Supporting Information

C(sp^3)-H Bond Functionalization of benzo[c]oxepines via C-O bond Cleavage: Formal [3+3] Synthesis of Multi-substituted Chromans

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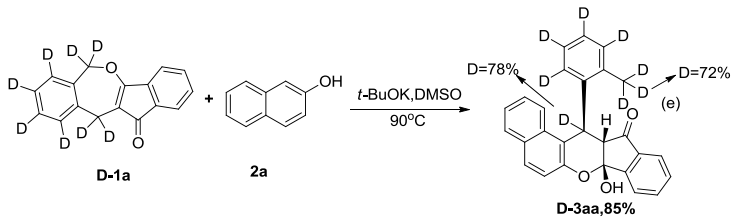
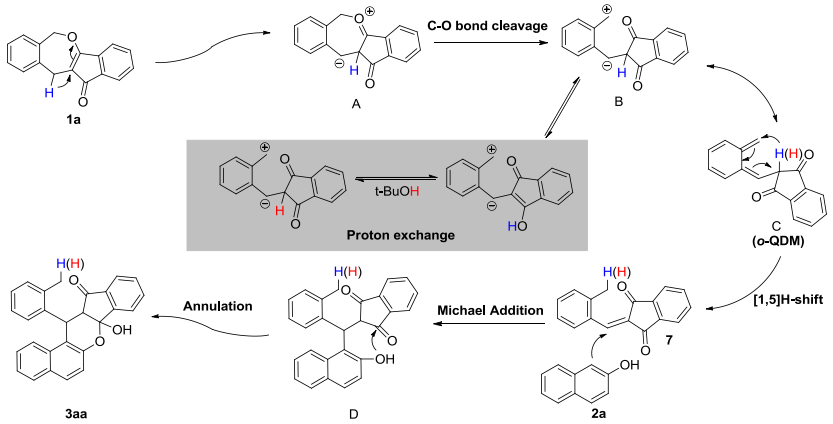
Table of Contents **page**

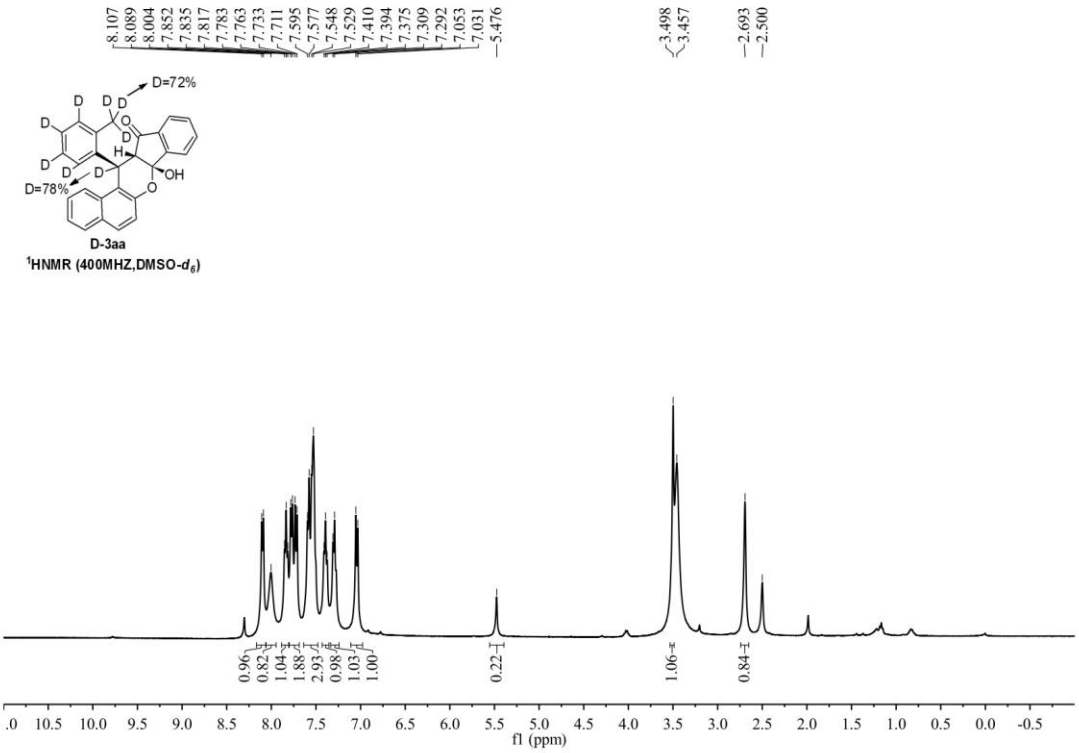
1. Evidence in support of the mechanism.



(1) The reaction of benzo[*c*]oxepine-d_8 (D-**1a**) and 2-naphthol (**2a**) under the standard conditions gave the deuterated product D-**3aa** in 85% yield with 72% deuterated methyl group. This means 0.16D was obtained, and indicated that an intramolecular H shift might involve in this transformation, but it was not the main pathway. The major pathway was showed in the paper, and the minor was showed below.



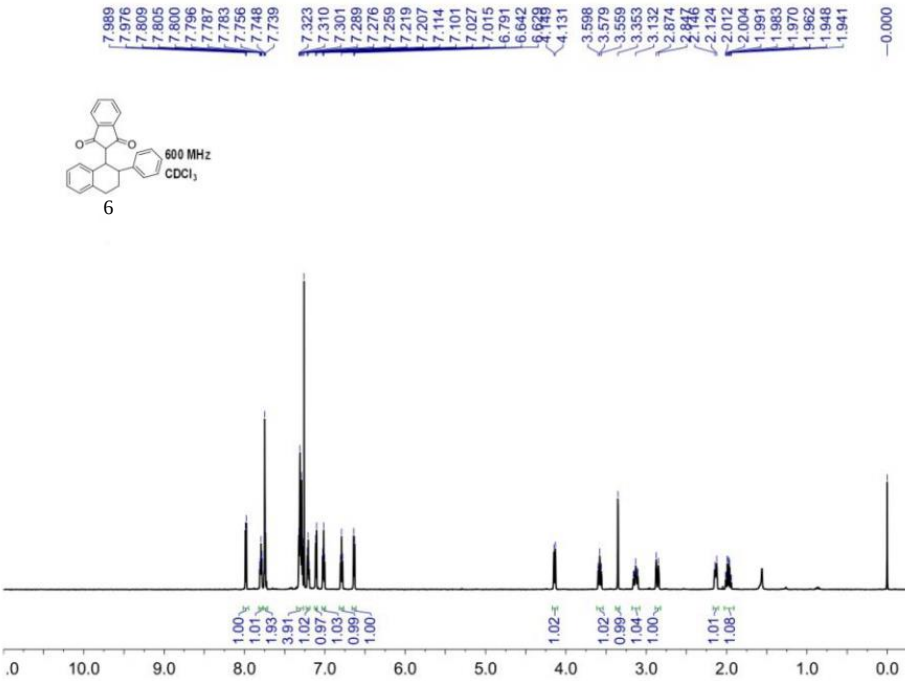
Scheme S1. An intramolecular H shift pathway for the possible mechanism.



(2) For the characterization of compond **6** and **7**, ^{1}H NMR and ^{13}C NMR was performed.

6: ^{1}H NMR (600 MHz, $CDCl_3$) δ = 7.98 (d, J= 7.8 Hz, 1H), 7.81- 7.78 (m, 1H), 7.76 -7.74 (m, 2H), 7.32-7.28 (m, 4H), 7.21 (t, J=7.2 Hz, 1H), 7.11 (d, J=7.8 Hz, 1H), 7.01 (t, J=7.2 Hz, 1H), 6.79 (t, J=7.8 Hz, 1H), 6.64 (d, J=7.8 Hz,1H), 4.14 (d, J=10.8 Hz,1H), 3.60 -3.56 (m,1H), 3.35 (s,1H), 3.18 -3.10 (m, 1H), 2.86 (d, J=16.2 Hz, 1H), 2.15-2.12 (m, 1H), 2.01-1.94 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ= 200.6, 199.3, 144.7,142.7,141.9,137.9,136.2,135.1,129.3,128.7,127.9,126.8,126.3,126.0,125.6, 122.9, 122.7, 56.8, 45.9, 43.7, 31.8, 30.6.

7: ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.54 (d, J=7.8 Hz, 1H), 8.24 (s, 1H), 8.01 (d, J=16.2 Hz, 2H), 7.82 (s, 2H), 7.42 (t, J=7.2 Hz, 1H), 7.33 (t, J=7.2 Hz,1H), 7.28 (s, 1H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ= 190.1, 188.6,144.1, 142.4,140.7, 139.9,135.3,135.1,132.7, 132.4,131.3,130.5, 129.0, 125.8, 123.2, 20.3.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7.976
7.809
7.805
7.800
7.796
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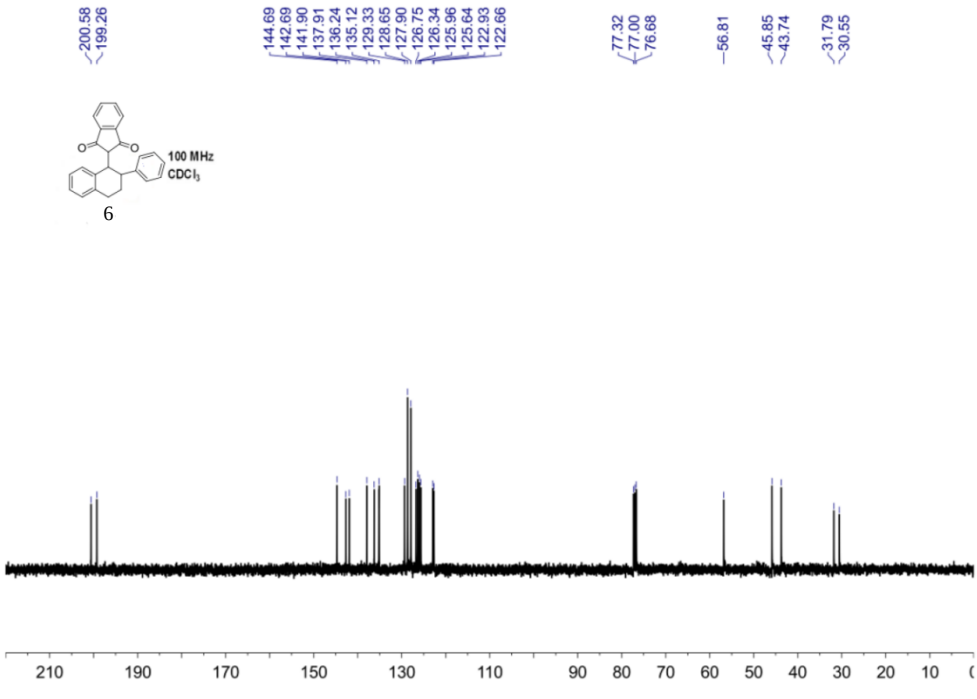
7.323
7.310
7.301
7.289
7.276
7.259
7.219
7.207
7.114
7.101
7.027
7.015
6.791
6.642
4.131
3.598
3.579
3.559
3.353
3.132
2.874
2.124
2.012
2.004
1.991
1.983
1.970
1.962
1.948
1.941
0.000
600 MHz
CDCl3
6
1.00
1.01
1.93
3.91
1.02
0.97
1.03
0.99
1.00
1.02
1.02
0.99
1.04
1.00
1.01
1.08
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0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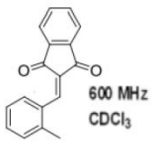
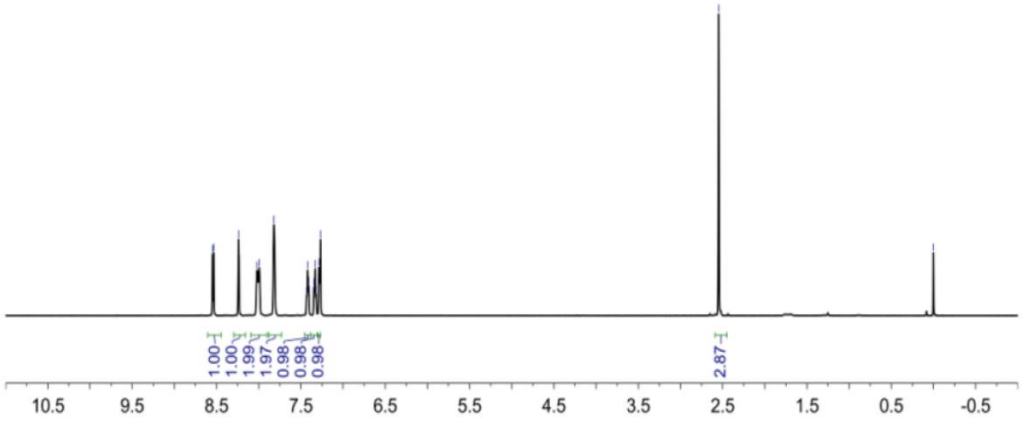
144.69
142.69
141.90
137.91
136.24
135.12
129.33
128.65
127.90
126.75
126.34
125.96
125.64
122.93
122.66
77.32
77.00
76.68
56.81
45.85
43.74
31.79
30.55
100 MHz
CDCl3
6
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10


600 MHz
CDCl3

7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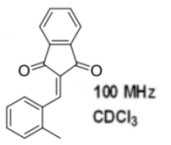
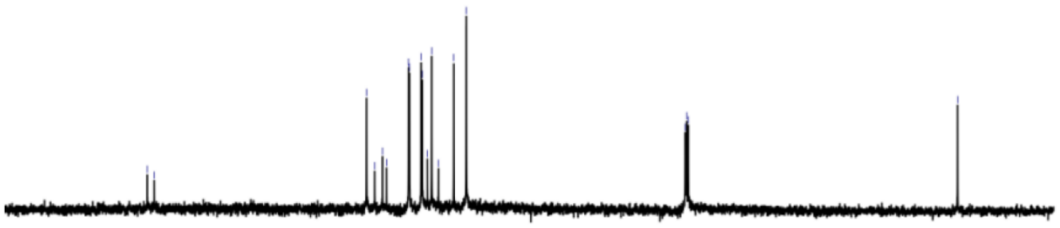
1.00
1.99
1.97
0.98
0.98
0.98
2.87
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5

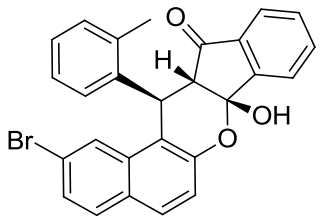

190.05
188.61
144.09
142.38
140.74
139.90
135.28
135.09
132.67
132.41
131.34
130.45
129.04
125.81
123.18
77.32
77.00
76.68
20.25


100 MHz
CDCl3

7



2. Crystallographic data of 3ai and 3am.



3ai

2-bromo-7a-hydroxy-13-(o-tolyl)-12a,13-dihydrobenzo[f]indeno[1,2-b]chromen-12(7aH)-one: (3ai)

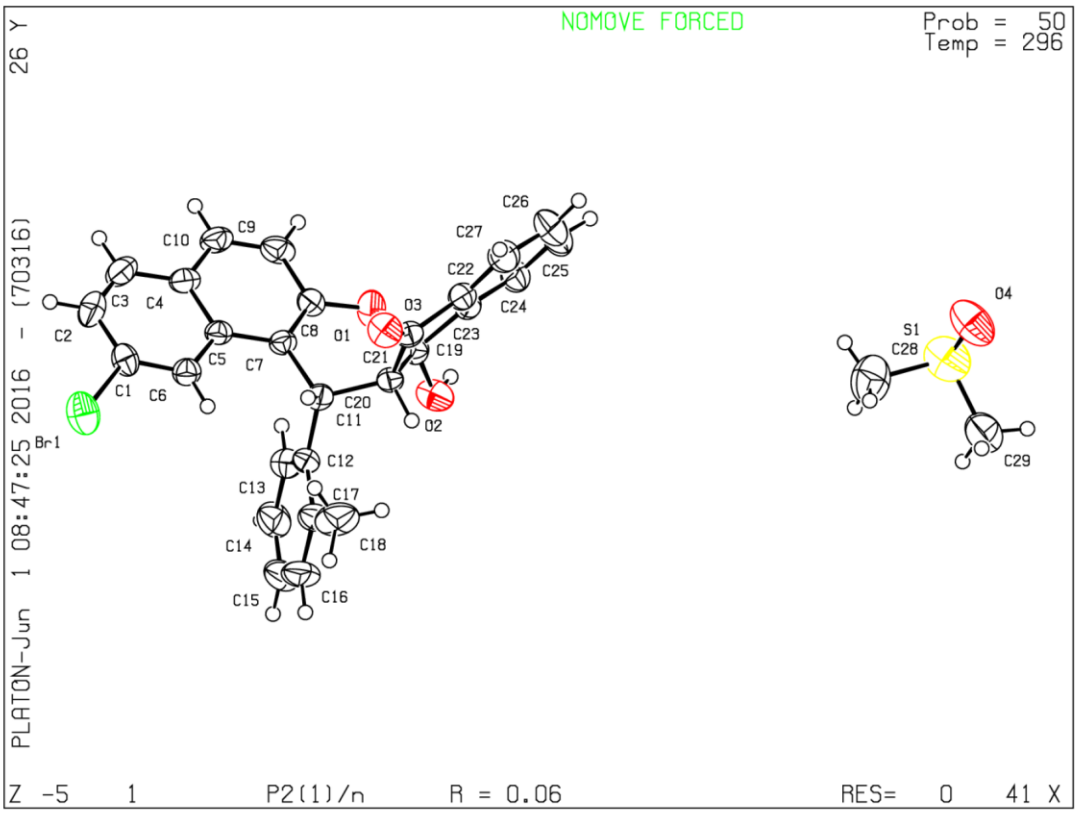


Figure S1. X-ray crystal structure of 3ai.

