Supporting Information

for

Synthesis of β-Aminoenones via Cross-Coupling of In-Situ-Generated Isocyanides with 1,3-Dicarbonyl Compounds

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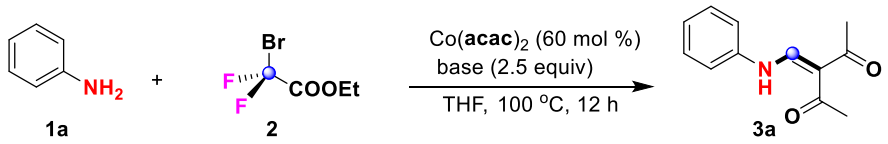
1. General information

All chemicals were purchased from Adamas Reagent, energy chemical company, J&K Scientific Ltd, Bide Pharmatech Ltd and Tansoole. Unless otherwise stated, all experiments were conducted in a sealed tube under N_2 atmosphere. THF or CH_3CN was a optional solvent. Reactions were monitored by TLC or GC-MS analysis. Flash column chromatography was performed over silica gel (200-300 mesh).

^{1}H-NMR and ^{13}C-NMR spectra were recorded in $CDCl_3$ on a Bruker Avance III 500MHz NMR spectrometer (500 MHz ^{1}H, 125 MHz ^{13}C) at room temperature. Chemical shifts were reported in ppm on the scale relative to $CDCl_3$ (δ = 7.26 for ^{1}H-NMR, δ = 77.00 for ^{13}C-NMR) as an internal reference. Coupling constants (*J*) were reported in Hertz (Hz).

2. Optimization of experiment conditions for 3a

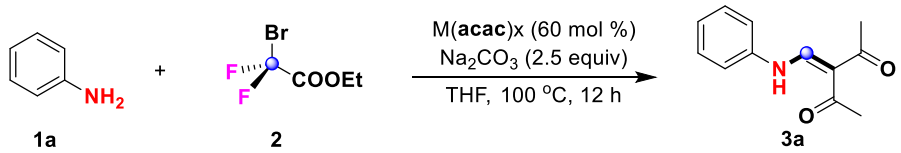
Table S1. Optimization of the the effect of base



entry	base	solvent	yield (%)[a]
1	K_2CO_3	THF	81
2	Na_2CO_3	THF	88 (83[b])
3	$NaHCO_3$	THF	79
4	Na_3PO_4	THF	77
5	DBU	THF	56
6	NaOH	THF	61
7	Cs_2CO_3	THF	55
8	NaOAc	THF	43
9	*t*-BuOK	THF	58

Reaction condition: **1a** (0.2 mmol), **2** (1.2 equiv), base (2.5 equiv), Co(**acac**)$_2$ (60 mol %), solvent (2 mL), at N_2 for 12 h under 100 °C, [a] GC yield. [b] isolated yield

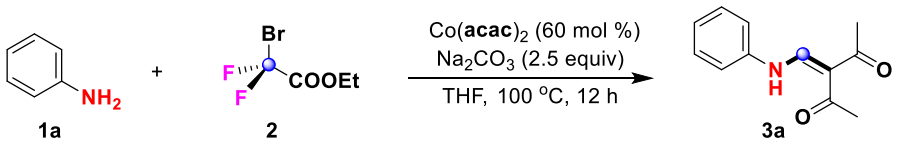
Table S2. Optimization of the M(acac)$_x$ for reaction



entry	M(acac)x (60 mol%)	solvent	yield (%)[a]
1	Cu(**acac**)$_2$	THF	67
2	Co(**acac**)$_2$	THF	88 (83[b])
3	Fe(**acac**)$_2$	THF	71
4	Ni(**acac**)$_2$	THF	78
5	Fe(**acac**)$_3$	THF	65
6	Mn(**acac**)$_2$	THF	45

Reaction condition: **1a** (0.2 mmol), **2** (1.2 equiv), Na_2CO_3 (2.5 equiv), M(**acac**)$_x$ (60 mol %), solvent (2 mL), at N_2 for 12 h under 100 °C, [a] GC yield. [b] isolated yield

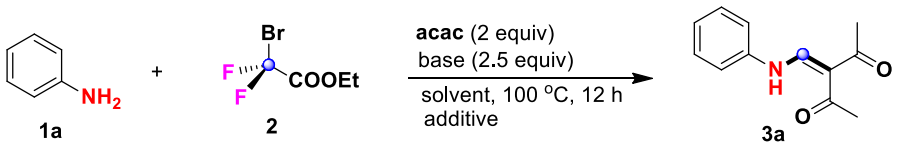
Table S3. Optimization of the solvent for reaction



entry	base	solvent	yield (%)[a]
1	Na_2CO_3	CH_3CN	84
2	Na_2CO_3	THF	88 (83[b])
3	Na_2CO_3	toluene	trace
4	Na_2CO_3	acetone	79
5	Na_2CO_3	CH_3OH	78
6	Na_2CO_3	DMSO	34
7	Na_2CO_3	DMF	22
8	Na_2CO_3	dioxane	55
9	Na_2CO_3	DCE	63

Reaction condition: **1a** (0.3 mmol), **2** (1.2 equiv), Na_2CO_3 (2.5 equiv), Co(**acac**)$_2$ (60 mol %), solvent (2 mL), at N_2 for 12 h under 100 °C, [a] GC yield. [b] isolated yield

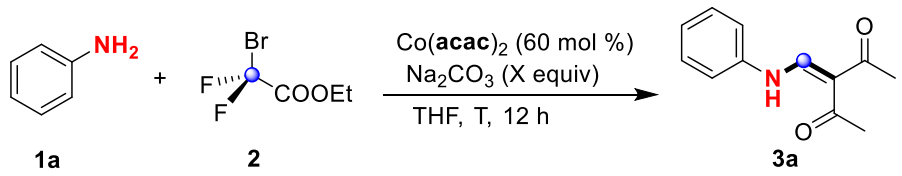
Table S4. Optimization of the reaction for other 1,3-dicardonyl compounds



entry	base	additive	solvent	yield (%)[a]
1	Na_2CO_3	3 Å MS	toluene	trace
2	Na_2CO_3	3 Å MS	THF	34
3	Na_2CO_3	3 Å MS	CH_3CN	53
4	K_2CO_3	3 Å MS	CH_3CN	48
5	$NaHCO_3$	3 Å MS	CH_3CN	32
6	$LiOCH_3$	3 Å MS	CH_3CN	77 (72)[b]
7	$LiOCH_3$	----	CH_3CN	64
8	$LiOCH_3$	4 Å MS	CH_3CN	62
9	$LiOCH_3$	5 Å MS	CH_3CN	59

Reaction condition: **1a** (0.3 mmol), **2** (1.2 equiv), Na_2CO_3 (2.5 equiv), **acac** (2 equiv), solvent (2 mL), additive (50 mg), at N_2 for 12 h under 100 °C, [a] GC yield. [b] isolated yield

Table S5. Optimization of the reaction for the scope of temperature and the dosage of base

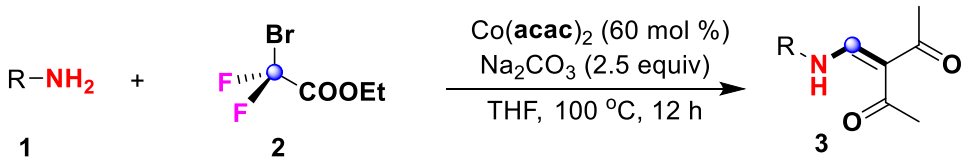


1a **2** **3a**

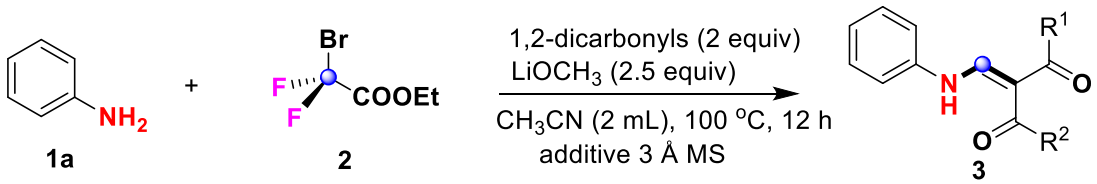
entry	T (^{o}C)	Na_2CO_3 (X equiv)	yield (%)[a]
1	100	2.5	88 (83[b])
2	80	2.5	69
3	60	2.5	34
4	50	2.5	31
5	RT	2.5	trace
6	100	2.0	84
7	100	1.5	54
8	100	1	39
9	100	0.5	trace
10	100	0	trace
11[c]	100	2.5	36

Reaction condition: **1a** (0.2 mmol), **2** (1.2 equiv), Na_2CO_3 (X equiv), Co(**acac**)$_2$ (60 mol %), THF (2 mL), at N_2 for 12 h under T ^{o}C, [a] GC yield. [b] isolated yield, [c] 5 h

3. General process for the synthesis of 3



In a dried Schlenk tube were placed **1** (0.2 mol, 1 equiv), Na_2CO_3 (0.75 mol, 2.5 equiv), Co(**acac**)$_2$ (0.18 mmol, 0.6 equiv), **2** (0.24 mmol, 1.2 equiv) and solvent was added the mixture under N_2 atmosphere. The resulting mixture was stirred at 100 ^oC for 12 h. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatograph (silica gel, petroleum ether : EtOAc = 50:1, v/v) to give the desired product **3**.

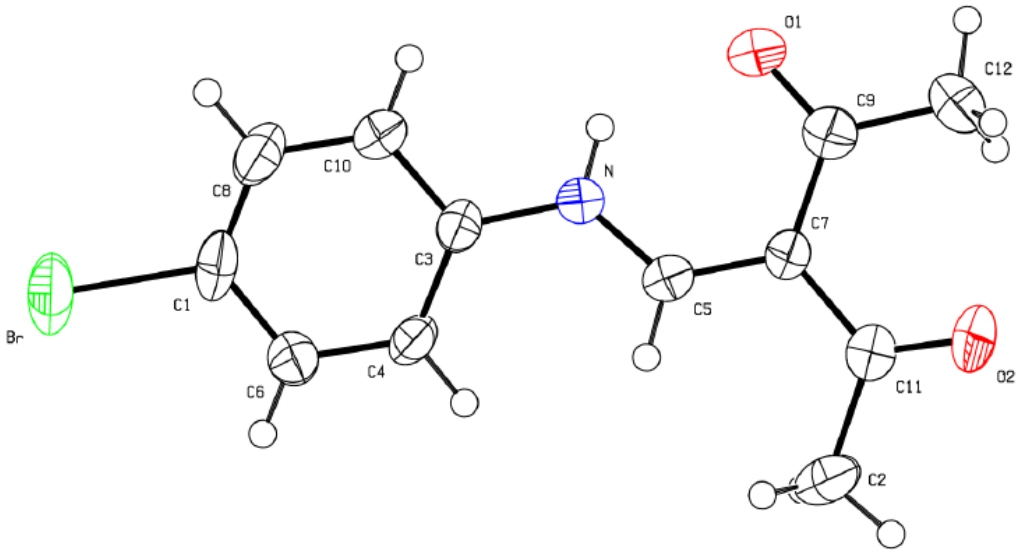


In a dried Schlenk tube were placed **1a** (0.2 mol, 1 equiv), $LiOCH_3$ (0.75 mol, 2.5 equiv), 1,3-dicarbonyl compounds (0.4 mmol, 2 equiv), **2** (0.24 mmol, 1.2 equiv), 3Å MS (50 mg) as additive and solvent was added the mixture under N_2 atmosphere. The resulting mixture was stirred at 100 ^oC for 12 h. Upon completion of the reaction, the solvent was evaporated under reduced pressure and the residue was purified by flash column chromatograph (silica gel, petroleum ether : EtOAc = 50:1, v/v) to give the desired product **3**.

4. Crystal data of 3l

Crystallographic data for compound **3l** (CCDC-1823240) has been deposited with the Cambridge Crystallographic Data Centre, Copies of the data can be obtained, free of

charge, on application to CCDC (Email:deposit@ccdc.cam.ac.uk).



Bond precision: C-C = 0.0087 A Wavelength=0.71073

Cell: a=7.6810(13) b=7.6878(19) c=11.2198(13)
alpha=103.279(15) beta=91.274(11) gamma=114.93(2)
Temperature: 293 K

	Calculated	Reported
Volume	579.4(2)	579.36(19)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C12 H12 Br N O2	?
Sum formula	C12 H12 Br N O2	C12 H12 Br N O2
Mr	282.13	282.14
Dx,g cm-3	1.617	1.617
Z	2	2
Mu (mm-1)	3.531	3.531
F000	284.0	284.0
F000'	283.55	
h,k,lmax	9,9,13	9,9,13
Nref	2037	2029
Tmin,Tmax		0.244,1.000
Tmin'		

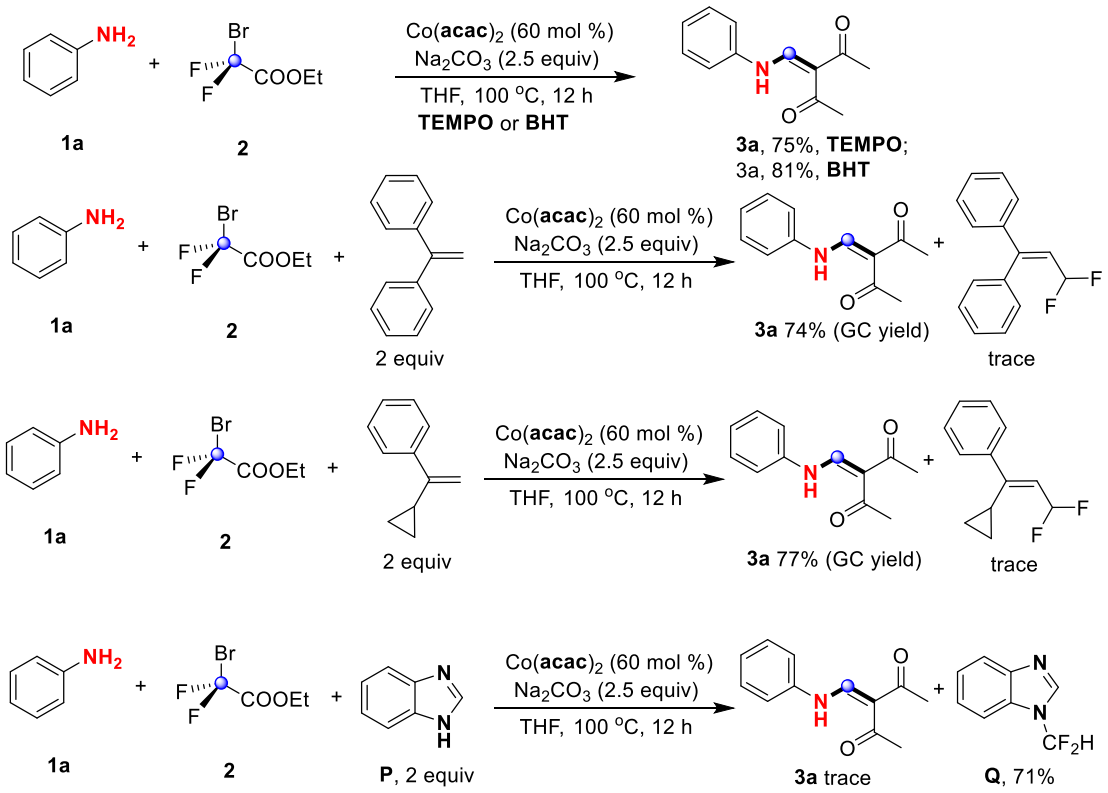
Correction method= # Reported T Limits: Tmin=0.244 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 25.000

R(reflections)= 0.0617(1362) wR2(reflections)= 0.1520(2029)

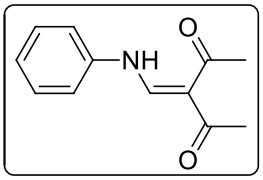
S = 1.002 Npar= 145

5. Radical trapping experiments.



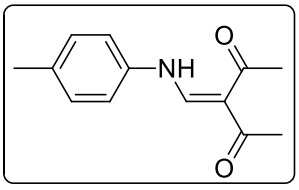
6. Characterization data for products

3-((phenylamino)methylene)pentane-2,4-dione (3a)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (33.7 mg, 83%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.74 (d, *J* = 10.9 Hz, 1H), 8.23 (d, *J* = 12.7 Hz, 1H), 7.45 – 7.34 (m, 2H), 7.24 – 7.07 (m, 3H), 2.54 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 194.8, 151.9, 139.1, 130.0, 125.8, 117.9, 113.3, 32.1, 27.4.
HRMS (ESI, m/z) calcd for $C_{12}H_{14}NO_2[M+H]^+$: 204.1025; found: 204.1022.

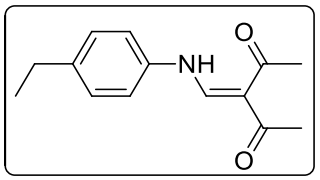
3-((p-tolylamino)methylene)pentane-2,4-dione (3b)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (36 mg, 83%). 1H NMR (500 MHz, CDCl3) δ 12.73 (d, J = 11.9 Hz, 1H), 8.19 (d, J = 12.8 Hz, 1H), 7.19 (d, J = 8.1 Hz, 2H), 7.06 (d, *J* = 8.4 Hz, 2H), 2.54 (s, 3H), 2.35 (d, J = 8.3 Hz, 6H). 13C NMR (125 MHz, CDCl3) δ 201.0, 194.8, 152.1, 136.6, 135.8, 130.5, 117.9, 113.0, 32.1, 27.4, 20.9.

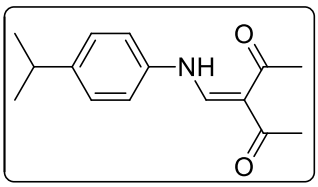
HRMS (ESI, m/z) calcd for $C_{13}H_{16}NO_2[M+H]^+$: 218.1181; found: 218.1175.

3-(((4-ethylphenyl)amino)methylene)pentane-2,4-dione (3c)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (39.3 mg, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.74 (d, *J* = 12.1 Hz, 1H), 8.20 (d, *J* = 12.8 Hz, 1H), 7.22 (d, *J* = 8.5 Hz, 2H), 7.09 (d, *J* = 8.5 Hz, 2H), 2.64 (q, *J* = 7.6 Hz, 2H), 2.54 (s, 3H), 2.36 (s, 3H), 1.23 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.0, 194.8, 152.2, 142.3, 136.8, 129.3, 118.0, 113.0, 32.1, 28.3, 27.4, 15.6.
HRMS (ESI, m/z) calcd for $C_{14}H_{18}NO_2[M+H]^+$: 232.1338; found: 232.1332.

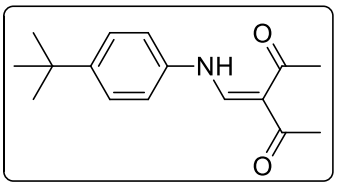
3-(((4-isopropylphenyl)amino)methylene)pentane-2,4-dione (3d)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a yellow oil (39.7 mg, 81%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.76 (d, *J* = 12.2 Hz, 1H), 8.23 (d, *J* = 12.8 Hz, 1H), 7.27 (d, *J* = 8.7 Hz, 2H), 7.12 (d, *J* = 8.5 Hz, 2H), 2.93 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.56 (s, 3H), 2.38 (s, 3H), 1.26 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.0, 194.8, 152.2, 146.9, 136.9, 127.9, 118.0, 113.0 33.6, 32.1, 27.4, 24.0.

HRMS (ESI, m/z) calcd for $C_{15}H_{20}NO_2[M+H]^+$: 246.1494; found: 246.1490.

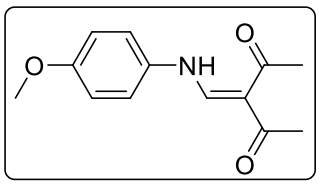
3-(((4-(tert-butyl)phenyl)amino)methylene)pentane-2,4-dione (3e)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a yellow oil (44 mg, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.73 (d, *J* = 12.4 Hz, 1H), 8.21 (d, *J* = 12.8 Hz, 1H), 7.41 (d, *J* = 8.7 Hz, 2H), 7.11 (d, *J* = 8.7 Hz, 2H), 2.54 (s, 3H), 2.36 (s, 3H), 1.31 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.0, 194.8, 152.2, 149.2, 136.6, 126.8, 117.7, 113.0, 34.6, 32.1, 31.3, 27.4.

HRMS (ESI, m/z) calcd for $C_{16}H_{22}NO_2[M+H]^+$: 260.1651; found: 260.1646.

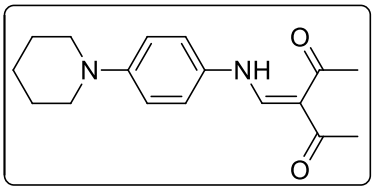
3-(((4-methoxyphenyl)amino)methylene)pentane-2,4-dione (3f)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (43.3 mg, 93%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.77 (d, *J* = 12.1 Hz, 1H), 8.13 (d, *J* = 12.8 Hz, 1H), 7.10 (d, *J* = 8.9 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 3.80 (s, 3H), 2.53 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.9, 194.7, 157.8, 152.5, 132.4, 119.5, 115.1, 112.8, 55.6, 32.0, 27.4.

HRMS (ESI, m/z) calcd for $C_{13}H_{16}NO_3[M+H]^+$: 234.1130; found: 234.1125.

3-(((4-(piperidin-1-yl)phenyl)amino)methylene)pentane-2,4-dione (3g)

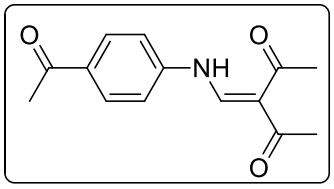


The reaction was performed following the general procedure. The residue was purified by flash column

chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (48.7 mg, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.79 (d, *J* = 12.6 Hz, 1H), 8.14 (d, *J* = 12.9 Hz, 1H), 7.12 – 7.02 (m, 2H), 6.96 – 6.85 (m, 2H), 3.19 – 3.09 (m, 4H), 2.54 (s, 3H), 2.35 (s, 3H), 1.70 (dt, *J* = 11.3, 5.7 Hz, 4H), 1.61 – 1.55 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.7, 194.7, 152.2, 150.5, 130.7, 119.1, 117.2, 112.5, 50.5, 32.0, 27.4, 25.7, 24.2.

HRMS (ESI, m/z) calcd for $C_{17}H_{23}N_2O_2[M+H]^+$: 287.1760; found: 287.1757.

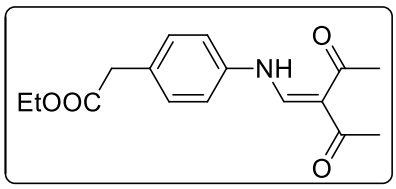
3-(((4-acetylphenyl)amino)methylene)pentane-2,4-dione (3h)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (37.7 mg, 77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.75 (d, *J* = 12.1 Hz, 1H), 8.25 (d, *J* = 12.5 Hz, 1H), 8.05 – 7.92 (m, 2H), 7.22 (d, *J* = 8.7 Hz, 2H), 2.57 (s, 3H), 2.53 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.6, 196.4, 195.0, 150.3, 142.8, 134.0, 130.5, 117.1, 114.4, 32.1, 27.4, 26.5.

HRMS (ESI, m/z) calcd for $C_{14}H_{16}N_3O_2[M+H]^+$: 246.1130; found: 246.1123.

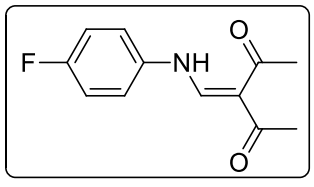
ethyl 2-(4-((2-acetyl-3-oxobut-1-en-1-yl)amino)phenyl)acetate (3i)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (41.6 mg, 72%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.74 (d, *J* = 12.5 Hz, 1H), 8.21 (d, *J* = 12.7 Hz, 1H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.14 (d, *J* = 8.5 Hz, 2H), 4.16 (q, *J* = 7.1 Hz, 2H), 3.61 (s, 2H), 2.55 (s, 3H), 2.37 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 194.8, 171.2, 151.9, 138.1, 131.8, 130.9, 118.1, 113.3, 61.1, 40.7, 32.1, 27.4, 14.2.

HRMS (ESI, m/z) calcd for $C_{16}H_{20}NO_4[M+H]^+$: 290.1392; found: 290.1388.

3-(((4-fluorophenyl)amino)methylene)pentane-2,4-dione (3j)

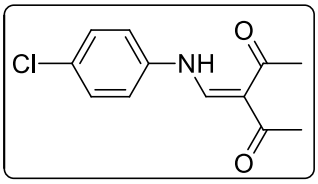


The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (37.6 mg, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.76 (d, *J* = 11.3 Hz, 1H),

8.13 (d, *J* = 12.6 Hz, 1H), 7.17 – 7.06 (m, 4H), 2.53 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 194.7, 161.5, 159.5, 152.3, 135.41 (d, *J* = 2.9 Hz), 119.67 (d, *J* = 8.3 Hz), 117.0, 116.8, 113.3, 32.0, 27.4.

HRMS (ESI, m/z) calcd for $C_{12}H_{13}FNO_2[M+H]^+$: 222.0930; found: 222.0928.

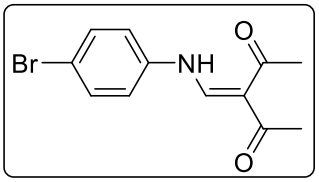
3-(((4-chlorophenyl)amino)methylene)pentane-2,4-dione (3k)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (42.3 mg, 89%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.73 (d, *J* = 11.9 Hz, 1H), 8.15 (d, *J* = 12.6 Hz, 1H), 7.48 – 7.27 (m, 2H), 7.19 – 7.05 (m, 2H), 2.53 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.3, 194.8, 151.5, 137.7, 131.1, 130.1, 119.0, 113.6, 32.1, 27.4.

HRMS (ESI, m/z) calcd for $C_{12}H_{13}ClNO_2[M+H]^+$: 238.0635; found: 238.0632.

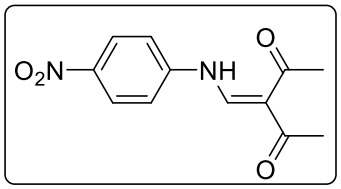
3-(((4-bromophenyl)amino)methylene)pentane-2,4-dione (3l)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (49 mg, 87%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.71 (d, *J* = 12.0 Hz, 1H), 8.15 (d, *J* = 12.6 Hz, 1H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.04 (d, *J* = 8.8 Hz, 2H), 2.52 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.3, 194.8, 151.3, 138.2, 133.0, 119.3, 118.6, 113.7, 32.1, 27.4.

HRMS (ESI, m/z) calcd for $C_{12}H_{13}BrNO_2[M+H]^+$: 282.0130; found: 282.0128.

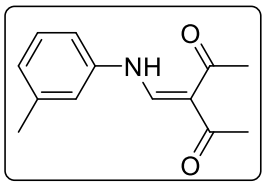
3-(((4-nitrophenyl)amino)methylene)pentane-2,4-dione (3m)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a yellow solid (38.2 mg, 77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.83 (d, *J* = 11.0 Hz, 1H), 8.29 (d, *J* = 8.7 Hz, 2H), 8.23 (d, *J* = 12.2 Hz, 1H), 7.32 – 7.23 (m, 2H), 2.56 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.9, 194.9, 149.5, 144.5, 144.4, 126.0, 117.2, 115.3, 32.2, 27.5.

HRMS (ESI, m/z) calcd for $C_{10}H_{14}N_3O_2[M+H]^+$: 208.1081; found: 208.1080.

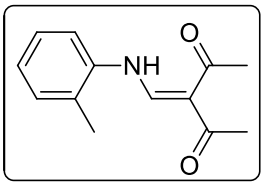
3-((m-tolylamino)methylene)pentane-2,4-dione (3n)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a yellow oil (36 mg, 83%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.70 (d, *J* = 11.7 Hz, 1H), 8.22 (d, *J* = 12.8 Hz, 1H), 7.31 – 7.25 (m, 1H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.99 – 6.94 (m, 2H), 2.54 (s, 3H), 2.37 (d, *J* = 2.0 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.1, 194.8, 151.9, 140.1, 139.0, 129.8, 126.7, 118.6, 114.9, 113.2, 32.1, 27.4, 21.5.

HRMS (ESI, m/z) calcd for $C_{13}H_{16}NO_2[M+H]^+$: 218.1181; found: 218.1180.

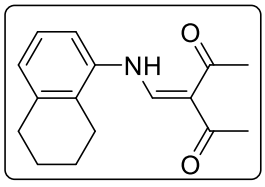
3-((o-tolylamino)methylene)pentane-2,4-dione (3o)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (34.3 mg, 79%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.95 (d, *J* = 10.8 Hz, 1H), 8.26 (d, *J* = 12.5 Hz, 1H), 7.31 – 7.20 (m, 3H), 7.14 (td, *J* = 7.4, 1.2 Hz, 1H), 2.57 (s, 3H), 2.39 (d, *J* = 7.2 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 194.8, 152.3, 137.8, 131.5, 128.3, 127.5, 125.8, 115.8, 113.4, 32.0, 27.4, 17.6.

HRMS (ESI, m/z) calcd for $C_{13}H_{16}NO_2[M+H]^+$: 218.1181; found: 218.1176.

