Supporting Information

Alkali-metal Organomagnesiate Complexes as Catalysts for Highly Chemselective Crossed-Tishchenko Reaction

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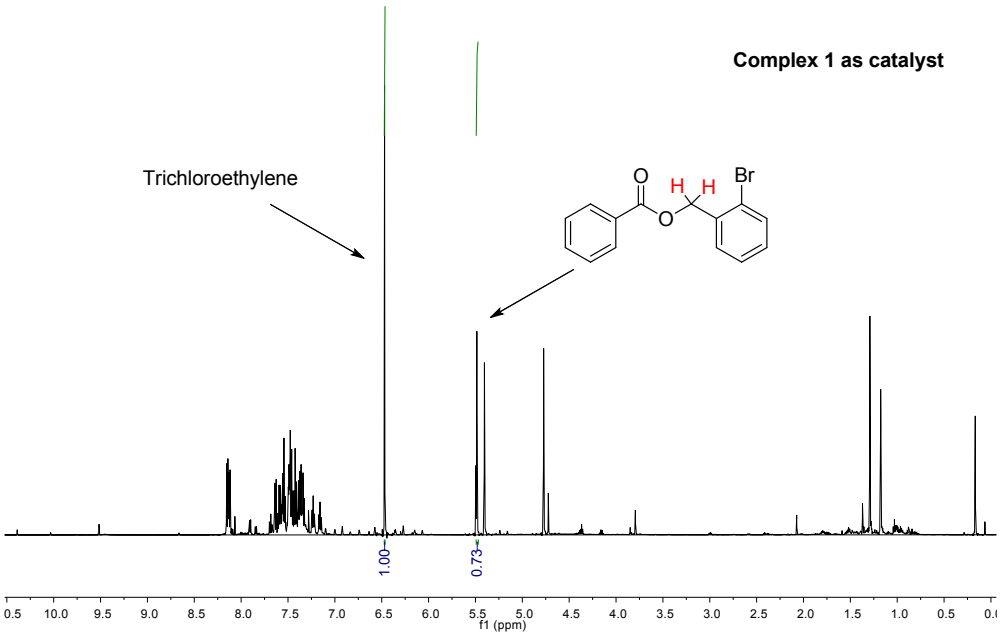
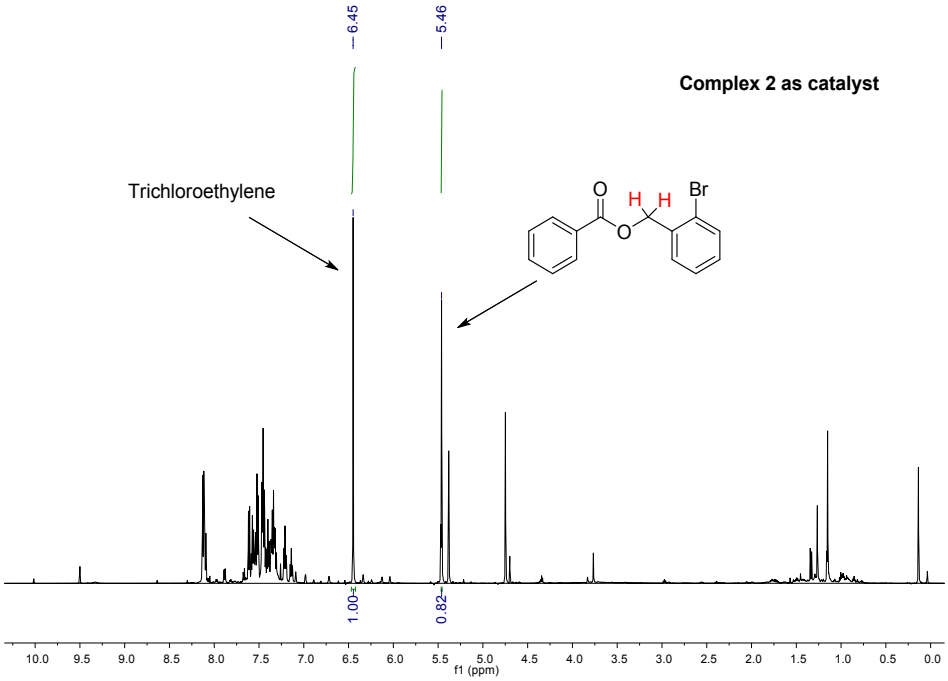
Experimental Procedures

1. The Procedure for Crossed-Tishchenko Reaction Catalyzed by Complex 1-5

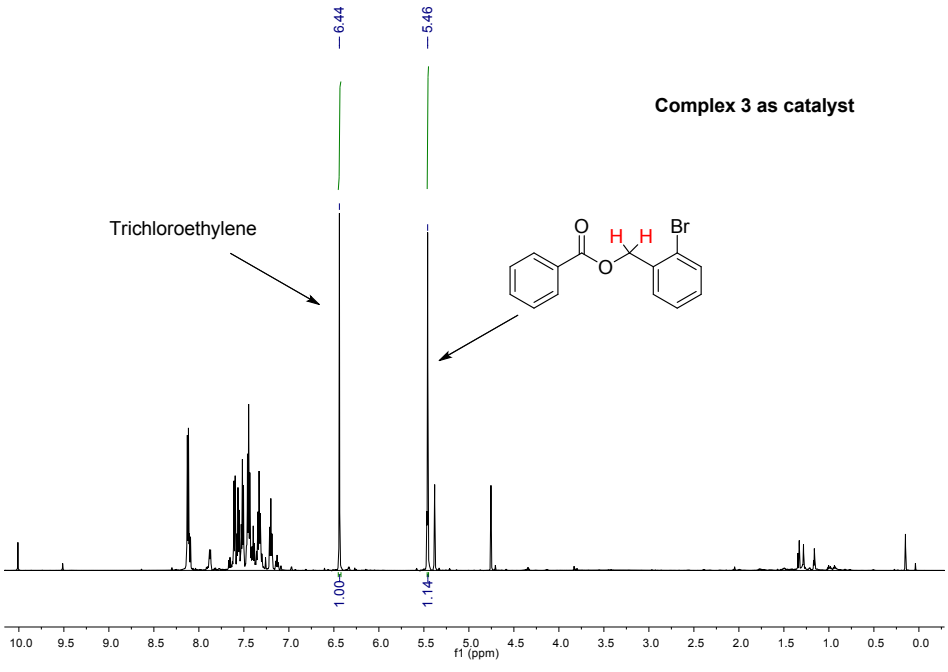
(a) In a glovebox, to a 50 mL sealed tube with a magnetic stirring bar, was successively added benzaldehyde (102 uL, 1.0 mmol), *o*-bromobenzaldehyde (117 uL, 1.0 mmol) catalyst **1** (0.0312 g, 0.05 mmol). The mixture was stirred at 30 °C for 3 h. The reaction was then quenched with H_2O (10 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The yields were determined by ^1H NMR spectroscopy with trichloroethylene (90 μL, 1 mmol) as an internal standard. The NMR yield of 2-bromobenzyl benzoate is 37%.



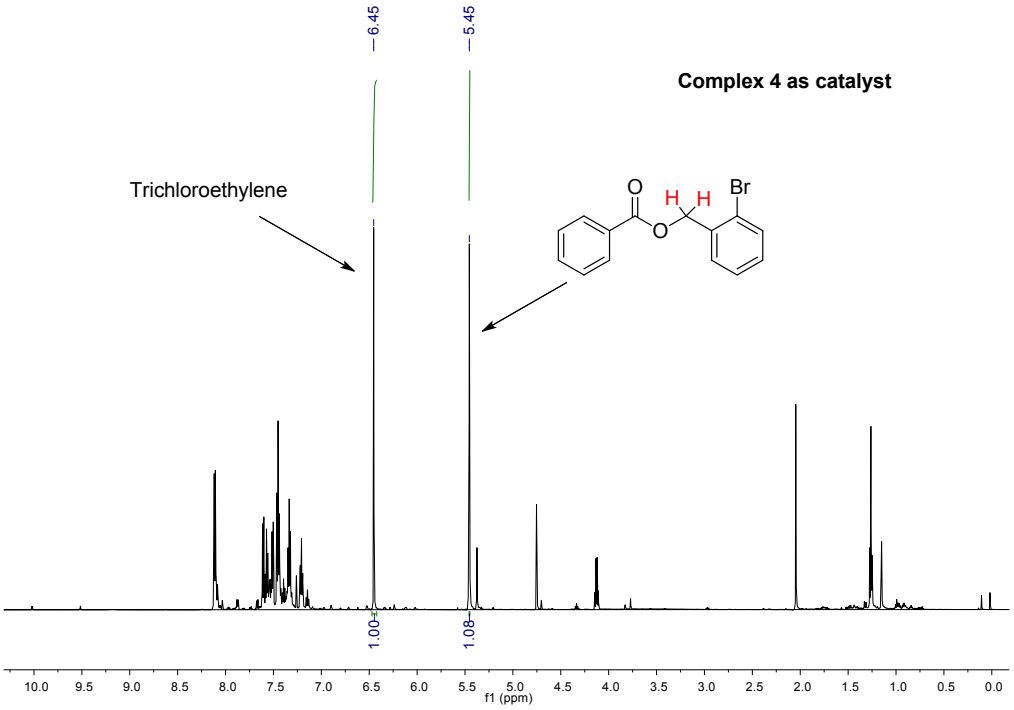
(b) In a glovebox, to a 50 mL sealed tube with a magnetic stirring bar, was successively added benzaldehyde (102 uL, 1.0 mmol), *o*-bromobenzaldehyde (117 uL, 1.0 mmol) catalyst **2** (0.0282 g, 0.05 mmol). The mixture was stirred at 30 °C for 3 h. The reaction was then quenched with H_2O (10 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The yields were determined by ^1H NMR spectroscopy with trichloroethylene (90 μL, 1 mmol) as an internal standard. The NMR yield of 2-bromobenzyl benzoate is 41%.



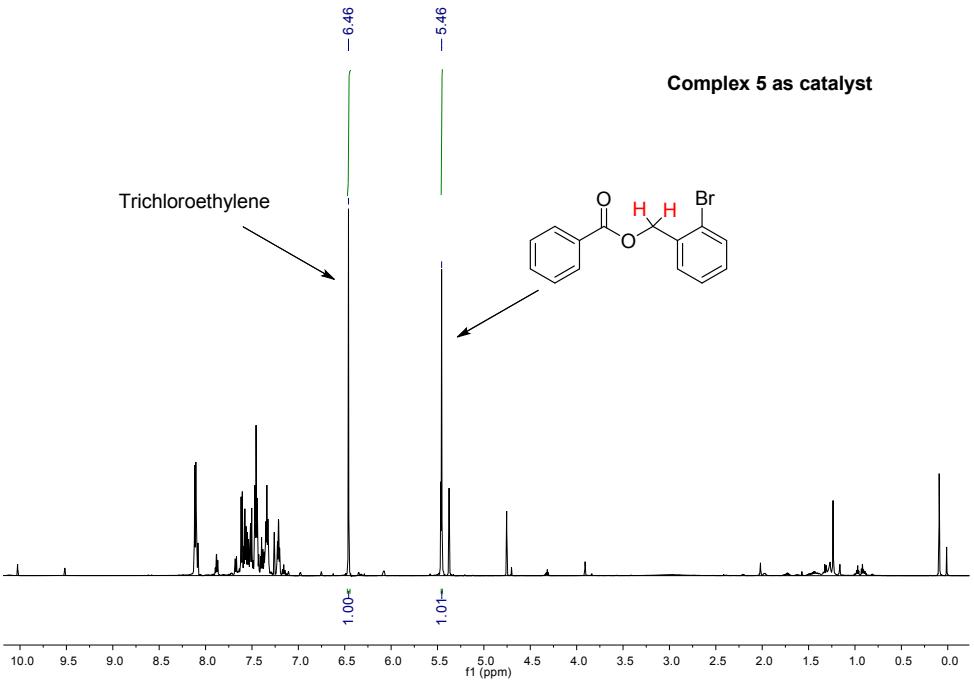
(c) In a glovebox, to a 50 mL sealed tube with a magnetic stirring bar, was successively added benzaldehyde (102 uL, 1.0 mmol), *o*-bromobenzaldehyde (117 uL, 1.0 mmol) catalyst **3** (0.0329 g, 0.05 mmol). The mixture was stirred at 30 °C for 3 h. The reaction was then quenched with H_2O (10 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The yields were determined by ^1H NMR spectroscopy with trichloroethylene (90 µL, 1 mmol) as an internal standard. The NMR yield of 2-bromobenzyl benzoate is 57%.



(d) In a glovebox, to a 50 mL sealed tube with a magnetic stirring bar, was successively added benzaldehyde (102 uL, 1.0 mmol), *o*-bromobenzaldehyde (117 uL, 1.0 mmol) catalyst **4** (0.0371 g, 0.05 mmol). The mixture was stirred at 30 °C for 3 h. The reaction was then quenched with H_2O (10 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The yields were determined by ^1H NMR spectroscopy with trichloroethylene (90 μL, 1 mmol) as an internal standard. The NMR yield of 2-bromobenzyl benzoate is 54%.