Table S1. Crystal data and structure refinement for compound 3ai (CCDC: 1587437)

Bond precision: C-C = 0.0080 A Wavelength=0.71073

Cell: a=11.508(4) b=9.580(4) c=23.335(9)
alpha=90 beta=101.596(6) gamma=90
Temperature: 296 K

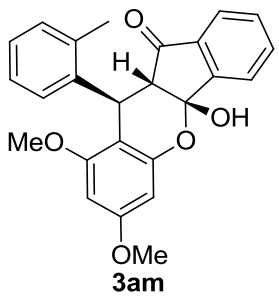
	Calculated	Reported
Volume	2520.1(17)	2520.3(17)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
Moiety formula	C27 H19 Br O3, C2 H6 O S	?
Sum formula	C29 H25 Br O4 S	C29 H25 Br O4 S
Mr	549.45	549.46
Dx,g cm-3	1.448	1.448
Z	4	4
Mu (mm-1)	1.748	1.748
F000	1128.0	1128.0
F000'	1127.81	
h,k,lmax	13,11,27	13,11,27
Nref	4449	4448
Tmin,Tmax	0.688,0.730	0.700,0.744
Tmin'	0.674	

Correction method= # Reported T Limits: Tmin=0.700 Tmax=0.744
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.0609(3209) wR2(reflections)= 0.1951(4448)

S = 0.825 Npar= 328



3am

4b-hydroxy-7,9-dimethoxy-10-(o-tolyl)-10,10a-dihydroindeno[1,2-b]chromen-11(4bH)-one: (3am)

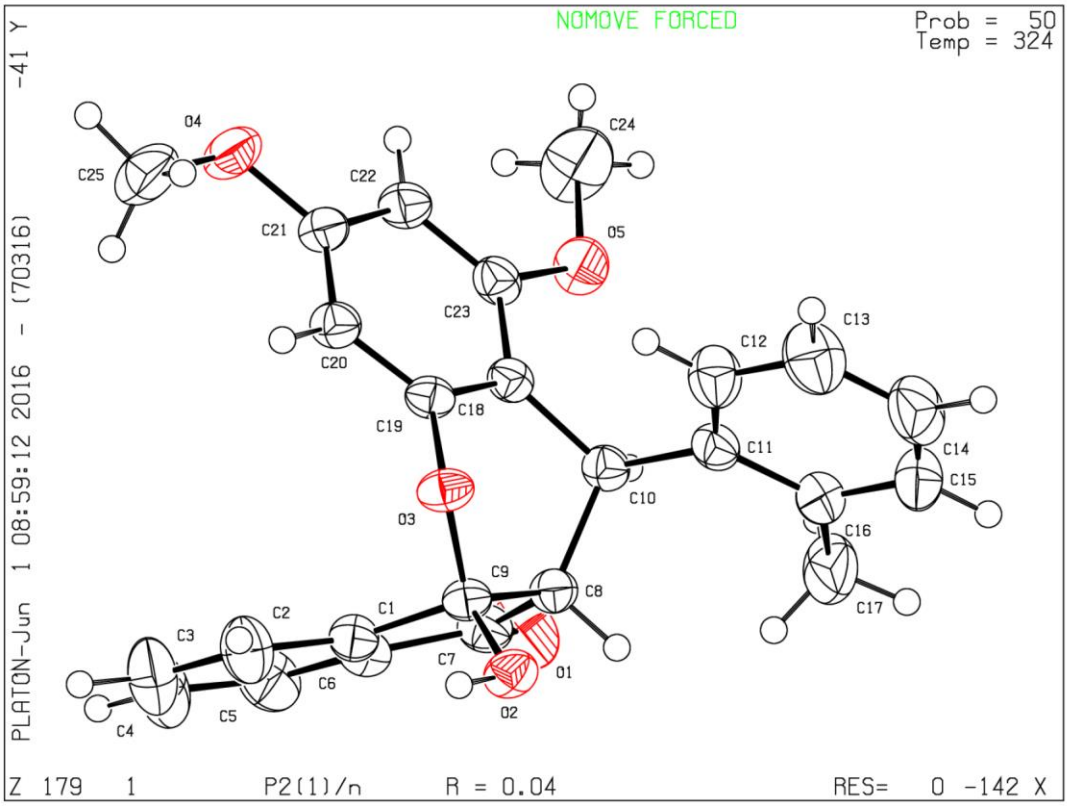


Figure S2. X-ray crystal structure of 3am.

Table S2. Crystal data and structure refinement for compound 3am (CCDC: 1587446)

Bond precision: C-C = 0.0021 A		Wavelength=0.71073	
Cell:	a=8.6534(11)	b=20.771(3)	c=11.3478(14)
	alpha=90	beta=93.146(2)	gamma=90
Temperature:	324 K		
	Calculated		Reported
Volume	2036.6(5)		2036.6(4)
Space group	P 21/n		P2(1)/n
Hall group	-P 2yn		?
Moiety formula	C25 H22 O5		?
Sum formula	C25 H22 O5		C25 H22 O5
Mr	402.43		402.43
Dx,g cm-3	1.313		1.312
Z	4		4
Mu (mm-1)	0.091		0.091
F000	848.0		848.0
F000'	848.45		
h,k,lmax	10,24,13		10,24,13
Nref	3596		3589
Tmin,Tmax	0.980,0.984		0.980,0.984
Tmin'	0.980		

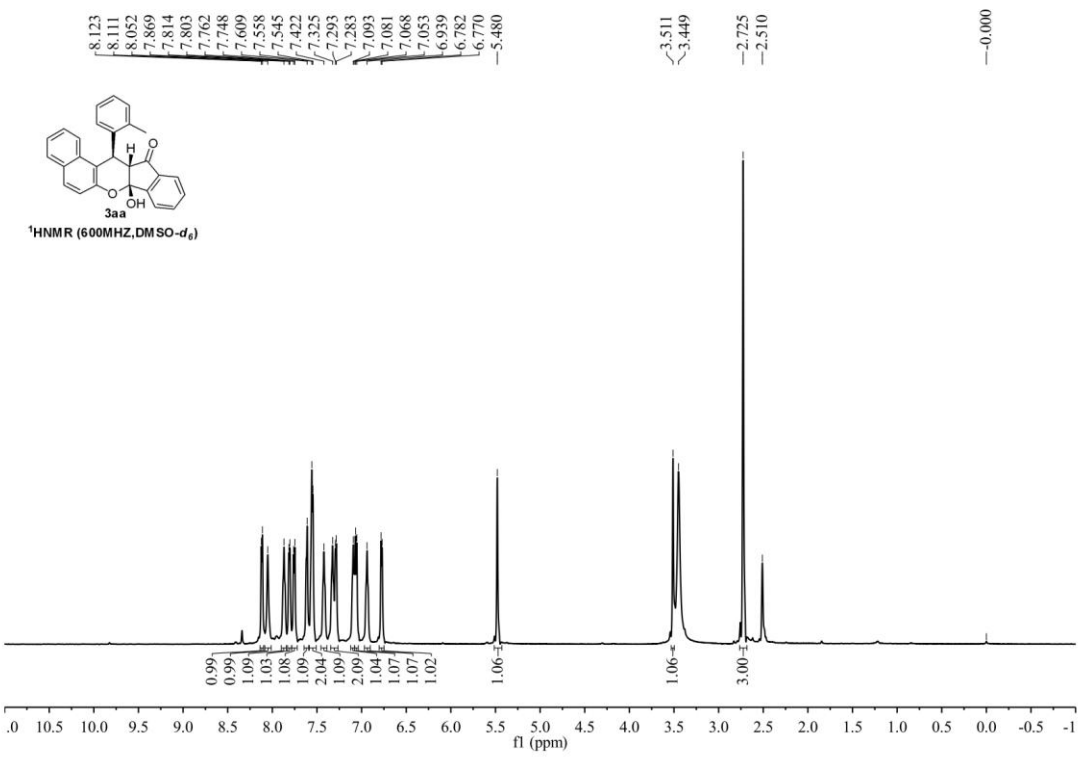
Correction method= # Reported T Limits: Tmin=0.980 Tmax=0.984
AbsCorr = MULTI-SCAN

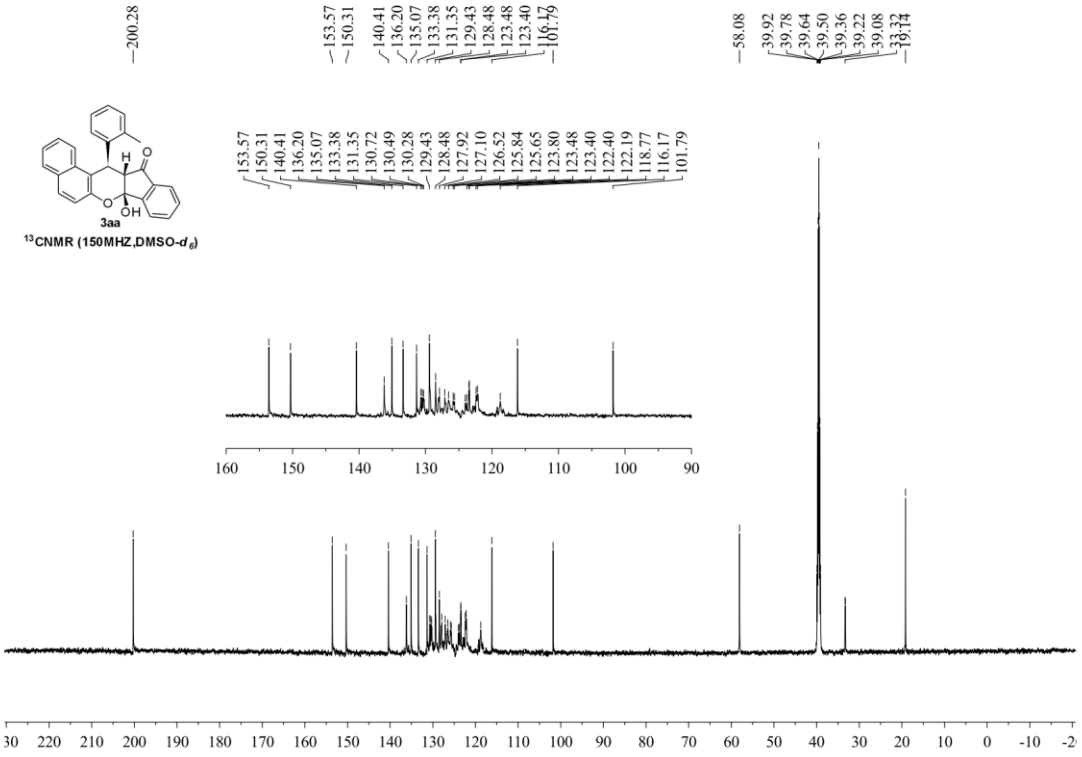
Data completeness= 0.998 Theta(max)= 25.000

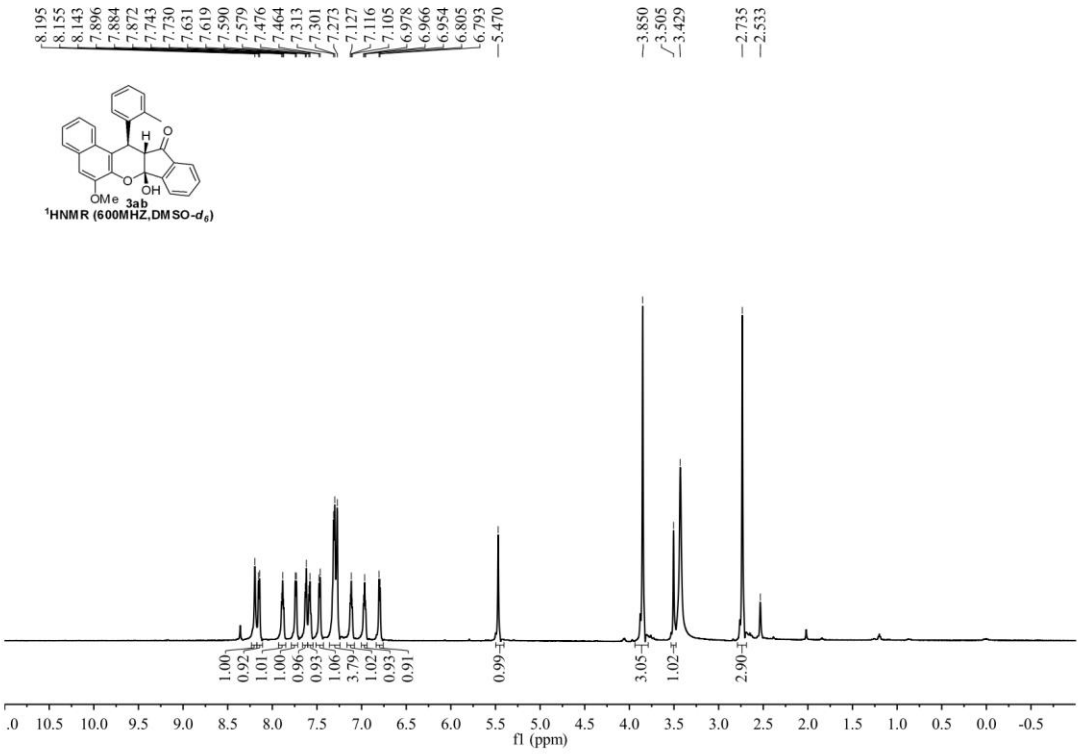
R(reflections)= 0.0425(3249) wR2(reflections)= 0.1238(3589)

