Supporting Information for

Enantioselective Construction of Tetrahydroquinolin-5-one-based Spirooxindole Scaffold via An Organocatalytic Asymmetric Multicomponent [3+3] Cyclization

Qiu-Ning Zhu, Yu-Chen Zhang, Meng-Meng Xu, Xiao-Xue Sun, Xue Yang and Feng Shi*

Jiangsu Key Laboratory of Green Synthetic Chemistry for Functional Materials, School of Chemistry & Chemical Engineering, Jiangsu Normal University, Xuzhou, 221116, China

E-mail: fshi@jsnu.edu.cn

Contents:

1. Screening of catalysts and optimization of reaction conditions (S2-S3)

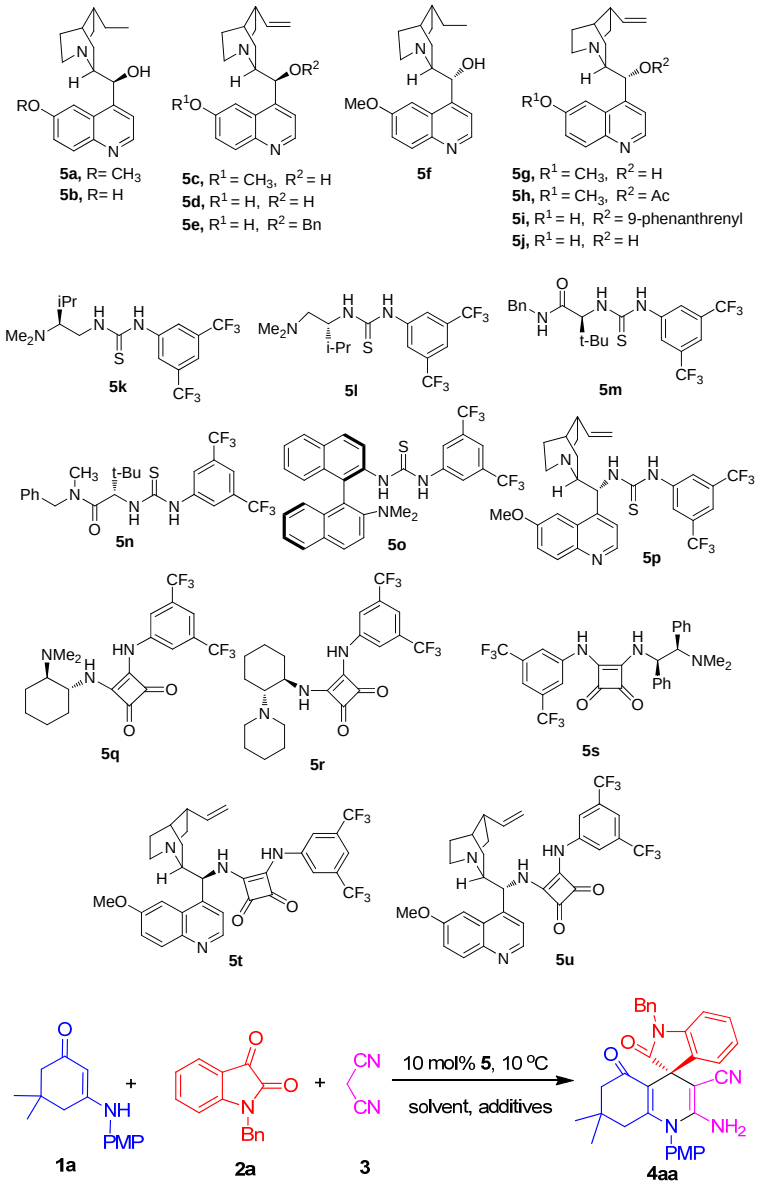
2. NMR spectra of products 4, 6 and 7 (S4-S28)

3. HPLC spectra of products 4, 6 and 7 (S29-S52)

4. X-ray single crystal data for compound4aa (S53-S54)

1. Screening of catalysts and optimization of reaction conditions

Table 1. Screening of catalysts and optimization of reaction conditions[a]



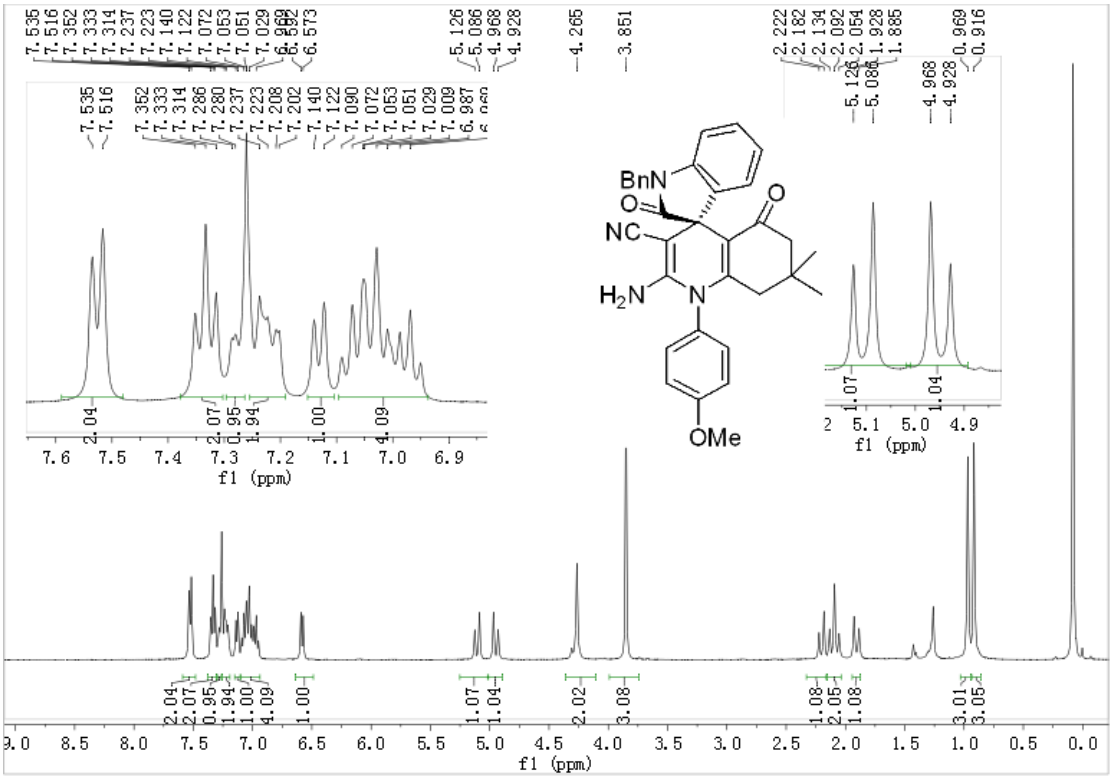
entry	**Cat.**	solvent	**1a**:**2a**:**3**	additives	yield (%)[b]	er[c]
1	**5a**	chloroform	1.2:1:1	5 Å MS	22	53:47
2	**5b**	chloroform	1.2:1:1	5 Å MS	69	70:30
3	**5c**	chloroform	1.2:1:1	5 Å MS	39	52:48
4	**5d**	chloroform	1.2:1:1	5 Å MS	46	79:21
5	**5e**	chloroform	1.2:1:1	5 Å MS	61	44:56
6	**5f**	chloroform	1.2:1:1	5 Å MS	54	57:43
7	**5g**	chloroform	1.2:1:1	5 Å MS	99	52:48
8	**5h**	chloroform	1.2:1:1	5 Å MS	17	50:50
9	**5i**	chloroform	1.2:1:1	5 Å MS	20	49:51
10	**5d**	toluene	1.2:1:1	5 Å MS	22	77:23
11	**5d**	THF	1.2:1:1	5 Å MS	trace	-

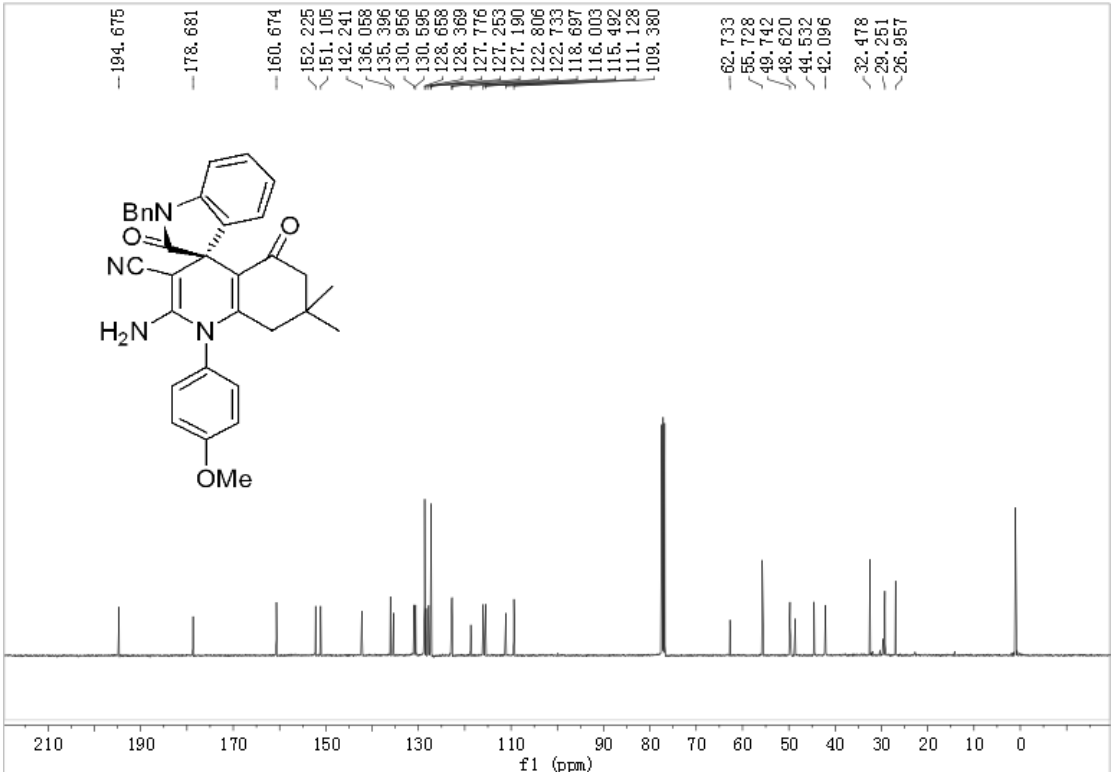
12	**5d**	acetonitrile	1.2:1:1	5 Å MS	38	52:48
13	**5d**	EtOAc	1.2:1:1	5 Å MS	trace	-
14	**5d**	acetone	1.2:1:1	5 Å MS	trace	-
15	**5j**	chloroform	1.2:1:1	5 Å MS	50	88:12
16	**5k**	chloroform	1.2:1:1	5 Å MS	trace	-
17	**5l**	chloroform	1.2:1:1	5 Å MS	47	53:47
18	**5m**	chloroform	1.2:1:1	5 Å MS	25	51:49
19	**5n**	chloroform	1.2:1:1	5 Å MS	28	61:39
20	**5o**	chloroform	1.2:1:1	5 Å MS	trace	-
21	**5p**	chloroform	1.2:1:1	5 Å MS	14	57:43
22	**5q**	chloroform	1.2:1:1	5 Å MS	trace	-
23	**5r**	chloroform	1.2:1:1	5 Å MS	15	49:51
24	**5s**	chloroform	1.2:1:1	5 Å MS	25	53:47
25	**5t**	chloroform	1.2:1:1	5 Å MS	36	50:50
26	**5u**	chloroform	1.2:1:1	5 Å MS	23	50:50
27	**5j**	chloroform	1.2:1:1	3 Å MS	62	82:18
28	**5j**	chloroform	1.2:1:1	4 Å MS	81	88:12
29	**5j**	chloroform	1.2:1:1	$MgSO_4$	47	81:19
30[d]	**5j**	chloroform	1.2:1:1	4 Å MS	80	90:10
31[e]	**5j**	chloroform	1.2:1:1	4 Å MS	54	94:6
32[e]	**5j**	chloroform	1:1.5:1.5	4 Å MS	75	94:6
33[f]	**5j**	chloroform	1:1.5:1.5	4 Å MS	45	95:5
34[e,g]	**5j**	chloroform	1:1.5:1.5	4 Å MS	43	94:6
35[e,h]	**5j**	chloroform	1:1.5:1.5	4 Å MS	80	94:6
36[e,h]	**5j**	chloroform	1:4:4	4 Å MS	91	96:4

[a]Unless otherwise indicated, the reaction was carried out at the 0.05 mmol scale and catalyzed by 10 mol% **5** in a solvent (0.5 mL) with additives (100mg) at 10 °C for 2days. [b]Isolated yield.[c]The er value was determined by HPLC. [d]The volume of solvent was 1 mL.[e]The volume of solvent was 2 mL.[f]The volume of solvent was 3 mL.[g]Performed at 0 °C.[h]The reaction time was 4 days.

