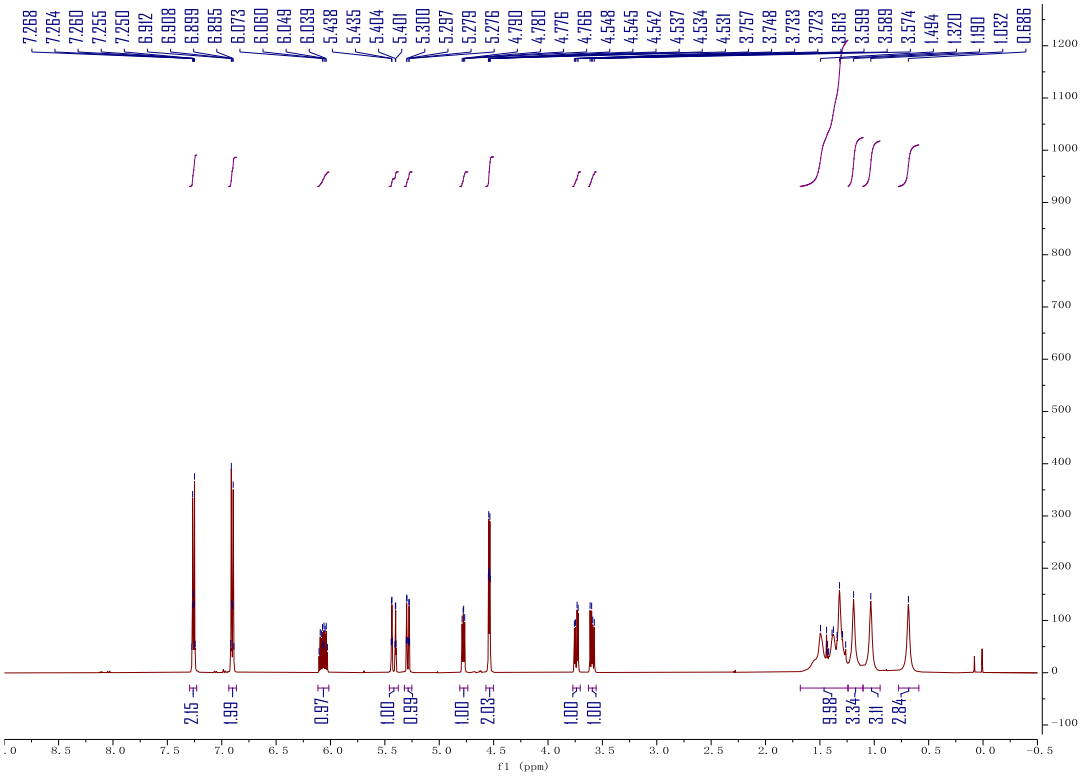
5u, ^{1}H NMR, 500 MHz, $CDCl_3$.



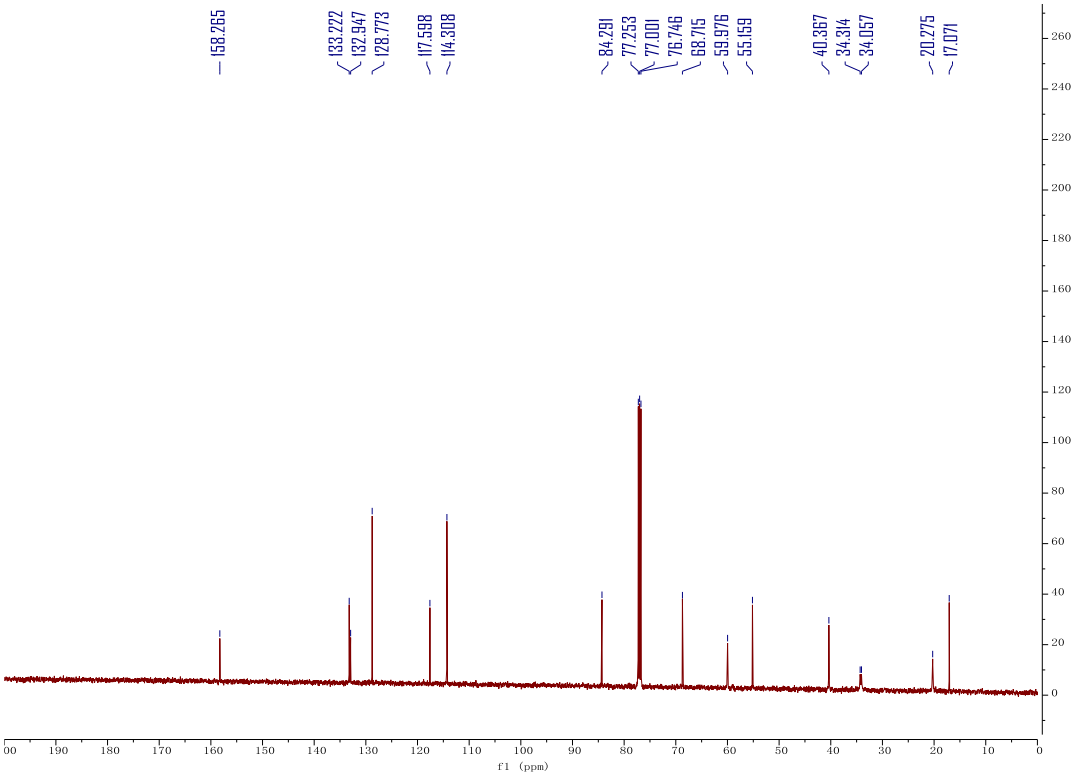
5u, ^{13}C NMR, 126 MHz, $CDCl_3$.

