Supporting Information

Synthesis of Phthalic Acid Derivatives via Pd-Catalyzed Alkoxycarbonylation of Aromatic C–H Bonds with Alkyl Chloroformates

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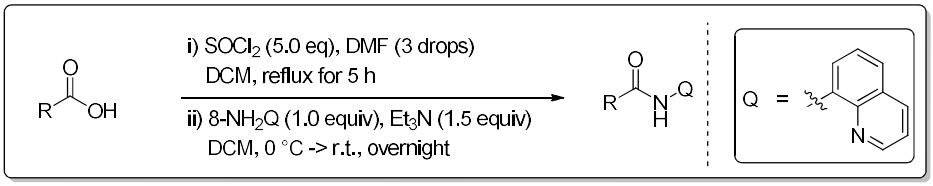
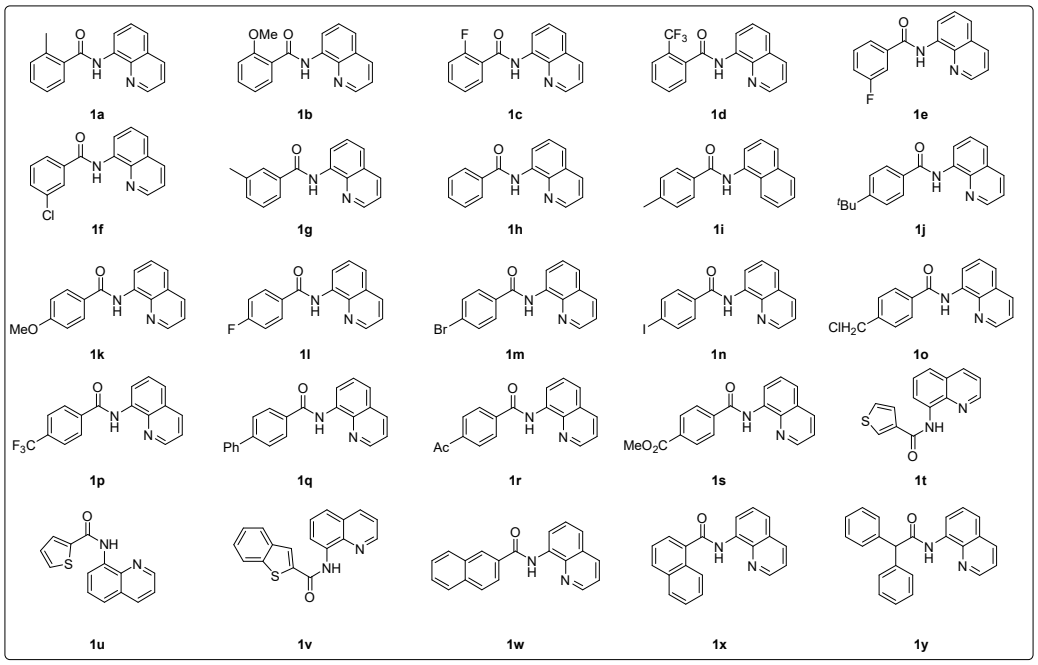
General Information: Unless otherwise noted, all commercial materials were used without further purification. Solvents obtained from Aladdin were used directly without further purification, and solvents obtained from other commercial suppliers were used after purification as specified in *Purification of Laboratory Chemicals, 6th Ed*. Nuclear magnetic resonance (NMR) spectra were recorded with a Bruker AVANCE 400MHz instrument. ^{1}H and ^{13}C chemical shifts are reported in ppm downfield of tetramethylsilane and referenced to residual solvent peak ($CHCl_3$ = 7.26 (^{1}H NMR), DMSO = 2.50 (^{1}H NMR), $CDCl_3$ = 77.16 (^{13}C NMR)) unless otherwise noted. ^{19}F NMR chemical shifts were determined relative to internal standard ($CFCl_3$ = 0.0 (^{19}F NMR)). Multiplicities are reported using the following abbreviations: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad resonance. High-resolution mass spectra for new compounds were recorded at Mass Spectrometry Facilities, Zhejiang University. X-ray diffraction experiments were performed at X-Ray Facilities, Zhejiang University.

Experimental Procedures:

Preparation of Aromatic Acid Substrates

1. General Procedures (GP1) for the Preparation of Aromatic Acid Substrates



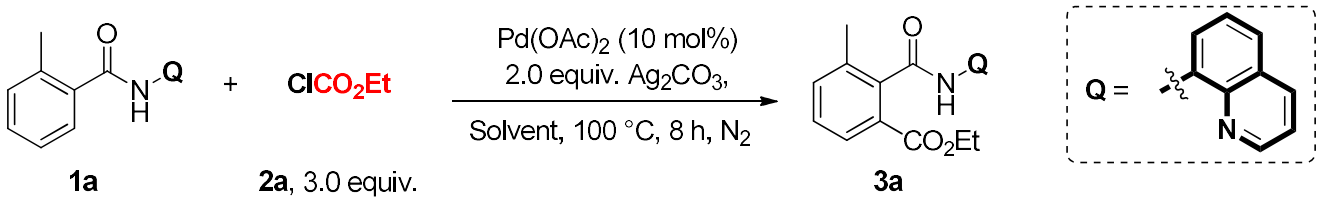


The Aromatic acid (24 mmol), thionyl chloride (8.70 mL, 120 mmol), and 3 drops of DMF were heated in DCM (50 mL) at 55 °C for 5 h. After the reaction, DCM and excess of thionyl chloride were removed under vacuum. The acid chloride was then dissolved in dry DCM (50 mL) and used for the coupling with 8-aminoquinoline (8-NH_2Q).

To a stirred solution of 8-NH_2Q (2.88g, 20 mmol) and Et_3N (4.0 mL, 30 mmol) in dry DCM (50 mL)was added the solution of the acid chloride (20 mmol) in DCM (50 mL) slowly at 0 °C. After the solution was stirred overnight, the mixture was quenched by DCM (30 mL). Then the mixture was filtered through a pad of Celite to remove the undissolved salts and washed by DCM (30 mL). The collected solution was then washed by aqueous HCl (50 mL, 1 M), saturated $NaHCO_3$ (50 mL), brine (50 mL), and dried over anhydrous $MgSO_4$. Evaporation of the solvent and purification by column chromatography or recrystallization afforded pure 8-aminoquinoline amides. All the substrates were prepared according to literature.[1]

Optimization of Reaction Conditions for Alkoxycarbonylation of C(sp^2)–H Bonds

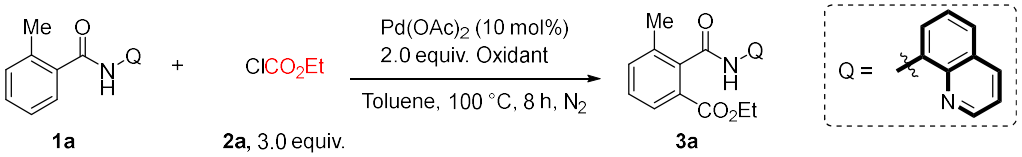
Table S1 Screening of solvents



Entry	Solvent	Yield of **3a** (%)	**1a** (%)
1	DCE	72	4
2	CH_3CN	n.d.	72
3	DMF	n.d.	76
4	DMSO	n.d	81
5	HFIP	n.d	64
6	CH_3OH	n.d.	62
7	*t*BuOH	38	37
8	*t*-AmylOH	55	20
9	HOAc	n.d	69
10	1, 4-dioxane	73	26
11	THF	39	21
12	Toluene	83 (81)[b]	--
13[c]	Toluene	42	28
14[d]	Toluene	trace	76%
15[e]	Toluene	76	--
16[f]	Toluene	76	--

[a]Reaction conditions: **1a** (0.15 mmol), **2a** (3.0 equiv), $Pd(OAc)_2$ (10 mol%), Ag_2CO_3 (0.3 mmol) in 2.0 mL solvent at 100 °C under N_2 for 8 h. Yields were determined by ^1H NMR using CH_2Br_2 as the internal standard. [b] Isolated yield in parenthesis. [c] 1.0 equiv. Ag_2CO_3 was used. [d] Without Ag_2CO_3. [e] 2.0 equiv.$ClCO_2Et$ was used. [f] Under air. n.d. = no detected.

Table S2 Screening of oxidant

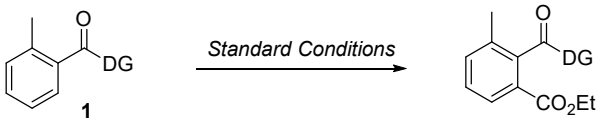


1a **2a**, 3.0 equiv. **3a**

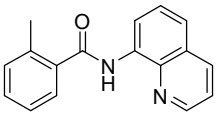
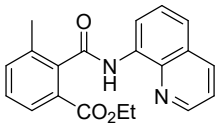
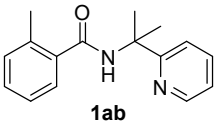
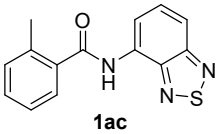
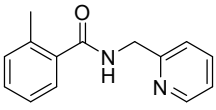
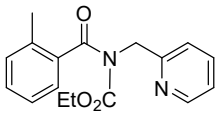
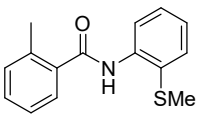
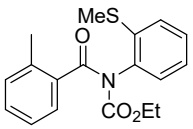
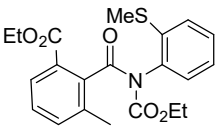
Entry	Oxidant	Yield (%)[a]	S.M. (%)
1	Oxone	8	51
2	TBHP	4	72
3	BQ	5	75
4	AgOAc	59	--
5	Ag_2O	8	23
6	$AgNO_3$	8	29
7	AgTFA	--	61
8	Ag_3PO_4	--	11
9	AgF	44	30
10	AgOTs	7	19

[a] Yields were determined by ^1H NMR using CH_2Br_2 as the internal standard.

Table S3 Screening of directing groups



1

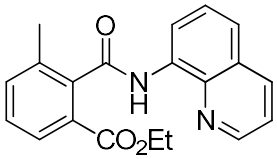
Entry	Starting Material	Product
1	 **1a**	 **3a**, 81%
2	 **1ab**	n.d.
3	 **1ac**	n.d.
4	 **1ad**	 **3ad**, 54%
5	 **1ae**	 **3ae**, 33% +  **3af**, 31%

Standard Conditions: **1** (0.15 mmol), $ClCO_2Et$ (0.45 mmol, 3.0 equiv), $Pd(OAc)_2$ (10 mol%), Ag_2CO_3 (0.3 mmol) in 2.0 mL toluene at 100 °C under N_2 for 8 h. isolated yield.

General Procedures (GP) for Alkoxycarbonylation of C(sp^2)–H Bonds

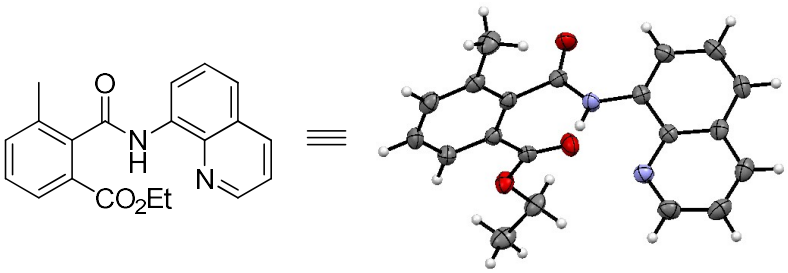
To a 50 mL Schlenk tube, were added **1** (0.15 mmol), $Pd(OAc)_2$ (3.5 mg, 0.015 mmol), Ag_2CO_3 (82.7 mg, 0.3 mmol), $ClCO_2R$ (0.45 mmol, 3.0 equiv.) and toluene (2.0 mL). The tube was sealed under N_2. The mixture was stirred at room temperature for 5 minutes then heated at 100 °C for 8 h. After cooling to room temperature, the reaction mixture was diluted with EtOAc (10 mL) and filtered through a pad of Celite. Evaporation of the solvent under vaccum and further purification column chromatography afforded the pure corresponding products.

Ethyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (3a)



The title compound **3a** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3a** was obtained as pale yellow solid (40.6 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 9.00 (dd, *J* = 7.6, 1.3 Hz, 1H), 8.77 – 8.65 (m, 1H), 8.15 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.53 (d, *J* = 8.2 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 7.44 – 7.38 (m, 2H), 4.20 (q, *J* = 7.1 Hz, 2H), 2.48 (s, 3H), 1.09 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 166.1, 148.3, 138.6, 138.5, 136.4, 135.9, 134.7, 129.0, 128.2, 128.1, 128.1, 127.5, 121.8, 121.7, 116.8, 61.4, 19.3, 14.0; HRMS (EI): calc. for $C_{20}H_{18}N_2O_3$ (M^+): 334.1312; Found: 334.1310;

X-ray Crystal Structure for 3a



Bond precision:	C-C = 0.0027 A		Wavelength=0.71073
Cell:	a=13.2268(10)	b=8.5916 (5)	c=15.6448 (13)
	α=90	*β*=108.955 (9)	*γ*=90
Temperature:	170 K		
	Calculated		Reported
Volume	1681.5 (2)		1681.5 (2)
Space group	P 21/c		P 1 21/c 1
Hall group	-P 2ybc		-P 2ybc
Moiety formula	C20 H18 N2 O3		C20 H18 N2 O3
Sum formula	C20 H18 N2 O3		C20 H18 N2 O3
Mr	334.36		334.36

Dx, g cm^{-3}	1.321	1.321
Z	4	4
Mu (mm^{-1})	0.090	0.090
F000	704.0	704.0
F000’	704.32	
h, k, l*max*	15, 10, 18	15, 10, 18
N*ref*	3070	3061
T*min,* T*max*	0.959, 0.972	0.968, 1.000
T*min*’	0.959	

Correction method= # Reported T Limits: T*min*=0.968 T*max*=1.000

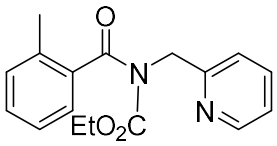
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(*max*)= 25.350

R(reflections)= 0.0426 (2326) wR2(reflections)= 0.1148(3061)

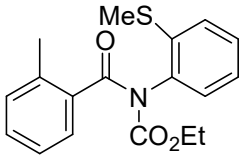
S = 1.034 N*par*= 228

Ethyl (2-methylbenzoyl)(pyridin-2-ylmethyl)carbamate (3ad)



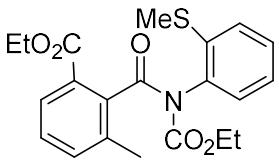
The title compound **3ad** was prepared according to GP and was purified by column chromatography (petroleum ether: ethyl acetate = 6: 1). **3ad** was obtained as an oil (24.0 mg, 54%).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, J = 5.0 Hz, 1H), 7.66 (td, J = 7.7, 1.8 Hz, 1H), 7.34 (d, J = 7.7 Hz, 1H), 7.32 – 7.26 (m, 2H), 7.18 (m, 3H), 5.21 (s, 2H), 3.96 (q, J = 7.1 Hz, 2H), 2.38 (s, 3H), 0.83 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 172.83, 156.87, 154.53, 149.53, 138.12, 136.60, 135.06, 130.40, 129.50, 125.87, 125.39, 122.24, 121.20, 63.09, 49.38, 19.44, 13.49. HRMS (EI): calc. for $C_{17}H_{18}N_2O_3$(M^+): 298.1312; Found: 298.1315.

Ethyl (2-methylbenzoyl)(2-(methylthio)phenyl)carbamate (3ae)



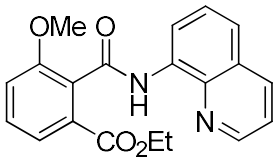
The title compound **3ae** was prepared according to GP and was purified by column chromatography (petroleum ether: ethyl acetate = 8: 1). **3ae** was obtained as pale yellow oil (16.1 mg, 33%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.42 – 7.36 (m, 2H), 7.32 (td, *J* = 7.5, 1.4 Hz, 1H), 7.29 – 7.20 (m, 4H), 4.03 (q, *J* = 6.9 Hz, 2H), 2.48 (s, 3H), 2.48 (s, 3H), 0.96 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 153.6, 138.0, 137.4, 136.5, 135.7, 130.6, 129.8, 129.4, 129.3, 127.7, 126.3, 126.1, 125.4, 63.3, 19.7, 15.9, 13.8. HRMS (EI): calc. for $C_{18}H_{19}NSO_3$(M^+): 329.1080; Found: 329.1083.

Ethyl 2-((ethoxycarbonyl)(2-(methylthio)phenyl)carbamoyl)-3-methylbenzoate (3af)



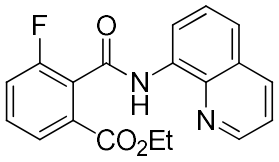
The title compound **3af** was prepared according to GP and was purified by column chromatography (petroleum ether: ethyl acetate = 8: 1). **3af** was obtained as pale yellow oil (18.3 mg, 31%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 7.8 Hz, 1H), 7.79 (d, J = 7.7 Hz, 1H), 7.45 – 7.39 (m, 2H), 7.38 – 7.30 (m, 3H), 4.47 – 4.28 (m, 2H), 4.12 – 3.89 (m, 2H), 2.56 (s, 3H), 2.48 (s, 3H), 1.39 (t, J = 7.1 Hz, 3H), 0.99 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.4, 166.2, 153.1, 140.6, 137.6, 135.9, 135.3, 134.6, 129.6, 129.2, 128.0, 127.2, 126.6, 126.3, 126.1, 63.0, 61.3, 19.8, 15.7, 14.4, 13.9. HRMS (EI): calc. for $C_{21}H_{23}NSO_5(M^+)$: 401.1291; Found: 401.1290.

Ethyl 3-methoxy-2-(quinolin-8-ylcarbamoyl)benzoate (3b)



The title compound **3b** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3b** was obtained as a white solid (32.0 mg, 61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.22 (s, 1H), 8.99 (dd, J = 7.6, 1.1 Hz, 1H), 8.74 (dd, J = 4.2, 1.6 Hz, 1H), 8.16 (dd, J = 8.3, 1.5 Hz, 1H), 7.59 (t, J = 7.6 Hz, 2H), 7.53 (dd, J = 8.2, 1.1 Hz, 1H), 7.48 (t, J = 8.1 Hz, 1H), 7.42 (dd, J = 8.3, 4.2 Hz, 1H), 7.18 (d, J = 8.1 Hz, 1H), 4.25 (q, J = 7.1 Hz, 2H), 3.90 (s, 3H), 1.12 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 165.3, 156.9, 148.2, 138.6, 136.4, 135.1, 131.1, 130.6, 128.1, 127.7, 127.5, 122.3, 121.7, 121.6, 116.9, 115.2, 61.6, 56.4, 14.0; HRMS (EI): calc. for $C_{20}H_{18}N_2O_4(M^+)$: 350.1261; Found: 350.1258.

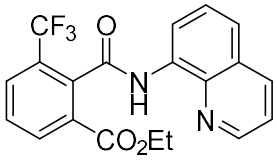
Ethyl 3-fluoro-2-(quinolin-8-ylcarbamoyl)benzoate (3c)



The title compound **3c** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3c** was obtained as a white solid (36.0 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.12 (s, 1H), 8.97 (d, J = 7.2 Hz, 1H), 8.80 – 8.71 (m, 1H), 8.19 (dd, J = 8.2, 1.1 Hz, 1H), 7.88 (d, J = 7.8 Hz, 1H), 7.65 – 7.50 (m, 3H), 7.46 (dd, J = 8.3, 4.2 Hz, 1H), 7.39 (t, J = 8.6 Hz, 1H), 4.28 (q, J = 7.1 Hz, 2H), 1.14 (t, J = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.0. ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3 (d, $J_{C\text{-}F}$ = 3.1 Hz), 162.7, 159.4 (d, $J_{C\text{-}F}$ = 249.8 Hz), 148.4, 138.5, 136.5, 134.5, 131.2 (d, $J_{C\text{-}F}$ = 3.2 Hz) , 131.0 (d, $J_{C\text{-}F}$ = 8.4 Hz), 128.1, 127.6, 126.7 (d, $J_{C\text{-}F}$ = 20.0 Hz), 126.3 (d, $J_{C\text{-}F}$ = 3.2 Hz),

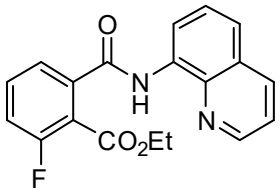
122.2, 121.8, 120.2(d, J_{C-F} = 22.3 Hz), 117.1, 61.9, 13.9. HRMS (EI): calc. for $C_{19}H_{15}FN_2O_3(M^+)$: 338.1061; Found: 338.1063;

Ethyl 2-(quinolin-8-ylcarbamoyl)-3-(trifluoromethyl)benzoate (3d)



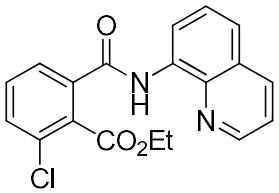
The title compound **3d** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3d** was obtained as a white solid (30.3mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.93 (dd, J = 7.4, 1.4 Hz, 1H), 8.73 (dd, J = 4.2, 1.6 Hz, 1H), 8.28 (d, J = 7.9 Hz, 1H), 8.17 (dd, J = 8.3, 1.5 Hz, 1H), 7.95 (d, J = 7.9 Hz, 1H), 7.67 (t, J = 7.9 Hz, 1H), 7.64 – 7.53 (m, 2H), 7.43 (dd, J = 8.3, 4.2 Hz, 1H), 4.23 (q, J = 7.1 Hz, 2H), 1.09 (t, J = 7.1 Hz, 4H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.0. ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.2, 164.6, 148.4, 138.5, 136.7(q, J_{C-F} = 4.5 Hz), 136.5, 134.6, 134.3, 130.7, 130.2(q, J_{C-F} = 4.9 Hz), 129.7, 128.7(q, J_{C-F} = 31.9 Hz), 128.1, 127.6, 123.5(d, J_{C-F} = 275.6 Hz), 122.2, 121.8, 117.1, 62.2, 13.9. HRMS (EI): calc. for $C_{20}H_{15}FN_2O_3(M^+)$: 388.1029; Found: 388.1028.

Ethyl 2-fluoro-6-(quinolin-8-ylcarbamoyl)benzoate (3e)



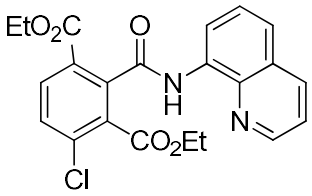
The title compound **3e** was prepared under the optimized conditions and purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3e** was obtained as a a white solid (21.3 mg, 42%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.91 (dd, J = 7.2, 1.2 Hz, 1H), 8.76 (dd, J = 4.2, 1.5 Hz, 1H), 8.18 (dd, J = 8.3, 1.6 Hz, 1H), 8.07 (dd, J = 8.7, 5.4 Hz, 1H), 7.65 – 7.53 (m, 2H), 7.46 (dd, J = 8.3, 4.2 Hz, 1H), 7.37 (dd, J = 8.3, 2.5 Hz, 1H), 7.23 (td, J = 8.3, 2.6 Hz, 1H), 4.24 (q, J = 7.1 Hz, 2H), 1.12 (t, J = 7.1 Hz, 3H). ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.42. ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3 (d, J_{C-F} = 6.7 Hz), 165.5, 164.7 (d, J_{C-F} = 256.7 Hz), 148.5, 141.4(d, J_{C-F} = 7.6 Hz), 138.5, 136.5, 134.5, 133.4(d, J_{C-F} = 9.1 Hz), 128.1, 127.6, 125.4(d, J_{C-F} = 3.4 Hz), 122.23, 121.9, 117.0, 116.9(d, J_{C-F} = 21.5 Hz), 115.3 (d, J_{C-F} = 23.6 Hz), 61.8, 14.0. HRMS (EI): calc. for $C_{19}H_{15}FN_2O_3$ (M^+): 338.1061; Found: 338.1060.

Ethyl 2-chloro-6-(quinolin-8-ylcarbamoyl)benzoate (3fa)



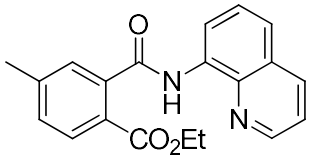
The title compound **3fa** was prepared according to **GP3** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3fa** was obtained as a white solid (23.9 mg, 45%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.90 (dd, *J* = 7.1, 1.0 Hz, 1H), 8.76 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.18 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 2.0 Hz, 1H), 7.62 – 7.54 (m, 2H), 7.52 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.24 (q, *J* = 7.1 Hz, 2H), 1.12 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 165.6, 148.4, 140.3, 138.7, 138.5, 136.5, 134.5, 132.1, 130.0, 128.09, 123.0, 127.6, 127.6, 122.2, 121.9, 117.0, 61.9, 14.0; HRMS (EI): calc. for $C_{19}H_{15}ClN_2O_3$ (M^+): 354.0766; Found: 354.0752

Diethyl 4-chloro-2-(quinolin-8-ylcarbamoyl)isophthalate (3fb)



The title compound **3fb** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3f'** was obtained as a white solid (9.6 mg, 15%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.86 (dd, *J* = 6.9, 2.1 Hz, 1H), 8.76 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.04 (d, *J* = 7.6 Hz, 1H), 7.65 – 7.53 (m, 3H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.39 – 3.90 (m, 4H), 1.13 (t, *J* = 7.1 Hz, 3H), 1.07 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.1, 165.0, 164.5, 148.5, 138.5, 138.5, 136.4, 136.0, 134.5, 133.0, 132.7, 131.0, 128.1, 128.0, 127.5, 122.3, 121.9, 117.0, 62.6, 62.2, 13.9; HRMS (EI): calc. for $C_{19}H_{15}ClN_2O_3$ (M^+): 354.0766; Found: 354.0760.

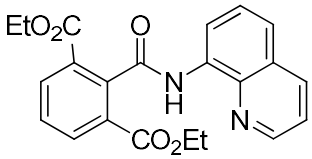
Ethyl 4-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (3g)



The title compound **3g** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3g** was obtained as a white solid (38.6 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 8.94 (d, *J* = 7.4 Hz, 1H), 8.74 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.56 – 7.50 (m, 1H), 7.46 (s, 1H), 7.43 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 4.22 (q, *J* = 7.1 Hz, 2H), 2.45 (s, 3H), 1.11 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 166.4, 148.3, 143.2, 139.0, 138.5, 136.4, 134.8, 130.6, 130.5, 128.3,

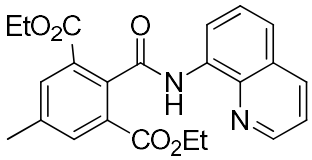
128.1, 127.6, 126.3, 121.9, 121.7, 116.8, 61.4, 21.6, 14.0; HRMS (EI): calc. for $C_{20}H_{18}N_2O_3$ (M^+): 334.1312; Found: 334.1314;

Diethyl 2-(quinolin-8-ylcarbamoyl)isophthalate (**3h**)



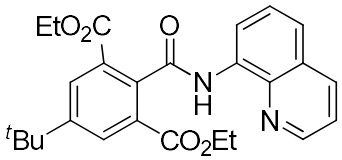
The title compound **3h** was prepared according to **GP** and was purified by column chromatography (petroleum ether: tetrahydrofuran = 3: 1). **3h** was obtained as a white solid (47.0 mg, 80%). ^{1}H NMR (400 MHz, CDCl3) δ 9.85 (s, 1H), 8.89 (dd, *J* = 7.6, 1.2 Hz, 1H), 8.63 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.18 (d, *J* = 7.9 Hz, 2H), 8.09 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.54 (td, *J* = 7.8, 2.5 Hz, 2H), 7.46 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.34 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.15 (q, *J* = 7.1 Hz, 4H), 1.01 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 165.6, 148.2, 136.4, 135.0, 134.6, 129.9, 129.3, 128.1, 127.7, 121.7, 116.9, 61.9, 13.9. HRMS (EI): calc. for $C_{22}H_{20}N_2O_5$ (M^+): 392.1367; Found: 392.1368.

Diethyl 5-methyl-2-(quinolin-8-ylcarbamoyl)isophthalate (**3i**)



The title compound **3i** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3i** was obtained as a white solid (46.3 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.95 (dd, *J* = 7.6, 0.8 Hz, 1H), 8.69 (d, *J* = 4.1 Hz, 1H), 8.14 (d, *J* = 8.2 Hz, 1H), 8.04 (s, 2H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.51 (d, *J* = 8.2 Hz, 1H), 7.40 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.20 (q, *J* = 7.1 Hz, 4H), 2.48 (s, 3H), 1.07 (t, *J* = 7.1 Hz, 6H).^{13}C NMR (101 MHz, $CDCl_3$) δ 166.8, 165.7, 148.2, 139.6, 138.4, 136.6, 136.3, 135.0, 134.9, 129.8, 128.0, 127.6, 121.6, 121.5, 116.7, 61.8, 21.1, 13.9; HRMS (EI): calc. for $C_{23}H_{22}N_2O_5$(M^+): 406.4306; Found: 406.4301.

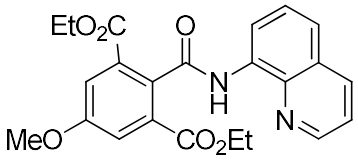
Diethyl 5-(tert-butyl)-2-(quinolin-8-ylcarbamoyl)isophthalate (**3j**)



The title compound **3j** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate =4: 1). **3j** was obtained as a white solid (51.8 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.90 (s, 1H), 8.95 (dd, *J* = 7.6, 1.1 Hz, 1H), 8.69 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.24 (s, 2H), 8.14 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.51 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.40 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.20 (q, *J* = 7.1 Hz, 4H), 1.40 (s, 9H), 1.05 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ

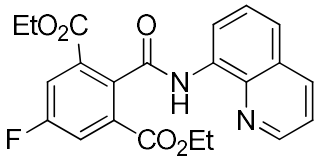
166.9, 166.1, 152.8, 148.2, 138.4, 136.4, 136.4, 135.0, 131.5, 129.7, 128.1, 127.6, 121.6, 121.6, 116.7, 61.8, 35.1, 31.1, 13.9; HRMS (EI): calc. for $C_{26}H_{28}N_2O_5$ (M^+): 448.1993; Found: 448.1990.

Diethyl 5-methoxy-2-(quinolin-8-ylcarbamoyl)isophthalate (3k)



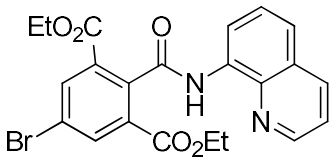
The title compound **3k** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3k** was obtained as a white solid (49.2 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 8.94 (dd, *J* = 7.6, 1.2 Hz, 1H), 8.70 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.14 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.72 (s, 2H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.51 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.40 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.20 (q, *J* = 7.1 Hz, 4H), 3.92 (s, 3H), 1.06 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 165.5, 159.6, 148.2, 138.5, 136.4, 135.1, 131.9, 131.5, 128.1, 127.7, 121.6, 121.5, 119.6, 116.7, 62.0, 56.0, 13.9; HRMS (EI): calc. for $C_{23}H_{22}N_2O_6$ (M^+): 422.1472; Found: 422.1470.

Diethyl 5-fluoro-2-(quinolin-8-ylcarbamoyl)isophthalate (3l)



The title compound **3l** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3l** was obtained as a white solid (46.8 mg, 76%). ^{11}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.93 (d, *J* = 7.5 Hz, 1H), 8.71 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.42 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.23 (q, *J* = 7.1 Hz, 4H), 1.09 (t, *J* = 7.1 Hz, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.6 (s, 1F); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 164.4 (d, $J_{C\text{-}F}$ = 2.5 Hz), 162.0 (d, $J_{C\text{-}F}$ = 252.4 Hz), 148.3, 138.4, 136.5, 135.5 (d, $J_{C\text{-}F}$ = 3.9 Hz), 134.8, 132.2 (d, $J_{C\text{-}F}$ = 7.2 Hz), 128.1, 127.7, 121.8, 121.7, 121.6 (d, $J_{C\text{-}F}$ = 23.5 Hz), 116.9, 62.4, 13.9. HRMS (EI): calc. for $C_{22}H_{19}FN_2O_5$ (M^+): 410.1273; Found: 410.1360.

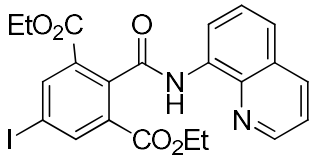
Diethyl 5-bromo-2-(quinolin-8-ylcarbamoyl)isophthalate (3m)



The title compound **3m** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 3:1). **3m** was obtained as a white solid (24.7 mg, 35%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 8.92 (d, *J* = 7.4 Hz, 1H), 8.71 (dd, *J* = 4.1, 1.3 Hz, 1H), 8.37 (s, 2H), 8.17 (dd,

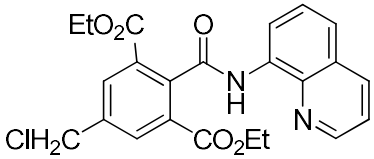
J = 8.2, 1.2 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.2 Hz, 1H), 4.23 (q, *J* = 7.1 Hz, 4H), 1.10 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 164.3, 148.3, 138.5, 137.9, 137.3, 136.5, 134.8, 131.5, 128.1, 127.7, 123.3, 121.9, 121.8, 116.9, 62.4, 13.9; HRMS (EI): calc. for $C_{22}H_{19}BrN_2O_5$ (M^+): 470.0472; Found: 470.0458.

Diethyl 5-iodo-2-(quinolin-8-ylcarbamoyl)isophthalate (**3n**)



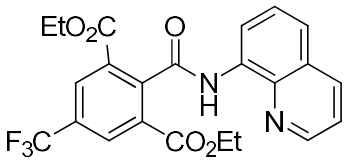
The title compound **3n** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 3 :1). **3n** was obtained as a white solid (24.1 mg, 31%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.90 (s, 1H), 8.92 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.71 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.56 (s, 2H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.54 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.43 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.22 (q, *J* = 7.1 Hz, 4H), 1.09 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 164.2, 148.3, 143.1, 138.5, 138.4, 136.5, 134.8, 131.3, 128.1, 127.7, 121.9, 121.8, 116.9, 94.3, 62.4, 13.9; HRMS (EI): calc. for $C_{22}H_{19}IN_2O_5$ (M^+): 518.0333; Found: 518.0333.

Diethyl 5-(chloromethyl)-2-(quinolin-8-ylcarbamoyl)isophthalate (**3o**)



The title compound **3o** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3o** was obtained as a colourless oil (34.3 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.08 (s, 1H), 8.92 (dd, *J* = 7.3, 1.0 Hz, 1H), 8.75 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.18 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.02 (d, *J* = 1.4 Hz, 1H), 7.72 – 7.64 (m, 2H), 7.63 – 7.54 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.67 (s, 2H), 4.27 (q, *J* = 7.1 Hz, 2H), 1.15 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.2, 166.2, 148.4, 139.6, 138.6, 136.5, 134.7, 132.2, 130.5, 130.2, 128.3, 128.1, 127.6, 122.1, 121.8, 116.9, 61.9, 45.1, 14.0; HRMS (EI): calc. for $C_{23}H_{21}ClN_2O_5$ (M^+): 440.1134; Found: 440.1123.

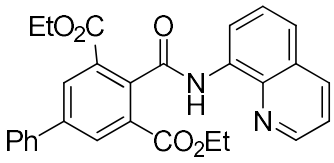
Diethyl 2-(quinolin-8-ylcarbamoyl)-5-(trifluoromethyl)isophthalate (**3p**)



The title compound **3p** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 3: 1). **3p** was obtained as white solid (48.3 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 8.93 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.70 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.51 (s, 2H),

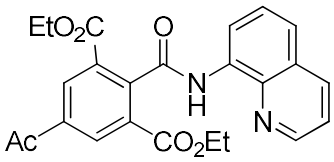
8.17 (dd, J = 8.3, 1.5 Hz, 1H), 7.61 (t, J = 7.9 Hz, 1H), 7.55 (dd, J = 8.3, 1.2 Hz, 1H), 7.43 (dd, J = 8.3, 4.2 Hz, 1H), 4.26 (q, J = 7.1 Hz, 4H), 1.11 (t, J = 7.1 Hz, 6H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1; ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.2, 163.3, 147.4, 140.9, 137.4, 135.5, 133.6, 130.9 (q, J_{C-F} =34.3Hz), 130.4 (q, J_{C-F} =3.6 Hz), 130.0, 127.1, 126.7, 122.0(q, J_{C-F} =274.0 Hz), 121.1, 120.8, 116.0, 61.6, 12.9; HRMS (ESI): calc. for $C_{23}H_{19}FN_2O_5$(M^+): 460.1241; Found: 460.1221.

Diethyl 4-(quinolin-8-ylcarbamoyl)-[1,1'-biphenyl]-3,5-dicarboxylate (3q)



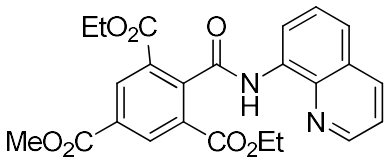
The title compound **3q** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4:1). **3q** was obtained as a white solid (42.8 mg, 61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.98 (d, J = 6.8 Hz, 1H), 8.72 (dd, J = 4.1, 1.5 Hz, 1H), 8.46 (s, 2H), 8.17 (dd, J = 8.3, 1.4 Hz, 1H), 7.69 (d, J = 7.3 Hz, 2H), 7.63 (t, J = 7.9 Hz, 1H), 7.53 (dd, J = 14.1, 7.3 Hz, 3H), 7.48 – 7.38 (m, 2H), 4.25 (q, J = 7.1 Hz, 4H), 1.10 (t, J = 7.1 Hz, 6H).; ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 165.7, 148.3, 142.5, 138.6, 138.5, 137.7, 136.4, 135.0, 132.9, 130.5, 129.3, 128.7, 128.1, 127.7, 127.4, 121.7, 116.9, 62.1, 14.0; HRMS (EI): calc. for $C_{28}H_{24}N_2O_5$ (M^+): 468.1680; Found: 468.1768.

Diethyl 5-acetyl-2-(quinolin-8-ylcarbamoyl)isophthalate (3r)



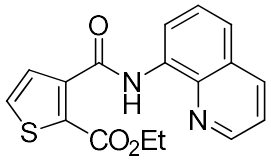
The title compound **3r** was prepared according to **GP** at 120 °C for 12 h and was purified by column chromatography (petroleum ether: ethyl acetate = 2: 1). **3r** was obtained as a white solid (49.5 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.98 (s, 1H), 8.95 (d, J = 7.4 Hz, 1H), 8.78 (s, 2H), 8.71 (dd, J = 4.0, 1.0 Hz, 1H), 8.24 – 8.12 (m, 1H), 7.62 (t, J = 7.9 Hz, 1H), 7.56 (d, J = 7.9 Hz, 1H), 7.43 (dd, J = 8.3, 4.2 Hz, 1H), 4.26 (q, J = 7.1 Hz, 4H), 2.72 (s, 3H), 1.12 (t, J = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.8, 165.6, 164.8, 148.2, 142.2, 138.3, 137.4, 136.4, 134.6, 133.9, 130.6, 128.0, 127.6, 121.9, 121.7, 116.9, 62.3, 26.9, 13.8; HRMS (ESI): calc. for $C_{24}H_{22}N_2O_6$(M^+): 434.1472; Found: 434.1472.

1,3-diethyl 5-methyl 2-(quinolin-8-ylcarbamoyl)benzene-1,3,5-tricarboxylate (3s)



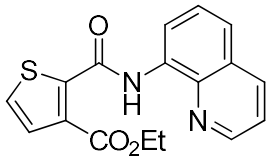
The title compound **3s** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 3: 1). **3s** was obtained as a white solid (45.3 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 8.93 (dd, *J* = 7.5, 1.1 Hz, 1H), 8.85 (s, 2H), 8.69 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.53 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.40 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.24 (q, *J* = 7.1 Hz, 4H), 3.99 (s, 3H), 1.11 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 165.0, 164.7, 148.3, 142.4, 138.4, 136.4, 135.3, 134.7, 131.2, 130.5, 128.1, 127.6, 121.9, 121.7, 116.9, 62.2, 52.9, 13.9; HRMS (EI): calc. for $C_{24}H_{22}N_2O_7$(M^+): 450.1422; Found: 450.1420.

