Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.


# *Supporting Information for*

## Catalytic Asymmetric C2-Nucleophilic Substitutions of C3-Substituted Indoles with *ortho*-Hydroxybenzyl Alcohols

Jia-Le Wu, Jing-Yi Wang, Ping Wu, Guang-Jian Mei and Feng Shi*

*School of Chemistry & Material Science, Jiangsu Normal University, Xuzhou, 221116, China*

*E-mail: fshi@jsnu.edu.cn*

**Contents:**

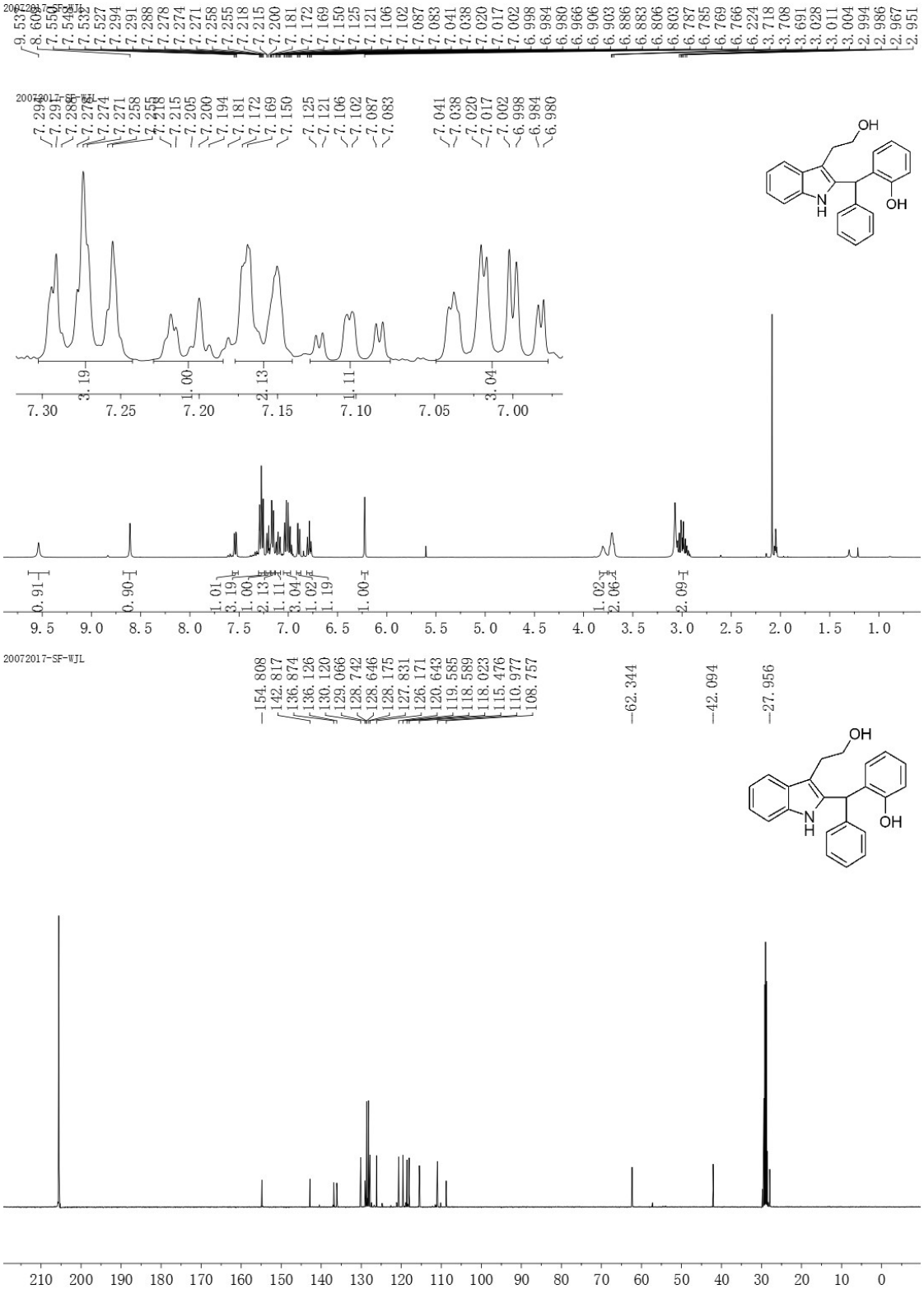
**1. NMR spectra of all products (S2-S51)**

**2. HPLC spectra of all products (S52-S101)**

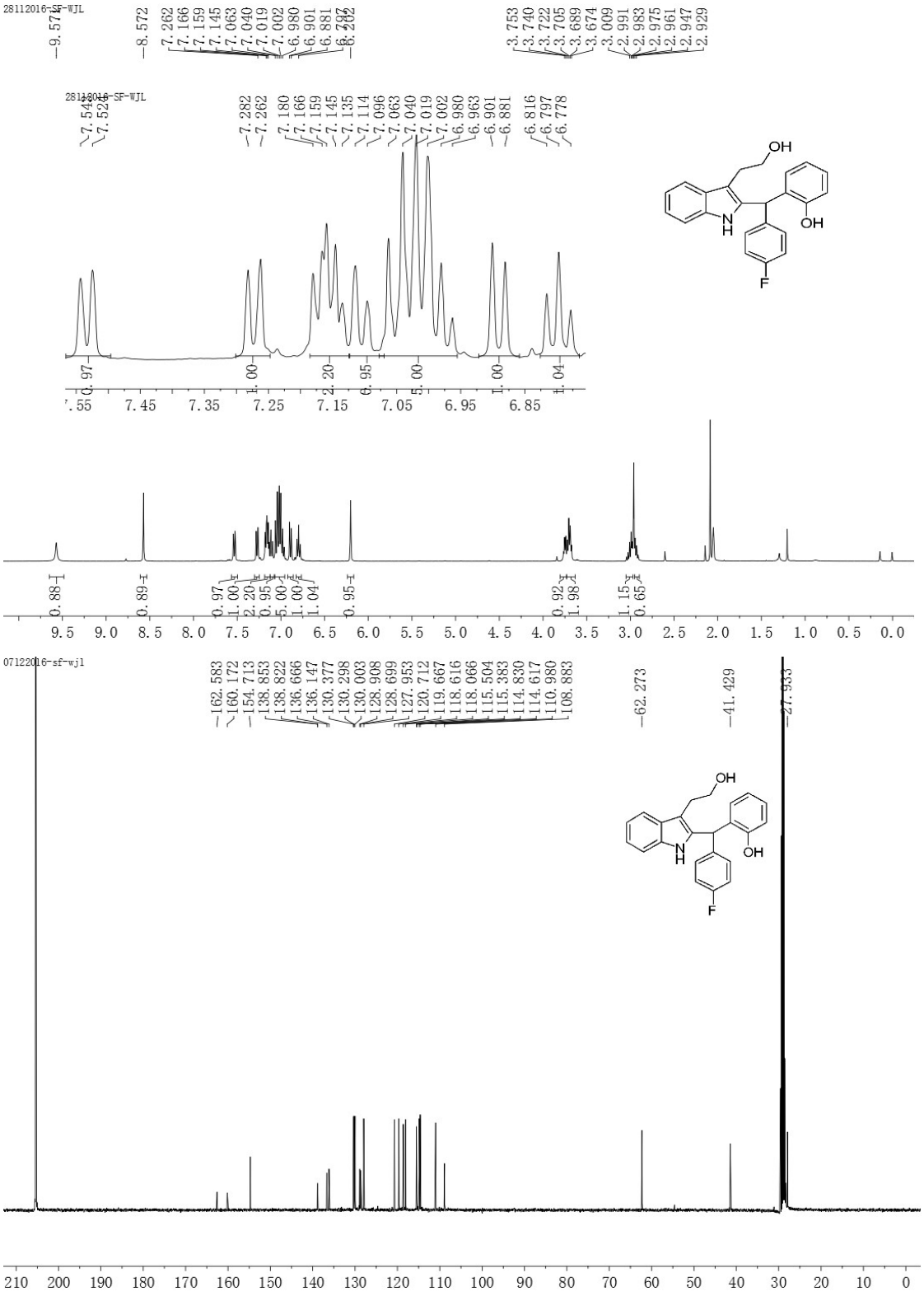
**3. X-ray single crystal data for compounds 3aa and 8aa (S102-S105)**

# 1. NMR spectra of all products

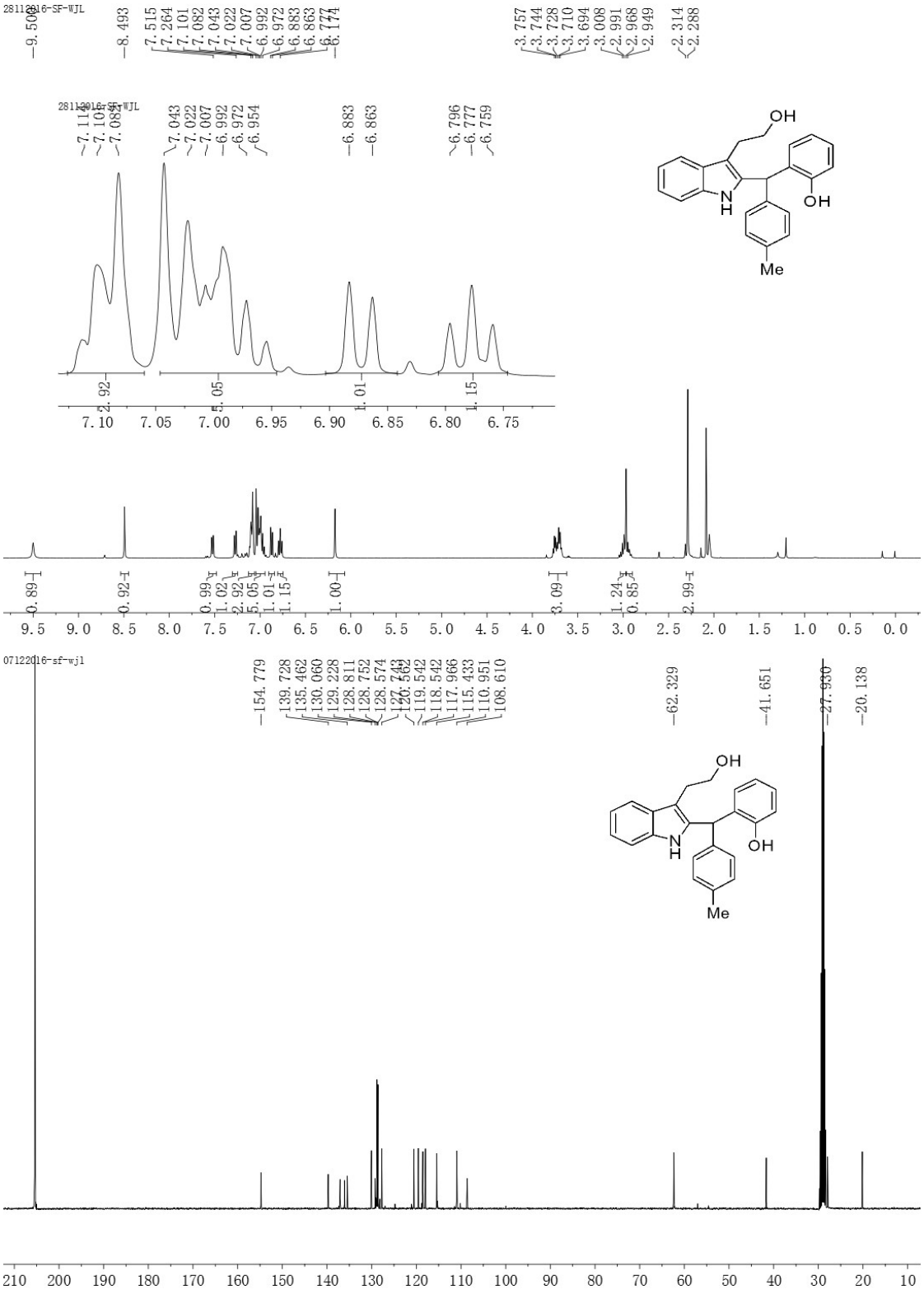
## 3aa



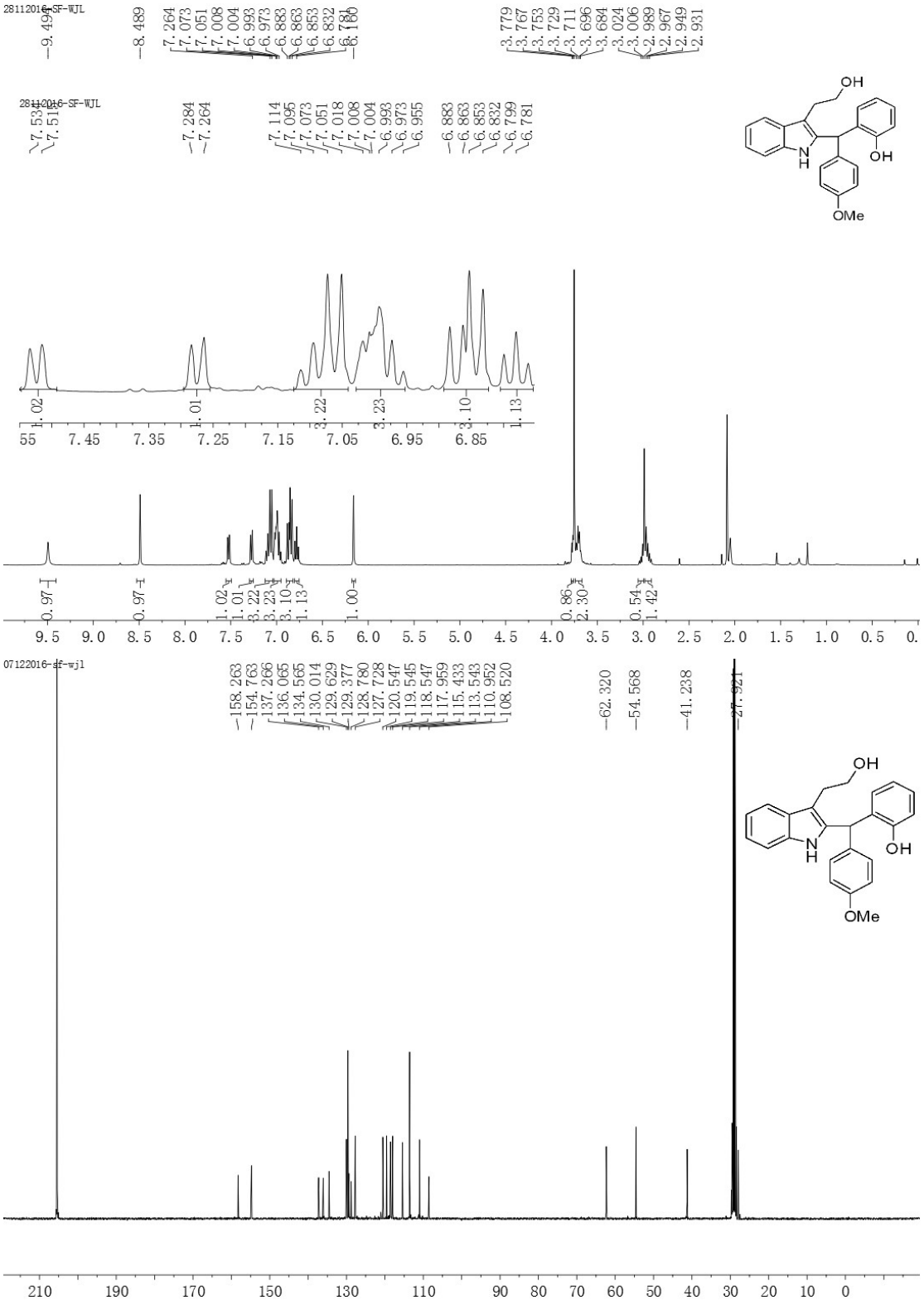
## 3ba


28112016-SF-WJL
9.574
8.572
7.262
7.166
7.159
7.145
7.063
7.040
7.019
7.002
6.980
6.901
6.881
6.797
6.202
3.753
3.740
3.722
3.705
3.689
3.674
3.009
2.991
2.983
2.975
2.961
2.947
2.929
28112016-SF-WJL
7.544
7.524
7.282
7.262
7.180
7.166
7.159
7.145
7.135
7.114
7.096
7.063
7.040
7.019
7.002
6.980
6.963
6.901
6.881
6.816
6.797
6.778
OH
OH
N
H
F
0.97
1.00
2.20
6.95
5.00
1.00
1.04
0.88
0.89
0.97
1.00
2.20
0.95
5.00
1.00
1.04
0.95
0.92
1.98
1.15
0.65
07122016-sf-wjl
162.583
160.172
154.713
138.853
138.822
136.666
136.147
130.377
130.298
130.003
128.908
128.699
127.953
120.712
119.667
118.616
118.066
115.504
115.383
114.830
114.617
110.980
108.883
62.273
41.429
27.933
OH
OH
N
H
F

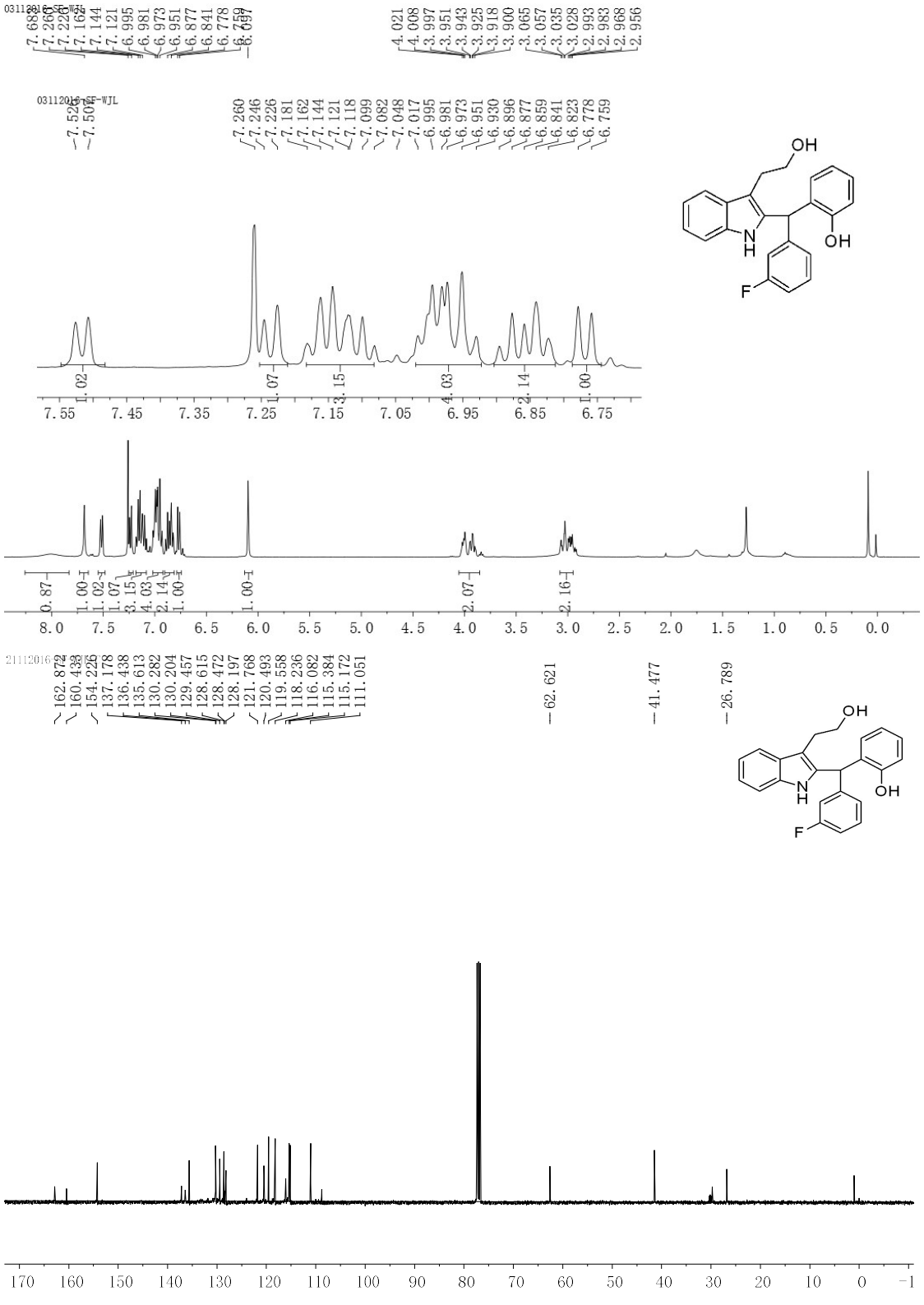
## 3ca


OH
OH
N
H
Me
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

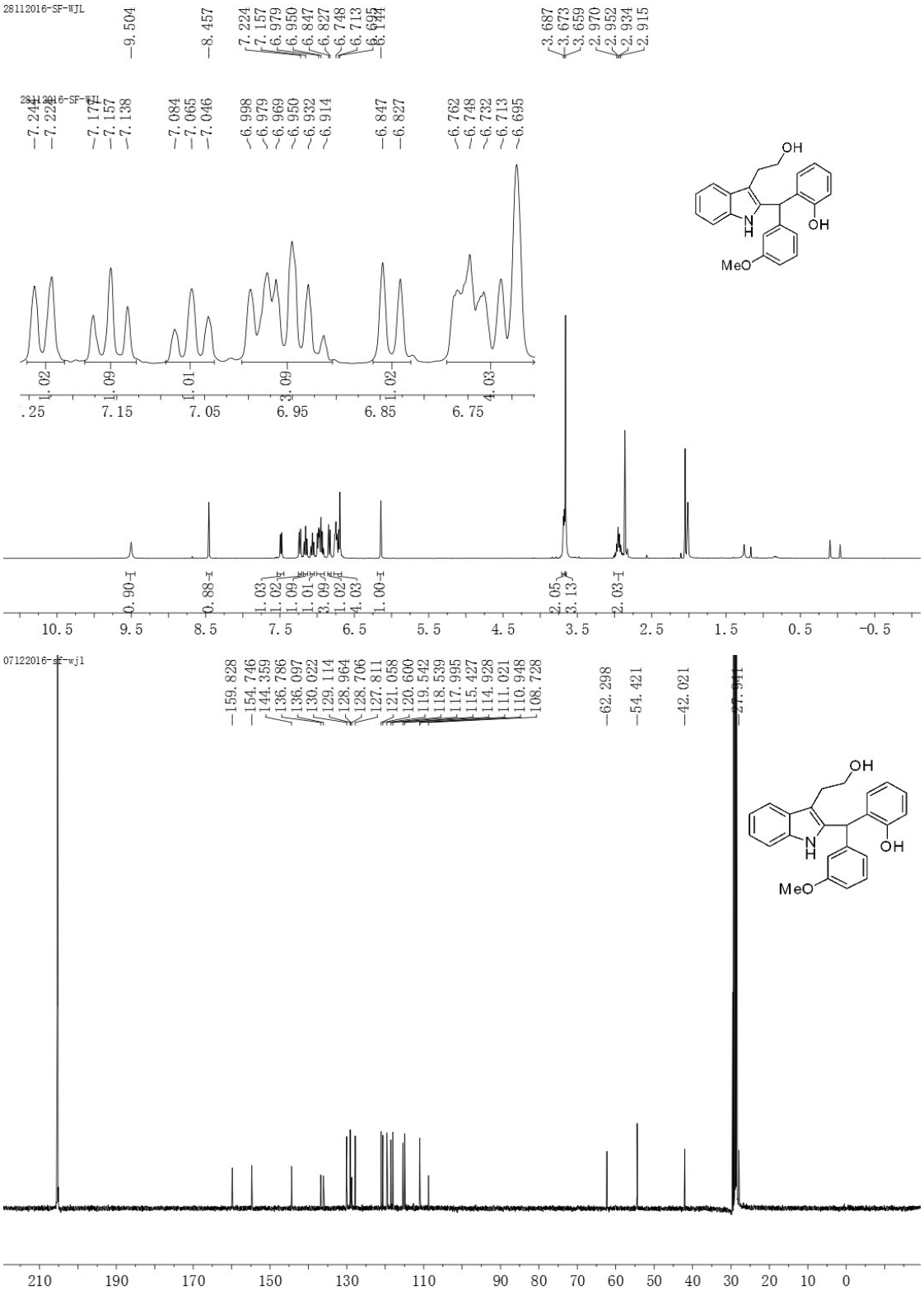
## 3da


28112016-SF-WJL
9.496
8.489
7.264
7.073
7.051
7.008
7.004
6.993
6.973
6.883
6.863
6.853
6.832
6.781
6.180
3.779
3.767
3.753
3.729
3.711
3.696
3.684
3.024
3.006
2.989
2.967
2.949
2.931
28112016-SF-WJL
7.538
7.518
7.284
7.264
7.114
7.095
7.073
7.051
7.018
7.008
7.004
6.993
6.973
6.955
6.883
6.863
6.853
6.832
6.799
6.781
OH
OH
N
H
OMe
1.02
1.01
3.22
3.23
3.10
1.13
55
7.45
7.35
7.25
7.15
7.05
6.95
6.85
0.97
0.97
1.02
1.01
3.22
3.23
3.10
1.13
1.00
0.86
2.30
0.54
1.42
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
07122016-sf-wjl
158.263
154.763
137.266
136.065
134.565
130.014
129.629
129.377
128.780
127.728
120.547
119.545
118.547
117.959
115.433
113.543
110.952
108.520
62.320
54.568
41.238
27.921
OH
OH
N
H
OMe
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

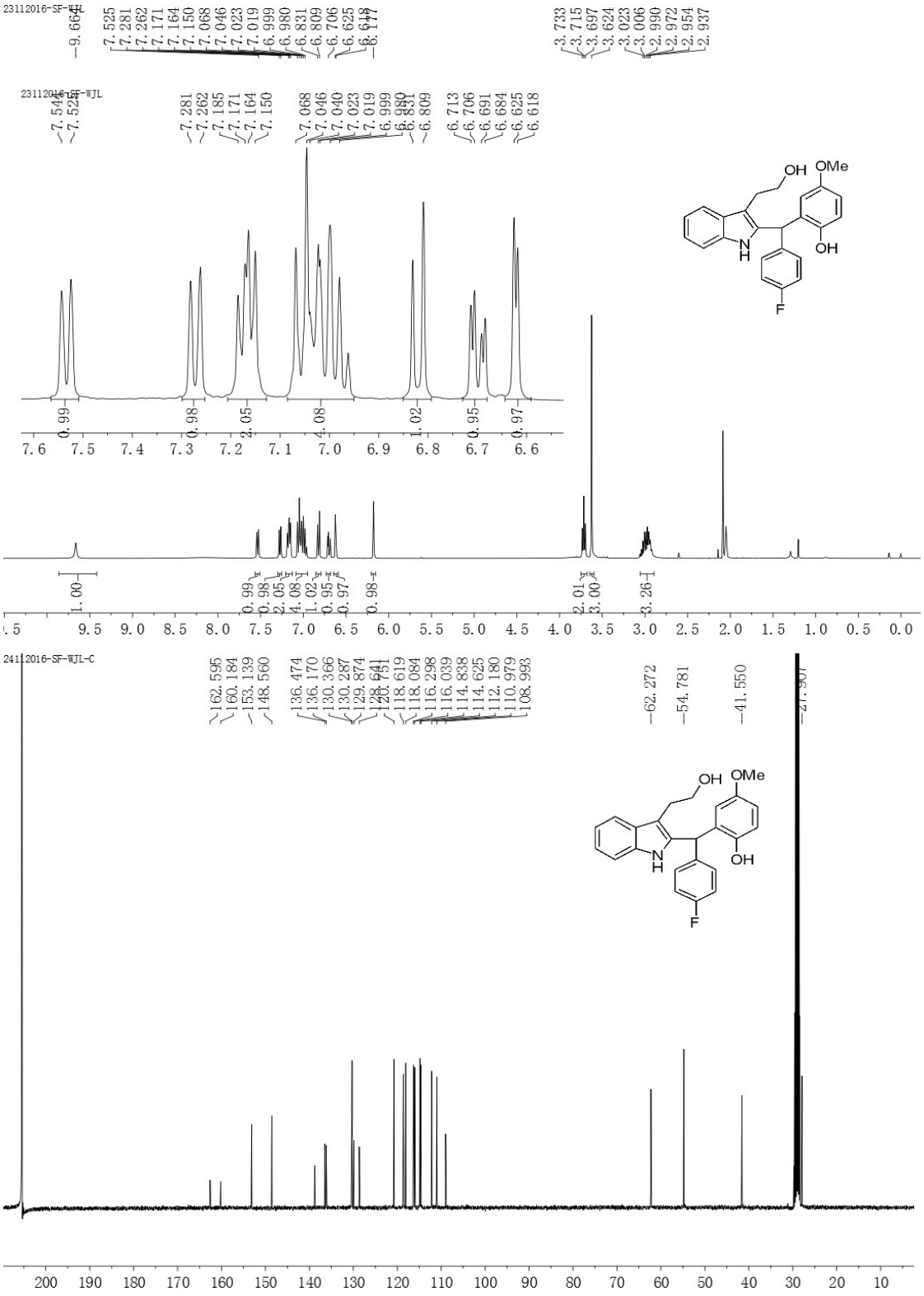
## 3ea



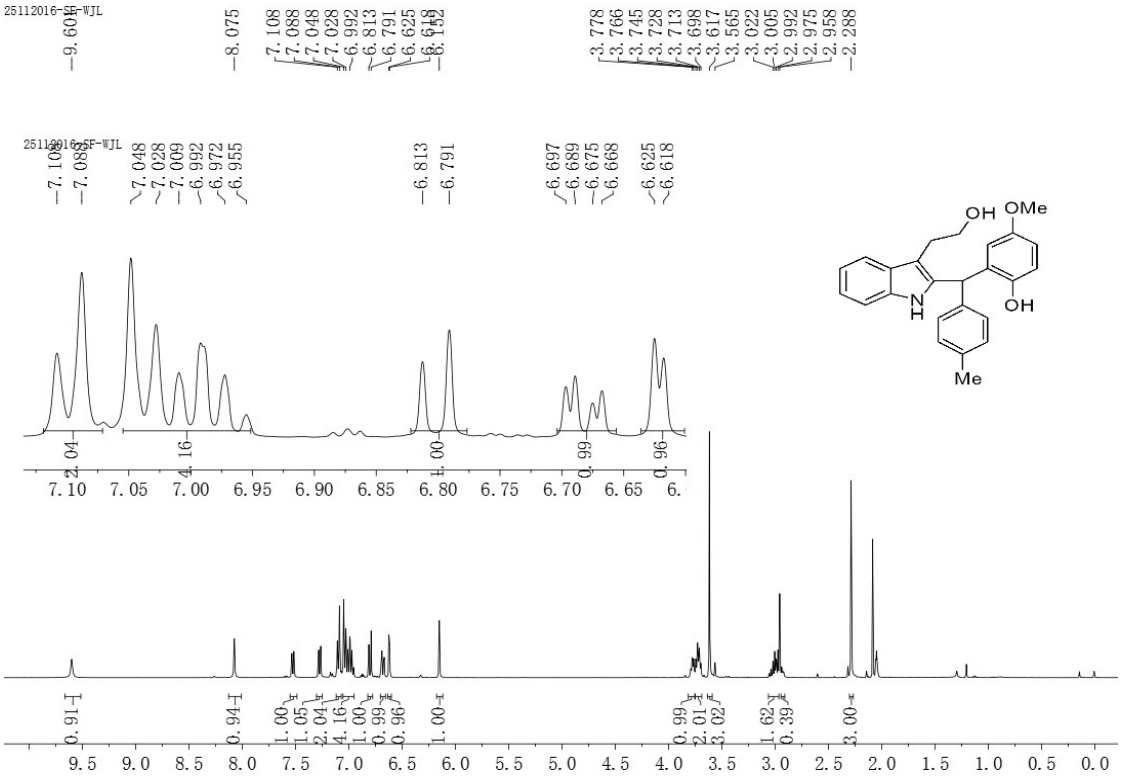
## 3fa

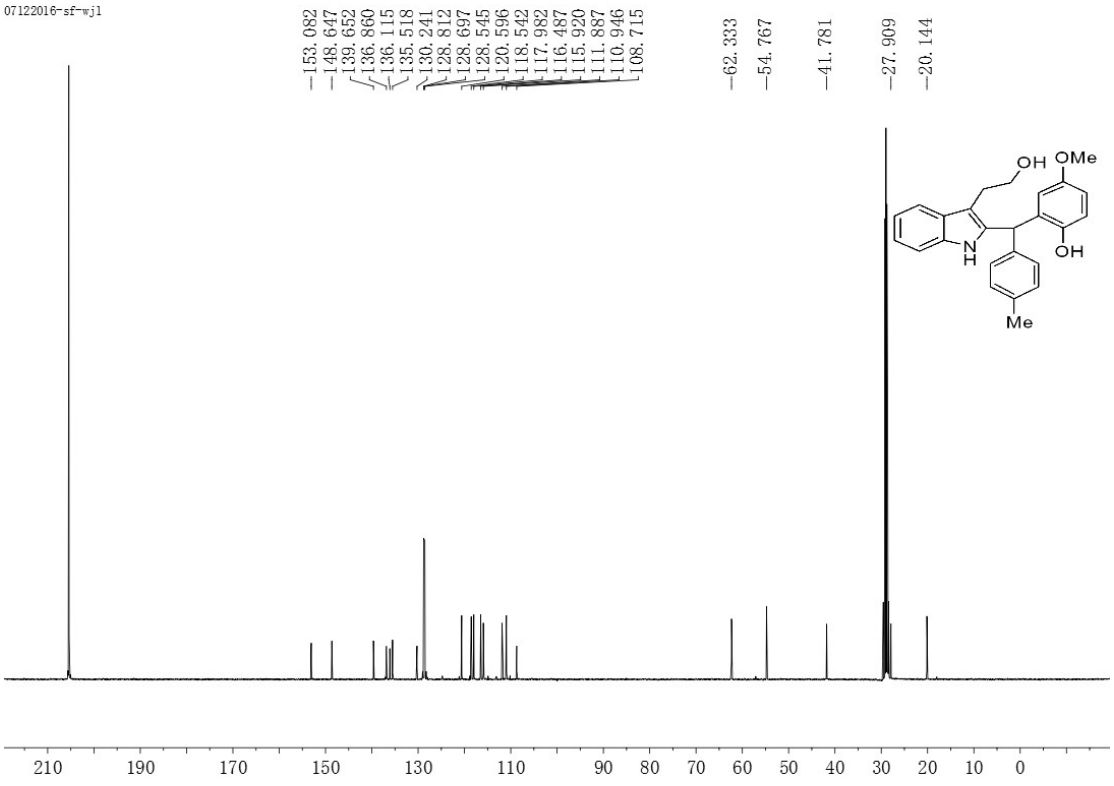

28112016-SF-WJL
9.504
8.457
7.224
7.157
6.979
6.950
6.847
6.827
6.748
6.713
3.687
3.673
3.659
2.970
2.952
2.934
2.915
7.084
7.065
7.046
6.998
6.979
6.969
6.950
6.932
6.914
6.847
6.827
6.762
6.748
6.732
6.713
6.695
OH
OH
MeO
07122016-sf-wjl
159.828
154.746
144.359
136.786
136.097
130.022
129.114
128.964
128.706
127.811
121.058
120.600
119.542
118.539
117.995
115.427
114.928
111.021
110.948
108.728
62.298
54.421
42.021
27.941

## 3ga

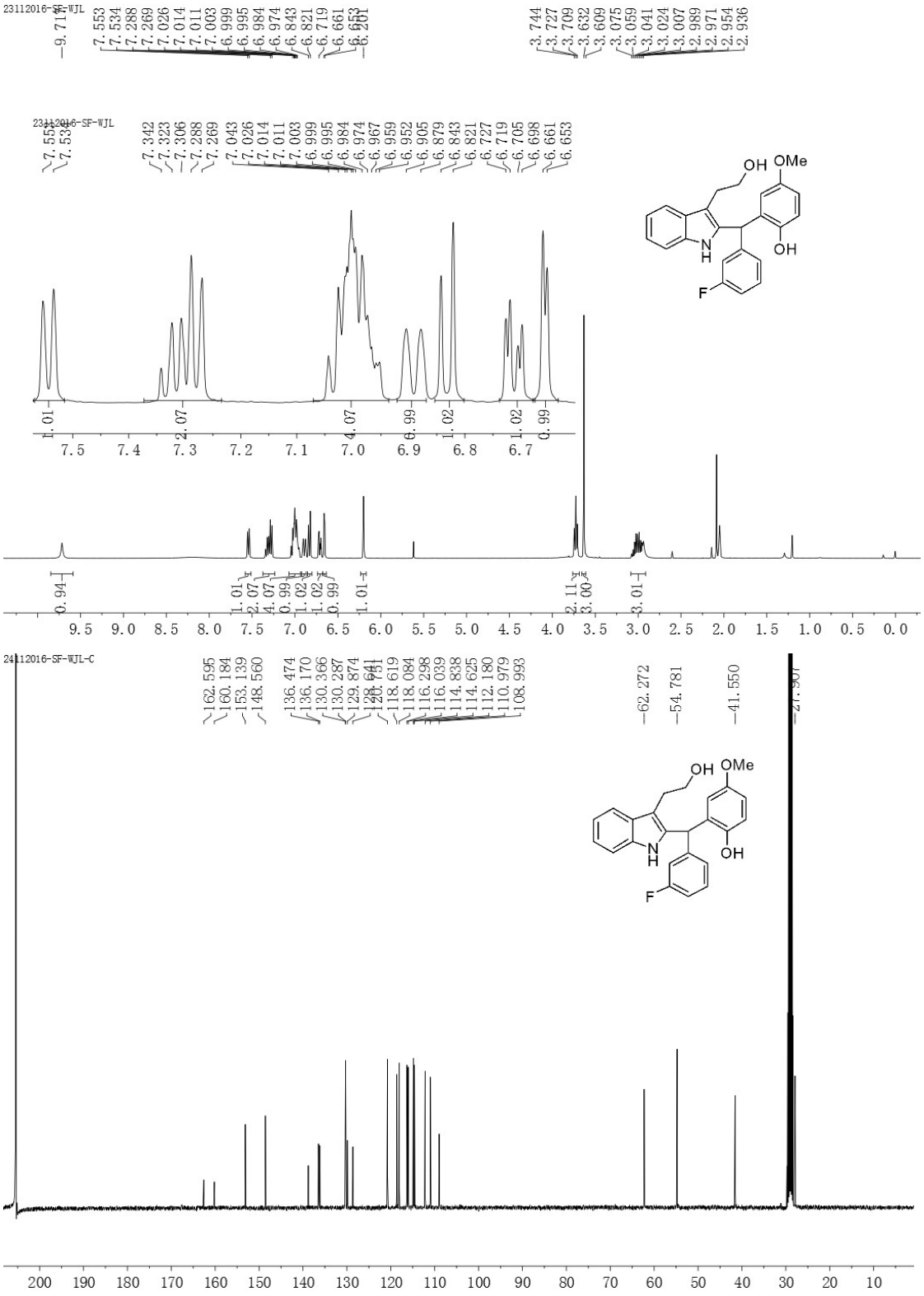


## 3ha

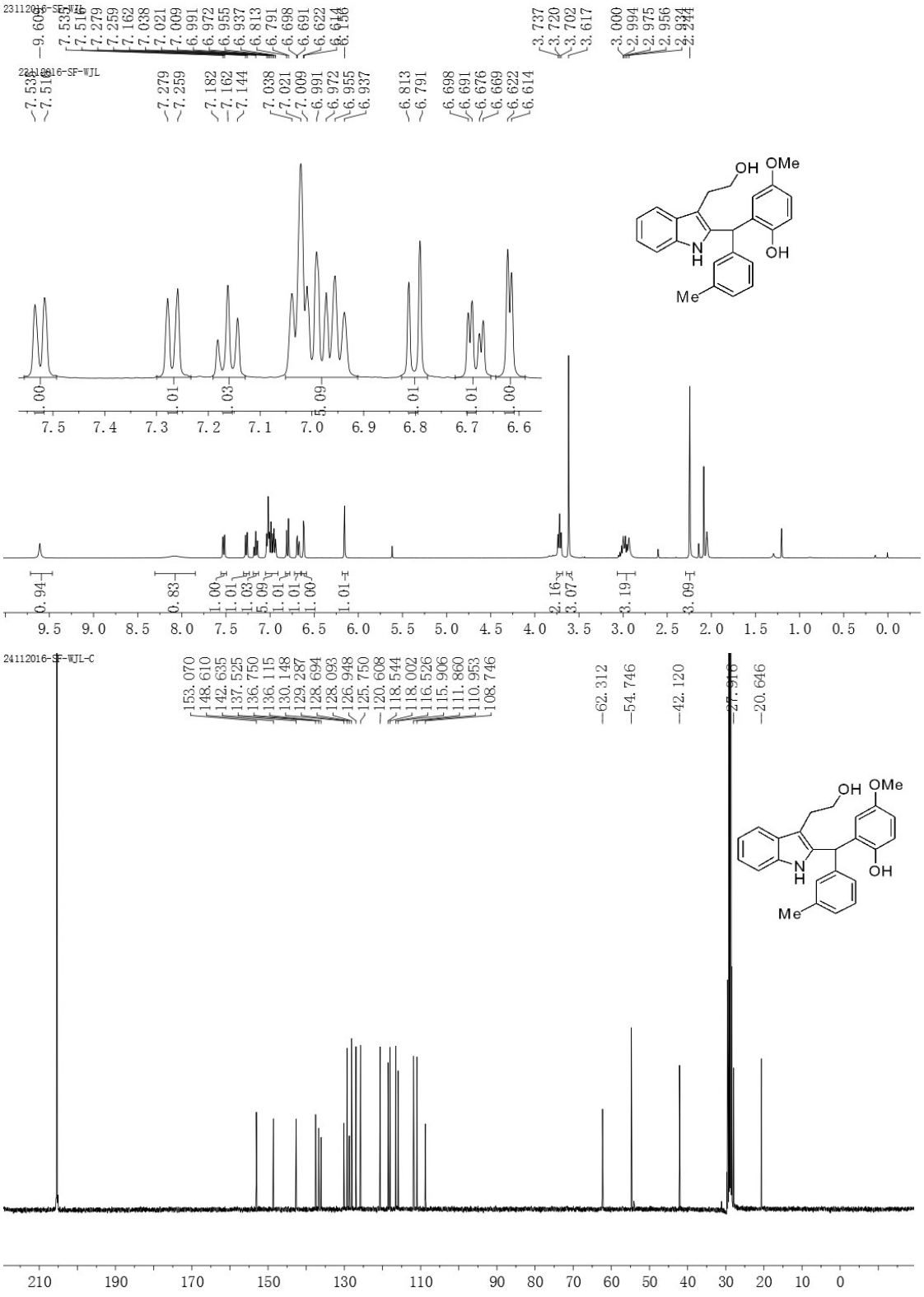

25112016-SF-WJL
9.604
8.075
7.108
7.088
7.048
7.028
6.992
6.813
6.791
6.625
6.618
6.152
3.778
3.766
3.745
3.728
3.713
3.698
3.617
3.565
3.022
3.005
2.992
2.975
2.958
2.288
OH
OMe
OH
Me


07122016-sf-wjl
153.082
148.647
139.652
136.860
136.115
135.518
130.241
128.812
128.697
128.545
120.596
118.542
117.982
116.487
115.920
111.887
110.946
108.715
62.333
54.767
41.781
27.909
20.144
OH
OMe
OH
Me

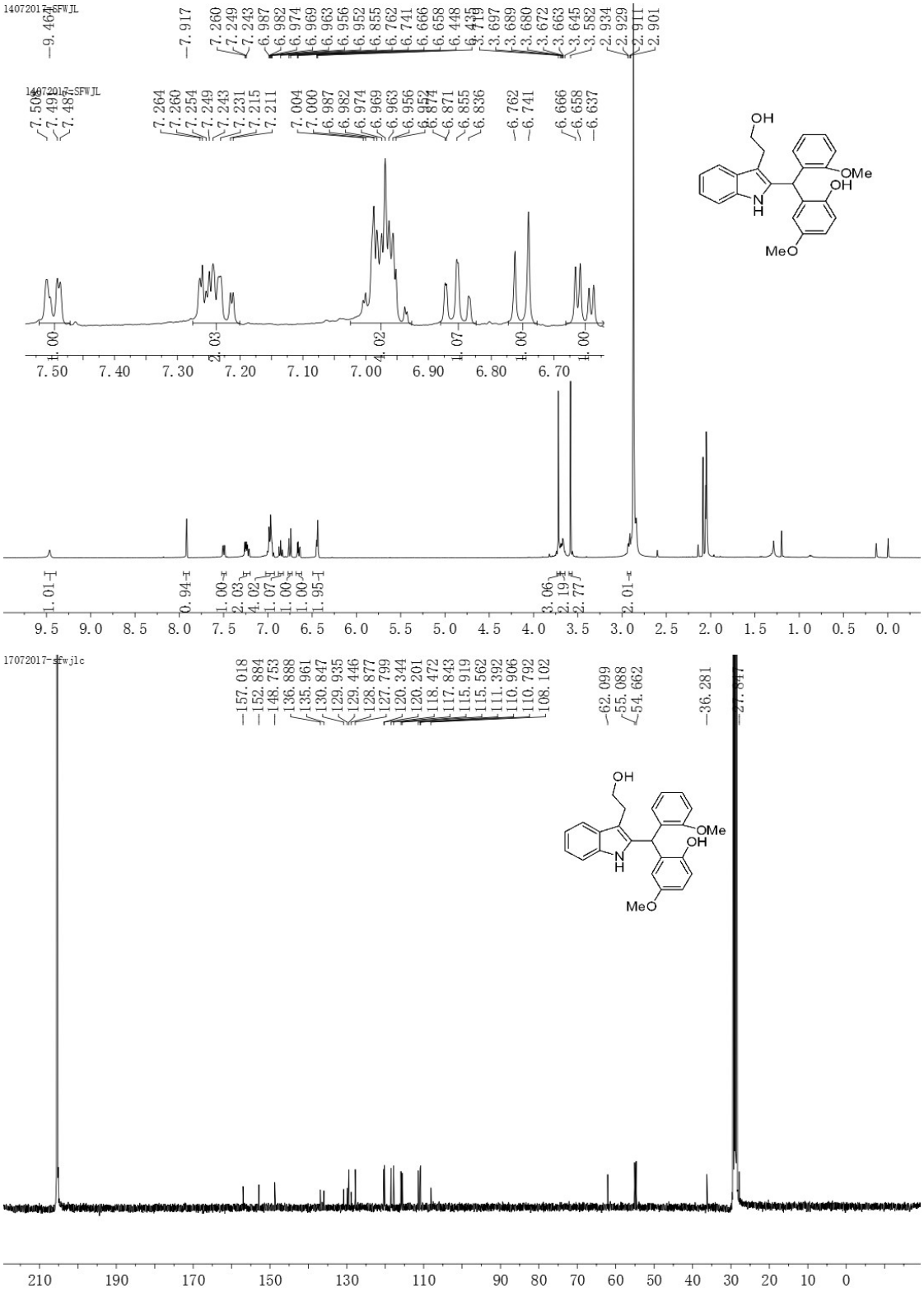
**3ia**



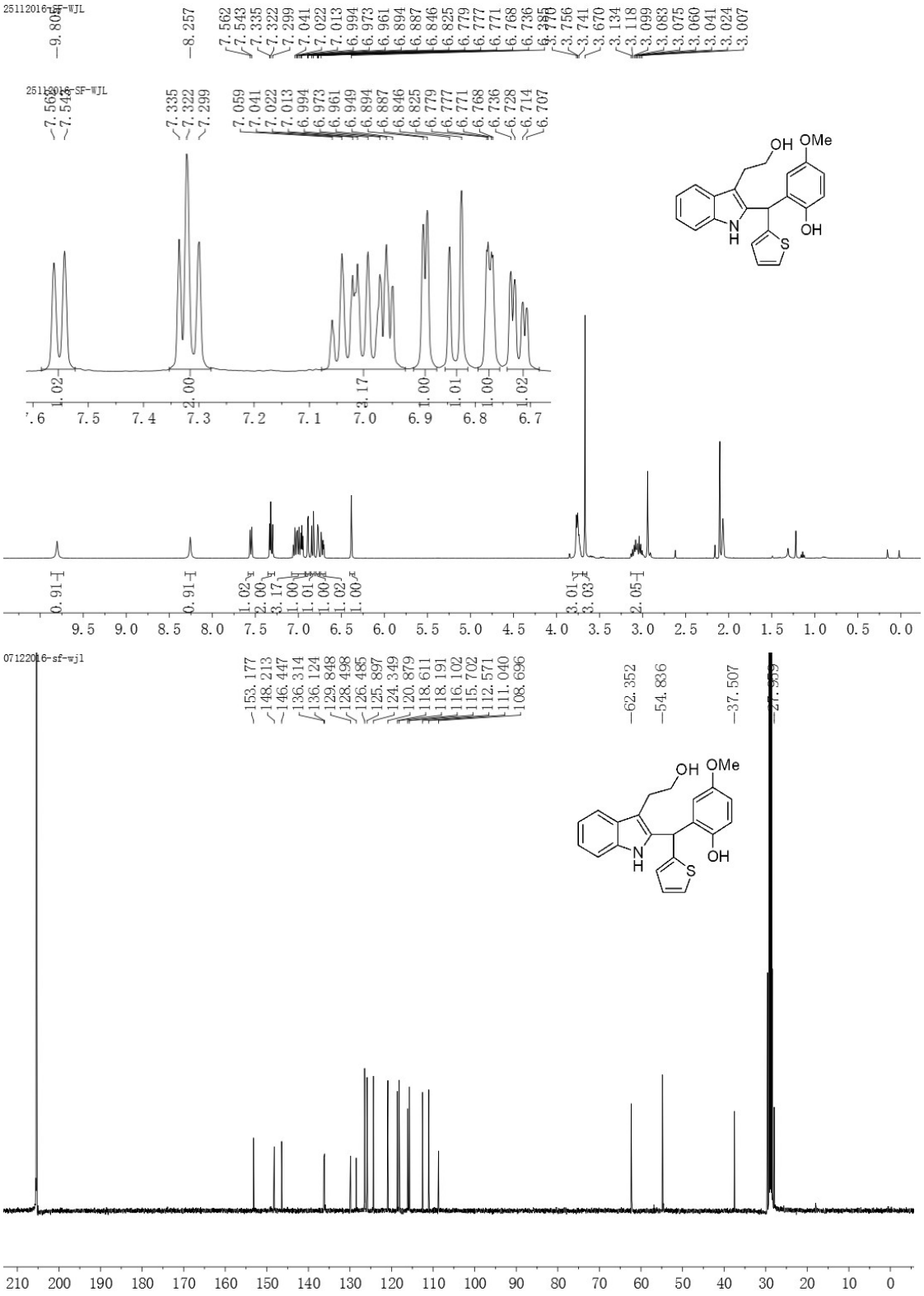
## 3ja


23112016-SF-WJL
9.604
7.538
7.516
7.279
7.259
7.162
7.038
7.021
7.009
6.991
6.972
6.955
6.937
6.813
6.791
6.698
6.691
6.622
6.614
6.144
3.737
3.720
3.702
3.617
3.000
2.994
2.975
2.956
2.934
2.244
OH
OMe
OH
N
H
Me
24112016-SF-WJL-C
153.070
148.610
142.635
137.525
136.750
136.115
130.148
129.287
128.694
128.093
126.948
125.750
120.608
118.544
118.002
116.526
115.906
111.860
110.953
108.746
62.312
54.746
42.120
27.916
20.646

