Copper-Catalyzed Oxyamination of Electron Deficient Alkenes with *N*-Acyloxyamines

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Supporting Information

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General information

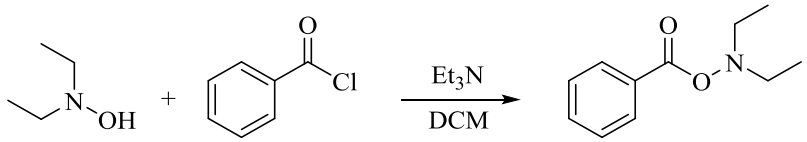
CuI, 2,2'-Dipyridine, Dioxane were purchased from commercial suppliers and used as received unless otherwise noted. All reactions were carried out under nitrogen atmosphere. Reactions were monitored through thin layer chromatography [Merck 60 F254 precoated silica gel plate (0.2 mm thickness)]. Subsequent to elution, spots were visualized using UV radiation (254 nm) on Spectroline Model ENF-24061/F 254 nm. Further visualization was possible using basic solution of potassium permanganate or acidic solution of ceric molybdate as stain, followed by heating on a hot plate. Flash chromatography was performed using Merck silica gel 60 with distilled solvents. HRMS spectra were recorded on a Waters Q–Tof Permier Spectrometer. ^{1}H NMR and ^{13}C NMR spectra were recorded using Bruker Avance 400 MHz spectrometers. Chemical shifts for ^{1}H NMR spectra are reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (δ 0.0) and relative to the signal of $SiMe_4$ (δ 0.00, singlet). Multiplicities were given as: s (singlet); brs (broad singlet); d (doublet); t (triplet); q (quartet); dd (doublets of doublet); ddd (doublets of doublets of doublet); td (triplet of doublet); m (multiplets); ddt (doublet of doublet of triplet) and etc. Coupling constants are reported as a *J* value in Hz. Carbon nuclear magnetic resonance spectra (^{13}C NMR) are reported as δ in units of parts per million (ppm) downfield from $SiMe_4$ (δ 0.0) and relative to the signal of chloroform-*d* (δ 77.00, triplet).

Experimental section

Substrate synthesis

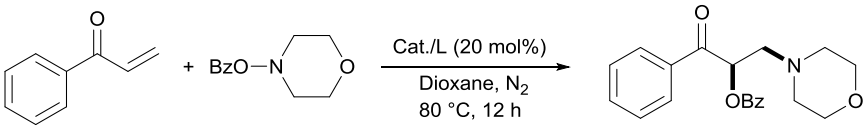
All the vinyl ketone derivatives were known compounds. Substrates **2d-2g** were prepared according to the general procedure A.

General procedure A:

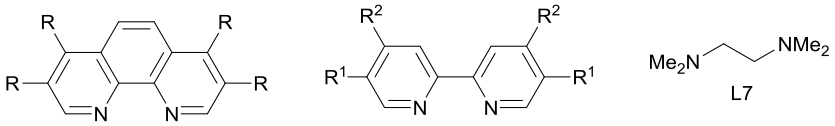


General Procedure for the preparation of *N,N*-dialkyl O-hydroxylamine derivatives: An oven-dried round bottom flask equipped with magnetic stir bar and addition funnel was charged with *N,N*-diethylhydroxylamine (0.89 g, 1.0 mL, 10 mmol), freshly distilled triethylamine (1.0 g, 1.4 mL, 10 mmol), and anhydrous dichloromethane (10 mL). The addition funnel was charged with benzoyl chloride (1.4 g, 1.2 mL, 10 mmol) and anhydrous dichloromethane (5 mL). The benzoyl chloride solution was added drop wise over 10 minutes and reaction mixture stirred at room temperature an additional 30 minutes. The reaction mixture was diluted with water (25 mL) and the organic layer was separated, washed with water (1 x 25mL), dried over sodium sulfate, and the solvent was removed under reduced pressure. The crude product was purified by flash chromatography, eluting with 15% ethyl acetate:hexanes, to afford *N,N*-diethyl-*O*-benzoylhydroxylamine (1.89 g, 9.8 mmol, 98 % yield) as a pale yellow oil.

Reaction condition optimization.[a]



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



L1, R = H
L2, R = Me

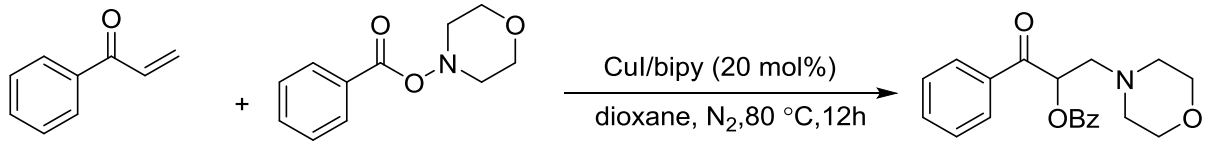
L3, R^1 = H, R^2 = *t*-Bu L5, R^1 = H, R^2 = Me
L4, R^1 = Me, R^2 = H L6, R^1 = R^2 = H

Entry	Catalyst	Ligand	Additive	Yield[b] (%)
1	CuI	L1	-	50
2	CuI	L3	-	58
3	CuI	L7	-	0
4	CuI	L4	-	70
5	CuI	L5	-	42
6	**CuI**	**L6**	**-**	**76**
7	CuI	L2	-	40
8	CuCl	L6	-	18
9	CuBr	L6	-	30
10	$Cu(MeCN)_4PF_6$	L6	-	0
11	$Cu(MeCN)_4BF_4$	L6	-	0
12	CuOAc	L6	-	0
13	CuBr·SMe_2	L6	-	52
14	CuI	-	-	0[c]
15	-	L6	-	0[d]
16	$Cu(MeCN)_4PF_6$	L6	Bu_4NI	76[e]

[a] Unless otherwise noted, the reactions were carried out at 80 °C using **1a** (0.1 mmol), **2a** (0.11 mmol), catalyst (0.02 mmol) and ligand (0.02 mmol) in solvent (1.0 mL) for 12 h. [b] Yield was determined by ^{1}H NMR using 1,1,2,2-tetrachloroethane as internal standard. [c] No ligand was added. [d] No catalyst was added. [e] 0.05 mmol Bu_4NI was added.

Copper-catalyzed oxyamination of electron deficient alkenes with *N*-acyloxyamines

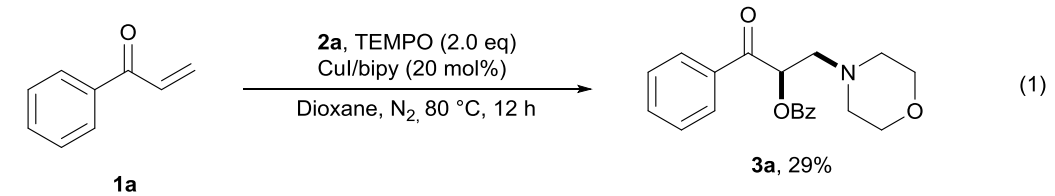
General procedure B:



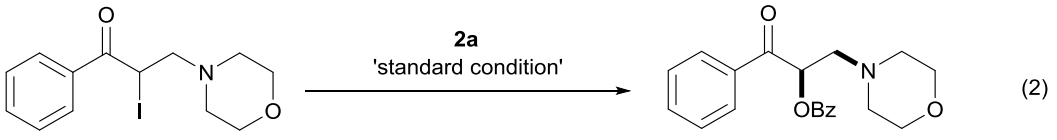
1a **2a** **3a**

Under nitrogen atmosphere, oven-dried 10mL schlenk tube was charged with 1-phenylprop-2-en-1-one **1a** (13.2 mg, 0.1 mmol), morpholino benzoate **2a** (22.8 mg, 0.11 mmol), CuI (3.8 mg, 0.02 mmol), 2,2'-dipyridine (3.1 mg, 0.02mmol) in sequence followed by adding dioxane (1 mL) through syringe. After stirring at 80 ℃ for 12h, the reaction was diluted with ethyl acetate, and the resulting mixture was filtered and concentrated in vacuo, the residue was purified via silica gel chromatography to afforded the desired product **3a** (26.7 mg, Yield: 76%).

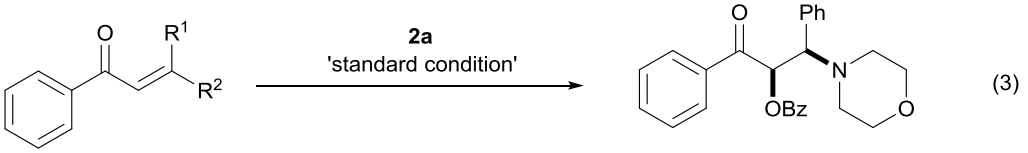
Control experiments



1a **3a**, 29% (1)



3a' **3a**, 30% (2)

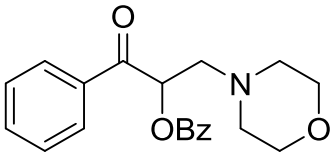


E- or *Z*-**1m**

R^1 = H, R^2 = Ph, dr = 2.4:1
R^1 = Ph, R^2 = H, dr = 2.6:1 (3)

Characterization of structurally novel compounds

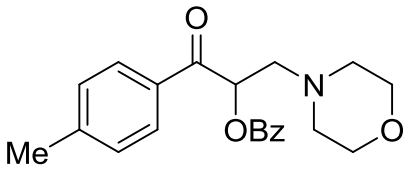
3-morpholino-1-oxo-1-phenylpropan-2-yl benzoate:



3a

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 – 8.05 (m, 2H), 8.05 – 7.97 (m, 2H), 7.62 – 7.54 (m, 2H), 7.53 – 7.42 (m, 4H), 6.32 (dd, J = 6.7, 4.2 Hz, 1H), 3.66 – 3.53 (m, 4H), 3.07 – 2.95 (m, 2H), 2.70 – 2.59 (m, 2H), 2.58 – 2.45 (m, 2H).ppm **^{13}C NMR (100 MHz, $CDCl_3$):** δ 195.51 (s), 165.85 (s), 135.33 (s), 133.43 (s), 133.36 (s), 129.84 (s), 129.37 (s), 128.73 (s), 128.45 (s), 128.36 (s), 74.14 (s), 66.86 (s), 58.95 (s), 53.79 (s).ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{22}NO_4$ $[M+H]^+$ 340.1549, found: 340.1551.

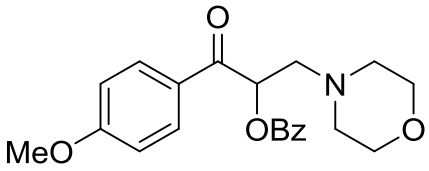
3-morpholino-1-oxo-1-(p-tolyl)propan-2-yl benzoate:



3b

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 – 8.05 (m, 2H), 7.92 (d, J = 8.2 Hz, 2H), 7.61 – 7.55 (m, 1H), 7.48 – 7.40 (m, 2H), 7.28 (d, J = 8.0 Hz, 2H), 6.32 (dd, J = 6.9, 4.0 Hz, 1H), 3.67 – 3.57 (m, 4H), 3.07 – 2.95 (m, 2H), 2.66 (m , 2H), 2.60 – 2.51 (m, 2H), 2.42 (s, 3H).ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 194.87 (s), 165.84 (s), 144.46 (s), 133.32 (s), 132.55 (s), 129.84 (s), 129.45 (s), 128.53 (s), 128.42 (s), 128.23(s), 73.93 (s), 66.82 (s), 58.97 (s), 53.75 (s), 21.71 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{24}NO4$ $[M+H]^+$ 354.1705, found: 354.1708.

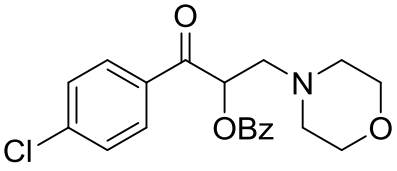
1-(4-methoxyphenyl)-3-morpholino-1-oxopropan-2-yl benzoate:



3c

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (d, J = 7.3 Hz, 2H), 8.02 (d, J = 8.9 Hz, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.7 Hz, 2H), 6.97 (d, J = 8.9 Hz, 2H), 6.29 (dd, J = 6.6, 4.4 Hz, 1H), 3.88 (s, 3H), 3.62 (t, J = 4.6 Hz, 4H), 3.08 – 2.93 (m, 2H), 2.60 (m, 4H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 193.70 (s), 165.88 (s), 163.86 (s), 133.31 (s), 130.81 (s), 129.85 (s), 129.49 (s), 128.43 (s), 127.99 (s), 113.98 (s), 73.71 (s), 66.92 (s), 59.18 (s), 55.50 (s), 53.83 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{21}H_{24}NO_5$ $[M+H]^+$ 370.1654, found: 370.1655.

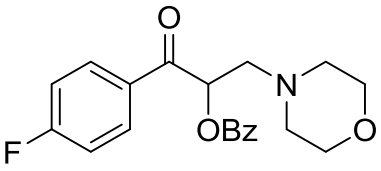
1-(4-chlorophenyl)-3-morpholino-1-oxopropan-2-yl benzoate:



3d

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 – 8.03 (m, 2H), 7.99 – 7.92 (m, 2H), 7.60 (t, J = 7.5 Hz, 1H), 7.50 – 7.43 (m, 4H), 6.23 (dd, J = 6.5, 4.4 Hz, 1H), 3.64 – 3.53 (m, 4H), 3.07 – 2.93 (m, 2H), 2.62 (dt, J = 9.2, 4.5 Hz, 2H), 2.57 – 2.47 (m, 2H). ppm; 13C NMR (100 MHz, CDCl3): δ 194.58 (s), 165.86 (s), 139.92 (s), 133.74 (s), 133.50 (s), 129.85 (s), 129.79 (s), 129.20 (s), 129.10 (s), 128.51 (s), 74.00 (s), 66.86 (s), 58.95 (s), 53.85 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{21}ClNO_4$ $[M+H]^+$ 374.1159, found: 374.1158.

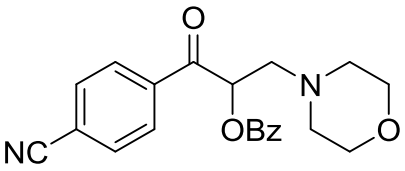
1-(4-fluorophenyl)-3-morpholino-1-oxopropan-2-yl benzoate:



3e

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 – 8.02 (m, 4H), 7.63 – 7.56 (m, 1H), 7.49 – 7.42 (m, 2H), 7.22 – 7.12 (m, 2H), 6.24 (dd, J = 6.6, 4.4 Hz, 1H), 3.64 – 3.54 (m, 4H), 3.07 – 2.94 (m, 2H), 2.63 (dt, J = 9.3, 4.6 Hz, 2H), 2.58 – 2.46 (m, 2H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 194.08 (s), 165.88 (d, J=255.5Hz), 165.86 (s), 133.46 (s), 131.73 (d, J = 3.0 Hz),131.08 (d, J = 9.3 Hz), 129.84 (s), 129.24 (s), 128.49 (s), 115.95 (d, J = 22.0 Hz), 73.92 (s), 66.86 (s), 58.98 (s), 53.84 (s).ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{21}FNO_4$ $[M+H]^+$ 358.1454, found: 358.1450.

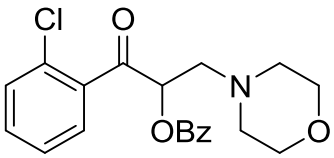
1-(4-cyanophenyl)-3-morpholino-1-oxopropan-2-yl benzoate:



3f

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 – 8.07 (m, 2H), 8.05 (dt, J = 8.5, 1.6 Hz, 2H), 7.82 – 7.76 (m, 2H), 7.64 – 7.58 (m, 1H), 7.50 – 7.43 (m, 2H), 6.19 (dd, J = 6.3, 4.7 Hz, 1H), 3.62 – 3.48 (m, 4H), 3.02 (qd, J = 13.8, 5.5 Hz, 2H), 2.67 – 2.55 (m, 2H), 2.55 – 2.42 (m, 2H).ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 195.11 (s), 165.86 (s), 138.98 (s), 133.68 (s), 132.53 (s), 129.84 (s), 128.89 (s), 128.69 (s), 128.58 (s), 117.78 (s), 116.50 (s), 74.09 (s), 66.76 (s), 58.78 (s), 53.85 (s). ppm; HRMS (ESI, m/z): calcd for $C_{21}H_{21}N_2O_4$ [M+H]+ 365.1501, found: 365.1505.

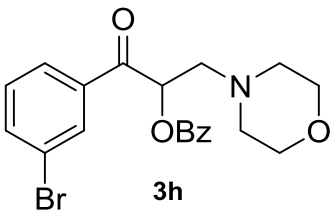
1-(2-chlorophenyl)-3-morpholino-1-oxopropan-2-yl benzoate:



3g

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 – 8.01 (m, 2H), 7.74 (dd, J = 7.5, 1.5 Hz, 1H), 7.59 (t, J = 7.4 Hz, 1H), 7.49 – 7.32 (m, 5H), 6.24 (dd, J = 6.1, 4.6 Hz, 1H), 3.63 – 3.48 (m, 4H), 2.98 (qd, J = 13.8, 5.4 Hz, 2H), 2.66 – 2.55 (m, 2H), 2.45 – 2.33 (m, 2H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 197.90 (s), 165.77 (s), 137.94 – 137.02 (m), 133.42 (s), 131.91 (s), 131.43 (s), 130.49 (s), 129.80 (s), 129.41 (s), 129.31 (s), 128.48 (s), 126.68 (s), 76.44 (s), 66.78 (s), 58.45 (s), 53.87 (s).ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{21}ClNO_4$ $[M+H]^+$ 374.1159, found: 374.1161.

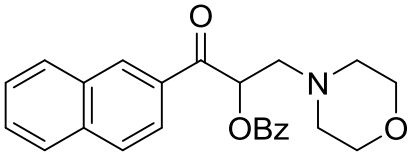
1-(3-bromophenyl)-3-morpholino-1-oxopropan-2-yl benzoate:



3h

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (t, J = 1.7 Hz, 1H), 8.10 – 8.03 (m, 2H), 7.93 (d, J = 7.8 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.60 (t, J = 7.5 Hz, 1H), 7.47 (t, J = 7.8 Hz, 2H), 7.38 (t, J = 7.9 Hz, 1H), 6.18 (dd, J = 6.3, 4.5 Hz, 1H), 3.66 – 3.50 (m, 4H), 3.01 (qd, J = 13.8, 5.5 Hz, 2H), 2.66 – 2.58 (m, 2H), 2.58 – 2.48 (m, 2H).ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 194.71 (s), 165.84 (s), 137.31 (s), 136.19 (s), 133.52 (s), 131.52 (s), 130.28 (s), 129.86 (s), 129.17 (s), 128.52 (s), 126.81 (s), 123.00 (s), 74.23 (s), 66.85 (s), 58.95 (s), 53.87 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{21}BrNO_4$ $[M+H]^+$ 418.0654, found: 418.0651.

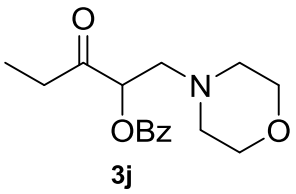
3-morpholino-1-(naphthalen-2-yl)-1-oxopropan-2-yl benzoate:



3i

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.59 (s, 1H), 8.14 – 8.08 (m, 2H), 8.05 (dd, J = 8.6, 1.7 Hz, 1H), 7.99 (d, J = 8.0 Hz, 1H), 7.91 (dd, J = 15.7, 8.4 Hz, 2H), 7.65-7.53 (m, 3H), 7.50-7.42 (t, J = 7.8, 2H), 6.48 (dd, J = 6.6, 4.1 Hz, 1H), 3.66 – 3.54 (m, 4H), 3.08 (qd, J = 14.0, 5.4 Hz, 2H), 2.74-2.61 (m, 2H), 2.62 – 2.48 (m, 2H).ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 195.42 (s), 165.91 (s), 135.69 (s), 133.39 (s), 132.60 (m), 132.41 (s), 130.08 (s), 129.87 (s), 129.63 (s), 129.37 (s), 128.72 (s), 128.69 (s), 128.47 (s), 127.81 (s), 126.92 (s), 124.05 (s), 74.25 (s), 66.87 (s), 59.13 (s), 53.82 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{24}H_{24}NO_4$ $[M+H]^+$ 390.1705, found: 390.1700.

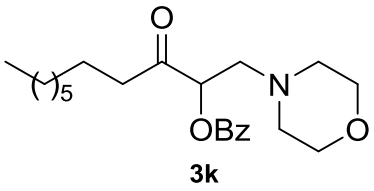
1-morpholino-3-oxopentan-2-yl benzoate:



3j

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 – 8.01 (m, 2H), 7.62 – 7.55 (m, 1H), 7.49 – 7.42 (m, 2H), 5.47 (dd, J = 6.7, 3.8 Hz, 1H), 3.71 – 3.59 (m, 4H), 2.99 (dd, J = 13.8, 6.8 Hz, 1H), 2.88 (dd, J = 13.8, 3.8 Hz, 1H), 2.70 – 2.48 (m, 6H), 1.10 (t, J = 7.2 Hz, 3H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 206.94 (s), 165.81 (s), 133.42 (s), 129.74 (s), 129.32 (s), 128.50 (s), 77.14 (s), 66.85 (s), 58.73 (s), 53.93 (s), 32.83 (s), 7.16 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{16}H_{22}NO_4$ $[M+H]^+$ 292.1549, found: 292.1547.

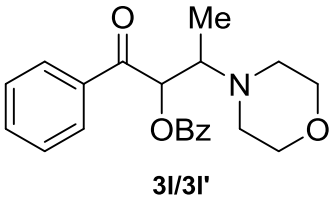
1-morpholino-3-oxoundecan-2-yl benzoate:



3k

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 – 8.03 (m, 2H), 7.62 – 7.56 (m, 1H), 7.49 – 7.43 (m, 2H), 5.46 (dd, J = 6.7, 3.7 Hz, 1H), 3.71 – 3.60 (m, 4H), 2.99 (dd, J = 13.8, 6.7 Hz, 1H), 2.87 (dd, J = 13.8, 3.7 Hz, 1H), 2.72 – 2.62 (m, 2H), 2.62 – 2.47 (m, 4H), 1.61 (dd, J = 14.4, 7.2 Hz, 2H), 1.35 – 1.14 (m, 10H), 0.87 (t, J = 6.9 Hz, 3H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 206.39 (s), 165.80 (s), 133.42 (s), 129.76 (s), 129.34 (s), 128.51 (s), 77.22 (s), 66.86 (s), 58.66 (s), 53.94 (s), 39.53 (s), 31.79 (s), 29.36 (s), 29.17 (s), 29.10 (s), 23.04 (s), 22.61 (s), 14.07 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{22}H_{34}NO_4$ $[M+H]^+$ 376.2488, found: 376.2493.

3-morpholino-1-oxo-1-phenylbutan-2-yl benzoate:

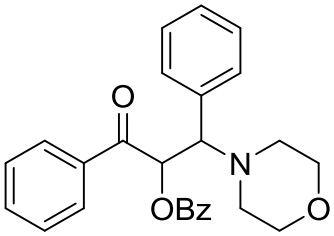


3l/3l'

(major diastereoisomer 3l) ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 – 7.98 (m, 4H), 7.63 – 7.54 (m, 2H), 7.53 – 7.41 (m, 4H), 6.14 (d, J = 6.8 Hz, 1H), 3.50 – 3.41 (m, 2H), 3.35 (p, J = 6.8 Hz, 1H), 3.28 (d, J = 4.6 Hz, 2H), 2.66 – 2.48 (m, 4H), 1.24 (d, J = 6.8 Hz, 3H).ppm; **^{13}C NMR (100 MHz, CDCl3):** δ 197.81 (s), 165.98 (s), 136.92 (s), 133.41 (s), 133.00 (s), 129.83 (s), 129.33 (s), 128.67 (s), 128.47 (s), 128.21 (s), 75.37 (s), 66.80 (s), 61.41 (s), 49.43 (s), 9.98 (s).ppm **(minal diastereoisomer 3l') ^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.11 – 8.07 (m, 2H), 7.99 – 7.92 (m, 2H), 7.62 – 7.53 (m, 2H), 7.50 – 7.44 (m, 4H), 6.26 (d, J = 6.0 Hz, 1H), 3.57 – 3.48 (m, 4H), 3.48 – 3.39 (m, 1H), 2.80 – 2.69 (m, 2H), 2.36 – 2.22 (m, 2H), 1.15 (d, J = 6.9 Hz, 3H).ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 195.24 (s), 165.91 (s), 136.55 (s), 133.30 (s), 132.79 (s), 129.77 (s), 129.63 (s), 128.57 (s), 128.50 (s),

128.01 (s), 78.97 (s), 67.19 (s), 60.25 (s), 49.30 (s), 9.03 (s).ppm; **HRMS (ESI, m/z):** calcd for $C_{21}H_{24}NO_4$ $[M+H]^+$ 354.1705, found: 354.1704.

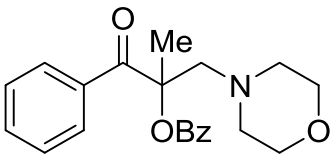
1-morpholino-3-oxo-1,3-diphenylpropan-2-yl benzoate:



3m

(major diastereoisomer) ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 – 8.04 (m, 1H), 7.86 (t, J = 10.6 Hz, 1H), 7.59 (t, J = 7.3 Hz, 1H), 7.51 (t, J = 8.0 Hz, 1H), 7.38 – 7.24 (m, 4H), 6.67 (d, J = 9.2 Hz, 1H), 4.31 (d, J = 9.2 Hz, 1H), 3.39 – 3.27 (m, 1H), 3.13 (s, 1H), 2.54 – 2.41 (m, 1H), 2.30 (s, 1H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 198.27 (s), 166.12 (s), 137.85 (s), 133.59 (s), 133.33 (s), 132.91 (s), 129.82 (s), 129.05 (s), 128.91 (s), 128.66 (s), 128.34 (s), 128.30 (s), 128.26 (s), 128.11 (s), 71.73 (s), 71.39 (s), 66.54 (s), 50.53 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{26}H_{26}NO_4$ $[M+H]^+$ 416.1862, found: 416.1868.

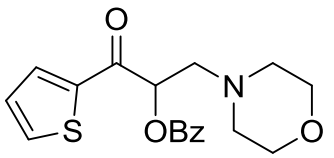
2-methyl-3-morpholino-1-oxo-1-phenylpropan-2-yl benzoate:



3n

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 – 8.02 (m, 2H), 7.95 – 7.88 (m, 2H), 7.59 – 7.53 (m, 1H), 7.46 – 7.38 (m, 3H), 7.36 – 7.28 (m, 2H), 3.67 – 3.56 (m, 4H), 3.23 (d, J = 14.4 Hz, 1H), 3.08 (d, J = 14.4 Hz, 1H), 2.67 – 2.54 (m, 4H), 1.89 (s, 3H). ppm. **^{13}C NMR (100 MHz, $CDCl_3$):** δ 199.48 (s), 165.41 (s), 135.65 (s), 133.24 (s), 132.23 (s), 130.09 (s), 129.53 (s), 128.55 (s), 128.48 (s), 128.20 (s), 88.08 (s), 67.05 (s), 64.20 (s), 55.14 (s), 22.09 (s) ppm. **HRMS (ESI, m/z):** calcd for $C_{21}H_{24}NO_4$ $[M+H]^+$ 354.1705, found: 354.1709.

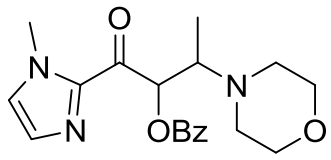
3-morpholino-1-oxo-1-(thiophen-2-yl)propan-2-yl benzoate:



3o

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 – 8.03 (m, 1H), 7.92 (d, J = 3.7 Hz, 1H), 7.70 (d, J = 4.9 Hz, 1H), 7.60 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.7 Hz, 1H), 7.20 – 7.13 (m, 1H), 6.09 (dd, J = 6.9, 4.6 Hz, 1H), 3.70 – 3.56 (m, 2H), 3.13 – 2.98 (m, 1H), 2.66 (dt, J = 9.3, 4.6 Hz, 1H), 2.62 – 2.54 (m, 1H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 188.14 (s), 165.78 (s), 141.31 (s), 134.49 (s), 133.46 (s), 132.77 (s), 129.90 (s), 129.28 (s), 128.50 (s), 128.25 (s), 74.60 (s), 66.92 (s), 59.42 (s), 53.83 (s). ppm. **HRMS (ESI, m/z):** calcd for $C_{18}H_{20}NO_4S$ $[M+H]^+$ 346.1113, found: 346.1118.