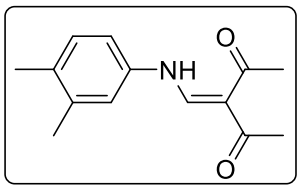
3-(((5,6,7,8-tetrahydronaphthalen-1-yl)amino)methylene)pentane-2,4-dione(3p)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (44.7 mg, 87%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.91 (d, *J* = 11.6 Hz, 1H), 8.26 (d, *J* = 12.5 Hz, 1H), 7.17 (t, *J* = 7.8 Hz, 1H), 7.06 (d, *J* = 7.9 Hz, 1H), 6.97 (d, *J* = 7.6 Hz, 1H), 2.79 (t, *J* = 6.2 Hz, 2H), 2.73 (t, *J* = 6.4 Hz, 2H), 2.57 (s, 3H), 2.37 (s, 3H), 1.92 – 1.86 (m, 2H), 1.80 – 1.76 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 194.8, 152.5, 139.5, 137.6, 127.5, 126.9, 126.4, 113.3, 113.1, 32.0, 29.8, 27.4, 24.4, 22.7, 22.4.

HRMS (ESI, m/z) calcd for $C_{16}H_{20}NO_2[M+H]^+$: 258.1494; found: 258.1491.

3-(((3,4-dimethylphenyl)amino)methylene)pentane-2,4-dione (3q)

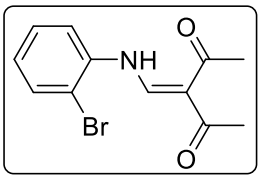


The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the

product as a white solid (35.2 mg, 76%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.70 (d, *J* = 12.0 Hz, 1H), 8.19 (d, *J* = 12.9 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 6.98 – 6.85 (m, 2H), 2.54 (s, 3H), 2.36 (s, 3H), 2.28 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.9, 194.8, 152.1, 138.5, 136.9, 134.5, 130.9, 119.3, 115.1, 112.9, 32.1, 27.4, 20.0, 19.3.

HRMS (ESI, m/z) calcd for $C_{14}H_{18}NO_2[M+H]^+$: 232.1338; found: 232.1334.

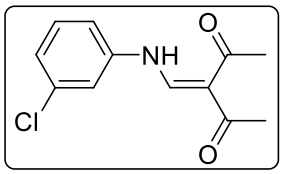
3-(((2-bromophenyl)amino)methylene)pentane-2,4-dione (3r)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a yellow oil (43.3 mg, 77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.00 (d, *J* = 11.3 Hz, 1H), 8.21 (d, *J* = 12.4 Hz, 1H), 7.62 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.43 – 7.35 (m, 1H), 7.30 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.12 – 7.02 (m, 1H), 2.57 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.1, 194.9, 150.7, 137.8, 133.8, 128.8, 126.4, 116.5, 114.6, 114.3, 32.0, 27.4.

HRMS (ESI, m/z) calcd for $C_{12}H_{13}BrNO_2[M+H]^+$: 282.0130; found: 282.0128.

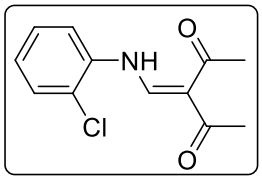
3-(((3-chlorophenyl)amino)methylene)pentane-2,4-dione (3s)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (34.2 mg, 72%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.69 (d, *J* = 11.8 Hz, 1H), 8.15 (d, *J* = 12.5 Hz, 1H), 7.31 (t, *J* = 8.3 Hz, 1H), 7.22 – 7.10 (m, 2H), 7.03 (ddd, *J* = 8.1, 2.0, 0.9 Hz, 1H), 2.52 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.4, 194.8, 151.2, 140.3, 135.8, 131.0, 125.6, 117.8, 116.2, 113.8, 32.1, 27.4.

HRMS (ESI, m/z) calcd for $C_{12}H_{13}ClNO_2[M+H]^+$: 238.0635; found: 238.0632.

3-(((2-chlorophenyl)amino)methylene)pentane-2,4-dione (3t)

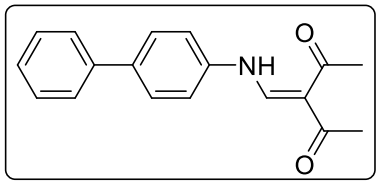


The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (37 mg, 78%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.04 (d, *J* = 11.4 Hz, 1H), 8.23 (d, *J* = 12.4 Hz, 1H), 7.50 – 7.41 (m, 1H), 7.32 (dt, *J* = 7.3, 3.6 Hz, 2H), 7.13 (ddd, *J* = 8.1, 6.3, 2.5 Hz, 1H), 2.56 (s, 3H), 2.39

(s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 194.9, 150.5, 136.3, 130.5, 128.1, 126.0, 124.6, 116.1, 114.3, 32.0, 27.4.

HRMS (ESI, m/z) calcd for $C_{12}H_{13}ClNO_2[M+H]^+$: 238.0635; found: 238.0632.

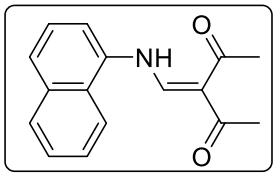
3-(([1,1'-biphenyl]-4-ylamino)methylene)pentane-2,4-dione (3u)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (48 mg, 86%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.82 (d, *J* = 12.5 Hz, 1H), 8.26 (d, *J* = 12.7 Hz, 1H), 7.66 – 7.60 (m, 2H), 7.59 – 7.53 (m, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 7.3 Hz, 1H), 7.27 – 7.21 (m, 2H), 2.57 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.2, 194.8, 151.5, 139.8, 138.8, 138.2, 129.0, 128.6, 127.6, 126.8, 118.2, 113.4, 32.1, 27.4.

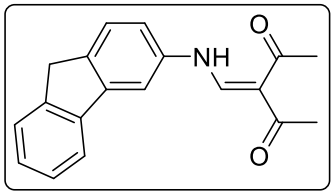
HRMS (ESI, m/z) calcd for $C_{18}H_{18}NO_2[M+H]^+$: 280.1338; found: 280.1336.

3-((naphthalen-1-ylamino)methylene)pentane-2,4-dione (3v)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (42 mg, 83%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.58 (d, *J* = 11.3 Hz, 1H), 8.37 (d, *J* = 12.2 Hz, 1H), 8.08 (d, *J* = 8.3 Hz, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.64 – 7.55 (m, 2H), 7.50 (t, *J* = 7.9 Hz, 1H), 7.36 (d, *J* = 7.4 Hz, 1H), 2.63 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.6, 194.9, 153.6, 135.6, 134.2, 128.6, 127.3, 127.1, 126.5, 125.7, 125.6, 120.8, 113.9, 32.1, 27.4.

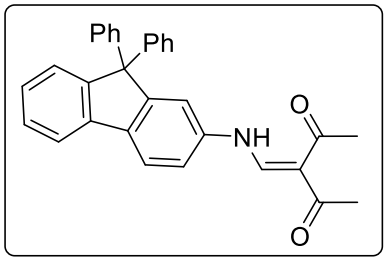
3-(((9H-fluoren-3-yl)amino)methylene)pentane-2,4-dione (3w)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (50 mg, 86%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.88 (d, *J* = 12.6 Hz, 1H), 8.26 (d, *J* = 12.7 Hz, 1H), 7.74 (dd, *J* = 7.7, 6.0 Hz, 2H), 7.53 (d, *J* = 7.4 Hz, 1H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.15 (dd, *J* = 8.2, 2.0 Hz, 1H), 3.89 (s, 2H), 2.57 (s, 3H), 2.40 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.1, 194.8, 151.6, 145.2, 143.0, 140.7, 139.7, 137.8, 127.1, 127.0, 125.1, 121.0, 119.8, 117.0, 114.4, 113.2, 37.0, 32.1, 27.5.

HRMS (ESI, m/z) calcd for $C_{19}H_{18}NO_2[M+H]^+$: 292.1338; found: 292.1335.

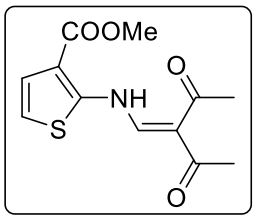
3-(((9,9-diphenyl-9H-fluoren-2-yl)amino)methylene)pentane-2,4-dion e (3x)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (72 mg, 81%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.84 (d, *J* = 12.6 Hz, 1H), 8.18 (d, *J* = 12.7 Hz, 1H), 7.81 – 7.77 (m, 1H), 7.75 (d, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.38 (td, *J* = 7.5, 0.9 Hz, 1H), 7.31 – 7.24 (m, 7H), 7.23 – 7.18 (m, 6H), 2.56 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.1, 194.8, 153.4, 151.7, 151.2, 145.3, 139.0, 138.6, 138.2, 128.5, 128.1, 128.0, 127.8, 127.1, 126.3, 121.6, 120.2, 117.1, 116.4, 113.3, 65.7, 32.1, 27.4.

HRMS (ESI, m/z) calcd for $C_{31}H_{26}NO_2[M+H]^+$: 444.1964; found: 444.1959.

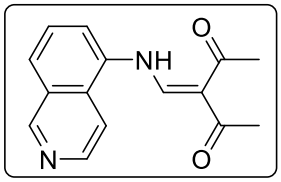
ethyl 2-((2-acetyl-3-oxobut-1-en-1-yl)amino)thiophene-3-carboxylate (3y)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (36.3 mg, 68%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.92 (d, *J* = 12.0 Hz, 1H), 7.90 (d, *J* = 12.4 Hz, 1H), 7.24 (d, *J* = 5.7 Hz, 1H), 6.74 (dd, *J* = 5.7, 0.6 Hz, 1H), 3.95 (s, 3H), 2.55 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.6, 195.0, 163.6, 152.1, 149.5, 127.6, 115.7, 115.1, 114.1, 52.2, 32.0, 27.3.

HRMS (ESI, m/z) calcd for $C_{12}H_{14}NS[M+H]^+$: 268.0644; found: 268.0638.

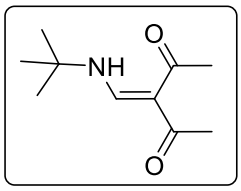
3-((isoquinolin-6-ylamino)methylene)pentane-2,4-dione (3z)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 50:1, v/v) to give the product as a white solid (33.5 mg, 66%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.61 (d, *J* = 11.9 Hz, 1H), 9.32 (s, 1H), 8.67 (d, *J* = 6.0 Hz, 1H), 8.38 (d, *J* = 12.0 Hz, 1H), 7.97 – 7.85 (m, 2H), 7.67 (t, *J* = 7.9 Hz, 1H), 7.60 (d, *J* = 7.4 Hz, 1H), 2.64 (s, 3H), 2.43 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 201.9, 153.0, 152.7, 144.3, 134.9, 129.1, 128.4, 127.3, 125.6, 117.1, 114.5, 113.8, 32.1, 27.5.

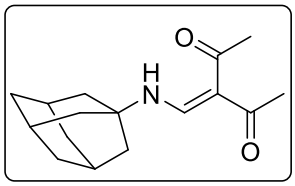
HRMS (ESI, m/z) calcd for $C_{15}H_{15}N_2O_2[M+H]^+$: 255.1134; found: 255.1133.

3-((tert-butylamino)methylene)pentane-2,4-dione (3aa CAS Number: 53630-82-3)[1]



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 10:1, v/v) to give the product as a white solid (27 mg, 74%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.41 (d, *J* = 4.3 Hz, 1H), 7.87 (d, *J* = 13.7 Hz, 1H), 2.45 (s, 3H), 2.26 (s, 3H), 1.36 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.1, 194.5, 155.4, 111.0, 53.7, 32.0, 29.8, 27.5.

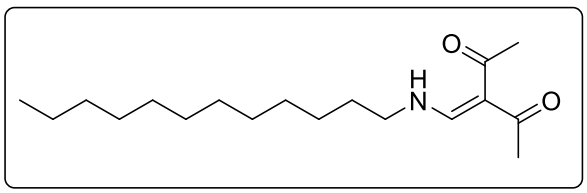
3-((adamantan-1-ylamino)methylene)pentane-2,4-dione (3ab)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 10:1, v/v) to give the product as a white solid (38.6 mg, 74%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.35 (d, *J* = 11.7 Hz, 1H), 7.87 (d, *J* = 13.8 Hz, 1H), 2.45 (s, 3H), 2.25 (s, 3H), 1.83 (d, *J* = 2.5 Hz, 7H), 1.69 (dd, *J* = 38.5, 12.0 Hz, 8H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.0, 194.5, 154.4, 111.0, 53.8, 42.9, 35.7, 32.0, 29.2, 27.5.

HRMS (ESI, m/z) calcd for $C_{16}H_{24}NO_2[M+H]^+$: 262.1807; found: 262.1804.

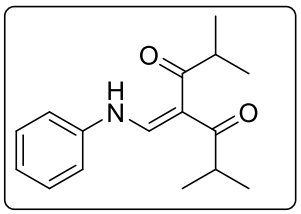
4-((dodecylamino)methylene)-2,6-dimethylheptane-3,5-dione (3ac)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 10:1, v/v) to give the product as a yellow oil (30.7 mg, 52%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.06 (s, 1H), 7.72 (d, *J* = 13.3 Hz, 1H), 3.34 (q, *J* = 6.8 Hz, 2H), 2.47 (s, 3H), 2.25 (s, 3H), 1.61 (dd, *J* = 14.6, 7.1 Hz, 2H), 1.39 – 1.20 (m, 20H), 0.87 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 200.3, 194.3, 159.9, 111.3, 50.5, 31.9, 31.9, 30.6, 29.6, 29.5, 29.4, 29.3, 29.1, 27.3, 26.5, 22.7, 14.1.

HRMS (ESI, m/z) calcd for $C_{18}H_{34}NO_2[M+H]^+$: 296.2590; found: 296.2594.

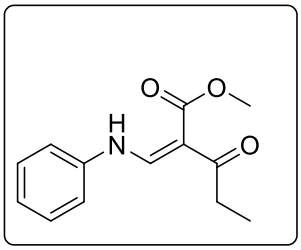
2,6-dimethyl-4-((phenylamino)methylene)heptane-3,5-dione (3ad)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 10:1, v/v) to give the product as a yellow oil (42 mg, 81%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.67 (d, *J* = 12.0 Hz, 1H), 8.19 (d, *J* = 12.6 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.24 – 7.12 (m, 3H), 3.70 (dt, *J* = 13.5, 6.8 Hz, 1H), 3.15 (dt, *J* = 13.5, 6.8 Hz, 1H), 1.19 (d, *J* = 6.8 Hz, 6H), 1.11 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 208.8, 202.4, 150.4, 139.3, 130.0, 129.4, 126.2, 125.5, 120.4, 117.6, 111.1, 37.8 35.9, 19.9, 19.4.

HRMS (ESI, m/z) calcd for $C_{16}H_{22}NO[M+H]^+$: 260.1651; found: 260.1644.

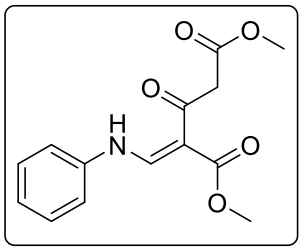
methyl-3-oxo-2-((phenylamino)methylene)pentanoate (3ae)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 10:1, v/v) to give the product as a yellow oil (32.6 mg, 70%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.67 (d, *J* = 12.0 Hz, 1H), 8.19 (d, *J* = 12.6 Hz, 1H), 7.41 – 7.36 (m, 2H), 7.24 – 7.12 (m, 3H), 3.70 (dt, *J* = 13.5, 6.8 Hz, 1H), 3.15 (dt, *J* = 13.5, 6.8 Hz, 1H), 1.19 (d, *J* = 6.8 Hz, 6H), 1.11 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 203.4, 167.3, 152.0, 139.1, 129.9, 125.5, 117.7, 102.0, 51.2, 35.5, 8.7.

HRMS (ESI, m/z) calcd for $C_{13}H_{16}NO_3[M+H]^+$: 234.1130; found: 234.1128.

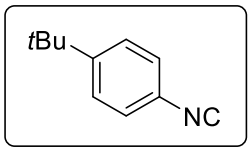
dimethyl-3-oxo-2-((phenylamino)methylene)pentanedioate (3af)



The reaction was performed following the general procedure. The residue was purified by flash column chromatograph (silica gel, petroleum ether:AcOEt = 10:1, v/v) to give the product as a yellow oil (26.6 mg, 48%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 12.70 (d, *J* = 12.9 Hz, 1H), 8.56 (d, *J* = 13.5 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.25 – 7.19 (m, 3H), 3.98 (s, 2H), 3.77 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.0, 169.4, 166.8, 153.0, 138.7, 123.0, 126.2, 118.1, 101.6, 52.1, 51.4, 49.1.

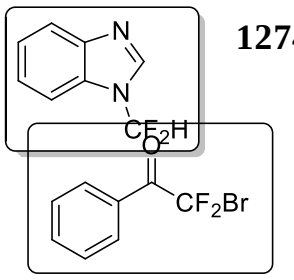
HRMS (ESI, m/z) calcd for $C_{14}H_{15}NO_5[M+H]^+$: 278.1028; found: 278.1025.

1-(*tert*-butyl)-4-isocyanobenzene (2,CAS Number: 602262-03-3)[2]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.37 (m, 2H), 7.30 (d, *J* = 8.5 Hz, 2H), 1.31 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1, 152.8, 126.4, 126.0, 34.9, 31.1, 26.9.

2-bromo-2,2-difluoro-1-phenylethan-1-one (3, CAS Number: 127427-45-6)[3]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.62 – 7.54 (m, 2H), 7.44 – 7.36 (m, 2H), 7.23 (d, *J* = 7.5 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.53 (t, *J* = 4.1 Hz), 135.3, 129.4, 126.3, 120.4, 111.5 (t, *J* = 315 Hz), 100.0.

1-(difluoromethyl)-1*H*-benzo[*d*]imidazole (Q)[4]

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (s, 1H), 7.93 – 7.76 (m, 1H), 7.61 (dd, *J* = 5.4, 3.6 Hz, 1H), 7.37 (ddd, *J* = 85.8, 55.8, 43.2 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.9, 139.1, 130.6, 124.8, 124.2, 121.0, 111.1, 109.0 (t, *J* = 248.8 Hz) ^{19}F NMR (470 MHz, $CDCl_3$) δ -93.7.

7. References

1. Ito,Y.; Inubushi, Y.; Seagusa, T. *Tetrahedron Lett.* **2001**, *15*, 1283.

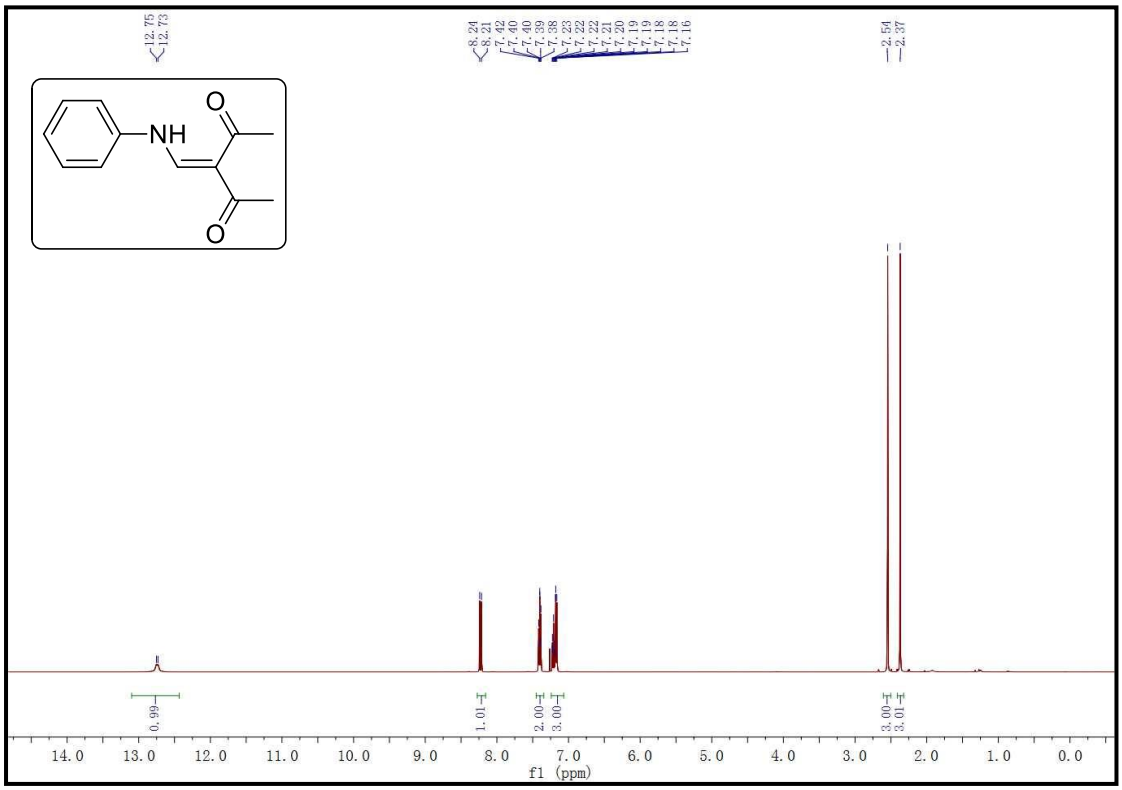
2. Leifert, D.; Artiukhin, D. G.; Neugebauer, J.; Galstyan, A.; Strasserta, C. A.; Studer, A. *Chem. Commun.* **2016**, *52*, 5997.

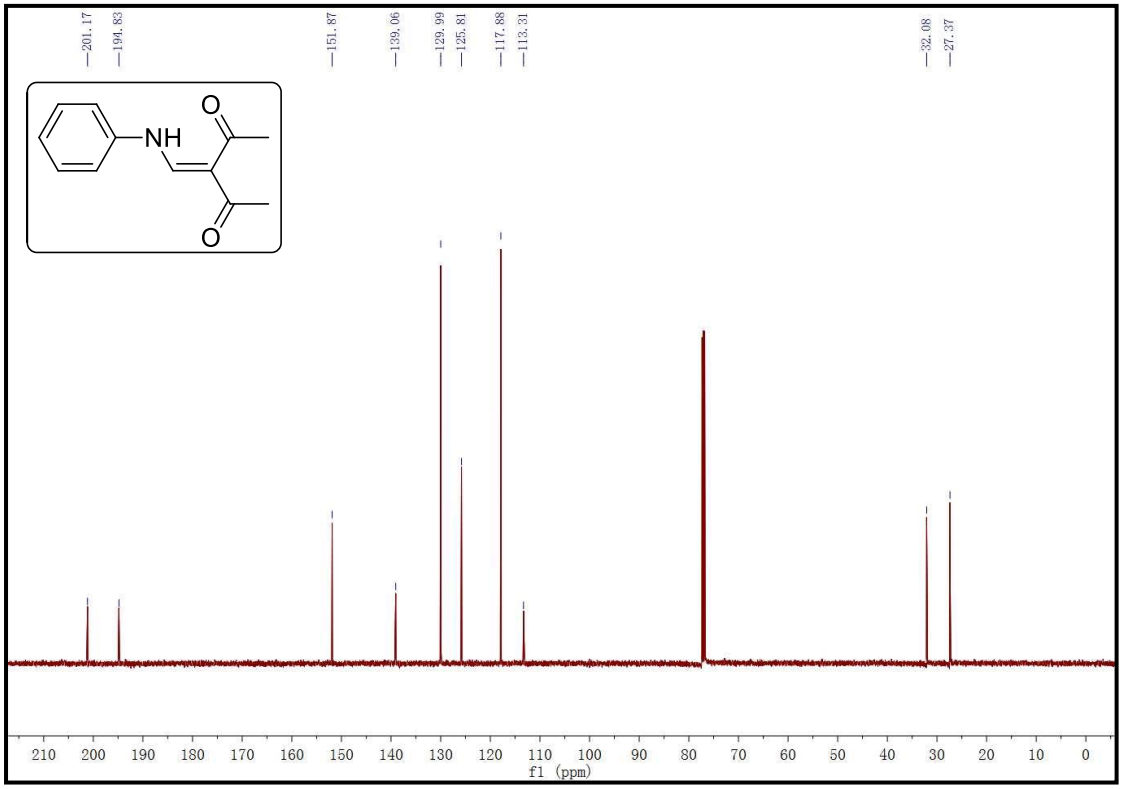
3. Ke, M.; Song, Q. *Chem. Commun.* **2017**, *53*, 2222.

4. Prakash, G. K. S.; Krishnamoorthy, S.; Ganesh, S.; K.; Kulkarni, A.; Haiges, R.; G.; Olah, A. *Org. Lett.* **2014**, *16*, 54.

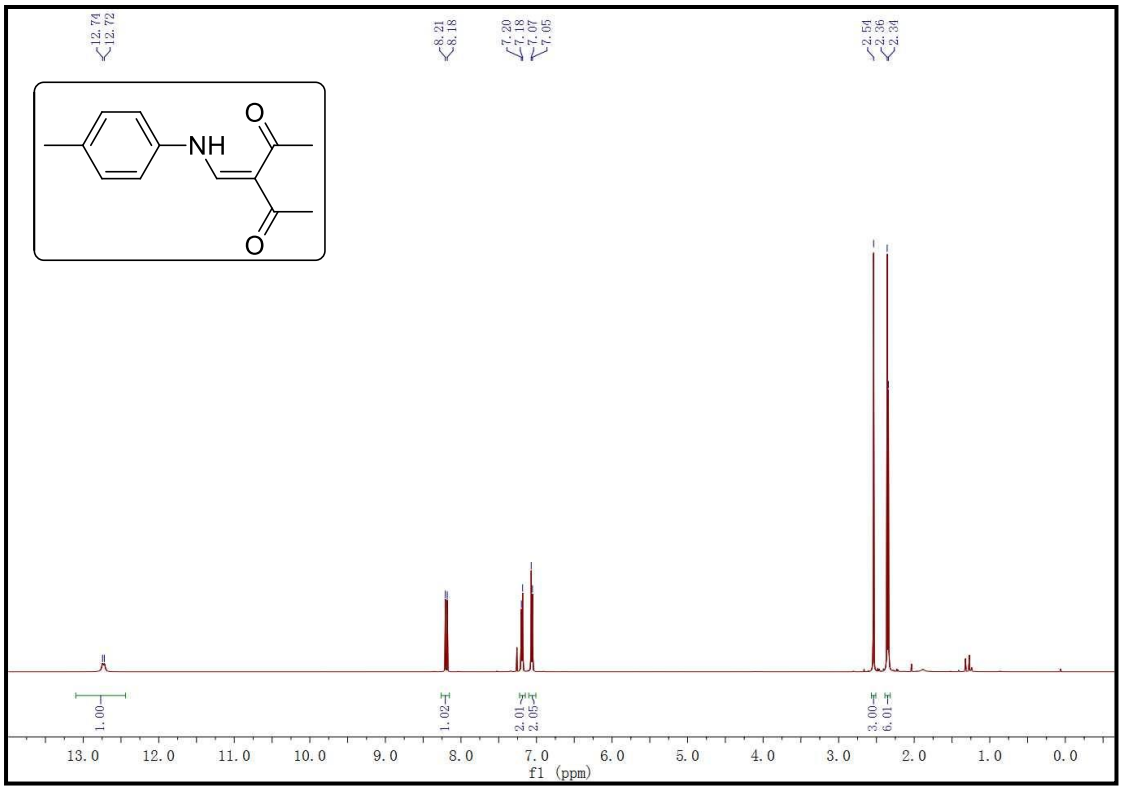
8. NMR spectroscopic data

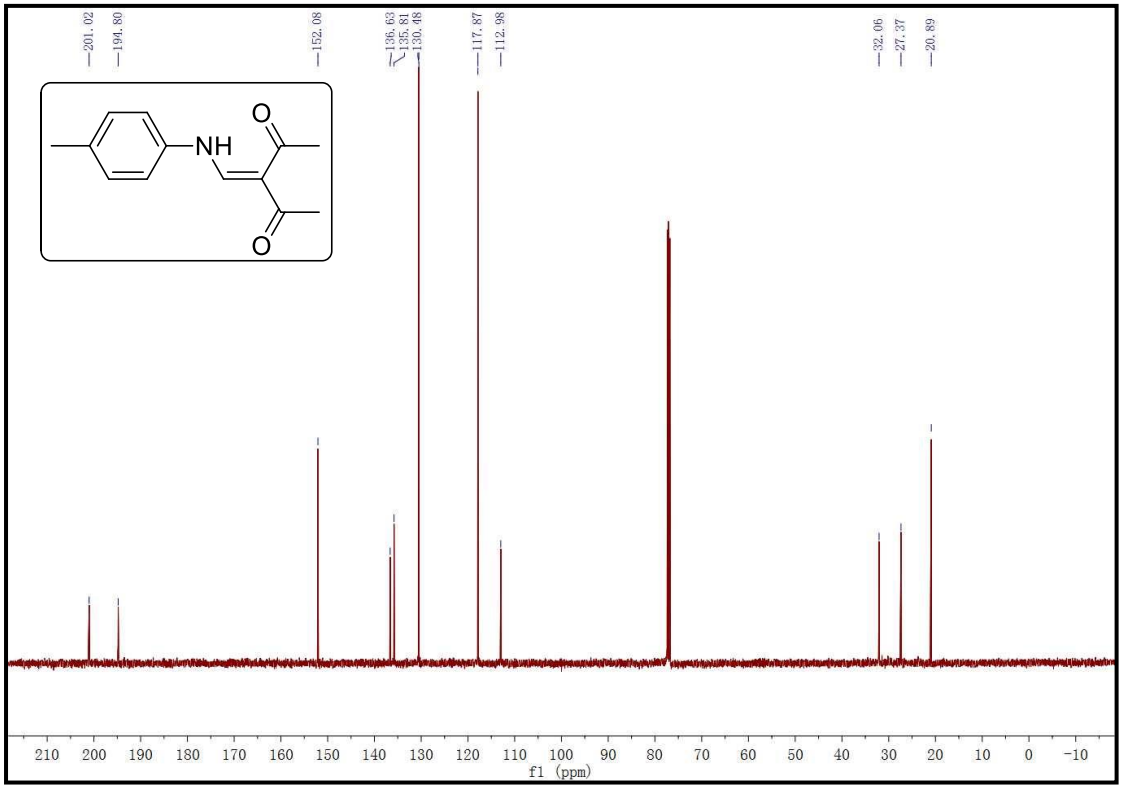
3-((phenylamino)methylene)pentane-2,4-dione (3a)



