Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

Diastereo- and Enantioselective Construction of Biologically Important Pyrrolo[1,2-*a*]indole Scaffolds via Catalytic Asymmetric [3+2] Cyclodimerizations of 3-Alkyl-2-vinylindoles

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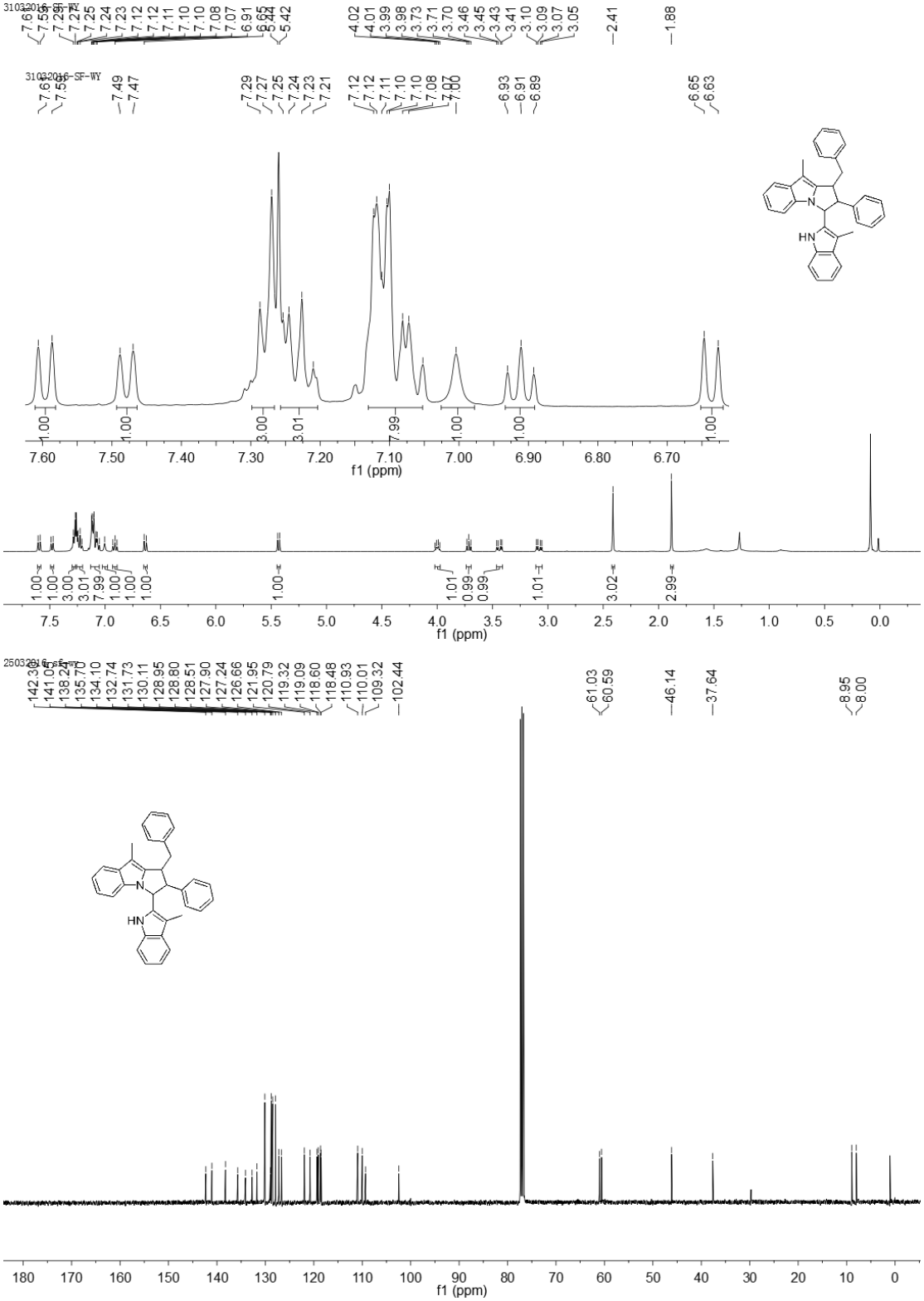
2a



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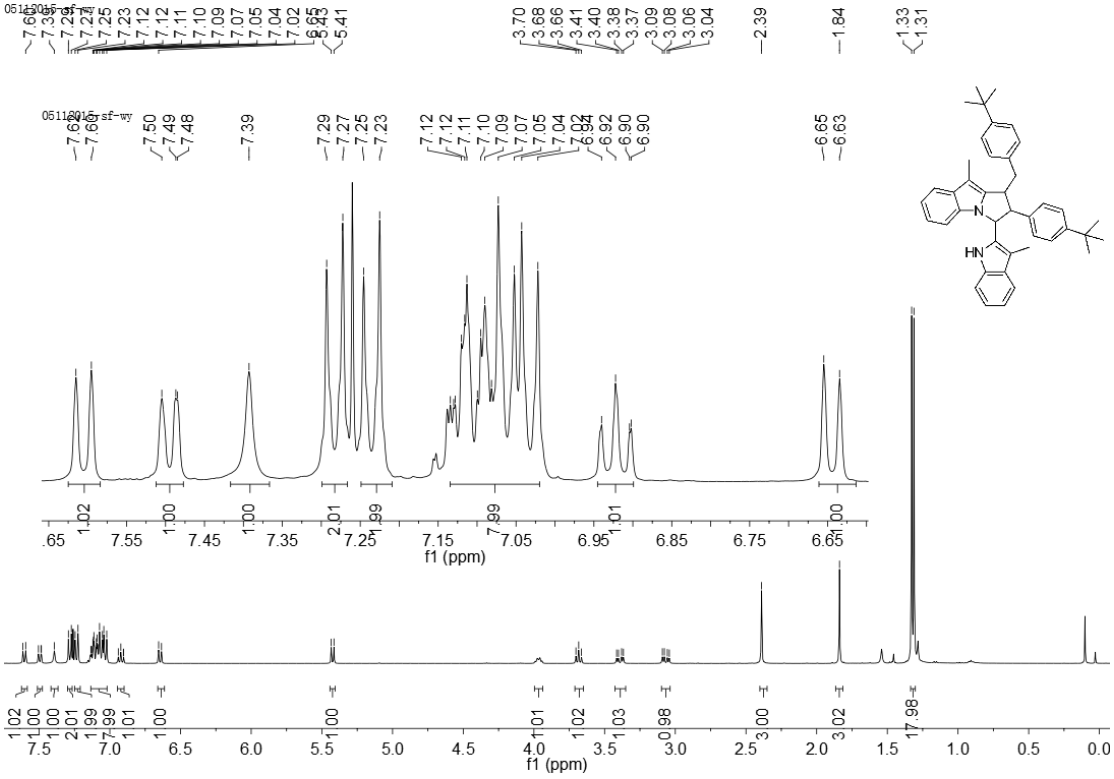

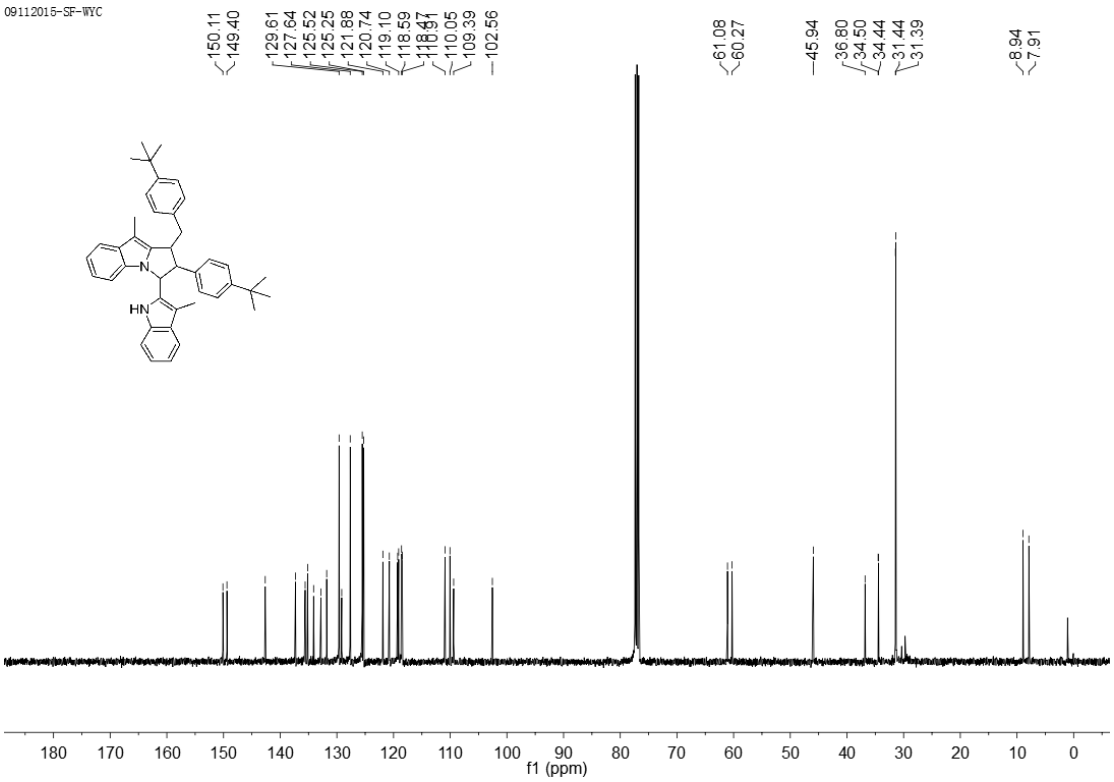

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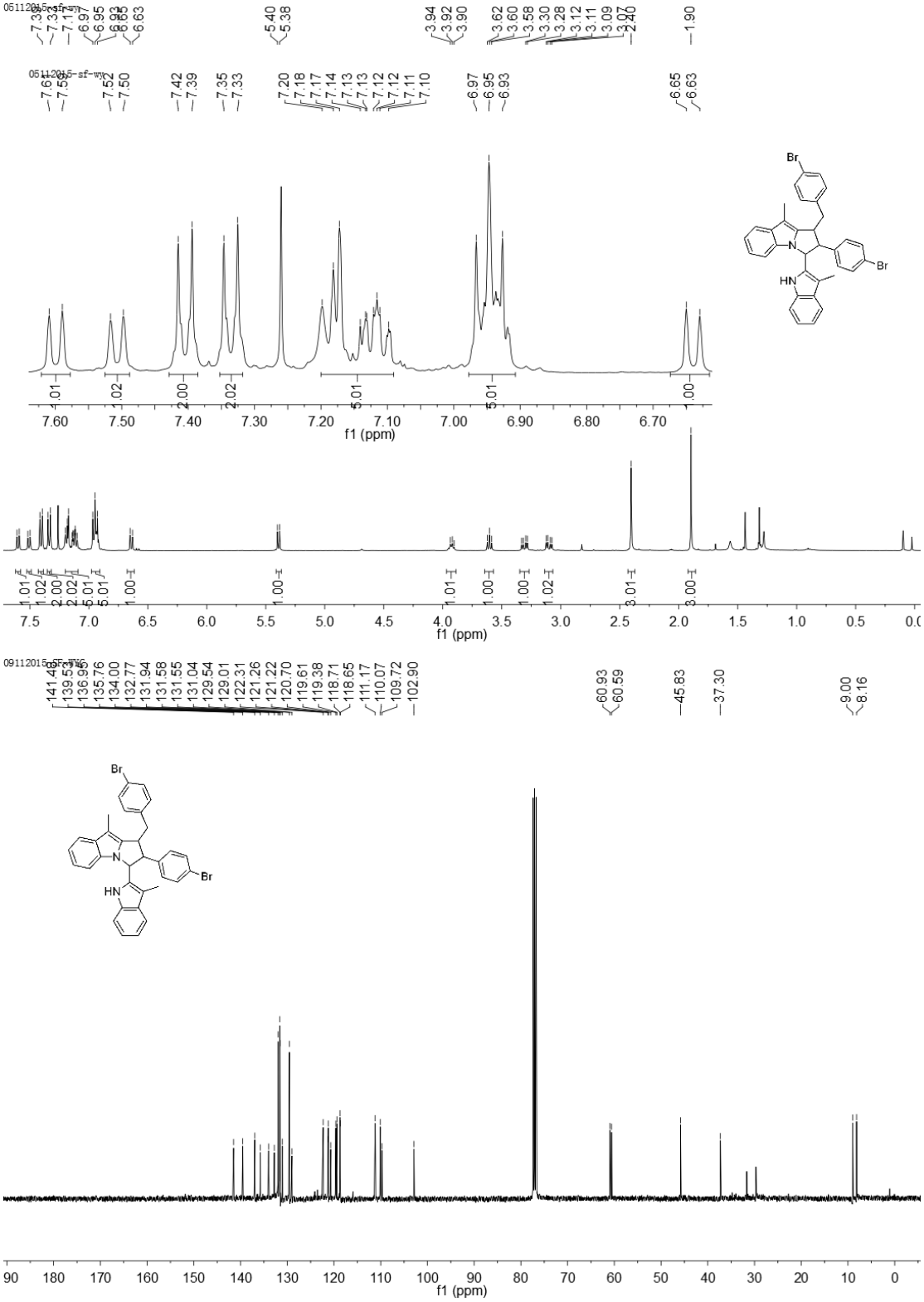

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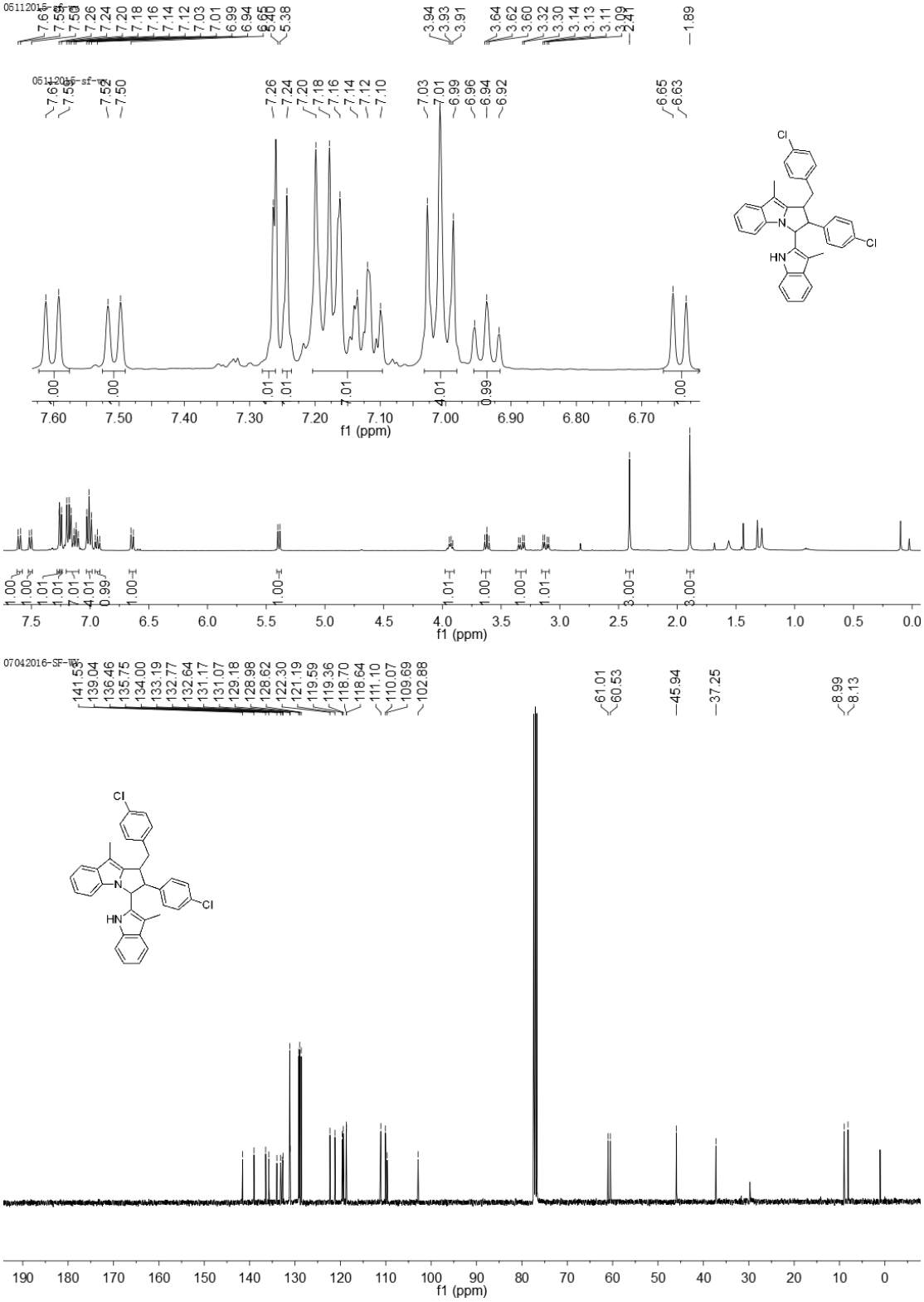
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3.94
3.93
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3.14
3.13
3.11
3.09
2.41
1.89
Cl
Cl
HN
f1 (ppm)
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139.04
136.46
135.75
134.00
133.19
132.77
132.64
131.17
131.07
129.18
128.98
128.62
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118.70
118.64
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f1 (ppm)

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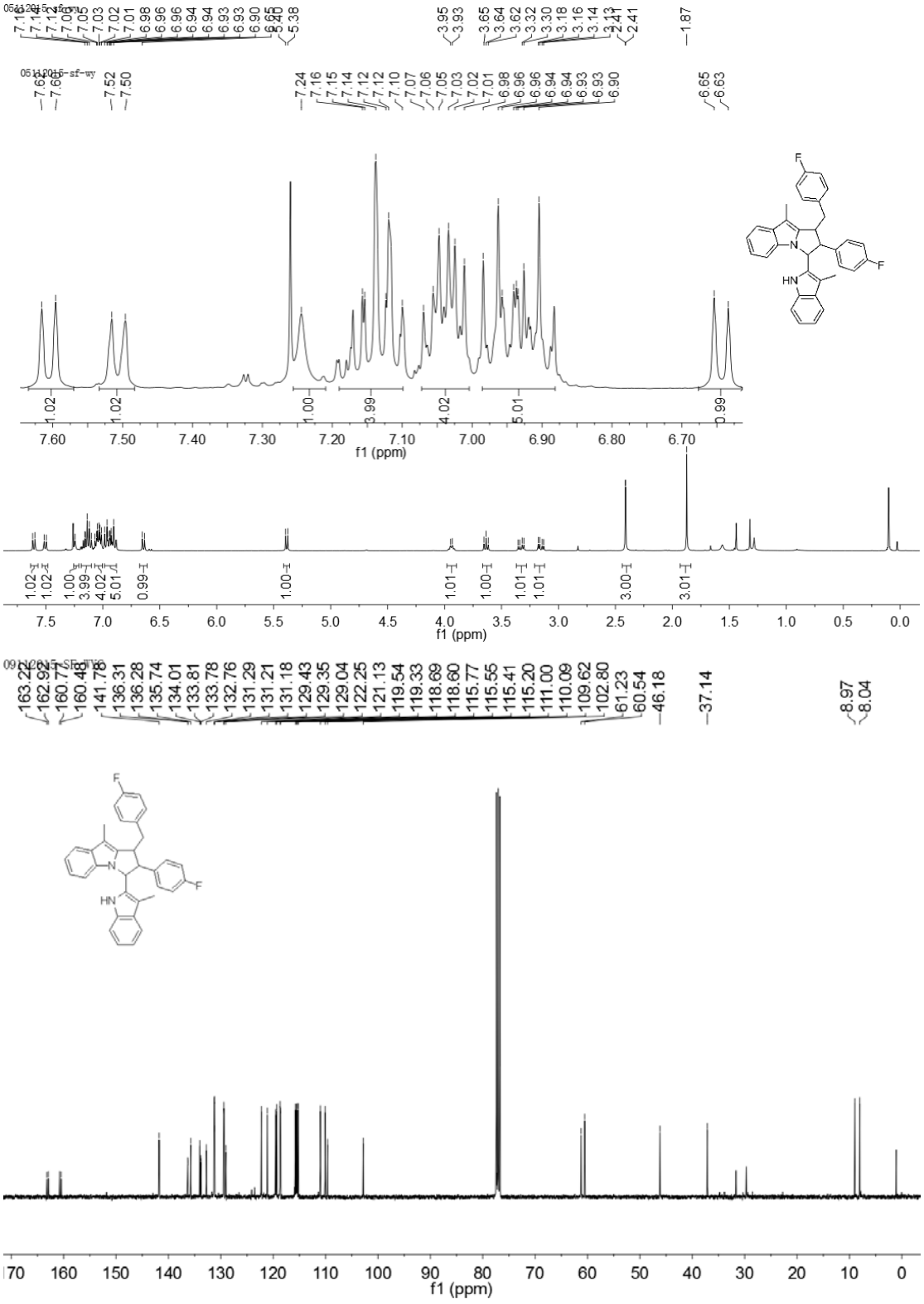

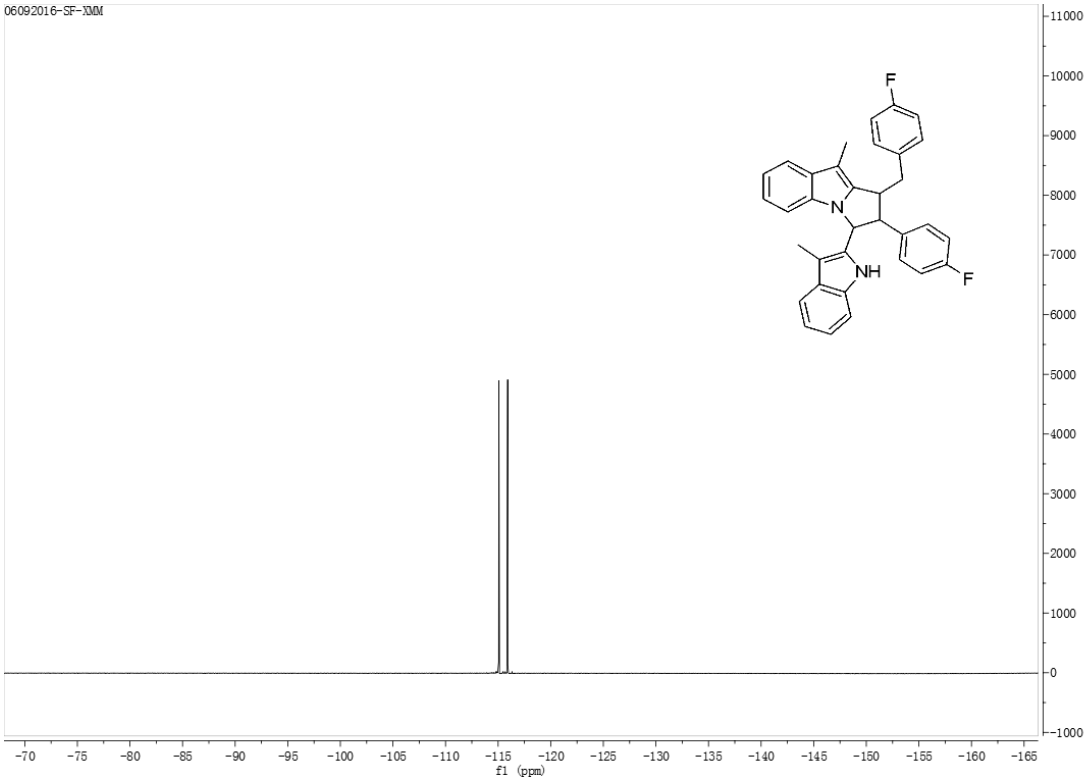

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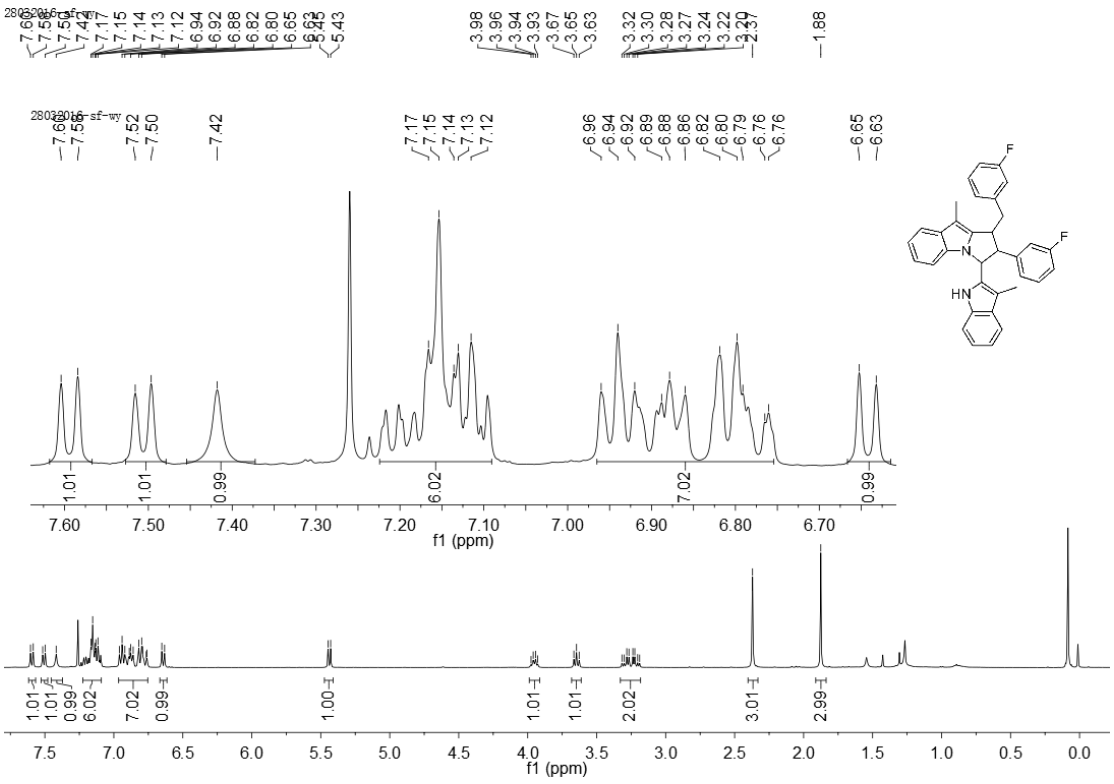

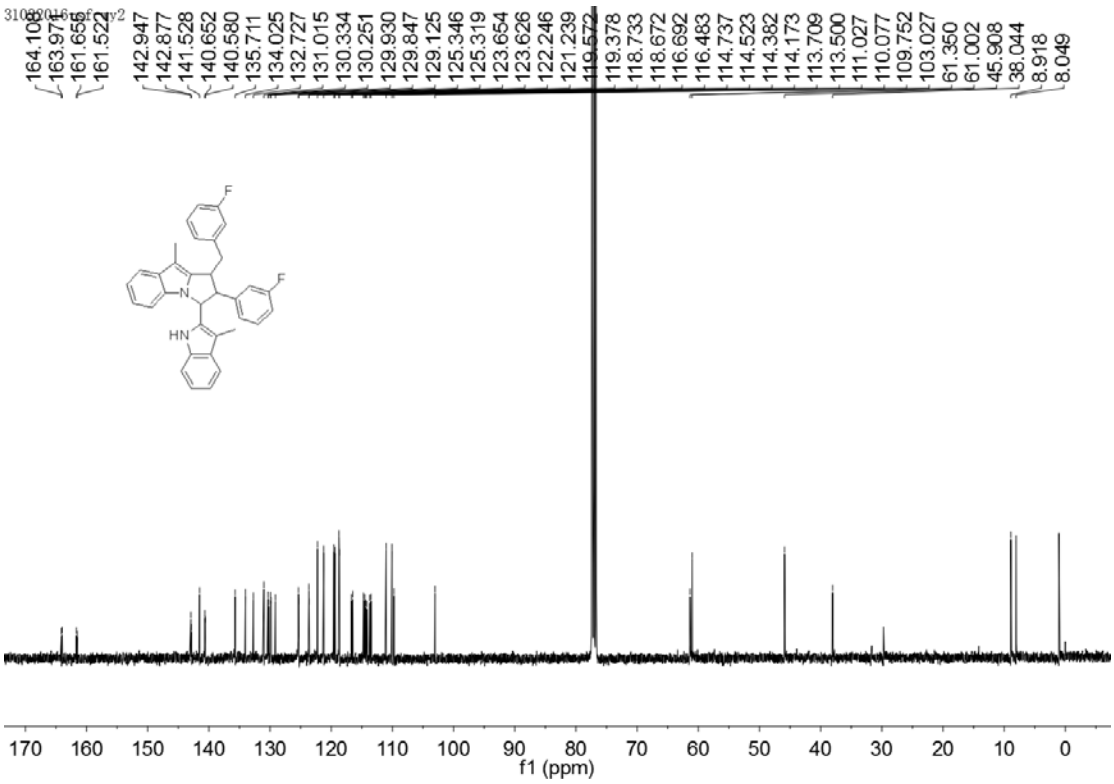
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129.930
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123.654
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122.246
121.239
119.572
119.378
118.733
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114.737
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113.500
111.027
110.077
109.752
103.027
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F
N
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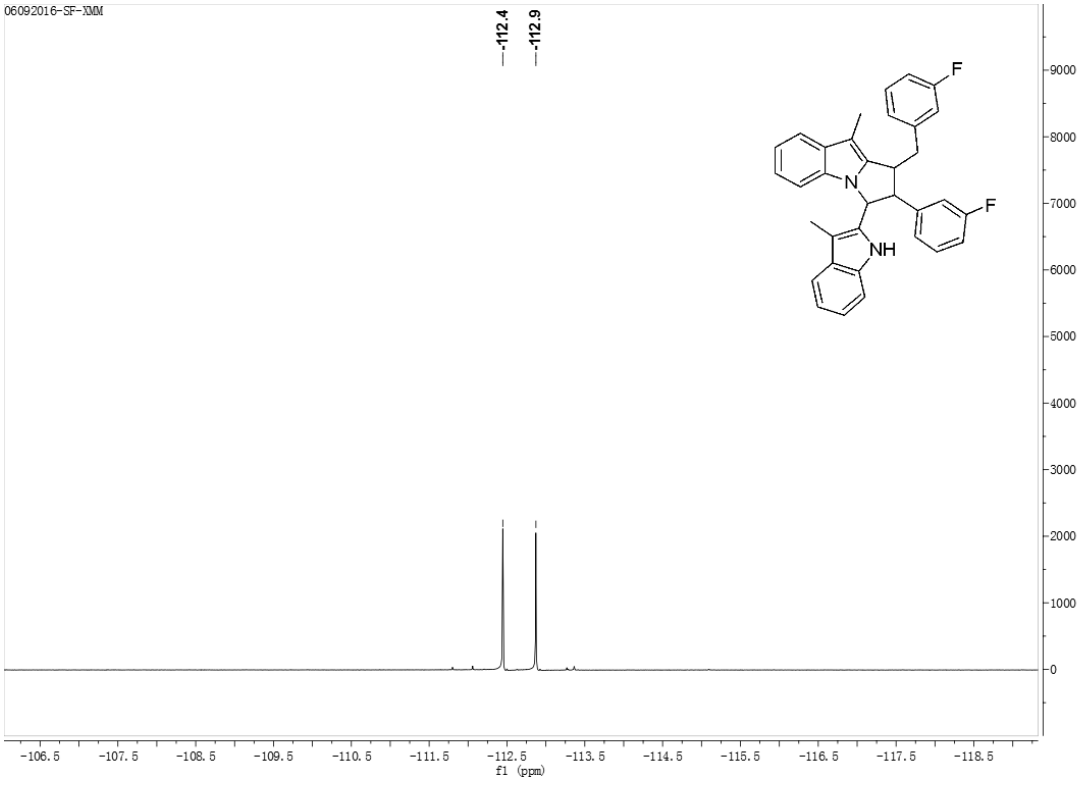
f1 (ppm)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0
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f1 (ppm)

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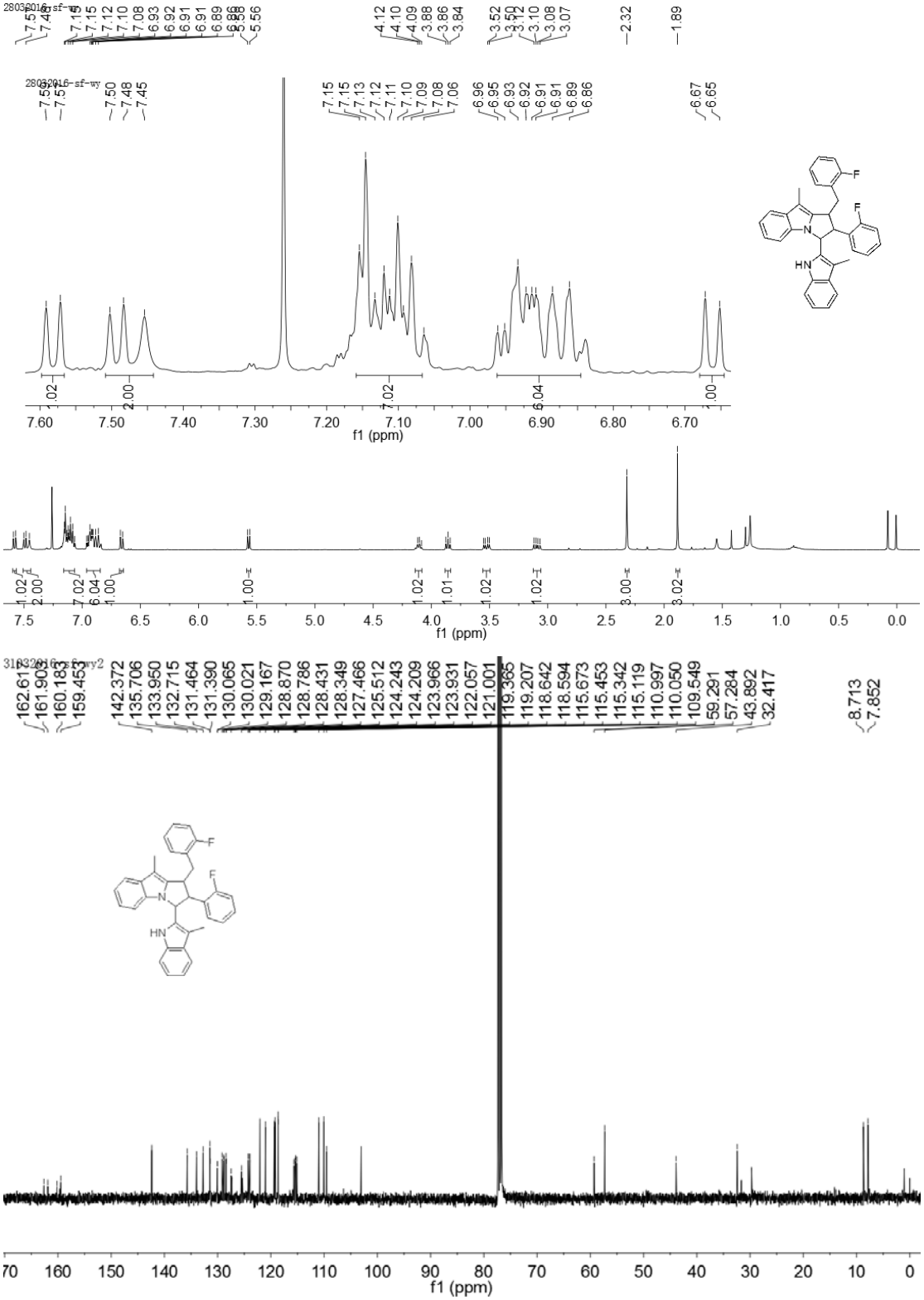

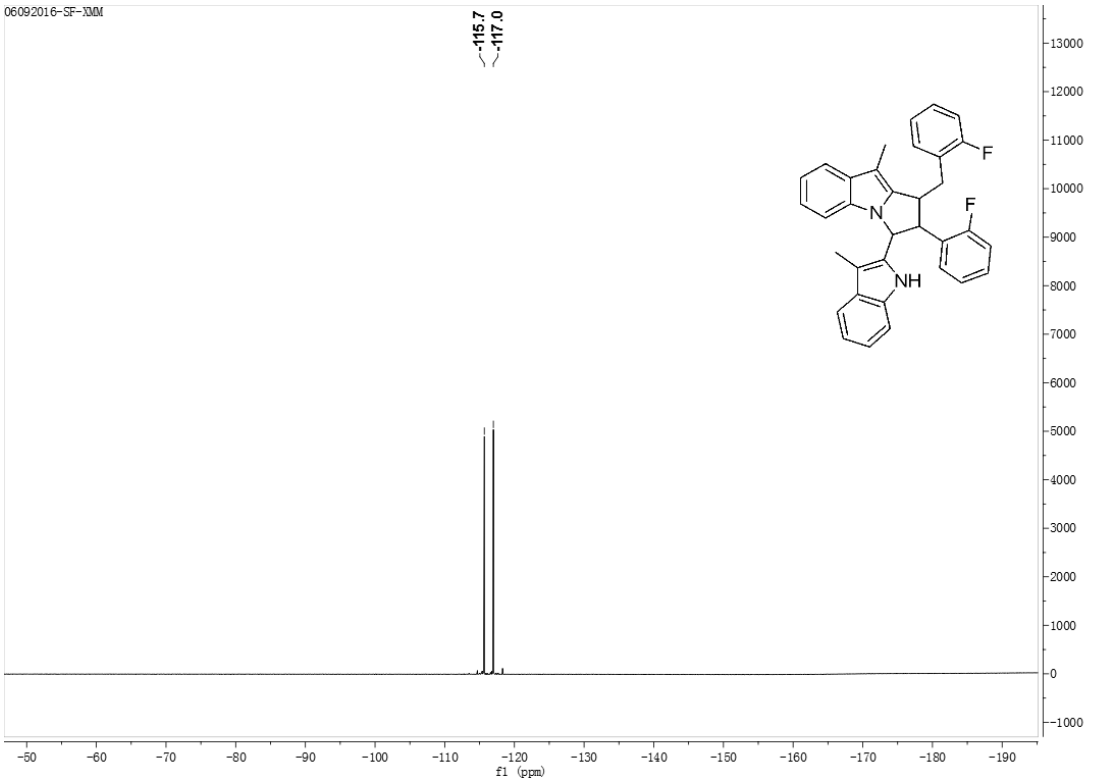
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F
F
N
NH
f1 (ppm)