Ethyl 3-(quinolin-8-ylcarbamoyl)thiophene-2-carboxylate (**3t**)



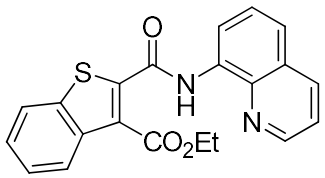
The title compound **3t** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 2: 1). **3t** was obtained as a yellow solid (26.0 mg, 53%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.06 (s, 1H), 8.95 (dd, *J* = 7.2, 1.6 Hz, 1H), 8.83 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.63 – 7.51 (m, 4H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 162.1, 148.6, 142.6, 139.2, 136.4, 134.8, 131.3, 131.2, 130.8, 128.2, 127.5, 122.4, 121.7, 117.8, 62.2, 14.2; HRMS (EI): calc. for $C_{17}H_{14}N_2O_3S$(M^+): 326.0720; Found: 326.0721;

Ethyl 2-(quinolin-8-ylcarbamoyl)thiophene-3-carboxylate (**3u**)



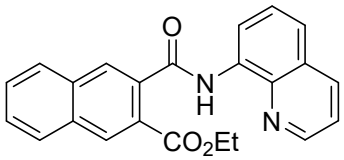
The title compound **3u** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 3: 1). **3u** was obtained as a yellow solid (39.6 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 12.42 (s, 1H), 9.11 – 8.78 (m, 2H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.62 – 7.54 (m, 3H), 7.47 – 7.42 (m, 2H), 4.47 (q, *J* = 7.1 Hz, 2H), 1.36 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.2, 162.1, 148.6, 142.6, 139.2, 136.4, 134.8, 131.3, 131.2, 130.8, 128.2, 127.5, 122.4, 121.7, 117.8, 62.2, 14.2; HRMS (EI): calc. for $C_{17}H_{14}N_2O_3S$(M^+): 326.0720; Found: 326.0723;

Ethyl 2-(quinolin-8-ylcarbamoyl)benzo[b]thiophene-3-carboxylate (**3v**)



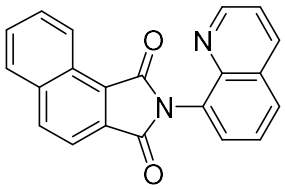
The title compound **3v** was prepared according to **GP3** at 140 °C and was purified by column chromatography (petroleum ether: ethyl acetate = 3: 1). **3v** was obtained as a yellow solid (44.0 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.00 (s, 1H), 8.92 (dd, *J* = 6.7, 2.2 Hz, 1H), 8.82 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.40 (dd, *J* = 7.2, 1.7 Hz, 1H), 8.18 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.88 (dd, *J* = 6.9, 1.5 Hz, 1H), 7.63 – 7.55 (m, 2H), 7.54 – 7.38 (m, 3H), 4.44 (q, *J* = 7.1 Hz, 2H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 160.7, 148.6, 145.4, 139.0, 138.9, 137.6, 136.5, 134.5, 128.2, 127.5, 126.6, 126.0, 126.0, 125.7, 122.7, 122.4, 121.9, 117.7, 61.9, 14.1; HRMS (EI): calc. for $C_{21}H_{16}SN_2O_3$(M^+): 376.0876; Found: 376.0886.

Ethyl 3-(quinolin-8-ylcarbamoyl)-2-naphthoate (3w)



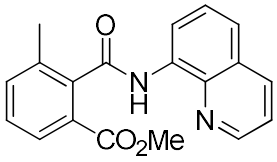
The title compound **3w** was prepared according to **GP3** at 100 °C and was purified by column chromatography (petroleum ether: ethyl acetate = 3: 1, Note: 5% Et_3N was added). **3w** was obtained as a white solid (28.3 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.25 (s, 1H), 8.98 (d, J = 7.4 Hz, 1H), 8.75 (dd, J = 4.2, 1.7 Hz, 1H), 8.53 (s, 1H), 8.24 – 8.11 (m, 2H), 8.02 – 7.90 (m, 2H), 7.68 – 7.59 (m, 3H), 7.55 (dd, J = 8.3, 1.4 Hz, 1H), 7.43 (dd, J = 8.2, 4.2 Hz, 1H), 4.33 (q, J = 7.1 Hz, 2H), 1.21 (t, J = 7.2 Hz, 3H). 13C NMR (101 MHz, $CDCl_3$) δ 167.8, 166.9, 148.4, 138.6, 136.5, 135.0, 134.9, 134.1, 133.0, 132.0, 129.1, 128.9, 128.4, 128.1, 127.7, 127.6, 127.2, 121.9, 121.8, 116.8, 61.7, 14.1. HRMS (EI): calc. for $C_{23}H_{18}N_2O_3$(M^+): 370.1312; Found: 370.1312.

2-(quinolin-8-yl)-1*H*-benzo[*e*]isoindole-1,3(2*H*)-dione (3x)



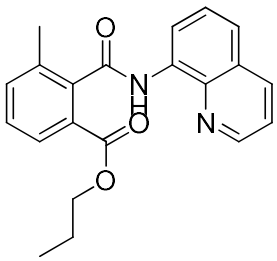
1x (0.15 mmol), $Pd(OAc)_2$ (3.5 mg, 0.015 mmol), Ag_2CO_3 (82.7 mg, 0.3 mmol), $ClCO_2Et$ (0.45 mmol, 3.0 equiv.) and toluene (2.0 mL). The tube was sealed under N_2. The mixture was stirred at room temperature for 5 minutes then heated at 100 °C for 8 h. After cooling to room temperature, the reaction mixture was diluted with EtOAc (10 mL) and filtered through a pad of Celite. Evaporation of the solvent under vaccum. The reaction mixture was stirred in 1.0 mL HOAc for 6 h and was further purified by column chromatography afforded the pure corresponding products. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.28 – 8.18 (m, 2H), 8.04 – 7.93 (m, 3H), 7.81 (dd, *J* = 7.2, 1.4 Hz, 1H), 7.78 – 7.64 (m, 3H), 7.43 (ddd, *J* = 8.3, 4.2, 1.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3, 168.7, 151.1, 144.7, 136.9, 136.3, 135.3, 131.9, 130.6, 130.1, 129.7, 129.6, 129.5, 128.9, 128.9, 128.5, 127.9, 126.3, 125.4, 122.0, 119.1. HRMS (EI): calc. for $C_{21}H_{12}N_2O_2$ (M^+): 324.0893; Found: 324.0894.

Methyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (**4a**)



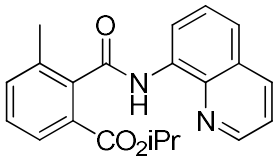
The title compound **4a** was prepared according to **GP** at 120 ºC for 12 h and was purified by column chromatography (petroleum ether: ethyl acetate = 3: 1). **4a** was obtained as a while solid (35.0 mg, 73%). ^{1}H NMR (400 MHz, CDCl3) δ 9.86 (s, 1H), 8.99 (d, *J* = 7.5 Hz, 1H), 8.71 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.93 (d, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.56 – 7.52 (m, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.44 – 7.37 (m, 2H), 3.76 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 166.5, 148.3, 138.9, 138.6, 136.4, 136.1, 135.0, 134.8, 129.1, 128.2, 128.1, 127.8, 127.7, 121.9, 121.7, 116.9, 52.5, 19.3; HRMS (EI): calc. for $C_{19}H_{16}N_2O_3(M^+)$: 320.1155; Found: 320.1153.

Propyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (**4b**)



The title compound **4b** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **4b** was obtained as a white solid (41.8 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 9.00 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.71 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.54 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.47 (d, *J* = 7.1 Hz, 1H), 7.44 – 7.37 (m, 2H), 4.12 (t, *J* = 6.6 Hz, 2H), 2.48 (s, 3H), 1.58 – 1.45 (m, 2H), 0.79 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 166.2, 148.3, 138.69,7 138.6, 136.4, 136.0, 134.8, 129.0, 128.2, 128.1, 127.6, 121.9, 121.7, 116.9, 67.2, 21.9, 19.3, 10.5; HRMS (ESI): calc. for $C_{21}H_{20}N_2O_3(M^+)$: 348.1468; Found: 348.1467.

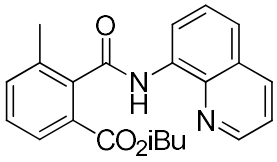
Isopropyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (**4c**)



The title compound **4c** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **4c** was obtained as a white solid (41.3 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.90 (dd, *J* = 7.6, 1.2 Hz, 1H), 8.61 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.06 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.84 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.51 (t, *J* = 7.9 Hz, 1H), 7.44 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.39 – 7.27 (m, 3H), 5.09 – 4.94 (m, 1H), 2.38 (s, 3H), 0.98 (d, *J* = 6.3 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ

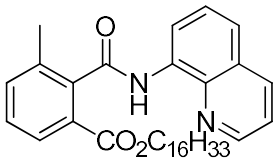
168.1, 165.7, 148.3, 138.5, 138.5, 136.4, 136.0, 134.9, 134.6, 129.0, 128.7, 128.2, 128.1, 127.6, 121.8, 121.7, 116.9, 69.1, 21.6, 19.3; HRMS (EI): calc. for $C_{21}H_{20}N_2O_3(M^+)$: 348.1468; Found: 348.1469.

Isobutyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (4d)



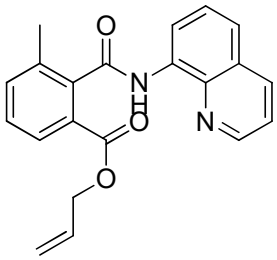
The title compound **4d** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate =4: 1). **4d** was obtained as a white solid (45.7 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 9.00 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.71 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.98 – 7.92 (m, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 7.54 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.47 (d, *J* = 7.0 Hz, 1H), 7.45 – 7.38 (m, 2H), 3.96 (d, *J* = 6.7 Hz, 2H), 2.49 (s, 3H), 1.92 – 1.76 (m, 1H), 0.82 (d, *J* = 6.7 Hz, 6H); ^{13}C ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.04, 166.17, 148.25, 138.75, 138.57, 136.41, 136.04, 134.81, 134.78, 129.04, 128.17, 128.09, 127.60, 121.85, 121.68, 116.91, 71.76, 27.71, 19.30, 19.18; HRMS (EI): calc. for $C_{22}H_{22}N_2O_3(M^+)$: 362.1625; Found: 362.1622.

Hexadecyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (4e)



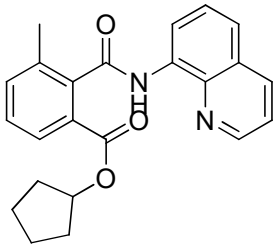
The title compound **4e** was prepared according to **GP** and was purified by column chromatography (petroleum ether : ethyl acetate = 6 : 1). **4e** was obtained as a colourless oil (59.7 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.88 (s, 1H), 9.00 (dd, *J* = 7.5, 1.4 Hz, 1H), 8.72 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.95 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.55 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.47 (d, *J* = 6.9 Hz, 1H), 7.45 – 7.40 (m, 2H), 4.14 (t, *J* = 6.6 Hz, 2H), 2.49 (s, 3H), 1.50 – 1.40 (m, 2H), 1.33 – 1.09 (m, 22H), 1.05 – 0.94 (m, 4H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 166.3, 148.3, 138.6, 138.6, 136.4, 136.0, 134.8, 134.8, 129.1, 128.3, 128.3, 128.2 127.6, 121.9, 121.7, 116.9, 65.9, 32.1, 29.8, 29.8, 29.7, 29.7, 29.5, 29.5, 29.3, 28.5, 26.0, 22.8, 19.3, 14.3; HRMS (EI): calc. for $C_{34}H_{46}N_2O_3(M^+)$: 530.3503; Found: 530.3503.

Allyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (4f)



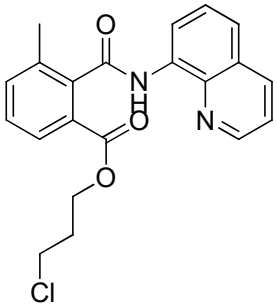
The title compound **4f** was prepared according to **GP** and was purified by column chromatography (petroleum ether : ethyl acetate = 3: 1). **4f** was obtained as a colourless oil (30.7 mg, 59%). ^{1}H ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.87 (s, 1H), 8.98 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.72 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.55 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.49 (d, *J* = 7.4 Hz, 1H), 7.46 – 7.39 (m, 2H), 5.90 – 5.62 (m, 1H), 5.17 (dd, *J* = 17.2, 1.4 Hz, 1H), 4.98 (dd, *J* = 10.4, 1.0 Hz, 1H), 4.65 (d, *J* = 5.9 Hz, 2H), 2.50 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 165.8, 148.3, 138.9, 138.6, 136.4, 136.1, 135.0, 134.8, 131.8, 129.1, 128.2, 128.1, 128.0, 127.6, 121.9, 121.7, 118.7, 117.0, 66.2, 19.3; HRMS (EI): calc. for $C_{21}H_{18}N_2O_3(M^+)$: 346.1312; Found: 346.1310.

Cyclopentyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (**4g**)



The title compound **4g** was prepared according to **GP** and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **4g** was obtained as a colourless oil (39.8 mg, 71%). ^{1}H^{1}H NMR (400 MHz, $CDCl_3$) δ 9.79 (s, 1H), 8.93 (dd, *J* = 7.5, 1.2 Hz, 1H), 8.64 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.10 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.88 – 7.76 (m, 1H), 7.54 (t, *J* = 7.9 Hz, 1H), 7.48 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.42 – 7.30 (m, 3H), 5.20 (dq, *J* = 8.9, 2.9 Hz, 1H), 2.40 (s, 3H), 1.68 – 1.47 (m, 4H), 1.38 – 1.23 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 166.0, 148.3, 138.6, 138.4, 136.5, 136.0, 134.8, 134.7, 129.0, 128.6, 128.3, 128.1, 127.6, 121.9, 121.8, 116.9, 78.6, 32.6, 23.7, 19.4; HRMS (EI): calc. for $C_{23}H_{22}N_2O_3(M^+)$: 374.1625; Found: 374.1620.

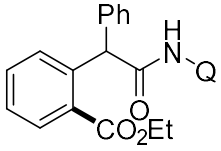
3-chloropropyl 3-methyl-2-(quinolin-8-ylcarbamoyl)benzoate (**4h**)



The title compound **4h** was prepared according to **GP** purified by column chromatography (petroleum ether: ethyl acetate = 3: 1). **4h** was obtained as a pale yellow solid (41.9 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.98 (dd, *J* = 7.5, 1.3 Hz, 1H), 8.72 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.65 – 7.59 (m, 1H), 7.56 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.49 (d, *J* = 7.2 Hz, 1H), 7.46 – 7.40 (m, 2H), 4.30 (t, *J* = 5.9 Hz, 2H), 3.43 (t, *J* = 6.5 Hz, 2H), 2.49 (s, 3H), 1.99 – 1.81 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.0, 166.0, 148.4, 138.6, 138.5, 136.5, 136.1, 135.1, 134.6, 129.2,

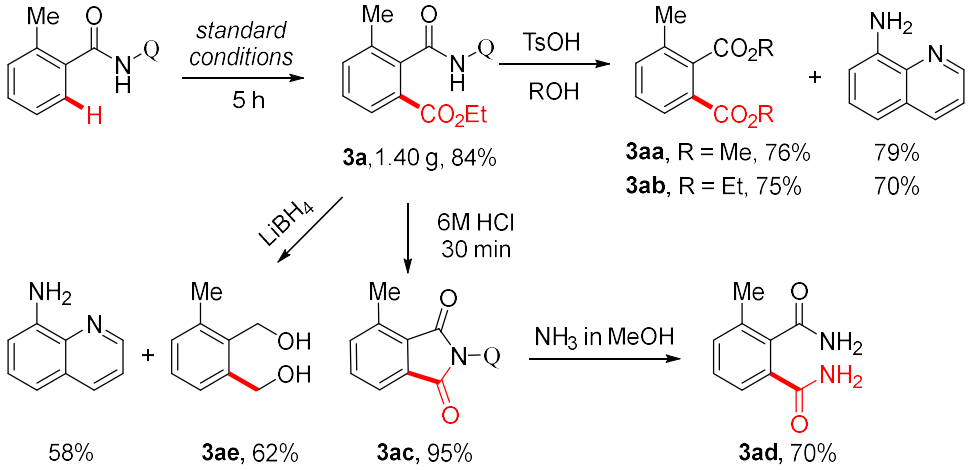
128.4, 128.2, 127.7, 127.6, 122.1, 121.8, 116.9, 62.3, 41.3, 31.6, 19.3; HRMS (EI): calc. for $C_{21}H_{19}ClN_2O_3(M^+)$: 382.1079; Found: 382.1077.

Ethyl 2-(2-oxo-1-phenyl-2-(quinolin-8-ylamino)ethyl)benzoate (5)



To a 50 mL Schlenk tube, were added **1w** (0.15 mmol), $Pd(OTFA)_2$ (5.0 mg, 0.015 mmol), Ag_2CO_3 (82.7 mg, 0.3 mmol), $ClCO_2Et$ (0.45 mmol, 3.0 equiv.) and toluene (2.0 mL). The tube was sealed under N_2. The mixture was stirred at room temperature for 5 minutes then heated at 100 °C for 16 h. After cooling to room temperature, the reaction mixture was diluted with EtOAc (10 mL) and filtered through a pad of Celite. Evaporation of the solvent under vaccum and further purification with column chromatography. **5** was obtained as a white solid (27.7mg, 45%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.85 (dd, *J* = 7.3, 1.6 Hz, 1H), 8.68 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.11 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.99 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.61 – 7.27 (m, 11H), 6.38 (s, 1H), 4.35 (qd, *J* = 7.1, 1.4 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 167.8, 148.3, 140.6, 139.4, 138.7, 136.3, 134.8, 132.3, 130.9, 130.9, 130.4, 129.5, 128.9, 128.0, 127.5, 127.3, 127.2, 121.7, 121.6, 116.5, 61.4, 56.1, 14.3. HRMS (EI): calc. for $C_{26}H_{22}N_2O_3(M^+)$: 410.1625; Found: 410.1620.

Synthetic Applications



1. Gram-scale Synthesis

Compound **3a** was prepared according to **GP** in 5.0 mmol scale (1.31 g) and was purified by column chromatography (petroleum ether: ethyl acetate = 4: 1). **3a** was obtained as a pale yellow solid (1.40 g, 84%).

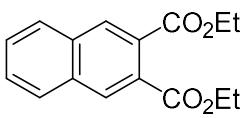
2. Removal of Directing Group

To a 50 mL Schlenk tube were added substrate **3** (0.2 mmol) and ROH (2.0 mL). TsOH(344.4 mg, 2.0 mmol) was added to the solution in one portion and the resulting mixture was stirred for 36 hours at 120 °C. The reaction was quenched with an saturated aqueous solution of $NaHCO_3$ (10 ml), then the mixture was extracted with ethyl acetate three times. The combined organic layer was dried over $MgSO_4$. Evaporation of the solvent under vaccum and further purification by column chromatography (petroleum ether: ethyl acetate = 4: 1).

For substrate **3a**, when MeOH was used as reaction solution, the product **5** was obtained as a white oil (31.6 mg, 76 %), and the 8-aminoquinoline was gave in 79% (22.7 mg) . When EtOH was used as reaction solution, the product **6** was obtained as a white oil (35.4 mg, 75%), and the 8-aminoquinoline was gave in 70% yield (20.2 mg).

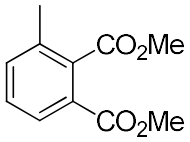
For substrate **3w**, a 50 mL Schlenk tube were added **3w** (66.8 mg, 0.1 mmol) and EtOH (1.0 mL). TsOH(172.2 mg, 1.0 mmol) was added to the solution in one portion and the resulting mixture was stirred for 36 hours at 120 °C. The reaction was quenched with an saturated aqueous solution of $NaHCO_3$ (10 ml), then the mixture was extracted with ethyl acetate three times. The product **3wa** was obtained as an oil in 42% yield (11.5 mg).

Diethyl naphthalene-2,3-dicarboxylate (3wa)



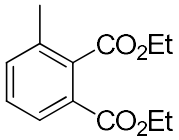
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 2H), 7.97 – 7.87 (m, 2H), 7.66 – 7.57 (m, 2H), 4.42 (q, *J* = 7.2 Hz, 4H), 1.41 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.9, 133.5, 130.2, 129.0, 128.8, 128.6, 61.8, 14. 3. This compound was known[2]

Dimethyl 3-methylphthalate (6)



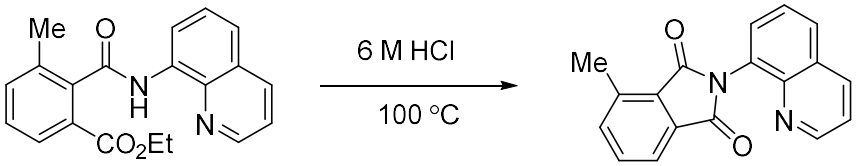
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.43 – 7.32 (m, 2H), 3.94 (s, 3H), 3.88 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.0, 166.5, 135.7, 135.4, 134.6, 129.2, 127.9, 127.6, 52.6, 52.6, 19.2. HRMS (EI): calc. for $C_{11}H_{12}O_4(M^+)$: 208.0730; Found: 208.0730.

Diethyl 3-methylphthalate (7)

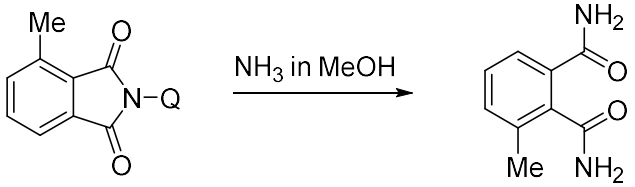


^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.80 (m, 1H), 7.41 – 7.29 (m, 2H), 4.41 (q, *J* = 7.2 Hz, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 2.35 (s, 3H), 1.48 – 1.20 (m, 6H); ^{13}C NMR (101 MHz, CDCl3) δ 169.5, 166.0, 135.5, 134.4, 129.0, 128.2, 127.6, 61.5, 61.5, 19.1, 14.3, 14.2. HRMS (EI): calc. for $C_{13}H_{16}O_4(M^+)$: 236.1043; Found: 236.1040.

3. **Synthesis of Phthalamide 9**

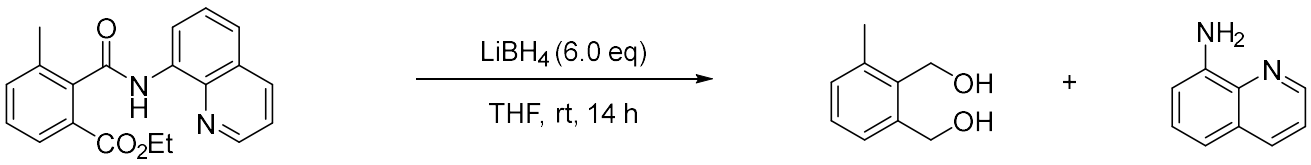


To a 50 mL Schlenk tube were added **3a** (66.8 mg, 0.2 mmol) and HCl (2.0 mL, 6 M) for 30 minutes at 100 °C. The reaction was quenched with an saturated aqueous solution of Na_2CO_3 (20 ml), then the mixture was extracted with ethyl acetate three times. The combined organic layer was dried over $MgSO_4$. Evaporation of the solvent under vaccum and further purification by column chromatography (petroleum ether: ethyl acetate = 4: 1). The product **8** was obtained as a pale yellow solid (54.8 mg, 95%),^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.87 (dd, J = 4.1, 1.6 Hz, 1H), 8.21 (dd, J = 8.4, 1.6 Hz, 1H), 7.95 (dd, J = 8.2, 1.3 Hz, 1H), 7.82 (d, J = 7.3 Hz, 1H), 7.74 (dd, J = 7.2, 1.3 Hz, 1H), 7.67 (d, J = 8.4 Hz, 1H), 7.64 (d, J = 7.7 Hz, 1H), 7.54 (d, J = 7.9 Hz, 1H), 7.43 (dd, J = 8.3, 4.2 Hz, 1H), 2.76 (s, 3H). This compound is known.[1g] The product could also obtain via **3a** stirred in HOAc for 6 h.



To a 50 mL Schlenk tube were added **8** (28.8 mg, 0.1 mmol) and NH_3 in MeOH (5.0 mL, 7M) for 24 hours at rt. Evaporation of the solvent under vaccum and further purification by column chromatography (DCM: MeOH = 10: 1). The product **9** was obtained as a white solid (12.5 mg, 70%). ^{1}H NMR (400 MHz, DMSO) δ 7.73 – 7.00 (m, 7H), 2.31 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 170.7, 169.4, 137.4, 134.1, 134.1, 131.6, 127.7, 125.0, 19.1; HRMS (EI): calc. for $C_9H_{10}O_2N_2(M^+)$: 178.0737; Found: 178.0737.

4. Synthesis of 1,2-dibenzyl alcohol 10



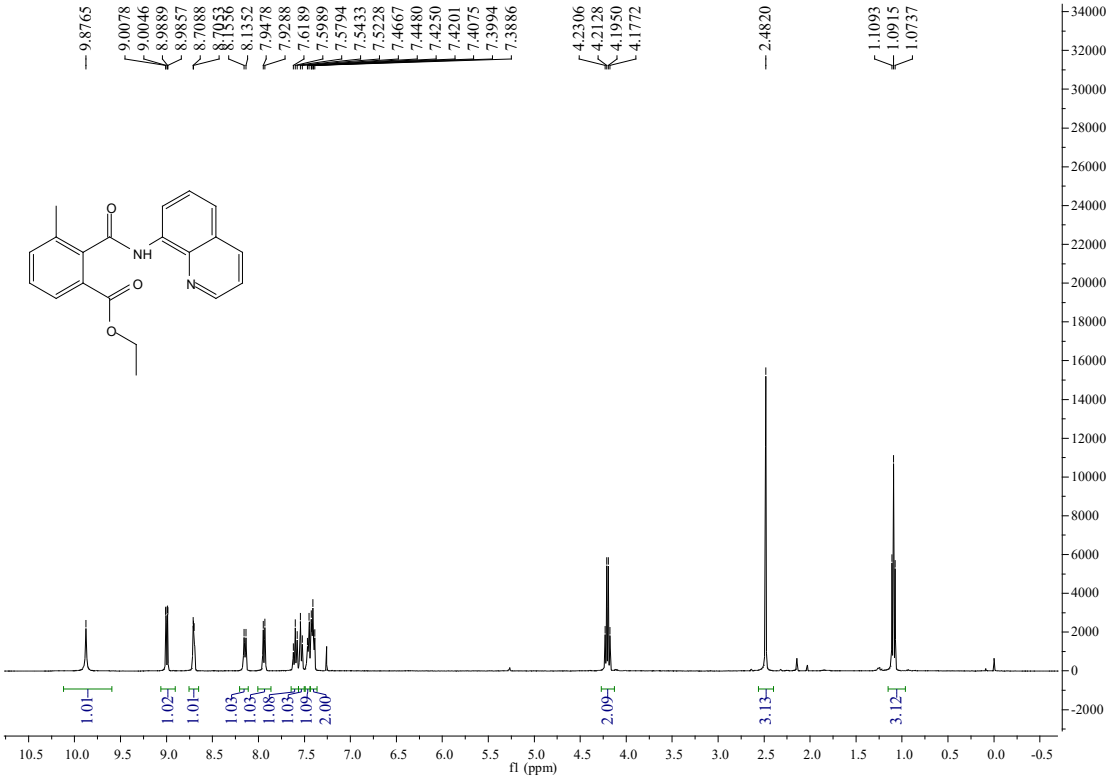
To a 50 mL Schlenk tube were added **3a** (33.4 mg, 0.1 mmol) and dry THF (2.0 mL). The Solid $LiBH_4$ was added slowly. The reaction was stirred at rt overnight. The reaction was quenched by 2M HCl solution. The mixture was extracted ethyl acetate three times. The combined organic layer was dried over $MgSO_4$. Evaporation of the solvent under vaccum and further purification by column chromatography (petroleum ether: ethyl acetate = 1: 1). The product **10** was obtained in 62% yield (9.4 mg). The 8-aminoquinoline was recovered by extraction and further purification by column chromatography and was obtained in 58% yield (8.4 mg). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.13 (m, 3H), 4.74 (s, 2H), 4.71 (s, 2H), 3.09 (s, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.0, 137.9, 137.8, 131.1, 128.3, 127.8, 65.0, 59.2, 19.6; HRMS (EI): calc. for $C_9H_{11}O_2(M^+)$: 151.0754; Found: 151.0758.

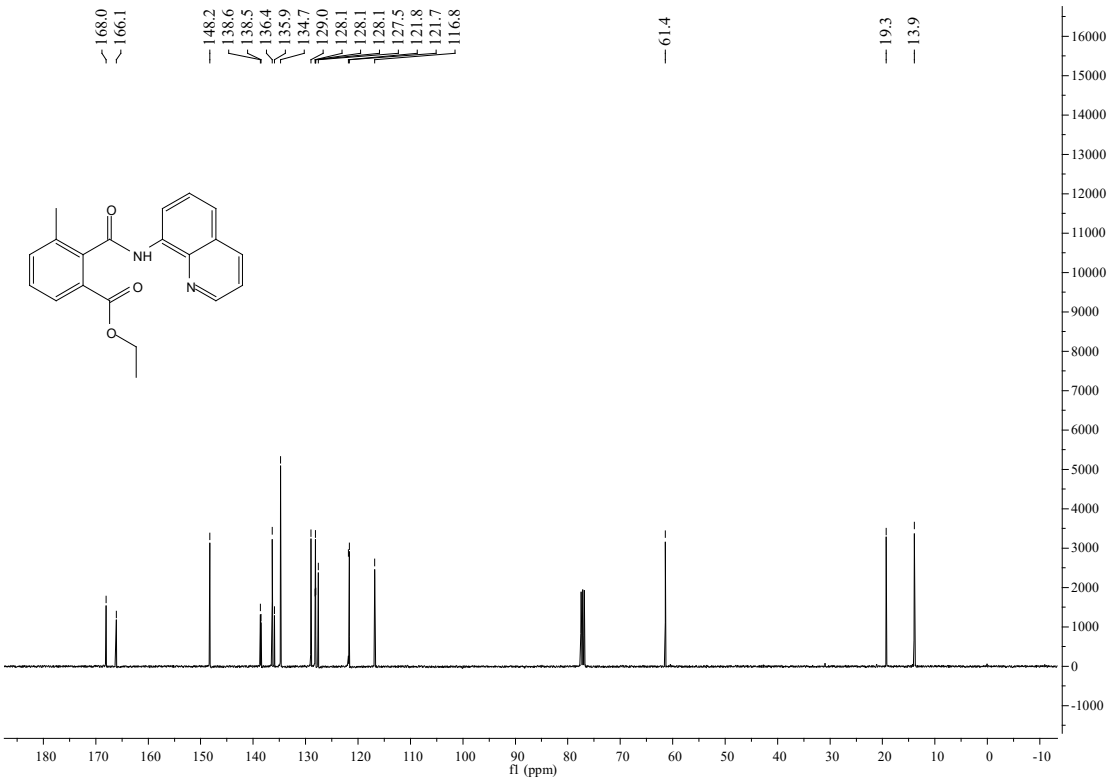
References

[1] a) L. D. Tran, I. Popov, O. Daugulis, *J. Am. Chem. Soc.* **2012**, *134*, 18237; b) T. Truong, K. Klimovica, O. Daugulis, *J. Am. Chem. Soc.* **2013**, *135*, 9342; c) L. D. Tran, J. Roane, O. Daugulis, *Angew. Chem., Int. Ed.* **2013**, *52*, 6043; d) J. Roane, O. Daugulis, *Org. Lett.* **2013**, *15*, 5842; e) M. Nishino, K. Hirano, T. Satoh, M. Miura, *Angew. Chem. Int. Ed.* **2013**, *52*, 4457. f) L.Grigorjeva,O.Daugulis,*Org. Lett*.,**2014**, *16*, 4684-4687; g) L.Grigorjeva, O. Daugulis. *Org. Lett*., **2014**, *16*, 4688; h) R.Shang, L.Ilies,E. Nakamura. *J. Am. Chem. Soc*., **2015**, *137*, 7660; i) N.Barsu, D.Kalsi, B. Sundararaju. *Chem. Eur. J.* **2015**, *21*, 9364.
[2] C.-H. Lin, K.-H. Lin, B. Pal, L.-D. Tsou, *Chem. Commun.* **2009**, 803-805

NMR Spectrum

3a





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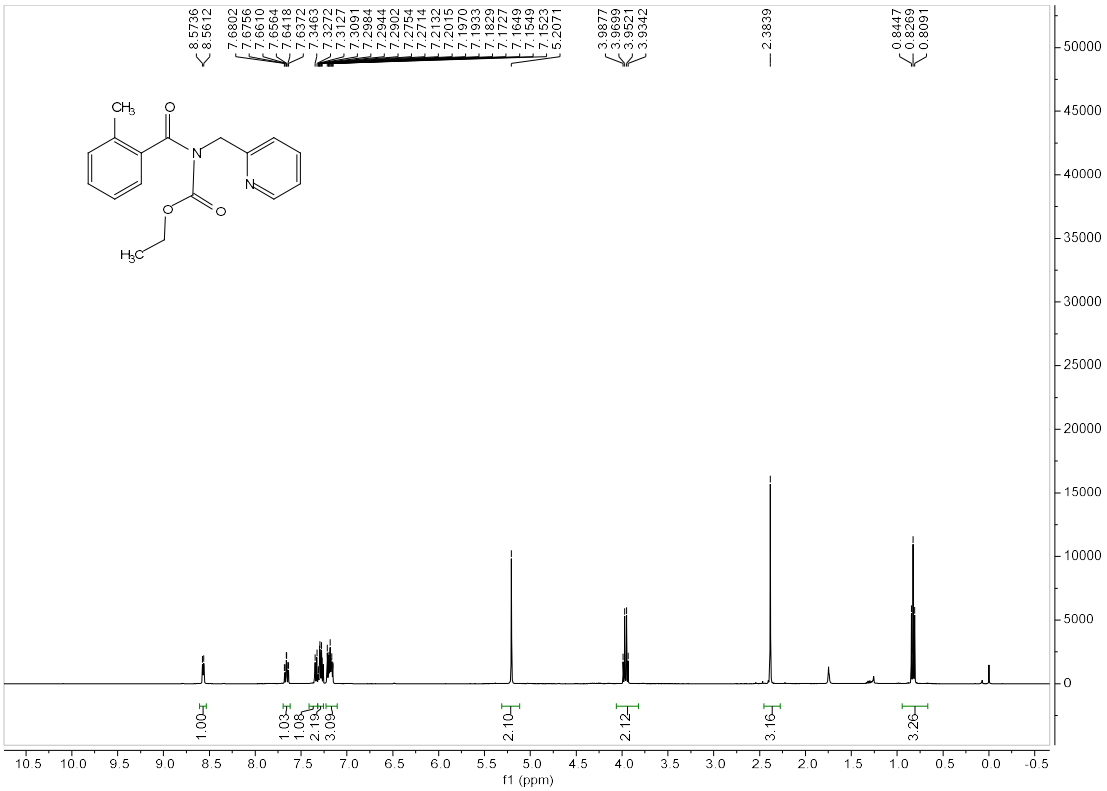
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7.2902
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2.10
2.12
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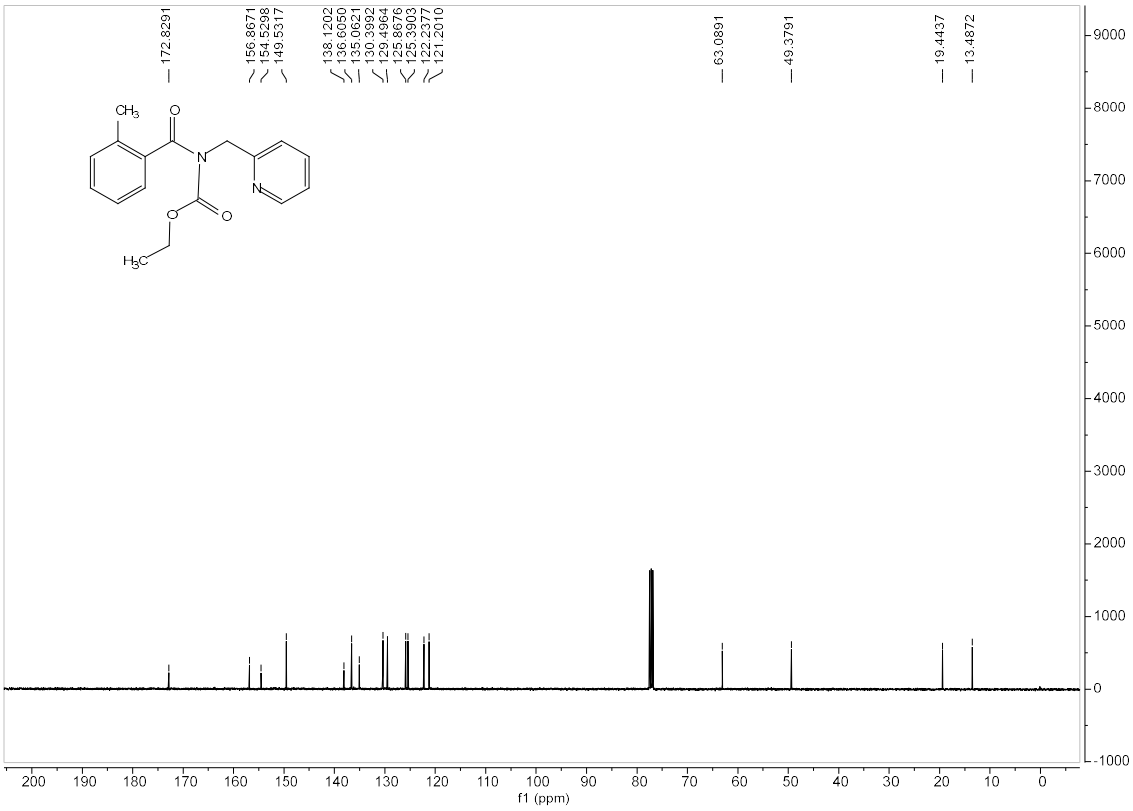
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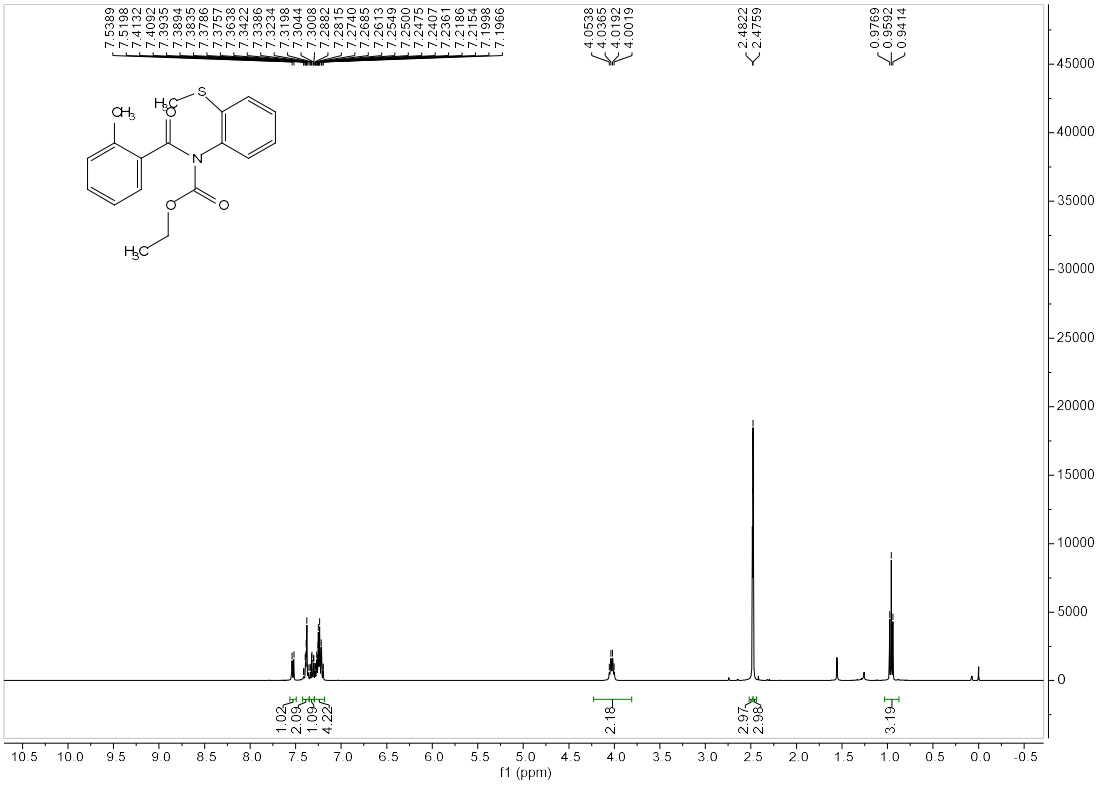
3ae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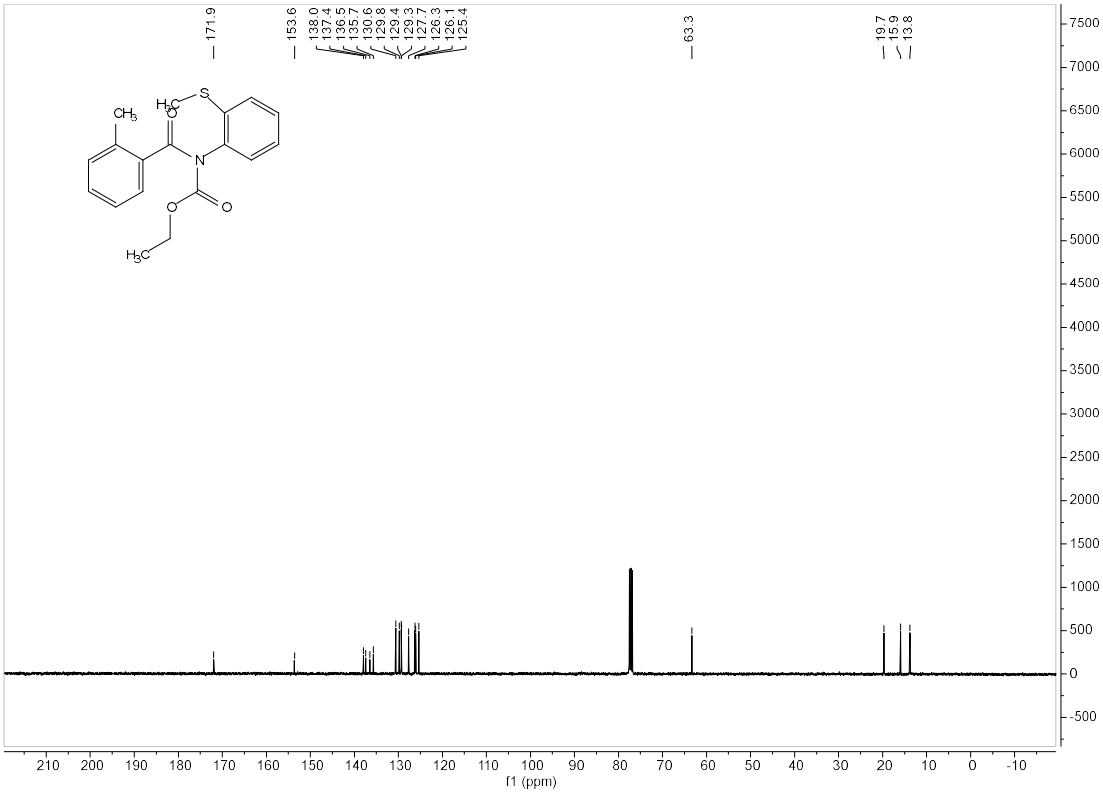
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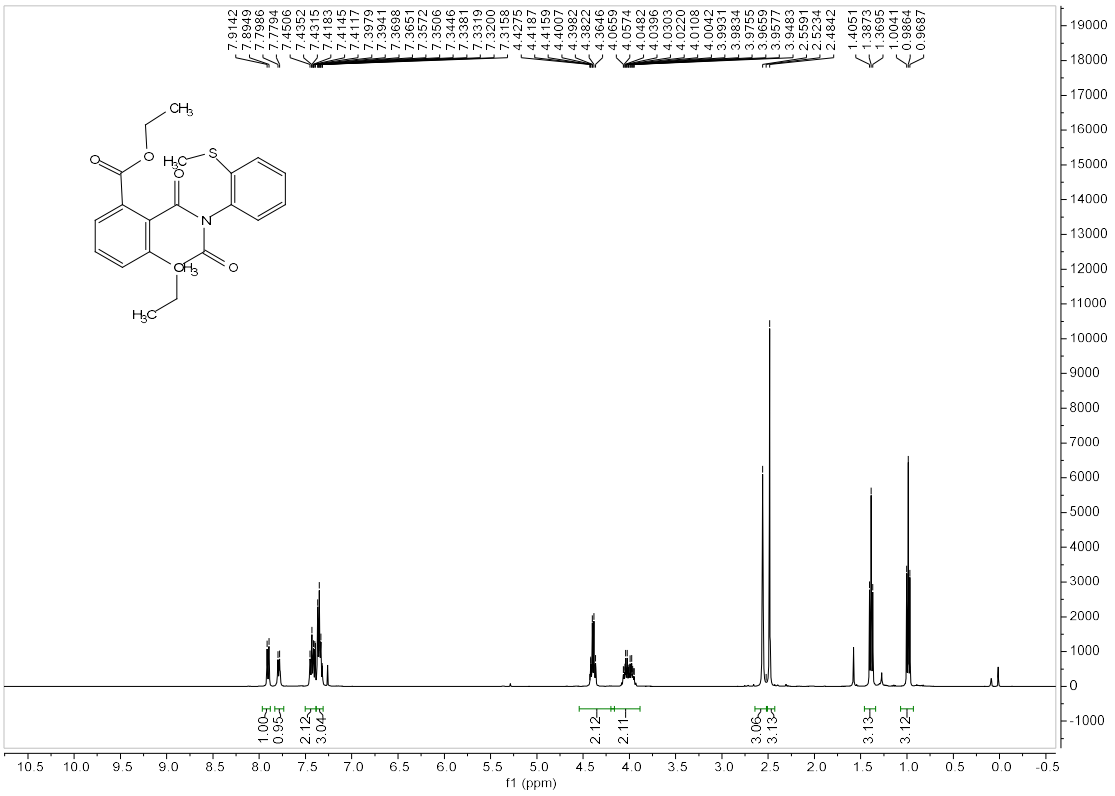
f1 (ppm)