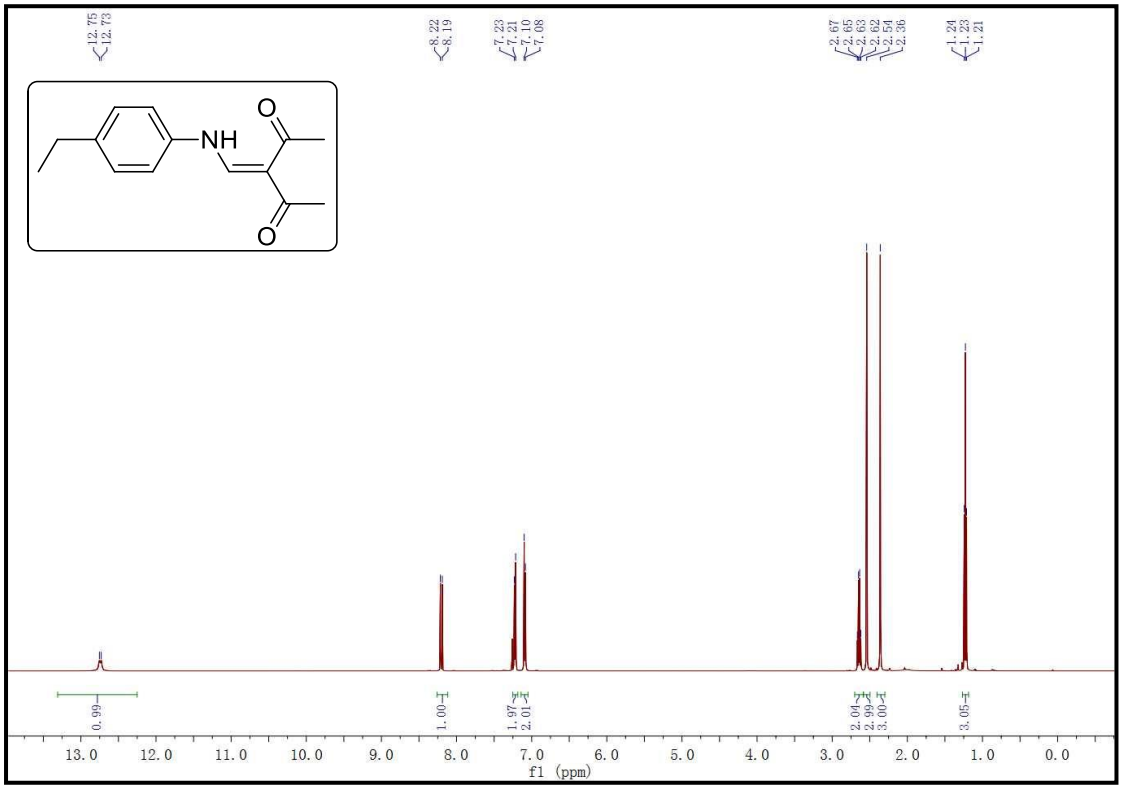


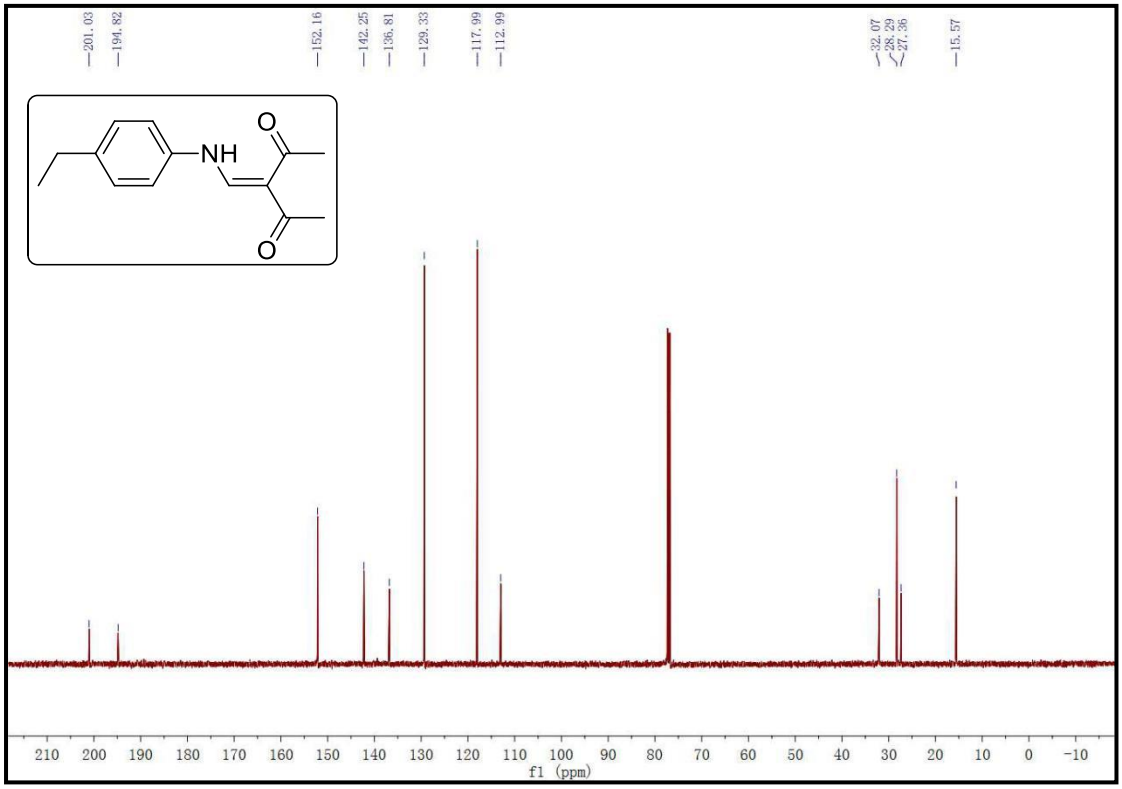
3-((p-tolylamino)methylene)pentane-2,4-dione (3b)



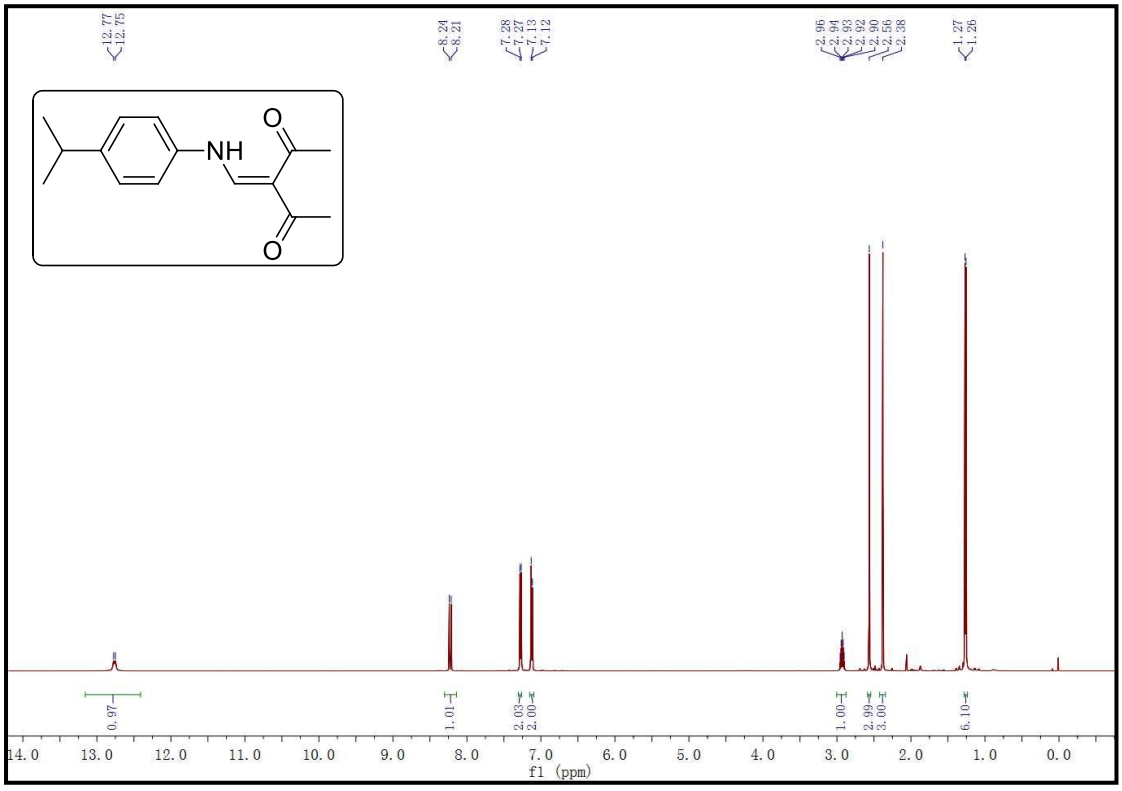


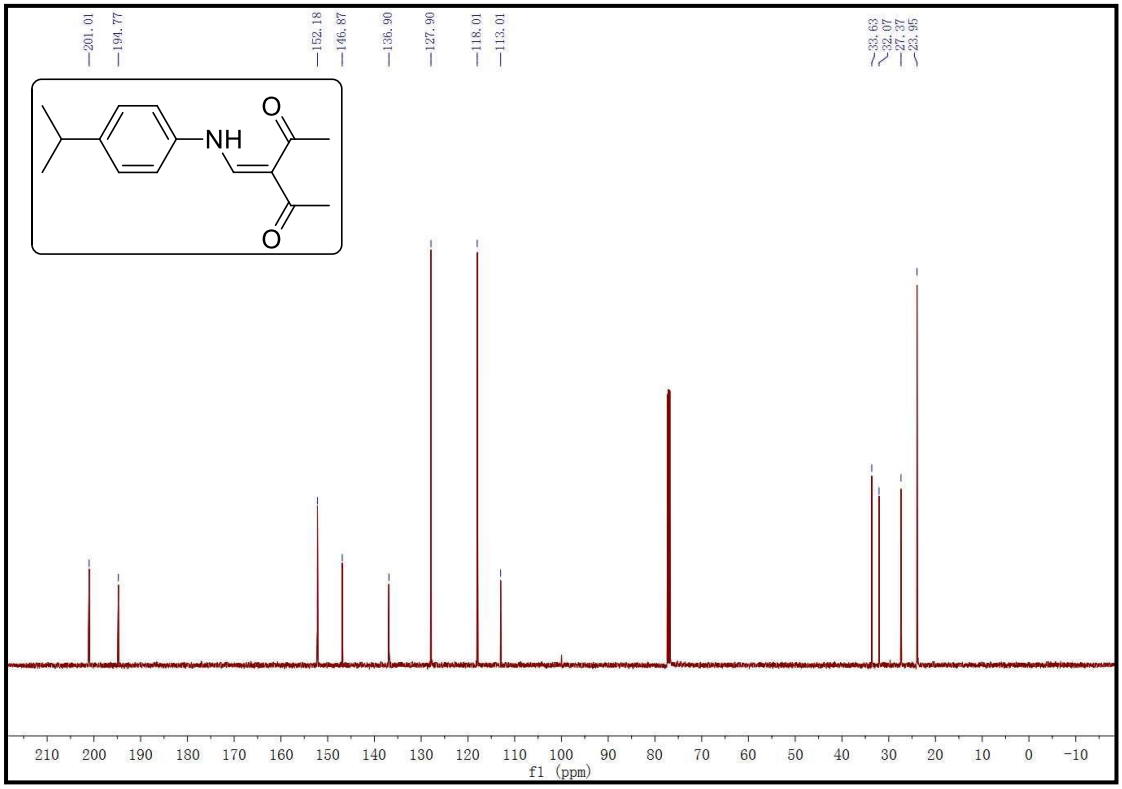
3-(((4-ethylphenyl)amino)methylene)pentane-2,4-dione (3c)



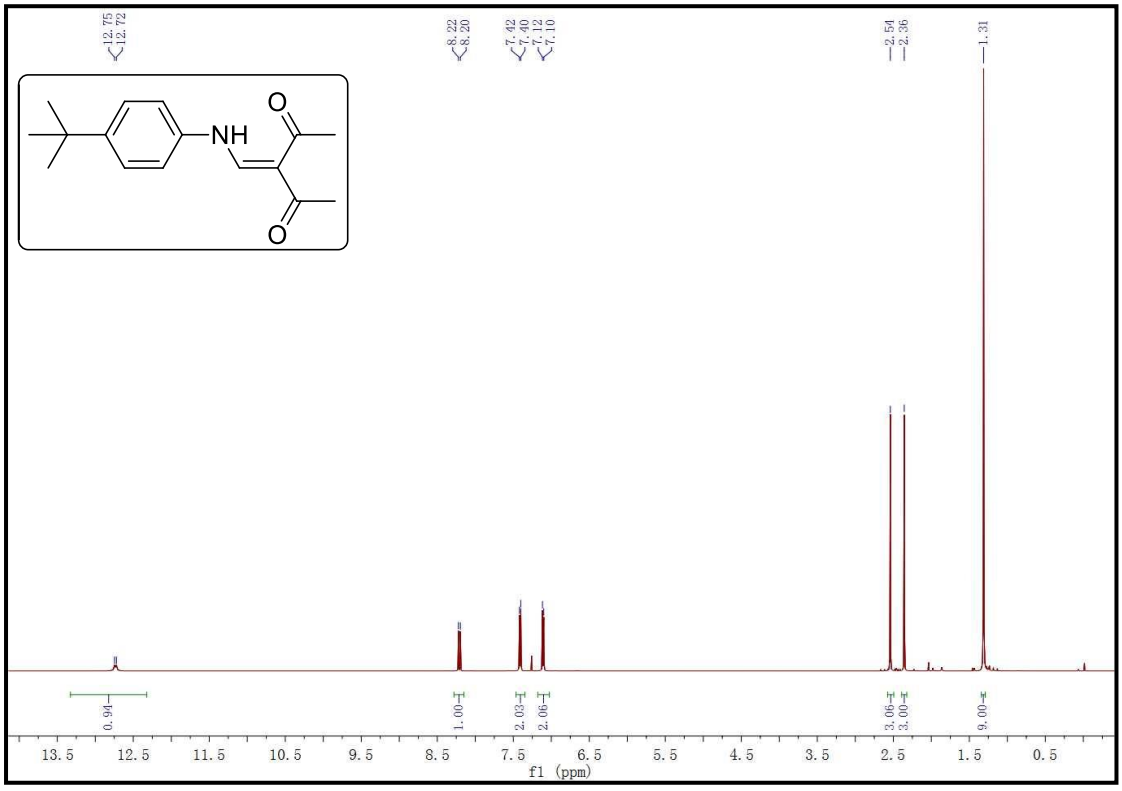


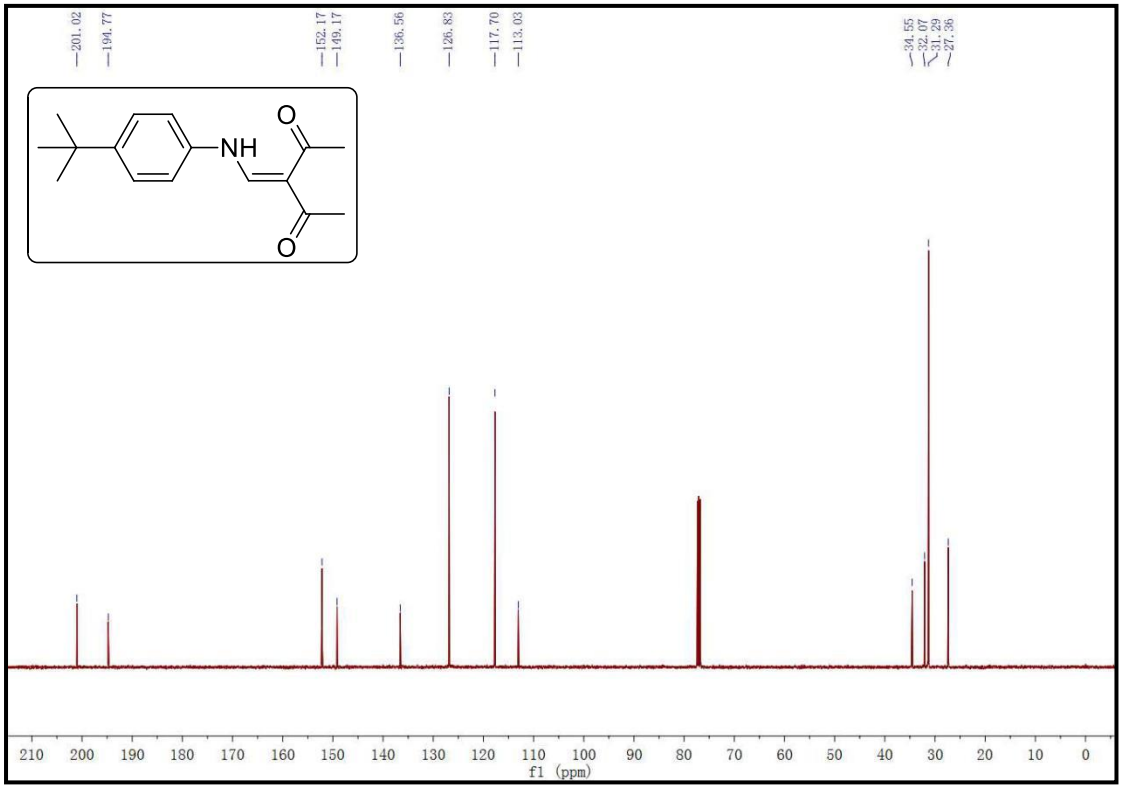
3-(((4-isopropylphenyl)amino)methylene)pentane-2,4-dione (3d)



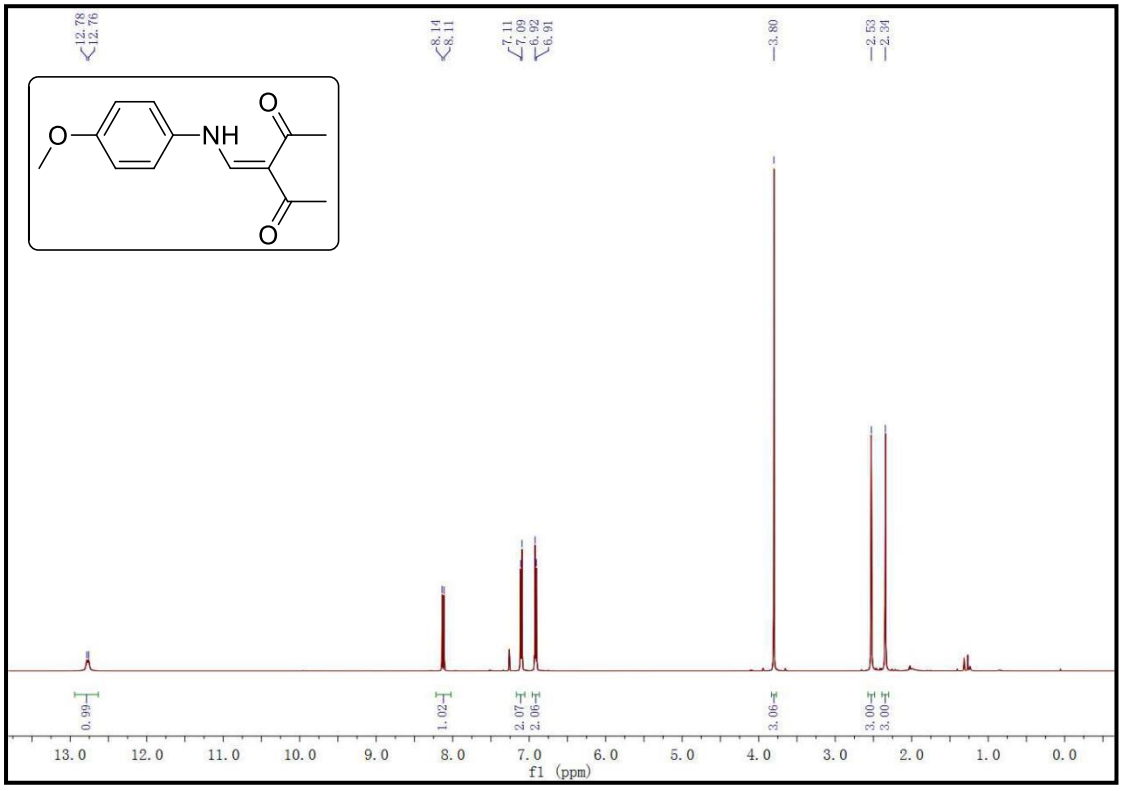


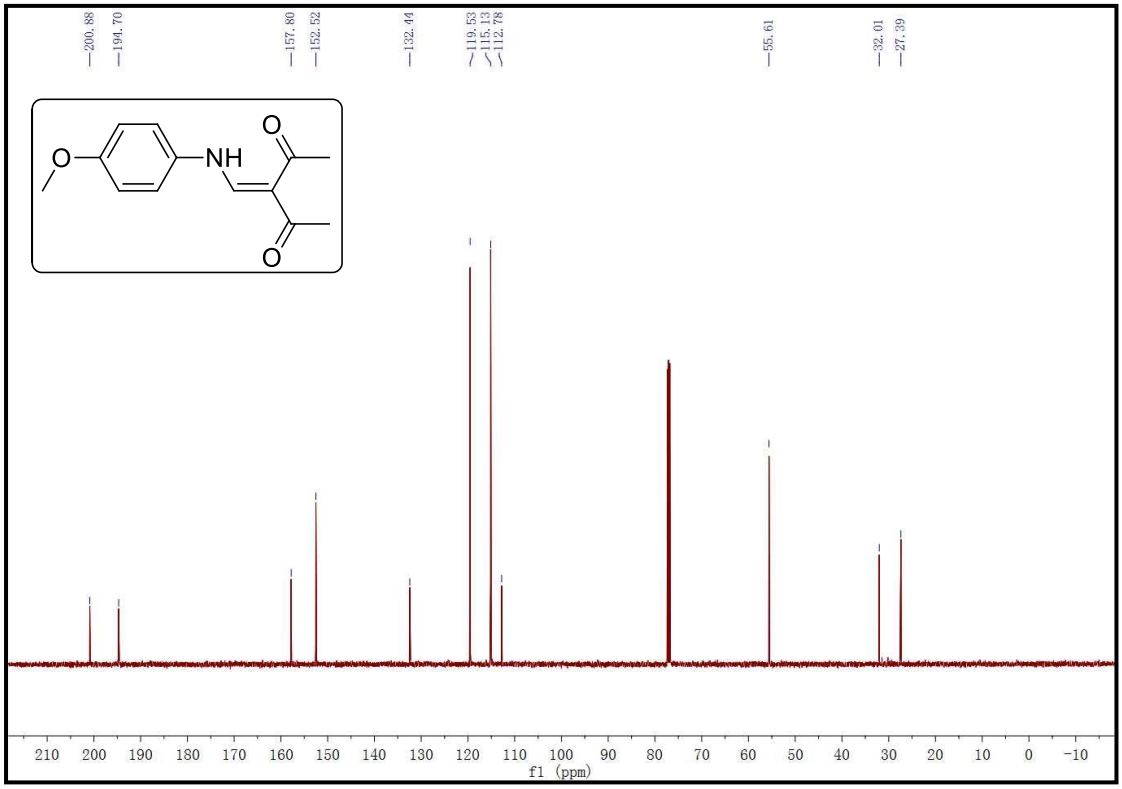
3-(((4-(tert-butyl)phenyl)amino)methylene)pentane-2,4-dione (3e)



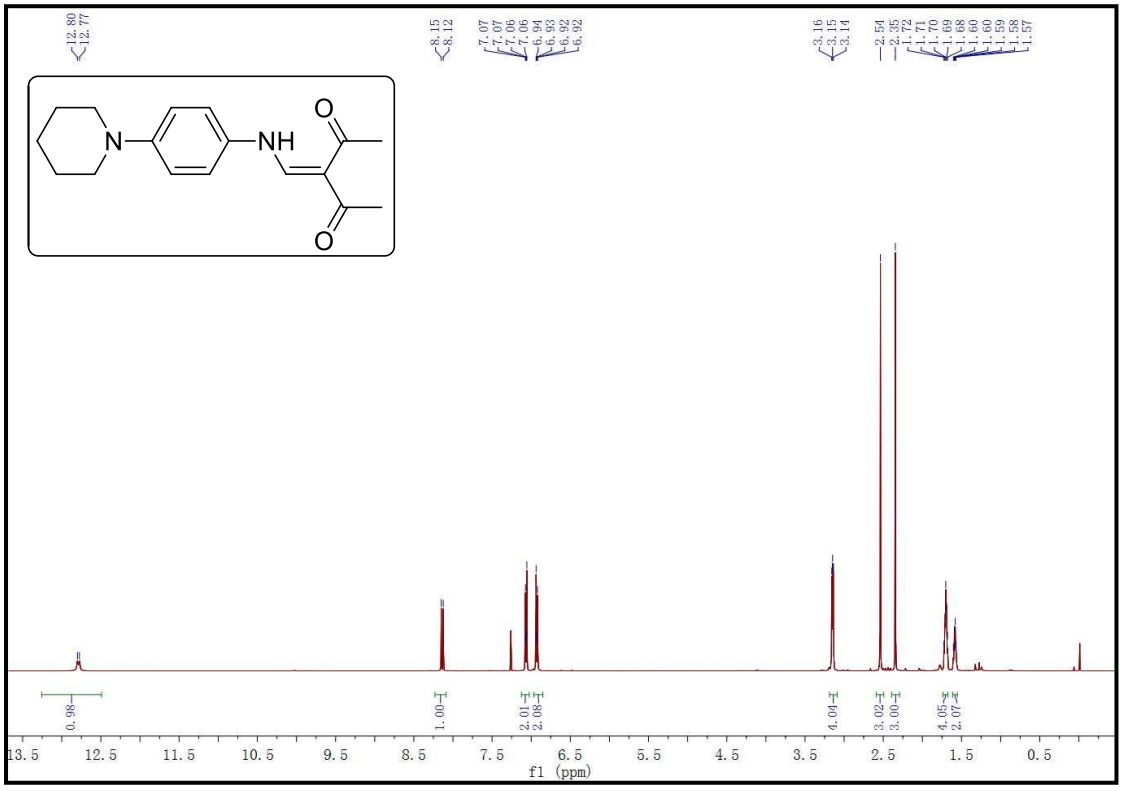


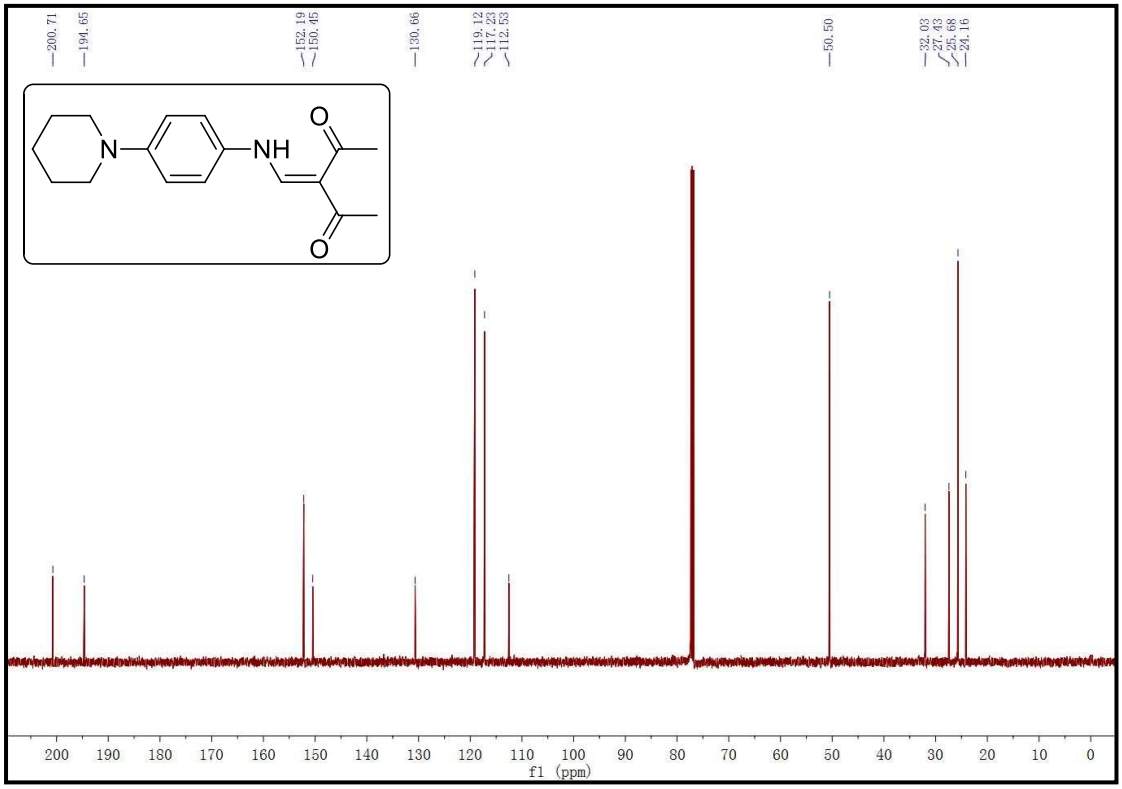
3-(((4-methoxyphenyl)amino)methylene)pentane-2,4-dione (3f)



