Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Chemoselective C(α)-C(β) bond cleavage of saturated aryl ketones with amines leading to α-ketoamides: A copper-catalyzed aerobic oxidation process with air

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Contents

1. General information

Reagents: Commercially available reagents were used without any further purification. Commercially unavailable ketones in Table **2** have been prepared according to the literatures: 3-hydroxy-1-phenyl-1-propanone (entry 25),[1] 3-methoxy-1-phenyl-1-propanone (entry 26),[1,2] 3-benzoyl-propionitrile (entry 27).[3]

Solvents: All organic solvents were also of reagent grade quality without any further purification.

Chromatography: Flash column chromatography was performed using silicycle silica gel (200-300 mesh).

Analytical thin-layer chromatography (TLC) was performed on 0.2 mm coated silica gel plates (HSGF 254) and visualized using a UV lamp (254 nm or 365 nm).

Nuclear Magnetic Resonance Spectroscopy:

^{1}H NMR was recorded on magnet system 400'54 ascend purchased from Bruker Biospin AG. ^{1}H NMR spectra chemical shifts (δ) are reported in parts per million (ppm) referenced to TMS (0 ppm).

^{13}C NMR spectra chemical shifts (δ) are reported in parts per million (ppm) were referenced to carbon resonances in the NMR solvent.

ESI-MS spectra were recorded on Agilent Q-TOF 6520.

2. Optimization data

2.1. Optimization data of selective cleavage of C(α)-C(β) bond of propiophenone

2.1.1. The base screening

Table S1. The base screening.[a]

Entry	Catalyst	Base (equiv)	Yield[b] (%)			Yield ratio (3a/4a)
			3a	4a	3a+4a	
1	$Cu(OAc)_2$	pyridine	76	16	92	4.75
2	$Cu(OAc)_2$	TEA	68	14	82	4.86
3	$Cu(OAc)_2$	AcONa	74	11	85	6.72
4	$Cu(OAc)_2$	DMAP	59	17	76	3.47
5	$Cu(OAc)_2$	K_2CO_3	trace	trace		
6	$Cu(OAc)_2$	Cs_2CO_3	trace	trace		
7	$Cu(OAc)_2$	DIPEA	40	7	47	5.71
8	$Cu(OAc)_2$	DBU	30	24	54	1.25

[a]Reaction conditions: 1a (1 mmol), 2a (3 mmol), $Cu(OAc)_2$ (0.2 mmol), base (2 mmol), toluene (1 mL), 70℃, O_2 (O_2 balloon), 18h. [b]Isolated yield.

2.1.2. The temperature and solvent screening

Table S2. The temperature and solvent screening.[a]

Entry	T (℃)	Solvent	Yield[b] (%)			Yield ratio (3a/4a)
			3a	4a	3a+4a	
1	100	toluene	76	17	93	4.47
2	90	toluene	83	12	95	6.91
3	80	toluene	81	14	95	5.78
4	70	toluene	83	10	93	8.30
5	60	toluene	69	19	88	3.63
6	50	toluene	57	20	77	2.85
7	70	Neat	66	9	75	7.33
8	70	DMSO	58	7	65	8.28
9	70	DMF	74	12	86	6.17
10	70	dioxane	72	16	88	4.50
11	70	H_2O	77	15	92	5.13
12	70	PhCN	78	15	93	5.20

[a]Reaction conditions: 1a (1 mmol), 2a (3 mmol), CuSCN (0.2 mmol), DMAP (2 mmol), solvent (1 mL), temperature, O_2 (O_2 balloon), 18h. [b]Isolated yield.

2.1.3 The equiv. of catalyst, amine and base screening

Table S3. The equiv. of catalyst, amine and base screening.[a]

Entry	Equiv. of catalyst	Equiv. of amine	Equiv. of DMAP	Yield[b] (%)			Yield ratio (3a/4a)
				3a	4a	3a+4a	
1	0.20	3.00	2	82	13	95	6.31
2	0.20	3.00	1.5	83	10	93	8.30
3	0.20	3.00	1	79	12	91	6.58
4	0.20	3.00	0.5	72	19	91	3.79
5	0.20	4.00	1.5	83	11	94	7.54
6	0.20	3.50	1.5	82	10	92	8.20
7	0.20	3.00	1.5	83	10	93	8.30
8	0.20	2.50	1.5	78	10	88	7.80
9	0.15	2.50	1.5	79	11	90	7.18
10	0.10	2.50	1.5	81	10	91	8.10
11	0.05	2.50	1.5	83	10	93	8.30

[a]Reaction conditions: 1a (1 mmol), 2a, CuSCN, DMAP, solvent (1 mL), 70℃, O_2 (O_2 balloon), 18h. [b]Isolated yield.

2.2. Optimization data of selective cleavage of C(O)-C(α) bond of propiophenone

As for the formation of C(O)-C(α) bond cleavage product 4a, solvent screening indicated that H_2O was best choice with 9.75 yield ratio of 4a to 3a (Table S4, entries 1-6). However, the conversion was unsatisfactory (Table S4, entry 5). To our delight, 89% 4a was isolated with only trace amounts of 3a when the reaction was performed in H_2O using $Cu(hfacac)_2$ as the catalyst (Table S4, entry 7).

Table S4. The selective cleavage of C(O)-C(α) bond of propiophenone.[a]

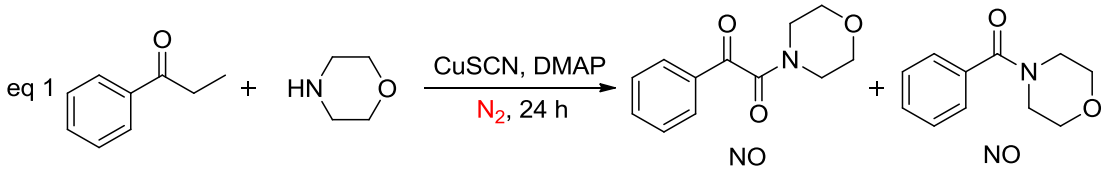
Entry	Catalyst	Solvent	Yield[b] (%)			Yield ratio (4a/3a)
			3a	4a	3a+4a	
1	$CuCl_2•2H_2O$	Neat	50	43	93	0.86
2	$CuCl_2•2H_2O$	DMSO	8	37	45	4.62
3	$CuCl_2•2H_2O$	DMF	47	42	89	0.89
4	$CuCl_2•2H_2O$	dioxane	29	50	79	1.72
5	$CuCl_2•2H_2O$	H_2O	4	39	43	9.75
6	$CuCl_2•2H_2O$	PhCN	49	30	78	0.61
7	$Cu(hfacac)_2$	H_2O	trace	89	89	

[a]Reaction conditions: 1a (1 mmol), 2a (3 mmol), catalyst (0.2 mmol), solvent (1 mL), 70℃, O_2 (O_2 balloon), 36h. [b]Isolated yield.

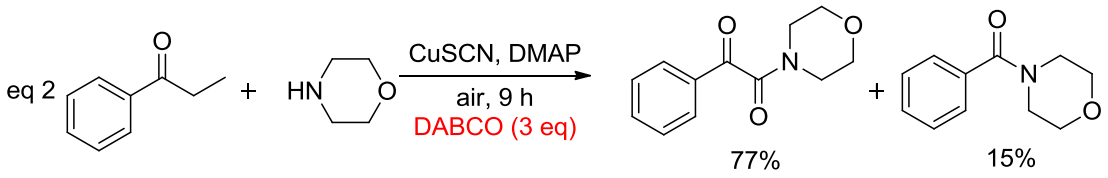
3. General experimental details for the synthesis of C (α)-C (β) bond cleavage products

To a solution of the specific ketone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq) and amine (3 mmol, 3eq). The mixture was stirred at 70℃ under the open air for about 5-48 h. After the TLC revealed that the full conversion of corresponding ketone was completed, the reaction mixture was cooled and diluted with ethyl acetate (30 mL). The crude product was washed with saturated NH_4Cl solution (30 mL) and water (30 mL). The separated organic layer was dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexanes/ethyl acetate or dichloromethane/methanol to afford the desired product.

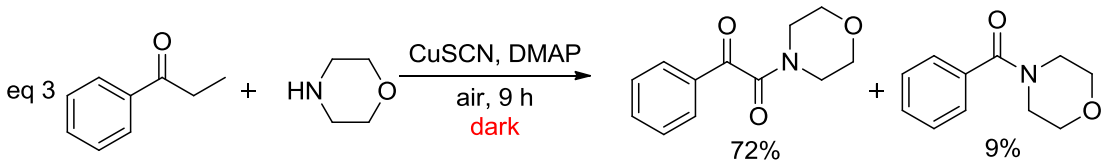
4. Control experiments



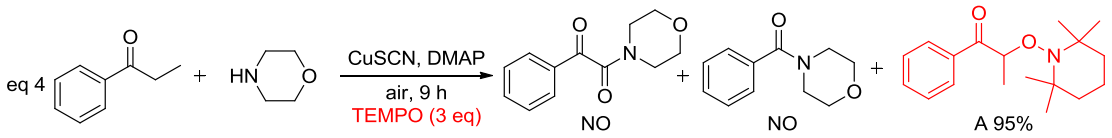
To a solution of propiophenone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq) and morpholine (3 mmol, 3eq). The mixture was stirred at 70℃ under N_2 for 24 h. The TLC revealed that no desired product was generated.



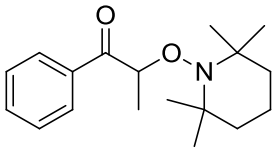
To a solution of propiophenone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq), DABCO (3 mmol, 3 eq) and morpholine (3 mmol, 3eq). The mixture was stirred at 70℃ under the open air for 9 h. Then, the reaction mixture was cooled and diluted with ethyl acetate (30 mL). The crude product was washed with saturated NH_4Cl solution (30 mL) and water (30 mL). The separated organic layer was dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexanes/ethyl acetate (6:1) to afford the desired product (3a, 168.7 mg, 77%; 4a, 28.7 mg, 15%).



To a solution of propiophenone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq) and morpholine (3 mmol, 3eq). The mixture was stirred at 70℃ under the open air in the dark for 9 h. Then, the reaction mixture was cooled and diluted with ethyl acetate (30 mL). The crude product was washed with saturated NH_4Cl solution (30 mL) and water (30 mL). The separated organic layer was dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexanes/ethyl acetate (6:1) to afford the desired product (3a, 157.7 mg, 72%; 4a, 17.2 mg, 9%).

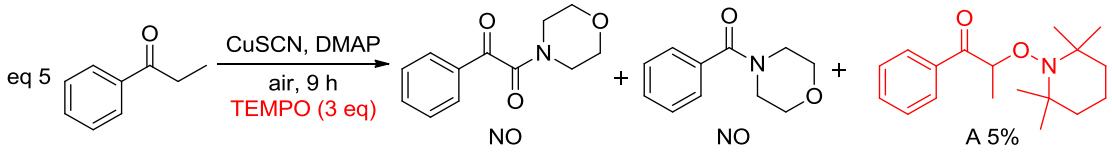


To a solution of propiophenone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq), TEMPO (3 mmol, 3 eq) and morpholine (3 mmol, 3eq). The mixture was stirred at 70℃ under the open air for 9 h. Then, the reaction mixture was cooled and diluted with ethyl acetate (30 mL). The crude product was washed with saturated NH_4Cl solution (30 mL) and water (30 mL). The separated organic layer was dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexanes/ethyl acetate (200:1) to afford the Intermediate A (274.7 mg, 95%).

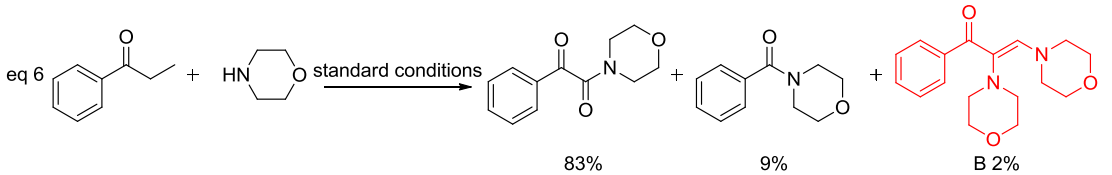


1-Phenyl-2-(2,2,6,6-tetramethylpiperidin-1-yloxy)propan-1-one:[4]

^{1}H NMR (300 MHz, DMSO) δ 8.01 (dt, *J* = 7.2, 1.5 Hz, 2H), 7.64 (tt, *J* = 7.5, 1.2 Hz, 1H), 7.53 (tt, *J* = 7.2, 1.5 Hz, 2H), 5.00 (q, *J* = 7.0 Hz, 1H), 1.58 – 1.30 (m, 8H), 1.25 (s, 4H), 1.11 (s, 3H), 0.97 (s, 3H), 0.78 (s, 3H); ^{13}C NMR (75 MHz, DMSO) δ 201.30, 135.21, 133.83, 129.25, 129.15, 85.36, 59.65, 40.16, 34.07, 33.62, 20.48, 20.40, 19.29, 17.05; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{18}H_{27}NO_2$ 290.2115 found 290.2100.

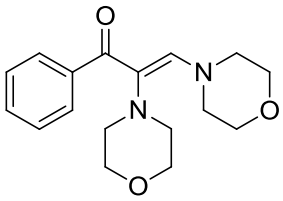


To a solution of propiophenone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq) and TEMPO (3 mmol, 3 eq). The mixture was stirred at 70℃ under the open air for 9 h. Then, the reaction mixture was cooled and diluted with ethyl acetate (30 mL). The crude product was washed with saturated NH_4Cl solution (30 mL) and water (30 mL). The separated organic layer was dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexanes/ethyl acetate (200:1) to afford the Intermediate A (14.5 mg, 5%).



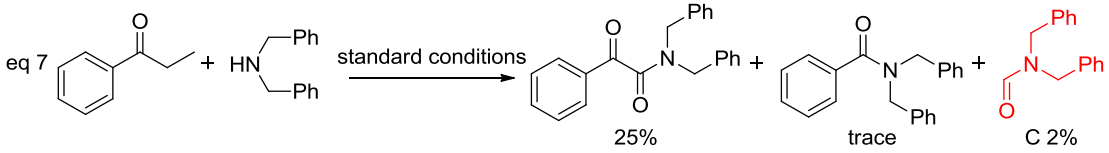
To a solution of propiophenone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq) and morpholine (3 mmol, 3eq). The mixture was

stirred at 70℃ under the open air for 9 h. Then, the reaction mixture was cooled and diluted with ethyl acetate (30 mL). The crude product was washed with saturated NH_4Cl solution (30 mL) and water (30 mL). The separated organic layer was dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexanes/ethyl acetate (6:1) to afford the byproduct B (6.0 mg, 2%).

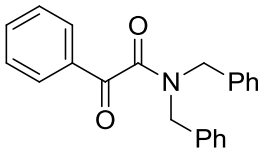


2,3-di-4-morpholinyl-1-phenyl-2-propen-1-one:[5]

^{1}H NMR (400 MHz, DMSO) δ 7.46 – 7.36 (m, 5H), 6.52 (s, 1H), 3.75 (s, 4H), 3.64 – 3.55 (m, 8H), 3.03 (s, 4H); ^{13}C NMR (101 MHz, DMSO) δ 193.87, 150.23, 142.25, 130.03, 128.65, 128.41, 122.19, 66.93, 66.78, 50.98, 50.25; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{17}H_{22}N_2O_3$ 325.1523 found 325.1532.

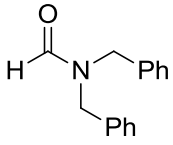


To a solution of propiophenone (1 mmol, 1eq) in toluene (1 mL) was added CuSCN (0.05 mmol, 0.05 eq), DMAP (1.5 mmol, 1,5 eq) and dibenzylamine (3 mmol, 3eq). The mixture was stirred at 70℃ under the open air for 9 h. Then, the reaction mixture was cooled and diluted with ethyl acetate (30 mL). The crude product was washed with saturated NH_4Cl solution (30 mL) and water (30 mL). The separated organic layer was dried over by anhydrous Na_2SO_4 and filtered. The filtrate was concentrated under reduced pressure and the residue was chromatographed on silica gel using hexanes/ethyl acetate (9:1) to afford the desired product (82.3 mg, 25%) and the corresponding formamide C (4.5 mg, 2%).



N,N-Dibenzyl-2-oxo-2-phenylacetamide:[6]

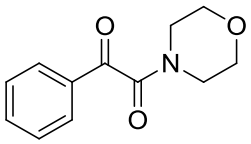
^{1}H NMR (500 MHz, DMSO) δ 7.93 (d, *J* = 7.3 Hz, 2H), 7.78 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.7 Hz, 2H), 7.43 (t, *J* = 7.3 Hz, 2H), 7.38-7.31 (m, 5H), 7.30 – 7.23 (m, 3H), 4.62 (s, 2H), 4.38 (s, 2H); ^{13}C NMR (126 MHz, DMSO) δ 191.78, 167.54, 136.58, 135.63, 135.60, 133.09, 129.76, 129.19, 129.05, 128.53, 128.33, 128.24, 128.08, 50.60, 47.05; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{22}H_{19}NO_2$ 352.1308 found 352.1318.



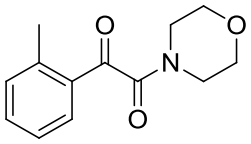
N,N-Bis(phenylmethyl)formamide:[7]

^{1}H NMR (500 MHz, DMSO) δ 8.50 (s, 1H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.35 (q, *J* = 6.8 Hz, 3H), 7.31 – 7.24 (m, 3H), 7.20 (d, *J* = 7.3 Hz, 2H), 4.39 (s, 2H), 4.32 (s, 2H); ^{13}C NMR (126 MHz, DMSO) δ 163.66, 137.14, 137.01, 129.12, 128.95, 128.28, 128.26, 128.14, 127.68, 50.16, 44.70; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{15}H_{15}NO$ 248.1046 found 248.1046.

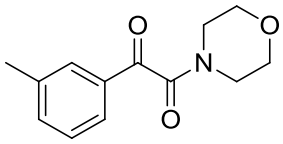
5. Characterization data



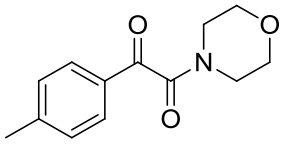
1-Morpholino-2-phenylethane-1,2-dione:[6]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 7.3 Hz, 2H), 7.65 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.7 Hz, 2H), 3.78 (brs, 4H), 3.67 – 3.60 (m, 2H), 3.40 – 3.33 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.29, 165.59, 135.08, 133.20, 129.82, 129.24, 66.88, 66.81, 46.41, 41.76; HRMS (TOF) m/z $[M + Na]^+$ Calcd for $C_{12}H_{13}NO_3$ 242.0788 found 242.0783.



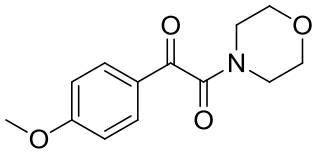
1-Morpholino-2-(o-tolyl)ethane-1,2-dione:[8]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, J = 6.8 Hz, 1H),7.50 (t, J = 6.9 Hz, 1H), 7.33 (dd, J = 10.0, 7.7 Hz, 2H), 3.79 (d, J = 3.1 Hz, 4H), 3.69 – 3.65 (m, 2H), 3.42 – 3.37 (m, 2H), 2.66 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 193.21, 166.30, 141.75, 134.00, 132.82, 131.80, 131.58, 126.33, 66.77, 66.75, 46.38, 41.72, 21.94; HRMS (TOF) m/z $[M + H]^+$Calcd for $C_{13}H_{15}NO_3$ 234.1125 found 234.1122.



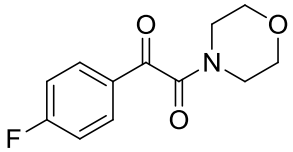
1-Morpholino-2-(m-tolyl)ethane-1,2-dione:[9]
Purified by column chromatography (hexanes/ethyl acetate 6:1); White solid; ^{1}H NMR (300 MHz, DMSO) δ 7.71 (s, 2H), 7.55 (dd, *J* = 19.2, 7.1 Hz, 2H), 3.68 (dd, *J* = 14.2, 3.5 Hz, 4H), 3.52 (t, *J* = 4.2 Hz, 2H), 3.28 (t, *J* = 5.1 Hz, 2H), 2.41 (s, 3H);^{113}C NMR (75 MHz, DMSO) δ 191.70, 164.97, 138.98, 135.83, 132.69, 129.25, 129.23, 126.72, 66.03, 65.83, 45.67, 40.99, 20.71; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{13}H_{15}NO_3$ 234.1125 found 234.1112.



1-Morpholino-2-(p-tolyl)ethane-1,2-dione:[8]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 8.1 Hz, 2H), 7.30 (d, J = 8.2 Hz, 2H), 3.77 (brs, 4H), 3.64 – 3.60 (m, 2H), 3.37 – 3.33 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 190.98, 165.75, 146.36, 130.73, 129.90, 129.86, 66.82, 66.74, 46.34, 41.64, 22.00; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{13}H_{15}NO_3$ 234.1125 found 234.1106.

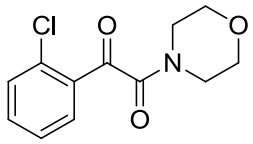


1-(4-Methoxyphenyl)-2-morpholinoethane-1,2-dione:[9]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (t, J = 12.9 Hz, 2H), 6.94 (t, J = 12.3 Hz, 2H), 3.88 – 3.79 (m, 3H), 3.73 (d, J = 25.3 Hz, 4H), 3.60 (t, J = 10.4 Hz, 2H), 3.33 (t, J = 10.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.91, 165.89, 165.11, 132.23, 126.24, 114.51, 66.86, 66.76, 55.76, 46.38, 41.64; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{13}H_{15}NO_4$ 250.1074 found 250.1072.

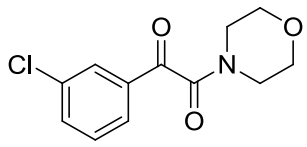


1-(4-fluorophenethyl)-2-morpholinoethane-1,2-dione:[8]

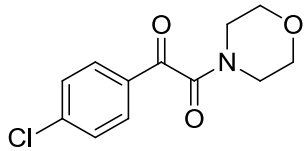
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 – 7.95 (m, 2H), 7.19 (t, J = 8.5 Hz, 2H), 3.79 (s, 4H), 3.70 – 3.62 (m, 2H), 3.43 – 3.34 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.50, 166.94 (d, J=256.7), 165.22, 132.69 (d, J=9.8), 129.75 (d, J=2.8), 116.70, 116.48, 66.89, 66.79, 46.44, 41.84; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{12}H_{12}FNO_3$ 238.0874 found 238.0876.



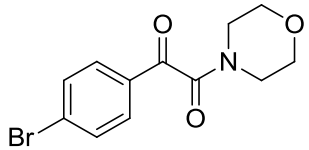
1-(2-Chlorophenyl)-2-morpholinoethane-1,2-dione:[10]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (300 MHz, DMSO) δ 7.85 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.69 (ddd, *J* = 8.7, 6.0, 1.7 Hz, 1H), 7.65 – 7.51 (m, 2H), 3.72-3.66 (m, 2H), 3.65-3.55 (m, 4H), 3.44 (t, *J* = 5.1 Hz, 2H); ^{13}C NMR (75 MHz, DMSO) δ 190.04, 165.26, 135.70, 133.27, 132.88, 132.74, 131.50, 128.38, 66.10, 65.97, 46.12, 41.78; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{12}H_{12}ClNO_3$ 276.0398 found 276.0366.



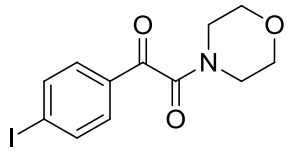
1-(3-Chlorophenyl)-2-morpholinoethane-1,2-dione:[11]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (300 MHz, DMSO) δ 7.92 – 7.79 (m, 3H), 7.66 (t, *J* = 7.7 Hz, 1H), 3.74 – 3.67 (m, 2H), 3.67 – 3.61 (m, 2H), 3.54 (t, *J* = 4.5 Hz, 2H), 3.32 (t, *J* = 4.8 Hz, 2H). ^{13}C NMR (75 MHz, DMSO) δ 190.48, 164.64, 135.31, 134.91, 134.68, 131.88, 128.81, 66.52, 66.24, 46.13, 41.62; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{12}H_{12}ClNO_3$ 276.0398 found 276.0394.



1-(4-Chlorophenyl)-2-morpholinoethane-1,2-dione:[6]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 – 7.85 (m, 2H), 7.56 – 7.46 (m, 2H), 3.82 – 3.74 (m, 4H), 3.69 – 3.63 (m, 2H), 3.42 – 3.34 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.83, 164.04, 140.76, 130.61, 130.18, 128.64, 65.88, 65.79, 45.43, 40.85; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{12}H_{12}ClNO_3$ 276.0398 found 276.0391.

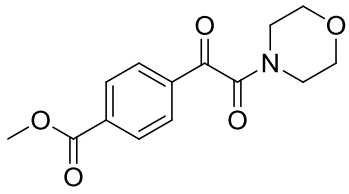


1-(4-bromophenethyl)-2-morpholinoethane-1,2-dione:[8]
Purified by column chromatography (hexanes/ethyl acetate 6:1); White solid; ^{1}H NMR (300 MHz, DMSO) δ 7.84 (s, 4H), 3.74-3.68 (m, 2H), 3.67-3.62 (m, 2H), 3.53 (t, *J* = 4.2 Hz, 2H), 3.30 (t, *J* = 4.5 Hz, 2H); ^{13}C NMR (75 MHz, DMSO) δ 190.51, 164.42, 132.53, 131.65, 131.16, 129.52, 66.05, 65.77, 45.66, 41.09; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{12}H_{12}BrNO_3$ 319.9893 found 319.9872.

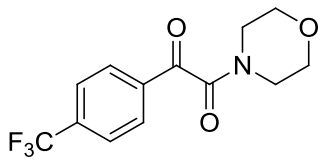


1-(4-iodophenyl)-2-morpholinoethane-1,2-dione:[12]
Purified by column chromatography (hexanes/ethyl acetate 6:1); White solid; ^{1}H NMR (300 MHz, DMSO) δ 8.02 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 8.1 Hz, 2H), 3.72 – 3.67 (m, 2H), 3.65 – 3.60 (m, 2H), 3.52 (t, *J* = 5.1 Hz, 2H), 3.27 (t, *J* = 4.5 Hz, 2H); ^{13}C NMR (75 MHz, DMSO) δ 191.41, 164.94, 138.87, 132.37, 131.19, 105.07, 66.52, 66.25, 46.12, 41.54; HRMS (TOF) m/z [M + Na]$^+$ Calcd

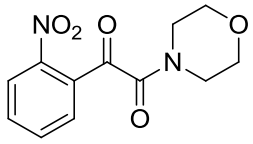
for $C_{12}H_{12}INO_3$ 367.9754 found 367.9756.



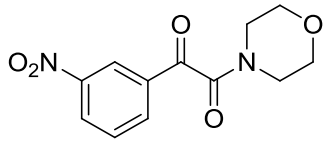
Methyl 4-(2-morpholino-2-oxoacetyl)benzoate:[9]
Purified by column chromatography (hexanes/ethyl acetate 4:1); Yellow solid; ^{1}H NMR (300 MHz, DMSO) δ 8.15 (d, *J* = 8.1 Hz, 2H), 8.04 (d, *J* = 8.1 Hz, 2H), 3.90 (s, 3H), 3.76 – 3.59 (m, 4H), 3.53 (t, *J* = 4.2 Hz, 2H), 3.30 (t, *J* = 5.8 Hz, 2H); ^{13}C NMR (75 MHz, DMSO) δ 191.26, 165.76, 164.82, 136.30, 135.26, 130.42, 130.10, 66.51, 66.24, 53.10, 46.14, 41.62; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{14}H_{15}NO_5$ 300.0842 found 300.0844.



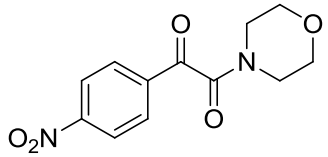
1-Morpholino-2-(4-(trifluoromethyl)phenyl)ethane-1,2-dione:[8]
Purified by column chromatography (hexanes/ethyl acetate 5:1); White solid; ^{1}H NMR (300 MHz, DMSO) δ 8.12 (d, *J* = 8.4 Hz, 2H), 7.98 (d, *J* = 8.4 Hz, 2H), 3.74 – 3.69 (m, 2H), 3.68 – 3.63 (m, 2H), 3.54 (t, *J* = 5.1 Hz, 2H), 3.33 (t, *J* = 4.5 Hz, 2H); ^{13}C NMR (75 MHz, DMSO) δ 190.79, 164.63, 136.18, 134.74, 134.30, 130.68, 126.79 (q, *J* = 3.4 Hz), 125.79, 66.54, 66.24, 46.13, 41.65; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{13}H_{12}NO_3F_3$ 310.0661 found 310.0672.



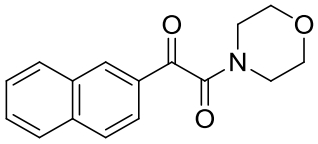
1-Morpholino-2-(2-nitrophenyl)ethane-1,2-dione:[13]
Purified by column chromatography (hexanes/ethyl acetate 4:1); Yellow solid; ^{1}H NMR (400 MHz, DMSO) δ 8.19 (dd, *J* = 8.0, 0.9 Hz, 1H), 7.95 (td, *J* = 7.5, 1.1 Hz, 1H), 7.91 – 7.82 (m, 2H), 3.75 (d, *J* = 1.2 Hz, 4H), 3.65 (t, *J* = 4.4 Hz 2H), 3.55 (t, *J* = 5.2 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 187.03, 161.75, 147.07, 134.83, 133.48, 131.71, 131.14, 124.15, 66.01 (d, *J* = 16.8 Hz), 45.98, 42.11; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{12}H_{12}N_2O_5$ 287.0638 found 287.0637.



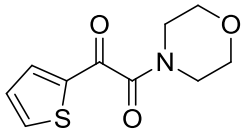
1-Morpholino-2-(3-nitrophenyl)ethane-1,2-dione:[8]
Purified by column chromatography (hexanes/ethyl acetate 4:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (t, J = 1.8 Hz, 1H), 8.48 (ddd, J = 8.2, 2.2, 1.0 Hz, 1H), 8.34 – 8.27 (m, 1H), 7.74 (t, J = 8.0 Hz, 1H), 3.83 – 3.79 (m, 4H), 3.72 – 3.67 (m, 2H), 3.46 – 3.42 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 188.25, 164.00, 148.73, 135.24, 134.66, 130.48, 128.96, 124.64, 66.85, 66.74 46.48, 42.10; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{12}H_{12}N_2O_5$ 287.0638 found 287.0623.



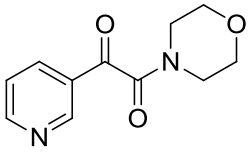
1-Morpholino-2-(4-nitrophenyl)ethane-1,2-dione:[8]
Purified by column chromatography (hexanes/ethyl acetate 4:1); Yellow solid; ^{1}H NMR (400 MHz, DMSO) δ 8.41 (d, *J* = 8.4 Hz, 2H), 8.18 (d, *J* = 8.4 Hz, 2H), 3.74 (t, *J* = 4.4 Hz, 2H), 3.67 (t, *J* = 5.2 Hz, 2H), 3.56 (t, *J* = 4.4 Hz, 2H), 3.36 (t, *J* = 4.8 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 189.78, 163.89, 150.90, 136.96, 130.84, 124.37, 66.05, 65.73, 45.66, 41.23; HRMS (TOF) m/z [M + K]$^+$ Calcd for $C_{12}H_{12}N_2O_5$ 303.0378 found 303.0330.



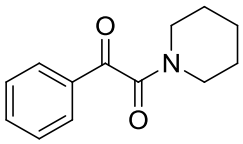
1-Morpholino-2-(naphthalen-2-yl)ethane-1,2-dione:[13] Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.04 – 7.86 (m, 4H), 7.61 (dt, J = 28.4, 7.3 Hz, 2H), 3.84 (s, 4H), 3.72 – 3.61 (m, 2H), 3.47 – 3.36 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.34, 165.70, 136.54, 133.16, 132.53, 130.53, 130.02, 129.66, 129.30, 128.08, 127.35, 123.68, 66.87, 66.82, 46.47, 41.83; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{16}H_{15}NO_3$ 270.1125 found 270.1140.



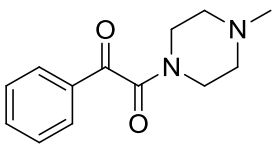
1-Morpholino-2-(thiophen-2-yl)ethane-1,2-dione:[8] Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (ddd, J = 5.9, 4.4, 1.0 Hz, 2H), 7.17 (dd, J = 4.8, 4.0 Hz, 1H), 3.78 – 3.71 (m, 4H), 3.69 – 3.62 (m, 2H), 3.51 – 3.44 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 182.90, 164.41, 140.36, 136.87, 136.37, 128.82, 66.89, 66.70, 46.52, 42.03; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{10}H_{11}NO_3S$ 226.0532 found 226.0552.



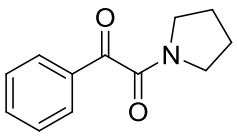
1-Morpholino-2-(pyridine-3-yl)ethane-1,2-dione:[8] Purified by column chromatography (hexanes/ethyl acetate 4:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.81 – 8.75 (m, 1H), 8.19 (dd, J = 8.0, 2.0 Hz, 1H), 7.46 – 7.37 (m, 1H), 3.72 (s, 4H), 3.63 – 3.58 (m, 2H), 3.38 – 3.33 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 189.45, 164.13, 154.80, 151.17, 136.73, 128.77, 123.92, 66.68, 66.55, 46.25, 41.79; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{11}H_{12}N_2O_3$ 221.0921 found 221.0928.



1-Phenyl-2-(piperidin-1-yl)ethane-1,2-dione:[8] Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 1.4 Hz, 2H), 7.65 – 7.59 (m, 1H), 7.49 (t, J = 7.7 Hz, 2H), 3.69 (s, 2H), 3.31 – 3.23 (m, 2H), 1.71 – 1.64 (m, 4H), 1.57 – 1.47 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.05, 165.54, 134.74, 133.36, 129.65, 129.09, 47.12, 42.24, 26.29, 25.54, 24.47; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{13}H_{15}NO_2$ 218.1184 found 218.1184.

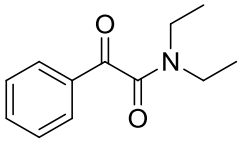


1-(4-Methylpiperazin-1-yl)-2-phenylethane-1,2-dione:[11] Purified by column chromatography (dichloromethane/methanol 30:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.87 (m, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.48 (t, J = 7.7 Hz, 2H), 3.82 – 3.71 (m, 2H), 3.39 – 3.28 (m, 2H), 2.51 – 2.45 (m, 2H), 2.36 – 2.32 (m, 2H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.54, 165.44, 134.88, 133.16, 129.69, 129.11, 54.95, 54.49, 46.04, 45.81, 41.20; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{13}H_{16}N_2O_2$ 233.1285 found 233.1281.

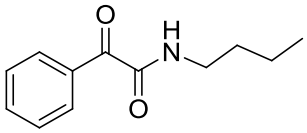


1-Phenyl-2-(pyrrolidin-1-yl)ethane-1,2-dione:[6] Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.94 (m, 2H), 7.62 (t, J = 8.0 Hz, 1H), 7.48 (t, J = 7.7 Hz, 2H), 3.64 (t, J = 6.8 Hz, 2H), 3.40 (t, J =

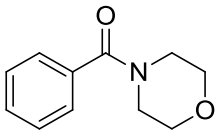
6.2 Hz, 2H), 2.00 – 1.87 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.59, 164.93, 134.59, 132.86, 129.80, 128.91, 46.62, 45.19, 25.85, 23.96; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{12}H_{13}NO_2$ 204.1019 found 204.1026.



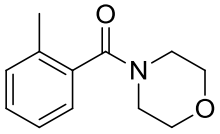
N,N-Diethyl-2-oxo-2-phenylacetamide:[6]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 – 7.85 (m, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.7 Hz, 2H), 3.53 (q, J = 7.2 Hz, 2H), 3.21 (q, J = 7.1 Hz, 2H), 1.25 (t, J = 7.2 Hz, 3H), 1.12 (t, J = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.66, 166.80, 134.64, 133.28, 129.64, 129.01, 42.16, 38.85, 14.14, 12.87; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{12}H_{15}NO_2$ 206.1176 found 206.1191.



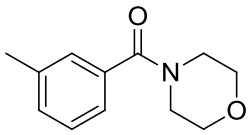
N-Butyl-2-oxo-2-phenylacetamide:[13]
Purified by column chromatography (hexanes/ethyl acetate 7:1); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 – 8.23 (m, 2H), 7.54 (t, J = 7.4 Hz, 1H), 7.40 (t, J = 7.8 Hz, 2H), 7.07 (s, 1H), 3.32 (dd, J = 13.4, 7.0 Hz, 2H), 1.56 – 1.47 (m, 2H), 1.38-1.28 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 186.93, 160.75, 133.32, 132.35, 130.17, 127.44, 38.13, 30.30, 19.03, 12.68; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{12}H_{15}NO_2$ 206.1176 found 206.1193.



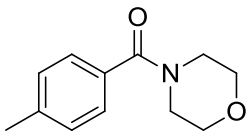
Morpholino(phenyl)methanone:[14]
Purified by column chromatography (hexanes/ethyl acetate 6:1); White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.38 (m, 5H), 3.90–3.36 (m, 8H); ^{13}C NMR (101 MHz, $CDCl_3$) 169.4, 134.3, 128.9, 127.5, 126.1, 65.9, 47.3, 41.6; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{11}H_{13}NO_2$ 191.1019 found 191.1039.



(2-methylphenyl)(morpholino)methanone:[14]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23–7.17 (m, 1H), 7.17–7.10 (m, 2H), 7.10-7.55 (m, 1H), 3.79–3.65 (m, 4H), 3.49 (s, 2H), 3.16 (d, *J* = 4.5 Hz, 2H), 2.24 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.07, 134.60, 133.15, 129.48, 128.03, 124.98, 124.80, 65.96, 65.91, 46.23, 40.88, 17.99; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{12}H_{15}NO_2$ 206.1136 found 206.1153.

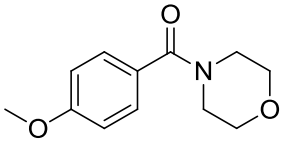


(3-methylphenyl)(morpholino)methanone:[15]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.18 (m, 1H), 7.17-7.13 (m, 2H), 7.09 (d, *J* = 7.4 Hz, 1H), 3.74 – 3.31 (m, 8H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.59, 137.47, 134.28, 129.54, 127.34, 126.67, 122.95, 65.87, 47.15, 41.50, 20.34; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{12}H_{15}NO_2$ 206.1136 found 206.1149.

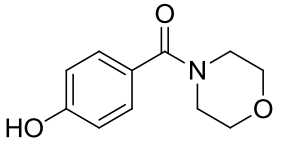


(4-methylphenyl)(morpholino)methanone:[14]
Purified by column chromatography (hexanes/ethyl acetate 6:1);

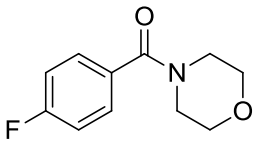
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 3.89-3.41 (m, 8H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.64, 139.08, 131.31, 128.13, 126.21, 65.90, 20.37; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{12}H_{15}NO_2$ 206.1136 found 206.1147.



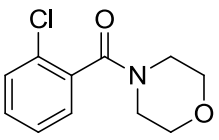
(4-methoxyphenyl)(morpholino)methanone:[14]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (dt, *J* = 8.8, 2.0 Hz, 2H), 6.92 (dt, *J* = 8.8, 2.0 Hz, 2H), 3.84 (s, 3H), 3.76 – 3.54 (m, 8H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.43, 159.90, 128.19, 126.32, 112.78, 65.92, 54.35; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{12}H_{15}NO_3$ 222.1085 found 222.1094.