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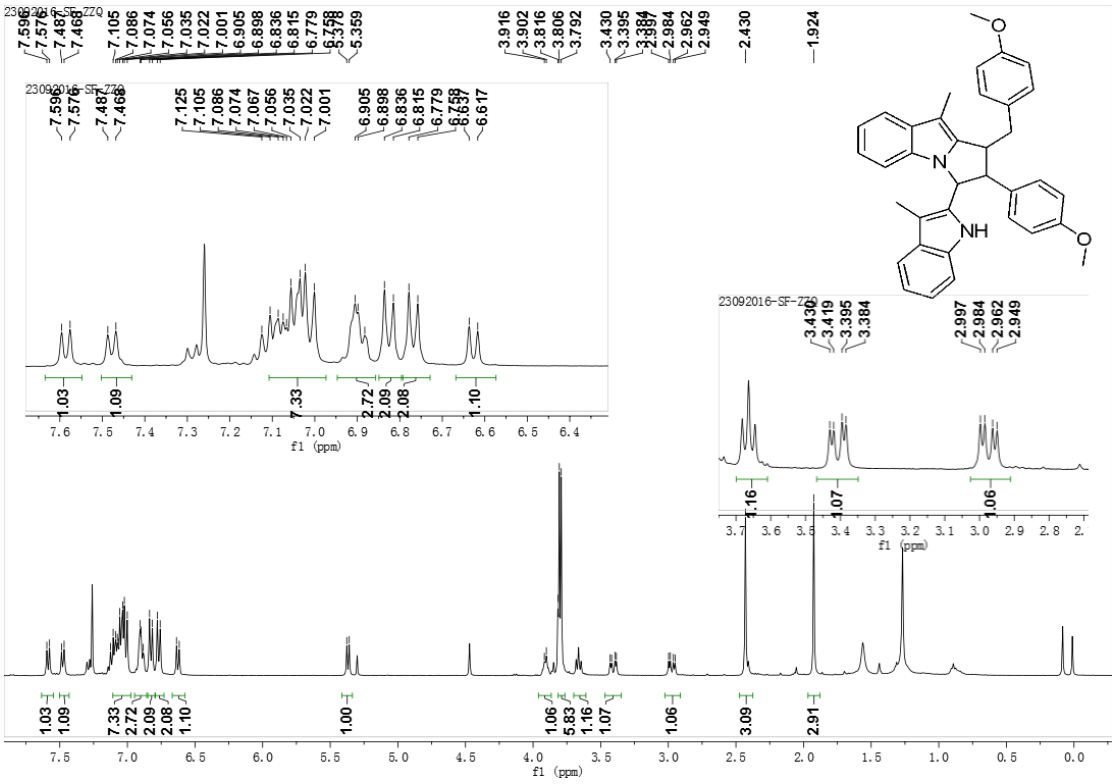
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6.815
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3.806
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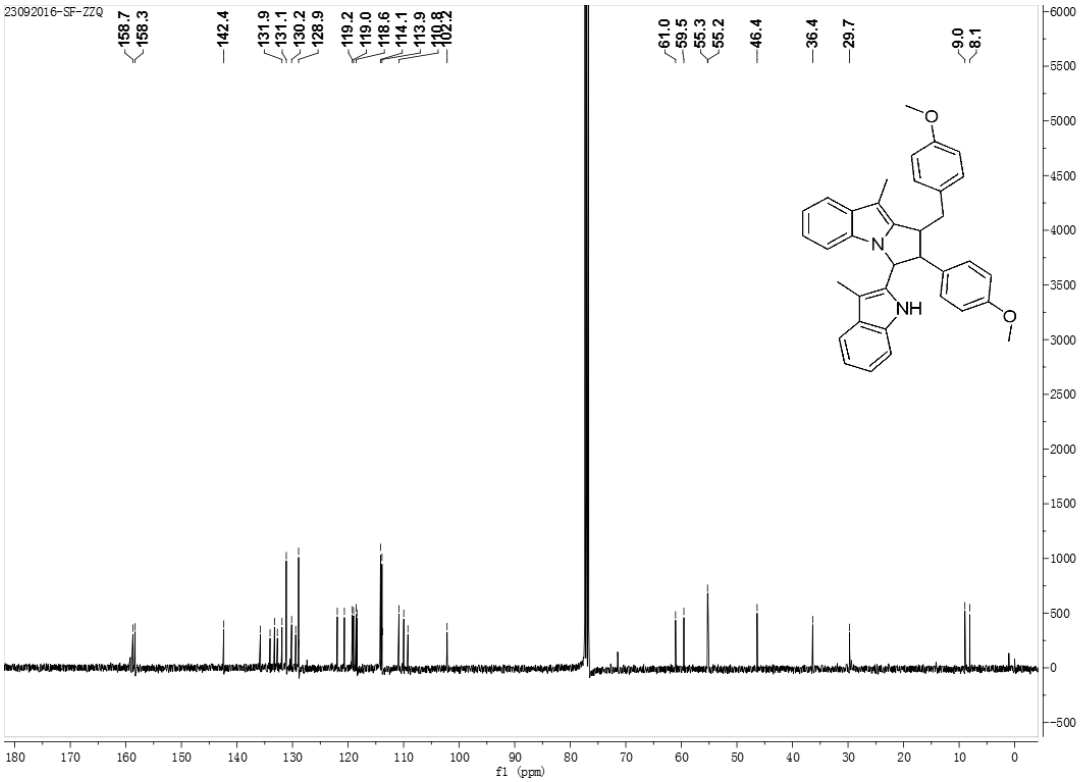
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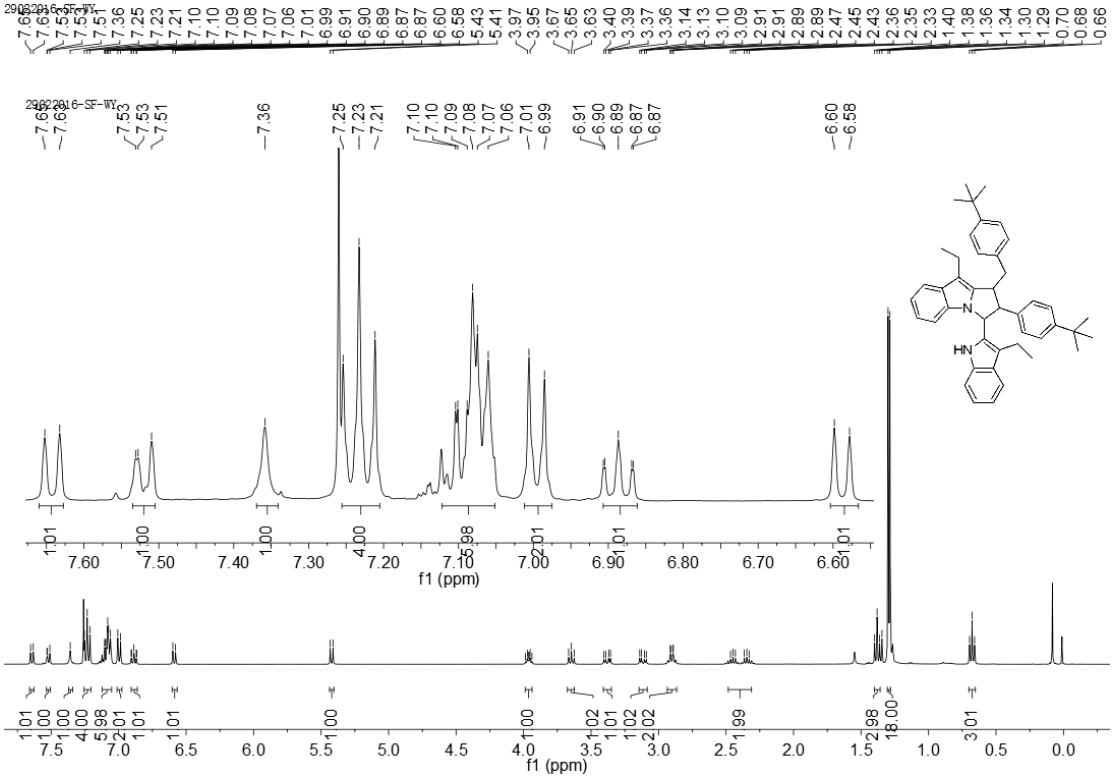
NH
f1 (ppm)

***ent*-2i**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7.08
7.07
7.06
7.01
6.99
6.91
6.90
6.89
6.87
6.60
6.58
5.43
3.97
3.95
3.67
3.65
3.63
3.40
3.39
3.37
3.36
3.14
3.13
3.10
3.09
2.91
2.91
2.89
2.89
2.47
2.45
2.43
2.36
2.35
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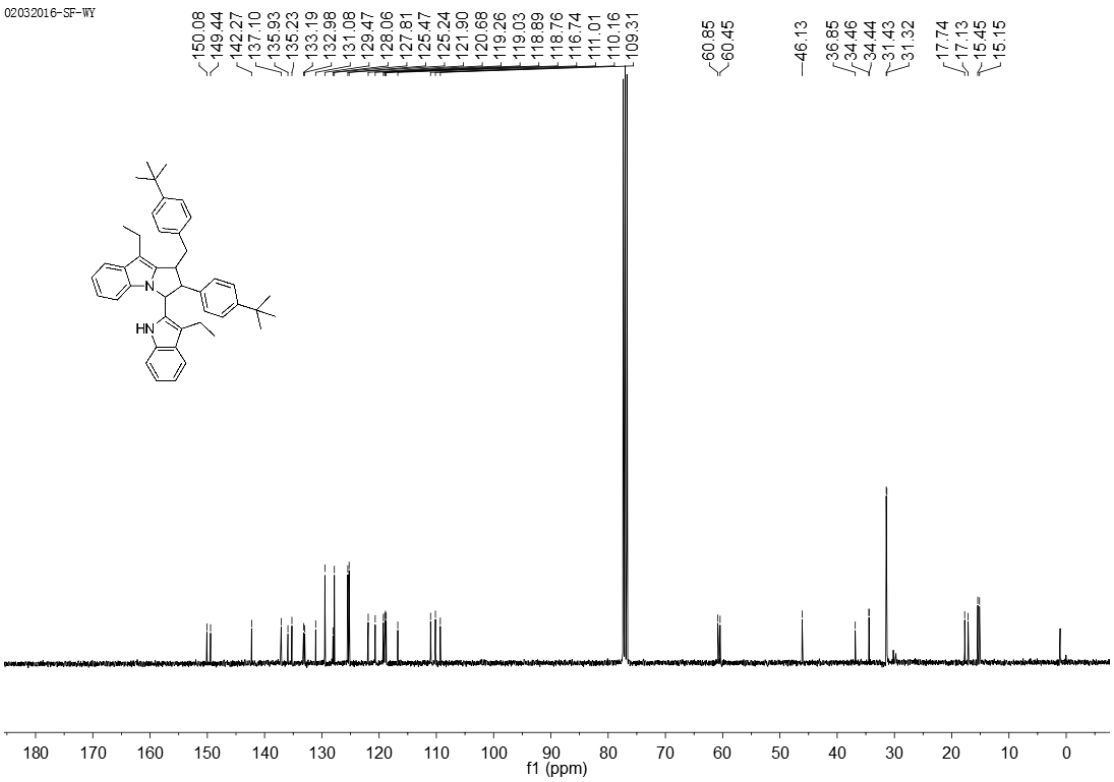
0.66
HN
f1 (ppm)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119.26
119.03
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116.74
111.01
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60.45
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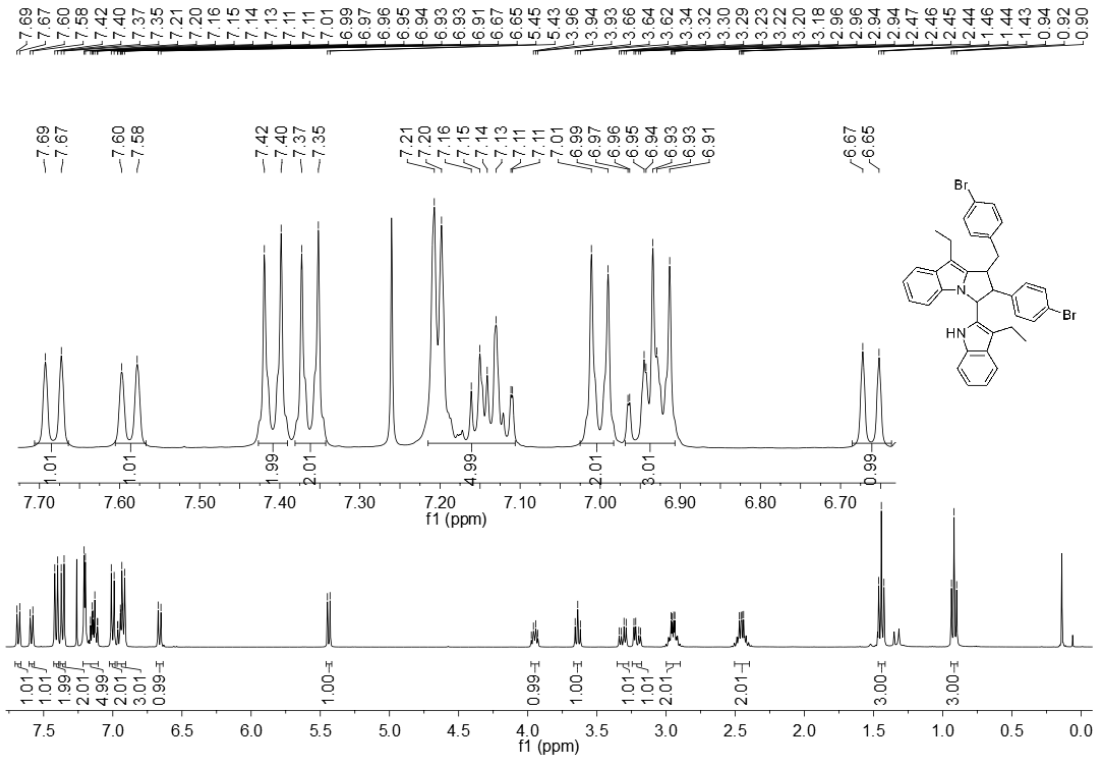
HN
f1 (ppm)

2j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7.13
7.11
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7.01
6.99
6.97
6.96
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6.93
6.93
6.91
6.67
6.65
Br
Br
HN
1.01
1.01
1.99
2.01
4.99
2.01
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2.01
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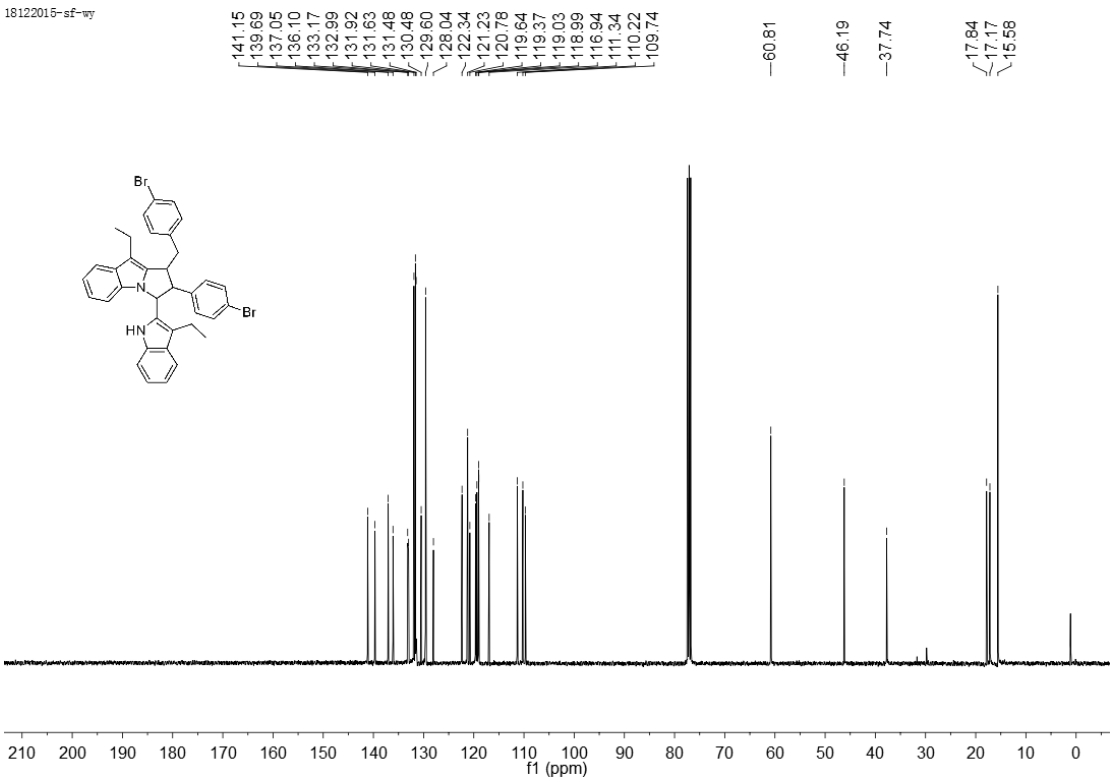
3.00
f1 (ppm)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128.04
122.34
121.23
120.78
119.64
119.37
119.03
118.99
116.94
111.34
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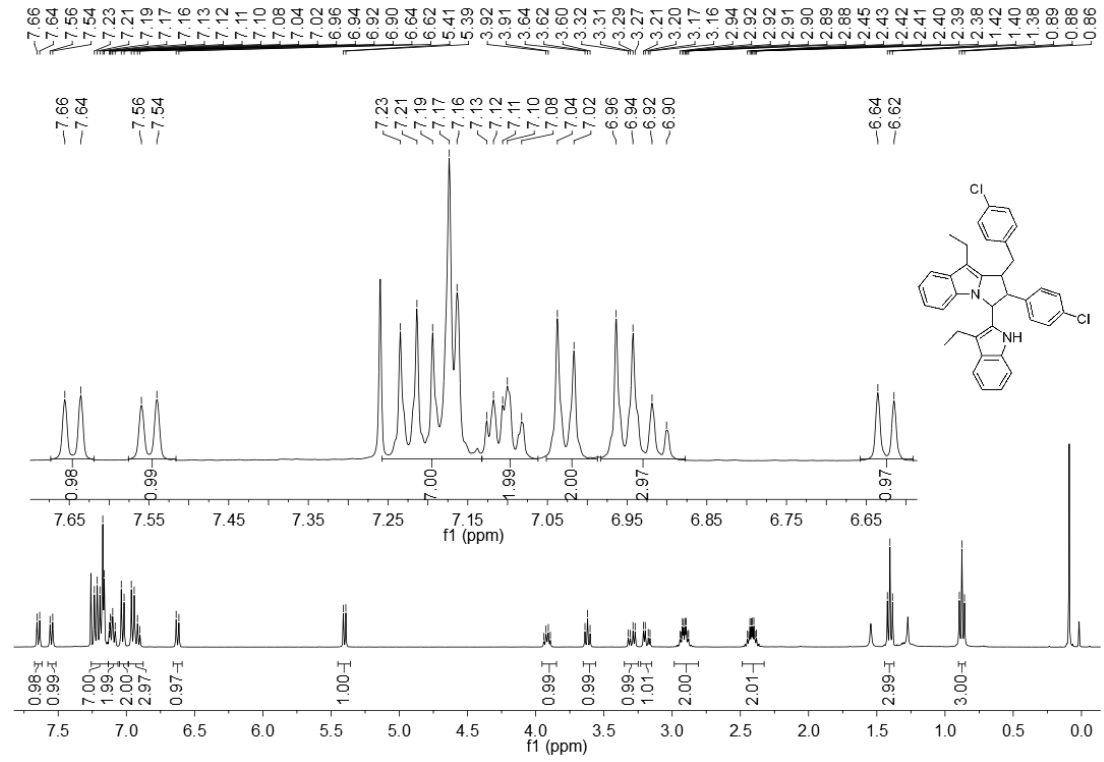
Br
Br
HN
f1 (ppm)

2k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7.08
7.04
7.02
6.96
6.94
6.92
6.90
6.64
6.62
5.41
5.39
3.92
3.91
3.64
3.62
3.60
3.32
3.31
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3.20
3.17
3.16
2.94
2.92
2.91
2.90
2.89
2.88
2.45
2.43
2.42
2.41
2.40
2.39
2.38
1.42
1.40
1.38
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0.88
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1.99
2.00
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0.97
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2.99
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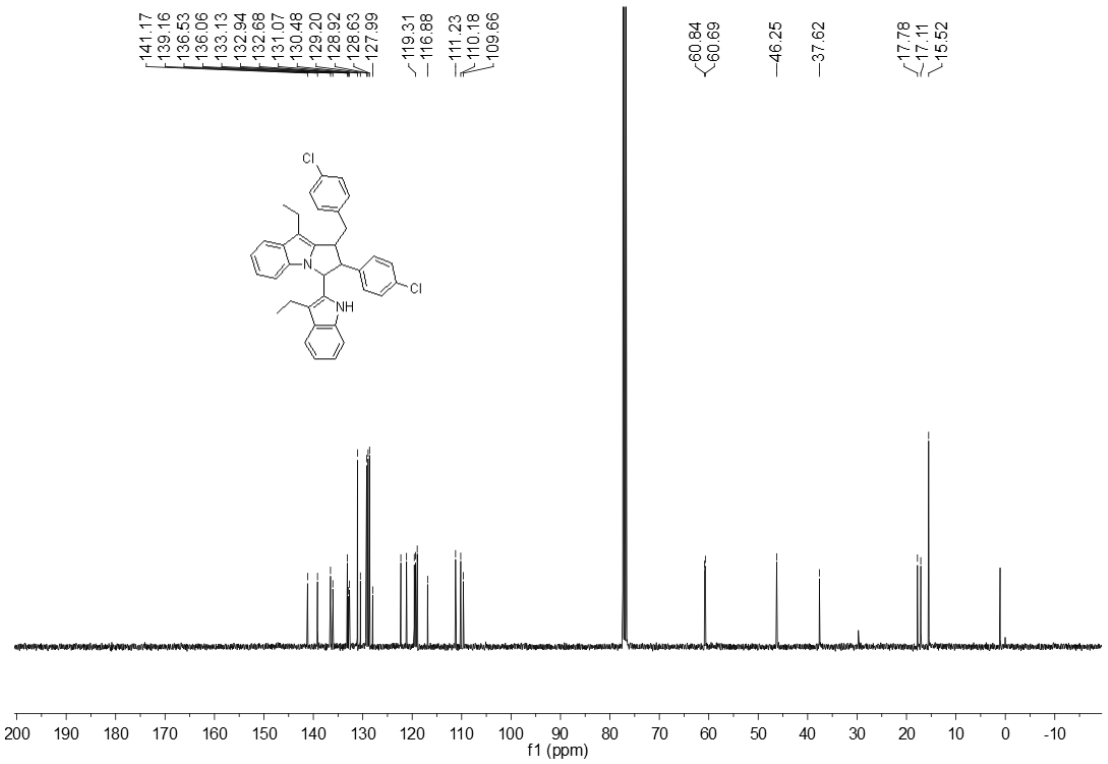
Cl
Cl
NH
f1 (ppm)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127.99
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116.88
111.23
110.18
109.66
60.84
60.69
46.25
37.62
17.78
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N
NH
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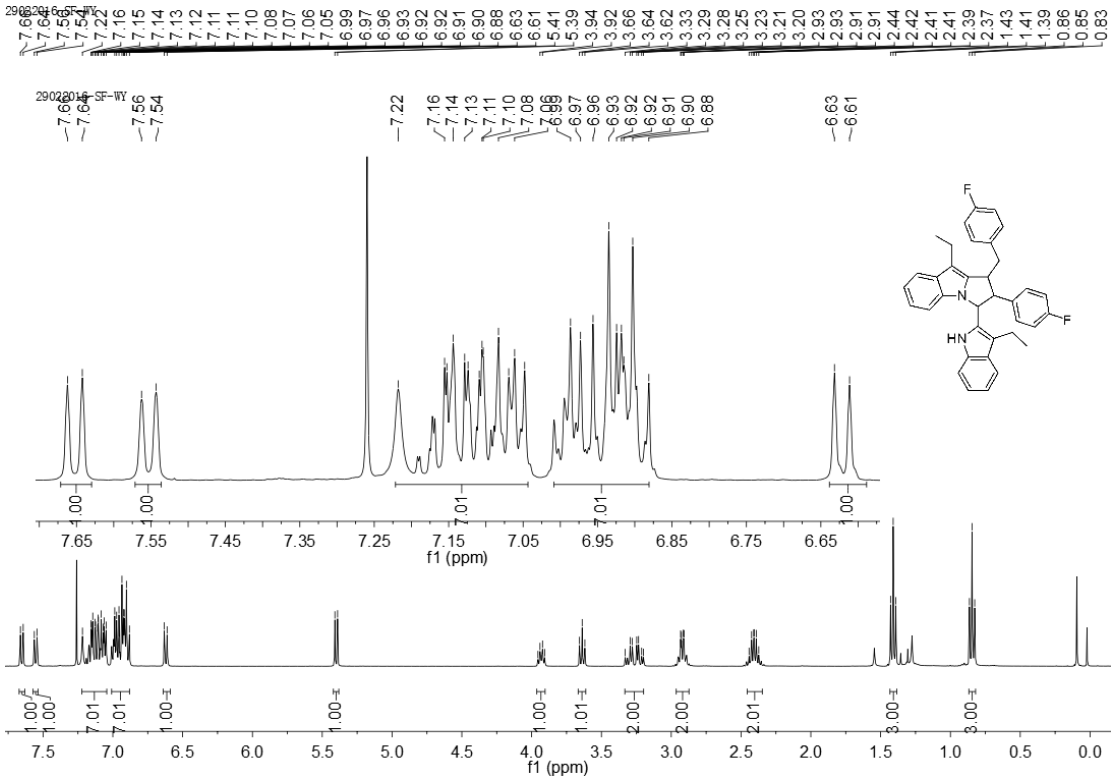
f1 (ppm)

***ent*-2l**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7.10
7.08
6.97
6.96
6.93
6.92
6.91
6.90
6.88
6.63
6.61
F
F
N
HN
1.00
1.00
7.01
7.01
1.00
7.65 7.55 7.45 7.35 7.25 7.15 7.05 6.95 6.85 6.75 6.65
f1 (ppm)
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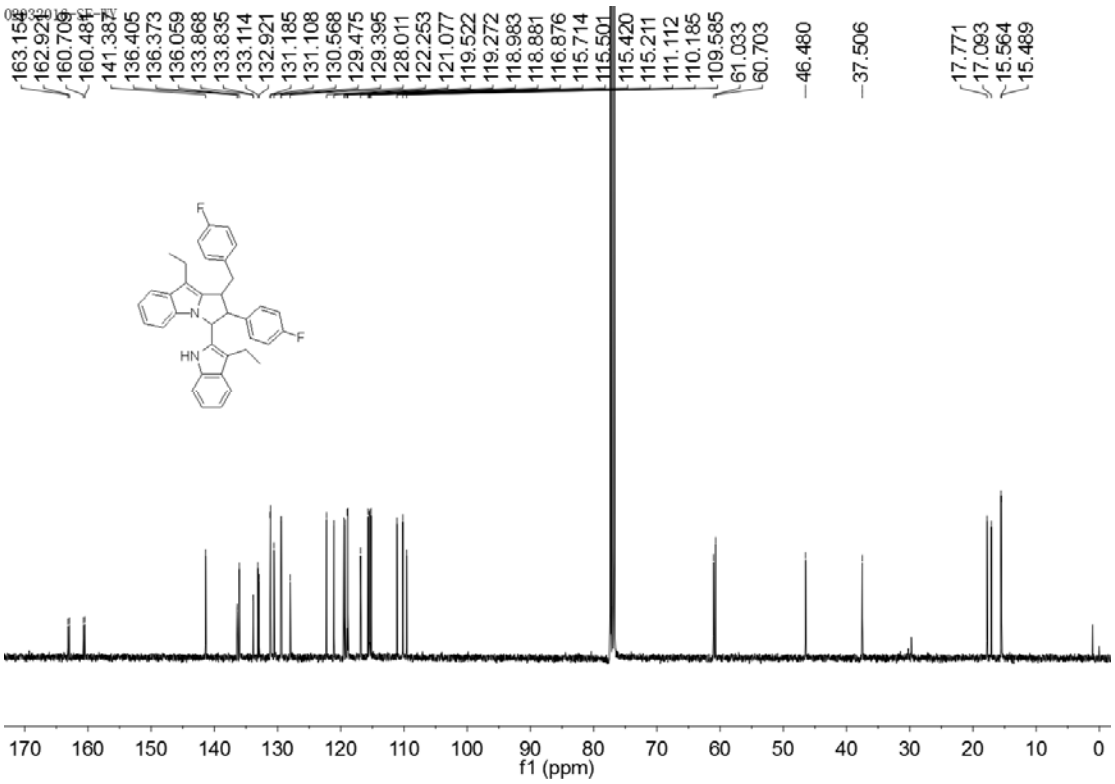
f1 (ppm)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129.475
129.395
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121.077
119.522
119.272
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116.876
115.714
115.501
115.420
115.211
111.112
110.185
109.585
61.033
60.703
46.480
37.506
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HN
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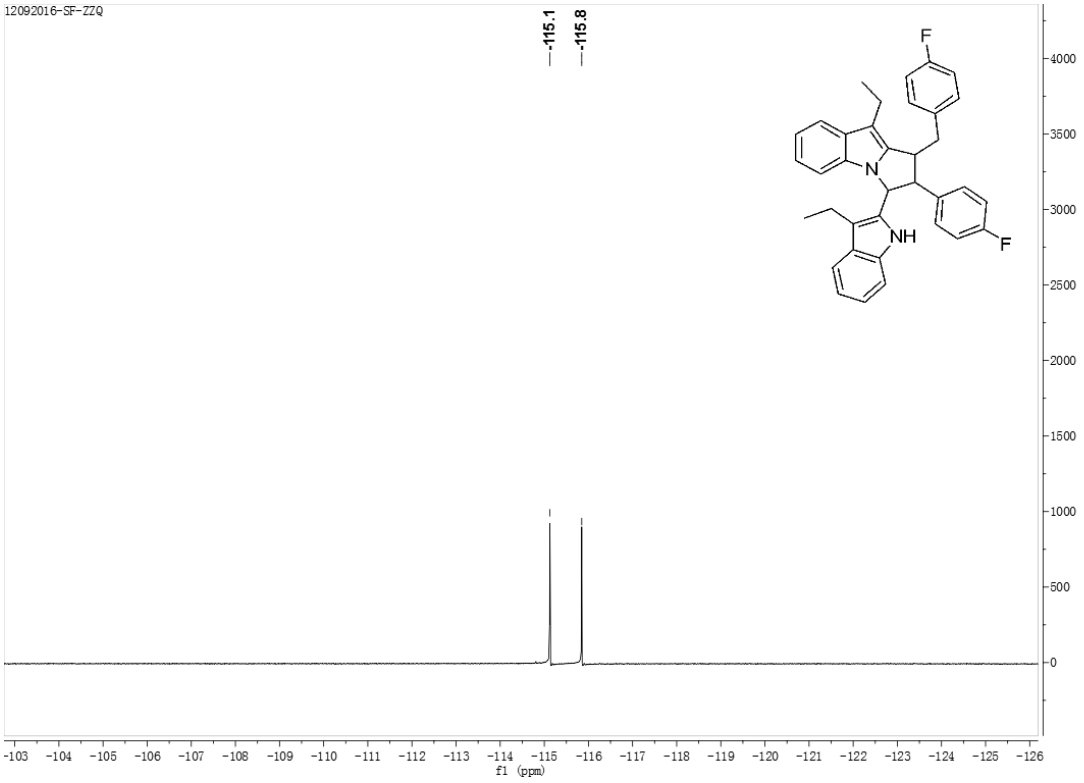
f1 (ppm)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NH
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3500
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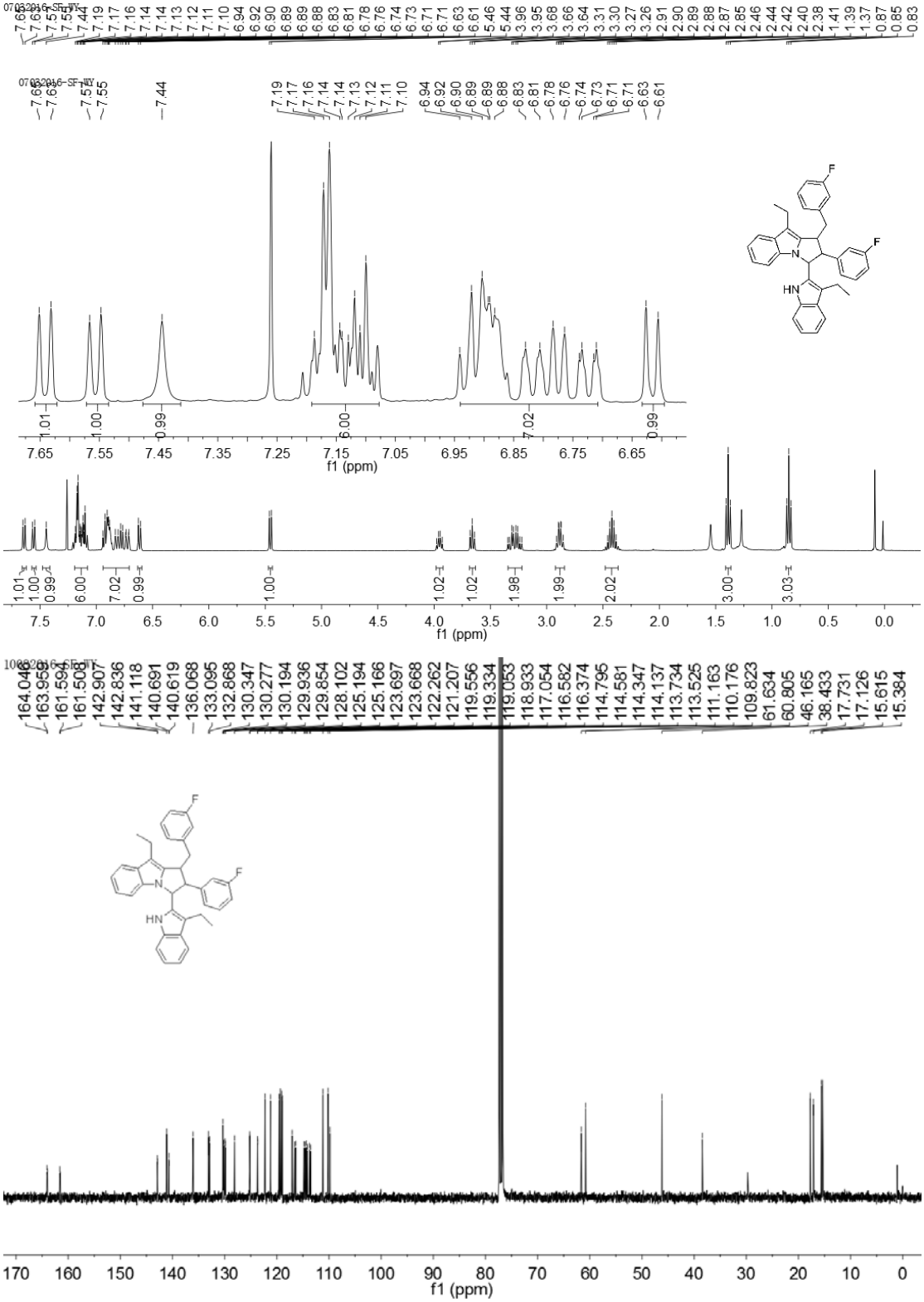
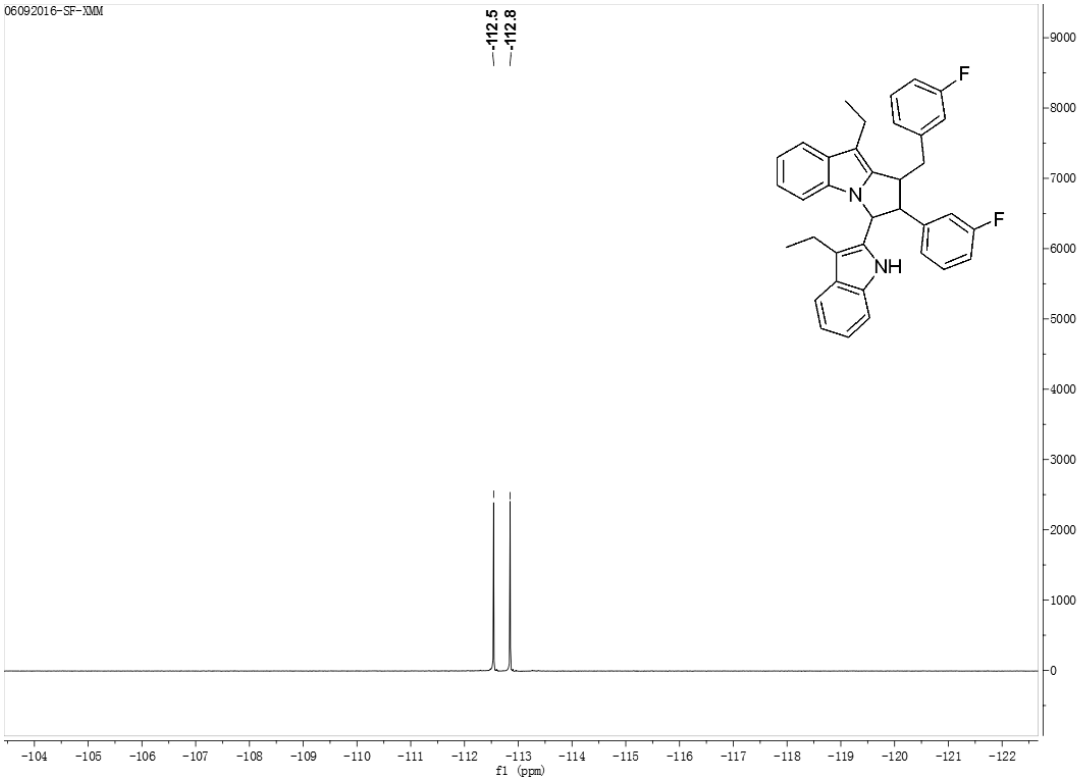
2500
2000
1500
1000
500
0
-103 -104 -105 -106 -107 -108 -109 -110 -111 -112 -113 -114 -115 -116 -117 -118 -119 -120 -121 -122 -123 -124 -125 -126
f1 (ppm)