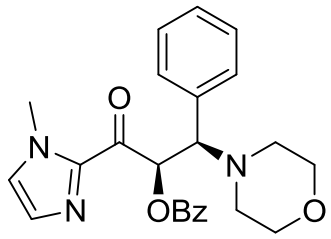
1-(1-methyl-1H-imidazol-2-yl)-3-morpholino-1-oxobutan-2-yl benzoate:



3p/3p'

(major diastereoisomer 3p) ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 – 8.03 (m, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.44 (t, J = 7.7 Hz, 2H), 7.18 (s, 1H), 7.05 (s, 1H), 6.49 (d, J = 7.0 Hz, 1H), 3.99 (s, 3H), 3.54 – 3.42 (m, 3H), 3.28 (s, 2H), 2.82 – 2.72 (m, 2H), 2.64 – 2.53 (m, 2H), 1.26 (d, J = 6.8 Hz, 3H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 188.82 (s), 165.66 (s), 142.25 (s), 133.24 (s), 129.81 (s), 129.49 (s), 128.40 (s), 126.66 (s), 75.52 (s), 67.29 (s), 61.70 (s), 49.40 (s), 35.80 (s), 10.55 (s). **(minal diastereoisomer 3p')^{1}H NMR (400 MHz, $CDCl_3$):** δ 8.12 – 8.07 (m, 2H), 7.59 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.7 Hz, 2H), 7.16 (s, 1H), 7.05 (s, 1H), 6.39 (d, J = 5.5 Hz, 1H), 4.10 – 4.02 (m, 1H), 4.03 – 3.96 (m, 3H), 3.58 – 3.39 (d, J = 3.9 Hz, 4H), 2.86 – 2.74 (m, 2H), 2.41 – 2.27 (m, 2H), 1.21 (d, J = 7.0 Hz, 3H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 185.77 (s), 165.71 (s), 141.58 (s), 133.20 (s), 129.72 (s), 128.98 (s), 128.49 (s), 126.31 (s), 80.62 (s), 67.50 (s), 60.48 (s), 49.15 (s), 35.81 (s), 8.21 (s). ppm; ppm **HRMS (ESI, m/z):** calcd for $C_{19}H_{24}N_3O_4$ $[M+H]^+$ 358.1767, found: 358.1772.

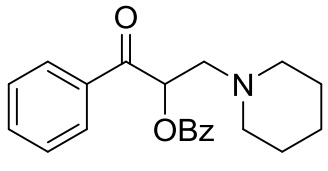
1-(1-methyl-1H-imidazol-2-yl)-3-morpholino-1-oxo-3-phenylpropan-2-yl benzoate:



3q

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, J = 7.2 Hz, 2H), 7.49 (t, J = 7.5 Hz, 1H), 7.38 – 7.29 (m, 7H), 7.25 (s, 1H), 7.08 (d, J = 8.0 Hz, 2H), 4.40 (d, J = 9.2 Hz, 1H), 3.97 (s, 3H), 3.43 – 3.33 (m, 2H), 3.27–3.09 (m, 2H), 2.76 – 2.67 (m, 2H), 2.37 – 2.22 (m, 2H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 188.51 (s), 165.76 (s), 142.75 (s), 134.03 (s), 133.12 (s), 129.82 (s), 129.58 (s), 129.27 (s), 128.99 (s), 128.27 (s), 128.15 (s), 127.96 (s), 126.70 (s), 72.51 (s), 71.45 (s), 67.11 (s), 50.36 (s), 35.73 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{24}H_{26}N_3O_4$ $[M+H]^+$ 420.1923, found: 420.1918.

1-oxo-1-phenyl-3-(piperidin-1-yl)propan-2-yl benzoate:

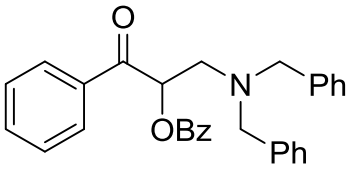


3r

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 – 8.06 (m, 2H), 8.06 – 7.96 (m, 2H), 7.58 (ddd, J = 7.4, 2.3, 1.1 Hz, 2H), 7.47 (dt, J = 13.3, 7.6 Hz, 4H), 6.29 (dd, J = 6.6, 4.4 Hz, 1H), 3.07 – 2.91 (m, 2H), 2.64 – 2.42 (m, 4H), 1.55 –

1.42 (m, 4H), 1.41 – 1.29 (m, 2H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 196.10 (s), 165.99 (s), 135.37 (s), 133.32 (s), 133.25 (s), 129.89 (s), 129.55 (s), 128.66 (s), 128.47 (s), 128.40 (s), 74.45 (s), 59.37 (s), 54.73 (s), 25.96 (s), 23.96 (s).ppm; **HRMS (ESI, m/z):** calcd for $C_{21}H_{24}NO_3$ $[M+H]^+$ 338.1756, found: 338.1757.

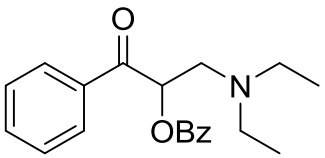
3-(dibenzylamino)-1-oxo-1-phenylpropan-2-yl benzoate:



3s

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.08 (dd, J = 5.2, 3.3 Hz, 2H), 7.71 (dd, J = 8.3, 1.2 Hz, 2H), 7.61 – 7.55 (m, 1H), 7.55 – 7.49 (m, 1H), 7.44 (dd, J = 10.6, 4.7 Hz, 2H), 7.34 (t, J = 7.8 Hz, 2H), 7.3 – 7.17 (m, 10H), 6.29 (dd, J = 8.1, 3.3 Hz, 1H), 3.81 (d, J = 13.5 Hz, 2H), 3.72 – 3.63 (m, 2H), 3.25 – 3.05 (m, 2H).ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 195.17 (s), 166.01 (s), 138.85 (s), 134.72 (s), 133.39 (s), 133.30 (s), 129.94 (s), 129.45 (s), 128.88 (s), 128.67 (s), 128.42 (s), 128.36 (s), 128.31 (s), 127.10 (s), 75.34 (s), 59.08 (s), 54.10 (s).ppm; **HRMS (ESI, m/z):** calcd for $C_{30}H_{28}NO_3$ $[M+H]^+$ 450.2069, found: 450.2073.

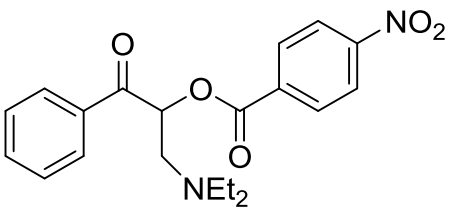
3-(diethylamino)-1-oxo-1-phenylpropan-2-yl benzoate:



3t

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 – 8.06 (m, 2H), 8.06 – 8.00 (m, 2H), 7.61 – 7.54 (m, 2H), 7.51 – 7.42 (m, 4H), 6.24 (dd, J = 6.7, 4.7 Hz, 1H), 3.15 – 3.02 (m, 2H), 2.68 – 2.57 (m, 4H), 0.98 (t, J = 7.1 Hz, 6H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 196.35 (s), 166.06 (s), 135.56 (s), 133.34 (s), 133.22 (s), 129.87 (s), 129.58 (s), 128.66 (s), 128.52 (s), 128.39 (s), 74.99 (s), 53.71 (s), 47.62 (s), 11.89 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{24}NO_3$ $[M+H]^+$ 326.17656, found: 326.1763.

3-(diethylamino)-1-oxo-1-phenylpropan-2-yl 4-nitrobenzoate:

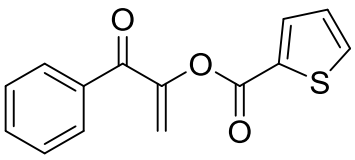


3u

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.35 – 8.21 (m, 4H), 8.06 – 7.97 (m, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.6 Hz, 2H), 6.29 (dd, J = 7.0, 4.4 Hz, 1H), 3.16 – 3.00 (m, 2H), 2.70 – 2.53 (m, 4H), 0.97 (t, J = 7.1 Hz, 6H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 195.57 (s), 164.23

(s), 150.69 (s), 135.21 (s), 135.03 (s), 133.65 (s), 130.96 (s), 128.78 (s), 128.46 (s), 123.57 (s), 75.95 (s), 53.77 (s), 47.62 (s), 11.86 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{20}H_{23}N_2O_5$ $[M+H]^+$ 371.1607, found: 371.1605.

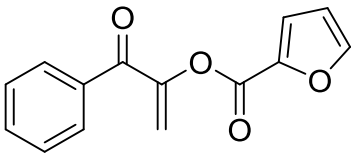
3-oxo-3-phenylprop-1-en-2-yl thiophene-2-carboxylate：



3v

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 – 7.87 (m, 3H), 7.66 (dd, J = 4.7, 0.9 Hz, 1H), 7.58 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.7 Hz, 2H), 7.17 – 7.12 (m, 1H), 5.86 (d, J = 2.2 Hz, 1H), 5.70 (d, J = 2.2 Hz, 1H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 189.42 (s), 160.01 (s), 150.93 (s), 136.12 (s), 135.19 (s), 134.00 (s), 132.98 (s), 131.59 (s), 129.60 (s), 128.38 (s), 128.07 (s), 114.72 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{14}H_{10}O_3SNa$ $[M+Na]^+$ 281.0248, found: 281.0253.

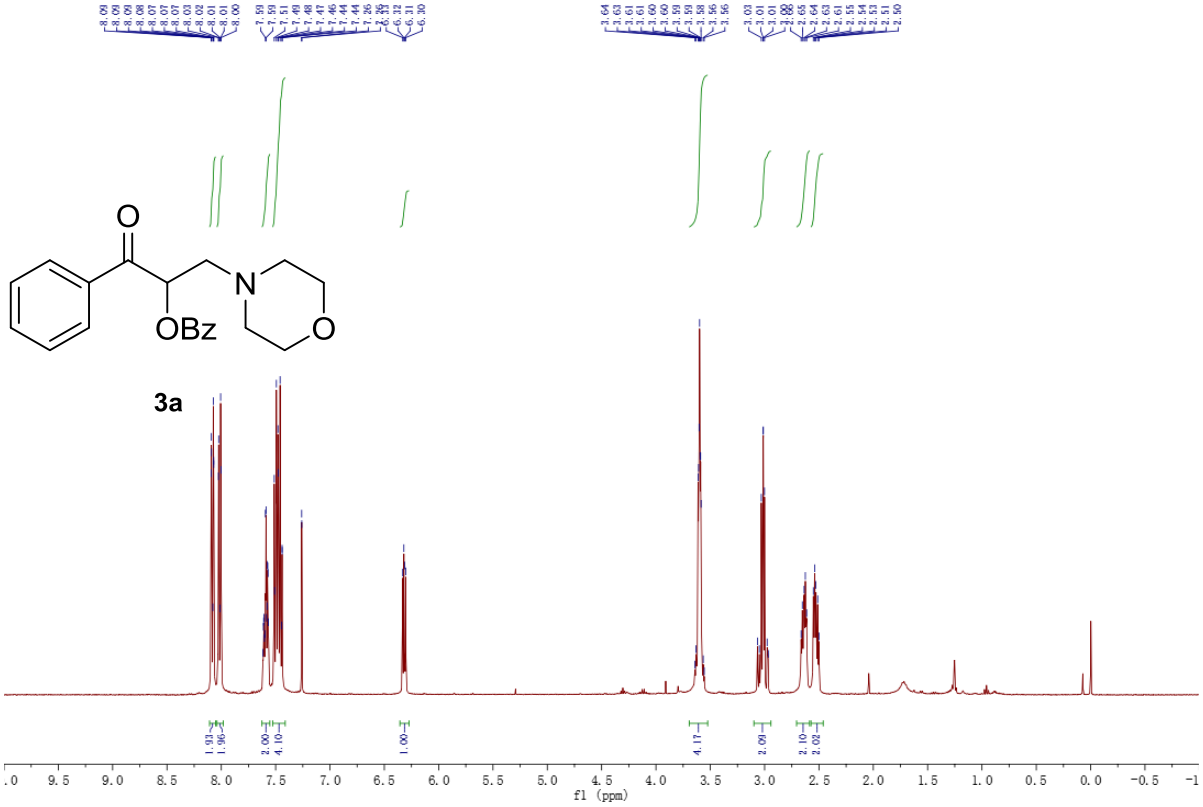
3-oxo-3-phenylprop-1-en-2-yl furan-2-carboxylate：

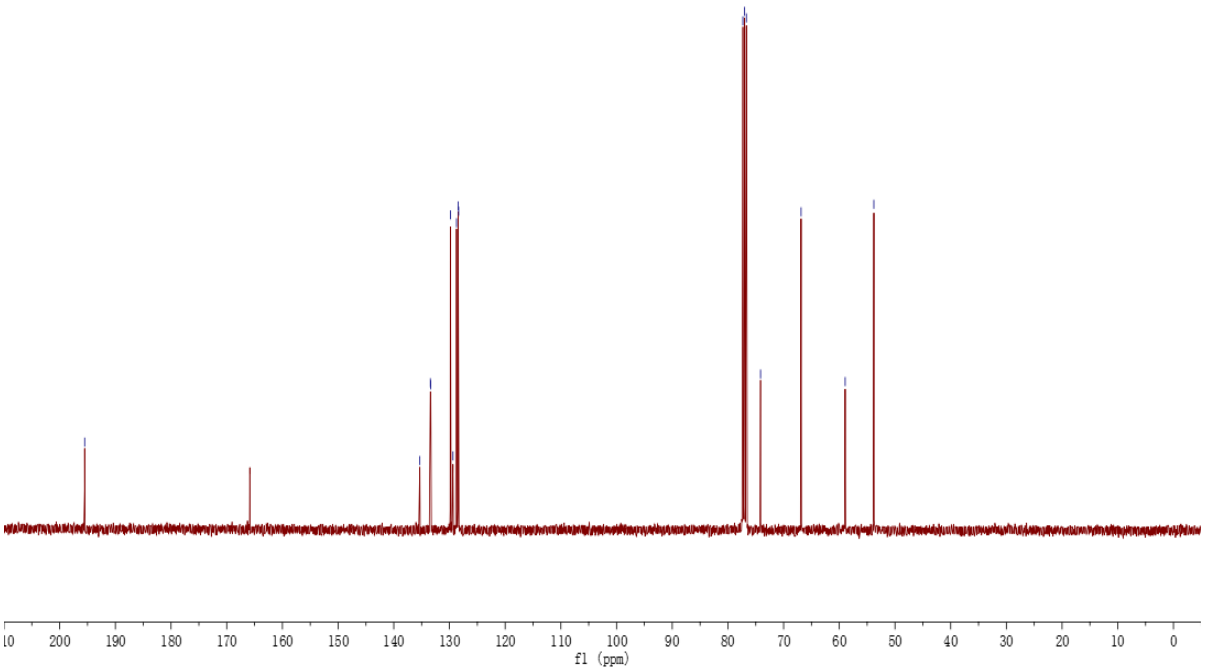


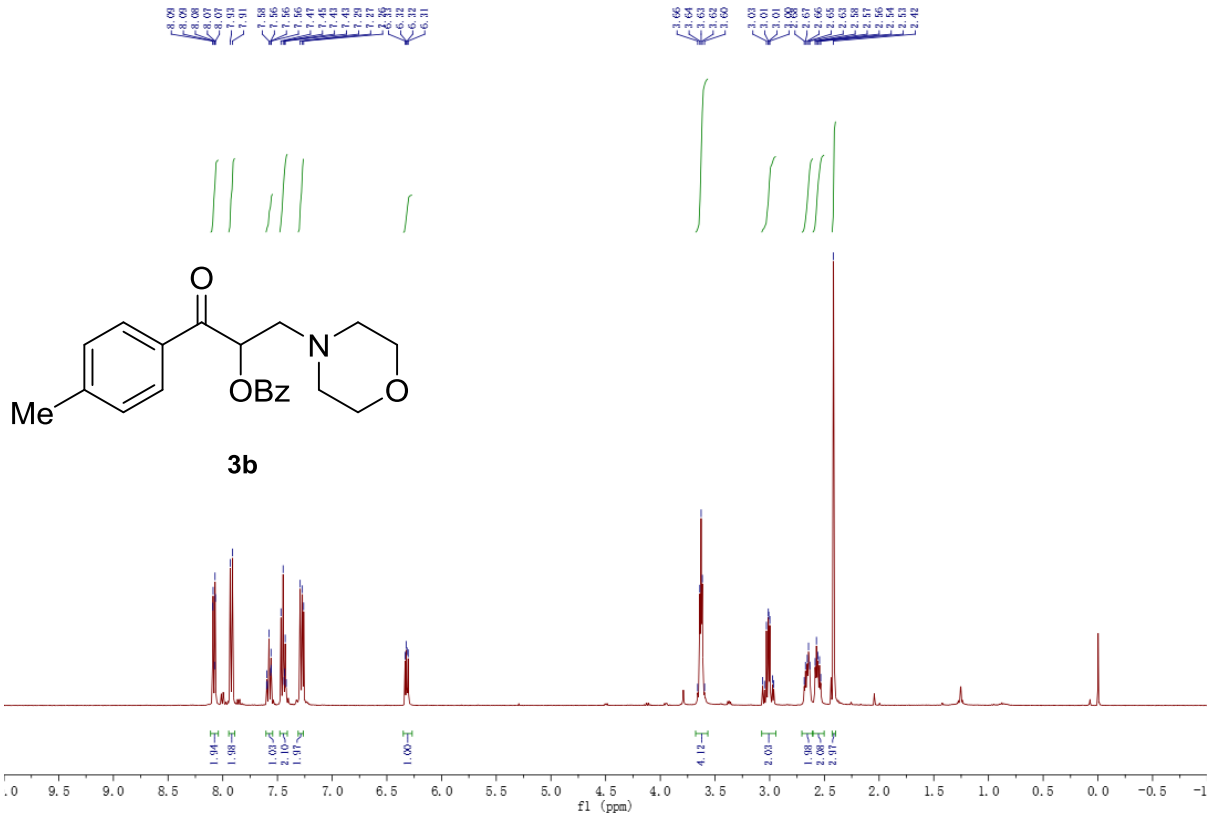
3w

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90 (dt, J = 8.4, 1.6 Hz, 2H), 7.65 (dt, J = 6.3, 3.1 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.50 – 7.44 (m, 2H), 7.36 (dd, J = 3.6, 0.8 Hz, 1H), 6.57 (dd, J = 3.5, 1.7 Hz, 1H), 5.88 (d, J = 2.3 Hz, 1H), 5.72 (d, J = 2.3 Hz, 1H). ppm; **^{13}C NMR (100 MHz, $CDCl_3$):** δ 189.24 (s), 156.12 (s), 150.58 (s), 147.43 (s), 143.13 (s), 136.11 (s), 132.98 (s), 129.57 (s), 128.39 (s), 120.16 (s), 115.21 (s), 112.25 (s). ppm; **HRMS (ESI, m/z):** calcd for $C_{14}H_{10}O_4Na$ $[M+Na]^+$ 265.0477, found: 265.0476.

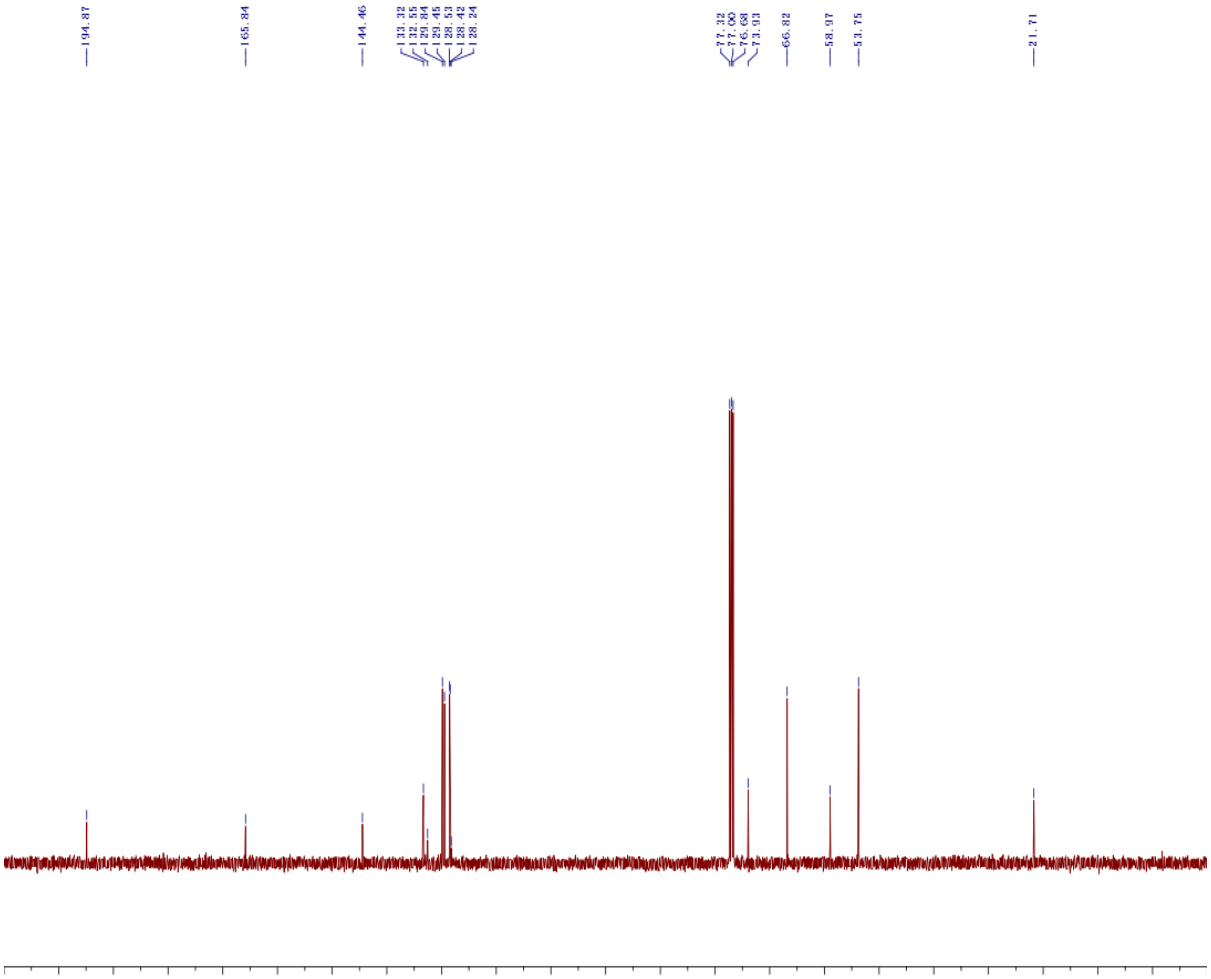
^{1}H and ^{13}C NMR spectra of structurally novel compounds

