ELECRONIC SUPPLEMENTARY INFORMATION

One Stone Two Birds：Cobalt Catalyzed *in situ* Generation of Isocyanate and Benzyl alcohol for the Synthesis of *N*-aryl Carbamates

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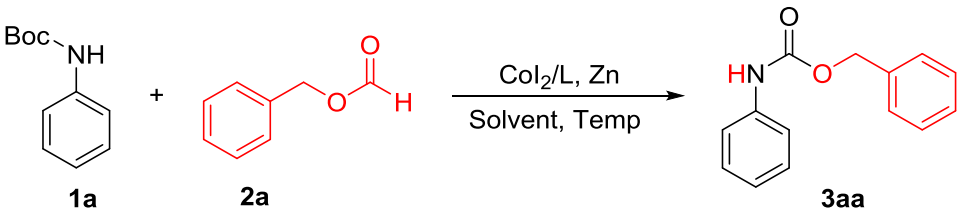
A: General Information

The reactions and manipulations were performed under an atmosphere of argon by using standard Schlenk techniques and glovebox (Mikrouna, Supper1220/750). Anhydrous toluene was distilled from sodium benzophenone ketyl prior to use. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-Avance 400 MHz spectrometer. $CDCl_3$ or CD_3OD were used as solvent. Chemical shifts (δ) were reported in ppm with tetramethylsilane as internal standard and *J* values were given in Hz. Melting points were measured on X-4 melting point apparatus and uncorrected. Column chromatography was performed with silica gel using petroleum ether and ethyl acetate as eluents.

B: Procedure of the reactions

Typical procedure for the synthesis of 3aa. CoI_2 (0.02 mmol), tris-(4-dimethylaminophenyl)-phosphine (0.048 mmol)，Zinc powder (0.6 mmol) and 1 mL of toluene were added to a Schlenk tube under an argon atmosphere in a glovebox. The mixture was stirred at room temperature for 30 min. Then *N*-Boc protected aniline **1a** (0.2 mmol), benzyl formate **2a** (0.6 mmol) and toluene (1 mL) were added. The reaction mixture was stirred under argon atmosphere at 120^{o}C for 24 h. After vacuum evaporation of the solvent, the residue was purified by silica gel column chromatography to provide the desired product **3aa** (42 mg, 92% yield).

C: Table S1: Screening of different Ligands and solvents[a]



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

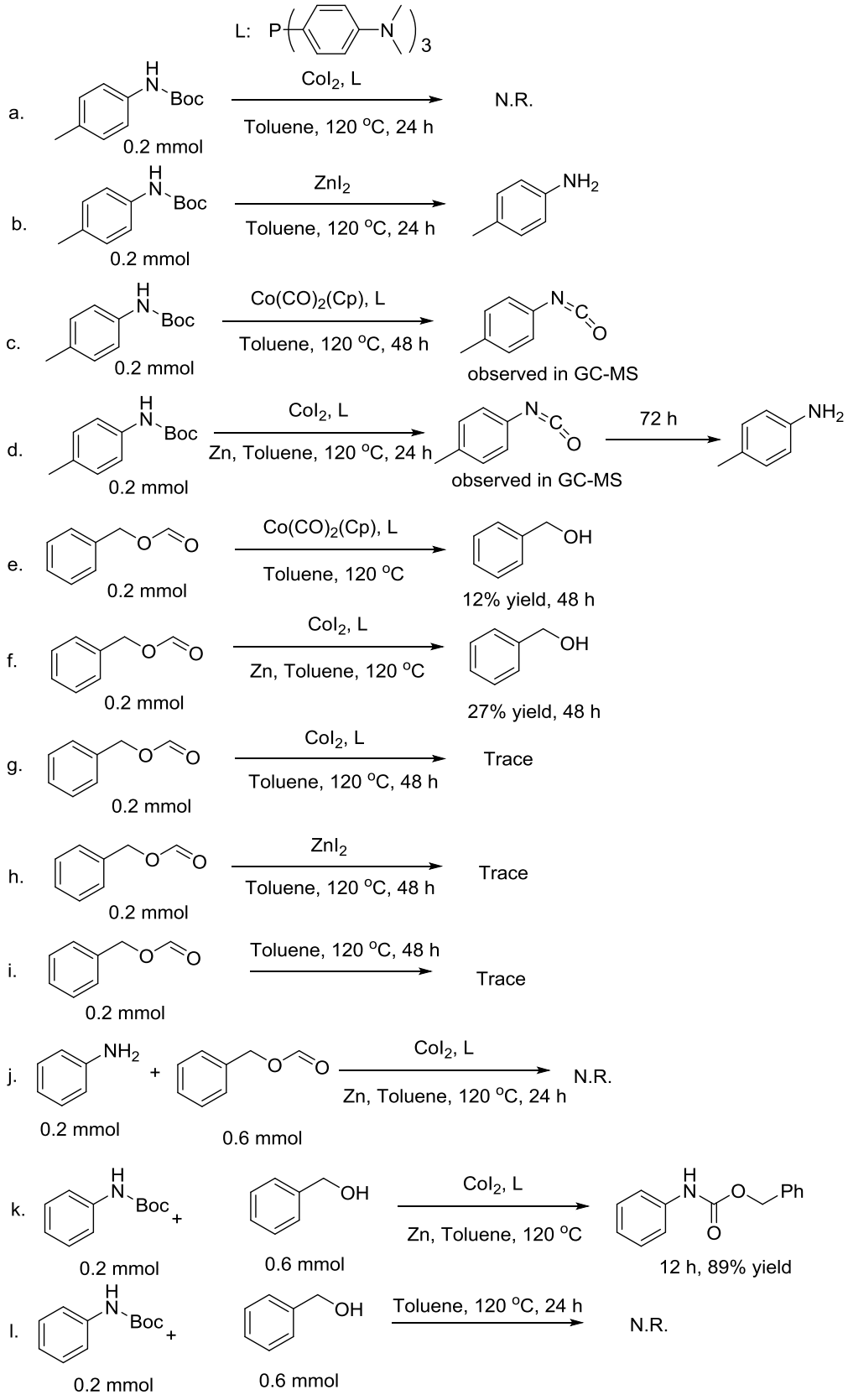
Entry	Ligand	Zinc (equiv)	Solvent	Temp (°C)	Time (h)	Yield (%)[b]
1	----	3	Toluene	100	72	39
2	Dppp	3	Toluene	100	48	53
3	Dppm	3	Toluene	100	24	74
4	Dppb	3	Toluene	100	72	Trace
5	Dppe	3	Toluene	100	72	71
6	PPh_3	3	Toluene	100	60	50
7	Tricyclohexyl phosphine	3	Toluene	100	72	89
8	1,10-Phenanthroline	3	Toluene	100	72	Trace
9	(±)-BINAP	3	Toluene	100	72	Trace
10	tris-(3,5-dimethylphenyl)-phosphine	3	Toluene	100	48	N.R.
11	tris-(4-methoxyphenyl)-phosphine	3	Toluene	100	48	80
12	tris-(4-dimethylaminophenyl)-phosphine	3	Toluene	100	72	93
13	tri-(furan-2-yl)-phosphine	3	Toluene	100	72	20
14	tris-(4-dimethylaminophenyl)-phosphine	3	1,4-dioxane	100	72	Trace
15	tris-(4-dimethylaminophenyl)-phosphine	3	DCE	100	72	Trace
16	tris-(4-dimethylaminophenyl)-phosphine	3	THF	100	72	Trace
17	tris-(4-dimethylaminophenyl)-phosphine	3	DMF	100	48	62
18	tris-(4-dimethylaminophenyl)-phosphine	3	DMSO	100	48	83
19	tris-(4-dimethylaminophenyl)-phosphine	3	MeCN	100	96	44
20	tris-(4-dimethylaminophenyl)-phosphine	**3**	**Toluene**	**120**	**24**	**92**
21	tris-(4-dimethylaminophenyl)-phosphine	1	Toluene	120	48	77
22	tris-(4-dimethylaminophenyl)-phosphine	0.5	Toluene	120	48	48
23	tris-(4-dimethylaminophenyl)-phosphine	-	Toluene	120	48	NR
24[c]	tris-(4-dimethylaminophenyl)-phosphine	3	Toluene	120	48	NR

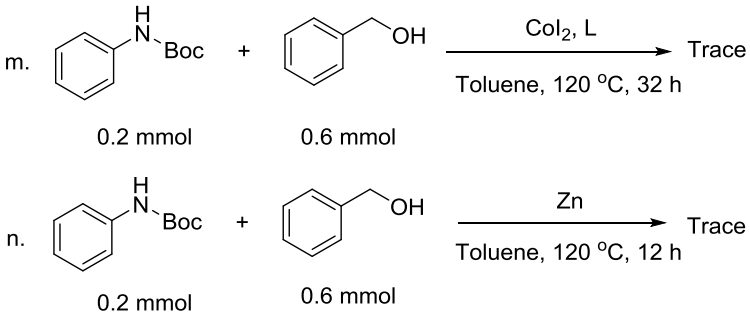
[a]*Reaction conditions:* CoI_2 (10 mol%), monophosphine ligands (24 mol%) or diphosphine ligands (12 mol%) and zinc powder were stirred in solvent (1 mL) for 30 minutes at room temperature under Ar. *N*-Boc protected aniline **1a** (0.2 mmol), benzyl formate **2a** (0.6 mmol) and 1 mL solvent were added. The reaction mixture was stirred under argon atmosphere at 100 °C or 120 °C. The reaction was monitored by TLC.

[b]Isolated yields.

[c]Mn (3 equiv.) was used instead of Zn.

