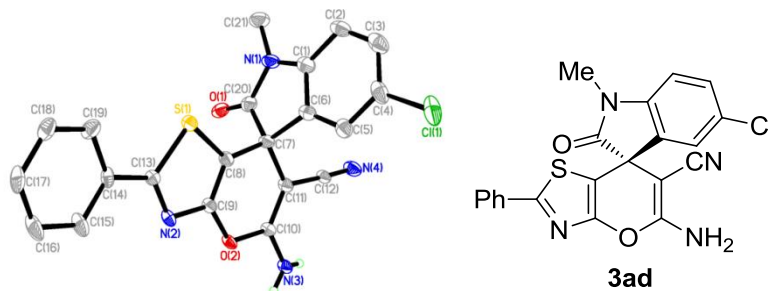


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| 4. Copies of HPLC spectra | Page 27 – Page 45 |
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1. Crystallography data of Compound **3ad**

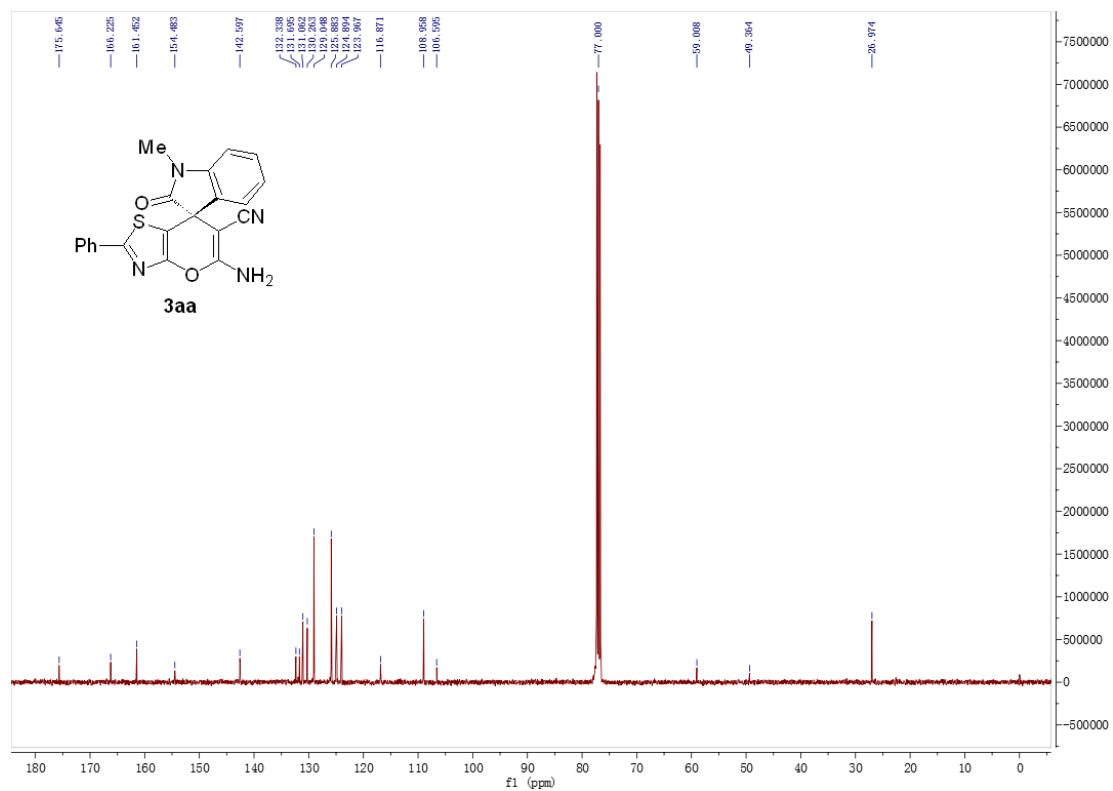
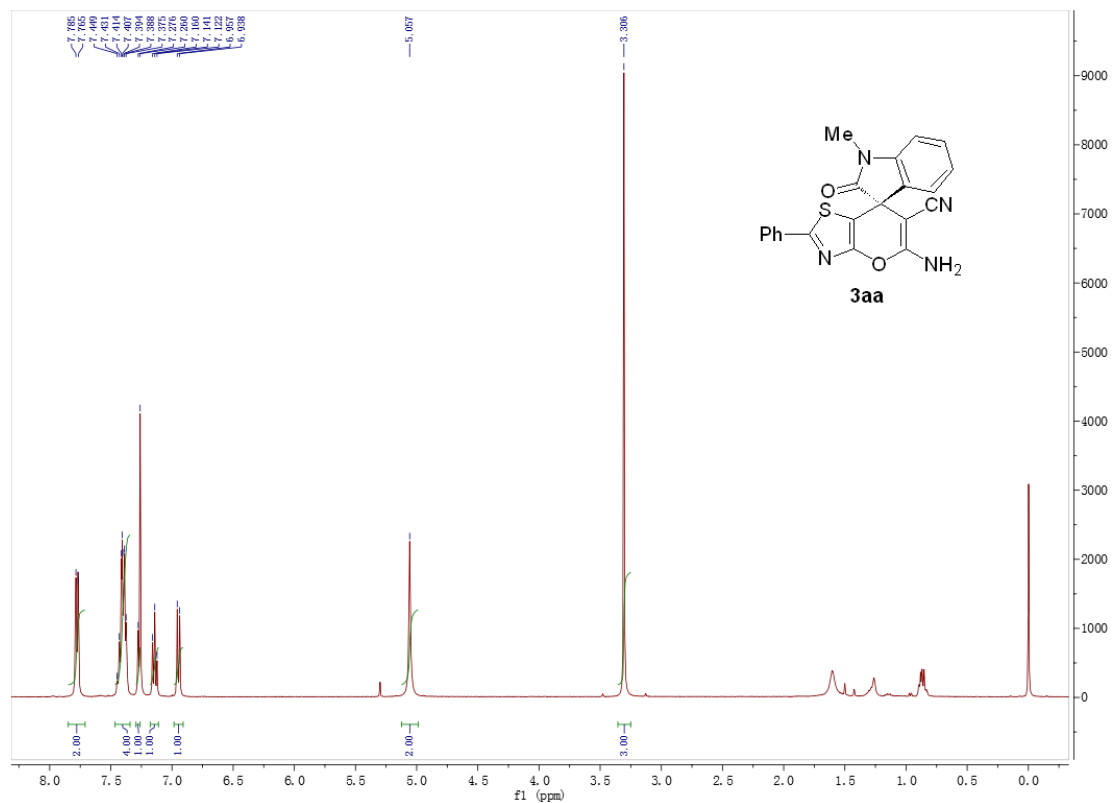


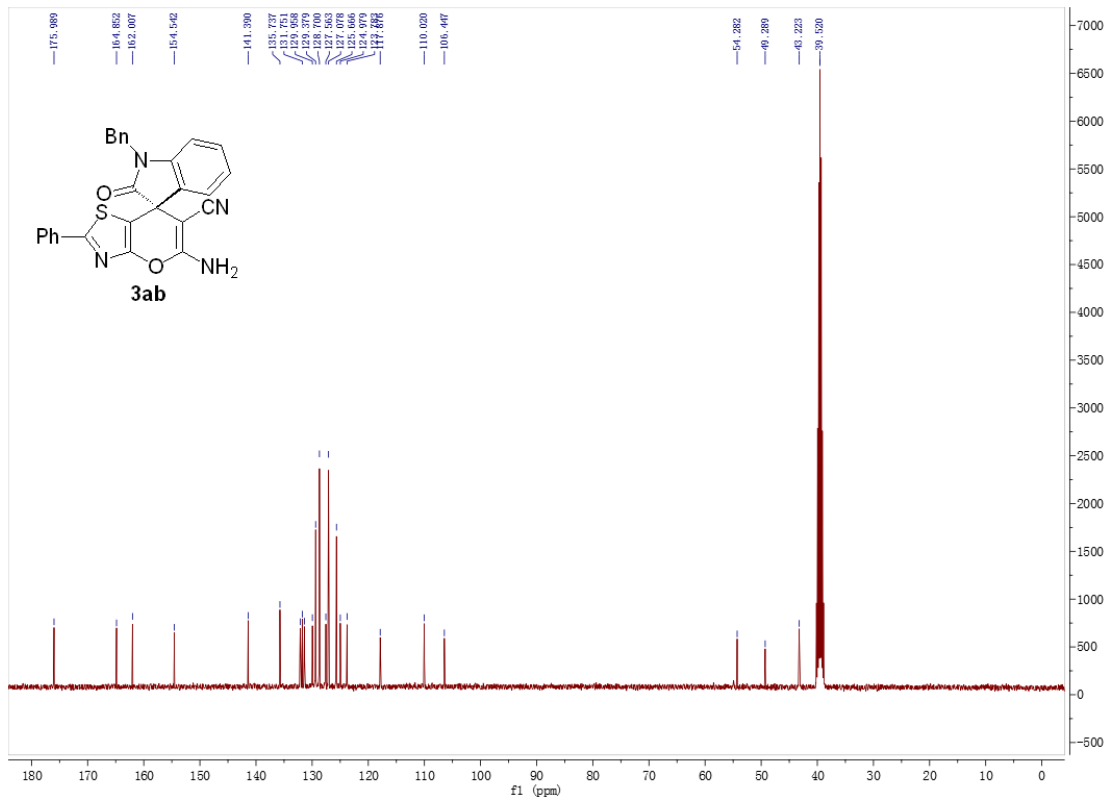
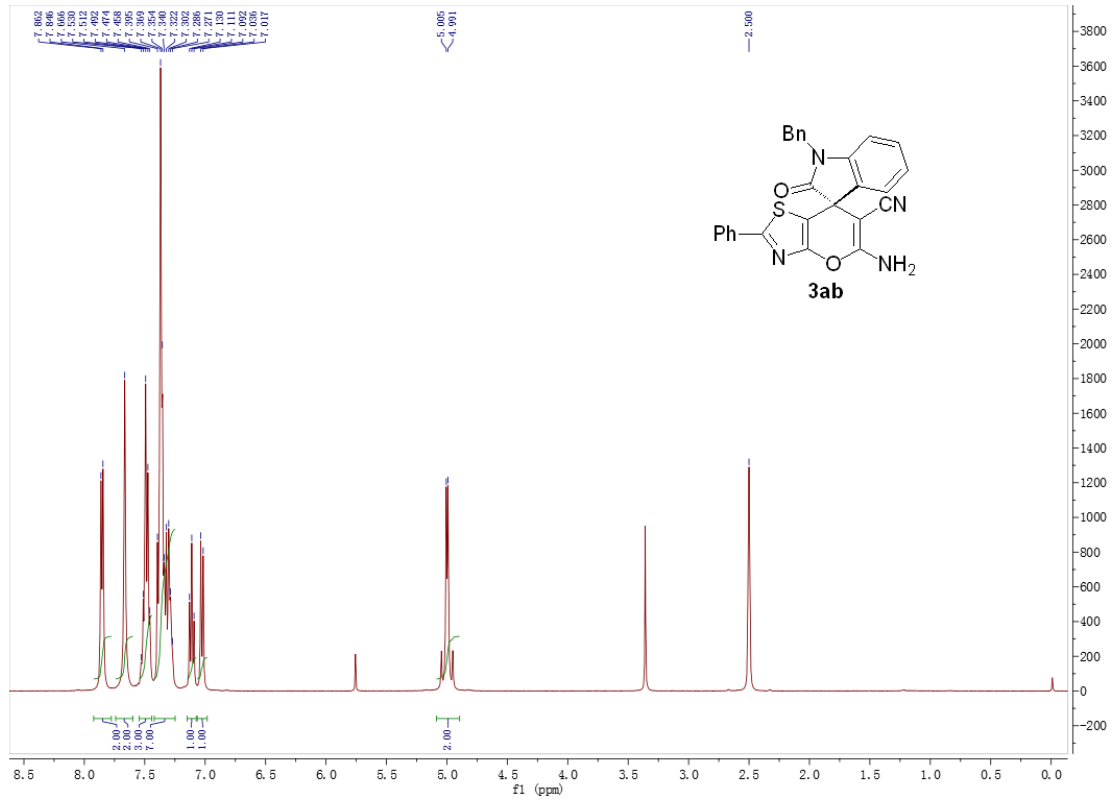
Identification code	m20151228d
Empirical formula	C _{22.25} H _{15.50} Cl _{3.50} N ₄ O ₂ S
Formula weight	527.02
Temperature	113(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 12.4973(2) Å alpha = 90 deg. b = 24.2521(3) Å beta = 90 deg. c = 30.8995(4) Å gamma = 90 deg.
Volume	9365.2(2) Å ³
Z, Calculated density	16, 1.495 Mg/m ³
Absorption coefficient	0.566 mm ⁻¹
F(000)	4296
Crystal size	0.200 x 0.180 x 0.120 mm
Theta range for data collection	1.563 to 25.019 deg.
Limiting indices	-14 ≤ h ≤ 14, -28 ≤ k ≤ 28, -36 ≤ l ≤ 36
Reflections collected / unique	66384 / 16530 [R(int) = 0.0293]
Completeness to theta = 67.687	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.50244
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	16530 / 160 / 1280
Goodness-of-fit on F ²	1.094
Final R indices [I > 2σ(I)]	R1 = 0.0587, wR2 = 0.1683
R indices (all data)	R1 = 0.0621, wR2 = 0.1720
Absolute structure parameter	0.016(11)
Extinction coefficient	n/a

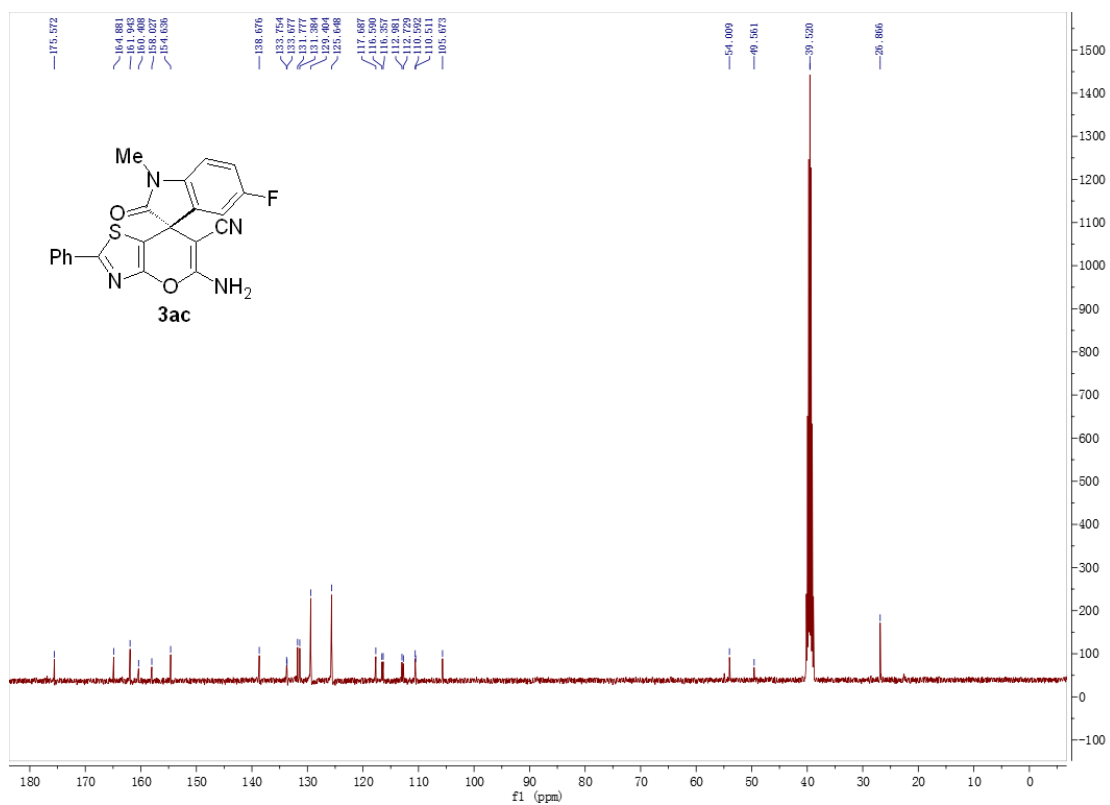
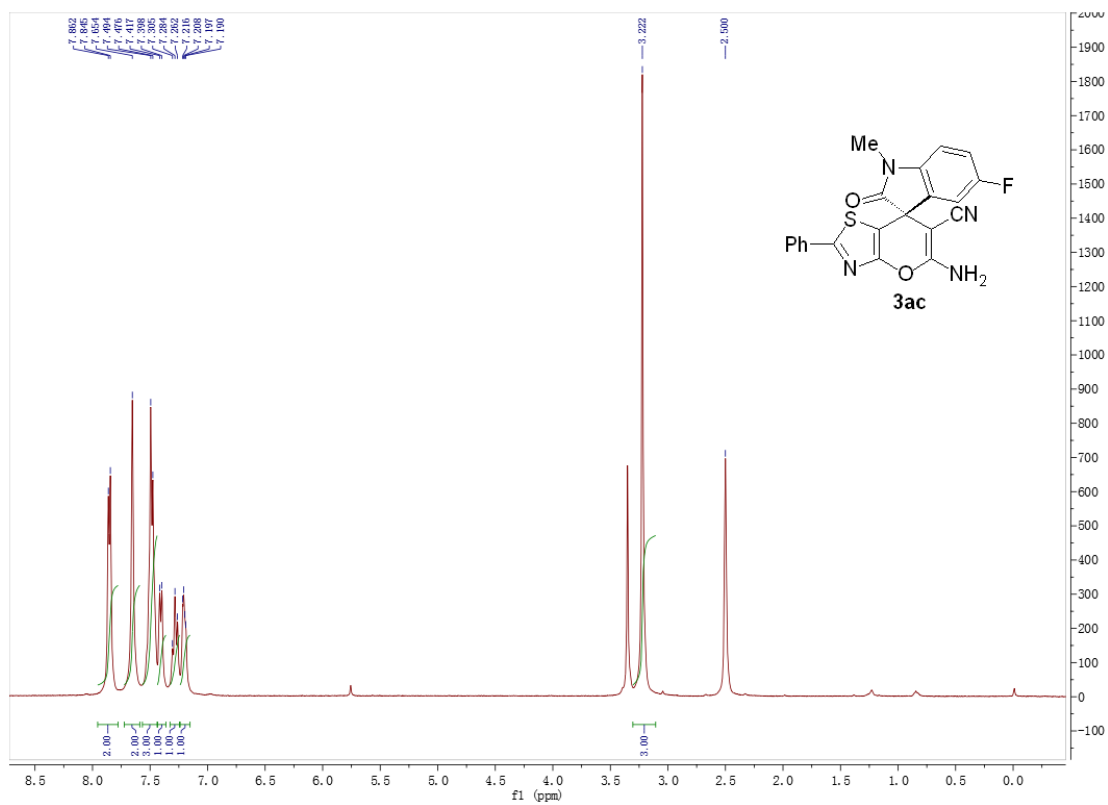
Largest diff. peak and hole

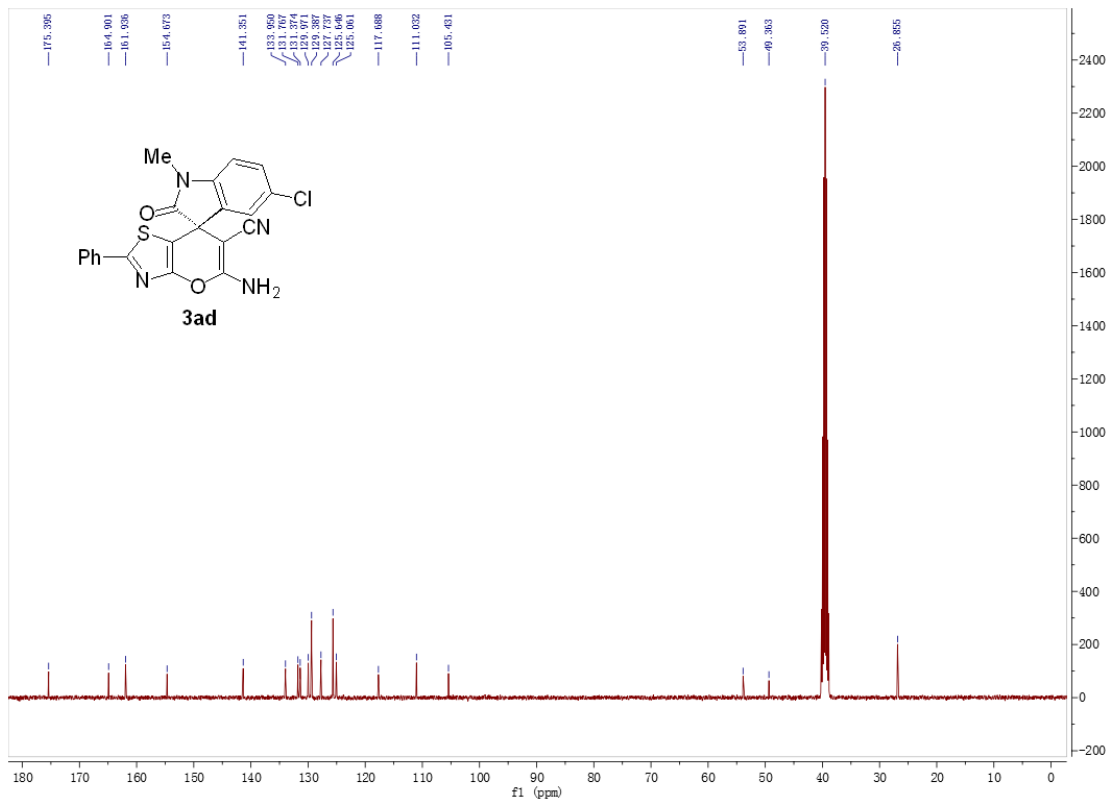
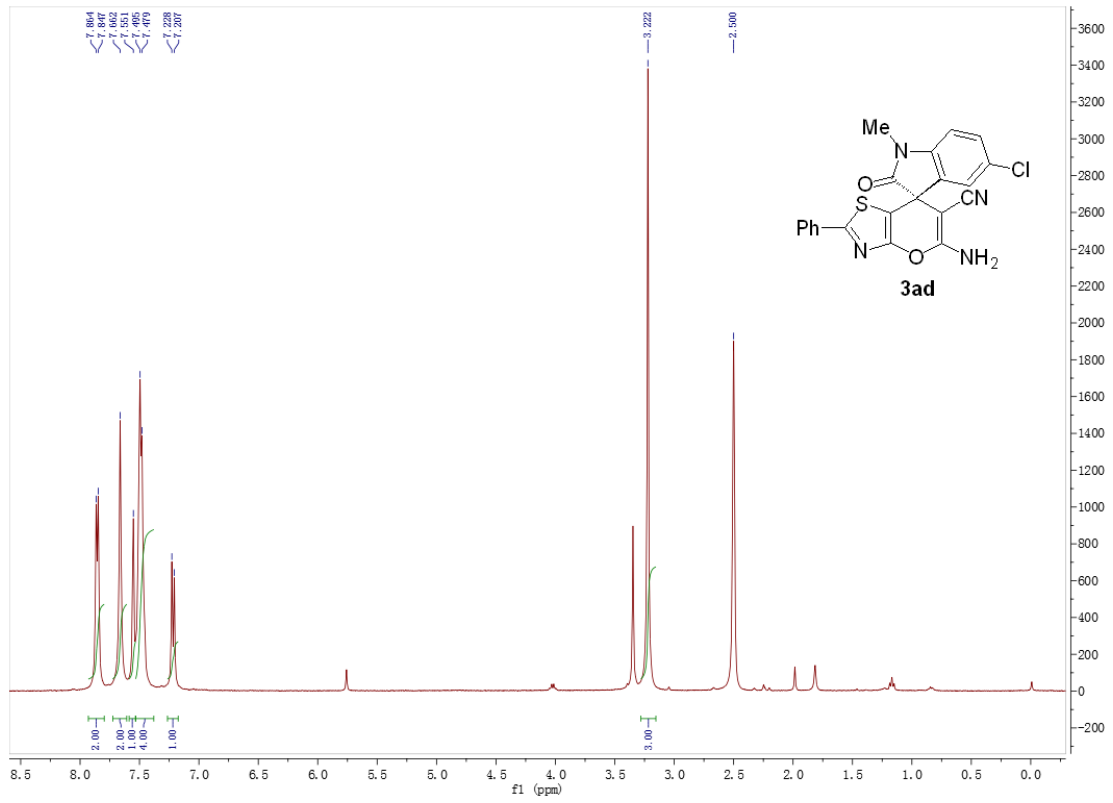
1.111 and -0.667 e.A⁻³