S = 1.048 Npar= 283

3. Copies of ^{1}HNMR, ^{13}CNMR.



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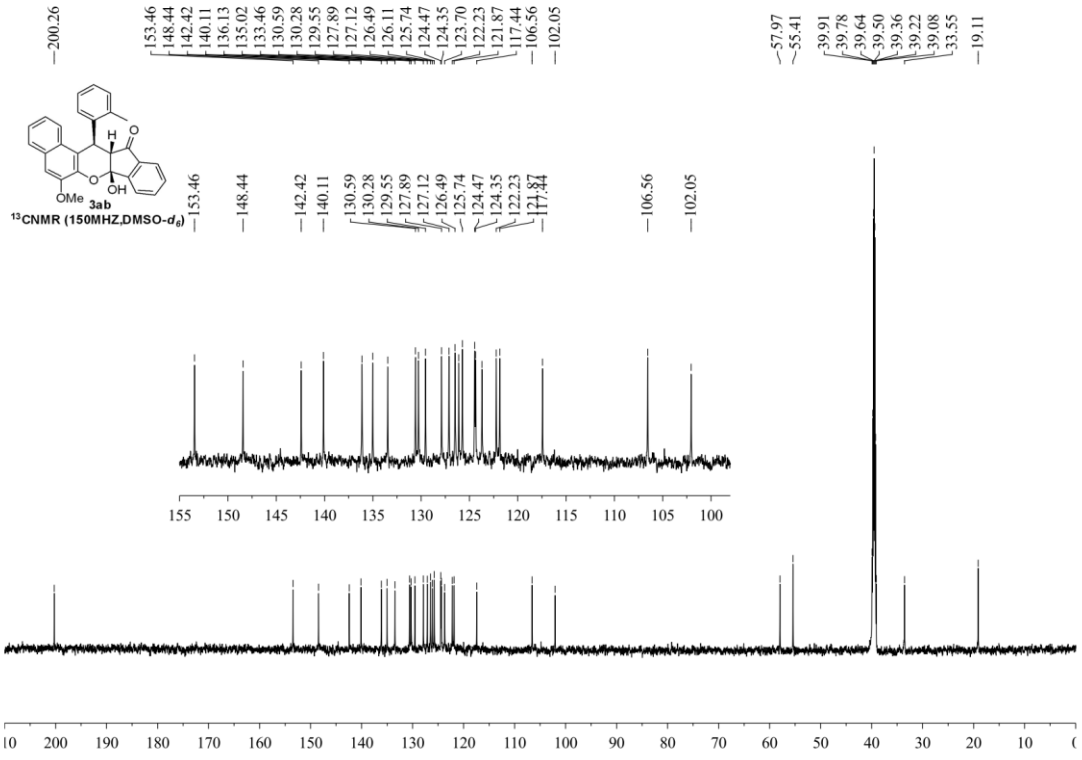
7.872
7.743
7.730
7.631
7.619
7.590
7.579
7.476
7.464
7.313
7.301
7.273
7.127
7.116
7.105
6.978
6.966
6.954
6.805
6.793
5.470
3.850
3.505
3.429
2.735
2.533
OMe
OH
3ab
1HNMR (600MHZ,DMSO-d6)
1.00
0.92
1.01
1.00
0.96
0.93
1.06
3.79
1.02
0.93
0.91
0.99
3.05
1.02
2.90
f1 (ppm)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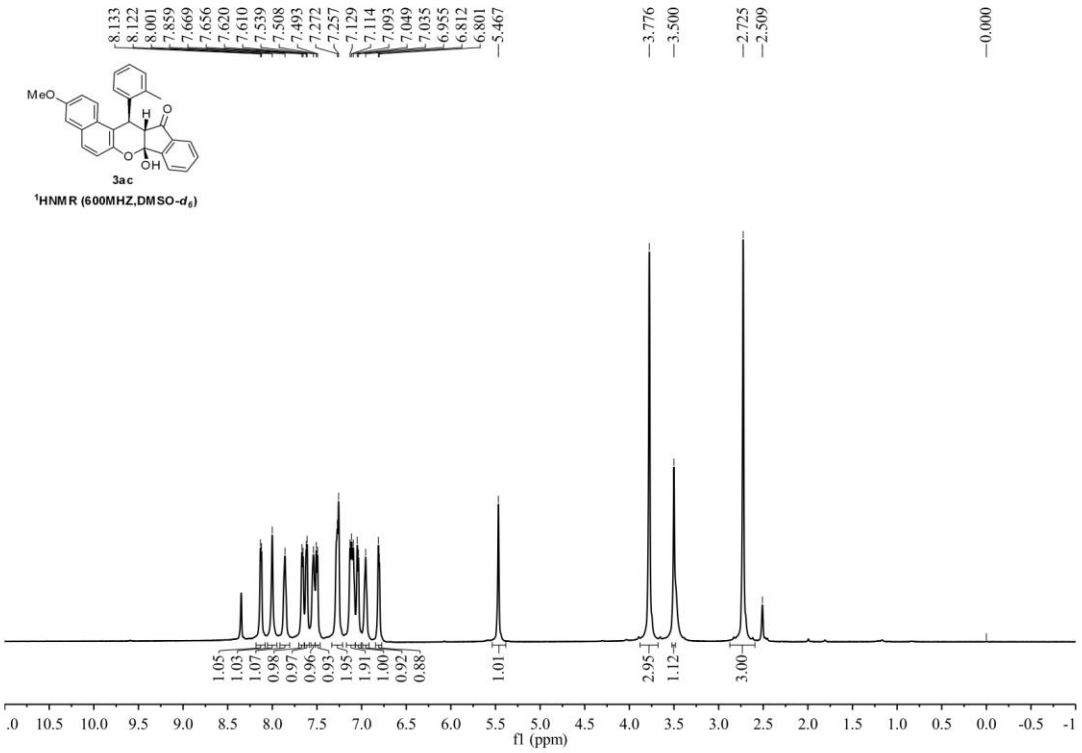
127.12
126.49
126.11
125.74
124.47
124.35
123.70
122.23
121.87
117.44
106.56
102.05
57.97
55.41
39.91
39.78
39.64
39.50
39.36
39.22
39.08
33.55
19.11
OMe
OH
3ab
13CNMR (150MHZ,DMSO-d6)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7.656
7.620
7.610
7.539
7.508
7.493
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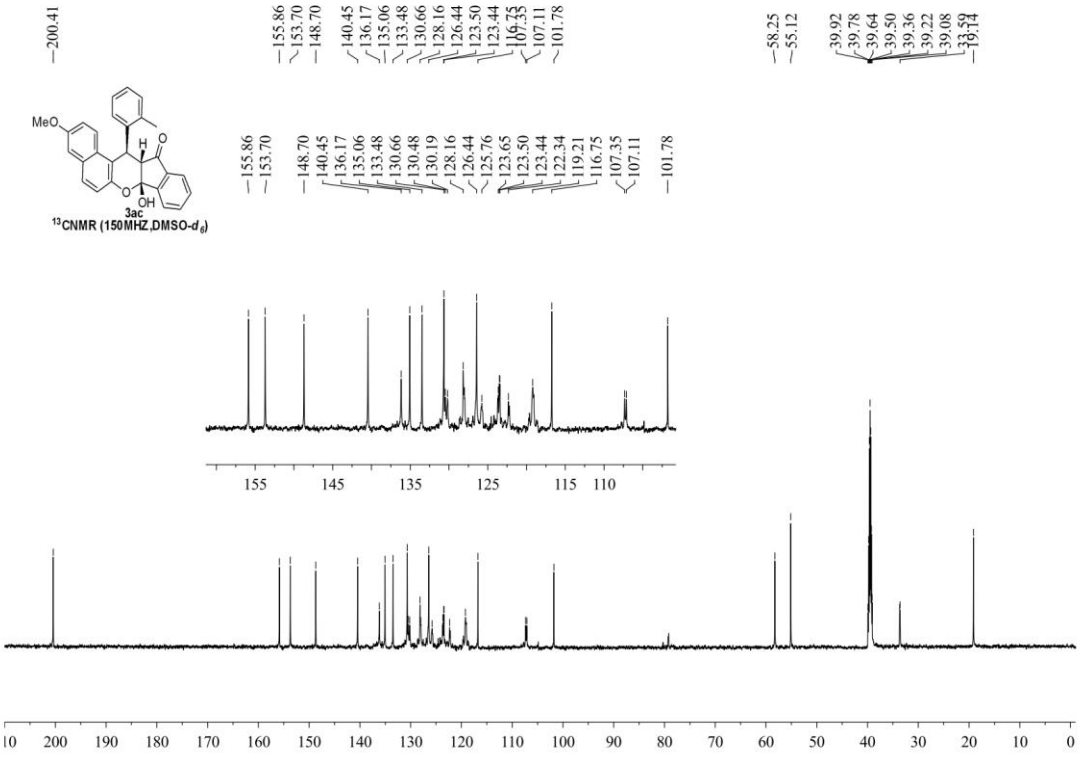
7.257
7.129
7.114
7.093
7.049
7.035
6.955
6.812
6.801
5.467
3.776
3.500
2.725
2.509
0.000
MeO
H
O
O
OH
3ac
1HNMR (600MHZ,DMSO-d6)
1.05
1.03
1.07
0.98
0.97
0.96
0.93
1.95
1.91
1.00
0.92
0.88
1.01
2.95
1.12
3.00
f1 (ppm)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153.70
148.70
140.45
136.17
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133.48
130.66
128.16
126.44
123.50
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107.11
101.78
58.25
55.12
39.92
39.78
39.64
39.50
39.36
39.22
39.08
MeO
H
O
O
OH
3ac
13CNMR (150MHZ,DMSO-d6)
155.86
153.70
148.70
140.45
136.17
135.06
133.48
130.66
130.48
130.19
128.16
126.44
125.76
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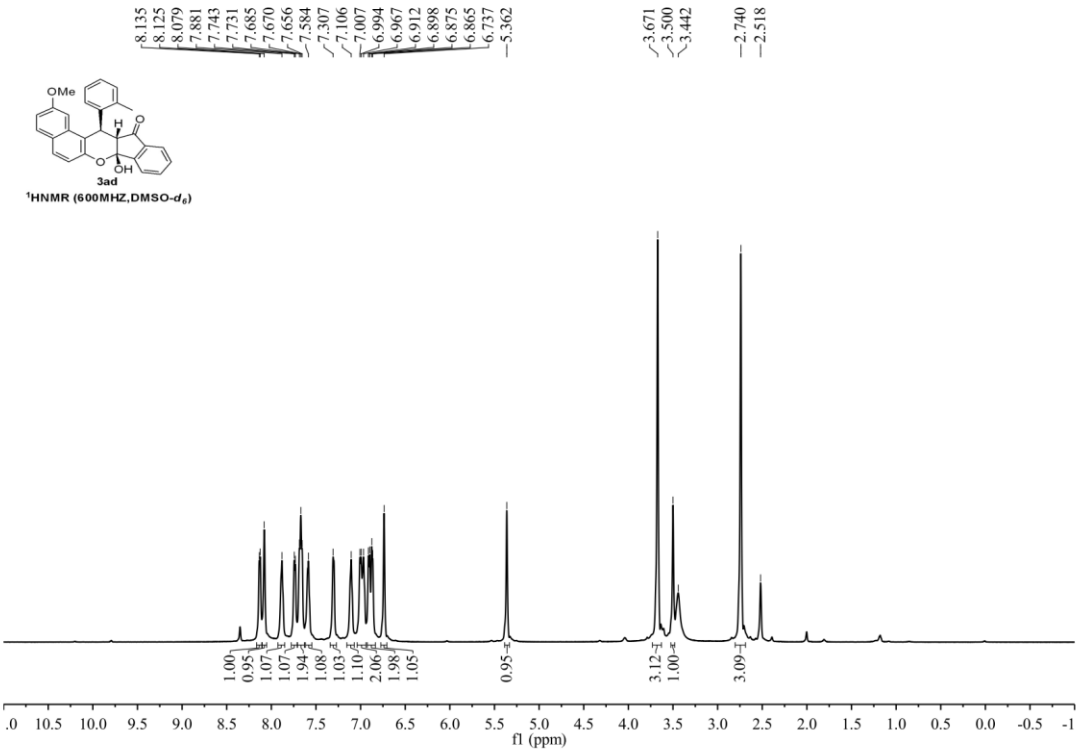
107.11
101.78
155
145
135
125
115
110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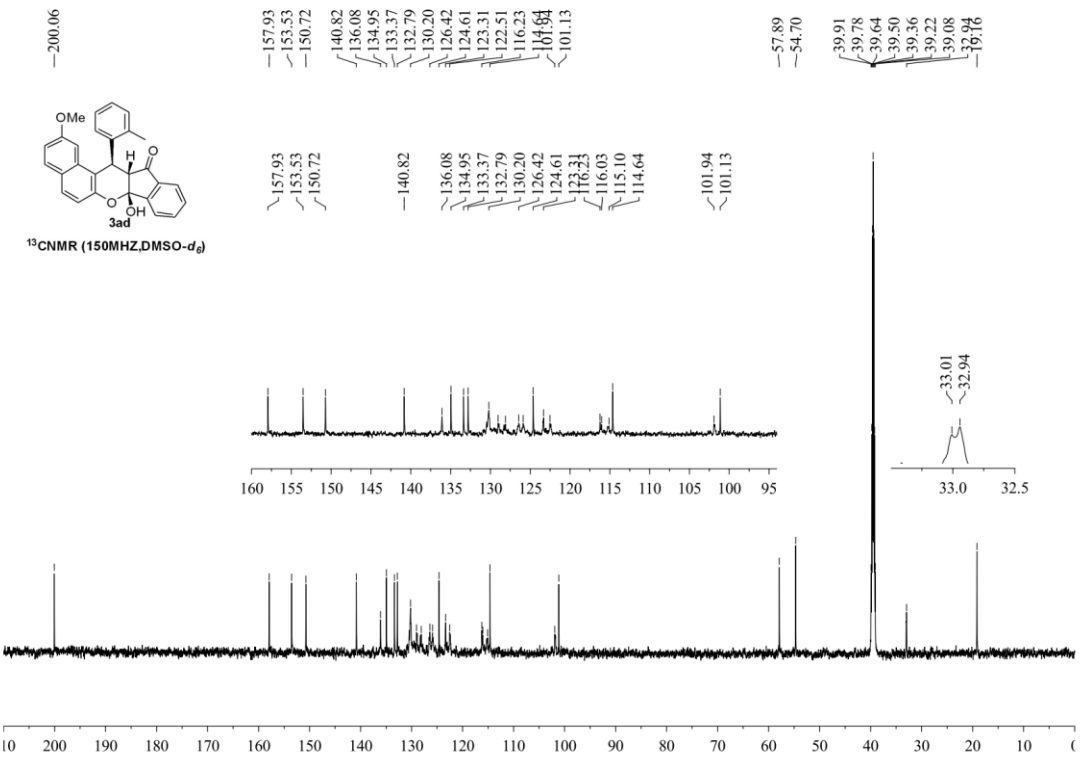
7.007
6.994
6.967
6.912
6.898
6.875
6.865
6.737
5.362
3.671
3.500
3.442
2.740
2.518
OMe
H
O
OH
3ad
1HNMR (600MHZ,DMSO-d6)
1.00
0.95
1.07
1.07
1.94
1.08
1.03
1.10
2.06
1.98
1.05
0.95
3.12
1.00
3.09
f1 (ppm)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157.93
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150.72
140.82
136.08
134.95
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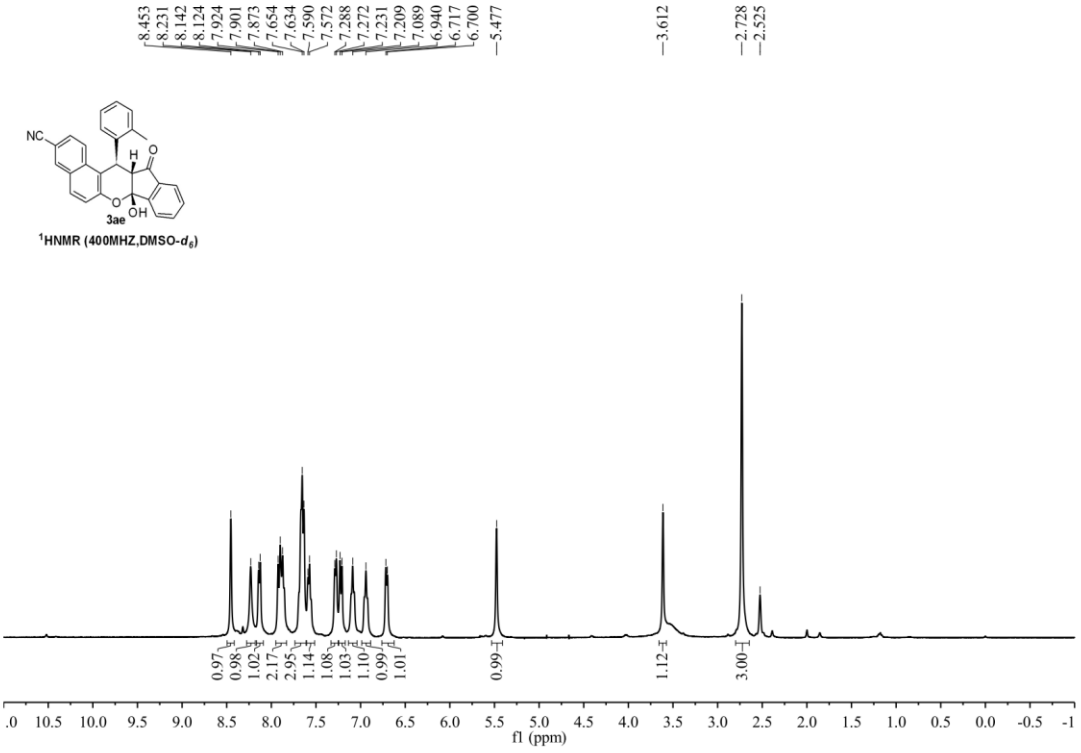
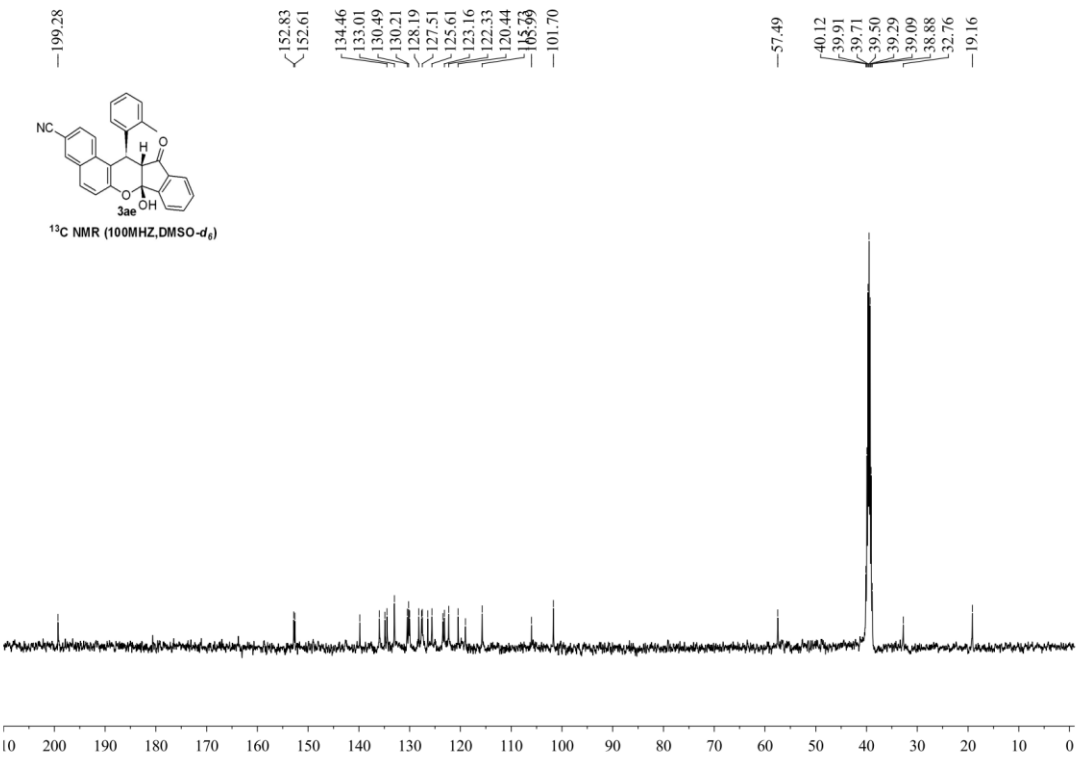
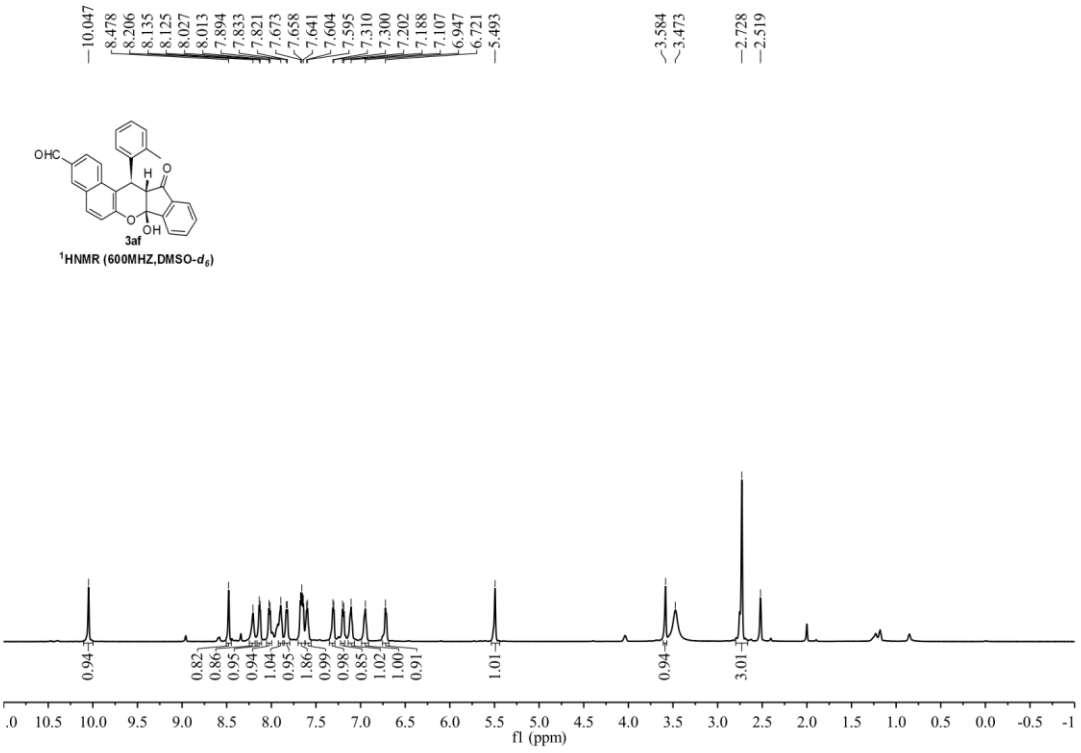
124.61
123.31
122.51
116.23
114.64
101.94
101.13
57.89
54.70
39.91
39.78
39.64
39.50
39.36
39.22
39.08
32.94
19.16
OMe
H
O
OH
3ad
13CNMR (150MHZ,DMSO-d6)
33.01
32.94



^{1}HNMR (400MHZ,DMSO-d_6)



