Supporting Information

Highly Enantioselective Asymmetric Alkynylation of Aldehydes Catalyzed by a New Oxazolidine-Titanium Complex

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Copy of HRMS, ^{1}H, ^{13}C NMR and IR Spectra for Ligands

Figure-1 : HRMS spectrum of ligand **2a**

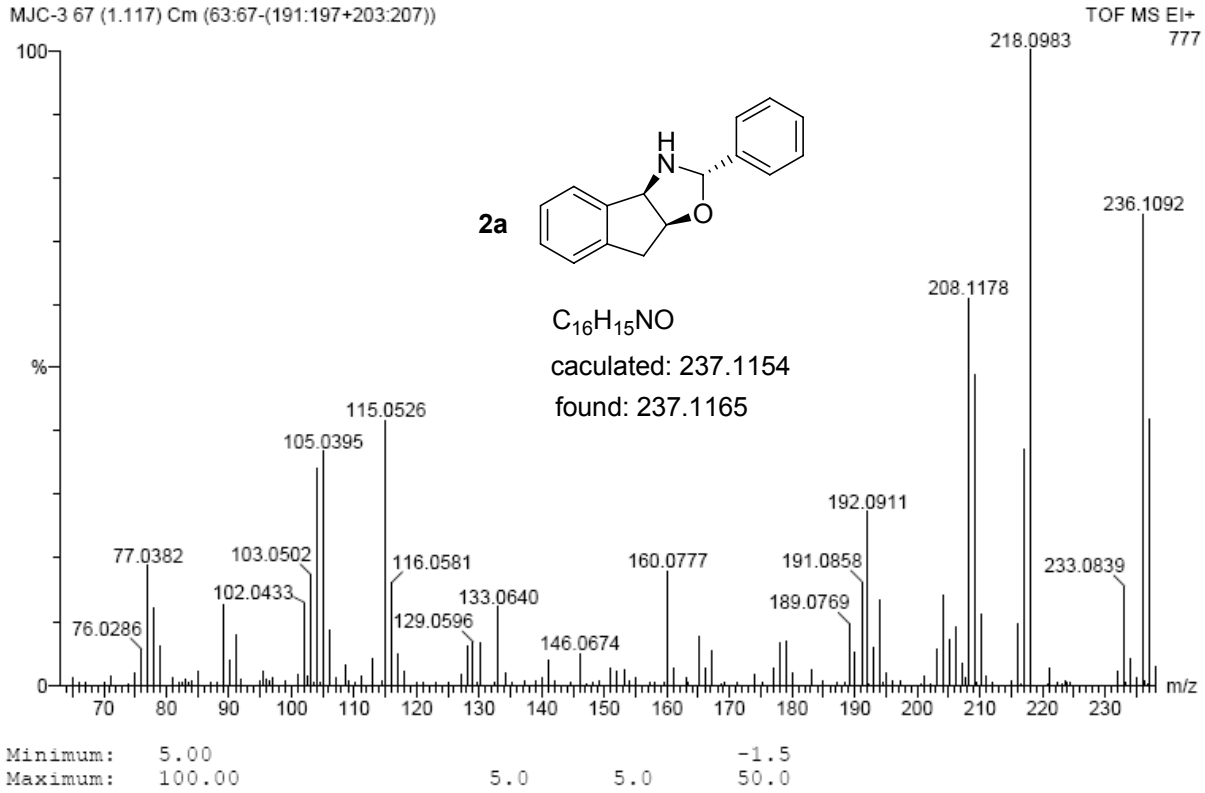


Figure-2 : HRMS spectrum of ligand **2b**

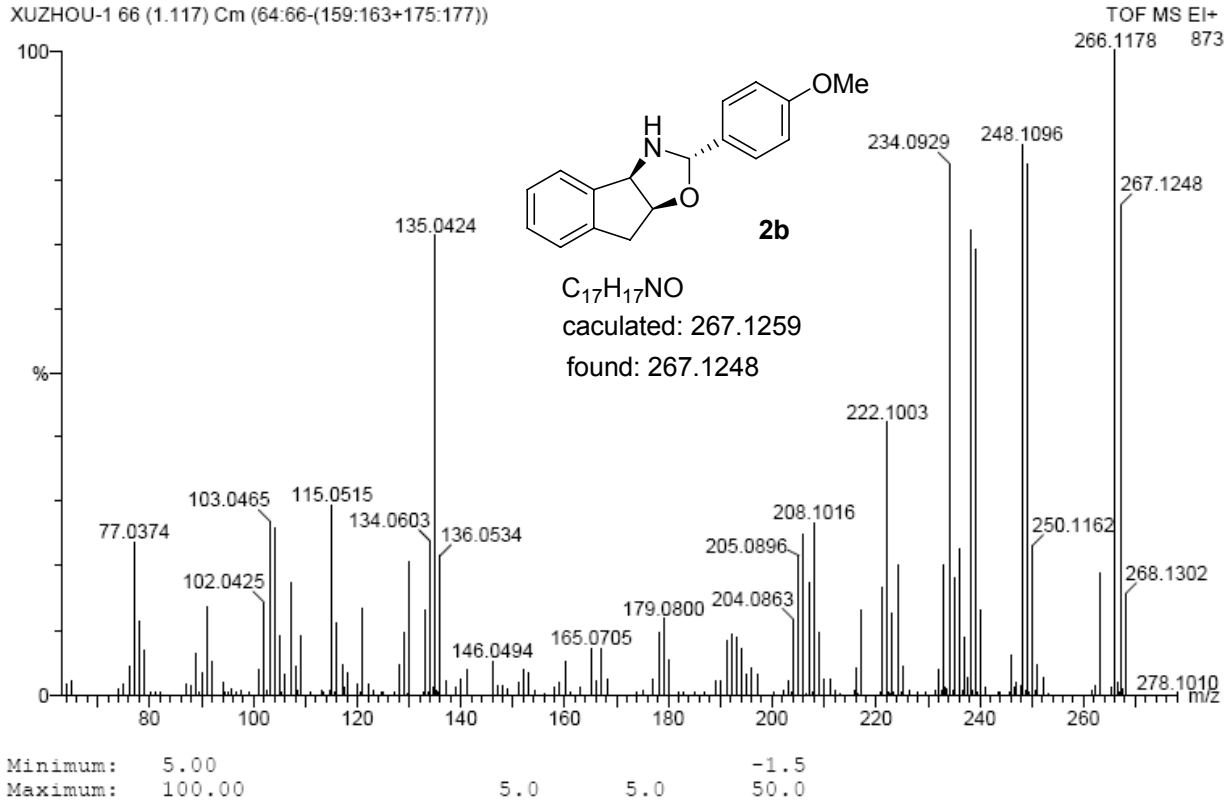


Figure-3 : HRMS spectrum of ligand **2c**

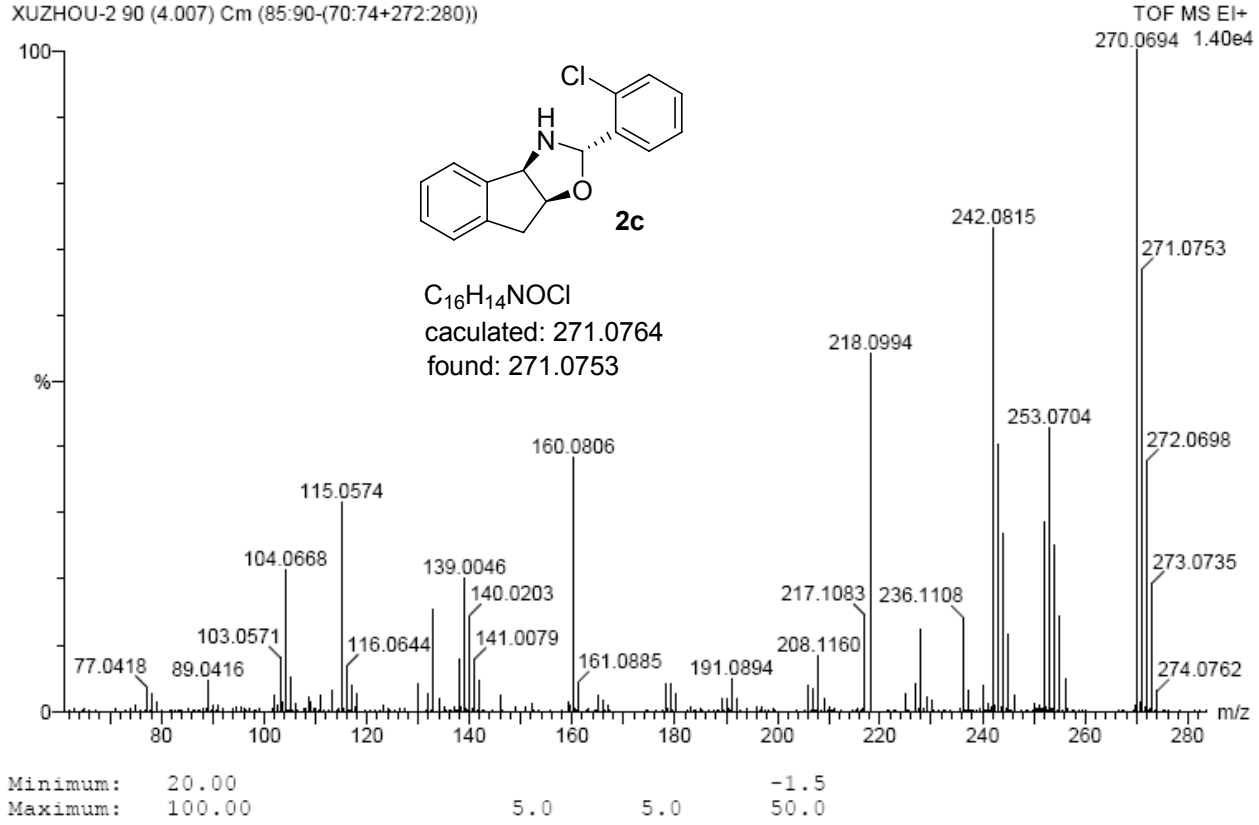


Figure-4 : HRMS spectrum of ligand 2**d**