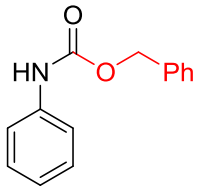
D: Scheme S1: Control reactions to identify the reaction intermediates





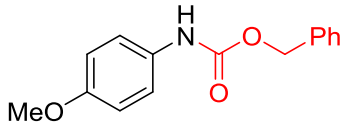
E: Characterization Data of Products

Benzyl phenylcarbamate (*3aa*)



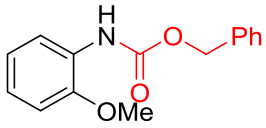
White solid, 42 mg, 92% yield, mp 70-72 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42-7.29 (m, 9H), 7.07 (t, J = 7.4 Hz, 1H), 6.75(s, 1H), 5.20(s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.37, 137.77, 136.04, 129.11, 128.67, 128.42, 128.37, 123.56, 118.67, 67.05.

Benzyl (4-methoxyphenyl)carbamate (*3ba*)



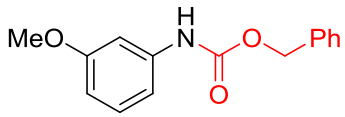
White solid, 46 mg, 90% yield, mp 98-100 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40-7.29 (m, 7H), 6.86-6.82 (m, 2H), 6.76 (s, 1H), 5.19 (s, 2H), 3.78 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.98, 153.85, 136.22, 130.91, 128.64, 128.33, 120.72, 114.26, 66.94, 55.53.

Benzyl (2-methoxyphenyl)carbamate (*3ca*)



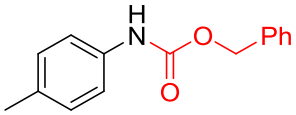
White solid, 44 mg, 86% yield, mp 72-74 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (s, 1H), 7.44 -7.33 (m, 6H), 7.03-6.95 (m, 2H), 6.87-6.85 (m, 1H), 5.22 (s, 2H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.30, 147.60, 136.20, 128.66, 128.39, 127.56, 122.85, 121.14, 118.15, 109.98, 66.96, 55.63.

Benzyl (3-methoxyphenyl)carbamate (*3da*)



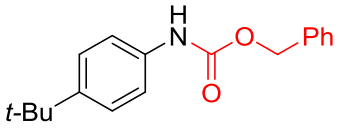
Colorless oil, 44 mg, 86% yield.^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41-7.32 (m, 5H), 7.19 (t, J = 8.2, 1H), 7.14 (s, 1H), 6.89-6.84 (m, 2H), 6.63 (dd, J = 8.2, 2.3 Hz, 1H), 5.20 (s, 2H), 3.79 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.30, 153.33, 139.10, 136.05, 129.78, 128.65, 128.39, 128.32, 110.96, 109.33, 104.44, 67.03, 55.28.

Benzyl *p*-tolylcarbamate (*3ea*)



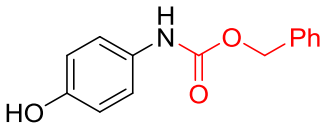
White solid, 40 mg, 82% yield, mp 77-79 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39-7.30 (m, 5H), 7.27-7.24 (m, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.78 (s, 1H), 5.17 (s, 2H), 2.29 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.56, 136.19, 135.25, 130.09, 129.57, 128.63, 128.50, 128.34, 118.87, 66.94, 20.78.

Benzyl (4-(tert-butyl)phenyl)carbamate (*3fa*)



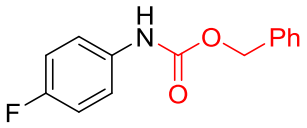
White solid, 47 mg, 83% yield, mp 102-104 ºC.^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42 -7.33 (m, 9H), 6.78 (s, 1H), 5.21 (s, 2H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.60, 146.51, 136.21, 135.19, 128.64, 128.34, 128.32, 125.90, 118.65, 66.97, 34.31, 31.43.

Benzyl (4-hydroxyphenyl)carbamate (*3ga*)



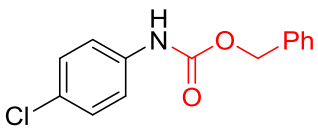
White solid, 20 mg, 41% yield, mp 160-162 ºC.^{1}H NMR (400 MHz, Methanol-*d4*) δ 7.40-7.29 (m, 5H), 7.21-7.20 (m, 2H), 6.73-6.69 (m, 2H), 5.14 (d, *J* = 2.1 Hz, 2H).^{13}C NMR (101 MHz, Methanol-*d4*) δ 153.20, 136.84, 130.53, 128.11, 127.66, 127.53, 120.72, 114.87, 66.00.

Benzyl (4-fluorophenyl)carbamate (*3ha*)



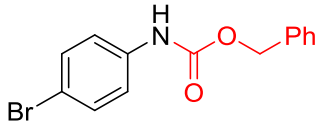
White solid, 46 mg, 94% yield, mp 76-78 ºC.^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40-7.32 (m, 7H), 7.02-6.96 (m, 2H), 6.82 (s, 1H), 5.19 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.26, 157.85, 153.62, 135.99, 133.79, 128.66, 128.43, 128.33, 120.56, 115.79, 115.57, 67.13.

Benzyl (4-chlorophenyl)carbamate (*3ia*)



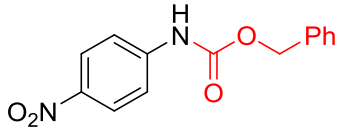
White solid, 46 mg, 89% yield, mp 109-111 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37-7.30(m, 7H), 7.24-7.22 (m, 2H), 6.84 (s, 1H), 5.17(s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.39, 136.45, 135.88, 129.05, 128.68, 128.48, 128.35, 120.02, 67.22.

Benzyl (4-bromophenyl)carbamate (*3ja*)



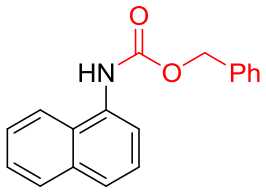
White solid, 37 mg, 60% yield, mp 115-117 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.42-7.33(m, 7H), 7.29-7.27 (m, 2H), 6.72 (s, 1H), 5.19 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.20, 136.91, 135.81, 132.02, 128.70, 128.40, 120.21, 116.05, 67.25.

Benzyl (4-nitrophenyl)carbamate (*3ka*)



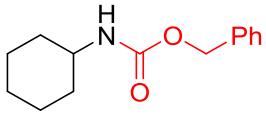
White solid, 44 mg, 80% yield, mp 163-165 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21-8.17(m, 2H), 7.56-7.54 (m, 2H), 7.41-7.35 (m, 5H), 7.13 (s, 1H), 5.23 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 152.64, 143.81, 143.09, 135.33, 128.75, 128.71, 128.48, 125.24, 117.78, 67.75.

Benzyl naphthalen-1-ylcarbamate (*3la*)



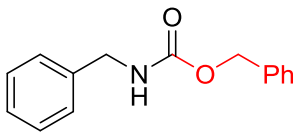
White solid, 40 mg, 72% yield, mp 130-132 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85-7.81(m, 3H), 7.63 (d, *J* = 8.1 Hz, 1H), 7.47-7.32 (m, 8H), 7.08 (s, 1H), 5.23 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 154.33, 136.11, 134.09, 132.44, 128.77, 128.69, 128.45, 126.29, 126.06, 125.85, 125.15, 120.51, 67.35.

Benzyl cyclohexylcarbamate (*3ma*)



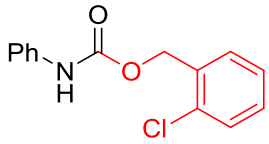
White solid, 38 mg, 82% yield, mp 64-66 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37-7.28(m, 5H), 5.08 (s, 2H), 4.71 (d, *J* = 4.9 Hz, 1H), 3.54-3.47 (m, 1H), 1.94-1.91 (m, 2H), 1.72-1.66 (m, 2H), 1.60-1.57 (m, 1H), 1.38-1.25 (m, 2H), 1.20-1.07 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 155.58, 136.70, 128.54, 128.18, 128.09, 66.48, 49.90, 33.41, 25.49, 24.82.

Benzyl benzylcarbamate (*3na*)



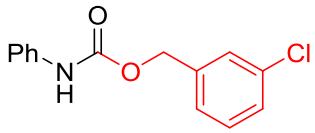
White solid, 26 mg, 54% yield, mp 64-66 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37-7.26 (m, 10H), 5.14 (s, 3H), 4.38 (d, *J* = 5.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.46, 138.41, 136.49, 128.70, 128.56, 128.18, 127.54, 66.90, 45.16.

2-chlorobenzyl phenylcarbamate (*3ab*)



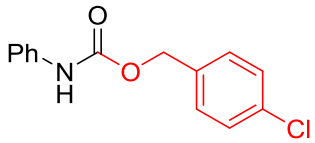
White solid, 34 mg, 64% yield, mp 82-84 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37-7.28(m, 4H), 7.22-7.13 (m, 4H), 6.97 (t, *J* = 7.4 Hz, 1H), 6.79 (s, 1H), 5.22 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.21, 137.73, 133.80, 133.78, 130.12, 129.69, 129.63, 129.12, 126.98, 123.63, 118.70, 64.33.

3-chlorobenzyl phenylcarbamate (*3ac*)



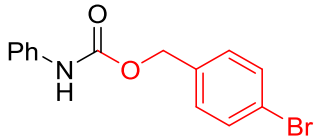
White solid, 20 mg, 38% yield, mp 91-93 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39-7.25(m, 8H), 7.09-7.05 (m, 1H), 6.75 (s, 1H), 5.17 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.10, 138.11, 137.59, 134.50, 129.92, 129.13, 128.47, 128.19, 126.19, 123.71, 118.76, 66.05.

4-chlorobenzyl phenylcarbamate (*3ad*)



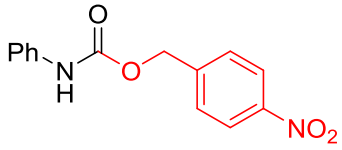
White solid, 34 mg, 65% yield, mp 94-96 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40-7.28(m, 9H), 7.08 (t, *J* = 7.3 Hz, 1H), 6.83 (s, 1H), 5.15 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.25, 137.65, 134.61, 134.25, 129.68, 129.11, 128.81, 123.68, 118.77, 66.16.