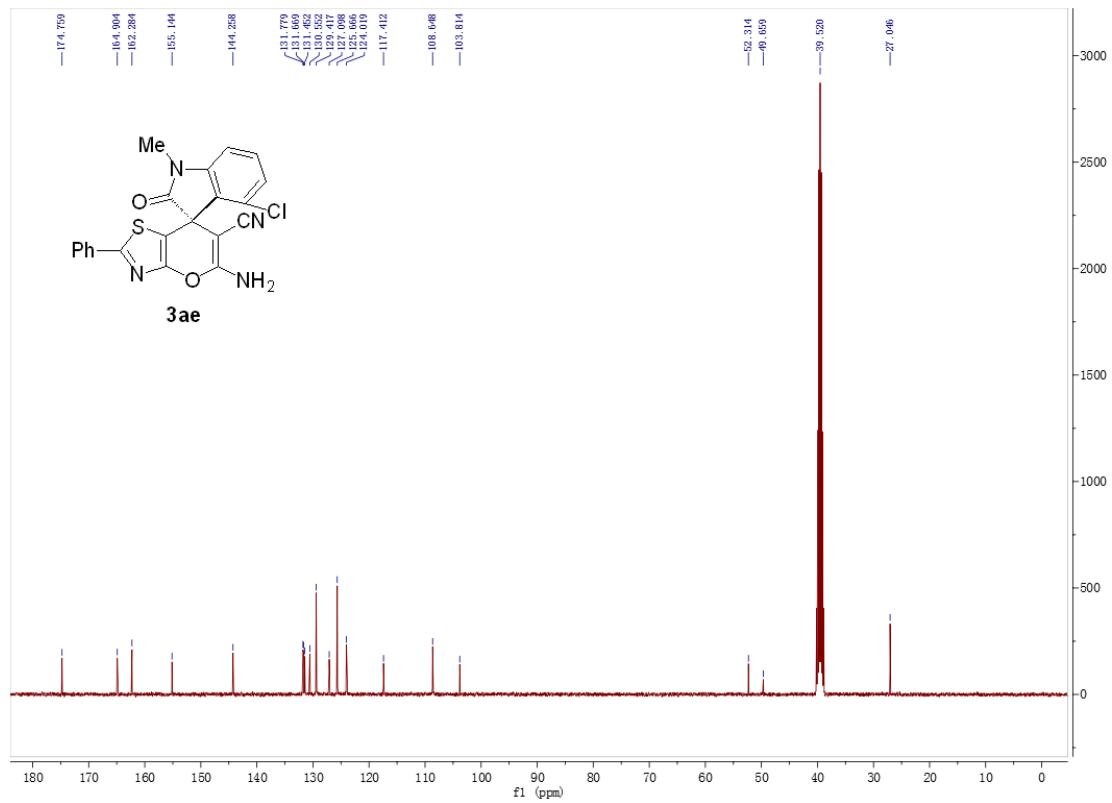
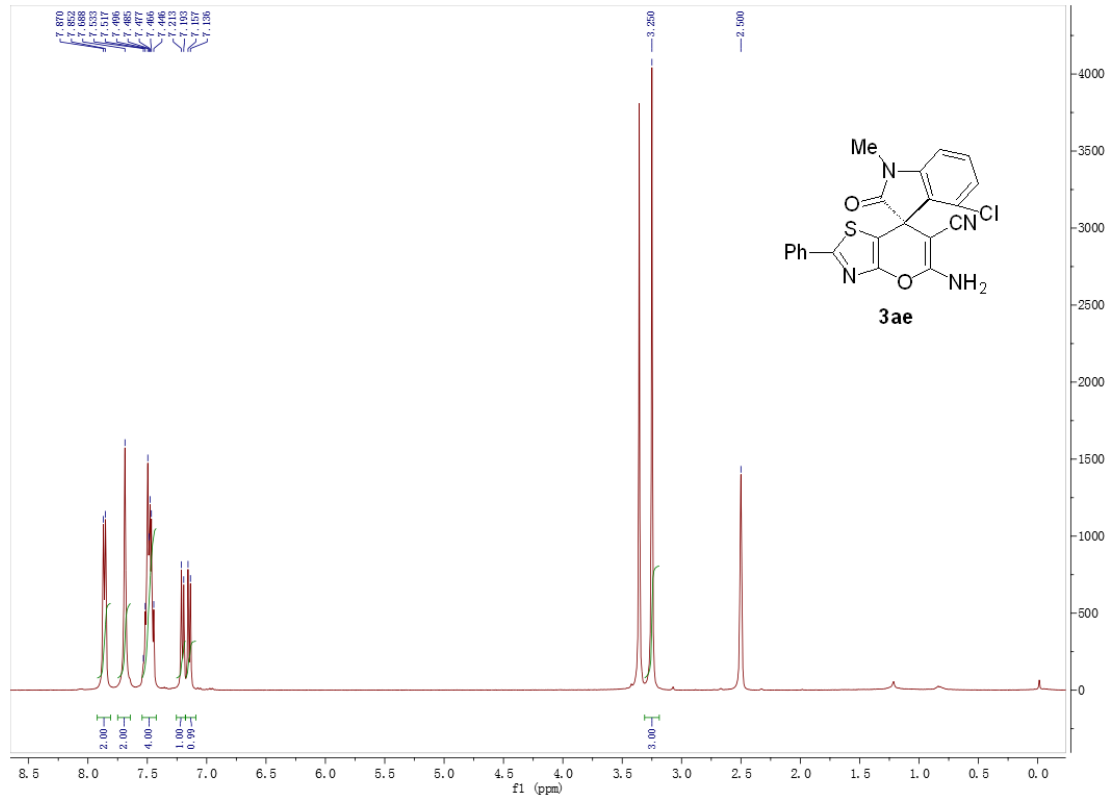
2. Copies of ¹H and ¹³C NMR Spectra

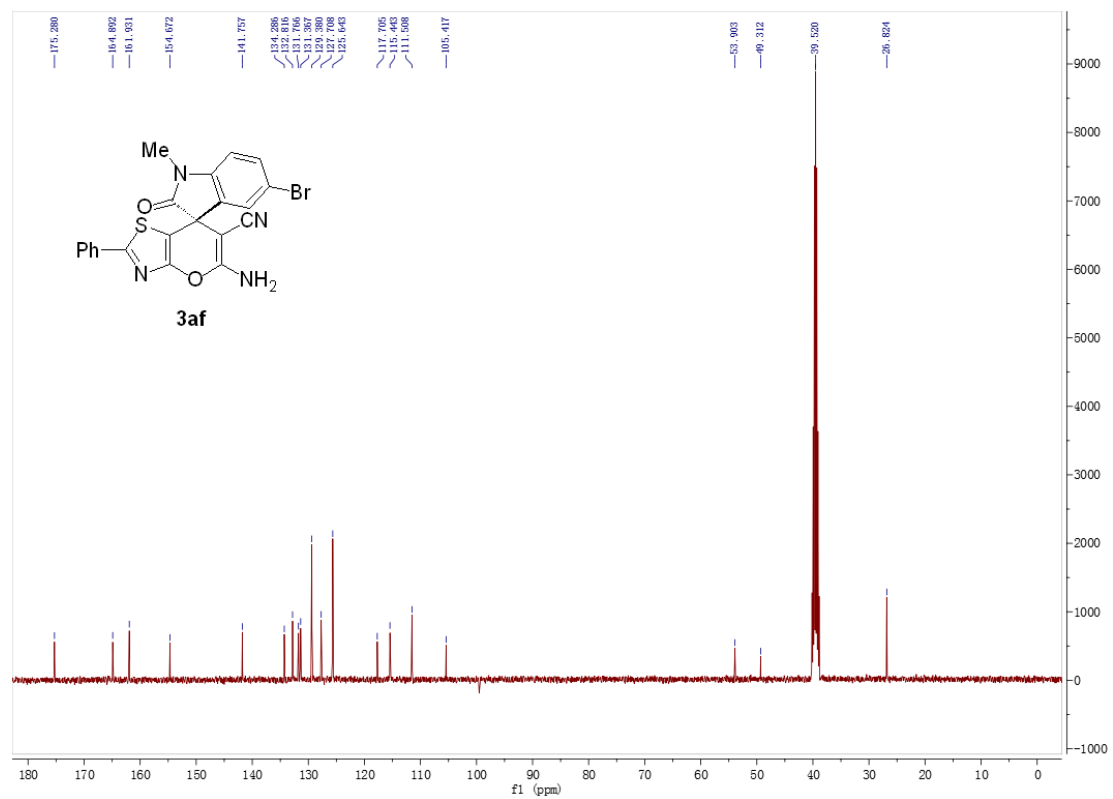
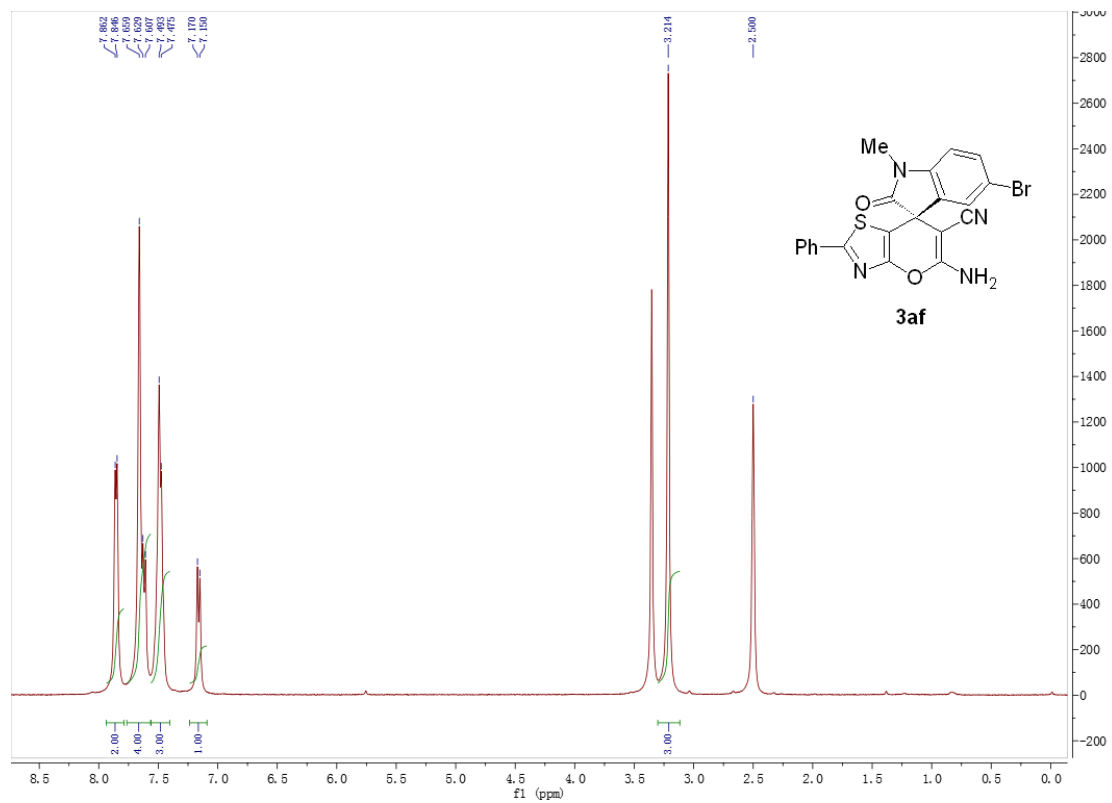


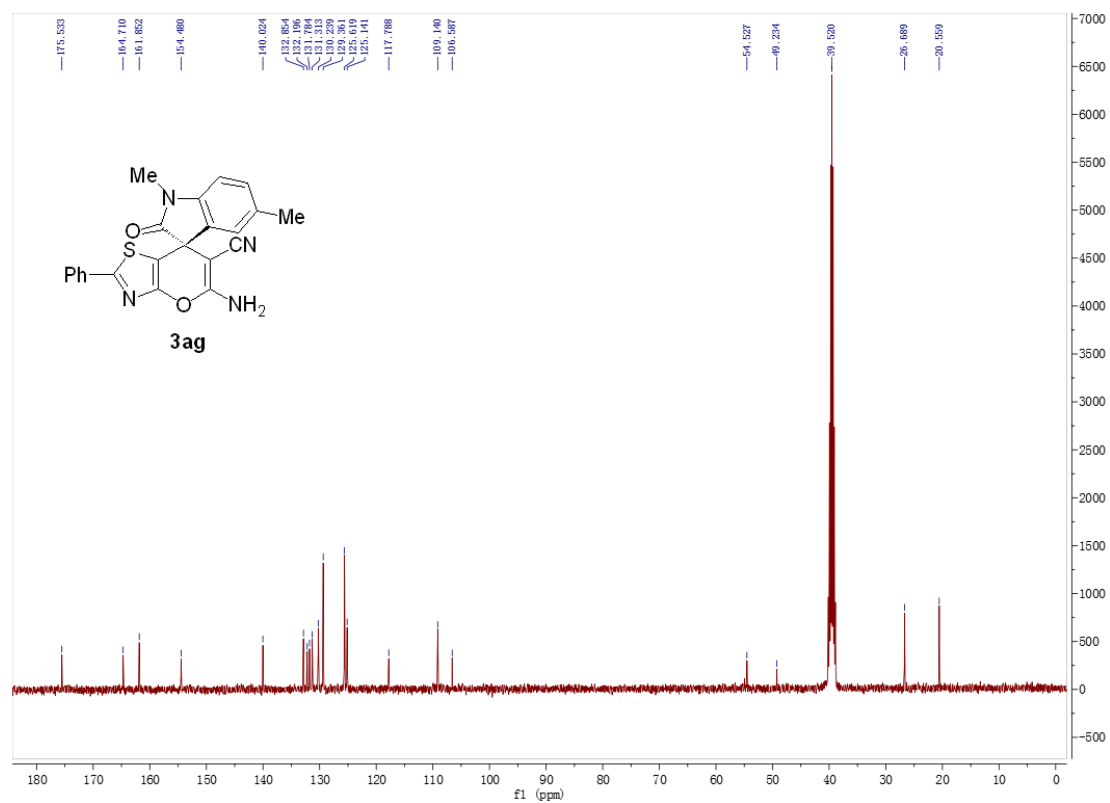
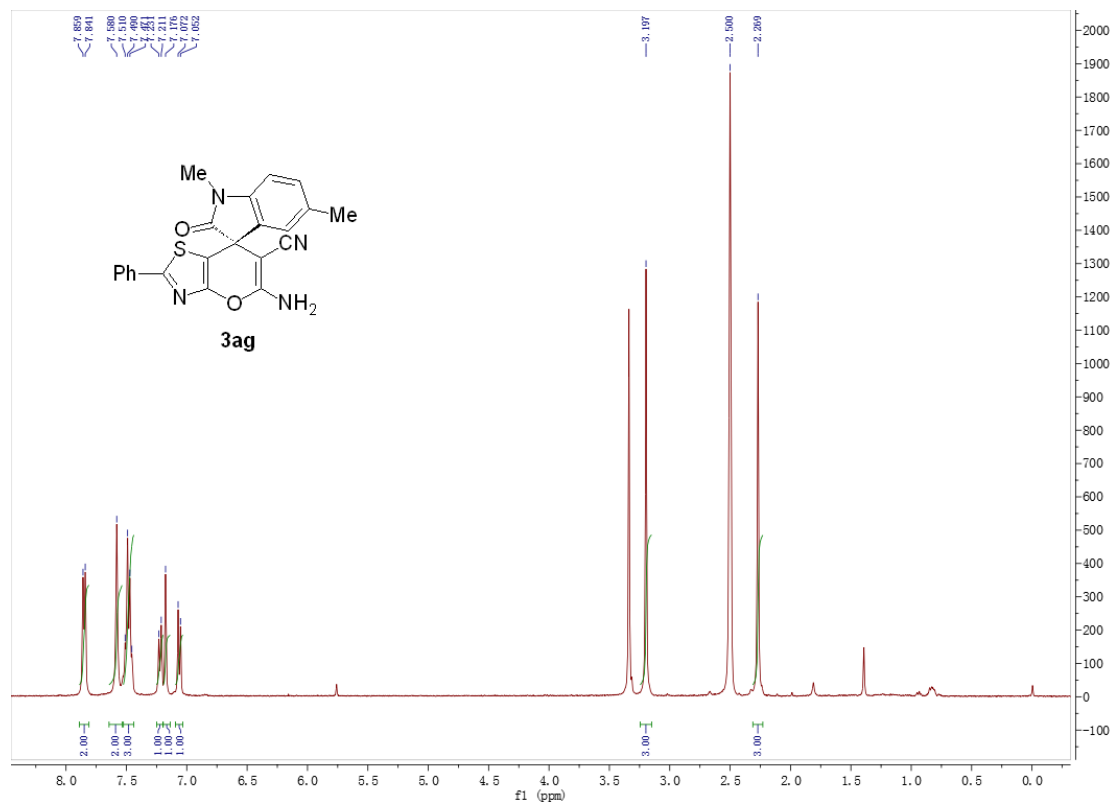


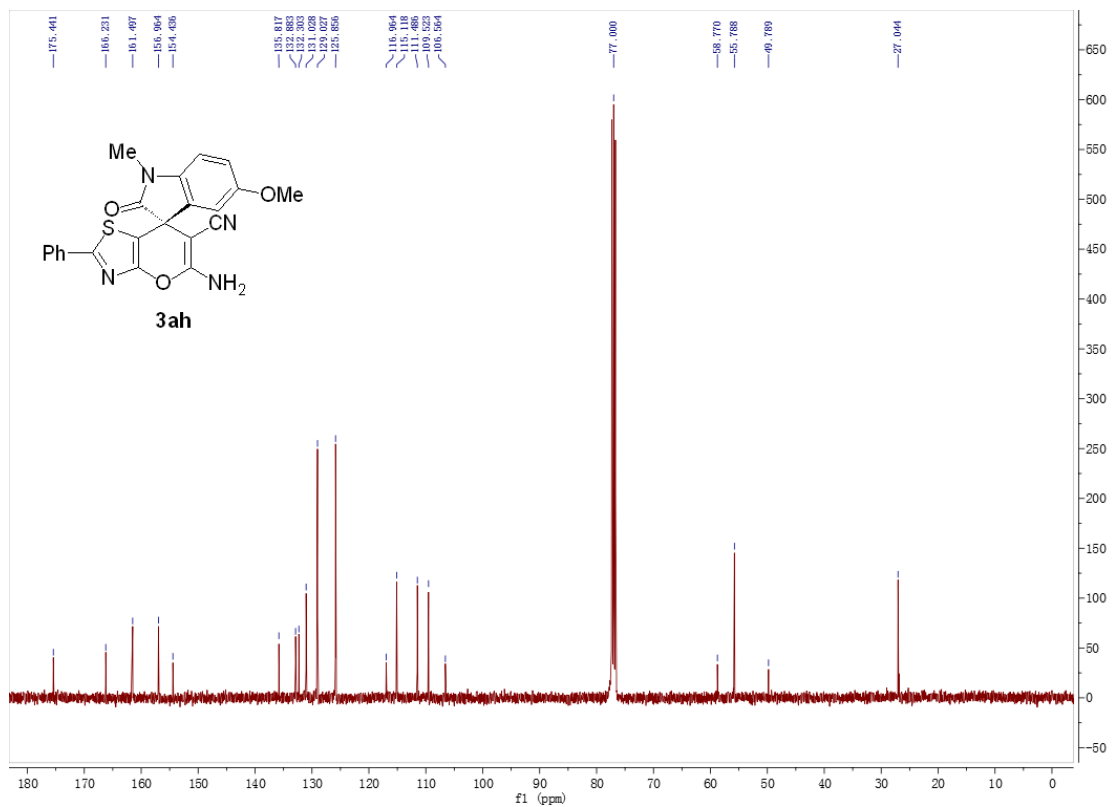
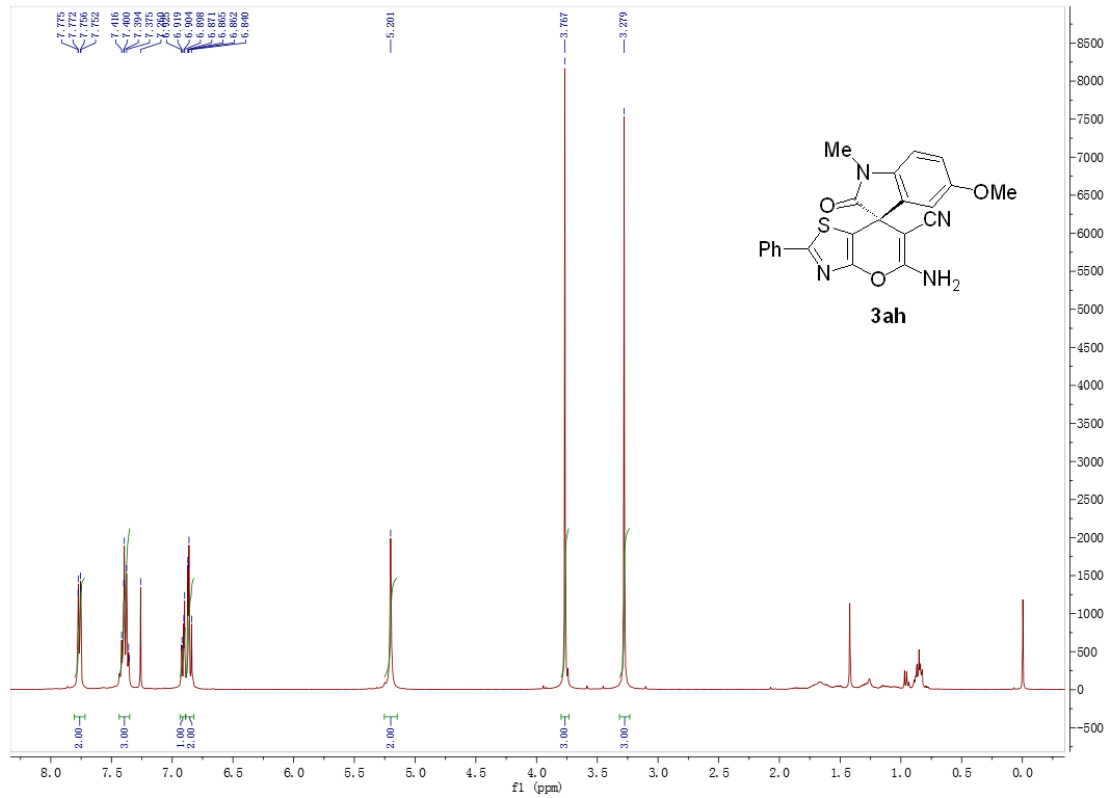


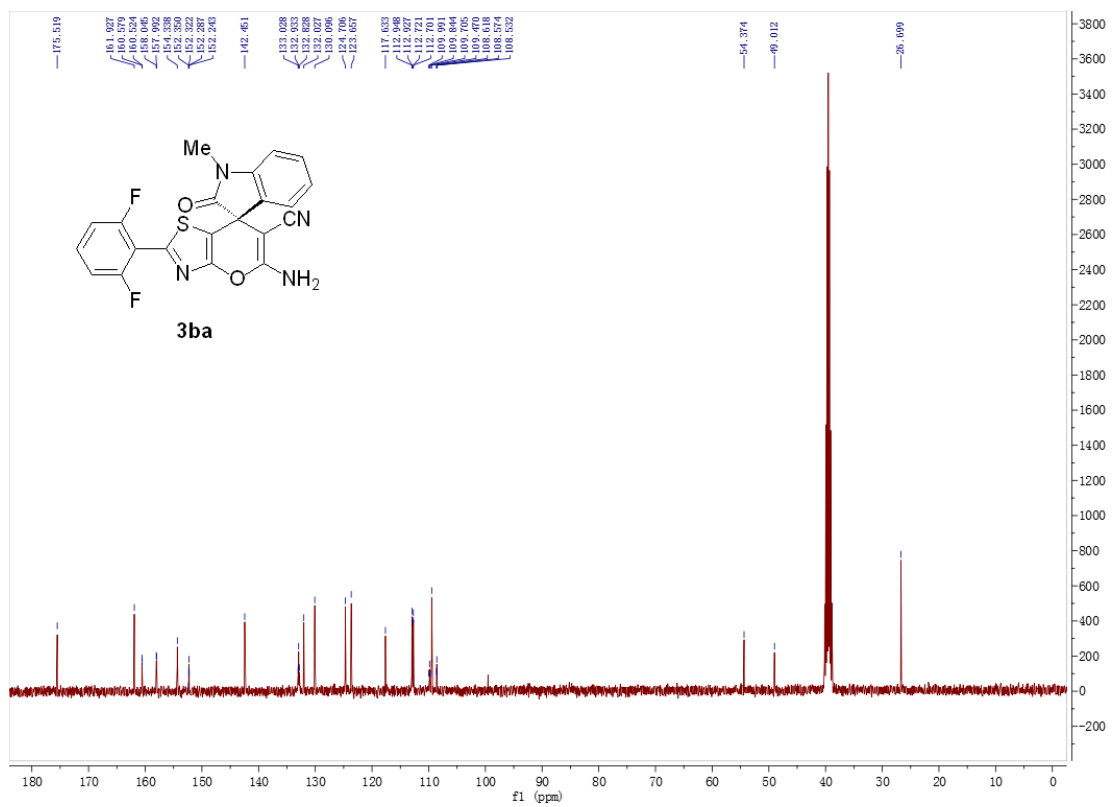
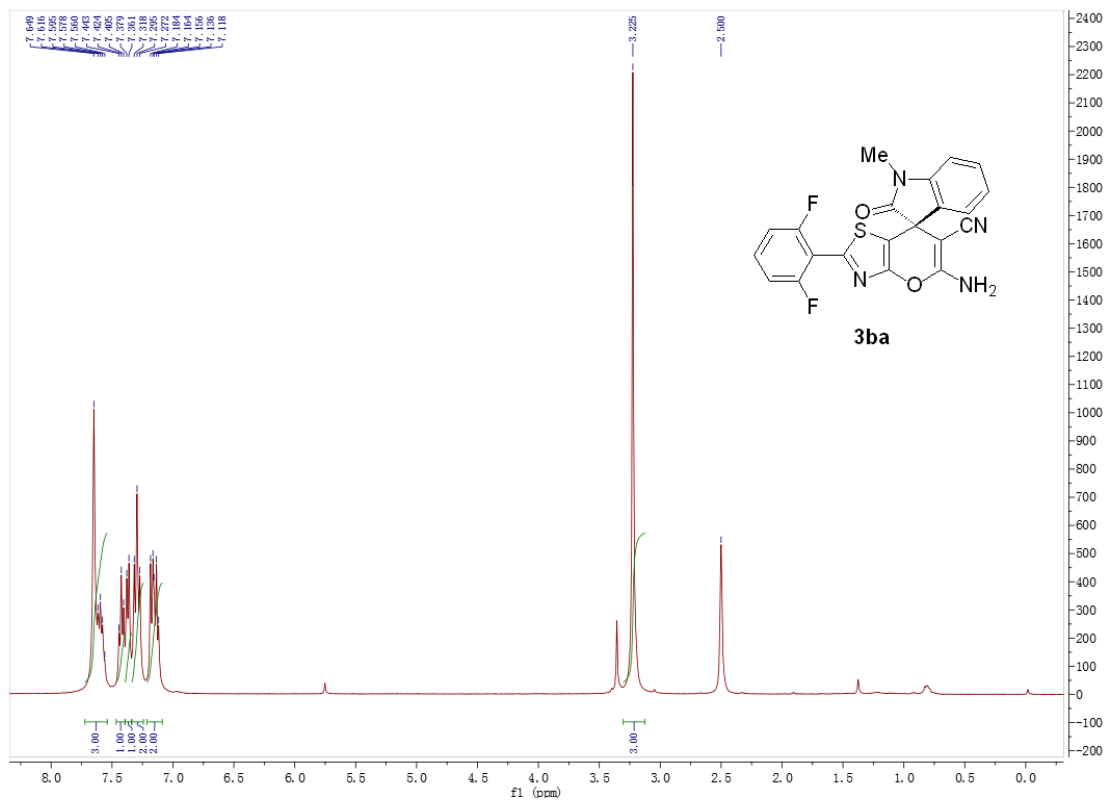


