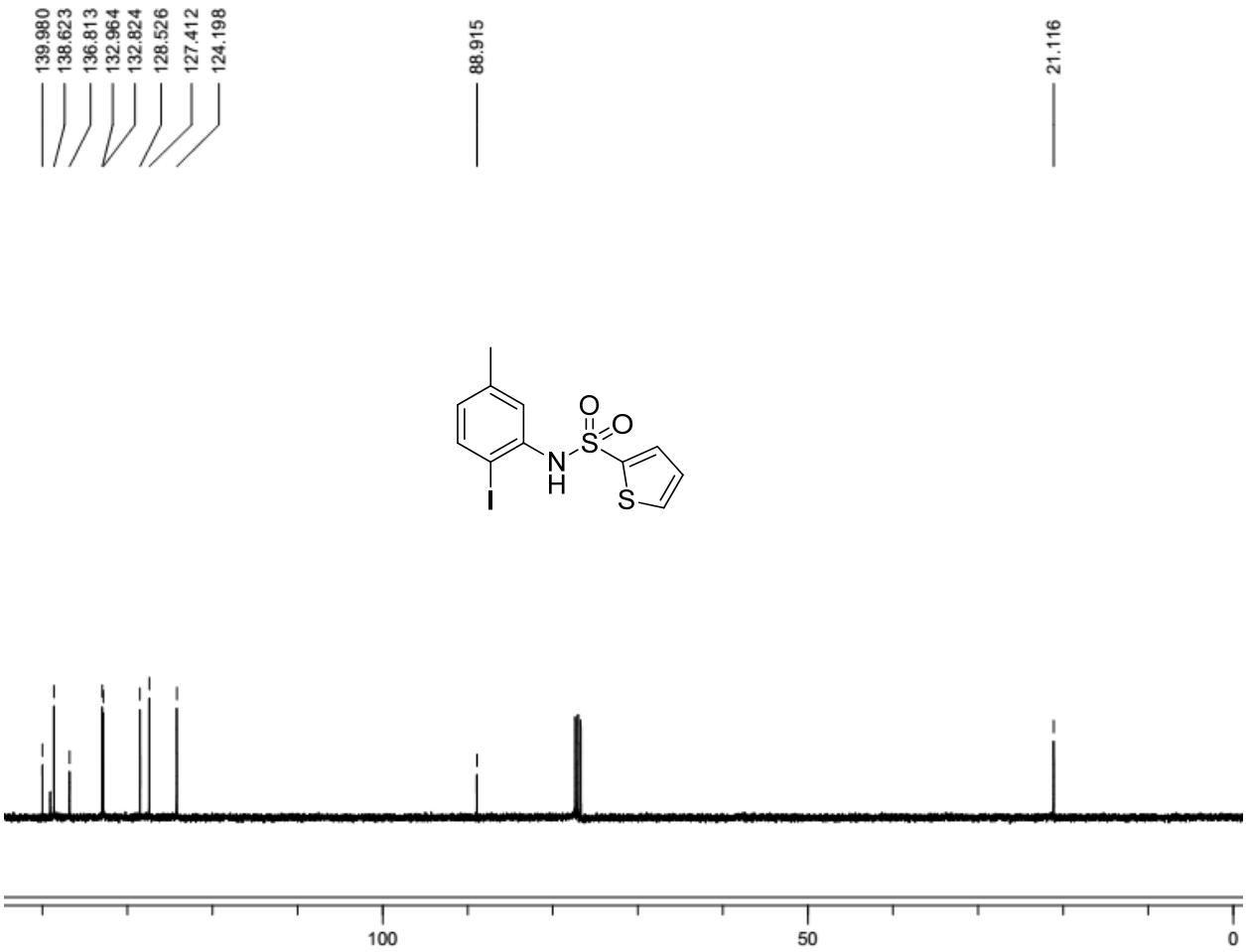
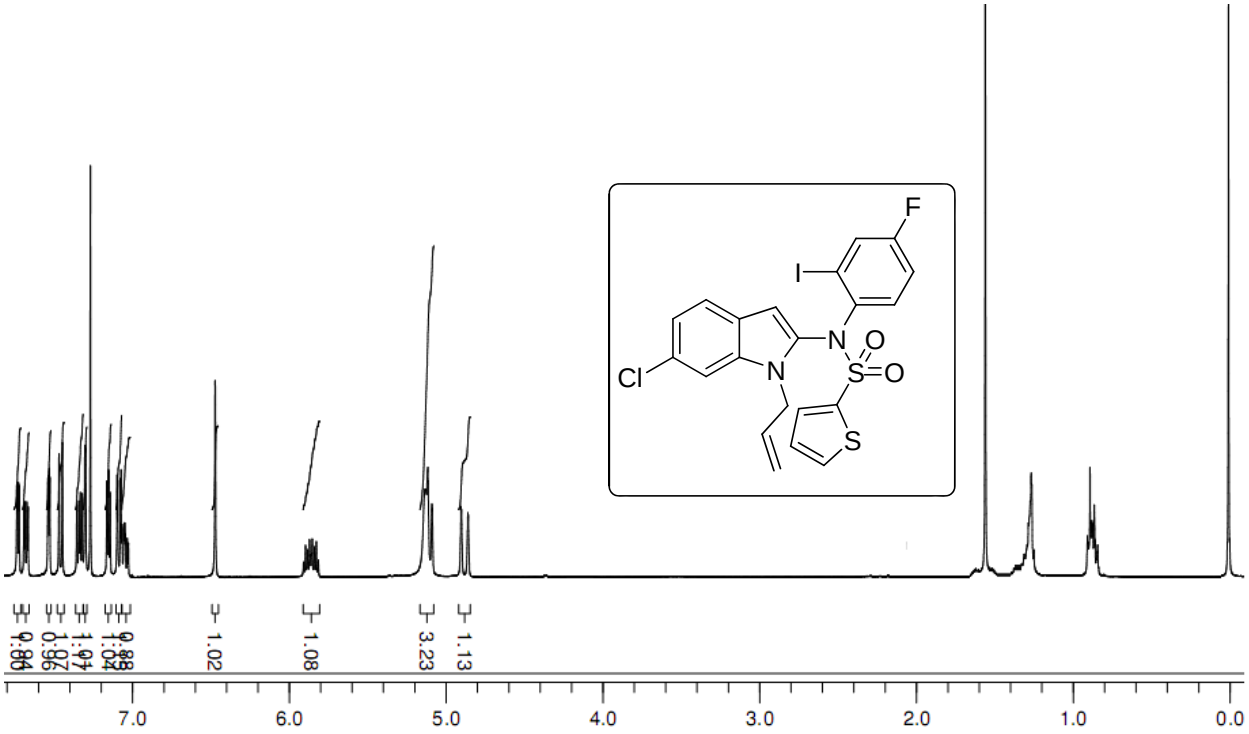
Electronic Supplementary Material (ESI) for Chemical Communications.

Copies of spectra

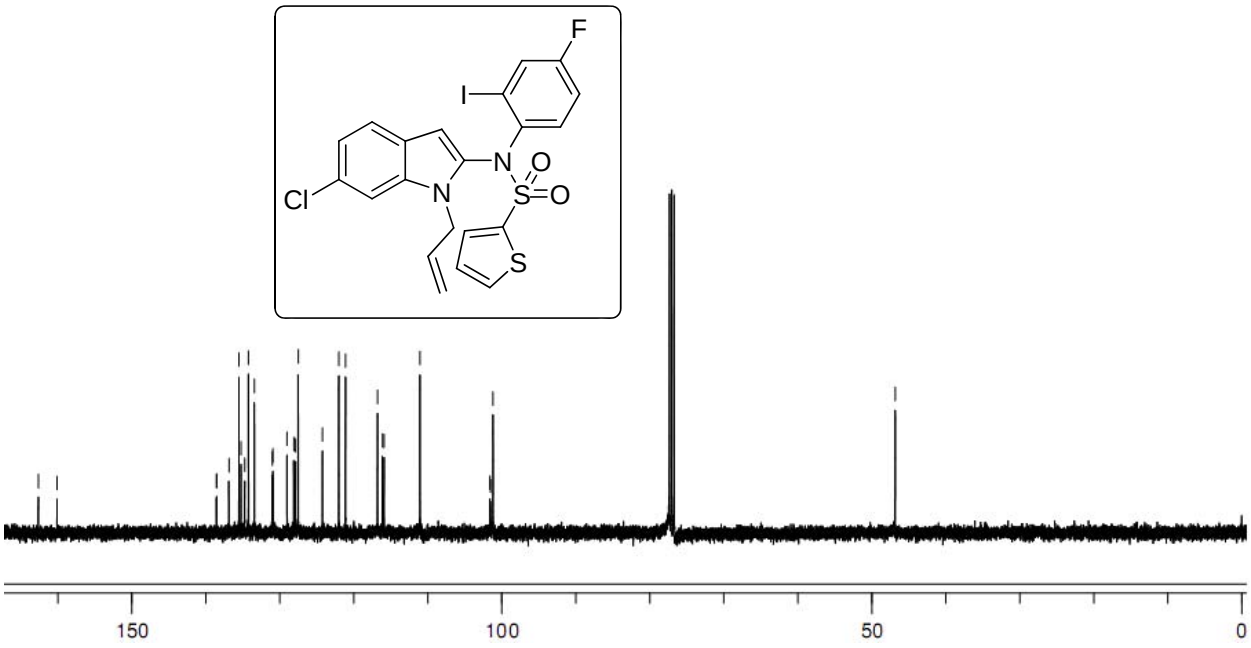
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1S1** in $CDCl_3$



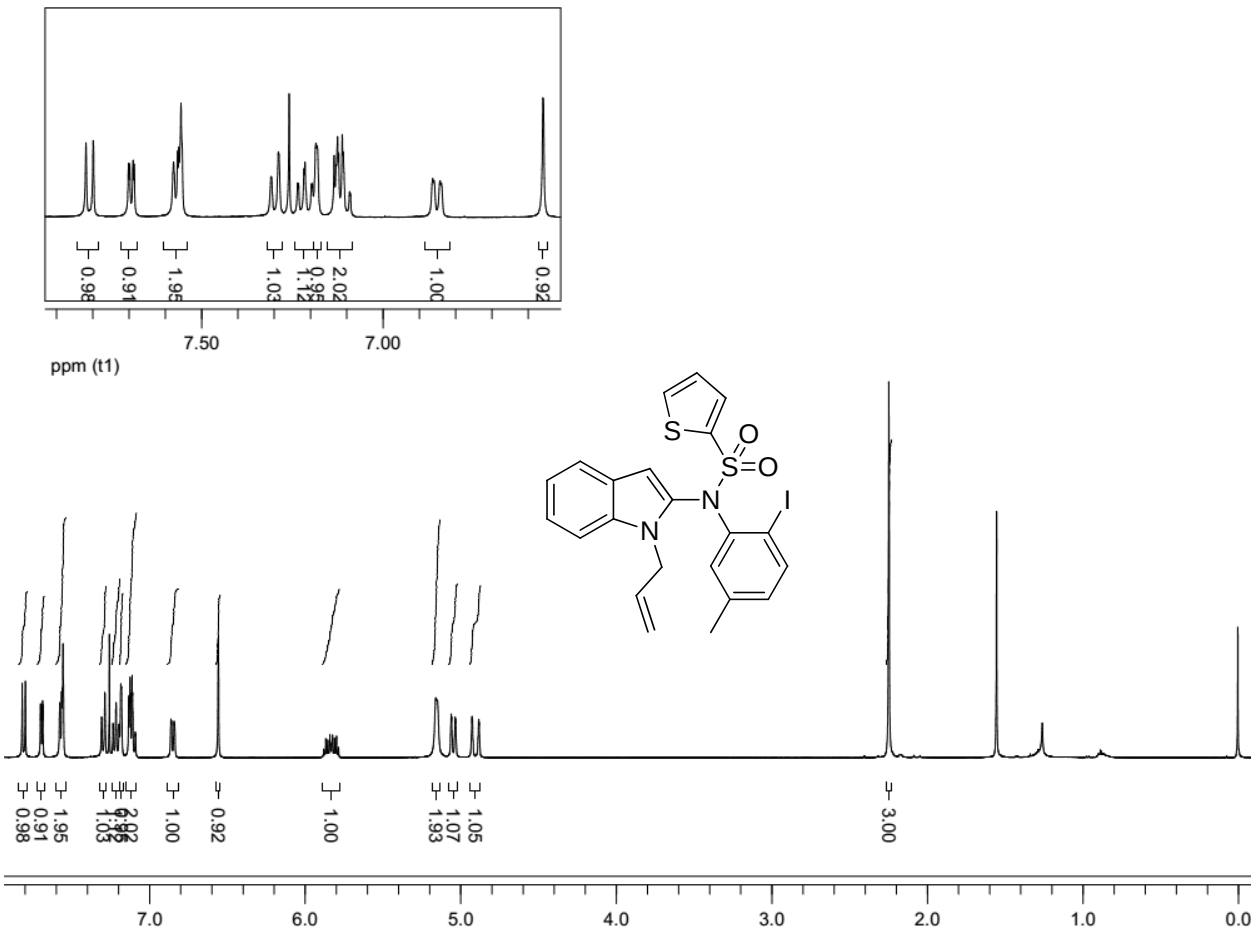
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1S1** in $CDCl_3$



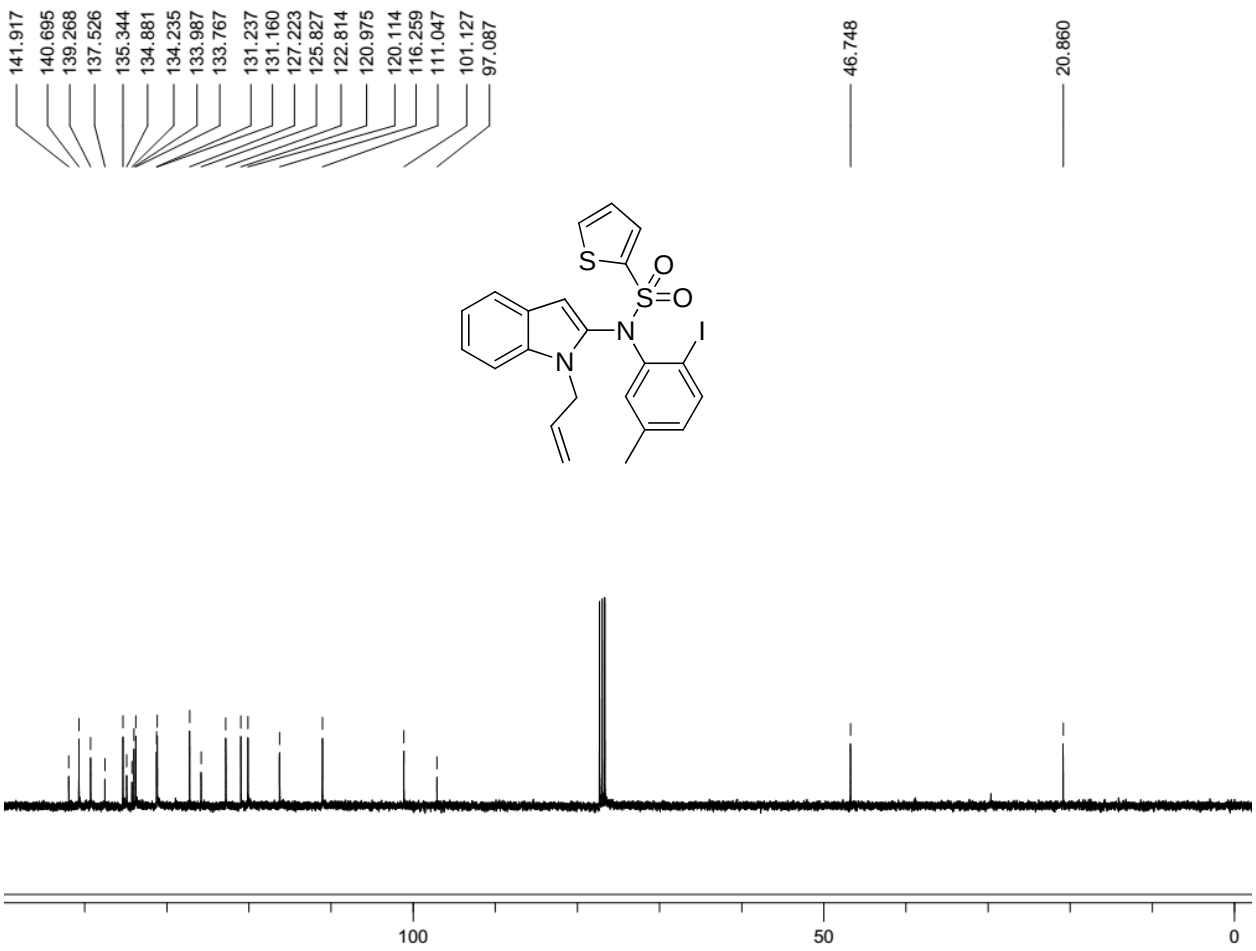
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1S4r** in $CDCl_3$



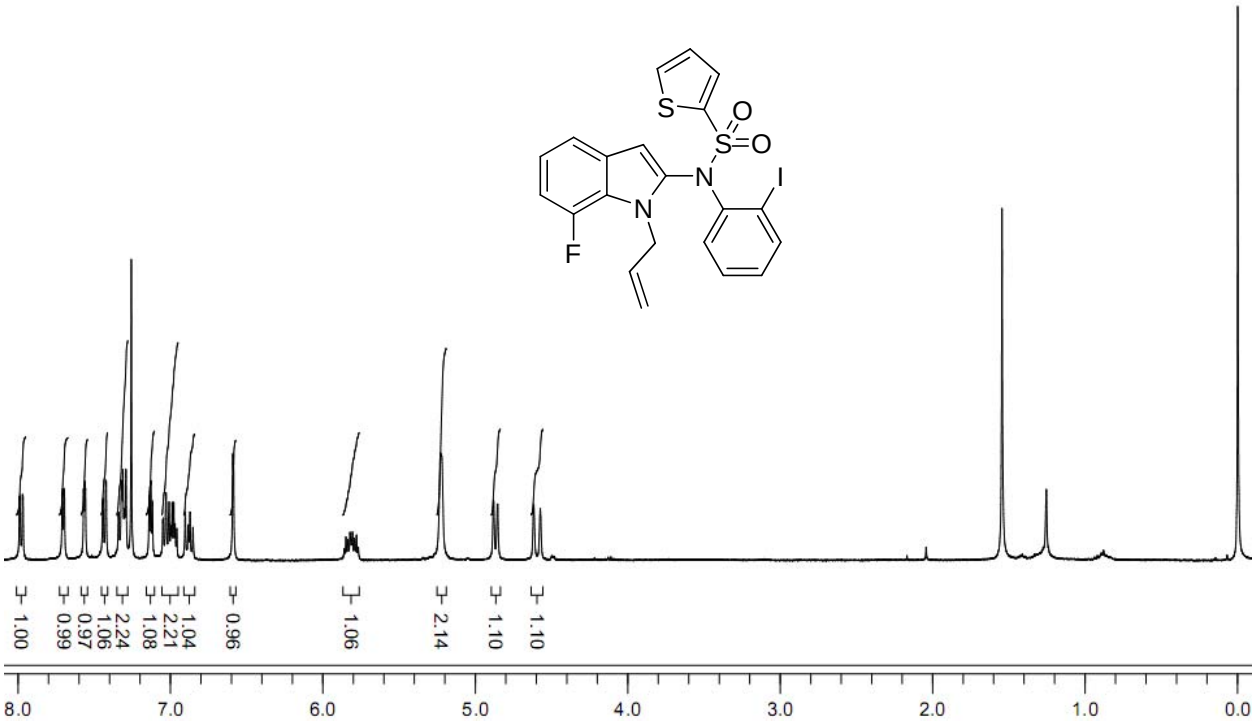
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1S4r** in $CDCl_3$



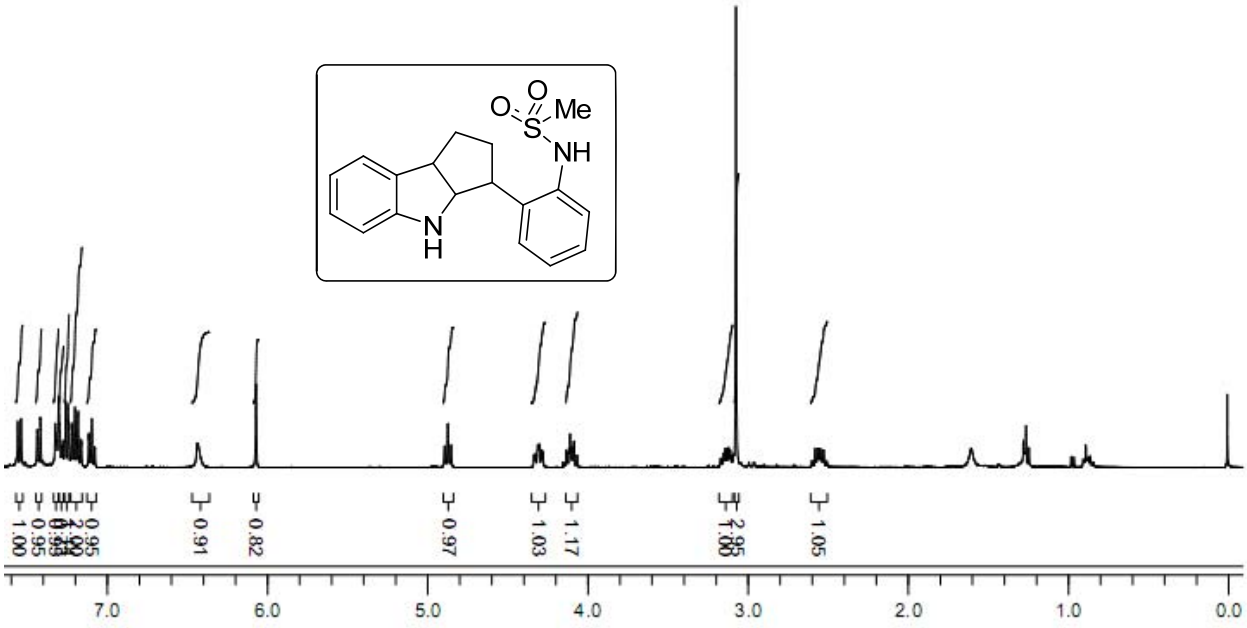
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1S4s** in $CDCl_3$



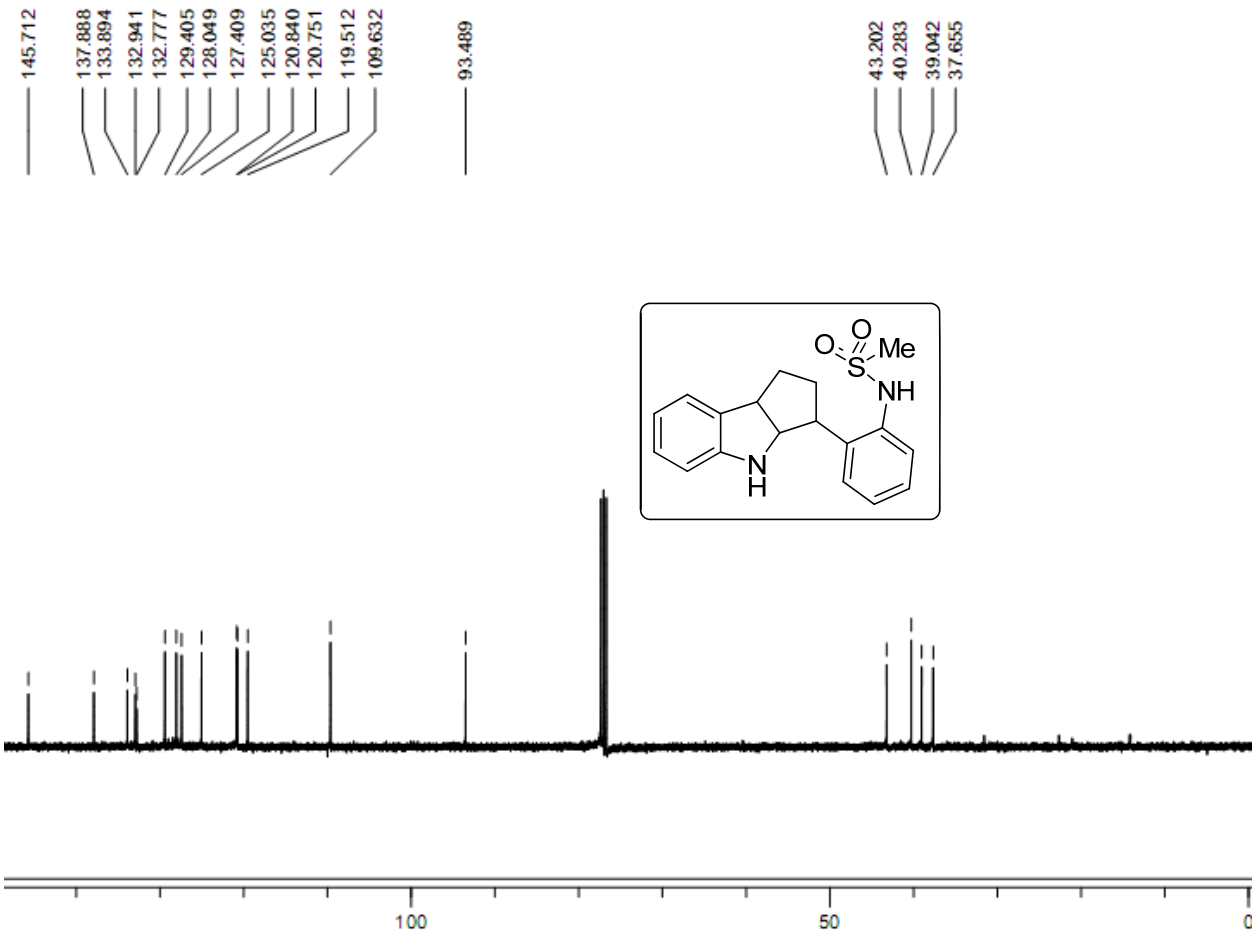
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1S4s** in $CDCl_3$



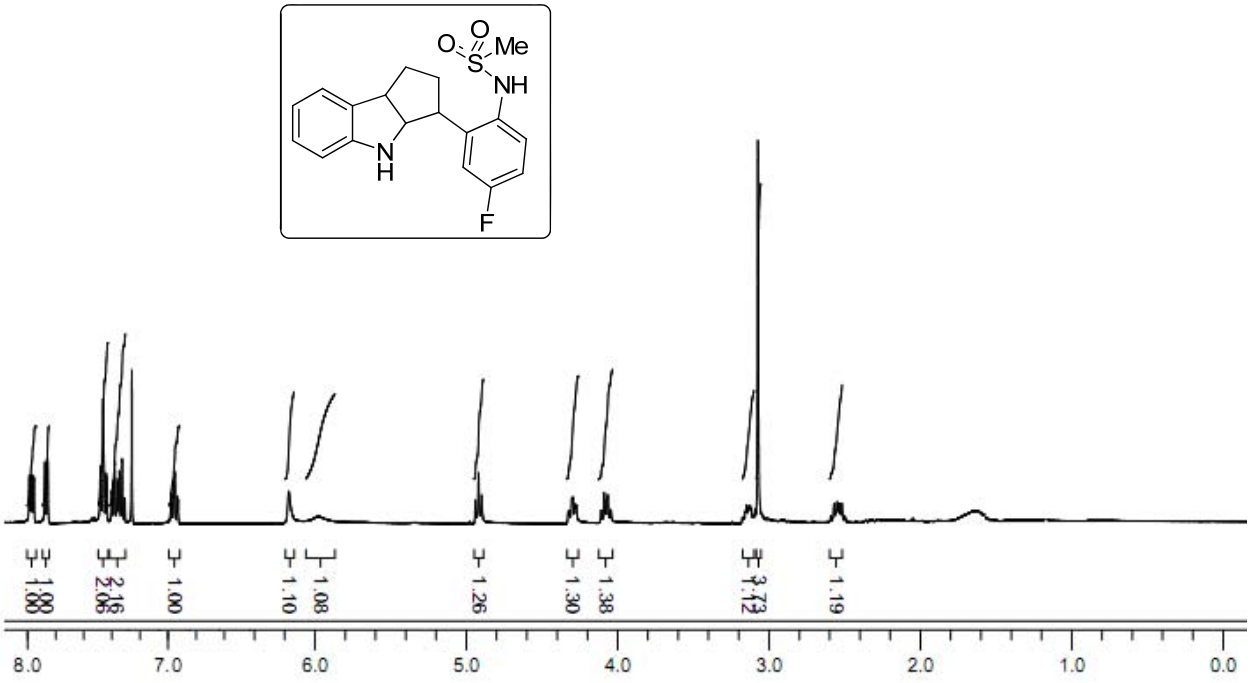
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1S4t** in $CDCl_3$



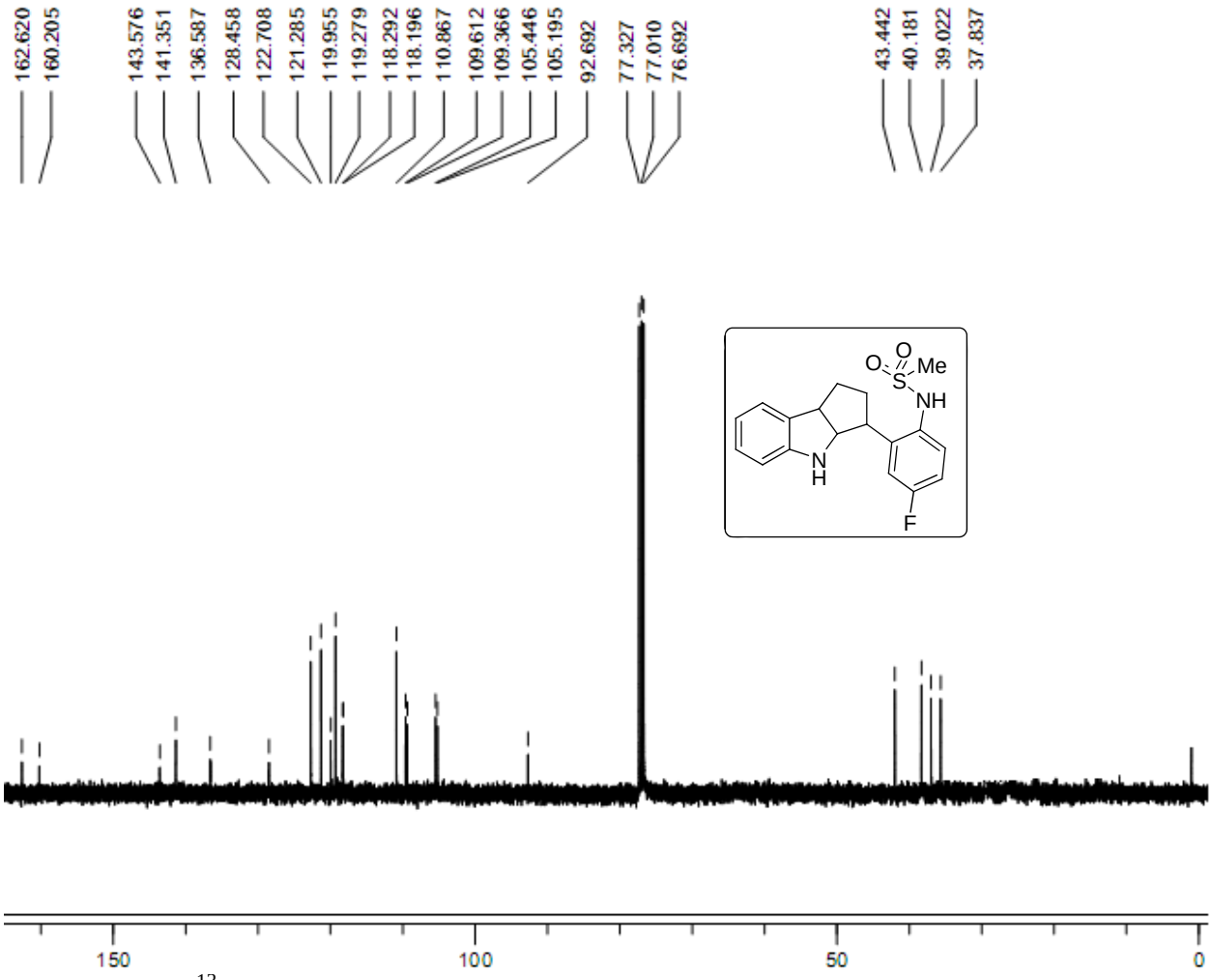
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1a** in $CDCl_3$



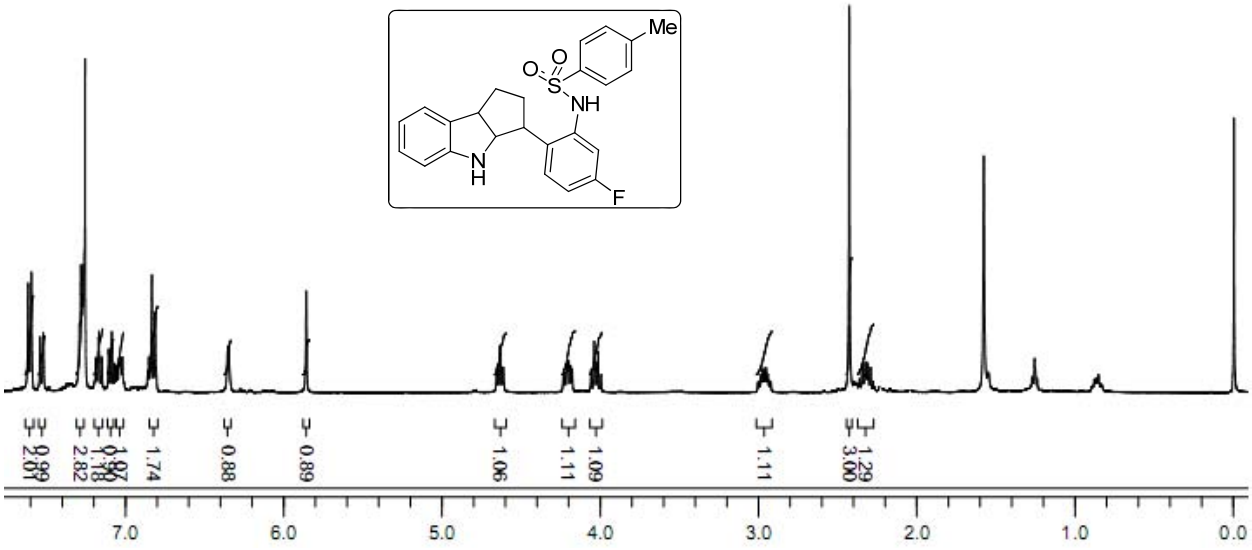
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1a** in $CDCl_3$



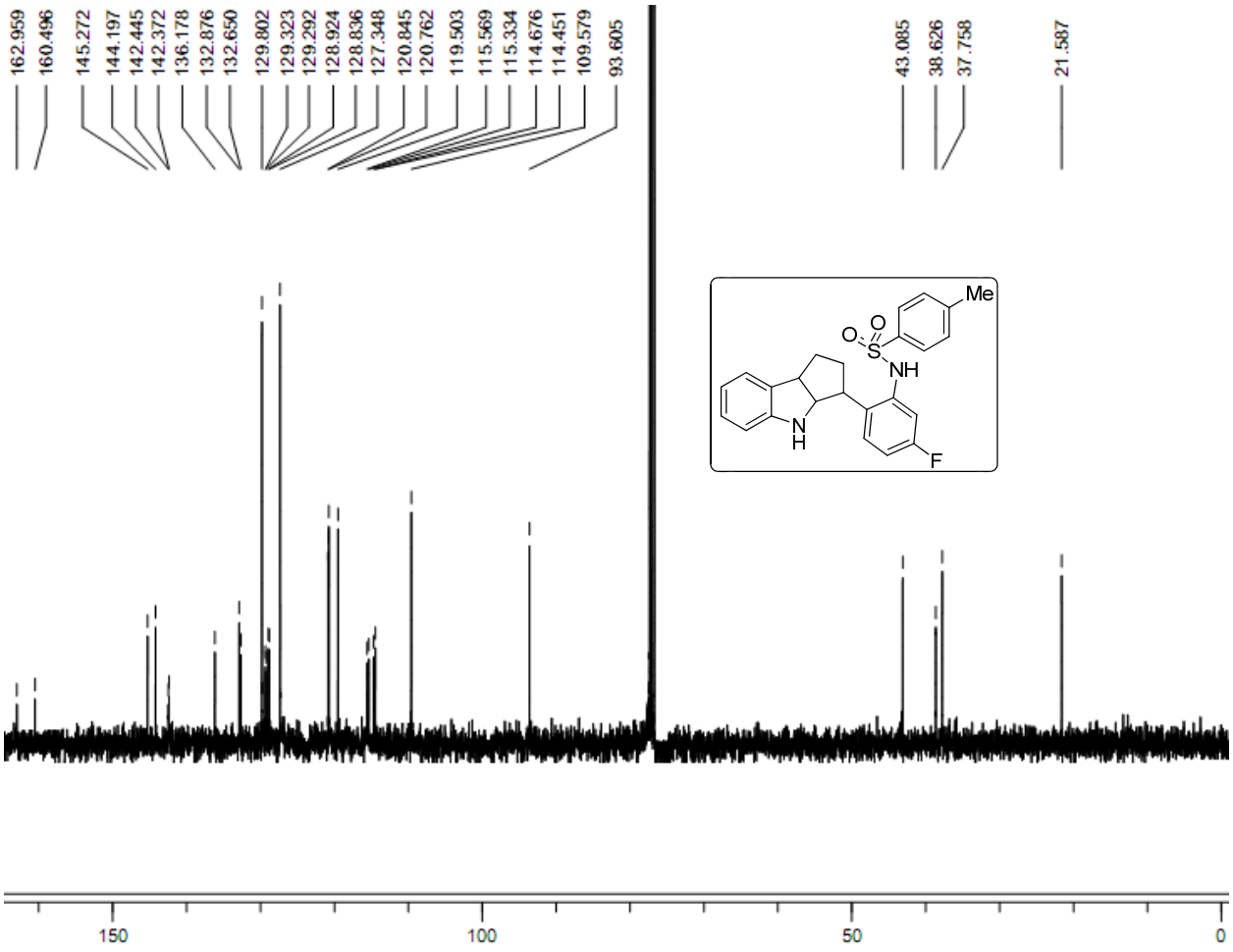
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1f** in $CDCl_3$



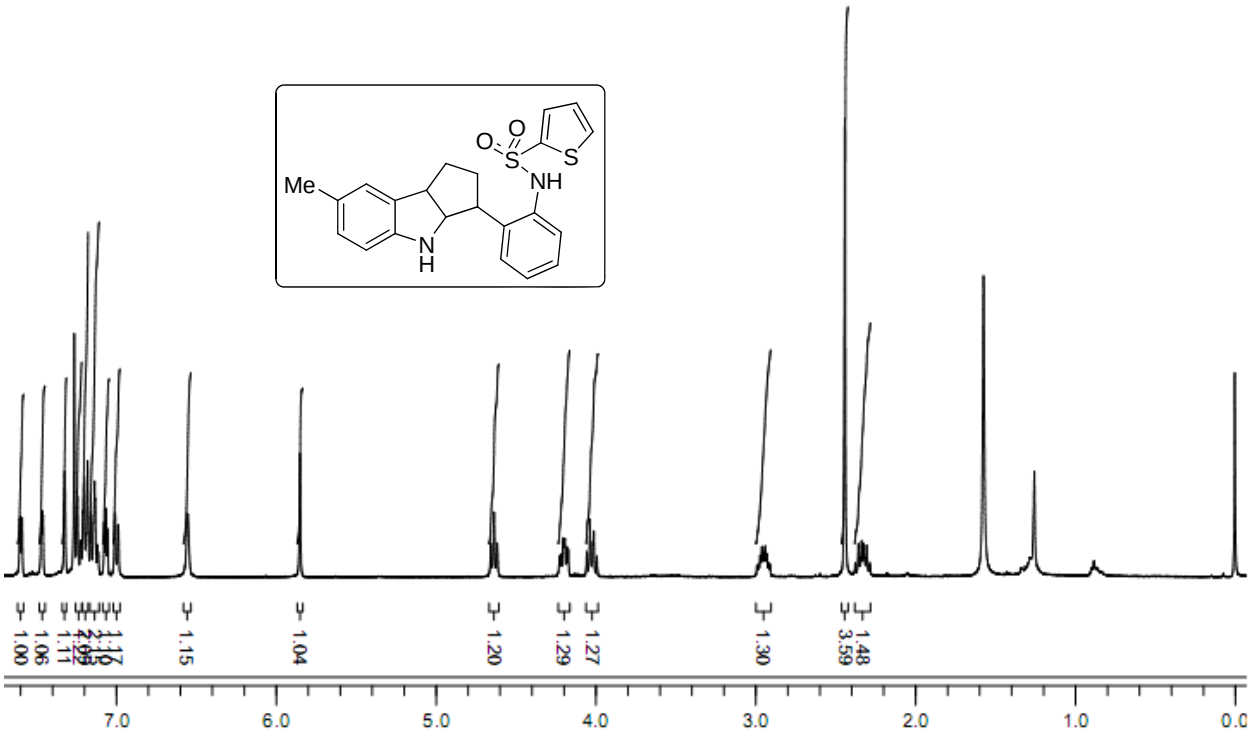
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1f** in $CDCl_3$



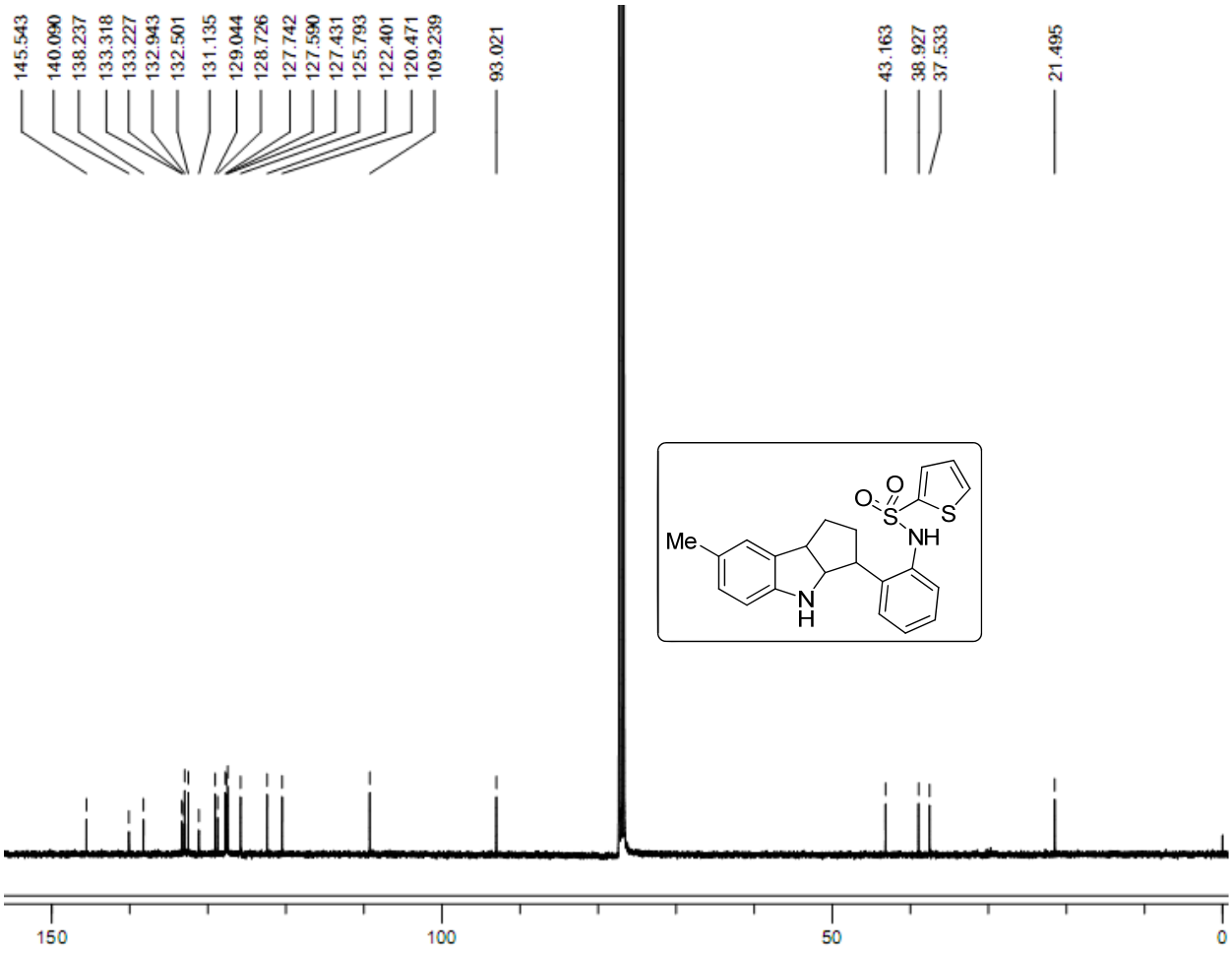
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1g** in $CDCl_3$