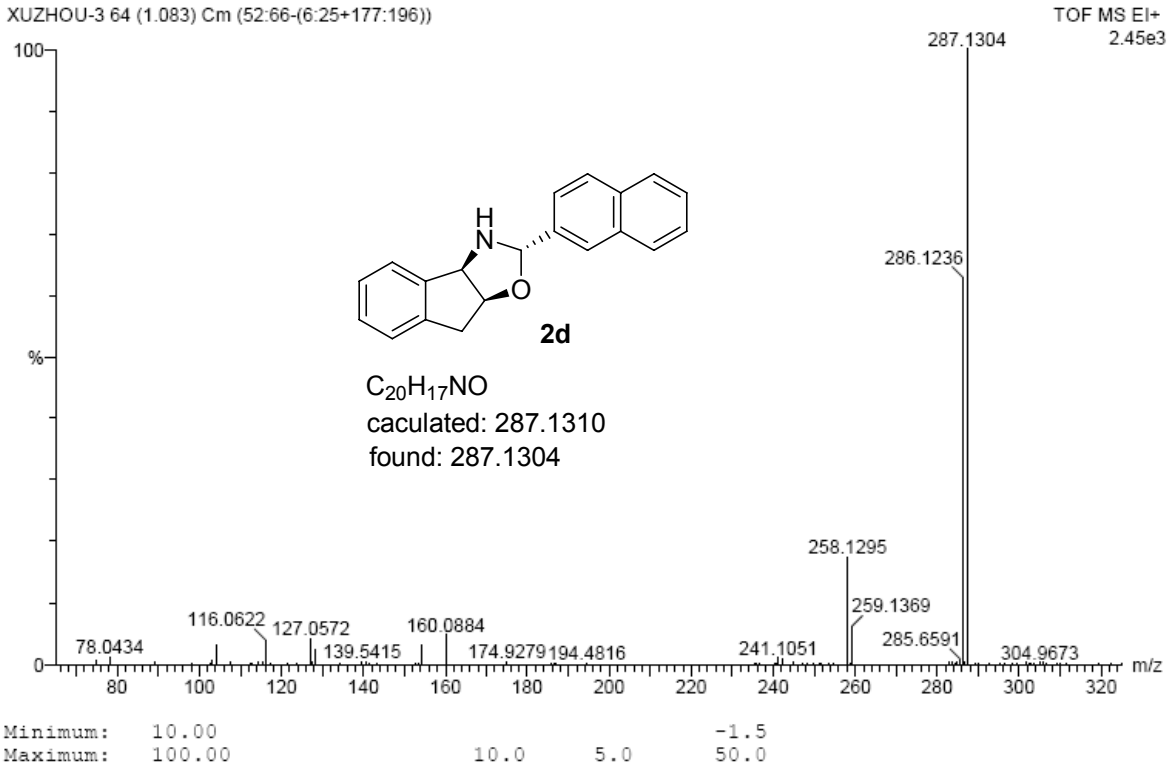


Figure-5 : ^{1}H NMR spectra of ligand **2a**

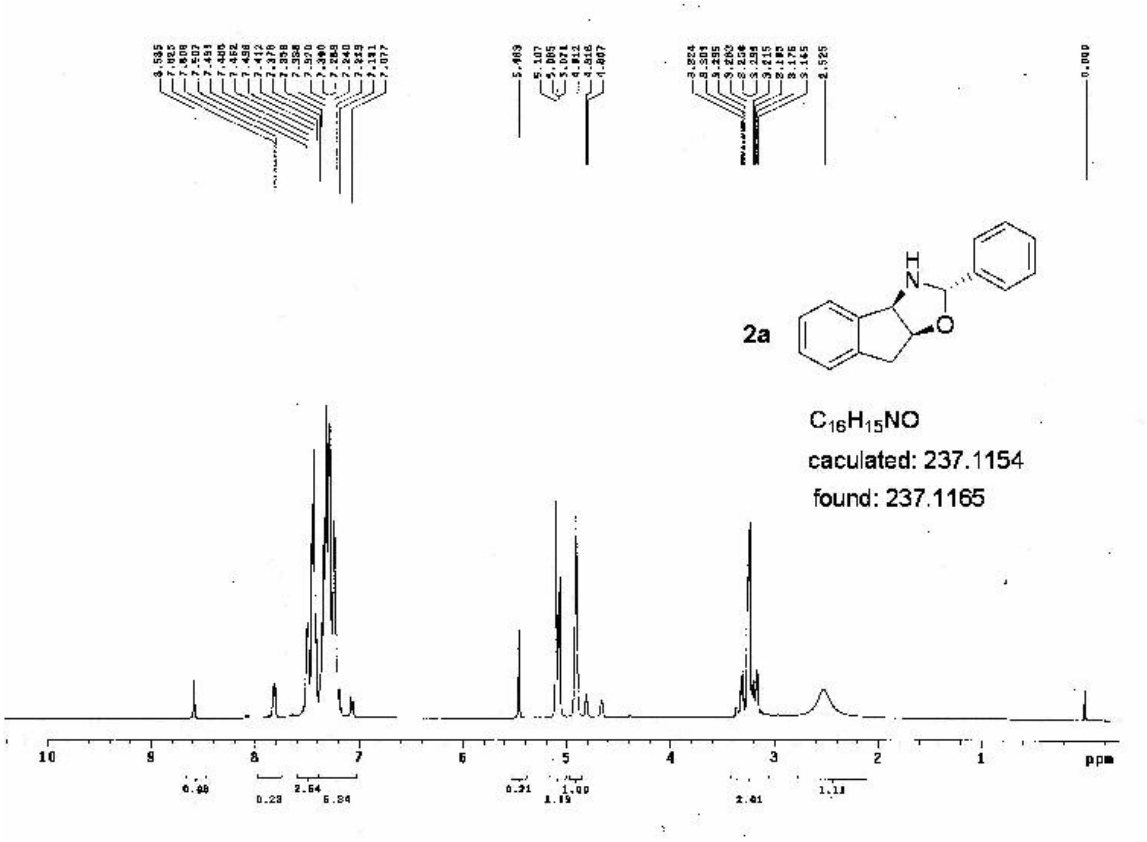


Figure-6 : ^{1}H NMR spectra of ligand **2b**

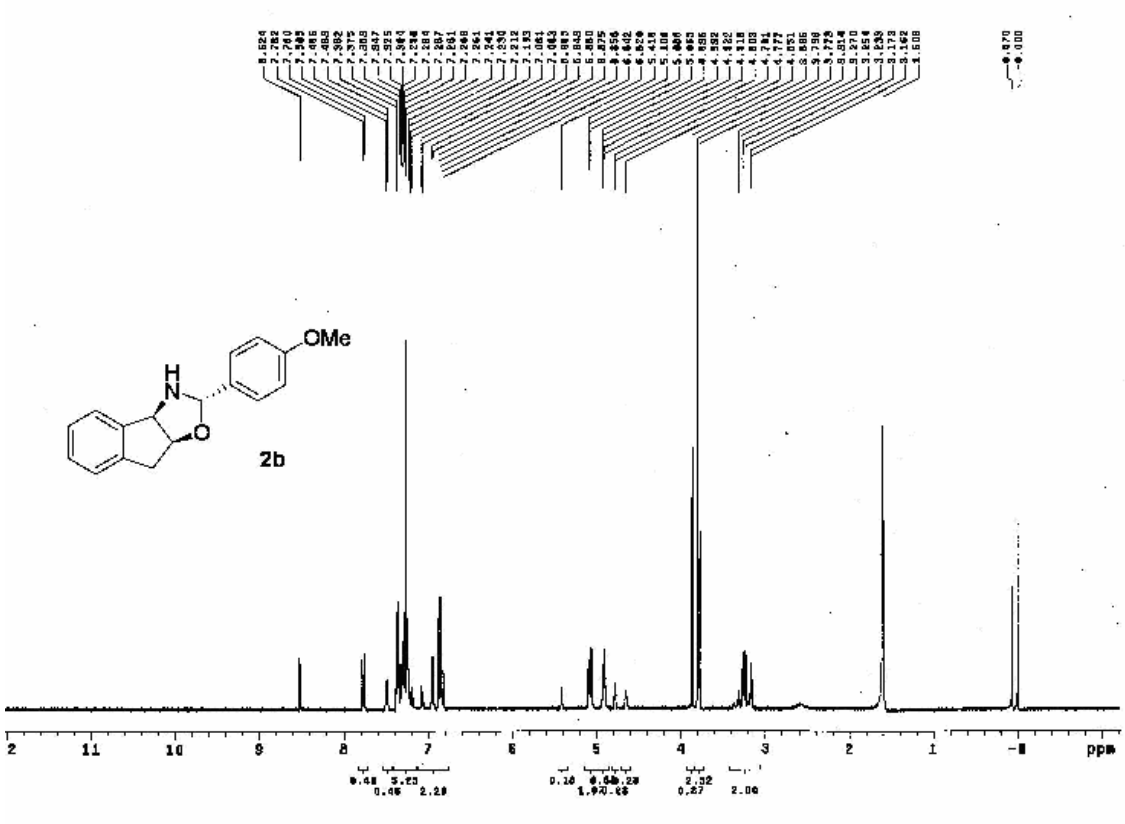


Figure-7 : ^{1}H NMR spectra of ligand **2c**

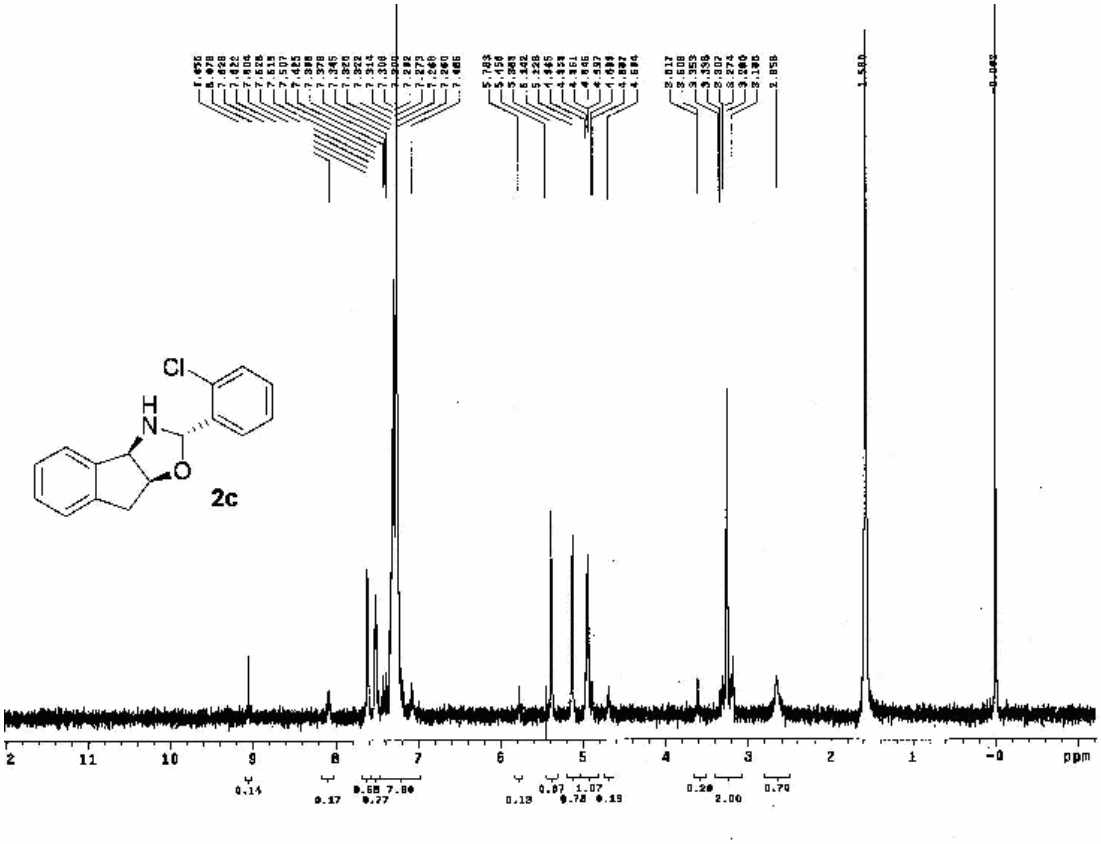


Figure-8 : ^{1}H NMR spectra of ligand **2d**

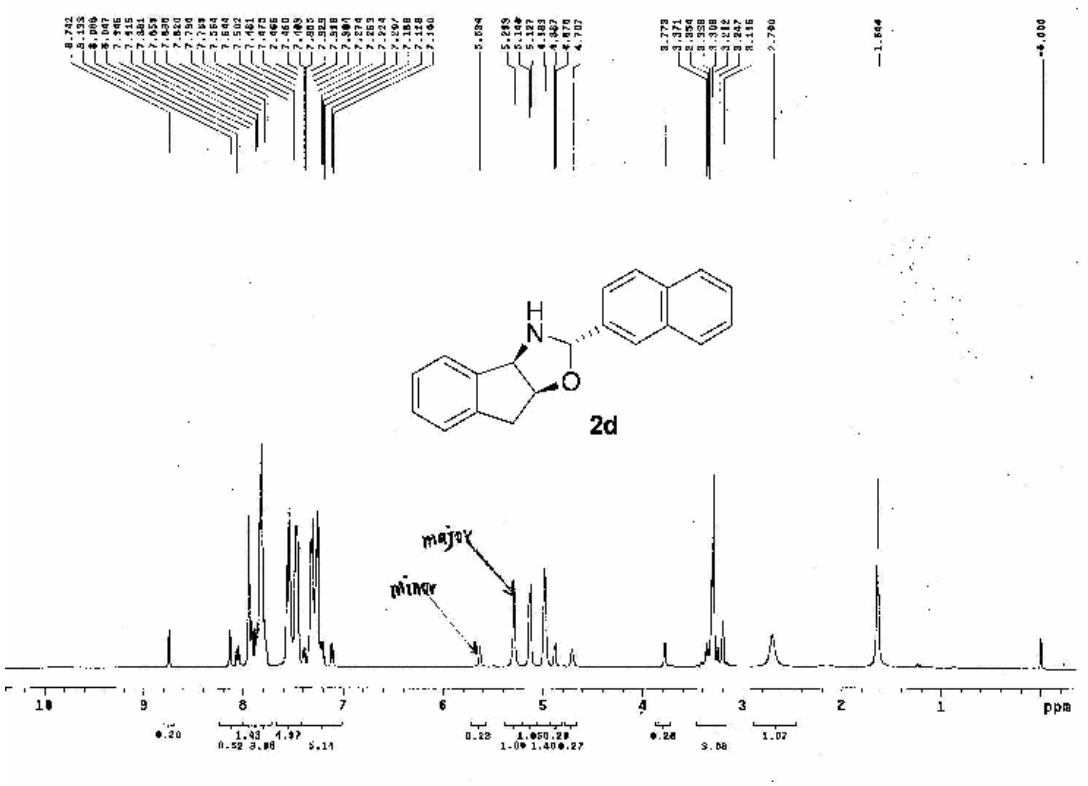


Figure-9 : ^{13}C NMR NMR spectra of ligand **2a**

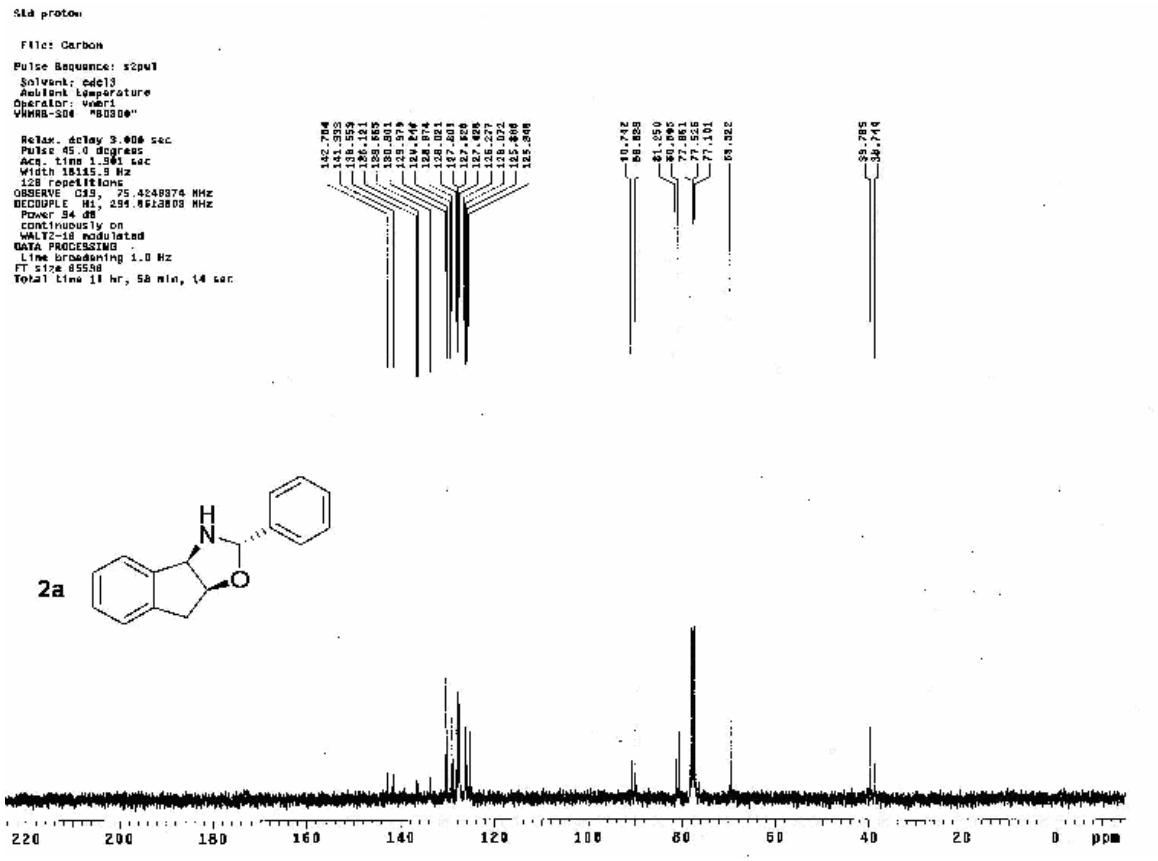


Figure-10 : ^{13}C NMR NMR spectra of ligand **2b**

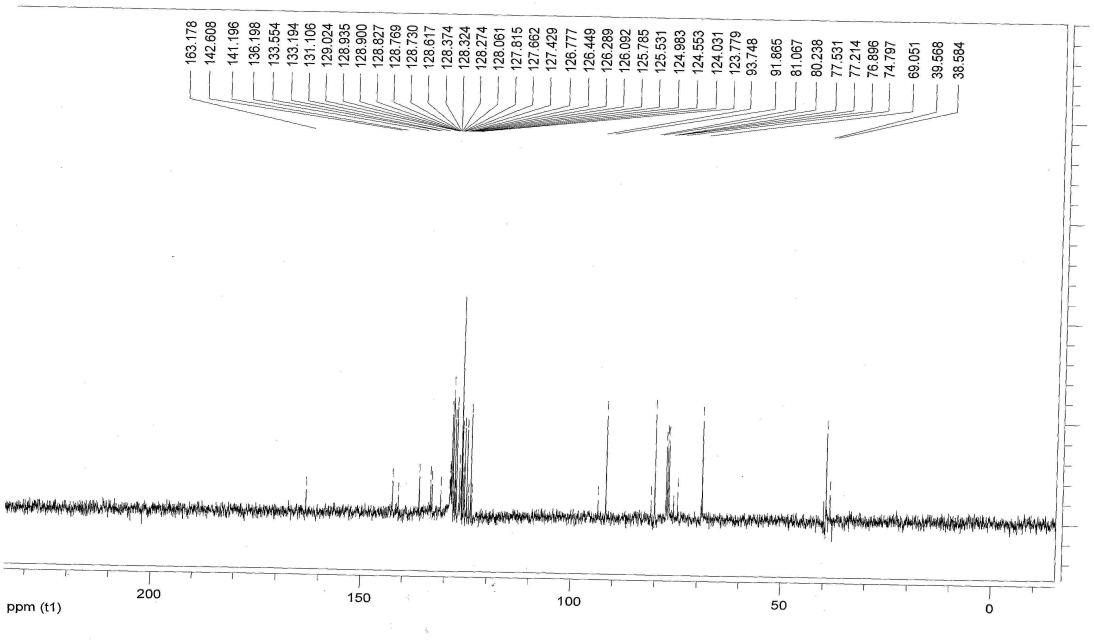