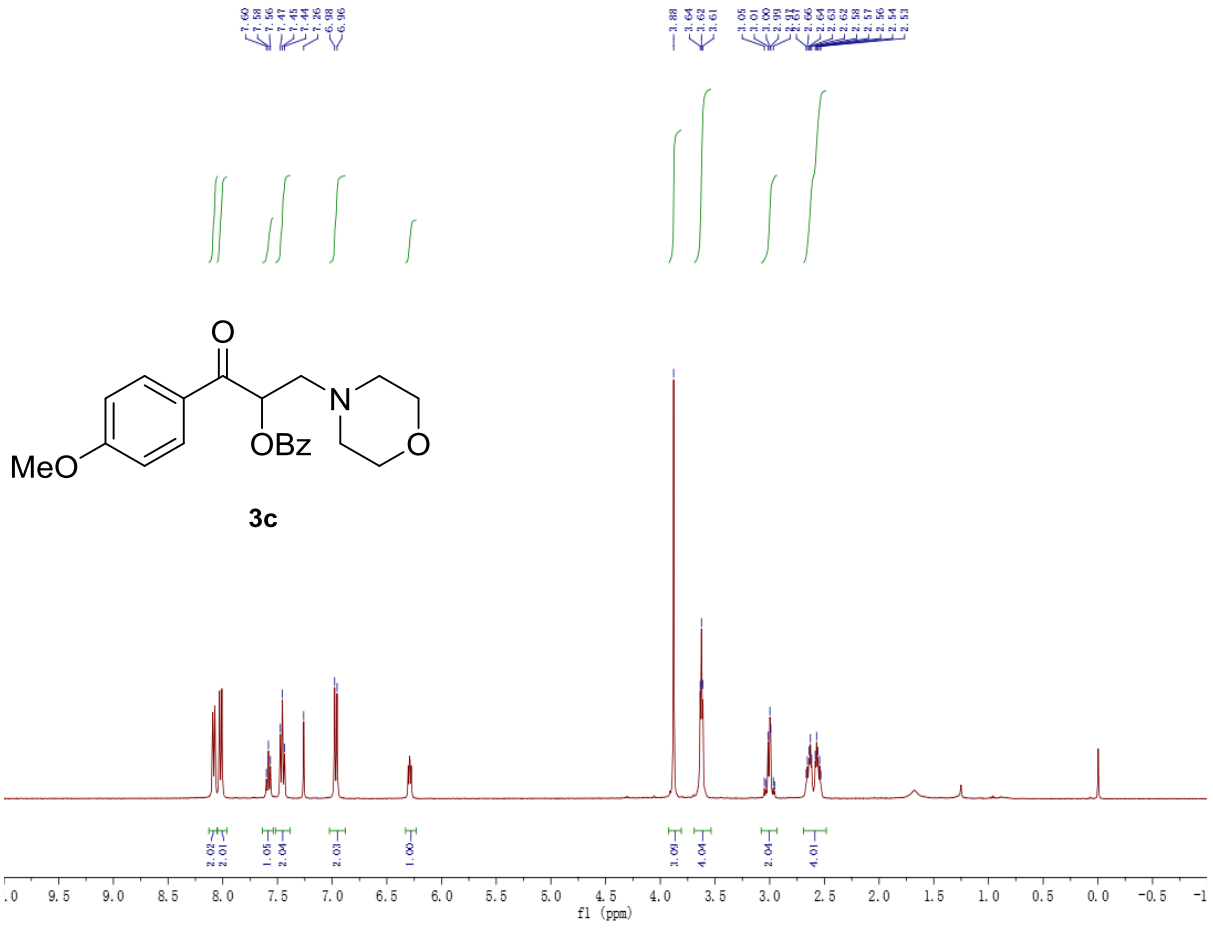




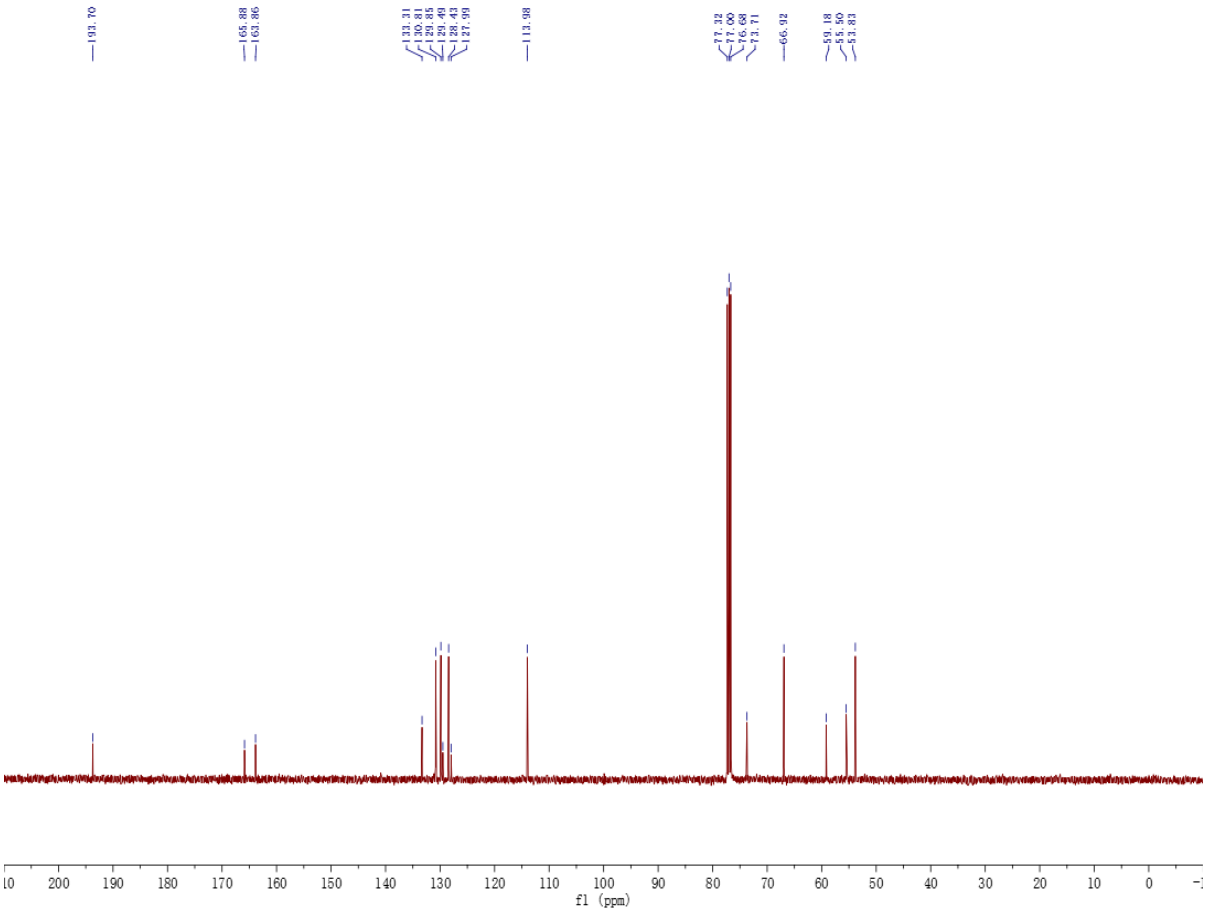


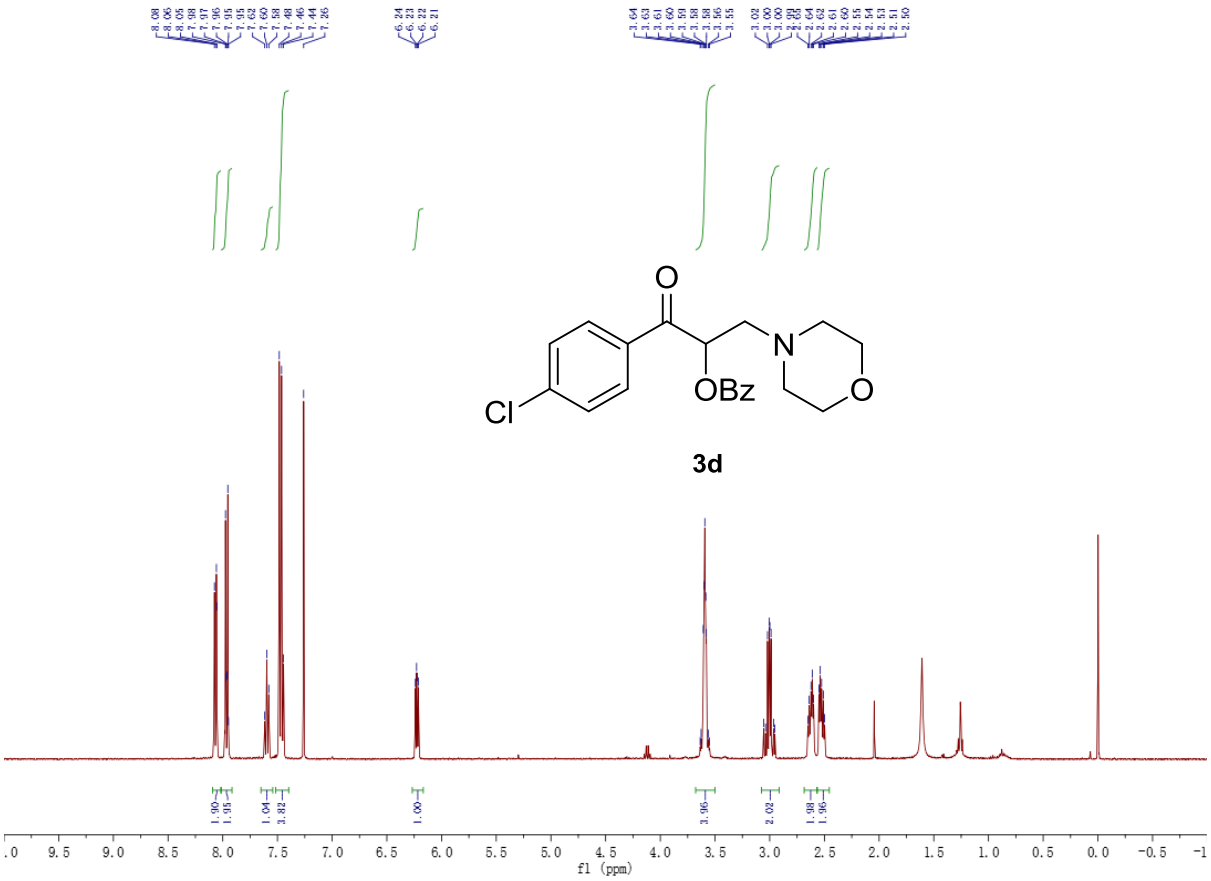
3b



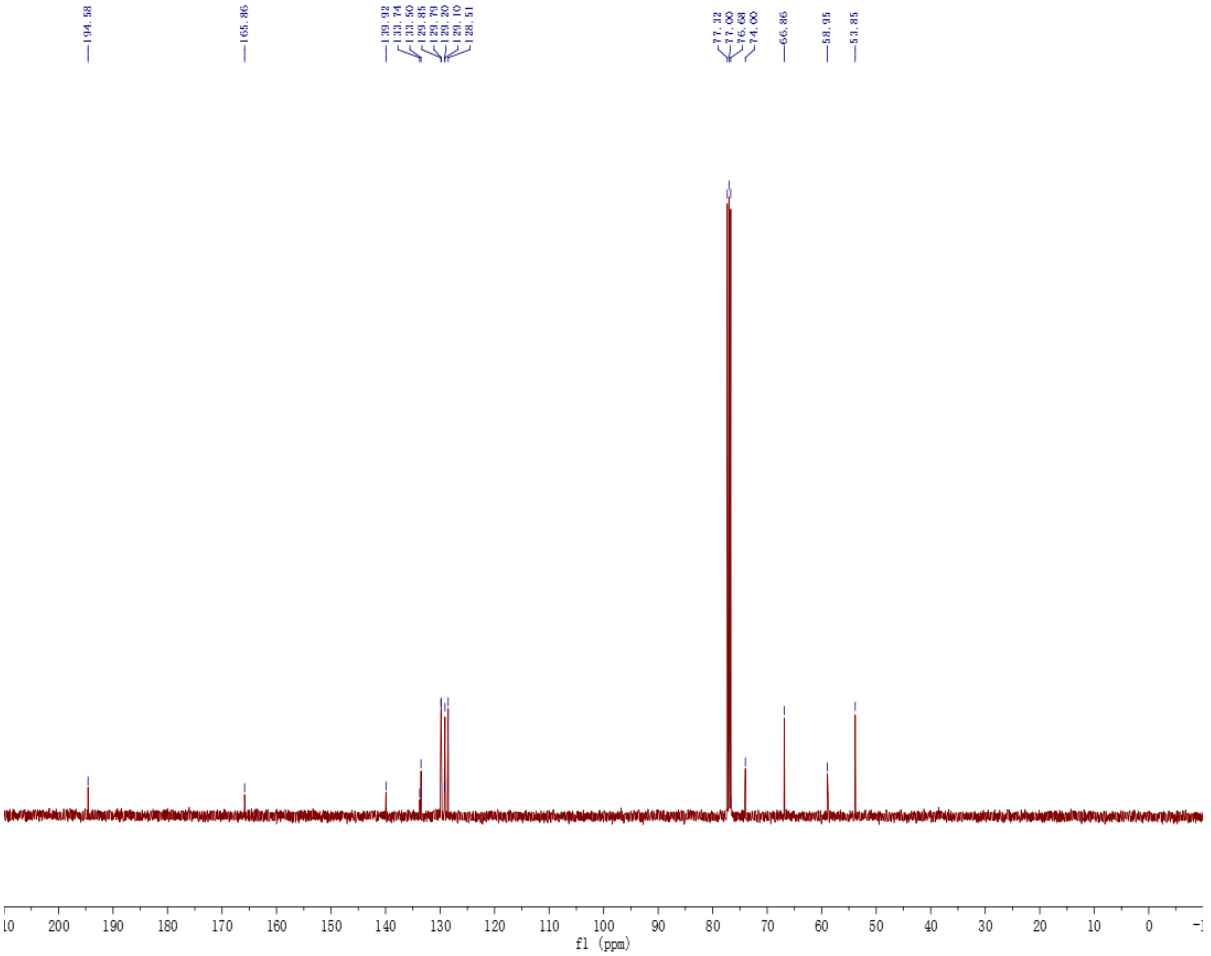


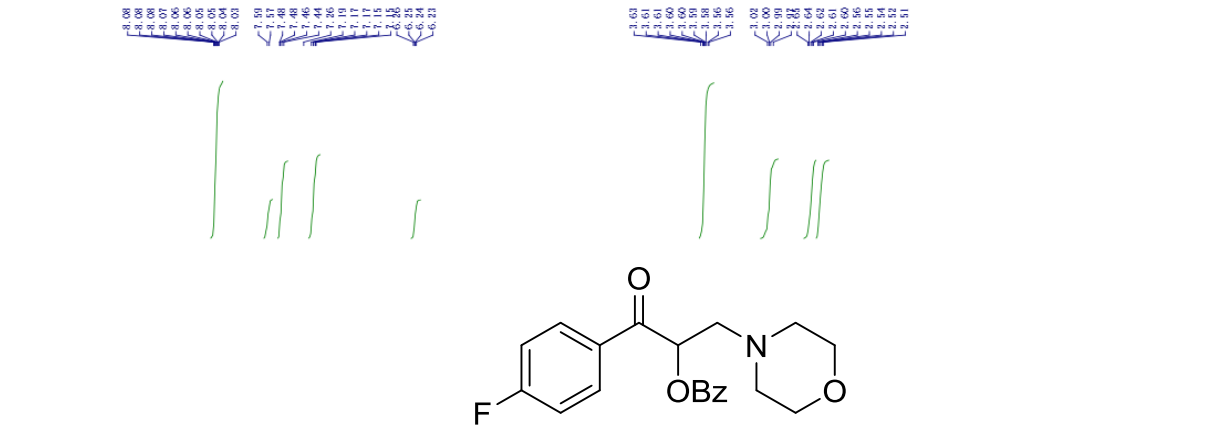
3c





3d





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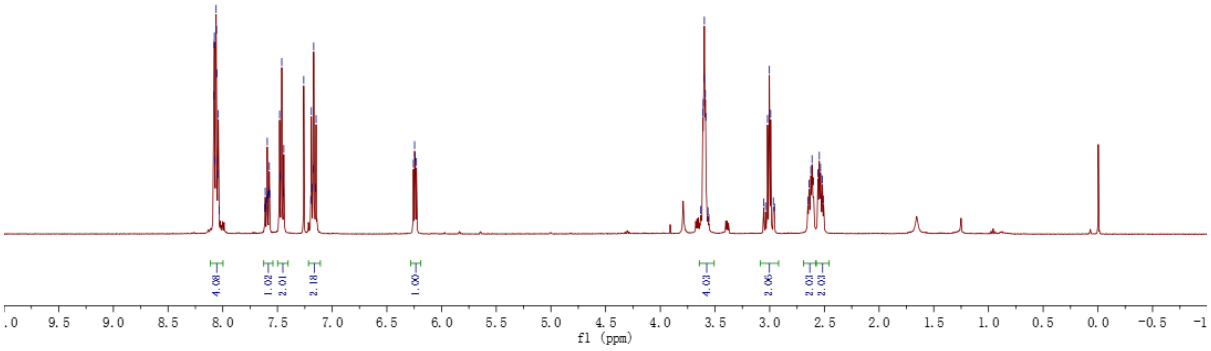