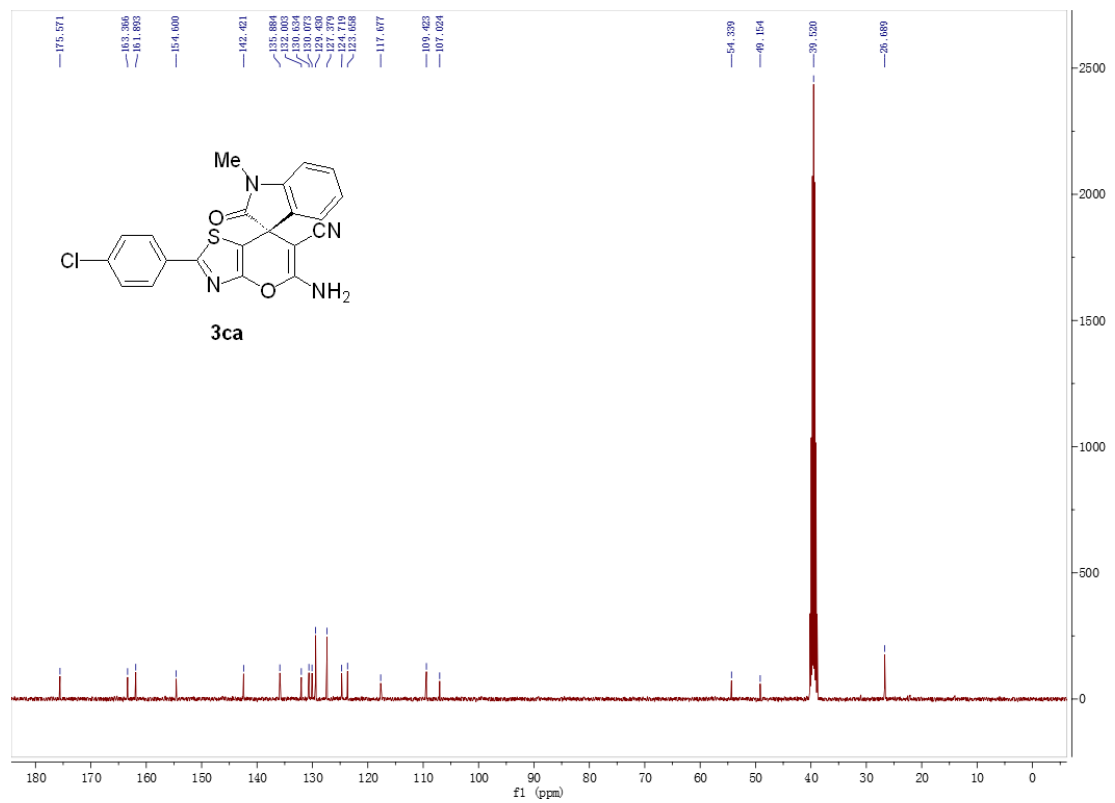
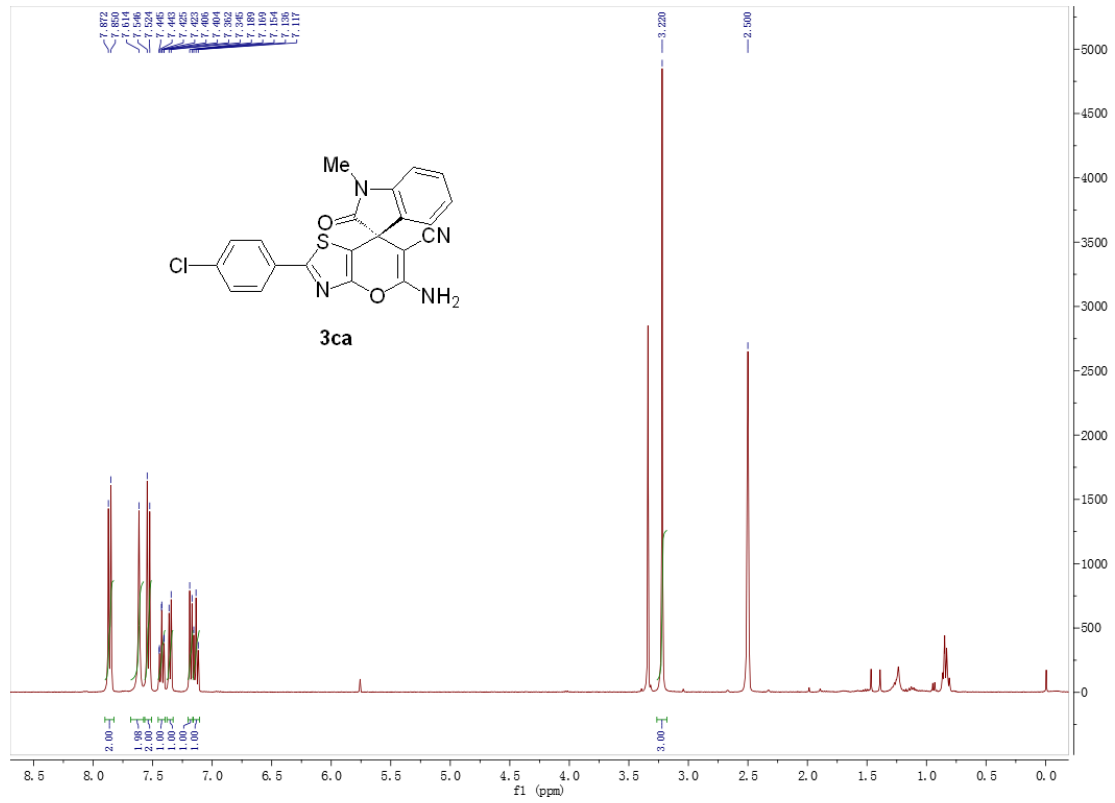


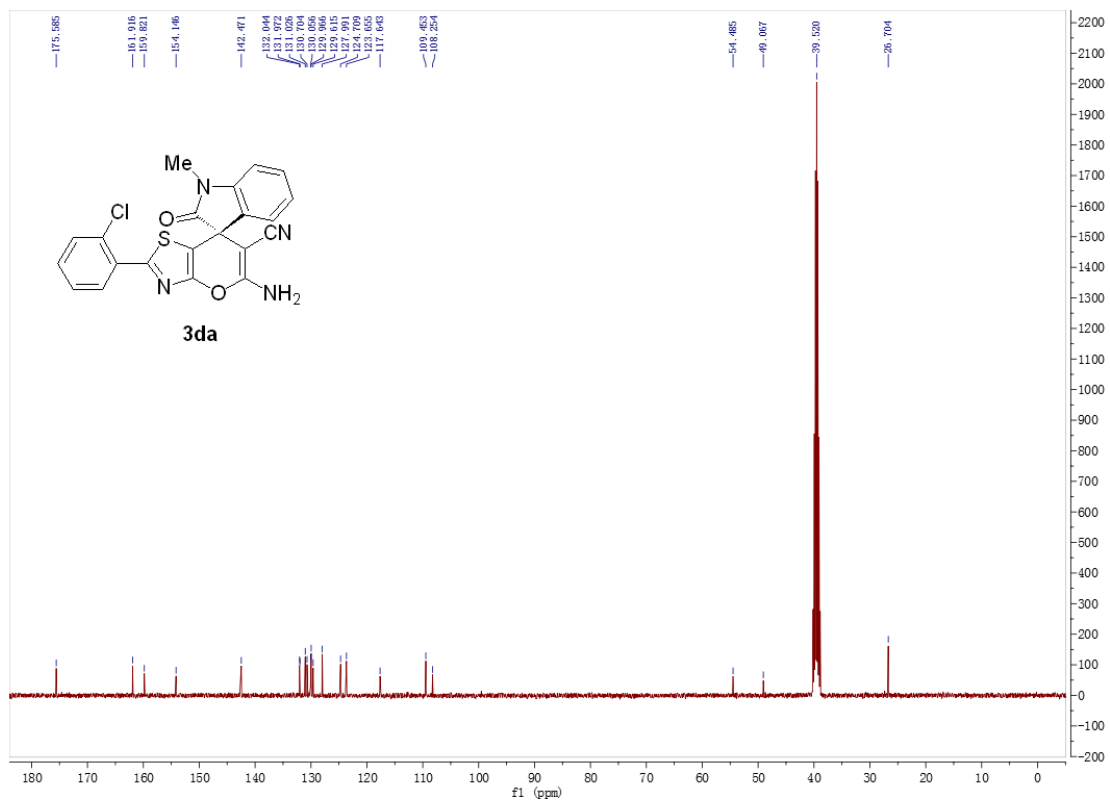
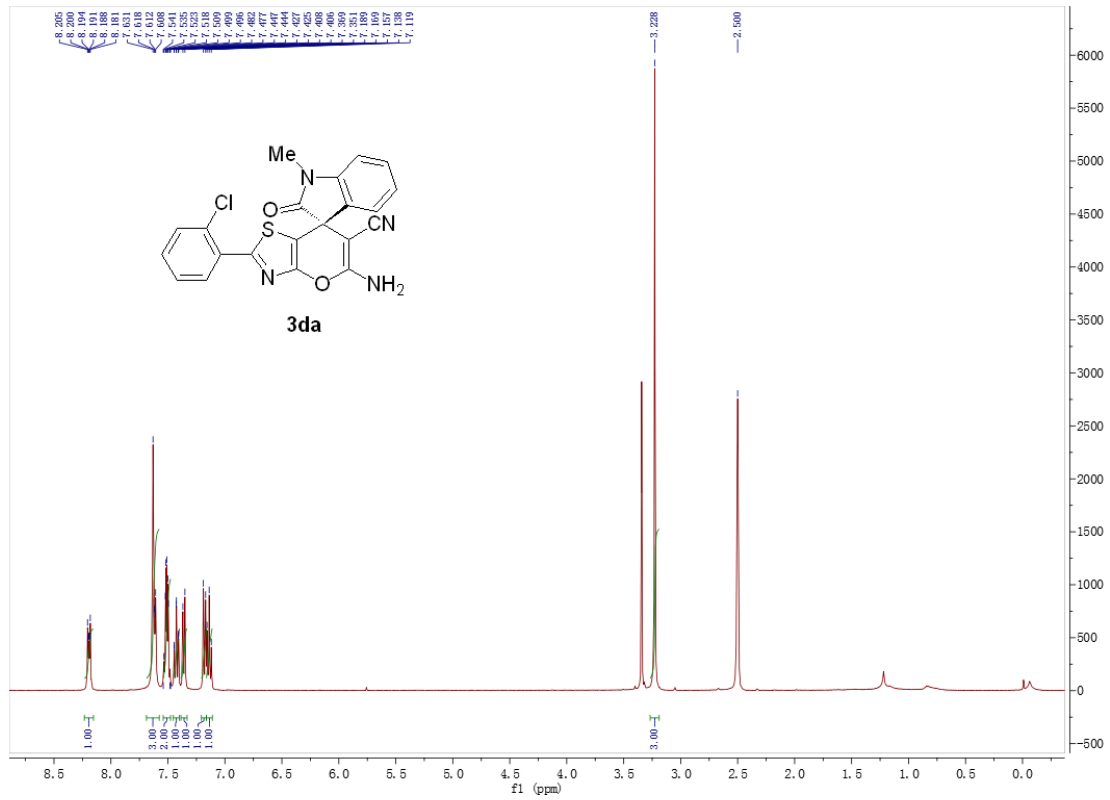


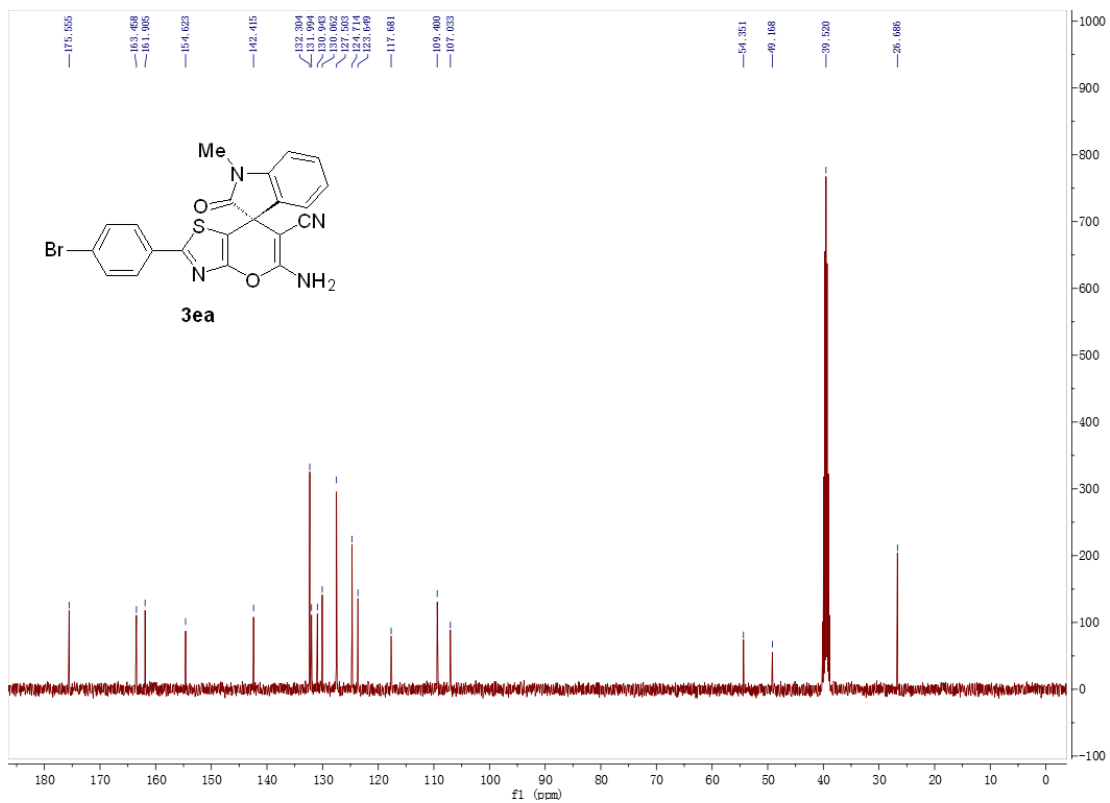
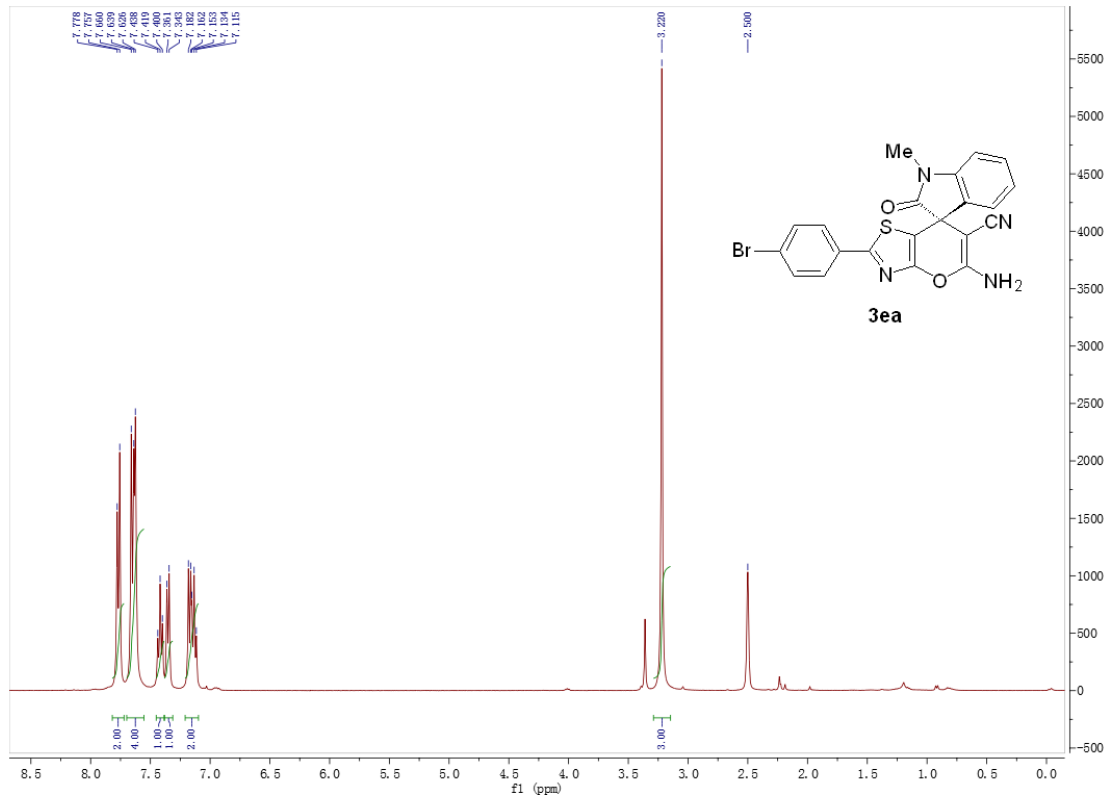


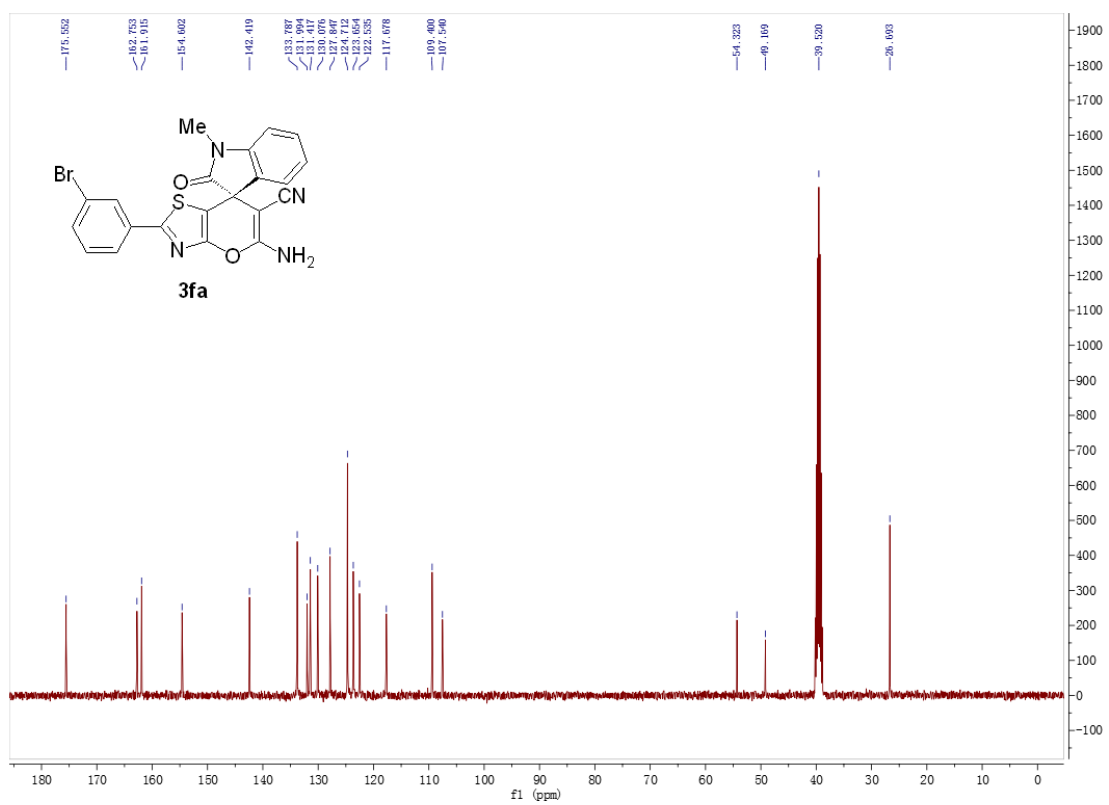
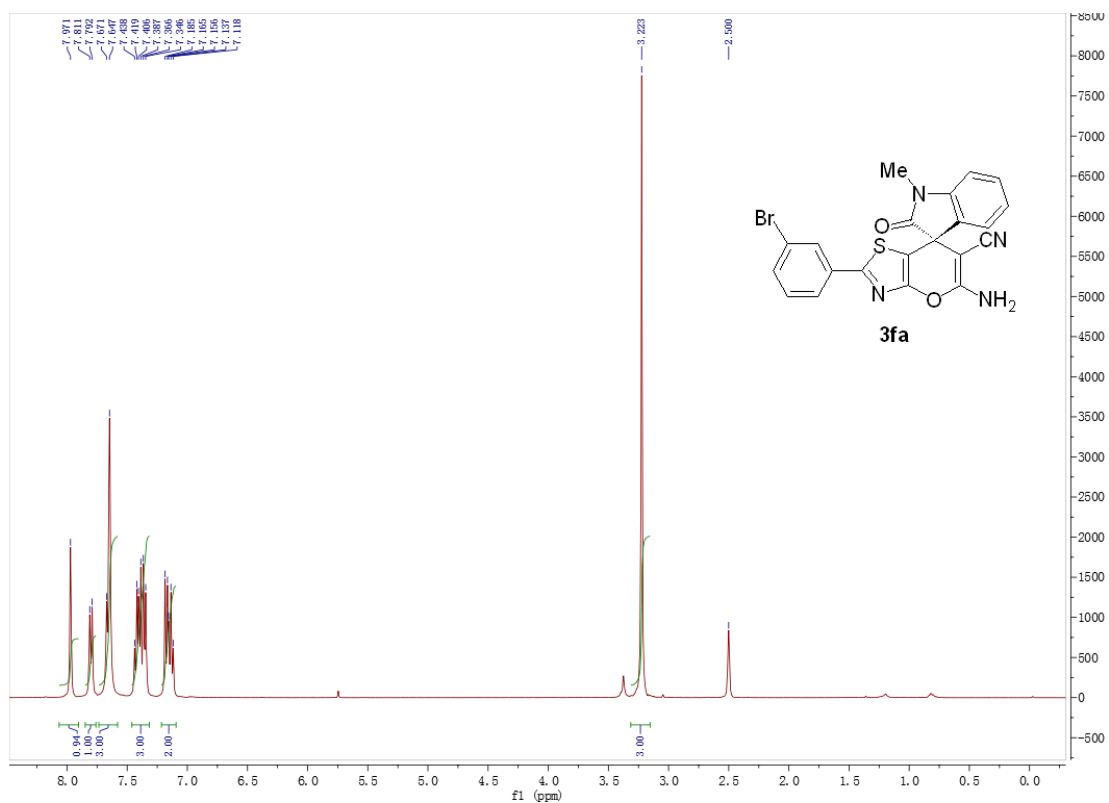