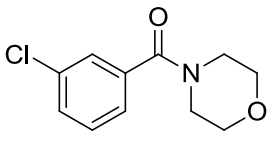
(4-hydroxyphenyl)(morpholino)methanone:[16]
Purified by column chromatography (hexanes/ethyl acetate 3:1); white solid; ^{1}H NMR (500 MHz, DMSO) δ 9.85 (s, 1H), 7.29 (d, *J* = 8.1 Hz, 2H), 6.83 (d, *J* = 8.3 Hz, 2H), 3.60 (t, *J* = 4.2 Hz, 4H), 3.51 (s, 4H); ^{13}C NMR (126 MHz, DMSO) δ 169.83, 159.24, 129.72, 126.24, 115.36, 66.60; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{11}H_{13}NO_2$ 230.0788 found 230.0794.



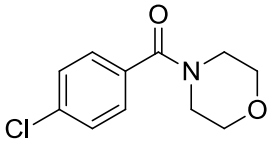
(4-fluorophenyl)(morpholino)methanone:[17]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (500 MHz, DMSO) δ 7.51-7.25 (m, 2H), 7.27 (tt, *J* = 9.1, 2.1 Hz, 2H), 3.70-3.31 (m, 8H); ^{13}C NMR (126 MHz, DMSO) δ 168.11, 163.47, 161.51, 131.92, 131.90, 129.58, 129.51, 115.37, 115.20, 65.96; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{11}H_{12}FNO_2$ 232.0744 found 232.0752.



(2-chlorophenyl)(morpholino)methanone:[18]
Purified by column chromatography (hexanes/ethyl acetate 6:1); white solid; ^{1}H NMR (500 MHz, DMSO) δ 7.58 – 7.53 (m, 1H), 7.50 – 7.39 (m, 3H), 3.74-3.64 (m, 4H), 3.56 (t, *J* = 4.7 Hz, 2H), 3.15 (t, *J* = 4.5 Hz, 2H); ^{13}C NMR (126 MHz, DMSO) δ 165.54, 135.38, 130.46, 129.30, 129.07, 127.92, 127.52, 66.00, 65.84, 46.58, 41.47; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{11}H_{12}ClNO_2$ 248.0449 found 248.0459.

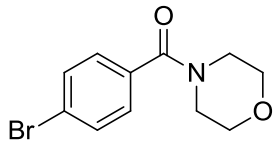


(3-chlorophenyl)(morpholino)methanone:[18]
Purified by column chromatography (hexanes/ethyl acetate 6:1); colorless liquid; ^{1}H NMR (500 MHz, DMSO) δ 7.54 – 7.46 (m, 3H), 7.42 – 7.38 (m, 1H), 3.63 (s, 6H), 3.36 (s, 2H); ^{13}C NMR (126 MHz, DMSO) δ 167.38, 137.62, 133.22, 130.22, 129.33, 126.76, 125.42, 65.92, 47.47, 42.02; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{11}H_{12}ClNO_2$ 248.0449 found 248.0455.

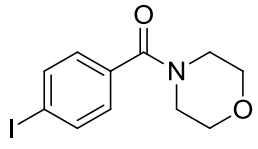


(4-chlorophenyl)(morpholino)methanone:[14]
Purified by column chromatography (hexanes/ethyl acetate 6:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (q, *J* = 8.5 Hz, 4H), 3.89-3.36 (m, 8H);

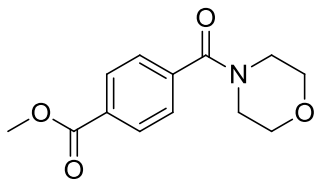
^{13}C NMR (101 MHz, $CDCl_3$) δ 168.37, 135.03, 132.61, 127.86, 127.65, 65.83; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{11}H_{12}ClNO_2$ 248.0449 found 248.0462.



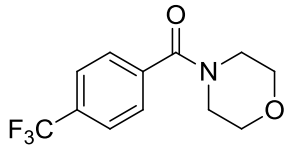
(4-bromophenethyl)(morpholino)methanone:[14]
Purified by column chromatography (hexanes/ethyl acetate 6:1); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (dt, *J* = 8.4, 2.0 Hz, 2H), 7.29 (dt, *J* = 8.4, 1.6 Hz, 2H), 3.85-3.40 (m, 8H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.38, 133.08, 130.82, 127.83, 123.25, 65.81; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{11}H_{12}BrNO_2$ 271.1260 found 271.1282.



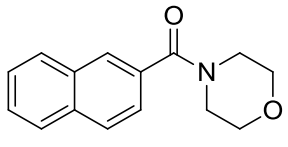
(4-iodophenyl)(morpholino)methanone:[15]
Purified by column chromatography (hexanes/ethyl acetate 6:1); White solid; ^{1}H NMR (500 MHz, DMSO) δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.2 Hz, 2H), 3.71-3.34 (m, 8H); ^{13}C NMR (126 MHz, DMSO) δ 168.19, 137.16, 134.94, 129.02, 96.25, 65.94; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{11}H_{12}INO_2$ 339.9805 found 339.9811.



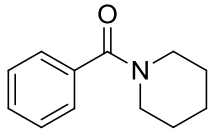
4-(4-Morpholinylcarbonyl)benzoic acid methyl ester:[21]
Purified by column chromatography (hexanes/ethyl acetate 4:1); white solid; ^{1}H NMR (500 MHz, DMSO) δ 8.04 (d, *J* = 7.9 Hz, 2H), 7.57 (d, *J* = 7.9 Hz, 2H), 3.90 (s, 3H), 3.78-3.52 m, 6H), 3.33 (s, 2H); ^{13}C NMR (126 MHz, DMSO) δ 168.55, 166.14, 140.56, 130.86, 129.76, 127.76, 66.47, 52.76; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{13}H_{15}NO_4$ 272.0896 found 272.0890.



(4-(trifluoromethyl)phenyl)(morpholino)methanone:[17]
Purified by column chromatography (hexanes/ethyl acetate 5:1); White solid; ^{1}H NMR (500 MHz, DMSO) δ 7.84 (d, *J* = 6.6 Hz, 2H), 7.67 (d, *J* = 7.7 Hz, 2H), 3.79-3.49 (m, 6H), 3.39-3.25 (m, 2H); ^{13}C NMR (126 MHz, DMSO) δ 168.17, 140.20, 130.21 (q, *J* = 32.2 Hz), 128.27, 127.62, 125.91 (q, *J* = 3.7 Hz), 125.45, 123.27 , 121.12, 66.45, 47.67, 42.32; HRMS (TOF) m/z [M + Na]$^+$ Calcd for $C_{12}H_{12}F_3NO_2$ 282.0712 found 282.0722.

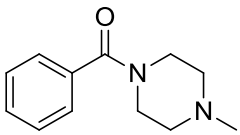


4-Morpholinyl-2-naphthalenylmethanone:[18]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Yellow solid; ^{1}H NMR (500 MHz, DMSO) δ 8.05 – 7.97 (m, 4H), 7.64 – 7.58 (m, 2H), 7.55 (d, *J* = 8.3 Hz, 1H), 3.65 (s, 8H); ^{13}C NMR (126 MHz, DMSO) δ 169.00, 133.04, 132.88, 132.16, 128.26, 127.97, 127.58, 127.02, 126.63, 126.47, 124.40, 66.05; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{15}H_{15}NO_2$ 242.1176 found 242.1191.



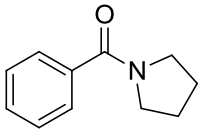
Phenyl(piperidin-1-yl)methanone:[17]
Purified by column chromatography (hexanes/ethyl acetate 6:1); Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (s, 5H), 3.63 (s, 2H), 3.27

(s, 2H), 1.70–1.35 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.29, 135.51, 128.32, 127.37, 125.76, 47.75, 42.11, 25.49, 24.63, 23.57; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{12}H_{15}NO$ 190.1187 found 190.1190.



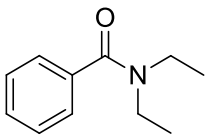
(4-Methyl-1-piperazinyl)phenylmethanone:[19]

Purified by column chromatography (dichloromethane/methanol 30:1); Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.34 (m, 5H), 3.78 (s, 2H), 3.39 (s, 2H), 2.53 – 2.27 (m, 7H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.33, 134.73, 128.68, 127.46, 126.01, 54.16, 53.63, 46.51, 44.89, 40.92; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{12}H_{16}N_2O$ 205.1296 found 205.1304.



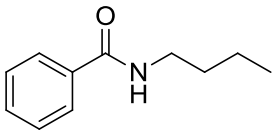
Phenyl(pyrrolidin-1-yl)methanone:[19]

Purified by column chromatography (hexanes/ethyl acetate 6:1); Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.41 (m, 2H), 7.35 – 7.28 (m, 3H), 3.46 (d, *J* = 78.4 Hz, 4H), 1.84 (s, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.74, 136.17, 128.76, 127.22, 126.05, 48.60, 45.18, 25.36, 23.46; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{11}H_{13}NO$ 176.1031 found 176.1042.



N,N-Diethylbenzamide:[19]

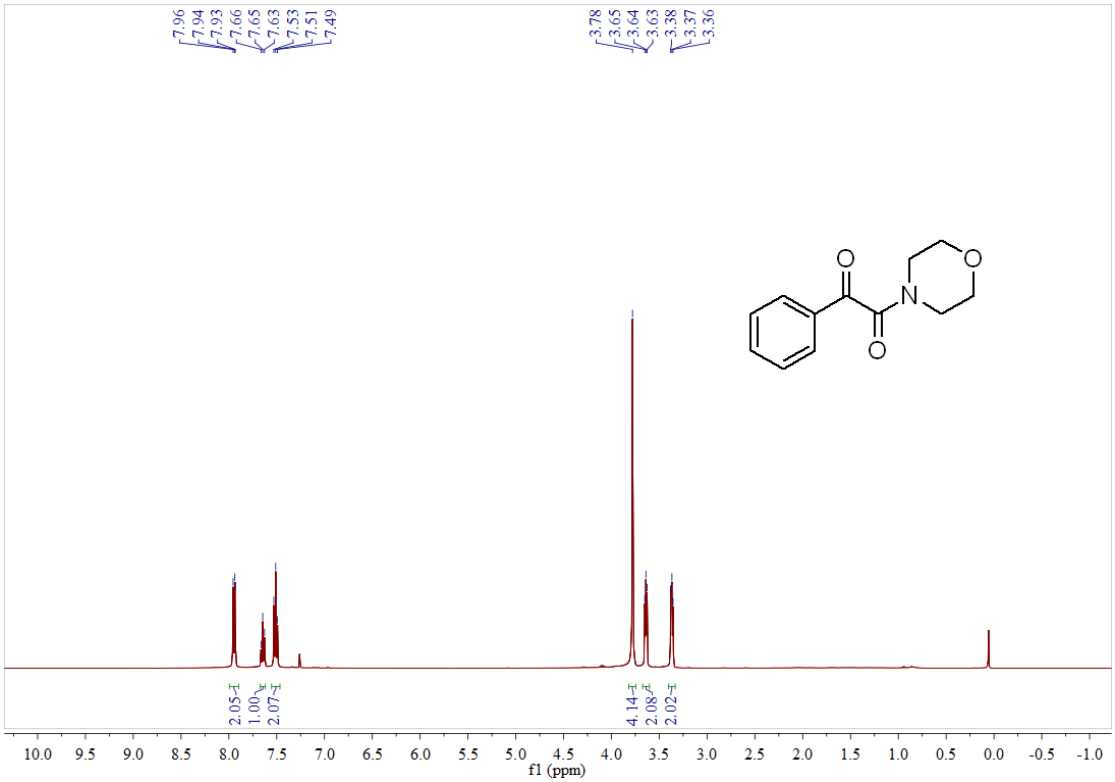
Purified by column chromatography (hexanes/ethyl acetate 6:1); Colourless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.31 (m, 5H), 3.54 (s, 2H), 3.25 (s, 2H), 1.27 – 0.99 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.32, 136.24, 128.08, 127.37, 125.26, 42.29, 38.21, 13.18, 11.91; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{11}H_{15}NO$ 178.1187 found 178.1189.

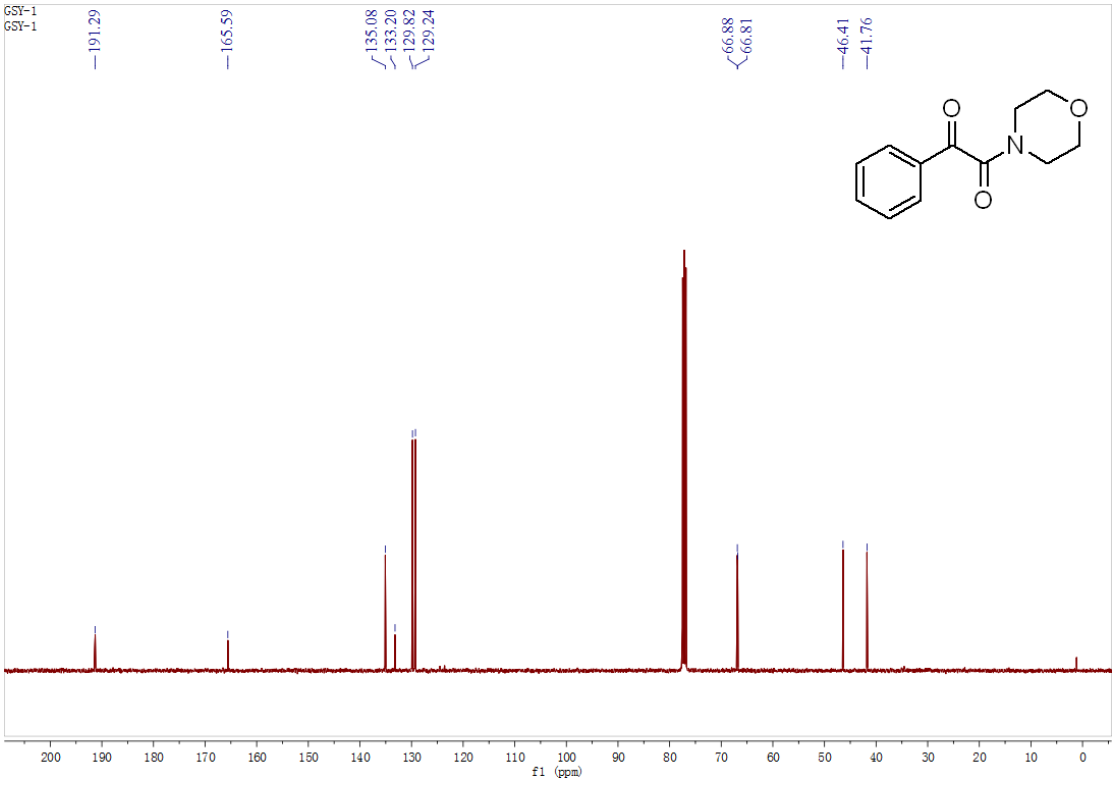


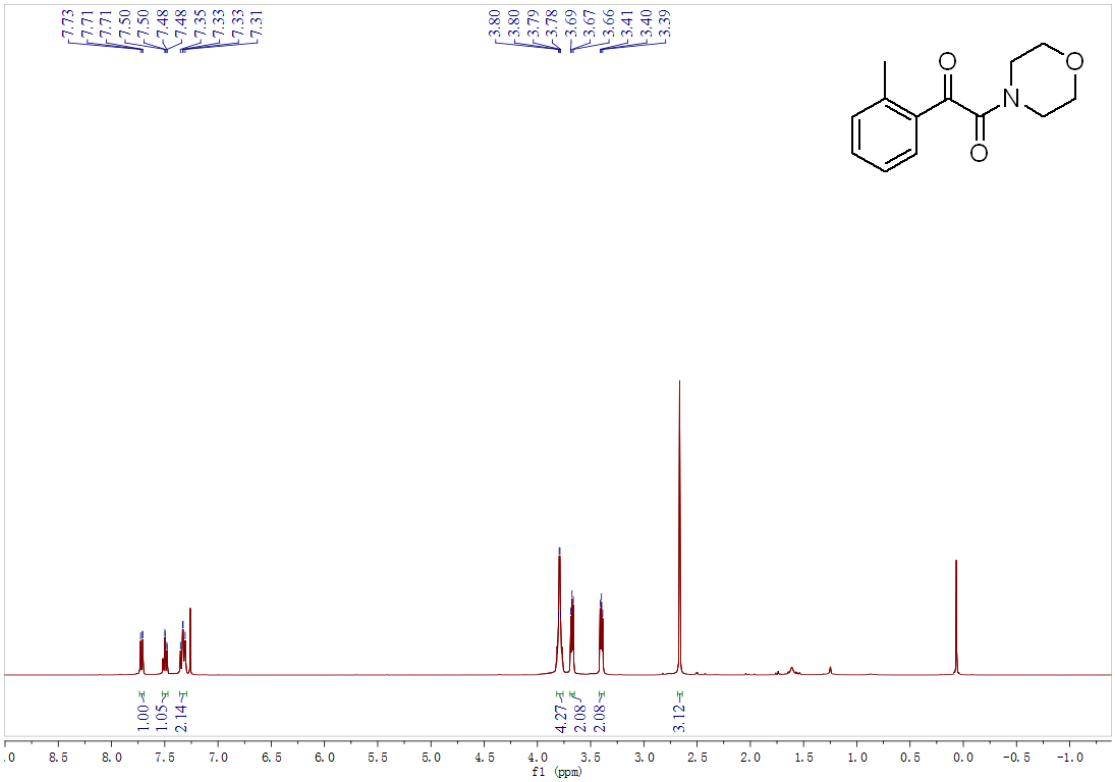
N-*n*-Butylbenzamide:[20]

Purified by column chromatography (hexanes/ethyl acetate 7:1); White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.51 (m, 2H), 7.48 – 7.09 (m, 3H), 6.40-6.07 (m, 1H), 3.53 – 3.11 (m, 2H), 1.65-1.50 (m, 2H), 1.45-1.31 (m, 2H), 0.99-0.82 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.57, 134.89, 131.25, 128.49, 126.85, 39.81, 31.74, 20.16, 13.77; HRMS (TOF) m/z [M + H]$^+$ Calcd for $C_{11}H_{15}NO$ 178.1187 found 178.1191.

6. NMR spectra of products in Table 2, Table 3 and Scheme 2



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7.71
7.50
7.50
7.48
7.48
7.35
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7.33
7.31
3.80
3.80
3.79
3.78
3.69
3.67
3.66
3.41
3.40
3.39
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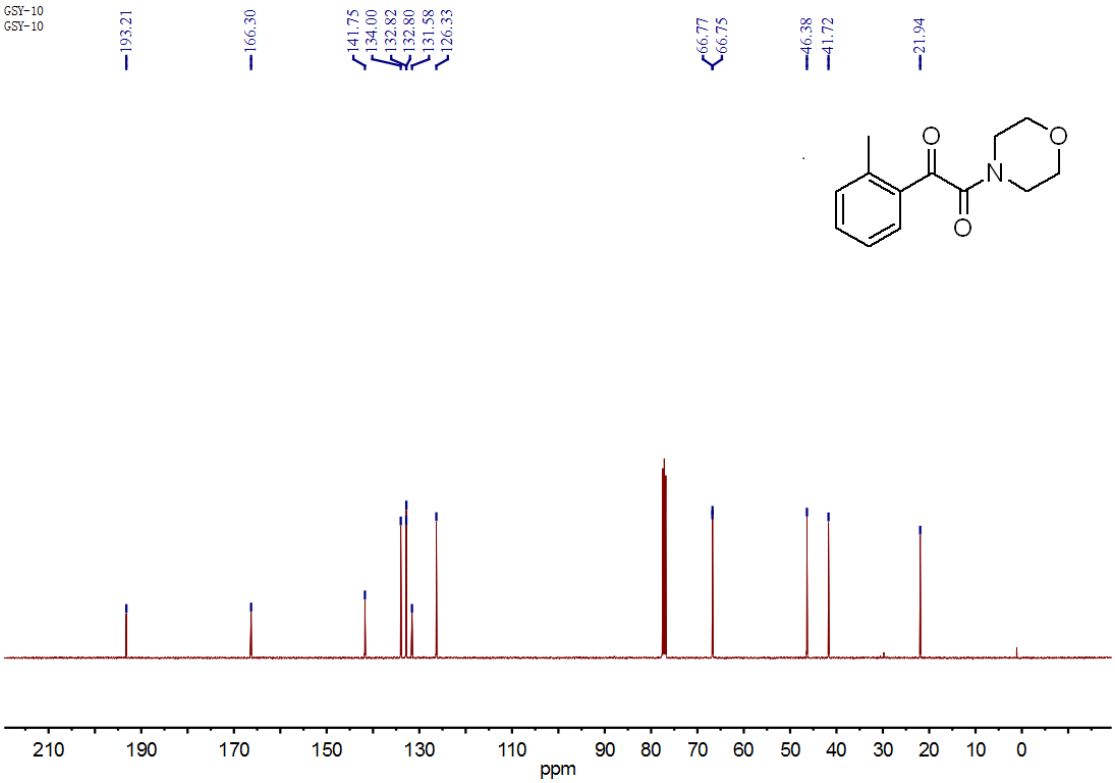
N
O
O
1.00
1.05
2.14
4.27
2.08
2.08
3.12
f1 (ppm)


GSY-10
GSY-10
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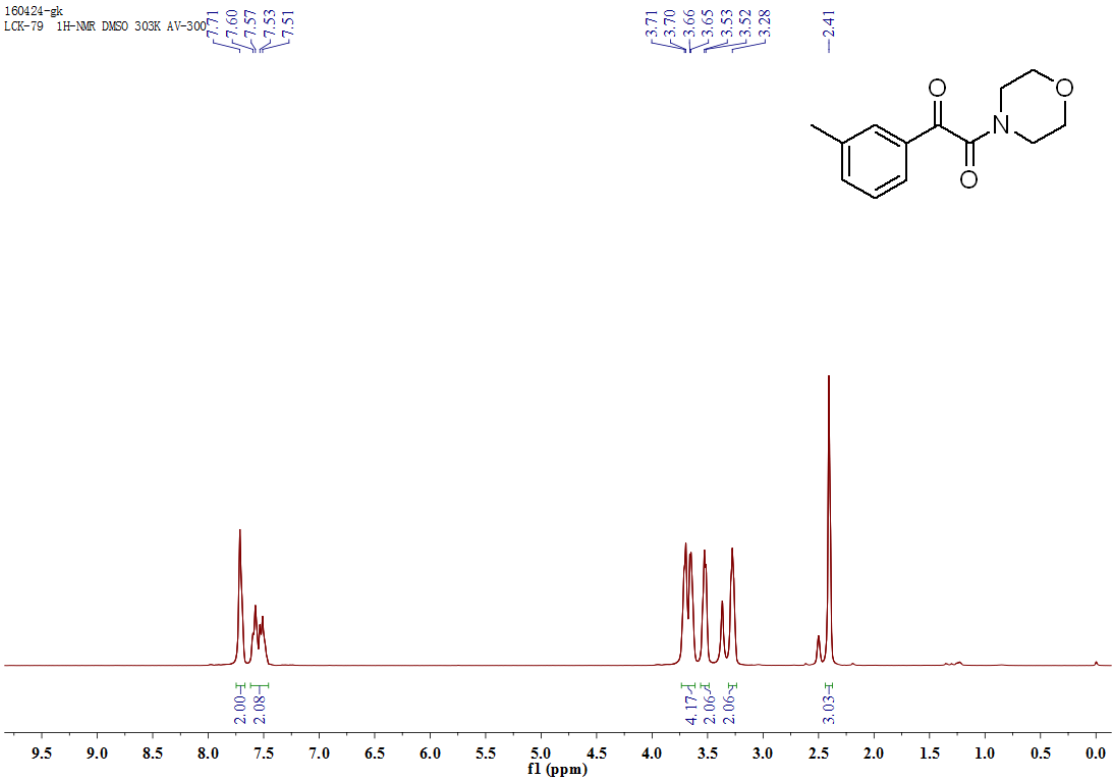
166.30
141.75
134.00
132.82
132.80
131.58
126.33
66.77
66.75
46.38
41.72
21.94
O
N
O
O
ppm


160424-gk
LCK-79 1H-NMR DMSO 303K AV-300
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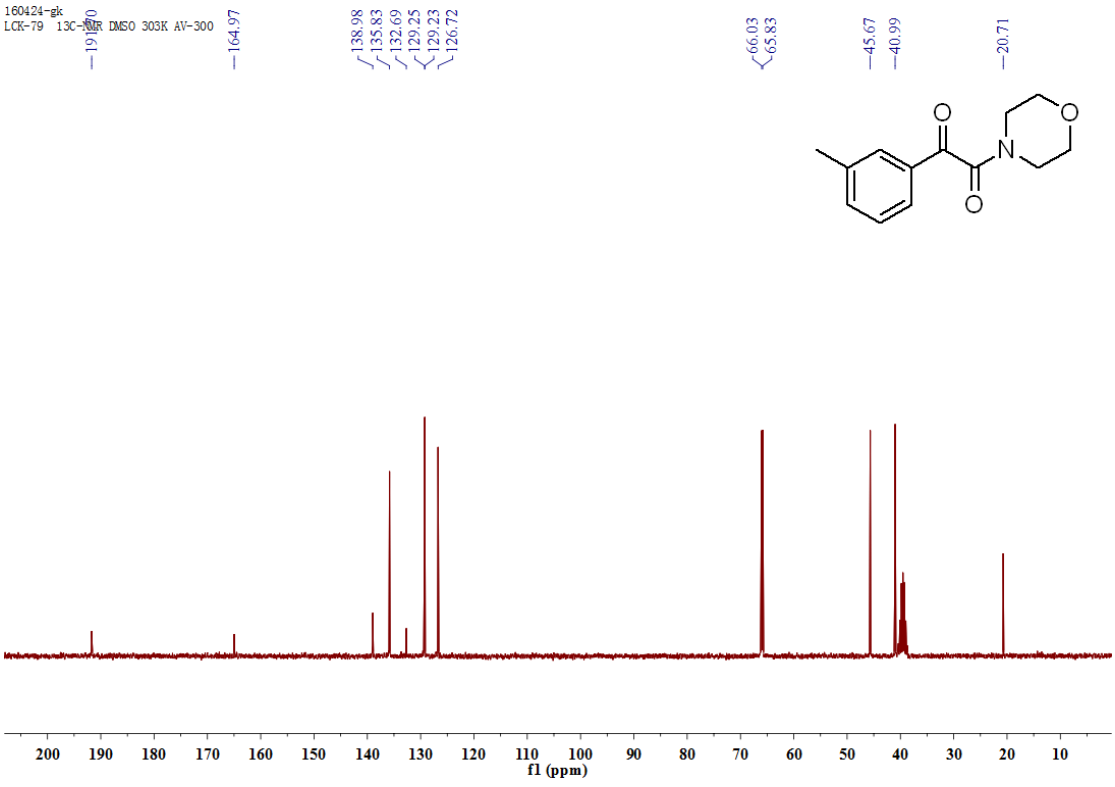
7.60
7.57
7.53
7.51
3.71
3.70
3.66
3.65
3.53
3.52
3.28
2.41
2.00
2.08
4.17
2.06
2.06
3.03
f1 (ppm)


160424-gk
LCK-79 13C-NMR DMSO 303K AV-300
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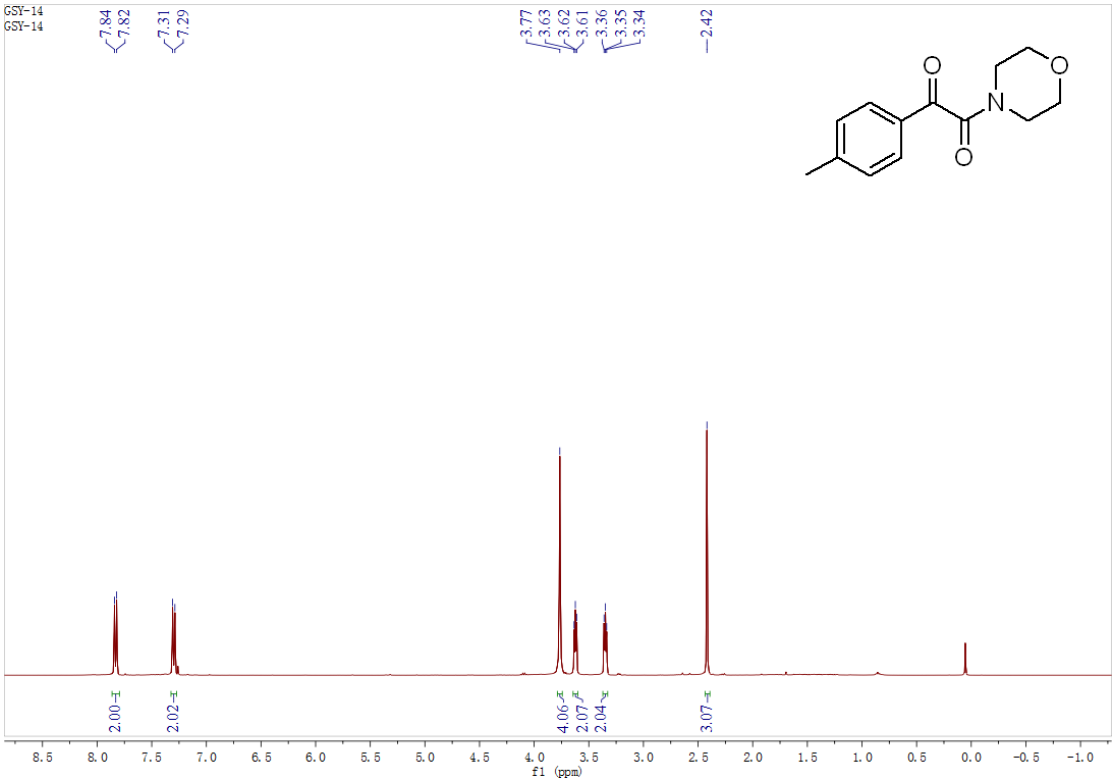
135.83
132.69
129.25
129.23
126.72
66.03
65.83
45.67
40.99
20.71
f1 (ppm)


GSY-14
GSY-14
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3.63
3.62
3.61
3.36
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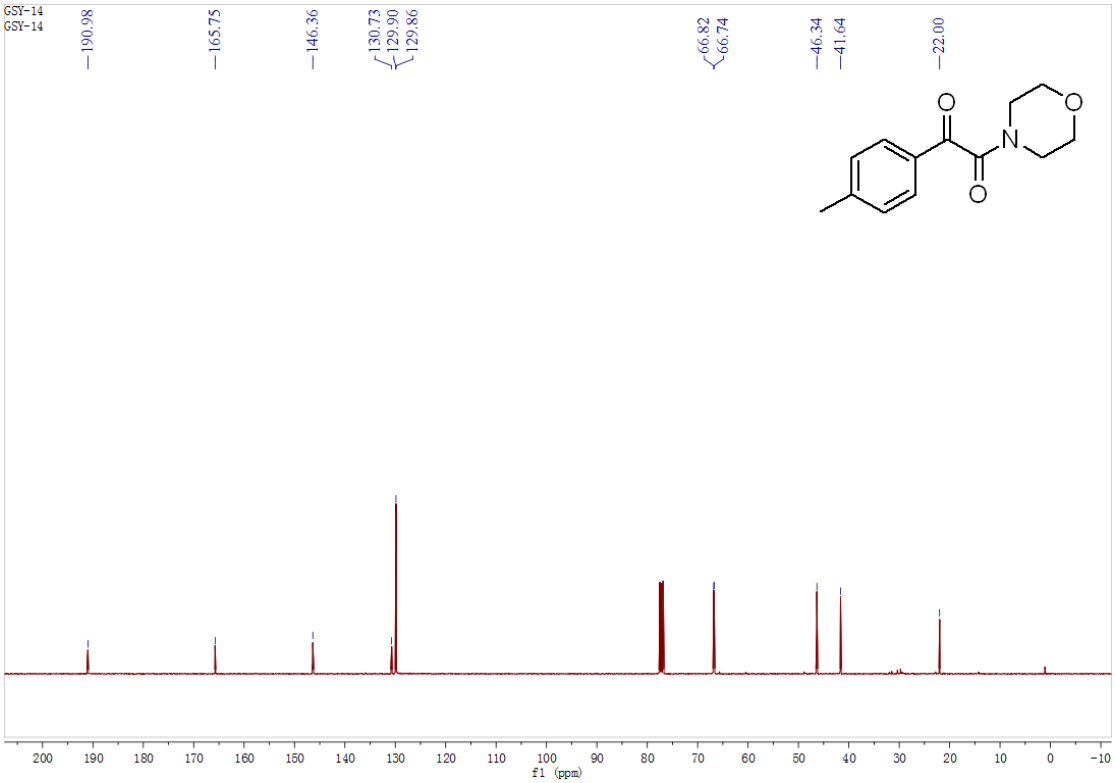
4.06
2.07
2.04
3.07
f1 (ppm)


GSY-14
GSY-14
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66.74
46.34
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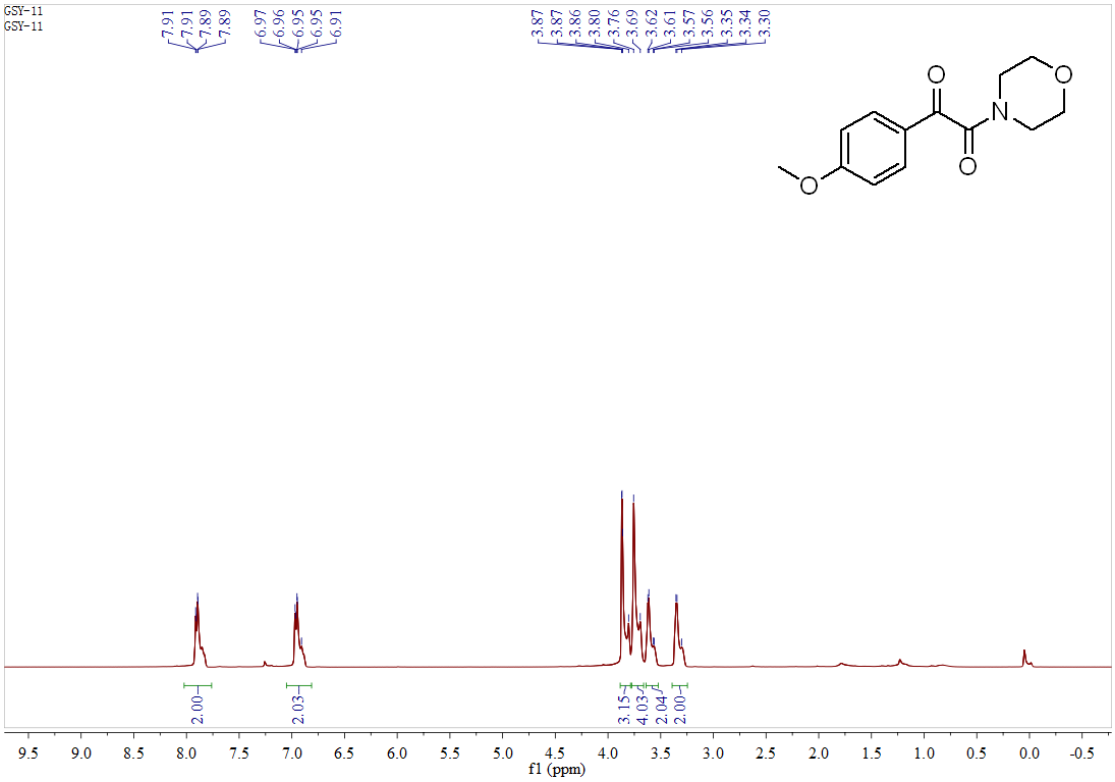
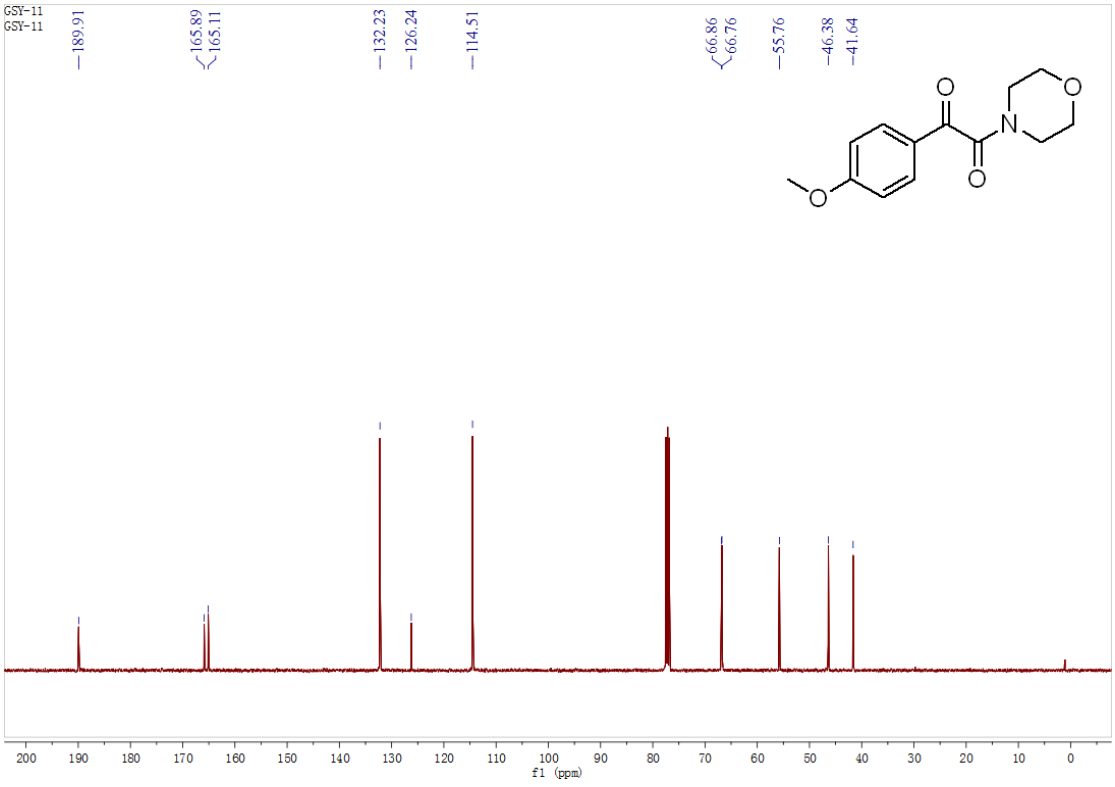
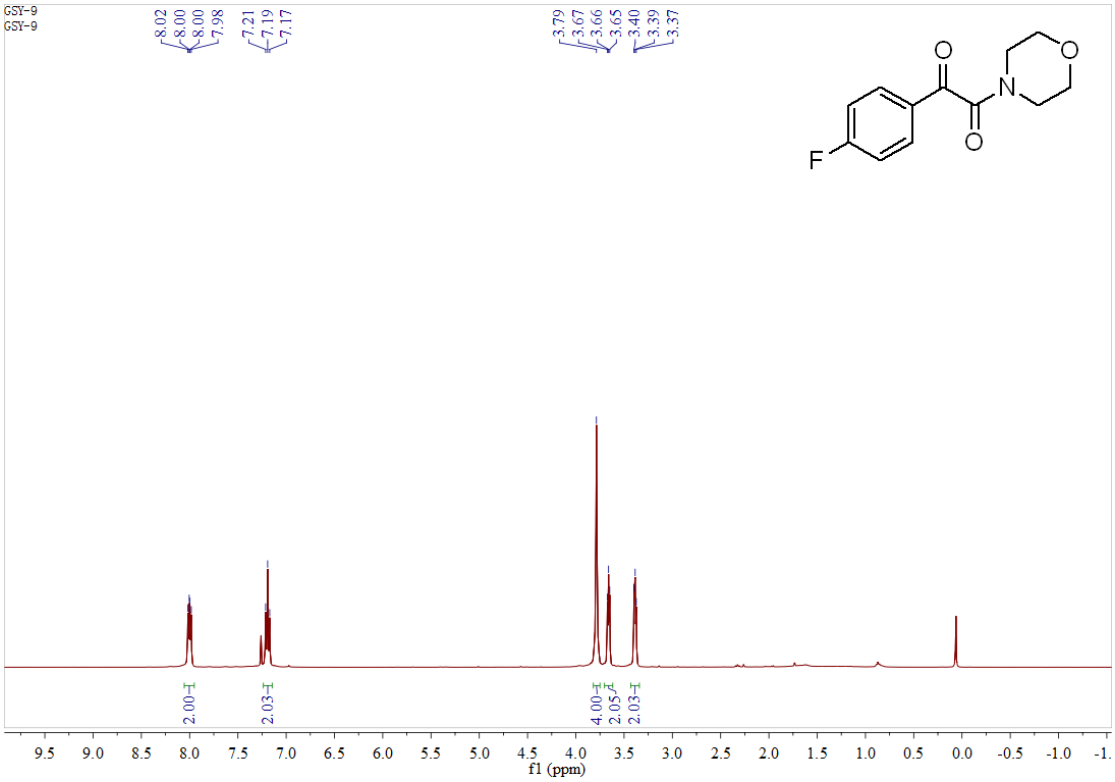
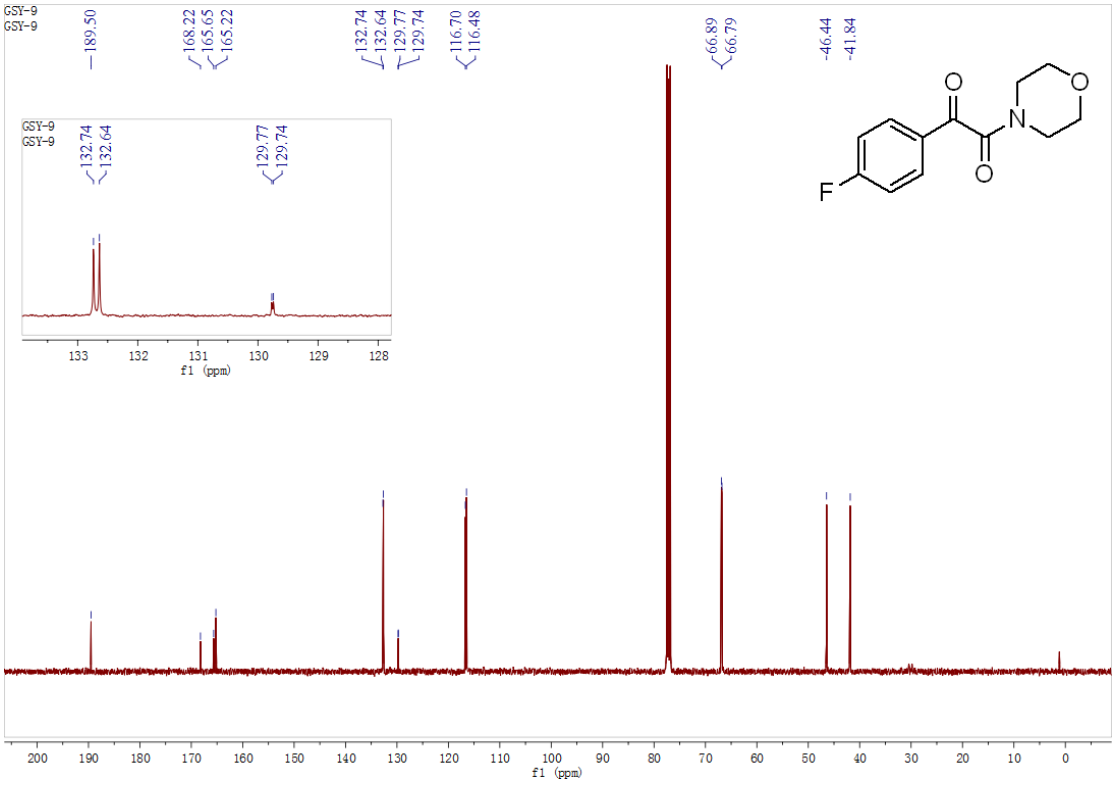
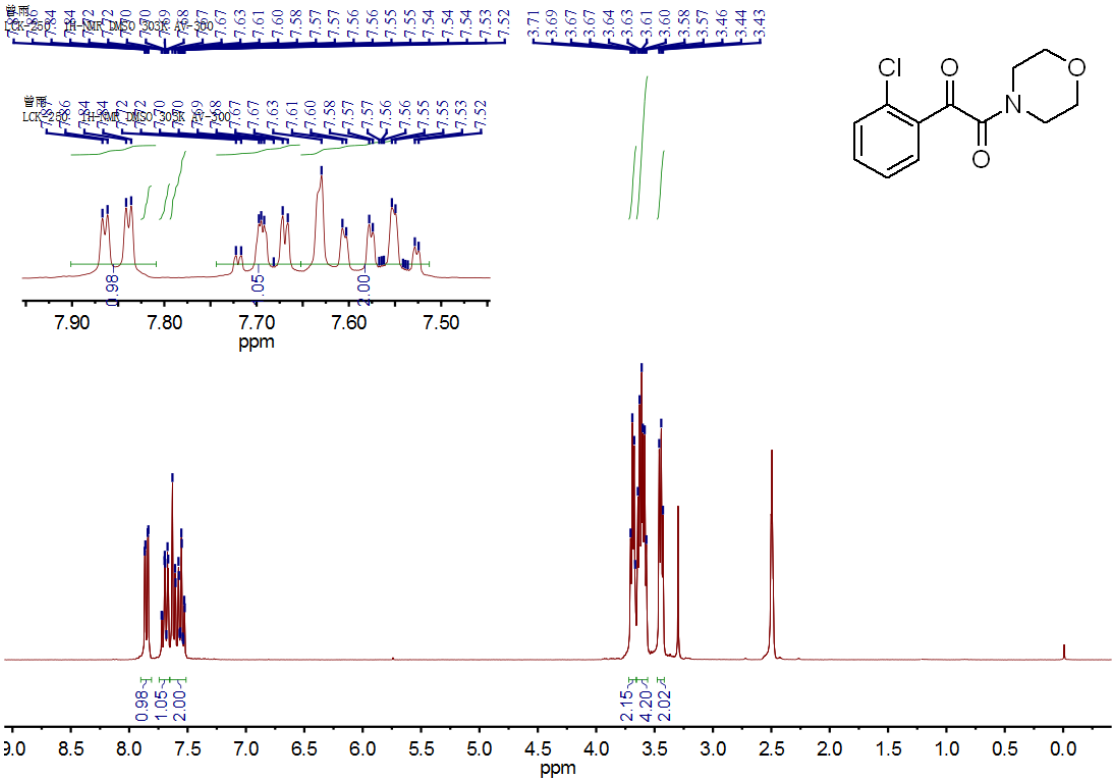
22.00
f1 (ppm)