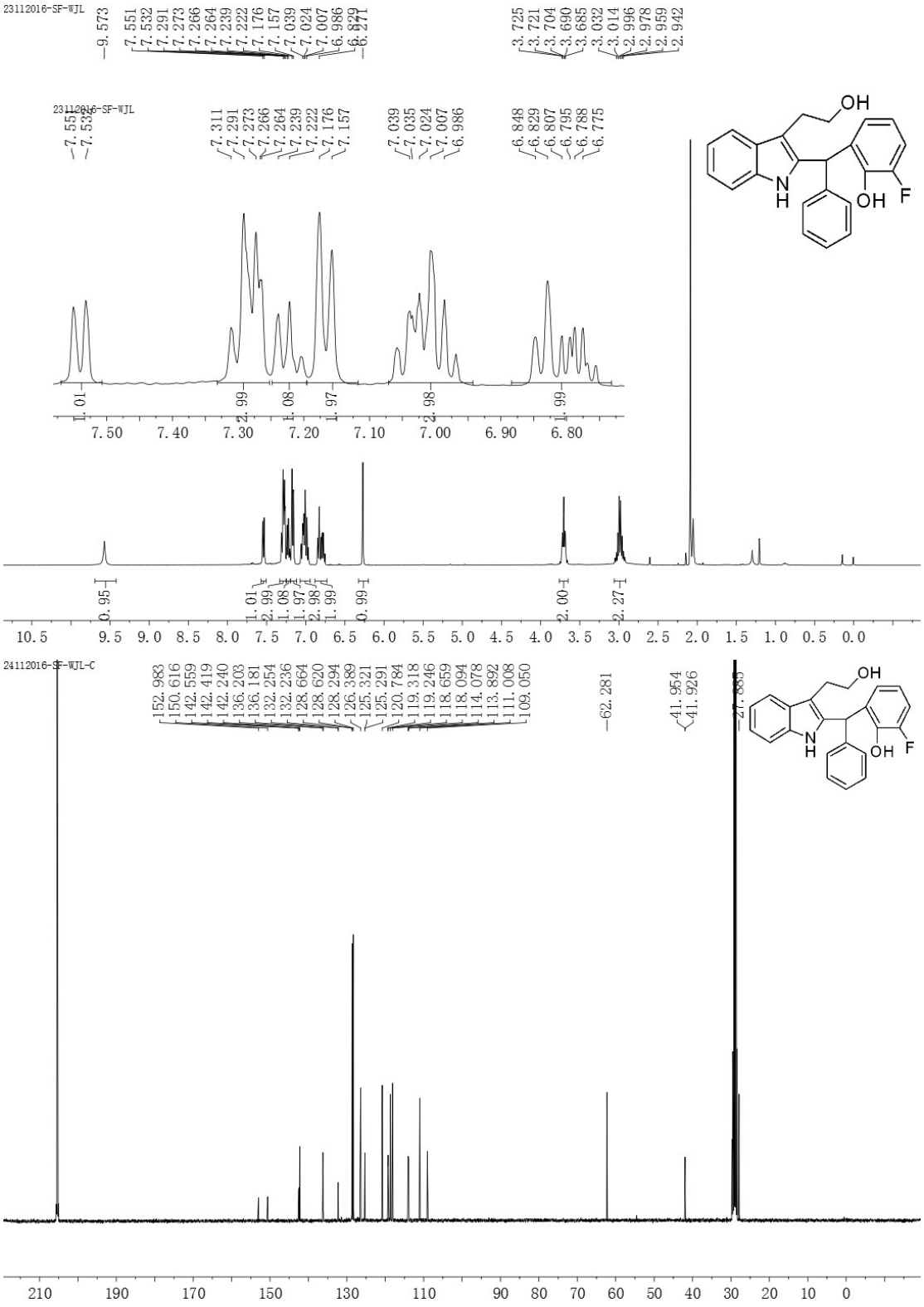
**3ka**



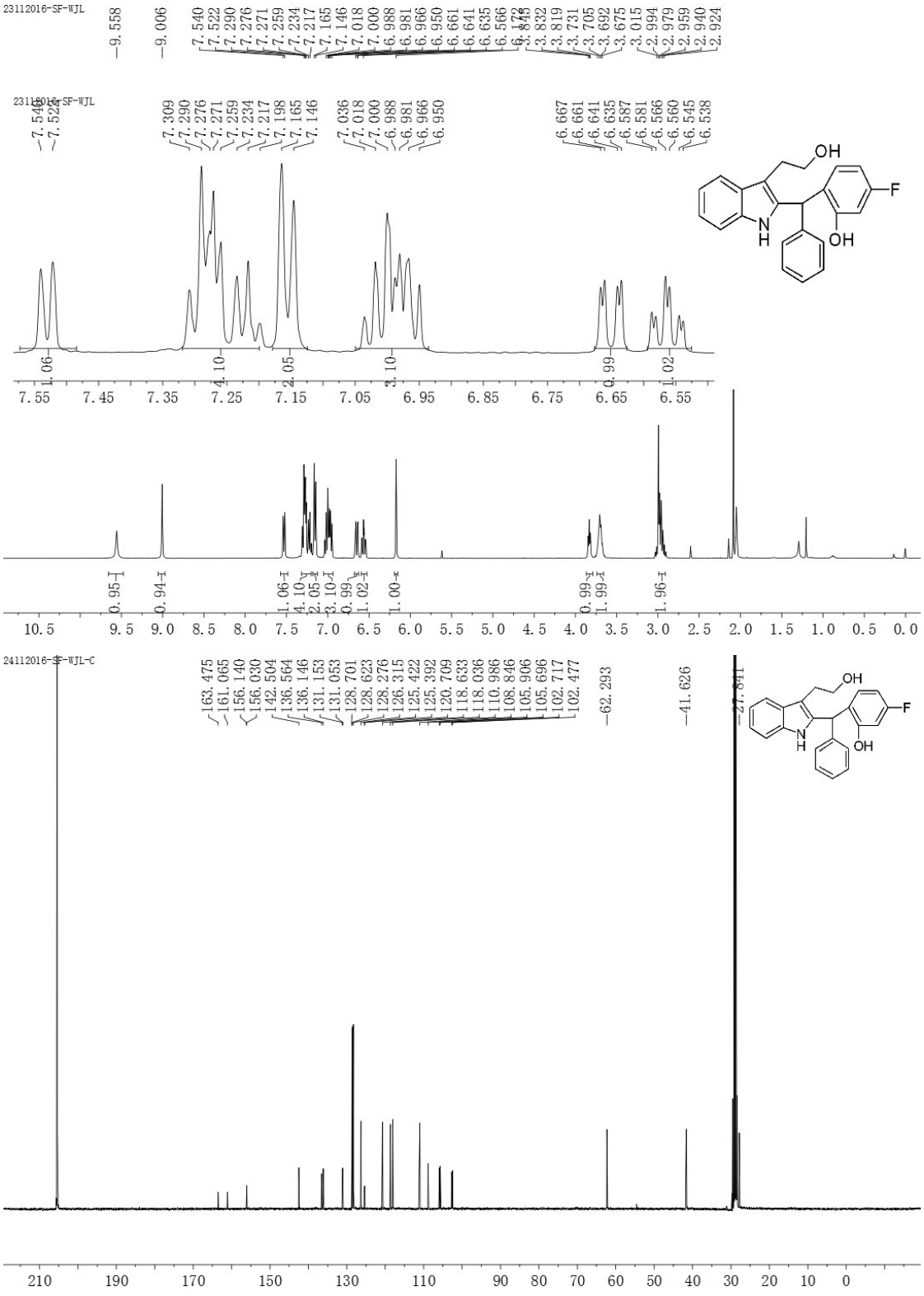
**3la**



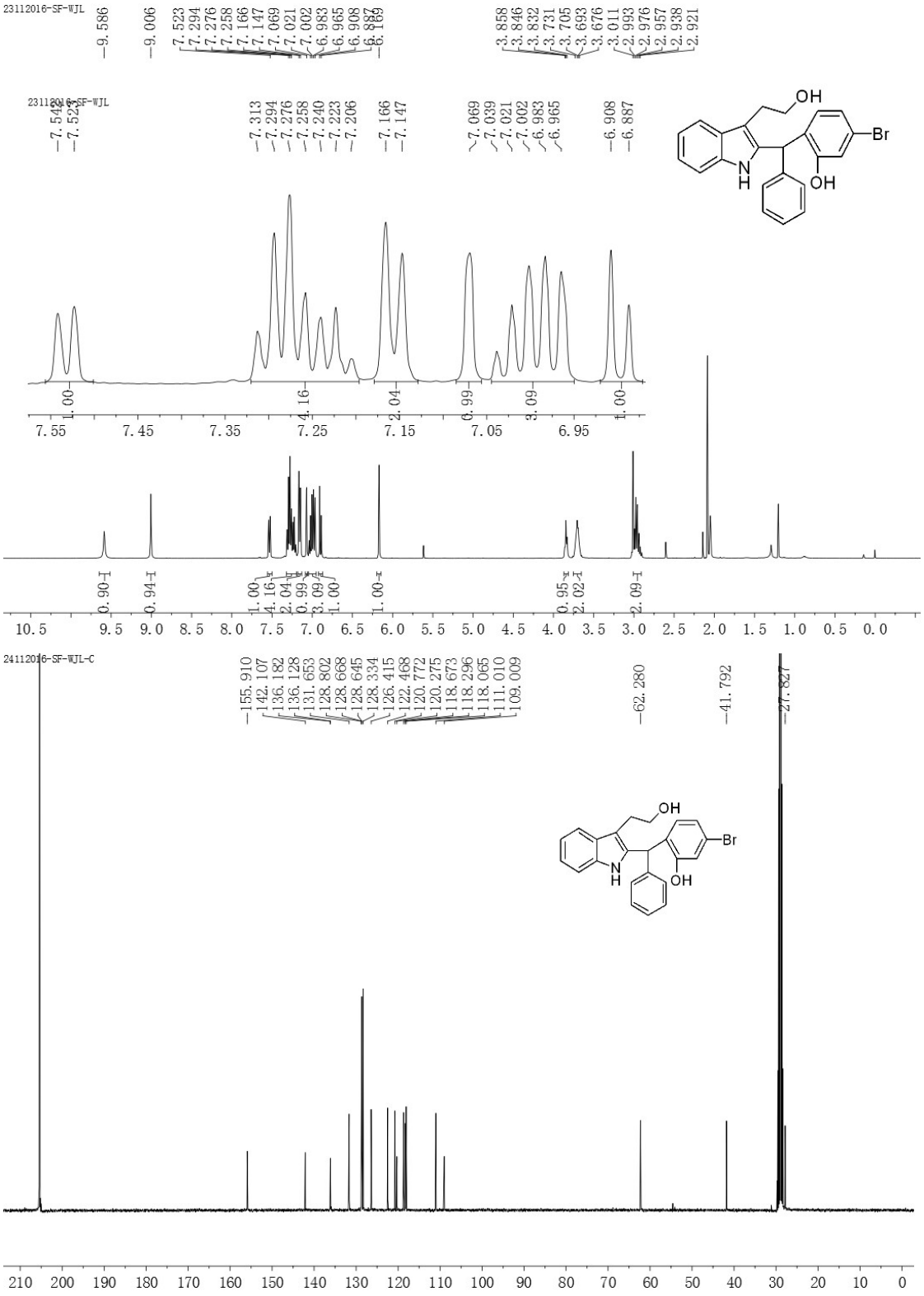
## 3ma



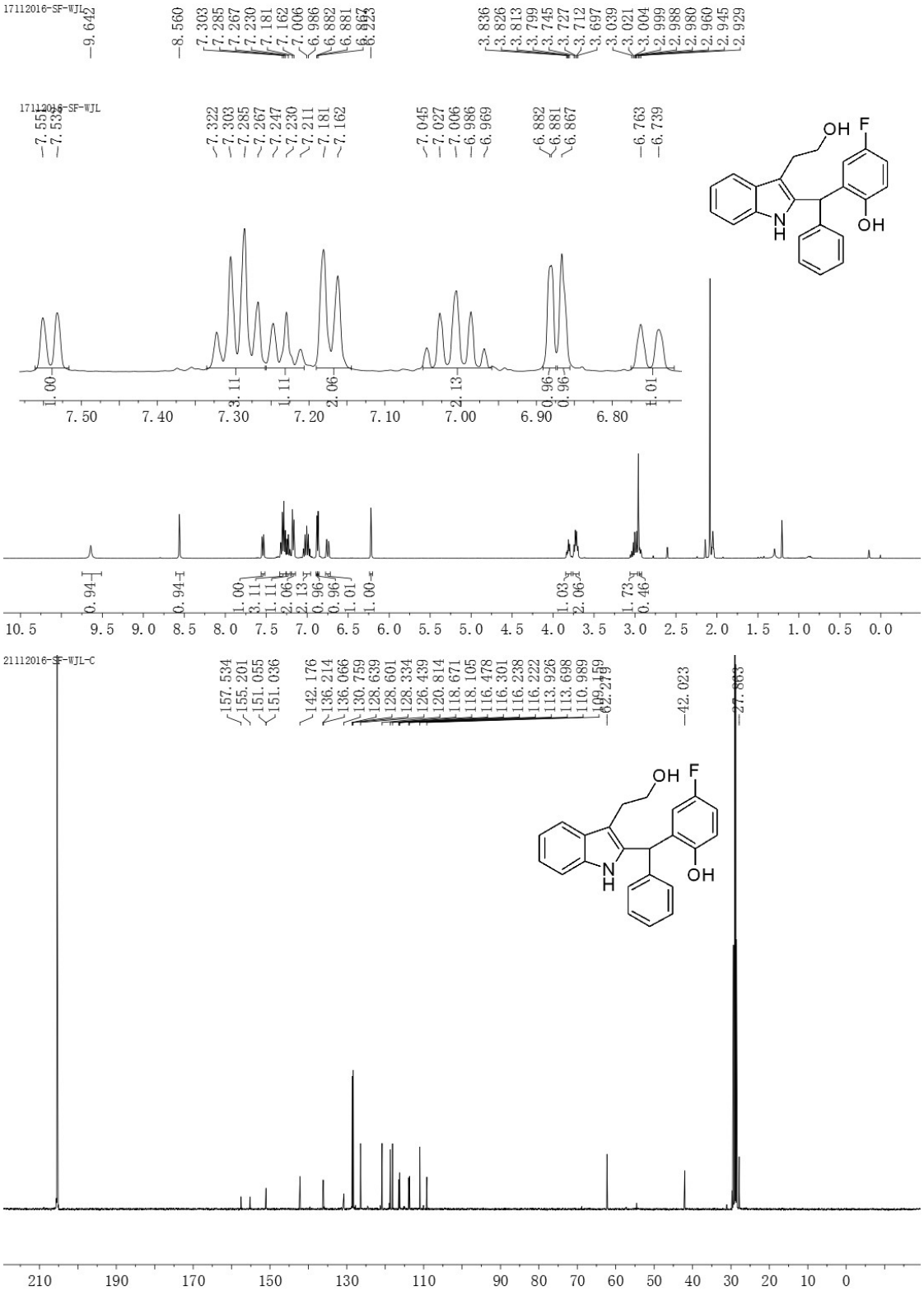
## 3na



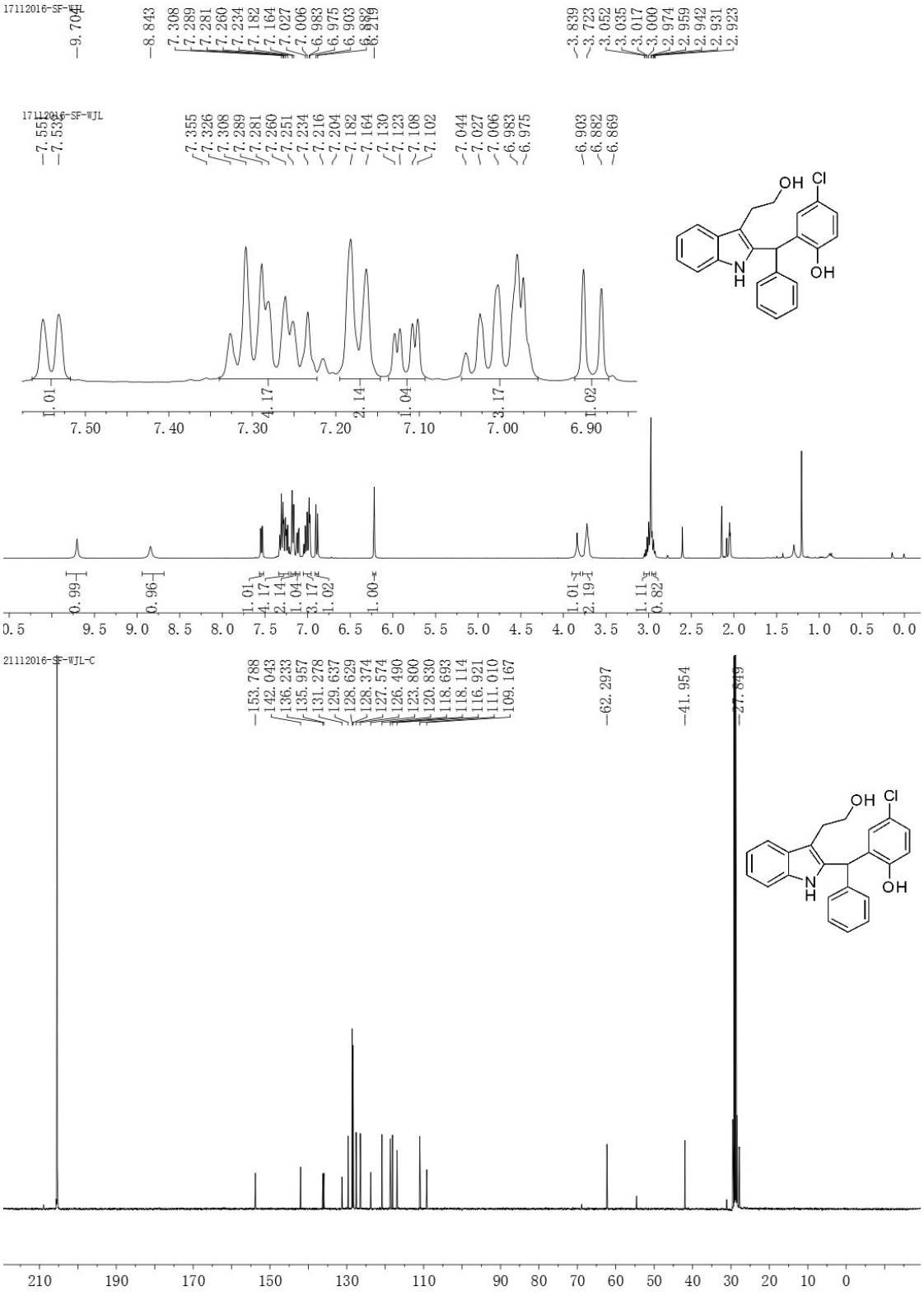
## 3oa


23112016-SF-WJL
9.586
9.006
7.523
7.294
7.276
7.258
7.166
7.147
7.069
7.021
7.002
6.983
6.965
6.908
6.887
3.858
3.846
3.832
3.731
3.705
3.693
3.676
3.011
2.993
2.976
2.957
2.938
2.921
OH
Br
N
H
OH
24112016-SF-WJL-C
155.910
142.107
136.182
136.128
131.653
128.802
128.668
128.645
128.334
126.415
122.468
120.772
120.275
118.673
118.296
118.065
111.010
109.009
62.280
41.792
27.827

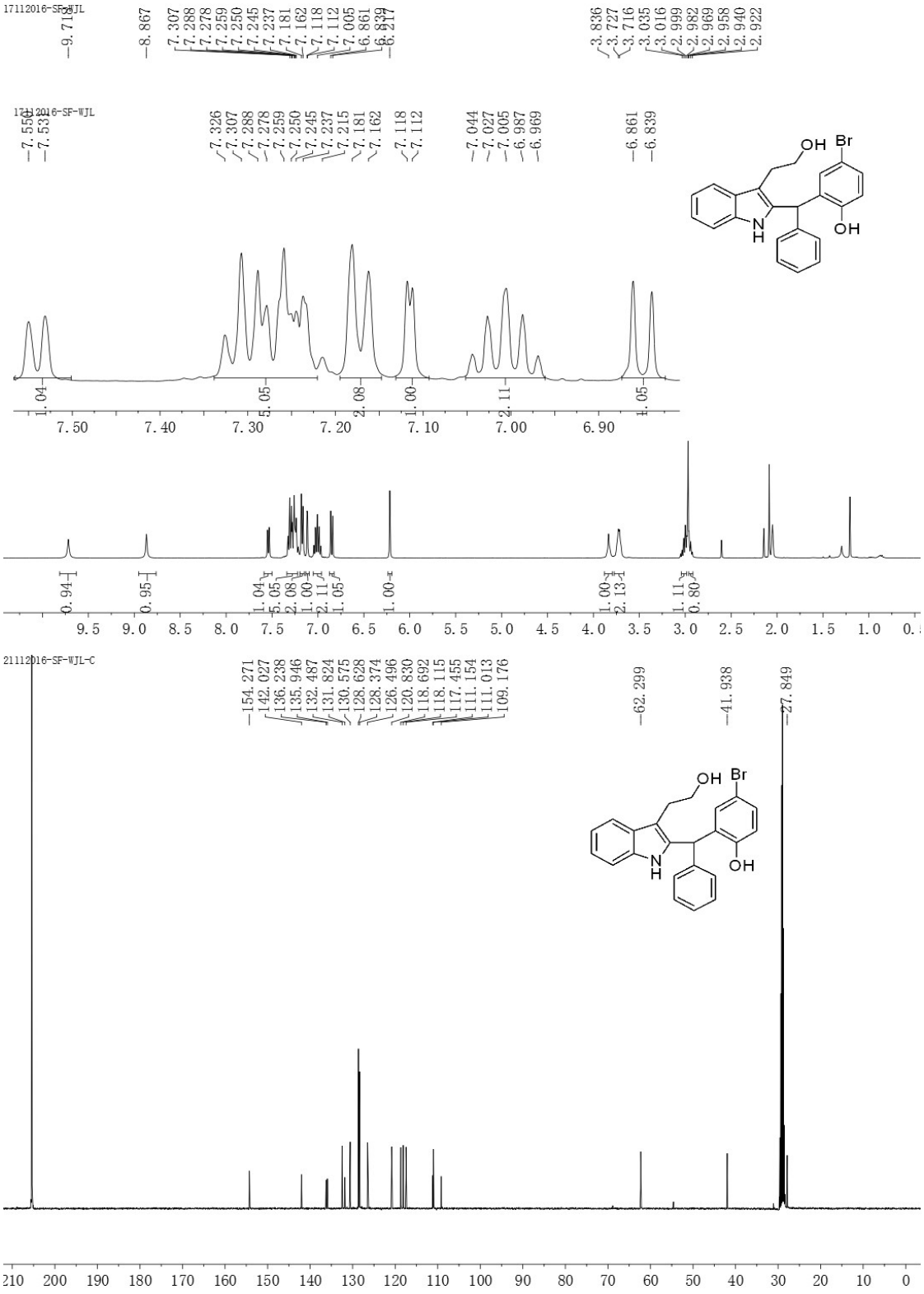
## 3pa



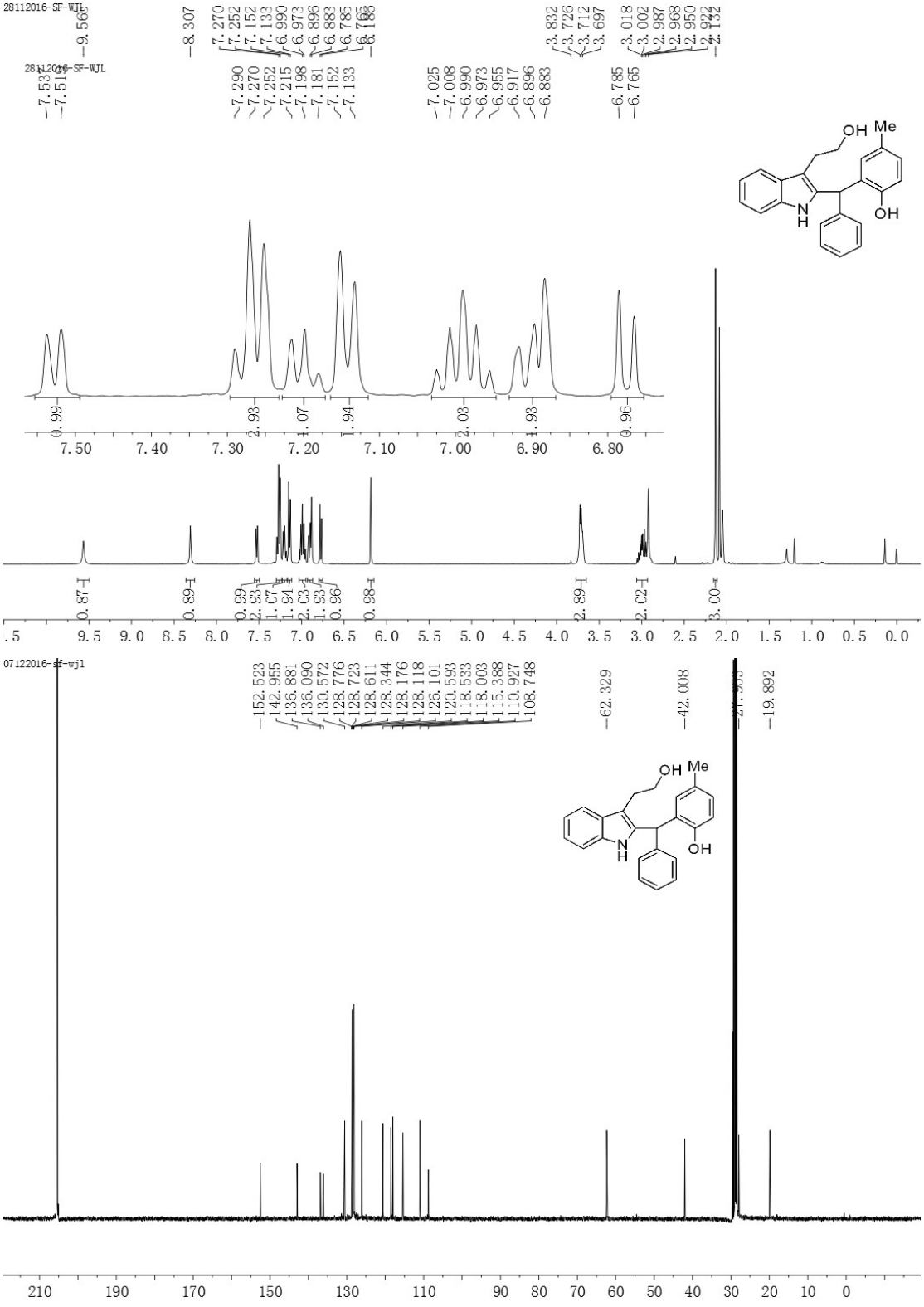
## 3qa


17112016-SF-WJL
9.704
8.843
7.308
7.289
7.281
7.260
7.234
7.182
7.164
7.027
7.006
6.983
6.975
6.903
6.882
6.219
3.839
3.723
3.052
3.035
3.017
3.000
2.974
2.959
2.942
2.931
2.923
17112016-SF-WJL
7.551
7.533
7.355
7.326
7.308
7.289
7.281
7.260
7.251
7.234
7.216
7.204
7.182
7.164
7.130
7.123
7.108
7.102
7.044
7.027
7.006
6.983
6.975
6.903
6.882
6.869
OH
Cl
N
H
OH
1.01
4.17
2.14
1.04
3.17
1.02
7.50
7.40
7.30
7.20
7.10
7.00
6.90
0.99
0.96
1.01
4.17
2.14
1.04
3.17
1.02
1.00
1.01
2.19
1.11
0.82
0.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
21112016-SF-WJL-C
153.788
142.043
136.233
135.957
131.278
129.637
128.629
128.374
127.574
126.490
123.800
120.830
118.693
118.114
116.921
111.010
109.167
62.297
41.954
27.849
OH
Cl
N
H
OH
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

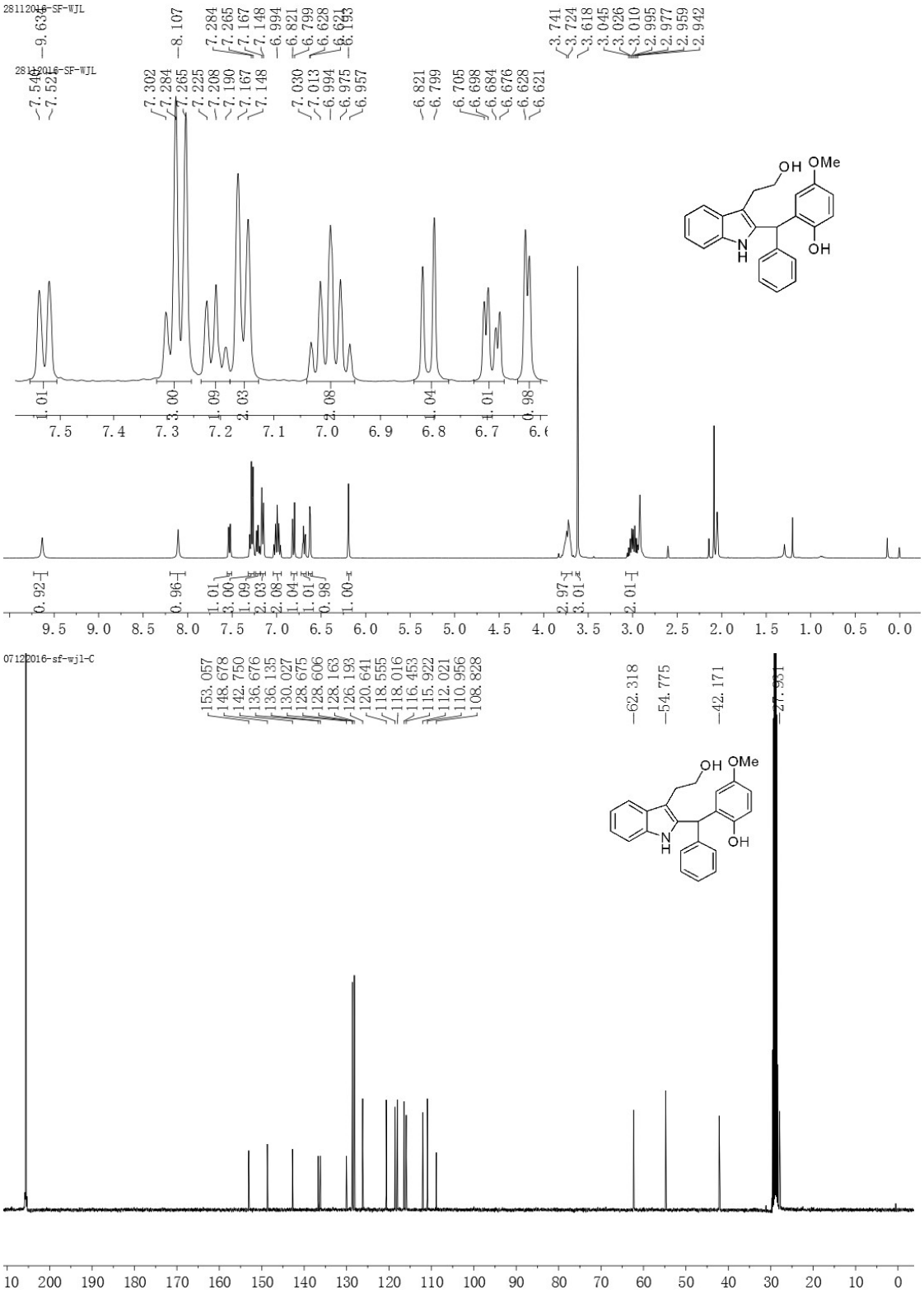
## 3ra


17112016-SF-WJL
9.718
8.867
7.307
7.288
7.278
7.259
7.250
7.245
7.237
7.181
7.162
7.118
7.112
7.005
6.861
6.839
6.817
3.836
3.727
3.716
3.035
3.016
2.999
2.982
2.969
2.958
2.940
2.922
7.556
7.531
7.326
7.307
7.288
7.278
7.259
7.250
7.245
7.237
7.215
7.181
7.162
7.118
7.112
7.044
7.027
7.005
6.987
6.969
6.861
6.839
OH
Br
N
H
OH
1.04
5.05
2.08
1.00
2.11
1.05
7.50
7.40
7.30
7.20
7.10
7.00
6.90
0.94
0.95
1.04
5.05
2.08
1.00
2.11
1.05
1.00
1.00
2.13
1.11
0.80
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
21112016-SF-WJL-C
154.271
142.027
136.238
135.946
132.487
131.824
130.575
128.628
128.374
126.496
120.830
118.692
118.115
117.455
111.154
111.013
109.176
62.299
41.938
27.849
OH
Br
N
H
OH
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

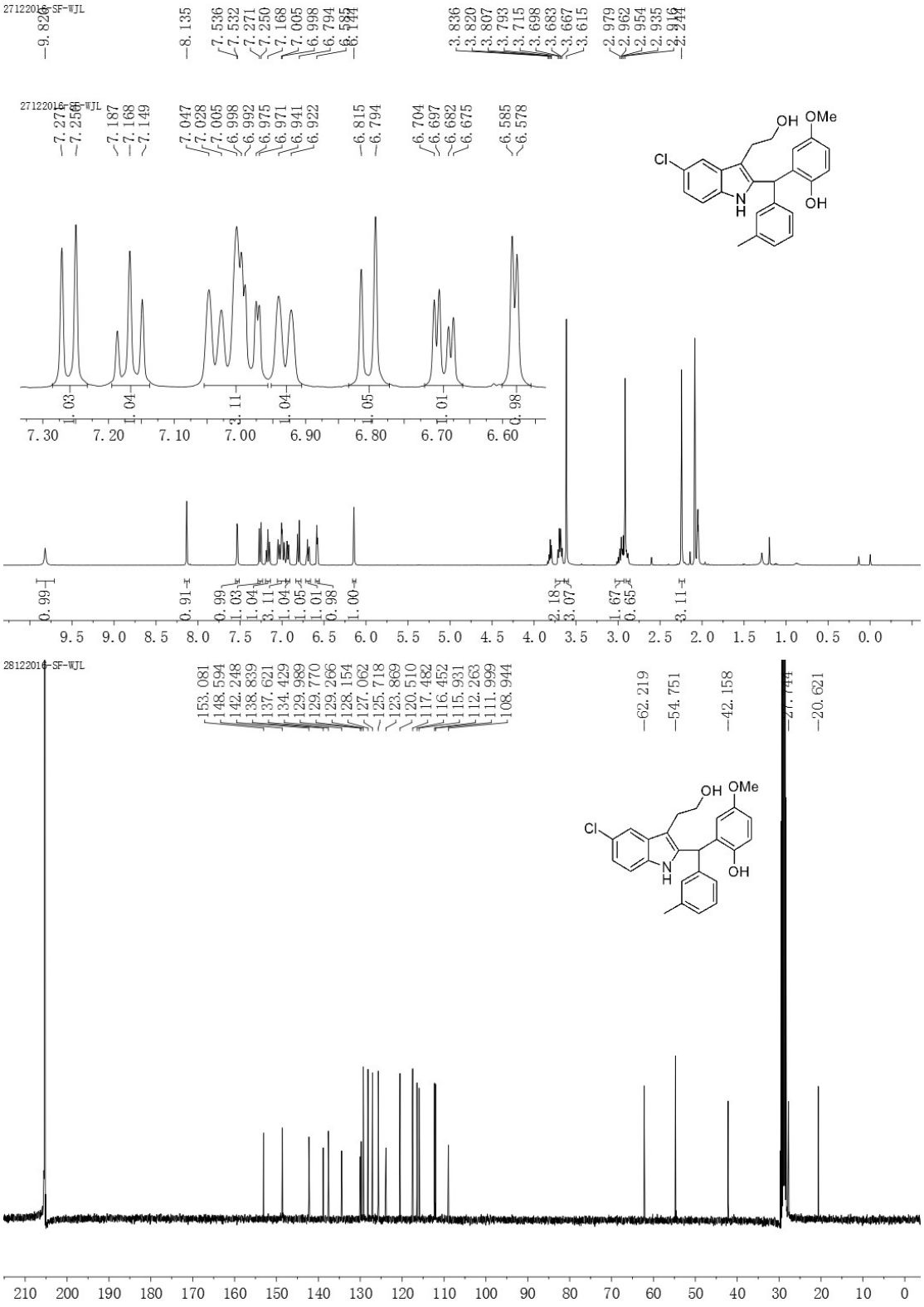
**3sa**


28112016-SF-WJL
9.565
8.307
7.270
7.252
7.152
7.133
6.990
6.973
6.896
6.883
6.785
6.765
3.832
3.726
3.712
3.697
3.018
3.002
2.987
2.968
2.950
2.922
2.132
7.537
7.517
7.290
7.270
7.252
7.215
7.198
7.181
7.152
7.133
7.025
7.008
6.990
6.973
6.955
6.917
6.896
6.883
6.785
6.765
OH
Me
N
H
OH
0.99
2.93
1.07
1.94
2.03
1.93
0.96
0.87
0.89
0.93
2.93
1.07
1.94
2.03
1.93
0.96
0.98
2.89
2.02
3.00
07122016-sf-wjl
152.523
142.955
136.881
136.090
130.572
128.776
128.723
128.611
128.344
128.176
128.118
126.101
120.593
118.533
118.003
115.388
110.927
108.748
62.329
42.008
21.365
19.892

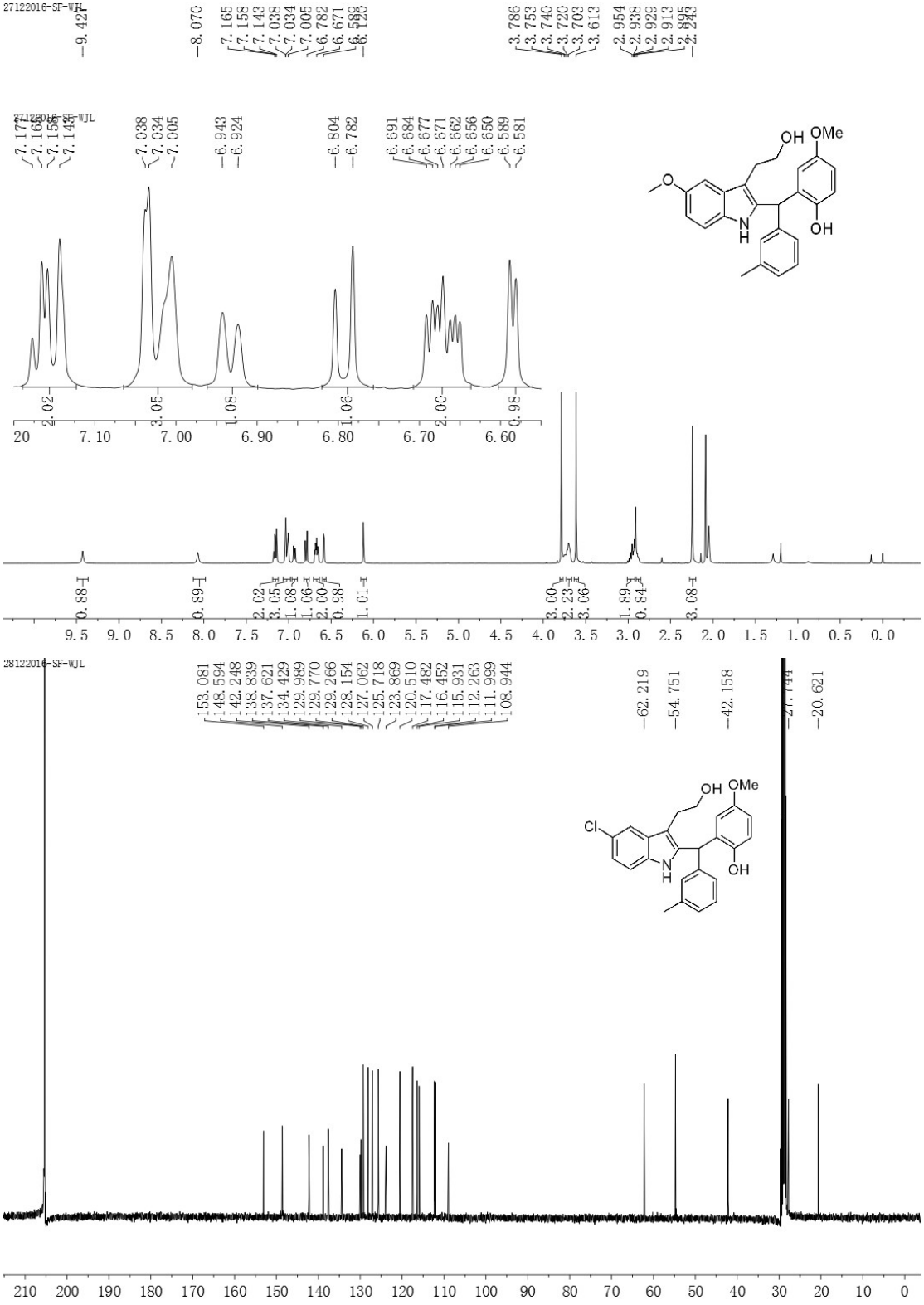
**3ta**


28112016-SF-WJL
9.634
8.107
7.541
7.522
7.302
7.284
7.265
7.225
7.208
7.190
7.167
7.148
6.994
6.821
6.799
6.628
6.621
6.193
6.030
6.013
6.994
6.975
6.957
6.821
6.799
6.705
6.698
6.684
6.676
6.628
6.621
3.741
3.724
3.618
3.045
3.026
3.010
2.995
2.977
2.959
2.942
OH
OMe
OH
N
H
07122016-sf-wjl-C
153.057
148.678
142.750
136.676
136.135
130.027
128.675
128.606
128.163
126.193
120.641
118.555
118.016
116.453
115.922
112.021
110.956
108.828
62.318
54.775
42.171
27.951

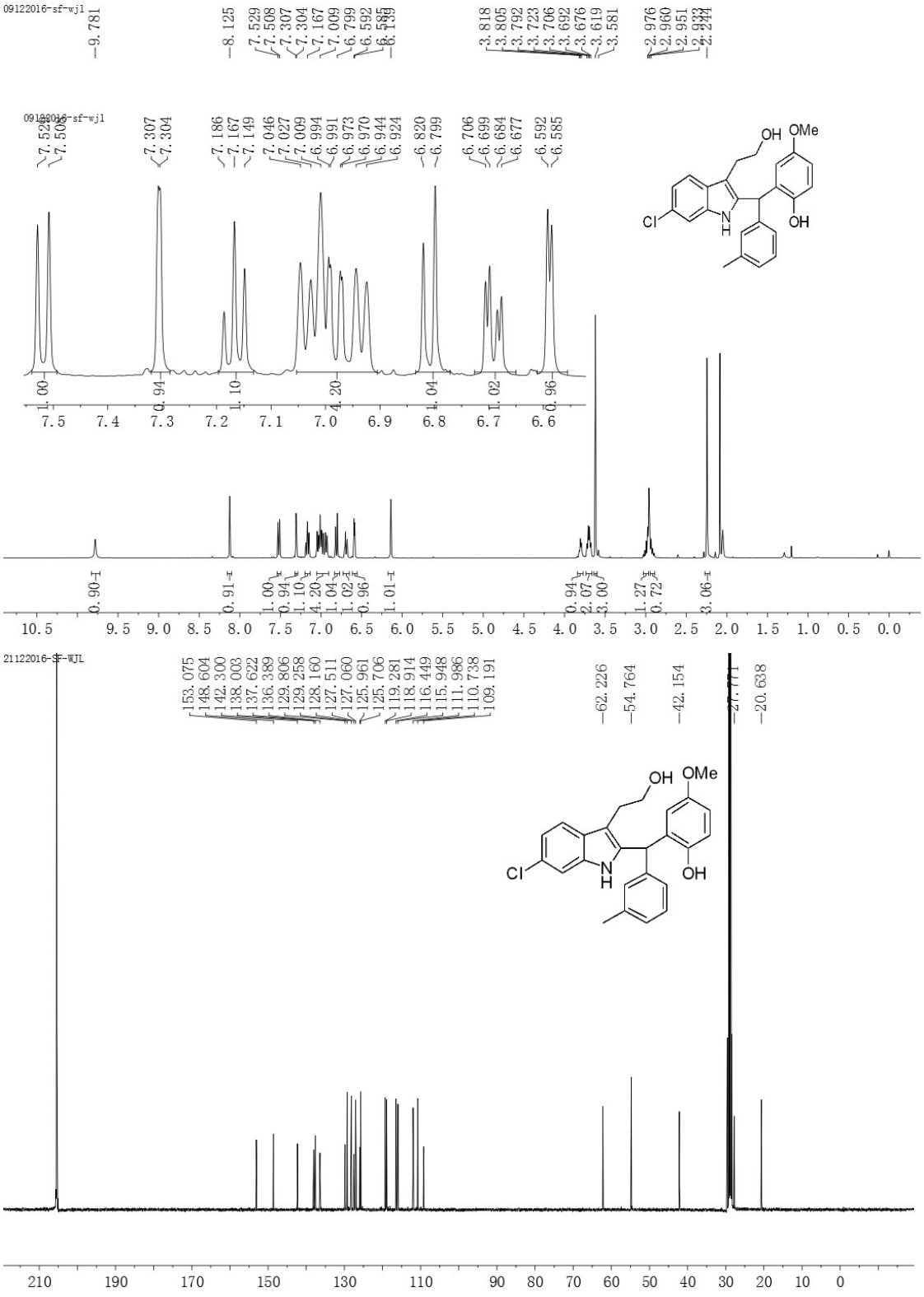
## 3jb



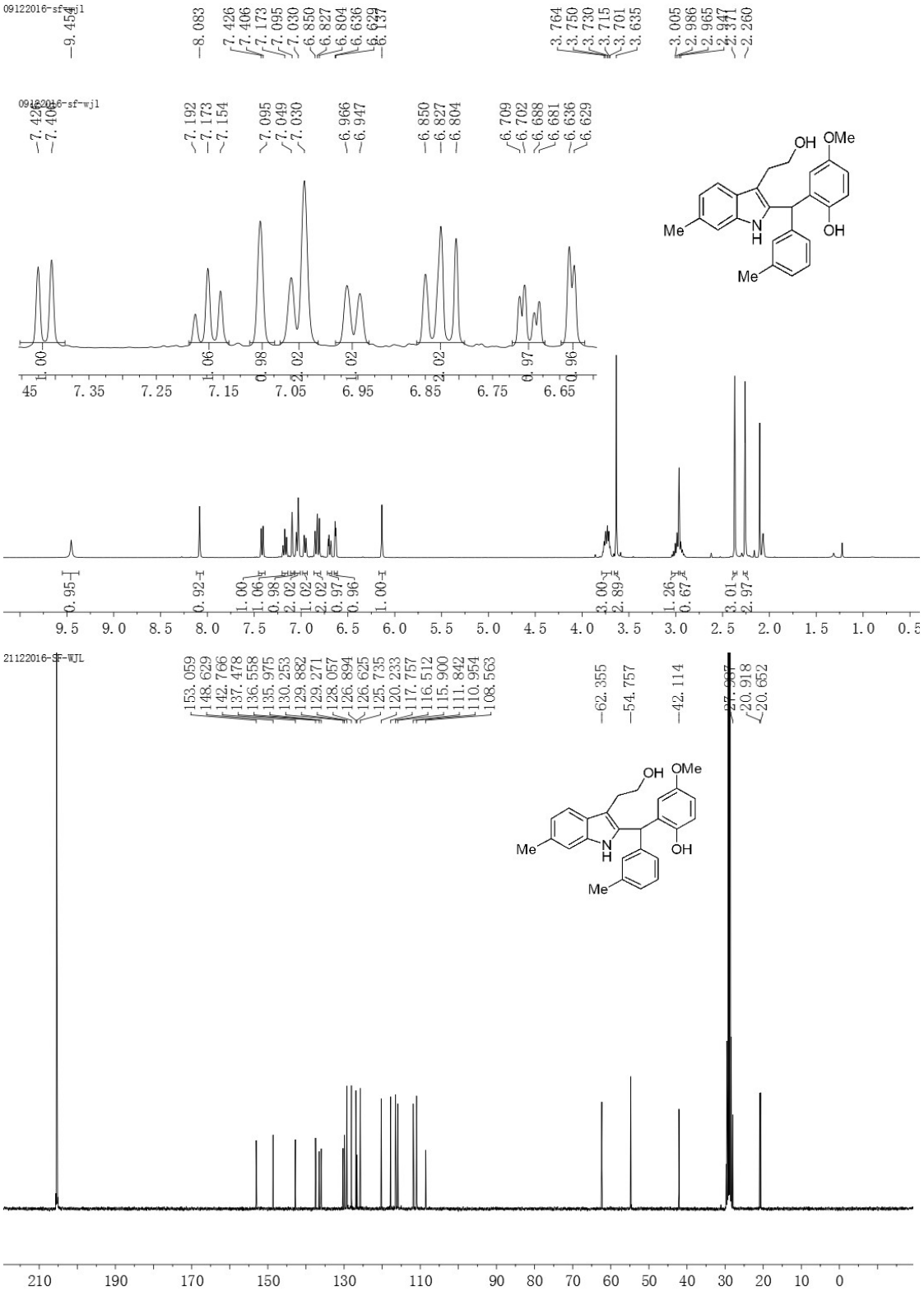
## 3jc


27122016-SF-WJL
9.427
8.070
7.165
7.158
7.143
7.038
7.034
7.005
6.782
6.671
6.120
3.786
3.753
3.740
3.720
3.703
3.613
2.954
2.938
2.929
2.913
7.038
7.034
7.005
6.943
6.924
6.804
6.782
6.691
6.684
6.677
6.671
6.662
6.656
6.650
6.589
6.581
OH
OMe
O
N
H
OH
2.02
3.05
1.08
1.06
2.00
0.98
1.01
3.00
2.23
3.06
1.89
0.84
3.08
28122016-SF-WJL
153.081
148.594
142.248
138.839
137.621
134.429
129.989
129.770
129.266
128.154
127.062
125.718
123.869
120.510
117.482
116.452
115.931
112.263
111.999
108.944
62.219
54.751
42.158
27.744
20.621
OH
OMe
Cl
N
H
OH

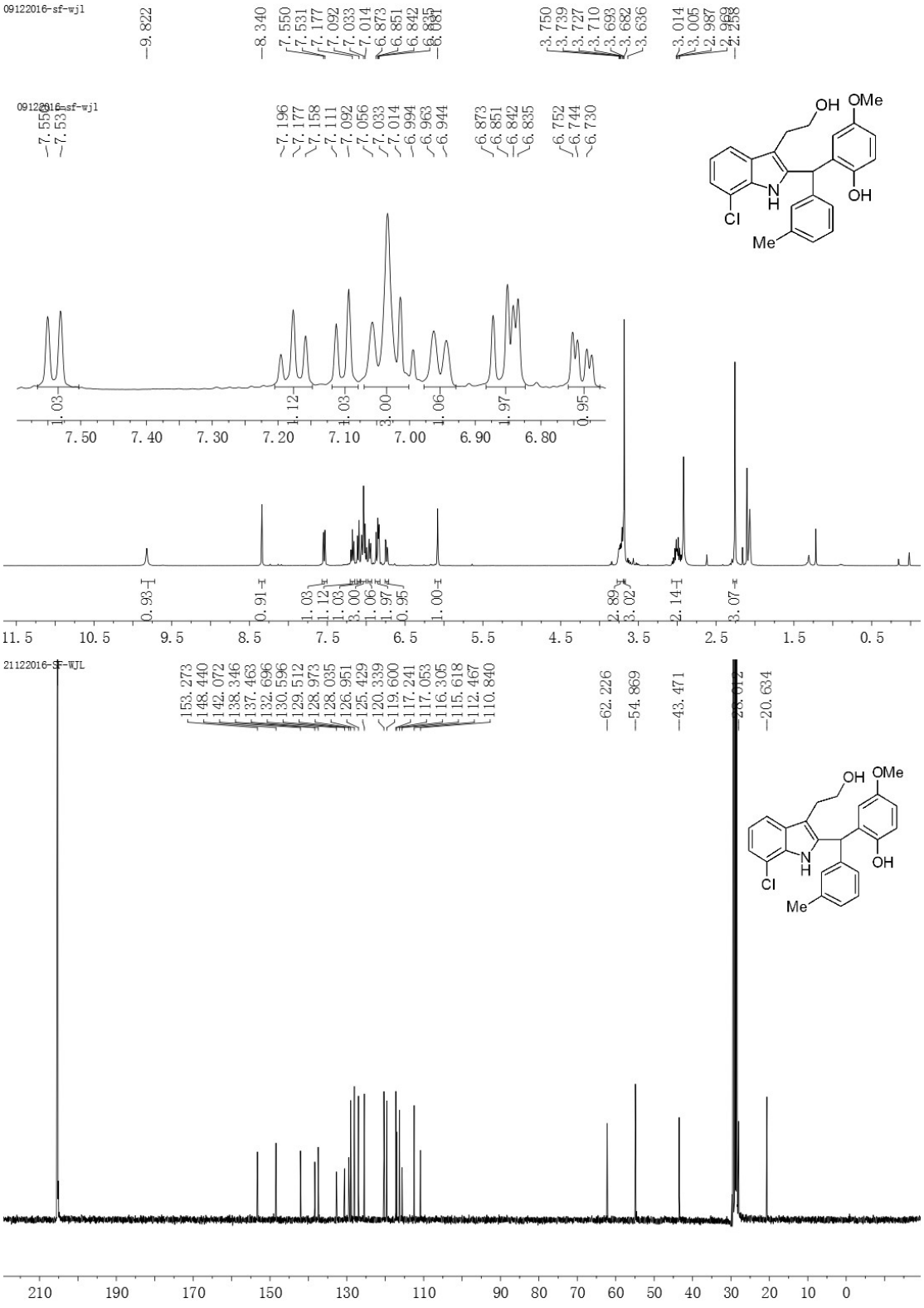
## 3jd



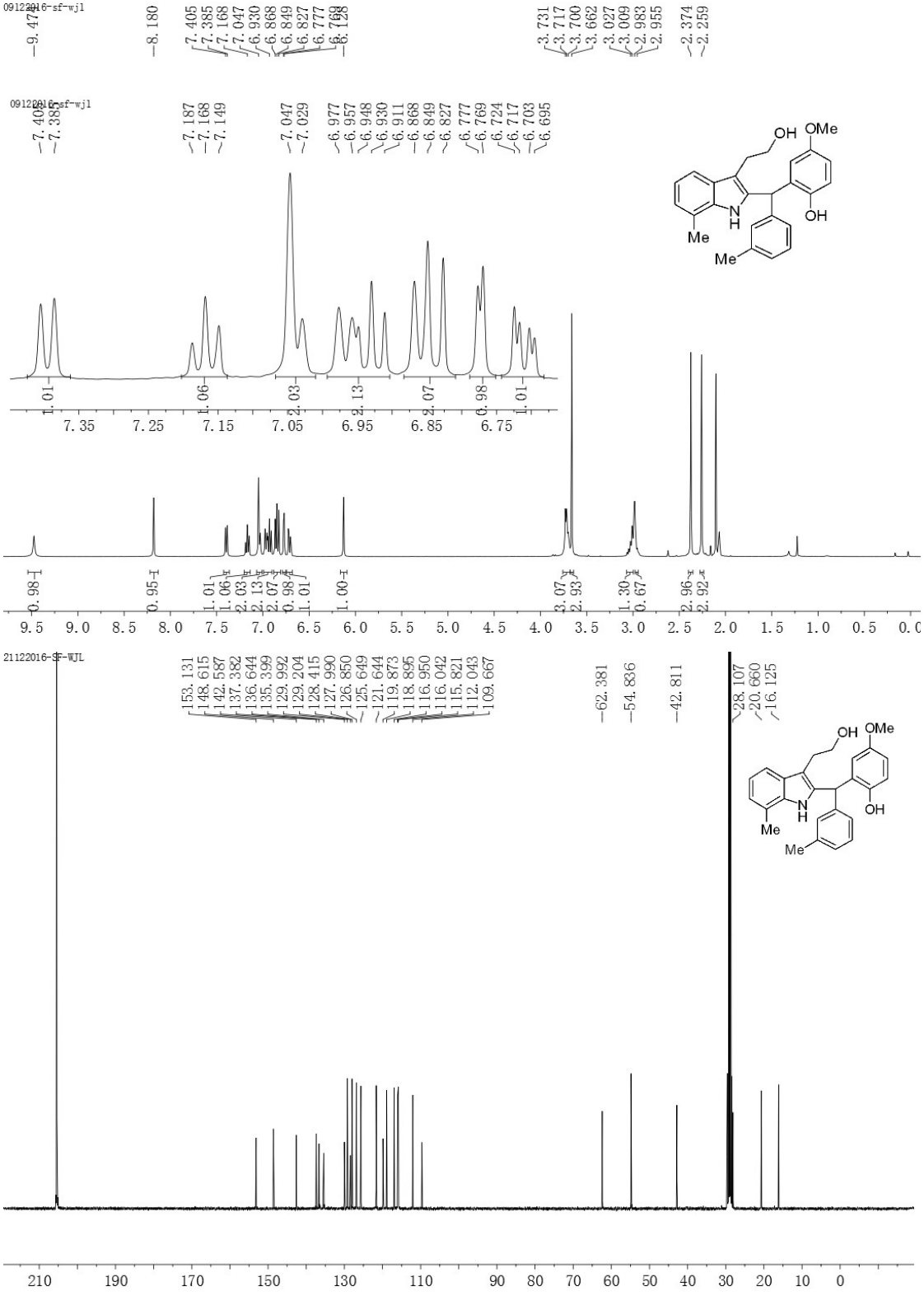
## 3je



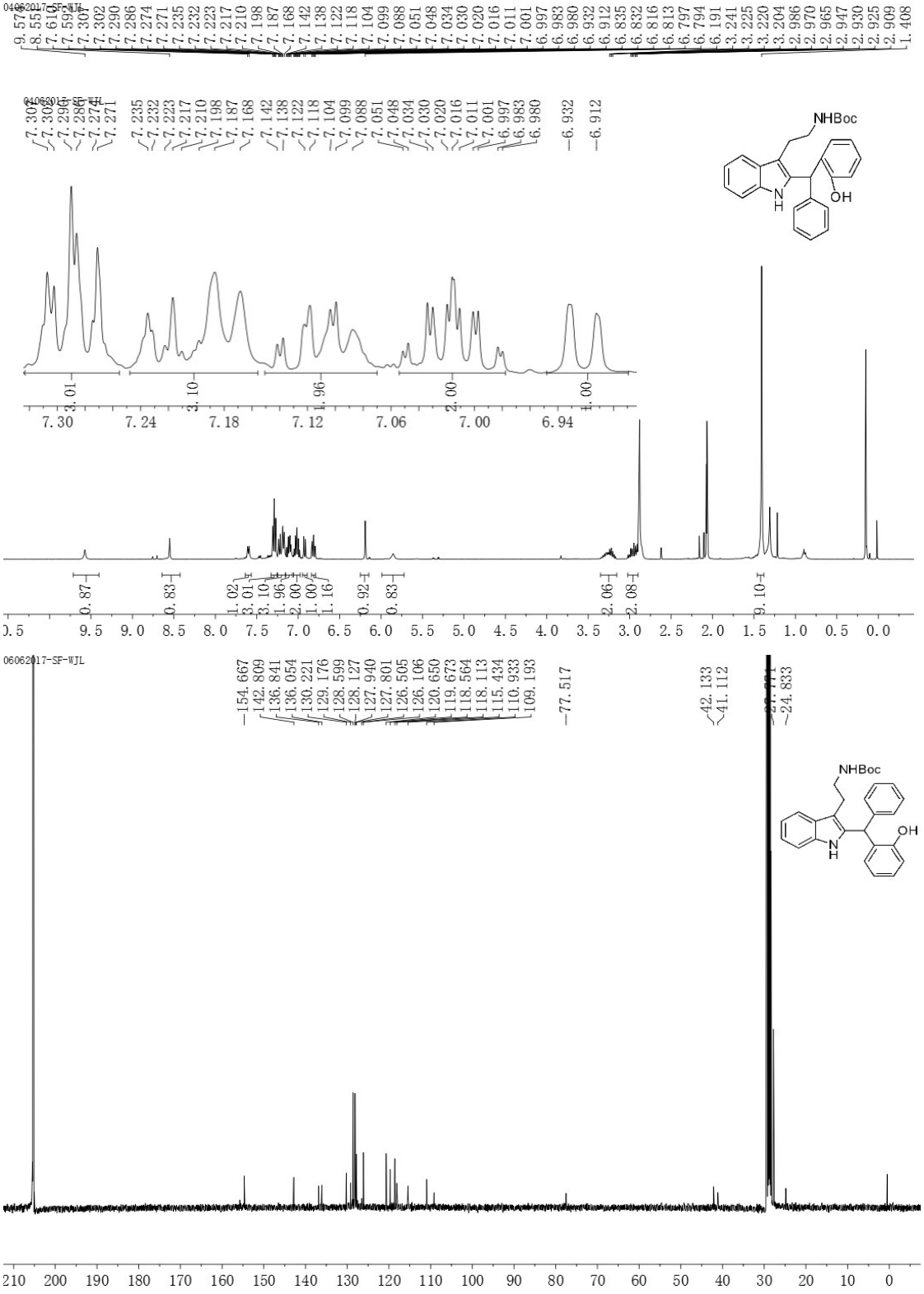
## 3jf



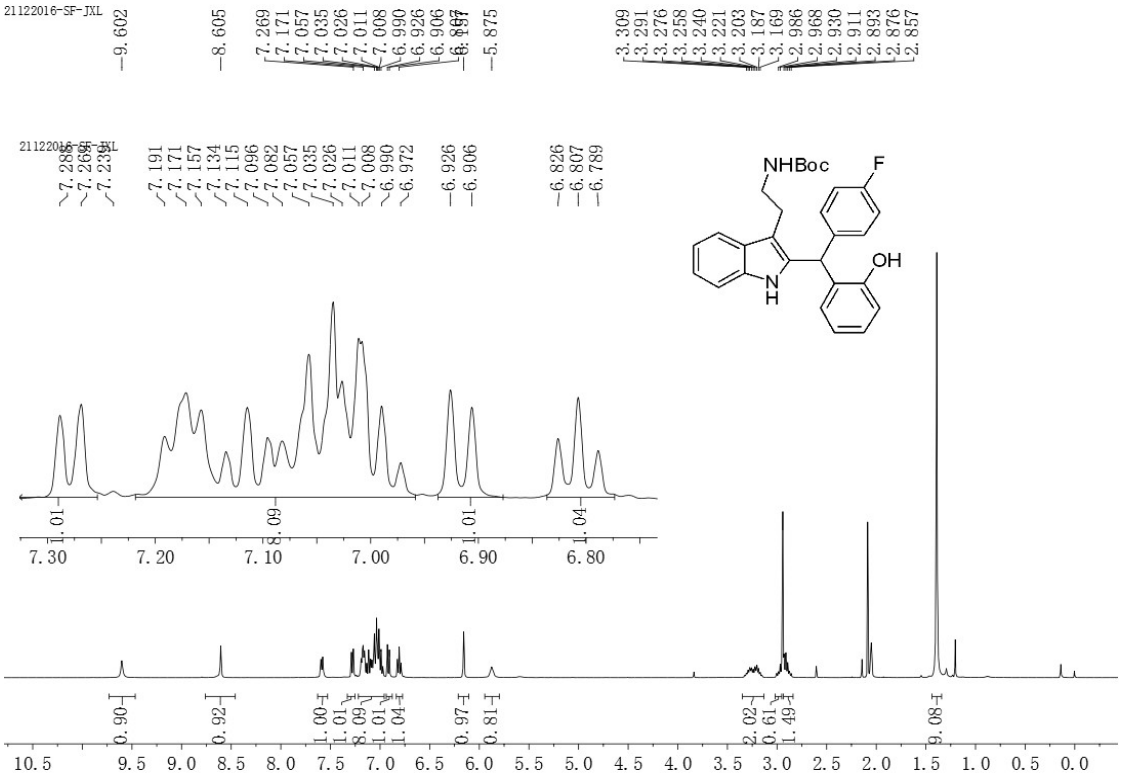
## 3jg

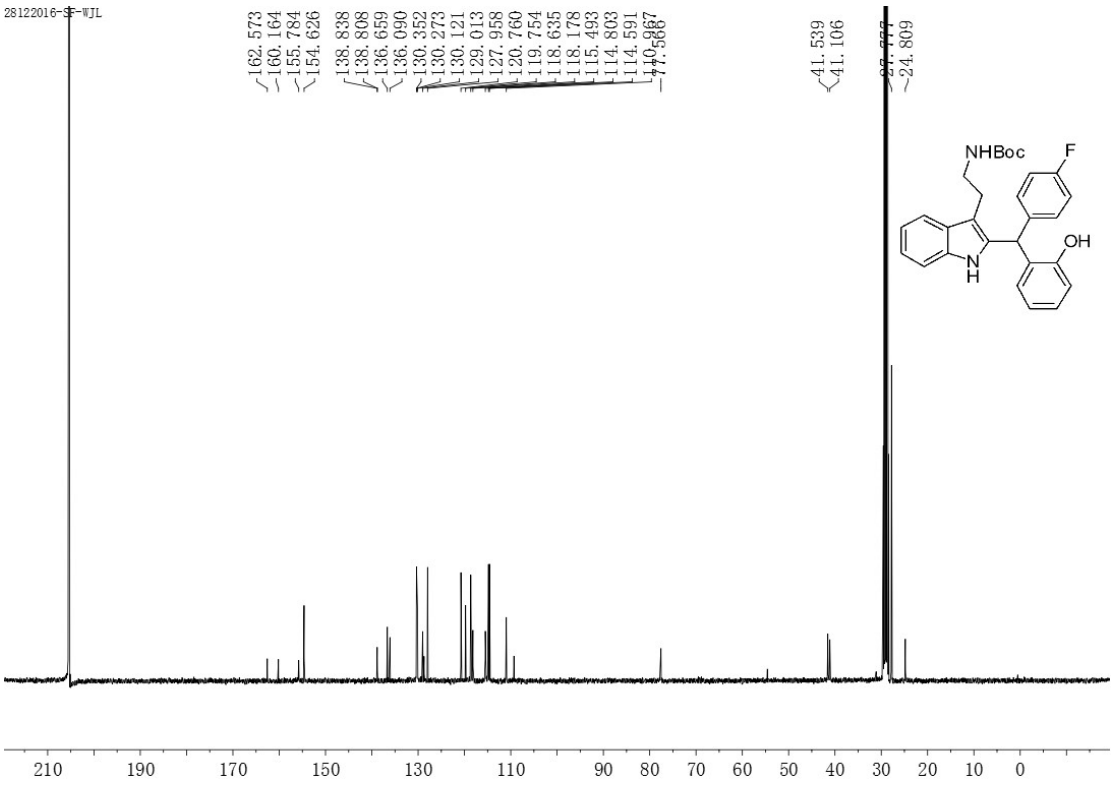

09122016-sf-wjl
9.474
8.180
7.405
7.385
7.168
7.047
6.930
6.868
6.849
6.827
6.777
6.769
6.128
3.731
3.717
3.700
3.662
3.027
3.009
2.983
2.955
2.374
2.259
7.187
7.168
7.149
7.047
7.029
6.977
6.957
6.948
6.930
6.911
6.868
6.849
6.827
6.777
6.769
6.724
6.717
6.703
6.695
OH
OMe
OH
N
H
Me
Me
1.01
1.06
2.03
2.13
2.07
6.98
1.01
7.35
7.25
7.15
7.05
6.95
6.85
6.75
0.98
0.95
1.01
1.06
2.03
2.13
2.07
0.98
1.01
1.00
3.07
2.93
1.30
0.67
2.96
2.92
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
21122016-SF-WJL
153.131
148.615
142.587
137.382
136.644
135.399
129.992
129.204
128.415
127.990
126.850
125.649
121.644
119.873
118.895
116.950
116.042
115.821
112.043
109.667
62.381
54.836
42.811
28.107
20.660
16.125
OH
OMe
OH
N
H
Me
Me
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