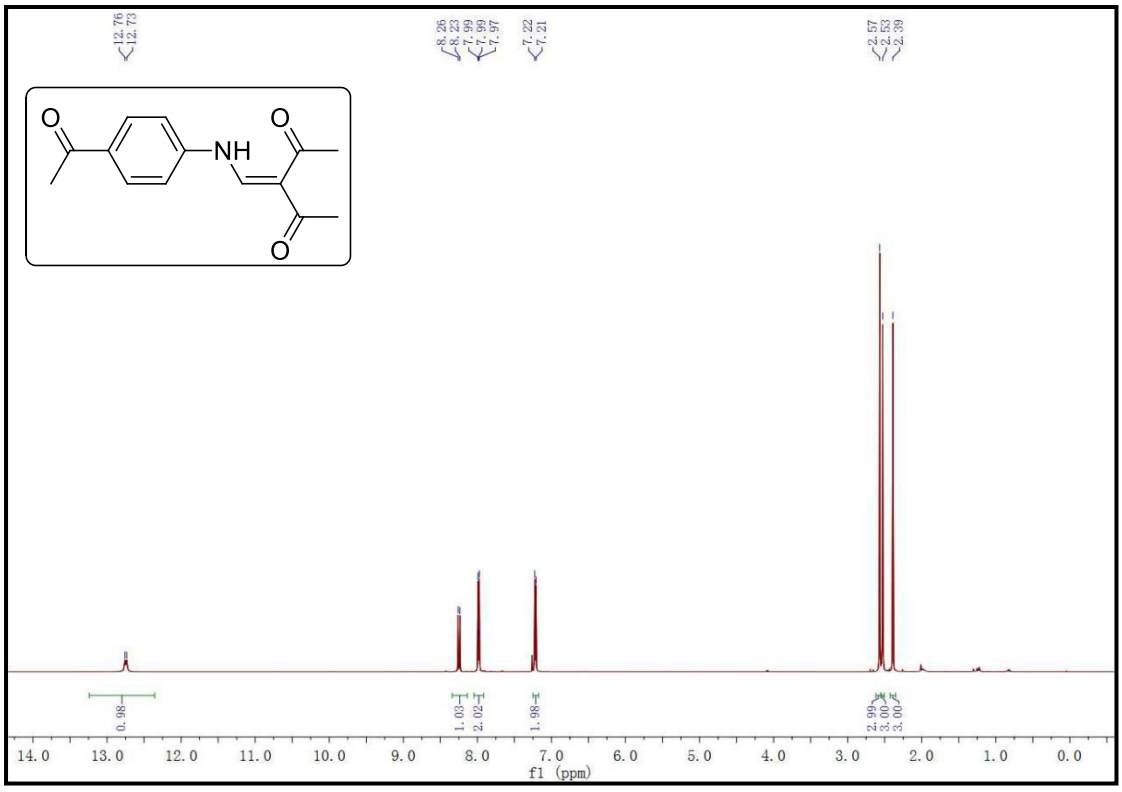


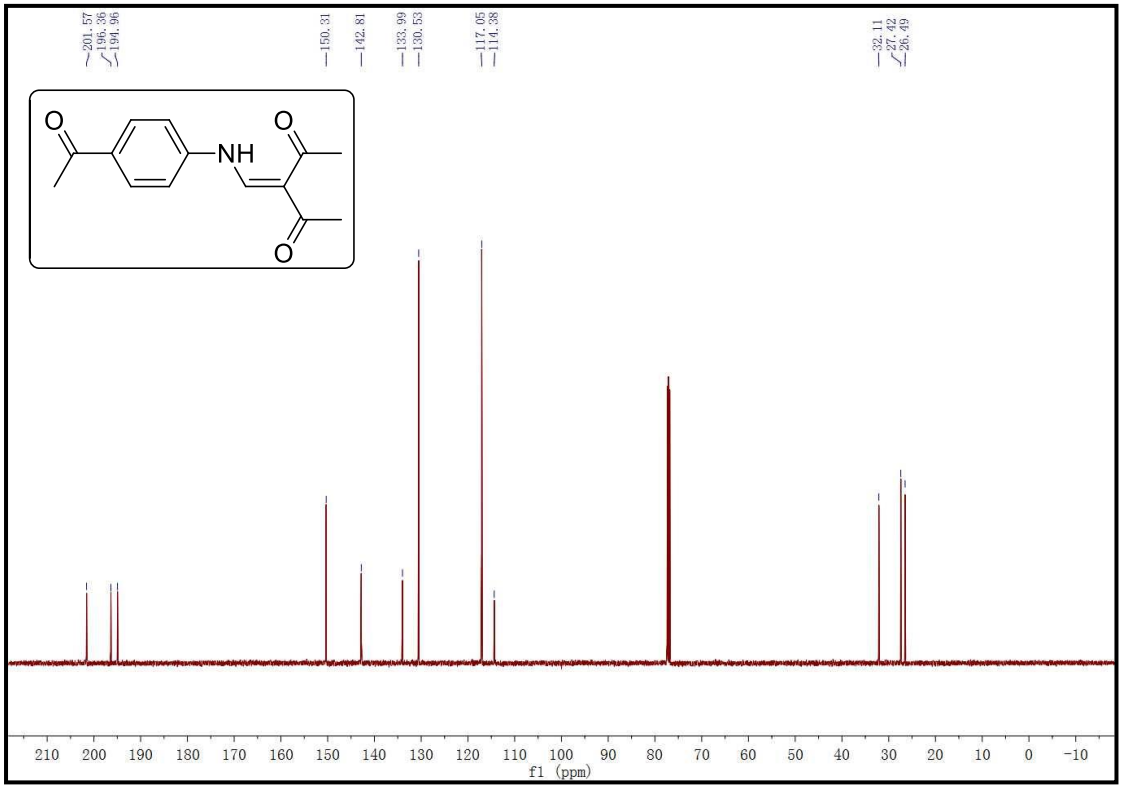
3-(((4-(piperidin-1-yl)phenyl)amino)methylene)pentane-2,4-dione (3g)



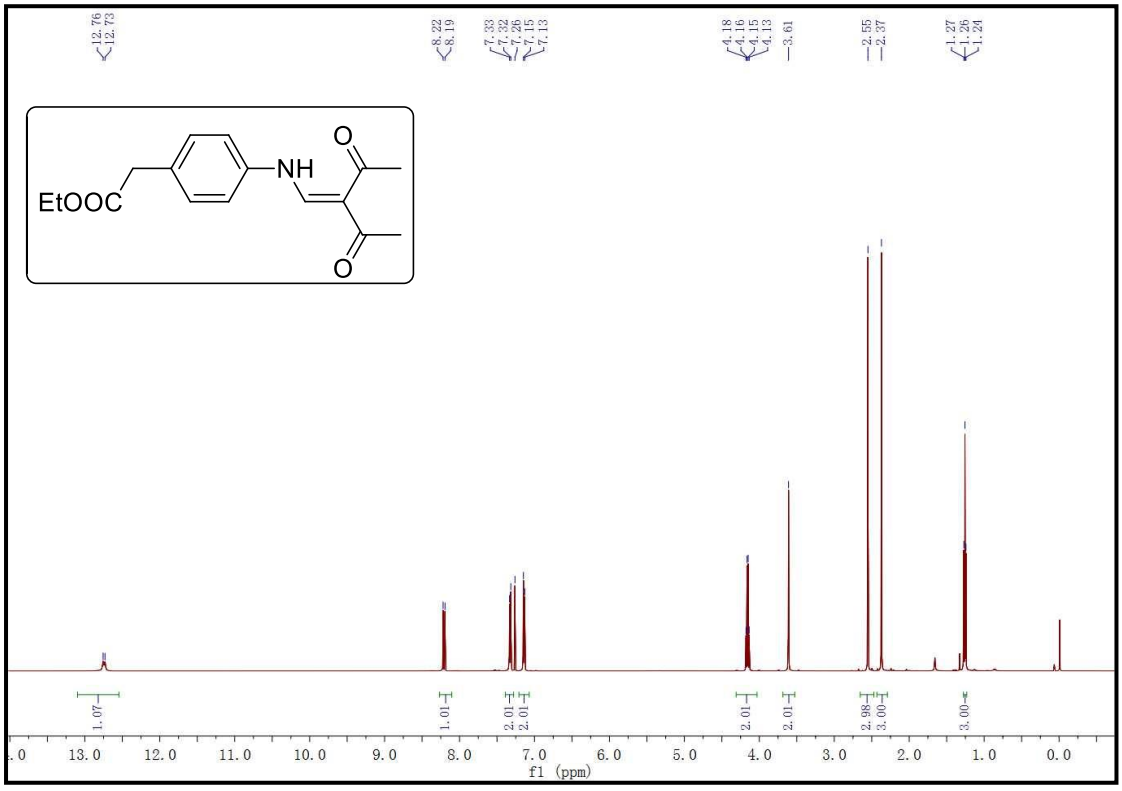


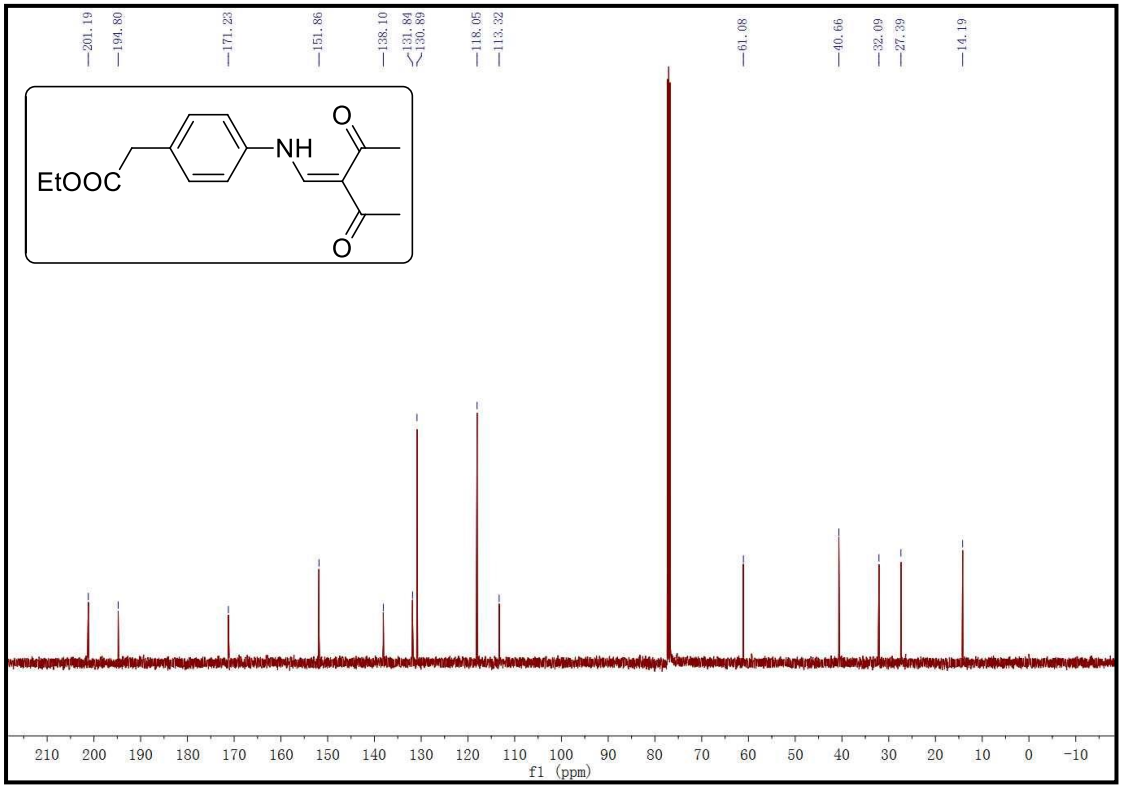
3-(((4-acetylphenyl)amino)methylene)pentane-2,4-dione (3h)



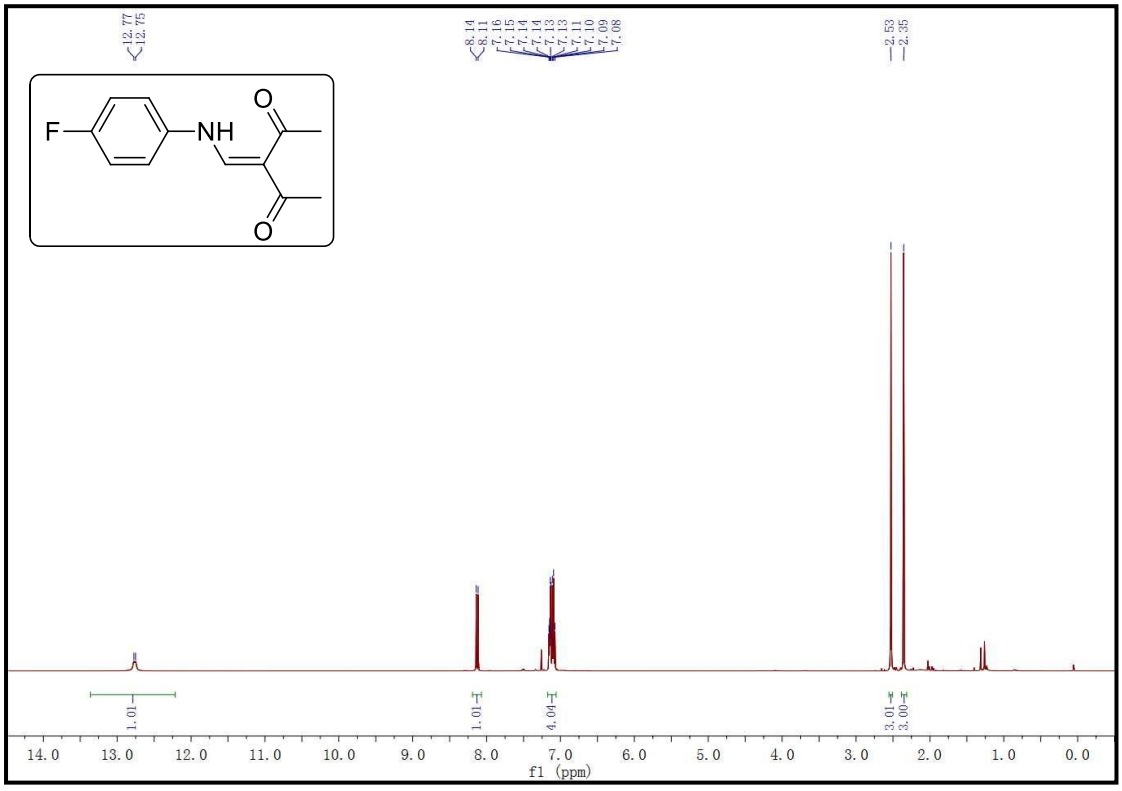


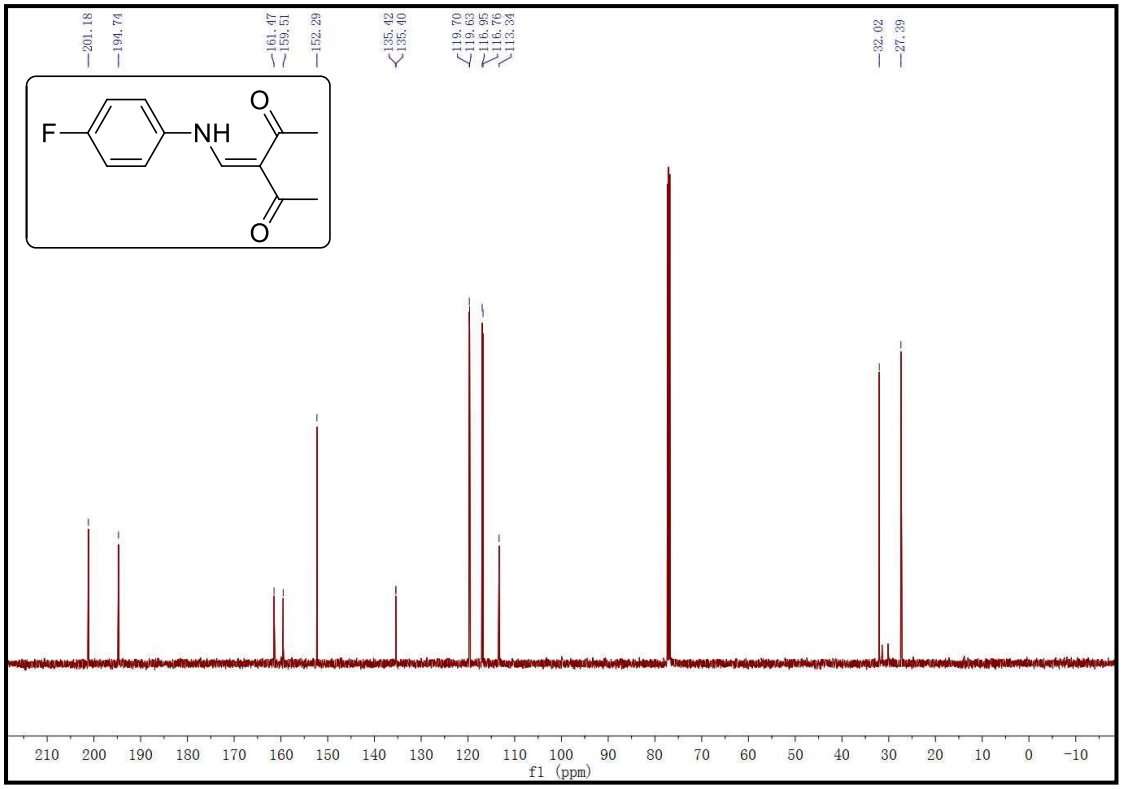
ethyl 2-(4-((2-acetyl-3-oxobut-1-en-1-yl)amino)phenyl)acetate (3i)



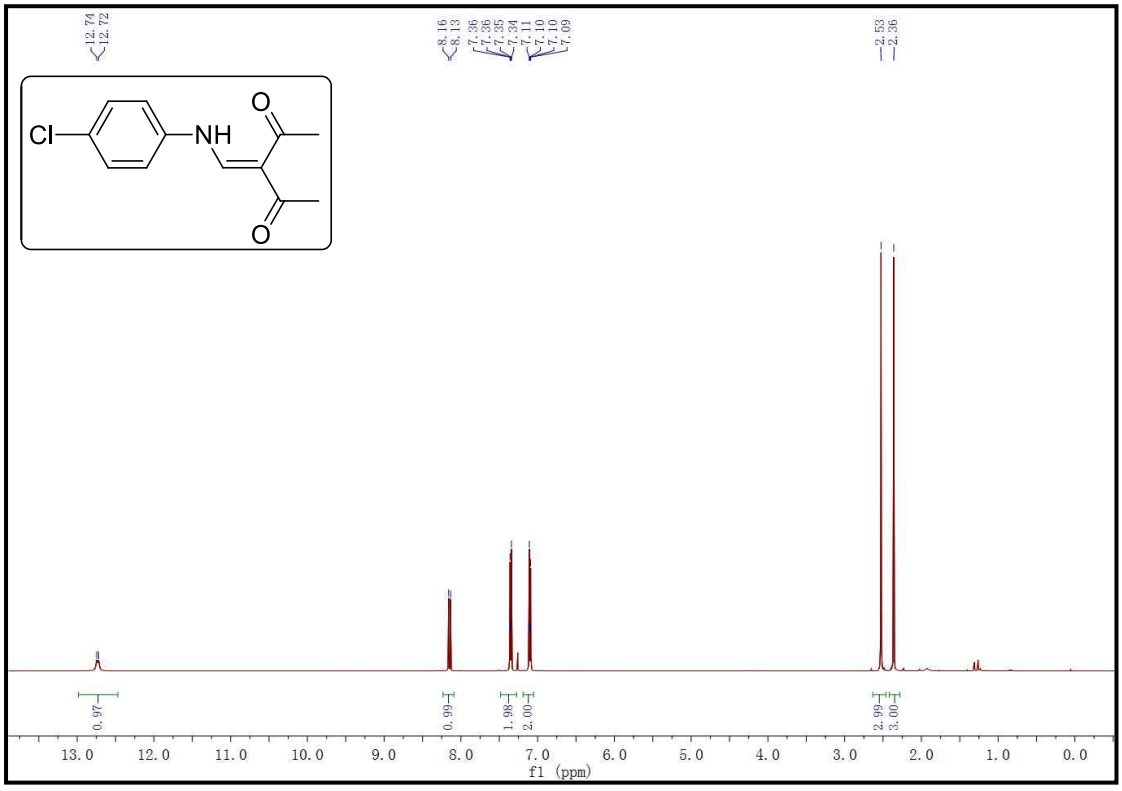


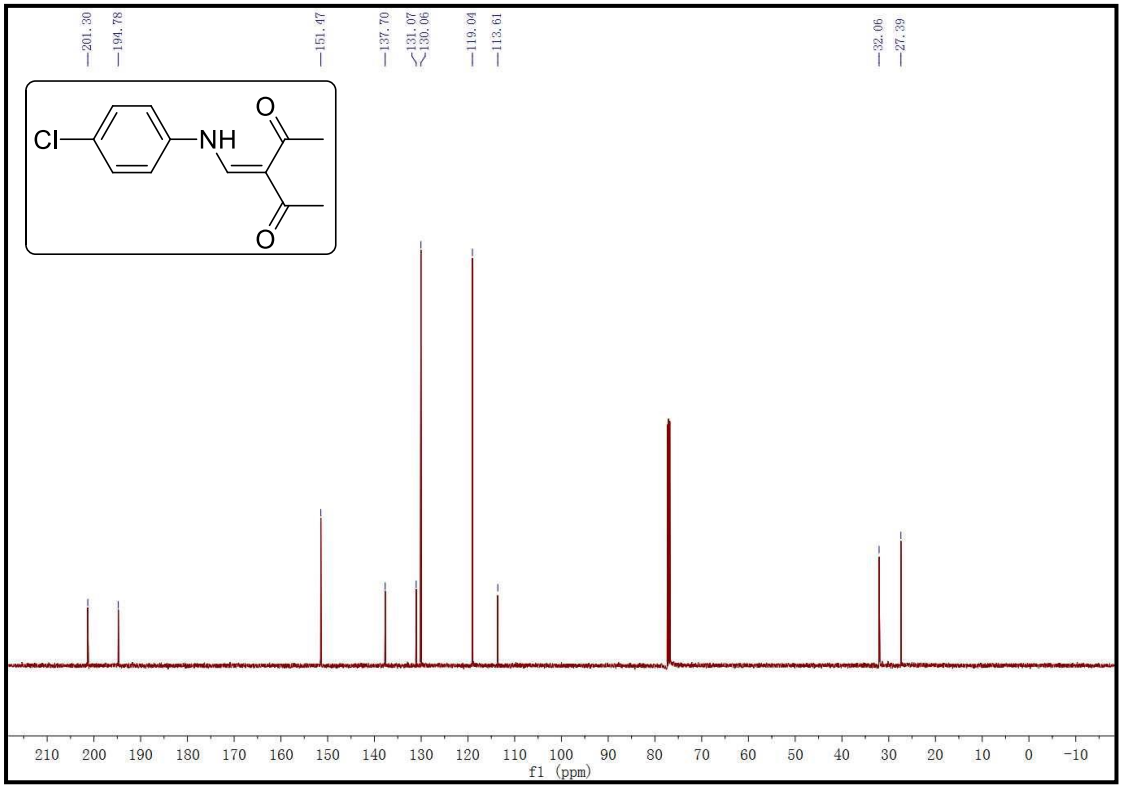
3-(((4-fluorophenyl)amino)methylene)pentane-2,4-dione (3j)



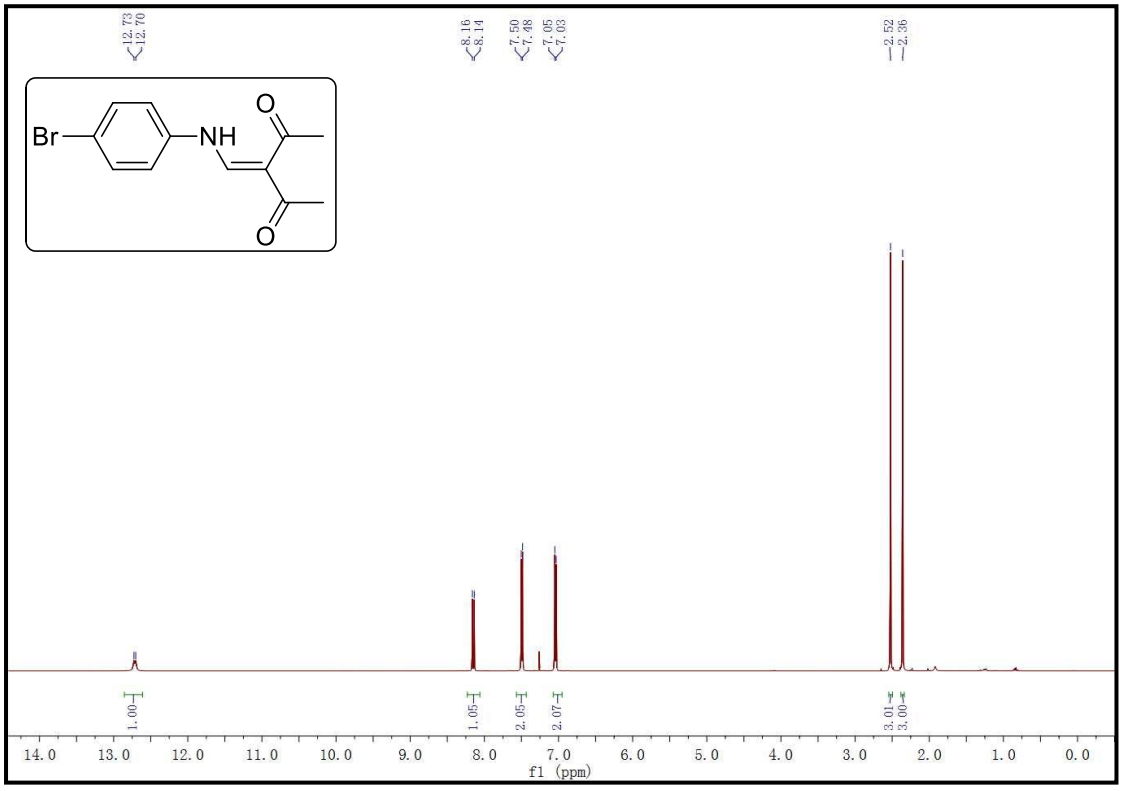


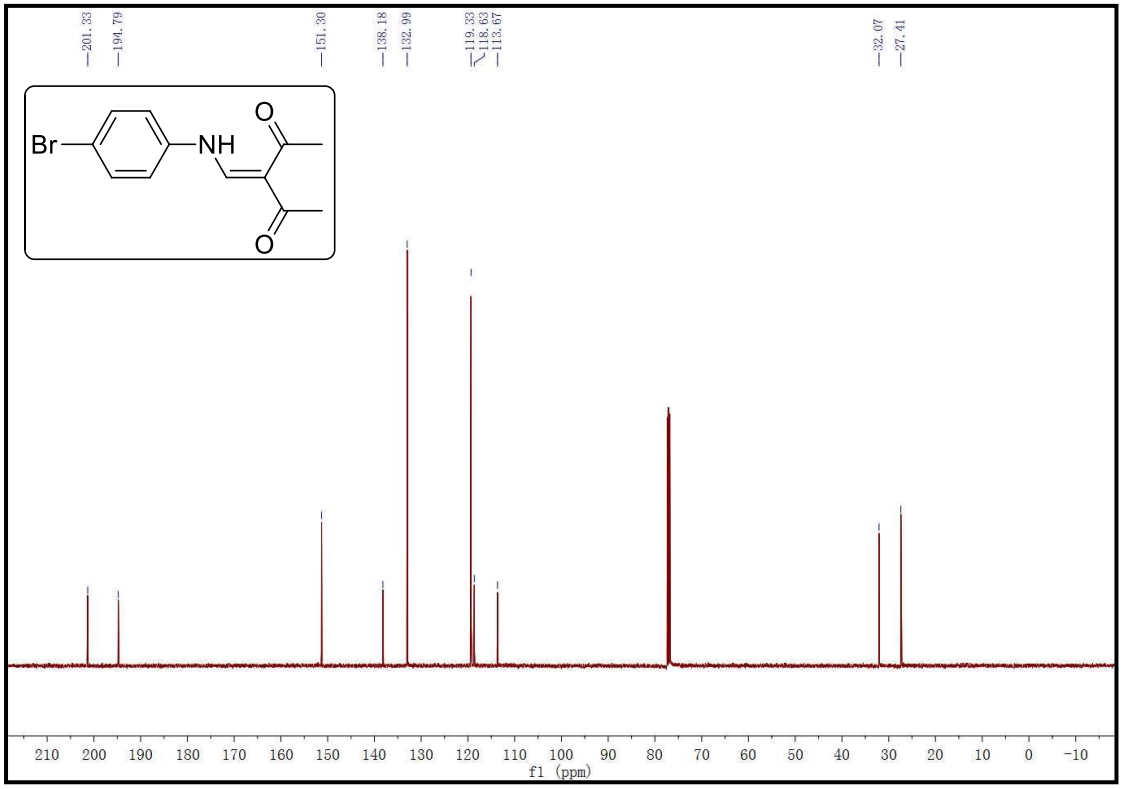
3-(((4-chlorophenyl)amino)methylene)pentane-2,4-dione (3k)