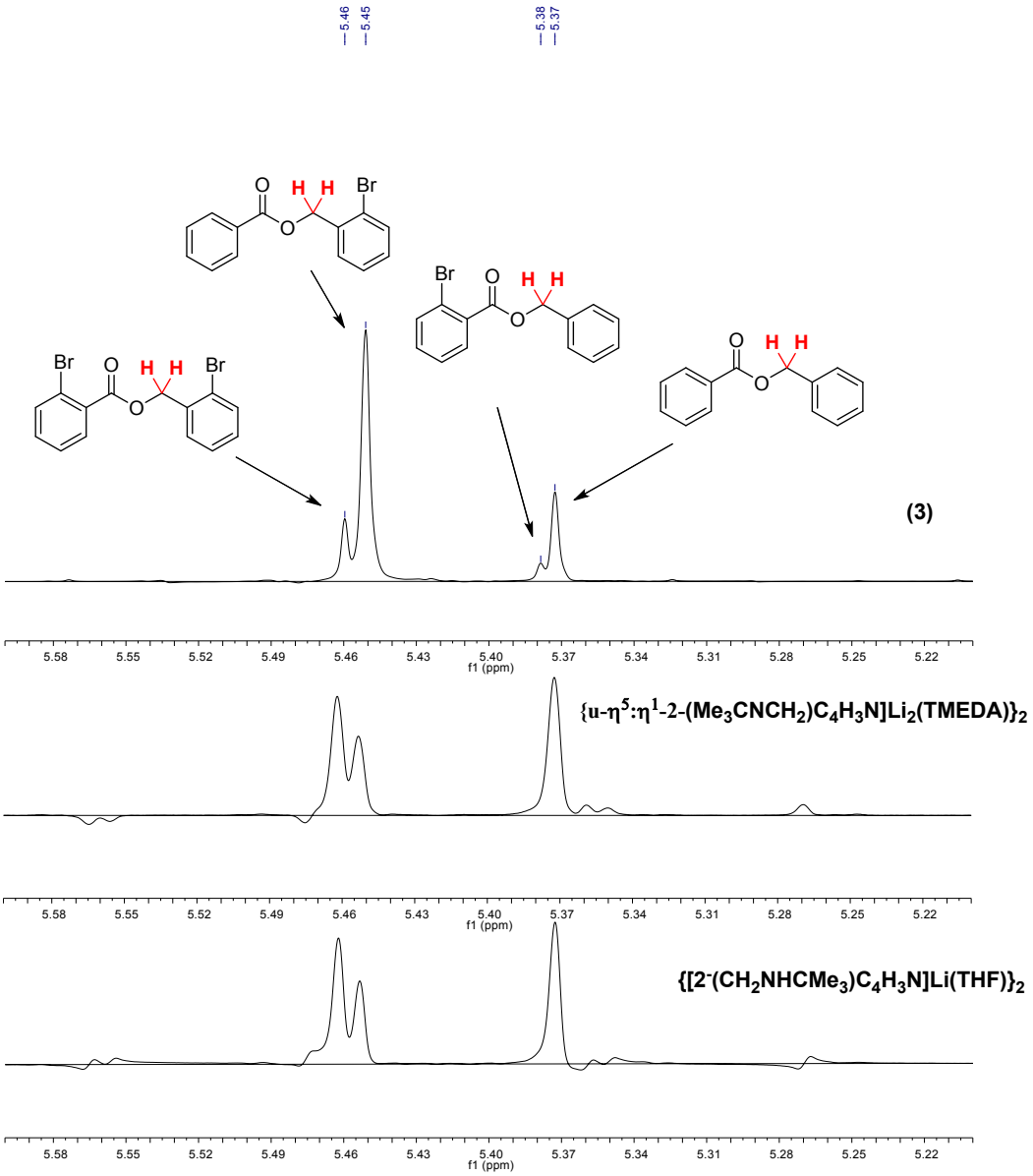


(e) In a glovebox, to a 50 mL sealed tube with a magnetic stirring bar, was successively added benzaldehyde (102 uL, 1.0 mmol), *o*-bromobenzaldehyde (117 uL, 1.0 mmol) catalyst **5** (0.0344 g, 0.05 mmol). The mixture was stirred at 30 °C for 3 h. The reaction was then quenched with H_2O (10 mL) and extracted with ethyl acetate (3 x 10 mL). The combined organic layers were dried over Na_2SO_4 and concentrated. The yields were determined by ^1H NMR spectroscopy with trichloroethylene (90 μL, 1 mmol) as an internal standard. The NMR yield of 2-bromobenzyl benzoate is 50%.


6.46
5.46
Complex 5 as catalyst
Trichloroethylene
O
H
H
Br
O
1.00
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

2. The Control Reactions.

In the same condition, the control reactions were carried out using 2-aminopyrr-olyl lithium complex $\{[2\text{-}(CH_2NHCMe_3)C_4H_3N]Li(THF)\}_2$, 2-aminopyrrolyl di-lithium compounds $\{\mu\text{-}\eta^5\text{:}\eta^1\text{-}2\text{-}(Me_3CNCH_2)C_4H_3N]Li_2(TMEDA)\}_2$ and sodium alkyl magnesiate $\{^nBuMg[2\text{-}(Me_3CNCH_2)C_4H_3N]Na(Et_2O)\}_\infty$ (**3**) with the same supporting ligand as catalysts. As shown in the following scheme, the NMR results show that mono-, di-lithioaminopyrroyl complex can catalyze Tishchenko reaction, but their selectivity is lower than that of sodium alkyl magnesiate.



Crystal data and Structure Refinement Details of 1, 3 and 4

Table S1. Single crystal X-ray data and structure refinement details for **1**, **3**, **4.**

Complex	**1**	**3**	**4**
Empirical formula	$C_{34}H_{60}Li_2MgN_4O_4$	$C_{34}H_{66}Mg_2N_4Na_2O_2$	$C_{38}H_{77}Mg_2N_8Na_2$
Formula weight	627.05	655.49	740.68
Temperature (K)	200(2)	136(2)	150(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Orthorhombic	Monoclinic
space group	C2/c	Pbca	P2(1)/c
a (Å)	22.586(2)	17.2336(6)	18.5707(7)
b (Å)	11.7778(12)	19.0795(6)	17.2230(6)
c (Å)	17.703(3)	24.5532(8)	15.7369(6)
α (deg)	90.00	90.00	90.00
β (deg)	126.618(2)	90.00	112.5610(10)
γ (deg)	90.00	90.00	90.00
Volume ($Å^3$)	3779.8(8)	8073.3(5)	4648.1(3)
Z	4	8	4
D_c (g/cm^{-3})	1.102	1.079	1.058
M (mm^{-1})	0.085	0.113	0.104
F(000)	1368	2864	1628
Crystal size (mm)	0.45 x 0.40 x 0.40	0.30 x 0.30 x 0.20	0.30 x 0.30 x 0.20
Theta range for data collection	3.27 to 28.81 deg.	2.89 to 28.28 deg.	2.85 to 27.34 deg.
Reflections collected / unique	27282 / 3320 [R(int) = 0.0801]	57967 / 7125 [R(int) = 0.0315]	34123 / 8183 [R(int) = 0.0341]
Completeness to theta = 25.05	98.8 %	99.7 %	99.5 %
Max. and min. transmission	0.967 and 0.963	0.9778 and 0.9670	0.9796 and 0.9696
Data / restraints / parameters	3320/ 1 / 207	7125/ 541 / 434	8183 / 43/ 476
Goodness-of-fit	0.989	1.062	1.048
R_1 / wR_2 [I>2sigma(I)]	0.0795 / 0.1336	0.0703/ 0.2013	0.0761/ 0.2040
R_1 / wR_2 (all data)	0.1635/ 0.1826	0.0808 / 0.2183	0.1000 / 0.2287

ORTEP Diagram of Compound 2a and 2e

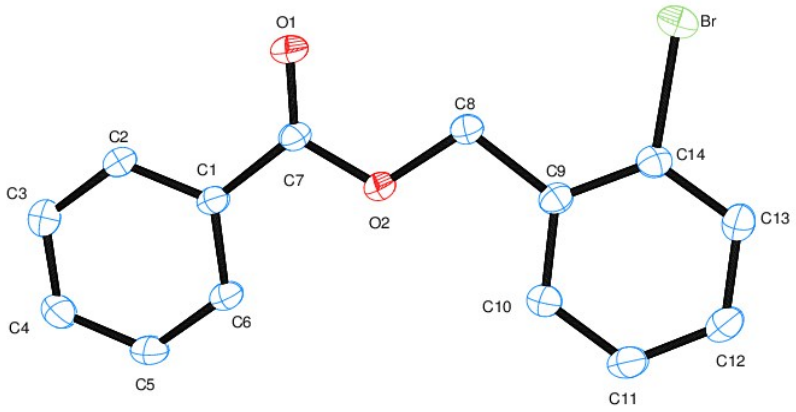


Figure S1. ORTEP diagram of compound **2a** with thermal ellipsoids at 30% probability (H not shown for clarity)

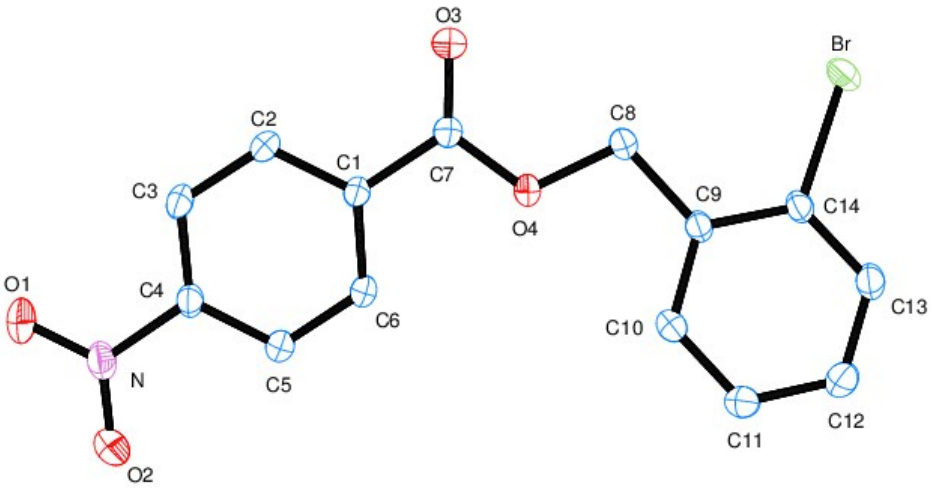


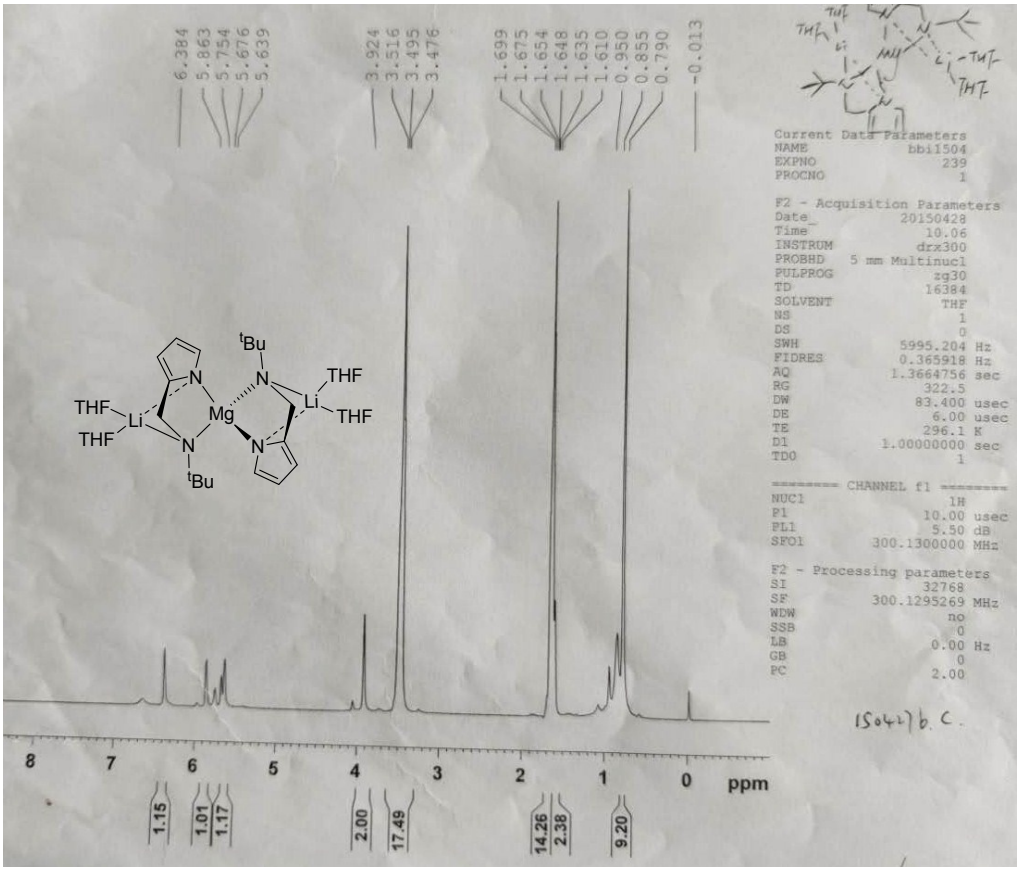
Figure S2. ORTEP diagram of compound **2e** with thermal ellipsoids at 30% probability (H not shown for clarity)

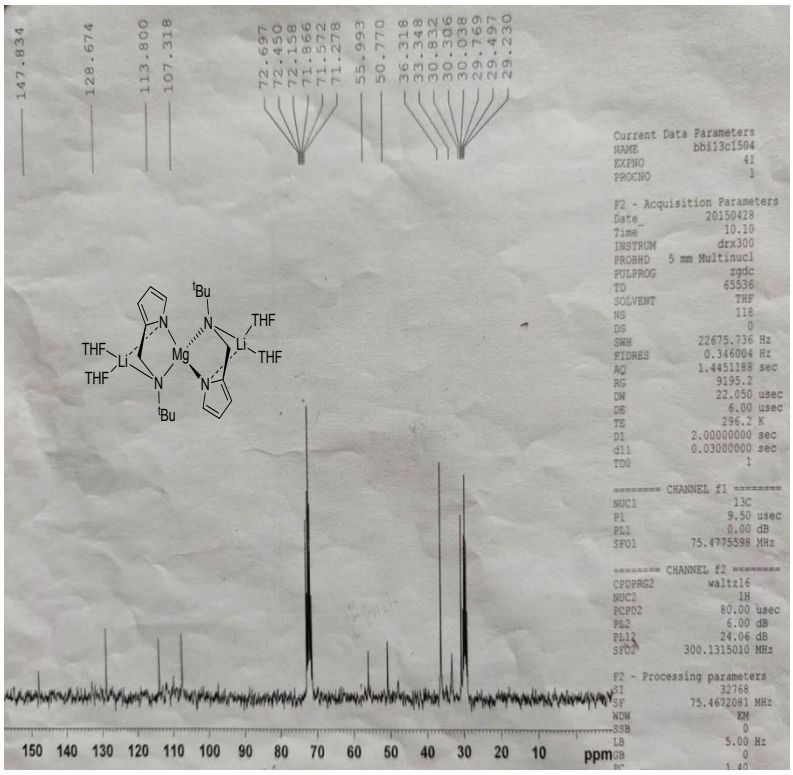
Crystal Data and Structure Refinement Details of 2a and 2e