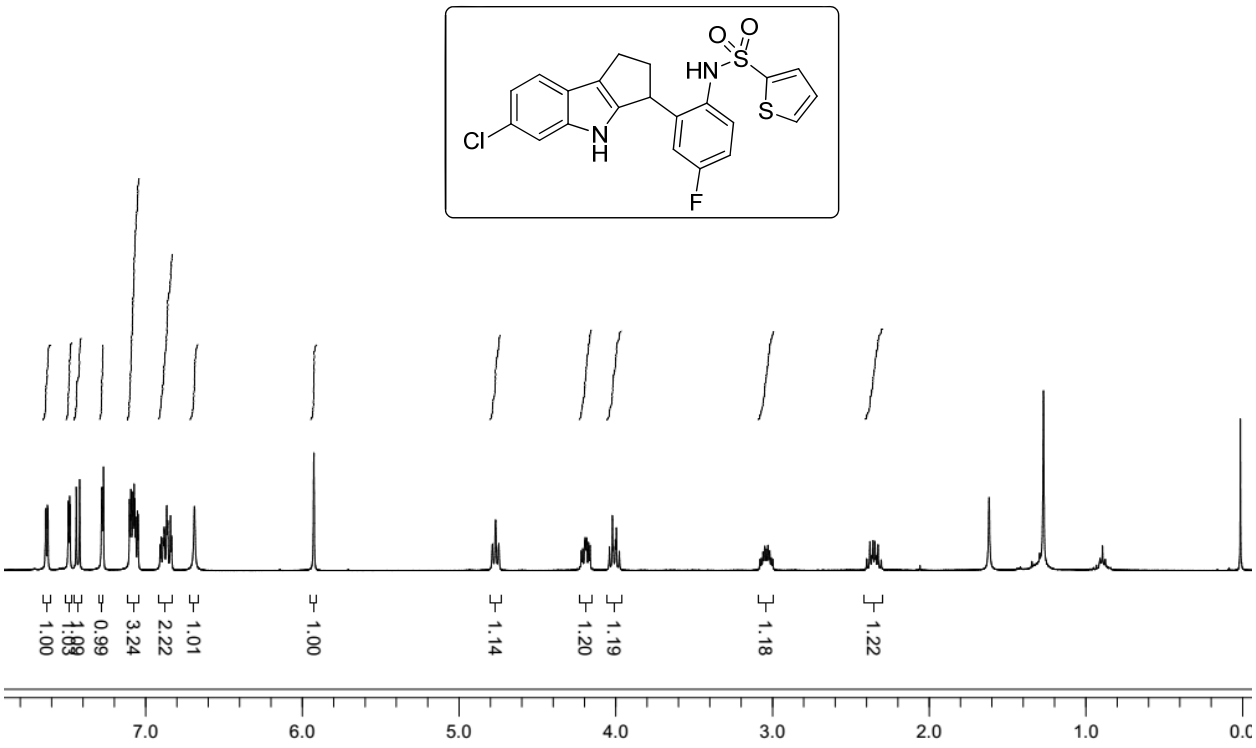
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1g** in $CDCl_3$



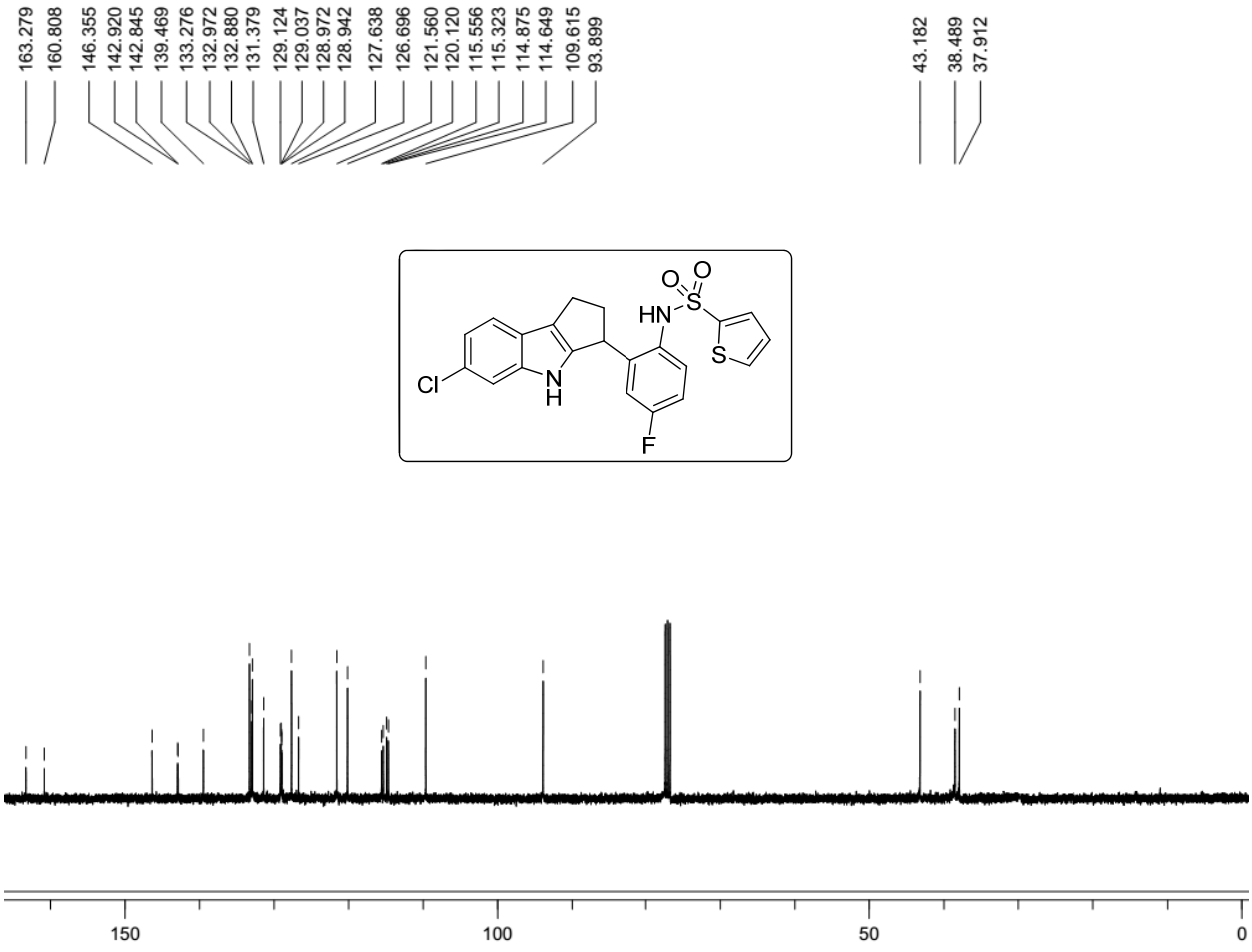
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1e** in $CDCl_3$



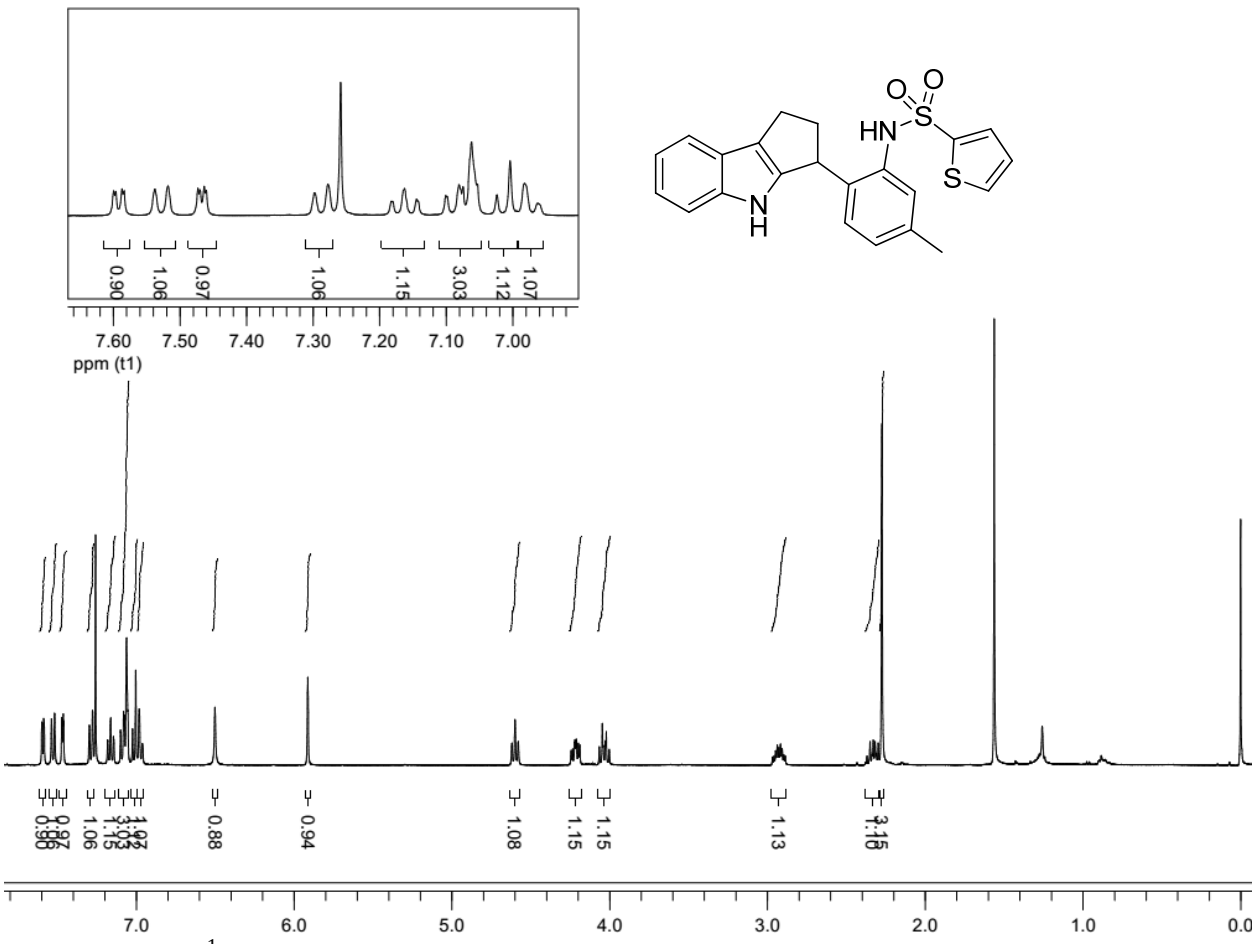
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1e** in $CDCl_3$



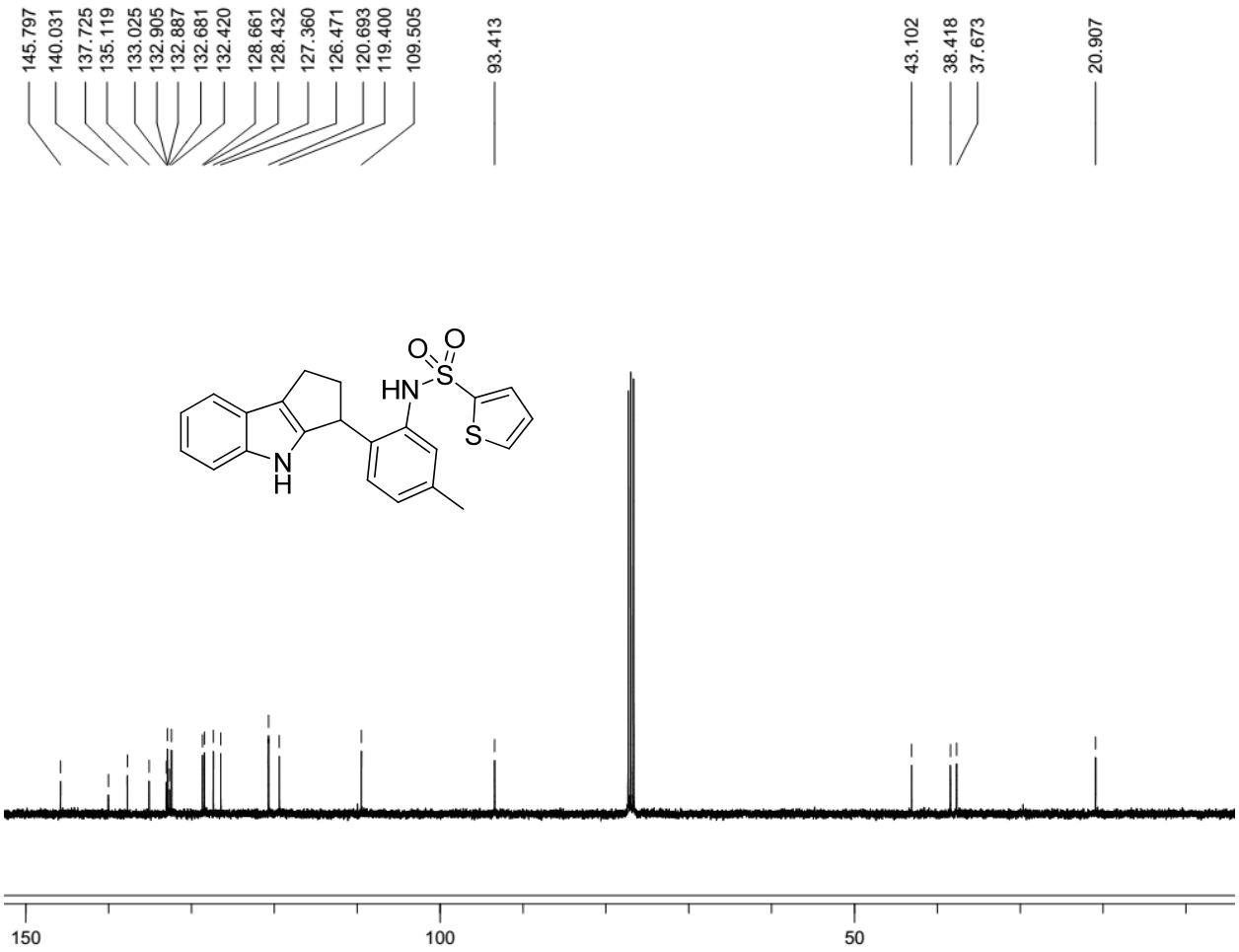
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1r** in $CDCl_3$



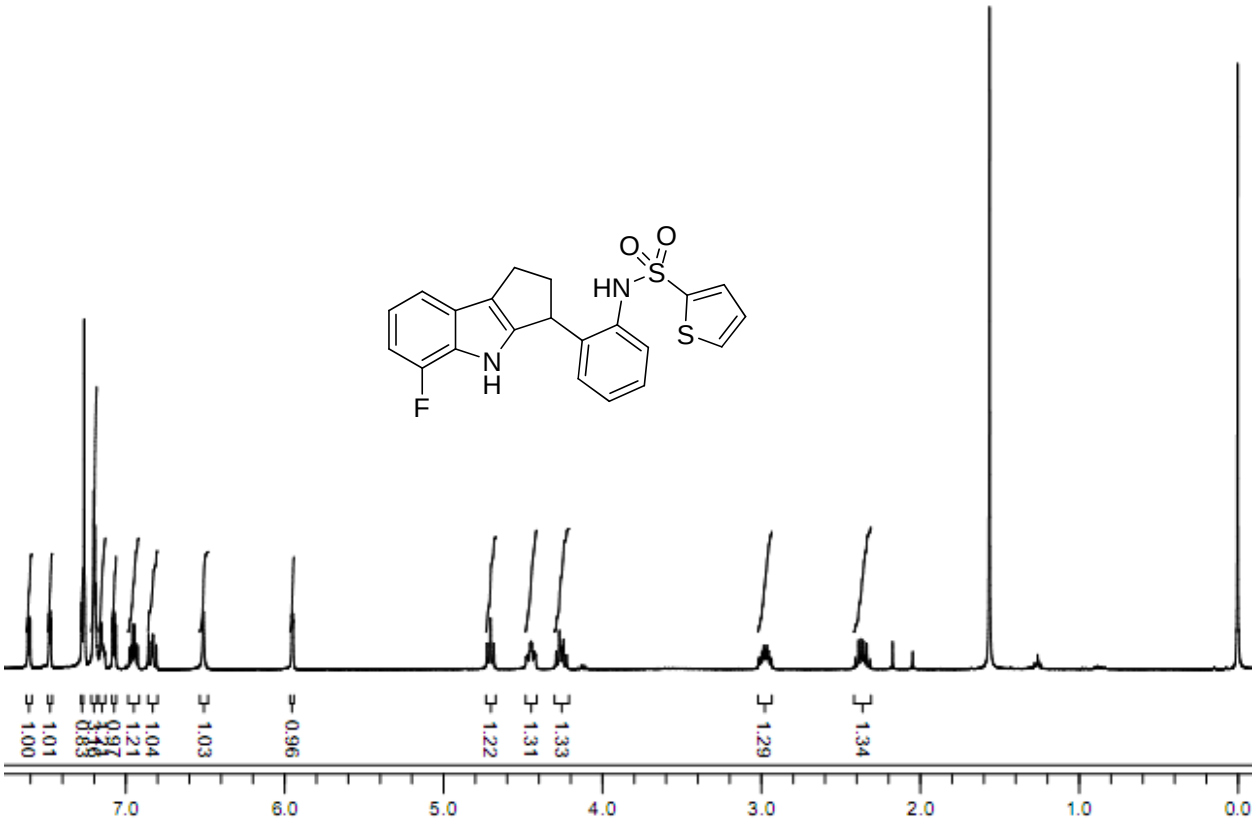
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1r** in $CDCl_3$



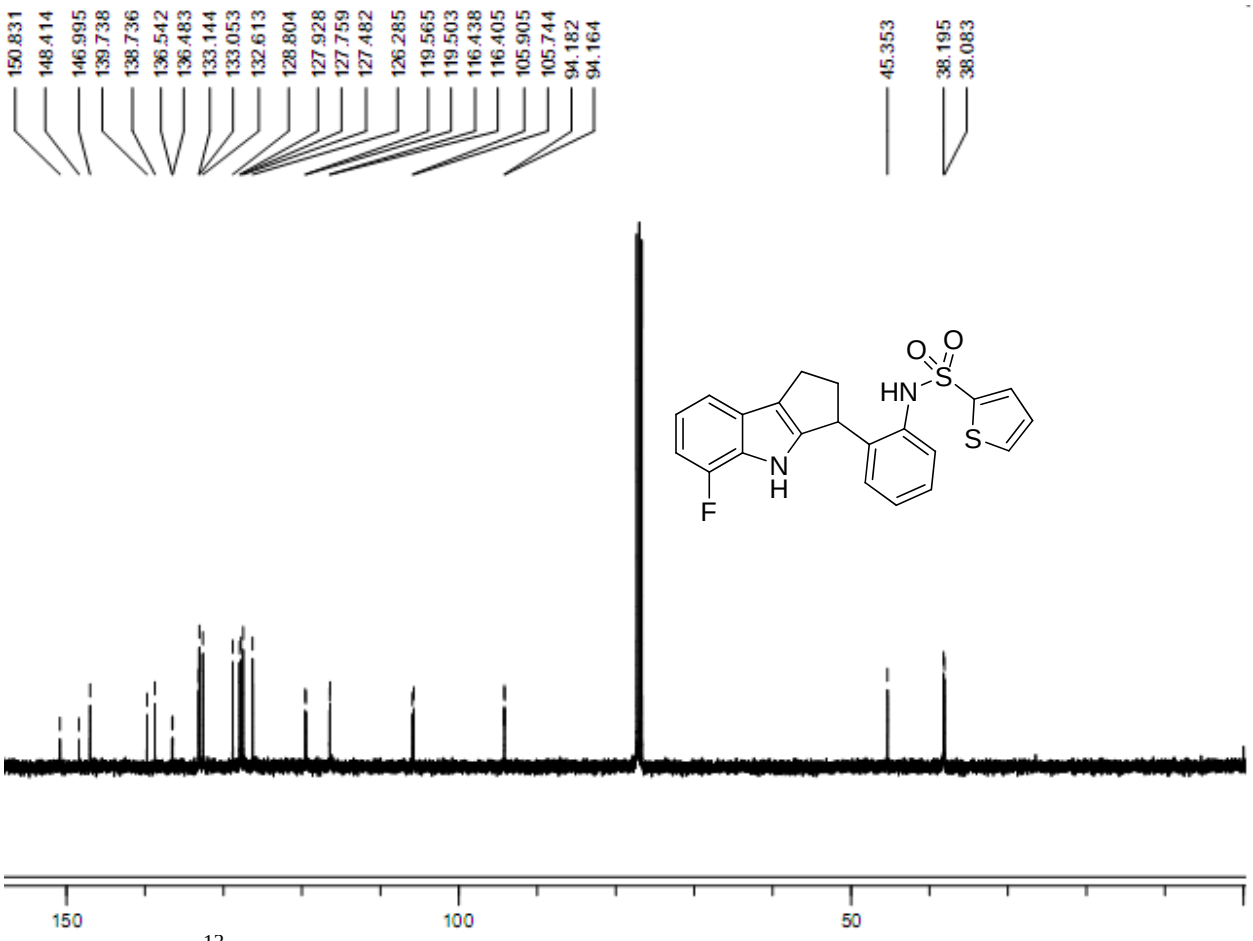
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1s** in $CDCl_3$



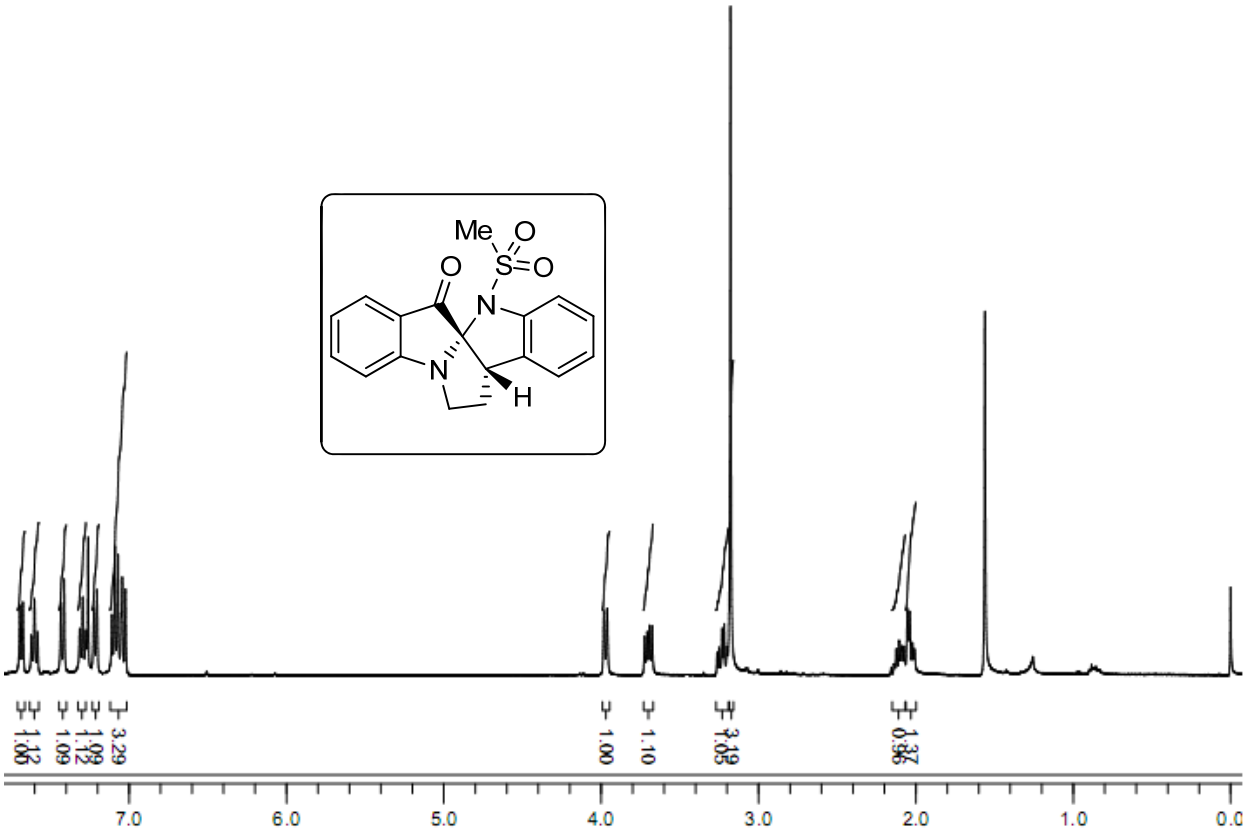
^{13}C NMR spectrum (Varian, 100 MHz) of compound **1s** in $CDCl_3$



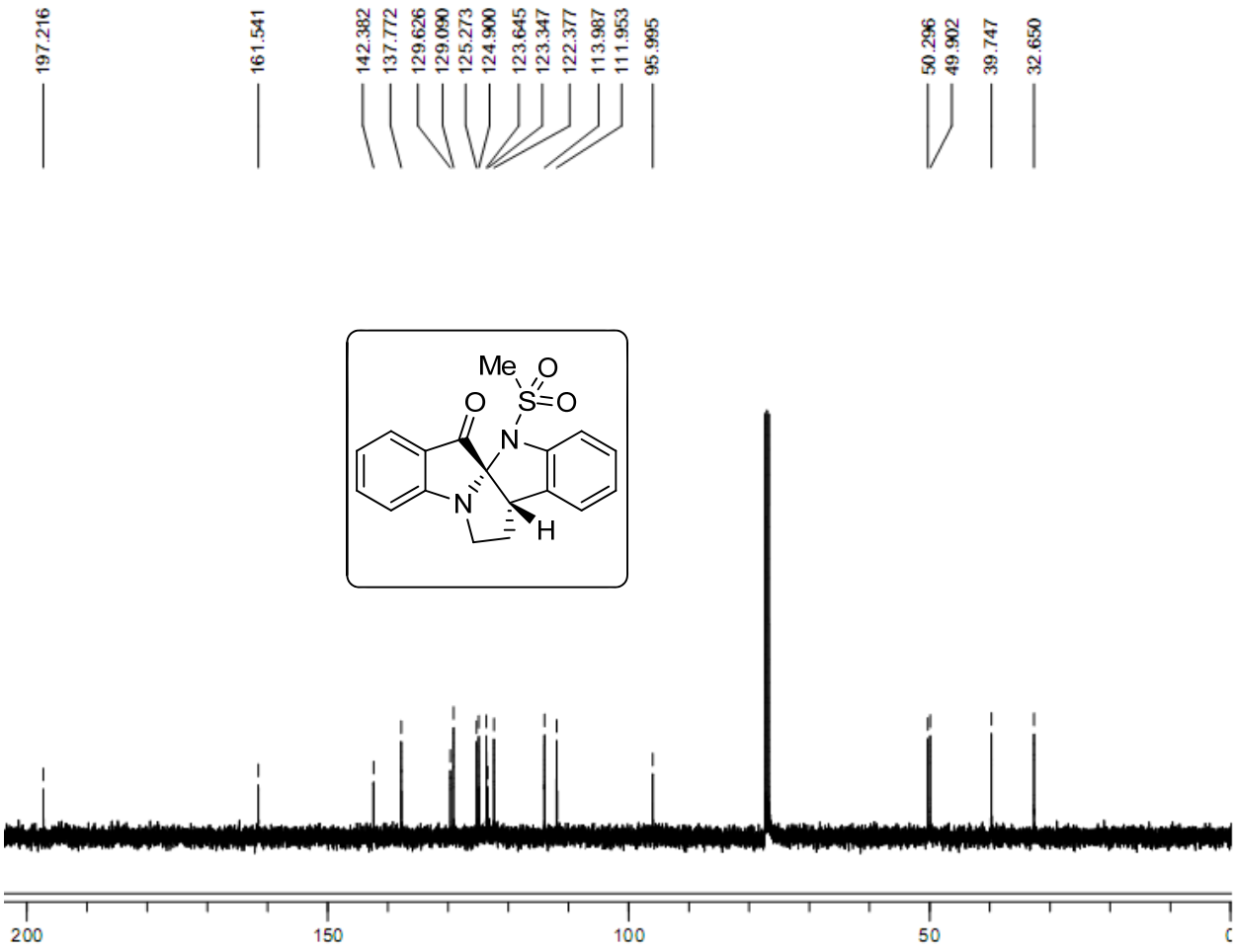
^{1}H NMR (Varian, 400 MHz) spectrum of compound **1t** in $CDCl_3$



^{13}C NMR spectrum (Varian, 100 MHz) of compound **1t** in $CDCl_3$



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2a** in $CDCl_3$

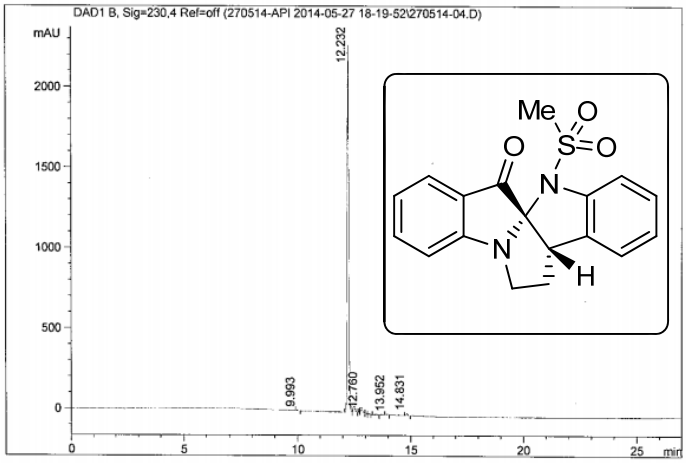


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2a** in $CDCl_3$

HPLC of compound **2a**

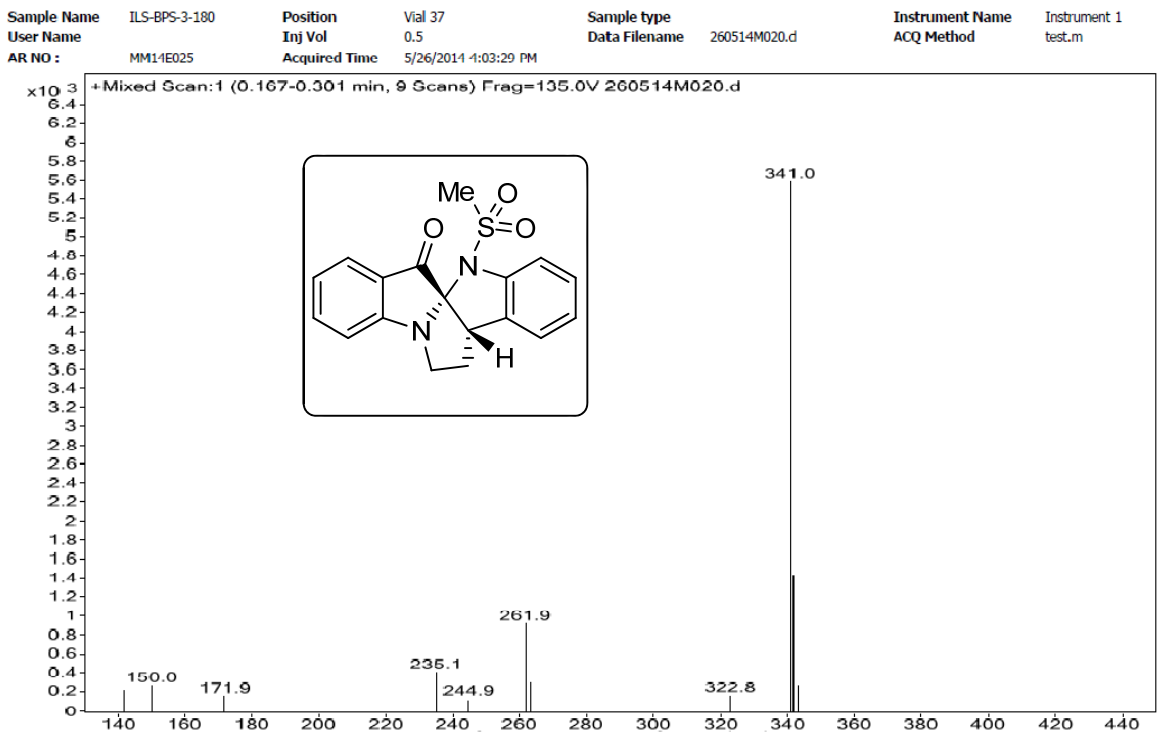
CPRI @ DRILS
HPLC ANALYSIS REPORT

```
Inj Date        : Tue, 27. May. 2014          Acq Operator: SHASHIDHAR
Sample Name     : ILS-BPS-3-180                             Vial 14
A.R Number      : CM14E012                    ->Inj. Vol.   : 5µL
Acq. Method     : D:\chem32\1\DATA\270514-API 2014-05-27 18-19-52\API ->
Analysis Method : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info     : Column: X-Terra C-18 250*4.6mm, 5µm
                  Mobile phase: A) 5mm Ammonium Acetate  in water B) ACN
                  T/%B:0/20,3/20,12/95,23/95,25/20,30/20
                  Flow:1.0ml/min  Diluent: ACN:WATER(50:50)
```

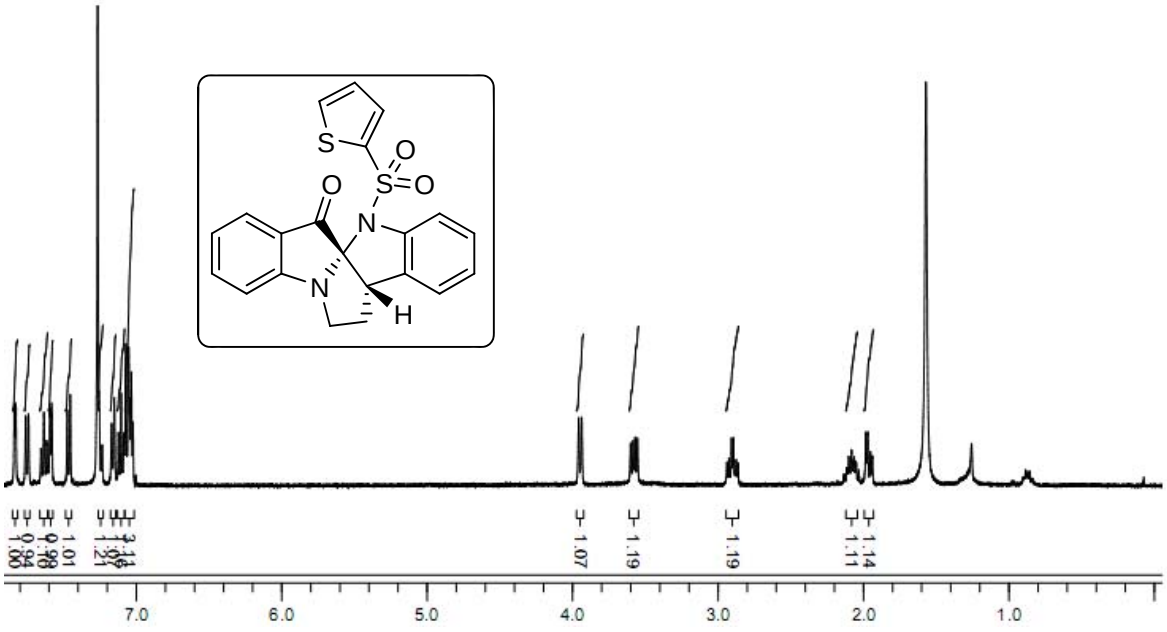


Signal 1: DAD1 B, Sig=230,4 Ref=off

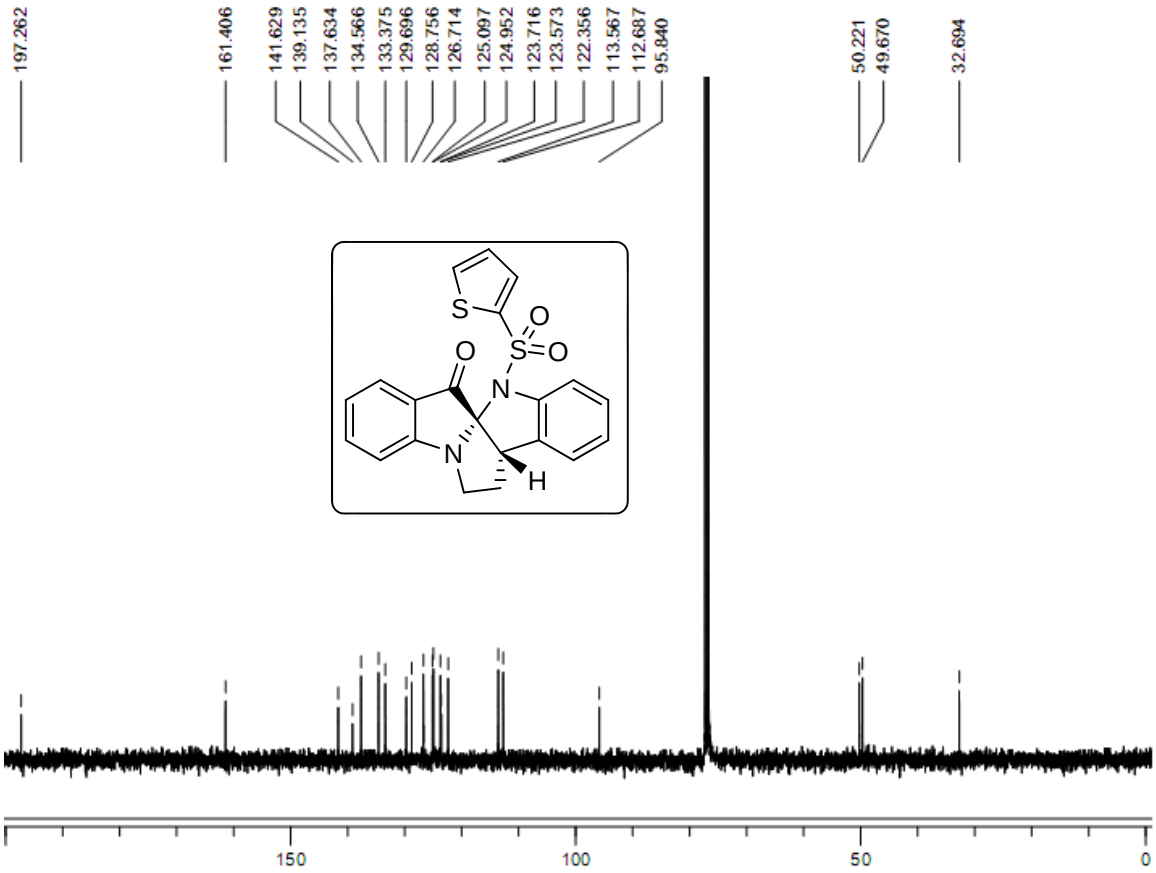
Peak #	RT [min]	Area	Area %
1	9.993	14.972	0.131
2	12.232	10840.727	96.465
3	12.501	186.677	1.635
4	12.760	20.405	0.179
5	12.833	206.185	1.806
6	13.027	27.736	0.743
7	13.154	21.844	0.191
8	13.465	25.585	0.224
9	13.952	15.275	0.134
10	14.831	56.059	0.491



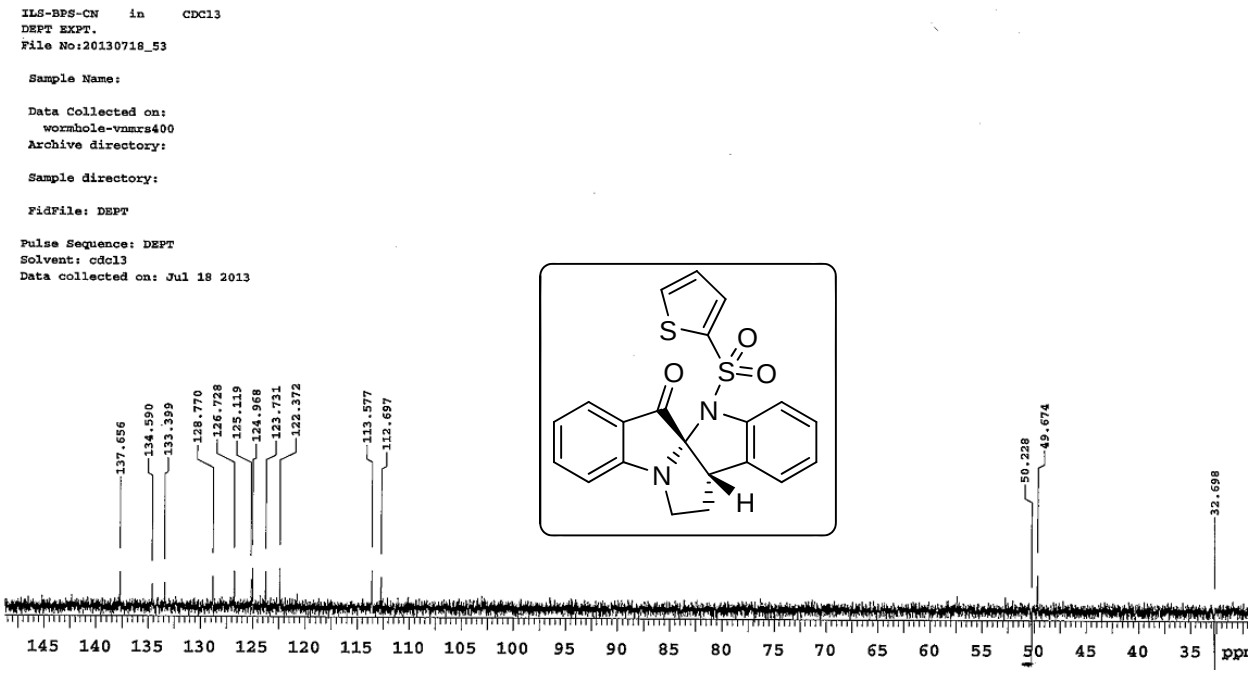
Mass spectra of compound **2a**



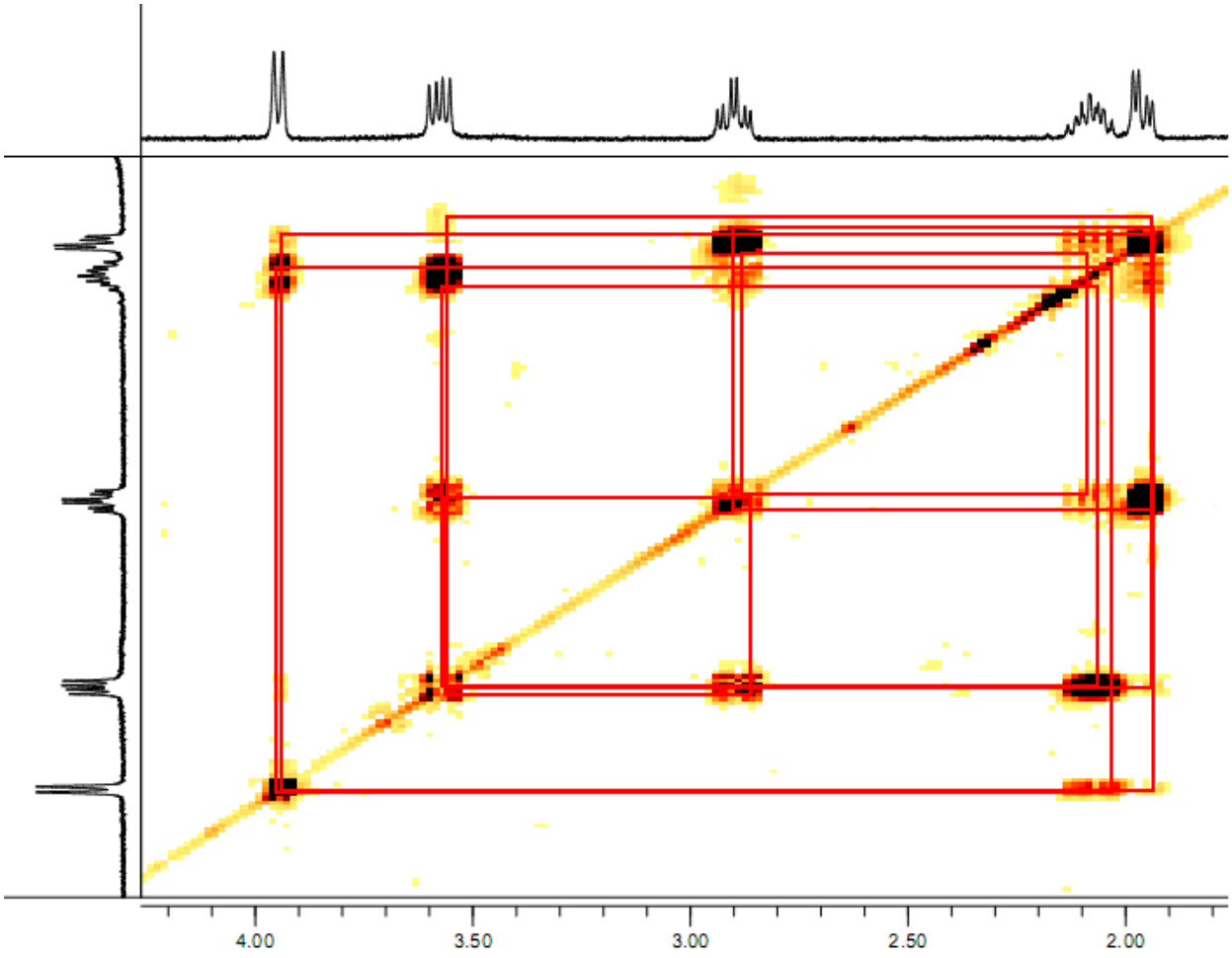
^{1}H NMR (Varian, 400 MHz) spectrum of compound **2b** in $CDCl_3$