^{13}C NMR (100MHZ,DMSO-d_6)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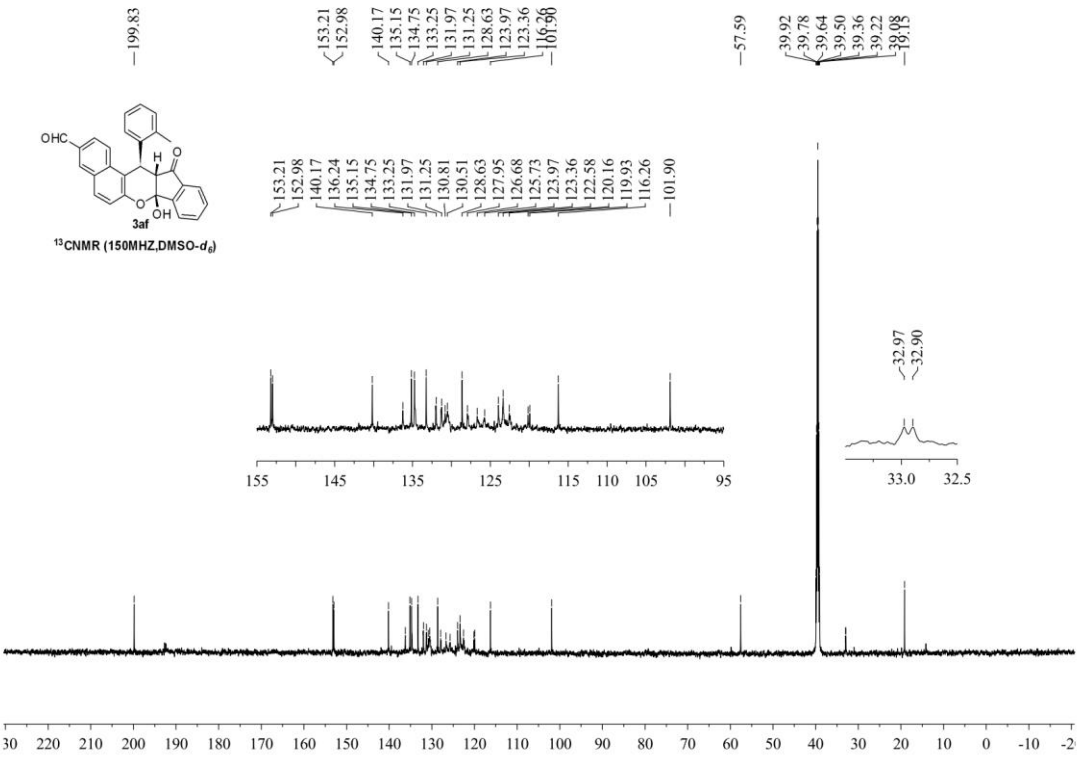
7.658
7.641
7.604
7.595
7.310
7.300
7.202
7.188
7.107
6.947
6.721
5.493
3.584
3.473
2.728
2.519
OHC
H
O
O
OH
3af
1HNMR (600MHZ,DMSO-d6)
0.94
0.82
0.86
0.95
0.94
1.04
0.95
1.86
0.99
0.98
0.85
1.02
1.00
0.91
1.01
0.94
3.01
f1 (ppm)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152.98
140.17
135.15
134.75
133.25
131.97
131.25
128.63
123.97
123.36
116.26
101.90
57.59
39.92
39.78
39.64
39.50
39.36
39.22
39.08
38.93
OHC
H
O
O
OH
3af
13CNMR (150MHZ,DMSO-d6)
153.21
152.98
140.17
136.24
135.15
134.75
133.25
131.97
131.25
130.81
130.51
128.63
127.95
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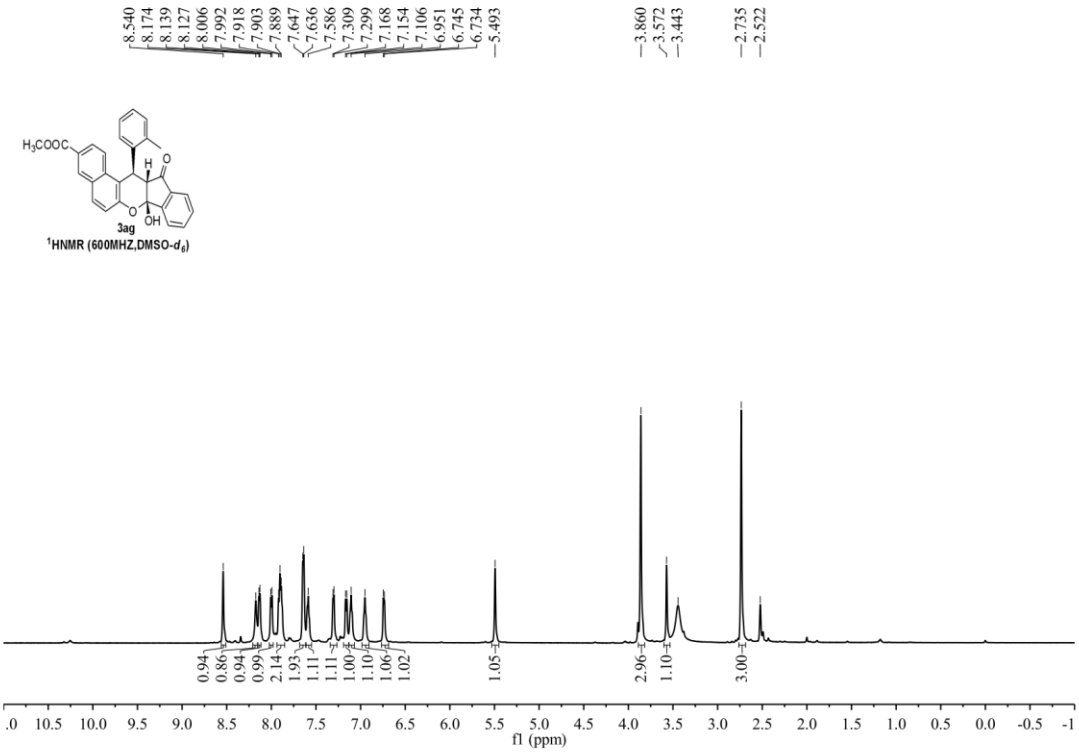
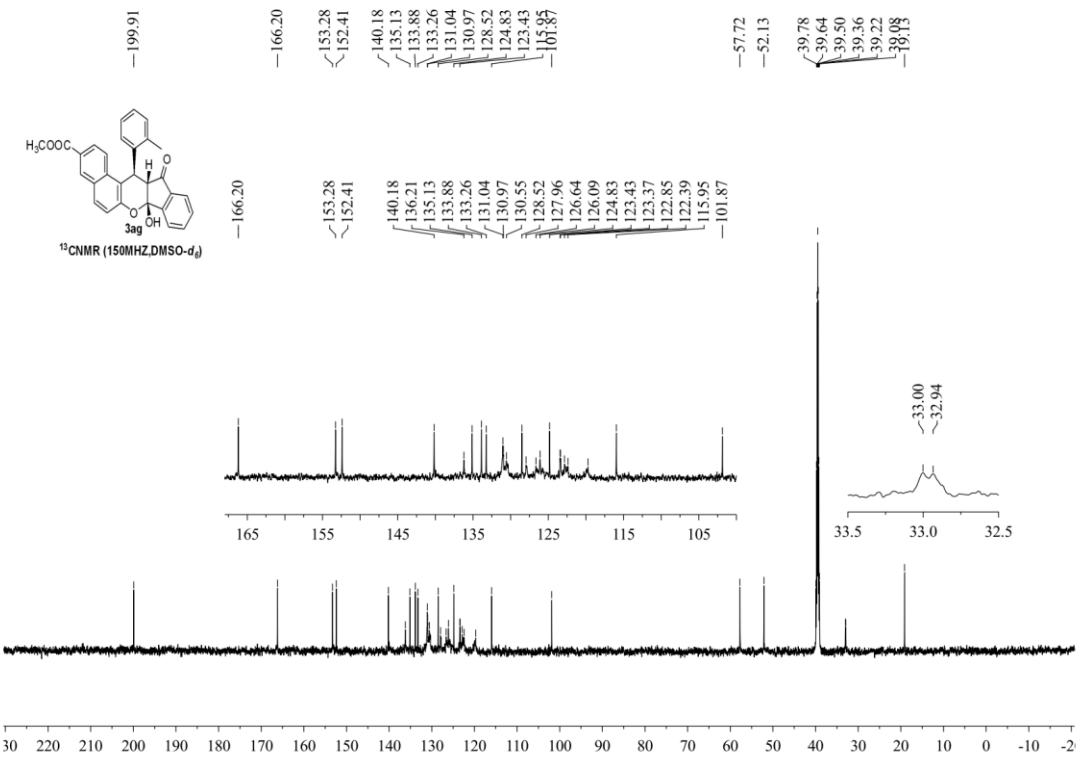
120.16
119.93
116.26
101.90
32.97
32.90


8.540
8.174
8.139
8.127
8.006
7.992
7.918
7.903
7.889
7.647
7.636
7.586
7.309
7.299
7.168
7.154
7.106
6.951
6.745
6.734
5.493
3.860
3.572
3.443
2.735
2.522
H3COOC
H
O
O
OH
3ag
1HNMR (600MHZ,DMSO-d6)
0.94
0.86
0.94
0.99
2.14
1.93
1.11
1.11
1.00
1.10
1.06
1.02
1.05
2.96
1.10
3.00
f1 (ppm)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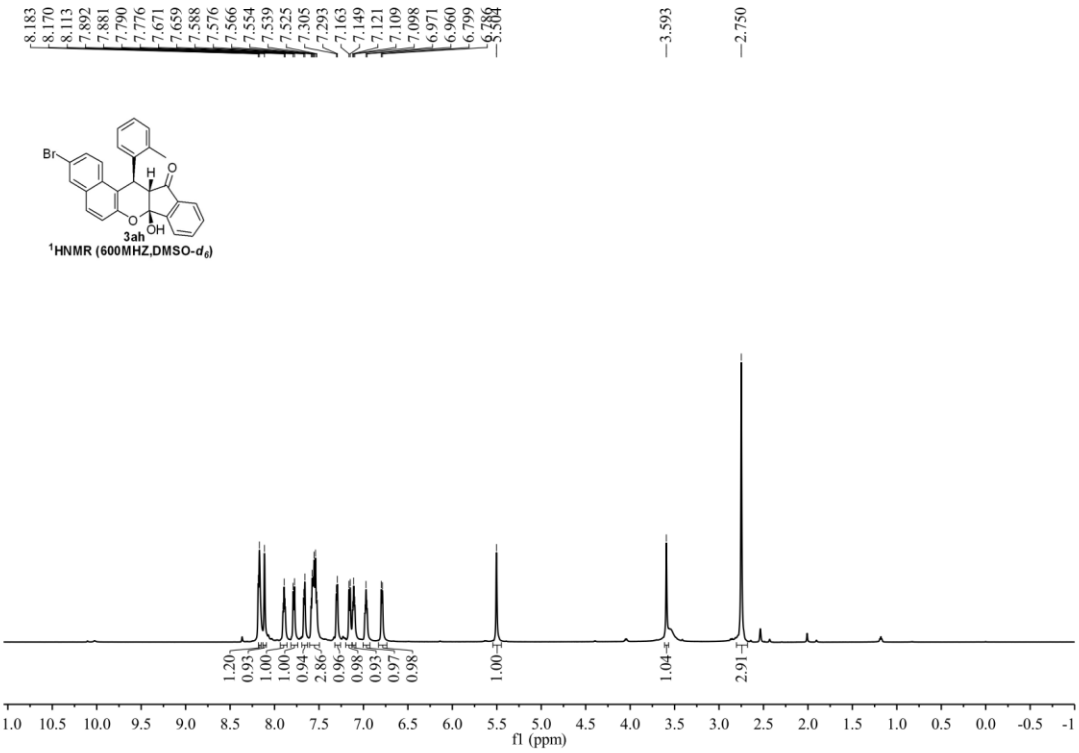
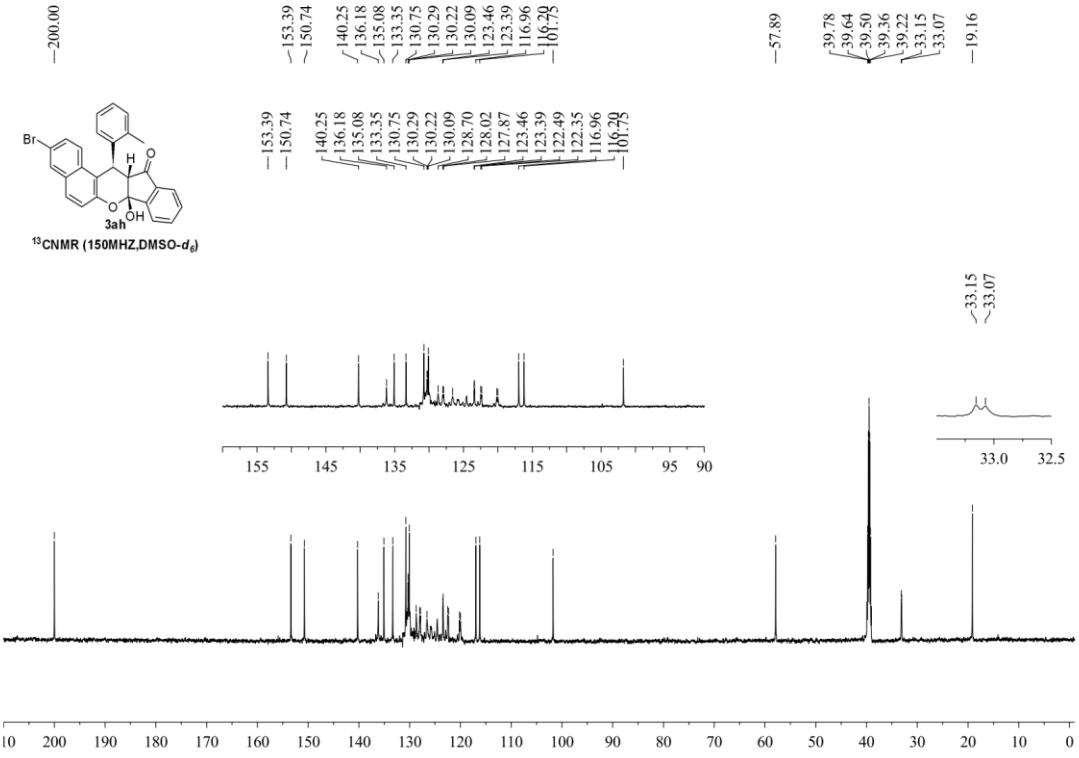
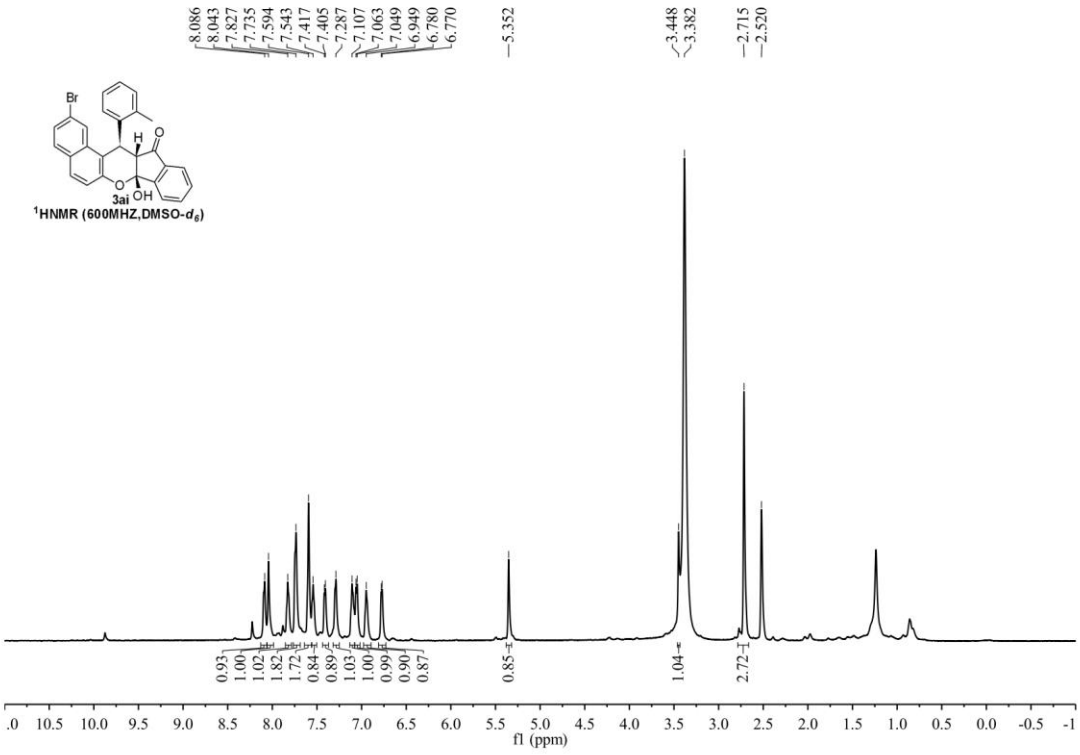
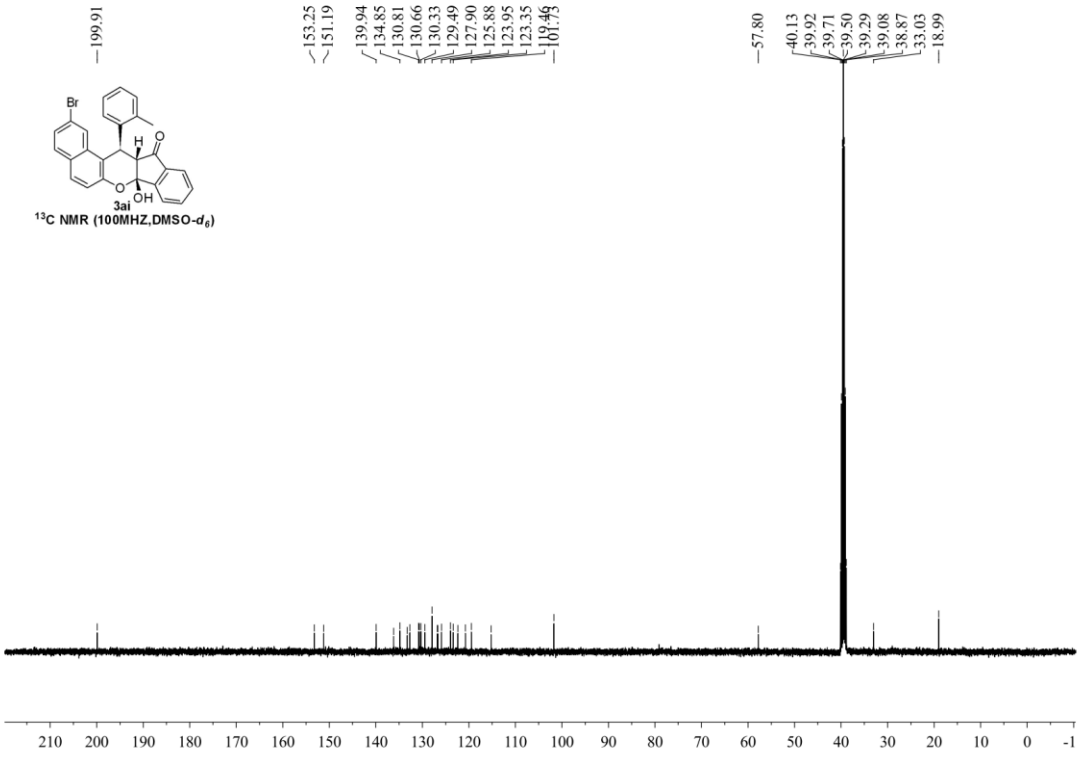
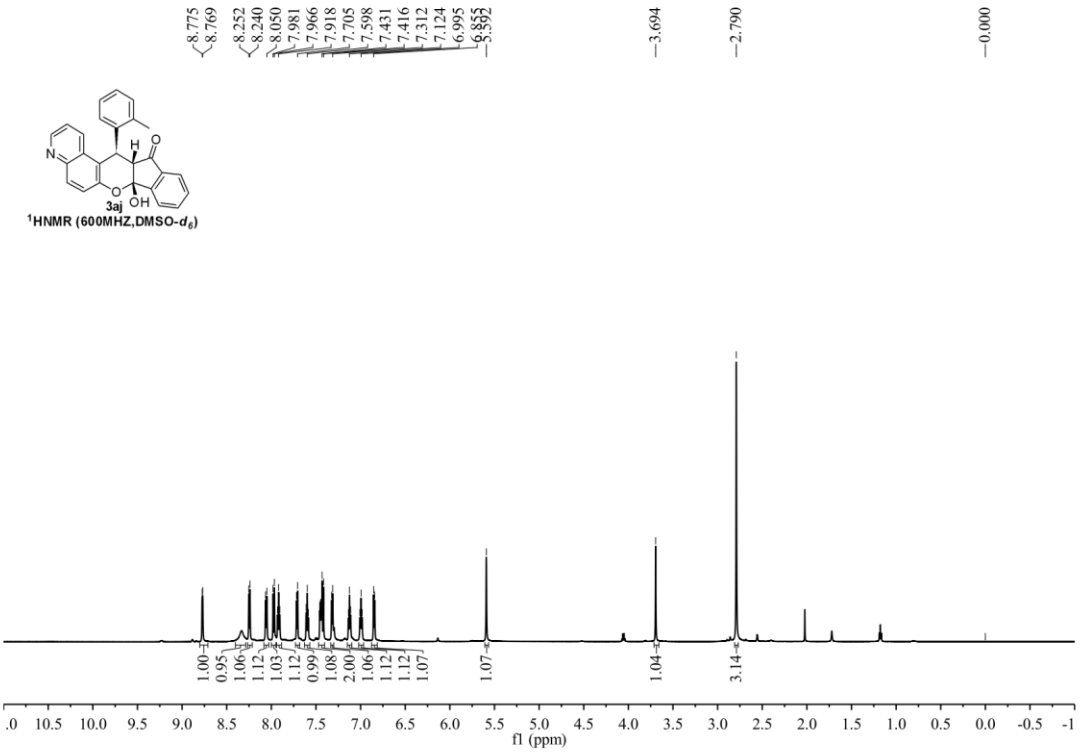
166.20
153.28
152.41
140.18
135.13
133.88
133.26
131.04
130.97
128.52
124.83
123.43
115.95
101.87
57.72
52.13
39.78
39.64
39.50
39.36
39.22
39.08
38.93
H3COOC
H
O
O
OH
3ag
13CNMR (150MHZ,DMSO-d6)
166.20
153.28
152.41
140.18
136.21
135.13
133.88
133.26
131.04
130.97
130.55
128.52
127.96
126.64
126.09
124.83
123.43
123.37
122.85
122.39
115.95
101.87
33.00
32.94