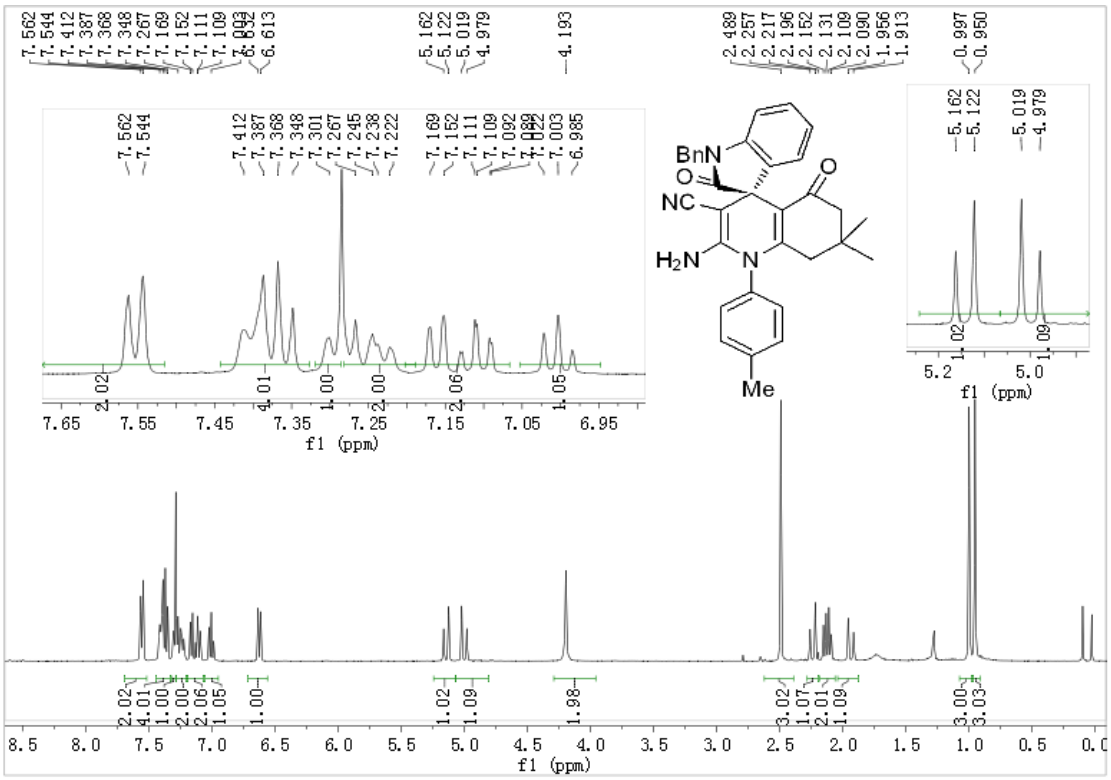
2. NMR spectra of products 4, 6 and 7

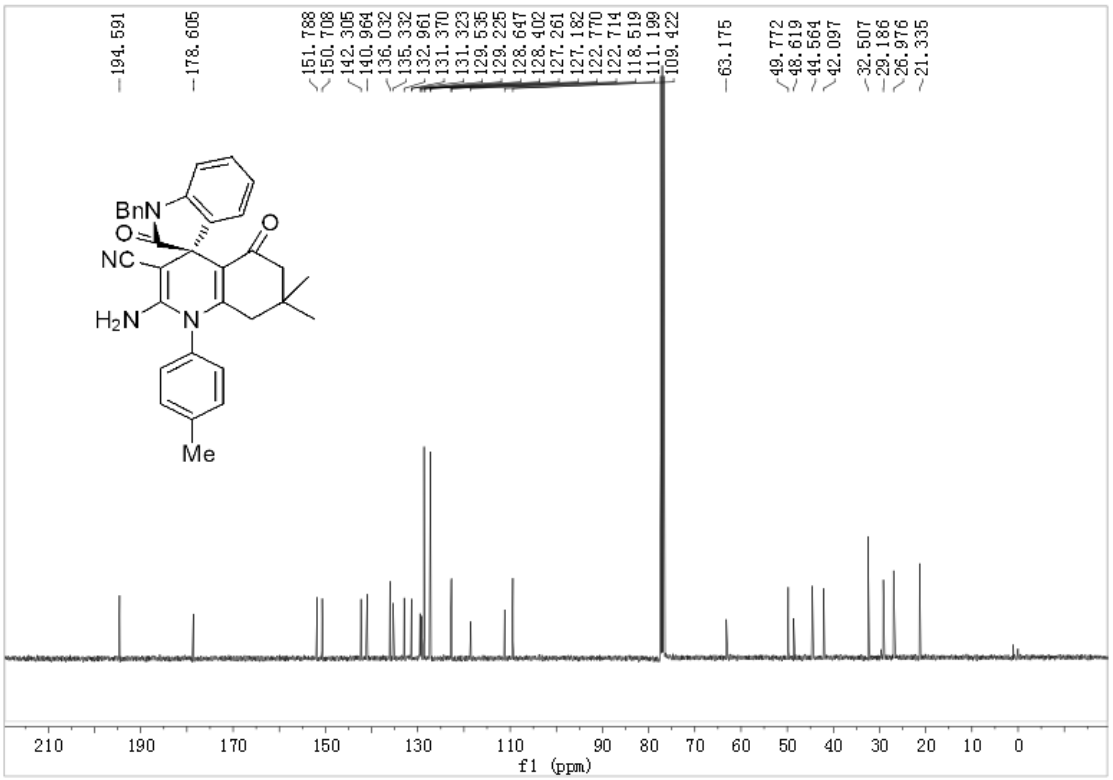
4aa



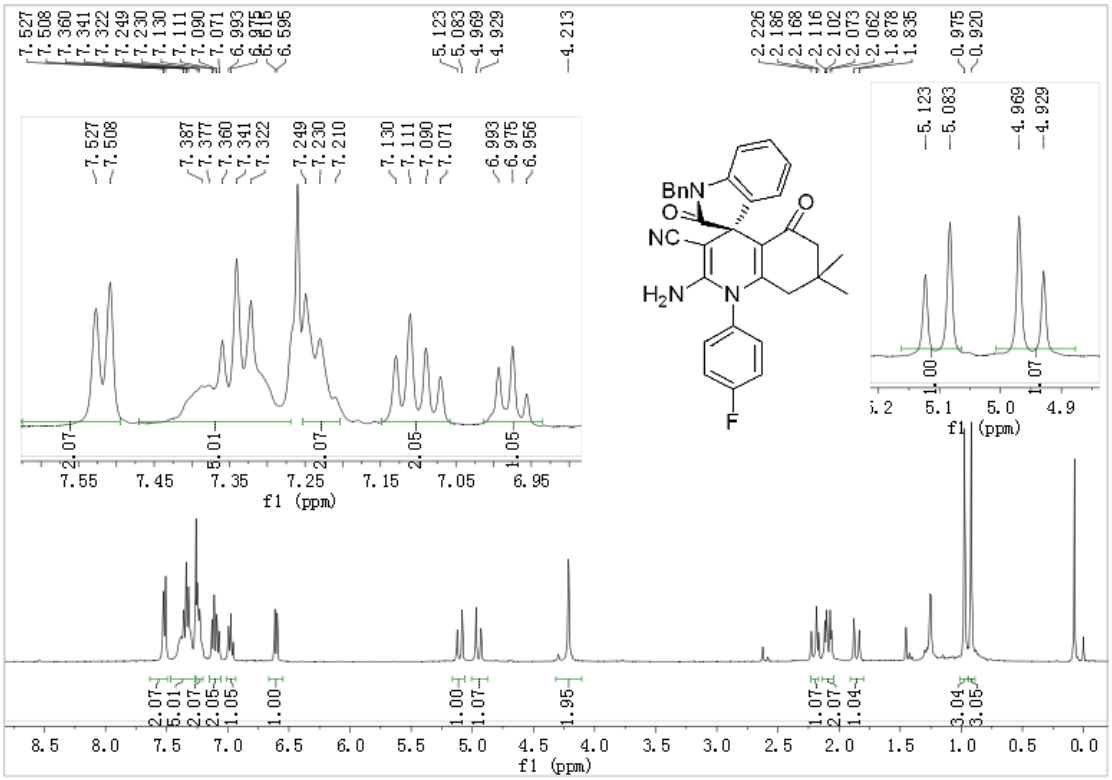


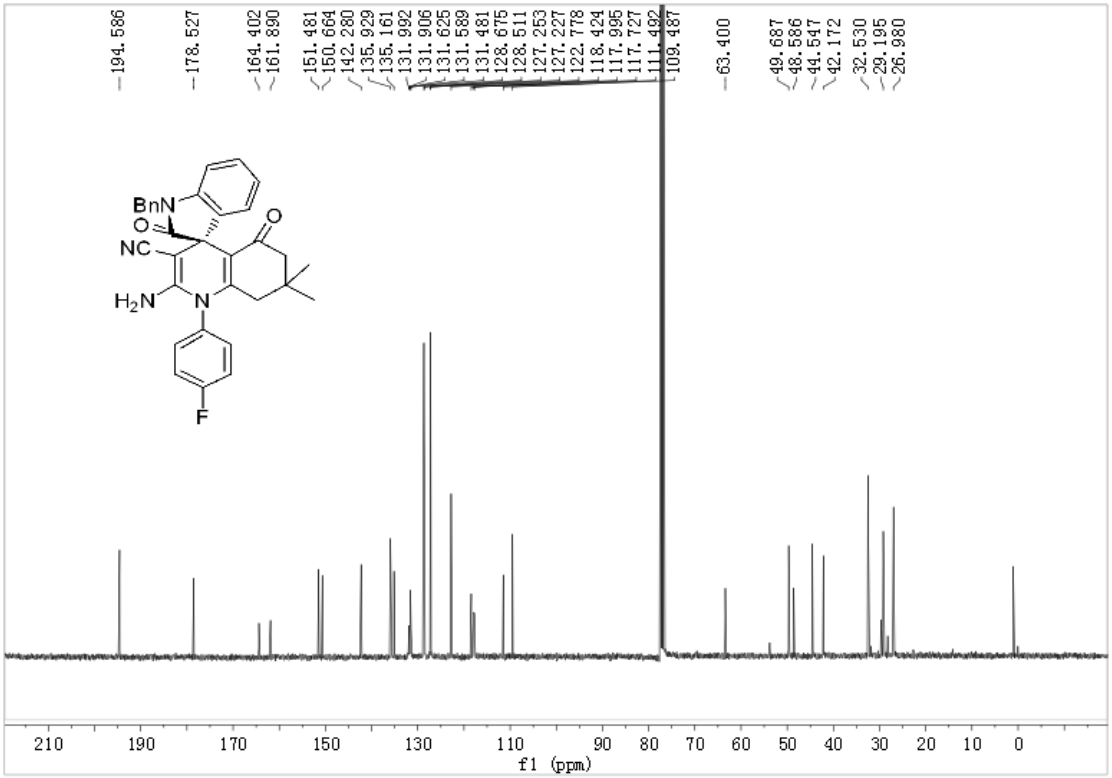
4ba



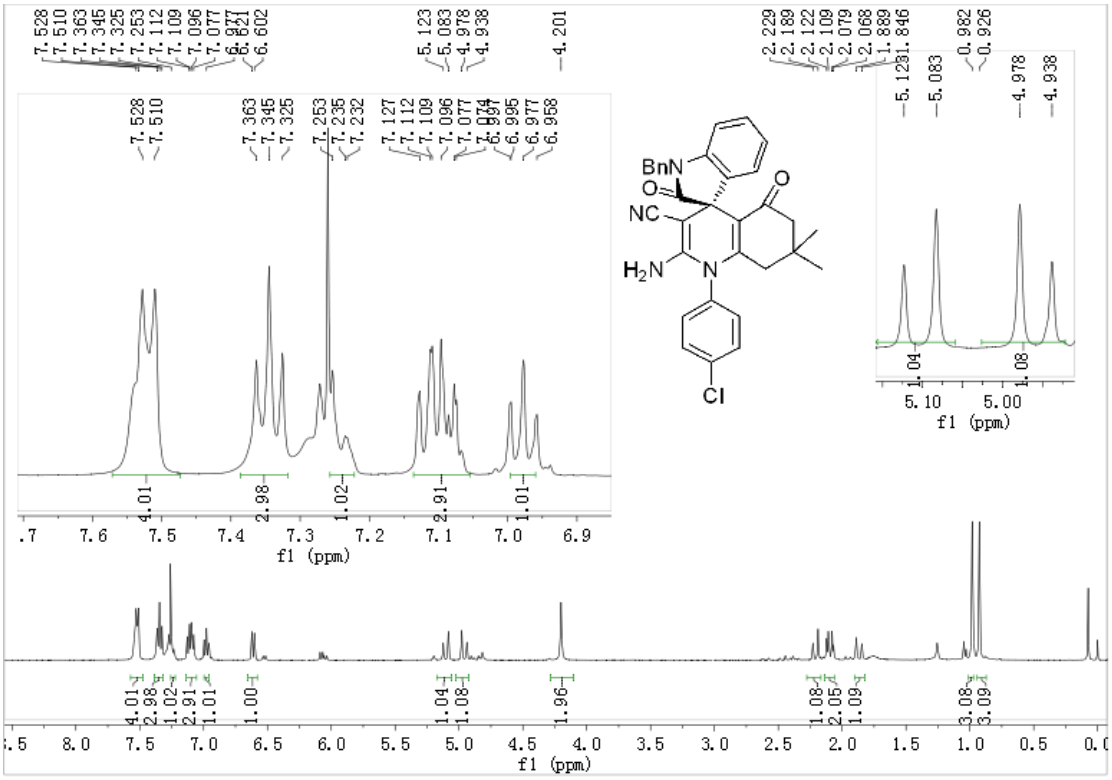


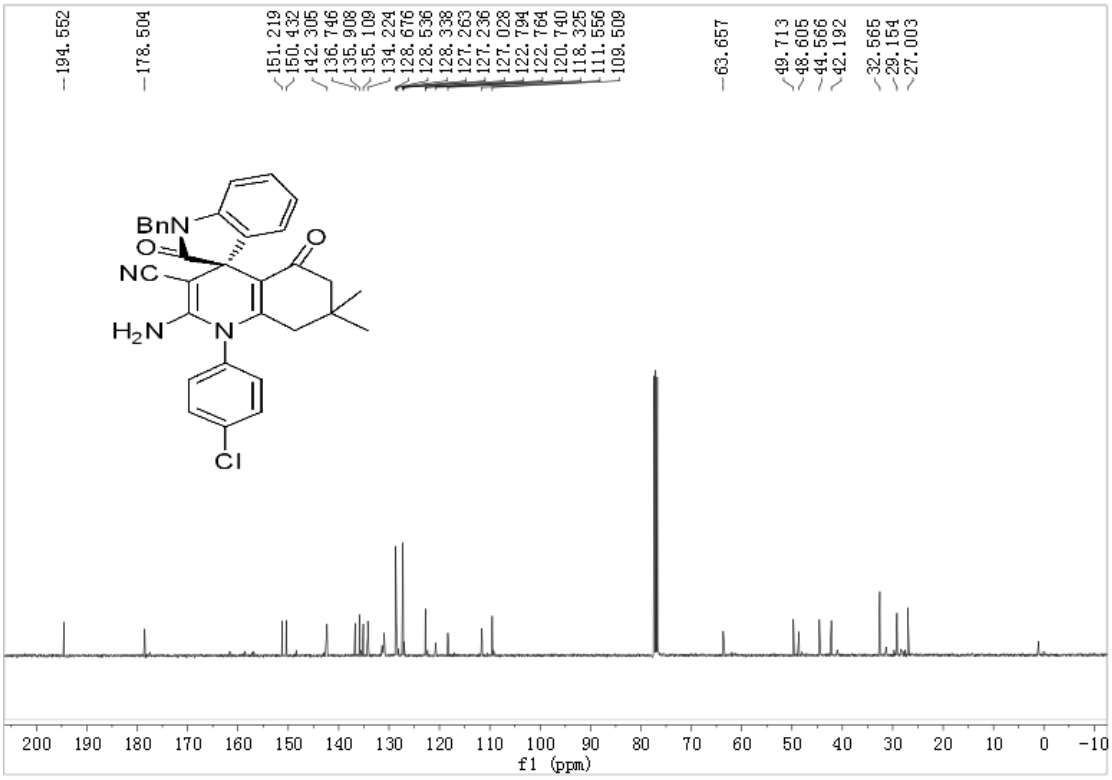
4ca



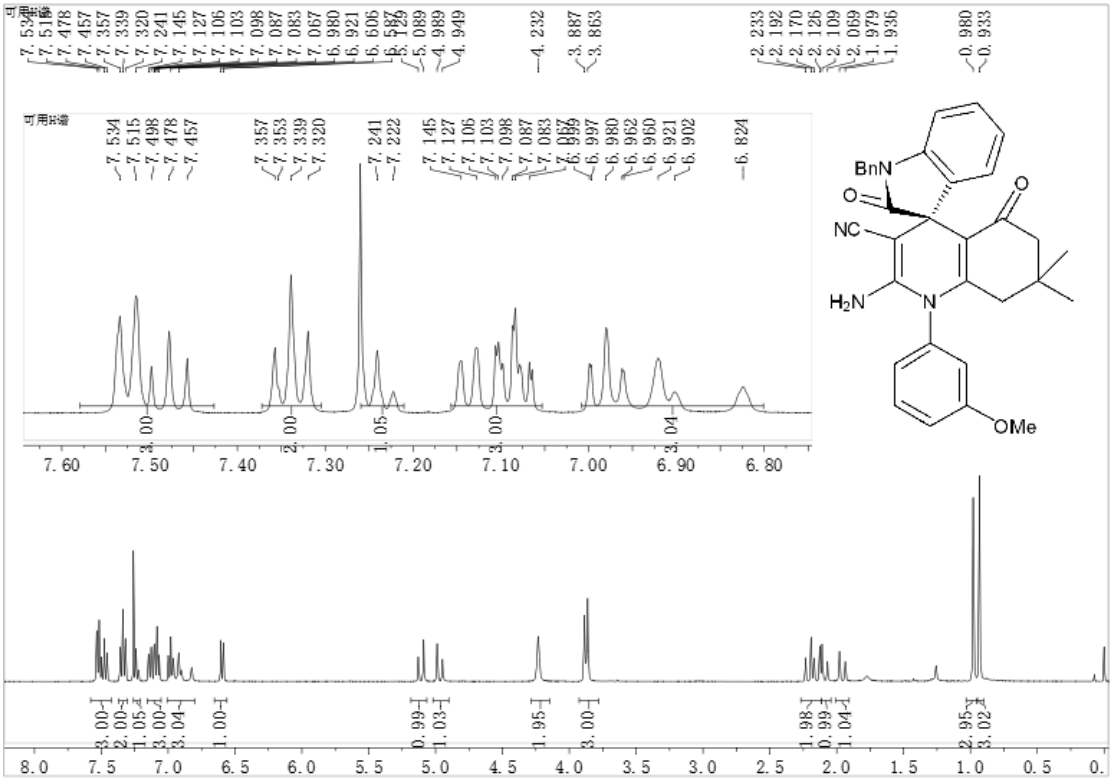


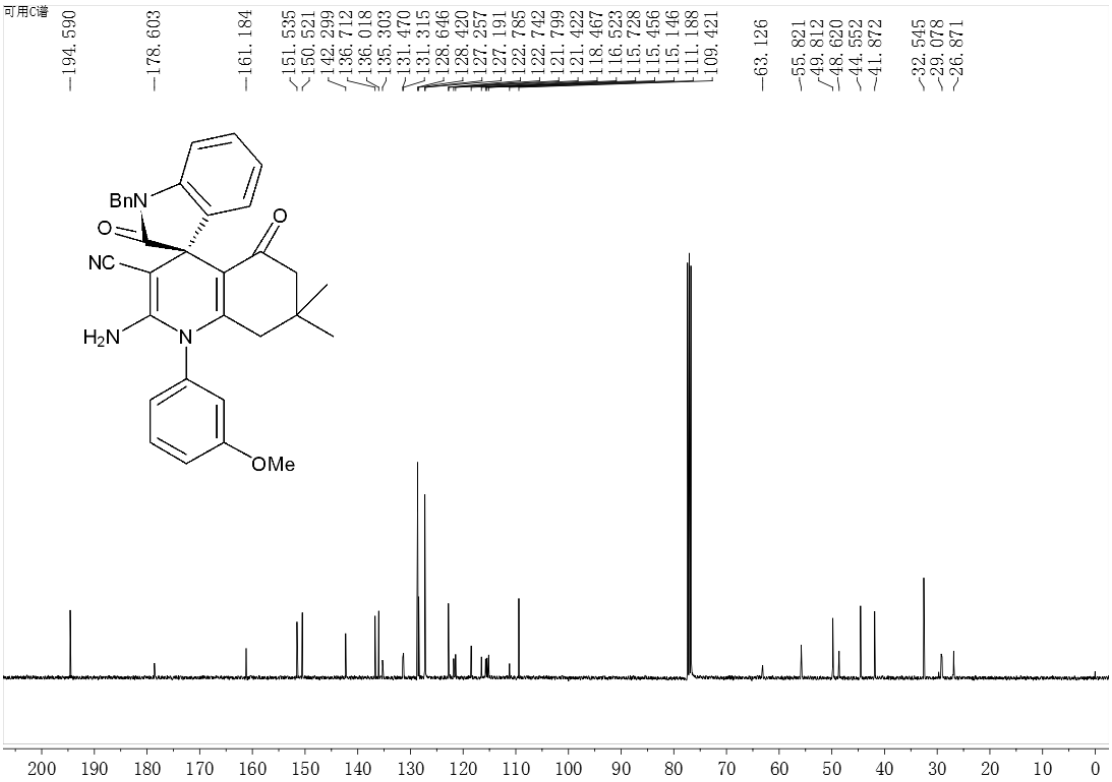
4da



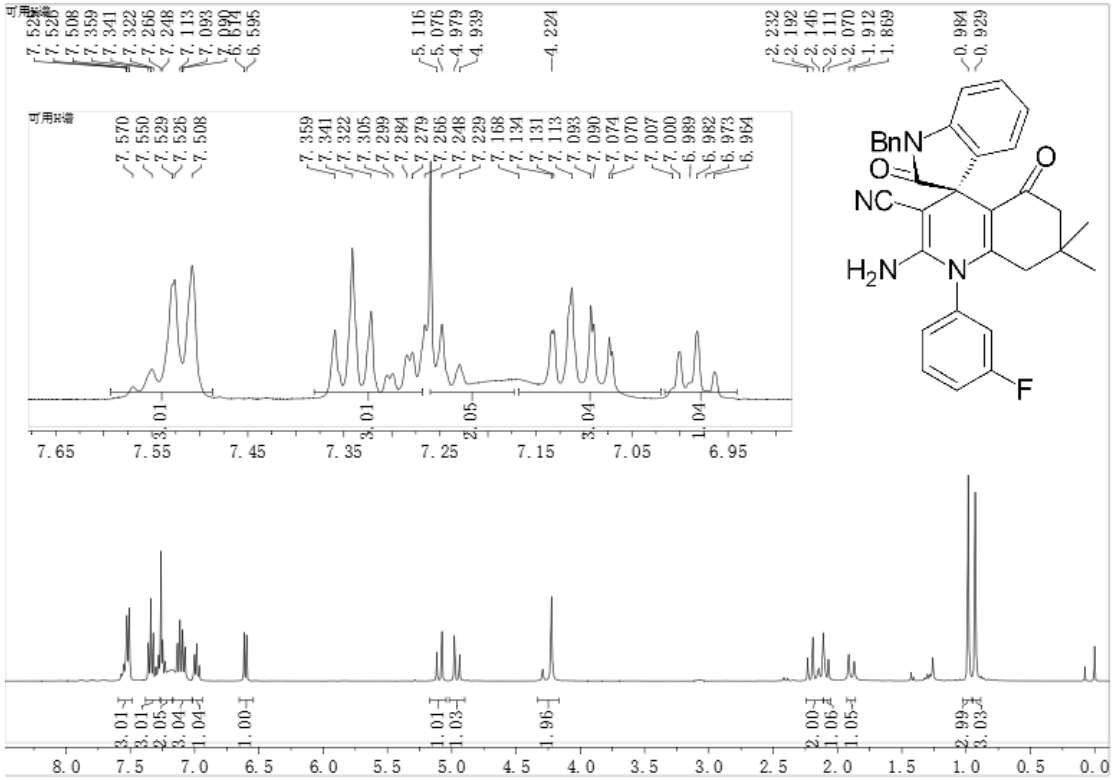


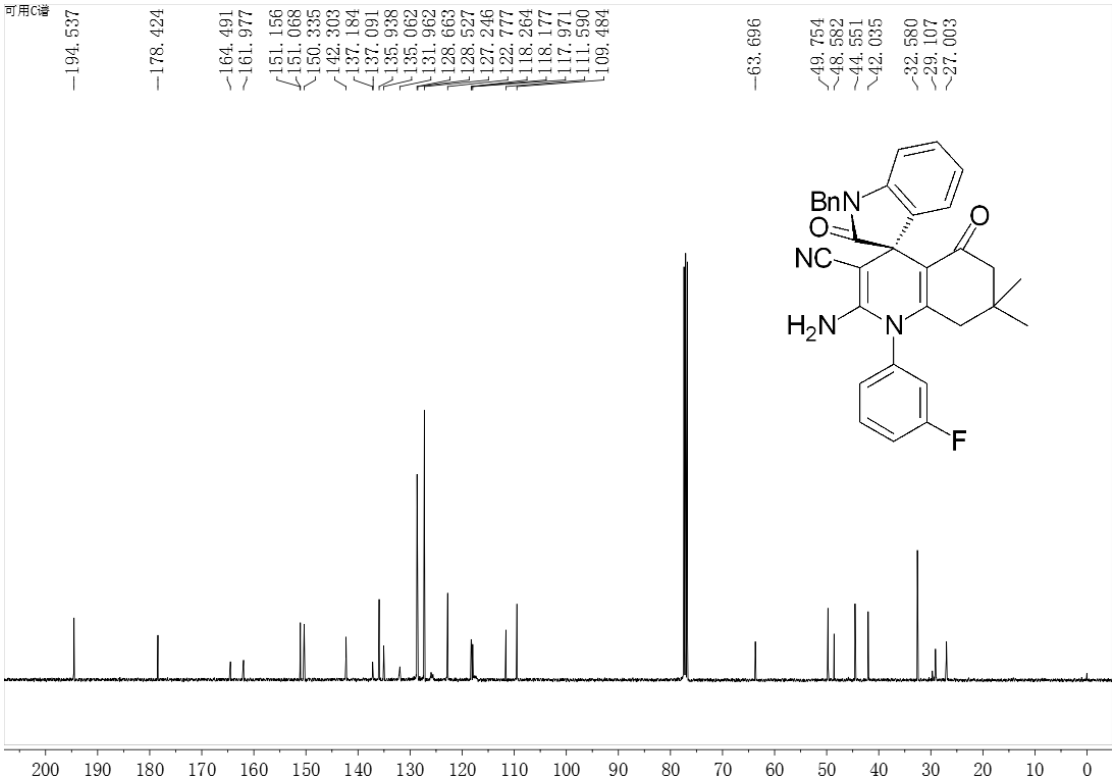
4ea



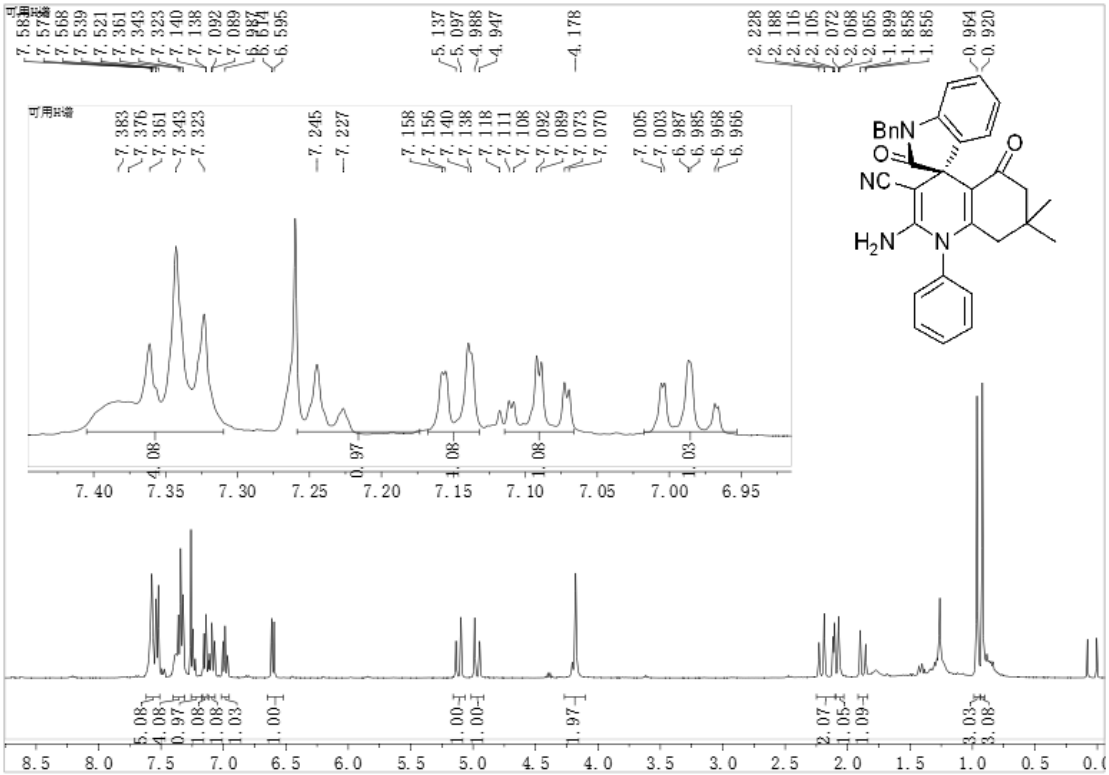


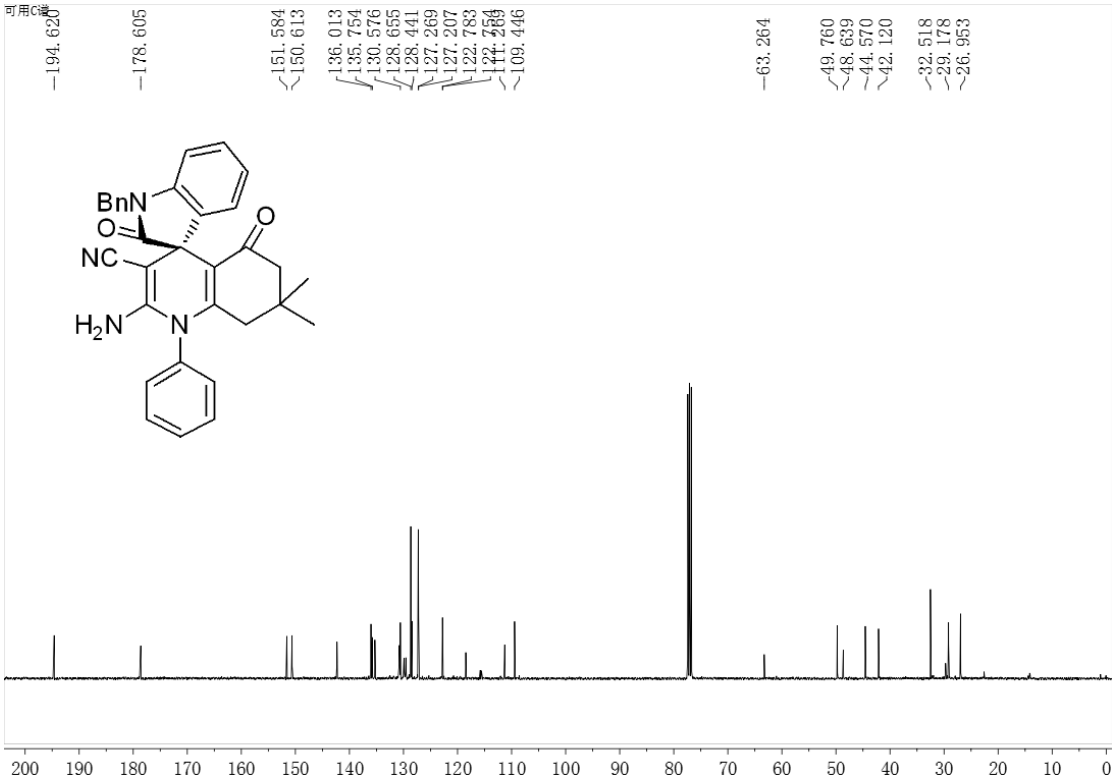
4fa



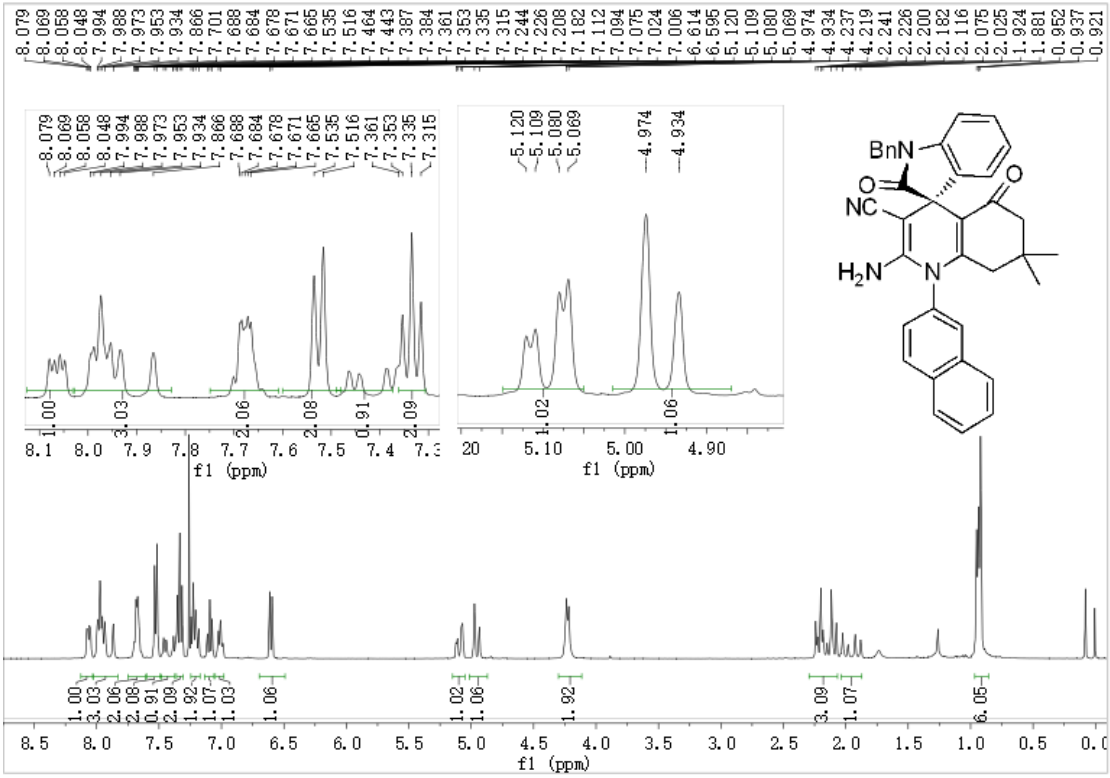


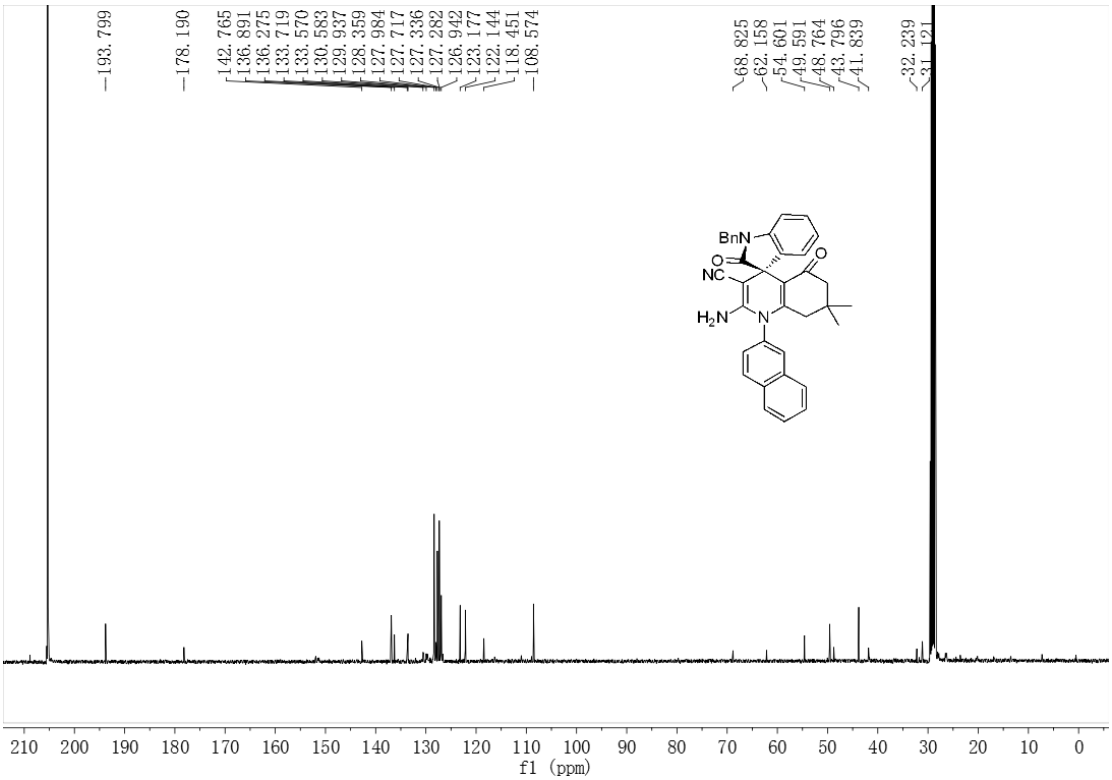
4ga



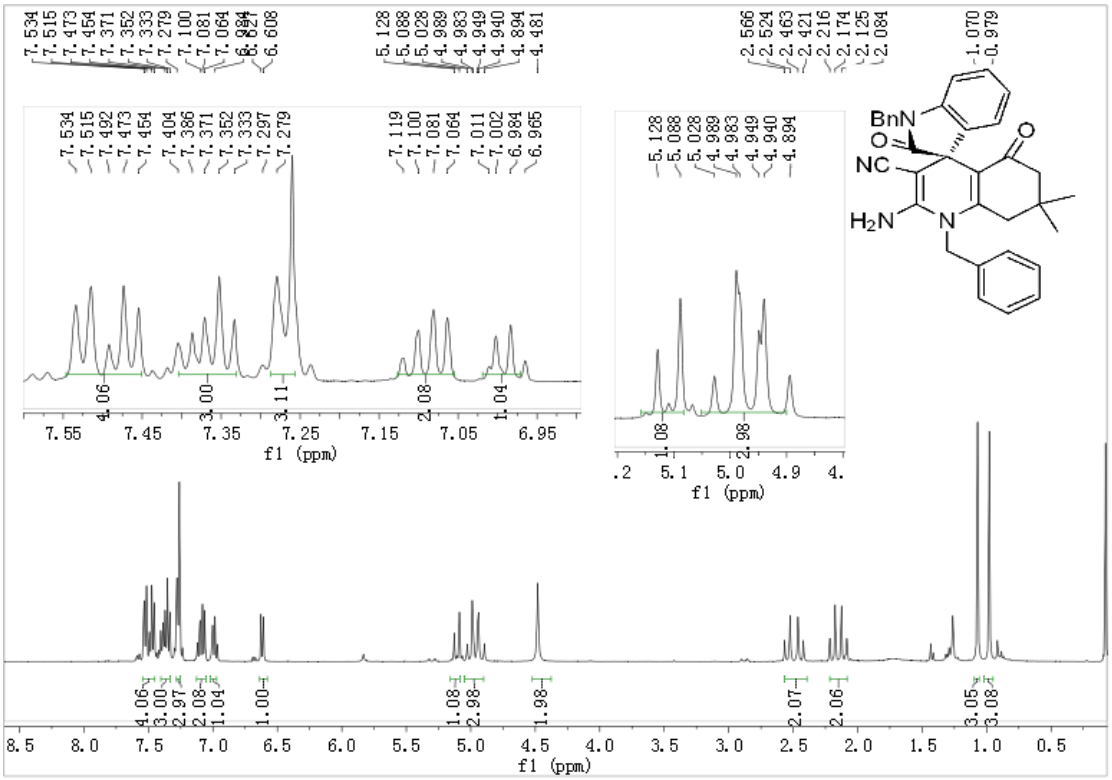


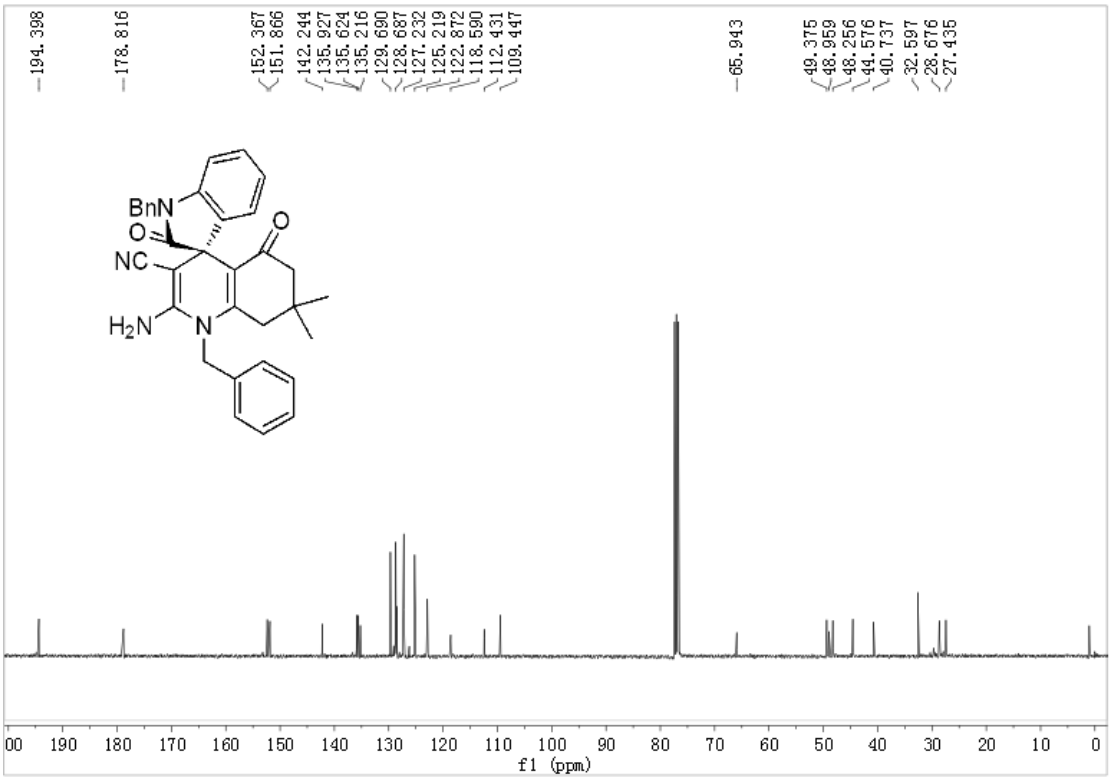
4ha



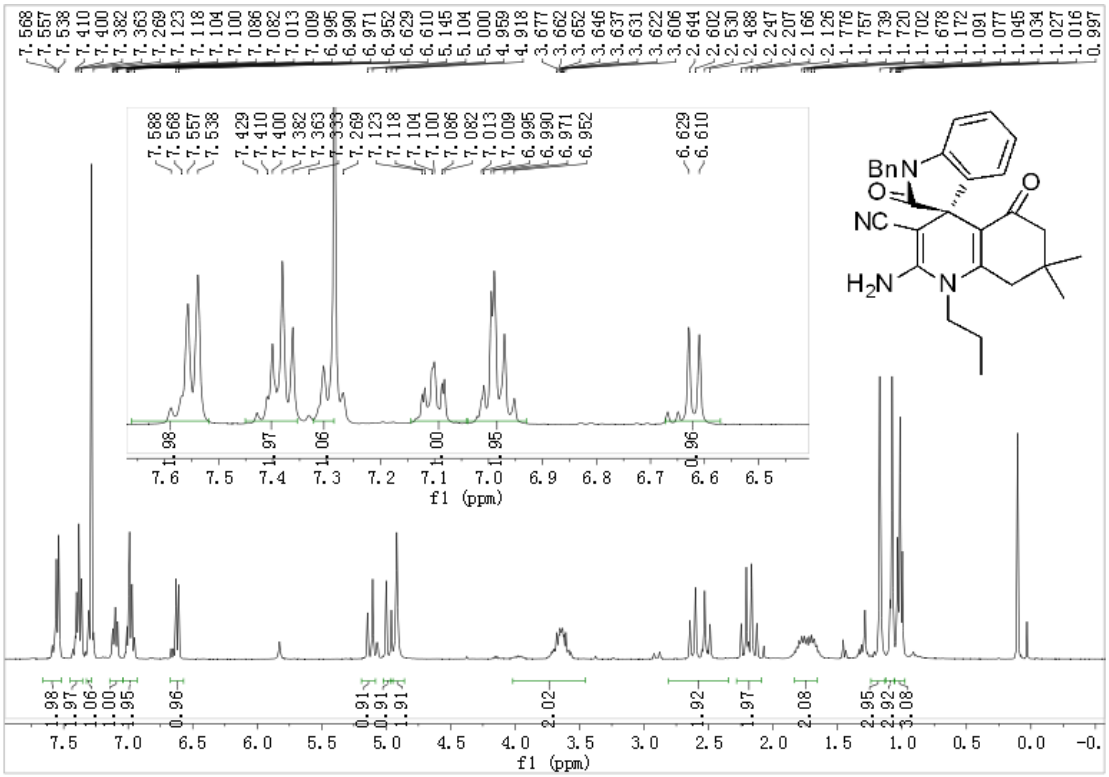


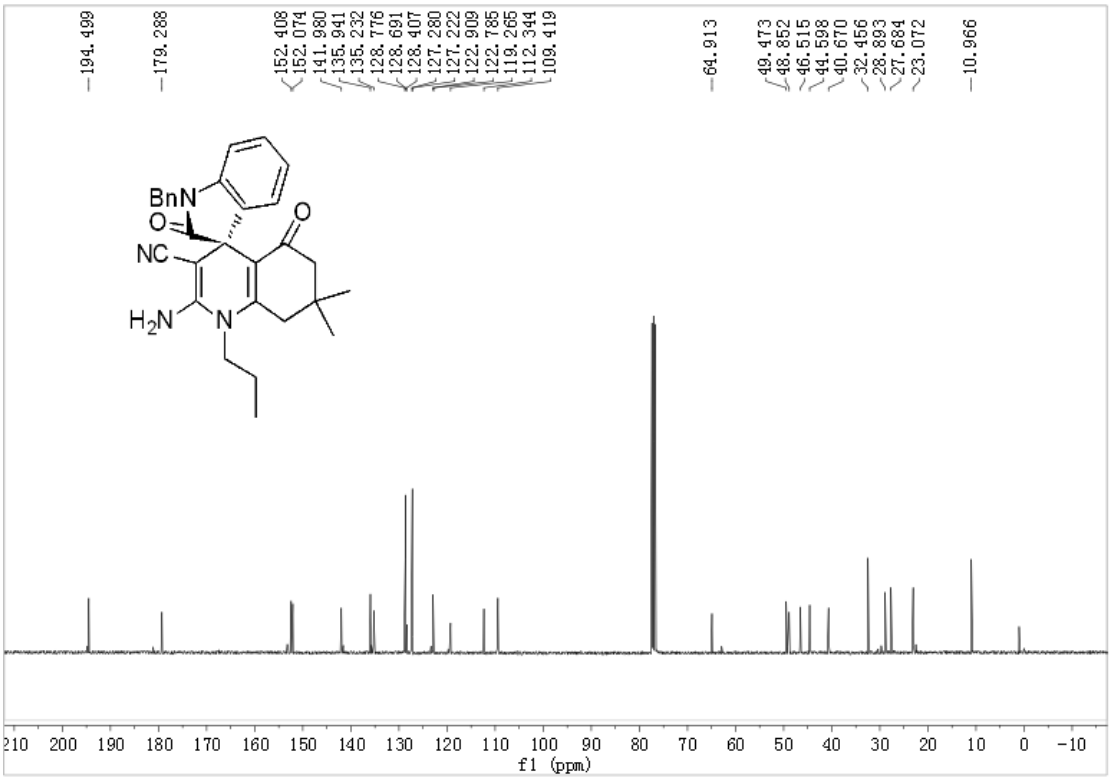
4ia



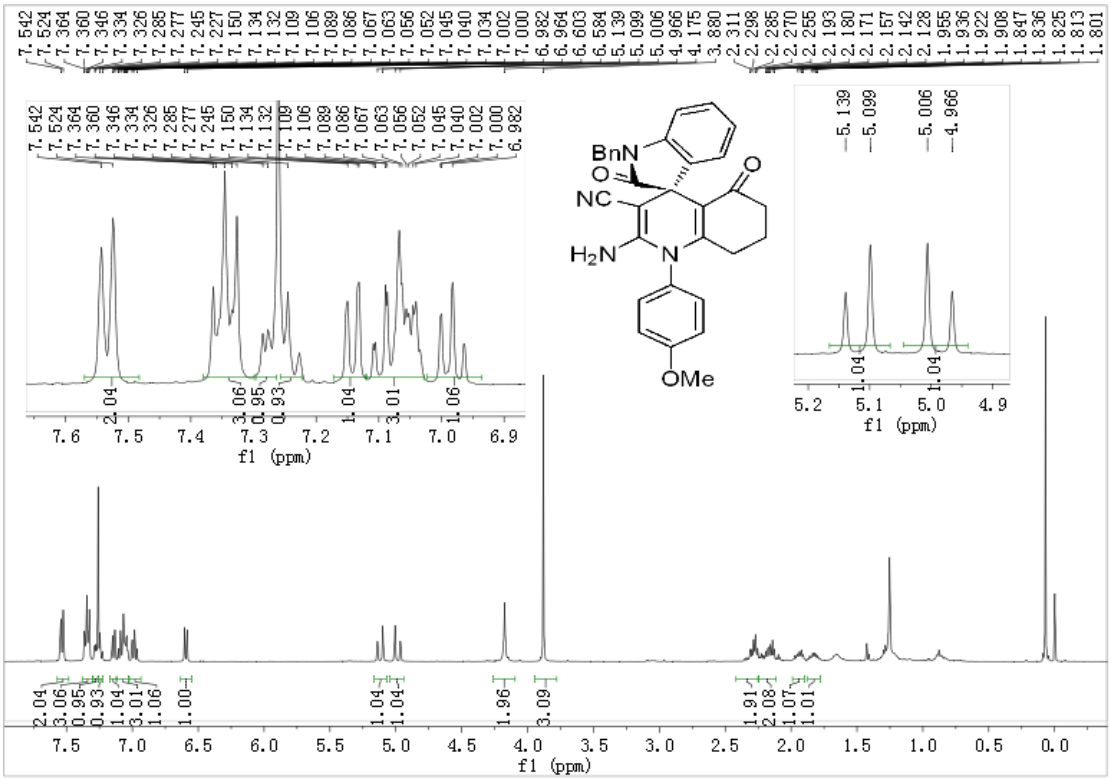


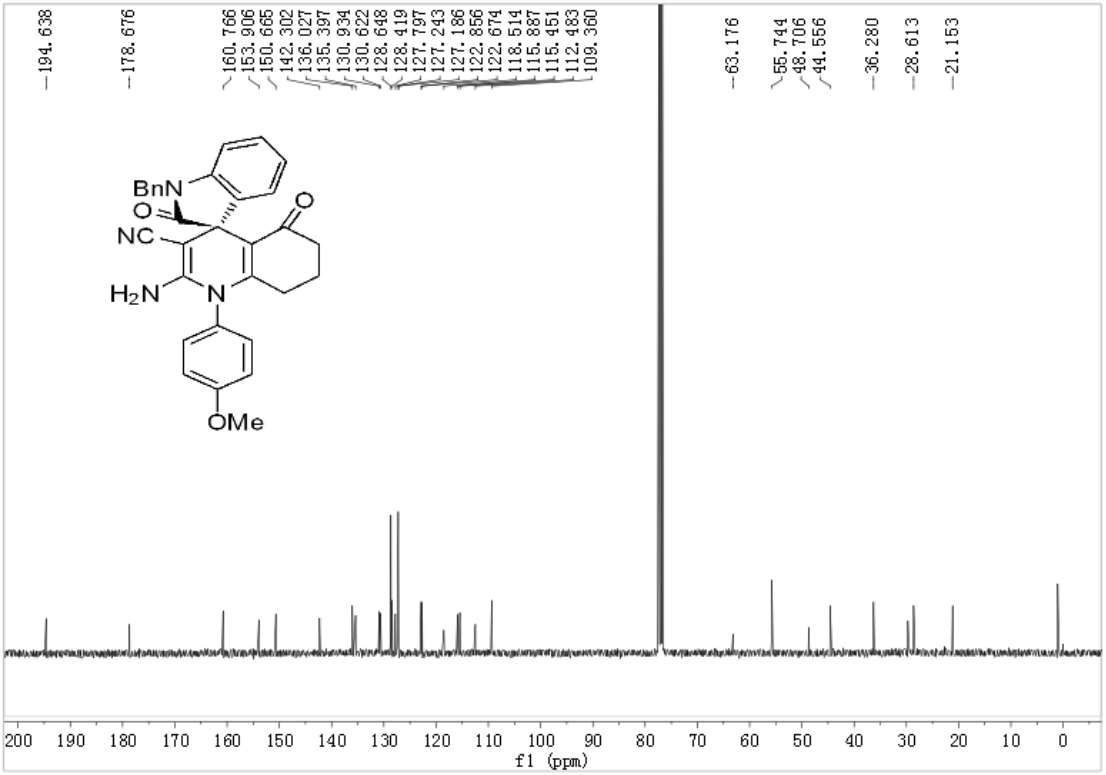
4ja



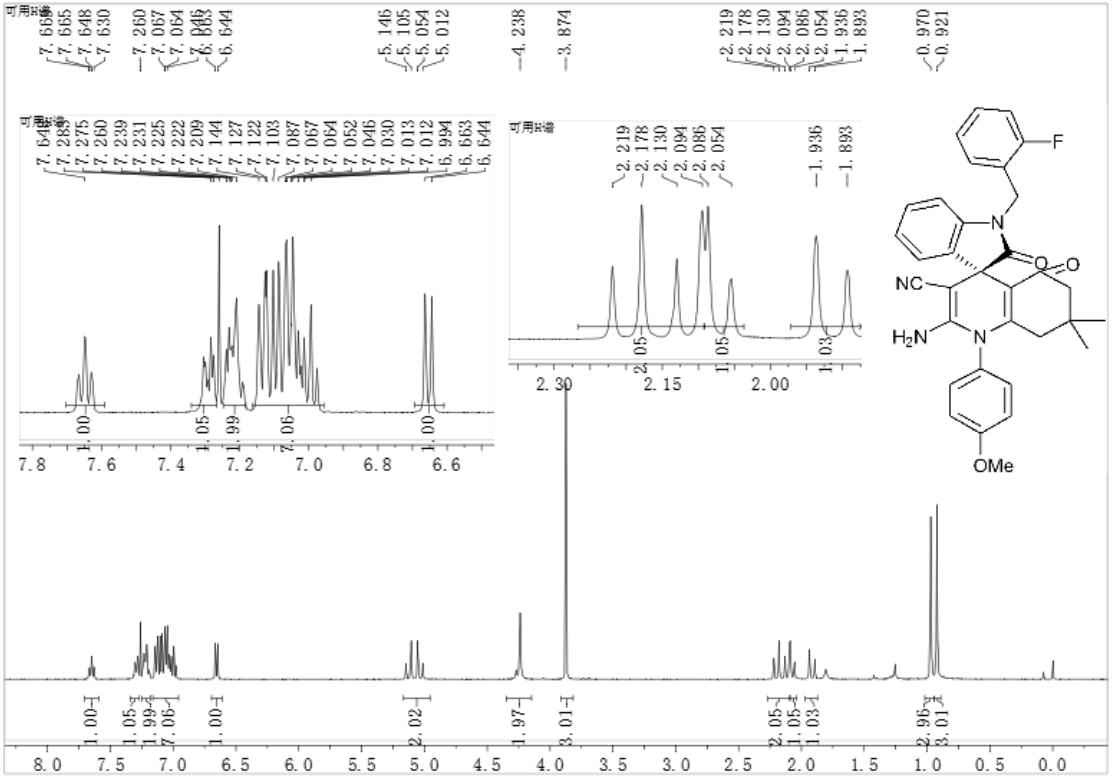