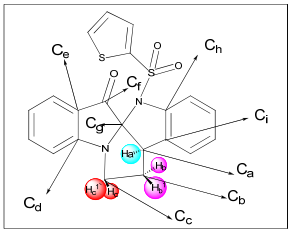
^{13}C NMR spectrum (Varian, 100 MHz) of compound **2b** in $CDCl_3$

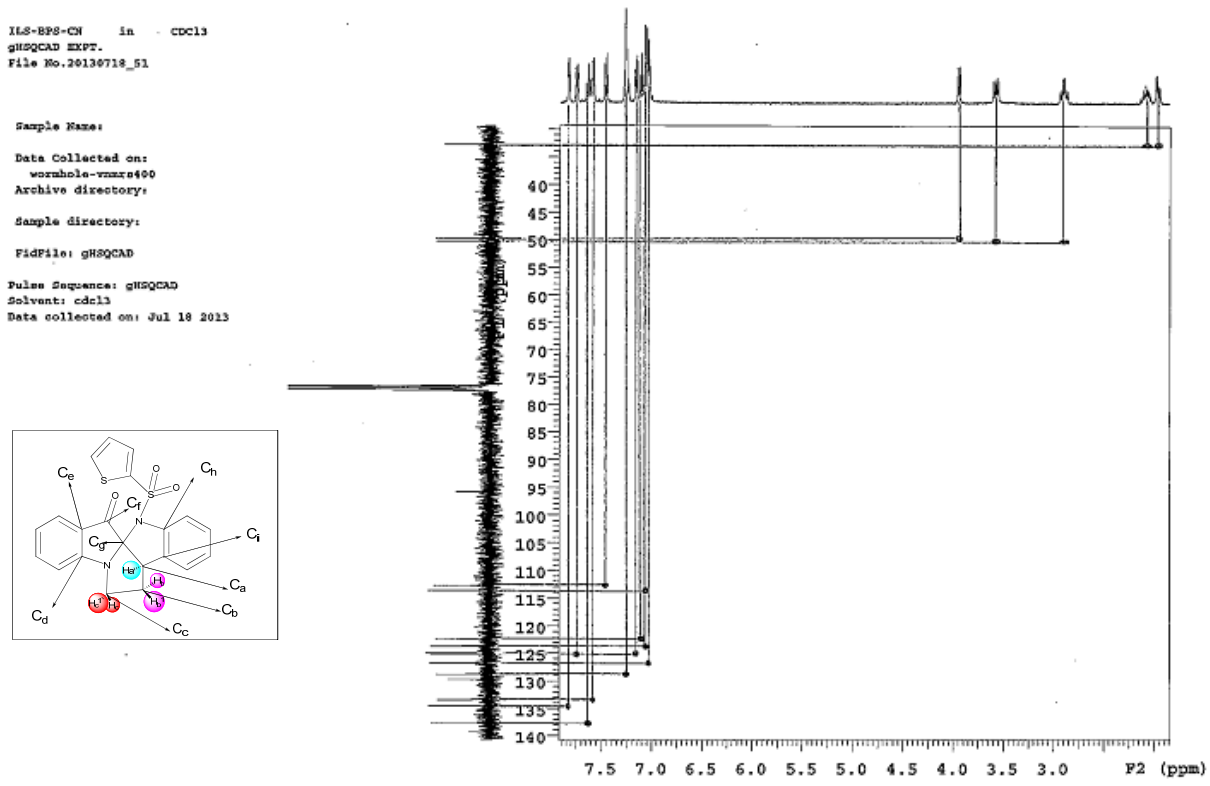


DEPT of compound **2b**

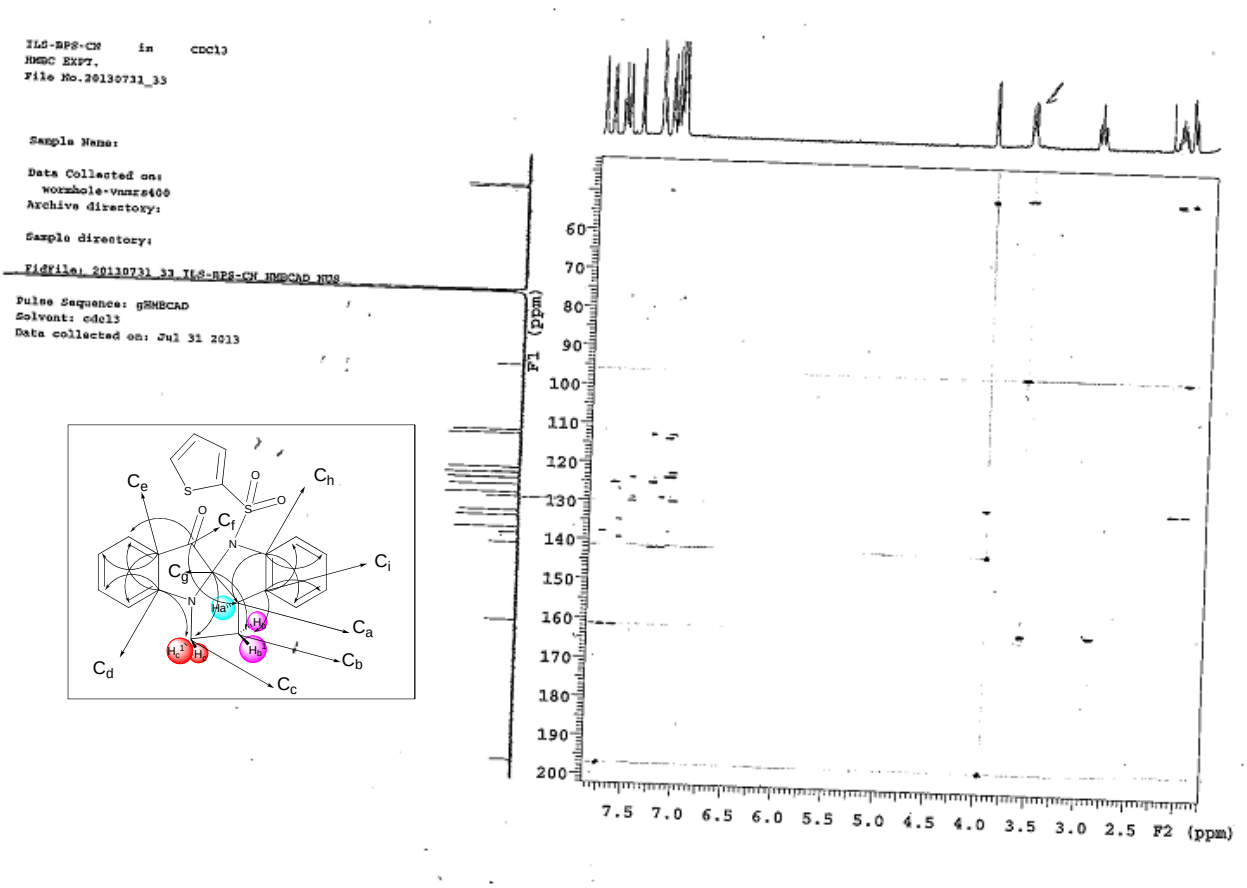


^{1}H-^{1}H COSY of compound **2b**





HSQC of compound **2b**

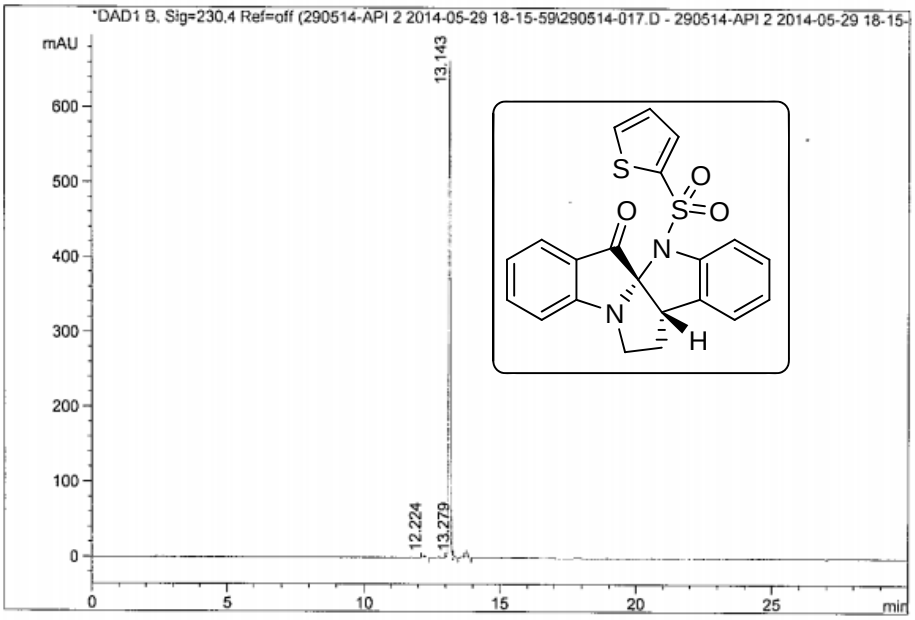


HMBC of compound **2b**

HPLC of compound **2b**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Inj Date : Thu, 29. May. 2014 Acq Operator: SHASHIDHAR
Sample Name : ILS-BPS-3-79 Vial 52
A.R Number : CM14E018 ->Inj. Vol. : 5µL
Acq. Method : D:\chem32\1\DATA\290514-API 2 2014-05-29 18-15-59\AP->
Analysis Method : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info : Column: X-Terra C-18 250*4.6mm, 5µm
Mobile phase: A) 5mm Ammonium Acetate in water B) ACN
T/%B:0/20,3/20,12/95,23/95,25/20,30/20
Flow:1.0ml/min Diluent: ACN:WATER(50:50)

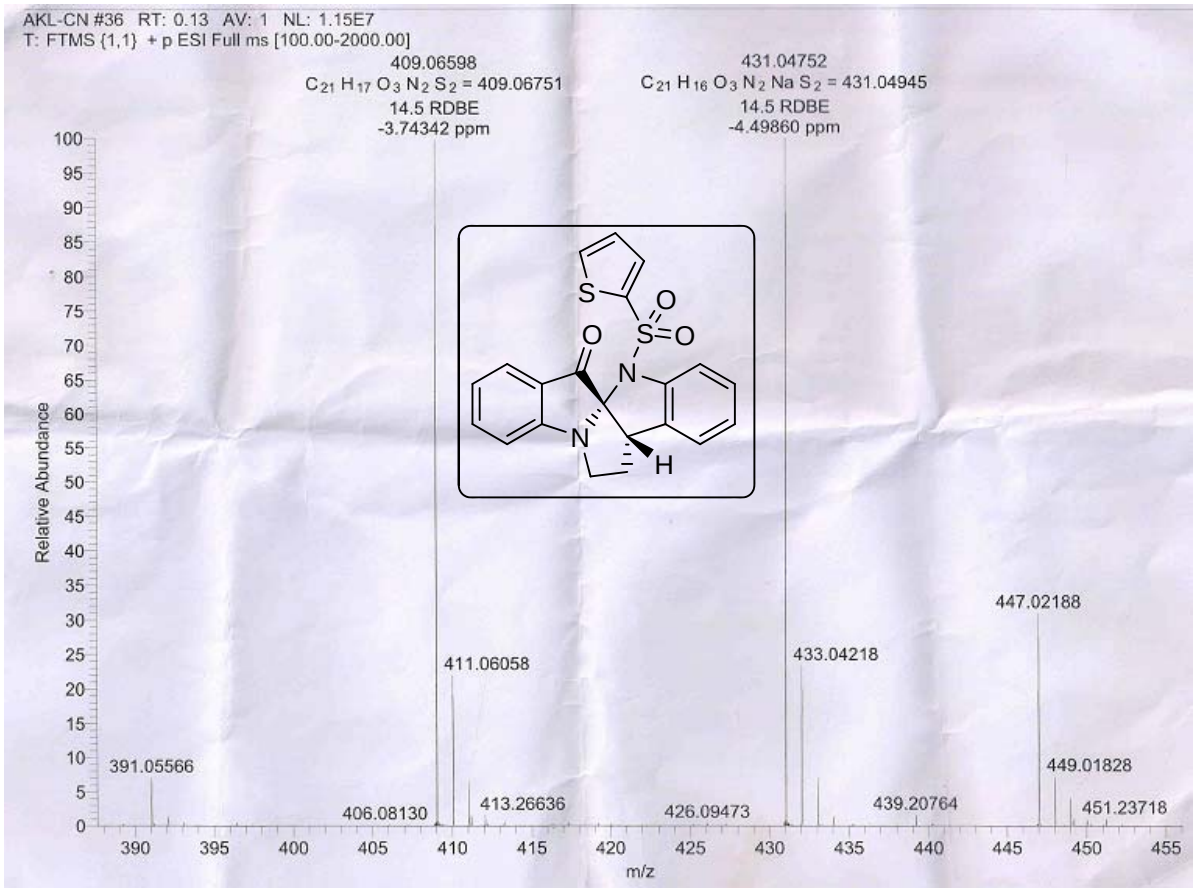


Signal 1: DAD1 B, Sig=230,4 Ref=off

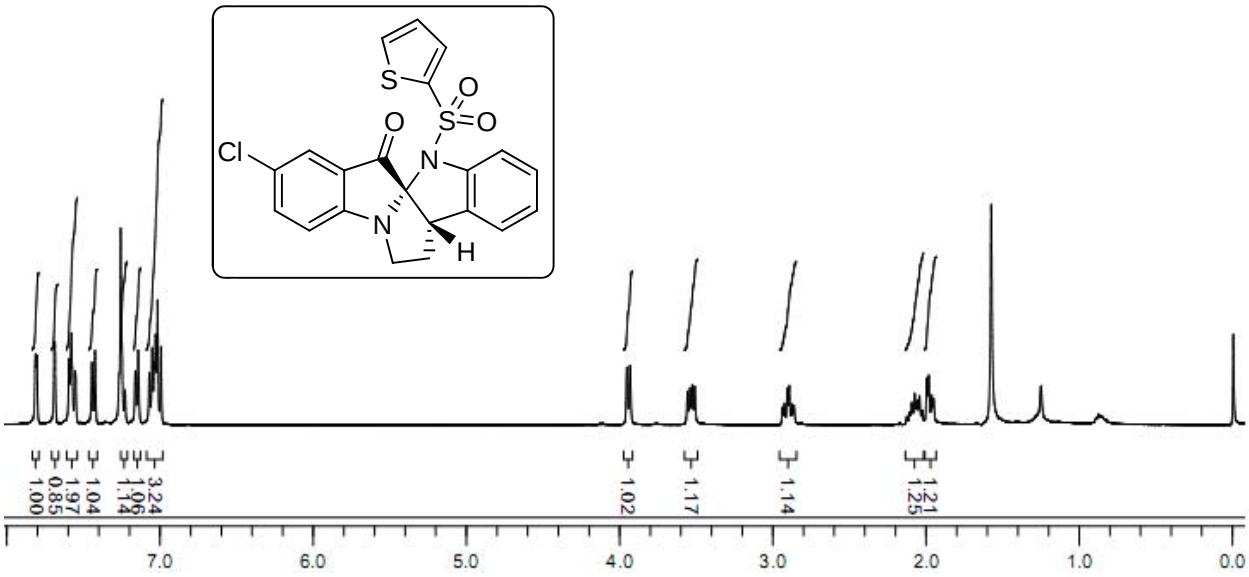
Peak #	RT [min]	Area	Area %
1	12.224	11.089	0.367
2	13.143	2960.202	97.887
3	13.279	8.671	0.287
4	13.773	44.138	1.460

Analysed by : 30/05/14

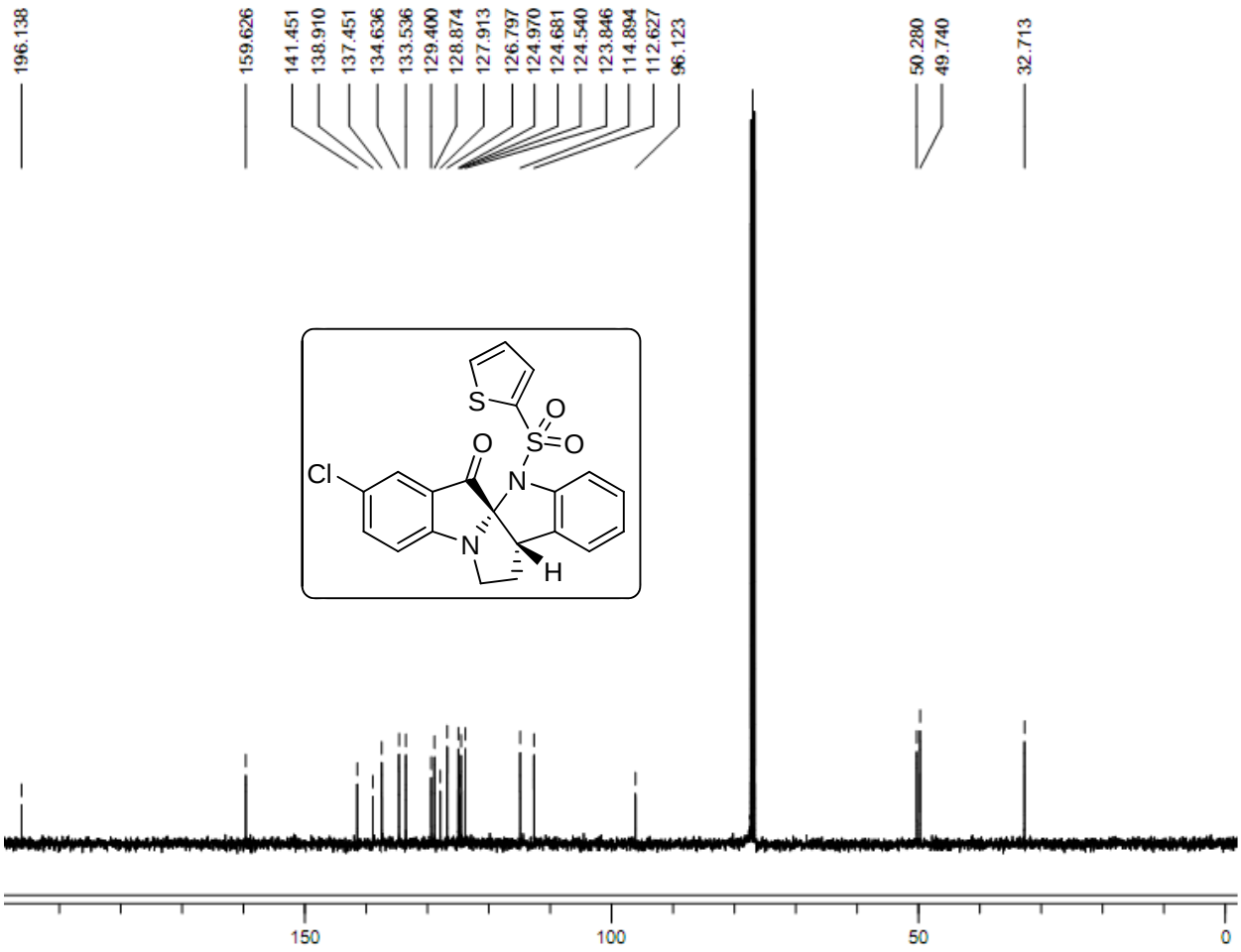
Checked by : 30/5/14



HRMS of compound **2b**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2c** in $CDCl_3$

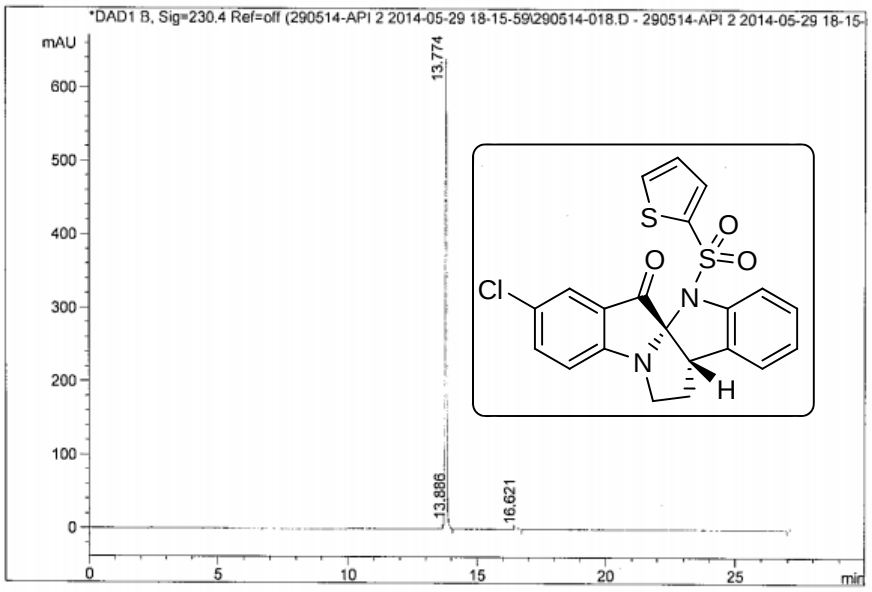


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2c** in $CDCl_3$

HPLC of compound **2c**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Inj Date : Thu, 29. May. 2014 Acq Operator: SHASHIDHAR
Sample Name : ILS-BPS-3-62 Vial 53
A.R Number : CM14E020 ->Inj. Vol. : 5µL
Acq. Method : D:\chem32\1\DATA\290514-API 2 2014-05-29 18-15-59\AP->
Analysis Method : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info : Column: X-Terra C-18 250*4.6mm, 5µm
Mobile phase: A) 5mm Ammonium Acetate in water B) ACN
T/%B:0/20,3/20,12/95,23/95,25/20,30/20
Flow:1.0ml/min Diluent: ACN:WATER(50:50)



Signal 1: DAD1 B, Sig=230,4 Ref=off

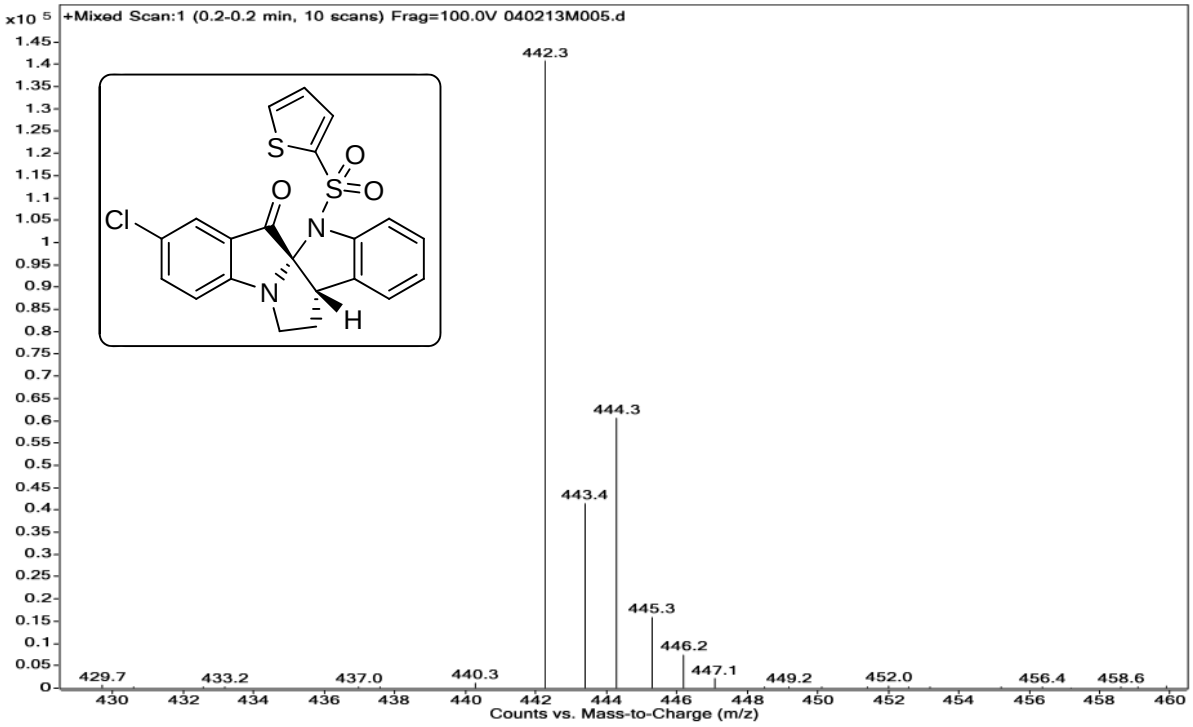
Peak #	RT [min]	Area	Area %
1	13.774	2858.811	99.049
2	13.886	18.771	0.650
3	16.621	8.689	0.301

Analysed by : 30/05/14

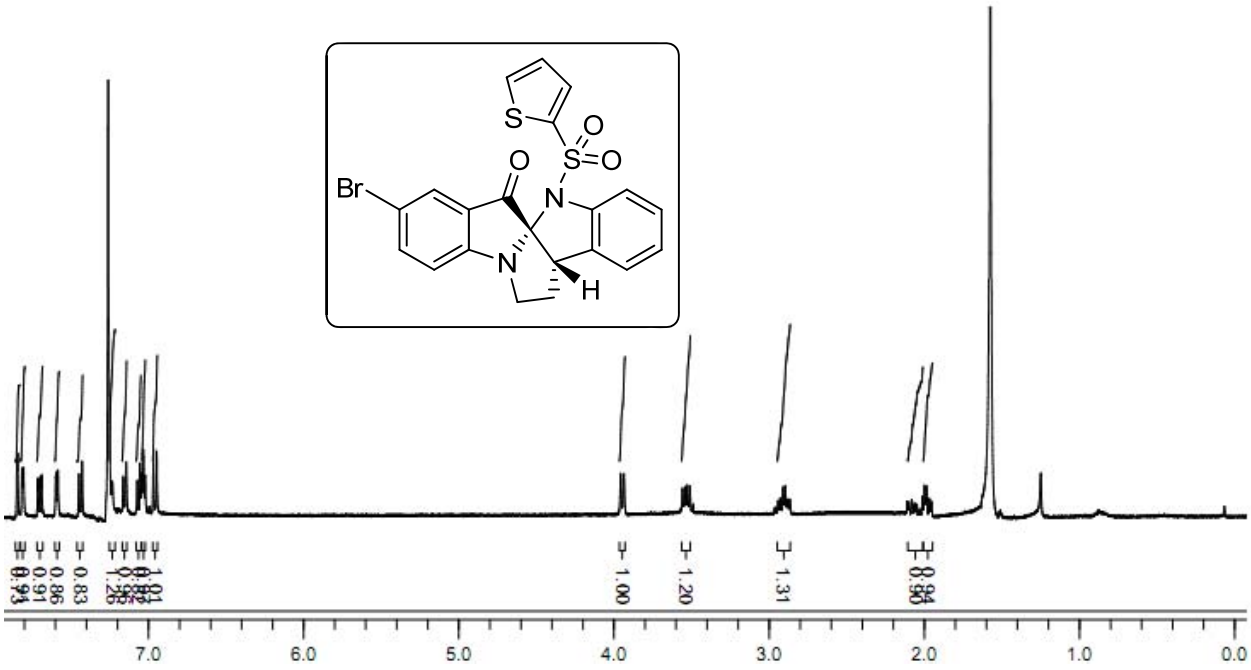
Checked by : 30/5/14

trument 1 Fri, 30. May. 2014 10:23:00 am Page 1 of 1

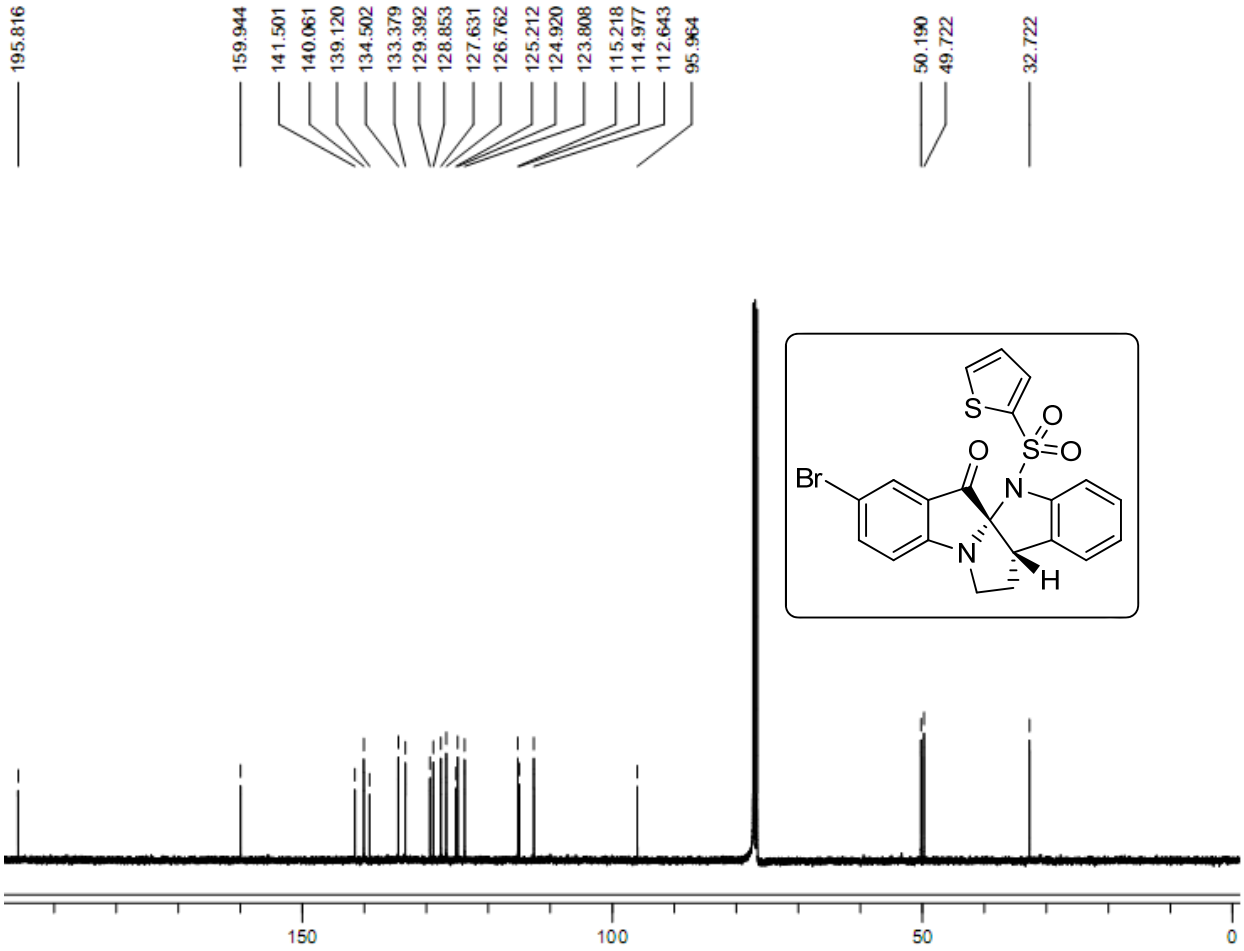
Sample Name	ILS/BPS/3-62	**Position**	Vial 2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0.5	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	040213M005.d	**ACQ Method**	ILS.m	**Comment**		**Acquired Time**	2/4/2013 12:51:35 PM



Mass spectra of compound **2c**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2d** in $CDCl_3$

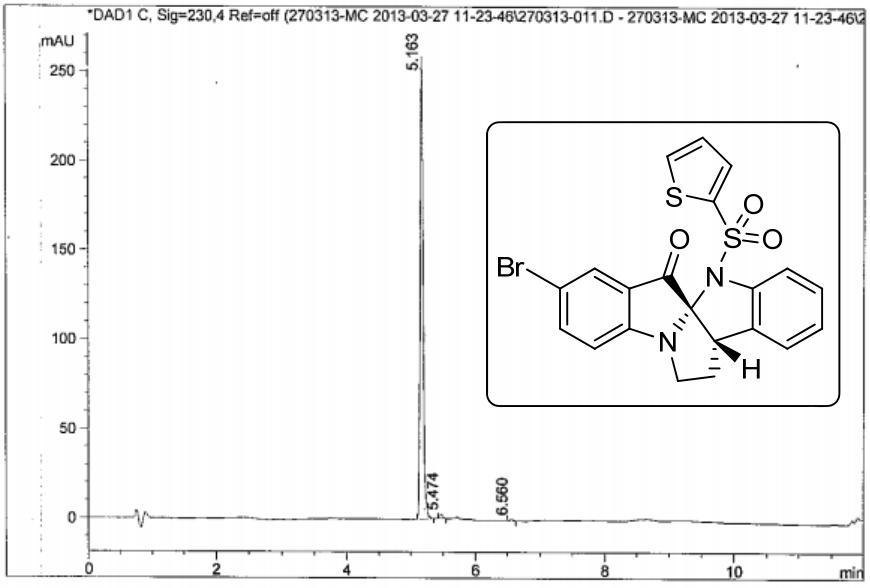


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2d** in $CDCl_3$

HRMS of compound **2d**

COSMIC DISCOVERIES @ ILS
HPLC ANALYSIS REPORT

		Seq Line :	11
Injection Date	: Wed, 27. Mar. 2013	Location :	Vial 58
Sample Name	: ILS-BPS-3-85	Inj. No. :	1
Acq Operator	: VARMA	Inj. Vol. :	5 µl
Acq. Method	: D:\Chem32\1\DATA\270313-MC 2013-03-27 11-23-46\C-18 ->		
Analysis Method	: D:\CHEM32\1\METHODS\C-18 A80B20GM.M		
Method Info	: Column:Symmetry C-18 75*4.6mm,3.5µ		
	Mobile phase: A) 0.1% HCOOH in water,B) ACN(GRADIENT) T/		
	B%:0/20,0.5/20,4/98,10/98,10.5/20,12/20		
	Flow:1.0 ml/min Diluent: ACN:Water(80:20)		



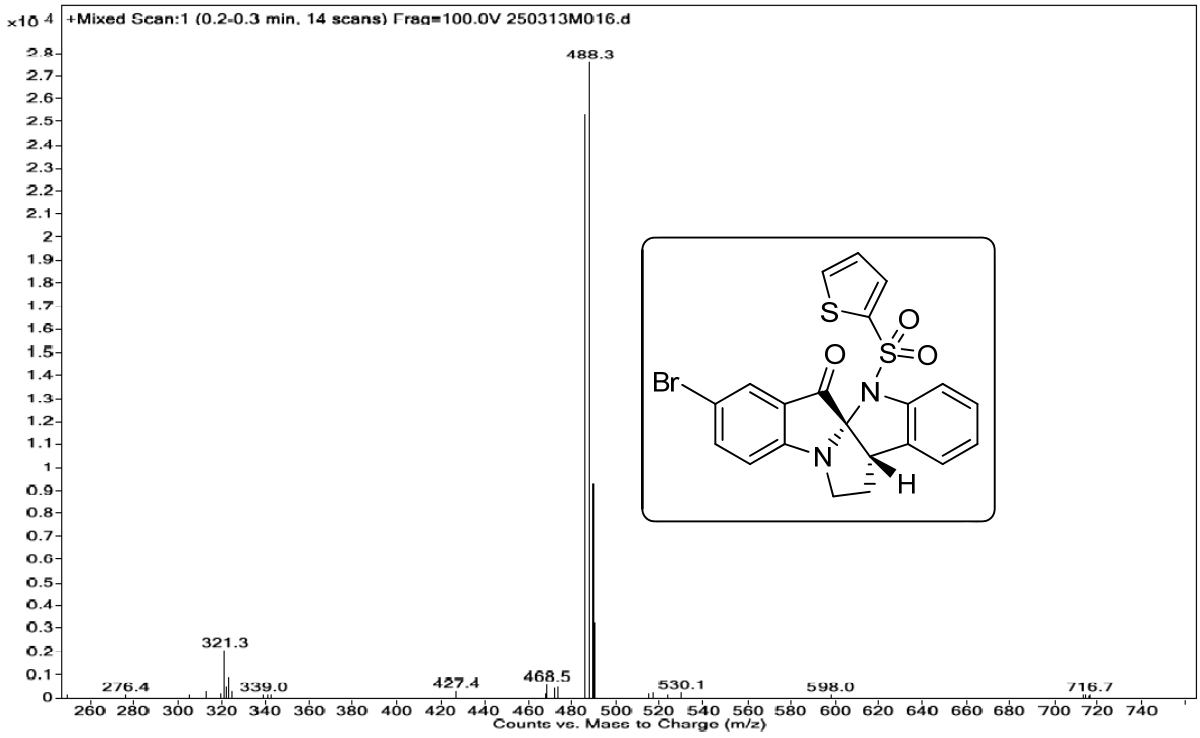
Signal 1: DAD1 C, Sig=230,4 Ref=off

Peak #	RT [min]	Area	Area %
1	5.163	841.146	99.003
2	5.474	6.264	0.737
3	6.560	2.204	0.259

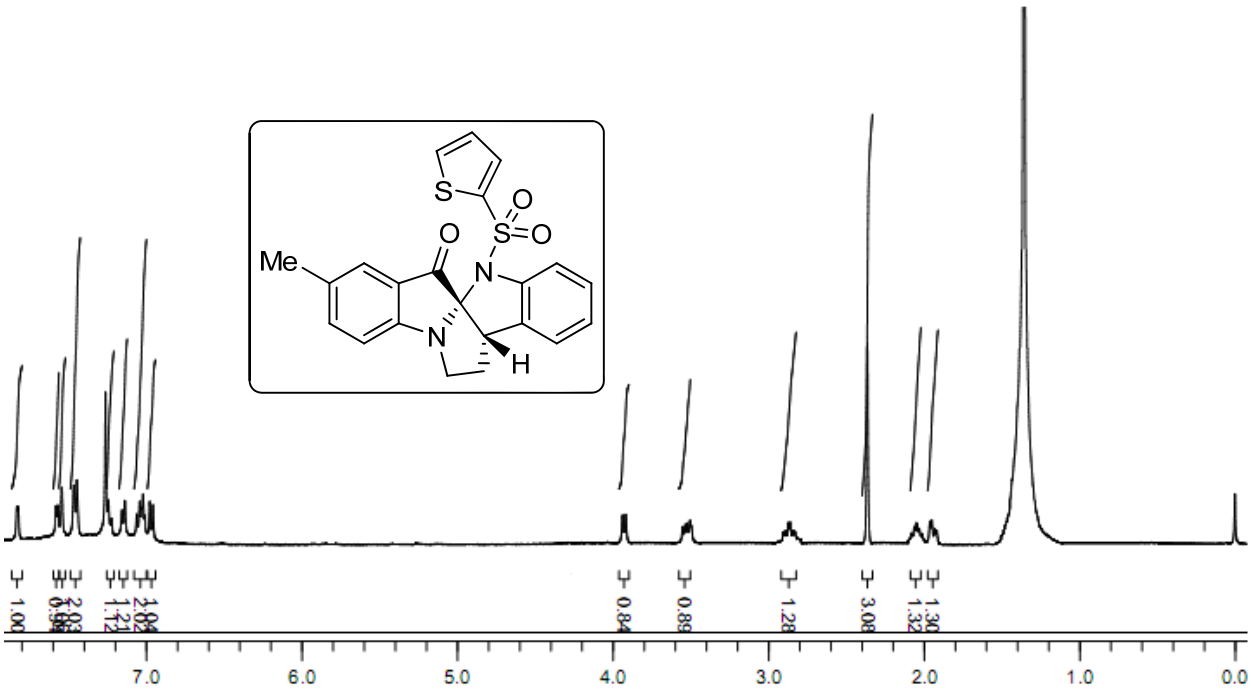
Pages 27/03/13

*** End of Report ***

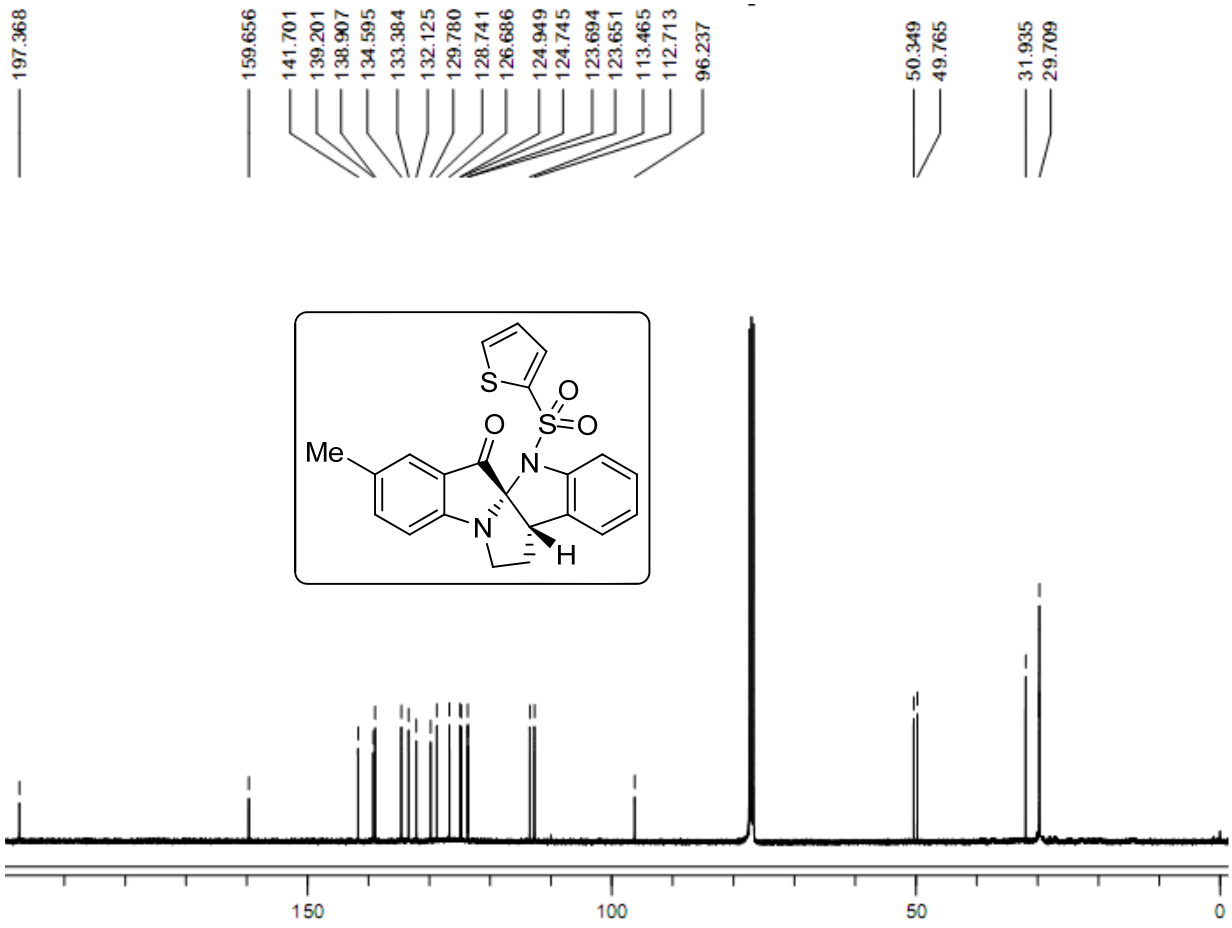
Sample Name	ILS/BPS/3-85	**Position**	Vial 15	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0.5	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	250313M016.d	**ACQ Method**	ILS.m	**Comment**		**Acquired Time**	3/25/2013 6:13:44 PM