Figure-11 : ^{13}C NMR NMR spectra of ligand **2c**

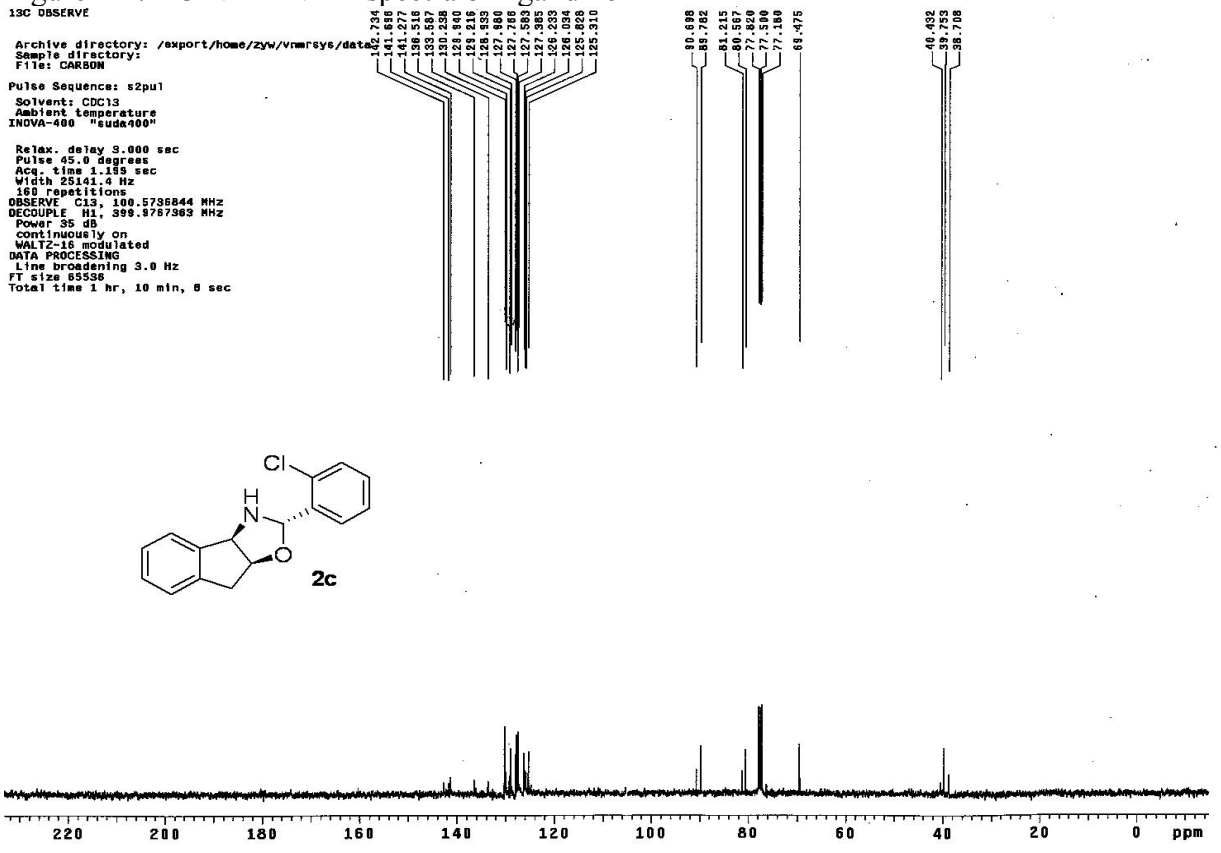


Figure-12 : ^{13}C NMR NMR spectra of ligand **2d**

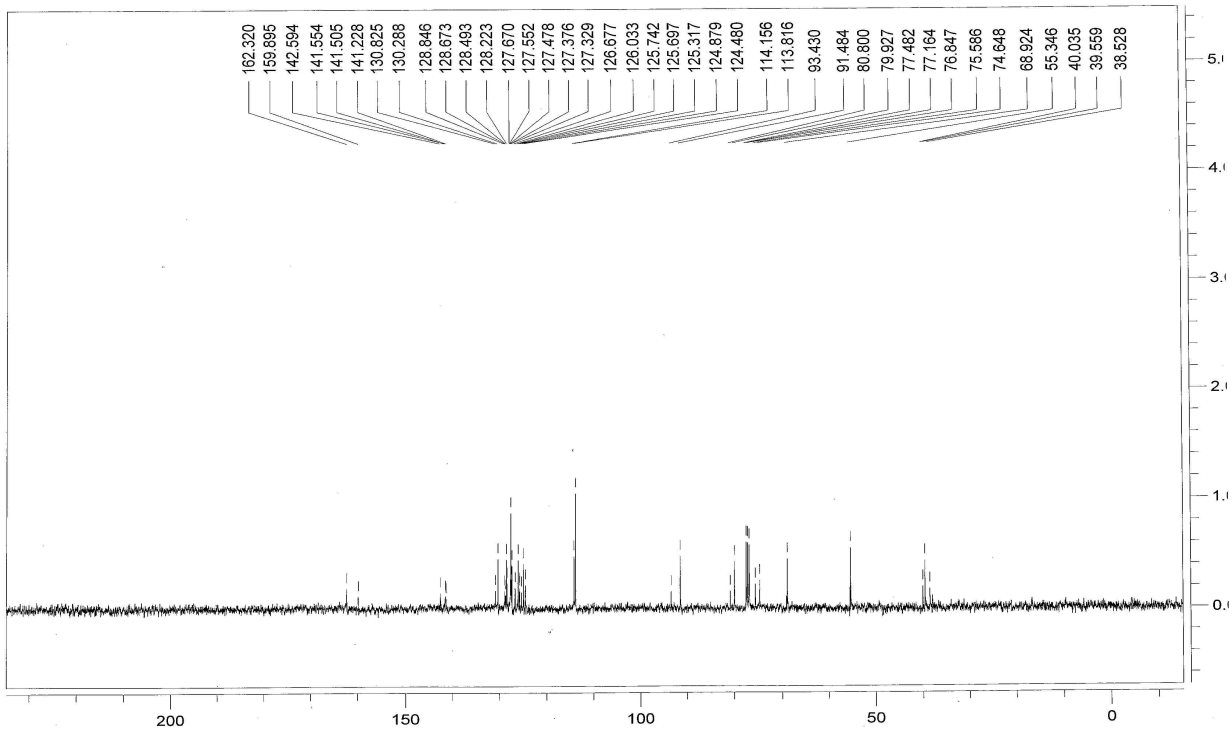


Figure-13: IR spectra of ligand **2a**

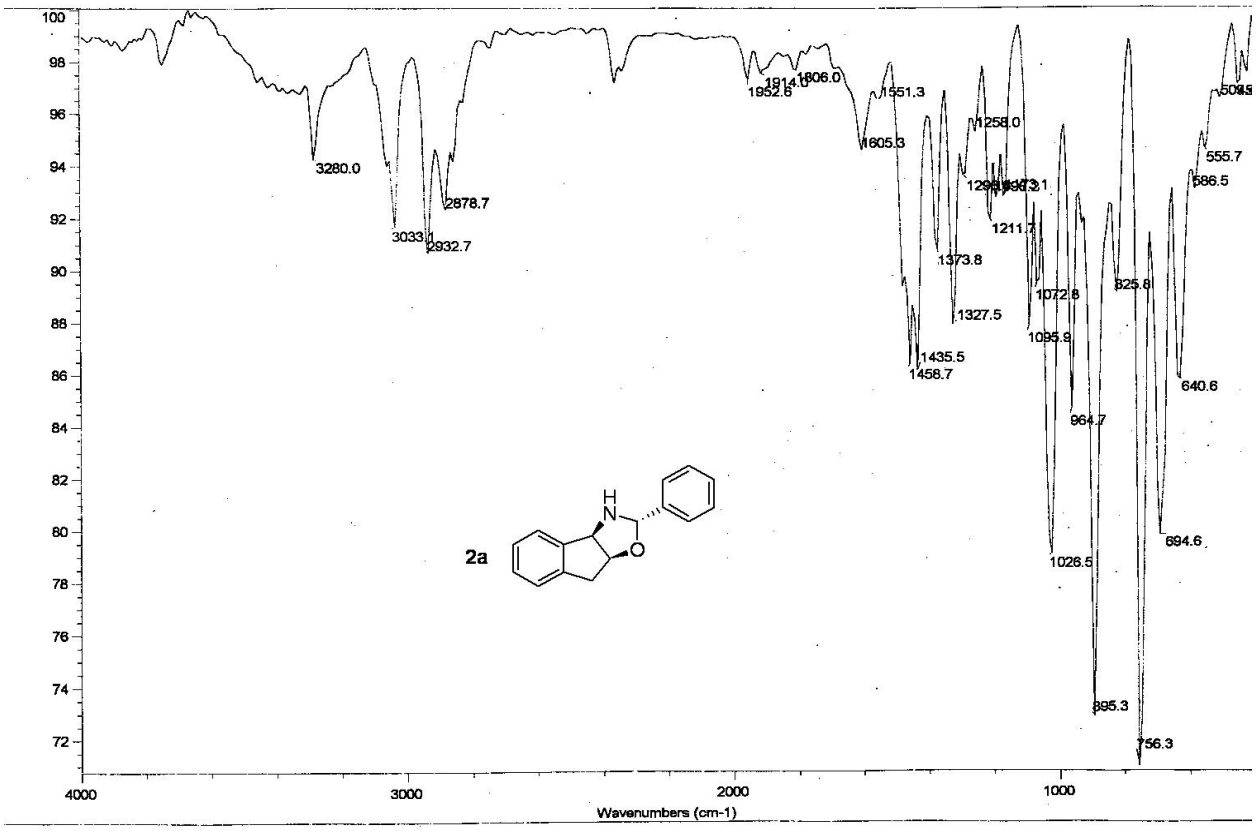


Figure-14: IR spectra of ligand **2b**

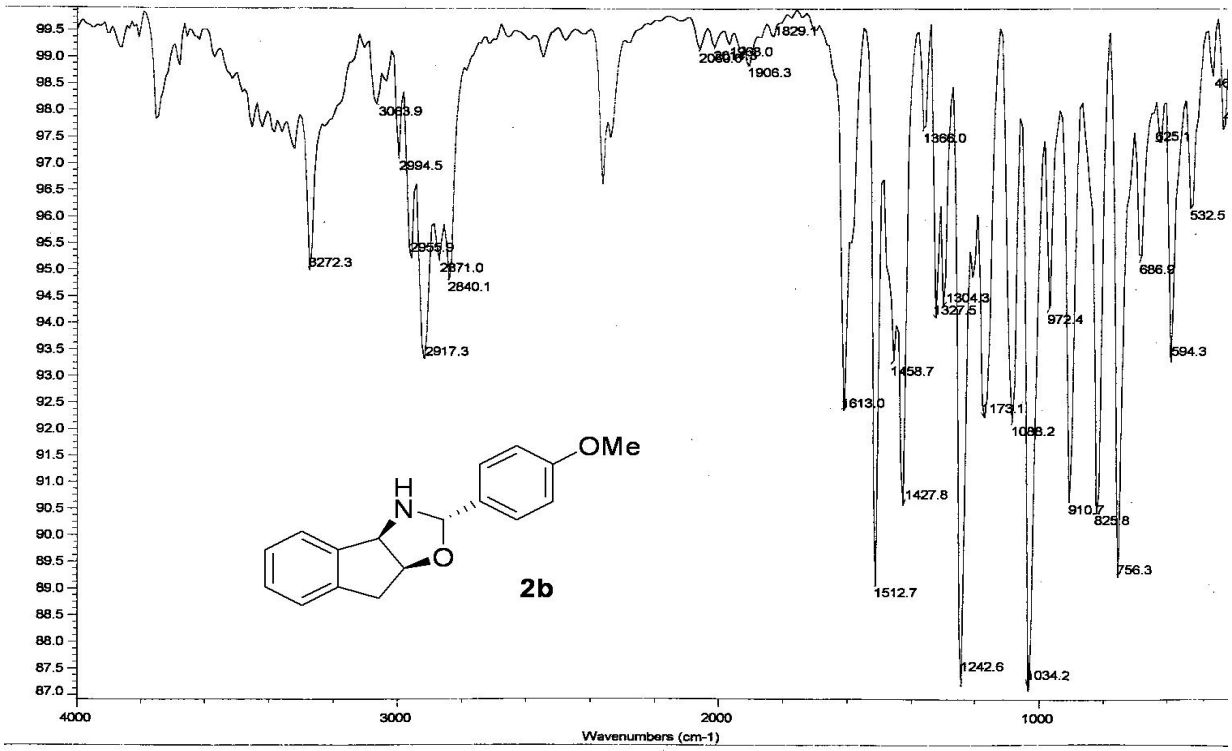


Figure-15: IR spectra of ligand **2c**

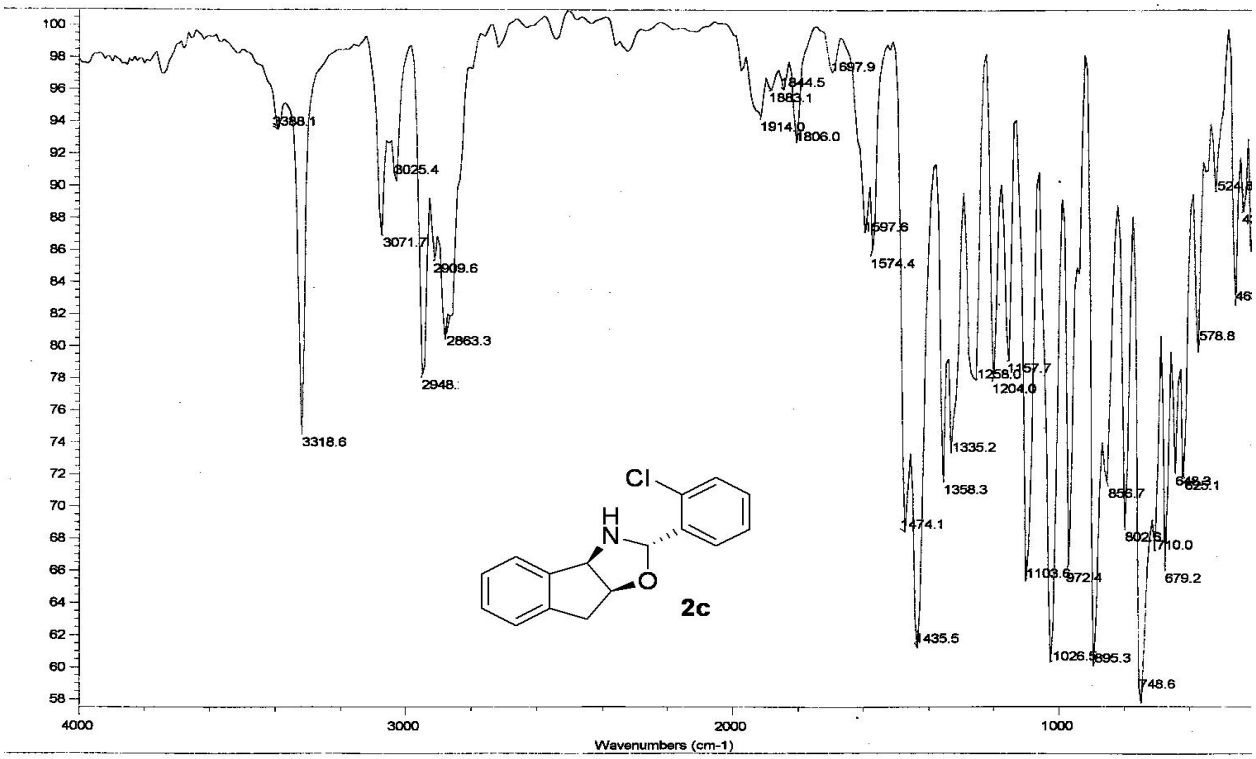
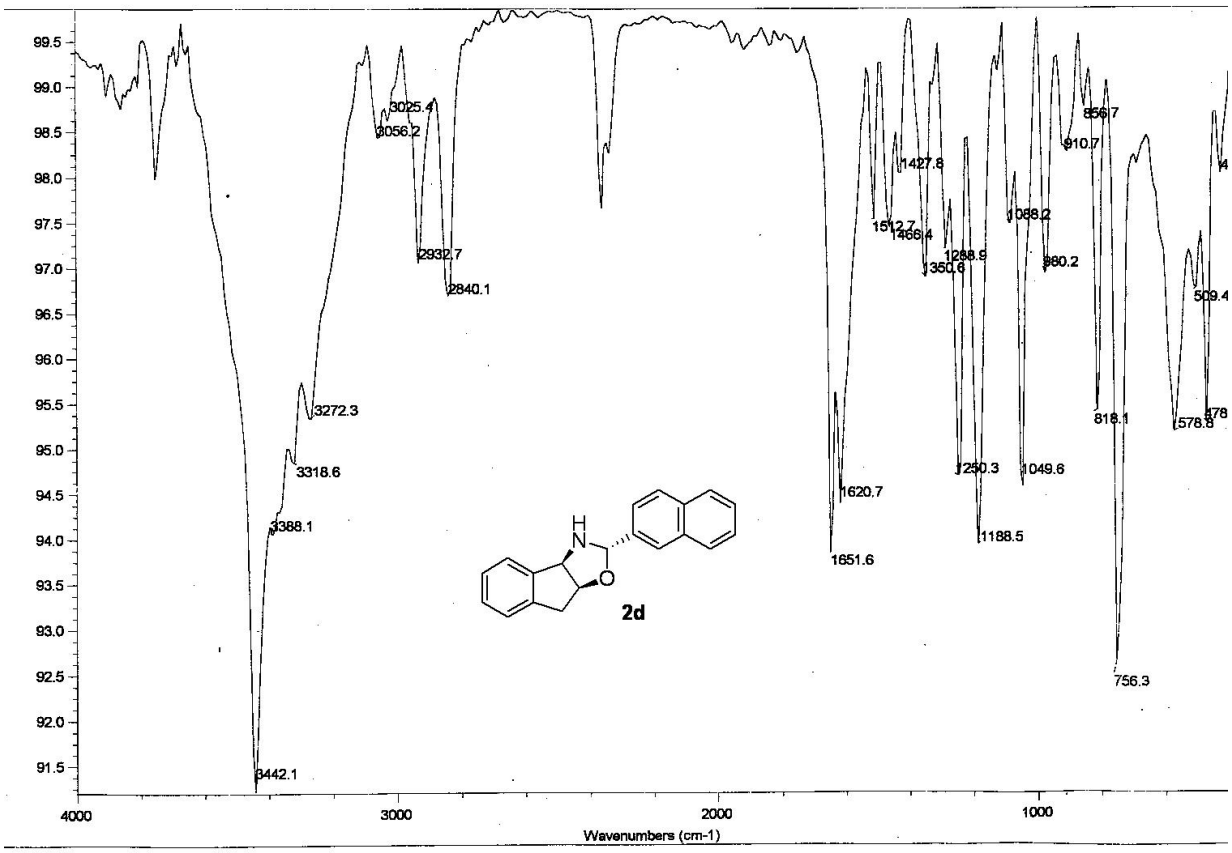
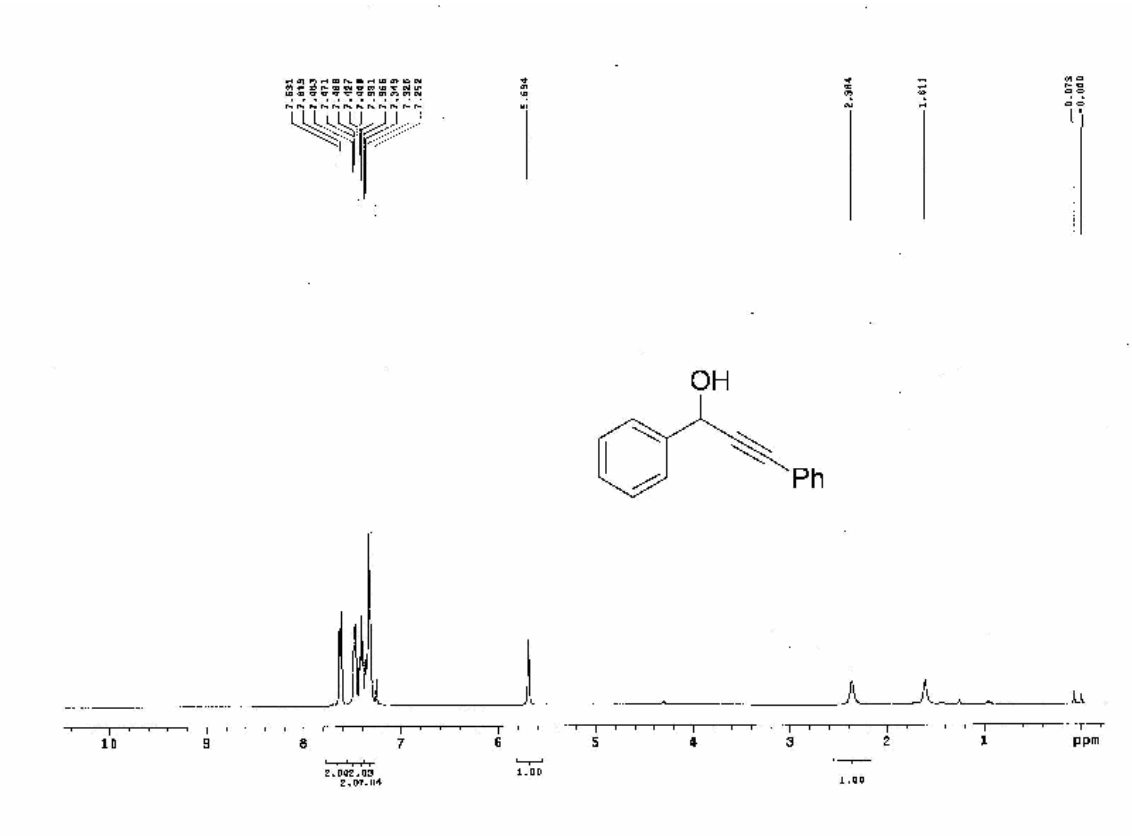
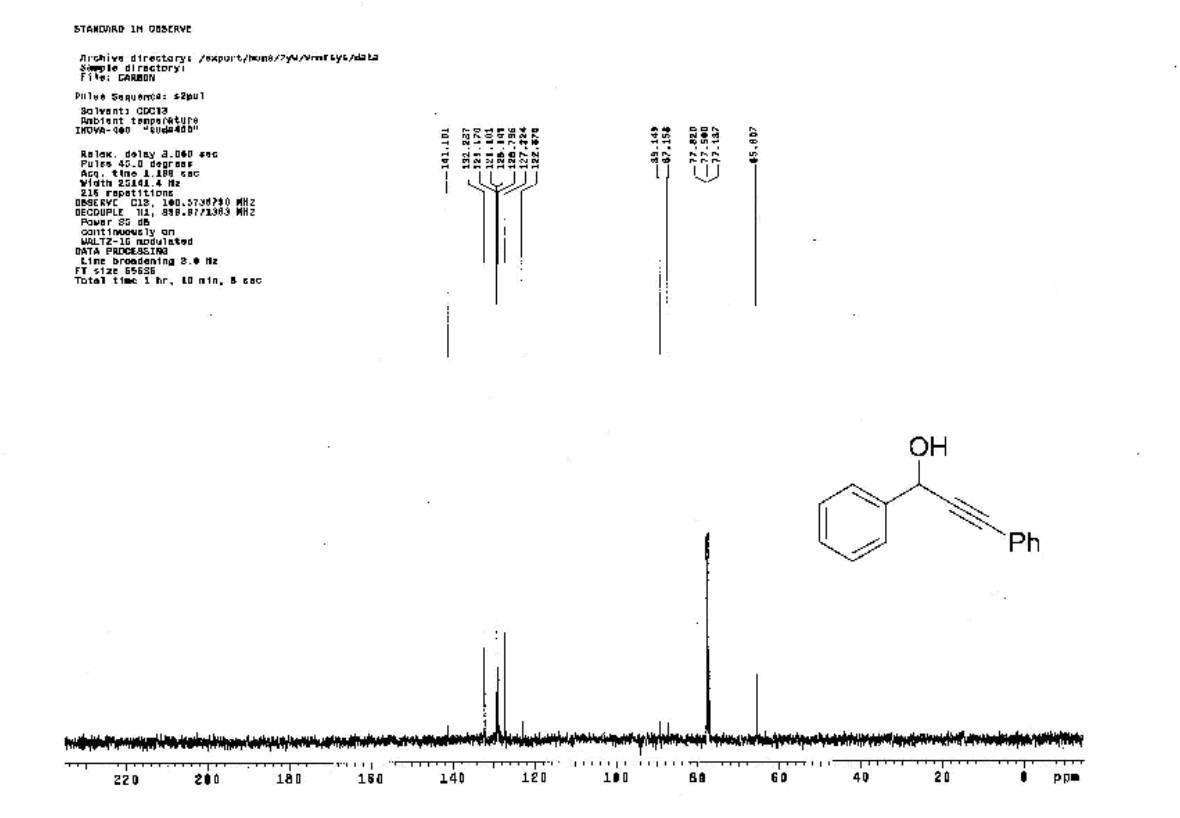