Table S2. Single crystal X-ray data and structure refinement details for **2a** and **2e**

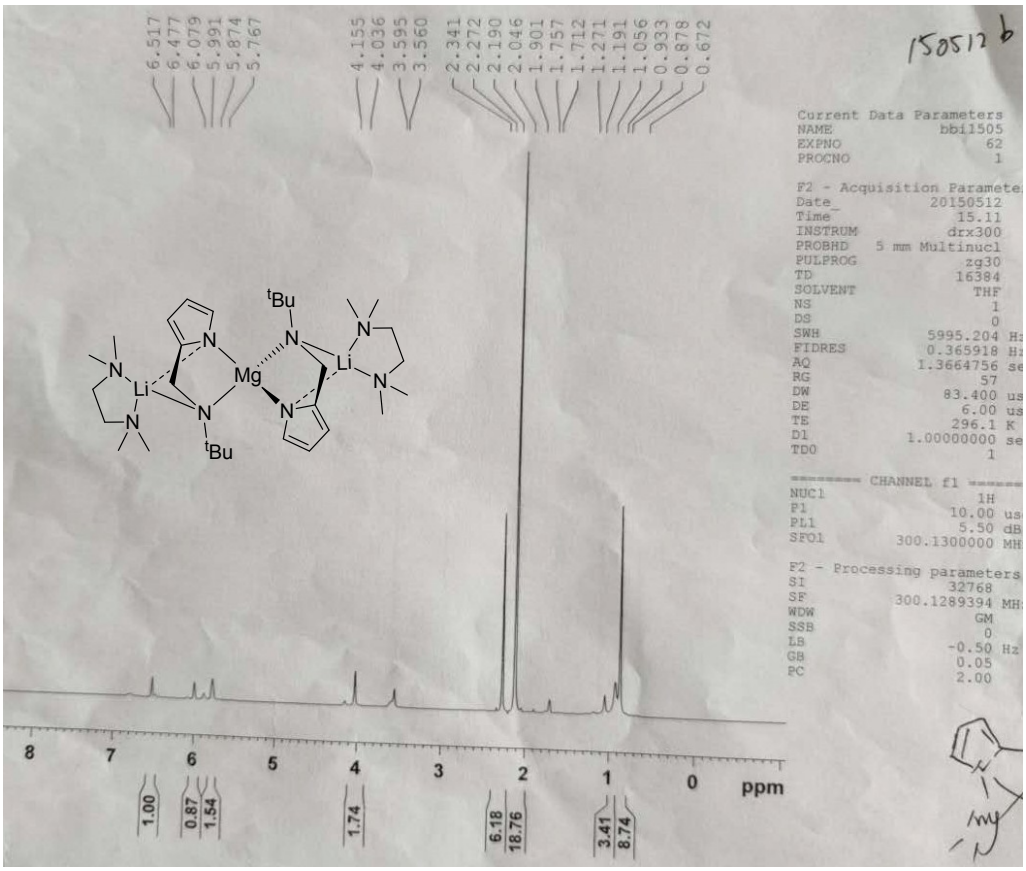
Complex	**2a**	**2e**
Empirical formula	$C_{14}H_{11}BrO_2$	$C_{14}H_{10}BrNO_4$
Formula weight	291.14	336.14
Temperature (K)	296(2)	298(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
space group	P-1	P-1
a (Å)	8.2096(12)	7.1524(7)
b (Å)	8.2608(12)	9.2277(10)
c (Å)	9.3910(13)	10.9410(11)
α (deg)	76.231(6)	76.639(4)
β (deg)	81.102(5)	70.963(4)
γ (deg)	84.399(5)	77.997(3)
Volume ($Å^3$)	609.90(15)	657.20(12)
Z	2	2
D_c (g/cm^{-3})	1.585	1.699
M (mm^{-1})	3.356	3.140
F(000)	292	336
Crystal size (mm)	0.31 x 0.30 x 0.25	0.30 x 0.20 x 0.20
Theta range for data collection	2.99 to 28.29 deg.	3.12 to 34.75 deg.
Reflections collected / unique	9515 / 2107 [R(int) = 0.0501]	13798 / 2298 [R(int) = 0.0277]
Completeness to theta = 25.05	98.5 %	98.8 %
Max. and min. transmission	0.488 and 0.423	0.572 and 0.453
Data / restraints / parameters	2107 / 0 / 155	2293 / 0 / 182
Goodness-of-fit	1.129	1.06
R_1 / wR_2 [I>2sigma(I)]	0.0448 / 0.0859	0.0248 / 0.0816
R_1 / wR_2 (all data)	0.0567 / 0.0899	0.0269 / 0.0851

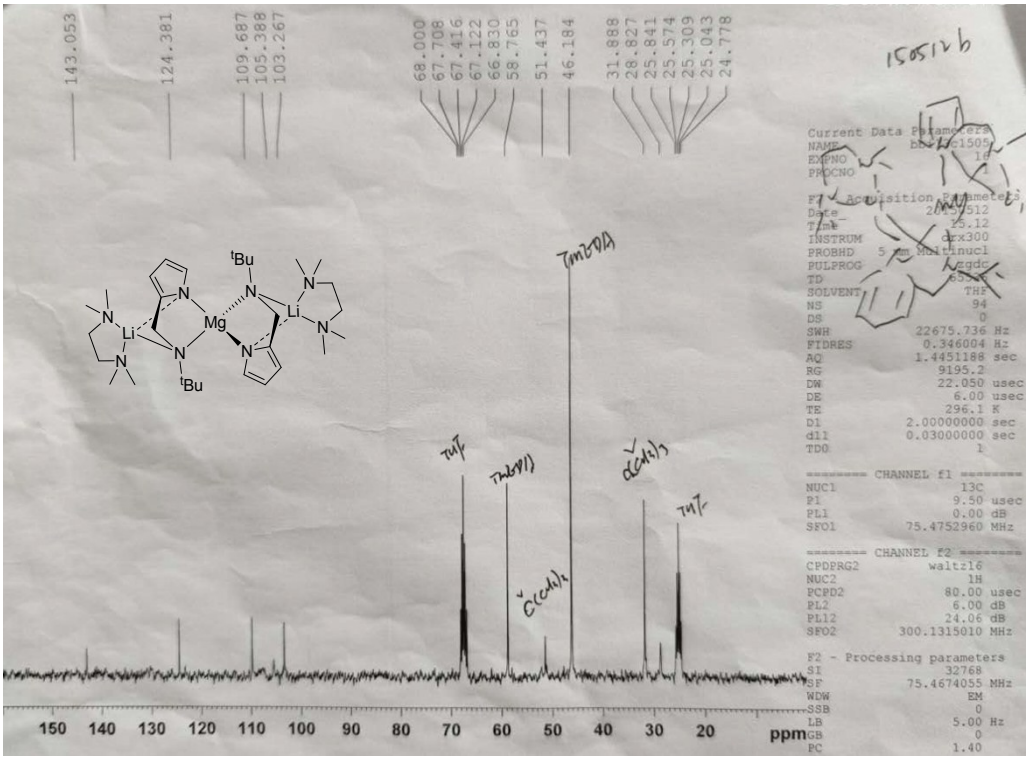
^{1}H and ^{13}C NMR Spectra of Alkali-metal Organomagnesiate Complexes