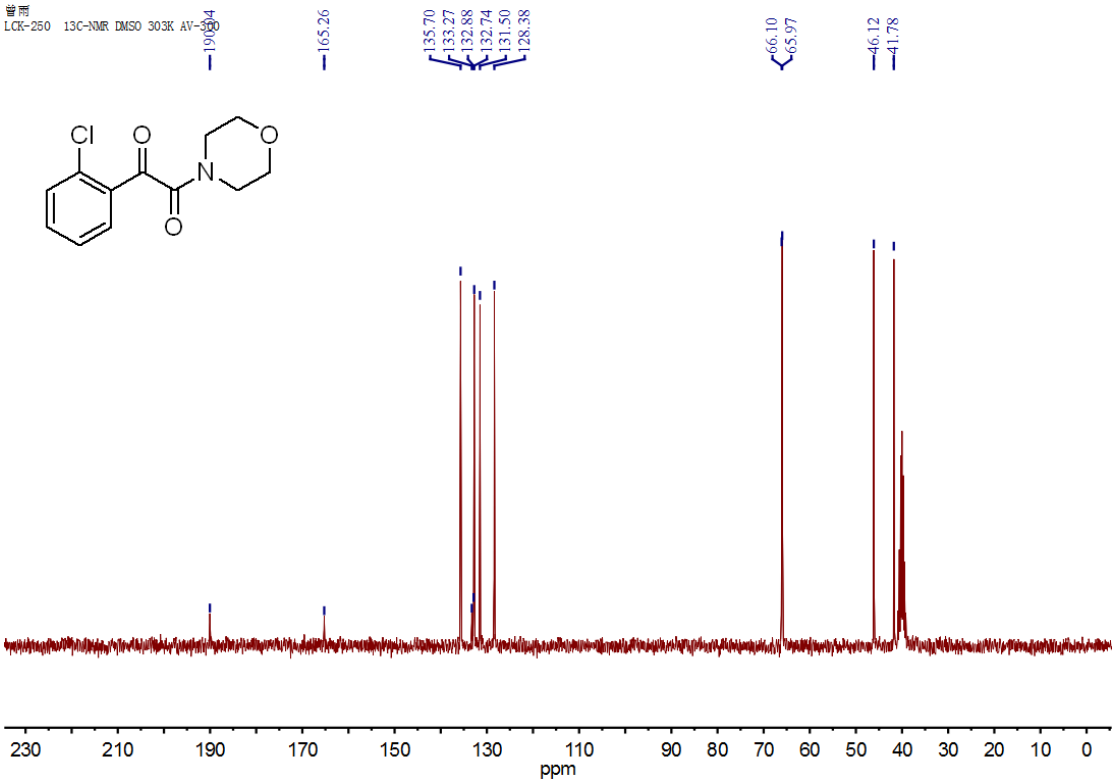

GSY-11
GSY-11
7.91
7.91
7.89
7.89
6.97
6.96
6.95
6.95
6.91
3.87
3.87
3.86
3.80
3.76
3.69
3.62
3.61
3.57
3.56
3.35
3.34
3.30
2.00
2.03
3.15
4.03
2.04
2.00
f1 (ppm)

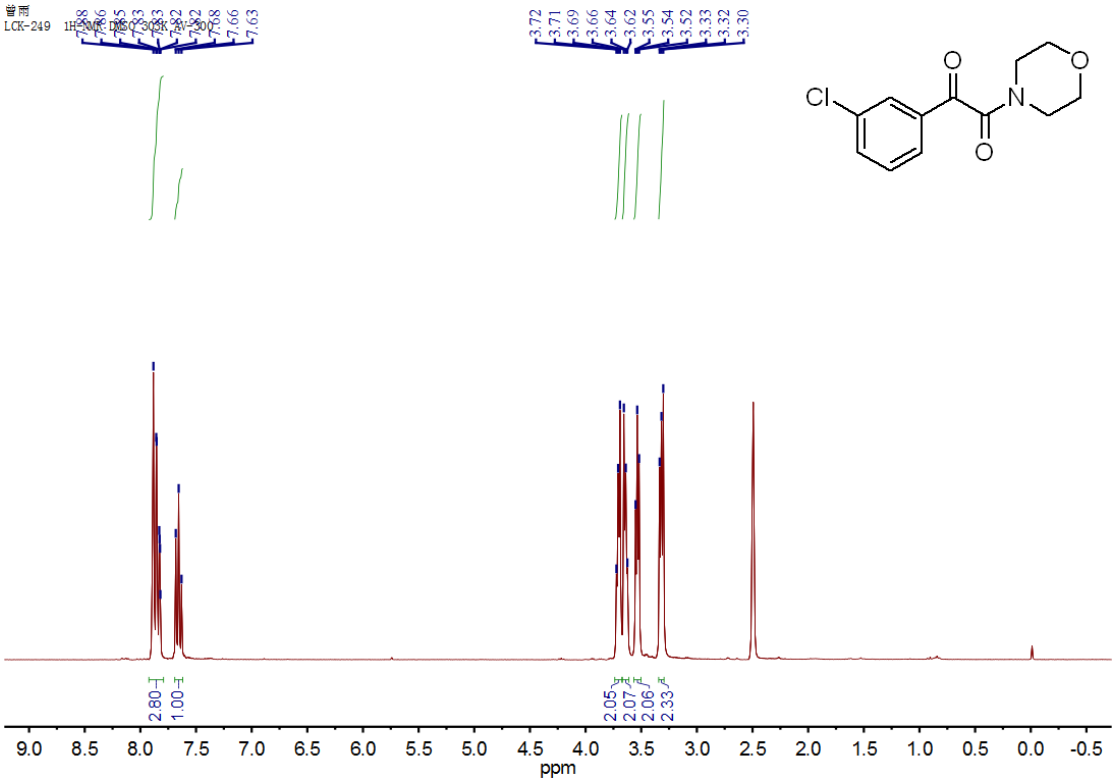

GSY-11
GSY-11
189.91
165.89
165.11
132.23
126.24
114.51
66.86
66.76
55.76
46.38
41.64
f1 (ppm)

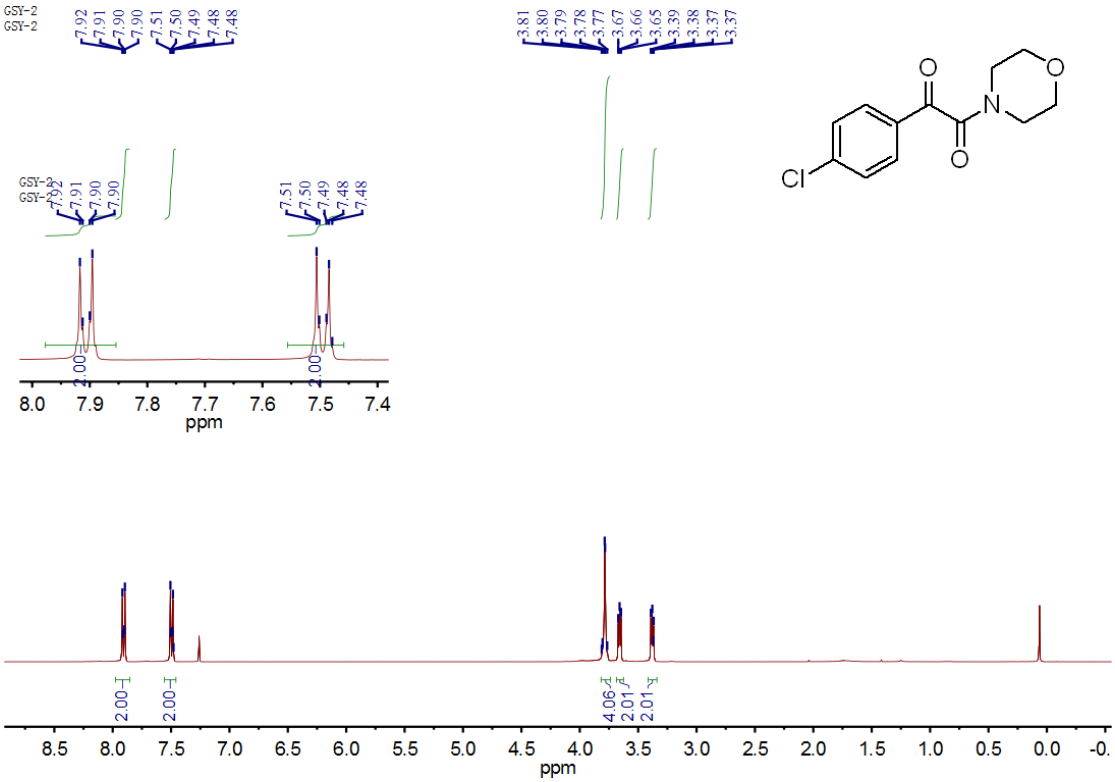

GSY-9
GSY-9
8.02
8.00
8.00
7.98
7.21
7.19
7.17
3.79
3.67
3.66
3.65
3.40
3.39
3.37
2.00
2.03
4.00
2.05
2.03
f1 (ppm)

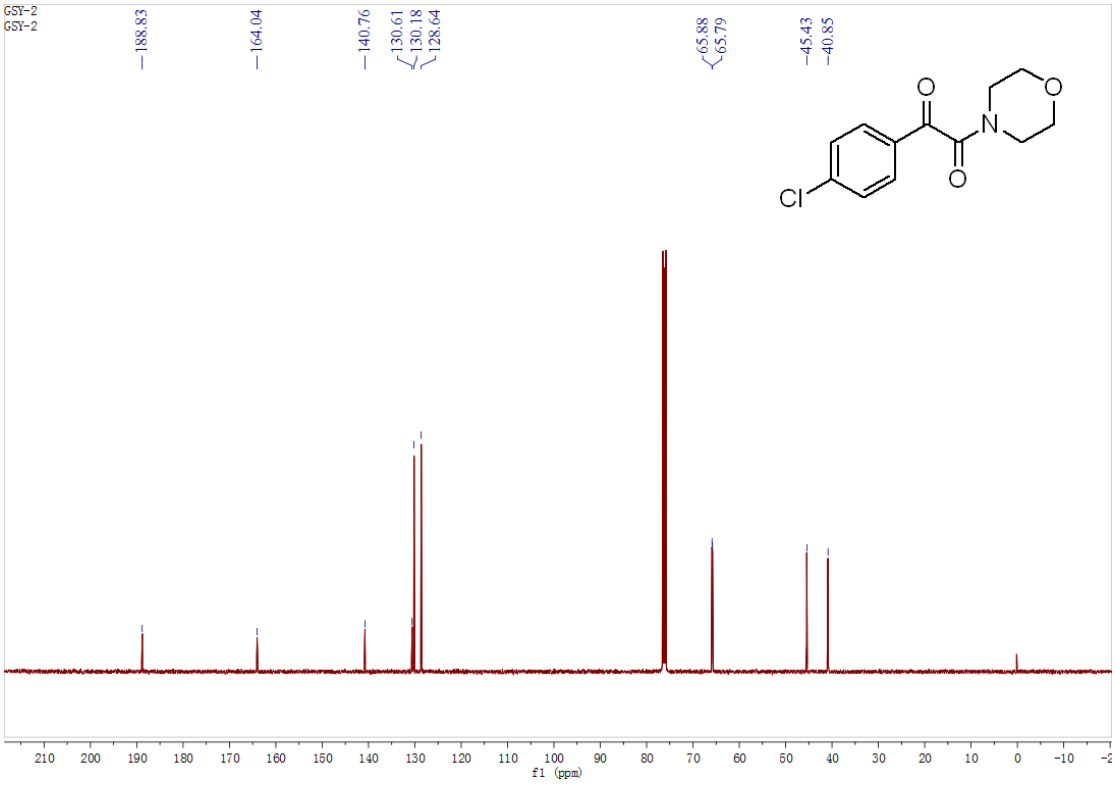

GSY-9
GSY-9
189.50
168.22
165.65
165.22
132.74
132.64
129.77
129.74
116.70
116.48
66.89
66.79
46.44
41.84
f1 (ppm)

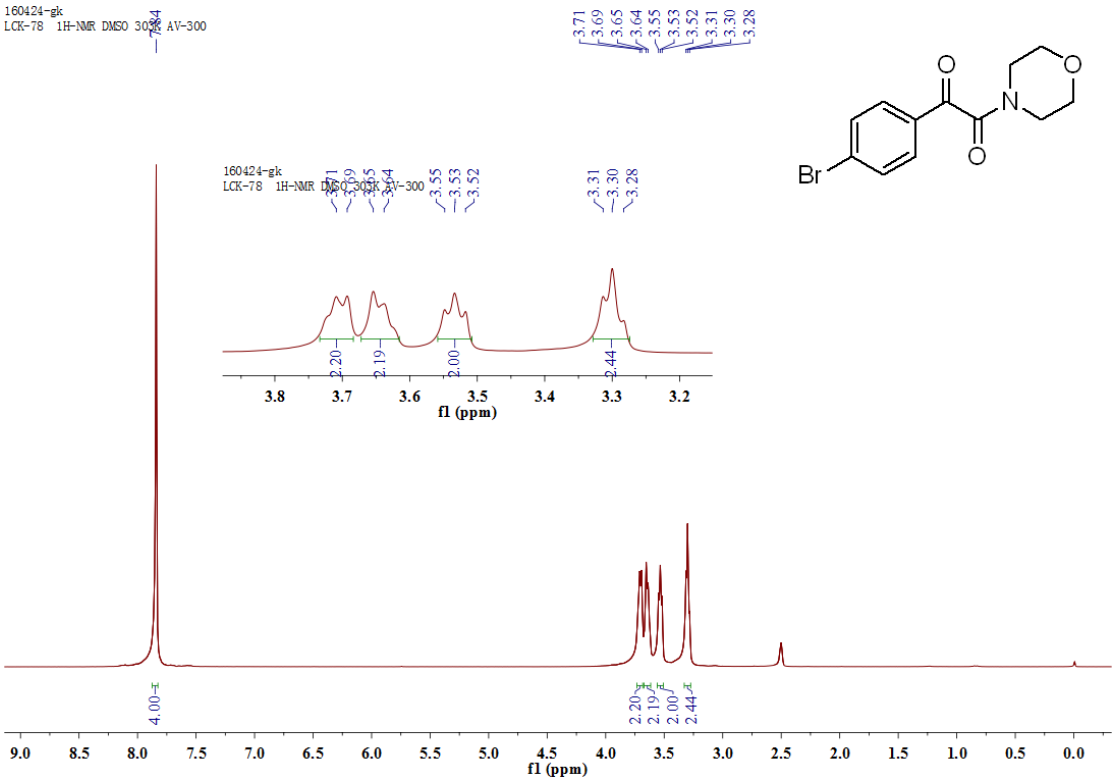

Cl
O
O
N
O
ppm

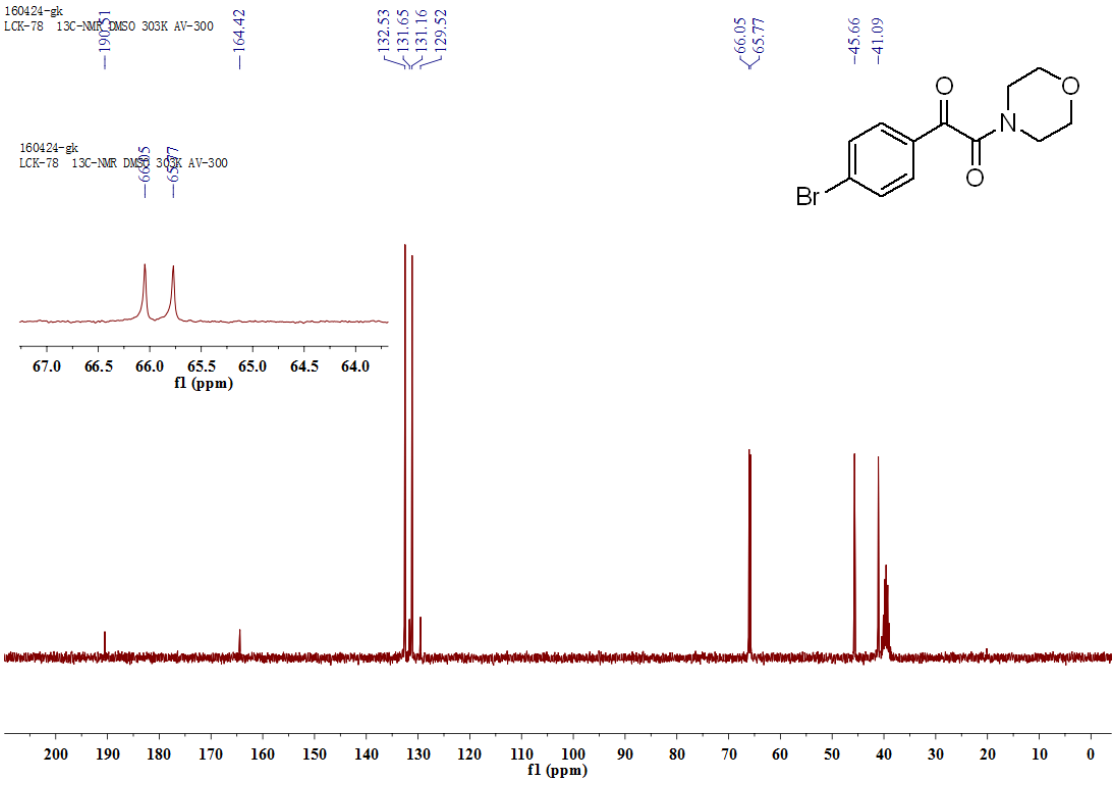

Cl
O
O
N
O
ppm

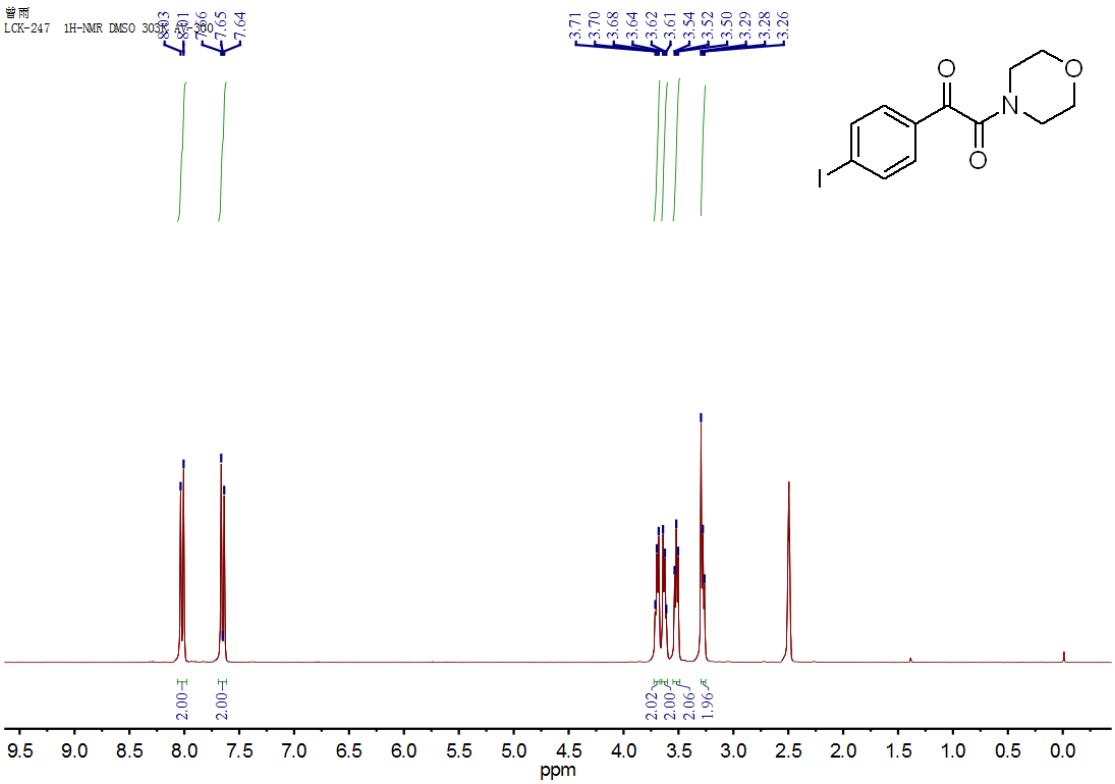

LCK-249 1H-NMR DMSO 303K AV-500
7.68
7.66
7.65
7.63
7.63
7.62
7.62
7.62

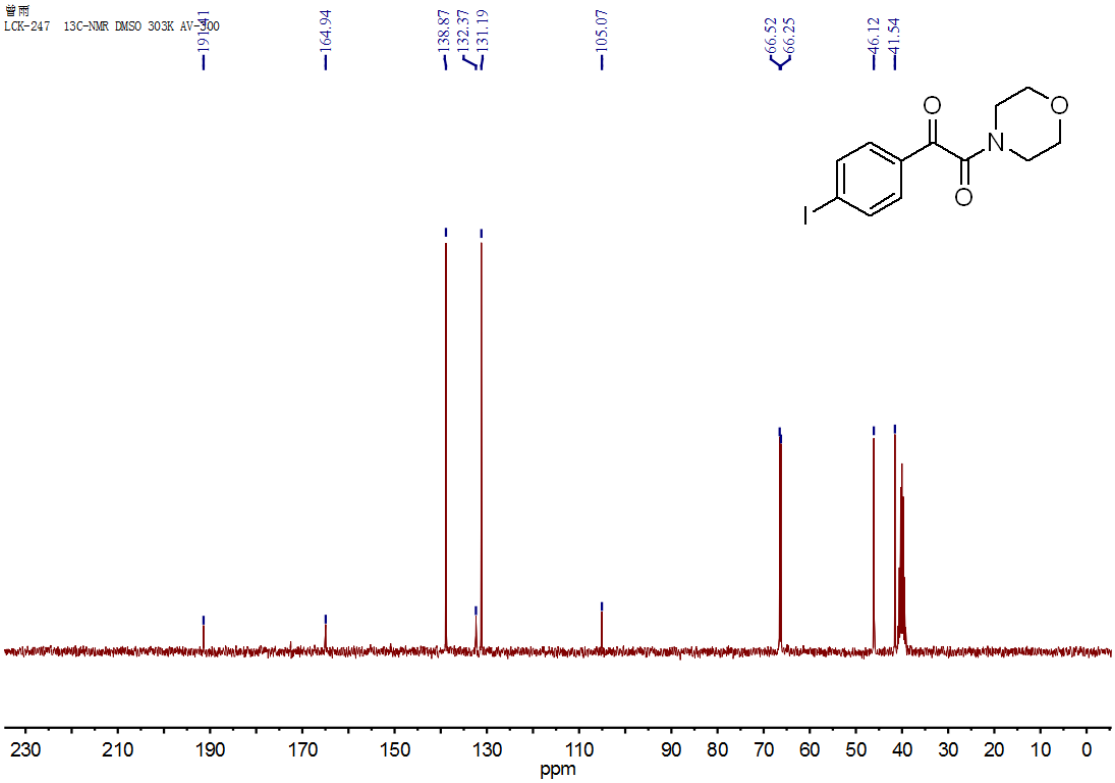

GSY-2
GSY-2
7.92
7.91
7.90
7.90
7.51
7.50
7.49
7.48
7.48
3.81
3.80
3.79
3.78
3.77
3.67
3.66
3.65
3.39
3.38
3.37
3.37
Cl
O
N
O
O
2.00
2.00
8.0
7.9
7.8
7.7
7.6
7.5
7.4
ppm
2.00
2.00
4.06
2.01
2.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

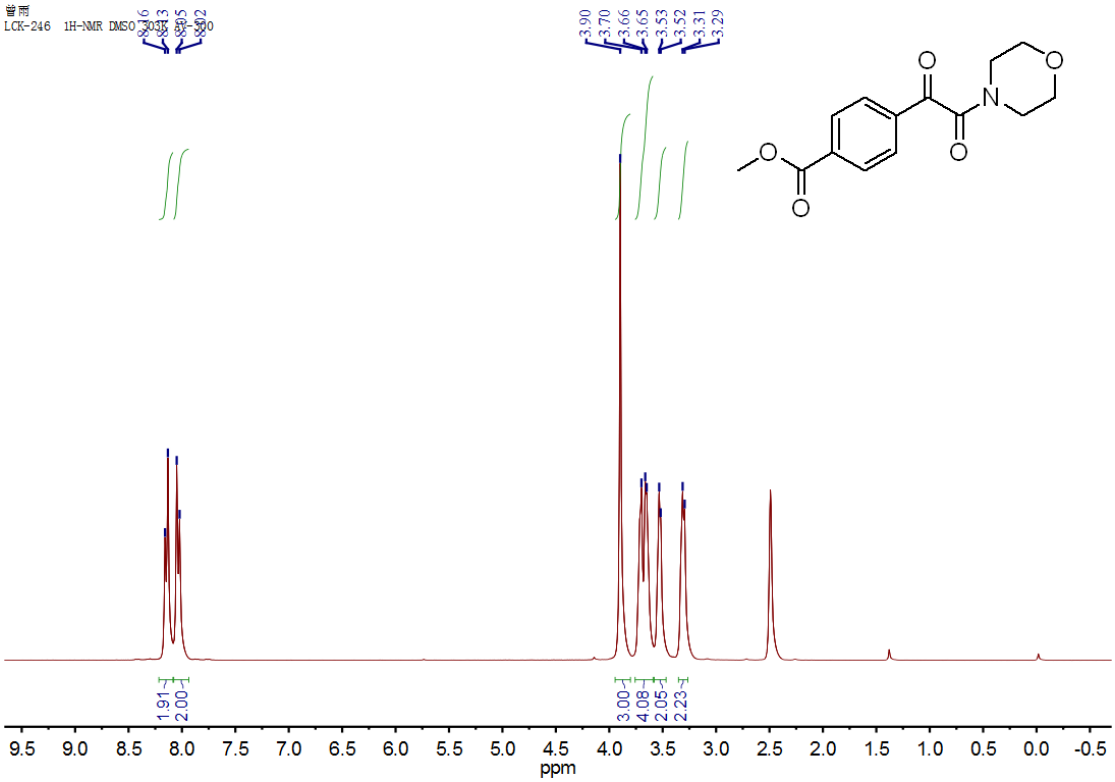

GSY-2
GSY-2
188.83
164.04
140.76
130.61
130.18
128.64
65.88
65.79
45.43
40.85
Cl
O
N
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

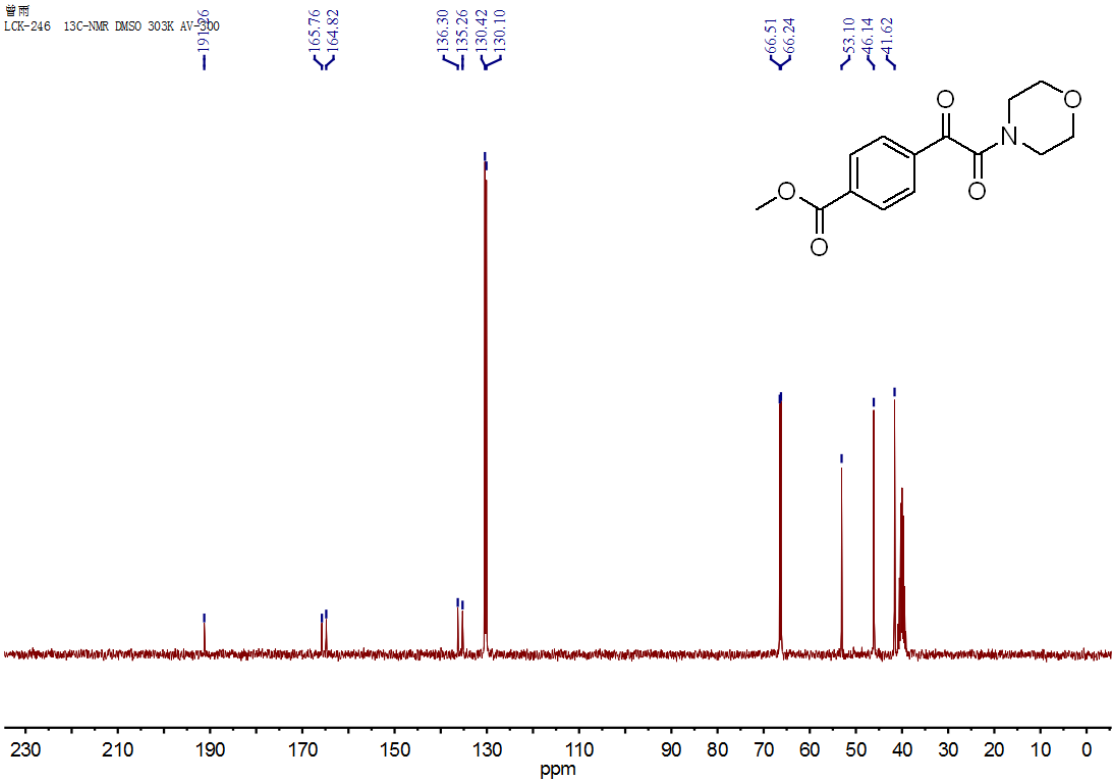

160424-gk
LCK-78 1H-NMR DMSO 303K AV-300
7.84
3.71
3.69
3.65
3.64
3.55
3.53
3.52
3.31
3.30
3.28
Br
O
N
O
O
160424-gk
LCK-78 1H-NMR DMSO 303K AV-300
2.20
2.19
2.00
2.44
3.8
3.7
3.6
3.5
3.4
3.3
3.2
f1 (ppm)
4.00
2.20
2.19
2.00
2.44
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

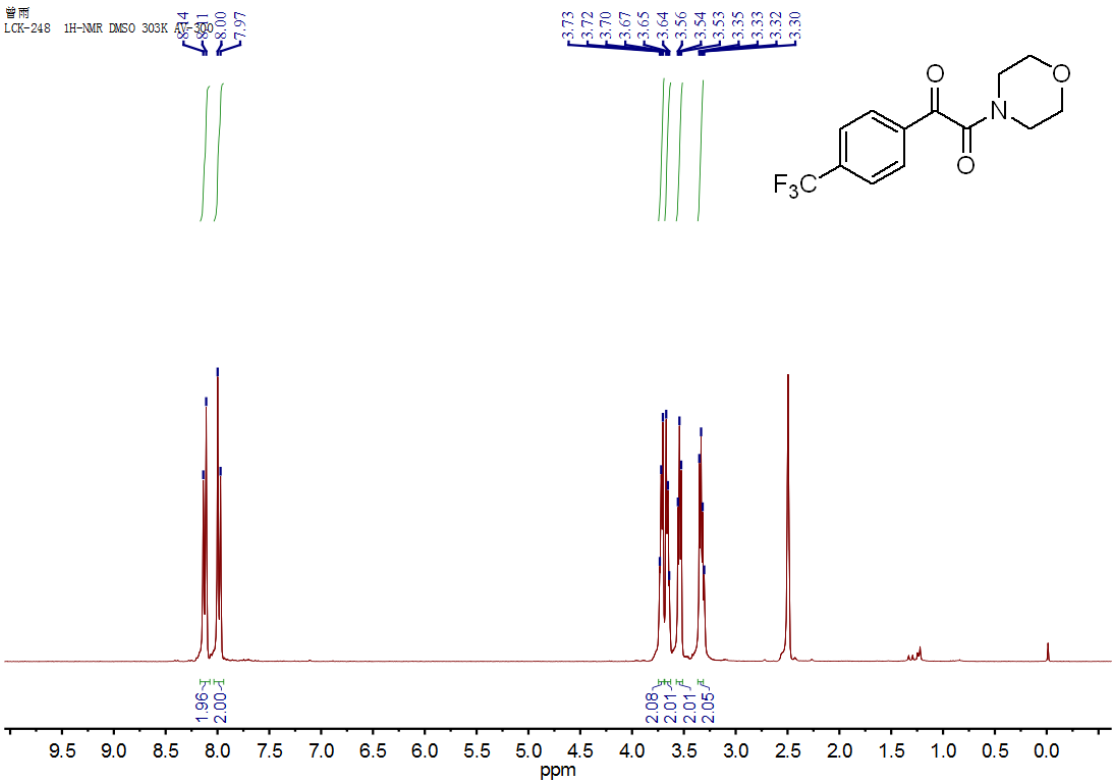

160424-gk
LCK-78 13C-NMR DMSO 303K AV-300
190.51
164.42
132.53
131.65
131.16
129.52
66.05
65.77
45.66
41.09
Br
O
N
O
O
160424-gk
LCK-78 13C-NMR DMSO 303K AV-300
66.05
65.77
67.0
66.5
66.0
65.5
65.0
64.5
64.0
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