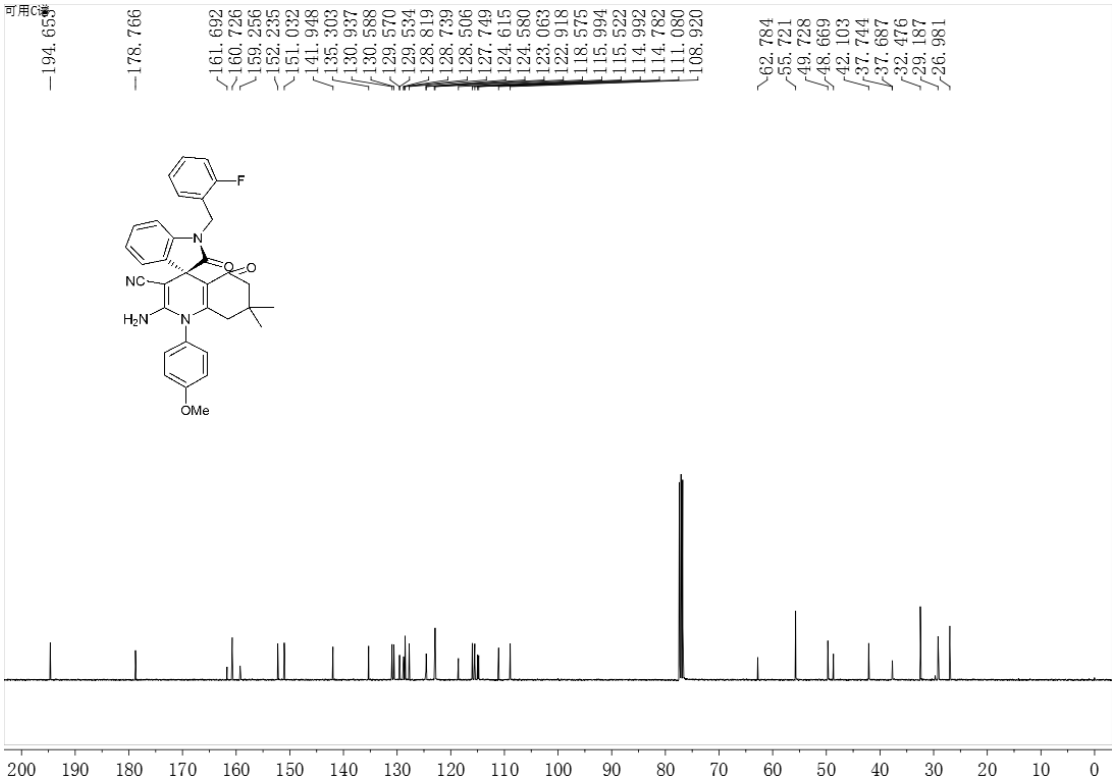
4ka



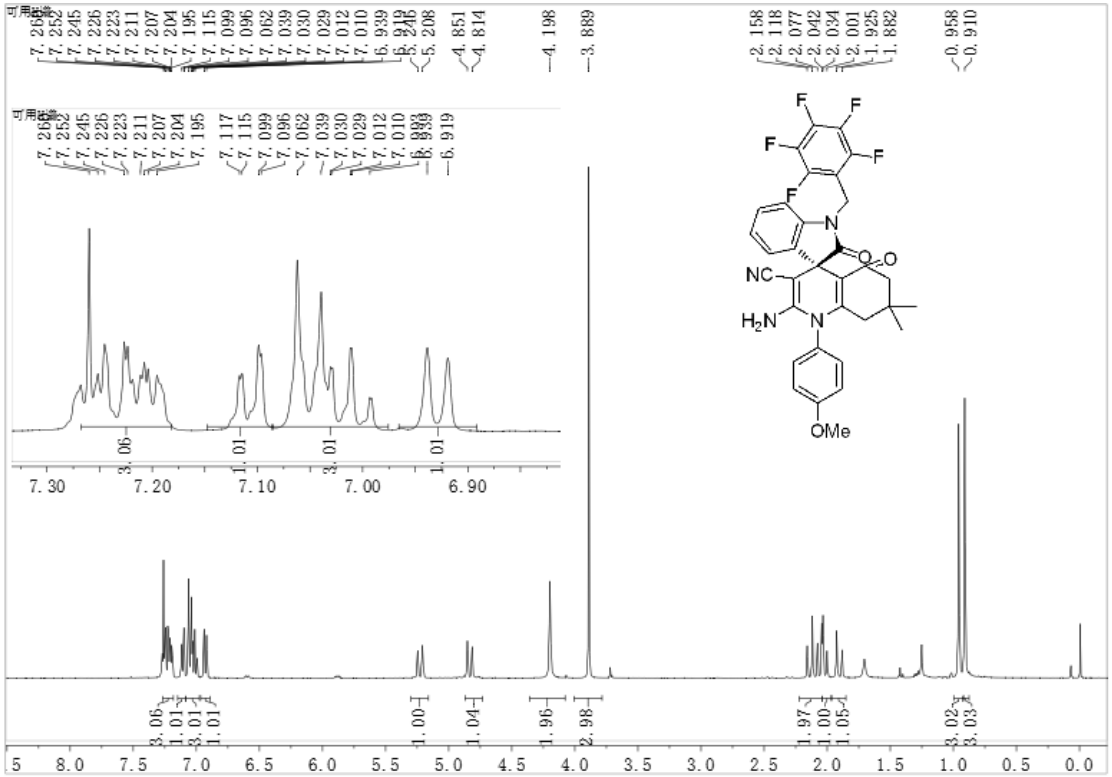


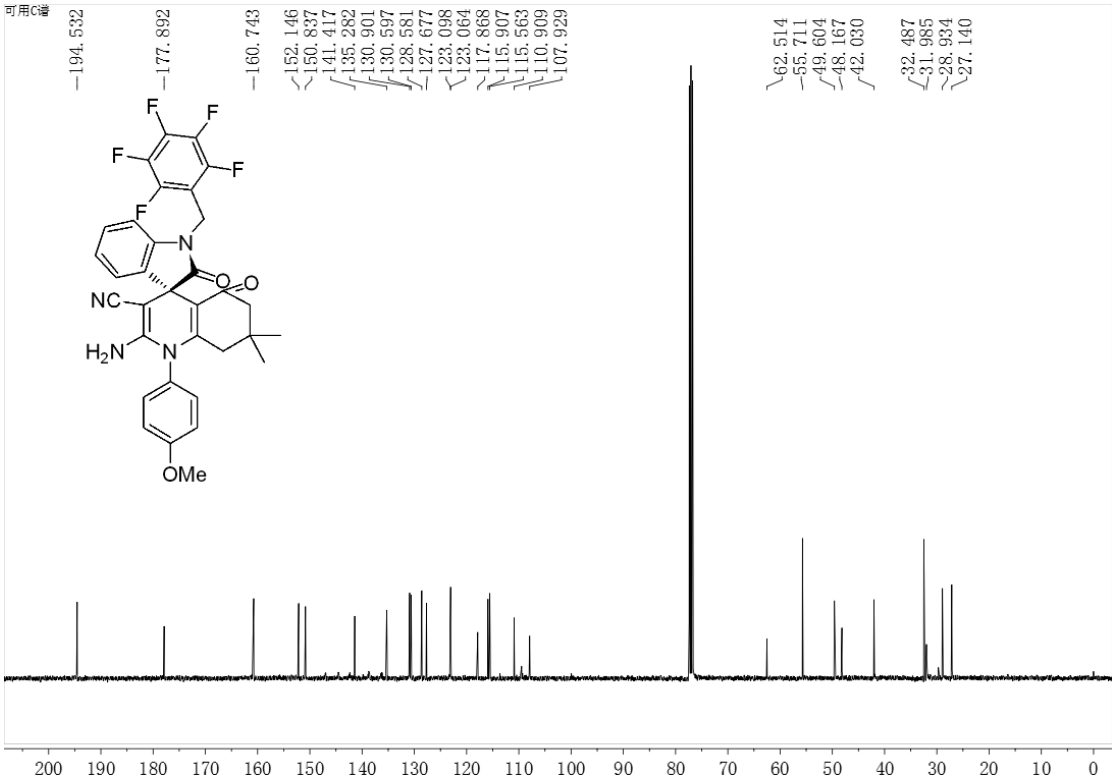
4ab



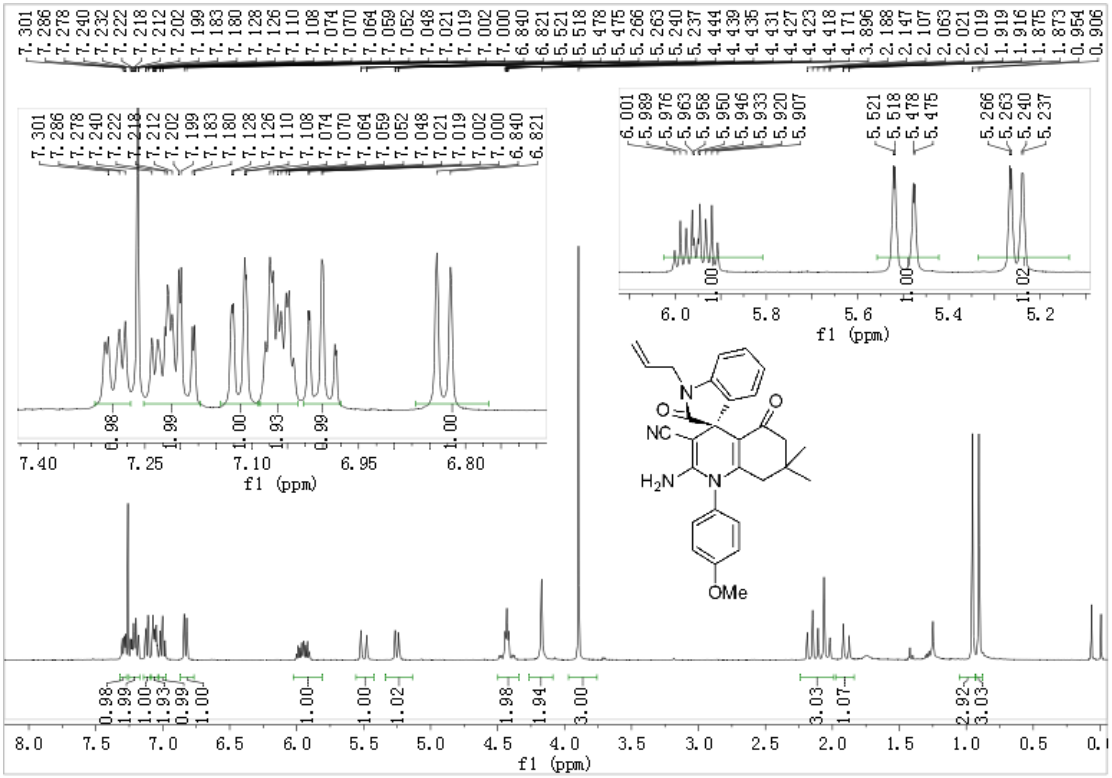


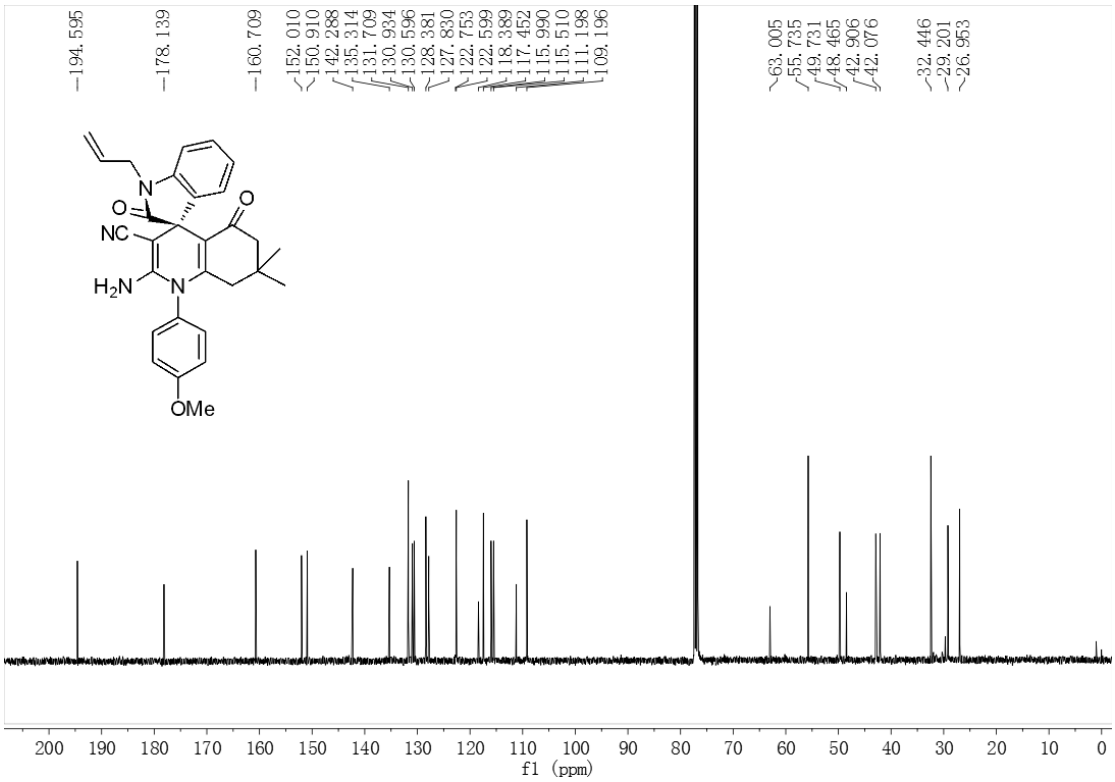
4ac



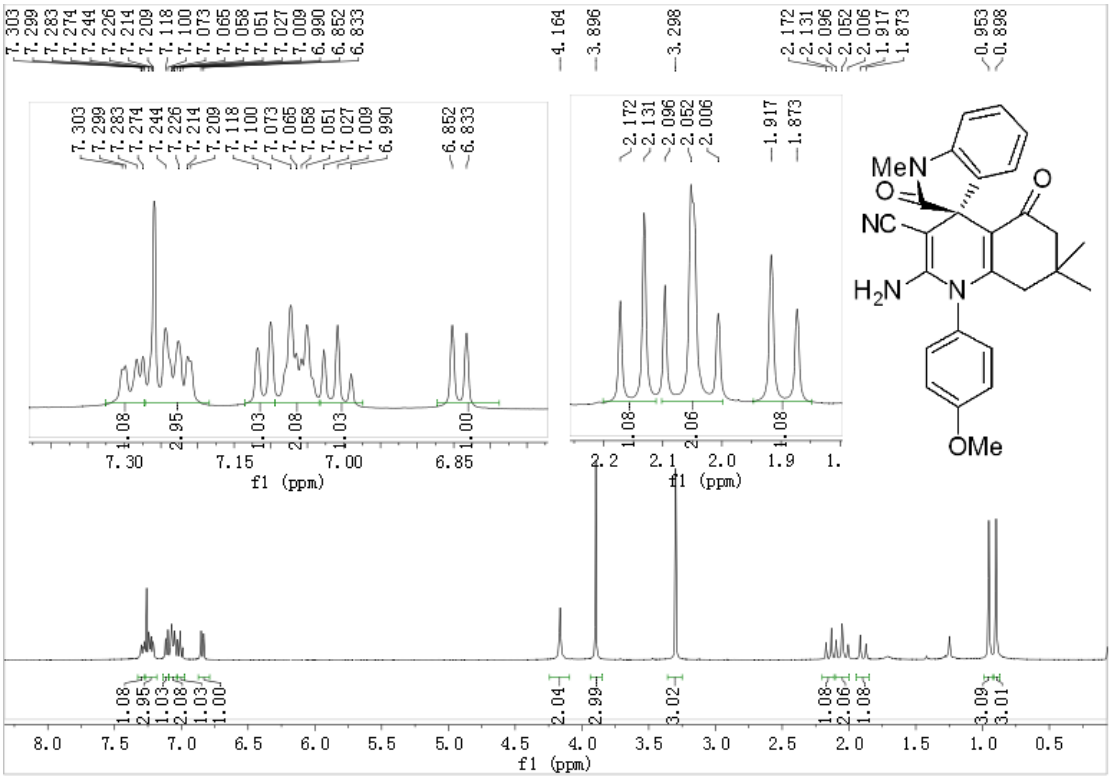


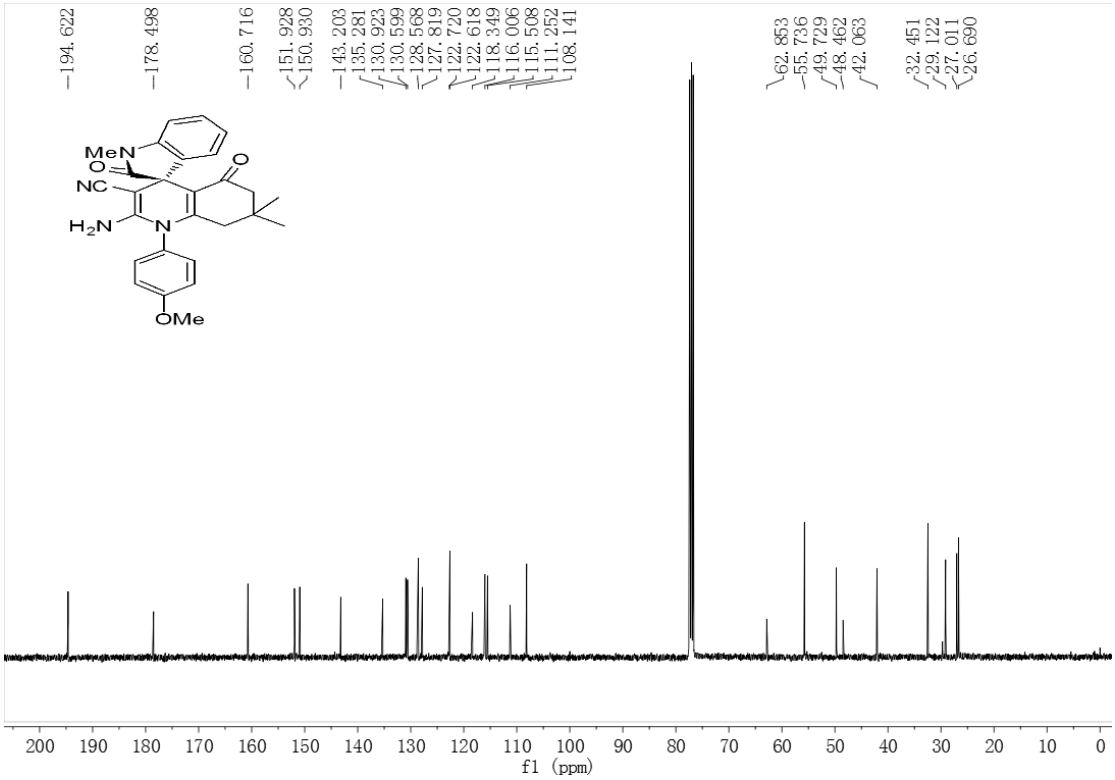
4ad



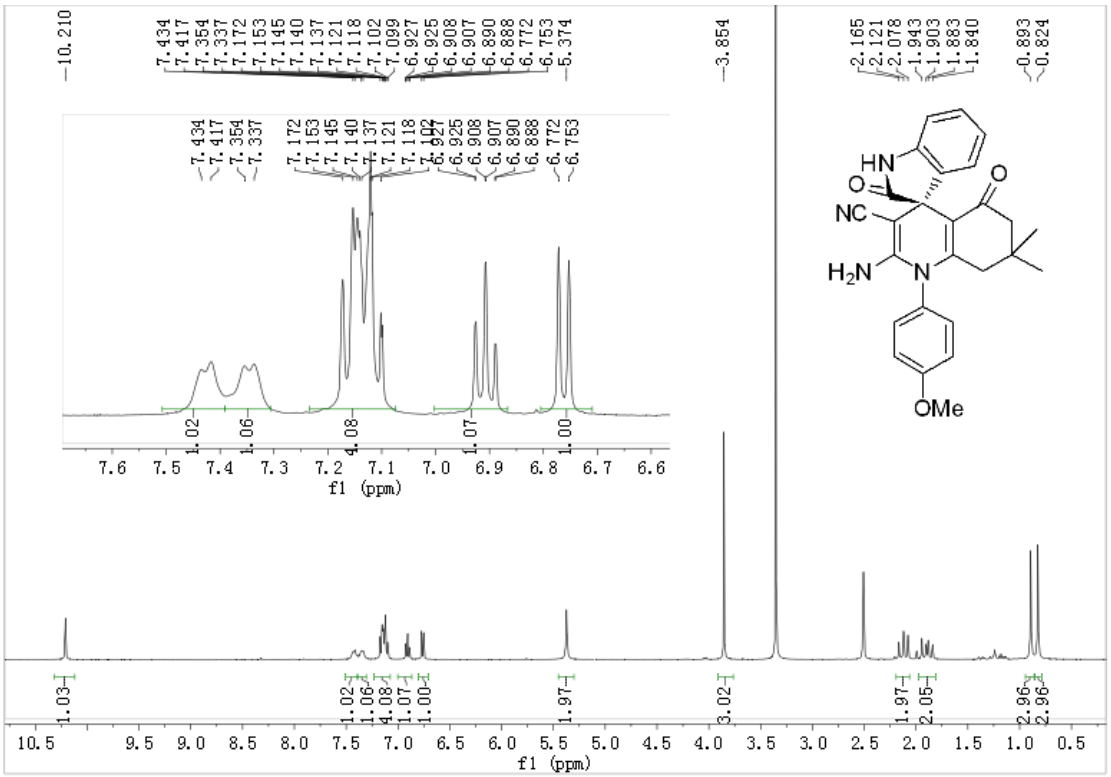


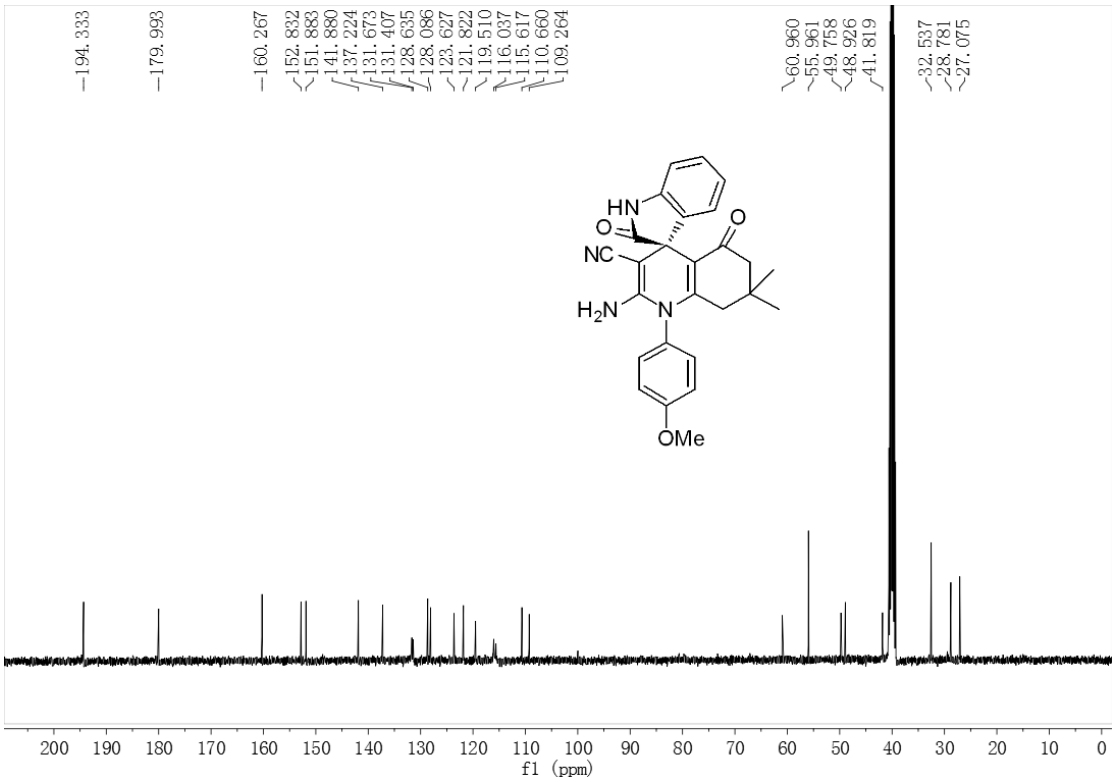
4ae


7.303
7.299
7.283
7.274
7.244
7.226
7.214
7.209
7.118
7.100
7.073
7.065
7.058
7.051
7.027
7.009
6.990
6.852
6.833
4.164
3.896
3.298
2.172
2.131
2.096
2.052
2.006
1.917
1.873
0.953
0.898
1.08
2.95
1.03
2.08
1.03
1.00
2.04
2.99
3.02
1.08
2.06
1.08
3.09
3.01
f1 (ppm)
MeN
O
NC
H2N
N
OMe

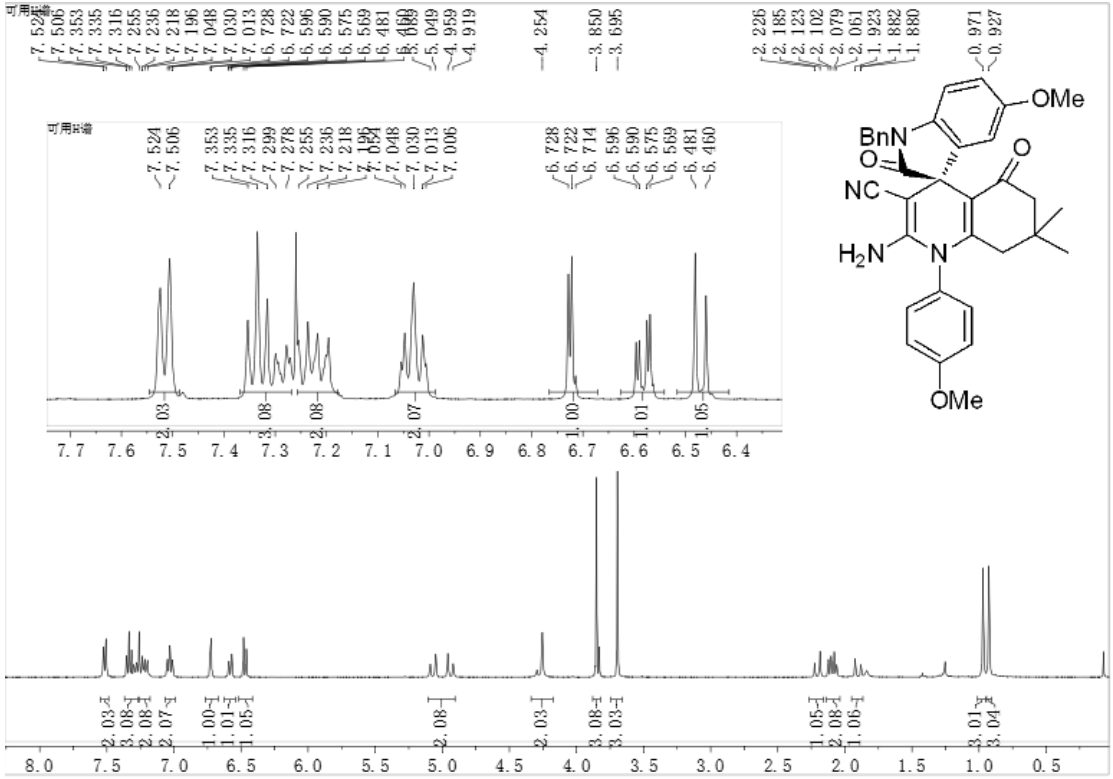

194.622
178.498
160.716
151.928
150.930
143.203
135.281
130.923
130.599
128.568
127.819
122.720
122.618
118.349
116.006
115.508
111.252
108.141
62.853
55.736
49.729
48.462
42.063
32.451
29.122
27.011
26.690
MeN
O
NC
H2N
N
OMe
f1 (ppm)