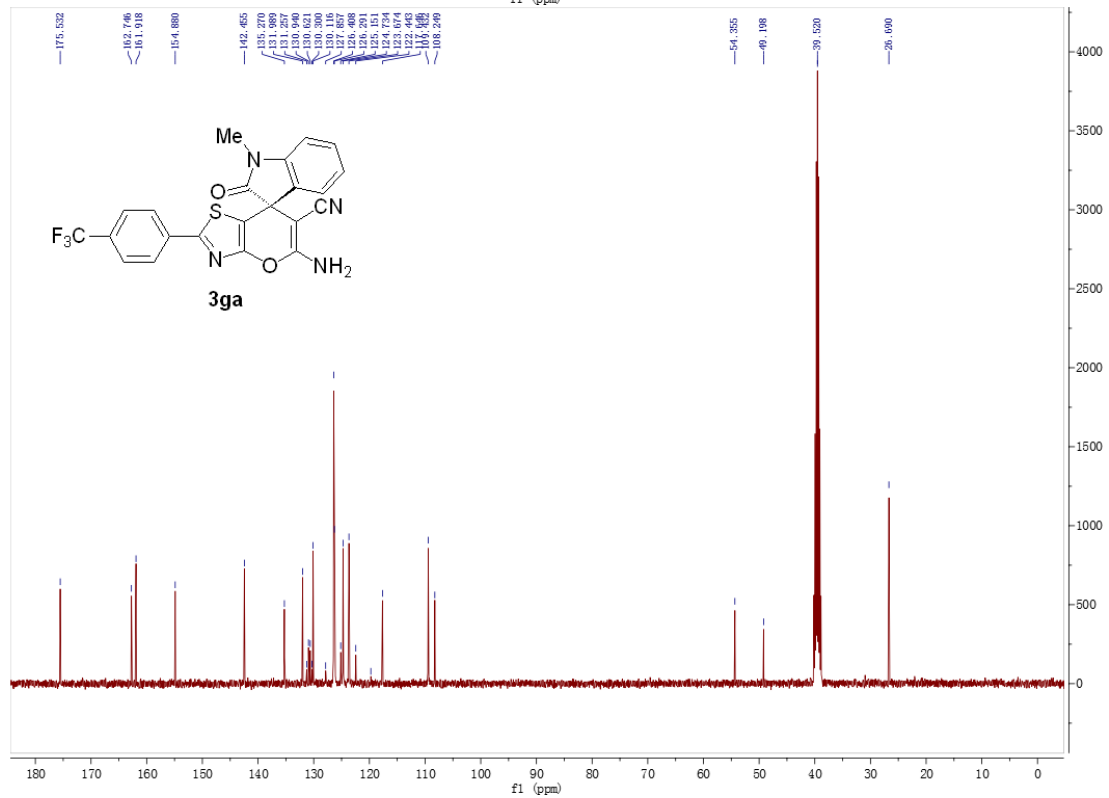
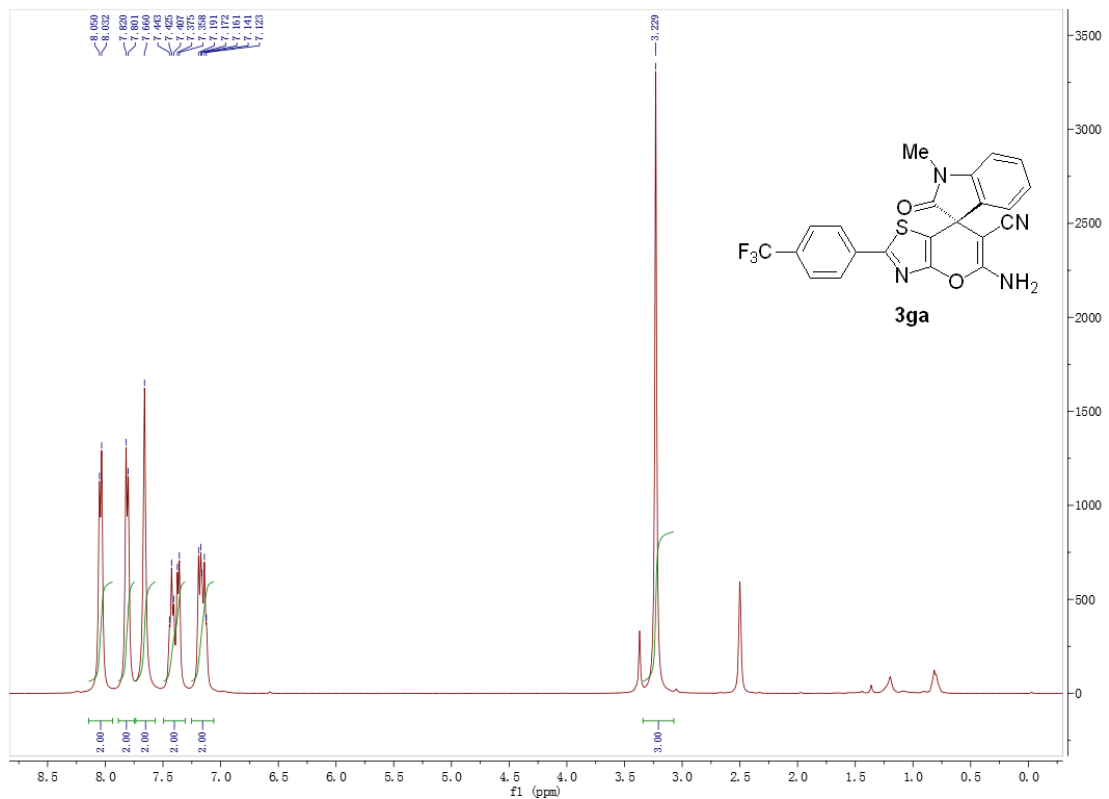


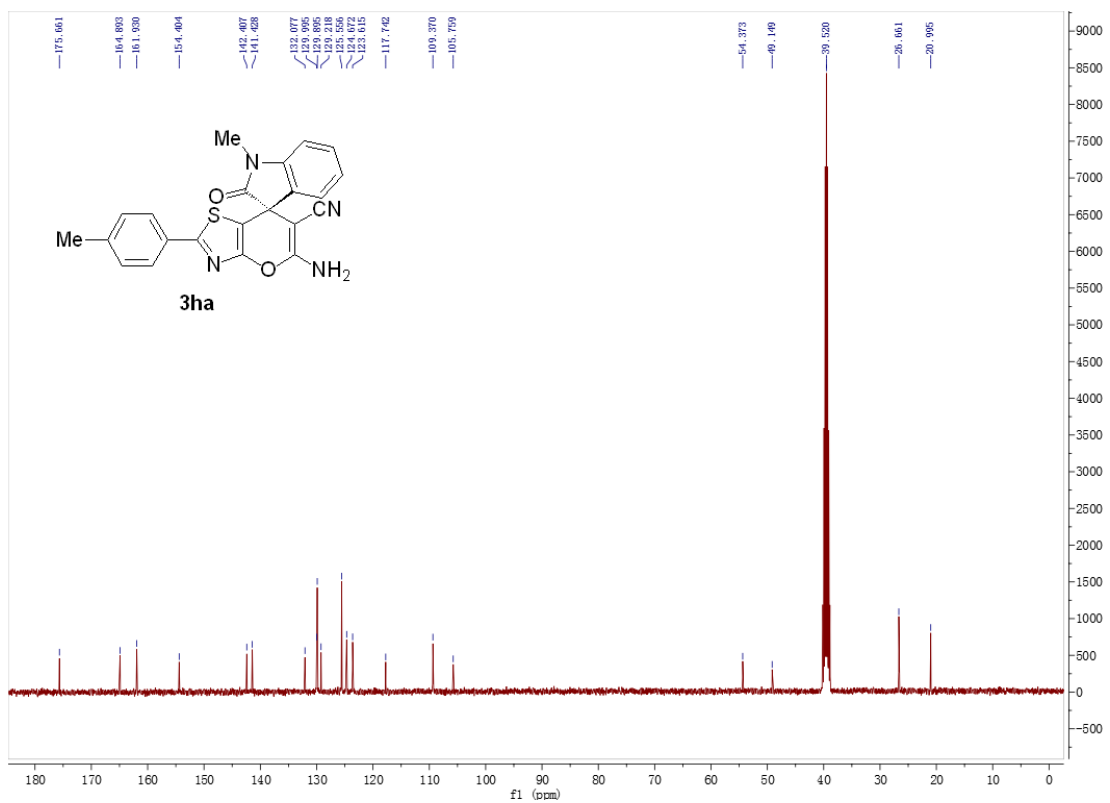
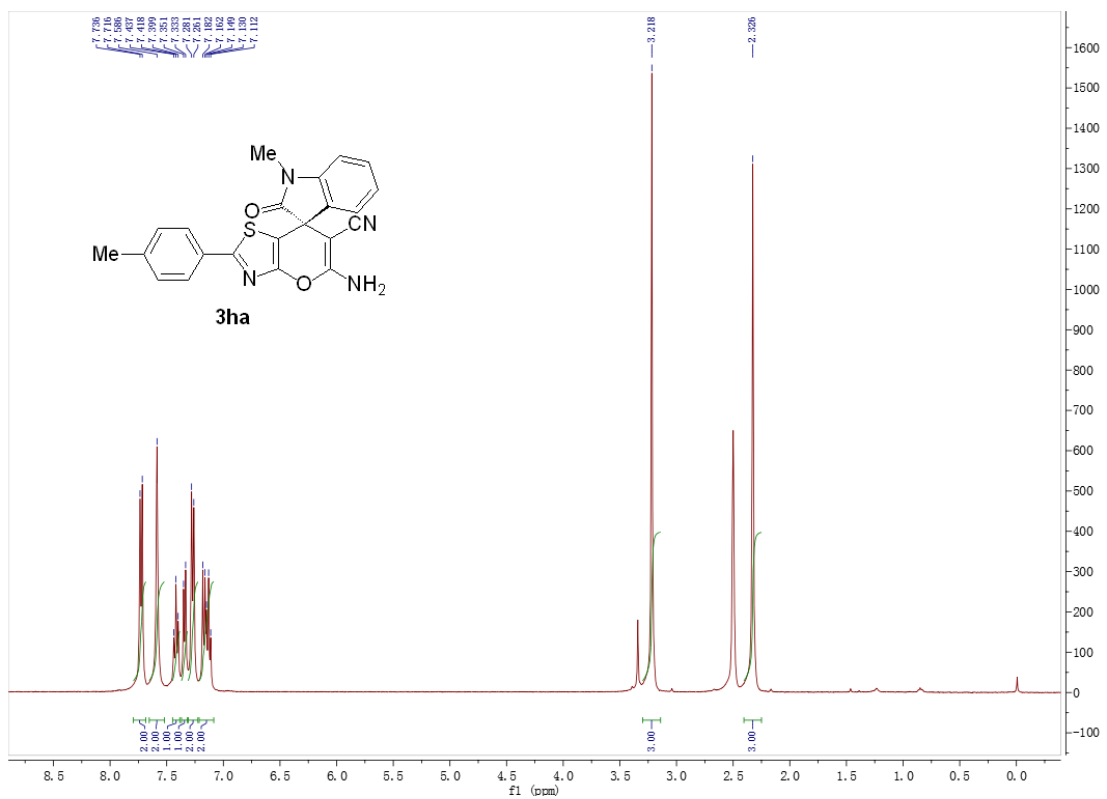


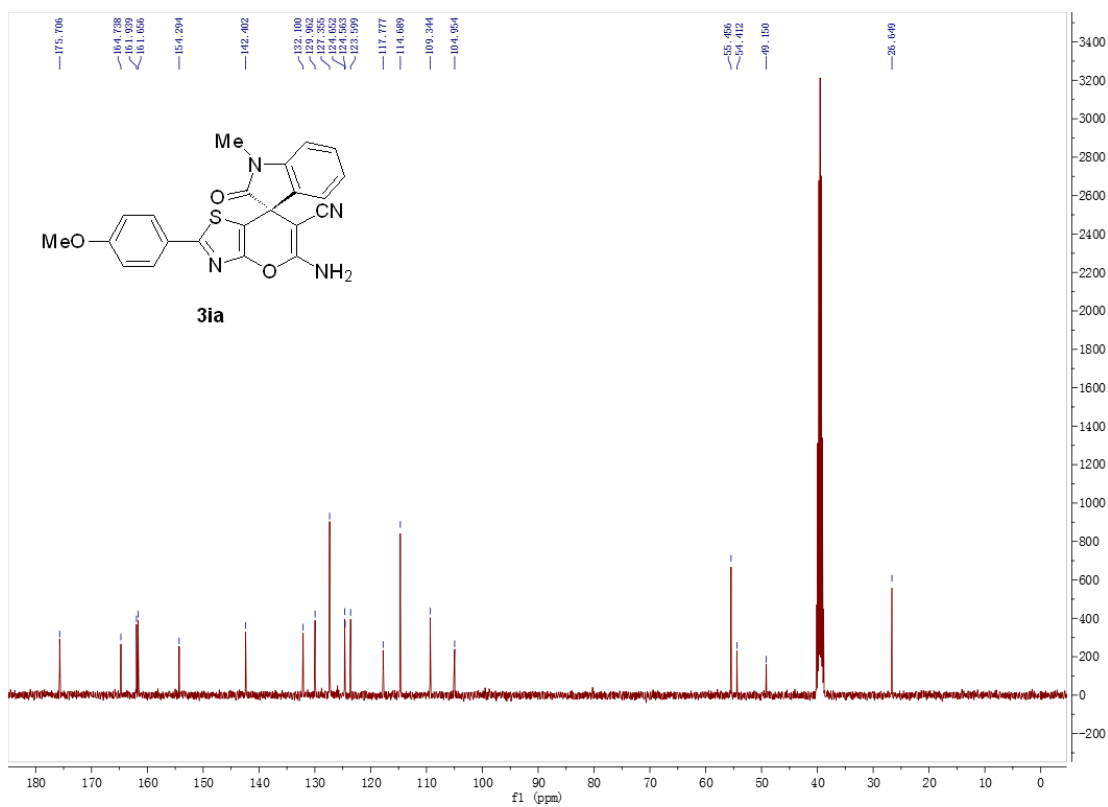
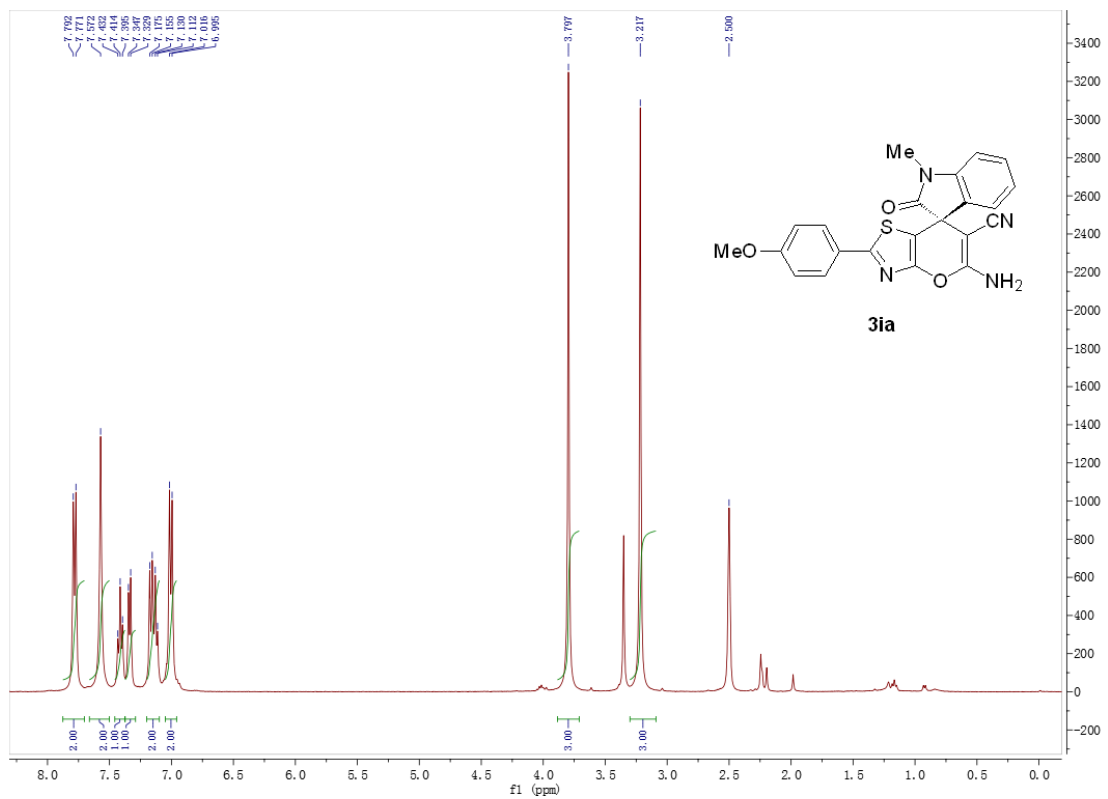


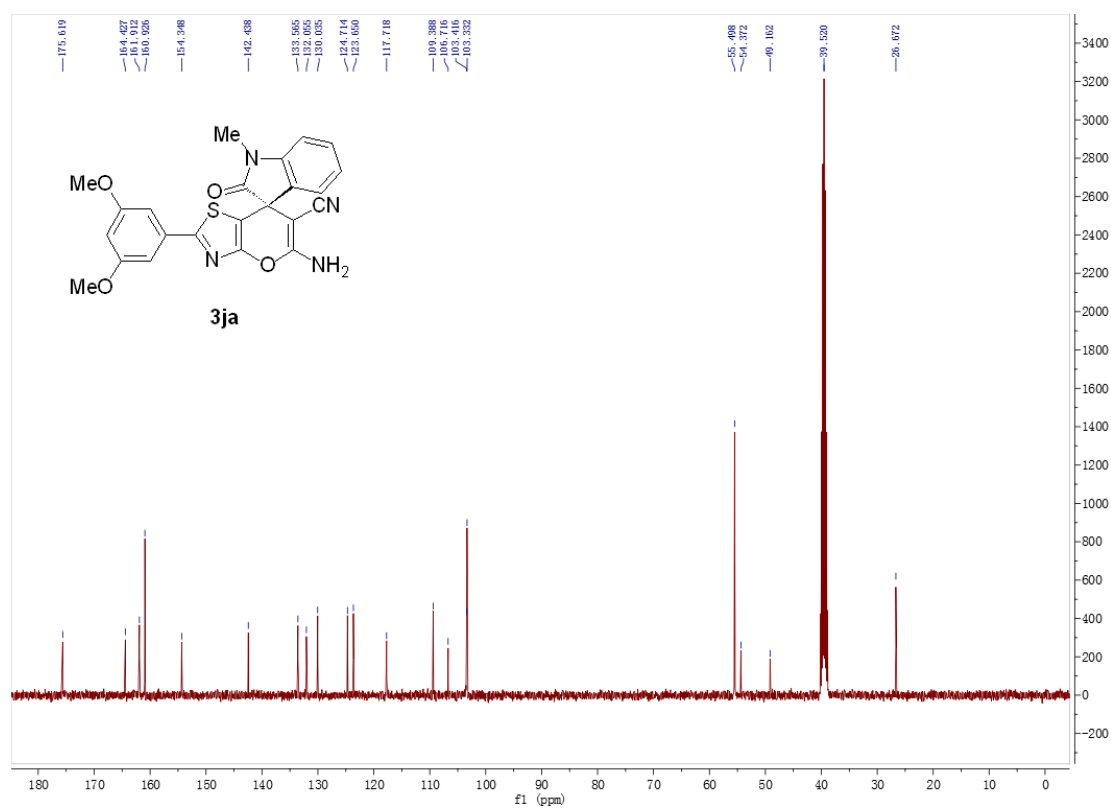
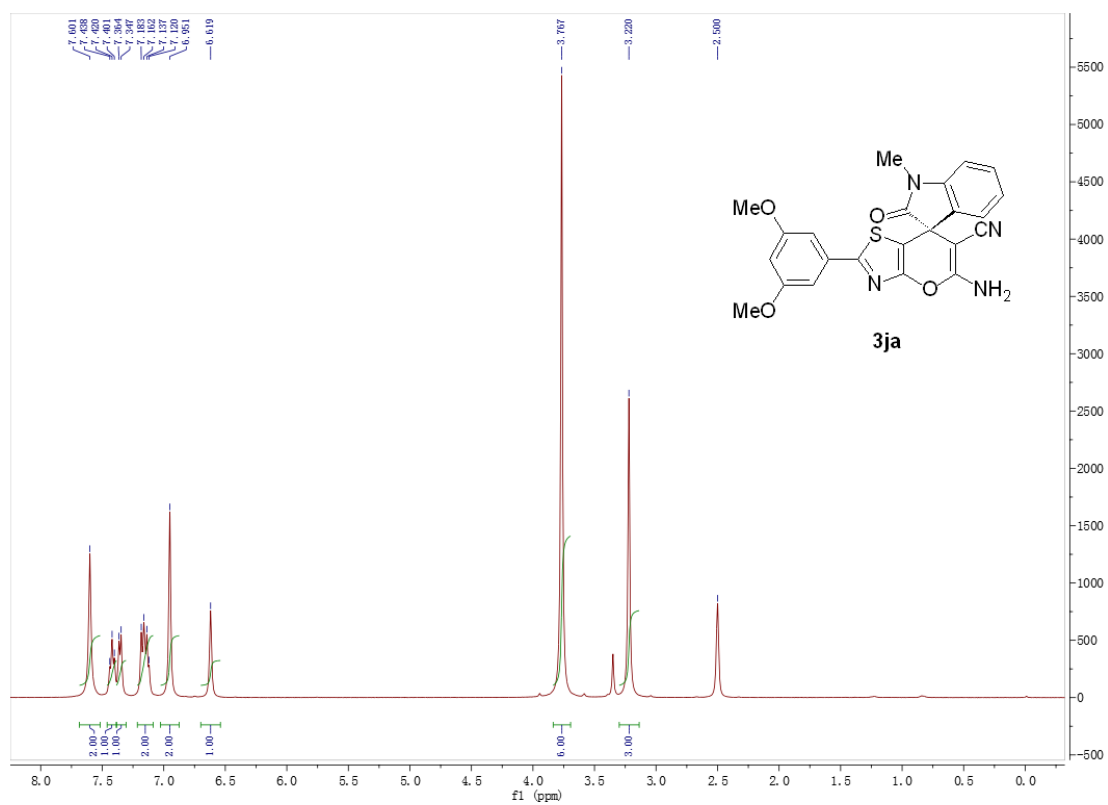