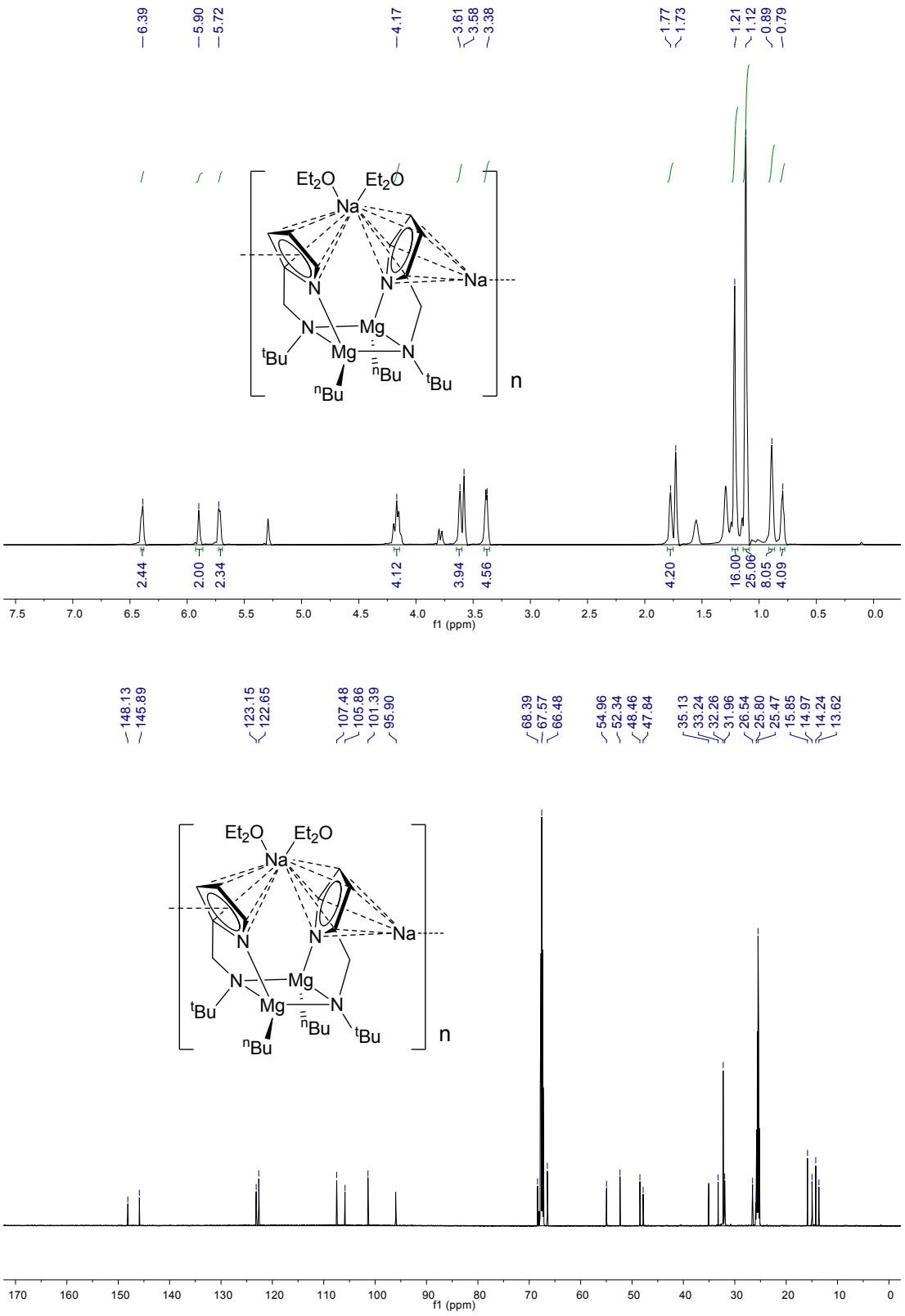


^{1}H NMR and ^{13}C NMR spectrum of complex (**1**) in d_8-THF

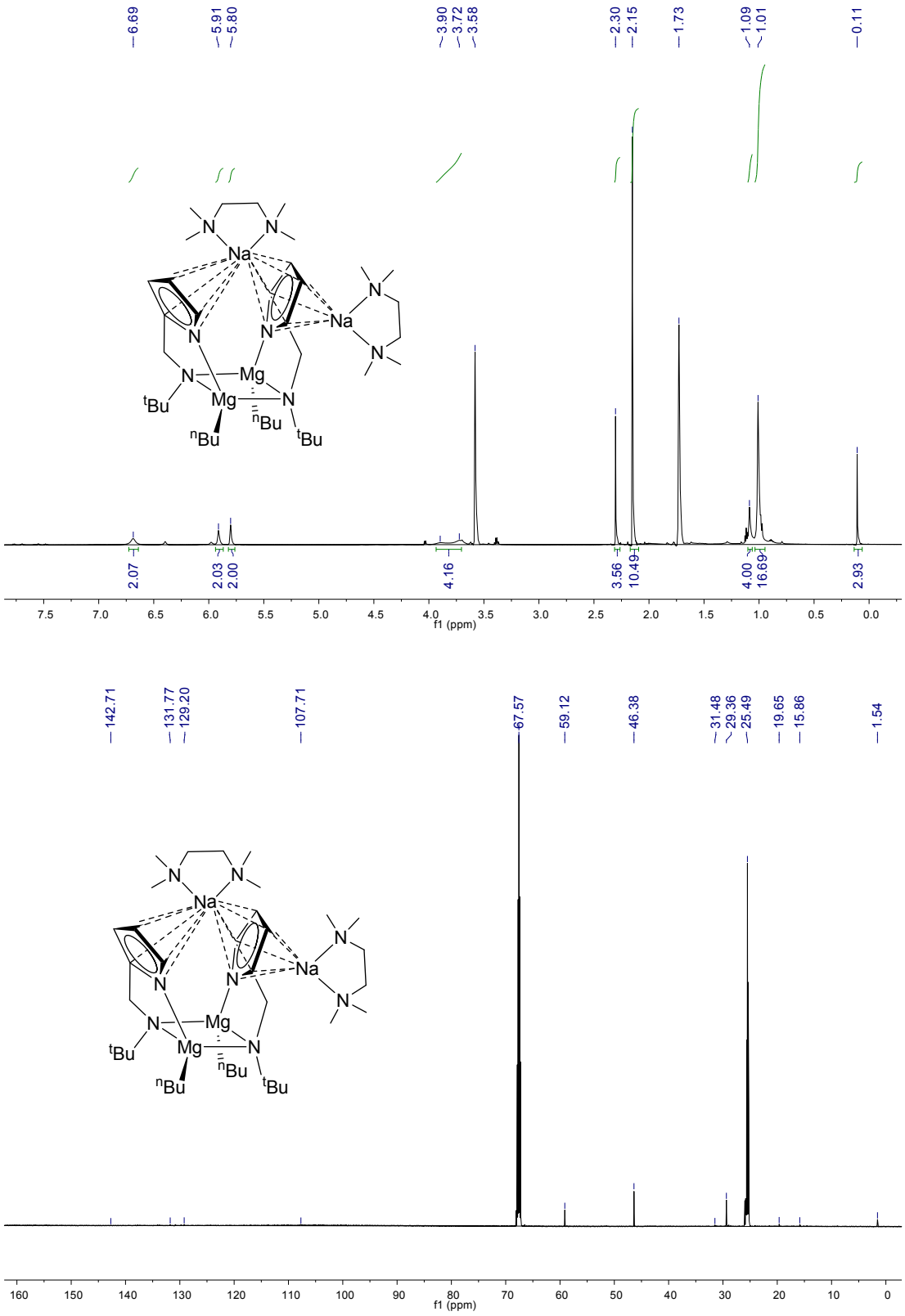




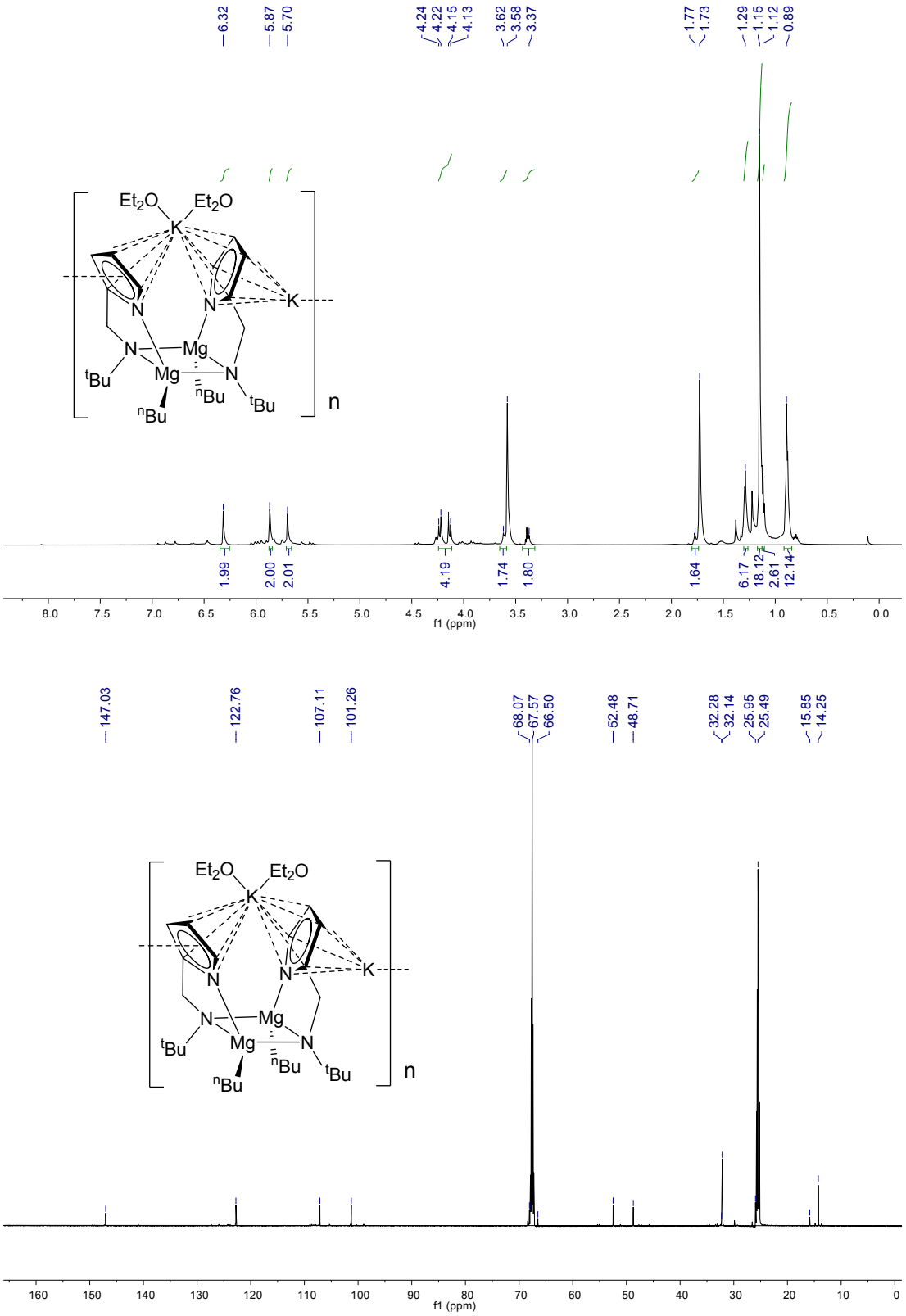
^{1}H NMR and ^{13}C NMR spectrum of complex (**2**) in d_8-THF



^{1}H NMR and ^{13}C NMR spectrum of complex (**3**) in d_8-THF



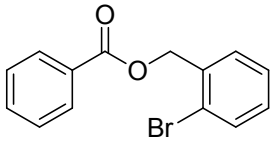
^{1}H NMR and ^{13}C NMR spectrum of complex (**4**) in d_8-THF



^{1}H NMR and ^{13}C NMR spectrum of complex (**5**) in d_8-THF

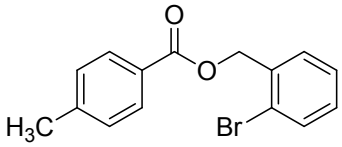
Characterization Data of the Ester Compounds

(The ester compounds were identified through comparisons with the corresponding ^{1}H NMR, ^{13}C NMR data reported in the literatures.)



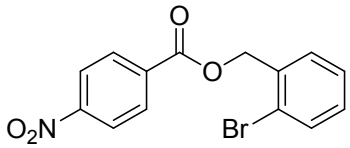
2-bromobenzyl benzoate[1]

White solid, yield: 58%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, J = 7.5 Hz, 2H), 7.61 (d, J = 8.0 Hz, 1H), 7.58 (t, J = 7.4 Hz, 1H), 7.51 (d, J = 7.6 Hz, 1H), 7.46 (t, J = 7.7 Hz, 2H), 7.34 (t, J = 7.5 Hz, 1H), 7.22 (t, J = 7.7 Hz, 1H), 5.46 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.33 (s), 135.55 (s), 133.30 (s), 133.06 (s), 129.98 (dd, J = 22.7, 4.8 Hz), 128.58 (s), 127.67 (s), 123.65 (s), 66.37 (s).



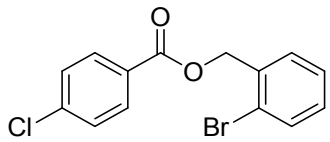
2-bromobenzyl-4-methylbenzoate

Colourless liquid, yield: 54%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, J = 8.2 Hz, 2H), 7.59 (d, J = 8.0 Hz, 1H), 7.49 (d, J = 7.7 Hz, 1H), 7.32 (t, J = 8.0 Hz, 1H), 7.24 (d, J = 7.9 Hz, 2H), 7.19 (t, J = 7.7 Hz, 1H), 5.42 (s, 2H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.36 (s), 143.99 (s), 135.67 (s), 132.99 (s), 130.02-129.68 (m), 129.27 (s), 127.63 (s), 127.30 (s), 123.54 (s), 66.15 (s), 21.78 (s).



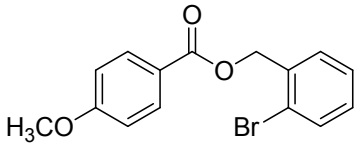
2-bromobenzyl-4-nitrobenzoate

Yellow solid, yield: 65%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (dd, J = 22.9, 9.0 Hz, 4H), 7.63 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.36 (t, J = 7.5 Hz, 1H), 7.27-7.23 (m, 1H), 5.49 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.47 (s), 150.77 (s), 135.43 (s), 134.73 (s), 133.25 (s), 131.03 (s), 130.58 (s), 130.39 (s), 127.79 (s), 124.05 (s), 123.74 (s), 67.33 (s).



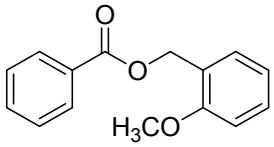
2-bromobenzyl-4-chlorobenzoate [2]

Colourless liquid, yield: 69%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.6 Hz, 2H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 8.6 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.22 (t, *J* = 7.7 Hz, 1H), 5.44 (s, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.49 (s), 139.78 (s), 135.27 (s), 133.12 (s), 131.30 (s), 130.21 (s), 130.05 (s), 128.94 (s), 128.50 (s), 127.71 (s), 123.79 (s), 66.63 (s).



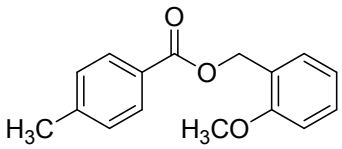
2-bromobenzyl-4-methoxybenzoate

Colourless liquid, yield: 48%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.9 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 6.93 (d, *J* = 8.9 Hz, 2H), 5.41 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.04 (s), 163.66 (s), 135.77 (s), 132.99 (s), 131.94 (s), 129.91 (s), 129.75 (s), 127.63 (s), 123.54 (s), 122.44 (s), 113.81 (s), 66.05 (s), 55.57 (s).



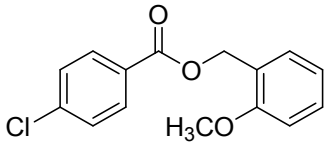
2-Methoxybenzyl benzoate [2]

Colourless liquid, yield: 72%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 8.4, 1.3 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.44-7.40 (m, 3H), 7.31 (t, *J* = 7.9 Hz, 1H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 5.42 (s, 2H), 3.84 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.64 (s), 157.61 (s), 132.97 (s), 130.51 (s), 129.80 (s), 129.54 (d, *J* = 11.0 Hz), 128.42 (s), 124.46 (s), 120.53 (s), 110.56 (s), 62.28 (s), 55.53 (s).



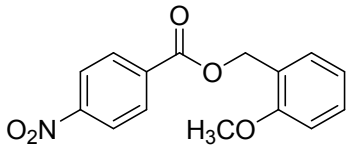
2-Methoxybenzyl-4-methylbenzoate[3]

Colourless liquid, yield: 75%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.89 (d, *J* = 8.2 Hz, 1H), 5.40 (s, 2H), 3.83 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.65 (s), 157.52 (s), 143.57 (s), 129.79 (s), 129.40 (d, *J* = 14.3 Hz), 129.10 (s), 127.73 (s), 124.64 (s), 120.48 (s), 110.49 (s), 62.03 (s), 55.46 (s), 21.70 (s).



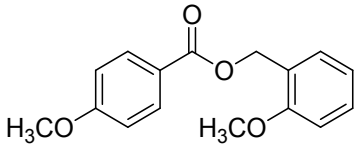
2-methoxybenzyl-4-chlorobenzoate[2]

White solid, yield: 79%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.03-7.99 (m, 2H), 7.42-7.38 (m, 3H), 7.33 (td, *J* = 8.1, 1.7 Hz, 1H), 6.97 (t, *J* = 7.1 Hz, 1H), 6.92 (d, *J* = 8.2 Hz, 1H), 5.41 (s, 2H), 3.86 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.85 (s), 157.74 (s), 139.45 (s), 131.25 (s), 129.78 (d, *J* = 9.6 Hz), 129.01 (s), 128.81 (s), 124.28 (s), 120.59 (s), 110.65 (s), 62.61 (s), 55.60 (s).



2-Methoxybenzyl-4-nitrobenzoate[3]

White solid, yield: 66%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.25 (d, *J* = 15.4 Hz, 4H), 7.45-7.31 (m, 2H), 7.02-6.89 (m, 2H), 5.46 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.79 (s), 157.86 (s), 150.61 (s), 135.95 (s), 130.94 (s), 130.14 (d, *J* = 12.1 Hz), 123.64 (d, *J* = 7.4 Hz), 120.61 (s), 110.72 (s), 63.35 (s), 55.60 (s).