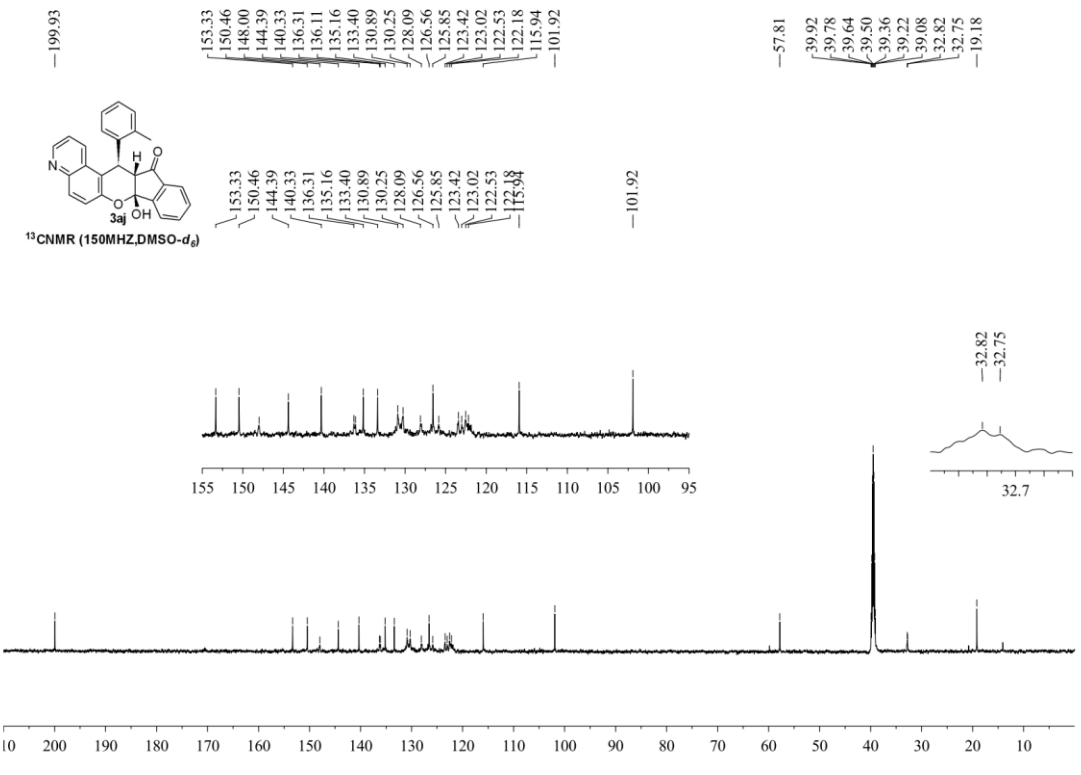

8.183
8.170
8.113
7.892
7.881
7.790
7.776
7.671
7.659
7.588
7.576
7.566
7.554
7.539
7.525
7.305
7.293
7.163
7.149
7.121
7.109
7.098
6.971
6.960
6.799
6.786
5.504
3.593
2.750
Br
H
O
O
OH
3ah
1HNMR (600MHZ,DMSO-d6)
1.20
0.93
1.00
1.00
0.94
2.86
0.96
0.98
0.93
0.97
0.98
1.00
1.04
2.91
f1 (ppm)

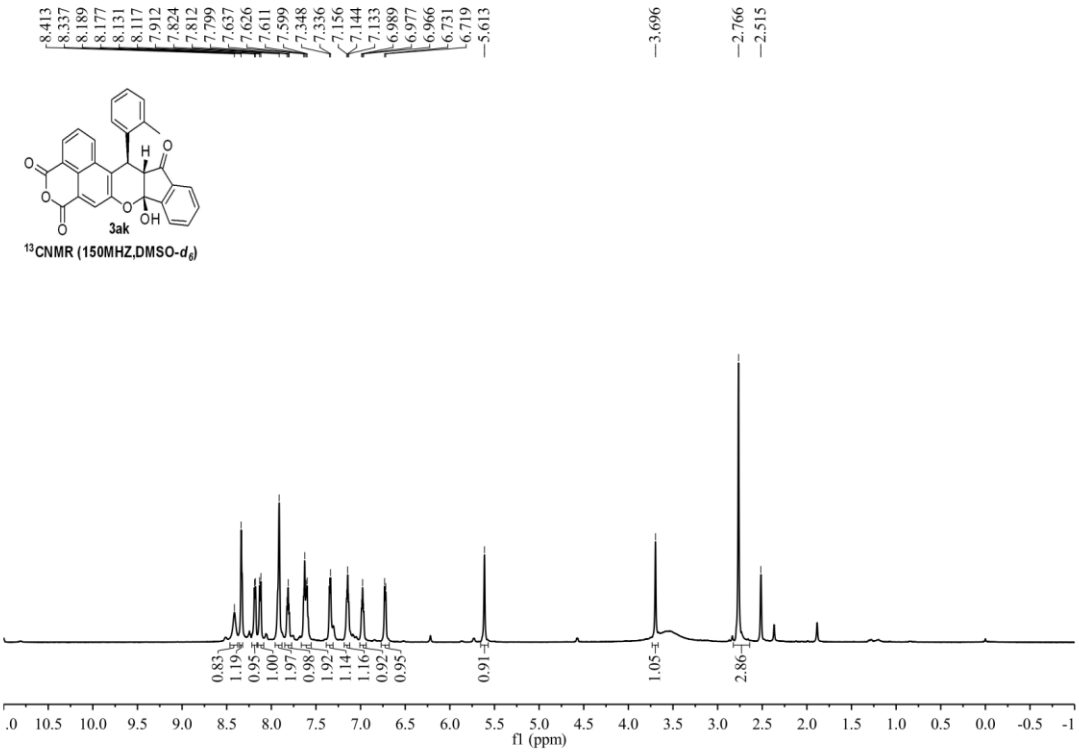

200.00
153.39
150.74
140.25
136.18
135.08
133.35
130.75
130.29
130.22
130.09
123.46
123.39
116.96
116.20
101.75
57.89
39.78
39.64
39.50
39.36
39.22
33.15
33.07
19.16
128.70
128.02
127.87
122.49
122.35
Br
H
O
O
OH
3ah
13CNMR (150MHZ,DMSO-d6)


8.086
8.043
7.827
7.735
7.594
7.543
7.417
7.405
7.287
7.107
7.063
7.049
6.949
6.780
6.770
5.352
3.448
3.382
2.715
2.520
Br
H
O
O
OH
3ai
¹HNMR (600MHZ,DMSO-d6)
0.93
1.00
1.02
1.82
1.72
0.84
0.89
1.03
1.00
0.99
0.90
0.87
0.85
1.04
2.72
f1 (ppm)


199.91
153.25
151.19
139.94
134.85
130.81
130.66
130.33
129.49
127.90
125.88
123.95
123.35
57.80
40.13
39.92
39.71
39.50
39.29
39.08
38.87
33.03
18.99
Br
H
O
O
OH
3ai
¹³C NMR (100MHZ,DMSO-d6)


8.775
8.769
8.252
8.240
8.050
7.981
7.966
7.918
7.705
7.598
7.431
7.416
7.312
7.124
6.995
6.855
5.392
3.694
2.790
0.000
3aj
OH
1HNMR (600MHZ,DMSO-d6)
1.00
0.95
1.06
1.12
1.03
1.12
0.99
1.08
2.00
1.06
1.12
1.12
1.07
1.07
1.04
3.14
f1 (ppm)