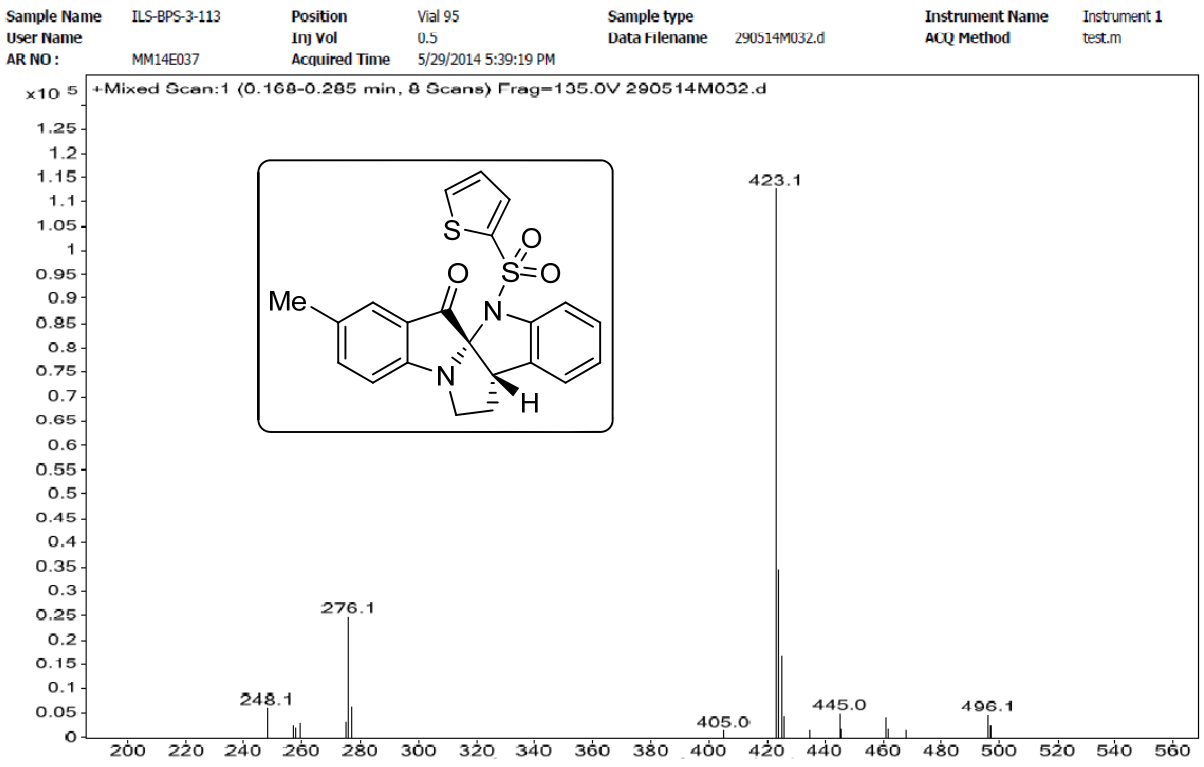
Mass spectra of compound **2d**



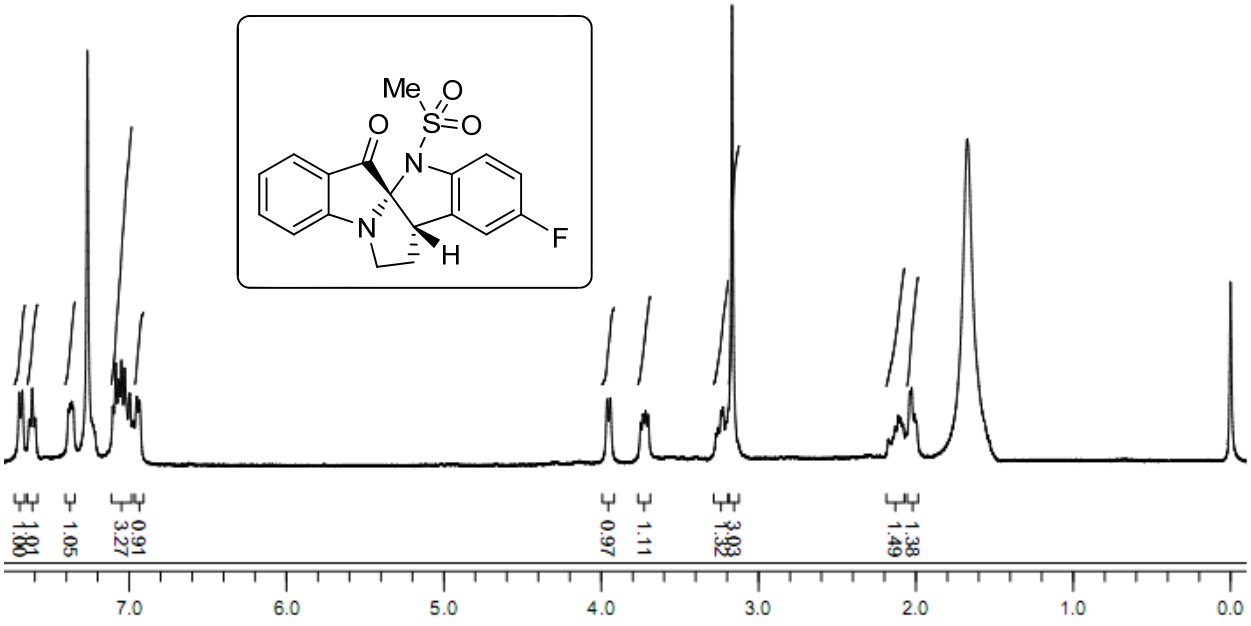
^{1}H NMR (Varian, 400 MHz) spectrum of compound **2e** in $CDCl_3$



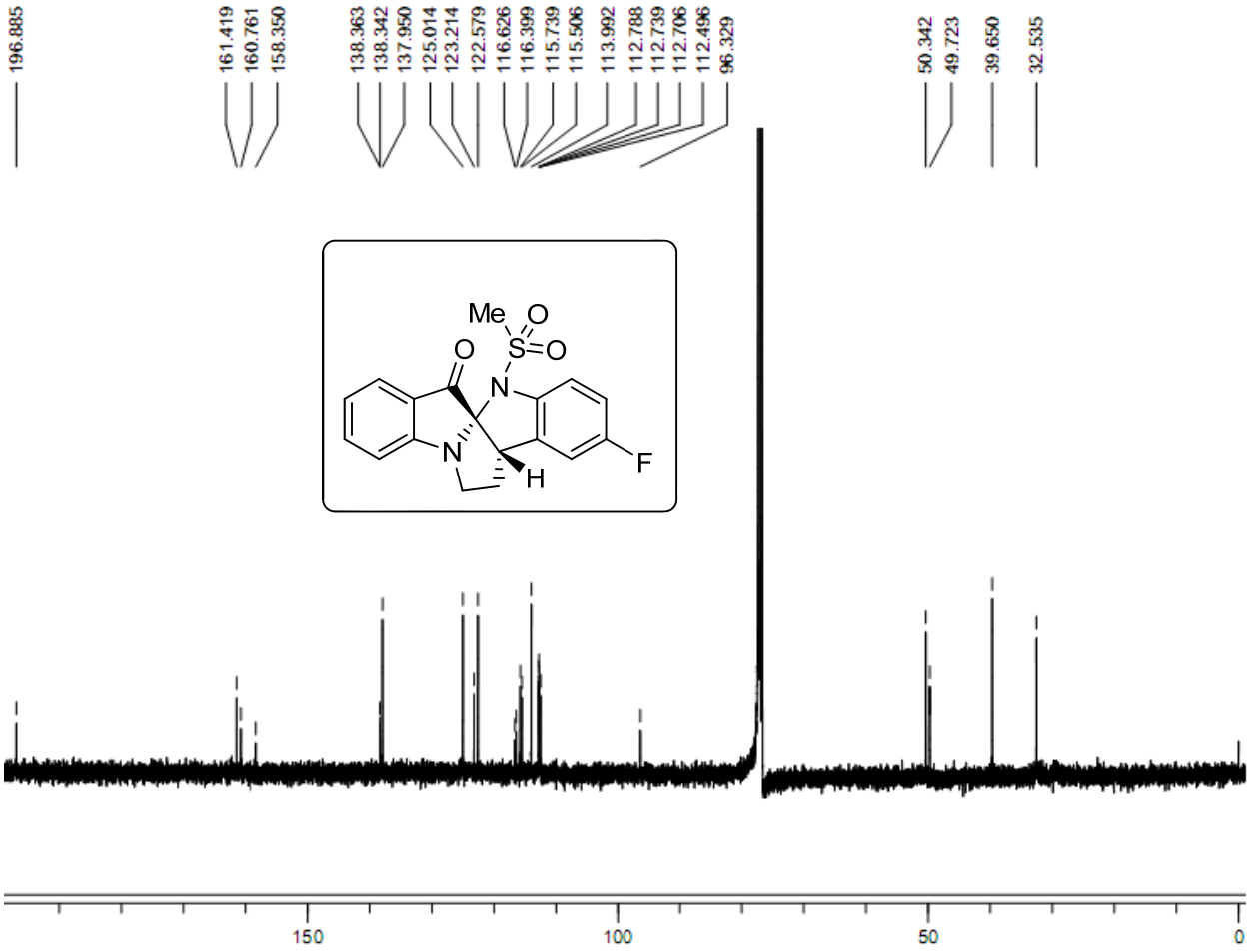
^{13}C NMR spectrum (Varian, 100 MHz) of compound **2e** in $CDCl_3$



Mass spectra of compound **2e**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2f** in $CDCl_3$

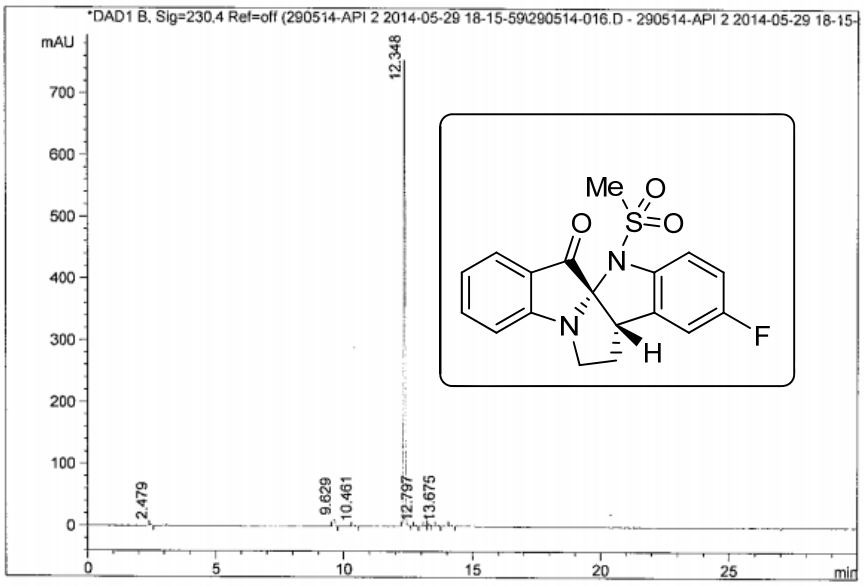


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2f** in $CDCl_3$

HPLC of compound **2f**

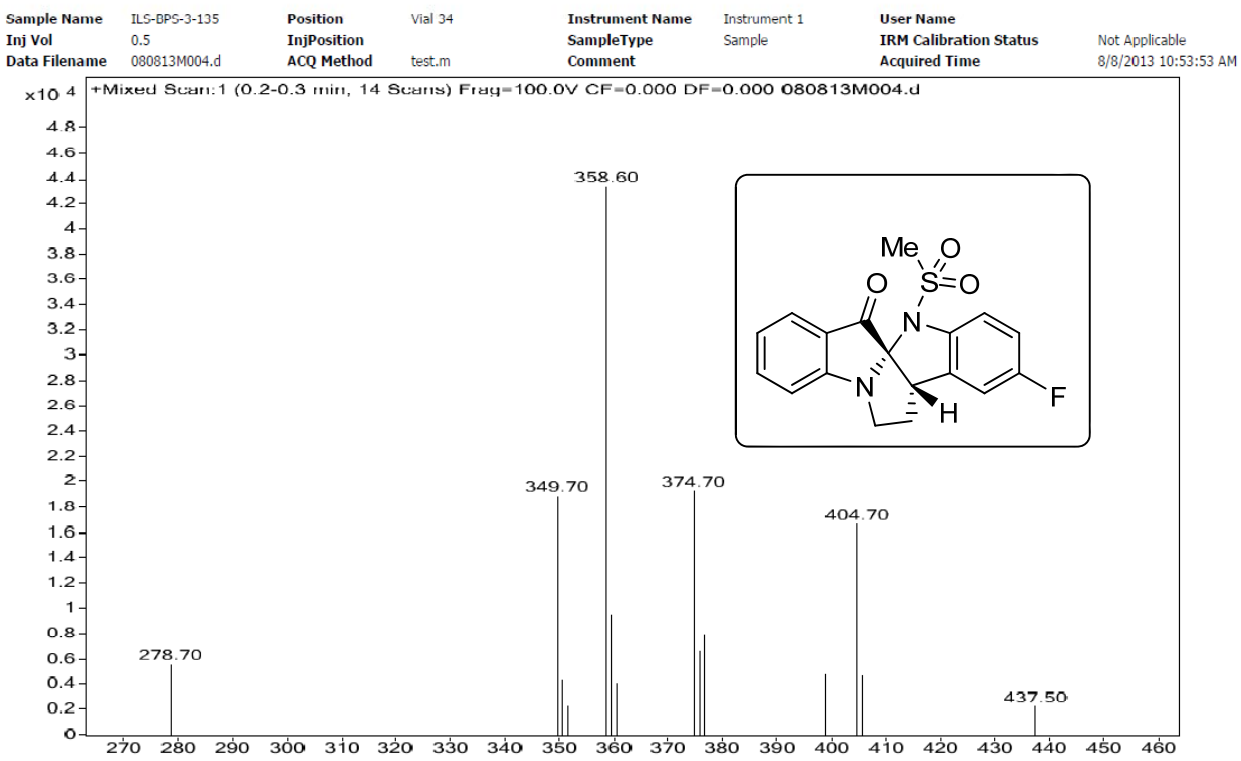
CPRI @ DRILS
HPLC ANALYSIS REPORT

```
Inj Date          : Thu, 29. May. 2014          Acq Operator: SHASHIDHAR
Sample Name       : ILS-BPS-3-135                             Vial 51
A.R Number        : CM14E017                  ->Inj. Vol.   : 5µL
Acq. Method       : D:\chem32\1\DATA\290514-API 2 2014-05-29 18-15-59\AP->
Analysis Method   : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info       : Column: X-Terra C-18 250*4.6mm, 5µm
                    Mobile phase: A) 5mm Ammonium Acetate  in water B) ACN
                    T/%B:0/20,3/20,12/95,23/95,25/20,30/20
                    Flow:1.0ml/min  Diluent: ACN:WATER(50:50)
```

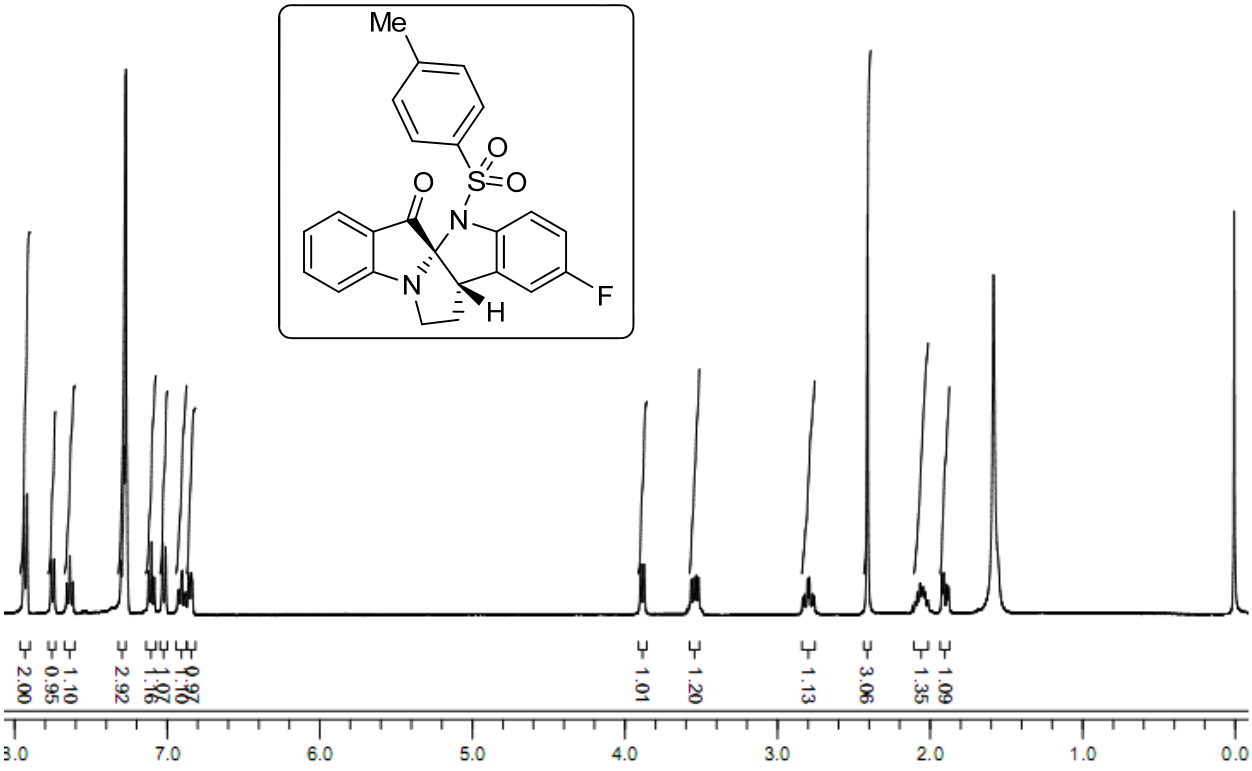


Signal 1: DAD1 B, Sig=230,4 Ref=off

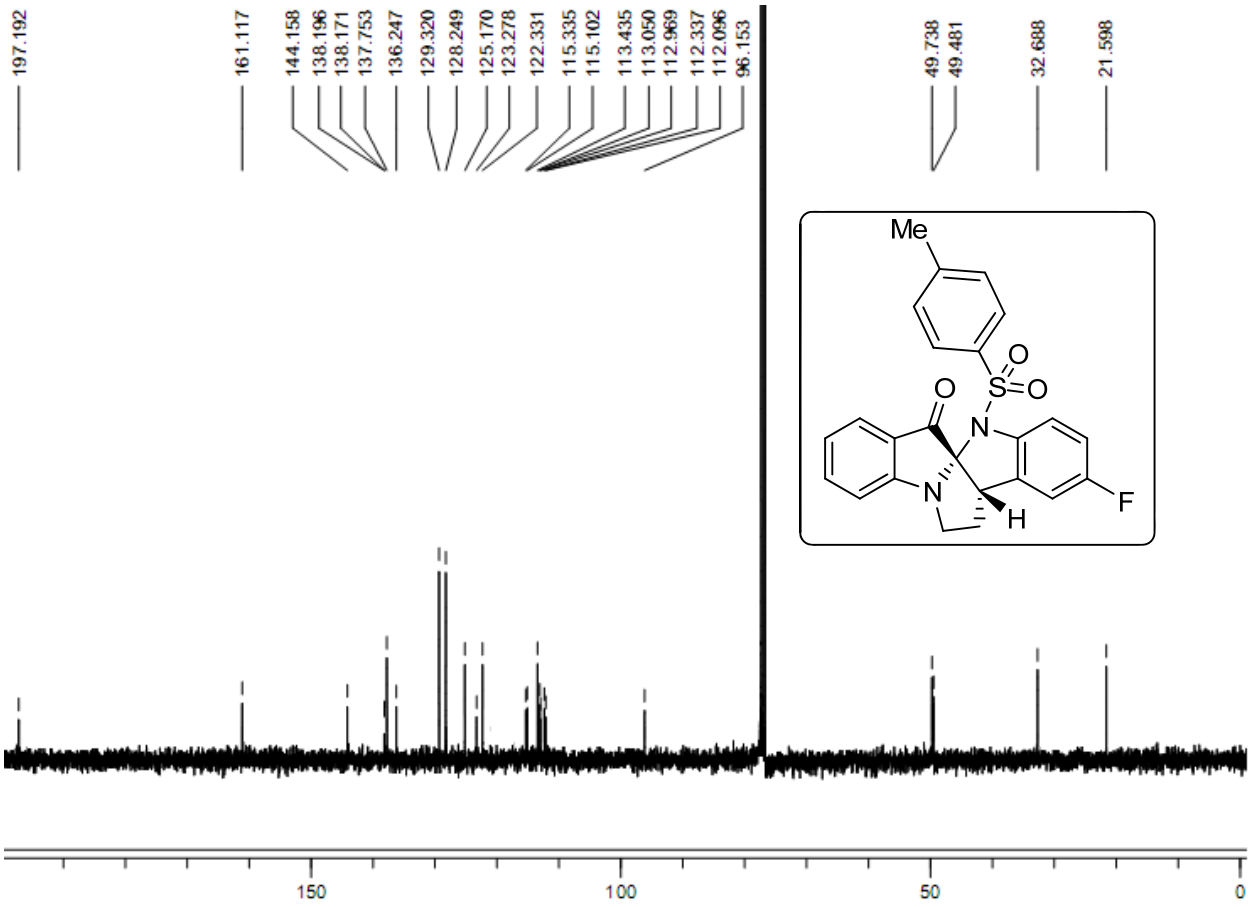
Peak #	RT [min]	Area	Area %
1	2.479	7.857	0.231
2	9.629	51.959	1.526
3	10.461	6.799	0.200
4	12.348	3296.286	96.790
5	12.797	5.788	0.170
6	13.188	7.891	0.232
7	13.308	11.549	0.339
8	13.675	5.793	0.170
9	14.164	11.693	0.343



Mass spectra of compound **2f**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2g** in $CDCl_3$

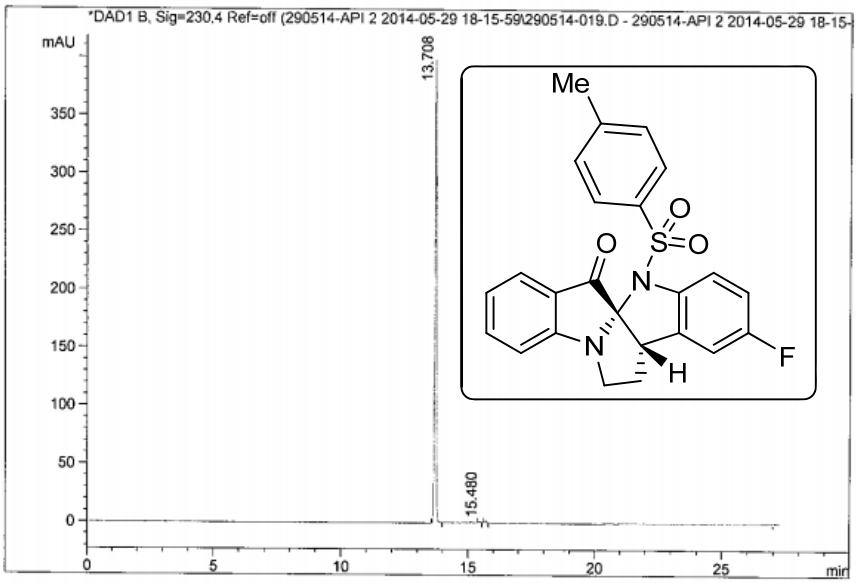


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2g** in $CDCl_3$

HPLC of compound **2g**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Inj Date : Fri, 30. May. 2014 Acq Operator: SHASHIDHAR
Sample Name : ILS-BPS-3-117 Vial 54
A.R Number : CM14E019 Inj. Vol. : 5µL
Acq. Method : D:\chem32\1\DATA\290514-API 2 2014-05-29 18-15-59\AP->
Analysis Method : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info : Column: X-Terra C-18 250*4.6mm, 5µm
Mobile phase: A) 5mm Ammonium Acetate in water B) ACN
T/%B:0/20,3/20,12/95,23/95,25/20,30/20
Flow:1.0ml/min Diluent: ACN:WATER(50:50)

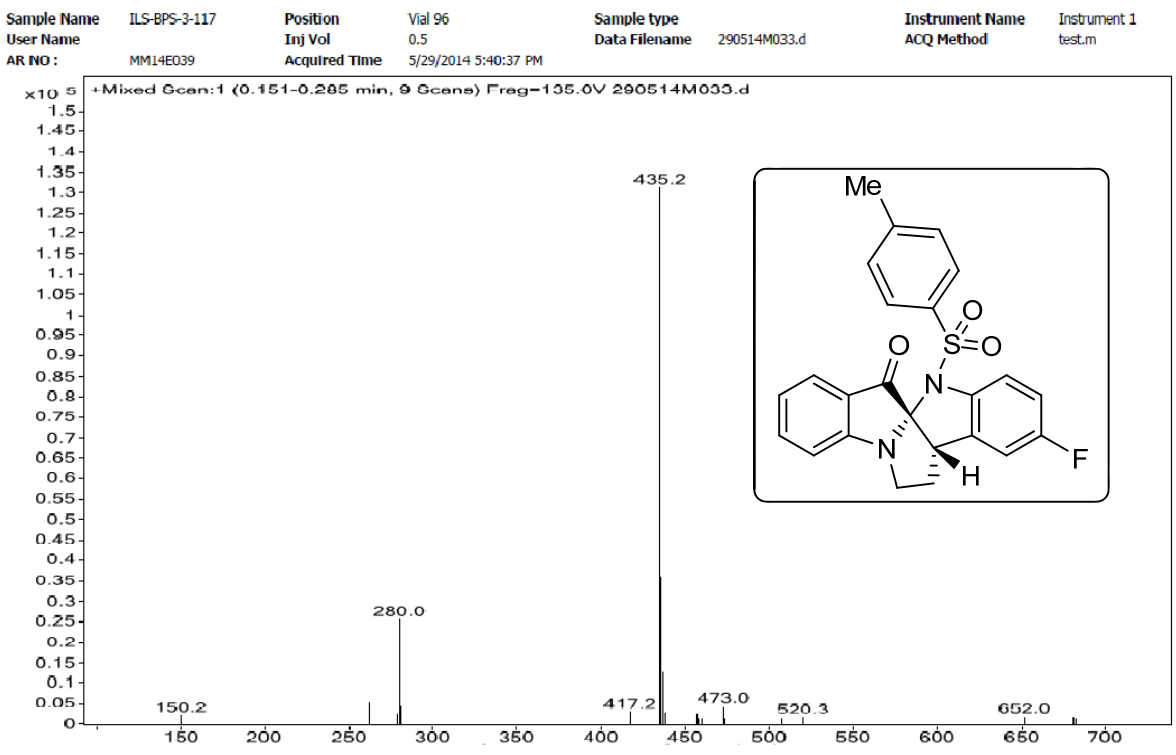


Signal 1: DAD1 B, Sig=230,4 Ref=off

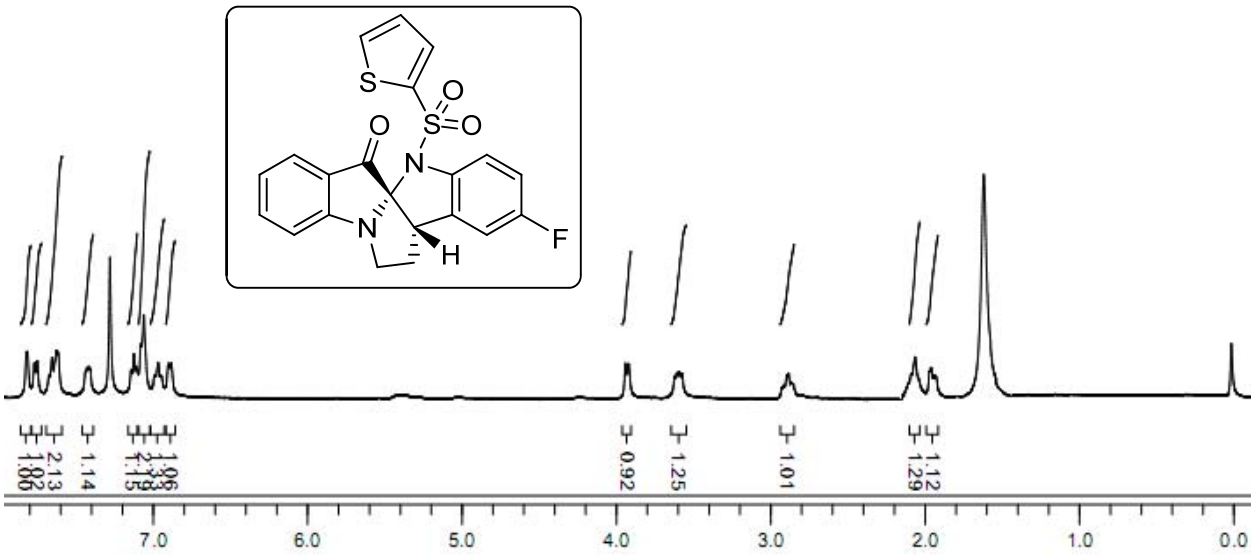
Peak #	RT [min]	Area	Area %
1	13.708	1782.930	99.291
2	15.480	5.937	0.331
3	15.707	6.795	0.378

Analysed by : 30/05/14

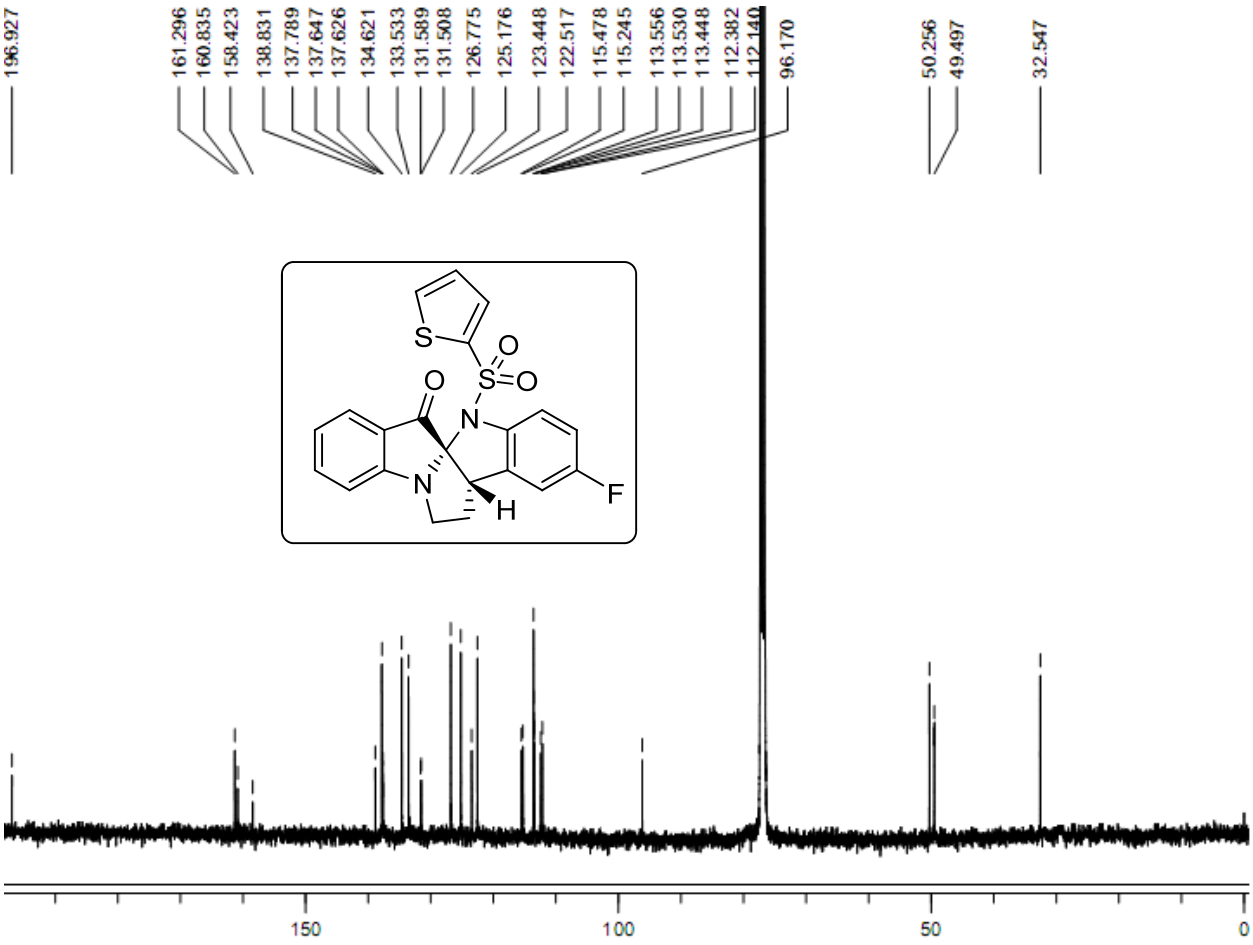
Checked by : 30/5/14



Mass spectra of compound **2g**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2h** in $CDCl_3$

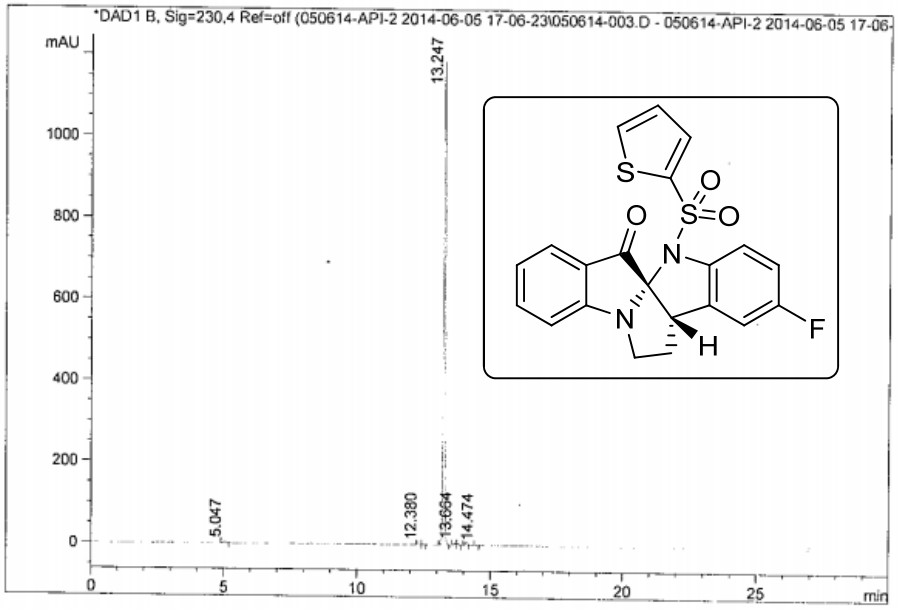


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2h** in $CDCl_3$

HPLC of compound **2h**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Inj Date : Thu, 5. Jun. 2014 Acq Operator: SHASHIDHAR
Sample Name : ILS-BPS-3-141 Vial 14
A R Number CM14F001 -> Inj. Vol. : 5µL
Acq. Method : D:\chem32\1\DATA\050614-API-2 2014-06-05 17-06-23\AP->
Analysis Method : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info : Column: X-Terra C-18 250*4.6mm, 5µm
Mobile phase: A) 5mm Ammonium Acetate in water B) ACN
T/%B:0/20,3/20,12/95,23/95,25/20,30/20
Flow:1.0ml/min Diluent: ACN:WATER(50:50)

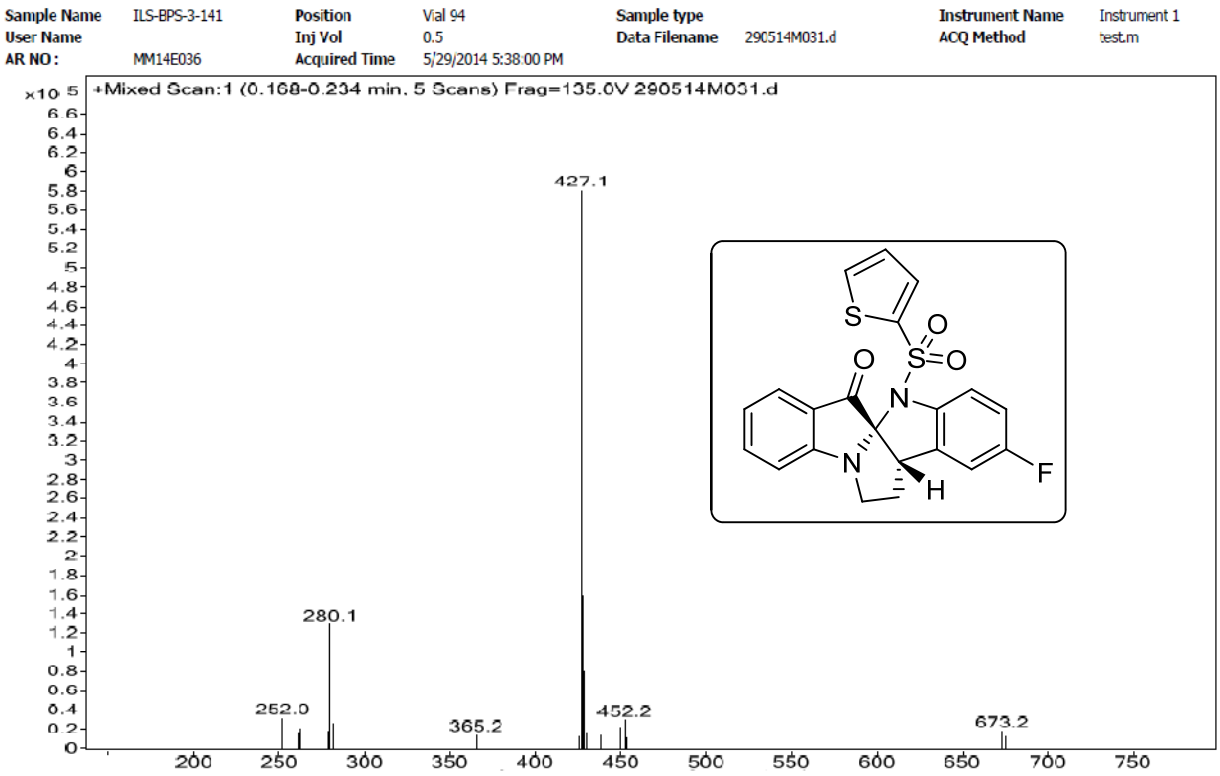


Signal 1: DAD1 B, Sig=230,4 Ref=off

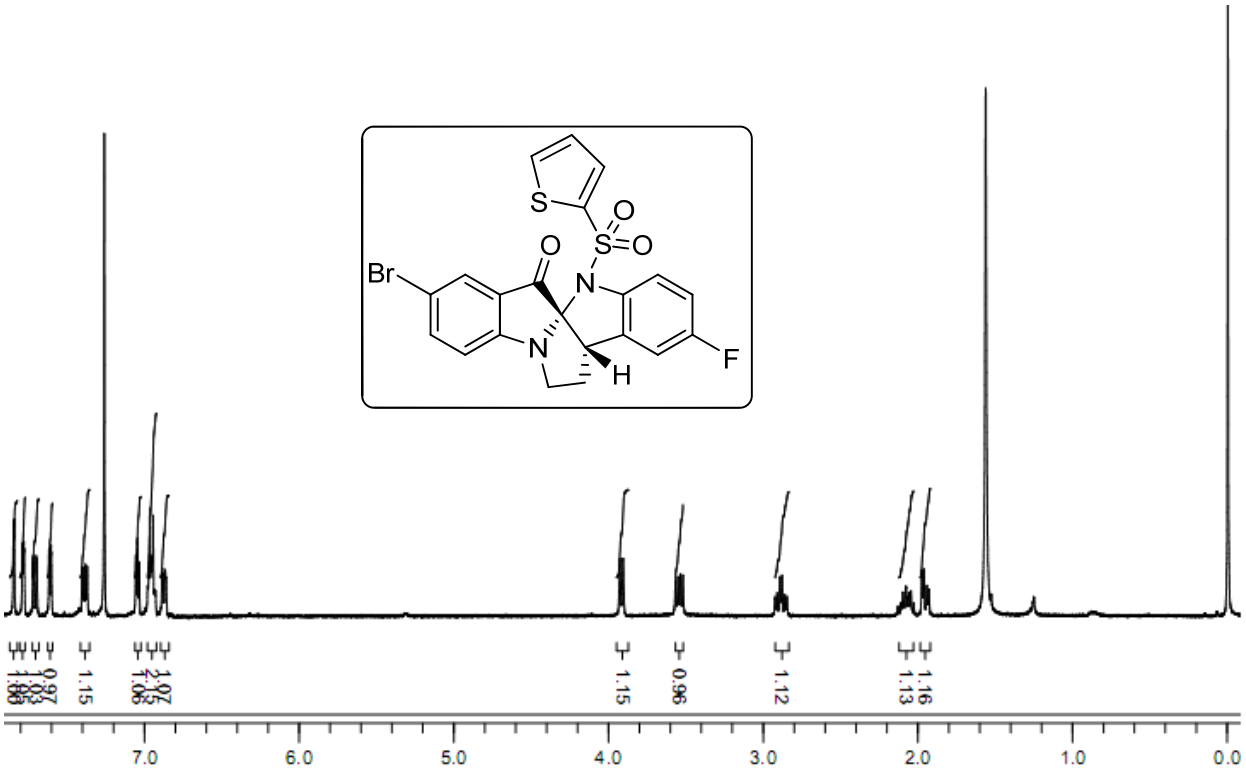
Peak #	RT [min]	Area	Area %
1	5.047	18.914	0.353
2	12.380	5.234	0.098
3	12.505	6.563	0.123
4	13.247	5243.596	97.982
5	13.664	19.120	0.357
6	13.771	21.259	0.397
7	14.104	29.528	0.552
8	14.474	7.351	0.137

Analysed by : 06/06/14

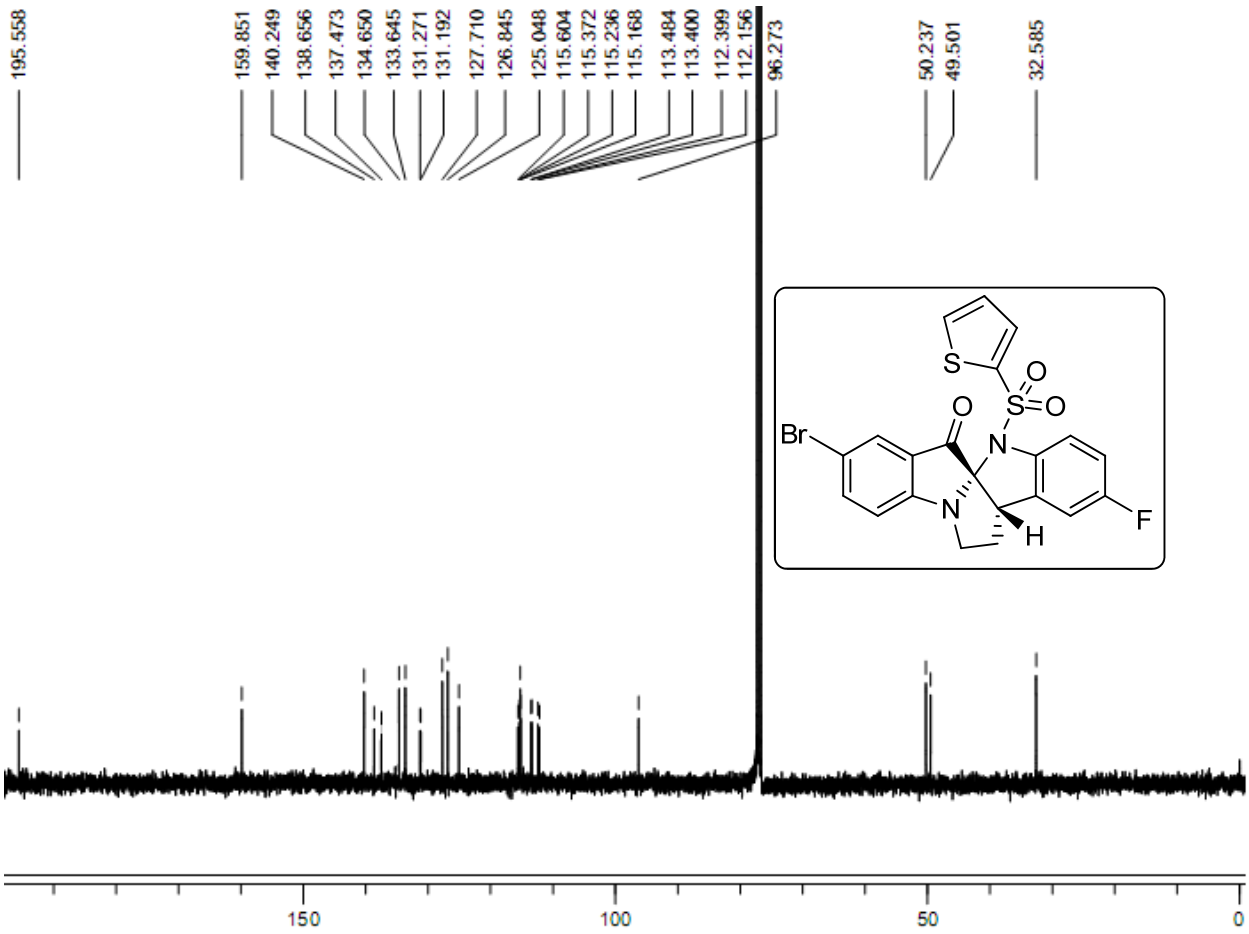
Checked by : 06/06/14



Mass spectra of compound **2h**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2i** in $CDCl_3$