2m





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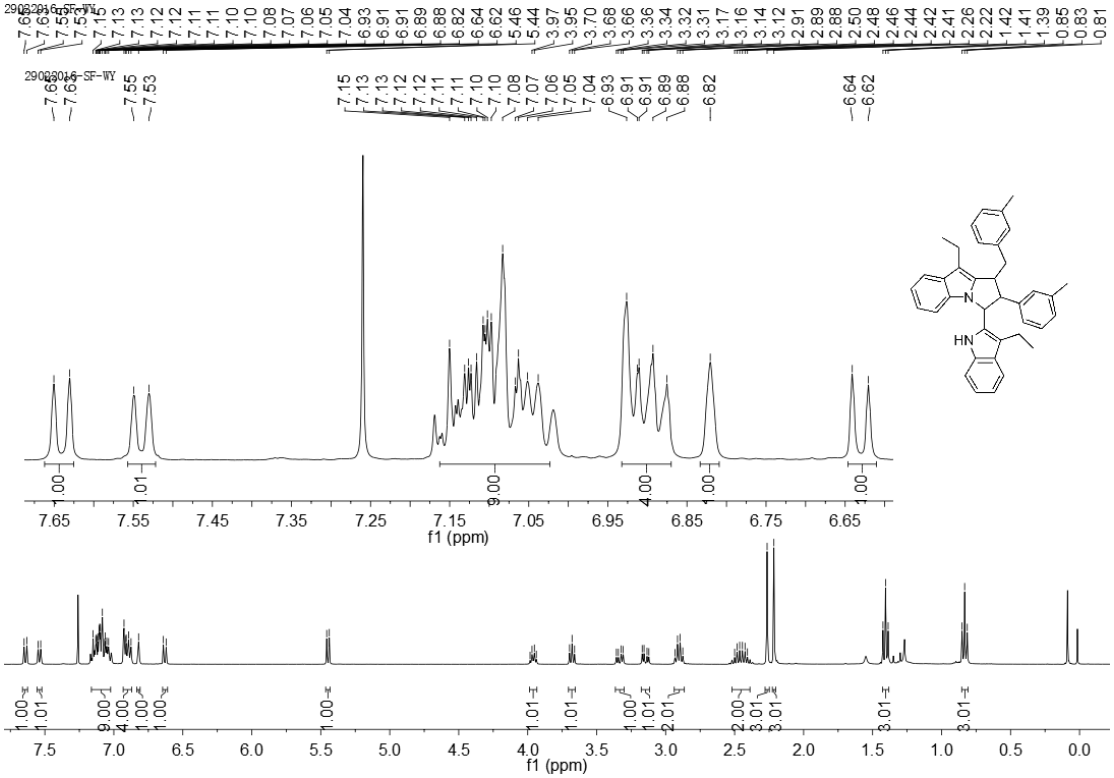

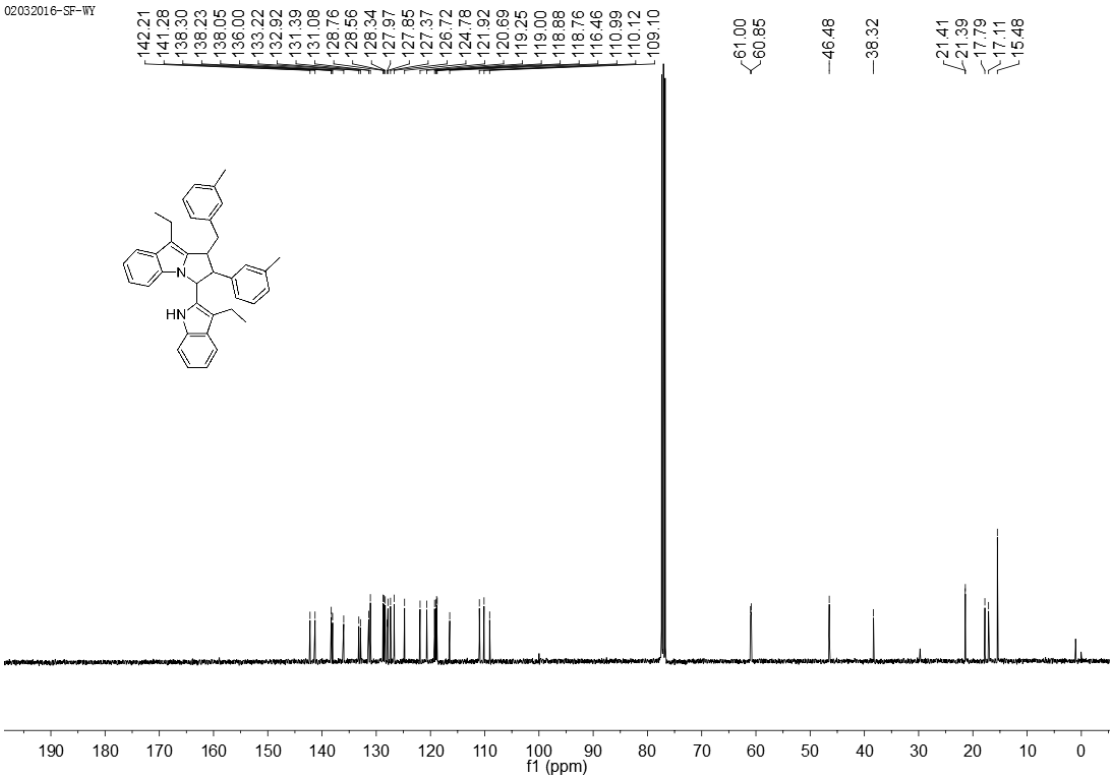
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132.92
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131.08
128.76
128.56
128.34
127.97
127.85
127.37
126.72
124.78
121.92
120.69
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118.88
118.76
116.46
110.99
110.12
109.10
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17.11
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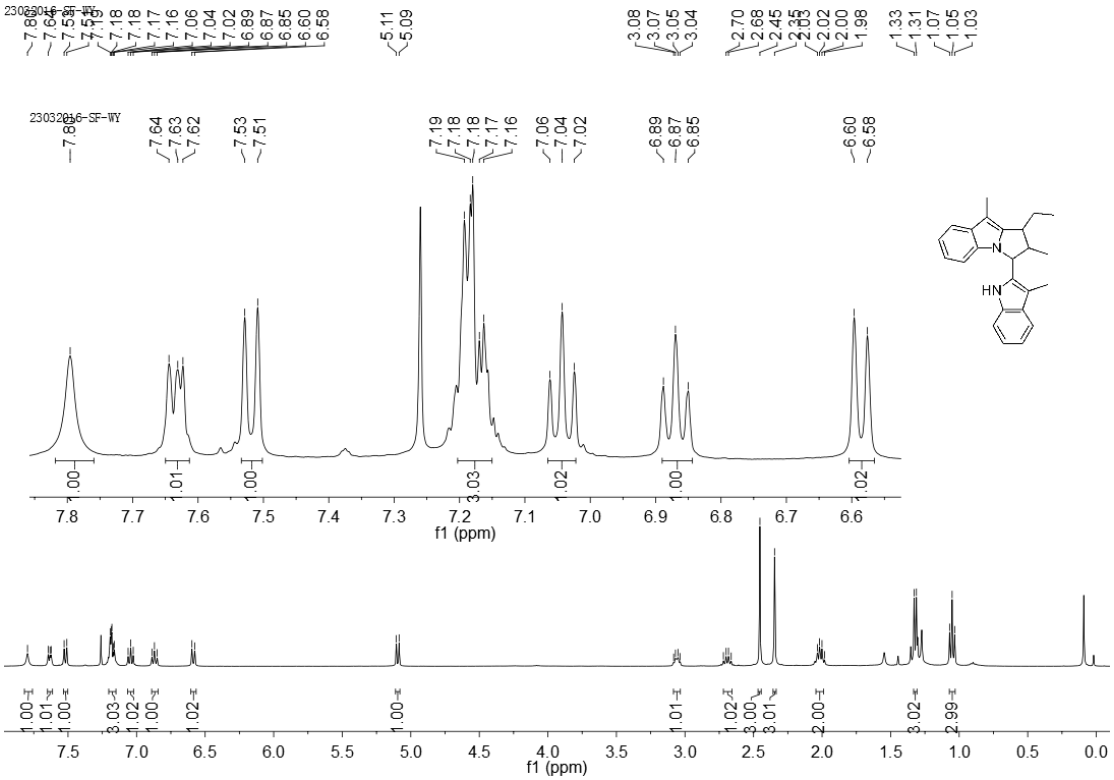
HN
f1 (ppm)

2o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7.18
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7.04
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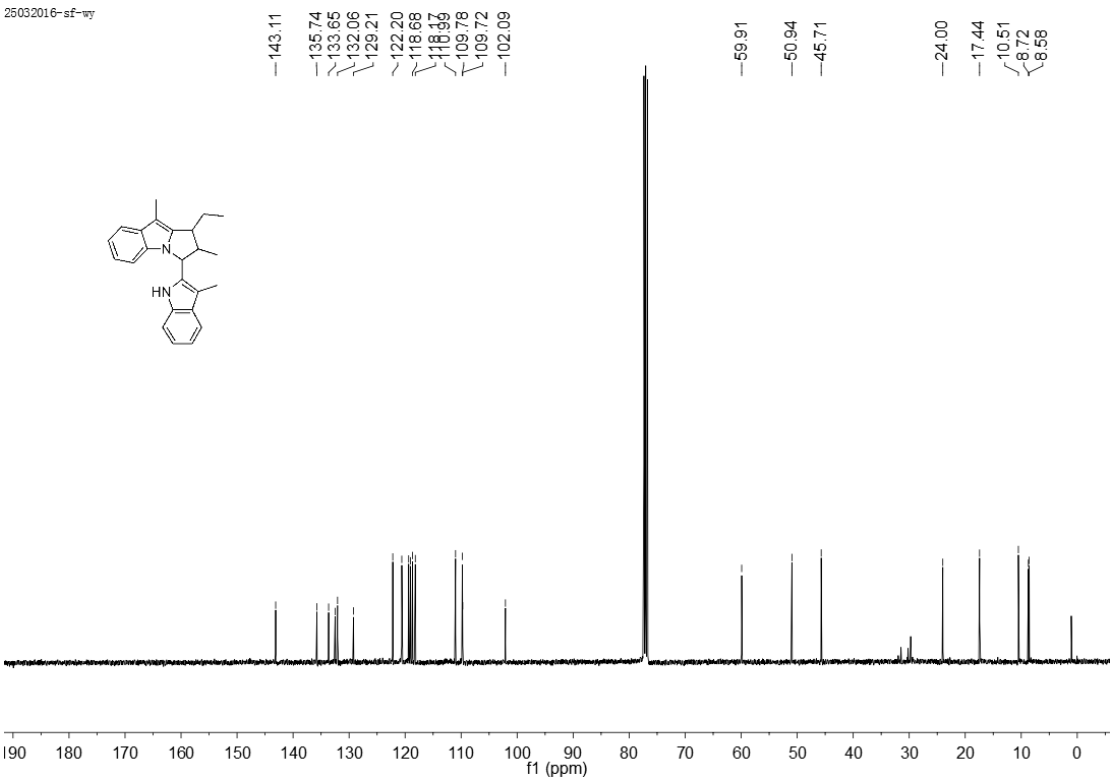
6.85
6.60
6.58
HN
f1 (ppm)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109.72
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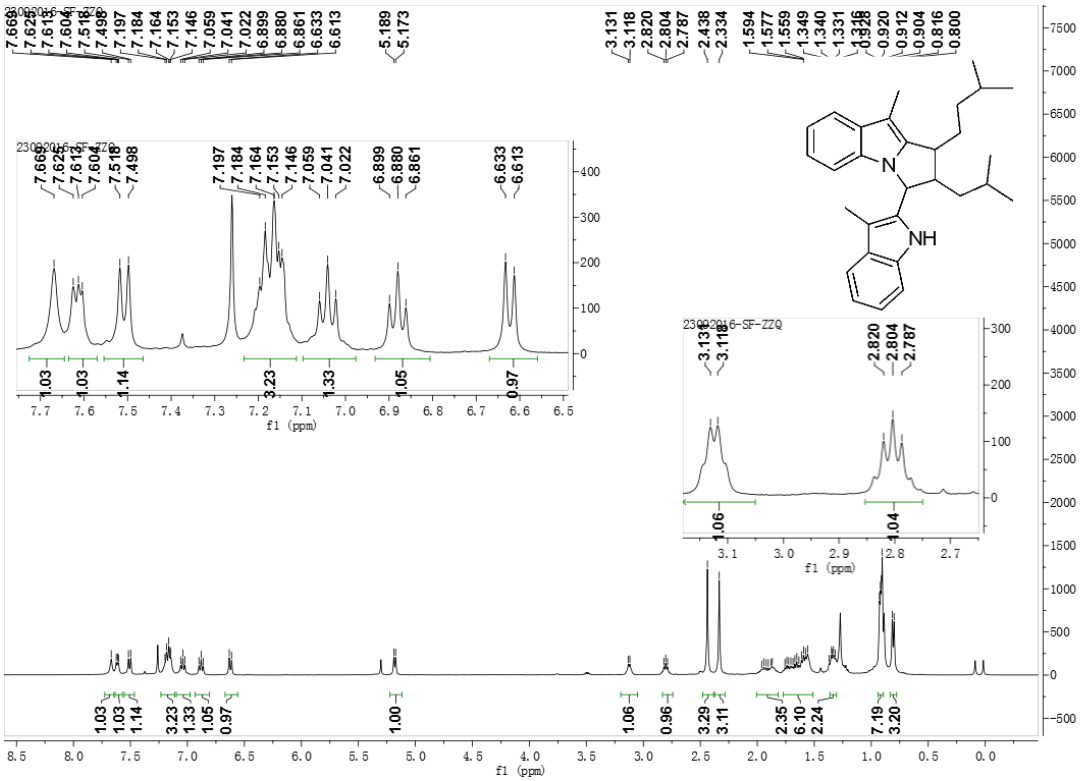
8.72
8.58
HN
f1 (ppm)

2q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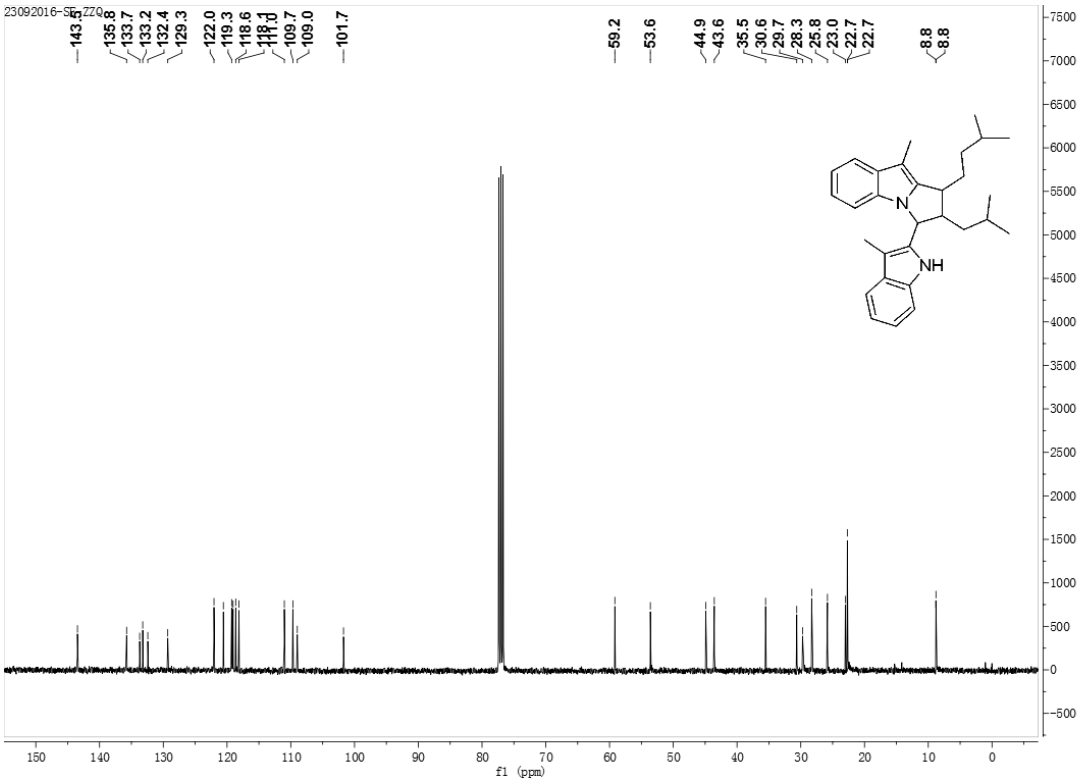
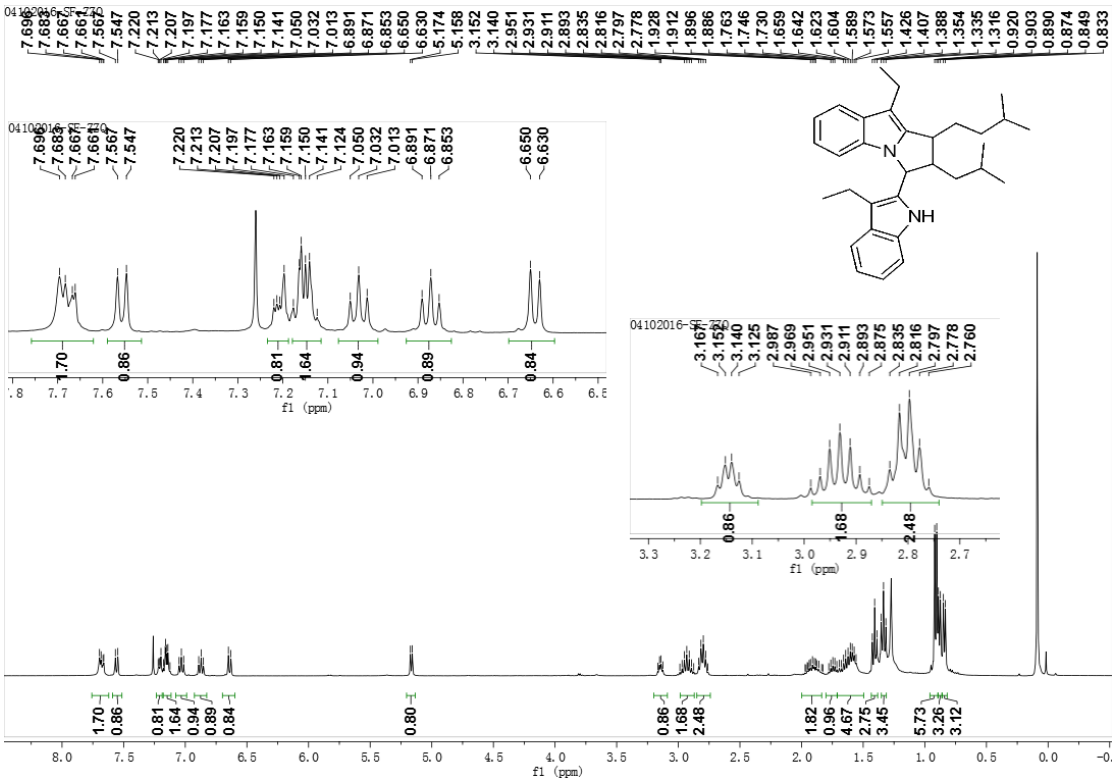
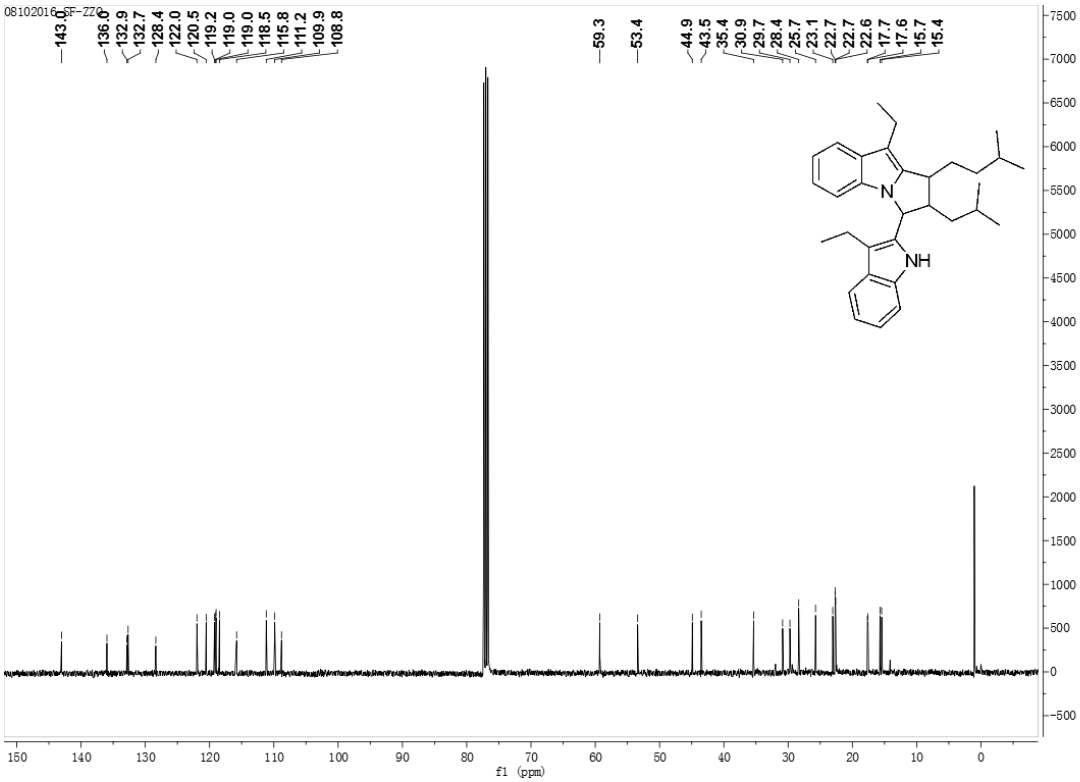
NH
f1 (ppm)



2r

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122.0
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119.0
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115.8
111.2
109.9
108.8
59.3
53.4
44.9
43.5
35.4
30.9
29.7
28.4
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22.7
22.6
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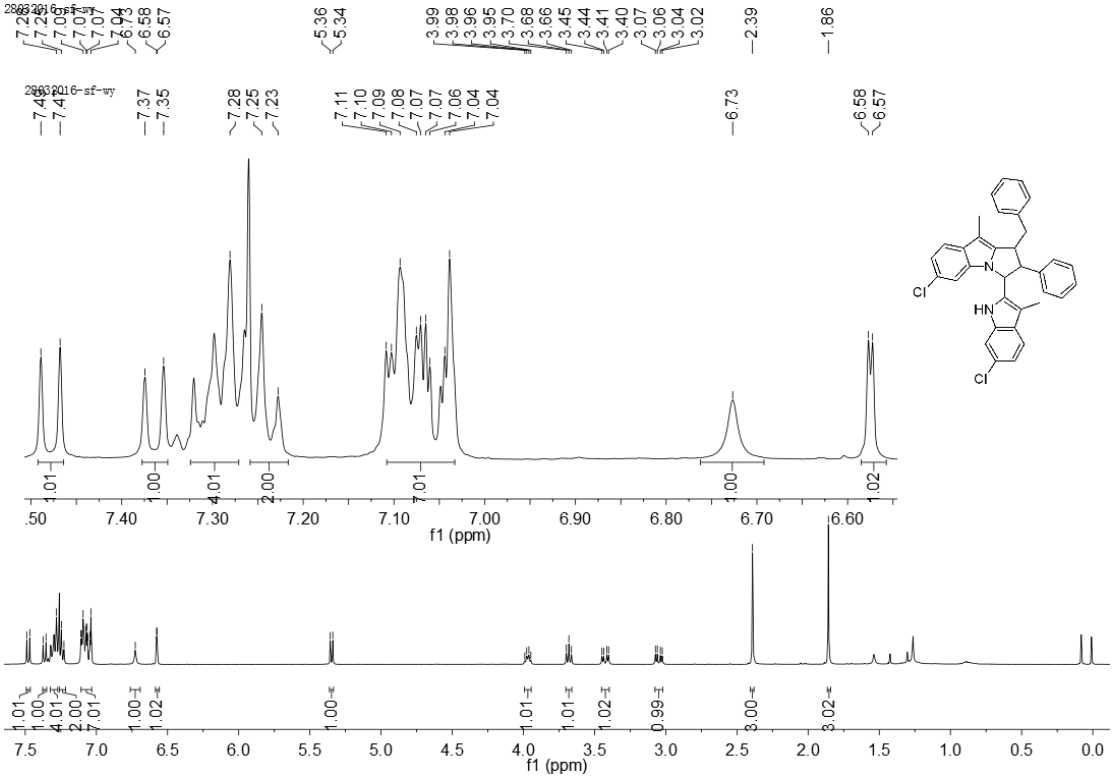
15.7
15.4
N
NH
f1 (ppm)

2s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7.01
7.01
7.01
6.94
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5.36
5.34
3.99
3.98
3.96
3.95
3.70
3.68
3.66
3.45
3.44
3.41
3.40
3.07
3.06
3.04
3.02
2.39
1.86
2803216-sf-wy
7.44
7.42
7.37
7.35
7.28
7.25
7.23
7.11
7.10
7.09
7.08
7.07
7.07
7.06
7.04
7.04
6.73
6.58
6.57
Cl
HN
Cl
1.01
1.00
4.01
2.00
7.01
1.00
1.02
f1 (ppm)
1.01
1.00
4.01
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1.02
1.00
1.01
1.01
1.02
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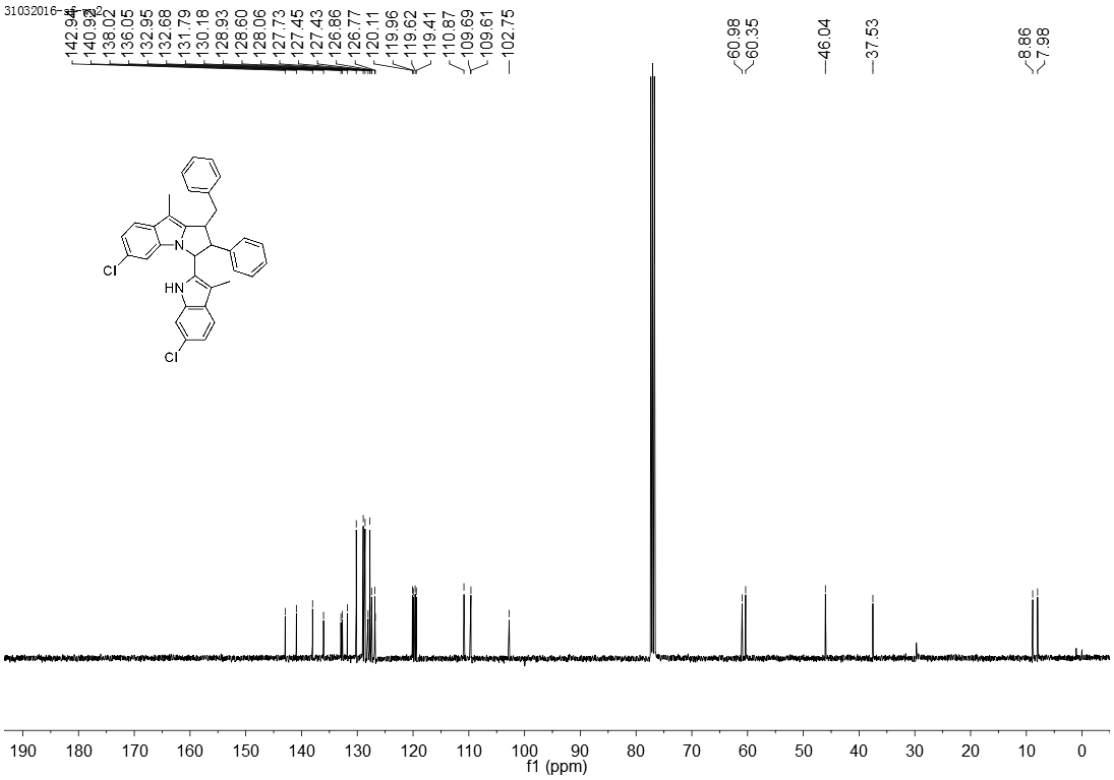
3.02
f1 (ppm)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127.43
126.86
126.77
120.11
119.96
119.62
119.41
110.87
109.69
109.61
102.75
60.98
60.35
46.04
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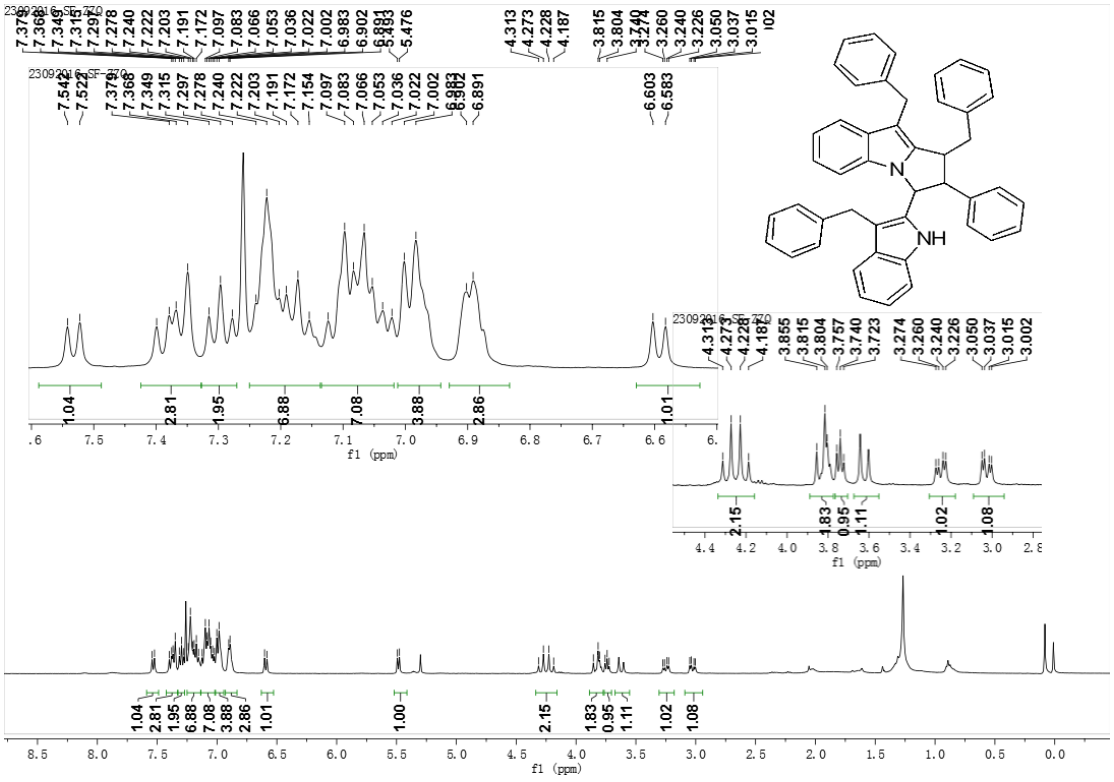
8.86
7.98
Cl
HN
Cl
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

***ent*-2t**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7.036
7.022
7.002
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6.891
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6.583
4.313
4.273
4.228
4.187
3.855
3.815
3.804
3.757
3.740
3.723
3.274
3.260
3.240
3.226
3.050
3.037
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3.002
N
NH
1.04
2.81
1.95
6.88
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1.02
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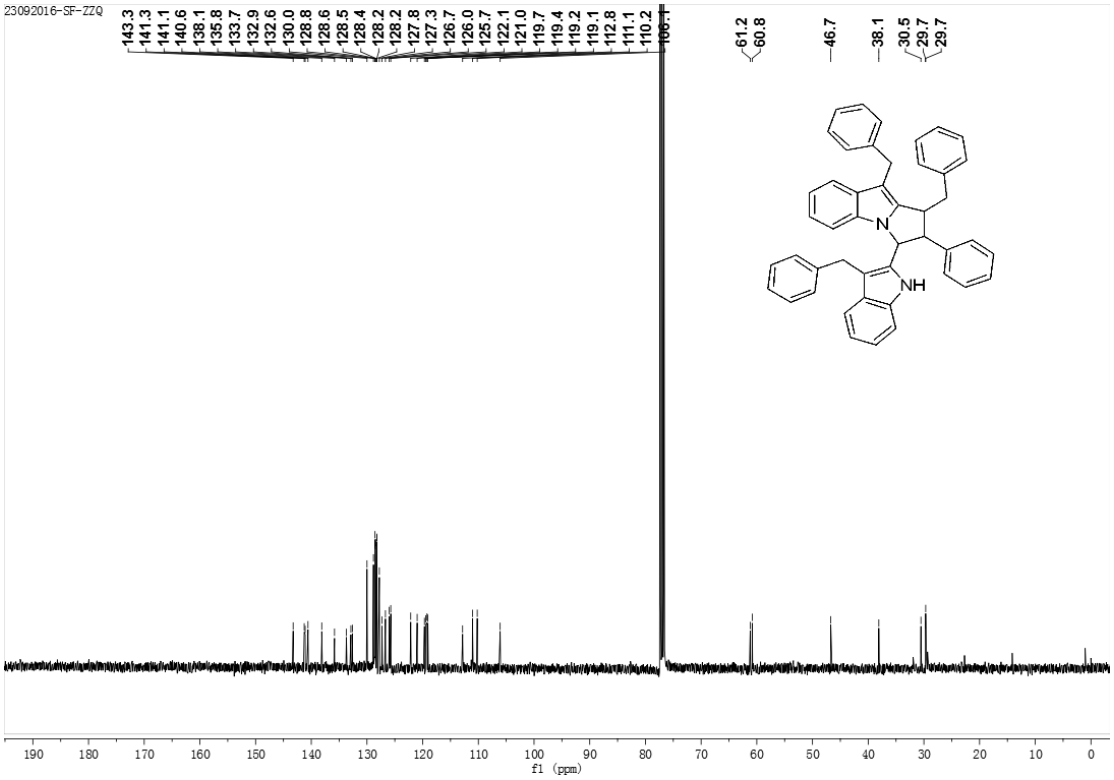
f1 (ppm)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132.6
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128.6
128.5
128.4
128.2
128.2
127.8
127.3
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126.0
125.7
122.1
121.0
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119.4
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46.7
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29.7
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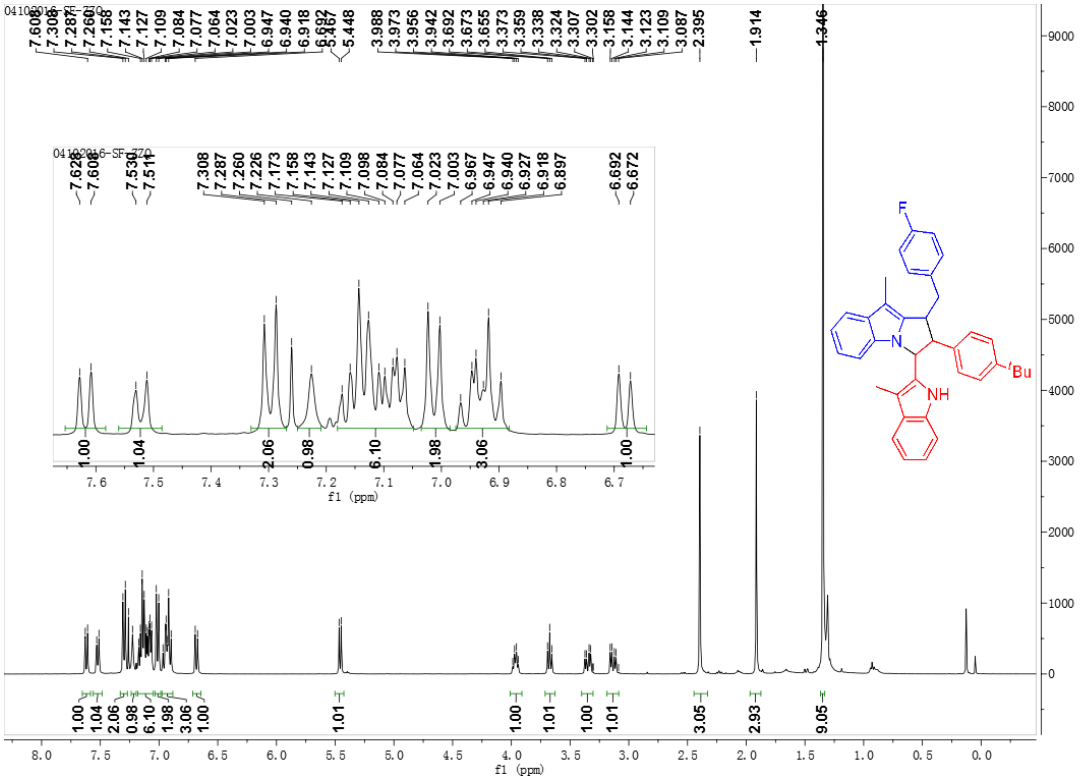
NH
f1 (ppm)