3af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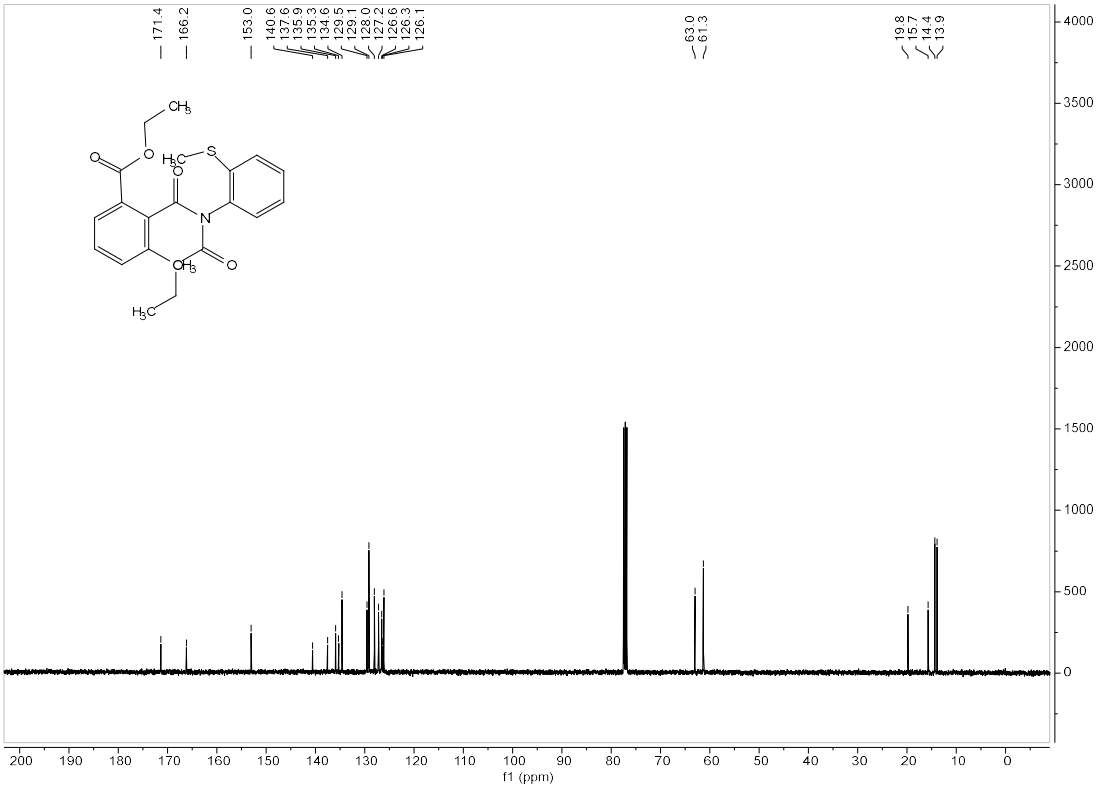
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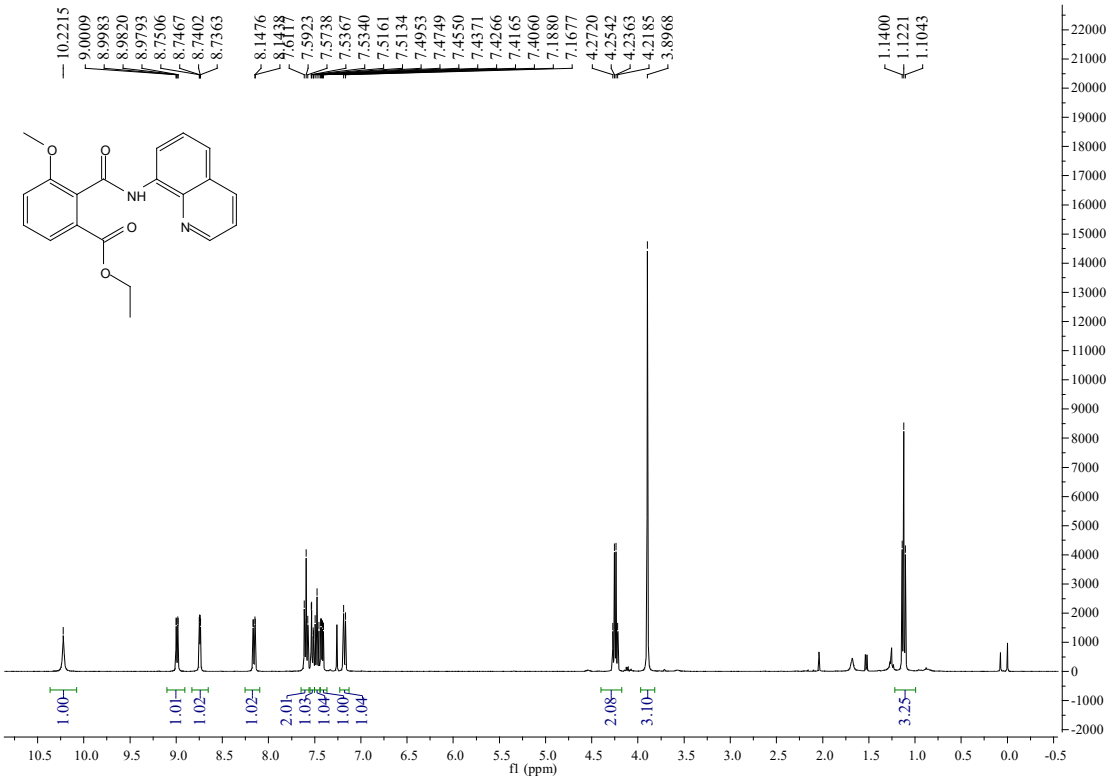
f1 (ppm)

3b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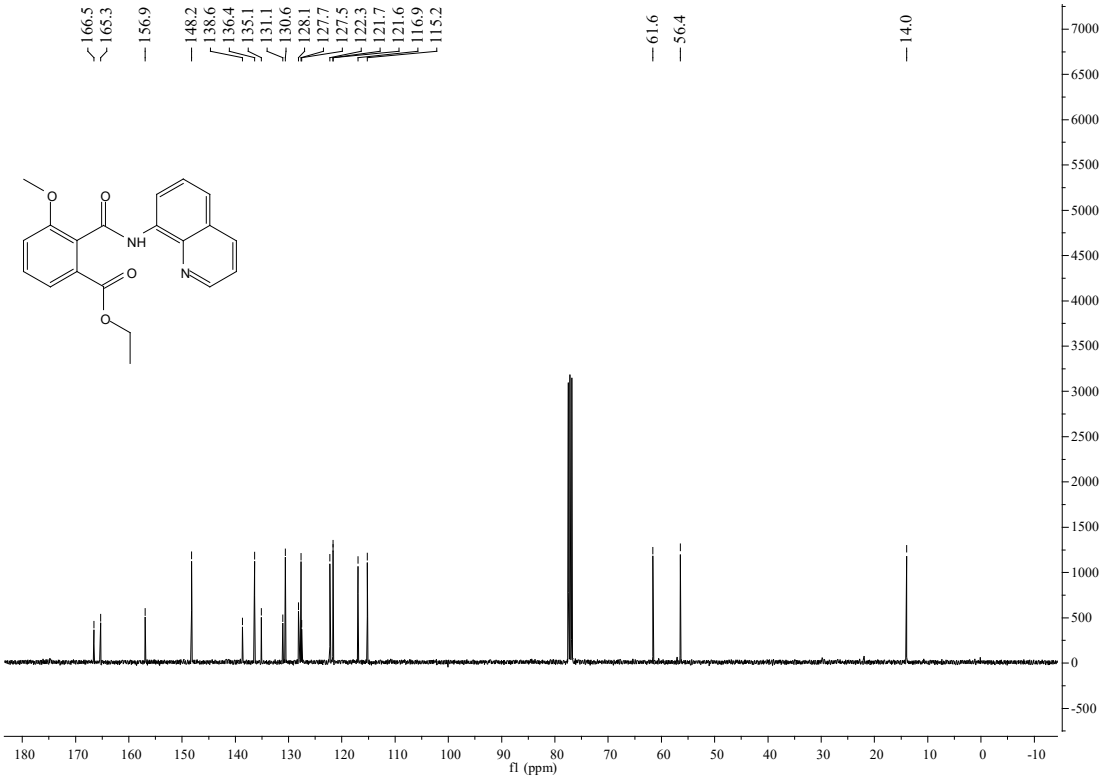
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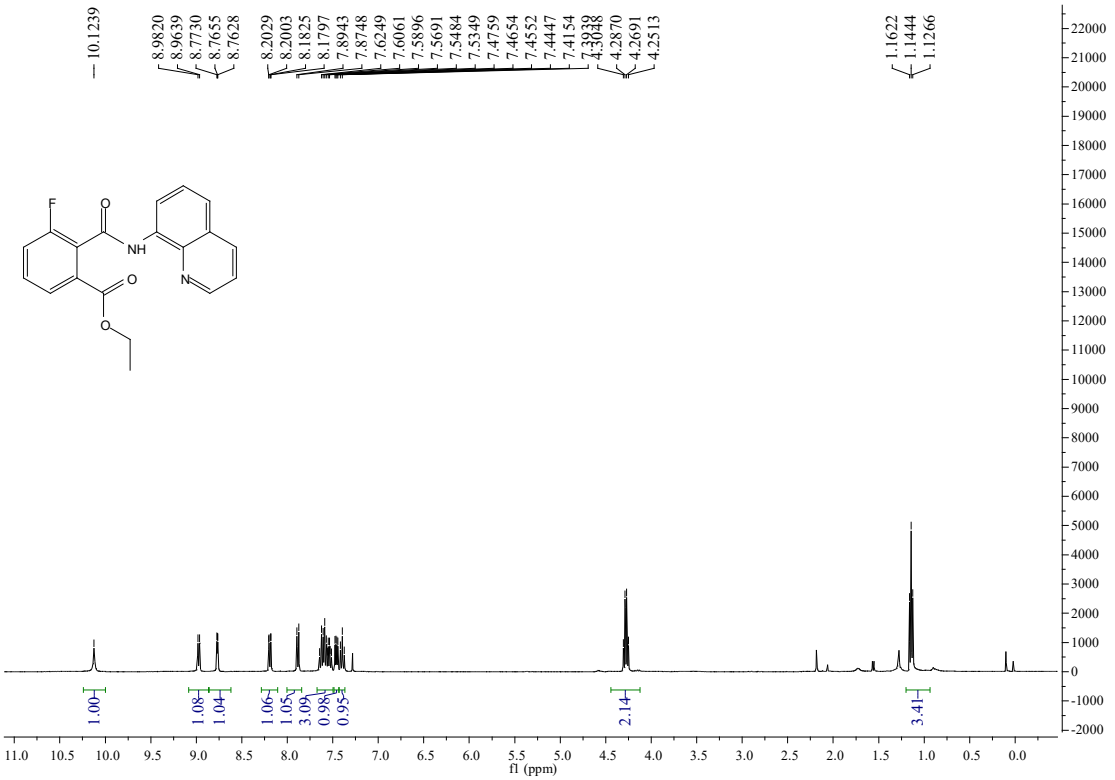
3c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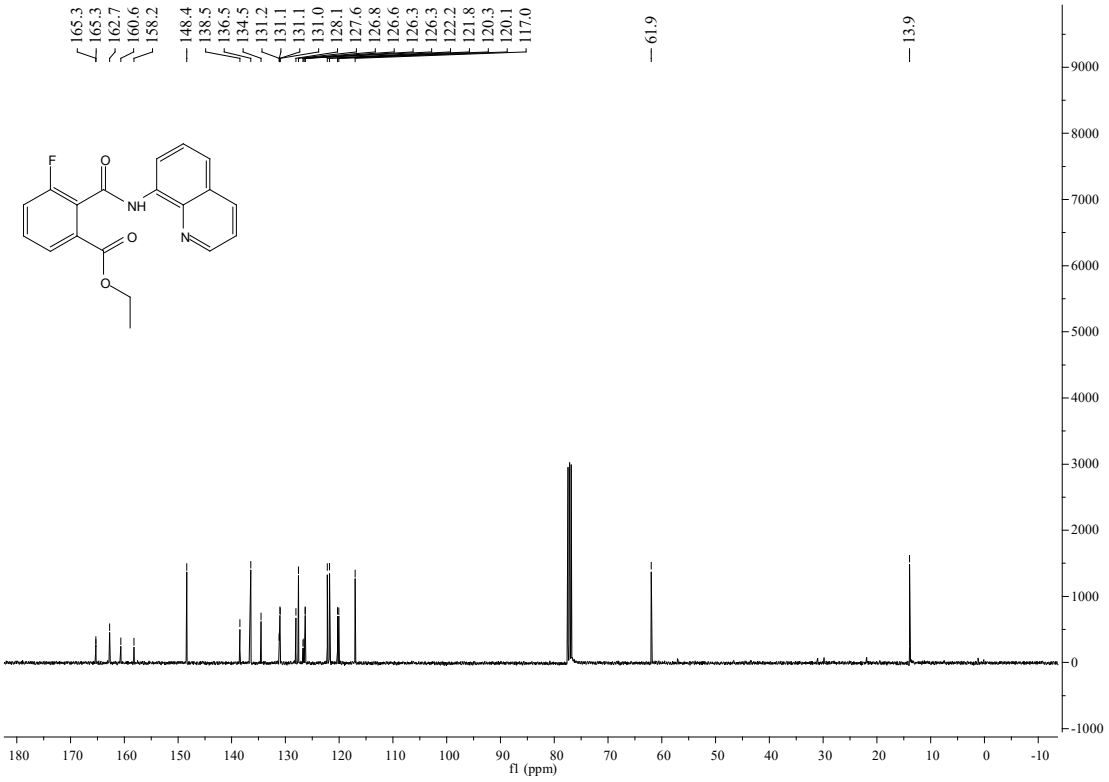
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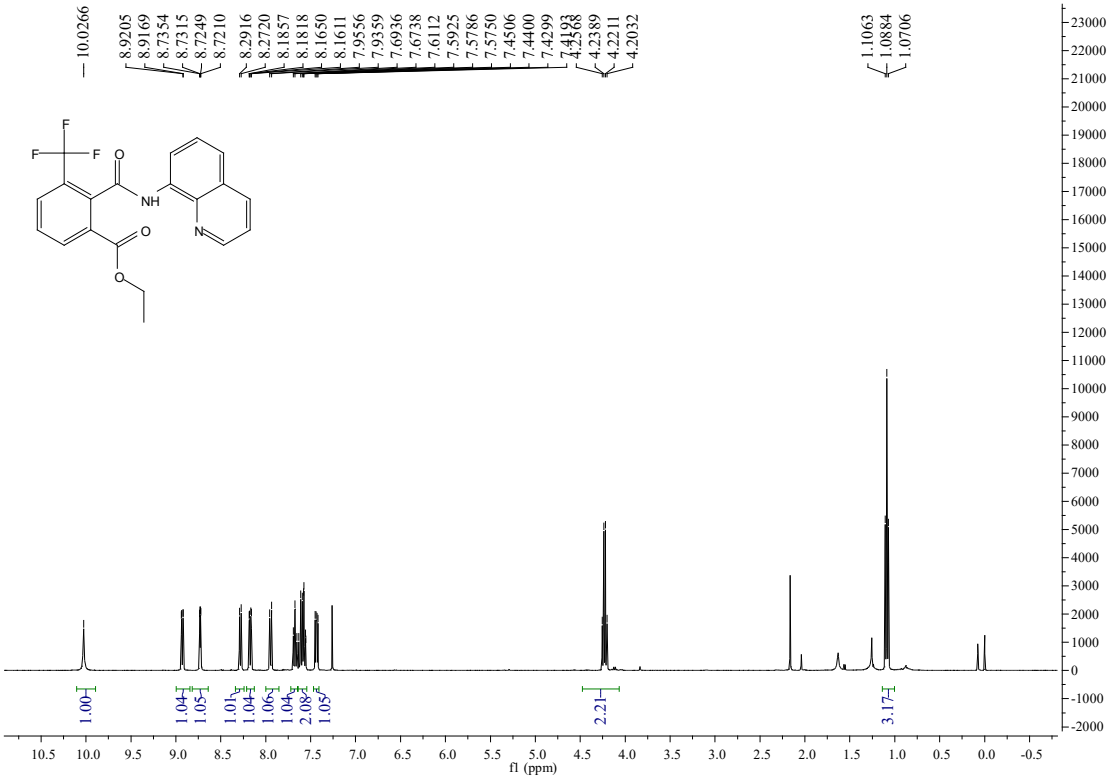
2000
1000
0
-1000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3d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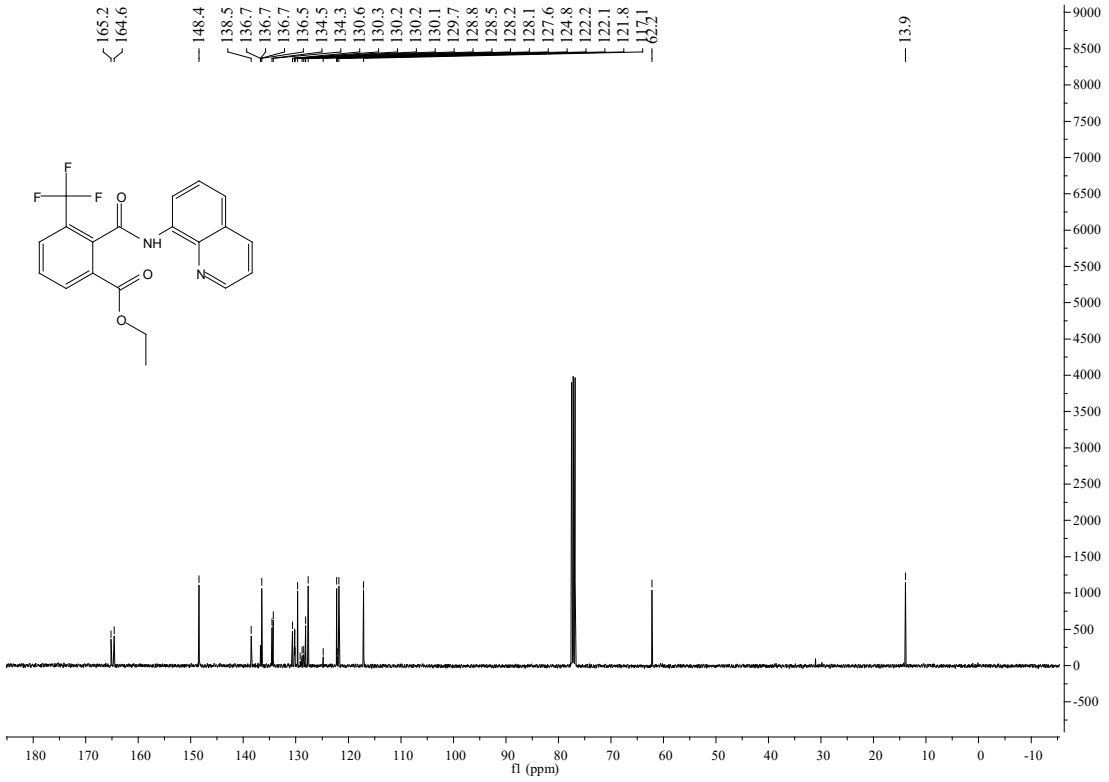
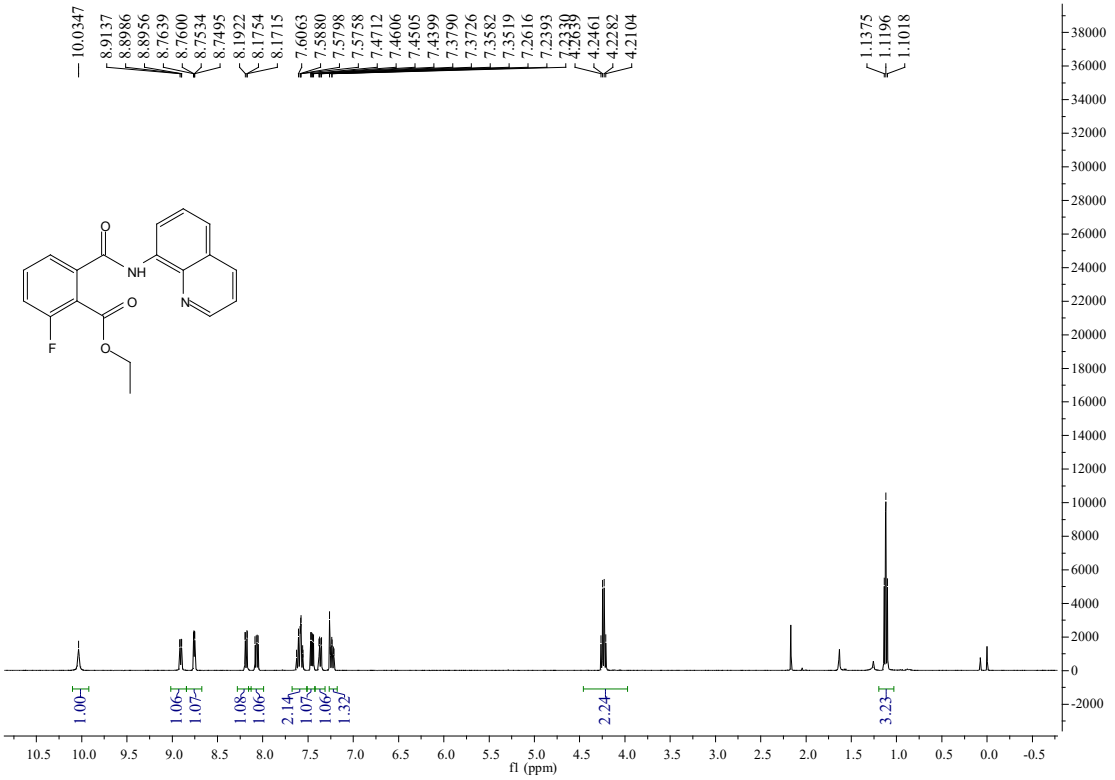
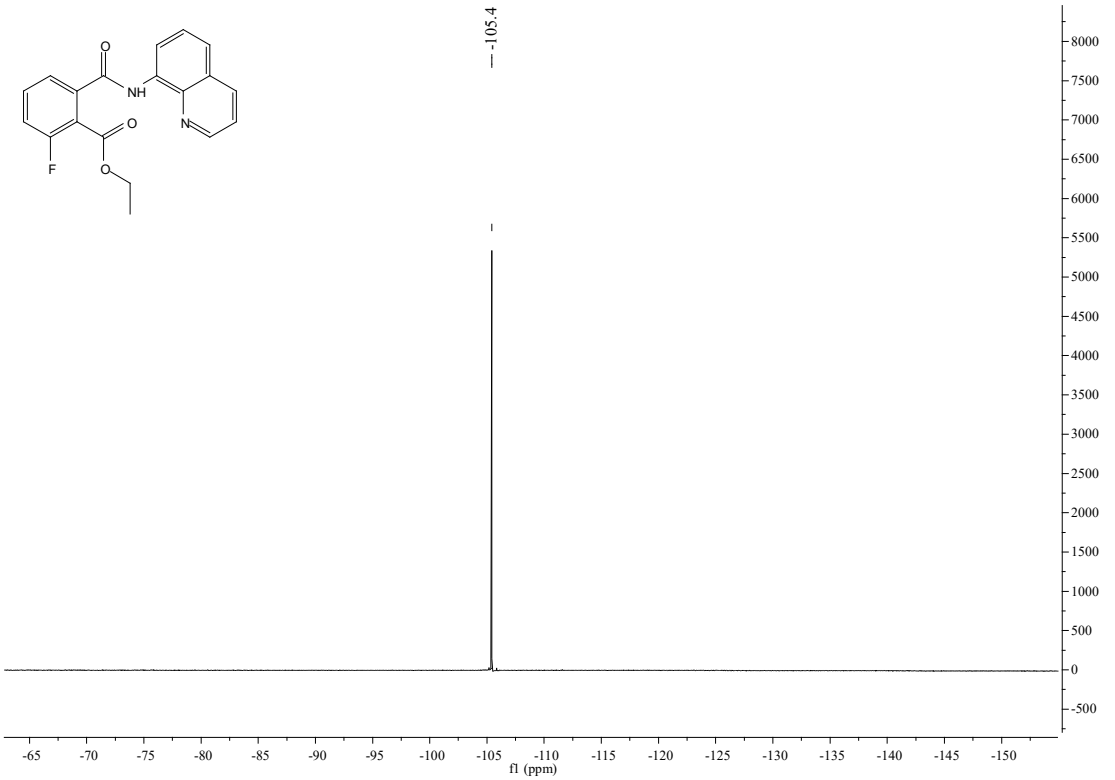
8.9205
8.9169
8.7354
8.7315
8.7249
8.7210
8.2916
8.2720
8.1857
8.1818
8.1650
8.1611
7.9556
7.9359
7.6936
7.6738
7.6112
7.5925
7.5786
7.5750
7.4506
7.4400
7.4299
7.4193
4.2568
4.2389
4.2211
4.2032
1.1063
1.0884
1.0706
F
F
F
O
NH
O
N
O
1.00
1.04
1.05
1.01
1.04
1.06
1.04
2.08
1.05
2.21
3.17
f1 (ppm)

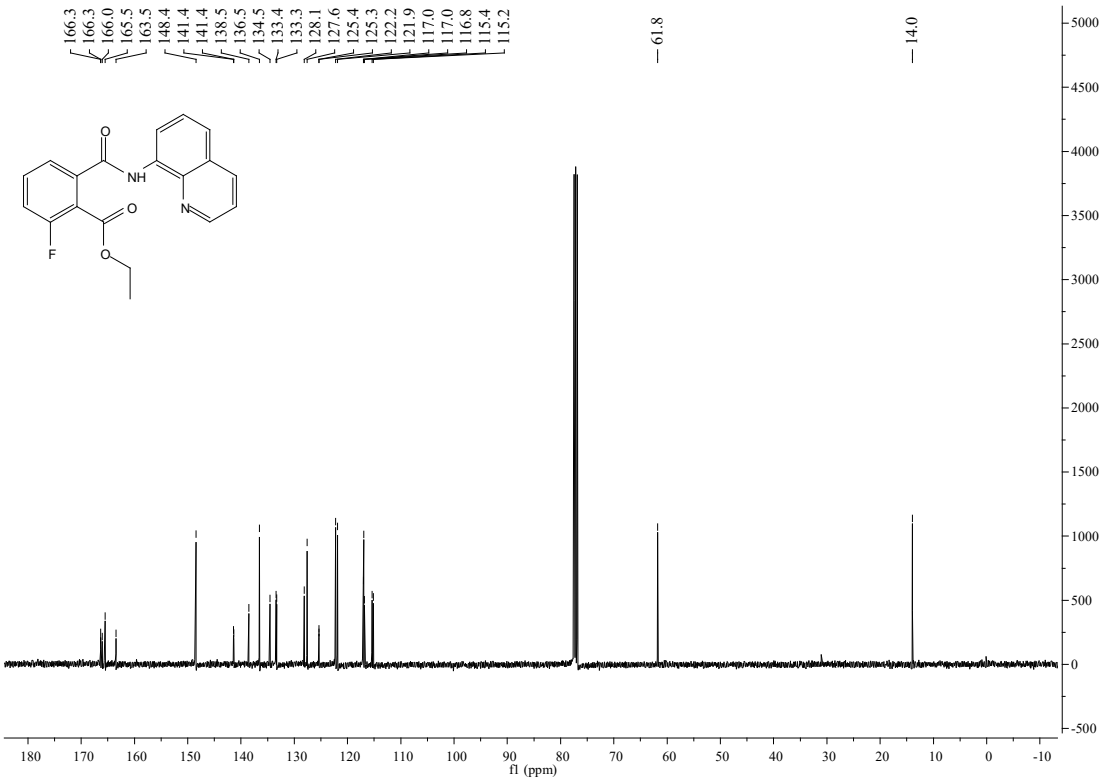

-58.7
F
F
F
O
NH
O
N
O
f1 (ppm)


165.2
164.6
148.4
138.5
136.7
136.7
136.7
136.5
134.5
134.3
130.6
130.3
130.2
130.2
130.1
129.7
128.8
128.5
128.2
128.1
127.6
124.8
122.2
122.1
121.8
117.1
62.2
13.9
F
F
F
O
NH
O
N
O
9000
8500
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

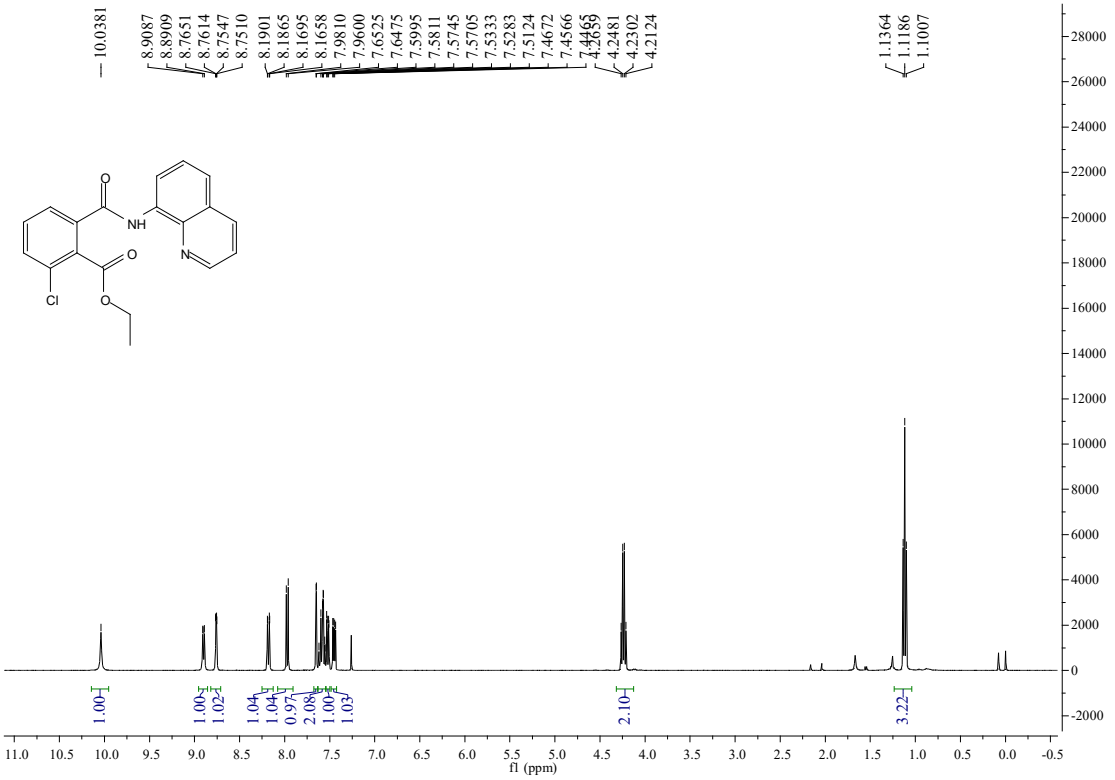
3e

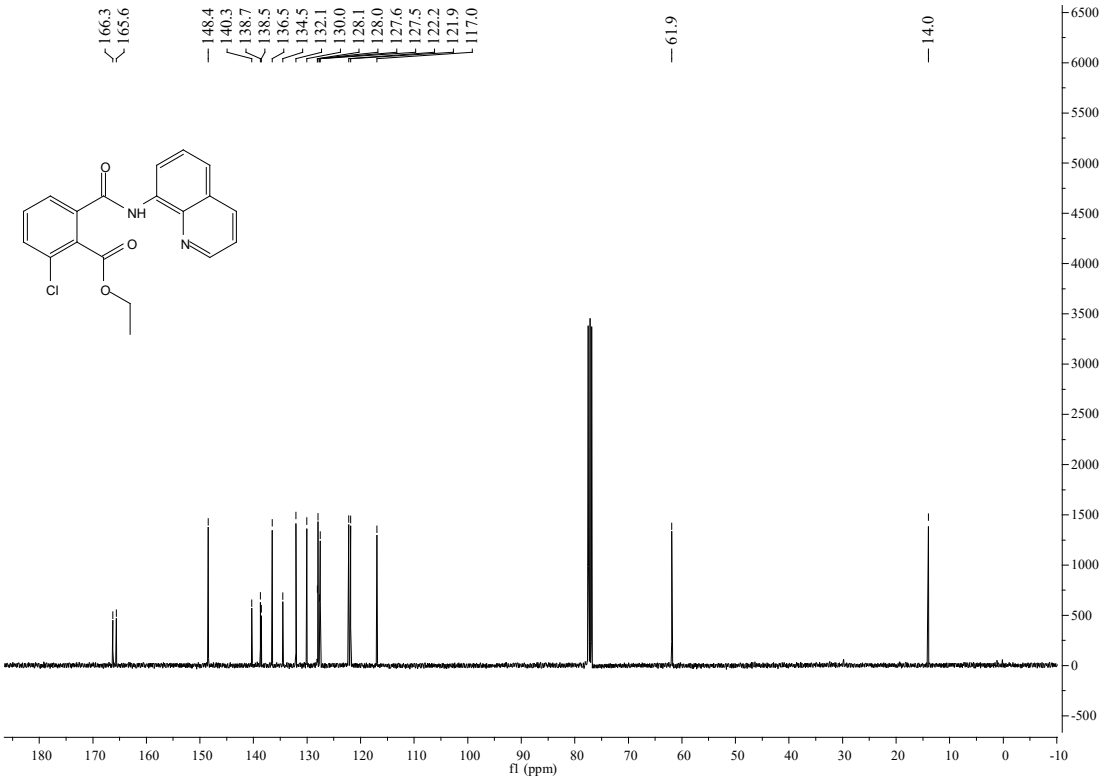

10.0347
8.9137
8.8986
8.8956
8.7639
8.7600
8.7534
8.7495
8.1922
8.1754
8.1715
7.6063
7.5880
7.5798
7.5758
7.4712
7.4606
7.4505
7.4399
7.3790
7.3726
7.3582
7.3519
7.2616
7.2393
7.2330
4.2639
4.2461
4.2282
4.2104
1.1375
1.1196
1.1018
O
NH
N
O
F
O
1.00
1.06
1.07
1.08
1.06
2.14
1.07
1.06
1.32
2.24
3.23
fl (ppm)


