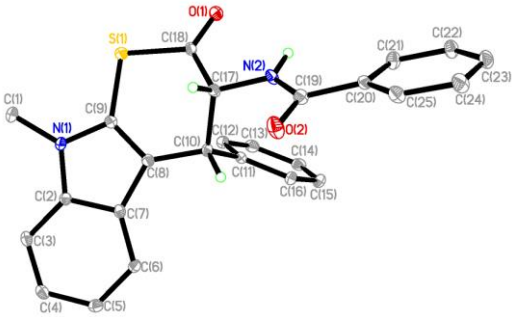
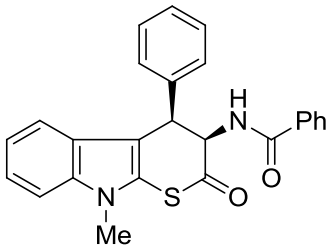
Table of Contents

1. Crystallography data of Compound 3aa

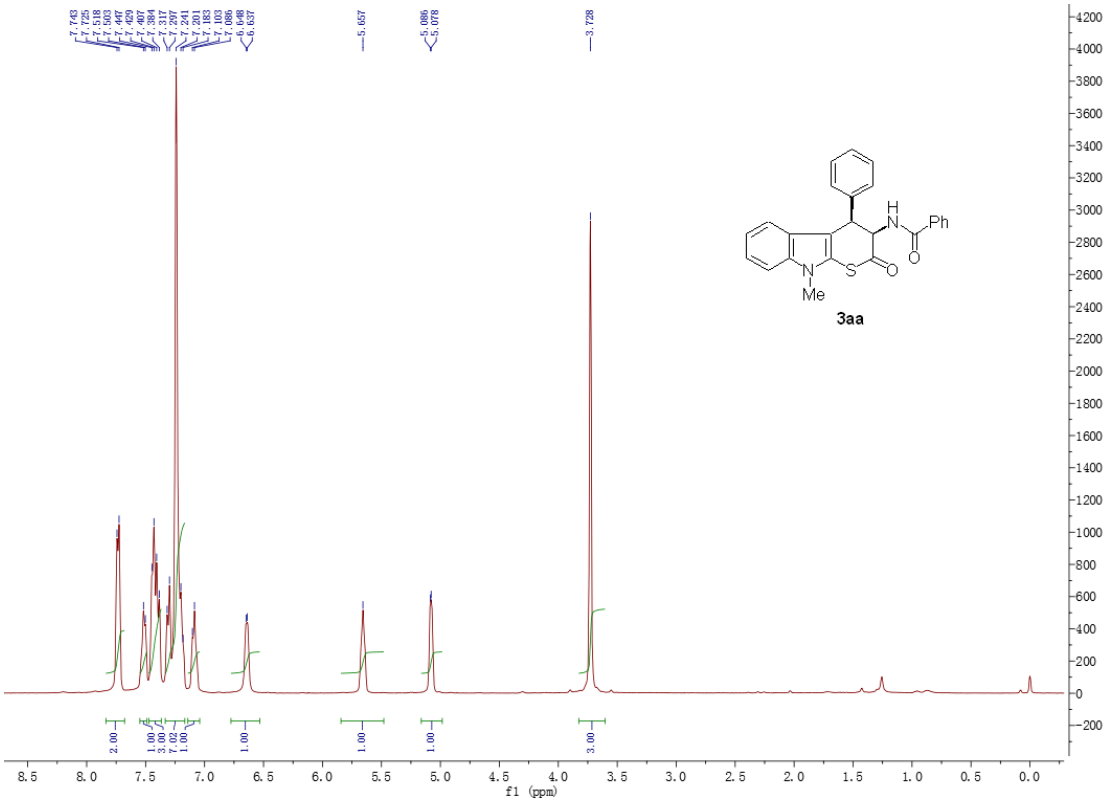


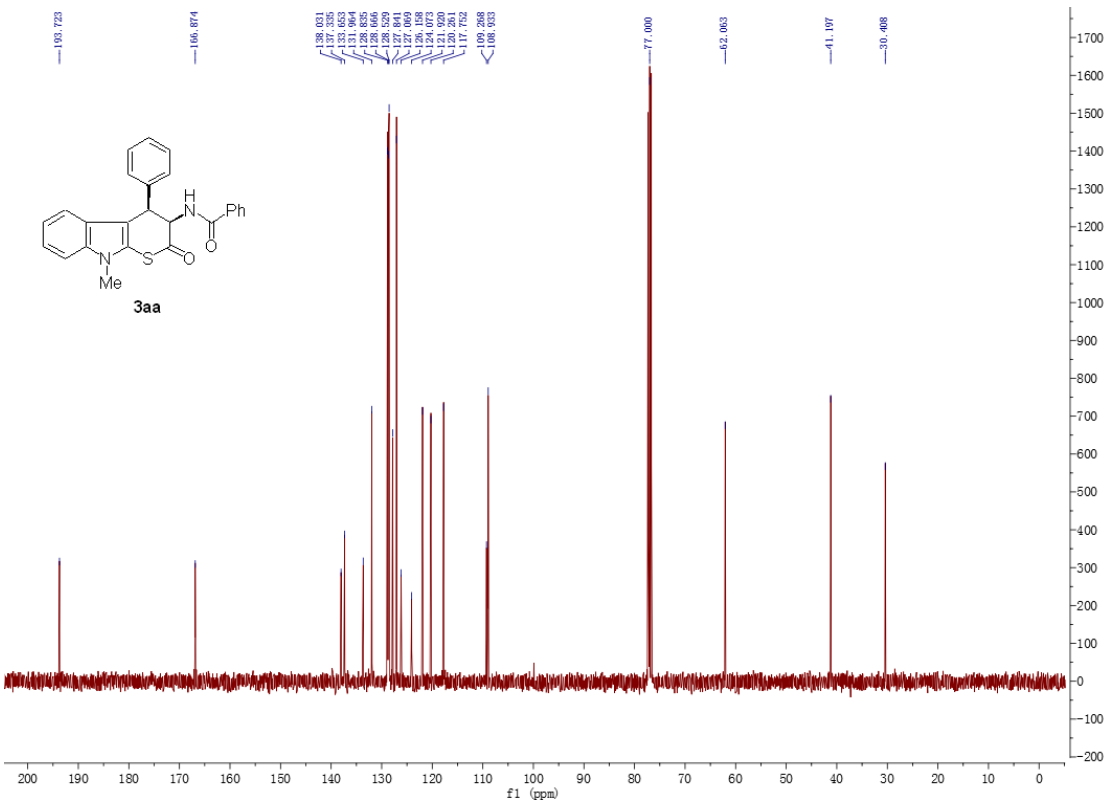


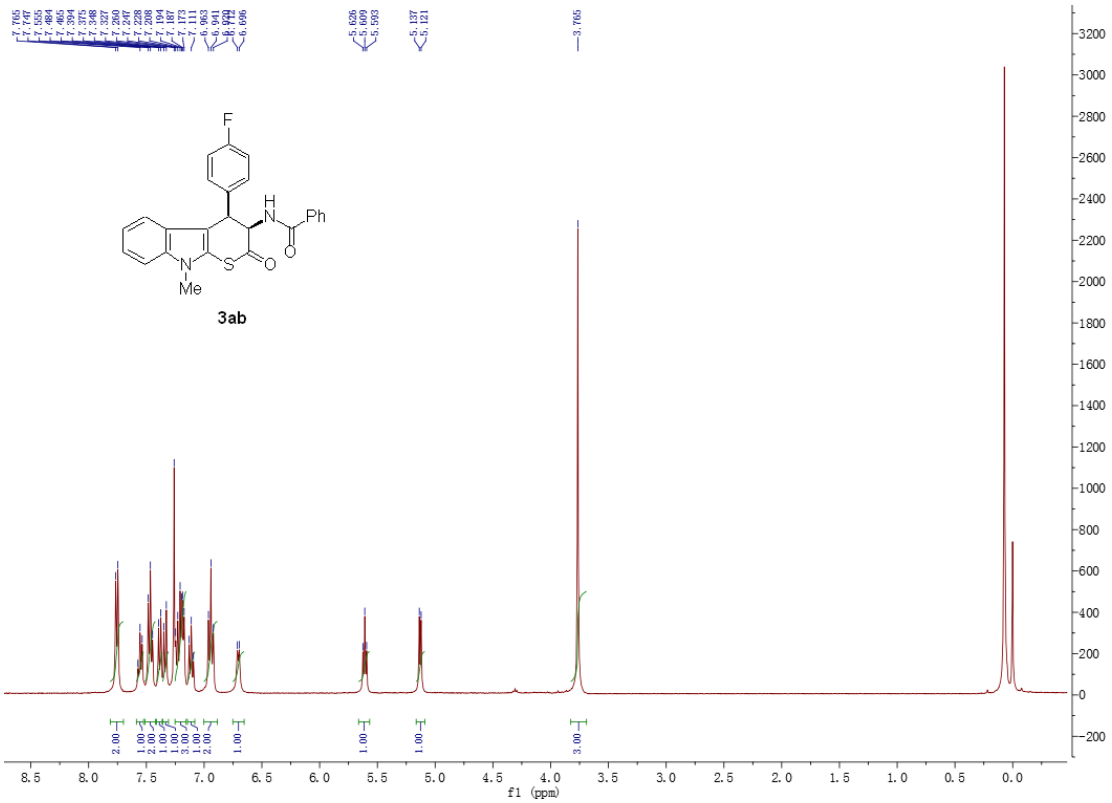
3aa

Identification code	Shelxl
Empirical formula	C25 H20 N2 O2 S
Formula weight	412.49
Temperature	113(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, Cc
Unit cell dimensions	a = 19.897(4) A alpha = 90 deg. b = 12.667(3) A beta = 108.18(3) deg. c = 8.4207(17) A gamma = 90 deg.
Volume	2016.3(7) A^3
Z, Calculated density	4, 1.359 Mg/m^3
Absorption coefficient	0.186 mm^-1
F(000)	864
Crystal size	0.20 x 0.18 x 0.12 mm
Theta range for data collection	1.94 to 27.89 deg.
Limiting indices	-26<=h<=25, -16<=k<=16, -10<=l<=11
Reflections collected / unique	9734 / 4166 [R(int) = 0.0392]
Completeness to theta = 27.89	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9781 and 0.9638
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4166 / 3 / 277
Goodness-of-fit on F^2	0.971
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0692
R indice s (all data)	R1 = 0.0405, wR2 = 0.0722
Absolute structure parameter	-0.03(5)
Extinction coefficient	0.0133(7)
Largest diff. peak and hole	0.246 and -0.186 e.A^-3