4-bromobenzyl phenylcarbamate (*3ae*)



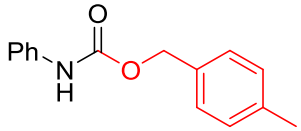
White solid, 48 mg, 79% yield, mp 95-96 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52-7.48 (m, 2H), 7.38-7.36 (m, 2H), 7.32-7.27 (m, 4H), 7.09-7.06 (m, 1H), 6.66 (s, 1H), 5.15 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.28, 137.67, 135.14, 131.78, 129.96, 129.12, 123.71, 122.40, 118.83, 66.19.

4-nitrobenzyl phenylcarbamate (*3af*)



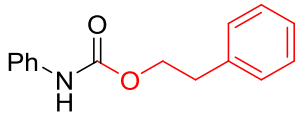
White solid, 47 mg, 87% yield, mp 124-126 ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (d, *J* = 8.7Hz, 2H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.40-7.38 (m, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.09 (t, *J* = 7.3 Hz, 1H), 6.78 (s, 1H), 5.29 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 147.73, 143.47, 137.34, 129.20, 128.38, 123.88, 118.76, 65.44.

4-methylbenzyl phenylcarbamate (*3ag*)



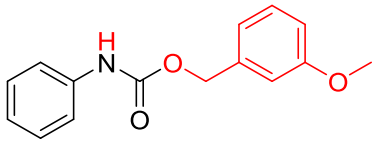
White solid, 29 mg, 62% yield, mp 76-78ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40-7.38(m, 2H), 7.33-7.28 (m, 4H), 7.19 (d, *J* = 7.9Hz, 2H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.74 (s, 1H), 5.17 (s, 2H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.44, 138.30, 137.83, 133.02, 129.35, 129.09, 128.56, 123.50, 118.66, 67.02, 21.28.

Phenethyl phenylcarbamate (*3ah*)



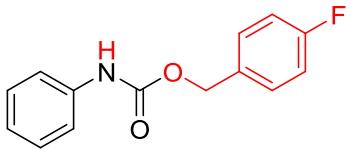
White solid, 29 mg, 62% yield, mp 77-79ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34-7.21 (m, 9H), 7.07-7.02 (m, 1H), 6.67 (s, 1H), 4.38 (t, *J* = 7.0 Hz, 2H), 2.98 (t, *J* = 7.0 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.50, 137.82, 129.08, 128.96, 128.59, 126.65, 123.49, 118.68, 65.65, 35.41.

3-methoxybenzyl phenylcarbamate (*3aj*)



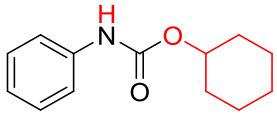
Colorless oil, 45 mg, 87% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41-7.39 (m, 2H), 7.33-7.28 (m, 3H), 7.09-7.05 (m, 1H), 6.99 (d, *J* = 7.6 *Hz*, 1H), 6.95-6.94 (m, 1H), 6.90-6.86 (m, 2H), 5.18 (s, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.8, 153.4, 137.8, 137.6, 129.7, 129.1, 123.5, 120.5, 118.7, 113.9, 113.7, 66.9, 55.3.

4-fluorobenzyl phenylcarbamate (*5ab)*



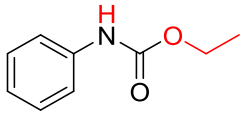
White solid, 47 mg, 96% yield, mp 79-80ºC. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40-7.37 (m, 4H), 7.31 (t, *J* = 7.4 *Hz*, 2H), 7.09-7.03 (m, 3H), 6.71 (s, 1H), 5.16 (s, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 163.9, 161.5, 153.2, 137.7, 131.9, 131.9, 130.4, 130.3, 129.1, 123.6, 118.7, 115.6, 115.4, 66.3.

Cyclohexyl phenylcarbamate (*5ac*)



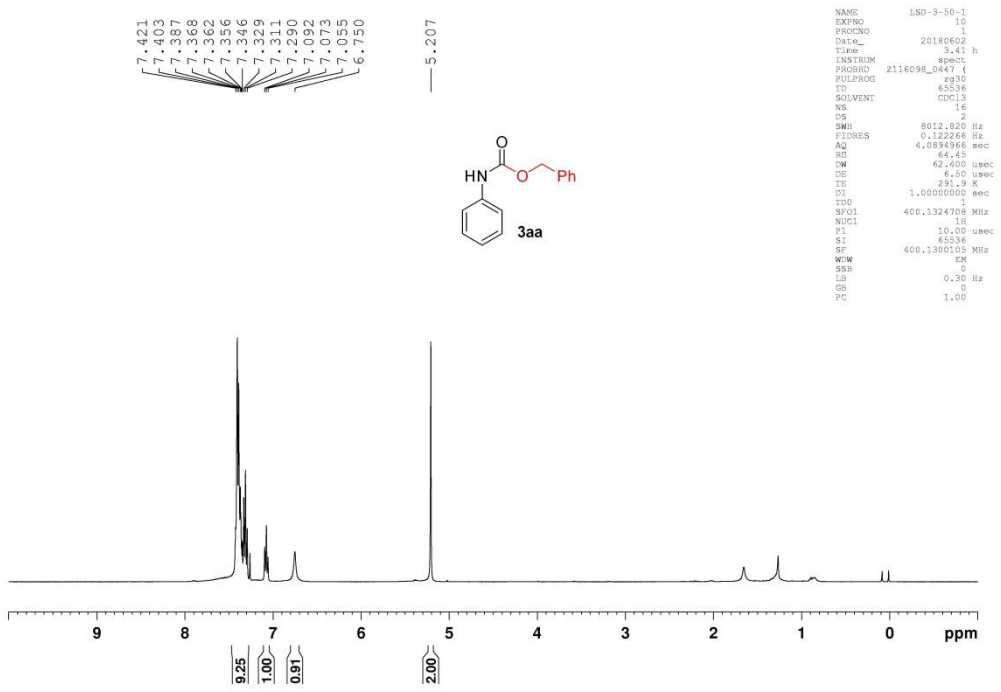
Colorless oil, 43 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40-7.38 (m, 2H), 7.31-7.27 (m, 2H), 7.07-7.02 (m, 1H), 6.71 (s, 1H), 4.78-4.72 (m, 1H), 1.96-1.91 (m, 2H), 1.77-1.71 (m, 2H), 1.58-1.53 (m, 1H), 1.50-1.33 (m, 4H), 1.30-1.21 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.3, 138.2, 129.0, 123.2, 118.5, 73.6, 31.9, 25.4, 23.8.

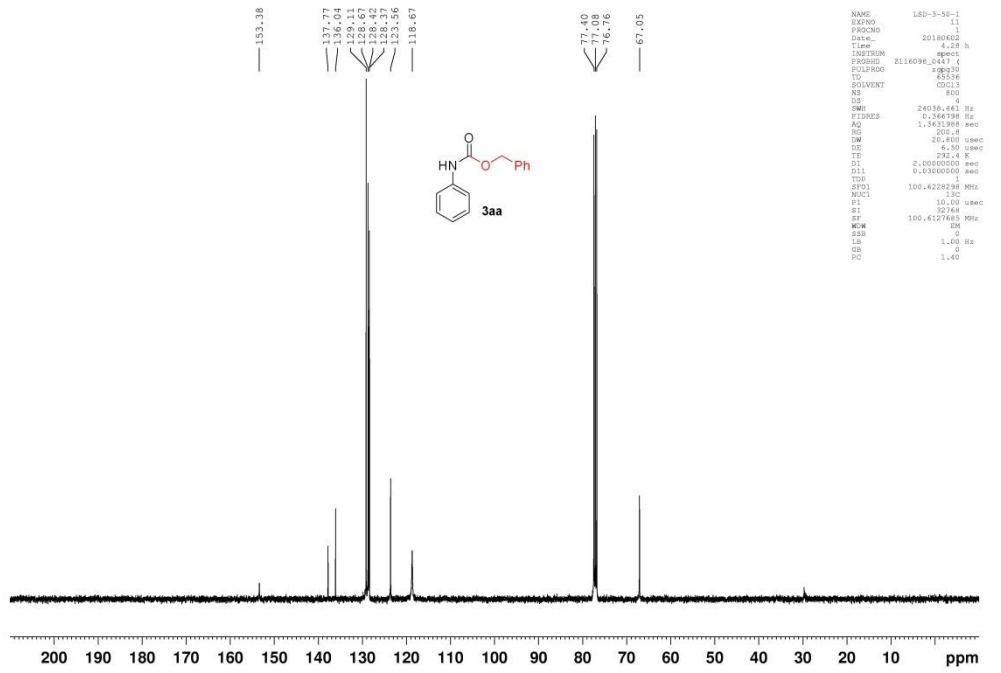
Ethyl phenylcarbamate (*5ad*)

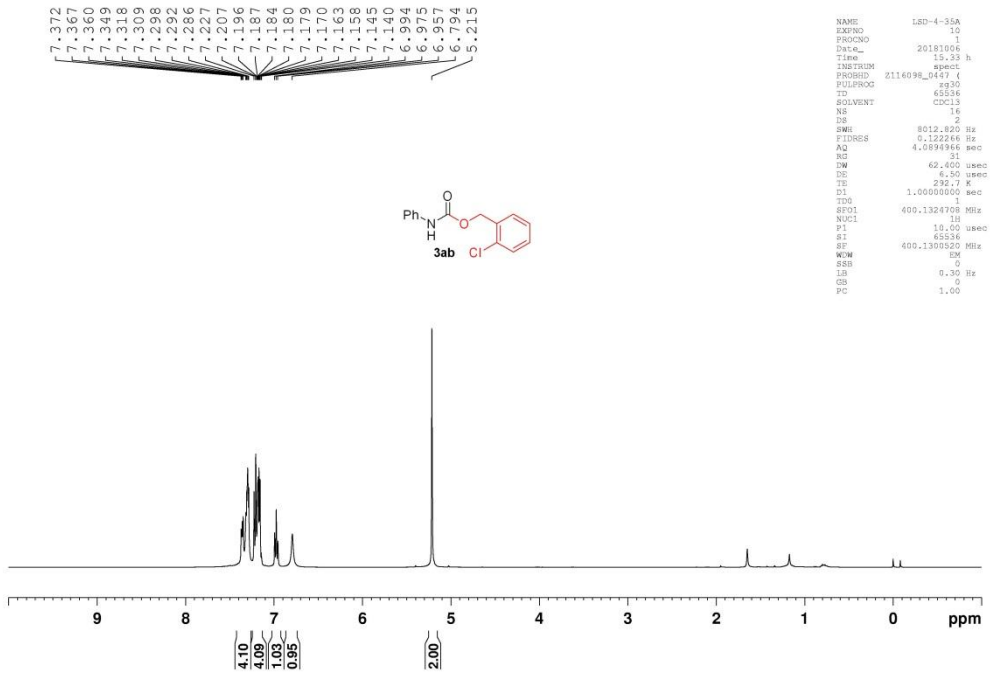


Colorless oil, 27 mg, 82% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40-7.35 (m, 2H), 7.32-7.27 (m, 2H), 7.08-7.03 (m, 1H), 6.77 (s, 1H), 4.22 (q, *J* = 7.1 *Hz*, 2H), 1.31 (t, *J* = 7.1 *Hz*, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.7, 138.0, 129.1, 123.3, 118.6, 61.2, 28.4, 14.6.