**8aa**

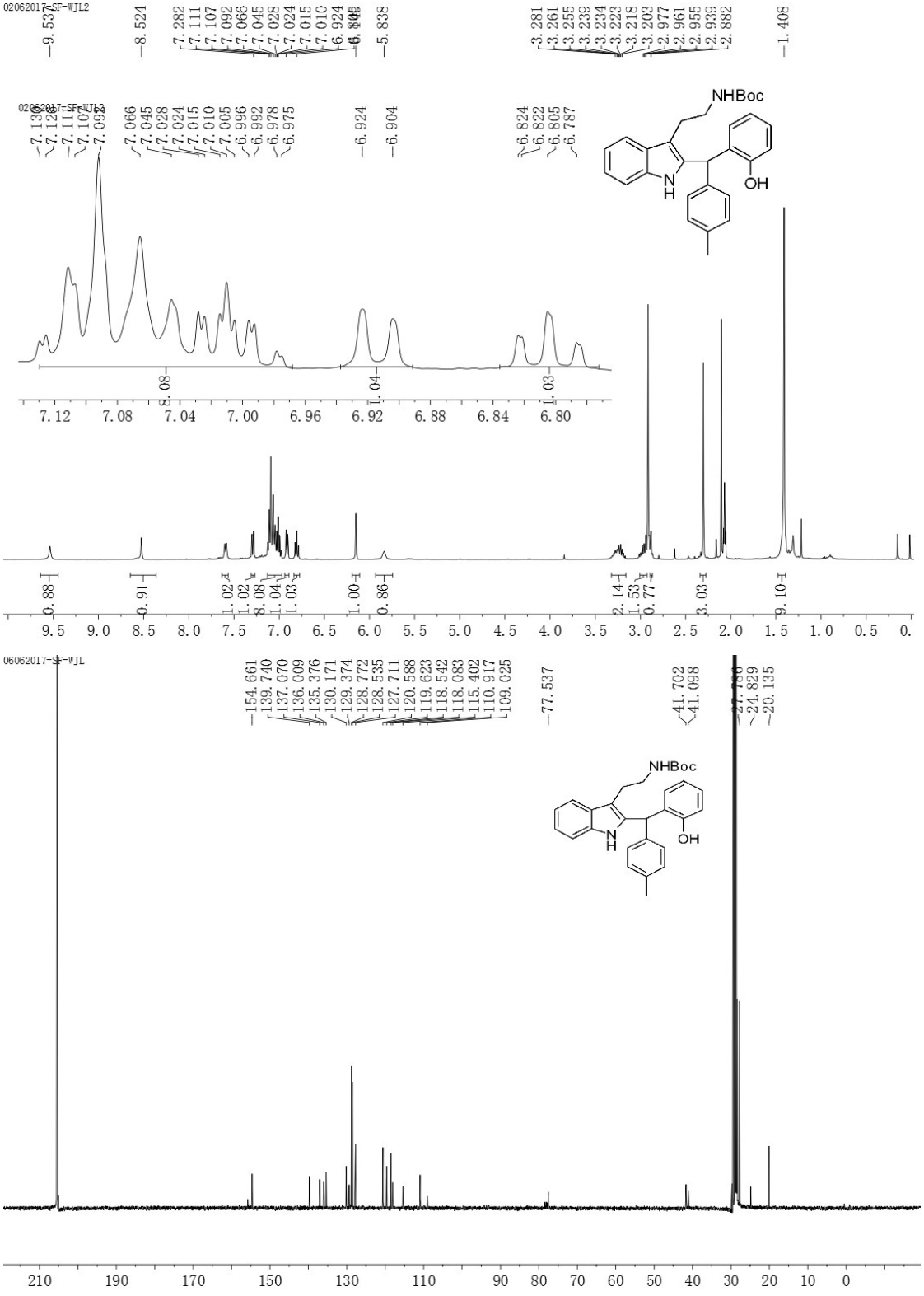


## 8ba

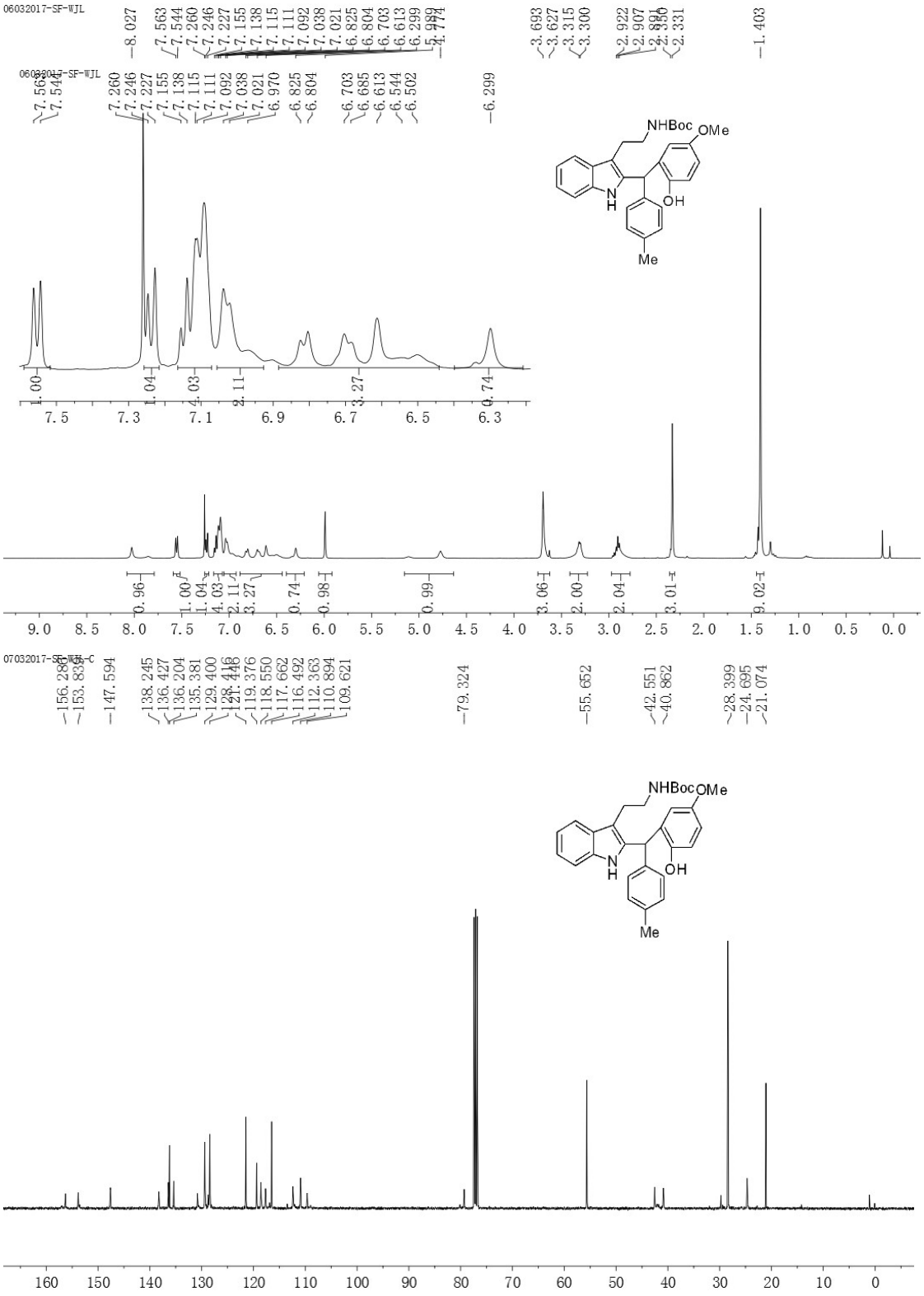


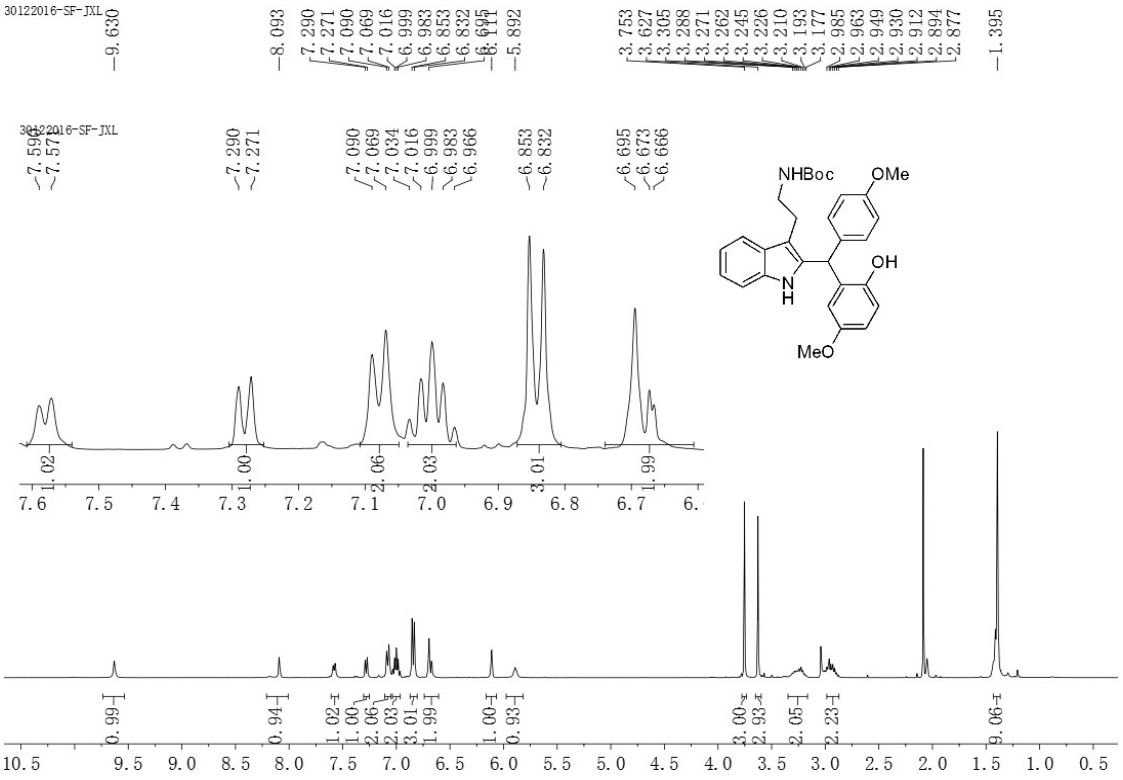
## 8ca

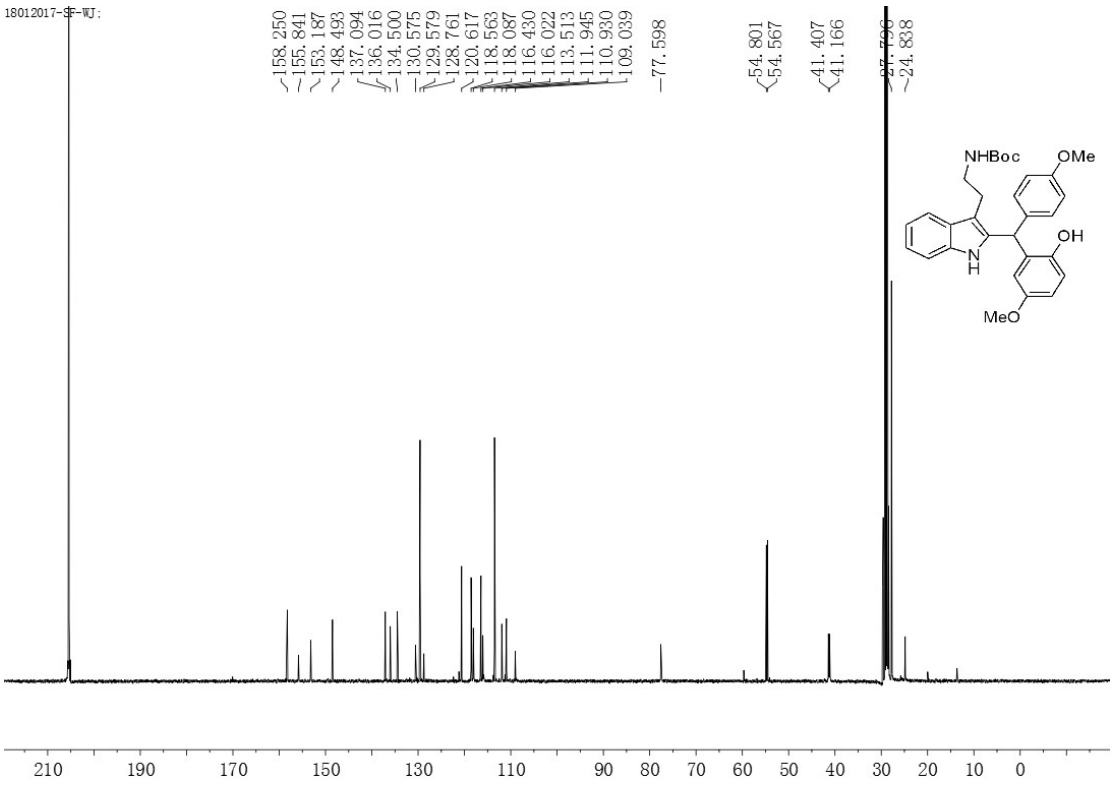


## 8ha

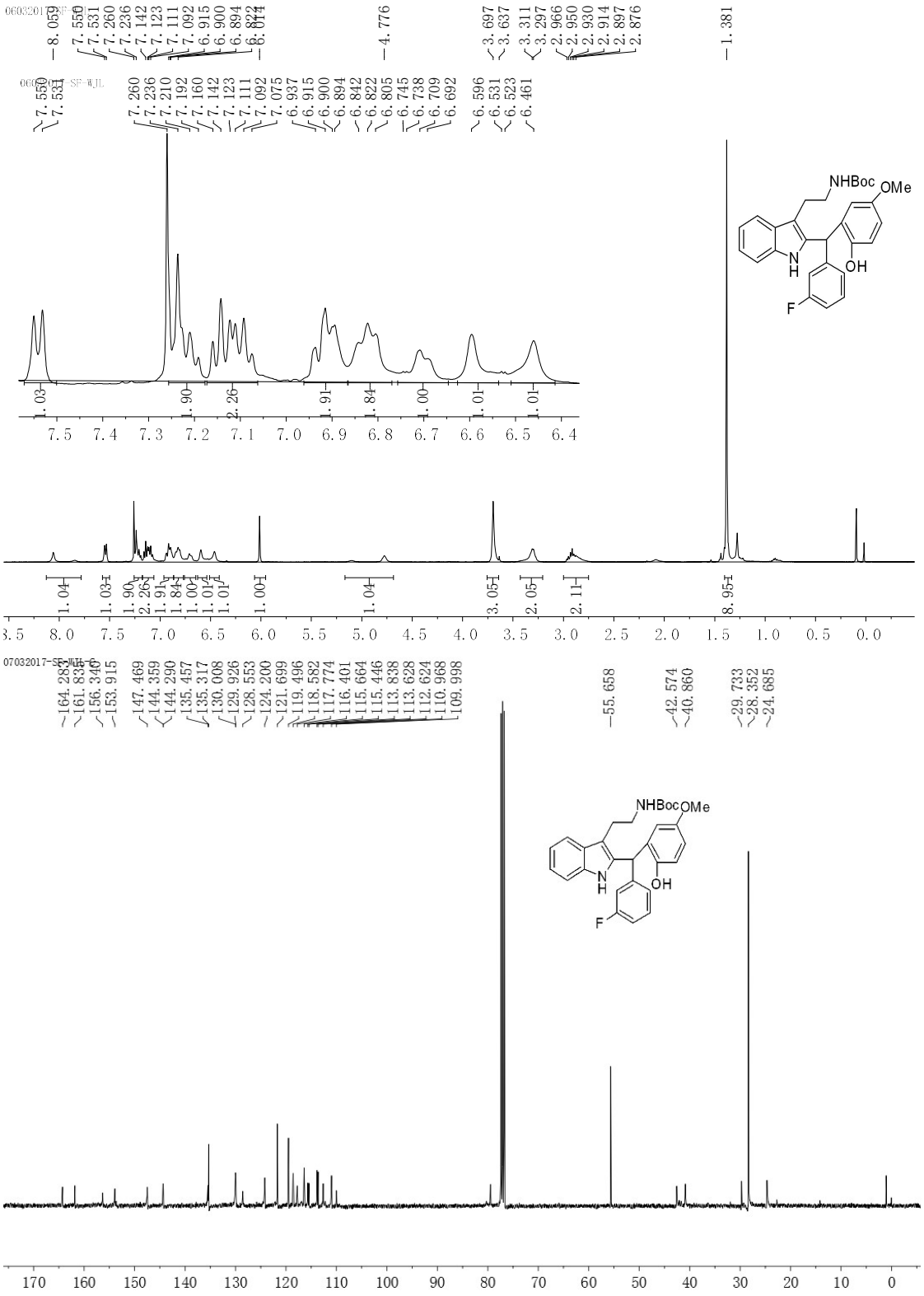


## 3ua

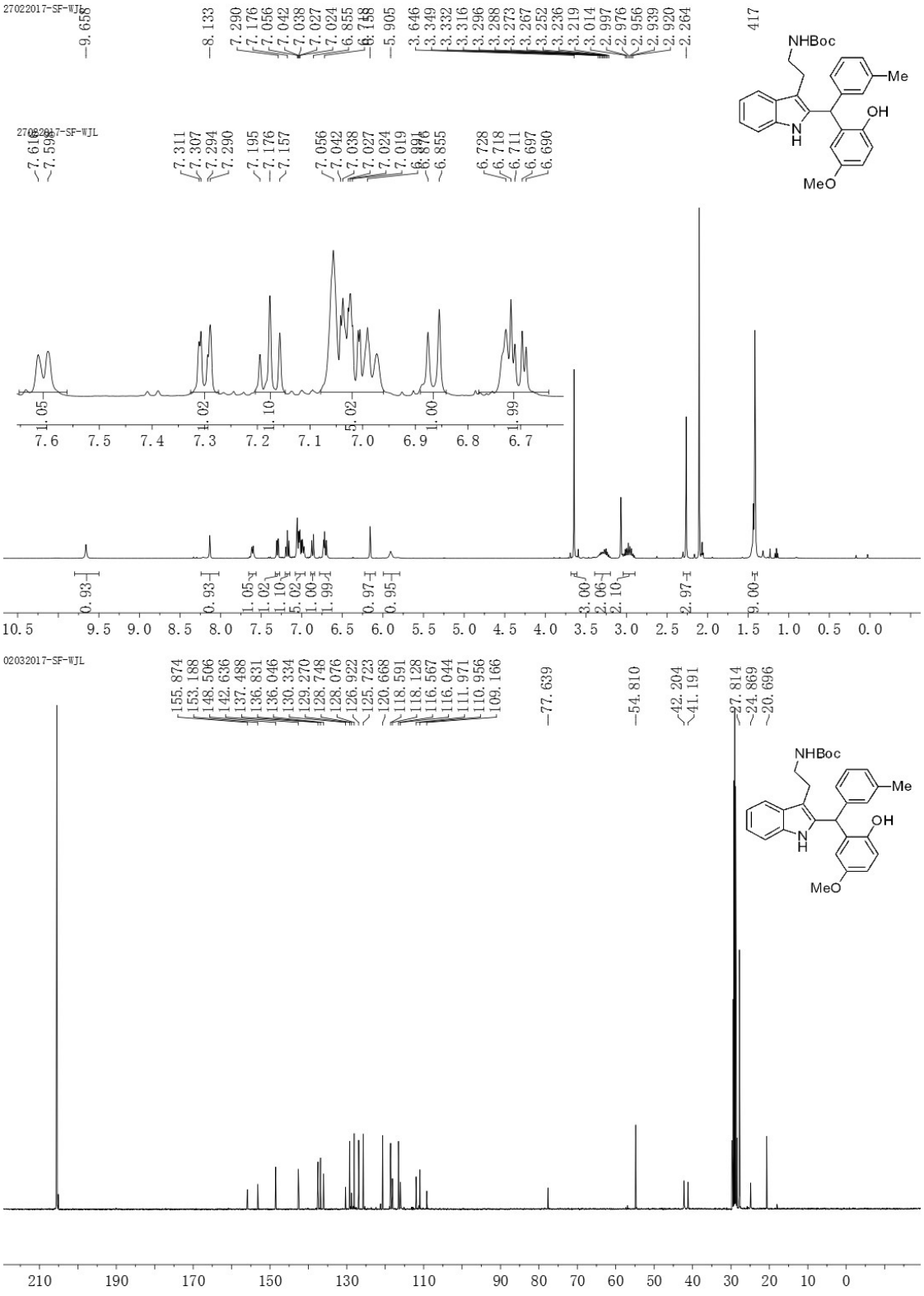

30122016-SF-JXL
NHBoc
OMe
OH
MeO


18012017-SF-WJ:
NHBoc
OMe
OH
MeO

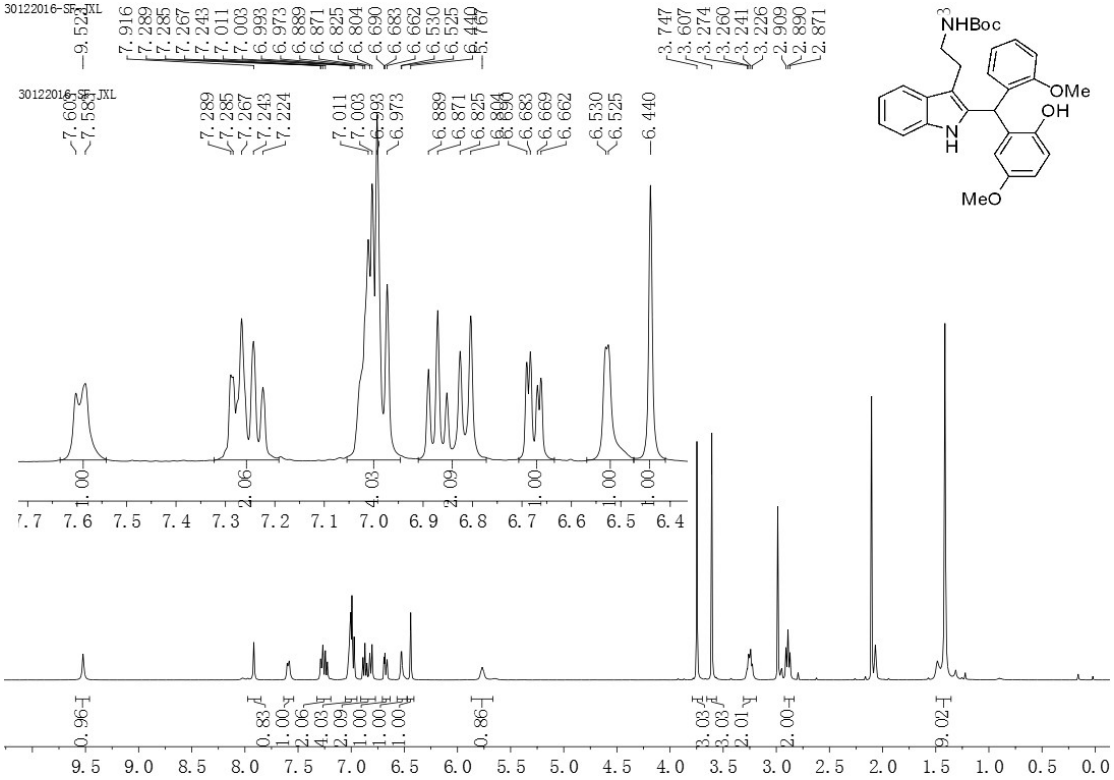
**8ia**

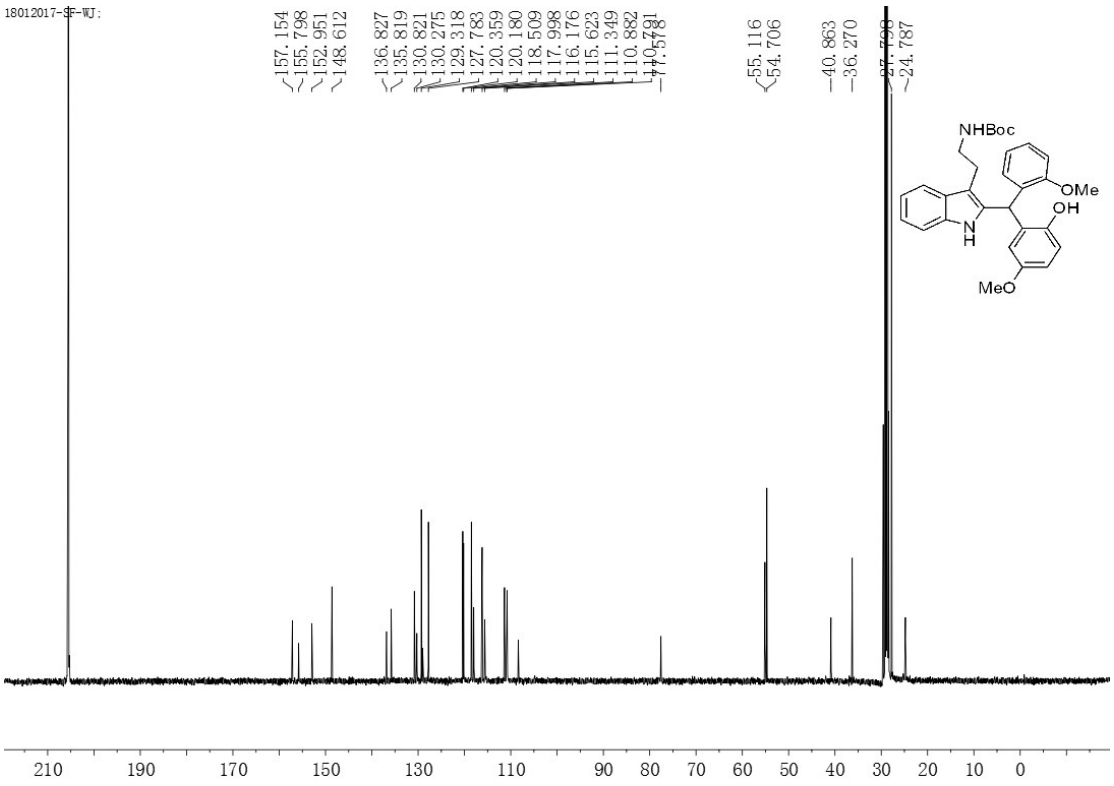


## 8ja

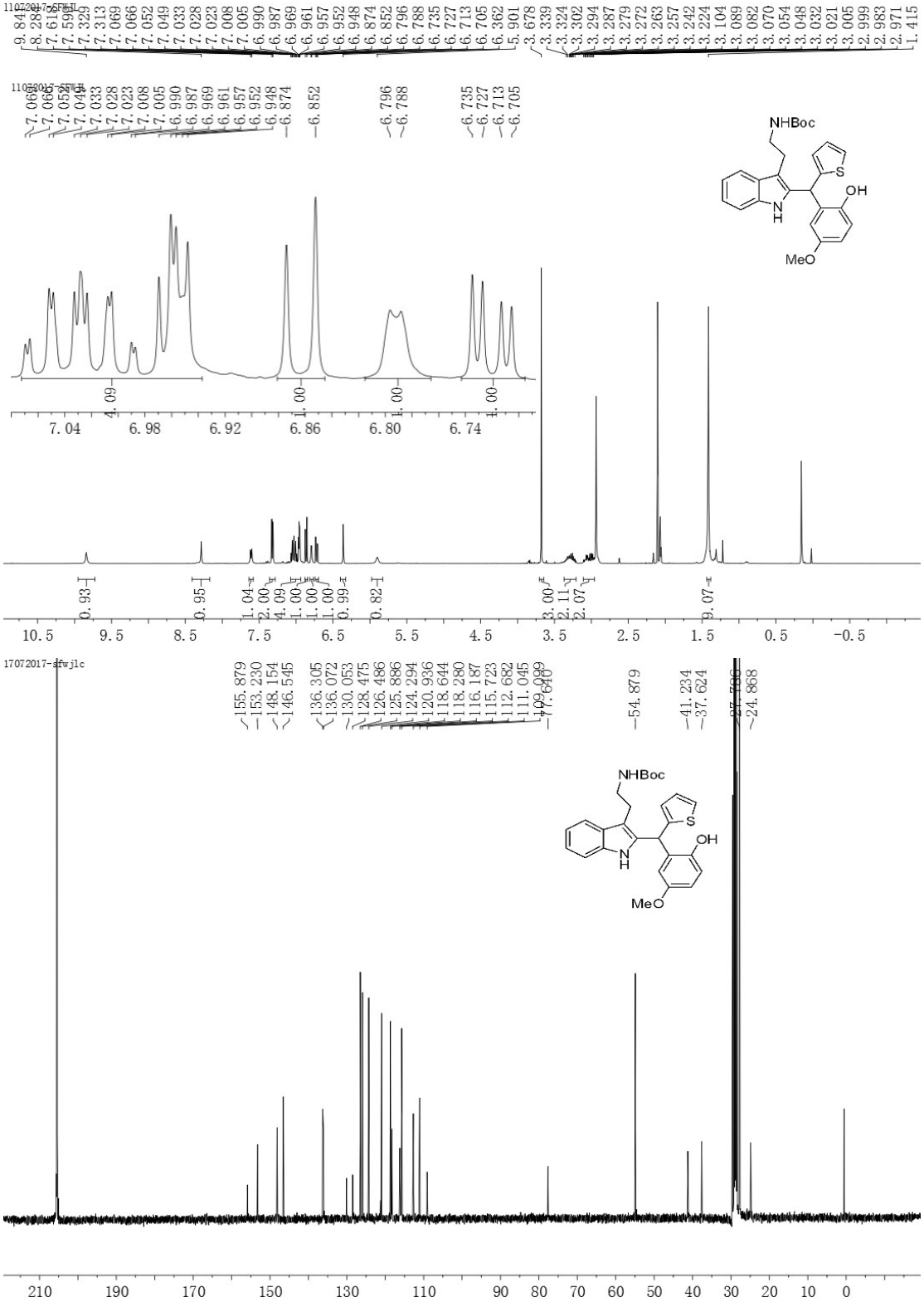


## 8ka

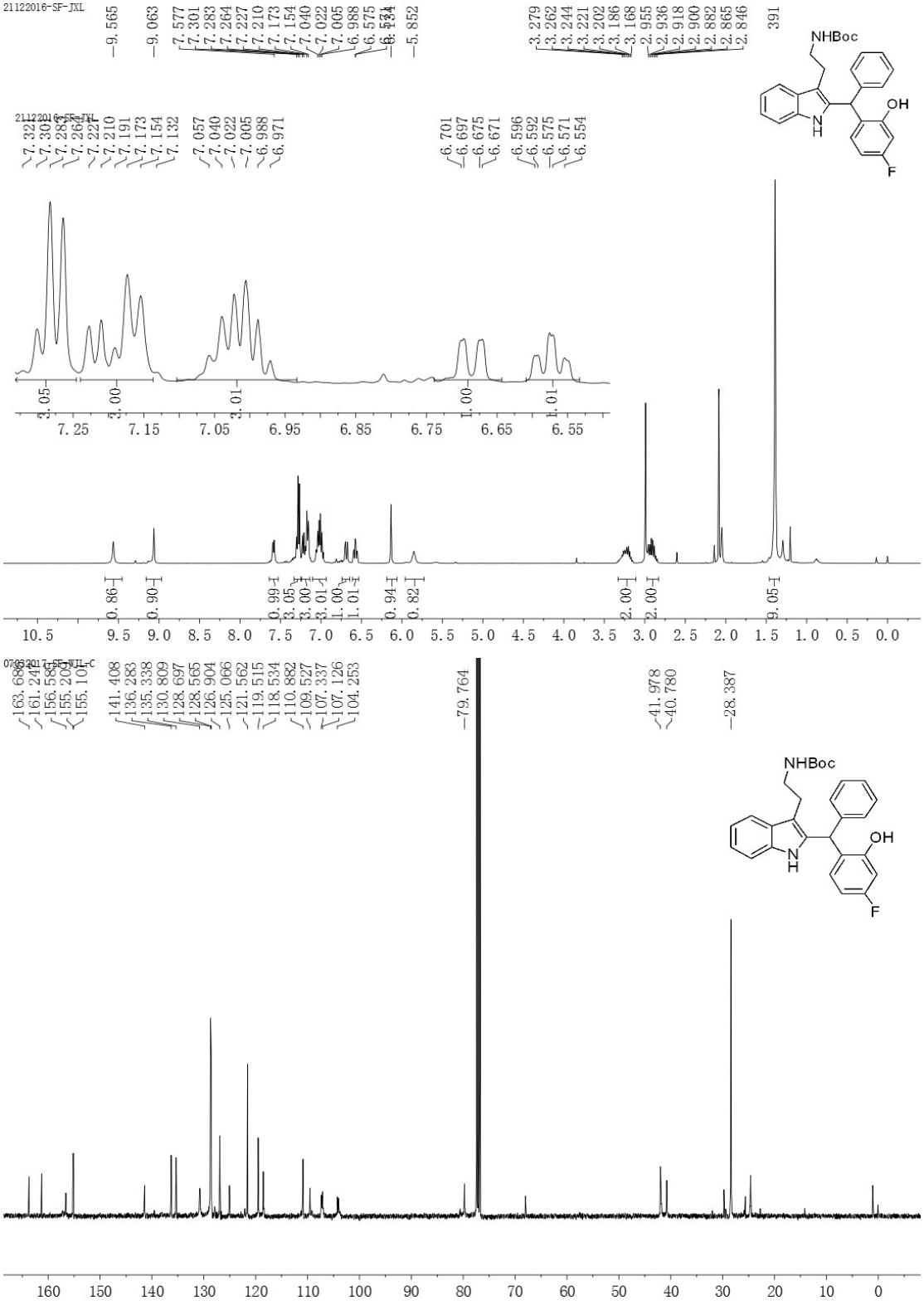

30122016-SF-JXL
NHBoc
OMe
OH
MeO


18012017-SF-WJ:
NHBoc
OMe
OH
MeO

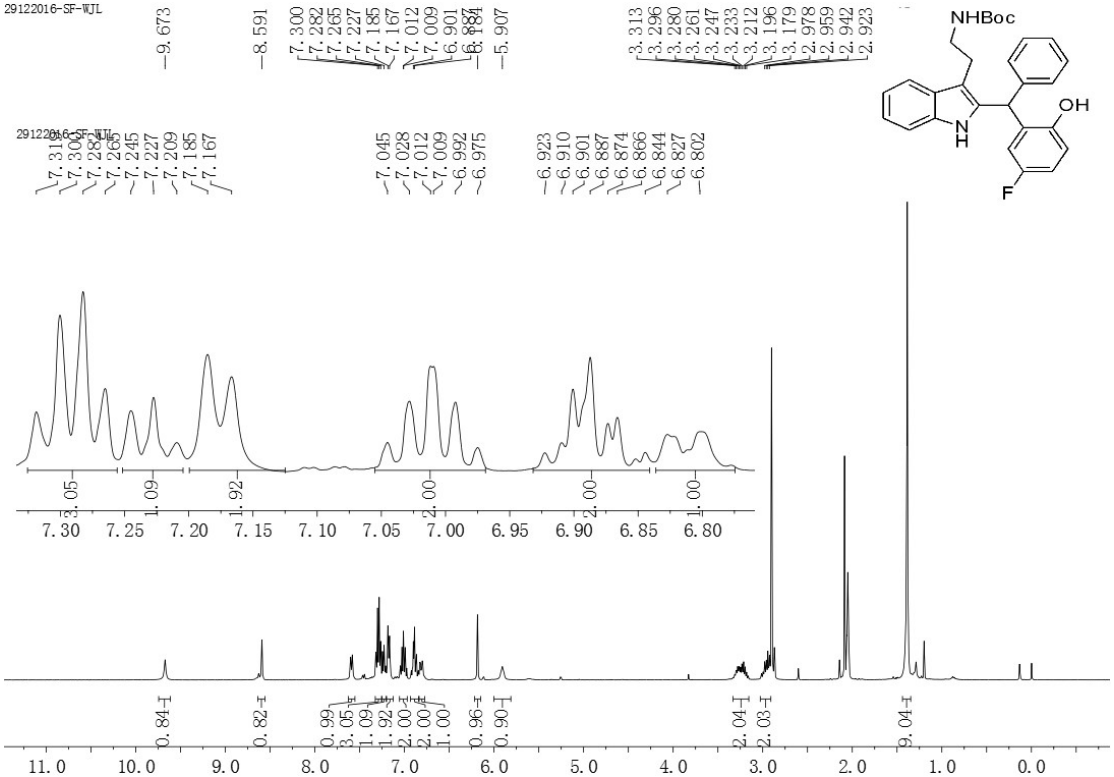
**8la**

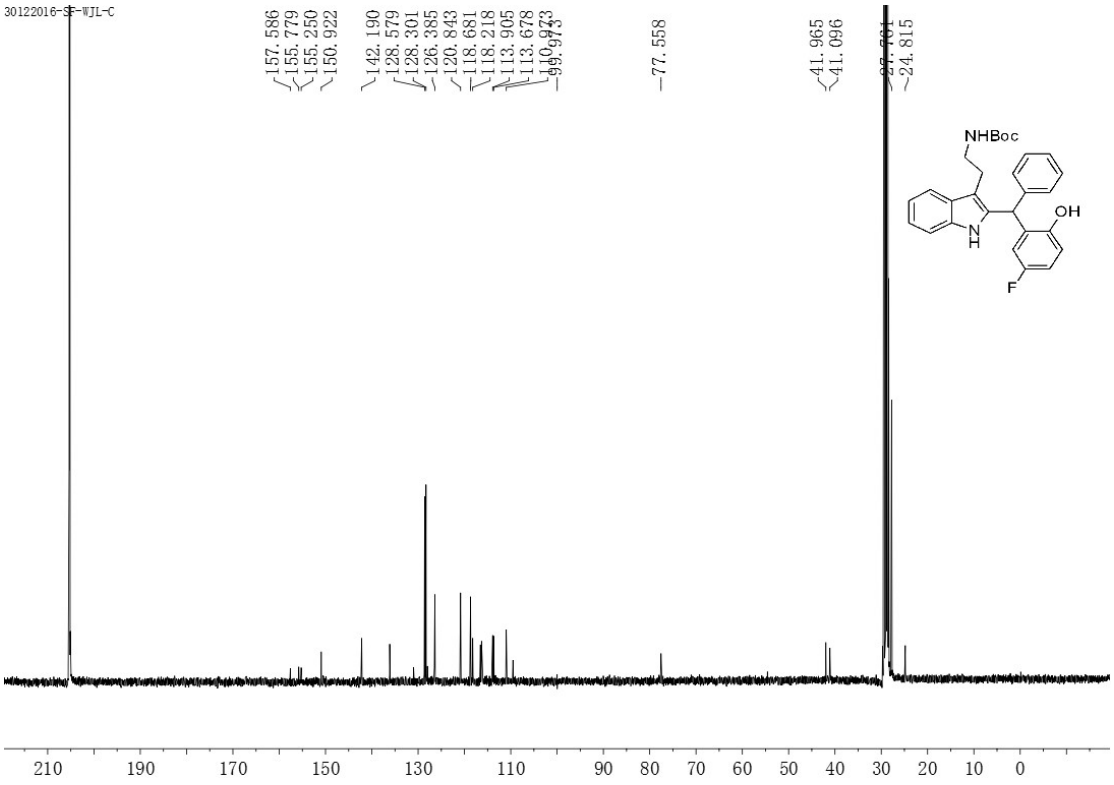

NHBoc
OH
MeO
S
N
H
7.04
6.98
6.92
6.86
6.80
6.74
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0

## 8na

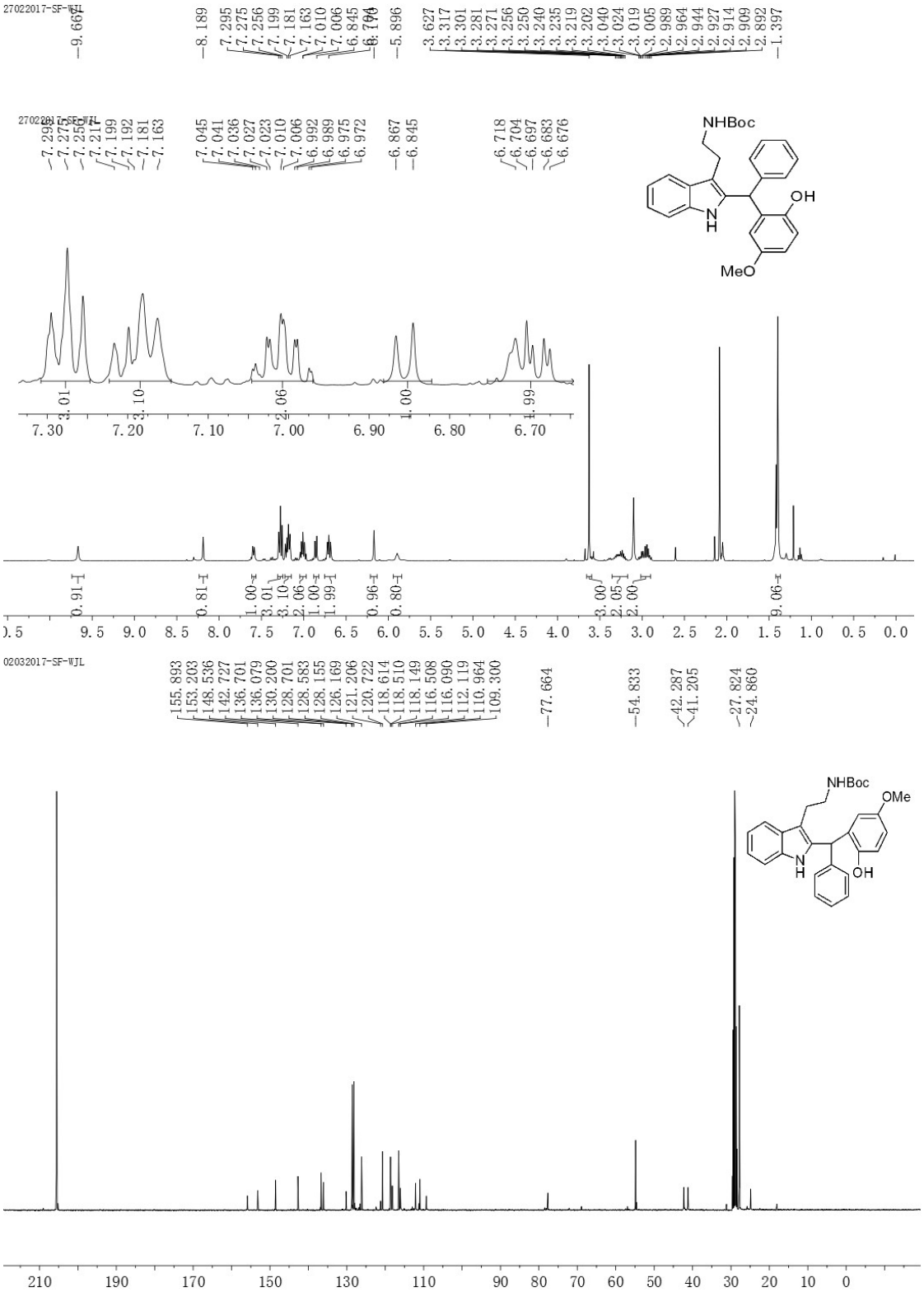

21122016-SF-JXL
NHBoc
OH
F
7.25
7.15
7.05
6.95
6.85
6.75
6.65
6.55
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