2. Copies of ^{1}H and ^{13}C NMR Spectra



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S
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Me
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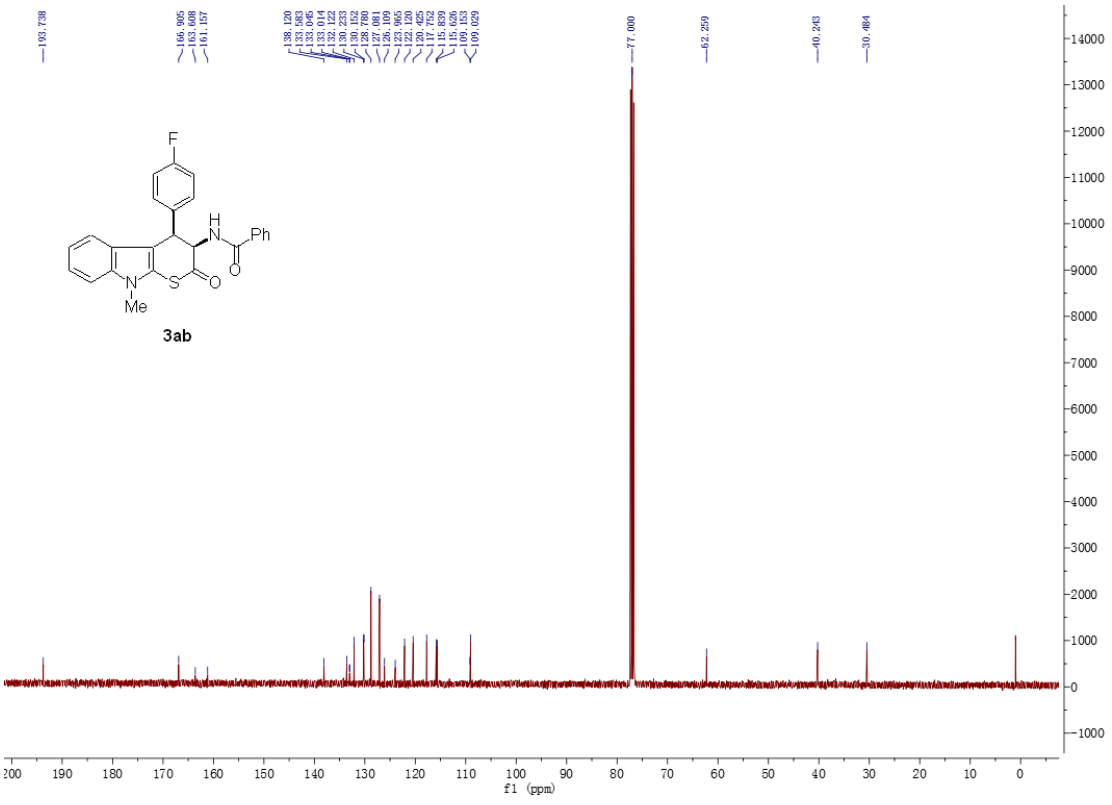
f1 (ppm)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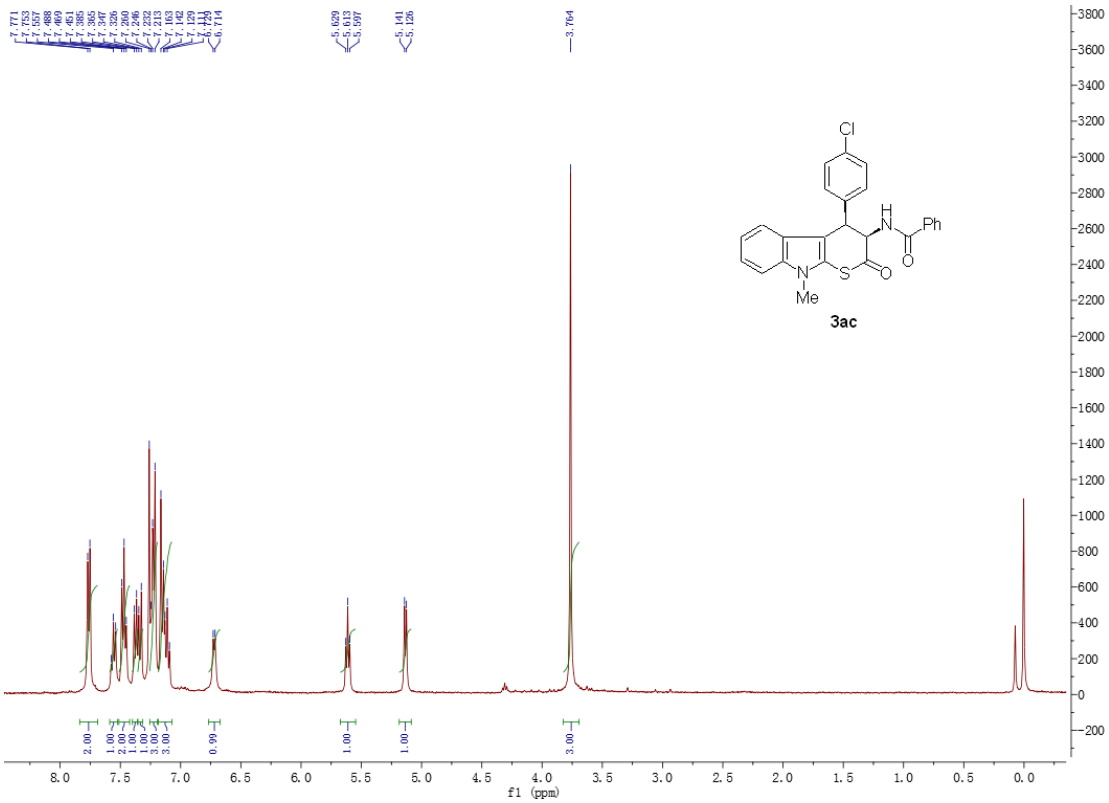
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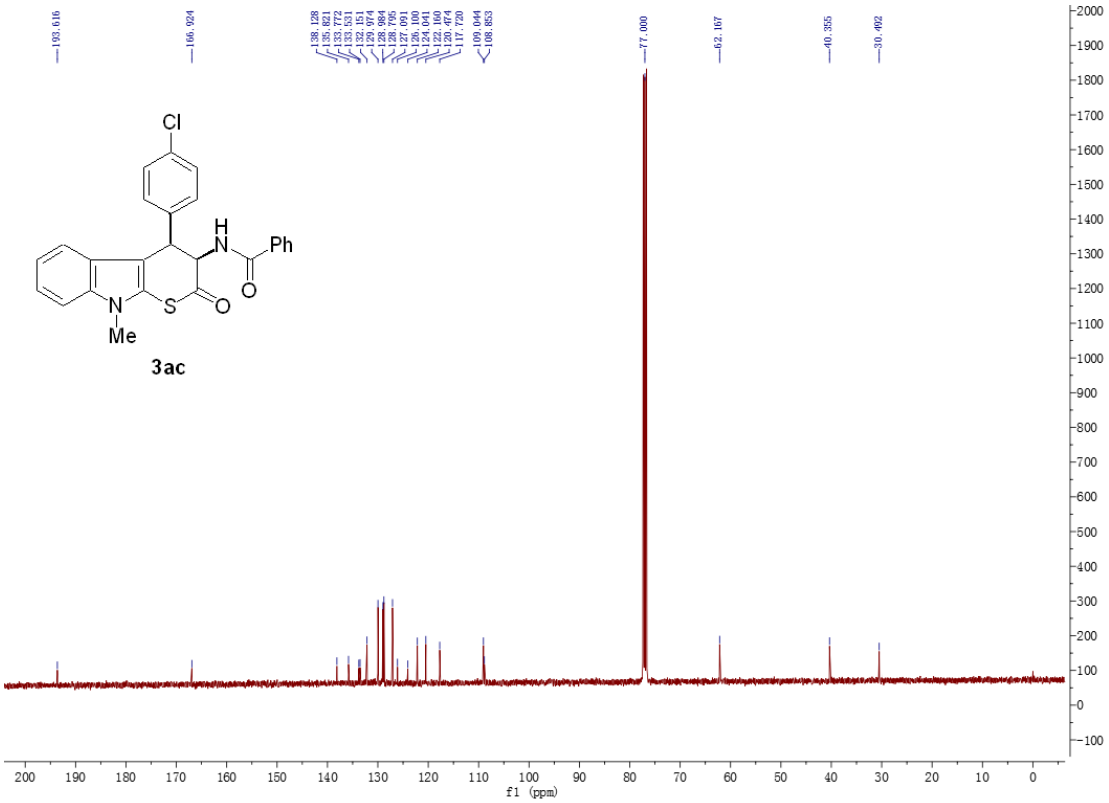
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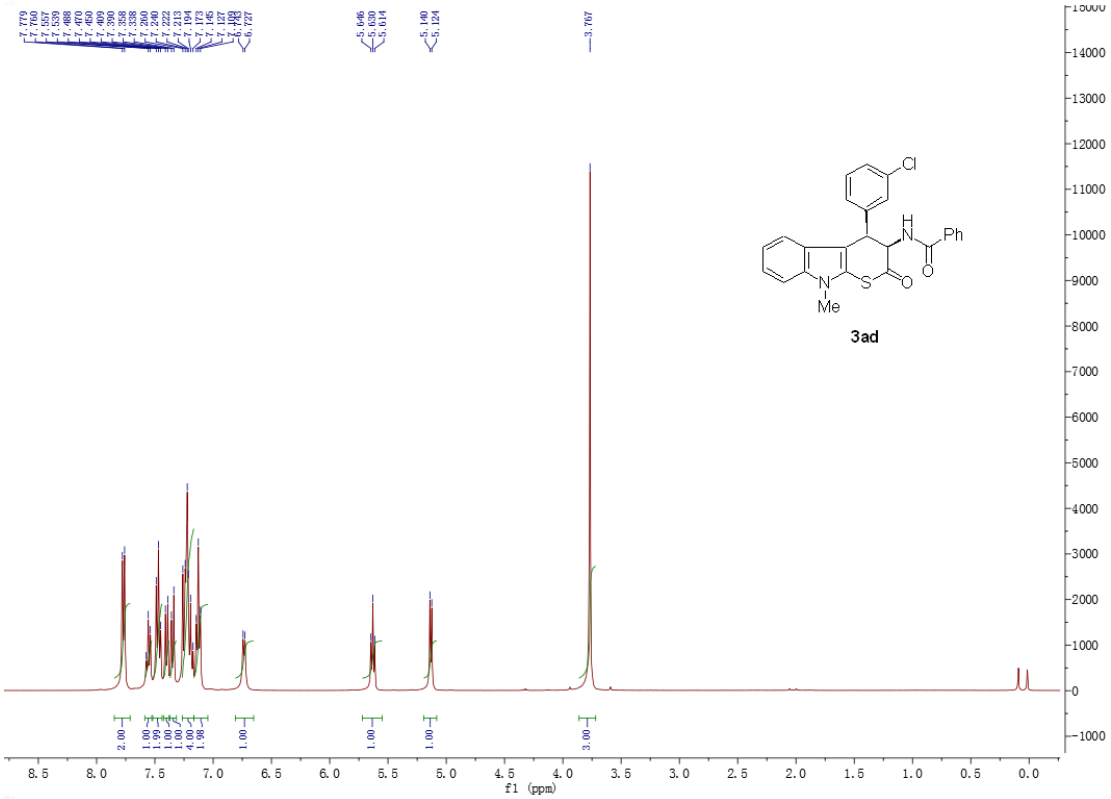
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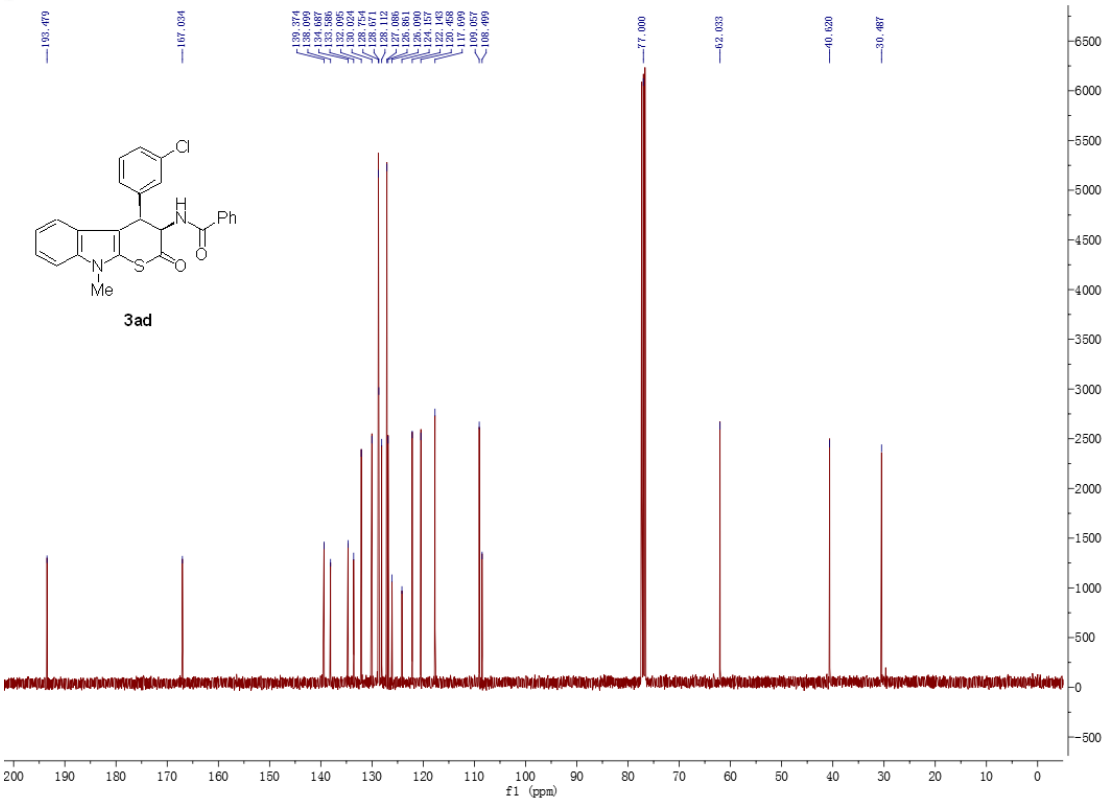
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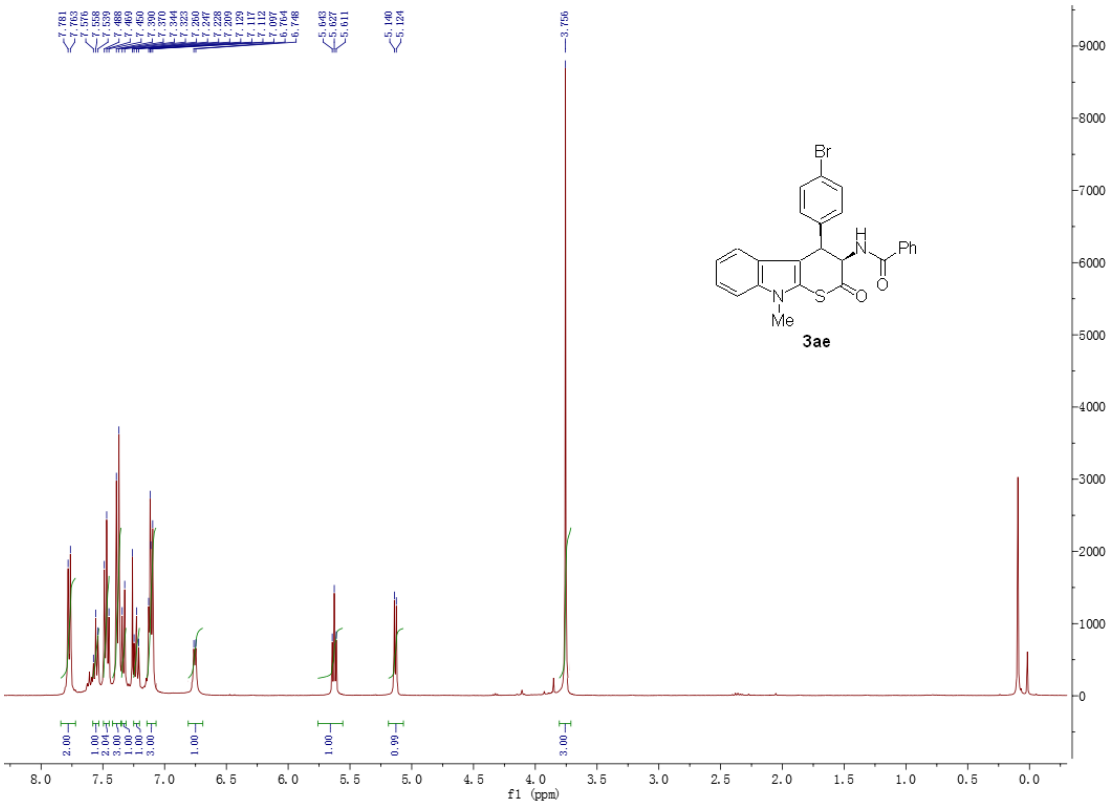
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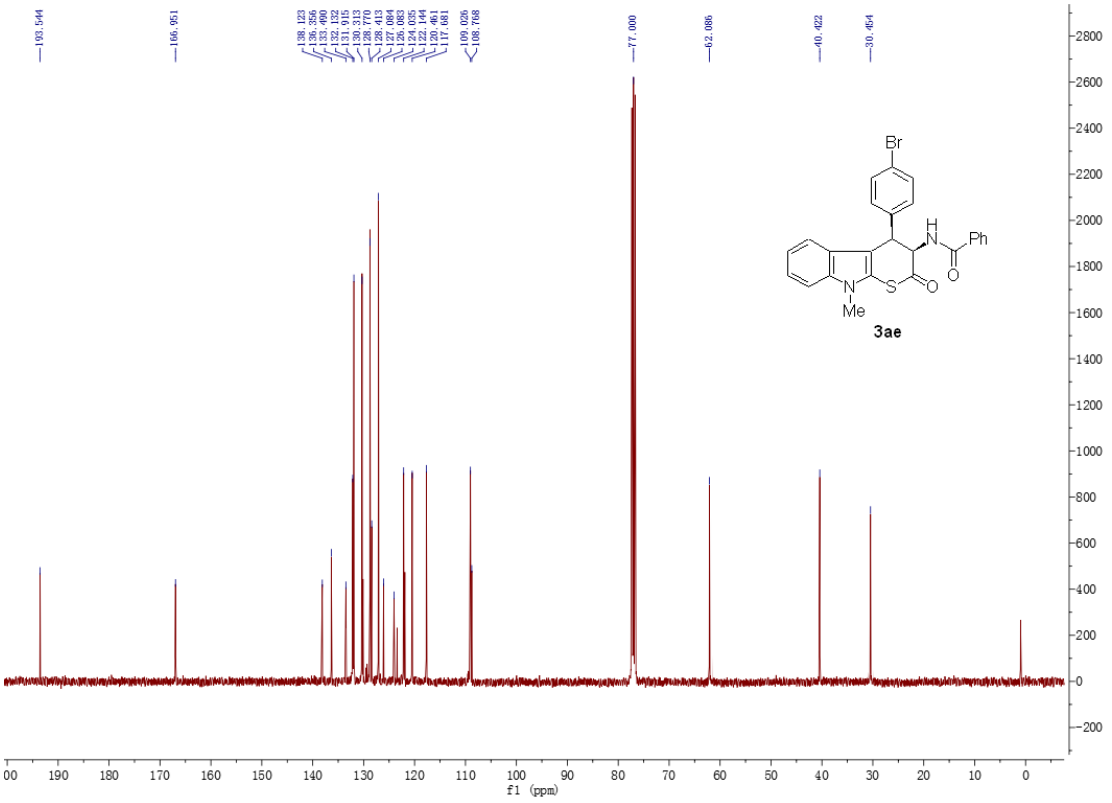
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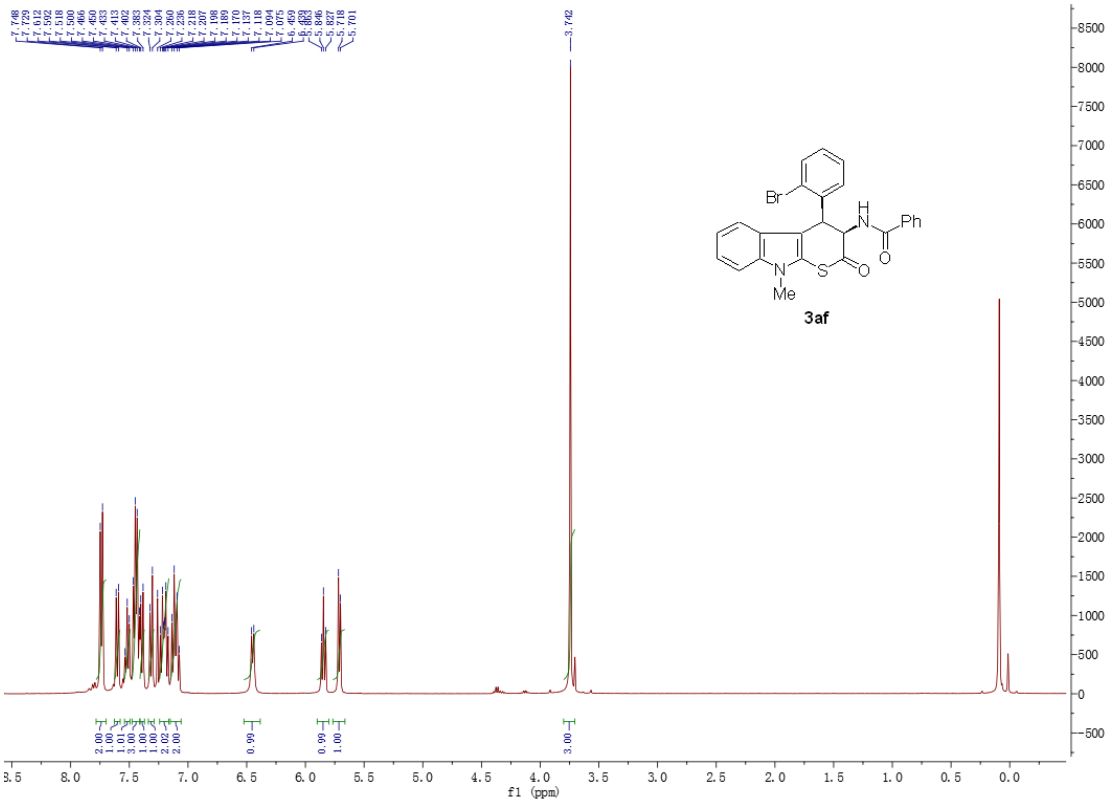
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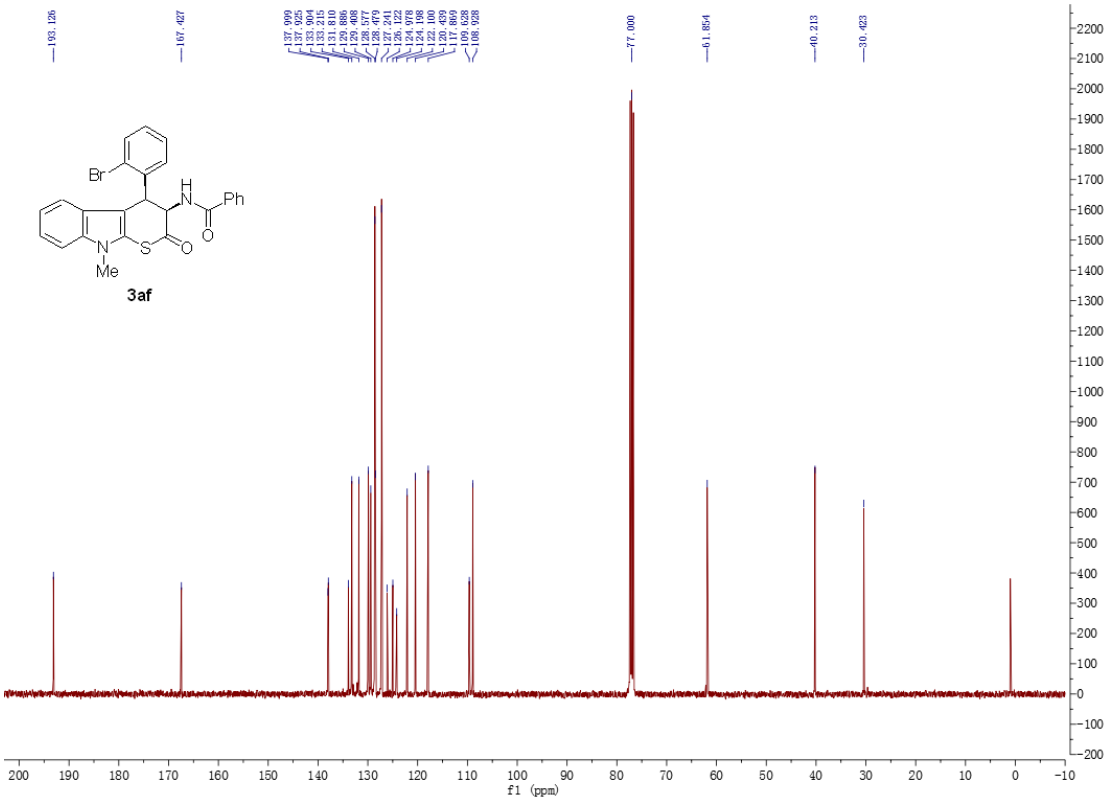
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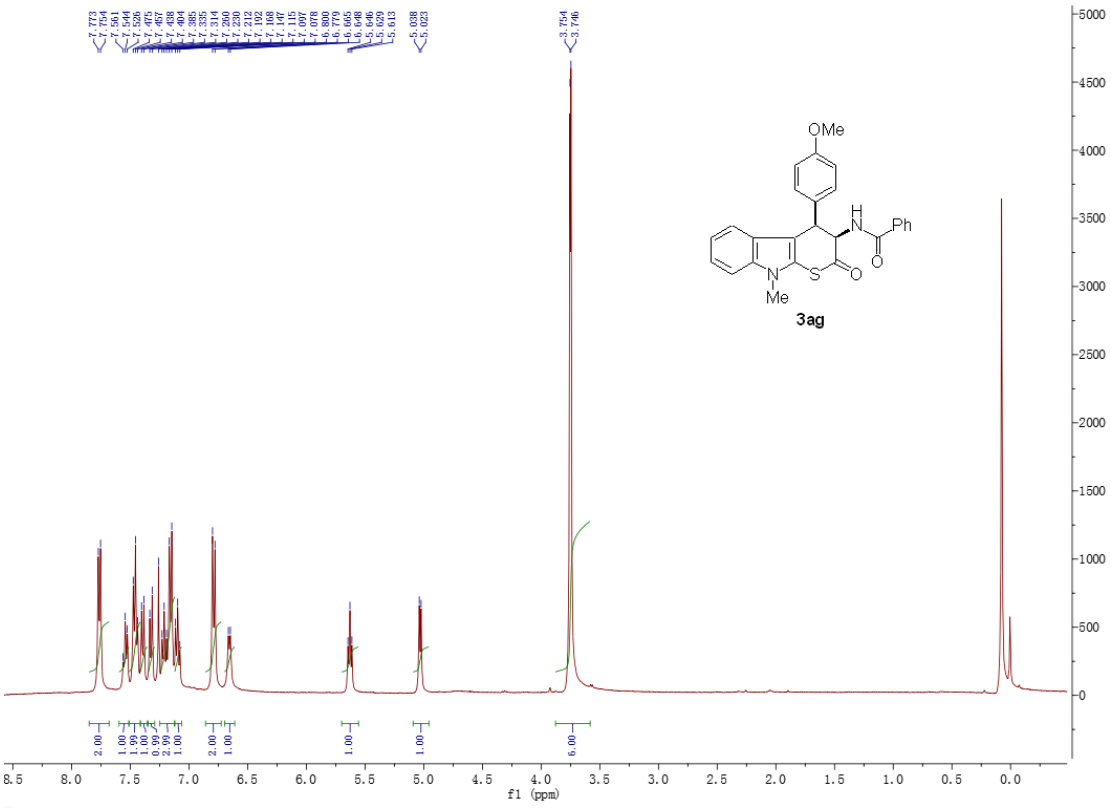
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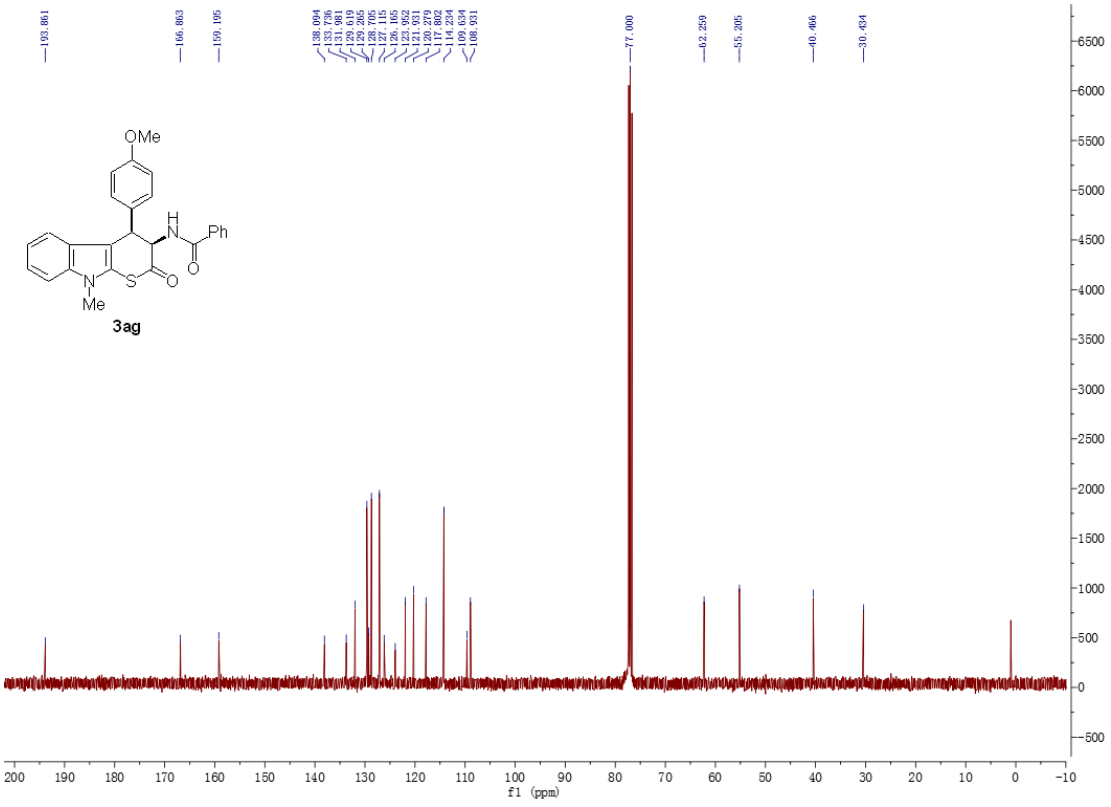
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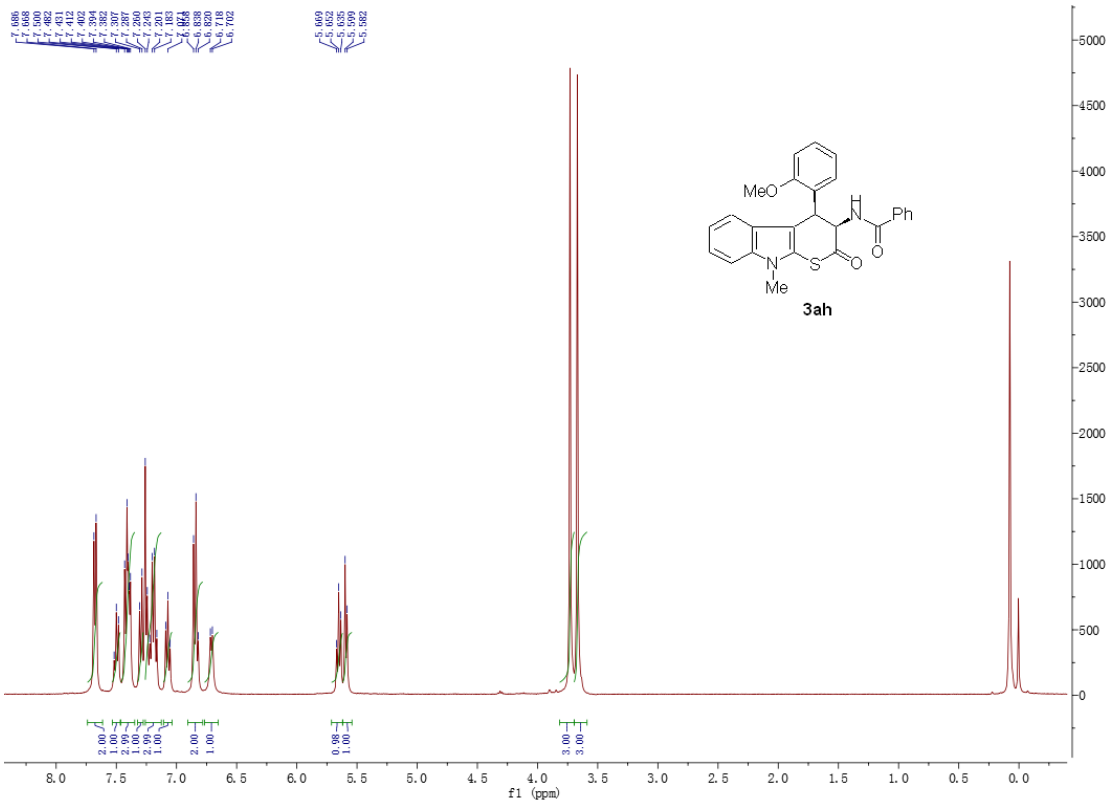
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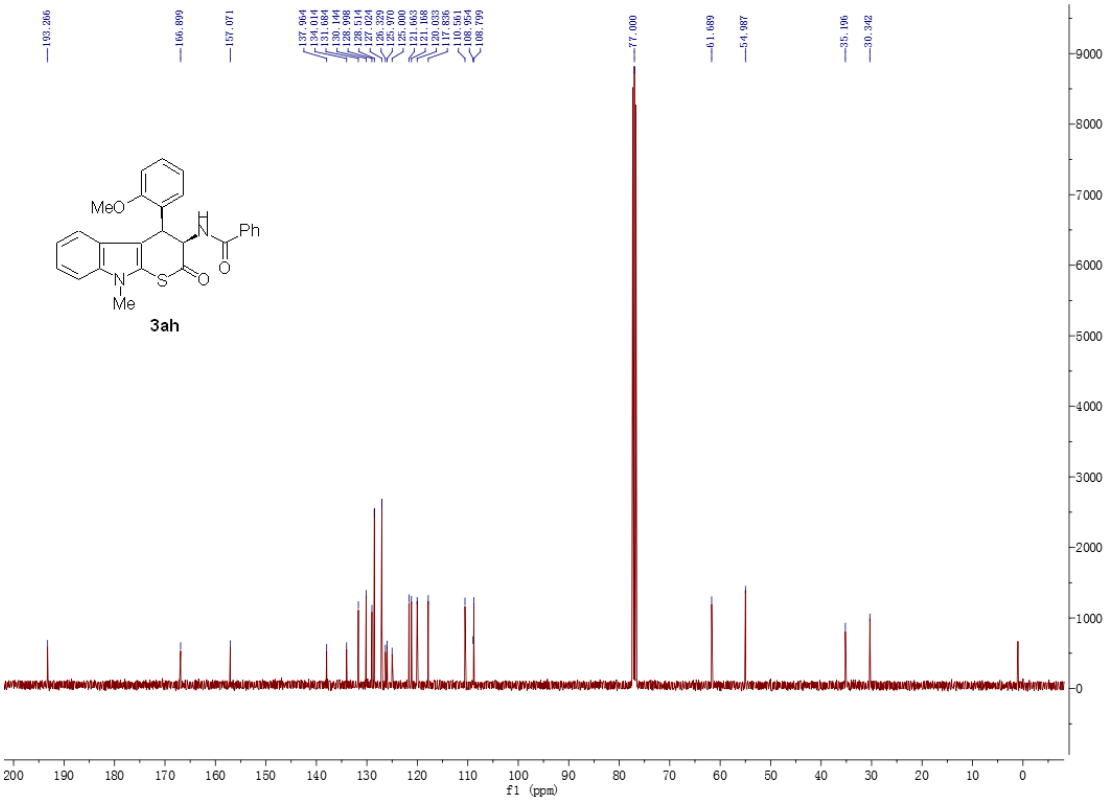
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S
O
Me
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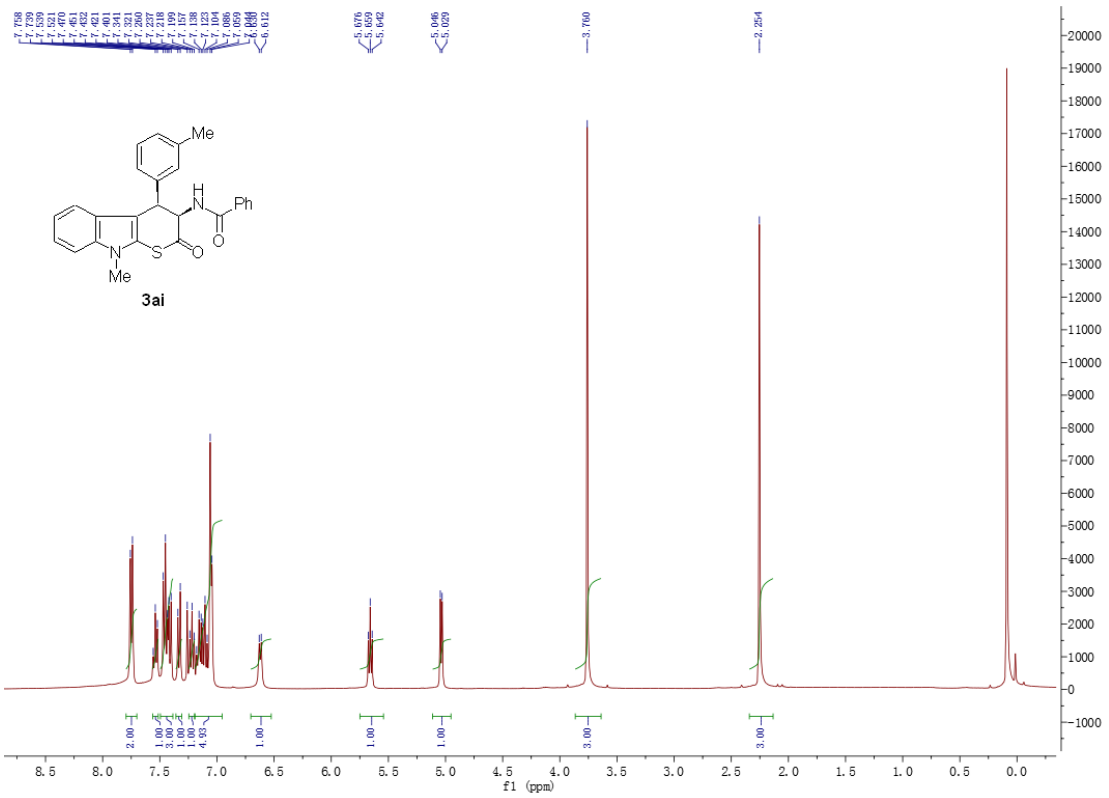
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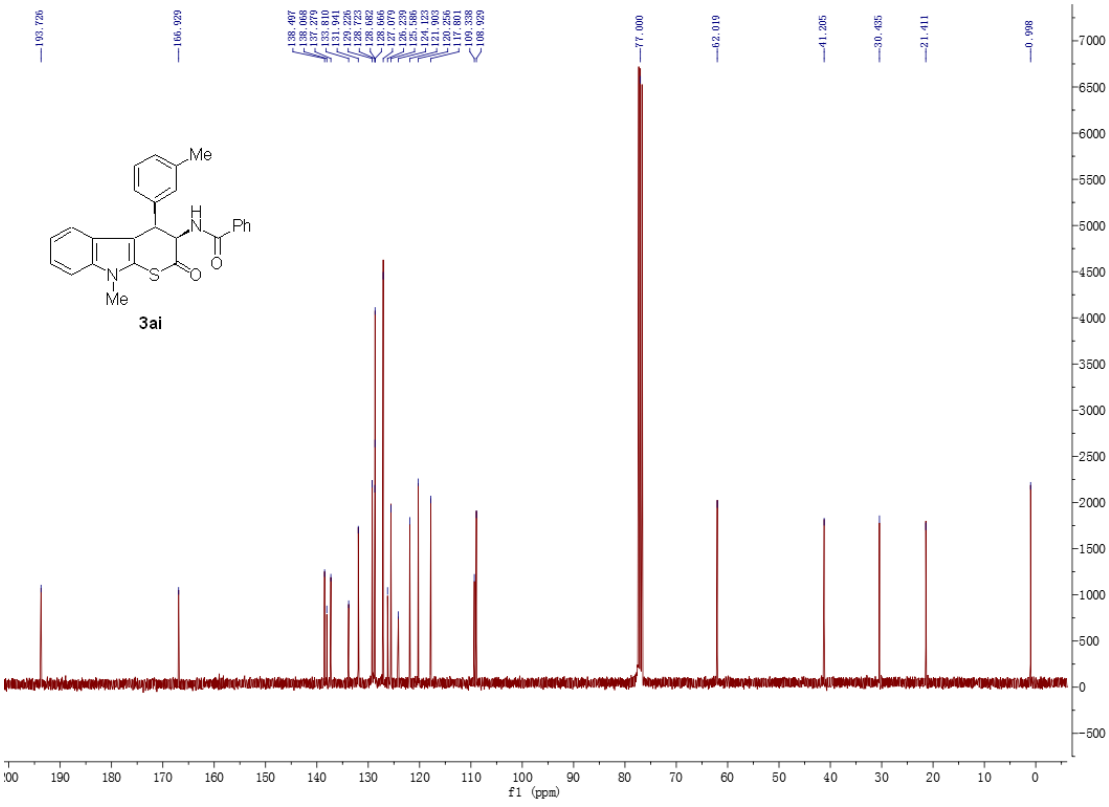
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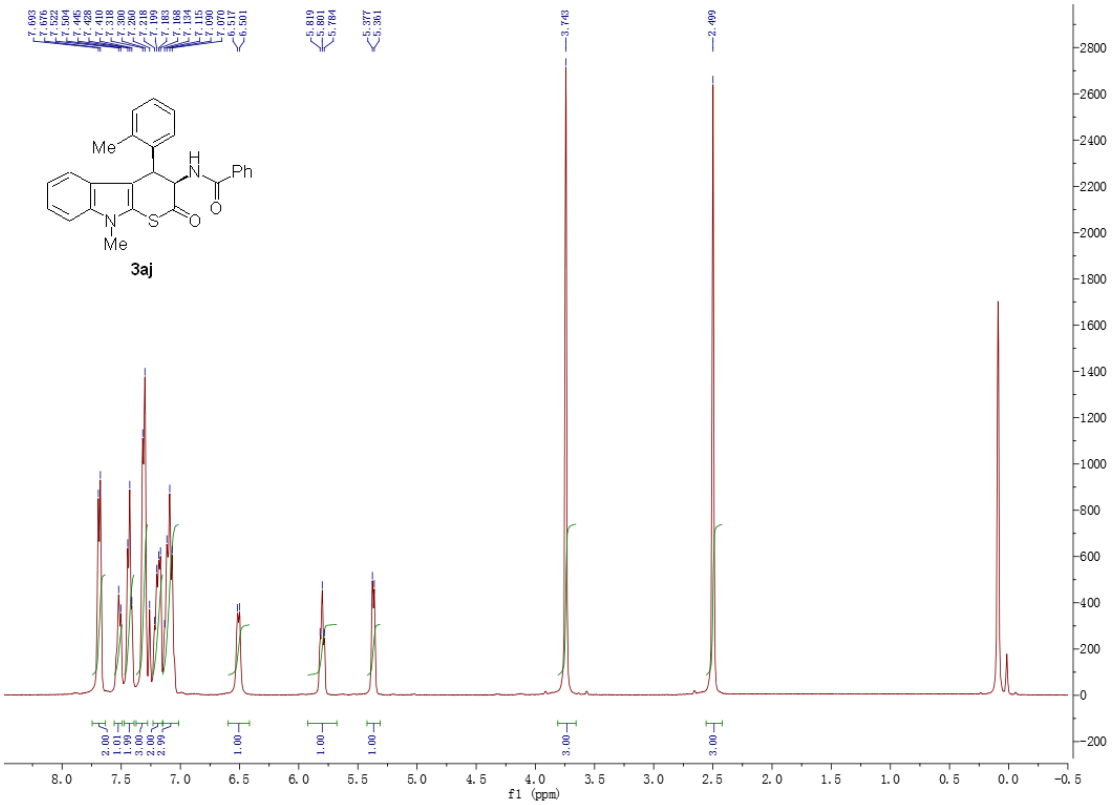
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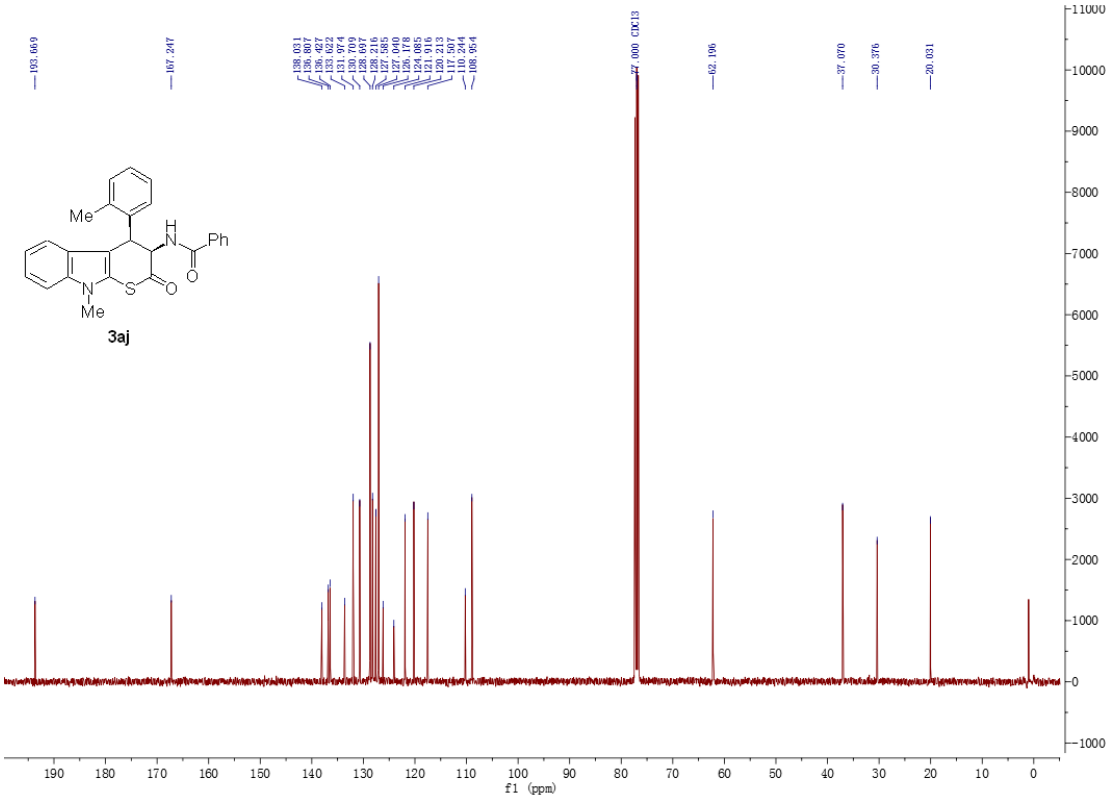
3.00
f1 (ppm)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Ph
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S
O
N
Me
3aj
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131.974
130.709
128.697
128.216
127.585
127.040
126.178
124.085
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110.244
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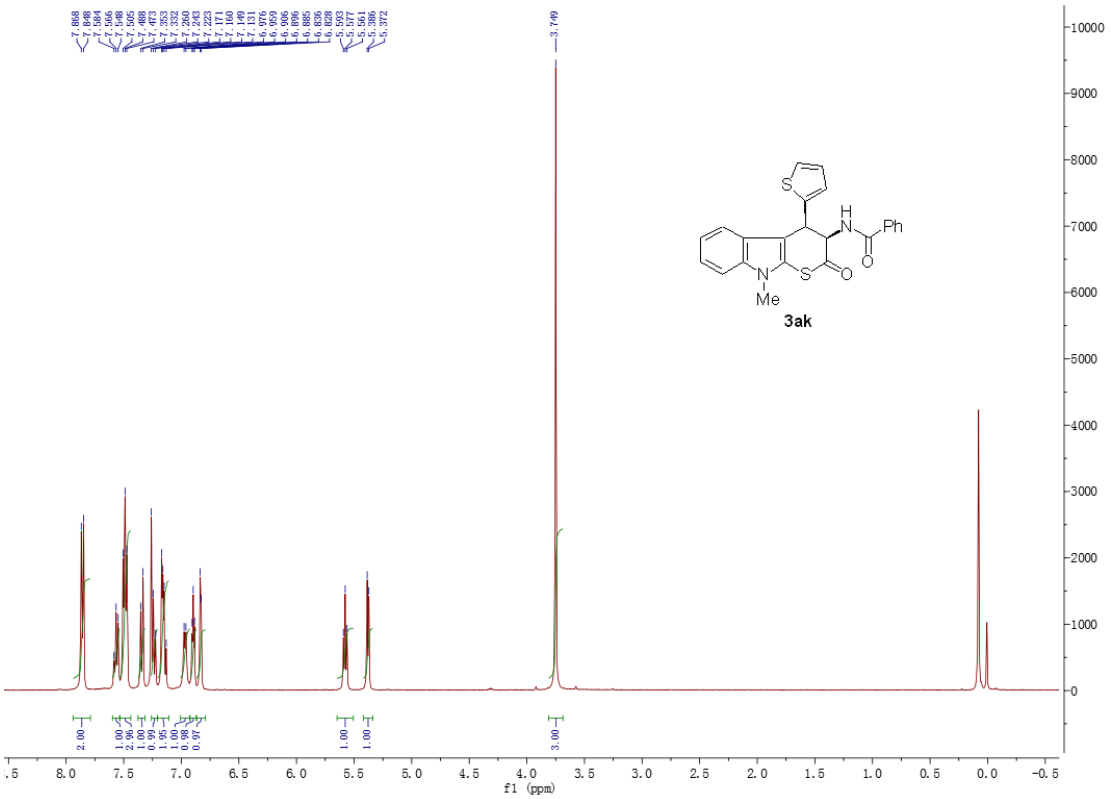
37.070
30.376
20.031