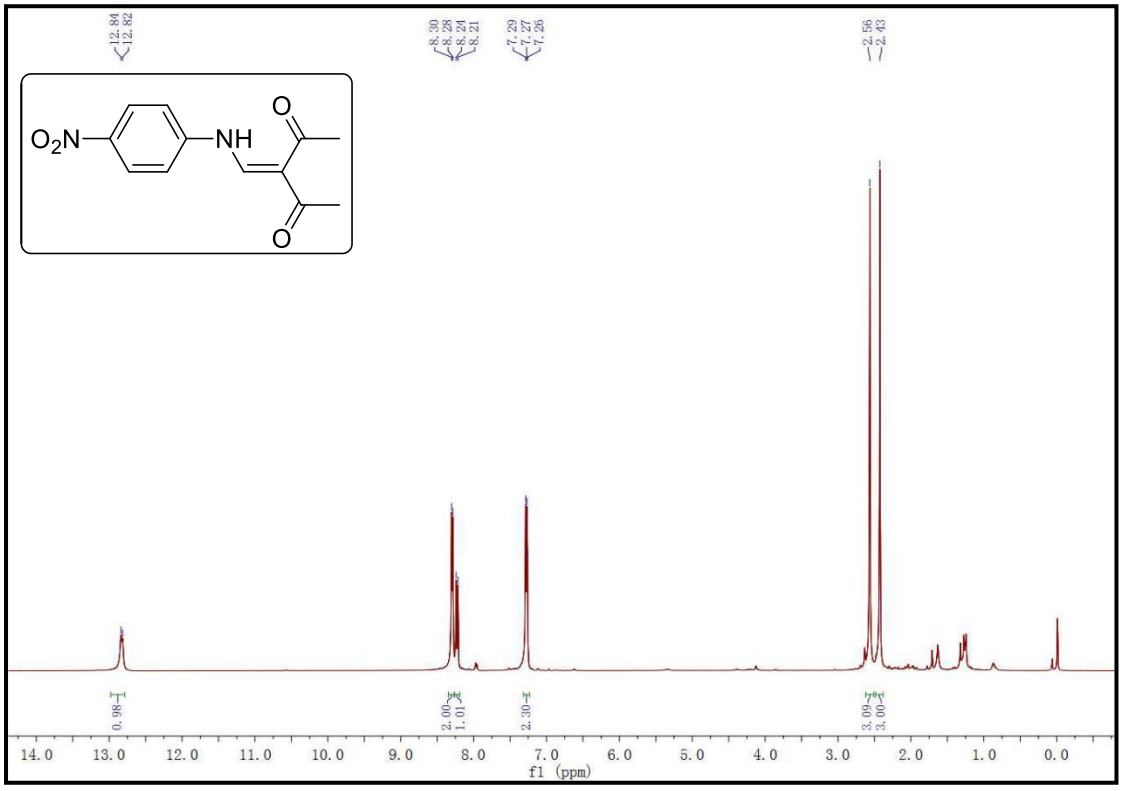


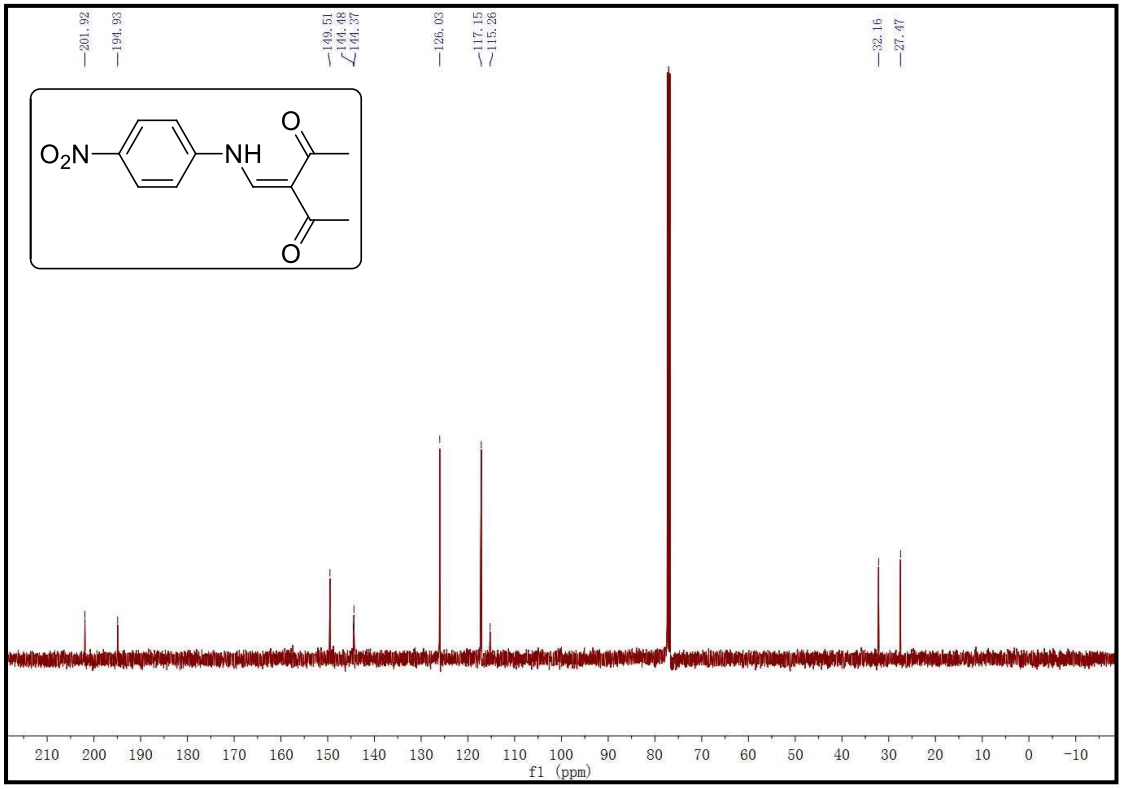
3-(((4-bromophenyl)amino)methylene)pentane-2,4-dione (3l)



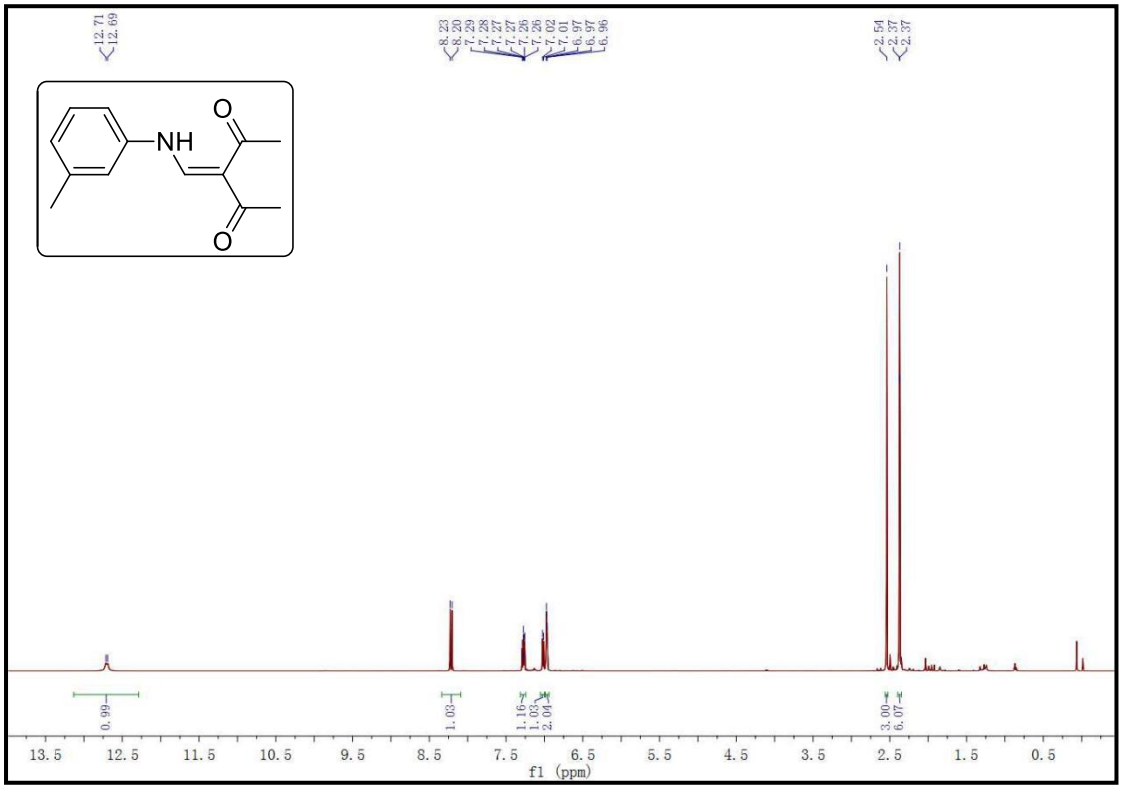


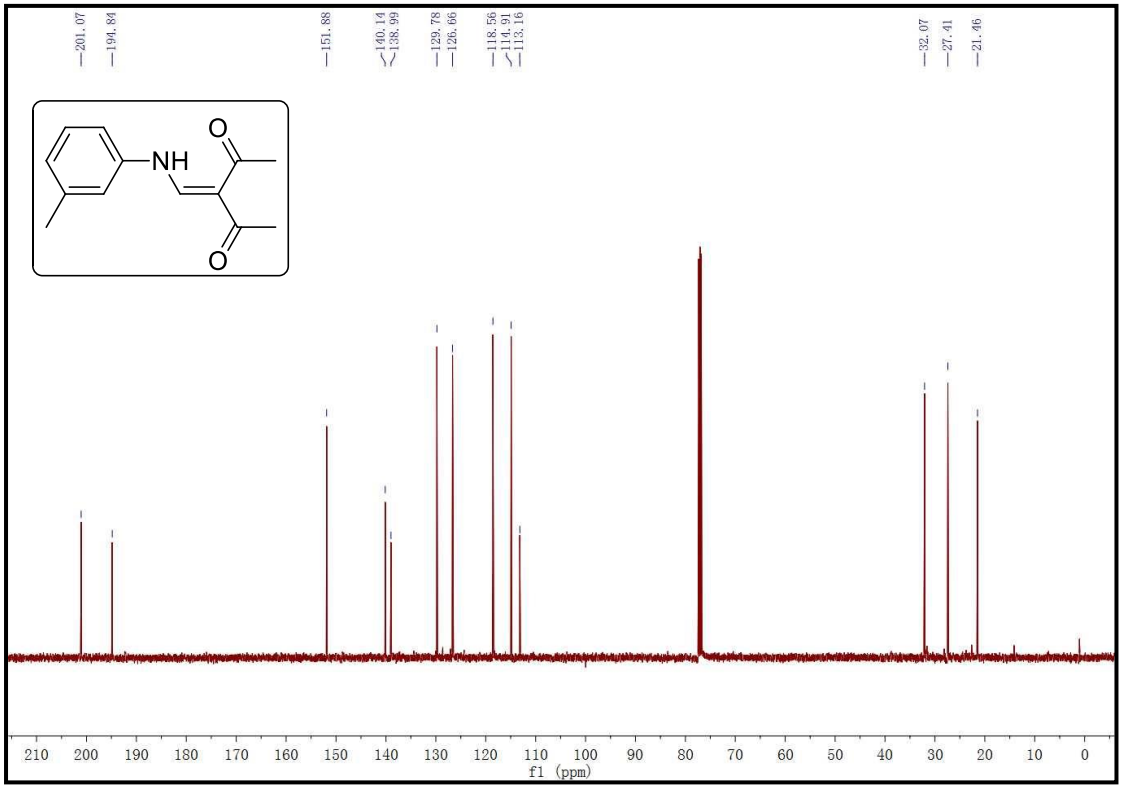
3-(((4-nitrophenyl)amino)methylene)pentane-2,4-dione (3m)



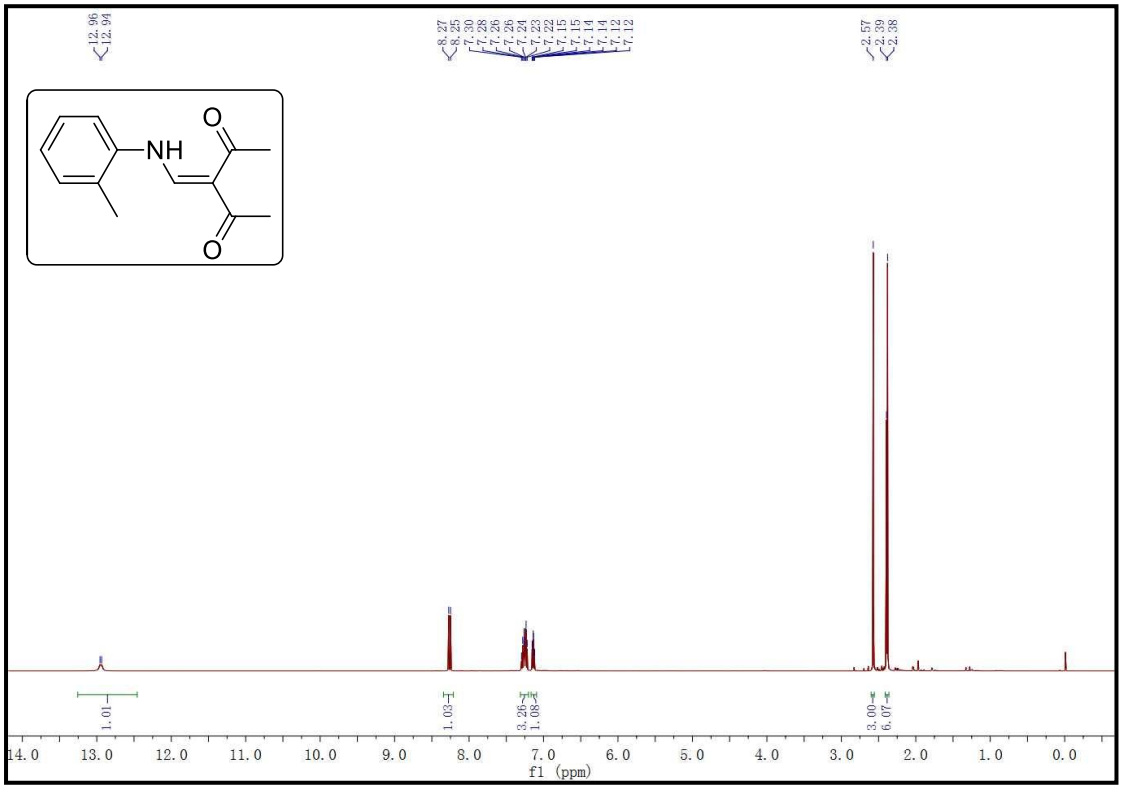


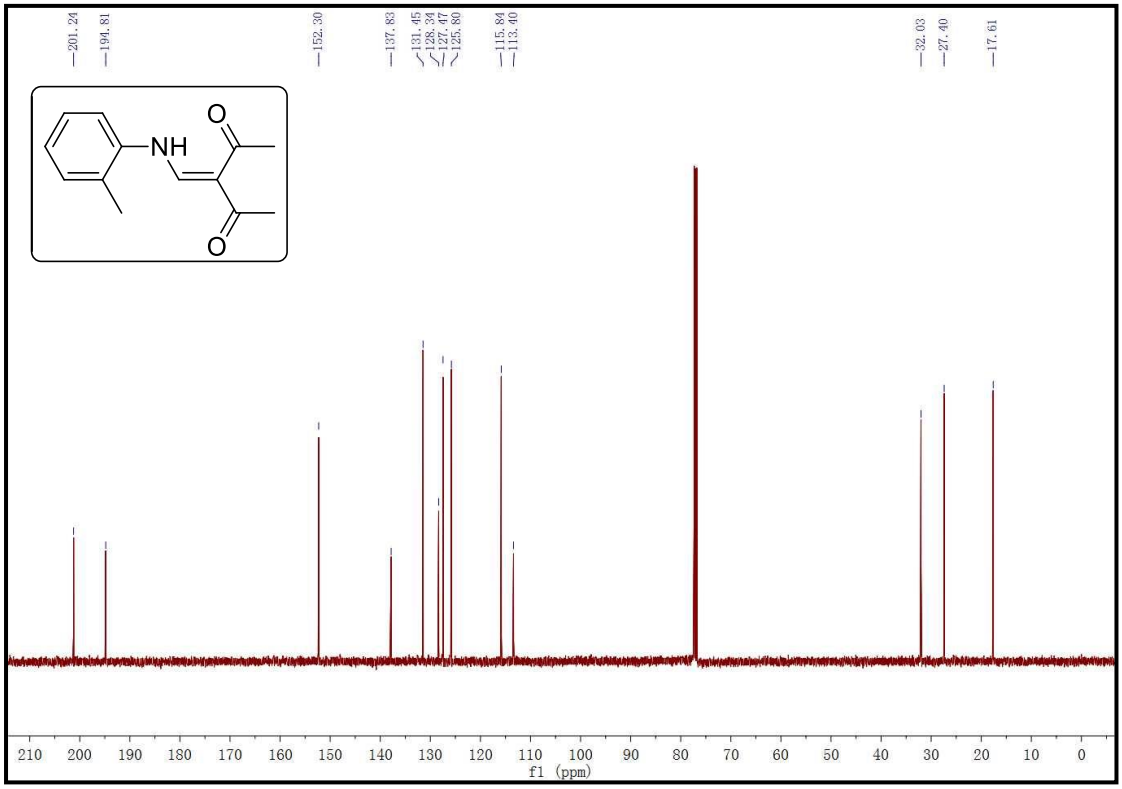
3-((m-tolylamino)methylene)pentane-2,4-dione (3n)



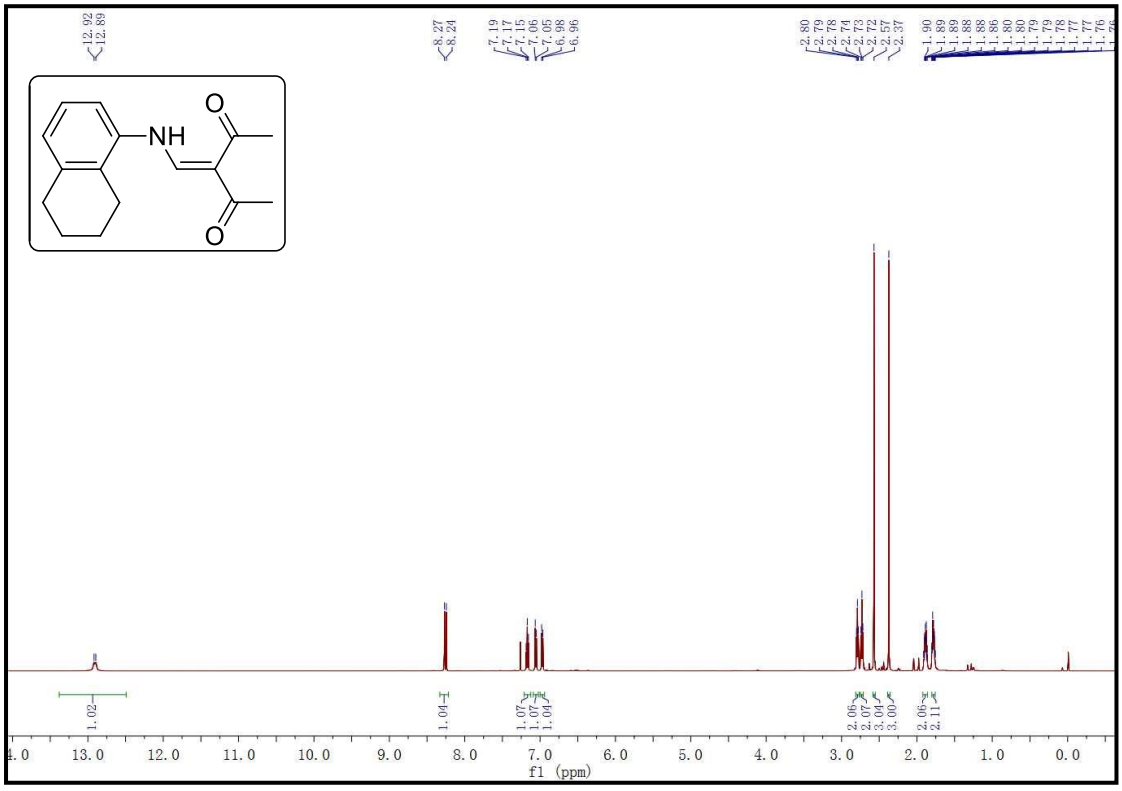


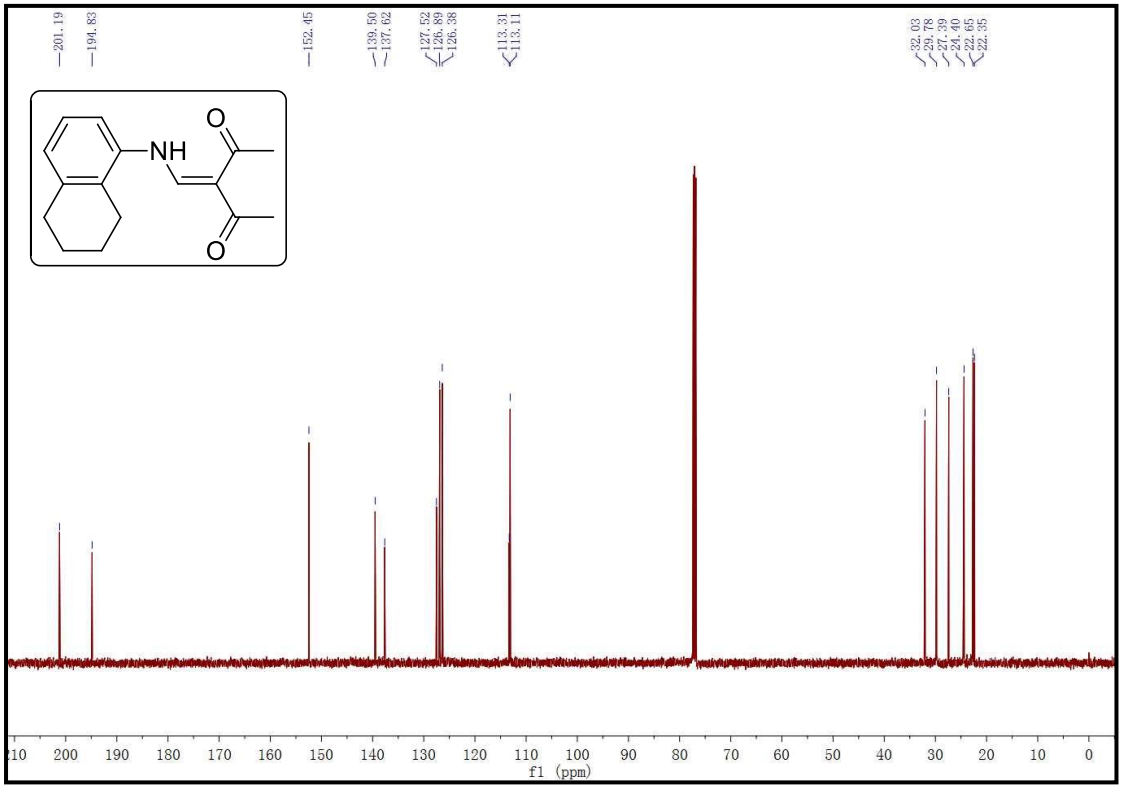
3-((o-tolylamino)methylene)pentane-2,4-dione (3o)



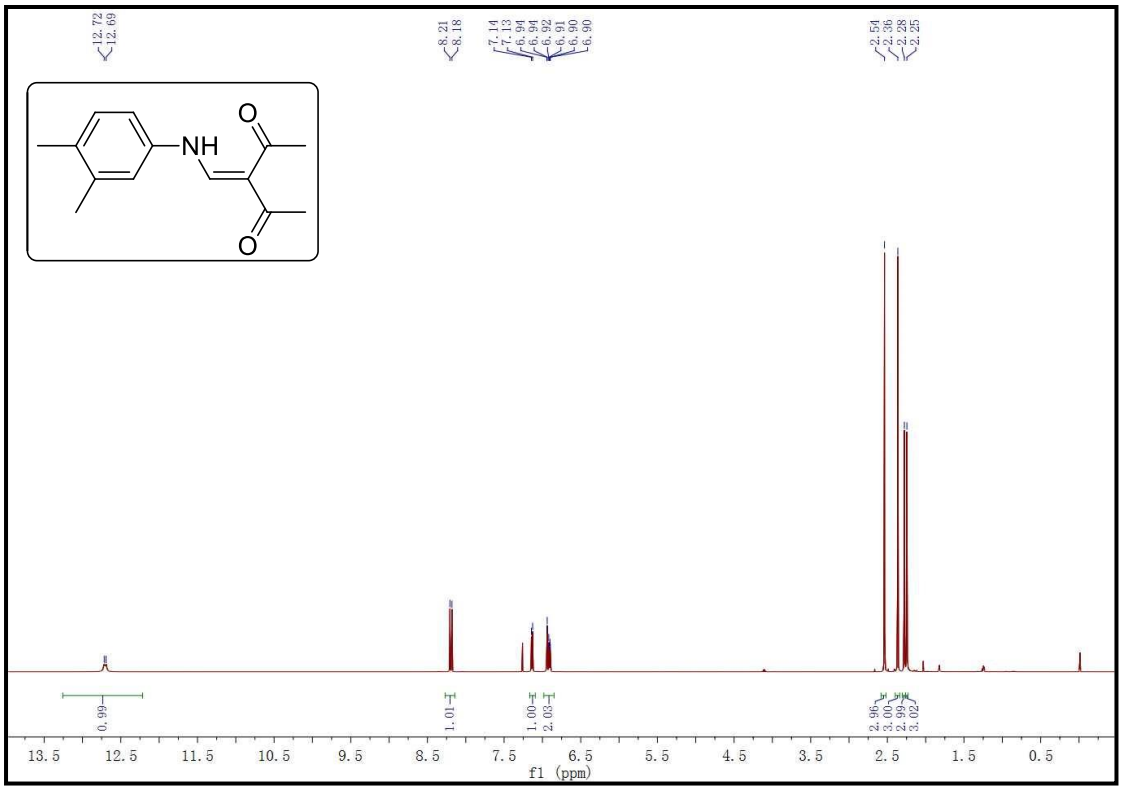


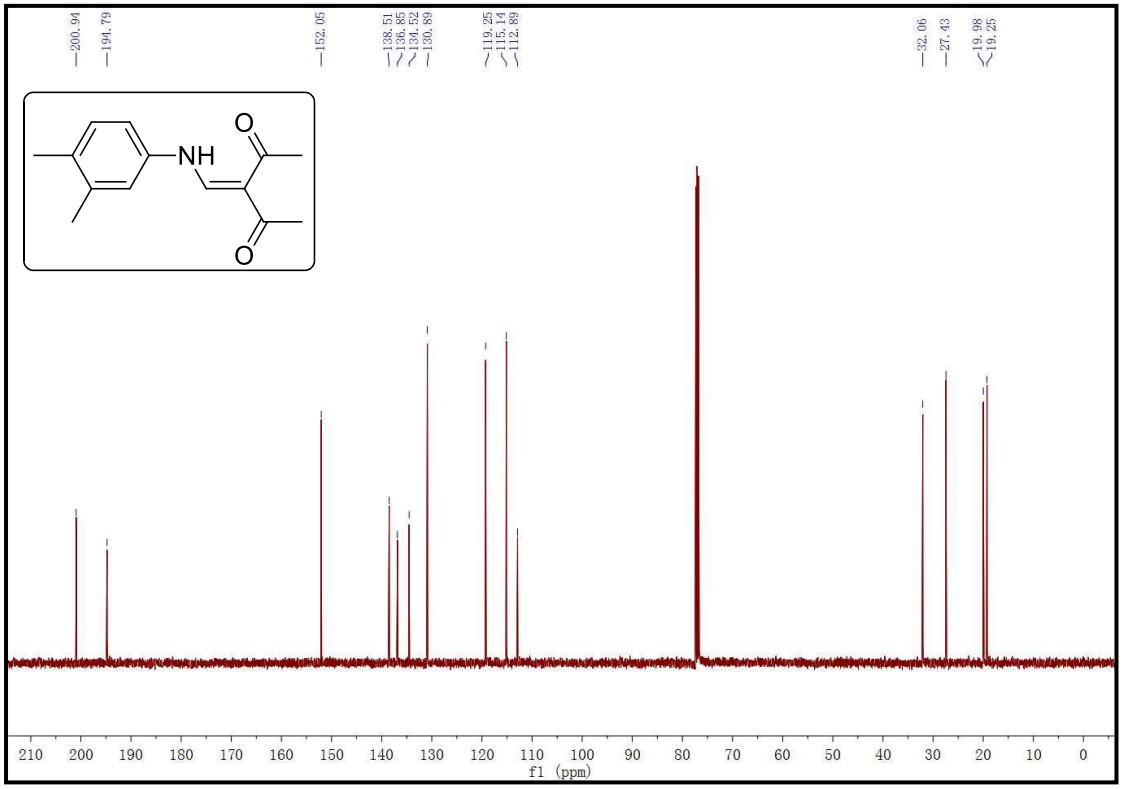
3-(((5,6,7,8-tetrahydronaphthalen-1-yl)amino)methylene)pentane-2,4-dione(3p)