F: NMR Spectra of Products



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7.184
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7.179
7.170
7.163
7.158
7.145
7.140
6.994
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6.794
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O
Cl
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PROCNO 1
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RG 31
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DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
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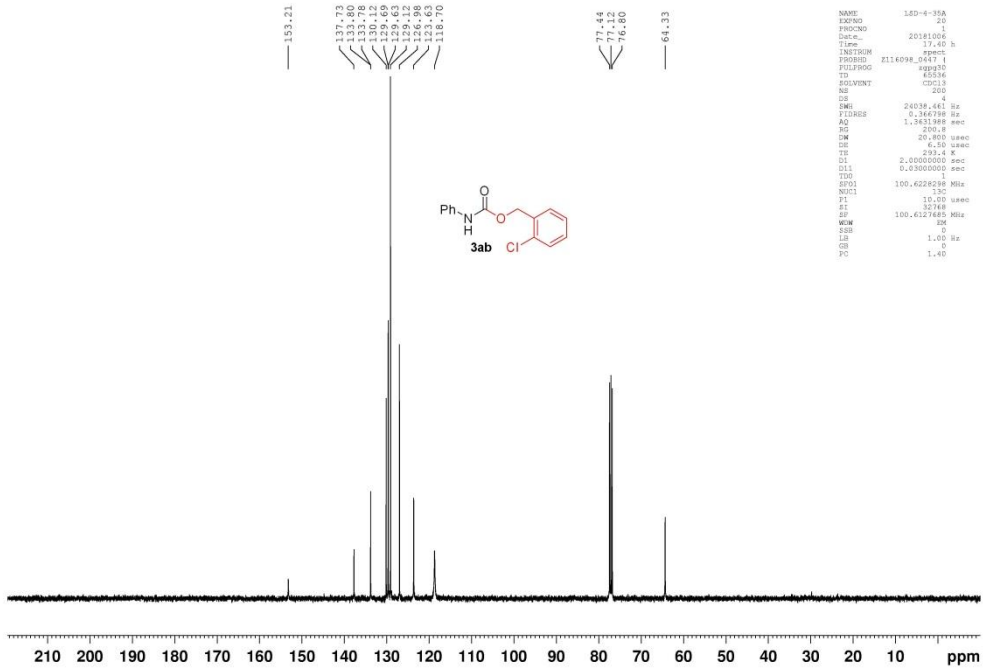
2.00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Cl
3ab
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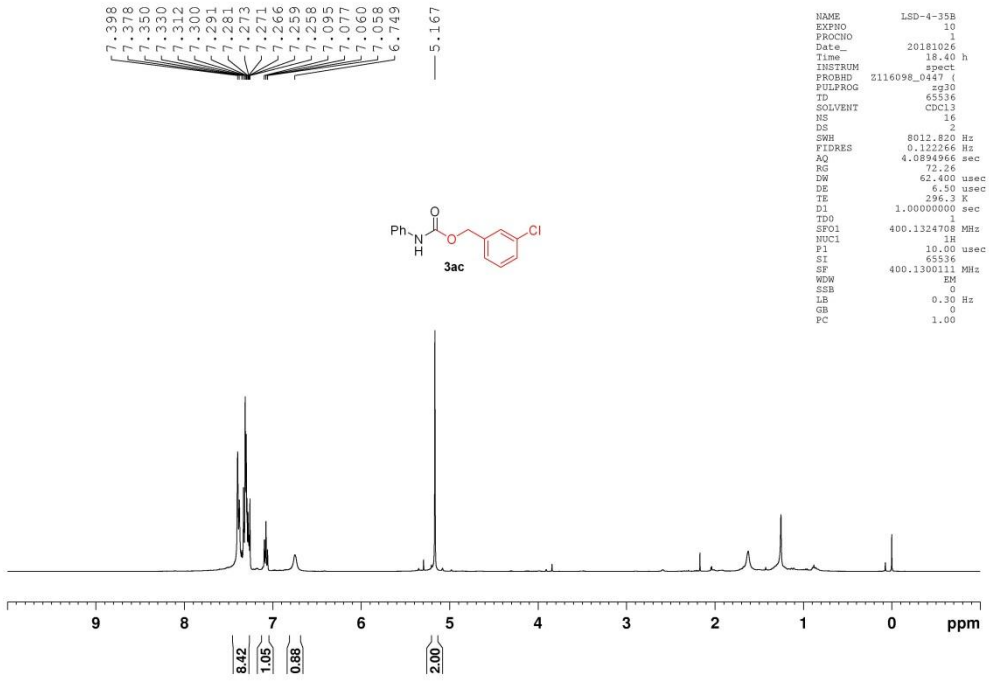
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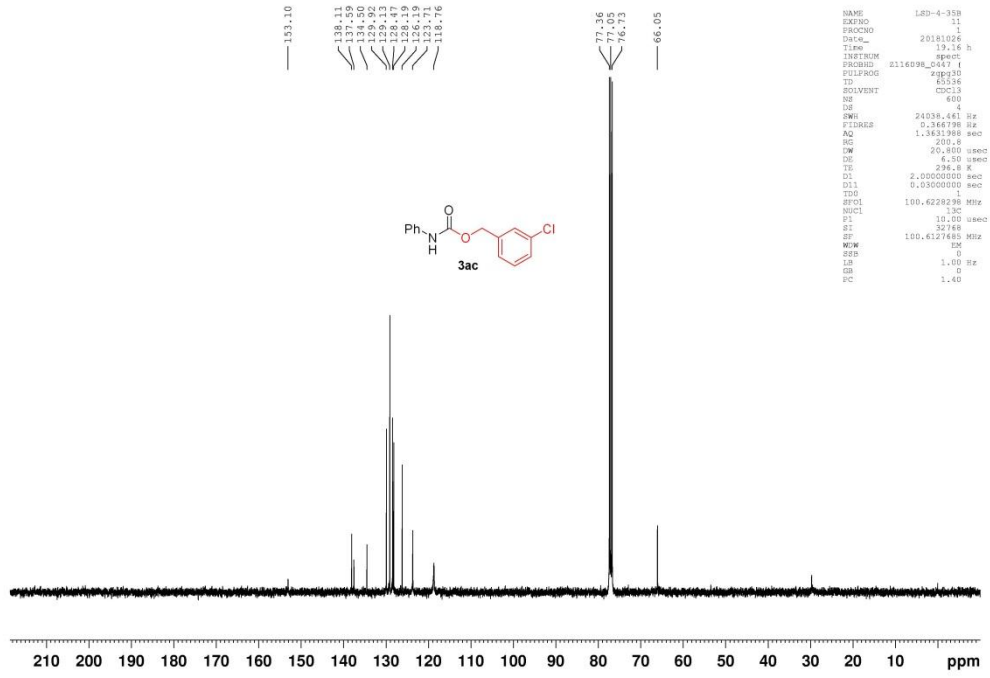
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128.19
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76.93