f1 (ppm)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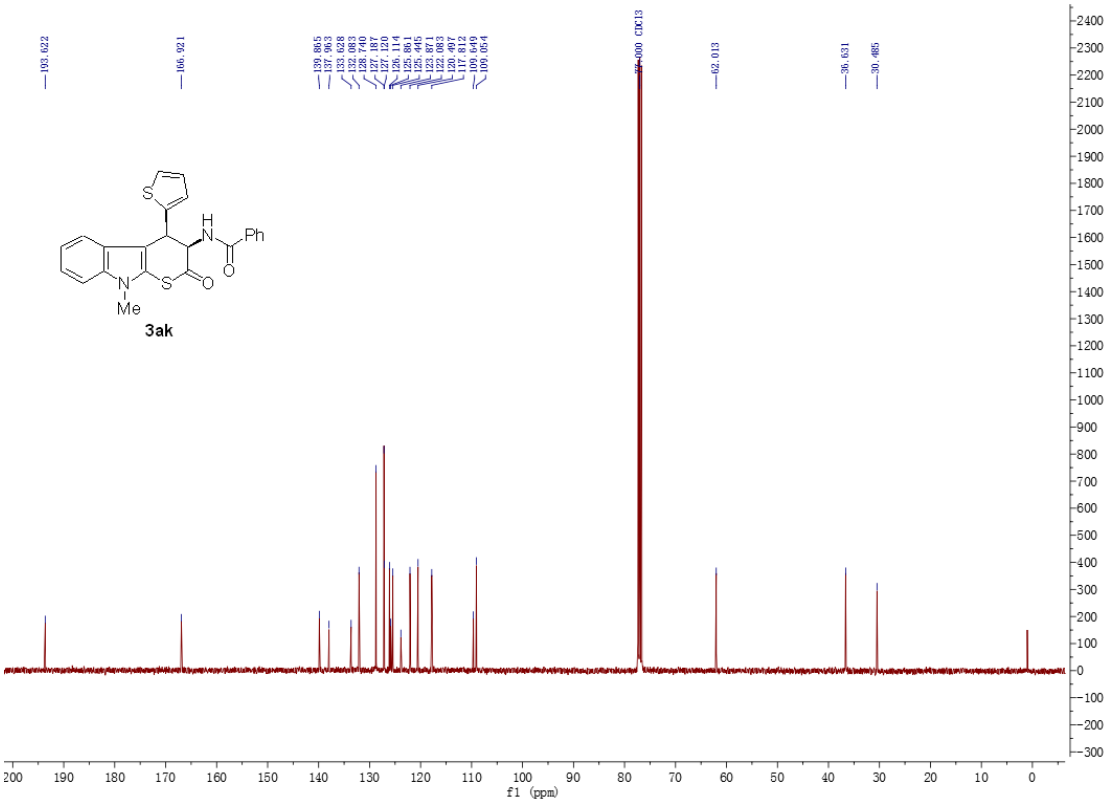
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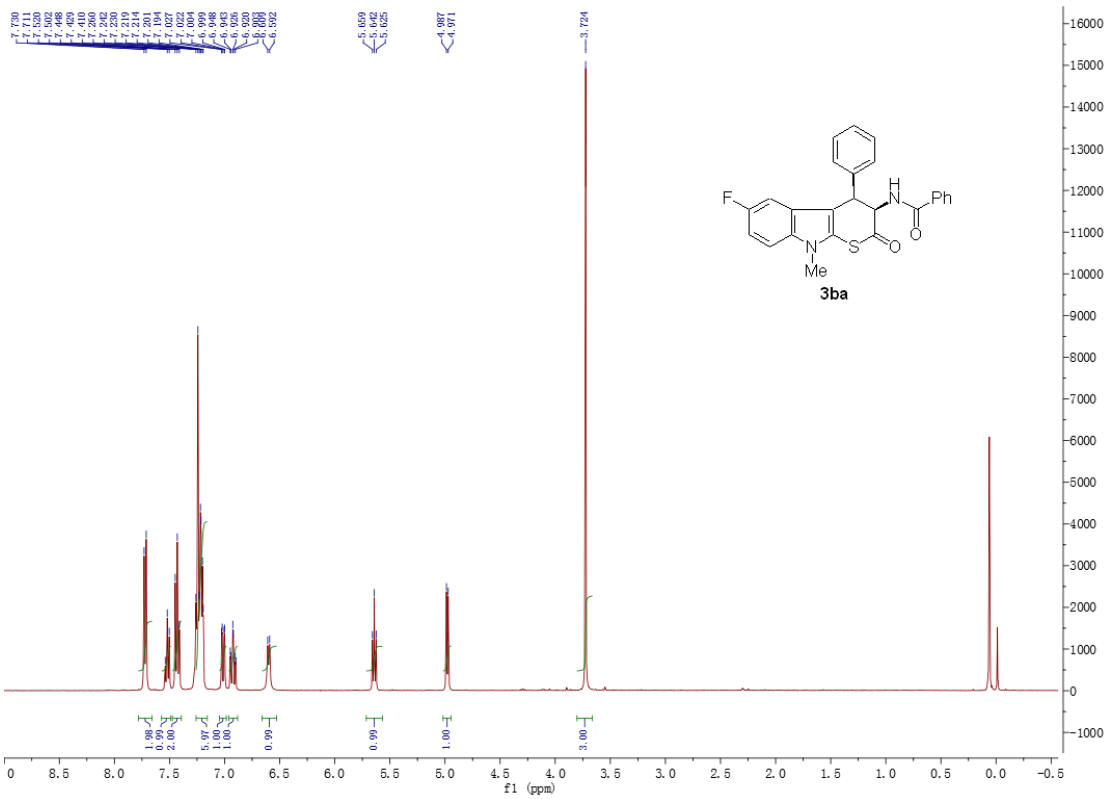
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7.077
7.022
7.004
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6.948
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6.926
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5.659
5.642
5.625
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F
N
H
Ph
O
S
O
N
Me
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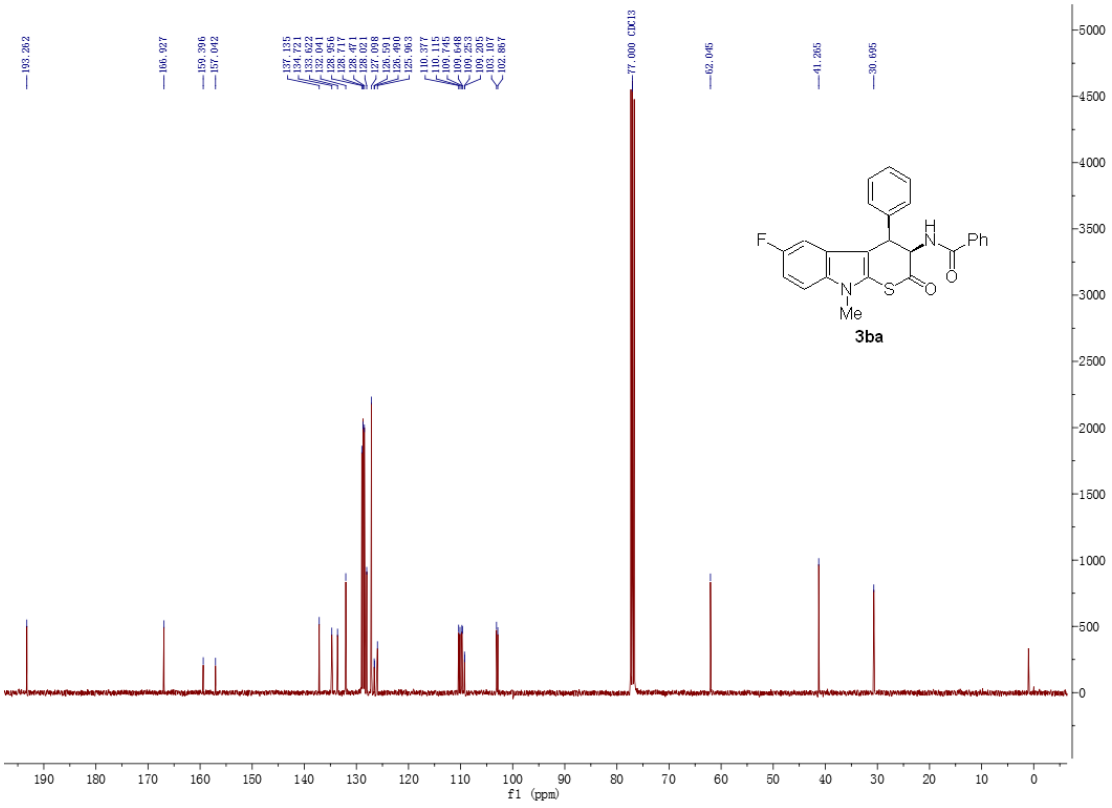
3.00
f1 (ppm)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109.205
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102.867
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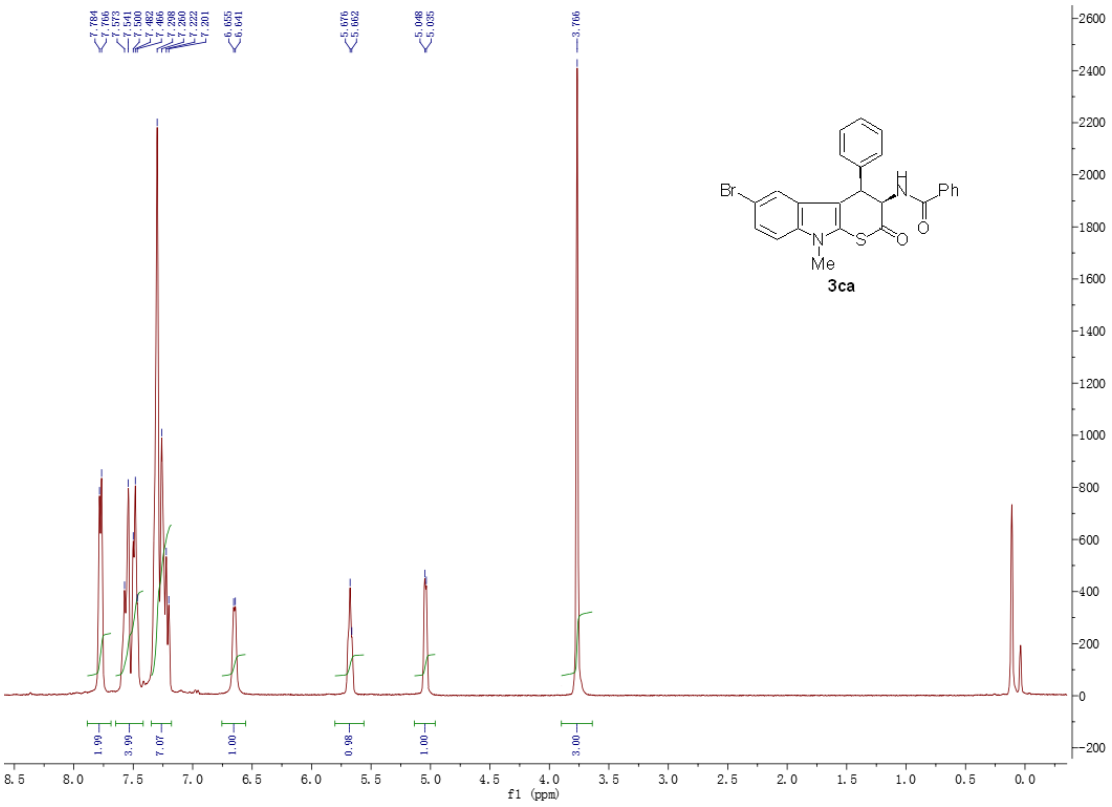
Me
3ba
f1 (ppm)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6.641
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5.662
5.048
5.035
3.766
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3.99
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1.00
3.00
f1 (ppm)
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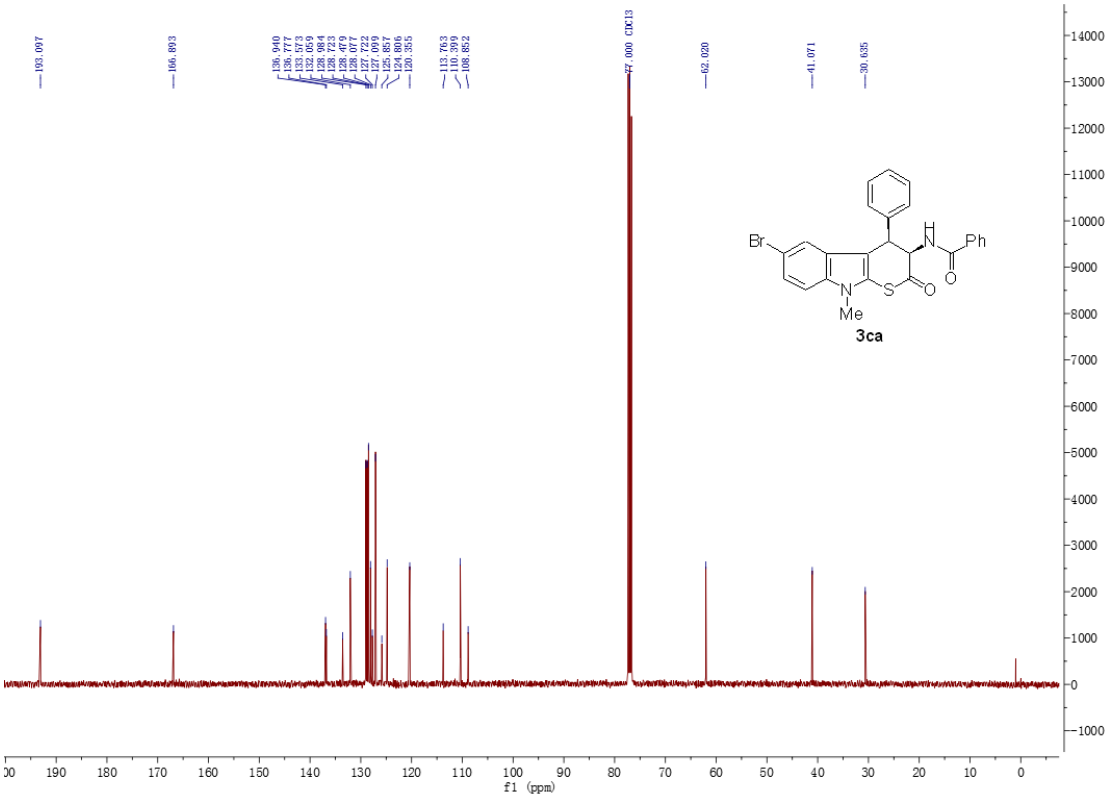
Ph
N
H
O
S
O
N
Me
3ca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110.399
108.852
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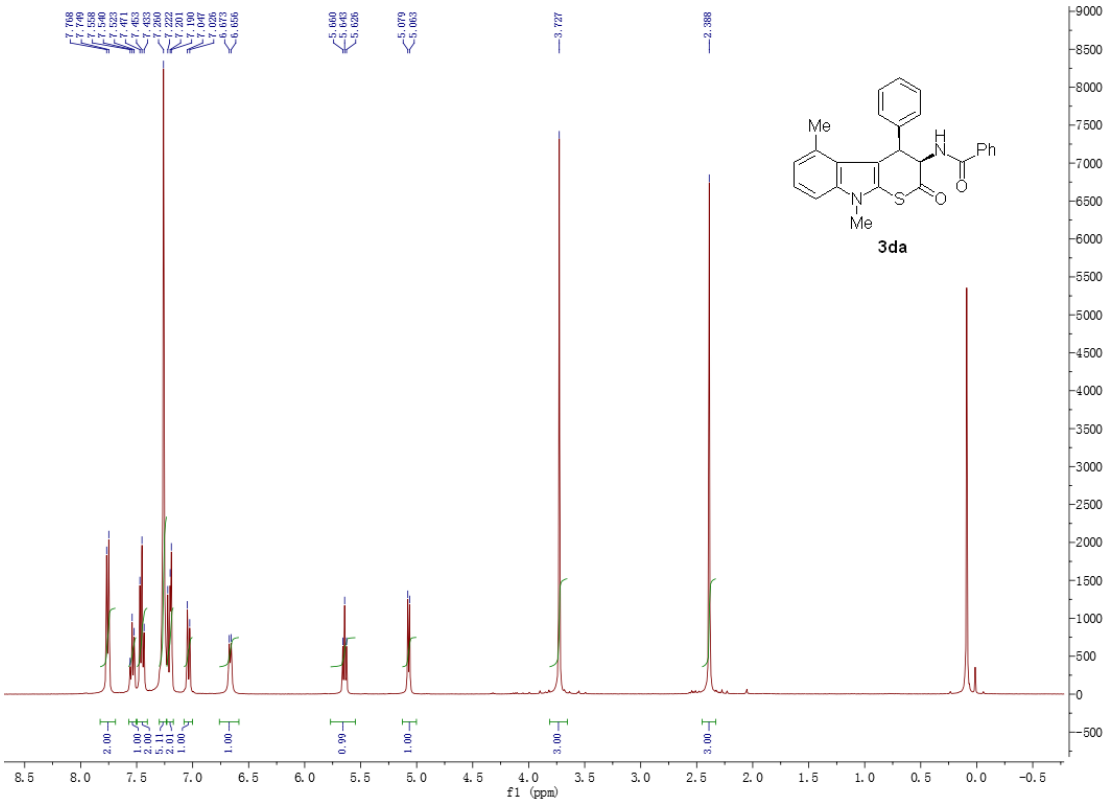
H
O
S
O
N
Me
3ca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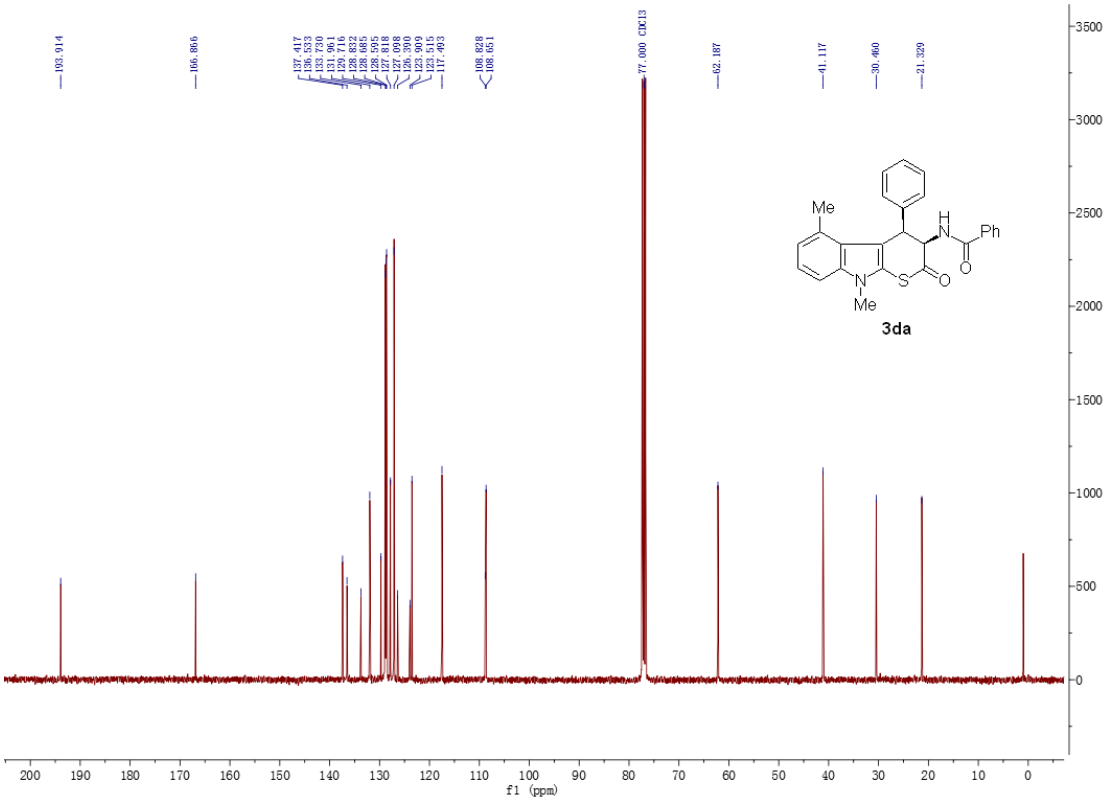
3.00
f1 (ppm)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S
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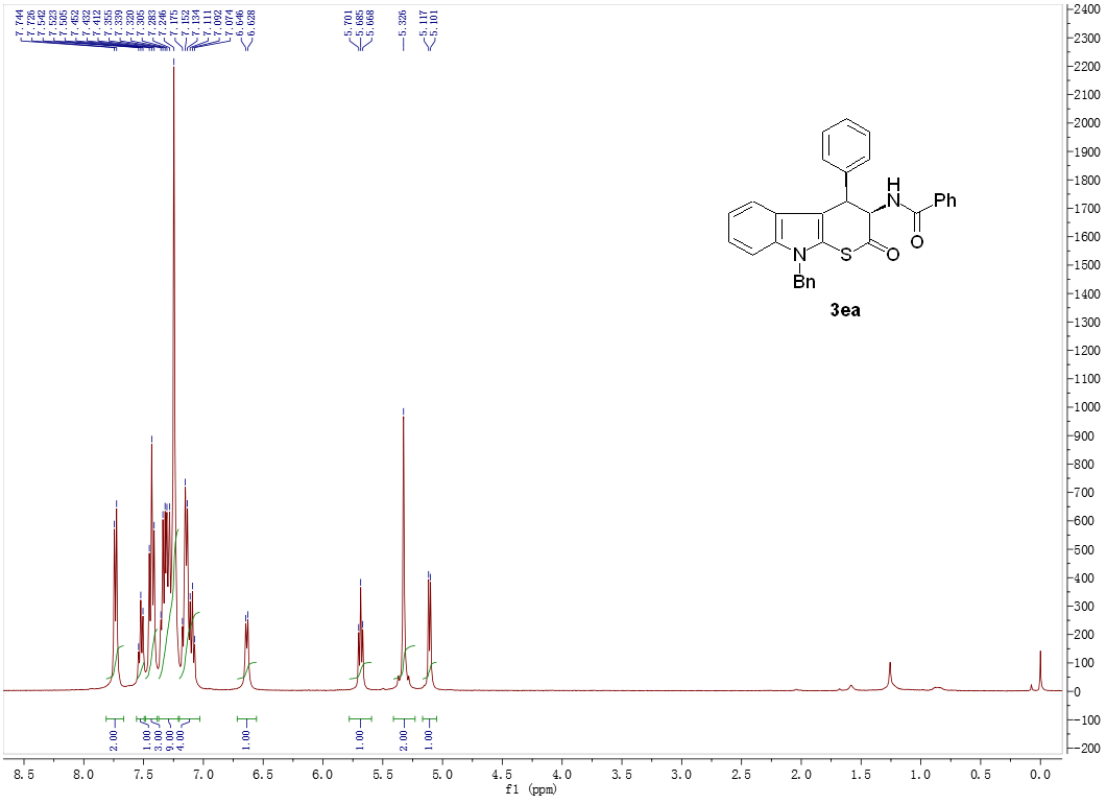
Me
3da
f1 (ppm)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7.283
7.246
7.175
7.152
7.134
7.111
7.092
7.074
6.646
6.628
5.701
5.685
5.668
5.326
5.117
5.101
2.00
1.00
3.00
9.00
4.00
1.00
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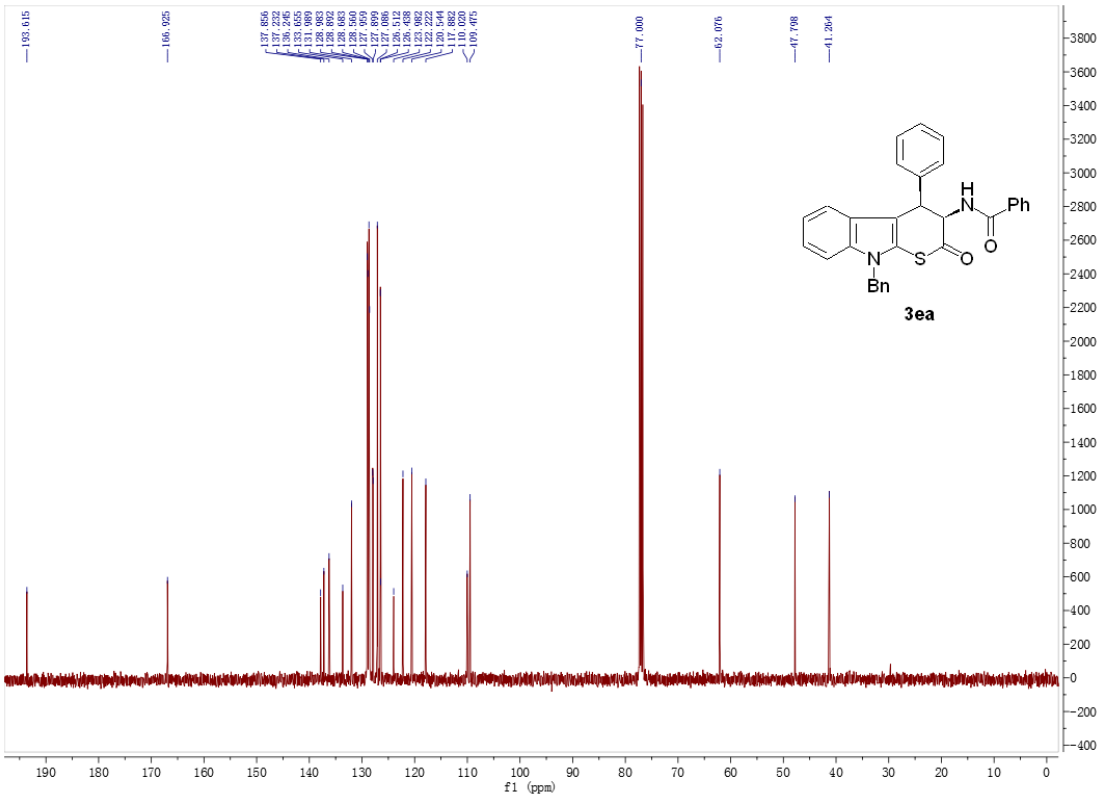
2.00
1.00
f1 (ppm)
H
N
Ph
O
N
S
O
Bn
3ea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110.020
109.476
77.000
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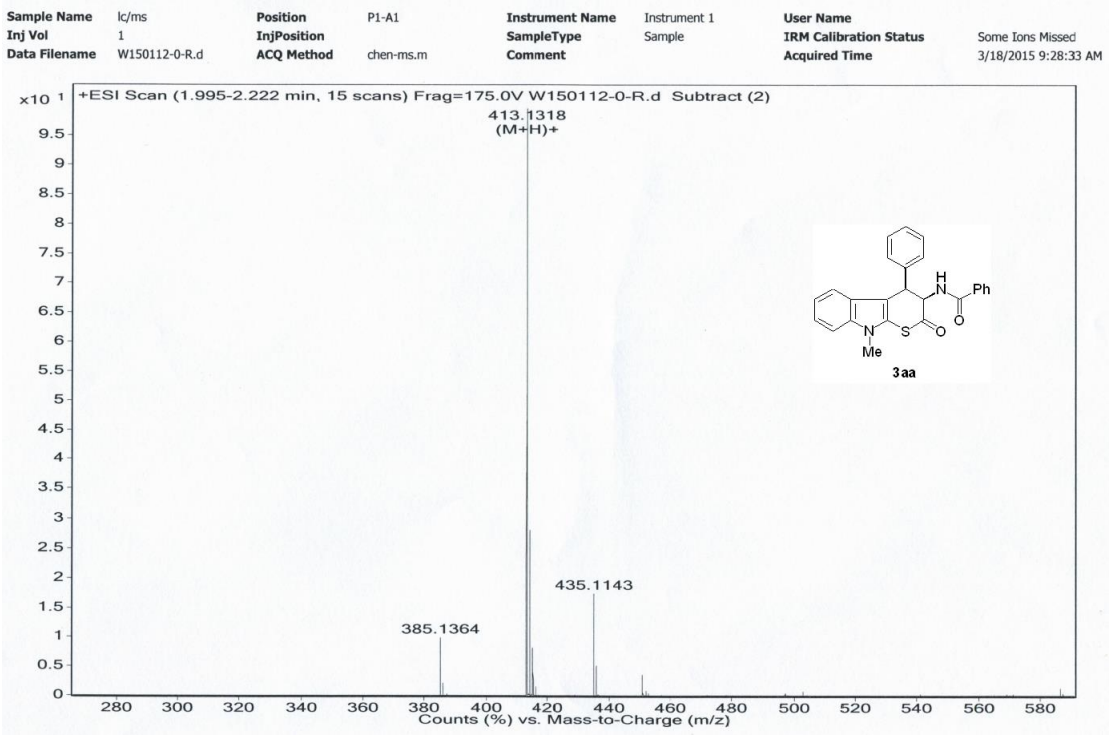
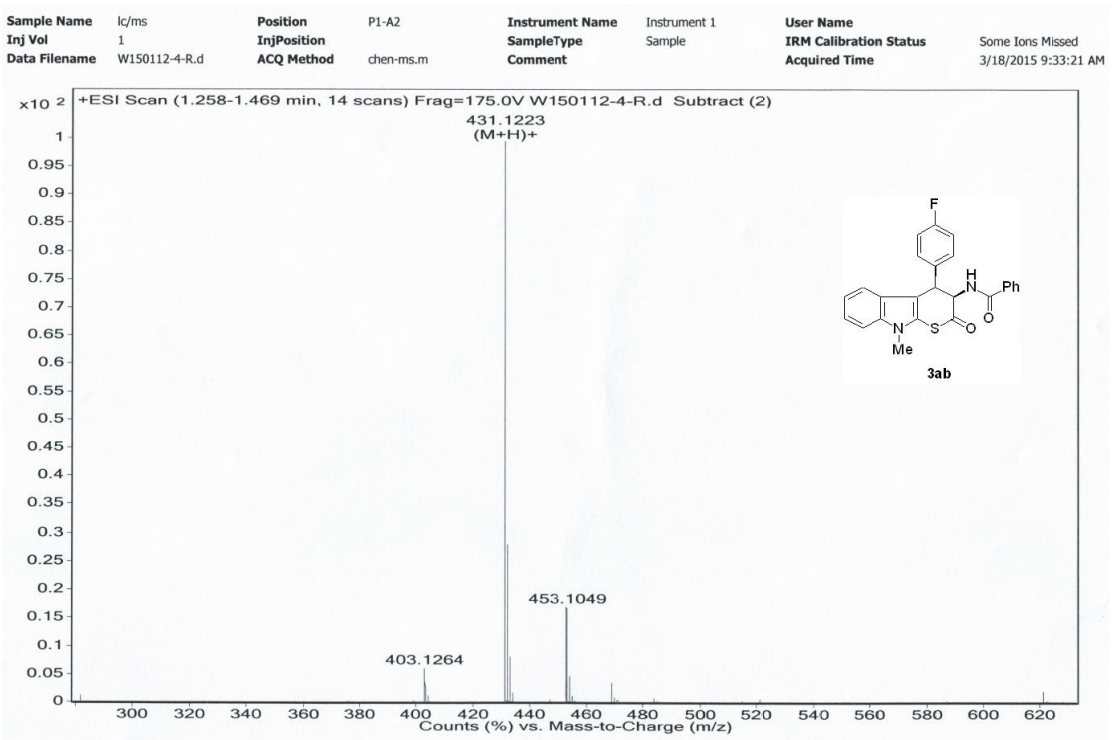
f1 (ppm)
H
N
Ph
O
N
S
O
Bn
3ea