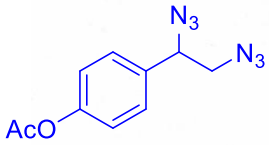


5v, ^{1}H NMR, 500 MHz, $CDCl_3$.



5v, ^{13}C NMR, 126 MHz, $CDCl_3$.





2i, HRMS

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename 20170417-9.d
Sample Name 9
User Name
Acquired Time 4/14/2017 11:15:06 AM
Instrument
Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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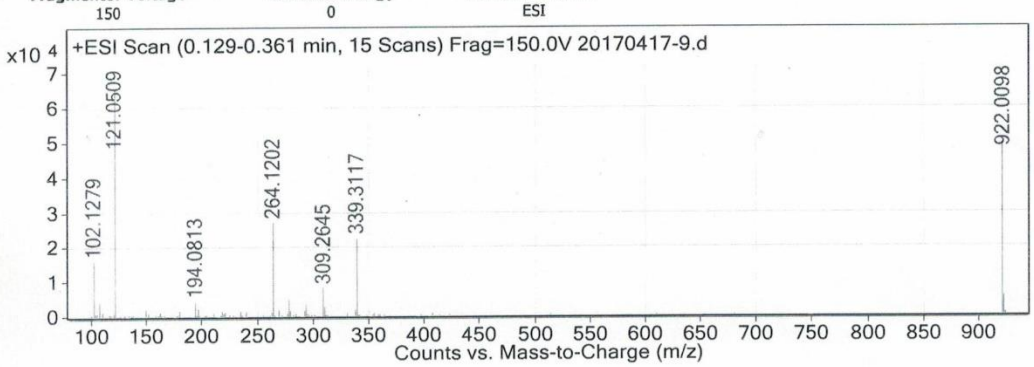


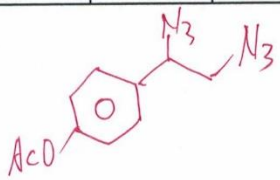
Peak List

m/z	z	Abund	Formula	Ion
102.1279		15860.1		
108.0574		4083		
121.0509		65950.6		
194.0813		4144		
264.1202		26867.7	C10 H14 N7 O2	(M+NH4)+
279.1589		4676.7		
309.2645		8031.2		
339.3117		22427.4		
922.0098	1	48965.5		
923.0122	1	5644.2		

Formula Calculator Results

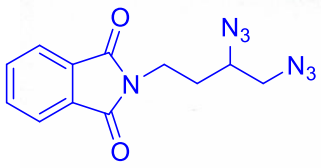
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 H14 N7 O2	264.1202	264.1203	0.66	88.91

--- End Of Report ---



Agilent Technologies Page 1 of 1 Printed at: 10:12 AM on: 4/17/2017

1



2t, HRMS

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	1APCI.d
Sample Name	1
User Name	
Acquired Time	2/23/2017 9:33:07 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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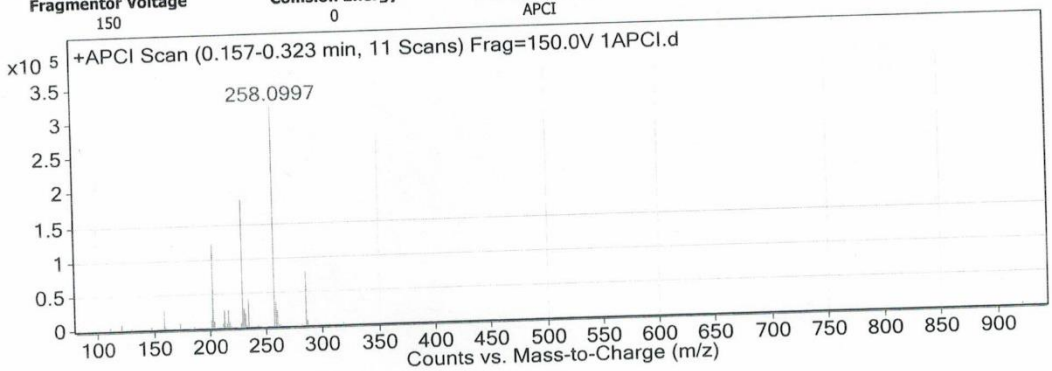