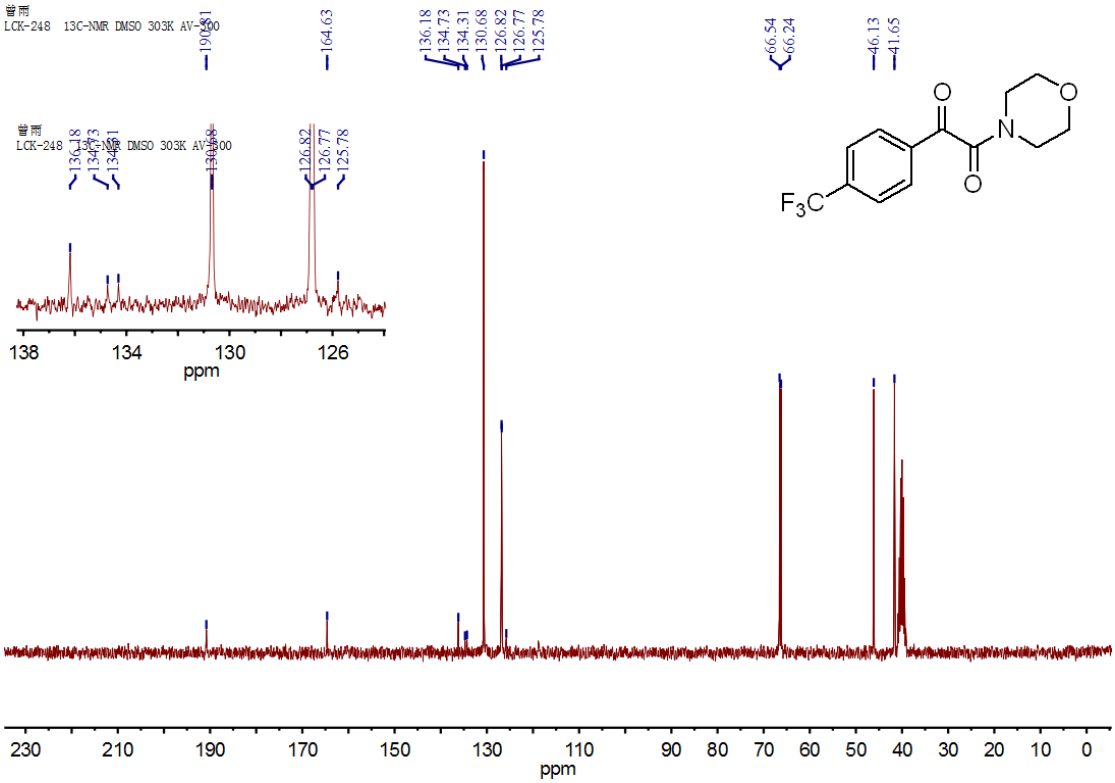

LCK-247 1H-NMR DMSO 303K
8.03
8.01
7.66
7.65
7.64
3.71
3.70
3.68
3.64
3.62
3.61
3.54
3.52
3.50
3.29
3.28
3.26
O
N
O
O
I
2.00
2.00
2.02
2.00
2.06
1.96
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

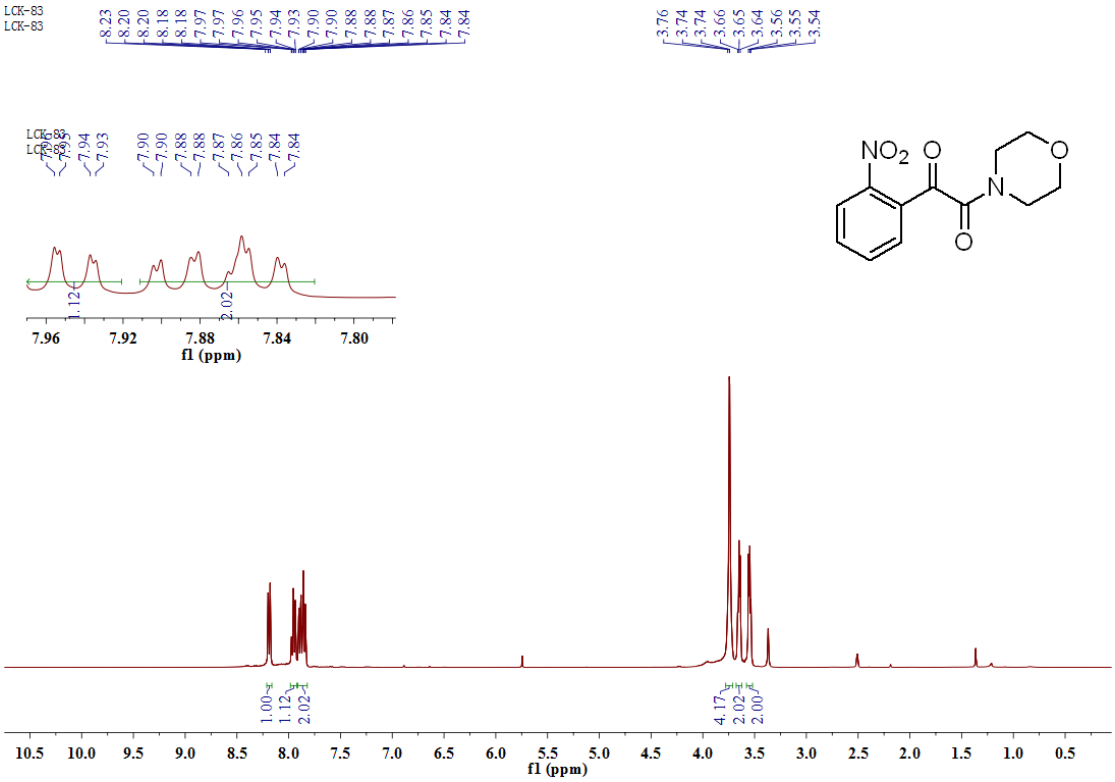

LCK-247 13C-NMR DMSO 303K AV-500
191.41
164.94
138.87
132.37
131.19
105.07
66.52
66.25
46.12
41.54
O
N
O
O
I
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
ppm

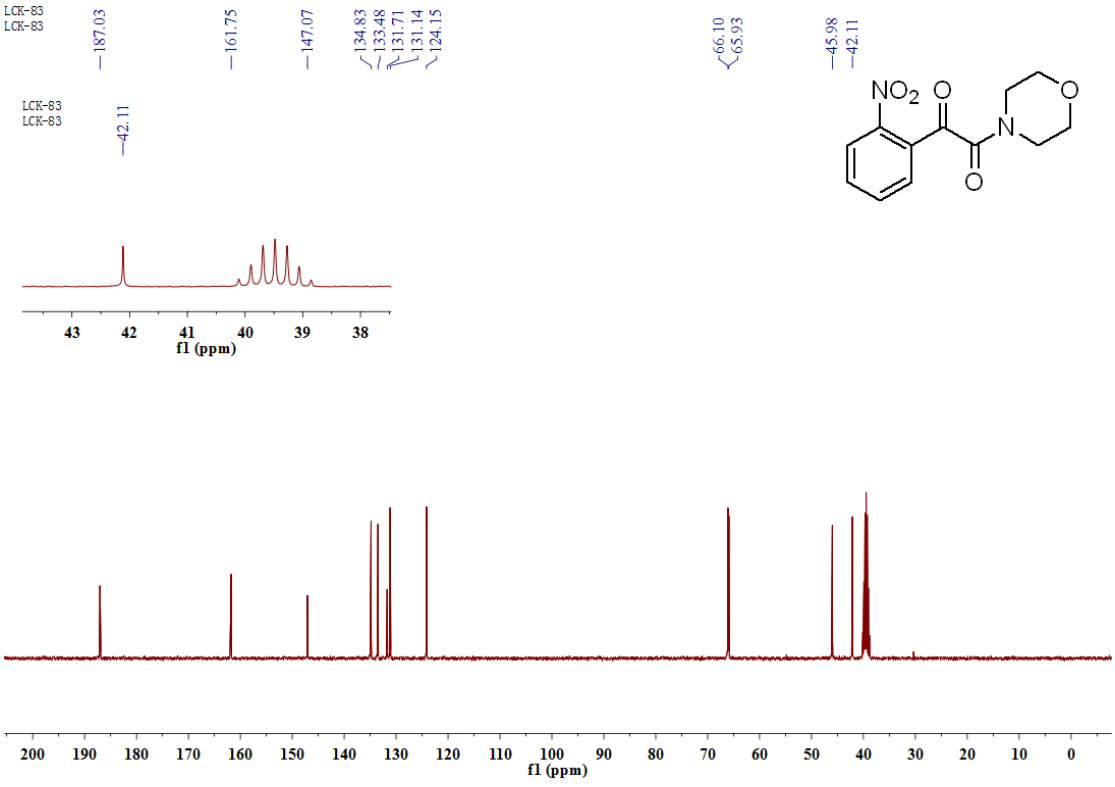

LCK-246 1H-NMR DMSO 303K AV-500
8.16
8.13
8.05
8.02
3.90
3.70
3.66
3.65
3.53
3.52
3.31
3.29
1.91
2.00
3.00
4.08
2.05
2.23
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

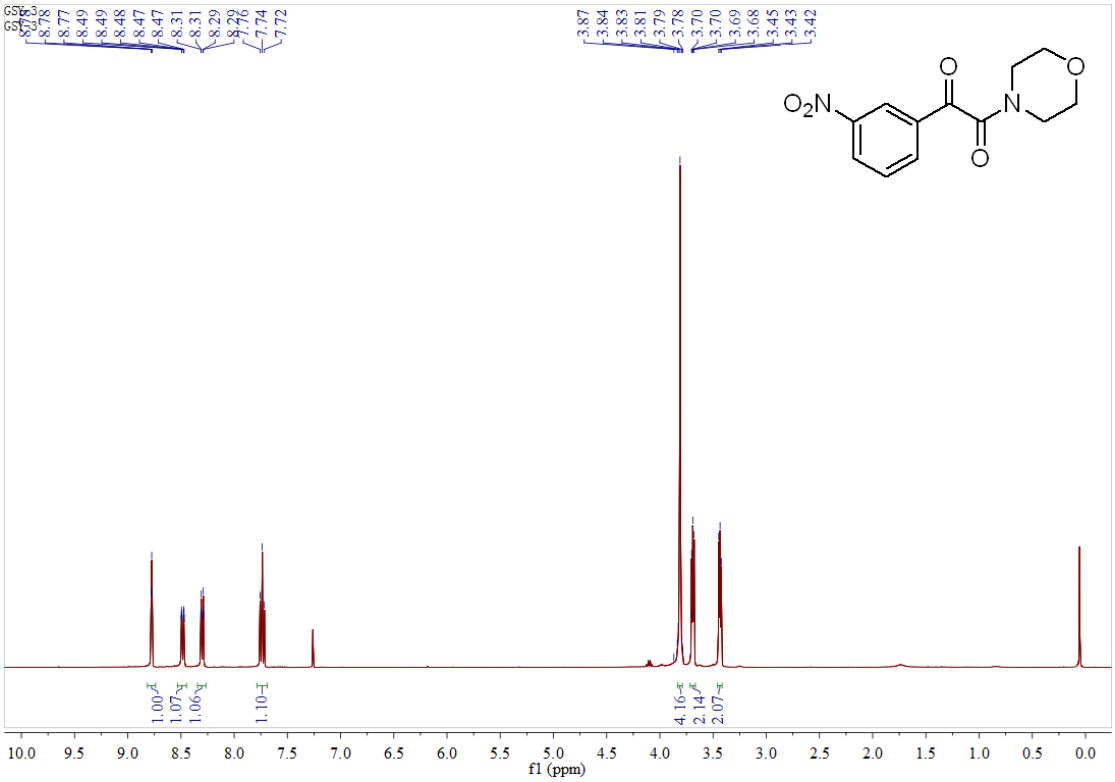

LCK-246 13C-NMR DMSO 303K AV-500
191.26
165.76
164.82
136.30
135.26
130.42
130.10
66.51
66.24
53.10
46.14
41.62
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
ppm

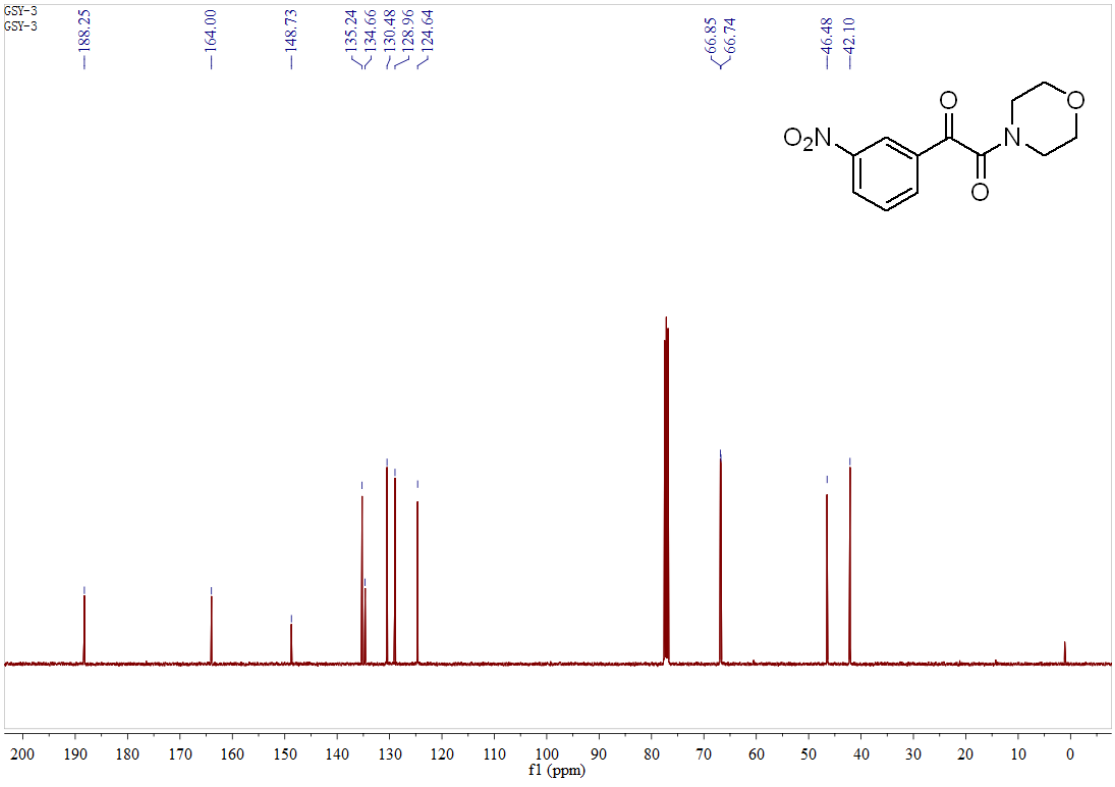

LCK-248 1H-NMR DMSO 303K AV-500
8.14
8.11
8.00
7.97
3.73
3.72
3.70
3.67
3.65
3.64
3.56
3.54
3.53
3.35
3.33
3.32
3.30
O
O
N
O
F3C
1.96
2.00
2.08
2.01
2.01
2.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

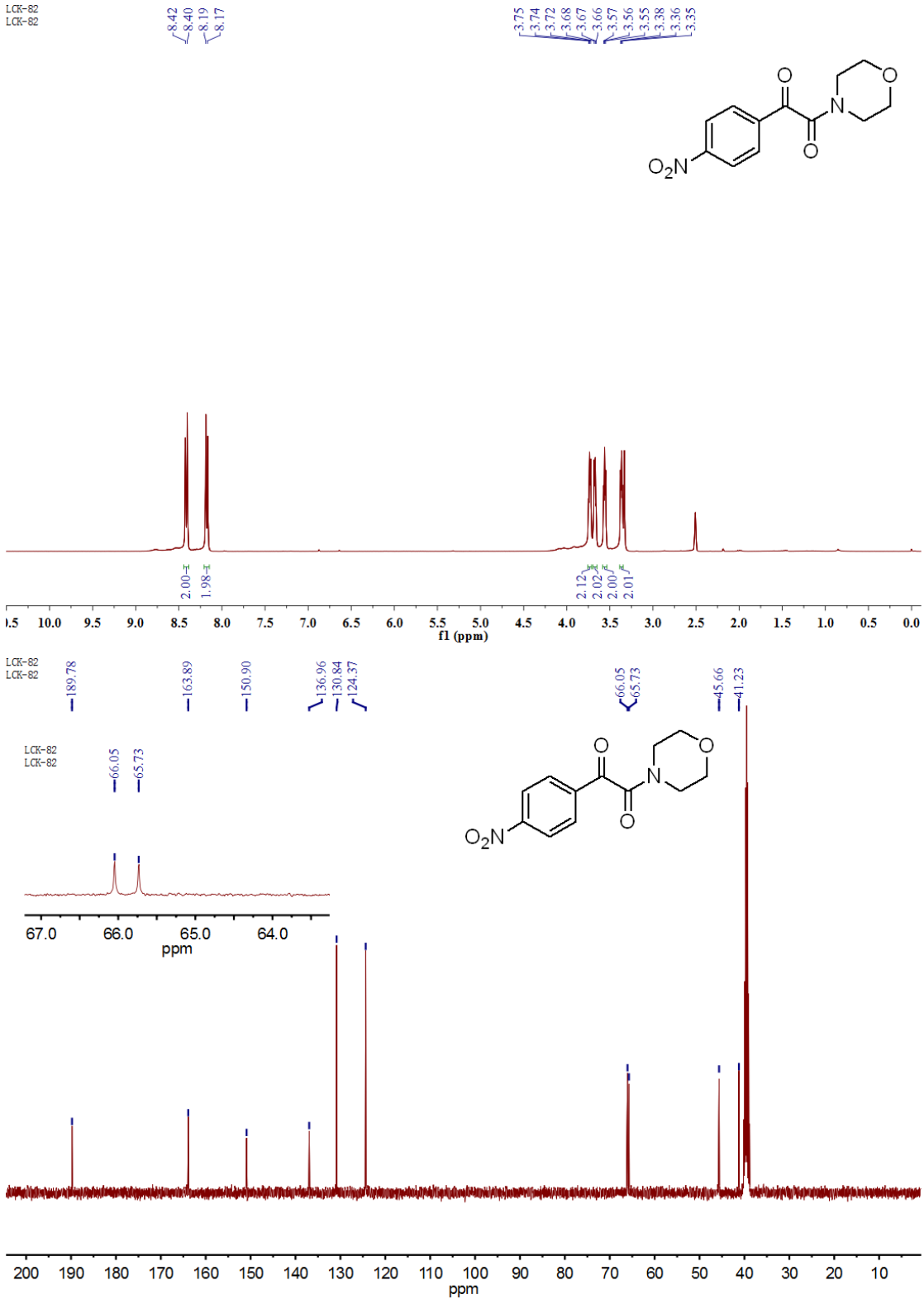

LCK-248 13C-NMR DMSO 303K AV-500
190.81
164.63
136.18
134.73
134.31
130.68
126.82
126.77
125.78
66.54
66.24
46.13
41.65
O
O
N
O
F3C
138 134 130 126
ppm
230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
ppm

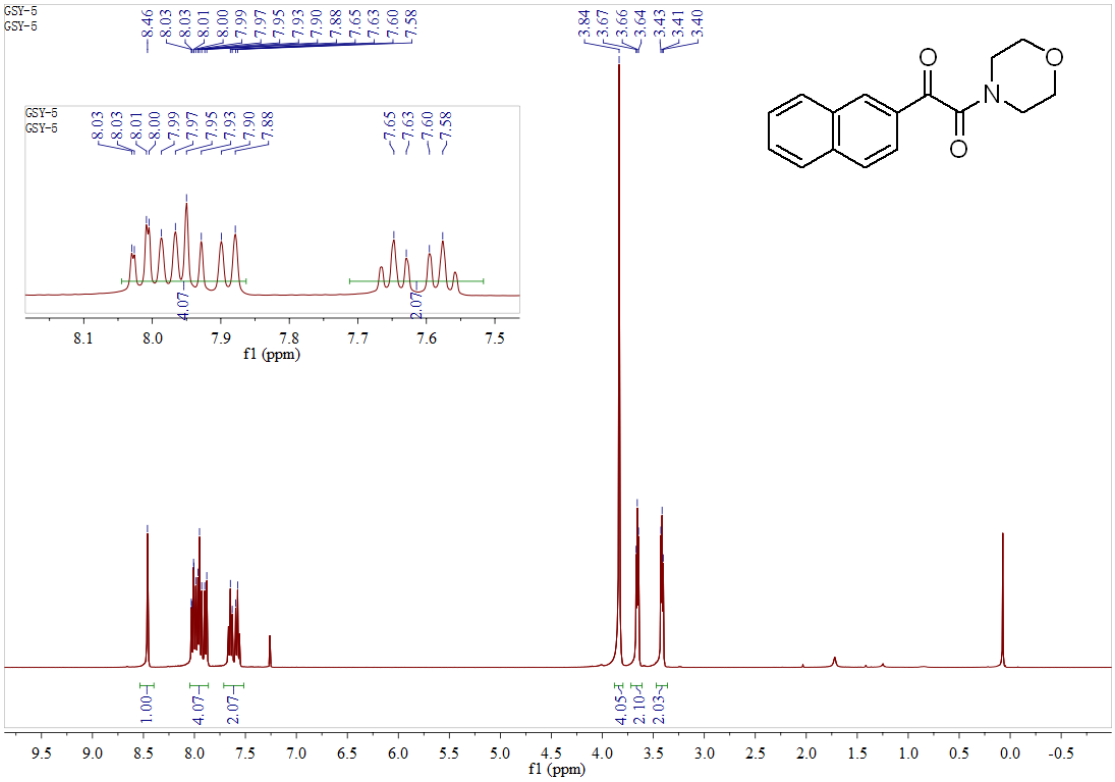

LCK-83
LCK-83
8.23
8.20
8.20
8.18
8.18
7.97
7.97
7.96
7.95
7.94
7.93
7.90
7.90
7.88
7.88
7.87
7.86
7.85
7.84
7.84
3.76
3.74
3.74
3.66
3.65
3.64
3.56
3.55
3.54
NO2
O
O
N
O
1.12
2.02
7.96
7.92
7.88
7.84
7.80
f1 (ppm)
1.00
1.12
2.02
4.17
2.02
2.00
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

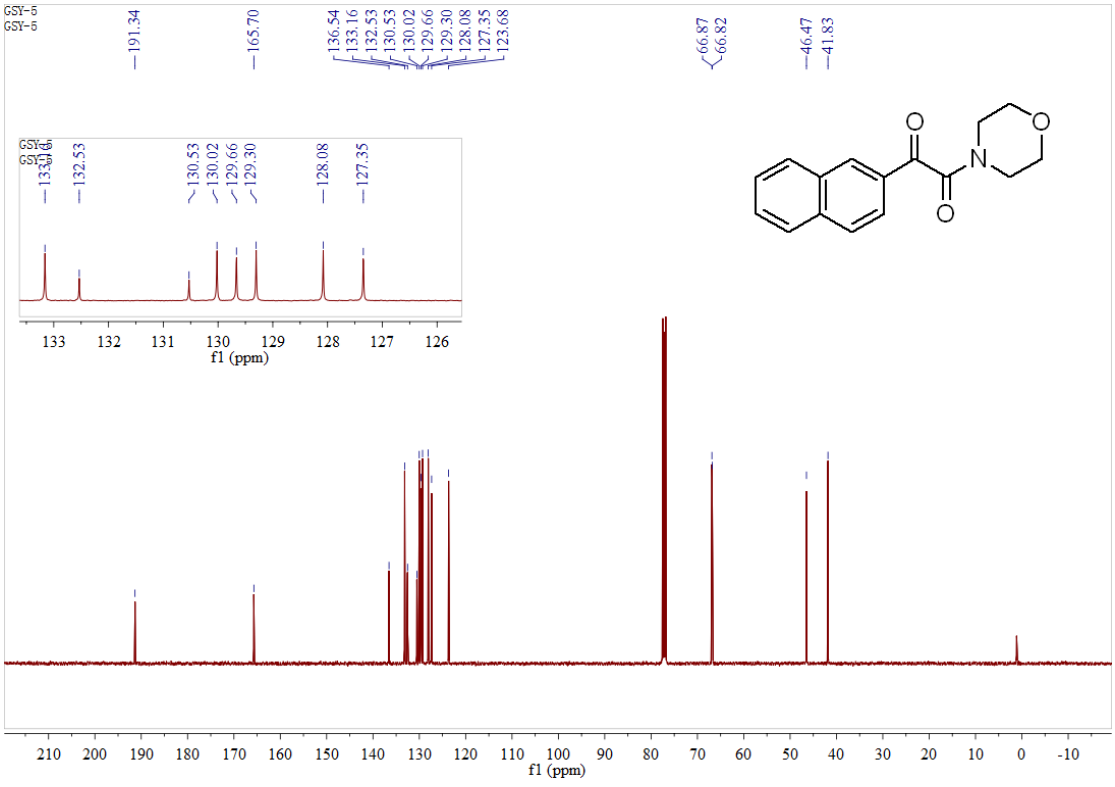

LCK-83
LCK-83
187.03
161.75
147.07
134.83
133.48
131.71
131.14
124.15
66.10
65.93
45.98
42.11
NO2
O
O
N
O
LCK-83
LCK-83
42.11
43
42
41
40
39
38
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

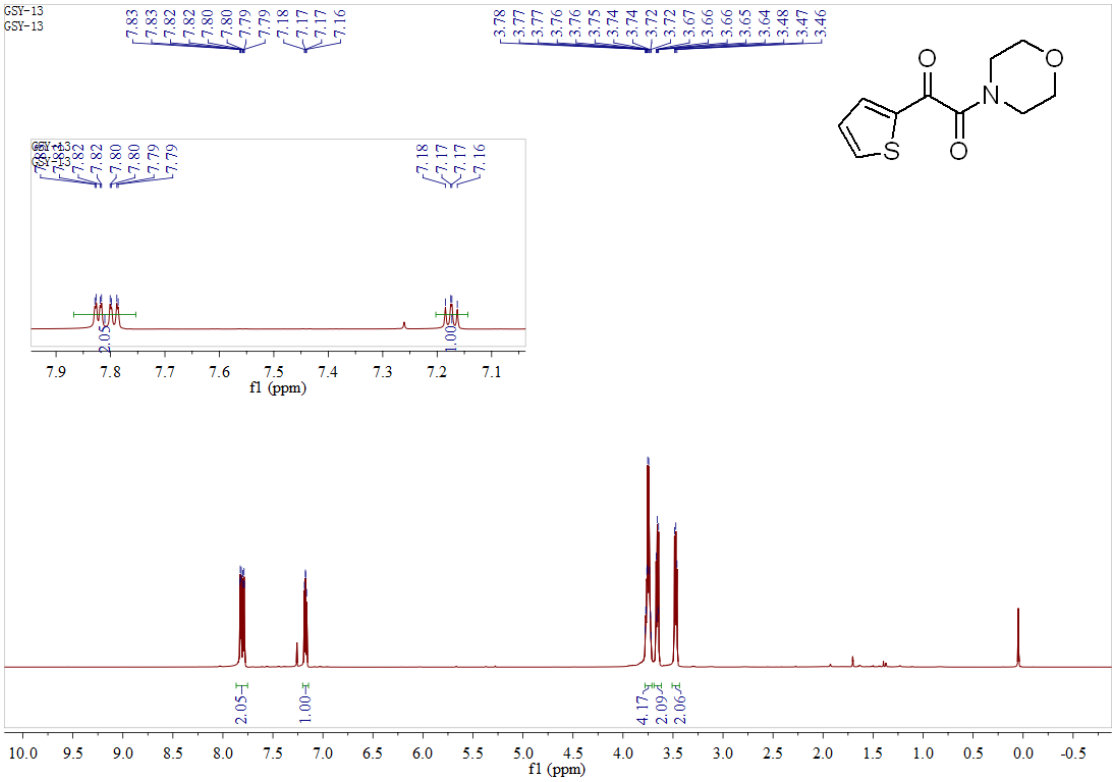

GSY-3
8.78
8.77
8.49
8.49
8.48
8.47
8.47
8.31
8.31
8.29
8.29
7.76
7.74
7.72
3.87
3.84
3.83
3.81
3.79
3.78
3.70
3.70
3.69
3.68
3.45
3.43
3.42
O2N
O
N
O
O
1.00
1.07
1.06
1.10
4.16
2.14
2.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

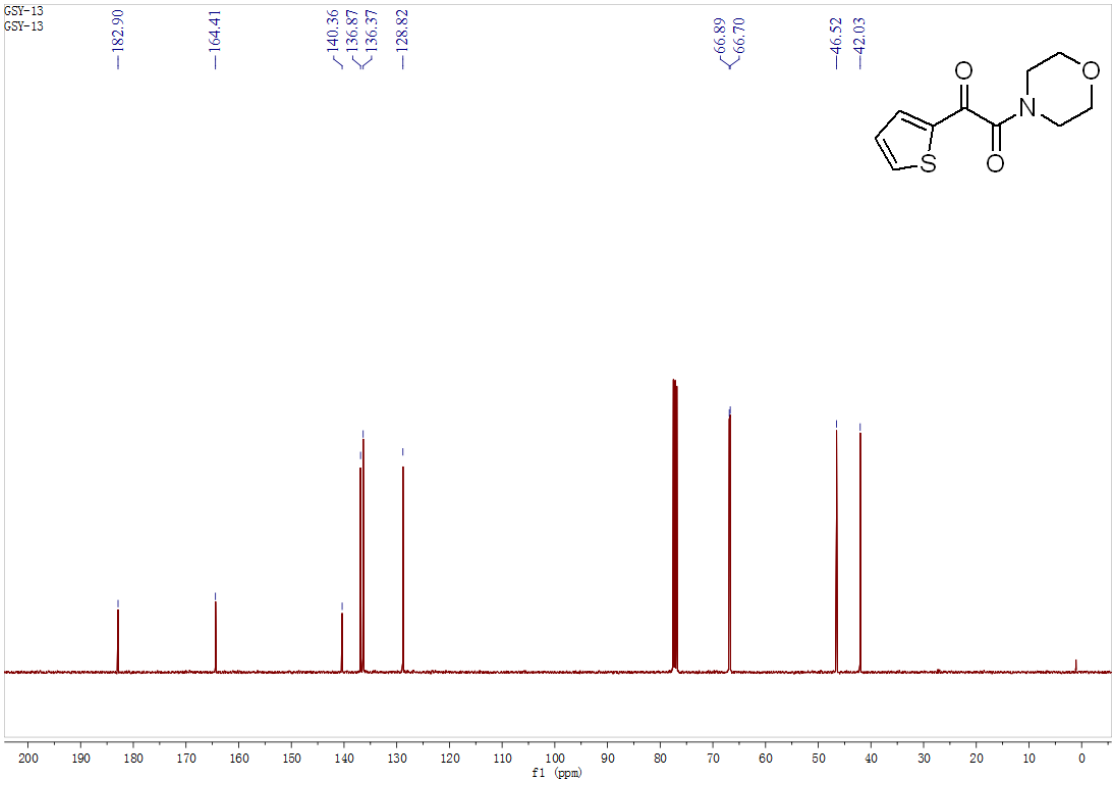

GSY-3
GSY-3
188.25
164.00
148.73
135.24
134.66
130.48
128.96
124.64
66.85
66.74
46.48
42.10
O2N
O
N
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

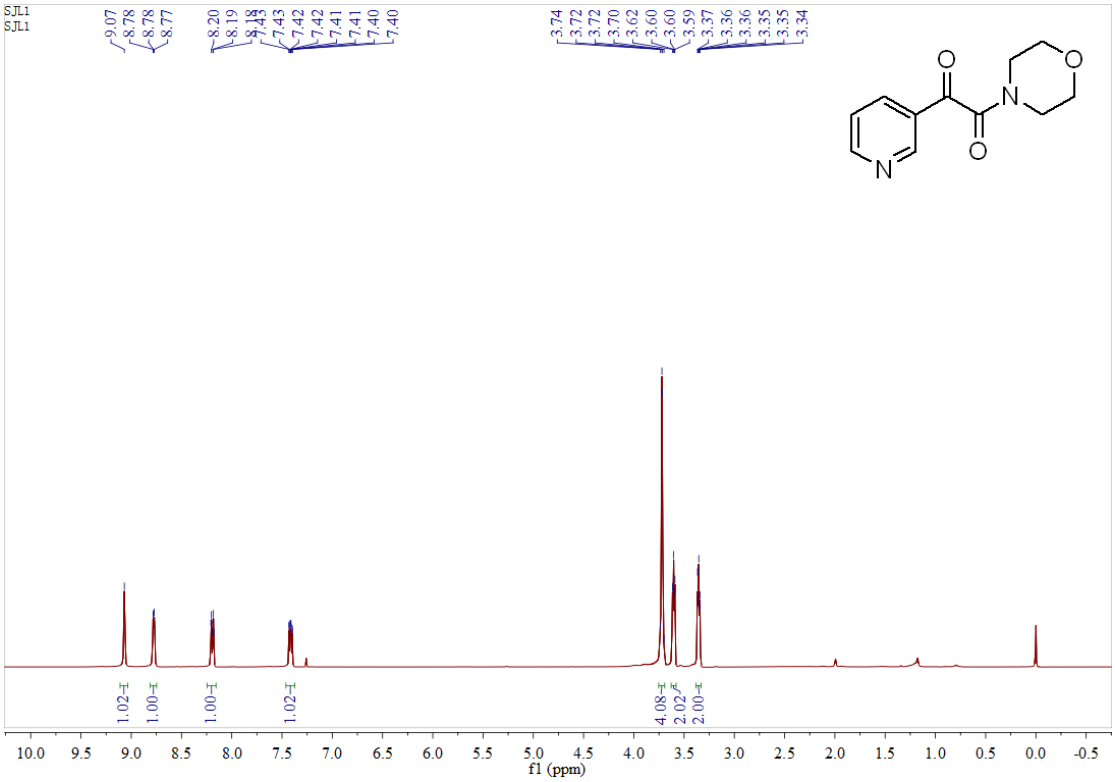

LCK-82
LCK-82
8.42
8.40
8.19
8.17
3.75
3.74
3.72
3.68
3.67
3.66
3.57
3.56
3.55
3.38
3.36
3.35
O
N
O
O
O2N
2.00
1.98
2.12
2.02
2.00
2.01
f1 (ppm)
LCK-82
LCK-82
189.78
163.89
150.90
136.96
130.84
124.37
66.05
65.73
45.66
41.23
LCK-82
LCK-82
66.05
65.73
67.0
66.0
65.0
64.0
ppm
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

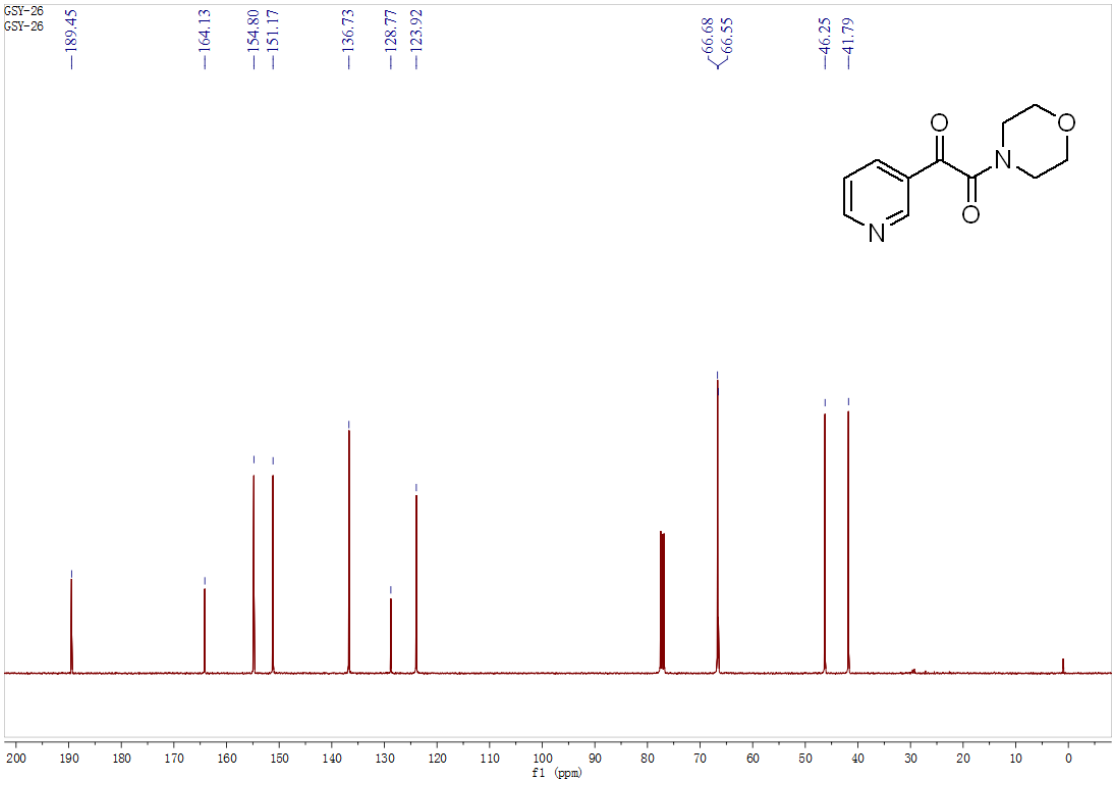

GSY-5
GSY-5
8.46
8.03
8.03
8.01
8.00
7.99
7.97
7.95
7.93
7.90
7.88
7.65
7.63
7.60
7.58
3.84
3.67
3.66
3.64
3.43
3.41
3.40
4.07
2.07
1.00
4.07
2.07
4.05
2.10
2.03
f1 (ppm)

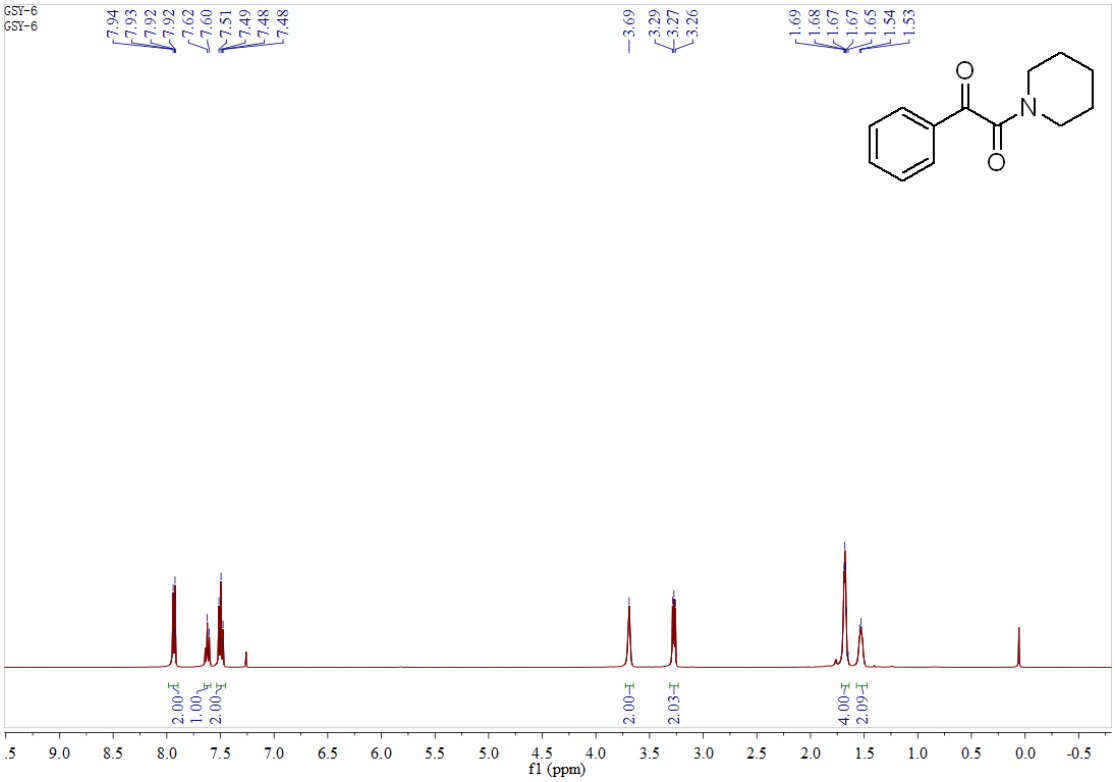

GSY-5
GSY-5
191.34
165.70
136.54
133.16
132.53
130.53
130.02
129.66
129.30
128.08
127.35
123.68
66.87
66.82
46.47
41.83
f1 (ppm)