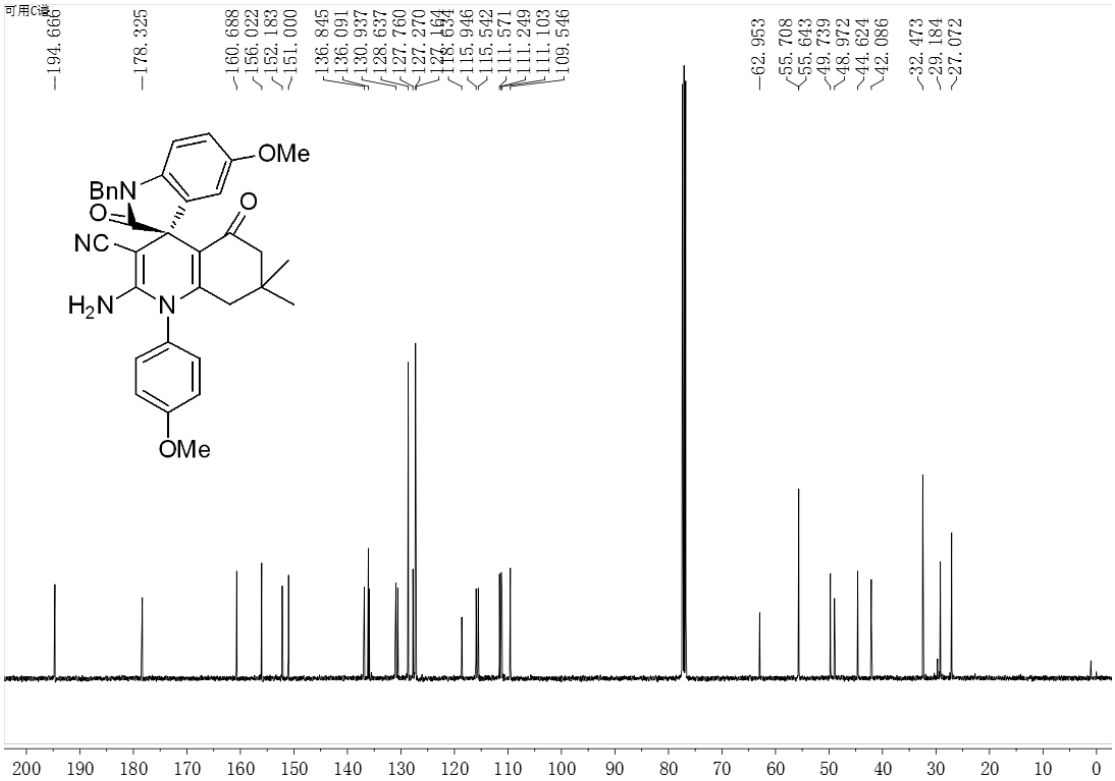
4af


10.210
7.434
7.417
7.354
7.337
7.172
7.153
7.145
7.140
7.137
7.121
7.118
7.102
7.099
6.927
6.925
6.908
6.907
6.890
6.888
6.772
6.753
5.374
3.854
2.165
2.121
2.078
1.943
1.903
1.883
1.840
0.893
0.824
HN
O
NC
H2N
N
OMe
1.03
1.02
1.06
4.08
1.07
1.00
1.97
3.02
1.97
2.05
2.96
2.96
f1 (ppm)

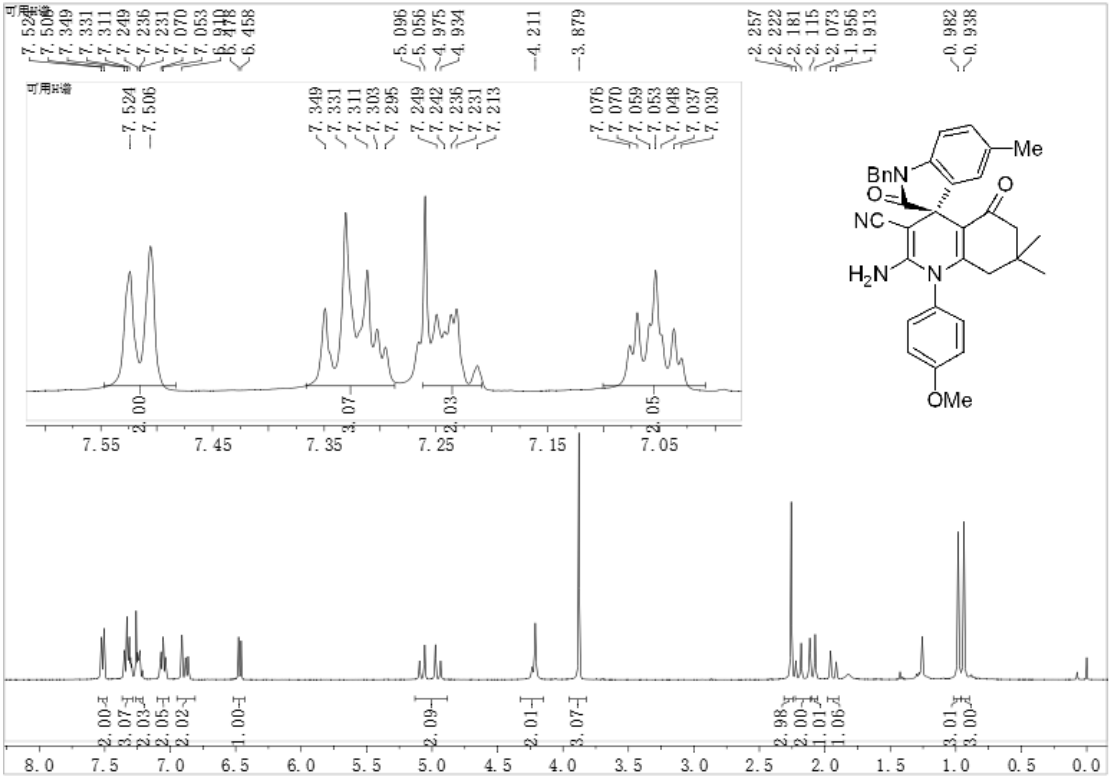

194.333
179.993
160.267
152.832
151.883
141.880
137.224
131.673
131.407
128.635
128.086
123.627
121.822
119.510
116.037
115.617
110.660
109.264
60.960
55.961
49.758
48.926
41.819
32.537
28.781
27.075
HN
O
NC
H2N
N
OMe
f1 (ppm)

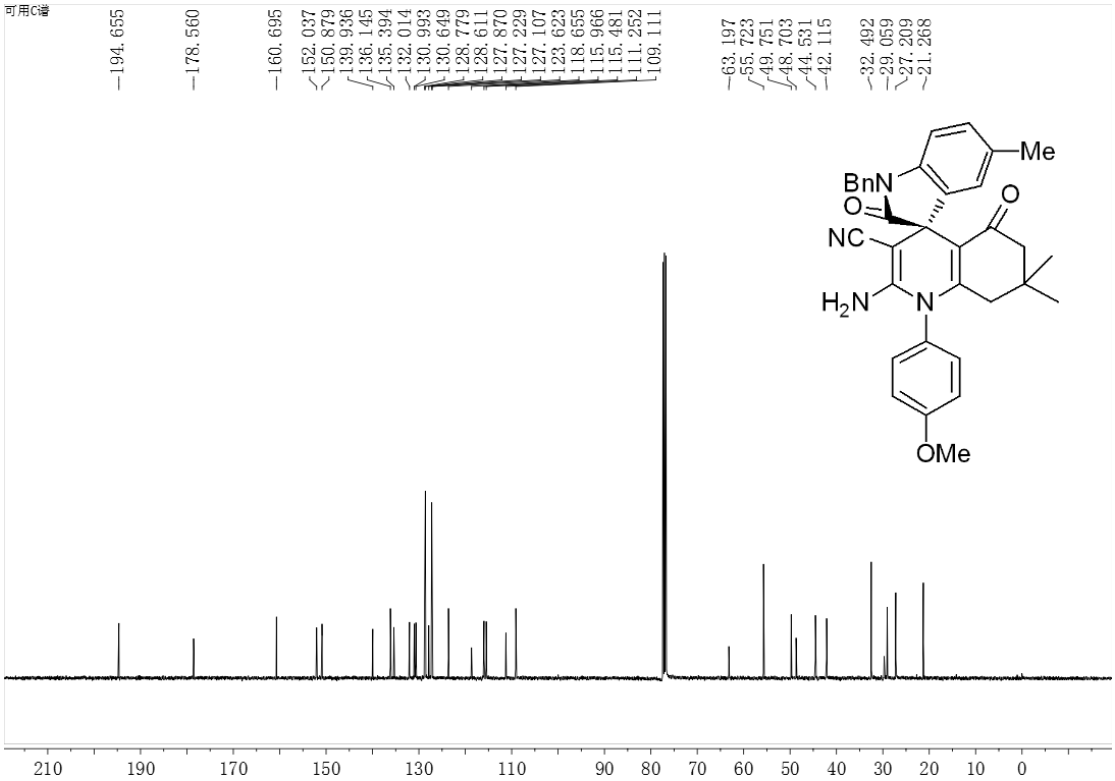
4ag



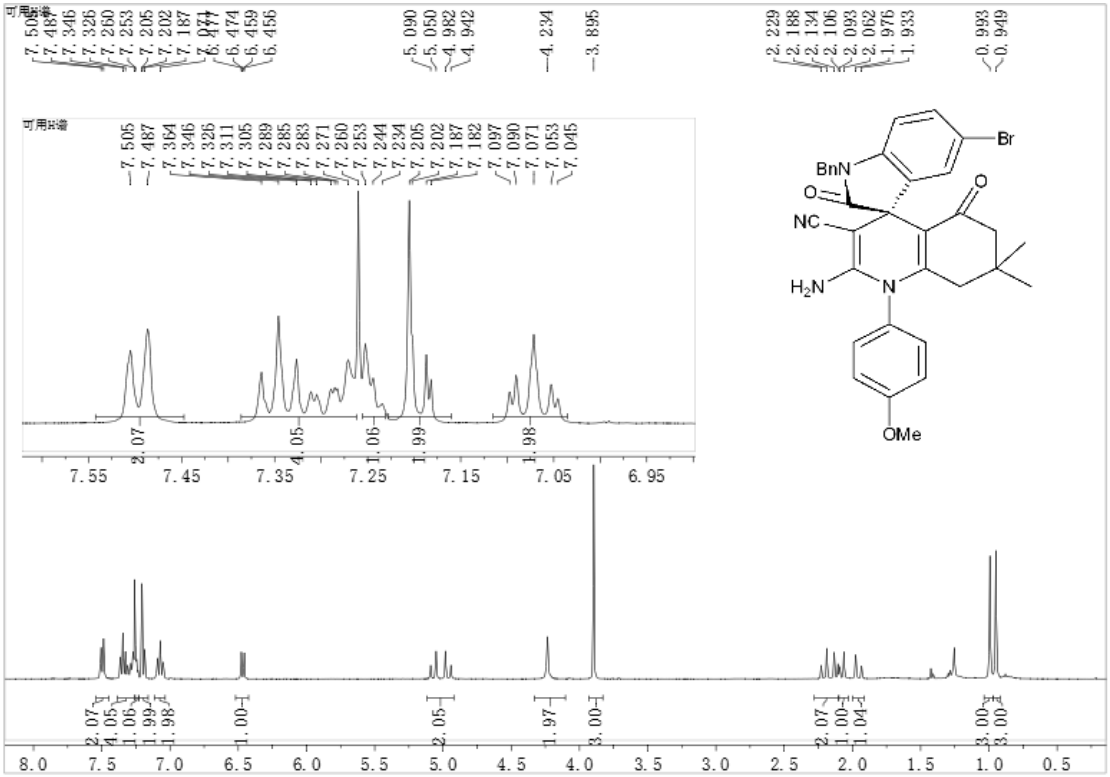


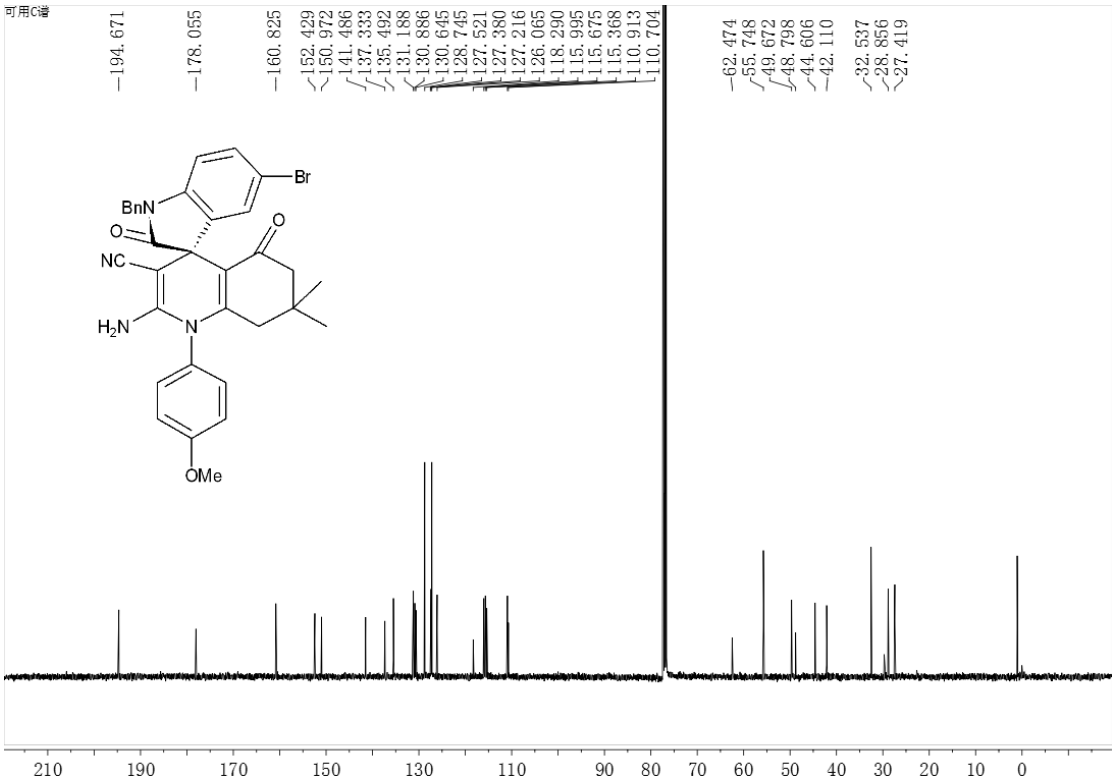
4ah



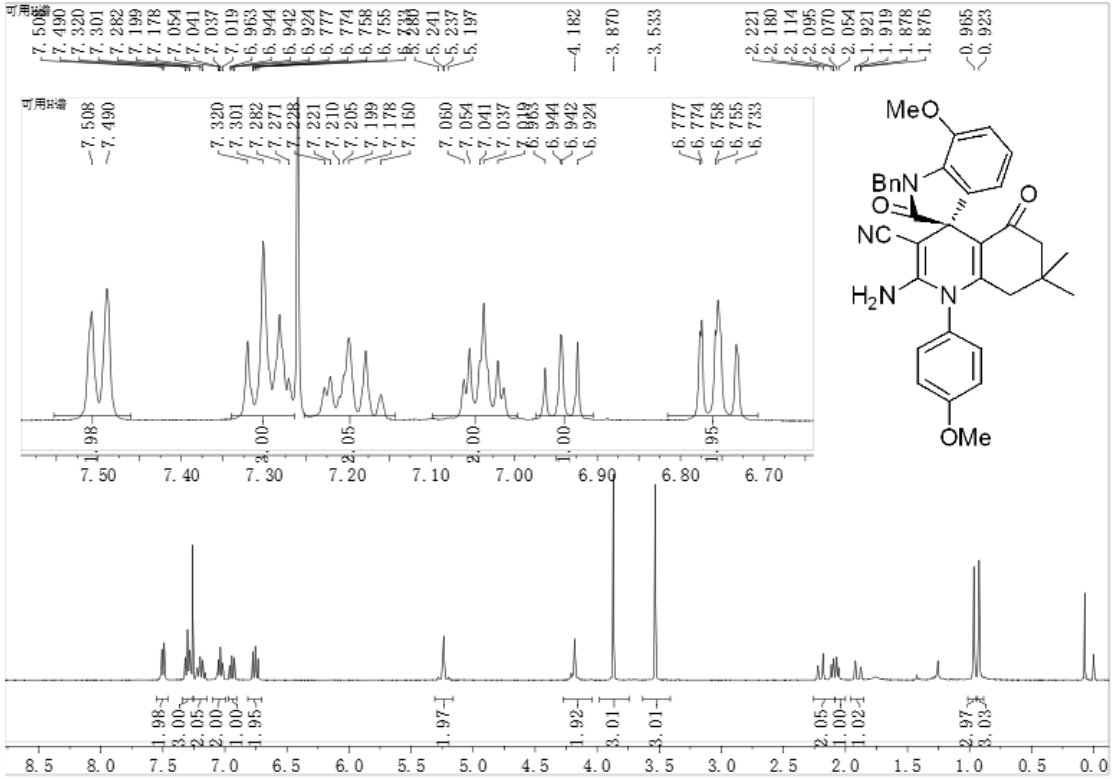


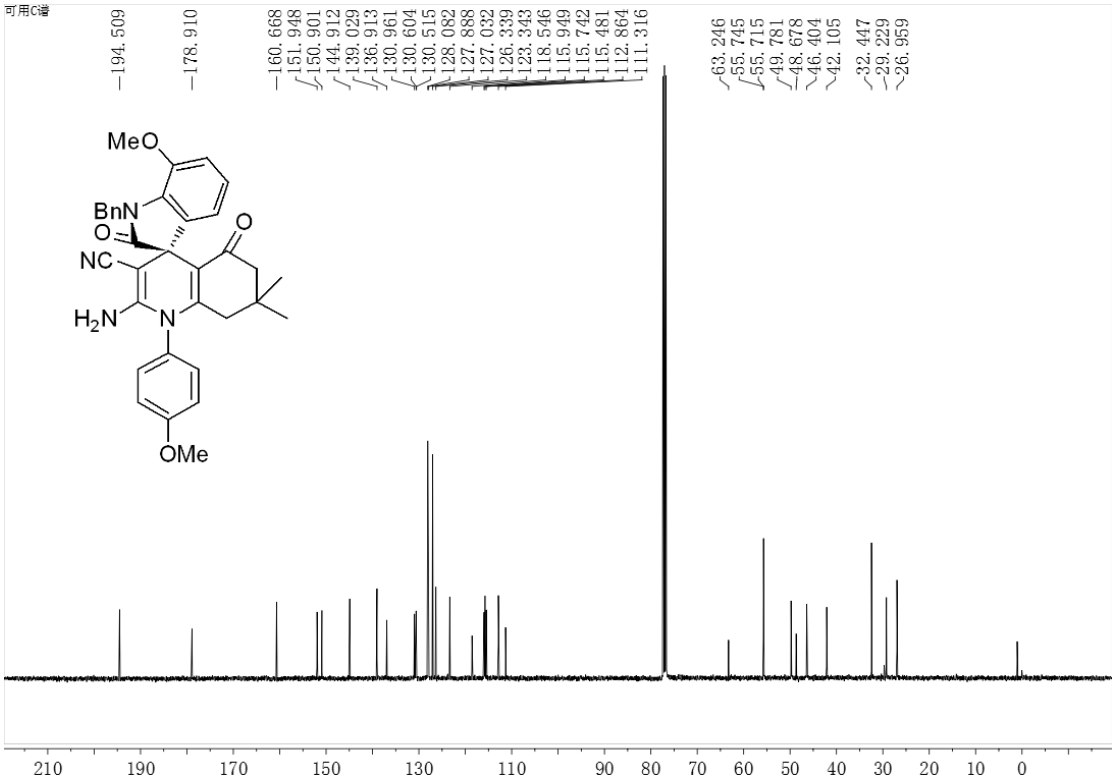
4ai



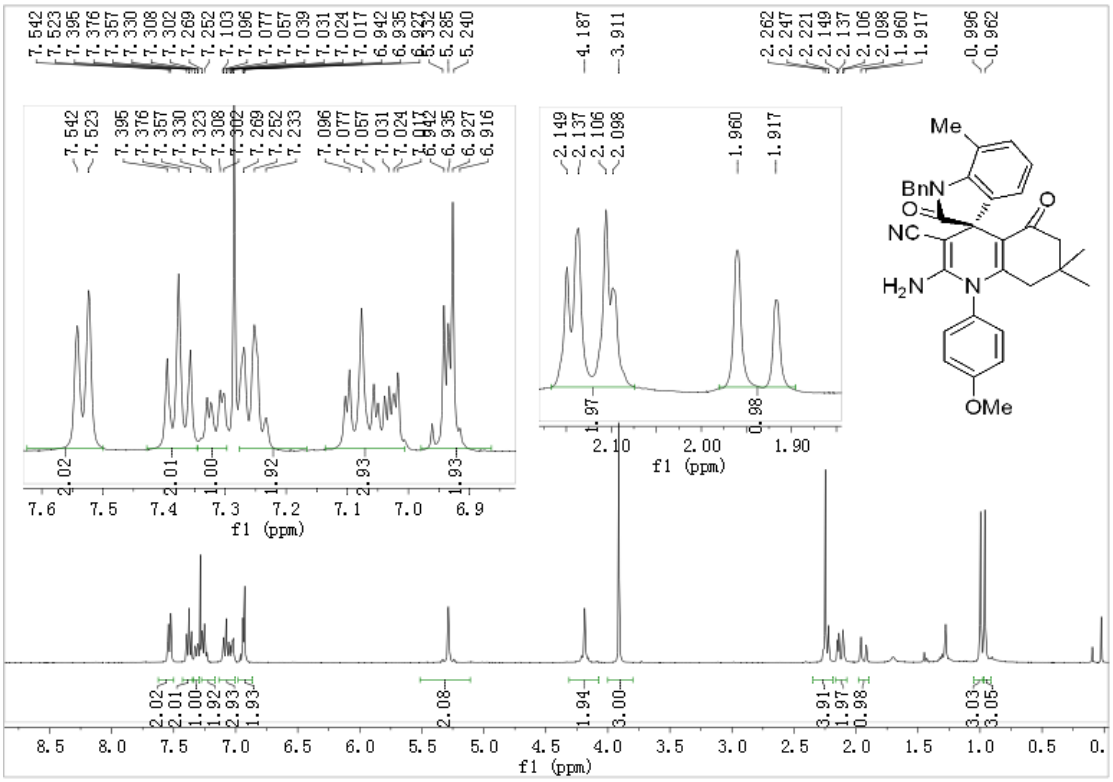


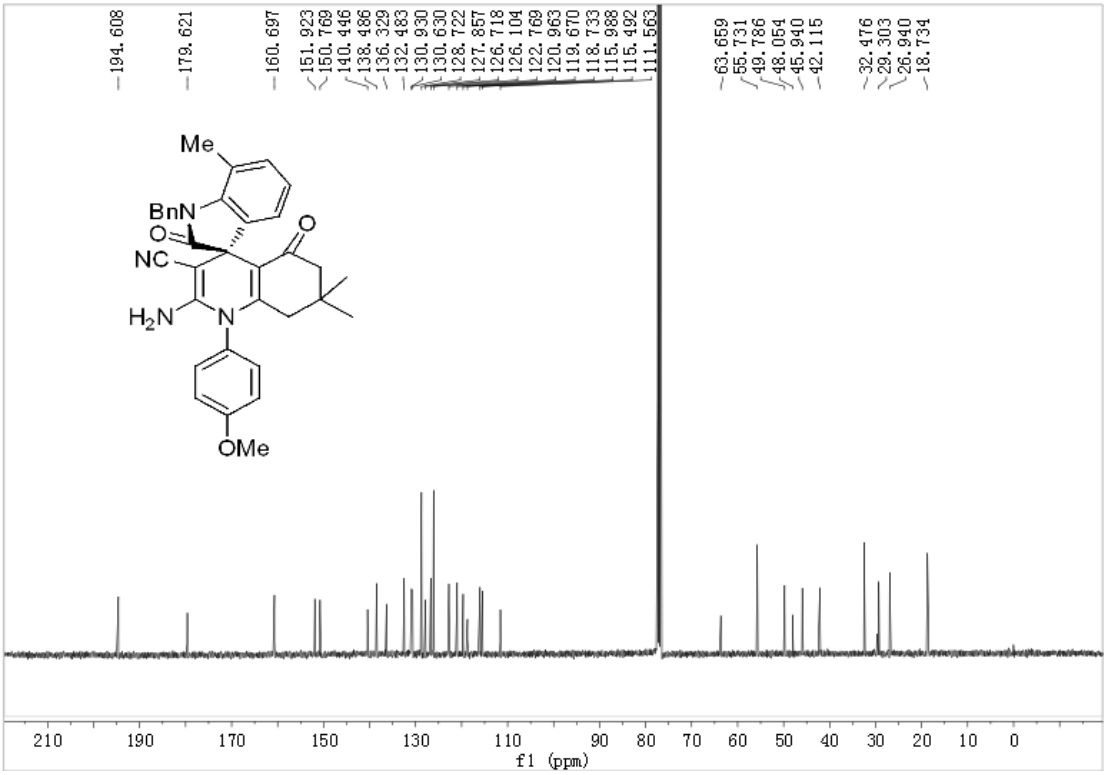
4aj



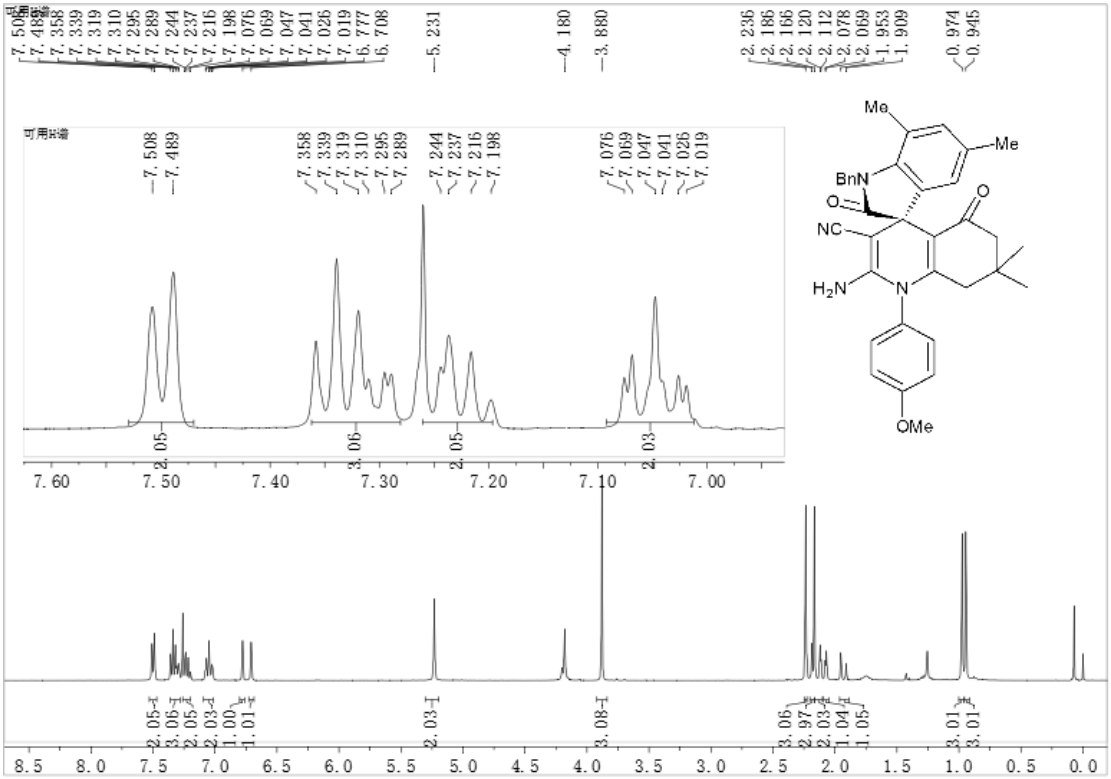


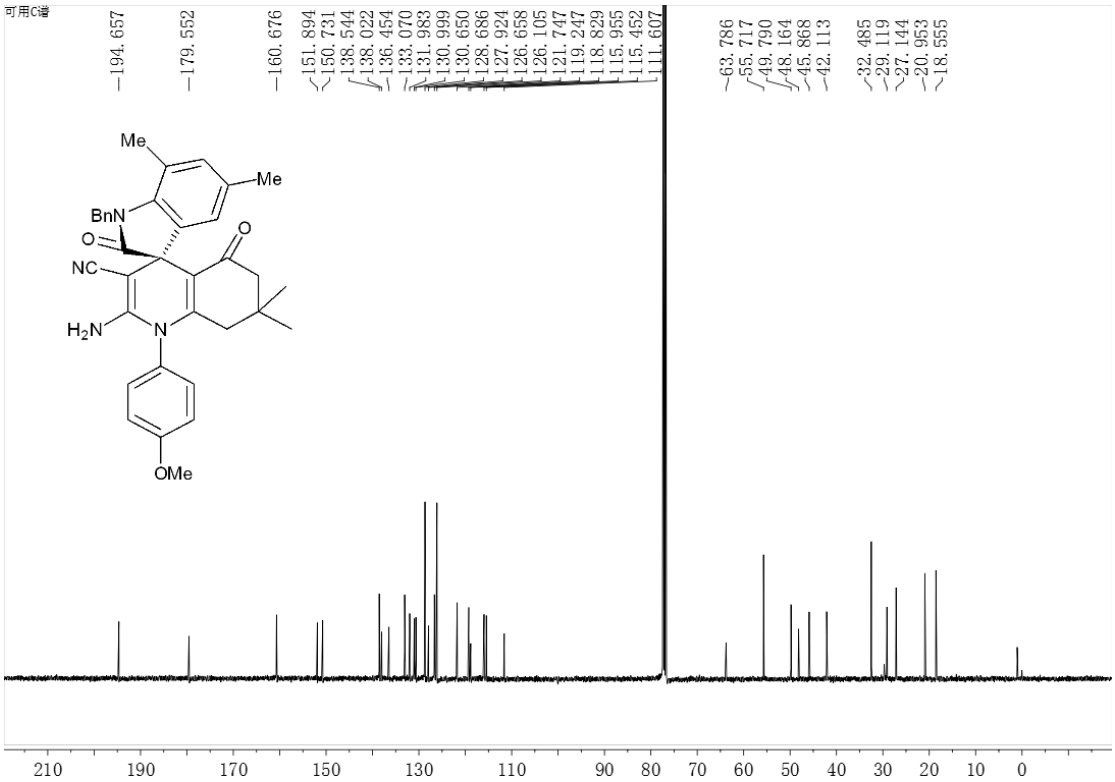
4ak



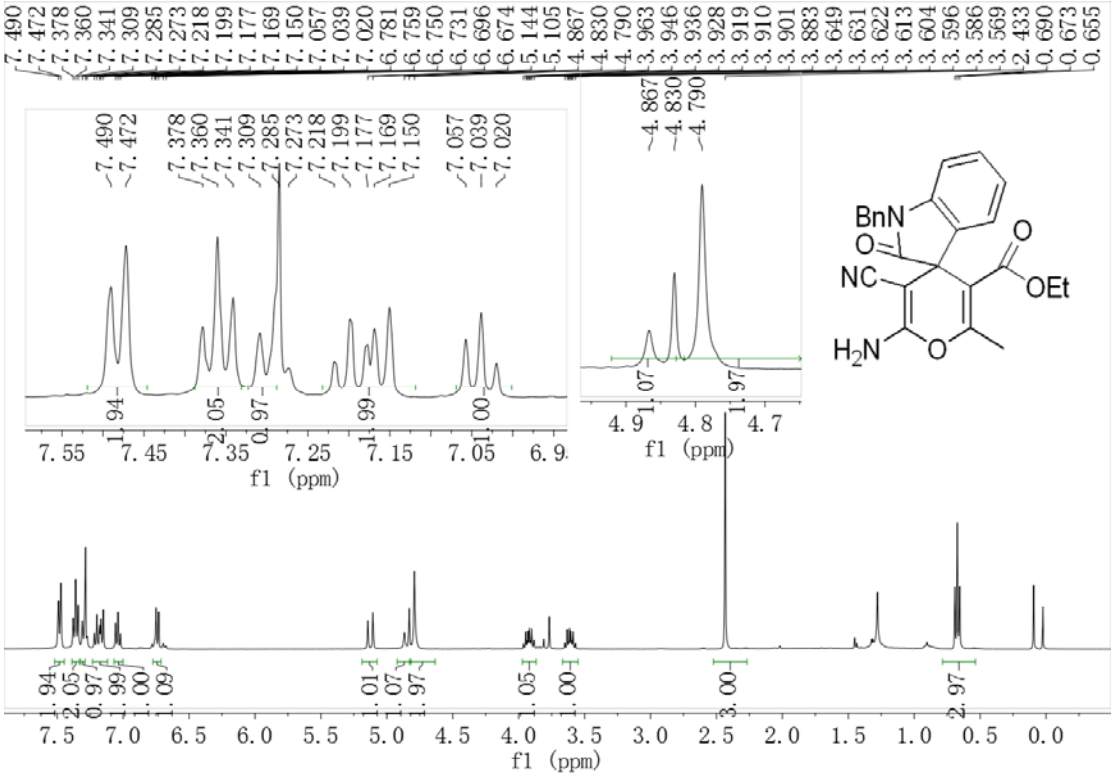


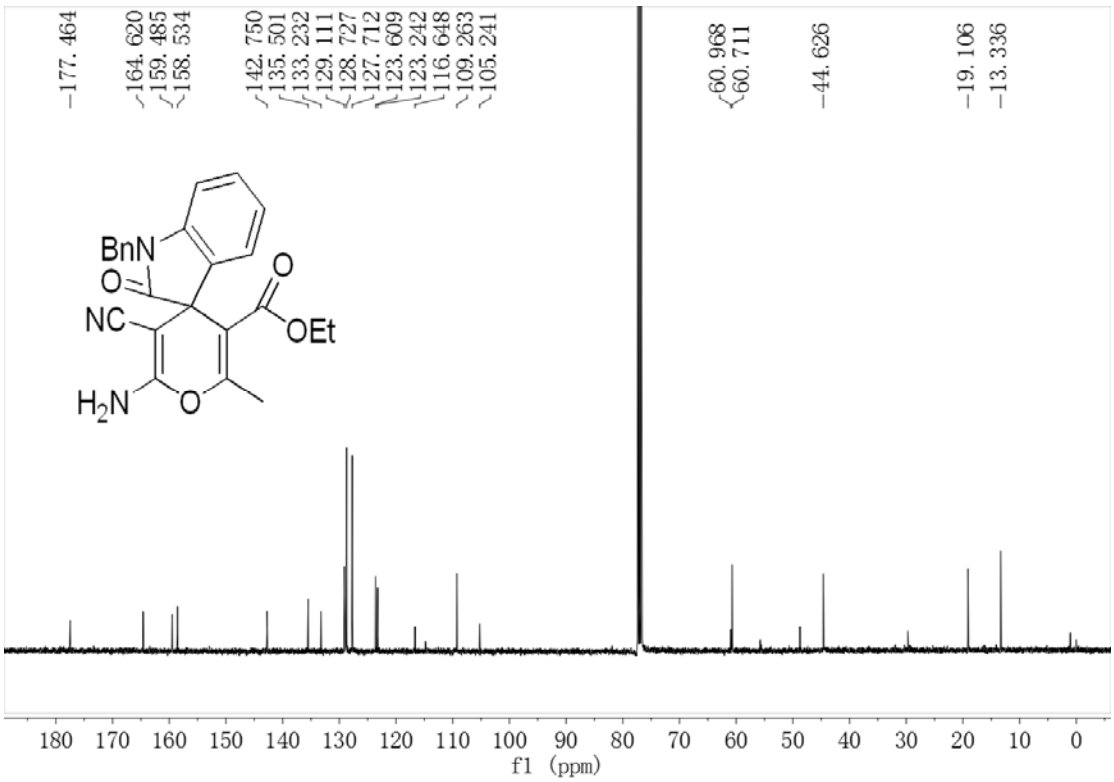
4al


7.508
7.489
7.358
7.339
7.319
7.310
7.295
7.289
7.244
7.237
7.216
7.198
7.076
7.069
7.047
7.041
7.026
7.019
5.231
4.180
3.880
0.974
0.945
Me
Me
BnN
O
NC
H2N
N
OMe
7.60
7.50
7.40
7.30
7.20
7.10
7.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

