Supporting Information

Cu-catalysed synthesis of benzo[f]indole-2,4,9(3H)-triones by reaction of 2-amino-1,4-napthoquinones with α-bromocarboxylates

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[b] College of public health, Zhengzhou University, Zhengzhou 450001, China

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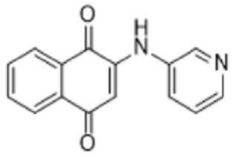
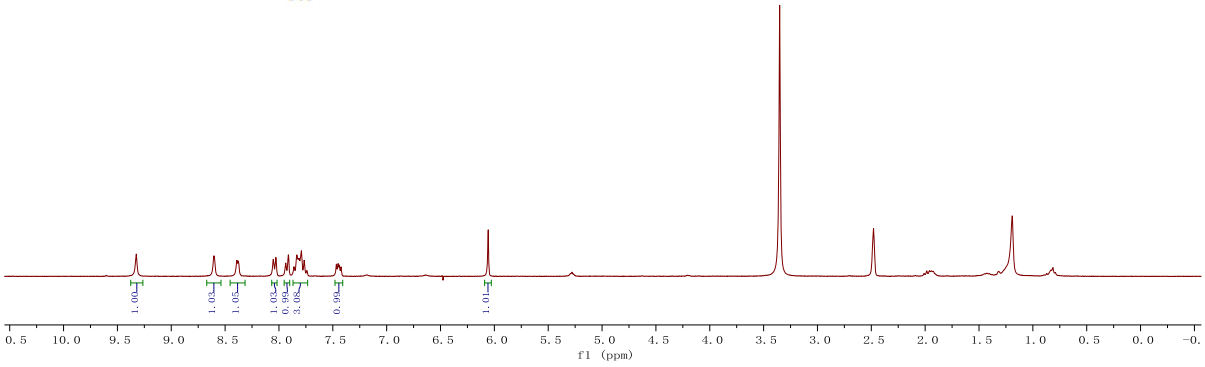
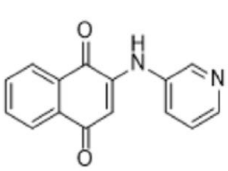
^{1}H NMR in DMSO-d_6 for **1n**



1n



^{13}C NMR in DMSO-d_6 for **1n**



1n

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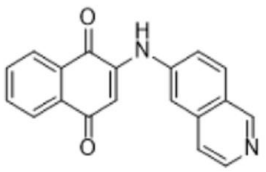

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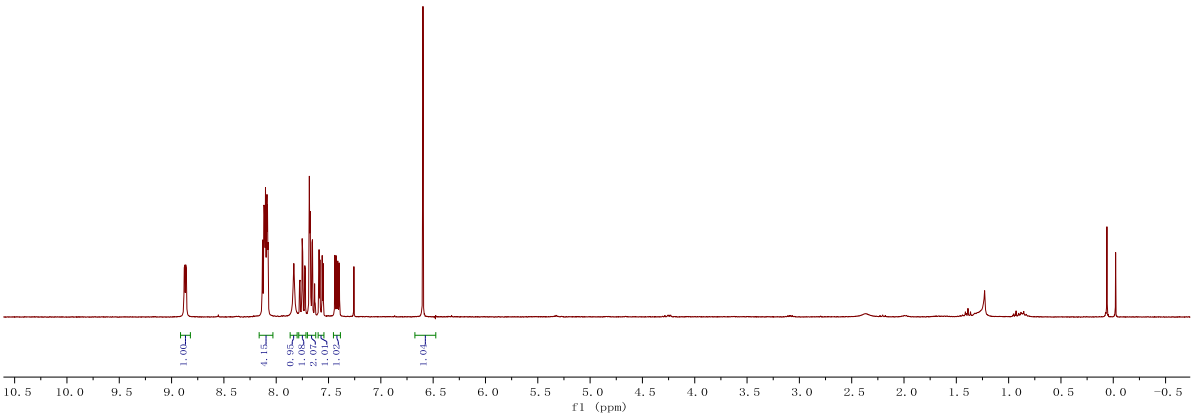

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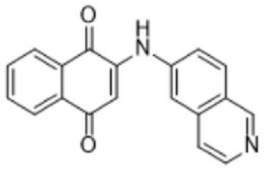
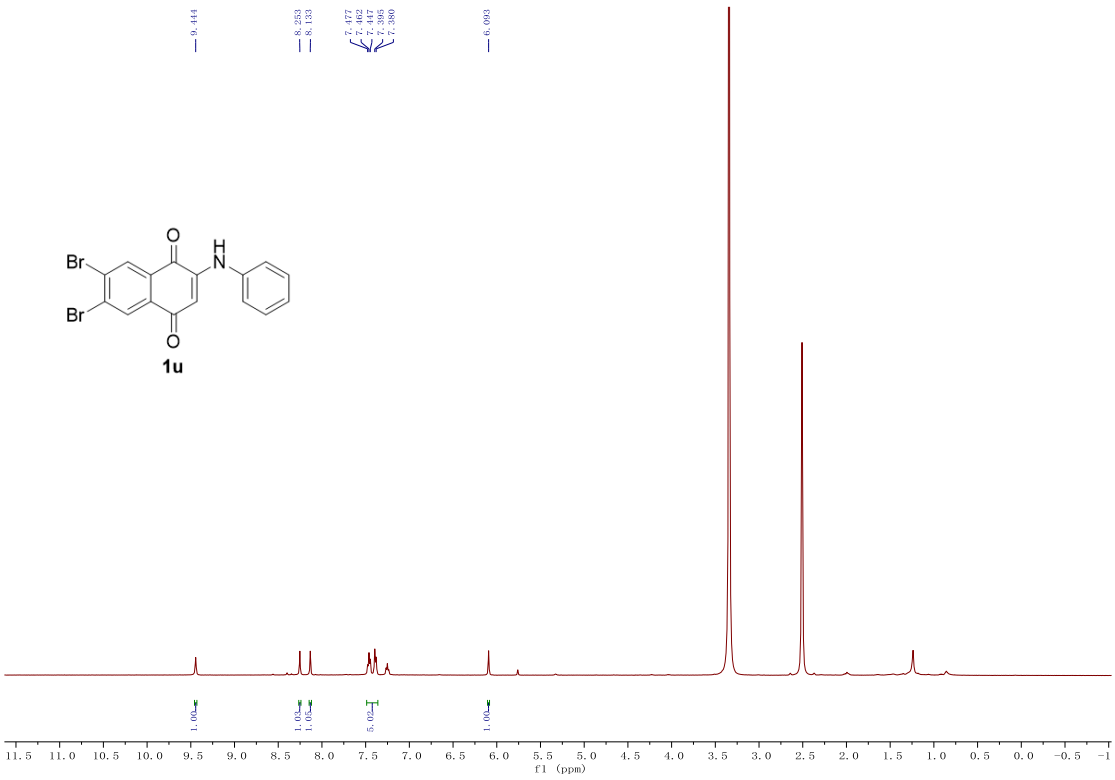
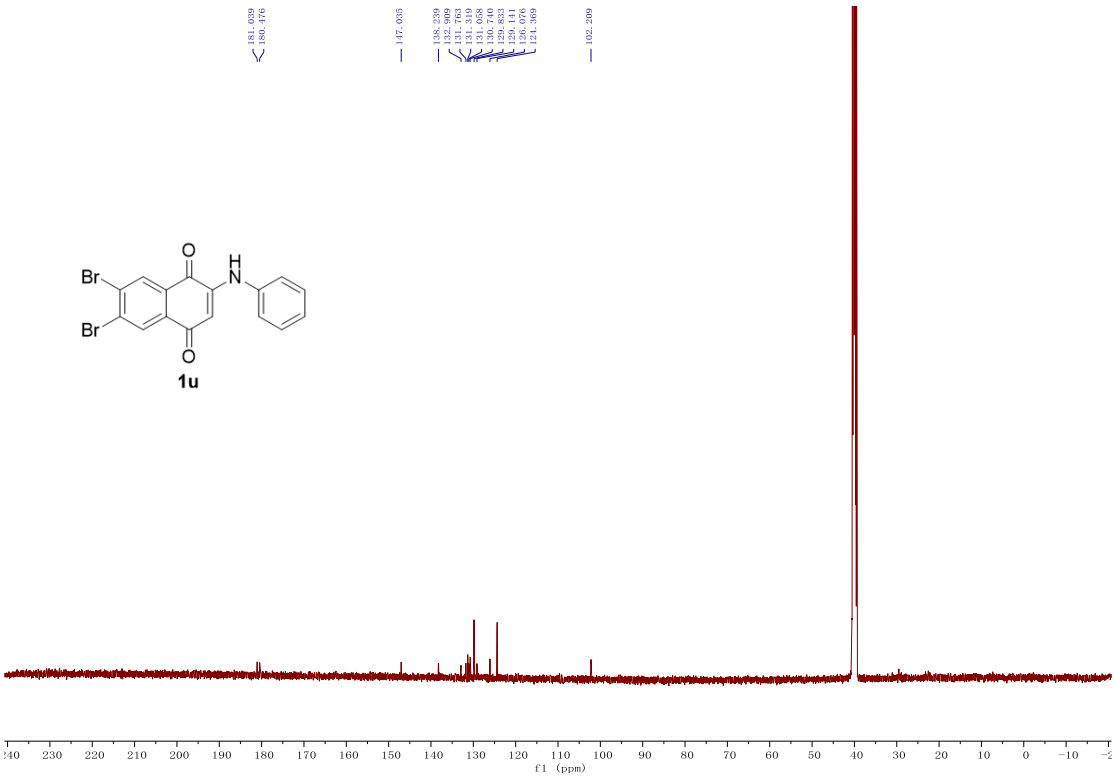


1o


9.444
8.253
8.183
7.477
7.462
7.447
7.395
7.380
6.093
1.00
1.02
1.02
5.02
1.00
f1 (ppm)

O
H
N
Br
Br
O

1u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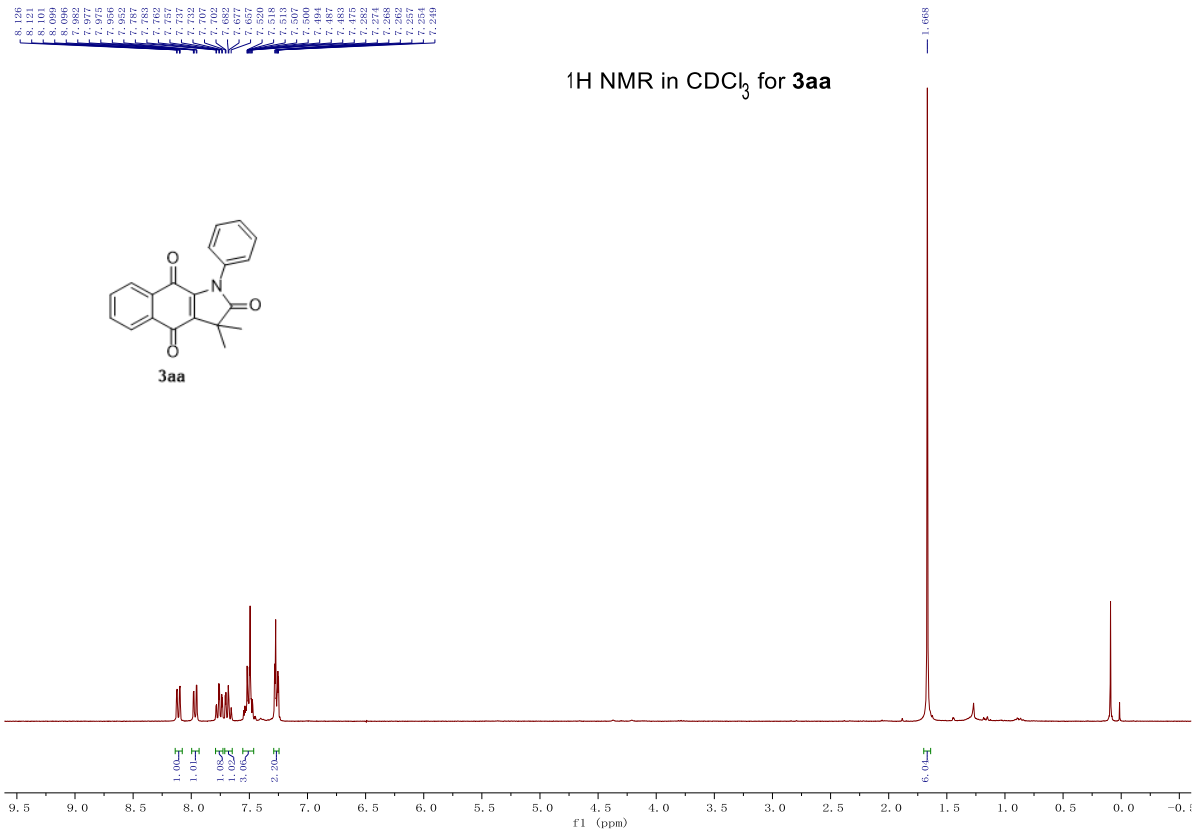
180.476
147.035
138.939
132.909
131.763
131.319
131.098
130.040
129.833
129.141
126.076
124.869
102.209
f1 (ppm)

O
H
N
Br
Br
O

1u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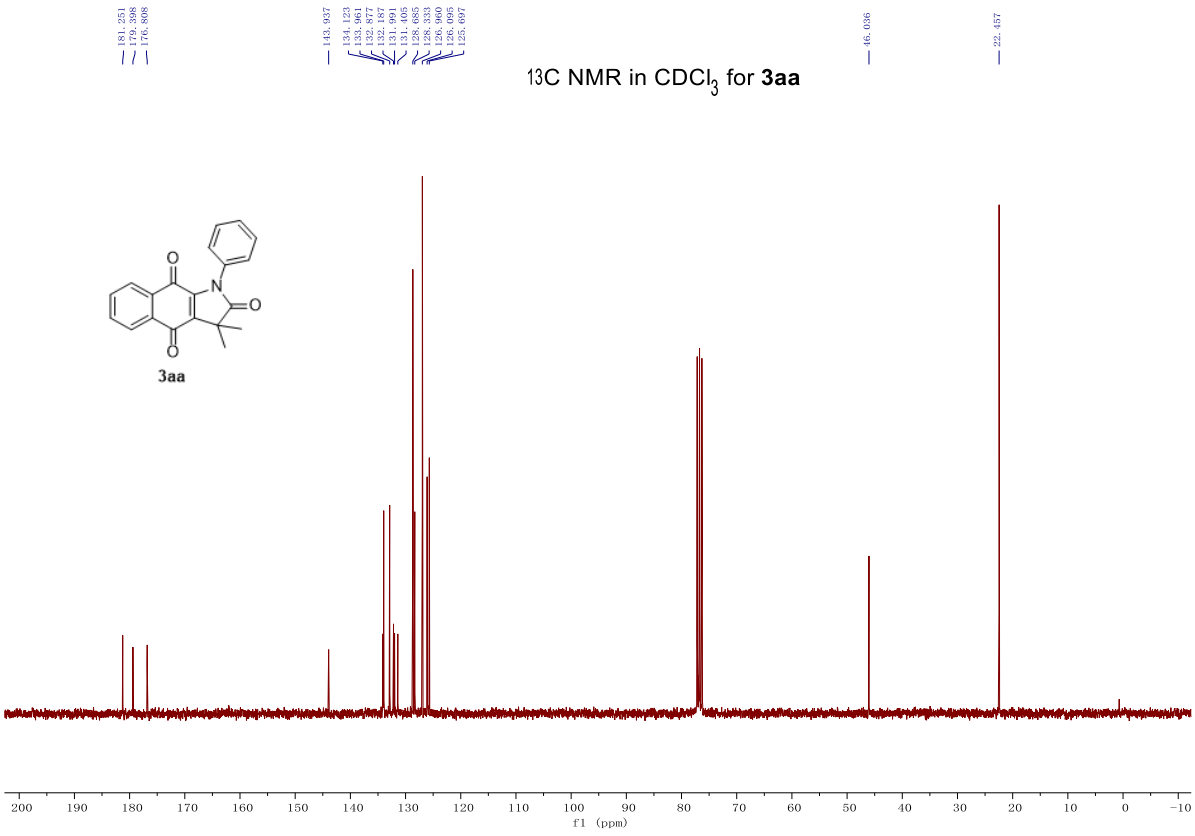
8.101
8.099
8.096
7.982
7.977
7.975
7.956
7.952
7.787
7.783
7.762
7.757
7.737
7.732
7.707
7.702
7.682
7.677
7.657
7.520
7.518
7.513
7.507
7.500
7.494
7.487
7.483
7.475
7.282
7.274
7.268
7.262
7.257
7.254
7.249
1.668
1H NMR in CDCl3 for 3aa
3aa
1.00
1.01
1.08
1.02
3.06
2.20
6.04
f1 (ppm)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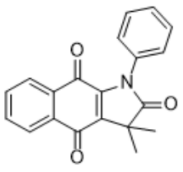
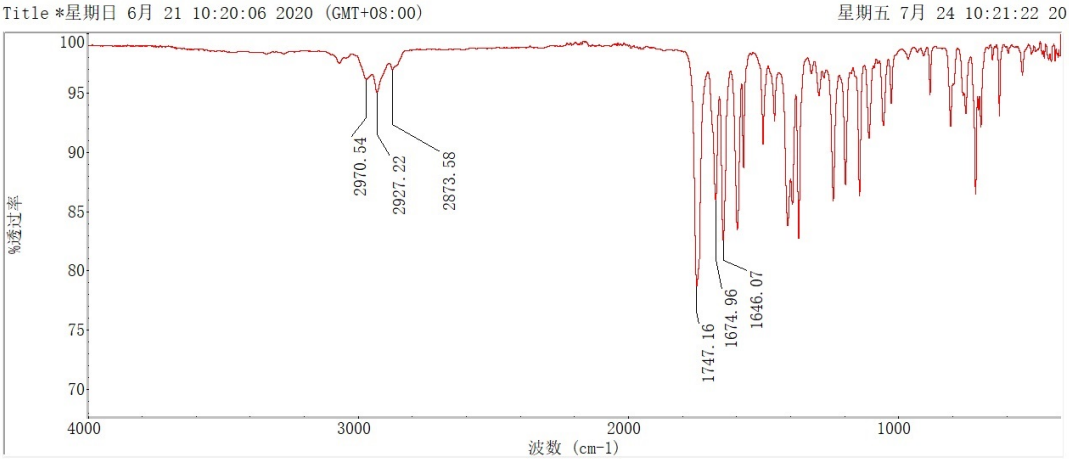
143.957
134.123
133.961
132.877
132.487
131.901
131.405
128.685
128.333
126.960
126.695
125.697
46.036
22.457
13C NMR in CDCl3 for 3aa
3aa
f1 (ppm)