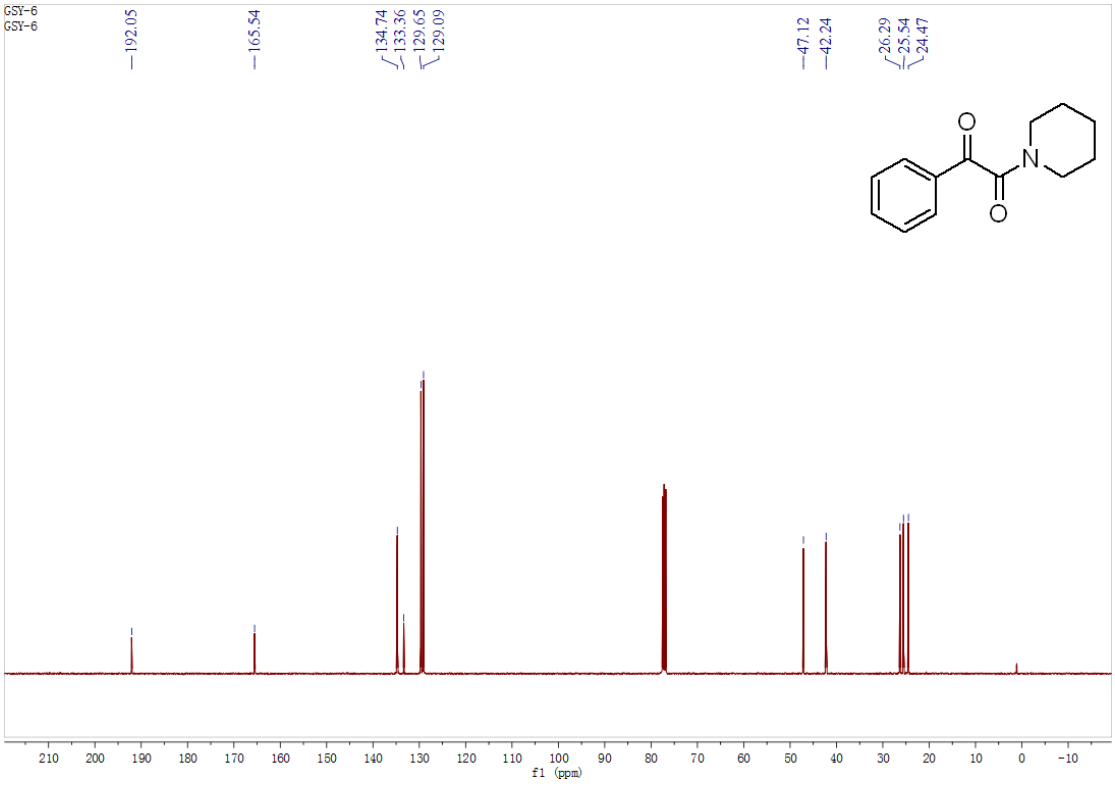

GSY-13
GSY-13
7.83
7.83
7.82
7.82
7.80
7.80
7.79
7.79
7.18
7.17
7.17
7.16
3.78
3.77
3.77
3.76
3.76
3.75
3.74
3.74
3.72
3.72
3.67
3.66
3.66
3.65
3.64
3.48
3.47
3.46
O
N
O
S
O
2.05
1.00
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
2.05
1.00
4.17
2.09
2.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

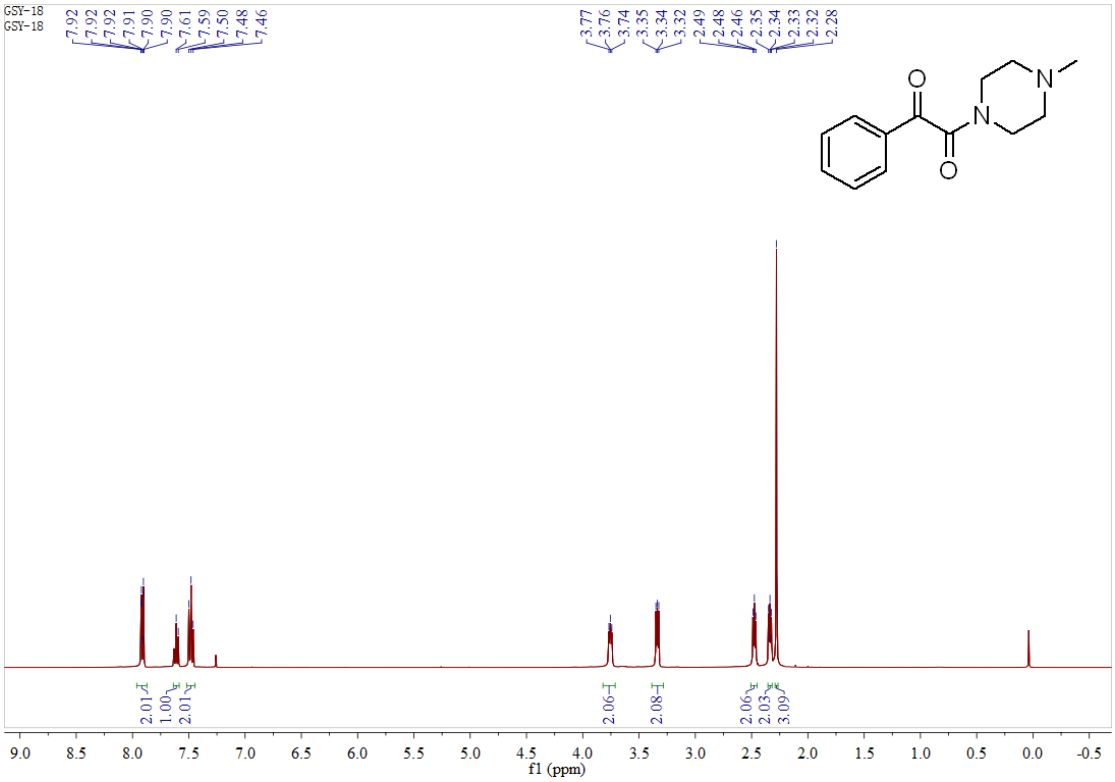

GSY-13
GSY-13
182.90
164.41
140.36
136.87
136.37
128.82
66.89
66.70
46.52
42.03
O
N
O
S
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

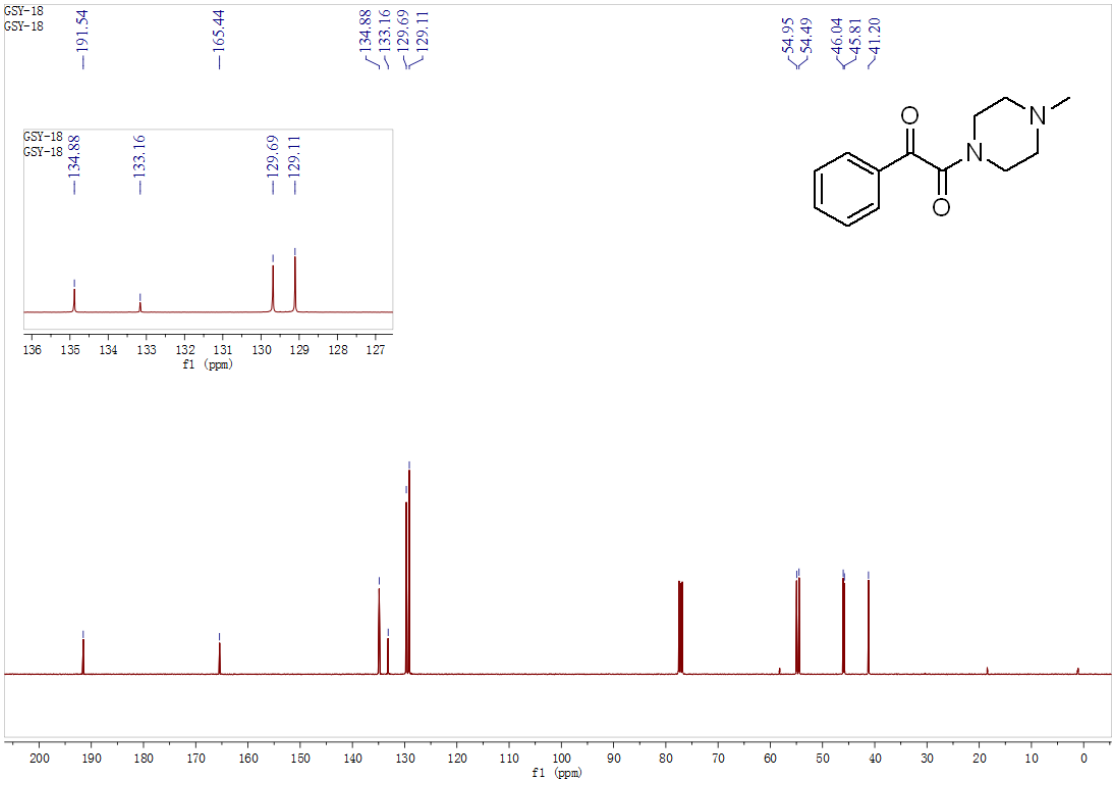

SJL1
SJL1
9.07
8.78
8.78
8.77
8.20
8.19
8.18
8.18
7.43
7.42
7.42
7.41
7.41
7.40
7.40
3.74
3.72
3.72
3.70
3.62
3.60
3.60
3.59
3.37
3.36
3.36
3.35
3.35
3.34
O
N
O
N
O
1.02
1.00
1.00
1.02
4.08
2.02
2.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

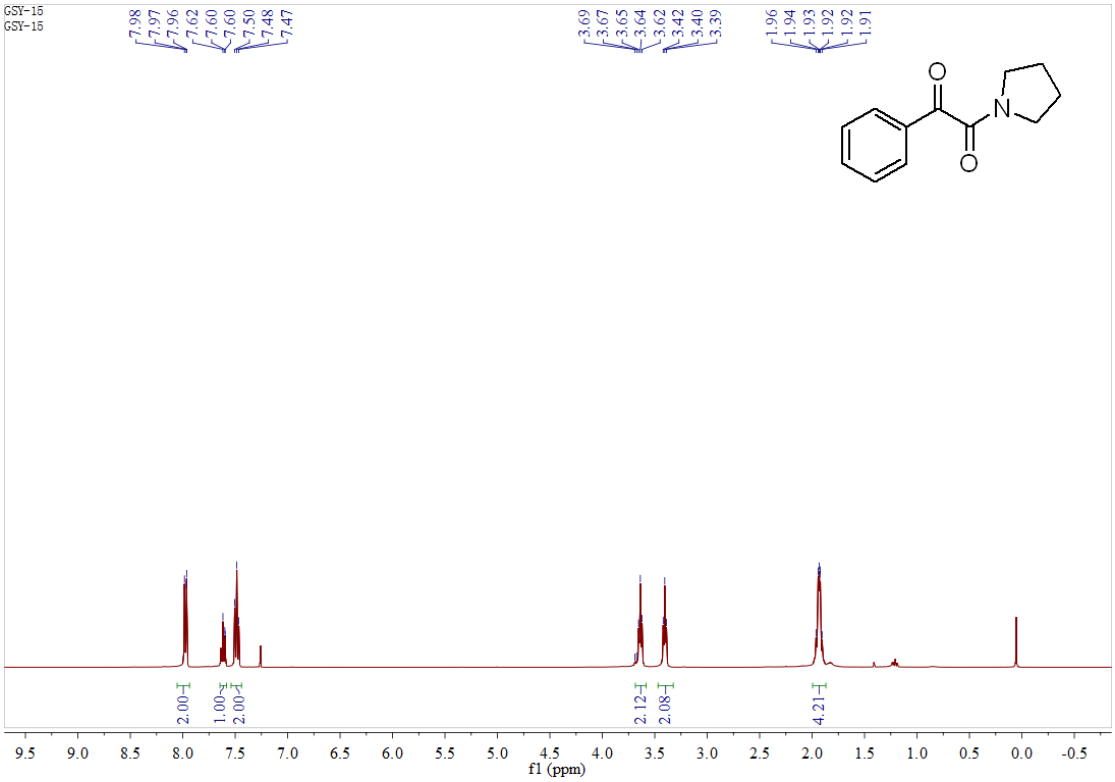

GSY-26
GSY-26
189.45
164.13
154.80
151.17
136.73
128.77
123.92
66.68
66.55
46.25
41.79
O
N
O
N
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

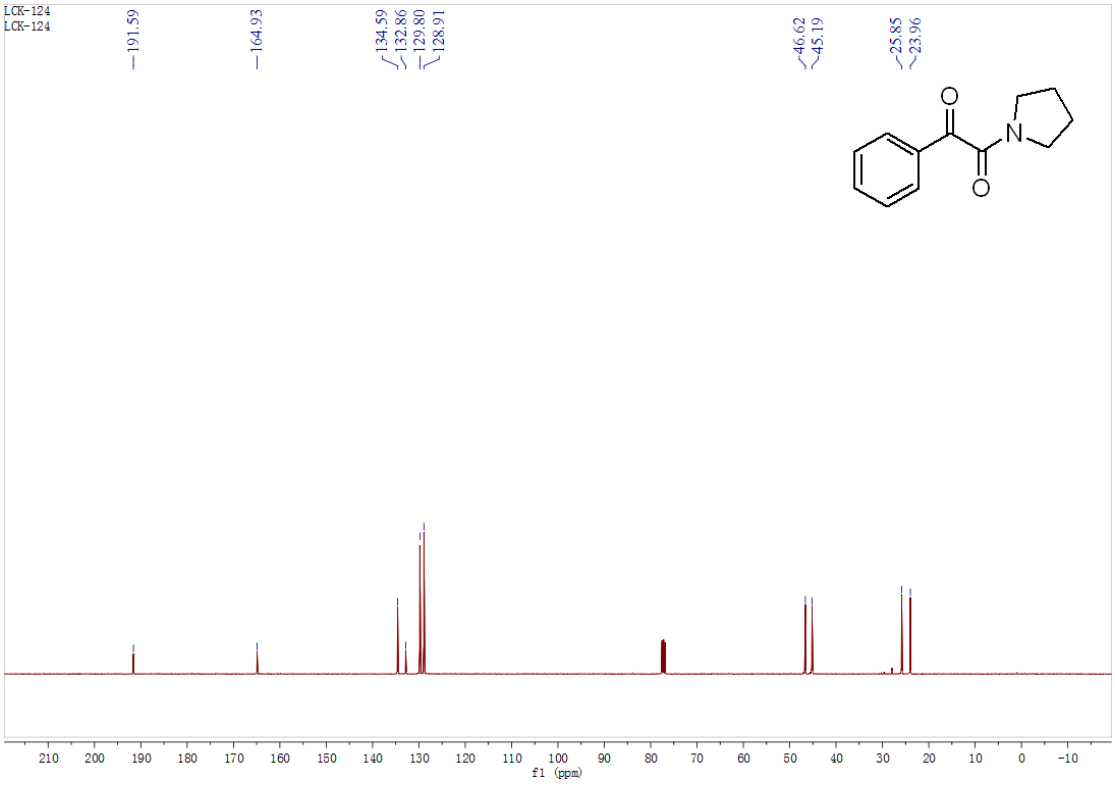

GSY-6
GSY-6
7.94
7.93
7.92
7.92
7.62
7.60
7.51
7.49
7.48
7.48
3.69
3.29
3.27
3.26
1.69
1.68
1.67
1.67
1.65
1.54
1.53
O
N
O
2.00
1.00
2.00
2.00
2.03
4.00
2.09
f1 (ppm)

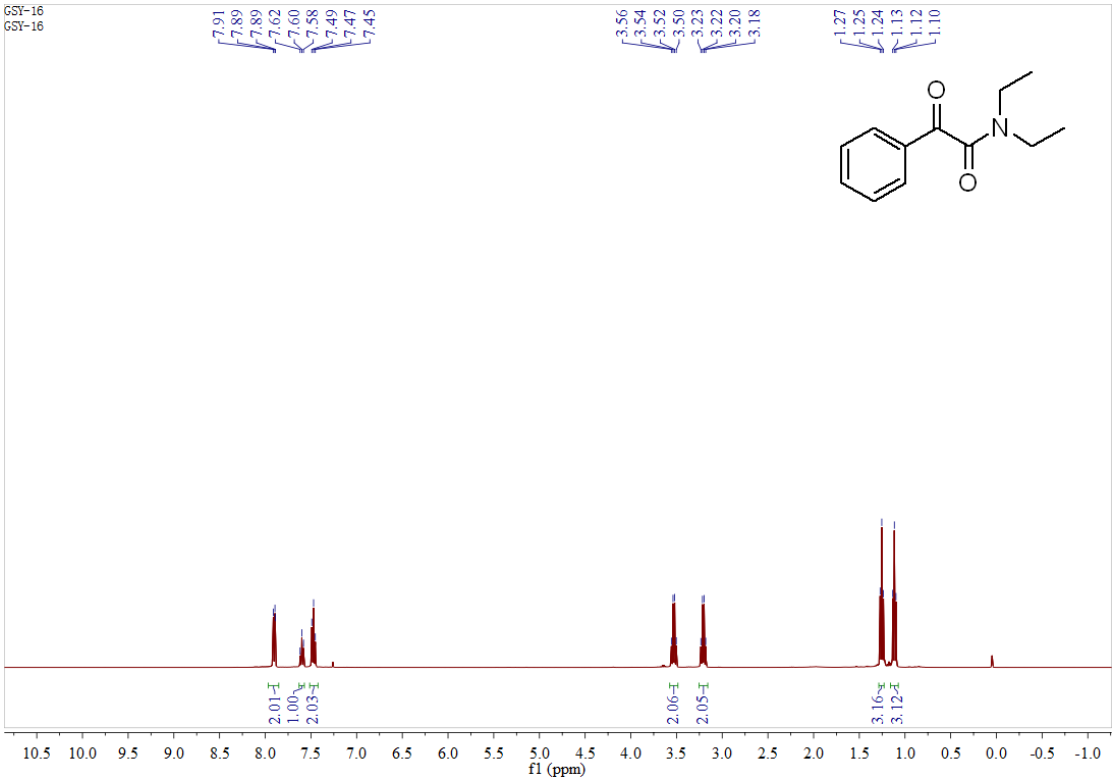

GSY-6
GSY-6
192.05
165.54
134.74
133.36
129.65
129.09
47.12
42.24
26.29
25.54
24.47
O
N
O
f1 (ppm)

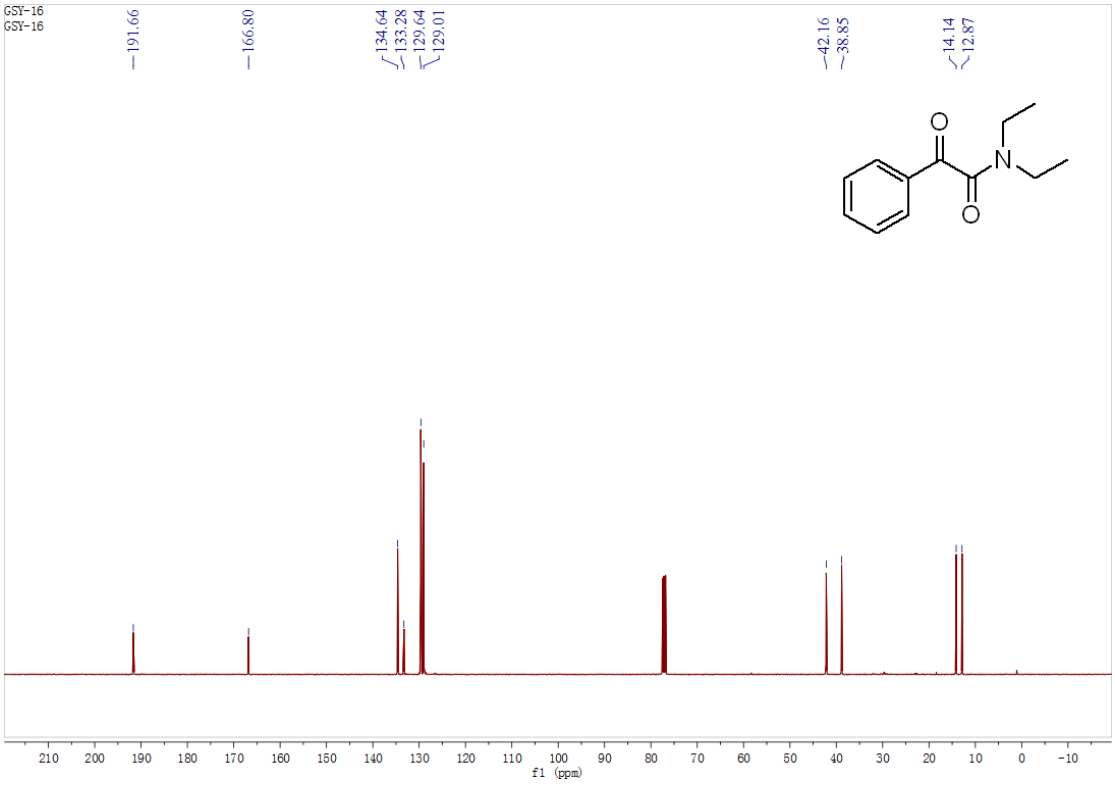

GSY-18
GSY-18
7.92
7.92
7.92
7.91
7.90
7.90
7.61
7.59
7.50
7.48
7.46
3.77
3.76
3.74
3.35
3.34
3.32
2.49
2.48
2.46
2.35
2.34
2.33
2.32
2.28
O
N
N
O
2.01
1.00
2.01
2.06
2.08
2.06
2.03
3.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

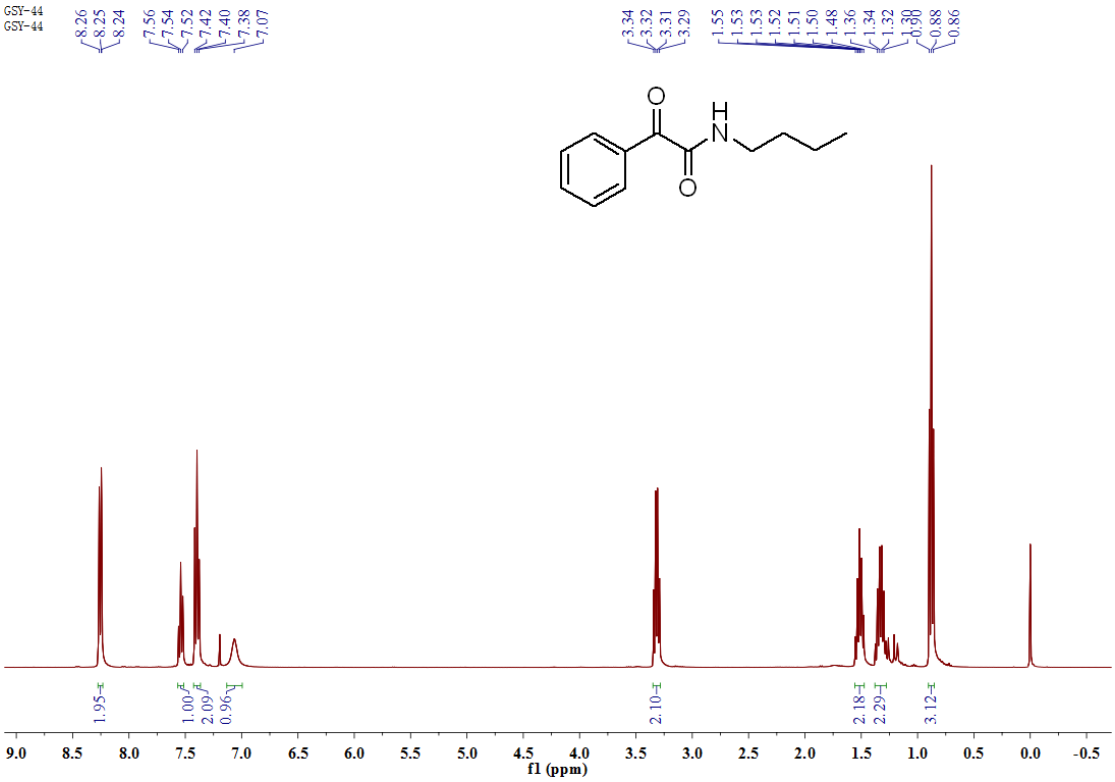

GSY-18
GSY-18
191.54
165.44
134.88
133.16
129.69
129.11
54.95
54.49
46.04
45.81
41.20
GSY-18
GSY-18
134.88
133.16
129.69
129.11
136
135
134
133
132
131
130
129
128
127
f1 (ppm)
O
N
N
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

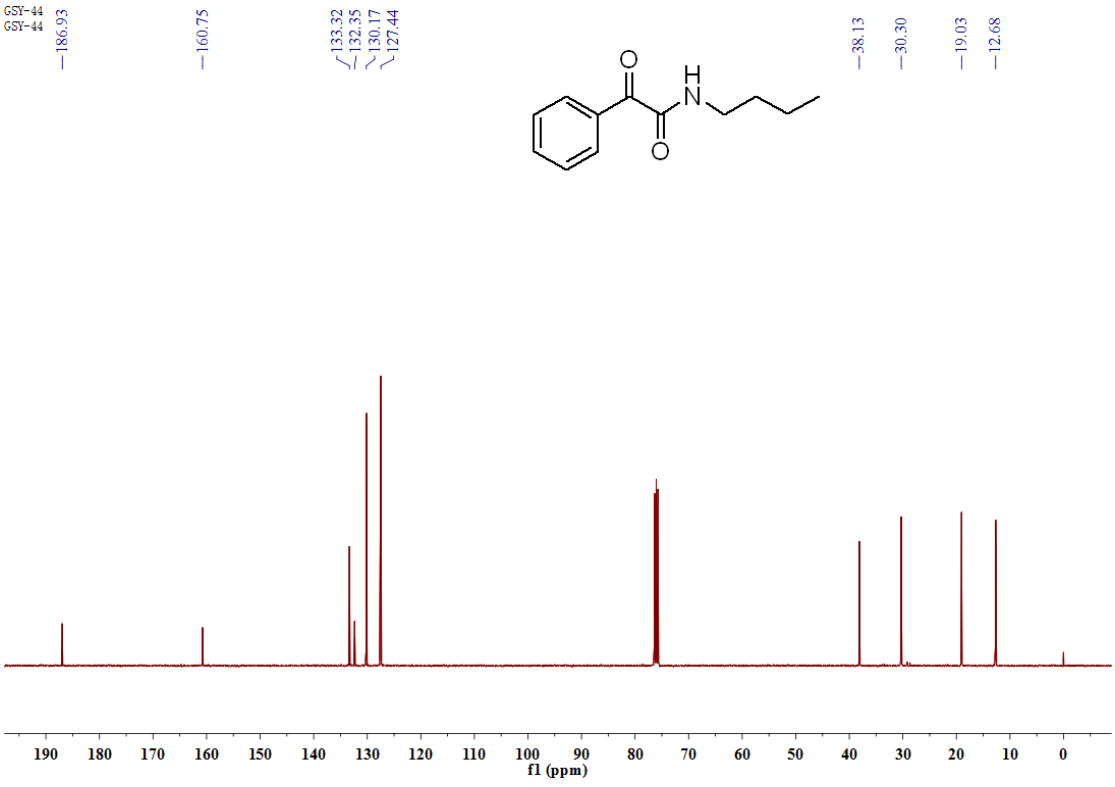

GSY-15
GSY-15
7.98
7.97
7.96
7.62
7.60
7.60
7.50
7.48
7.47
3.69
3.67
3.65
3.64
3.62
3.42
3.40
3.39
1.96
1.94
1.93
1.92
1.92
1.91
O
N
O
2.00
1.00
2.00
2.12
2.08
4.21
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

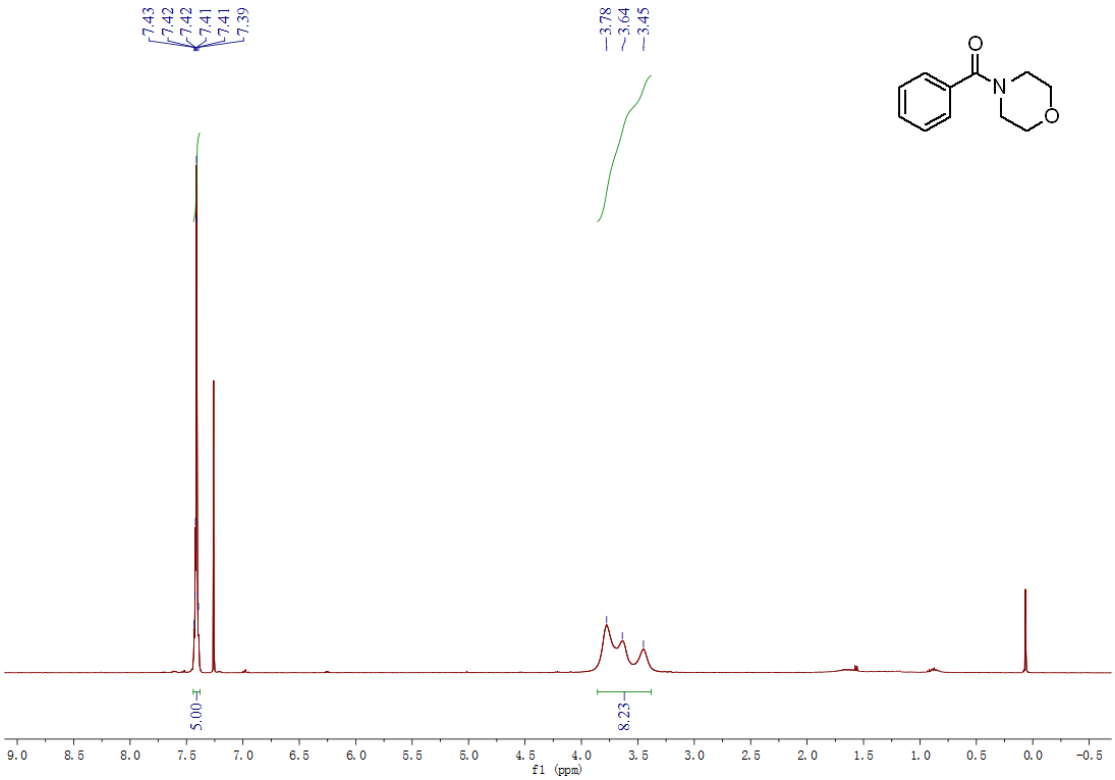

LCK-124
LCK-124
191.59
164.93
134.59
132.86
129.80
128.91
46.62
45.19
25.85
23.96
O
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

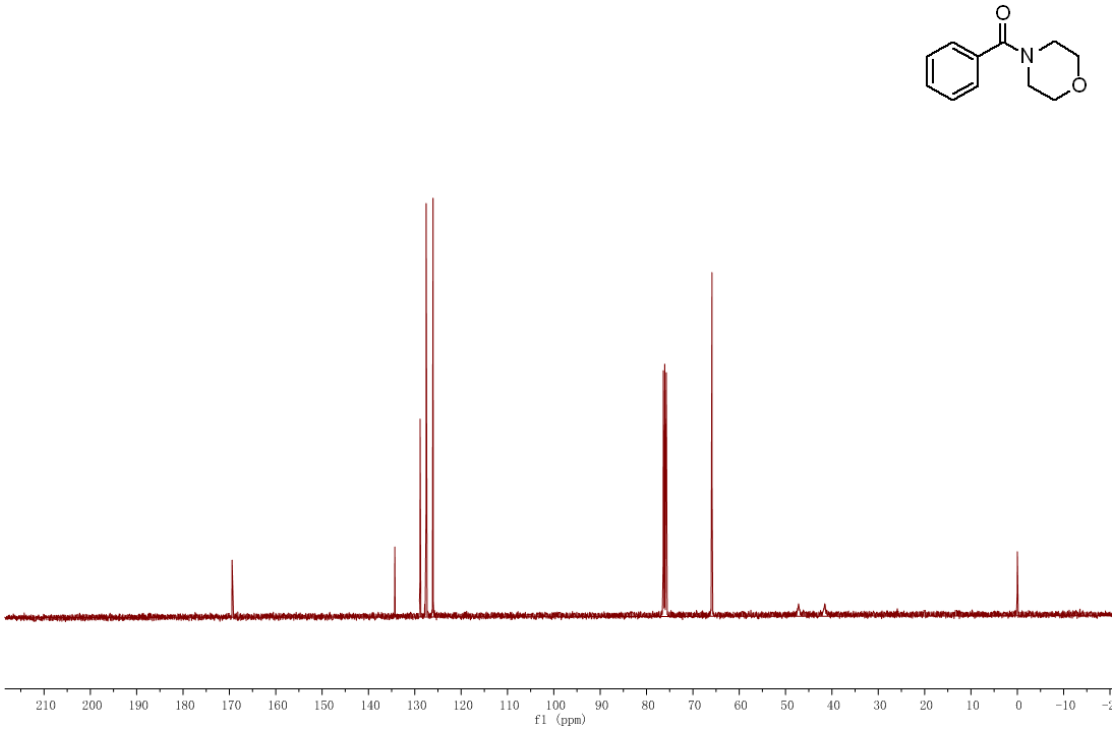

GSY-16
GSY-16
7.91
7.89
7.89
7.62
7.60
7.58
7.49
7.47
7.45
3.56
3.54
3.52
3.50
3.23
3.22
3.20
3.18
1.27
1.25
1.24
1.13
1.12
1.10
2.01
1.00
2.03
2.06
2.05
3.16
3.12
f1 (ppm)

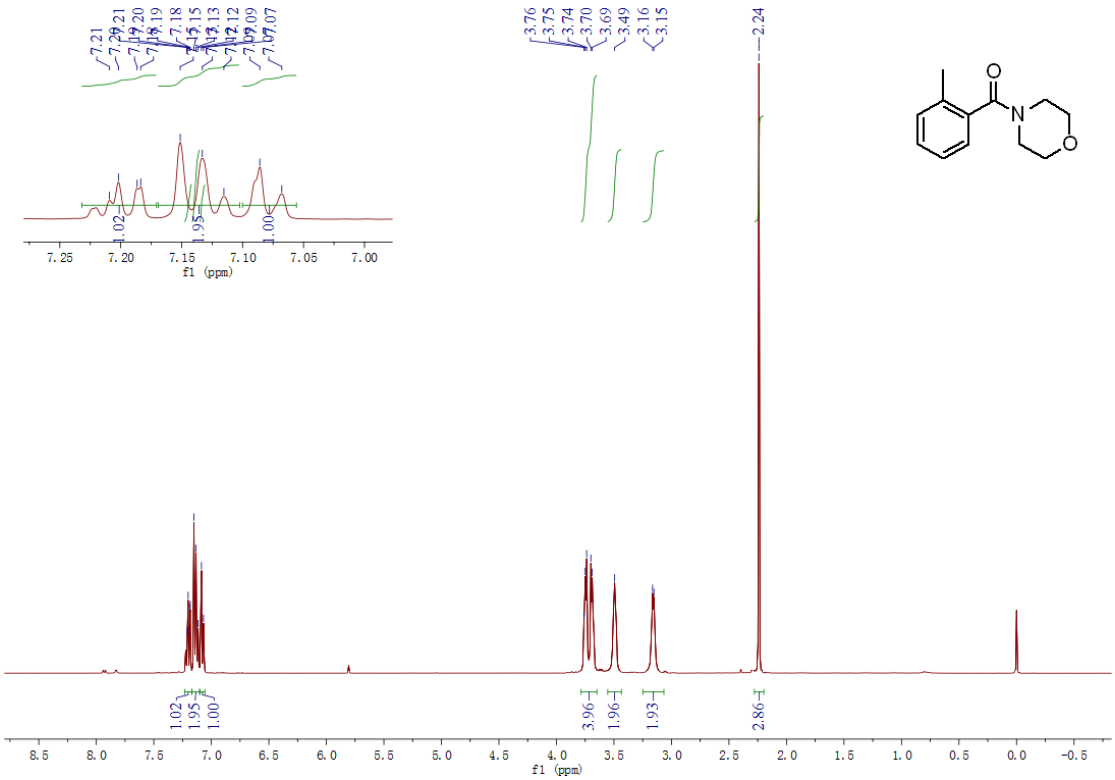

GSY-16
GSY-16
191.66
166.80
134.64
133.28
129.64
129.01
42.16
38.85
14.14
12.87
f1 (ppm)

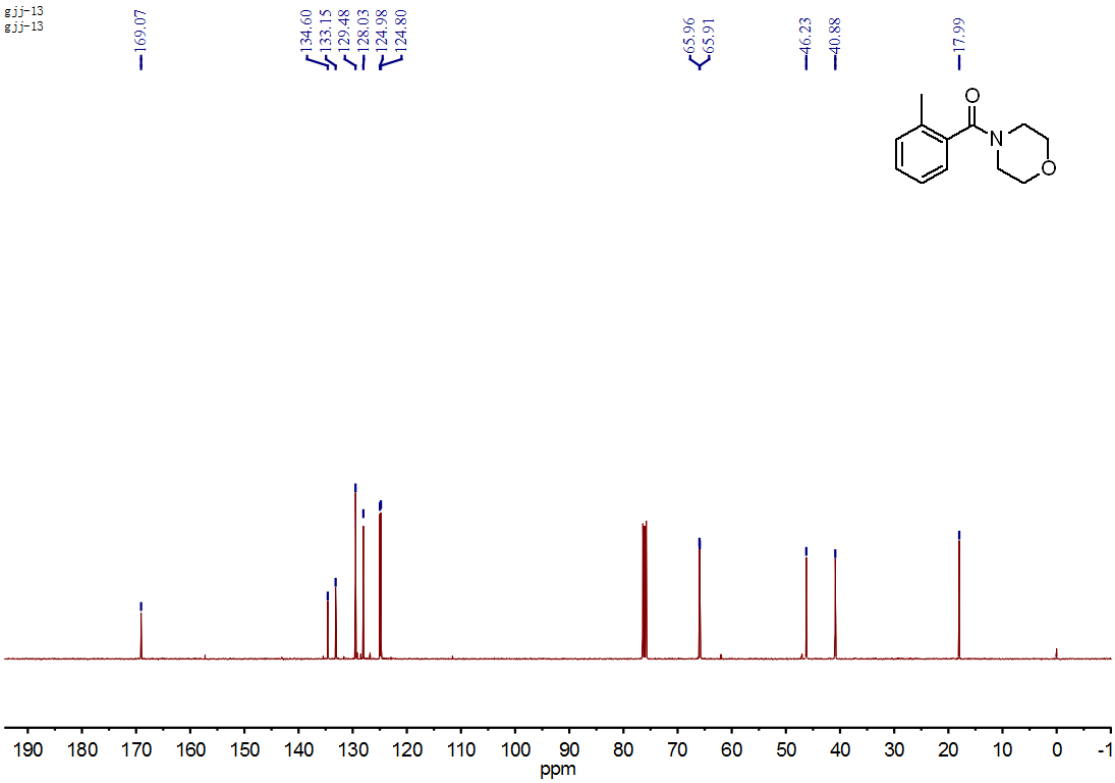

GSY-44
GSY-44
8.26
8.25
8.24
7.56
7.54
7.52
7.42
7.40
7.38
7.07
3.34
3.32
3.31
3.29
1.55
1.53
1.53
1.52
1.51
1.50
1.48
1.36
1.34
1.32
1.30
0.90
0.88
0.86
O
N
H
O
1.95
1.00
2.09
0.96
2.10
2.18
2.29
3.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