199.93
153.33
150.46
148.00
144.39
140.33
136.31
136.11
135.16
133.40
130.89
130.25
128.09
126.56
125.85
123.42
123.02
122.53
122.18
115.94
101.92
57.81
39.92
39.78
39.64
39.50
39.36
39.22
39.08
32.82
32.75
19.18
3aj
OH
13CNMR (150MHZ,DMSO-d6)
32.7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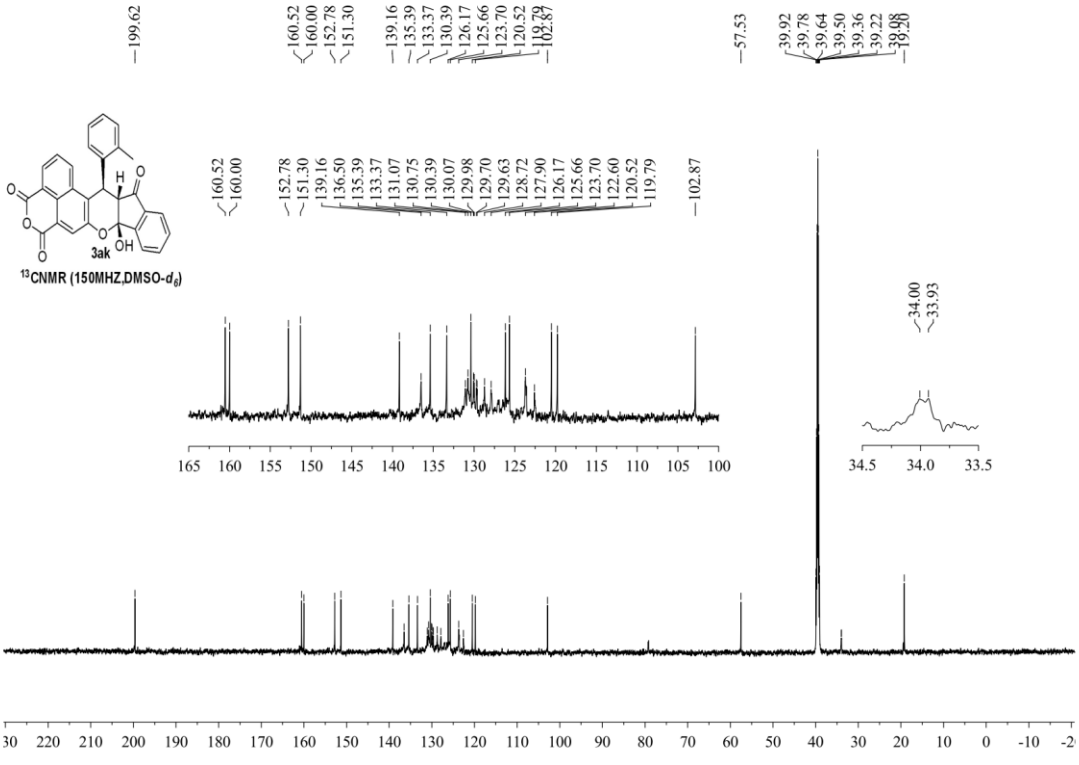
8.337
8.189
8.177
8.131
8.117
7.912
7.824
7.812
7.799
7.637
7.626
7.611
7.599
7.348
7.336
7.156
7.144
7.133
6.989
6.977
6.966
6.731
6.719
5.613
3.696
2.766
2.515
3ak
13CNMR (150MHZ,DMSO-d6)
0.83
1.19
0.95
1.00
1.97
0.98
1.92
1.14
1.16
0.92
0.95
0.91
1.05
2.86
f1 (ppm)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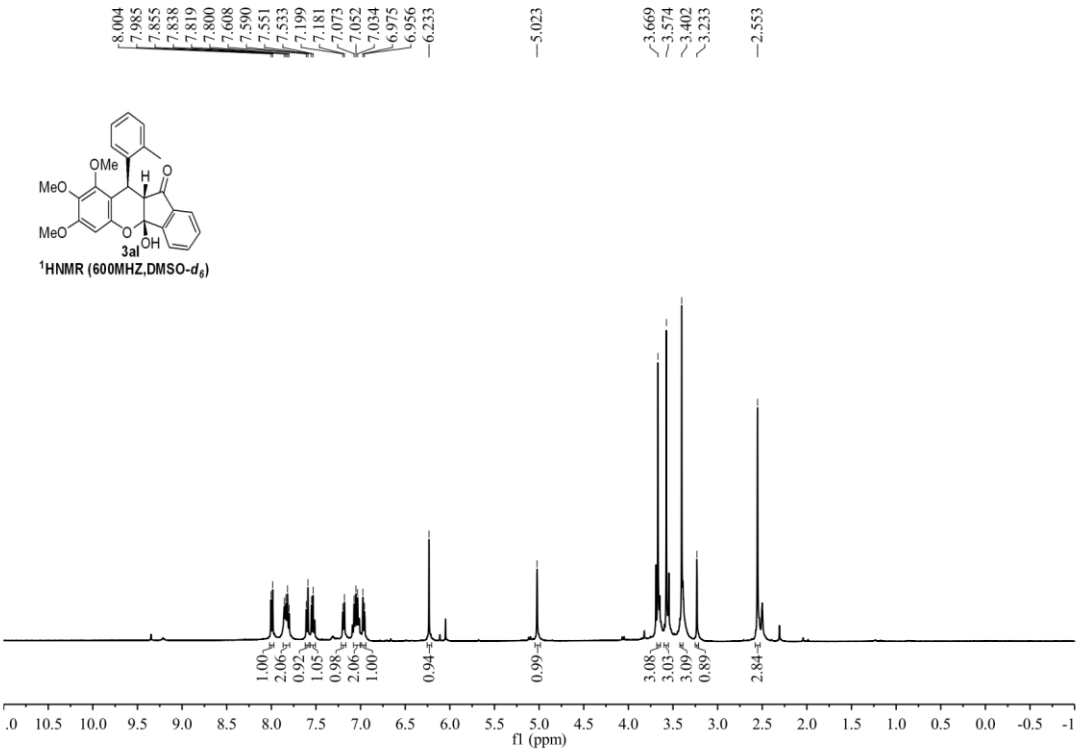
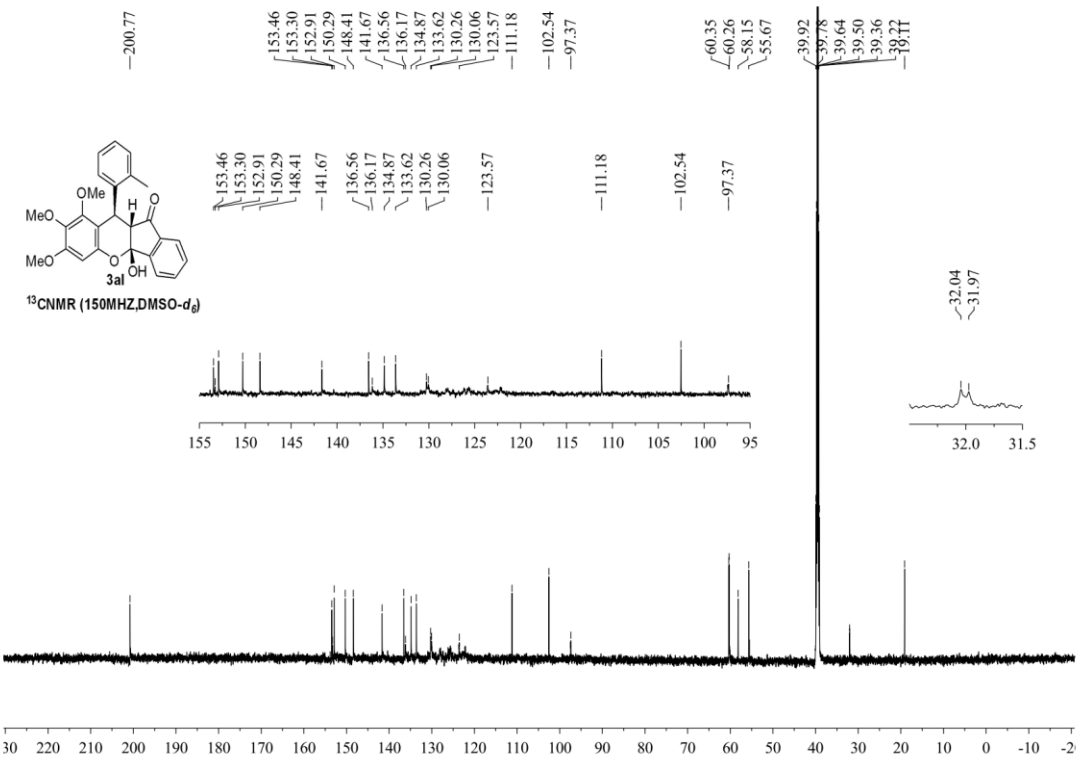
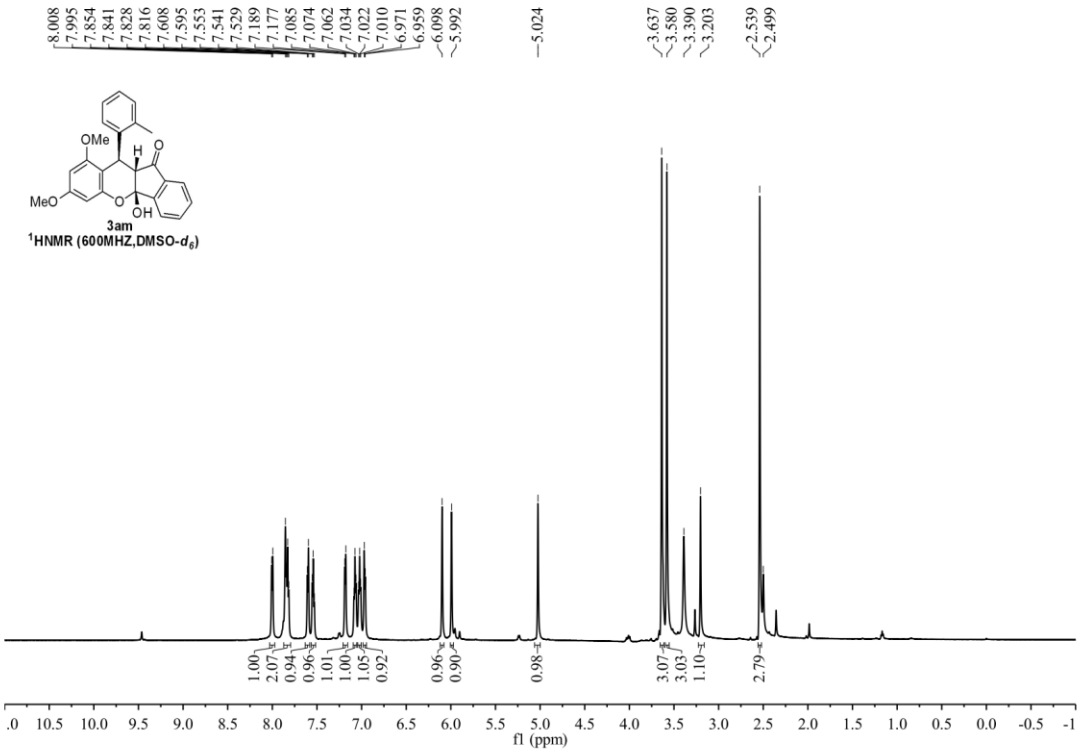
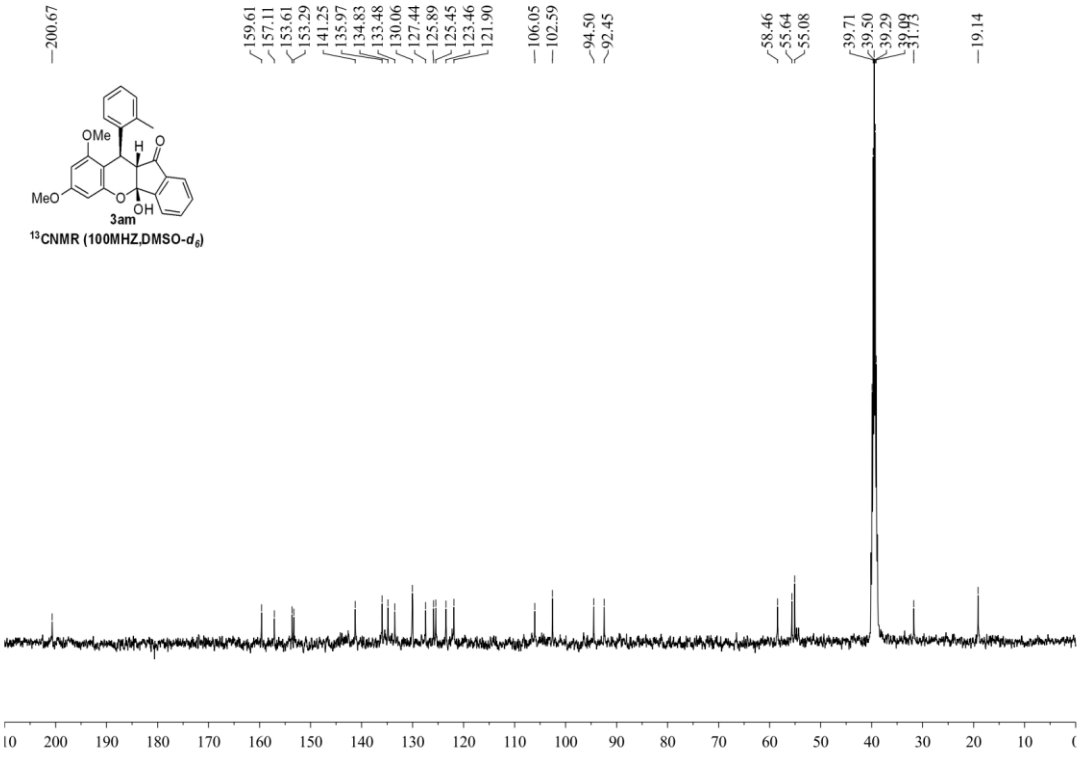
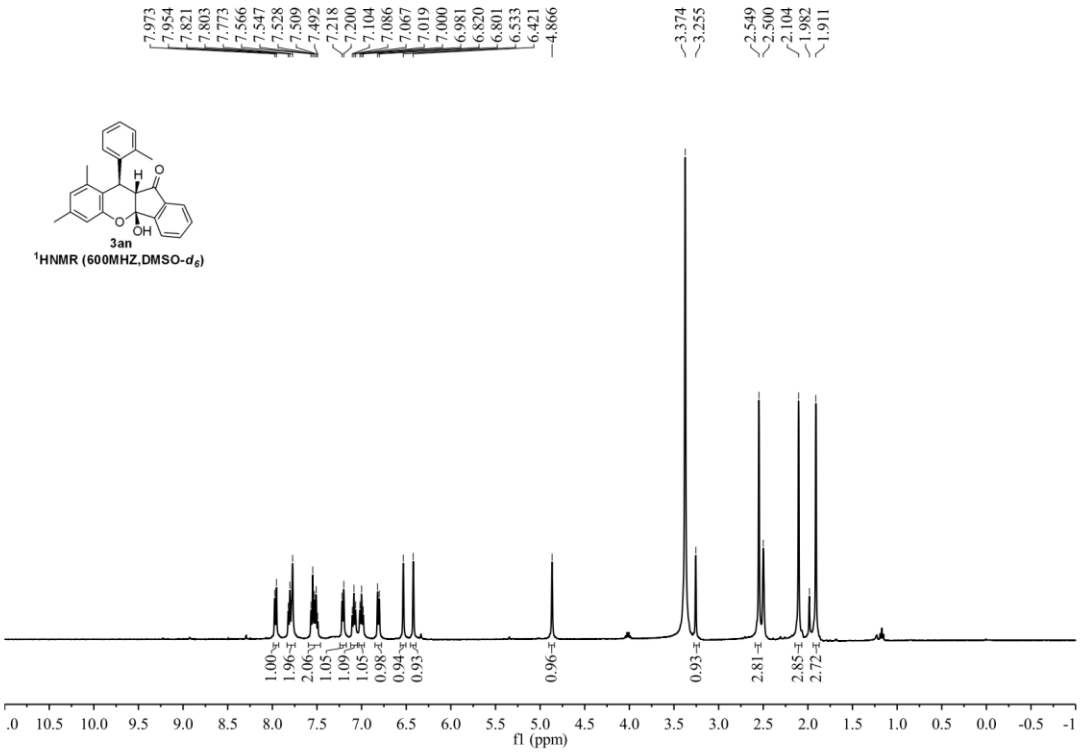
160.52
160.00
152.78
151.30
139.16
135.39
133.37
130.39
126.17
125.66
123.70
120.52
102.87
57.53
39.92
39.78
39.64
39.50
39.36
39.22
3ak
13CNMR (150MHZ,DMSO-d6)
152.78
151.30
139.16
136.50
135.39
133.37
131.07
130.75
130.39
130.07
129.98
129.70
129.63
128.72
127.90
126.17
125.66
123.70
122.60
120.52
119.79
34.00
33.93

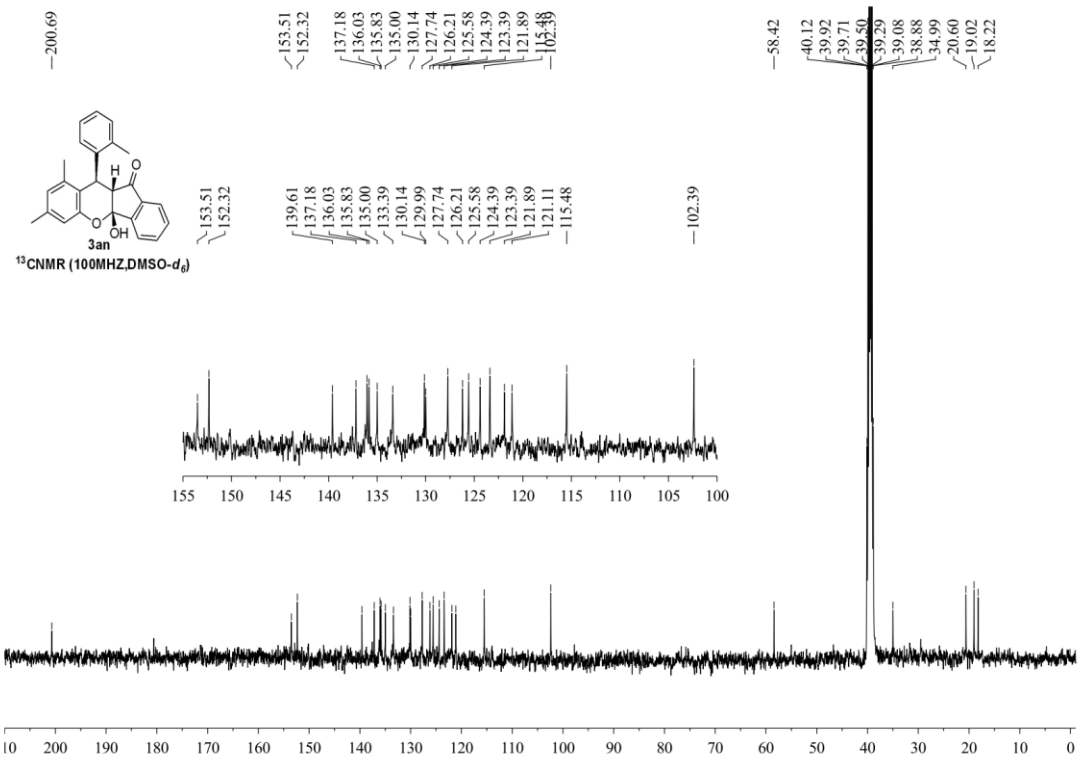

8.004
7.985
7.855
7.838
7.819
7.800
7.608
7.590
7.551
7.533
7.199
7.181
7.073
7.052
7.034
6.975
6.956
6.233
5.023
3.669
3.574
3.402
3.233
2.553
OMe
MeO
MeO
H
O
O
OH
3al
1HNMR (600MHZ,DMSO-d6)
1.00
2.06
0.92
1.05
0.98
2.06
1.00
0.94
0.99
3.08
3.03
3.09
0.89
2.84
f1 (ppm)

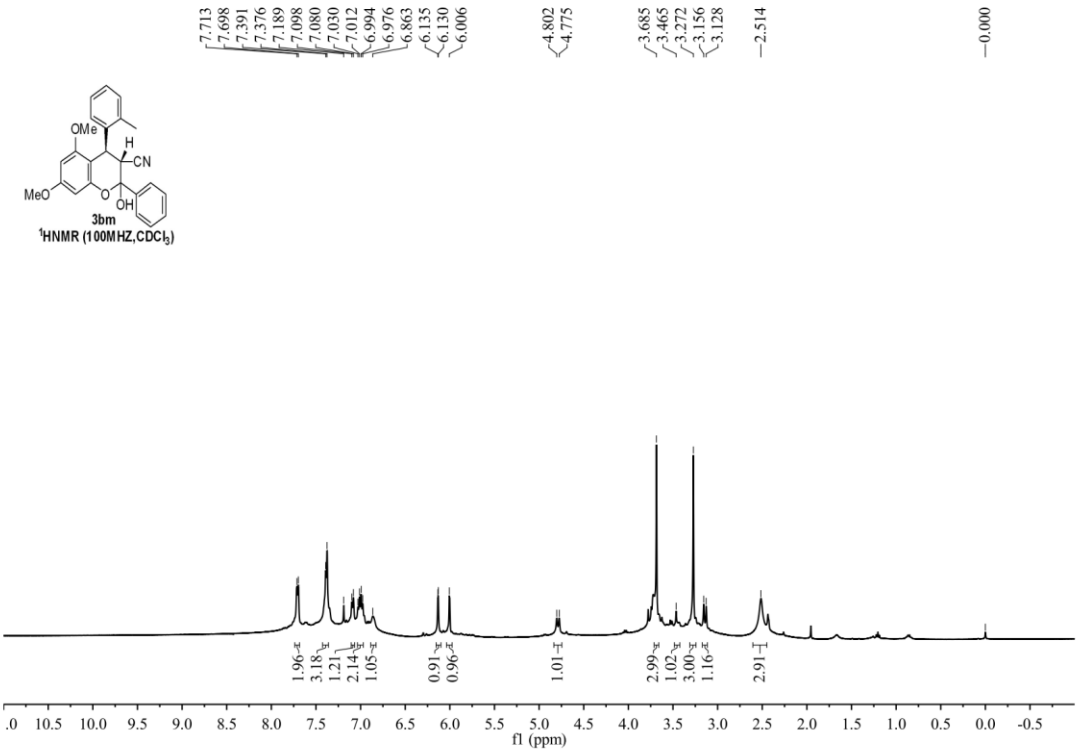

200.77
153.46
153.30
152.91
150.29
148.41
141.67
136.56
136.17
134.87
133.62
130.26
130.06
123.57
111.18
102.54
97.37
60.35
60.26
58.15
55.67
39.92
39.78
39.64
39.50
39.36
39.22
39.11
32.04
31.97
OMe
MeO
MeO
H
O
O
OH
3al
13CNMR (150MHZ,DMSO-d6)


8.008
7.995
7.854
7.841
7.828
7.816
7.608
7.595
7.553
7.541
7.529
7.189
7.177
7.085
7.074
7.062
7.034
7.022
7.010
6.971
6.959
6.098
5.992
5.024
3.637
3.580
3.390
3.203
2.539
2.499
OMe
H
O
MeO
O
OH
3am
1HNMR (600MHZ,DMSO-d6)
1.00
2.07
0.94
0.96
1.01
1.00
1.05
0.92
0.96
0.90
0.98
3.07
3.03
1.10
2.79
f1 (ppm)

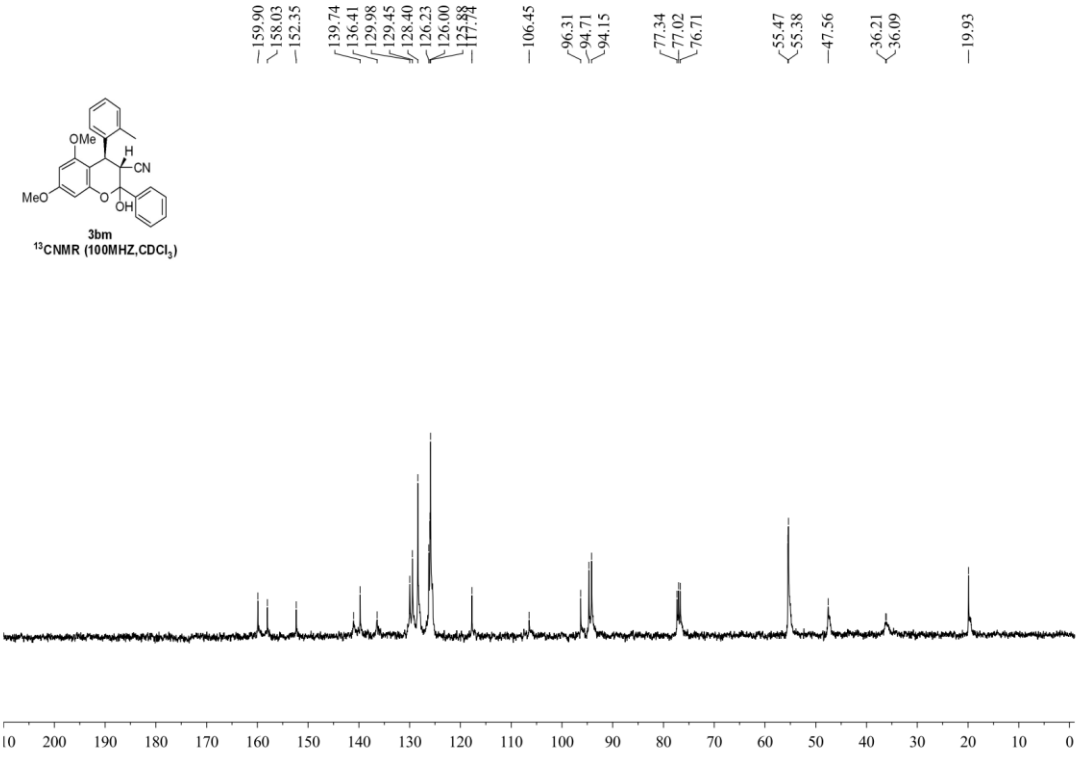

200.67
159.61
157.11
153.61
153.29
141.25
135.97
134.83
133.48
130.06
127.44
125.89
125.45
123.46
121.90
106.05
102.59
94.50
92.45
58.46
55.64
55.08
39.71
39.50
39.29
39.09
31.73
19.14
OMe
H
O
MeO
O
OH
3am
13CNMR (100MHZ,DMSO-d6)