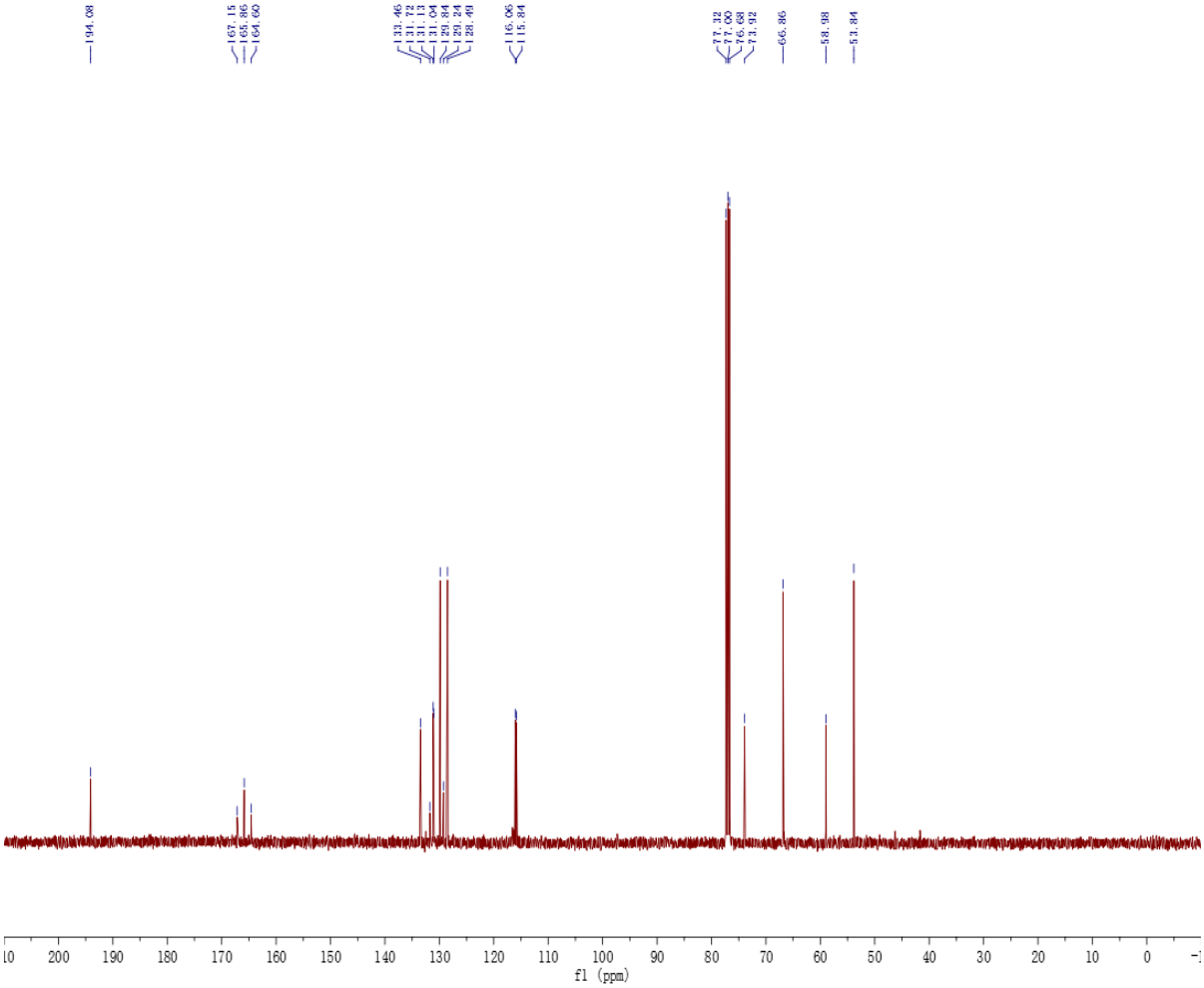

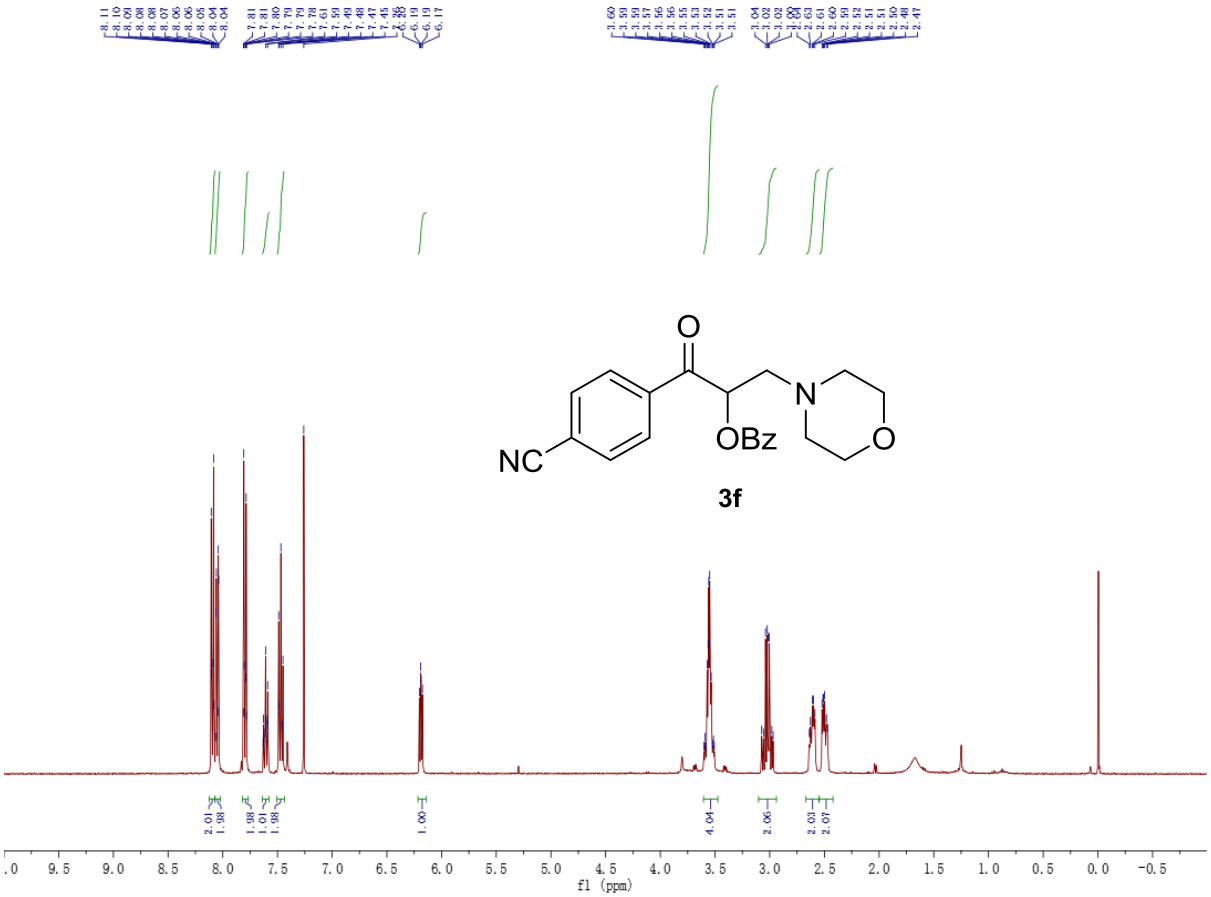
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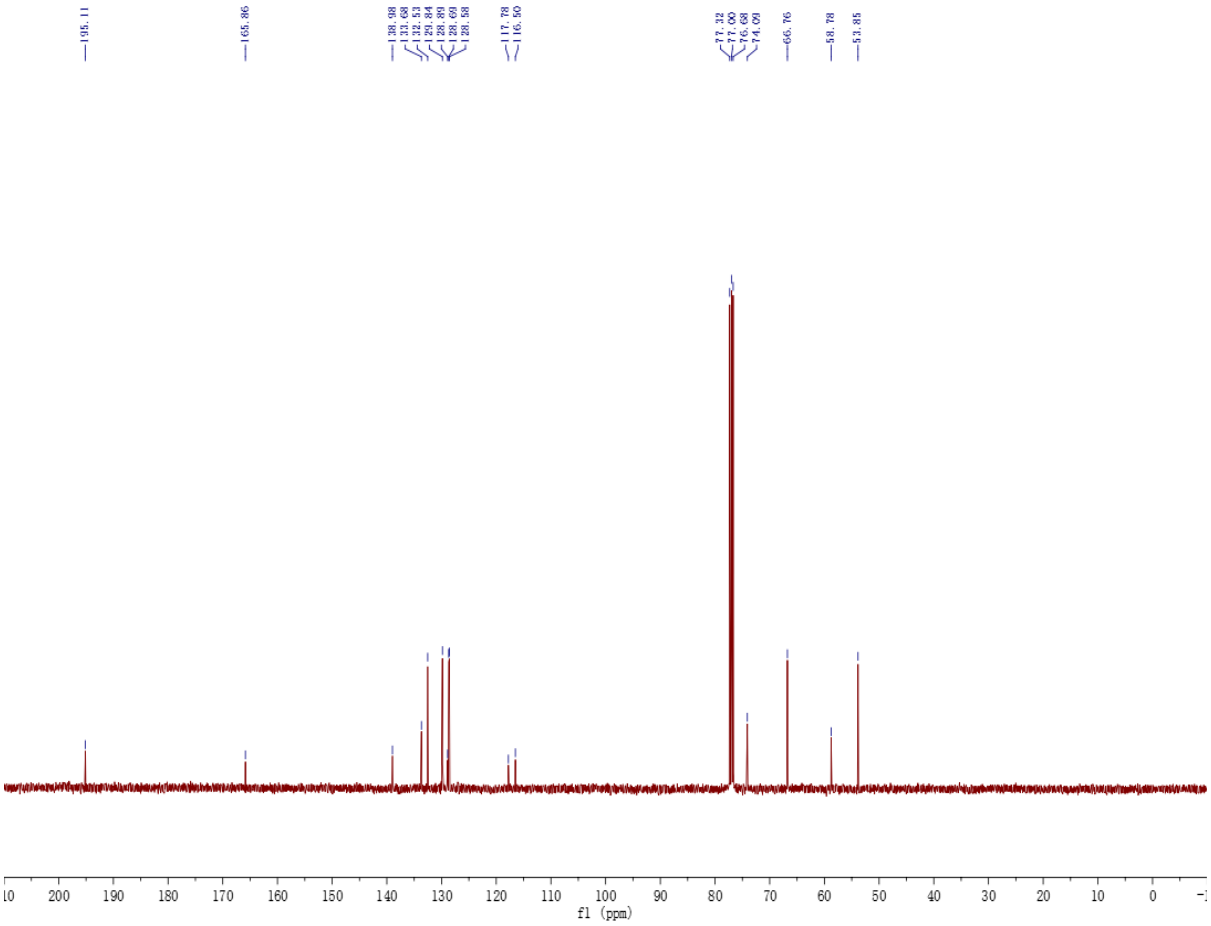
OBz
NC
O
3f
f1 (ppm)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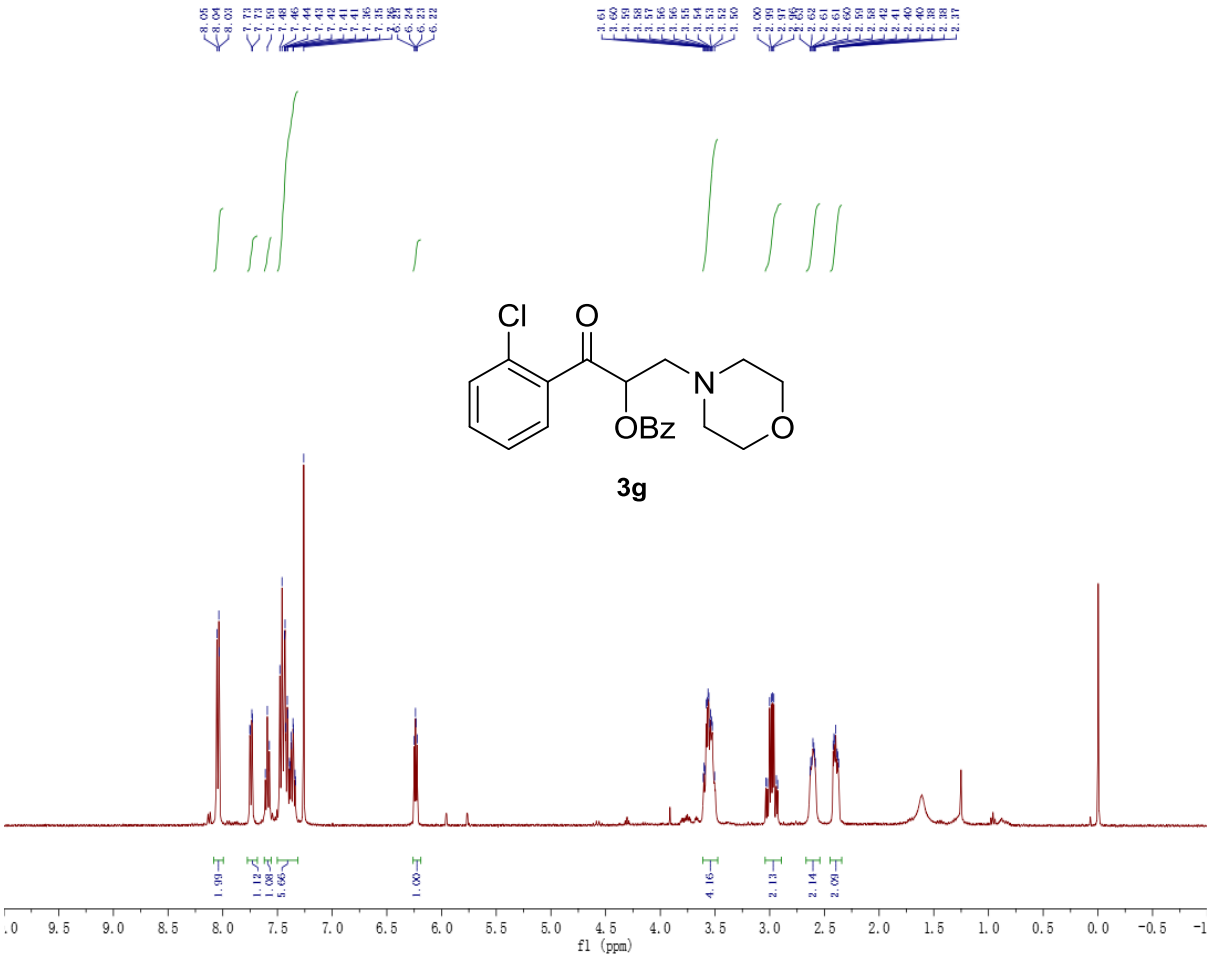
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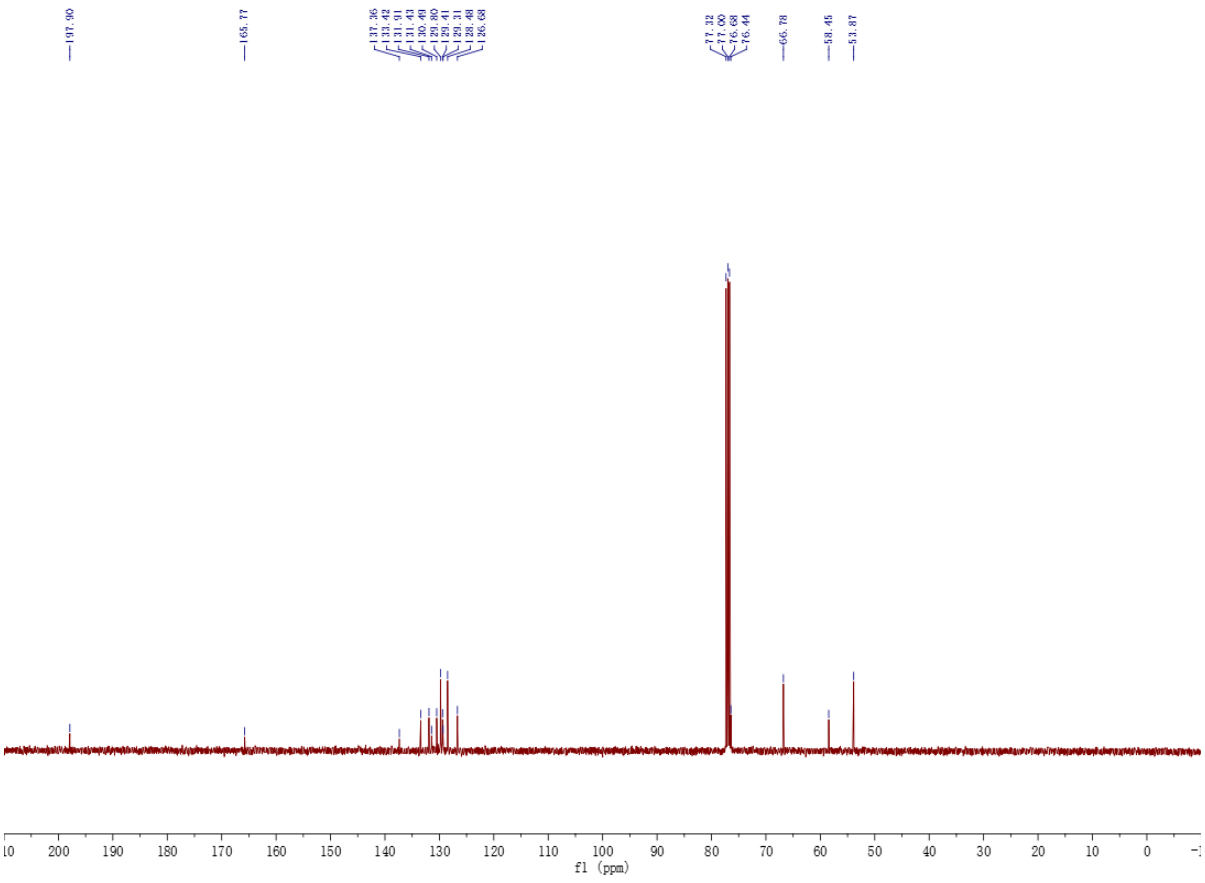
OBz
O
3g
f1 (ppm)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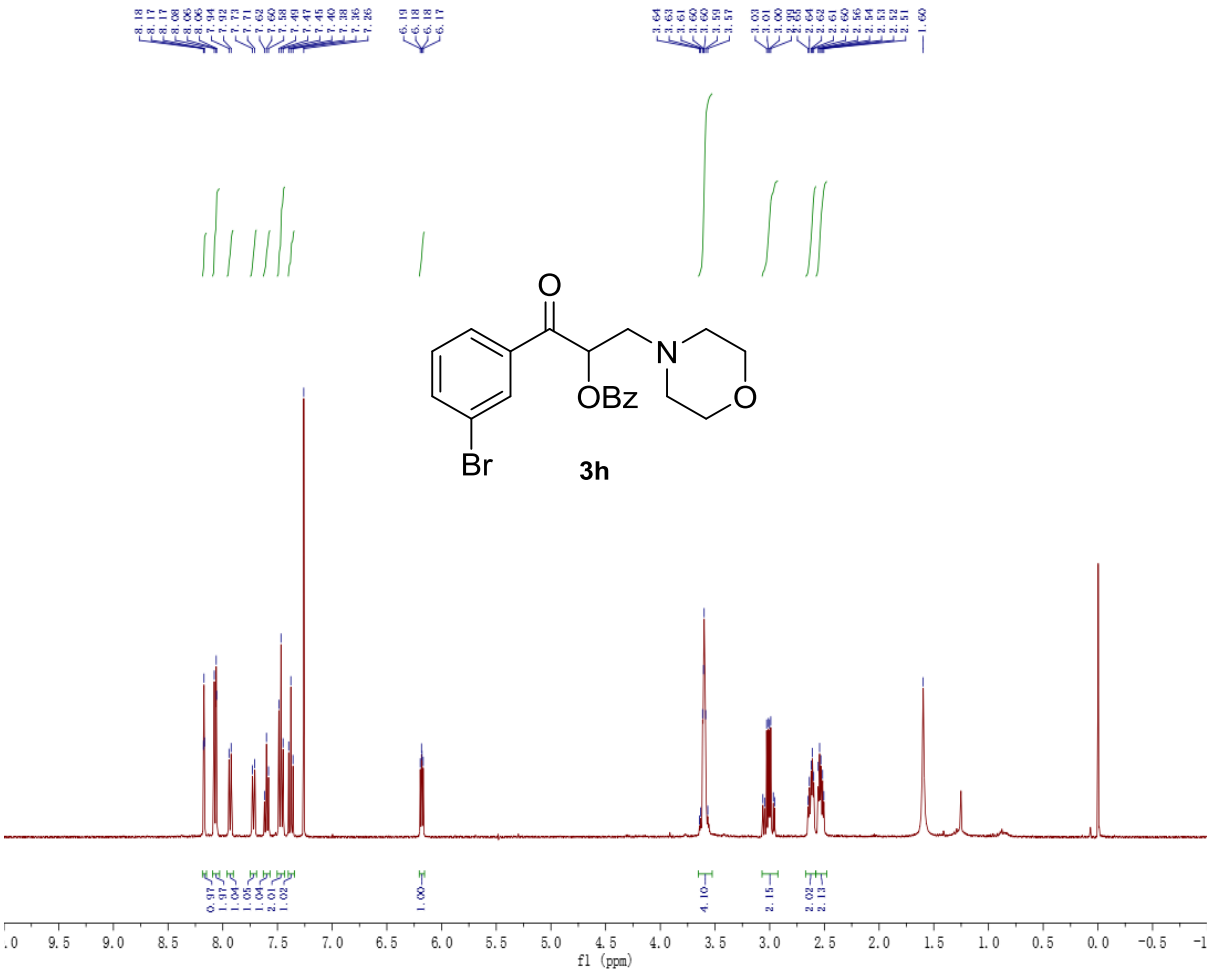
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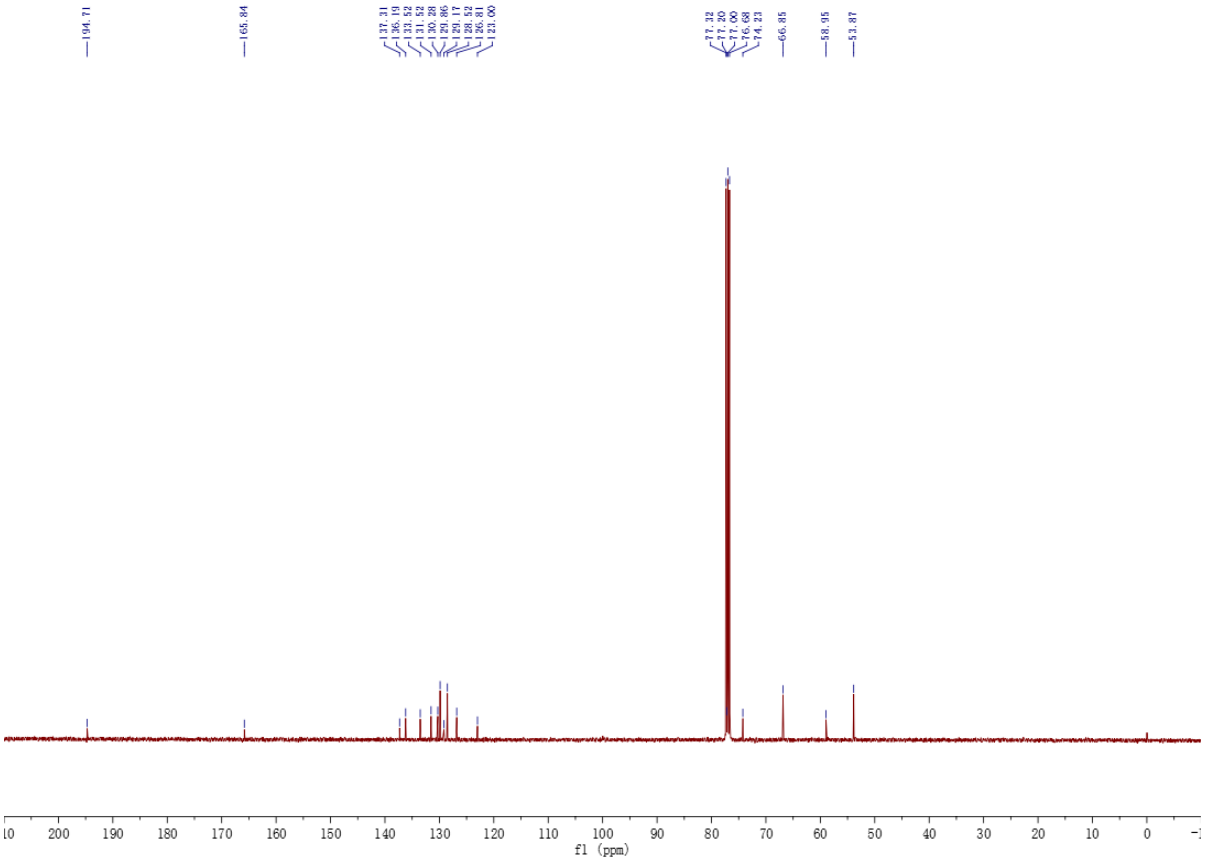
O
OBz
Br
3h
f1 (ppm)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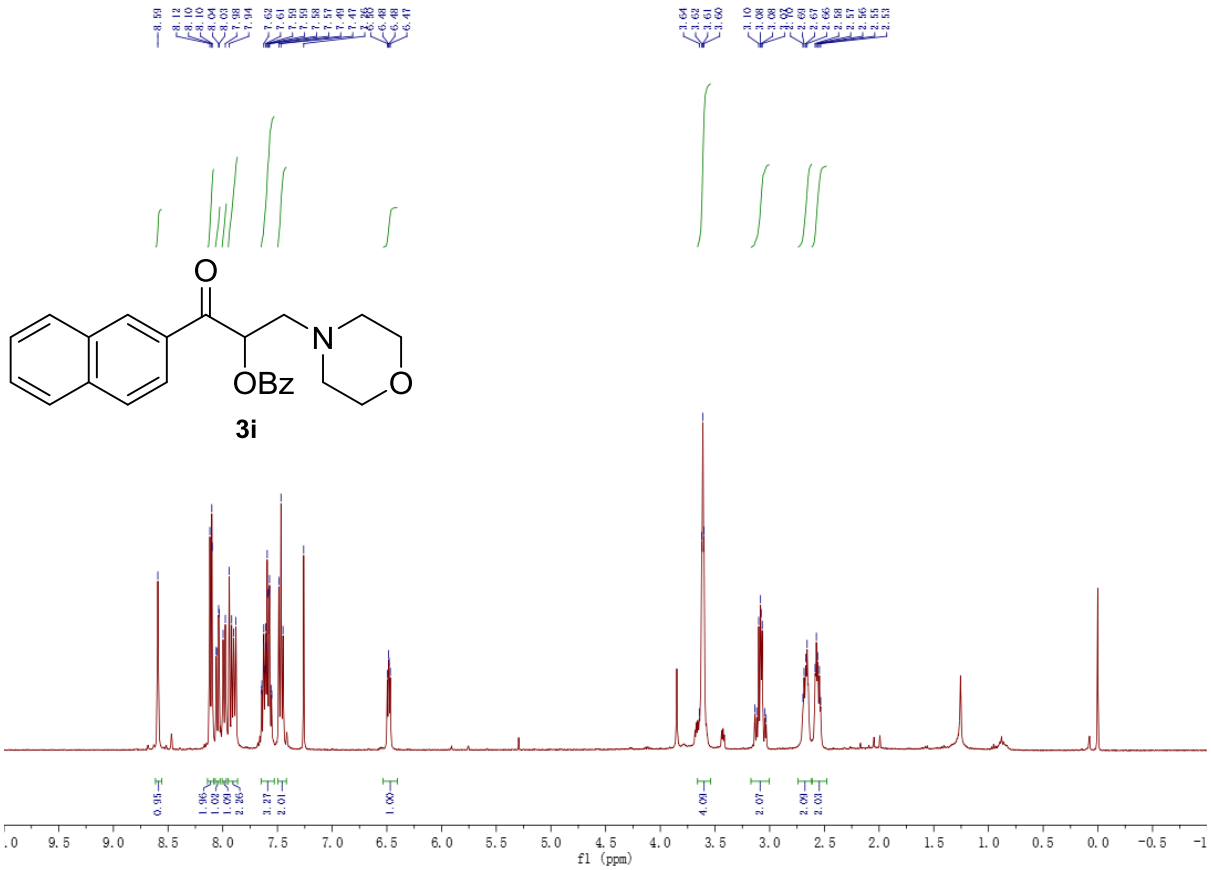
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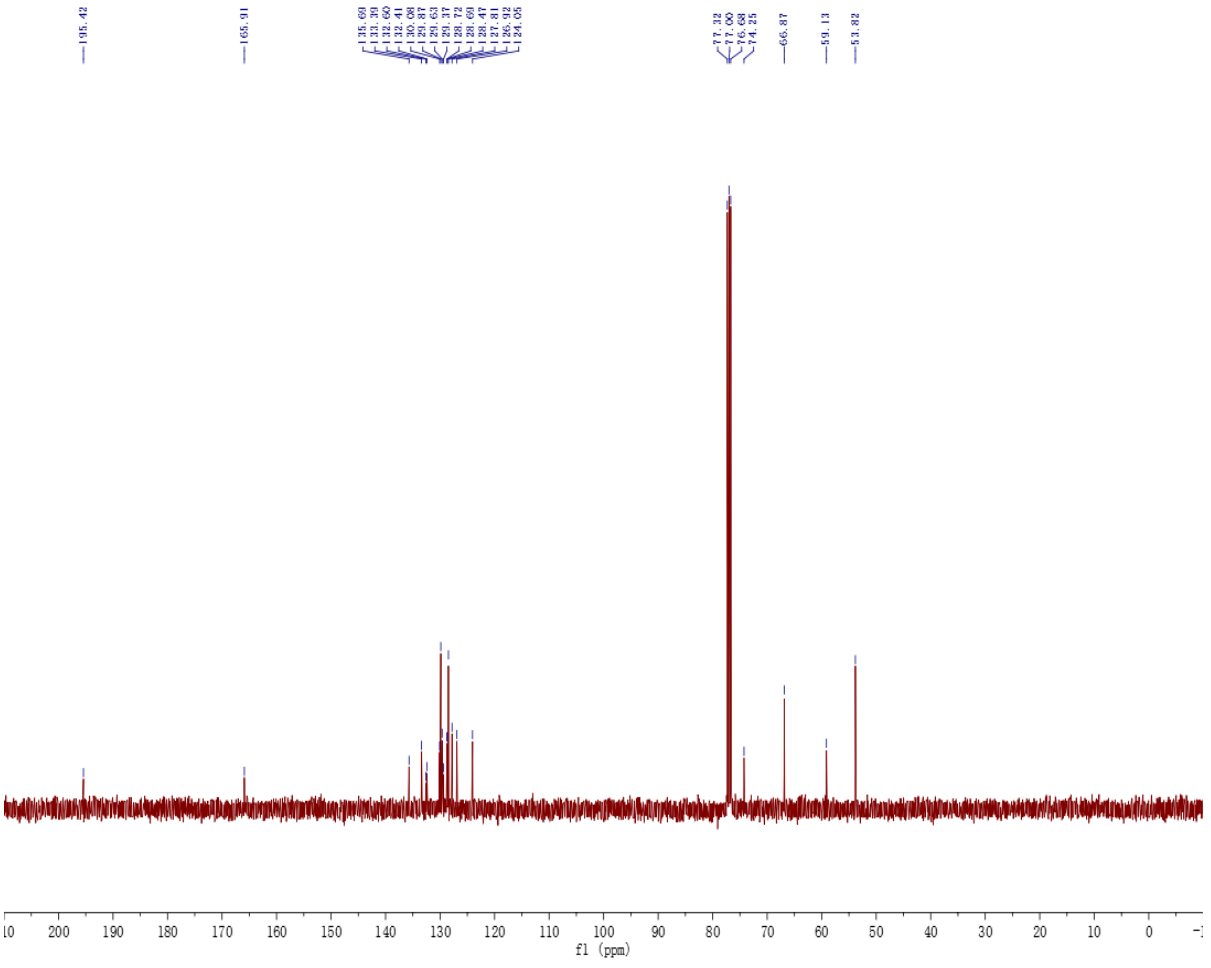
OBz
O
3i
f1 (ppm)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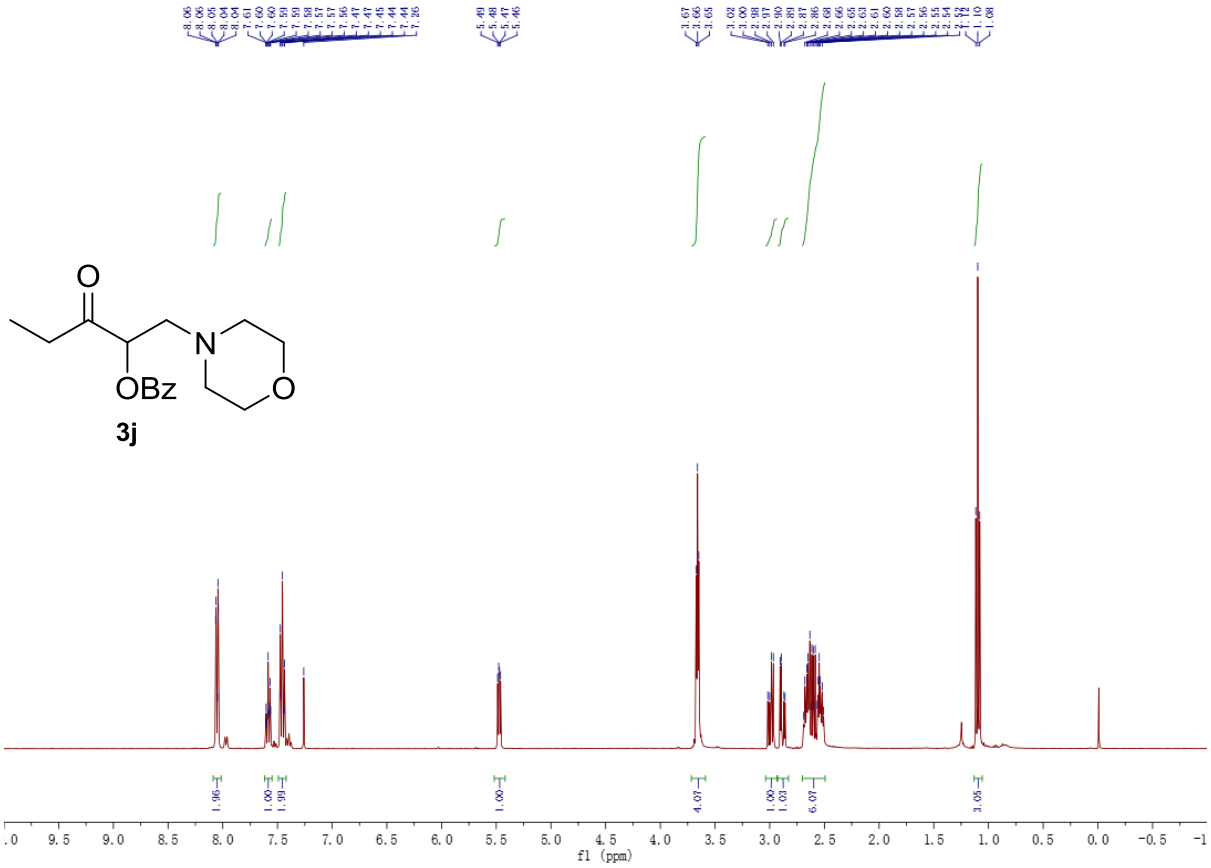
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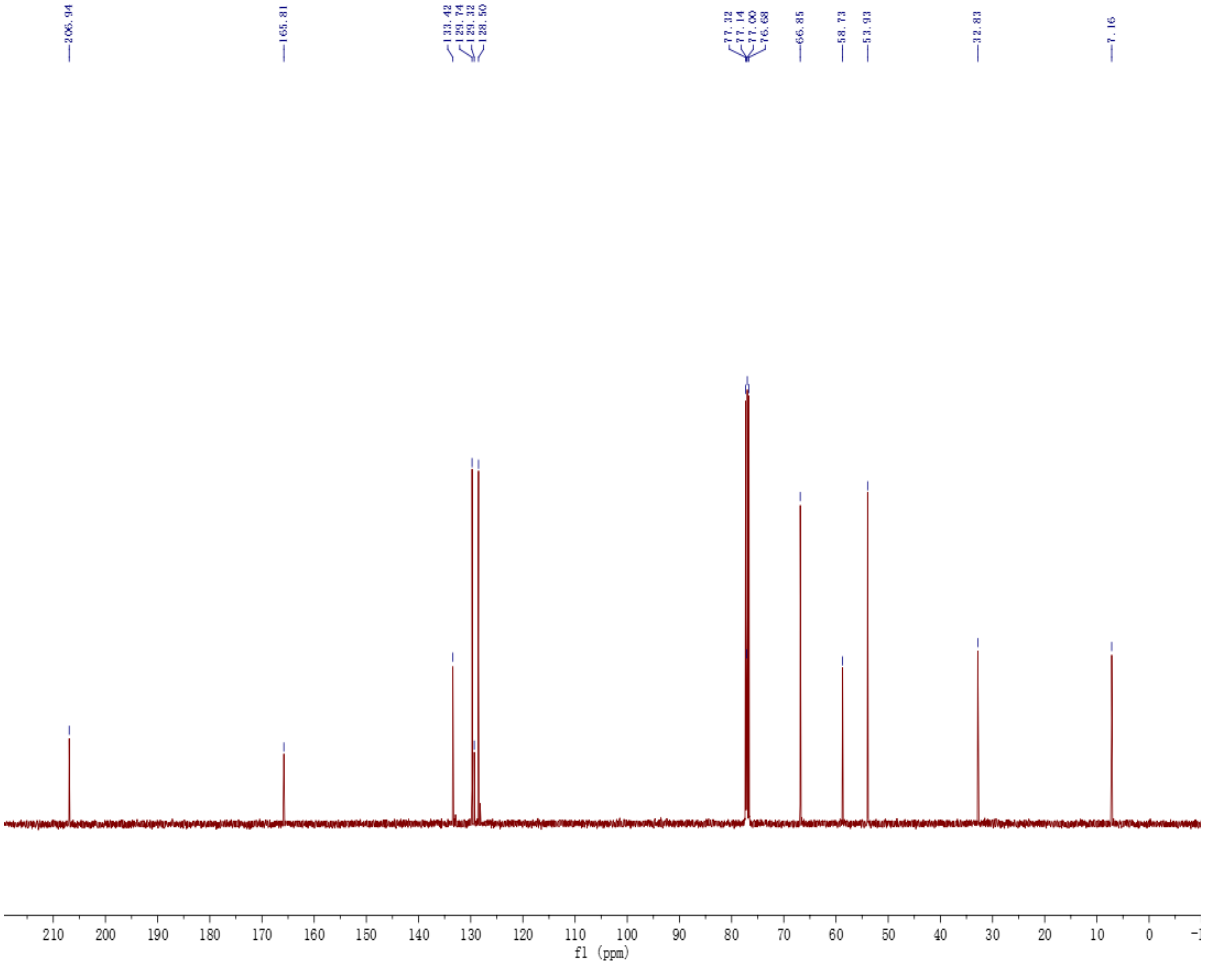
OBz
O
3j
f1 (ppm)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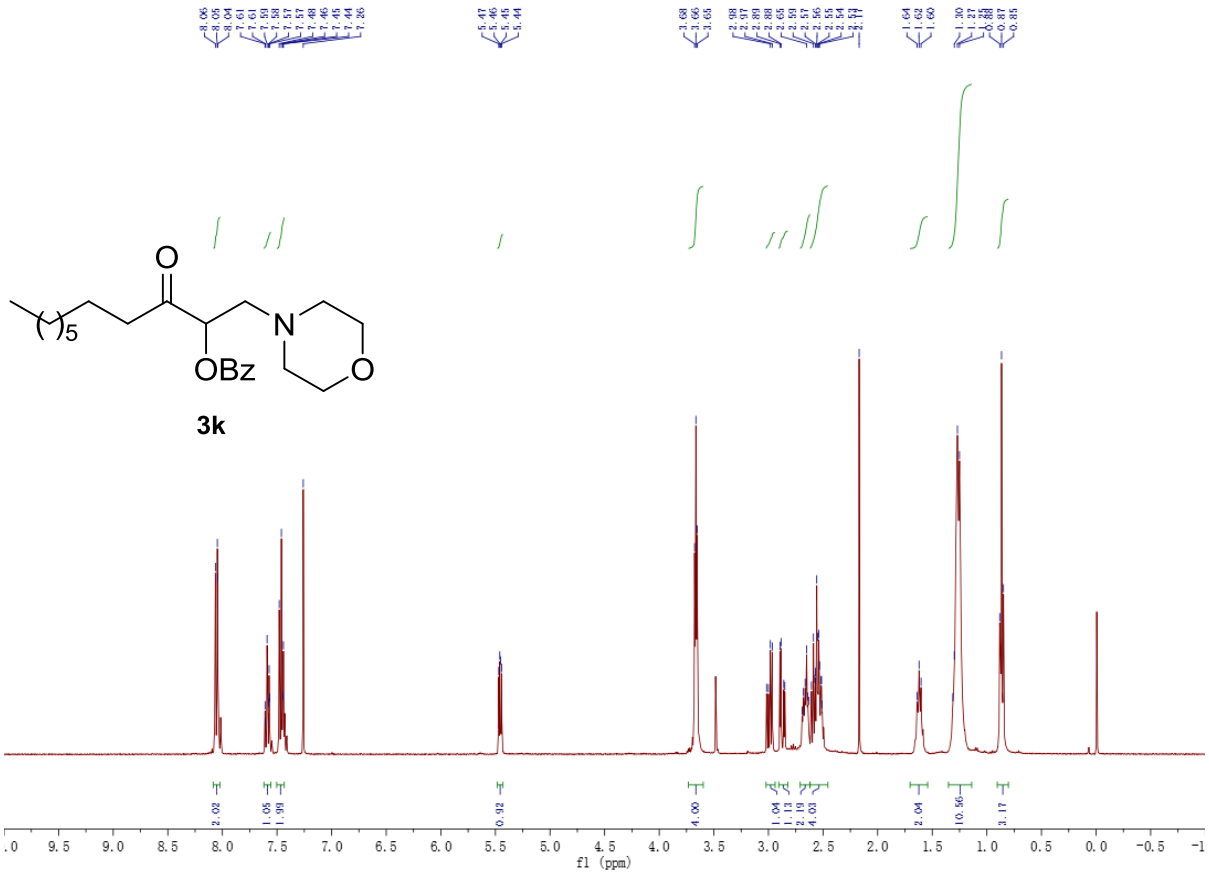
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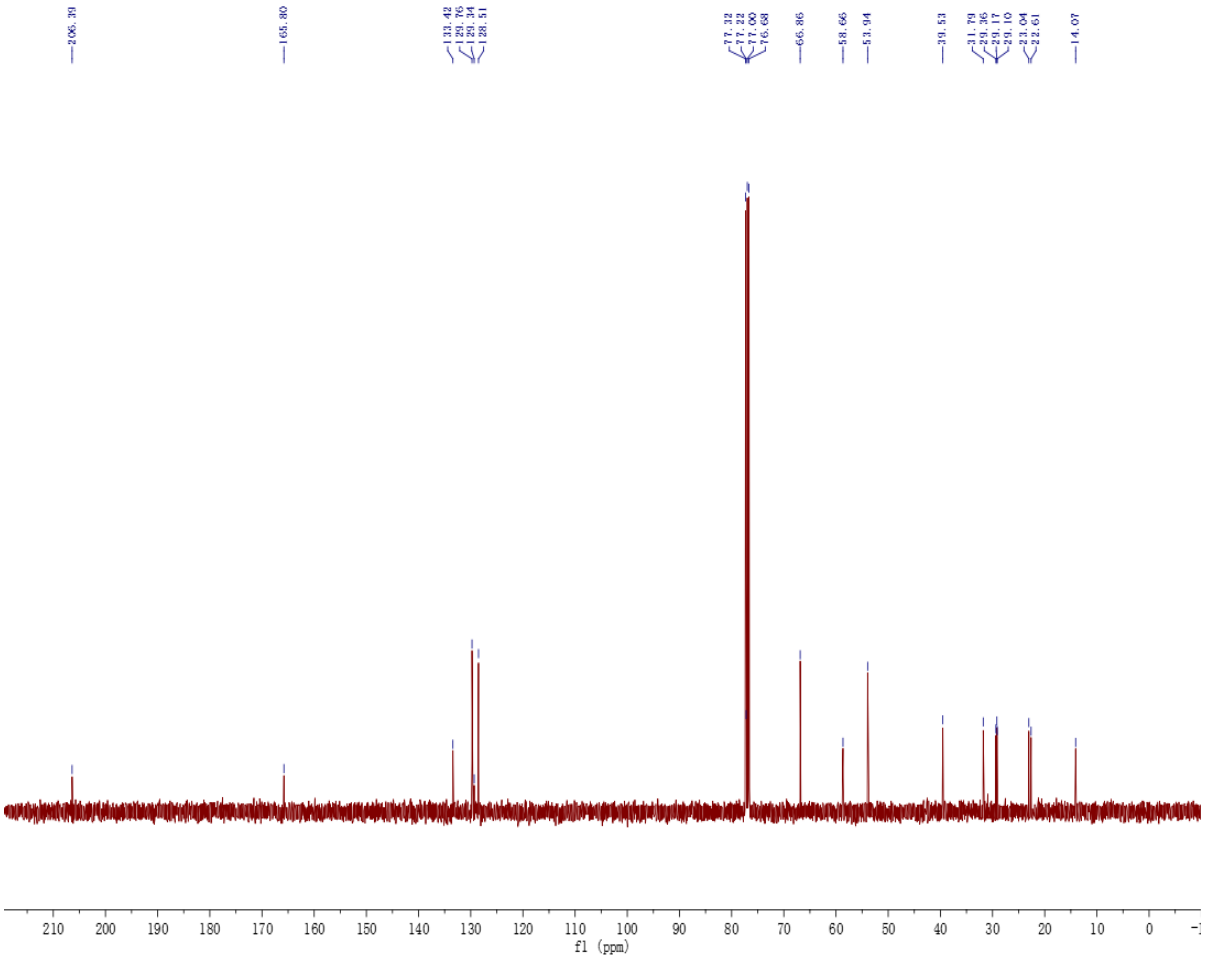
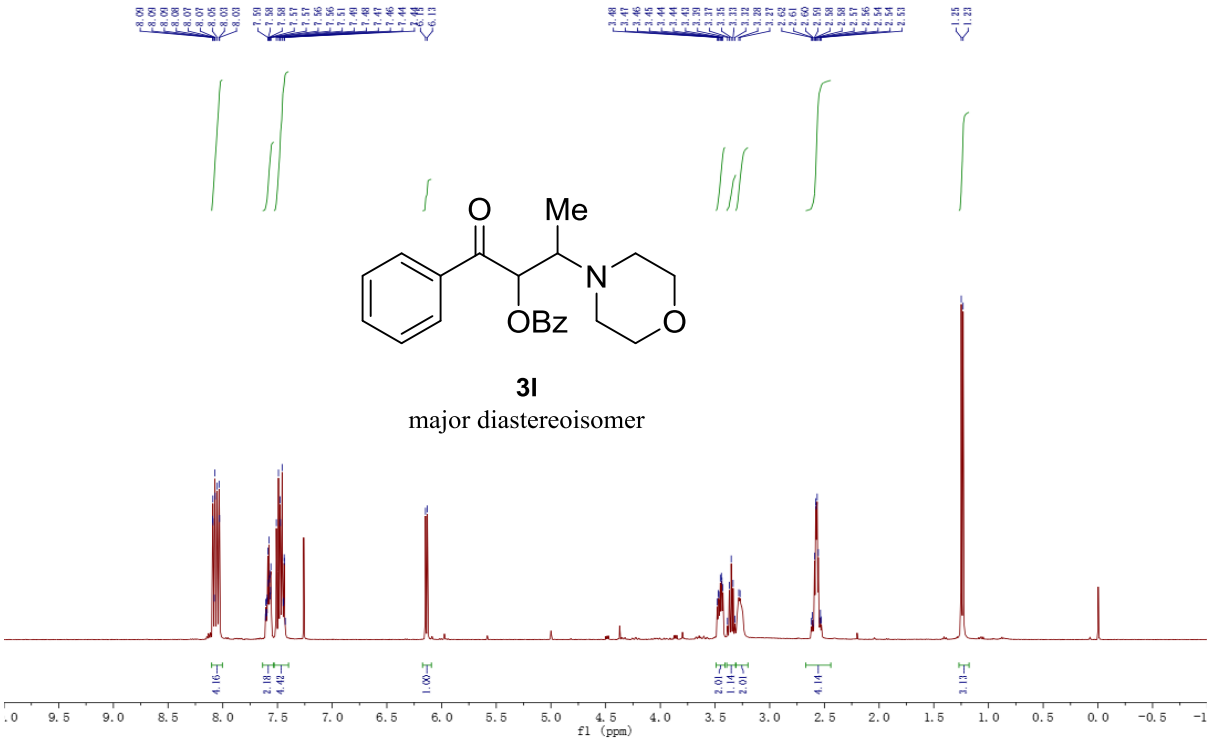
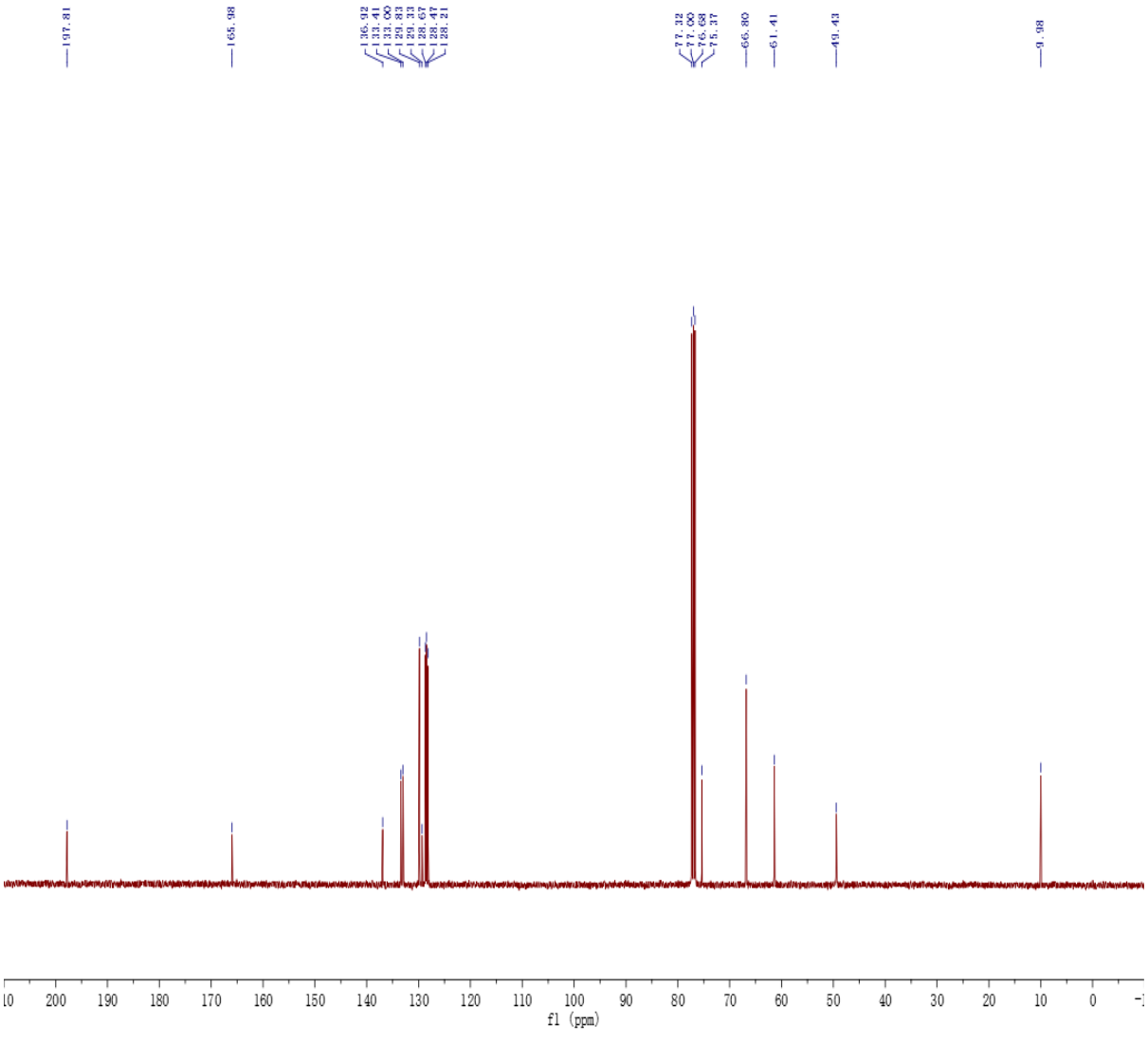
N
O
OBz
5
3k