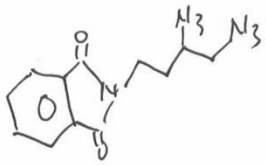
Peak List

m/z	z	Abund	Formula	Ion
160.0402		26790.3		
203.0825		125108		
213.0673		26141.2		
216.1143		25472.1		
230.0935	1	185025.3		
231.0885	1	26809.1		
234.1249		39479.1		
258.0997	1	319854.9		
259.1027	1	33914.6		
286.1059		78049.2	C12 H12 N7 O2	(M+H)+

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C12 H12 N7 O2	286.1059	286.1047	-4.2	70.99

--- End Of Report ---



Agilent Technologies Page 1 of 1 Printed at: 9:37 AM on: 2/23/2017

2

2x, HRMS

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : M170694

Sample Serial Number: 11

Operator : HUAQIN Date: 2017/04/17

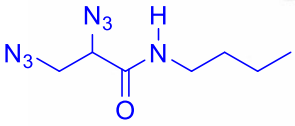
Operation Mode: DART Positive

Elemental composition search on mass 293.11

m/z= 288.11-298.11

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
293.1141	293.1145	-1.38	12.5	$C_{15}H_{13}ON_6$
	293.1132	3.18	7.5	$C_{14}H_{17}O_5N_2$

3



State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

2y, HRMS

Data Filename 5.d
Sample Name 5
User Name
Acquired Time 2/23/2017 9:04:00 AM
Instrument
Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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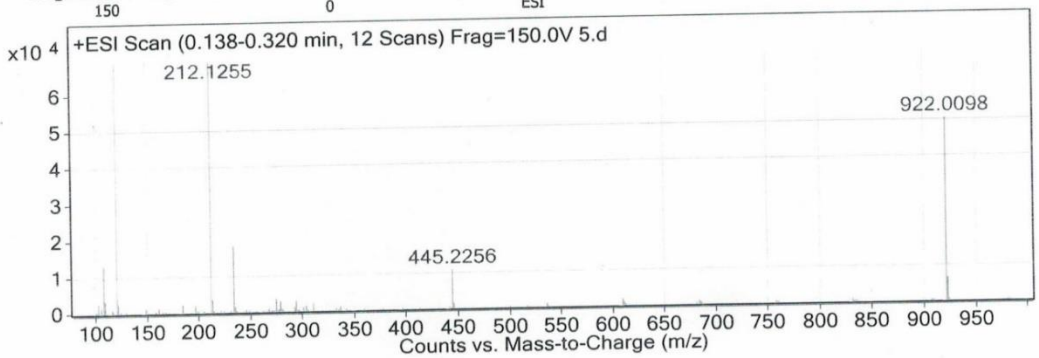


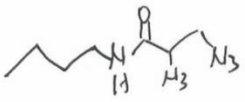
Peak List

m/z	z	Abund	Formula	Ion
108.0577		13018.2		
121.0509		74742.2		
212.1255		69080.2	C7 H14 N7 O	(M+H)+
234.1075		18137.7		
445.2256		10719		
922.0098	1	50191.3		
923.0124	1	6239.3		

Formula Calculator Results

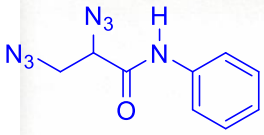
IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C7 H14 N7 O	212.1255	212.1254	-0.14	91.89

--- End Of Report ---



Agilent Technologies Page 1 of 1 Printed at: 4:25 PM on: 2/23/2017

4



State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

2z, HRMS

Data Filename	3.d
Sample Name	3
User Name	
Acquired Time	2/23/2017 8:59:11 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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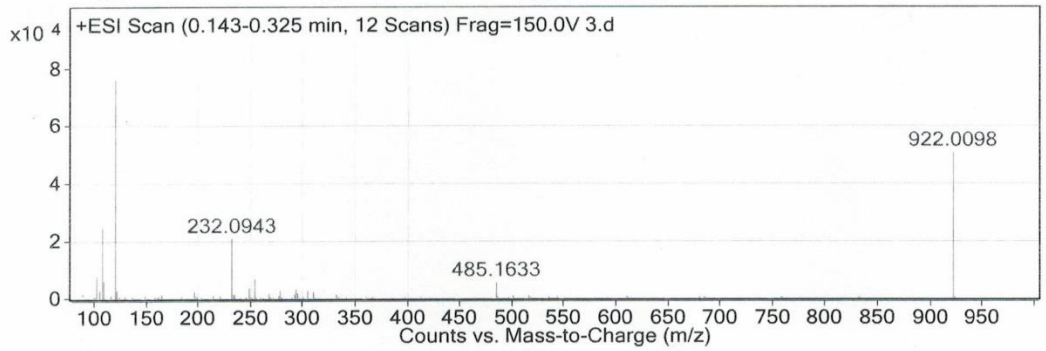