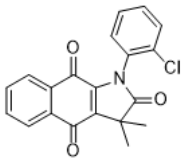


3aa

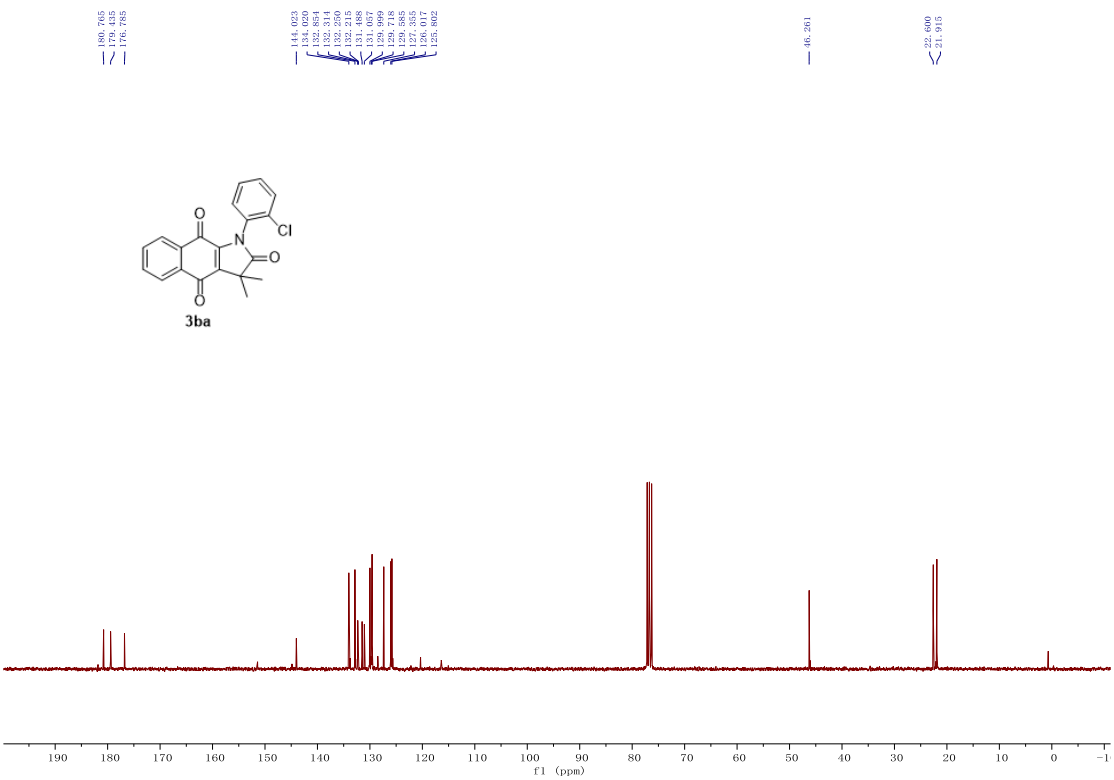
IR (KBr) spectrum of compound **3aa**

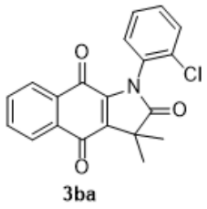


1H NMR in $CDCl_3$ for **3ba**

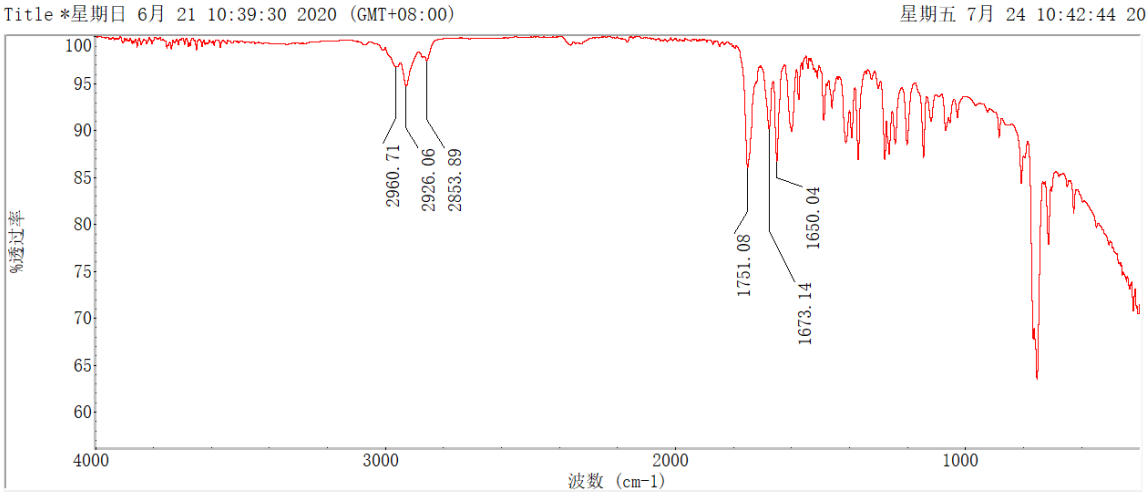


3ba





IR (KBr) spectrum of compound **3ba**



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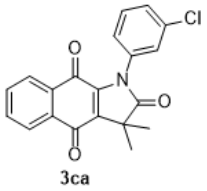
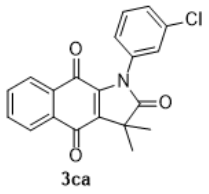
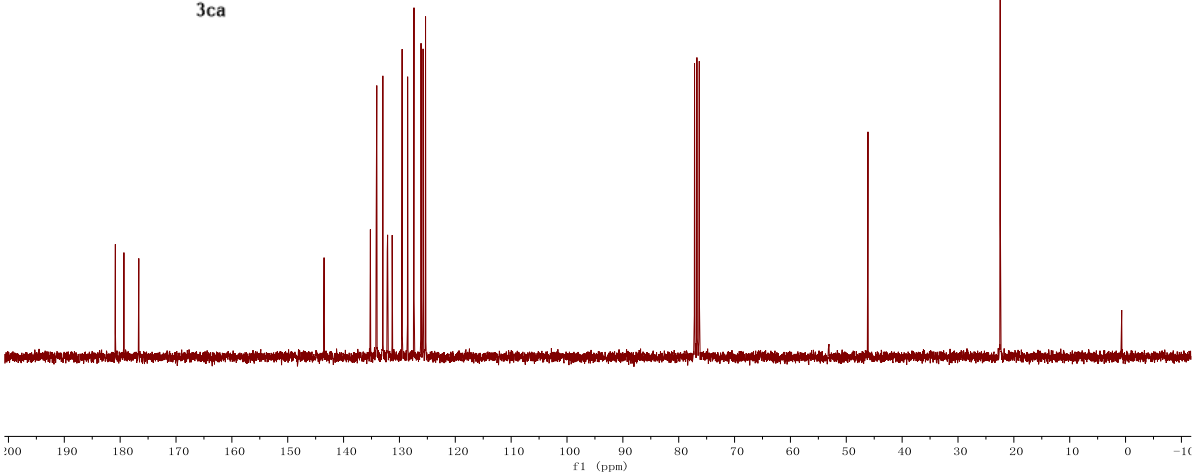


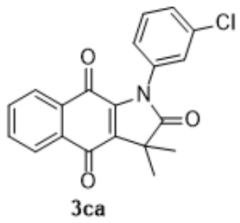
3ca

13C NMR in $CDCl_3$ for **3ca**



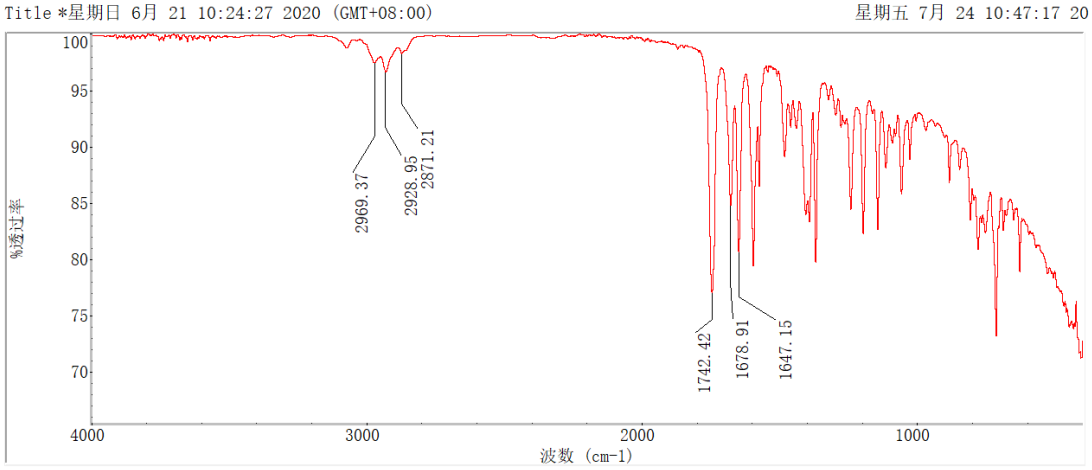
3ca





3ca

IR (KBr) spectrum for compound **3ca**



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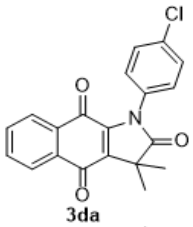
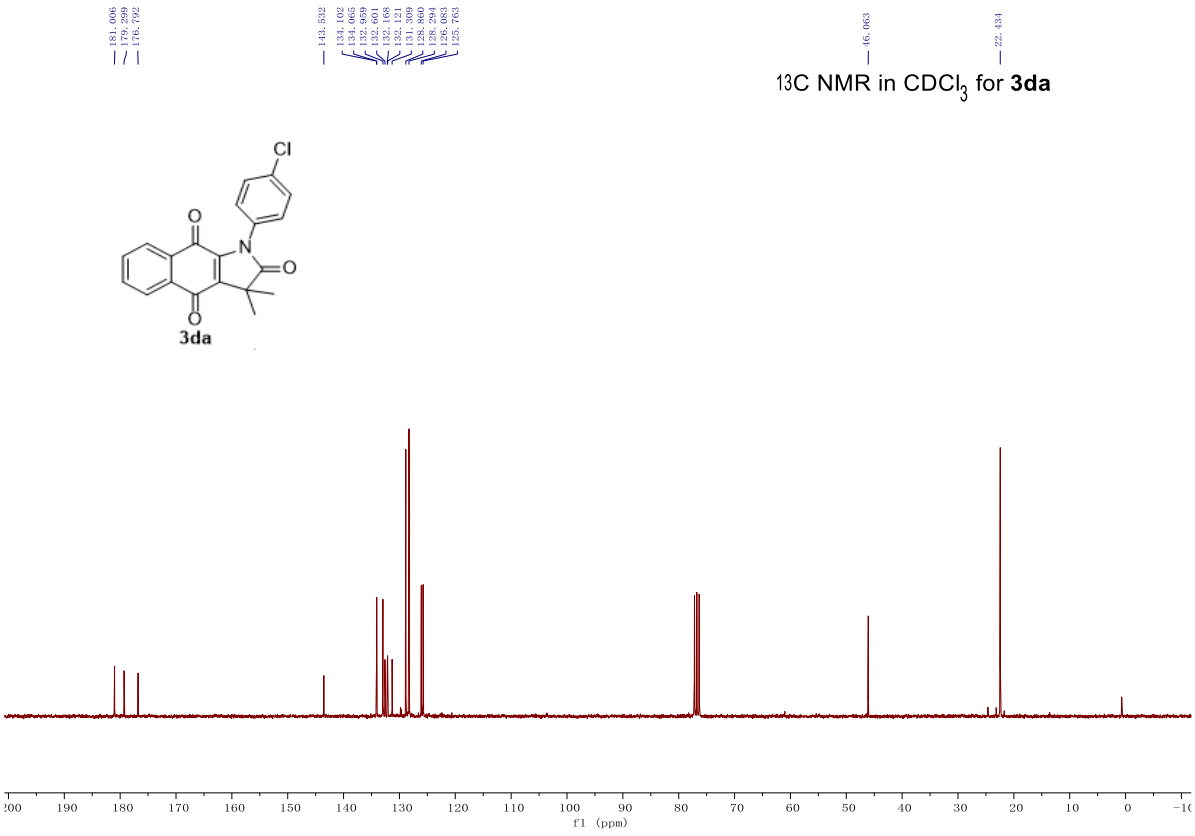


3da



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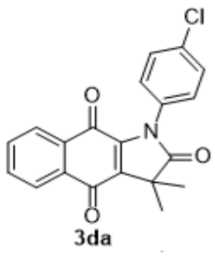
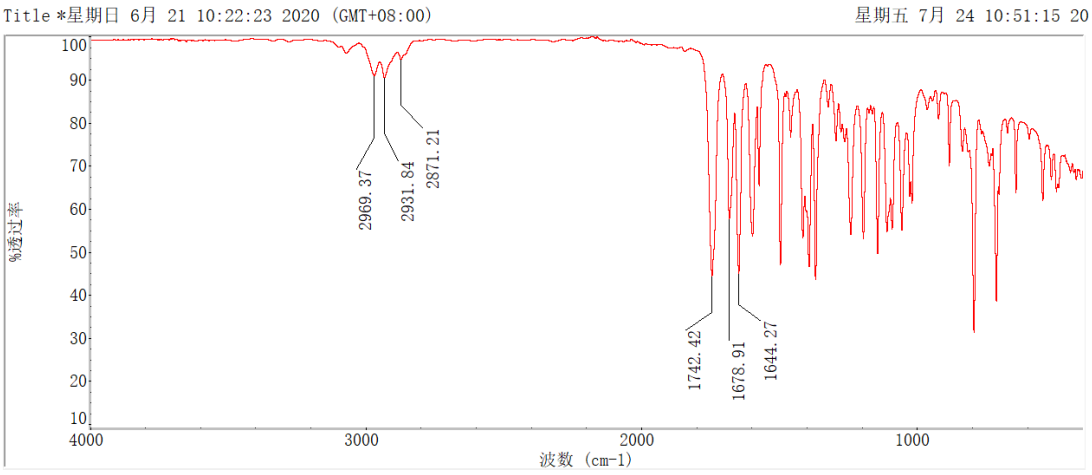


IR (KBr) spectrum for compound **3da**



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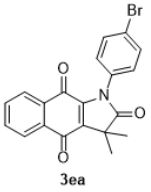
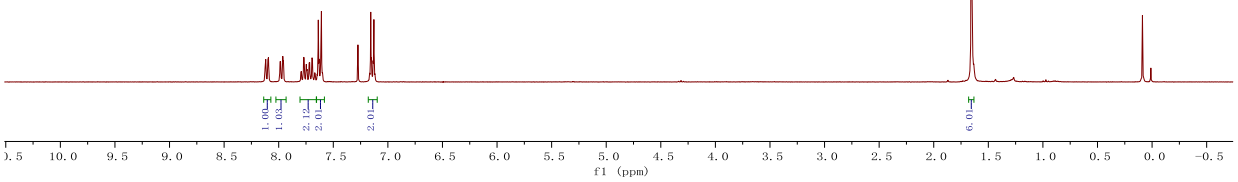
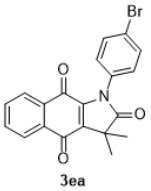


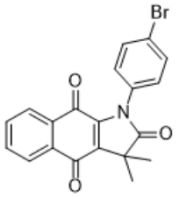
3ea



^{13}C NMR in $CDCl_3$ for **3ea**

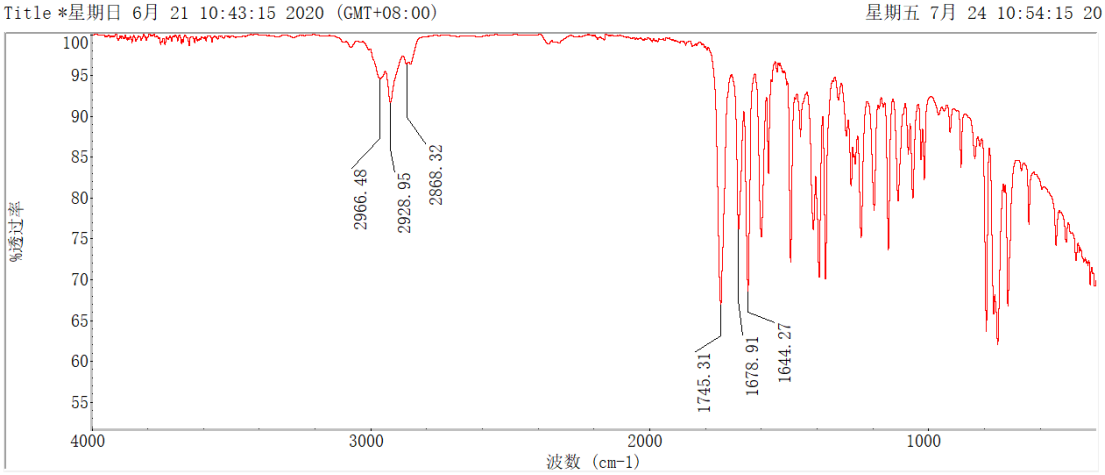


3ea



3ea

IR (KBr) spectrum for compound **3ea**



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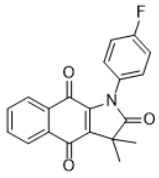
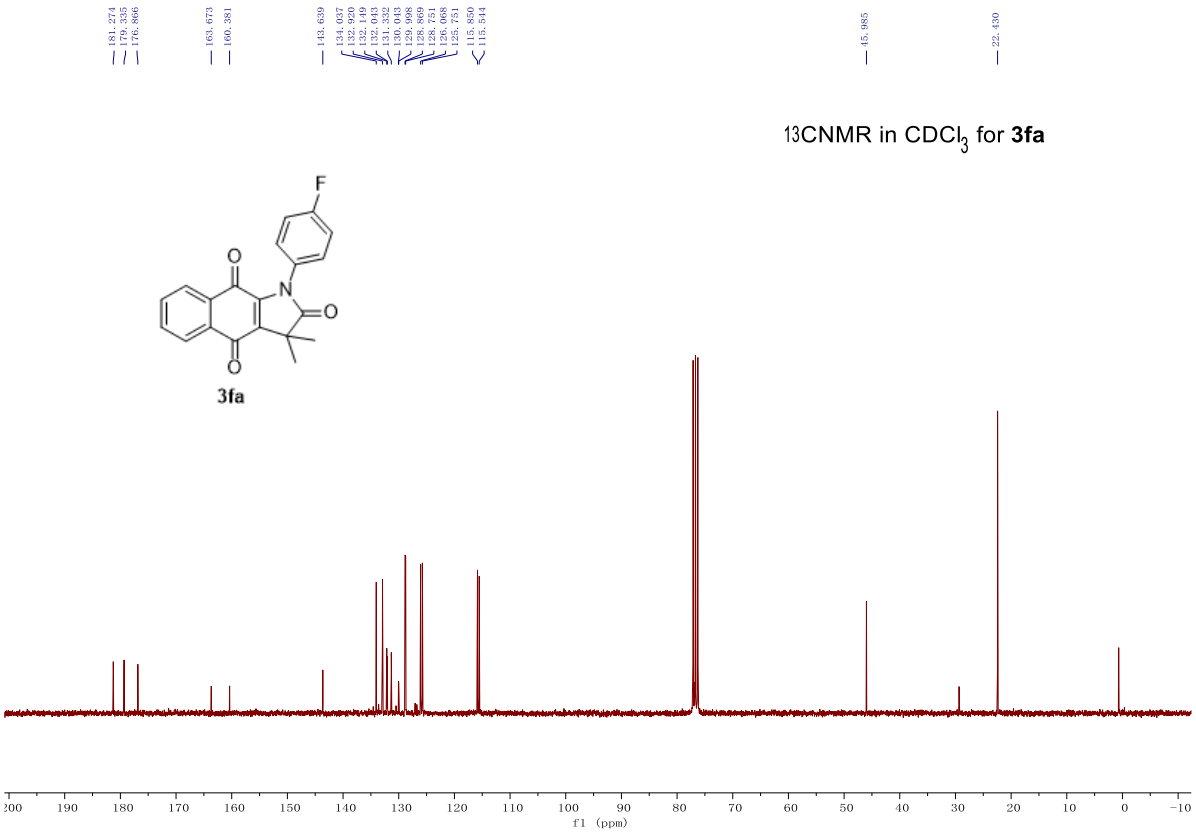
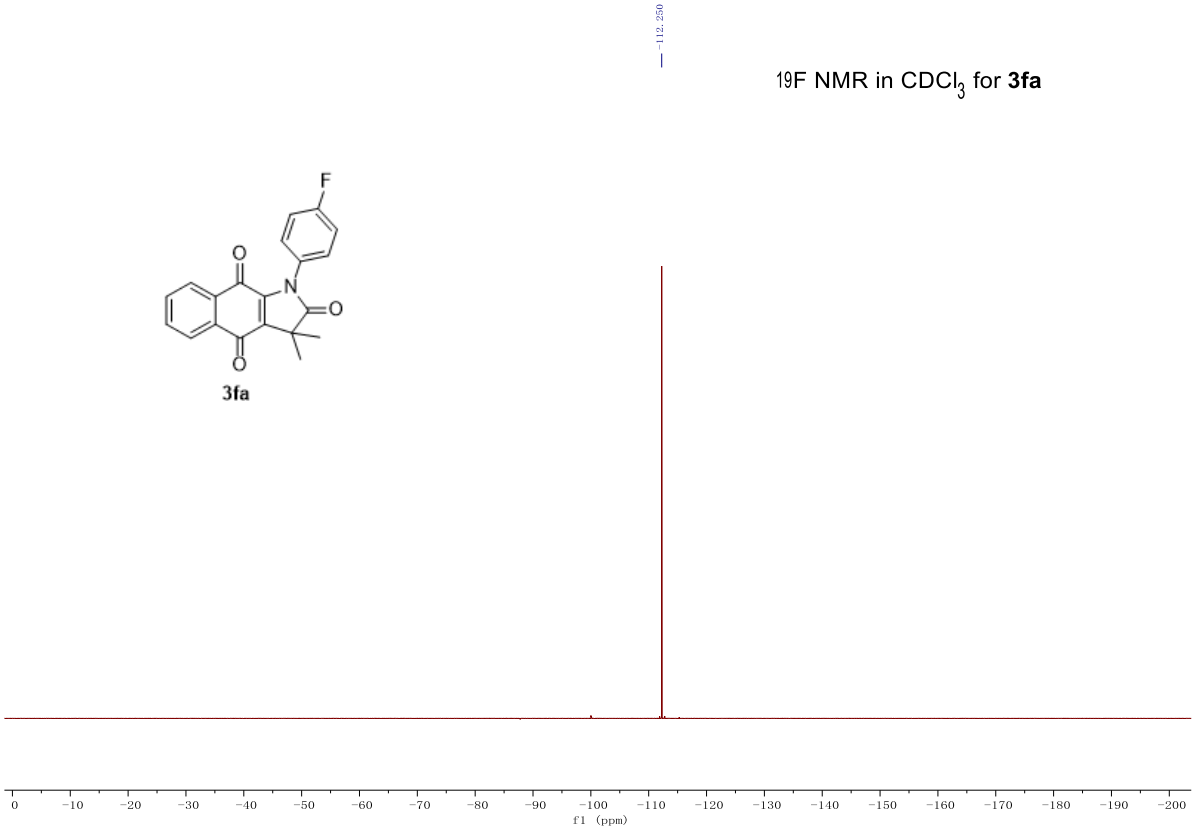