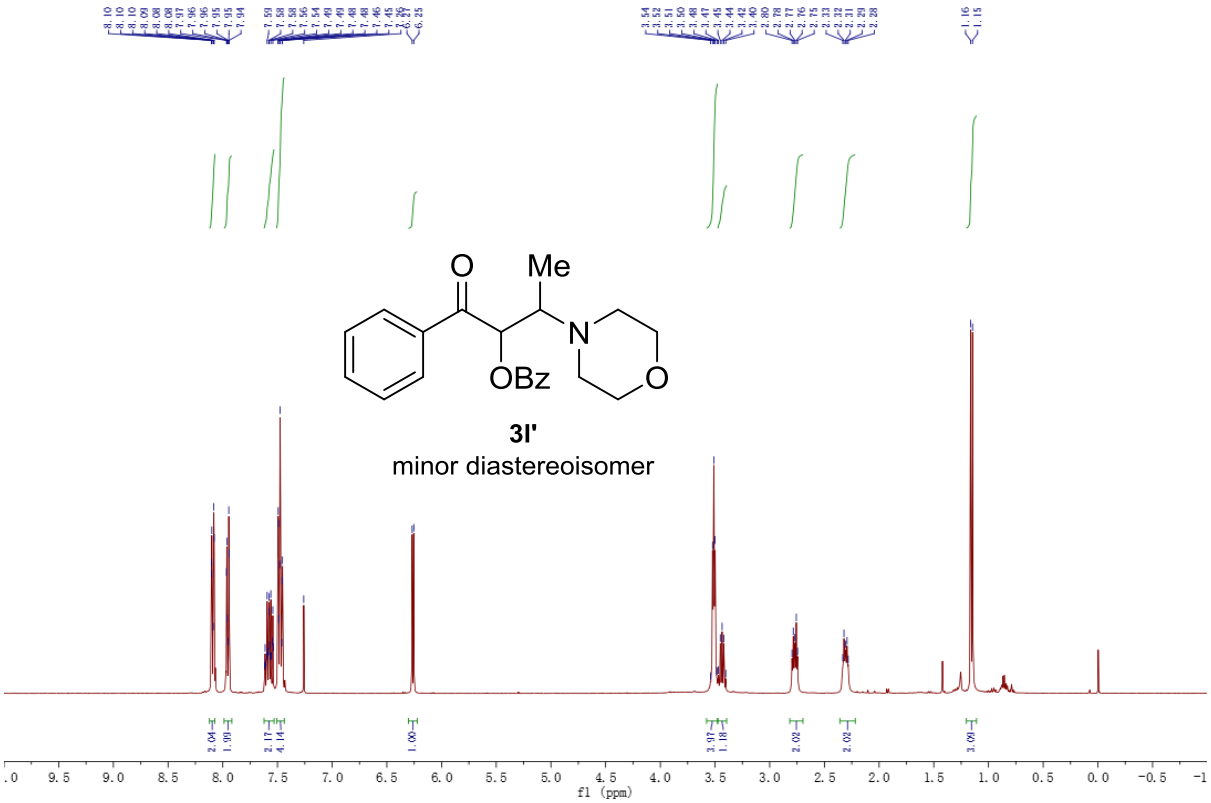


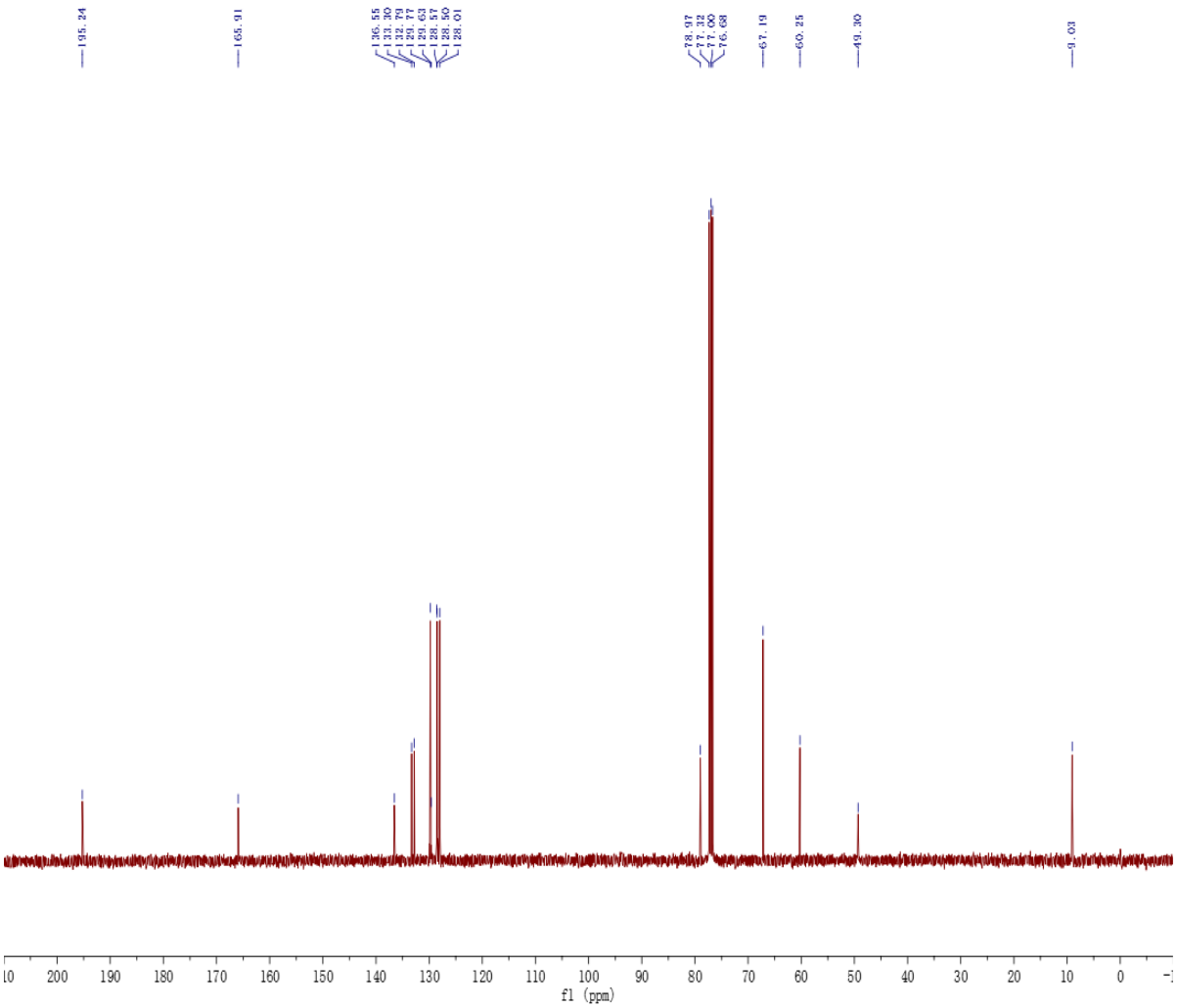


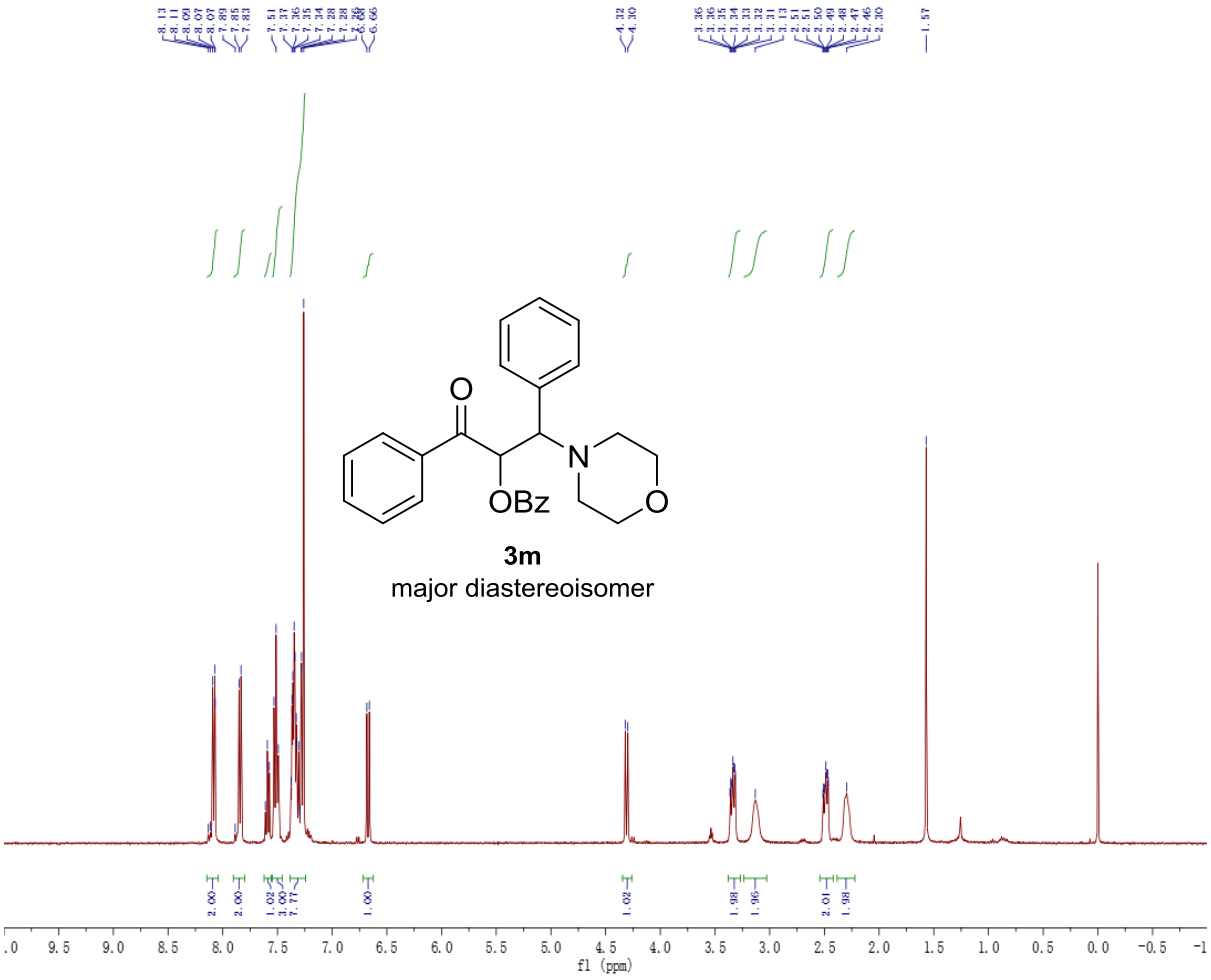
3l

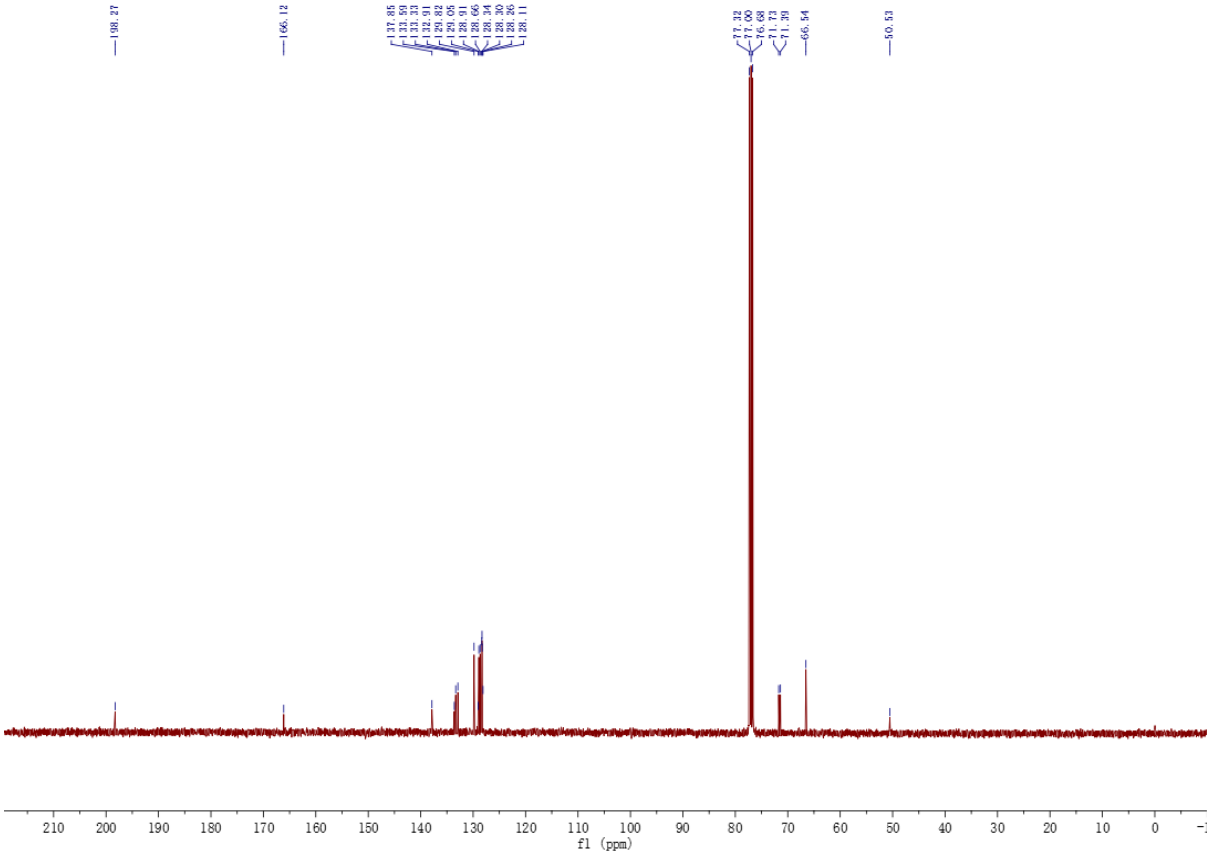
major diastereoisomer




O
Me
N
OBz
O
3l'
minor diastereoisomer
f1 (ppm)


f1 (ppm)


O
N
OBz
O
3m
major diastereoisomer
f1 (ppm)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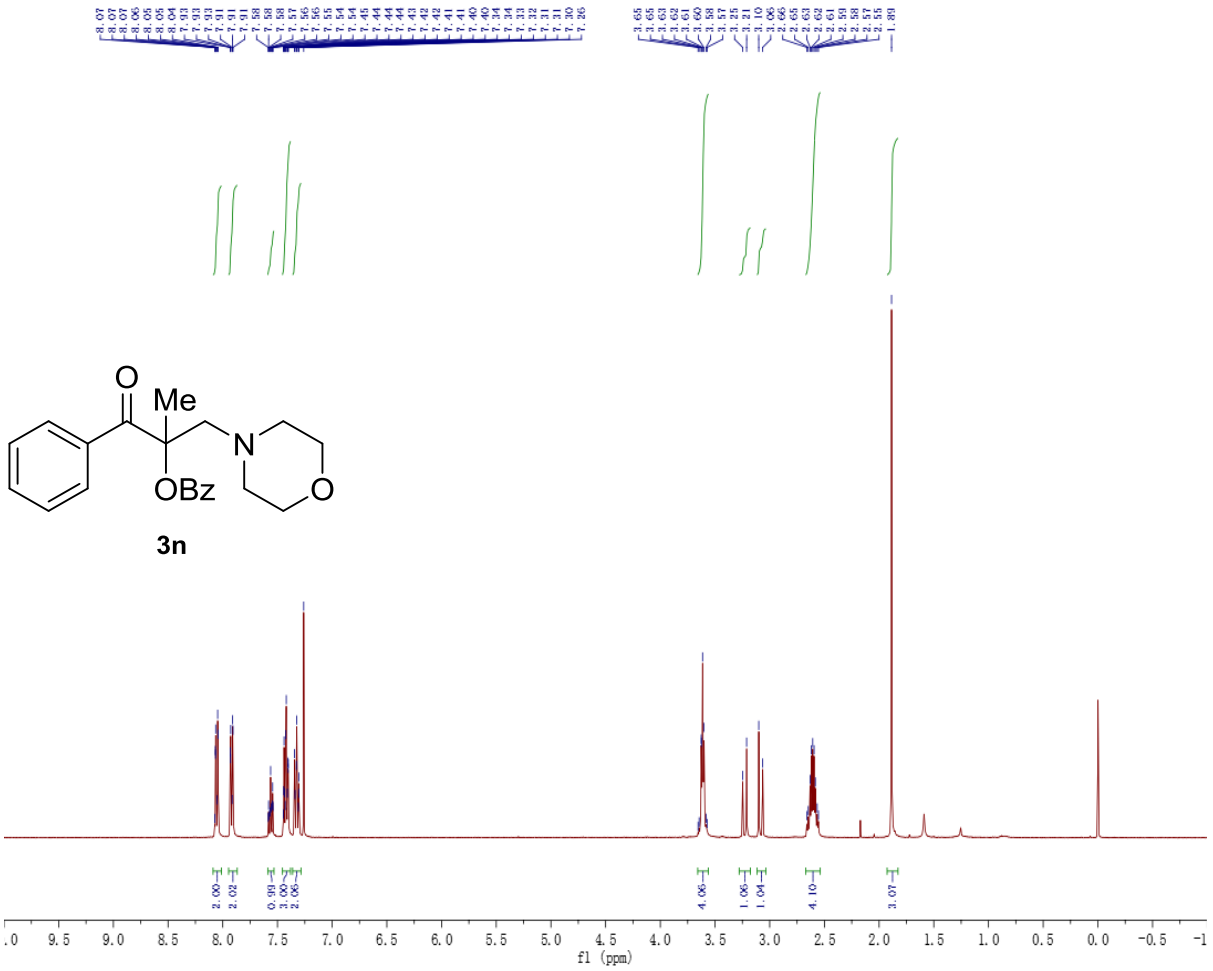