-105.4
O
NH
N
O
F
O
fl (ppm)

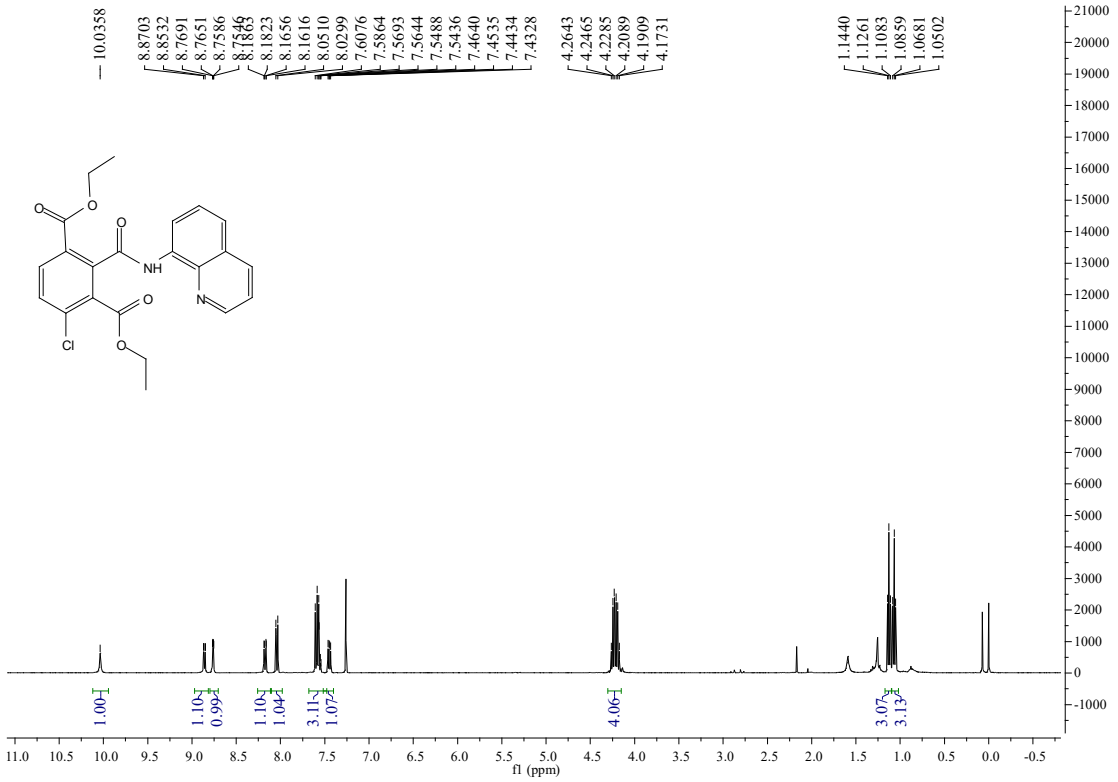

166.3
166.3
166.0
165.5
163.5
148.4
141.4
141.4
138.5
136.5
134.5
133.4
133.3
128.1
127.6
125.4
125.3
122.2
121.9
117.0
117.0
116.8
115.4
115.2
61.8
14.0
O
NH
O
N
F
O
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

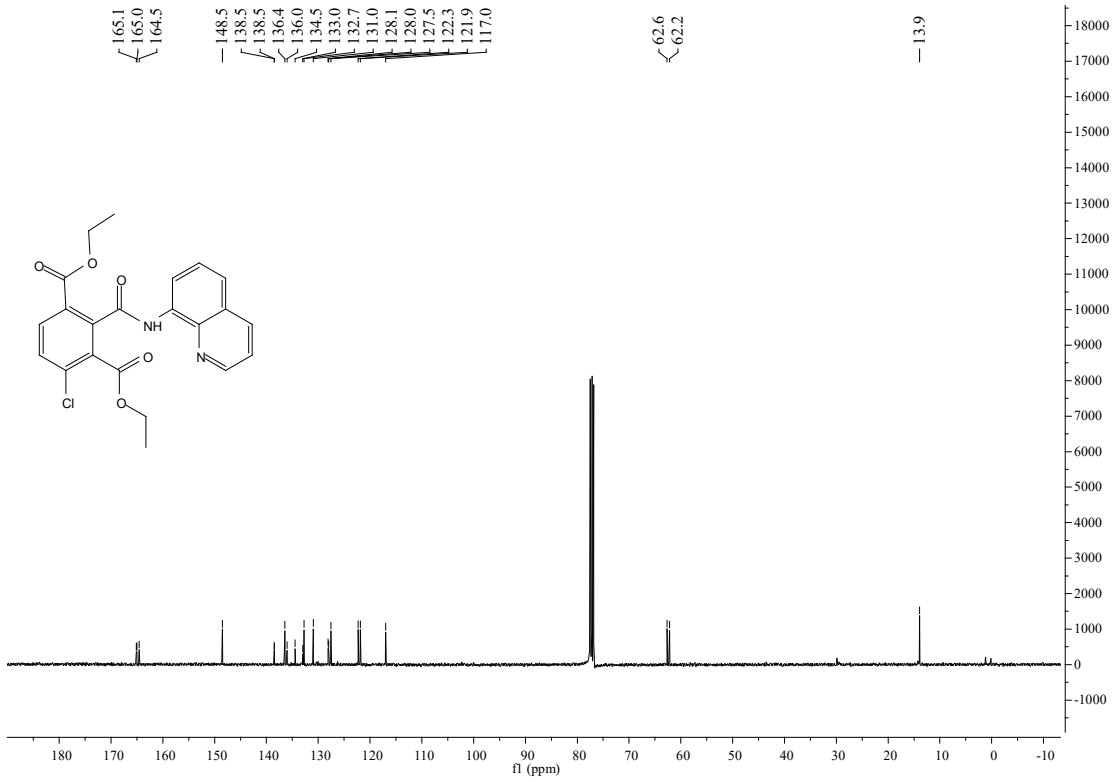
3fa


10.0381
8.9087
8.8909
8.7651
8.7614
8.7547
8.7510
8.1901
8.1865
8.1695
8.1658
7.9810
7.9600
7.6525
7.6475
7.5995
7.5811
7.5745
7.5705
7.5333
7.5283
7.5124
7.4672
7.4566
4.2481
4.2302
4.2124
1.1364
1.1186
1.1007
NH
N
O
Cl
1.00
1.00
1.02
1.04
1.04
0.97
2.08
1.00
1.03
2.10
3.22
fl (ppm)

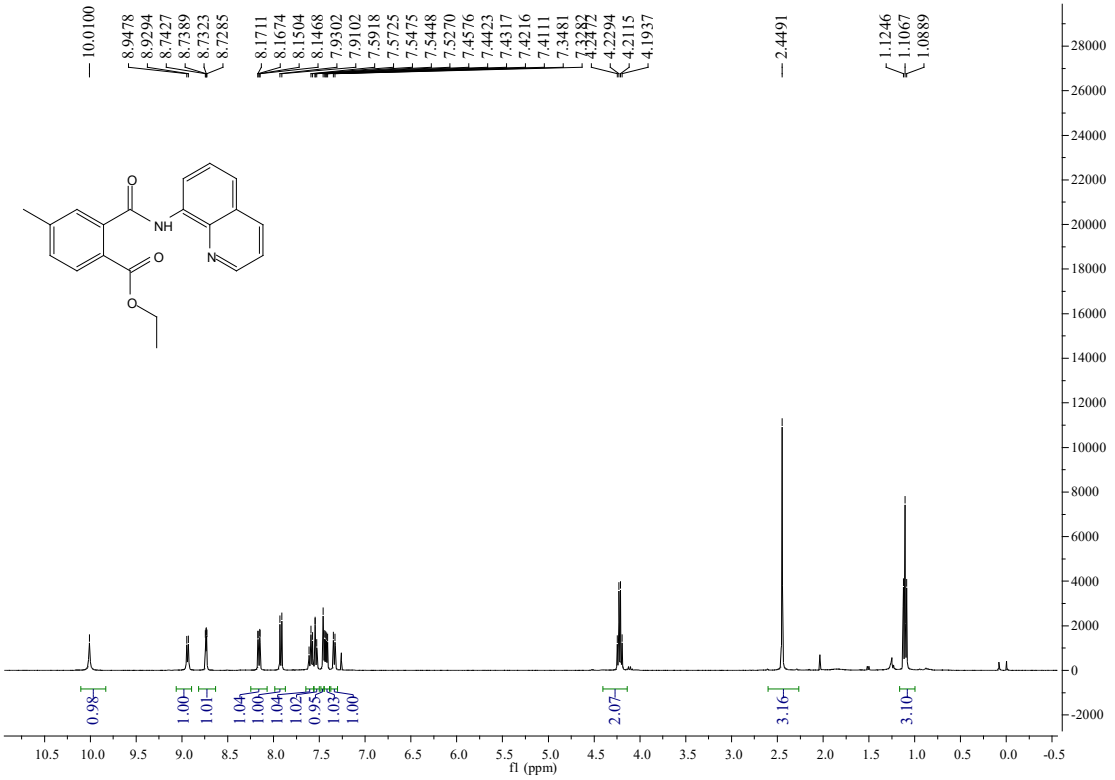

166.3
165.6
148.4
140.3
138.7
138.5
136.5
134.5
132.1
130.0
128.1
128.0
127.6
127.5
122.2
121.9
117.0
61.9
14.0
NH
N
O
Cl
fl (ppm)

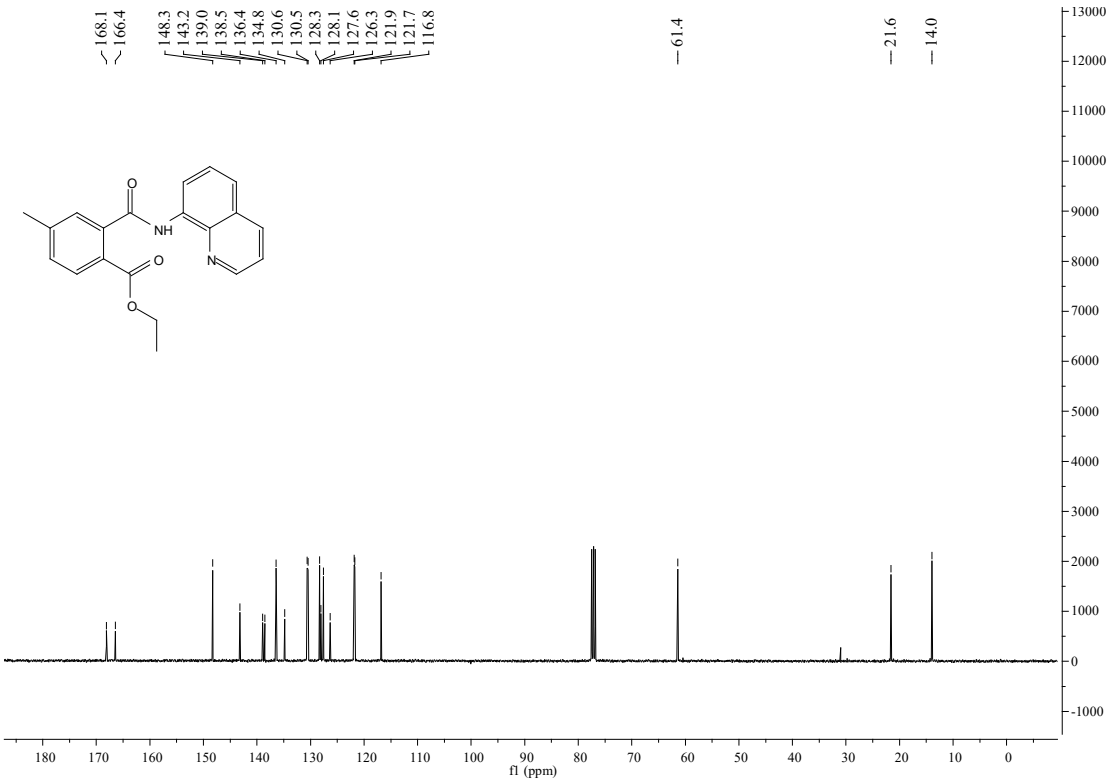
3fb


10.0358
8.8703
8.8532
8.7691
8.7651
8.7586
8.1823
8.1656
8.1616
8.0510
8.0299
7.6076
7.5864
7.5693
7.5644
7.5488
7.5436
7.4640
7.4535
7.4434
7.4328
4.2643
4.2465
4.2285
4.2089
4.1909
4.1731
1.1440
1.1261
1.1083
1.0859
1.0681
1.0502
1.00
1.10
0.99
1.10
1.04
3.11
1.07
4.06
3.07
3.13
f1 (ppm)

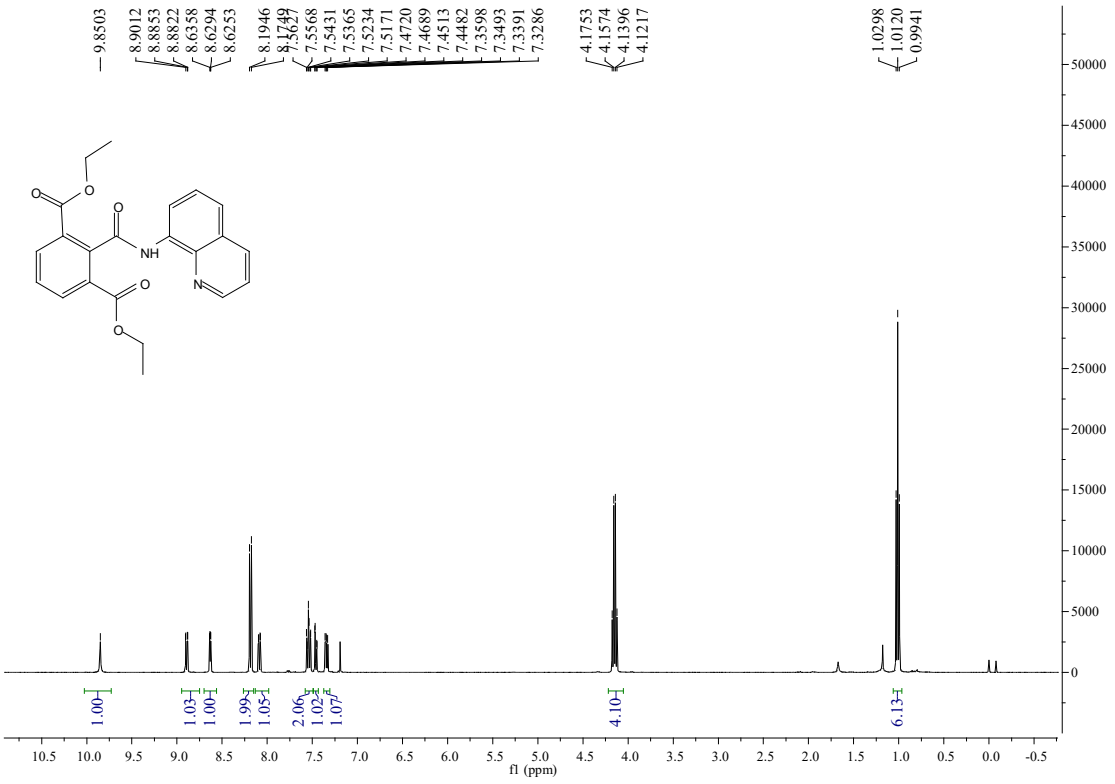

165.1
165.0
164.5
148.5
138.5
138.5
136.4
136.0
134.5
133.0
132.7
131.0
128.1
128.0
127.5
122.3
121.9
117.0
62.6
62.2
13.9
f1 (ppm)

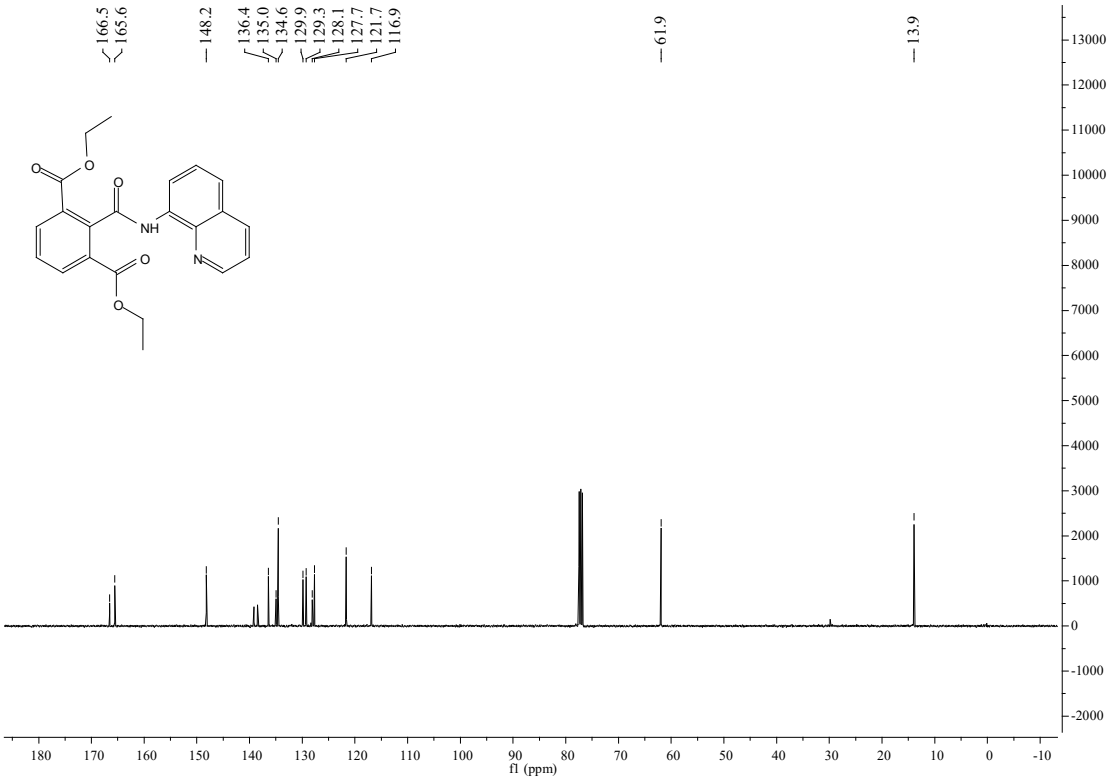
3g


10.0100
8.9478
8.9294
8.7427
8.7389
8.7323
8.7285
8.1711
8.1674
8.1504
8.1468
7.9302
7.9102
7.5918
7.5725
7.5475
7.5448
7.5270
7.4576
7.4423
7.4317
7.4216
7.4111
7.3481
7.3282
4.2472
4.2294
4.2115
4.1937
2.4491
1.1246
1.1067
1.0889
O
NH
N
O
O
0.98
1.00
1.01
1.04
1.00
1.04
1.02
0.95
1.03
1.00
2.07
3.16
3.10
fl (ppm)

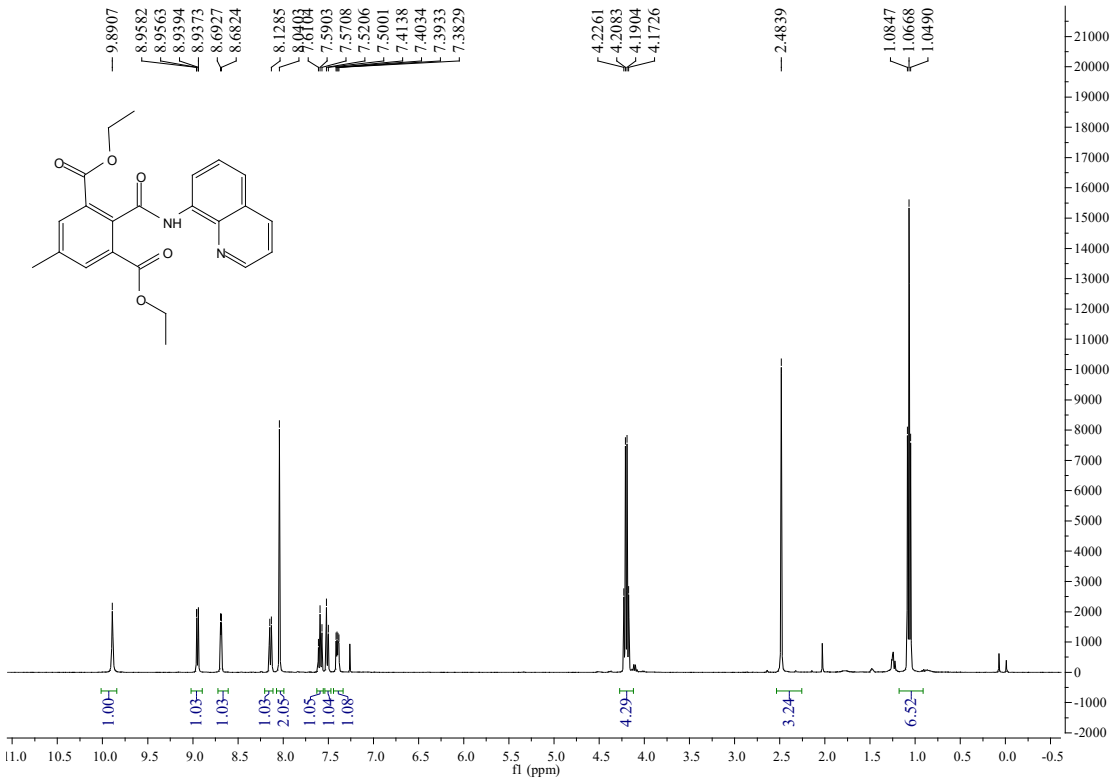

168.1
166.4
148.3
143.2
139.0
138.5
136.4
134.8
130.6
130.5
128.3
128.1
127.6
126.3
121.9
121.7
116.8
61.4
21.6
14.0
O
NH
N
O
O
fl (ppm)

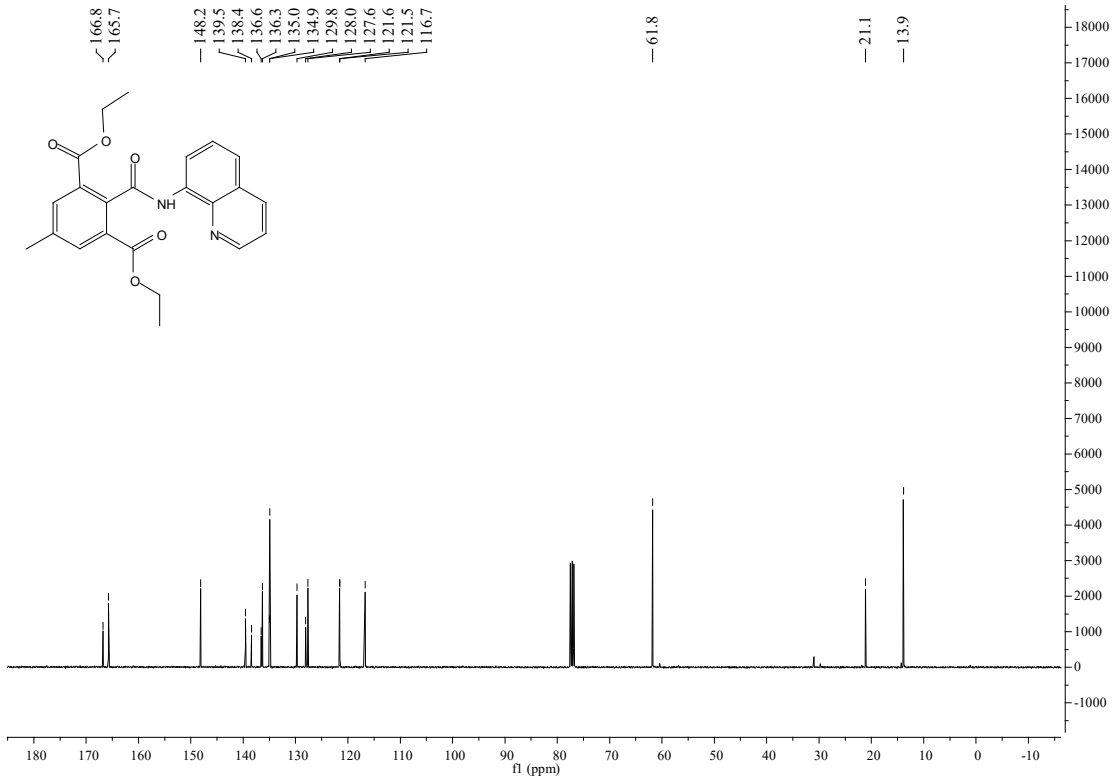
3h


9.8503
8.9012
8.8853
8.8822
8.6358
8.6294
8.6253
8.1946
8.1749
8.1627
7.5568
7.5431
7.5365
7.5234
7.5171
7.4720
7.4689
7.4513
7.4482
7.3598
7.3493
7.3391
7.3286
4.1753
4.1574
4.1396
4.1217
1.0298
1.0120
0.9941
1.00
1.03
1.00
1.99
1.05
2.06
1.02
1.07
4.10
6.13
f1 (ppm)

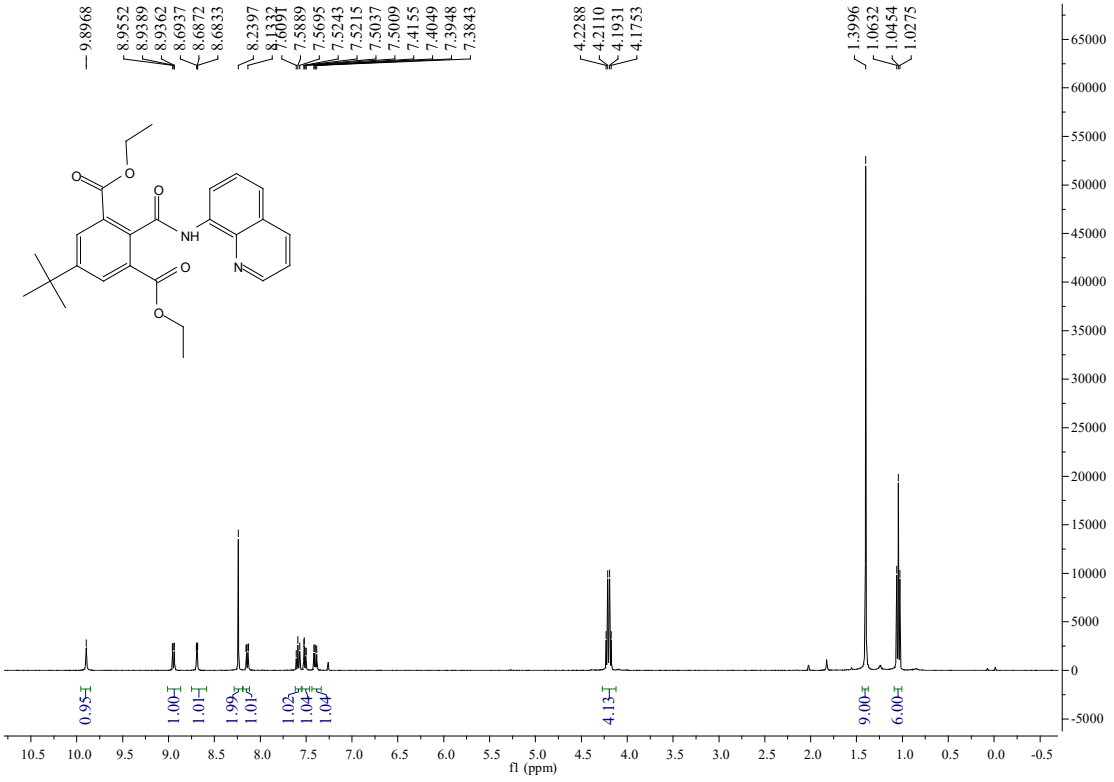

166.5
165.6
148.2
136.4
135.0
134.6
129.9
129.3
128.1
127.7
121.7
116.9
61.9
13.9
f1 (ppm)

3i


9.8907
8.9582
8.9563
8.9394
8.9373
8.6927
8.6824
8.1285
8.0403
7.6104
7.5903
7.5708
7.5206
7.5001
7.4138
7.4034
7.3933
7.3829
4.2261
4.2083
4.1904
4.1726
2.4839
1.0847
1.0668
1.0490
1.00
1.03
1.03
1.03
2.05
1.05
1.04
1.08
4.29
3.24
6.52
f1 (ppm)


166.8
165.7
148.2
139.5
138.4
136.6
136.3
135.0
134.9
129.8
128.0
127.6
121.6
121.5
116.7
61.8
21.1
13.9
f1 (ppm)

3j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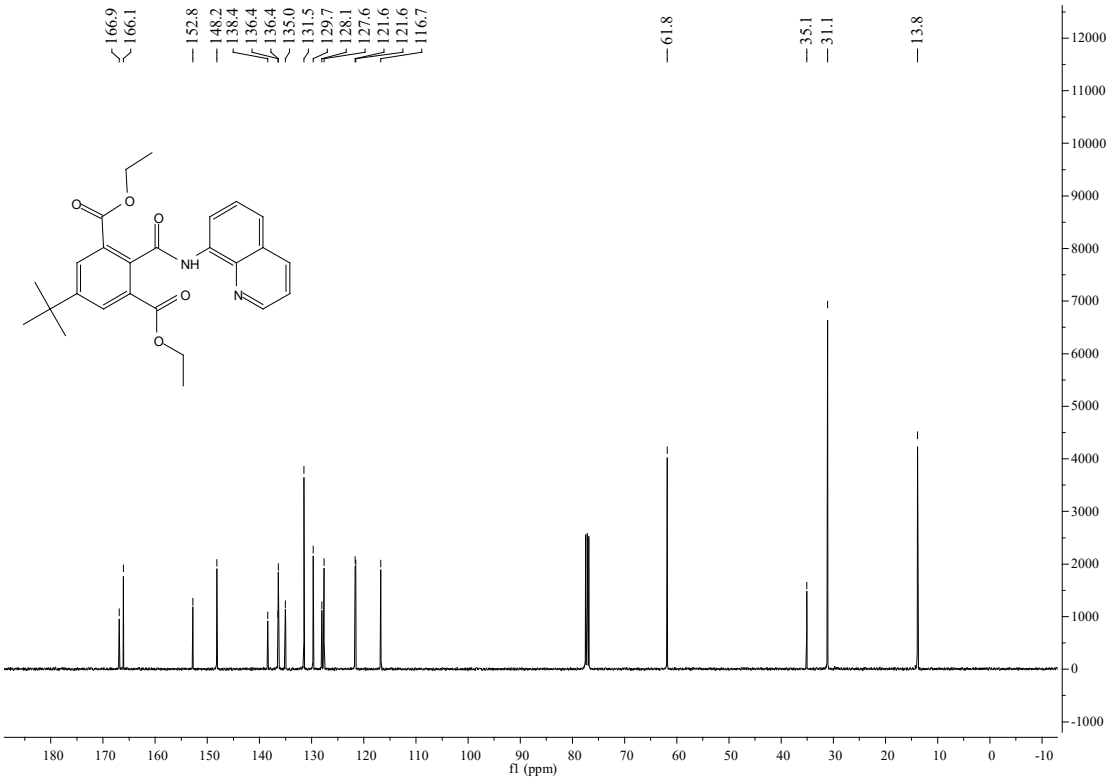
8.9362
8.6937
8.6872
8.6833
8.2397
8.1332
7.6091
7.5889
7.5695
7.5243
7.5215
7.5037
7.5009
7.4155
7.4049
7.3948
7.3843
4.2288
4.2110
4.1931
4.1753
1.3996
1.0632
1.0454
1.0275
0.95
1.00
1.01
1.99
1.01
1.02
1.04
1.04
4.13
9.00
6.00
f1 (ppm)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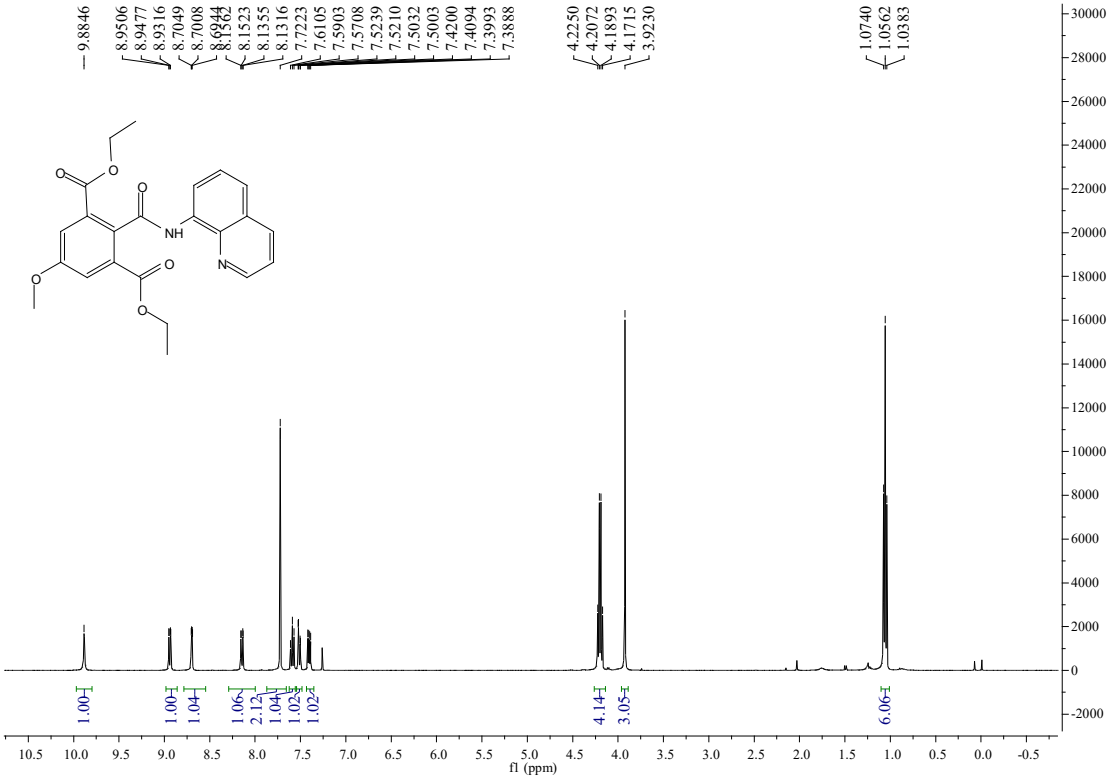
166.1
152.8
148.2
138.4
136.4
136.4
135.0
131.5
129.7
128.1
127.6
121.6
121.6
116.7
61.8
35.1
31.1
13.8
f1 (ppm)

3k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8.9477
8.9316
8.7049
8.7008
8.6944
8.6862
8.1523
8.1355
8.1316
7.7223
7.6105
7.5903
7.5708
7.5239
7.5210
7.5032
7.5003
7.4200
7.4094
7.3993
7.3888
4.2250
4.2072
4.1893
4.1715
3.9230
1.0740
1.0562
1.0383
NH
N
1.00
1.00
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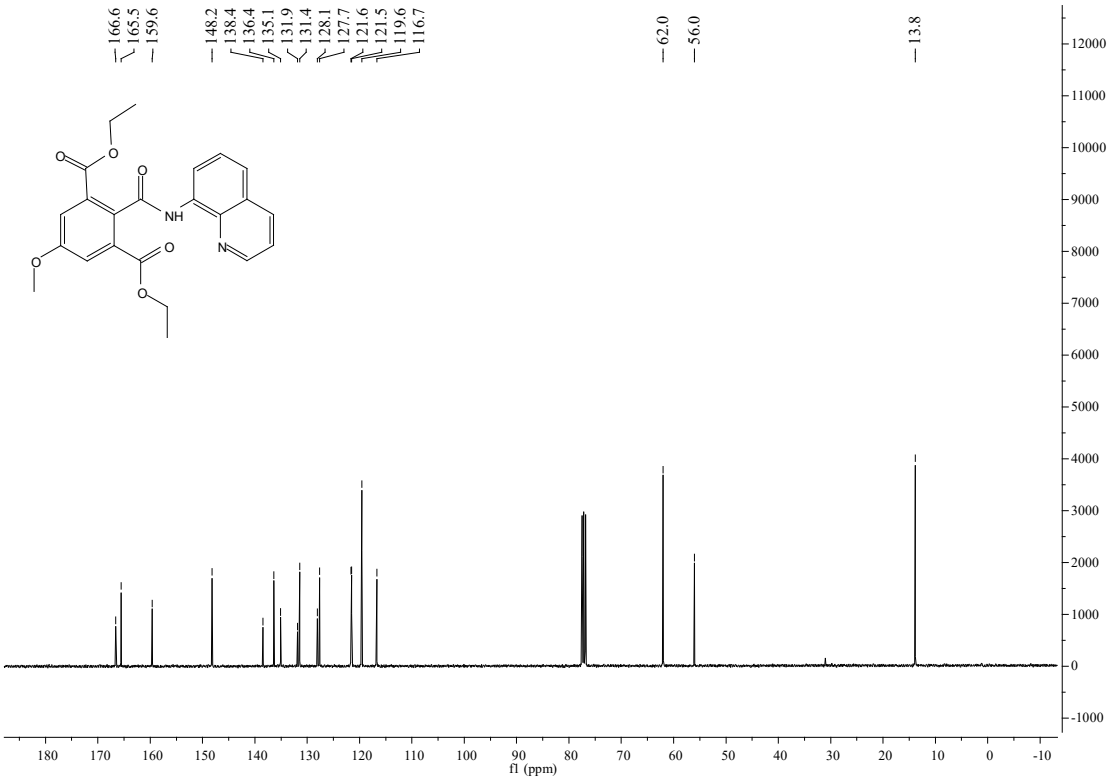
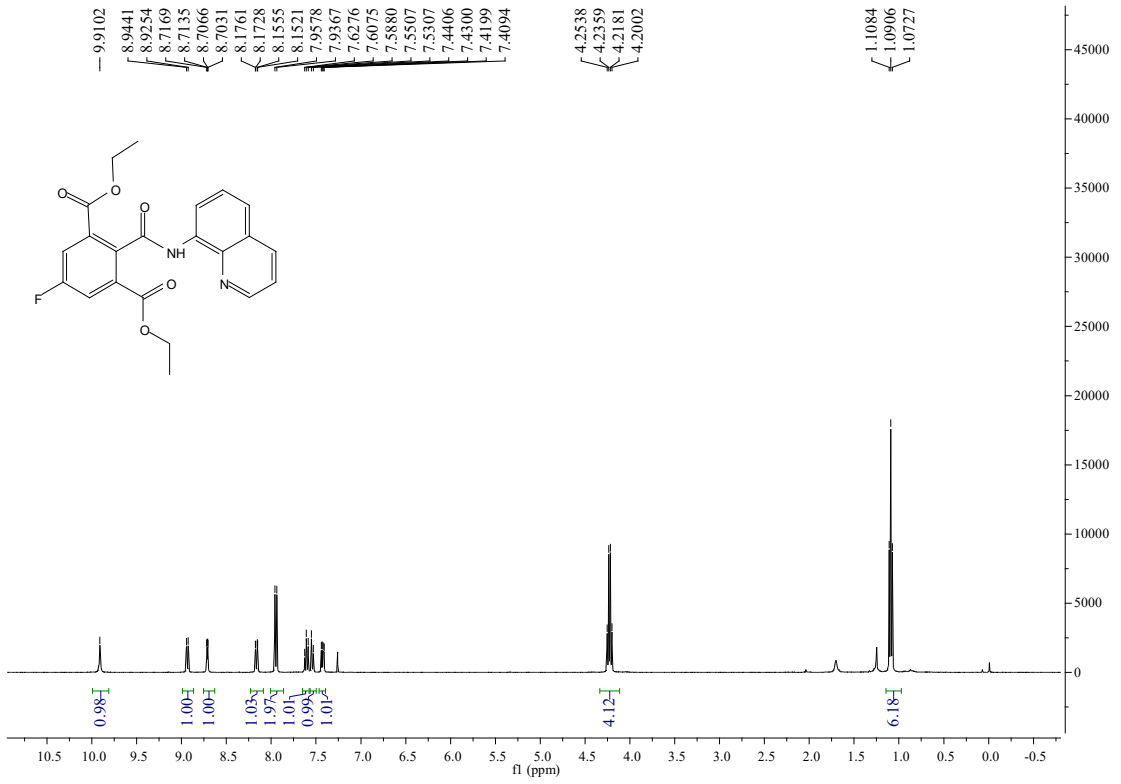
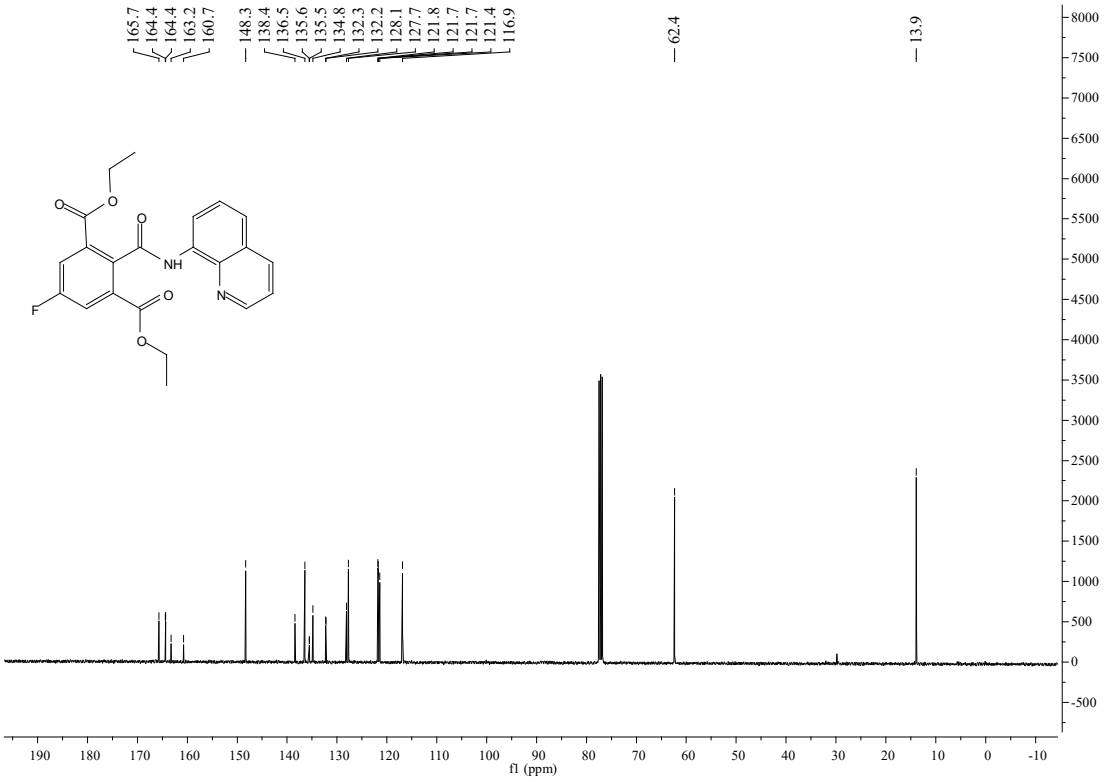
1.06
2.12
1.04
1.02
1.02
4.14
3.05
6.06
f1 (ppm)