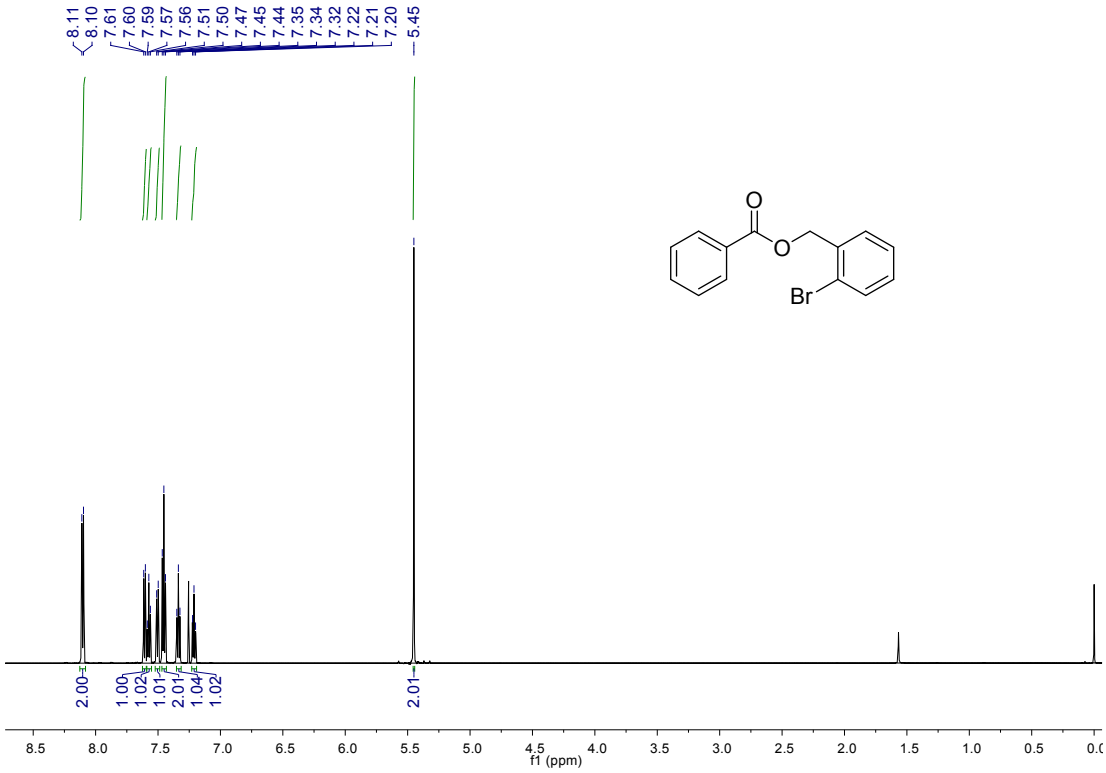
2-methoxybenzyl 4-chlorobenzoate[2]

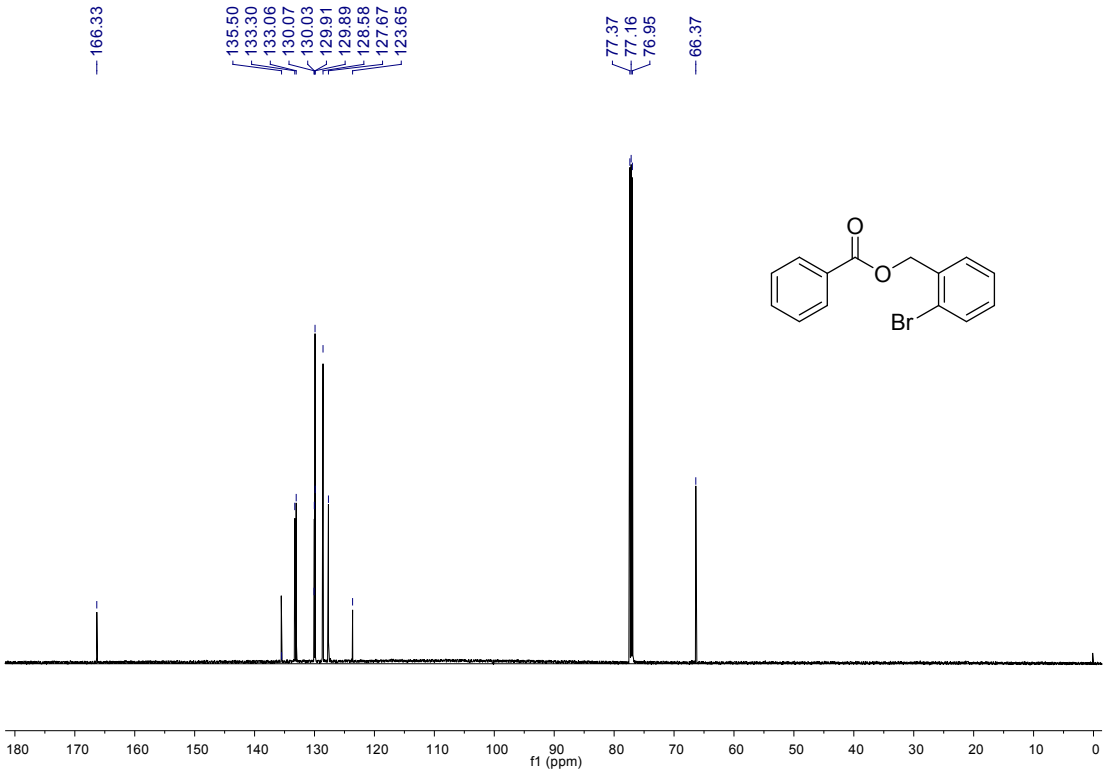
White solid, yield: 65%. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 9.0 Hz, 2H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.32-7.28 (m, 1H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.91 (t, *J* = 5.9 Hz, 3H), 5.39 (s, 2H), 3.84 (d, *J* = 3.6 Hz, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.39 (s),

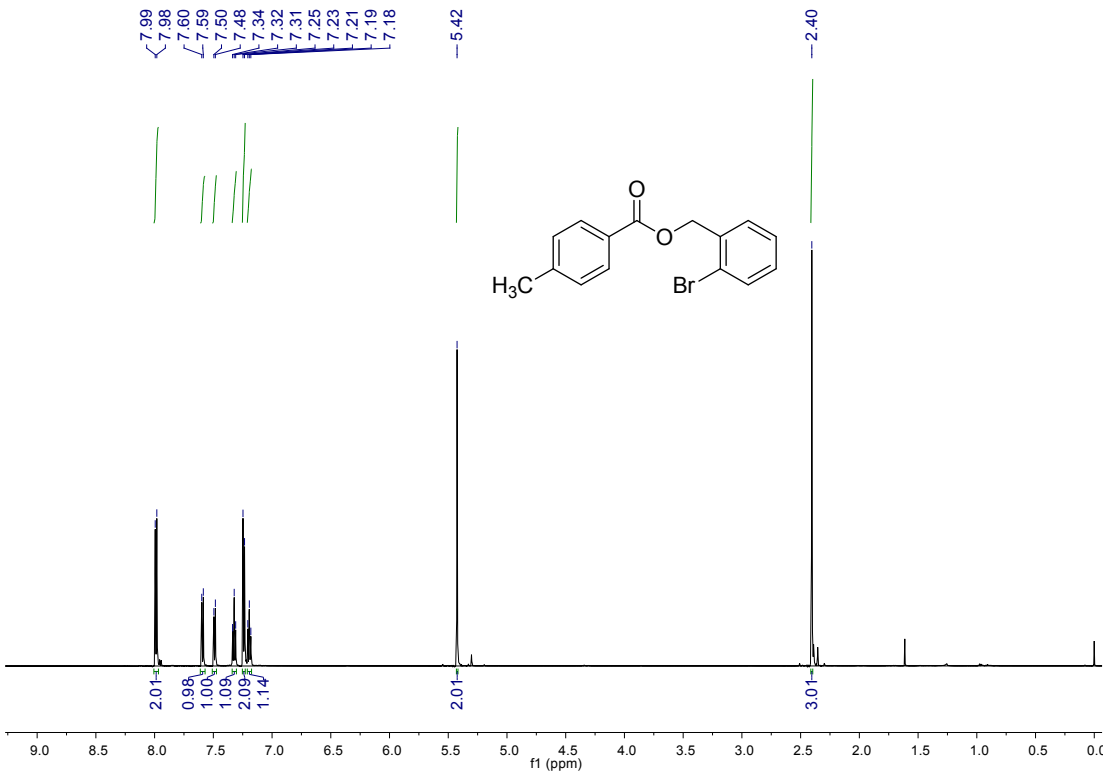
163.42 (s), 157.55 (s), 131.82 (s), 129.41 (d, J = 10.4 Hz), 124.76 (s), 122.94 (s), 120.52 (s), 113.66 (s), 110.53 (s), 61.96 (s), 55.53 (d, J = 4.7 Hz).