3. Copies of HRMS spectra





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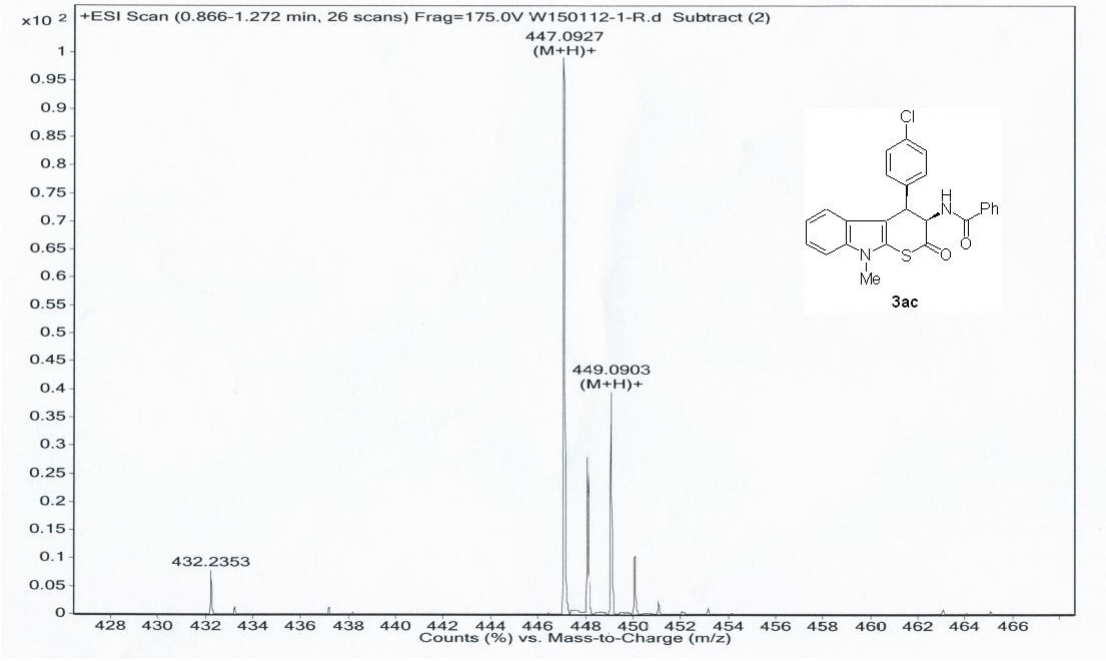