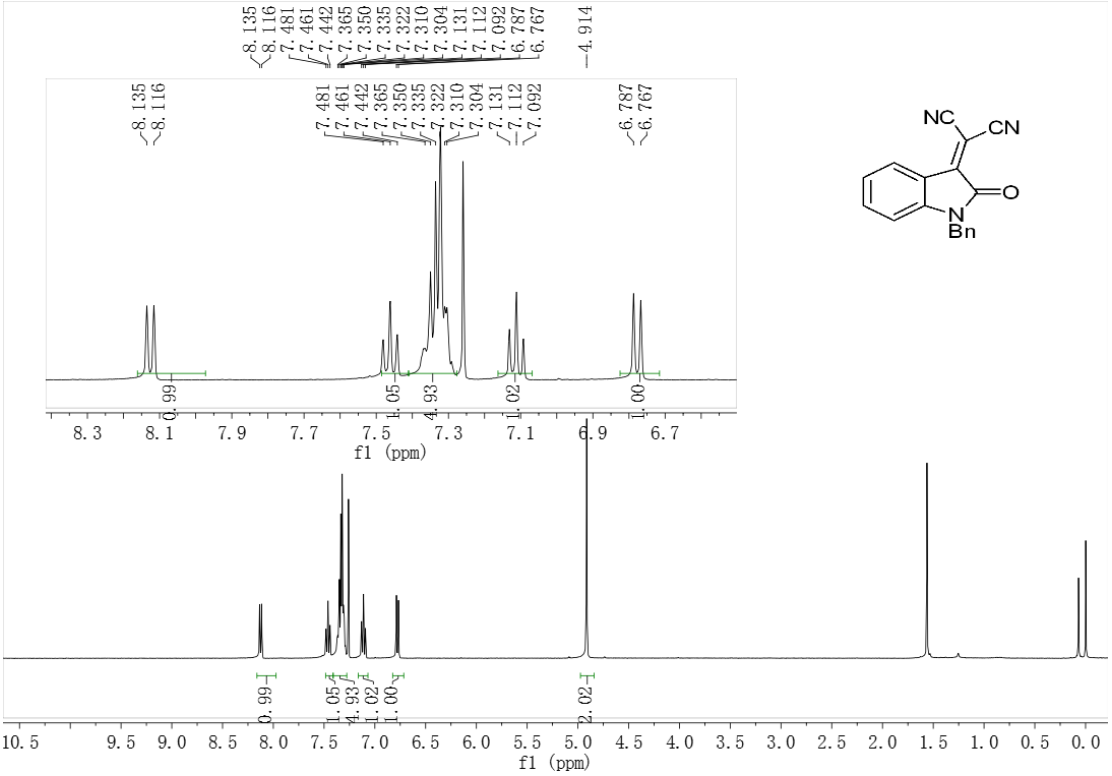

194.657
179.552
160.676
151.894
150.731
138.544
138.022
136.454
133.070
131.983
130.999
130.650
128.686
127.924
126.658
126.105
121.747
119.247
118.829
115.955
115.452
111.607
63.786
55.717
49.790
48.164
45.868
42.113
32.485
29.119
27.144
20.953
18.555
Me
Me
BnN
O
NC
H2N
N
OMe
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

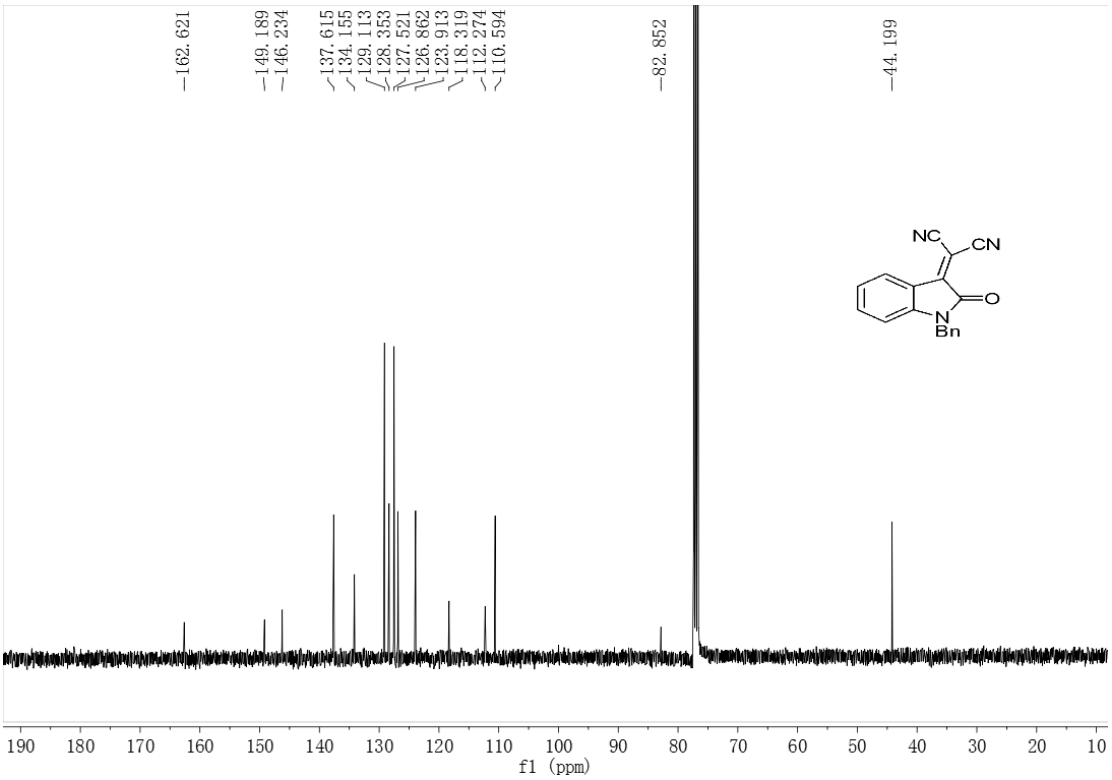
Compound 6:



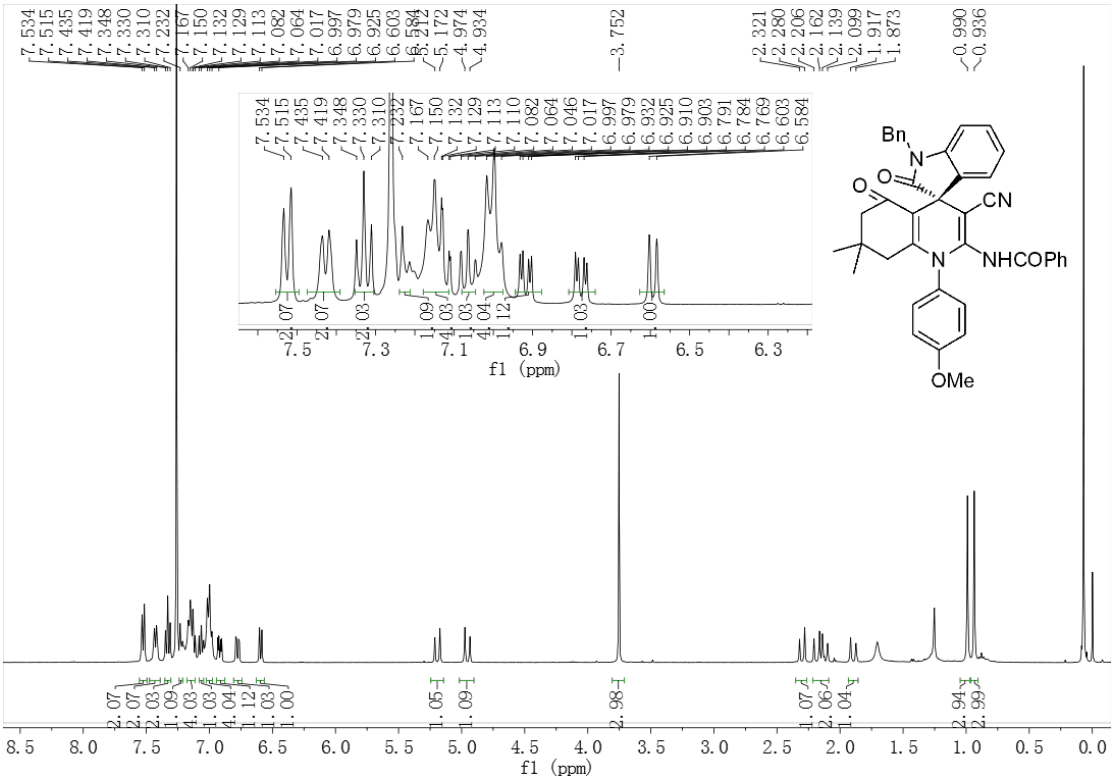


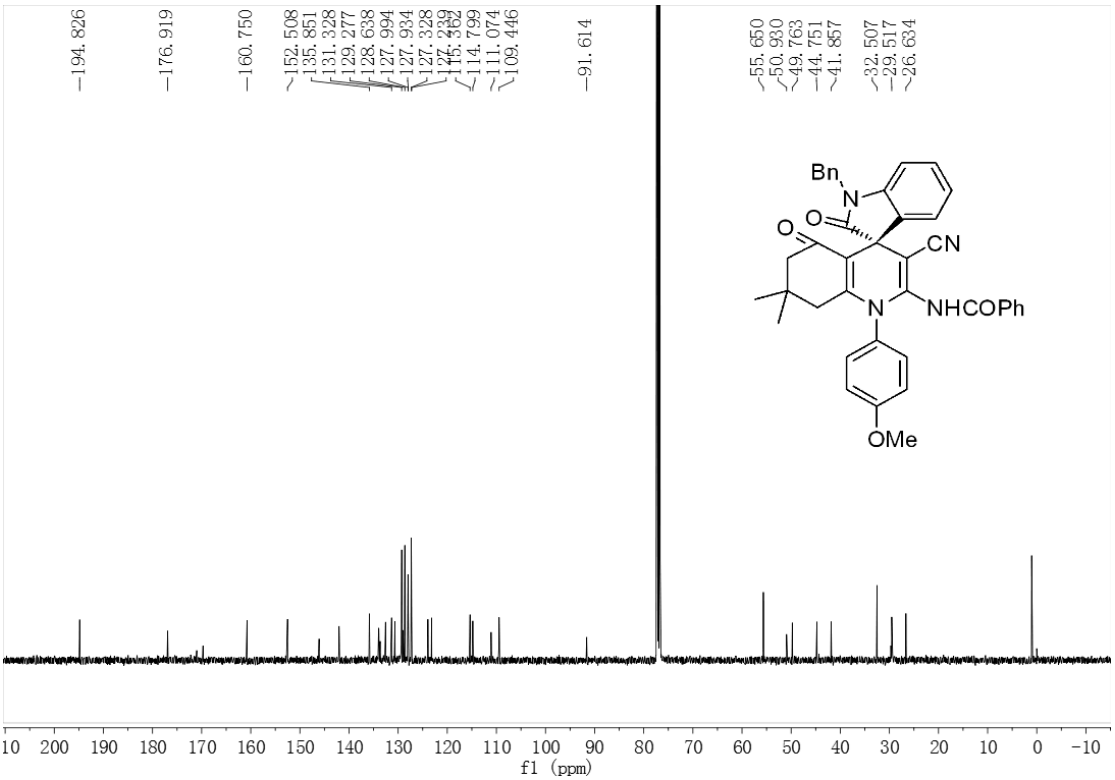
Intermediate A:





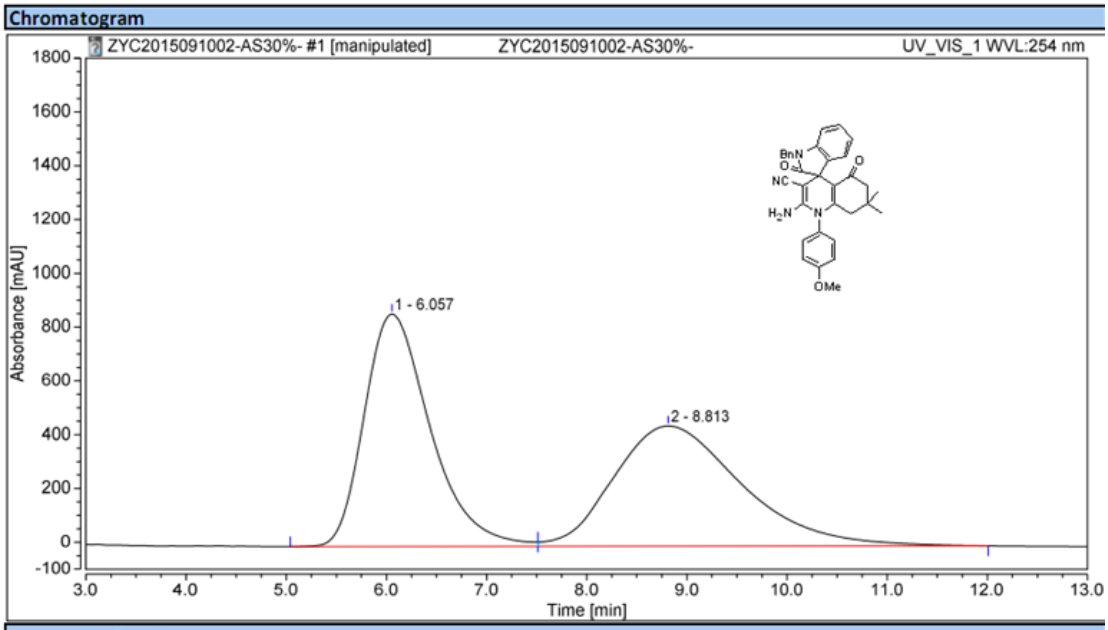
Compound 7





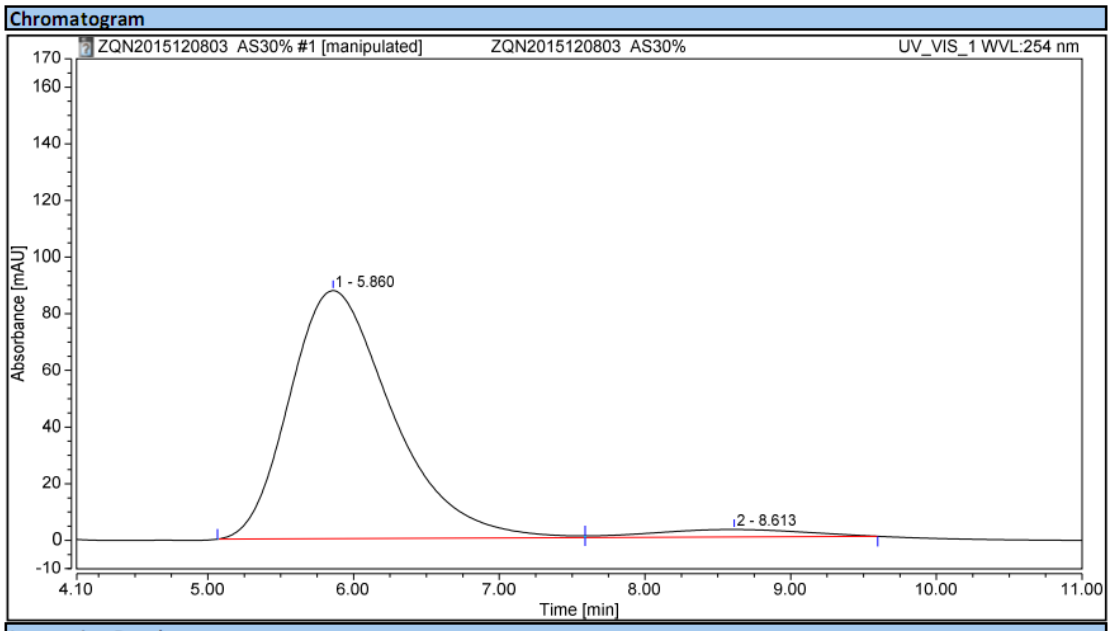
3. HPLC spectra of products 4, 6 and 7

4aa



Integration Results

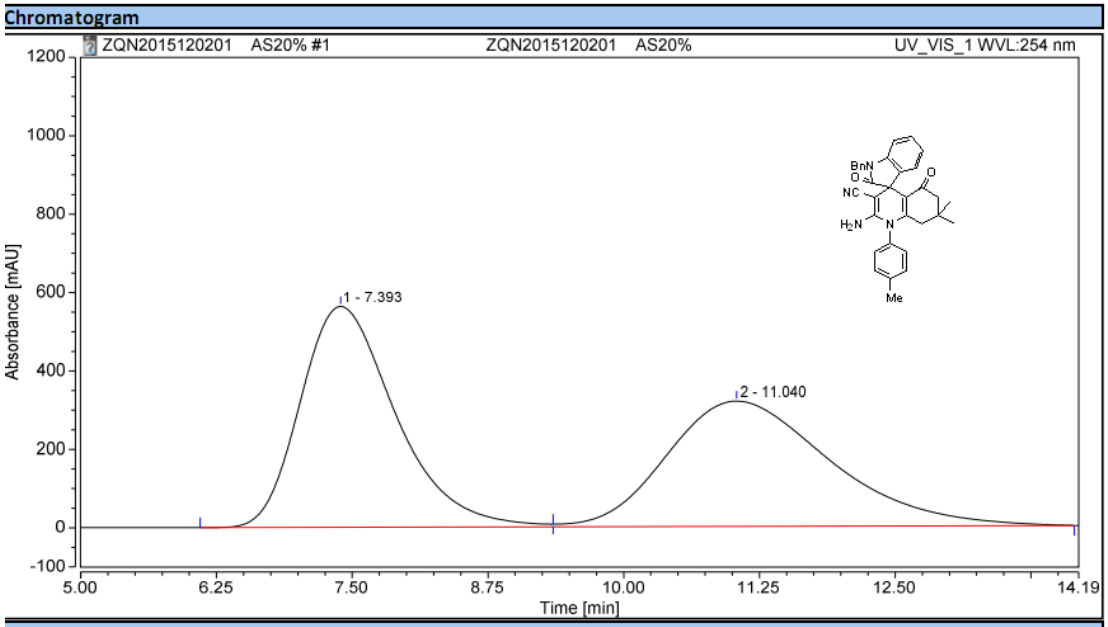
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.057	660.087	864.042	49.97	65.90	n.a.



Integration Results

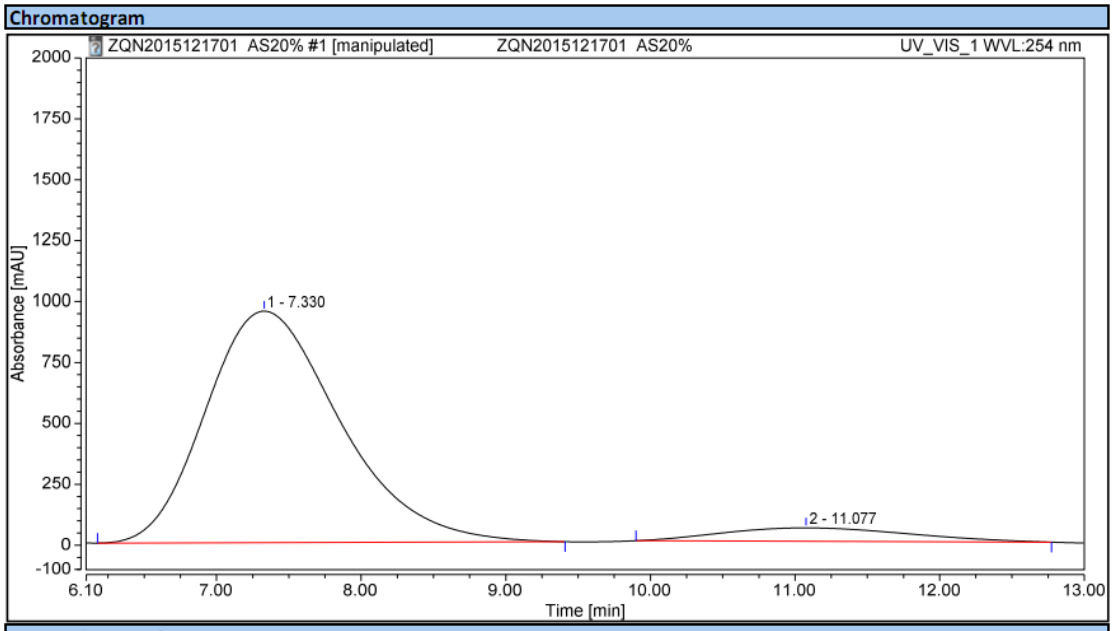
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.860	71.574	87.550	95.80	97.09	n.a.
2		8.613	3.136	2.622	4.20	2.91	n.a.
Total:			**74.710**	**90.172**	**100.00**	**100.00**	

4ba



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.393	571.500	563.000	50.70	63.81	n.a.
2		11.040	555.663	319.264	49.30	36.19	n.a.
Total:			**1127.163**	**882.264**	**100.00**	**100.00**	

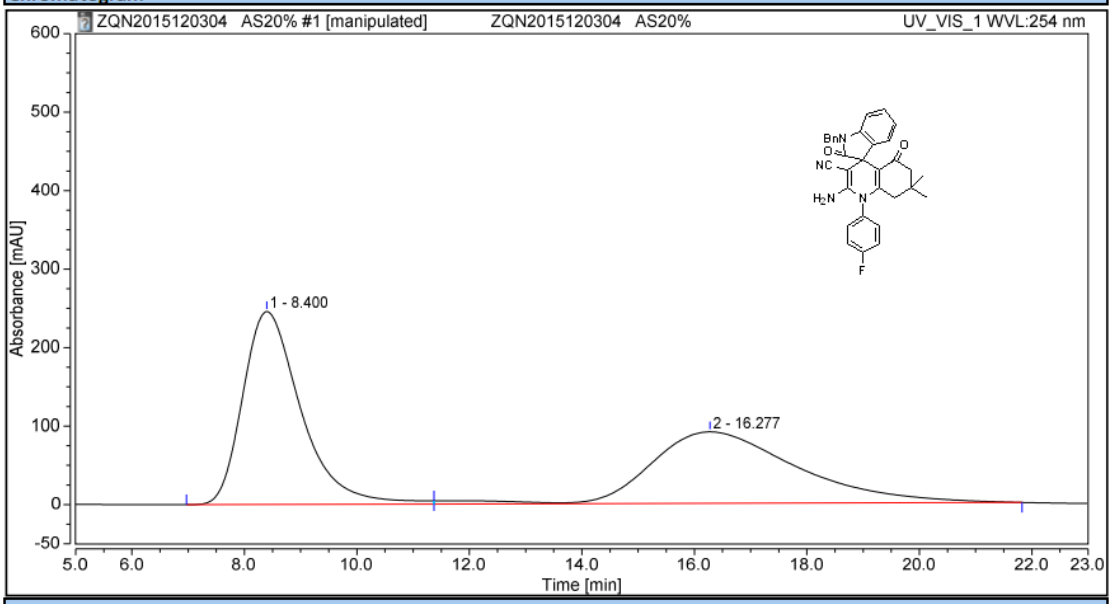


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.330	1022.873	950.063	92.53	94.50	n.a.
2		11.077	82.569	55.247	7.47	5.50	n.a.
Total:			**1105.441**	**1005.310**	**100.00**	**100.00**	

4ca

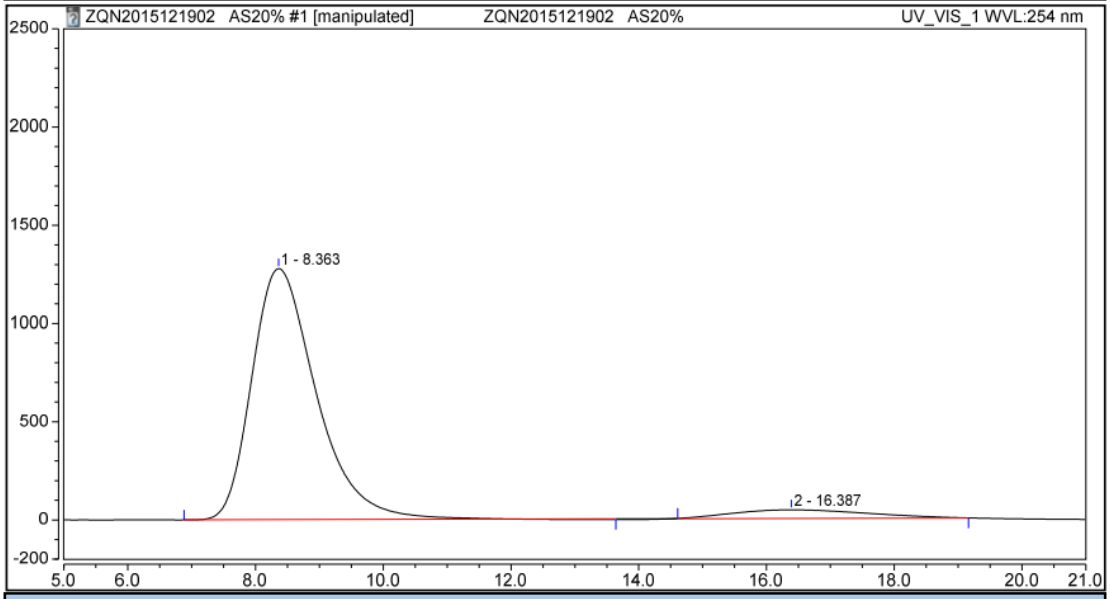
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.400	294.272	245.772	51.65	72.98	n.a.
2		16.277	275.459	91.016	48.35	27.02	n.a.
Total:			**569.731**	**336.788**	**100.00**	**100.00**	

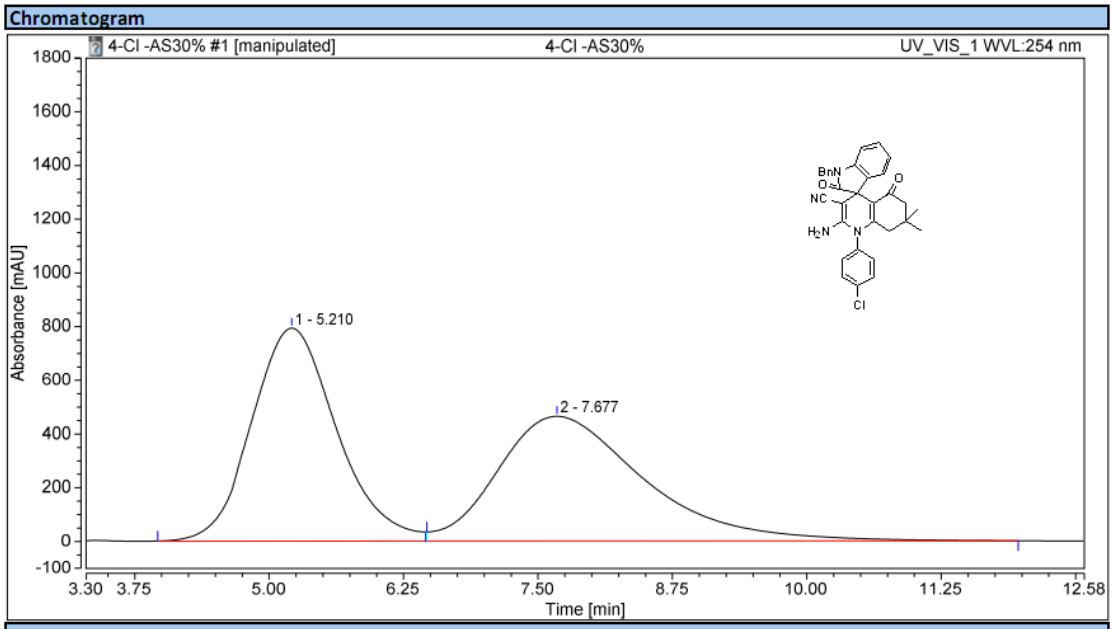
Chromatogram



Integration Results

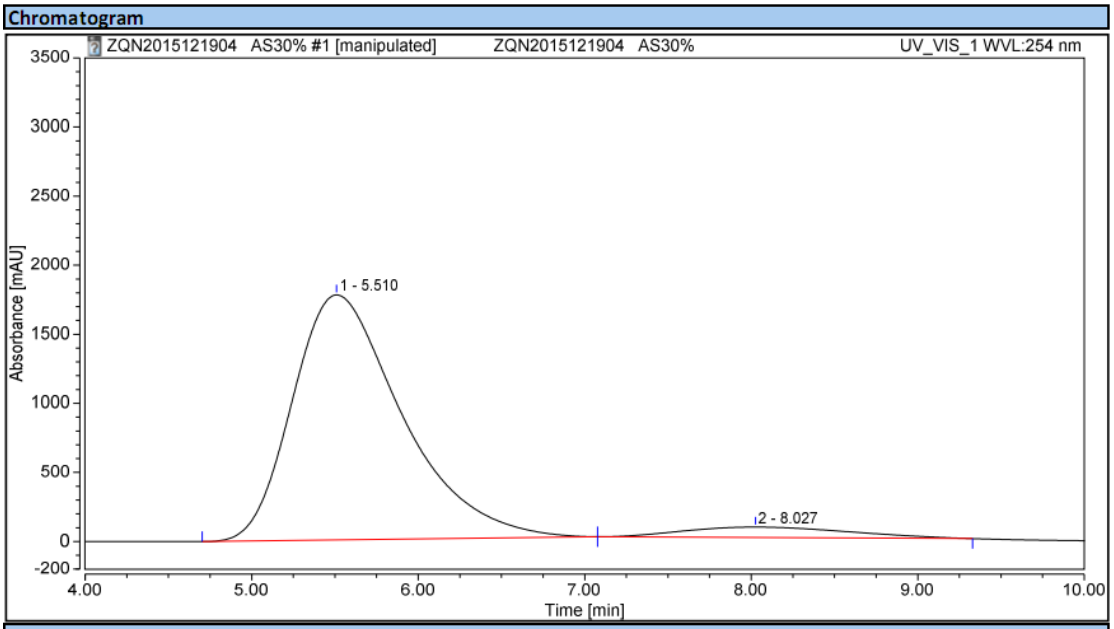
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.363	1487.443	1277.805	93.37	96.71	n.a.
2		16.387	105.662	43.435	6.63	3.29	n.a.
Total:			**1593.105**	**1321.240**	**100.00**	**100.00**	

4da



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.210	726.509	793.291	49.92	63.06	n.a.
2		7.677	728.747	464.644	50.08	36.94	n.a.
Total:			**1455.257**	**1257.935**	**100.00**	**100.00**	