166.6
165.5
159.6
148.2
138.4
136.4
135.1
131.9
131.4
128.1
127.7
121.6
121.5
119.6
116.7
62.0
56.0
13.8
NH
N
f1 (ppm)

3l


9.9102
8.9441
8.9254
8.7169
8.7135
8.7066
8.7031
8.1761
8.1728
8.1555
8.1521
7.9578
7.9367
7.6276
7.6075
7.5880
7.5507
7.5307
7.4406
7.4300
7.4199
7.4094
4.2538
4.2359
4.2181
4.2002
1.1084
1.0906
1.0727
0.98
1.00
1.00
1.03
1.97
1.01
0.99
1.01
4.12
6.18
f1 (ppm)


-109.6
f1 (ppm)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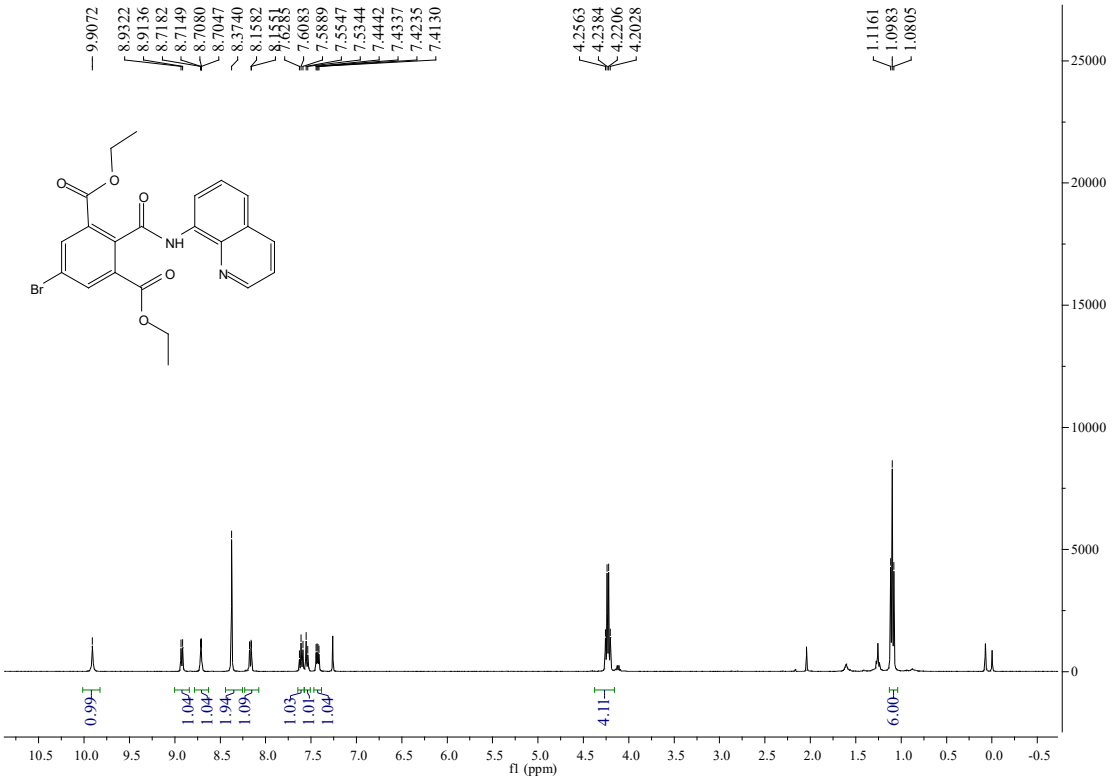
164.4
164.4
163.2
160.7
148.3
138.4
136.5
135.6
135.5
134.8
132.3
132.2
128.1
127.7
121.8
121.7
121.7
121.4
116.9
62.4
13.9
O
O
NH
O
F
O
O
N
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3m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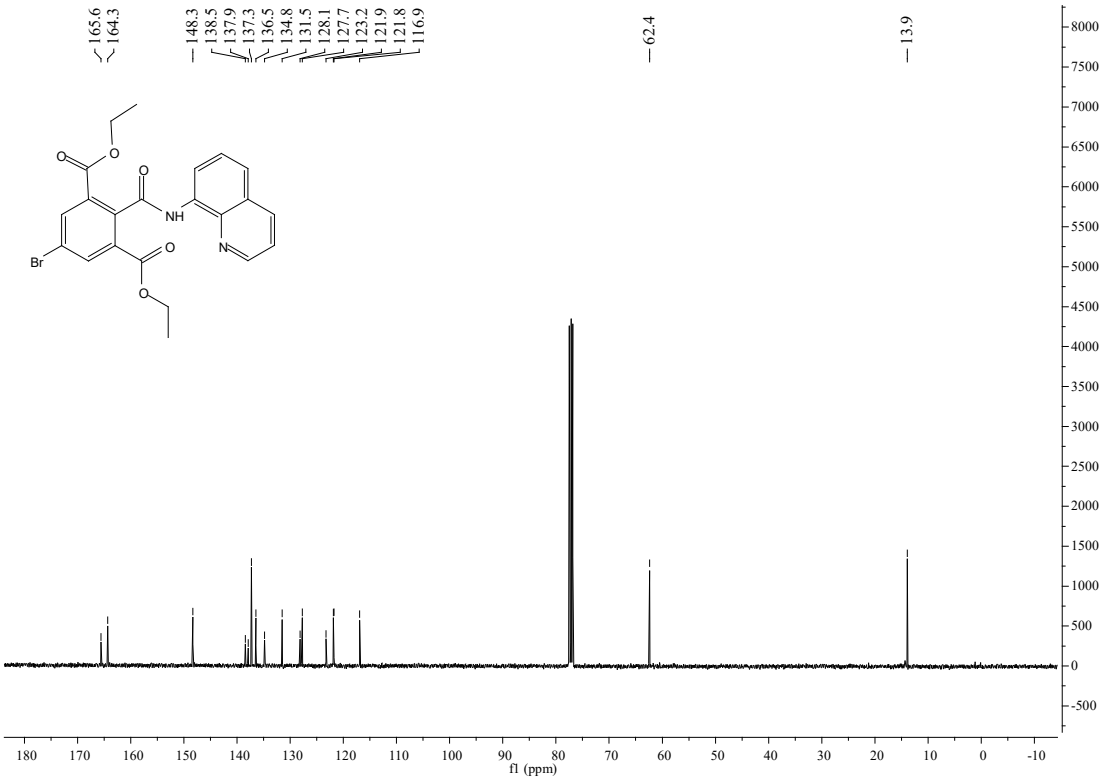
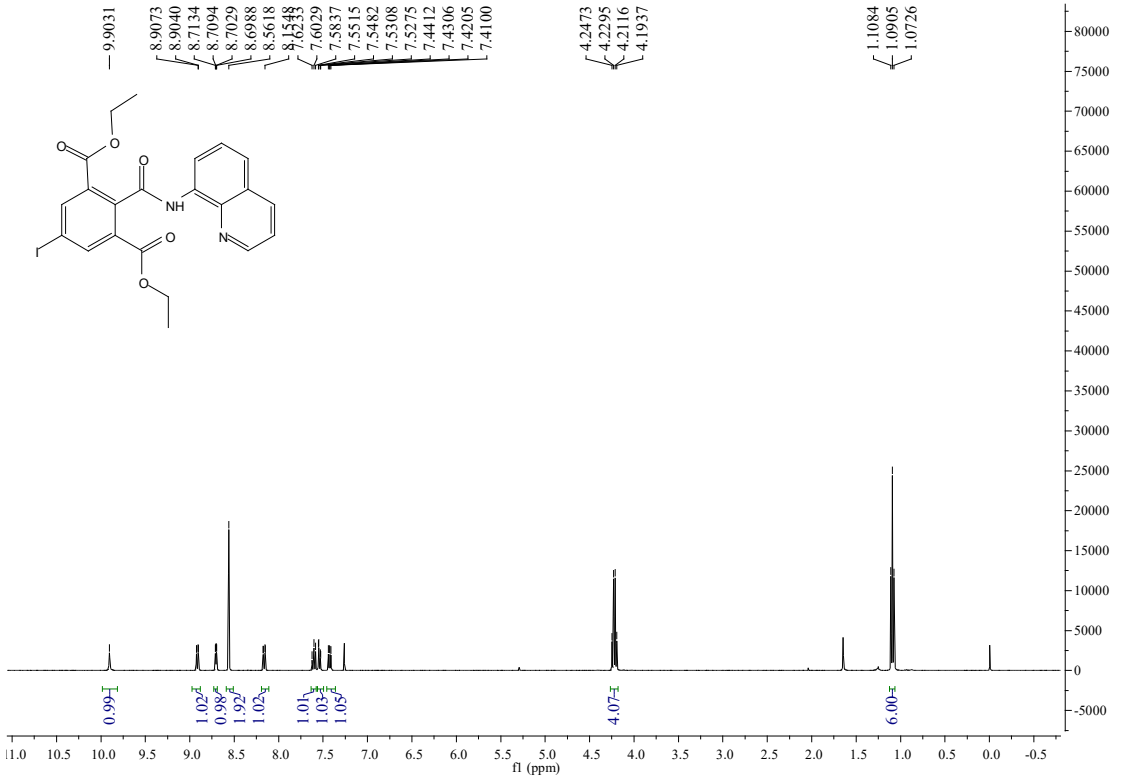
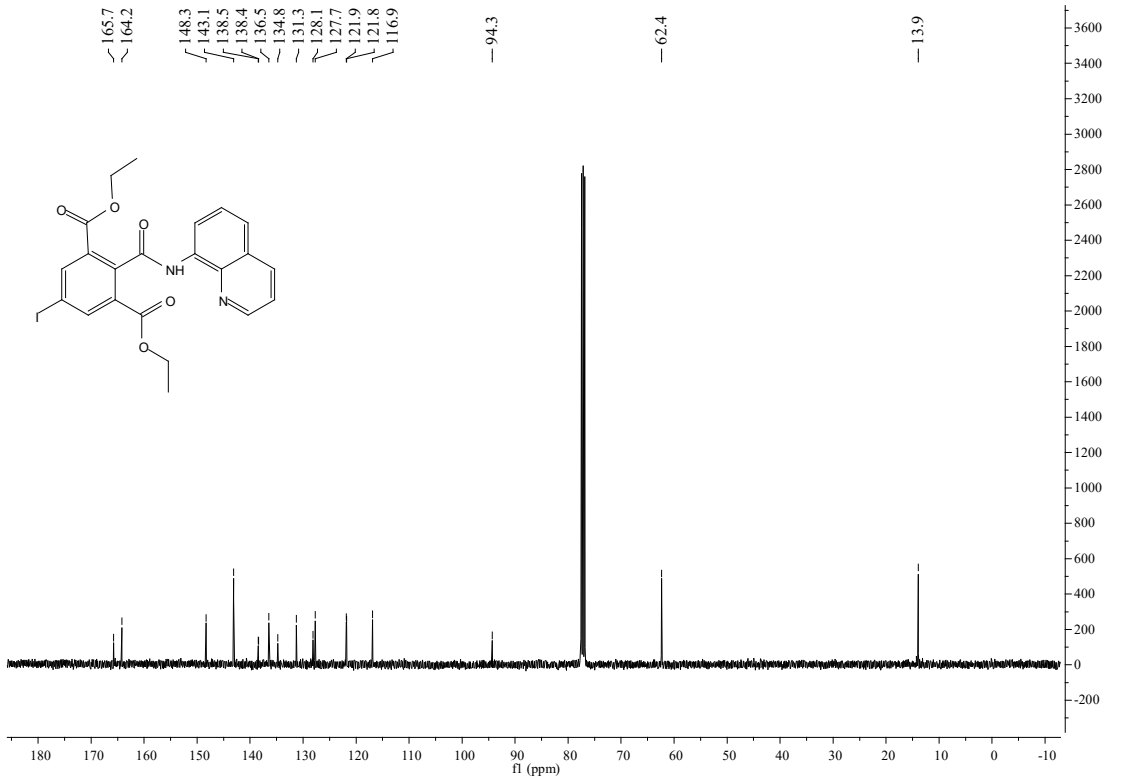
8.7047
8.3740
8.1582
8.1551
7.6285
7.6083
7.5889
7.5547
7.5344
7.4442
7.4337
7.4235
7.4130
4.2563
4.2384
4.2206
4.2028
1.1161
1.0983
1.0805
0.99
1.04
1.04
1.94
1.09
1.03
1.01
1.04
4.11
6.00
f1 (ppm)

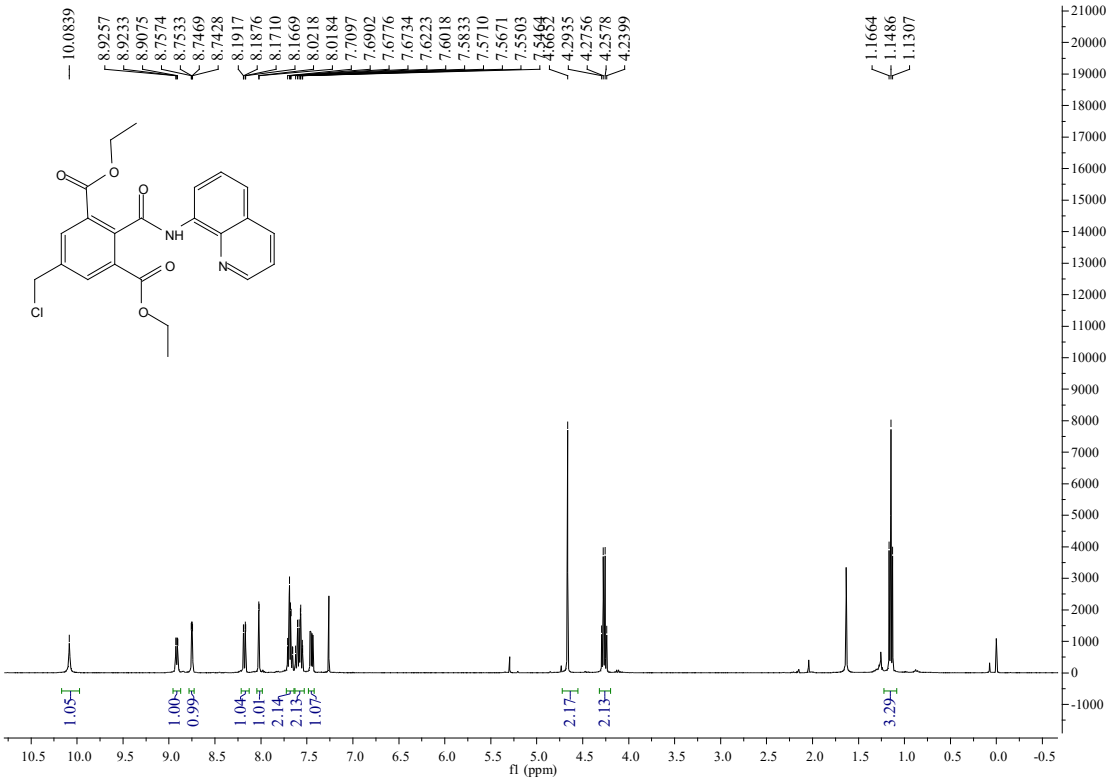

165.6
164.3
148.3
138.5
137.9
137.3
136.5
134.8
131.5
128.1
127.7
123.2
121.9
121.8
116.9
62.4
13.9
f1 (ppm)

3n


9.9031
8.9073
8.9040
8.7134
8.7094
8.7029
8.6988
8.5618
8.1548
8.1533
7.6233
7.6029
7.5837
7.5515
7.5482
7.5308
7.5275
7.4412
7.4306
7.4205
7.4100
4.2473
4.2295
4.2116
4.1937
1.1084
1.0905
1.0726
0.99
1.02
0.98
1.92
1.02
1.01
1.03
1.05
4.07
6.00
f1 (ppm)


165.7
164.2
148.3
143.1
138.5
138.4
136.5
134.8
131.3
128.1
127.7
121.9
121.8
116.9
94.3
62.4
13.9
f1 (ppm)

3o


10.0839
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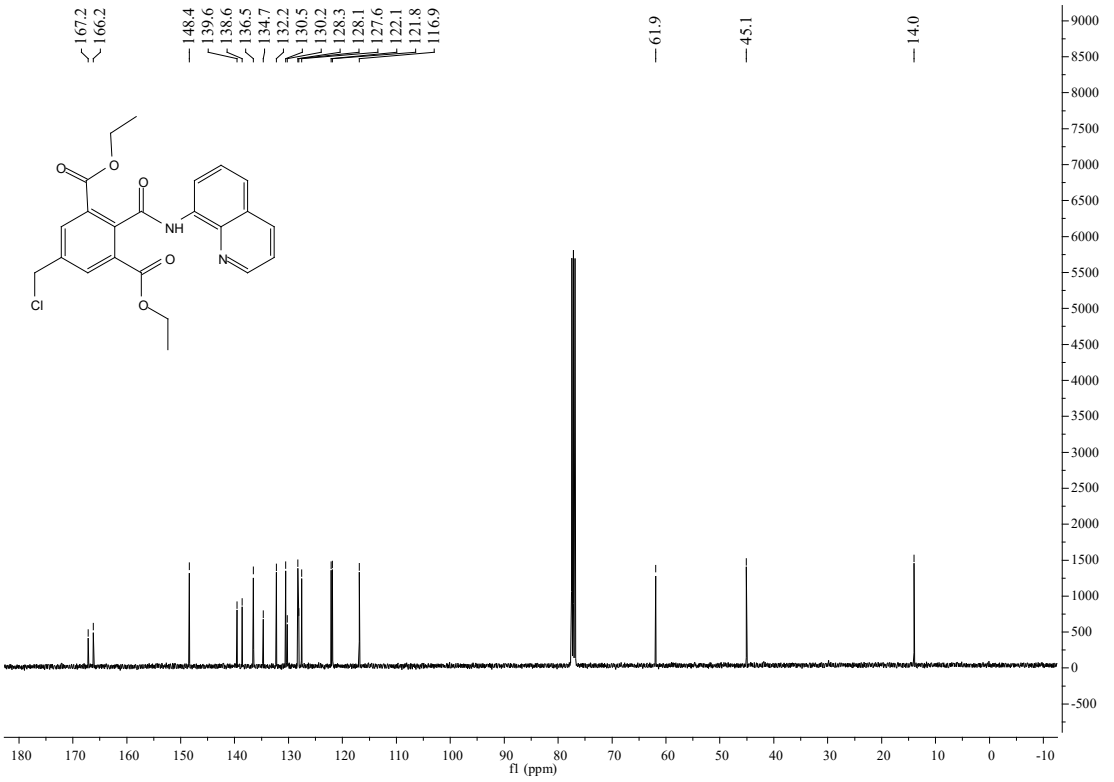
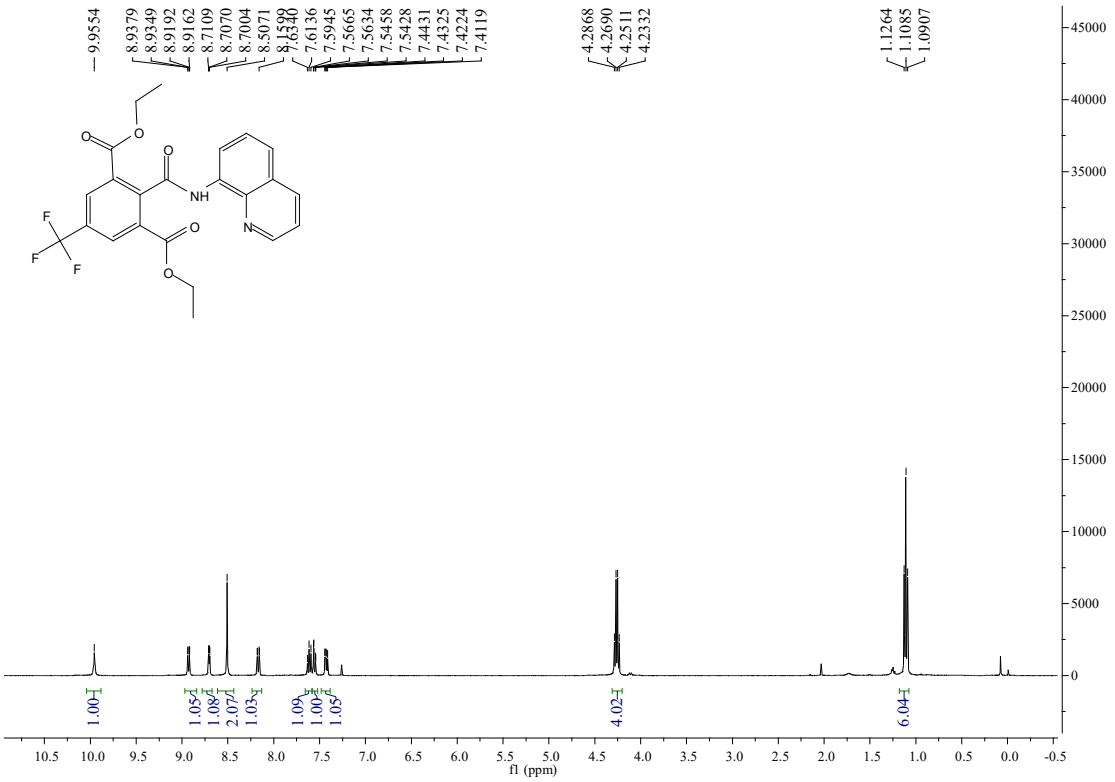
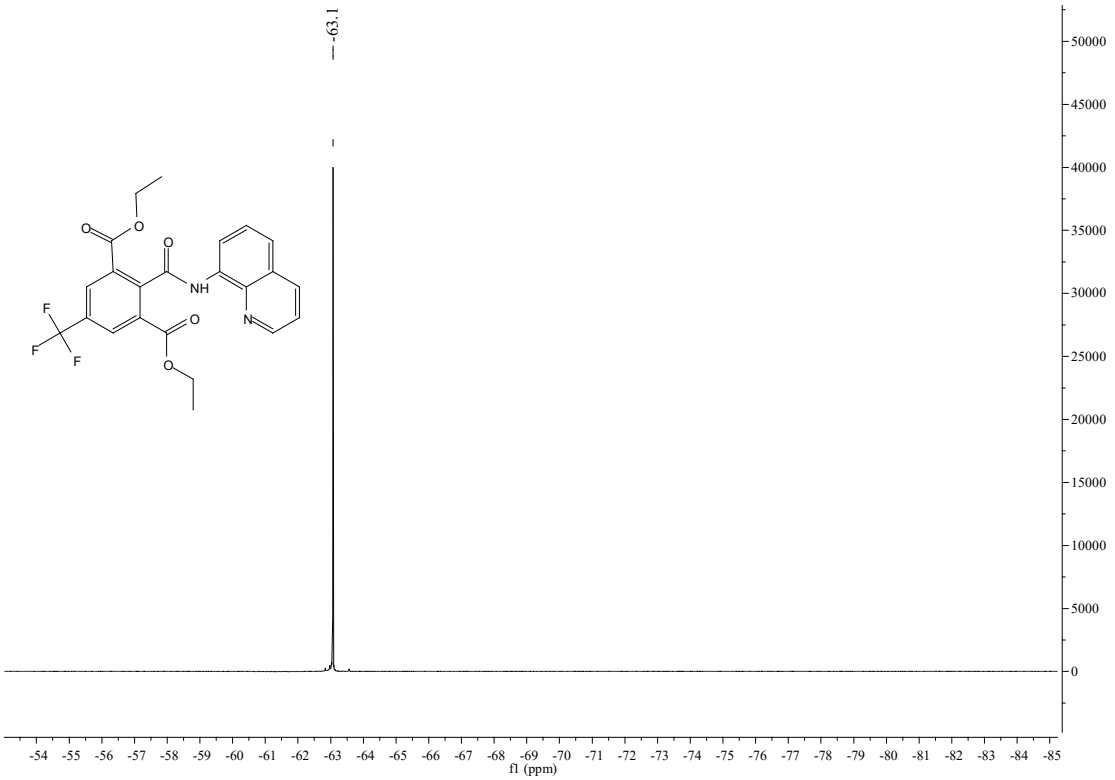
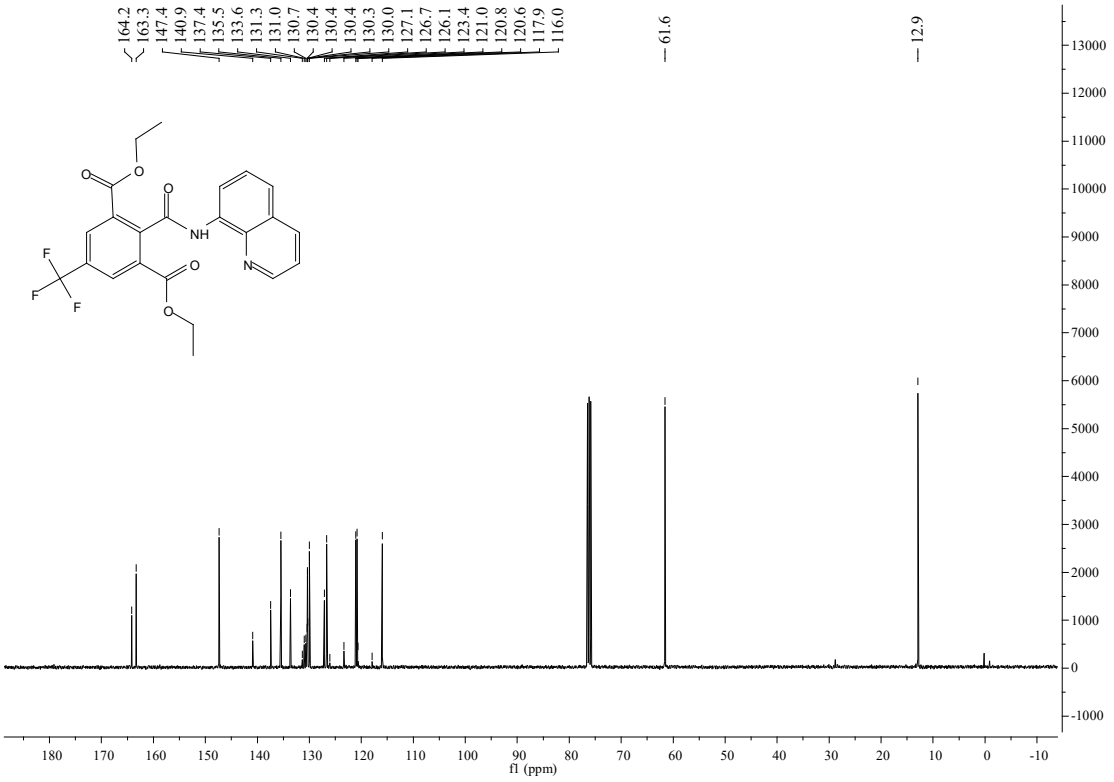
8.9233
8.9075
8.7574
8.7533
8.7469
8.7428
8.1917
8.1876
8.1710
8.1669
8.0218
8.0184
7.7097
7.6902
7.6776
7.6734
7.6223
7.6018
7.5833
7.5710
7.5671
7.5503
7.5464
4.6652
4.2935
4.2756
4.2578
4.2399
1.1664
1.1486
1.1307
1.05
1.00
0.99
1.04
1.01
2.14
2.13
1.07
2.17
2.13
3.29
fl (ppm)


167.2
166.2
148.4
139.6
138.6
136.5
134.7
132.2
130.5
130.2
128.3
128.1
127.6
122.1
121.8
116.9
61.9
45.1
14.0
fl (ppm)

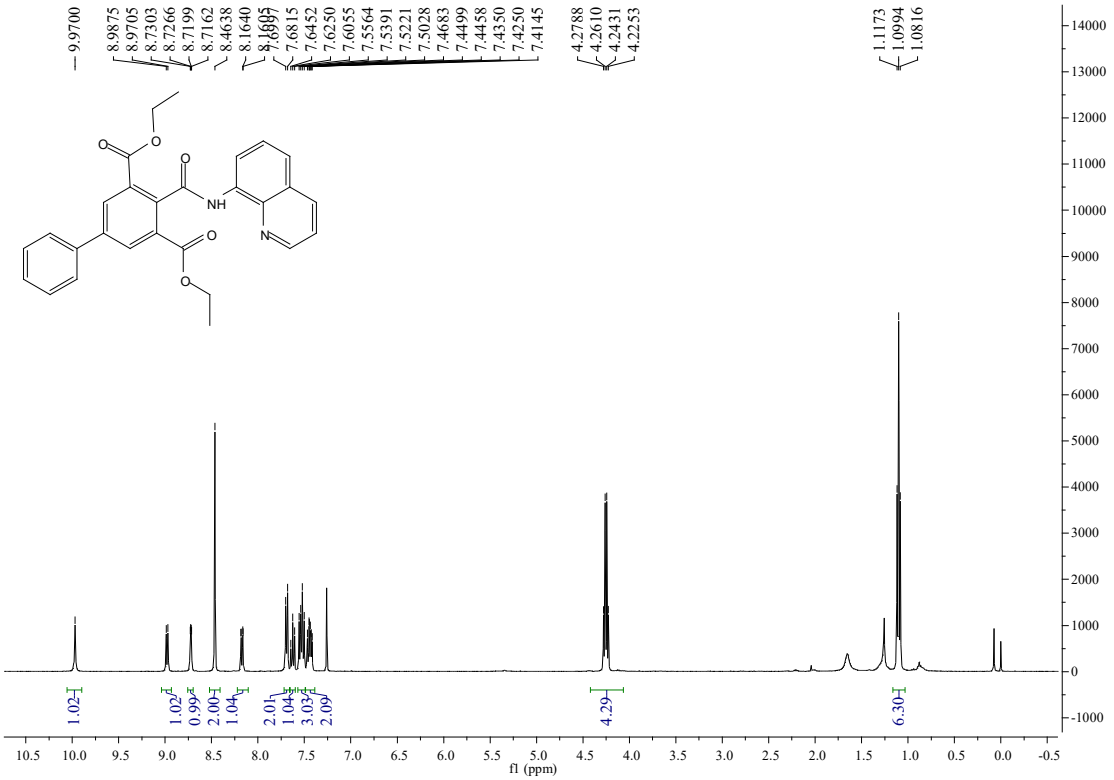
3p

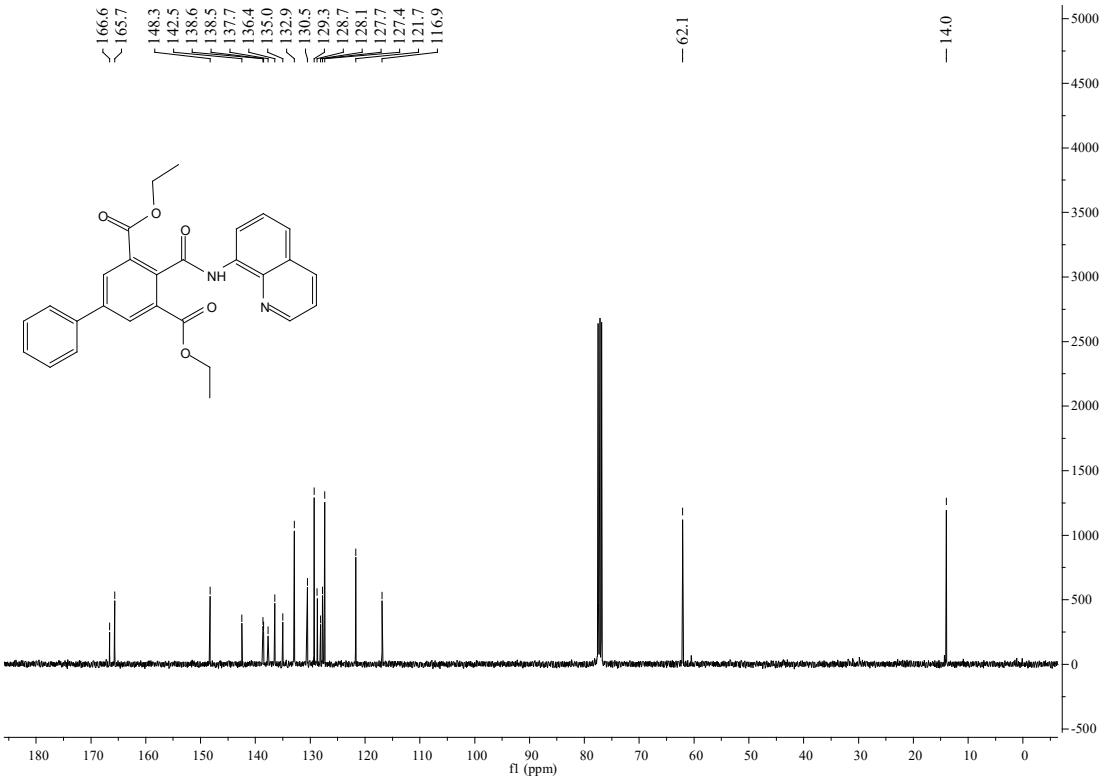

9.9554
8.9379
8.9349
8.9192
8.9162
8.7109
8.7070
8.7004
8.5071
8.1599
8.1340
7.6136
7.5945
7.5665
7.5634
7.5458
7.5428
7.4431
7.4325
7.4224
7.4119
4.2868
4.2690
4.2511
4.2332
1.1264
1.1085
1.0907
1.00
1.05
1.08
2.07
1.03
1.09
1.00
1.05
4.02
6.04
f1 (ppm)


-63.1
f1 (ppm)

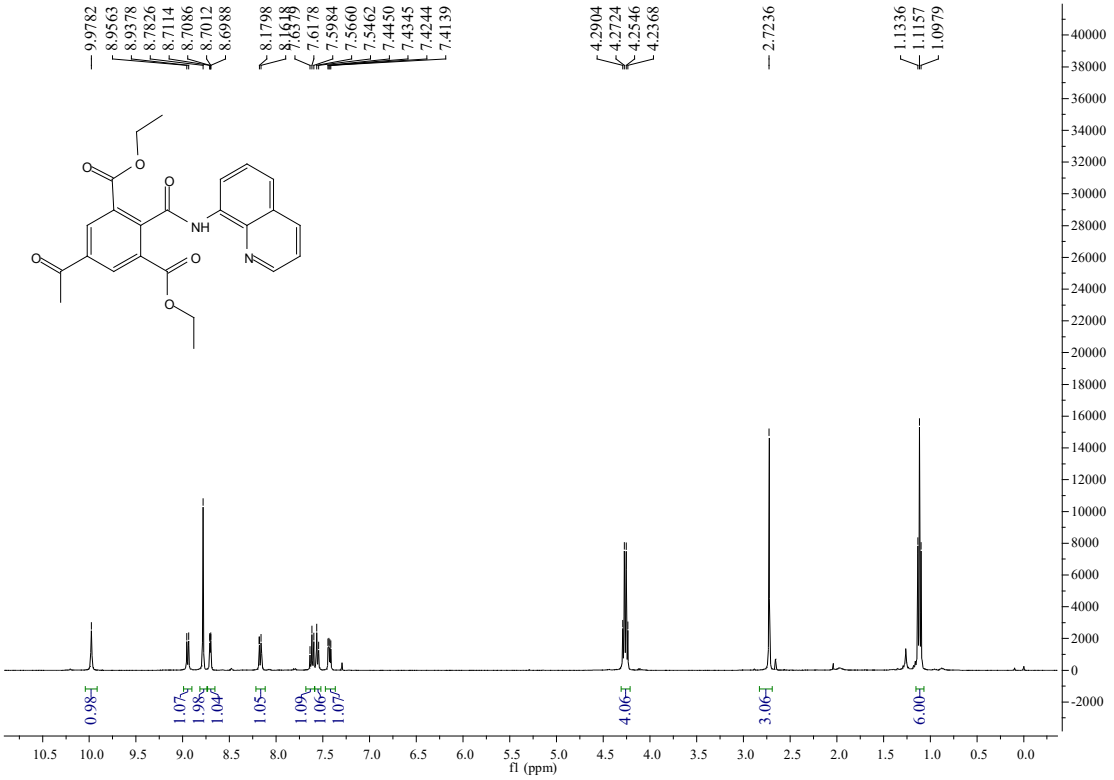

164.2
163.3
147.4
140.9
137.4
135.5
133.6
131.3
131.0
130.7
130.4
130.4
130.4
130.3
130.0
127.1
126.7
126.1
123.4
121.0
120.8
120.6
117.9
116.0
61.6
12.9
O
O
O
NH
N
F
F
F
O
O
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