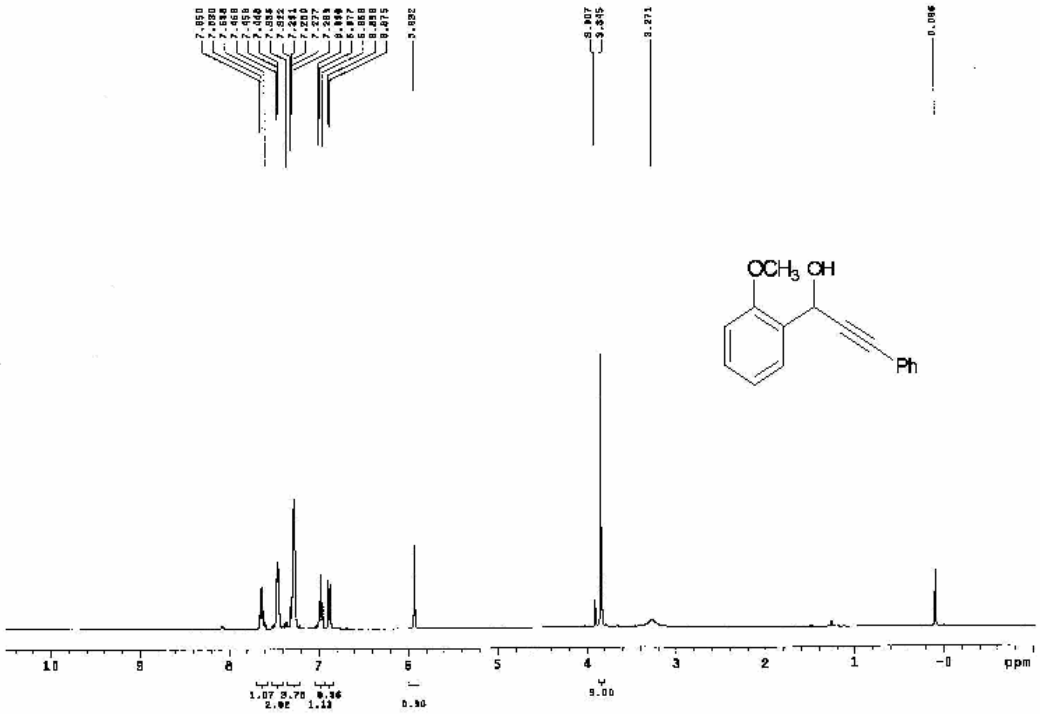
Figure-16: IR spectra of ligand **2d**



Copies of ^{1}H, ^{13}C NMR for Products



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Ph
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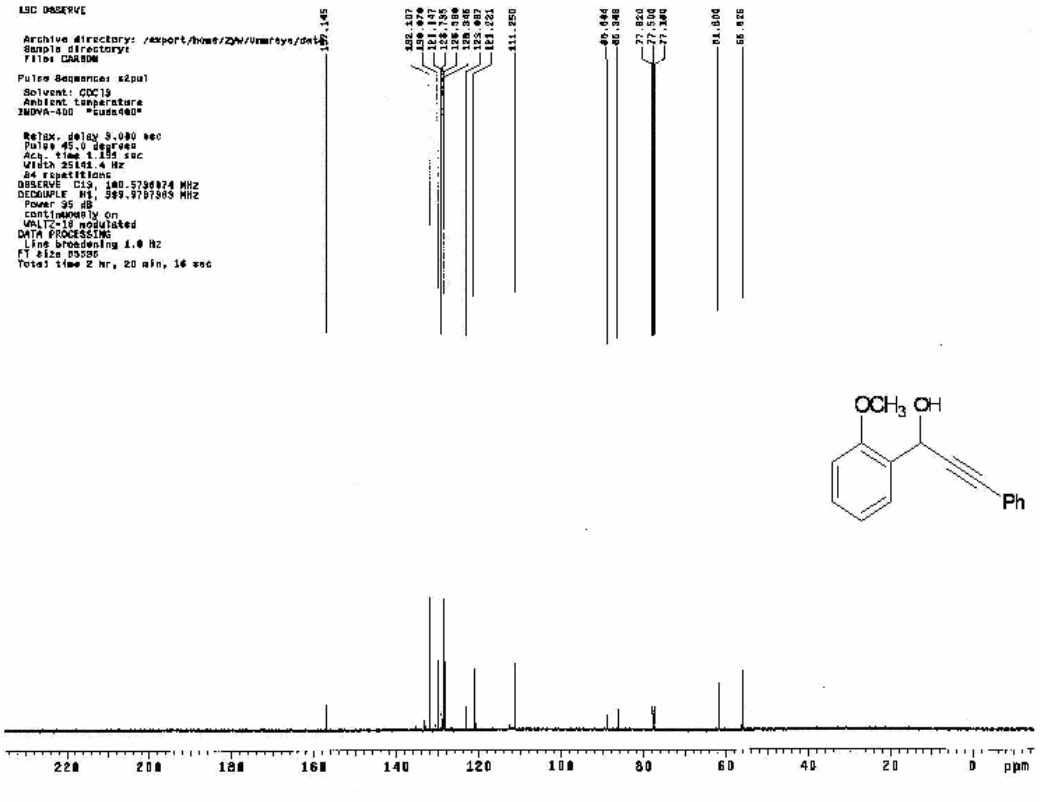
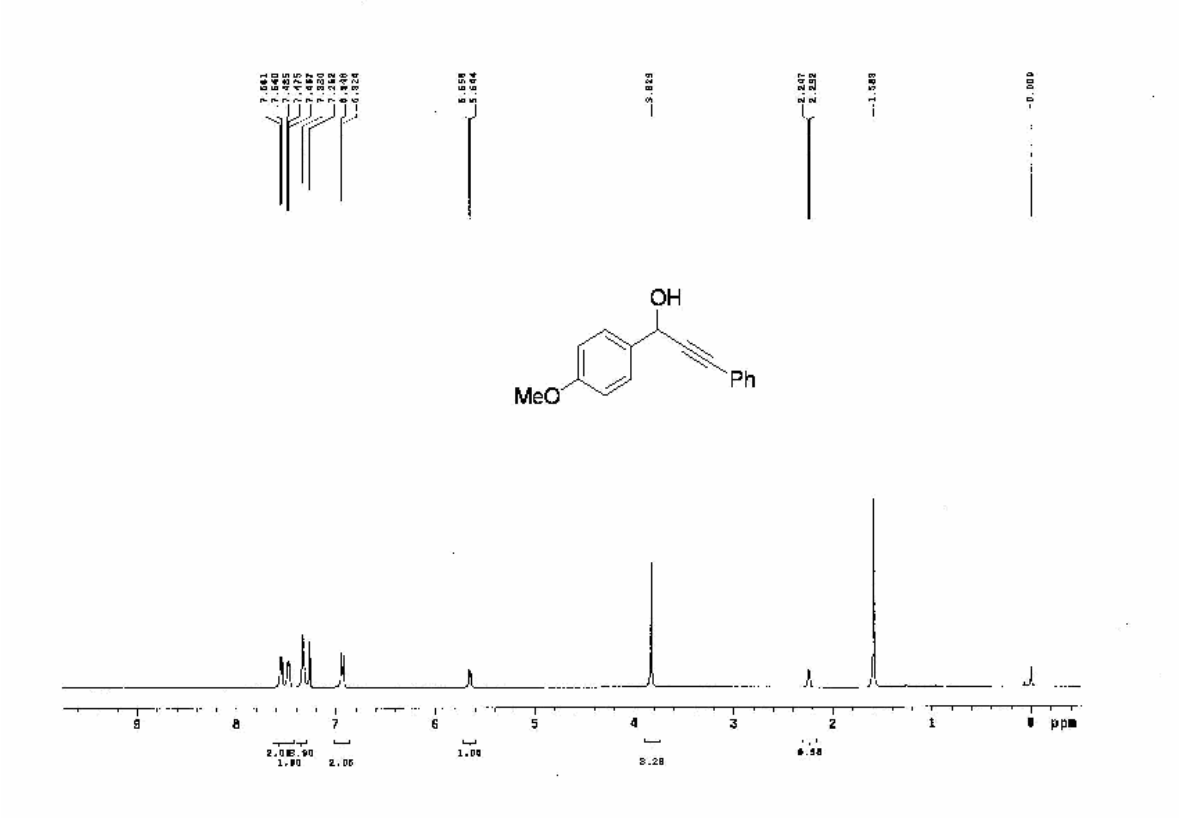

OCH3 OH
Ph
ppm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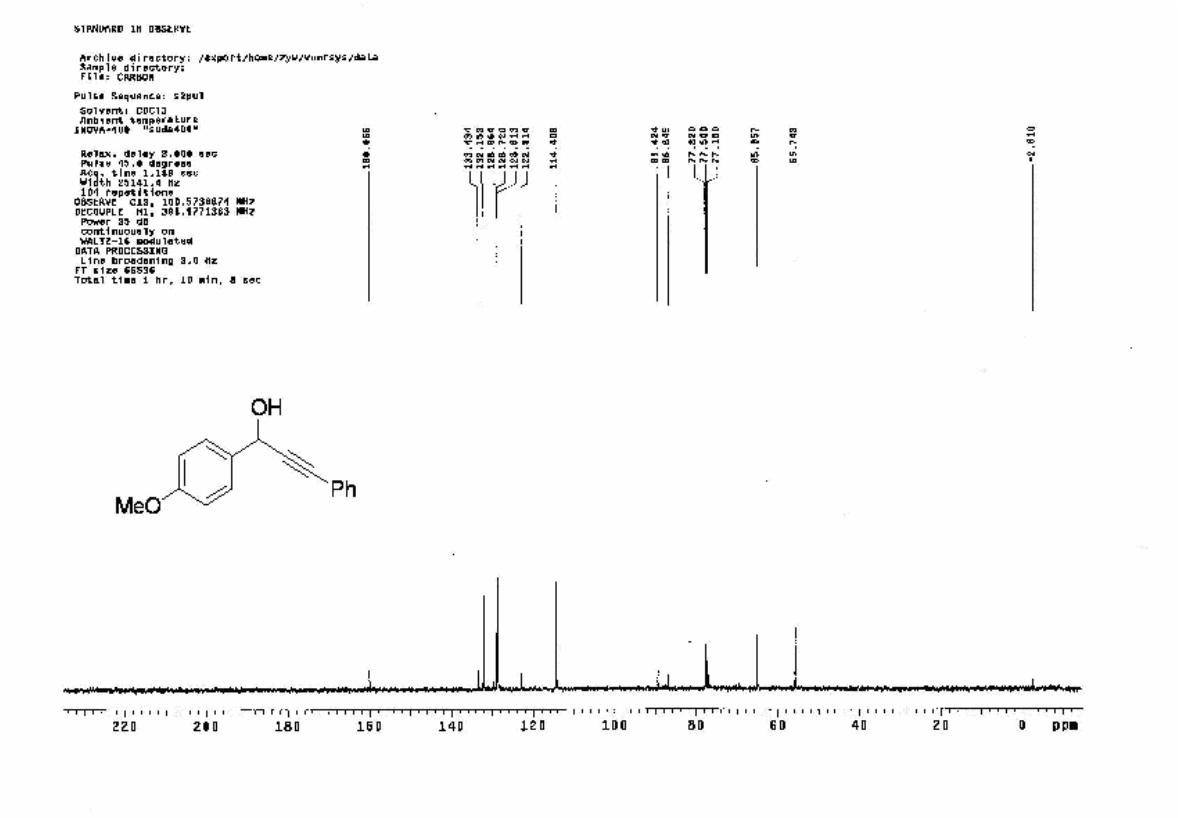
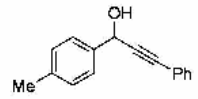
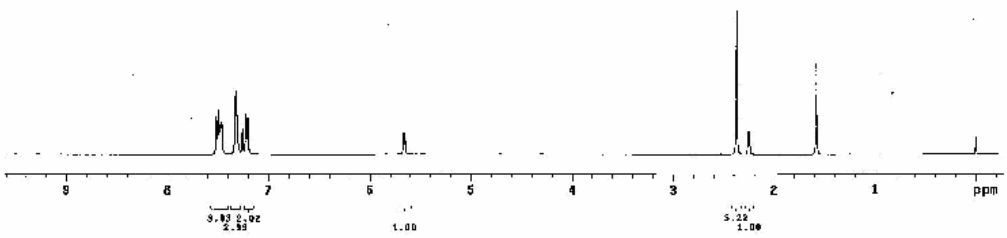
MeO
Ph
ppm


OH
MeO
Ph
ppm



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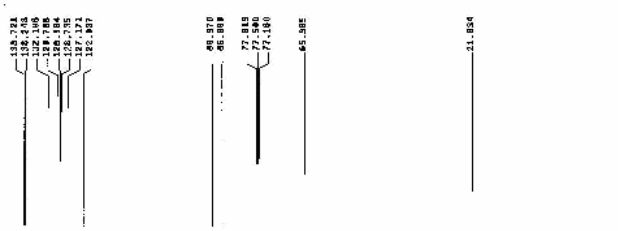
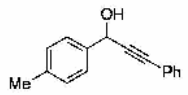
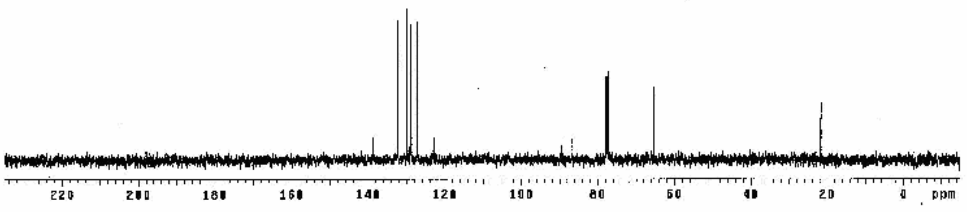
 Sample directory:
 File: CARBON