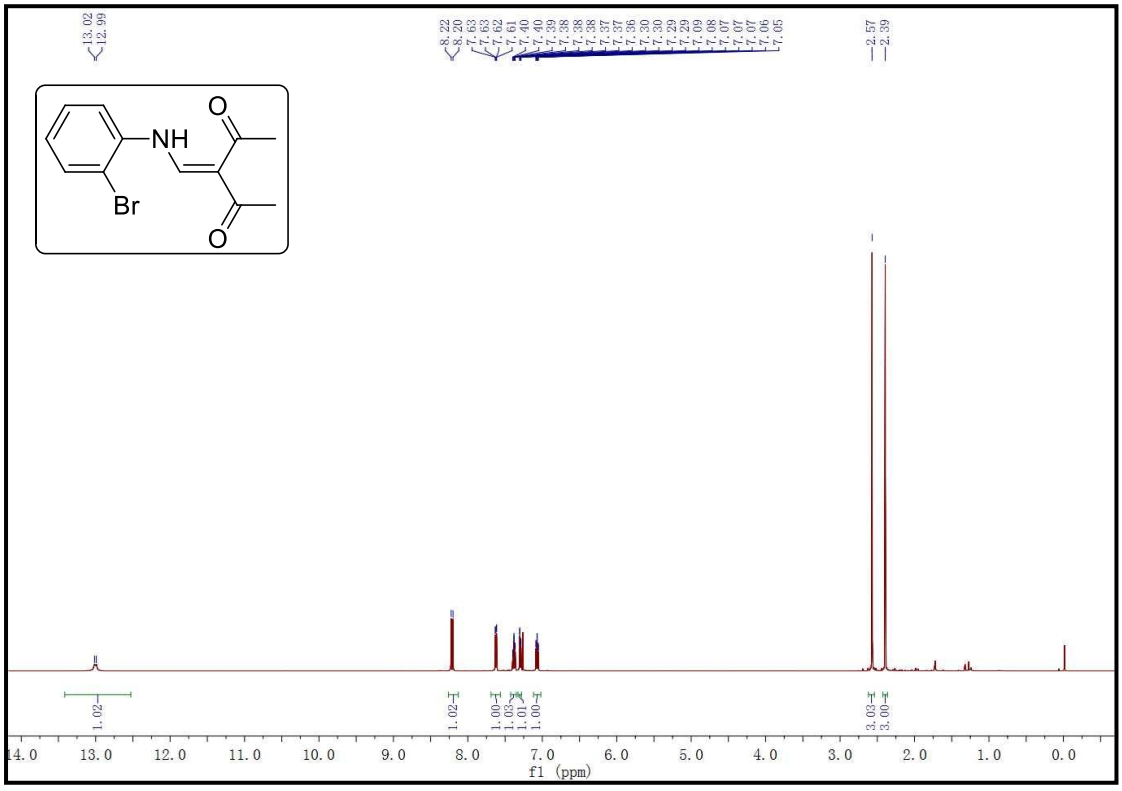


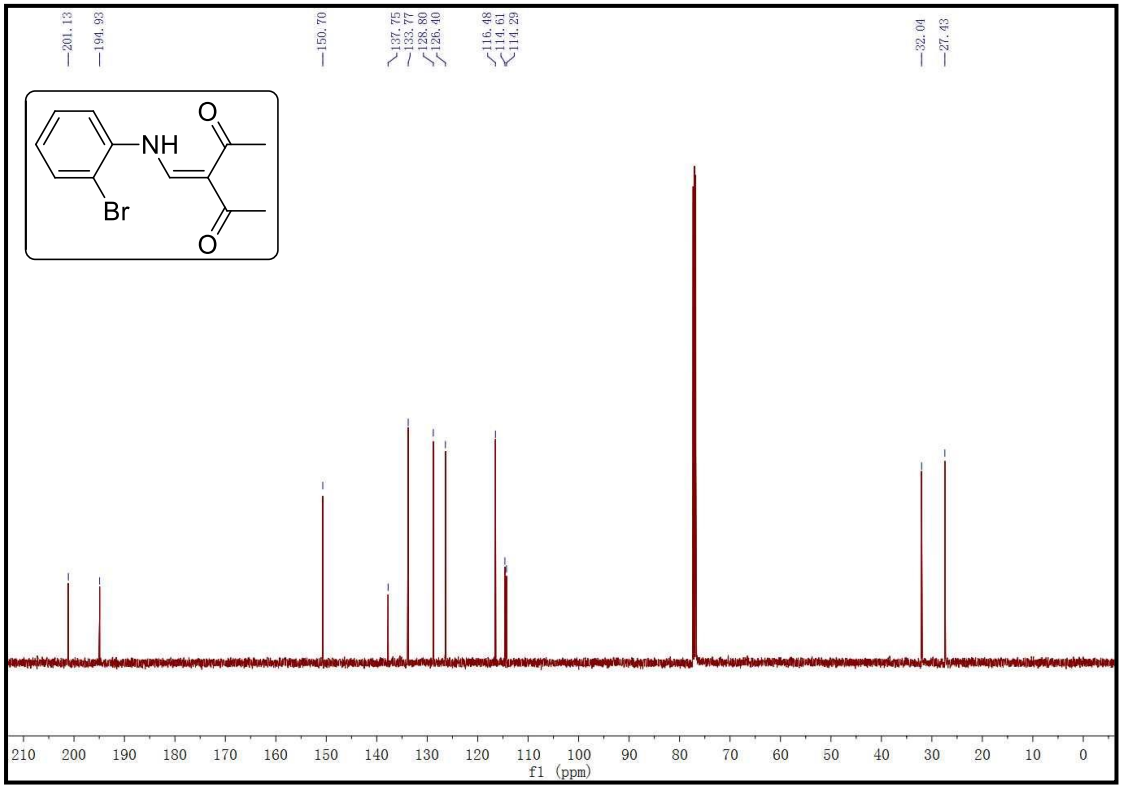
3-(((3,4-dimethylphenyl)amino)methylene)pentane-2,4-dione (3q)



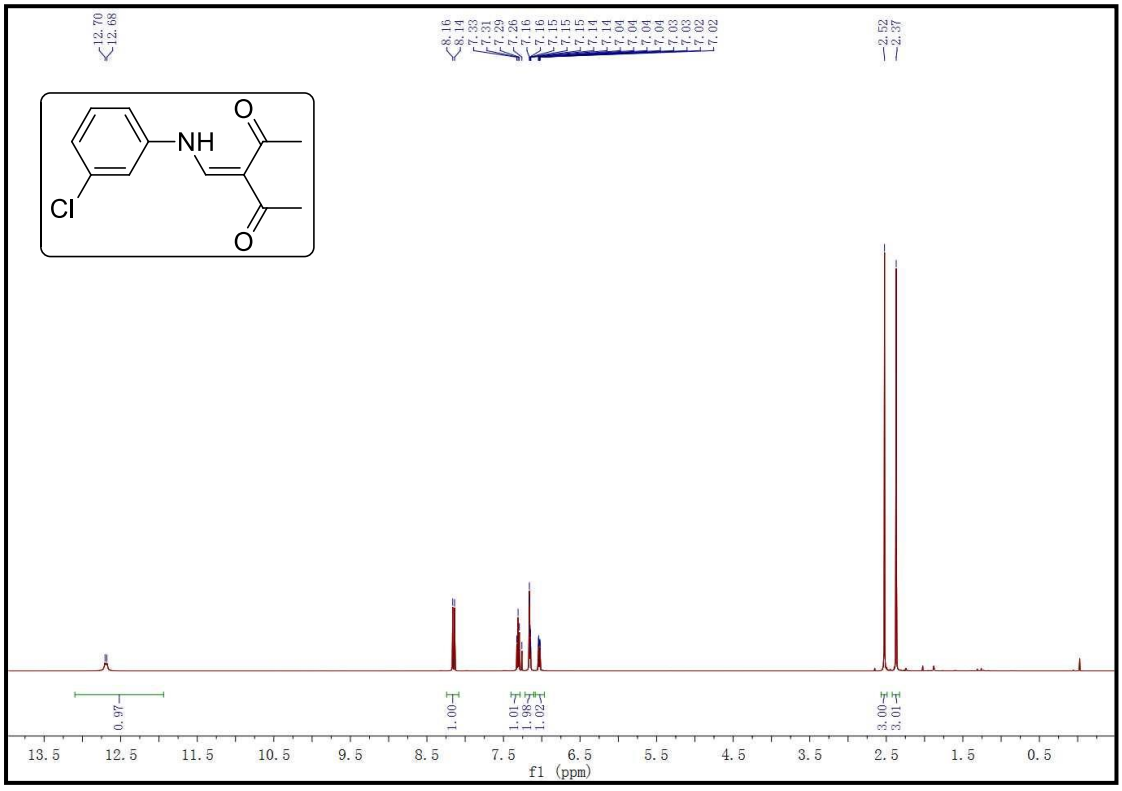


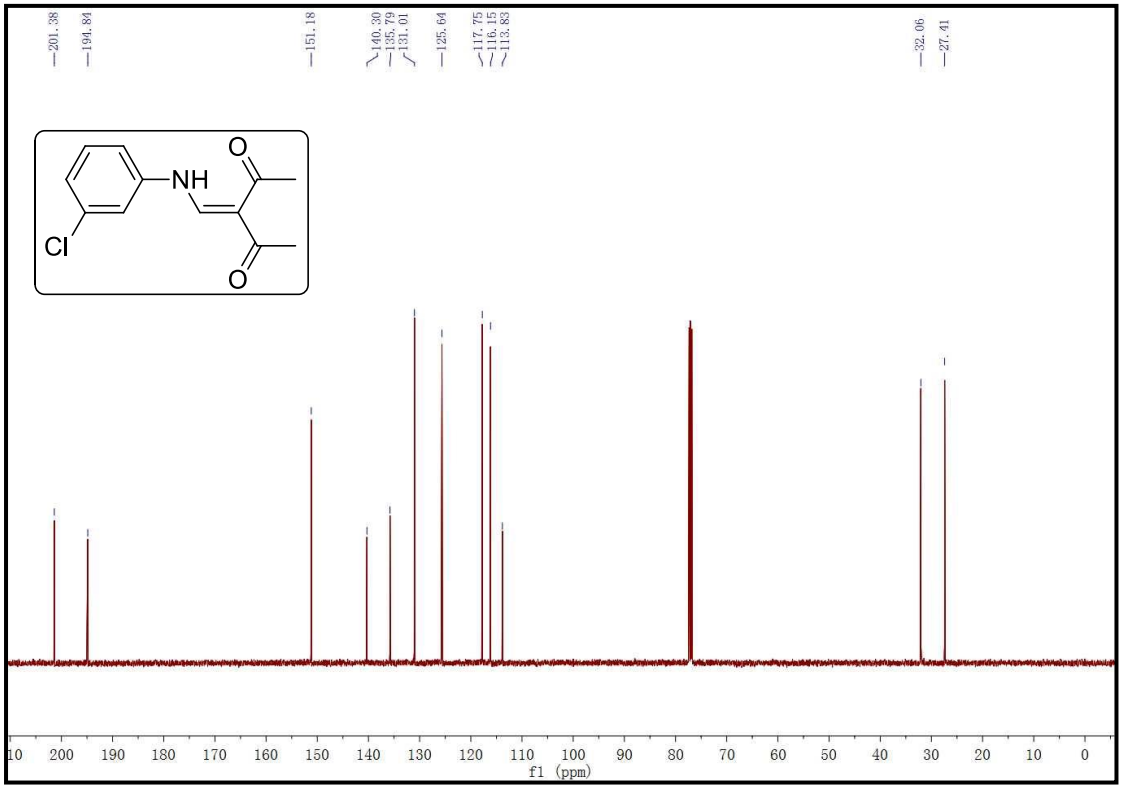
3-(((2-bromophenyl)amino)methylene)pentane-2,4-dione (3r)



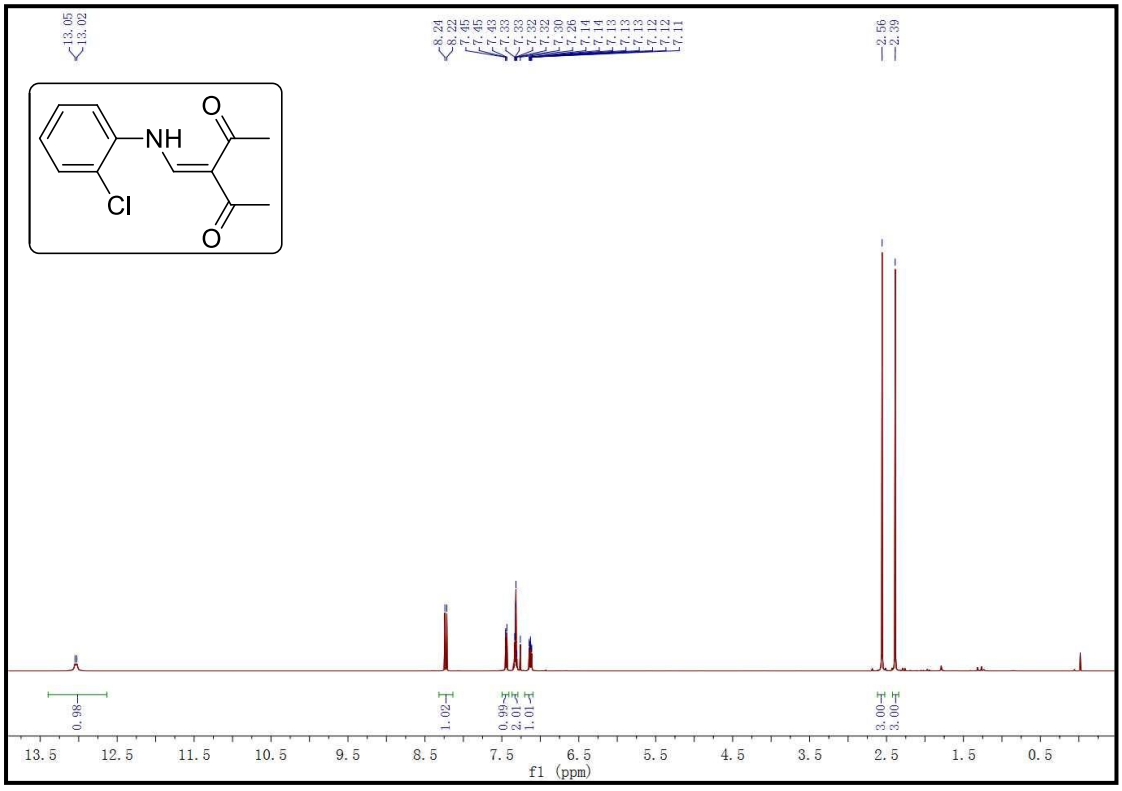


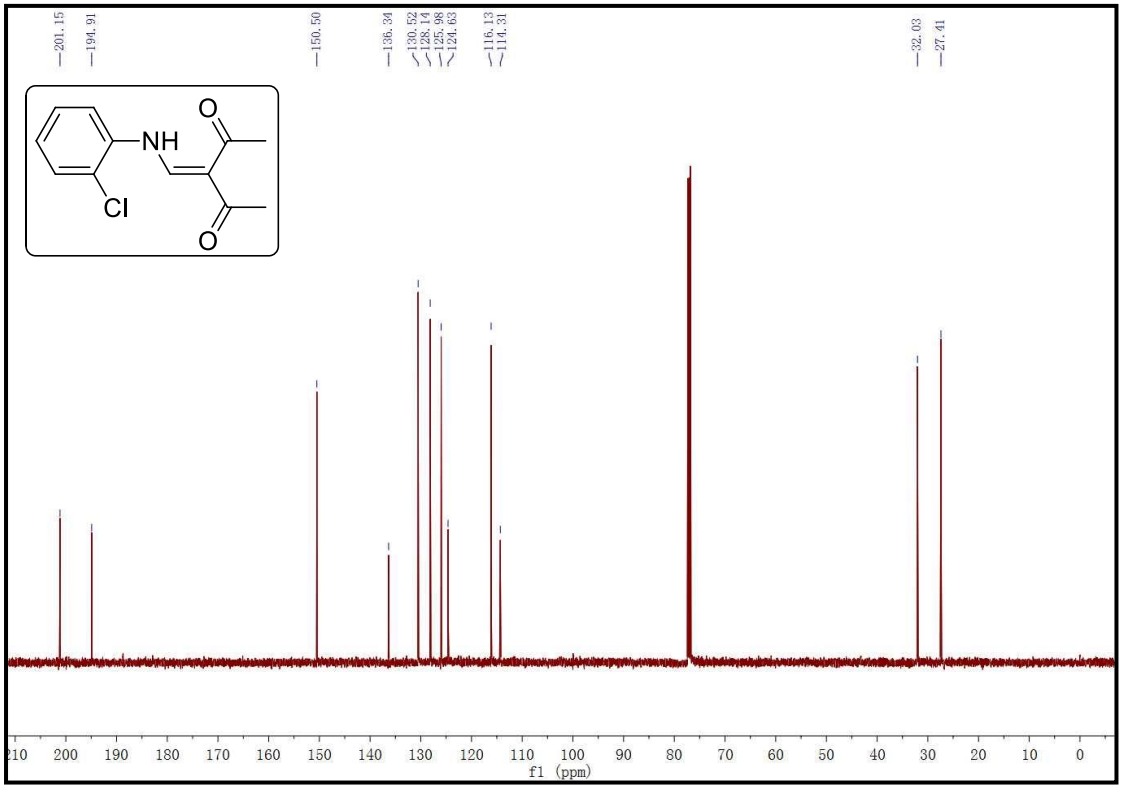
3-(((3-chlorophenyl)amino)methylene)pentane-2,4-dione (3s)



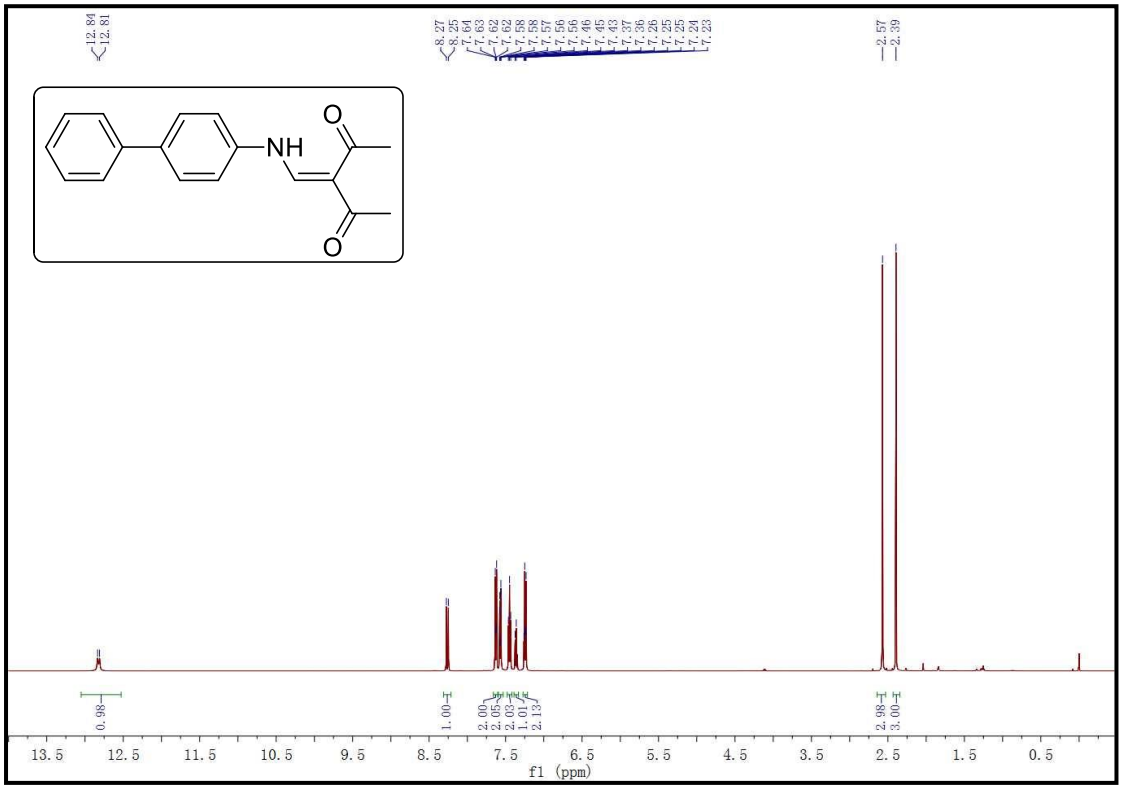


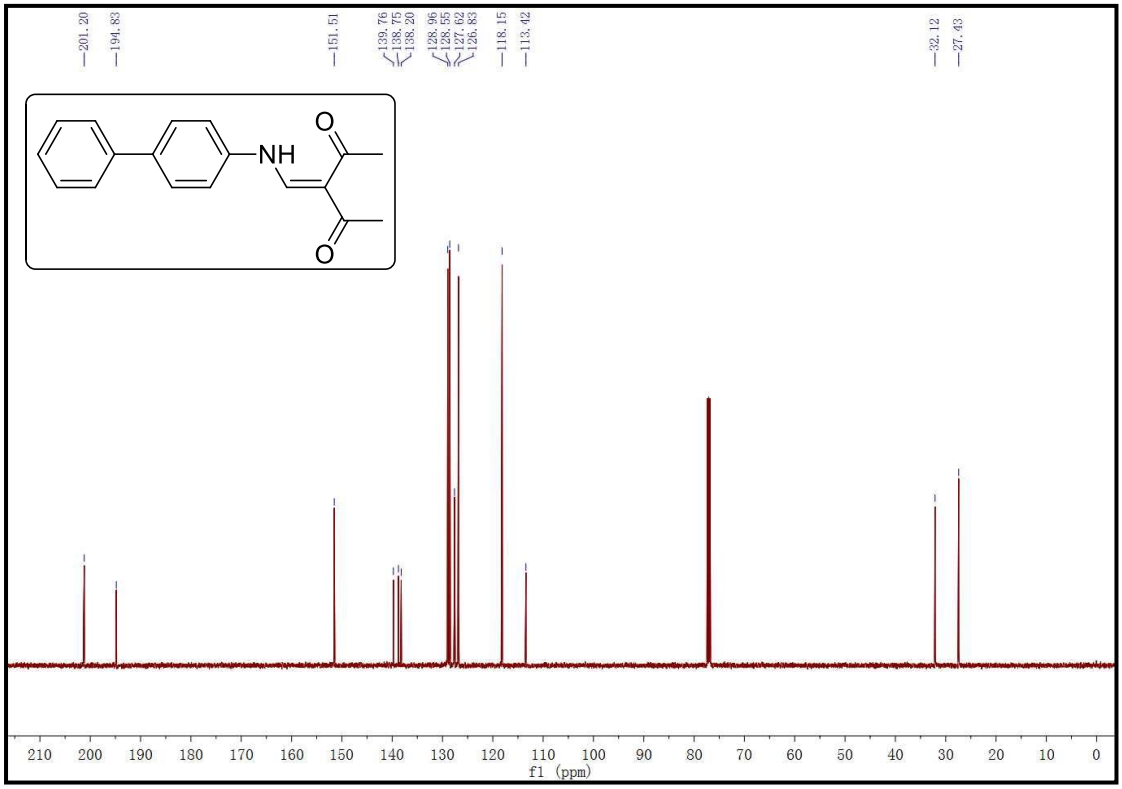
3-(((2-chlorophenyl)amino)methylene)pentane-2,4-dione (3t)



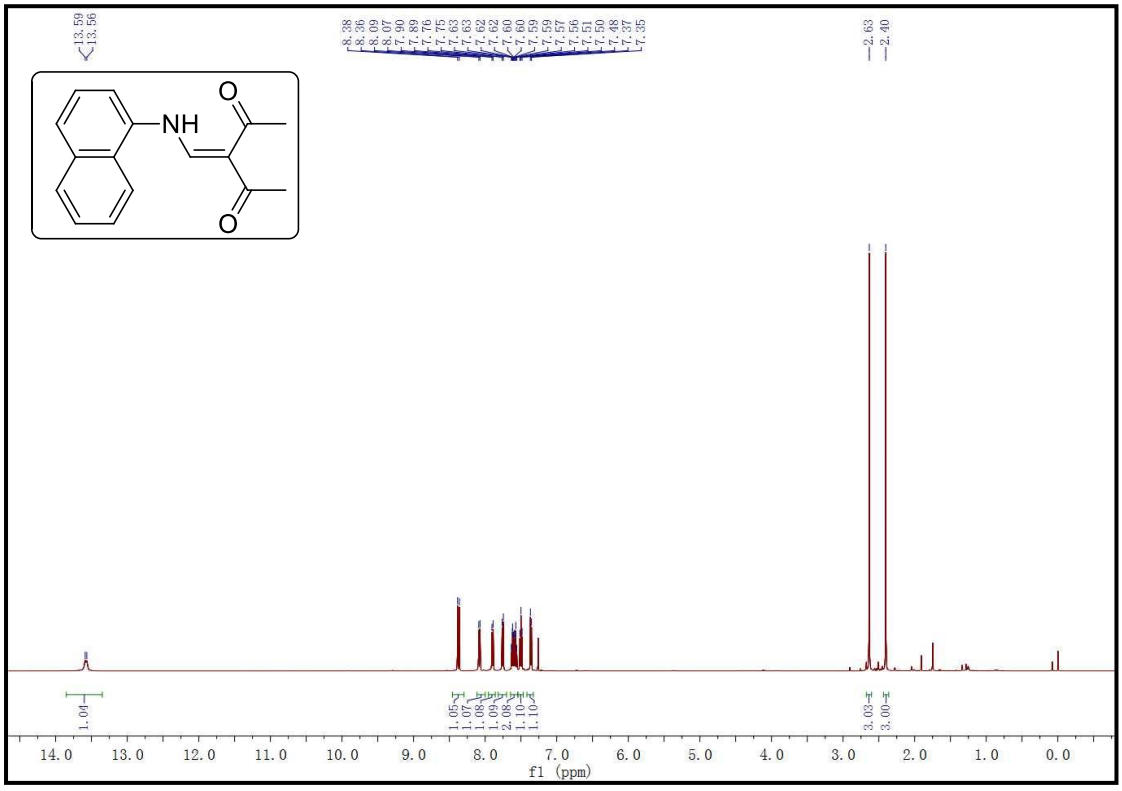


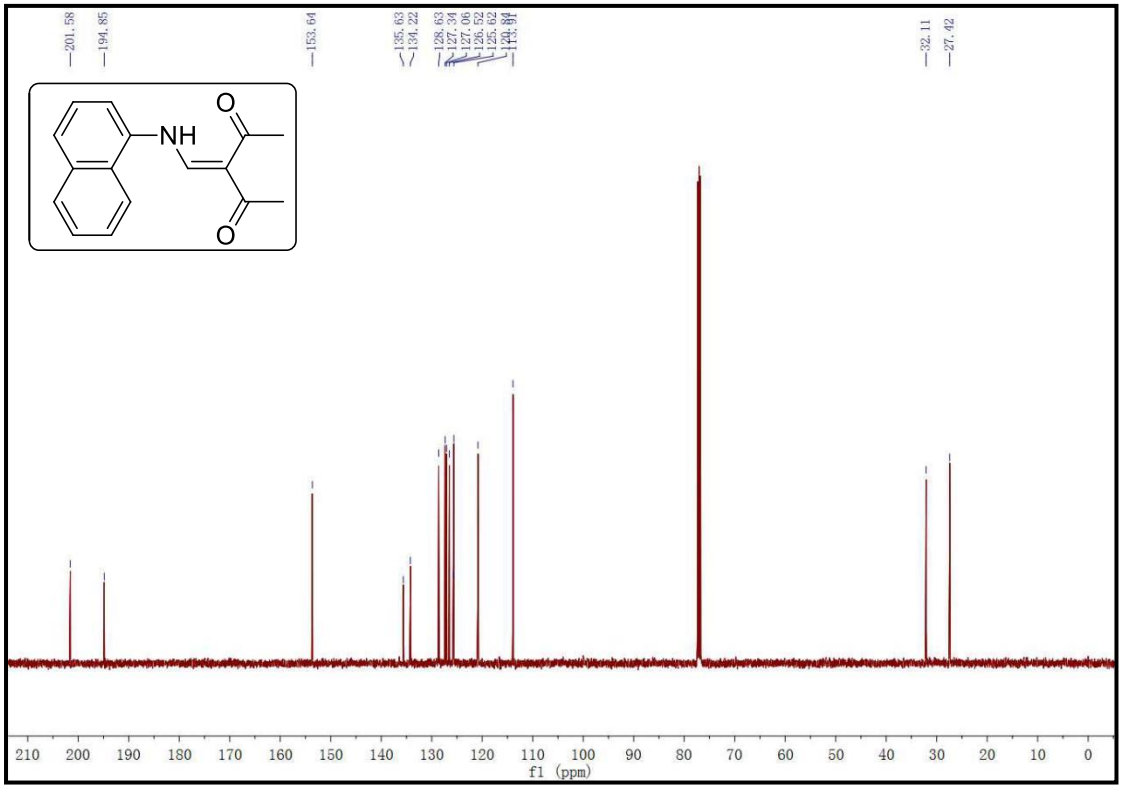
3-(([1,1'-biphenyl]-4-ylamino)methylene)pentane-2,4-dione (3u)