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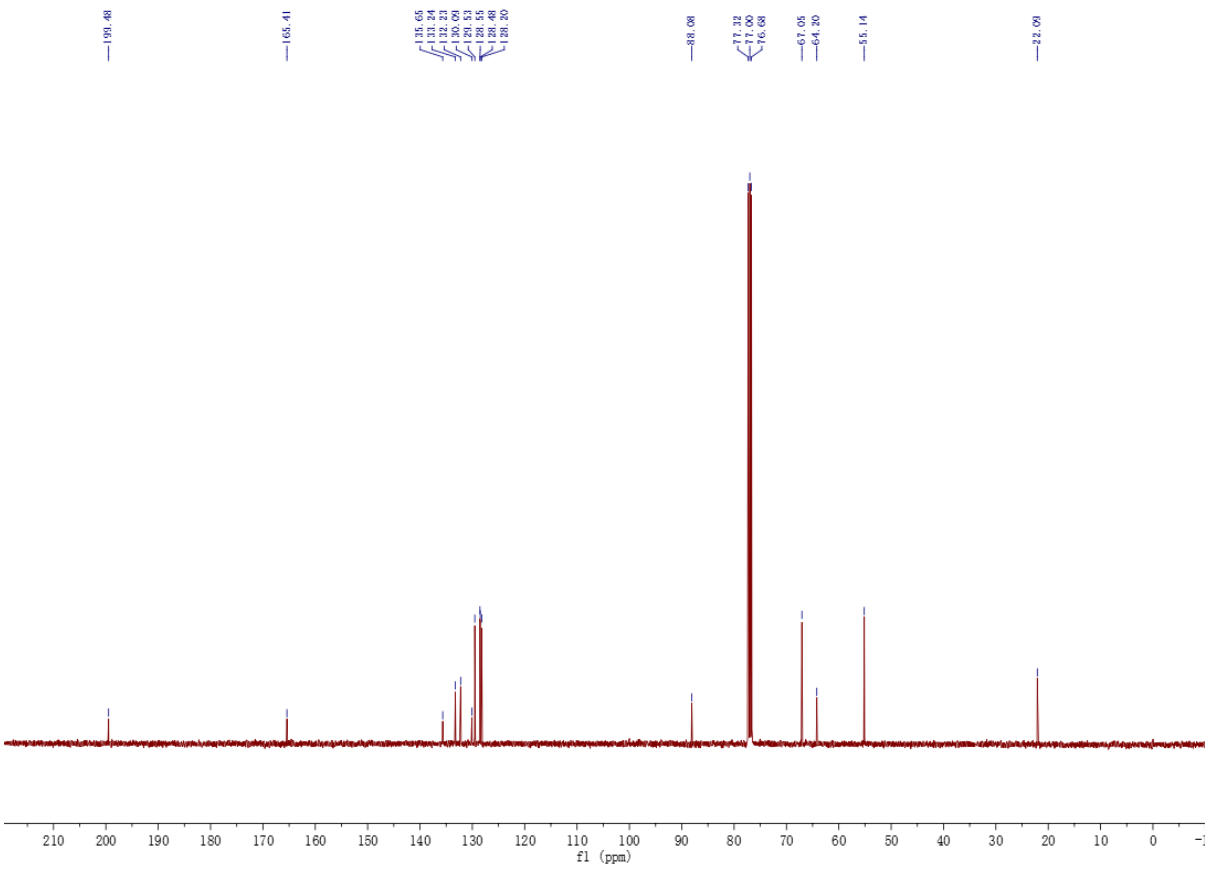
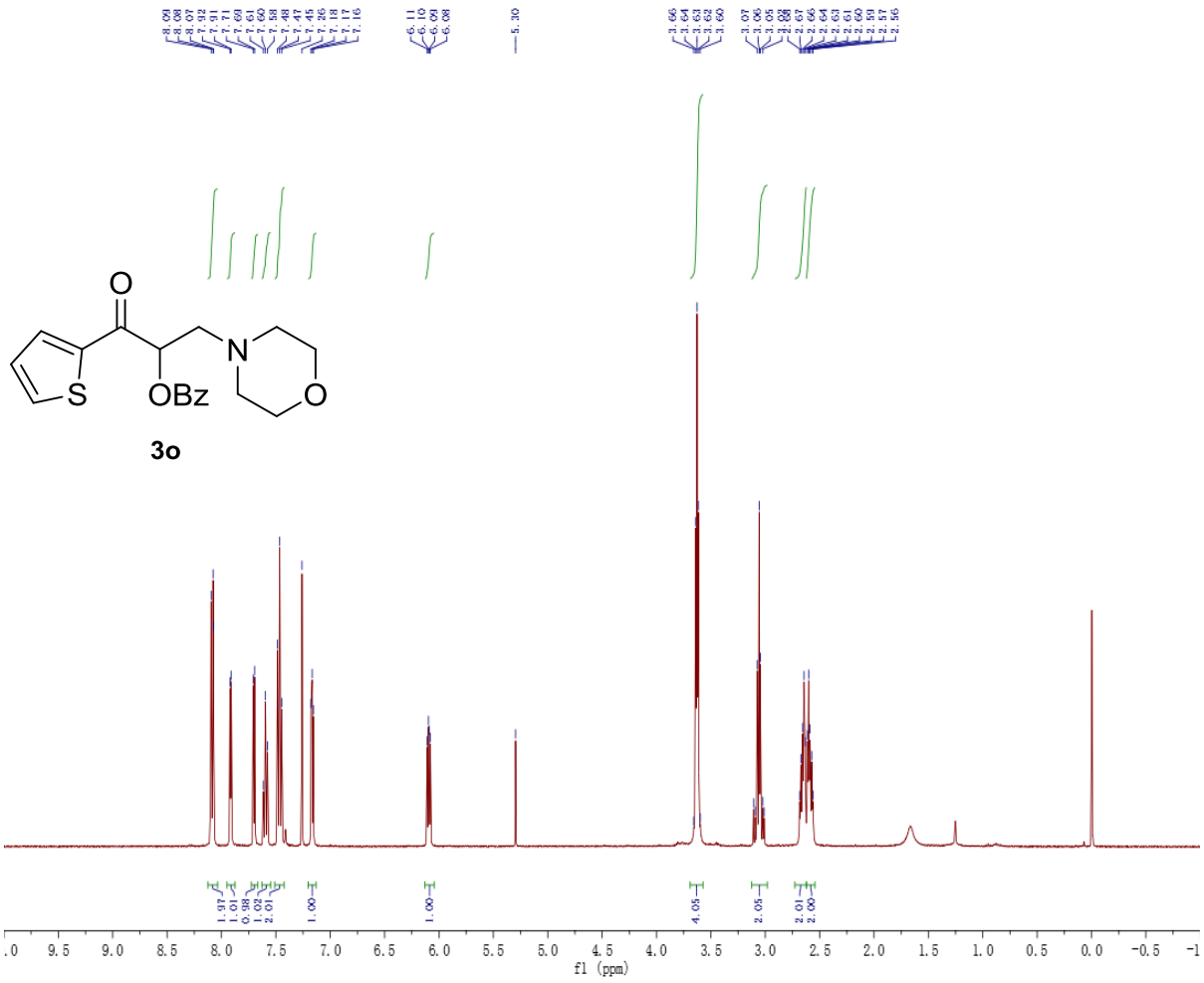
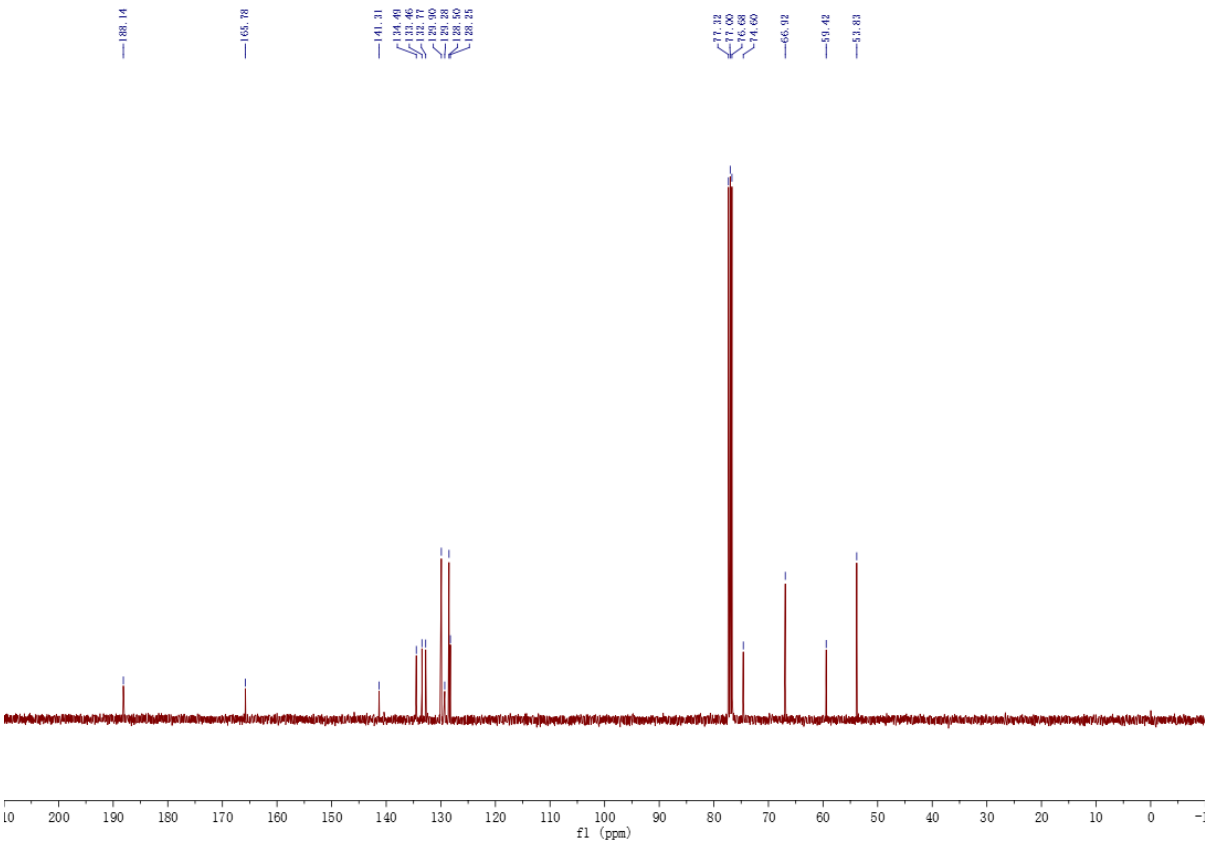
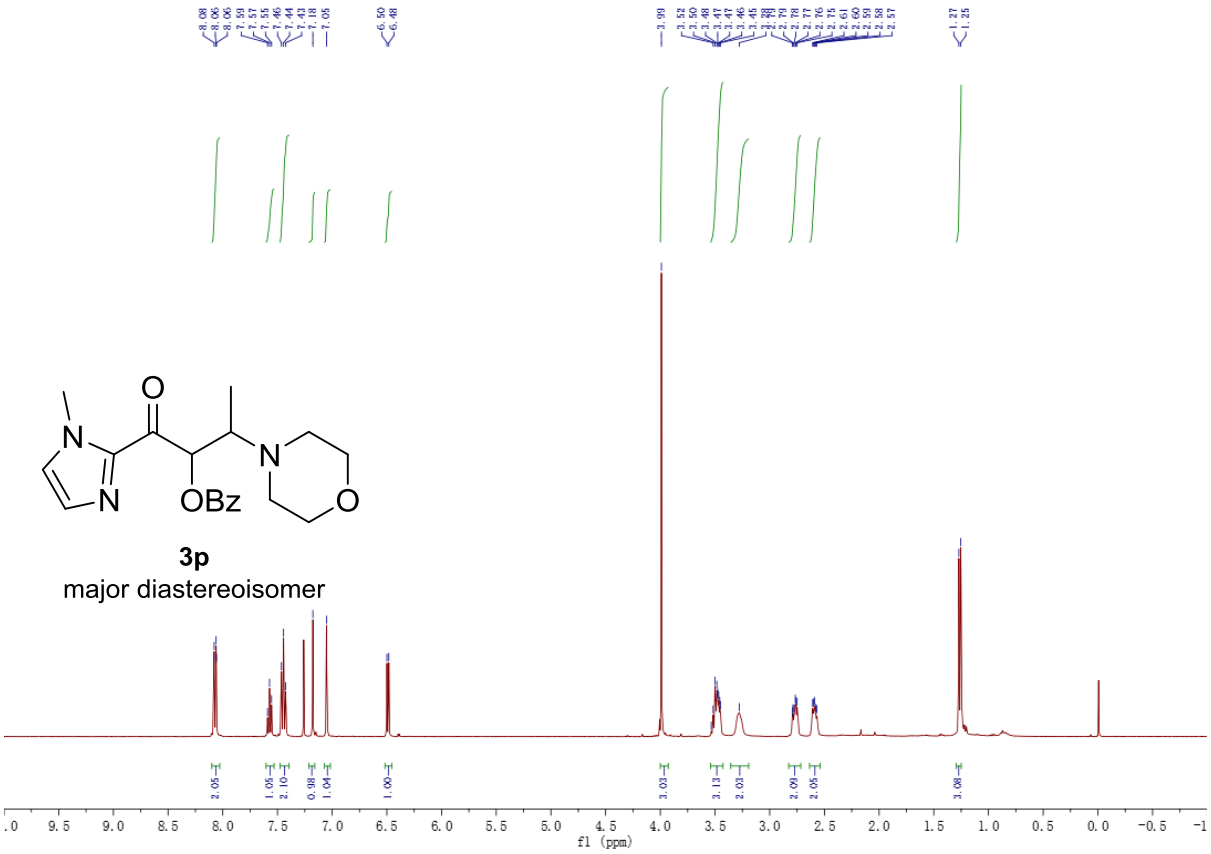
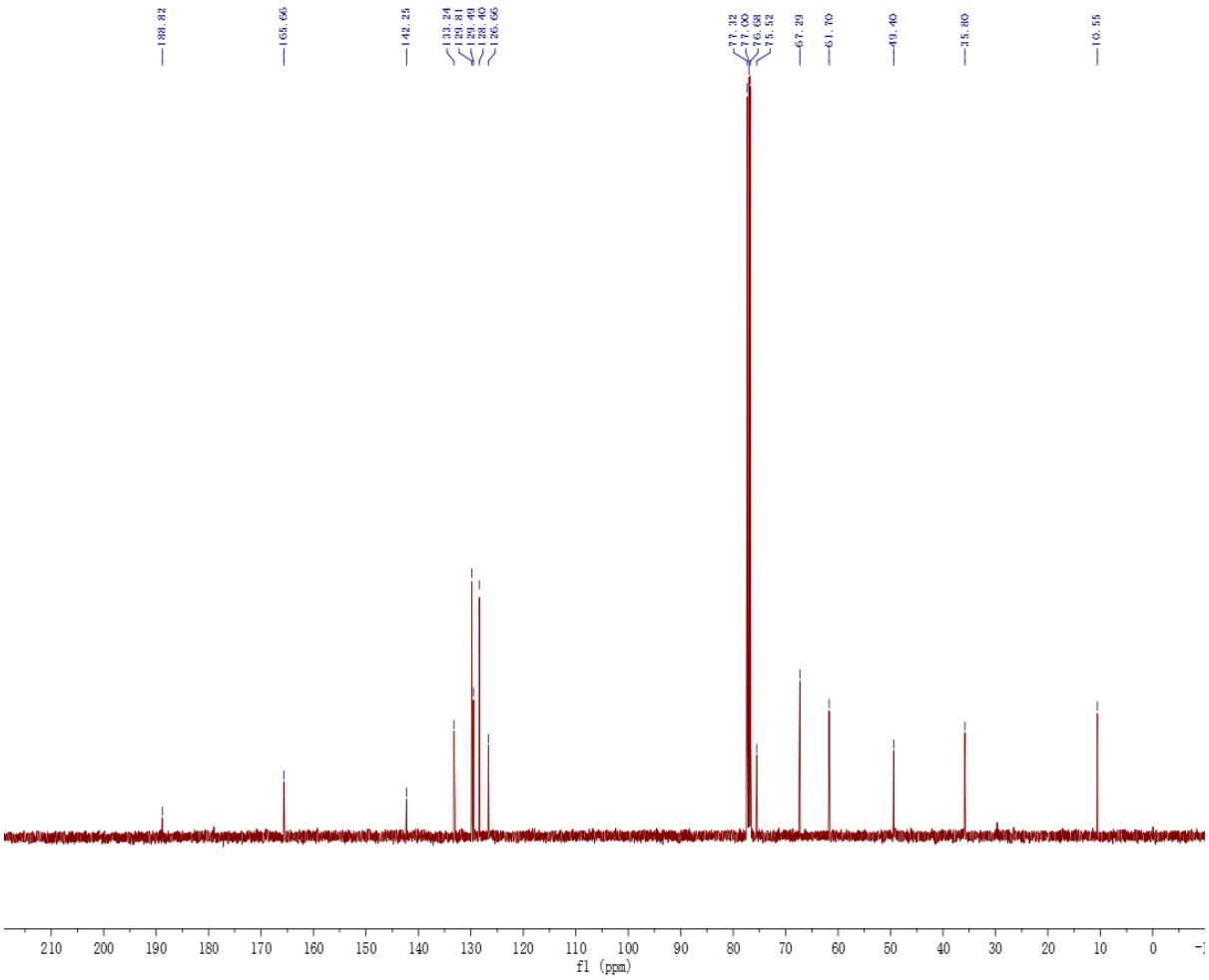


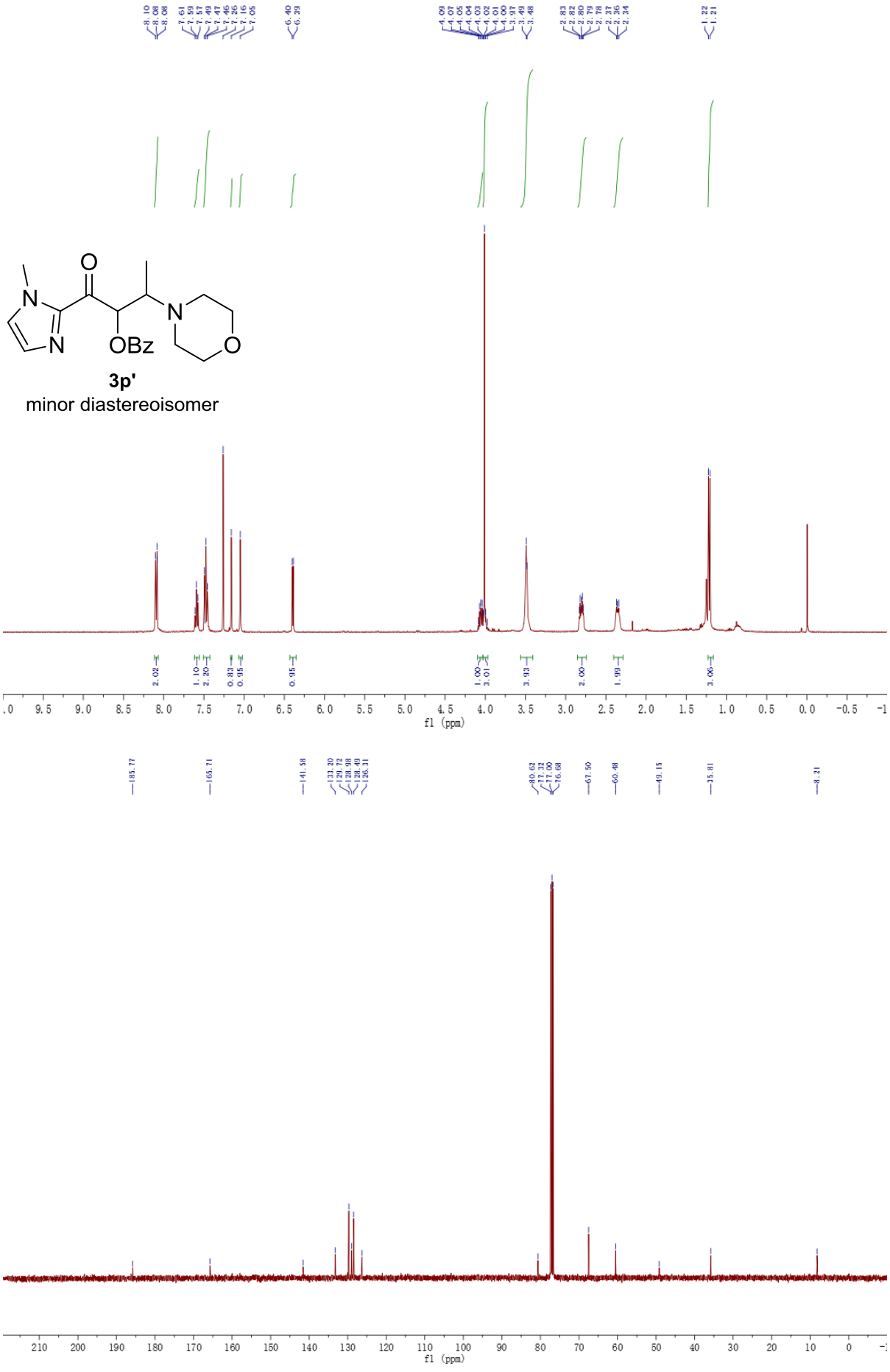

O
N
S
OBz
3o
f1 (ppm)


f1 (ppm)



3p
major diastereoisomer

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8.08
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7.59
7.57
7.49
7.47
7.46
7.26
7.16
7.05
6.40
6.39
4.09
4.07
4.05
4.04
4.03
4.02
4.01
4.00
3.97
3.49
3.48
2.83
2.82
2.80
2.79
2.78
2.37
2.36
2.34
1.22
1.21
O
N
N
OBz
N
O
3p'
minor diastereoisomer
2.02
1.10
2.20
0.83
0.95
0.95
1.00
1.01
3.93
2.00
1.99
3.06
f1 (ppm)
185.77
165.71
141.58
133.20
129.72
128.98
128.49
126.31
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76.68
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49.15
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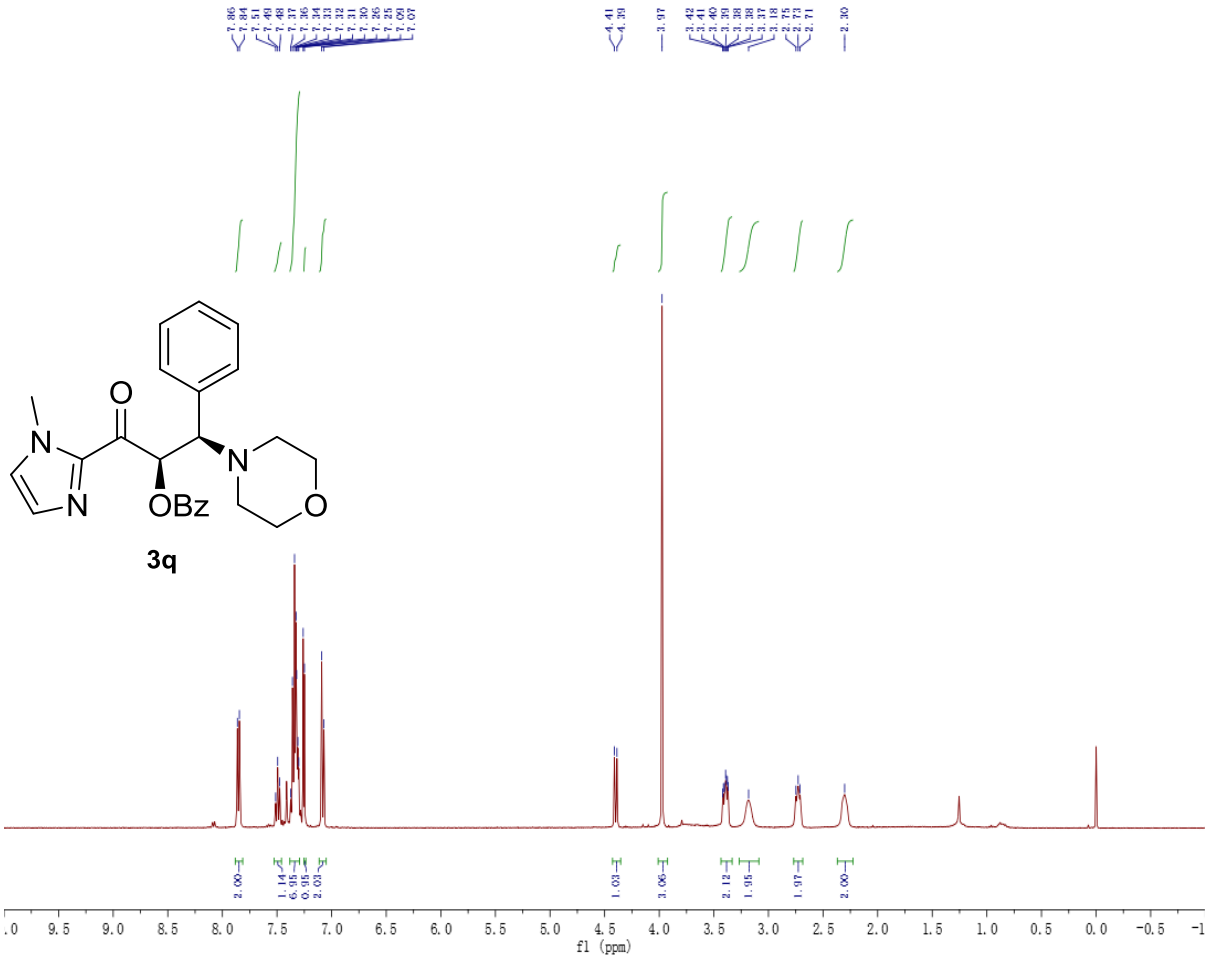
8.21
f1 (ppm)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7.33
7.32
7.31
7.30
7.26
7.25
7.09
7.07
4.41
4.39
3.97
3.42
3.41
3.40
3.39
3.38
3.38
3.37
3.18
2.75
2.73
2.71
2.30
O
N
N
N
OBz
O
2.00
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6.95
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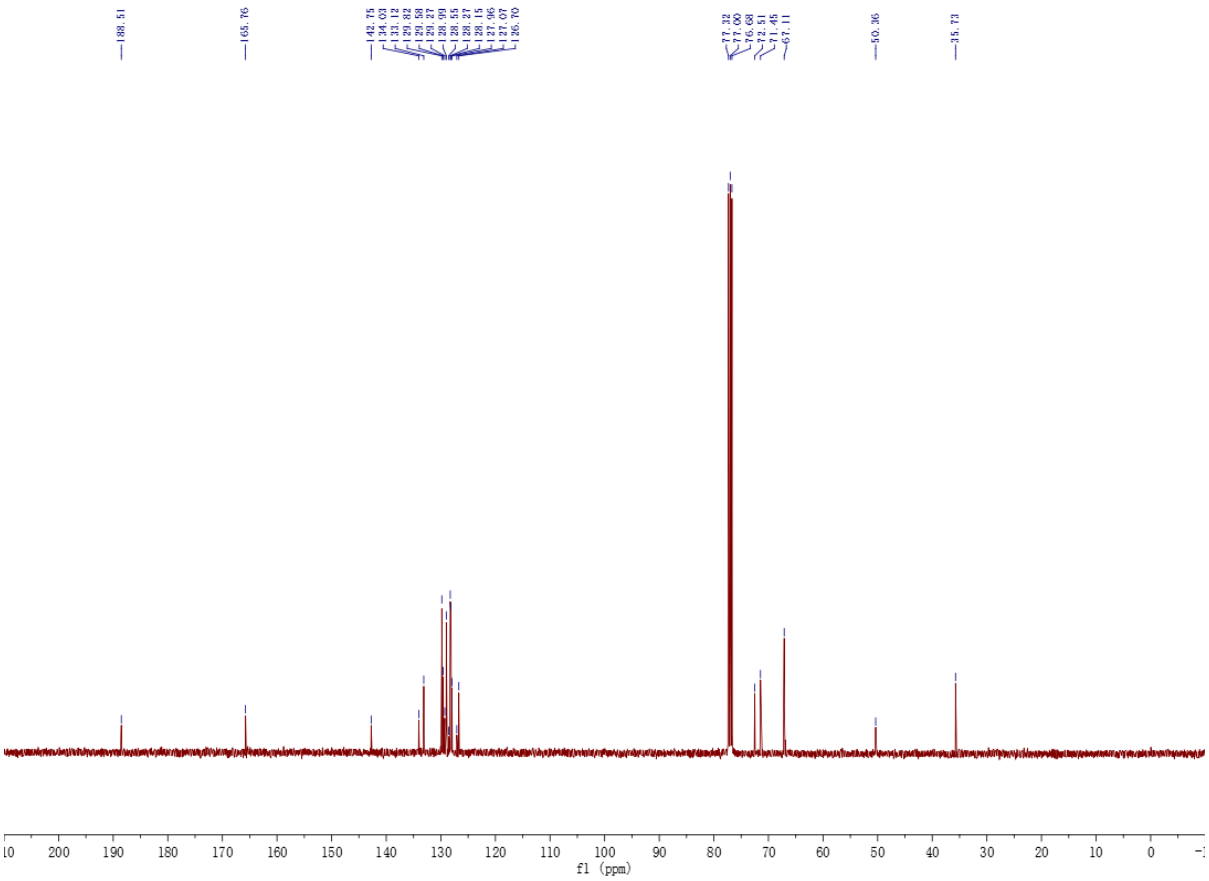
2.03
1.03
3.06
2.12
1.95
1.97
2.00
f1 (ppm)