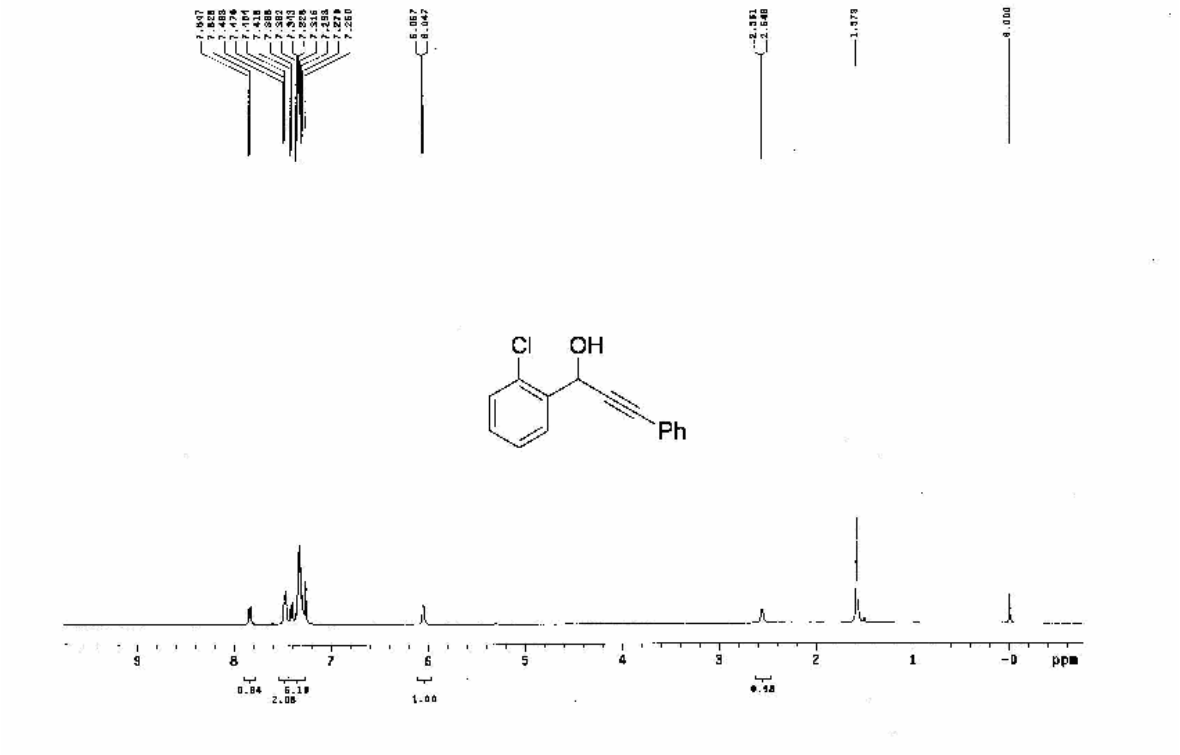
Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
INOVA-400  "suda400"