References

^{1}H and ^{13}C NMR Spectra of the Ester Compounds



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7.18
5.42
2.40
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O
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Br
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1.00
1.05
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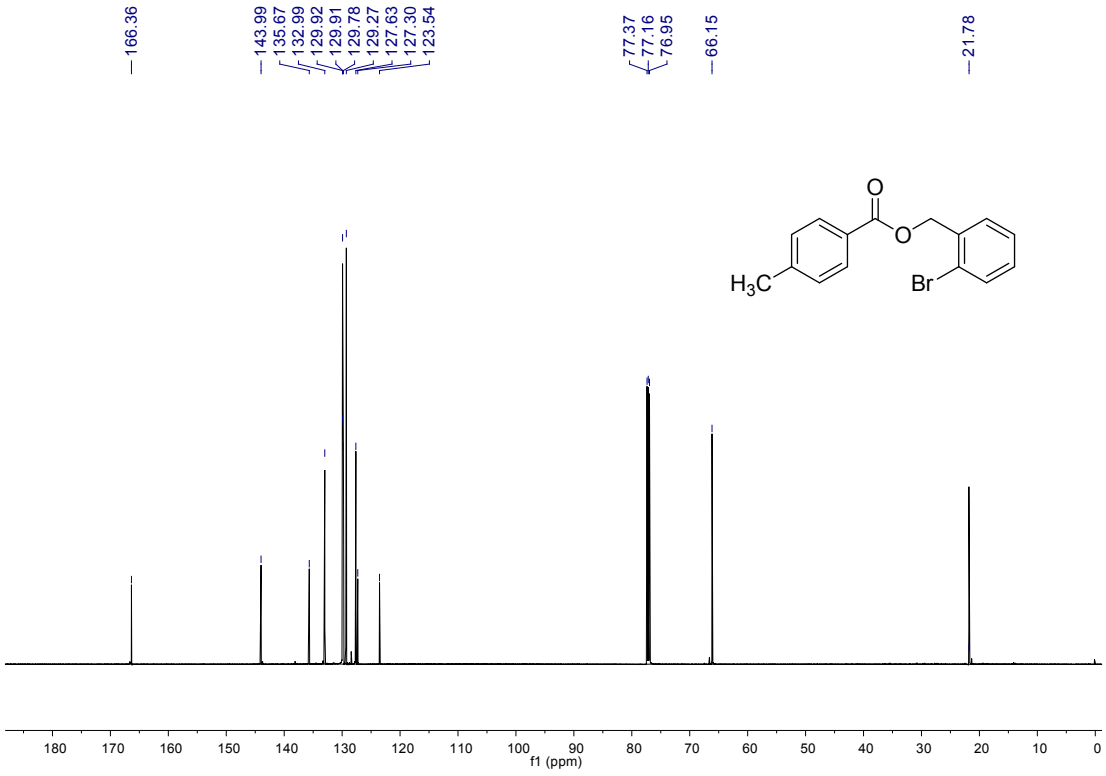
1.14
2.01
3.01
f1 (ppm)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O
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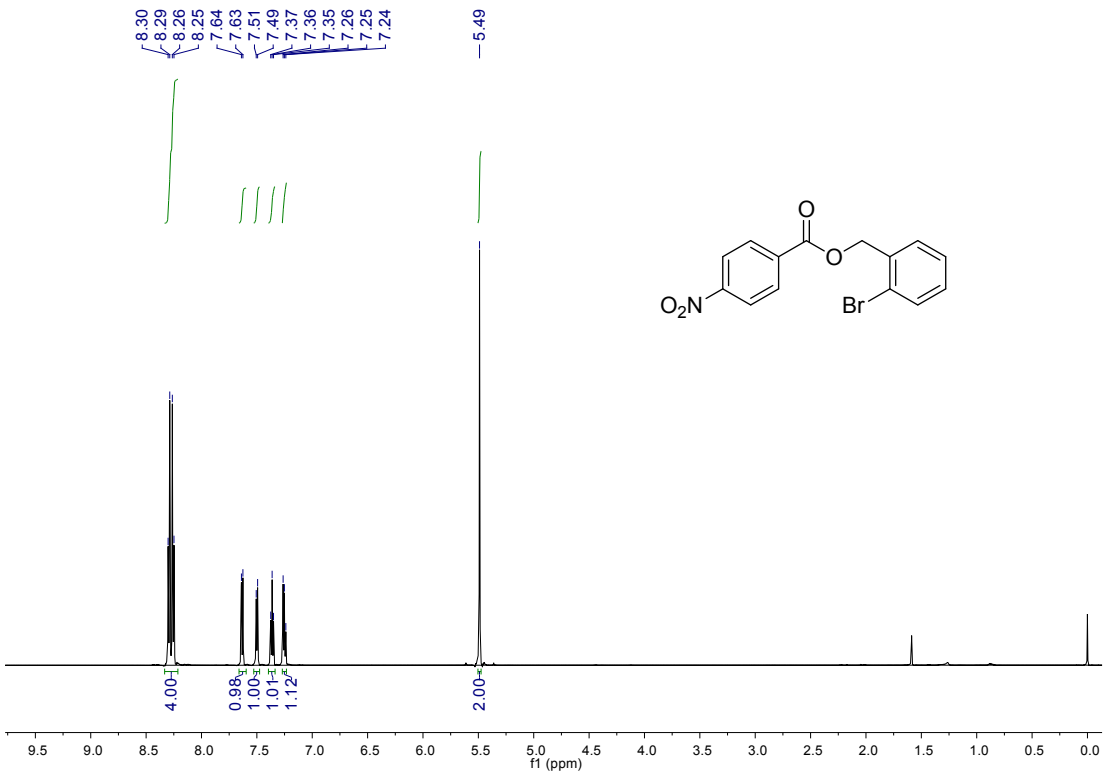
Br
f1 (ppm)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7.25
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2.00
f1 (ppm)
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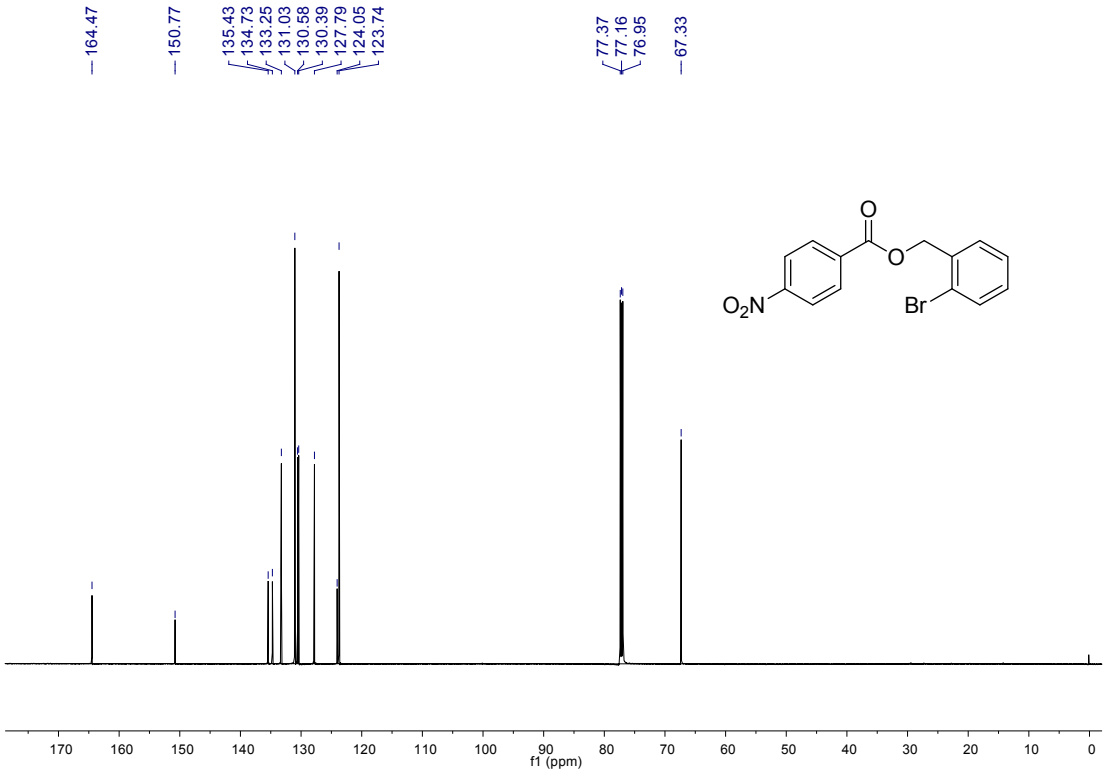
O