2be: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7.077
7.064
7.023
7.003
6.947
6.940
6.918
5.448
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3.973
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3.942
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3.673
3.655
3.373
3.359
3.338
3.324
3.307
3.302
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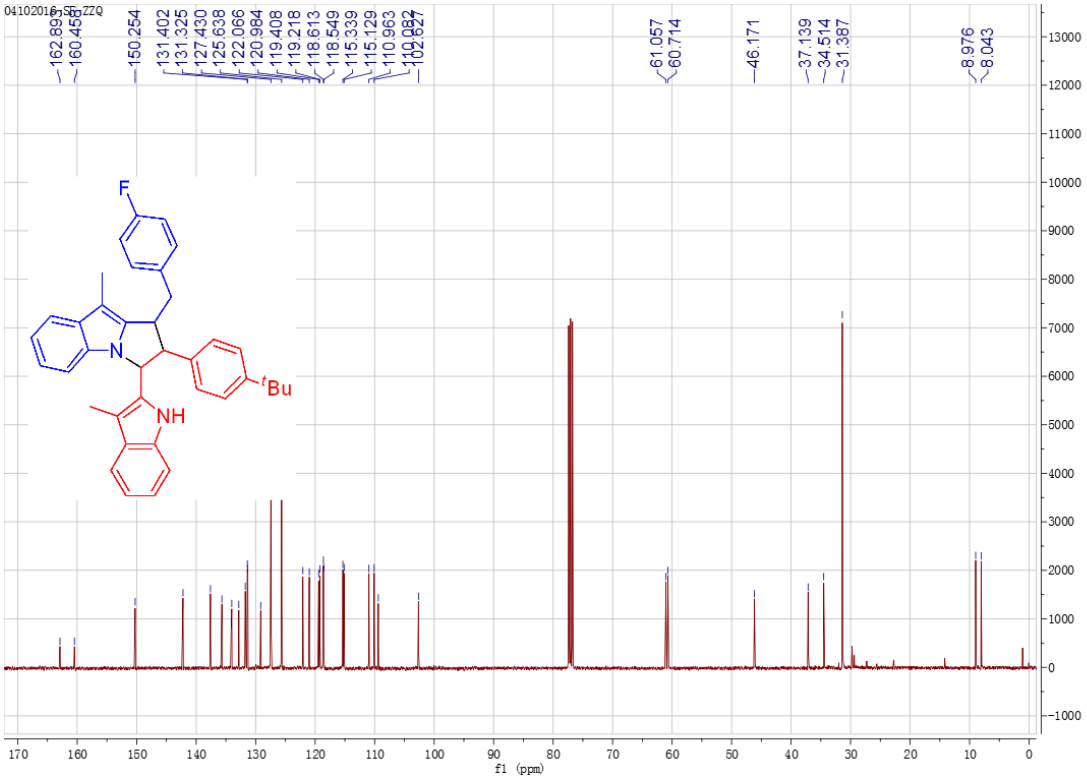
3.144
3.123
3.109
3.087
2.395
1.914
1.346
F
N
NH
tBu
f1 (ppm)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115.129
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102.627
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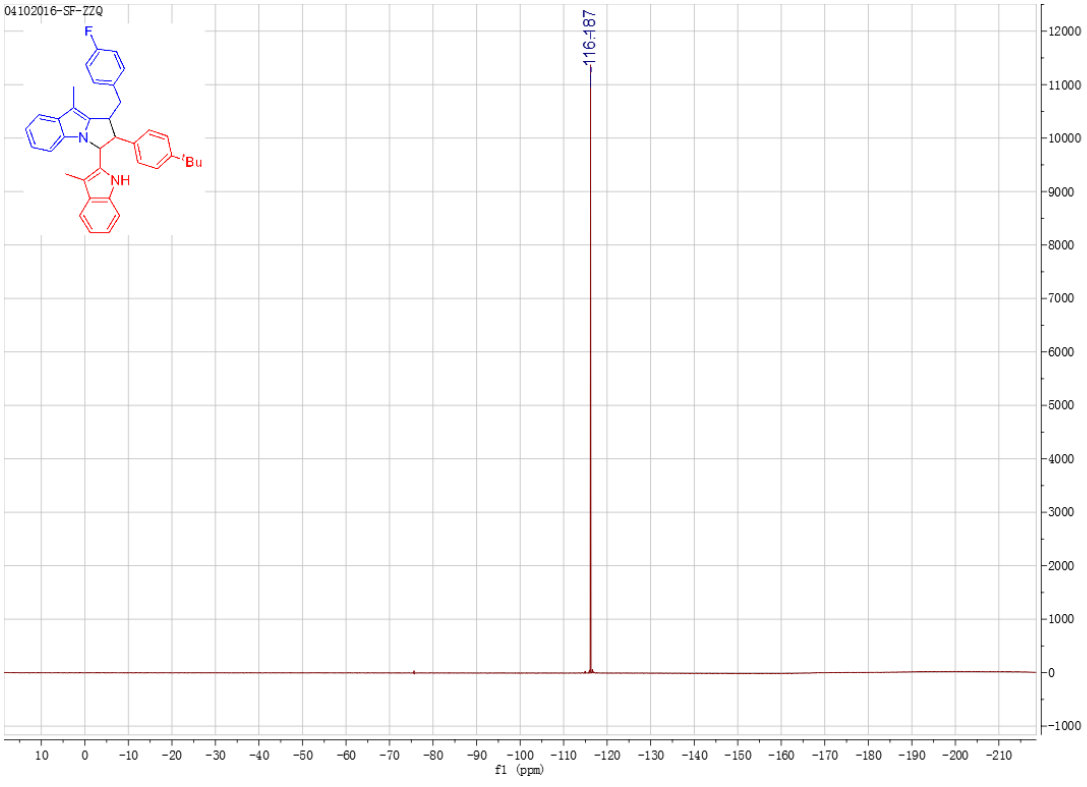
8.043
F
N
NH
tBu
f1 (ppm)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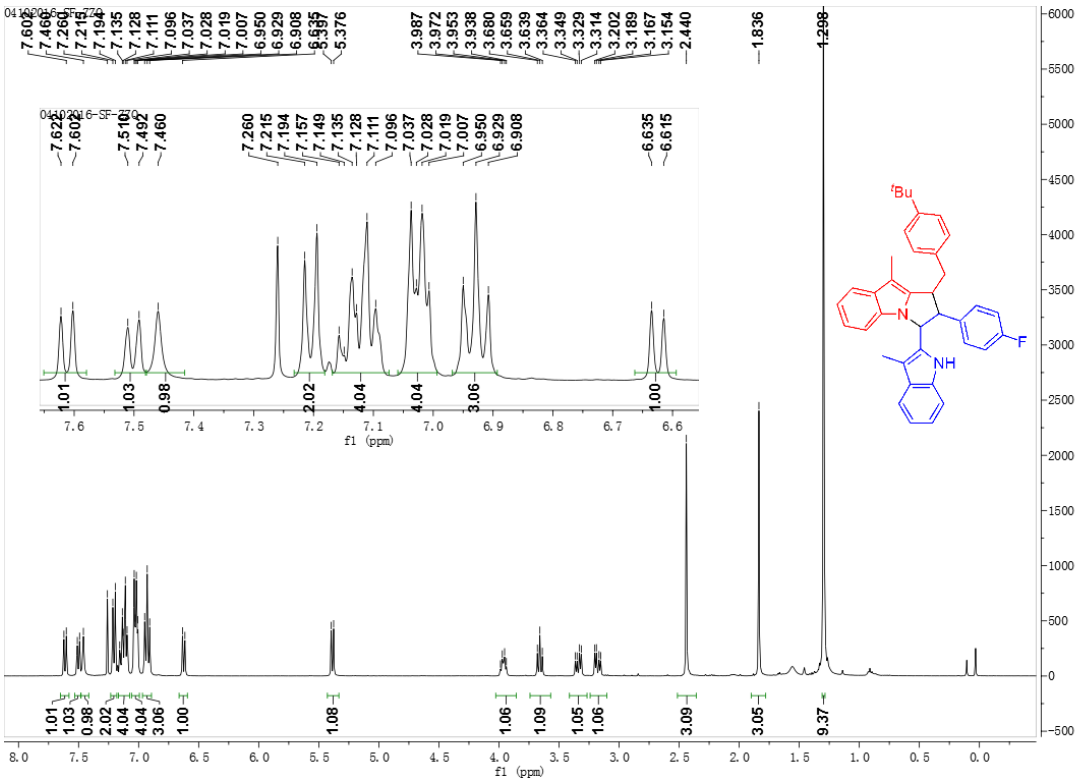
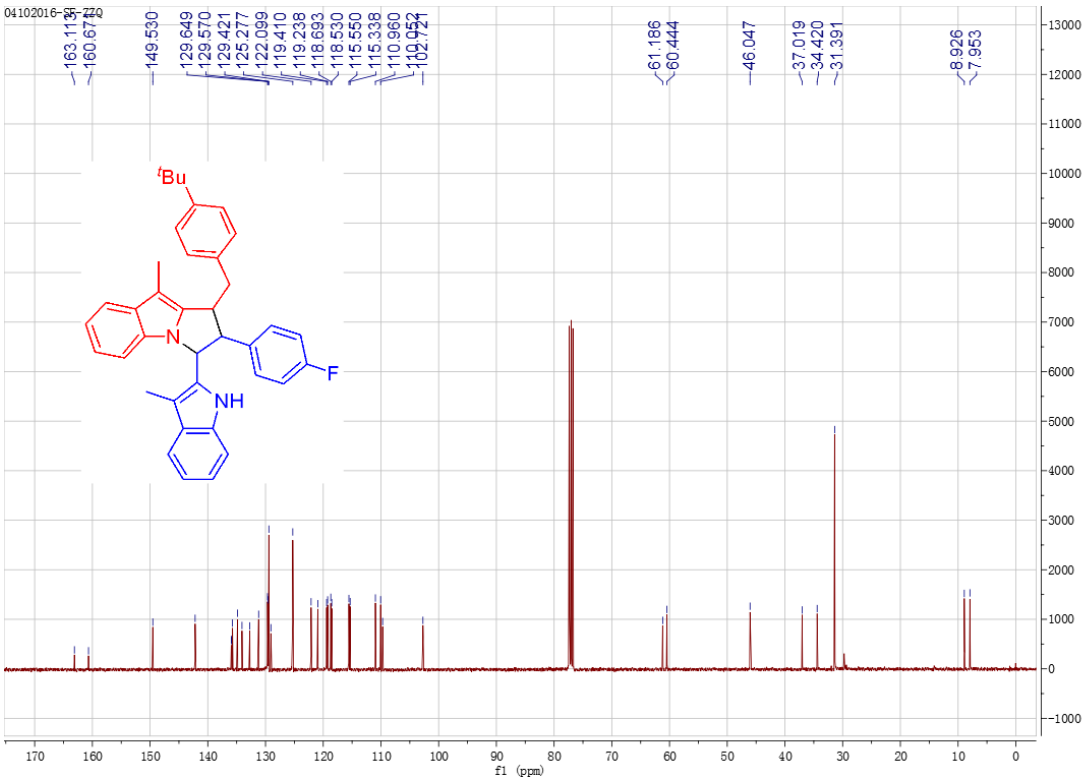
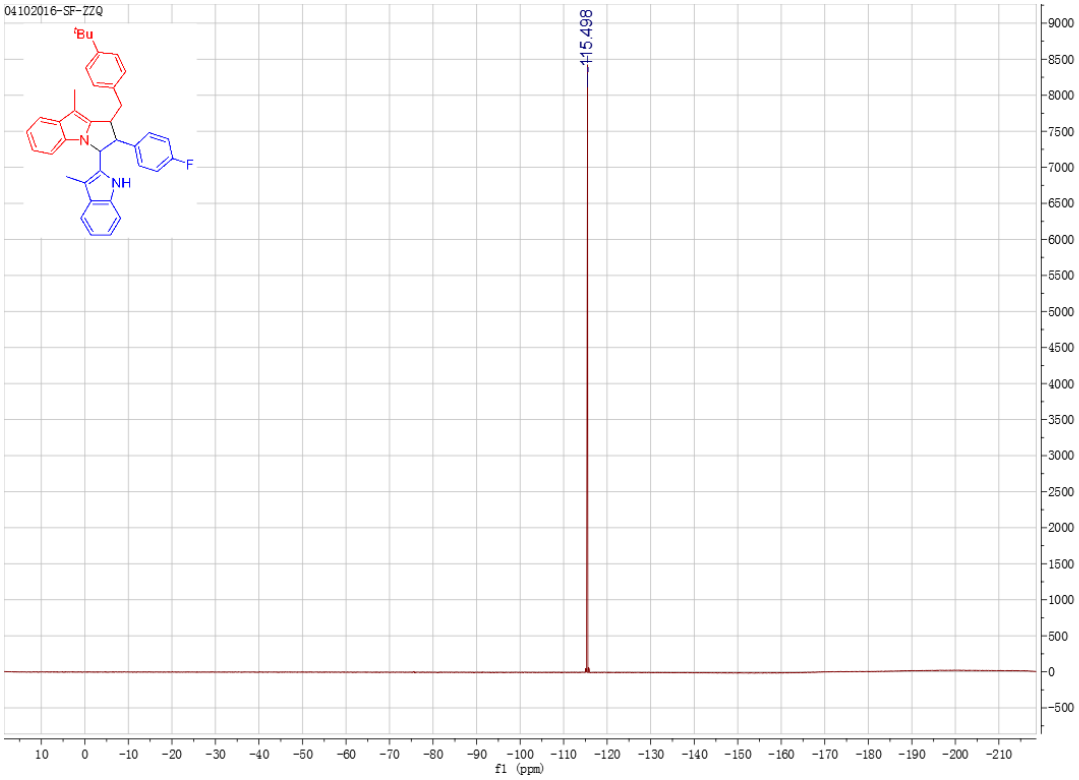
N
NH
tBu
f1 (ppm)

2be':



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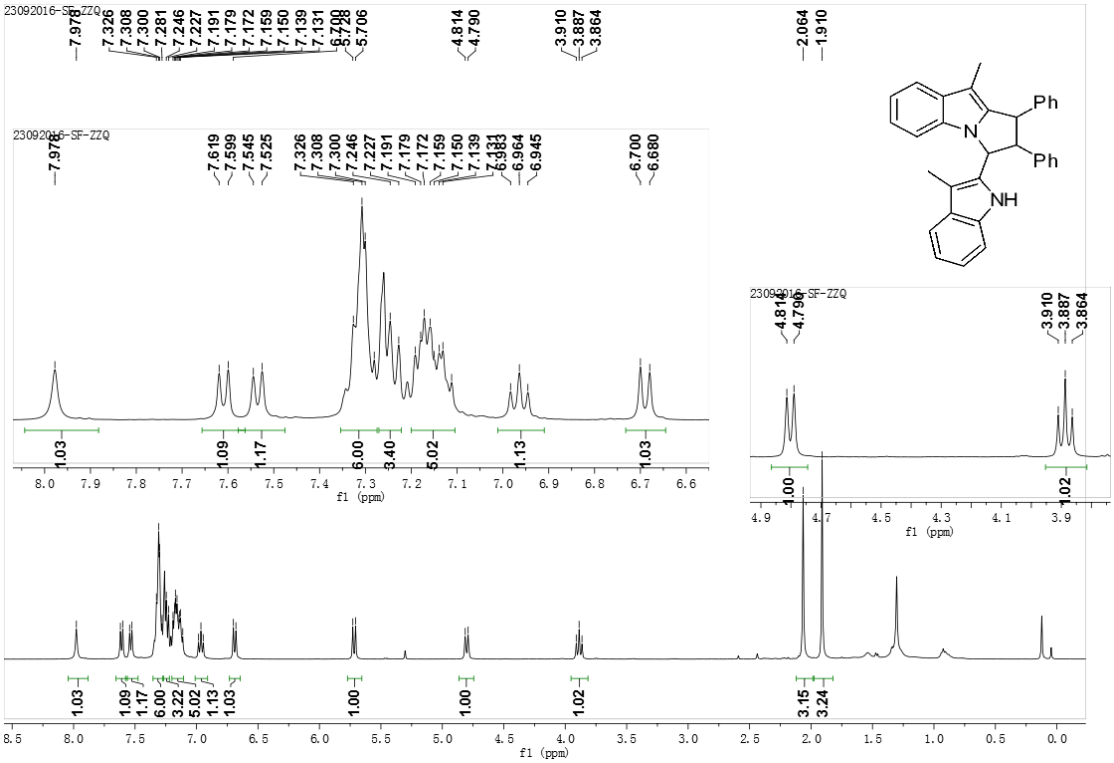
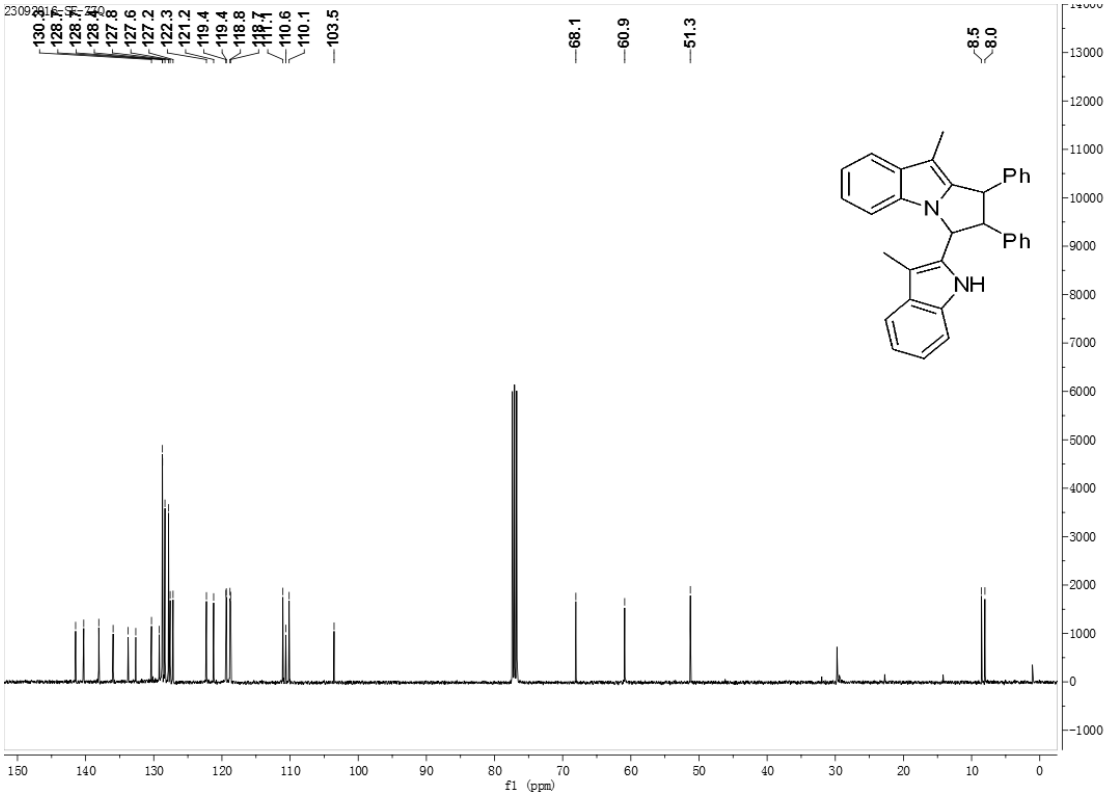
tBu
F
NH
-115.498
f1 (ppm)

Compound 6


23092016-SF-ZZQ
Ph
Ph
NH
f1 (ppm)


130.3
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121.2
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119.4
118.8
111.1
110.6
110.1
103.5
68.1
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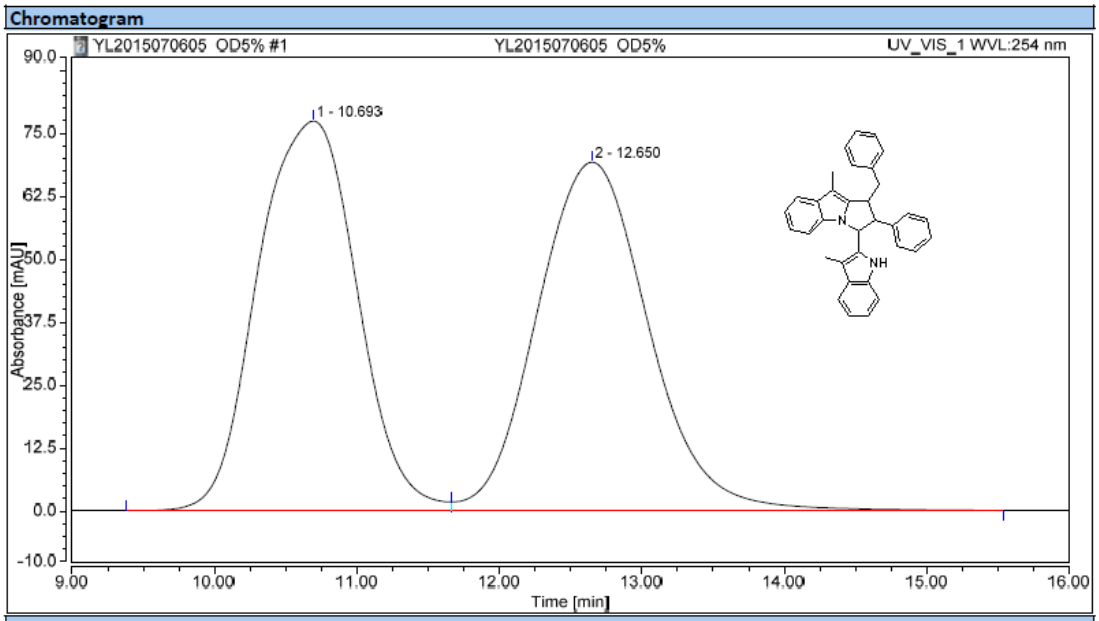
51.3
8.5
8.0
Ph
Ph
N
NH
f1 (ppm)

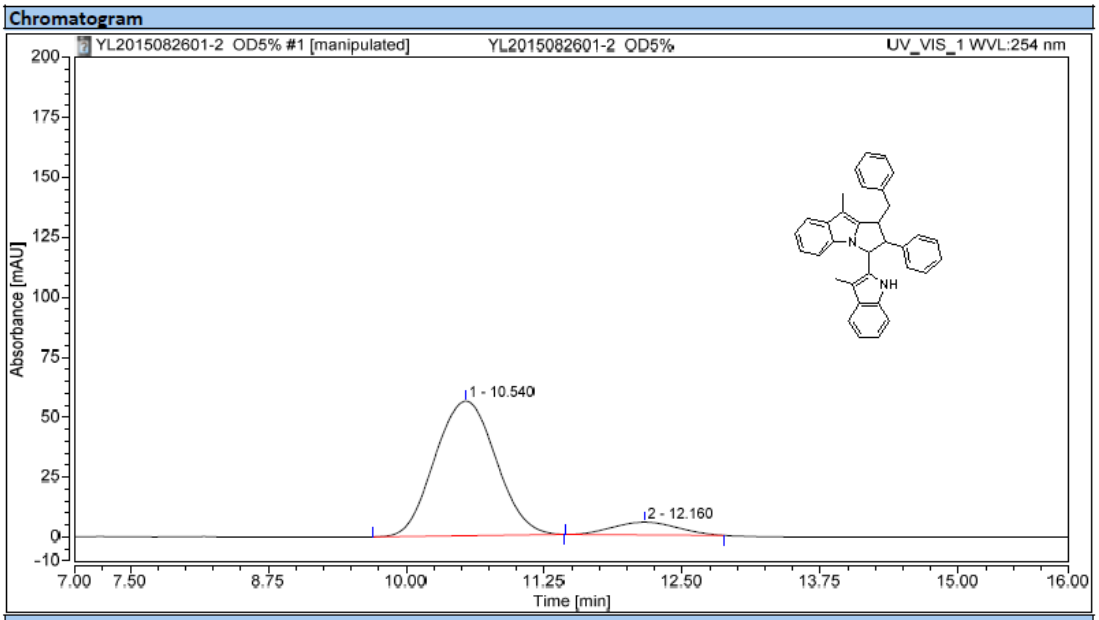
2. HPLC spectra of all products 2

2a



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.693	62.334	77.244	49.93	52.79	n.a.
2		12.650	62.516	69.071	50.07	47.21	n.a.
Total:			**124.851**	**146.316**	**100.00**	**100.00**	

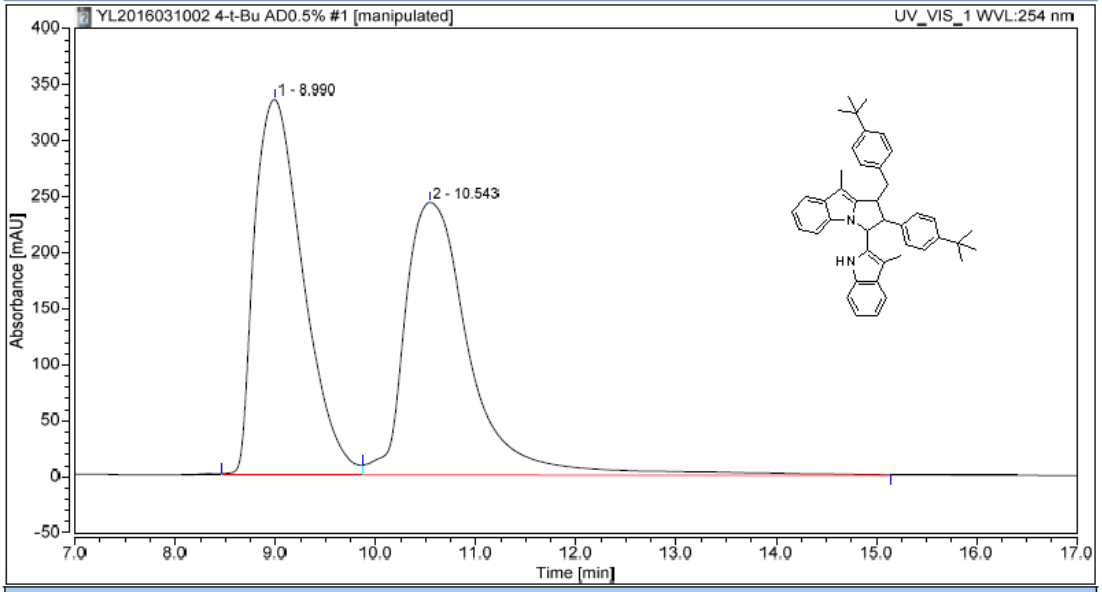


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10.540	36.017	56.126	90.84	91.35	n.a.
2		12.160	3.633	5.317	9.16	8.65	n.a.
Total:			**39.650**	**61.443**	**100.00**	**100.00**	

2b

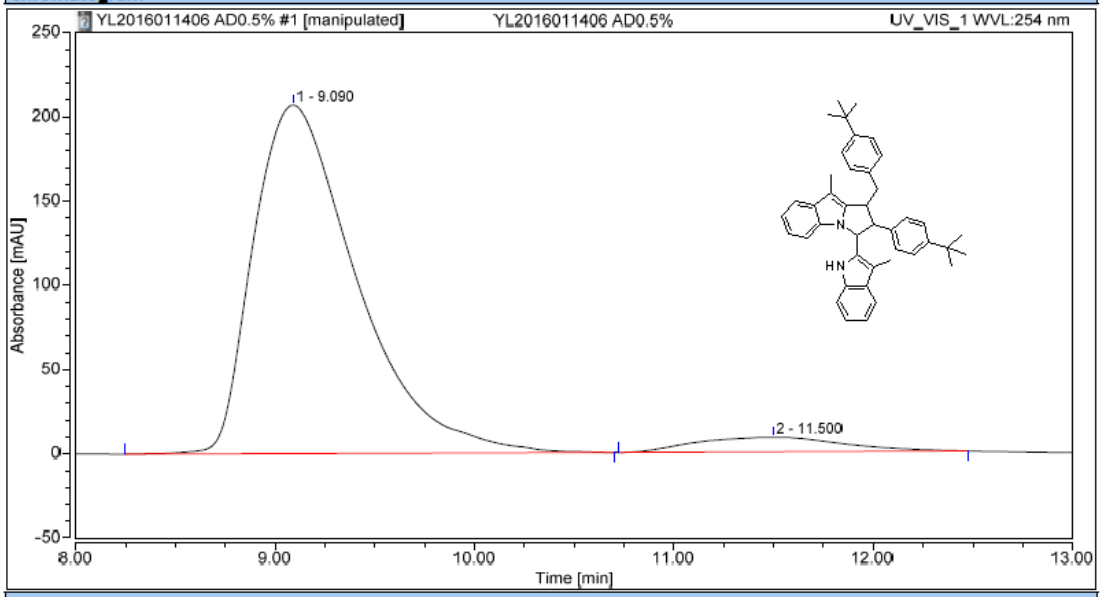
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.990	187.687	335.158	50.61	57.93	n.a.
2		10.543	183.195	243.362	49.39	42.07	n.a.
Total:			**370.882**	**578.520**	**100.00**	**100.00**	

Chromatogram

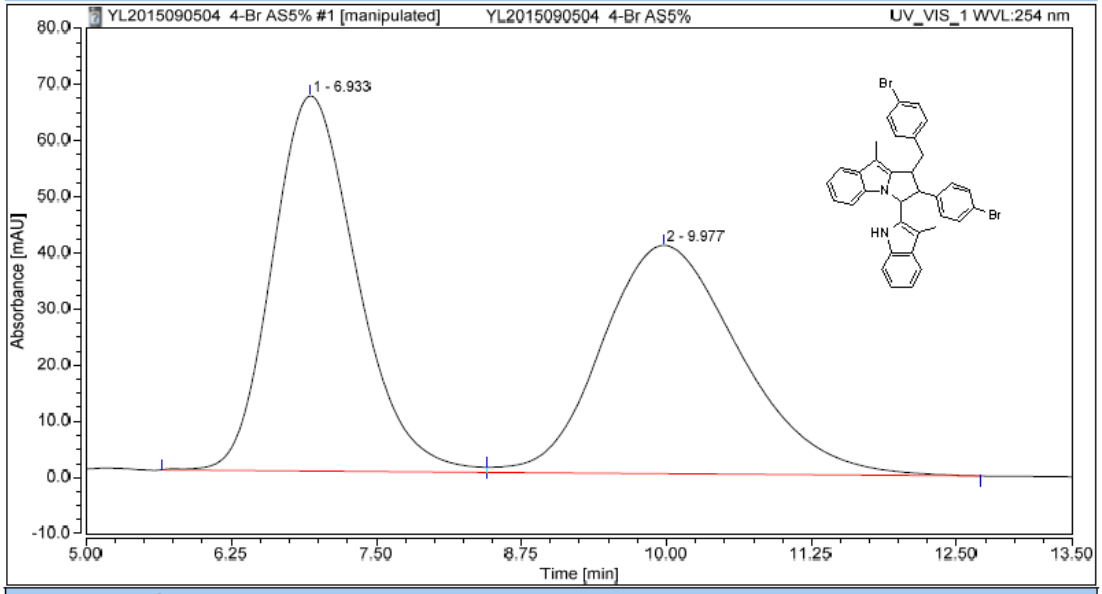


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.090	123.922	206.862	94.39	95.98	n.a.
2		11.500	7.365	8.656	5.61	4.02	n.a.
Total:			**131.287**	**215.518**	**100.00**	**100.00**	

2c

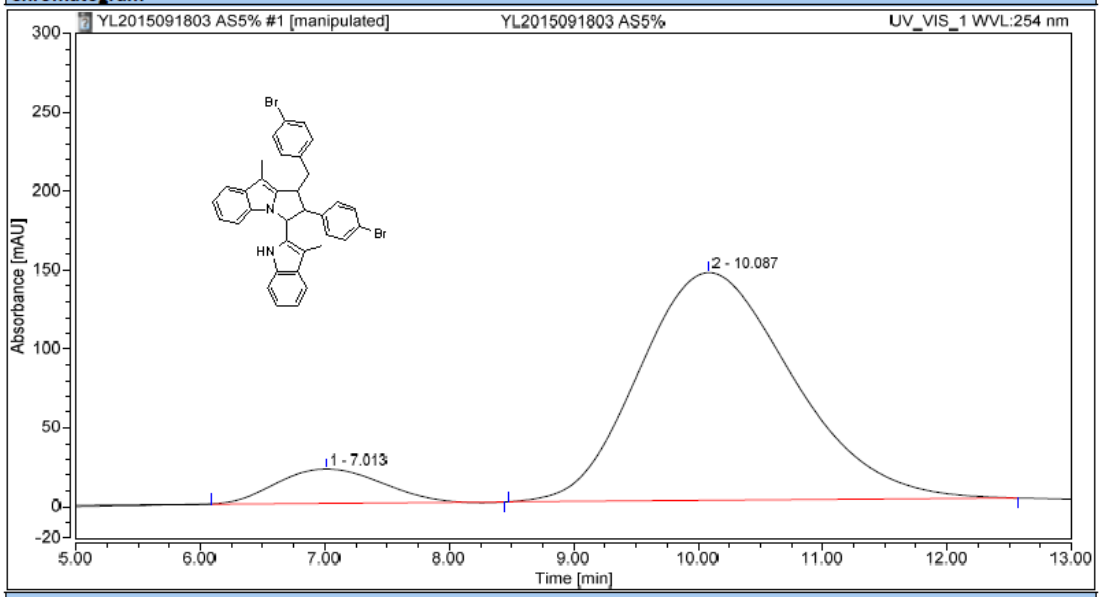
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.933	56.541	66.811	50.15	62.17	n.a.
2		9.977	56.207	40.649	49.85	37.83	n.a.
Total:			**112.748**	**107.461**	**100.00**	**100.00**	

Chromatogram

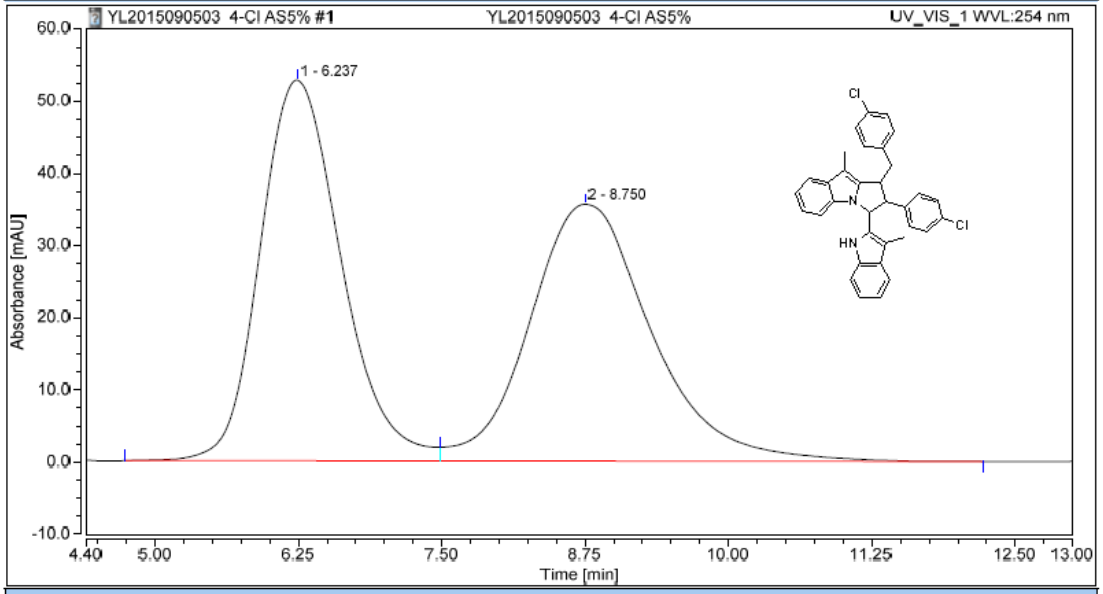


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.013	21.318	21.740	9.37	13.08	n.a.
2		10.087	206.285	144.414	90.63	86.92	n.a.
Total:			**227.603**	**166.154**	**100.00**	**100.00**	