^{13}C NMR spectrum (Varian, 100 MHz) of compound **2i** in $CDCl_3$

HPLC of compound **2i**

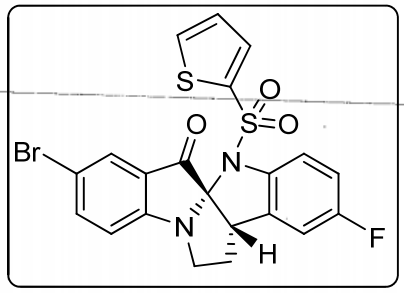
Empower 2 software

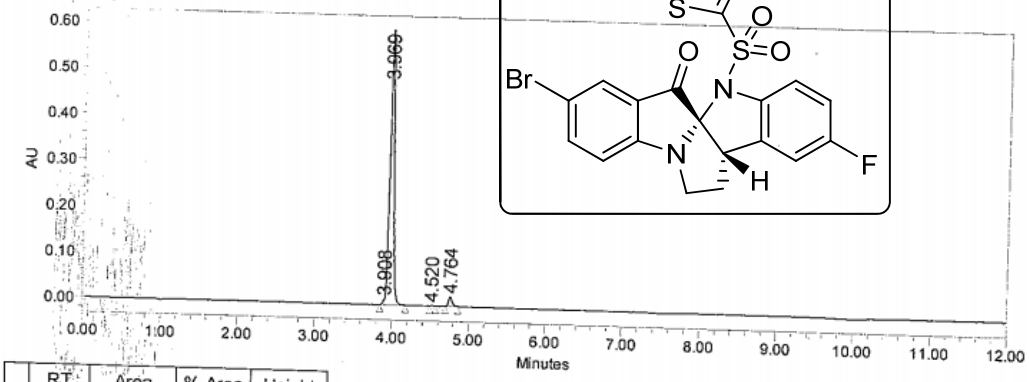
CPRI@DRILS

SAMPLE INFORMATION

Sample Name:	ILS-BPS-3-175		
A.R Number:	CM14D002		
Vial:	4		
Injection #:	1		
Injection Volume:	5.00 ul		
Run Time:	12.0 Minutes		
Sample Set Name:	040414		
Date Acquired:	4/4/2014 12:47:36 PM IST		
Date Processed:	4/4/2014 1:58:44 PM IST		
		Acq operator:	Vaishnavi
		Acq. Method Set:	METHOD
		Processing Method:	METHOD_PRO
		Channel Name:	235.0nm
		Proc. Chnl. Descr.:	PDA 235.0 nm Blank Subtracted

Column: Symmetry C-18 75*4.6mm 3µm
Mobile phase: A) 0.1% TFA in water B) ACN
T/%B: 0/50, 1/50, 3/98,10/98, 10.5/50, 12/50
Flow: 1.0 ml/min, Diluent: ACN





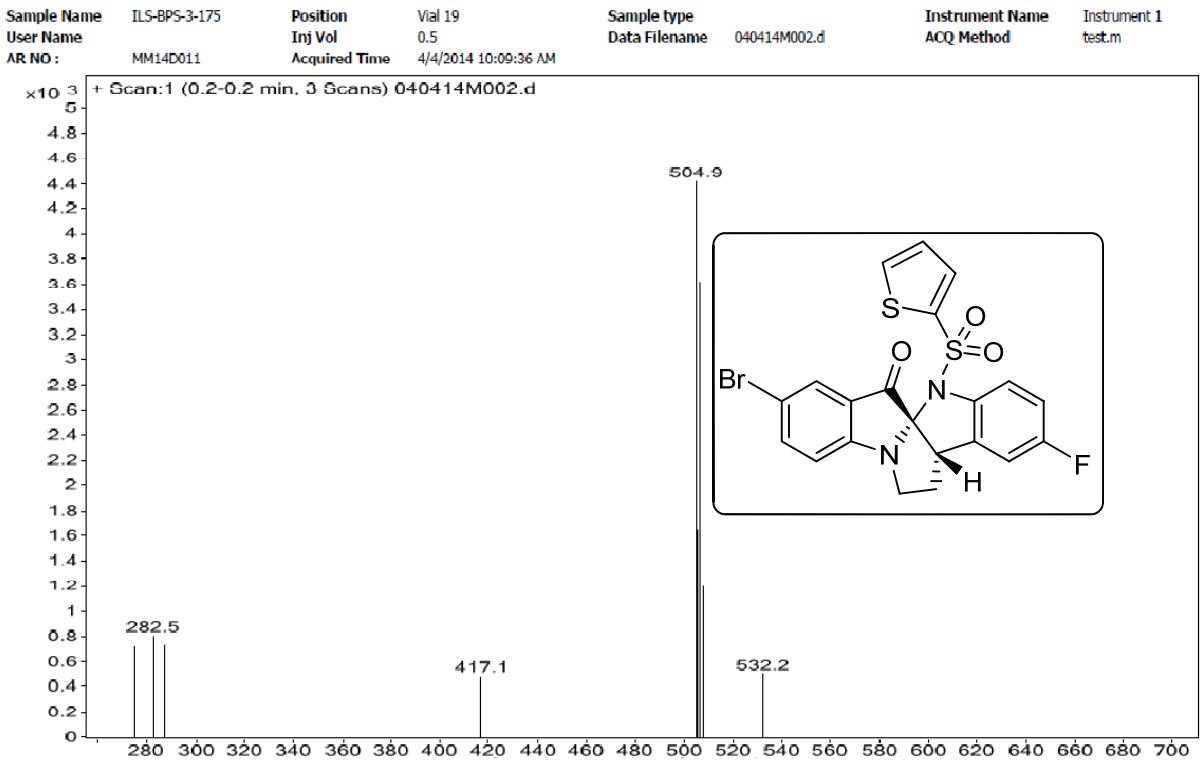
	RT	Area	% Area	Height
1	3.908	16849	0.76	12850
2	3.969	2120119	95.97	596912
3	4.520	3631	0.16	1266
4	4.764	68451	3.10	20688

Analysed By 04/04/14

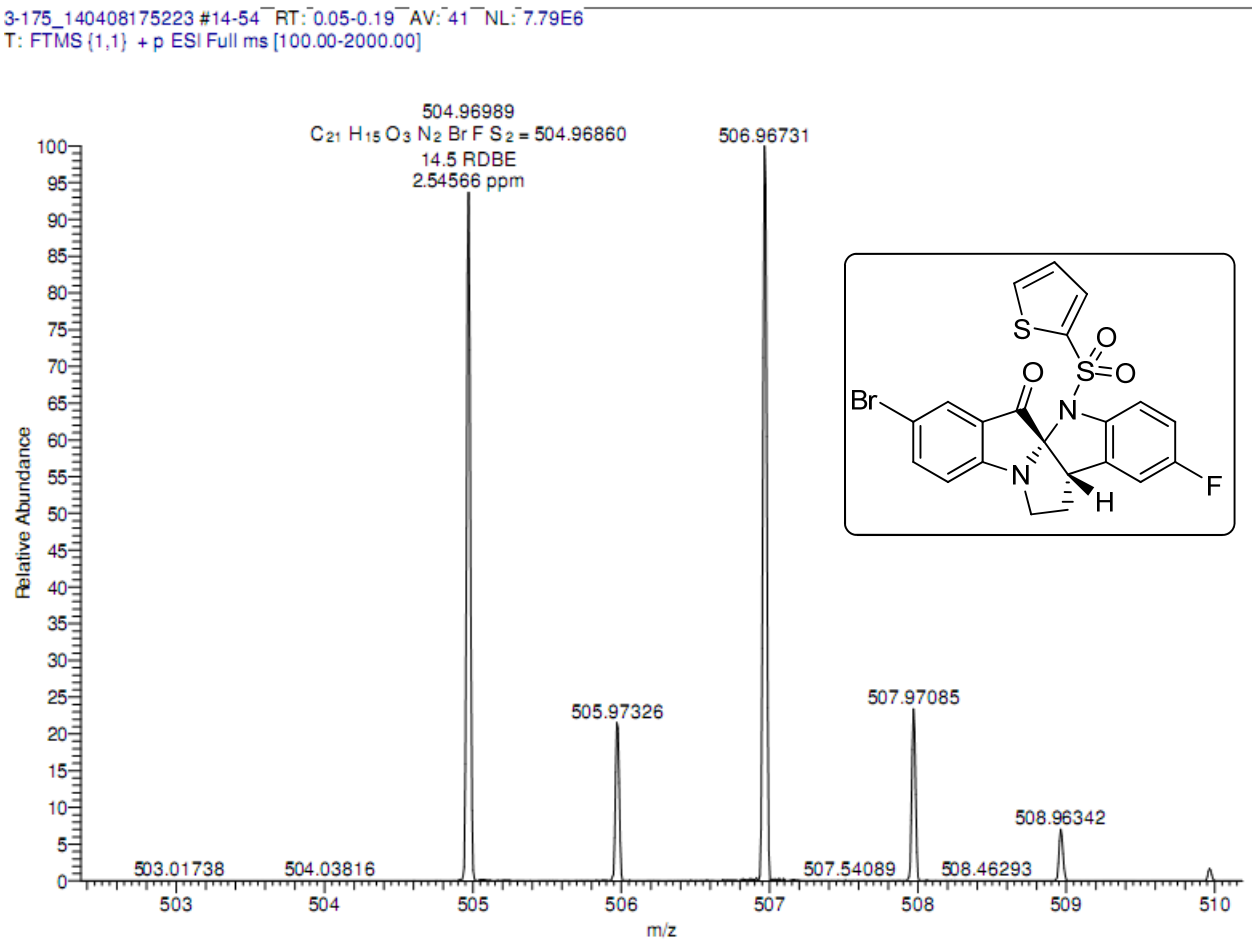
Checked By 04/04/14

Reported by User: System
Report Method: CPRI@DRILS
Report Method ID: 3377
Page 1 of 1

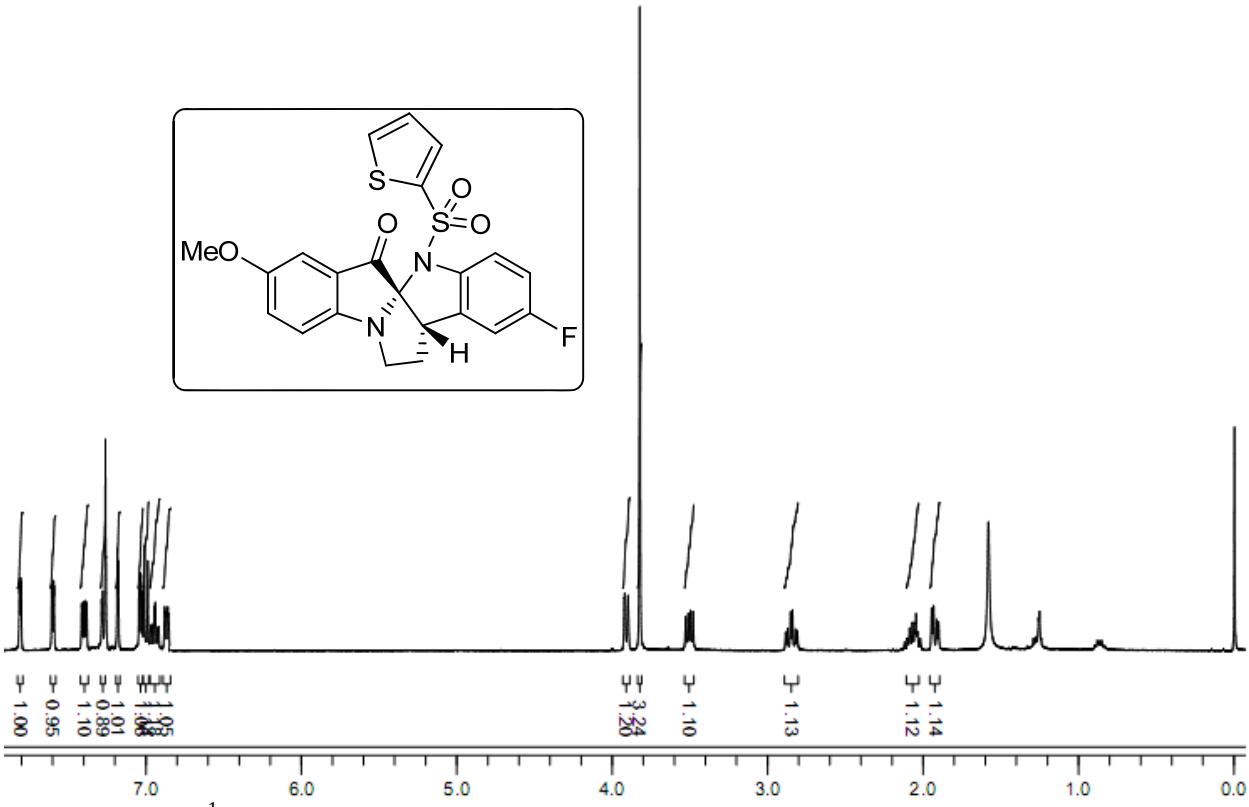
Project Name: APRIL_2014
Date Printed: 4/4/2014
2:01:37 PM Asia/Calcutta



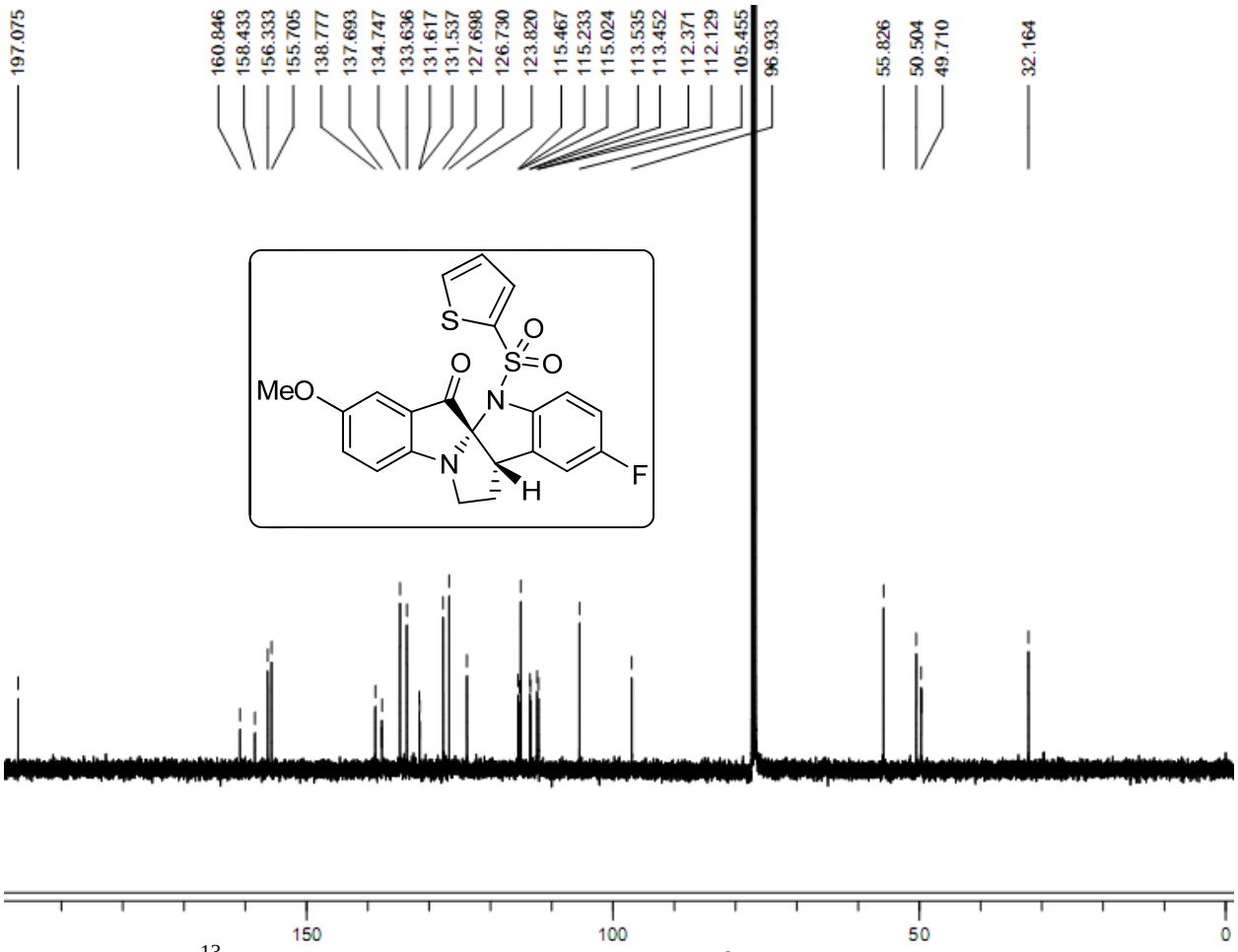
Mass spectra of compound **2i**



HRMS of compound **2i**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2j** in $CDCl_3$

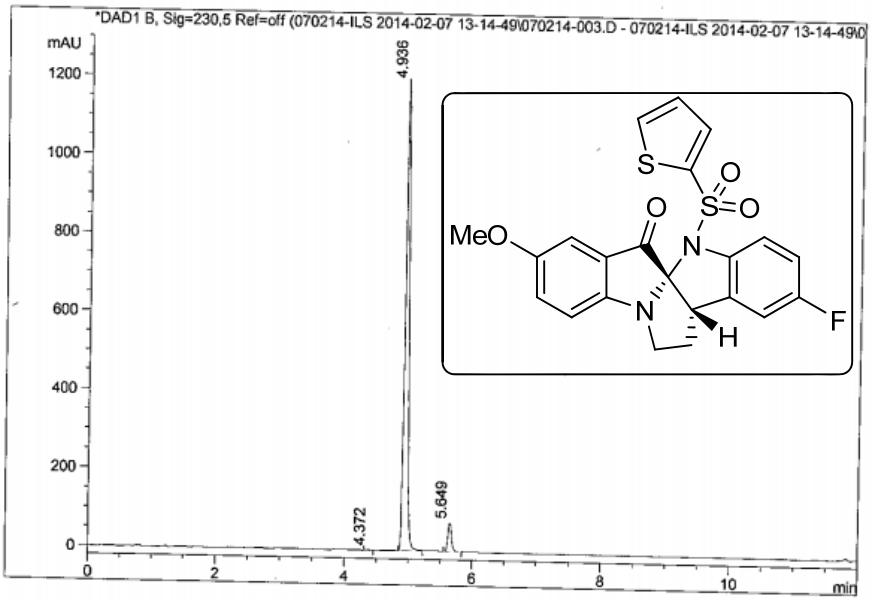


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2j** in $CDCl_3$

HPLC of compound **2j**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Injection Date	: Fri, 7. Feb. 2014	Seq Line :	3
Sample Name	: ILS-BPS-3-172	Location :	Vial 5
Acq Operator	: RADHA	Inj. No. :	1
Acq. Method	: D:\chem32\1\DATA\070214-ILS 2014-02-07 13-14-49\C-18->	Inj. Vol. :	10 µl
Analysis Method	: D:\CHEM32_002\1\METHODS\C-18 A80B20GS.M		
Method Info	: Column : Symmetry C-18 75*4.6mm,3.5µm		
	Mobile phase: A) 0.1% HCOOH in Water , B) ACN		
	T/B%:0/20,0.5/20,4/98,10/98,10.5/20,12/20		
	Flow: 1.0 ml/min, Diluent: ACN:Water(80:20)		



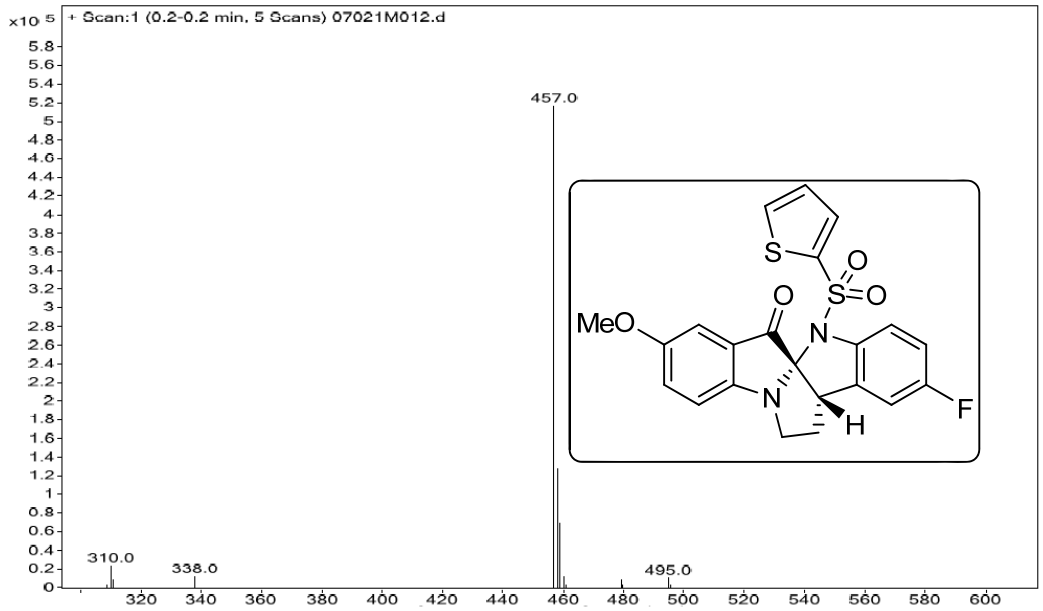
Signal 1: DAD1 B, Sig=230,5 Ref=off

Peak #	RT [min]	Area	Area %
1	4.372	5.081	0.100
2	4.936	4799.861	94.264
3	5.649	286.973	5.636

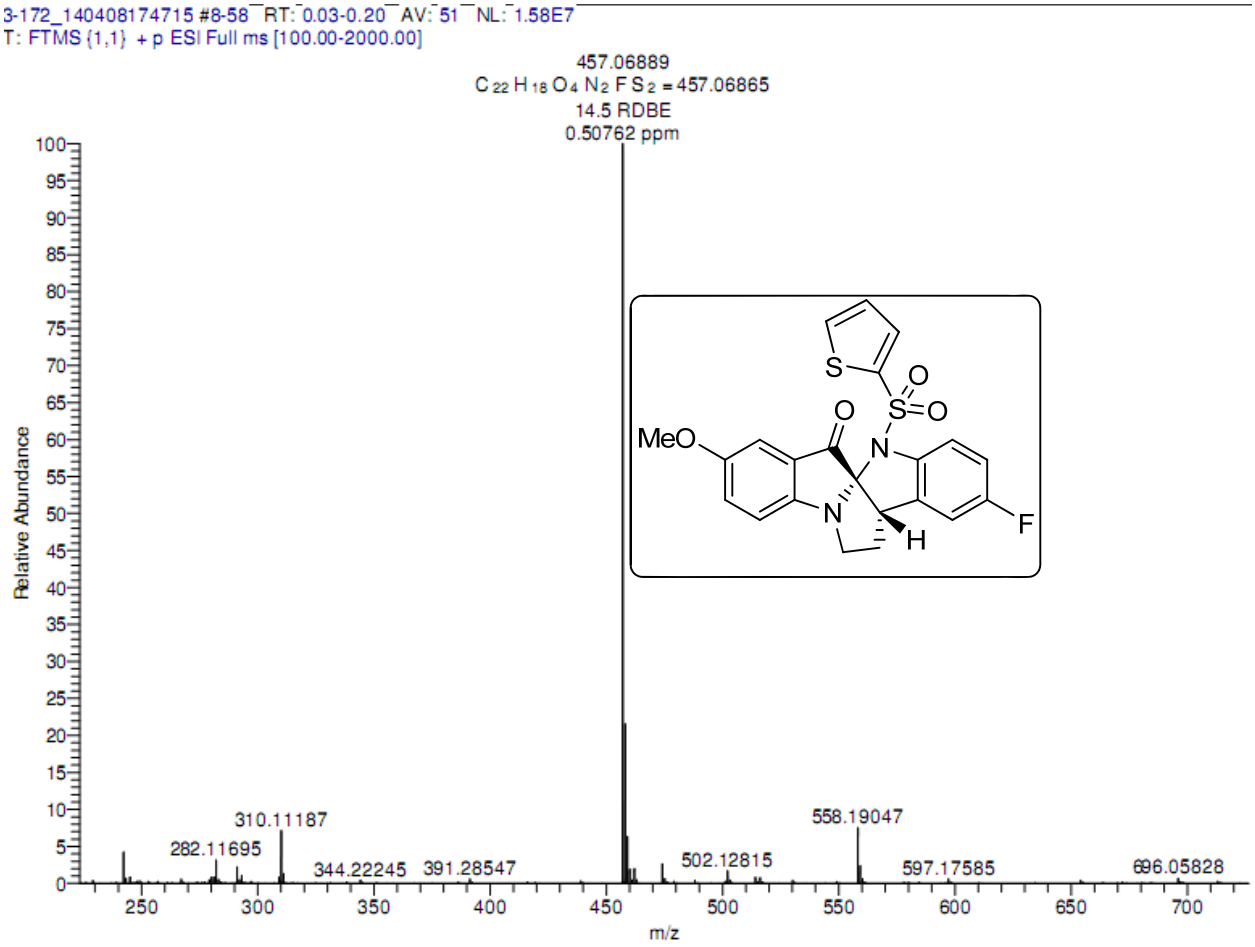
07/02/14

*** End of Report ***

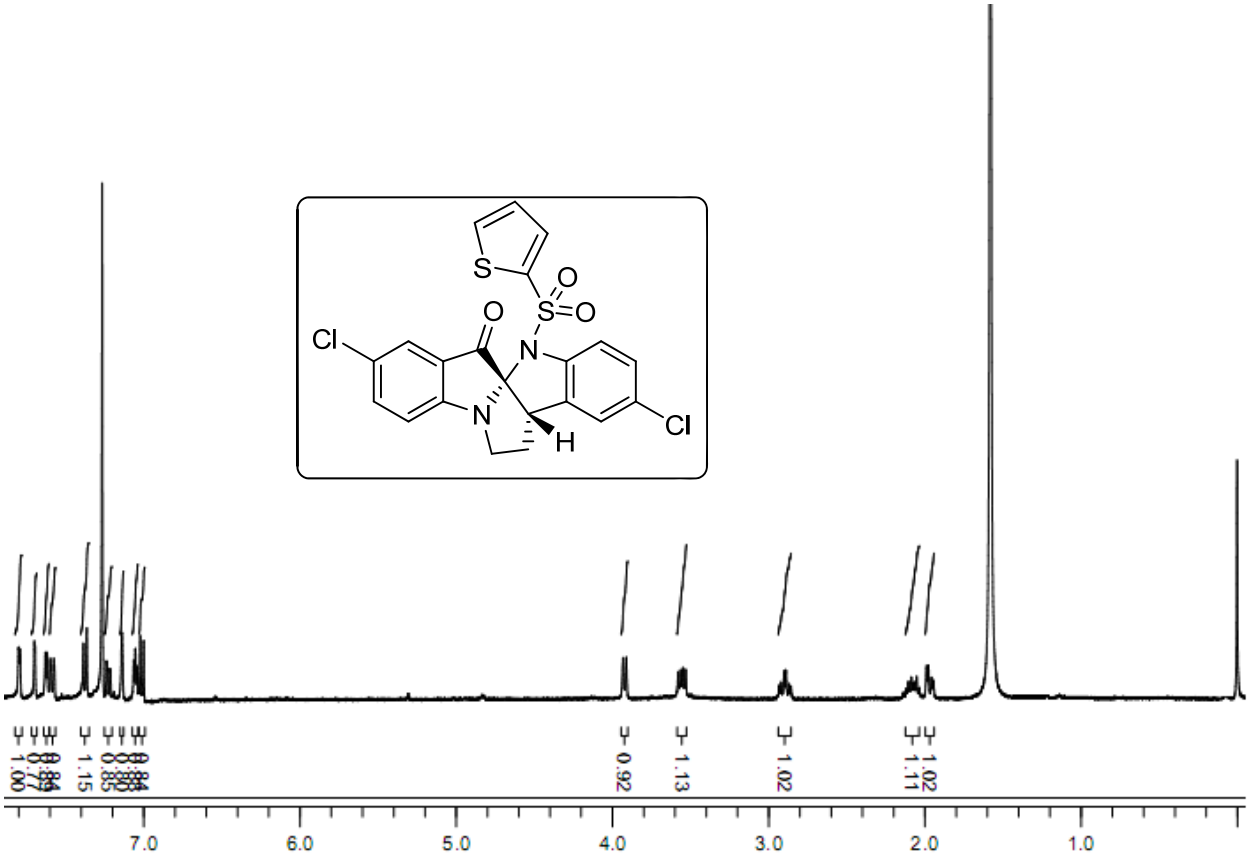
Sample Name	ILS-BPS-3-172	**Position**	Vial 64	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0.5	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	07021M012.d	**ACQ Method**	test.m	**Comment**		**Acquired Time**	2/7/2014 2:56:45 PM



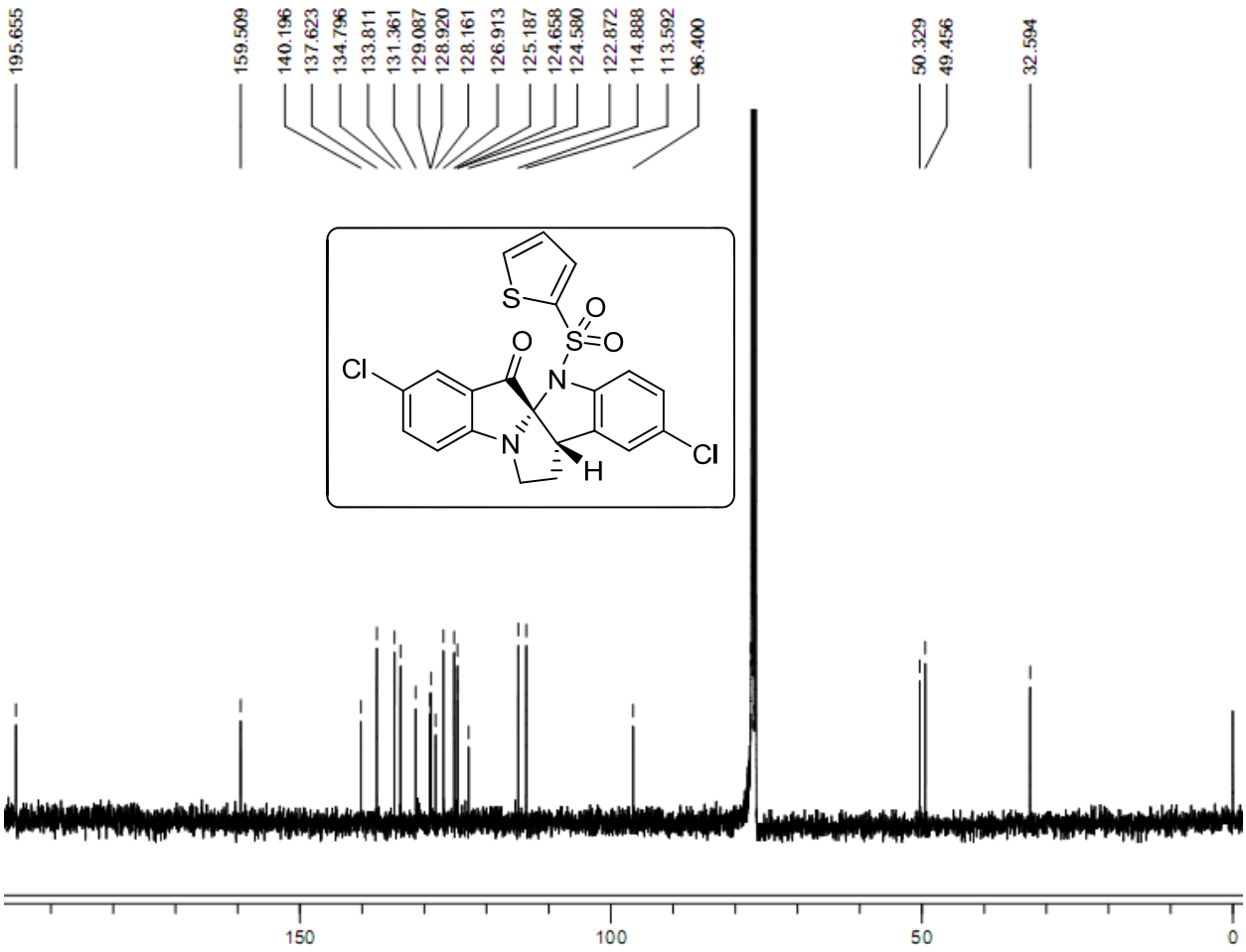
Mass spectra of compound **2j**



HRMS of compound **2j**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2k** in $CDCl_3$



^{13}C NMR spectrum (Varian, 100 MHz) of compound **2k** in $CDCl_3$

HPLC of compound 2k

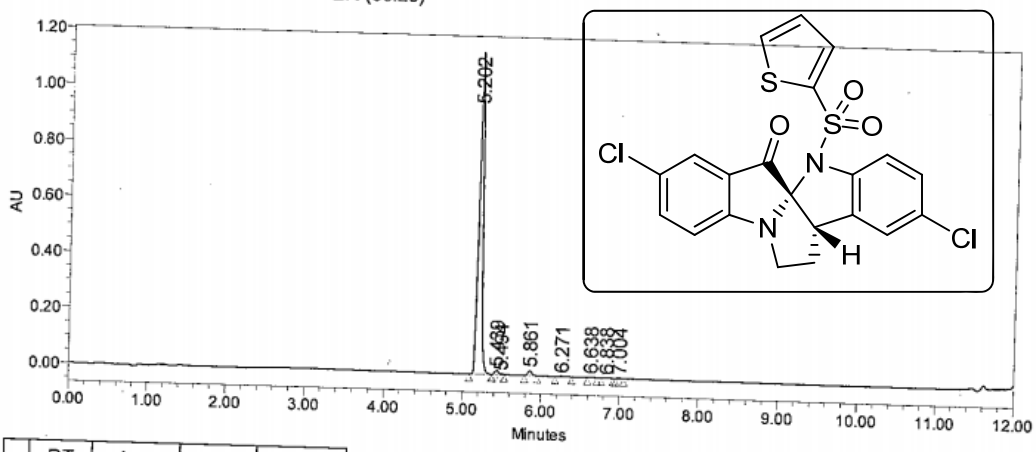
Empower 2 software

CPRI@DRILS

SAMPLE INFORMATION

Sample Name:	ILS-BPS-3-173	Sample Set Name:	240214
Sample Type:	Unknown	Acq. Method Set:	METHOD
Vial:	49	Processing Method:	METHOD PRO
Injection #:	1	Channel Name:	230.0nm
Injection Volume:	5.00 ul	Proc. Chnl. Descr.:	PDA 230.0 nm Blank Subtracted
Run Time:	12.0 Minutes		
Date Acquired:	2/24/2014 1:38:48 PM IST		
Date Processed:	2/24/2014 2:14:20 PM IST		

Column: SYMMETRY C-18 75*4.6mm 3.5µm
Mobile phase: A) 0.1% FA in water B) ACN
T/%B: 0/20, 0.5/20, 4/98, 10/98, 10.5/20, 12/20
Flow: 1.0 ml /min, Diluent: ACN: WATER (80:20)

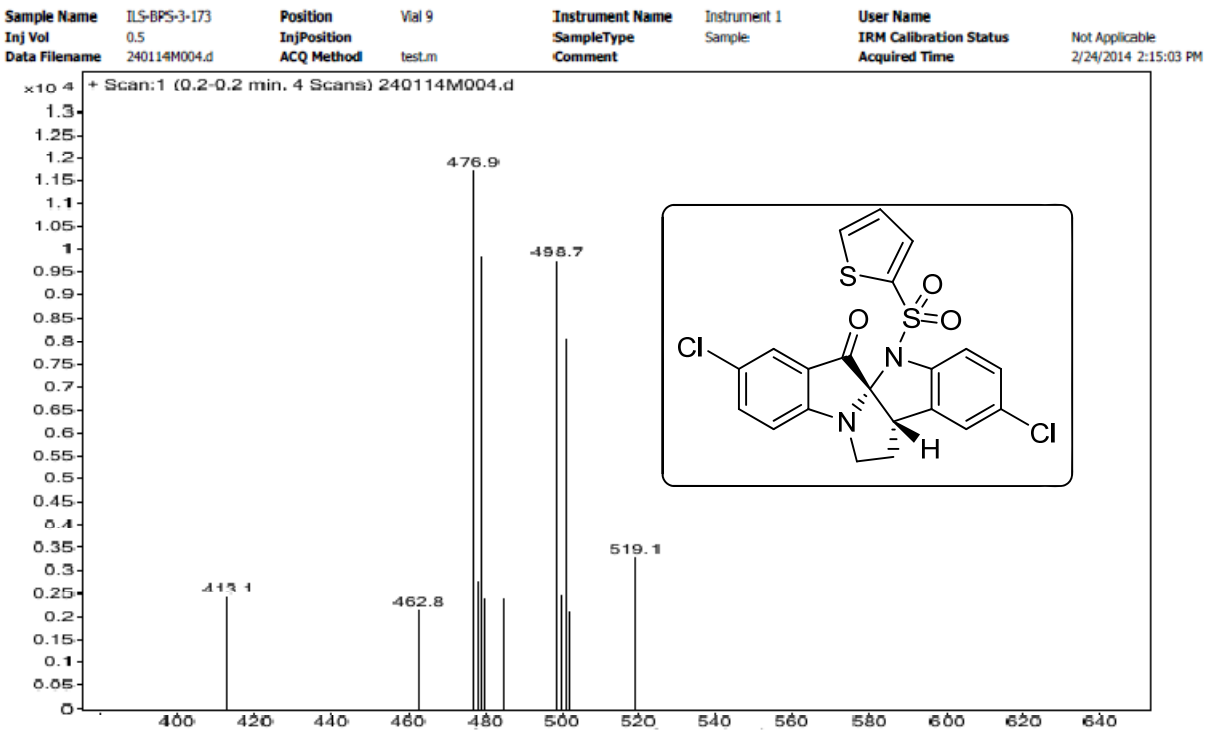


	RT	Area	% Area	Height
1	5.202	3935070	96.52	1149119
2	5.439	46820	1.15	14753
3	5.494	3874	0.10	2005
4	5.861	53377	1.31	17312
5	6.271	11931	0.29	2116
6	6.638	9319	0.23	2658
7	6.838	10427	0.26	2364
8	7.004	6112	0.15	1886

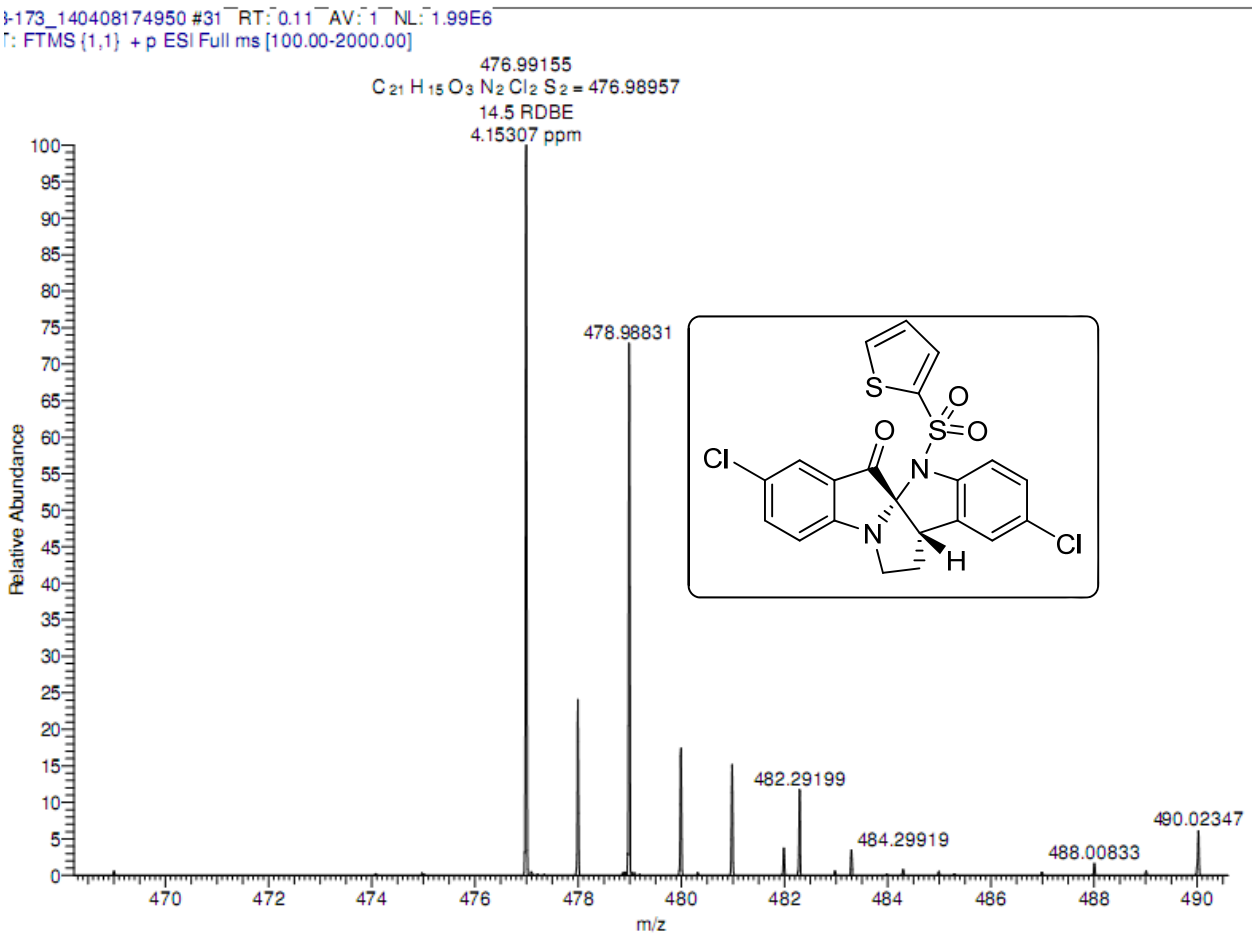
Analysed By 24.02.14

Reported by User: System
Report Method: CPRI@DRILS
Report Method ID: 3330
Page: 1 of 1