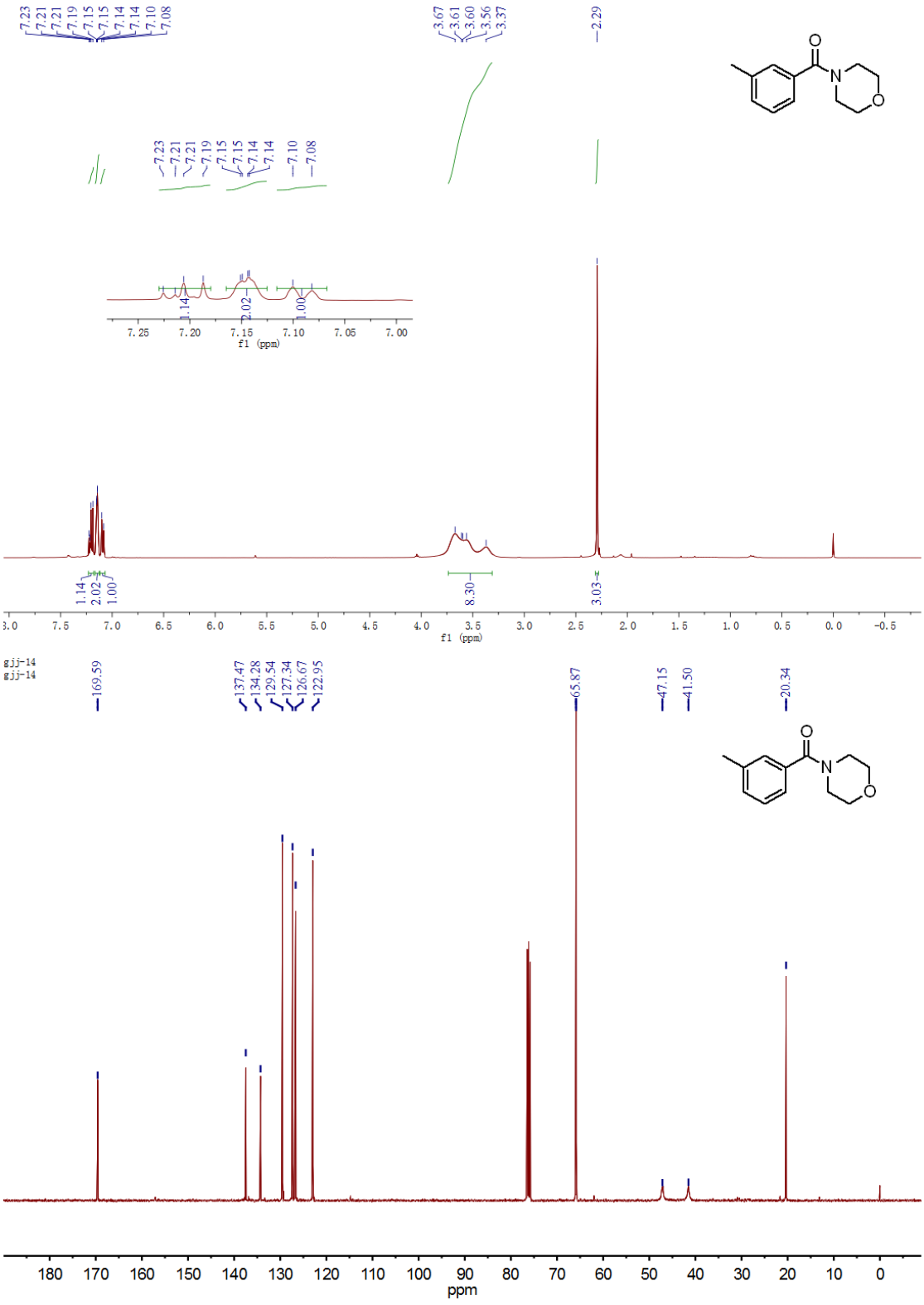

GSY-44
GSY-44
186.93
160.75
133.32
132.35
130.17
127.44
38.13
30.30
19.03
12.68
O
N
H
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

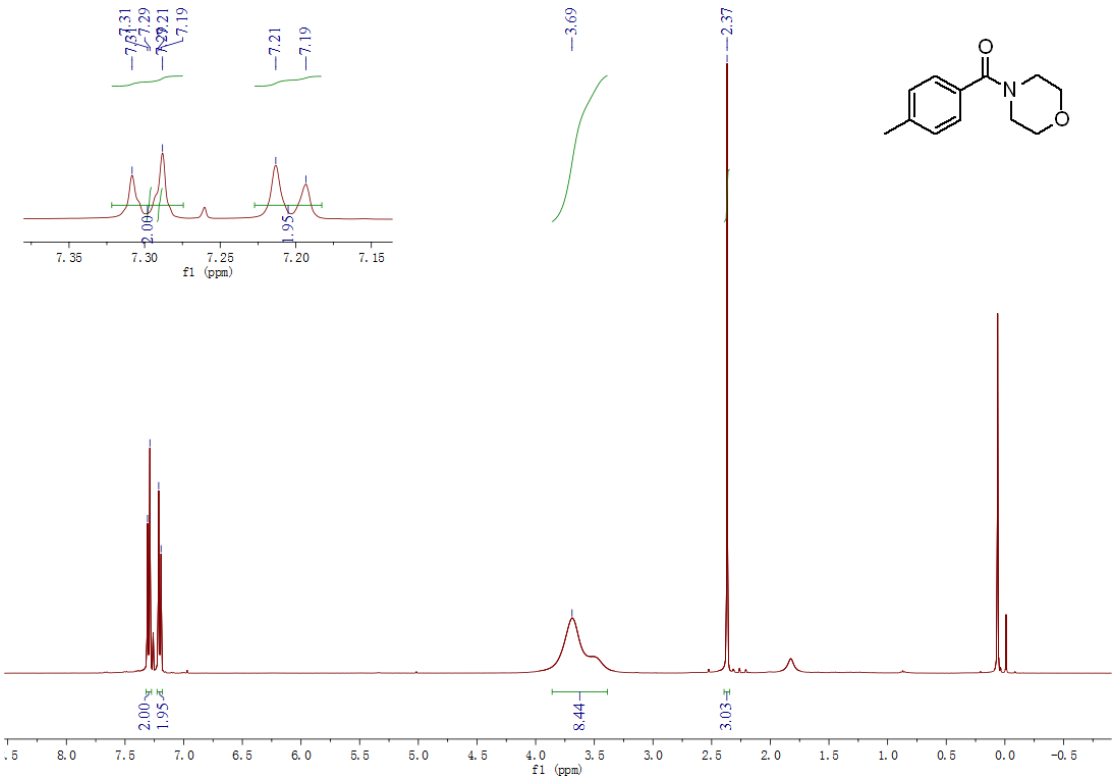

7.43
7.42
7.42
7.41
7.41
7.39
3.78
3.64
3.45
5.00
8.23
f1 (ppm)

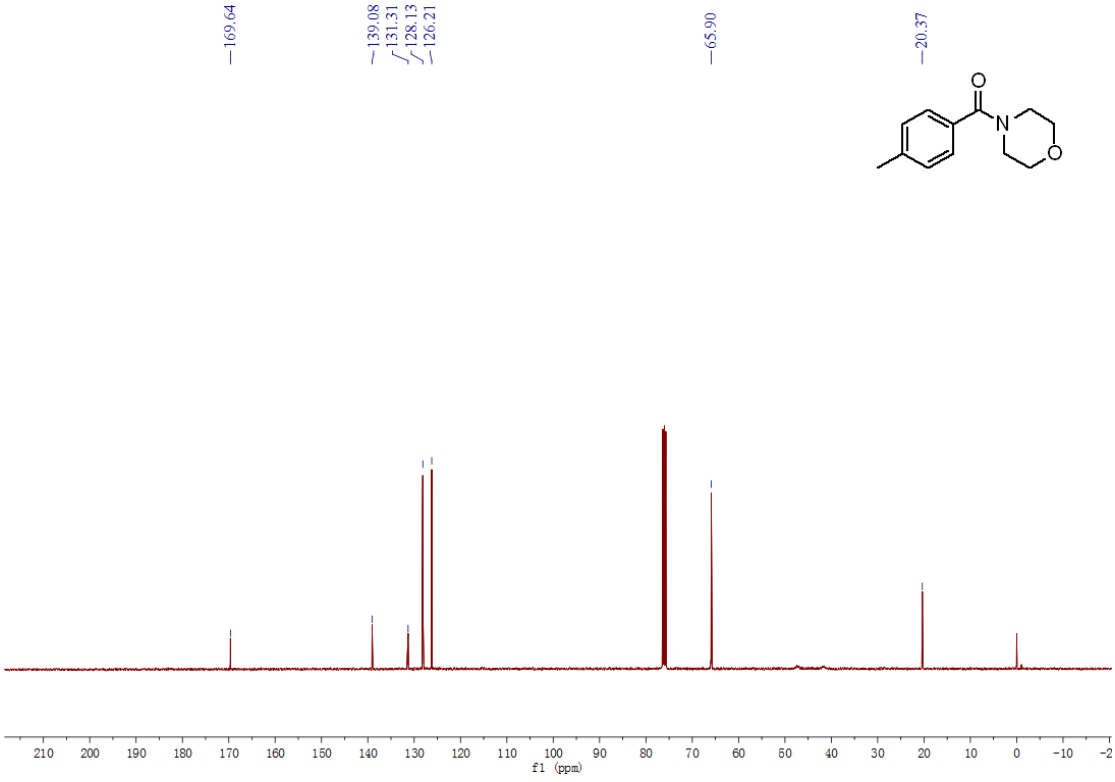

f1 (ppm)

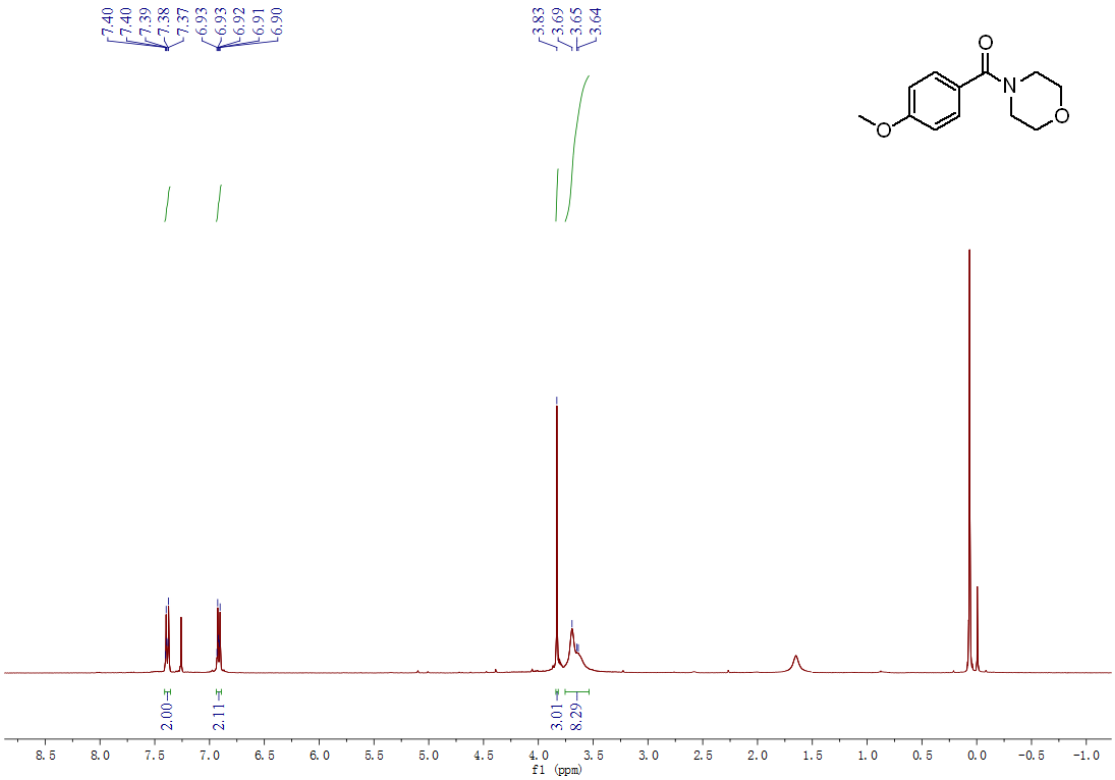

7.21
7.20
7.19
7.18
7.15
7.13
7.12
7.09
7.07
1.02
1.95
1.00
7.25
7.20
7.15
7.10
7.05
7.00
f1 (ppm)
3.76
3.75
3.74
3.70
3.69
3.49
3.16
3.15
2.24
O
N
O
1.02
1.95
1.00
3.96
1.96
1.93
2.86
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

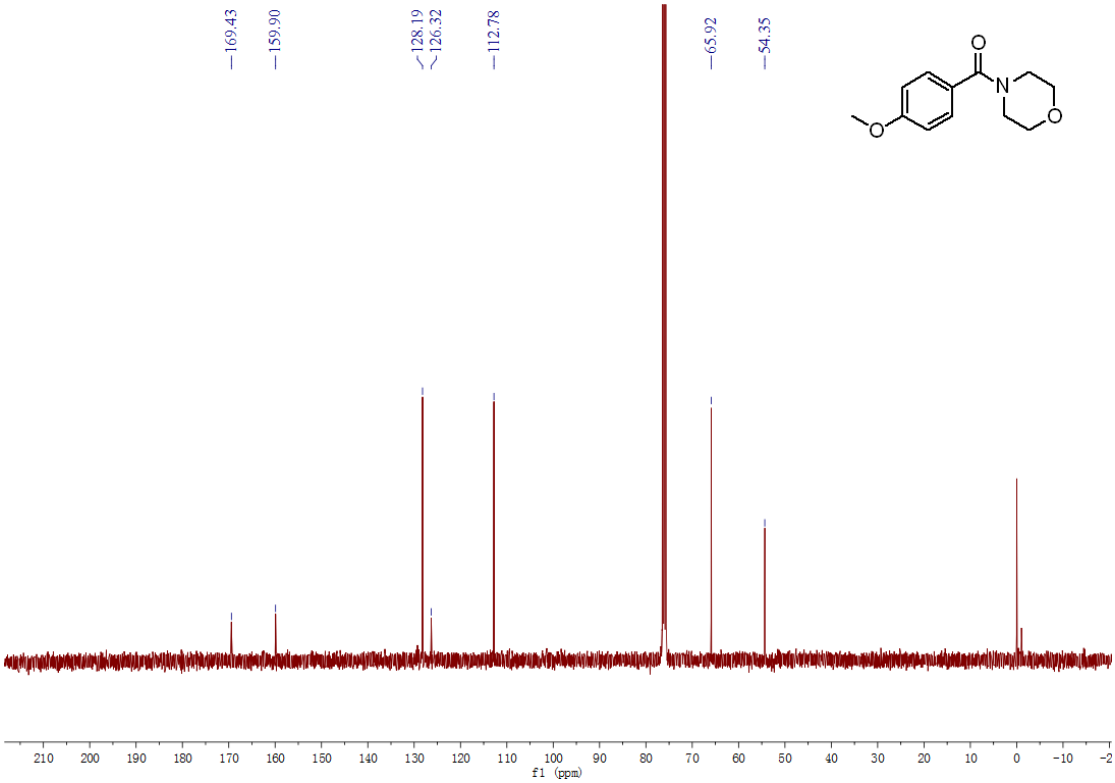

gjj-13
gjj-13
169.07
134.60
133.15
129.48
128.03
124.98
124.80
65.96
65.91
46.23
40.88
17.99
O
N
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
ppm

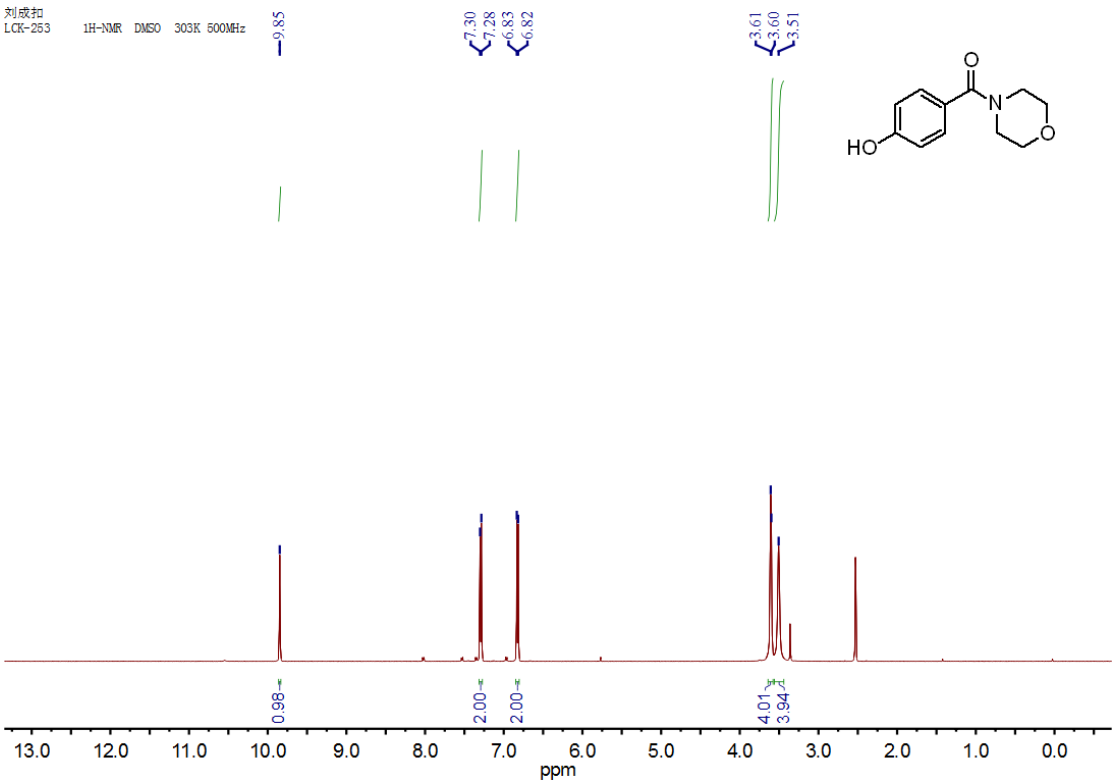

7.23
7.21
7.21
7.19
7.15
7.15
7.14
7.14
7.10
7.08
3.67
3.61
3.60
3.56
3.37
2.29
1.14
2.02
1.00
8.30
3.03
f1 (ppm)
gjj-14
gjj-14
169.59
137.47
134.28
129.54
127.34
126.67
122.95
65.87
47.15
41.50
20.34
ppm

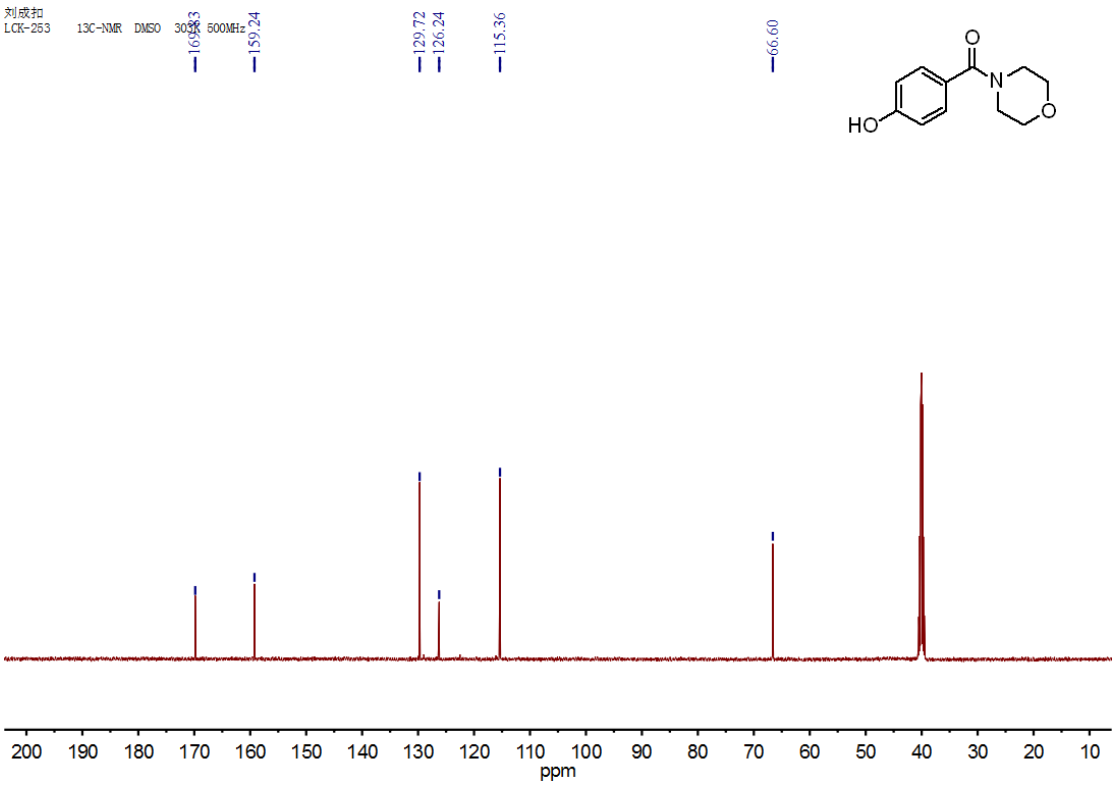

7.31
7.29
7.21
7.19
7.21
7.19
2.00
1.95
7.36
7.30
7.25
7.20
7.15
f1 (ppm)
3.69
2.37
2.00
1.95
8.44
3.03
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
O
N
O

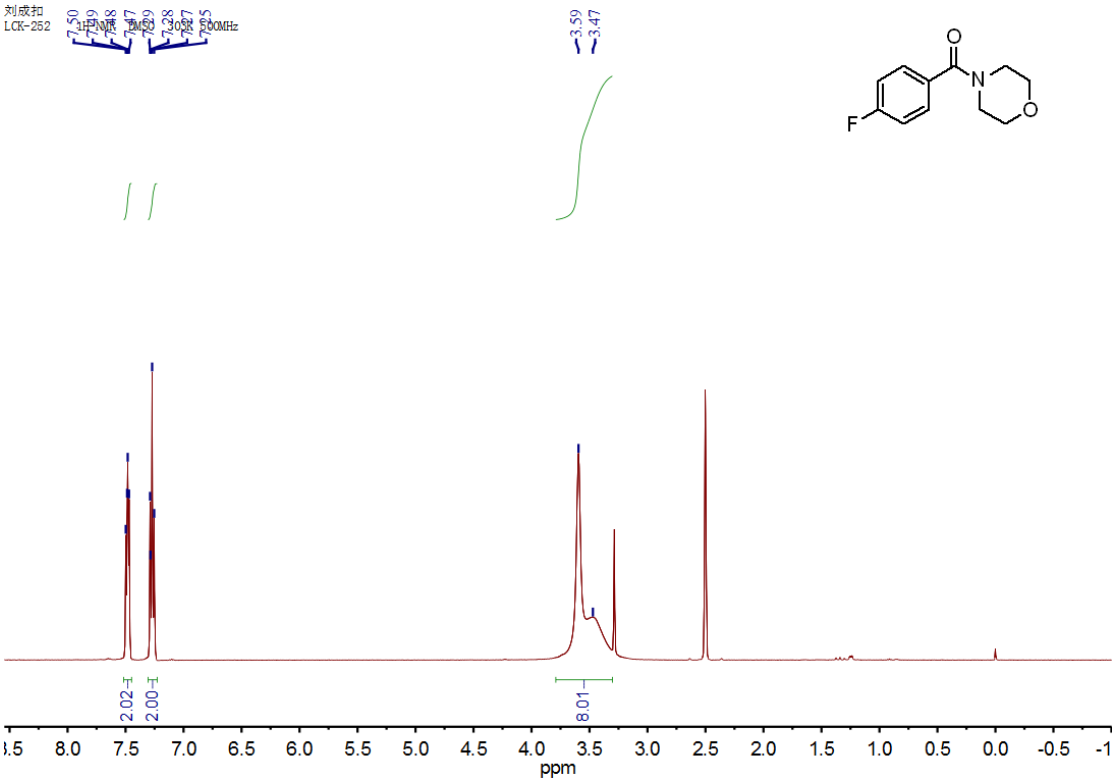

169.64
139.08
131.31
128.13
126.21
65.90
20.37
O
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-2
f1 (ppm)

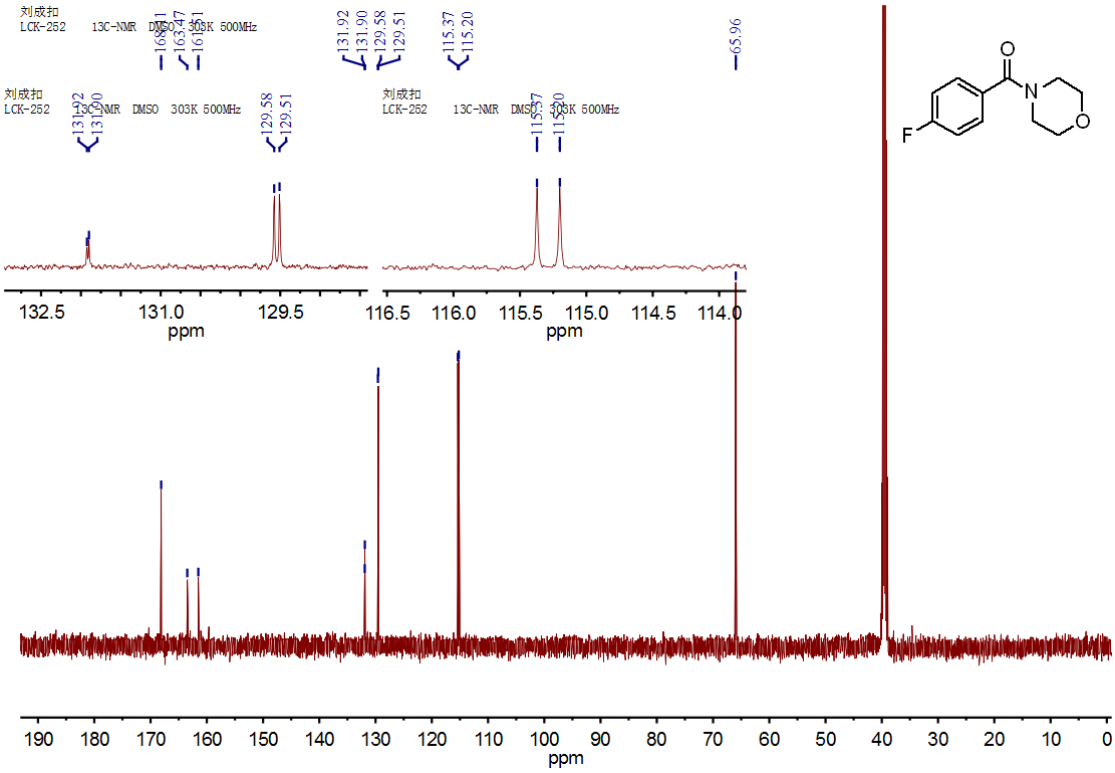

7.40
7.40
7.39
7.38
7.37
6.93
6.92
6.91
6.90
3.83
3.69
3.65
3.64
O
N
O
O
2.00
2.11
3.01
8.29
f1 (ppm)

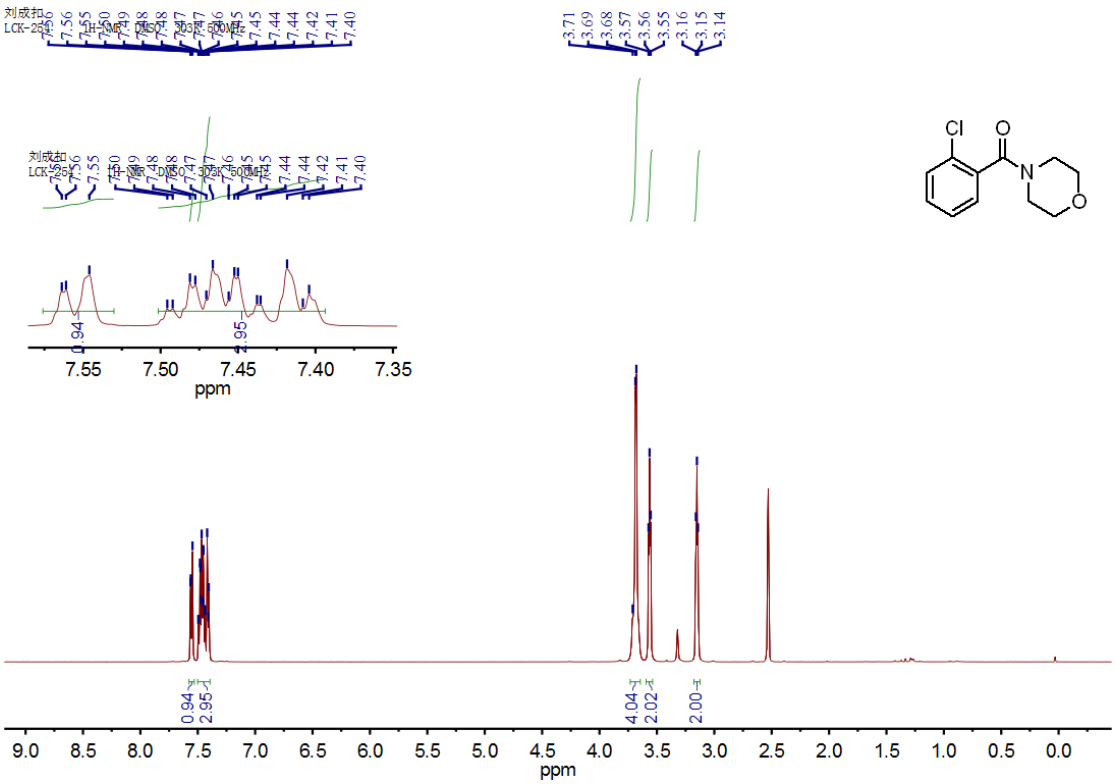

169.43
159.90
128.19
126.32
112.78
65.92
54.35
O
N
O
O
f1 (ppm)

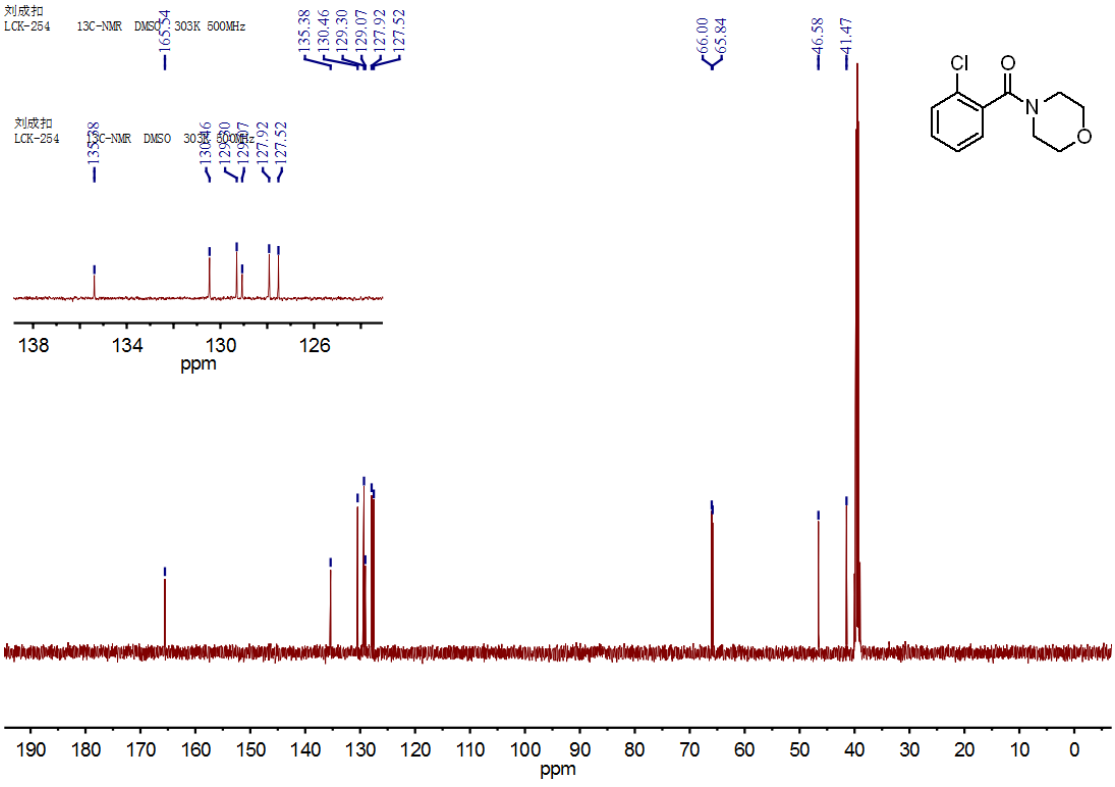

刘成扣
LCK-253 1H-NMR DMSO 303K 500MHz
9.85
7.30
7.28
6.83
6.82
3.61
3.60
3.51
O
N
O
HO
0.98
2.00
2.00
4.01
3.94
13.0 12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
ppm

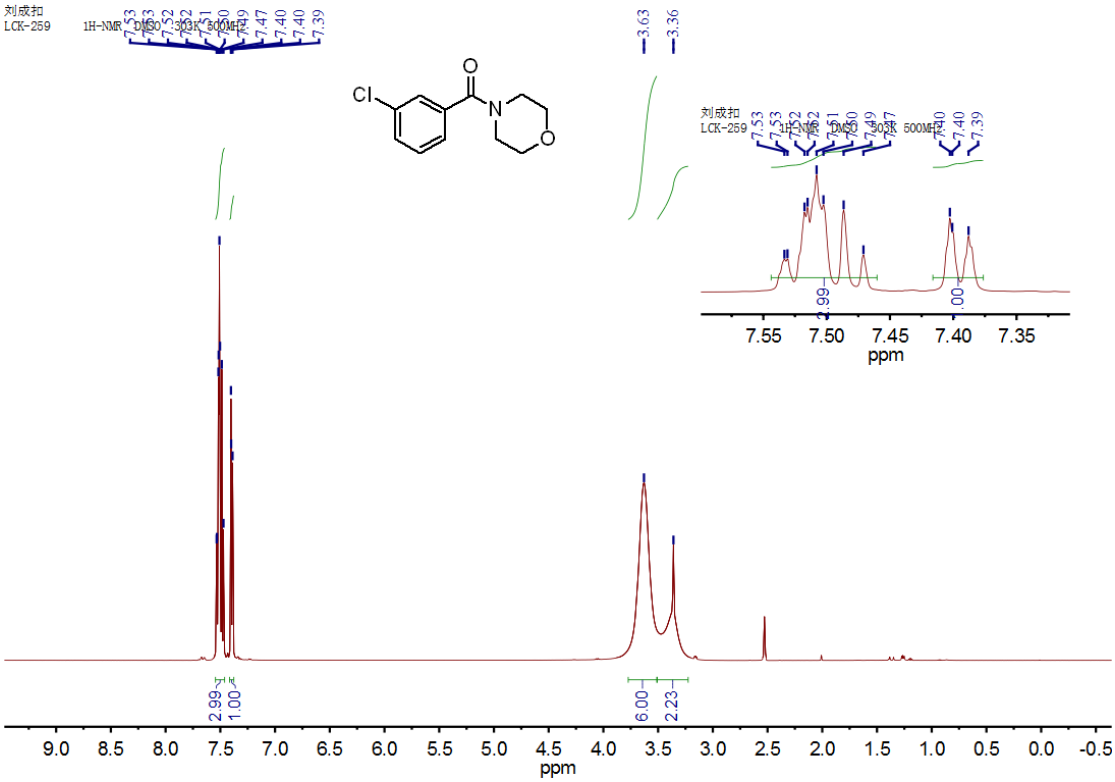

刘成扣
LCK-253 13C-NMR DMSO 303K 500MHz
169.83
159.24
129.72
126.24
115.36
66.60
O
N
O
HO
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

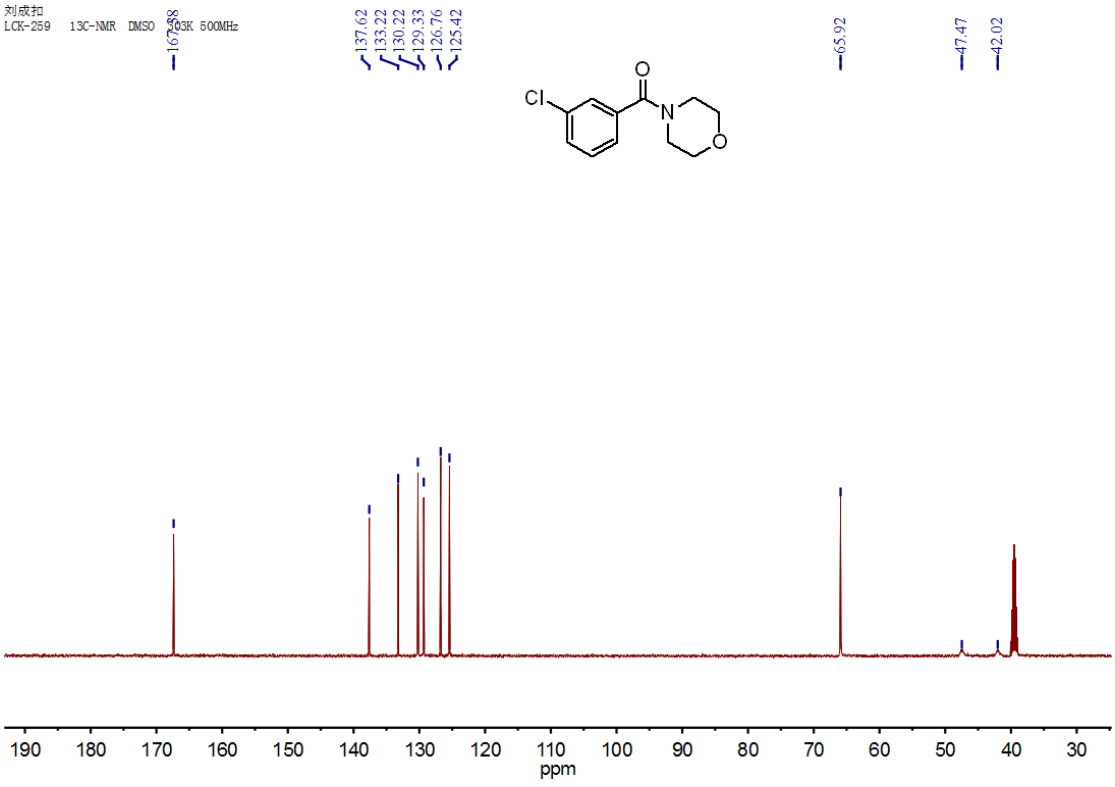

刘成扣
LCK-252
1H-NMR DMSO 303K 500MHz
7.50
7.49
7.48
7.47
7.29
7.28
7.27
7.25
3.59
3.47
2.02
2.00
8.01
ppm