3fa



^{13}CNMR in $CDCl_3$ for **3fa**



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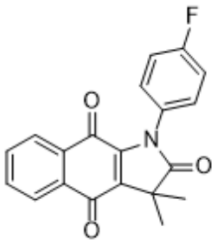
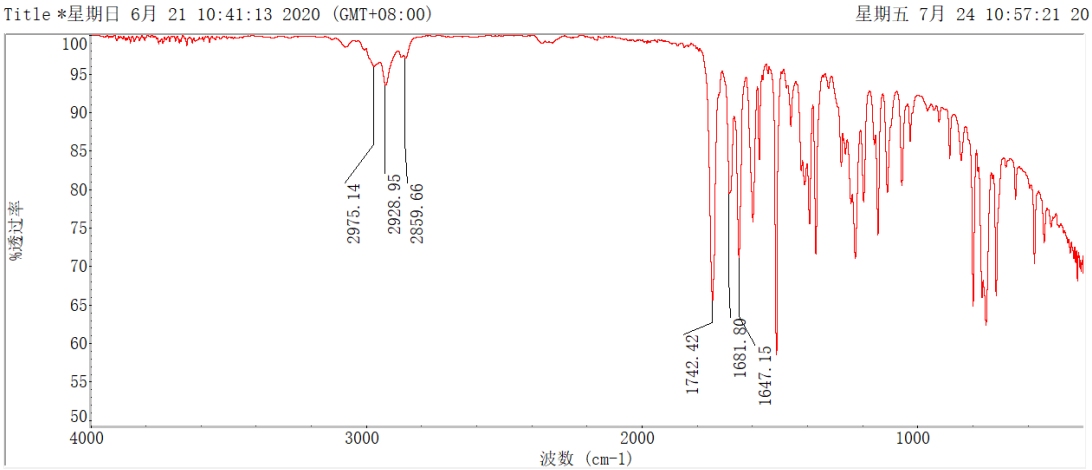
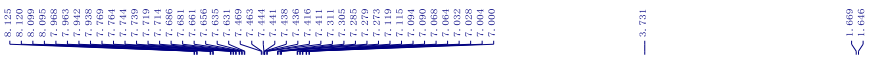