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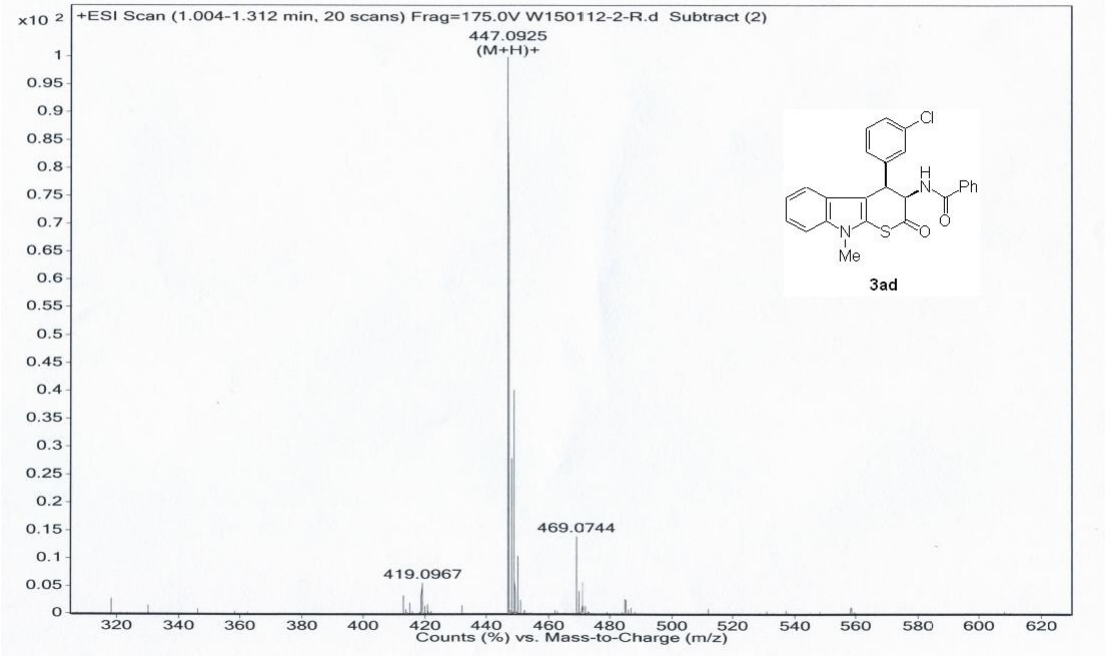

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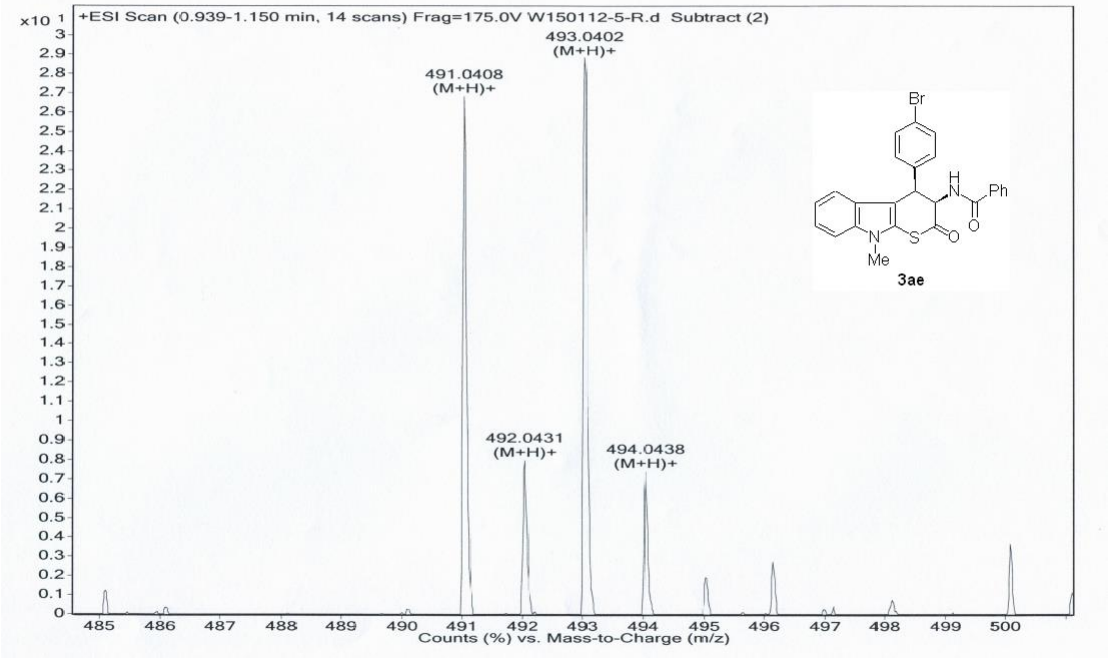
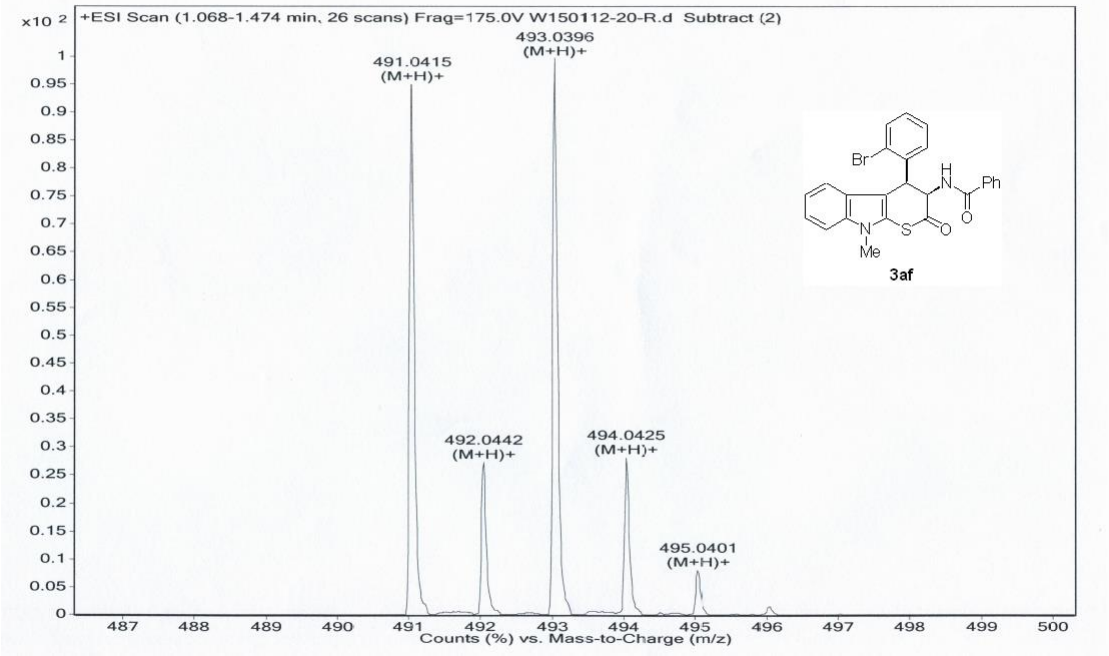
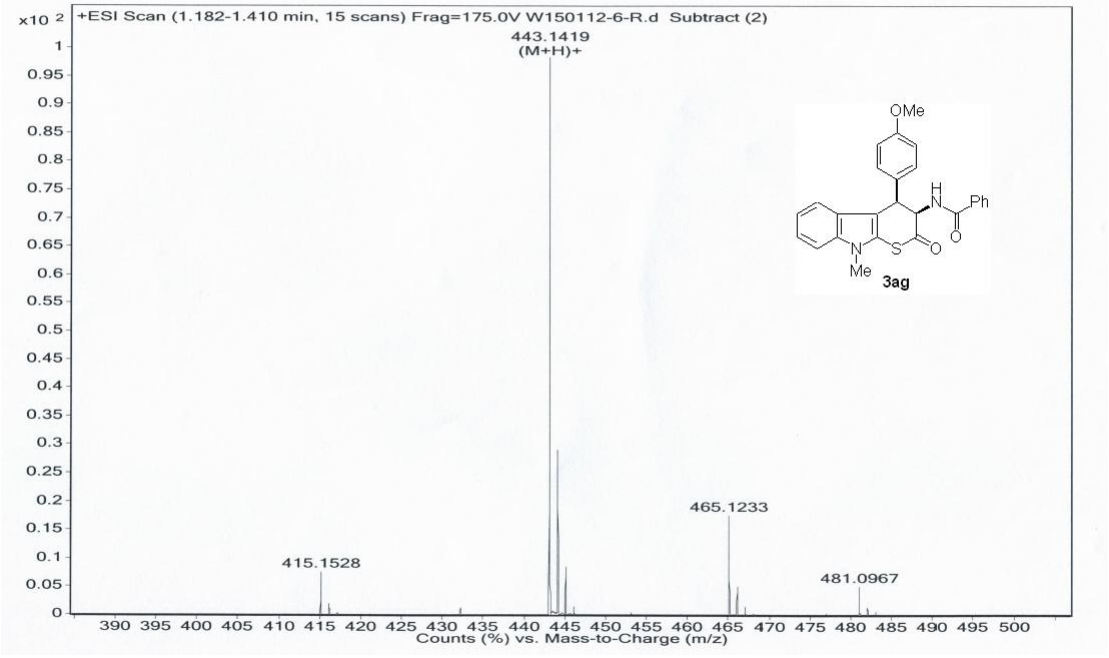


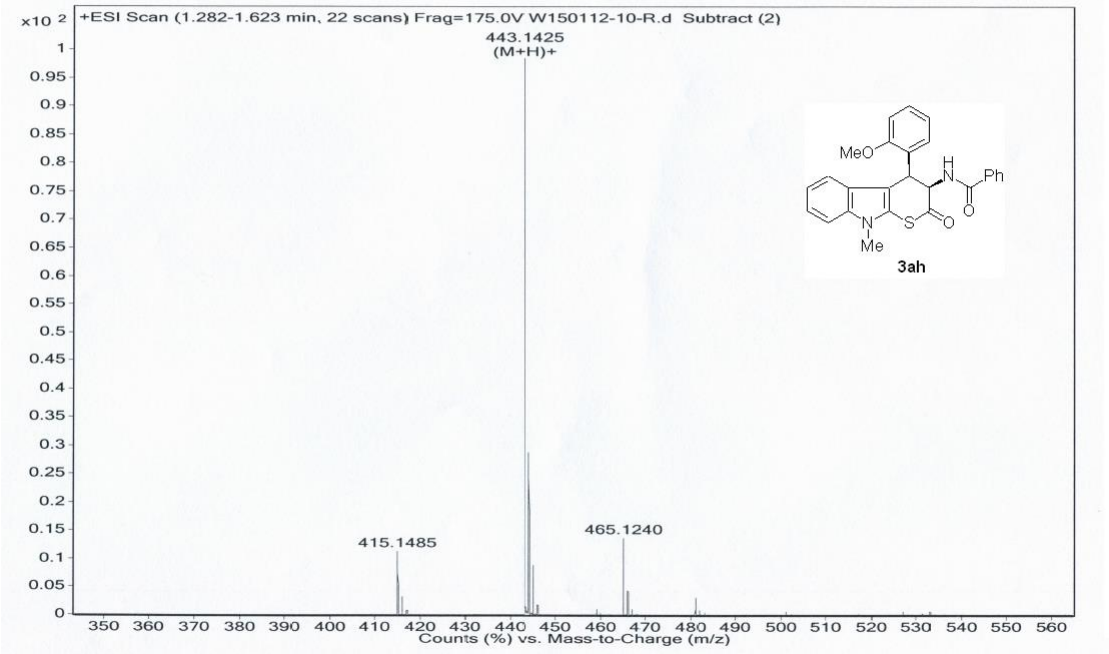
Sample Name	lc/ms	**Position**	P1-A6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-20-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 9:52:25 AM



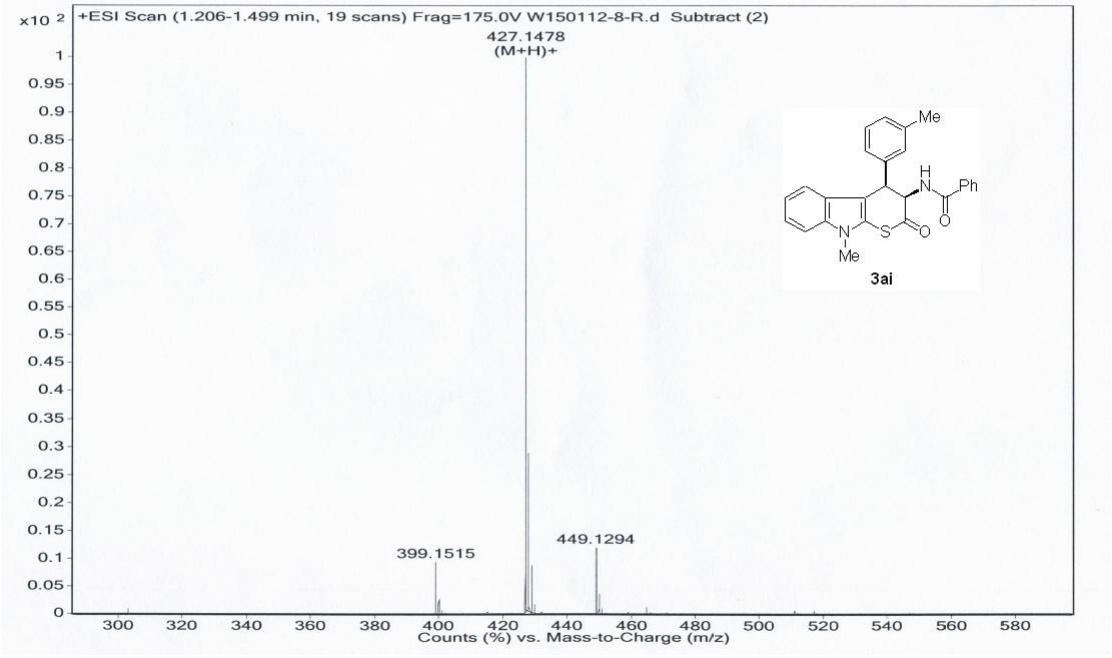
Sample Name	lc/ms	**Position**	P1-A7	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-6-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 9:57:09 AM



Sample Name	lc/ms	**Position**	P1-A8	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-10-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 10:01:54 AM

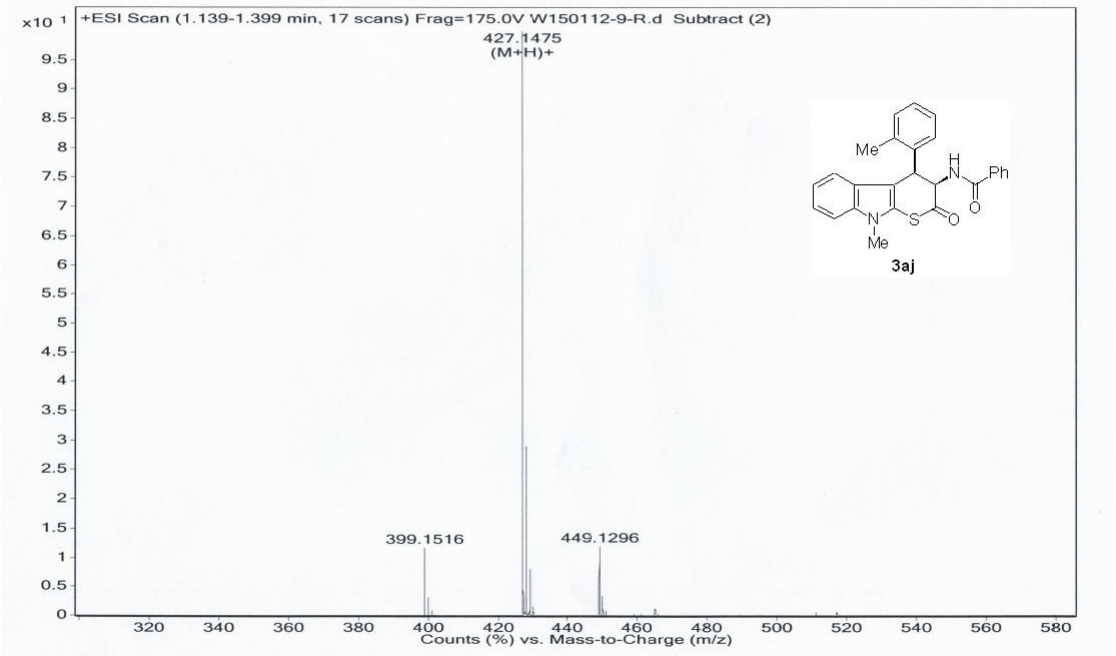


Sample Name	lc/ms	**Position**	P1-A9	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-8-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 10:06:39 AM



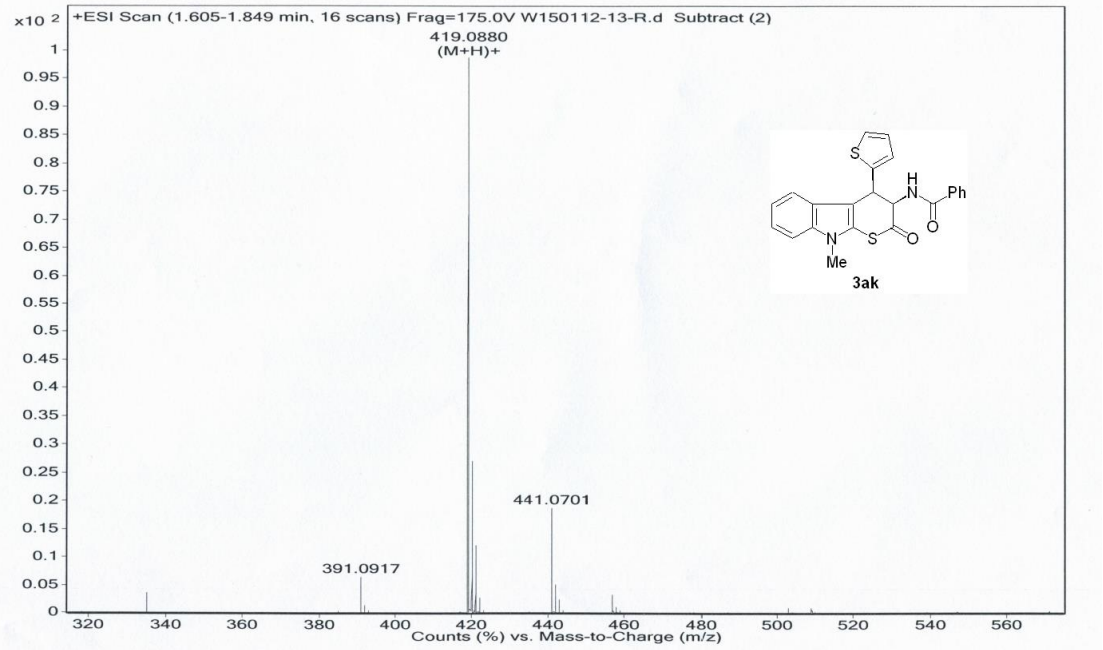
3ai

Sample Name	lc/ms	**Position**	P1-B1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-9-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 10:11:25 AM