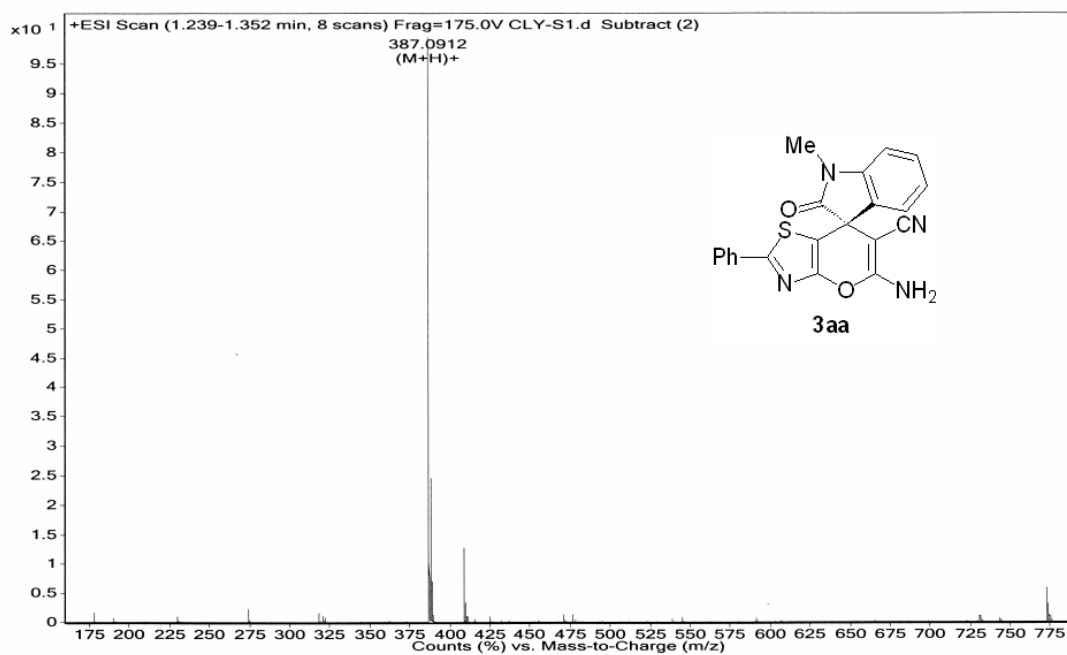




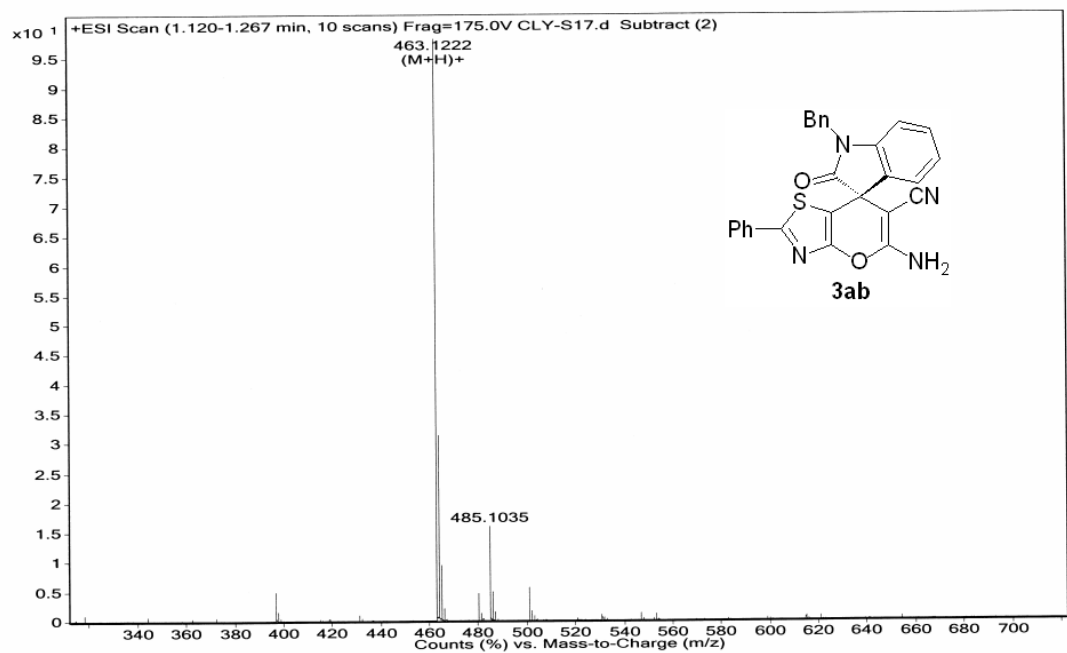


3. Copies of HRMS Spectra

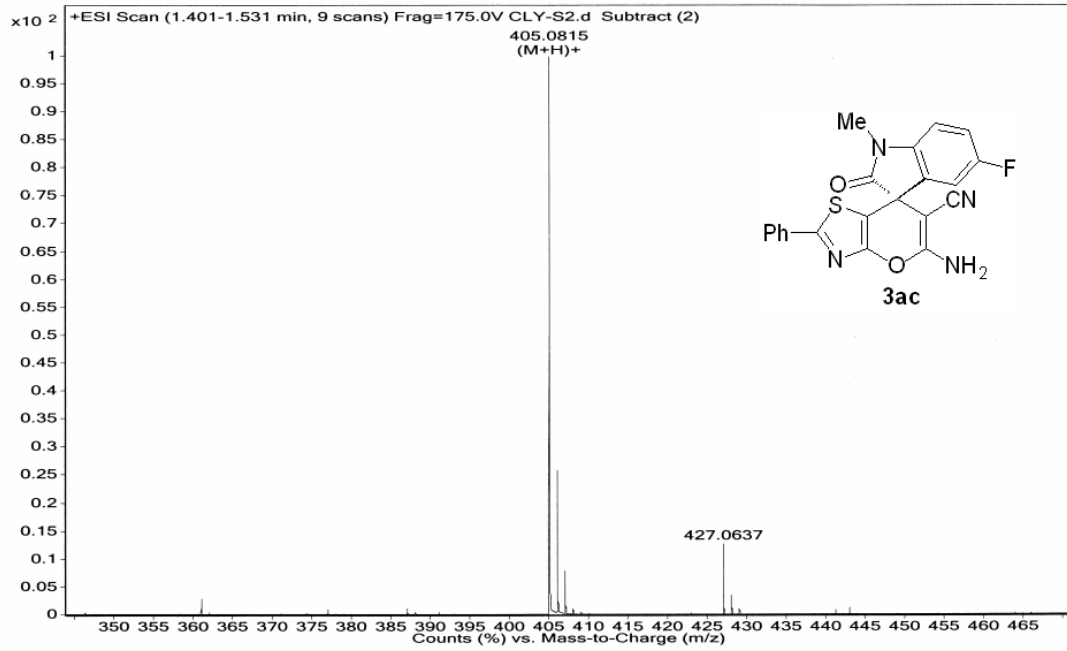
Sample Name	Sample55	Position	P2-A1	Instrument Name	Instrument 1	User Name	
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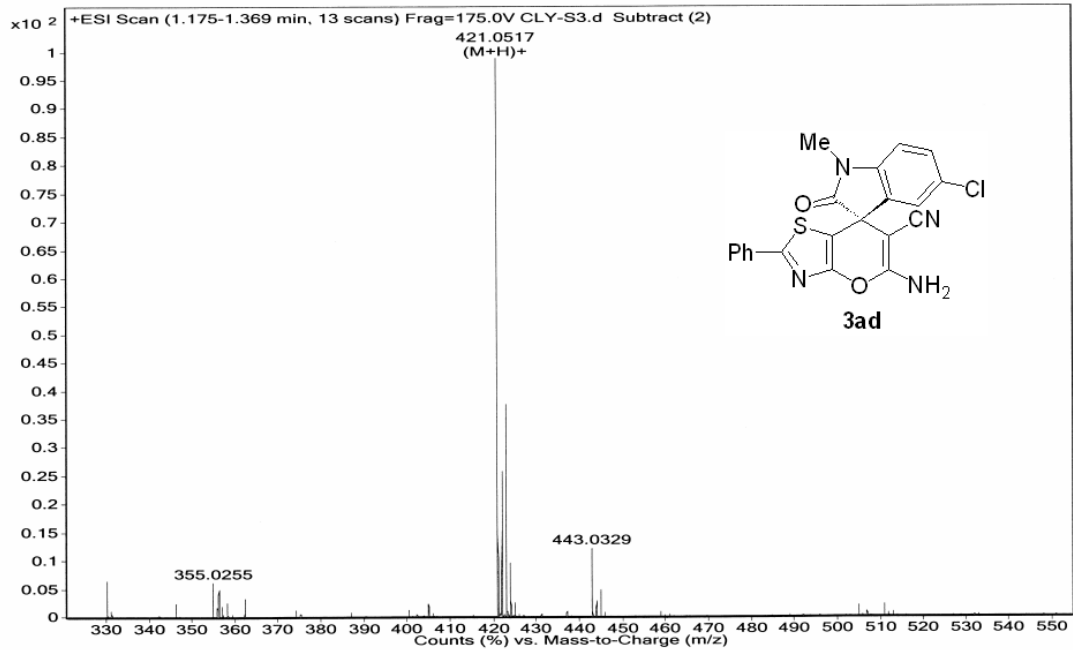
Sample Name	Sample71	Position	P2-B8	Instrument Name	Instrument 1	User Name	
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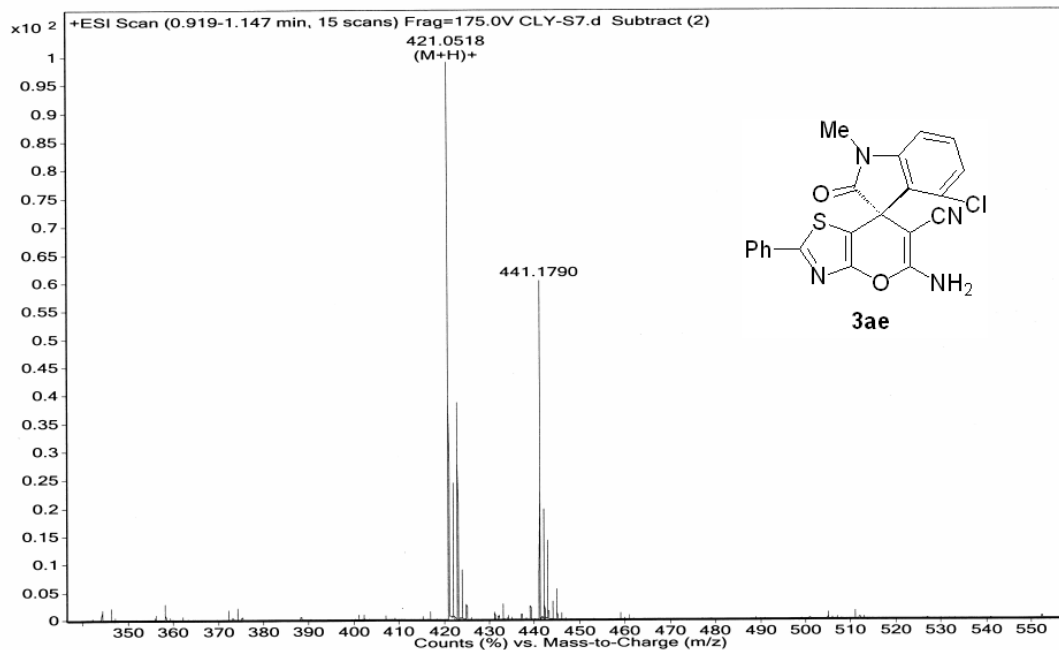
Sample Name	Sample56	Position	P2-A2	Instrument Name	Instrument 1	User Name	
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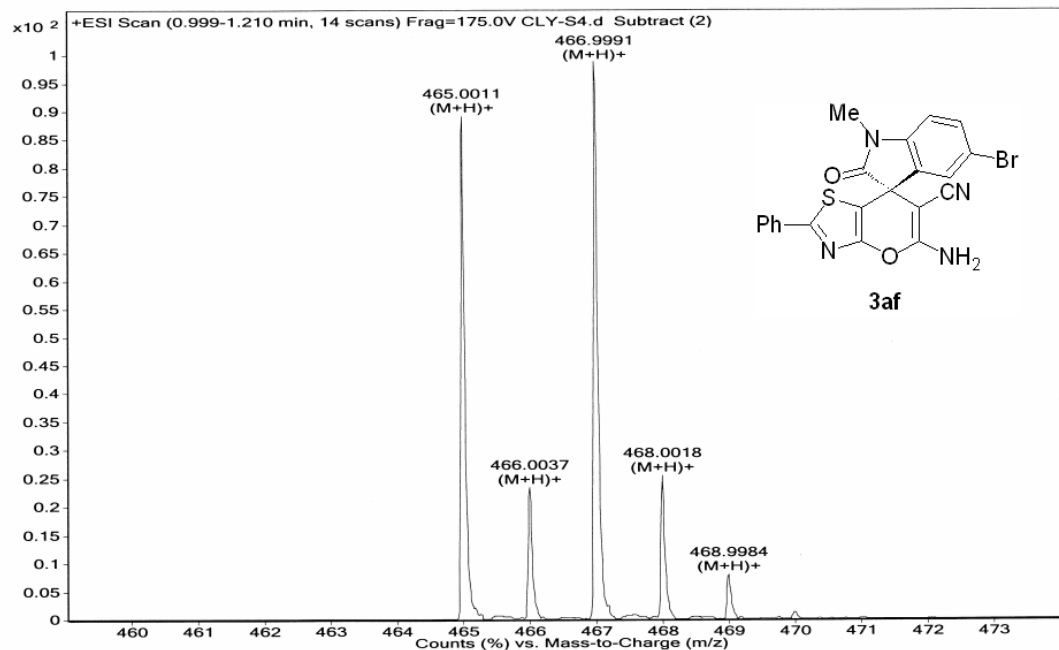
Sample Name	Sample57	Position	P2-A3	Instrument Name	Instrument 1	User Name	
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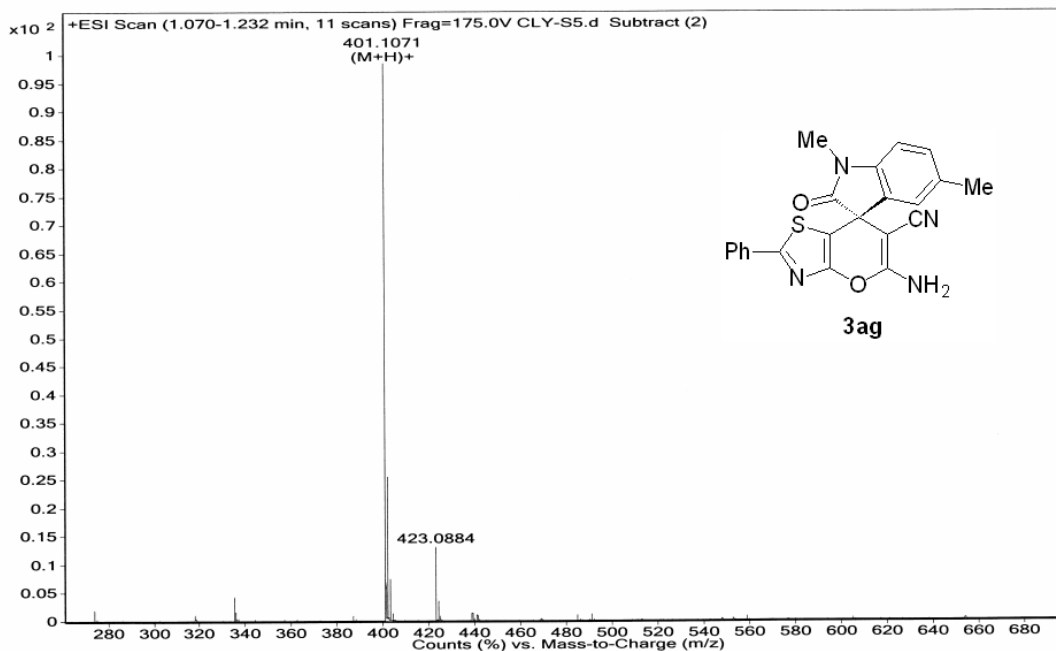
Sample Name	Sample61	Position	P2-A7	Instrument Name	Instrument 1	User Name	
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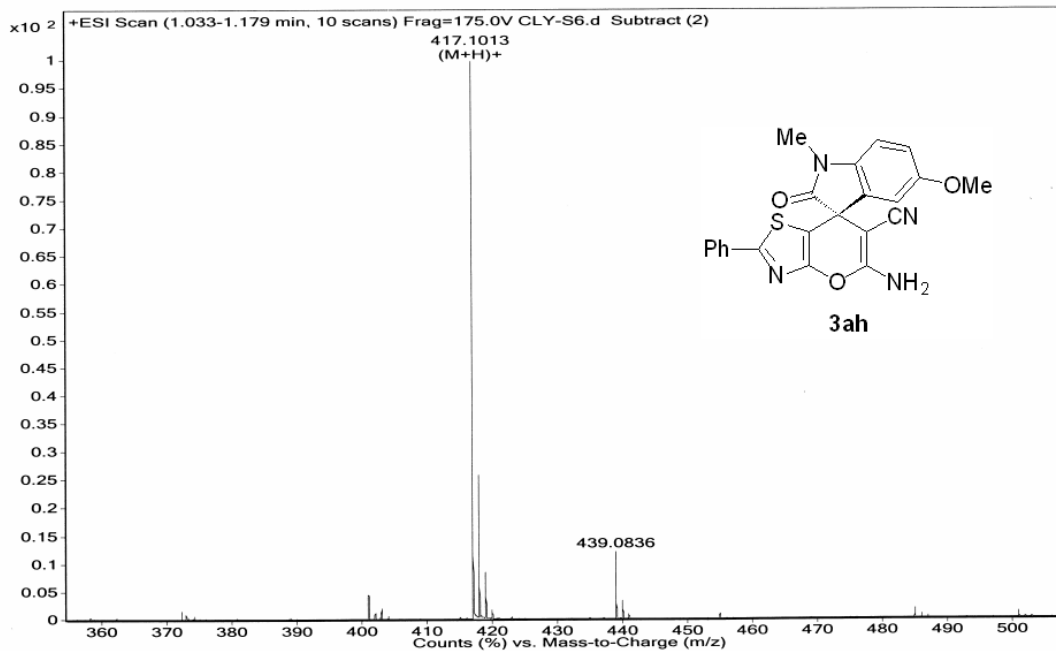
Sample Name	Sample58	Position	P2-A4	Instrument Name	Instrument 1	User Name	
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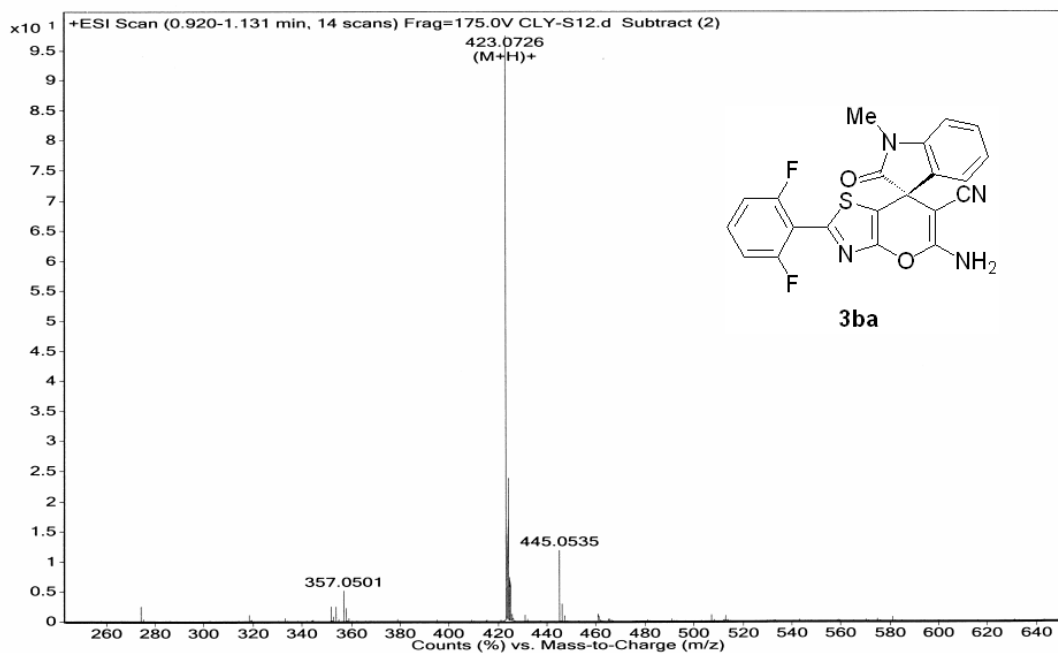
Sample Name	Sample59	Position	P2-A5	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
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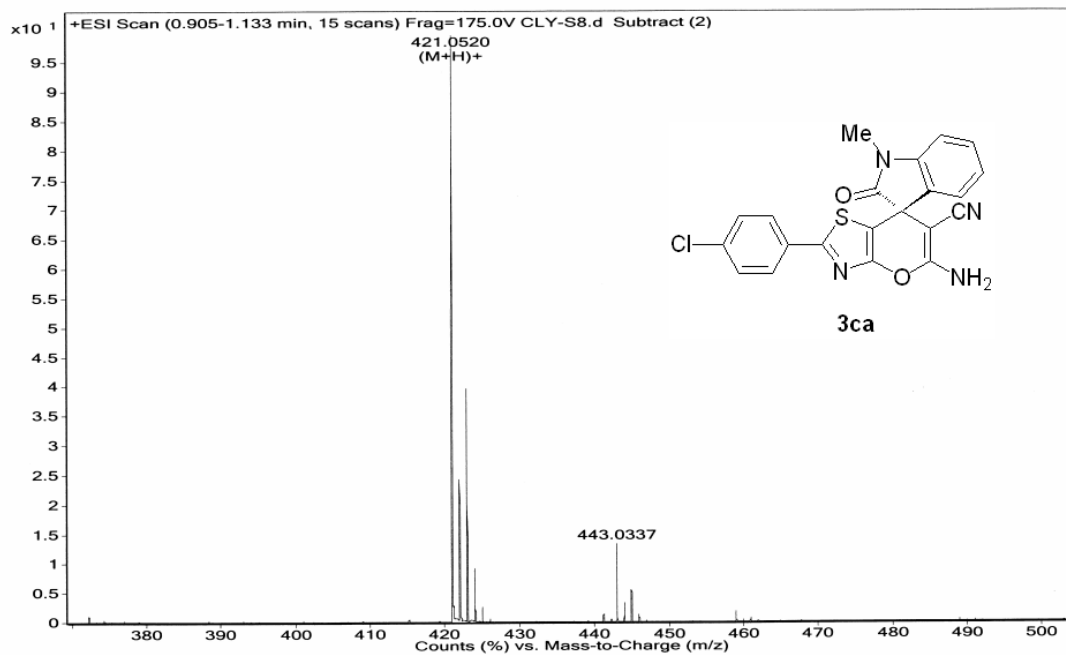
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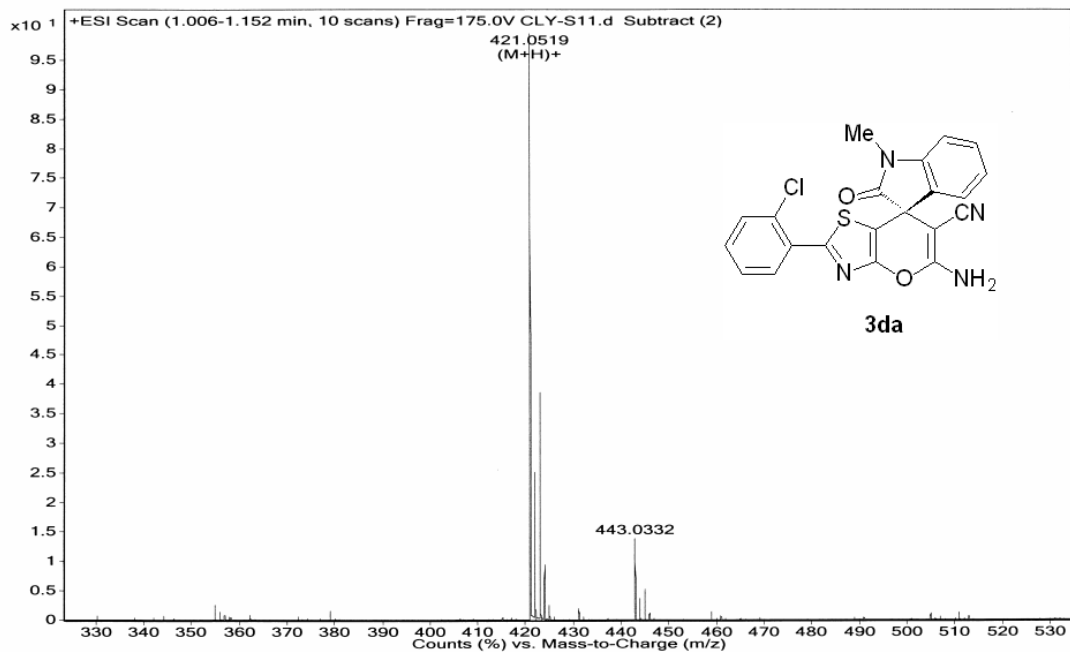
Sample Name	Sample66	Position	P2-B3	Instrument Name	Instrument 1	User Name	
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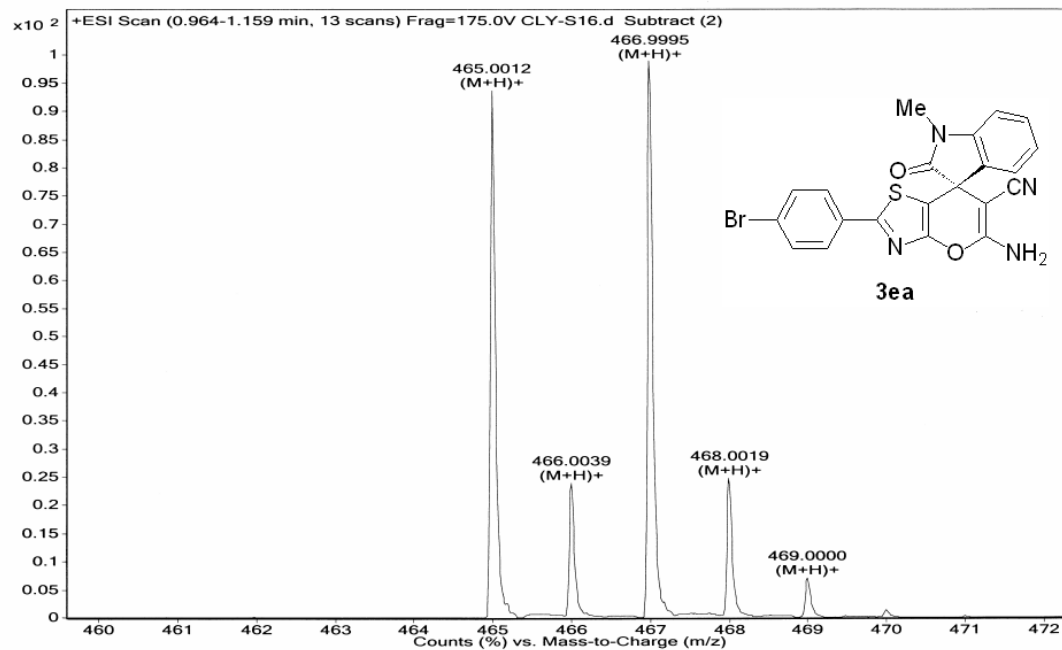
Sample Name	Sample62	Position	P2-A8	Instrument Name	Instrument 1	User Name	
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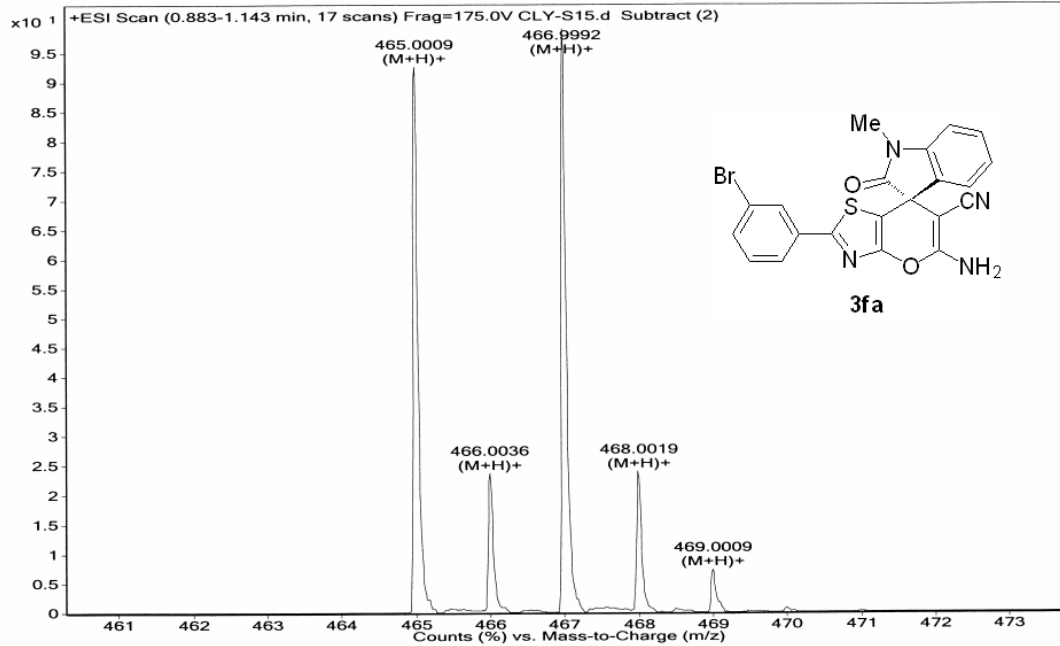
Sample Name	Sample65	Position	P2-B2	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
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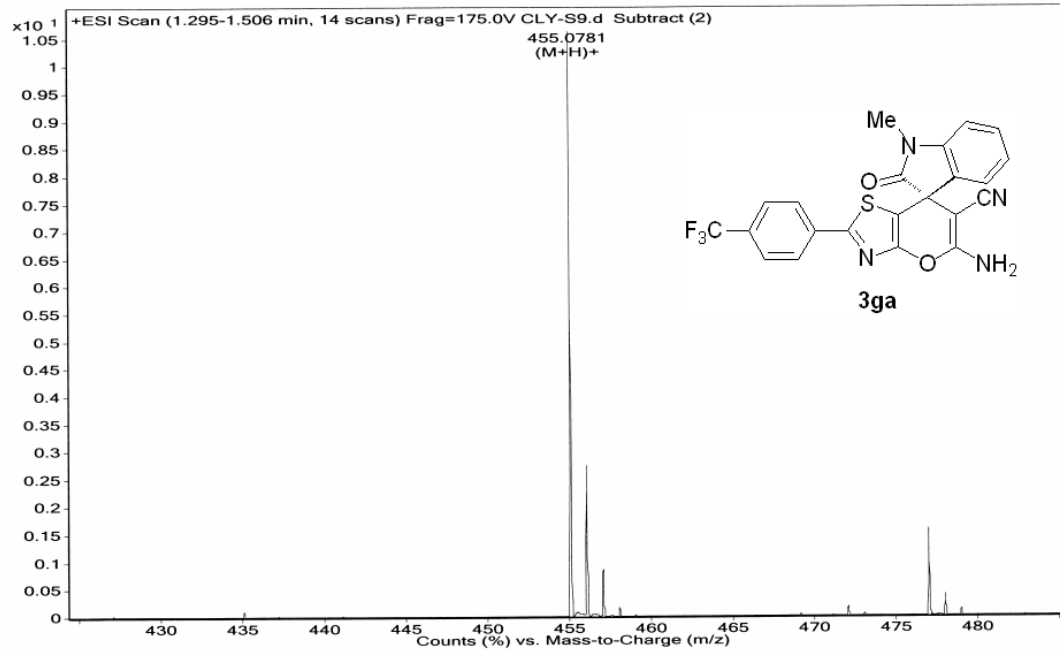
Sample Name	Sample70	Position	P2-B7	Instrument Name	Instrument 1	User Name	
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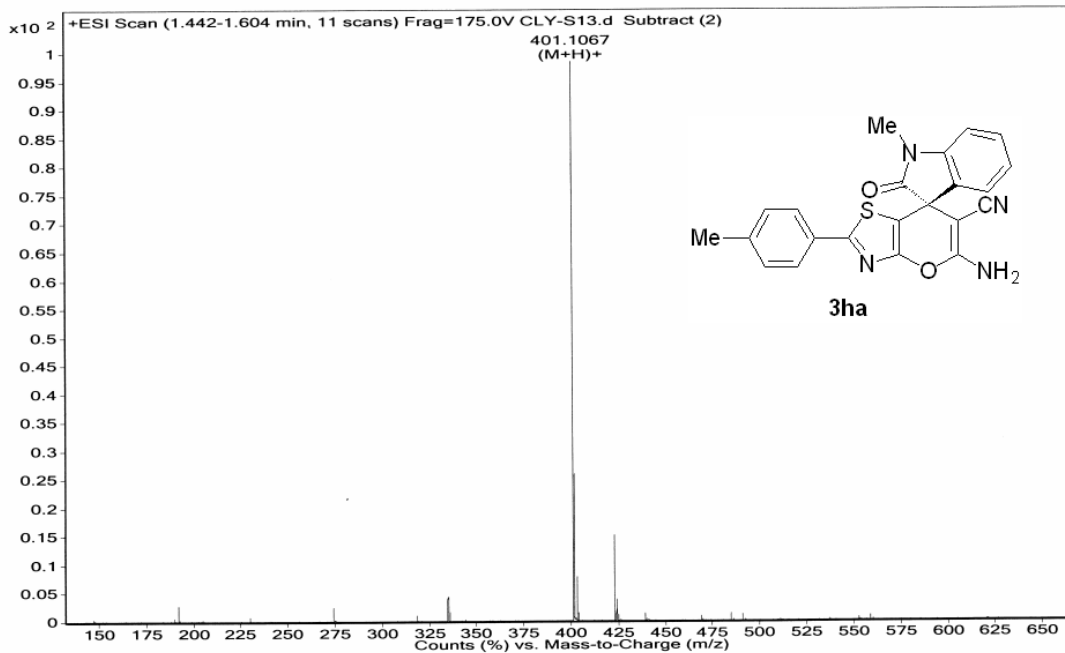
Sample Name	Sample69	Position	P2-B6	Instrument Name	Instrument 1	User Name	
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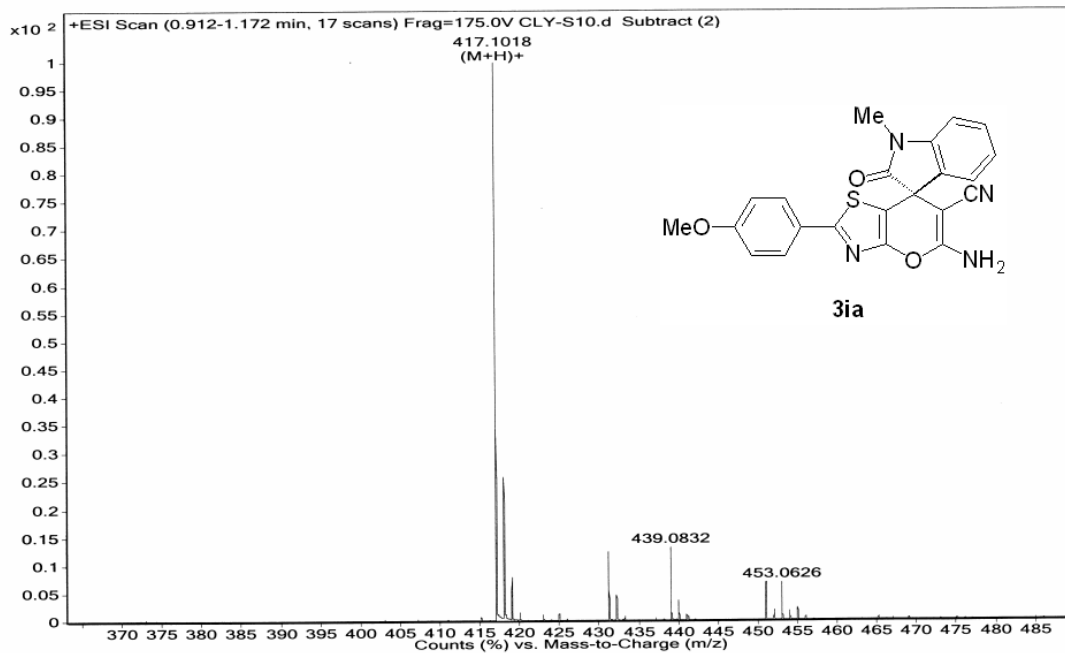
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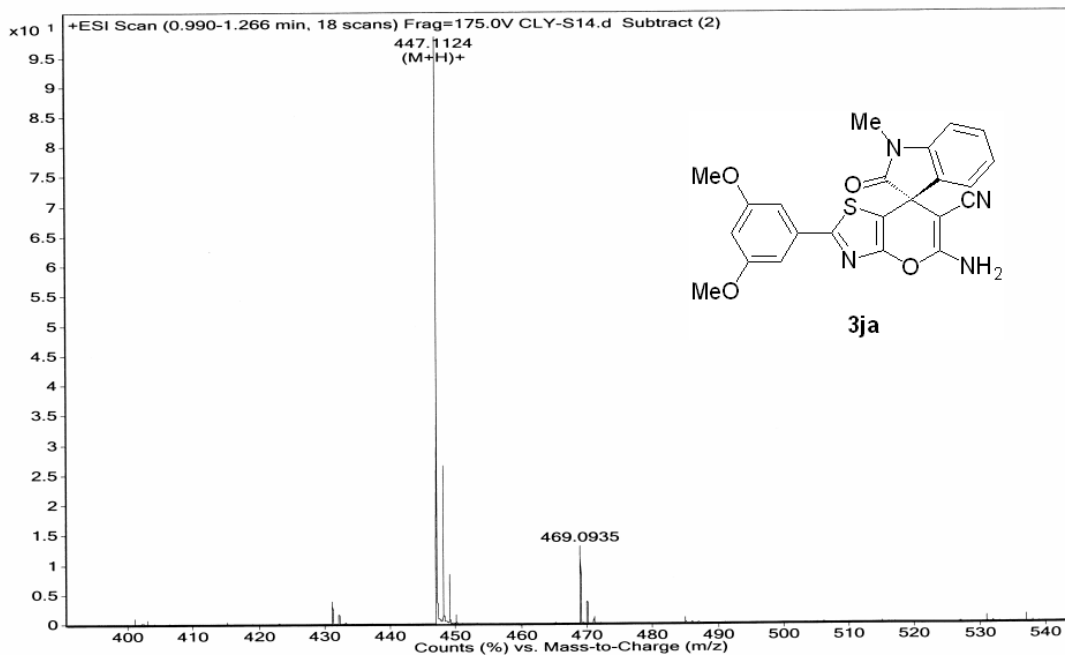
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Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
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Sample Name	Sample64	Position	P2-B1	Instrument Name	Instrument 1	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
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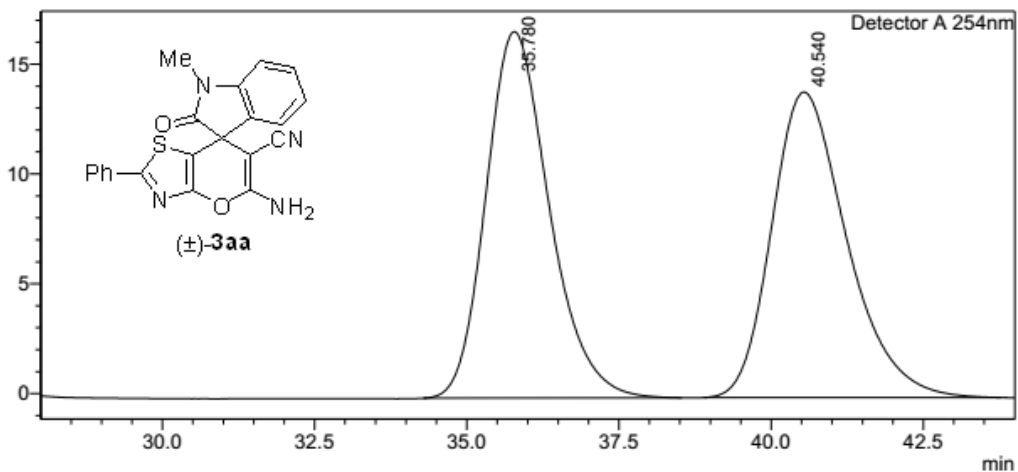
Sample Name Sample68 **Position** P2-B5 **Instrument Name** Instrument 1 **User Name**
Inj Vol -1 **InjPosition** **SampleType** Sample **IRM Calibration Status**
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4. Copies of HPLC Spectra