3q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128.27
128.15
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127.07
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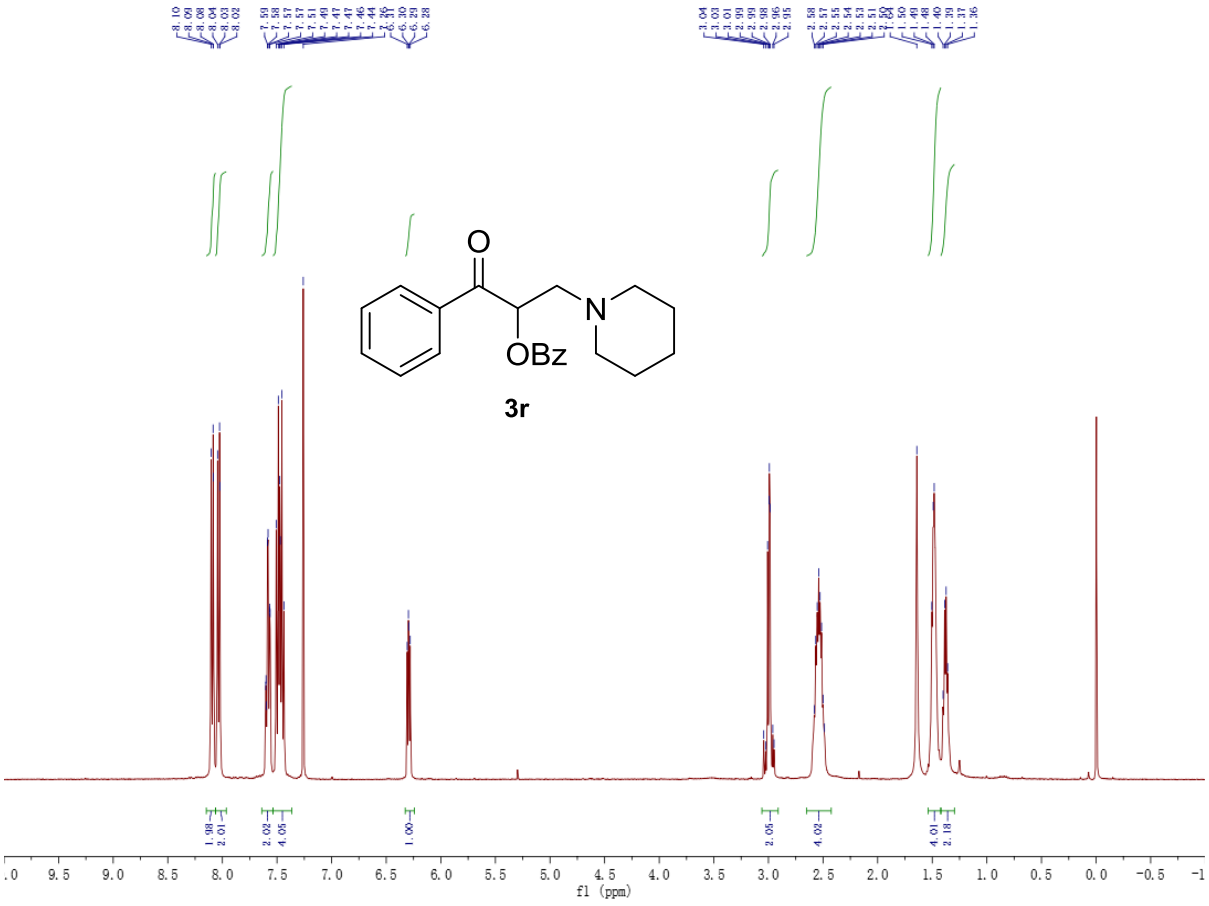
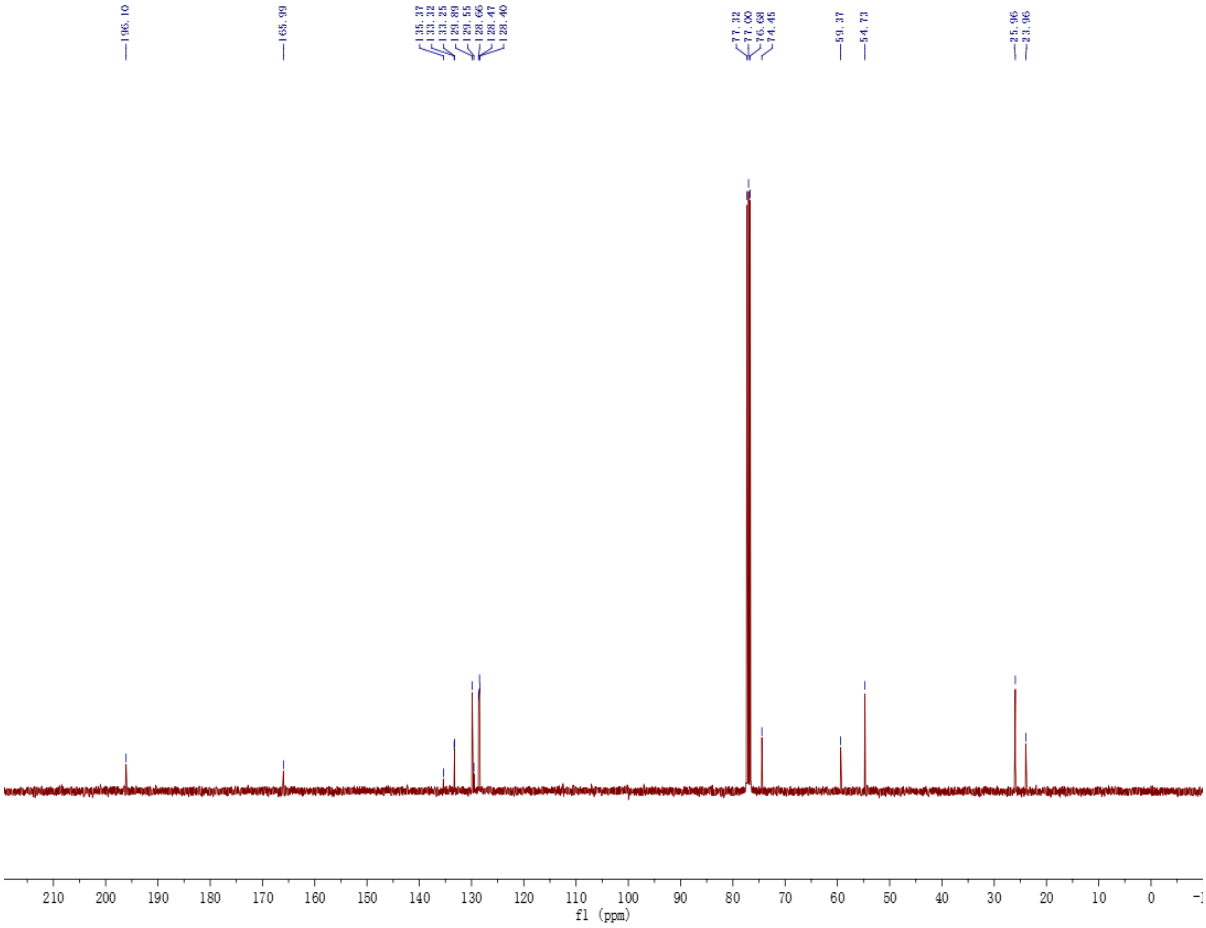
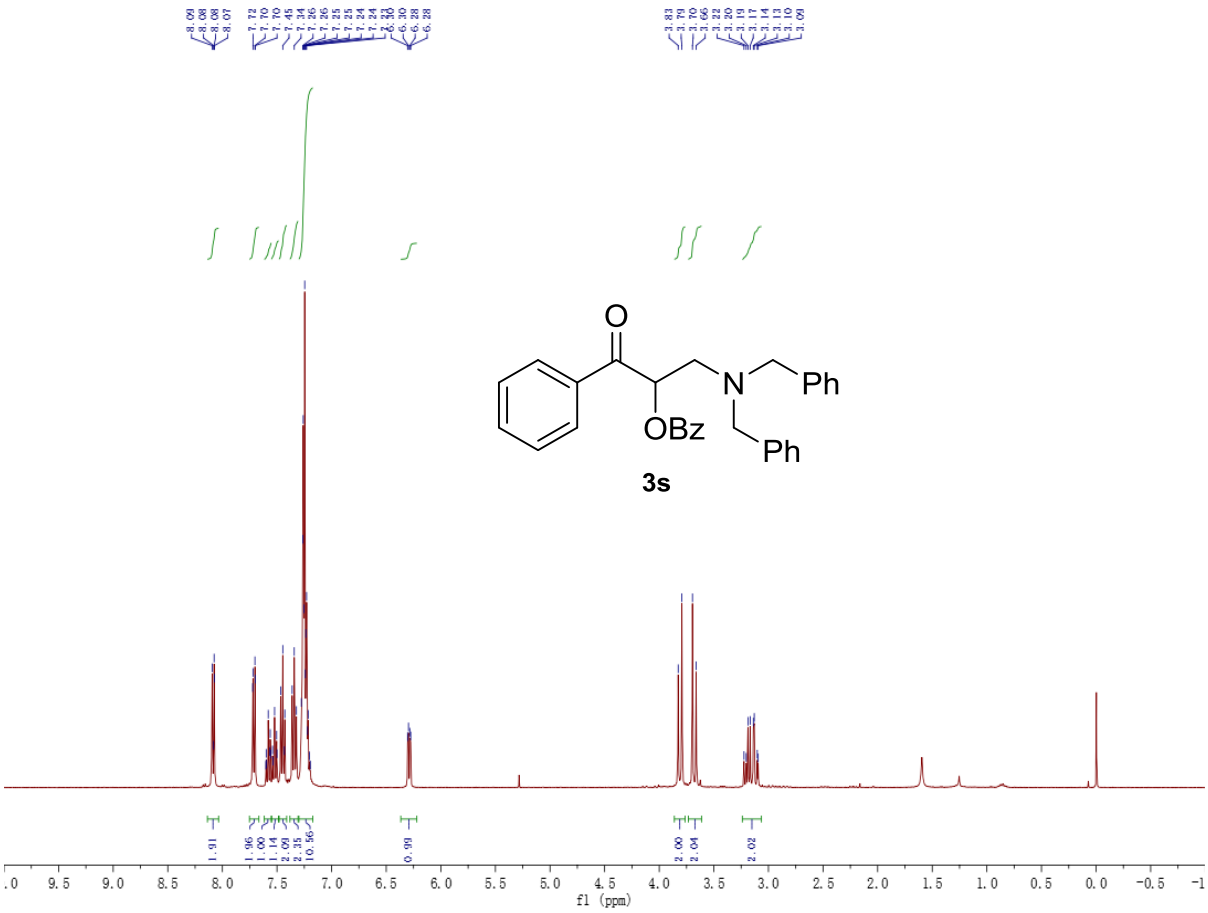
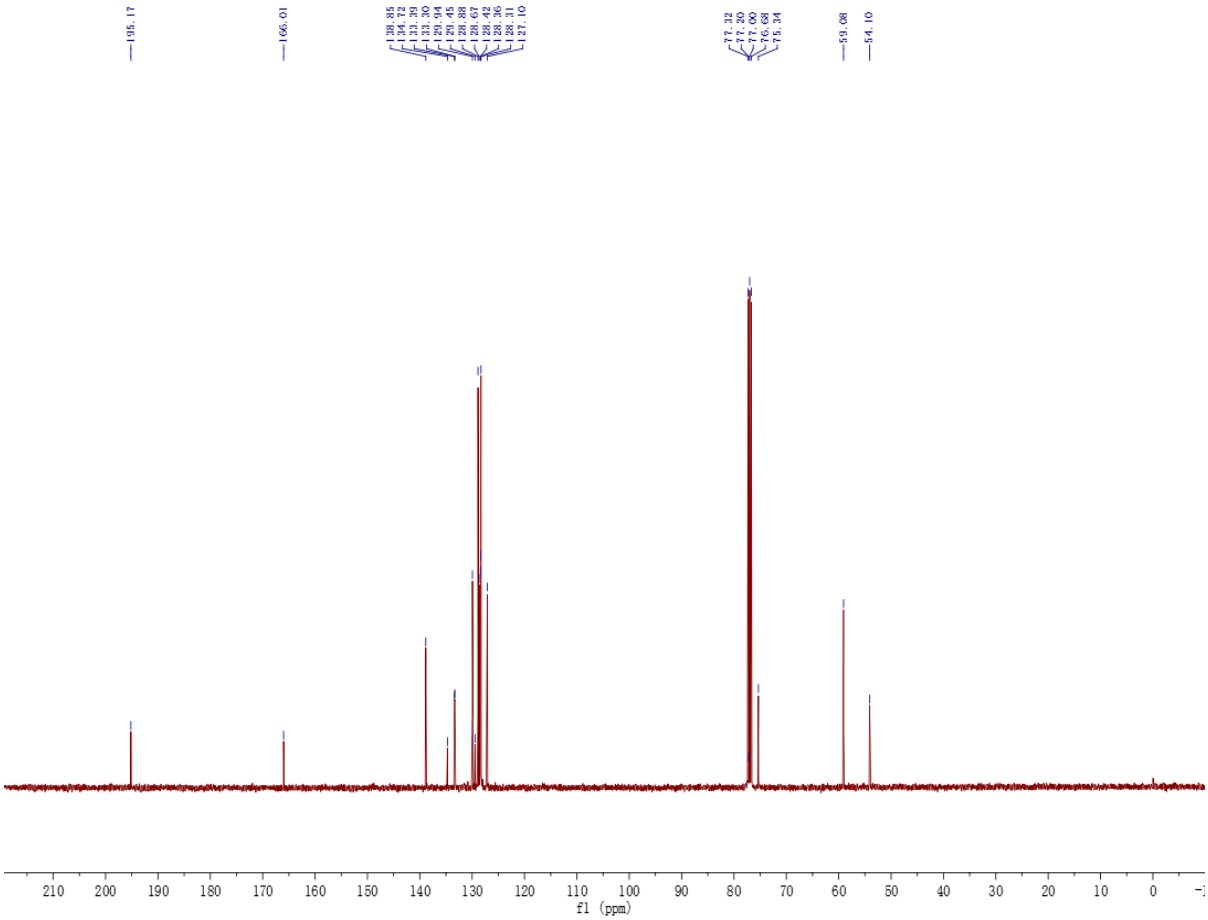
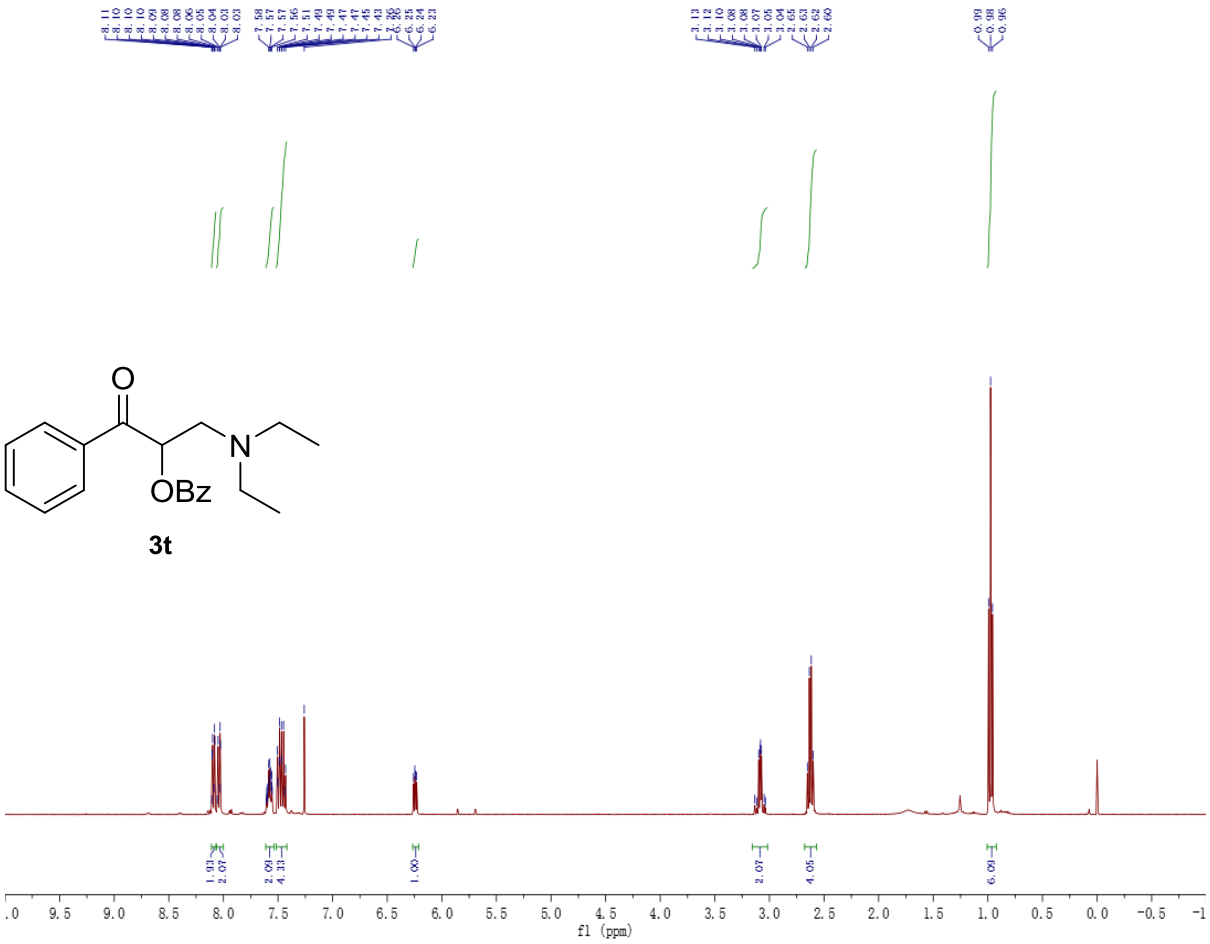
77.32
77.00
76.68
72.51
71.45
67.11
50.36
35.73
f1 (ppm)


O
N
OBz
3r
f1 (ppm)

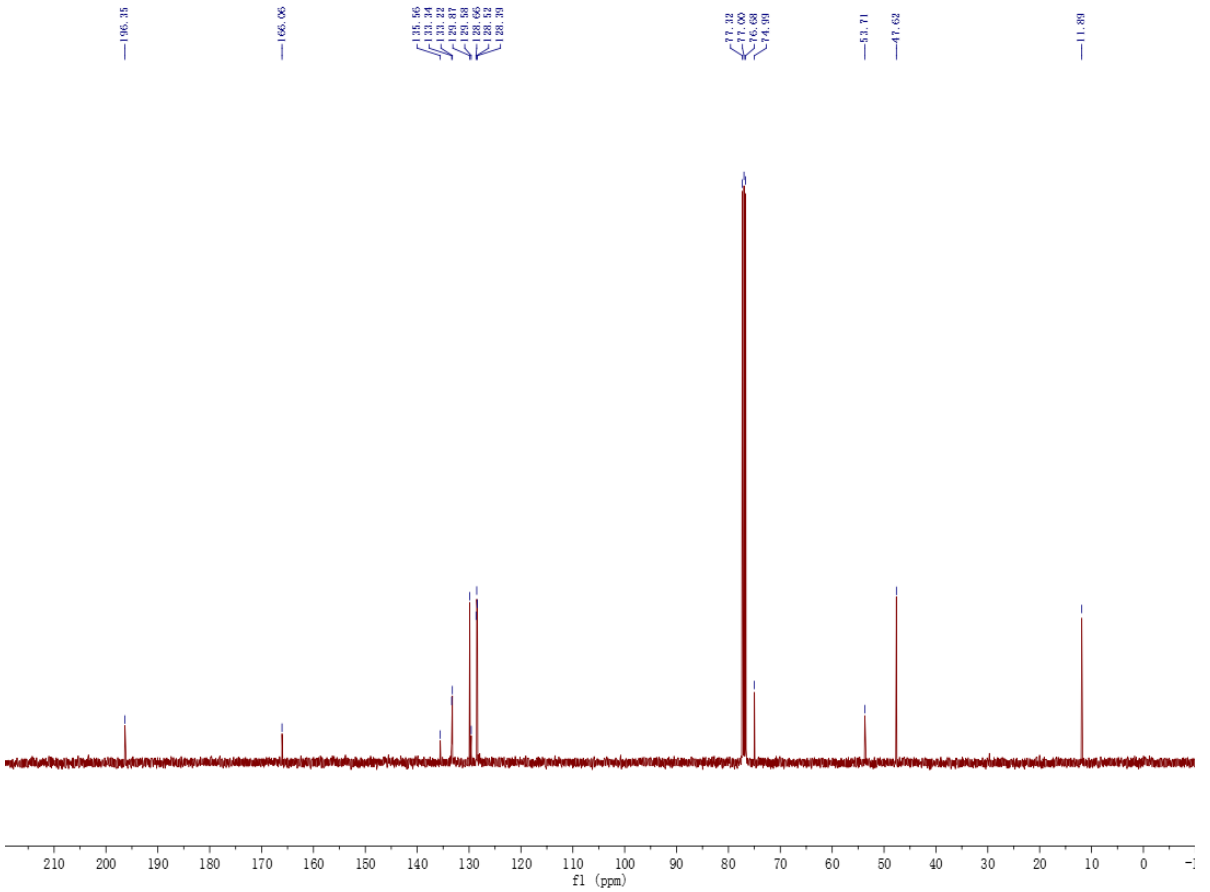

f1 (ppm)

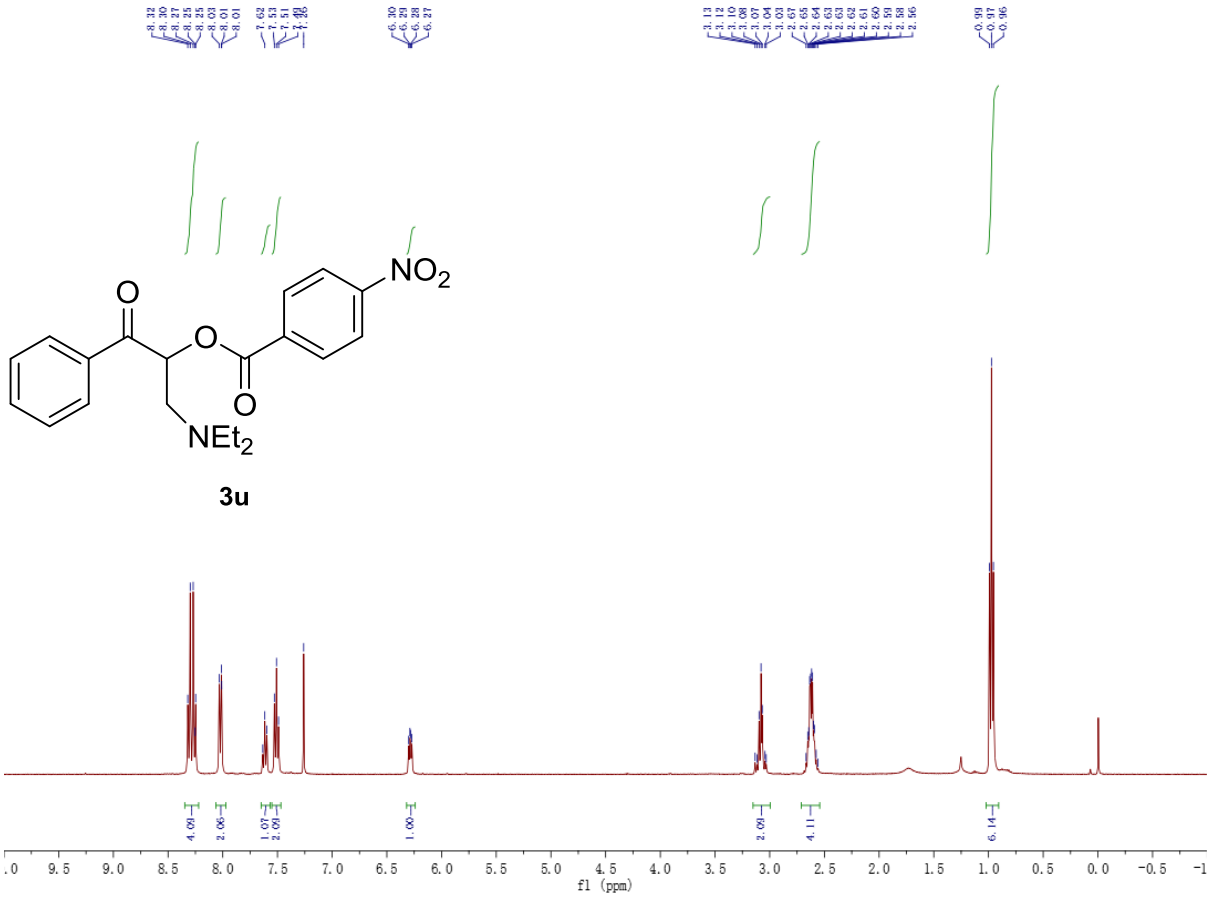

O
N
Ph
Ph
OBz
3s
f1 (ppm)


f1 (ppm)