 Relax. delay 3.000 sec
 Pulse 45.0 degrees
 Acq. time 1.159 sec
 Width 18141.4 Hz
 64 repetitions
OBSERVE   C13, 100.5786844 MHz
DECOUPLE  H1, 399.9771363 MHz
 Power 35 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 3.0 Hz
FT size 65536
Total time 1 hr, 16 min, 8 sec
```








Cl
OH
Ph
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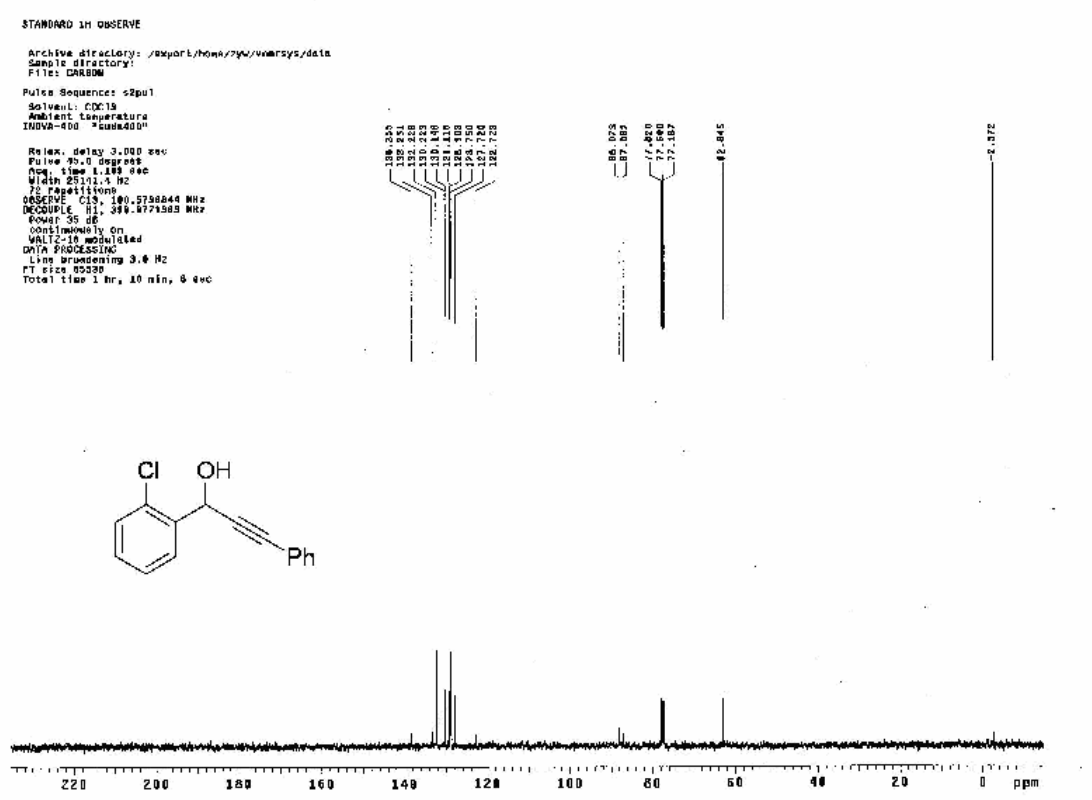
8
7
6
5
4
3
2
1
-0
ppm
0.84
2.08
1.00
0.98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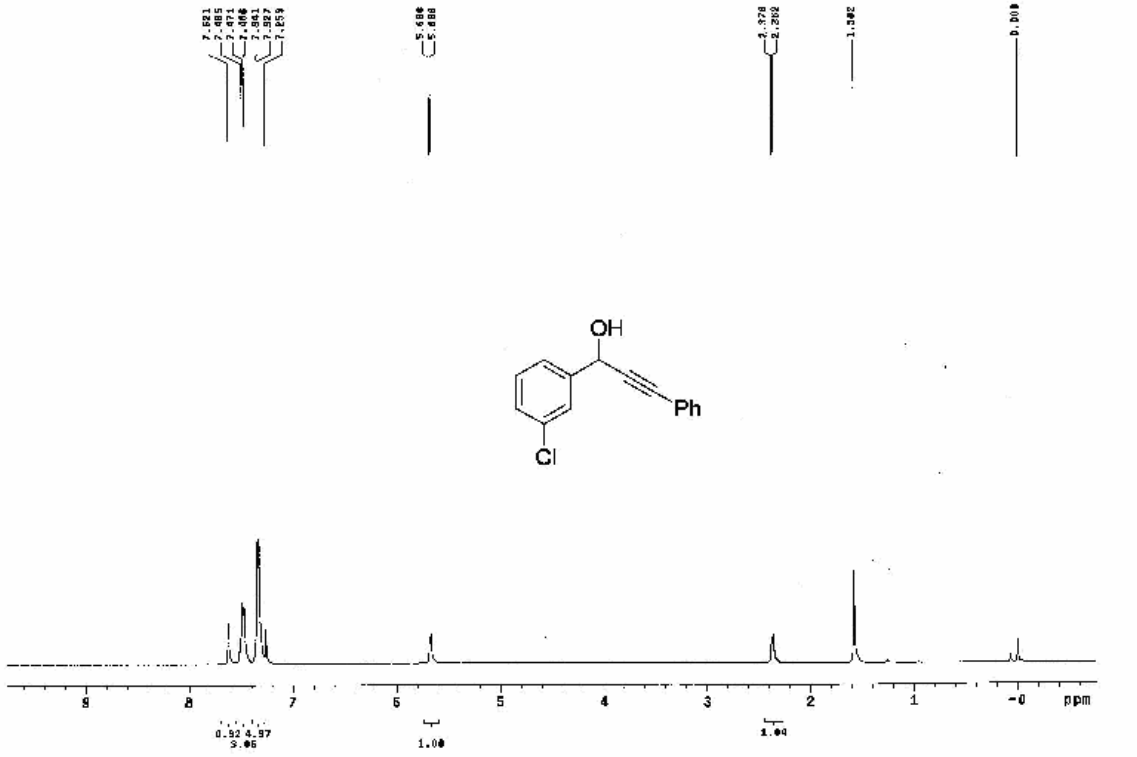
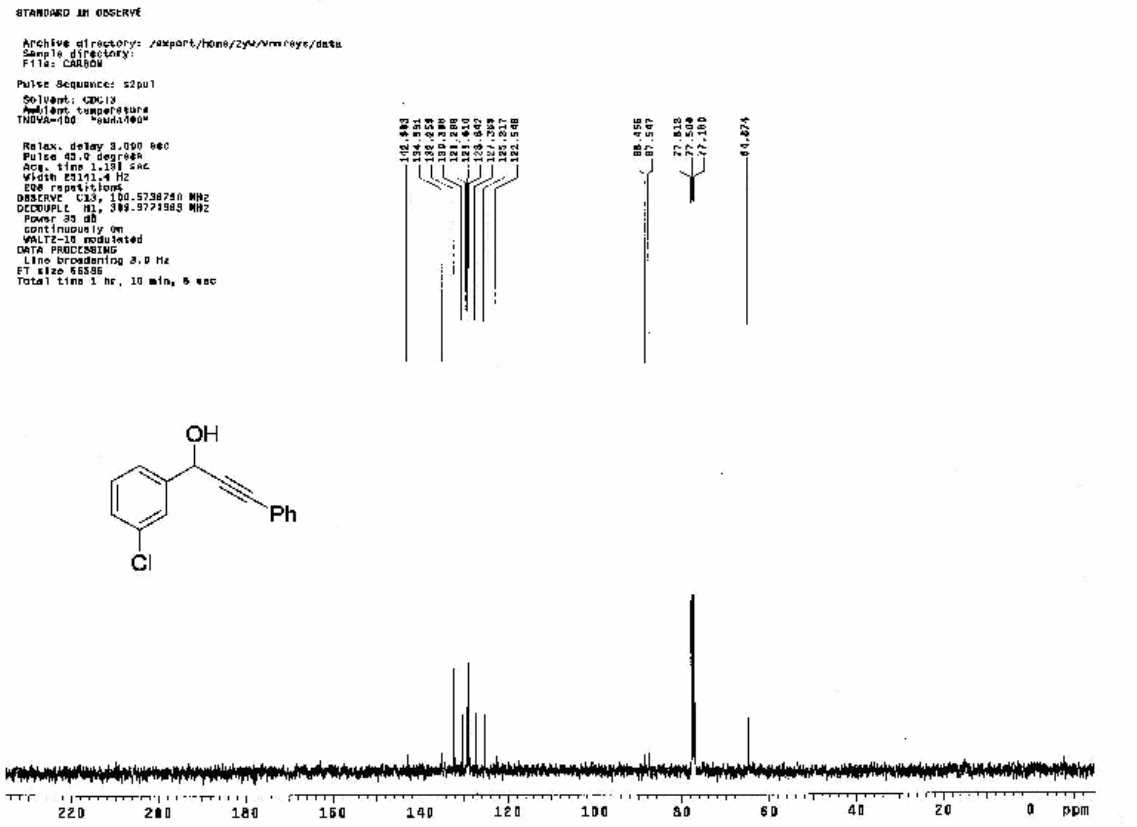
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-400 "sunm400"
Relax. delay 3.000 sec
Pulse 90.0 degrees
Acq. time 1.189 sec
Width 25141.4 Hz
75 repetitions
OBSERVE C13, 100.5798844 MHz
DECOUPLE H1, 399.9779989 MHz
Power 35 dB
continuously On
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 65536
Total time 1 hr, 10 min, 6 sec
Cl
OH
Ph
220
200
180
160
140
120
100
80
60
40
20
0
ppm


OH
Ph
Cl
9
8
7
6
5
4
3
2
1
-0
ppm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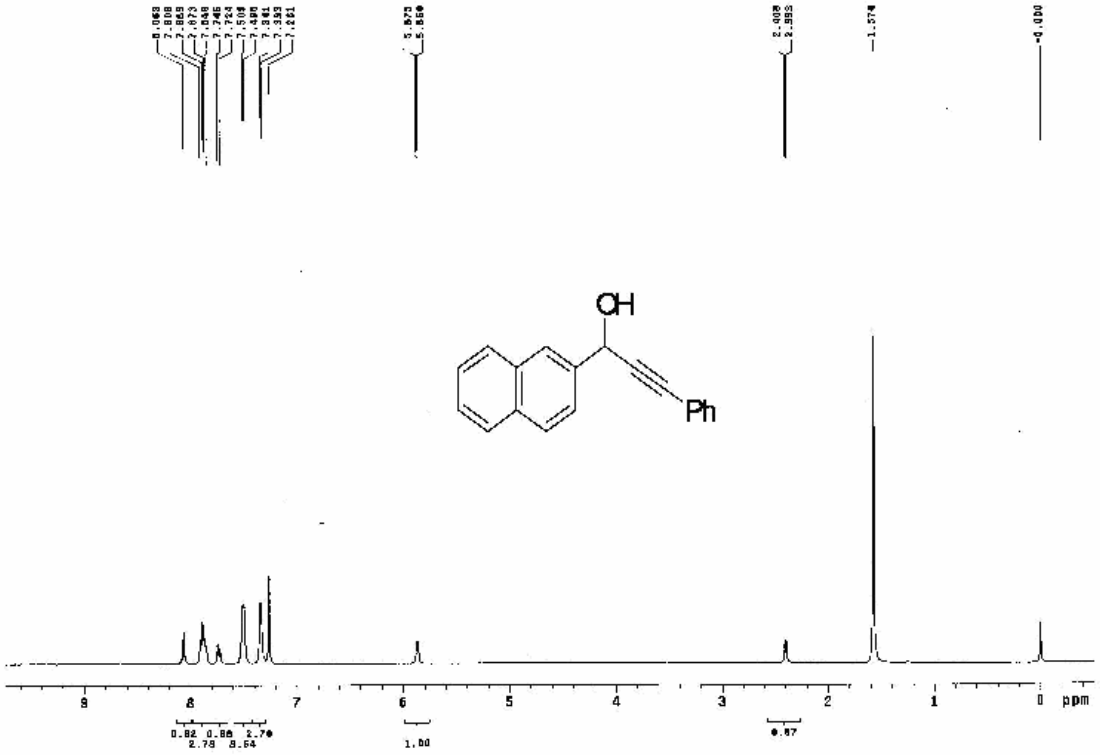
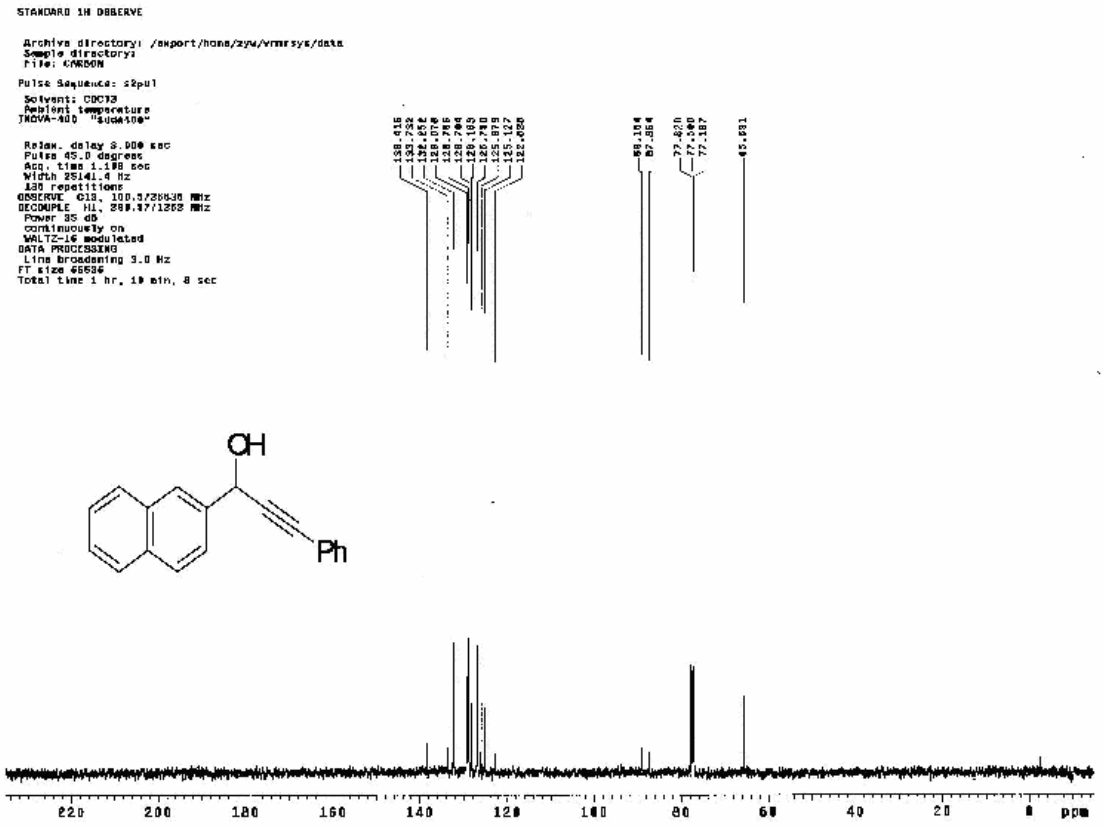
Solvent: CDCl3
Ambient temperature
INOVA-400 "wuxi400"
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.191 sec
Width 8191.4 Hz
256 repetitions
OBSERVE C13, 100.5738750 MHz
DECOUPLE H1, 399.9721985 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 65536
Total time 1 hr, 10 min, 5 sec
OH
Ph
Cl
220
200
180
160
140
120
100
80
60
40
20
0
ppm


OH
Ph
ppm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Sample directory:
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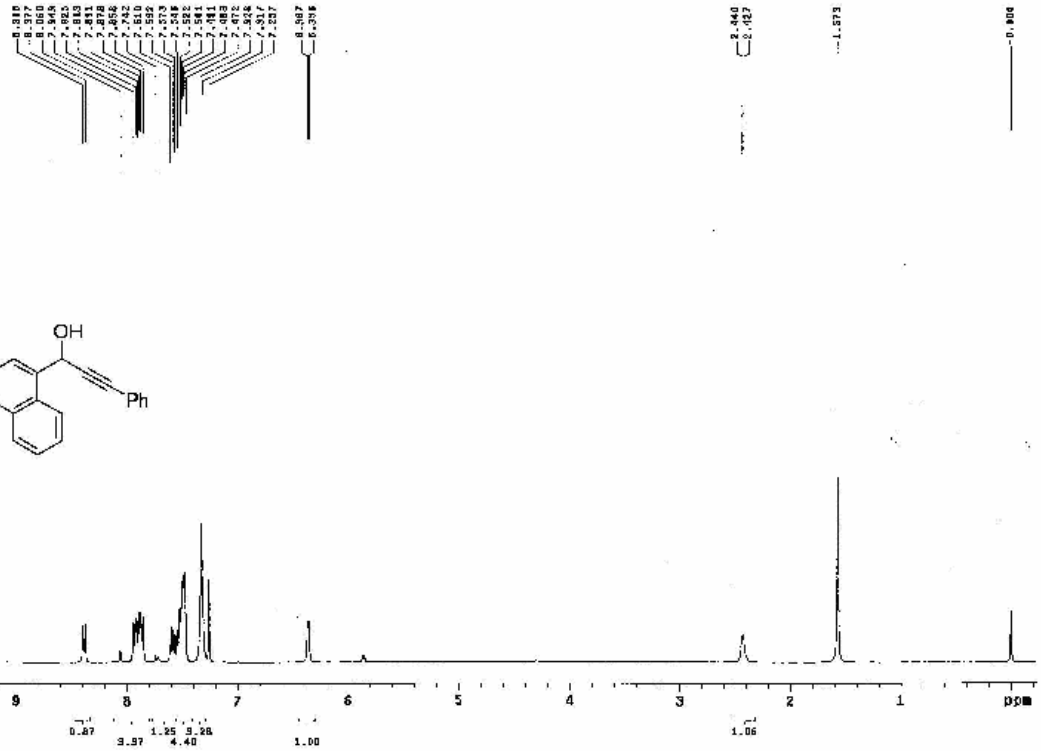
Solvent: CDCl3
Ambient temperature
INOVA-400 "sumston"
Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.188 sec
Width 25141.4 Hz
438 repetitions
OBSERVE C13, 100.5728538 MHz
DECOUPLE H1, 399.97/1268 MHz
Power 35 db
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 65536
Total time 1 hr, 19 min, 8 sec
OH
Ph
ppm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Ph
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4
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2
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ppm
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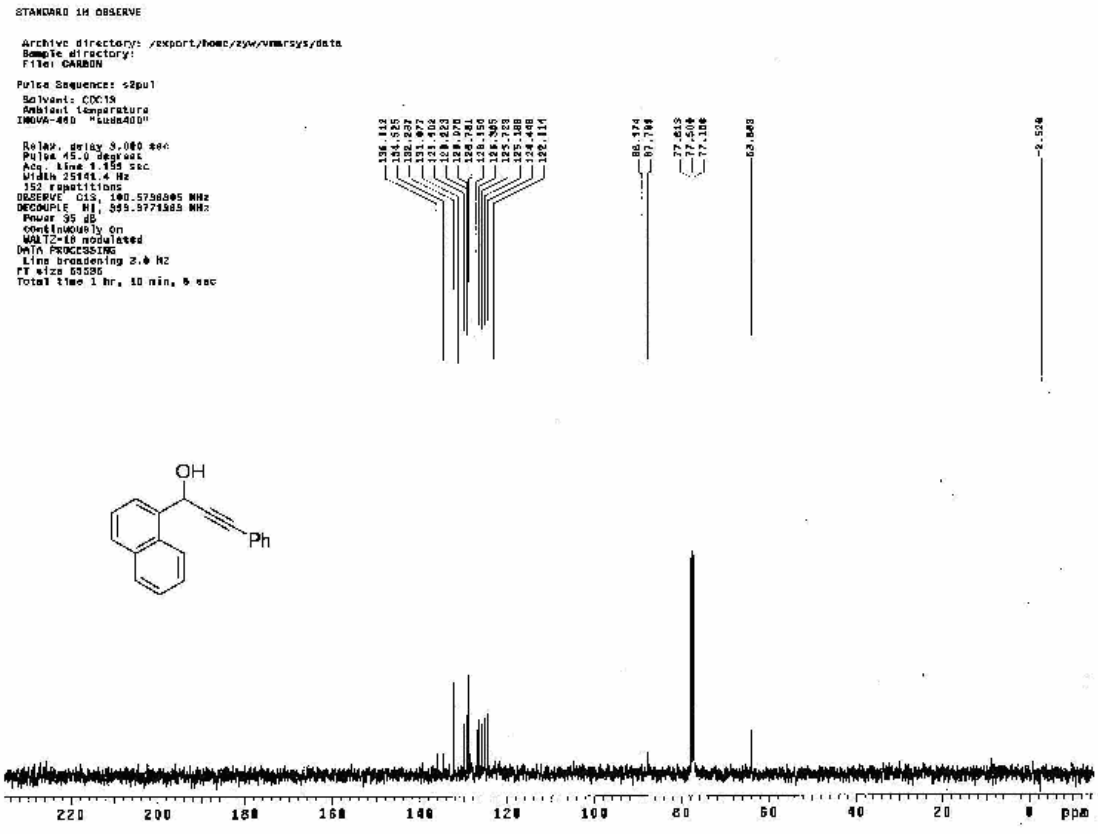
3.28
3.97
4.40
1.00
1.06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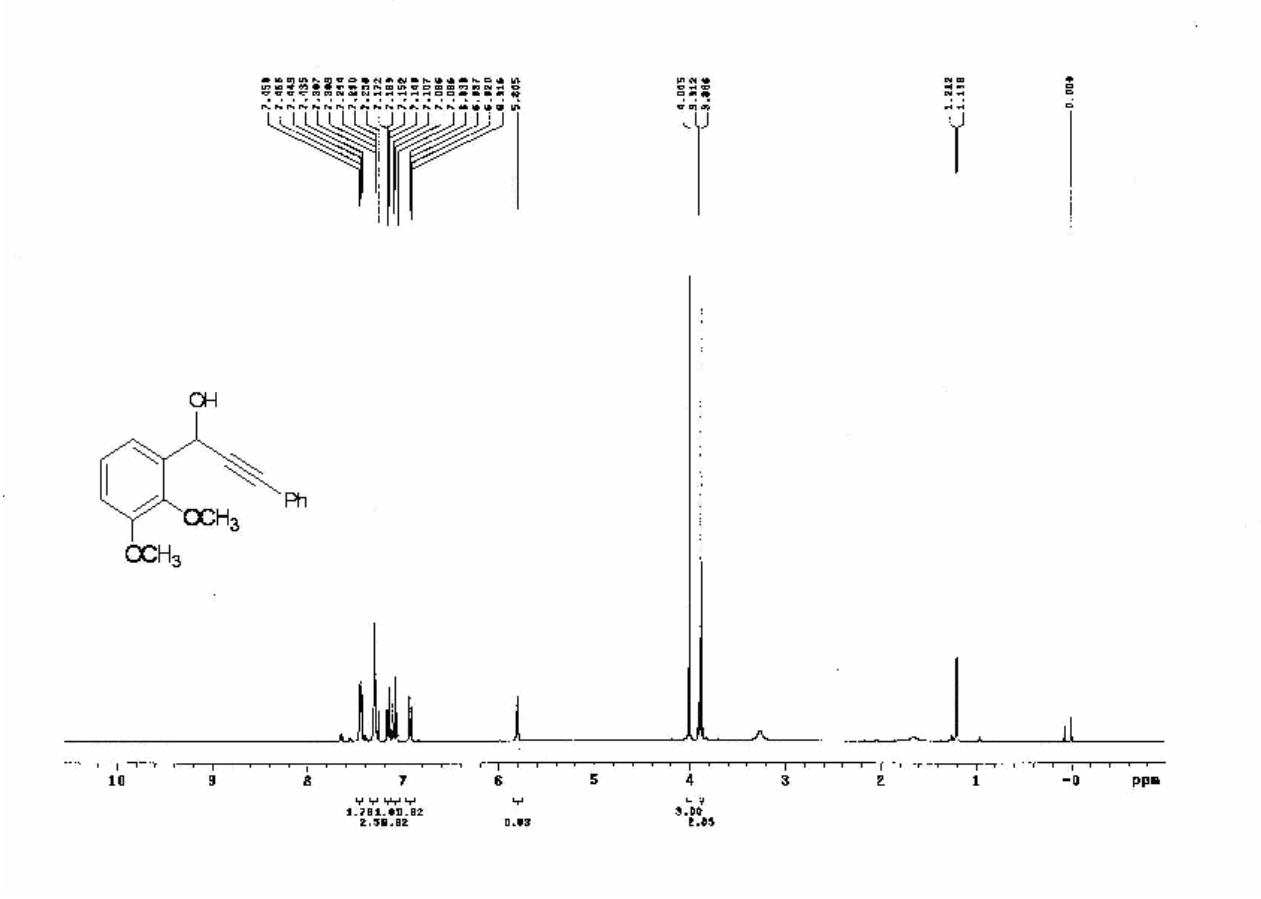
Solvent: CDCl3
Ambient temperature
INOVA-400 "Linda400"
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.199 sec
Width 25141.4 Hz
152 repetitions
OBSERVE C13, 100.5798805 MHz
DECOUPLE H1, 399.5771383 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 1 hr, 10 min, 6 sec
OH
Ph
220
200
180
160
140
120
100
80
60
40
20
0
ppm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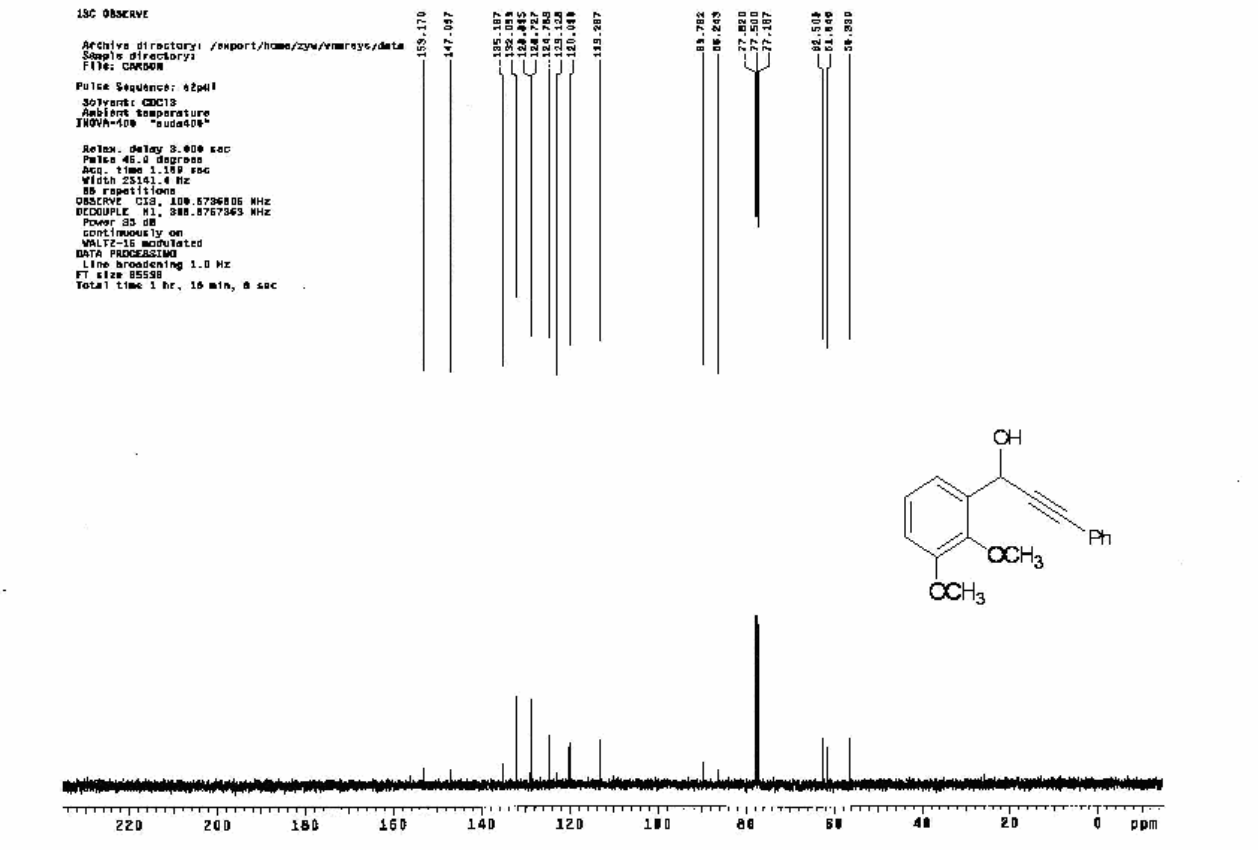
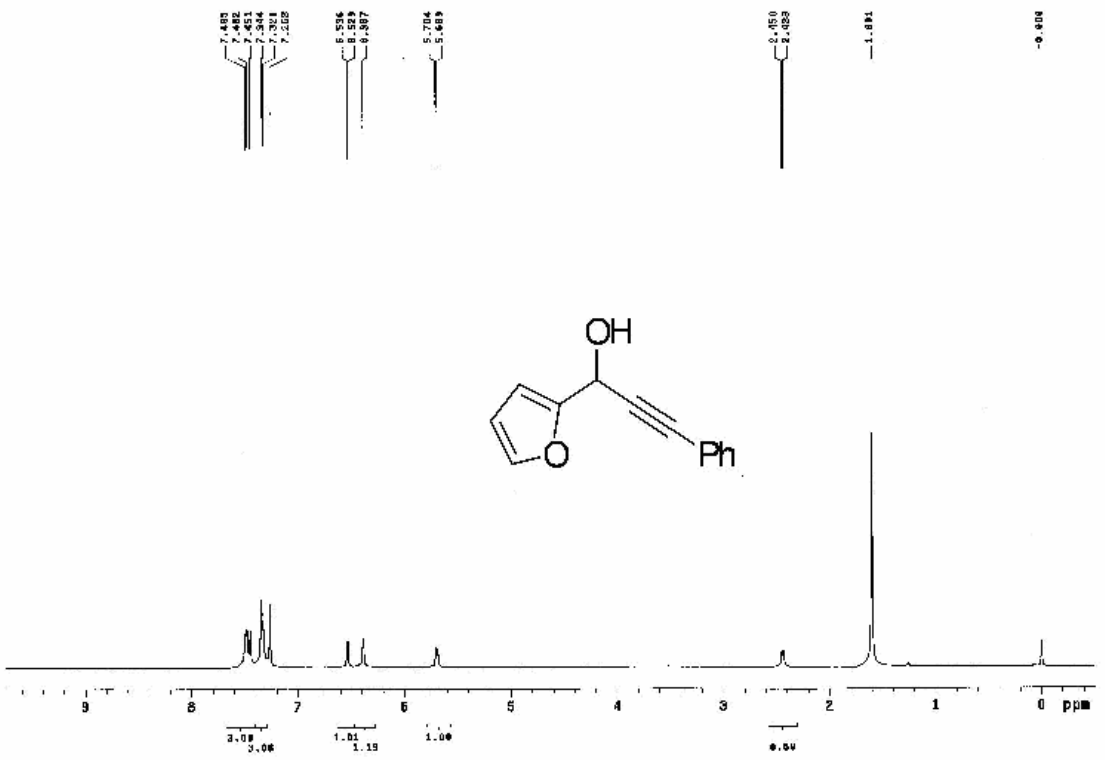
Ph
OCH3
OCH3
10
9
8
7
6
5
4
3
2
1
-0
ppm


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-400 "suda405"
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.189 sec
Width 25141.4 Hz
85 repetitions
OBSERVE C13, 100.5796805 MHz
DECOUPLE H1, 399.8767363 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 85598
Total time 1 hr, 16 min, 8 sec
OH
Ph
OCH3
OCH3
220
200
180
160
140
120
100
80
60
40
20
0
ppm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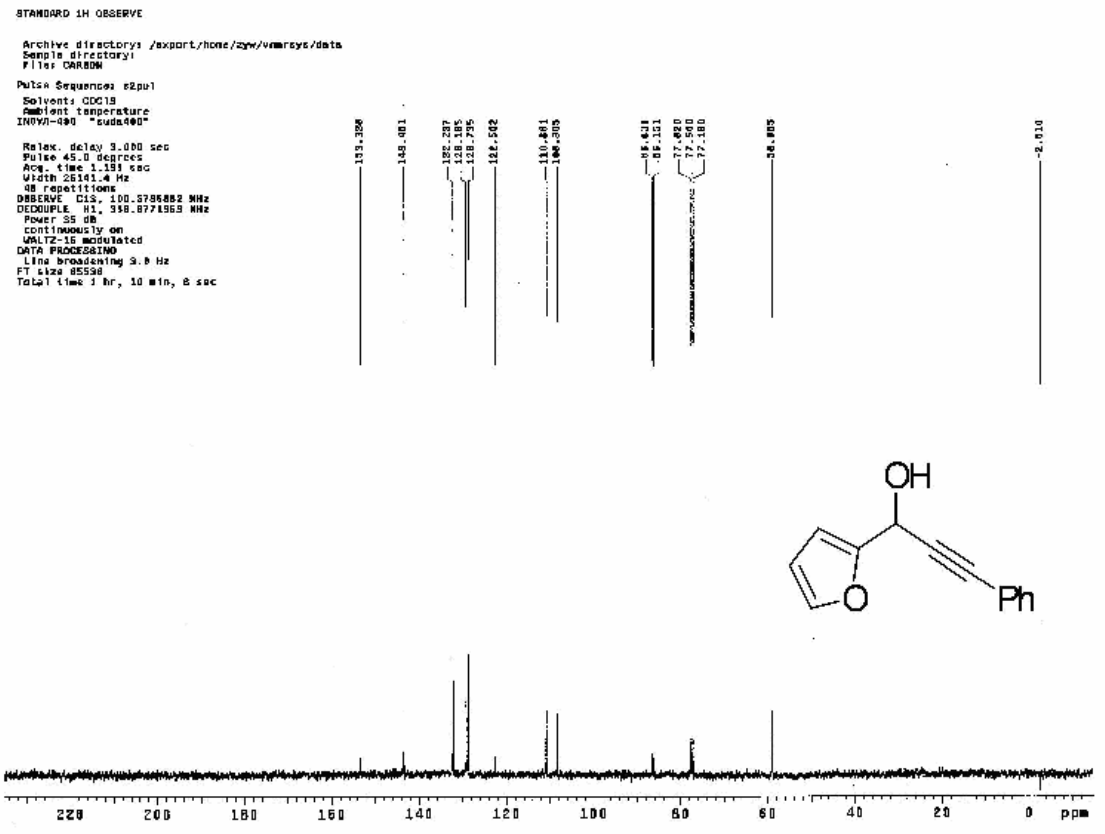
O
Ph
9
8
7
6
5
4
3
2
1
0
ppm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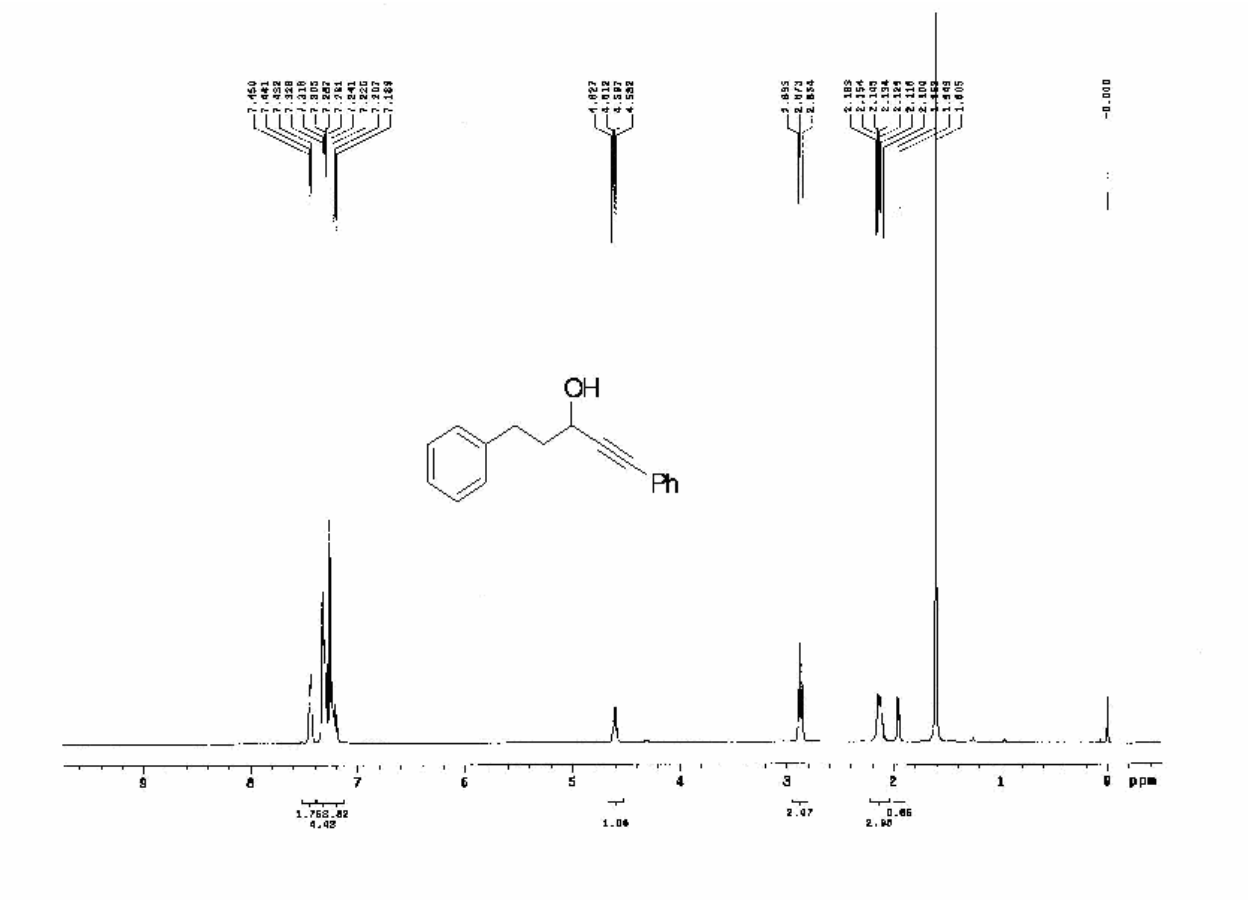
Solvent: CDCl3
Ambient temperature
INOVA-400 "suda400"
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.191 sec
Width 26141.4 Hz
48 repetitions
OBSERVE C13, 100.5786882 MHz
DECOUPLE H1, 399.8771969 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 65536
Total time 1 hr, 10 min, 8 sec
OH
O
Ph
220
200
180
160