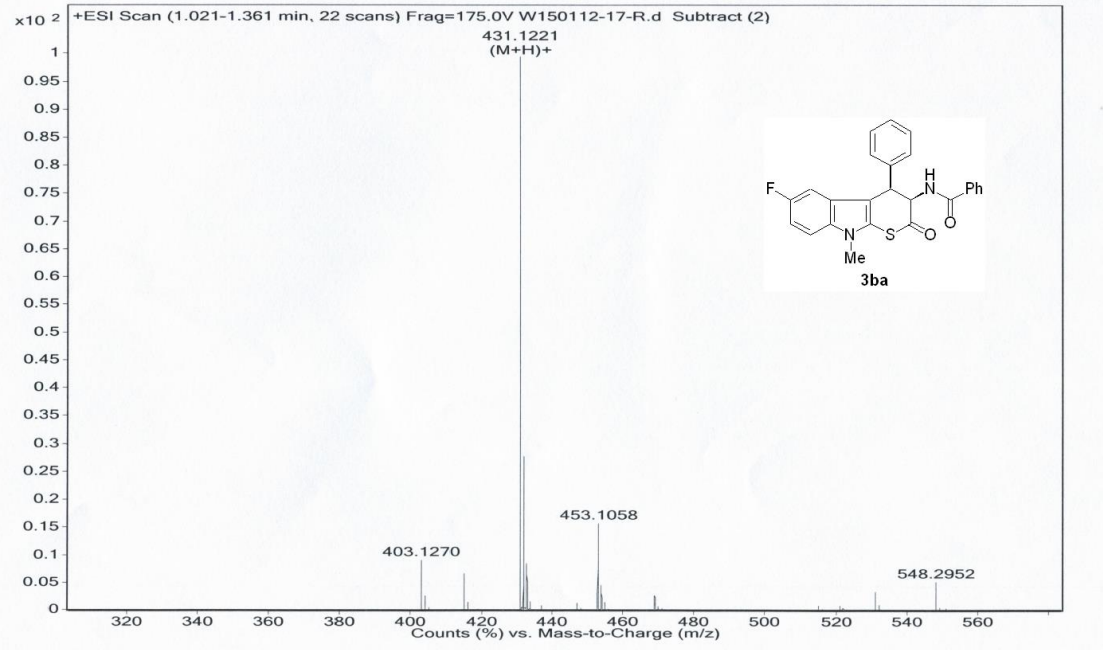


3aj

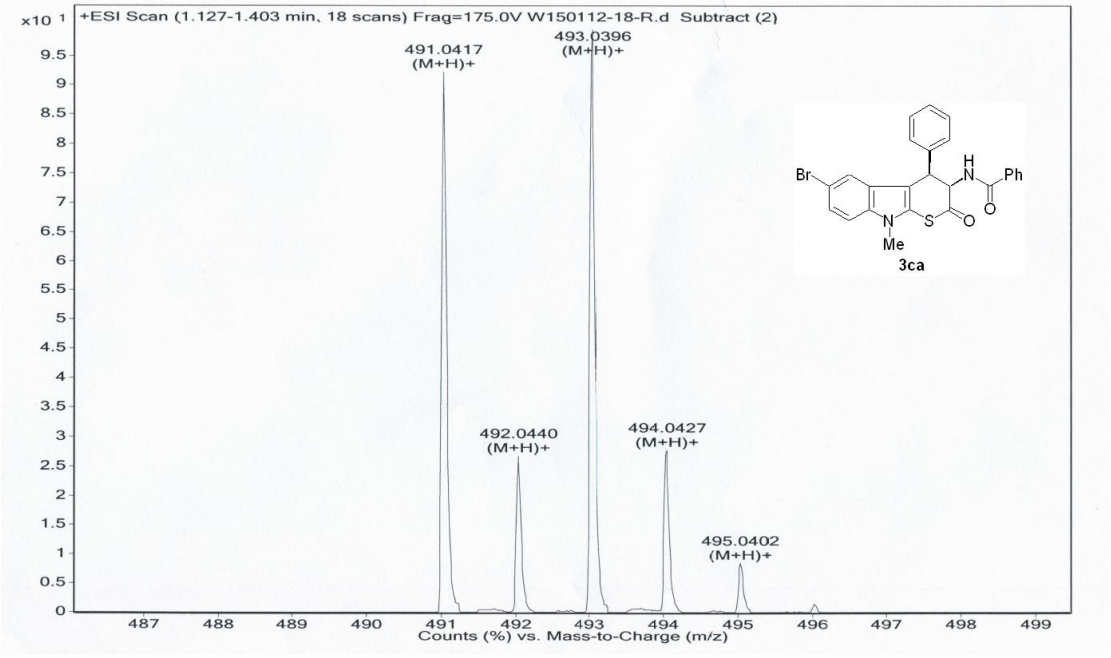
Sample Name	lc/ms	**Position**	P1-B2	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-13-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 10:16:08 AM



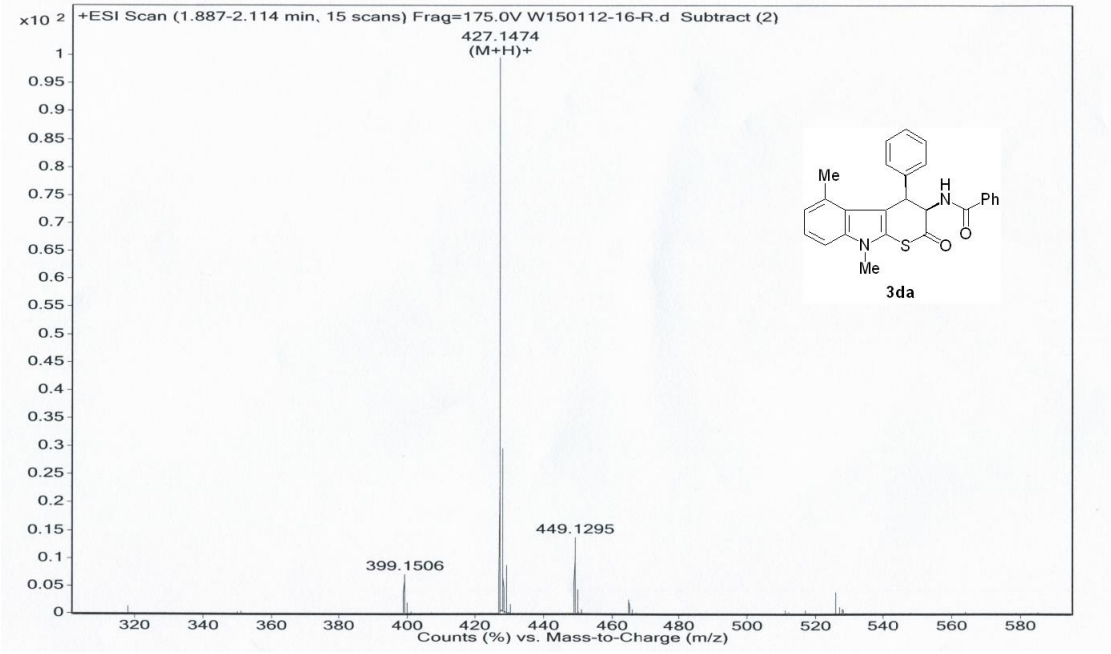
Sample Name	lc/ms	**Position**	P1-B5	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-17-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 10:30:24 AM

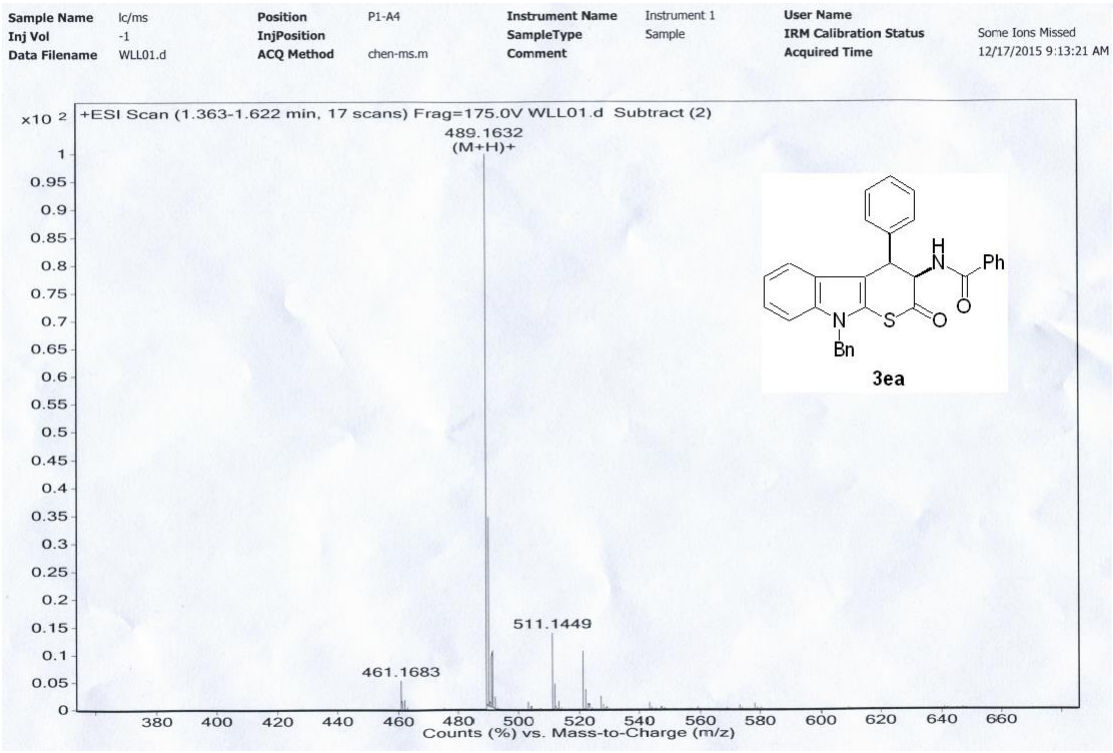


Sample Name	lc/ms	**Position**	P1-B6	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-18-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 10:35:08 AM



Sample Name	lc/ms	**Position**	P1-B4	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	W150112-16-R.d	**ACQ Method**	chen-ms.m	**Comment**		**Acquired Time**	3/18/2015 10:25:39 AM





4. Copies of HPLC data

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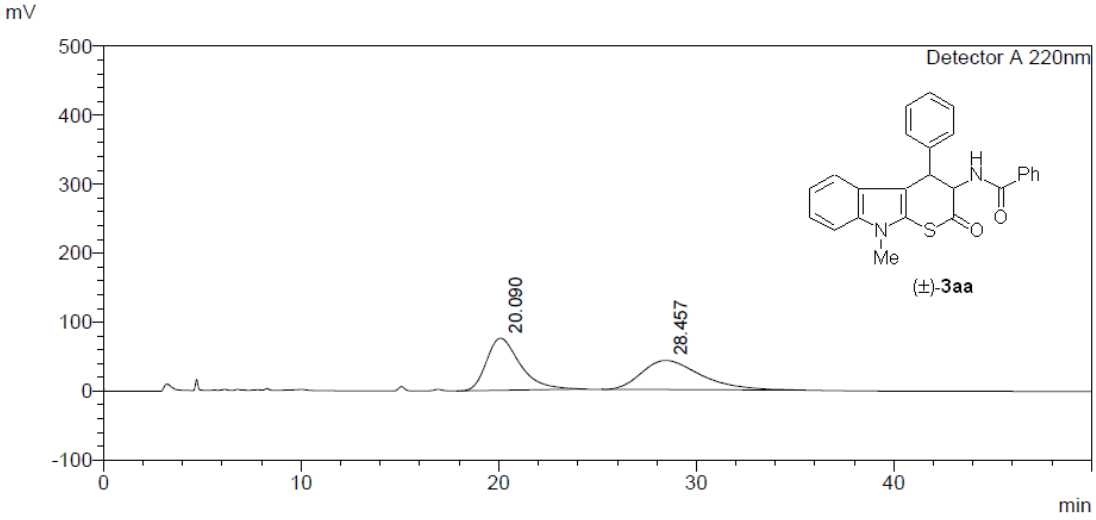

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	20.090	8939093	75487	50.276	64.093	50.276
2	28.457	8841007	42290	49.724	35.907	49.724
Total		17780100	117777		100.000	100.000

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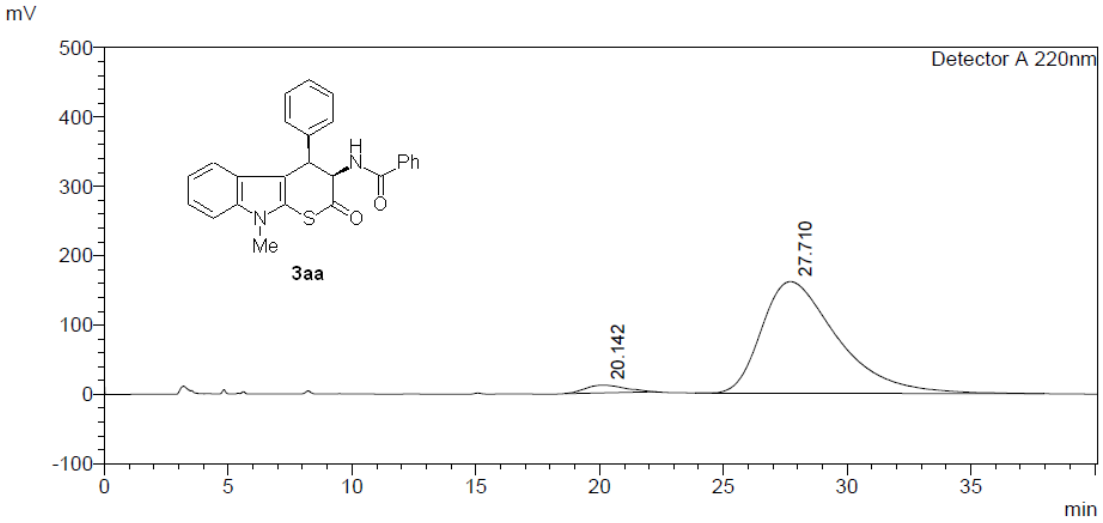

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	20.142	1242878	11257	3.484	6.534	3.484
2	27.710	34434964	161033	96.516	93.466	96.516
Total		35677842	172290		100.000	100.000

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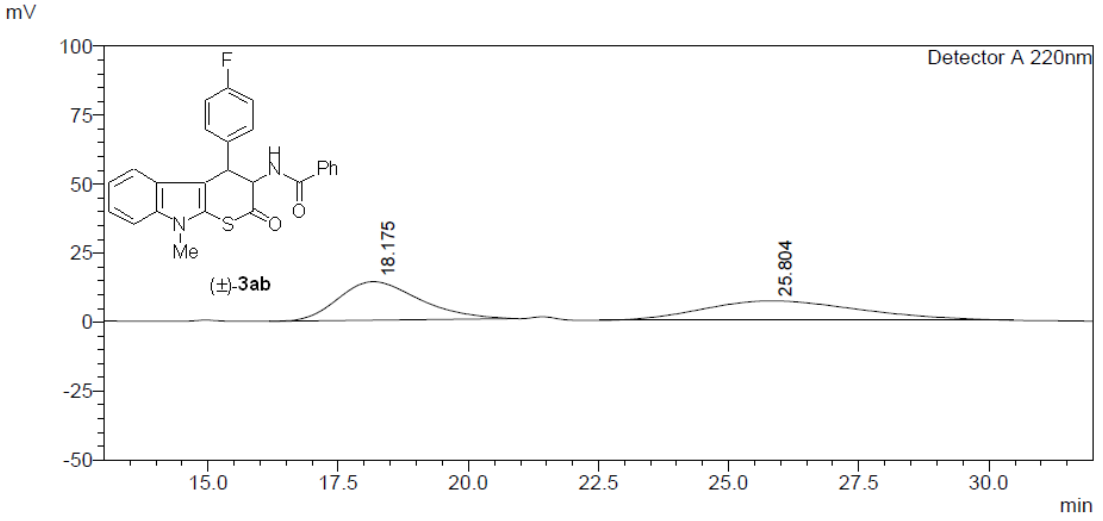

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	18.175	1520309	13959	50.873	66.682	50.873
2	25.804	1468105	6975	49.127	33.318	49.127
Total		2988414	20933		100.000	100.000

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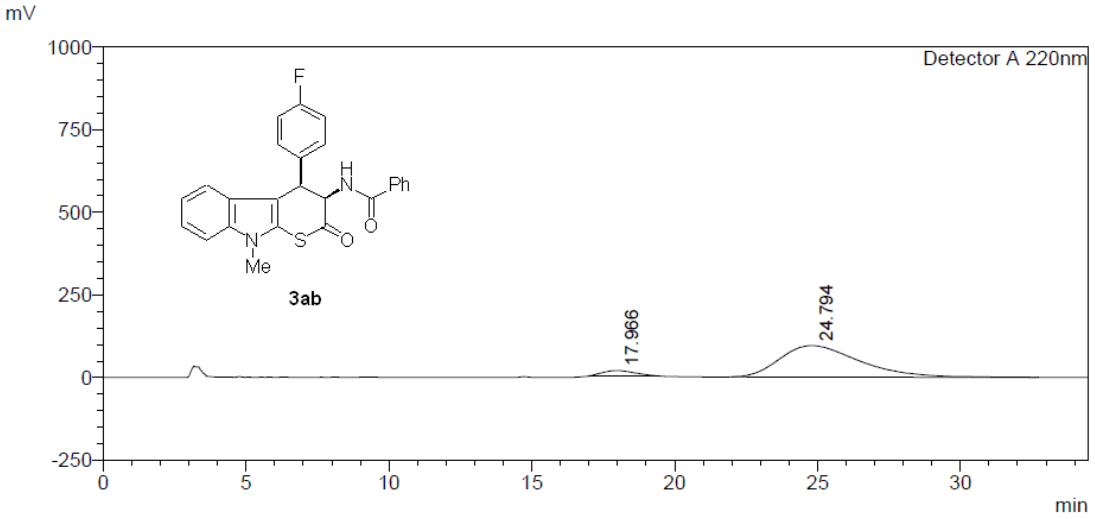

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	17.966	1261677	15936	6.387	14.330	6.387
2	24.794	18491761	95271	93.613	85.670	93.613
Total		19753438	111207		100.000	100.000

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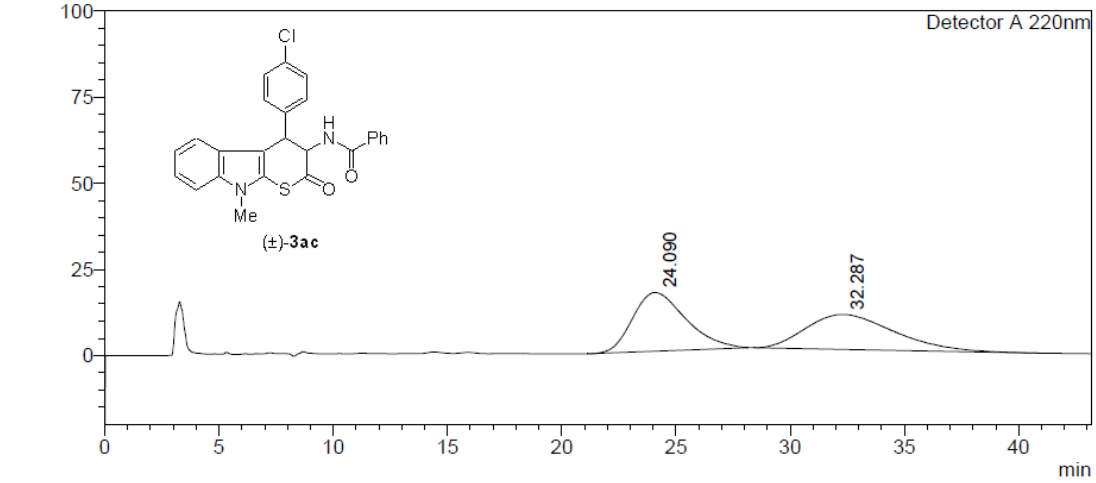

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	24.090	2756439	17024	50.195	62.698	50.195
2	32.287	2735061	10129	49.805	37.302	49.805
Total		5491501	27153		100.000	100.000

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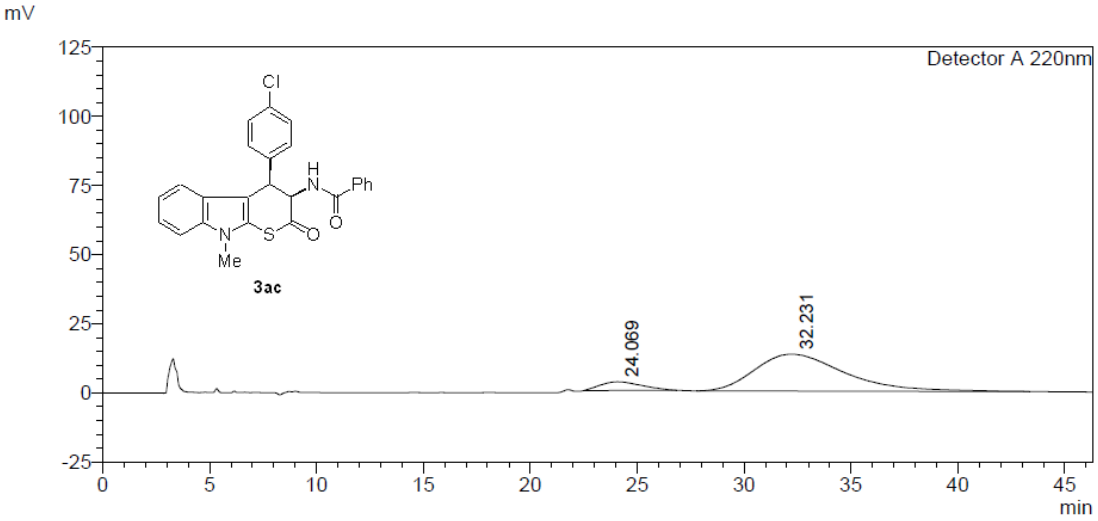

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	24.069	416799	3071	9.666	18.716	9.666
2	32.231	3895294	13335	90.334	81.284	90.334
Total		4312093	16406		100.000	100.000

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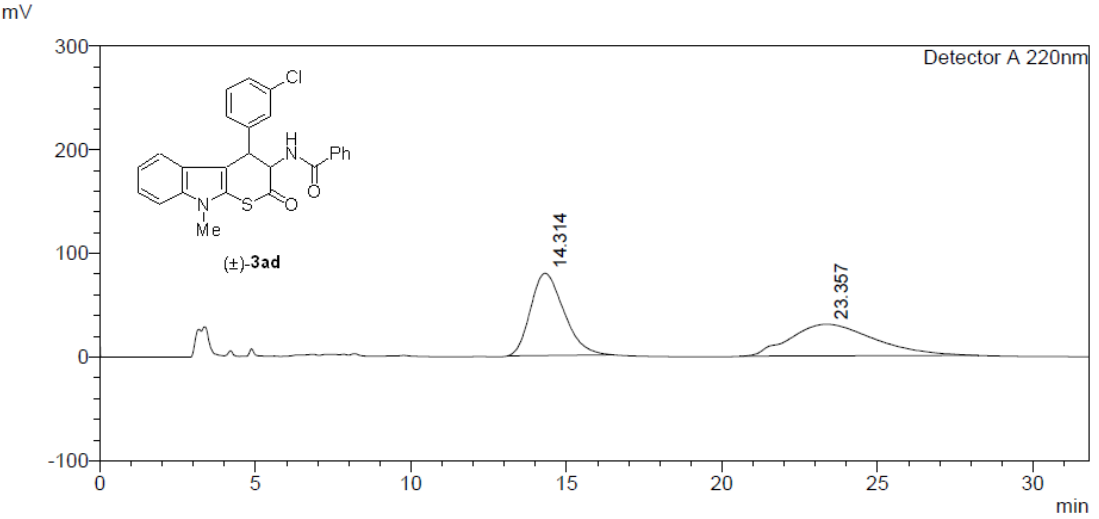