3t





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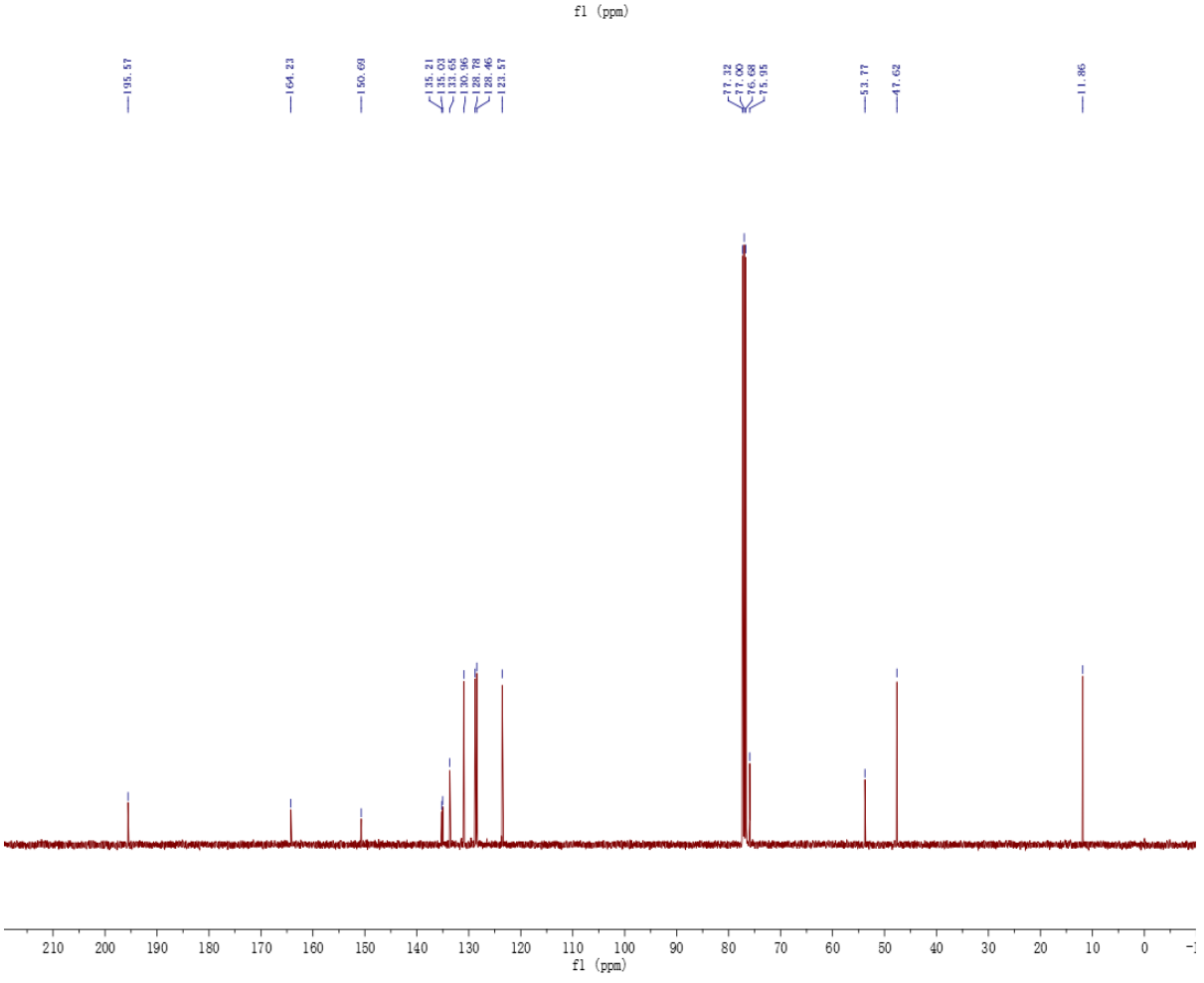

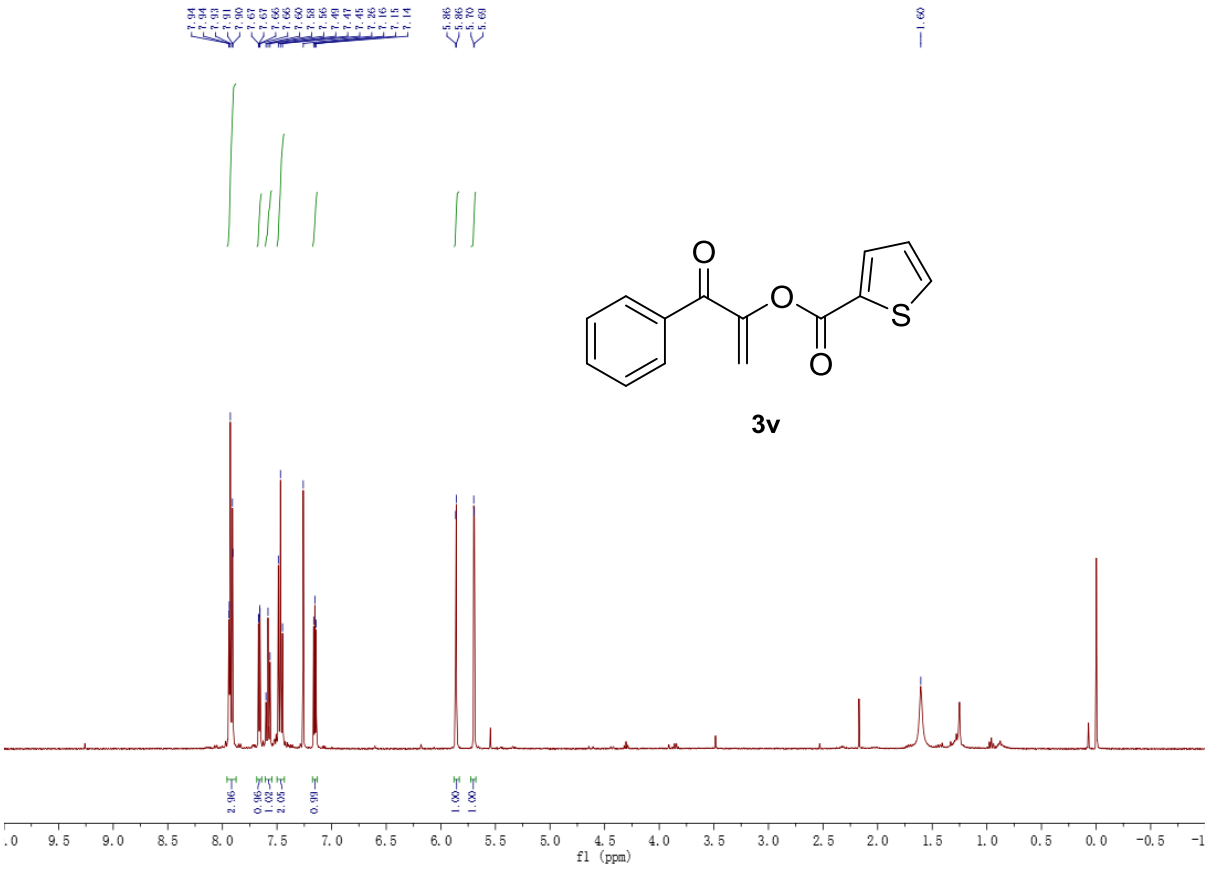
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7.45
7.36
7.16
7.15
7.14
5.86
5.86
5.70
5.69
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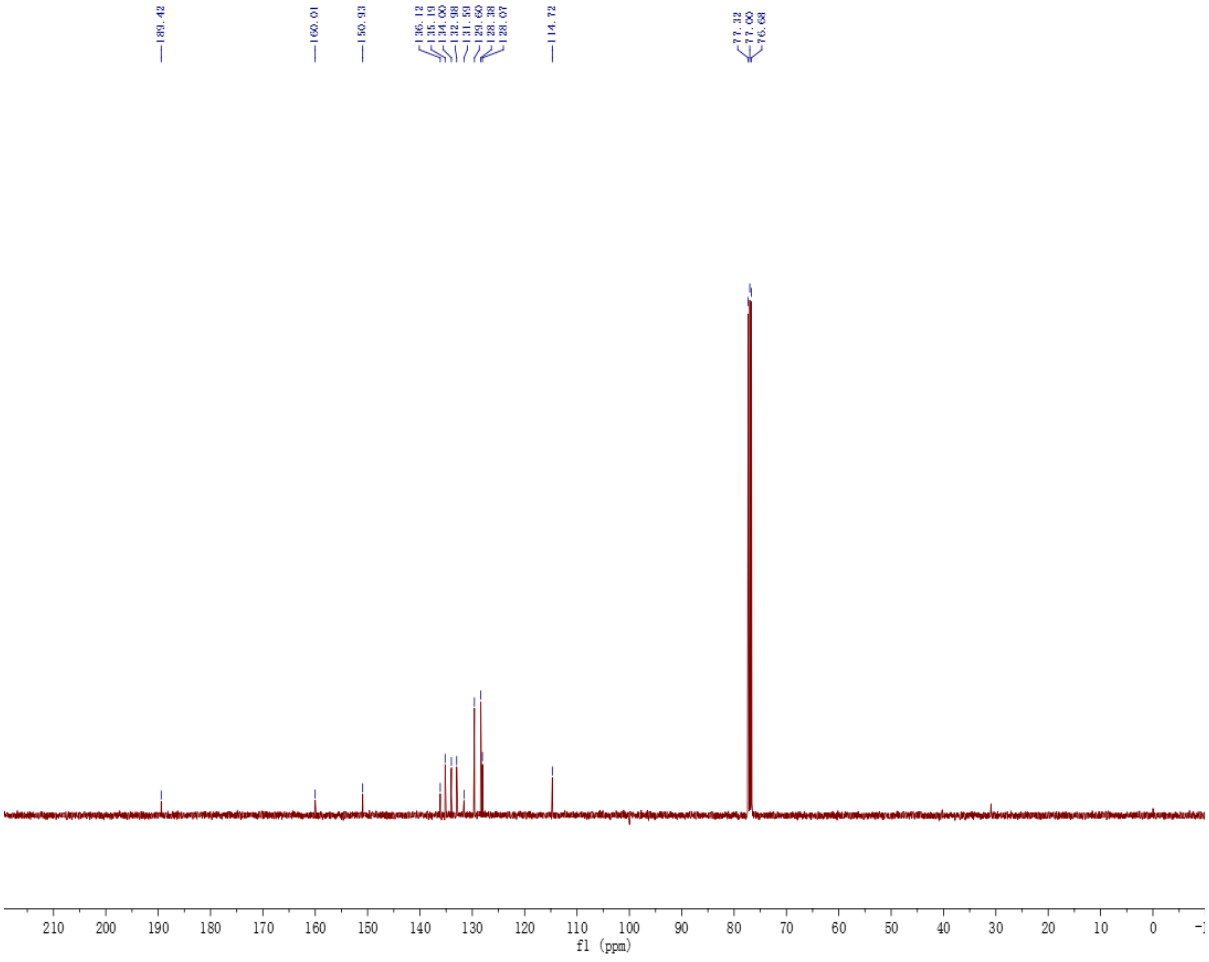
O
O
O
S
2.96
0.96
1.02
2.05
0.99
1.00
1.00
f1 (ppm)

3v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136.12
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131.59
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128.38
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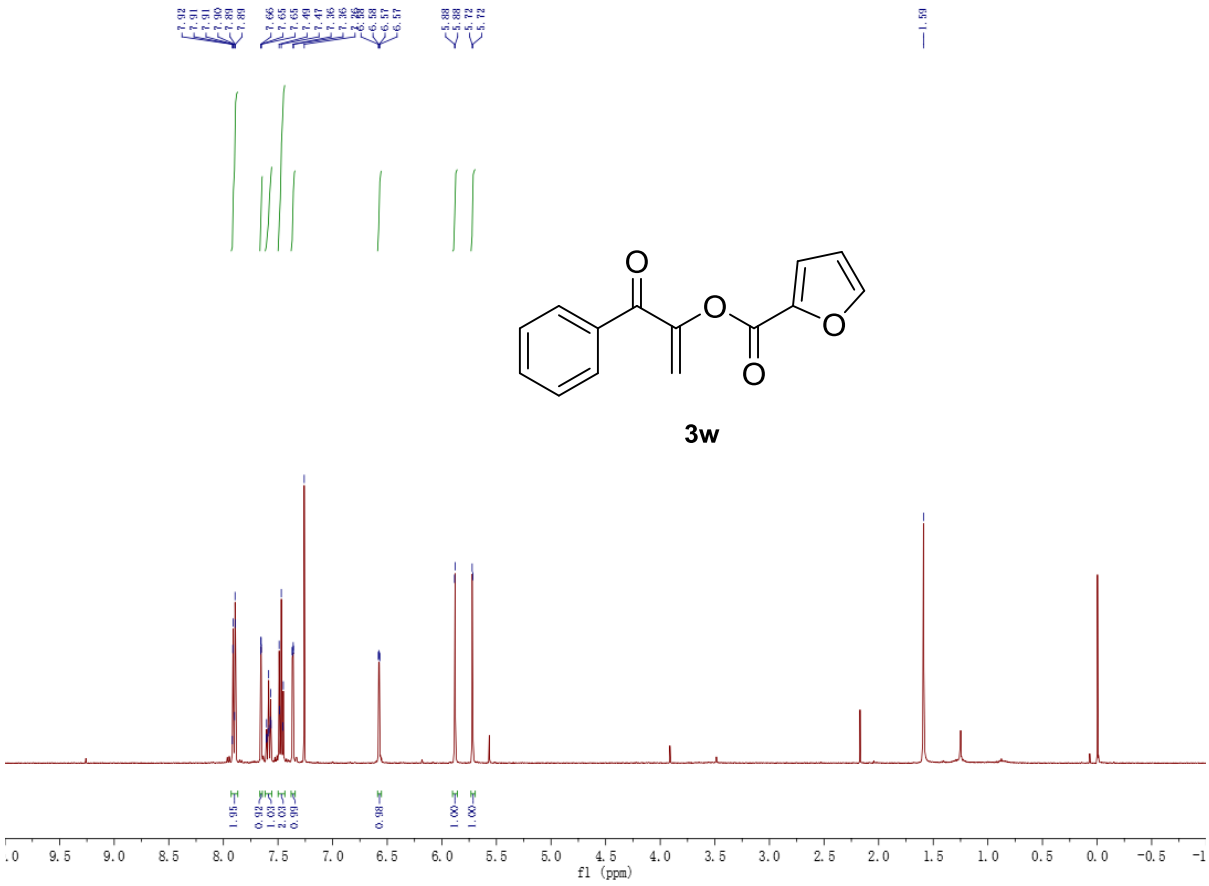
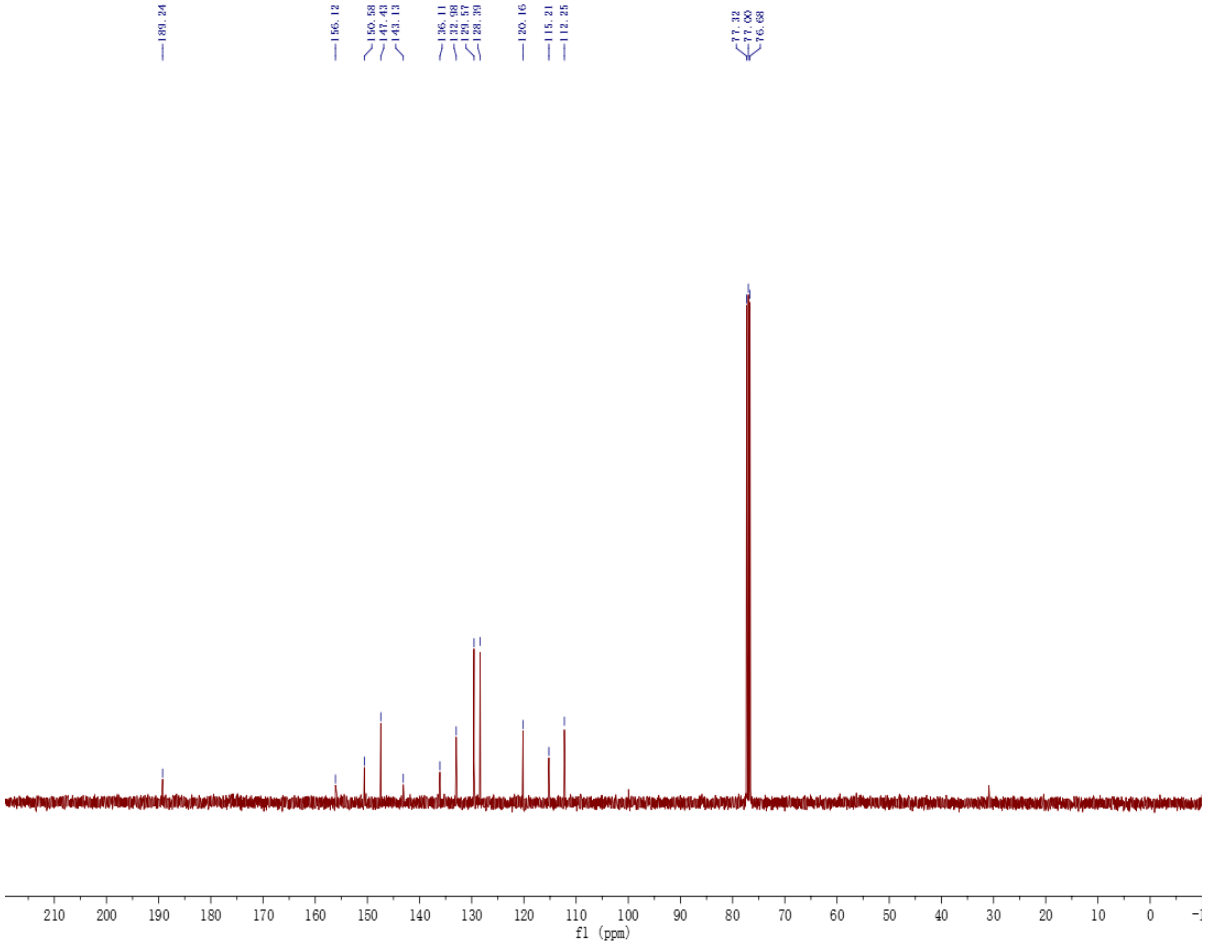
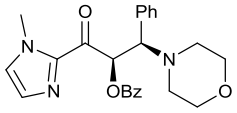
77.32
77.00
76.68
f1 (ppm)



3w



X-ray Data



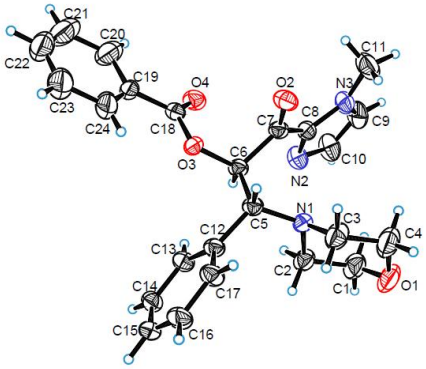


Table 1 Crystal data and structure refinement for rsc-1.

Identification code	rsc-1
Empirical formula	$C_{24}H_{25}N_3O_4$
Formula weight	419.47
Temperature/K	291(2)
Crystal system	monoclinic
Space group	I2/a
a/Å	22.3944(3)
b/Å	10.7588(2)
c/Å	19.4913(3)
α/°	90
β/°	105.440(2)
γ/ °	90
Volume/$Å^3$	4526.69(13)
Z	8
$\rho_{calc}g/cm^3$	1.231
μ/mm^{-1}	0.691
F(000)	1776.0
Crystal size/mm^3	0.220 × 0.200 × 0.150
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.192 to 142.528
Index ranges	$-21 \leq h \leq 27$, $-12 \leq k \leq 12$, $-23 \leq l \leq 22$
Reflections collected	19485
Independent reflections	4333 [R_{int} = 0.0167, R_{sigma} = 0.0099]
Data/restraints/parameters	4333/34/281
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0707, wR_2 = 0.1977
Final R indexes [all data]	R_1 = 0.0787, wR_2 = 0.2049
Largest diff. peak/hole / e $Å^{-3}$	0.57/-0.32

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for rsc-1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O3	4382.5(7)	7292.5(17)	4825.8(8)	56.5(4)
O2	5199.2(9)	8610.1(19)	4230.7(10)	70.1(5)
N1	5890.9(9)	8170.0(19)	5958(1)	54.4(5)
O4	4444.5(10)	5912(2)	3979.1(10)	76.1(6)
N3	6257.5(11)	7262(3)	4029.8(13)	73.7(7)
N2	6066.5(11)	5836(2)	4767.1(14)	72.4(6)
O1	7133.4(11)	8519(3)	6748.9(15)	111.4(9)
C12	4902.8(11)	7743(2)	6326.7(11)	52.2(5)
C8	5893.9(11)	6922(3)	4457.9(13)	57.7(6)
C7	5376.5(11)	7658(2)	4558.6(11)	53.4(5)
C6	5050.4(10)	7186(2)	5107.7(11)	52.1(5)
C5	5207.8(11)	8074(2)	5737.2(11)	52.4(5)
C13	4751.0(12)	6543(2)	6462.5(13)	60.4(6)
C18	4140.4(12)	6565(3)	4250.9(13)	61.2(6)
C14	4520.1(12)	6279(3)	7041.1(14)	64.9(7)
C17	4803.5(13)	8682(3)	6767.6(13)	65.5(7)
C15	4445.8(13)	7210(3)	7488.5(13)	68.4(7)
C16	4585.1(15)	8412(3)	7352.3(15)	75.6(8)
C2	6218.1(12)	7215(3)	6436.6(16)	70.6(7)
C19	3460.3(14)	6726(3)	3991.5(16)	80.8(10)
C3	6123.5(15)	9393(3)	6218(2)	84.9(9)
C1	6900.5(14)	7328(4)	6515(2)	94.5(11)
C9	6675.8(15)	6320(4)	4088(2)	95.6(11)
C10	6557.9(15)	5474(4)	4539(2)	93.7(11)
C11	6224.5(19)	8391(4)	3600(2)	110.5(14)
C24	3141.5(17)	7457(5)	4333(2)	105.9(12)
C22	2220(2)	6920(6)	3476(3)	136.2(16)
C4	6804.2(18)	9434(4)	6287(3)	119.6(15)
C20	3149(2)	6086(4)	3380(2)	118.0(14)
C23	2502(2)	7592(5)	4083(3)	130.6(14)
C21	2506(3)	6186(6)	3131(3)	150.4(19)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for rsc-1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O3	45.4(8)	77.5(11)	44.9(8)	-4.0(7)	9.0(6)	-0.3(7)
O2	75.3(12)	80.3(13)	59.2(10)	14.6(9)	25.8(9)	12.9(9)
N1	48.8(10)	64.2(12)	47.7(10)	-0.4(8)	8.7(8)	-0.7(9)
O4	91.8(14)	83.9(13)	54.8(10)	-13.1(9)	23.1(10)	-13.0(11)
N3	62.2(13)	92.9(17)	75.5(14)	-2.8(13)	34.8(11)	-4.5(12)
N2	67.7(14)	71.9(15)	86.3(16)	-2.3(12)	35.8(12)	10.2(11)
O1	67.1(14)	126(2)	115.0(19)	13.9(16)	-21.6(13)	-26.1(14)
C12	54.9(12)	59.5(14)	43.1(11)	-1.8(9)	15.0(9)	6.2(10)
C8	50.5(12)	74.9(16)	50.9(12)	-7.1(11)	19(1)	-1.3(11)
C7	54.3(13)	64.8(15)	41.4(11)	-1.4(10)	13.4(9)	3.3(10)
C6	49.7(12)	62.7(14)	44.3(11)	0.1(10)	13.6(9)	7.3(10)
C5	53.9(13)	58.5(13)	44.7(11)	-1.7(10)	13.2(9)	4.8(10)
C13	67.4(15)	61.0(15)	57.2(13)	-1.7(11)	24.4(11)	5.2(11)
C18	65.9(15)	71.6(16)	45.0(12)	7.3(11)	12.8(11)	-13.6(12)
C14	63.1(15)	73.0(17)	60.9(14)	12.7(13)	20.8(12)	3.2(12)
C17	81.6(17)	64.7(15)	57.0(13)	-9.3(12)	30.2(12)	-2.4(13)
C15	64.2(15)	99(2)	44.1(12)	0.2(13)	18.7(11)	-5.5(14)
C16	90(2)	89(2)	56.6(14)	-18.4(14)	33.3(14)	-6.2(16)
C2	55.9(15)	78.2(18)	70.6(16)	4.8(14)	4.3(12)	4.4(12)
C19	59.1(16)	105(2)	67.4(16)	36.1(16)	-2.8(13)	-25.3(16)
C3	75.0(19)	72.7(19)	96(2)	-0.6(16)	4.1(16)	-12.4(15)
C1	55.0(16)	113(3)	105(3)	12(2)	2.9(16)	4.3(17)
C9	67.8(18)	115(3)	122(3)	-12(2)	56.3(19)	8.9(18)
C10	78(2)	89(2)	130(3)	2(2)	56(2)	18.7(17)
C11	93(2)	142(4)	116(3)	32(3)	61(2)	3(2)
C24	66.1(16)	139(3)	111(2)	37(2)	20.7(18)	-2.3(19)
C22	80(2)	159(3)	147(3)	58(3)	-8(2)	-32(2)
C4	87(3)	115(3)	134(3)	22(3)	-10(2)	-38(2)
C20	107(3)	120(3)	100(2)	22(2)	-19(2)	-27(2)
C23	75.5(17)	169(3)	145(3)	45(2)	25(2)	1(2)
C21	130(3)	150(4)	129(3)	22(3)	-39(2)	-38(3)

Table 4 Bond Lengths for rsc-1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O3	C18	1.356(3)	C8	C7	1.459(3)
O3	C6	1.454(3)	C7	C6	1.534(3)
O2	C7	1.217(3)	C6	C5	1.521(3)
N1	C2	1.449(3)	C13	C14	1.389(4)
N1	C3	1.456(4)	C18	C19	1.482(4)
N1	C5	1.478(3)	C14	C15	1.367(4)
O4	C18	1.196(3)	C17	C16	1.385(4)
N3	C8	1.362(3)	C15	C16	1.373(4)
N3	C9	1.364(4)	C2	C1	1.500(4)
N3	C11	1.465(5)	C19	C24	1.351(6)
N2	C8	1.324(4)	C19	C20	1.393(5)
N2	C10	1.350(4)	C3	C4	1.495(5)
O1	C4	1.403(5)	C9	C10	1.340(5)
O1	C1	1.413(5)	C24	C23	1.392(5)
C12	C13	1.379(4)	C22	C21	1.310(8)
C12	C17	1.382(3)	C22	C23	1.387(8)
C12	C5	1.527(3)	C20	C21	1.396(7)

Table 5 Bond Angles for rsc-1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C18	O3	C6	114.29(19)	C6	C5	C12	114.0(2)
C2	N1	C3	110.1(2)	C12	C13	C14	120.7(2)
C2	N1	C5	116.4(2)	O4	C18	O3	123.8(2)
C3	N1	C5	114.3(2)	O4	C18	C19	124.9(3)
C8	N3	C9	105.0(3)	O3	C18	C19	111.3(3)
C8	N3	C11	128.7(3)	C15	C14	C13	120.2(3)
C9	N3	C11	126.3(3)	C12	C17	C16	120.6(3)
C8	N2	C10	105.6(3)	C14	C15	C16	119.6(2)
C4	O1	C1	110.1(3)	C15	C16	C17	120.3(3)
C13	C12	C17	118.5(2)	N1	C2	C1	109.6(3)
C13	C12	C5	123.0(2)	C24	C19	C20	120.1(4)
C17	C12	C5	118.4(2)	C24	C19	C18	122.0(3)
N2	C8	N3	111.5(2)	C20	C19	C18	117.9(4)
N2	C8	C7	124.3(2)	N1	C3	C4	108.7(3)
N3	C8	C7	124.2(3)	O1	C1	C2	112.6(3)
O2	C7	C8	123.1(2)	C10	C9	N3	108.0(3)

O2	C7	C6	119.7(2)	C9	C10	N2	109.9(3)
C8	C7	C6	117.2(2)	C19	C24	C23	121.2(5)
O3	C6	C5	104.44(17)	C21	C22	C23	125.2(5)
O3	C6	C7	110.06(17)	O1	C4	C3	112.7(3)
C5	C6	C7	107.7(2)	C19	C20	C21	119.5(5)
N1	C5	C6	106.19(18)	C22	C23	C24	115.9(5)
N1	C5	C12	115.64(18)	C22	C21	C20	118.1(5)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for rsc-1.

Atom	*x*	*y*	*z*	U(eq)
H6	5174	6332	5255	62
H5	5049	8892	5556	63
H13	4804	5902	6163	72
H14	4416	5467	7124	78
H17	4884	9503	6671	79
H15	4302	7030	7883	82
H16	4533	9049	7654	91
H2A	6075	6401	6249	85
H2B	6136	7304	6898	85
H3A	6046	9548	6677	102
H3B	5913	10029	5889	102
H1A	7118	6710	6853	113
H1B	6982	7154	6060	113
H9	6988	6274	3856	115
H10	6781	4744	4674	112
H11A	5838	8408	3239	166
H11B	6560	8395	3380	166
H11C	6254	9108	3900	166
H24	3353	7877	4743	127
H22	1792	6997	3299	163
H4A	6874	9323	5821	144
H4B	6962	10247	6462	144
H20	3369	5595	3138	142
H23	2278	8102	4309	157
H21	2288	5745	2733	180