66.05
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FIDRES 0.366798 Hz
AQ 1.3631986 sec
RG 200.8
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
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O
O
Cl
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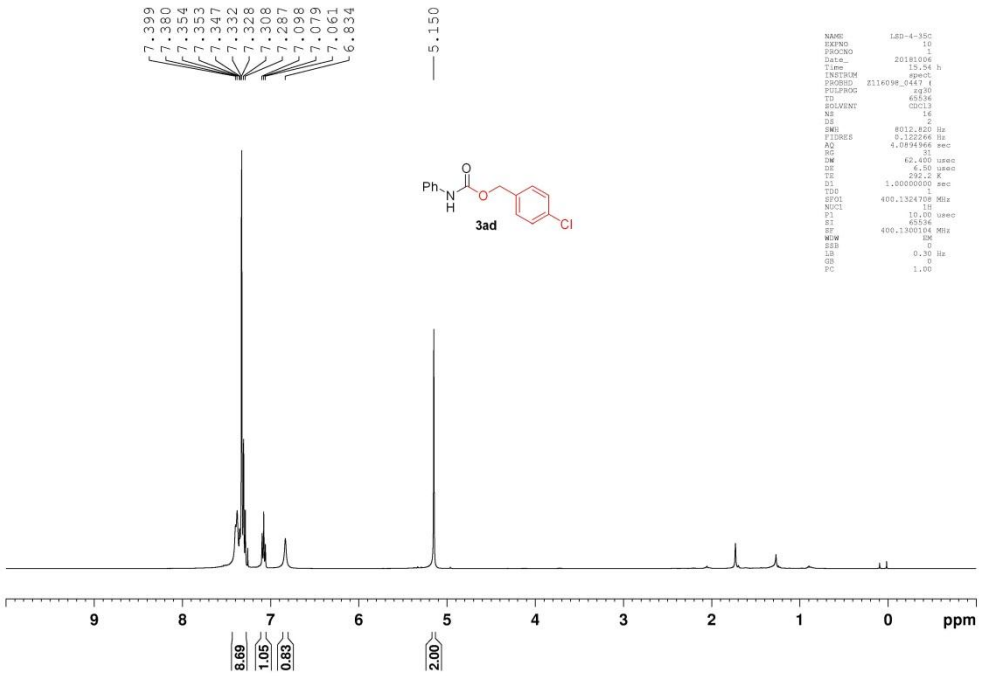
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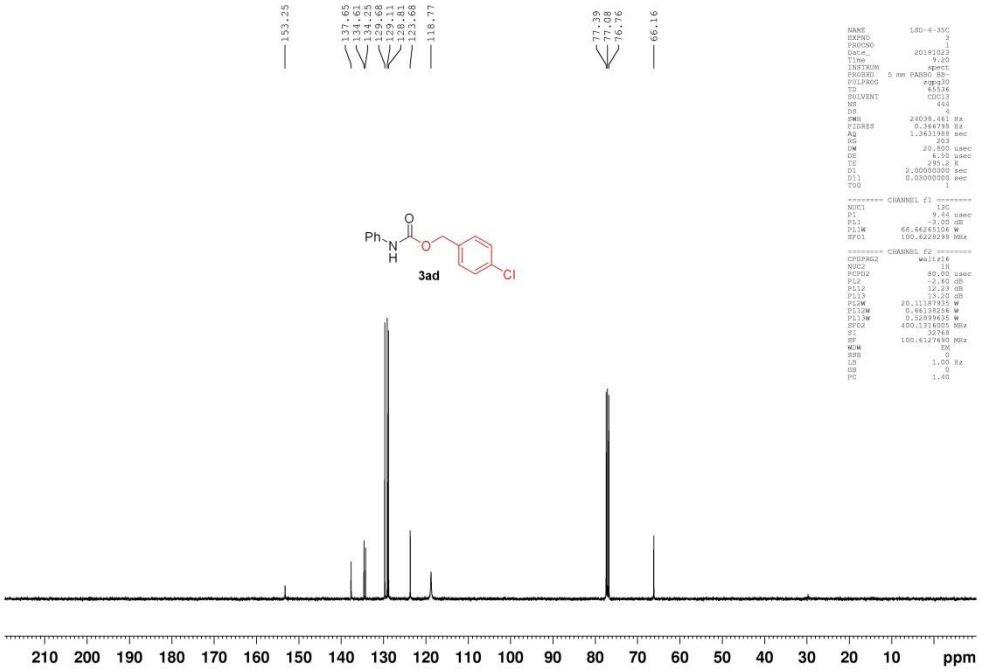
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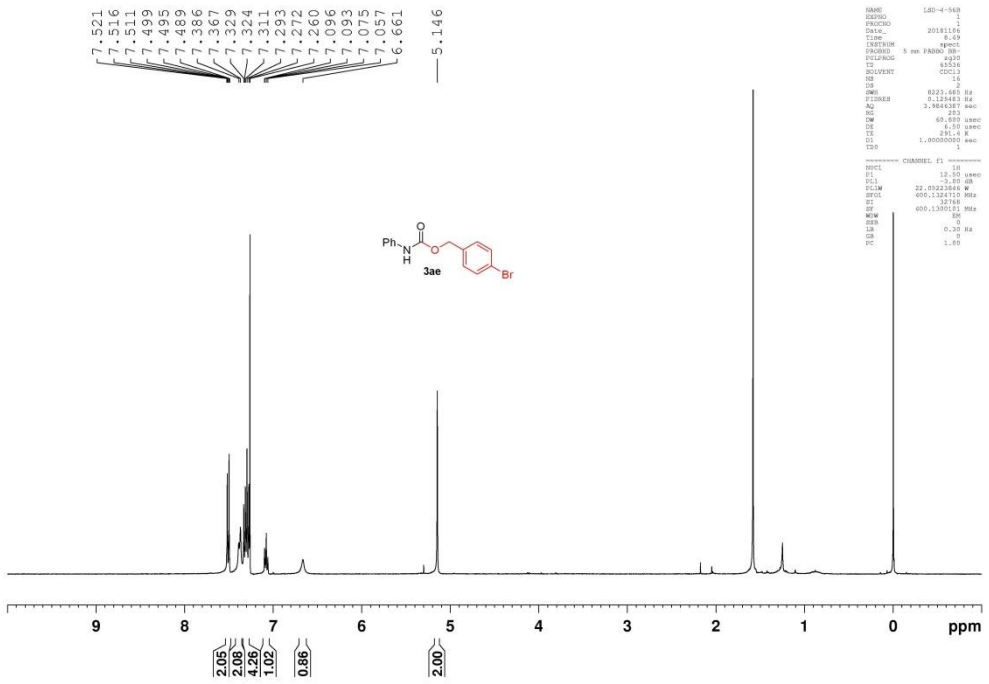
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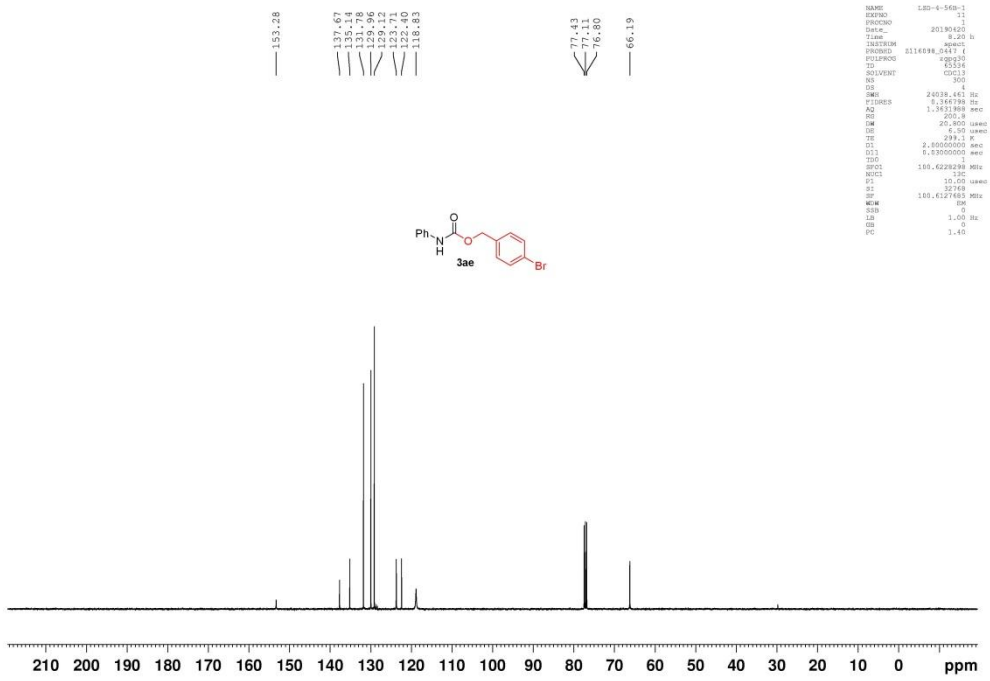
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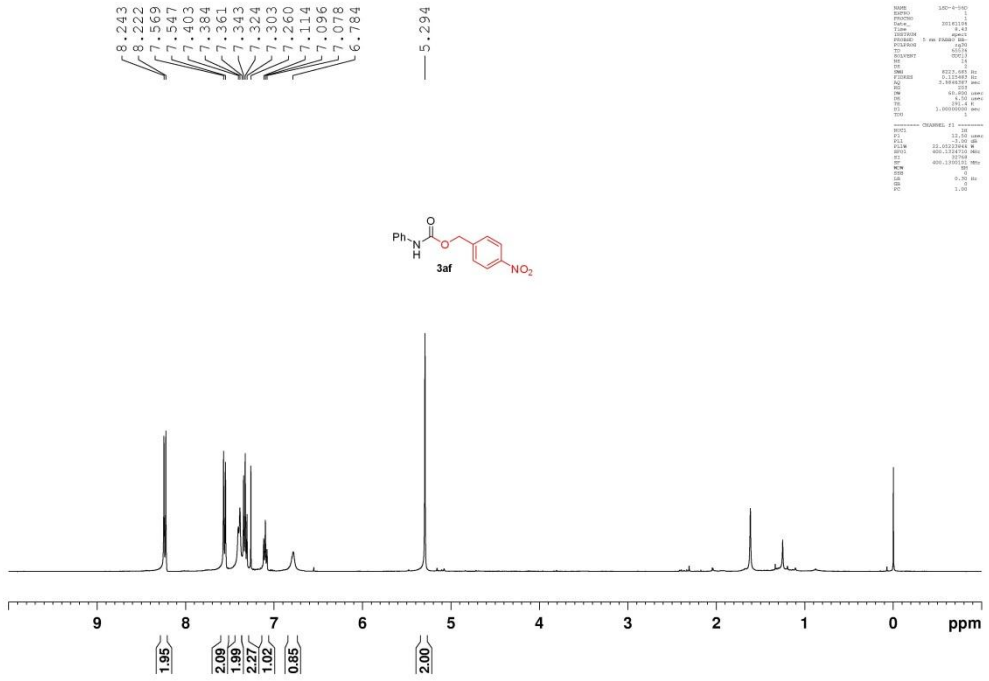
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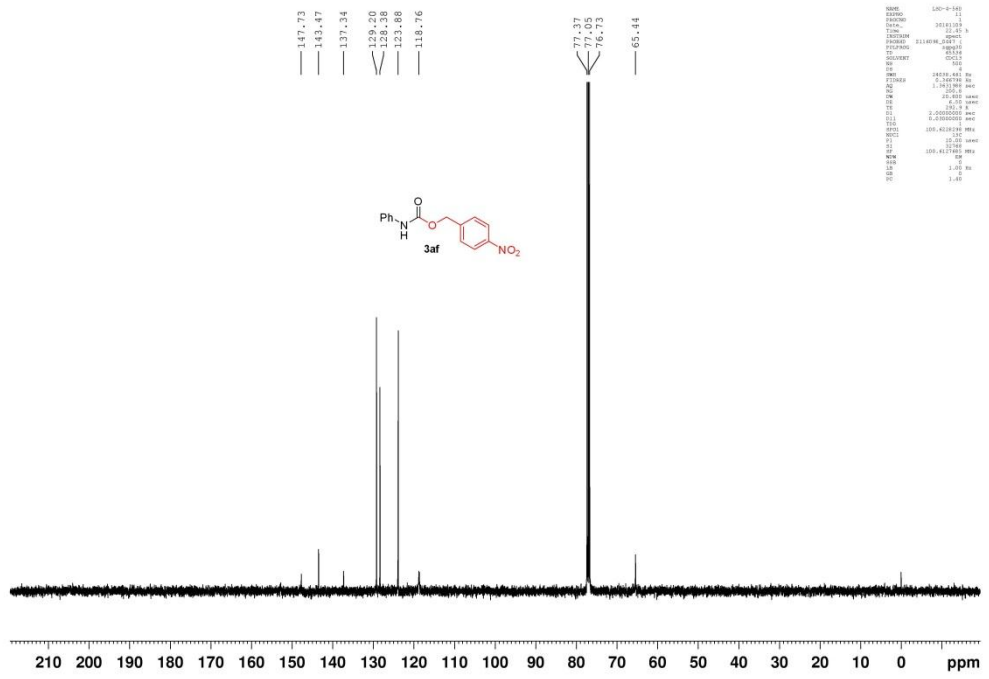
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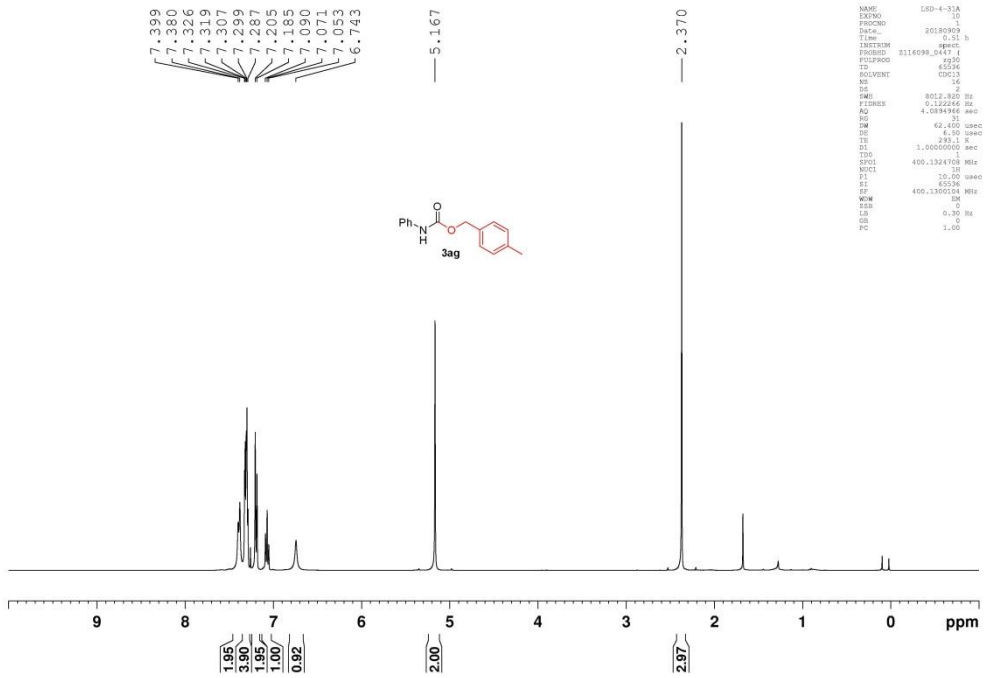
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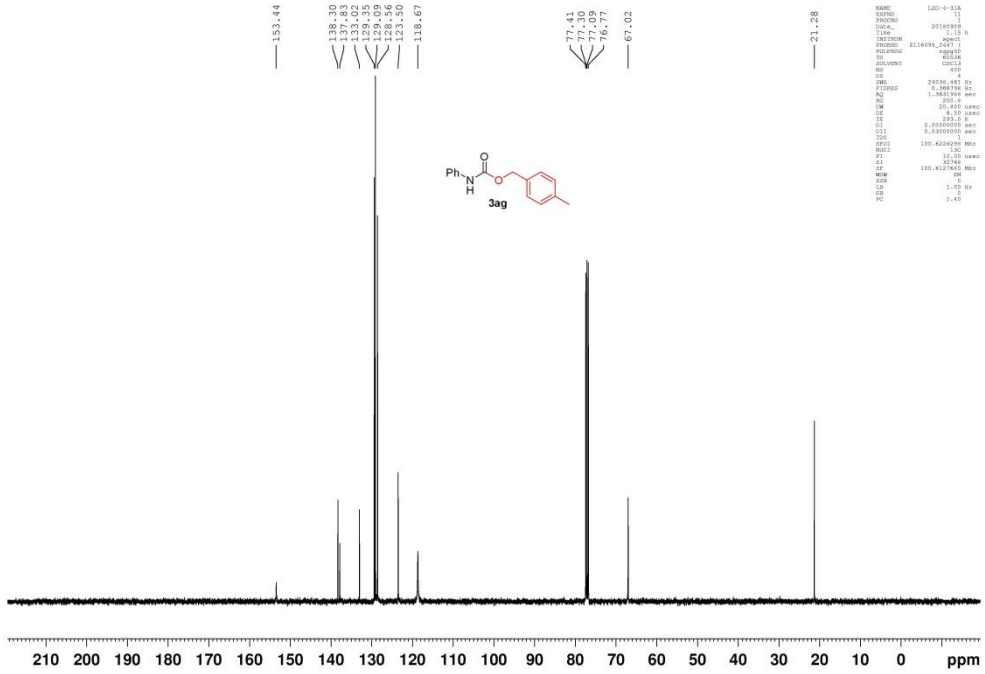