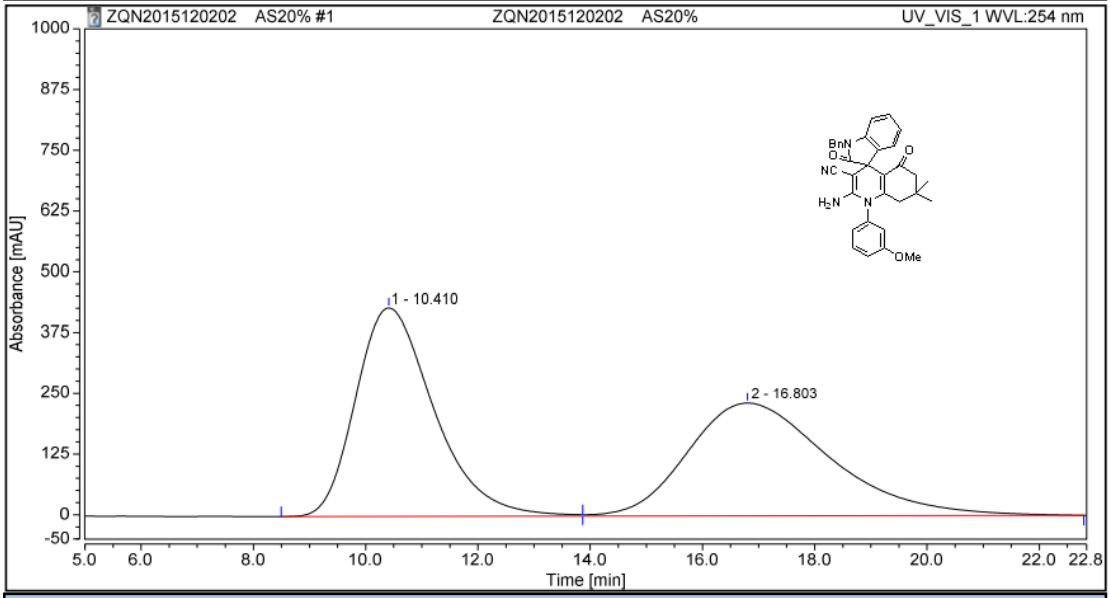


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.510	1352.301	1773.704	93.93	95.90	n.a.
2		8.027	87.394	75.874	6.07	4.10	n.a.
Total:			**1439.695**	**1849.578**	**100.00**	**100.00**	

4ea

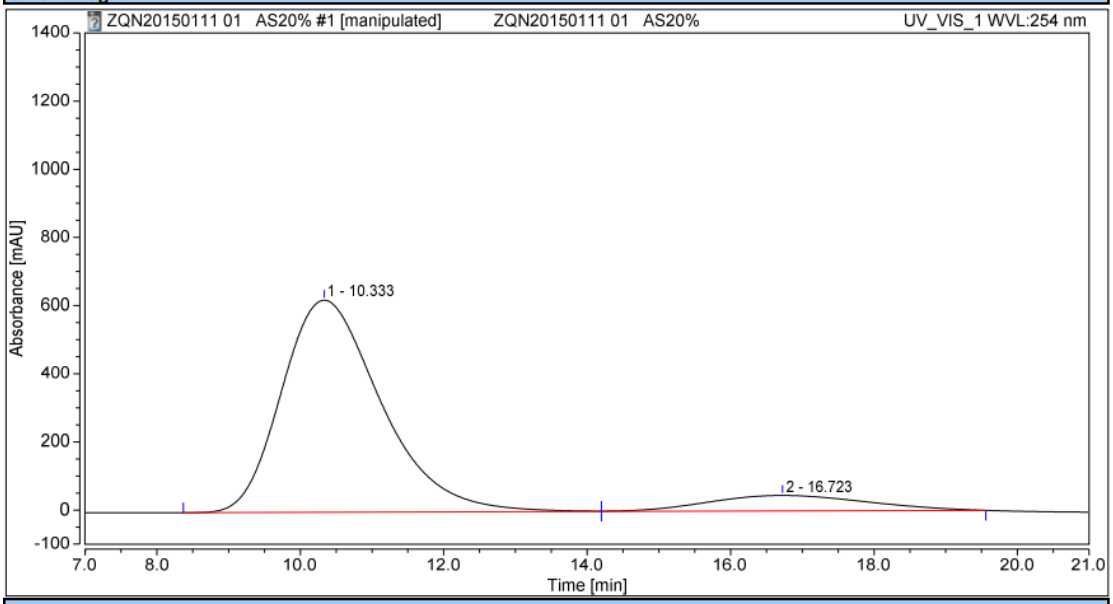
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.410	692.944	429.005	50.48	64.88	n.a.
2		16.803	679.635	232.268	49.52	35.12	n.a.
Total:			**1372.578**	**661.273**	**100.00**	**100.00**	

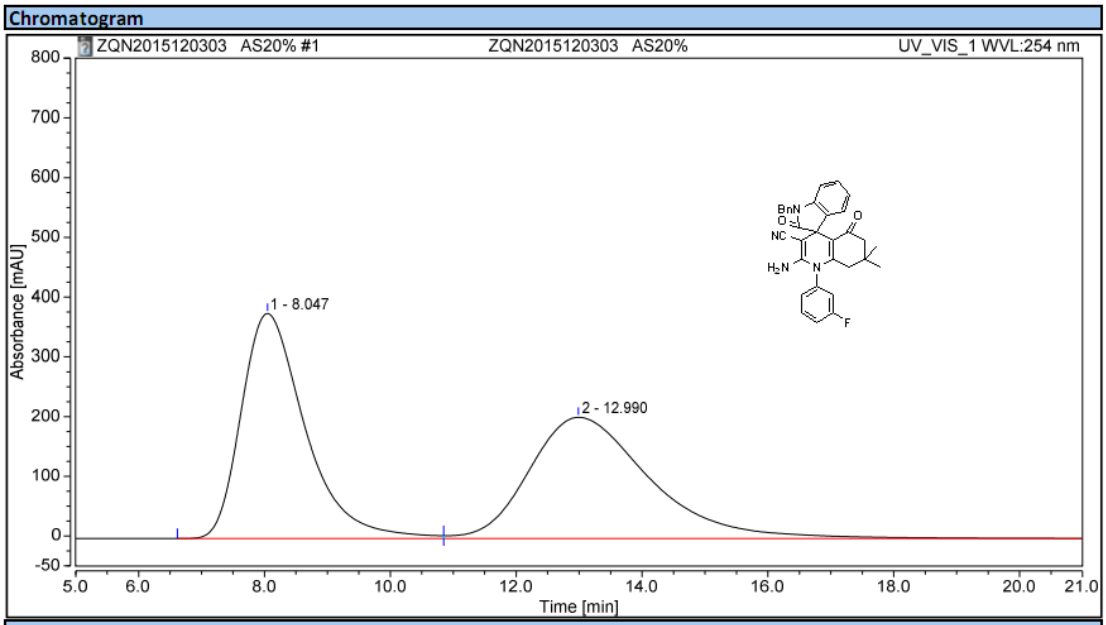
Chromatogram



Integration Results

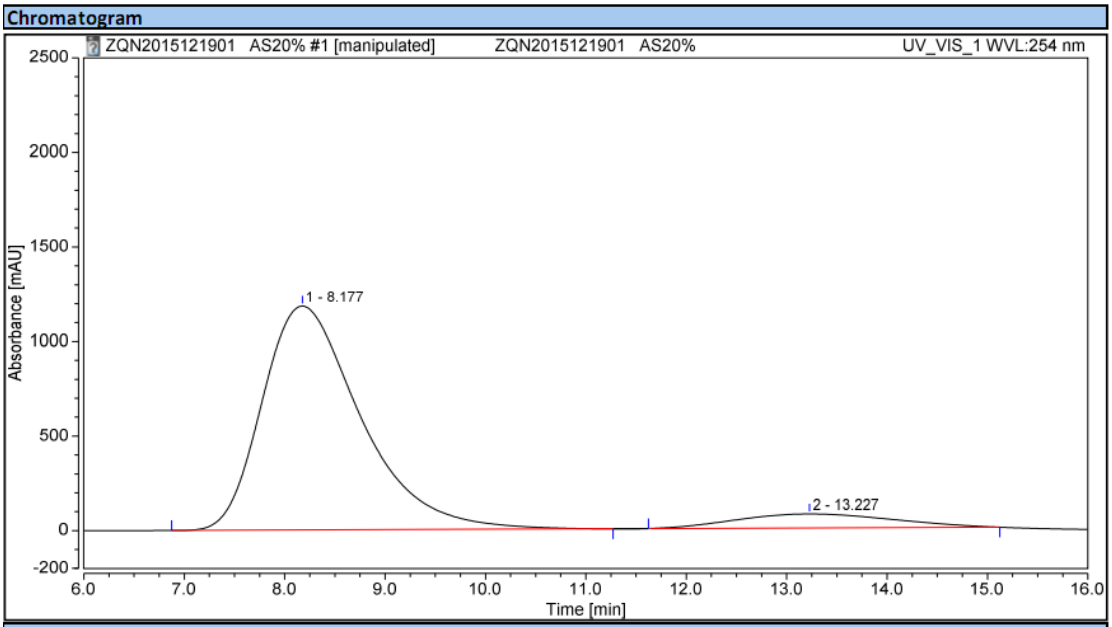
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.333	1002.226	622.573	89.57	93.18	n.a.
2		16.723	116.719	45.562	10.43	6.82	n.a.
Total:			**1118.945**	**668.135**	**100.00**	**100.00**	

4fa



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.047	442.741	376.625	49.54	64.99	n.a.
2		12.990	451.008	202.881	50.46	35.01	n.a.
Total:			**893.749**	**579.505**	**100.00**	**100.00**	

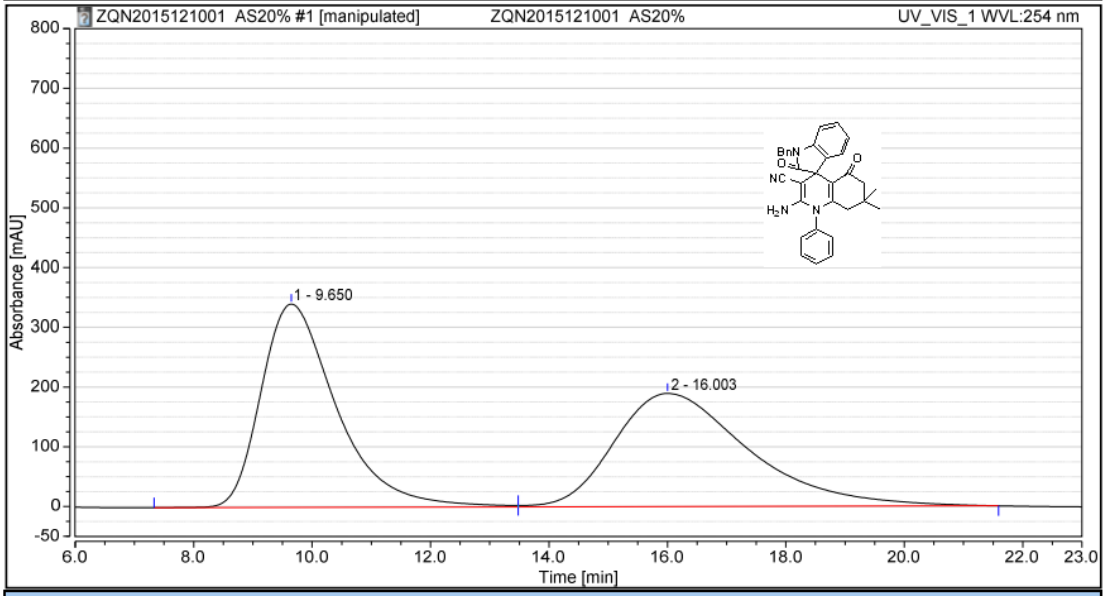


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.177	1348.421	1184.232	90.95	94.10	n.a.
2		13.227	134.126	74.245	9.05	5.90	n.a.
Total:			**1482.548**	**1258.477**	**100.00**	**100.00**	

4ga

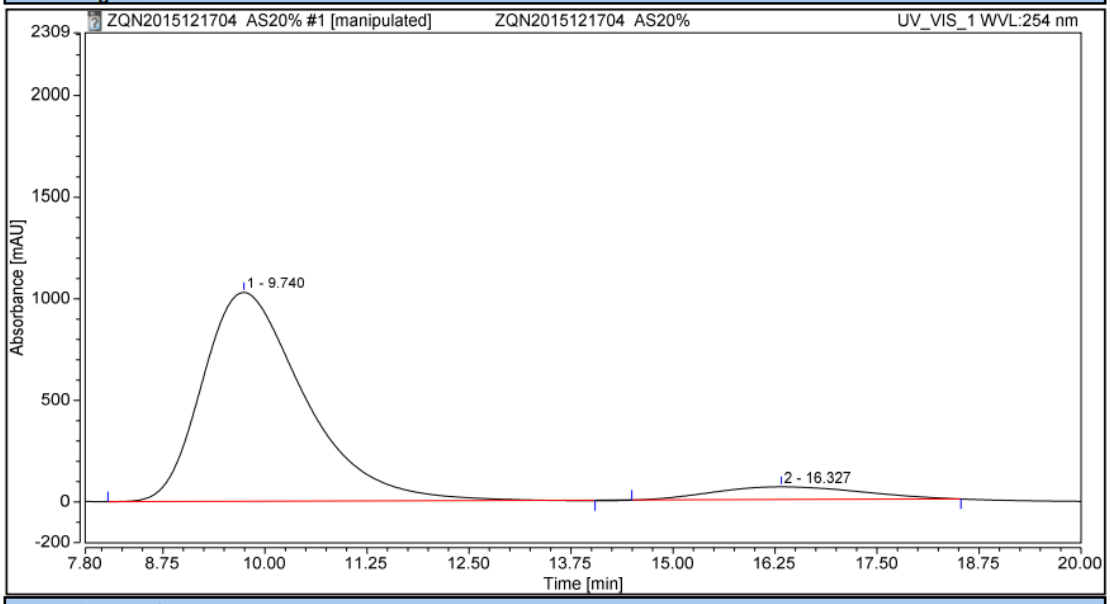
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.650	502.987	340.292	50.28	64.25	n.a.
2		16.003	497.471	189.356	49.72	35.75	n.a.
Total:			**1000.458**	**529.648**	**100.00**	**100.00**	

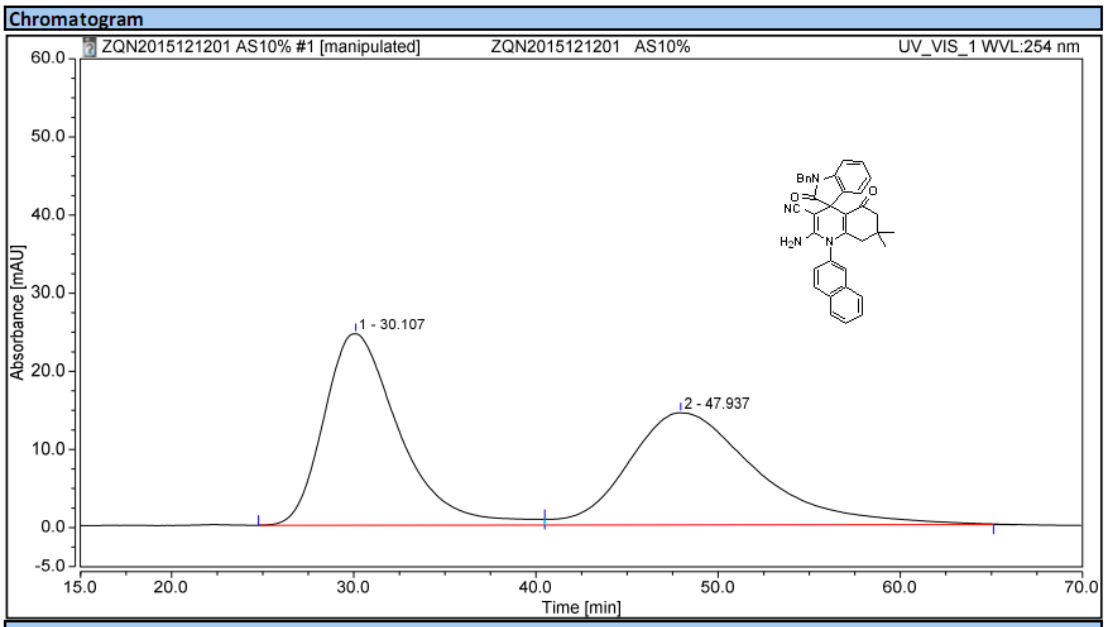
Chromatogram



Integration Results

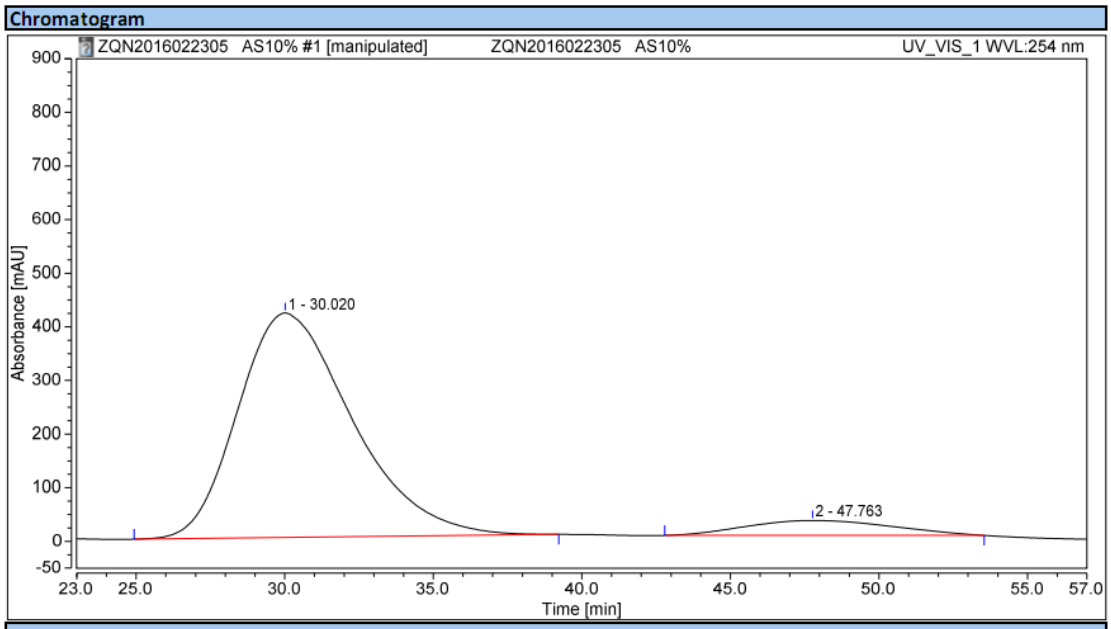
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.740	1487.201	1027.440	91.92	94.24	n.a.
2		16.327	130.698	62.752	8.08	5.76	n.a.
Total:			**1617.899**	**1090.192**	**100.00**	**100.00**	

4ha



Integration Results

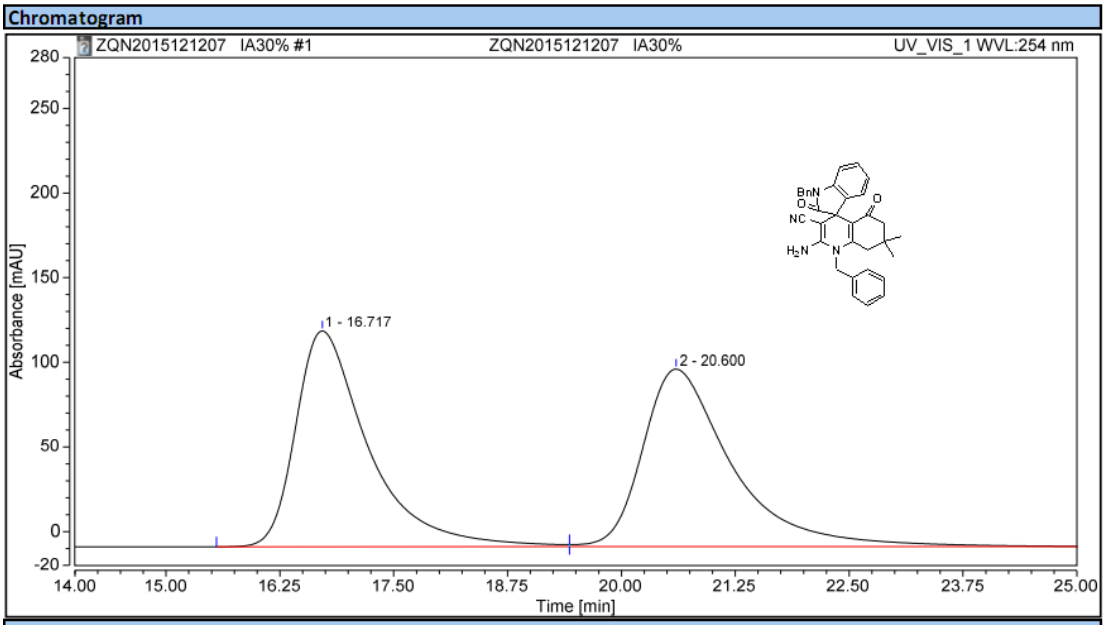
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		30.107	117.420	24.506	50.04	63.08	n.a.
2		47.937	117.235	14.341	49.96	36.92	n.a.
Total:			**234.655**	**38.848**	**100.00**	**100.00**	



Integration Results

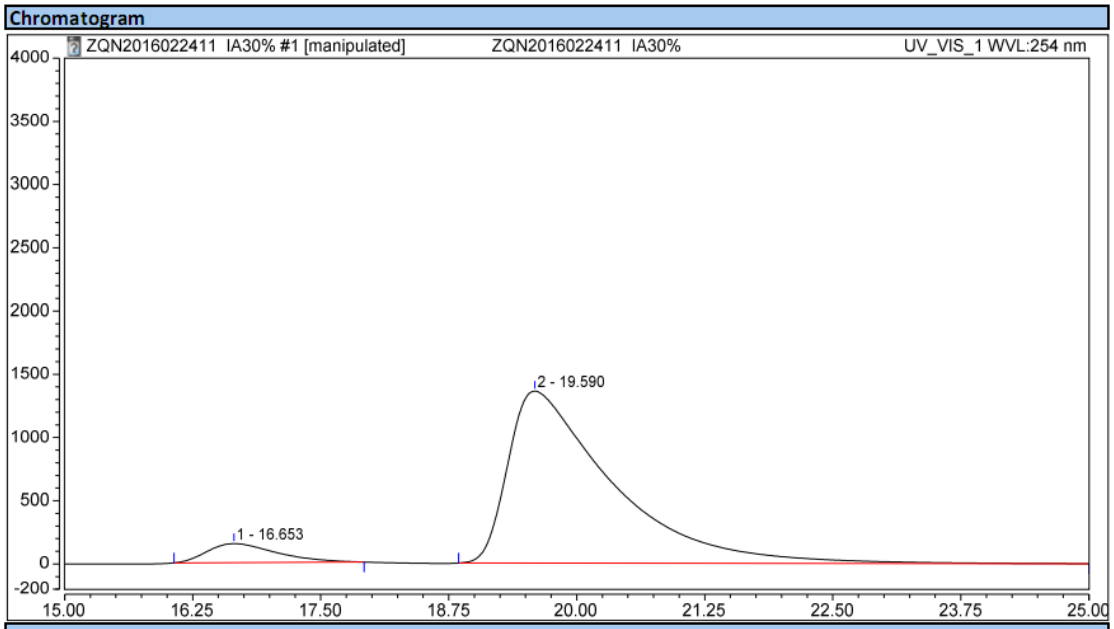
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		30.020	1865.381	418.679	92.16	93.77	n.a.
2		47.763	158.661	27.839	7.84	6.23	n.a.
Total:			**2024.042**	**446.518**	**100.00**	**100.00**	

4ia



Integration Results

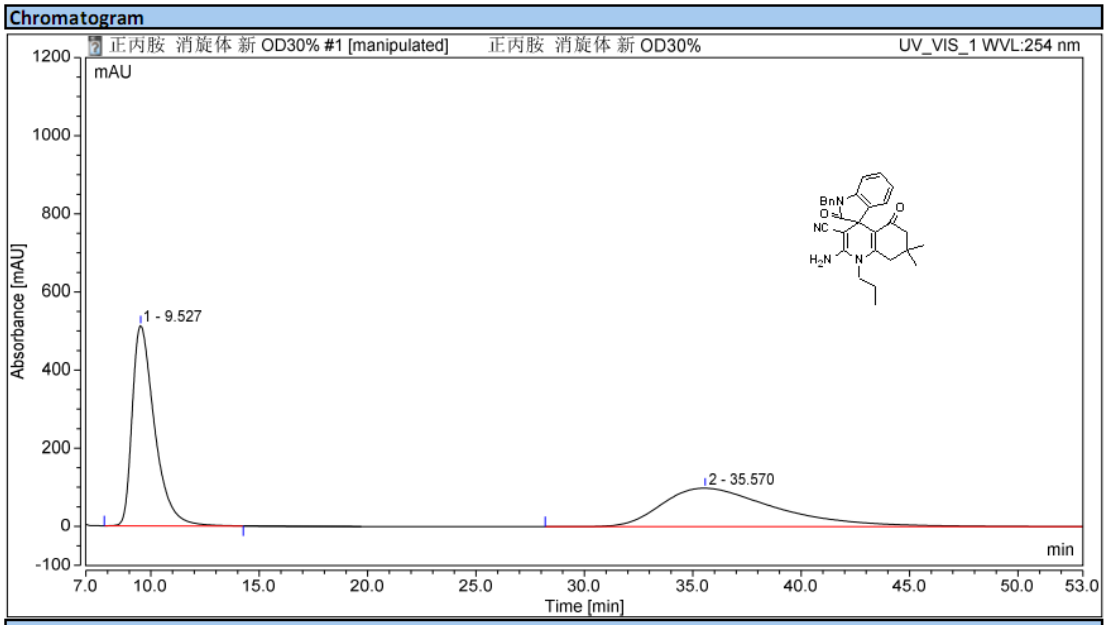
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16.717	117.960	127.500	49.71	54.87	n.a.
2		20.600	119.316	104.851	50.29	45.13	n.a.
Total:			**237.276**	**232.352**	**100.00**	**100.00**	



Integration Results

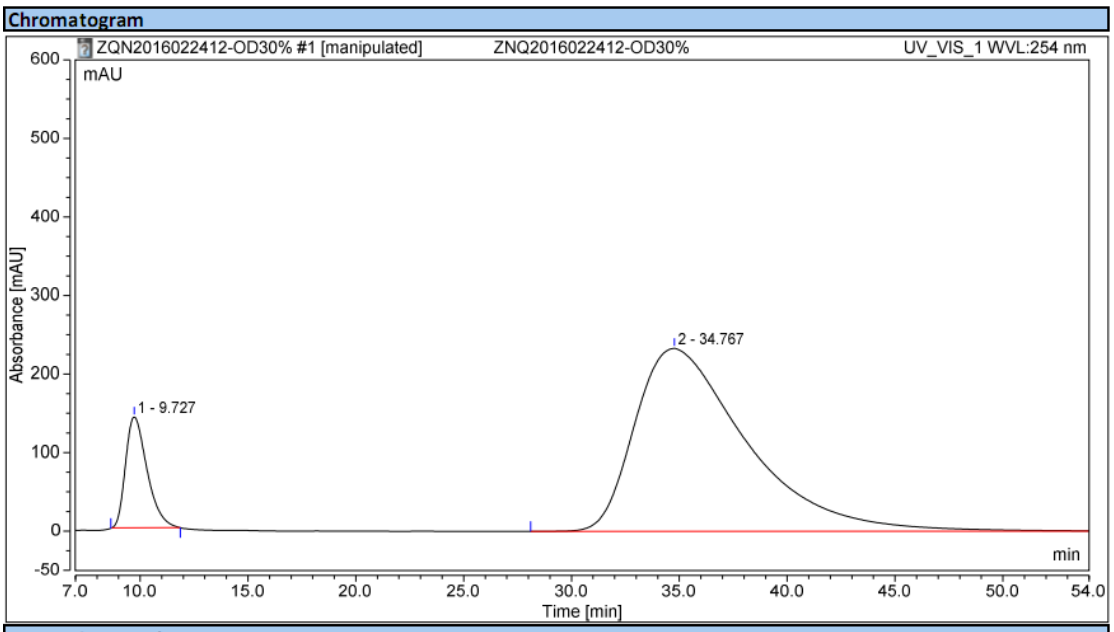
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16.653	117.486	150.123	6.82	9.93	n.a.
2		19.590	1606.282	1361.054	93.18	90.07	n.a.
Total:			**1723.768**	**1511.177**	**100.00**	**100.00**	

4ja



Integration Results

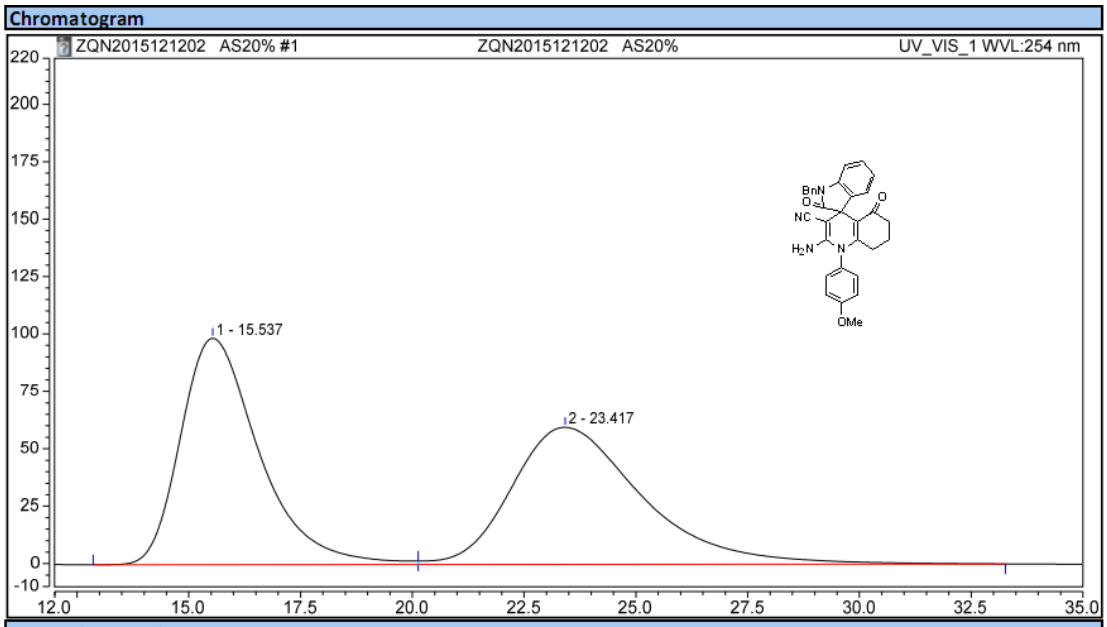
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.527	615.316	512.319	50.49	83.88	n.a.
2		35.570	603.340	98.449	49.51	16.12	n.a.
Total:			**1218.657**	**610.768**	**100.00**	**100.00**	



Integration Results

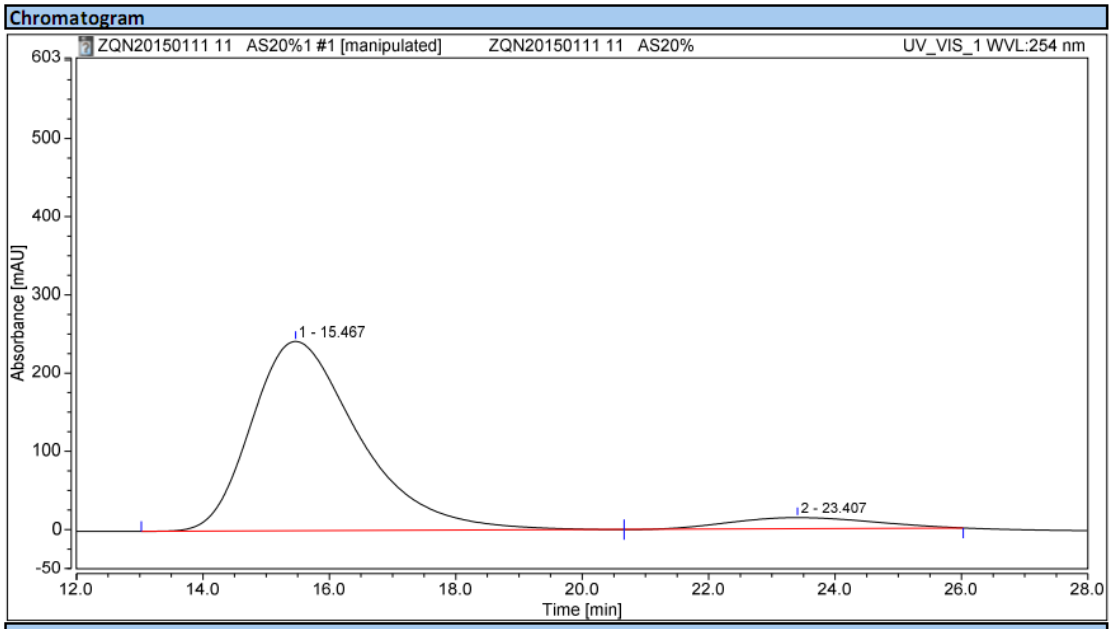
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.727	163.735	141.232	10.49	37.75	n.a.
2		34.767	1397.338	232.896	89.51	62.25	n.a.
Total:			**1561.073**	**374.128**	**100.00**	**100.00**	