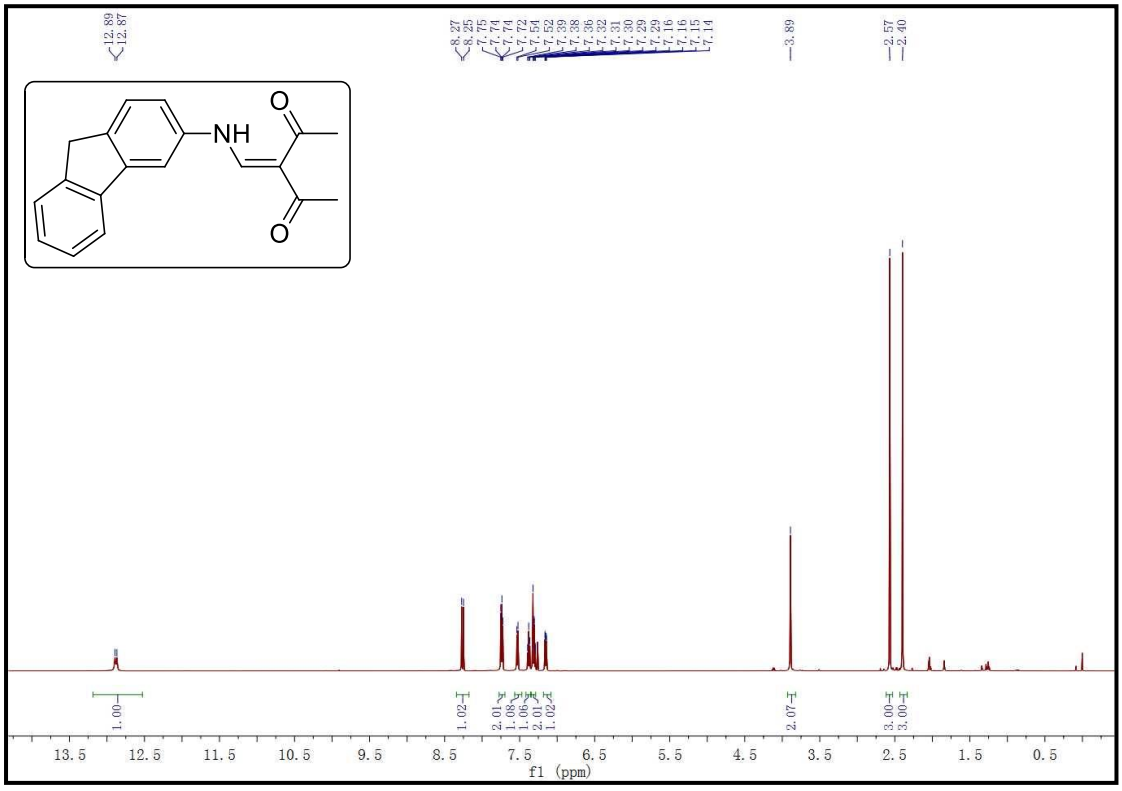


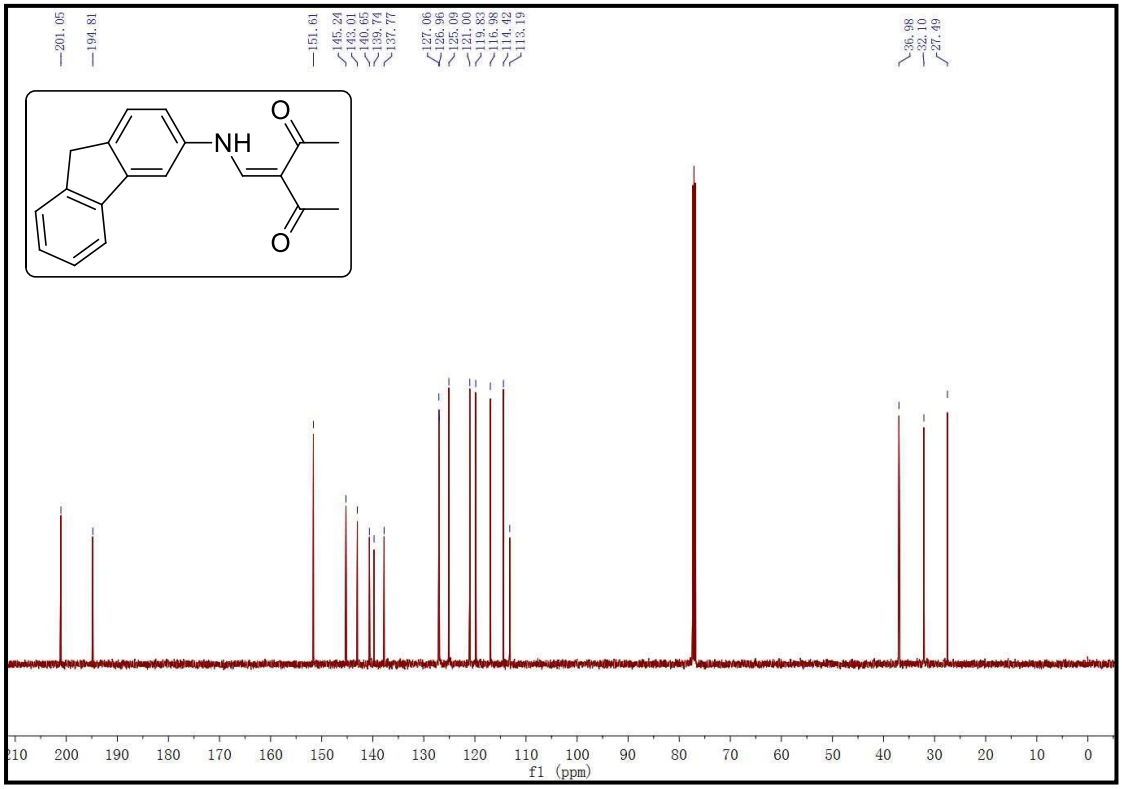
3-((naphthalen-1-ylamino)methylene)pentane-2,4-dione (3v)



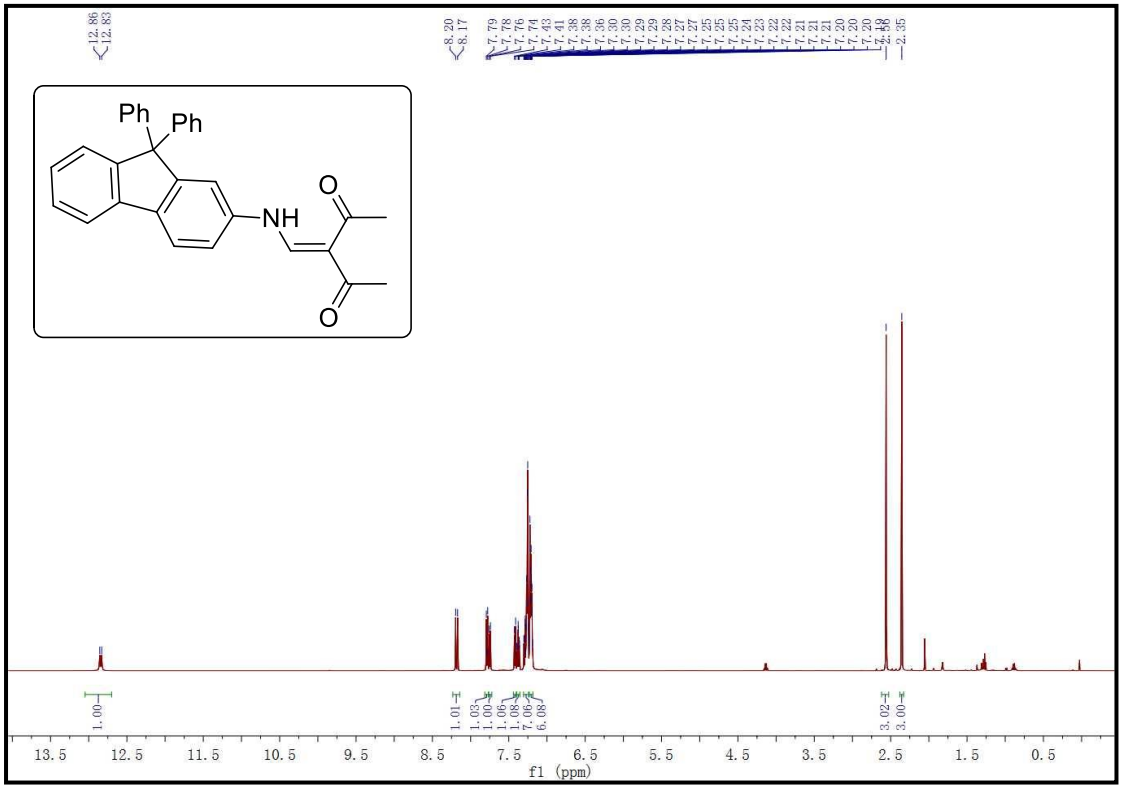


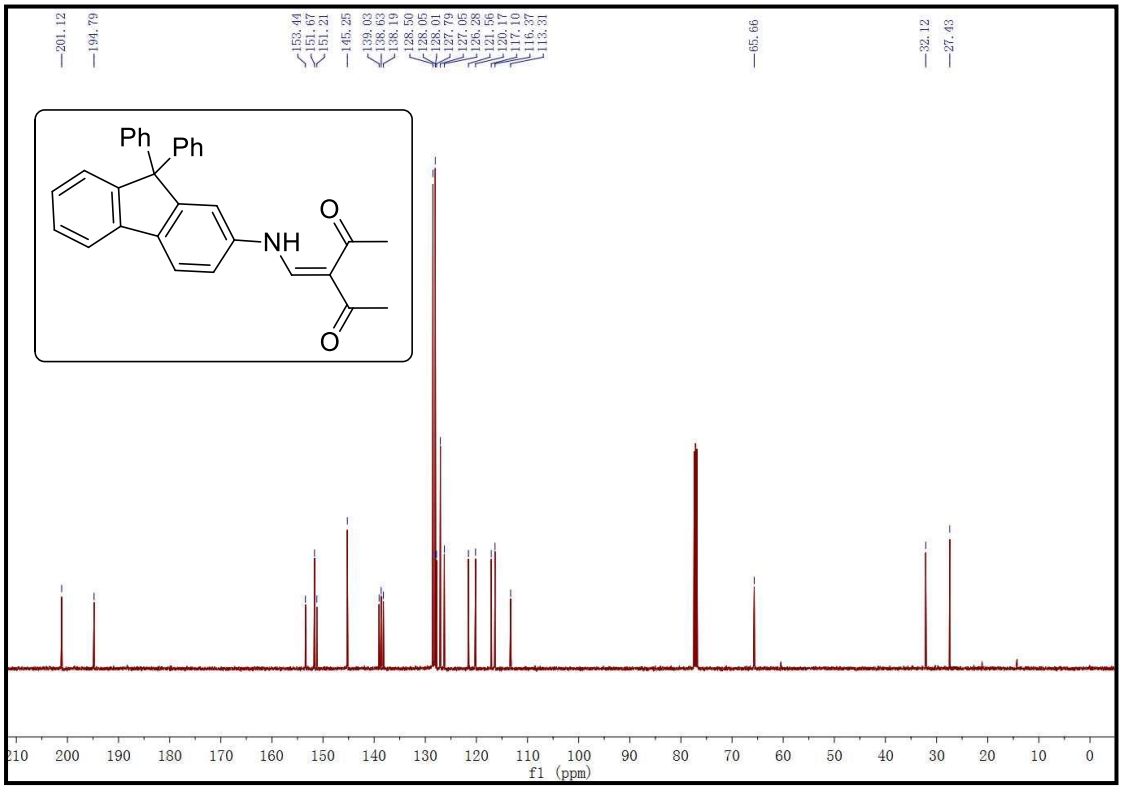
3-(((9H-fluoren-3-yl)amino)methylene)pentane-2,4-dione (3w)



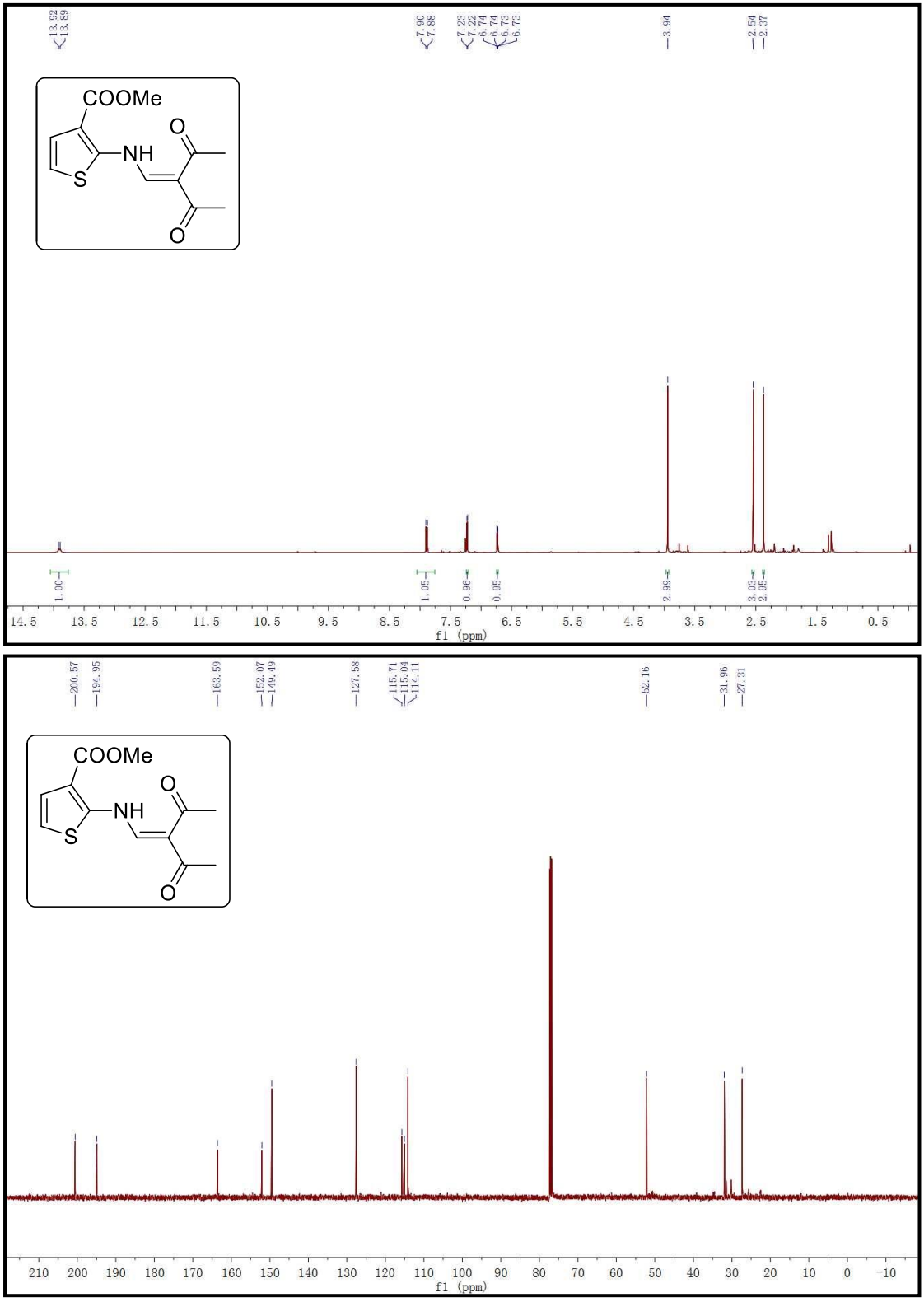


3-(((9,9-diphenyl-9H-fluoren-2-yl)amino)methylene)pentane-2,4-dion e (3x)

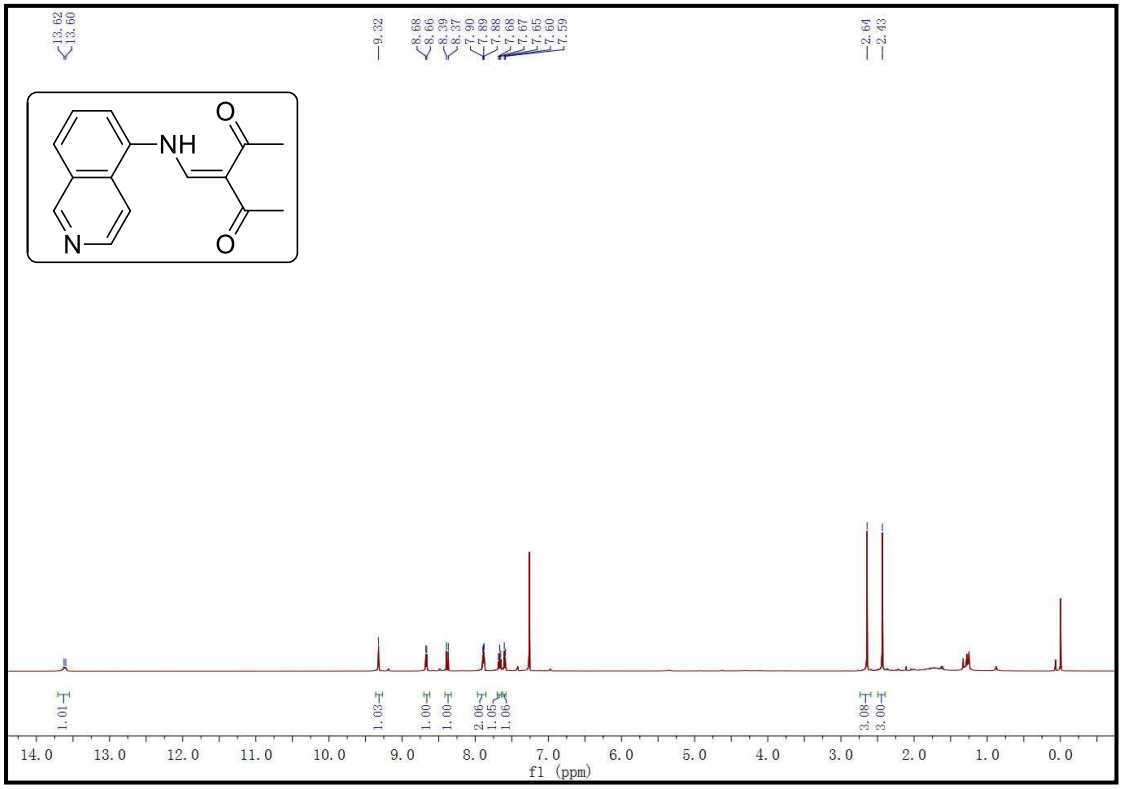


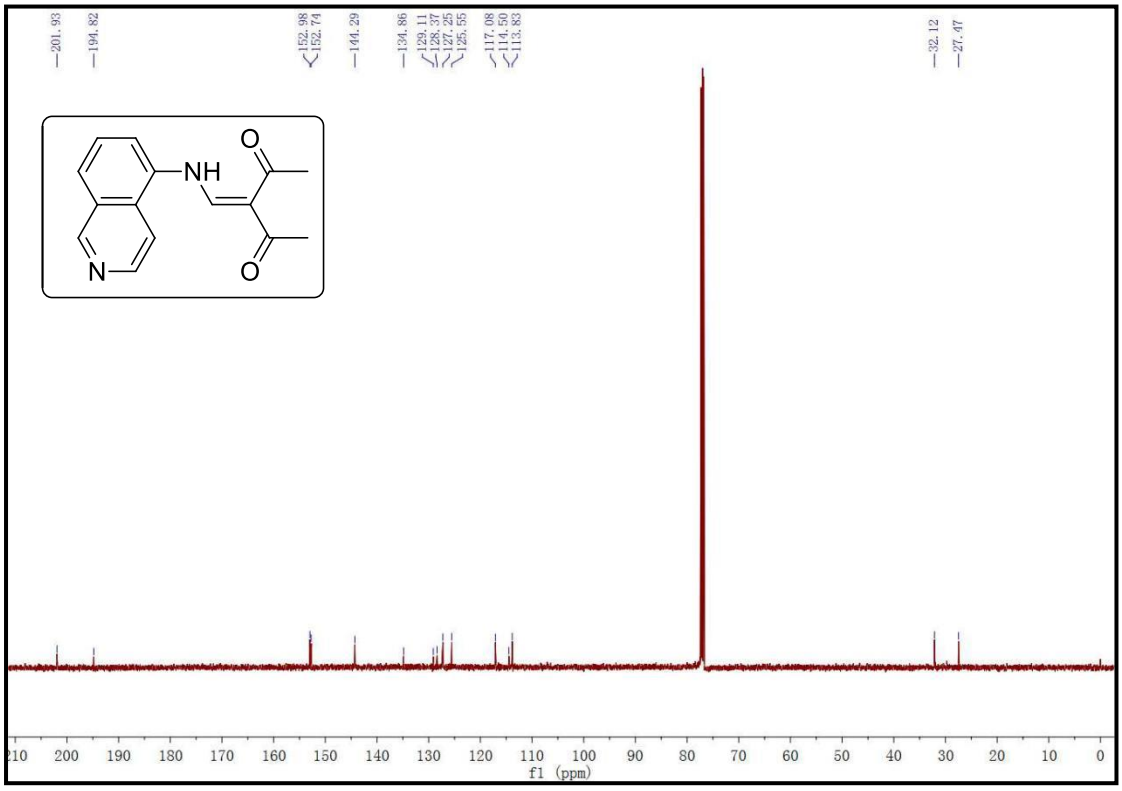


ethyl 2-((2-acetyl-3-oxobut-1-en-1-yl)amino)thiophene-3-carboxylate (3y)

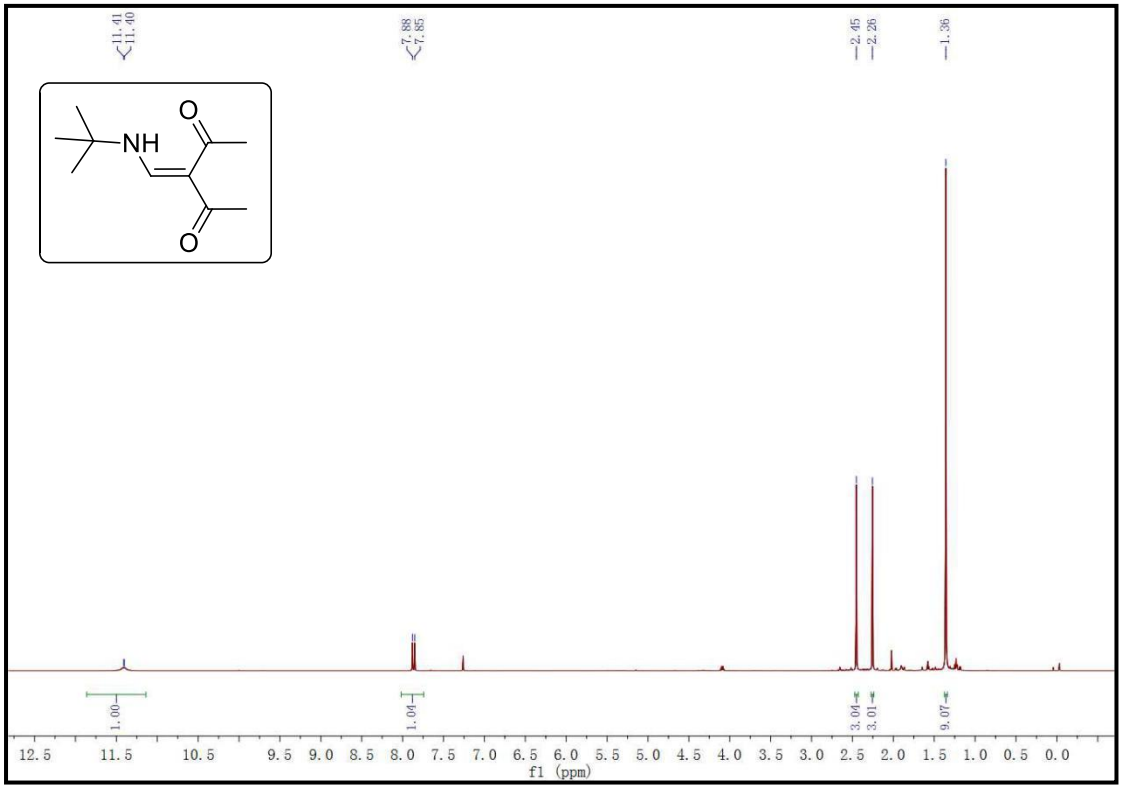


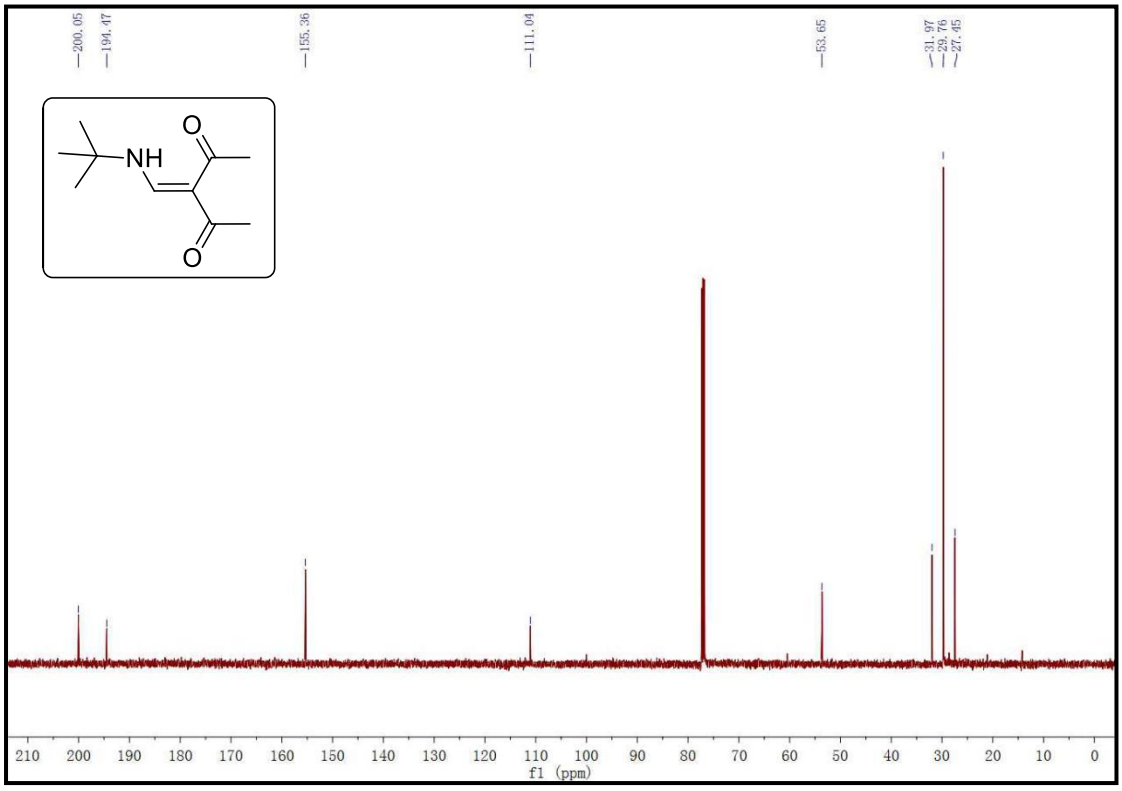
3-((isoquinolin-6-ylamino)methylene)pentane-2,4-dione (3z)



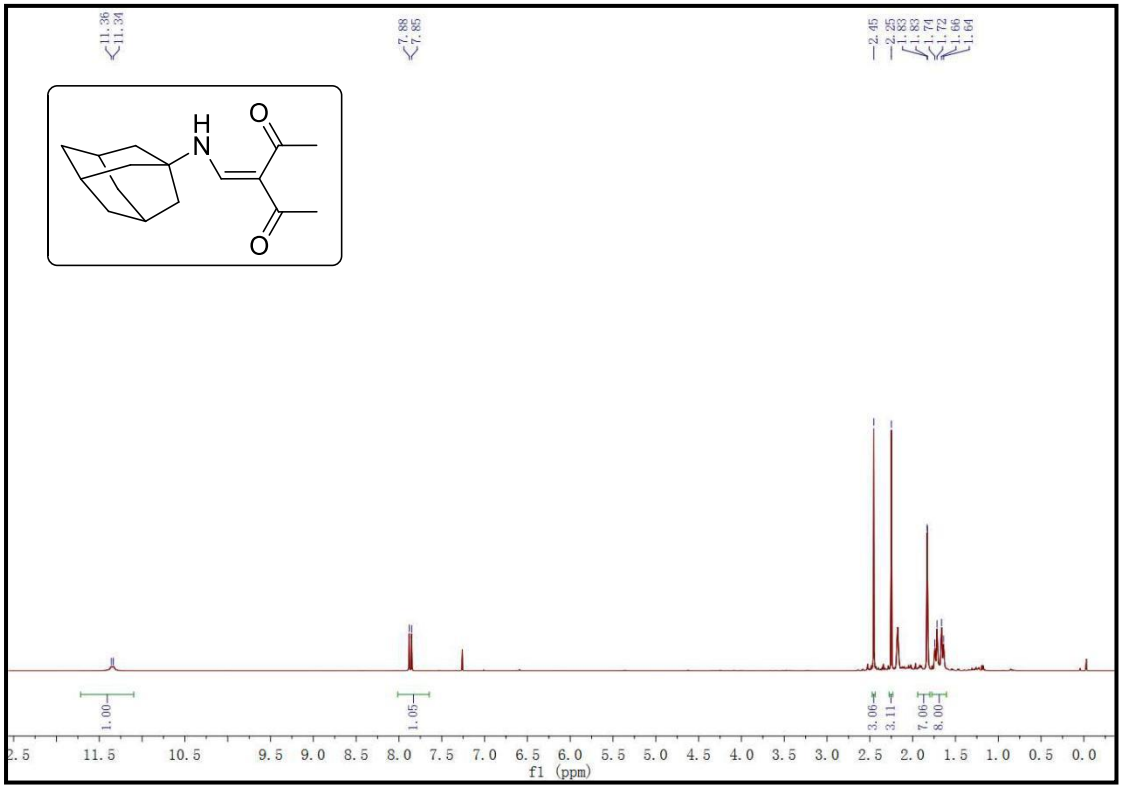


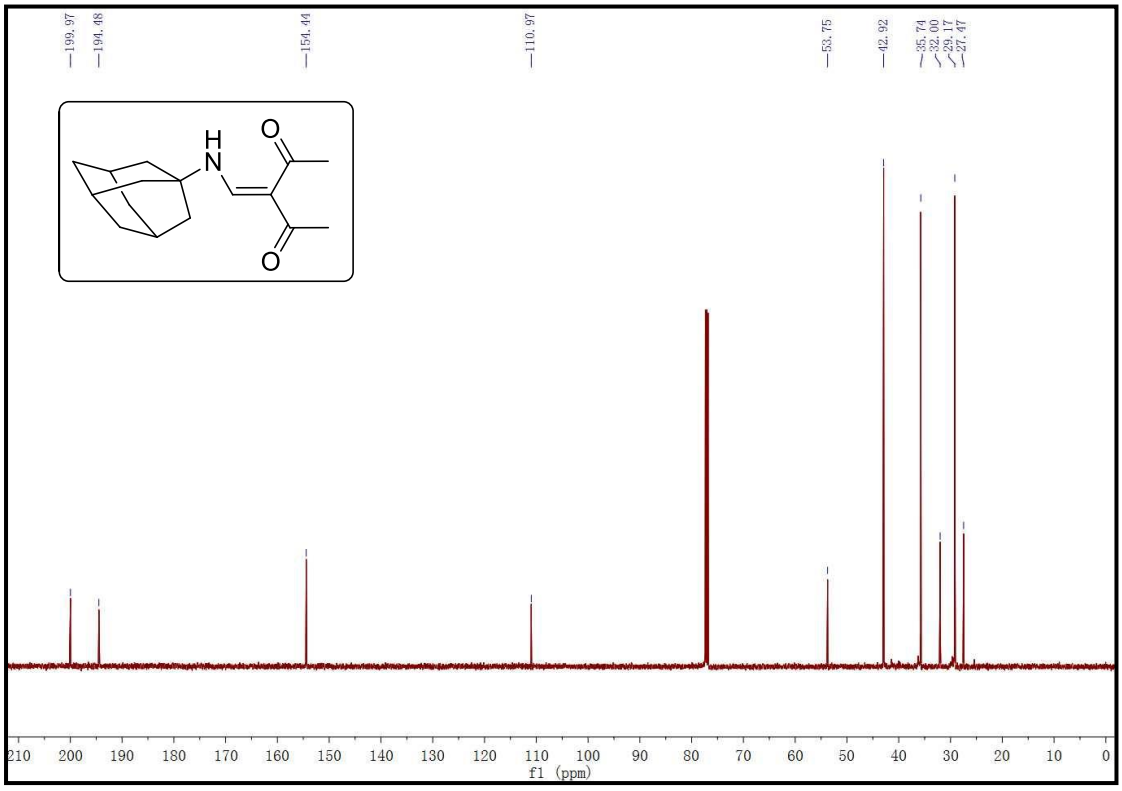
3-((tert-butylamino)methylene)pentane-2,4-dione (3aa)