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	14.314	5905118	79254	50.430	72.202	50.430
2	23.357	5804328	30513	49.570	27.798	49.570
Total		11709446	109767		100.000	100.000

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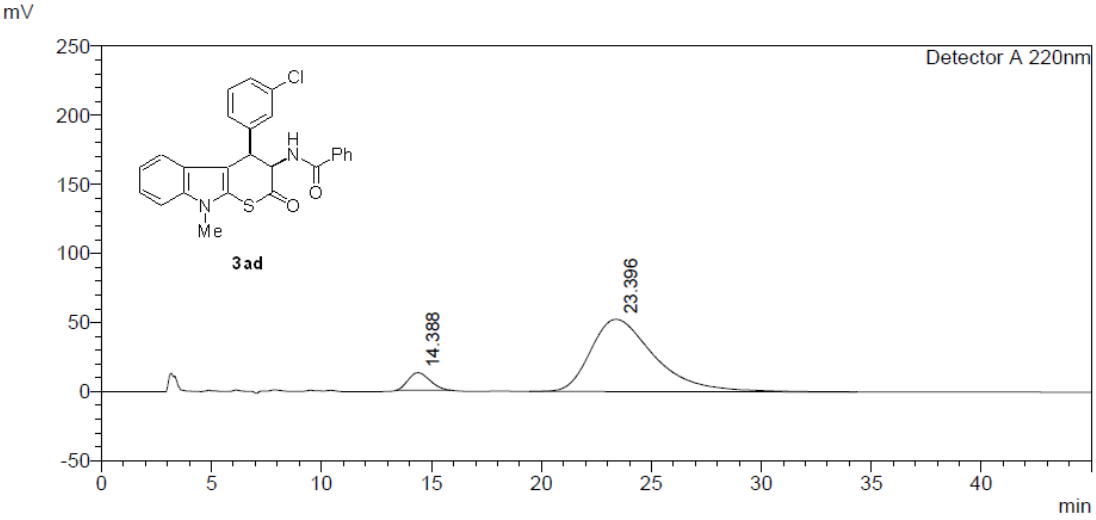

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	14.388	859315	12602	7.559	19.429	7.559
2	23.396	10508822	52258	92.441	80.571	92.441
Total		11368137	64859		100.000	100.000

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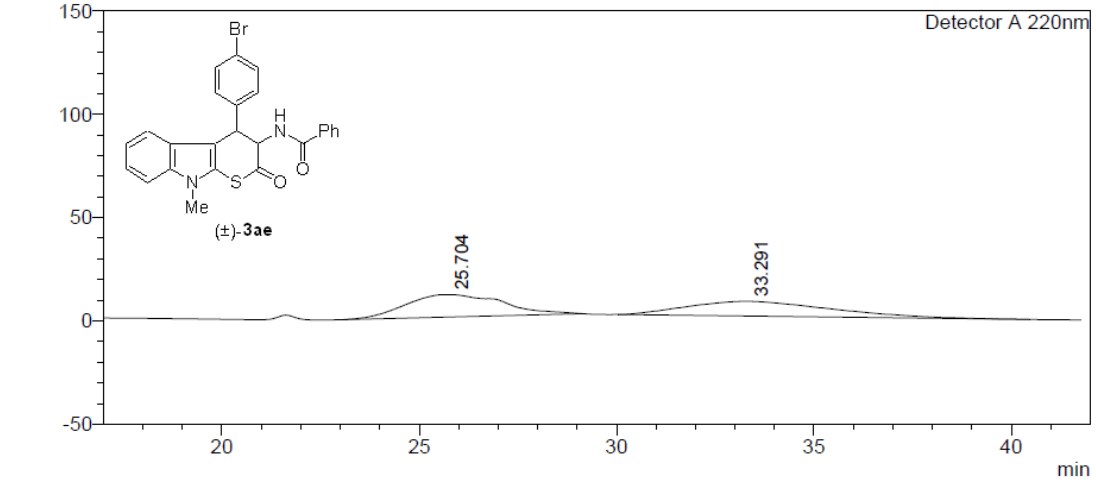

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	25.704	1846633	10898	50.599	60.720	50.599
2	33.291	1802945	7050	49.401	39.280	49.401
Total		3649578	17948		100.000	100.000

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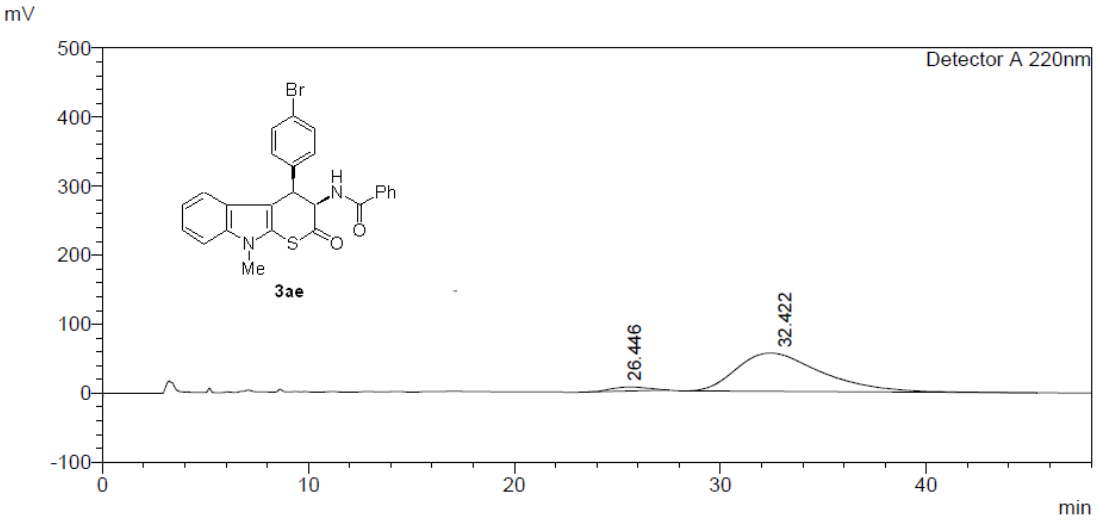

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	26.446	741015	6363	4.470	10.327	4.470
2	32.422	15836468	55250	95.530	89.673	95.530
Total		16577483	61613		100.000	100.000

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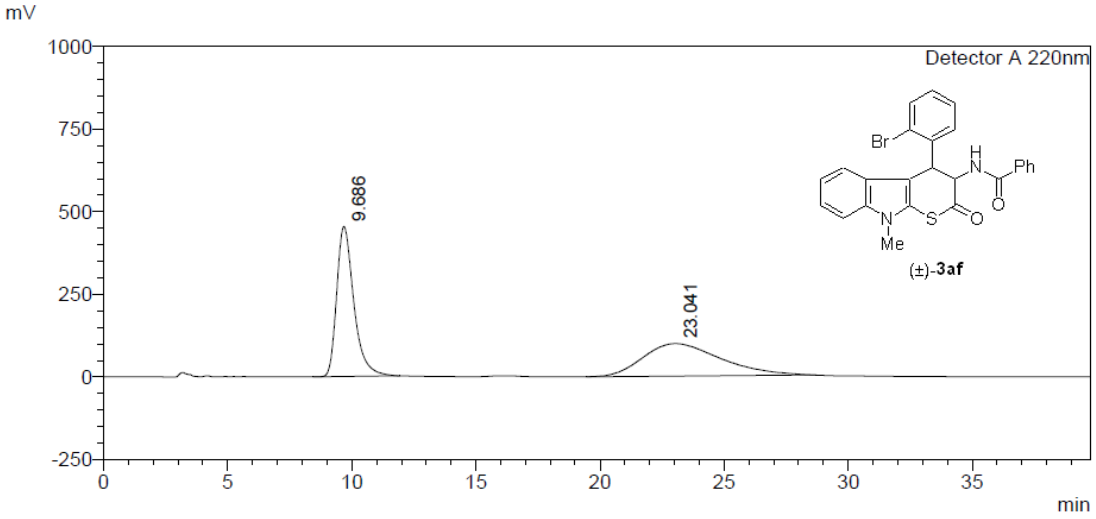
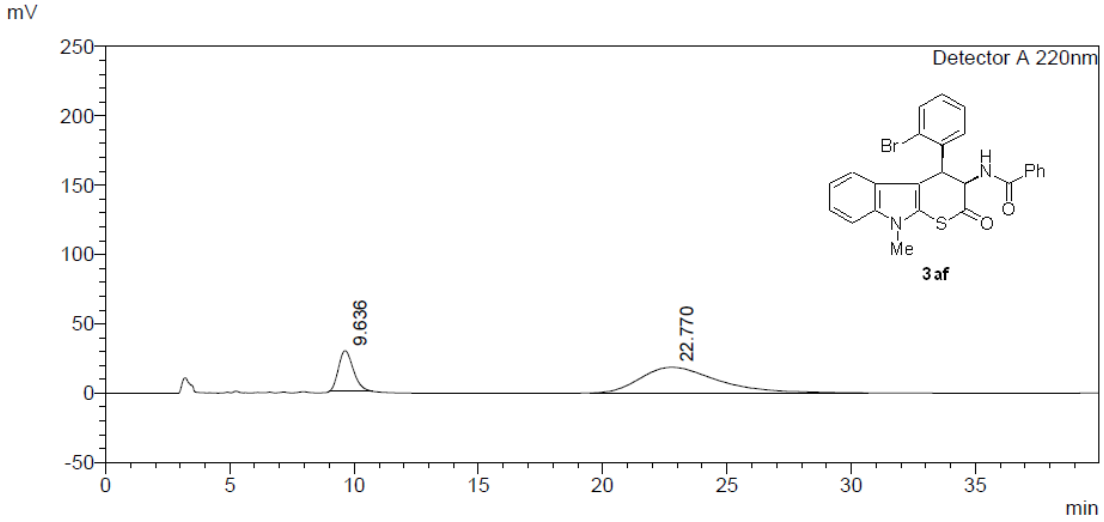


<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	9.686	21825501	454239	50.343	82.225	50.343
2	23.041	21528403	98197	49.657	17.775	49.657
Total		43353903	552436		100.000	100.000

<Chromatogram>



<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	9.636	1209923	29205	23.288	61.165	23.288
2	22.770	3985544	18543	76.712	38.835	76.712
Total		5195467	47748		100.000	100.000

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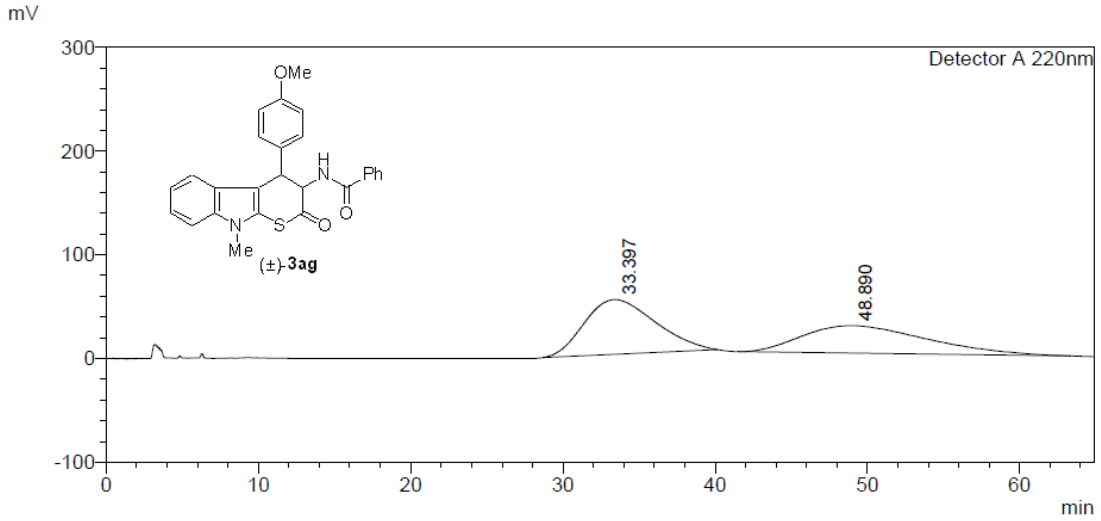

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	33.397	17016829	52592	53.049	66.682	53.049
2	48.890	15060936	26278	46.951	33.318	46.951
Total		32077766	78870		100.000	100.000

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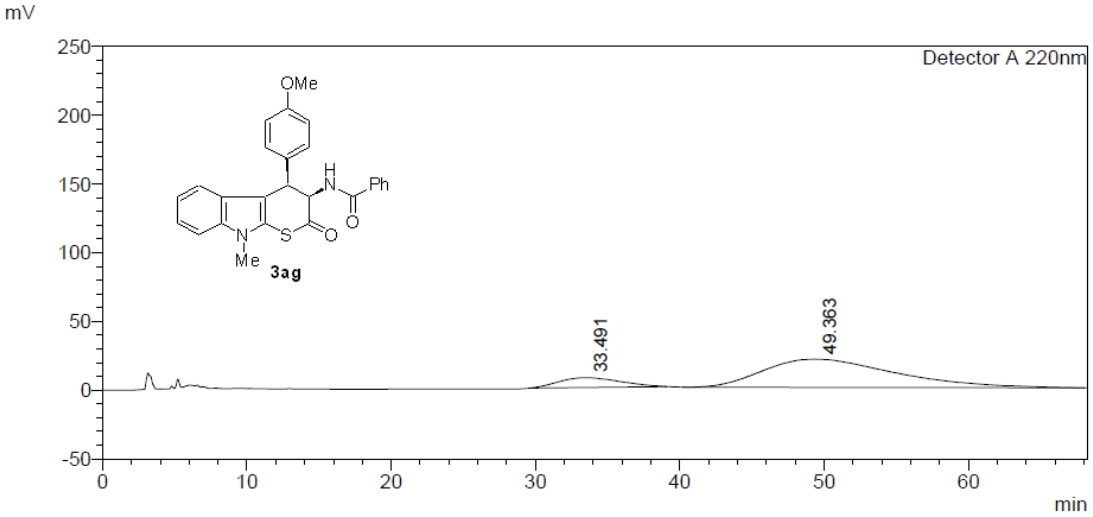

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	33.491	2078421	7093	13.728	25.621	13.728
2	49.363	13061377	20591	86.272	74.379	86.272
Total		15139798	27684		100.000	100.000

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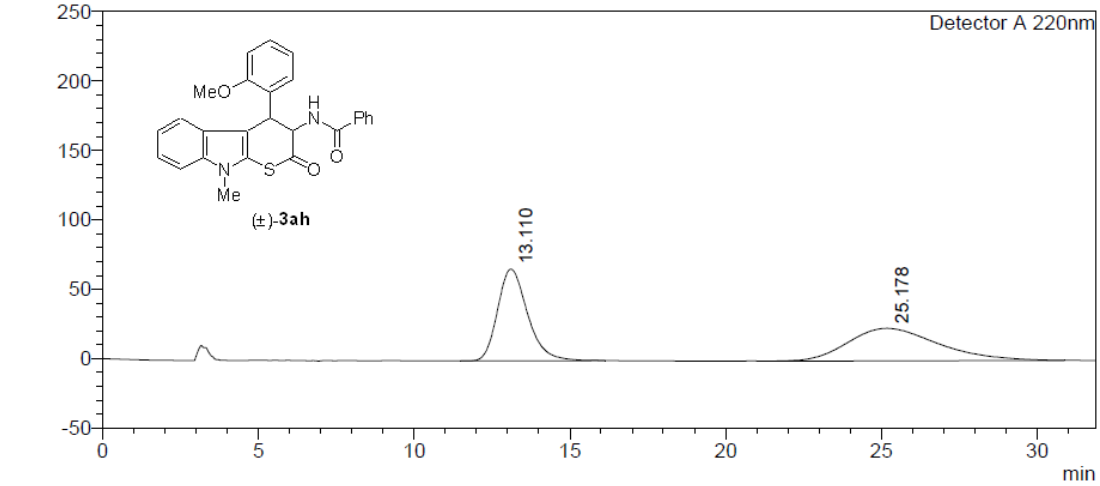

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	13.110	4434804	66123	48.546	73.900	48.546
2	25.178	4700529	23354	51.454	26.100	51.454
Total		9135332	89477		100.000	100.000

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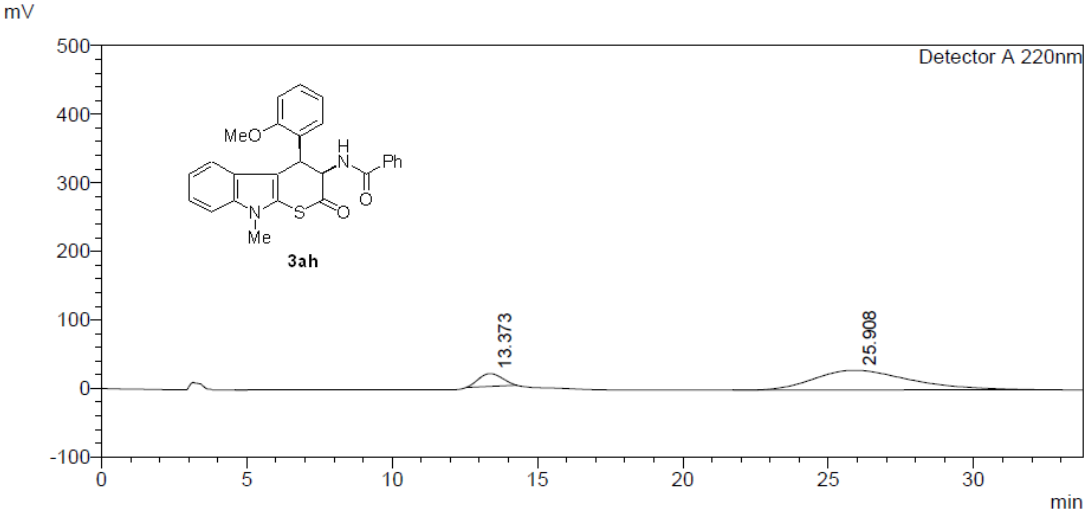

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	13.373	1048614	18459	13.867	39.275	13.867
2	25.908	6513157	28541	86.133	60.725	86.133
Total		7561770	47001		100.000	100.000

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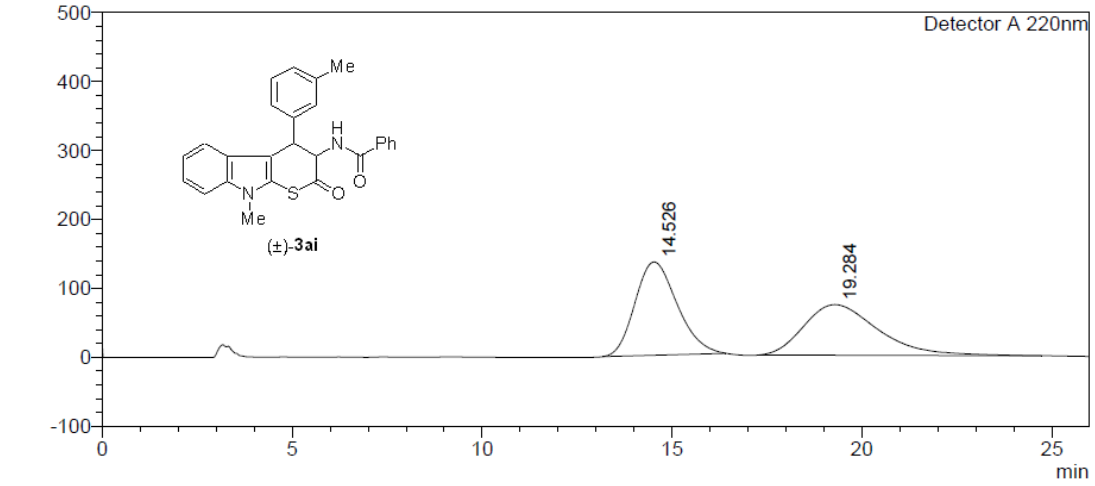

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	14.526	10448972	135255	51.064	64.817	51.064
2	19.284	10013575	73418	48.936	35.183	48.936
Total		20462547	208673		100.000	100.000

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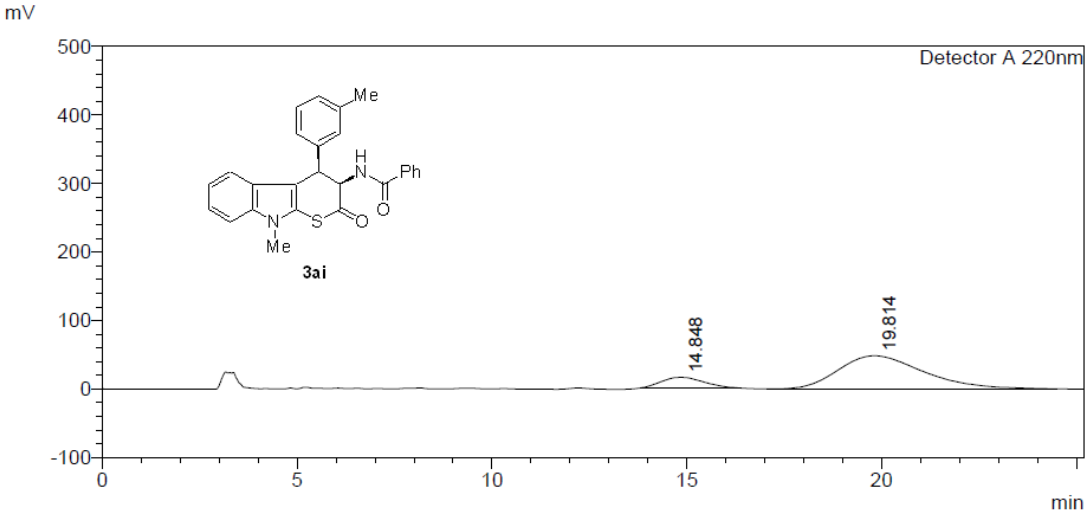

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	14.848	1201254	15833	14.022	24.669	14.022
2	19.814	7365627	48349	85.978	75.331	85.978
Total		8566881	64183		100.000	100.000