4ka



Integration Results

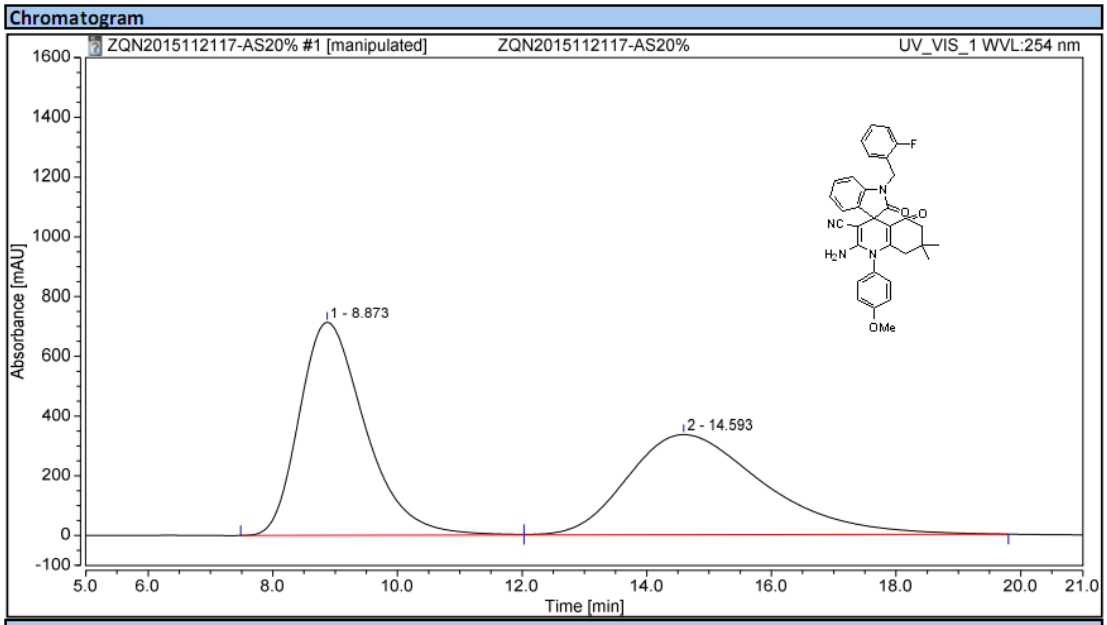
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.537	200.877	98.521	49.86	62.29	n.a.
2		23.417	202.035	59.642	50.14	37.71	n.a.
Total:			**402.912**	**158.163**	**100.00**	**100.00**	



Integration Results

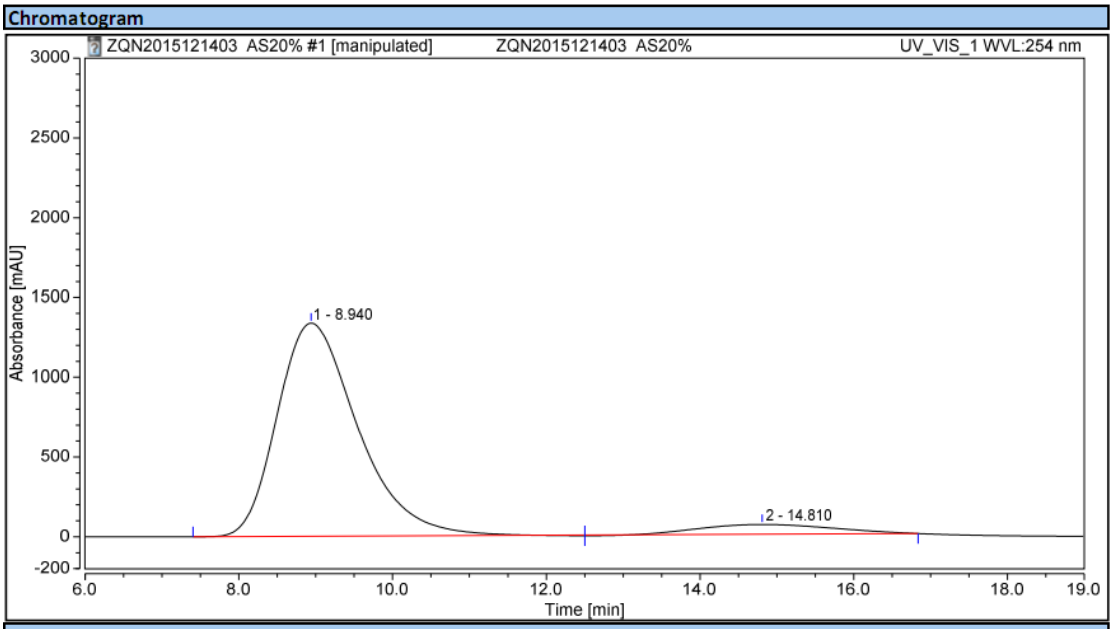
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.467	476.891	241.974	92.91	94.50	n.a.
2		23.407	36.387	14.074	7.09	5.50	n.a.
Total:			**513.278**	**256.048**	**100.00**	**100.00**	

4ab



Integration Results

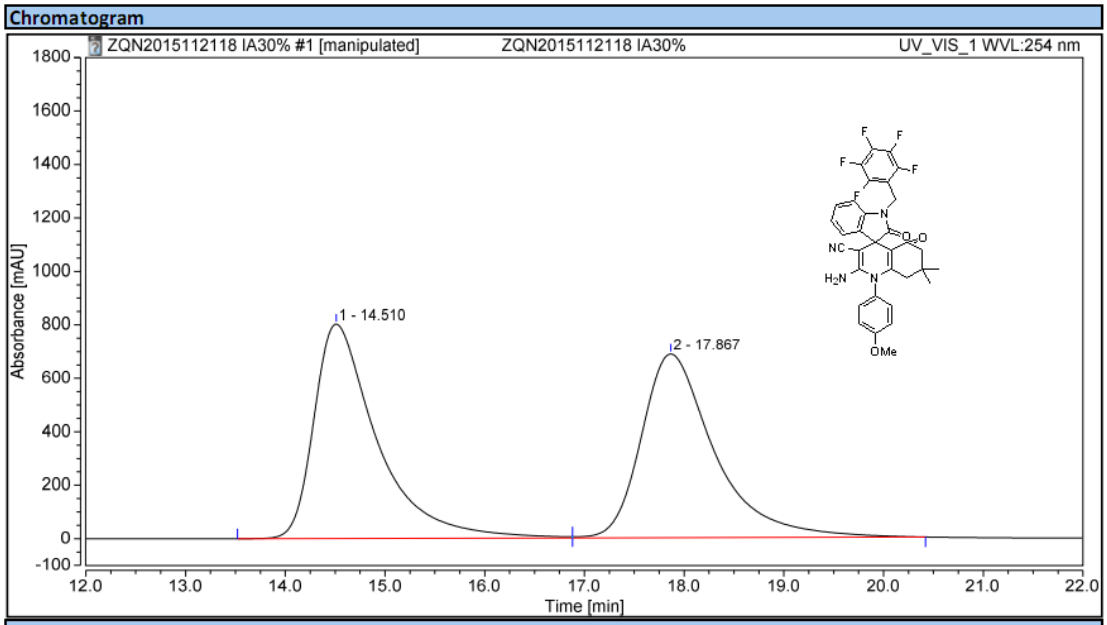
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.873	873.691	713.256	50.69	68.02	n.a.
2		14.593	849.808	335.361	49.31	31.98	n.a.
Total:			**1723.498**	**1048.617**	**100.00**	**100.00**	



Integration Results

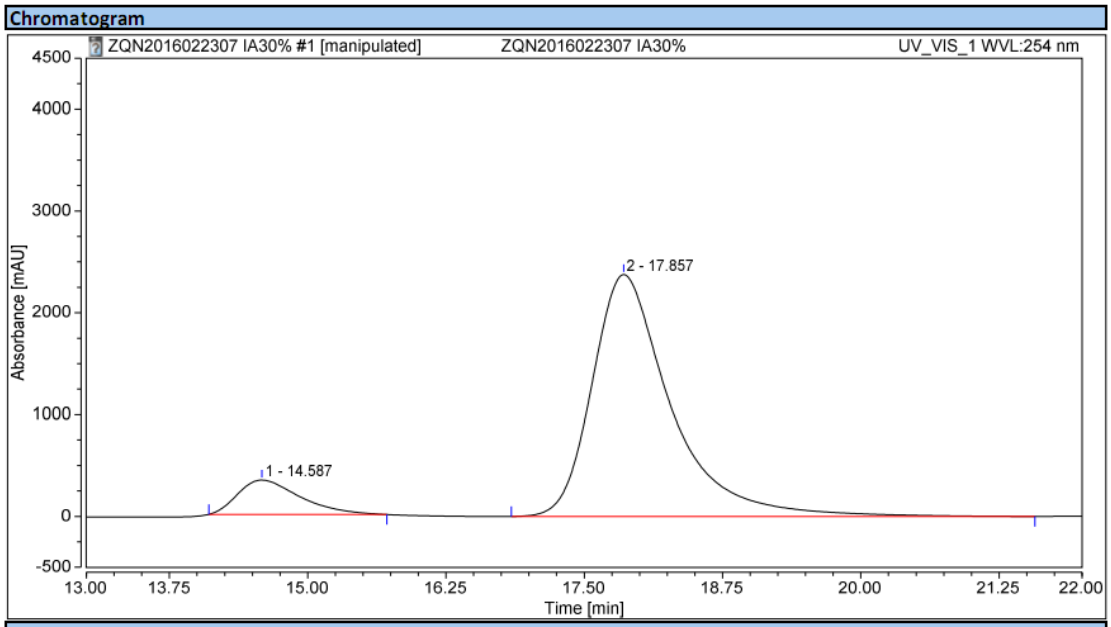
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.940	1617.089	1335.421	93.03	95.63	n.a.
2		14.810	121.182	61.057	6.97	4.37	n.a.
Total:			**1738.271**	**1396.478**	**100.00**	**100.00**	

4ac



Integration Results

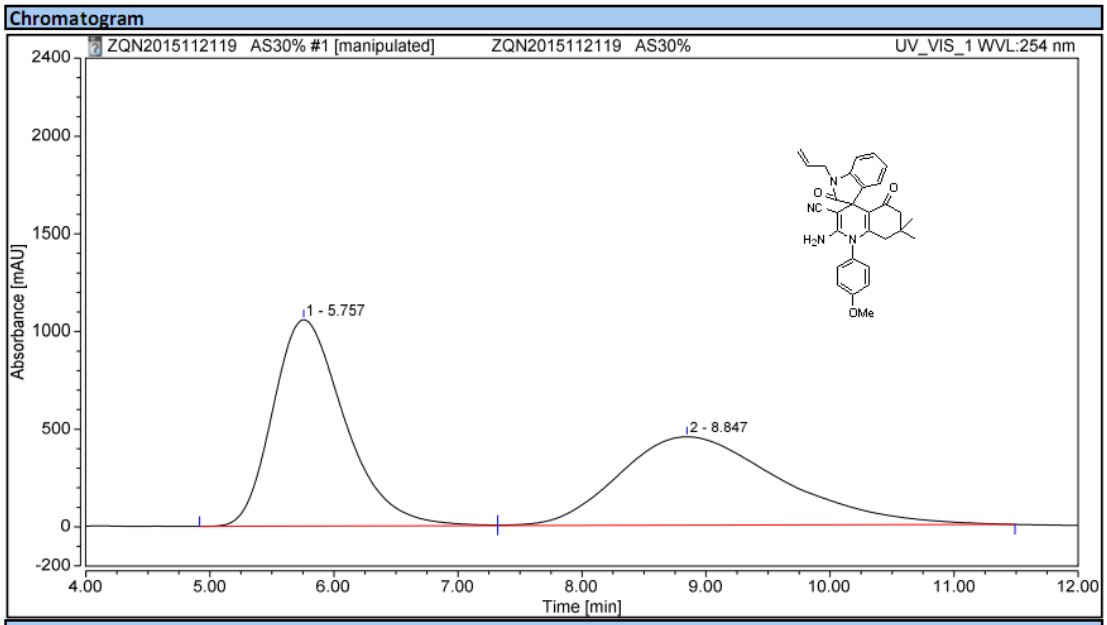
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.510	587.649	802.087	50.19	53.86	n.a.
2		17.867	583.189	687.183	49.81	46.14	n.a.
Total:			**1170.839**	**1489.270**	**100.00**	**100.00**	



Integration Results

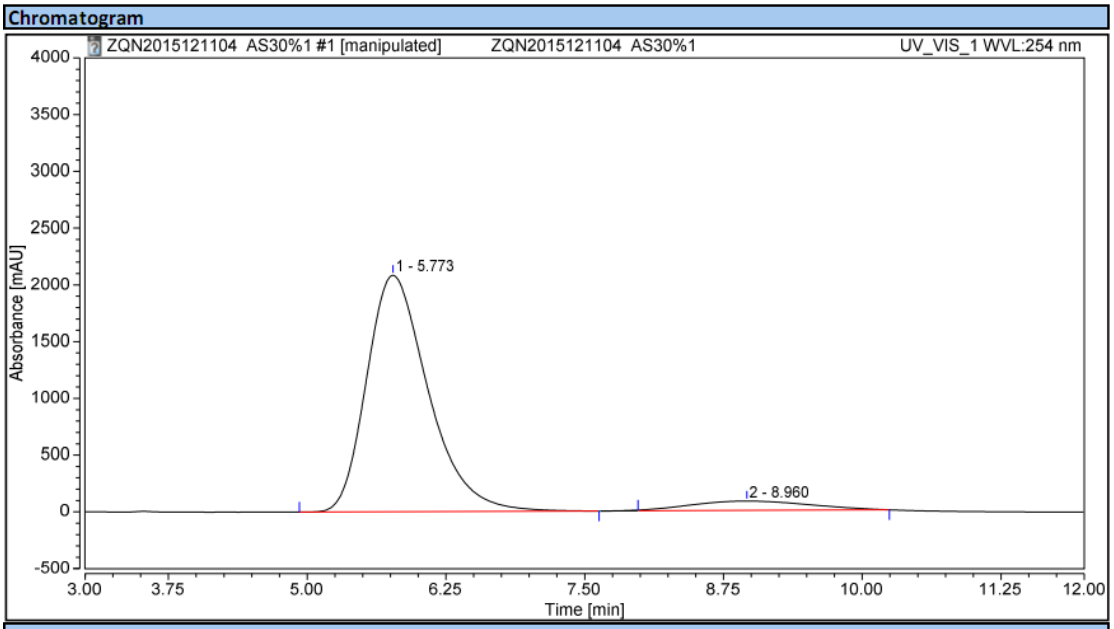
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.587	220.234	337.325	10.11	12.43	n.a.
2		17.857	1958.781	2376.637	89.89	87.57	n.a.
Total:			**2179.015**	**2713.963**	**100.00**	**100.00**	

4ad



Integration Results

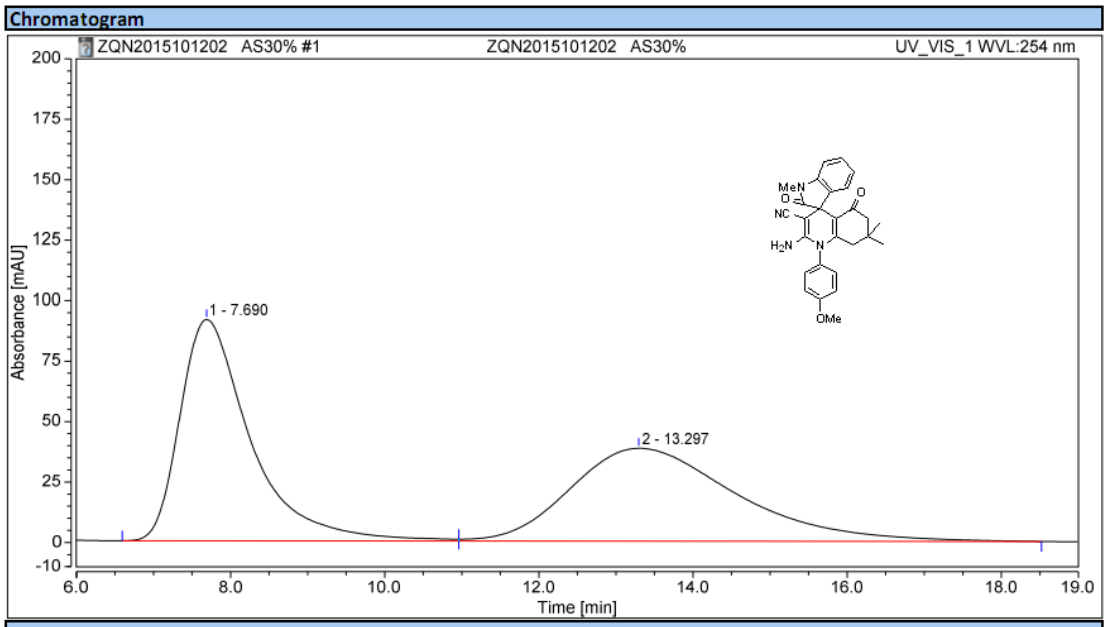
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.757	710.735	1057.199	50.94	70.02	n.a.
2		8.847	684.488	452.760	49.06	29.98	n.a.
Total:			**1395.223**	**1509.959**	**100.00**	**100.00**	



Integration Results

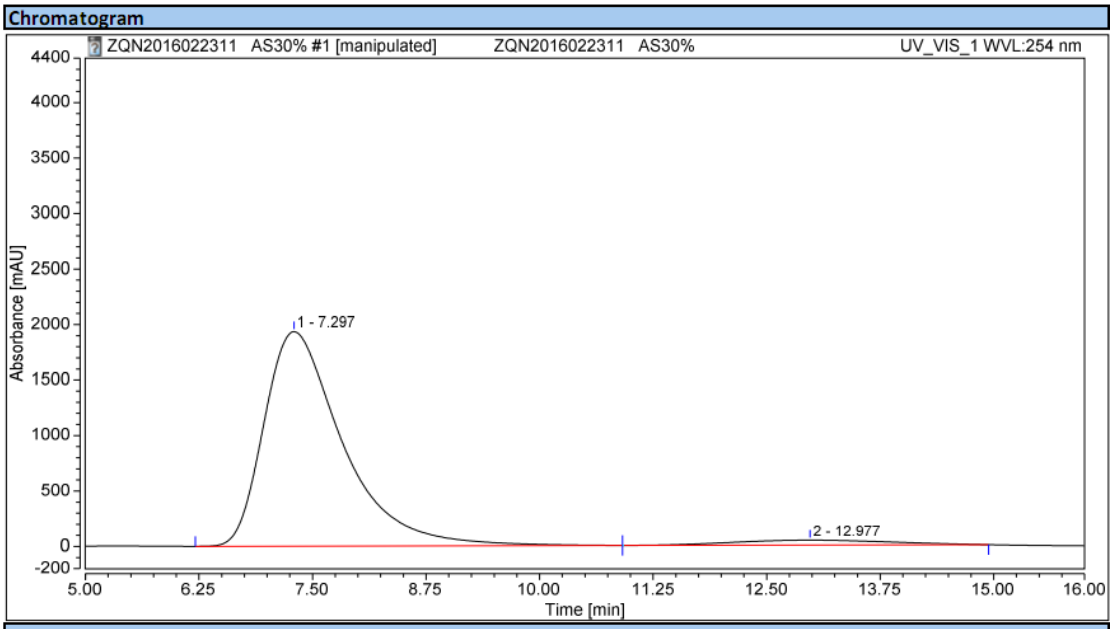
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.773	1338.939	2082.748	92.93	96.21	n.a.
2		8.960	101.942	82.156	7.07	3.79	n.a.
Total:			**1440.881**	**2164.905**	**100.00**	**100.00**	

4ae



Integration Results

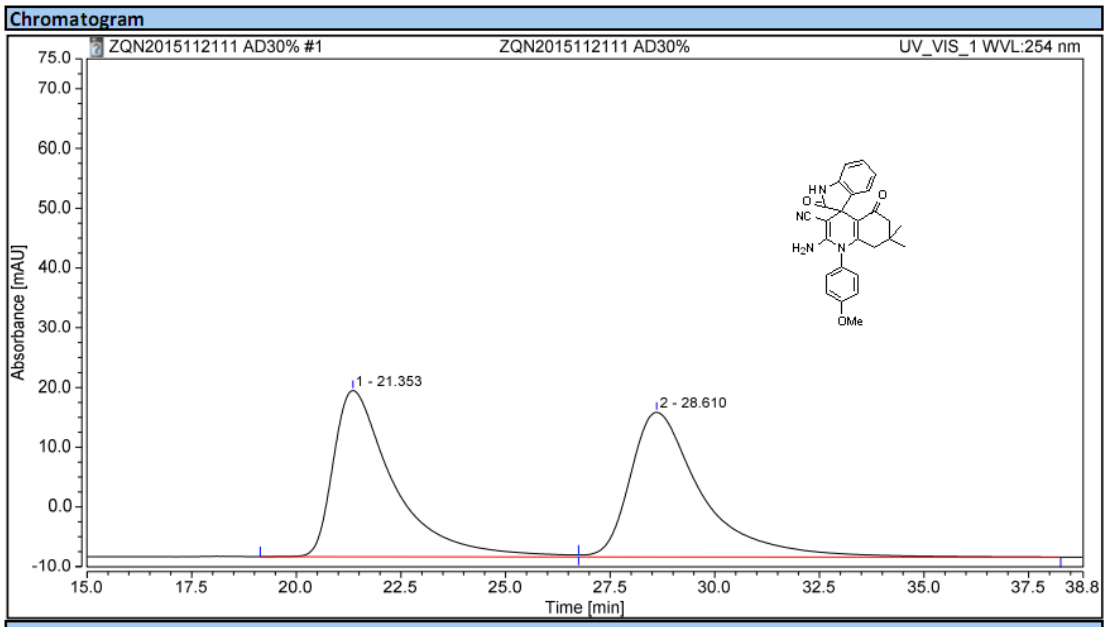
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.690	96.796	91.509	50.31	70.44	n.a.
2		13.297	95.593	38.395	49.69	29.56	n.a.
Total:			**192.389**	**129.904**	**100.00**	**100.00**	



Integration Results

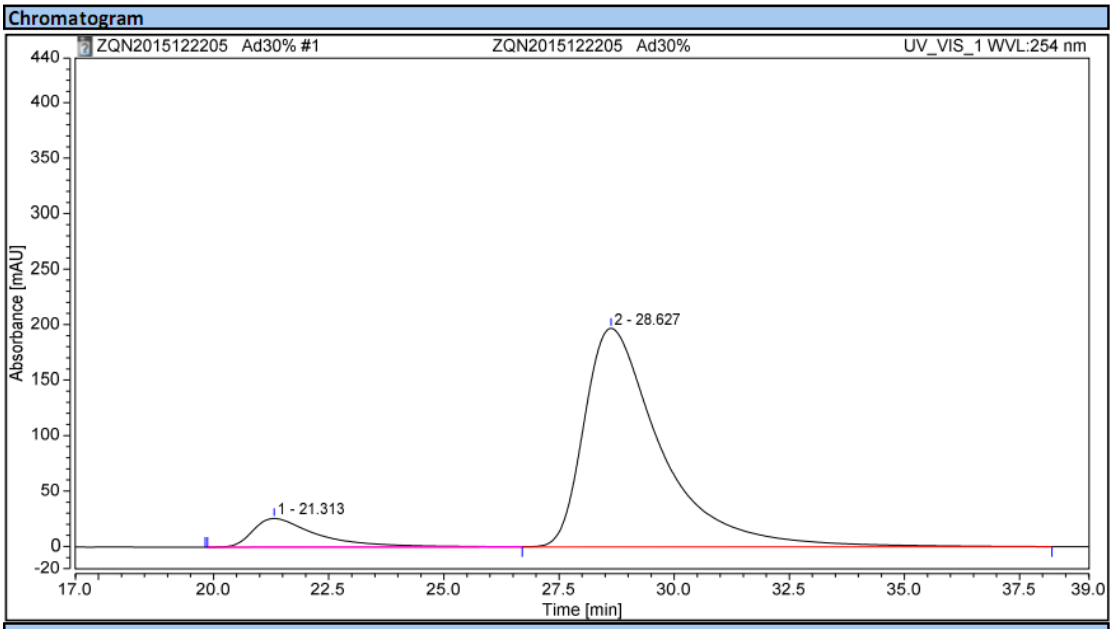
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.297	1939.683	1932.204	95.60	97.76	n.a.
2		12.977	89.307	44.289	4.40	2.24	n.a.
Total:			**2028.990**	**1976.494**	**100.00**	**100.00**	

4af



Integration Results

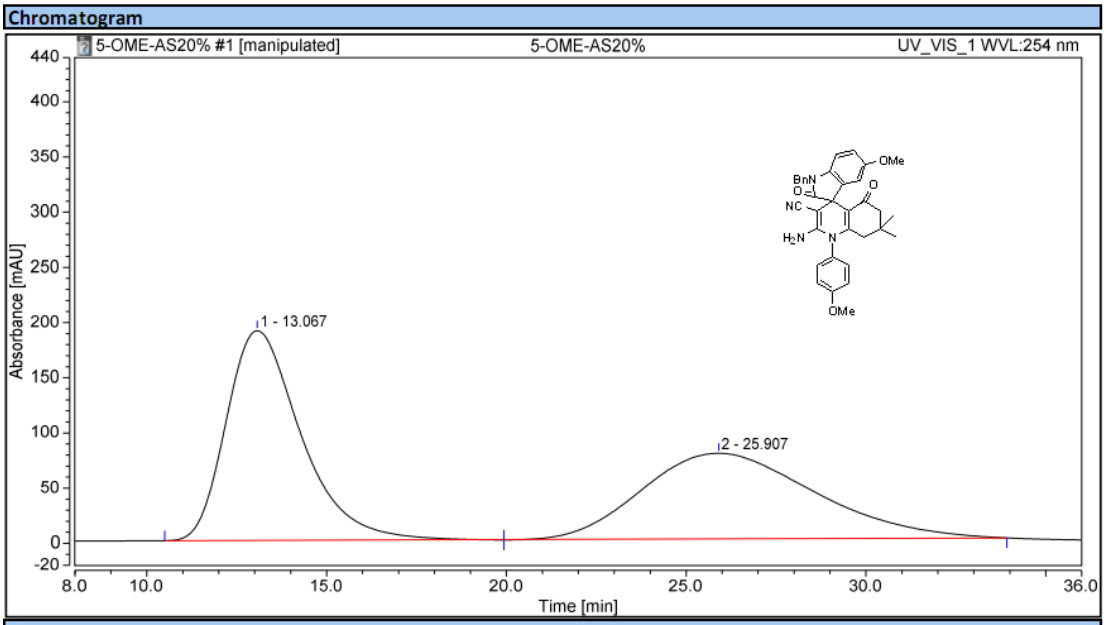
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		21.353	46.512	27.813	49.25	53.48	n.a.
2		28.610	47.928	24.196	50.75	46.52	n.a.
Total:			**94.440**	**52.009**	**100.00**	**100.00**	



Integration Results

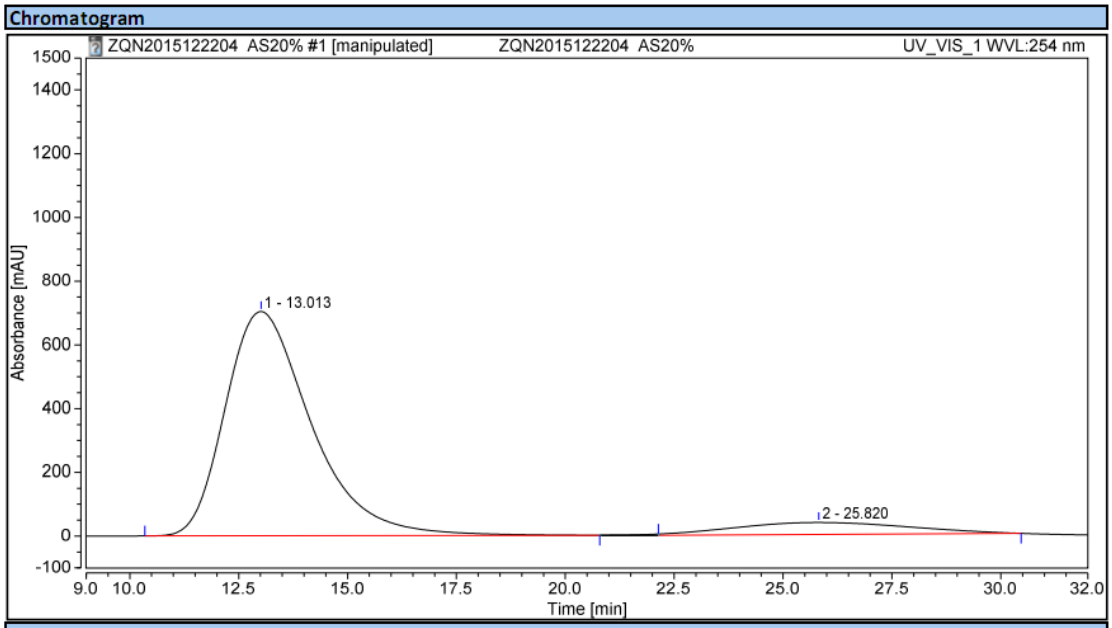
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		21.313	41.472	25.816	9.78	11.59	n.a.
2		28.627	382.400	196.936	90.22	88.41	n.a.
Total:			**423.872**	**222.752**	**100.00**	**100.00**	

4ag



Integration Results

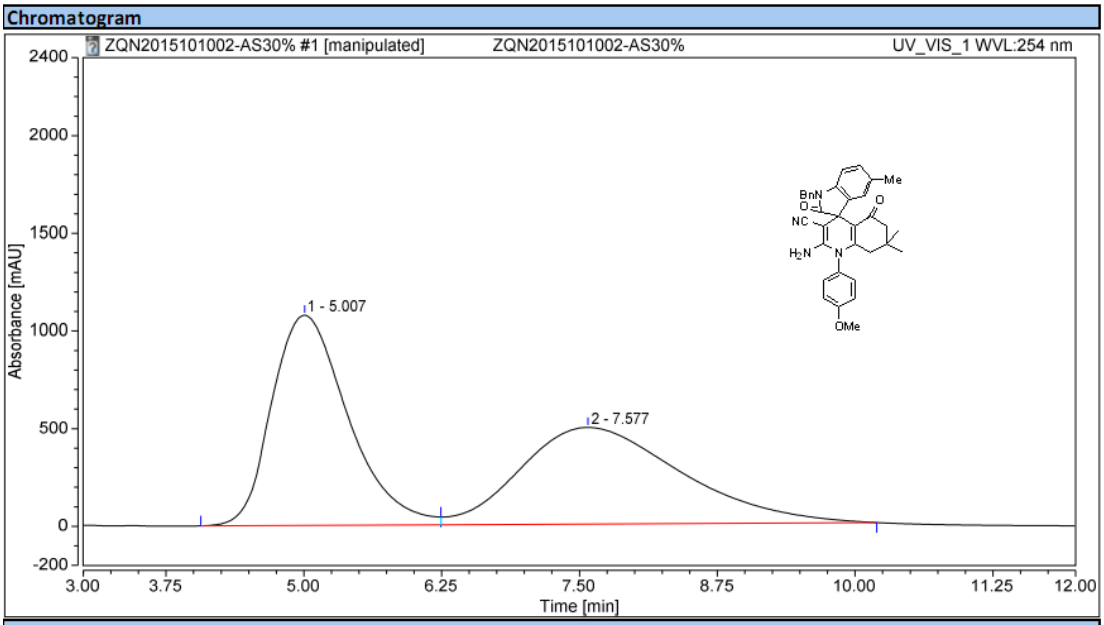
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13.067	457.169	189.915	51.51	71.02	n.a.
2		25.907	430.371	77.494	48.49	28.98	n.a.
Total:			**887.540**	**267.409**	**100.00**	**100.00**	



Integration Results

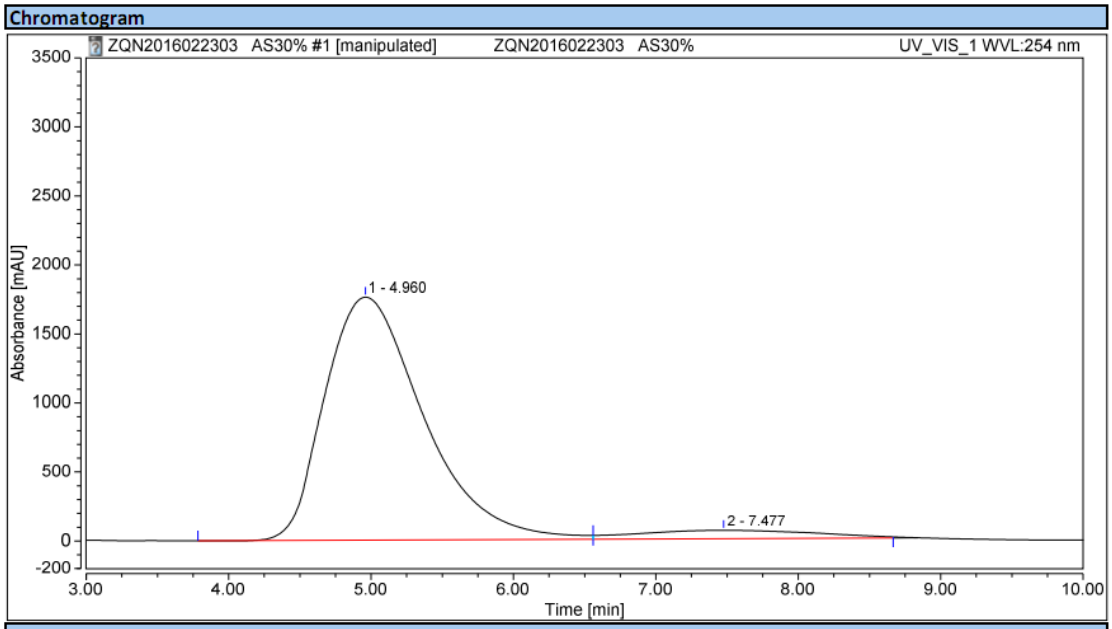
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13.013	1610.116	703.601	90.24	94.95	n.a.
2		25.820	174.062	37.432	9.76	5.05	n.a.
Total:			**1784.178**	**741.033**	**100.00**	**100.00**	