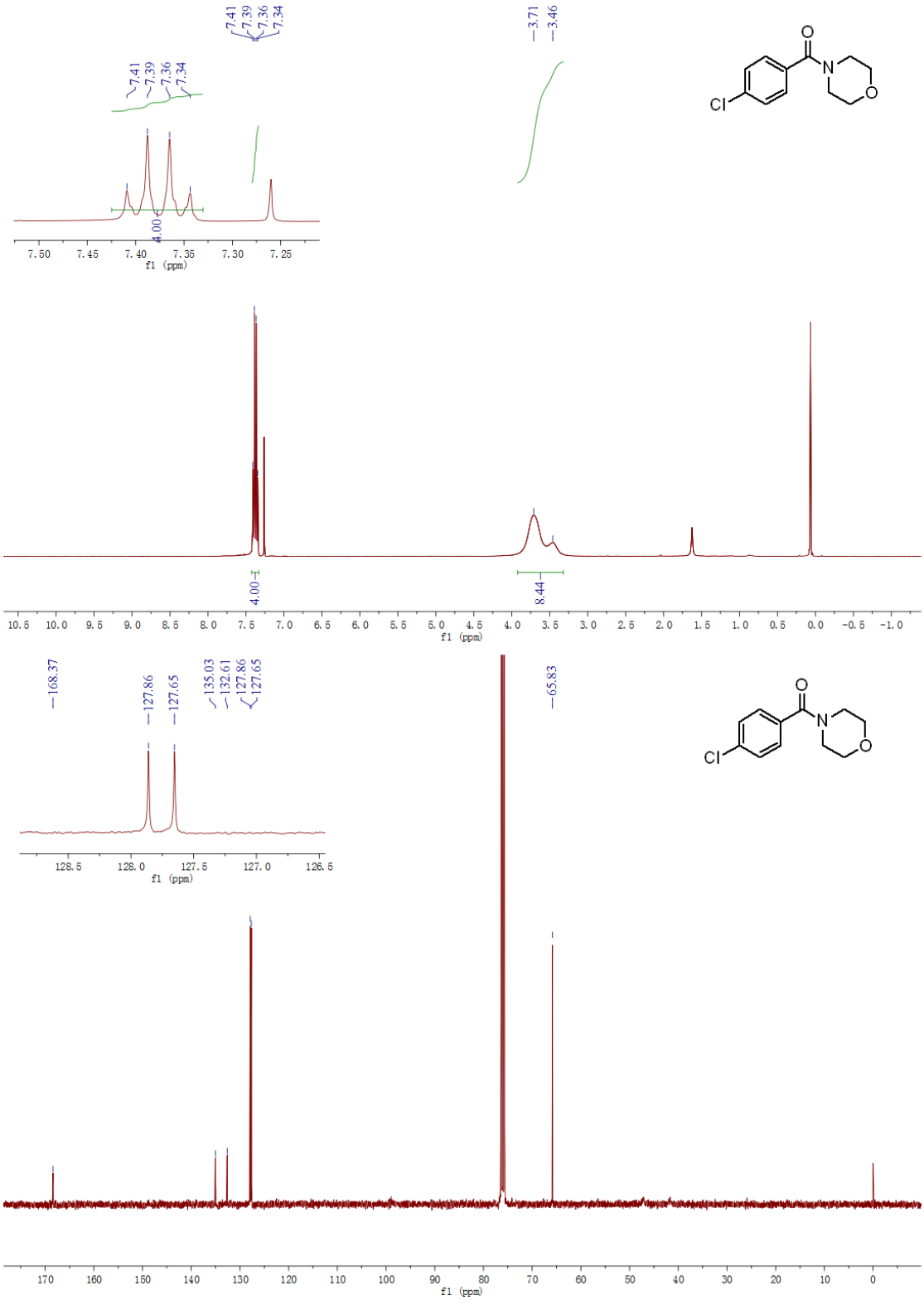

刘成扣
LCK-252
13C-NMR DMSO 303K 500MHz
131.92
131.90
129.58
129.51
115.37
115.20
65.96
ppm

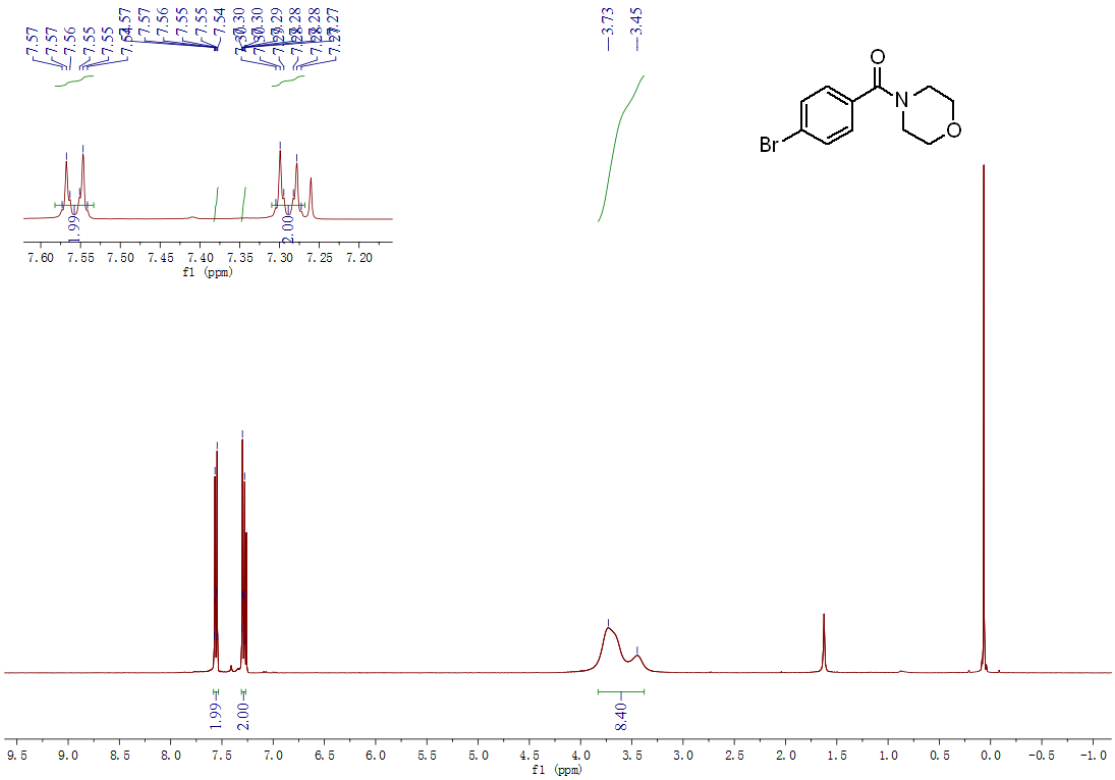

刘成扣
LCK-254
1H-NMR DMSO 303K 500MHz
7.56
7.55
7.50
7.49
7.48
7.47
7.45
7.44
7.42
7.41
7.40
3.71
3.69
3.68
3.57
3.56
3.55
3.16
3.15
3.14
0.94
2.95
4.04
2.02
2.00
7.55
7.50
7.45
7.40
7.35
ppm
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Cl
O
N
O

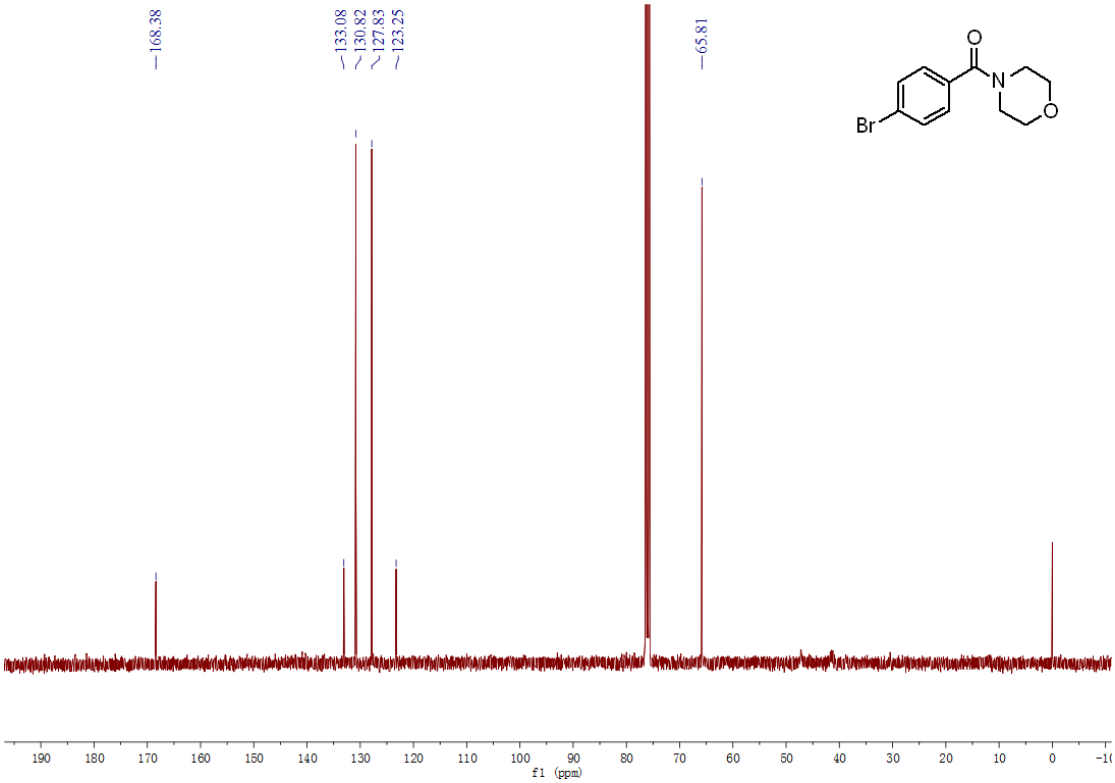

刘成扣
LCK-254
13C-NMR DMSO 303K 500MHz
165.54
135.38
130.46
129.30
129.07
127.92
127.52
66.00
65.84
46.58
41.47
138
134
130
126
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
Cl
O
N
O

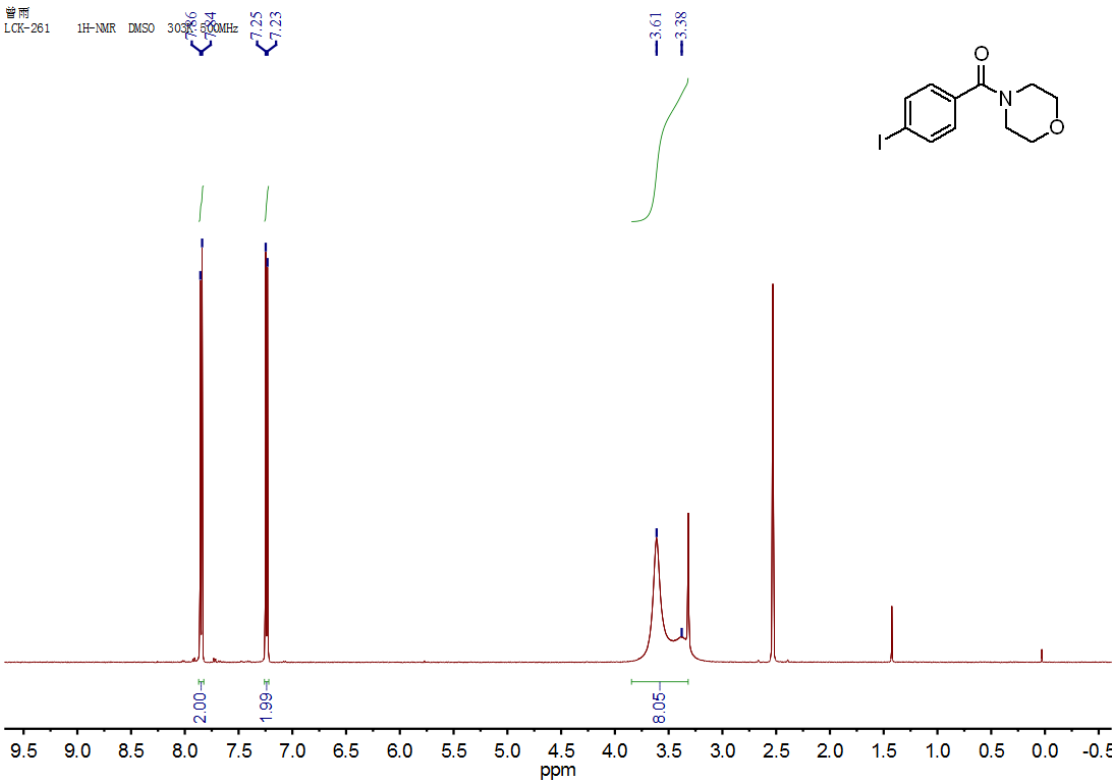

刘成扣
LCK-259
1H-NMR DMSO 303K 500MHz
7.53
7.52
7.51
7.50
7.49
7.47
7.40
7.39
3.63
3.36
Cl
O
N
O
2.99
1.00
6.00
2.23
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm
7.55 7.50 7.45 7.40 7.35
ppm

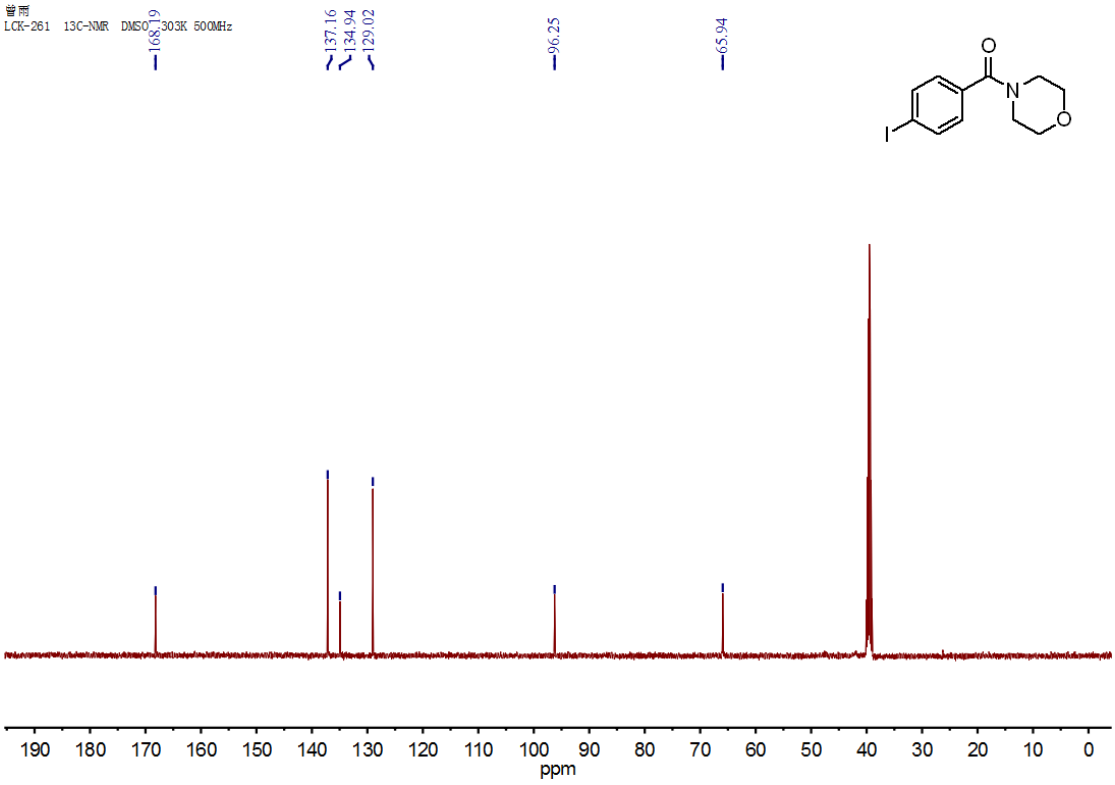

刘成扣
LCK-259
13C-NMR DMSO 303K 500MHz
167.88
137.62
133.22
130.22
129.33
126.76
125.42
65.92
47.47
42.02
Cl
O
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
ppm

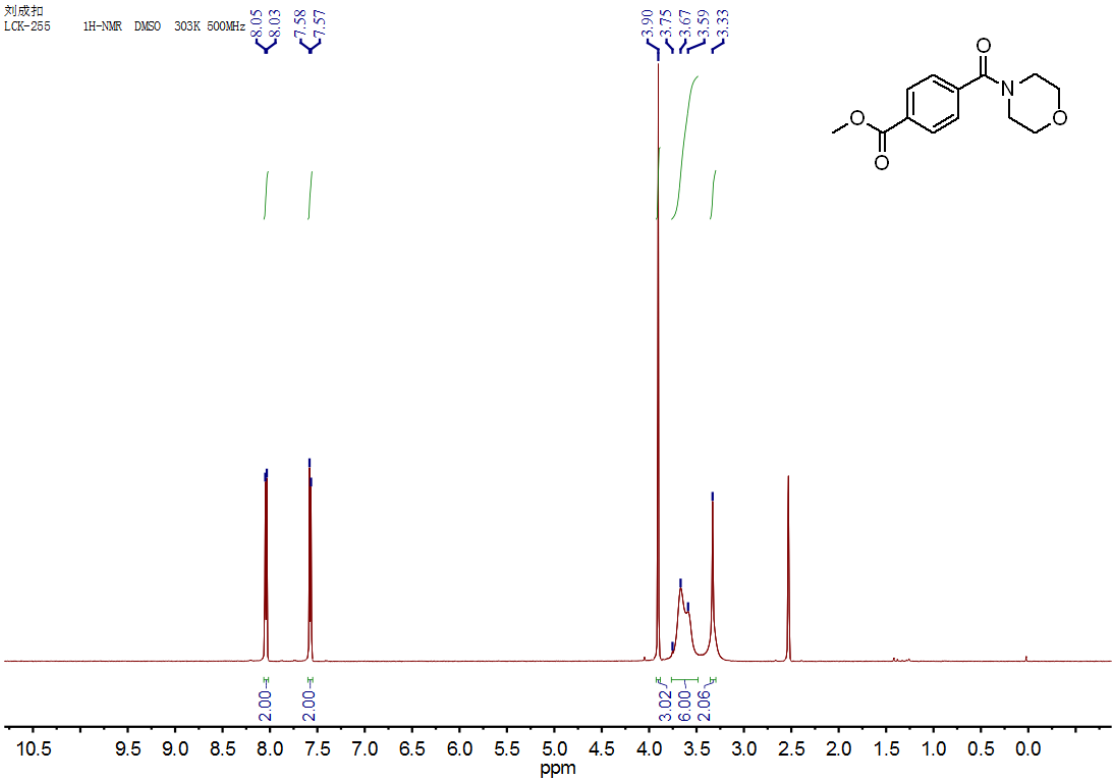

7.41
7.39
7.36
7.34
3.71
3.46
4.00
8.44
f1 (ppm)
168.37
127.86
127.65
135.03
132.61
127.86
127.65
65.83
f1 (ppm)

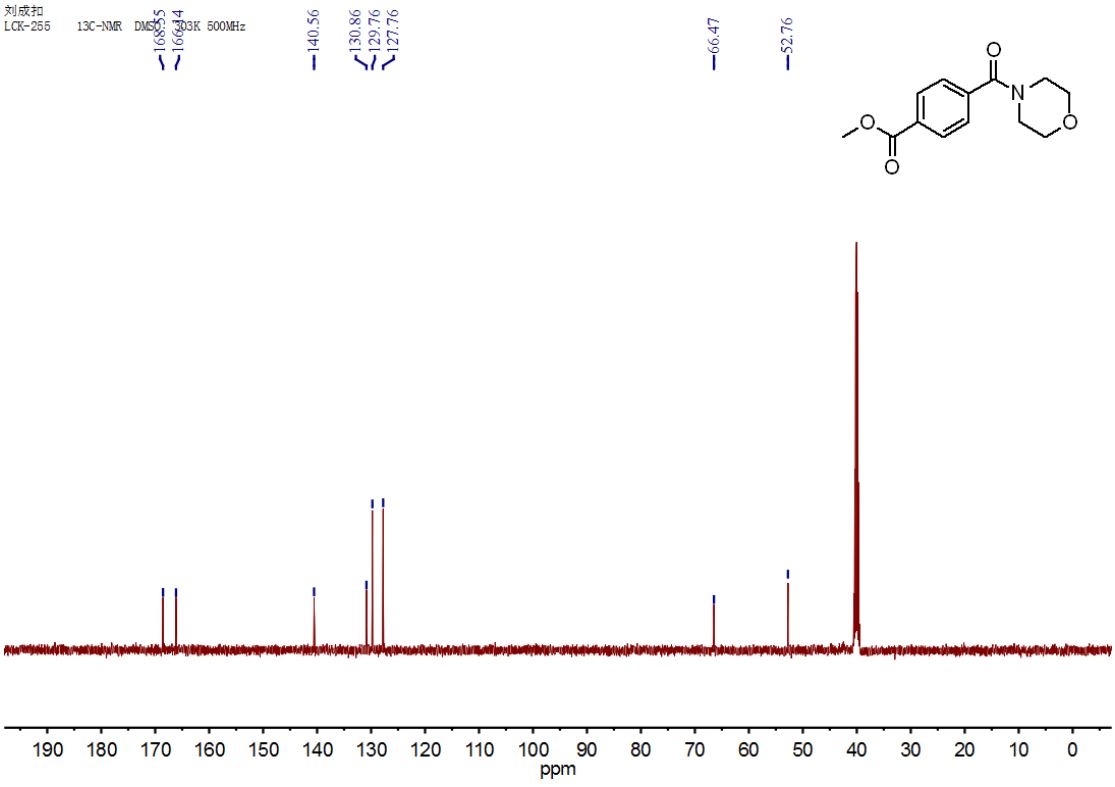

7.57
7.57
7.56
7.55
7.55
7.54
7.30
7.30
7.29
7.28
7.28
7.27
1.99
2.00
7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20
f1 (ppm)
3.73
3.45
Br
O
N
O
1.99
2.00
8.40
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

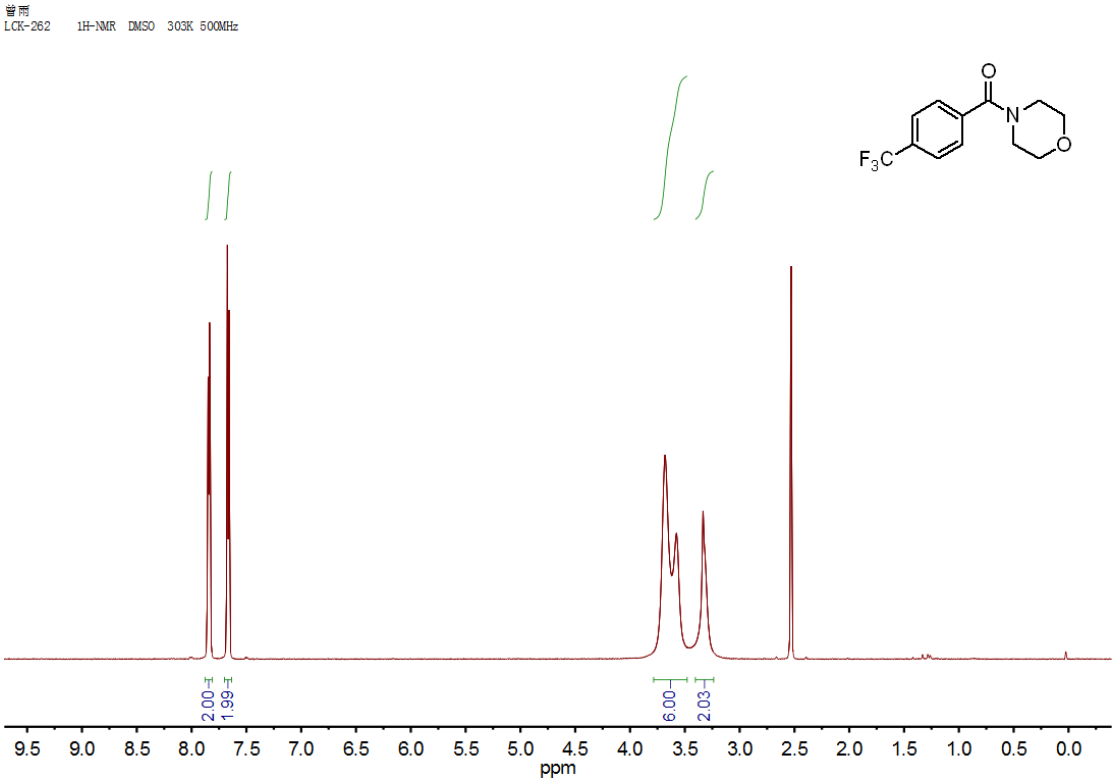

168.38
133.08
130.82
127.83
123.25
65.81
Br
O
N
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

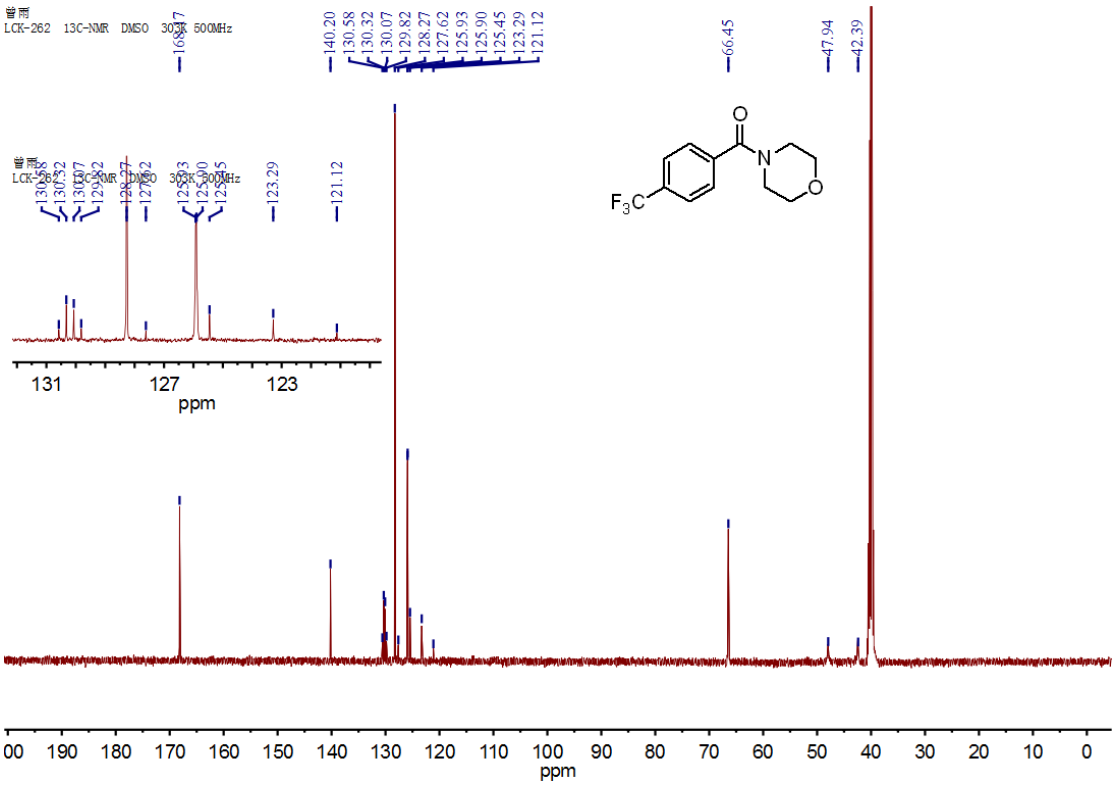

LCK-261 1H-NMR DMSO 303K 500MHz
7.86
7.84
7.25
7.23
3.61
3.38
2.00
1.99
8.05
ppm

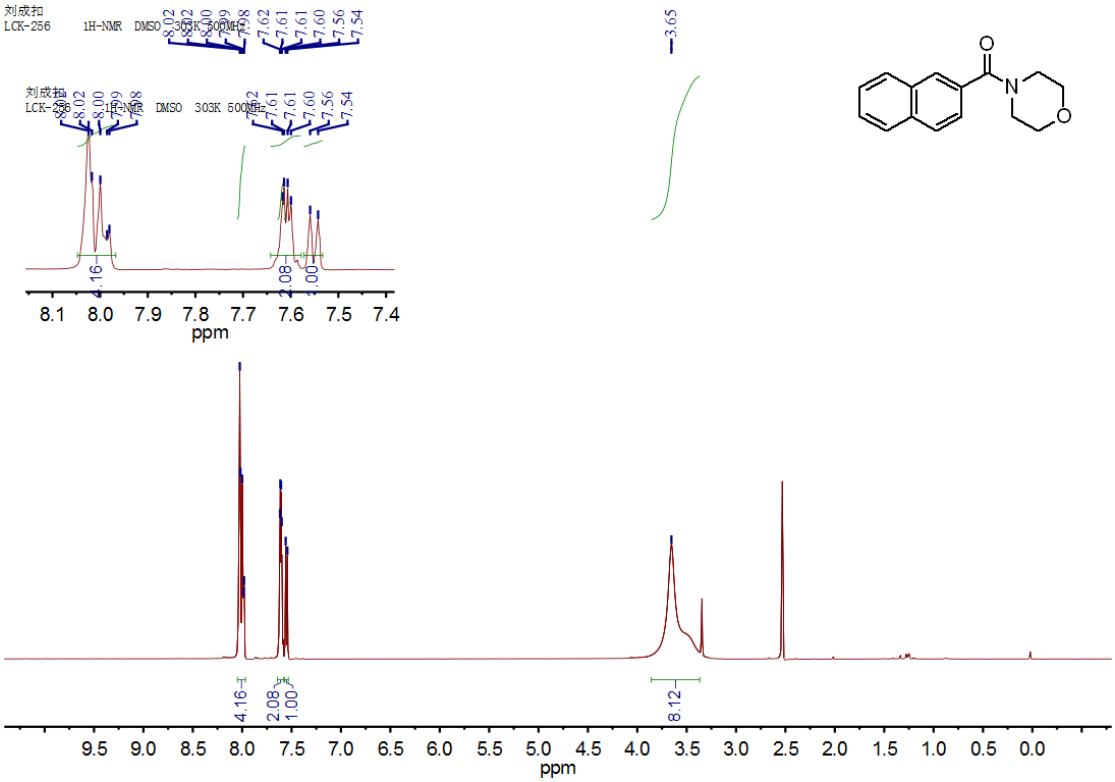

LCK-261 13C-NMR DMSO 303K 500MHz
168.19
137.16
134.94
129.02
96.25
65.94
ppm

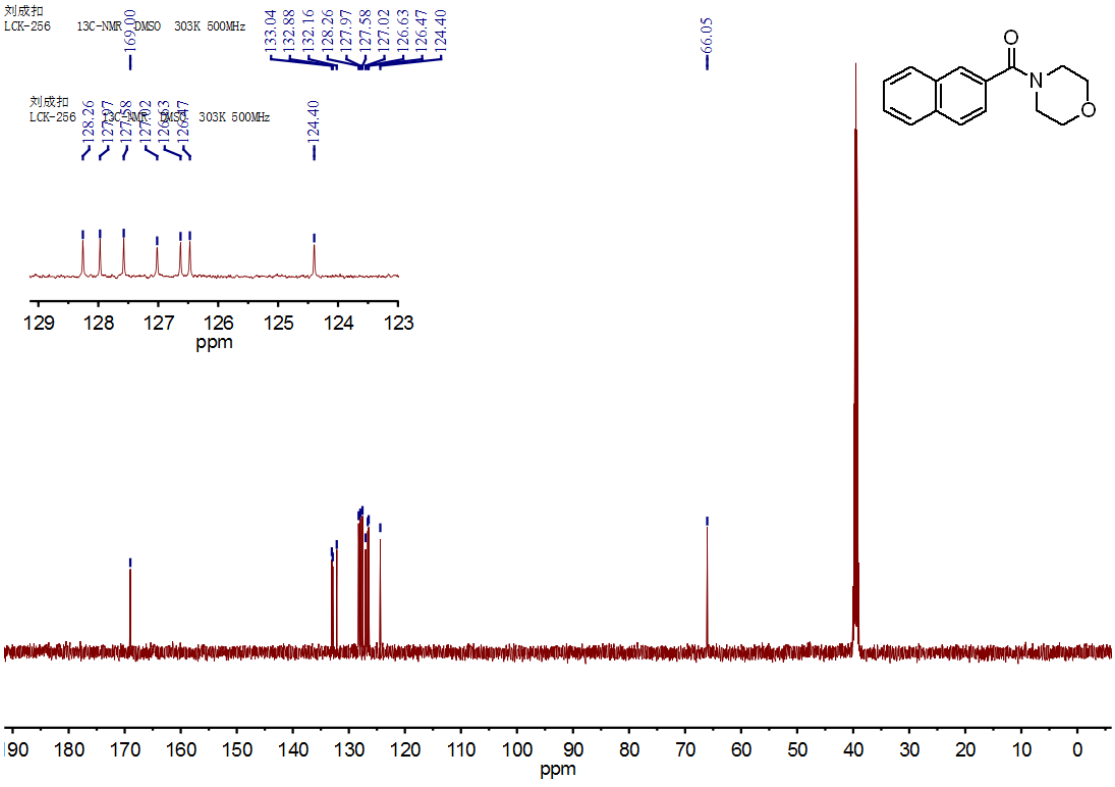

刘成扣
LCK-255 1H-NMR DMSO 303K 500MHz
8.05
8.03
7.58
7.57
3.90
3.75
3.67
3.59
3.33
2.00
2.00
3.02
6.00
2.06
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

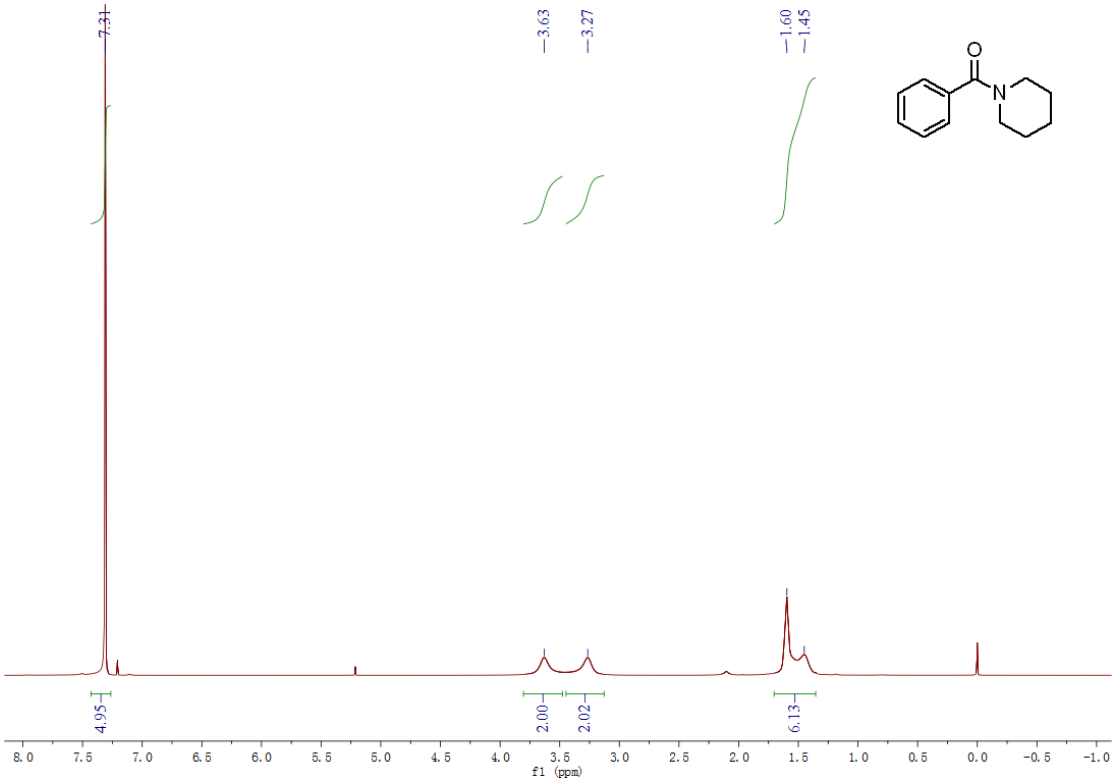

刘成扣
LCK-255 13C-NMR DMSO 303K 500MHz
168.55
168.44
140.56
130.86
129.76
127.76
66.47
52.76
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

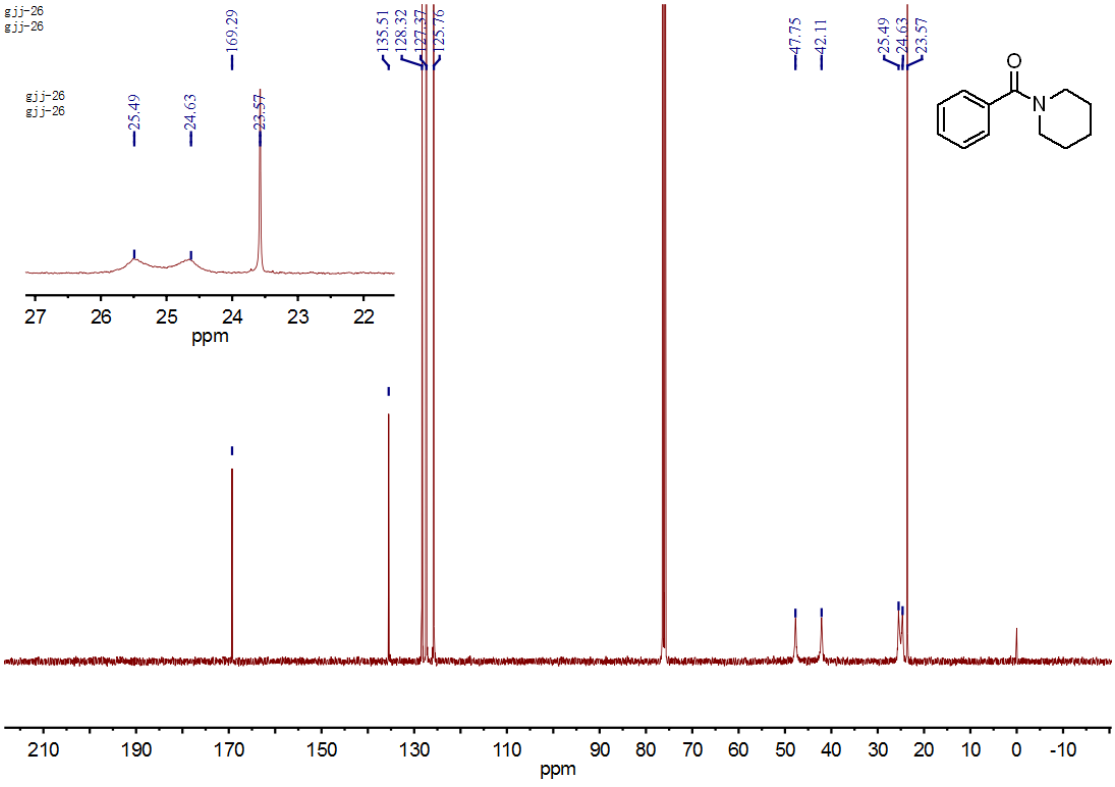

LCK-262 1H-NMR DMSO 303K 500MHz
2.00
1.99
6.00
2.03
ppm

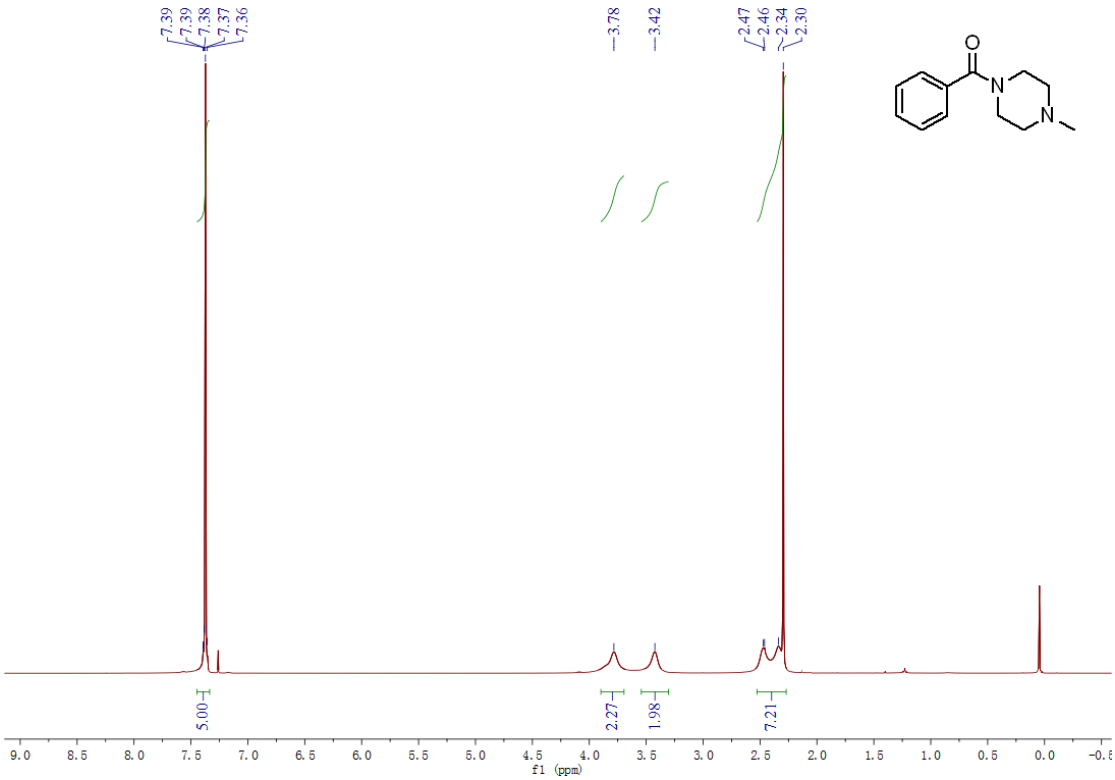

LCK-262 13C-NMR DMSO 303K 500MHz
140.20
130.58
130.32
130.07
129.82
128.27
127.62
125.93
125.90
125.45
123.29
121.12
66.45
47.94
42.39
131
127
123
ppm