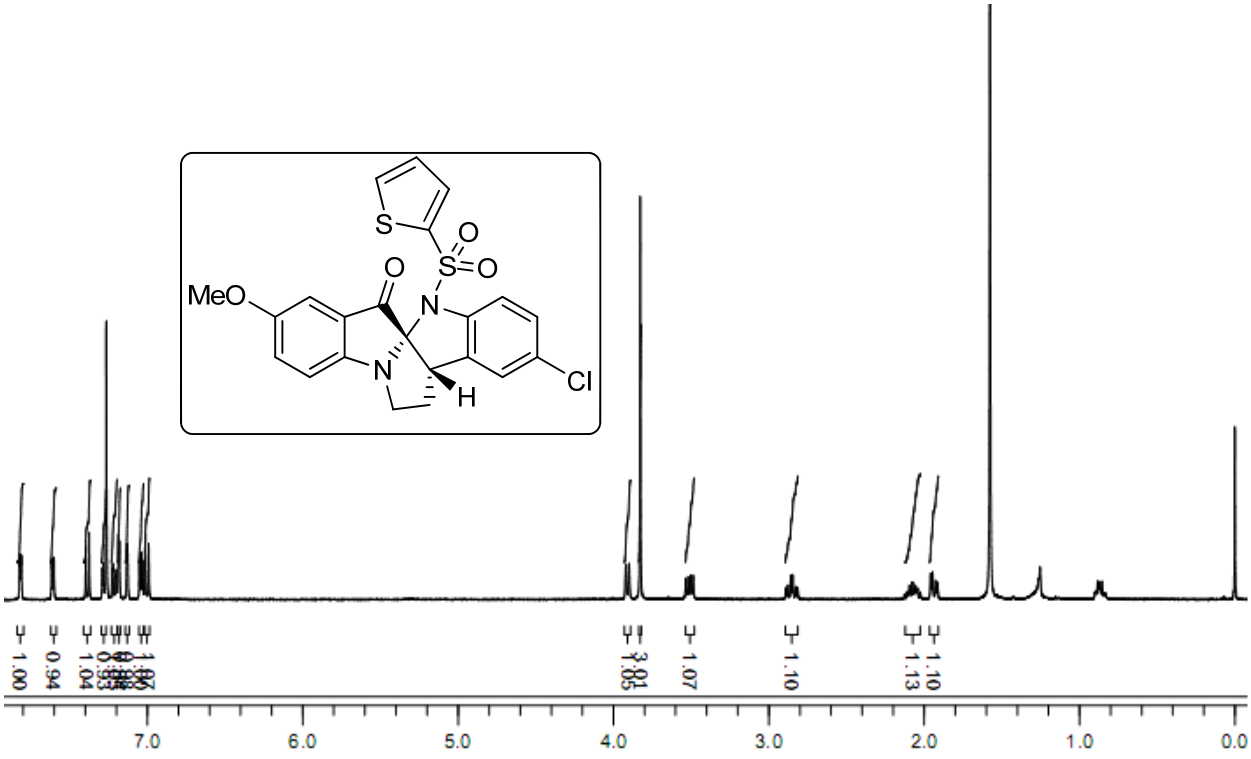
Project Name: FEB_2014
Date Printed:
2/24/2014
2:16:20 PM Asia/Calcutta



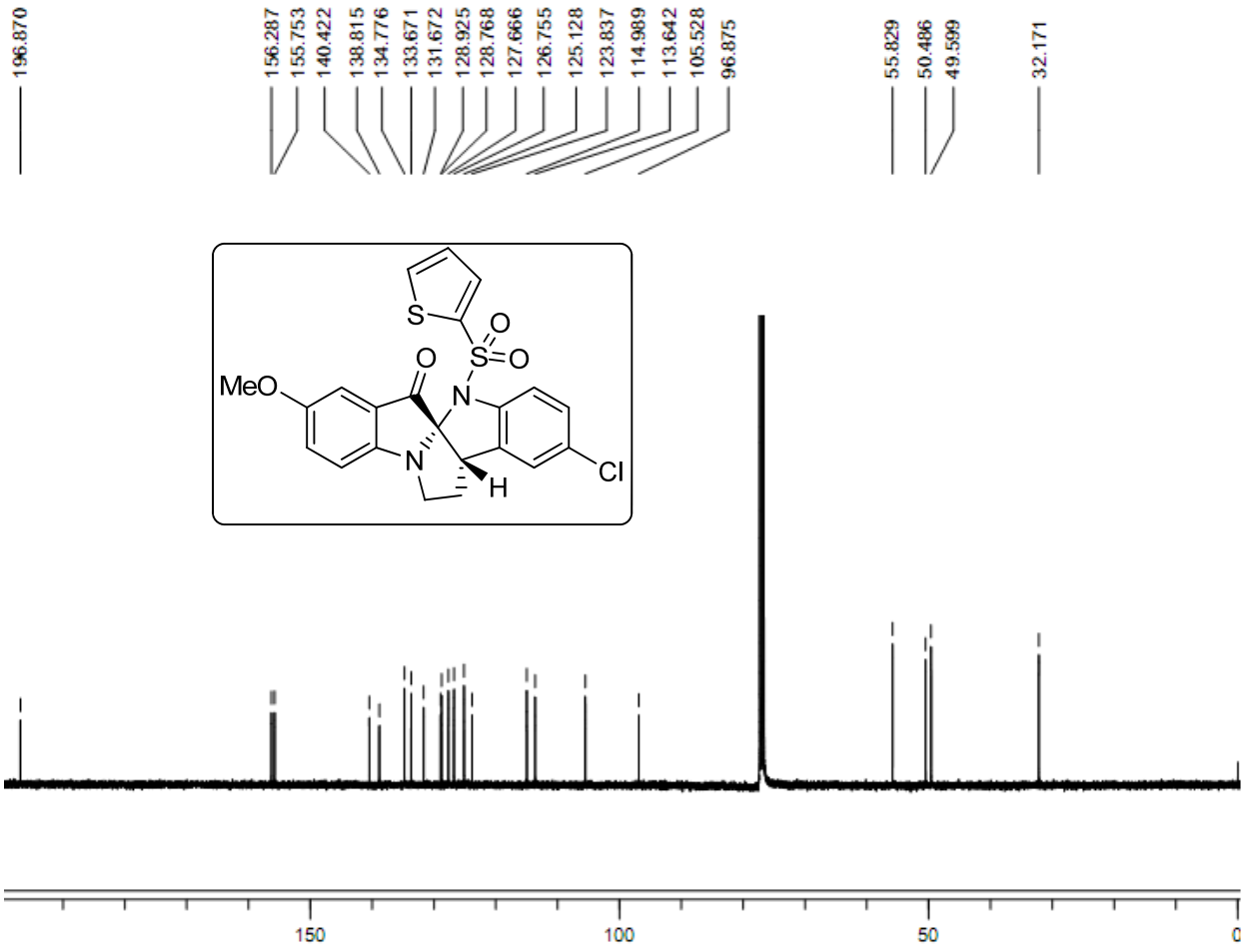
Mass spectra of compound **2k**



HRMS of compound **2k**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2l** in $CDCl_3$



^{13}C NMR spectrum (Varian, 100 MHz) of compound **2l** in $CDCl_3$

HPLC of compound 2l

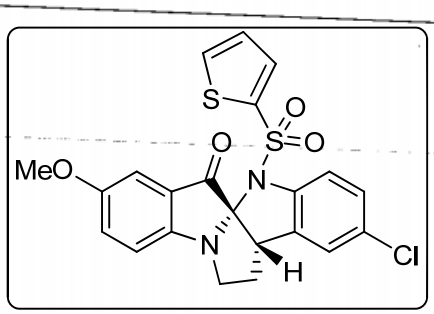
Empower 2 software

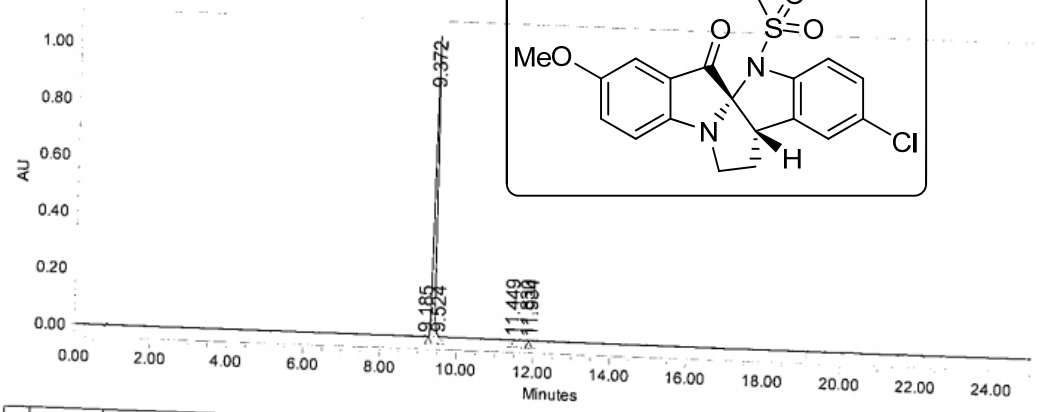
CPRI@DRILS

SAMPLE INFORMATION

Sample Name:	ILS-BPS-3-177		
A.R Number:	CM14D011		
Vial:	22		
Injection #:	1		
Injection Volume:	5.00 ul	Acq operator:	Vaishnavi
Run Time:	25.0 Minutes	Acq. Method Set:	SFV_A5
Sample Set Name:	220414	Processing Method:	SFV_A5 PRO
Date Acquired:	4/22/2014 8:19:11 PM IST	Channel Name:	235.0nm
Date Processed:	4/23/2014 9:29:14 AM IST	Proc. Chnl. Descr.:	PDA 235.0 nm Blank Subtracted

Column: Symmetry C-18 75*4.6mm 3.5lm
Mobile phase: A) 0.1% TFA in water B) ACN
T/%B: 0/20, 2/20, 10/95, 20/95, 22/20, 25/20
Flow: 1.0 ml /min, Diluent: ACN: WATER (80:20)





	RT	Area	% Area	Height
1	9.185	9136	0.22	2199
2	9.372	4100557	99.29	1059981
3	9.524	5187	0.13	3806
4	11.449	4995	0.12	1607
5	11.830	6085	0.15	1803
6	11.934	4036	0.10	1656

Analysed By

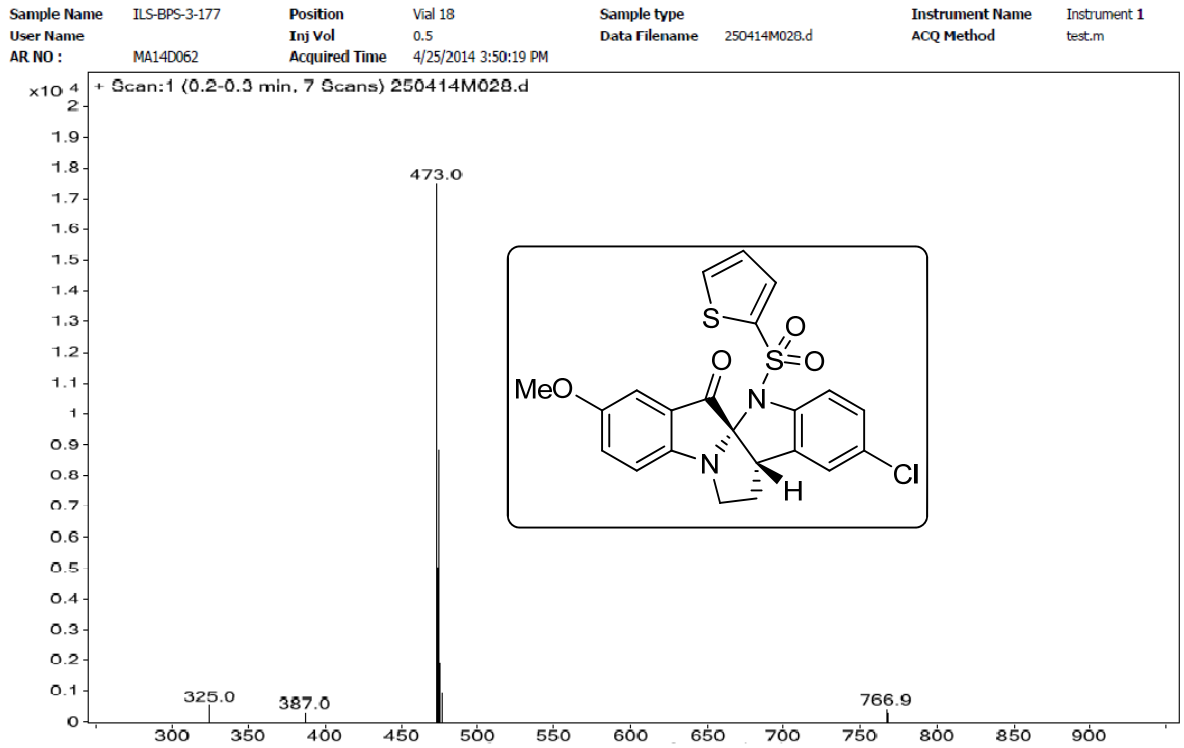
23/04/14

Checked By

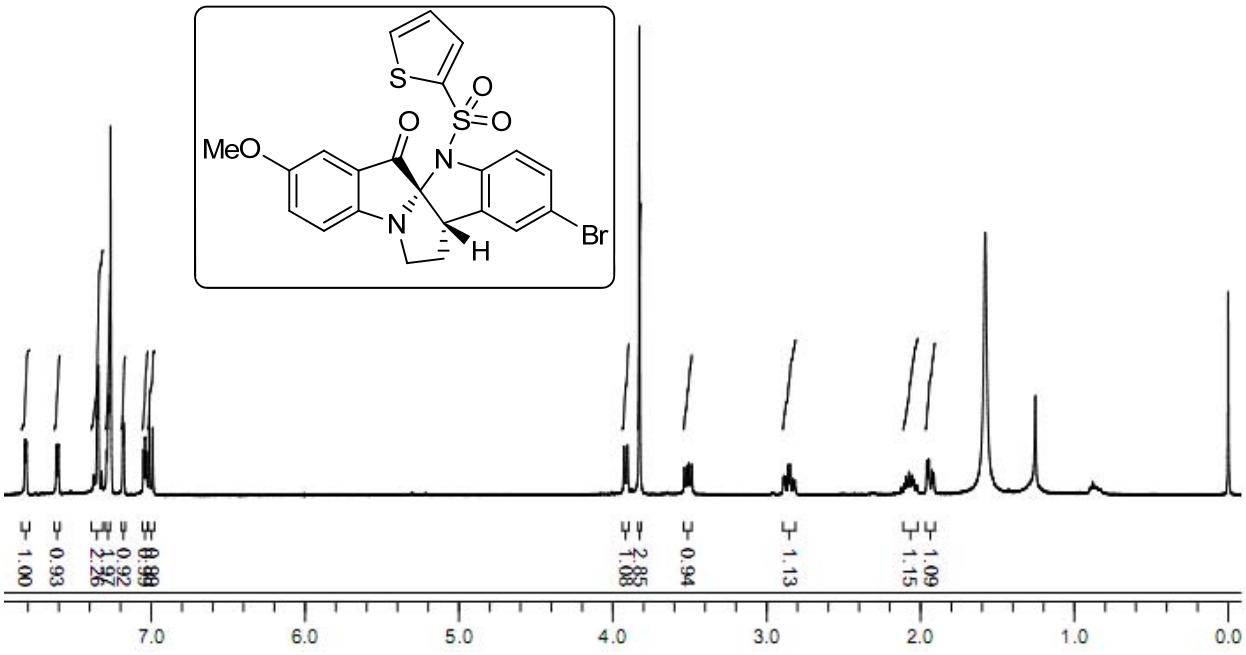
23/04/14

Reported by User: System
Report Method: CPRI@DRILS
Report Method ID: 6580
Page: 1 of 1

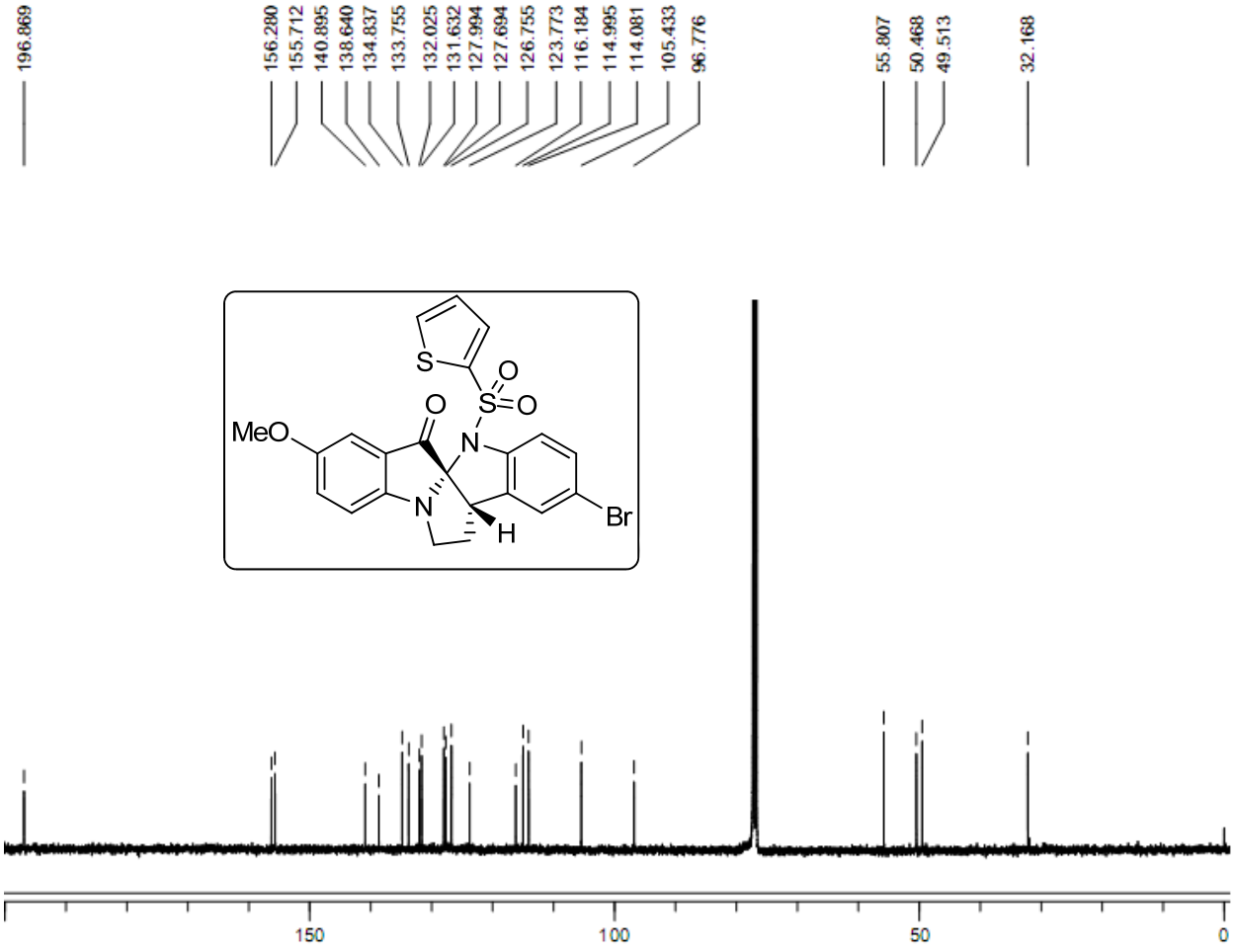
Project Name: APRIL_2014
Date Printed:
4/23/2014
10:03:43 AM Asia/Calcutta



Mass spectra of compound **2l**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2m** in $CDCl_3$



^{13}C NMR spectrum (Varian, 100 MHz) of compound **2m** in $CDCl_3$

HPLC of compound **2m**

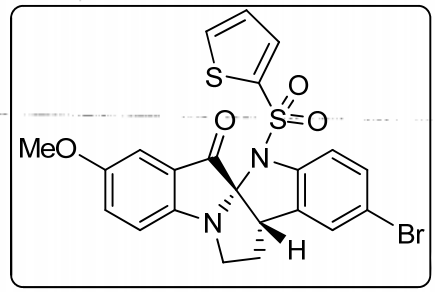
Empower 2 software

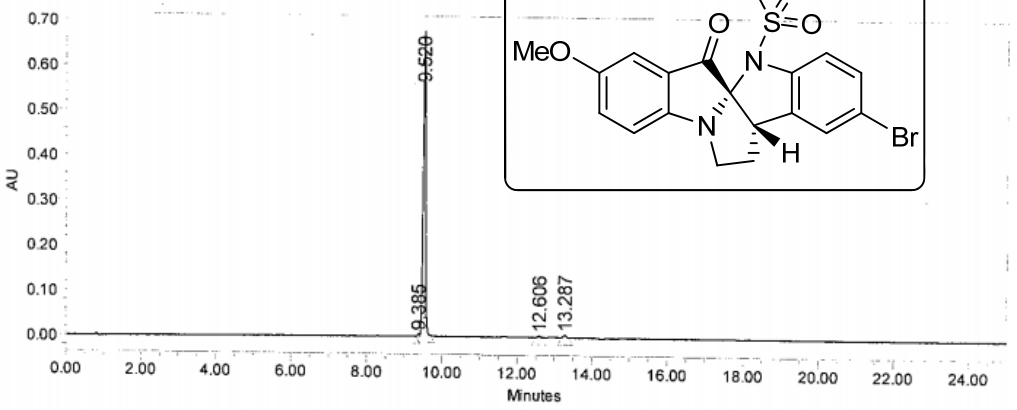
CPRI@DRILS

SAMPLE INFORMATION

Sample Name:	ILS-BPS-3-176		
A.R Number:	CM14D016		
Vial:	5	Acq operator:	Vaishnavi
Injection #:	1	Acq. Method Set:	SFV_A5
Injection Volume:	5.00 ul	Processing Method:	SFV_A5 PRO
Run Time:	25.0 Minutes	Channel Name:	235.0nm
Sample Set Name:	250414_1	Proc. Chnl. Descr.:	PDA 235.0 nm Blank Subtracted
Date Acquired:	4/25/2014 6:47:45 PM IST		
Date Processed:	4/26/2014 10:23:08 AM IST		

Column: Symmetry C-18 75*4.6mm 3.5µm
Mobile phase: A) 0.1% TFA in water B) ACN
T/%B: 0/20, 2/20, 10/95, 20/95, 22/20, 25/20
Flow: 1.0 ml /min, Diluent: ACN: WATER (80:20)





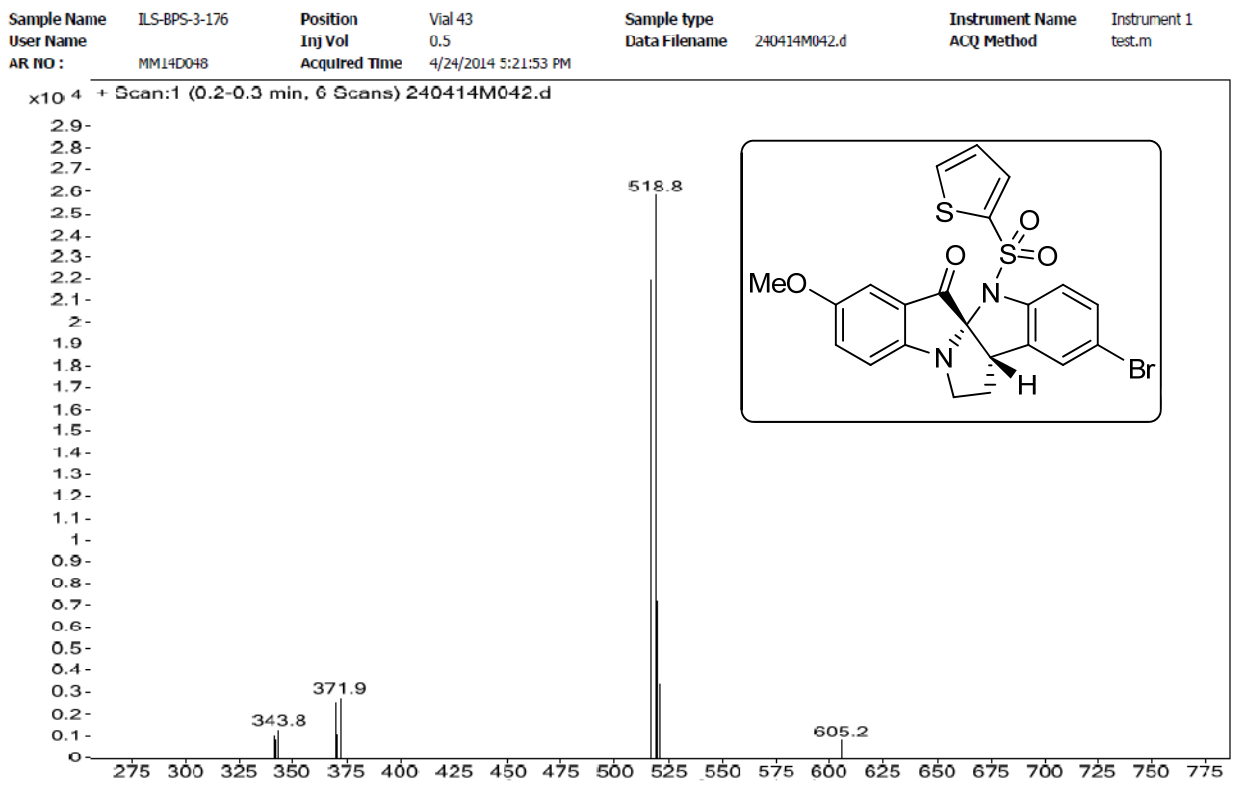
	RT	Area	% Area	Height
1	9.385	17153	0.58	4945
2	9.520	2900511	97.53	674925
3	12.606	22960	0.77	4009
4	13.287	33329	1.12	6188

Analysed By

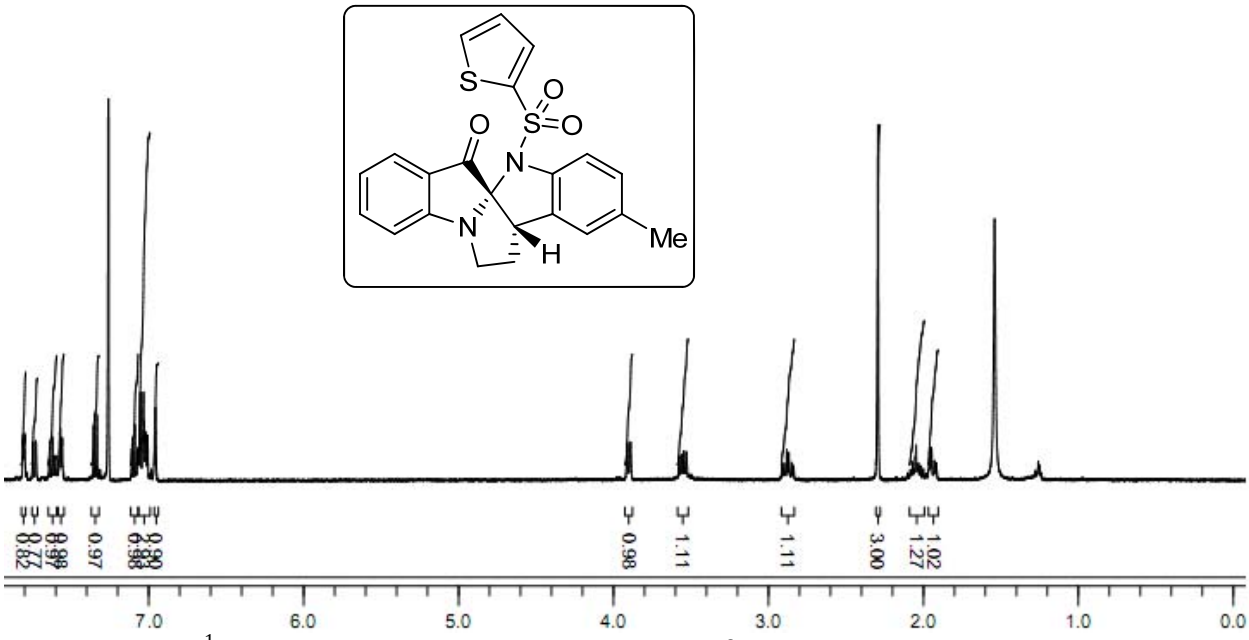
Checked By

Reported by User: System
Report Method: CPRI@DRILS
Report Method ID: 7305
Page: 1 of 1

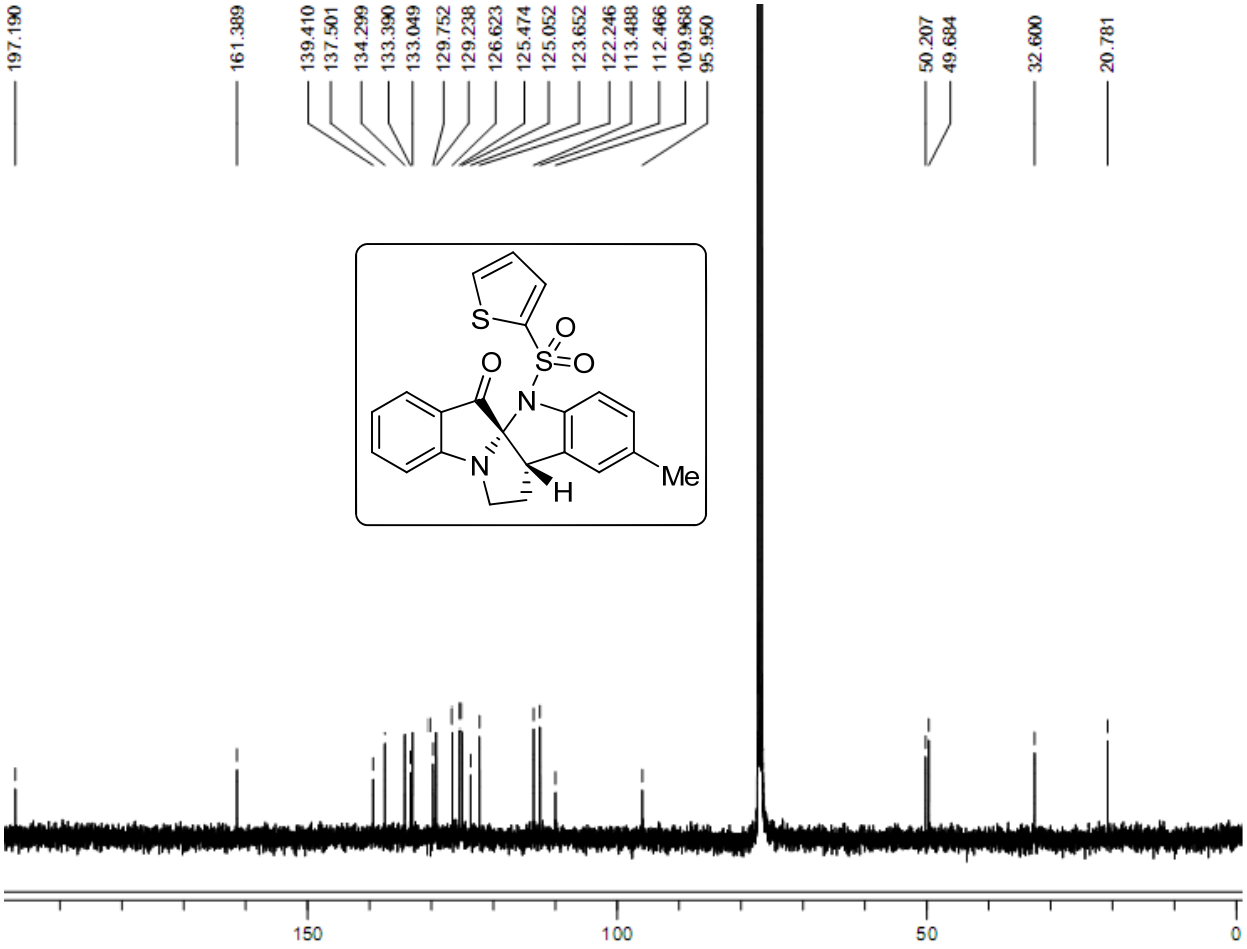
Project Name: APRIL_2014
Date Printed:
4/26/2014
10:23:18 AM Asia/Calcutta



Mass spectra of compound **2m**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2n** in $CDCl_3$

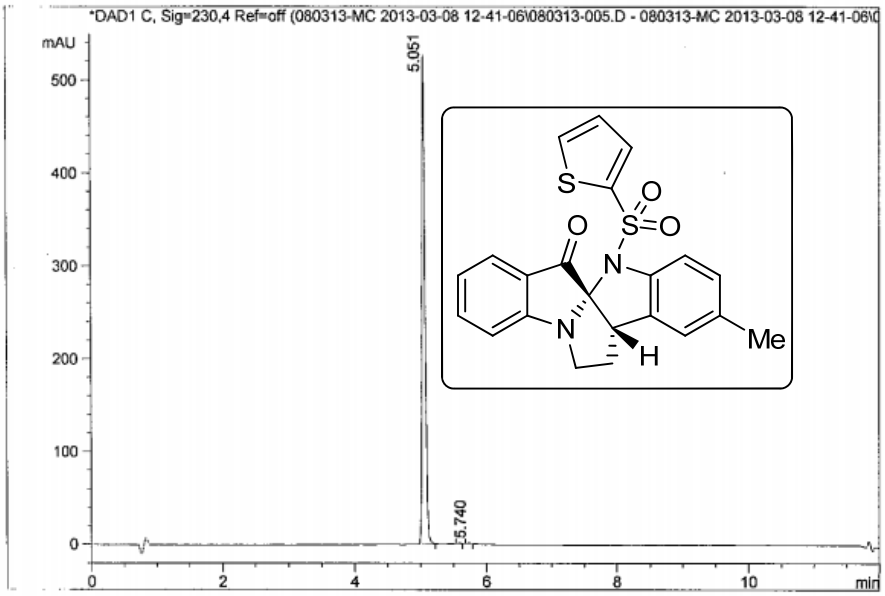


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2n** in $CDCl_3$

HPLC of compound **2n**

COSMIC DISCOVERIES @ ILS
HPLC ANALYSIS REPORT

		Seq Line :	4
Injection Date	: Fri, 8. Mar. 2013	Location :	Vial 14
Sample Name	: ILS-BPS-3-73	Inj. No. :	1
Acq Operator	: VARMA	Inj. Vol. :	5 µl
Acq. Method	: D:\Chem32\1\DATA\080313-MC 2013-03-08 12-41-06\C-18 ->		
Analysis Method	: D:\CHEM32\1\METHODS\C-18 A80B20GM.M		
Method Info	: Column:Symmetry C-18 75*4.6mm,3.5µ		
	Mobile phase: A) 0.1% HCOOH in water,B) ACN(GRADIENT) T/		
	B%:0/20,0.5/20,4/98,10/98,10.5/20,12/20		
	Flow:1.0 ml/min Diluent: ACN:Water(80:20)		



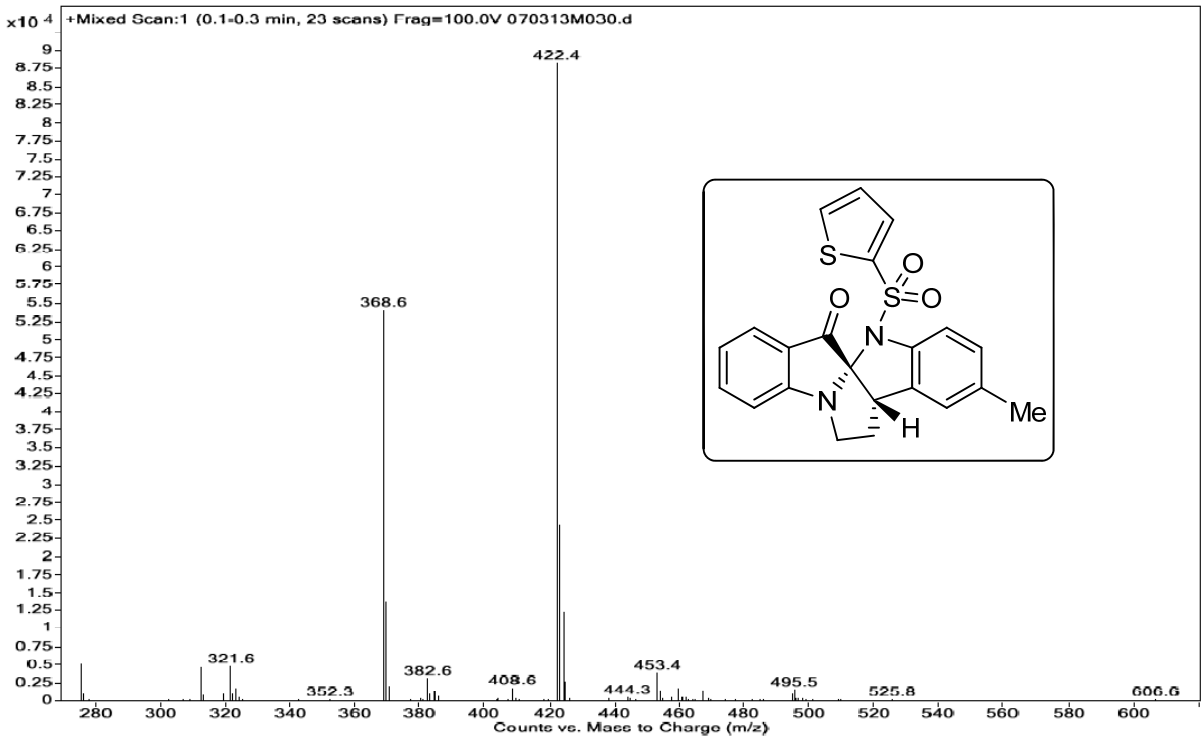
Signal 1: DAD1 C, Sig=230,4 Ref=off

Peak #	RT [min]	Area	Area %
1	5.051	1686.874	99.697
2	5.590	2.637	0.156
3	5.740	2.483	0.147

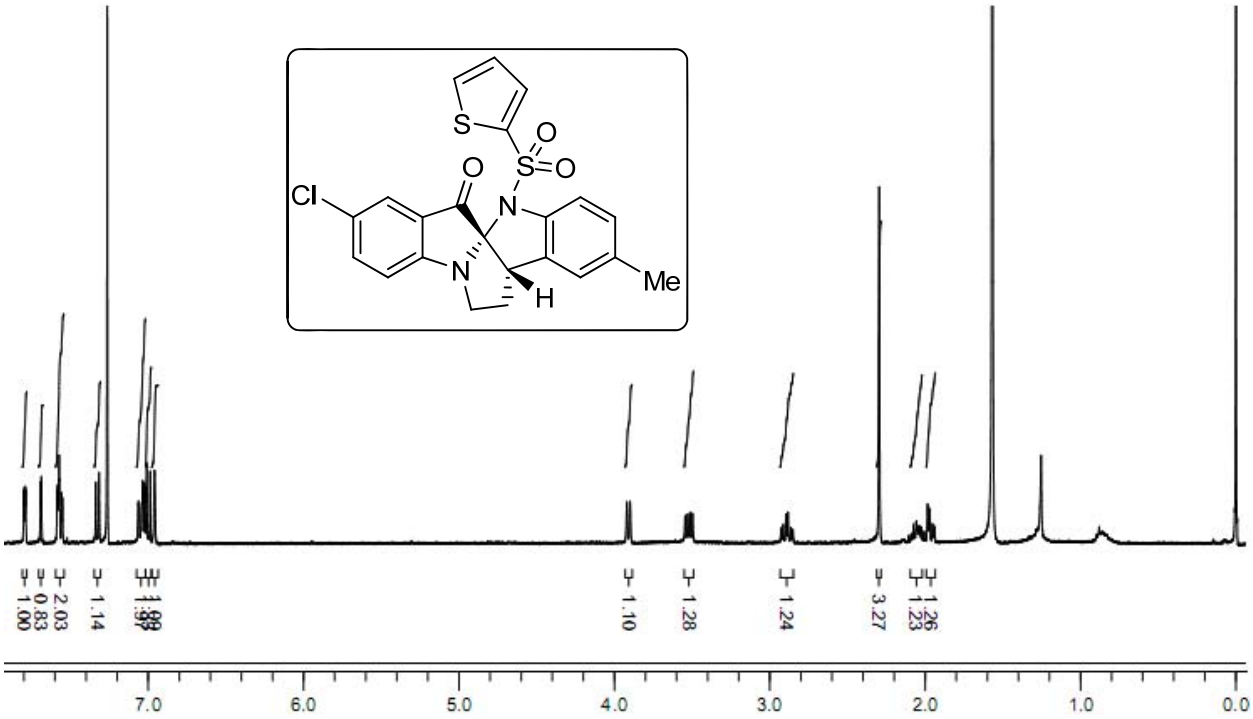
Rajesh 05/03/13

*** End of Report ***

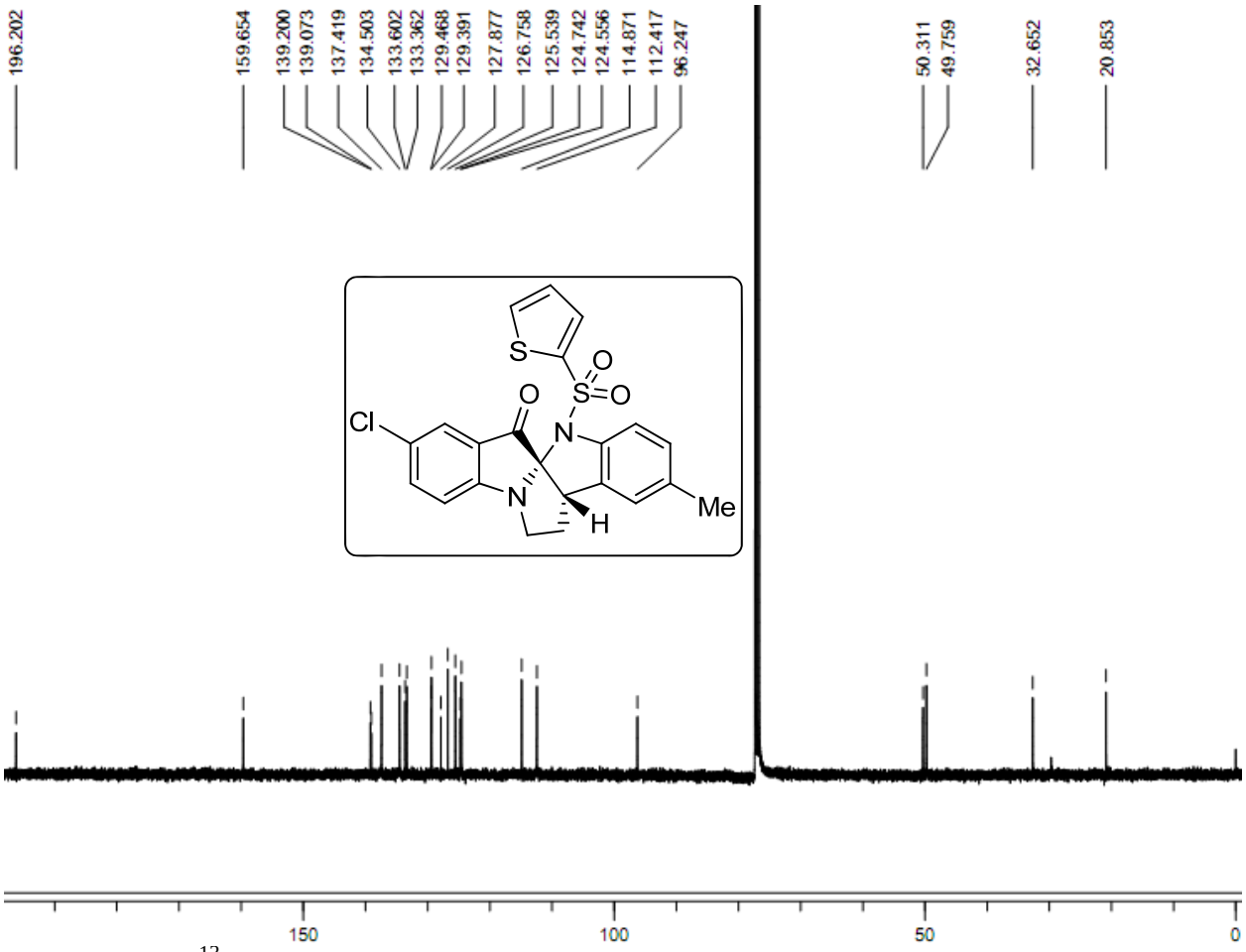
Sample Name	ILS/BPS/3-73	**Position**	Vial 27	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Not Applicable
Data Filename	070313M030.d	**ACQ Method**	ILS.m	**Comment**		**Acquired Time**	3/7/2013 1:07:24 PM



Mass spectra of compound **2n**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2o** in $CDCl_3$