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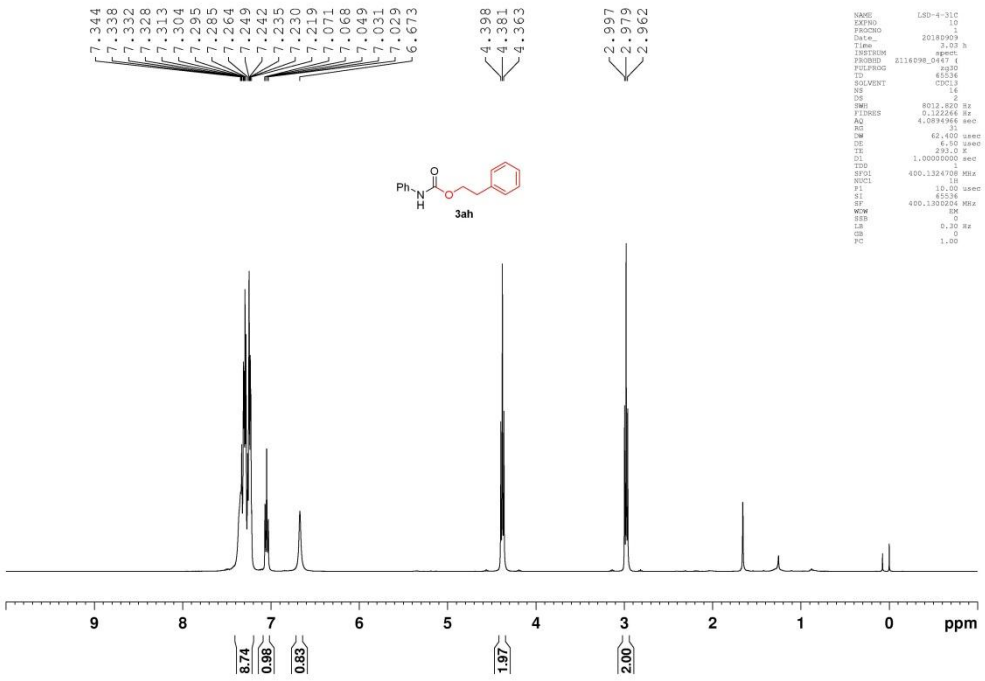
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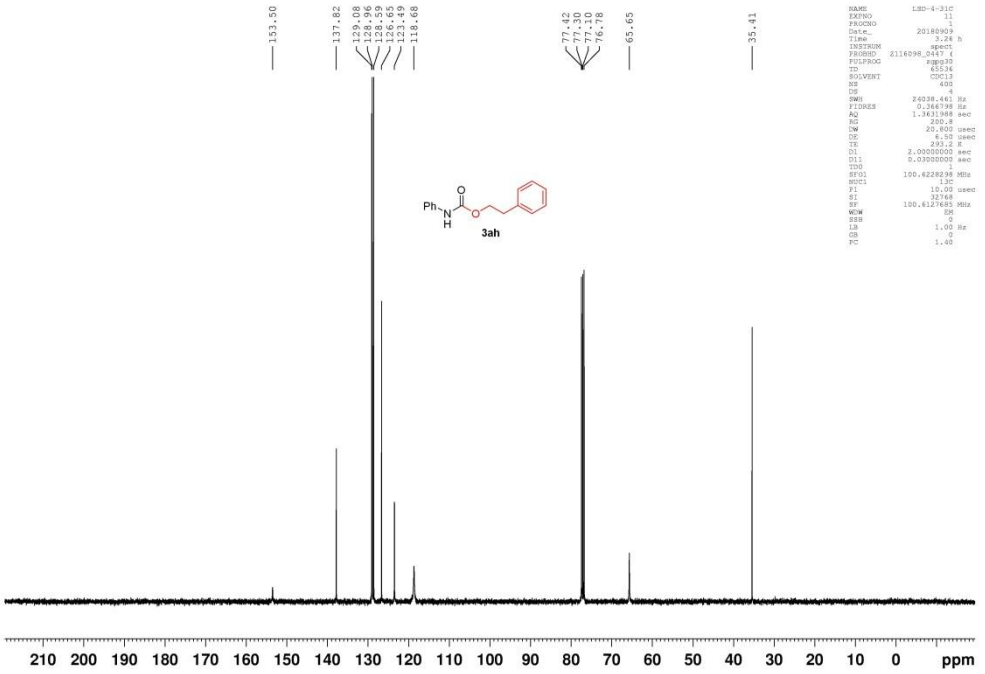
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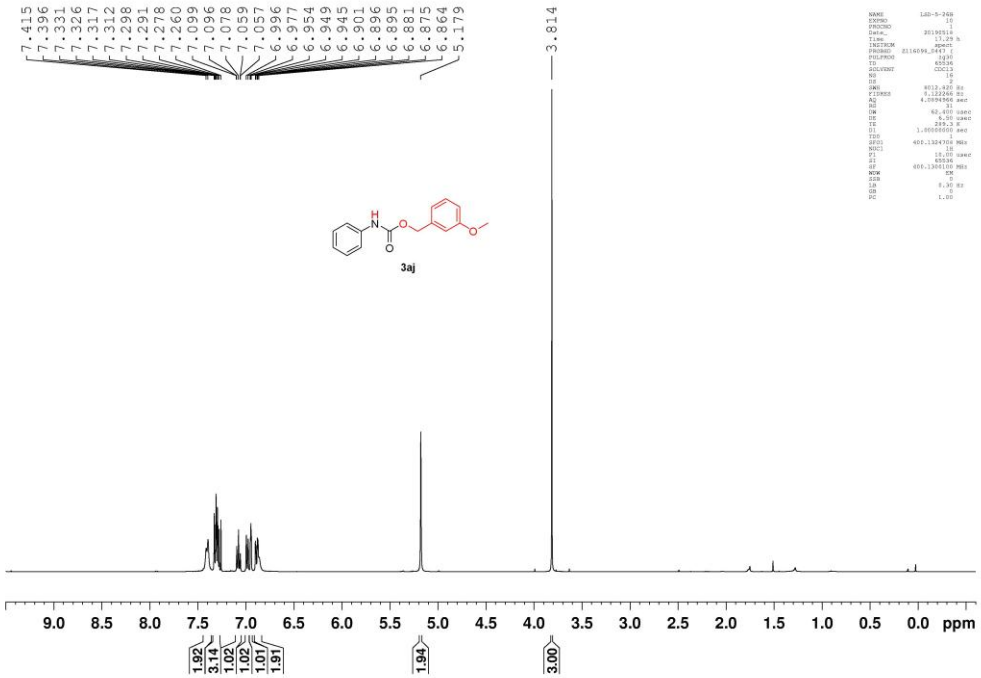
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3.814
3aj
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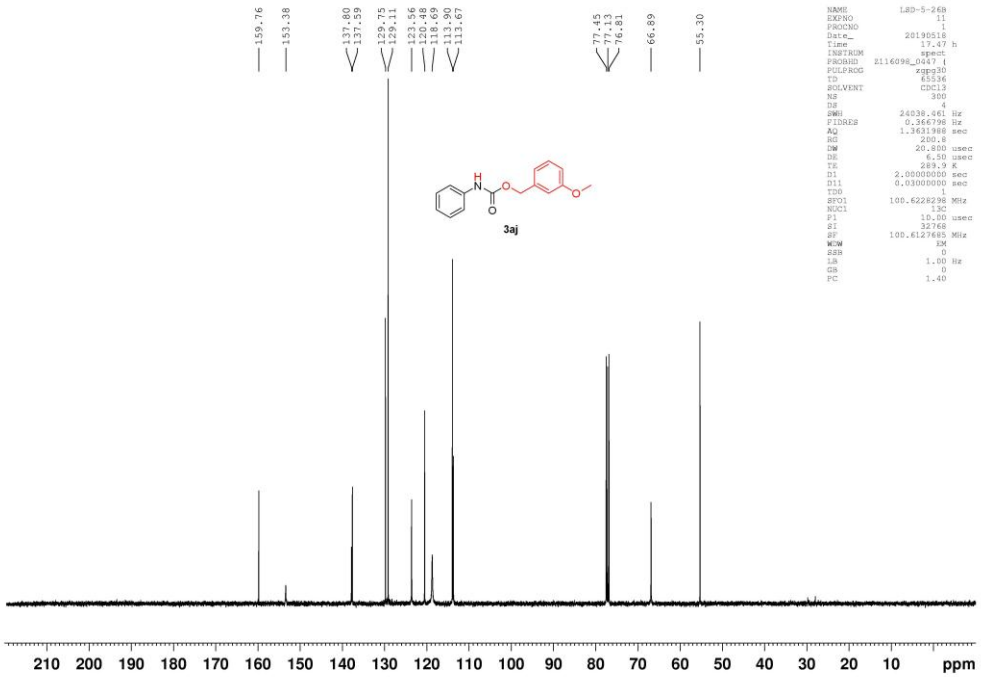
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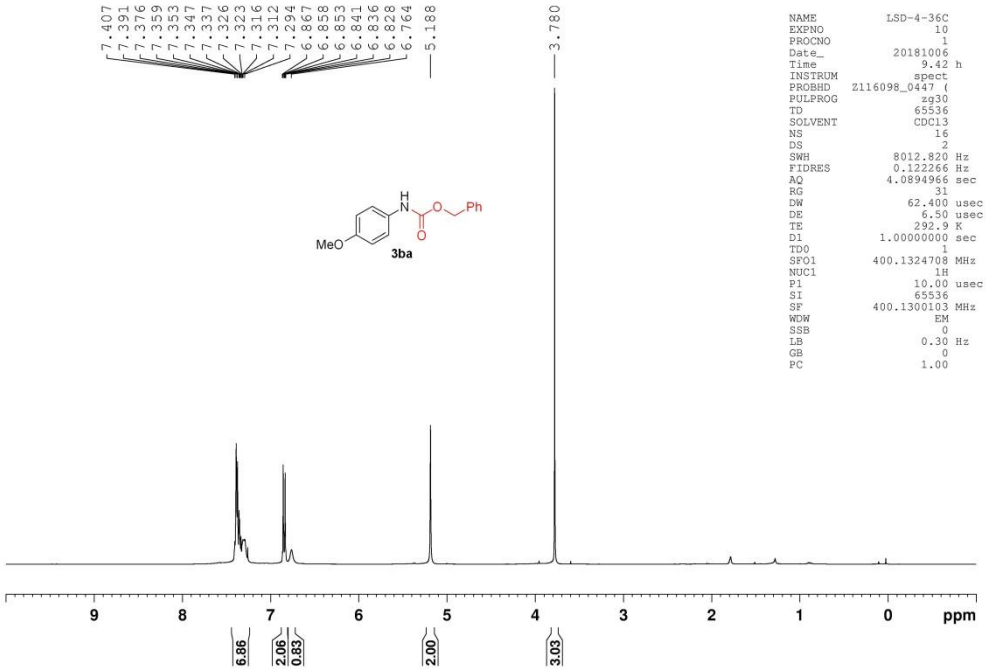
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FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 31
DW 62.400 usec
DE 6.50 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300103 MHz
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
Ph
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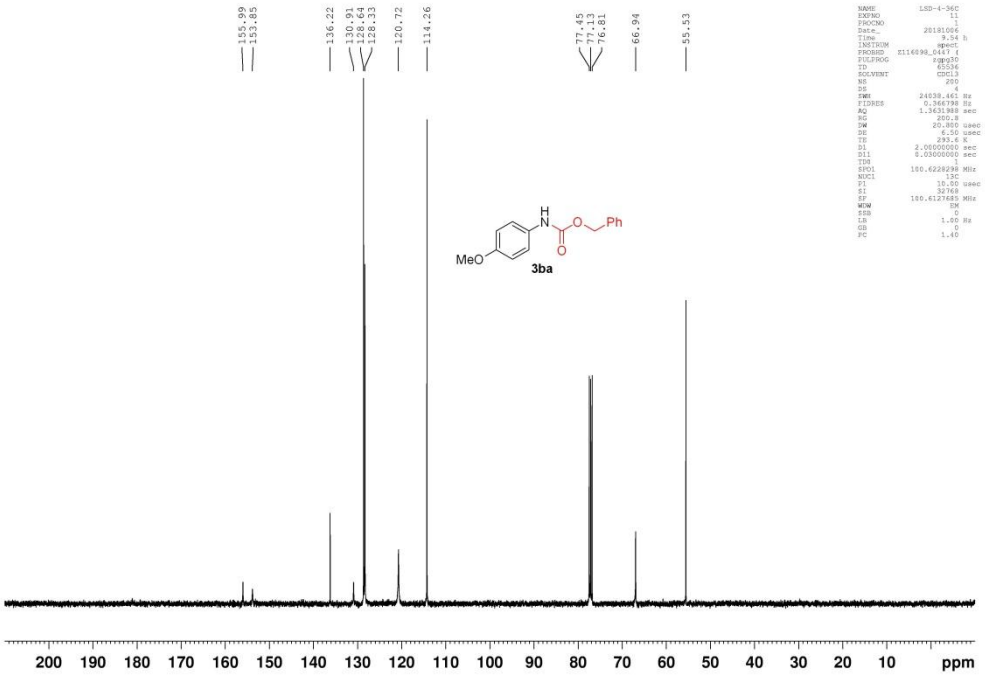
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Ph
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130