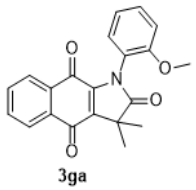
3fa

IR (KBr) spectrum for compound **3fa**



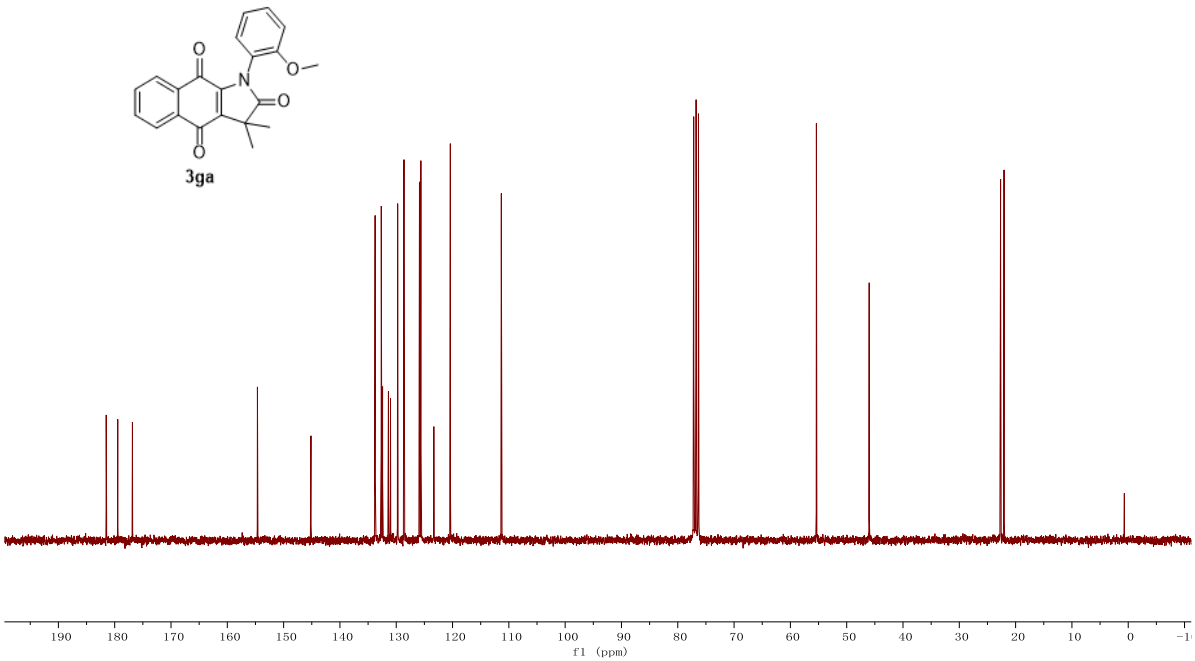


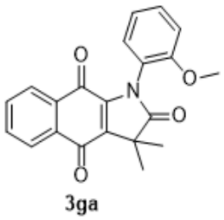
^{1}H NMR in $CDCl_3$ for **3ga**



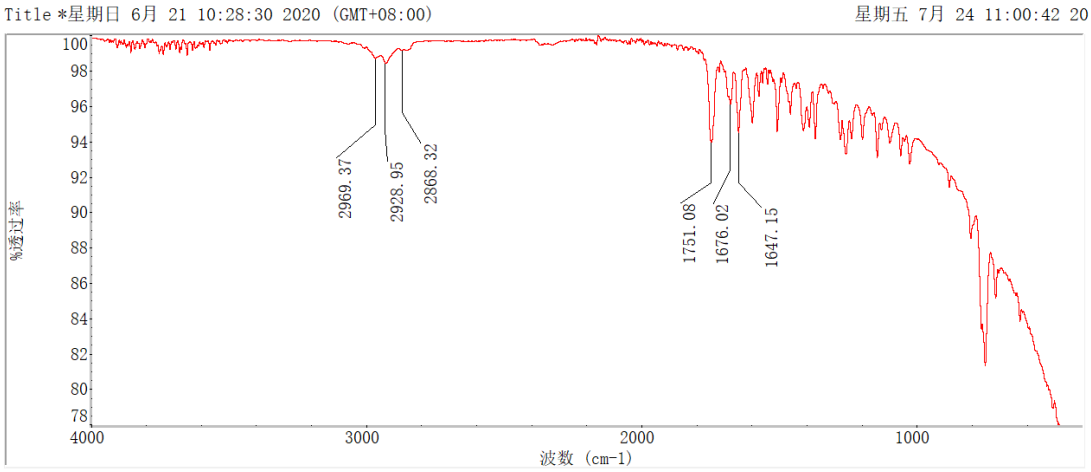
3ga

13C NMR in $CDCl_3$ for **3ga**

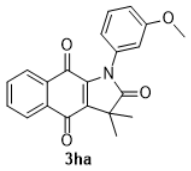




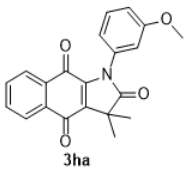
IR (KBr) spectrum for compound **3ga**

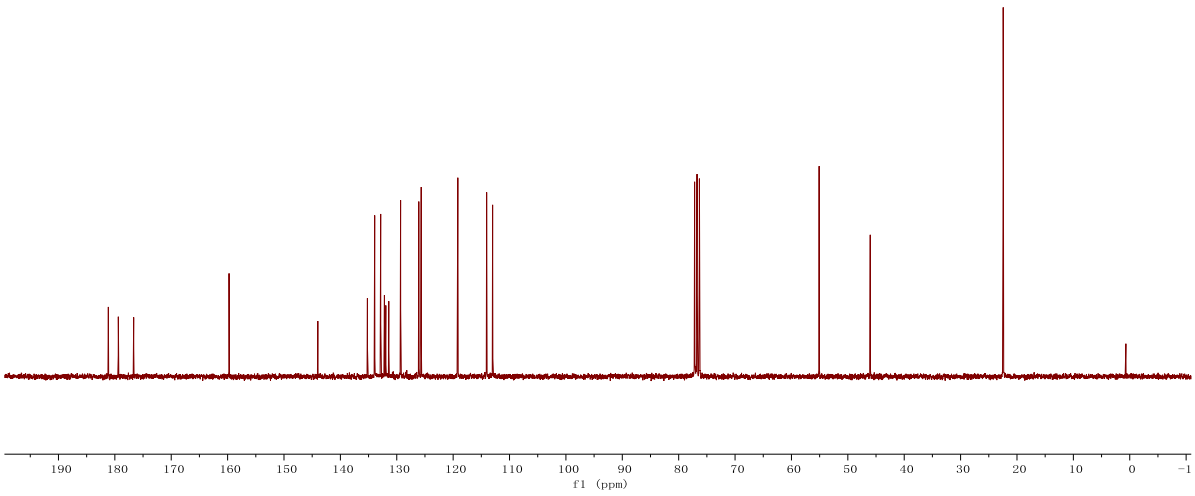


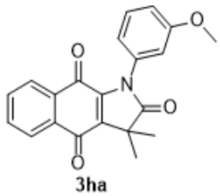
^{1}H NMR in $CDCl_3$ for **3ha**



^{13}C NMR in $CDCl_3$ for **3ha**

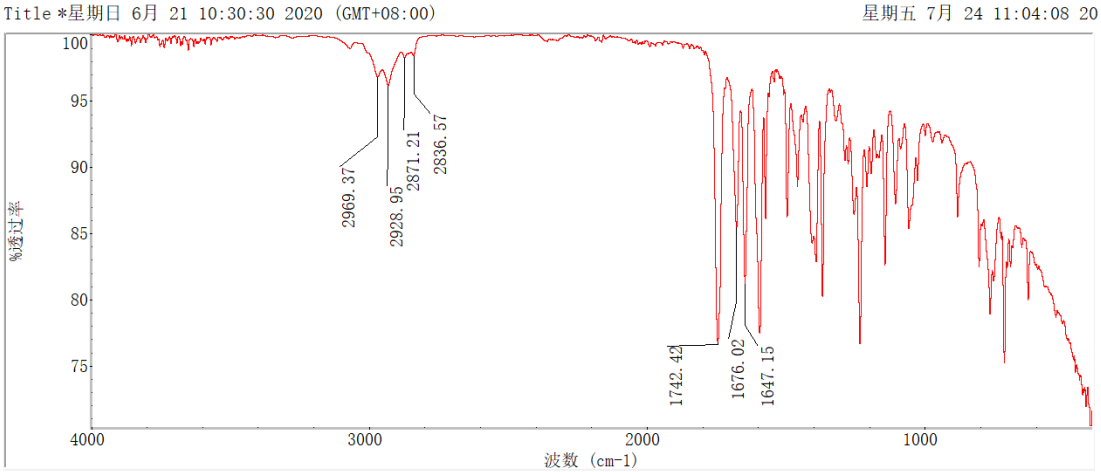




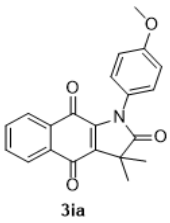


3ha

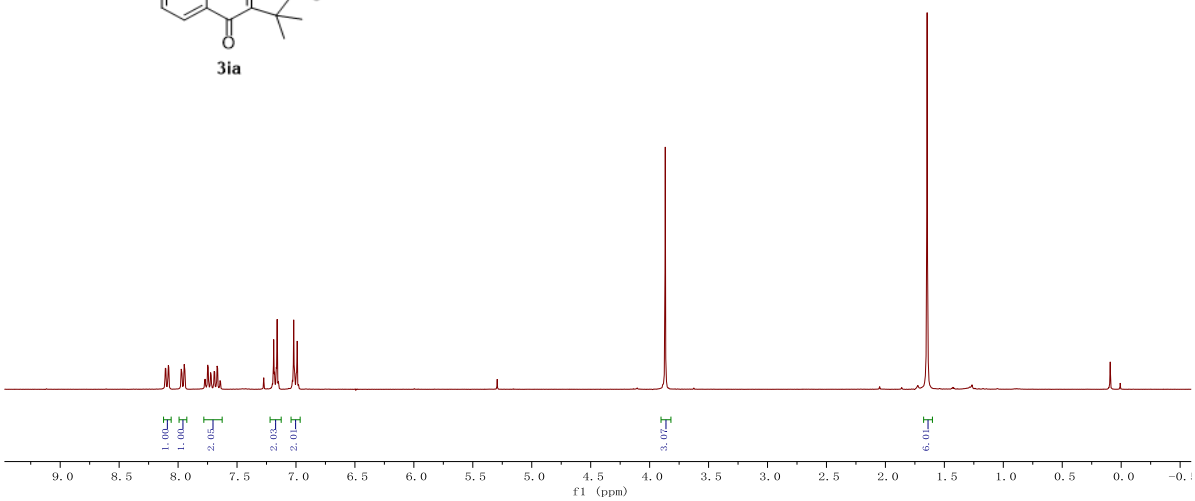
IR (KBr) spectrum for compound **3ha**

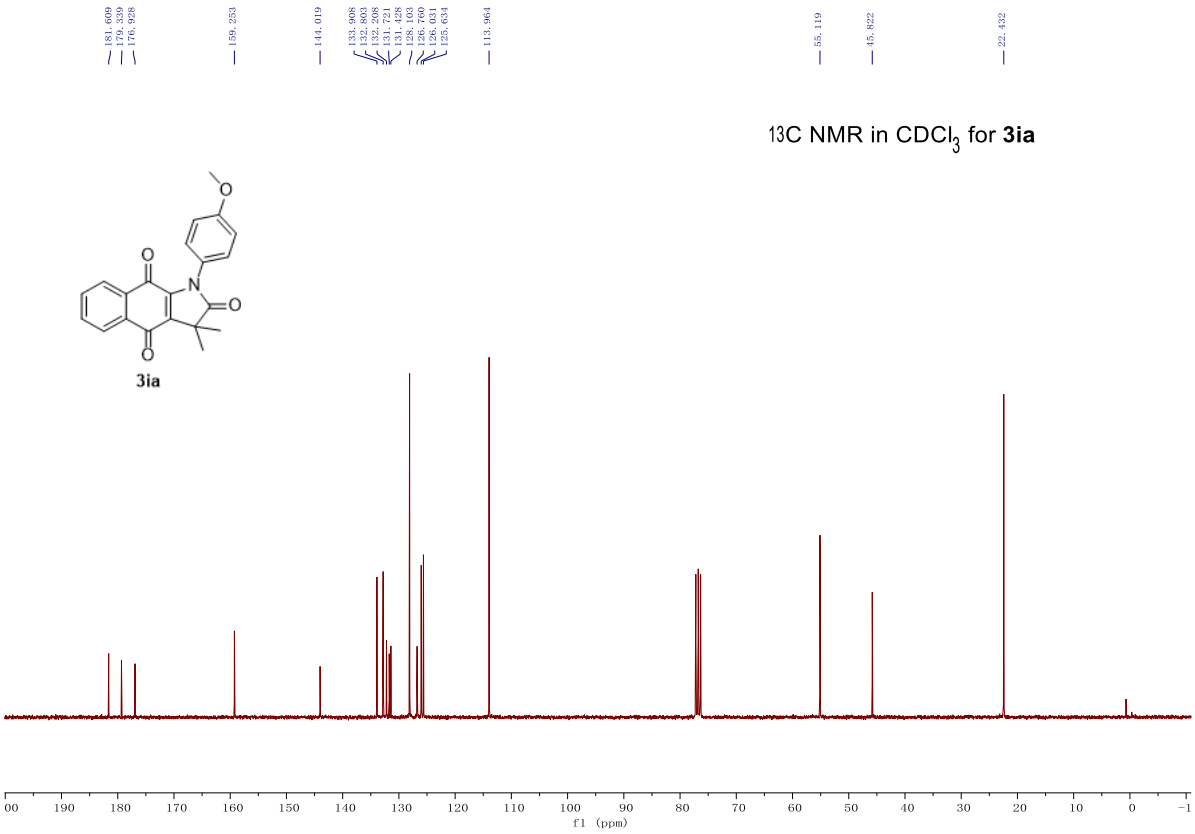


1H NMR in $CDCl_3$ for **3ia**

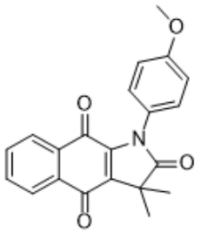


3ia



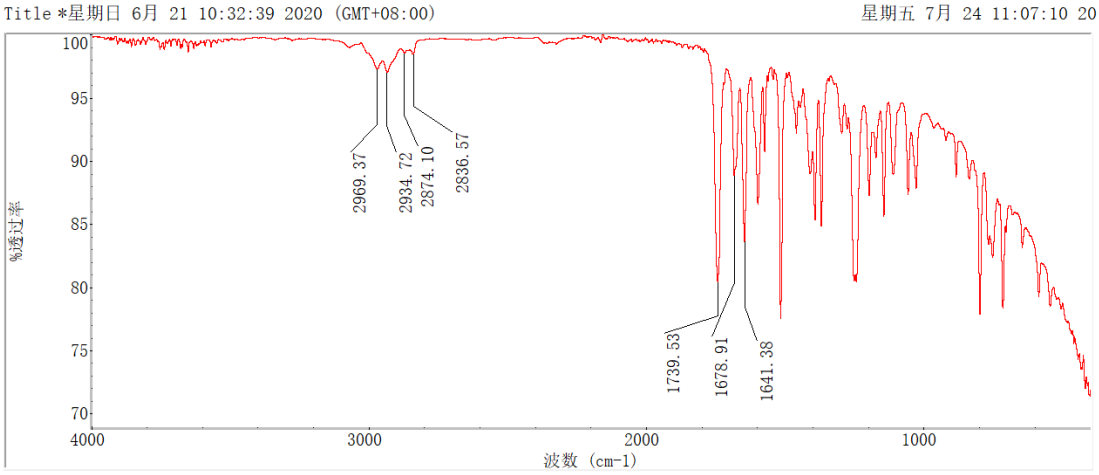


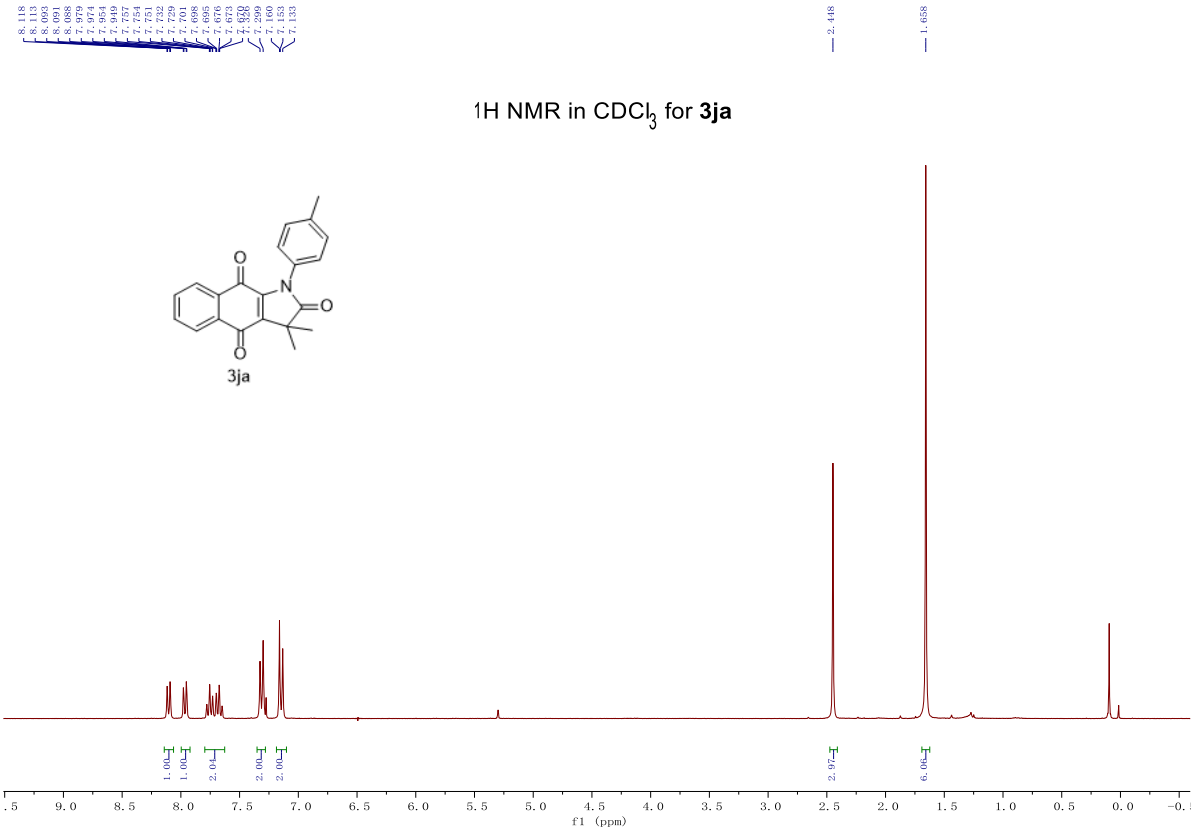
^{13}C NMR in $CDCl_3$ for **3ia**



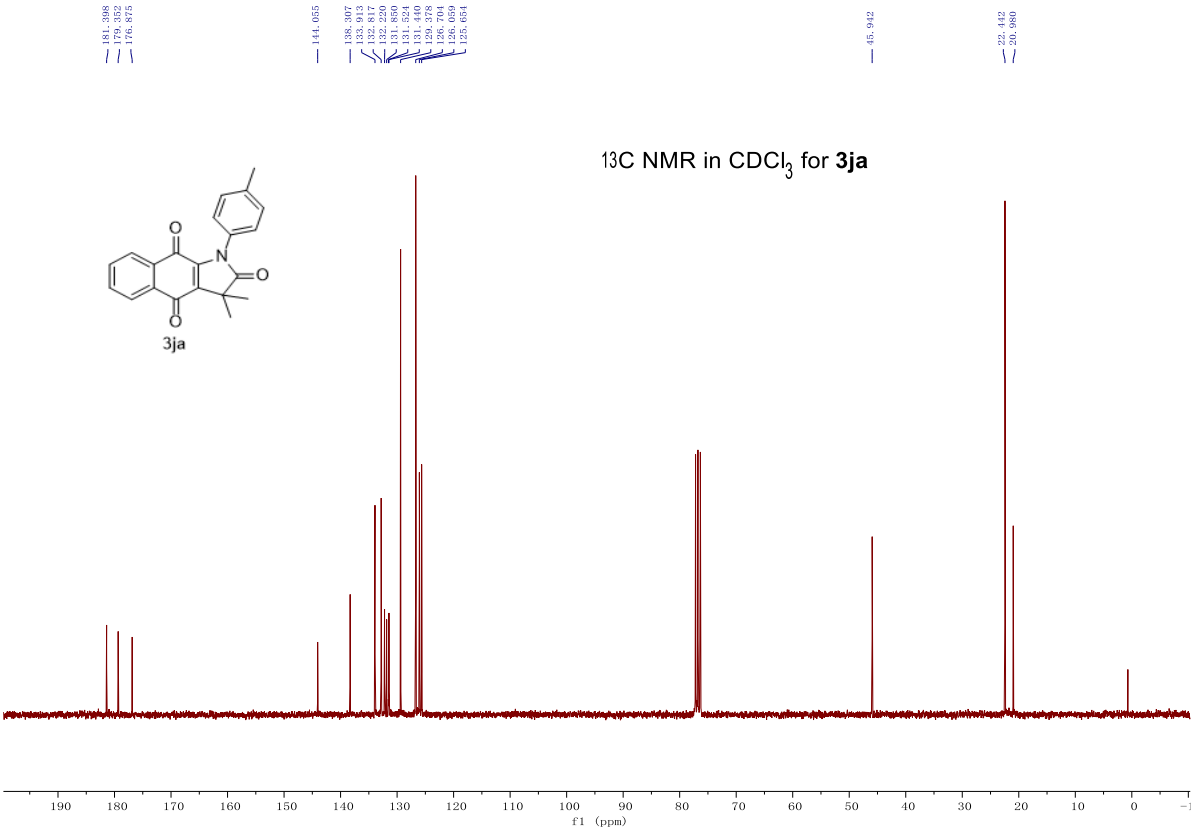
3ia

IR (KBr) spectrum for compound **3ia**

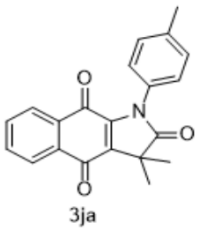




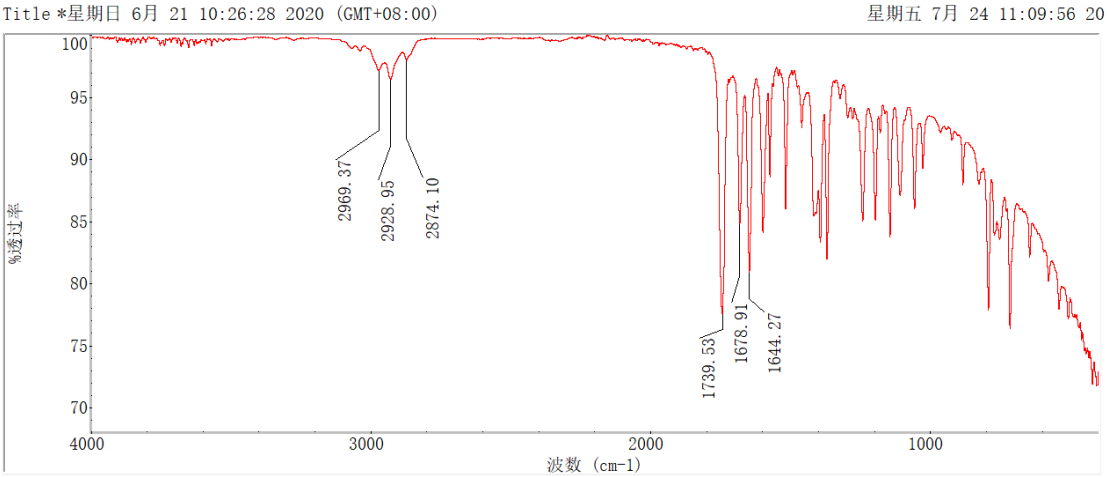
^{1}H NMR in $CDCl_3$ for **3ja**



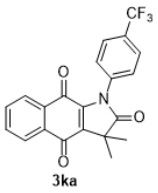
^{13}C NMR in $CDCl_3$ for **3ja**

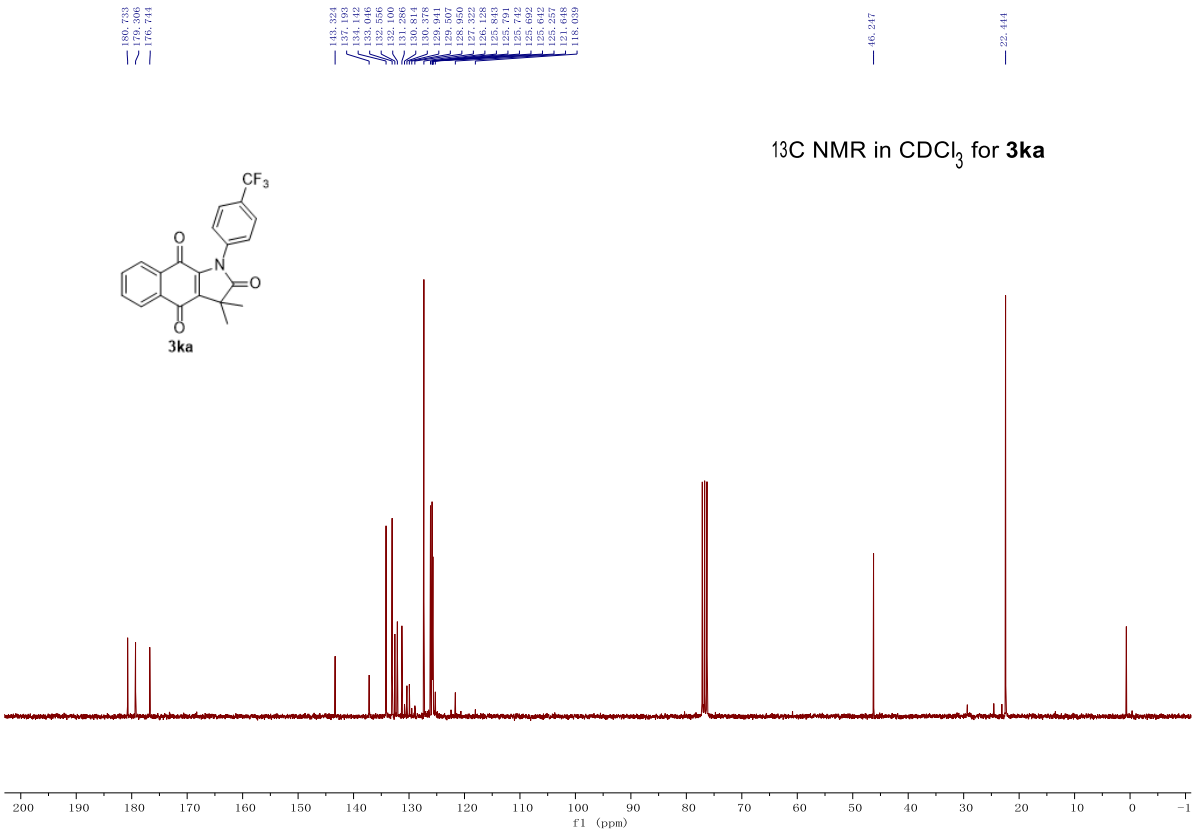


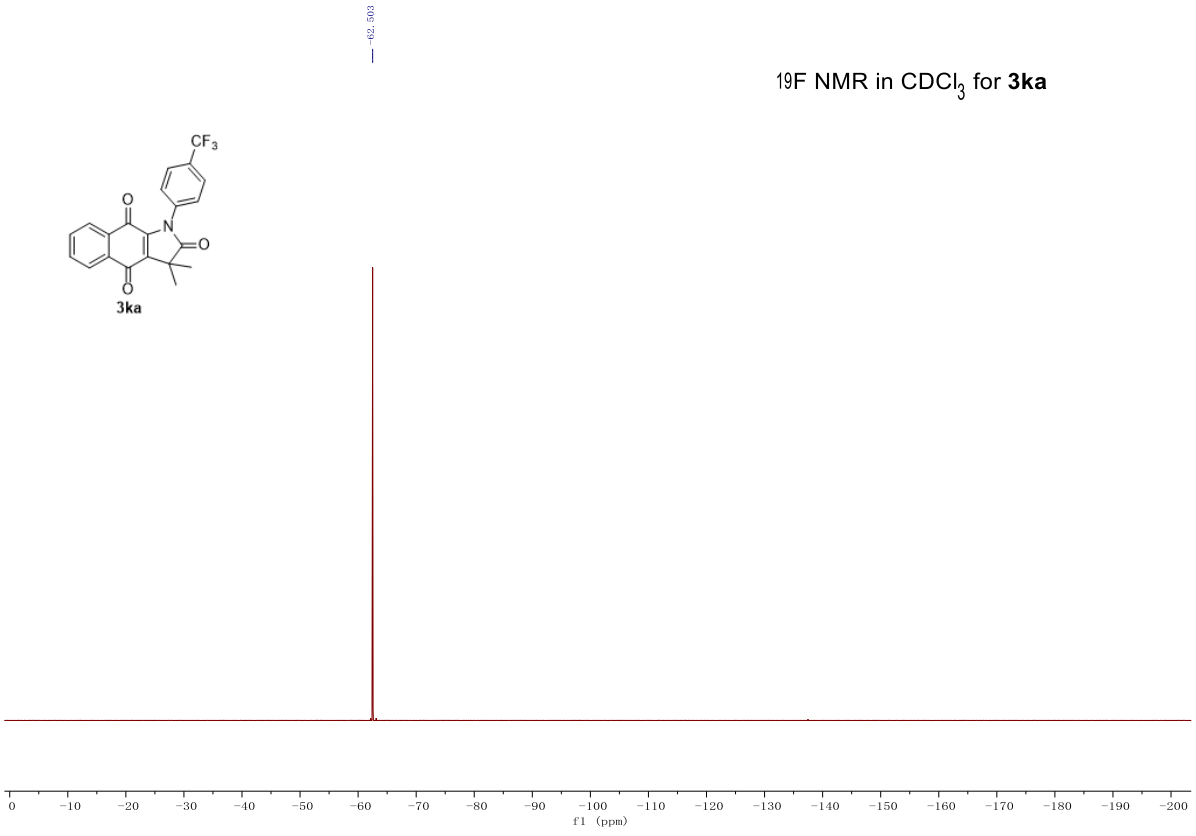
IR (KBr) spectrum for compound **3ja**

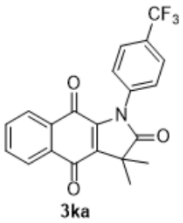


^{1}H NMR in $CDCl_3$ for **3ka**



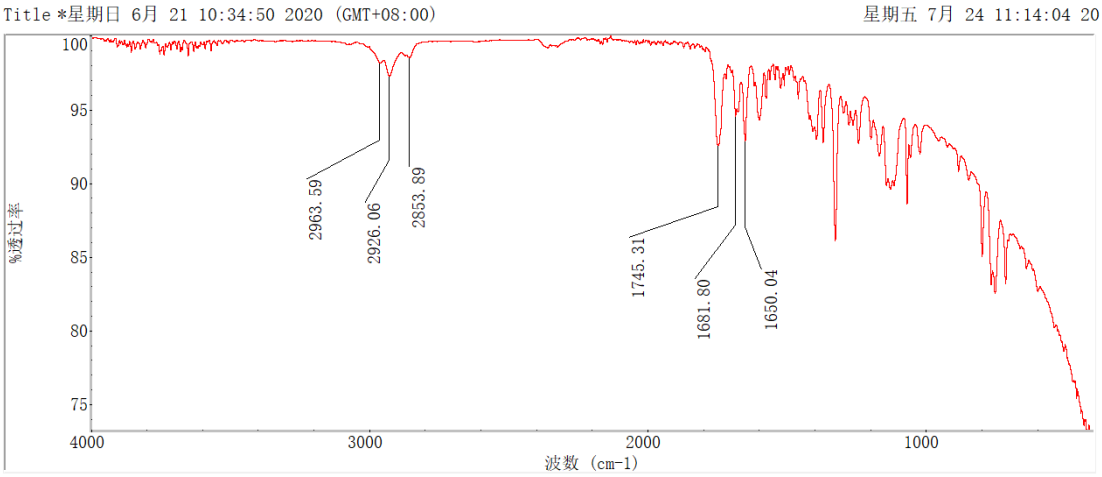

180.733
179.306
176.744
143.324
137.193
134.142
133.046
132.556
132.100
131.286
130.814
130.378
129.941
129.507
128.959
127.322
126.128
125.843
125.794
125.742
125.692
125.642
125.257
121.648
116.039
46.247
22.444
CF3
O
N
O
O
3ka
13C NMR in CDCl3 for 3ka
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−1
f1 (ppm)


−62.503
CF3
O
N
O
O
3ka
19F NMR in CDCl3 for 3ka
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
f1 (ppm)