O2N
Br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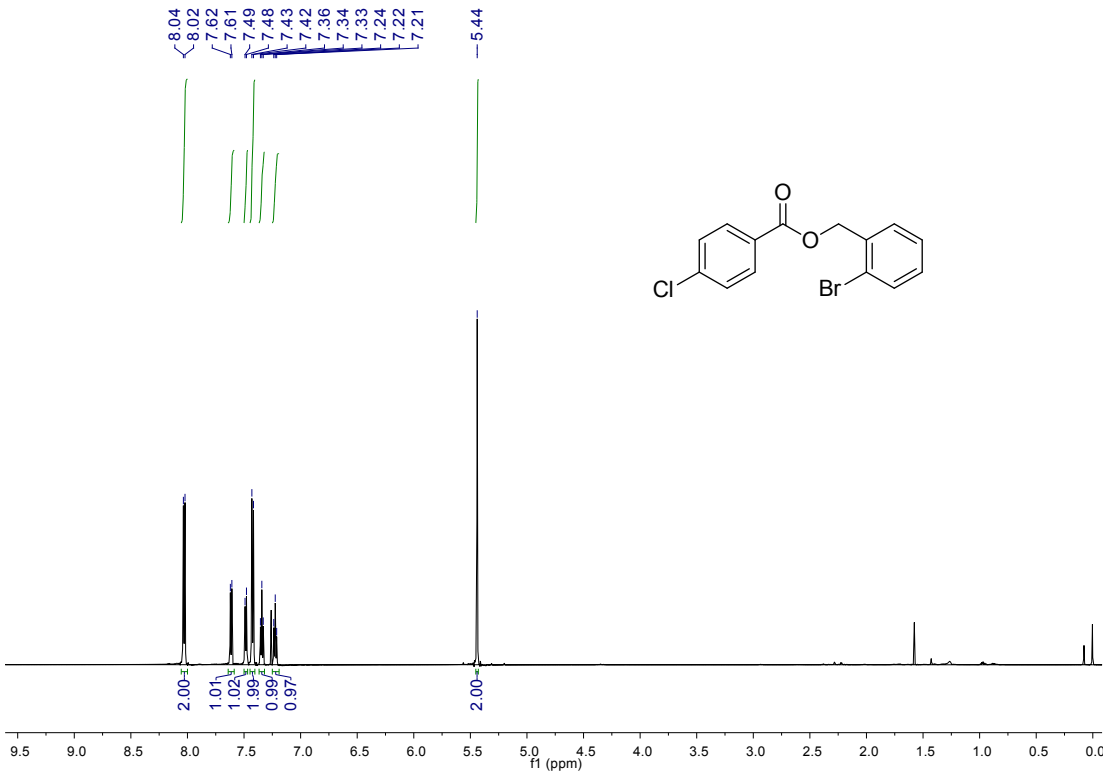
67.33
f1 (ppm)
O
O
O2N
Br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Br
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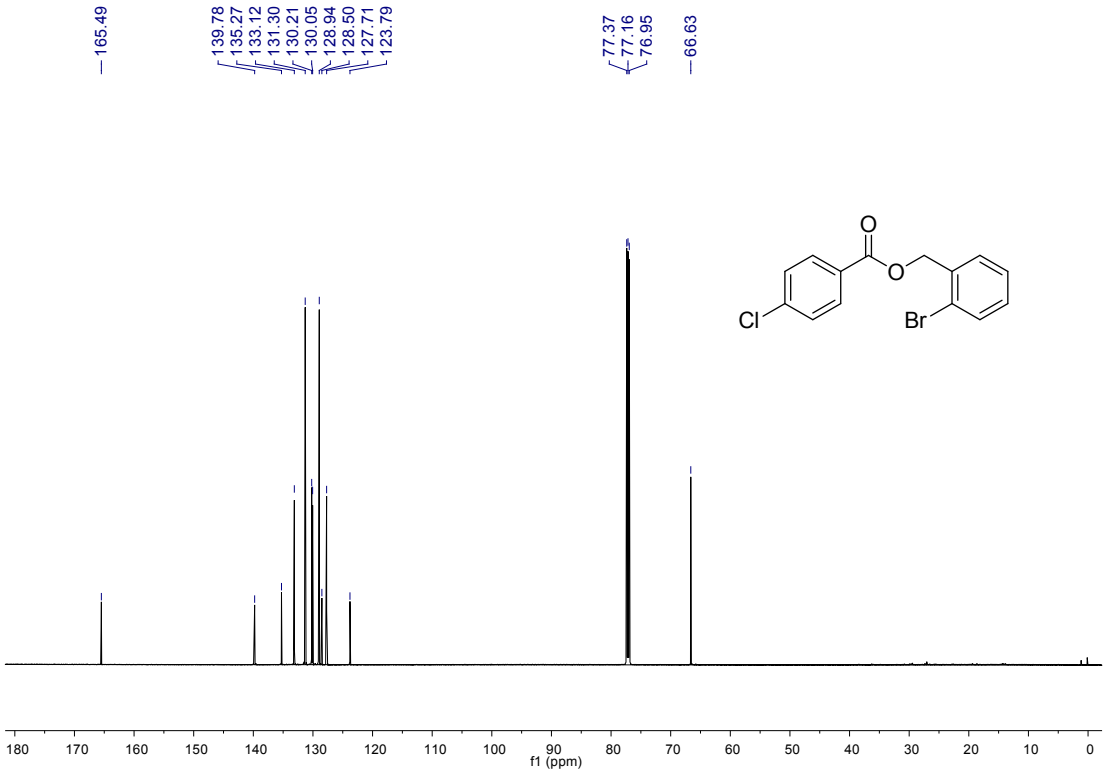
2.00
f1 (ppm)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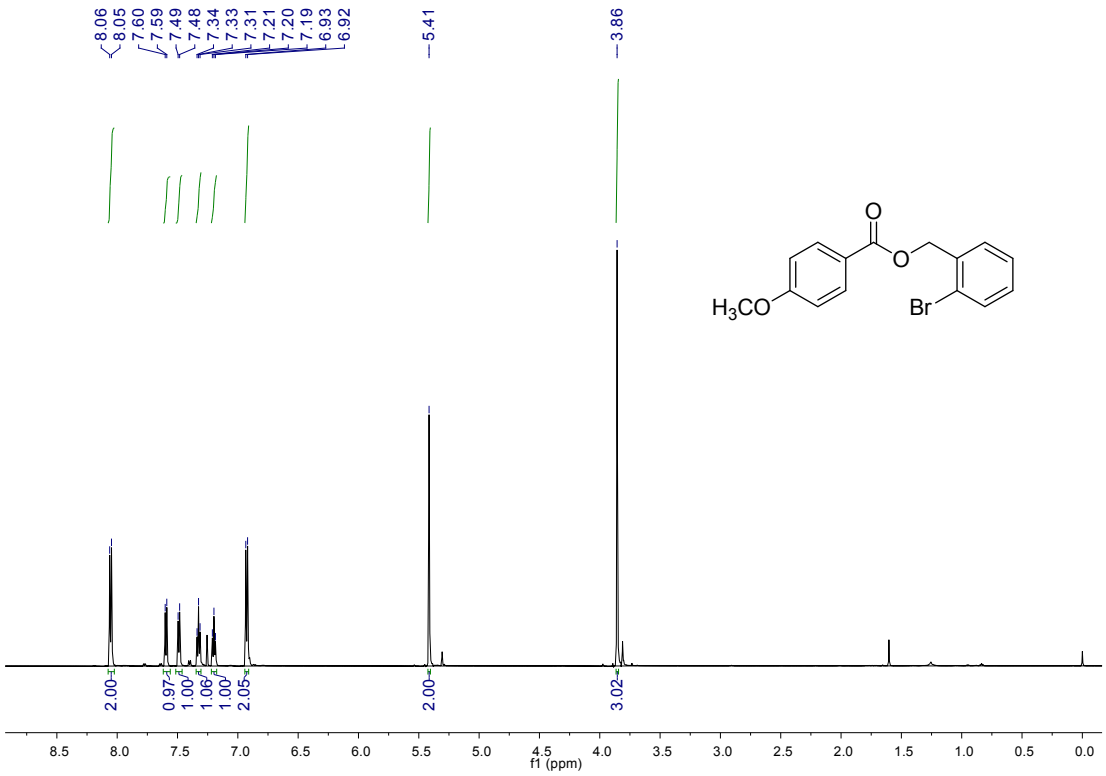
Cl
Br
f1 (ppm)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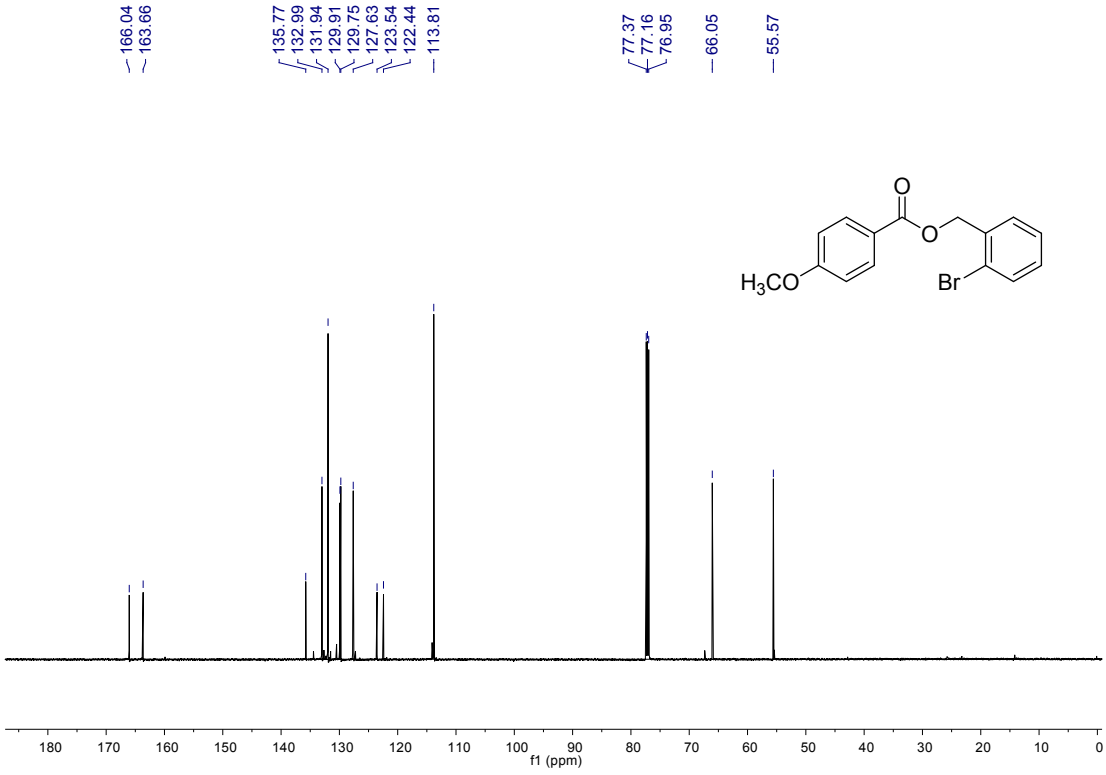
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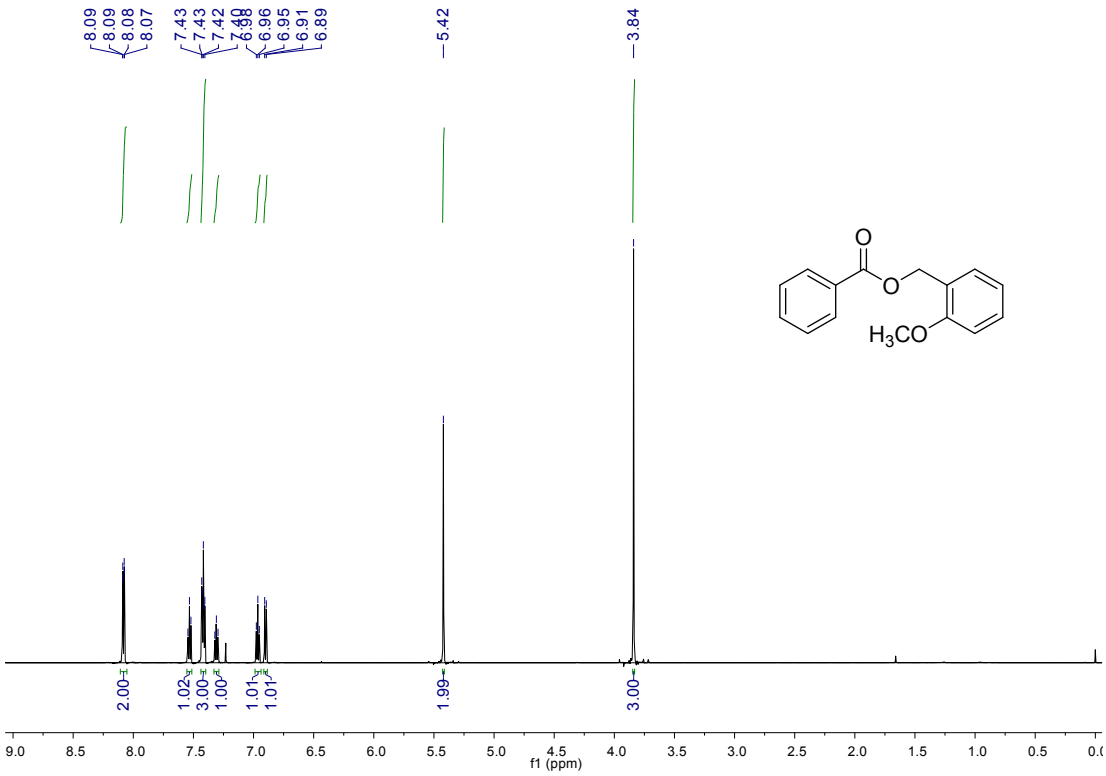
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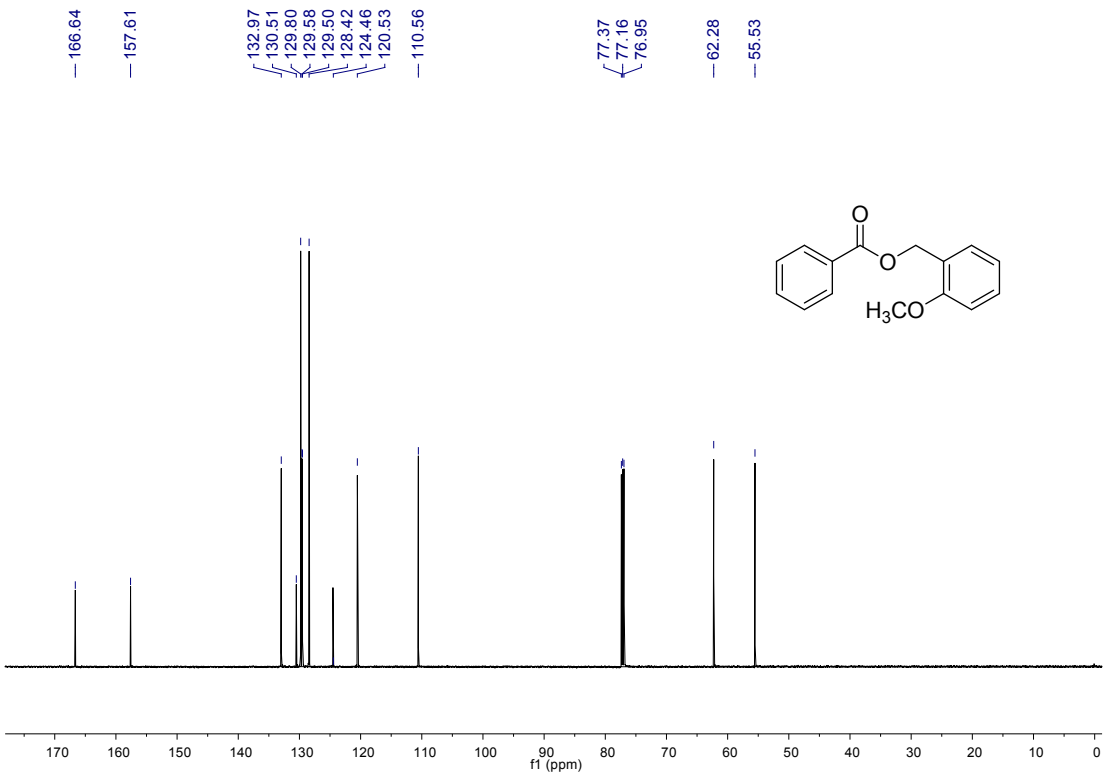
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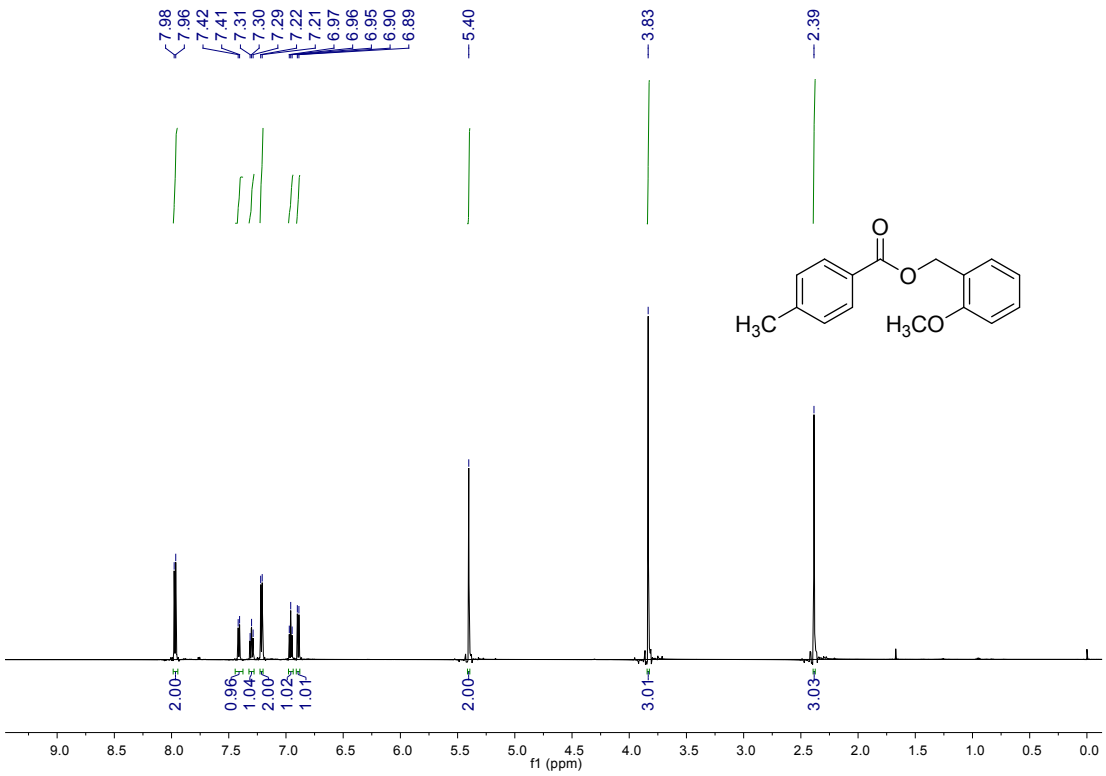