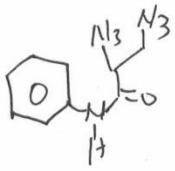
Peak List

m/z	z	Abund	Formula	Ion
102.128		7793.8		
108.0577		24955		
110.0548		6067.7		
121.0509		76051		
232.0943		20897.6	C9 H10 N7 O	(M+H)+
254.0764		6860.8		
485.1633		5583.4		
922.0098	1	50542.6		
923.0125	1	6266.9		

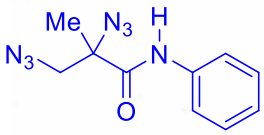
Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C9 H10 N7 O	232.0943	232.0941	-0.57	80.58

--- End Of Report ---



Agilent Technologies Page 1 of 1 Printed at: 4:25 PM on: 2/23/2017



State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

2aa, HRMS

Data Filename	2.d
Sample Name	2
User Name	
Acquired Time	2/23/2017 8:56:48 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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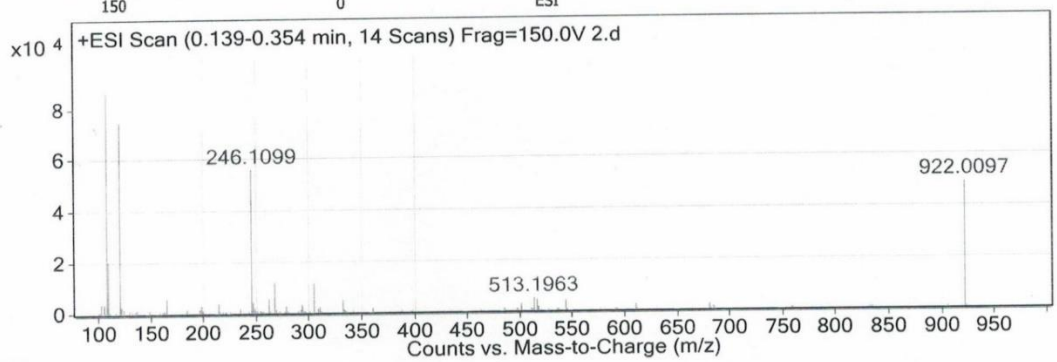


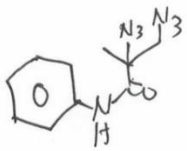
Peak List

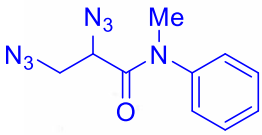
m/z	z	Abund	Formula	Ion
108.0576		86029.5		
108.08		6126		
110.0547		20690.4		
121.0509		74658.9		
165.1386		5790.2		
246.1099		55878.4	C10 H12 N7 O	(M+H)+
268.0911		11617.9		
304.2999		11161.8		
922.0097	1	49044.1		
923.0123	1	6061.8		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 H12 N7 O	246.1099	246.1098	-0.32	89.77

--- End Of Report ---





State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

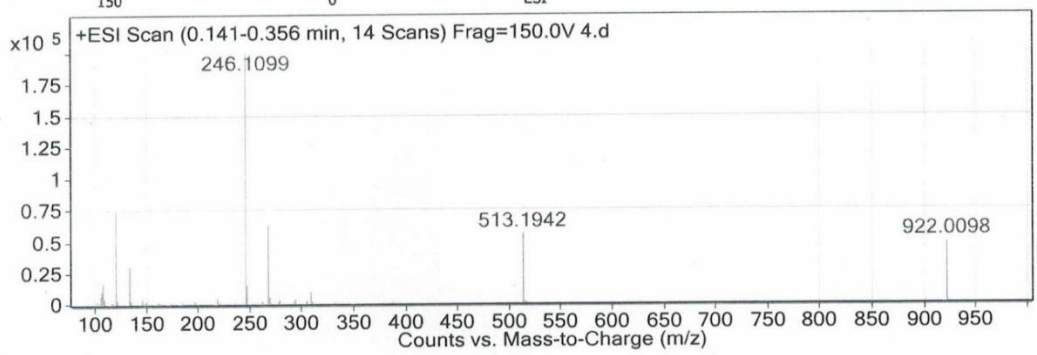
2ab, HRMS

Data Filename	4.d
Sample Name	4
User Name	
Acquired Time	2/23/2017 9:01:36 AM

Instrument
Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



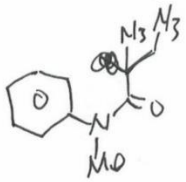
Peak List

m/z	z	Abund	Formula	Ion
106.0653		10536.3		
108.0577		16824.1		
121.0509		73858		
134.0601		30316.6		
246.1099	1	200135.9	C10 H12 N7 O	(M+H)+
247.1125	1	15681.4	C10 H12 N7 O	(M+H)+
268.0919		62554.3		
513.1942	1	55731.6		
514.1968	1	10071.3		
922.0098		48687.8		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 H12 N7 O	246.1099	246.1098	-0.4	90.78

--- End Of Report ---



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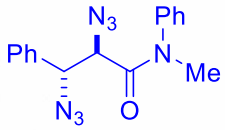