## 8pa

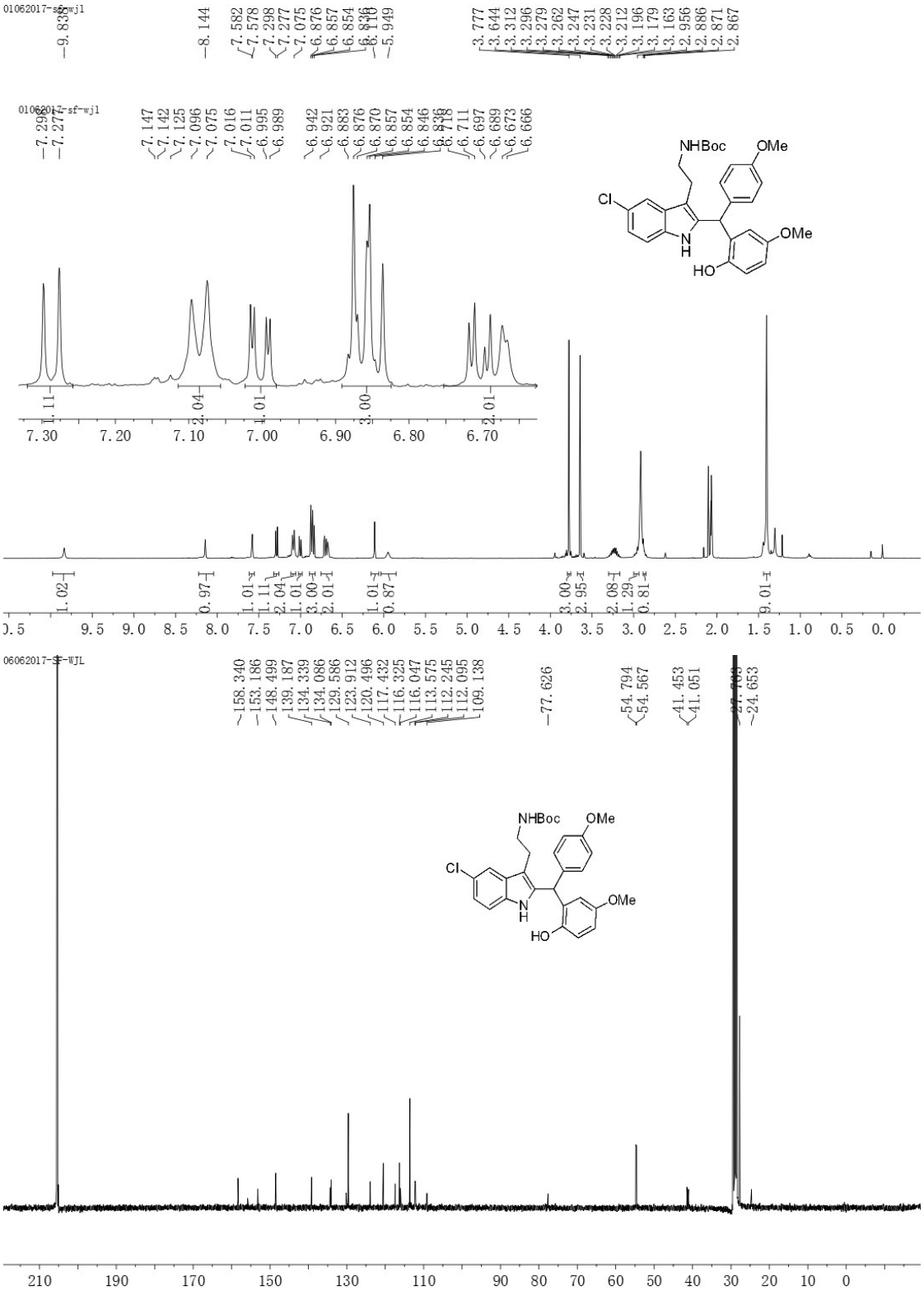


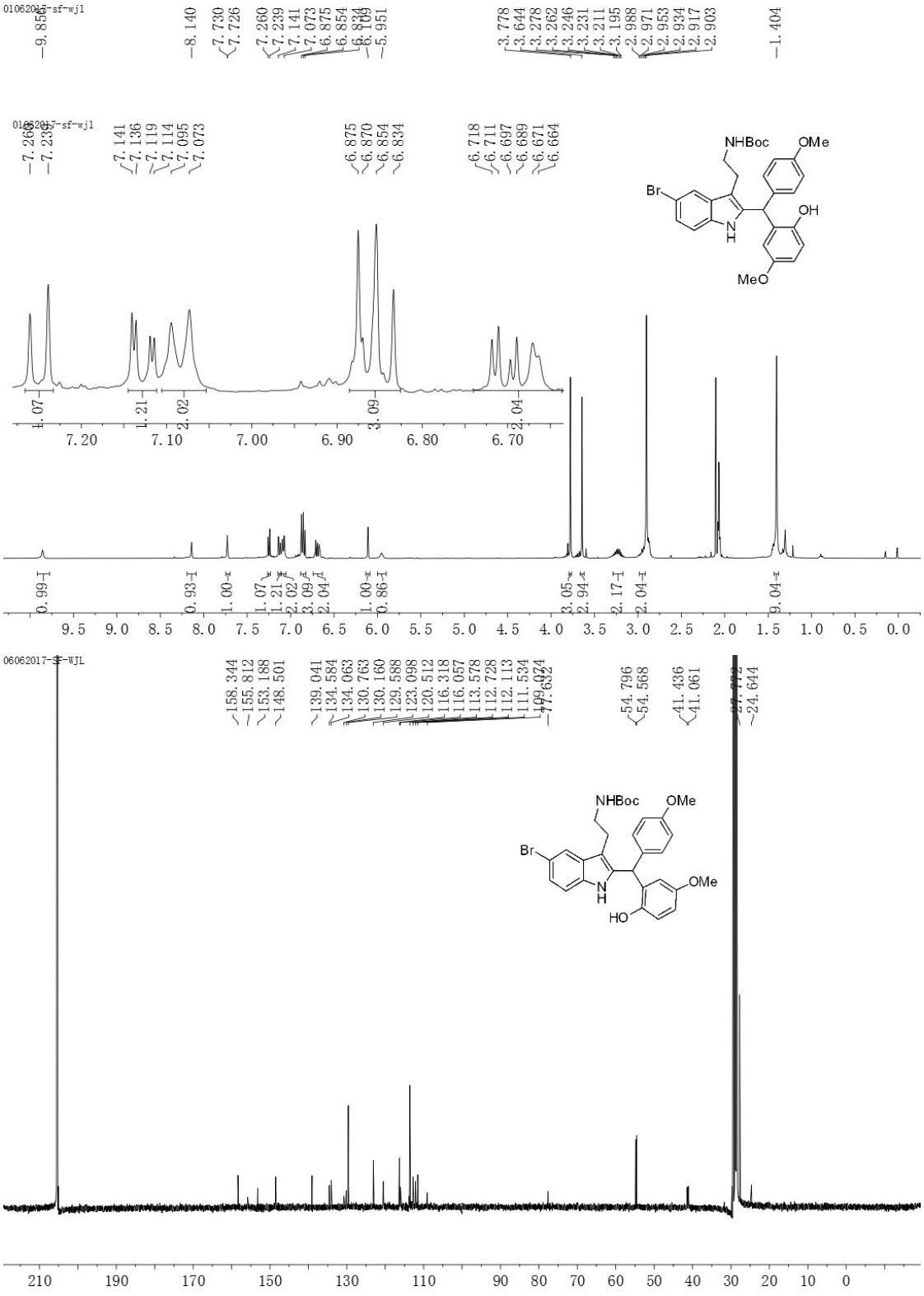
## 8ta



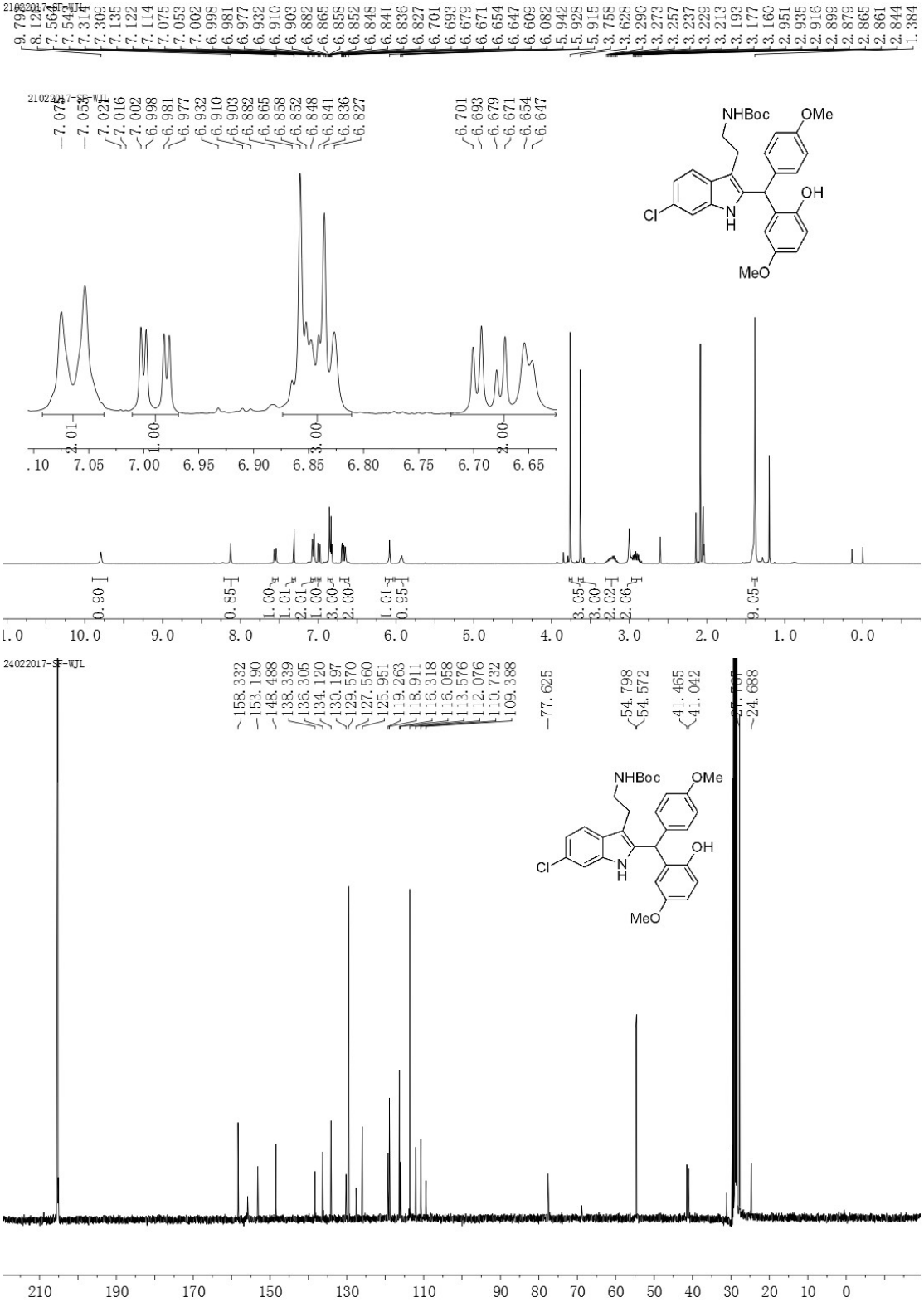
## 8ub



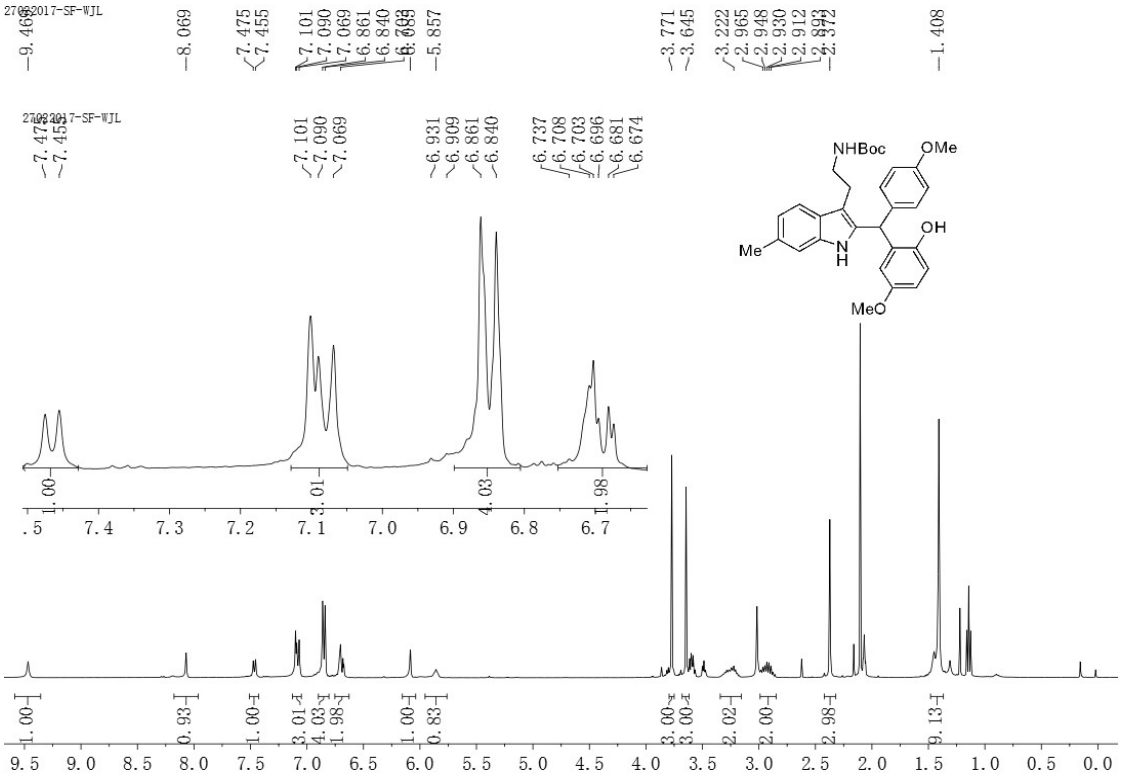
## 8uc

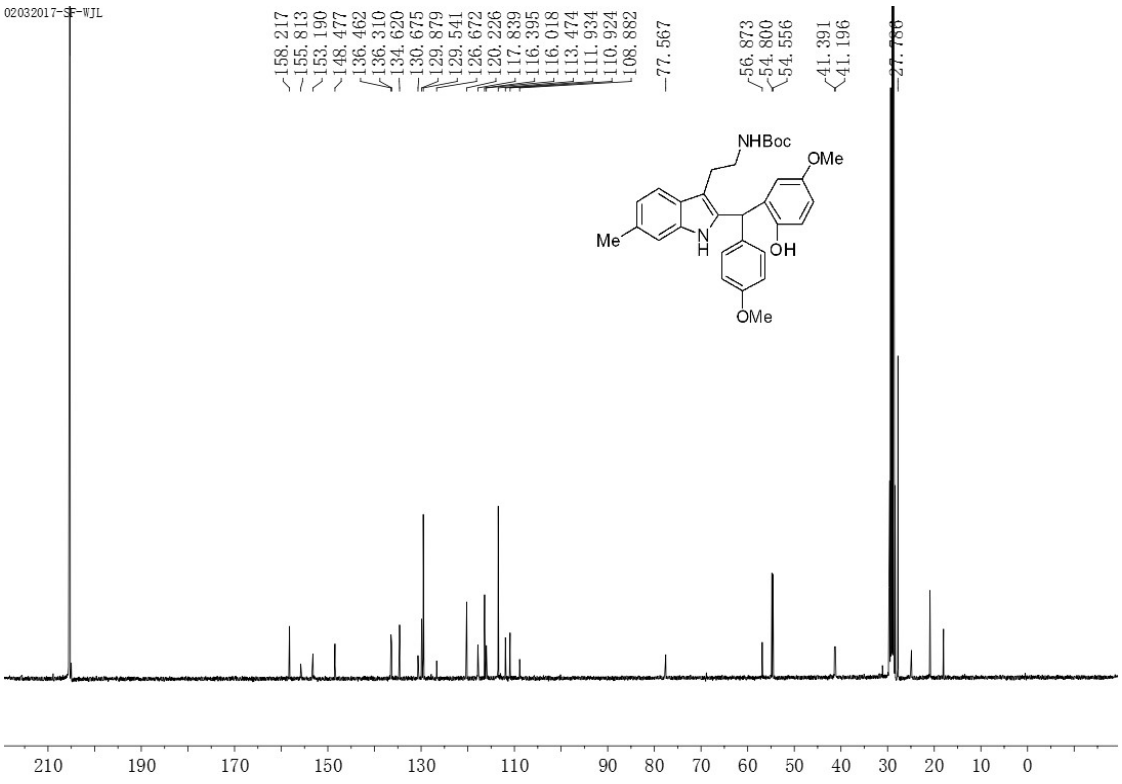


## 8ud

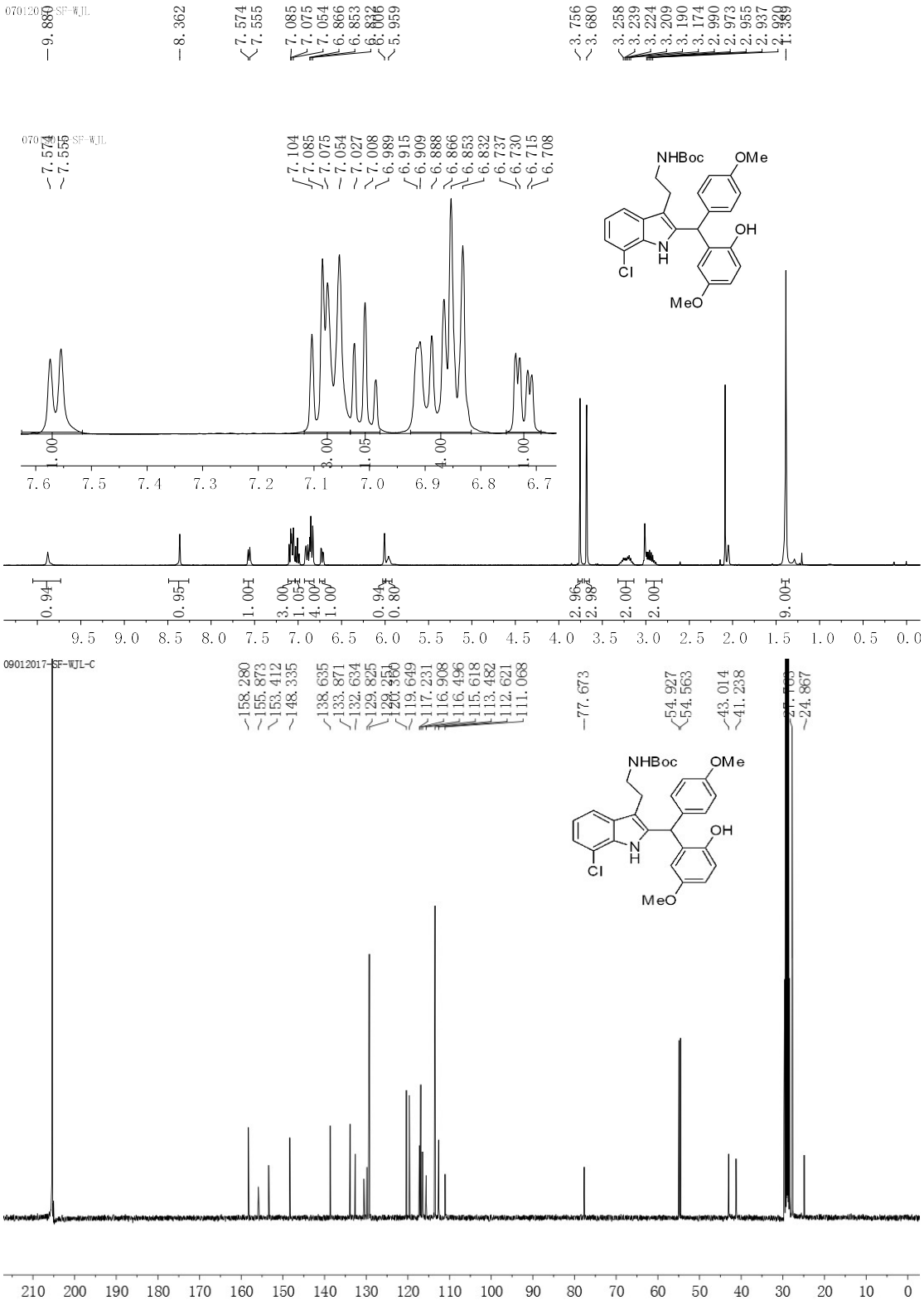


## 8ue

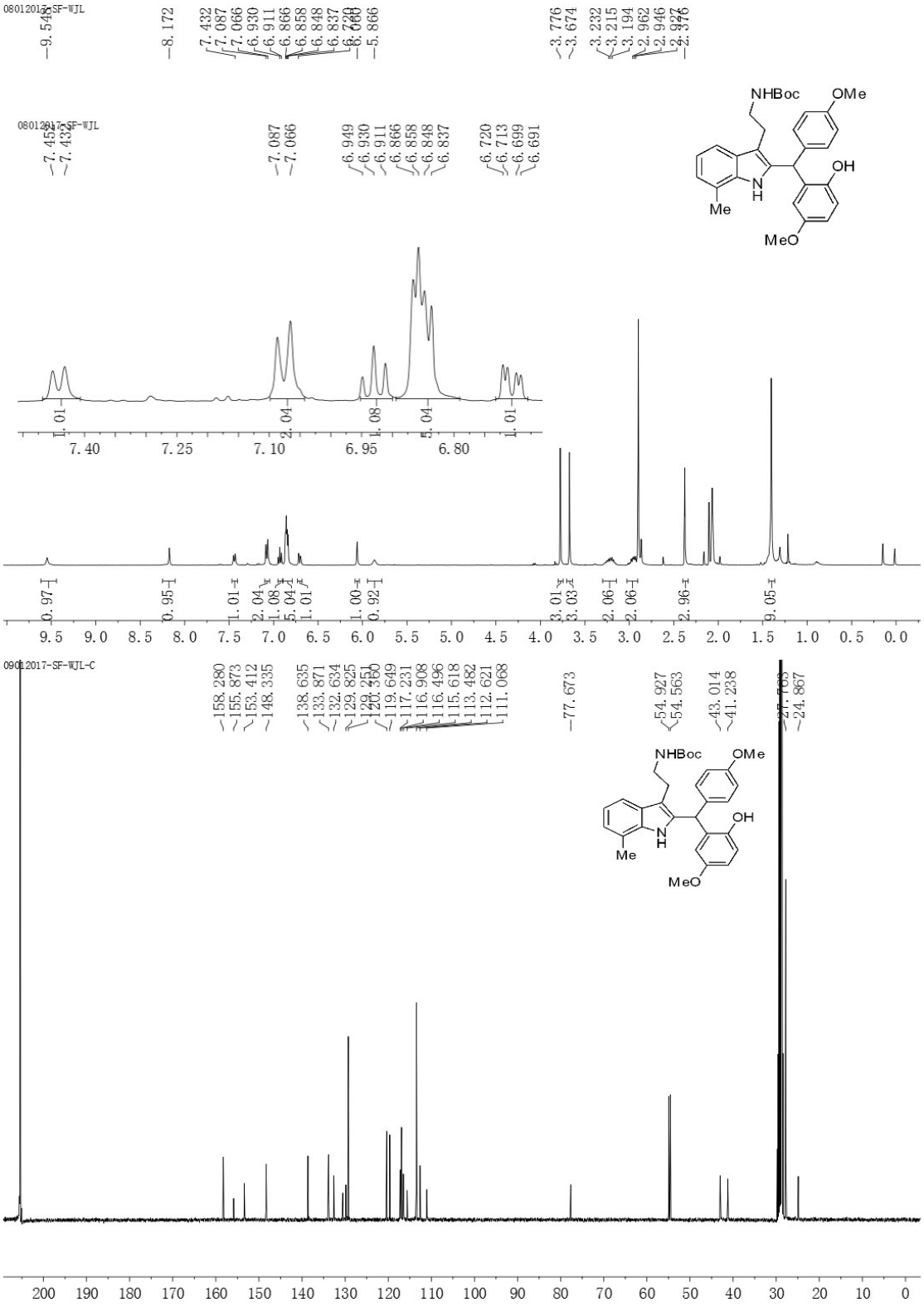


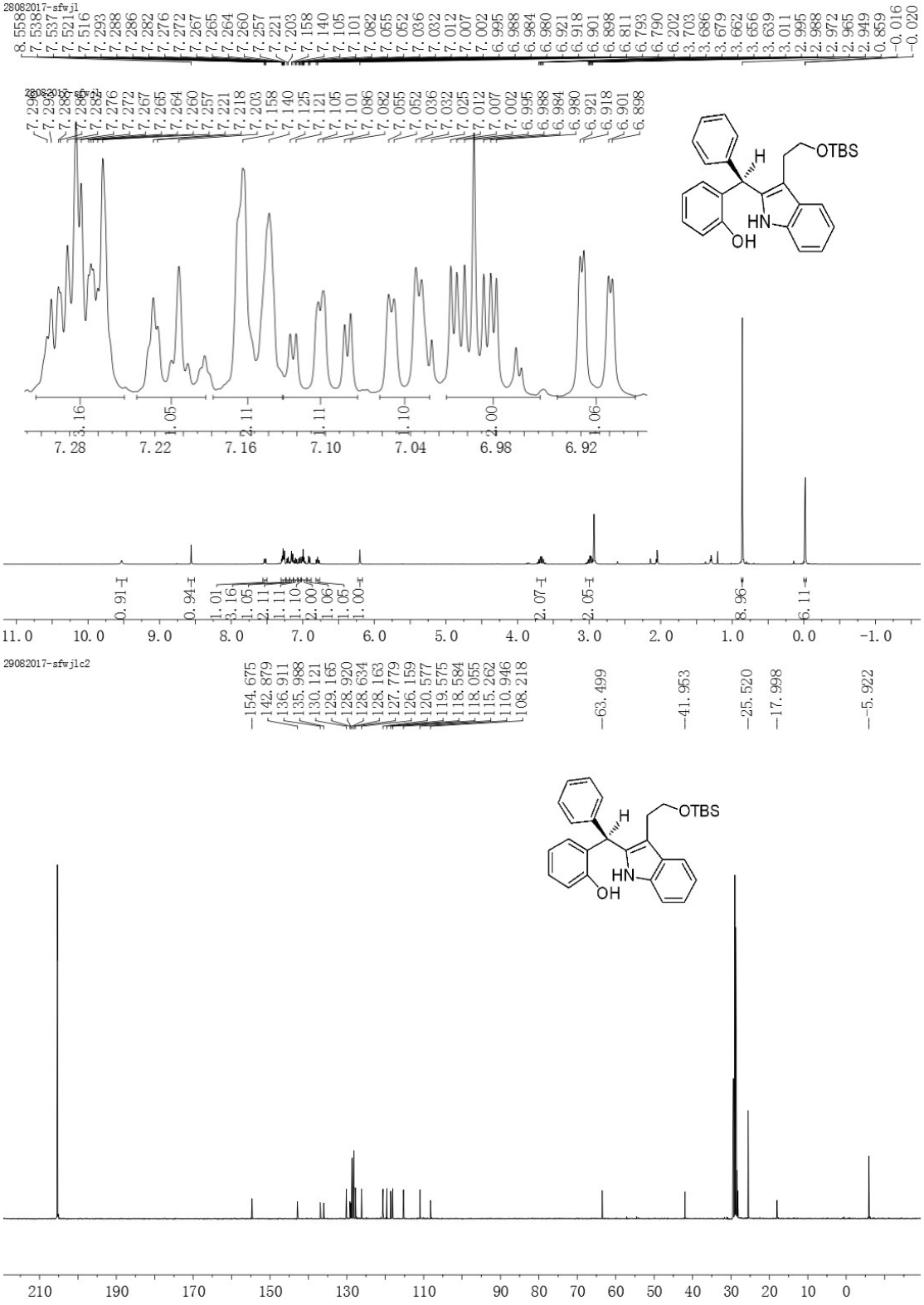
## 8uf



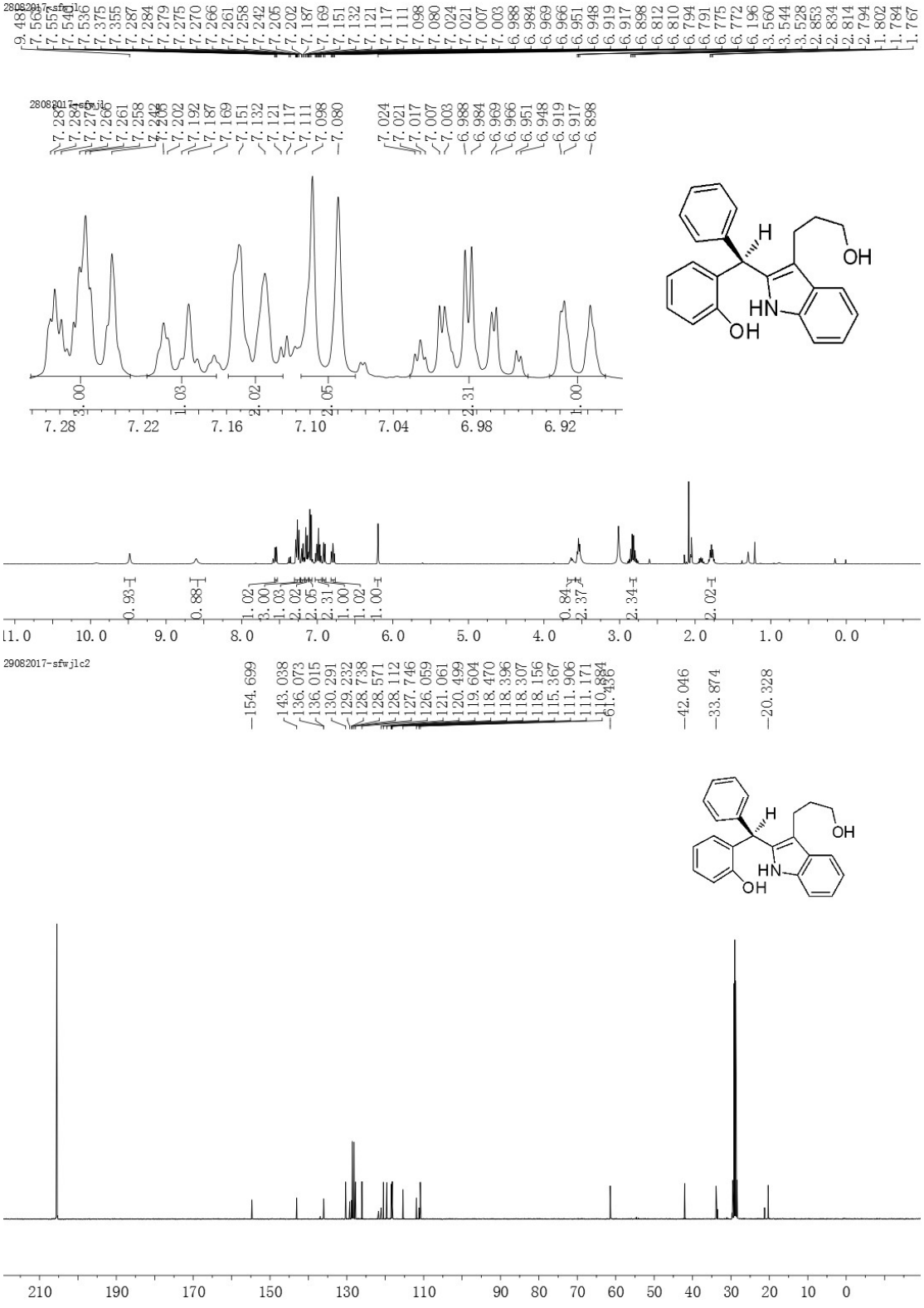
## 8ug



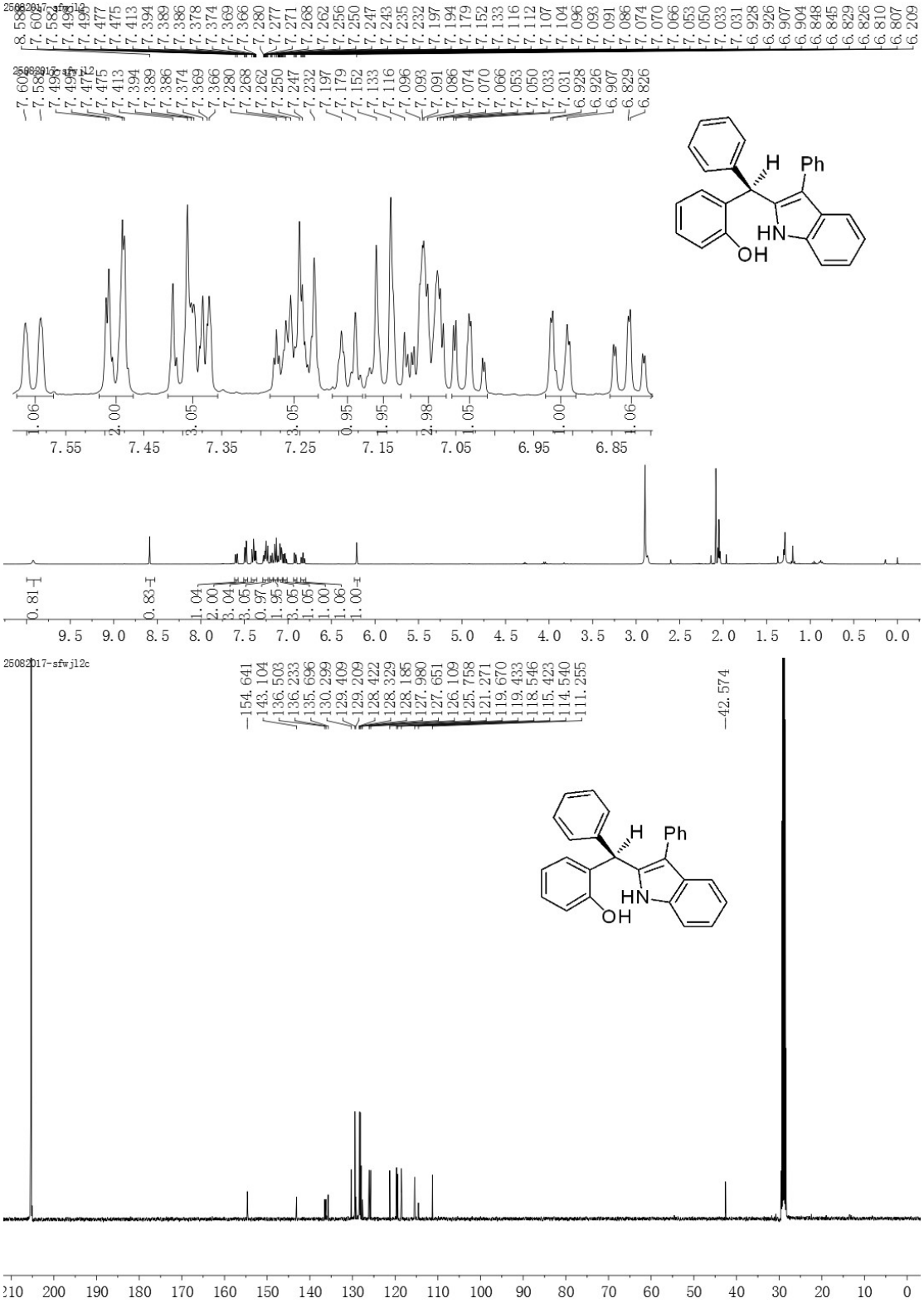
## 10aa



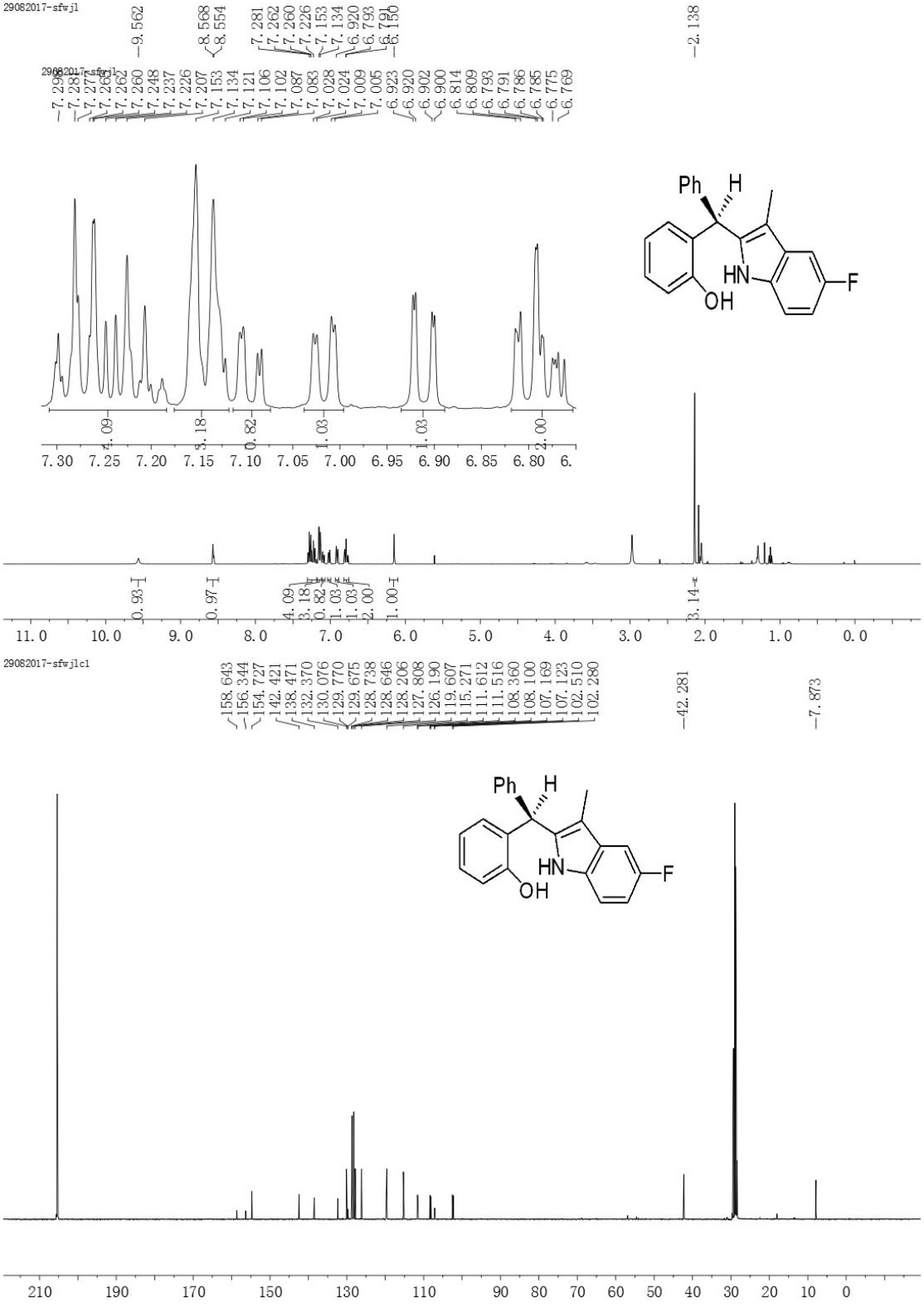
## 10ab



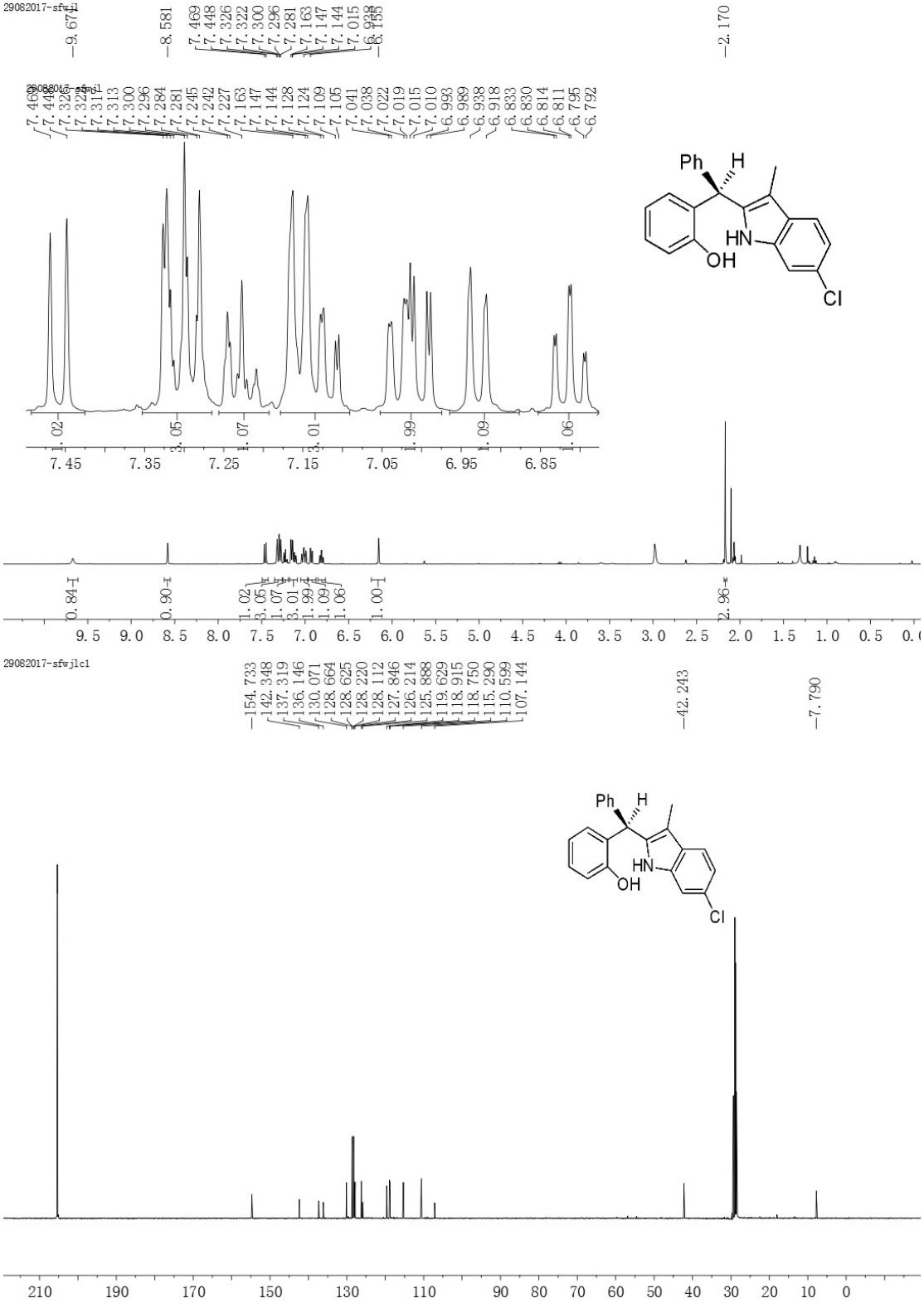
## 10ac



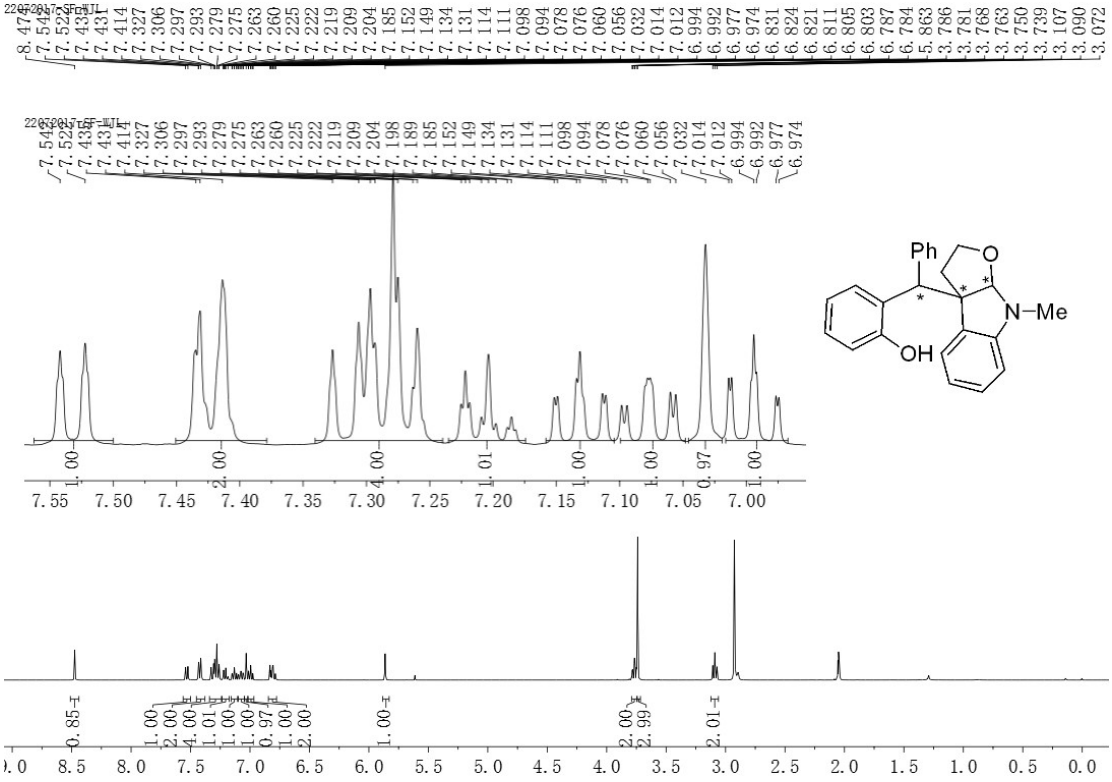
## 10ad

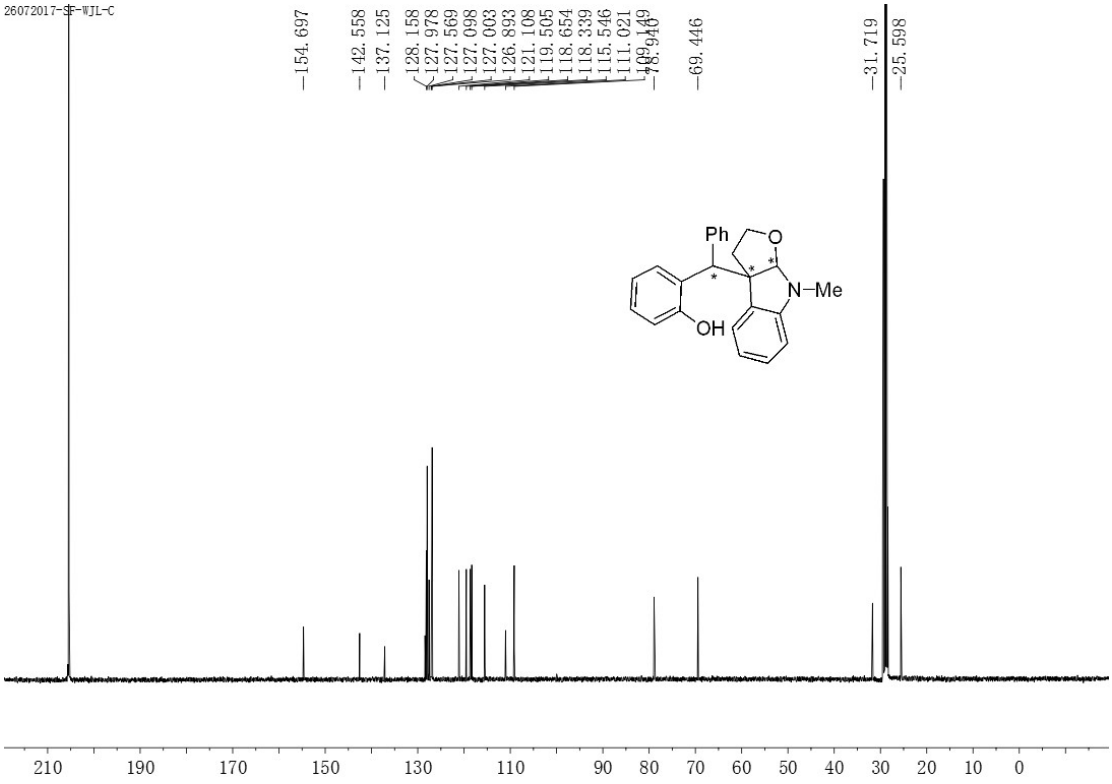


## 10ae



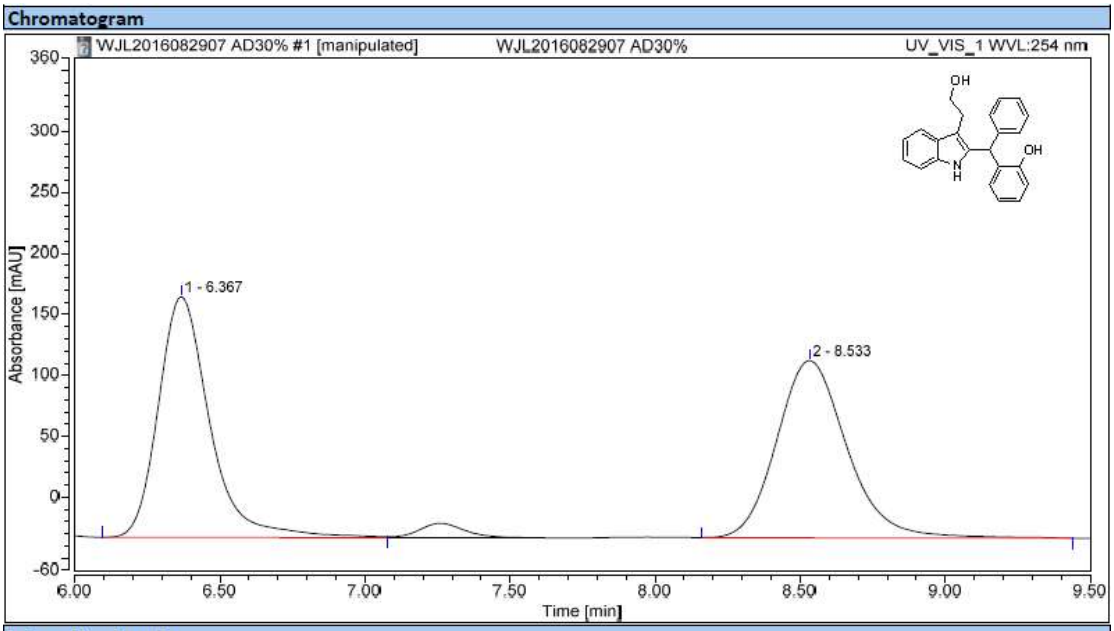
## 11ah



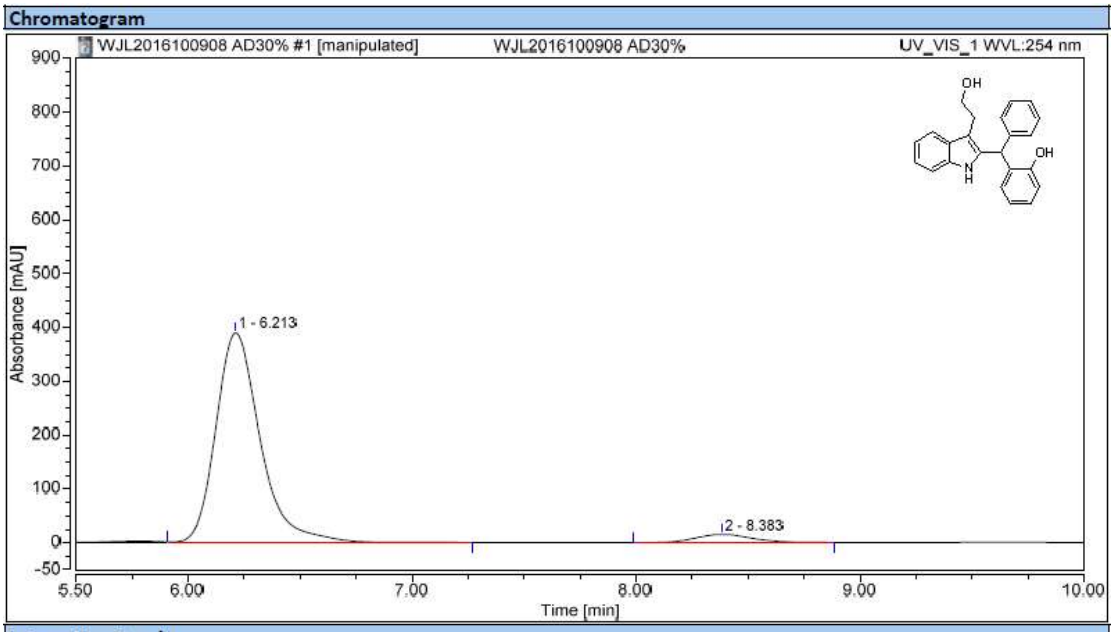
## 2. HPLC spectra of all products

### 3aa




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.367 | 40.426 | 197.362 | 49.80 | 57.60 | n.a. |
| 2 | | 8.533 | 40.745 | 145.252 | 50.20 | 42.40 | n.a. |
| **Total:** | | | **81.171** | **342.614** | **100.00** | **100.00** | |

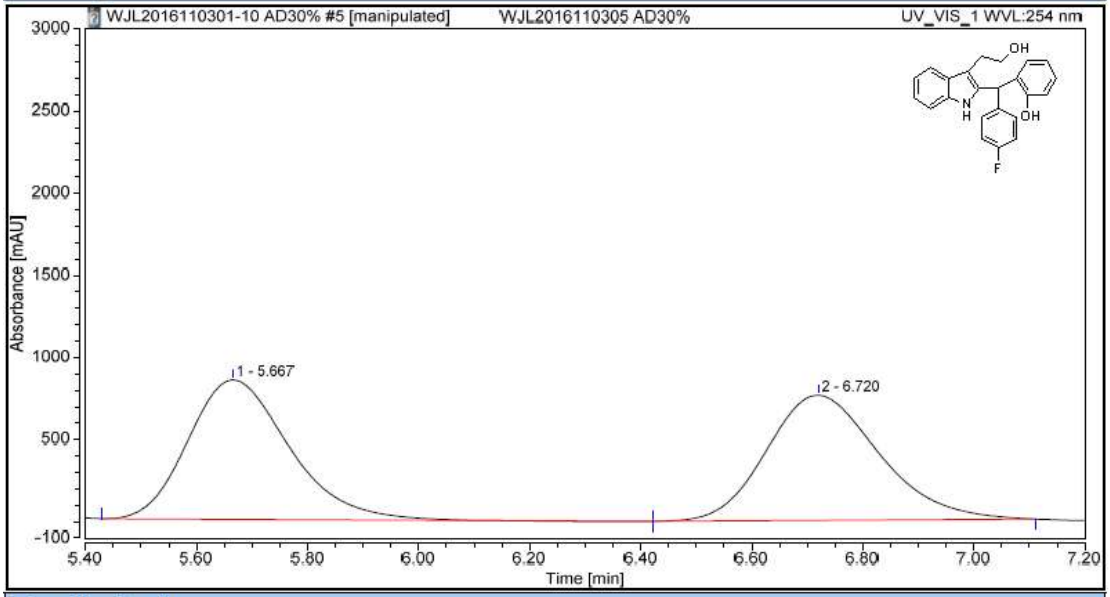



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.213 | 89.621 | 389.924 | 95.21 | 96.21 | n.a. |
| 2 | | 8.383 | 4.509 | 15.348 | 4.79 | 3.79 | n.a. |
| **Total:** | | | **94.130** | **405.272** | **100.00** | **100.00** | |

**3ba**

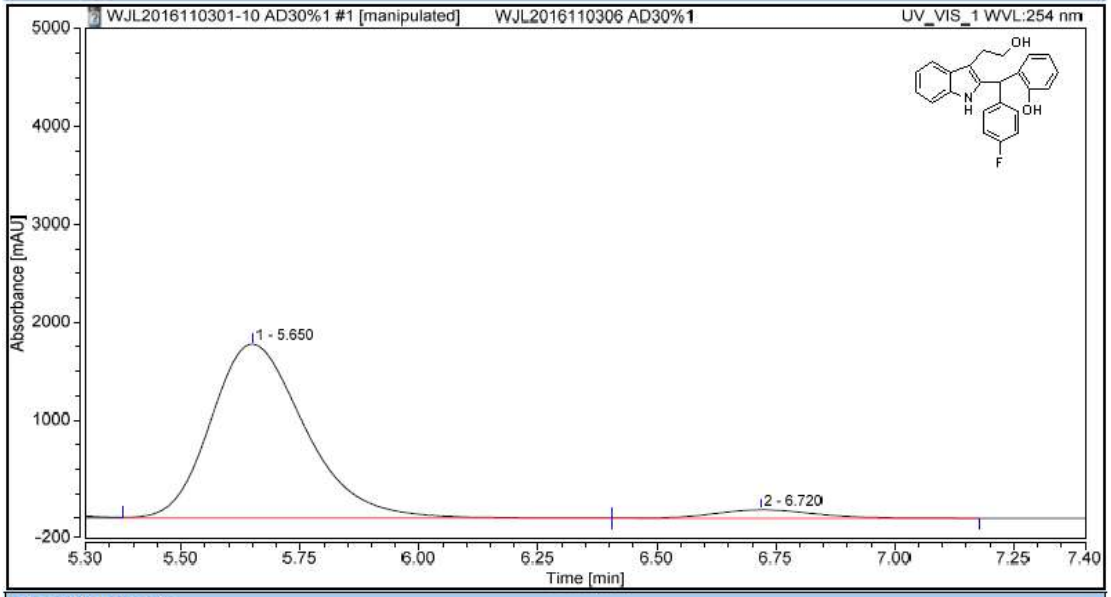
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.667 | 178.677 | 848.619 | 49.91 | 52.70 | n.a. |
| 2 | | 6.720 | 179.287 | 761.574 | 50.09 | 47.30 | n.a. |
| **Total:** | | | **357.963** | **1610.193** | **100.00** | **100.00** | |

**Chromatogram**

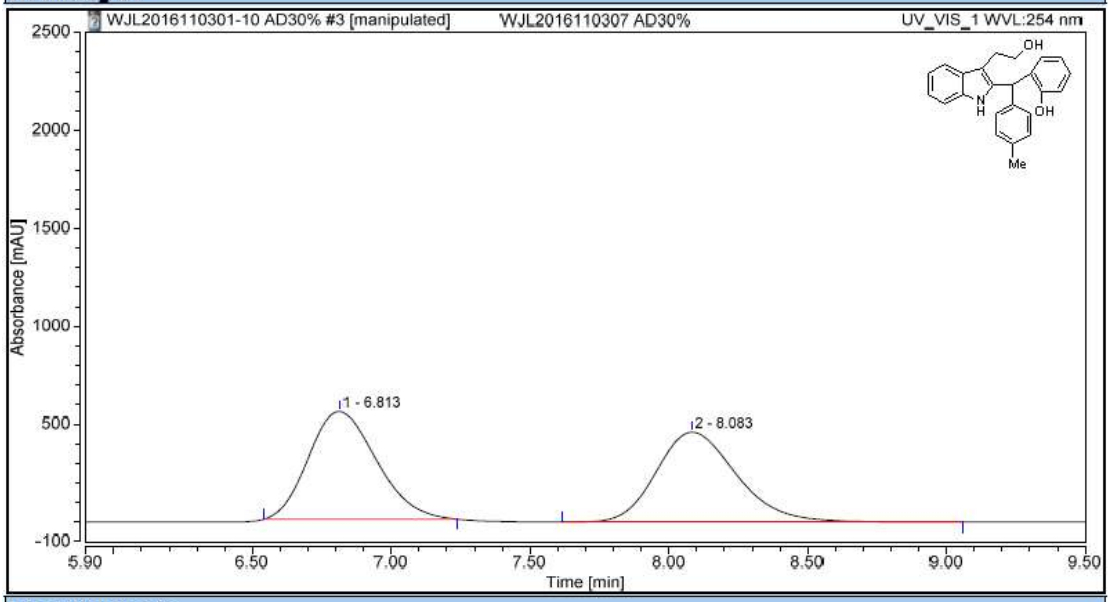



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.650 | 407.814 | 1775.506 | 95.06 | 95.37 | n.a. |
| 2 | | 6.720 | 21.205 | 86.188 | 4.94 | 4.63 | n.a. |
| **Total:** | | | **429.019** | **1861.694** | **100.00** | **100.00** | |

## 3ca

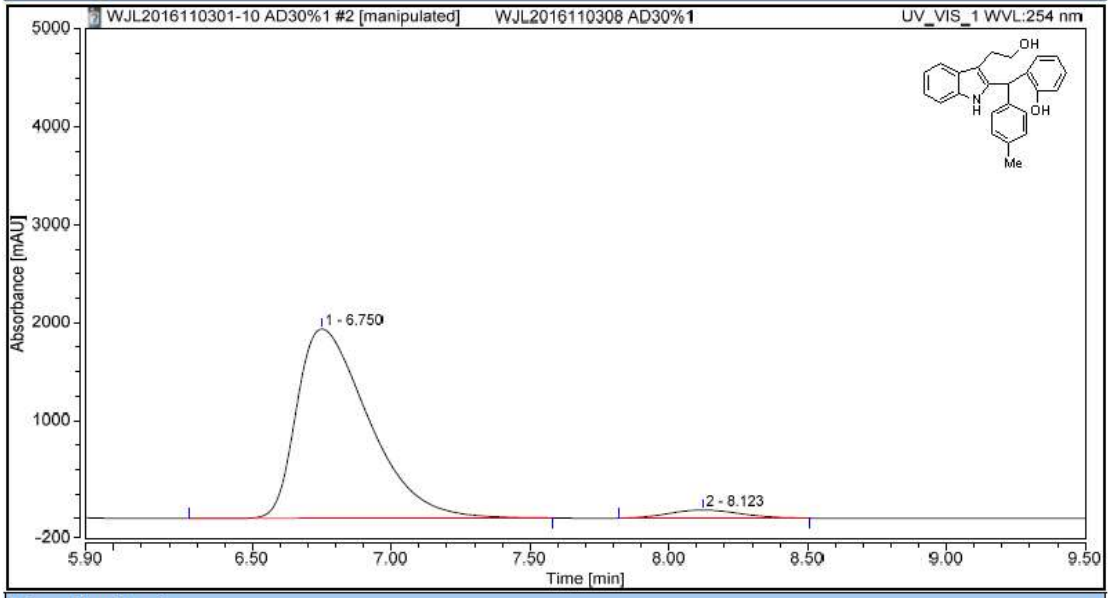
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.813 | 156.100 | 550.395 | 50.32 | 54.54 | n.a. |
| 2 | | 8.083 | 154.112 | 458.764 | 49.68 | 45.46 | n.a. |
| **Total:** | | | **310.212** | **1009.159** | **100.00** | **100.00** | |

**Chromatogram**

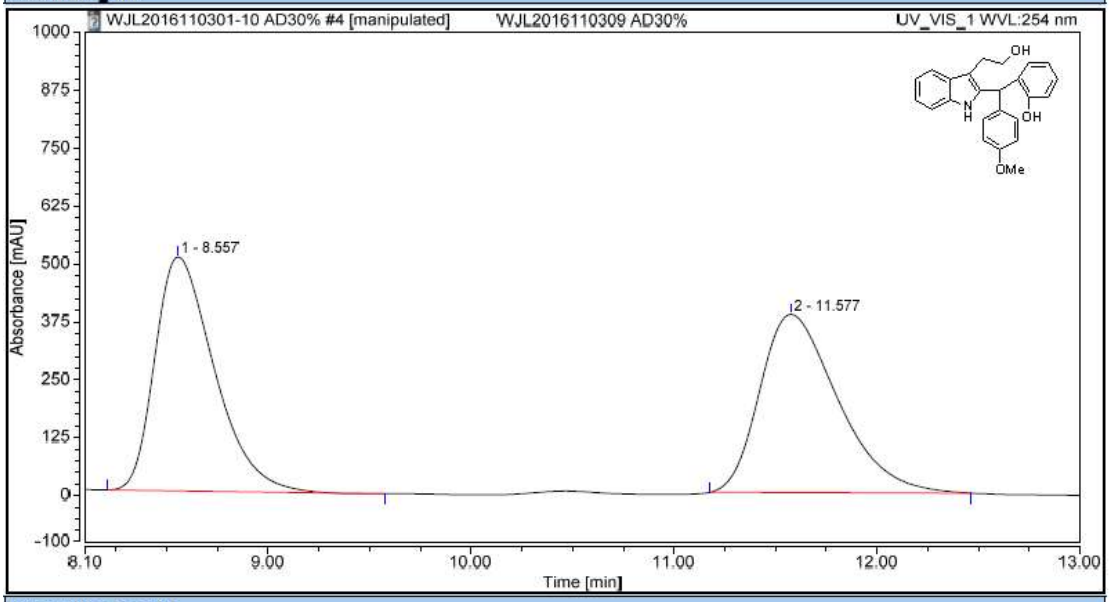



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.750 | 579.479 | 1932.275 | 95.91 | 95.89 | n.a. |
| 2 | | 8.123 | 24.712 | 82.841 | 4.09 | 4.11 | n.a. |
| **Total:** | | | **604.191** | **2015.115** | **100.00** | **100.00** | |

## 3da

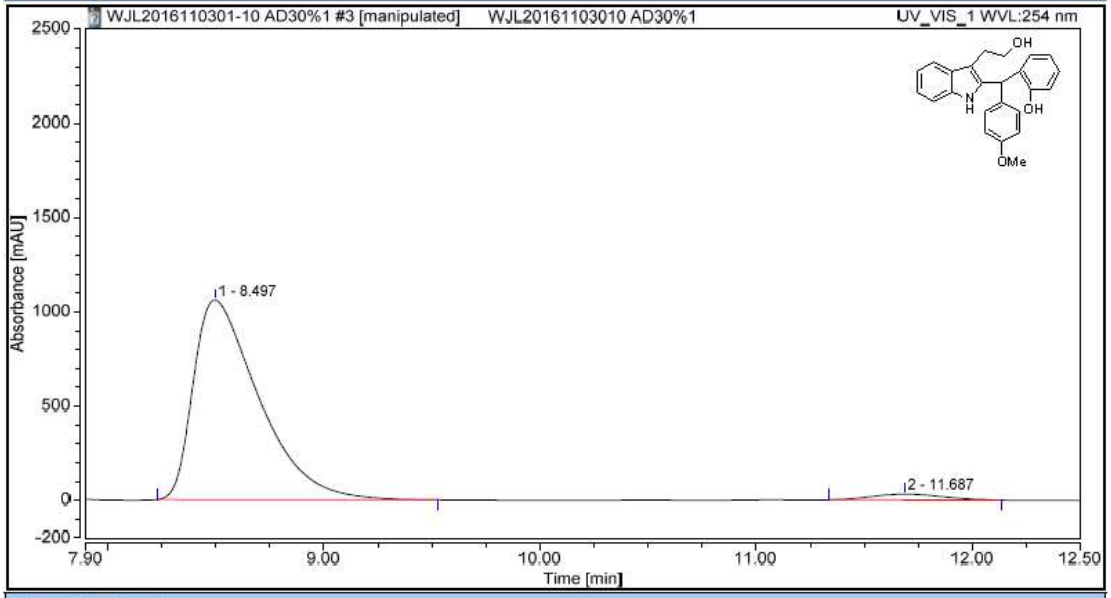
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.557 | 171.182 | 505.626 | 49.96 | 56.76 | n.a. |
| 2 | | 11.577 | 171.465 | 385.127 | 50.04 | 43.24 | n.a. |
| **Total:** | | | **342.647** | **890.753** | **100.00** | **100.00** | |