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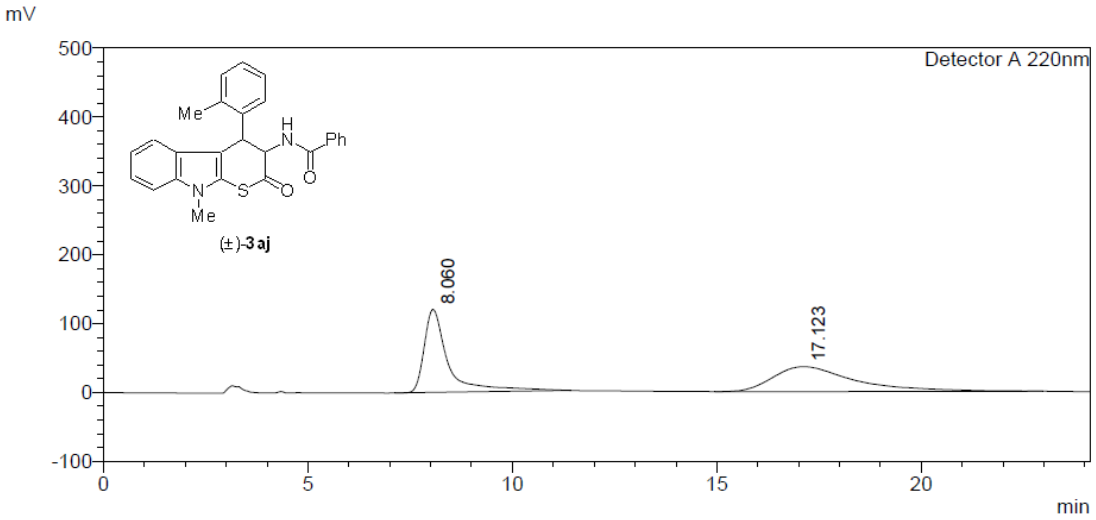

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	8.060	4870711	120195	49.082	76.835	49.082
2	17.123	5052900	36237	50.918	23.165	50.918
Total		9923610	156433		100.000	100.000

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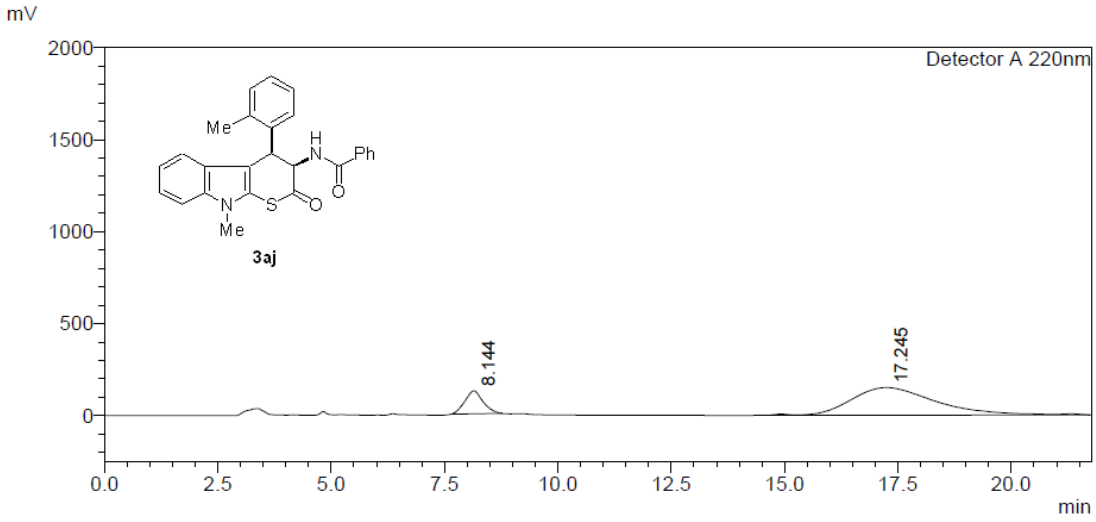

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	8.144	3476534	124432	15.176	45.479	15.176
2	17.245	19431015	149173	84.824	54.521	84.824
Total		22907549	273605		100.000	100.000

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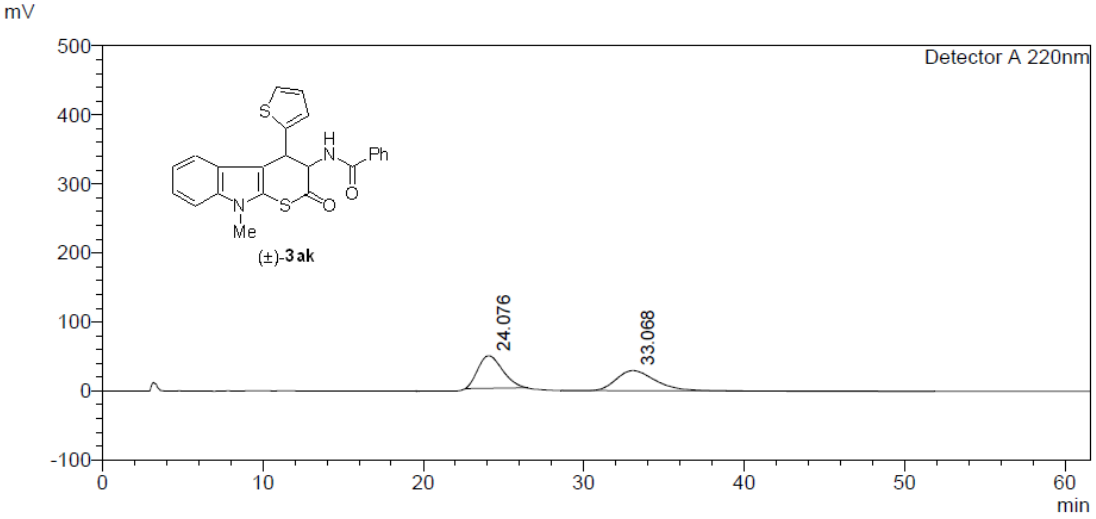

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	24.076	5071302	47285	51.361	61.855	51.361
2	33.068	4802553	29160	48.639	38.145	48.639
Total		9873855	76446		100.000	100.000

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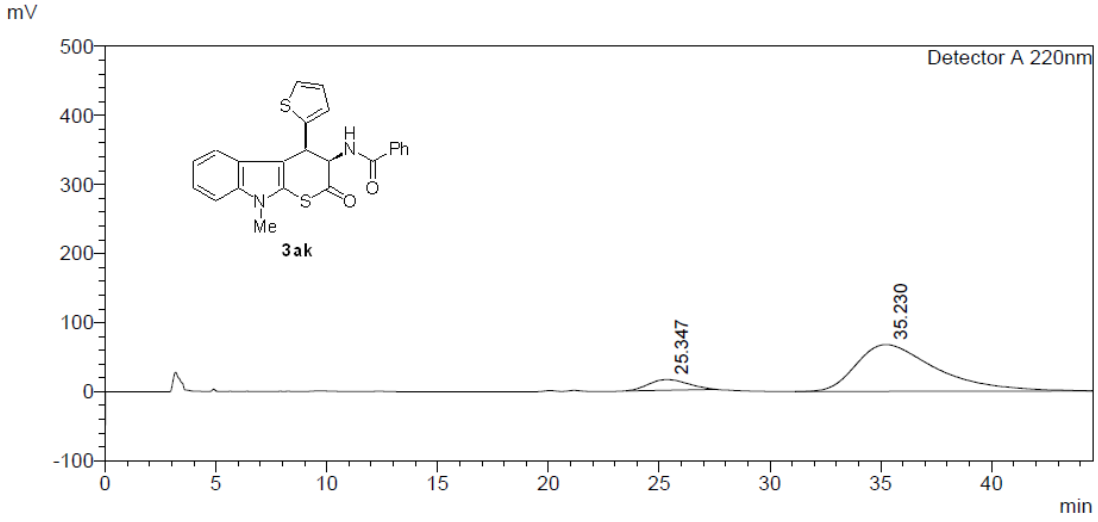

<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	25.347	1909121	15565	10.105	18.715	10.105
2	35.230	16984123	67604	89.895	81.285	89.895
Total		18893244	83169		100.000	100.000

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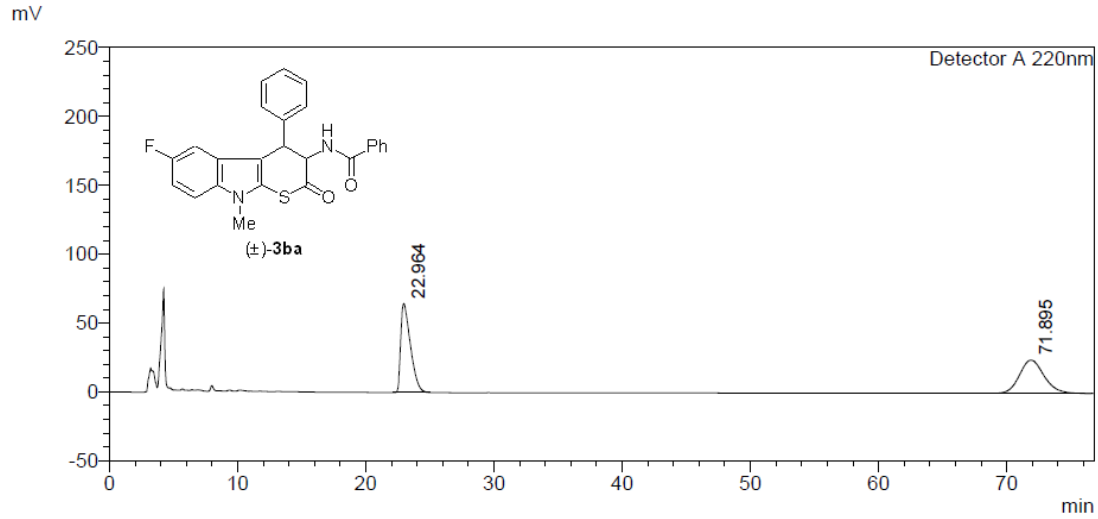
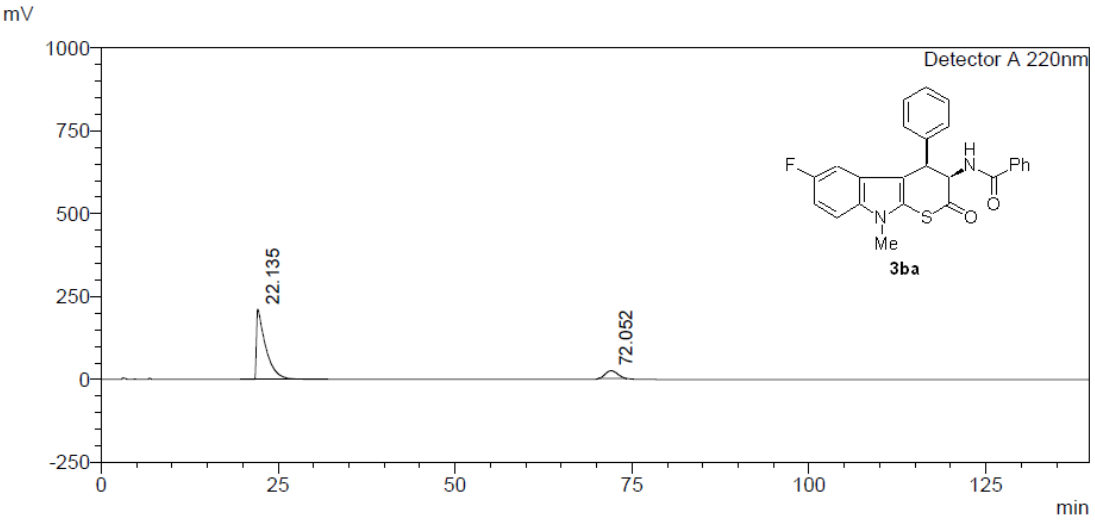


<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	22.964	3404894	64420	51.735	72.824	51.735
2	71.895	3176569	24040	48.265	27.176	48.265
Total		6581464	88460		100.000	100.000

<Chromatogram>



<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	22.135	19308683	212245	87.468	89.980	87.468
2	72.052	2766582	23636	12.532	10.020	12.532
Total		22075265	235880		100.000	100.000

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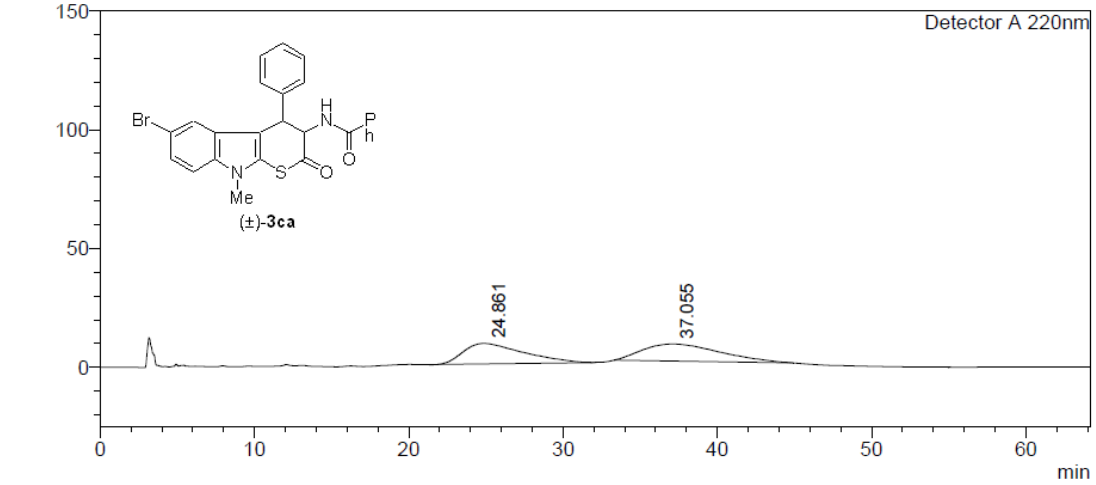
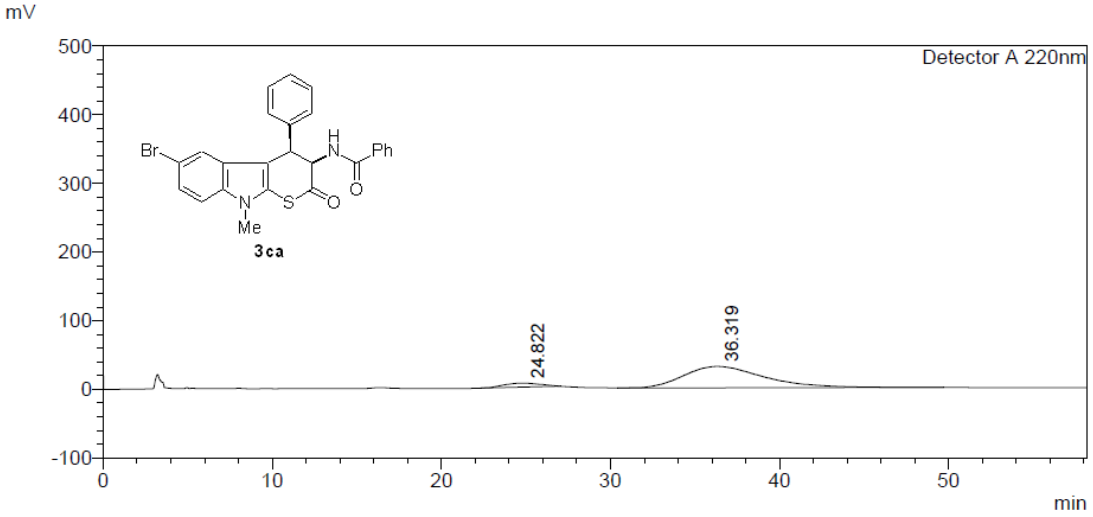


<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	24.861	2344571	8627	48.024	54.566	48.024
2	37.055	2537540	7184	51.976	45.434	51.976
Total		4882111	15811		100.000	100.000

<Chromatogram>

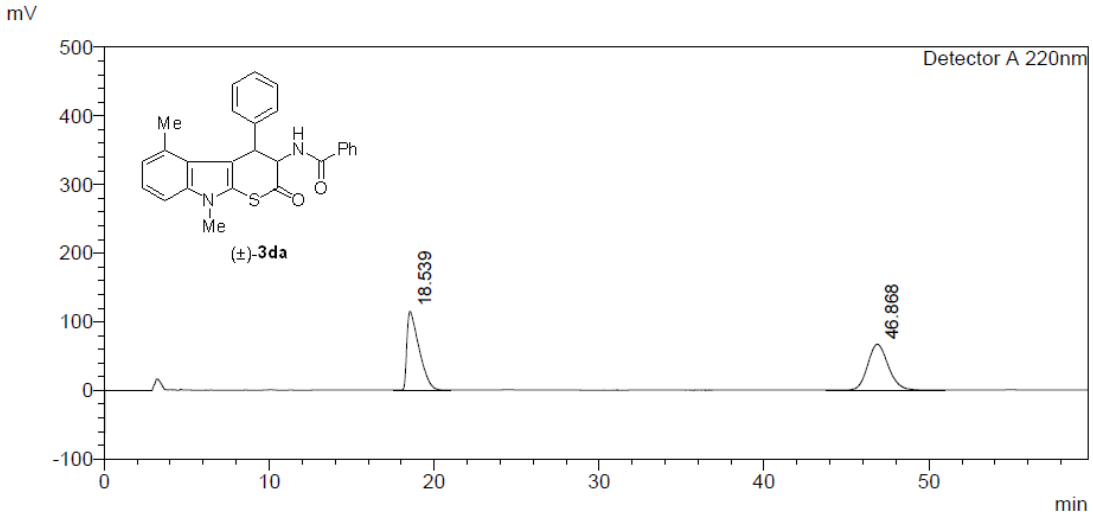


<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	24.822	908073	5976	8.087	16.089	8.087
2	36.319	10320606	31168	91.913	83.911	91.913
Total		11228680	37144		100.000	100.000

<Chromatogram>

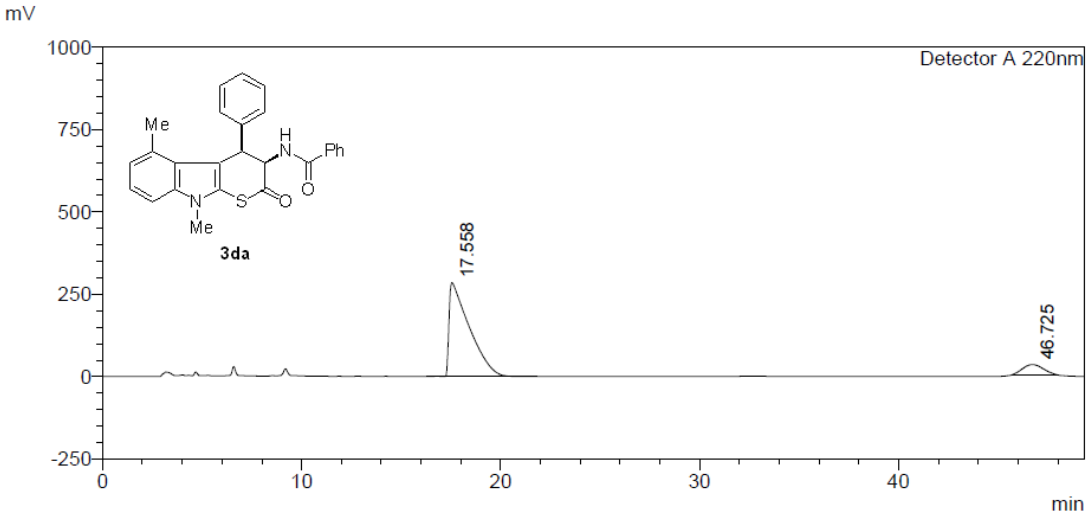


<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	18.539	5856219	114556	50.501	63.197	50.501
2	46.868	5740010	66714	49.499	36.803	49.499
Total		11596229	181270		100.000	100.000

<Chromatogram>

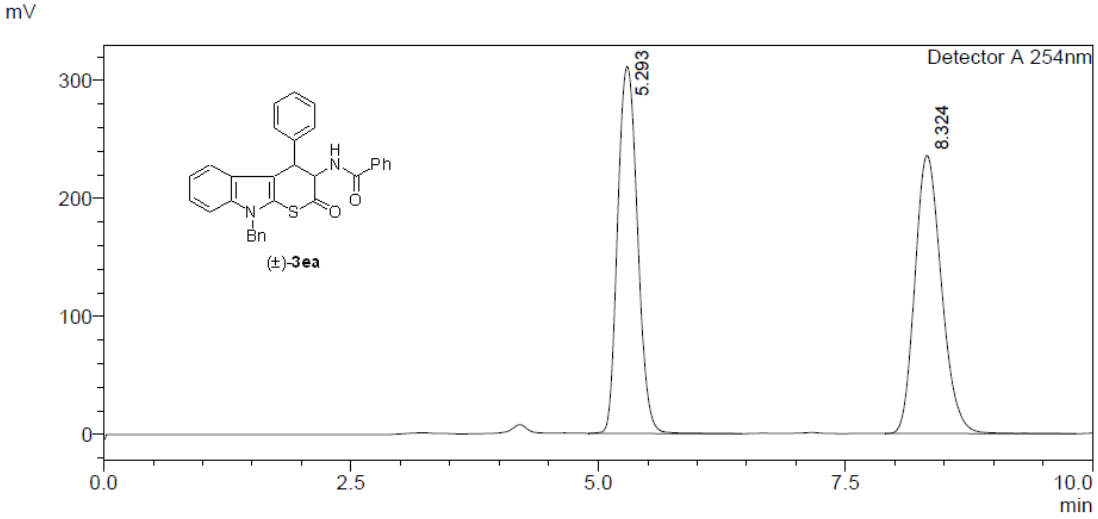


<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Height%	Area%
1	17.558	20187445	285276	89.806	90.039	89.806
2	46.725	2291450	31560	10.194	9.961	10.194
Total		22478895	316836		100.000	100.000

<Chromatogram>



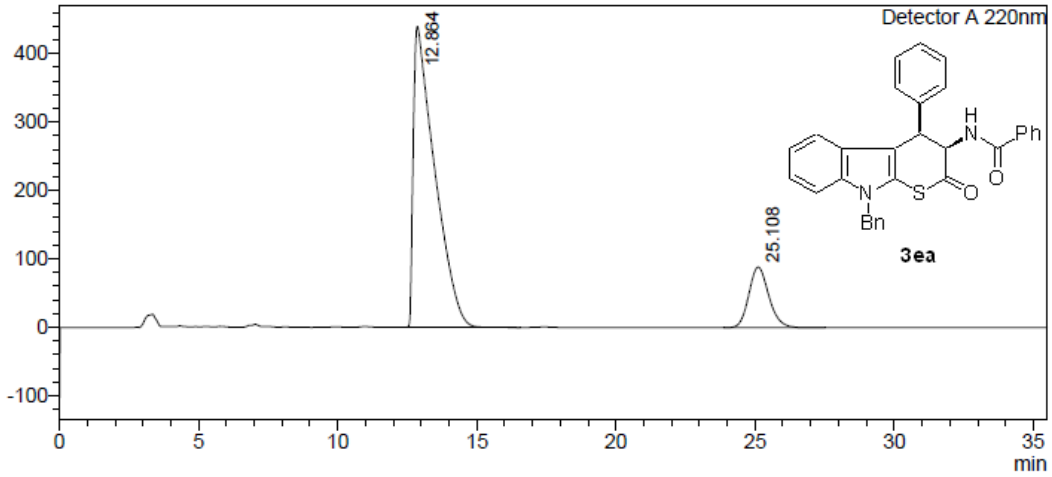
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	5.293	4351610	310996	49.653			
2	8.324	4412403	235719	50.347		S	
Total		8764013	546715				

<Chromatogram>

mV



<Peak Table>

Detector A 220nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.864	23440840	439318	84.221			
2	25.108	4391565	88277	15.779			
Total		27832405	527595				