140
120
100
80
60
40
20
0
ppm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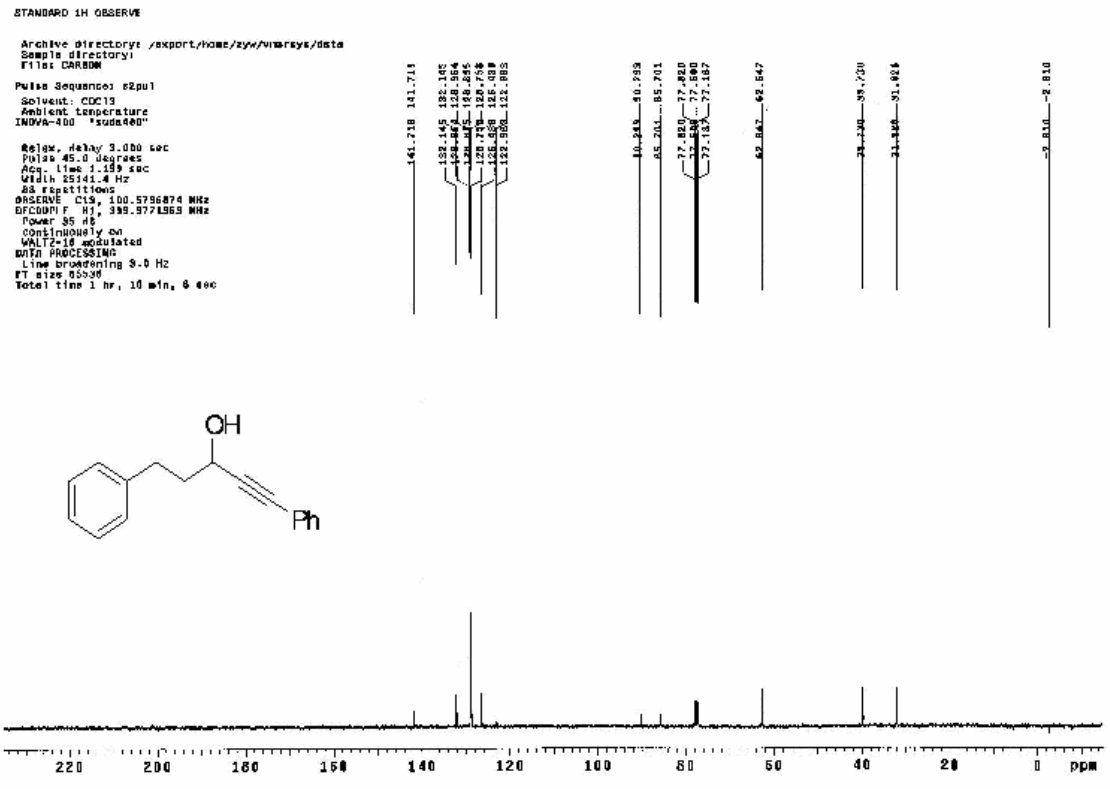
Ph
ppm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Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-400 "suda400"
Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.159 sec
Width 25141.4 Hz
88 repetitions
OBSERVE C13, 100.5796874 MHz
DECOUPLE H1, 399.9771963 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 65536
Total time 1 hr, 10 min, 8 sec
OH
Ph
ppm

Copies of the HPLC Data

Empower 2

SZX

SAMPLE INFORMATION

Sample Name:	xz-6	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
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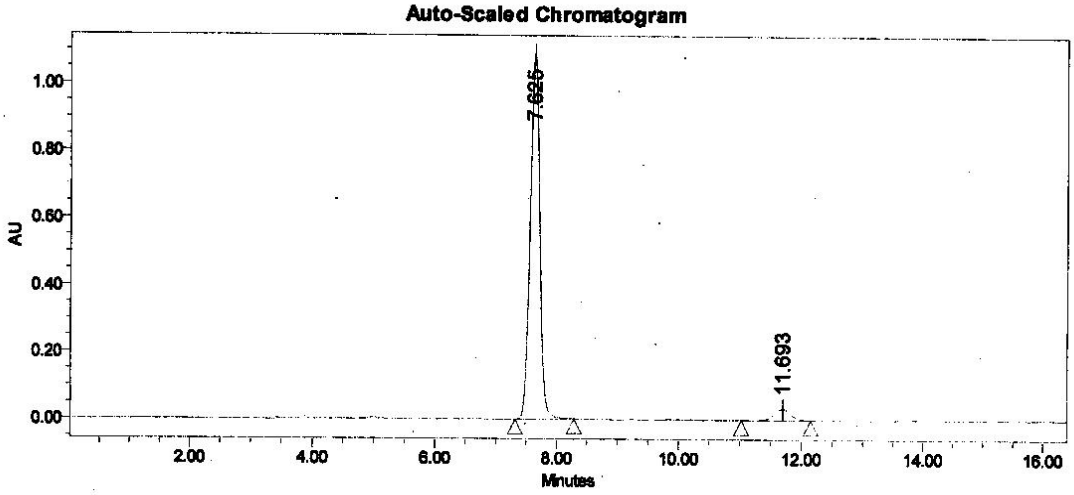
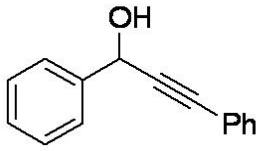
Injection #:	8	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	18.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-10 13:24:47 CST		
Date Processed:	2007-7-10 13:44:29 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	7.625	11916892	94.93	1094461		
2	11.693	635844	5.07	33875		



Reported by User: System
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2007-7-10
13:44:53 PRC

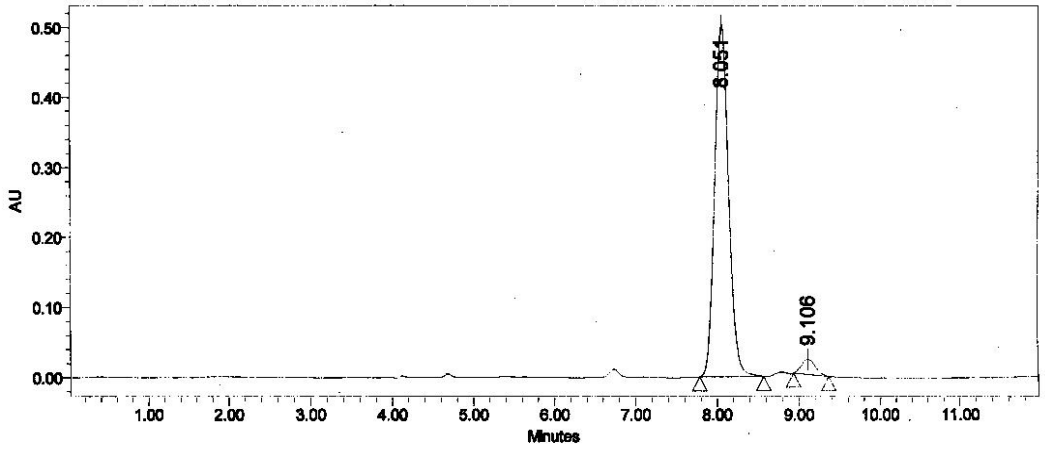
Empower 2

SZX

SAMPLE INFORMATION

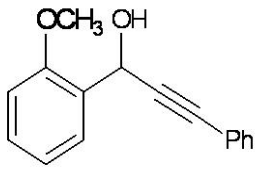
Sample Name:	xz-3	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	4	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	12.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-9-13 10:43:45 CST		
Date Processed:	2007-9-13 11:00:52 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	8.051	5963526	95.82	504405		
2	9.106	260384	4.18	21422		



Reported by User: System
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Project Name: szx
Date Printed:
2007-9-13
11:01:24 PRC

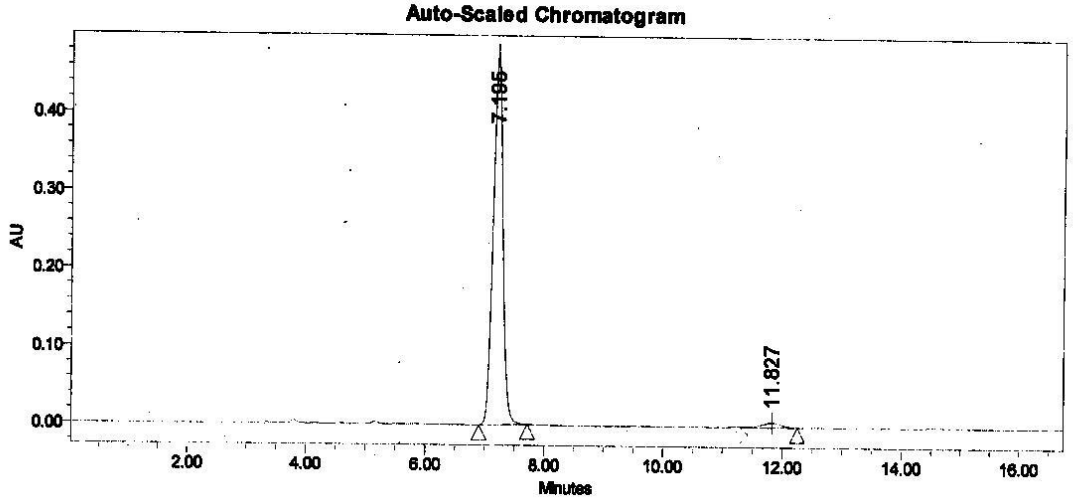
Empower 2

SZX

SAMPLE INFORMATION

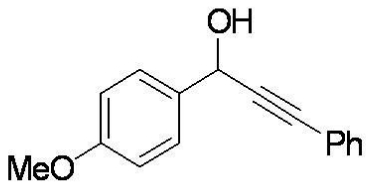
Sample Name:	xz-10	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	6	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	25.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-13 15:10:42 CST		
Date Processed:	2007-7-13 15:29:15 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	7.195	5422084	97.29	476875		
2	11.827	151249	2.71	6103		



Reported by User: System
Report Method: szx
Report Method ID 4116
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Project Name: szx
Date Printed:
2007-7-13
15:29:34 PRC

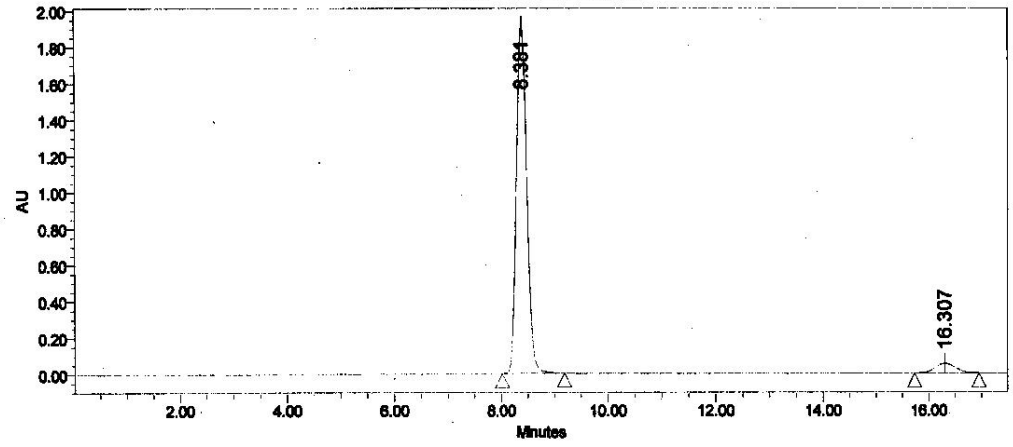
Empower 2

SZX

SAMPLE INFORMATION

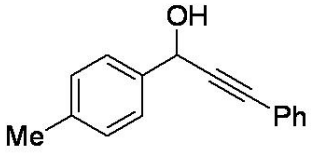
Sample Name:	xz-3	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	3	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-10 10:59:39 CST		
Date Processed:	2007-7-10 11:18:55 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	8.381	26007252	94.92	1912229		
2	16.307	1392076	5.08	52957		



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Project Name: szx
Date Printed:
2007-7-10
11:19:33 PRC

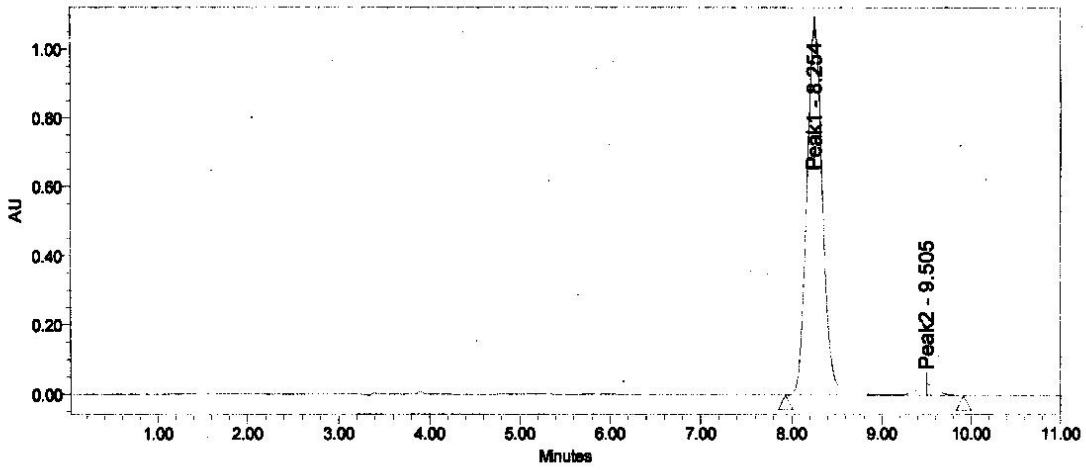
Empower 2

SZX

SAMPLE INFORMATION

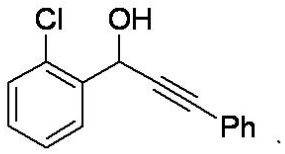
Sample Name:	xz-2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	2	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	11.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-10 10:48:06 CST		
Date Processed:	2007-7-10 11:01:10 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	8.254	12877327	96.31	1070312		
2	9.505	493541	3.69	33103		



Reported by User: System
Report Method: szx
Report Method ID 1050
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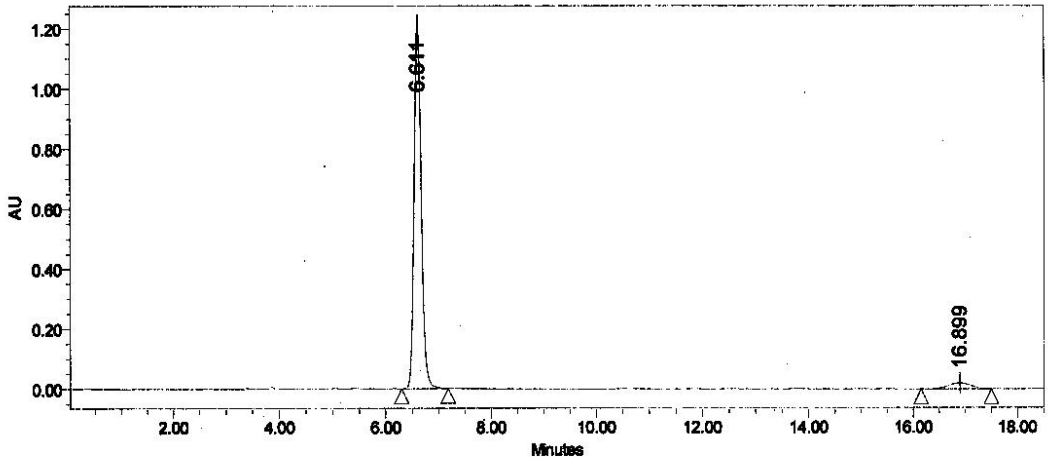
Project Name: szx
Date Printed:
2007-7-10
11:02:19 PRC

SAMPLE INFORMATION

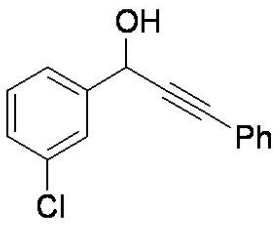
Sample Name:	xz-1	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	6	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	18.5 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-10 12:31:06 CST		