**Chromatogram**

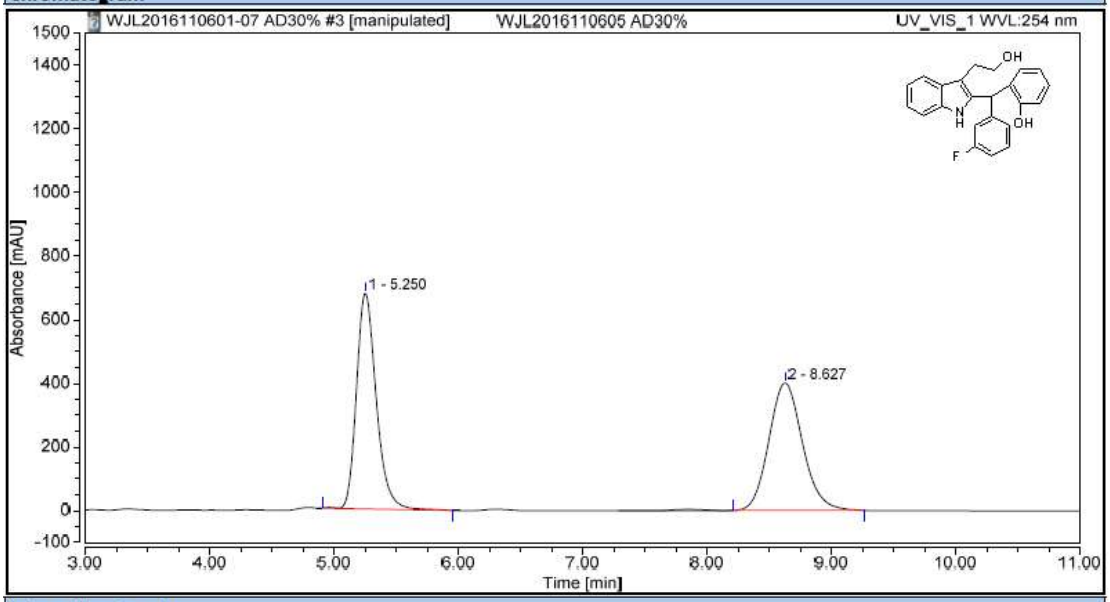



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.497 | 371.669 | 1059.026 | 96.91 | 97.14 | n.a. |
| 2 | | 11.687 | 11.836 | 31.180 | 3.09 | 2.86 | n.a. |
| **Total:** | | | **383.505** | **1090.207** | **100.00** | **100.00** | |

**3ea**

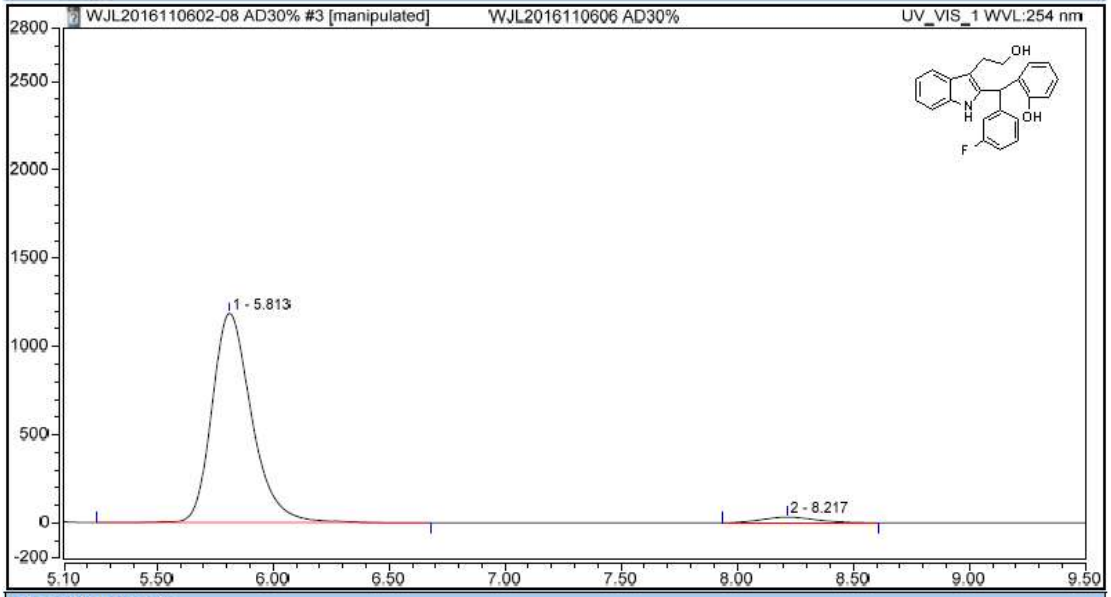
Chromatogram




Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.250 | 125.197 | 678.461 | 49.91 | 62.86 | n.a. |
| 2 | | 8.627 | 125.657 | 400.829 | 50.09 | 37.14 | n.a. |
| Total: | | | 250.854 | 1079.291 | 100.00 | 100.00 | |

Chromatogram

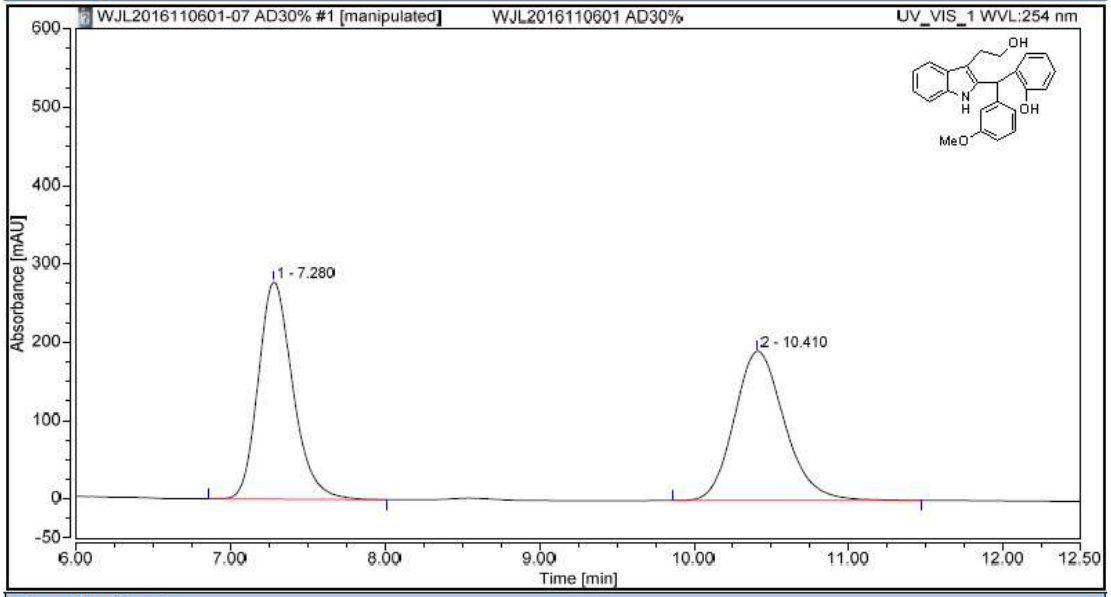



Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.813 | 234.915 | 1184.864 | 96.51 | 97.42 | n.a. |
| 2 | | 8.217 | 8.507 | 31.404 | 3.49 | 2.58 | n.a. |
| Total: | | | 243.422 | 1216.268 | 100.00 | 100.00 | |

**3fa**

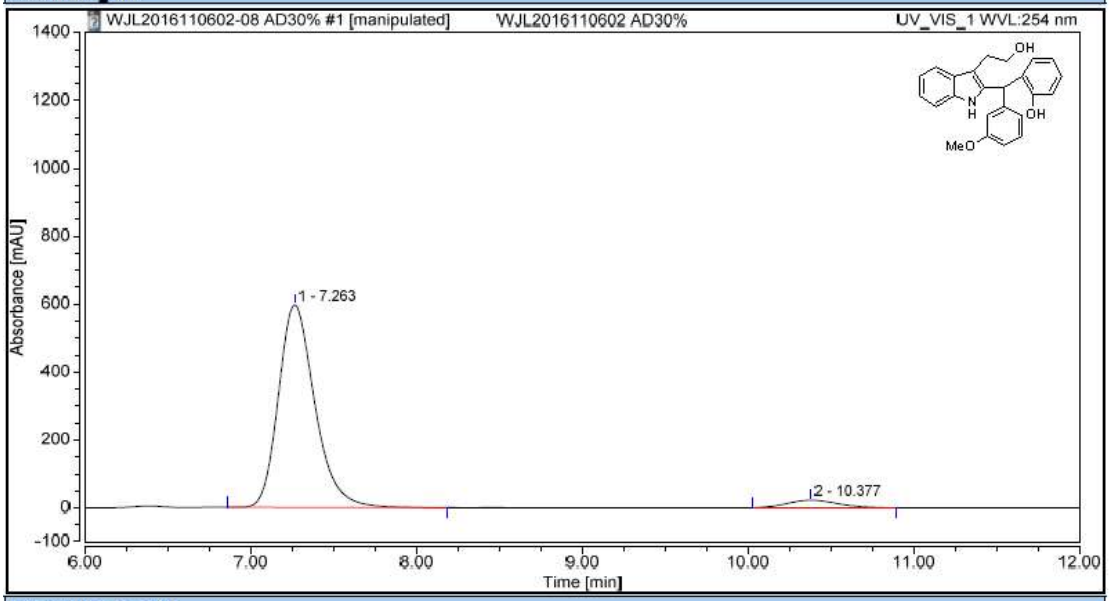
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 7.280 | 71.789 | 277.102 | 50.00 | 59.26 | n.a. |
| 2 | | 10.410 | 71.779 | 190.509 | 50.00 | 40.74 | n.a. |
| Total: | | | 143.568 | 467.611 | 100.00 | 100.00 | |

**Chromatogram**

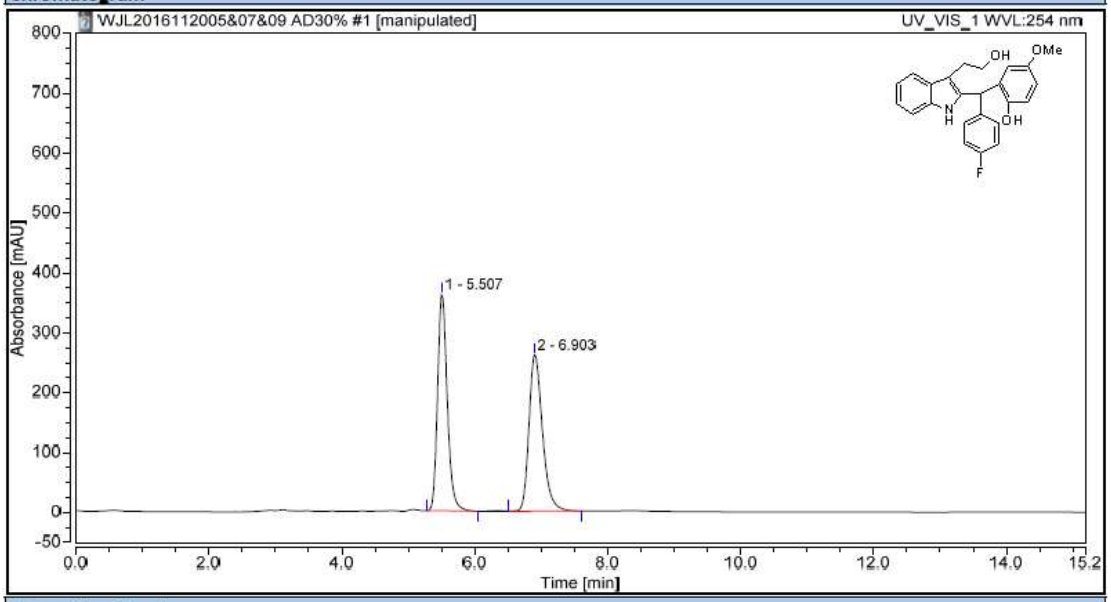



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 7.263 | 151.814 | 596.558 | 95.13 | 96.44 | n.a. |
| 2 | | 10.377 | 7.768 | 22.047 | 4.87 | 3.56 | n.a. |
| Total: | | | 159.582 | 618.605 | 100.00 | 100.00 | |

## 3ga

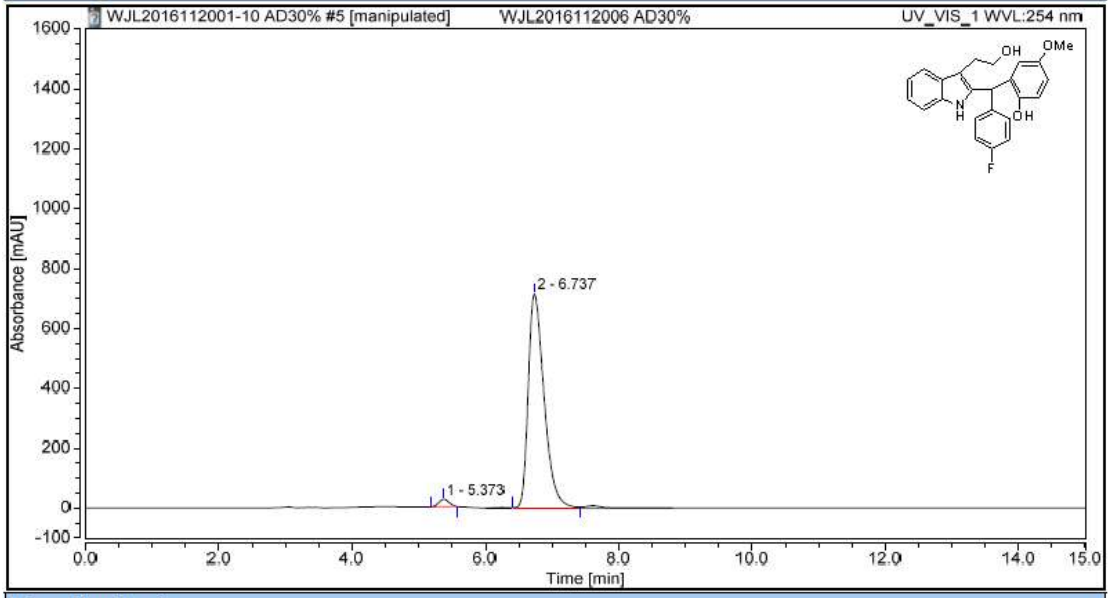
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.507 | 61.140 | 362.624 | 49.88 | 58.09 | n.a. |
| 2 | | 6.903 | 61.432 | 261.667 | 50.12 | 41.91 | n.a. |
| Total: | | | **122.572** | **624.291** | **100.00** | **100.00** | |

**Chromatogram**

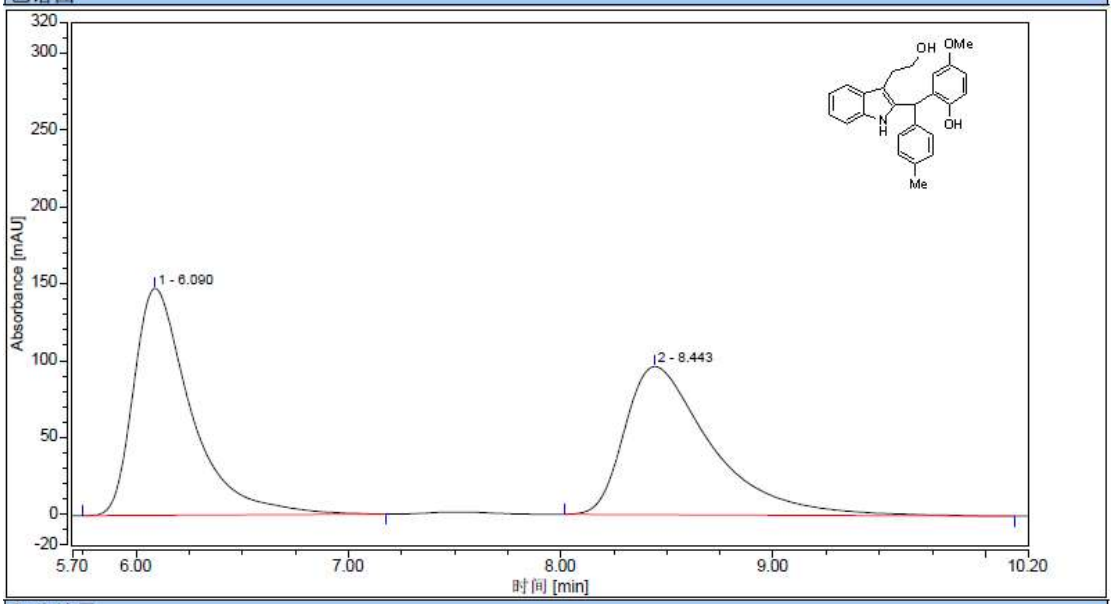



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.373 | 4.407 | 24.799 | 2.19 | 3.35 | n.a. |
| 2 | | 6.737 | 196.460 | 714.392 | 97.81 | 96.65 | n.a. |
| Total: | | | **200.868** | **739.191** | **100.00** | **100.00** | |

**3ha**

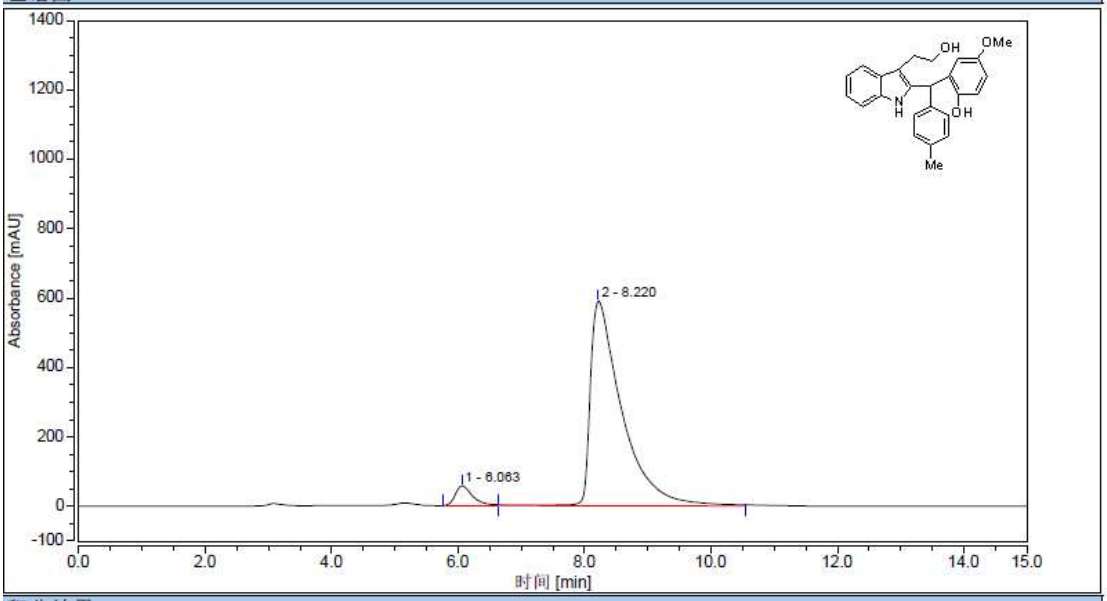
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.090 | 46.084 | 147.467 | 50.29 | 60.52 | n.a. |
| 2 | | 8.443 | 45.550 | 96.209 | 49.71 | 39.48 | n.a. |
| 总和: | | | 91.634 | 243.676 | 100.00 | 100.00 | |

色谱图

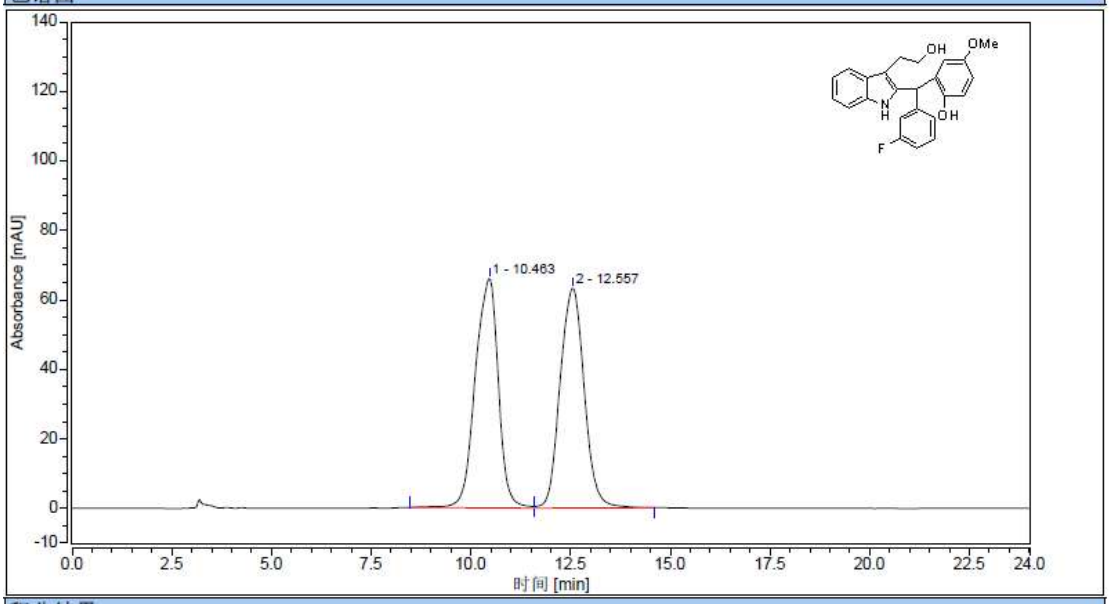



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.063 | 17.957 | 56.853 | 5.00 | 8.79 | n.a. |
| 2 | | 8.220 | 341.429 | 590.272 | 95.00 | 91.21 | n.a. |
| 总和: | | | 359.386 | 647.125 | 100.00 | 100.00 | |

**3ia**

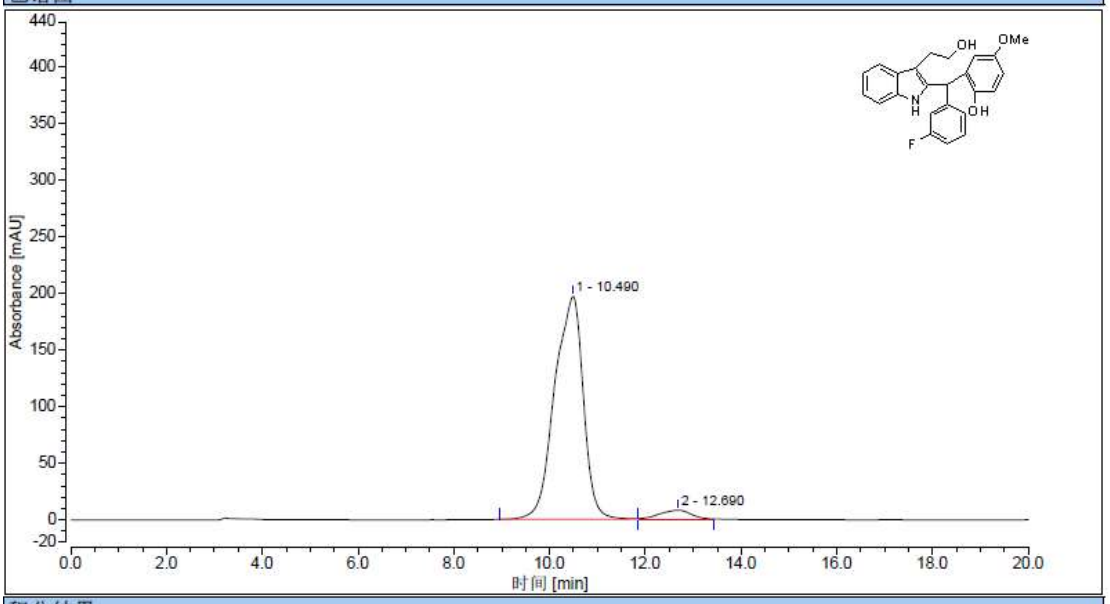
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 10.463 | 44.252 | 65.992 | 49.92 | 51.07 | n.a. |
| 2 | | 12.557 | 44.392 | 63.229 | 50.08 | 48.93 | n.a. |
| 总和: | | | **88.644** | **129.221** | **100.00** | **100.00** | |

色谱图

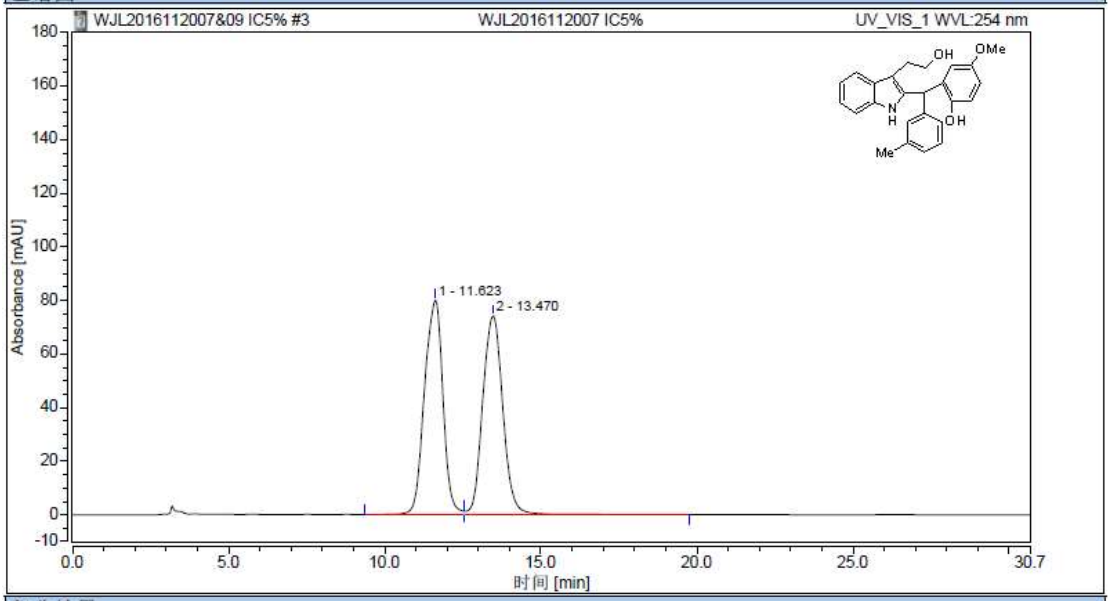



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 10.490 | 136.767 | 197.039 | 95.89 | 96.15 | n.a. |
| 2 | | 12.690 | 5.865 | 7.886 | 4.11 | 3.85 | n.a. |
| 总和: | | | **142.632** | **204.924** | **100.00** | **100.00** | |

**3ja**

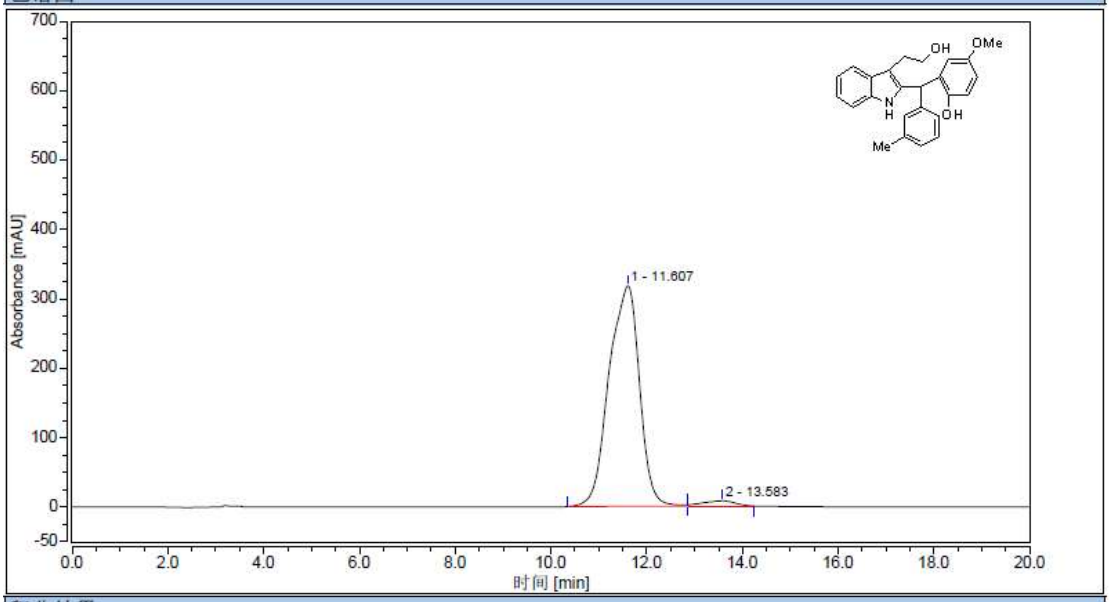
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 11.623 | 55.047 | 80.105 | 49.71 | 51.87 | n.a. |
| 2 | | 13.470 | 55.695 | 74.338 | 50.29 | 48.13 | n.a. |
| 总和: | | | **110.742** | **154.443** | **100.00** | **100.00** | |

色谱图

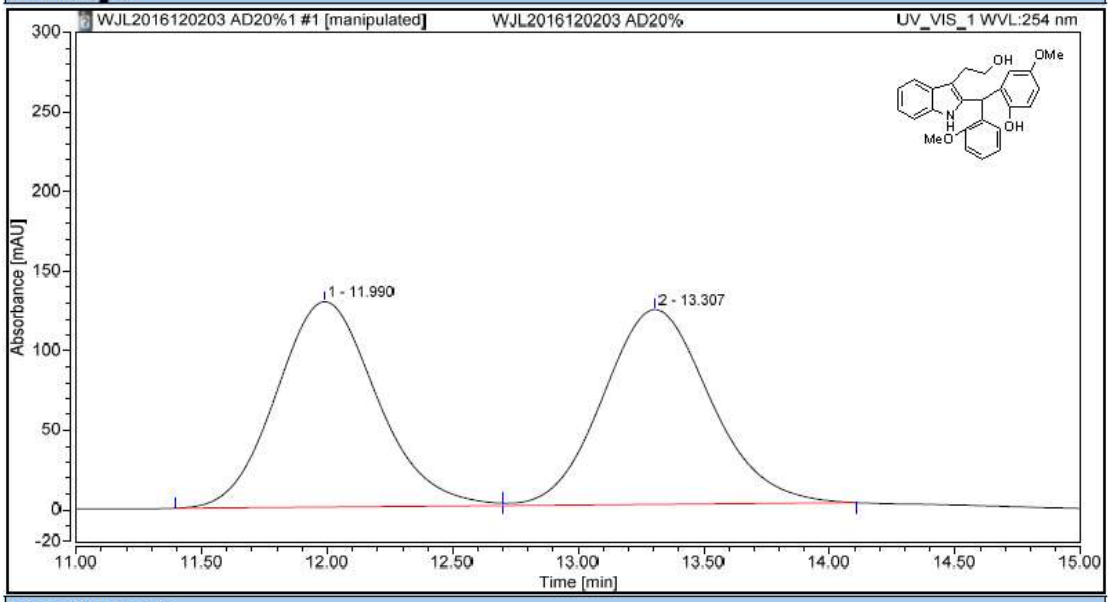



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 11.607 | 234.006 | 317.910 | 97.48 | 97.68 | n.a. |
| 2 | | 13.583 | 6.047 | 7.562 | 2.52 | 2.32 | n.a. |
| 总和: | | | **240.053** | **325.472** | **100.00** | **100.00** | |

## 3ka

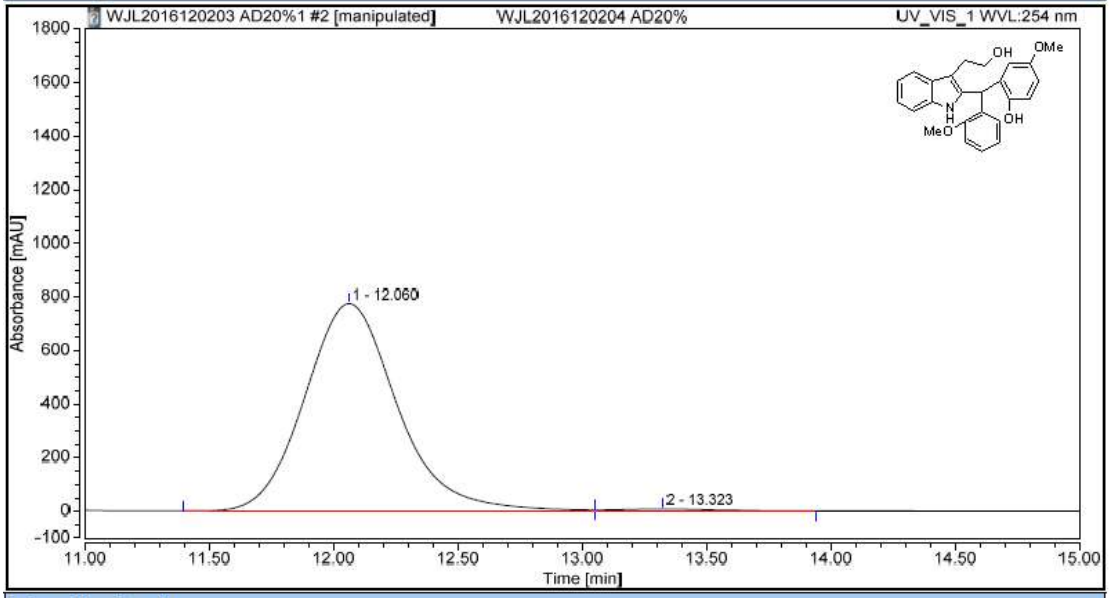
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 11.990 | 59.936 | 129.091 | 49.67 | 51.33 | n.a. |
| 2 | | 13.307 | 60.742 | 122.403 | 50.33 | 48.67 | n.a. |
| **Total:** | | | **120.677** | **251.494** | **100.00** | **100.00** | |

**Chromatogram**

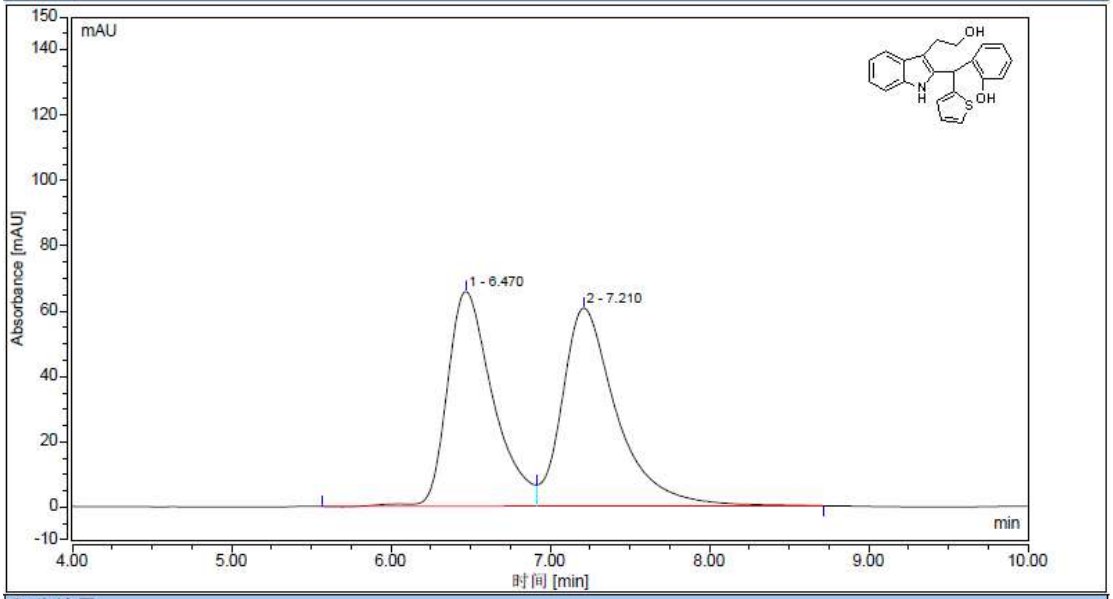



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 12.060 | 334.466 | 773.768 | 98.78 | 99.01 | n.a. |
| 2 | | 13.323 | 4.121 | 7.755 | 1.22 | 0.99 | n.a. |
| **Total:** | | | **338.587** | **781.524** | **100.00** | **100.00** | |

**3la**

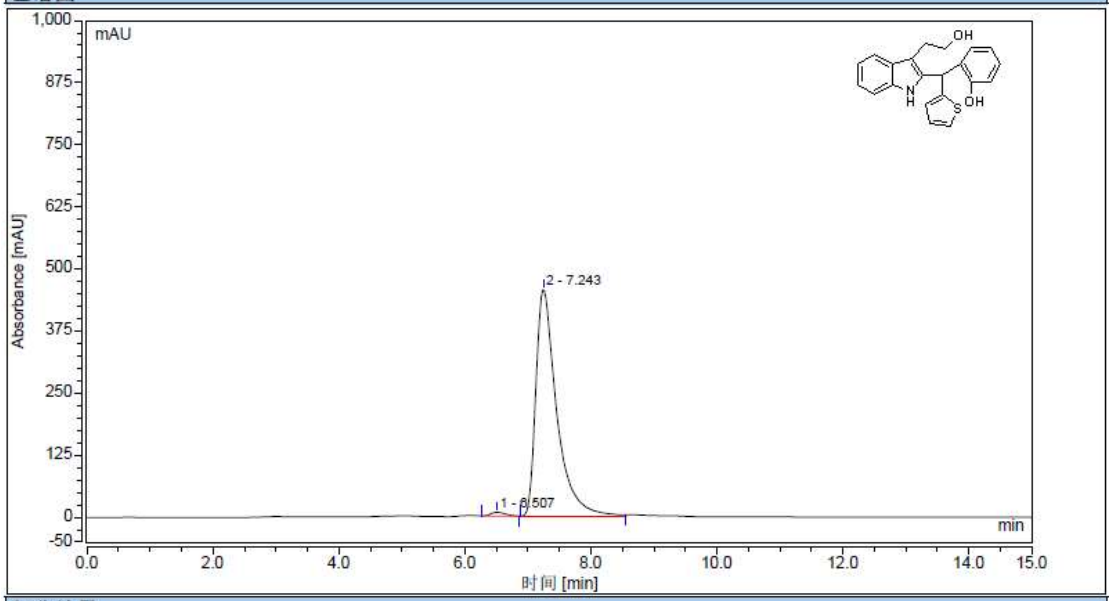
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.470 | 21.723 | 65.708 | 47.54 | 52.04 | n.a. |
| 2 | | 7.210 | 23.973 | 60.547 | 52.46 | 47.96 | n.a. |
| 总和: | | | **45.696** | **126.255** | **100.00** | **100.00** | |

色谱图

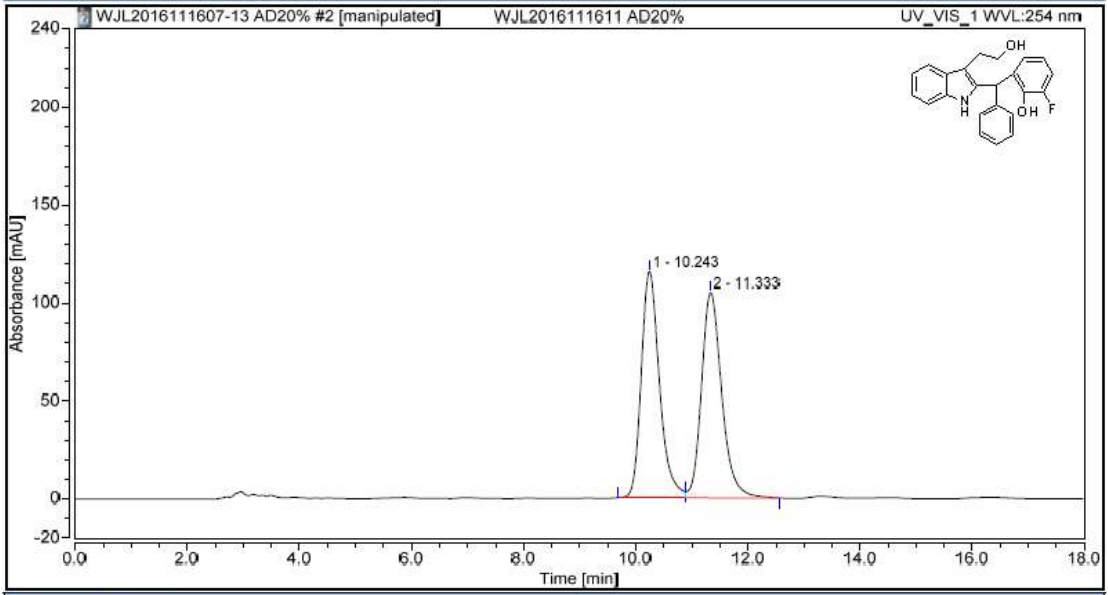



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.507 | 2.019 | 7.624 | 1.15 | 1.64 | n.a. |
| 2 | | 7.243 | 174.132 | 456.015 | 98.85 | 98.36 | n.a. |
| 总和: | | | **176.151** | **463.639** | **100.00** | **100.00** | |

**3ma**

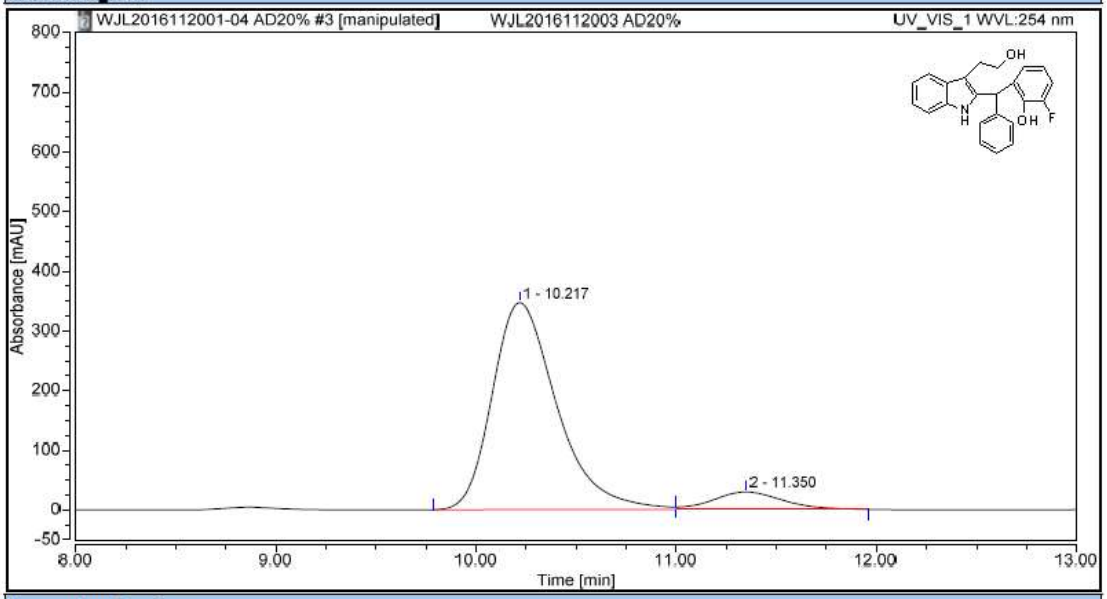
Chromatogram




Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 10.243 | 43.392 | 115.593 | 49.71 | 52.43 | n.a. |
| 2 | | 11.333 | 43.901 | 104.860 | 50.29 | 47.57 | n.a. |
| Total: | | | 87.292 | 220.453 | 100.00 | 100.00 | |

Chromatogram

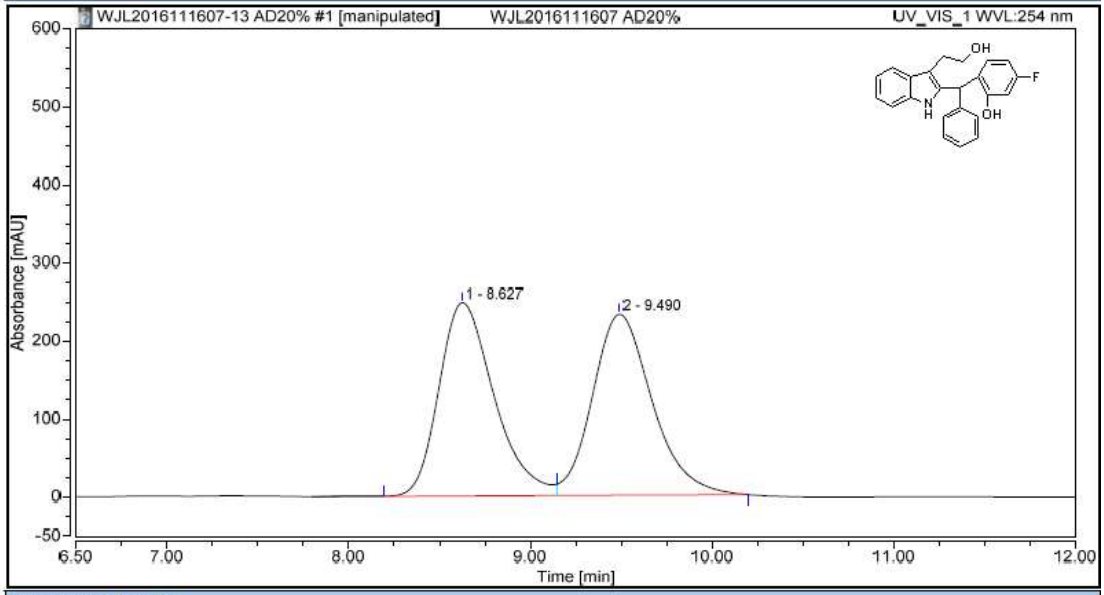



Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 10.217 | 129.533 | 346.728 | 91.65 | 92.20 | n.a. |
| 2 | | 11.350 | 11.807 | 29.338 | 8.35 | 7.80 | n.a. |
| Total: | | | 141.340 | 376.066 | 100.00 | 100.00 | |

**3na**

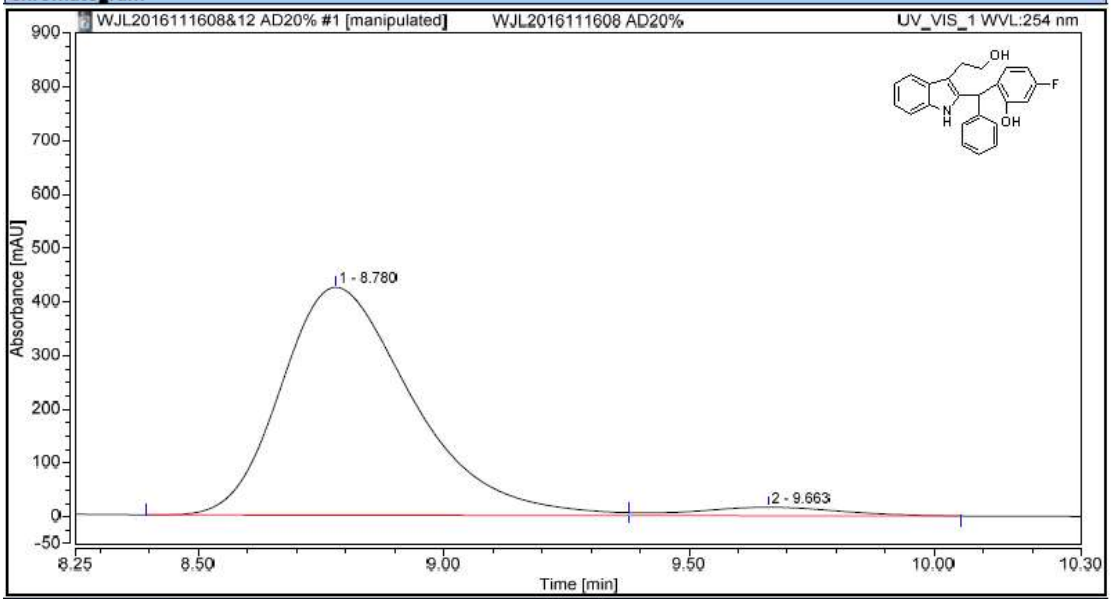
Chromatogram




Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.627 | 86.954 | 247.551 | 49.70 | 51.65 | n.a. |
| 2 | | 9.490 | 88.005 | 231.715 | 50.30 | 48.35 | n.a. |
| Total: | | | 174.960 | 479.266 | 100.00 | 100.00 | |

Chromatogram

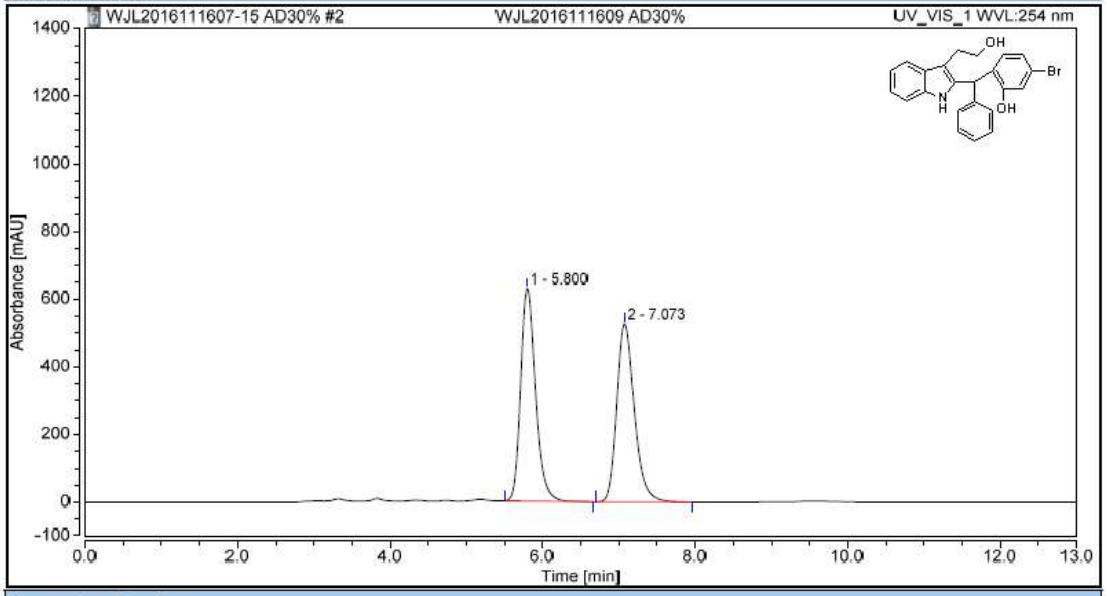



Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.780 | 131.731 | 423.838 | 96.09 | 96.37 | n.a. |
| 2 | | 9.663 | 5.366 | 15.950 | 3.91 | 3.63 | n.a. |
| Total: | | | 137.096 | 439.788 | 100.00 | 100.00 | |

**3oa**

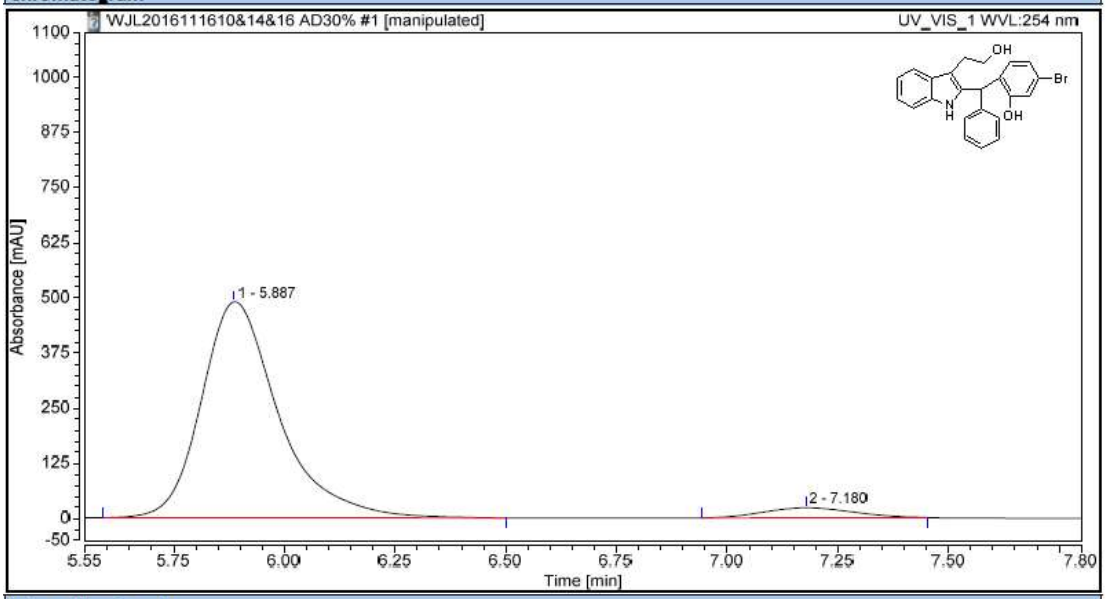
Chromatogram




Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.800 | 140.764 | 627.994 | 50.03 | 54.38 | n.a. |
| 2 | | 7.073 | 140.602 | 526.744 | 49.97 | 45.62 | n.a. |
| Total: | | | 281.366 | 1154.738 | 100.00 | 100.00 | |

Chromatogram

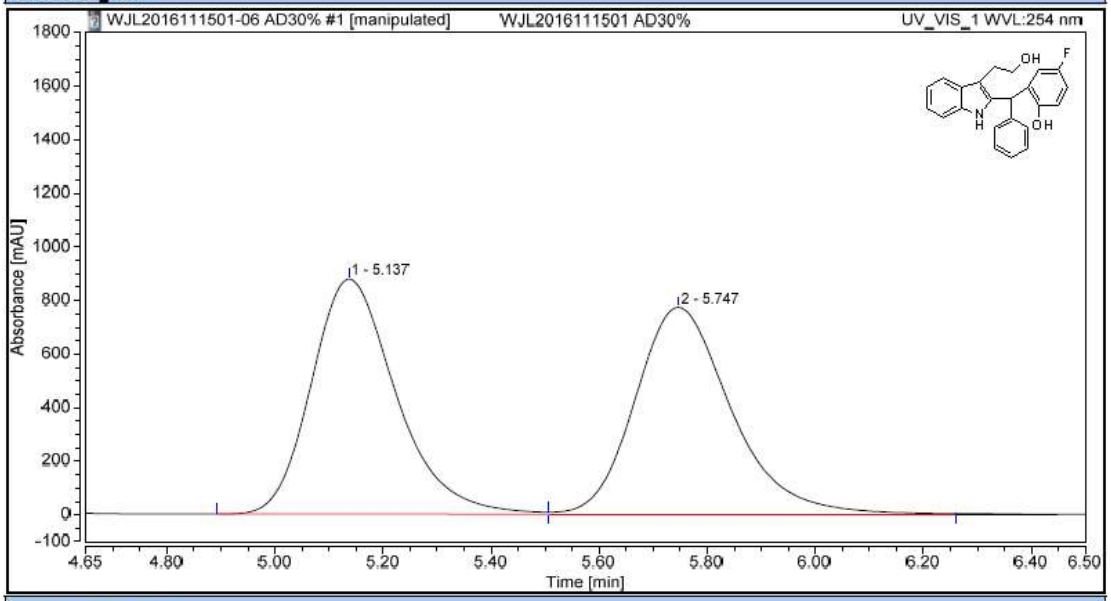



Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.887 | 99.257 | 489.734 | 94.95 | 95.59 | n.a. |
| 2 | | 7.180 | 5.278 | 22.579 | 5.05 | 4.41 | n.a. |
| Total: | | | 104.535 | 512.312 | 100.00 | 100.00 | |

## 3pa

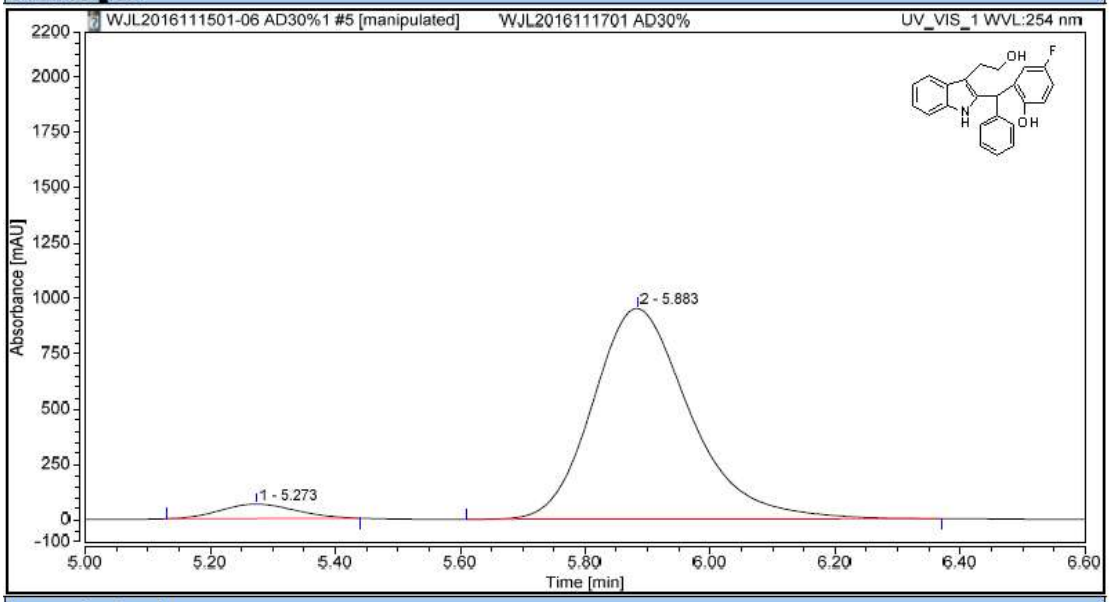
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.137 | 159.344 | 876.636 | 50.06 | 53.19 | n.a. |
| 2 | | 5.747 | 158.940 | 771.588 | 49.94 | 46.81 | n.a. |
| **Total:** | | | **318.284** | **1648.224** | **100.00** | **100.00** | |