2d

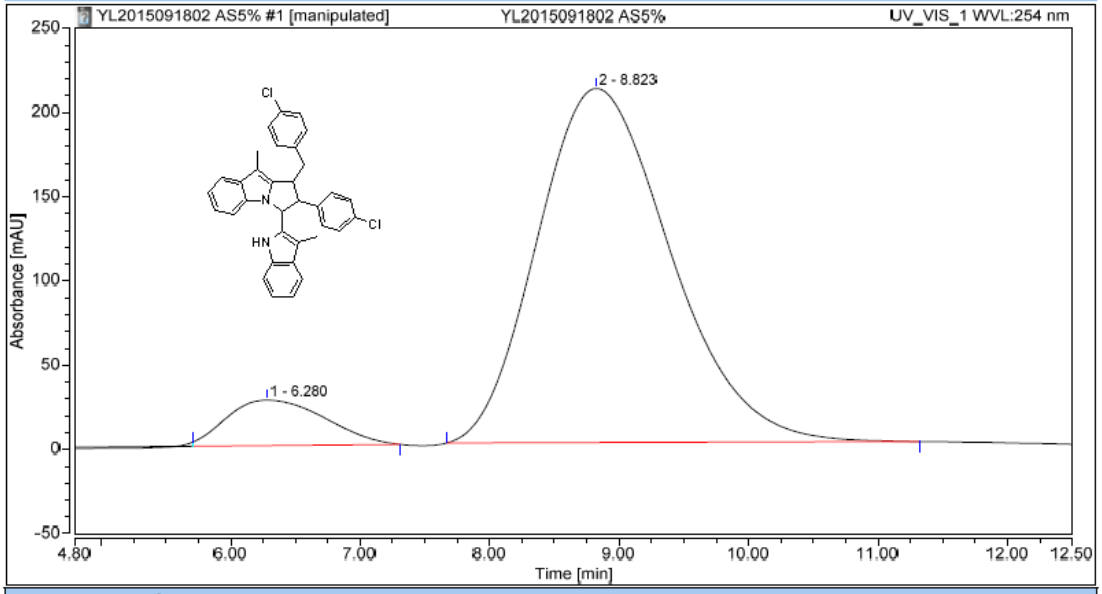
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.237	43.109	52.731	49.66	59.71	n.a.
2		8.750	43.703	35.580	50.34	40.29	n.a.
Total:			**86.811**	**88.311**	**100.00**	**100.00**	

Chromatogram

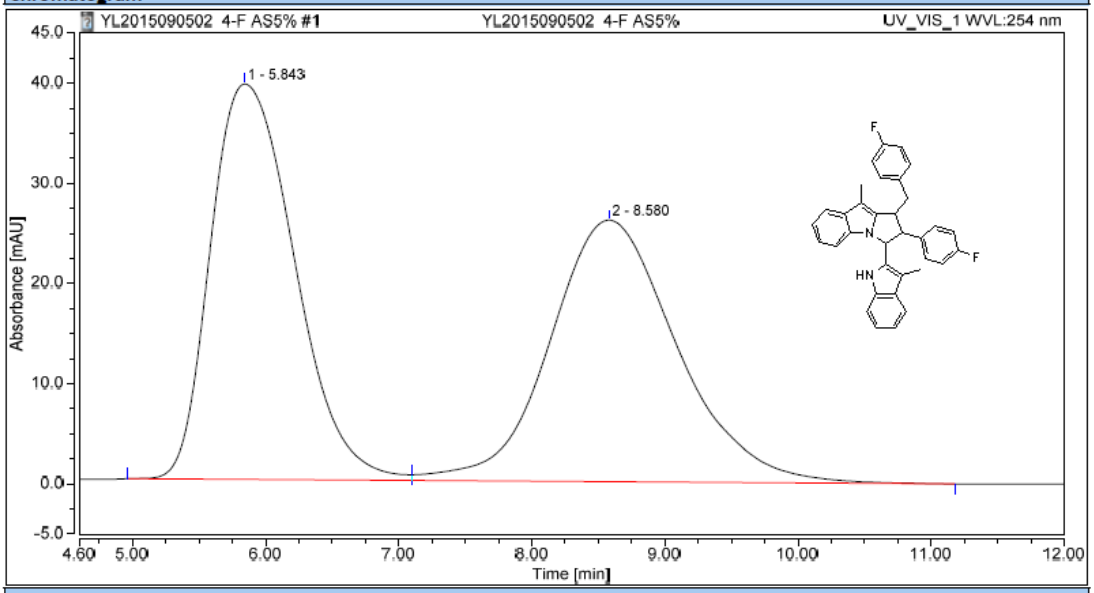


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.280	23.642	26.966	8.64	11.37	n.a.
2		8.823	250.077	210.219	91.36	88.63	n.a.
Total:			**273.719**	**237.185**	**100.00**	**100.00**	

2e

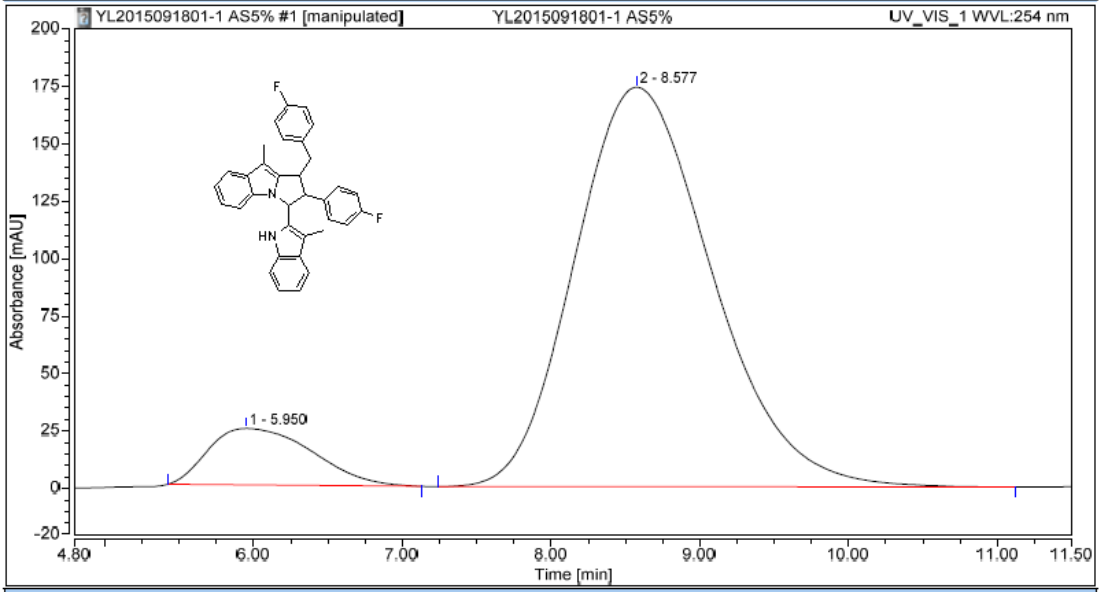
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.843	28.874	39.463	49.98	60.19	n.a.
2		8.580	28.898	26.102	50.02	39.81	n.a.
Total:			**57.772**	**65.565**	**100.00**	**100.00**	

Chromatogram

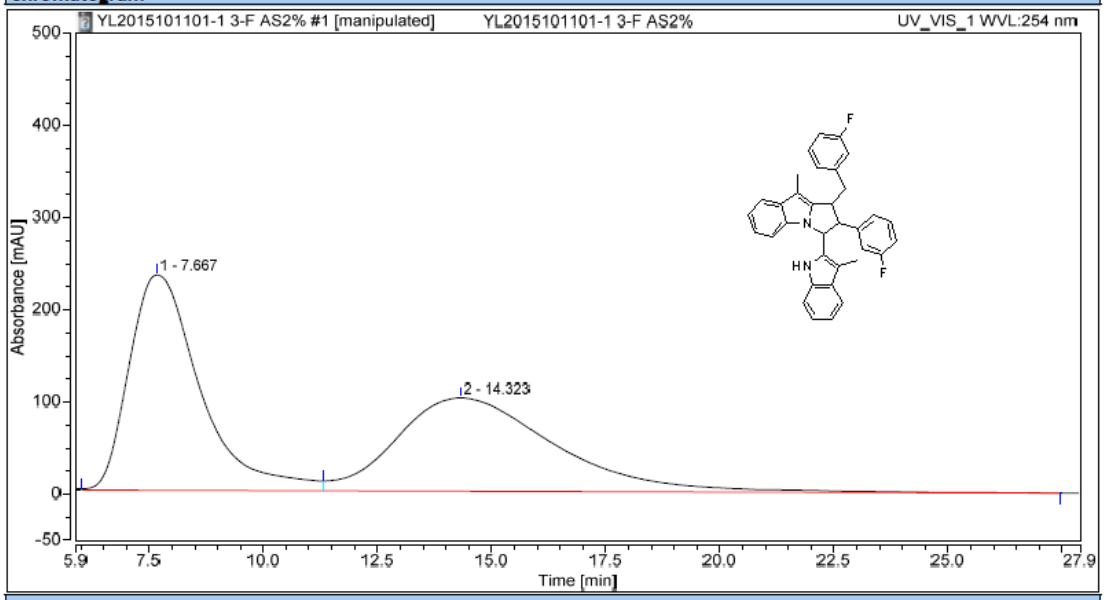


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.950	19.838	24.571	9.63	12.38	n.a.
2		8.577	186.169	173.946	90.37	87.62	n.a.
Total:			**206.007**	**198.517**	**100.00**	**100.00**	

2f

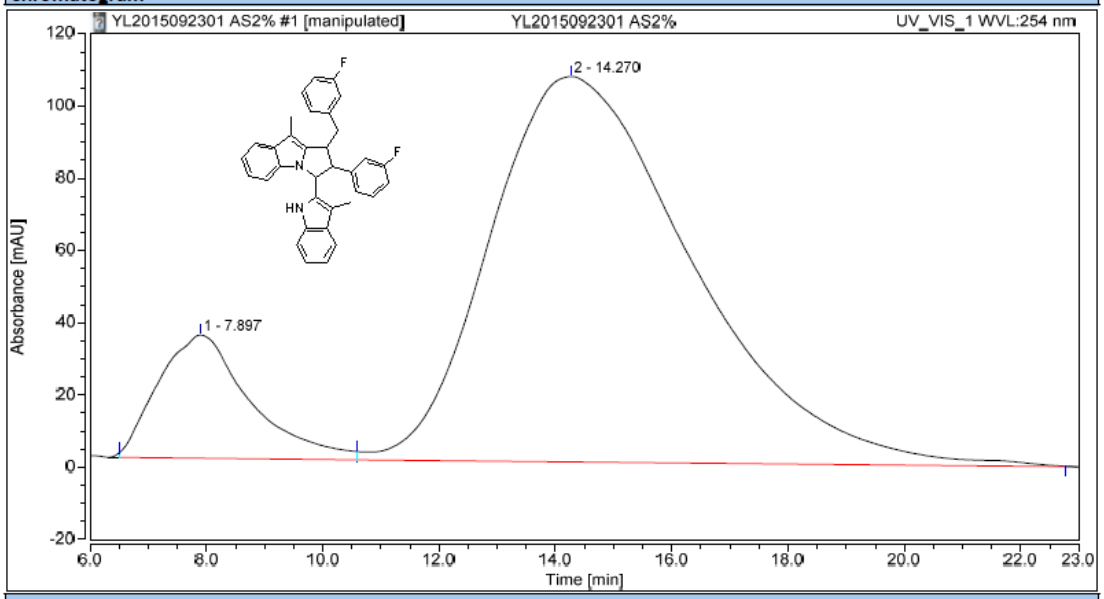
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.667	421.629	233.645	50.87	69.74	n.a.
2		14.323	407.286	101.400	49.13	30.26	n.a.
Total:			**828.915**	**335.046**	**100.00**	**100.00**	

Chromatogram

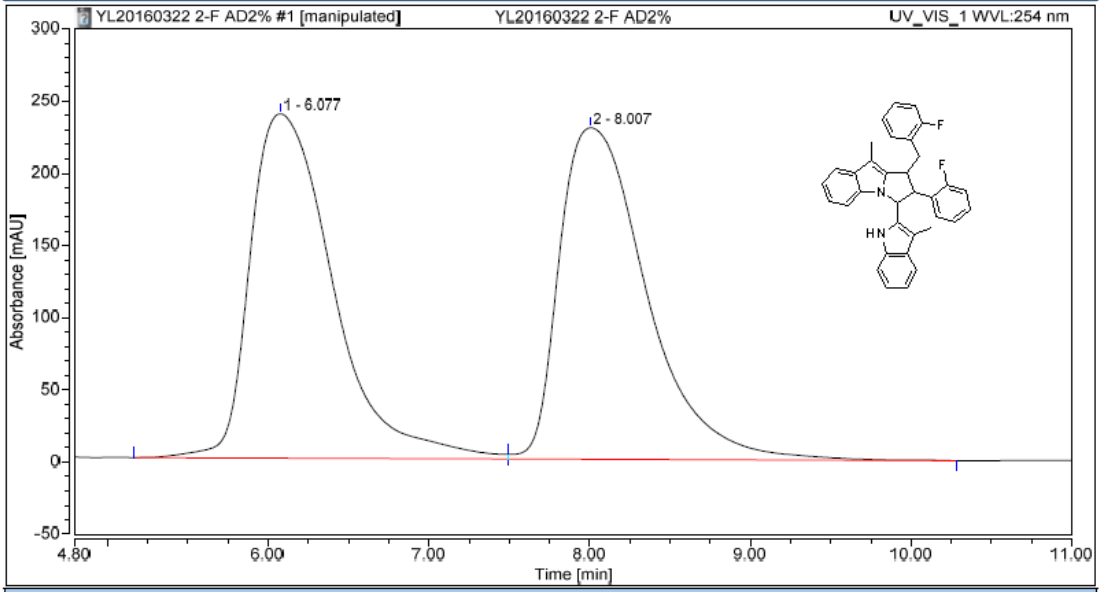


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.897	62.276	34.091	12.62	24.22	n.a.
2		14.270	431.170	106.652	87.38	75.78	n.a.
Total:			**493.446**	**140.743**	**100.00**	**100.00**	

***ent*-2g**

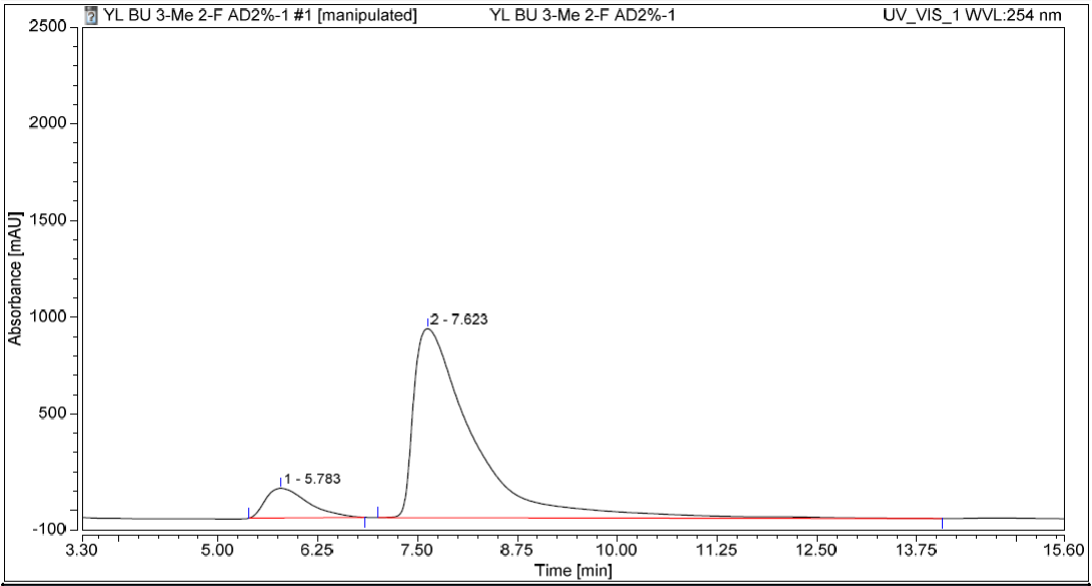
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6.077	142.658	238.628	49.62	50.95	n.a.
2		8.007	144.858	229.698	50.38	49.05	n.a.
Total:			**287.515**	**468.326**	**100.00**	**100.00**	

Chromatogram

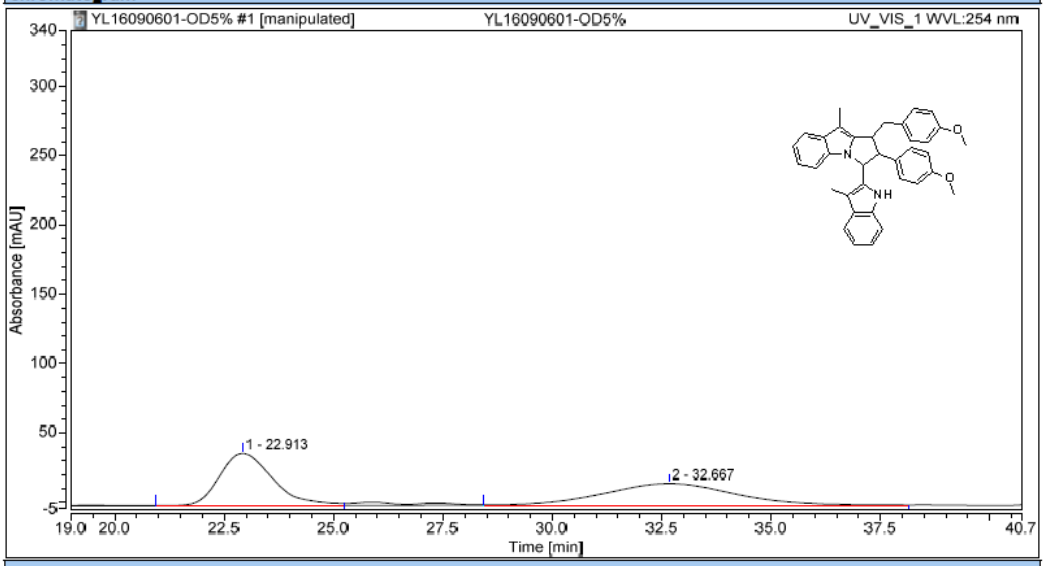


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.783	94.832	153.469	10.12	13.56	n.a.
2		7.623	842.045	978.325	89.88	86.44	n.a.
Total:			**936.877**	**1131.794**	**100.00**	**100.00**	

***ent*-2h**

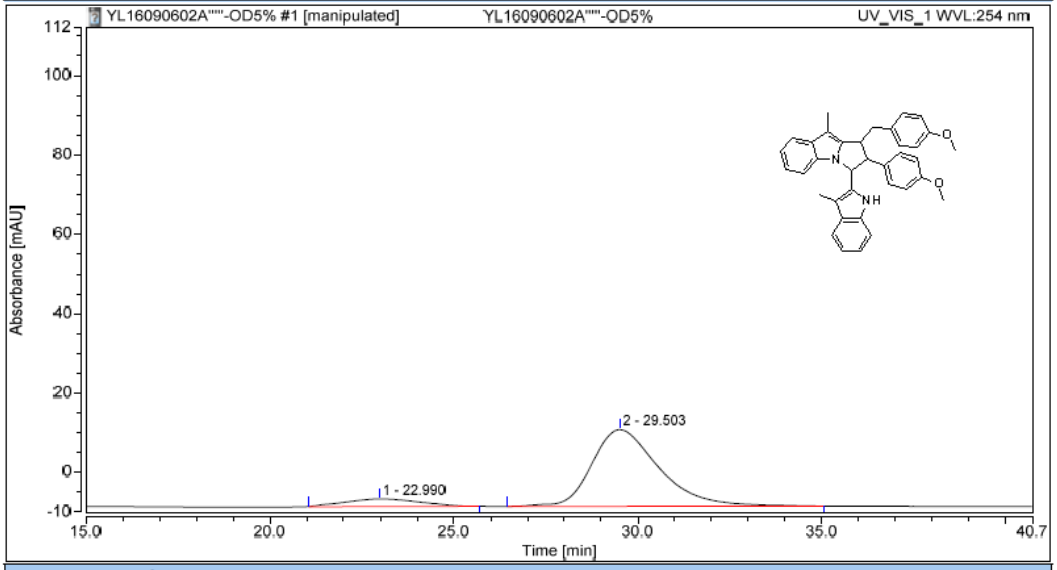
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		22.913	52.491	37.484	49.63	70.80	n.a.
2		32.667	53.268	15.461	50.37	29.20	n.a.
Total:			**105.759**	**52.945**	**100.00**	**100.00**	

Chromatogram

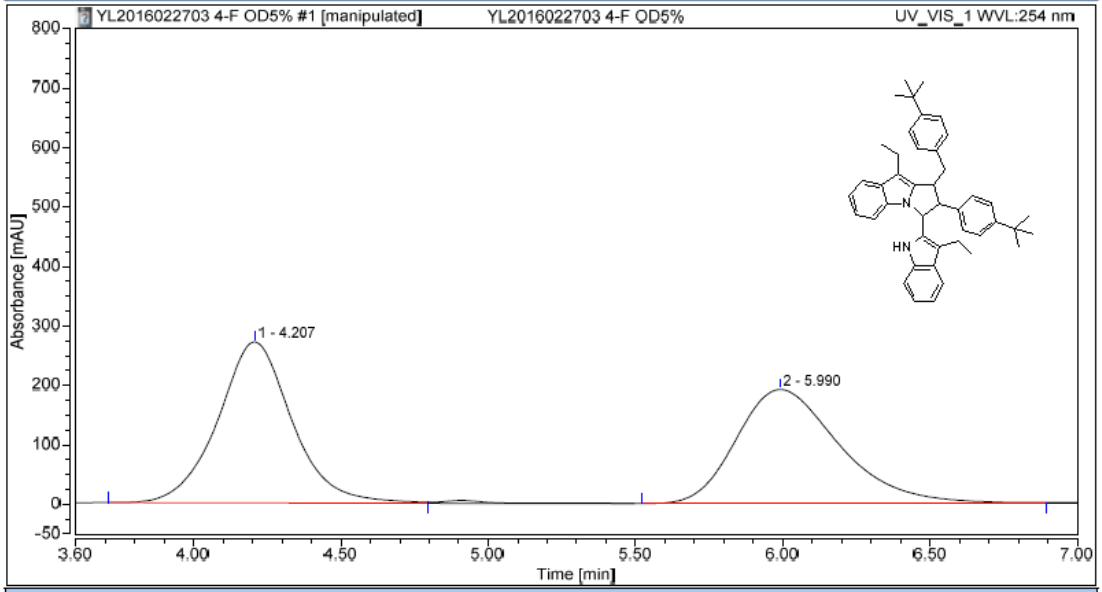


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		22.990	4.612	1.932	10.13	9.09	n.a.
2		29.503	40.904	19.316	89.87	90.91	n.a.
Total:			**45.517**	**21.247**	**100.00**	**100.00**	

***ent*-2i**

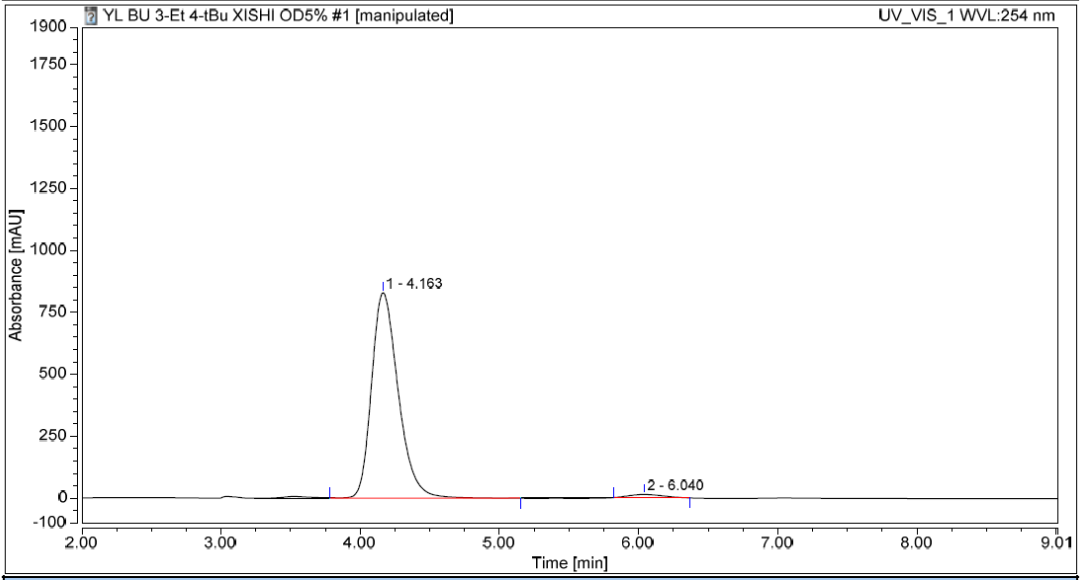
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.207	79.044	270.738	50.32	58.53	n.a.
2		5.990	78.038	191.840	49.68	41.47	n.a.
Total:			**157.082**	**462.578**	**100.00**	**100.00**	

Chromatogram

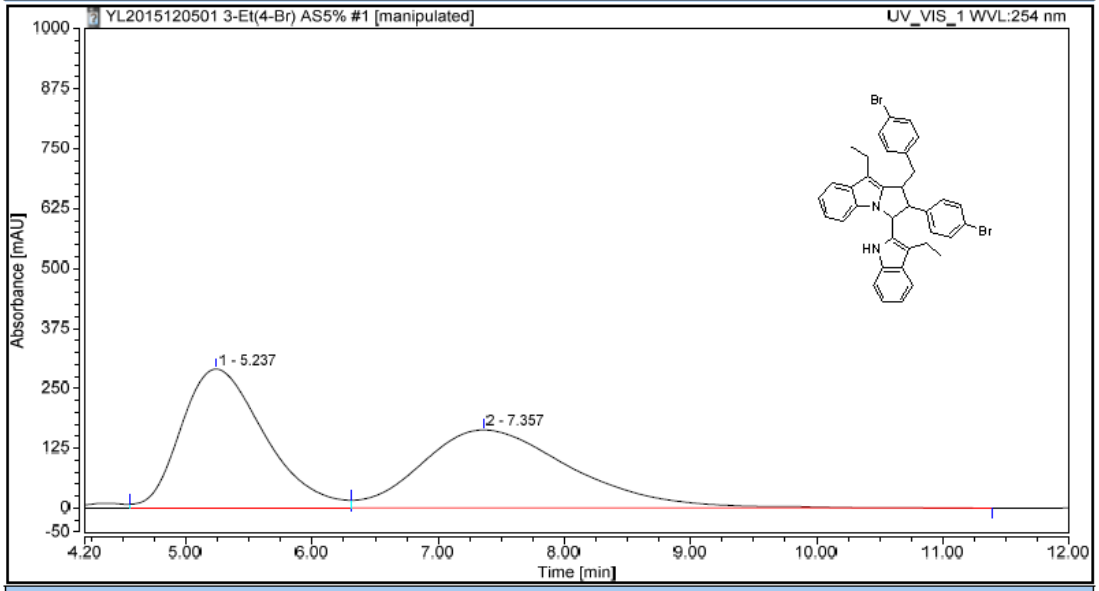


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.163	184.162	829.447	97.73	98.32	n.a.
2		6.040	4.274	14.141	2.27	1.68	n.a.
Total:			**188.436**	**843.588**	**100.00**	**100.00**	

2j

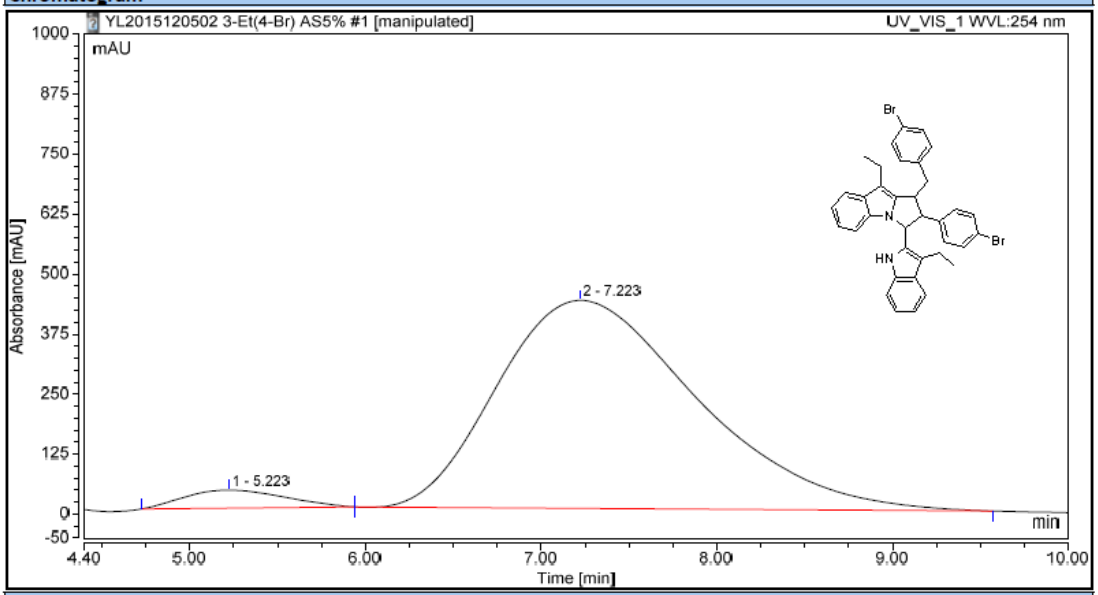
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.237	221.736	289.491	49.73	64.03	n.a.
2		7.357	224.126	162.635	50.27	35.97	n.a.
Total:			**445.862**	**452.126**	**100.00**	**100.00**	

Chromatogram

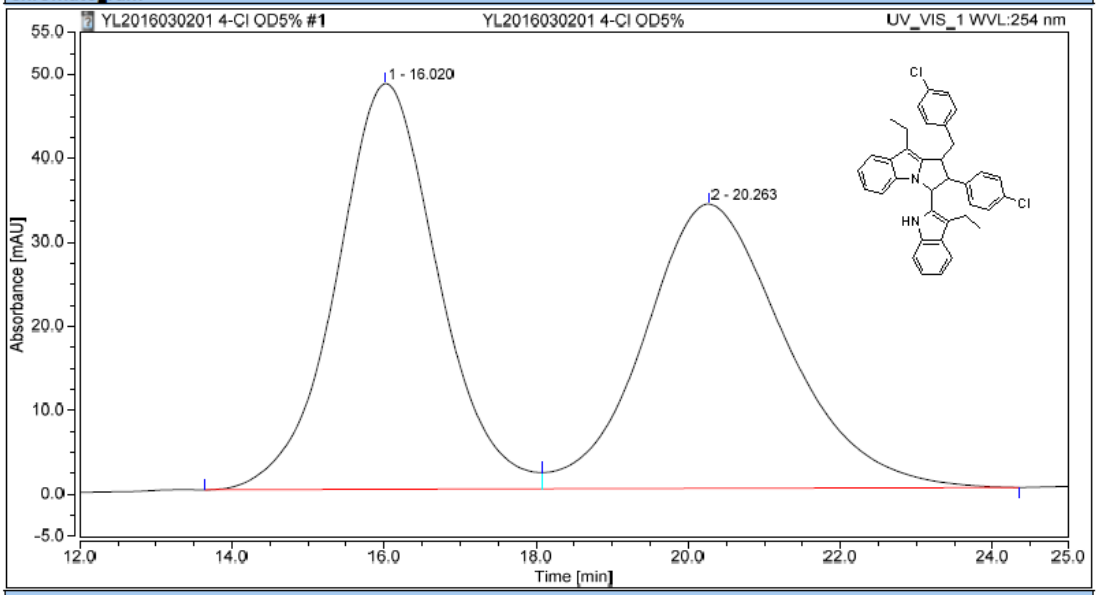


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.223	24.863	37.598	4.17	7.98	n.a.
2		7.223	571.862	433.321	95.83	92.02	n.a.
Total:			**596.725**	**470.919**	**100.00**	**100.00**	

2k

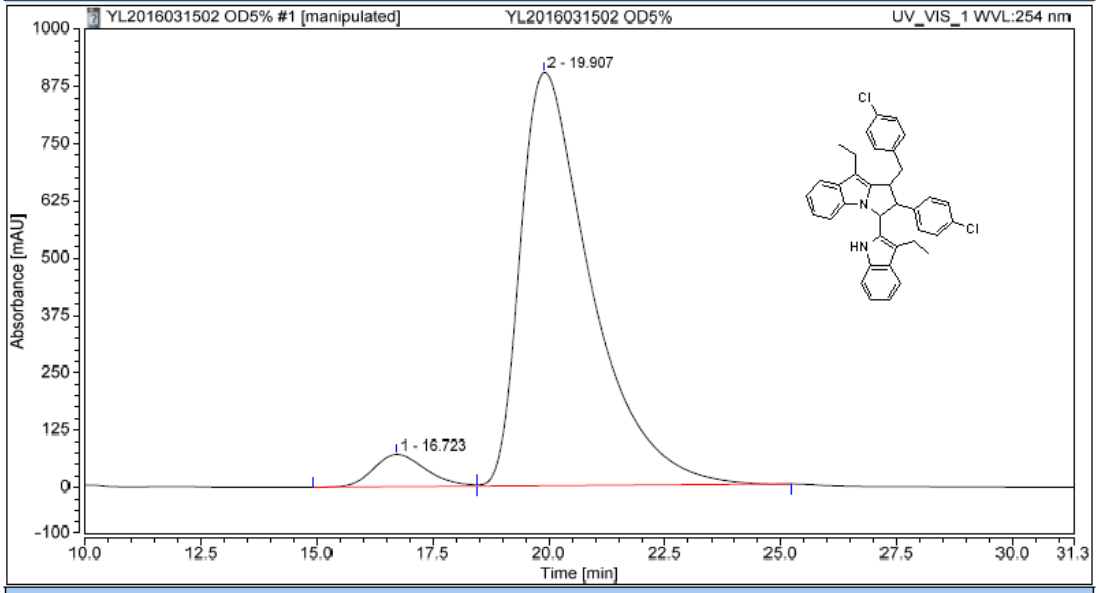
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16.020	74.759	48.292	50.67	58.79	n.a.
2		20.263	72.771	33.849	49.33	41.21	n.a.
Total:			**147.529**	**82.141**	**100.00**	**100.00**	

Chromatogram

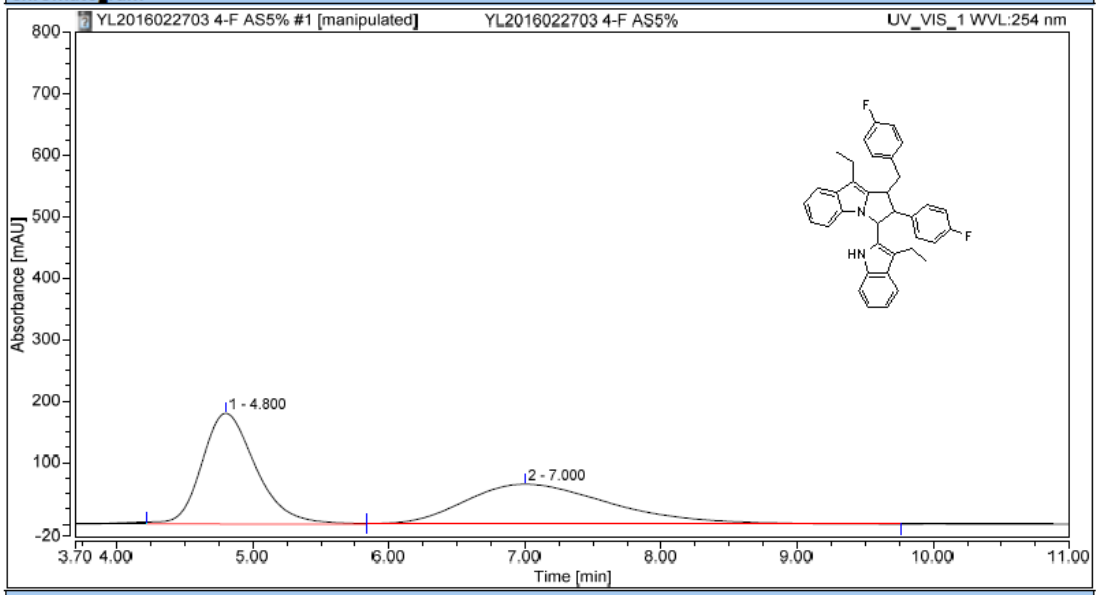


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16.723	90.839	69.972	5.40	7.20	n.a.
2		19.907	1589.870	902.202	94.60	92.80	n.a.
Total:			**1680.709**	**972.174**	**100.00**	**100.00**	

***ent*-2l**

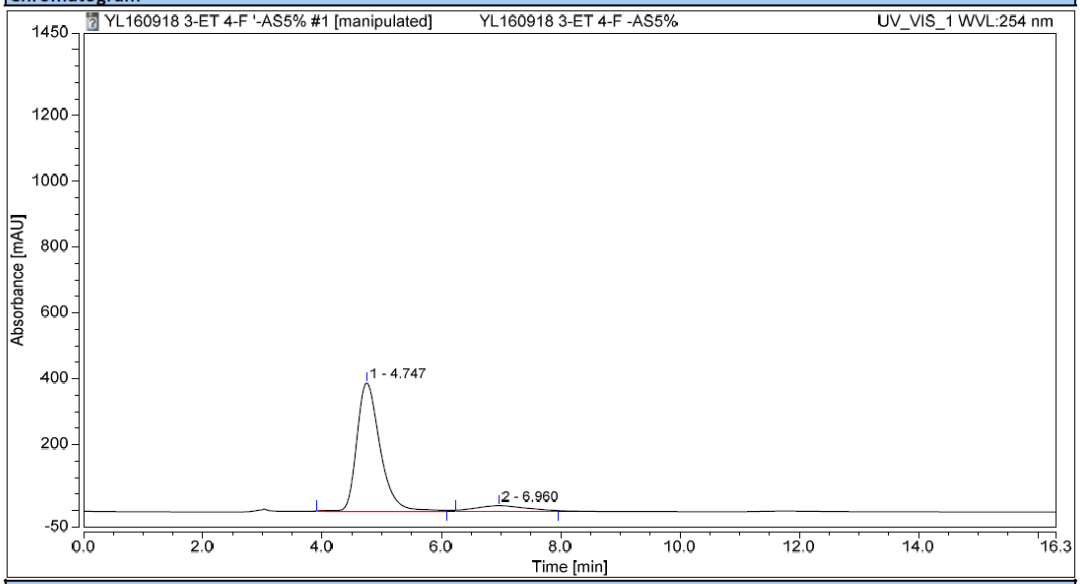
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.800	82.874	180.197	50.59	73.52	n.a.
2		7.000	80.949	64.904	49.41	26.48	n.a.
Total:			**163.823**	**245.101**	**100.00**	**100.00**	