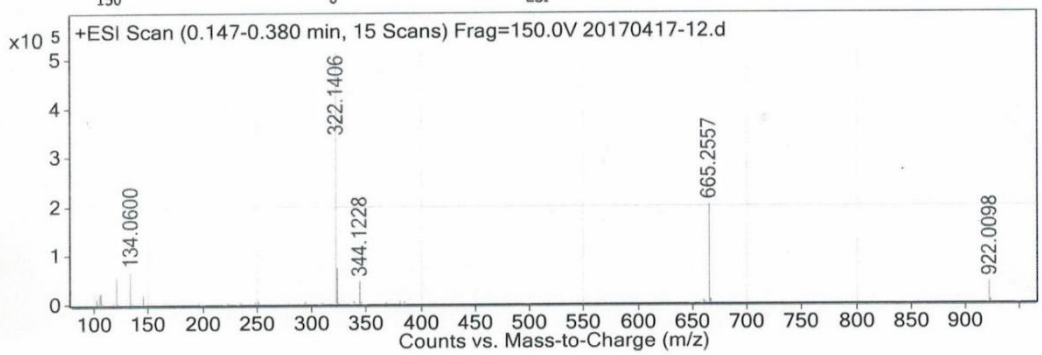
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

2ac, HRMS

Data Filename 20170417-12.d
Sample Name 12
User Name
Acquired Time 4/14/2017 11:22:09 AM
Instrument
Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



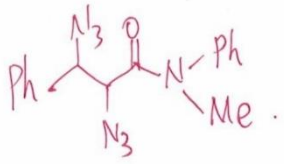
Peak List

m/z	z	Abund	Formula	Ion
121.0509		58324.9		
134.06		67922.3		
322.1406	1	517168.6	C16 H16 N7 O	(M+H)+
323.1435	1	73608.4	C16 H16 N7 O	(M+H)+
344.1228		46830.3		
665.2557	1	202896.5		
666.2587	1	64614.1		
922.0098		42948.5		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C16 H16 N7 O	322.1406	322.1411	1.49	91.46

--- End Of Report ---



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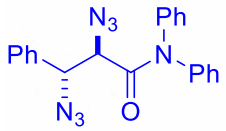


2ad, HRMS

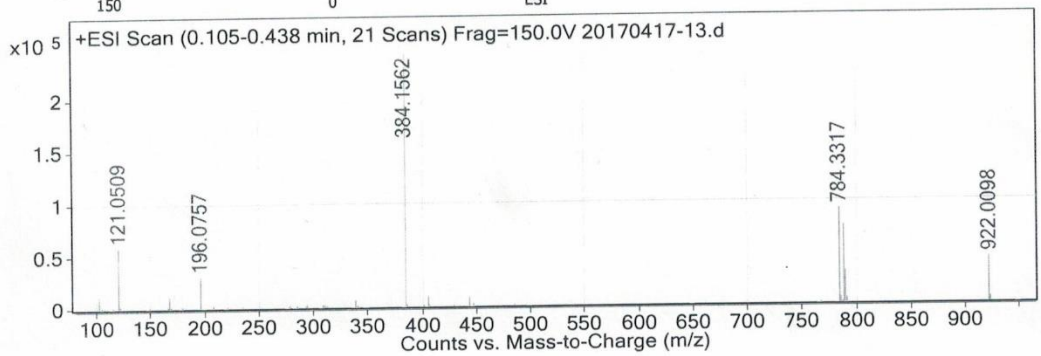
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	20170417-13.d
Sample Name	13
User Name	
Acquired Time	4/14/2017 11:24:32 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



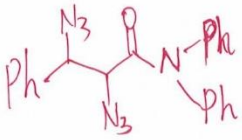
Peak List

m/z	z	Abund	Formula	Ion
121.0509		58747.1		
196.0757		30207		
384.1562	1	243006	C21 H18 N7 O	(M+H)+
385.1592	1	43046.1	C21 H18 N7 O	(M+H)+
784.3317	1	91008.6		
785.3349	1	38547.6		
789.2873	1	75501.5		
790.2905	1	31854.9		
922.0098		43845.5		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C21 H18 N7 O	384.1562	384.1567	1.5	88.34

--- End Of Report ---



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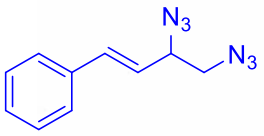