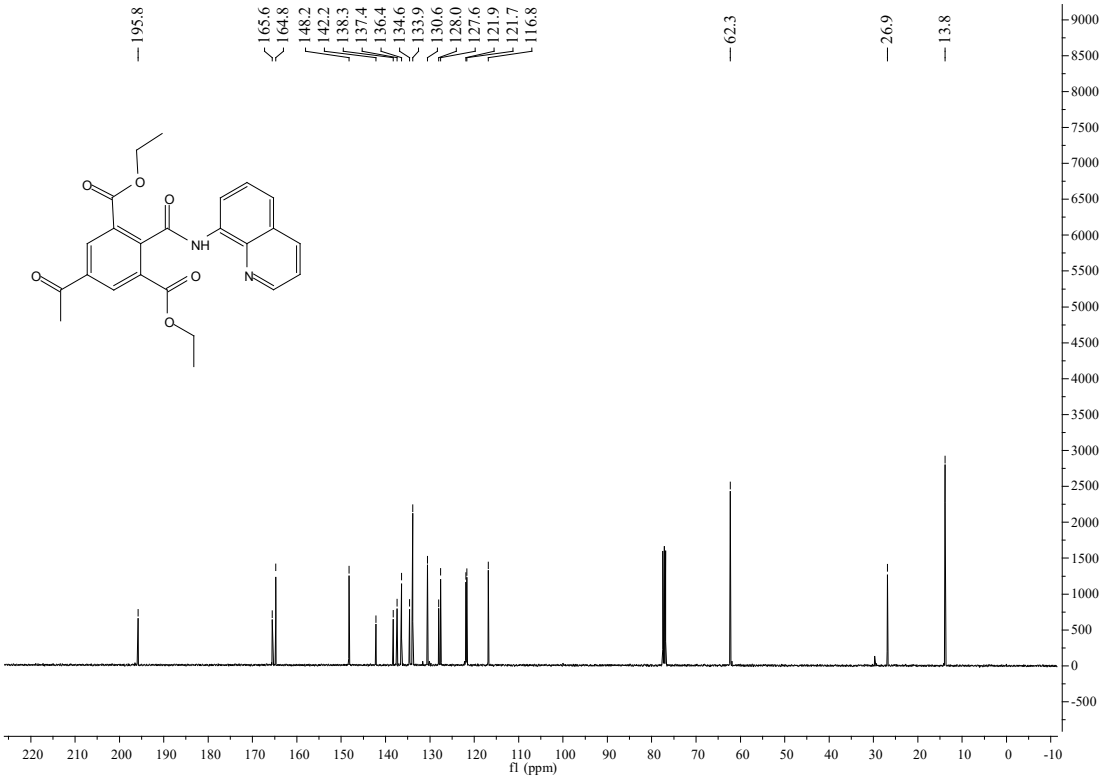
3q


9.9700
8.9875
8.9705
8.7303
8.7266
8.7199
8.7162
8.4638
8.1640
7.6815
7.6452
7.6250
7.6055
7.5564
7.5391
7.5221
7.5028
7.4683
7.4499
7.4458
7.4350
7.4250
7.4145
4.2788
4.2610
4.2431
4.2253
1.1173
1.0994
1.0816
1.02
1.02
0.99
2.00
1.04
2.01
1.04
3.03
2.09
4.29
6.30
O
O
O
NH
N
O
O
fl (ppm)

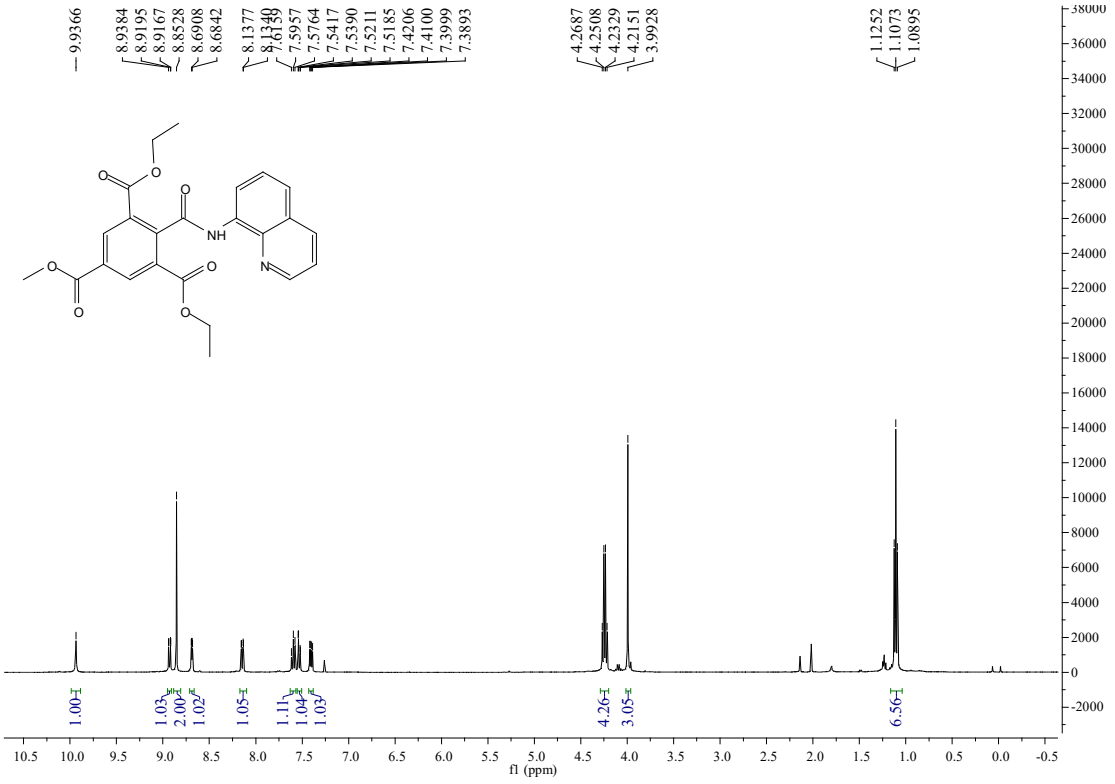

166.6
165.7
148.3
142.5
138.6
138.5
137.7
136.4
135.0
132.9
130.5
129.3
128.7
128.1
127.7
127.4
121.7
116.9
62.1
14.0
O
O
O
NH
N
O
O
fl (ppm)

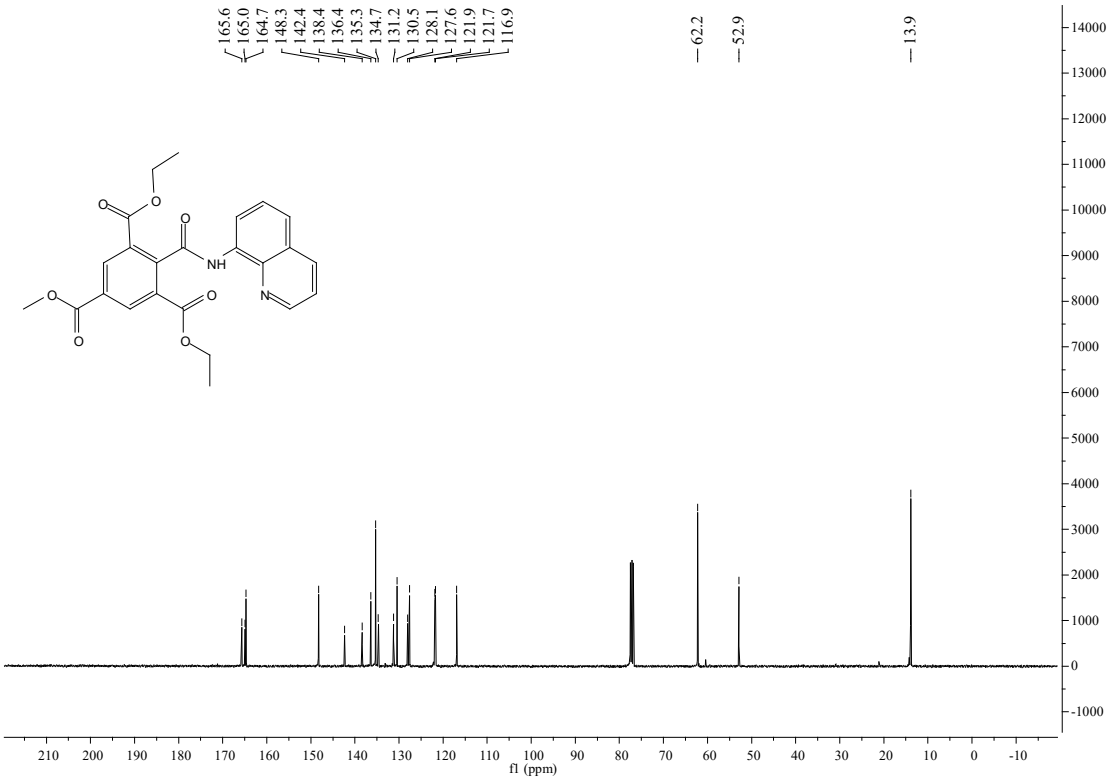
3r


9.9782
8.9563
8.9378
8.7826
8.7114
8.7086
8.7012
8.6988
8.1798
7.6178
7.5984
7.5660
7.5462
7.4450
7.4345
7.4244
7.4139
4.2904
4.2724
4.2546
4.2368
2.7236
1.1336
1.1157
1.0979
NH
N
0.98
1.07
1.98
1.04
1.05
1.09
1.06
1.07
4.06
3.06
6.00
f1 (ppm)

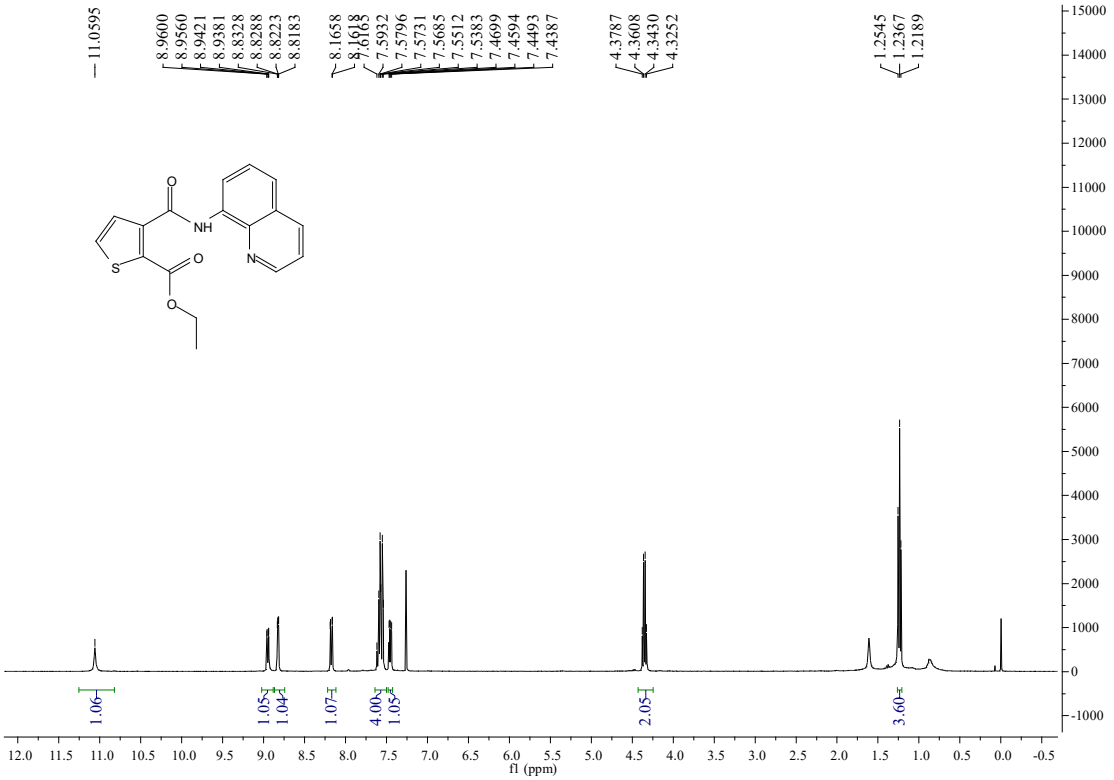

195.8
165.6
164.8
148.2
142.2
138.3
137.4
136.4
134.6
133.9
130.6
128.0
127.6
121.9
121.7
116.8
62.3
26.9
13.8
NH
N
f1 (ppm)

3s


9.9366
8.9384
8.9195
8.9167
8.8528
8.6908
8.6842
8.1377
8.1340
8.1139
7.5957
7.5764
7.5417
7.5390
7.5211
7.5185
7.4206
7.4100
7.3999
7.3893
4.2687
4.2508
4.2329
4.2151
3.9928
1.1252
1.1073
1.0895
1.00
1.03
2.00
1.02
1.05
1.11
1.04
1.03
4.26
3.05
6.56
fl (ppm)


165.6
165.0
164.7
148.3
142.4
138.4
136.4
135.3
134.7
131.2
130.5
128.1
127.6
121.9
121.7
116.9
62.2
52.9
13.9
fl (ppm)

3t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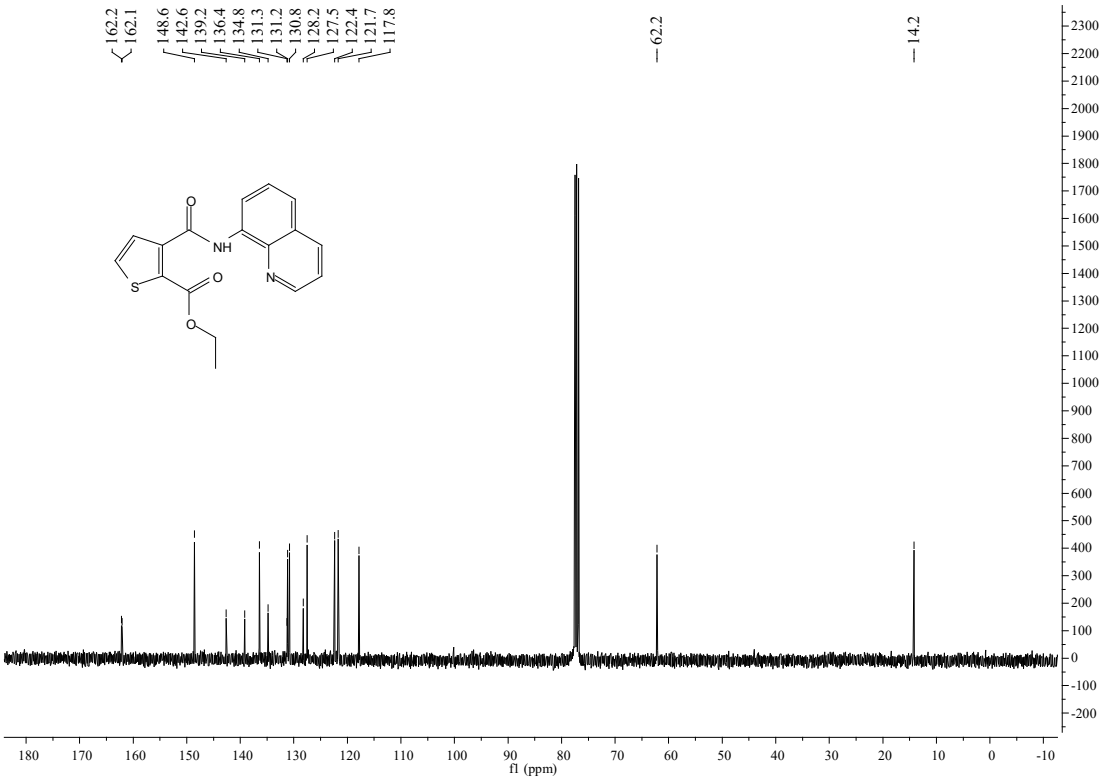
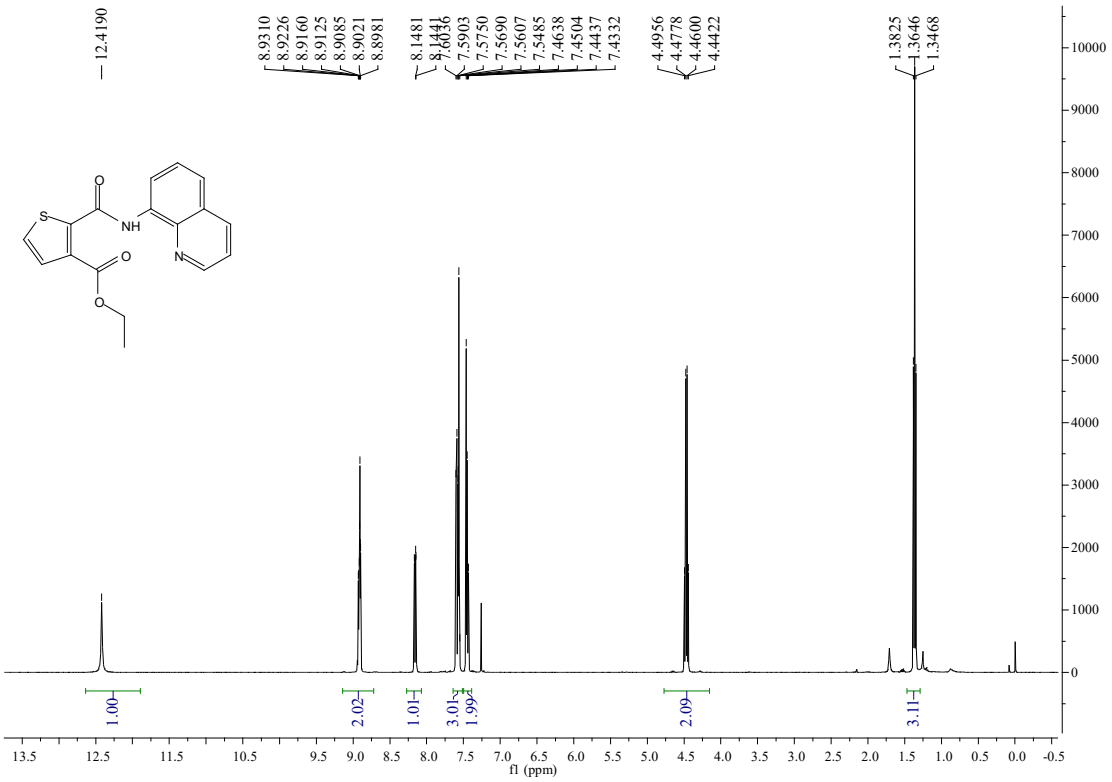
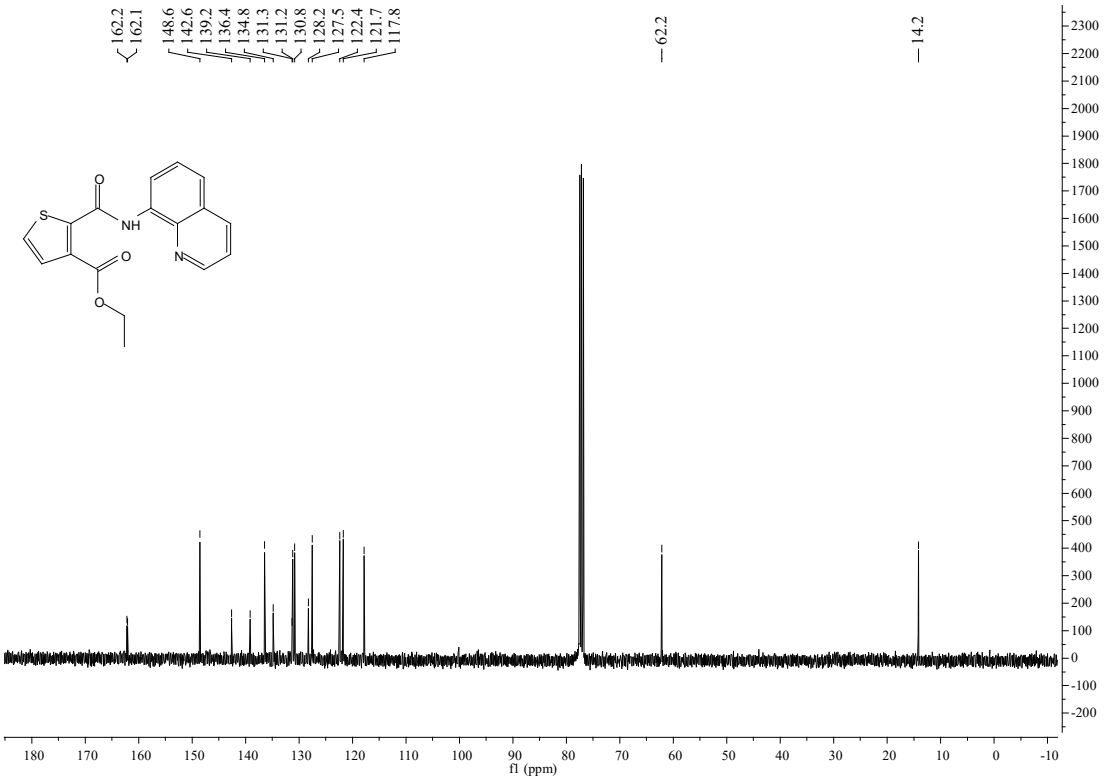
8.9600
8.9560
8.9421
8.9381
8.8328
8.8288
8.8223
8.8183
8.1658
8.1618
7.6165
7.5932
7.5796
7.5731
7.5685
7.5512
7.5383
7.4699
7.4594
7.4493
7.4387
4.3787
4.3608
4.3430
4.3252
1.2545
1.2367
1.2189
1.06
1.05
1.04
1.07
4.00
1.05
2.05
3.60
f1 (ppm)

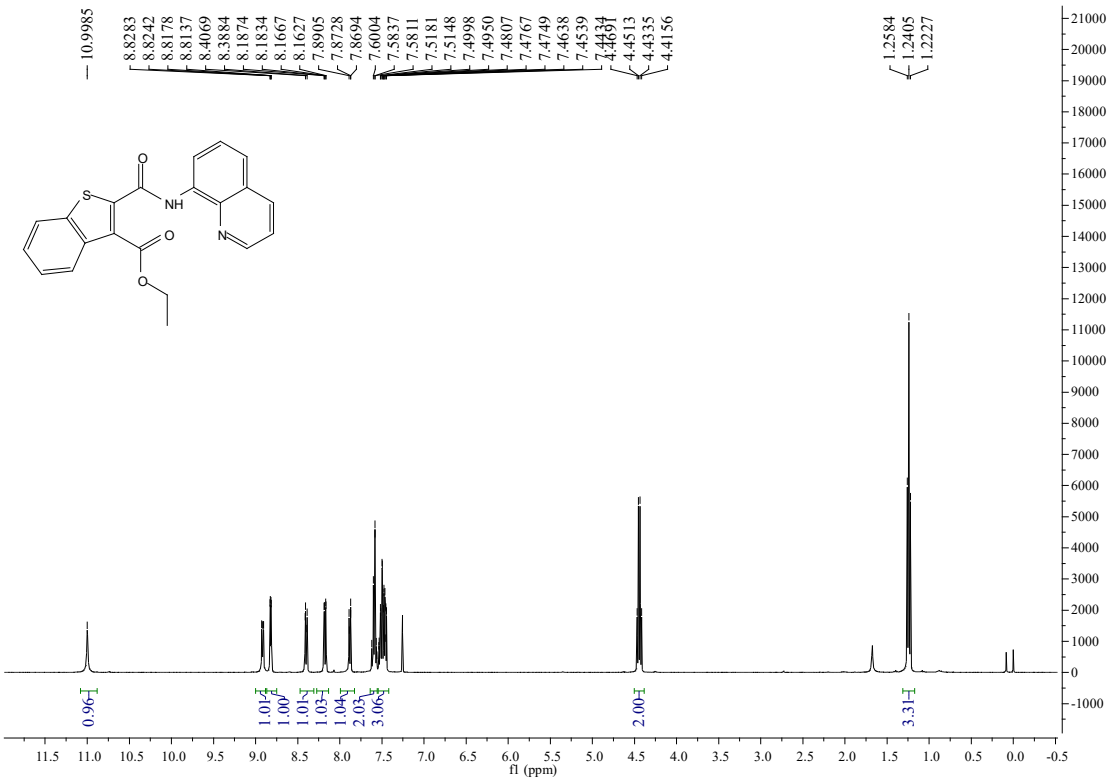

162.2
162.1
148.6
142.6
139.2
136.4
134.8
131.3
131.2
130.8
128.2
127.5
122.4
121.7
117.8
62.2
14.2
f1 (ppm)

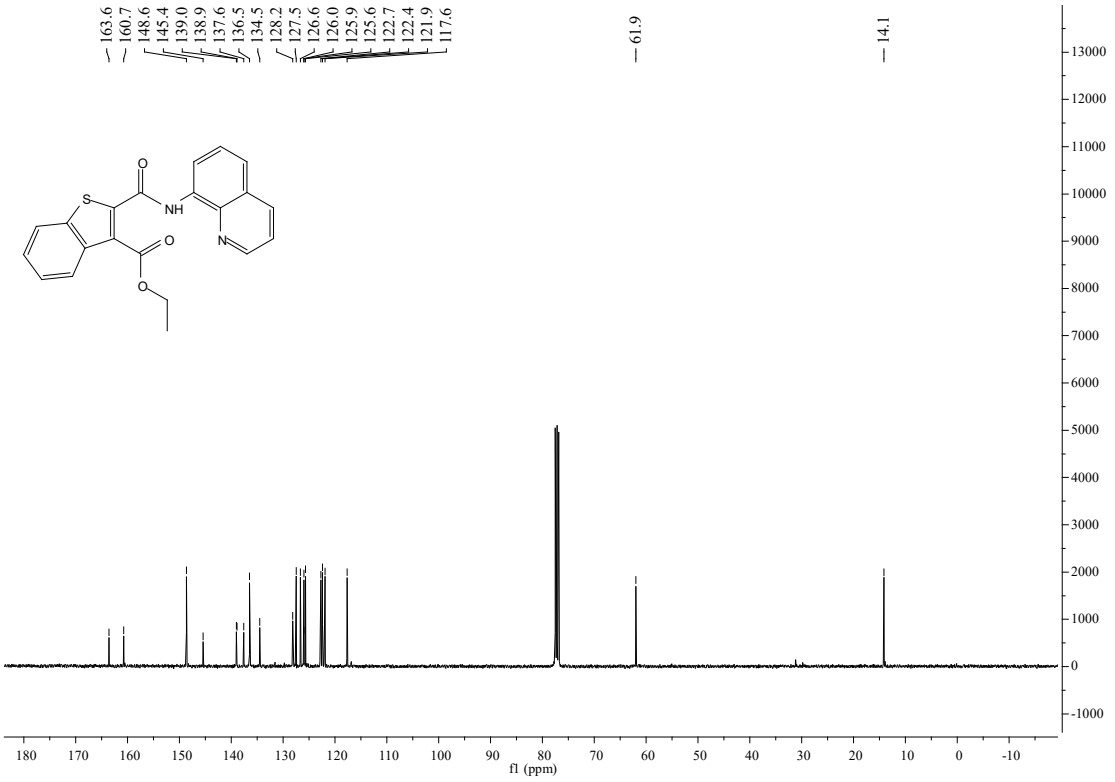
3u


12.4190
8.9310
8.9226
8.9160
8.9125
8.9085
8.9021
8.8981
8.1481
8.1441
7.6036
7.5903
7.5750
7.5690
7.5607
7.5485
7.4638
7.4504
7.4437
7.4332
4.4956
4.4778
4.4600
4.4422
1.3825
1.3646
1.3468
1.00
2.02
1.01
3.01
1.99
2.09
3.11
f1 (ppm)

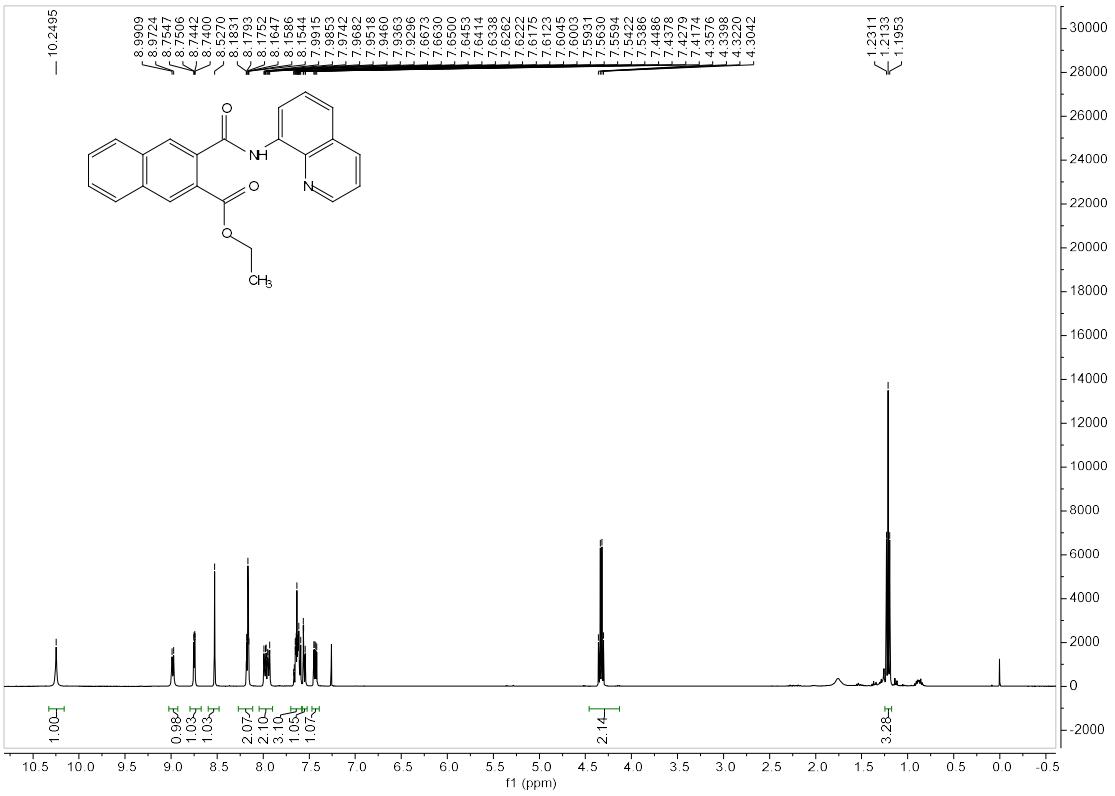

162.2
162.1
148.6
142.6
139.2
136.4
134.8
131.3
131.2
130.8
128.2
127.5
122.4
121.7
117.8
62.2
14.2
f1 (ppm)

3v


10.9985
8.8283
8.8242
8.8178
8.8137
8.4069
8.3884
8.1874
8.1834
8.1667
8.1627
7.8905
7.8728
7.8694
7.6004
7.5837
7.5811
7.5181
7.5148
7.4998
7.4950
7.4807
7.4767
7.4749
7.4638
7.4539
4.4513
4.4335
4.4156
1.2584
1.2405
1.2227
0.96
1.01
1.00
1.01
1.03
1.04
2.03
3.06
2.00
3.31
O
NH
S
N
O
O
fl (ppm)


163.6
160.7
148.6
145.4
139.0
138.9
137.6
136.5
134.5
128.2
127.5
126.6
126.0
125.9
125.6
122.7
122.4
121.9
117.6
61.9
14.1
O
NH
S
N
O
O
fl (ppm)

3w


10.2495
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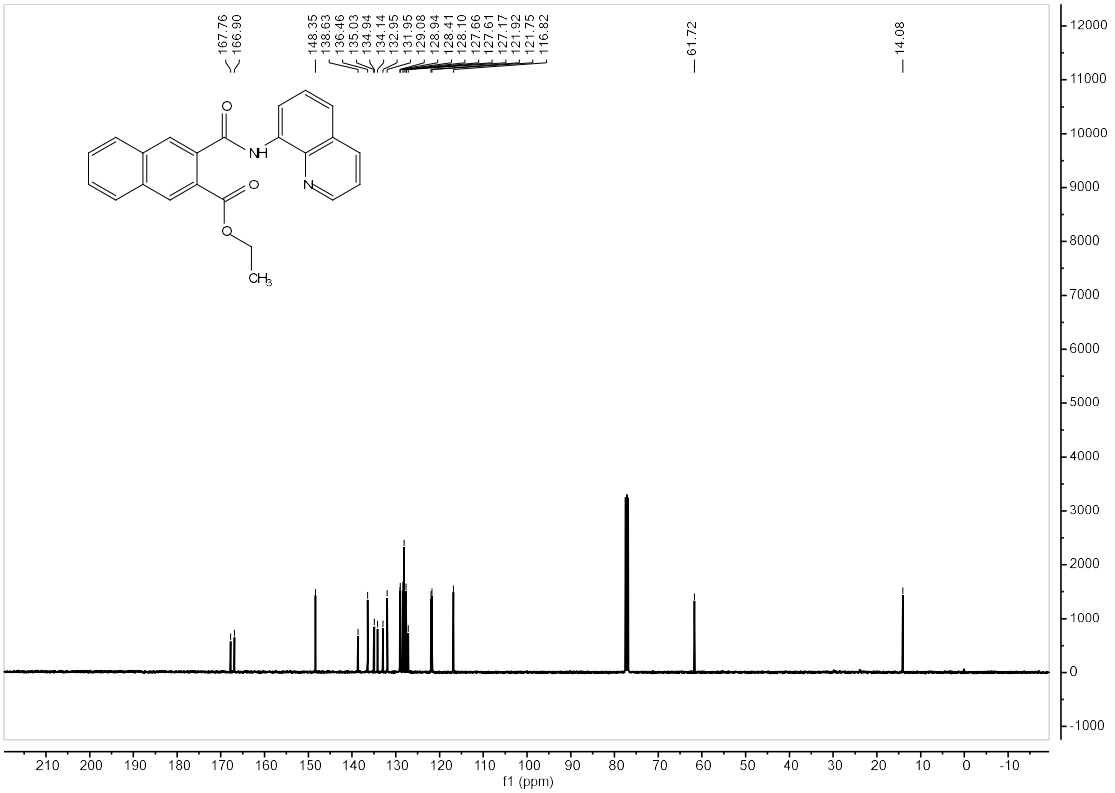
8.9724
8.7547
8.7506
8.7442
8.7400
8.5270
8.1831
8.1793
8.1732
8.1647
8.1586
8.1544
7.9915
7.9853
7.9742
7.9682
7.9518
7.9460
7.9363
7.9296
7.6673
7.6630
7.6500
7.6453
7.6414
7.6338
7.6262
7.6222
7.6175
7.6123
7.6045
7.6003
7.5931
7.5630
7.5594
7.5422
7.5386
7.4486
7.4378
7.4279
7.4174
4.3576
4.3398
4.3220
4.3042
1.2311
1.2133
1.1953
NH
O
N
CH3
1.00
0.98
1.03
1.03
2.07
2.10
3.10
1.05
1.07
2.14
3.28
f1 (ppm)


167.76
166.90
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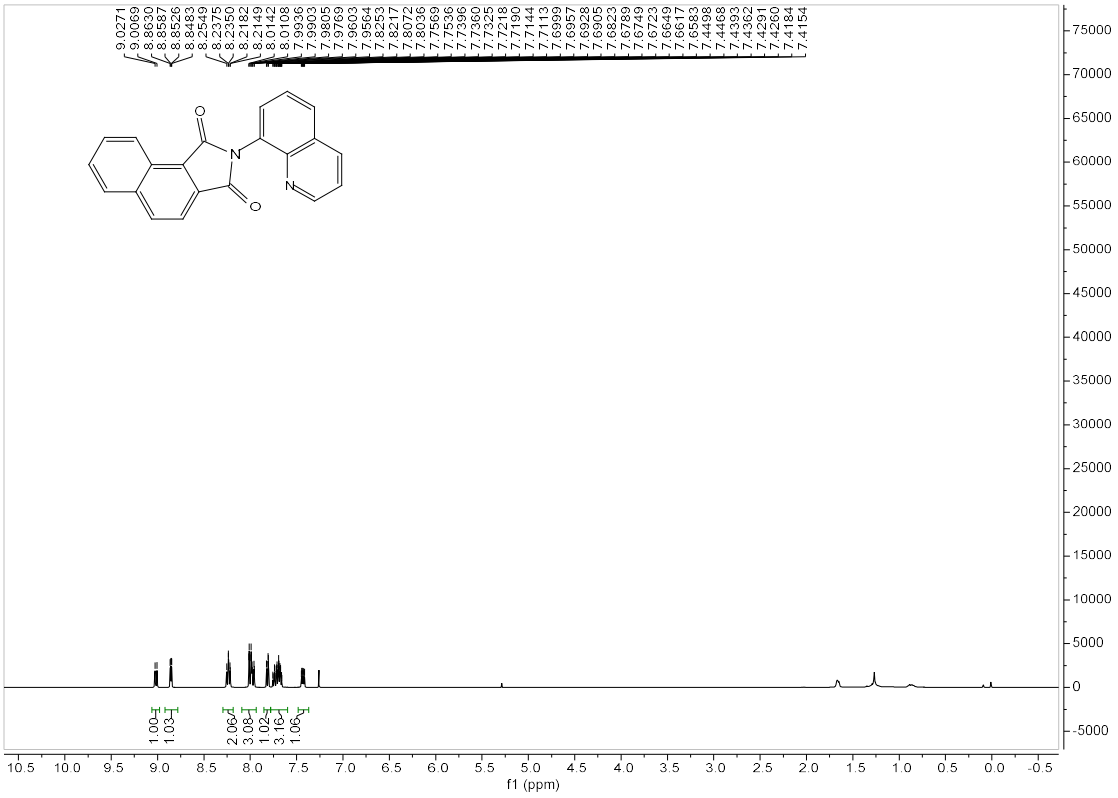
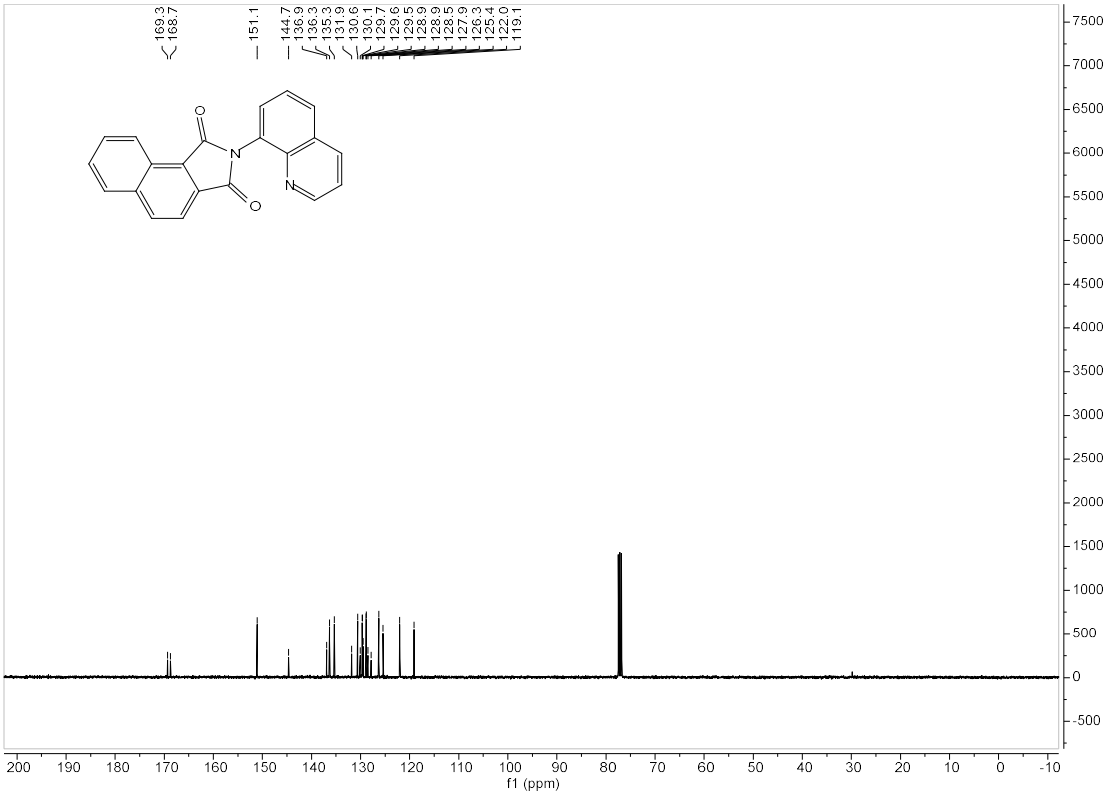
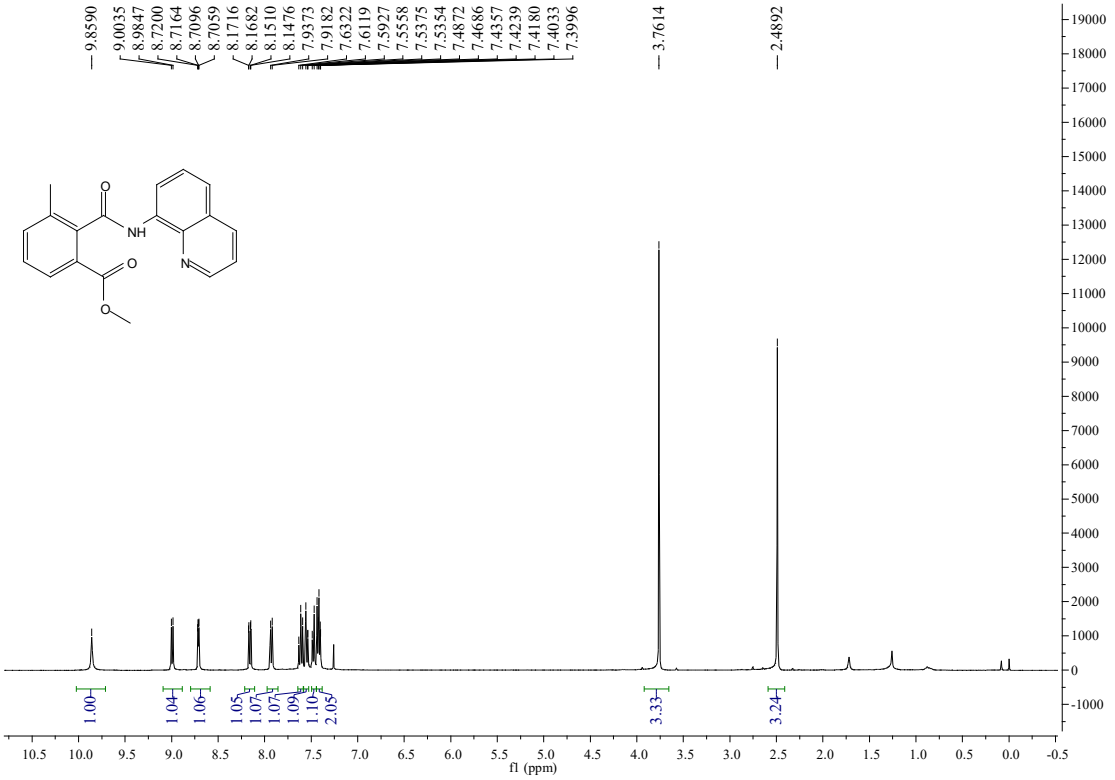
136.46
135.03
134.94
134.14
132.95
131.95
129.08
128.94
128.41
128.10
127.66
127.61
127.17
121.92
121.75
116.82
61.72
14.08
NH
O
N
CH3
f1 (ppm)