<Chromatogram>

mV



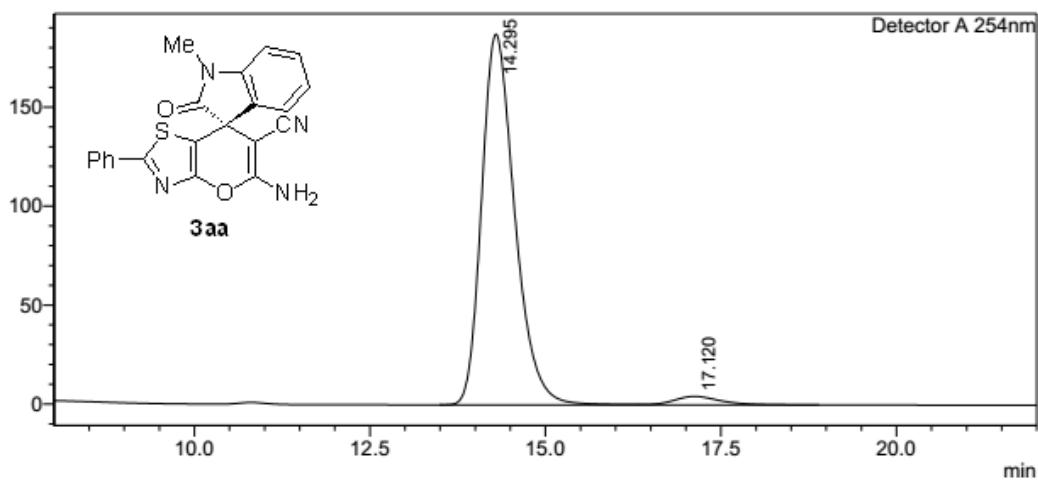
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	35.780	1206943	16681	50.268			
2	40.540	1194083	13907	49.732			
Total		2401026	30588				

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mV



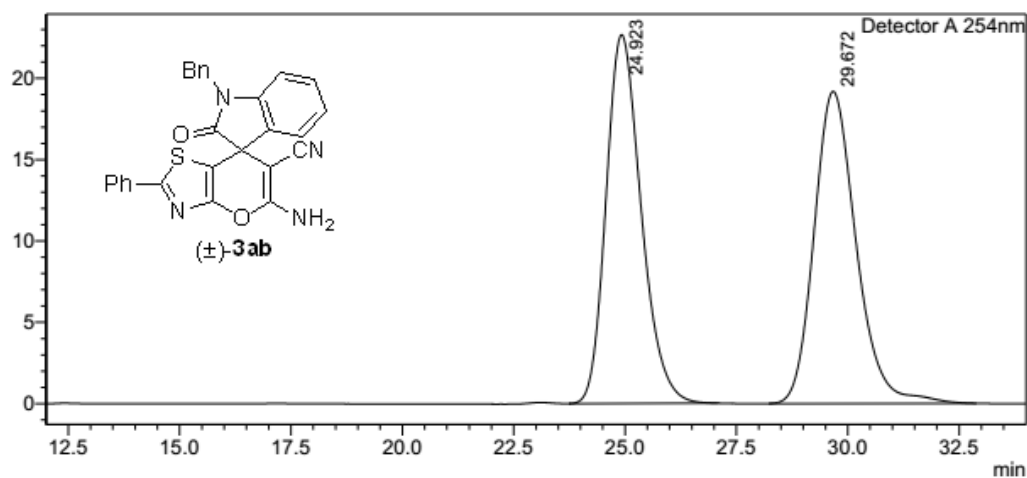
<Peak Table>

Detector A 254nm

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1	14.295	6151300	187120	96.896			
2	17.120	197037	4280	3.104		V	
Total		6348337	191401				

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mV



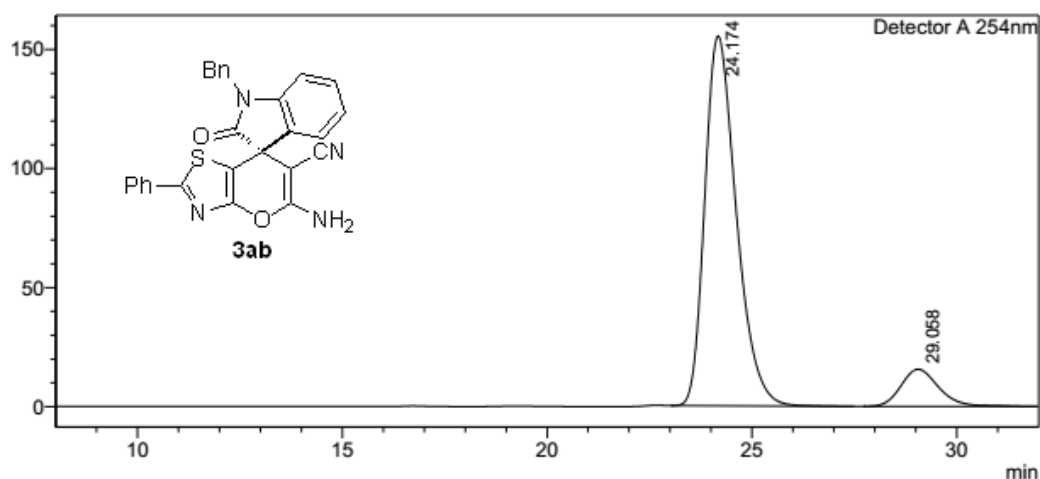
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	24.923	1243876	22672	49.628			
2	29.672	1262546	19187	50.372			
Total		2506422	41858				

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mV



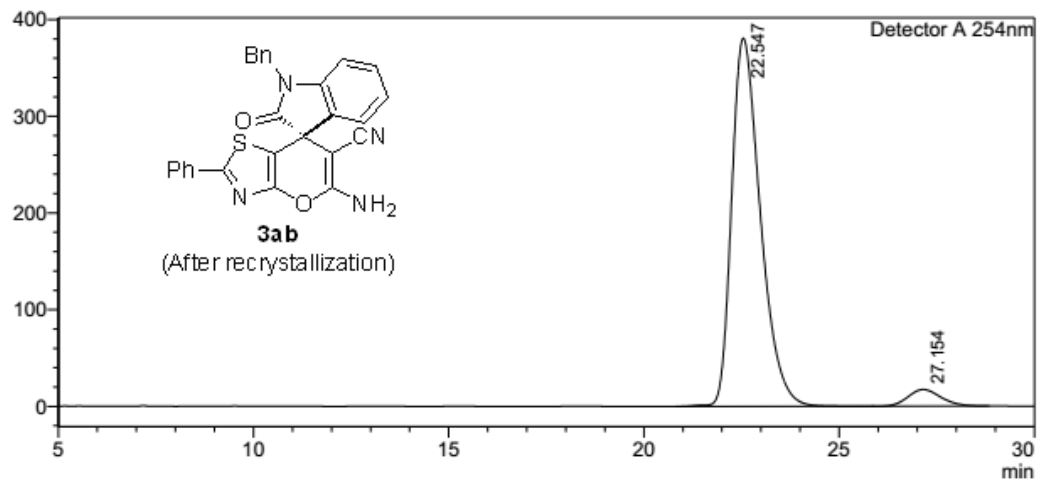
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	24.174	8322625	155365	89.225			
2	29.058	1005053	15603	10.775			
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mV



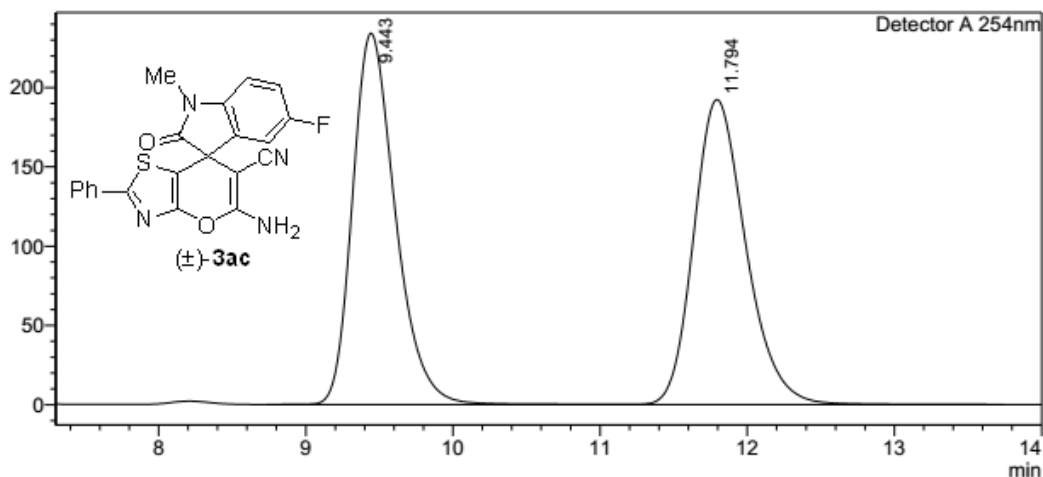
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	22.547	19500152	380594	95.077			
2	27.154	1009725	17202	4.923			
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mV



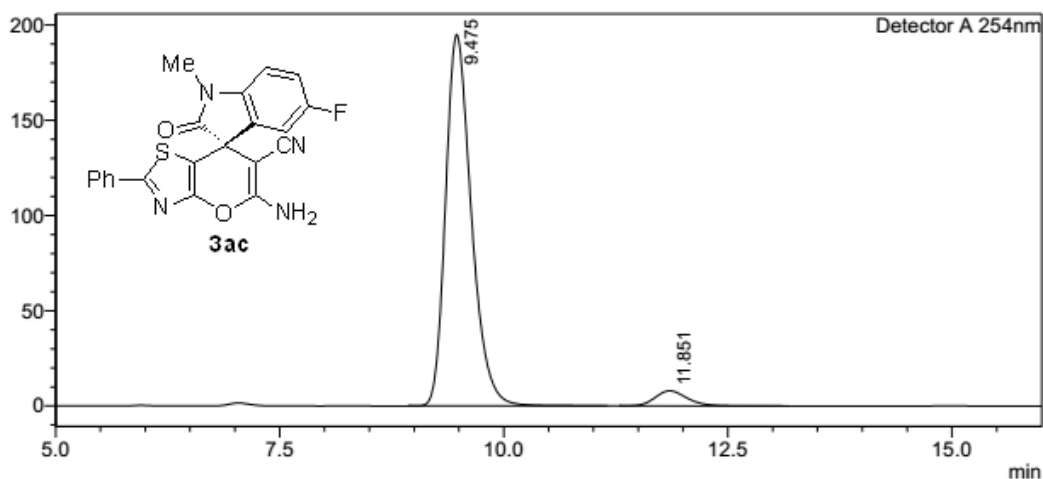
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.443	4748893	234130	50.032			
2	11.794	4742887	192286	49.968		V	
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mV



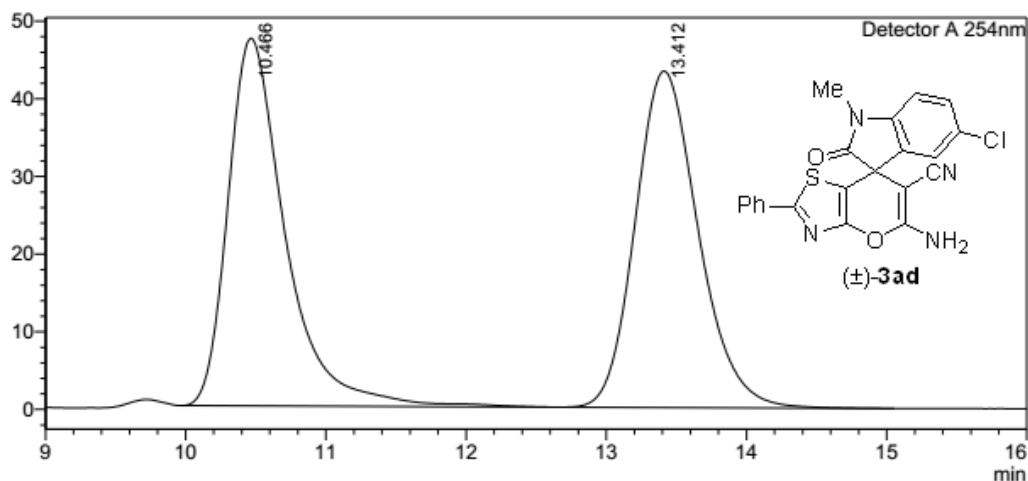
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
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2	11.851	196587	7909	4.799			
Total		4096107	202890				