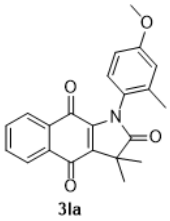


3ka

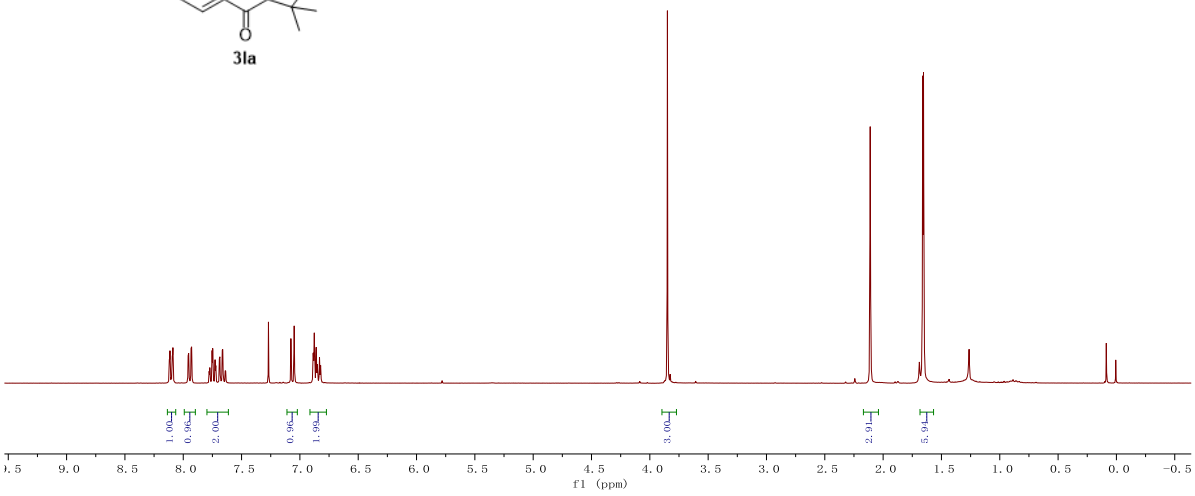
IR (KBr) spectrum for compound **3ka**

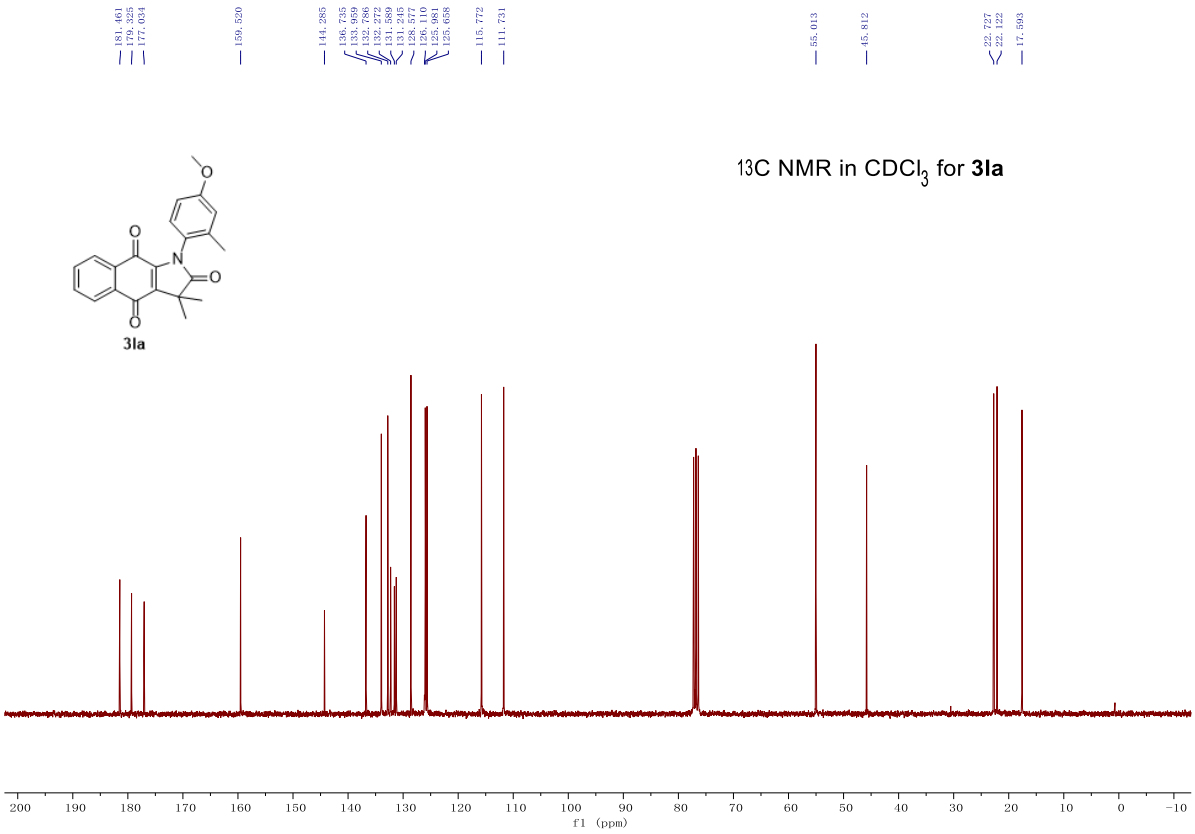


1H NMR in $CDCl_3$ for **3la**

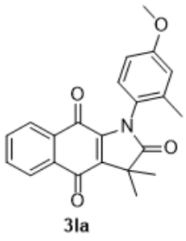


3la

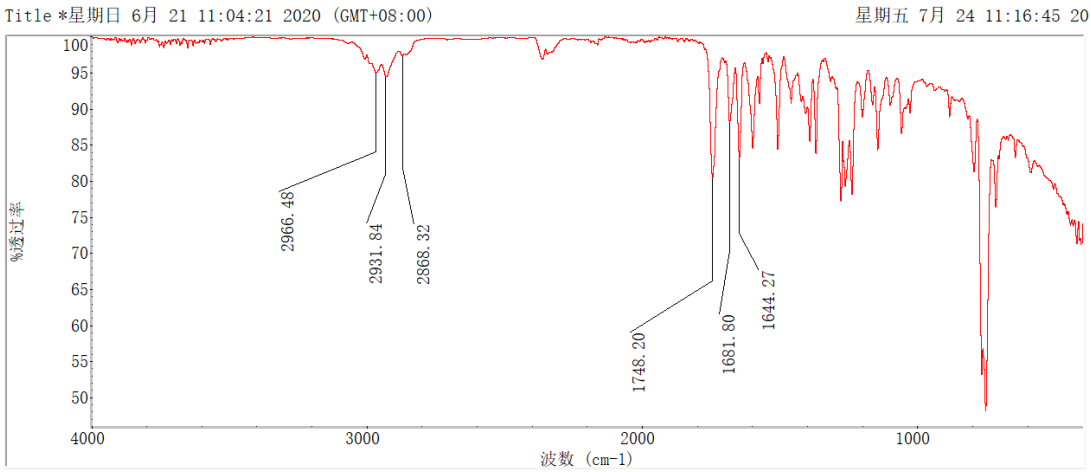


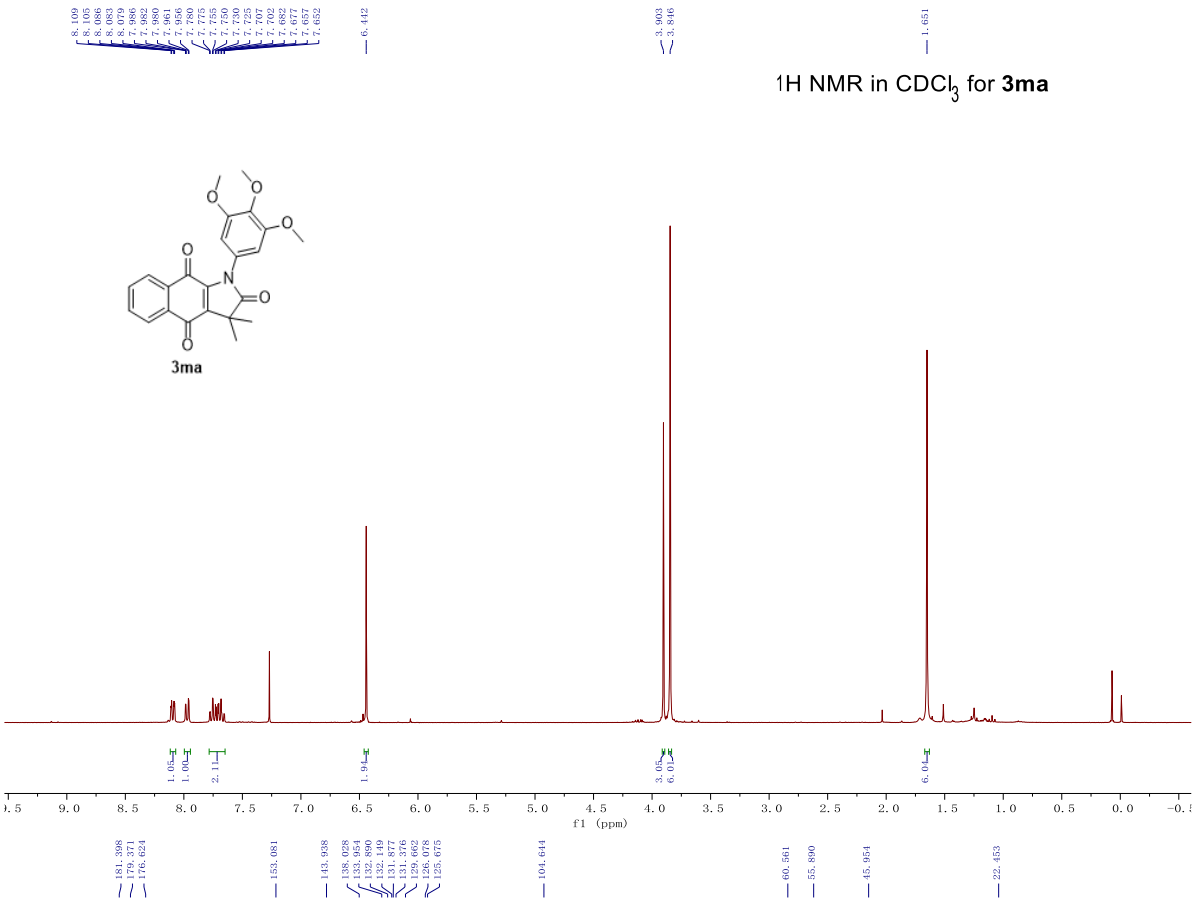


^{13}C NMR in $CDCl_3$ for **3la**

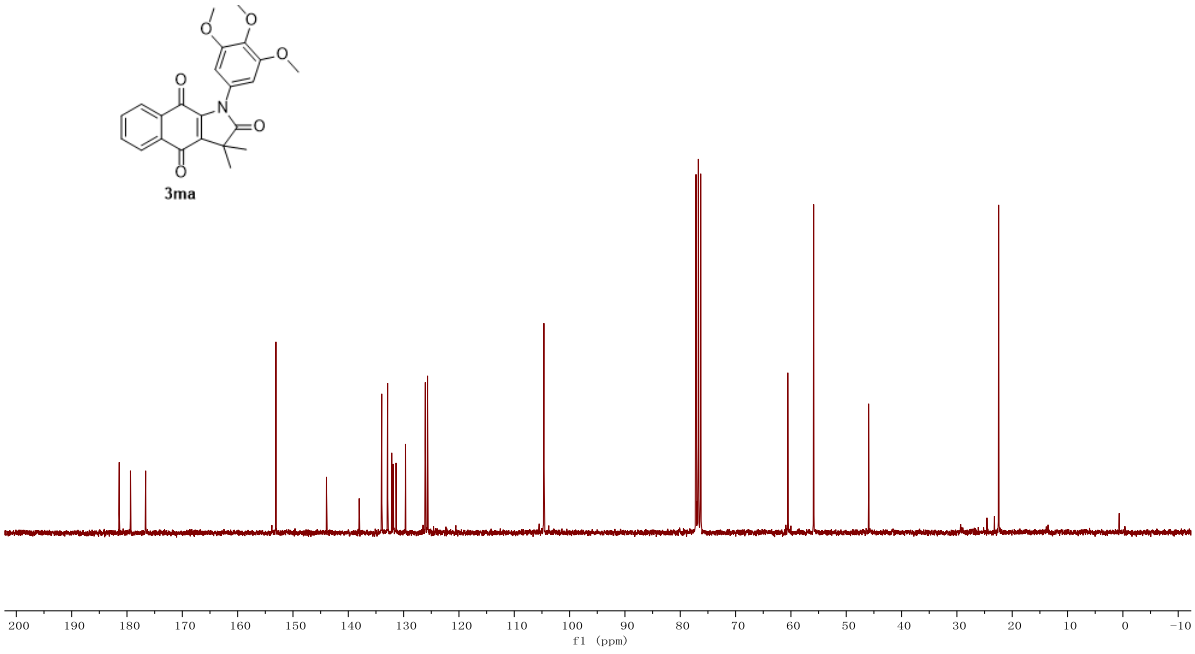


IR (KBr) spectrum for compound **3la**

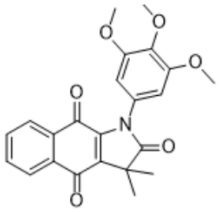




1H NMR in $CDCl_3$ for **3ma**

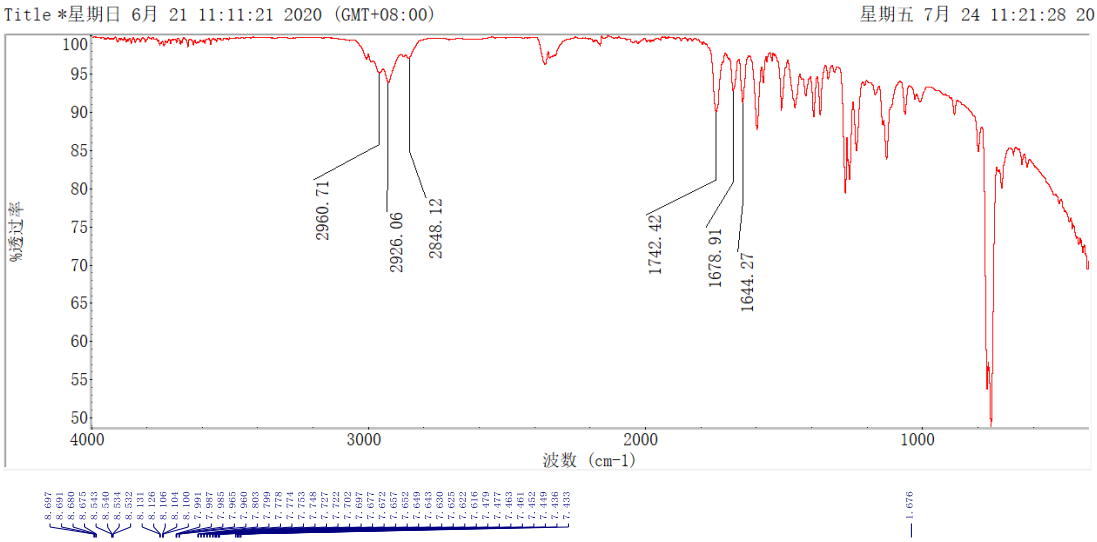


13C NMR in $CDCl_3$ for **3ma**

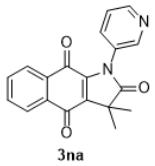


3ma

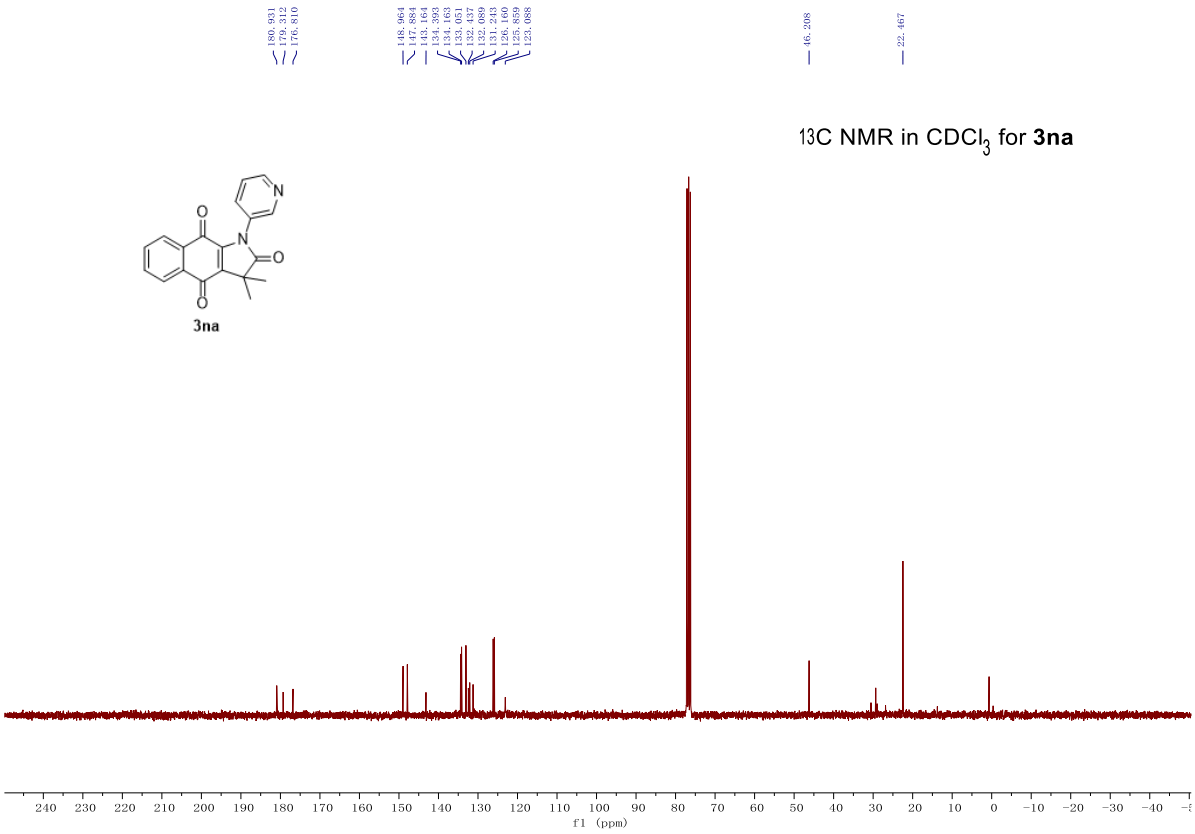
IR (KBr) spectrum for compound **3ma**



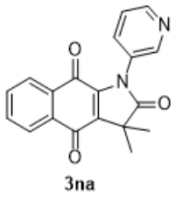
1H NMR in $CDCl_3$ for **3na**



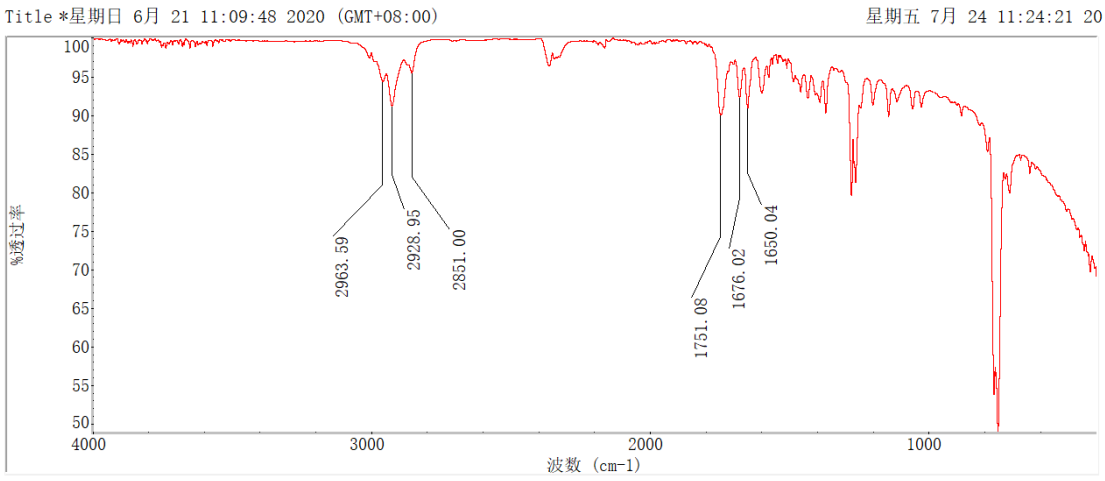
3na



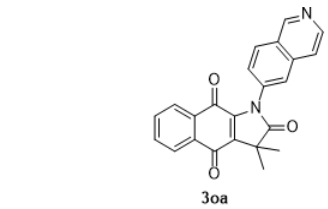
^{13}C NMR in $CDCl_3$ for **3na**

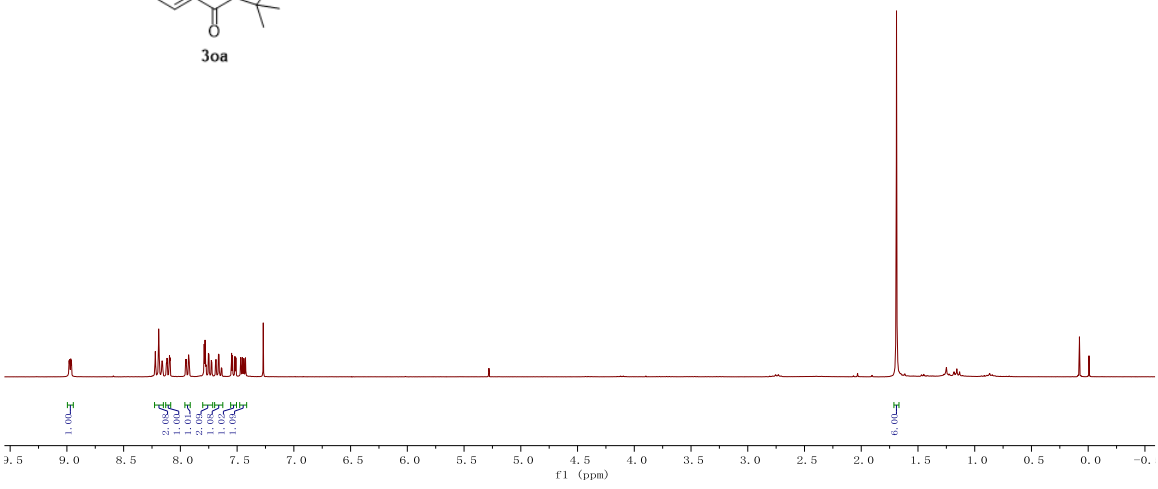


IR (KBr) spectrum for compound **3na**

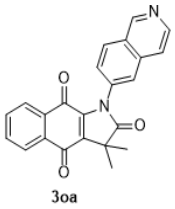


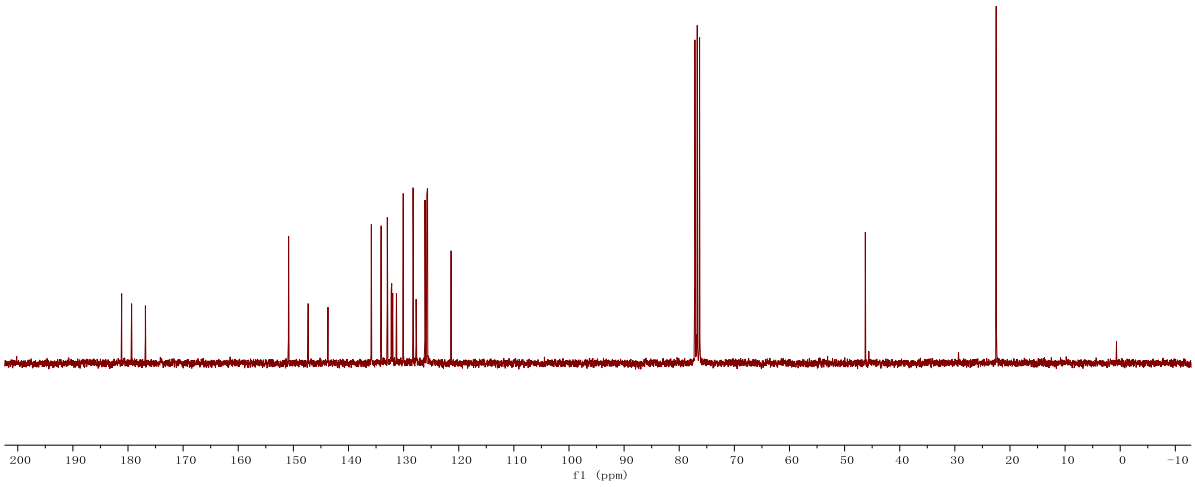
1H NMR in $CDCl_3$ for **3oa**

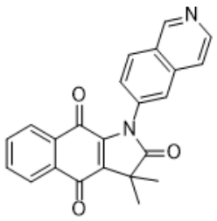




13C NMR in $CDCl_3$ for **3oa**

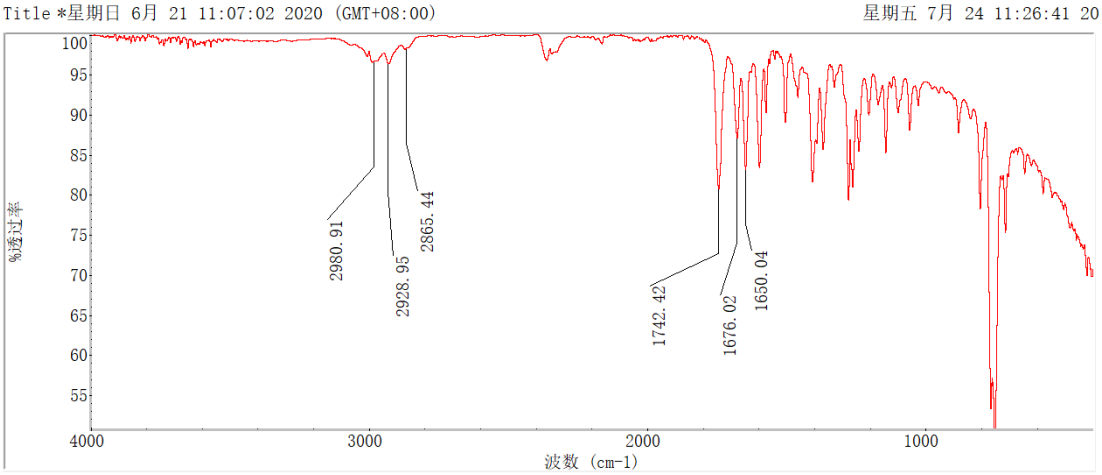




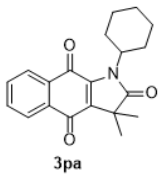


3oa

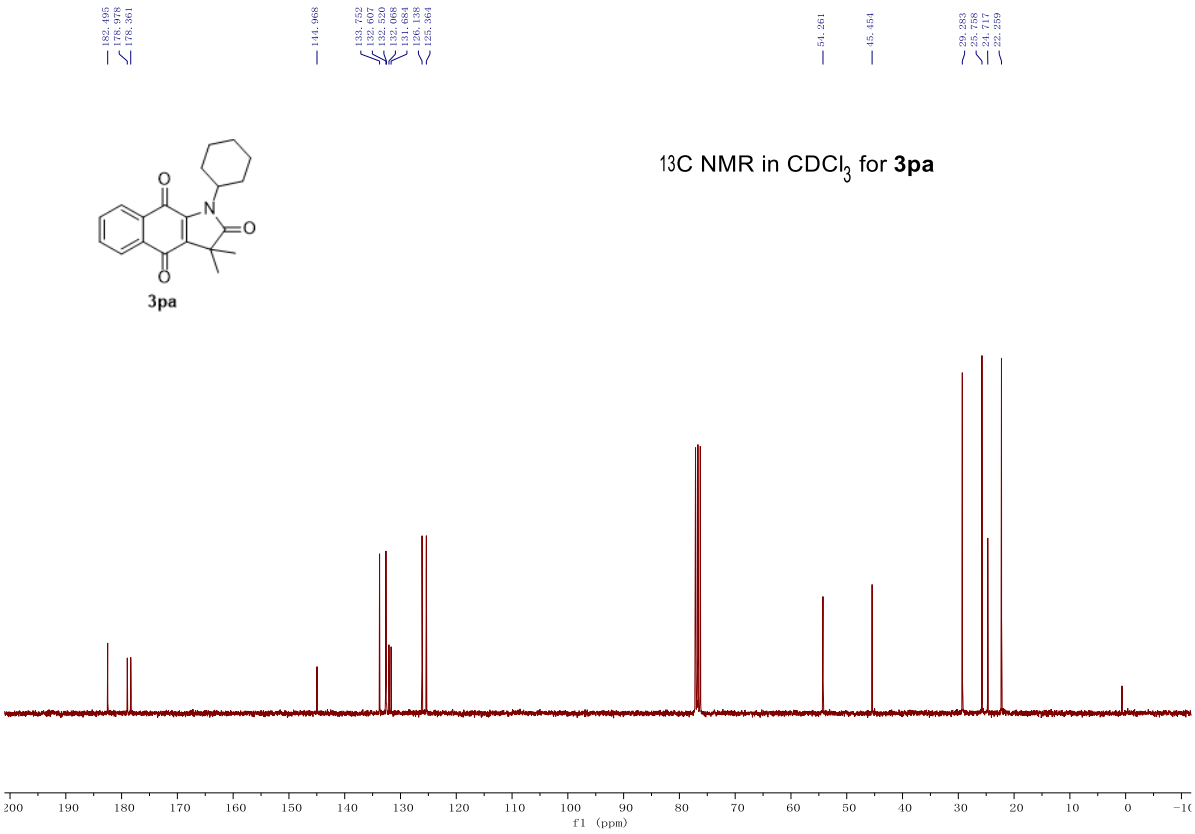
IR (KBr) spectrum for compound **3oa**



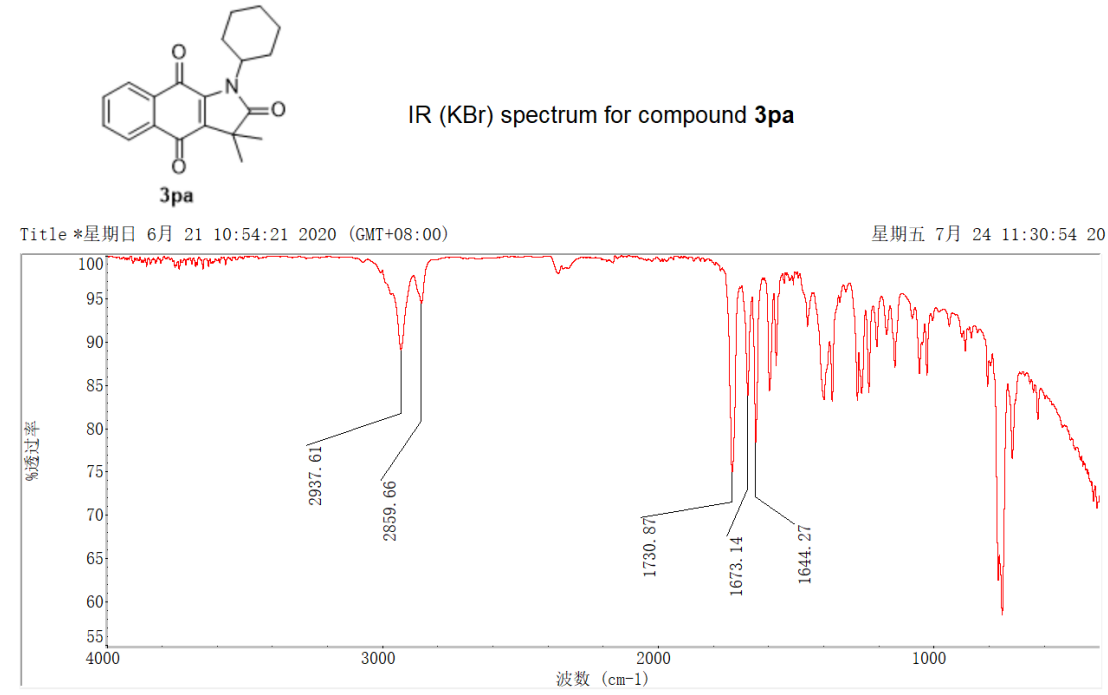
1H NMR in $CDCl_3$ for **3pa**



3pa