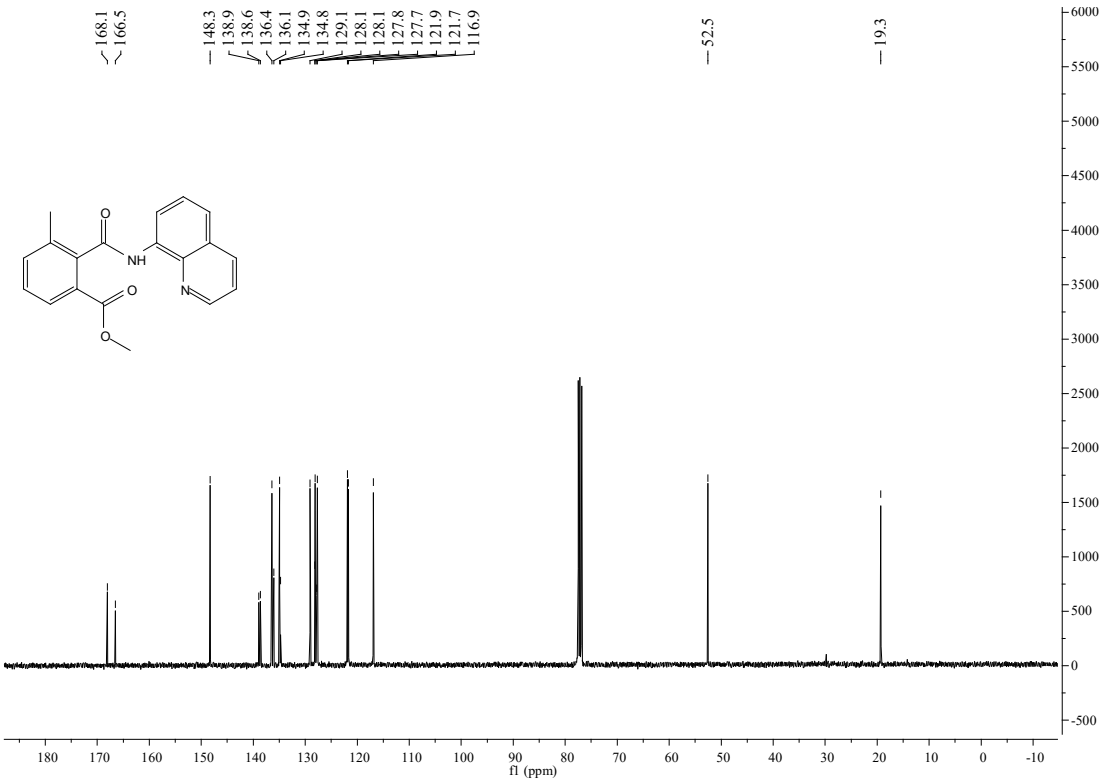
3x


9.0271
9.0069
8.8637
8.8587
8.8526
8.8483
8.2549
8.2375
8.2350
8.2182
8.2149
8.0142
8.0108
7.9936
7.9903
7.9805
7.9769
7.9603
7.9564
7.8253
7.8217
7.8072
7.8036
7.7569
7.7536
7.7396
7.7360
7.7325
7.7218
7.7190
7.7144
7.7113
7.6999
7.6957
7.6928
7.6905
7.6823
7.6789
7.6749
7.6723
7.6649
7.6617
7.6583
7.4498
7.4468
7.4393
7.4362
7.4291
7.4260
7.4184
7.4154
1.00
1.03
2.06
3.08
1.02
3.16
1.06
f1 (ppm)

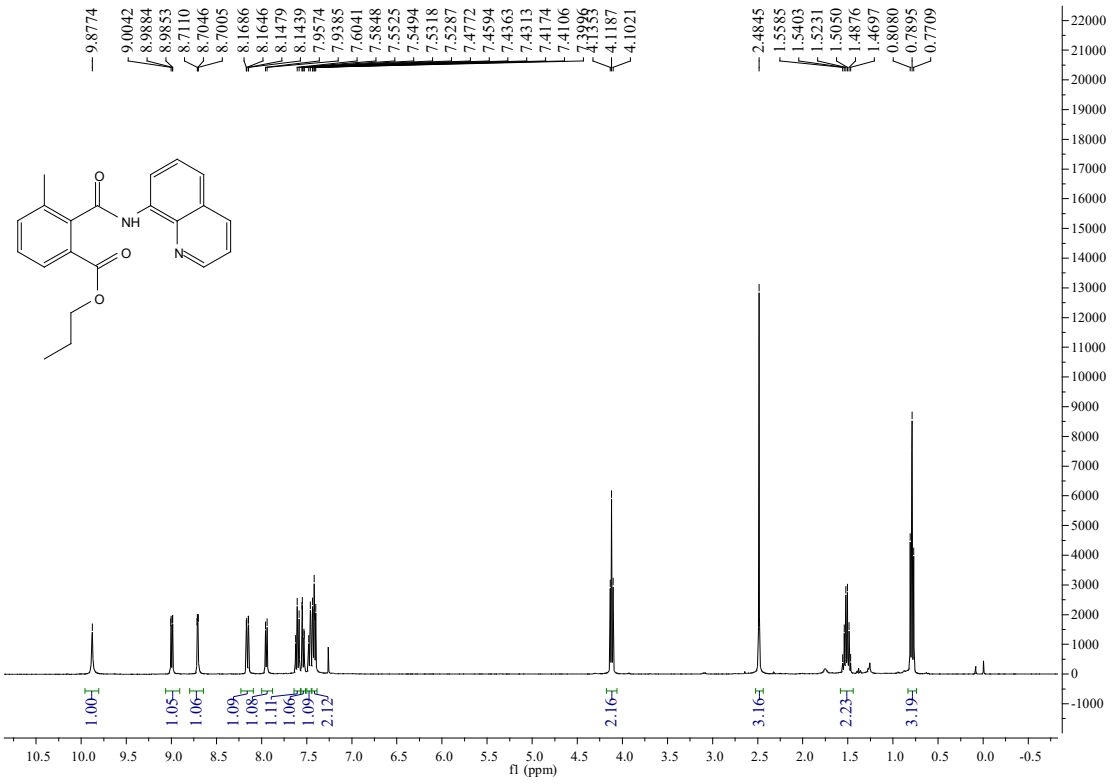

169.3
168.7
151.1
144.7
136.9
136.3
135.3
131.9
130.6
130.1
129.7
129.6
129.5
128.9
128.9
128.5
127.9
126.3
125.4
122.0
119.1
f1 (ppm)

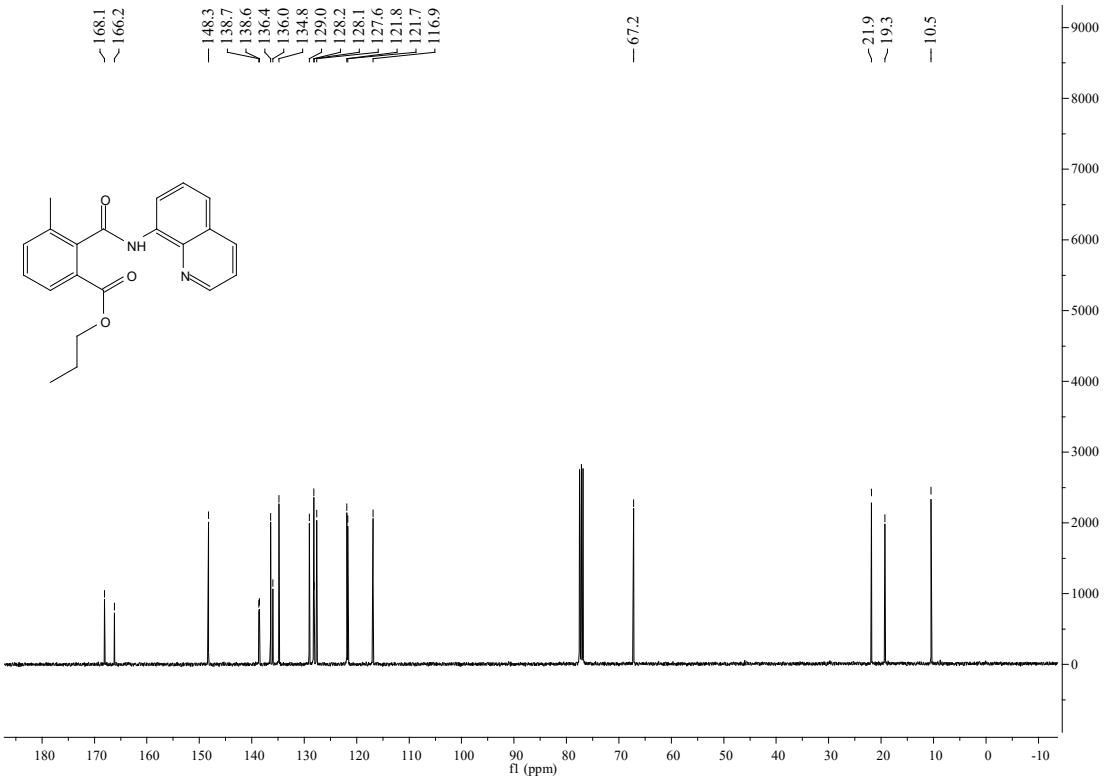
4a


9.8590
9.0035
8.9847
8.7200
8.7164
8.7096
8.7059
8.1716
8.1682
8.1510
8.1476
7.9373
7.9182
7.6322
7.6119
7.5927
7.5558
7.5375
7.5354
7.4872
7.4686
7.4357
7.4239
7.4180
7.4033
7.3996
3.7614
2.4892
O
NH
N
O
O
1.00
1.04
1.06
1.05
1.07
1.07
1.09
1.10
2.05
3.33
3.24
fl (ppm)

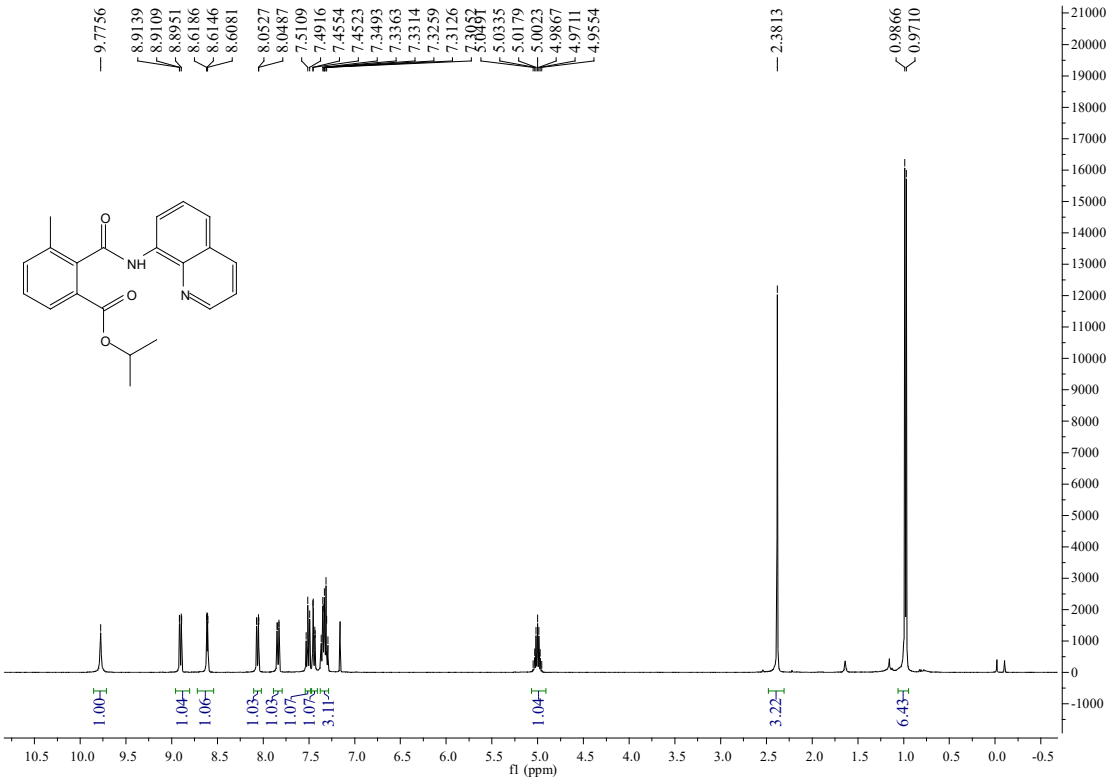

168.1
166.5
148.3
138.9
138.6
136.4
136.1
134.9
134.8
129.1
128.1
128.1
127.8
127.7
121.9
121.7
116.9
52.5
19.3
O
NH
N
O
O
fl (ppm)

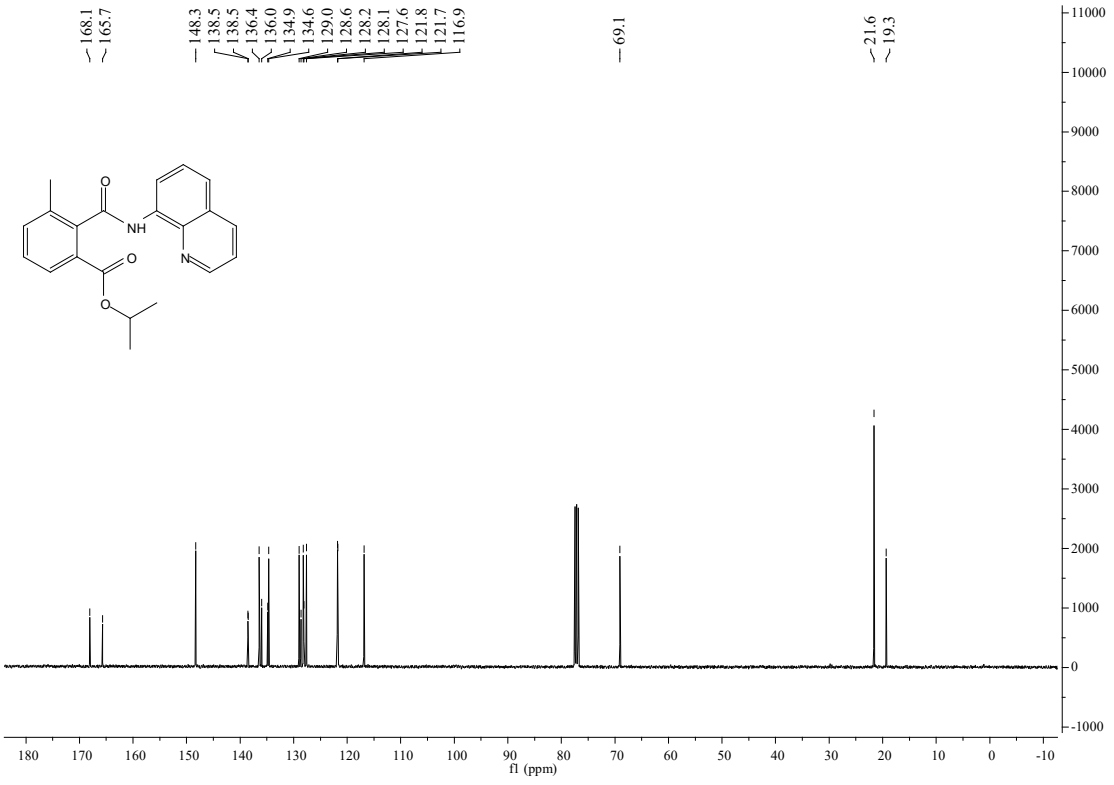
4b


9.8774
9.0042
8.9884
8.9853
8.7110
8.7046
8.7005
8.1686
8.1646
8.1479
8.1439
7.9574
7.9385
7.6041
7.5848
7.5525
7.5494
7.5318
7.5287
7.4772
7.4594
7.4363
7.4313
7.4174
7.4106
4.1187
4.1021
2.4845
1.5585
1.5403
1.5231
1.5050
1.4876
1.4697
0.8080
0.7895
0.7709
1.00
1.05
1.06
1.09
1.08
1.11
1.06
1.09
2.12
2.16
3.16
2.23
3.19
fl (ppm)


168.1
166.2
148.3
138.7
138.6
136.4
136.0
134.8
129.0
128.2
128.1
127.6
121.8
121.7
116.9
67.2
21.9
19.3
10.5
fl (ppm)

4c


9.7756
8.9139
8.9109
8.8951
8.6186
8.6146
8.6081
8.0527
8.0487
7.5109
7.4916
7.4554
7.4523
7.3493
7.3363
7.3314
7.3259
7.3126
5.0335
5.0179
5.0023
4.9867
4.9711
4.9554
2.3813
0.9866
0.9710
1.00
1.04
1.06
1.03
1.03
1.07
1.07
3.11
1.04
3.22
6.43
fl (ppm)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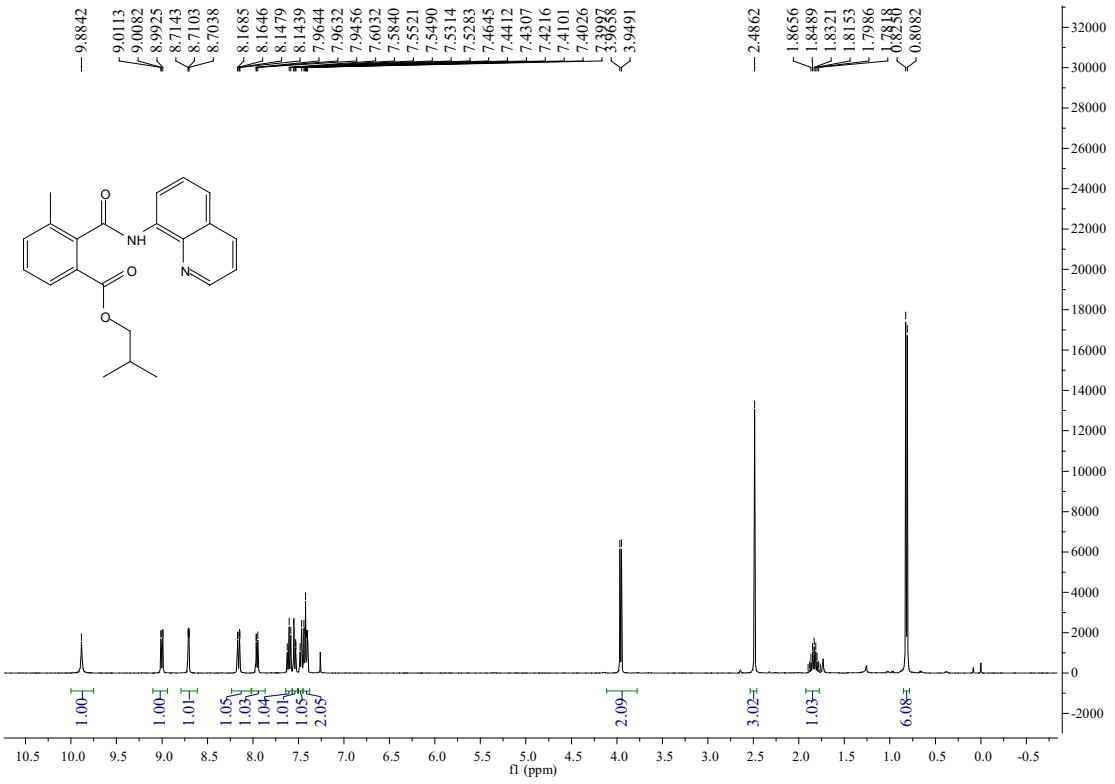
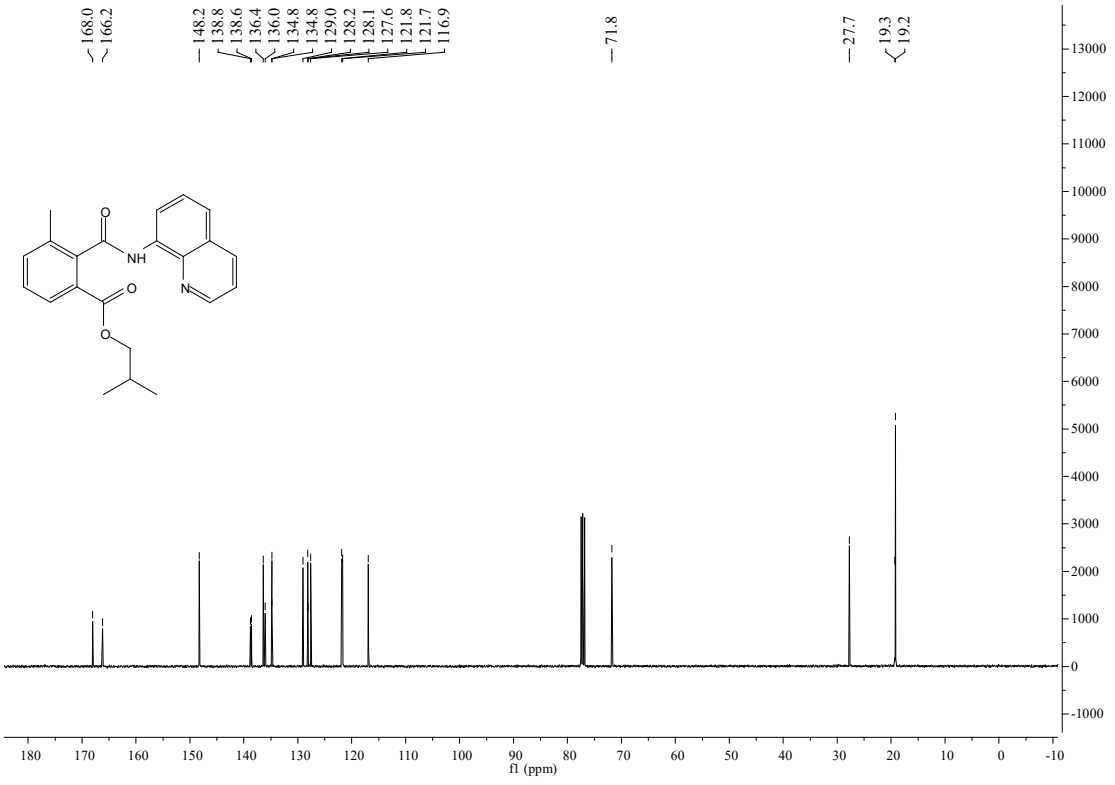
165.7
148.3
138.5
138.5
136.4
136.0
134.9
134.6
129.0
128.6
128.2
128.1
127.6
121.8
121.7
116.9
69.1
21.6
19.3
fl (ppm)

4d


9.8842
9.0113
9.0082
8.9925
8.7143
8.7103
8.7038
8.1685
8.1646
8.1479
8.1439
7.9644
7.9632
7.9456
7.6032
7.5840
7.5521
7.5490
7.5314
7.5283
7.4645
7.4412
7.4307
7.4216
7.4101
7.4026
3.9638
3.9491
2.4862
1.8656
1.8489
1.8321
1.8153
1.7986
0.8250
0.8082
O
NH
O
N
O
1.00
1.00
1.01
1.05
1.03
1.04
1.01
1.05
2.05
2.09
3.02
1.03
6.08
fl (ppm)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166.2
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138.8
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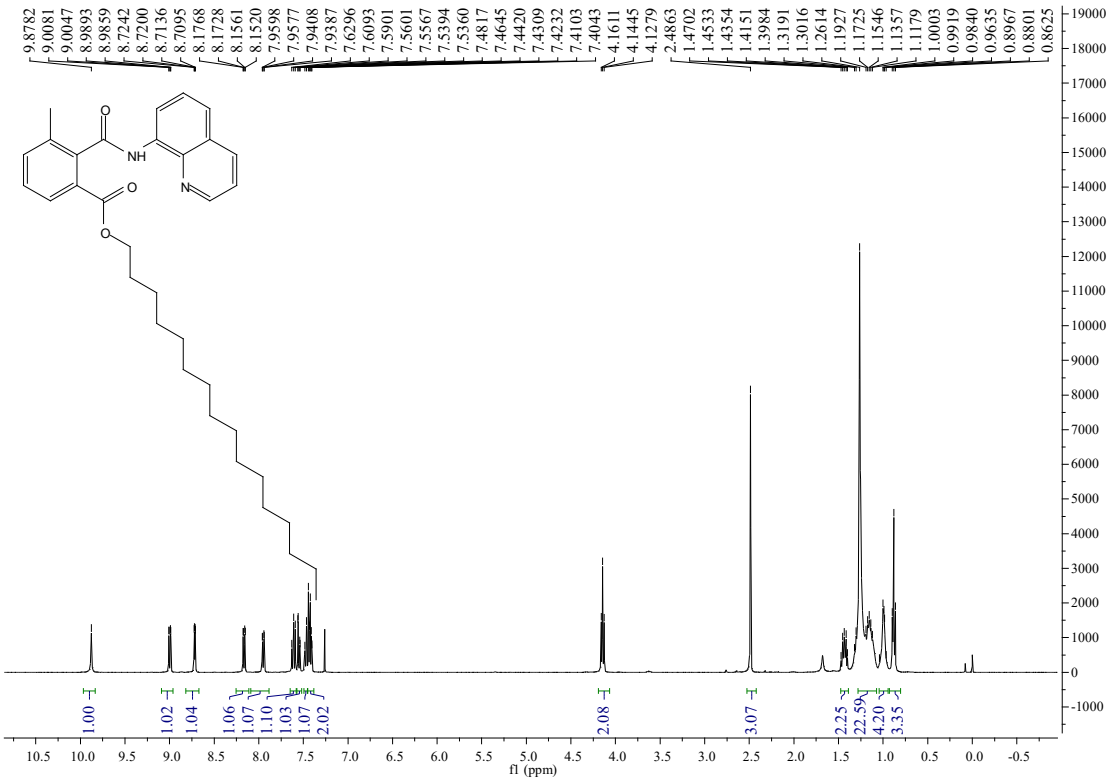
136.0
134.8
134.8
129.0
128.2
128.1
127.6
121.8
121.7
116.9
71.8
27.7
19.3
19.2
O
NH
O
N
O
fl (ppm)

4e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9.0047
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8.9859
8.7242
8.7200
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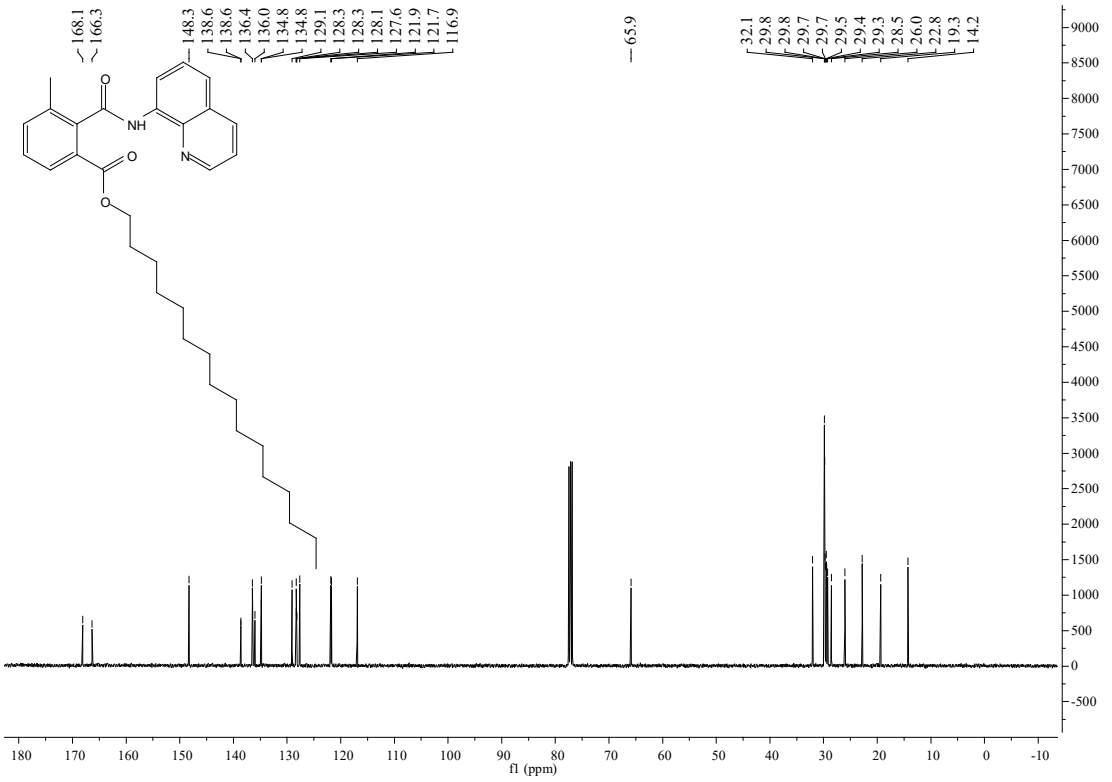
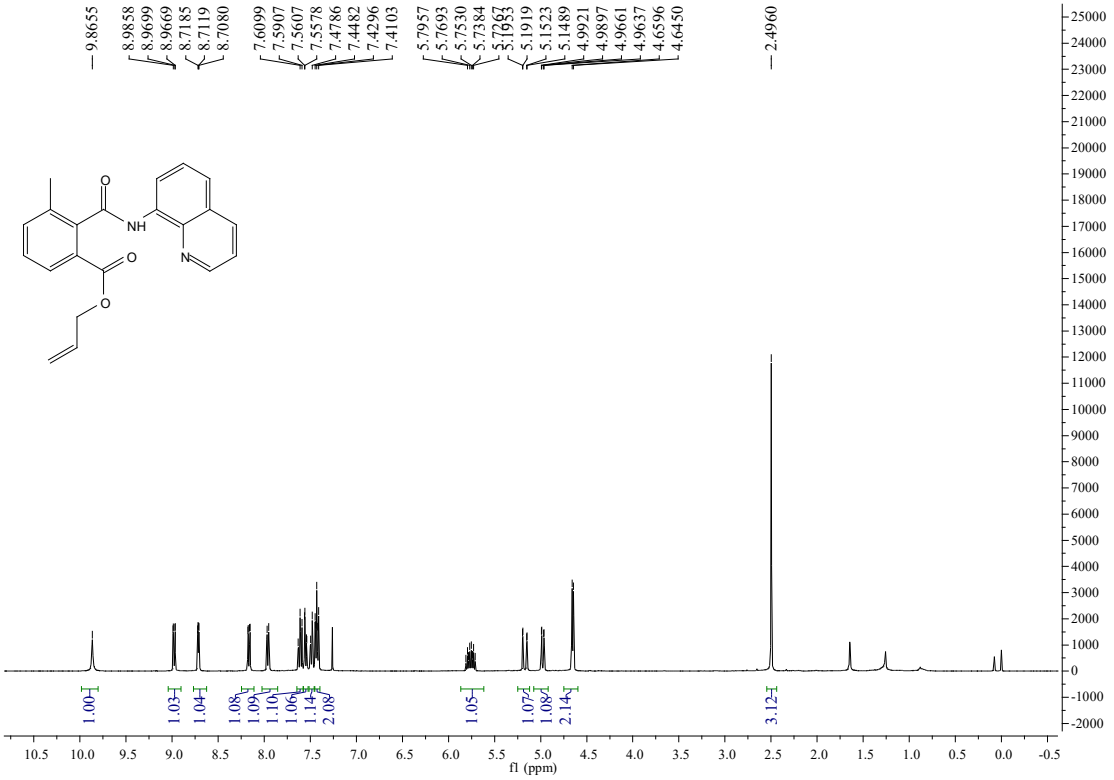
8.7095
8.1768
8.1728
8.1561
8.1520
7.9598
7.9577
7.9408
7.9387
7.6296
7.6093
7.5901
7.5601
7.5567
7.5394
7.5360
7.4817
7.4645
7.4420
7.4309
7.4232
7.4103
7.4043
4.1611
4.1445
4.1279
2.4863
1.4702
1.4533
1.4354
1.4151
1.3984
1.3191
1.3016
1.2614
1.1927
1.1725
1.1546
1.1357
1.1179
1.0003
0.9919
0.9840
0.9635
0.8967
0.8801
0.8625
O
NH
O
N
O
1.00
1.02
1.04
1.06
1.07
1.10
1.03
1.07
2.02
2.08
3.07
2.25
22.59
4.20
3.35
f1 (ppm)


168.1
166.3
148.3
138.6
138.6
136.4
136.0
134.8
134.8
129.1
128.3
128.3
128.1
127.6
121.9
121.7
116.9
65.9
32.1
29.8
29.8
29.7
29.7
29.5
29.4
29.3
28.5
26.0
22.8
19.3
14.2
O
NH
O
N
O
f1 (ppm)

4f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8.9699
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8.7185
8.7119
8.7080
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7.5907
7.5607
7.5578
7.4786
7.4482
7.4296
7.4103
5.7957
5.7693
5.7530
5.7384
5.7267
5.1983
5.1919
5.1523
5.1489
4.9921
4.9897
4.9661
4.9637
4.6596
4.6450
2.4960
O
NH
O
N
O
1.00
1.03
1.04
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1.06
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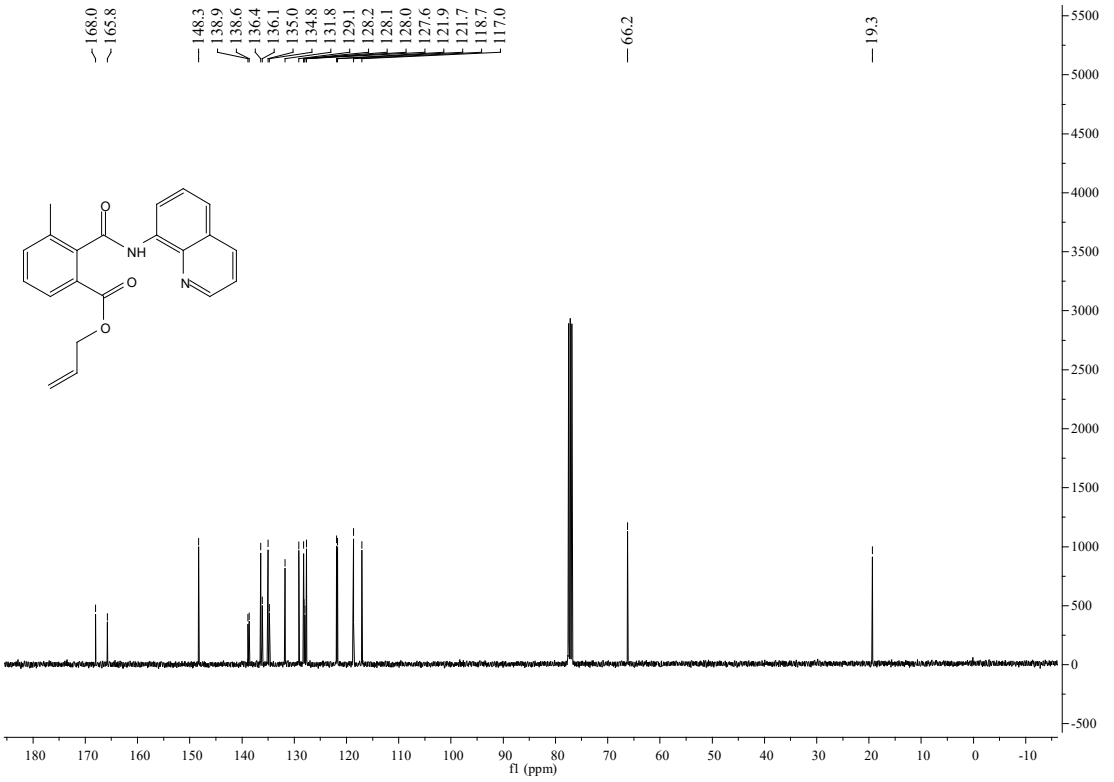
1.05
1.07
1.08
2.14
3.12
fl (ppm)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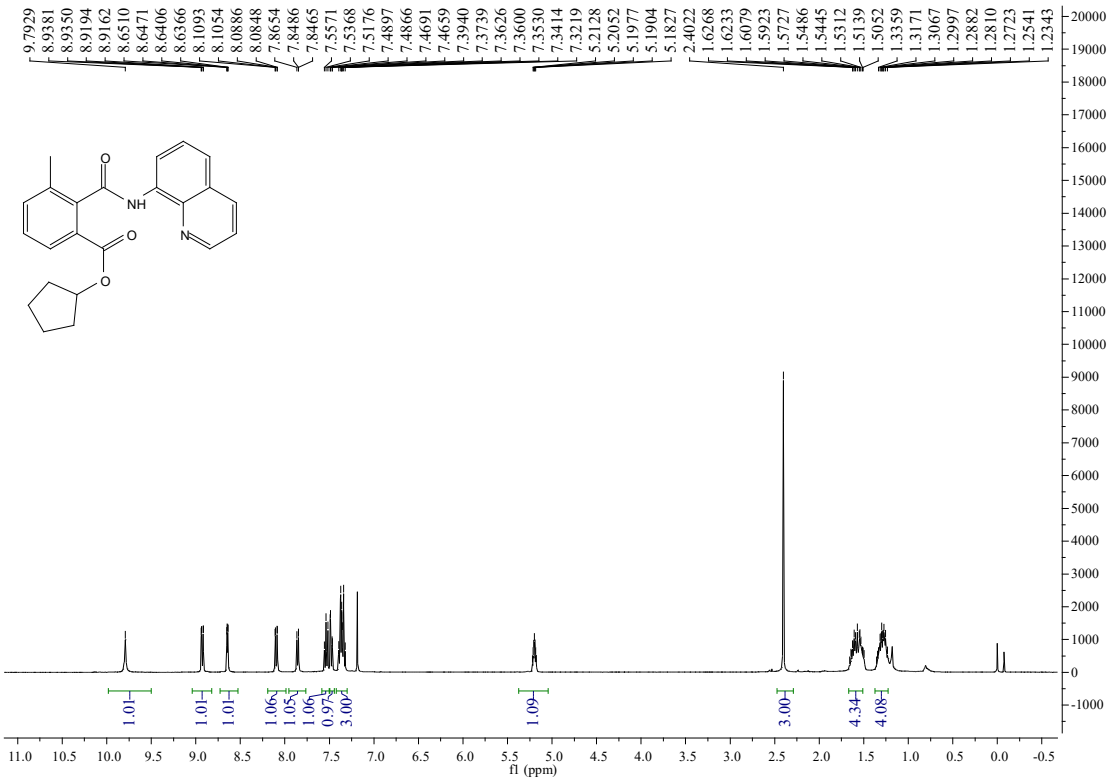
165.8
148.3
138.9
138.6
136.4
136.1
135.0
134.8
131.8
129.1
128.2
128.1
128.0
127.6
121.9
121.7
118.7
117.0
66.2
19.3
O
NH
O
N
O
fl (ppm)