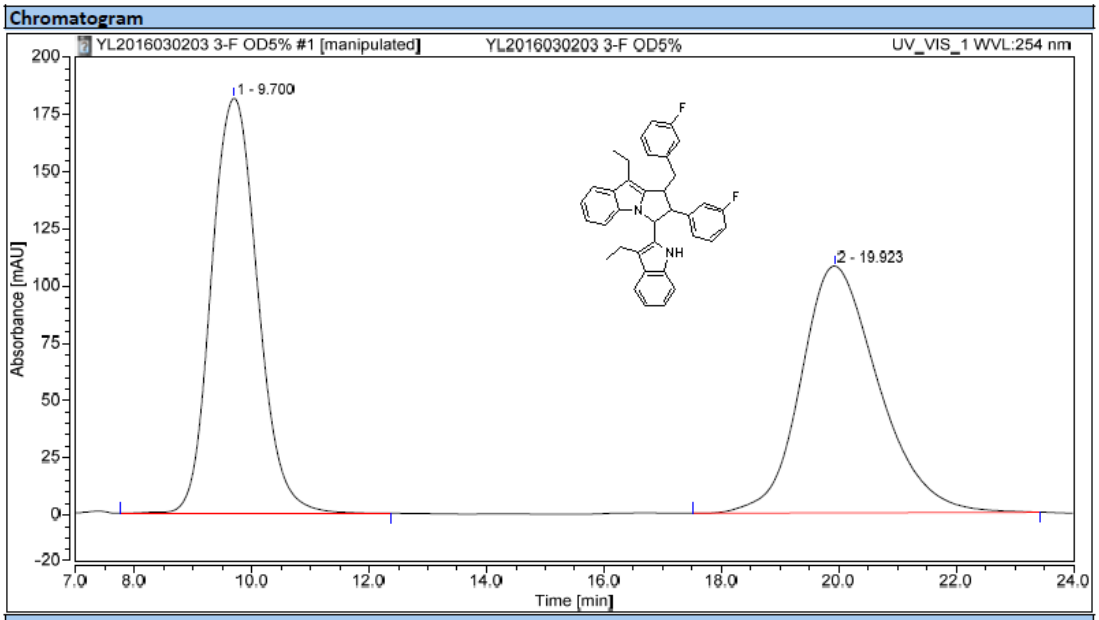
Chromatogram



Integration Results

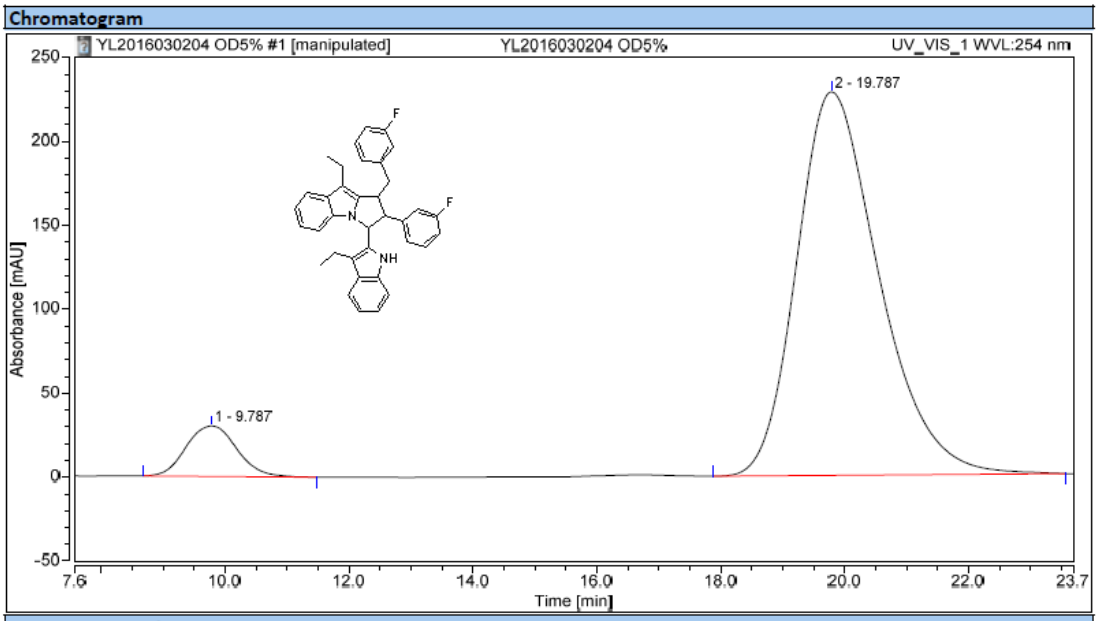
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.747	177.328	390.882	90.63	95.66	n.a.
2		6.960	18.334	17.750	9.37	4.34	n.a.
Total:			**195.662**	**408.632**	**100.00**	**100.00**	

2m



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.700	165.681	181.382	50.04	62.71	n.a.
2		19.923	165.430	107.843	49.96	37.29	n.a.
Total:			**331.111**	**289.225**	**100.00**	**100.00**	

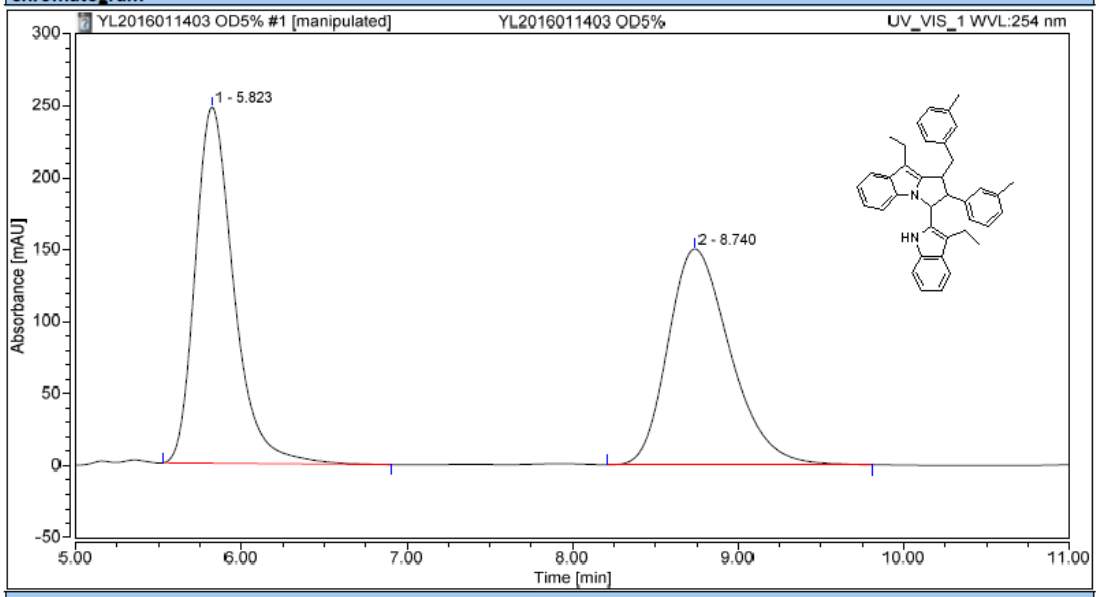


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		9.787	28.500	30.049	7.49	11.62	n.a.
2		19.787	351.817	228.487	92.51	88.38	n.a.
Total:			**380.317**	**258.536**	**100.00**	**100.00**	

2n

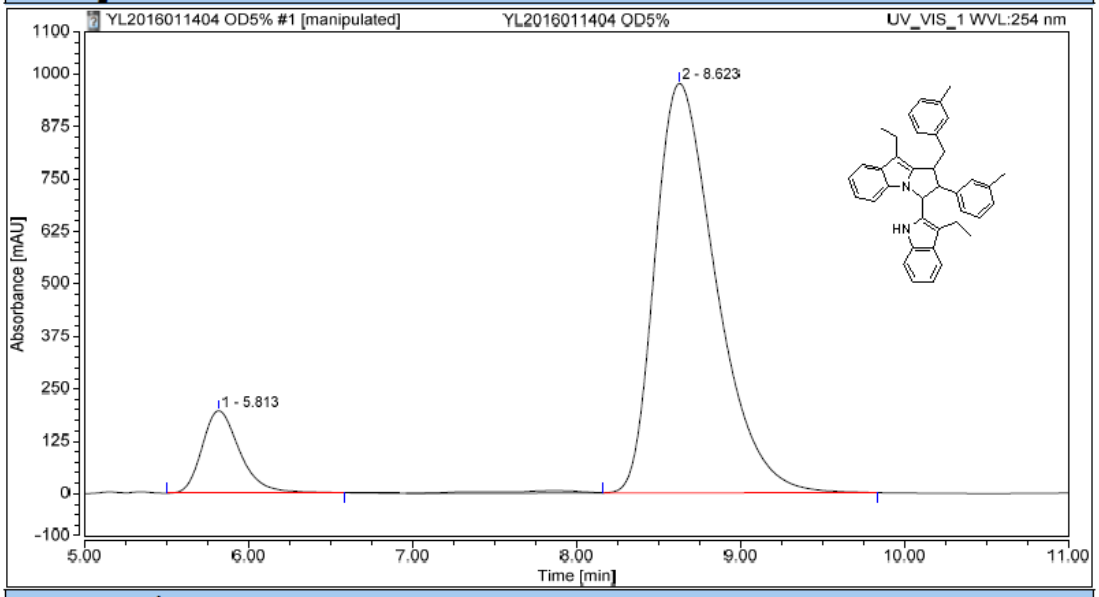
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.823	66.612	247.381	50.56	62.26	n.a.
2		8.740	65.129	149.980	49.44	37.74	n.a.
Total:			**131.741**	**397.361**	**100.00**	**100.00**	

Chromatogram

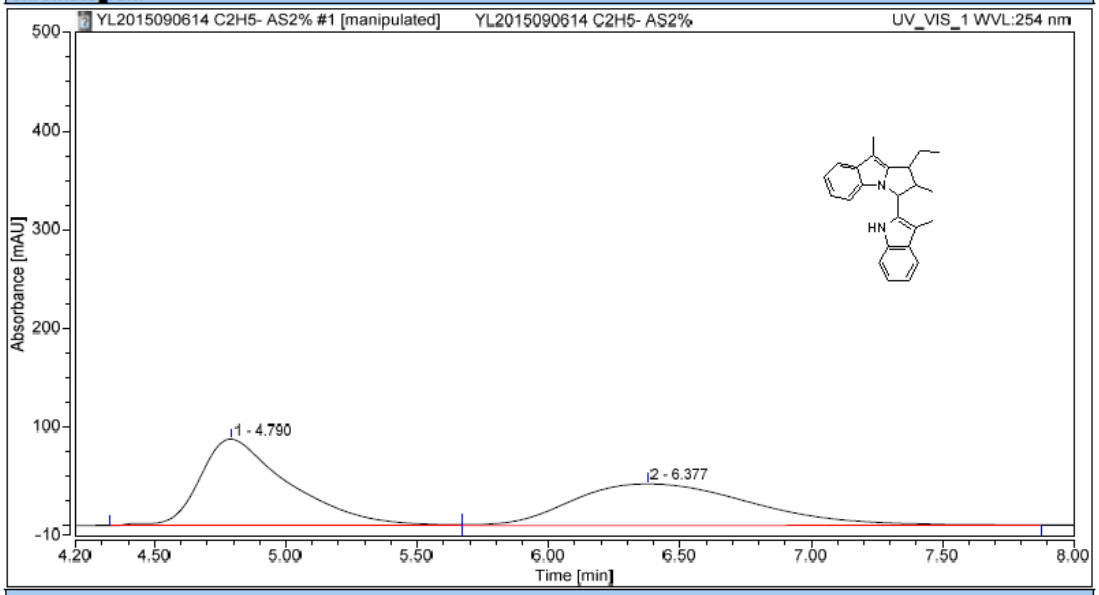


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.813	53.262	196.862	11.24	16.78	n.a.
2		8.623	420.499	976.033	88.76	83.22	n.a.
Total:			**473.761**	**1172.894**	**100.00**	**100.00**	

2o

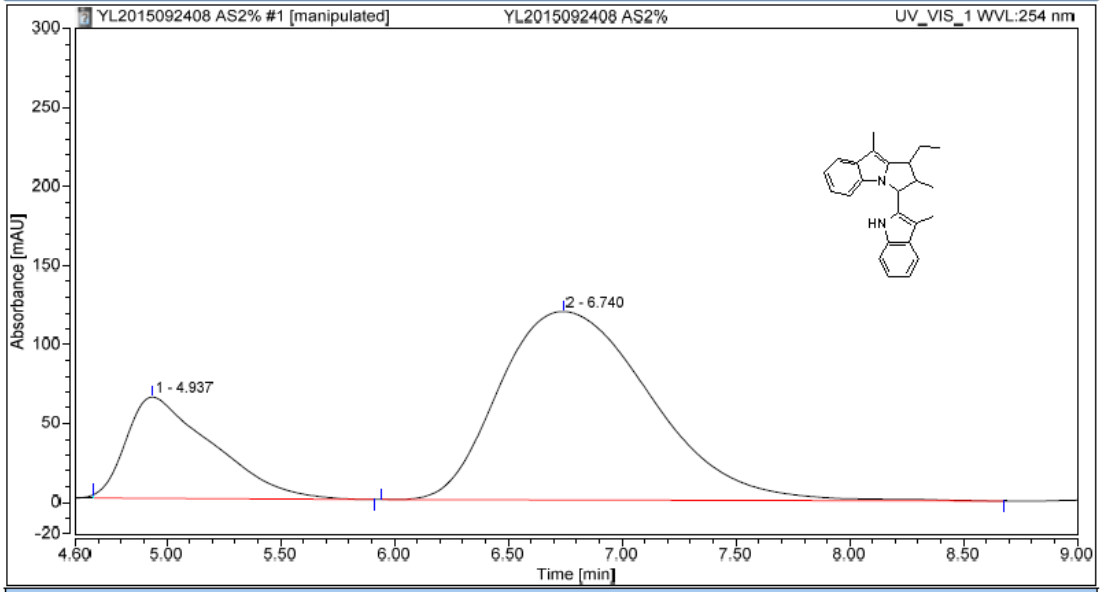
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.790	34.555	87.779	50.85	67.57	n.a.
2		6.377	33.399	42.131	49.15	32.43	n.a.
Total:			**67.955**	**129.910**	**100.00**	**100.00**	

Chromatogram

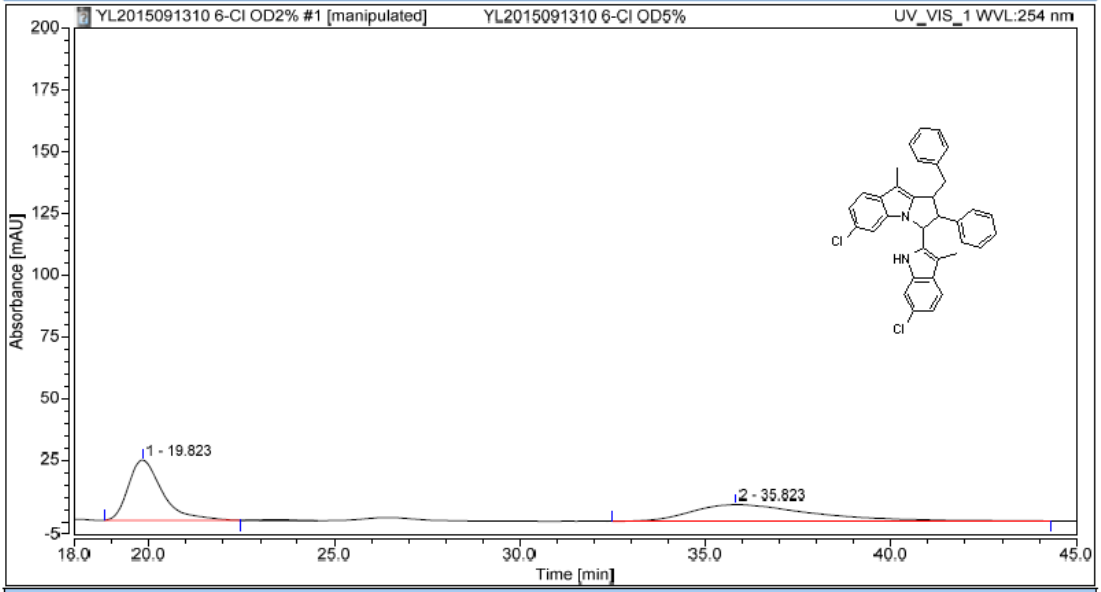


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4.937	28.220	64.195	23.44	34.98	n.a.
2		6.740	92.194	119.349	76.56	65.02	n.a.
Total:			**120.414**	**183.544**	**100.00**	**100.00**	

2s

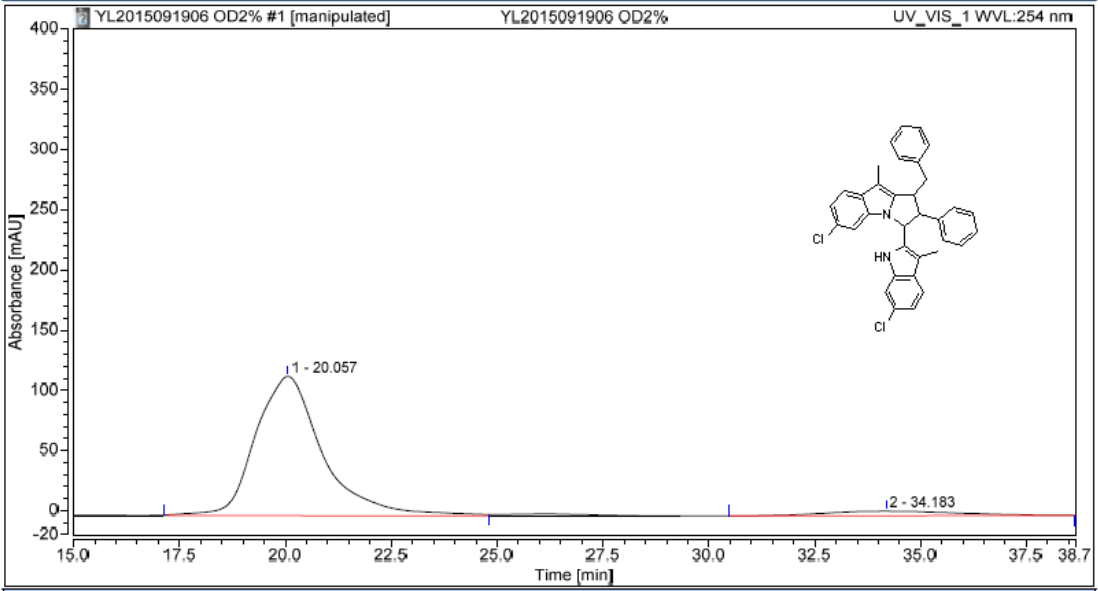
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		19.823	26.063	24.459	51.26	78.63	n.a.
2		35.823	24.782	6.649	48.74	21.37	n.a.
Total:			**50.844**	**31.109**	**100.00**	**100.00**	

Chromatogram

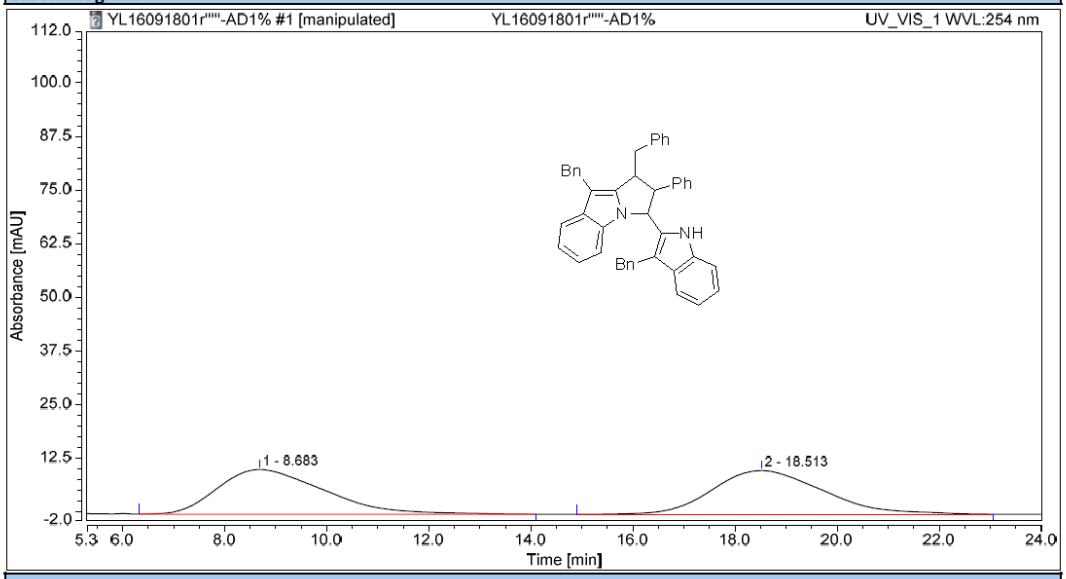


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		20.057	212.658	115.696	93.86	96.82	n.a.
2		34.183	13.911	3.798	6.14	3.18	n.a.
Total:			**226.569**	**119.495**	**100.00**	**100.00**	

***ent*-2t**

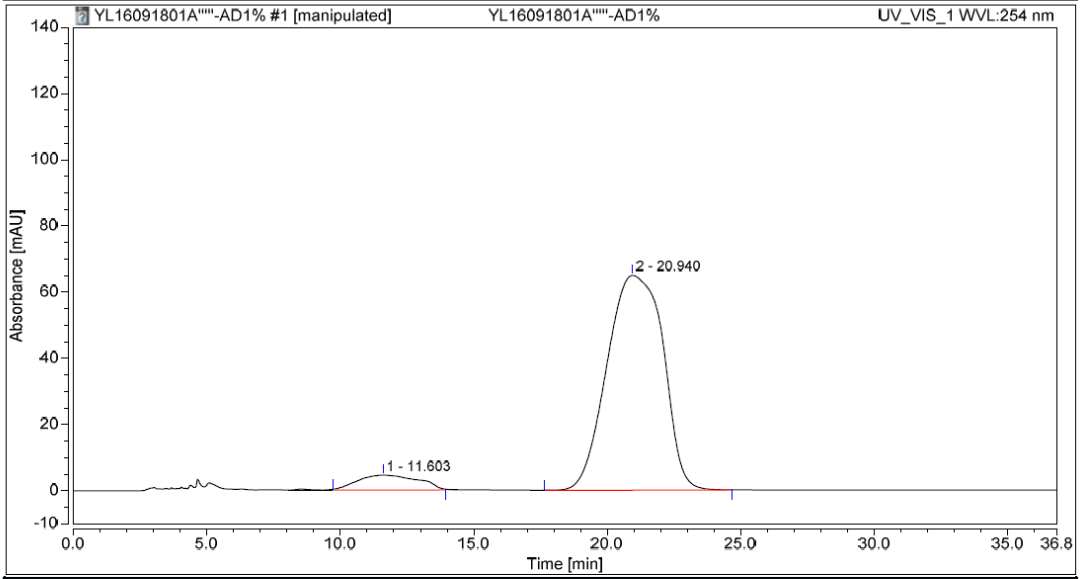
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.683	25.197	10.403	49.47	50.50	n.a.
2		18.513	25.738	10.197	50.53	49.50	n.a.
Total:			**50.935**	**20.600**	**100.00**	**100.00**	

Chromatogram



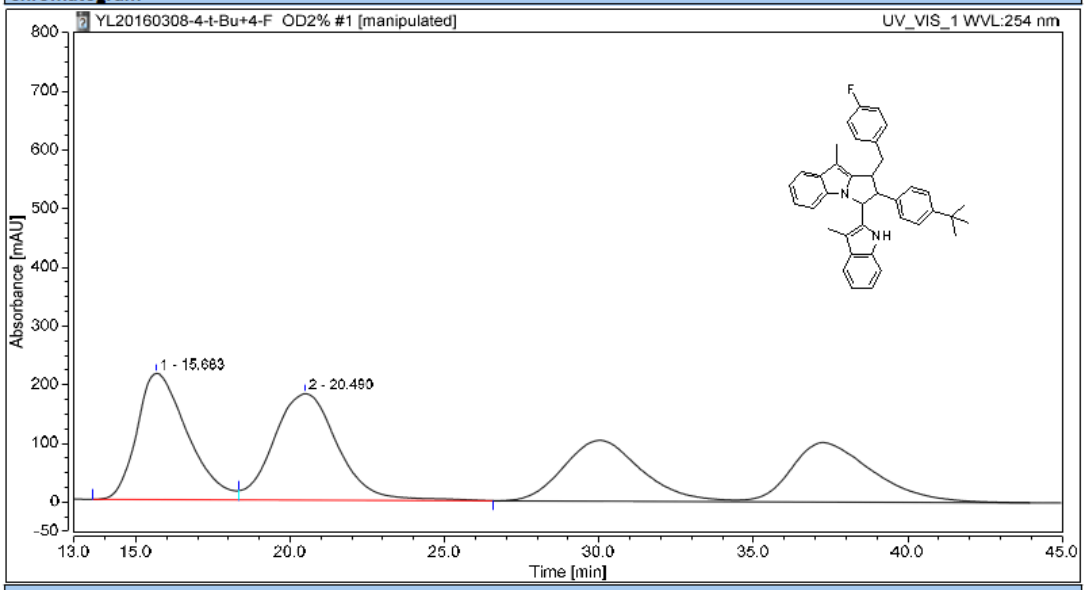
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.603	11.912	4.482	7.00	6.46	n.a.
2		20.940	158.297	64.881	93.00	93.54	n.a.
Total:			**170.209**	**69.363**	**100.00**	**100.00**	

2be and 2be' : inseparable isomers (61:39 molar ratio)

2be:

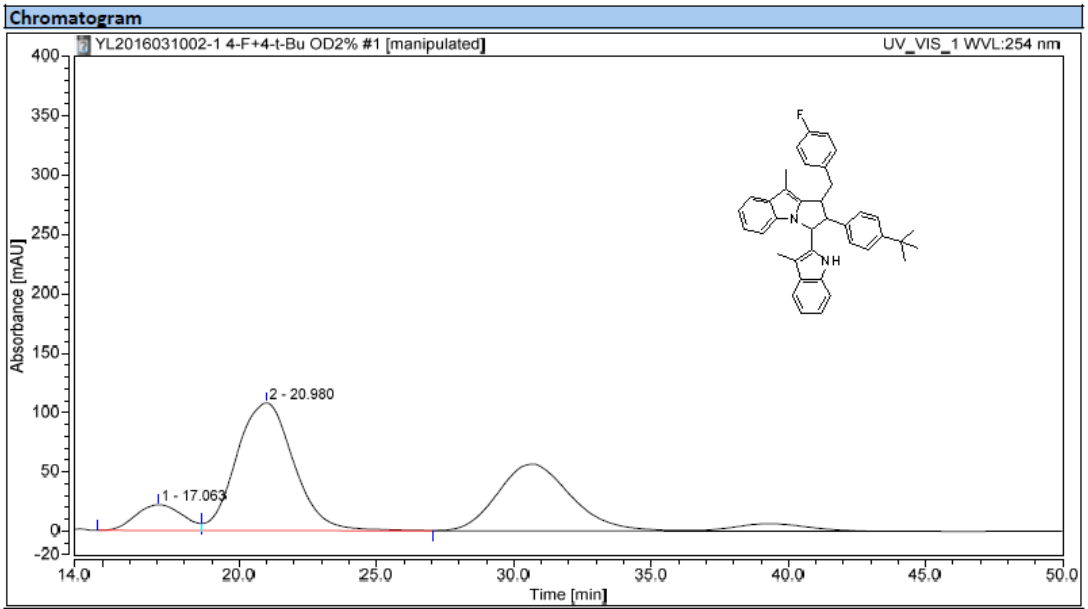
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.683	407.421	214.949	48.40	54.23	n.a.
2		20.490	434.429	181.435	51.60	45.77	n.a.
Total:			**841.849**	**396.384**	**100.00**	**100.00**	

Chromatogram

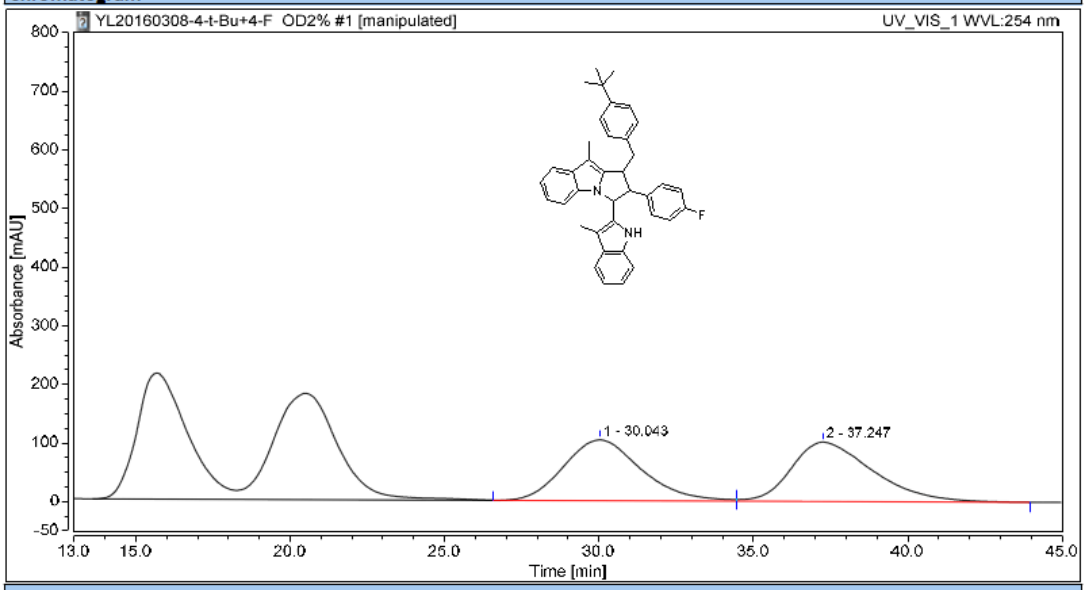


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17.063	42.807	21.737	14.12	16.81	n.a.
2		20.980	260.266	107.569	85.88	83.19	n.a.
Total:			**303.073**	**129.305**	**100.00**	**100.00**	

2be':

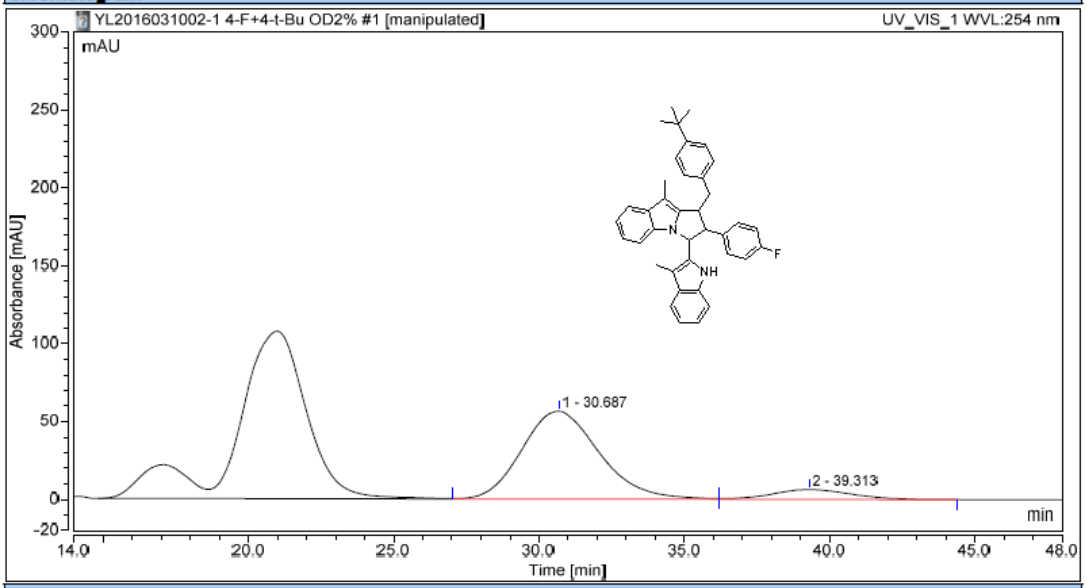
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		30.043	301.309	103.760	49.39	50.57	n.a.
2		37.247	308.813	101.429	50.61	49.43	n.a.
Total:			**610.122**	**205.189**	**100.00**	**100.00**	

Chromatogram

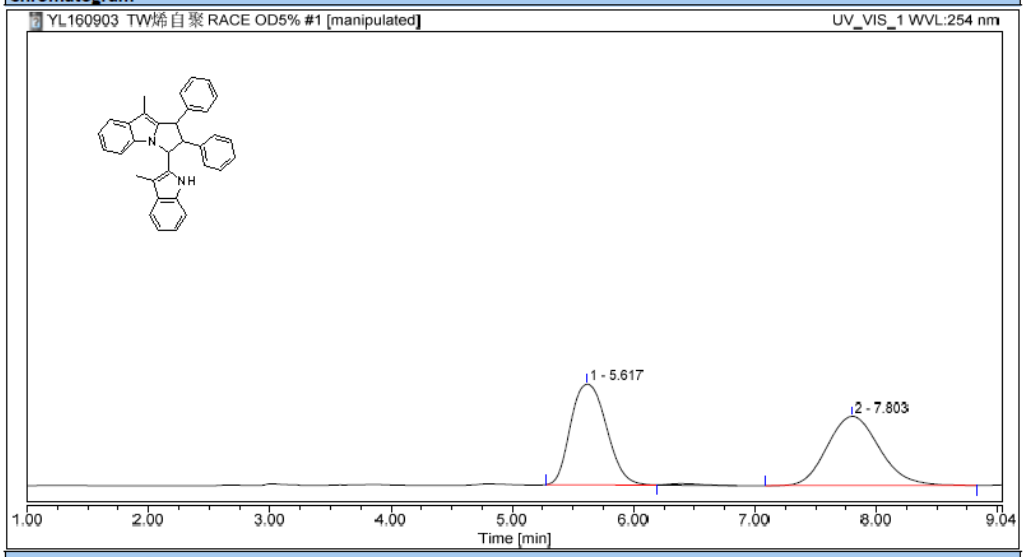


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		30.687	174.437	56.374	89.68	89.86	n.a.
2		39.313	20.083	6.363	10.32	10.14	n.a.
Total:			**194.519**	**62.736**	**100.00**	**100.00**	

Compound 6

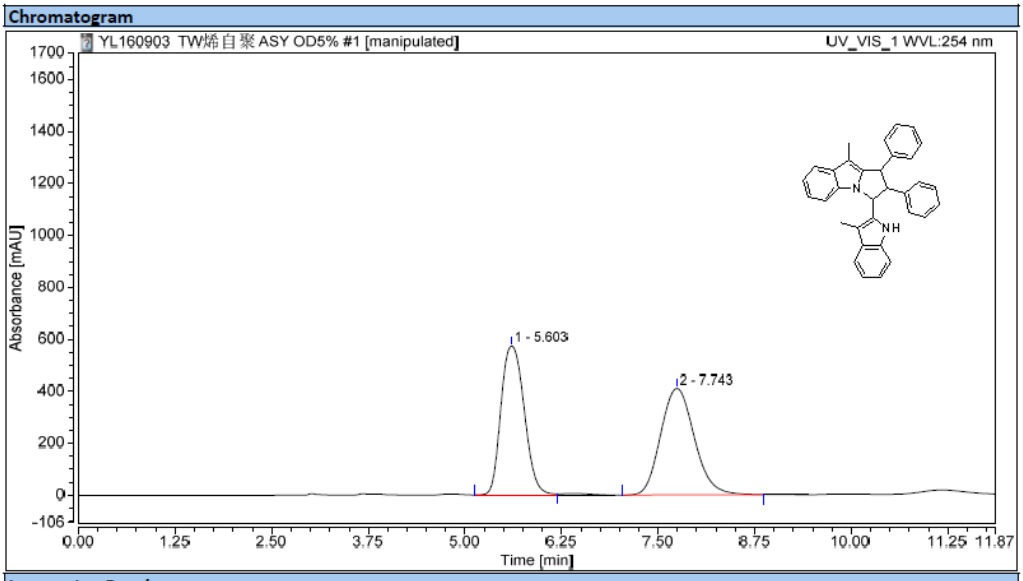
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.617	221.134	644.057	50.03	59.27	n.a.
2		7.803	220.895	442.630	49.97	40.73	n.a.
Total:			**442.029**	**1086.687**	**100.00**	**100.00**	

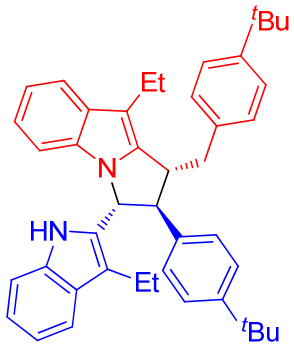
Chromatogram



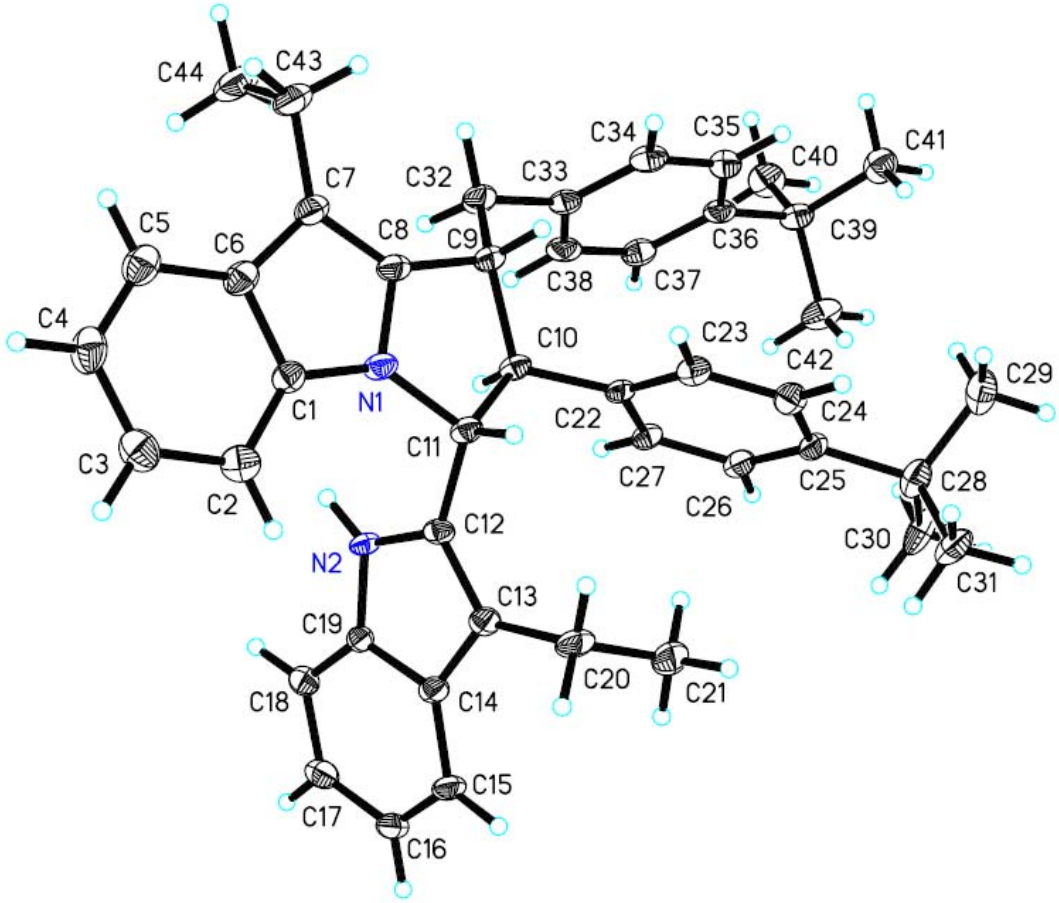
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		5.603	200.155	572.806	49.09	58.28	n.a.
2		7.743	207.588	409.965	50.91	41.72	n.a.
Total:			**407.743**	**982.771**	**100.00**	**100.00**	

3. X-ray single crystal data for racemic product 2i and chiral compound 4



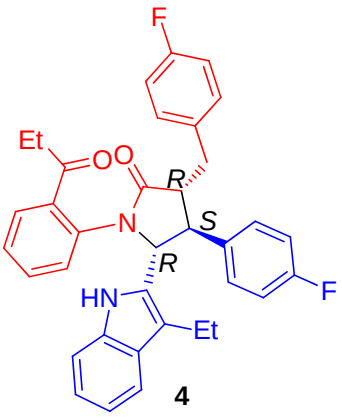
(±)-2i



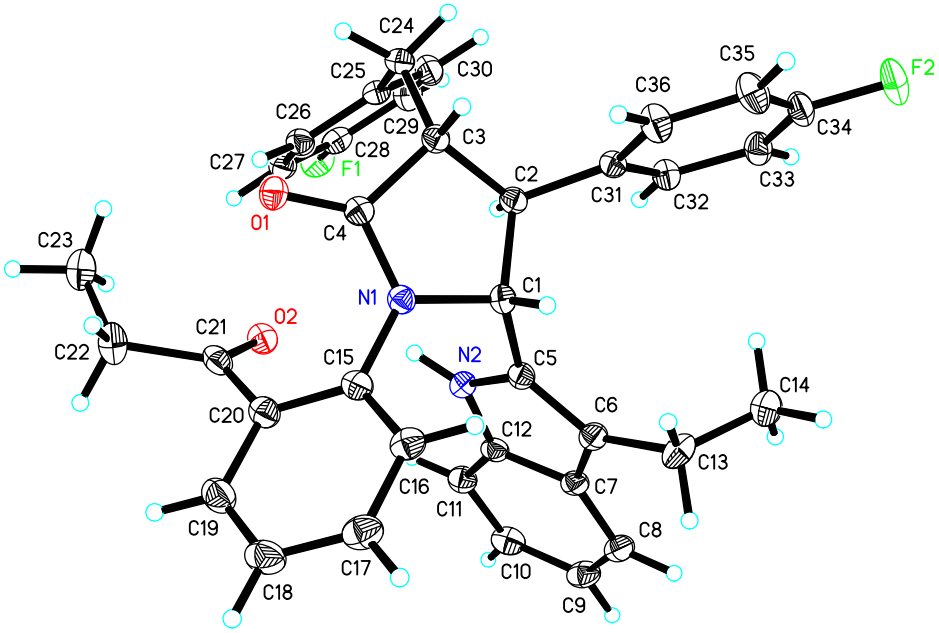
The thermal ellipsoid was drawn at the 30% probability level.