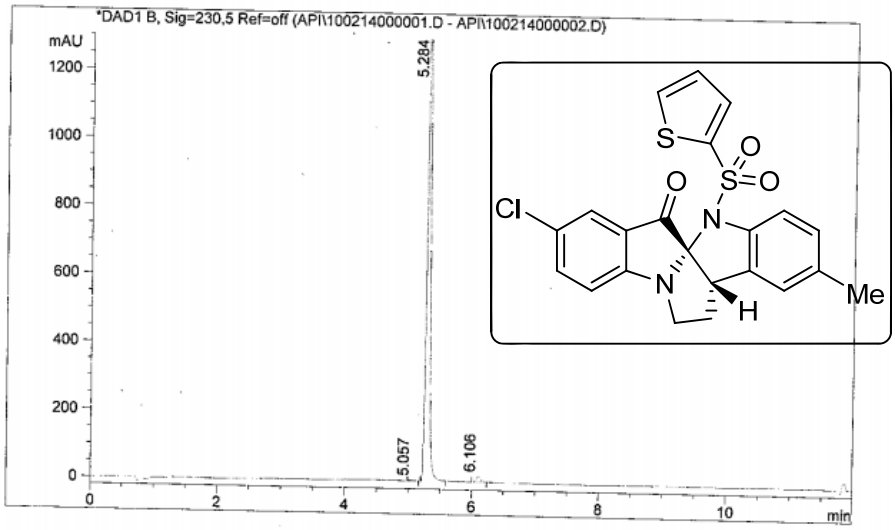


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2o** in $CDCl_3$

HPLC of compound **2o**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Injection Date	: Mon, 10. Feb. 2014	Seq Line :	0
Sample Name	: ILS-BPS-3-171	Location :	Vial 1
Acq Operator	: RADHA	Inj. No. :	0
Acq. Method	: D:\CHEM32_002\1\METHODS\C-18 A80B20GS.M	Inj. Vol. :	15 µl
Analysis Method	: D:\CHEM32_002\1\METHODS\C-18 A80B20GS.M		
Method Info	: Column : Symmetry C-18 75*4.6mm,3.5µm		
	Mobile phase: A) 0.1% HCOOH in Water , B) ACN		
	T/B%:0/20,0.5/20,4/98,10/98,10.5/20,12/20		
	Flow: 1.0 ml/min, Diluent: ACN:Water(80:20)		

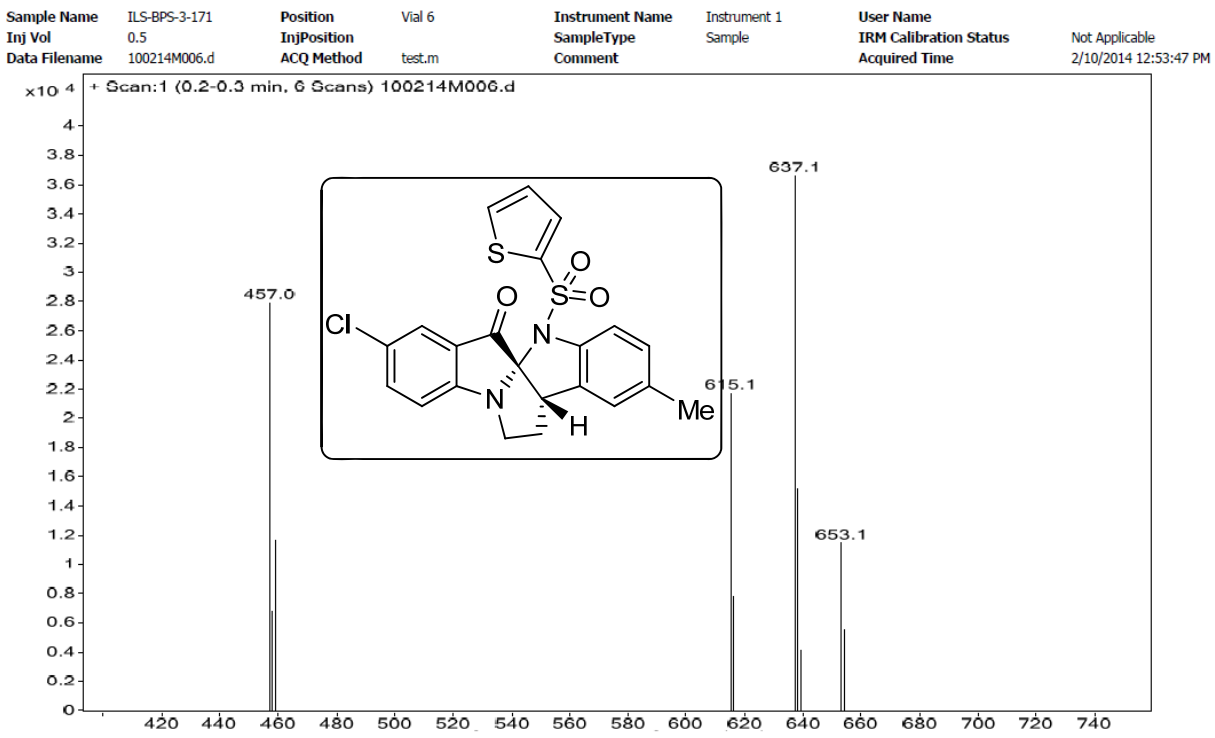


Signal 1: DAD1 B, Sig=230,5 Ref=off

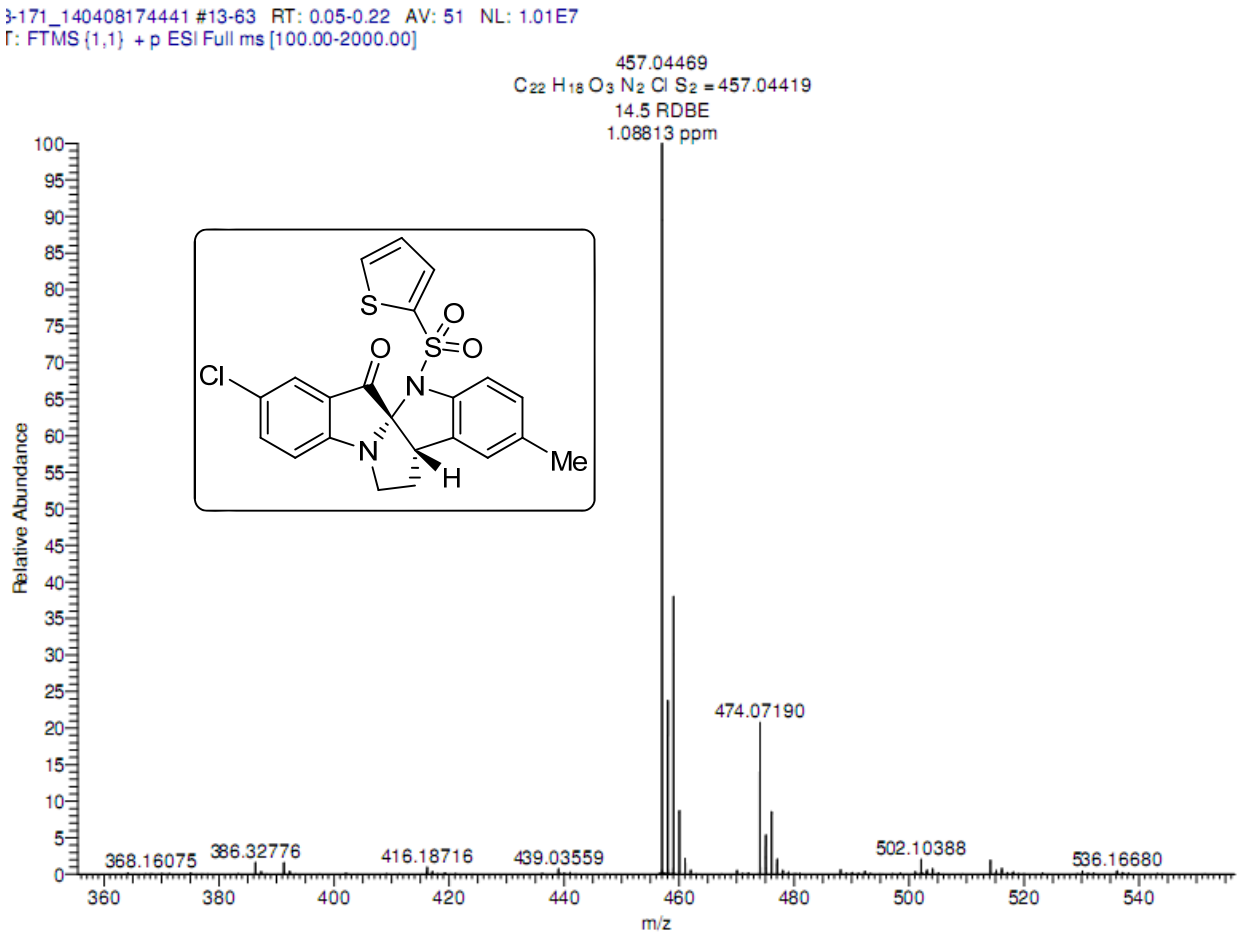
Peak #	RT [min]	Area	Area %
1	5.057	6.209	0.110
2	5.284	5550.146	98.465
3	6.106	80.288	1.424

10/02/14

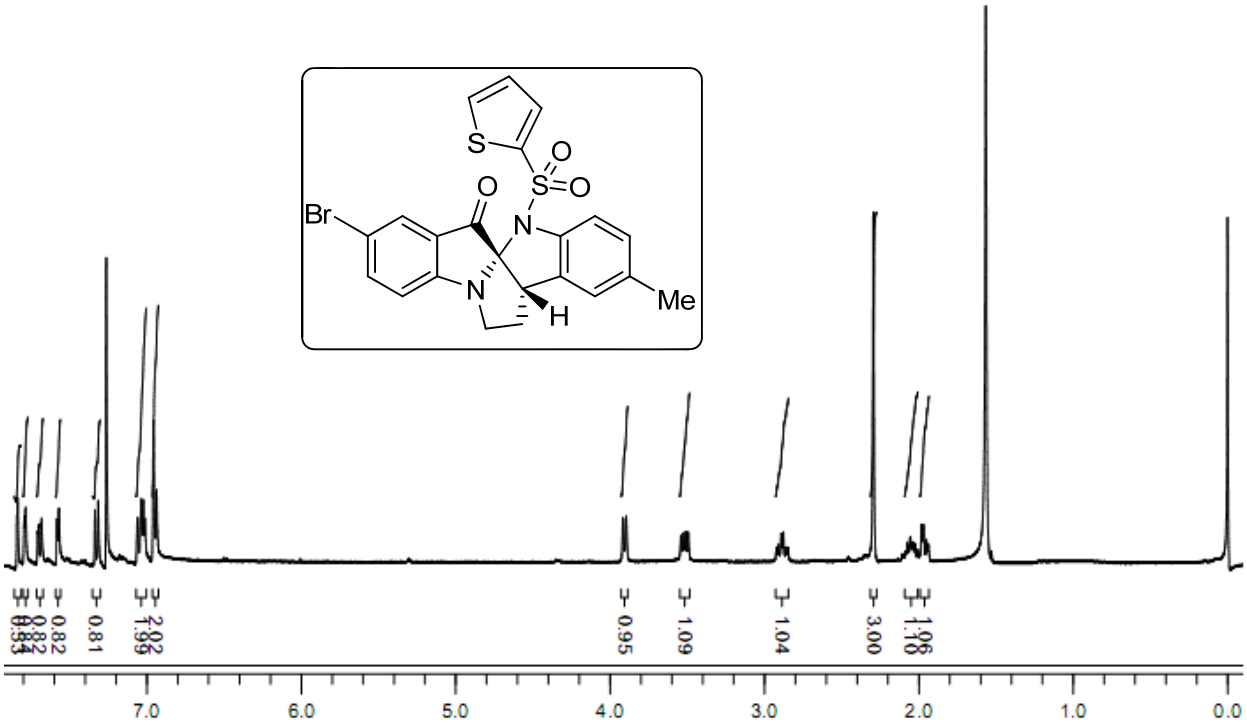
*** End of Report ***



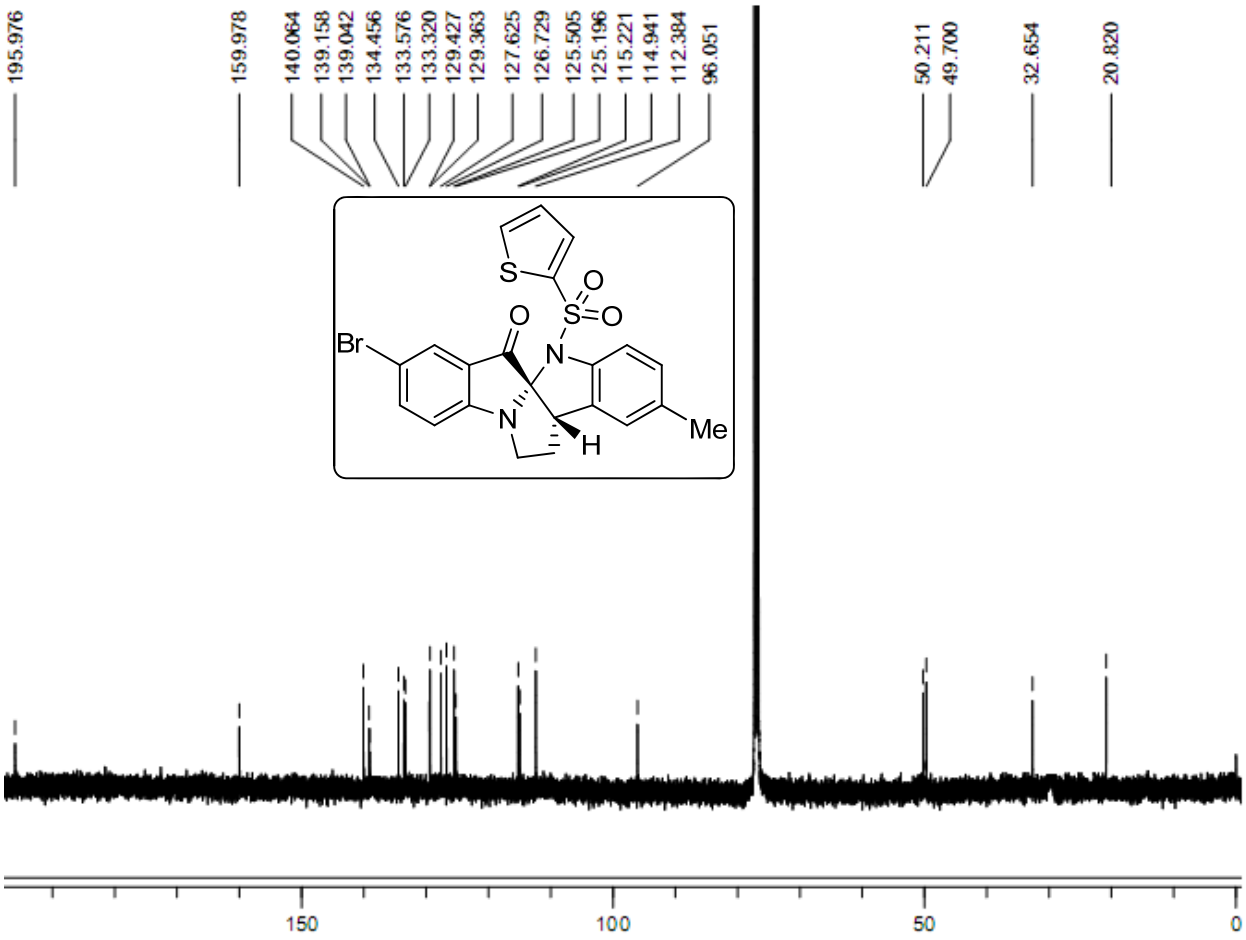
Mass spectra of compound **2o**



HRMS of compound **2o**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2p** in $CDCl_3$

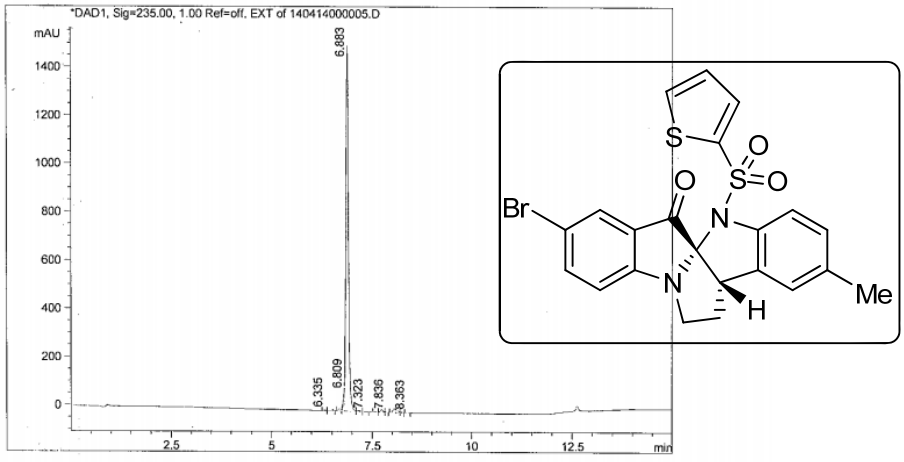


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2p** in $CDCl_3$

HPLC of compound **2p**

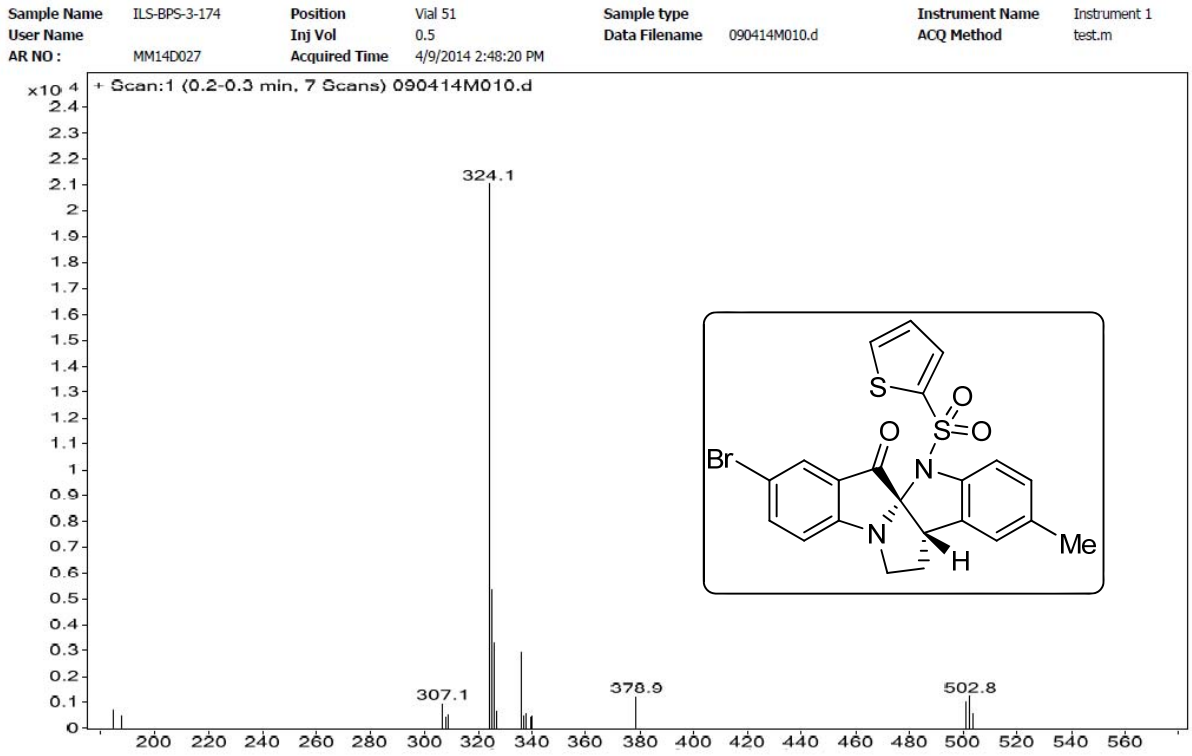
CPRI @ DRILS
HPLC ANALYSIS REPORT

Inj Date : Mon, 14. Apr. 2014 Acq Operator: SHASHIDHAR
Sample Name : ILS-BPS-3-174 Vial 3
A.R Number : CM14D008 -> Inj. Vol. : 10µL
Acq. Method : D:\CHEM32_002\1\METHODS\C-18 A80B20.M
Analysis Method : D:\CHEM32_002\1\METHODS\C-18 A80B20.M
Method Info : Column : Symmetry C-18 75*4.6mm3.5µm
Mobile phase: A) 0.1% TFA in water , B) ACN
T/B% : 0/20,1/20,6/98,10/98,12/20,15/20.
Flow: 1.0 ml/min Diluent: ACN:Water(80:20)

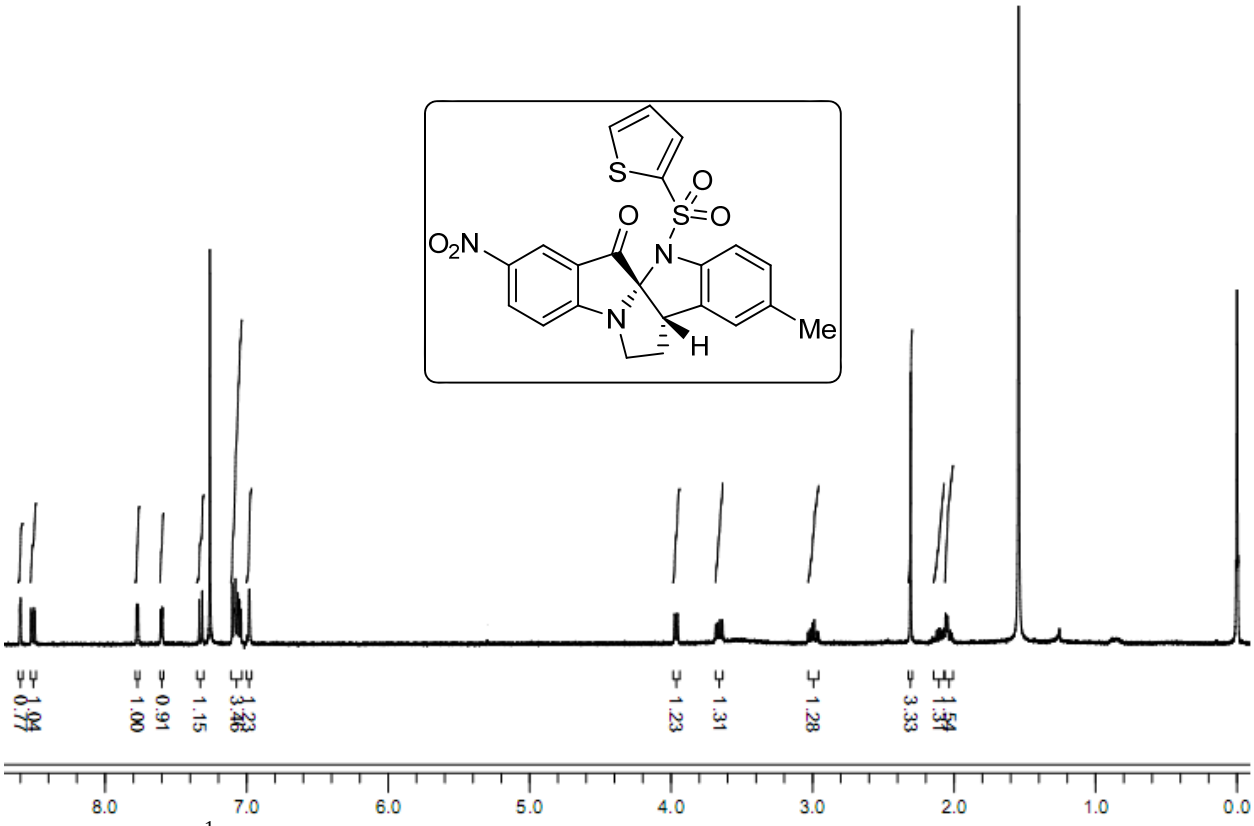


Signal 1: DAD1, Sig=235.00, 1.00 Ref=off, EXT

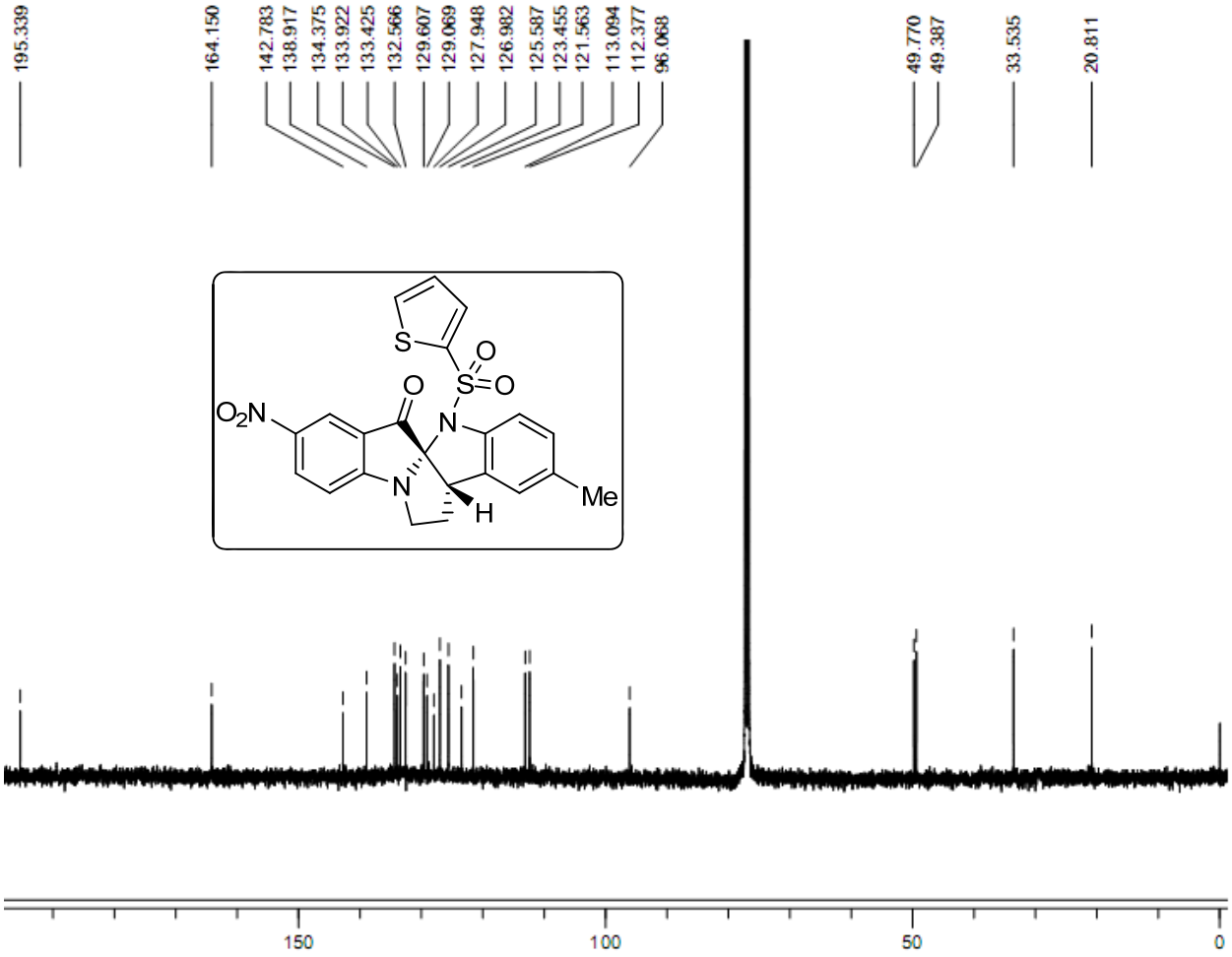
Peak #	RT [min]	Area	Area %
1	6.335	9.078	0.128
2	6.464	193.773	2.727
3	6.684	29.836	0.420
4	6.809	178.952	0.518
5	6.883	6501.815	93.496
6	7.164	17.489	0.246
7	7.323	6.065	0.085
8	7.579	7.627	0.107
9	7.730	40.471	0.570
10	7.836	2.209	0.031
11	8.052	66.167	0.931



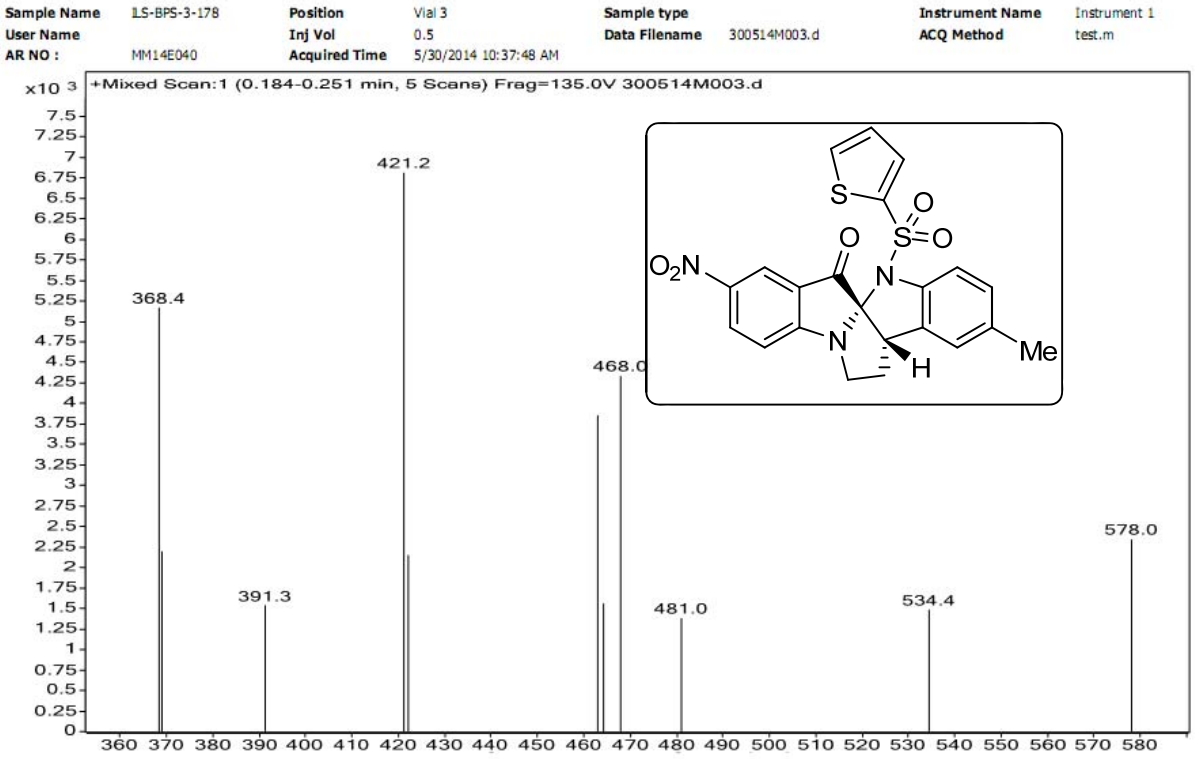
Mass spectra of compound **2p**



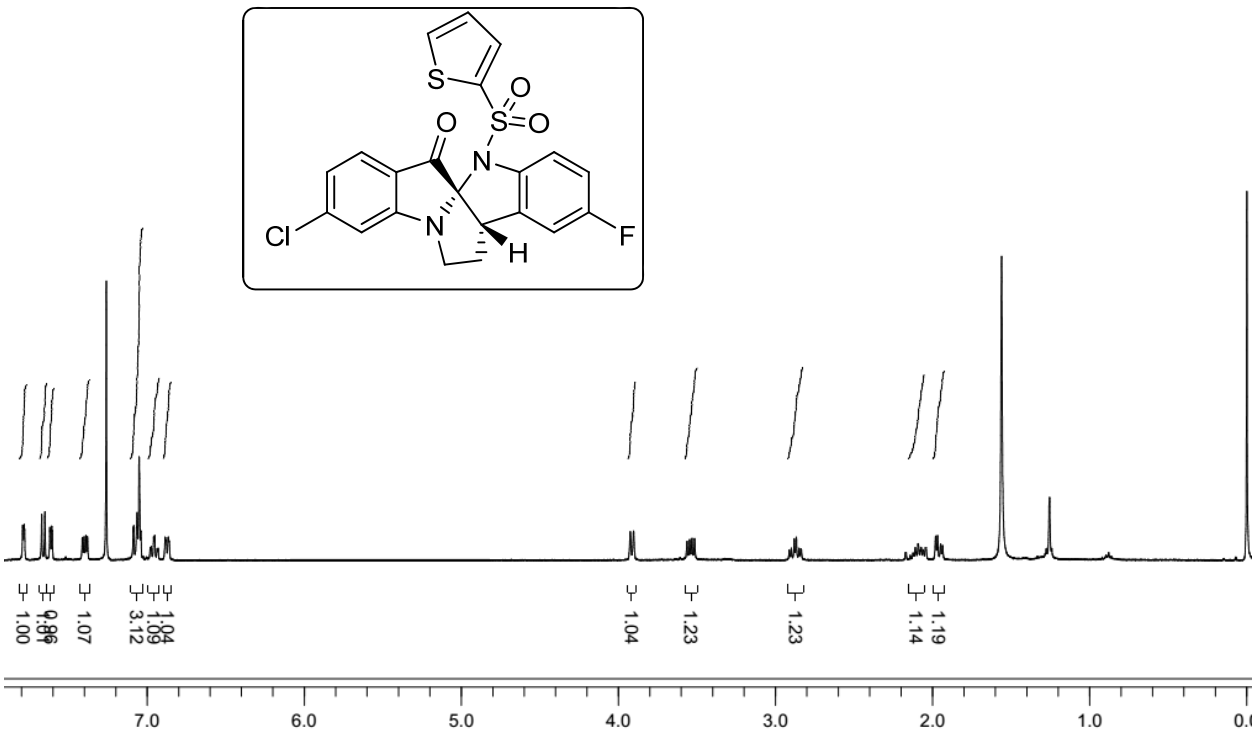
^{1}H NMR (Varian, 400 MHz) spectrum of compound **2q** in $CDCl_3$



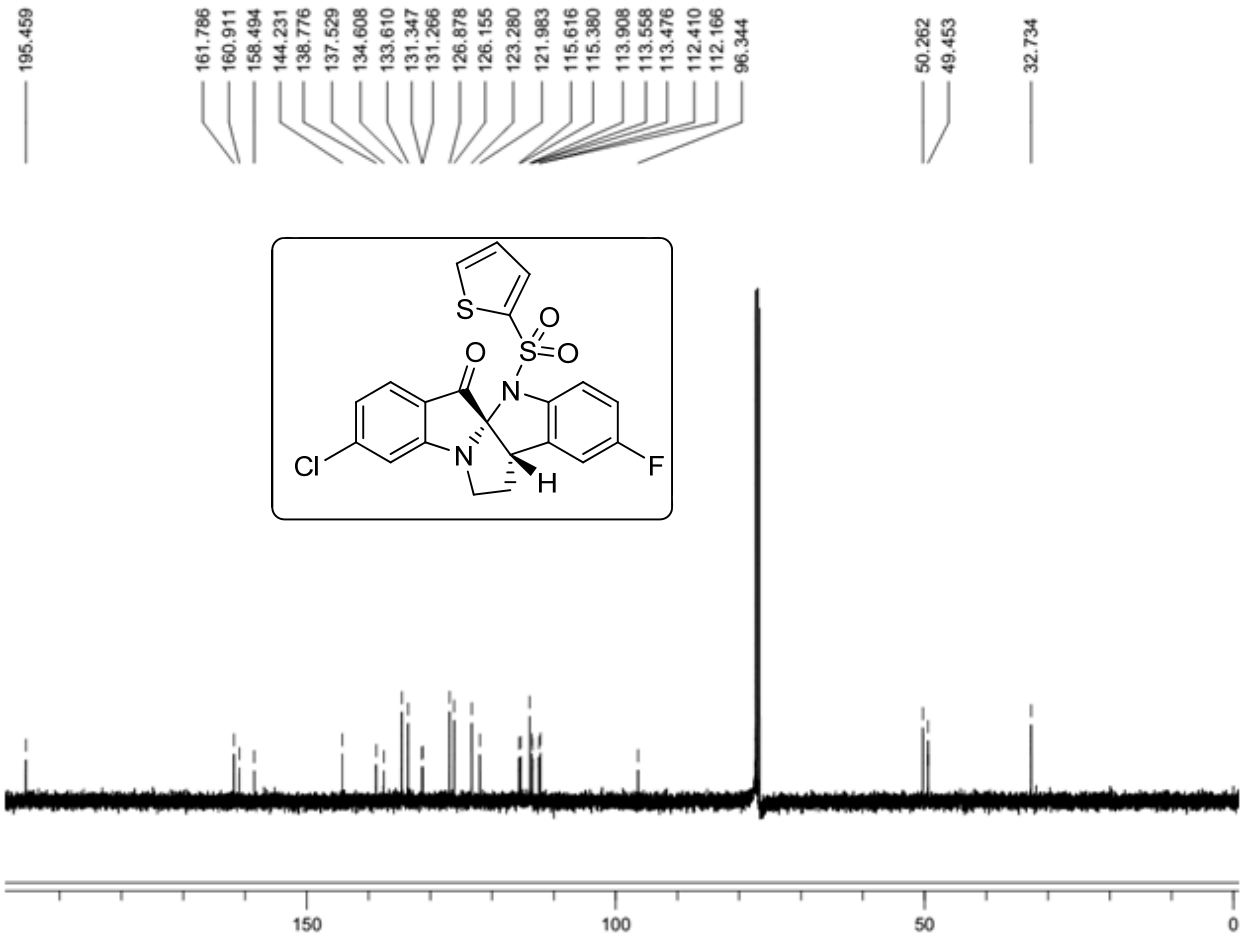
^{13}C NMR spectrum (Varian, 100 MHz) of compound **2q** in $CDCl_3$



Mass spectra of compound **2q**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2r** in $CDCl_3$

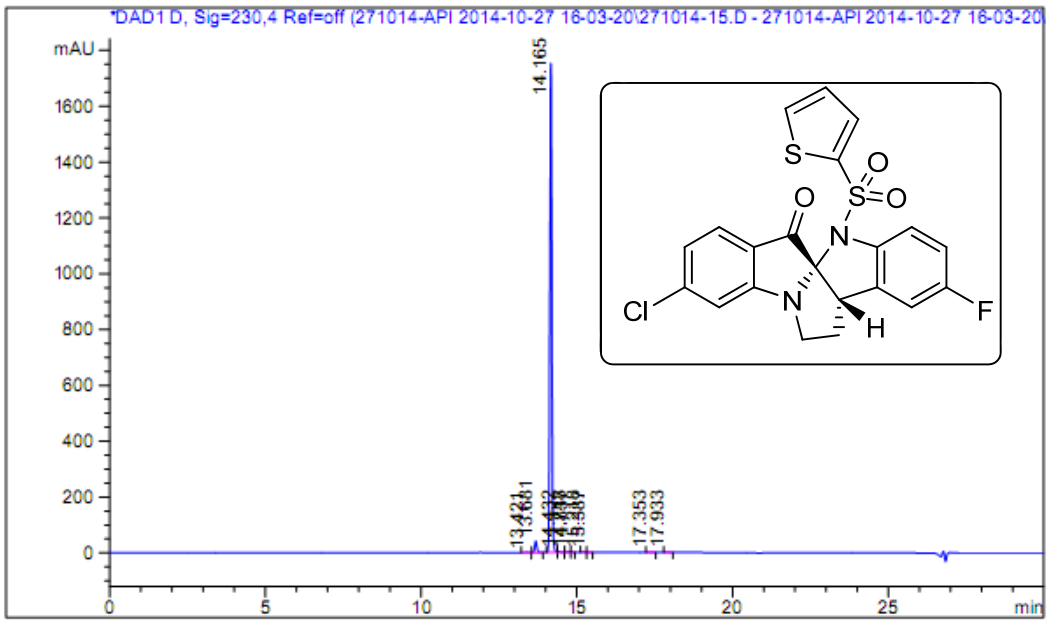


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2r** in $CDCl_3$

HPLC of compound **2r**

CPRI @ DRILS
HPLC ANALYSIS REPORT

```
Inj Date         : Mon, 27. Oct. 2014          Acq Operator: RADHA
Sample Name      : ILS-BPS-3-193                             Vial 42
A R Number       : CM14J011                  ->Inj. Vol.    : 7µL
Acq. Method      : D:\chem32\1\DATA\271014-API 2014-10-27 16-03-20\API ->
Analysis Method  : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info      : Column: X-Terra C-18 250*4.6mm, 5µm
                   Mobile phase: A) 5mm Ammonium Acetate in water B) ACN
                   T/%B:0/20,3/20,12/95,23/95,25/20,30/20
                   Flow:1.0ml/min Diluent: ACN:Water(80:20)
```

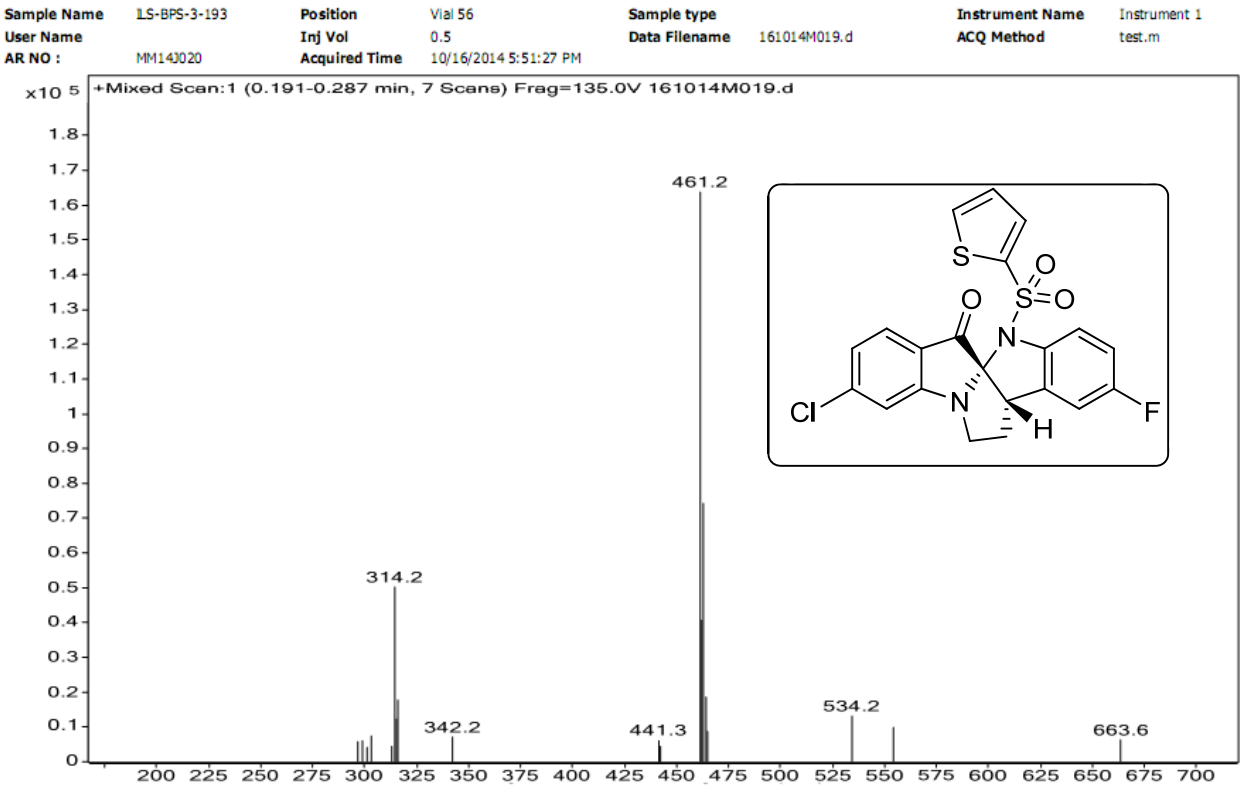


==========

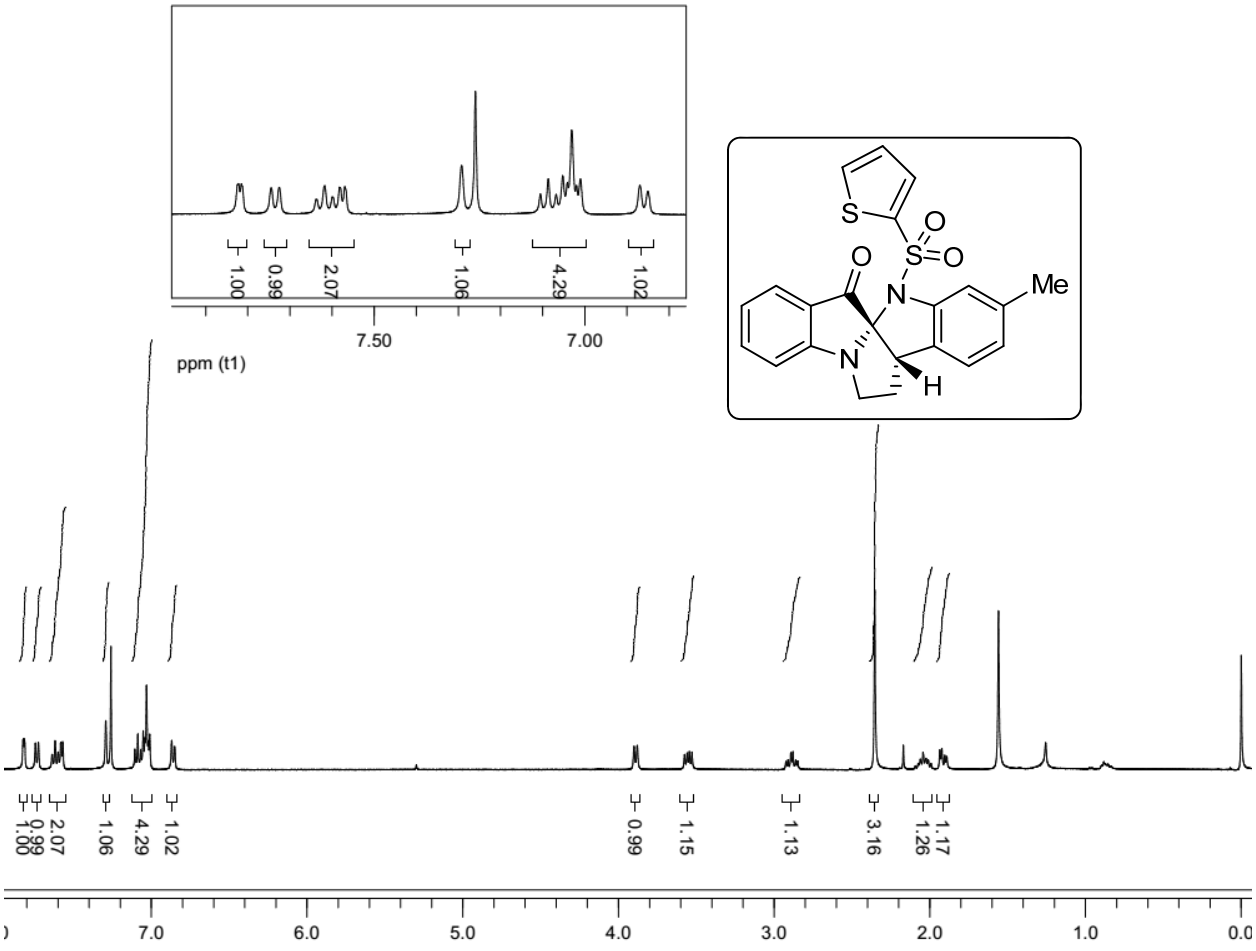
Signal 1: DAD1 D, Sig=230,4 Ref=off

Peak #	RT [min]	Area	Area %
1	13.421	6.645	0.082
2	13.681	198.157	2.453
3	14.165	7816.338	96.774
4	14.432	14.074	0.174
5	14.748	11.102	0.137
6	14.837	3.966	0.049
7	15.218	8.604	0.107
8	15.387	3.310	0.041
9	17.353	8.452	0.105
10	17.933	6.223	0.077