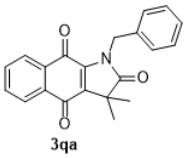


^{13}C NMR in $CDCl_3$ for **3pa**



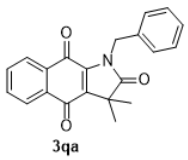
IR (KBr) spectrum for compound **3pa**

^{1}H NMR in $CDCl_3$ for **3qa**

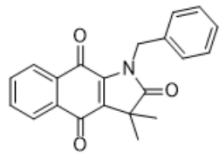


3qa

^{13}C NMR in $CDCl_3$ for **3qa**

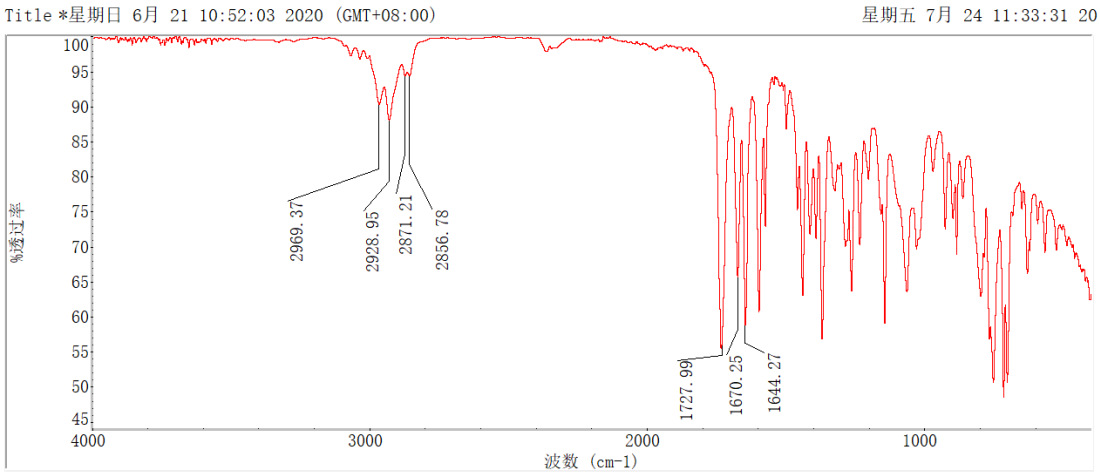


3qa

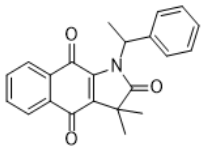


3qa

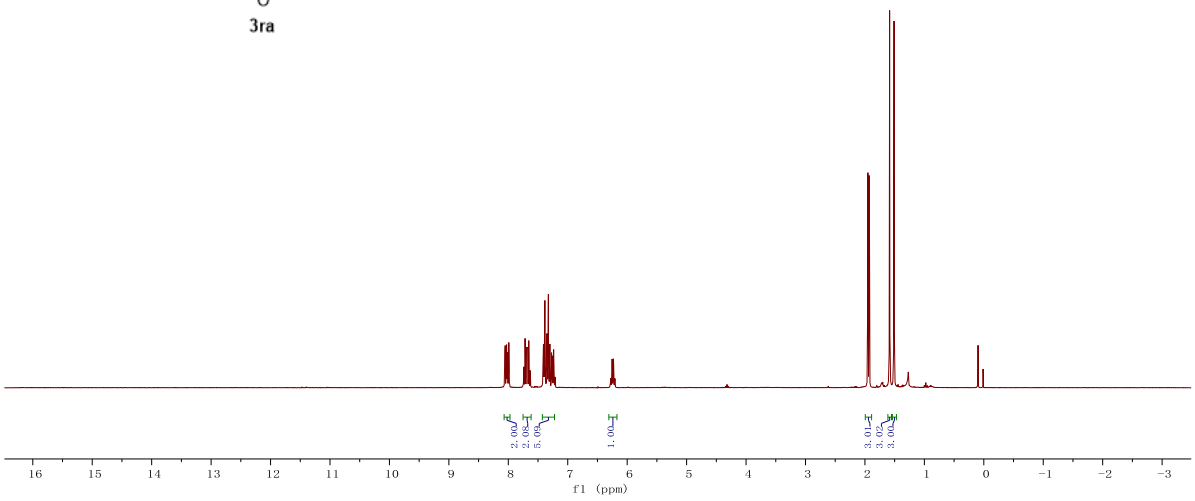
IR (KBr) spectrum for compound **3qa**

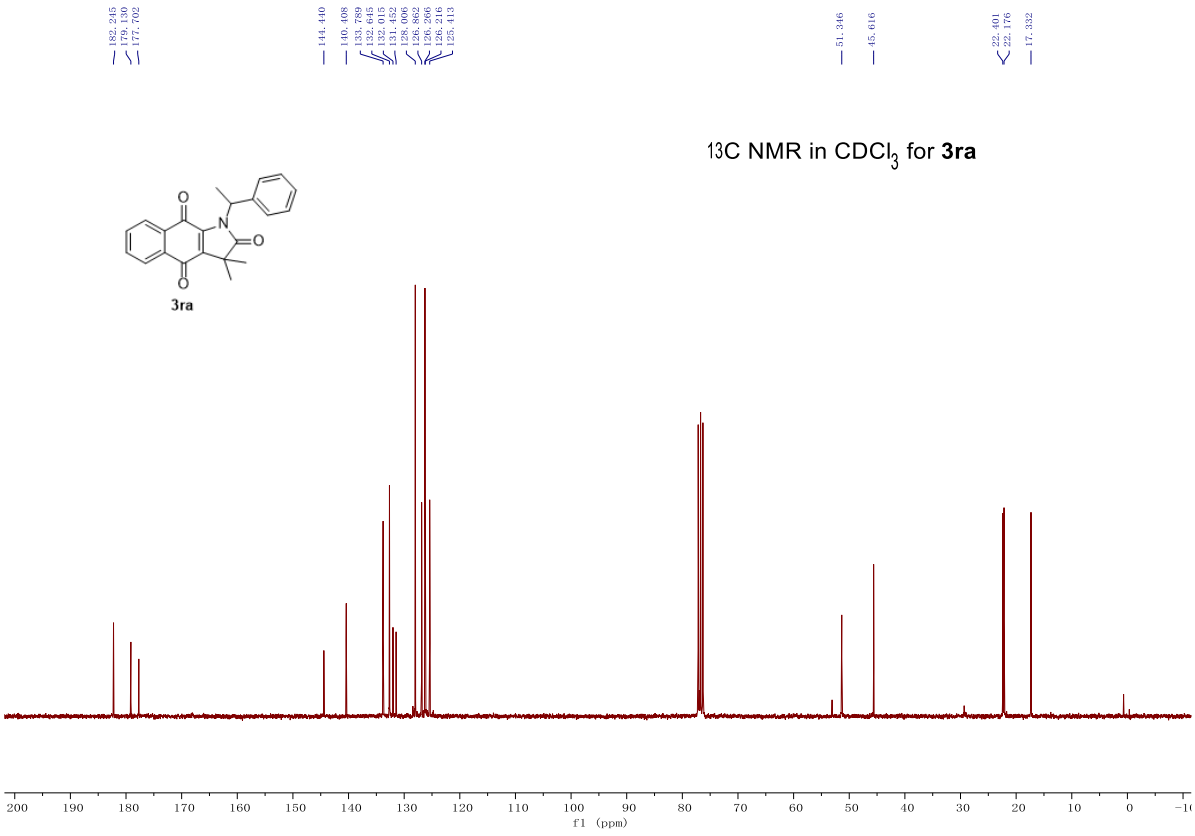


1H NMR in $CDCl_3$ for **3ra**

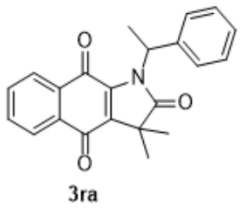


3ra

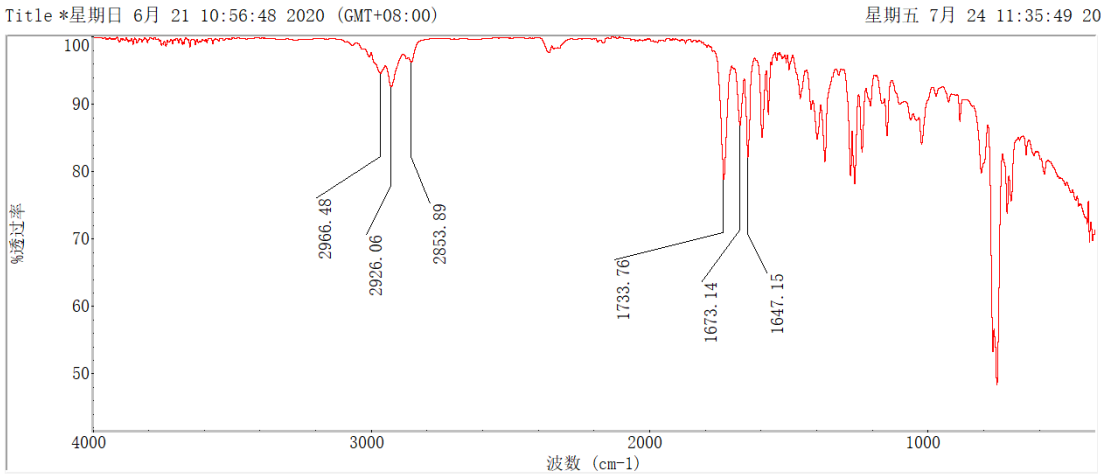


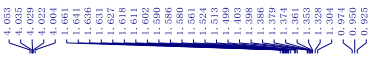


^{13}C NMR in $CDCl_3$ for **3ra**

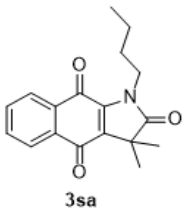


IR (KBr) spectrum for compound **3ra**



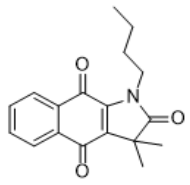


1H NMR in $CDCl_3$ for **3sa**

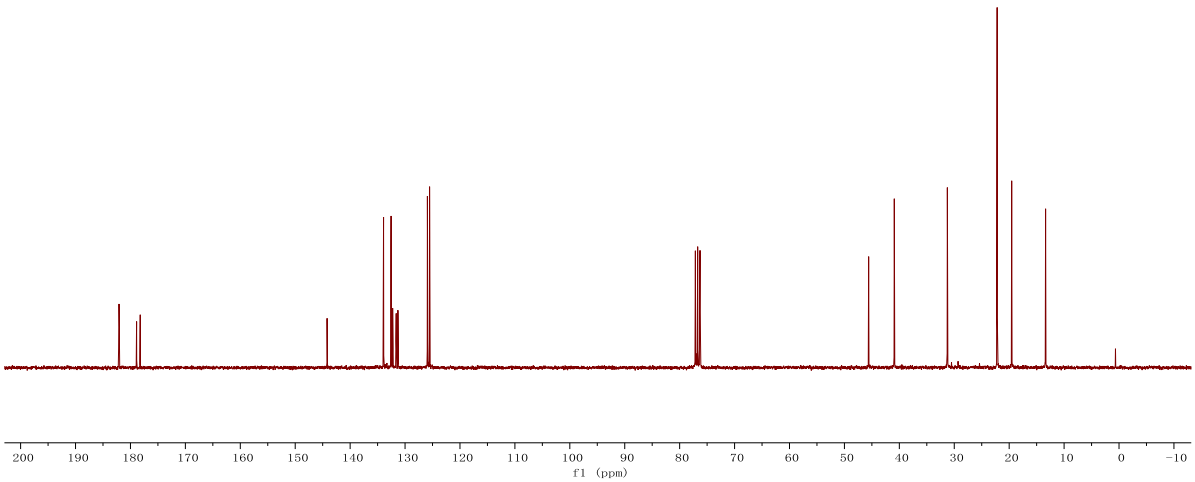


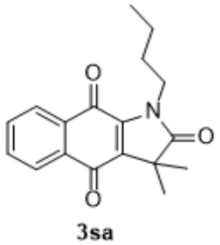
3sa

13C NMR in $CDCl_3$ for **3sa**



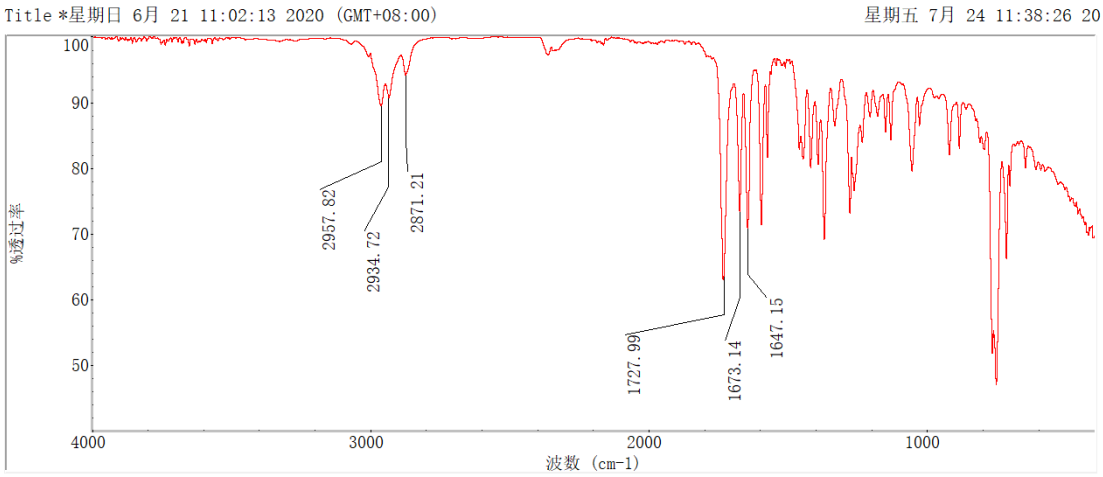
3sa



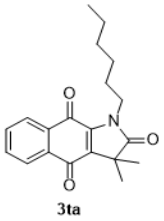


3sa

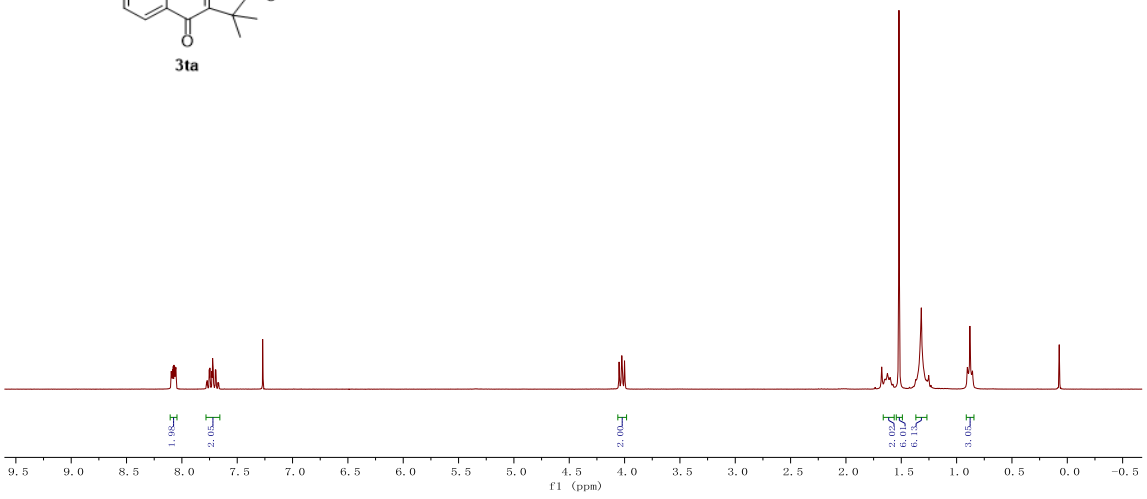
IR (KBr) spectrum for compound **3sa**



1H NMR in $CDCl_3$ for **3ta**

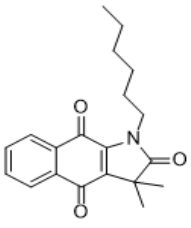


3ta

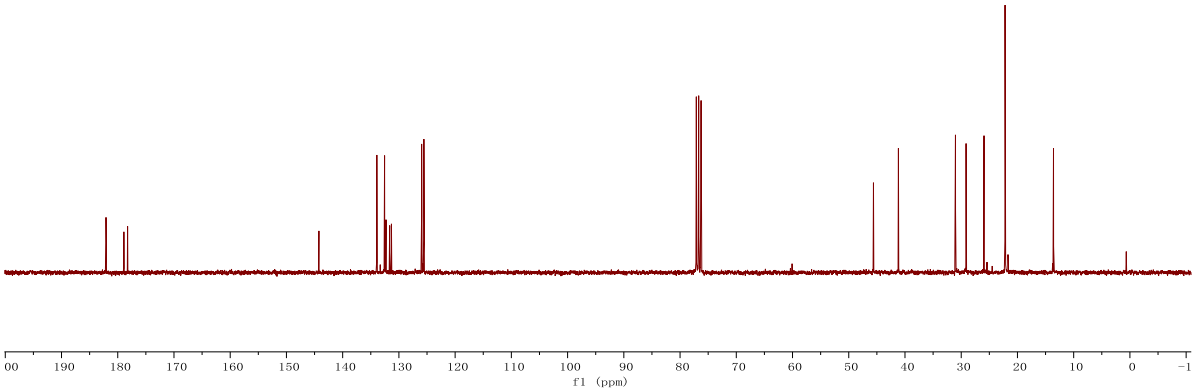


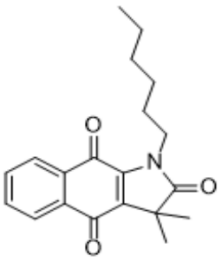
182.065
178.911
176.259
144.223
133.922
132.549
132.294
131.450
131.330
125.955
125.555
45.607
41.166
31.023
29.156
25.948
22.204
22.163
13.591