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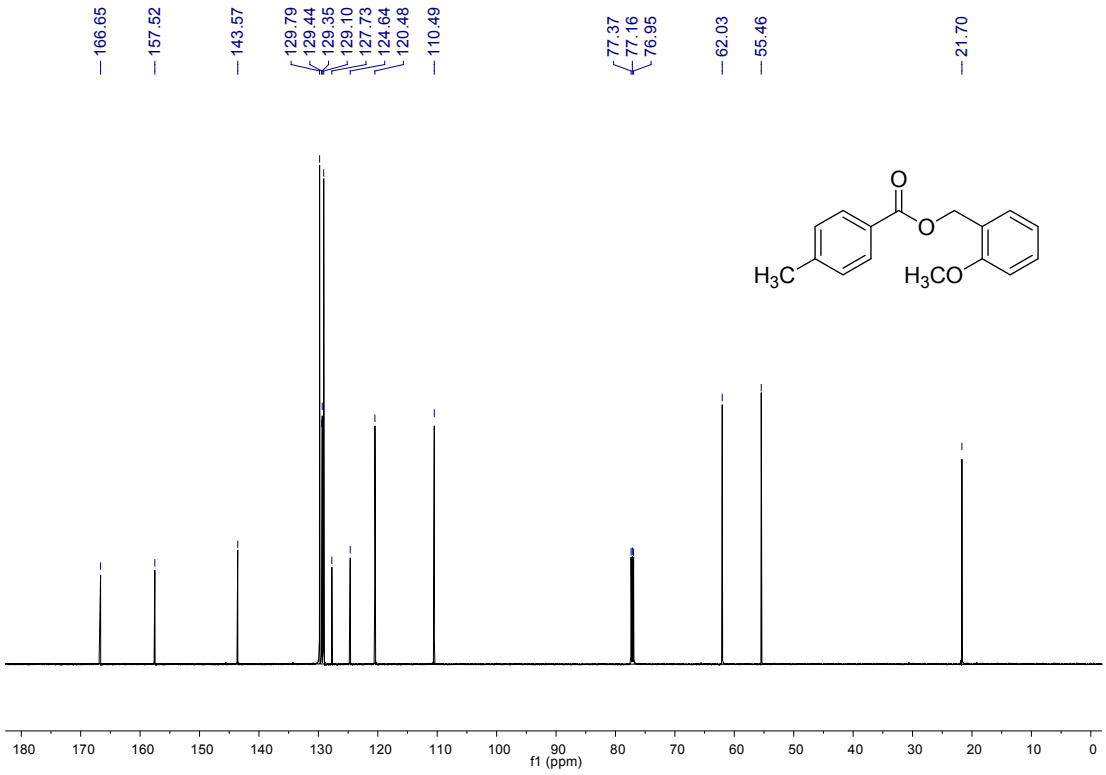
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H3CO
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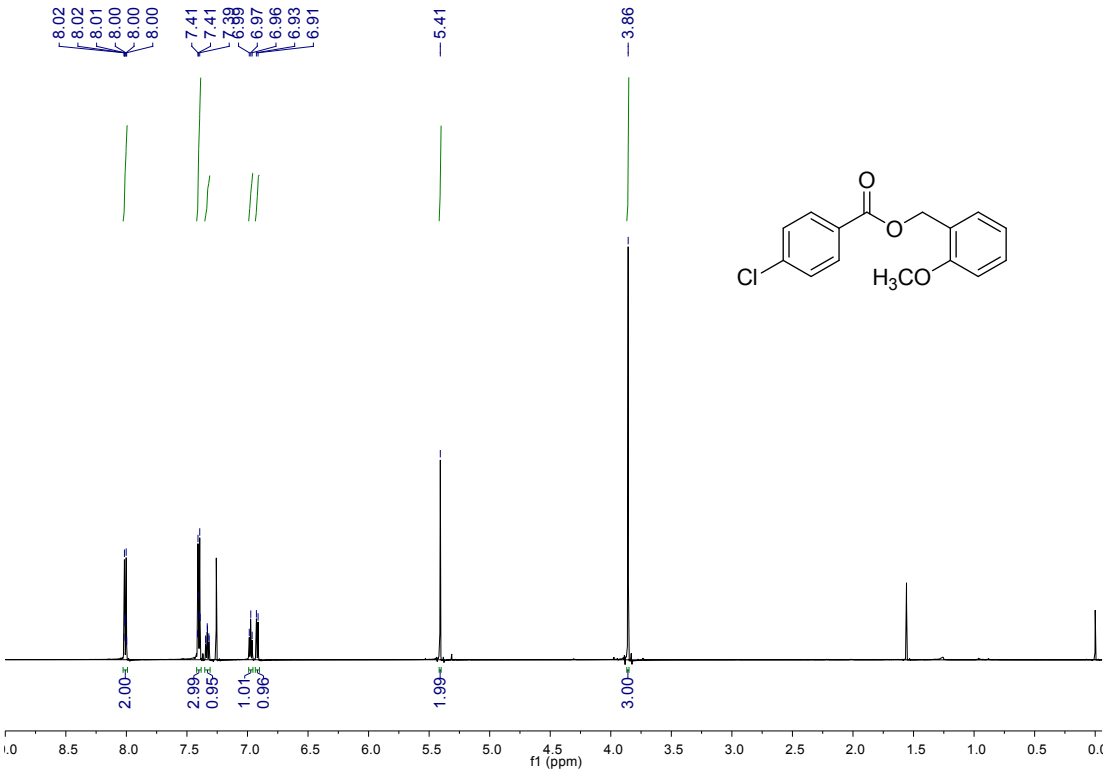
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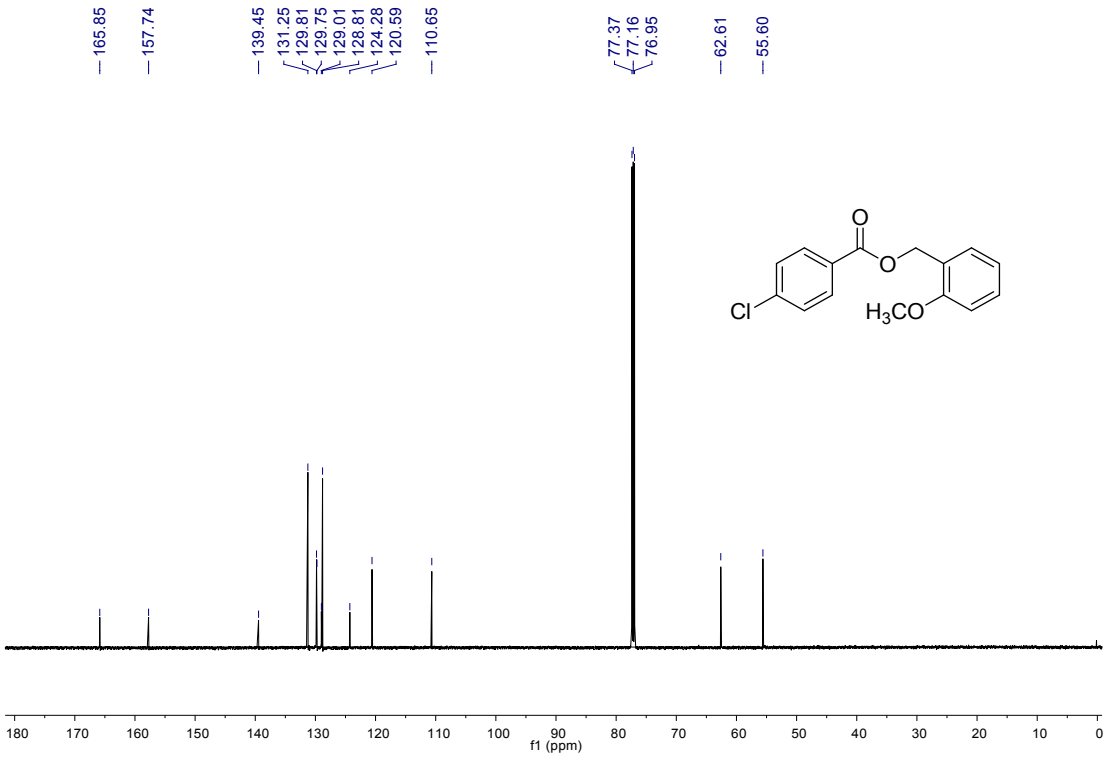
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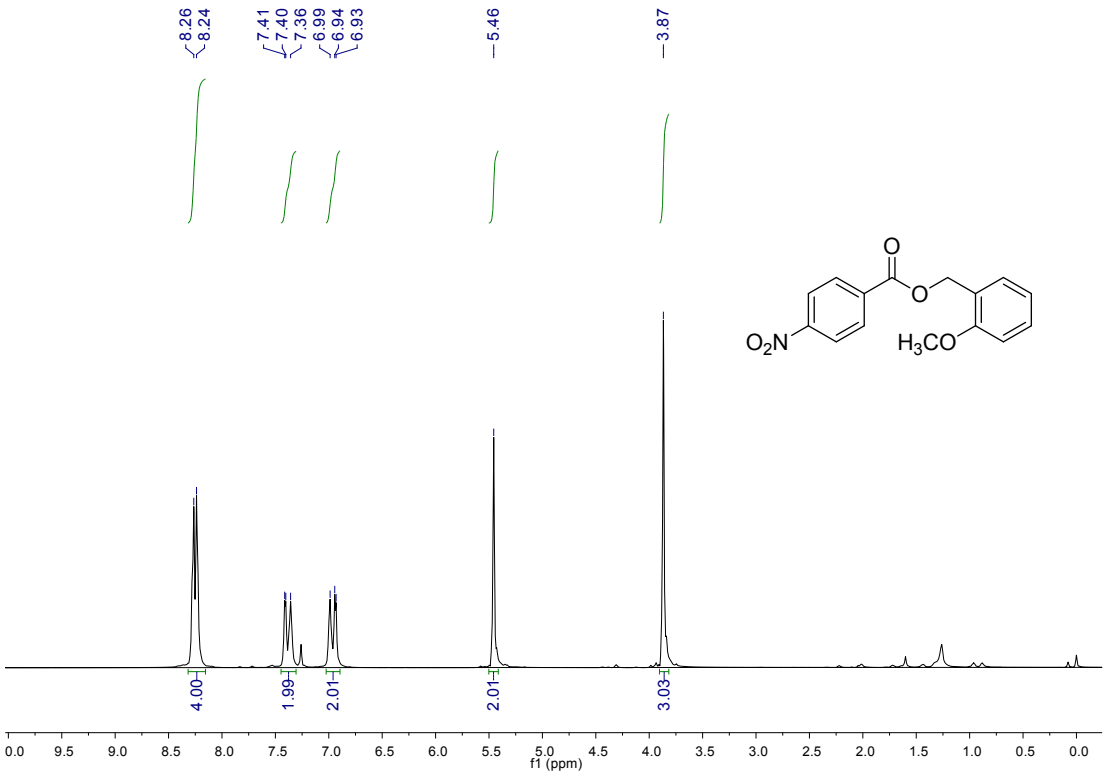
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2.01
3.03
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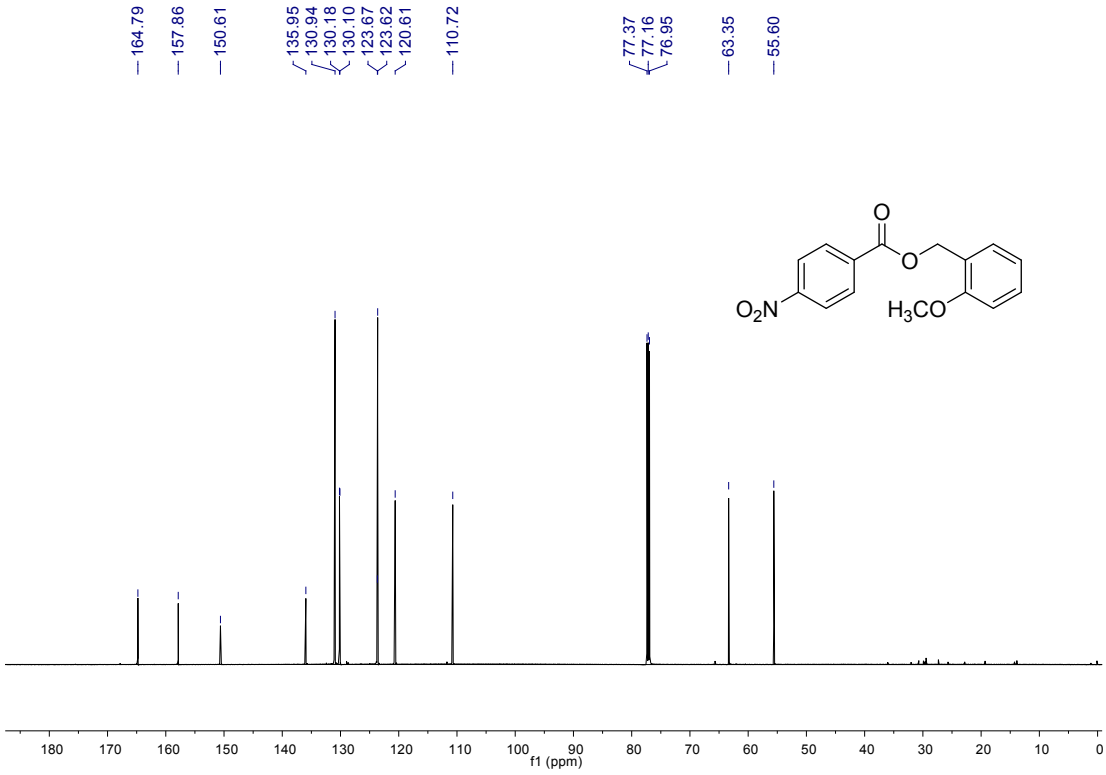
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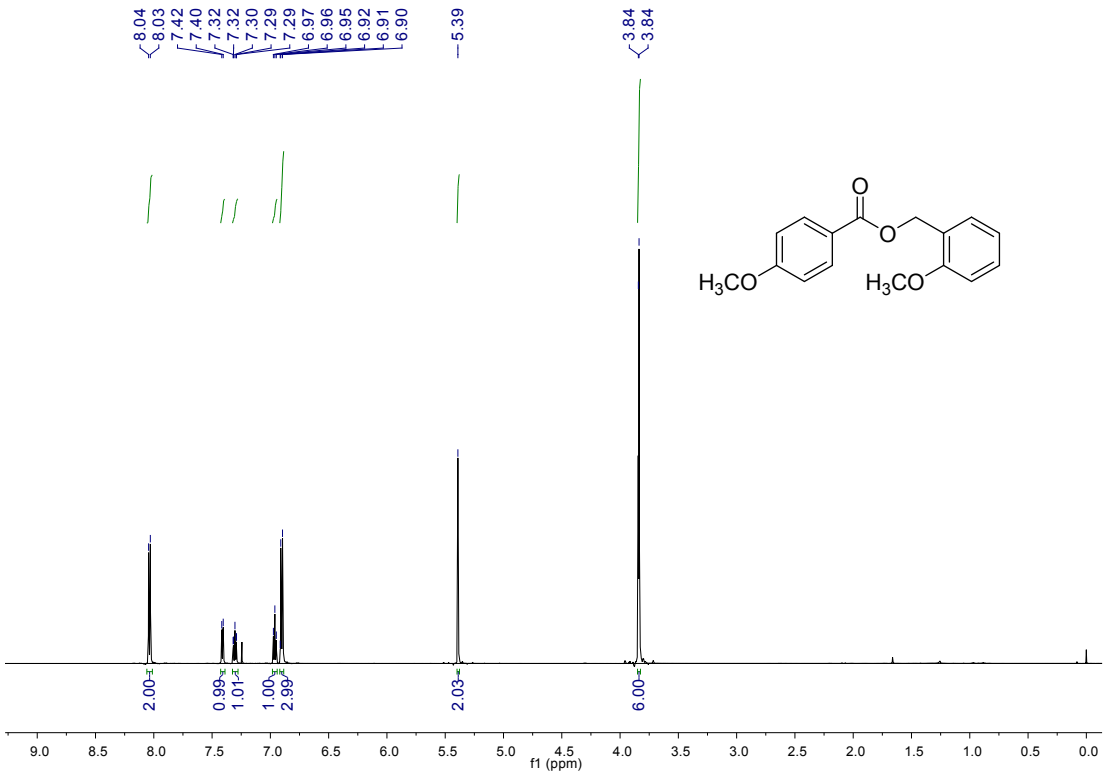
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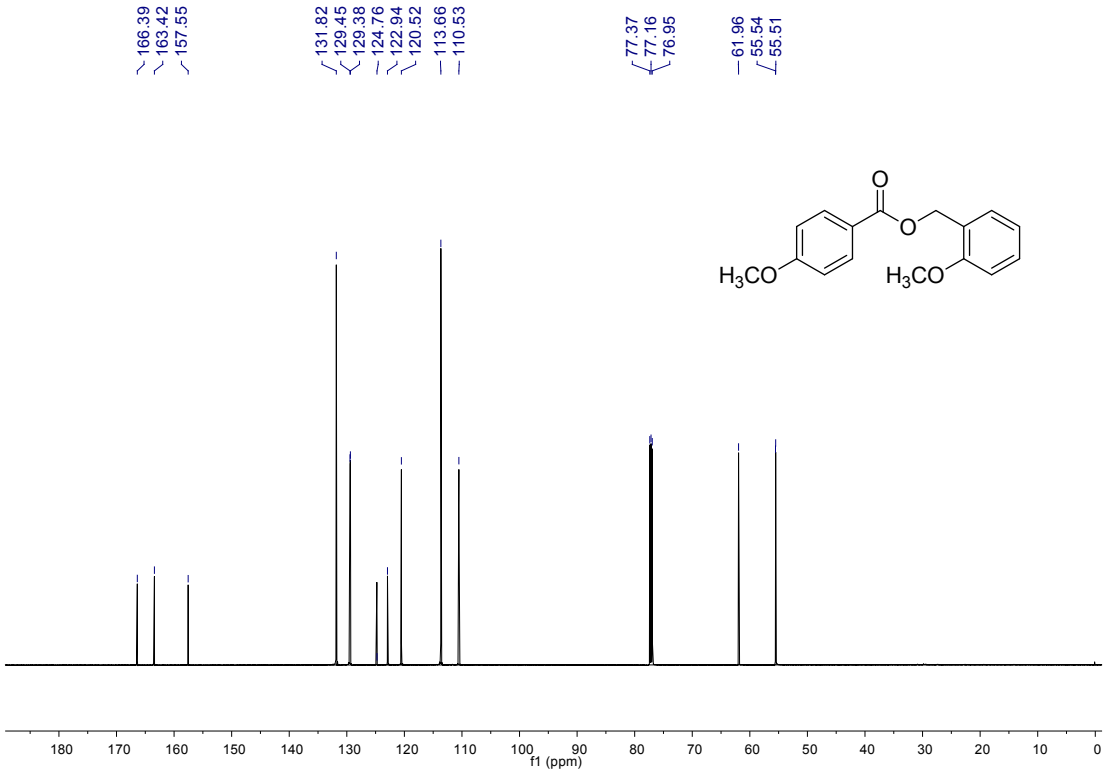
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H3CO
f1 (ppm)