4ah



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.007	861.618	1075.750	50.79	68.51	n.a.
2		7.577	834.760	494.565	49.21	31.49	n.a.
Total:			**1696.378**	**1570.315**	**100.00**	**100.00**	

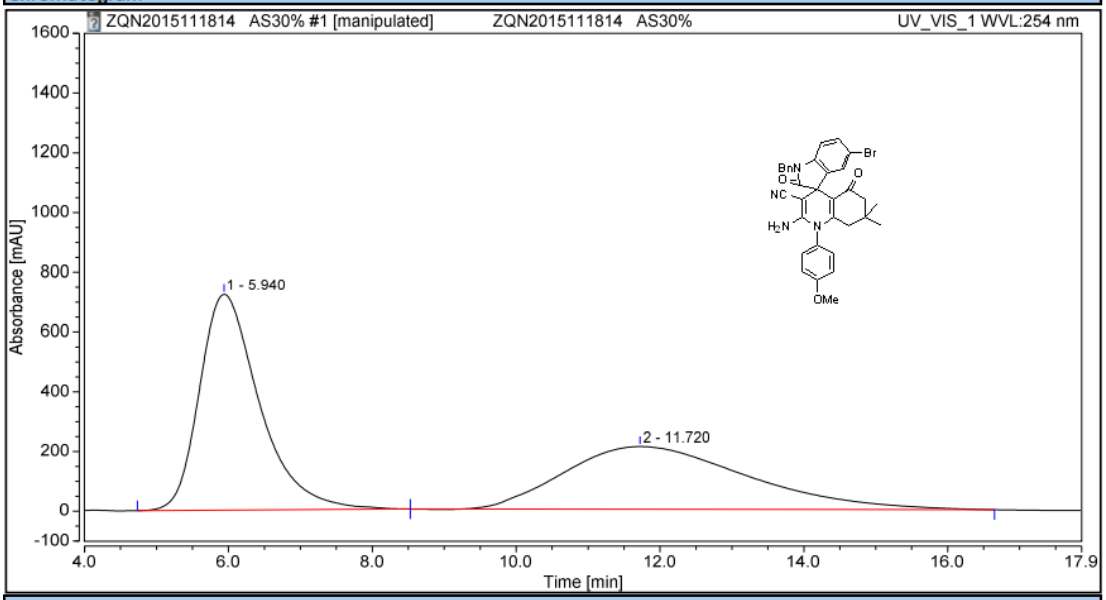


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.960	1413.045	1760.948	94.25	96.70	n.a.
2		7.477	86.243	60.119	5.75	3.30	n.a.
Total:			**1499.289**	**1821.068**	**100.00**	**100.00**	

4ai

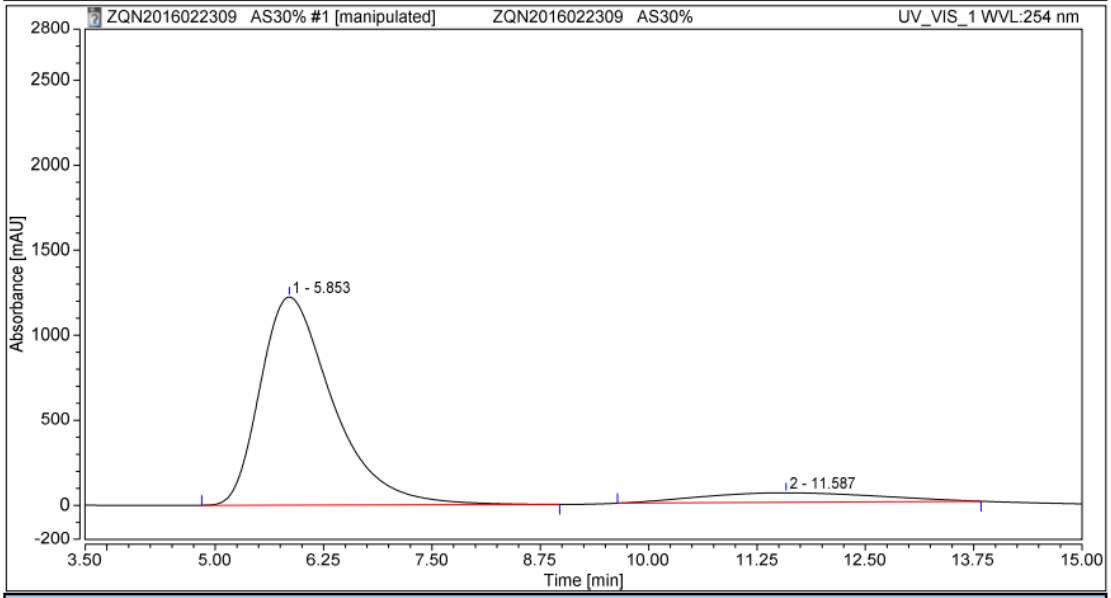
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.940	698.084	722.659	52.91	77.48	n.a.
2		11.720	621.247	210.046	47.09	22.52	n.a.
Total:			**1319.331**	**932.705**	**100.00**	**100.00**	

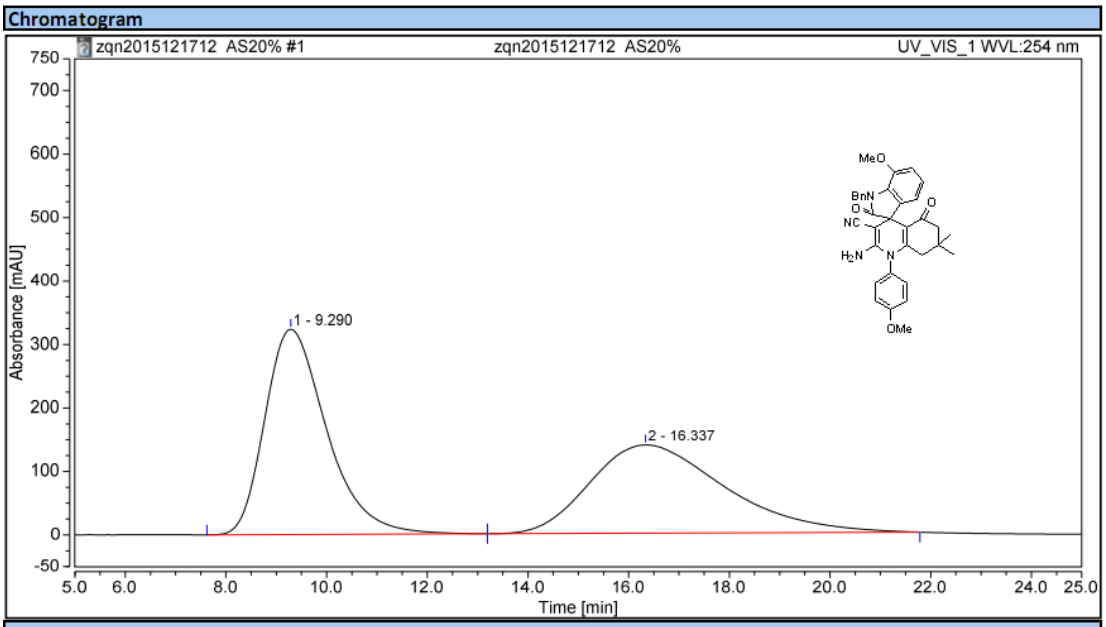
Chromatogram



Integration Results

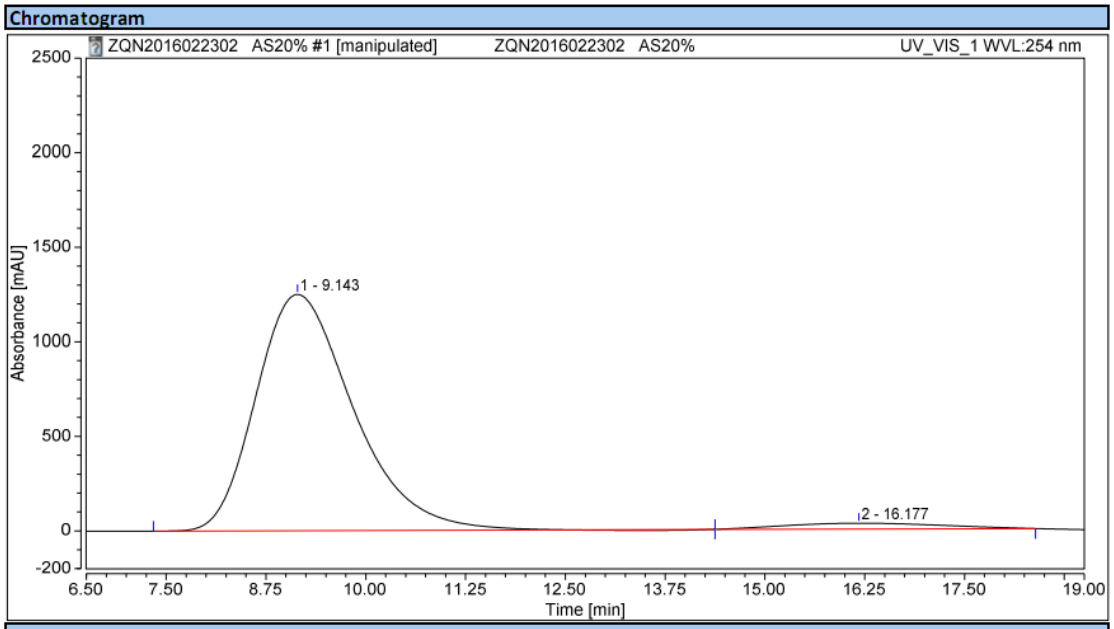
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.853	1186.937	1223.317	90.01	95.65	n.a.
2		11.587	131.716	55.648	9.99	4.35	n.a.
Total:			**1318.653**	**1278.966**	**100.00**	**100.00**	

4aj



Integration Results

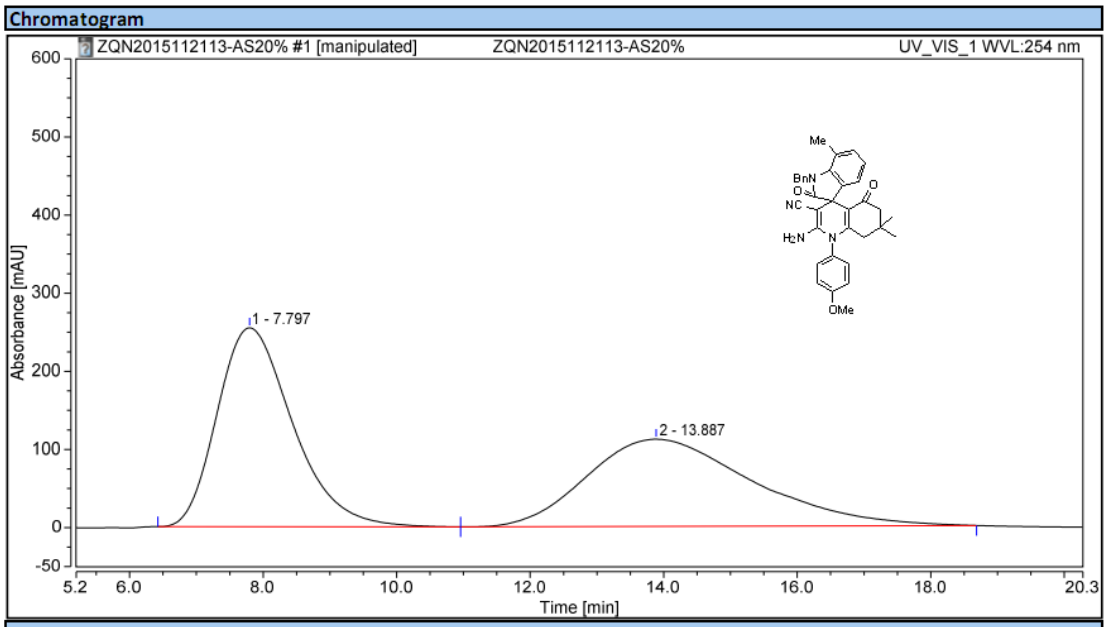
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.290	459.291	323.376	51.60	69.94	n.a.
2		16.337	430.736	138.995	48.40	30.06	n.a.
Total:			**890.027**	**462.370**	**100.00**	**100.00**	



Integration Results

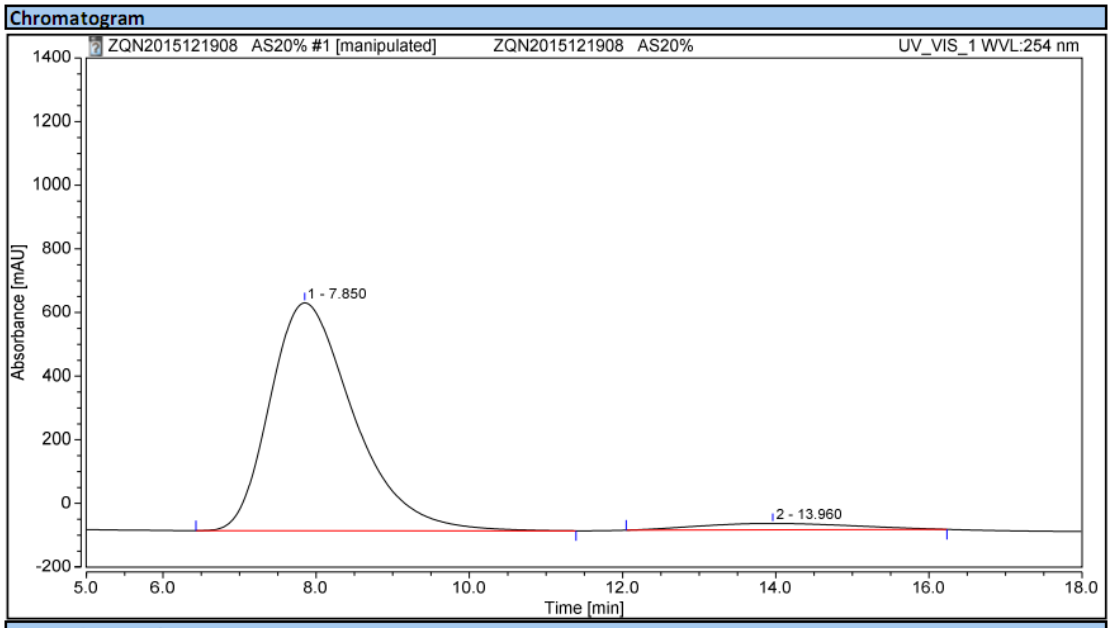
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.143	1762.442	1249.612	96.12	97.58	n.a.
2		16.177	71.184	30.976	3.88	2.42	n.a.
Total:			**1833.626**	**1280.588**	**100.00**	**100.00**	

4ak



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.797	333.472	254.632	51.09	69.53	n.a.
2		13.887	319.217	111.597	48.91	30.47	n.a.
Total:			**652.689**	**366.229**	**100.00**	**100.00**	

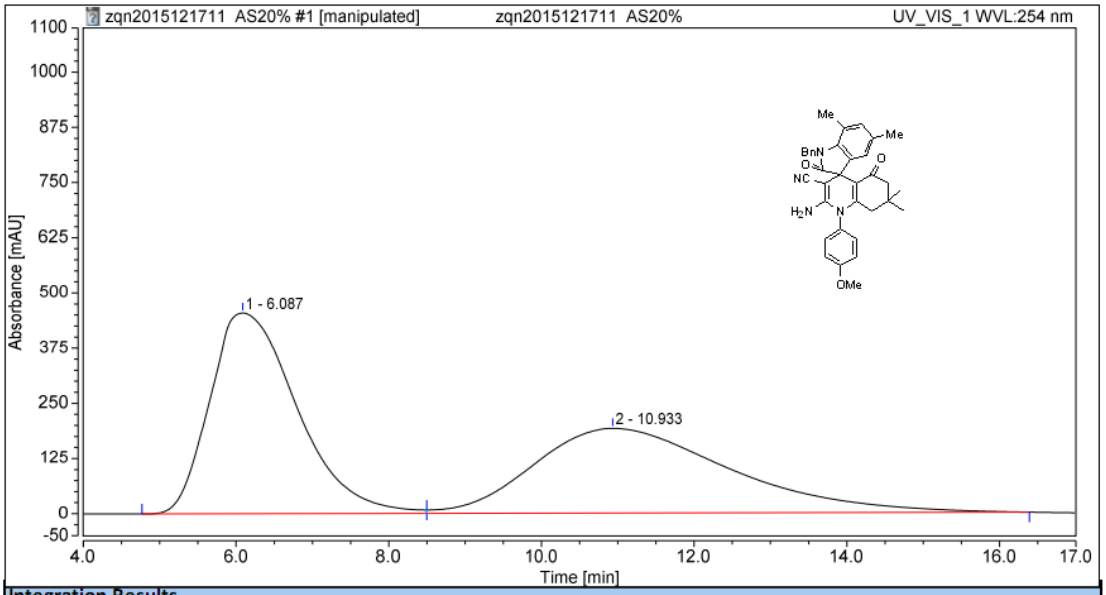


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.850	905.844	715.934	95.09	97.27	n.a.
2		13.960	46.744	20.062	4.91	2.73	n.a.
Total:			**952.587**	**735.996**	**100.00**	**100.00**	

4al

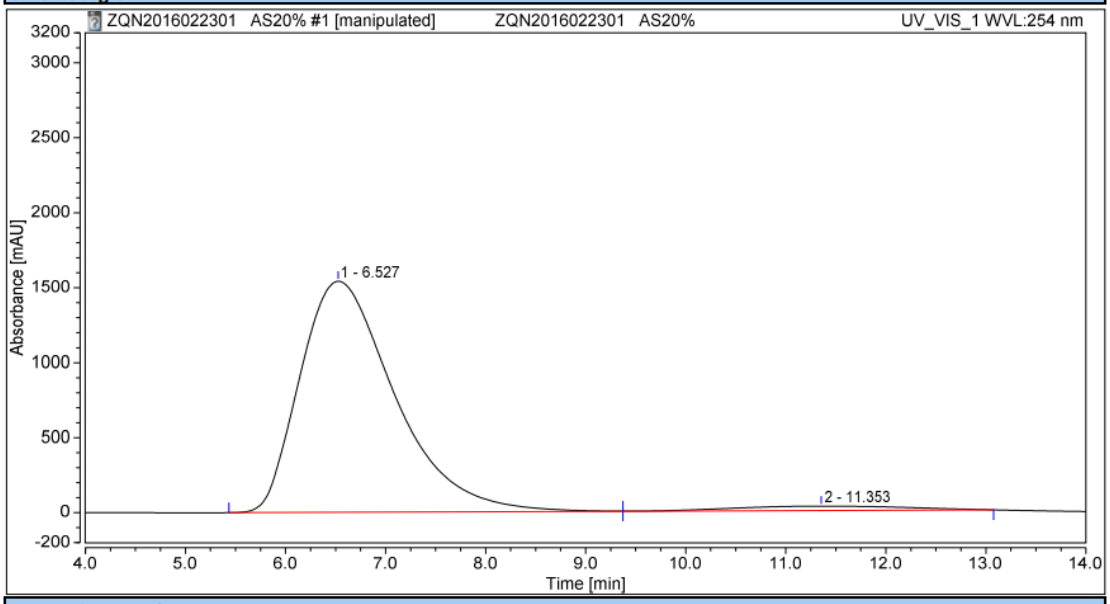
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.087	600.708	454.754	51.34	70.34	n.a.
2		10.933	569.358	191.769	48.66	29.66	n.a.
Total:			**1170.066**	**646.523**	**100.00**	**100.00**	

Chromatogram

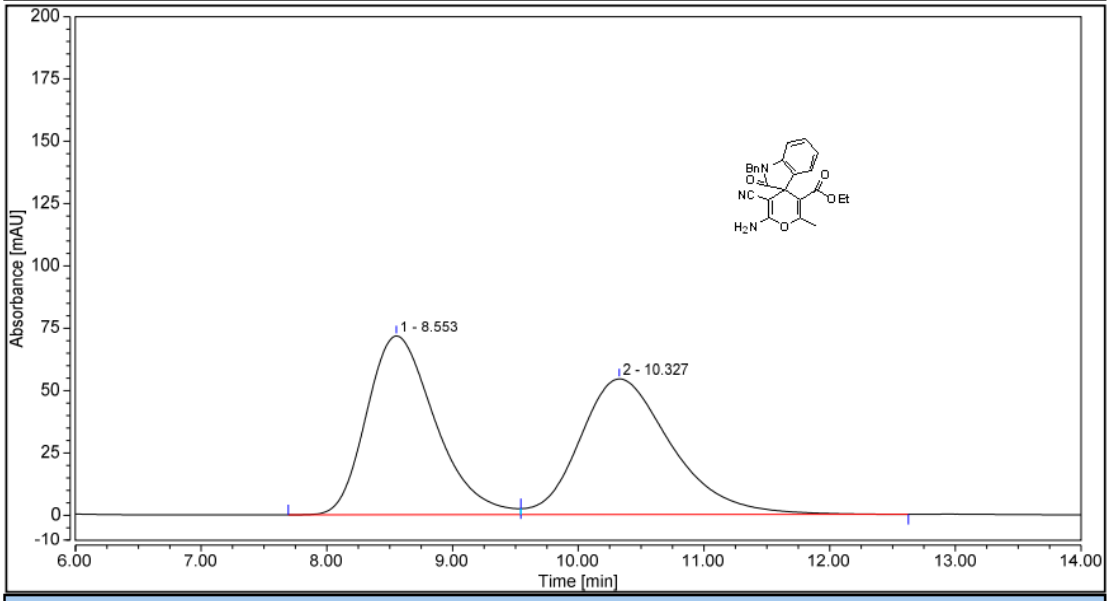


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.527	1688.976	1540.703	96.66	98.15	n.a.
2		11.353	58.347	29.076	3.34	1.85	n.a.
Total:			**1747.323**	**1569.779**	**100.00**	**100.00**	

Compound 6

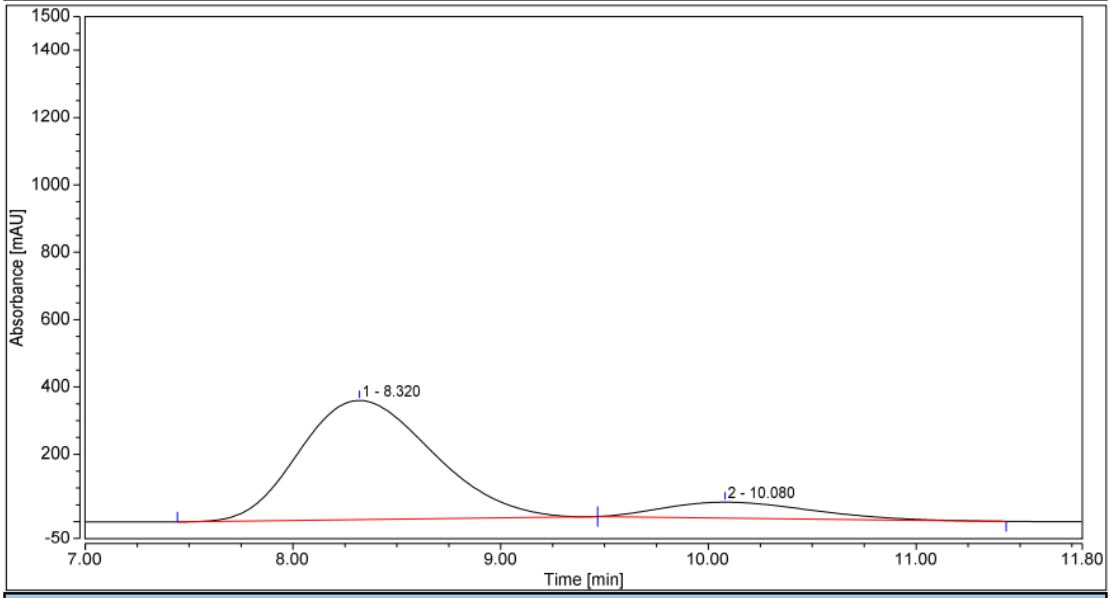
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.553	45.309	71.694	49.64	56.85	n.a.
2		10.327	45.972	54.416	50.36	43.15	n.a.
Total:			**91.281**	**126.110**	**100.00**	**100.00**	

Chromatogram

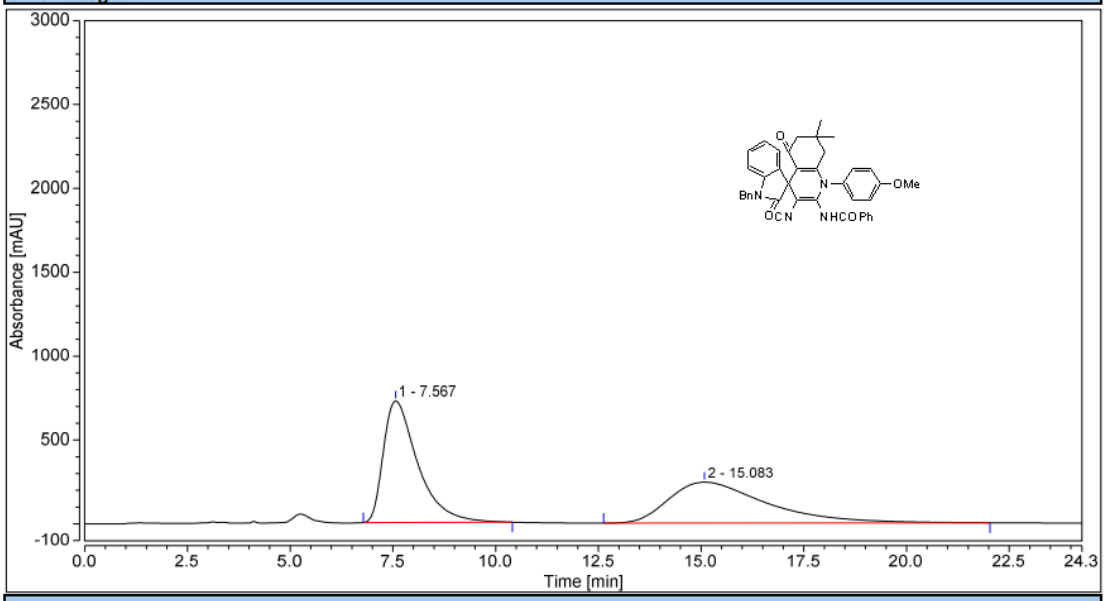


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.320	262.731	353.645	87.23	88.24	n.a.
2		10.080	38.450	47.133	12.77	11.76	n.a.
Total:			**301.181**	**400.778**	**100.00**	**100.00**	

Compound 7

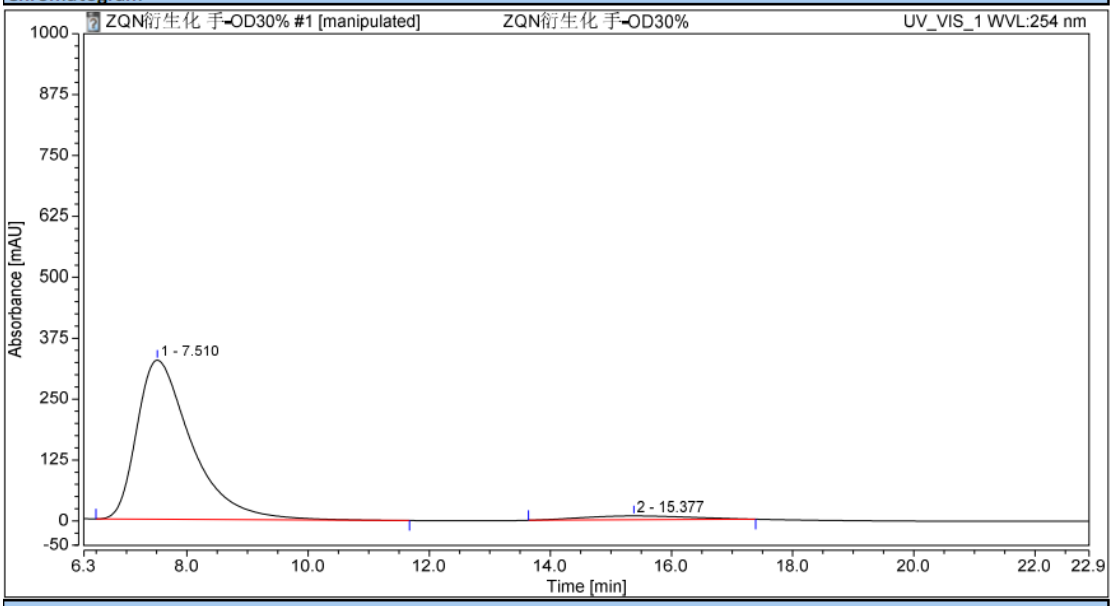
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.567	704.672	724.484	51.22	74.83	n.a.
2		15.083	671.064	243.674	48.78	25.17	n.a.
Total:			**1375.736**	**968.158**	**100.00**	**100.00**	

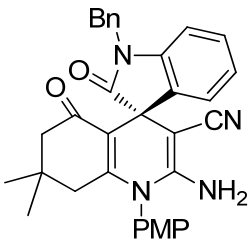
Chromatogram



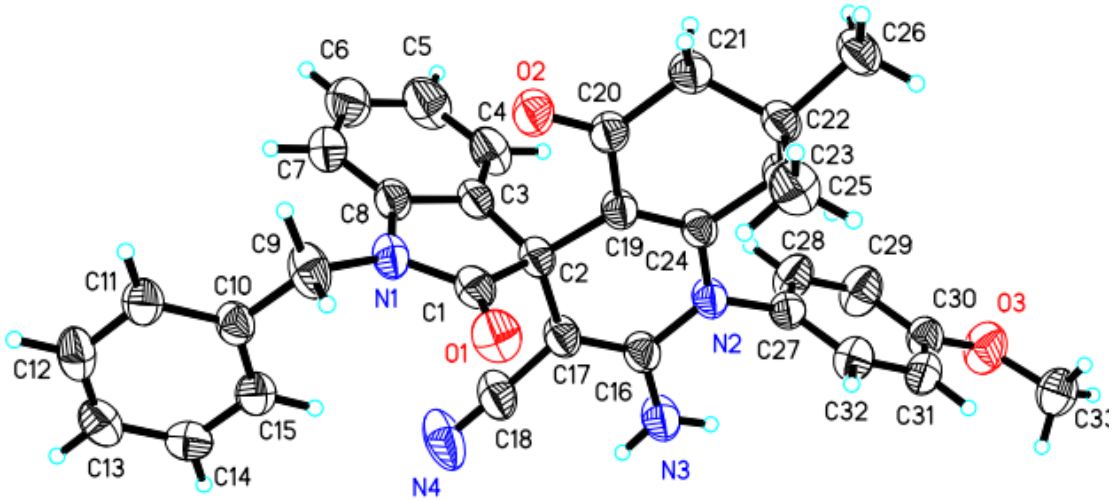
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.510	341.260	326.653	95.38	97.63	n.a.
2		15.377	16.514	7.945	4.62	2.37	n.a.
Total:			**357.773**	**334.597**	**100.00**	**100.00**	

4. X-ray single crystal data for compound 4aa



(*R*)-**4aa**



The thermal ellipsoid was drawn at the 30% probability level.

Identification code	cu_dm15841_0m	
Empirical formula	C33 H30 N4 O3	
Formula weight	530.61	
Temperature	296 K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C 1 2 1	
Unit cell dimensions	a = 32.0719(7) Å	α= 90°.
	b = 9.2396(2) Å	β= 109.7790(10)°.
	c = 20.2331(4) Å	γ = 90°.
Volume	5642.0(2) $Å^3$	
Z	8	
Density (calculated)	1.249 Mg/m^3	
Absorption coefficient	0.651 mm^{-1}	
F(000)	2240	

Crystal size	0.28 x 0.1 x 0.05 mm^3
Theta range for data collection	2.320 to 69.706°.
Index ranges	-38<=h<=36, -11<=k<=11, -24<=l<=24
Reflections collected	21205
Independent reflections	8811 [R(int) = 0.0344]
Completeness to theta = 67.679°	97.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7532 and 0.5863
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8811 / 1 / 729
Goodness-of-fit on F^2	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0540, wR2 = 0.1393
R indices (all data)	R1 = 0.0707, wR2 = 0.1557
Absolute structure parameter	-0.04(19)
Extinction coefficient	0.00069(9)
Largest diff. peak and hole	0.281 and -0.229 e.$Å^{-3}$