Empirical formula	C44 H50 N2	
Formula weight	606.86	
Temperature	130 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 19.661(13) Å	α= 90°.
	b = 10.710(7) Å	β= 97.306(11)°.

	c = 17.118(11) Å γ = 90°.
Volume	3575(4) $Å^3$
Z	4
Density (calculated)	1.127 Mg/m^3
Absorption coefficient	0.064 mm^{-1}
F(000)	1312
Crystal size	0.25 x 0.15 x 0.05 mm^3
Theta range for data collection	2.089 to 25.049°.
Index ranges	0<=h<=23, -12<=k<=0, -20<=l<=20
Reflections collected	6181
Independent reflections	6181 [R(int) = ?]
Completeness to theta = 25.049°	97.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.3807
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6181 / 0 / 424
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0877, wR2 = 0.1849
R indices (all data)	R1 = 0.1483, wR2 = 0.2210
Extinction coefficient	n/a
Largest diff. peak and hole	0.296 and -0.330 $e.Å^{-3}$



4



Identification code	cu_dm16560_0m	
Empirical formula	C36 H32 F2 N2 O2	
Formula weight	562.63	
Temperature	130 K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 11.5593(3) Å	α= 90°.
	b = 14.0068(3) Å	β= 90°.
	c = 17.8914(4) Å	γ = 90°.
Volume	2896.77(12) $Å^3$	
Z	4	

Density (calculated)	1.290 Mg/m^3
Absorption coefficient	0.719 mm^{-1}
F(000)	1184
Crystal size	0.12 x 0.1 x 0.05 mm^3
Theta range for data collection	4.008 to 65.664°.
Index ranges	-13<=h<=12, -16<=k<=16, -21<=l<=20
Reflections collected	16825
Independent reflections	4925 [R(int) = 0.0523]
Completeness to theta = 65.664°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7527 and 0.6319
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4925 / 0 / 381
Goodness-of-fit on F^2	0.821
Final R indices [I>2sigma(I)]	R1 = 0.0361, wR2 = 0.1029
R indices (all data)	R1 = 0.0409, wR2 = 0.1084
Absolute structure parameter	-0.05(10)
Extinction coefficient	n/a
Largest diff. peak and hole	0.169 and -0.161 $e.Å^{-3}$

4. Theoretical calculations to determine the absolute configuration of 2k

Table 1. Simulated and Experimental ECD spectra date at half peak width of 0.3 of (-)-**2k**

Wavelength(nm)	Exp.ECD	Wavelength(nm)	Cal.ECD
190.00	-12.6000	190.77	-0.7835
190.25	-9.0390	190.80	-0.7956
190.50	-5.8974	190.83	-0.8081
190.75	-3.5439	190.86	-0.8205
191.00	-2.2270	190.89	-0.8331
191.25	-1.9965	190.92	-0.8460
191.50	-2.6541	190.95	-0.8589
191.75	-3.7801	190.98	-0.8721
192.00	-4.8526	191.01	-0.8855
192.25	-5.4213	191.04	-0.8991
192.50	-5.2614	191.07	-0.9128
192.75	-4.4324	191.10	-0.9267
193.00	-3.2173	191.13	-0.9408
193.25	-1.9791	191.16	-0.9551
193.50	-1.0100	191.19	-0.9696
193.75	-0.4472	191.22	-0.9843
194.00	-0.2817	191.25	-0.9992
194.25	-0.4340	191.27	-1.0143
194.50	-0.8376	191.30	-1.0296
194.75	-1.4776	191.33	-1.0451
195.00	-2.3688	191.36	-1.0608
195.25	-3.4999	191.39	-1.0767
195.50	-4.7898	191.42	-1.0928
195.75	-6.0892	191.45	-1.1091
196.00	-7.2275	191.48	-1.1258
196.25	-8.0769	191.51	-1.1426
196.50	-8.5954	191.54	-1.1595
196.75	-8.8305	191.57	-1.1768
197.00	-8.8894	191.60	-1.1942
197.25	-8.8960	191.63	-1.2119
197.50	-8.9588	191.66	-1.2297
197.75	-9.1567	191.69	-1.2479
198.00	-9.5411	191.72	-1.2663
198.25	-10.1423	191.75	-1.2849
198.50	-10.9700	191.78	-1.3038
198.75	-12.0036	191.81	-1.3229
199.00	-13.1765	191.84	-1.3422
199.25	-14.3697	191.87	-1.3619
199.50	-15.4303	191.90	-1.3818
199.75	-16.2168	191.93	-1.4019
200.00	-16.6548	191.96	-1.4223

200.25	-16.7750	191.99	-1.4429
200.50	-16.7099	192.02	-1.4639
200.75	-16.6475	192.04	-1.4850
201.00	-16.7638	192.07	-1.5065
201.25	-17.1650	192.10	-1.5282
201.50	-17.8628	192.13	-1.5501
201.75	-18.7883	192.16	-1.5725
202.00	-19.8335	192.19	-1.5950
202.25	-20.8964	192.22	-1.6178
202.50	-21.9130	192.25	-1.6409
202.75	-22.8639	192.28	-1.6644
203.00	-23.7592	192.31	-1.6881
203.25	-24.6146	192.34	-1.7121
203.50	-25.4323	192.37	-1.7364
203.75	-26.1977	192.40	-1.7610
204.00	-26.8882	192.43	-1.7859
204.25	-27.4881	192.46	-1.8111
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205.00	-28.8477	192.55	-1.8887
205.25	-29.2528	192.58	-1.9152
205.50	-29.6859	192.61	-1.9419
205.75	-30.1677	192.64	-1.9691
206.00	-30.7137	192.67	-1.9967
206.25	-31.3377	192.70	-2.0244
206.50	-32.0515	192.73	-2.0526
206.75	-32.8589	192.76	-2.0811
207.00	-33.7488	192.79	-2.1099
207.25	-34.6901	192.82	-2.1390
207.50	-35.6338	192.85	-2.1686
207.75	-36.5230	192.88	-2.1984
208.00	-37.3061	192.91	-2.2287
208.25	-37.9525	192.94	-2.2593
208.50	-38.4637	192.97	-2.2904
208.75	-38.8755	193.00	-2.3217
209.00	-39.2473	193.03	-2.3534
209.25	-39.6416	193.06	-2.3855
209.50	-40.1029	193.09	-2.4180
209.75	-40.6466	193.12	-2.4509
210.00	-41.2631	193.15	-2.4840
210.25	-41.9309	193.18	-2.5176
210.50	-42.6311	193.21	-2.5517
210.75	-43.3519	193.24	-2.5862
211.00	-44.0857	193.27	-2.6210

211.25	-44.8235	193.30	-2.6562
211.50	-45.5554	193.33	-2.6919
211.75	-46.2772	193.36	-2.7279
212.00	-46.9982	193.39	-2.7644
212.25	-47.7424	193.42	-2.8013
212.50	-48.5387	193.45	-2.8386
212.75	-49.4064	193.48	-2.8763
213.00	-50.3430	193.51	-2.9145
213.25	-51.3225	193.54	-2.9531
213.50	-52.3056	193.57	-2.9922
213.75	-53.2539	193.60	-3.0317
214.00	-54.1417	193.63	-3.0716
214.25	-54.9599	193.66	-3.1121
214.50	-55.7132	193.70	-3.1529
214.75	-56.4159	193.73	-3.1943
215.00	-57.0873	193.76	-3.2360
215.25	-57.7470	193.79	-3.2783
215.50	-58.4078	193.82	-3.3209
215.75	-59.0675	193.85	-3.3641
216.00	-59.7052	193.88	-3.4079
216.25	-60.2893	193.91	-3.4520
216.50	-60.7950	193.94	-3.4967
216.75	-61.2214	193.97	-3.5418
217.00	-61.5952	194.00	-3.5874
217.25	-61.9554	194.03	-3.6336
217.50	-62.3264	194.06	-3.6803
217.75	-62.6996	194.09	-3.7274
218.00	-63.0351	194.12	-3.7751
218.25	-63.2855	194.15	-3.8232
218.50	-63.4239	194.18	-3.8720
218.75	-63.4587	194.21	-3.9212
219.00	-63.4280	194.24	-3.9710
219.25	-63.3785	194.27	-4.0212
219.50	-63.3439	194.30	-4.0721
219.75	-63.3342	194.33	-4.1235
220.00	-63.3354	194.36	-4.1754
220.25	-63.3155	194.39	-4.2279
220.50	-63.2305	194.42	-4.2810
220.75	-63.0298	194.45	-4.3346
221.00	-62.6610	194.48	-4.3887
221.25	-62.0760	194.52	-4.4435
221.50	-61.2387	194.55	-4.4988
221.75	-60.1332	194.58	-4.5548
222.00	-58.7681	194.61	-4.6112

222.25	-57.1751	194.64	-4.6683
222.50	-55.3987	194.67	-4.7259
222.75	-53.4819	194.70	-4.7843
223.00	-51.4503	194.73	-4.8431
223.25	-49.3036	194.76	-4.9026
223.50	-47.0161	194.79	-4.9628
223.75	-44.5436	194.82	-5.0234
224.00	-41.8355	194.85	-5.0847
224.25	-38.8448	194.88	-5.1467
224.50	-35.5360	194.91	-5.2094
224.75	-31.8894	194.94	-5.2725
225.00	-27.9019	194.97	-5.3364
225.25	-23.5850	195.00	-5.4009
225.50	-18.9638	195.04	-5.4662
225.75	-14.0756	195.07	-5.5319
226.00	-8.9702	195.10	-5.5985
226.25	-3.7091	195.13	-5.6655
226.50	1.6397	195.16	-5.7333
226.75	7.0076	195.19	-5.8019
227.00	12.3325	195.22	-5.8710
227.25	17.5611	195.25	-5.9408
227.50	22.6471	195.28	-6.0114
227.75	27.5465	195.31	-6.0825
228.00	32.2139	195.34	-6.1545
228.25	36.6011	195.37	-6.2271
228.50	40.6581	195.40	-6.3005
228.75	44.3357	195.44	-6.3746
229.00	47.5880	195.47	-6.4493
229.25	50.3745	195.50	-6.5247
229.50	52.6633	195.53	-6.6009
229.75	54.4337	195.56	-6.6779
230.00	55.6802	195.59	-6.7556
230.25	56.4150	195.62	-6.8340
230.50	56.6697	195.65	-6.9131
230.75	56.4940	195.68	-6.9930
231.00	55.9505	195.71	-7.0737
231.25	55.1077	195.74	-7.1552
231.50	54.0321	195.77	-7.2374
231.75	52.7812	195.81	-7.3203
232.00	51.3998	195.84	-7.4040
232.25	49.9186	195.87	-7.4885
232.50	48.3575	195.90	-7.5738
232.75	46.7300	195.93	-7.6599
233.00	45.0490	195.96	-7.7468

233.25	43.3306	195.99	-7.8345
233.50	41.5948	196.02	-7.9230
233.75	39.8636	196.05	-8.0123
234.00	38.1573	196.08	-8.1023
234.25	36.4927	196.12	-8.1933
234.50	34.8812	196.15	-8.2850
234.75	33.3285	196.18	-8.3775
235.00	31.8347	196.21	-8.4710
235.25	30.3950	196.24	-8.5652
235.50	29.0016	196.27	-8.6603
235.75	27.6461	196.30	-8.7563
236.00	26.3223	196.33	-8.8530
236.25	25.0275	196.36	-8.9507
236.50	23.7636	196.40	-9.0492
236.75	22.5356	196.43	-9.1485
237.00	21.3509	196.46	-9.2487
237.25	20.2169	196.49	-9.3498
237.50	19.1390	196.52	-9.4518
237.75	18.1178	196.55	-9.5547
238.00	17.1481	196.58	-9.6585
238.25	16.2196	196.61	-9.7632
238.50	15.3203	196.64	-9.8688
238.75	14.4404	196.68	-9.9752
239.00	13.5759	196.71	-10.0826
239.25	12.7290	196.74	-10.1909
239.50	11.9055	196.77	-10.3001
239.75	11.1116	196.80	-10.4102
240.00	10.3518	196.83	-10.5213
240.25	9.6276	196.86	-10.6332
240.50	8.9383	196.89	-10.7462
240.75	8.2821	196.93	-10.8600
241.00	7.6563	196.96	-10.9748
241.25	7.0580	196.99	-11.0906
241.50	6.4843	197.02	-11.2073
241.75	5.9327	197.05	-11.3249
242.00	5.4018	197.08	-11.4435
242.25	4.8903	197.11	-11.5632
242.50	4.3972	197.14	-11.6837
242.75	3.9211	197.18	-11.8053
243.00	3.4603	197.21	-11.9277
243.25	3.0135	197.24	-12.0513
243.50	2.5808	197.27	-12.1758
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244.25	1.3814	197.36	-12.5552
244.50	1.0175	197.40	-12.6837
244.75	0.6691	197.43	-12.8132
245.00	0.3339	197.46	-12.9437
245.25	0.0108	197.49	-13.0752
245.50	-0.2988	197.52	-13.2078
245.75	-0.5914	197.55	-13.3413
246.00	-0.8632	197.58	-13.4759
246.25	-1.1120	197.62	-13.6116
246.50	-1.3373	197.65	-13.7483
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247.25	-1.8979	197.74	-14.1645
247.50	-2.0572	197.77	-14.3054
247.75	-2.2062	197.80	-14.4473
248.00	-2.3454	197.84	-14.5902
248.25	-2.4744	197.87	-14.7342
248.50	-2.5925	197.90	-14.8794
248.75	-2.6998	197.93	-15.0255
249.00	-2.7966	197.96	-15.1728
249.25	-2.8836	197.99	-15.3210
249.50	-2.9608	198.03	-15.4704
249.75	-3.0280	198.06	-15.6210
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250.25	-3.1321	198.12	-15.9252
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251.25	-3.2827	198.25	-16.5467
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253.00	-3.2773	198.47	-17.6771
253.25	-3.2468	198.50	-17.8431
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254.00	-3.1604	198.60	-18.3477
254.25	-3.1266	198.63	-18.5183
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256.00	-2.7588	198.85	-19.7435
256.25	-2.6869	198.88	-19.9230
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258.25	-2.1816	199.14	-21.4016
258.50	-2.1319	199.17	-21.5916
258.75	-2.0845	199.20	-21.7829
259.00	-2.0400	199.24	-21.9753
259.25	-1.9982	199.27	-22.1688
259.50	-1.9577	199.30	-22.3635
259.75	-1.9159	199.33	-22.5593
260.00	-1.8702	199.36	-22.7564
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261.00	-1.6443	199.49	-23.5562
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262.00	-1.4485	199.62	-24.3747
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263.00	-1.2815	199.75	-25.2119
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264.50	-0.9855	199.94	-26.5028
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265.25	-0.8753	200.04	-27.1640
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265.75	-0.7927	200.10	-27.6105
266.00	-0.7546	200.14	-27.8355

266.25	-0.7242	200.17	-28.0617
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266.75	-0.6946	200.23	-28.5176
267.00	-0.6938	200.27	-28.7471
267.25	-0.6987	200.30	-28.9779
267.50	-0.7054	200.33	-29.2098
267.75	-0.7096	200.36	-29.4429
268.00	-0.7079	200.39	-29.6771
268.25	-0.6990	200.43	-29.9124
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268.75	-0.6689	200.49	-30.3866
269.00	-0.6573	200.52	-30.6252
269.25	-0.6543	200.56	-30.8651
269.50	-0.6620	200.59	-31.1061
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270.25	-0.7364	200.69	-31.8357
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271.00	-0.8369	200.78	-32.5754
271.25	-0.8703	200.82	-32.8241
271.50	-0.9037	200.85	-33.0740
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272.00	-0.9700	200.91	-33.5769
272.25	-1.0023	200.95	-33.8300
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279.00	-1.9908	201.83	-41.0535
279.25	-2.0184	201.86	-41.3346
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282.00	-2.1868	202.23	-44.4848
282.25	-2.1966	202.26	-44.7762
282.50	-2.2065	202.29	-45.0683
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283.00	-2.2353	202.36	-45.6551
283.25	-2.2593	202.39	-45.9495
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284.00	-2.3663	202.49	-46.8375
284.25	-2.4029	202.52	-47.1350
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285.00	-2.4852	202.62	-48.0317
285.25	-2.5081	202.65	-48.3320
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285.75	-2.5616	202.72	-48.9345
286.00	-2.5941	202.75	-49.2366
286.25	-2.6301	202.79	-49.5396
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287.00	-2.7490	202.89	-50.4519
287.25	-2.7901	202.92	-50.7572
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289.25	-3.1264	203.19	-53.2191
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290.00	-3.2516	203.29	-54.1505
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291.00	-3.3391	203.42	-55.3983
291.25	-3.3536	203.45	-55.7112
291.50	-3.3708	203.49	-56.0246
291.75	-3.3931	203.52	-56.3381
292.00	-3.4208	203.55	-56.6522
292.25	-3.4526	203.59	-56.9664
292.50	-3.4859	203.62	-57.2810
292.75	-3.5173	203.65	-57.5958
293.00	-3.5435	203.69	-57.9110
293.25	-3.5623	203.72	-58.2264
293.50	-3.5726	203.75	-58.5420
293.75	-3.5753	203.79	-58.8579
294.00	-3.5720	203.82	-59.1740
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295.00	-3.5365	203.95	-60.4401
295.25	-3.5217	203.99	-60.7569
295.50	-3.5024	204.02	-61.0740
295.75	-3.4784	204.06	-61.3911
296.00	-3.4508	204.09	-61.7084
296.25	-3.4206	204.12	-62.0256
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305.25	-1.1997	205.34	-73.3413
305.50	-1.1370	205.37	-73.6484
305.75	-1.0730	205.41	-73.9548
306.00	-1.0073	205.44	-74.2605
306.25	-0.9392	205.48	-74.5656
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306.75	-0.7955	205.54	-75.1737
307.00	-0.7226	205.58	-75.4766
307.25	-0.6531	205.61	-75.7788
307.50	-0.5905	205.65	-76.0802
307.75	-0.5375	205.68	-76.3808
308.00	-0.4952	205.71	-76.6805
308.25	-0.4622	205.75	-76.9794
308.50	-0.4357	205.78	-77.2775
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309.25	-0.3581	205.89	-78.1662
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313.25	0.0467	206.43	-82.7484
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315.00	0.1143	206.67	-84.6551
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316.00	0.1646	206.81	-85.7135
316.25	0.1655	206.85	-85.9743
316.50	0.1631	206.88	-86.2337
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318.00	0.1571	207.09	-87.7562
318.25	0.1640	207.12	-88.0043
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320.00	0.1953	207.37	-89.6912
320.25	0.1932	207.40	-89.9250
320.50	0.1947	207.44	-90.1569
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321.00	0.2088	207.50	-90.6150

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322.25	0.2183	207.68	-91.7261
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326.00	0.2037	208.20	-94.7444
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327.00	0.1817	208.34	-95.4636
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336.00	0.1332	209.61	-100.0800
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345.25	0.1144	210.93	-100.8440
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222.87	15.9708
222.91	16.3470
222.95	16.7214
222.99	17.0937
223.03	17.4642
223.07	17.8329
223.11	18.1995
223.15	18.5642
223.19	18.9270
223.23	19.2878
223.27	19.6466
223.31	20.0034
223.35	20.3583
223.39	20.7113
223.44	21.0621
223.48	21.4110
223.52	21.7580
223.56	22.1028
223.60	22.4457
223.64	22.7867
223.68	23.1255
223.72	23.4623
223.76	23.7971
223.80	24.1298
223.84	24.4605
223.88	24.7890
223.92	25.1157
223.96	25.4402
224.00	25.7627

224.04	26.0829
224.08	26.4012
224.12	26.7176
224.16	27.0317
224.20	27.3437
224.24	27.6537
224.28	27.9615
224.32	28.2674
224.37	28.5710
224.41	28.8726
224.45	29.1720
224.49	29.4695
224.53	29.7647
224.57	30.0579
224.61	30.3489
224.65	30.6378
224.69	30.9248
224.73	31.2095
224.77	31.4921
224.81	31.7724
224.85	32.0508
224.89	32.3271
224.93	32.6012
224.98	32.8731
225.02	33.1430
225.06	33.4107
225.10	33.6764
225.14	33.9399
225.18	34.2012
225.22	34.4606
225.26	34.7177
225.30	34.9727
225.34	35.2256
225.38	35.4762
225.43	35.7249
225.47	35.9714
225.51	36.2159
225.55	36.4581
225.59	36.6983
225.63	36.9363
225.67	37.1723
225.71	37.4061
225.75	37.6379
225.80	37.8674

225.84	38.0949
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225.92	38.5437
225.96	38.7648
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226.04	39.2010
226.08	39.4160
226.12	39.6287
226.17	39.8394
226.21	40.0482
226.25	40.2548
226.29	40.4592
226.33	40.6617
226.37	40.8621
226.41	41.0604
226.46	41.2566
226.50	41.4509
226.54	41.6430
226.58	41.8331
226.62	42.0212
226.66	42.2072
226.70	42.3911
226.75	42.5730
226.79	42.7529
226.83	42.9308
226.87	43.1067
226.91	43.2806
226.95	43.4523
226.99	43.6221
227.04	43.7900
227.08	43.9559
227.12	44.1197
227.16	44.2815
227.20	44.4414
227.24	44.5994
227.29	44.7554
227.33	44.9093
227.37	45.0614
227.41	45.2115
227.45	45.3596
227.49	45.5058
227.54	45.6501
227.58	45.7923
227.62	45.9329

227.66	46.0713
227.70	46.2080
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227.79	46.4754
227.83	46.6064
227.87	46.7354
227.91	46.8624
227.95	46.9877
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228.04	47.2328
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228.16	47.5863
228.21	47.7005
228.25	47.8128
228.29	47.9234
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228.54	48.5490
228.58	48.6471
228.63	48.7434
228.67	48.8379
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228.92	49.3689
228.96	49.4514
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229.13	49.7648
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229.26	49.9823
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229.39	50.1851
229.43	50.2494
229.47	50.3121

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229.60	50.4909
229.64	50.5475
229.69	50.6024
229.73	50.6556
229.77	50.7074
229.81	50.7576
229.86	50.8064
229.90	50.8536
229.94	50.8994
229.98	50.9436
230.03	50.9862
230.07	51.0275
230.11	51.0672
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230.20	51.1424
230.24	51.1778
230.28	51.2117
230.33	51.2441
230.37	51.2751
230.41	51.3048
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230.50	51.3599
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230.58	51.4094
230.63	51.4322
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230.71	51.4734
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230.84	51.5252
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231.14	51.6002
231.18	51.6057
231.23	51.6101
231.27	51.6132
231.31	51.6150
231.36	51.6156

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231.44	51.6132
231.49	51.6102
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231.57	51.6006
231.62	51.5940
231.66	51.5862
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231.75	51.5673
231.79	51.5561
231.83	51.5438
231.88	51.5303
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232.09	51.4463
232.14	51.4262
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232.66	51.1043
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232.75	51.0366
232.79	51.0014
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232.88	50.9280
232.92	50.8899
232.97	50.8509
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233.05	50.7702
233.10	50.7285
233.14	50.6859
233.18	50.6424
233.23	50.5982
233.27	50.5529

233.32	50.5068
233.36	50.4599
233.40	50.4122
233.45	50.3636
233.49	50.3141
233.54	50.2638
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233.62	50.1609
233.67	50.1083
233.71	50.0549
233.76	50.0006
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234.60	48.8318
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235.22	47.8212

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235.35	47.5904
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235.53	47.2754
235.58	47.1953
235.62	47.1149
235.67	47.0339
235.71	46.9524
235.76	46.8705
235.80	46.7880
235.85	46.7052
235.89	46.6220
235.94	46.5383
235.98	46.4541
236.03	46.3695
236.07	46.2845
236.12	46.1991
236.16	46.1133
236.21	46.0271
236.25	45.9404
236.30	45.8534
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236.39	45.6782
236.43	45.5900
236.48	45.5015
236.52	45.4125
236.57	45.3233
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236.66	45.1437
236.70	45.0534
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236.88	44.6888
236.93	44.5968
236.97	44.5047
237.02	44.4122
237.06	44.3193
237.11	44.2262
237.15	44.1327
237.20	44.0390

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237.29	43.8509
237.34	43.7562
237.38	43.6616
237.43	43.5665
237.47	43.4712
237.52	43.3757
237.56	43.2800
237.61	43.1840
237.65	43.0877
237.70	42.9912
237.75	42.8945
237.79	42.7976
237.84	42.7005
237.88	42.6032
237.93	42.5057
237.97	42.4079
238.02	42.3101
238.06	42.2120
238.11	42.1136
238.16	42.0152
238.20	41.9165
238.25	41.8176
238.29	41.7188
238.34	41.6196
238.39	41.5203
238.43	41.4209
238.48	41.3213
238.52	41.2215
238.57	41.1216
238.61	41.0216
238.66	40.9214
238.71	40.8210
238.75	40.7207
238.80	40.6202
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238.89	40.4187
238.94	40.3178
238.98	40.2168
239.03	40.1157
239.07	40.0146
239.12	39.9134
239.17	39.8120
239.21	39.7106

239.26	39.6090
239.31	39.5073
239.35	39.4056
239.40	39.3039
239.44	39.2021
239.49	39.1002
239.54	38.9982
239.58	38.8962
239.63	38.7942
239.68	38.6921
239.72	38.5899
239.77	38.4876
239.81	38.3855
239.86	38.2832
239.91	38.1807
239.95	38.0784
240.00	37.9760
240.05	37.8737
240.09	37.7712
240.14	37.6688
240.19	37.5662
240.23	37.4637
240.28	37.3613
240.33	37.2587
240.37	37.1562
240.42	37.0536
240.47	36.9512
240.51	36.8486
240.56	36.7461
240.61	36.6435
240.65	36.5411
240.70	36.4386
240.75	36.3362
240.79	36.2337
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240.93	35.9265
240.98	35.8241
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241.07	35.6195
241.12	35.5172
241.17	35.4150
241.21	35.3129
241.26	35.2107

241.31	35.1086
241.36	35.0066
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241.45	34.8026
241.50	34.7007
241.54	34.5989
241.59	34.4970
241.64	34.3953
241.68	34.2936
241.73	34.1919
241.78	34.0904
241.83	33.9890
241.87	33.8876
241.92	33.7862
241.97	33.6849
242.01	33.5837
242.06	33.4826
242.11	33.3815
242.16	33.2805
242.20	33.1796
242.25	33.0788
242.30	32.9780
242.35	32.8773
242.39	32.7768
242.44	32.6763
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242.54	32.4756
242.58	32.3754
242.63	32.2752
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243.20	31.0814
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243.34	30.7851

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244.16	29.1266
244.21	29.0301
244.26	28.9337
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244.45	28.5495
244.50	28.4538
244.54	28.3583
244.59	28.2627
244.64	28.1673
244.69	28.0722
244.74	27.9771
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244.98	27.5037
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245.08	27.3152
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245.22	27.0335
245.27	26.9399
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246.44	24.7341
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246.64	24.3743
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246.98	23.7500
247.03	23.6613
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247.13	23.4845
247.18	23.3963
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247.28	23.2203
247.33	23.1326
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247.42	22.9575
247.47	22.8701
247.52	22.7829
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248.42	21.2382
248.47	21.1538
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249.11	20.0699
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249.67	19.1726
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261.24	7.1232
261.29	7.1052
261.35	7.0878
261.40	7.0707

261.46	7.0541
261.51	7.0379
261.57	7.0220
261.63	7.0065
261.68	6.9915
261.74	6.9770
261.79	6.9627
261.85	6.9489
261.90	6.9356
261.96	6.9227
262.01	6.9101
262.07	6.8979
262.12	6.8862
262.18	6.8748
262.23	6.8639
262.29	6.8534
262.34	6.8433
262.40	6.8336
262.46	6.8243
262.51	6.8154
262.57	6.8070
262.62	6.7989
262.68	6.7913
262.73	6.7839
262.79	6.7772
262.85	6.7707
262.90	6.7646
262.96	6.7590
263.01	6.7538
263.07	6.7488
263.12	6.7445
263.18	6.7404
263.24	6.7368
263.29	6.7335
263.35	6.7307
263.40	6.7283
263.46	6.7262
263.52	6.7245
263.57	6.7232
263.63	6.7223
263.68	6.7218
263.74	6.7218
263.80	6.7221
263.85	6.7227

263.91	6.7238
263.96	6.7253
264.02	6.7271
264.08	6.7293
264.13	6.7320
264.19	6.7350
264.25	6.7383
264.30	6.7421
264.36	6.7463
264.41	6.7508
264.47	6.7556
264.53	6.7608
264.58	6.7665
264.64	6.7725
264.70	6.7788
264.75	6.7856
264.81	6.7926
264.87	6.8001
264.92	6.8079
264.98	6.8162
265.04	6.8246
265.09	6.8336
265.15	6.8429
265.21	6.8525
265.26	6.8624
265.32	6.8727
265.38	6.8834
265.43	6.8943
265.49	6.9057
265.55	6.9174
265.60	6.9294
265.66	6.9419
265.72	6.9545
265.78	6.9675
265.83	6.9810
265.89	6.9947
265.95	7.0088
266.00	7.0230
266.06	7.0377
266.12	7.0529
266.17	7.0682
266.23	7.0838
266.29	7.0998
266.35	7.1160

266.40	7.1327
266.46	7.1496
266.52	7.1667
266.58	7.1843
266.63	7.2021
266.69	7.2203
266.75	7.2387
266.80	7.2575
266.86	7.2764
266.92	7.2957
266.98	7.3154
267.03	7.3352
267.09	7.3554
267.15	7.3758
267.21	7.3965
267.26	7.4175
267.32	7.4388
267.38	7.4603
267.44	7.4822
267.50	7.5042
267.55	7.5266
267.61	7.5491
267.67	7.5720
267.73	7.5951
267.78	7.6185
267.84	7.6421
267.90	7.6659
267.96	7.6901
268.02	7.7144
268.07	7.7390
268.13	7.7637
268.19	7.7888
268.25	7.8141
268.31	7.8396
268.36	7.8654
268.42	7.8914
268.48	7.9175
268.54	7.9439
268.60	7.9704
268.65	7.9973
268.71	8.0243
268.77	8.0516
268.83	8.0789
268.89	8.1066

268.95	8.1344
269.00	8.1624
269.06	8.1906
269.12	8.2190
269.18	8.2475
269.24	8.2763
269.30	8.3052
269.36	8.3343
269.41	8.3636
269.47	8.3930
269.53	8.4225
269.59	8.4524
269.65	8.4822
269.71	8.5124
269.77	8.5425
269.82	8.5730
269.88	8.6034
269.94	8.6342
270.00	8.6649
270.06	8.6958
270.12	8.7269
270.18	8.7581
270.24	8.7894
270.29	8.8209
270.35	8.8524
270.41	8.8842
270.47	8.9160
270.53	8.9480
270.59	8.9799
270.65	9.0120
270.71	9.0443
270.77	9.0767
270.83	9.1091
270.89	9.1416
270.94	9.1742
271.00	9.2069
271.06	9.2396
271.12	9.2724
271.18	9.3054
271.24	9.3384
271.30	9.3714
271.36	9.4046
271.42	9.4379
271.48	9.4712

271.54	9.5045
271.60	9.5378
271.66	9.5712
271.72	9.6047
271.78	9.6383
271.84	9.6717
271.90	9.7053
271.95	9.7389
272.01	9.7727
272.07	9.8063
272.13	9.8400
272.19	9.8738
272.25	9.9075
272.31	9.9413
272.37	9.9750
272.43	10.0089
272.49	10.0427
272.55	10.0764
272.61	10.1103
272.67	10.1441
272.73	10.1778
272.79	10.2116
272.85	10.2455
272.91	10.2792
272.97	10.3130
273.03	10.3466
273.09	10.3803
273.15	10.4139
273.21	10.4477
273.27	10.4813
273.33	10.5147
273.39	10.5483
273.45	10.5818
273.51	10.6152
273.57	10.6485
273.64	10.6820
273.70	10.7151
273.76	10.7484
273.82	10.7816
273.88	10.8147
273.94	10.8477
274.00	10.8807
274.06	10.9136
274.12	10.9464

274.18	10.9791
274.24	11.0118
274.30	11.0444
274.36	11.0768
274.42	11.1092
274.48	11.1416
274.54	11.1737
274.61	11.2058
274.67	11.2379
274.73	11.2697
274.79	11.3015
274.85	11.3333
274.91	11.3648
274.97	11.3963
275.03	11.4276
275.09	11.4588
275.15	11.4900
275.21	11.5209
275.28	11.5518
275.34	11.5826
275.40	11.6132
275.46	11.6436
275.52	11.6739
275.58	11.7041
275.64	11.7342
275.70	11.7641
275.77	11.7938
275.83	11.8235
275.89	11.8529
275.95	11.8821
276.01	11.9114
276.07	11.9403
276.13	11.9691
276.20	11.9978
276.26	12.0263
276.32	12.0546
276.38	12.0828
276.44	12.1107
276.50	12.1385
276.57	12.1662
276.63	12.1937
276.69	12.2208
276.75	12.2480
276.81	12.2748