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100
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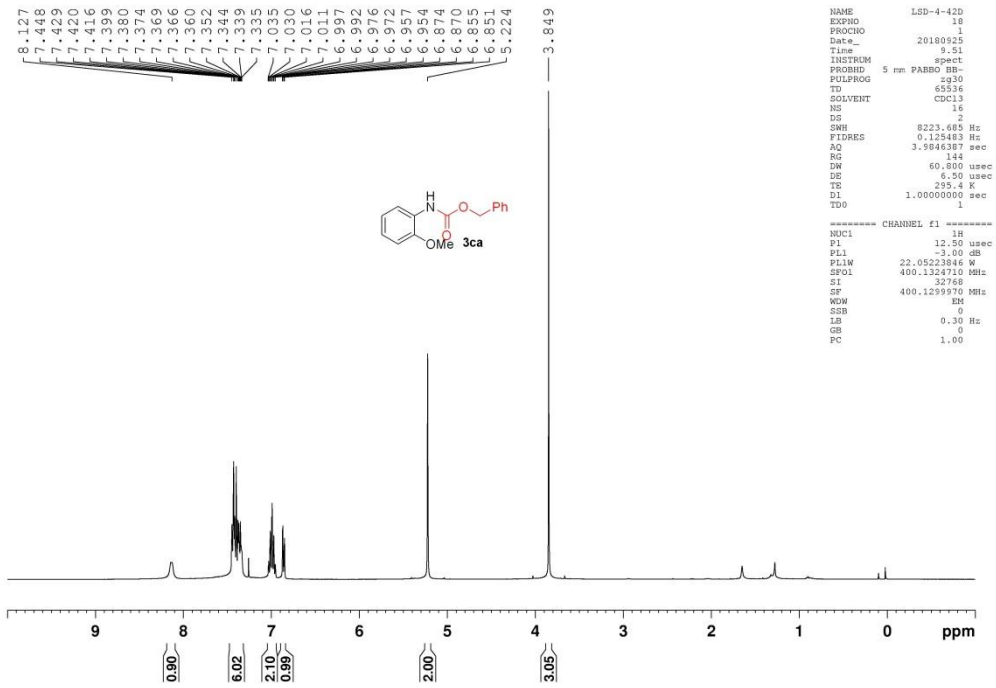
40
30
20
10
ppm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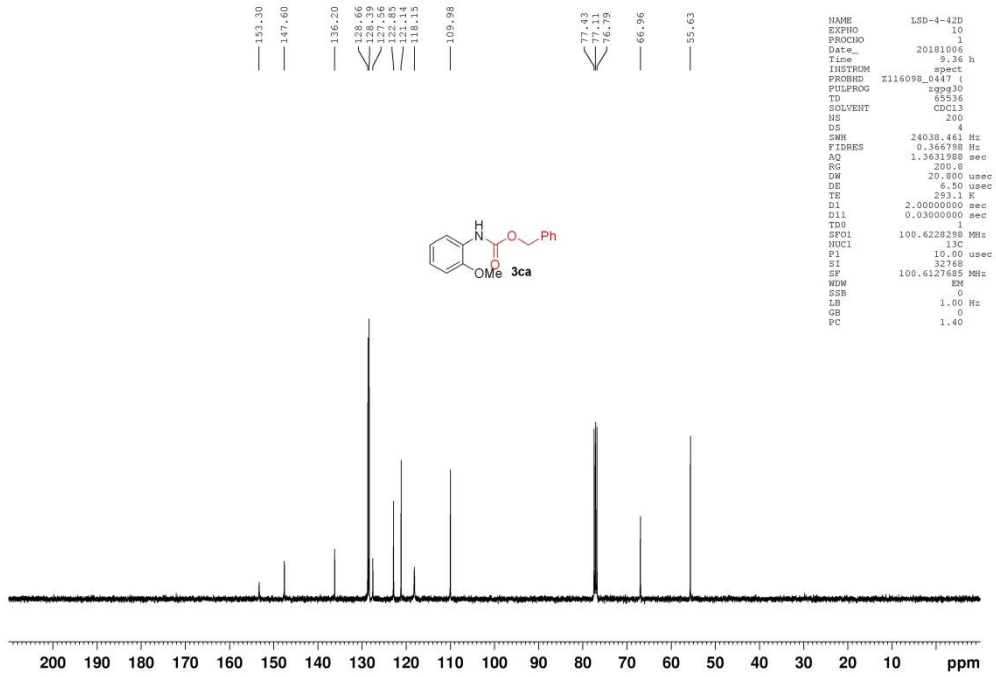
7.448
7.429
7.420
7.416
7.399
7.380
7.374
7.369
7.366
7.360
7.352
7.344
7.339
7.335
7.035
7.030
7.016
7.011
6.997
6.992
6.976
6.972
6.957
6.954
6.874
6.870
6.855
6.851
5.224
3.849
Ph
OMe
3ca
NAME LSD-4-42D
EXPNO 18
PROCNO 1
Date_ 20180925
Time 9.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1299970 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
0.90
6.02
2.10
0.99
2.00
3.05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147.60
136.20
128.66
128.59
127.56
122.85
121.14
118.15
109.98
77.43
77.11
76.79
66.96
55.63
Ph
OMe
3ca
NAME LSD-4-42D
EXPNO 10
PROCNO 1
Date_ 20181006
Time 9.36 h
INSTRUM spect
PROBHD Z116098_0447 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 200.8
DW 20.800 usec
DE 6.50 usec