**Chromatogram**

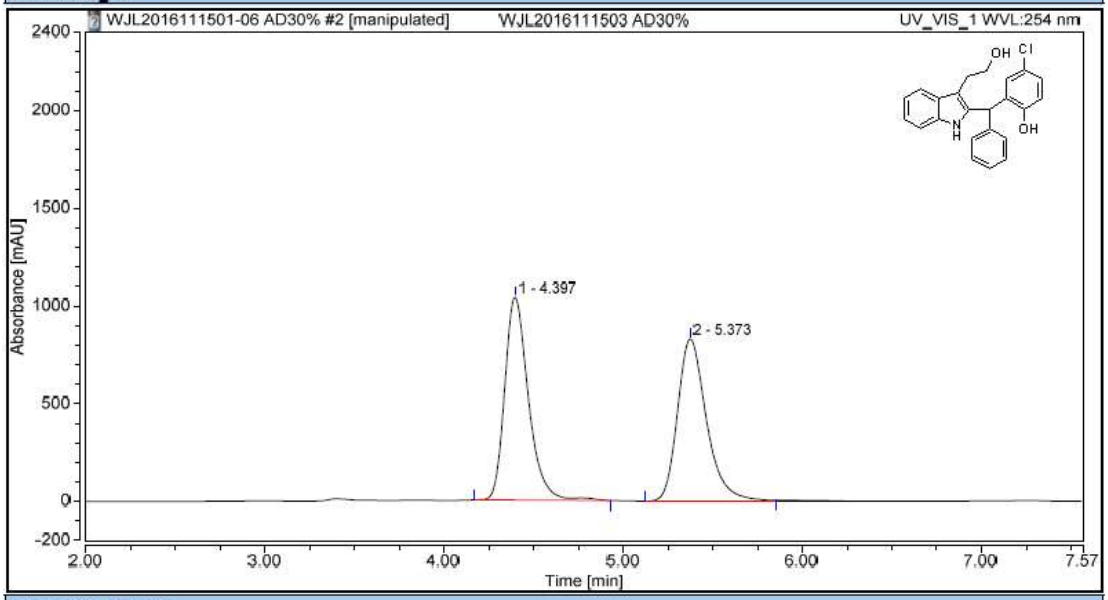



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.273 | 9.055 | 65.204 | 5.01 | 6.42 | n.a. |
| 2 | | 5.883 | 171.630 | 950.819 | 94.99 | 93.58 | n.a. |
| **Total:** | | | **180.685** | **1016.022** | **100.00** | **100.00** | |

## 3qa

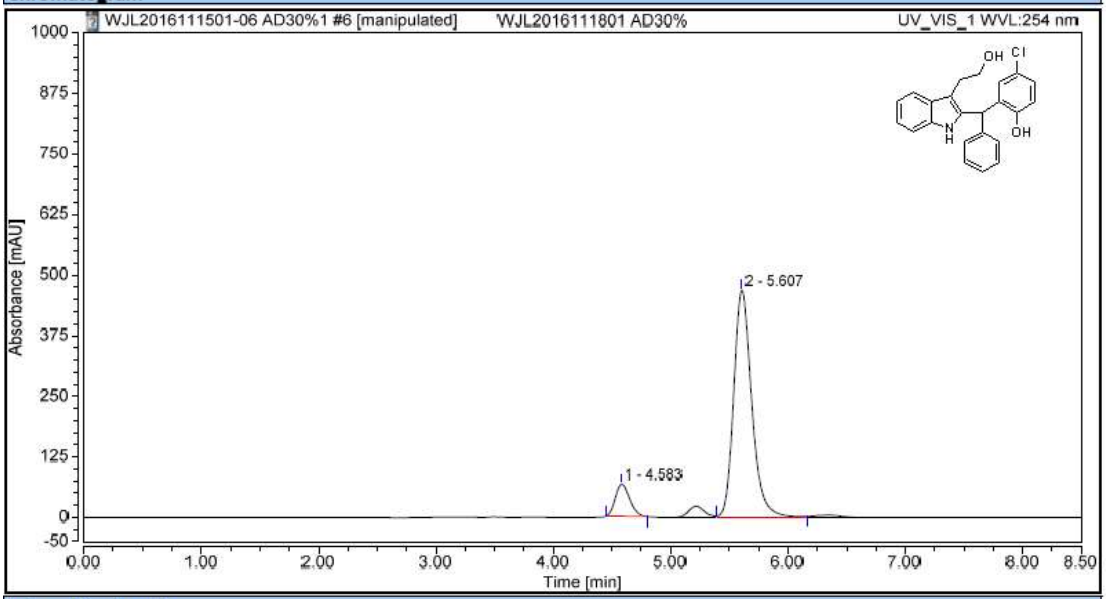
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.397 | 159.162 | 1038.726 | 50.57 | 55.59 | n.a. |
| 2 | | 5.373 | 155.601 | 829.989 | 49.43 | 44.41 | n.a. |
| Total: | | | 314.763 | 1868.716 | 100.00 | 100.00 | |

**Chromatogram**

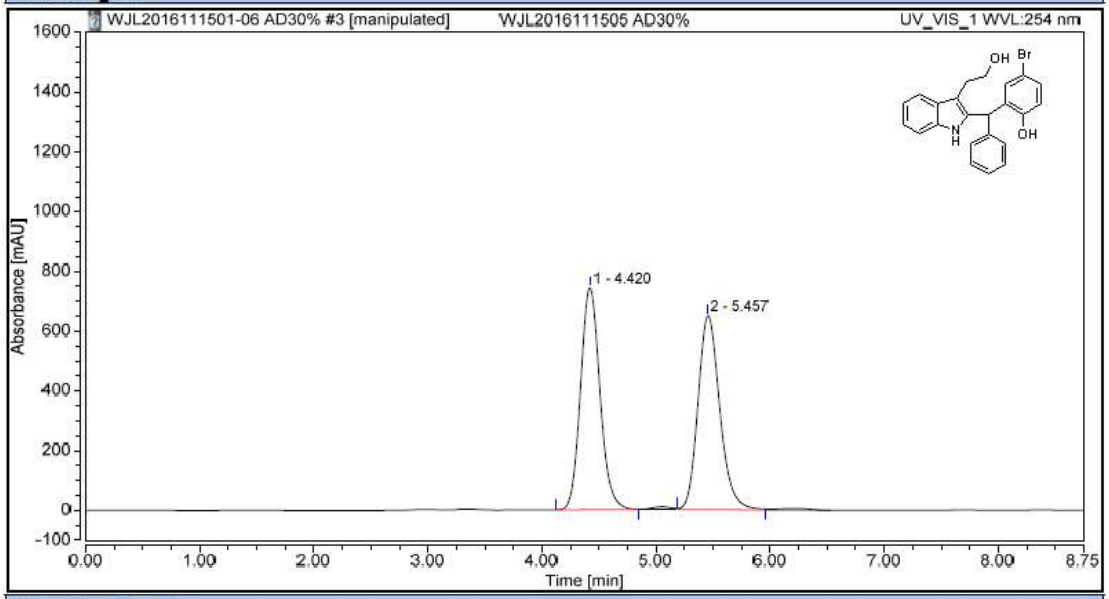



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.583 | 9.305 | 66.014 | 10.02 | 12.36 | n.a. |
| 2 | | 5.607 | 83.535 | 468.276 | 89.98 | 87.64 | n.a. |
| Total: | | | 92.839 | 534.290 | 100.00 | 100.00 | |

**3ra**

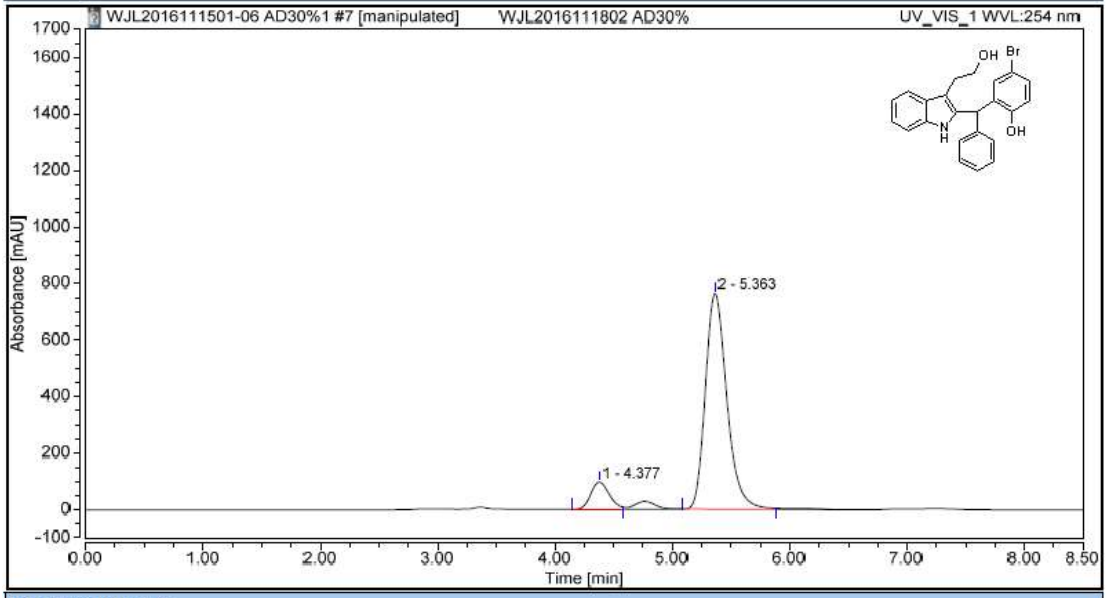
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.420 | 145.818 | 742.783 | 50.32 | 53.37 | n.a. |
| 2 | | 5.457 | 143.980 | 649.004 | 49.68 | 46.63 | n.a. |
| Total: | | | 289.798 | 1391.787 | 100.00 | 100.00 | |

**Chromatogram**

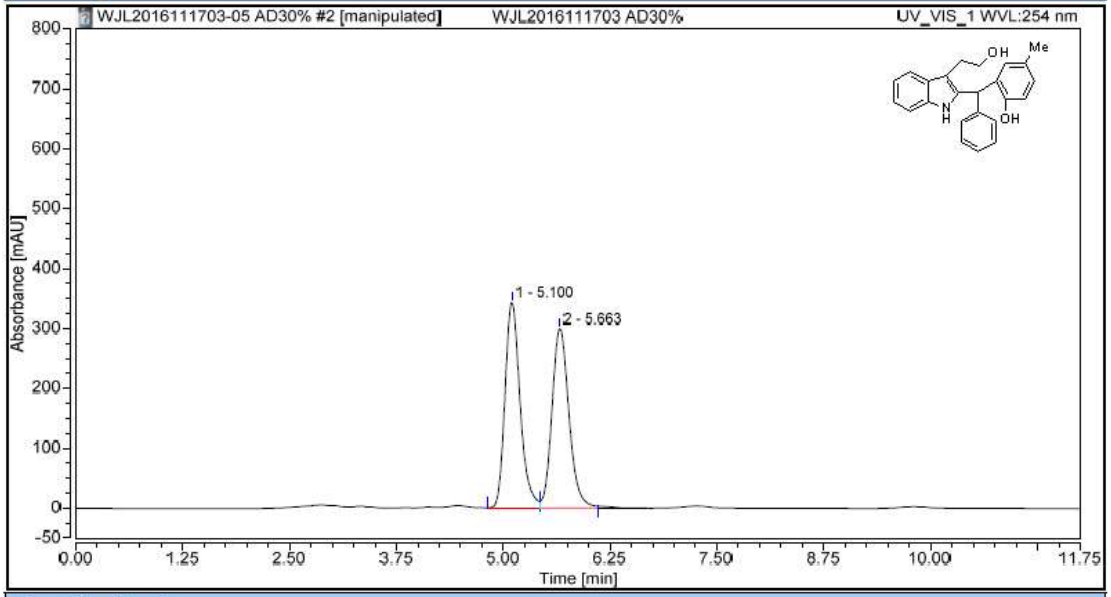



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.377 | 17.253 | 95.230 | 9.63 | 11.10 | n.a. |
| 2 | | 5.363 | 161.850 | 762.927 | 90.37 | 88.90 | n.a. |
| Total: | | | 179.103 | 858.157 | 100.00 | 100.00 | |

**3sa**

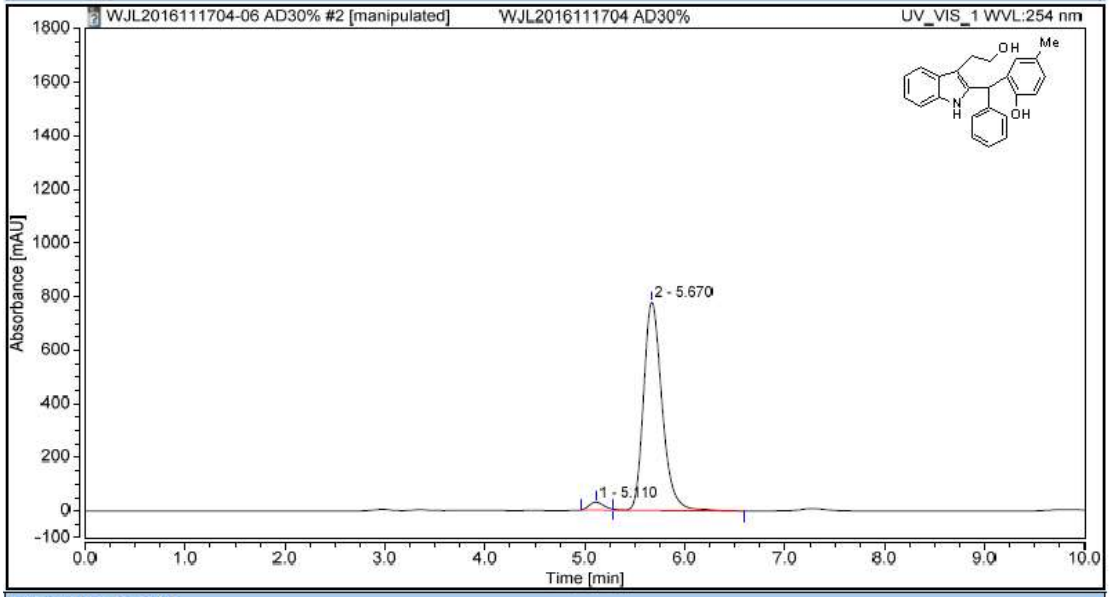
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.100 | 70.176 | 343.331 | 50.43 | 53.39 | n.a. |
| 2 | | 5.663 | 68.977 | 299.738 | 49.57 | 46.61 | n.a. |
| Total: | | | 139.153 | 643.068 | 100.00 | 100.00 | |

**Chromatogram**

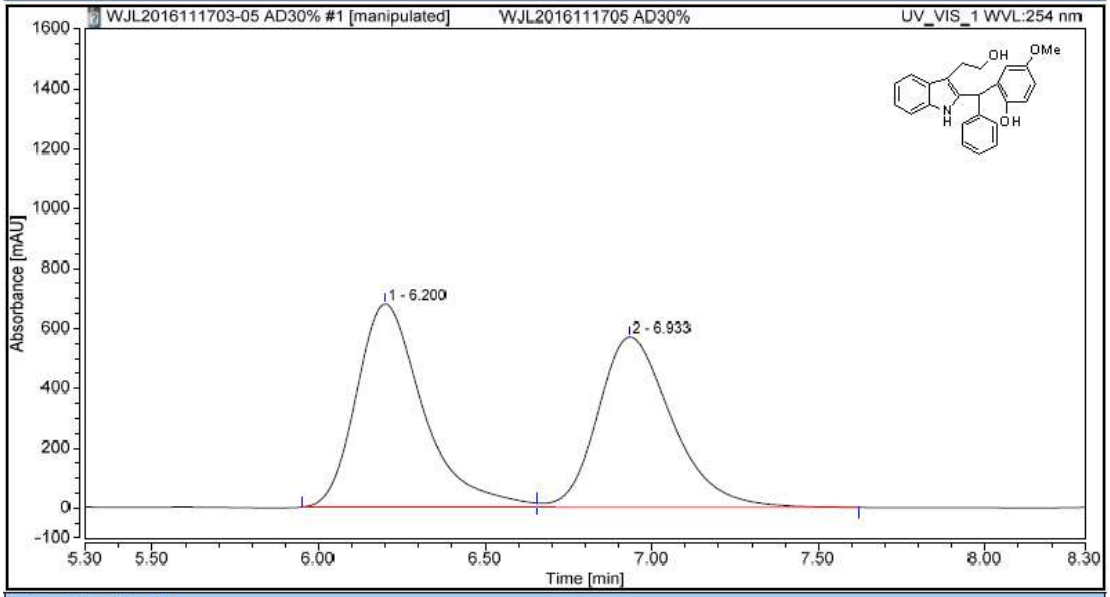



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.110 | 5.201 | 30.082 | 3.02 | 3.72 | n.a. |
| 2 | | 5.670 | 166.829 | 778.754 | 96.98 | 96.28 | n.a. |
| Total: | | | 172.031 | 808.836 | 100.00 | 100.00 | |

**3ta**

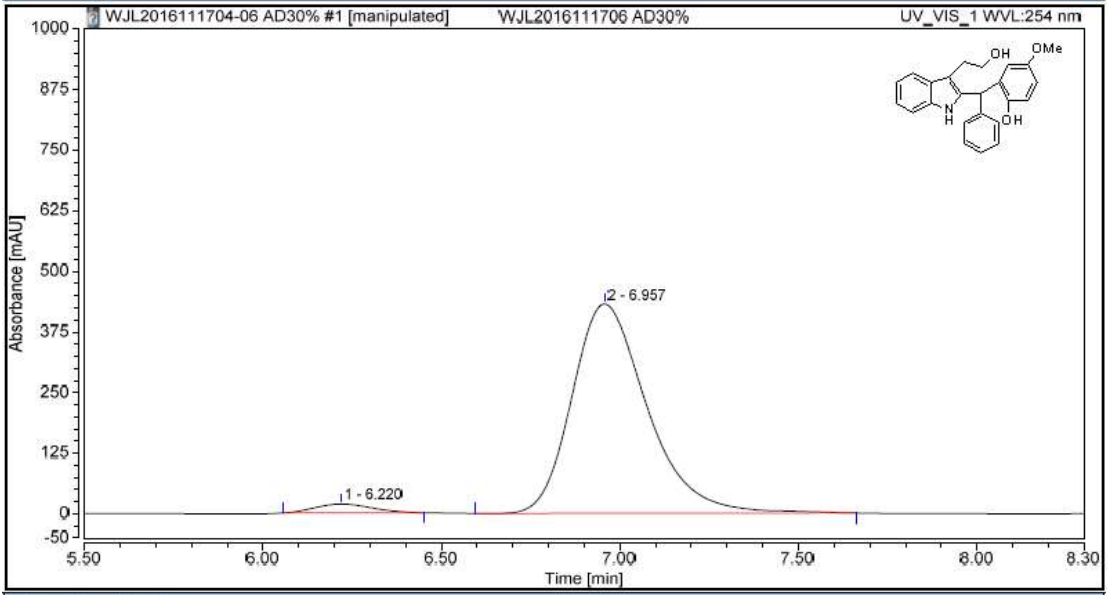
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.200 | 157.814 | 678.438 | 51.80 | 54.41 | n.a. |
| 2 | | 6.933 | 146.841 | 568.482 | 48.20 | 45.59 | n.a. |
| **Total:** | | | **304.655** | **1246.920** | **100.00** | **100.00** | |

**Chromatogram**

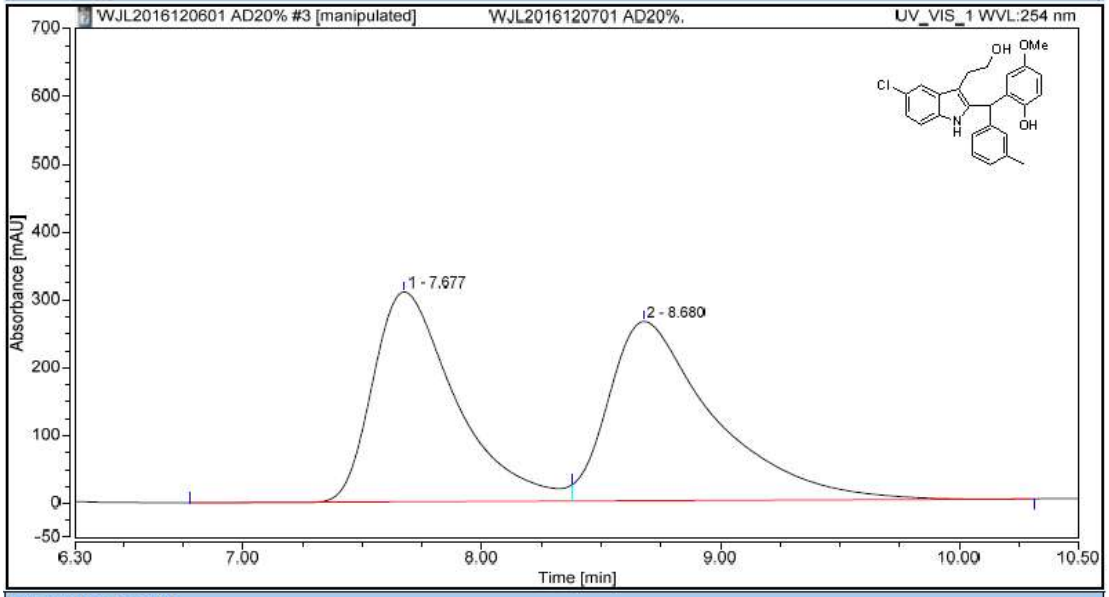



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.220 | 3.376 | 18.196 | 3.10 | 4.04 | n.a. |
| 2 | | 6.957 | 105.386 | 431.820 | 96.90 | 95.96 | n.a. |
| **Total:** | | | **108.762** | **450.016** | **100.00** | **100.00** | |

## 3jb

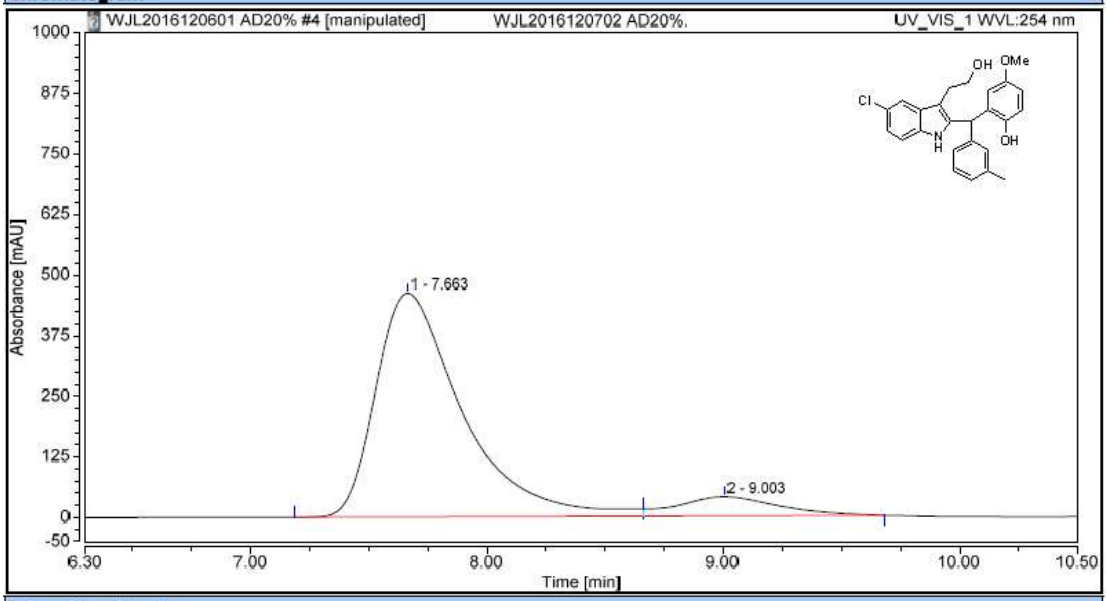
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 7.677 | 124.771 | 309.428 | 48.10 | 53.94 | n.a. |
| 2 | | 8.680 | 134.644 | 264.226 | 51.90 | 46.06 | n.a. |
| **Total:** | | | **259.415** | **573.654** | **100.00** | **100.00** | |

**Chromatogram**

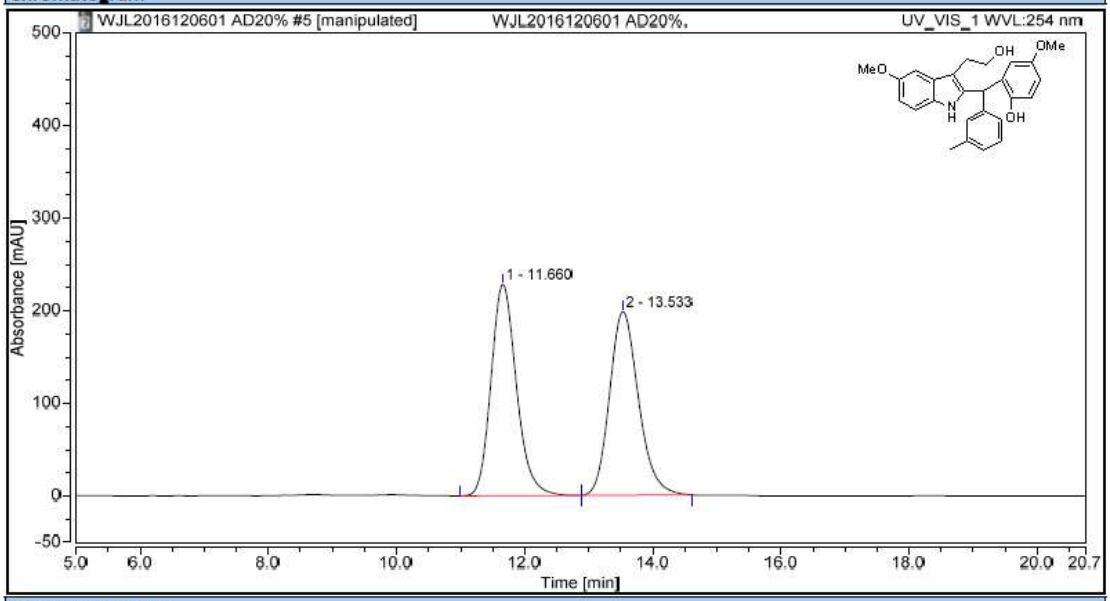



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 7.663 | 194.918 | 460.440 | 91.09 | 92.21 | n.a. |
| 2 | | 9.003 | 19.075 | 38.874 | 8.91 | 7.79 | n.a. |
| **Total:** | | | **213.993** | **499.315** | **100.00** | **100.00** | |

## 3jc

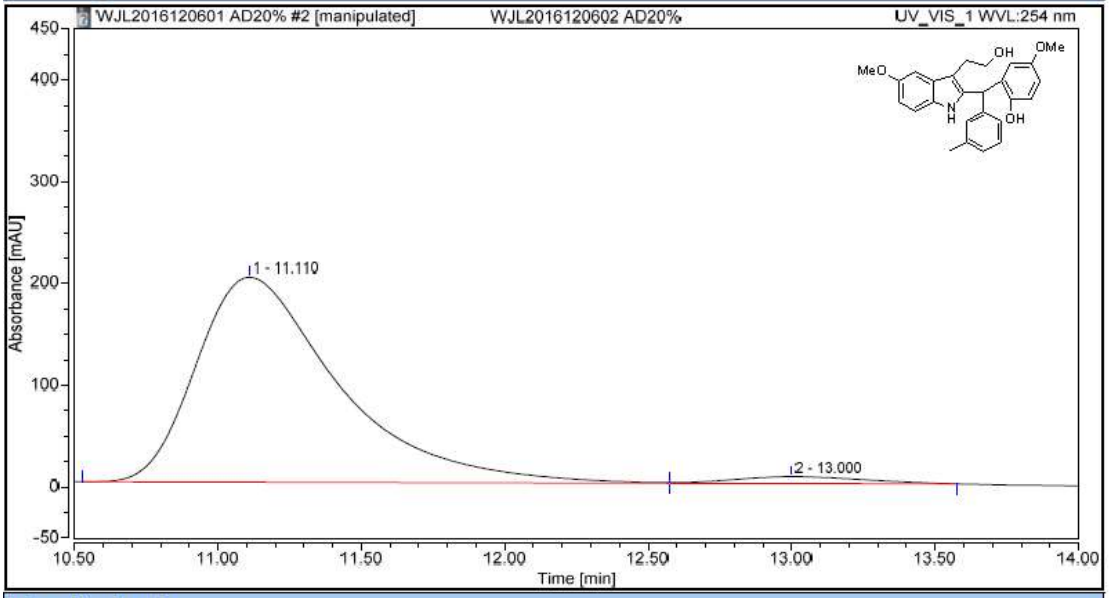
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 11.660 | 104.687 | 228.458 | 50.26 | 53.52 | n.a. |
| 2 | | 13.533 | 103.624 | 198.418 | 49.74 | 46.48 | n.a. |
| Total: | | | 208.311 | 426.876 | 100.00 | 100.00 | |

**Chromatogram**

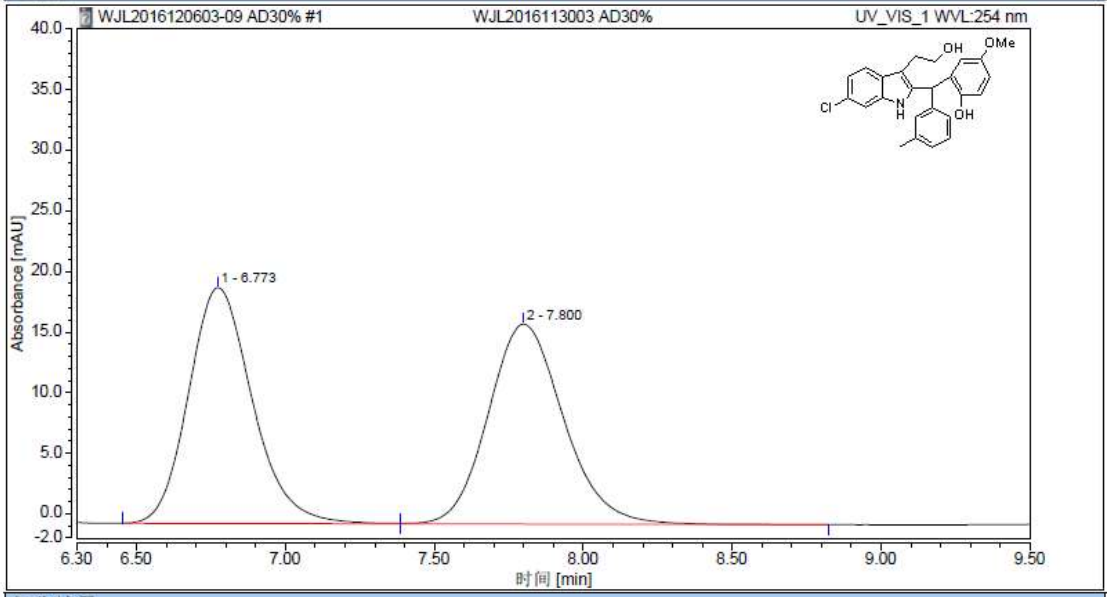



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 11.110 | 115.644 | 201.237 | 97.10 | 96.82 | n.a. |
| 2 | | 13.000 | 3.450 | 6.614 | 2.90 | 3.18 | n.a. |
| Total: | | | 119.094 | 207.851 | 100.00 | 100.00 | |

**3jd**

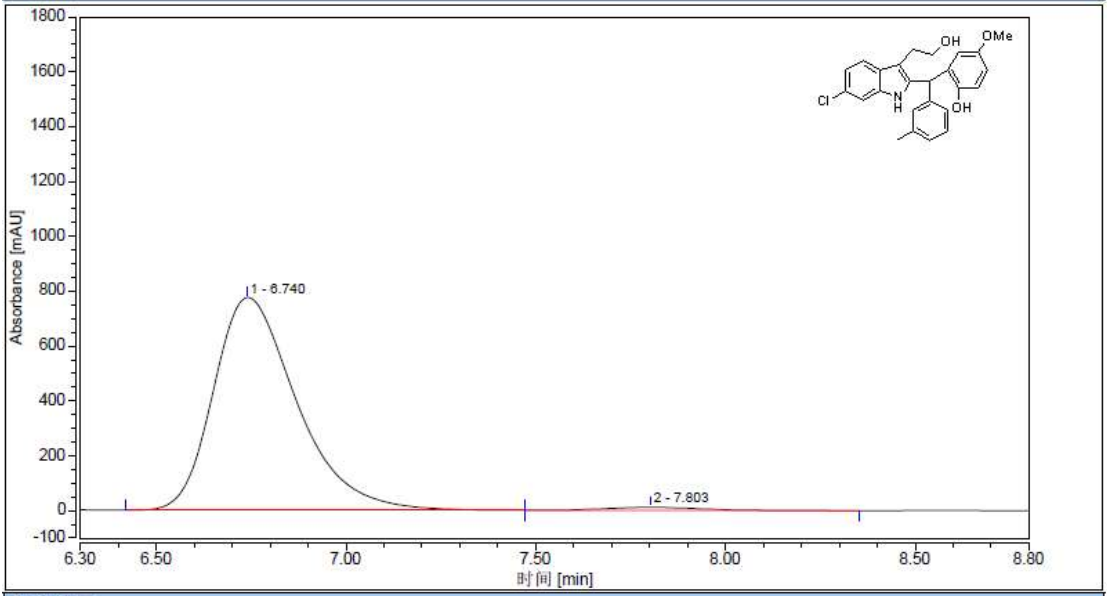
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.773 | 4.824 | 19.462 | 49.94 | 54.14 | n.a. |
| 2 | | 7.800 | 4.835 | 16.488 | 50.06 | 45.86 | n.a. |
| 总和: | | | 9.659 | 35.951 | 100.00 | 100.00 | |

色谱图

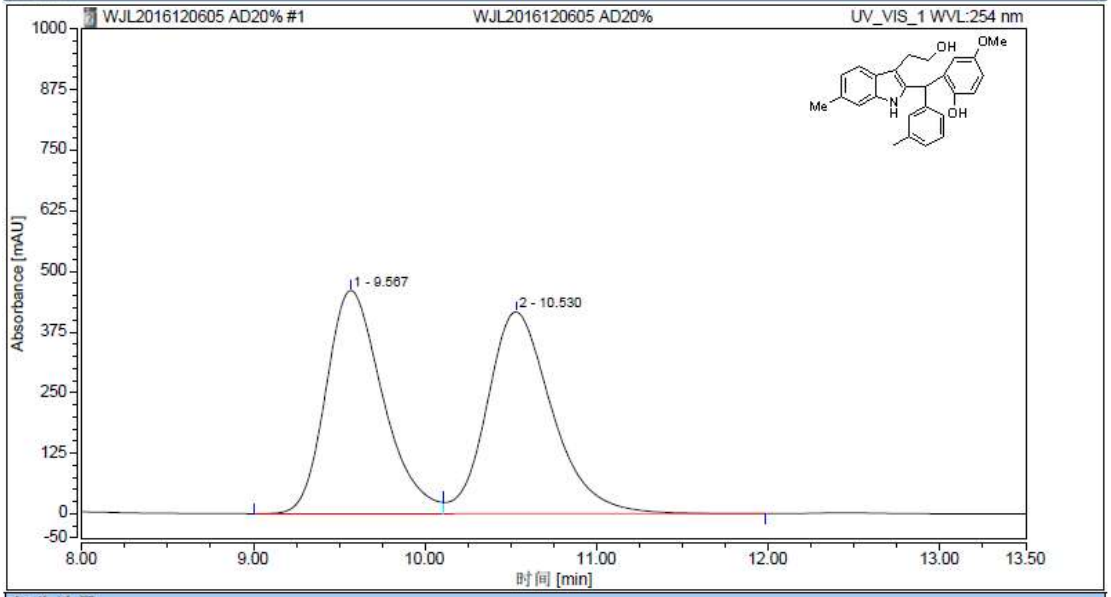



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 6.740 | 198.114 | 776.348 | 98.19 | 98.50 | n.a. |
| 2 | | 7.803 | 3.646 | 11.835 | 1.81 | 1.50 | n.a. |
| 总和: | | | 201.760 | 788.183 | 100.00 | 100.00 | |

**3je**

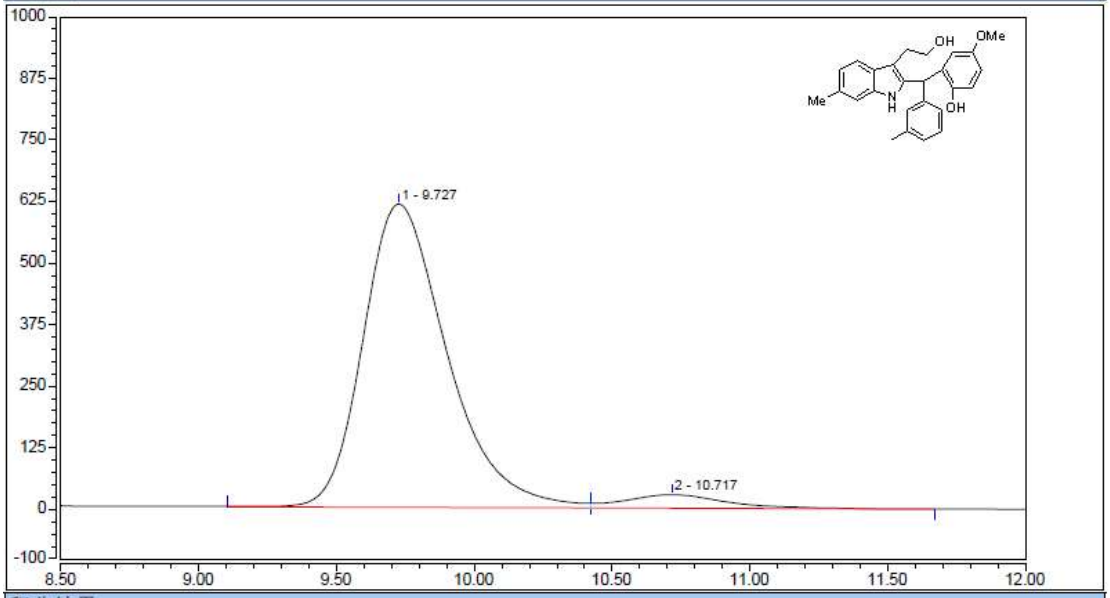
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 9.567 | 176.423 | 460.234 | 49.20 | 52.53 | n.a. |
| 2 | | 10.530 | 182.134 | 415.847 | 50.80 | 47.47 | n.a. |
| 总和: | | | 358.557 | 876.081 | 100.00 | 100.00 | |

色谱图

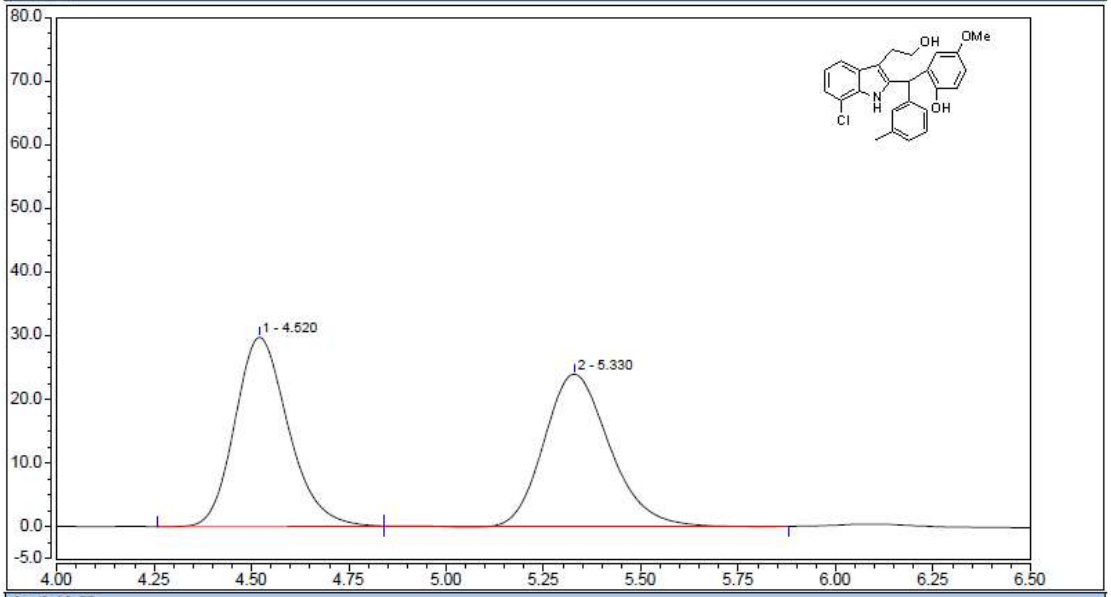



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 9.727 | 217.635 | 615.671 | 94.90 | 95.72 | n.a. |
| 2 | | 10.717 | 11.696 | 27.528 | 5.10 | 4.28 | n.a. |
| 总和: | | | 229.331 | 643.199 | 100.00 | 100.00 | |

**3jf**

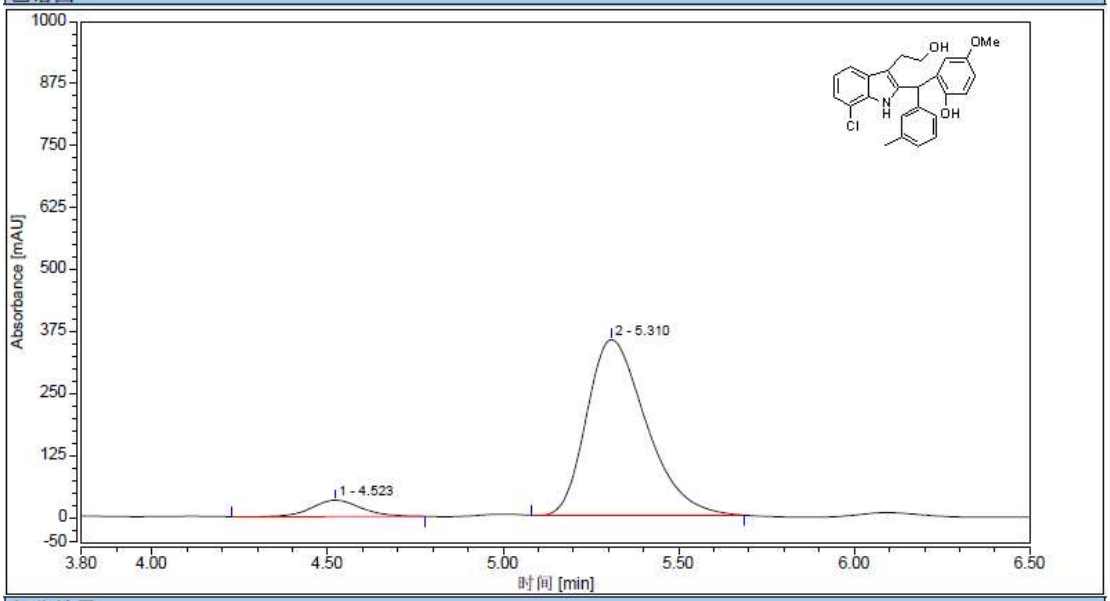
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.520 | 4.740 | 29.707 | 50.37 | 55.39 | n.a. |
| 2 | | 5.330 | 4.671 | 23.924 | 49.63 | 44.61 | n.a. |
| 总和: | | | **9.411** | **53.631** | **100.00** | **100.00** | |

色谱图

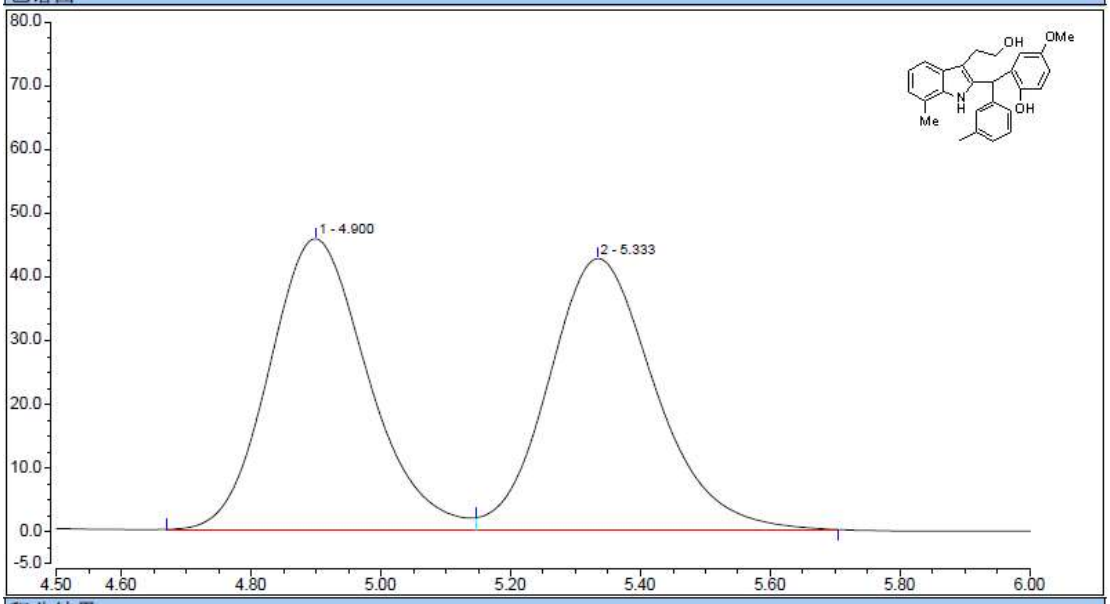



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.523 | 5.350 | 32.992 | 7.14 | 8.52 | n.a. |
| 2 | | 5.310 | 69.609 | 354.201 | 92.86 | 91.48 | n.a. |
| 总和: | | | **74.959** | **387.193** | **100.00** | **100.00** | |

**3jg**

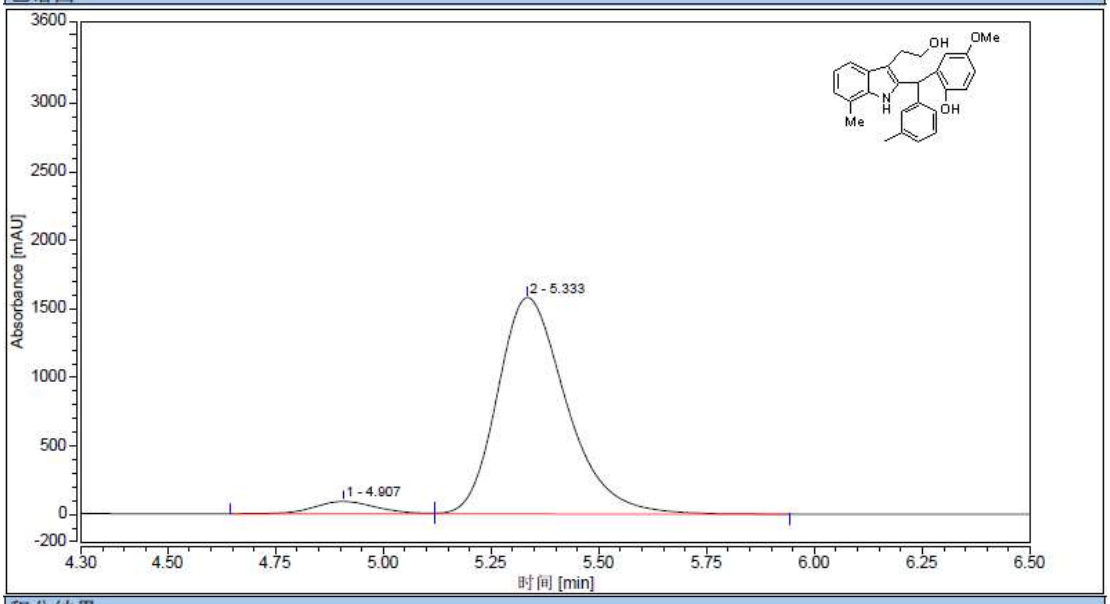
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.900 | 8.025 | 45.573 | 49.88 | 51.76 | n.a. |
| 2 | | 5.333 | 8.065 | 42.478 | 50.12 | 48.24 | n.a. |
| 总和: | | | **16.090** | **88.052** | **100.00** | **100.00** | |

色谱图

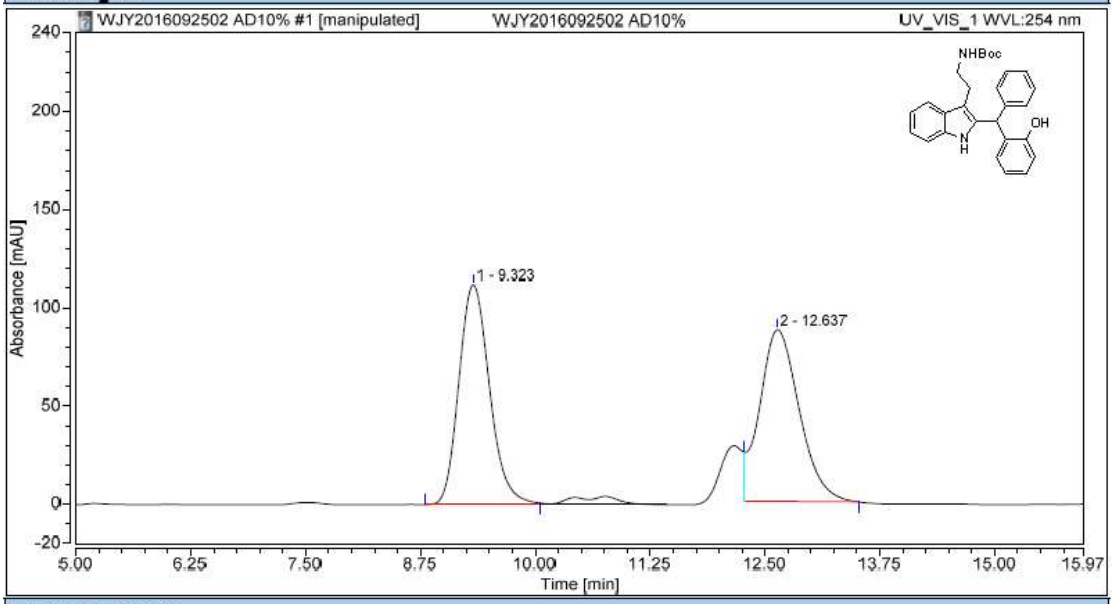



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.907 | 14.885 | 89.343 | 4.83 | 5.36 | n.a. |
| 2 | | 5.333 | 292.996 | 1578.967 | 95.17 | 94.64 | n.a. |
| 总和: | | | **307.881** | **1668.310** | **100.00** | **100.00** | |

**8aa**

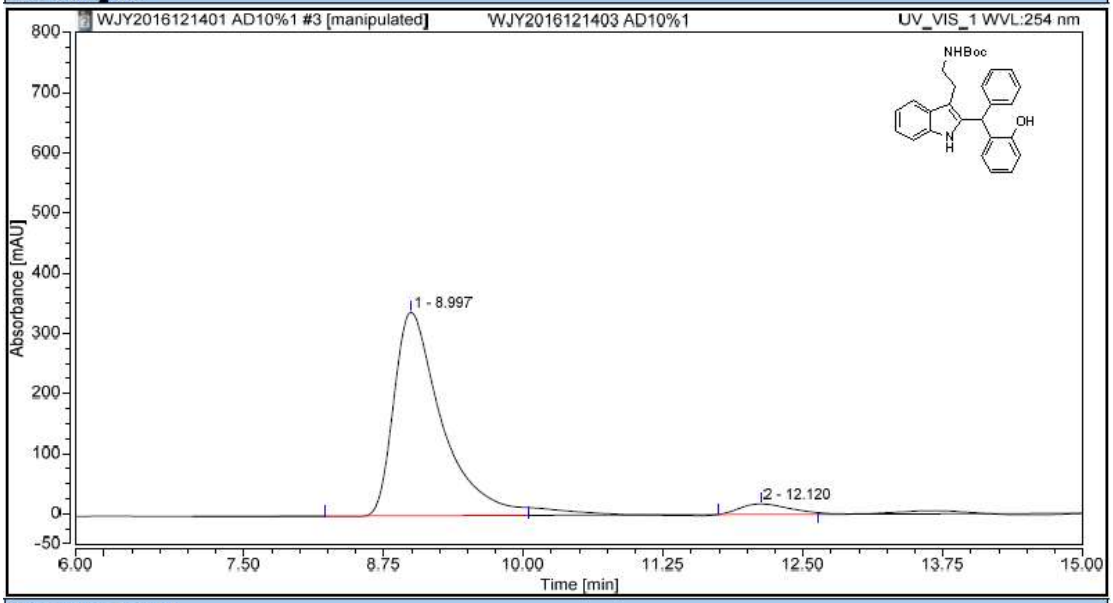
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 9.323 | 43.292 | 111.855 | 49.58 | 56.13 | n.a. |
| 2 | | 12.637 | 44.020 | 87.411 | 50.42 | 43.87 | n.a. |
| Total: | | | 87.311 | 199.266 | 100.00 | 100.00 | |

**Chromatogram**

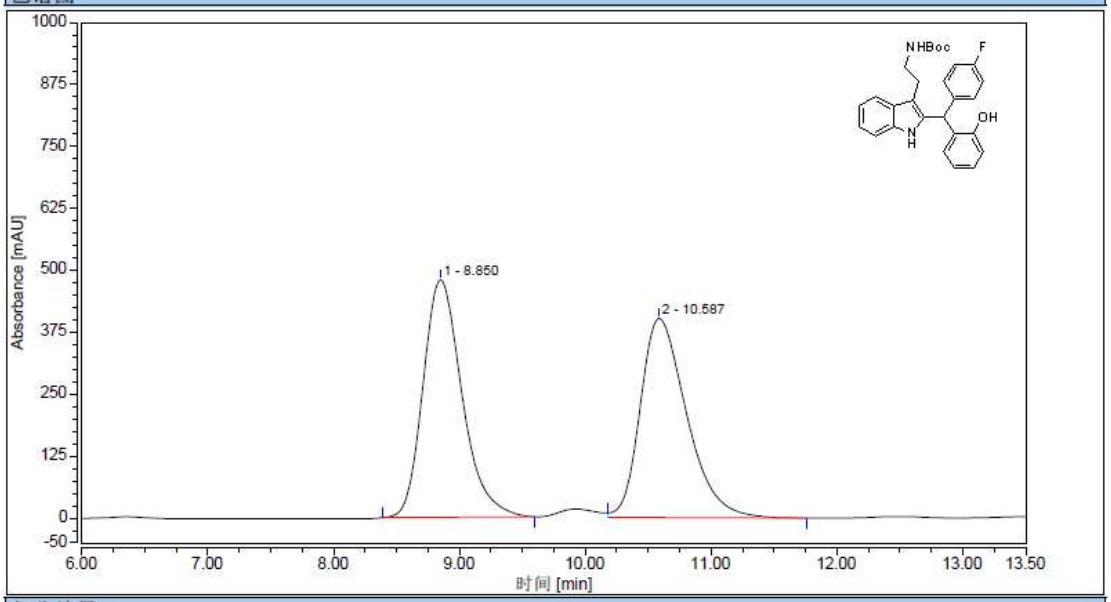



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.997 | 166.911 | 337.973 | 94.94 | 95.08 | n.a. |
| 2 | | 12.120 | 8.895 | 17.495 | 5.06 | 4.92 | n.a. |
| Total: | | | 175.805 | 355.467 | 100.00 | 100.00 | |