4g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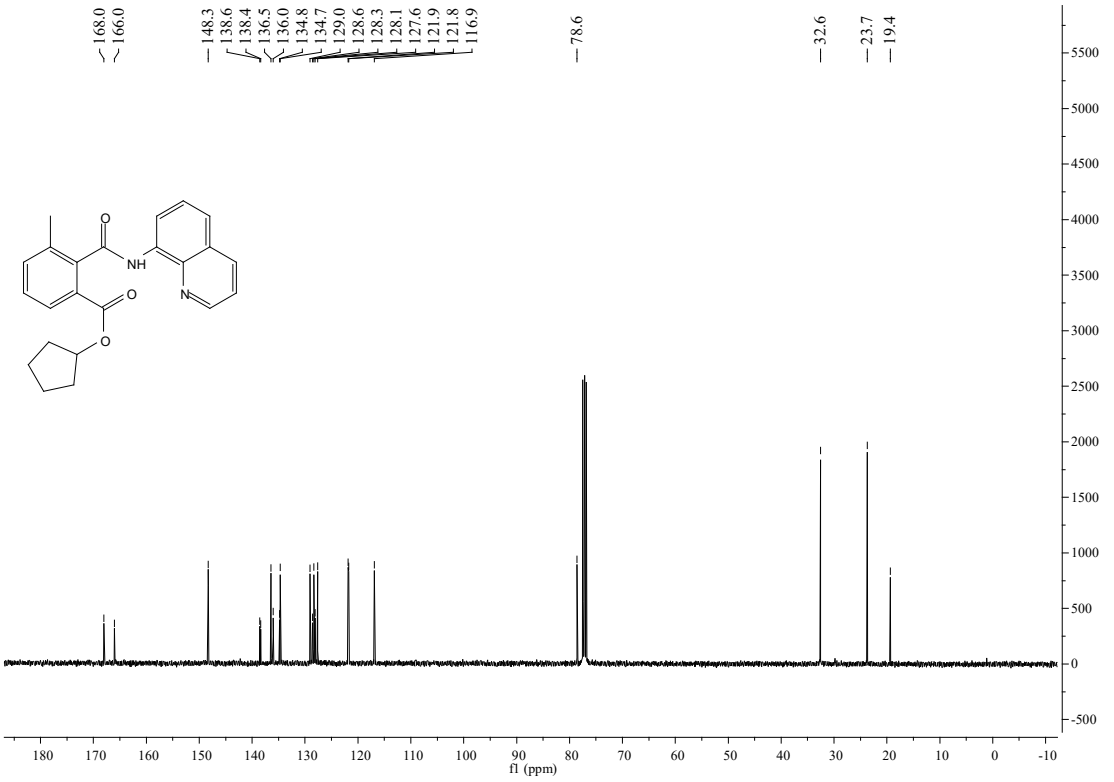
8.9381
8.9350
8.9194
8.9162
8.6510
8.6471
8.6406
8.6366
8.1093
8.1054
8.0886
8.0848
7.8654
7.8486
7.8465
7.5571
7.5368
7.5176
7.4897
7.4866
7.4691
7.4659
7.3940
7.3739
7.3626
7.3600
7.3530
7.3414
7.3219
5.2128
5.2052
5.1977
5.1904
5.1827
2.4022
1.6268
1.6233
1.6079
1.5923
1.5727
1.5486
1.5445
1.5312
1.5139
1.5052
1.3359
1.3171
1.3067
1.2997
1.2882
1.2810
1.2723
1.2541
1.2343
O
NH
O
N
O
1.01
1.01
1.01
1.06
1.05
1.06
0.97
3.00
1.09
3.00
4.34
4.08
fl (ppm)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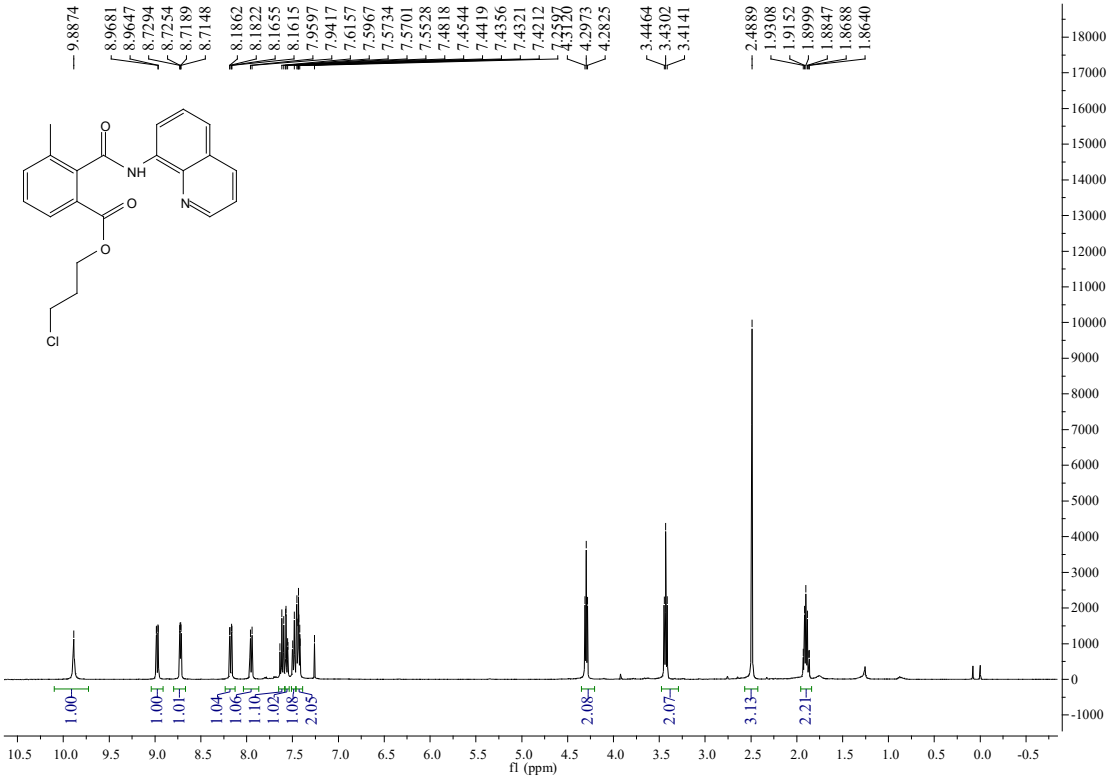
166.0
148.3
138.6
138.4
136.5
136.0
134.8
134.7
129.0
128.6
128.3
128.1
127.6
121.9
121.8
116.9
78.6
32.6
23.7
19.4
O
NH
O
N
O
fl (ppm)

4h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8.9647
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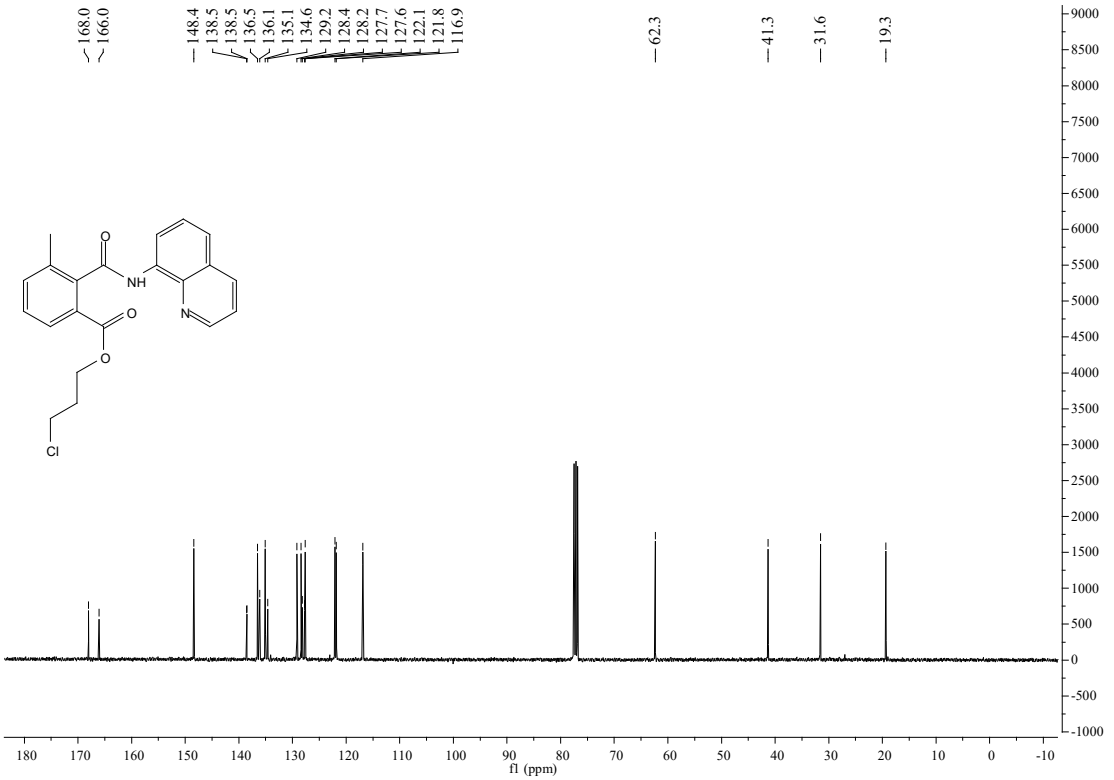
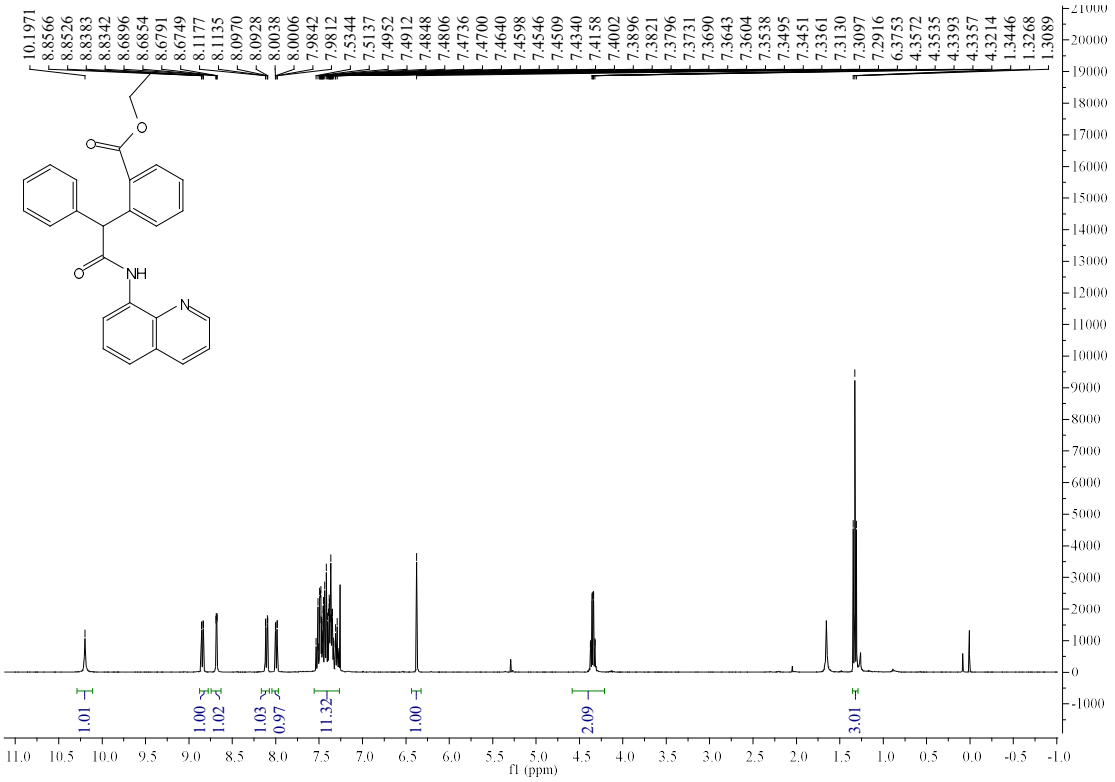
8.7254
8.7189
8.7148
8.1862
8.1822
8.1655
8.1615
7.9597
7.9417
7.6157
7.5967
7.5734
7.5701
7.5528
7.4818
7.4544
7.4419
7.4356
7.4321
7.4212
4.2973
4.2825
3.4464
3.4302
3.4141
2.4889
1.9308
1.9152
1.8999
1.8847
1.8688
1.8640
1.00
1.00
1.01
1.04
1.06
1.10
1.02
1.08
2.05
2.08
2.07
3.13
2.21
O
NH
N
O
O
Cl
f1 (ppm)


168.0
166.0
148.4
138.5
138.5
136.5
136.1
135.1
134.6
129.2
128.4
128.2
127.7
127.6
122.1
121.8
116.9
62.3
41.3
31.6
19.3
O
NH
N
O
O
Cl
f1 (ppm)

5


10.1971
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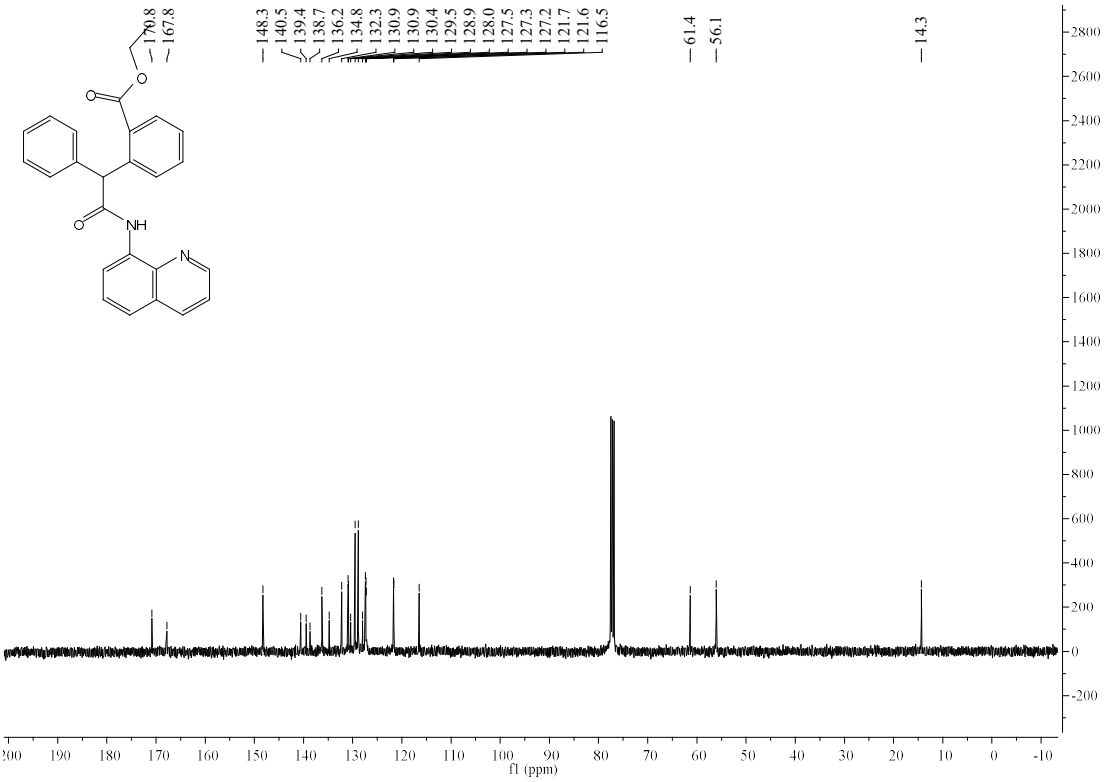
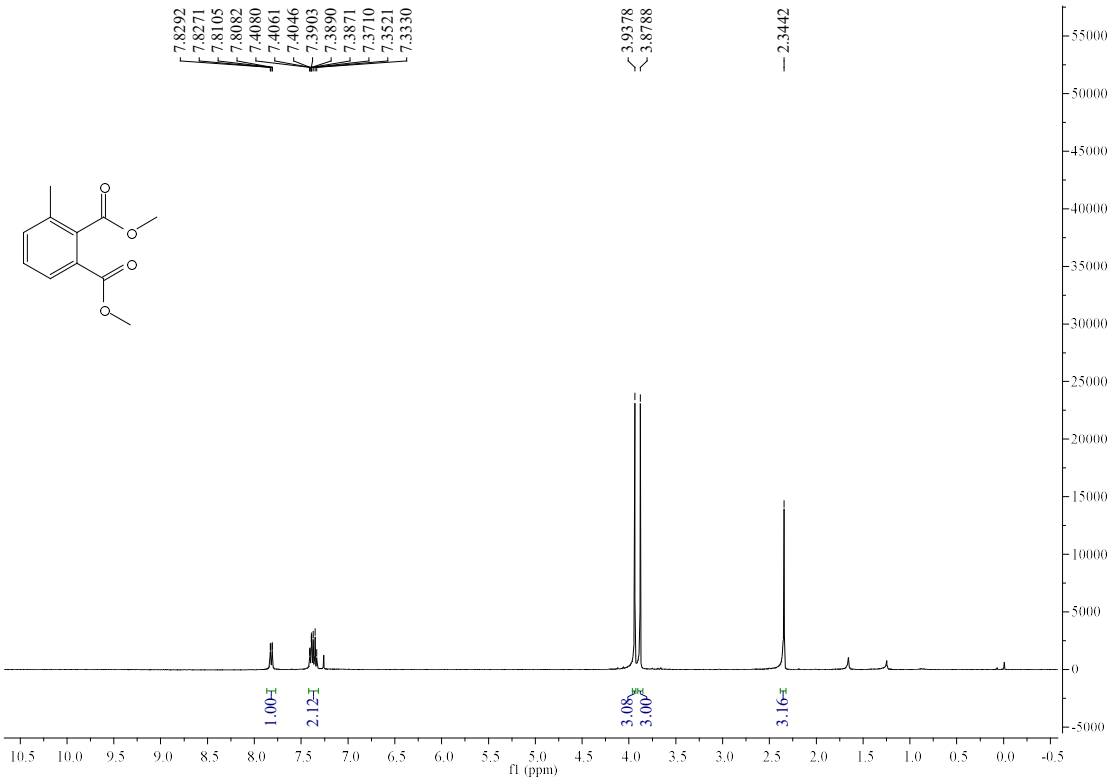
8.8526
8.8383
8.8342
8.6896
8.6854
8.6791
8.6749
8.1177
8.1135
8.0970
8.0928
8.0038
8.0006
7.9842
7.9812
7.5344
7.5137
7.4952
7.4912
7.4848
7.4806
7.4736
7.4700
7.4640
7.4598
7.4546
7.4509
7.4340
7.4158
7.4002
7.3896
7.3821
7.3796
7.3731
7.3690
7.3643
7.3604
7.3538
7.3495
7.3451
7.3361
7.3130
7.3097
7.2916
6.3753
4.3572
4.3535
4.3393
4.3357
4.3214
1.3446
1.3268
1.3089
O
O
NH
N
1.01
1.00
1.02
1.03
0.97
11.32
1.00
2.09
3.01
f1 (ppm)


170.8
167.8
148.3
140.5
139.4
138.7
136.2
134.8
132.3
130.9
130.9
130.4
129.5
128.9
128.0
127.5
127.3
127.2
121.7
121.6
116.5
61.4
56.1
14.3
O
O
NH
N
f1 (ppm)

6


7.8292
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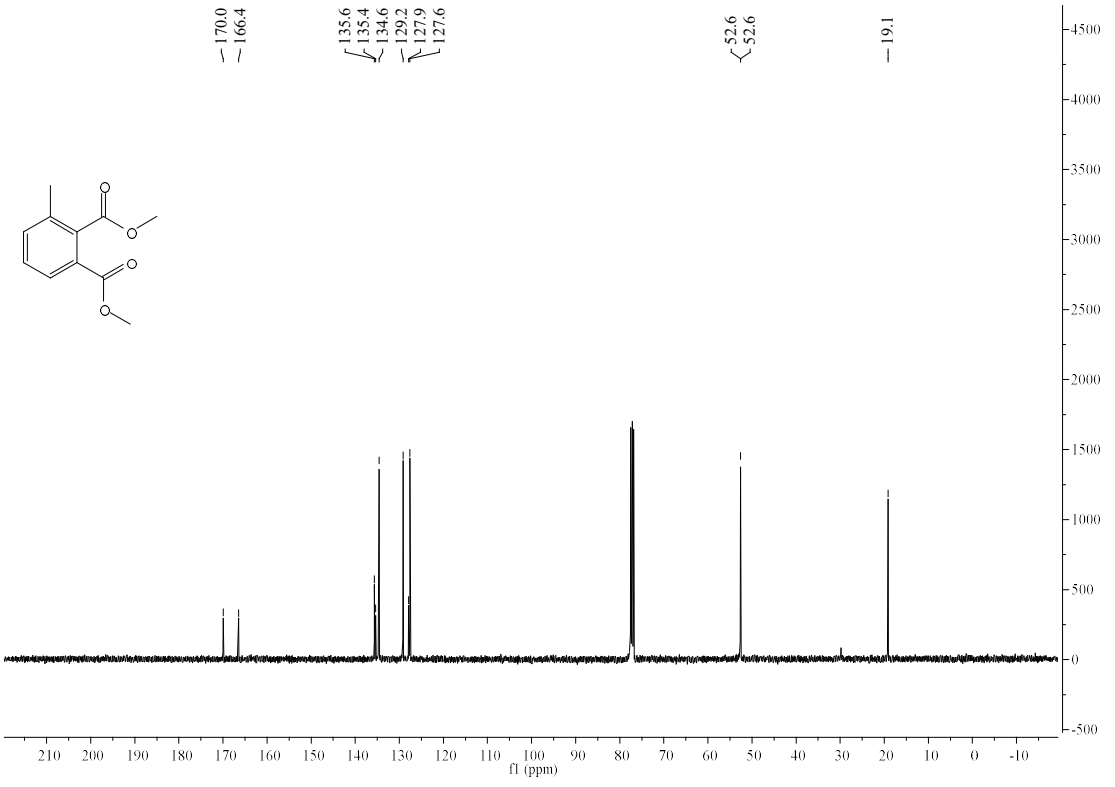
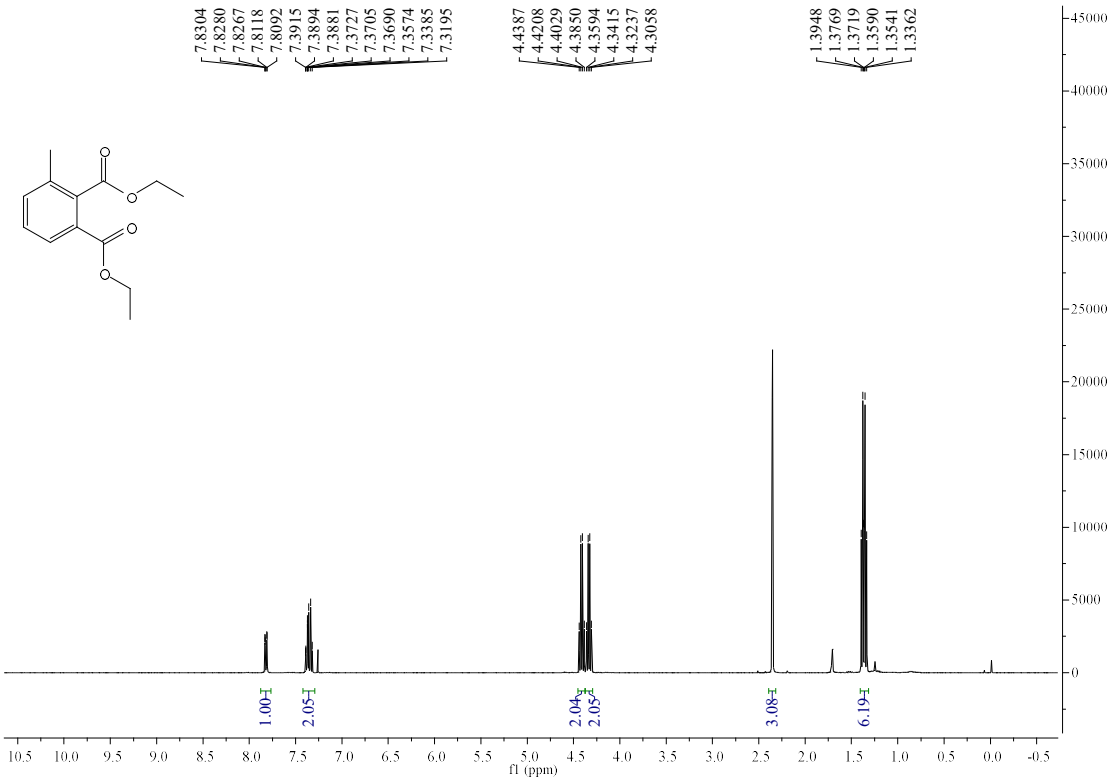
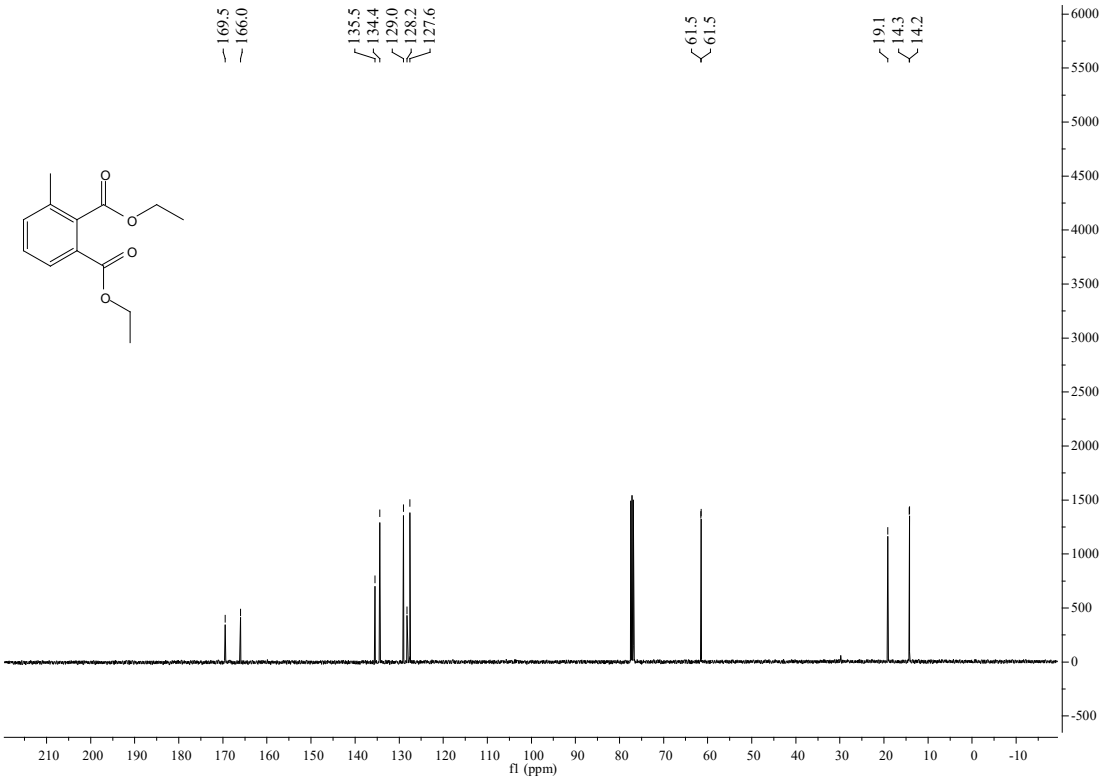
7.8105
7.8082
7.4080
7.4061
7.4046
7.3903
7.3890
7.3871
7.3710
7.3521
7.3330
3.9378
3.8788
2.3442
1.00
2.12
3.08
3.00
3.16
f1 (ppm)

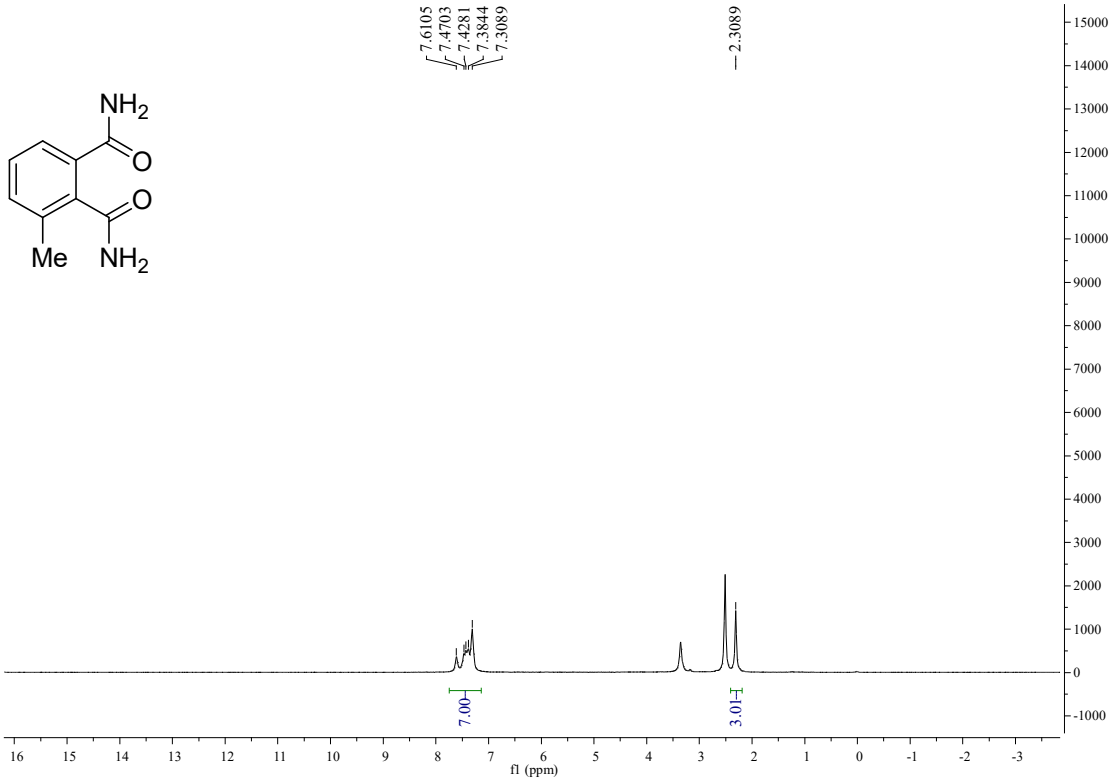

170.0
166.4
135.6
135.4
134.6
129.2
127.9
127.6
52.6
52.6
19.1
f1 (ppm)

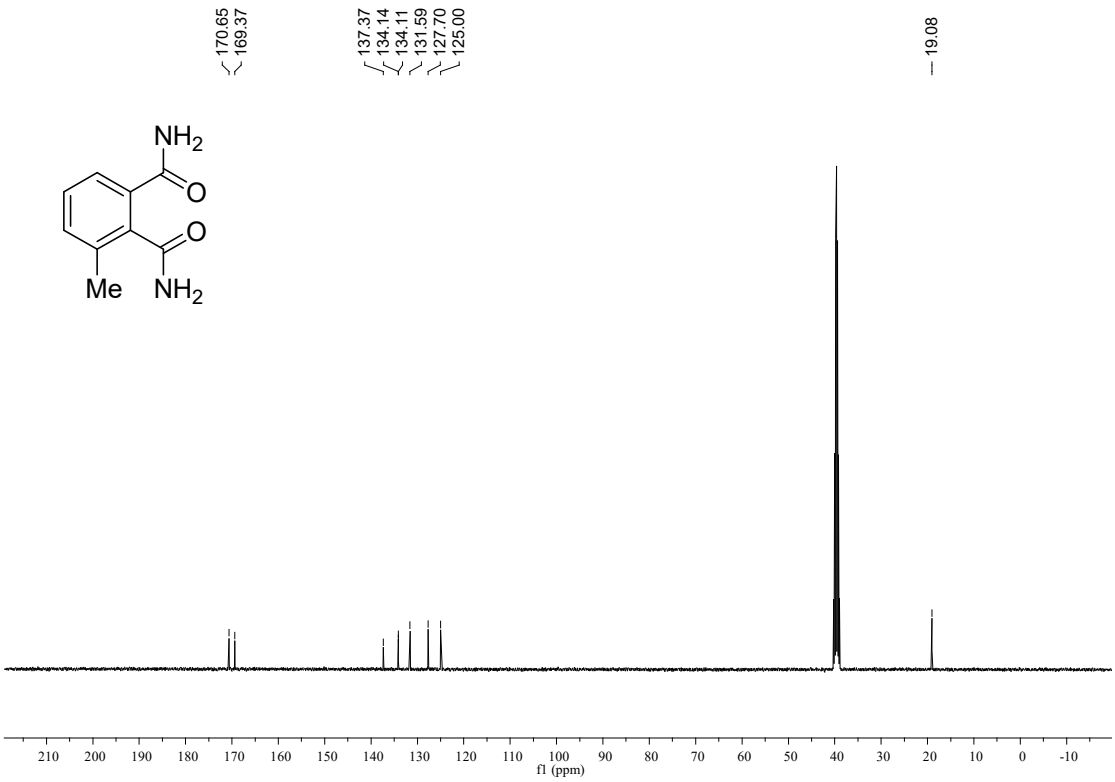
7


7.8304
7.8280
7.8267
7.8118
7.8092
7.3915
7.3894
7.3881
7.3727
7.3705
7.3690
7.3574
7.3385
7.3195
4.4387
4.4208
4.4029
4.3850
4.3594
4.3415
4.3237
4.3058
1.3948
1.3769
1.3719
1.3590
1.3541
1.3362
1.00
2.05
2.04
2.05
3.08
6.19
f1 (ppm)

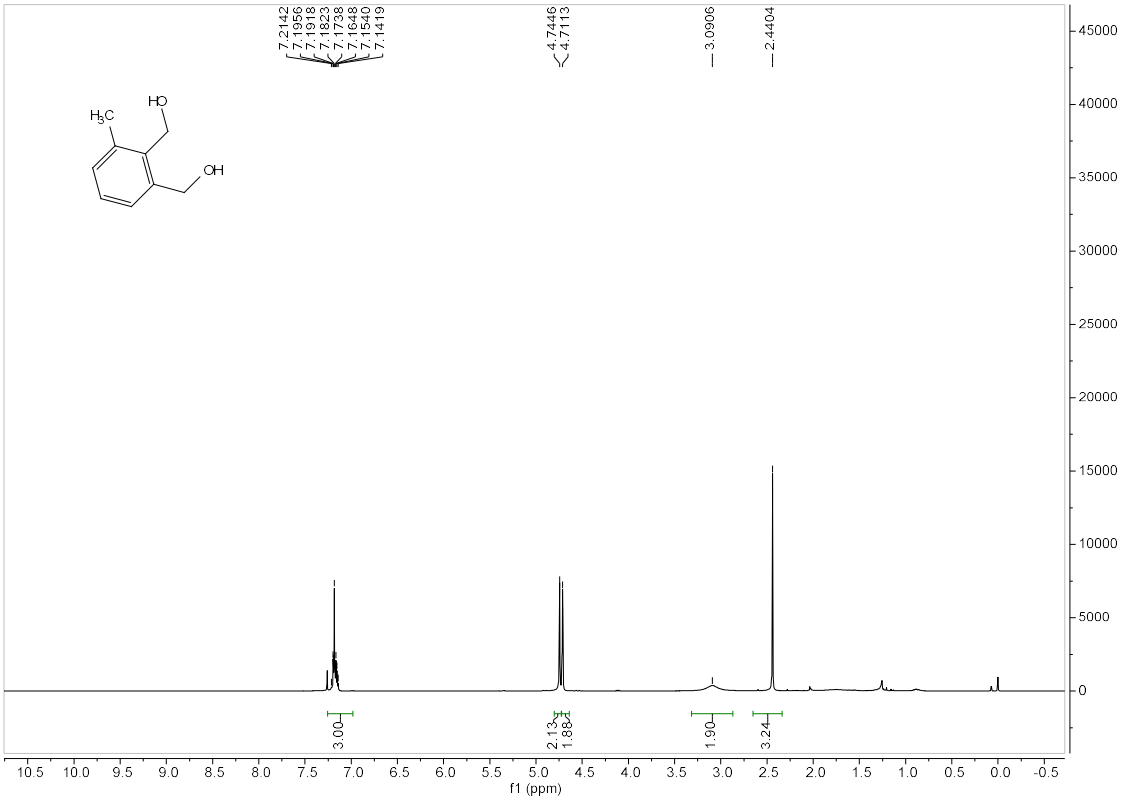

169.5
166.0
135.5
134.4
129.0
128.2
127.6
61.5
61.5
19.1
14.3
14.2
f1 (ppm)

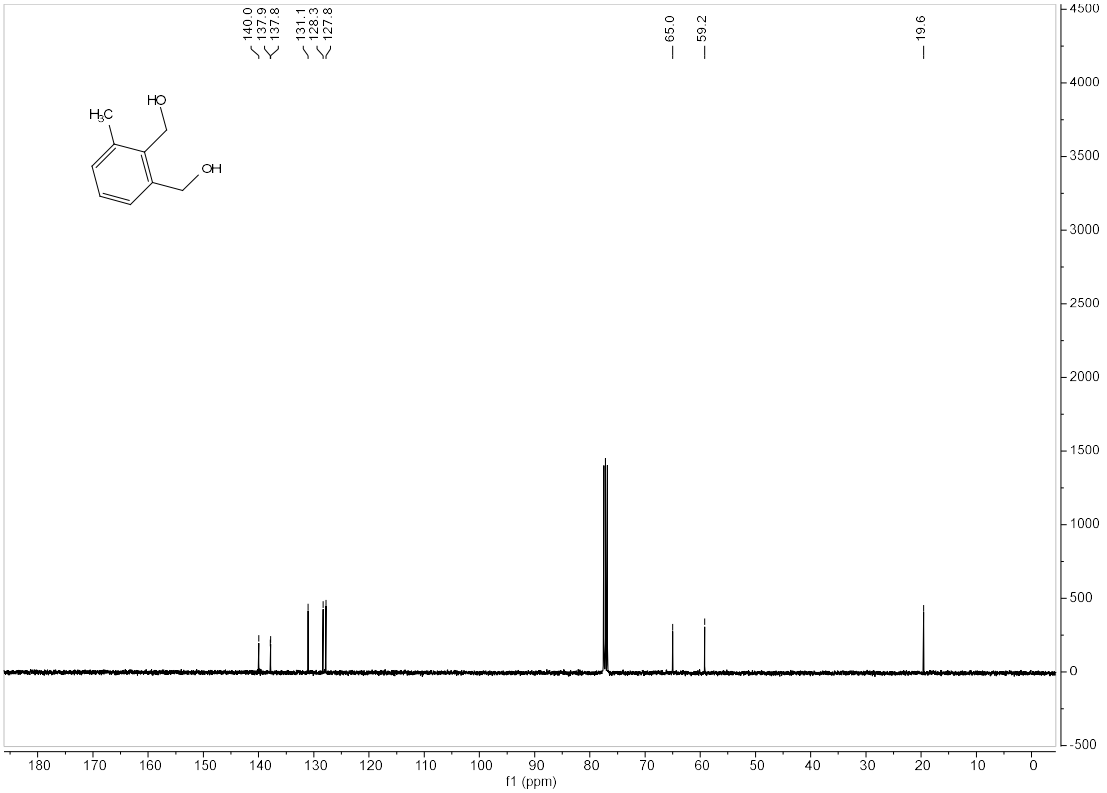
9


7.6105
7.4703
7.4281
7.3844
7.3089
2.3089
NH2
O
O
Me
NH2
7.00
3.01
f1 (ppm)


170.65
169.37
137.37
134.14
134.11
131.59
127.70
125.00
19.08
NH2
O
O
Me
NH2
f1 (ppm)

10


7.2142
7.1956
7.1918
7.1823
7.1738
7.1648
7.1540
7.1419
4.7446
4.7113
3.0906
2.4404
HO
H3C
OH
3.00
2.13
1.88
1.90
3.24
f1 (ppm)


140.0
137.9
137.8
131.1
128.3
127.8
65.0
59.2
19.6
HO
H3C
OH
f1 (ppm)