Date Processed:	2007-7-10 12:51:36 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	6.611	11588831	95.25	1217324		
2	16.899	577726	4.75	19771		



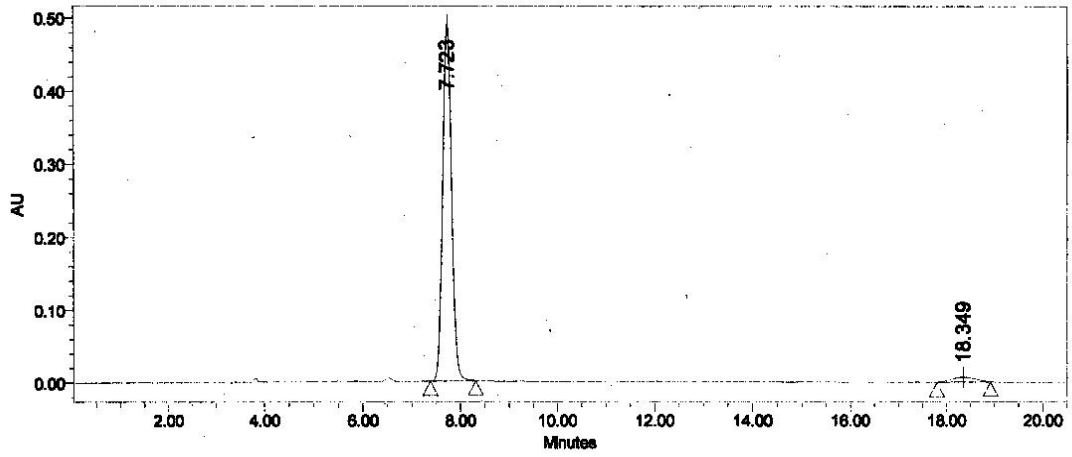
Empower 2

SZX

SAMPLE INFORMATION

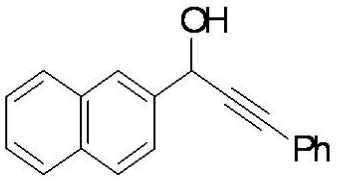
Sample Name:	xz-7	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	4	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	25.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-13 14:31:36 CST		
Date Processed:	2007-7-13 14:55:03 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	7.723	8254583	96.45	490735		
2	18.349	230220	3.55	6874		



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14:56:01 PRC

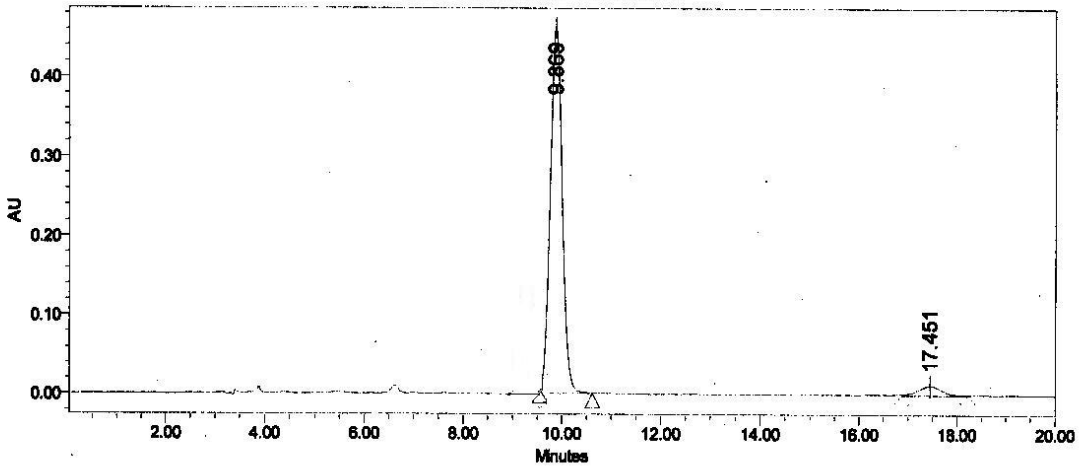
Empower 2

SZX

SAMPLE INFORMATION

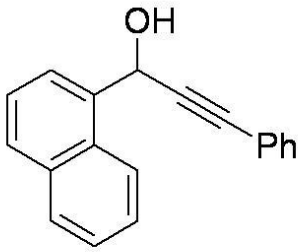
Sample Name:	xz-4	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	7	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-10 12:50:09 CST		
Date Processed:	2007-7-10 13:16:42 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	9.869	7799558	95.11	462514		
2	17.451	400764	4.89	11866		



Reported by User: System
Report Method: szx
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Project Name: szx
Date Printed:
2007-7-10
13:25:11 PRC

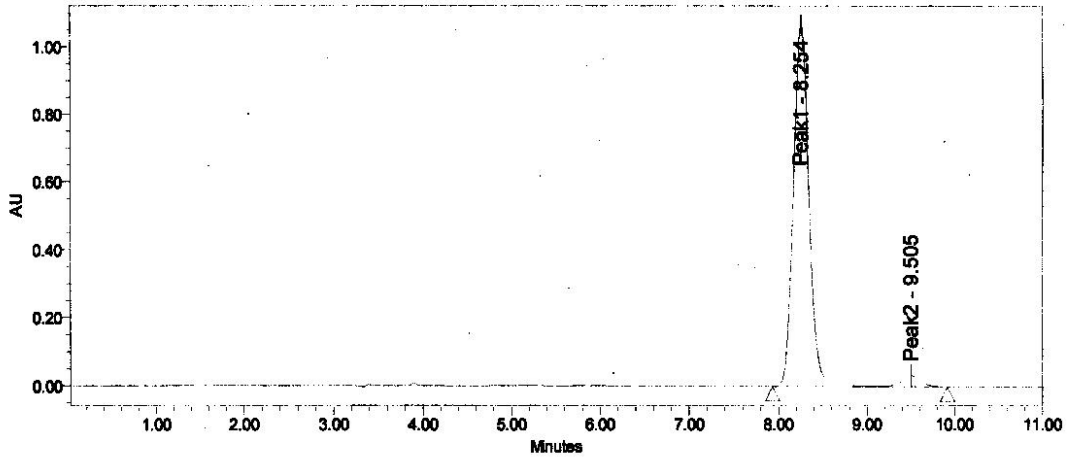
Empower 2

SZX

SAMPLE INFORMATION

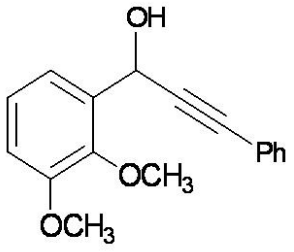
Sample Name:	xz-2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	2	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	11.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-10 10:48:06 CST		
Date Processed:	2007-7-10 11:01:10 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	8.254	12877327	96.31	1070312		
2	9.505	493541	3.69	33103		



Reported by User: System
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Report Method ID 1050
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Project Name: szx
Date Printed:
2007-7-10
11:02:19 PRC

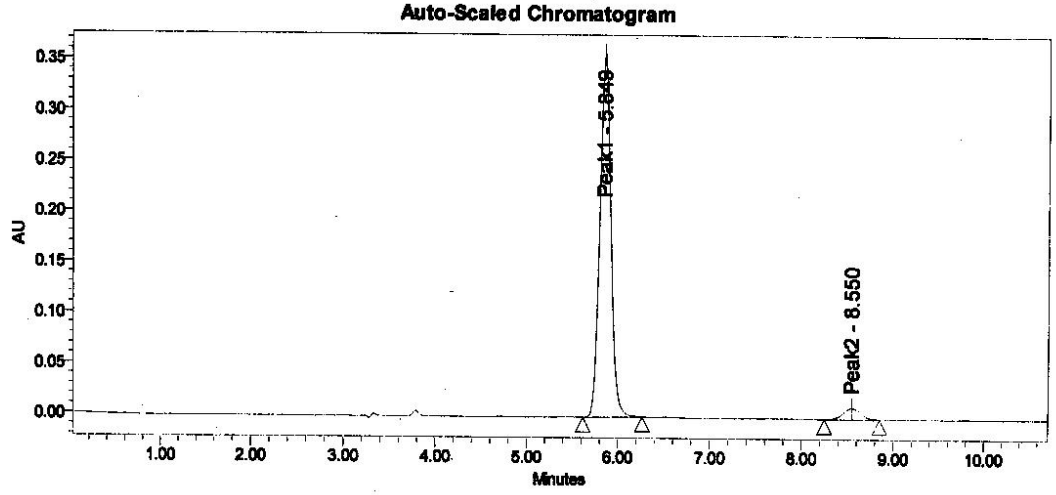
Empower 2

SZX

SAMPLE INFORMATION

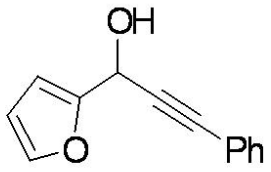
Sample Name:	xz-9	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	3	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	20.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-7-13 14:20:02 CST		
Date Processed:	2007-7-13 14:32:40 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	5.849	3014220	95.25	358139		
2	8.550	150408	4.75	11367		



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Date Printed:
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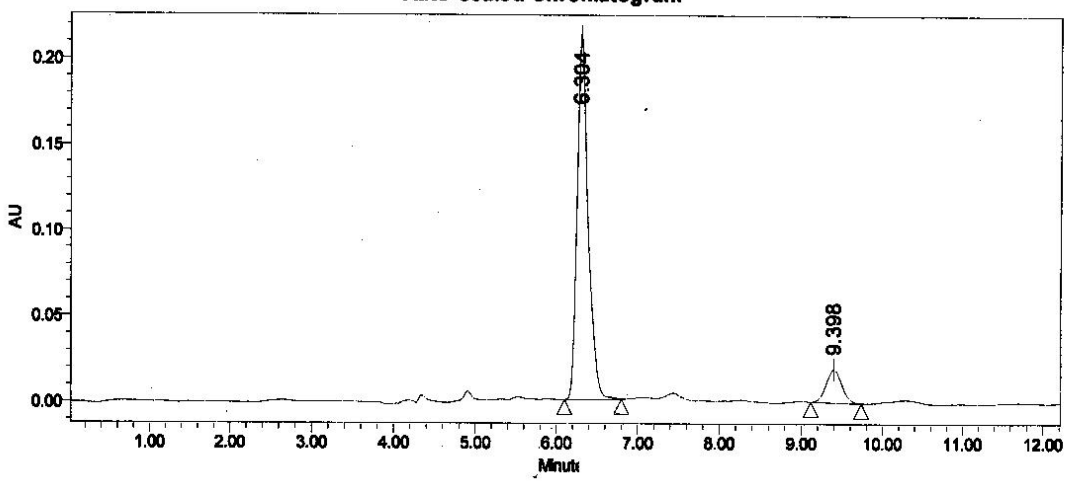
Empower 2

SZX

SAMPLE INFORMATION

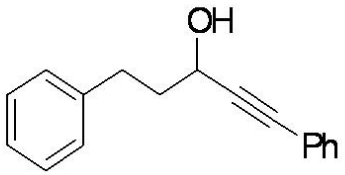
Sample Name:	xz-2	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	605	Acq. Method Set:	szx
Injection #:	5	Processing Method:	szx
Injection Volume:	20.00 ul	Channel Name:	254.0nm
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	PDA 254.0 nm
Date Acquired:	2007-9-13 10:56:26 CST		
Date Processed:	2007-9-13 11:10:05 CST		

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area	Height	Amount	Units
1	6.304	2003050	88.56	213202		
2	9.398	258670	11.44	19403		



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Project Name: szx
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The full data for Table 1: The relationship between ee values and the ratio of $Ti(O^iPr)_4$/ligand when different solvents were used.

Entry	Solvent	$Ti(O^iPr)_4$/**2a**	e.e
1	toluene	0.125/1	0
2	toluene	0.25/1	6
3	toluene	1/1	71
4	toluene	2/1	70
5	toluene	3/1	43
6	toluene	4/1	29
7	toluene	5/1	17
8	toluene	6/1	2
9	CH_2Cl_2	0.5/1	-3
10	CH_2Cl_2	1/1	79
11	CH_2Cl_2	2/1	71
12	CH_2Cl_2	3/1	57
13	THF	0/1	-20
14	THF	0.5/1	82
15	THF	2/1	85
16	THF	3/1	75
17	THF	4/1	81
18	THF	5/1	80
19	THF	6/1	80
20	THF	7/1	79