<Chromatogram>

mV



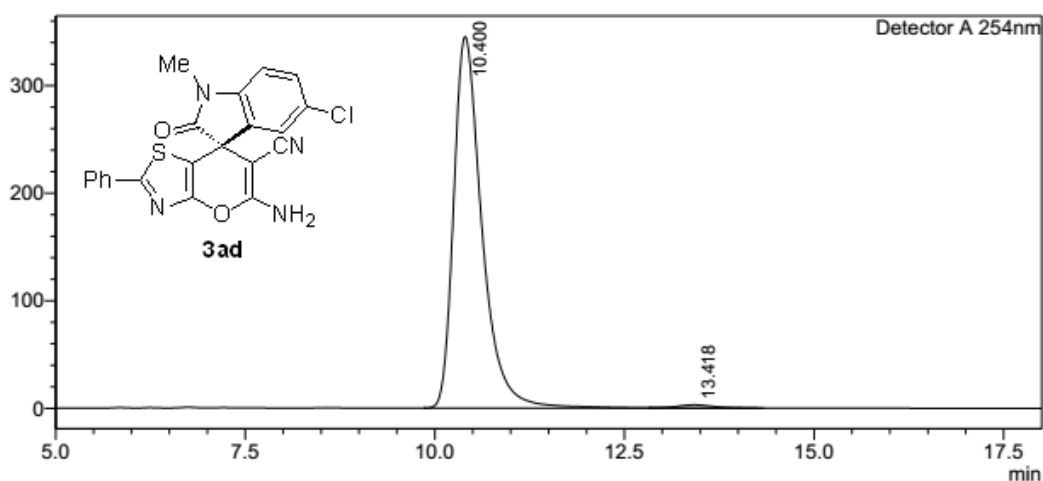
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.466	1345431	47340	49.801			
2	13.412	1356204	43329	50.199			
Total		2701636	90669				

<Chromatogram>

mV



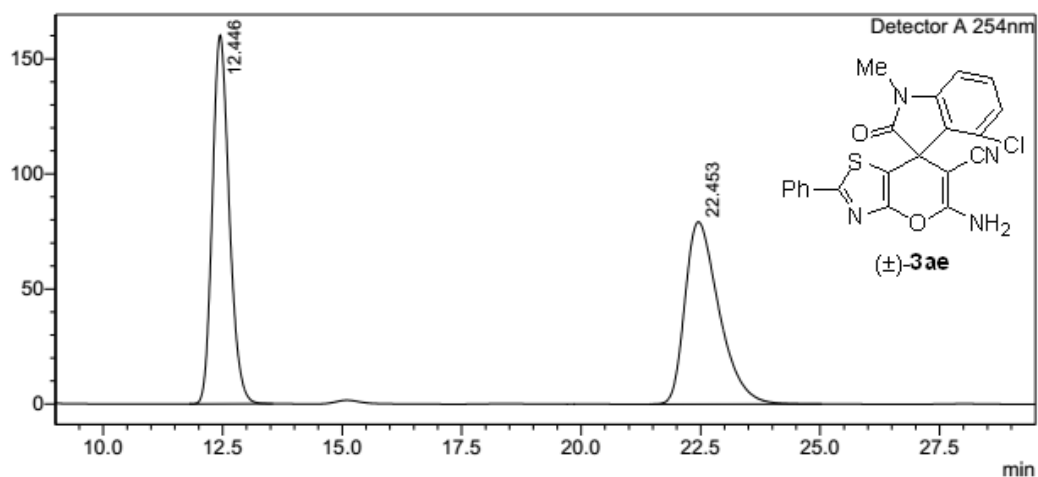
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.400	8969659	345268	99.060		S	
2	13.418	85099	2802	0.940		T	
Total		9054758	348071				

<Chromatogram>

mV



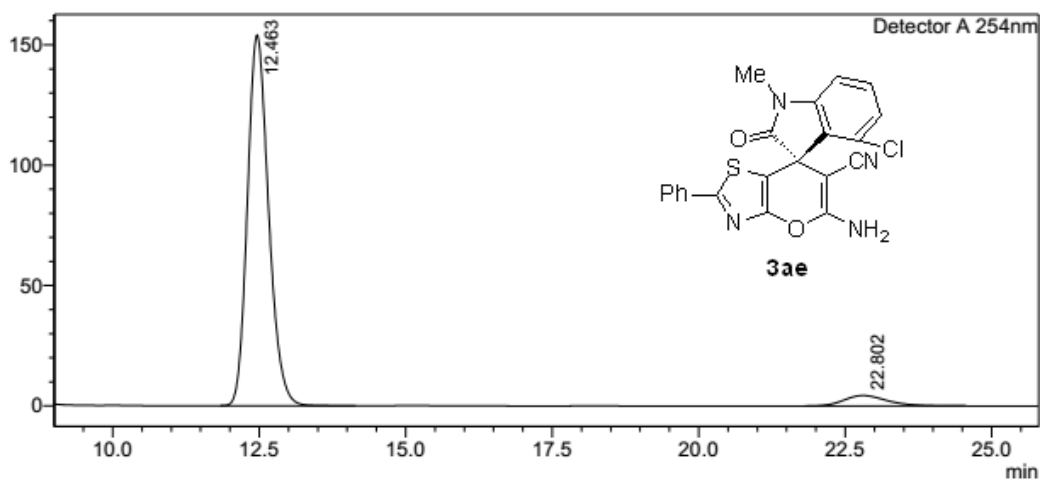
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.446	3935276	160166	50.056			
2	22.453	3926474	79148	49.944			
Total		7861750	239314				

<Chromatogram>

mV



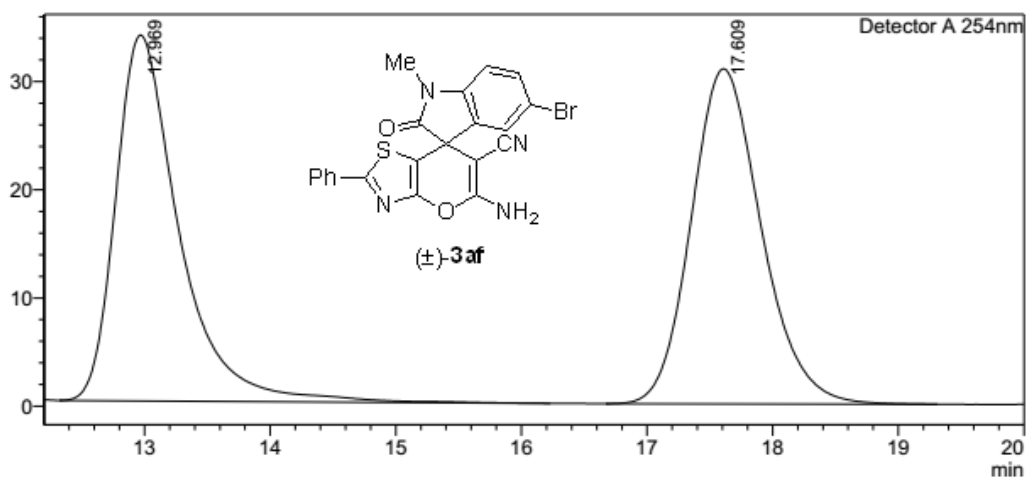
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.463	3871293	153965	94.604			
2	22.802	220792	4332	5.396			
Total		4092085	158297				

<Chromatogram>

mV



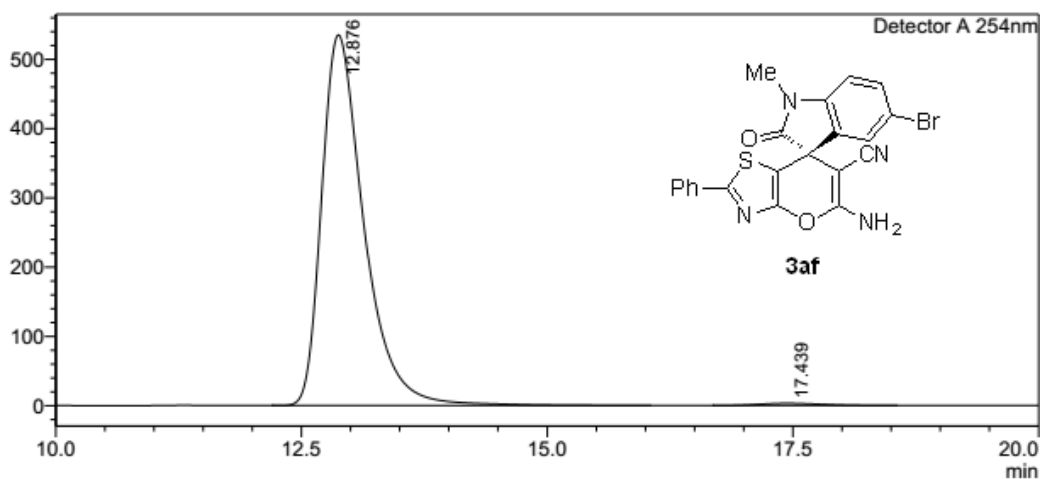
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.969	1187343	33815	49.692			
2	17.609	1202083	30967	50.308			
Total		2389426	64782				

<Chromatogram>

mV



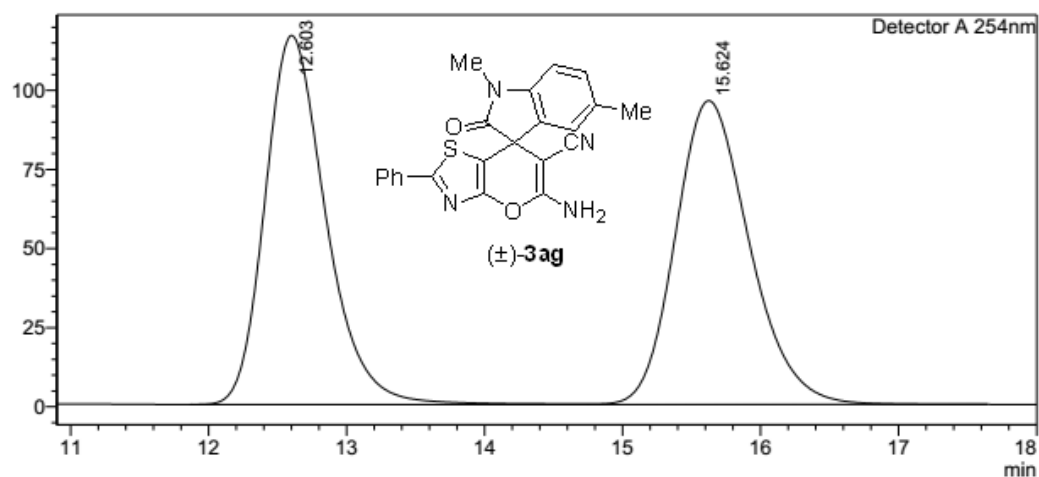
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.876	16011935	535053	99.188			
2	17.439	131081	3044	0.812			
Total		16143016	538097				

<Chromatogram>

mV



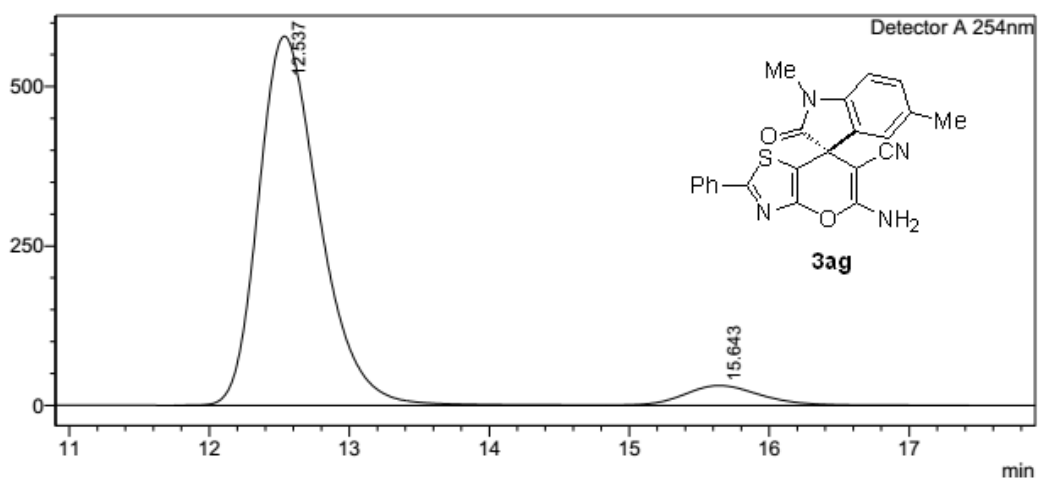
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.603	3583441	116653	49.968			
2	15.624	3588090	96043	50.032		V	
Total		7171531	212696				

<Chromatogram>

mV



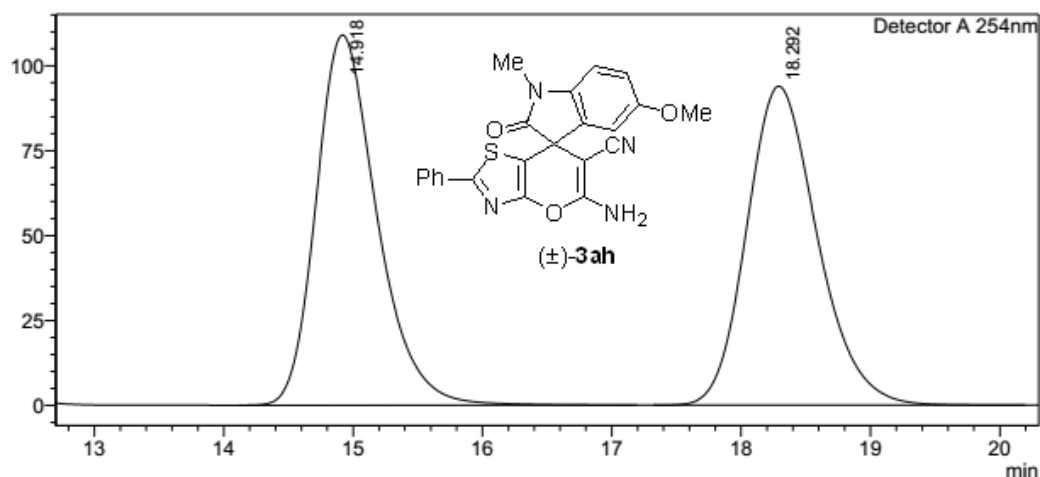
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.537	17503679	578745	93.717			
2	15.643	1173551	30949	6.283		V	
Total		18677231	609694				

<Chromatogram>

mV



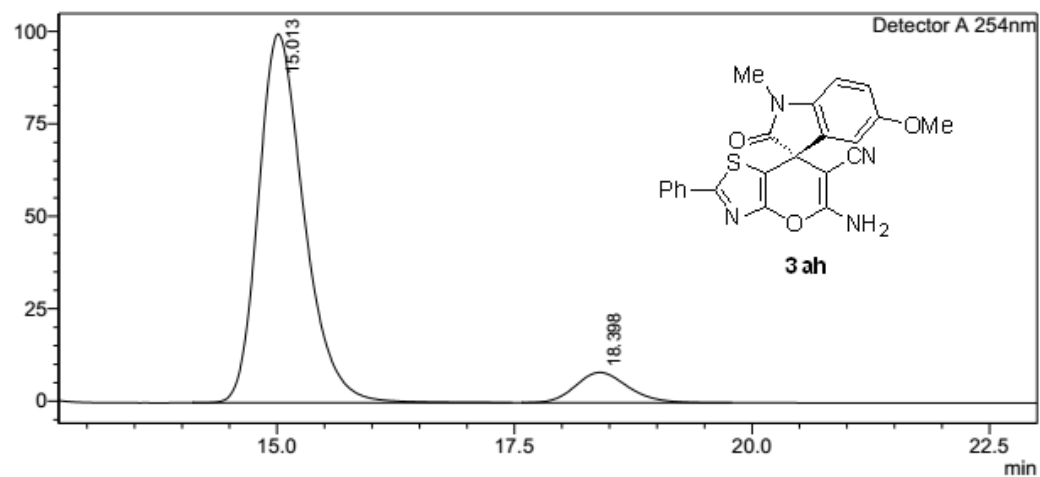
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	14.918	3568179	109003	49.998			
2	18.292	3568476	93889	50.002			
Total		7136655	202892				

<Chromatogram>

mV



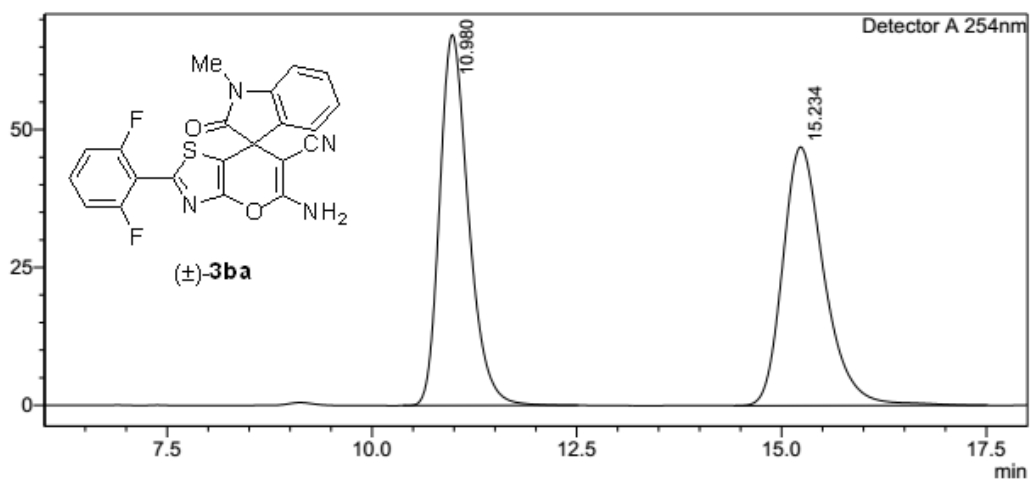
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.013	3329499	99678	91.365			
2	18.398	314655	8172	8.635			
Total		3644154	107850				

<Chromatogram>

mV



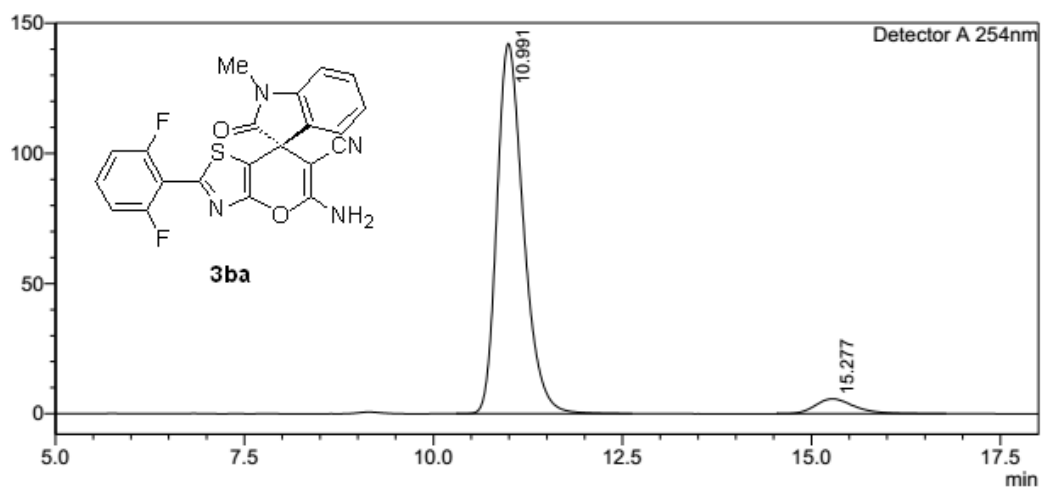
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.980	1654867	67278	50.016			
2	15.234	1653817	46904	49.984			
Total		3308684	114182				

<Chromatogram>

mV



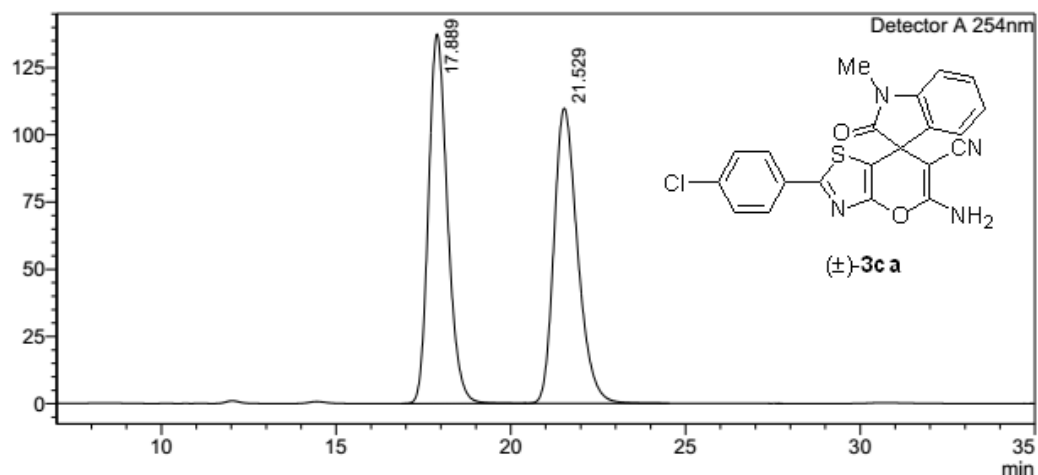
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.991	3464669	142165	94.396			
2	15.277	205676	5712	5.604			
Total		3670345	147878				

<Chromatogram>

mV



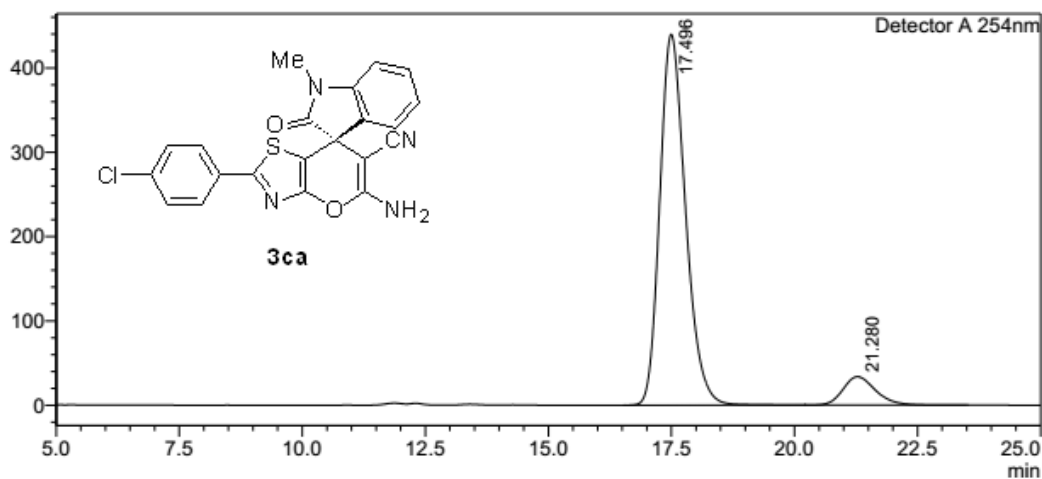
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	17.889	5186565	137329	50.099			
2	21.529	5166164	109750	49.901		V	
Total		10352729	247079				

<Chromatogram>

mV



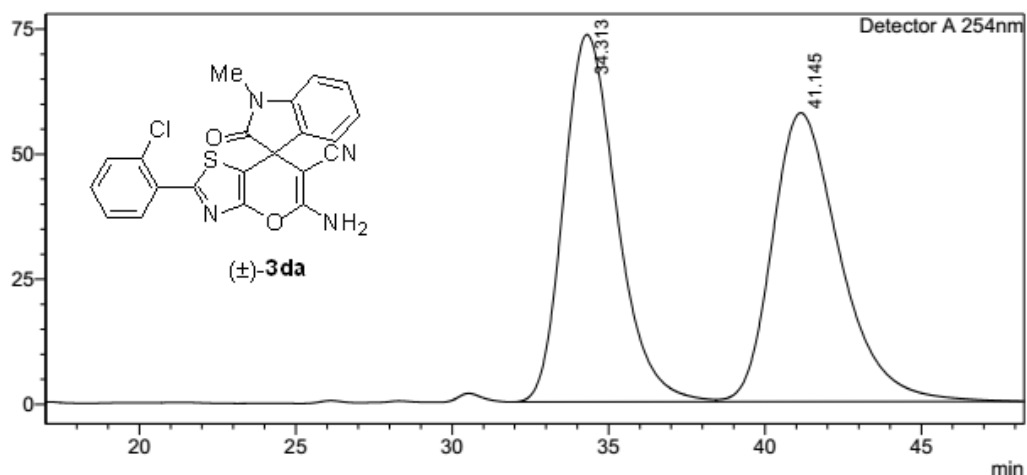
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	17.496	16011348	439641	91.151			
2	21.280	1554313	33653	8.849		V	
Total		17565662	473294				