**8ba**

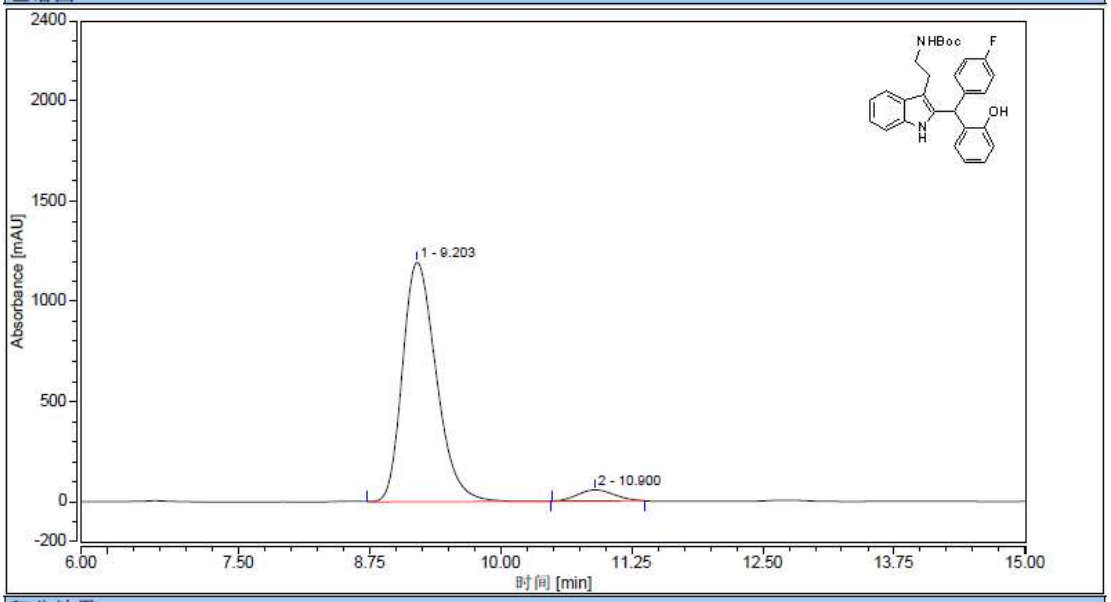
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.850 | 171.924 | 479.144 | 50.17 | 54.42 | n.a. |
| 2 | | 10.587 | 170.754 | 401.260 | 49.83 | 45.58 | n.a. |
| 总和: | | | 342.678 | 880.404 | 100.00 | 100.00 | |

色谱图

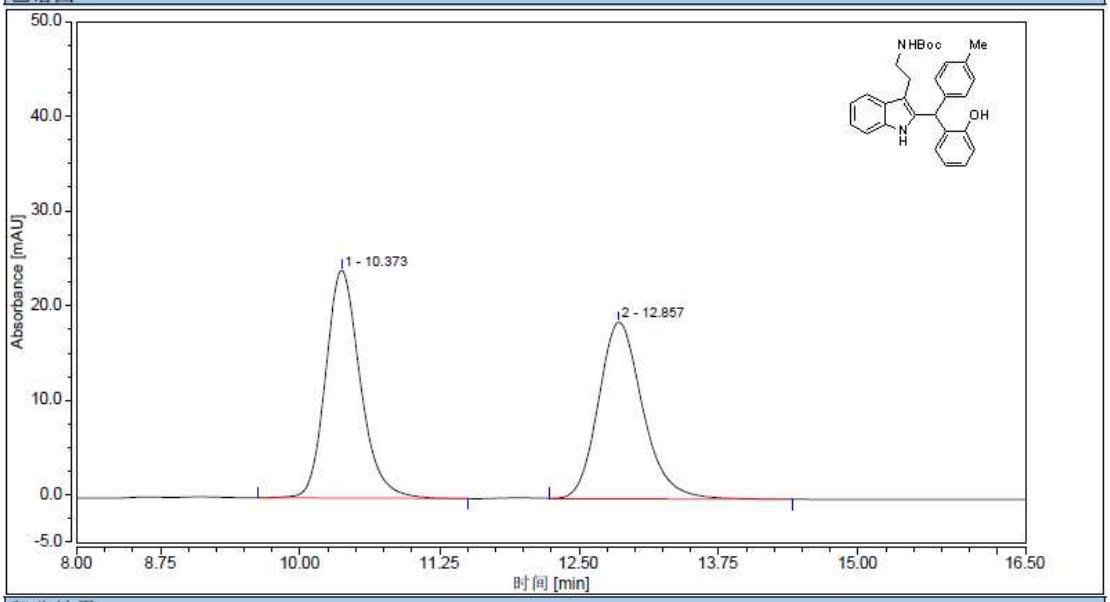



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 9.203 | 444.476 | 1194.662 | 95.27 | 95.60 | n.a. |
| 2 | | 10.900 | 22.051 | 54.970 | 4.73 | 4.40 | n.a. |
| 总和: | | | 466.528 | 1249.632 | 100.00 | 100.00 | |

**8ca**

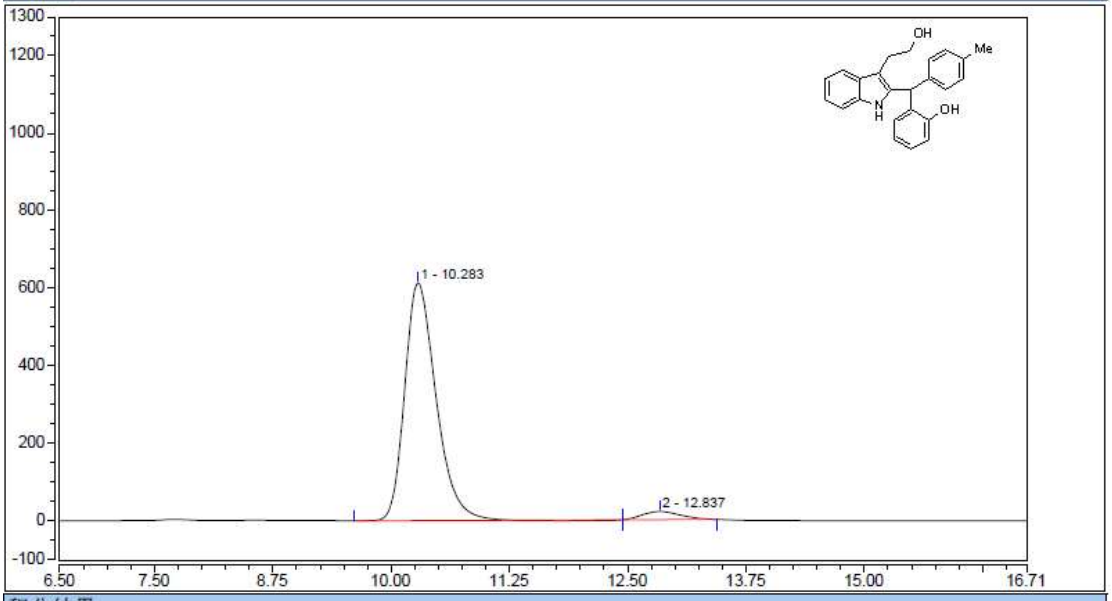
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 10.373 | 8.663 | 24.066 | 50.13 | 56.33 | n.a. |
| 2 | | 12.857 | 8.617 | 18.658 | 49.87 | 43.67 | n.a. |
| 总和: | | | **17.280** | **42.723** | **100.00** | **100.00** | |

色谱图

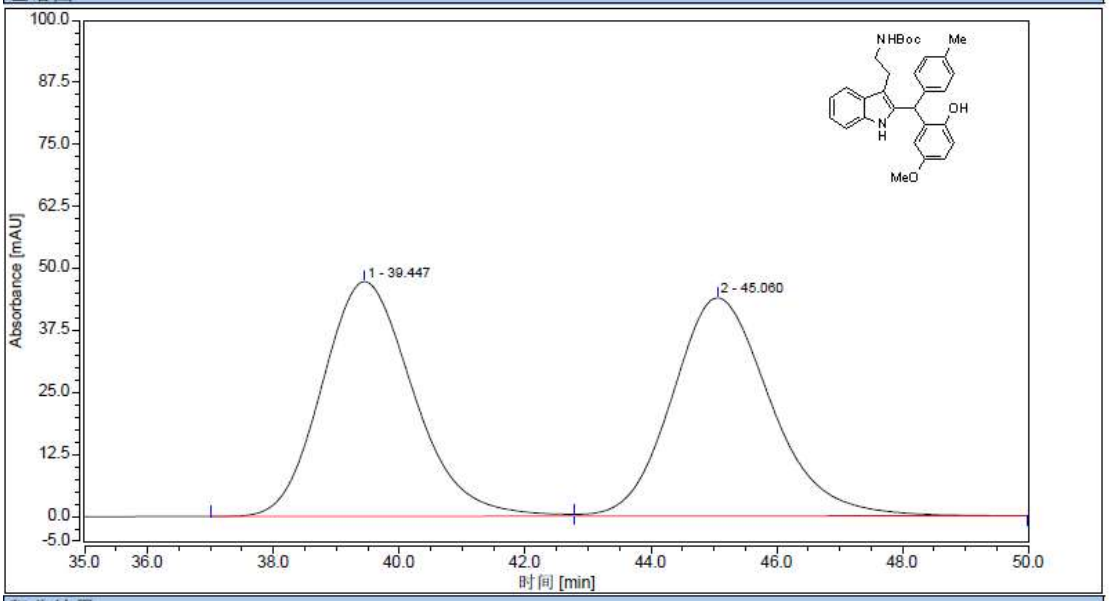



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 10.283 | 233.662 | 613.157 | 96.00 | 96.68 | n.a. |
| 2 | | 12.837 | 9.740 | 21.042 | 4.00 | 3.32 | n.a. |
| 总和: | | | **243.402** | **634.199** | **100.00** | **100.00** | |

## 8ha

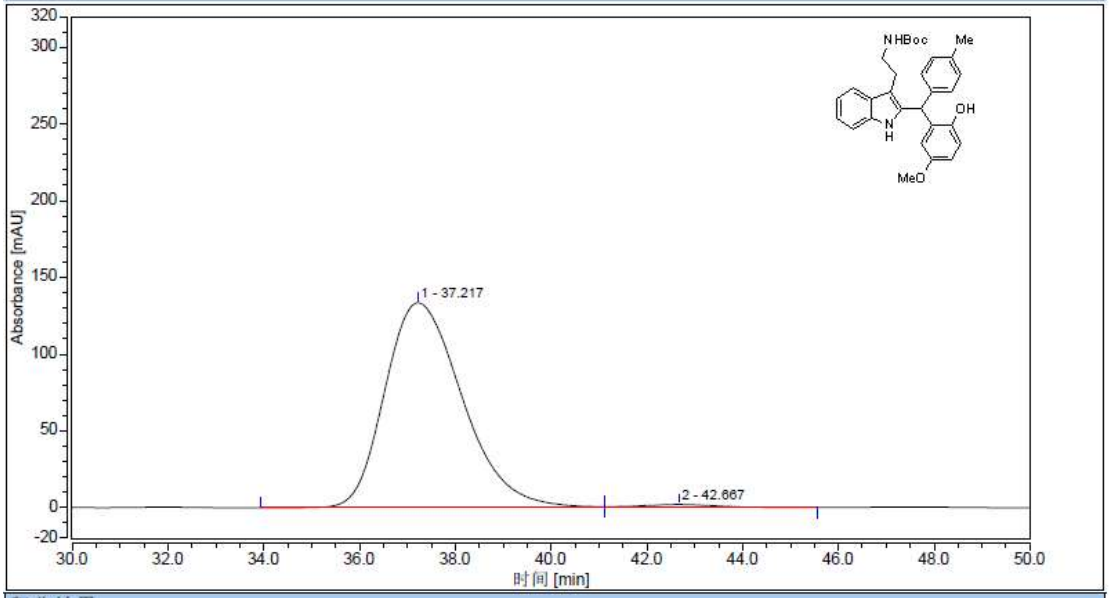
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 39.447 | 79.500 | 47.284 | 49.94 | 51.84 | n.a. |
| 2 | | 45.060 | 79.706 | 43.928 | 50.06 | 48.16 | n.a. |
| 总和: | | | **159.206** | **91.212** | **100.00** | **100.00** | |

色谱图

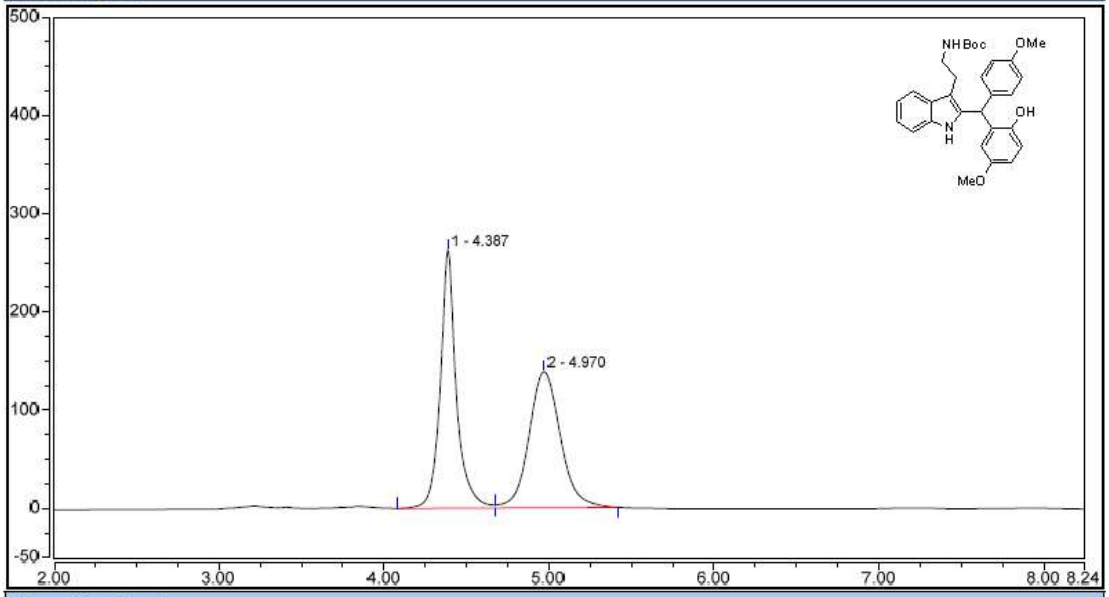



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 37.217 | 250.832 | 133.583 | 98.27 | 98.44 | n.a. |
| 2 | | 42.667 | 4.408 | 2.119 | 1.73 | 1.56 | n.a. |
| 总和: | | | **255.239** | **135.702** | **100.00** | **100.00** | |

## 8ua

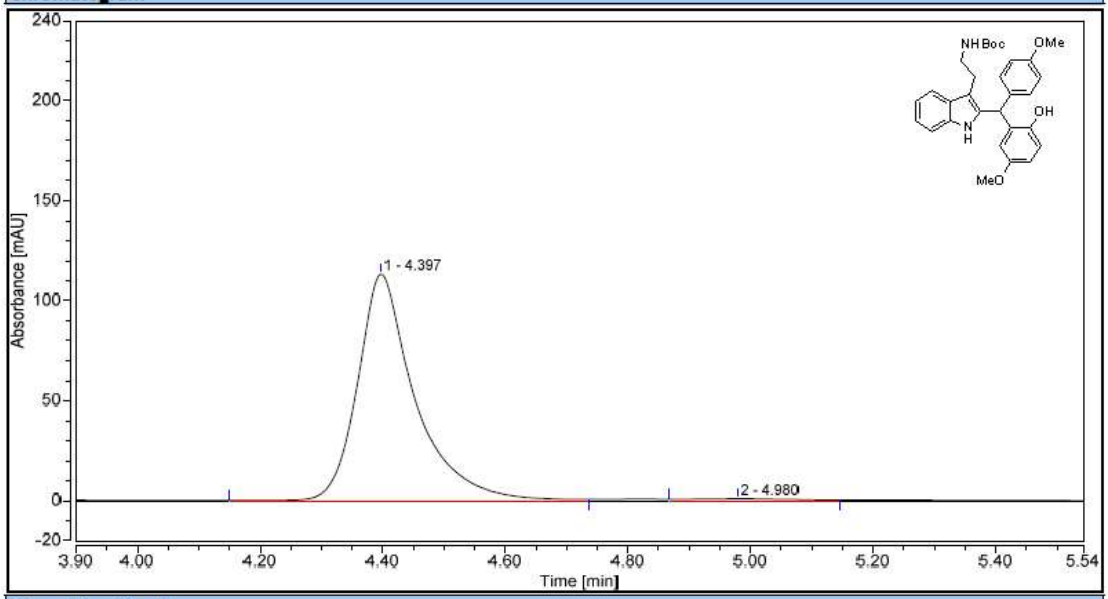
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.387 | 29.664 | 262.745 | 49.27 | 65.49 | n.a. |
| 2 | | 4.970 | 30.539 | 138.439 | 50.73 | 34.51 | n.a. |
| Total: | | | **60.202** | **401.184** | **100.00** | **100.00** | |

**Chromatogram**

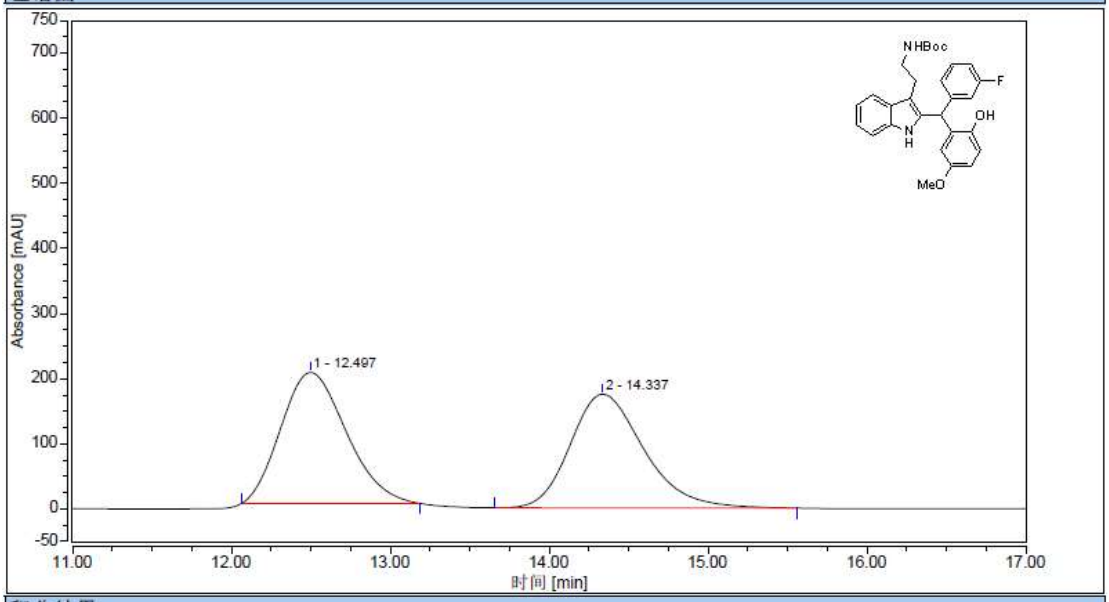



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.397 | 12.341 | 113.239 | 98.31 | 99.14 | n.a. |
| 2 | | 4.980 | 0.212 | 0.983 | 1.69 | 0.86 | n.a. |
| Total: | | | **12.553** | **114.222** | **100.00** | **100.00** | |

**8ia**

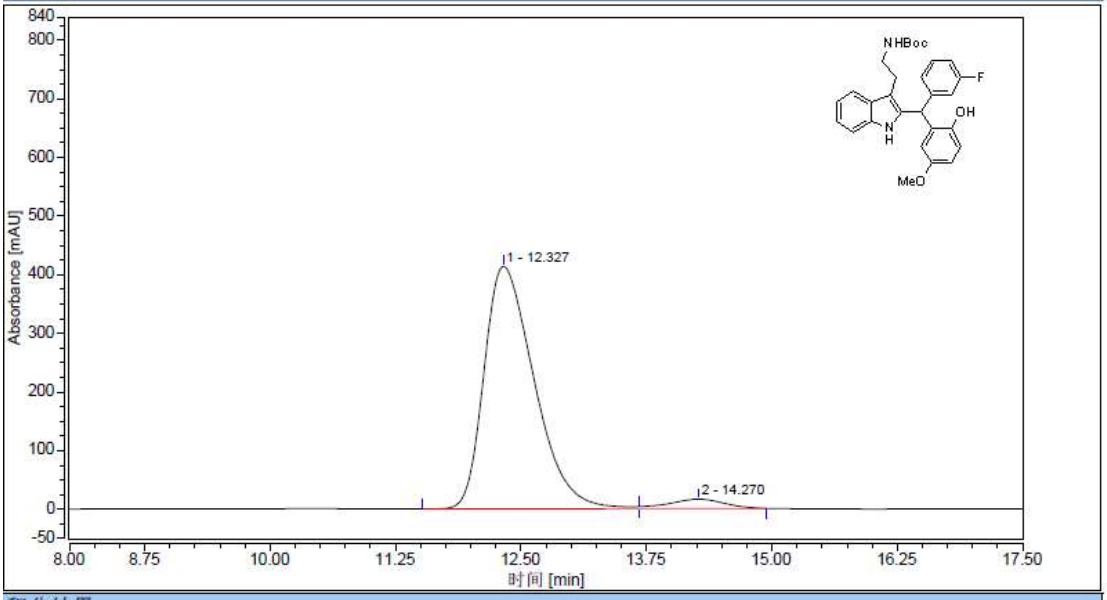
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 12.497 | 95.950 | 201.045 | 50.61 | 53.51 | n.a. |
| 2 | | 14.337 | 93.637 | 174.655 | 49.39 | 46.49 | n.a. |
| 总和: | | | 189.587 | 375.699 | 100.00 | 100.00 | |

色谱图

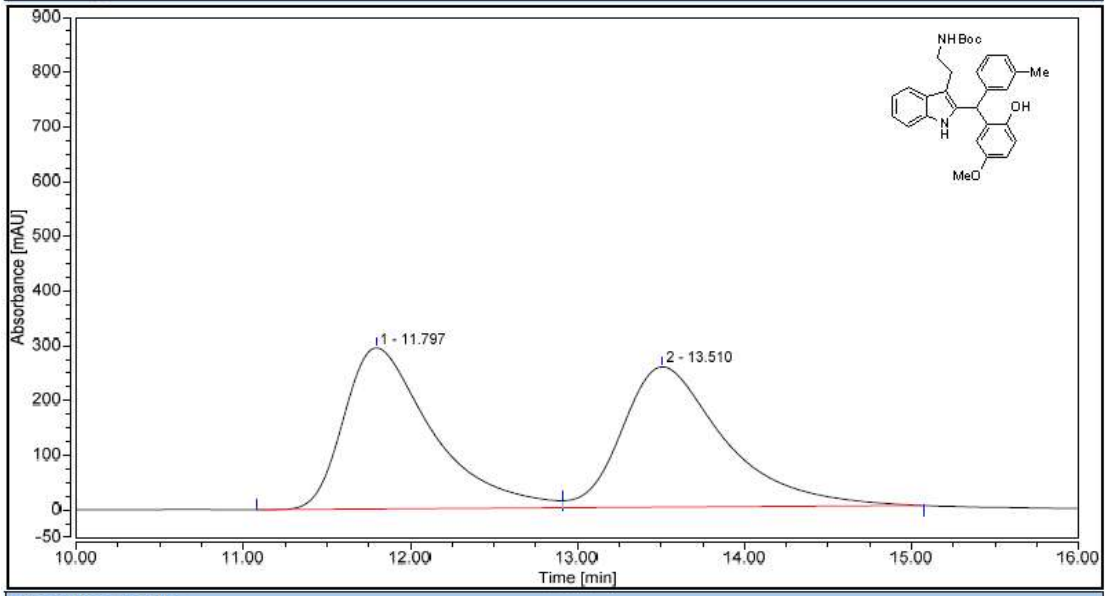



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 12.327 | 239.341 | 413.630 | 95.94 | 96.30 | n.a. |
| 2 | | 14.270 | 10.134 | 15.902 | 4.06 | 3.70 | n.a. |
| 总和: | | | 249.475 | 429.532 | 100.00 | 100.00 | |

**8ja**

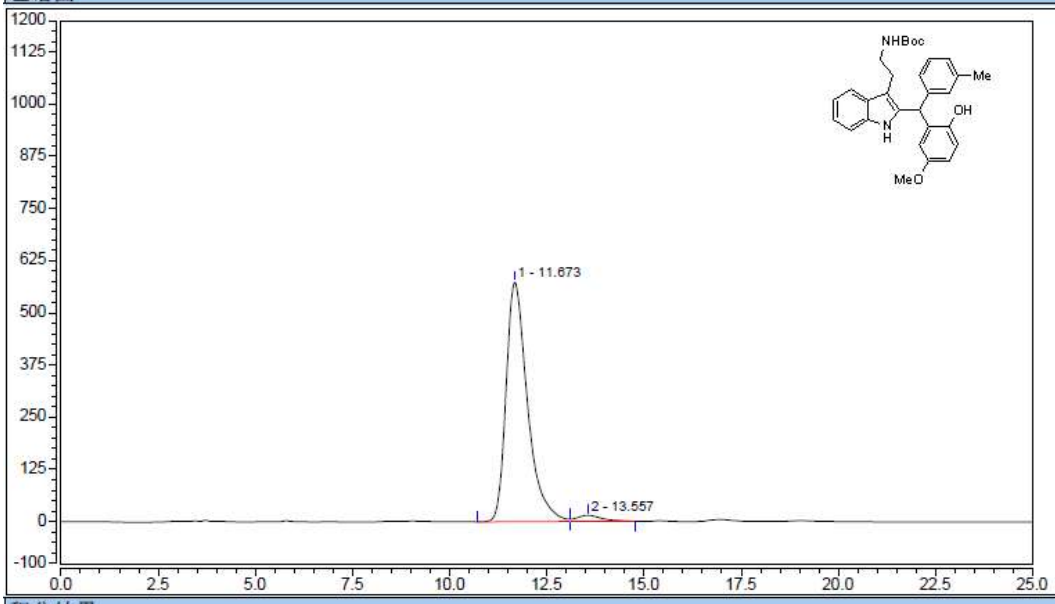
Chromatogram




Integration Results

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 11.797 | 180.356 | 294.140 | 49.73 | 53.44 | n.a. |
| 2 | | 13.510 | 182.310 | 256.284 | 50.27 | 46.56 | n.a. |
| Total: | | | 362.666 | 550.424 | 100.00 | 100.00 | |

色谱图

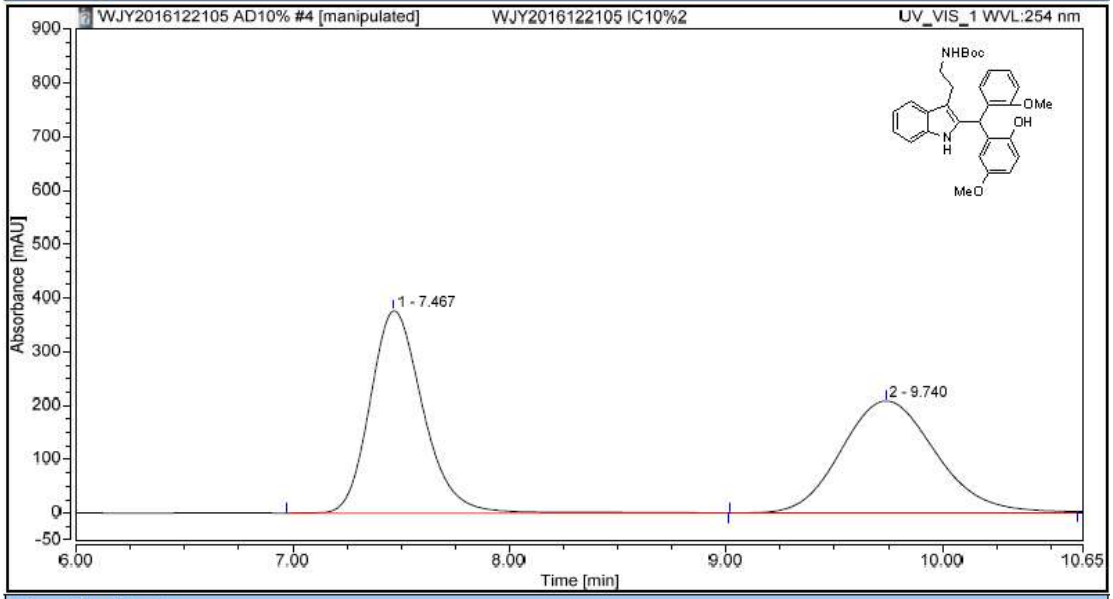



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 11.673 | 365.686 | 573.885 | 97.14 | 97.53 | n.a. |
| 2 | | 13.557 | 10.751 | 14.553 | 2.86 | 2.47 | n.a. |
| 总和: | | | 376.437 | 588.438 | 100.00 | 100.00 | |

## 8ka

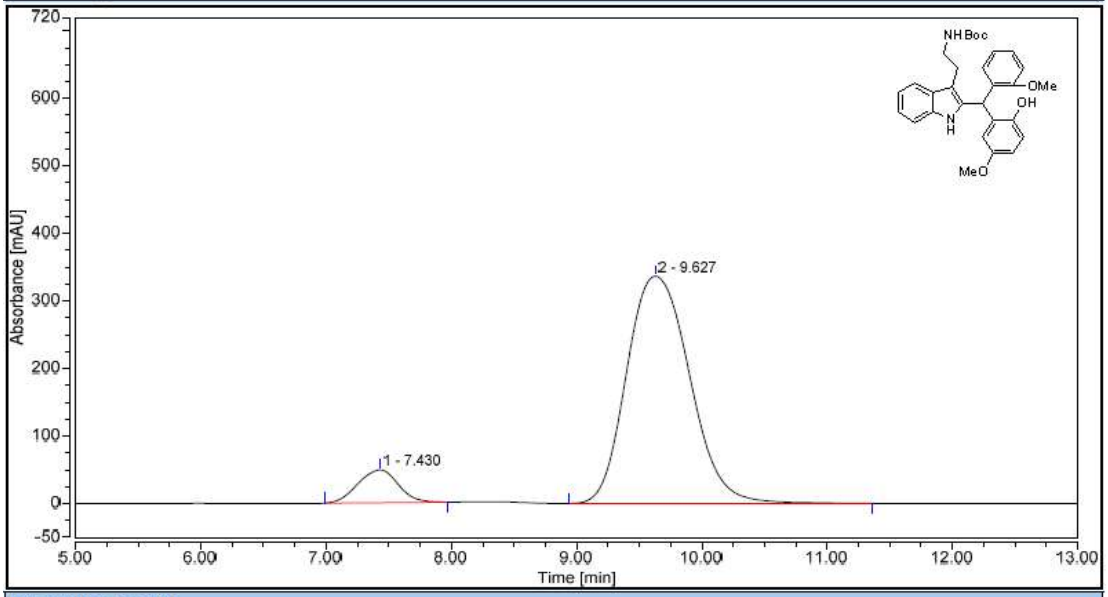
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 7.467 | 106.669 | 376.115 | 50.23 | 64.35 | n.a. |
| 2 | | 9.740 | 105.712 | 208.349 | 49.77 | 35.65 | n.a. |
| **Total:** | | | **212.381** | **584.464** | **100.00** | **100.00** | |

**Chromatogram**

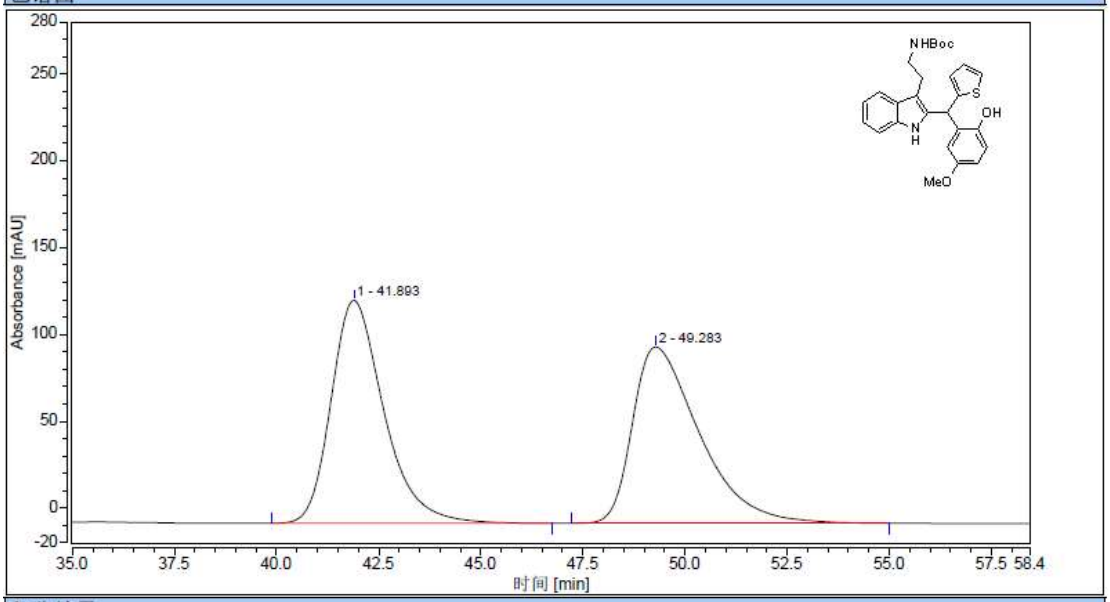



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 7.430 | 18.043 | 48.550 | 8.43 | 12.61 | n.a. |
| 2 | | 9.627 | 195.888 | 336.321 | 91.57 | 87.39 | n.a. |
| **Total:** | | | **213.931** | **384.870** | **100.00** | **100.00** | |

**8la**

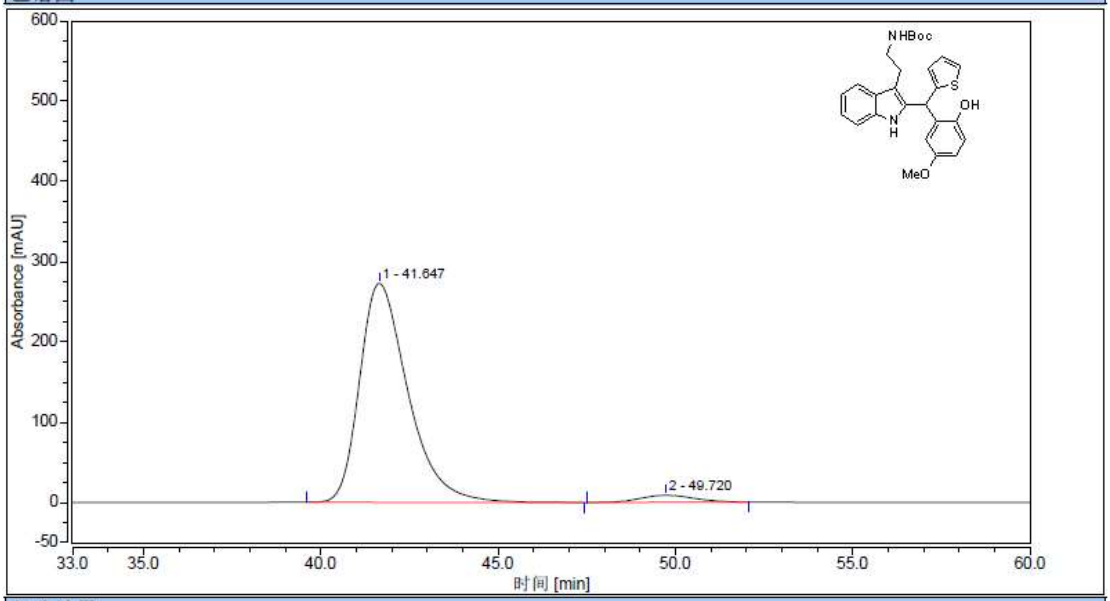
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 41.893 | 192.140 | 128.291 | 49.89 | 55.83 | n.a. |
| 2 | | 49.283 | 192.967 | 101.494 | 50.11 | 44.17 | n.a. |
| 总和: | | | 385.107 | 229.785 | 100.00 | 100.00 | |

色谱图

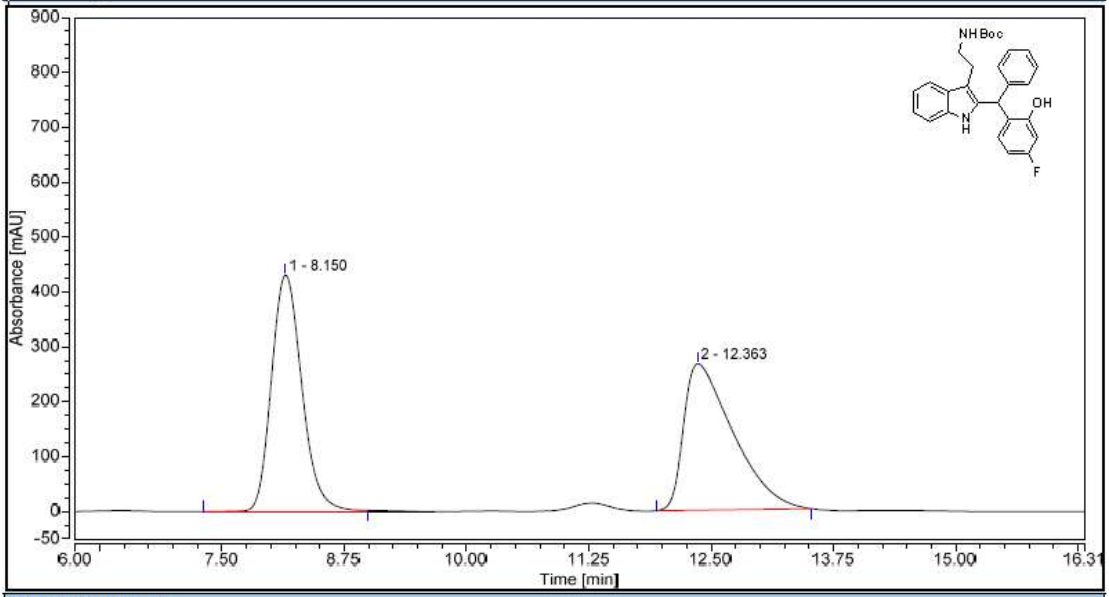



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 41.647 | 430.580 | 272.649 | 96.57 | 96.88 | n.a. |
| 2 | | 49.720 | 15.308 | 8.779 | 3.43 | 3.12 | n.a. |
| 总和: | | | 445.888 | 281.427 | 100.00 | 100.00 | |

## 8na

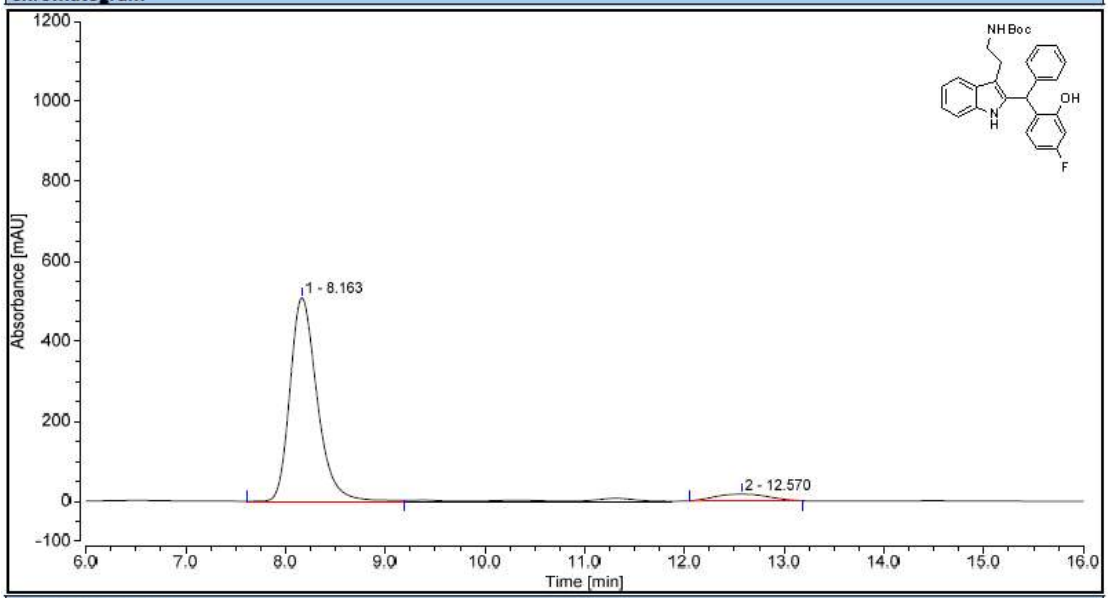
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.150 | 155.307 | 431.116 | 49.93 | 61.77 | n.a. |
| 2 | | 12.363 | 155.736 | 266.773 | 50.07 | 38.23 | n.a. |
| Total: | | | 311.043 | 697.889 | 100.00 | 100.00 | |

**Chromatogram**

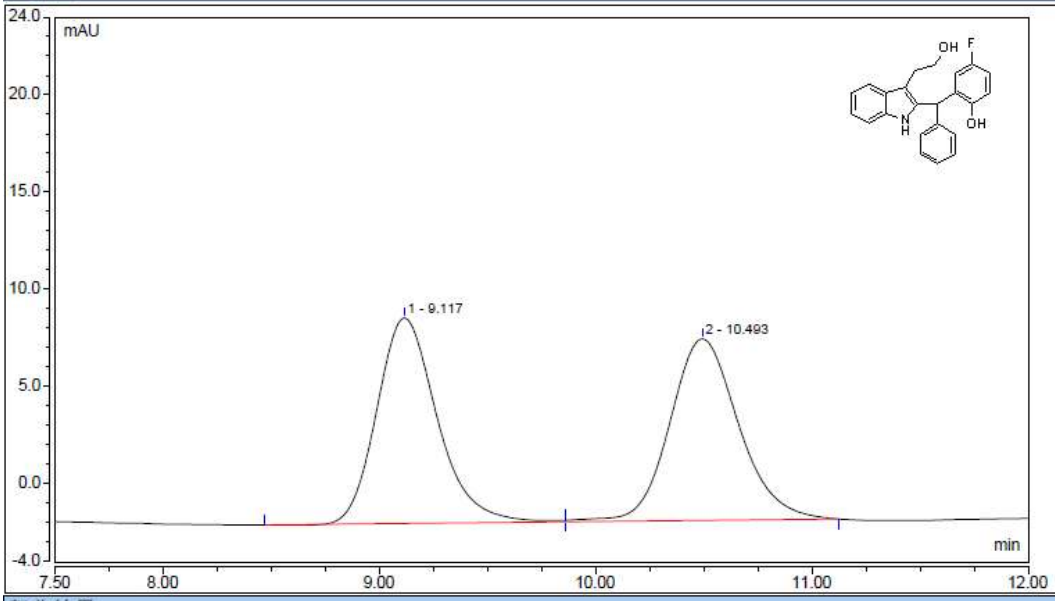



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 8.163 | 160.292 | 508.543 | 94.01 | 96.82 | n.a. |
| 2 | | 12.570 | 10.213 | 16.704 | 5.99 | 3.18 | n.a. |
| Total: | | | 170.506 | 525.247 | 100.00 | 100.00 | |

**3pa**

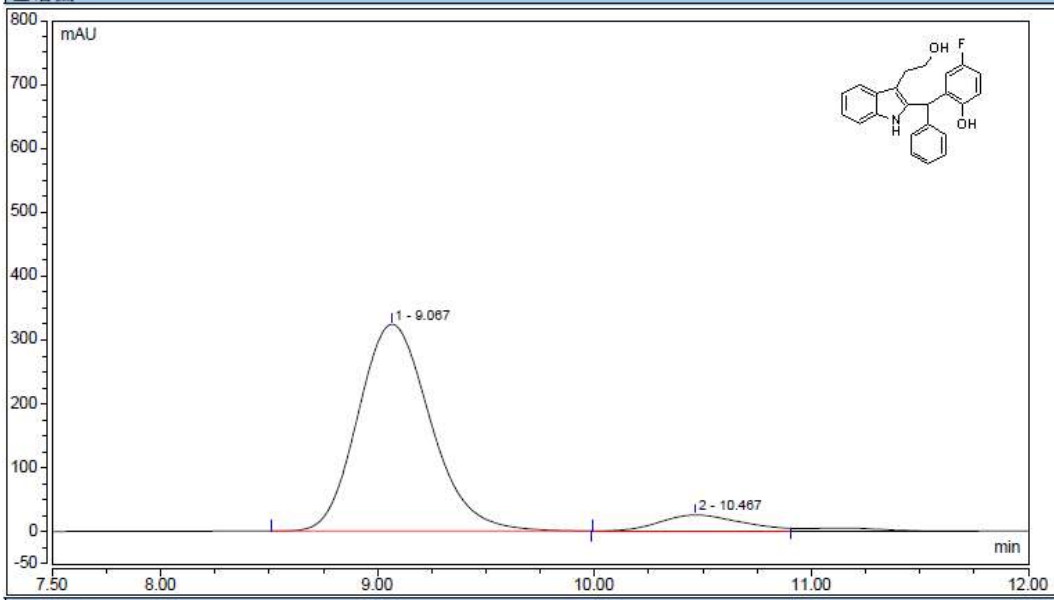
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 9.117 | 3.415 | 10.557 | 49.81 | 53.09 | n.a. |
| 2 | | 10.493 | 3.441 | 9.329 | 50.19 | 46.91 | n.a. |
| 总和: | | | 6.856 | 19.885 | 100.00 | 100.00 | |

色谱图

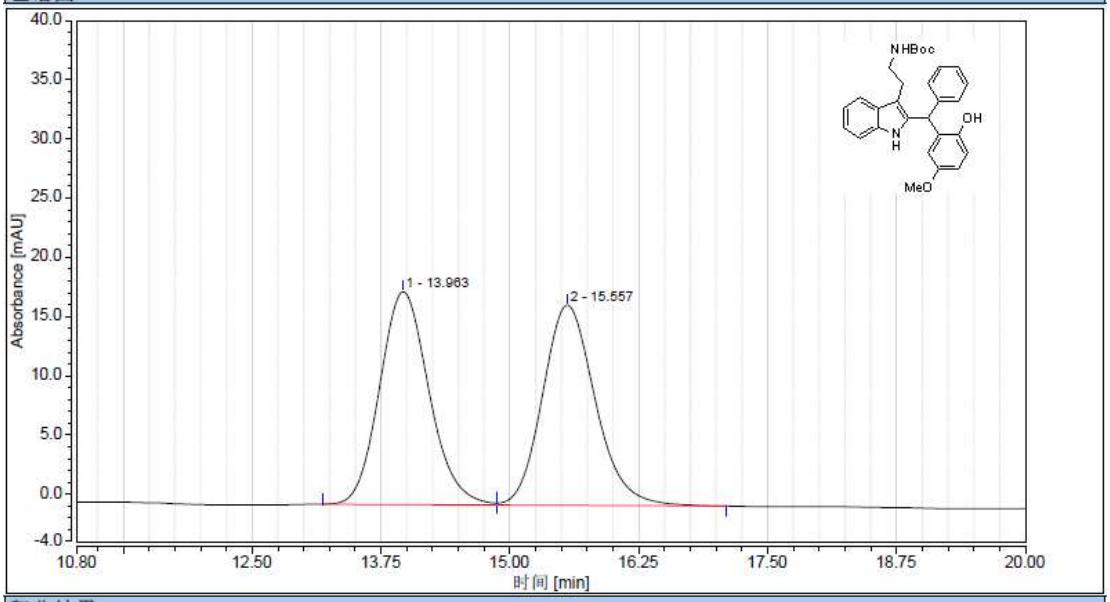



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 9.067 | 125.154 | 323.490 | 92.09 | 92.85 | n.a. |
| 2 | | 10.467 | 10.750 | 24.900 | 7.91 | 7.15 | n.a. |
| 总和: | | | 135.903 | 348.390 | 100.00 | 100.00 | |

**8ta**

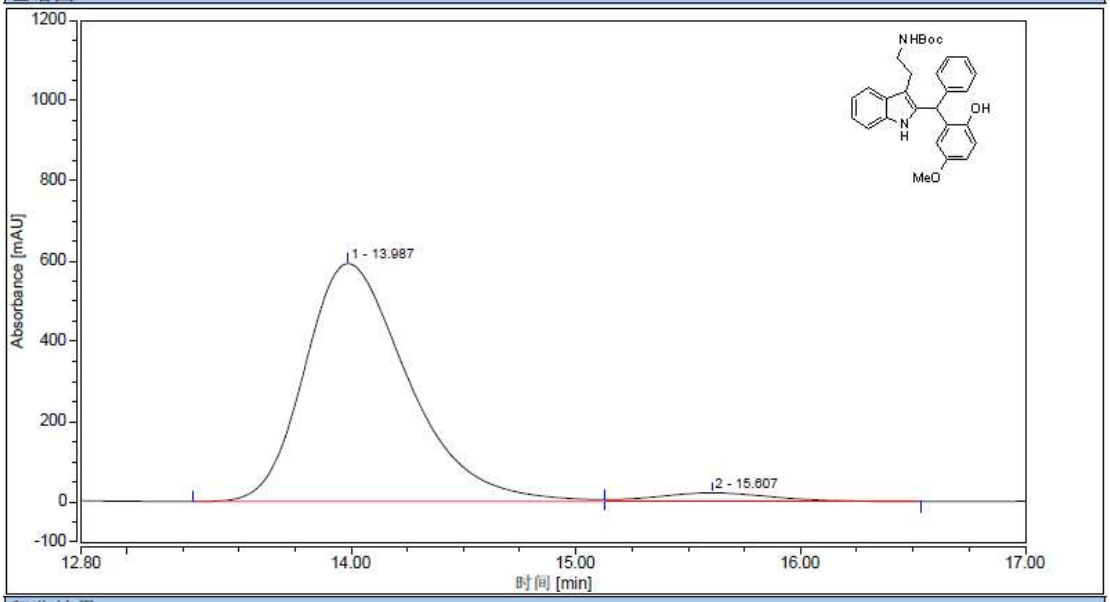
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 13.963 | 9.953 | 17.965 | 49.89 | 51.54 | n.a. |
| 2 | | 15.557 | 9.997 | 16.895 | 50.11 | 48.46 | n.a. |
| 总和: | | | 19.950 | 34.860 | 100.00 | 100.00 | |

色谱图

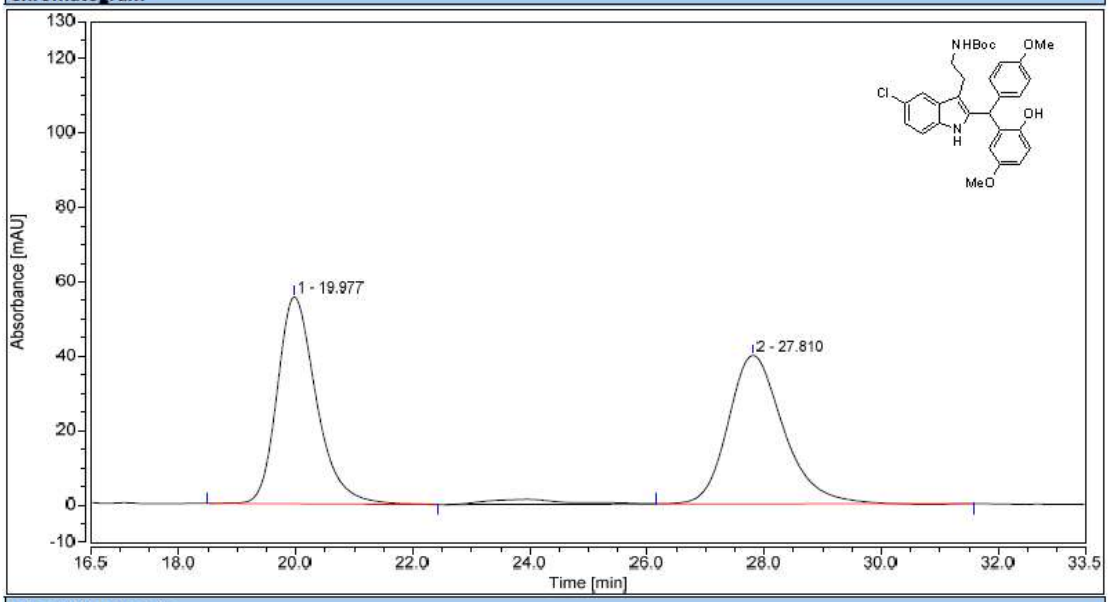



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 13.987 | 316.828 | 592.734 | 96.08 | 96.50 | n.a. |
| 2 | | 15.607 | 12.915 | 21.502 | 3.92 | 3.50 | n.a. |
| 总和: | | | 329.744 | 614.236 | 100.00 | 100.00 | |

## 8ub

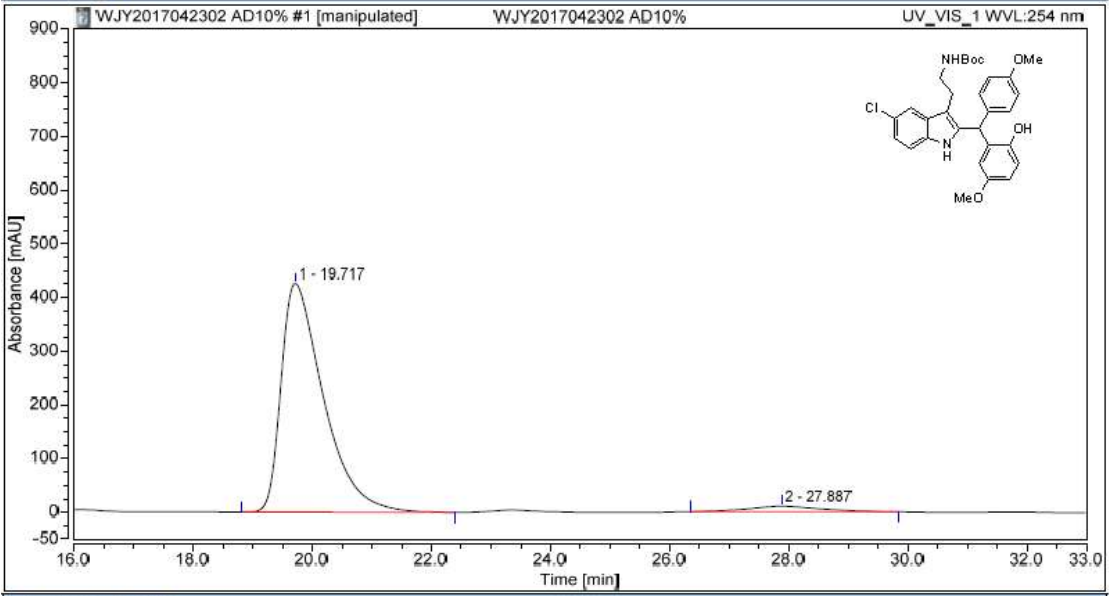
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 19.977 | 43.004 | 55.575 | 49.63 | 58.20 | n.a. |
| 2 | | 27.810 | 43.652 | 39.920 | 50.37 | 41.80 | n.a. |
| Total: | | | 86.656 | 95.495 | 100.00 | 100.00 | |

**Chromatogram**

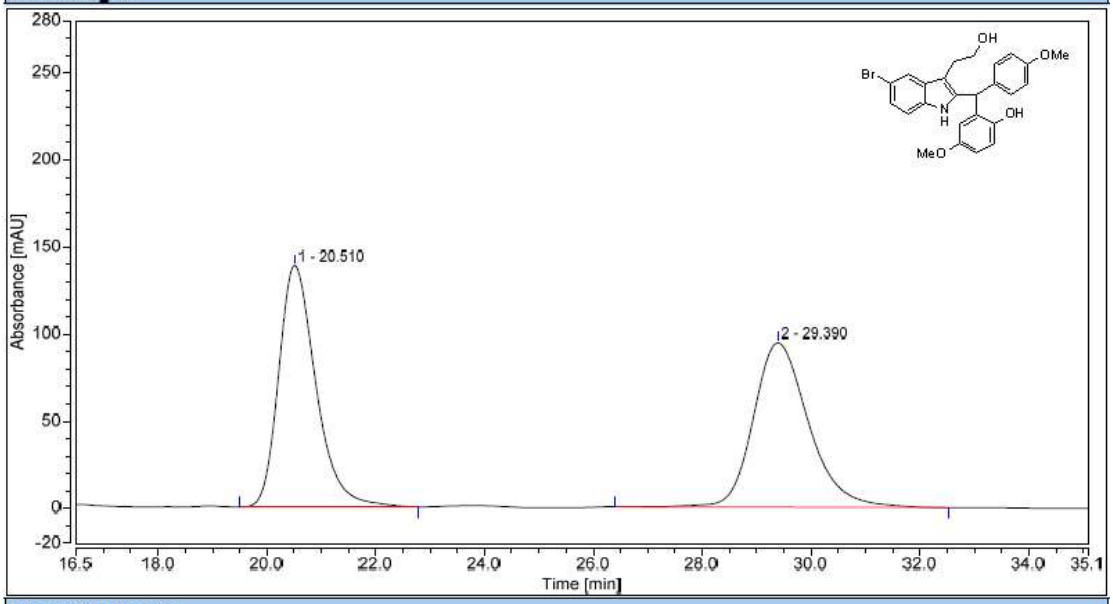



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 19.717 | 349.918 | 425.687 | 96.05 | 97.68 | n.a. |
| 2 | | 27.887 | 14.394 | 10.108 | 3.95 | 2.32 | n.a. |