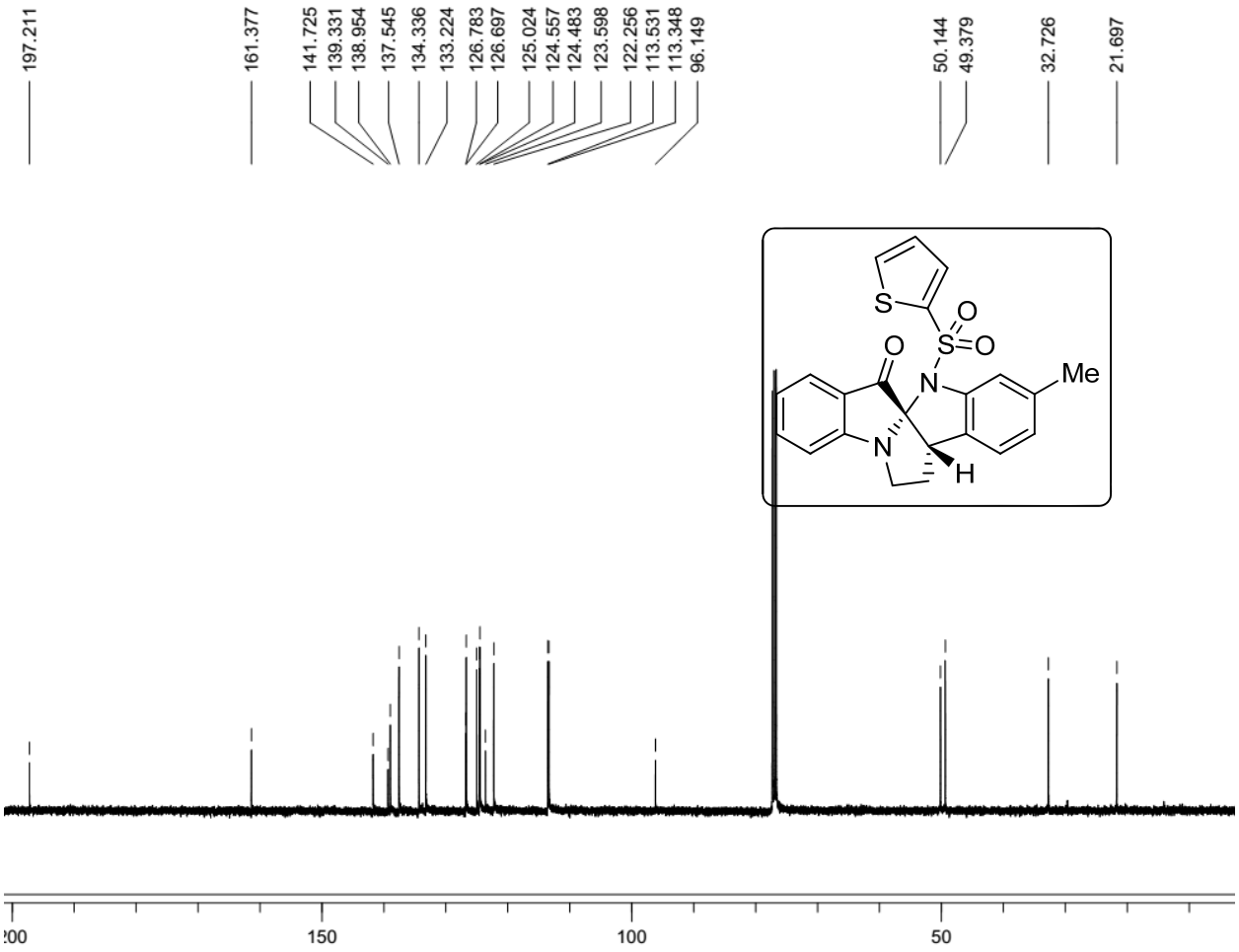
Analysed by : Checked by :



Mass spectra of compound **2r**



^{1}H NMR (Varian, 400 MHz) spectrum of compound **2s** in $CDCl_3$

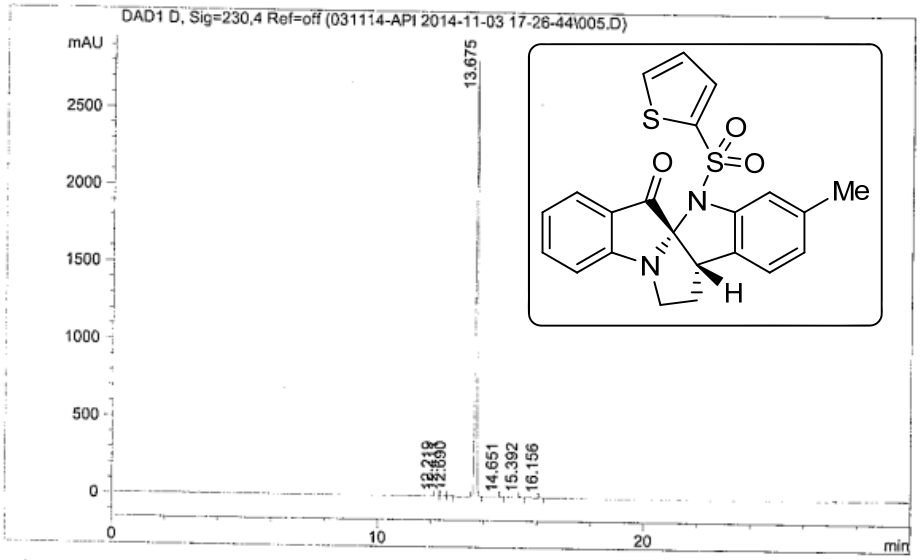


^{13}C NMR spectrum (Varian, 100 MHz) of compound **2s** in $CDCl_3$

HPLC of compound **2p**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Inj Date : Mon, 3. Nov. 2014 Acq Operator: RADHA
Sample Name : ILS-BPS-3-199 Vial 14
A R Number : CM14J023 ->Inj. Vol. : 5µL
Acq. Method : D:\chem32\1\DATA\031114-API 2014-11-03 17-26-44\API ->
Analysis Method : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info : Column: X-Terra C-18 250*4.6mm, 5µm
Mobile phase: A) 5mm Ammonium Acetate in water B) ACN
T/%B:0/20,3/20,12/95,23/95,25/20,30/20
Flow:1.0ml/min Diluent: ACN:Water(80:20)

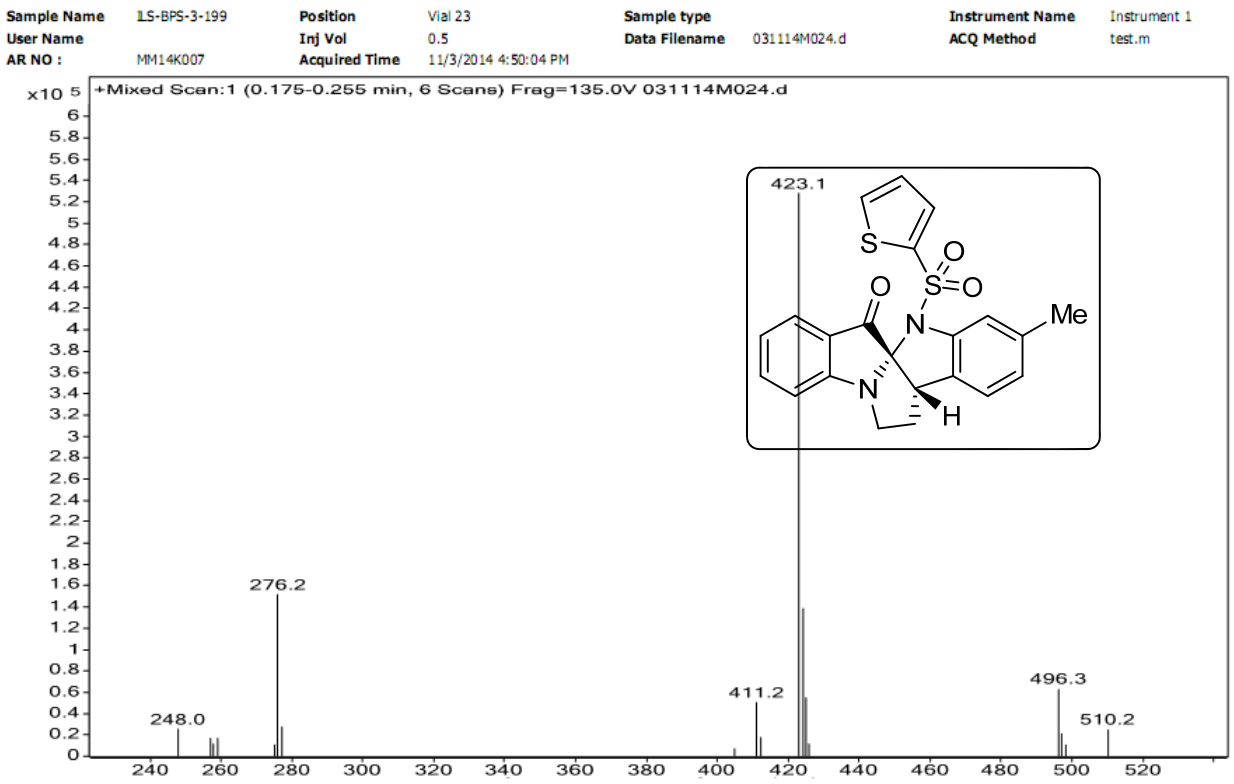


Signal 1: DAD1 D, Sig=230,4 Ref=off

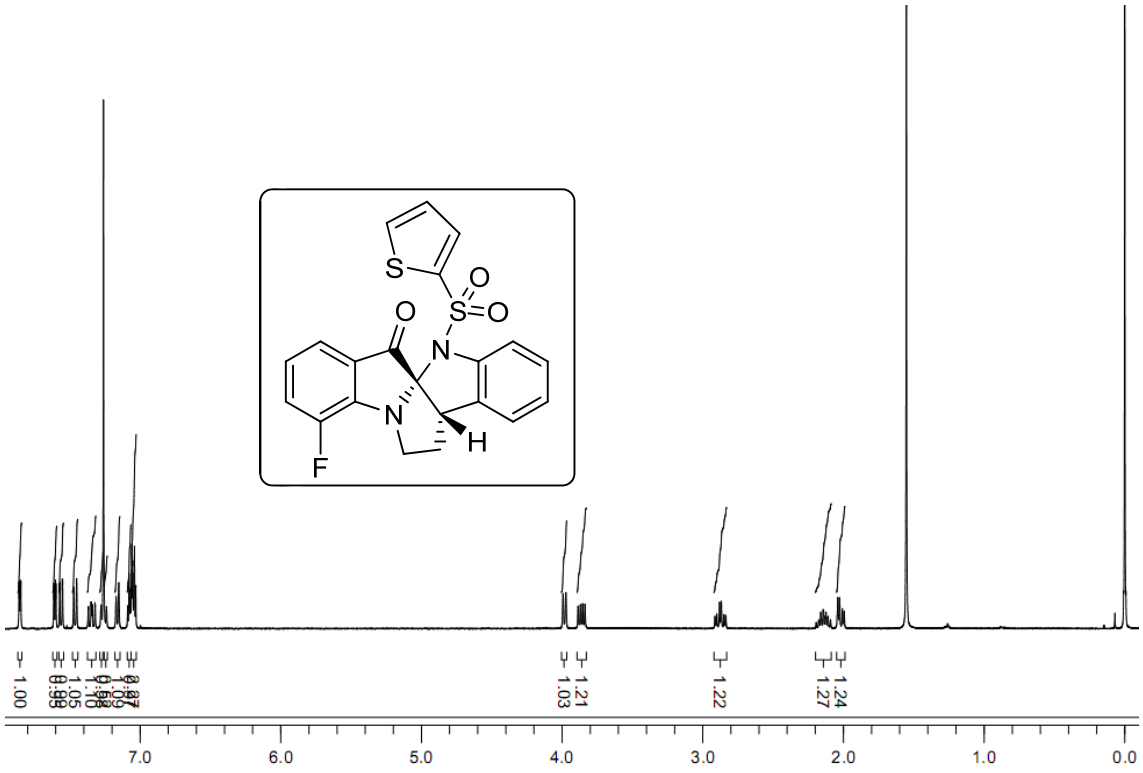
Peak #	RT [min]	Area	Area %
1	12.219	43.381	0.313
2	12.411	37.158	0.268
3	12.690	42.332	0.305
4	13.675	13688.322	98.694
5	14.651	13.987	0.101
6	15.392	20.441	0.147
7	16.156	23.829	0.172

Analysed by : 3/11/14 Checked by :

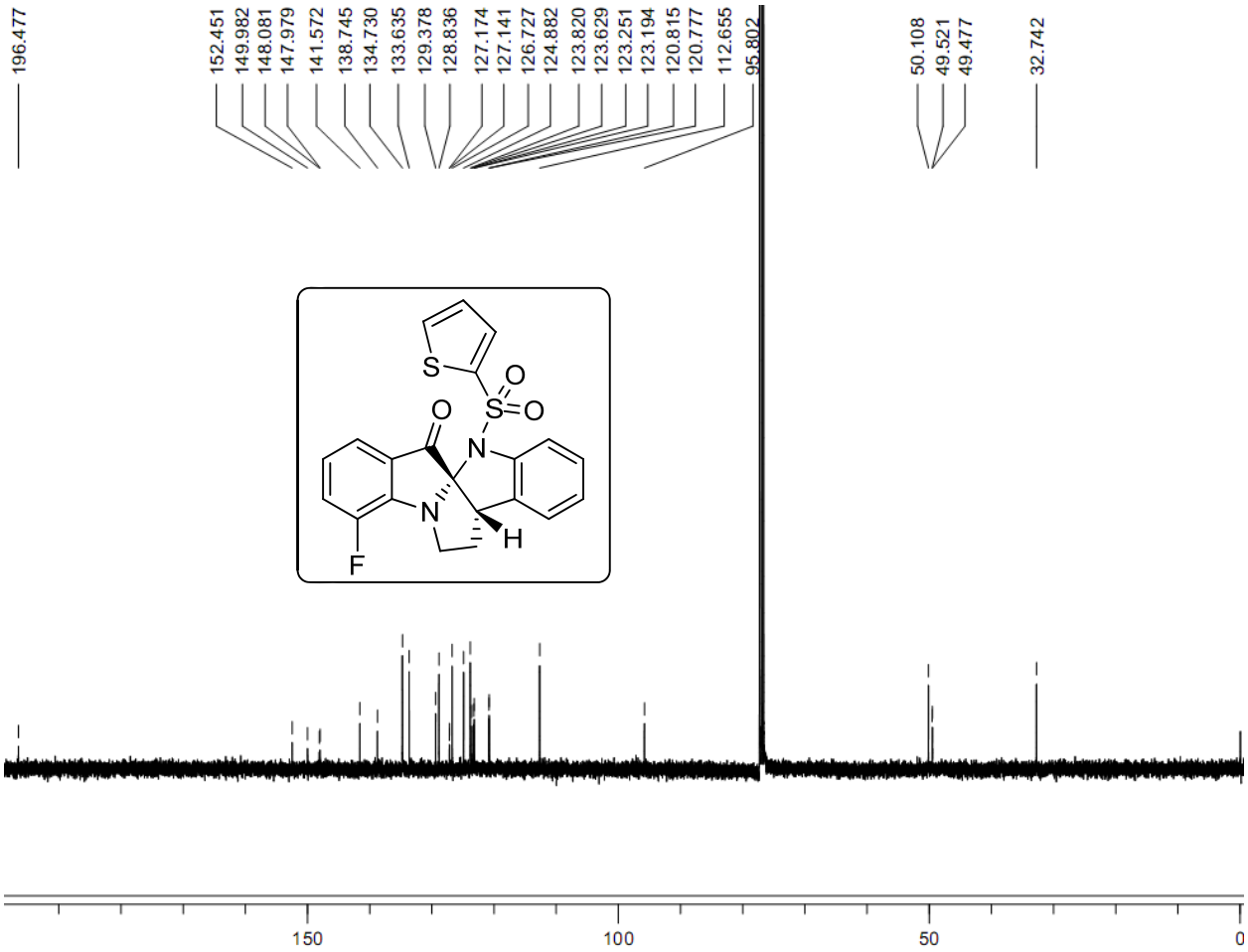
rument 1



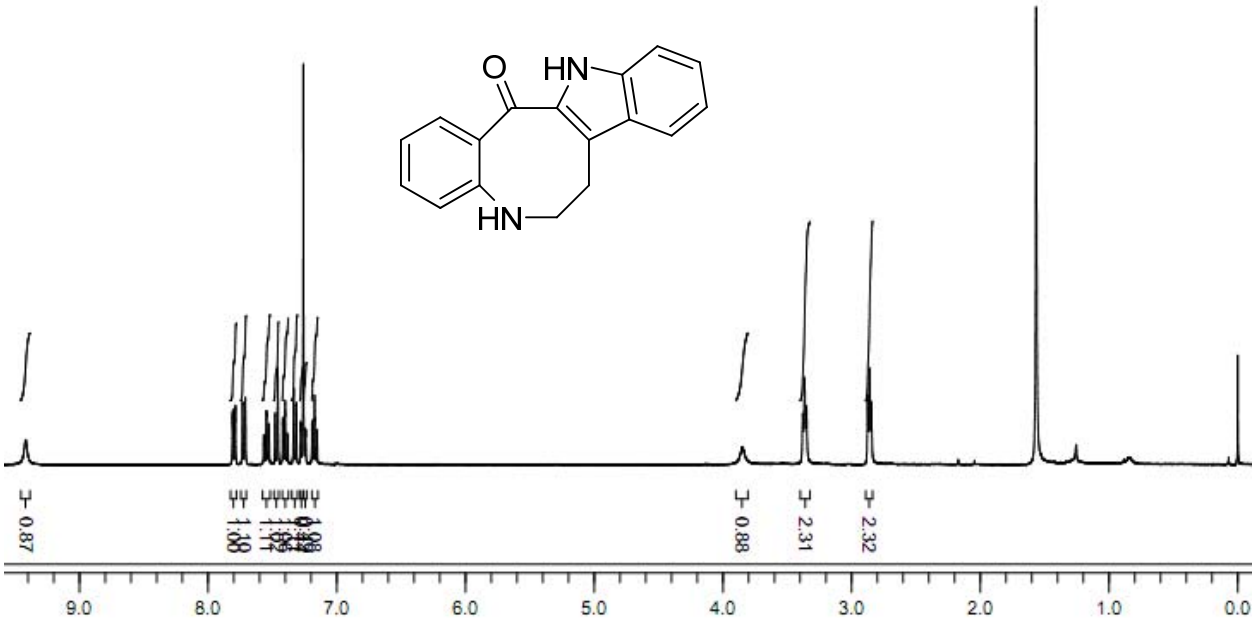
Mass spectra of compound **2s**



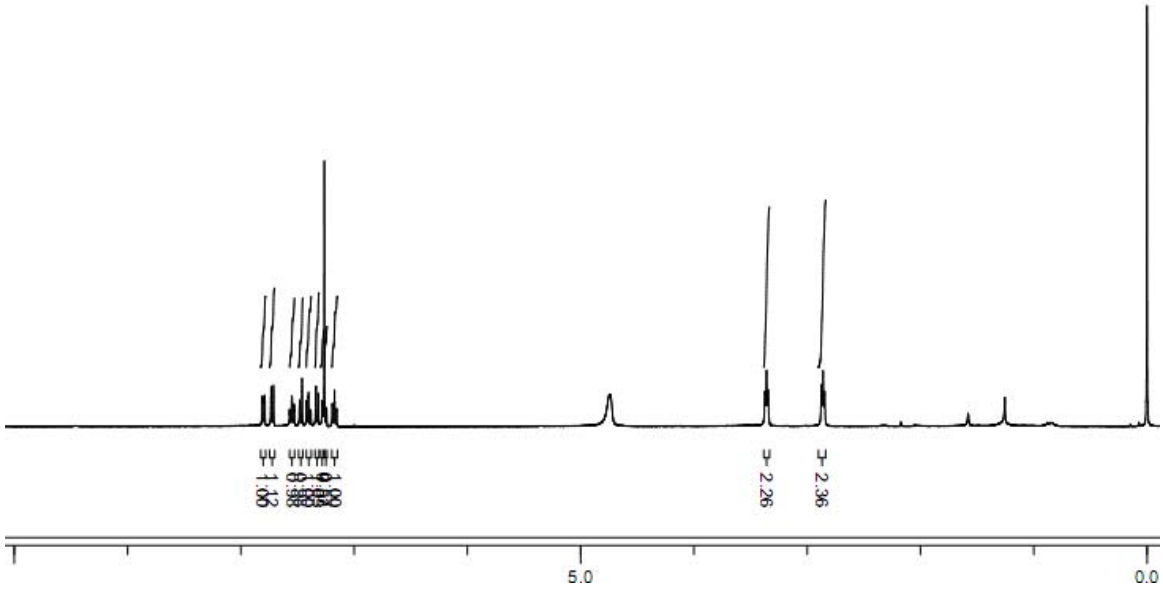
^{1}H NMR (Varian, 400 MHz) spectrum of compound **2t** in $CDCl_3$



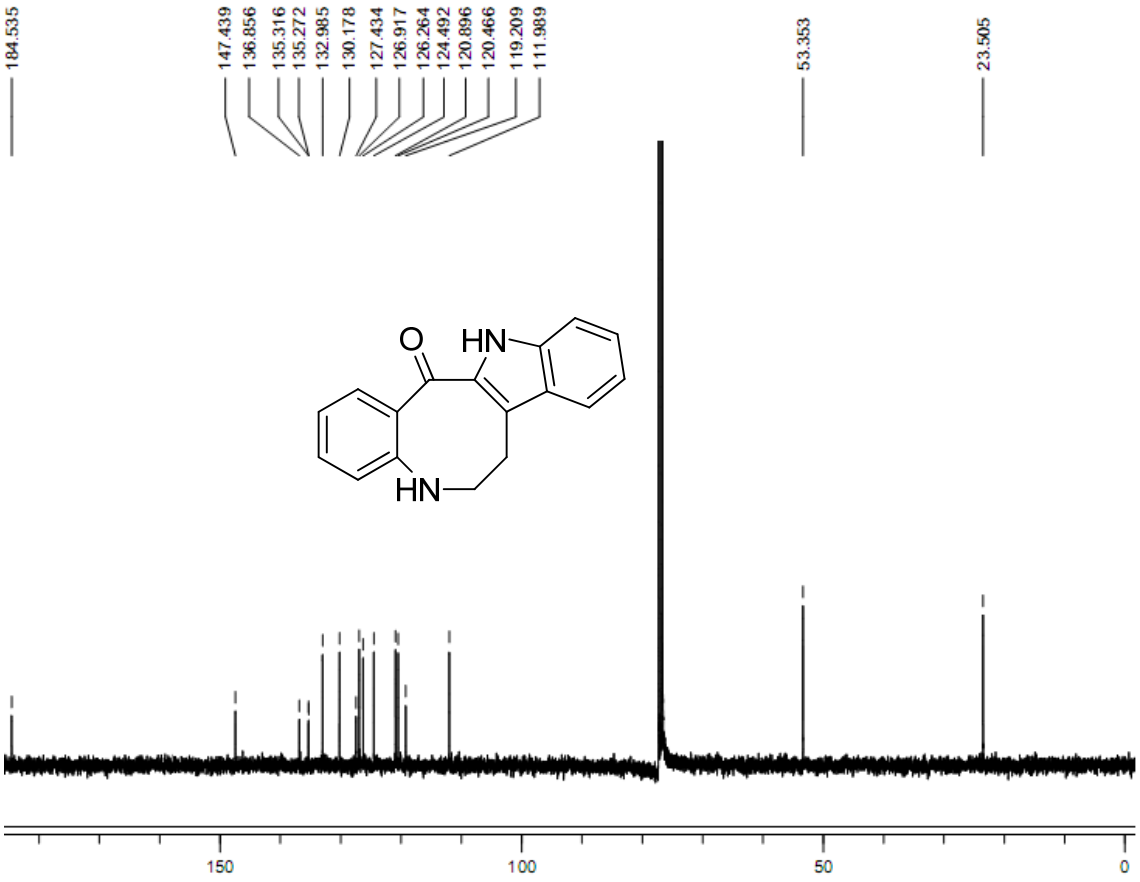
^{13}C NMR spectrum (Varian, 100 MHz) of compound **2t** in $CDCl_3$



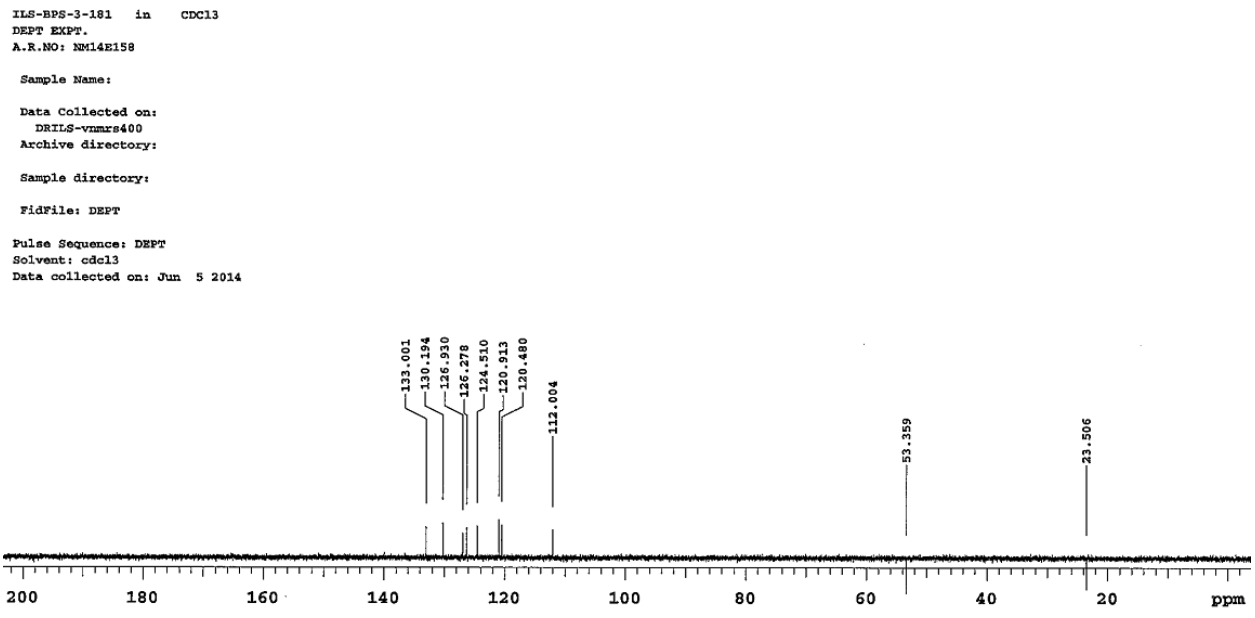
^{1}H NMR (Varian, 400 MHz) spectrum of compound **3** in $CDCl_3$



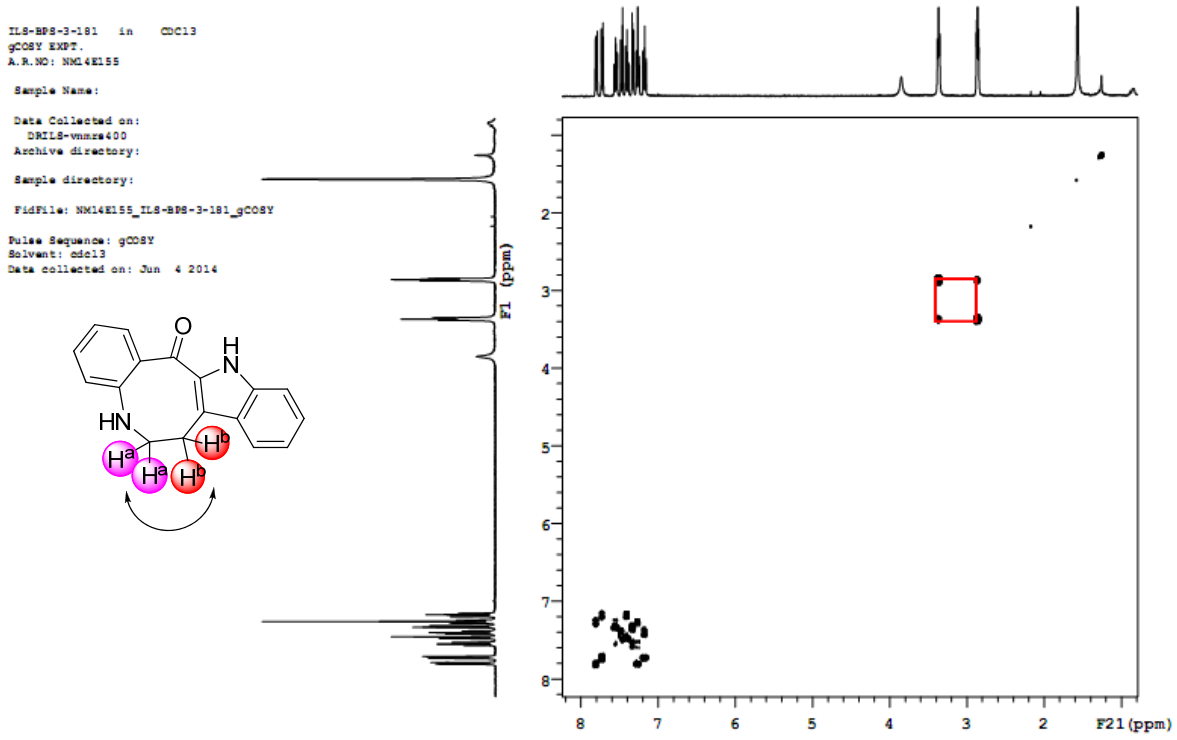
D_2O exchange spectrum of compound **3** in $CDCl_3$



^{13}C NMR spectrum (Varian, 100 MHz) of compound **3** in $CDCl_3$



DEPT of compound **3**

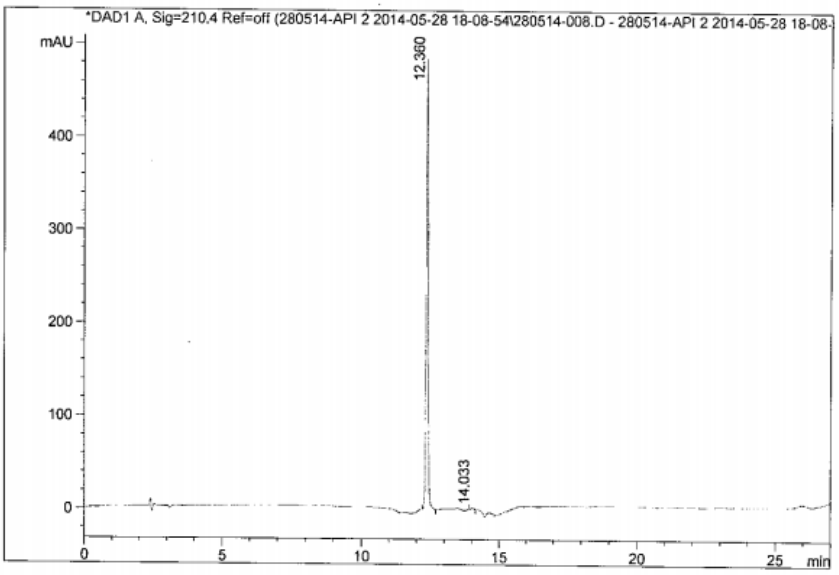


^{1}H-^{1}H COSY of compound **3**

HPLC of compound **3**

CPRI @ DRILS
HPLC ANALYSIS REPORT

Inj Date : Thu, 29. May. 2014 Acq Operator: SHASHIDHAR
Sample Name : ILS-BPS-3-181 Vial 26
A.R Number : CM14E013 ->Inj. Vol. : 5µL
Acq. Method : D:\chem32\1\DATA\280514-API 2 2014-05-28 18-08-54\AP->
Analysis Method : D:\CHEM32_002\1\METHODS\API DTV.M
Method Info : Column: X-Terra C-18 250*4.6mm, 5µm
Mobile phase: A) 5mm Ammonium Acetate in water B) ACN
T/%B:0/20,3/20,12/95,23/95,25/20,30/20
Flow:1.0ml/min Diluent: ACN:WATER(50:50)



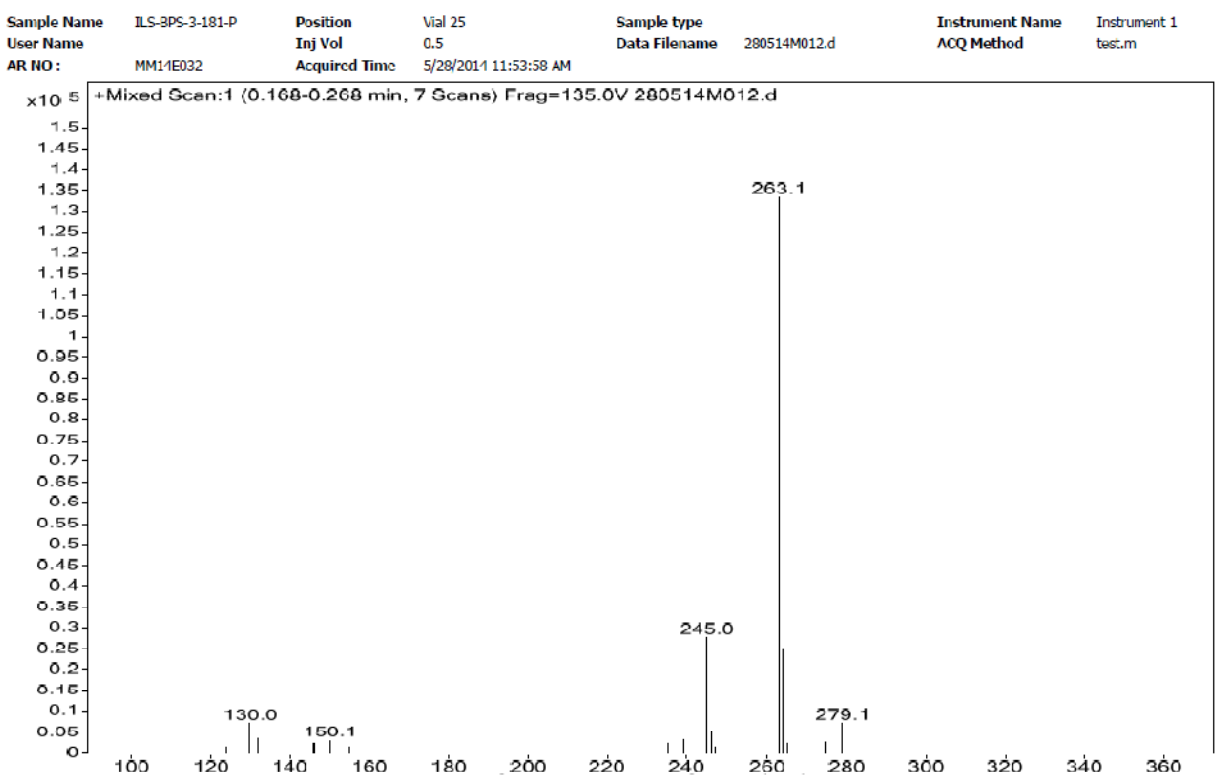
Signal 1: DAD1 A, Sig=210,4 Ref=off

Peak #	RT [min]	Area	Area %
1	12.360	2463.916	99.526
2	14.033	11.723	0.474

Analysed by : 29/5/14

Checked by : 29/5/14

ument 1 Thu, 29. May. 2014 09:49:36 am Page 1 of 1



Mass spectra of compound **3**

Chiral HPLC

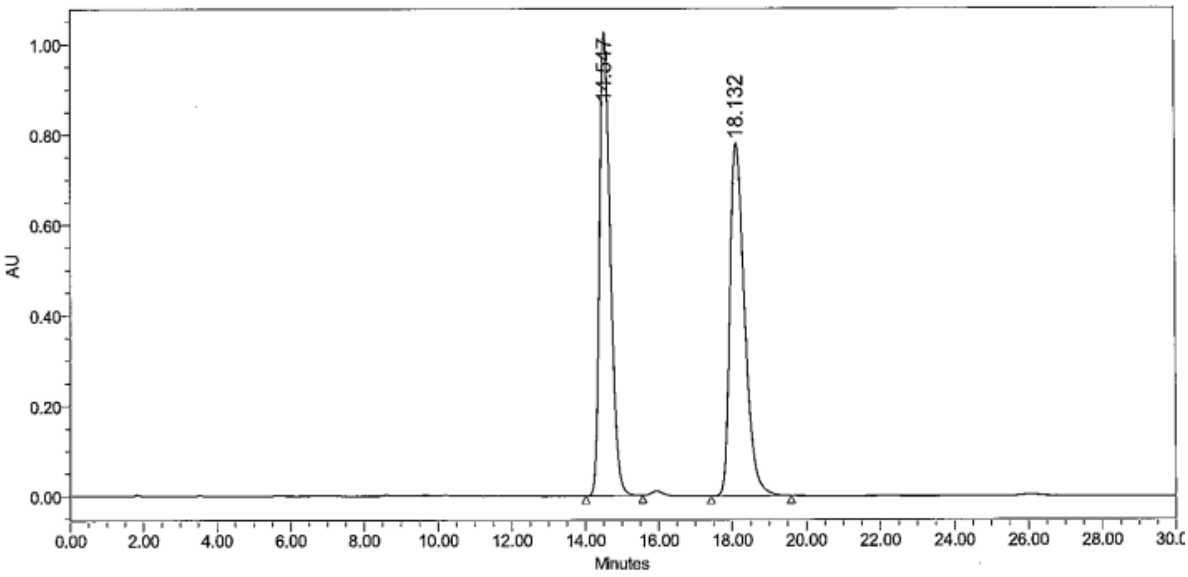
Empower 2 software

COSMIC@ILS

SAMPLE INFORMATION

Sample Name:	ILS-BPS-2-173	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	081112
Vial:	1	Acq. Method Set:	ILS
Injection #:	1	Processing Method:	chiral
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	30.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 235nm
Date Acquired:	11/8/2012 4:06:56 PM IST		
Date Processed:	11/8/2012 4:37:04 PM IST		

Column: Chiralpak IA-3 150*4.6mm 3µm
Mobile phase: n-Hexane:Ethanol (90:10)
Flow: 1.0mL/min
Diluent: Ethanol:n-Hexane(30:70)



	RT	Area	% Area	Height
1	14.547	21148926	49.55	1027100
2	18.132	21534405	50.45	781144

Analysed By:

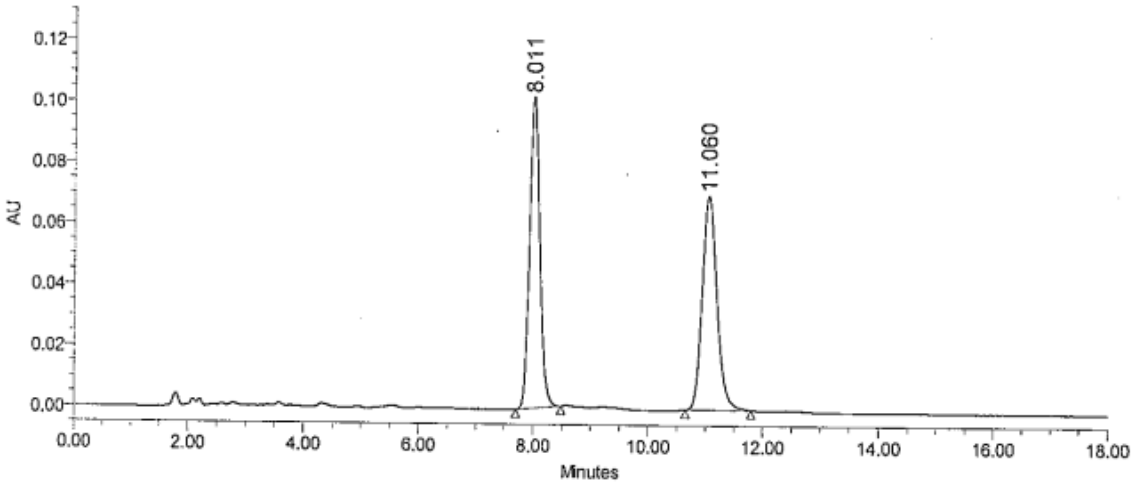
Empower 2 software

CPRI @ DRILS

SAMPLE INFORMATION

Sample Name:	ILS-BPS-3-62		
A.R.Number:	CM14G009	Analyst:	Varma
Vial:	9	Sample Set Name:	040714
Injection #:	1	Acq. Method Set:	CHIRAL
Injection Volume:	10.00 ul	Processing Method:	chiral1
Run Time:	35.0 Minutes	Proc. Chnl. Descr.:	W2489 ChB 220nm
Date Acquired:	7/4/2014 6:33:34 PM IST		
Date Processed:	7/7/2014 10:49:46 AM IST		

Column: Chiralpak IA-3, 150x4.6mm,3µm
Mobile phase: n-Hexane:Ethanol (80:20)
Flow: 1.0mL/min; Diluent:Mobile Phase.



	RT	Area	% Area	Height
1	8.011	1257339	50.00	102222
2	11.060	1257477	50.00	70135

Analysed By:

7/7/14