2ae, HRMS

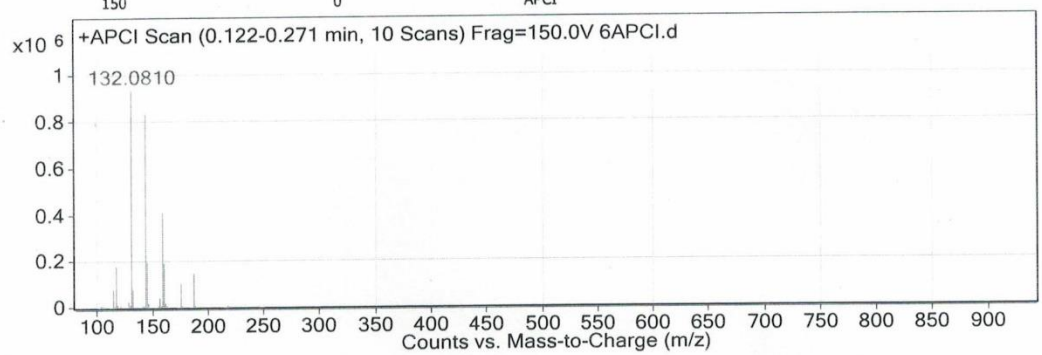
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	6APCI.d
Sample Name	6
User Name	
Acquired Time	2/23/2017 9:58:16 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	APCI



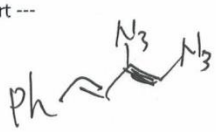
Peak List

m/z	z	Abund	Formula	Ion
115.0546		79231.2		
118.0656	1	179016.5		
132.081	1	936074.7		
144.081	1	835236.6		
145.0842	1	77811.3		
146.0966		198709.7		
159.0919		409573.7		
161.1076		188020.5		
176.1074		100123.9		
187.0981		146560.7	C10 H11 N4	(M+H)+

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C10 H11 N4	187.0981	187.0978	-1.37	87.14

--- End Of Report ---



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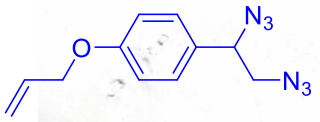


2af, HRMS

National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : M170692

Sample Serial Number: 8

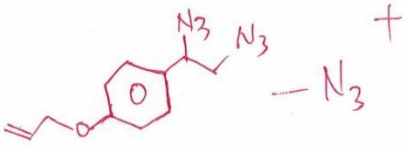
Operator : HUAQIN Date: 2017/04/17

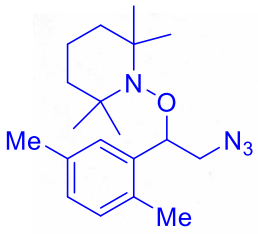
Operation Mode: DART Positive

Elemental composition search on mass 202.10

m/z= 197.10-207.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
202.0974	202.0975	-0.59	7.5	$C_{11}H_{12}ON_3$





5d, HRMS

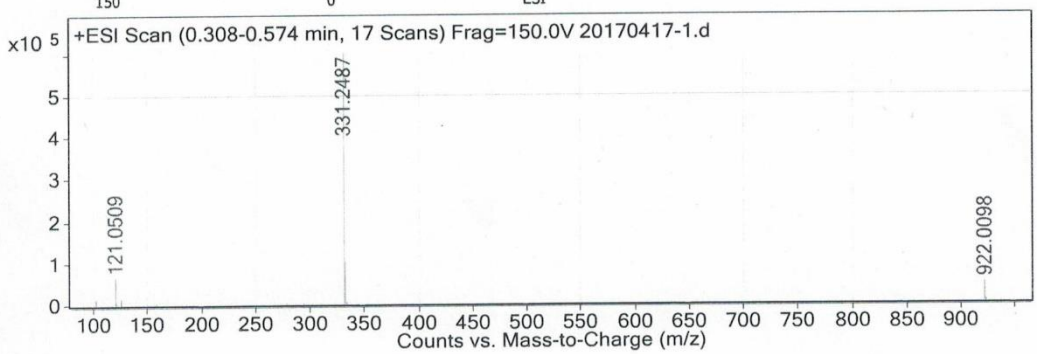
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	20170417-1.d
Sample Name	1
User Name	
Acquired Time	4/14/2017 10:56:08 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
121.0509		63994.6		
331.2487	1	602894.5	C19 H31 N4 O	(M+H)+
332.2519	1	102558.9	C19 H31 N4 O	(M+H)+
922.0098		47681.6		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C19 H31 N4 O	331.2487	331.2492	1.69	92.79

--- End Of Report ---

Agilent Technologies Page 1 of 1 Printed at: 10:12 AM on: 4/17/2017

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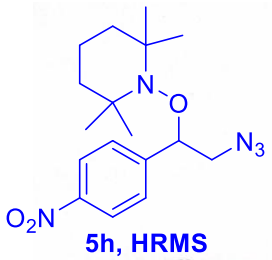