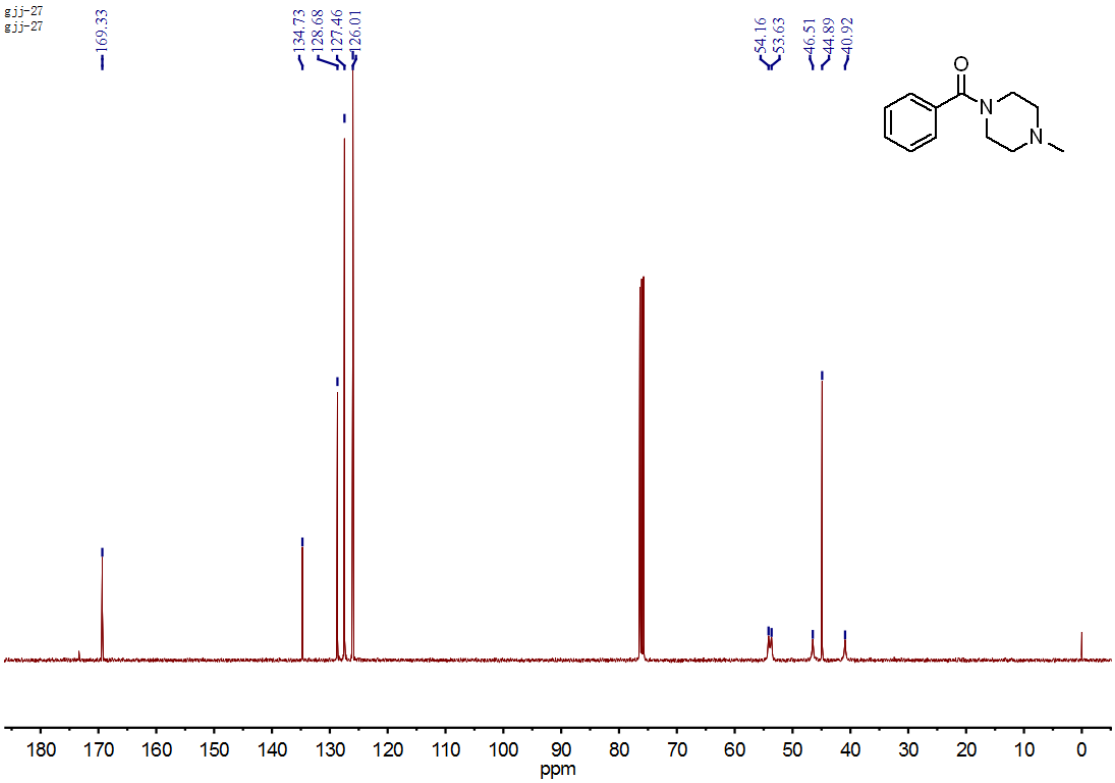

刘成扣
LCK-256
1H-NMR DMSO 303K 500MHz
8.02
8.00
7.99
7.98
7.62
7.61
7.61
7.60
7.56
7.54
3.65
4.16
2.08
1.00
8.12
ppm

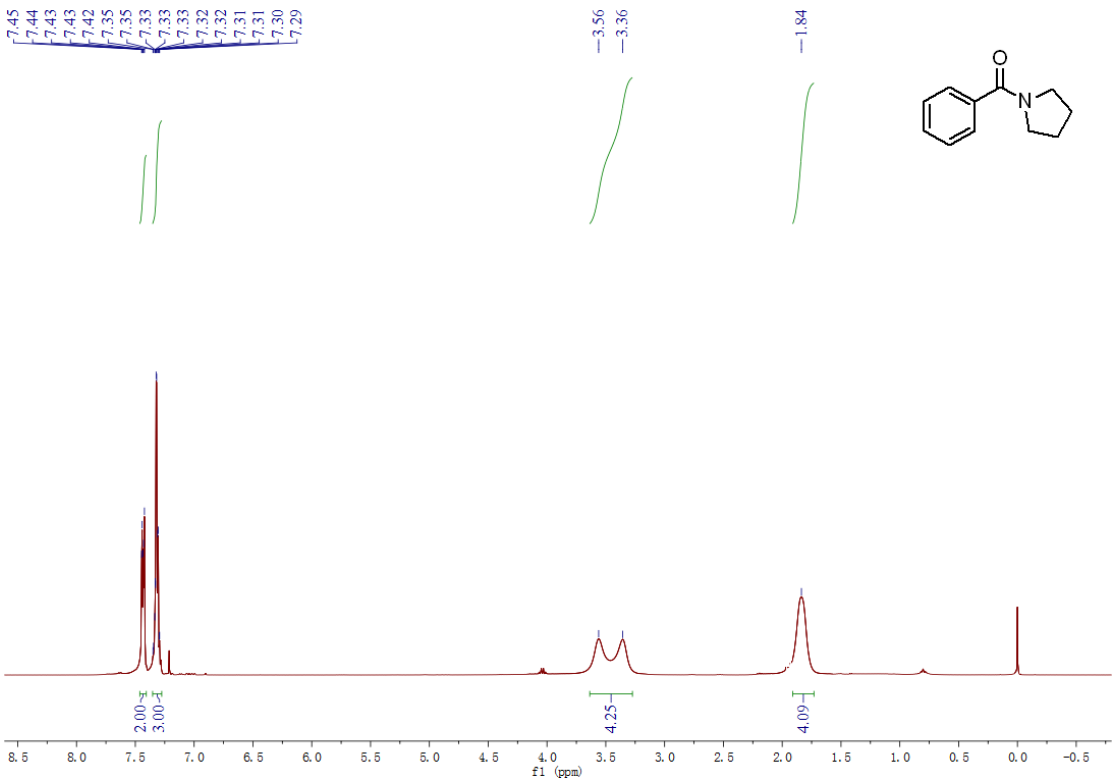

刘成扣
LCK-256
13C-NMR DMSO 303K 500MHz
169.00
133.04
132.88
132.16
128.26
127.97
127.58
127.02
126.63
126.47
124.40
66.05
ppm

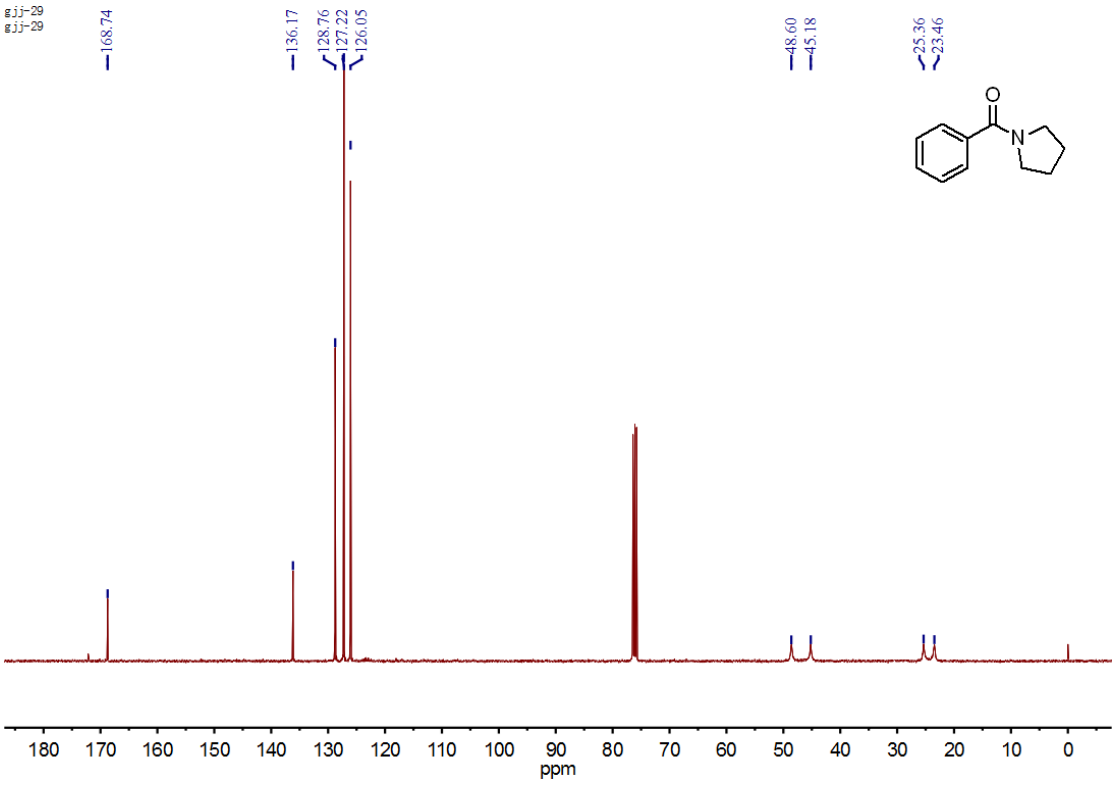

7.31
3.63
3.27
1.60
1.45
4.95
2.00
2.02
6.13
f1 (ppm)


gjj-26
gjj-26
169.29
135.51
128.32
127.32
125.76
47.75
42.11
25.49
24.63
23.57
ppm

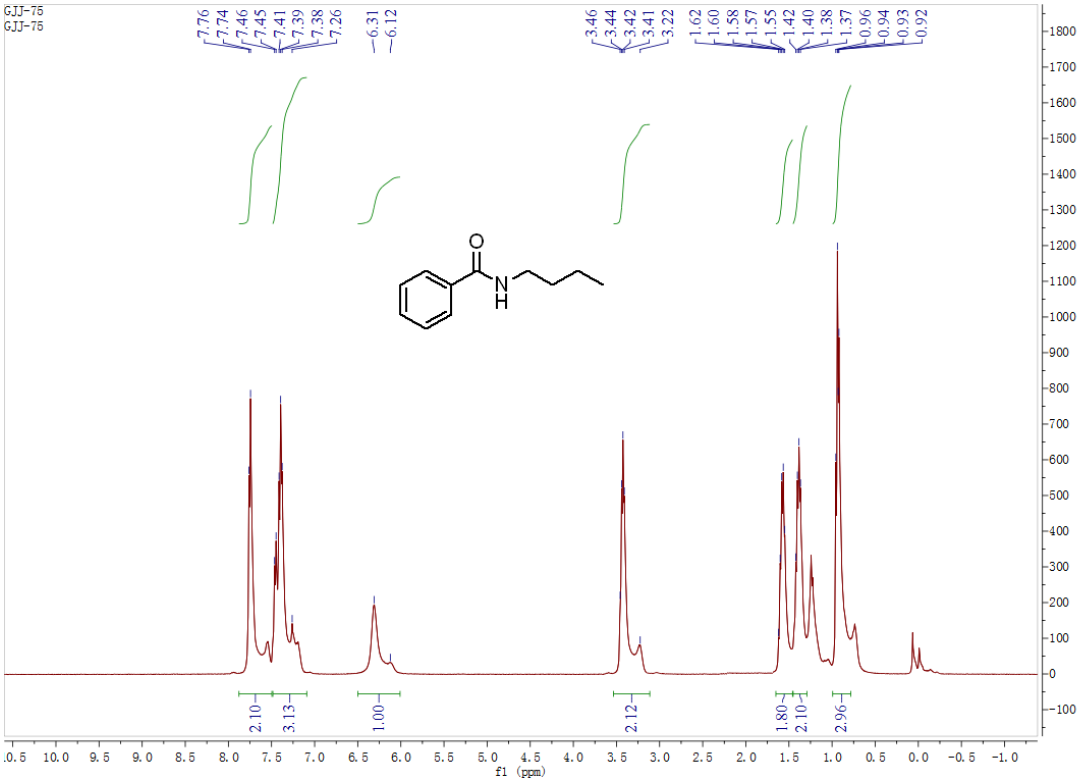

7.39
7.39
7.38
7.37
7.36
3.78
3.42
2.47
2.46
2.34
2.30
O
N
N
5.00
2.27
1.98
7.21
f1 (ppm)

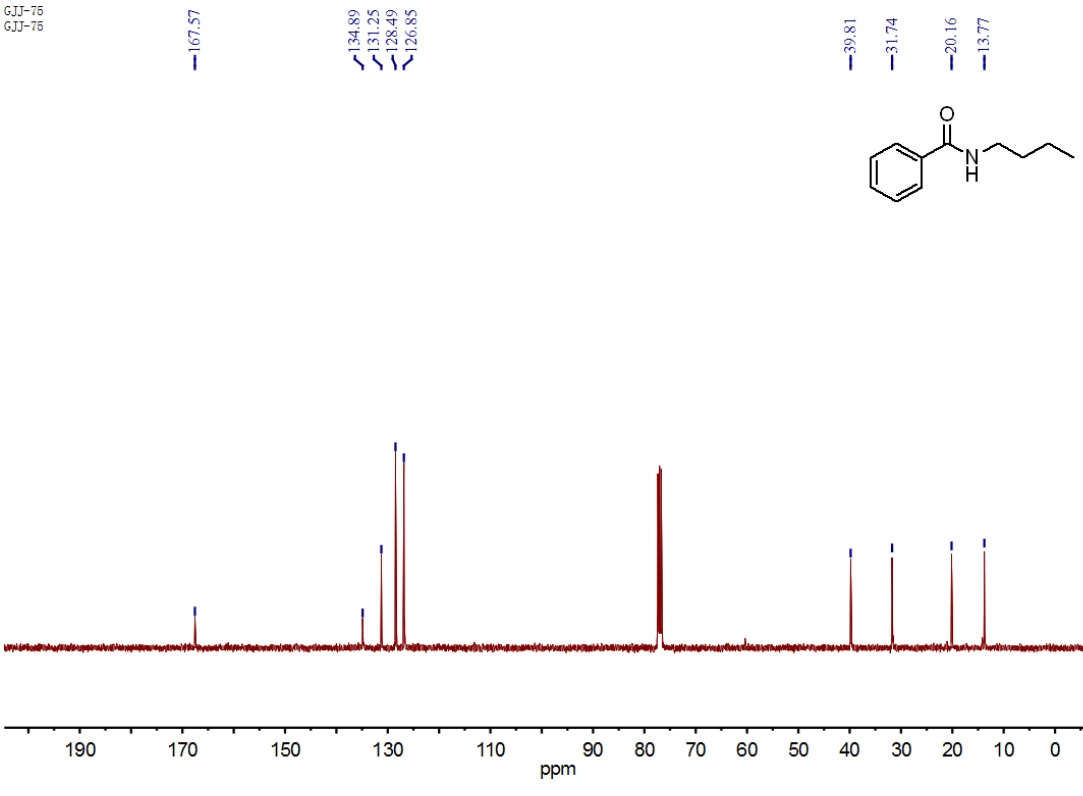

gjj-27
gjj-27
169.33
134.73
128.68
127.46
126.01
54.16
53.63
46.51
44.89
40.92
O
N
N
ppm

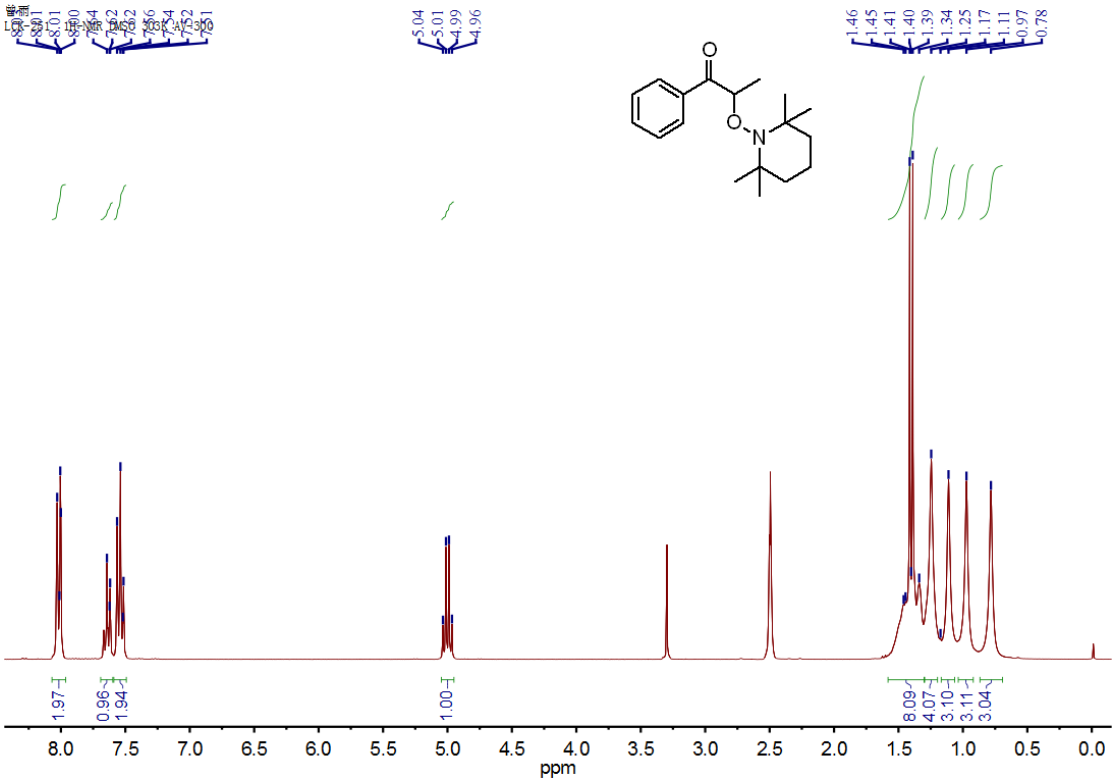

7.45
7.44
7.43
7.43
7.42
7.35
7.35
7.33
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.29
3.56
3.36
1.84
2.00
3.00
4.25
4.09
f1 (ppm)

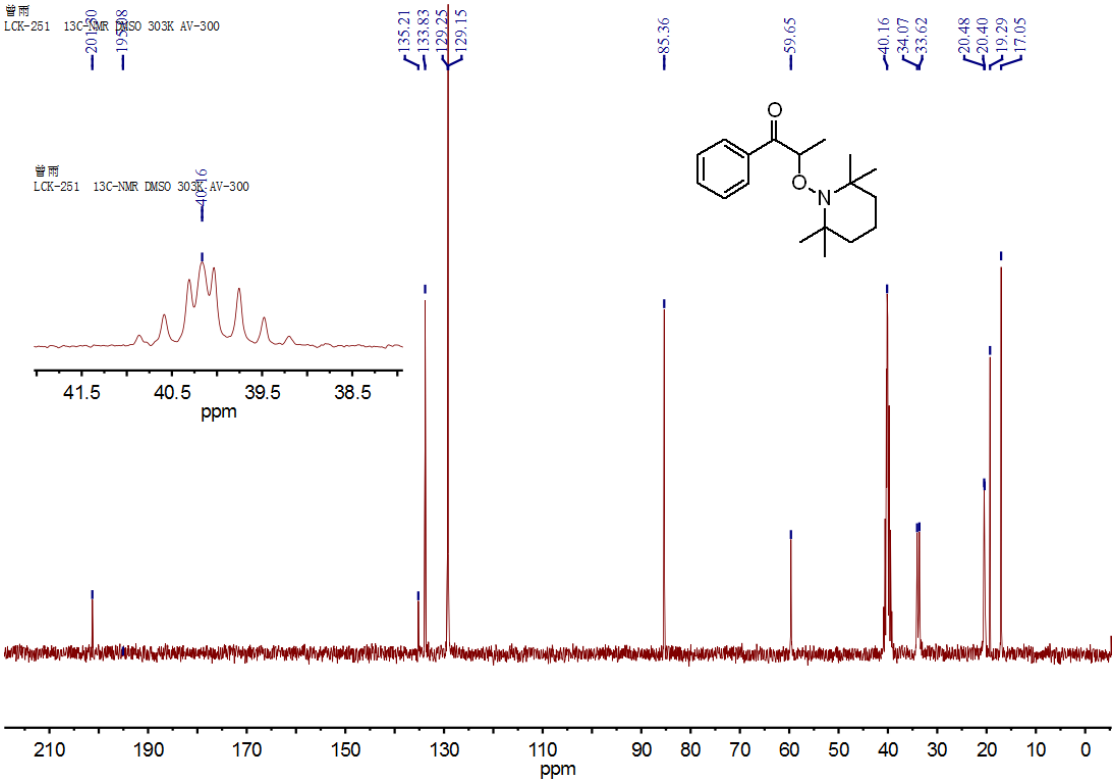

gjj-29
gjj-29
168.74
136.17
128.76
127.22
126.05
48.60
45.18
25.36
23.46
ppm

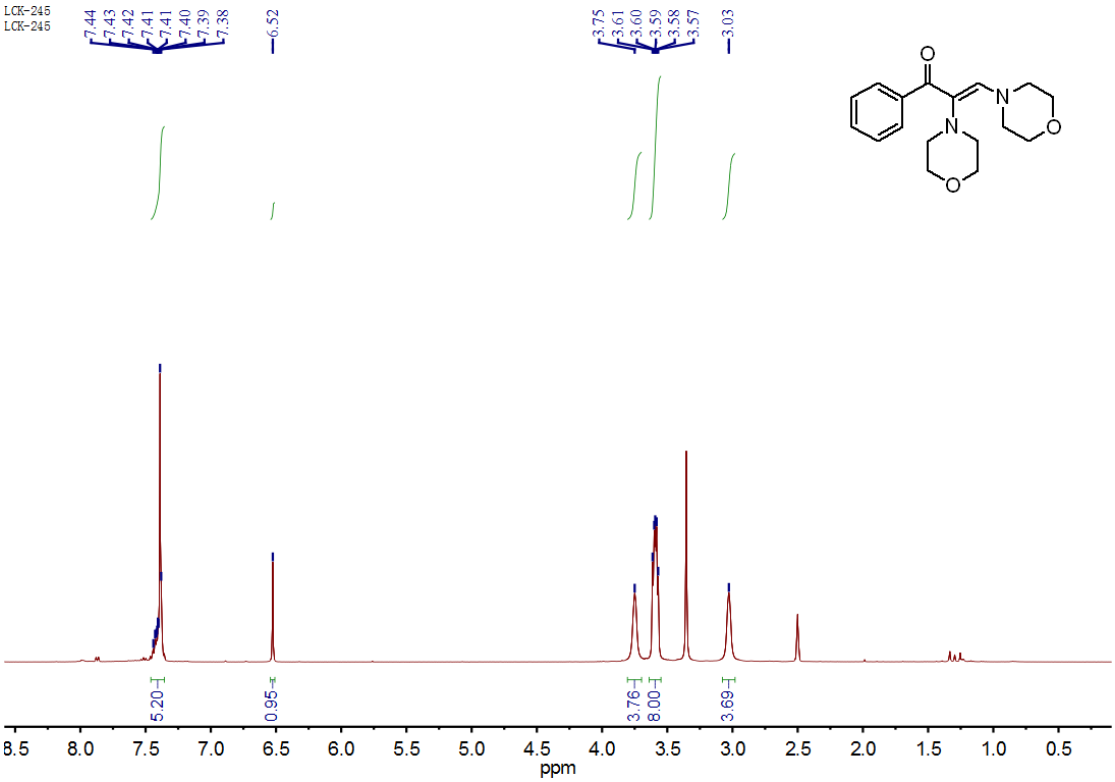

7.39
7.37
7.35
3.54
3.25
1.23
1.11
O
N
4.97
2.01
2.00
6.04
f1 (ppm)
gjj-33
gjj-33
170.32
136.24
128.08
127.37
125.26
42.29
38.21
13.18
11.91
O
N
ppm

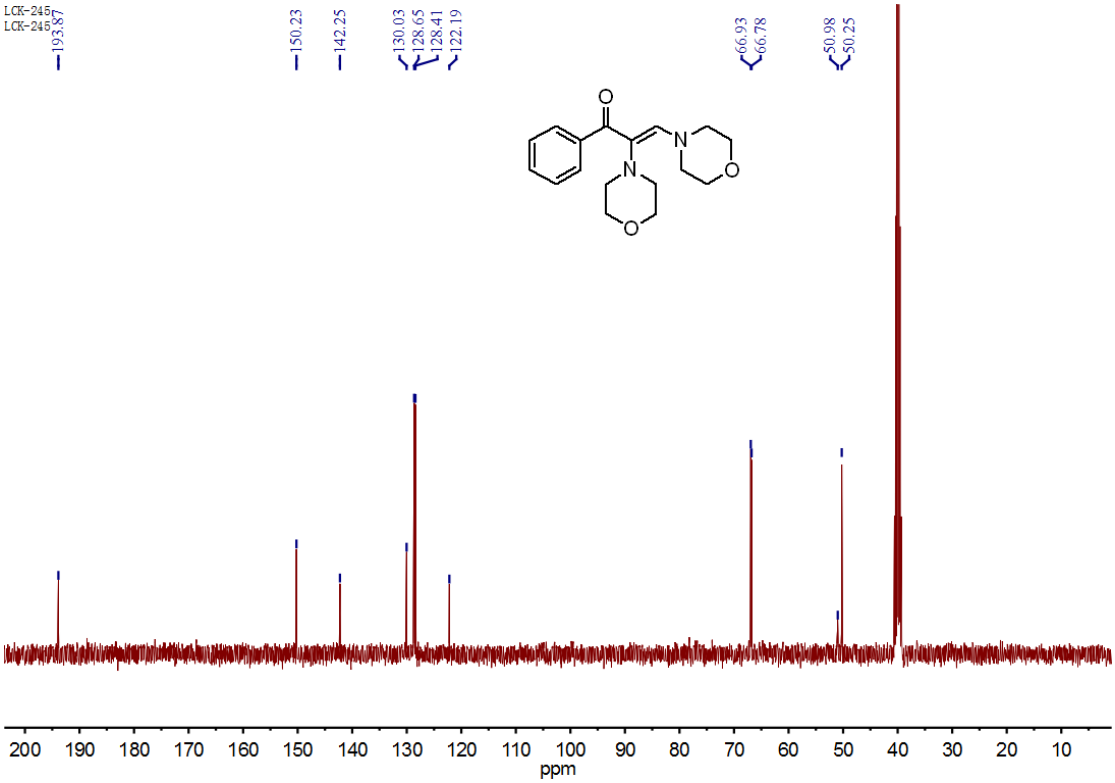

GJJ-75
GJJ-75
7.76
7.74
7.46
7.45
7.41
7.39
7.38
7.26
6.31
6.12
3.46
3.44
3.42
3.41
3.22
1.62
1.60
1.58
1.57
1.55
1.42
1.40
1.38
1.37
0.96
0.94
0.93
0.92
2.10
3.13
1.00
2.12
1.80
2.10
2.96
f1 (ppm)

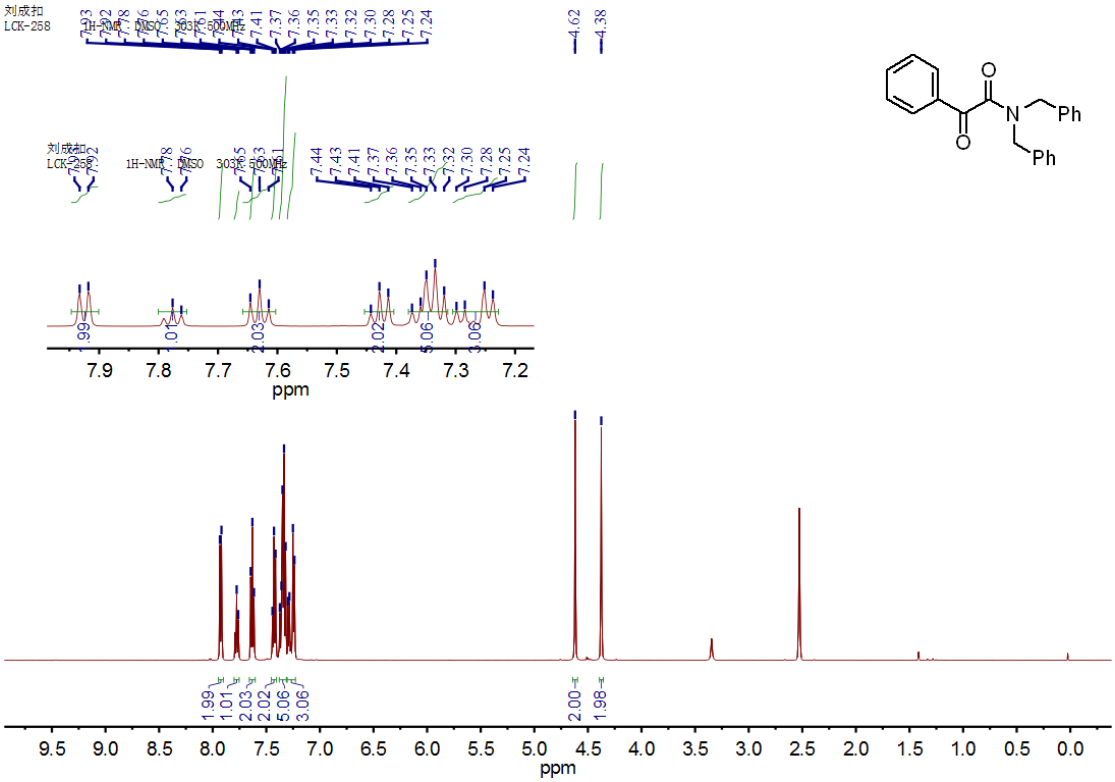

GJJ-75
GJJ-75
167.57
134.89
131.25
128.49
126.85
39.81
31.74
20.16
13.77
ppm

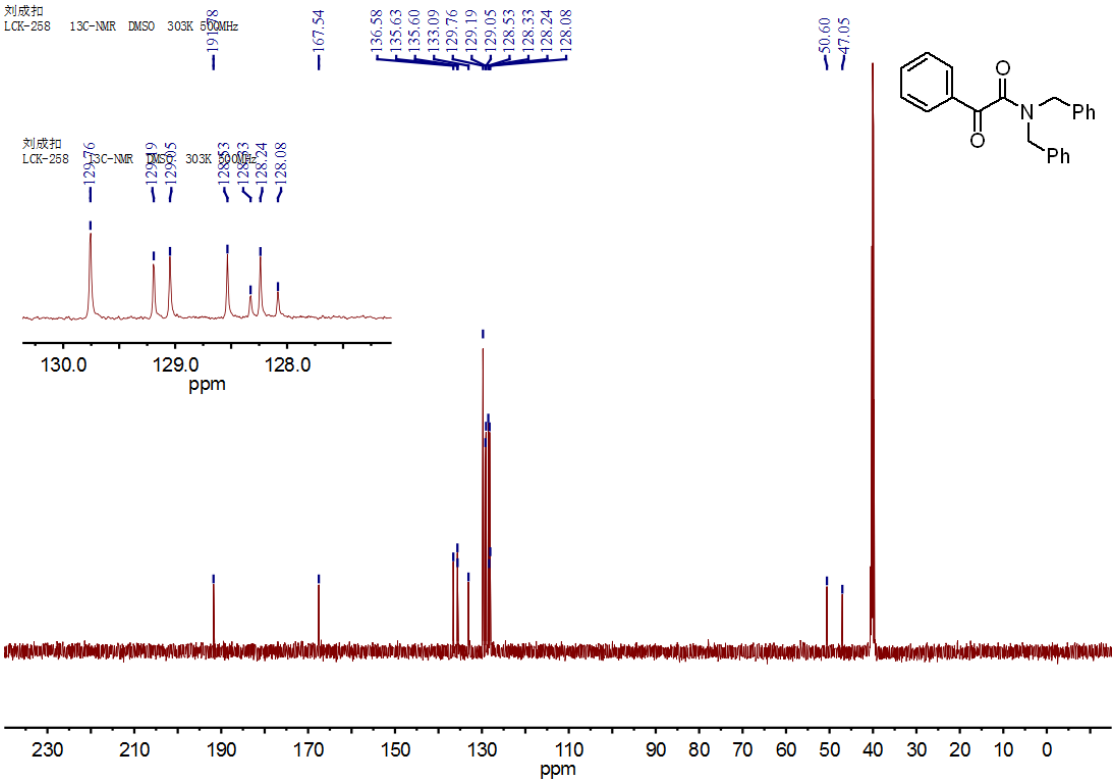

8.01
7.92
7.82
7.66
7.54
7.52
7.50
5.04
5.01
4.99
4.96
1.46
1.45
1.41
1.40
1.39
1.34
1.25
1.17
1.11
0.97
0.78
1.97
0.96
1.94
1.00
8.09
4.07
3.10
3.11
3.04
ppm

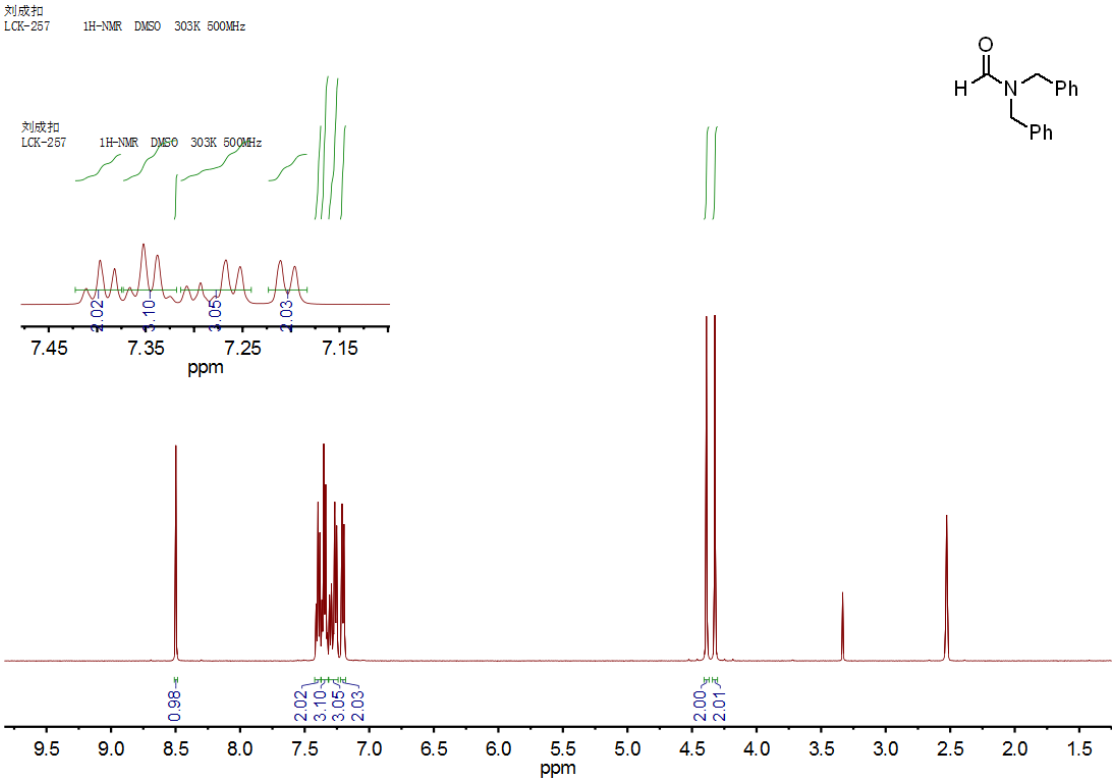

LCK-251 13C-NMR DMSO 303K AV-300
135.21
133.83
129.25
129.15
85.36
59.65
40.16
34.07
33.62
20.48
20.40
19.29
17.05
40.06
41.5
40.5
39.5
38.5
ppm

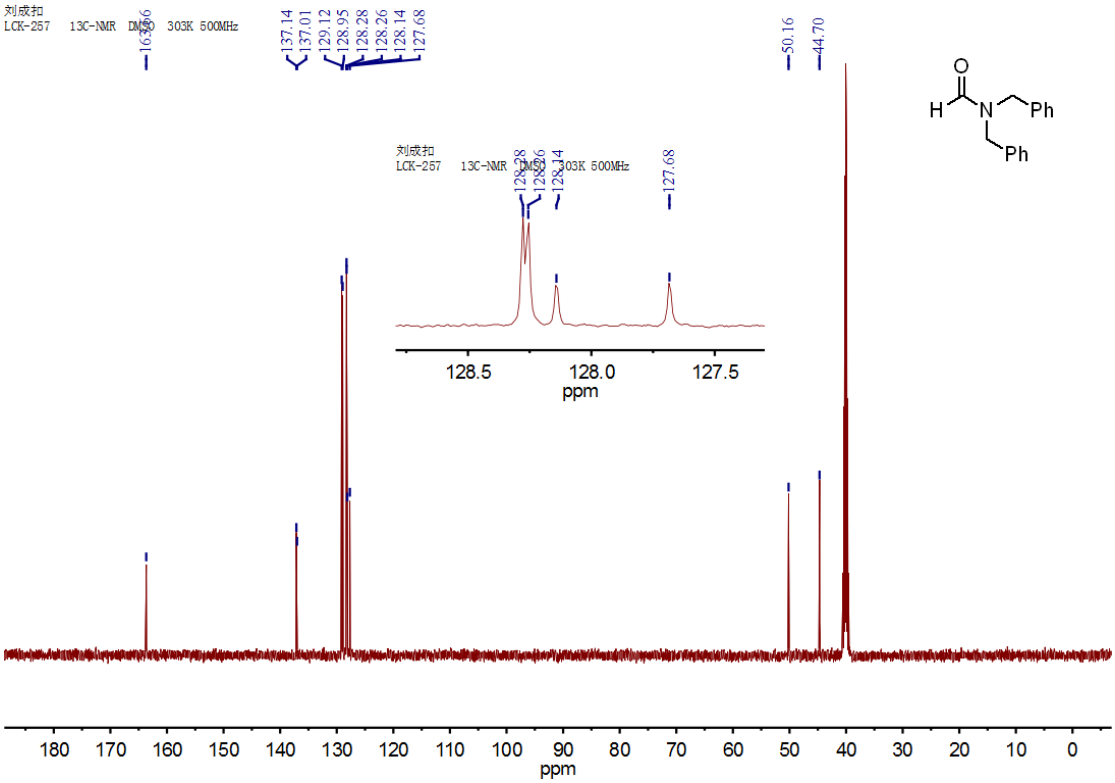

LCK-245
LCK-245
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.38
6.52
3.75
3.61
3.60
3.59
3.58
3.57
3.03
5.20
0.95
3.76
8.00
3.69
ppm


LCK-245
LCK-245
193.87
150.23
142.25
130.03
128.65
128.41
122.19
66.93
66.78
50.98
50.25
ppm


刘成扣
LCK-258
1H-NMR DMSO 303K 500MHz
ppm


刘成扣
LCK-258
13C-NMR DMSO 303K 500MHz
ppm


刘成扣
LCK-257 1H-NMR DMSO 303K 500MHz
O
H
N
Ph
Ph
2.02
3.10
3.05
2.03
7.45
7.35
7.25
7.15
ppm
0.98
2.02
3.10
3.05
2.03
2.00
2.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm


刘成扣
LCK-257 13C-NMR DMSO 303K 500MHz
137.14
137.01
129.12
128.95
128.28
128.26
128.14
127.68
50.16
44.70
O
H
N
Ph
Ph
128.28
128.26
128.14
127.68
128.5
128.0
127.5
ppm
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

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