^{13}C NMR in $CDCl_3$ for **3ta**



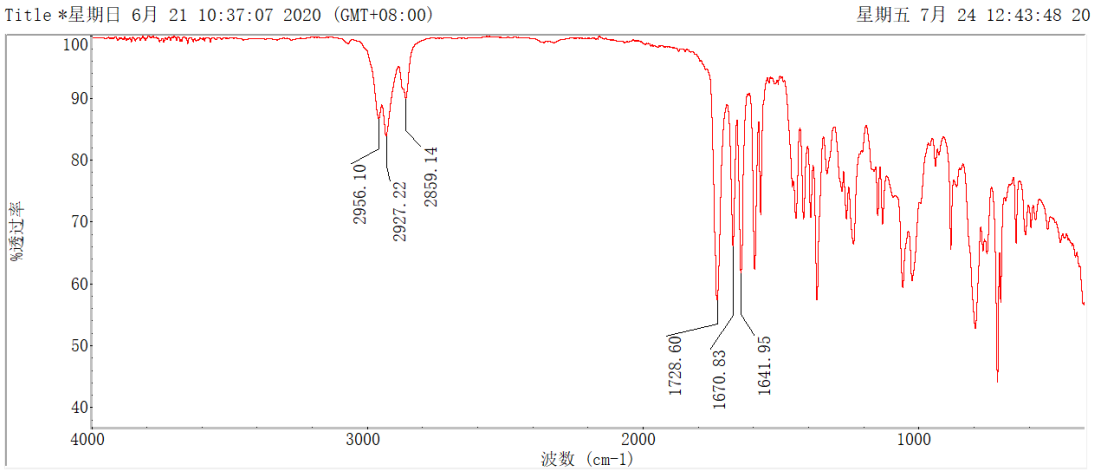
3ta



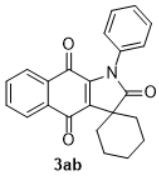


3ta

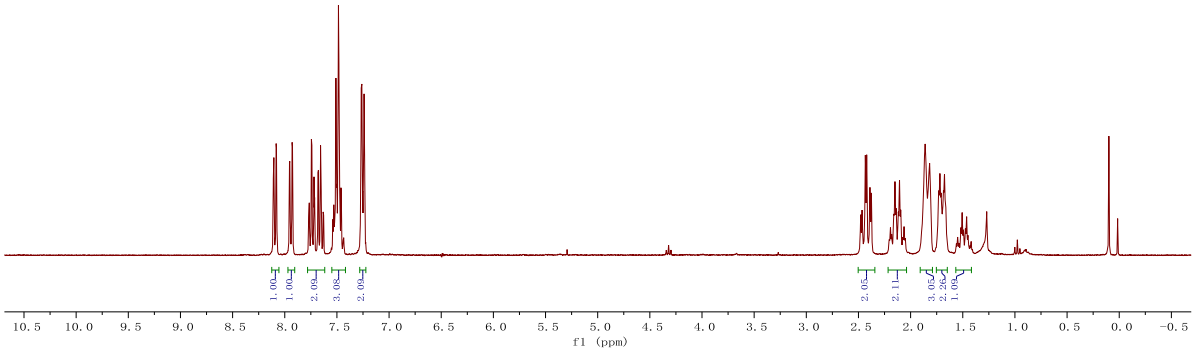
IR (KBr) sepctrum for compound **3ta**

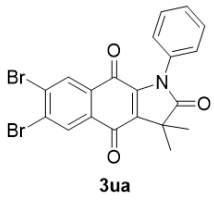


1H NMR in $CDCl_3$ for **3ab**

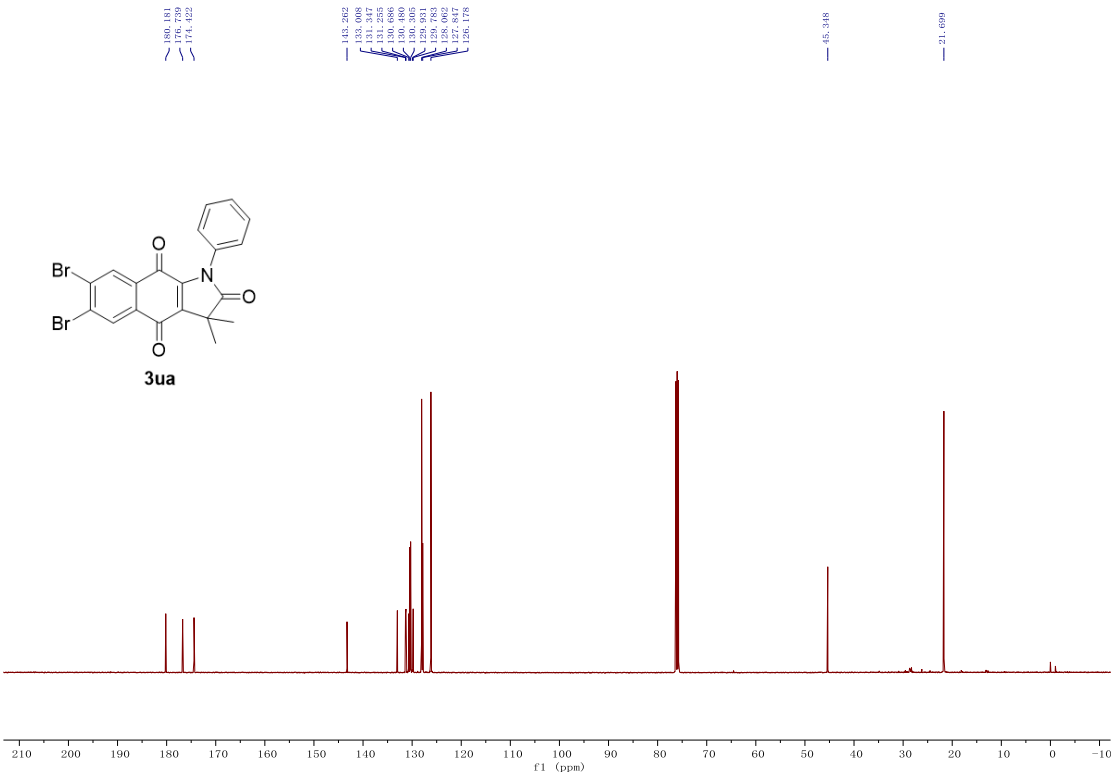


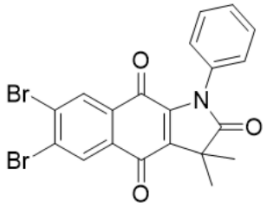
3ab



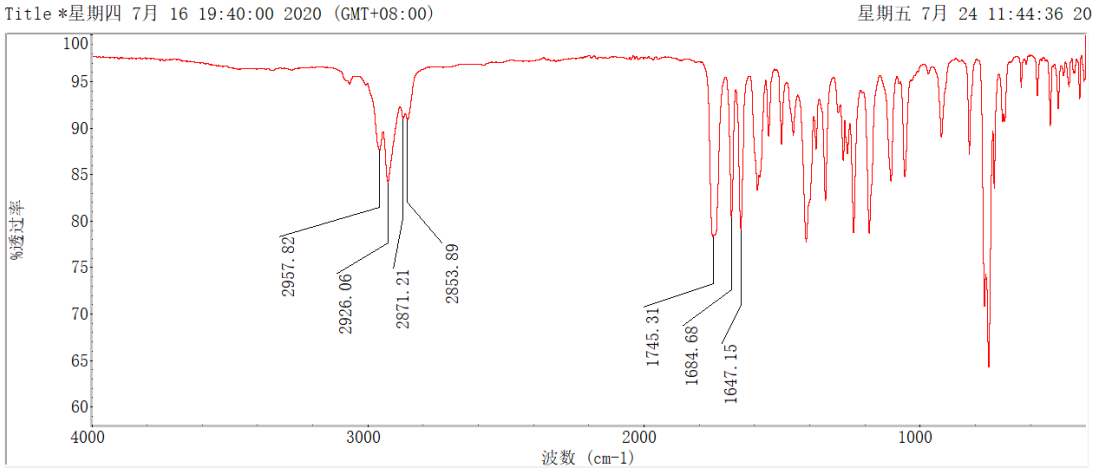


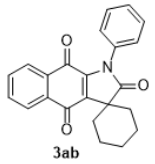
3ua



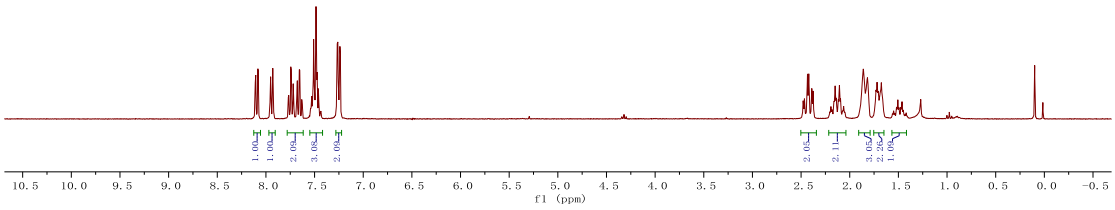


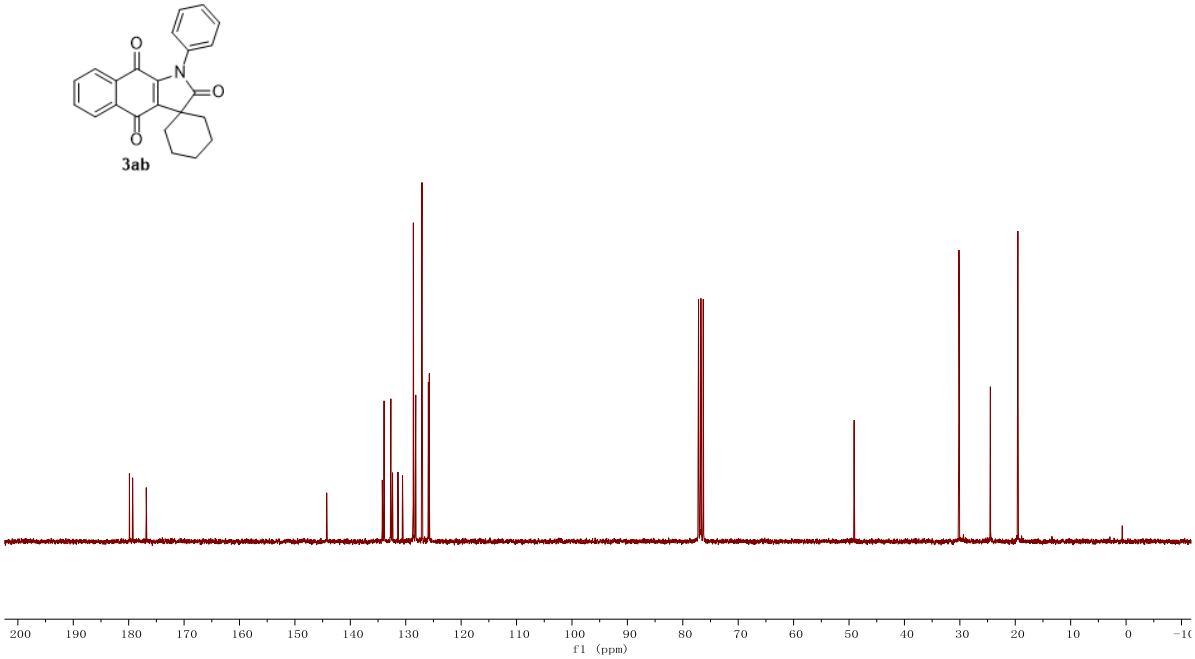
IR (KBr) spectrum for compound **3ua**





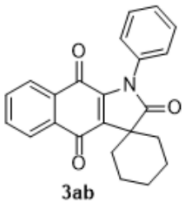
3ab





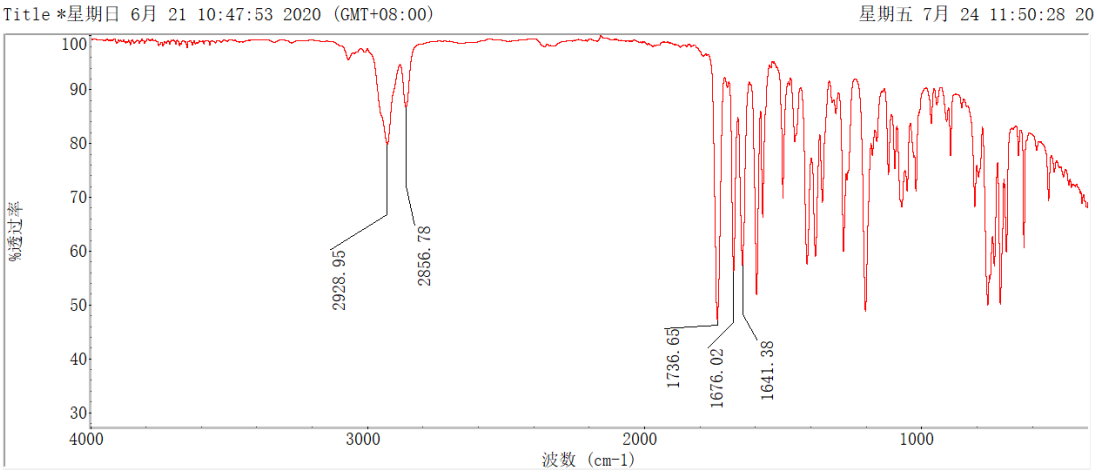
^{13}C NMR in $CDCl_3$ for **3ab**

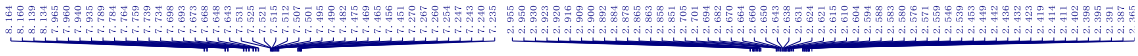
3ab



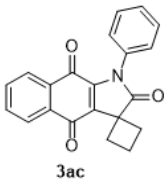
3ab

IR (KBr) spectrum for compound **3ab**

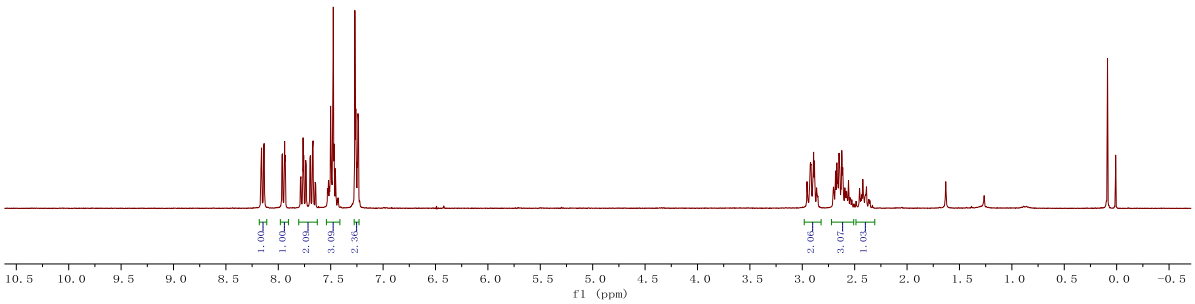


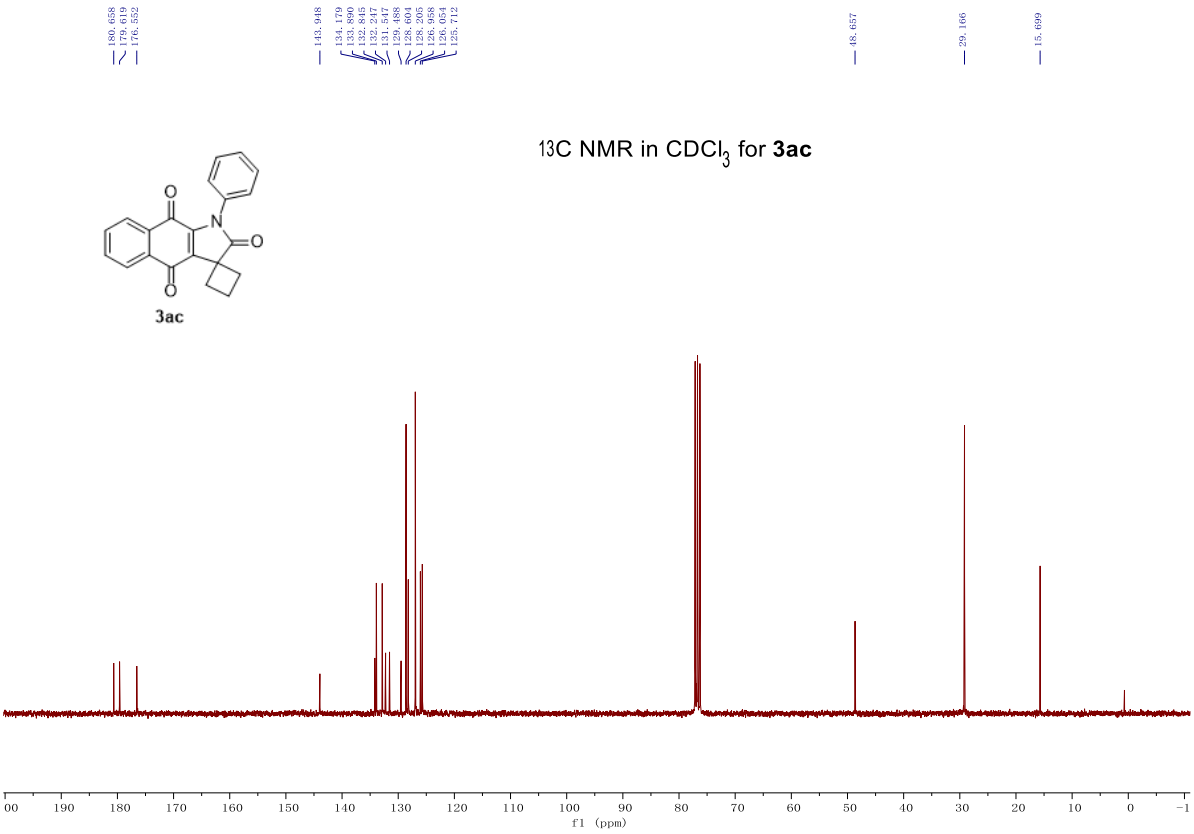


^{1}H NMR in $CDCl_3$ for **3ac**

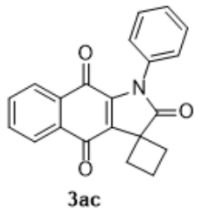


3ac

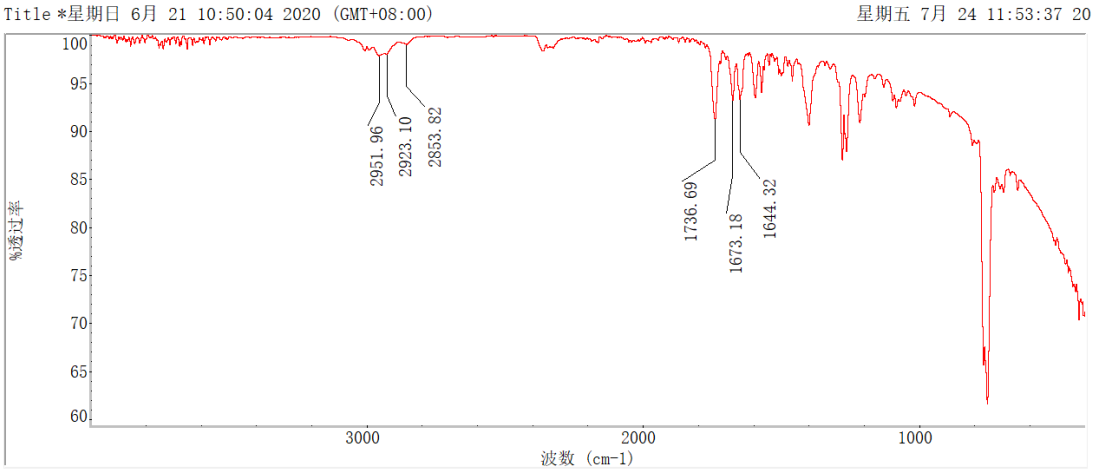




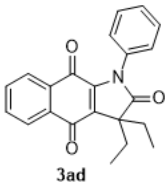
^{13}C NMR in $CDCl_3$ for **3ac**

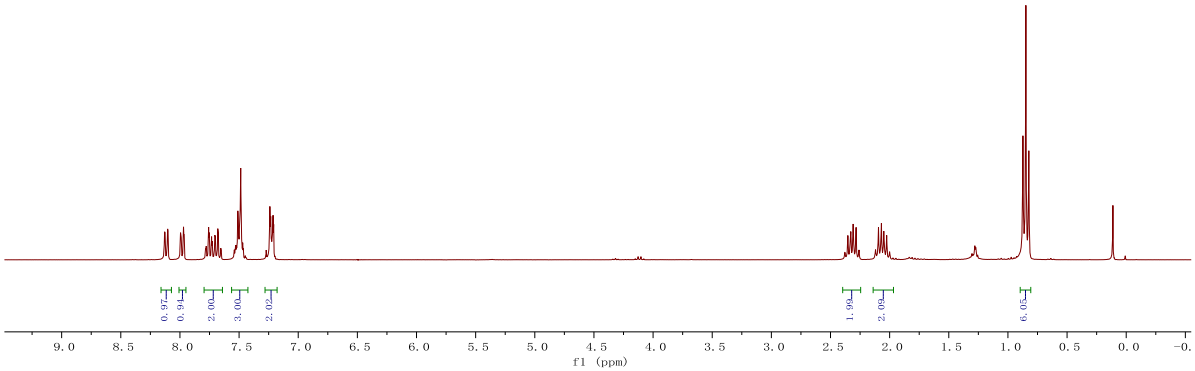


IR (KBr) spectrum for compound **3ac**

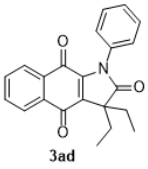


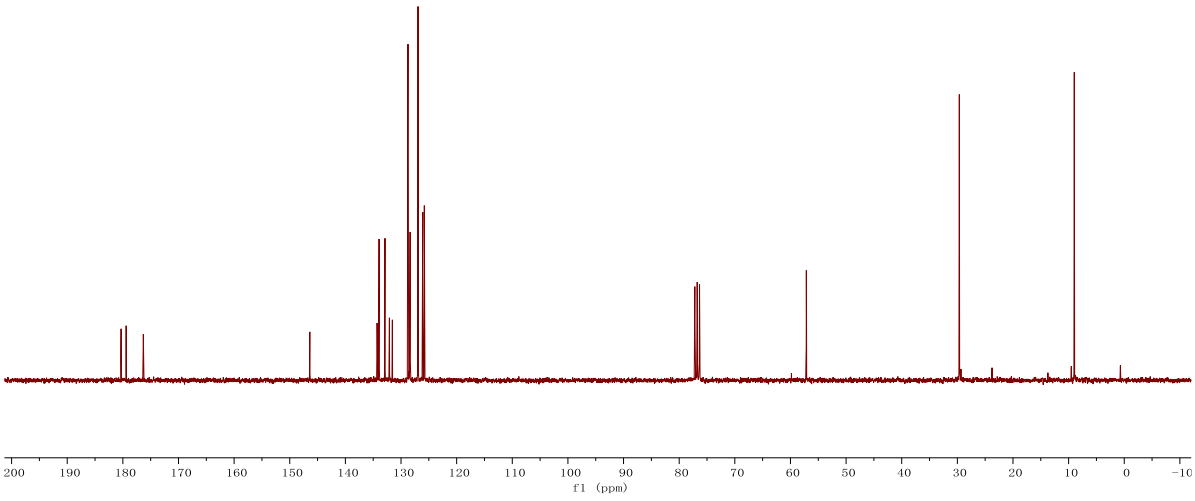
1H NMR in $CDCl_3$ for **3ad**

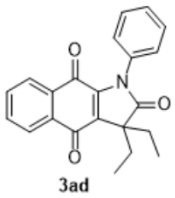




13C NMR in $CDCl_3$ for **3ad**

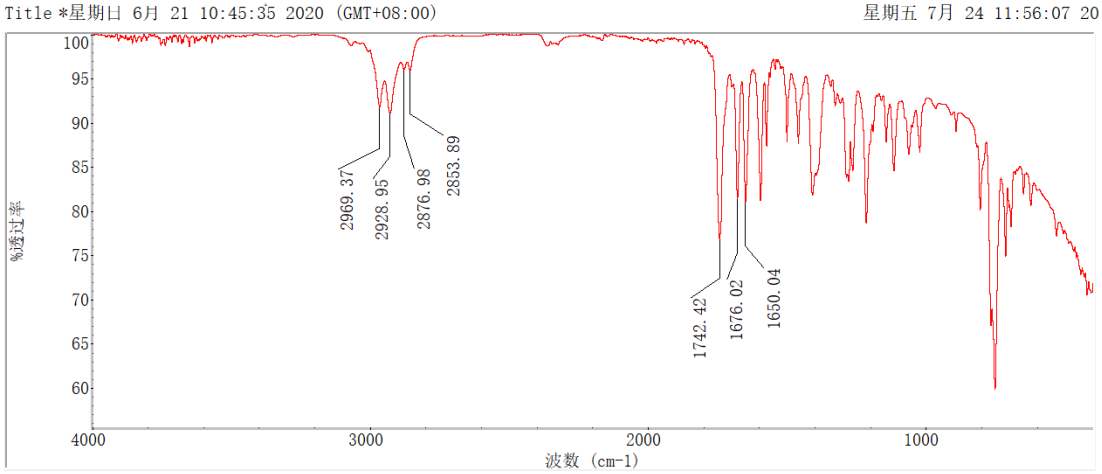




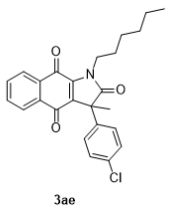


3ad

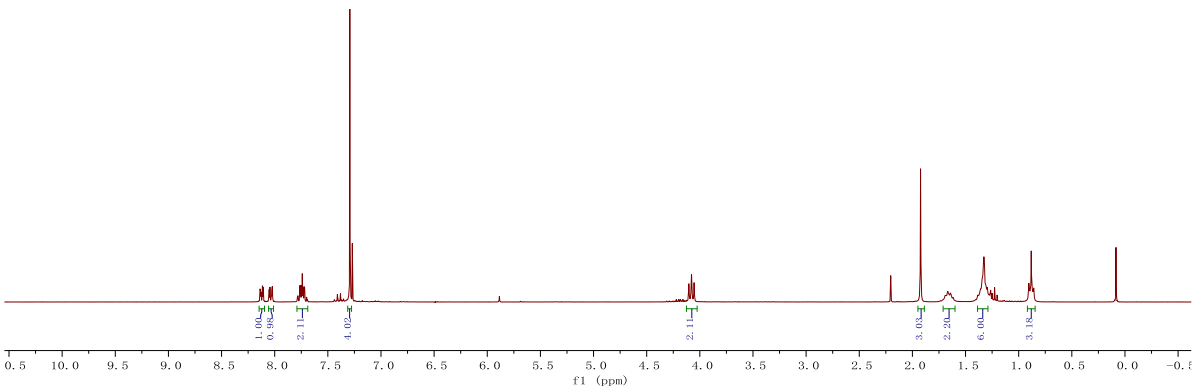
IR (KBr) spectrum for compound **3ad**