7.973
7.954
7.821
7.803
7.773
7.566
7.547
7.528
7.509
7.492
7.218
7.200
7.104
7.086
7.067
7.019
7.000
6.981
6.820
6.801
6.533
6.421
4.866
3.374
3.255
2.549
2.500
2.104
1.982
1.911
3an
1HNMR (600MHZ,DMSO-d6)
1.00
1.96
2.06
1.05
1.09
1.05
0.98
0.94
0.93
0.96
0.93
2.81
2.85
2.72
f1 (ppm)

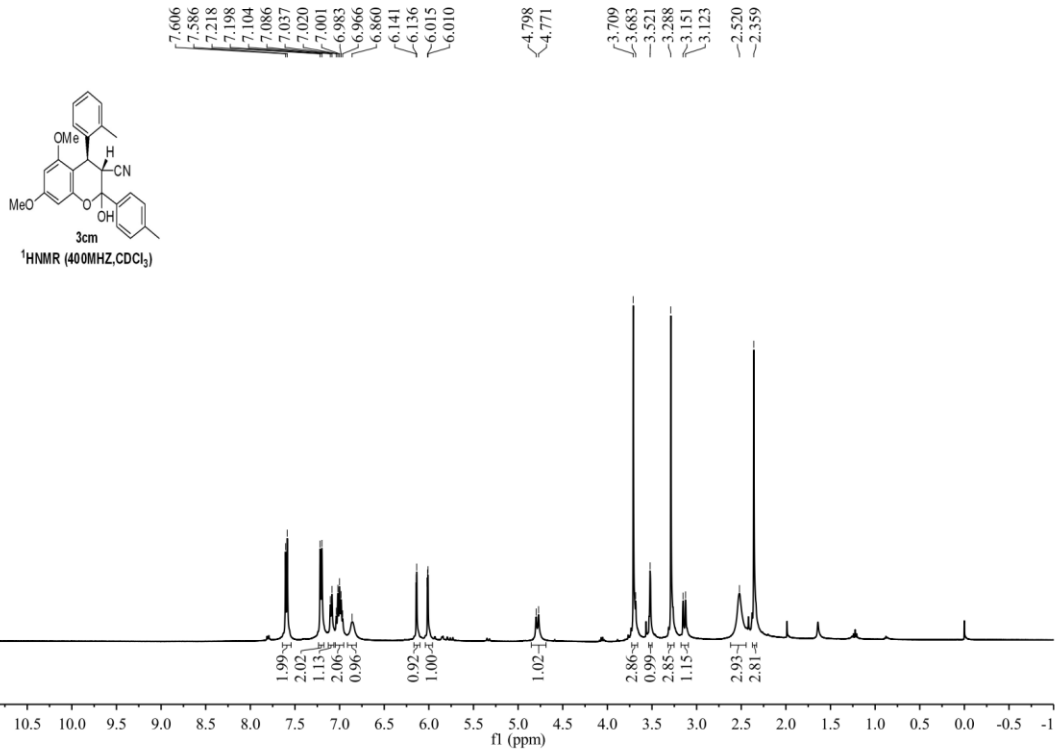

200.69
153.51
152.32
137.18
136.03
135.83
135.00
130.14
127.74
126.21
125.58
124.39
123.39
121.89
115.48
102.39
58.42
40.12
39.92
39.71
39.50
39.29
39.08
38.88
34.99
20.60
19.02
18.22
3an
13CNMR (100MHZ,DMSO-d6)

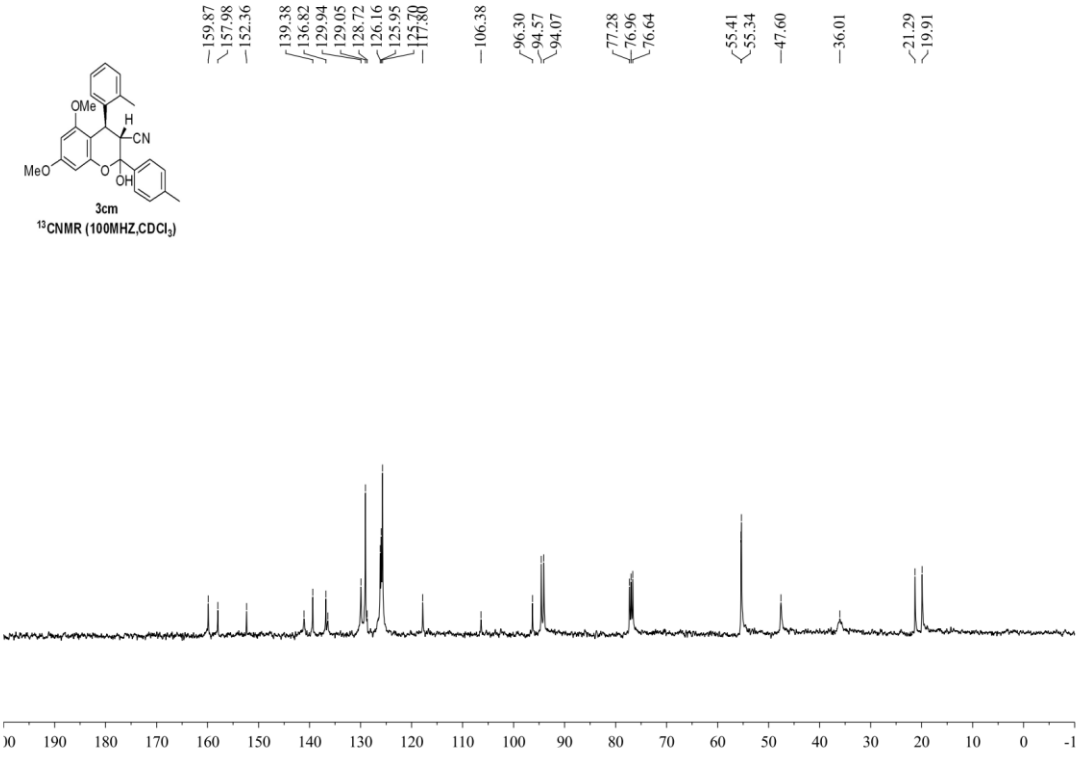


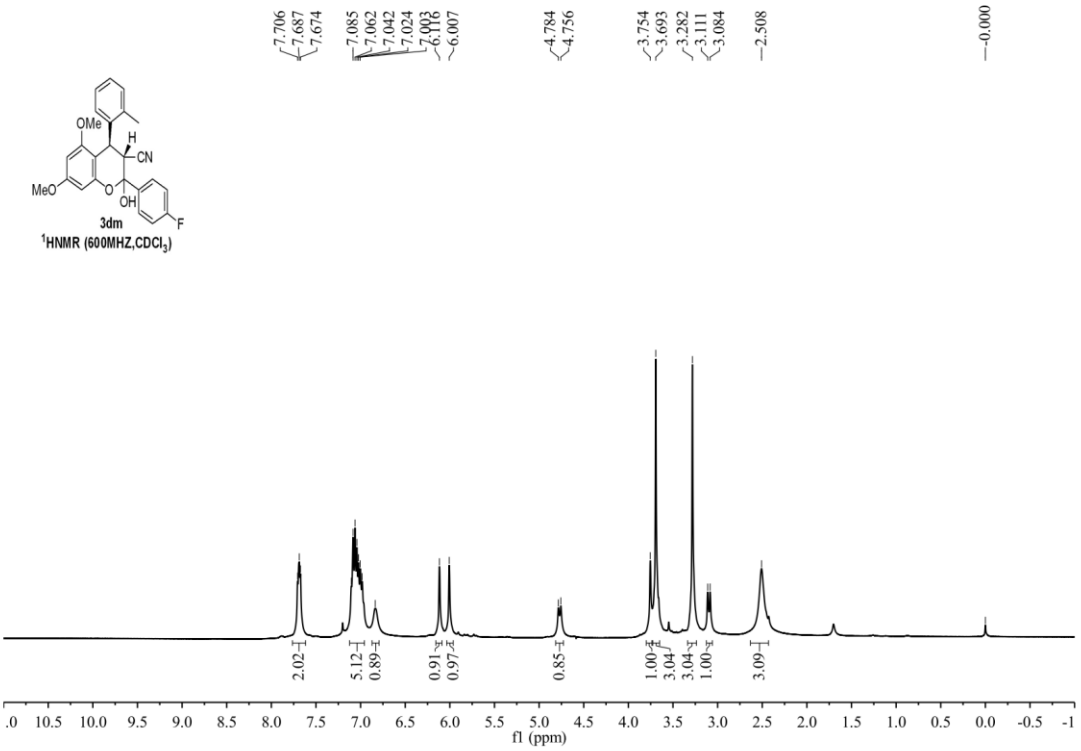
3bm
^{1}HNMR (100MHZ,$CDCl_3$)

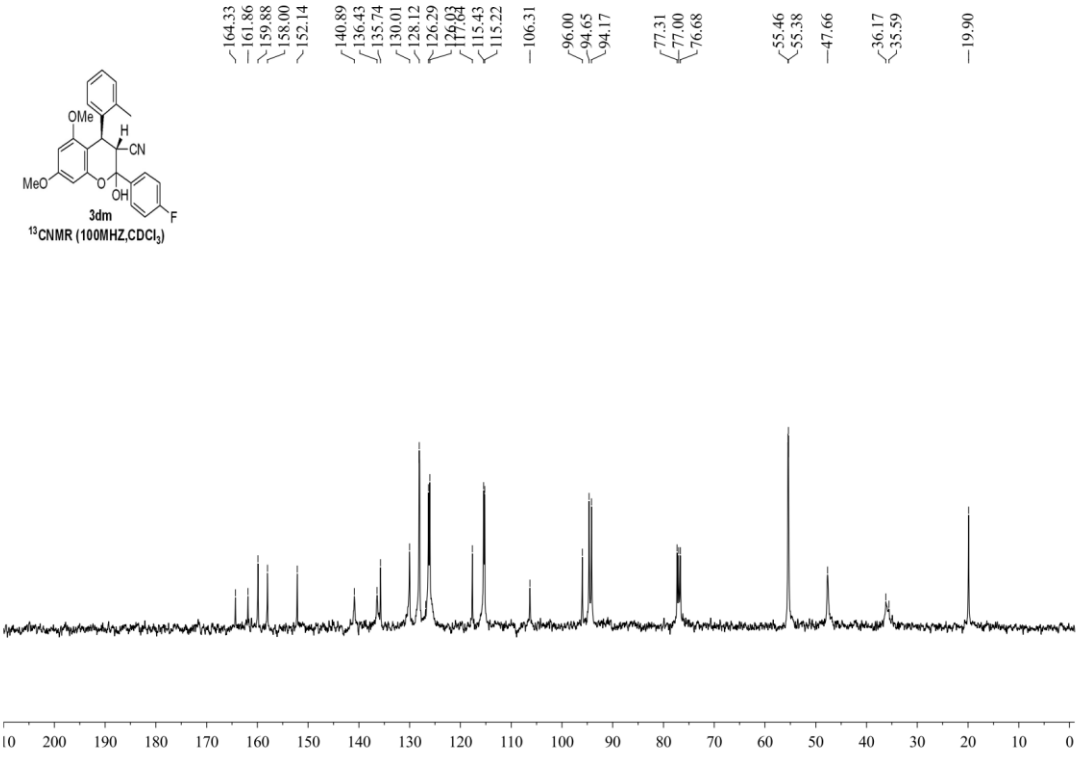


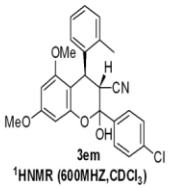
3bm
^{13}CNMR (100MHZ,$CDCl_3$)


7.606
7.586
7.218
7.198
7.104
7.086
7.037
7.020
7.001
6.983
6.966
6.860
6.141
6.136
6.015
6.010
4.798
4.771
3.709
3.683
3.521
3.288
3.151
3.123
2.520
2.359
OMe
H
CN
MeO
O
OH
3cm
1HNMR (400MHZ,CDCl3)
1.99
2.02
1.13
2.06
0.96
0.92
1.00
1.02
2.86
0.99
2.85
1.15
2.93
2.81
f1 (ppm)


159.87
157.98
152.36
139.38
136.82
129.94
129.05
128.72
126.16
125.95
125.70
117.80
106.38
96.30
94.57
94.07
77.28
76.96
76.64
55.41
55.34
47.60
36.01
21.29
19.91
OMe
H
CN
MeO
O
OH
3cm
13CNMR (100MHZ,CDCl3)

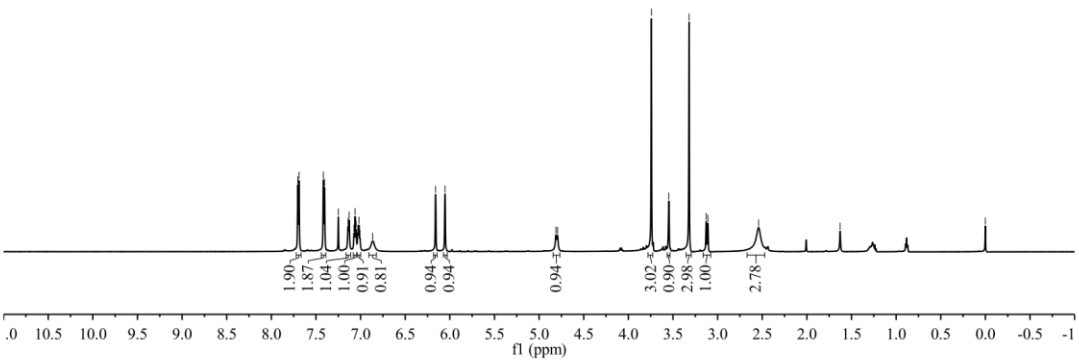

7.706
7.687
7.674
7.085
7.062
7.042
7.024
7.003
6.116
6.007
4.784
4.756
3.754
3.693
3.282
3.111
3.084
2.508
0.000
OMe
H
CN
MeO
O
OH
F
3dm
1HNMR (600MHZ,CDCl3)
2.02
5.12
0.89
0.91
0.97
0.85
1.00
3.04
3.04
1.00
3.09
f1 (ppm)

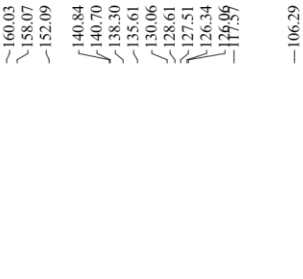

164.33
161.86
159.88
158.00
152.14
140.89
136.43
135.74
130.01
128.12
126.29
126.03
117.04
115.43
115.22
106.31
96.00
94.65
94.17
77.31
77.00
76.68
55.46
55.38
47.66
36.17
35.59
19.90
OMe
H
CN
MeO
O
OH
F
3dm
13CNMR (100MHZ,CDCl3)

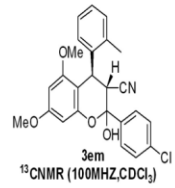


3em

^{1}HNMR (600MHZ,$CDCl_3$)