## 8uc

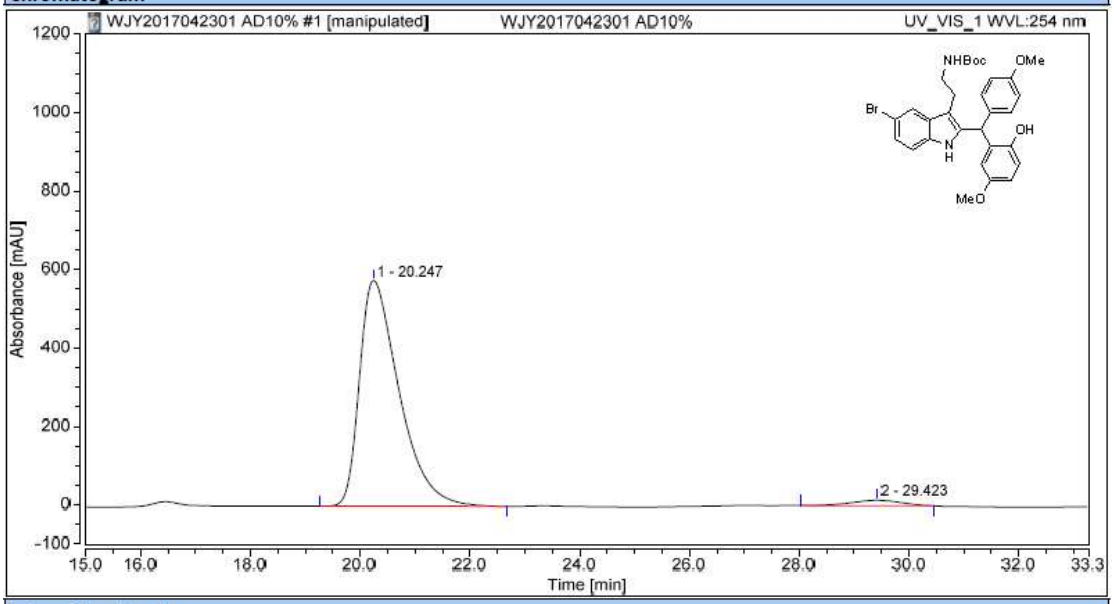
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 20.510 | 109.658 | 138.633 | 49.74 | 59.54 | n.a. |
| 2 | | 29.390 | 110.821 | 94.207 | 50.26 | 40.46 | n.a. |
| Total: | | | 220.479 | 232.840 | 100.00 | 100.00 | |

**Chromatogram**

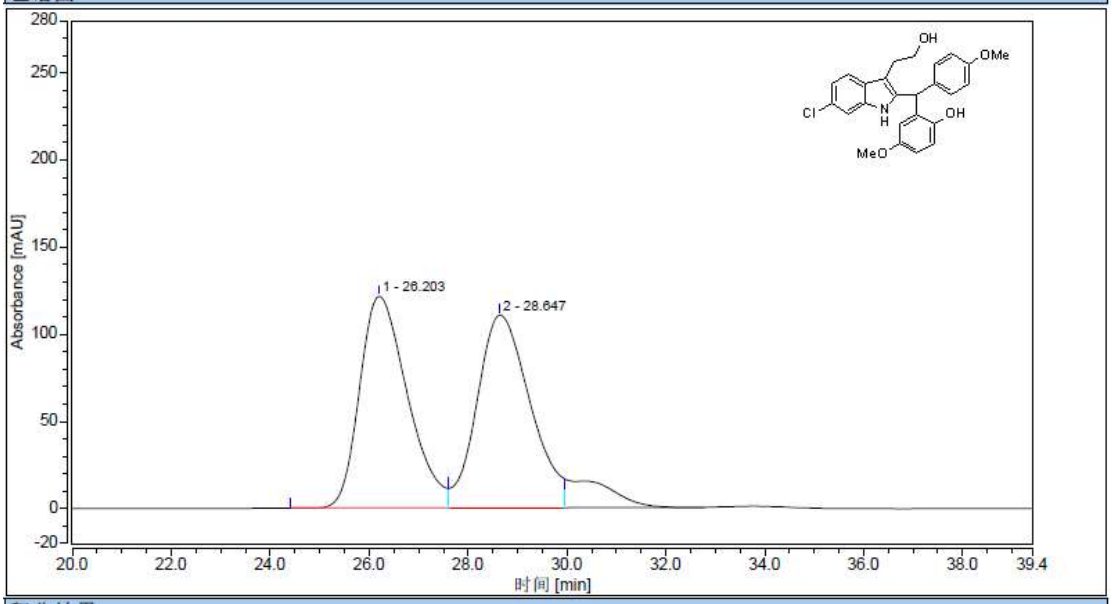



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 20.247 | 480.713 | 575.458 | 97.03 | 97.64 | n.a. |
| 2 | | 29.423 | 14.729 | 13.894 | 2.97 | 2.36 | n.a. |
| Total: | | | 495.443 | 589.352 | 100.00 | 100.00 | |

**8ud**

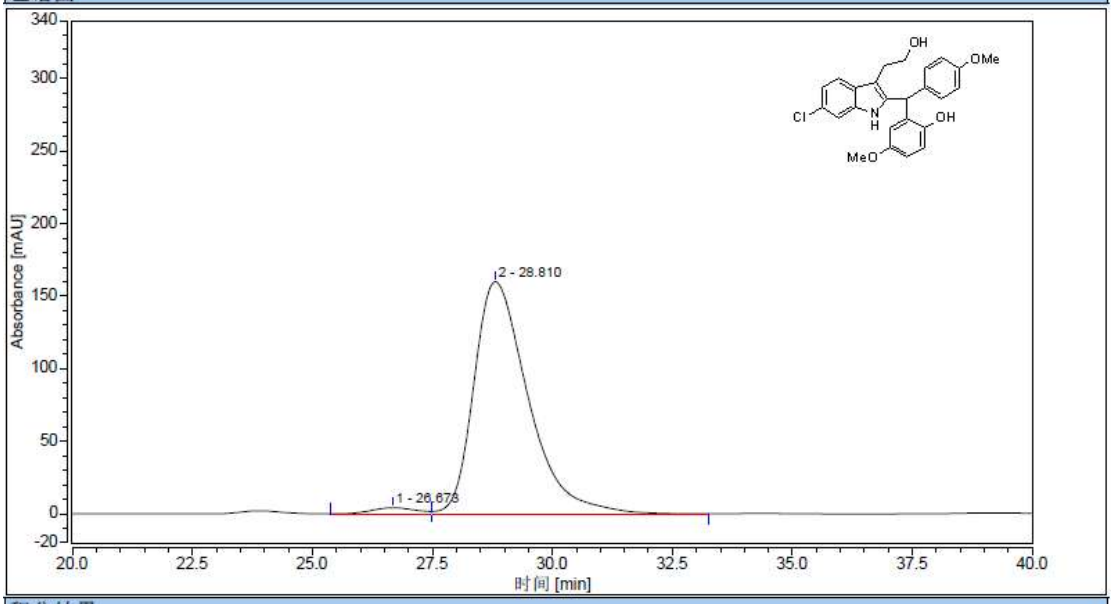
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 26.203 | 135.459 | 121.377 | 49.73 | 52.35 | n.a. |
| 2 | | 28.647 | 136.934 | 110.496 | 50.27 | 47.65 | n.a. |
| 总和: | | | **272.392** | **231.873** | **100.00** | **100.00** | |

色谱图

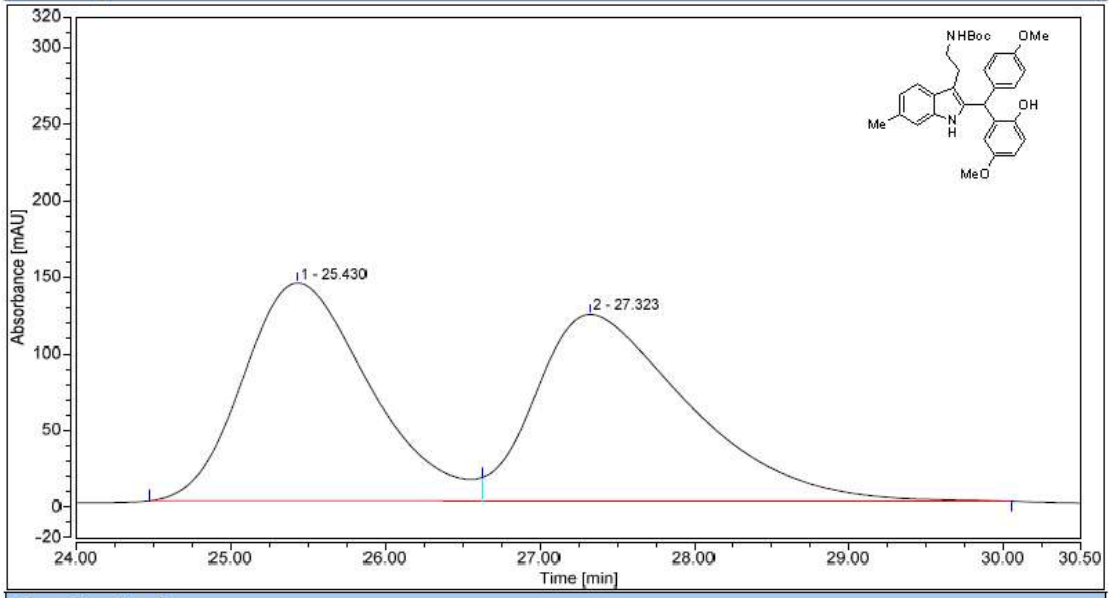



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 26.673 | 4.354 | 4.119 | 2.04 | 2.51 | n.a. |
| 2 | | 28.810 | 209.232 | 159.882 | 97.96 | 97.49 | n.a. |
| 总和: | | | **213.586** | **164.000** | **100.00** | **100.00** | |

## 8ue

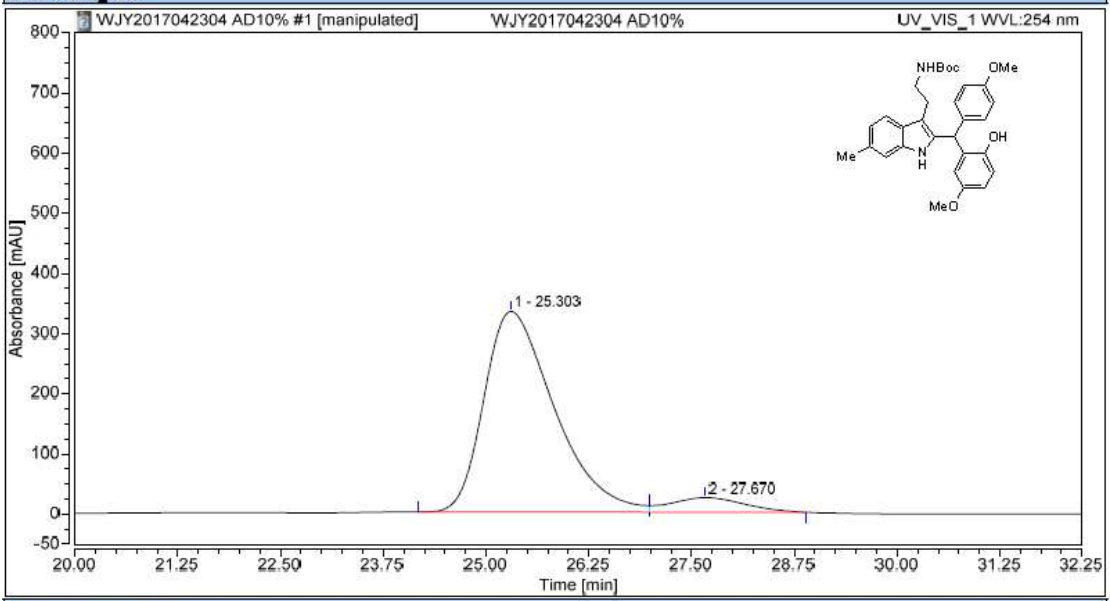
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 25.430 | 134.782 | 142.126 | 49.05 | 53.88 | n.a. |
| 2 | | 27.323 | 139.984 | 121.667 | 50.95 | 46.12 | n.a. |
| **Total:** | | | **274.766** | **263.793** | **100.00** | **100.00** | |

**Chromatogram**

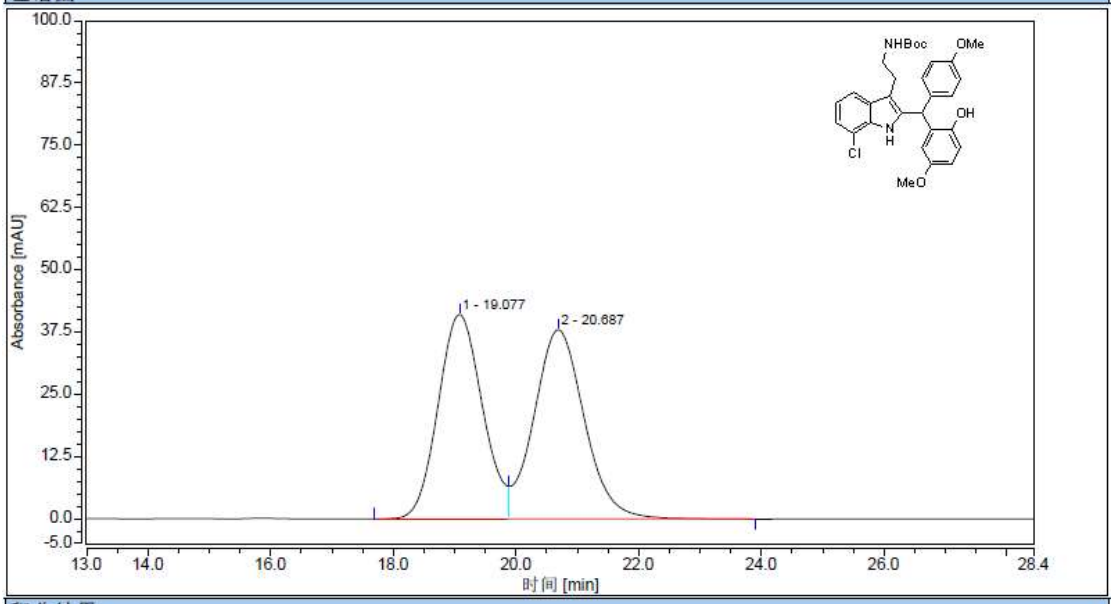



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 25.303 | 330.895 | 333.416 | 92.92 | 93.26 | n.a. |
| 2 | | 27.670 | 25.199 | 24.088 | 7.08 | 6.74 | n.a. |

**8uf**

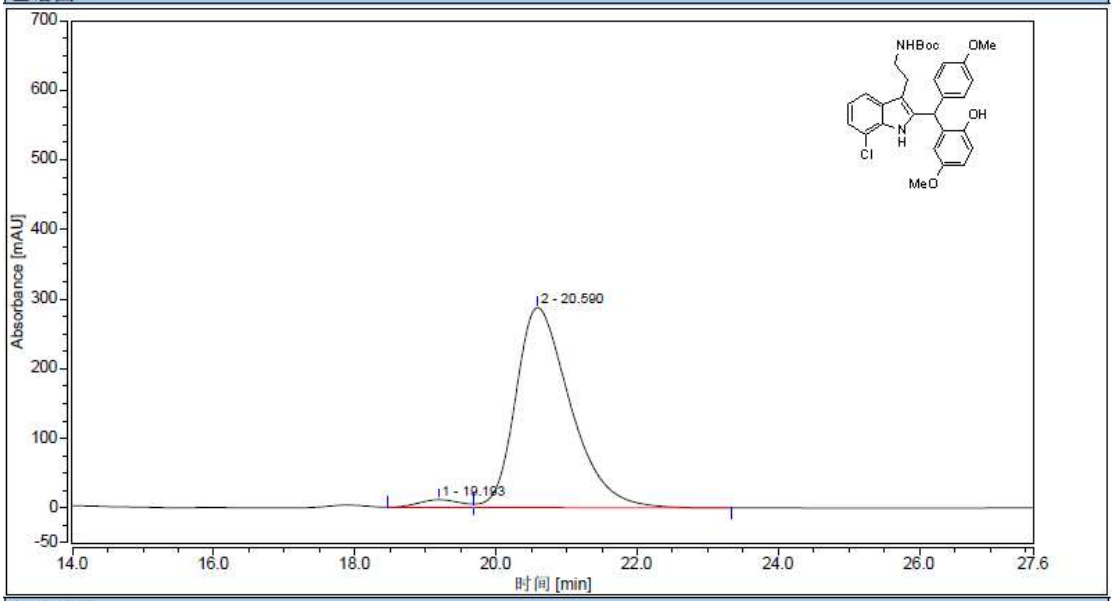
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 19.077 | 34.323 | 41.015 | 48.77 | 51.94 | n.a. |
| 2 | | 20.687 | 36.048 | 37.952 | 51.23 | 48.06 | n.a. |
| 总和: | | | **70.371** | **78.967** | **100.00** | **100.00** | |

色谱图

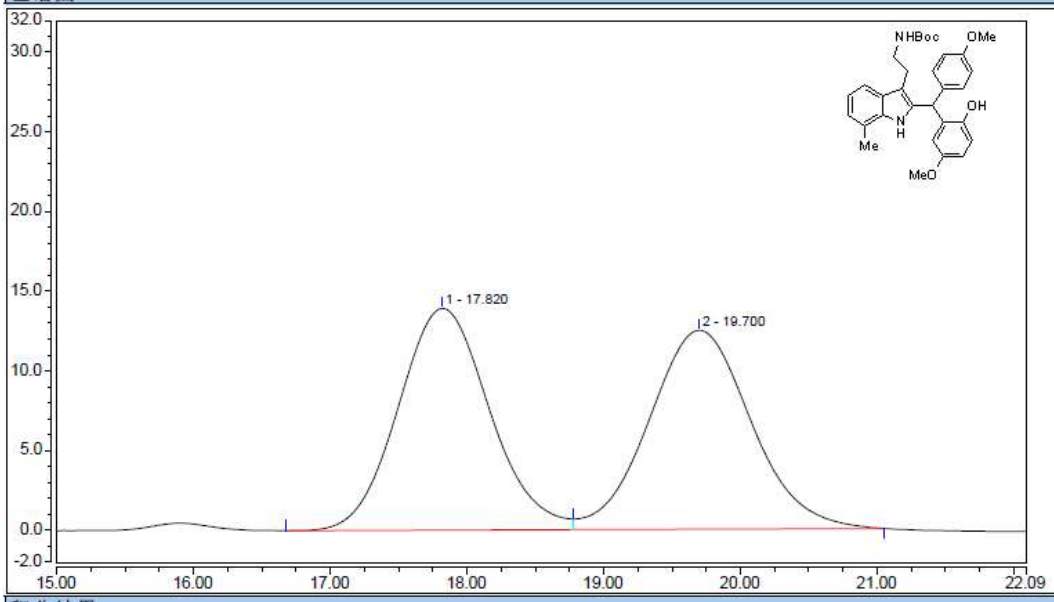



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 19.193 | 7.795 | 11.191 | 2.93 | 3.75 | n.a. |
| 2 | | 20.590 | 258.091 | 287.194 | 97.07 | 96.25 | n.a. |
| 总和: | | | **265.886** | **298.385** | **100.00** | **100.00** | |

**8ug**

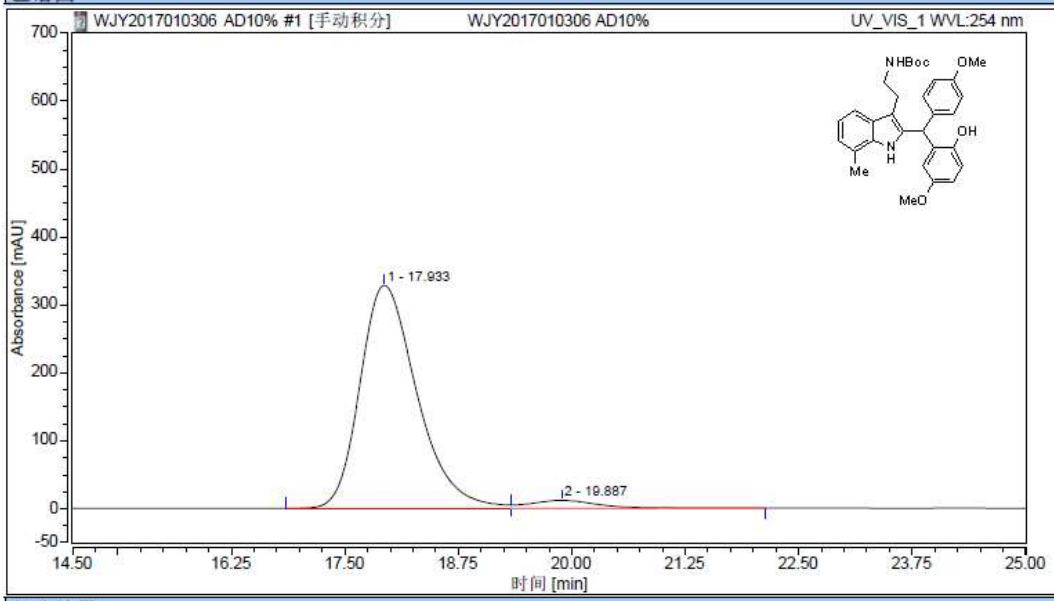
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 17.820 | 10.769 | 13.913 | 49.93 | 52.71 | n.a. |
| 2 | | 19.700 | 10.801 | 12.481 | 50.07 | 47.29 | n.a. |
| 总和: | | | **21.570** | **26.394** | **100.00** | **100.00** | |

色谱图

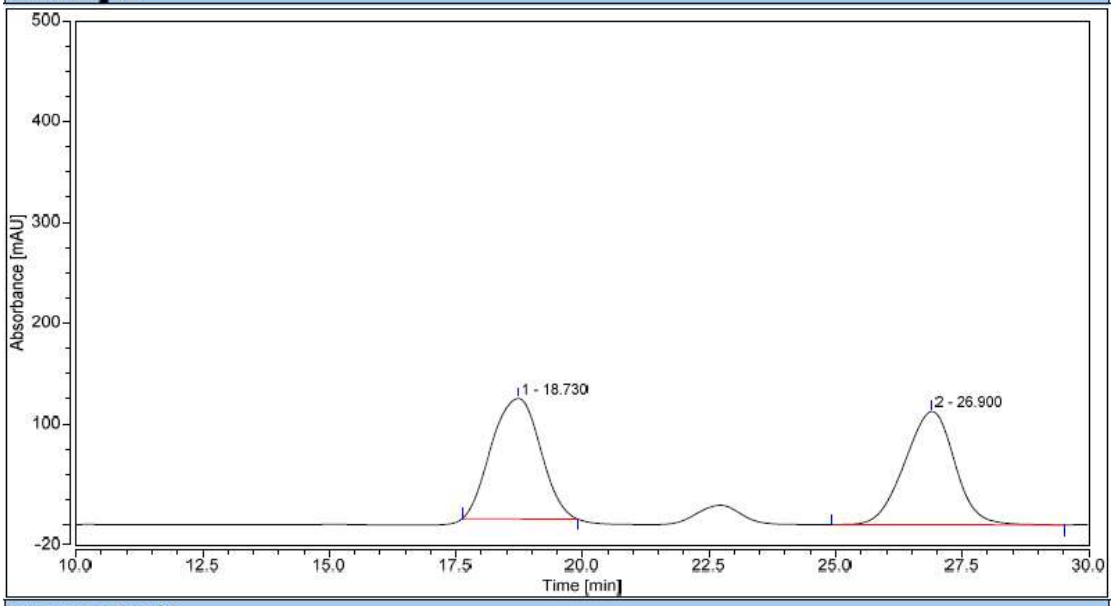



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 17.933 | 238.808 | 328.291 | 96.04 | 96.60 | n.a. |
| 2 | | 19.887 | 9.857 | 11.564 | 3.96 | 3.40 | n.a. |
| 总和: | | | **248.666** | **339.855** | **100.00** | **100.00** | |

## 10aa

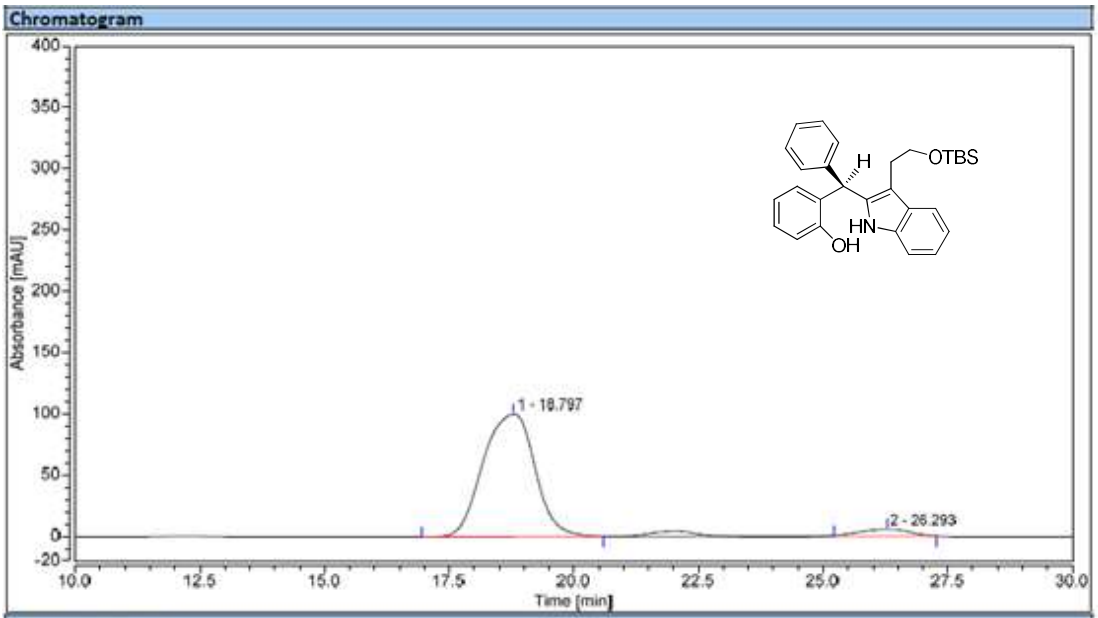
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 18.730 | 133.754 | 119.570 | 50.94 | 51.59 | n.a. |
| 2 | | 26.900 | 128.806 | 112.217 | 49.06 | 48.41 | n.a. |
| Total: | | | 262.560 | 231.787 | 100.00 | 100.00 | |

**Chromatogram**

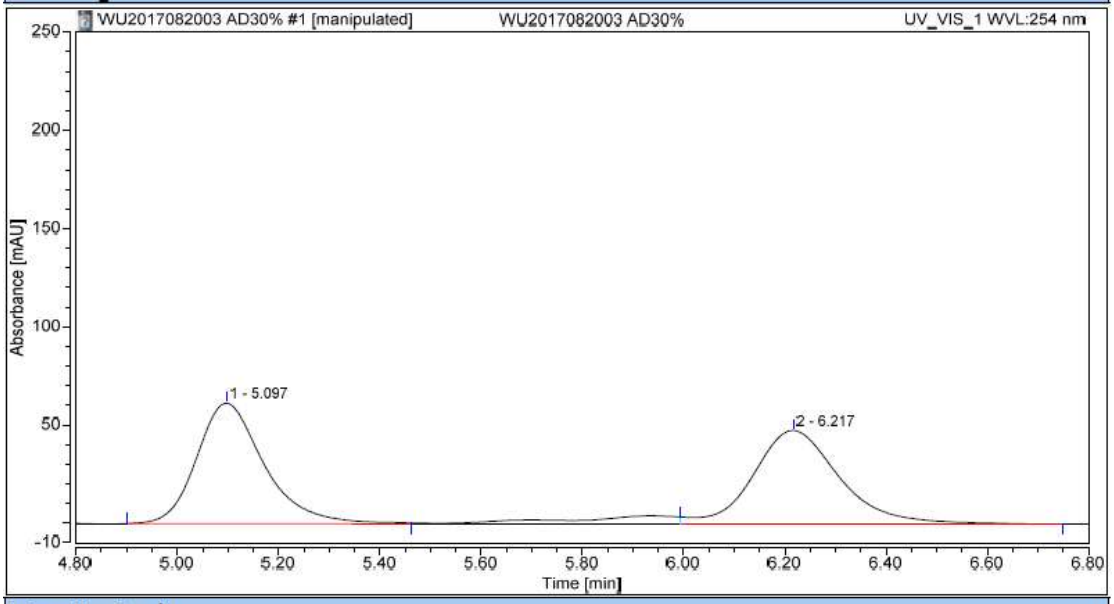



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 18.797 | 120.687 | 100.061 | 94.81 | 94.58 | n.a. |
| 2 | | 26.293 | 6.601 | 5.739 | 5.19 | 5.42 | n.a. |
| Total: | | | 127.288 | 105.800 | 100.00 | 100.00 | |

## 10ab

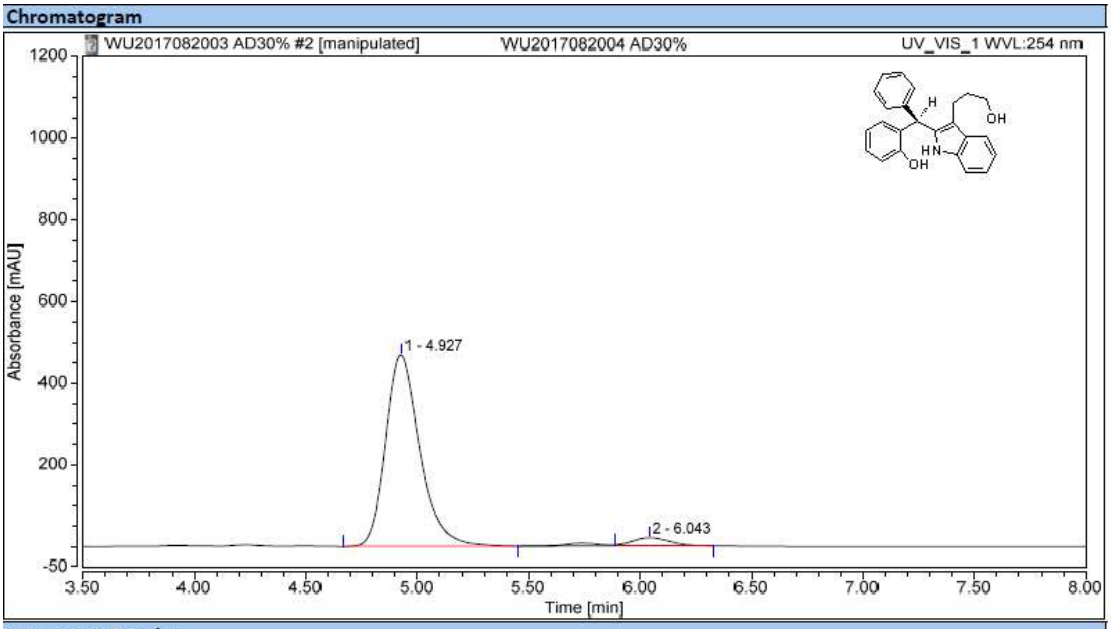
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 5.097 | 9.520 | 61.418 | 50.34 | 56.34 | n.a. |
| 2 | | 6.217 | 9.392 | 47.595 | 49.66 | 43.66 | n.a. |
| **Total:** | | | **18.912** | **109.014** | **100.00** | **100.00** | |

**Chromatogram**

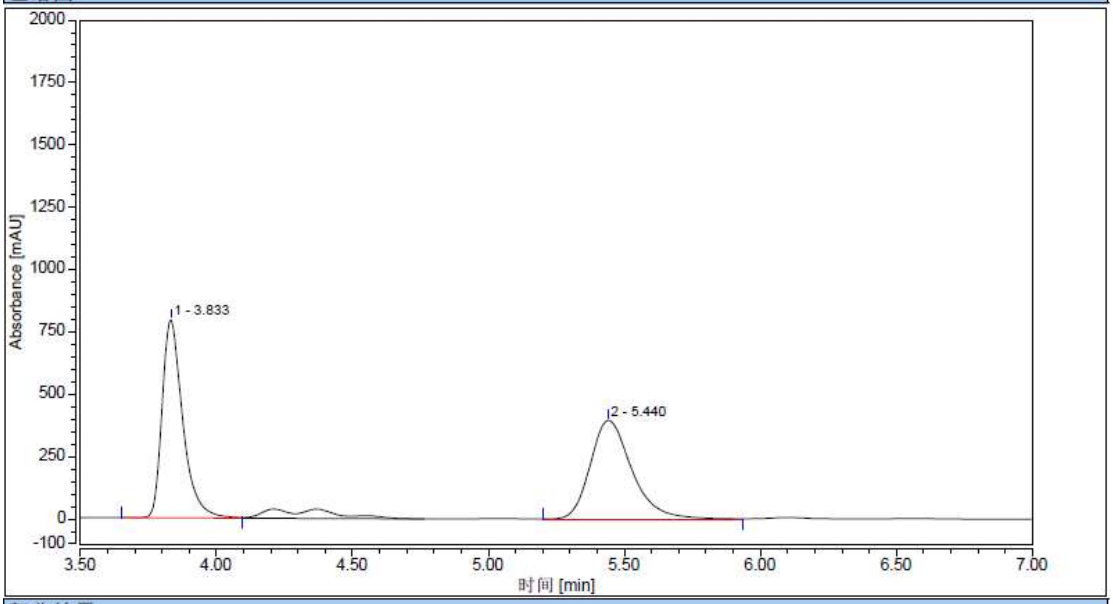



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 4.927 | 83.353 | 468.204 | 95.54 | 95.94 | n.a. |
| 2 | | 6.043 | 3.892 | 19.800 | 4.46 | 4.06 | n.a. |
| **Total:** | | | **87.245** | **488.003** | **100.00** | **100.00** | |

## 10ac

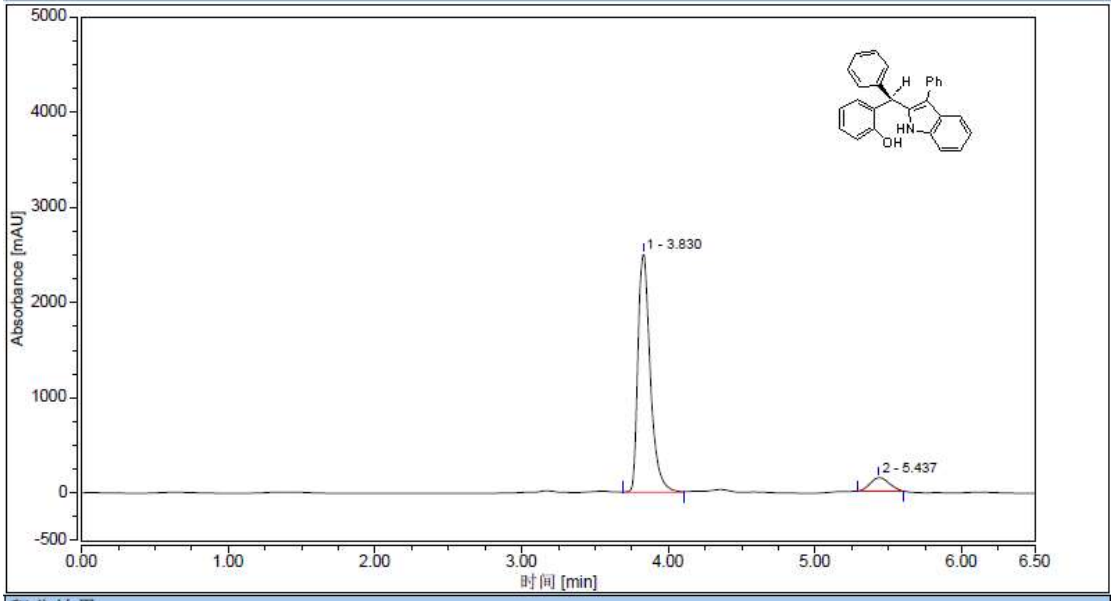
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 3.833 | 70.017 | 794.769 | 50.08 | 66.77 | n.a. |
| 2 | | 5.440 | 69.795 | 395.535 | 49.92 | 33.23 | n.a. |
| 总和: | | | **139.811** | **1190.304** | **100.00** | **100.00** | |

色谱图

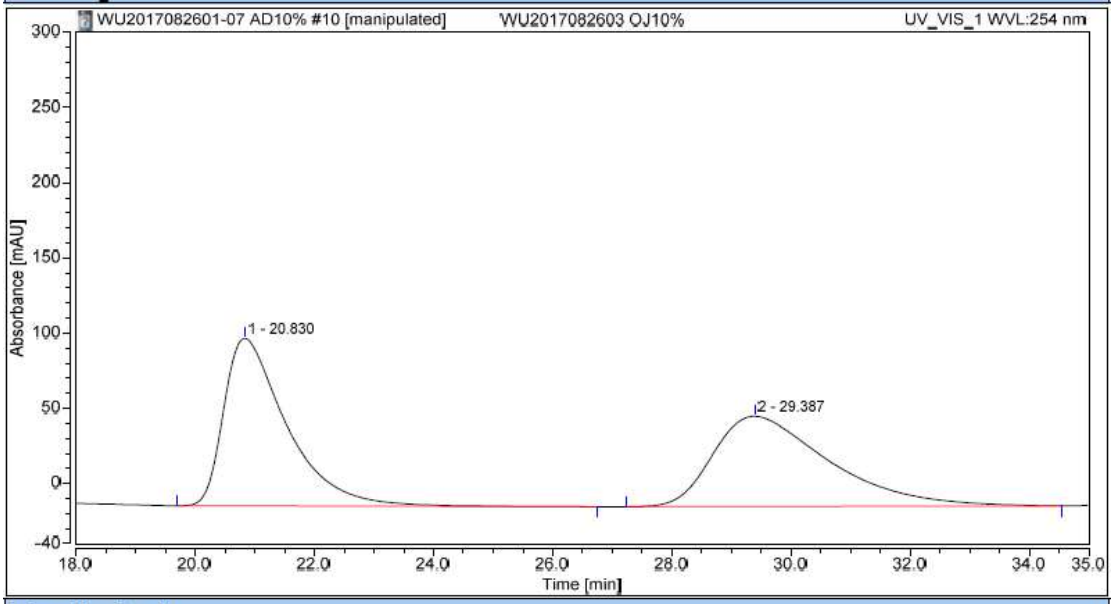



积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 3.830 | 244.574 | 2500.984 | 92.18 | 94.70 | n.a. |
| 2 | | 5.437 | 20.734 | 140.028 | 7.82 | 5.30 | n.a. |
| 总和: | | | **265.308** | **2641.012** | **100.00** | **100.00** | |

## 10ad

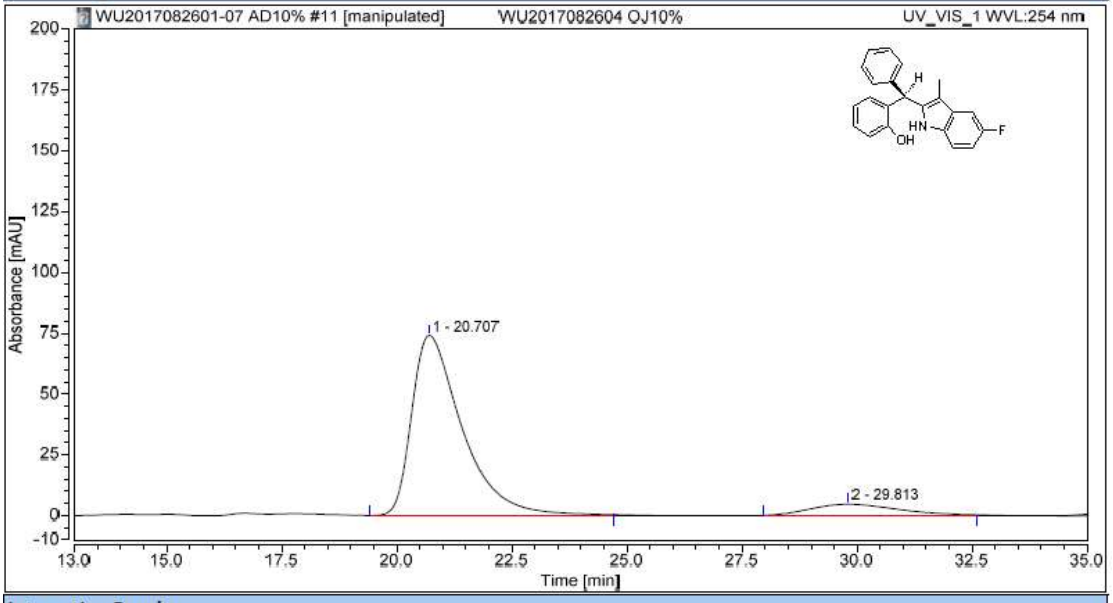
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 20.830 | 135.825 | 111.301 | 50.20 | 65.02 | n.a. |
| 2 | | 29.387 | 134.740 | 59.887 | 49.80 | 34.98 | n.a. |
| **Total:** | | | **270.565** | **171.188** | **100.00** | **100.00** | |

**Chromatogram**

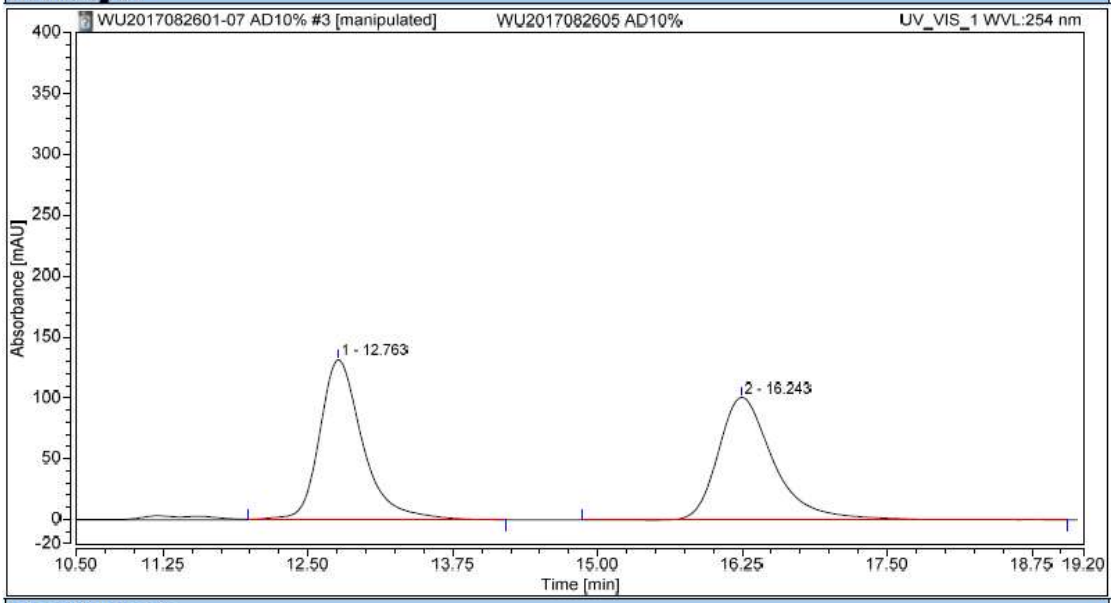



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 20.707 | 94.051 | 73.978 | 89.79 | 94.03 | n.a. |
| 2 | | 29.813 | 10.689 | 4.697 | 10.21 | 5.97 | n.a. |
| **Total:** | | | **104.741** | **78.676** | **100.00** | **100.00** | |

## 10ae

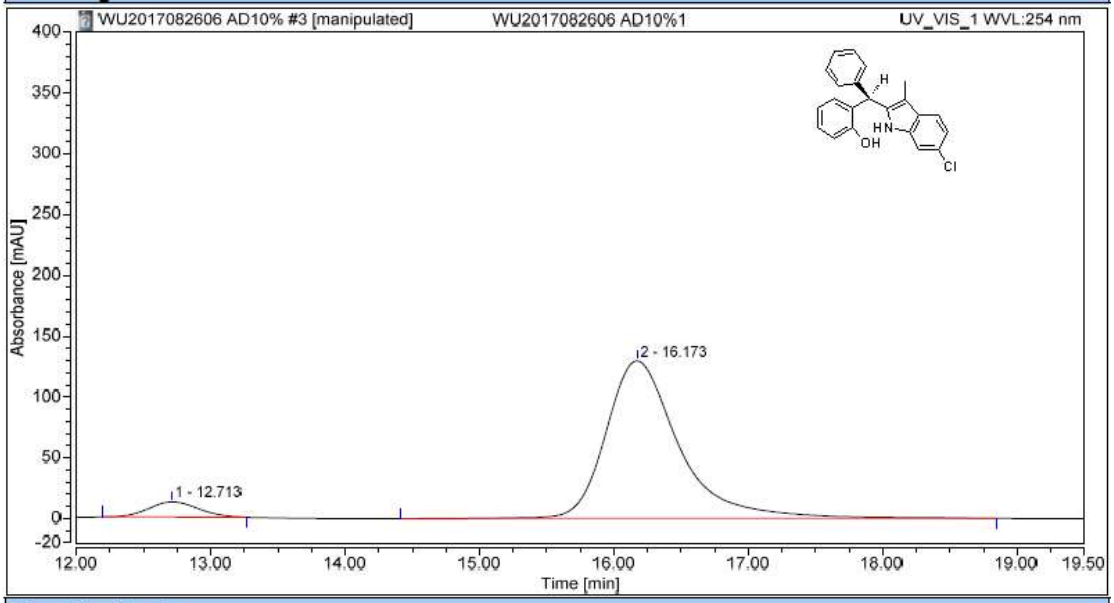
**Chromatogram**




**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 12.763 | 57.020 | 131.486 | 50.53 | 56.61 | n.a. |
| 2 | | 16.243 | 55.820 | 100.782 | 49.47 | 43.39 | n.a. |
| Total: | | | **112.840** | **232.268** | **100.00** | **100.00** | |

**Chromatogram**

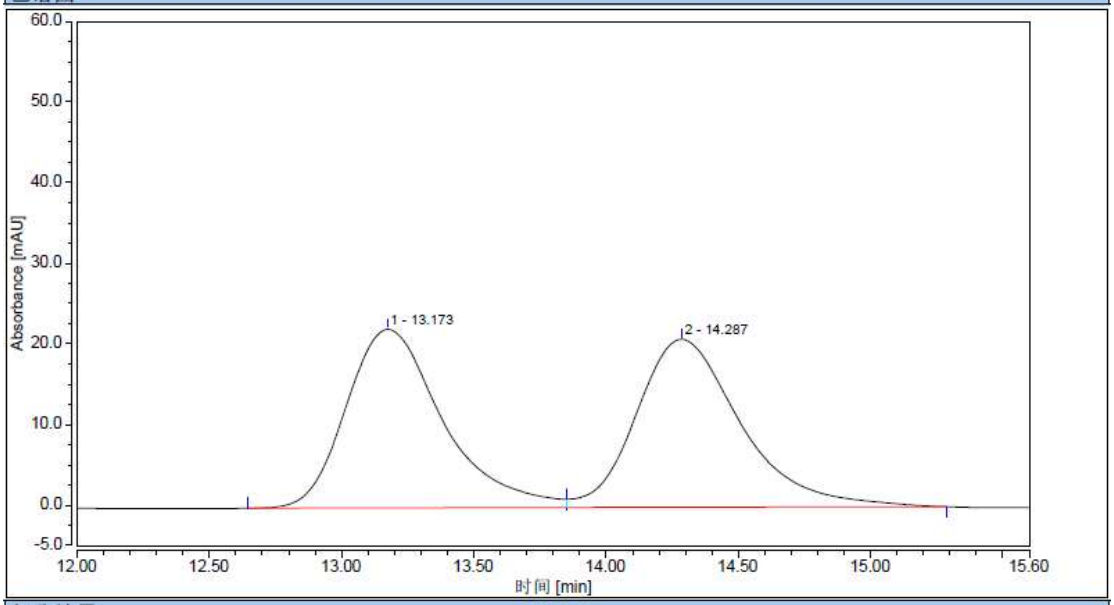



**Integration Results**

| No. | Peak Name | Retention Time min | Area mAU*min | Height mAU | Relative Area % | Relative Height % | Amount n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 12.713 | 5.374 | 12.479 | 6.16 | 8.79 | n.a. |
| 2 | | 16.173 | 81.828 | 129.540 | 93.84 | 91.21 | n.a. |
| Total: | | | **87.201** | **142.019** | **100.00** | **100.00** | |

## 11ah

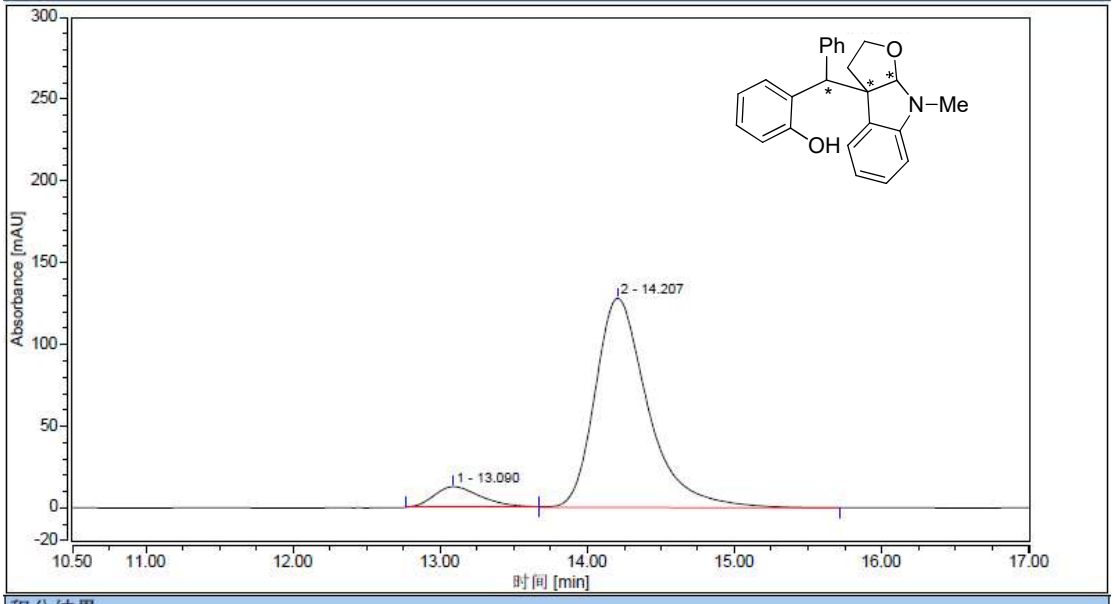
色谱图




积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 13.173 | 9.383 | 22.136 | 49.54 | 51.53 | n.a. |
| 2 | | 14.287 | 9.557 | 20.823 | 50.46 | 48.47 | n.a. |
| 总和: | | | **18.940** | **42.959** | **100.00** | **100.00** | |

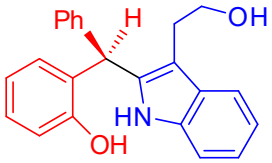
色谱图



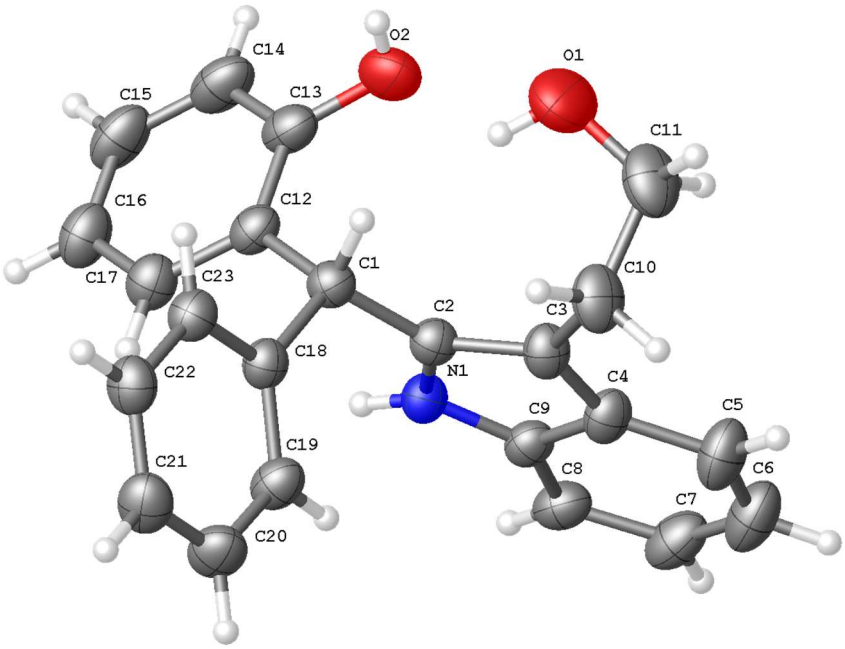

积分结果

| 序号 | 峰名称 | 保留时间 min | 峰面积 mAU*min | 峰高 mAU | 相对峰面积 % | 相对峰高 % | 样品量 n.a. |
|---|---|---|---|---|---|---|---|
| 1 | | 13.090 | 4.733 | 12.631 | 8.16 | 8.99 | n.a. |
| 2 | | 14.207 | 53.288 | 127.901 | 91.84 | 91.01 | n.a. |
| 总和: | | | **58.021** | **140.532** | **100.00** | **100.00** | |

## 3. X-ray single crystal data for compounds 3aa and 8aa



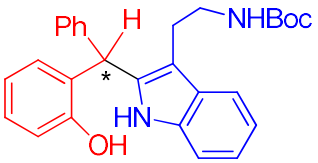

**(*R*)-3aa**



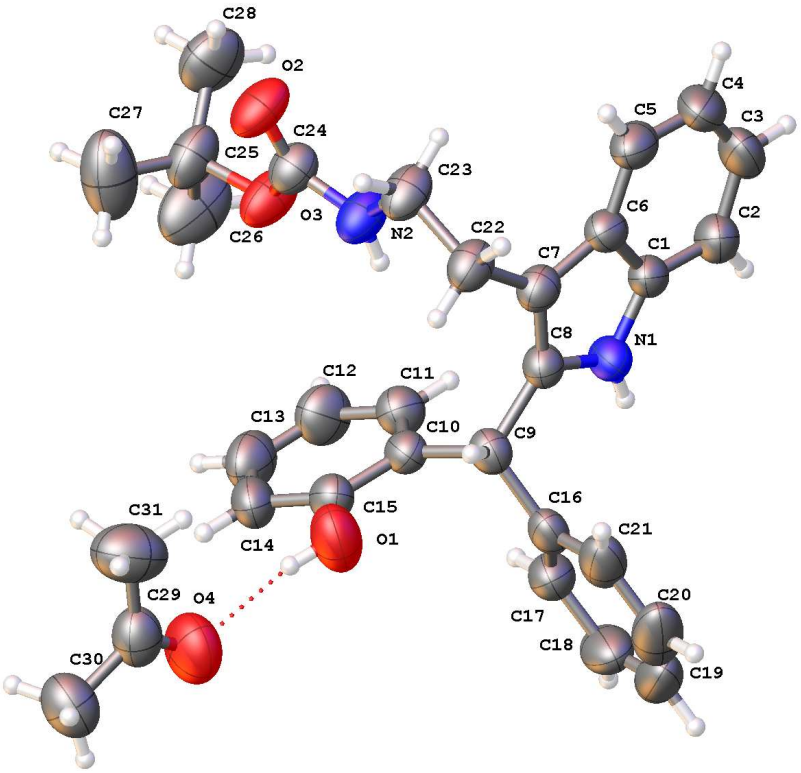

The thermal ellipsoid was drawn at the 30% probability level.

| | | |
|---|---|---|
| Identification code | cu_dm16869_0m | |
| Empirical formula | C23 H20 N O2 | |
| Formula weight | 342.40 | |
| Temperature | 296 K | |
| Wavelength | 1.54178 Å | |
| Crystal system | Hexagonal | |
| Space group | P 61 | |
| Unit cell dimensions | a = 18.5578(9) Å | α= 90°. |
| | b = 18.5578(9) Å | β= 90°. |
| | c = 9.8682(6) Å | γ = 120°. |
| Volume | 2943.2(3) $Å^3$ | |
| Z | 6 | |
| Density (calculated) | 1.159 $Mg/m^3$ | |
| Absorption coefficient | 0.583 $mm^{-1}$ | |
| F(000) | 1086 | |
| Crystal size | 0.12 x 0.03 x 0.02 $mm^3$ | |

| | |
|---|---|
| Theta range for data collection | 2.75 to 69.97°. |
| Index ranges | -22<=h<=22, -22<=k<=21, -11<=l<=9 |
| Reflections collected | 25185 |
| Independent reflections | 3259 [R(int) = 0.0822] |
| Completeness to theta = 67.496° | 99.5 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.7533 and 0.5113 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3259 / 1 / 237 |
| Goodness-of-fit on $F^2$ | 1.015 |
| Final R indices [I>2sigma(I)] | R1 = 0.0434, wR2 = 0.1186 |
| R indices (all data) | R1 = 0.0543, wR2 = 0.1284 |
| Absolute structure parameter | 0.3(3) |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.102 and -0.134 e.$Å^{-3}$ |




**8aa**




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

| | | |
|---|---|---|
| Identification code | dm16702 | |
| Empirical formula | C31 H36 N2 O4 | |
| Formula weight | 500.62 | |
| Temperature | 296.15 K | |
| Wavelength | 1.54178 Å | |
| Crystal system | Triclinic | |
| Space group | P -1 | |
| Unit cell dimensions | a = 8.4885(5) Å | α= 74.369(4)°. |
| | b = 10.6796(6) Å | β= 82.265(4)°. |
| | c = 16.8127(9) Å | γ = 75.011(5)°. |
| Volume | 1414.37(14) $Å^3$ | |
| Z | 2 | |
| Density (calculated) | 1.175 $Mg/m^3$ | |
| Absorption coefficient | 0.618 $mm^{-1}$ | |

| | |
|---|---|
| F(000) | 536 |
| Crystal size | 0.10 x 0.03 x 0.02 $mm^3$ |
| Theta range for data collection | 2.736 to 66.402°. |
| Index ranges | -9<=h<=9, -11<=k<=12, 0<=l<=19 |
| Reflections collected | 4709 |
| Independent reflections | 4709 [R(int) = ?] |
| Completeness to theta = 66.402° | 96.1 % |
| Absorption correction | Semi-empirical from equivalents |
| Max. and min. transmission | 0.7528 and 0.5492 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4709 / 0 / 341 |
| Goodness-of-fit on $F^2$ | 1.011 |
| Final R indices [I>2sigma(I)] | R1 = 0.0750, wR2 = 0.1876 |
| R indices (all data) | R1 = 0.1161, wR2 = 0.2188 |
| Extinction coefficient | n/a |
| Largest diff. peak and hole | 0.609 and -0.269 e.$Å^{-3}$ |