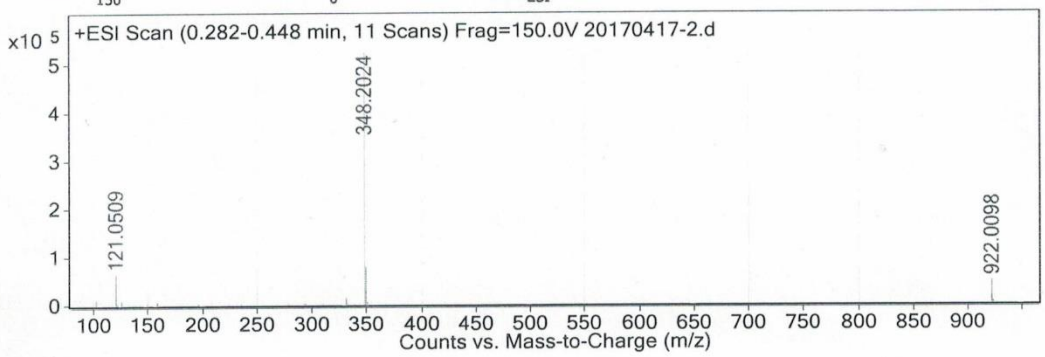
5h, HRMS

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename 20170417-2.d
Sample Name 2
User Name
Acquired Time 4/14/2017 10:58:28 AM
Instrument
Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



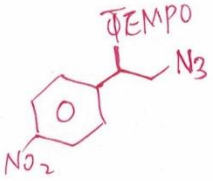
Peak List

m/z	z	Abund	Formula	Ion
121.0509		64356		
348.2024	1	527737.1	C17 H26 N5 O3	(M+H)+
349.2055	1	79932	C17 H26 N5 O3	(M+H)+
922.0098		48065.5		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C17 H26 N5 O3	348.2024	348.203	1.71	92.16

--- End Of Report ---



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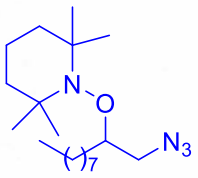


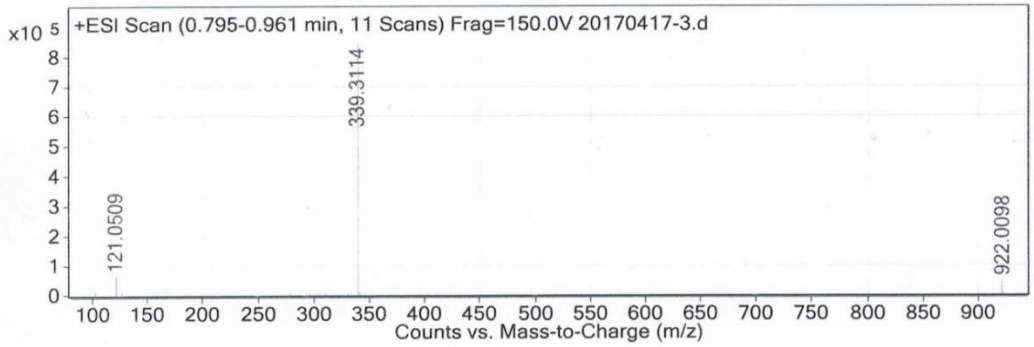
5p, HRMS

State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename 20170417-3.d
Sample Name 3
User Name
Acquired Time 4/14/2017 11:00:49 AM
Instrument
Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
121.0509		63675.5		
339.3114	1	845520.4	C19 H39 N4 O	(M+H)+
340.3146	1	145696.4	C19 H39 N4 O	(M+H)+
922.0098		47088.1		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C19 H39 N4 O	339.3114	339.3118	1.43	93.33

--- End Of Report ---

Agilent Technologies Page 1 of 1 Printed at: 10:12 AM on: 4/17/2017

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5q, HRMS

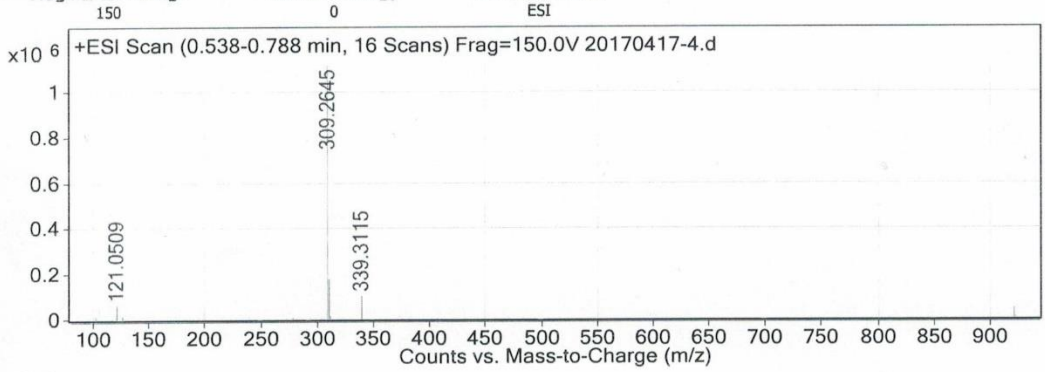
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	20170417-4.d
Sample Name	4
User Name	
Acquired Time	4/14/2017 11:03:10 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



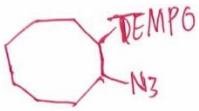
Peak List

m/z	z	Abund	Formula	Ion
121.0509		61677.3		
309.2645	1	1116477.8	C17 H33 N4 O	(M+H)+
310.2676	1	180788	C17 H33 N4 O	(M+H)+
339.3115		103784.7		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C17 H33 N4 O	309.2645	309.2649	1.4	95.39