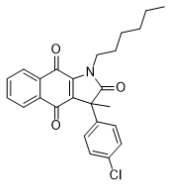
^{1}H NMR in $CDCl_3$ for **3ae**



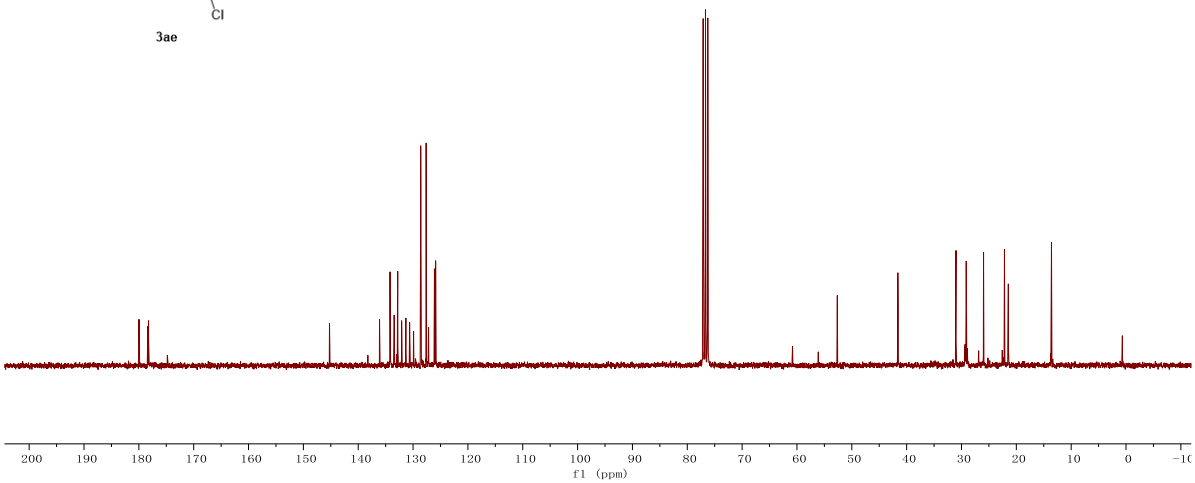
3ae

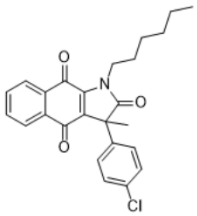


^{13}C NMR in $CDCl_3$ for **3ae**



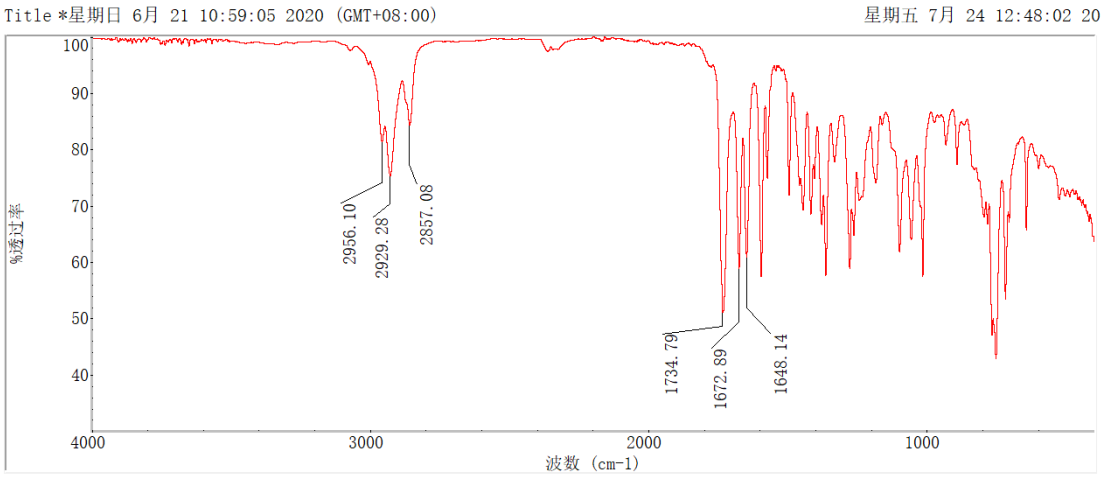
3ae





3ae

IR (KBr) sepctrum for compound **3ae**



Single crystallographic data for compound 3aa.

Single crystals of $C_{20}H_{15}NO_3$ (**3aa)** were obtained by slow evaporation of a solution containing **3aa** in the mixture of EtOH and DCM. A suitable crystal was selected and the crystal data and structure refinement results for compound **3aa** are listed in the Table S1.

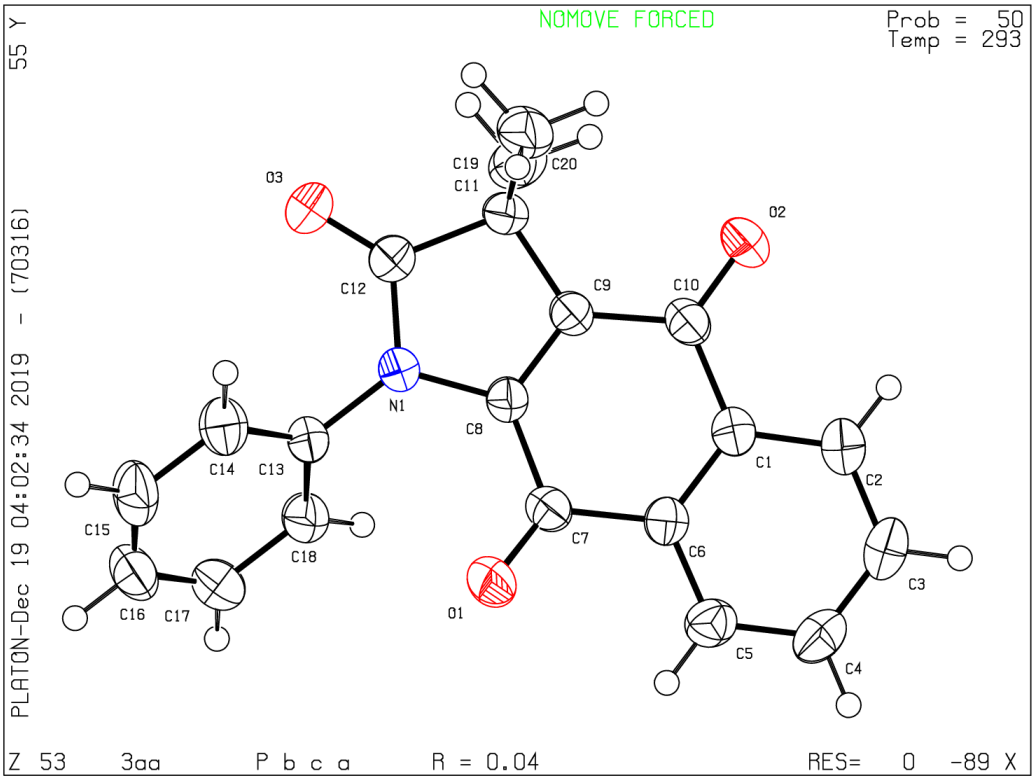


Figure S1. ORTEP view of the compound 3aa with thermal ellipsoids drawn at the 50% probability level

Table 1 Crystal data and structure refinement for 3aa.

Identification code	3AA
Empirical formula	$C_{20}H_{15}NO_3$
Formula weight	317.33
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	13.5094(16)
b/Å	11.0920(9)

c/Å	21.2668(18)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3186.8(5)
Z	8
ρ_{calc}g/cm^3	1.323
μ/mm^{-1}	0.089
F(000)	1328.0
Crystal size/mm^3	0.14 × 0.13 × 0.12
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.876 to 49.99
Index ranges	-16 ≤ h ≤ 10, -13 ≤ k ≤ 13, -25 ≤ l ≤ 24
Reflections collected	8730
Independent reflections	2800 [R_{int} = 0.0298, R_{sigma} = 0.0335]
Data/restraints/parameters	2800/0/219
Goodness-of-fit on F^2	1.075
Final R indexes [I>=2σ (I)]	R_1 = 0.0446, wR_2 = 0.1005
Final R indexes [all data]	R_1 = 0.0607, wR_2 = 0.1093
Largest diff. peak/hole / e Å^{-3}	0.14/-0.20