<Chromatogram>

mV



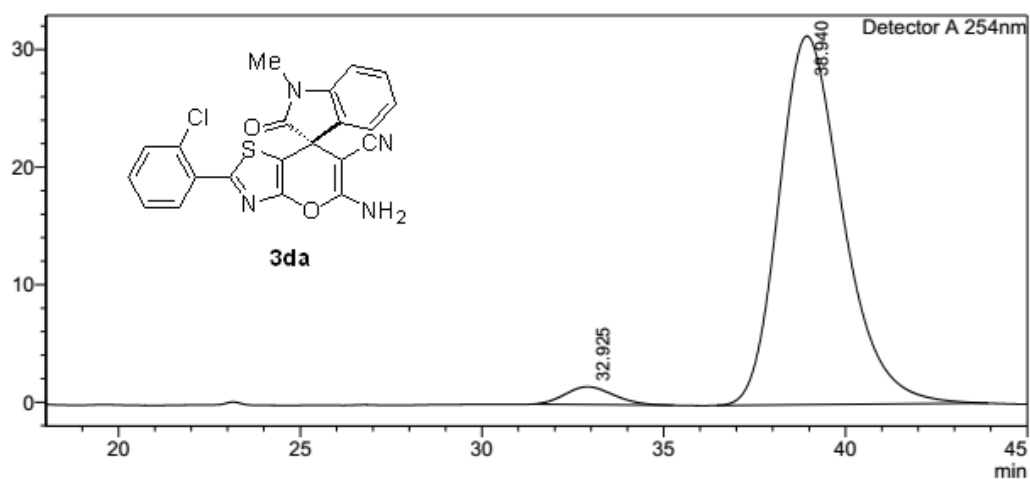
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	34.313	8678255	73437	49.969			
2	41.145	8688920	57731	50.031		V	
Total		17367175	131168				

<Chromatogram>

mV



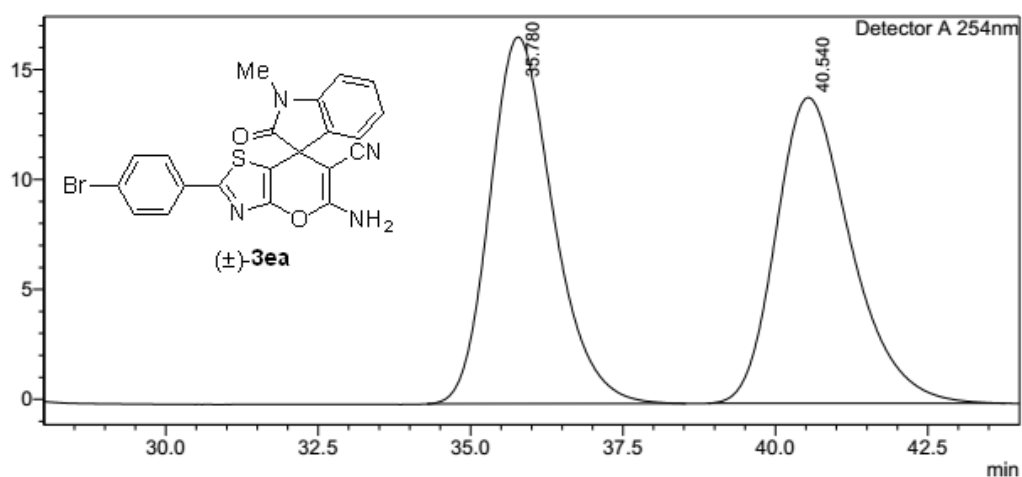
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	32.925	142042	1519	3.566			
2	38.940	3841261	31368	96.434			
Total		3983303	32888				

<Chromatogram>

mV



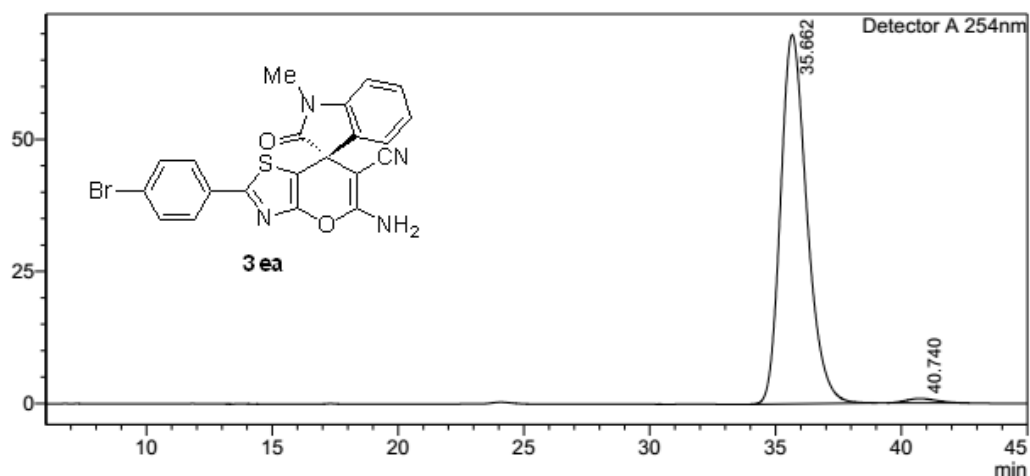
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	35.780	1206943	16681	50.268			
2	40.540	1194083	13907	49.732			
Total		2401026	30588				

<Chromatogram>

mV



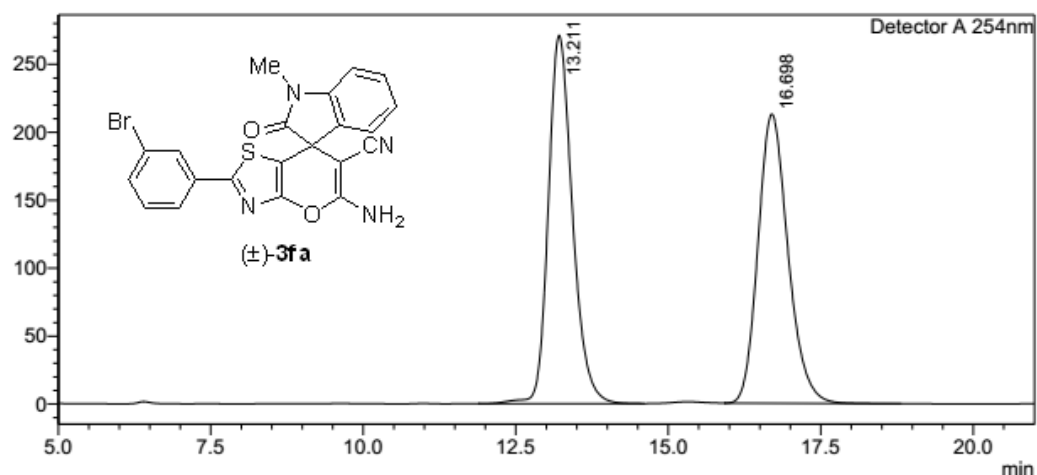
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	35.662	5075772	69872	98.626			
2	40.740	70738	845	1.374			
Total		5146510	70717				

<Chromatogram>

mV



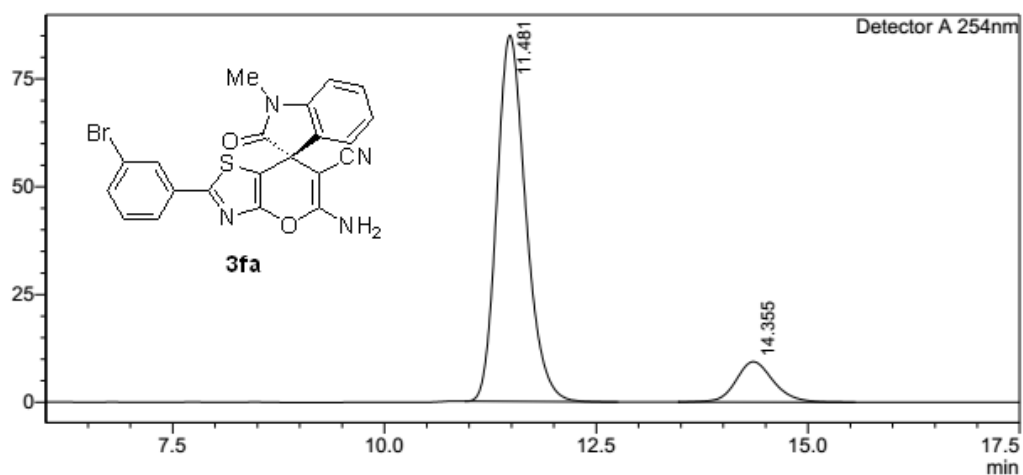
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.211	7475249	270996	50.645			
2	16.698	7284702	212738	49.355			
Total		14759951	483734				

<Chromatogram>

mV



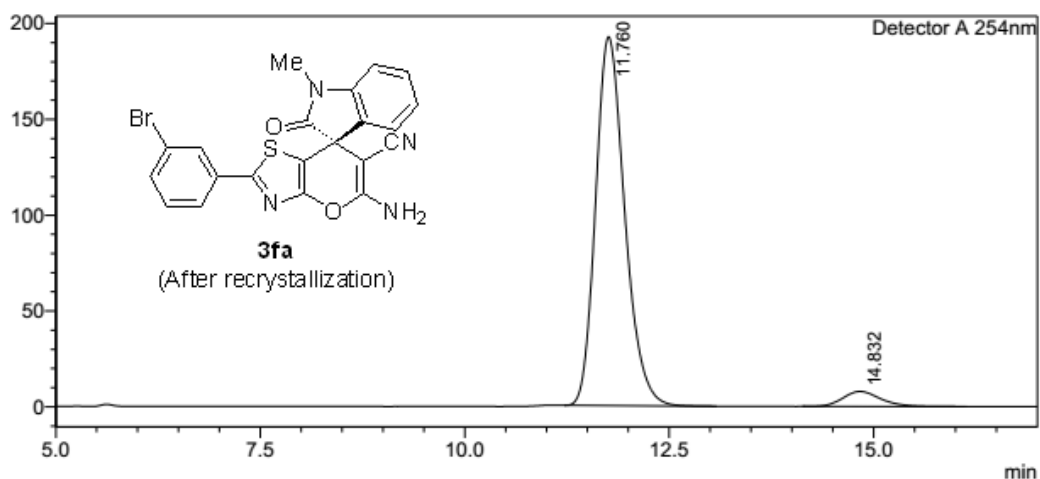
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	11.481	2022887	84906	87.533			
2	14.355	288109	9354	12.467			
Total		2310996	94261				

<Chromatogram>

mV



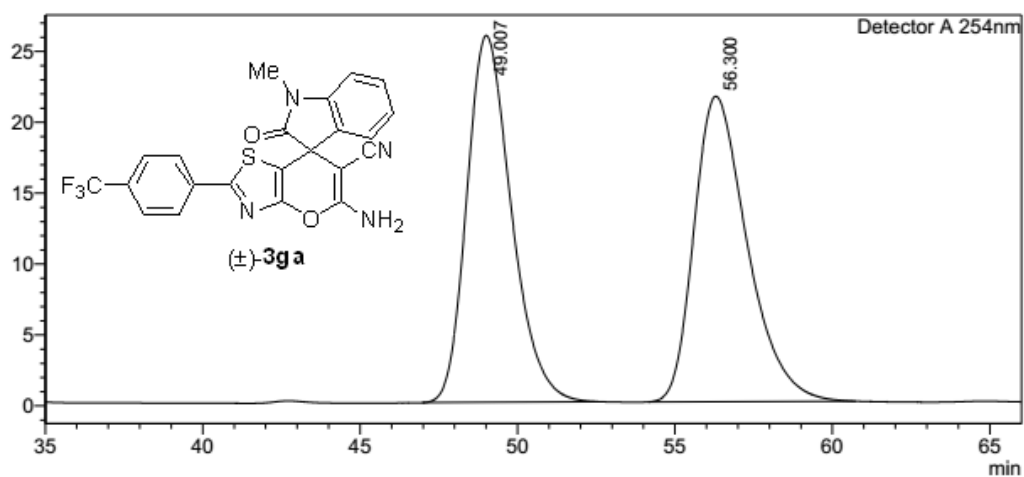
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	11.760	4773268	192412	95.000			
2	14.832	251232	7810	5.000			
Total		5024500	200222				

<Chromatogram>

mV



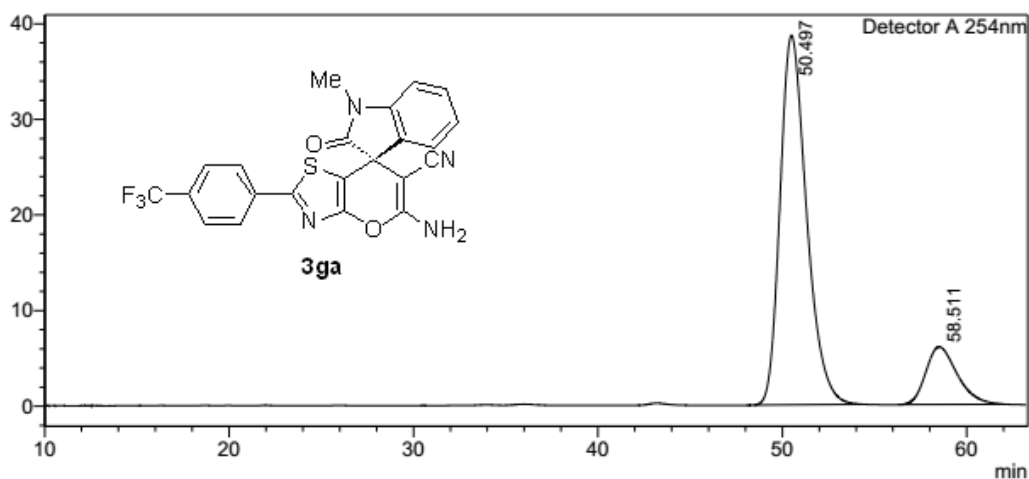
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	49.007	2551289	25874	50.195			
2	56.300	2531480	21537	49.805			
Total		5082770	47412				

<Chromatogram>

mV



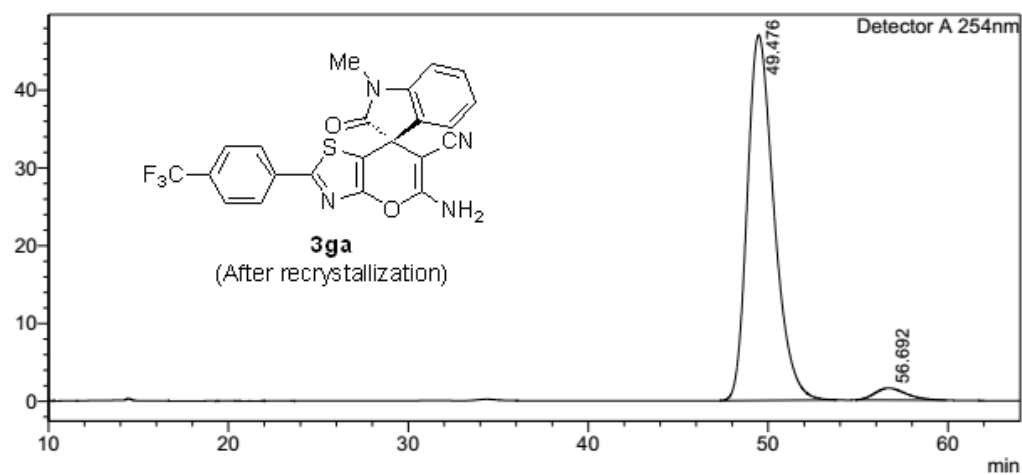
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	50.497	3862639	38608	84.349			
2	58.511	716738	6028	15.651			
Total		4579376	44636				

<Chromatogram>

mV



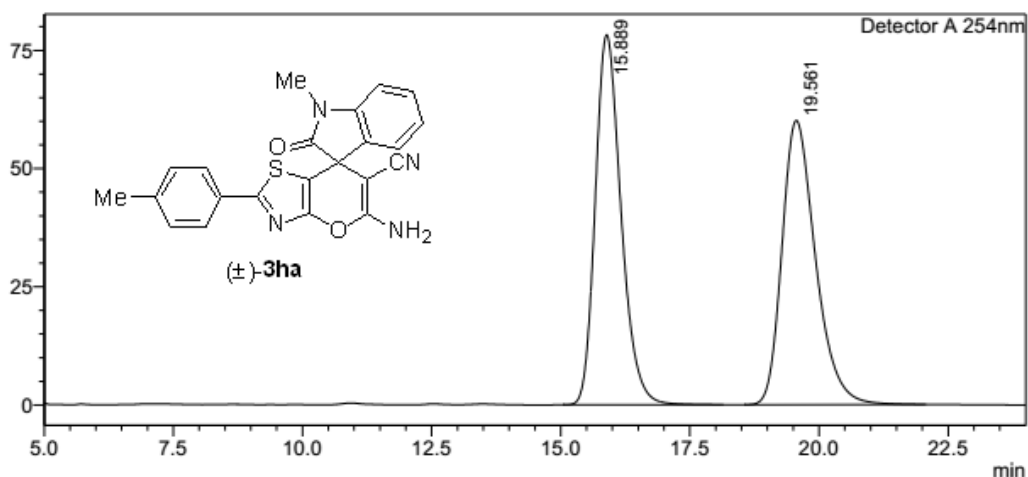
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	49.476	4848934	47010	96.338			
2	56.692	184312	1533	3.662			
Total		5033246	48543				

<Chromatogram>

mV



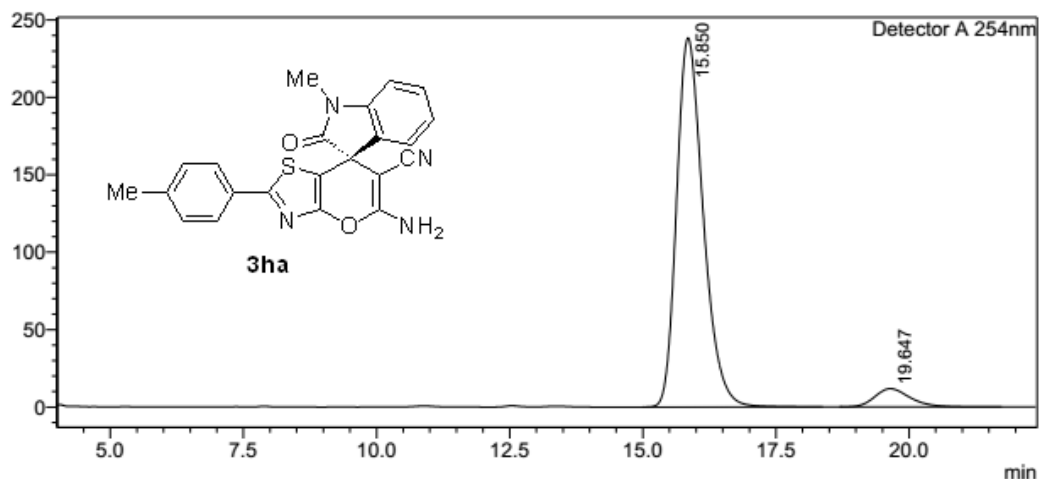
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.889	2721576	78240	50.056			
2	19.561	2715518	60112	49.944			
Total		5437094	138351				

<Chromatogram>

mV



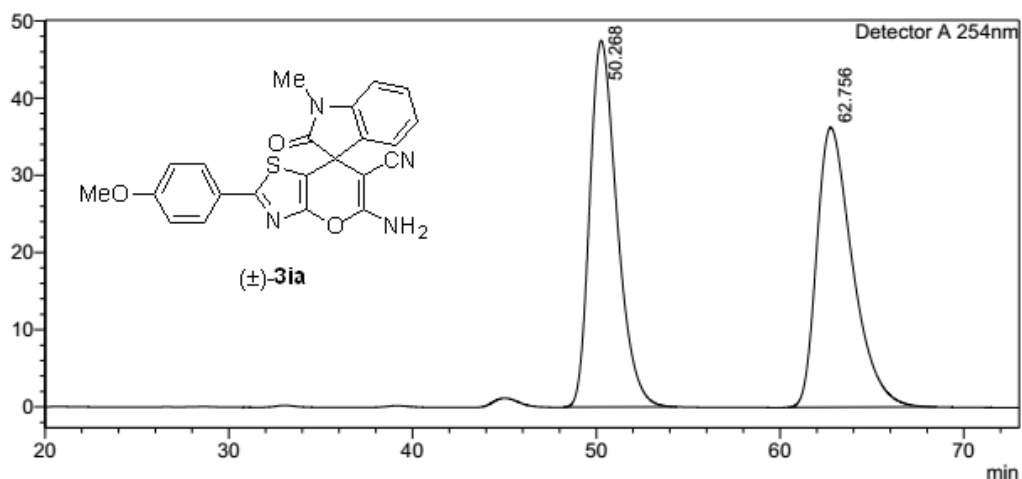
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.850	8307913	238440	93.852		S	
2	19.647	544193	11768	6.148			
Total		8852106	250207				

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mV



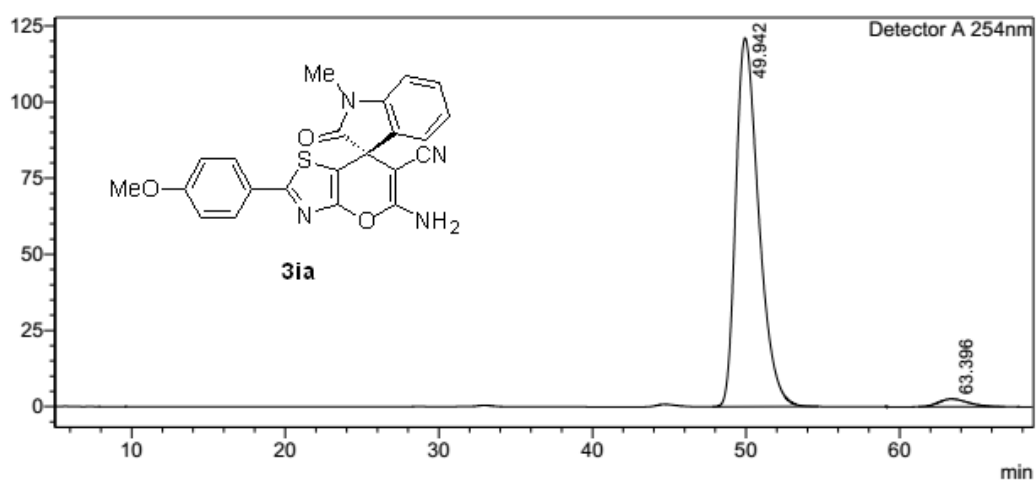
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	50.268	4899235	47465	50.066			
2	62.756	4886325	36237	49.934			
Total		9785561	83702				

<Chromatogram>

mV



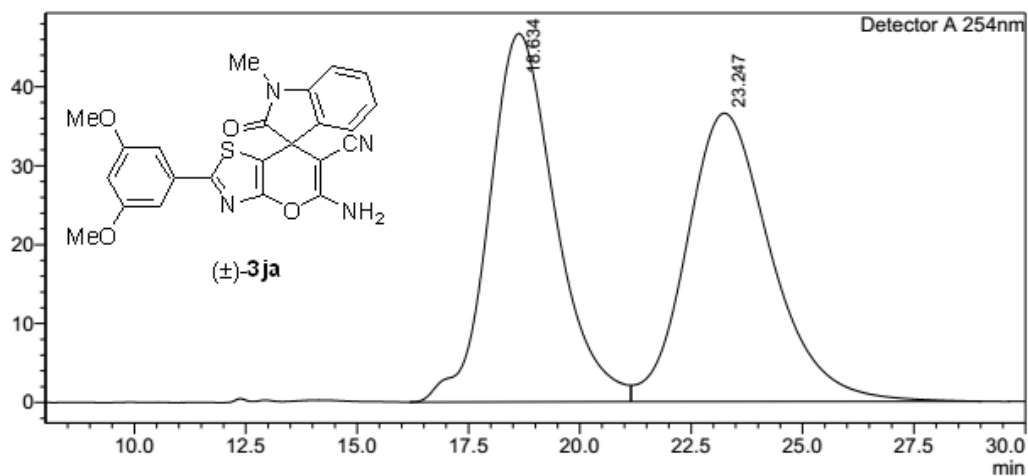
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	49.942	12581928	121031	97.381			
2	63.396	338346	2549	2.619			
Total		12920275	123580				

<Chromatogram>

mV



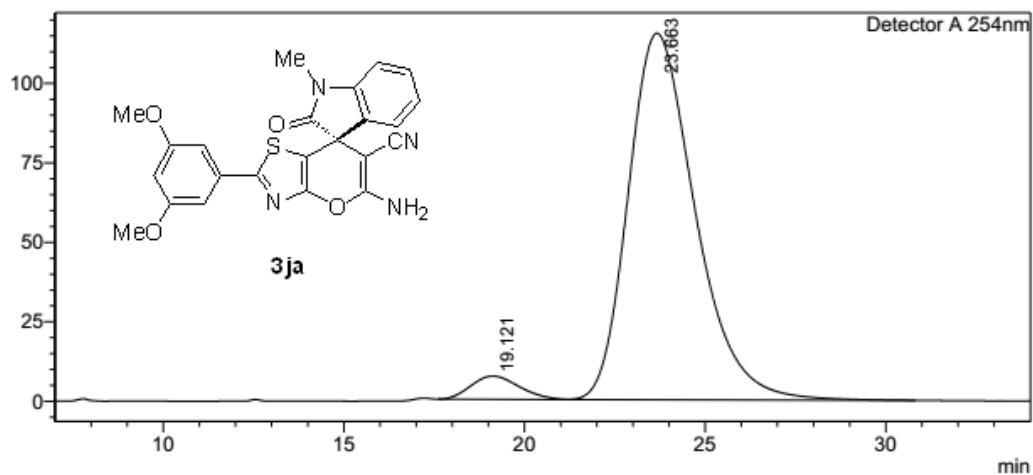
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	18.634	4817166	46672	49.998			
2	23.247	4817595	36547	50.002		V	
Total		9634761	83219				

<Chromatogram>

mV



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	19.121	679778	7318	4.370			
2	23.663	14877105	115323	95.630		V	
Total		15556883	122641				

5. Copies of HPLC Spectra