--- End Of Report ---



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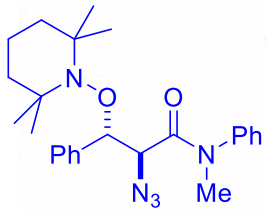


5u, HRMS

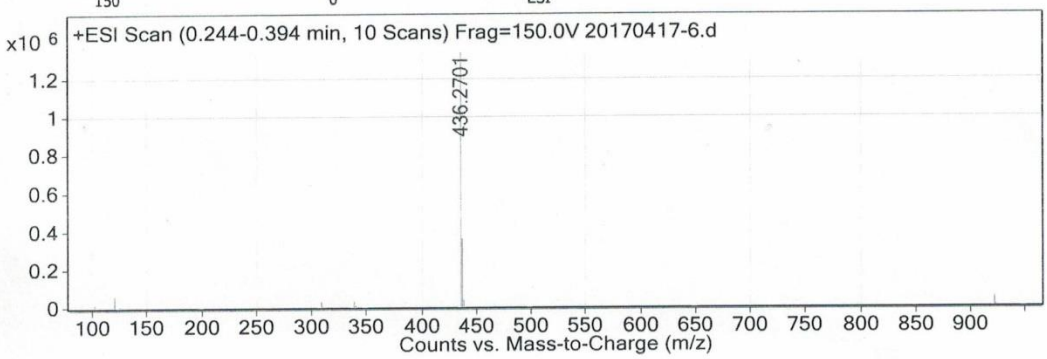
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	20170417-6.d
Sample Name	6
User Name	
Acquired Time	4/14/2017 11:07:58 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



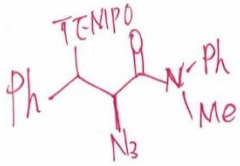
Peak List

m/z	z	Abund	Formula	Ion
436.2701	1	1337633.3	C25 H34 N5 O2	(M+H)+
437.2732	1	356145.8	C25 H34 N5 O2	(M+H)+

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C25 H34 N5 O2	436.2701	436.2707	1.42	97.37
C22 H36 N4 O5	436.2701	436.268	-4.74	89.69
C27 H36 N2 O3	436.2701	436.272	4.51	88.53

--- End Of Report ---



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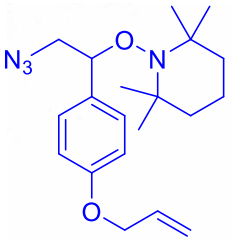


5v, HRMS

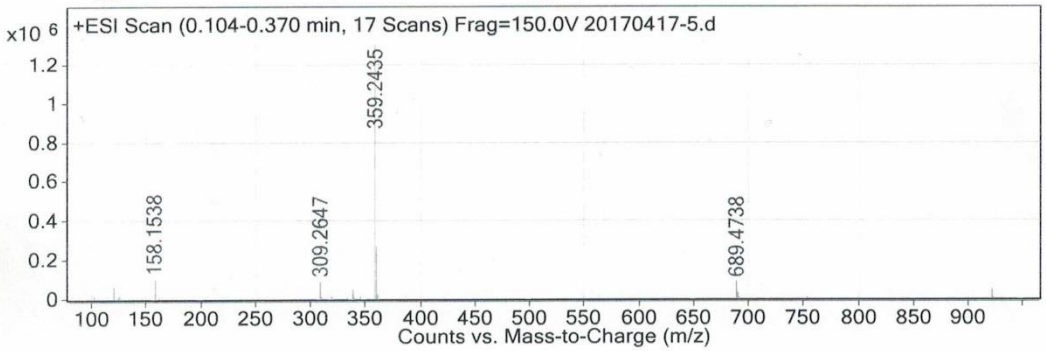
State Key Laboratory of Organometallic Chemistry
Shanghai Institute of Organic Chemistry
Chinese Academy of Sciences
ESI High Resolution MS Date Report

Data Filename	20170417-5.d
Sample Name	5
User Name	
Acquired Time	4/14/2017 11:05:36 AM
Instrument	

Agilent Technologies 6224 TOF LC/MS

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
150	0	ESI



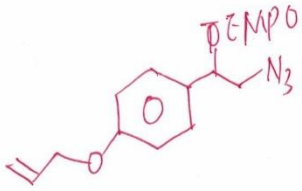
Peak List

m/z	z	Abund	Formula	Ion
158.1538		100874		
309.2647		88228.6		
359.2435	1	1299719.9	C20 H31 N4 O2	(M+H)+
360.2466	1	269034.6	C20 H31 N4 O2	(M+H)+
689.4738		84379.9		

Formula Calculator Results

IonFormula	Measured Mass	Tgt Mass	Diff (ppm)	Score
C20 H31 N4 O2	359.2435	359.2442	1.78	96.95

--- End Of Report ---



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