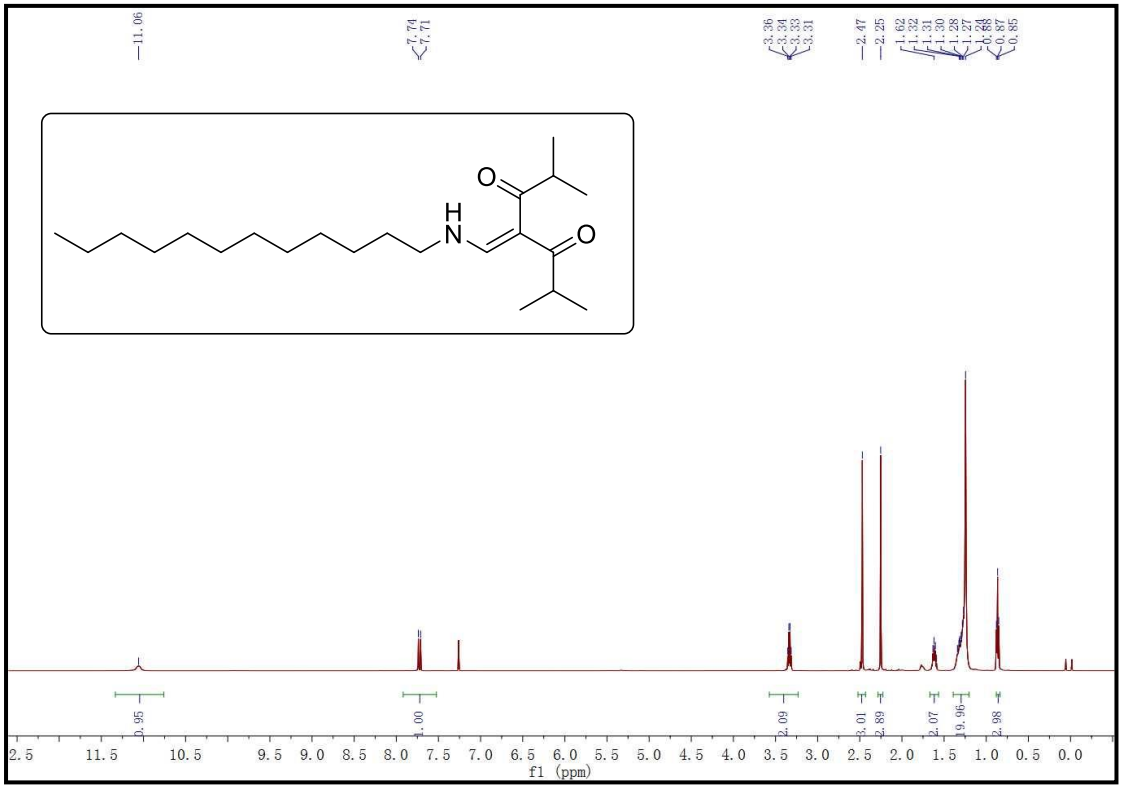


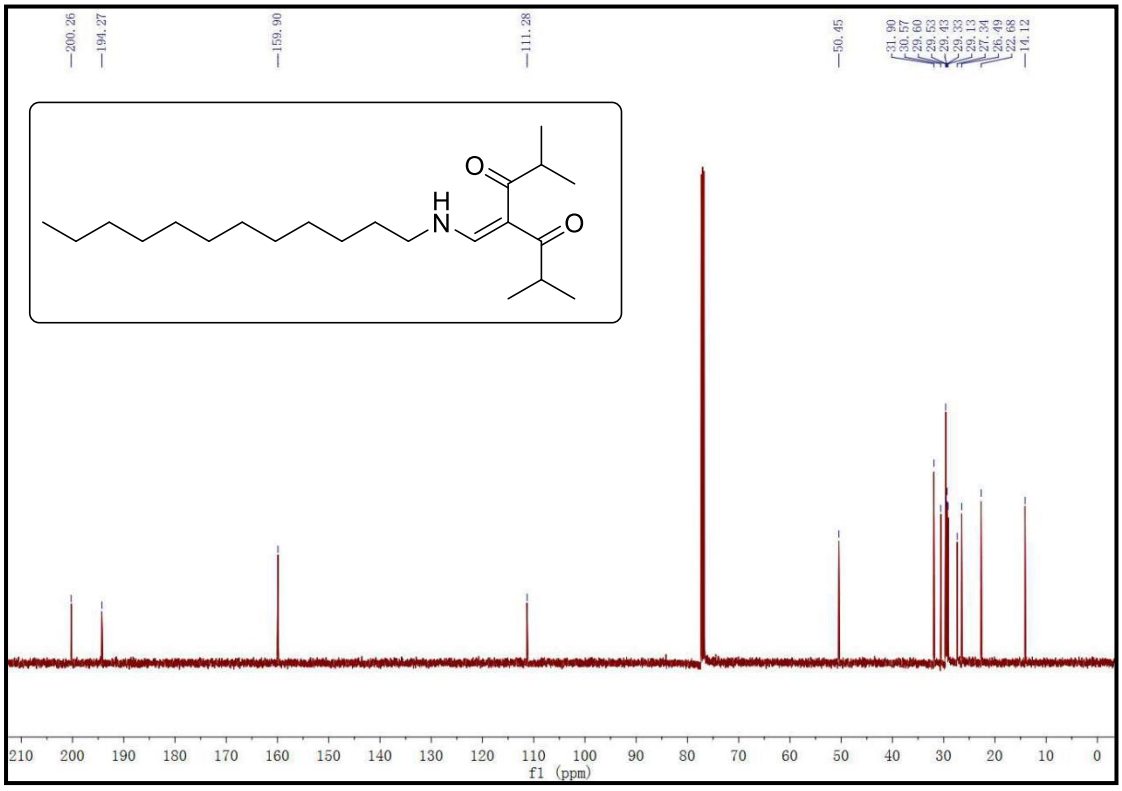
3-((adamantan-1-ylamino)methylene)pentane-2,4-dione (3ab)



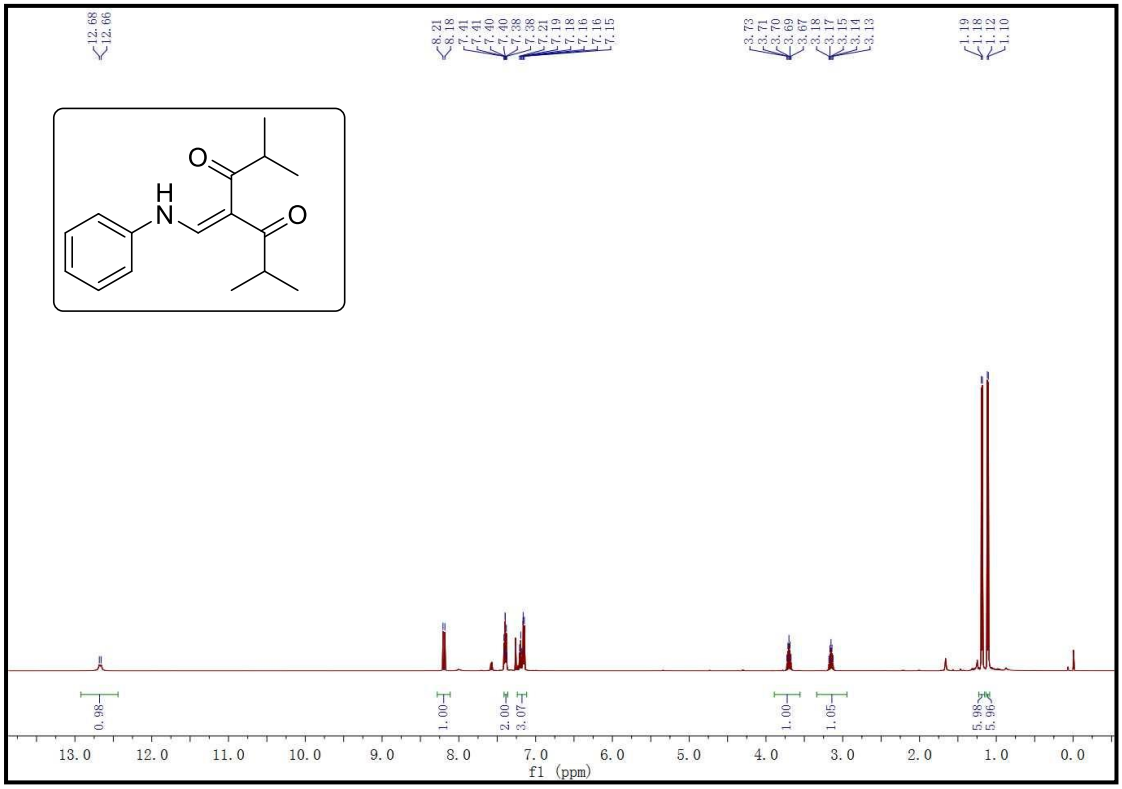


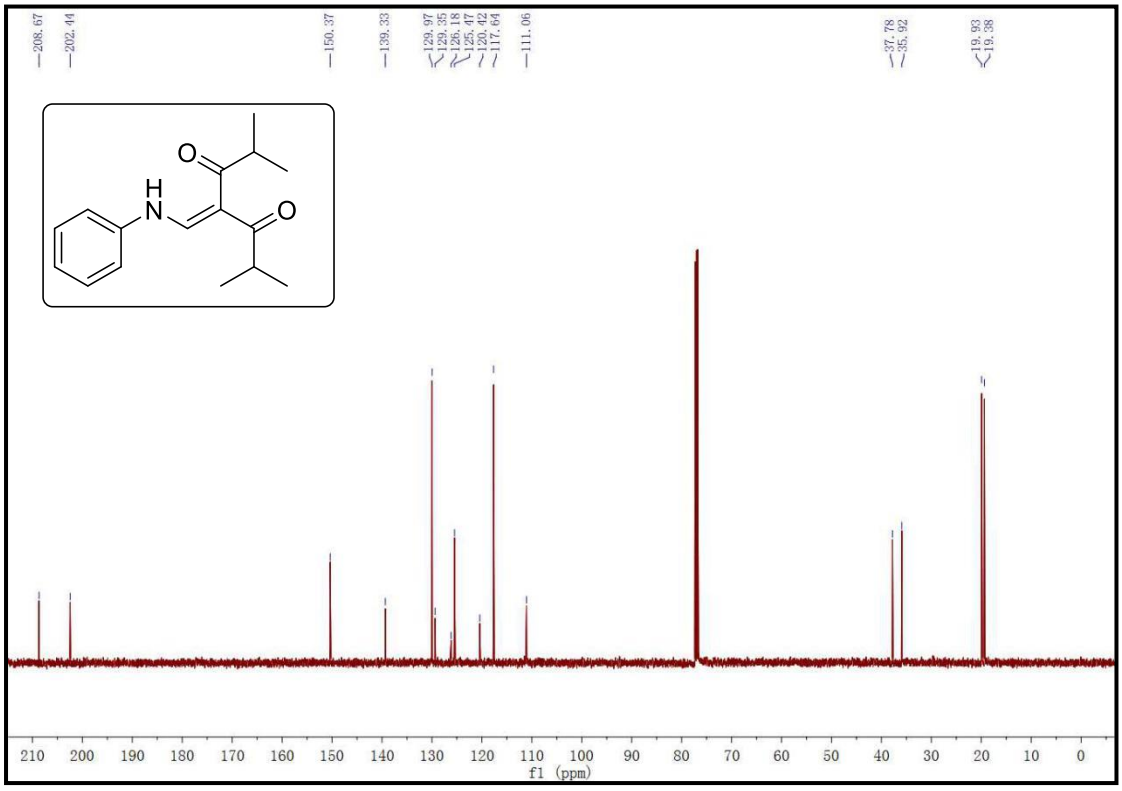
4-((dodecylamino)methylene)-2,6-dimethylheptane-3,5-dione (3ac)



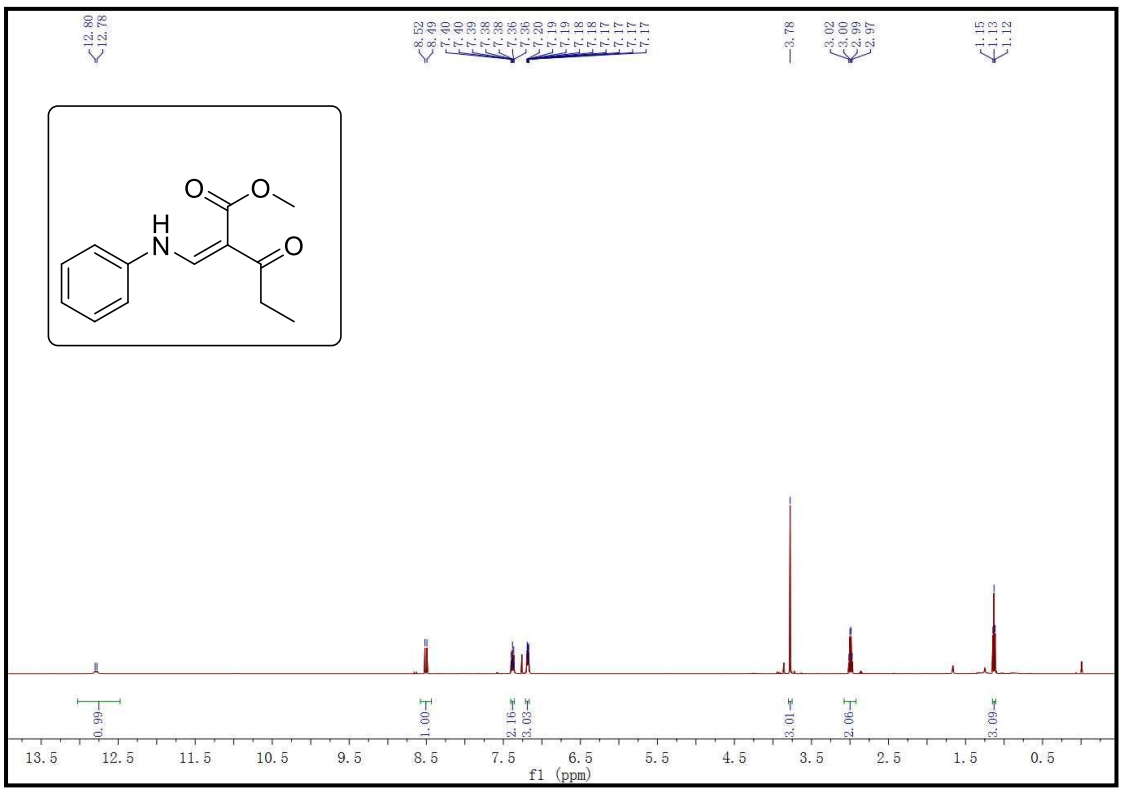


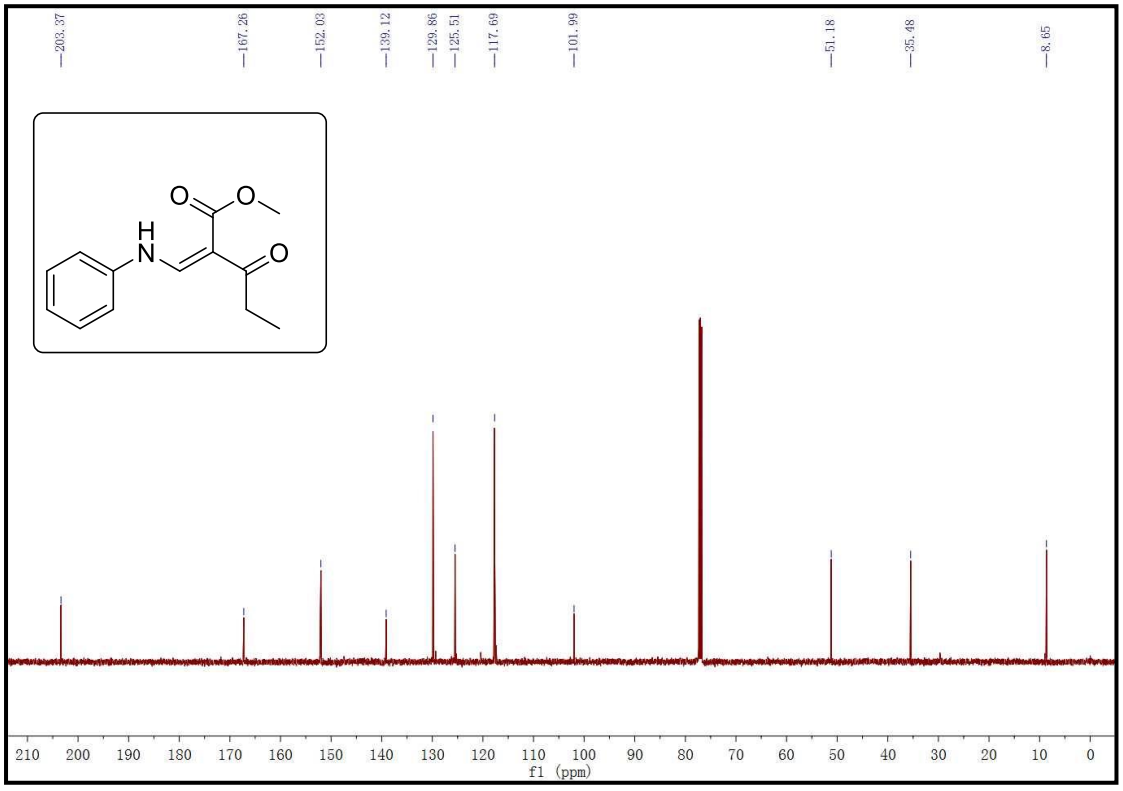
2,6-dimethyl-4-((phenylamino)methylene)heptane-3,5-dione (3ad)



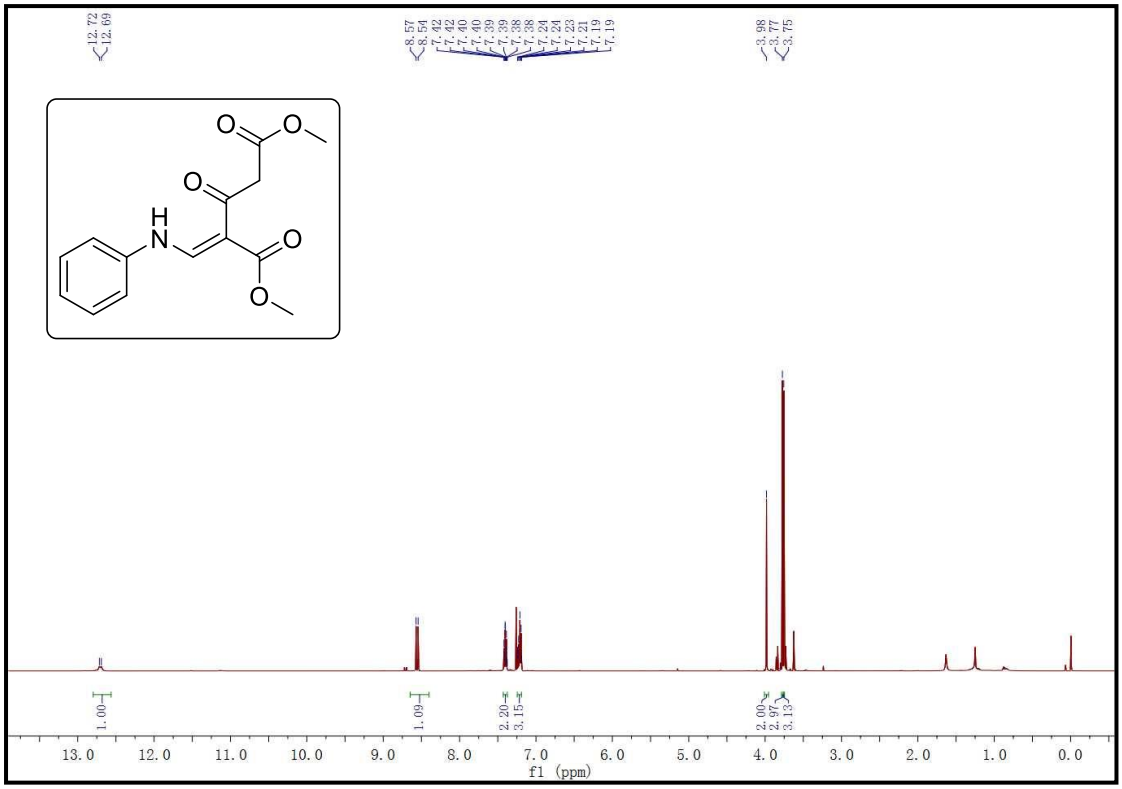


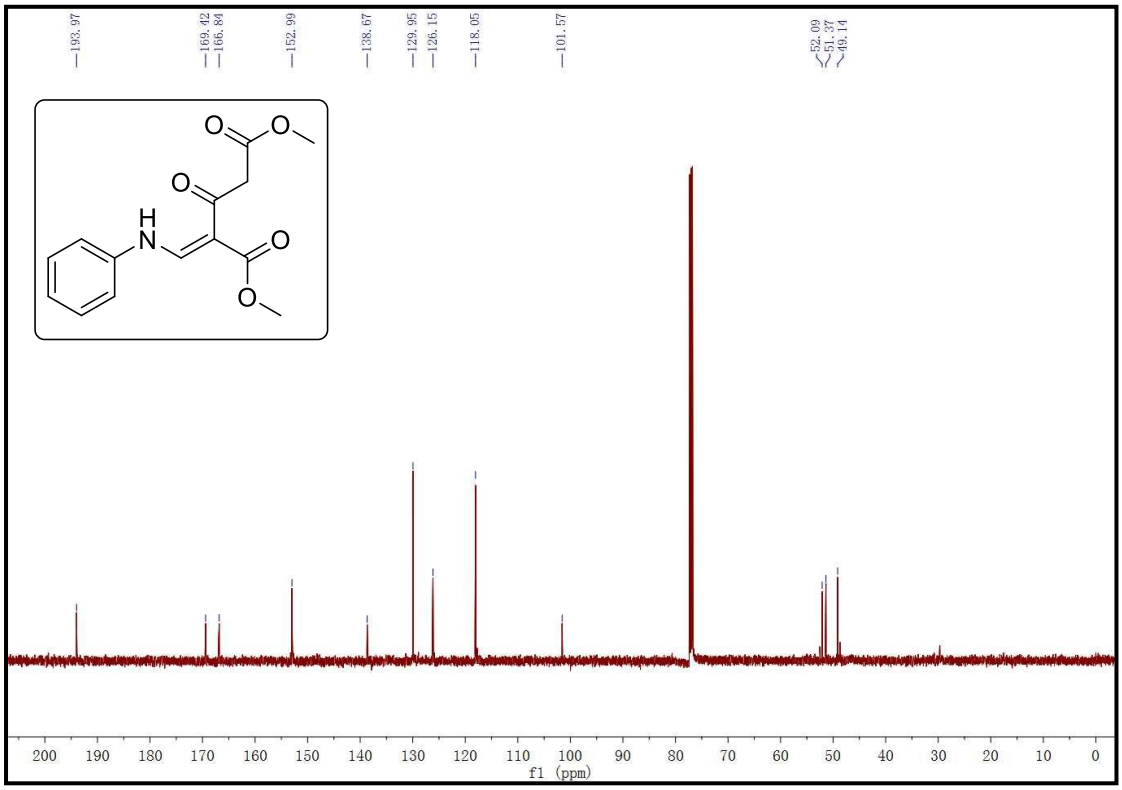
methyl-3-oxo-2-((phenylamino)methylene)pentanoate (3ae)


12.80
12.78
8.52
8.49
7.40
7.40
7.39
7.38
7.38
7.36
7.36
7.20
7.19
7.19
7.18
7.18
7.17
7.17
7.17
7.17
3.78
3.02
3.00
2.99
2.97
1.15
1.13
1.12
O
O
H
N
O
0.99
1.00
2.16
3.03
3.01
2.06
3.09
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

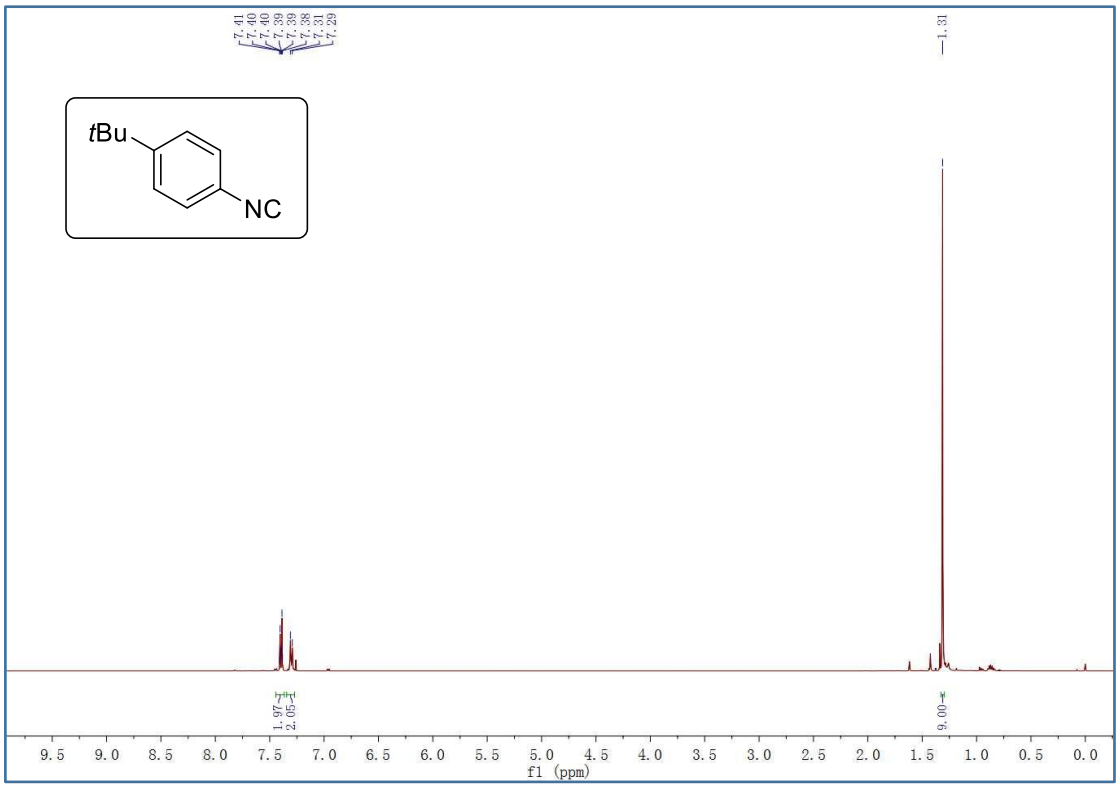

203.37
167.26
152.03
139.12
129.86
125.51
117.69
101.99
51.18
35.48
8.65
O
O
H
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

dimethyl-3-oxo-2-((phenylamino)methylene)pentanedioate (3af)





1-(*tert*-butyl)-4-isocyanobenzene (2)



2-bromo-2,2-difluoro-1-phenylethan-1-one (3)