276.87	12.3015
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277.00	12.3545
277.06	12.3806
277.12	12.4065
277.18	12.4322
277.25	12.4578
277.31	12.4830
277.37	12.5082
277.43	12.5331
277.49	12.5579
277.56	12.5823
277.62	12.6066
277.68	12.6308
277.74	12.6546
277.80	12.6783
277.87	12.7017
277.93	12.7250
277.99	12.7479
278.05	12.7707
278.12	12.7932
278.18	12.8156
278.24	12.8376
278.30	12.8595
278.37	12.8811
278.43	12.9024
278.49	12.9236
278.55	12.9446
278.62	12.9653
278.68	12.9857
278.74	13.0058
278.80	13.0257
278.87	13.0455
278.93	13.0650
278.99	13.0842
279.06	13.1031
279.12	13.1219
279.18	13.1403
279.24	13.1586
279.31	13.1765
279.37	13.1942
279.43	13.2117
279.50	13.2288
279.56	13.2458

279.62	13.2624
279.68	13.2789
279.75	13.2951
279.81	13.3110
279.87	13.3266
279.94	13.3419
280.00	13.3571
280.06	13.3719
280.13	13.3865
280.19	13.4007
280.25	13.4148
280.32	13.4285
280.38	13.4420
280.44	13.4552
280.51	13.4682
280.57	13.4808
280.63	13.4933
280.70	13.5054
280.76	13.5173
280.82	13.5288
280.89	13.5401
280.95	13.5510
281.02	13.5618
281.08	13.5723
281.14	13.5825
281.21	13.5924
281.27	13.6020
281.33	13.6113
281.40	13.6203
281.46	13.6292
281.53	13.6376
281.59	13.6458
281.65	13.6538
281.72	13.6614
281.78	13.6688
281.85	13.6758
281.91	13.6826
281.97	13.6890
282.04	13.6953
282.10	13.7012
282.17	13.7069
282.23	13.7123
282.30	13.7174
282.36	13.7220

282.42	13.7265
282.49	13.7309
282.55	13.7348
282.62	13.7384
282.68	13.7417
282.75	13.7448
282.81	13.7475
282.88	13.7501
282.94	13.7522
283.00	13.7541
283.07	13.7558
283.13	13.7571
283.20	13.7582
283.26	13.7589
283.33	13.7594
283.39	13.7597
283.46	13.7595
283.52	13.7592
283.59	13.7585
283.65	13.7576
283.72	13.7564
283.78	13.7549
283.85	13.7529
283.91	13.7510
283.98	13.7486
284.04	13.7459
284.11	13.7429
284.17	13.7397
284.24	13.7363
284.30	13.7324
284.37	13.7283
284.43	13.7240
284.50	13.7193
284.56	13.7145
284.63	13.7093
284.69	13.7039
284.76	13.6980
284.82	13.6920
284.89	13.6857
284.96	13.6791
285.02	13.6724
285.09	13.6652
285.15	13.6578
285.22	13.6502

285.28	13.6422
285.35	13.6340
285.41	13.6254
285.48	13.6167
285.55	13.6076
285.61	13.5983
285.68	13.5887
285.74	13.5789
285.81	13.5687
285.88	13.5584
285.94	13.5477
286.01	13.5368
286.07	13.5257
286.14	13.5143
286.21	13.5026
286.27	13.4906
286.34	13.4783
286.40	13.4658
286.47	13.4531
286.54	13.4402
286.60	13.4268
286.67	13.4133
286.73	13.3995
286.80	13.3856
286.87	13.3713
286.93	13.3568
287.00	13.3421
287.07	13.3269
287.13	13.3118
287.20	13.2962
287.27	13.2804
287.33	13.2644
287.40	13.2482
287.47	13.2317
287.53	13.2150
287.60	13.1979
287.67	13.1808
287.73	13.1633
287.80	13.1456
287.87	13.1277
287.93	13.1096
288.00	13.0911
288.07	13.0725
288.13	13.0538

288.20	13.0346
288.27	13.0154
288.34	12.9957
288.40	12.9761
288.47	12.9561
288.54	12.9359
288.60	12.9155
288.67	12.8948
288.74	12.8739
288.81	12.8528
288.87	12.8315
288.94	12.8100
289.01	12.7883
289.07	12.7664
289.14	12.7442
289.21	12.7218
289.28	12.6993
289.34	12.6765
289.41	12.6536
289.48	12.6303
289.55	12.6071
289.61	12.5834
289.68	12.5597
289.75	12.5357
289.82	12.5115
289.89	12.4871
289.95	12.4626
290.02	12.4379
290.09	12.4130
290.16	12.3878
290.23	12.3624
290.29	12.3369
290.36	12.3113
290.43	12.2855
290.50	12.2594
290.57	12.2331
290.63	12.2067
290.70	12.1802
290.77	12.1535
290.84	12.1265
290.91	12.0995
290.97	12.0722
291.04	12.0447
291.11	12.0171

291.18	11.9894
291.25	11.9615
291.32	11.9333
291.38	11.9051
291.45	11.8767
291.52	11.8481
291.59	11.8194
291.66	11.7905
291.73	11.7615
291.80	11.7323
291.86	11.7030
291.93	11.6735
292.00	11.6439
292.07	11.6141
292.14	11.5842
292.21	11.5542
292.28	11.5239
292.35	11.4936
292.42	11.4632
292.48	11.4326
292.55	11.4018
292.62	11.3711
292.69	11.3400
292.76	11.3090
292.83	11.2776
292.90	11.2463
292.97	11.2148
293.04	11.1831
293.11	11.1515
293.18	11.1197
293.25	11.0876
293.31	11.0556
293.38	11.0234
293.45	10.9911
293.52	10.9586
293.59	10.9262
293.66	10.8935
293.73	10.8608
293.80	10.8279
293.87	10.7949
293.94	10.7619
294.01	10.7288
294.08	10.6956
294.15	10.6622

294.22	10.6287
294.29	10.5953
294.36	10.5617
294.43	10.5279
294.50	10.4942
294.57	10.4603
294.64	10.4264
294.71	10.3923
294.78	10.3583
294.85	10.3241
294.92	10.2897
294.99	10.2554
295.06	10.2210
295.13	10.1865
295.20	10.1519
295.27	10.1172
295.34	10.0826
295.41	10.0478
295.48	10.0130
295.55	9.9780
295.62	9.9431
295.69	9.9081
295.76	9.8730
295.83	9.8379
295.90	9.8027
295.98	9.7674
296.05	9.7322
296.12	9.6968
296.19	9.6614
296.26	9.6260
296.33	9.5904
296.40	9.5549
296.47	9.5193
296.54	9.4838
296.61	9.4481
296.68	9.4124
296.75	9.3767
296.83	9.3408
296.90	9.3051
296.97	9.2693
297.04	9.2334
297.11	9.1974
297.18	9.1616
297.25	9.1256

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297.47	9.0176
297.54	8.9816
297.61	8.9454
297.68	8.9094
297.75	8.8733
297.82	8.8371
297.90	8.8011
297.97	8.7650
298.04	8.7288
298.11	8.6925
298.18	8.6564
298.25	8.6202
298.33	8.5841
298.40	8.5479
298.47	8.5118
298.54	8.4755
298.61	8.4393
298.69	8.4032
298.76	8.3670
298.83	8.3307
298.90	8.2946
298.97	8.2584
299.05	8.2223
299.12	8.1861
299.19	8.1500
299.26	8.1138
299.33	8.0777
299.41	8.0417
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299.70	7.8974
299.77	7.8614
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299.99	7.7535
300.06	7.7175
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300.28	7.6100
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300.42	7.5384

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300.57	7.4670
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300.79	7.3601
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300.93	7.2890
301.01	7.2536
301.08	7.2182
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301.22	7.1474
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301.37	7.0769
301.44	7.0416
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301.59	6.9714
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302.03	6.7617
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302.25	6.6578
302.33	6.6231
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303.21	6.2133
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303.36	6.1460
303.44	6.1124
303.51	6.0789
303.59	6.0455
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303.73	5.9787
303.81	5.9456
303.88	5.9124
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304.03	5.8464
304.11	5.8136
304.18	5.7807
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304.33	5.7153
304.41	5.6828
304.48	5.6504
304.55	5.6180
304.63	5.5856
304.70	5.5535
304.78	5.5212
304.85	5.4893
304.93	5.4572
305.00	5.4254
305.08	5.3936
305.15	5.3619
305.23	5.3303
305.30	5.2988
305.38	5.2673
305.45	5.2359
305.53	5.2047
305.61	5.1735
305.68	5.1425
305.76	5.1114
305.83	5.0807
305.91	5.0498
305.98	5.0192
306.06	4.9886
306.13	4.9580
306.21	4.9277
306.28	4.8974
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306.59	4.7771
306.66	4.7472
306.74	4.7175
306.82	4.6880
306.89	4.6584
306.97	4.6290

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307.12	4.5705
307.20	4.5414
307.27	4.5125
307.35	4.4835
307.42	4.4547
307.50	4.4261
307.58	4.3974
307.65	4.3691
307.73	4.3406
307.81	4.3124
307.88	4.2842
307.96	4.2561
308.04	4.2282
308.11	4.2003
308.19	4.1726
308.26	4.1450
308.34	4.1175
308.42	4.0901
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308.73	3.9815
308.80	3.9546
308.88	3.9278
308.96	3.9012
309.03	3.8747
309.11	3.8483
309.19	3.8219
309.26	3.7956
309.34	3.7695
309.42	3.7436
309.50	3.7176
309.57	3.6920
309.65	3.6663
309.73	3.6407
309.81	3.6153
309.88	3.5900
309.96	3.5648
310.04	3.5397
310.12	3.5147
310.19	3.4898
310.27	3.4650
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310.58	3.3671
310.66	3.3429
310.74	3.3188
310.82	3.2948
310.89	3.2709
310.97	3.2472
311.05	3.2235
311.13	3.2001
311.21	3.1767
311.28	3.1533
311.36	3.1302
311.44	3.1071
311.52	3.0842
311.60	3.0614
311.67	3.0386
311.75	3.0159
311.83	2.9934
311.91	2.9711
311.99	2.9487
312.07	2.9267
312.15	2.9046
312.22	2.8826
312.30	2.8608
312.38	2.8391
312.46	2.8175
312.54	2.7960
312.62	2.7746
312.70	2.7533
312.78	2.7321
312.85	2.7111
312.93	2.6901
313.01	2.6694
313.09	2.6487
313.17	2.6280
313.25	2.6076
313.33	2.5872
313.41	2.5670
313.49	2.5469
313.57	2.5268
313.65	2.5068
313.73	2.4870
313.80	2.4674

313.88	2.4477
313.96	2.4282
314.04	2.4089
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314.28	2.3514
314.36	2.3325
314.44	2.3136
314.52	2.2949
314.60	2.2763
314.68	2.2578
314.76	2.2394
314.84	2.2212
314.92	2.2029
315.00	2.1849
315.08	2.1669
315.16	2.1491
315.24	2.1314
315.32	2.1137
315.40	2.0961
315.48	2.0787
315.56	2.0615
315.64	2.0442
315.72	2.0271
315.80	2.0102
315.88	1.9932
315.96	1.9764
316.04	1.9598
316.12	1.9431
316.21	1.9268
316.29	1.9103
316.37	1.8941
316.45	1.8779
316.53	1.8618
316.61	1.8459
316.69	1.8300
316.77	1.8143
316.85	1.7985
316.93	1.7831
317.01	1.7676
317.10	1.7522
317.18	1.7370
317.26	1.7219
317.34	1.7067

317.42	1.6919
317.50	1.6770
317.58	1.6622
317.66	1.6476
317.75	1.6331
317.83	1.6185
317.91	1.6041
317.99	1.5899
318.07	1.5758
318.15	1.5617
318.23	1.5477
318.32	1.5338
318.40	1.5201
318.48	1.5063
318.56	1.4928
318.64	1.4793
318.73	1.4658
318.81	1.4526
318.89	1.4394
318.97	1.4262
319.05	1.4132
319.14	1.4003
319.22	1.3874
319.30	1.3746
319.38	1.3620
319.46	1.3494
319.55	1.3370
319.63	1.3245
319.71	1.3122
319.79	1.3001
319.88	1.2879
319.96	1.2759
320.04	1.2639
320.12	1.2521
320.21	1.2404
320.29	1.2287
320.37	1.2171
320.46	1.2056
320.54	1.1942
320.62	1.1828
320.70	1.1715
320.79	1.1604
320.87	1.1493
320.95	1.1382

321.04	1.1274
321.12	1.1165
321.20	1.1058
321.29	1.0952
321.37	1.0845
321.45	1.0740
321.54	1.0637
321.62	1.0533
321.70	1.0430
321.79	1.0328
321.87	1.0227
321.95	1.0127
322.04	1.0028
322.12	0.9929
322.20	0.9831
322.29	0.9734
322.37	0.9638
322.46	0.9542
322.54	0.9447
322.62	0.9354
322.71	0.9260
322.79	0.9168
322.88	0.9077
322.96	0.8985
323.04	0.8895
323.13	0.8805
323.21	0.8717
323.30	0.8628
323.38	0.8541
323.47	0.8454
323.55	0.8369
323.63	0.8283
323.72	0.8199
323.80	0.8115
323.89	0.8033
323.97	0.7950
324.06	0.7868
324.14	0.7787
324.23	0.7707
324.31	0.7628
324.40	0.7548
324.48	0.7470
324.57	0.7392
324.65	0.7316

324.74	0.7239
324.82	0.7164
324.91	0.7089
324.99	0.7014
325.08	0.6941
325.16	0.6867
325.25	0.6795
325.33	0.6723
325.42	0.6653
325.50	0.6582
325.59	0.6512
325.67	0.6443
325.76	0.6374
325.85	0.6306
325.93	0.6239
326.02	0.6171
326.10	0.6105
326.19	0.6039
326.27	0.5975
326.36	0.5910
326.45	0.5846
326.53	0.5783
326.62	0.5720
326.70	0.5658
326.79	0.5597
326.88	0.5535
326.96	0.5475
327.05	0.5415
327.13	0.5355
327.22	0.5297
327.31	0.5238
327.39	0.5181
327.48	0.5123
327.57	0.5067
327.65	0.5010
327.74	0.4955
327.83	0.4899
327.91	0.4845
328.00	0.4791
328.09	0.4737
328.17	0.4685
328.26	0.4632
328.35	0.4580
328.43	0.4529

328.52	0.4478
328.61	0.4427
328.70	0.4377
328.78	0.4328
328.87	0.4278
328.96	0.4229
329.05	0.4181
329.13	0.4133
329.22	0.4086
329.31	0.4040
329.39	0.3993
329.48	0.3947
329.57	0.3902
329.66	0.3857
329.75	0.3812
329.83	0.3768
329.92	0.3725
330.01	0.3681
330.10	0.3638
330.18	0.3596
330.27	0.3554
330.36	0.3512
330.45	0.3471
330.54	0.3431
330.62	0.3390
330.71	0.3350
330.80	0.3311
330.89	0.3272
330.98	0.3233
331.07	0.3195
331.15	0.3158
331.24	0.3120
331.33	0.3083
331.42	0.3045
331.51	0.3009
331.60	0.2973
331.69	0.2937
331.77	0.2903
331.86	0.2868
331.95	0.2834
332.04	0.2799
332.13	0.2765
332.22	0.2732
332.31	0.2699

332.40	0.2666
332.49	0.2633
332.58	0.2601
332.66	0.2570
332.75	0.2538
332.84	0.2507
332.93	0.2477
333.02	0.2447
333.11	0.2417
333.20	0.2387
333.29	0.2357
333.38	0.2328
333.47	0.2298
333.56	0.2270
333.65	0.2243
333.74	0.2214
333.83	0.2187
333.92	0.2160
334.01	0.2133
334.10	0.2106
334.19	0.2079
334.28	0.2054
334.37	0.2028
334.46	0.2003
334.55	0.1977
334.64	0.1952
334.73	0.1928
334.82	0.1902
334.91	0.1878
335.00	0.1854
335.09	0.1832
335.18	0.1808
335.27	0.1785
335.36	0.1761
335.45	0.1739
335.55	0.1718
335.64	0.1695
335.73	0.1673
335.82	0.1652
335.91	0.1631
336.00	0.1610
336.09	0.1589
336.18	0.1568
336.27	0.1548

336.37	0.1527
336.46	0.1508
336.55	0.1488
336.64	0.1469
336.73	0.1449
336.82	0.1430
336.91	0.1412
337.01	0.1392
337.10	0.1374
337.19	0.1356
337.28	0.1338
337.37	0.1320
337.46	0.1304
337.56	0.1286
337.65	0.1269
337.74	0.1253
337.83	0.1235
337.92	0.1218
338.02	0.1203
338.11	0.1187
338.20	0.1170
338.29	0.1155
338.38	0.1139
338.48	0.1124
338.57	0.1109
338.66	0.1094
338.75	0.1079
338.85	0.1065
338.94	0.1050
339.03	0.1035
339.13	0.1022
339.22	0.1008
339.31	0.0995
339.40	0.0981
339.50	0.0968
339.59	0.0954
339.68	0.0941
339.78	0.0927
339.87	0.0915
339.96	0.0903
340.06	0.0890
340.15	0.0878
340.24	0.0866
340.34	0.0854

340.43	0.0842
340.52	0.0830
340.62	0.0819
340.71	0.0807
340.80	0.0795
340.90	0.0785
340.99	0.0774
341.08	0.0762
341.18	0.0752
341.27	0.0741
341.37	0.0731
341.46	0.0720
341.55	0.0711
341.65	0.0701
341.74	0.0690
341.84	0.0681
341.93	0.0671
342.03	0.0662
342.12	0.0653
342.21	0.0644
342.31	0.0633
342.40	0.0624
342.50	0.0615
342.59	0.0608
342.69	0.0599
342.78	0.0590
342.88	0.0581
342.97	0.0573
343.07	0.0564
343.16	0.0557
343.26	0.0548
343.35	0.0540
343.45	0.0533
343.54	0.0525
343.64	0.0518
343.73	0.0510
343.83	0.0503
343.92	0.0495
344.02	0.0488
344.11	0.0480
344.21	0.0473
344.30	0.0467
344.40	0.0459
344.50	0.0453

344.59	0.0446
344.69	0.0440
344.78	0.0434
344.88	0.0426
344.98	0.0420
345.07	0.0414
345.17	0.0408
345.26	0.0402
345.36	0.0396
345.46	0.0390
345.55	0.0384
345.65	0.0378
345.75	0.0372
345.84	0.0368
345.94	0.0362
346.03	0.0356
346.13	0.0351
346.23	0.0345
346.32	0.0341
346.42	0.0335
346.52	0.0330
346.61	0.0324
346.71	0.0320
346.81	0.0315
346.91	0.0311
347.00	0.0306
347.10	0.0300
347.20	0.0296
347.29	0.0291
347.39	0.0287
347.49	0.0282
347.59	0.0279
347.68	0.0275
347.78	0.0270
347.88	0.0266
347.98	0.0261
348.07	0.0258
348.17	0.0254
348.27	0.0249
348.37	0.0246
348.47	0.0242
348.56	0.0239
348.66	0.0234
348.76	0.0231

348.86	0.0227
348.96	0.0224
349.05	0.0221
349.15	0.0216
349.25	0.0213
349.35	0.0210
349.45	0.0207
349.55	0.0203
349.65	0.0200
349.74	0.0197
349.84	0.0194
349.94	0.0191

Table 2. Energy and Percentage of each selected conformers for (*R*, *S, R*)-**2k** under method 1-4

conformer	Energy (a.u.)	Percentage(%)	OR	Net. OR
1-RSR_0009.log	-2460.740058	17.2	35.5	6.12
1-RSR_0010.log	-2460.739892	14.4	-35.83	-5.18
1-RSR_0011.log	-2460.739828	13.5	-20.57	-2.78
1-RSR_0012.log	-2460.739762	12.6	-103.55	-13.05
1-RSR_0007.log	-2460.739183	6.8	-256.99	-17.53
1-RSR_0008.log	-2460.739074	6.1	-197.67	-12.01
1-RSR_0002.log	-2460.738904	5.1	42.09	2.14
1-RSR_0003.log	-2460.738818	4.6	-22.92	-1.06
1-RSR_0005.log	-2460.738807	4.6	-82.33	-3.77
1-RSR_0006.log	-2460.738745	4.3	-47.14	-2.02
1-RSR_0001.log	-2460.738714	4.1	56.49	2.34
1-RSR_0004.log	-2460.738612	3.7	-8.33	-0.31
1-RSR_0016.log	-2460.737796	1.6	321.56	5.04
1-RSR_0015.log	-2460.737575	1.2	277.79	3.44
OR(Total)= -38.64				

Table 3. Coordination of the five minimum energy conformers for (*R,S,R*)-**2k** (>5% distribution)

Conformer 009

C	4.62088	2.80775	-1.30905
C	3.56559	1.90833	-1.40466
C	2.3593	2.26209	-0.79596
C	2.18846	3.49486	-0.10229
C	3.28017	4.37327	-0.01256
C	4.48123	4.02472	-0.61619
H	5.57179	2.5628	-1.77093
H	3.67939	0.96269	-1.92292
H	3.18947	5.3166	0.51769
H	5.32866	4.70003	-0.5539
C	0.82513	3.54925	0.38125

C	0.19522	4.69771	1.11913
H	-0.70759	4.3599	1.63813
H	0.87489	5.04561	1.90712
C	-0.16644	5.88832	0.21332
H	0.71246	6.2699	-0.31216
H	-0.89903	5.59702	-0.54472
H	-0.59287	6.71068	0.79603
C	0.24457	2.36912	-0.01616
N	1.1593	1.58505	-0.69653
C	-1.09526	1.68859	0.02547
H	-1.84377	2.33723	-0.44437
C	0.56466	0.4845	-1.45446
H	0.50727	0.77107	-2.5109
C	-0.88944	0.41063	-0.85691
H	-0.93143	-0.4691	-0.21209
C	-1.6349	1.38786	1.45659
H	-2.65191	0.99922	1.35459
H	-1.72631	2.33956	1.98896
C	-0.81825	0.42162	2.28779
C	0.42	0.78746	2.83492
C	-1.28468	-0.87414	2.53784
C	1.17289	-0.10987	3.59046
H	0.80761	1.7866	2.67055
C	-0.54812	-1.78444	3.29447
H	-2.24651	-1.18251	2.13921
C	0.68145	-1.39365	3.8116
H	2.12664	0.18835	4.00998
H	-0.92495	-2.78347	3.47883
C	-1.93658	0.23536	-1.97402
H	-1.93828	1.12913	-2.6079
H	-1.6181	-0.59487	-2.61409
C	-3.3376	-0.03857	-1.47315
C	-4.32511	0.95074	-1.48238
C	-3.67963	-1.30224	-0.97516
C	-5.6102	0.70154	-1.00128
H	-4.09766	1.93539	-1.88018
C	-4.95694	-1.5716	-0.49186
H	-2.93897	-2.09711	-0.97209
C	-5.91423	-0.56061	-0.50535
H	-5.21067	-2.55602	-0.11645
C	1.34083	-0.79356	-1.36353
C	1.7634	-1.65409	-2.35405
N	1.71441	-1.29385	-0.12384
H	1.6184	-0.79315	0.74689

C	1.57001	-1.53092	-3.83955
H	1.30708	-0.5011	-4.1026
H	2.52745	-1.72362	-4.33886
C	2.44947	-2.73643	-1.68823
C	2.40848	-2.47116	-0.29462
C	3.11274	-3.88995	-2.13912
H	3.1666	-4.12136	-3.19851
C	3.00442	-3.31753	0.64418
H	2.96242	-3.10302	1.70732
C	3.65188	-4.44927	0.16728
H	4.1241	-5.12749	0.87063
C	3.70738	-4.73296	-1.21125
H	4.22413	-5.62543	-1.54924
C	0.51052	-2.48453	-4.41862
H	-0.4785	-2.28082	-3.99832
H	0.44073	-2.37963	-5.50554
H	0.74793	-3.52796	-4.19767
Cl	1.62589	-2.53137	4.76547
Cl	-7.53105	-0.88924	0.10416
H	-6.36641	1.47752	-1.01715

Conformer 010

C	4.74249	2.68461	-0.85496
C	3.66747	1.82996	-1.06907
C	2.43022	2.20336	-0.53961
C	2.24847	3.41337	0.19043
C	3.35939	4.24592	0.4008
C	4.59128	3.87712	-0.12347
H	5.71731	2.42294	-1.25349
H	3.78973	0.90256	-1.61718
H	3.26059	5.16956	0.96319
H	5.45394	4.51713	0.03207
C	0.85517	3.49756	0.57452
C	0.20933	4.63637	1.31342
H	-0.74888	4.31409	1.73324
H	0.82934	4.91535	2.17478
C	-0.02281	5.88401	0.44289
H	0.91371	6.25313	0.01773
H	-0.6944	5.66174	-0.39125
H	-0.46837	6.69433	1.02807
C	0.26818	2.35447	0.08932
N	1.20517	1.56419	-0.55429
C	-1.09199	1.71862	0.01051
H	-1.78395	2.40563	-0.49066

C	0.62739	0.52206	-1.40213
H	0.64179	0.86215	-2.44412
C	-0.85968	0.46134	-0.89346
H	-0.95139	-0.43254	-0.27365
C	-1.74306	1.38772	1.38825
H	-2.76056	1.03516	1.1989
H	-1.84485	2.32239	1.94832
C	-1.01553	0.36669	2.23674
C	0.19397	0.67111	2.87715
C	-1.53672	-0.92108	2.40672
C	0.8682	-0.27748	3.64418
H	0.62165	1.66232	2.77669
C	-0.87966	-1.88227	3.17363
H	-2.47902	-1.18356	1.93519
C	0.32494	-1.55183	3.78308
H	1.80065	-0.02575	4.13596
H	-1.29818	-2.8744	3.29459
C	-1.84241	0.32503	-2.07258
H	-1.80037	1.23387	-2.68327
H	-1.49527	-0.49388	-2.71279
C	-3.27209	0.05308	-1.65881
C	-3.65627	-1.22264	-1.22643
C	-4.24527	1.05625	-1.68435
C	-4.96088	-1.49034	-0.82135
H	-2.92691	-2.02781	-1.21288
C	-5.55723	0.80882	-1.28111
H	-3.98434	2.05113	-2.03313
C	-5.90313	-0.46564	-0.8481
H	-6.30163	1.59581	-1.3084
C	1.3493	-0.78869	-1.32977
C	1.73167	-1.6521	-2.33356
N	1.65799	-1.34436	-0.09628
H	1.55704	-0.86767	0.78718
C	1.60181	-1.46657	-3.82063
H	1.17771	-2.3777	-4.26026
H	0.88024	-0.67428	-4.04376
C	2.31764	-2.79999	-1.68195
C	2.26391	-2.567	-0.28274
C	2.87153	-4.00458	-2.1468
H	2.92058	-4.21906	-3.21003
C	2.75525	-3.48724	0.64696
H	2.70527	-3.29562	1.71414
C	3.30247	-4.66488	0.15585
H	3.69085	-5.40143	0.85178

C	3.3578	-4.92328	-1.22769
H	3.78819	-5.85647	-1.57658
C	2.93097	-1.14377	-4.52521
H	3.68027	-1.91699	-4.33937
H	2.79123	-1.0658	-5.60765
H	3.34416	-0.1952	-4.17157
Cl	1.17078	-2.75479	4.74941
Cl	-7.55395	-0.79195	-0.33623
H	-5.24673	-2.48376	-0.49605

Conformer 011

C	4.66973	2.59243	-1.68712
C	3.61788	1.68492	-1.63756
C	2.40592	2.12991	-1.10545
C	2.22637	3.46032	-0.62747
C	3.31284	4.34784	-0.68415
C	4.51939	3.90867	-1.21353
H	5.62502	2.27768	-2.09448
H	3.73754	0.6671	-1.99176
H	3.21423	5.36796	-0.32539
H	5.36262	4.59023	-1.26366
C	0.85347	3.59373	-0.18645
C	0.20689	4.84188	0.3471
H	0.46733	5.68296	-0.30736
H	-0.88286	4.74788	0.28039
C	0.59427	5.20537	1.79138
H	0.26935	4.4378	2.49954
H	1.67657	5.31321	1.89946
H	0.13335	6.15061	2.09362
C	0.27894	2.36413	-0.39505
N	1.20305	1.47528	-0.91597
C	-1.06998	1.71259	-0.28785
H	-1.79748	2.29825	-0.8624
C	0.60421	0.29311	-1.53945
H	0.57407	0.44316	-2.625
C	-0.86324	0.31915	-0.97168
H	-0.93151	-0.45868	-0.20861
C	-1.64211	1.63197	1.15999
H	-2.67663	1.28436	1.09267
H	-1.68816	2.65063	1.55785
C	-0.88846	0.74335	2.12761
C	0.38361	1.08647	2.60857
C	-1.45171	-0.45687	2.57619
C	1.07366	0.25834	3.49238

H	0.84862	2.01289	2.2918
C	-0.77857	-1.29682	3.46258
H	-2.4402	-0.74533	2.23151
C	0.48549	-0.93221	3.9108
H	2.05393	0.54046	3.8588
H	-1.23113	-2.22198	3.79931
C	-1.88909	-0.00376	-2.07544
H	-1.85543	0.78349	-2.83667
H	-1.57676	-0.92824	-2.57357
C	-3.30688	-0.16627	-1.57291
C	-4.27223	0.82377	-1.77806
C	-3.68821	-1.319	-0.87447
C	-5.57291	0.68489	-1.29427
H	-4.01394	1.7209	-2.33299
C	-4.98177	-1.47773	-0.38535
H	-2.9664	-2.11511	-0.715
C	-5.91575	-0.46691	-0.59641
H	-5.26565	-2.37794	0.14707
C	1.35458	-0.97499	-1.27143
C	1.80709	-1.94475	-2.14067
N	1.66877	-1.33712	0.03127
H	1.53788	-0.74387	0.83707
C	1.67776	-1.98778	-3.63763
H	1.45006	-0.9902	-4.02718
H	2.65031	-2.25346	-4.0697
C	2.44777	-2.95276	-1.32931
C	2.35162	-2.53296	0.02301
C	3.10856	-4.15809	-1.61976
H	3.20136	-4.50733	-2.64361
C	2.89234	-3.27666	1.07535
H	2.80876	-2.94479	2.10537
C	3.53949	-4.46274	0.75598
H	3.96948	-5.06421	1.55034
C	3.64806	-4.89973	-0.57868
H	4.16242	-5.83123	-0.79204
C	0.62134	-2.98187	-4.15033
H	-0.37896	-2.71339	-3.79874
H	0.59836	-3.00021	-5.24414
H	0.82599	-3.99739	-3.80266
Cl	1.35119	-1.98226	5.02582
Cl	-7.55214	-0.65593	0.02023
H	-6.3109	1.46032	-1.46253

Conformer 012

C	4.76115	2.59643	-1.21083

C	3.69977	1.70067	-1.2719
C	2.45811	2.13717	-0.80579
C	2.25928	3.44703	-0.28159
C	3.35511	4.32288	-0.22589
C	4.59075	3.89287	-0.69216
H	5.73897	2.28766	-1.56589
H	3.8347	0.69713	-1.6593
H	3.24193	5.328	0.16883
H	5.44125	4.56624	-0.65616
C	0.86022	3.57829	0.06994
C	0.1917	4.80946	0.61561
H	0.50364	5.67575	0.0191
H	-0.89195	4.73247	0.47272
C	0.48539	5.10189	2.09754
H	0.10866	4.30581	2.74587
H	1.55886	5.19297	2.2817
H	0.01263	6.03701	2.41267
C	0.28913	2.3677	-0.23436
N	1.23864	1.48881	-0.72858
C	-1.07293	1.73363	-0.25771
H	-1.74846	2.35834	-0.85436
C	0.66609	0.36222	-1.46856
H	0.7069	0.58819	-2.54052
C	-0.83228	0.37228	-0.99191
H	-0.94748	-0.43724	-0.26872
C	-1.75126	1.59062	1.13878
H	-2.78338	1.26701	0.9784
H	-1.81012	2.58838	1.58493
C	-1.08449	0.63786	2.10955
C	0.15631	0.92751	2.69495
C	-1.69874	-0.57256	2.45071
C	0.76828	0.03855	3.57707
H	0.65753	1.85962	2.46126
C	-1.10372	-1.4736	3.33287
H	-2.66478	-0.82108	2.02168
C	0.13193	-1.16058	3.88657
H	1.72486	0.2799	4.02604
H	-1.59401	-2.40637	3.58526
C	-1.78677	0.09845	-2.17025
H	-1.70975	0.91855	-2.8928
H	-1.43952	-0.80318	-2.68741
C	-3.23247	-0.08952	-1.766
C	-4.1848	0.91327	-1.97027
C	-3.65413	-1.28155	-1.1635

C	-5.51263	0.74794	-1.57701
H	-3.89409	1.84158	-2.45322
C	-4.97509	-1.46691	-0.7654
H	-2.94167	-2.08696	-1.00889
C	-5.89587	-0.44323	-0.97228
H	-5.28977	-2.39717	-0.30713
C	1.37421	-0.93802	-1.24294
C	1.79518	-1.89044	-2.14594
N	1.63615	-1.37445	0.04821
H	1.49291	-0.82141	0.87992
C	1.72098	-1.84794	-3.6478
H	1.33217	-2.80611	-4.0137
H	0.99333	-1.09726	-3.97193
C	2.35714	-2.96902	-1.36766
C	2.24902	-2.6067	0.00049
C	2.93097	-4.20835	-1.69719
H	3.02167	-4.51951	-2.73343
C	2.70466	-3.43462	1.02992
H	2.61312	-3.14535	2.07208
C	3.27264	-4.64979	0.67168
H	3.63491	-5.31652	1.4475
C	3.38256	-5.03524	-0.67869
H	3.82785	-5.99449	-0.92233
C	3.07013	-1.56306	-4.3306
H	3.82697	-2.29678	-4.04278
H	2.97123	-1.5936	-5.41992
H	3.44979	-0.57501	-4.05667
Cl	0.90008	-2.28837	4.99722
Cl	-7.56686	-0.6654	-0.46977
H	-6.24036	1.53338	-1.74353

Conformer 007

C	5.23633	-2.09203	-1.0922
C	3.89689	-1.91172	-0.77
C	3.31129	-0.68827	-1.10467
C	4.04048	0.36	-1.74164
C	5.39159	0.13971	-2.05545
C	5.97461	-1.07796	-1.73102
H	5.7215	-3.03061	-0.84507
H	3.33136	-2.69225	-0.27175
H	5.97799	0.91038	-2.54652
H	7.0186	-1.25307	-1.97023
C	3.13852	1.47462	-1.9415
C	3.47001	2.79327	-2.58097

H	4.00871	2.61693	-3.52018
H	2.54304	3.30345	-2.86585
C	4.30943	3.72944	-1.69422
H	3.77571	3.98771	-0.77505
H	5.25325	3.26192	-1.40249
H	4.54596	4.6605	-2.21826
C	1.92916	1.0671	-1.43307
N	2.02596	-0.22136	-0.93521
C	0.52454	1.57341	-1.25896
H	0.15354	1.9933	-2.20011
C	0.79303	-0.74667	-0.35675
H	0.59505	-1.74921	-0.74385
C	-0.26729	0.26187	-0.93639
H	-1.03971	0.4469	-0.18879
C	0.40181	2.68317	-0.17699
H	1.08258	3.4956	-0.45083
H	0.75214	2.29421	0.78189
C	-1.00041	3.22884	-0.02154
C	-1.78774	2.89853	1.08628
C	-1.55348	4.07538	-0.99036
C	-3.08643	3.38651	1.22719
H	-1.38184	2.25606	1.86205
C	-2.84855	4.57183	-0.86886
H	-0.96216	4.36592	-1.85447
C	-3.60757	4.21819	0.24301
H	-3.68295	3.12643	2.0937
H	-3.26246	5.23015	-1.62365
C	-0.93843	-0.27458	-2.22452
H	-1.55363	0.53464	-2.63251
H	-0.16374	-0.47489	-2.9729
C	-1.80215	-1.50284	-2.04692
C	-3.05566	-1.41079	-1.42836
C	-1.3854	-2.75875	-2.49903
C	-3.86342	-2.53059	-1.25463
H	-3.4148	-0.44684	-1.07923
C	-2.17953	-3.8932	-2.33314
H	-0.4275	-2.85923	-3.00129
C	-3.41388	-3.76824	-1.70684
H	-1.84415	-4.8598	-2.69011
C	0.85814	-0.82466	1.15006
C	0.1355	-1.59363	2.03311
N	1.70702	0.02134	1.85576
H	2.47921	0.5108	1.43114
C	-0.8932	-2.64413	1.71938

H	-1.75654	-2.5122	2.38279
H	-1.28206	-2.50674	0.70715
C	0.57371	-1.21738	3.35714
C	1.57461	-0.2236	3.20748
C	0.21139	-1.62296	4.65225
H	-0.55833	-2.37368	4.80306
C	2.22964	0.34776	4.3004
H	3.00006	1.10142	4.16861
C	1.8575	-0.08087	5.5682
H	2.34678	0.34323	6.43899
C	0.85369	-1.05287	5.7426
H	0.58258	-1.36078	6.74733
C	-0.36626	-4.08247	1.86741
H	0.01387	-4.26841	2.87512
H	-1.15701	-4.81088	1.66578
H	0.45326	-4.27506	1.1691
Cl	-5.24636	4.83809	0.40667
Cl	-4.42548	-5.19041	-1.48778
H	-4.83255	-2.44477	-0.77748