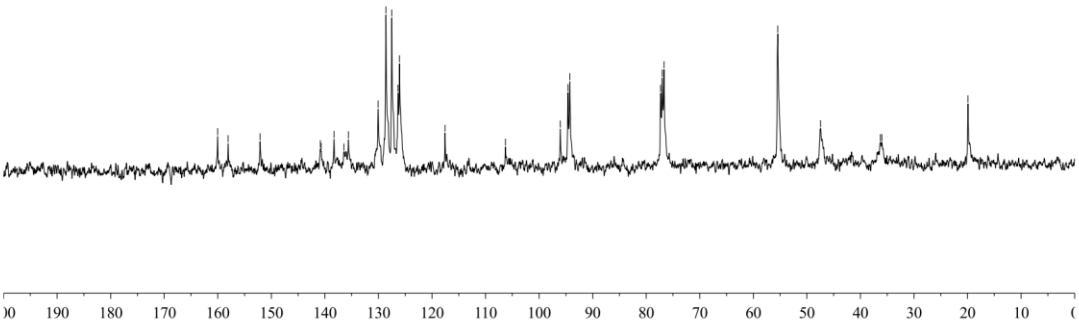


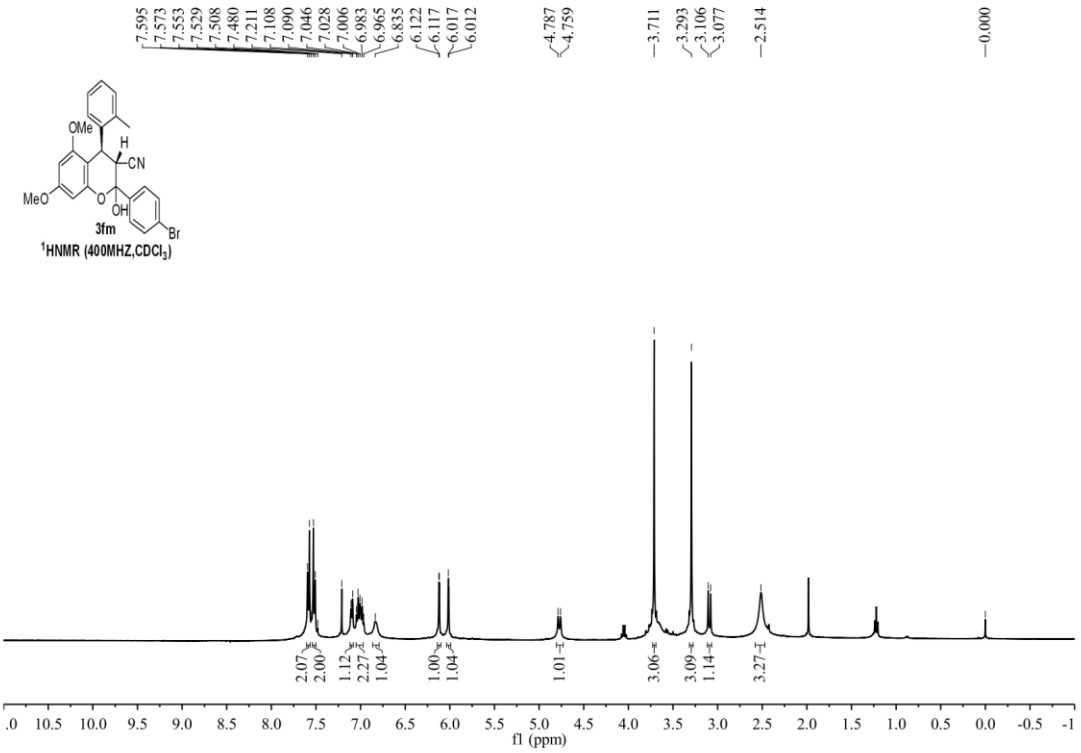


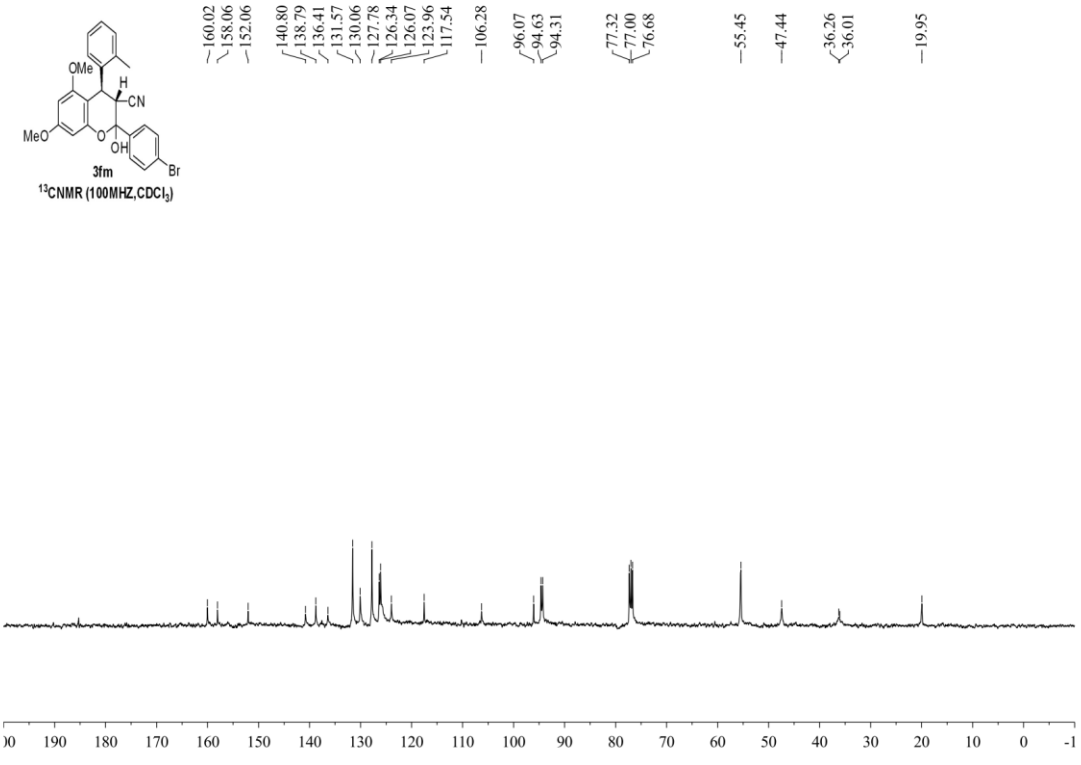


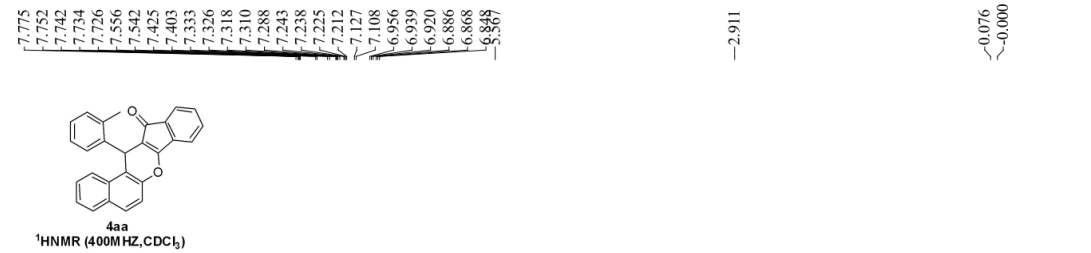
3em

^{13}CNMR (100MHZ,$CDCl_3$)

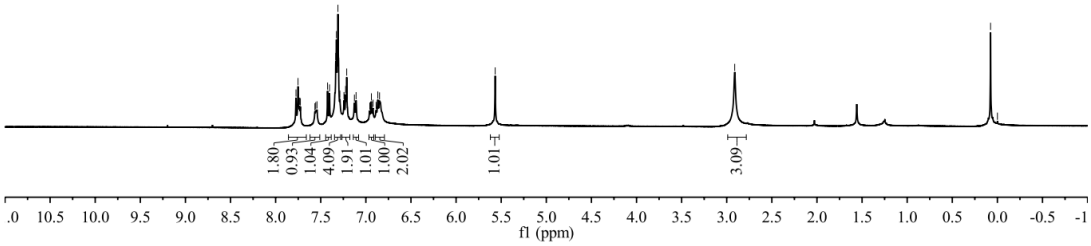


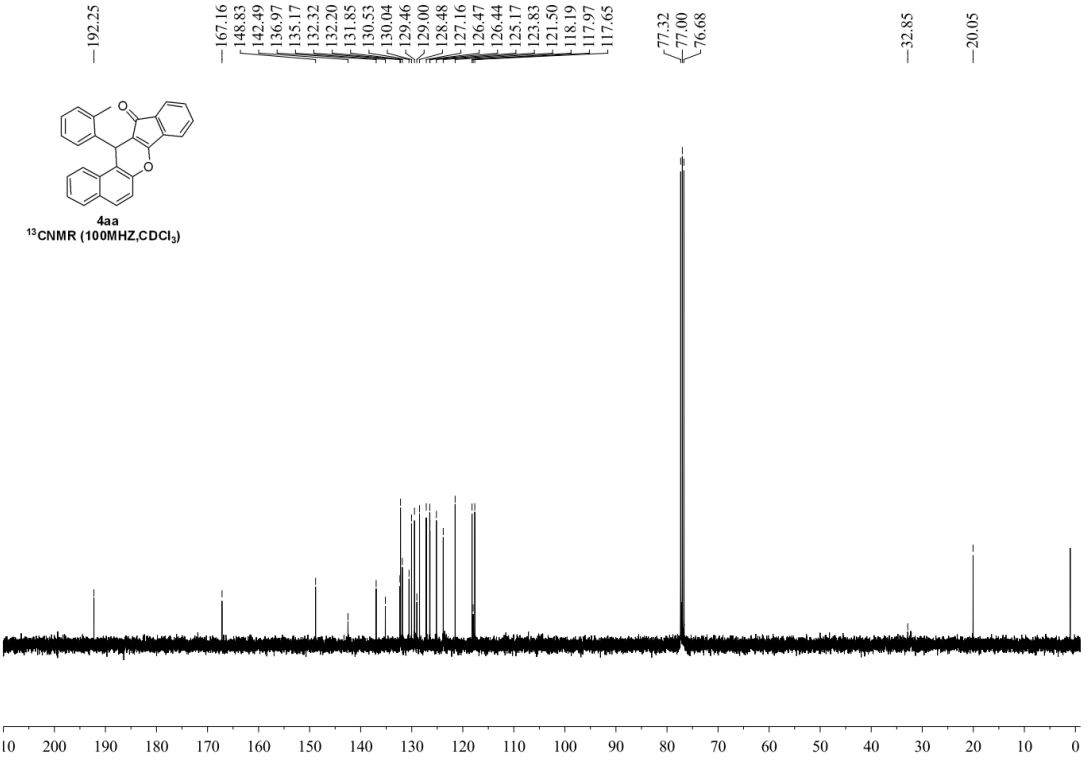

7.595
7.573
7.553
7.529
7.508
7.480
7.211
7.108
7.090
7.046
7.028
7.006
6.983
6.965
6.835
6.122
6.117
6.017
6.012
4.787
4.759
3.711
3.293
3.106
3.077
2.514
0.000
OMe
H
CN
MeO
O
OH
Br
3fm
1HNMR (400MHZ,CDCl3)
2.07
2.00
1.12
2.27
1.04
1.00
1.04
1.01
3.06
3.09
1.14
3.27
f1 (ppm)


160.02
158.06
152.06
140.80
138.79
136.41
131.57
130.06
127.78
126.34
126.07
123.96
117.54
106.28
96.07
94.63
94.31
77.32
77.00
76.68
55.45
47.44
36.26
36.01
19.95
OMe
H
CN
MeO
O
OH
Br
3fm
13CNMR (100MHZ,CDCl3)

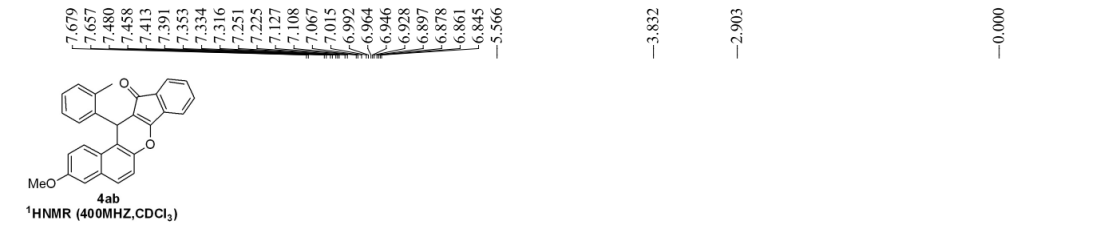


4aa
^{1}HNMR (400MHZ,CDCl$_3$)



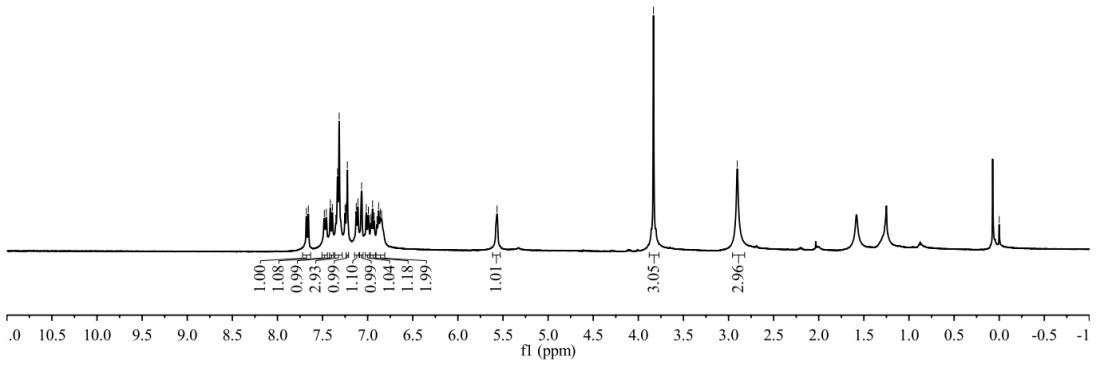


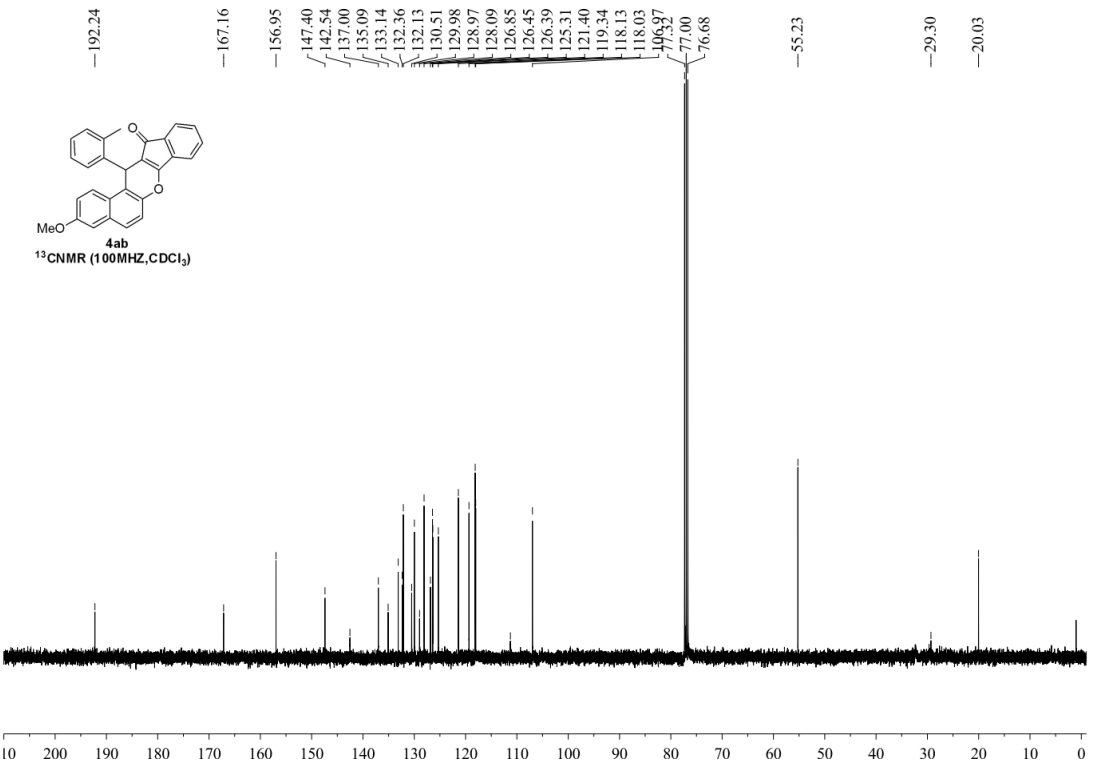
4aa
^{13}CNMR (100MHZ,CDCl$_3$)



4ab

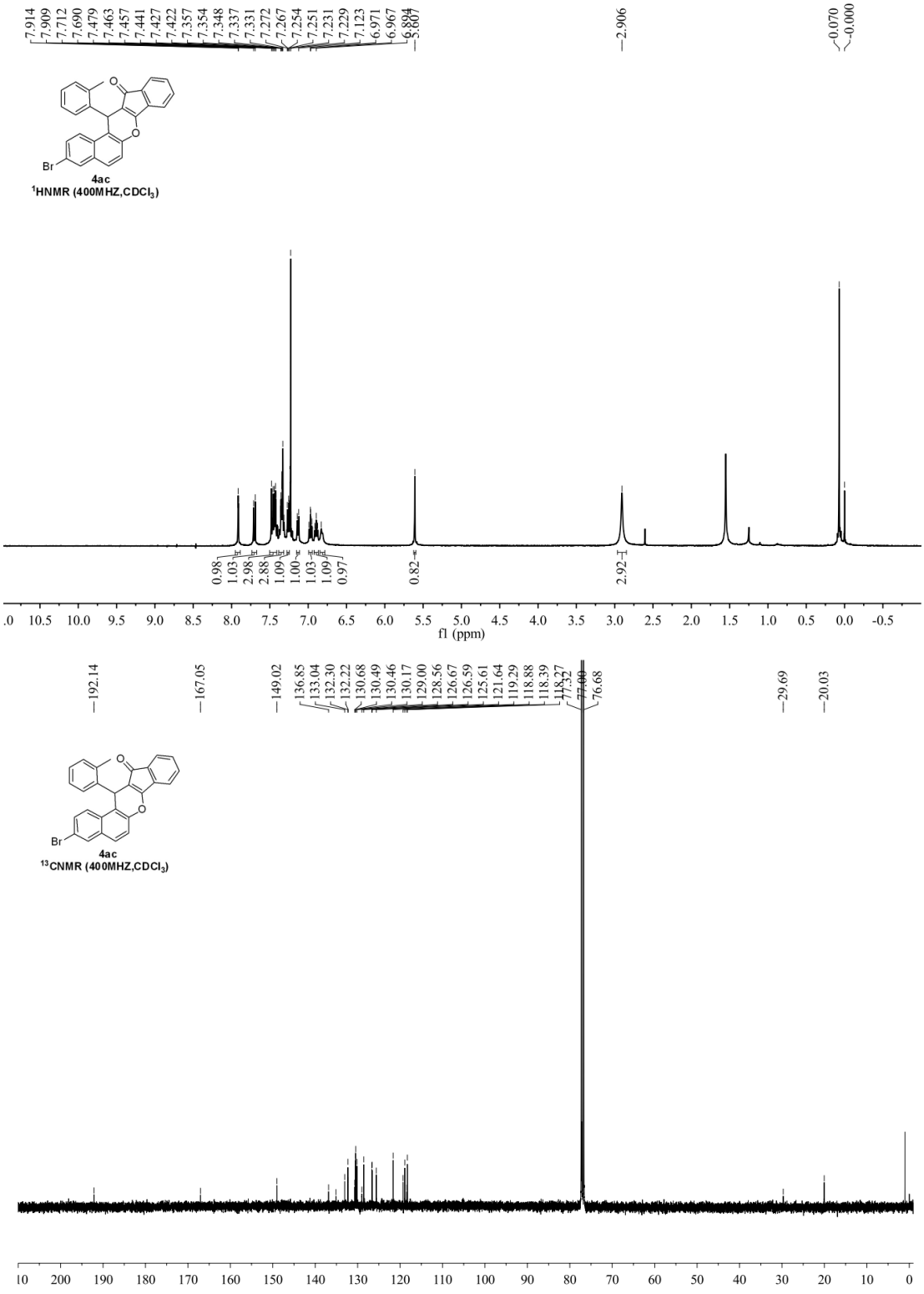
^{1}HNMR (400MHZ,CDCl$_3$)





4ab

^{13}CNMR (100MHZ,CDCl$_3$)


7.914
7.909
7.712
7.690
7.479
7.463
7.457
7.441
7.427
7.422
7.357
7.354
7.348
7.337
7.331
7.272
7.267
7.254
7.251
7.231
7.229
7.123
6.971
6.967
6.894
6.887
5.607
2.906
0.070
-0.000
Br
4ac
1HNMR (400MHZ,CDCl3)
0.98
1.03
2.98
2.88
1.09
1.00
1.03
1.09
0.97
0.82
2.92
f1 (ppm)
192.14
167.05
149.02
136.85
133.04
132.30
132.22
130.68
130.49
130.46
130.17
129.00
128.56
126.67
126.59
125.61
121.64
119.29
118.88
118.39
118.27
77.32
77.00
76.68
29.69
20.03
Br
4ac
13CNMR (400MHZ,CDCl3)