TE 293.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
190
180
170
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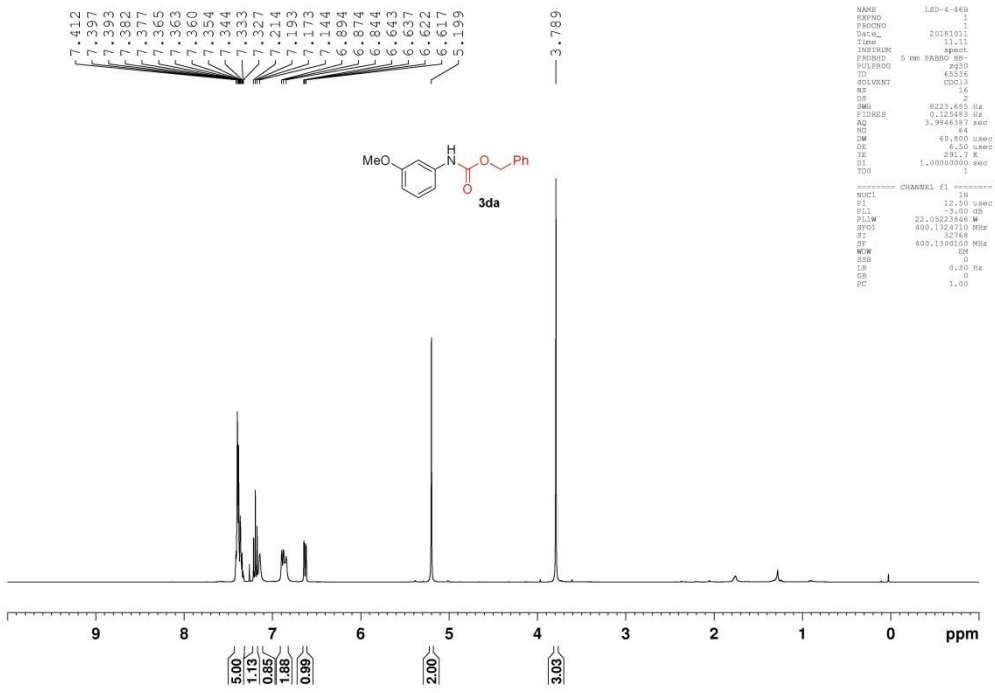
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.393
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7.365
7.363
7.360
7.354
7.344
7.333
7.327
7.214
7.193
7.173
7.144
6.894
6.874
6.844
6.643
6.637
6.622
6.617
5.199
3.789
MeO
H
N
O
O
Ph
3da
9
8
7
6
5
4
3
2
1
0
ppm
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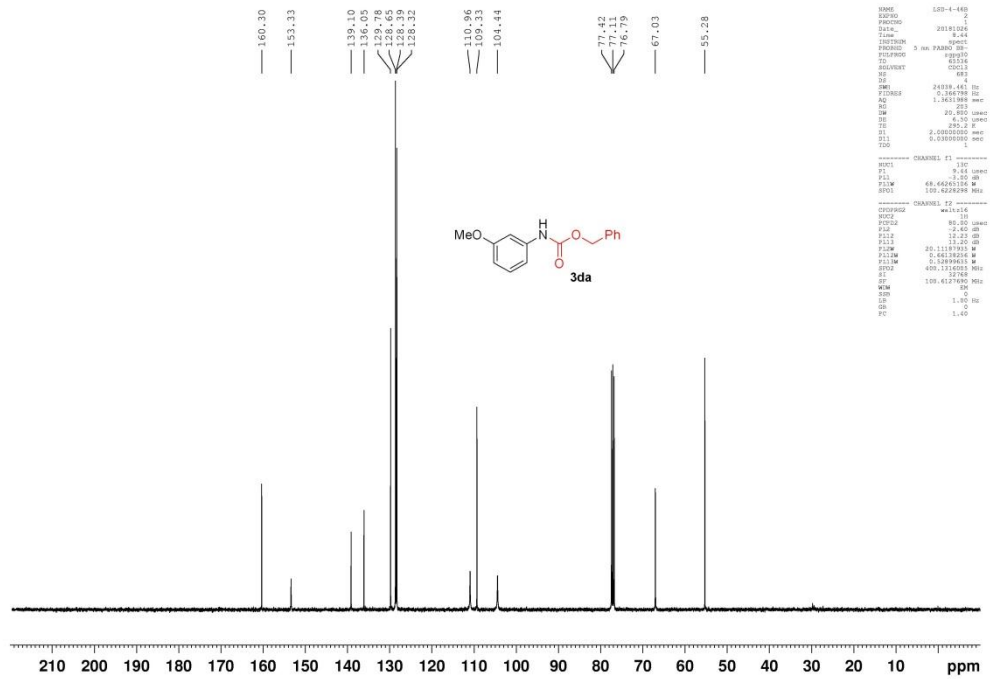
0.85
1.88
0.99
2.00
3.03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153.33
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129.78
128.65
128.39
120.32
110.96
109.33
104.44
77.42
77.11
76.79
67.03
55.28
MeO
H
N
O
O
Ph
3da
210
200
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150
140
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120
110
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70
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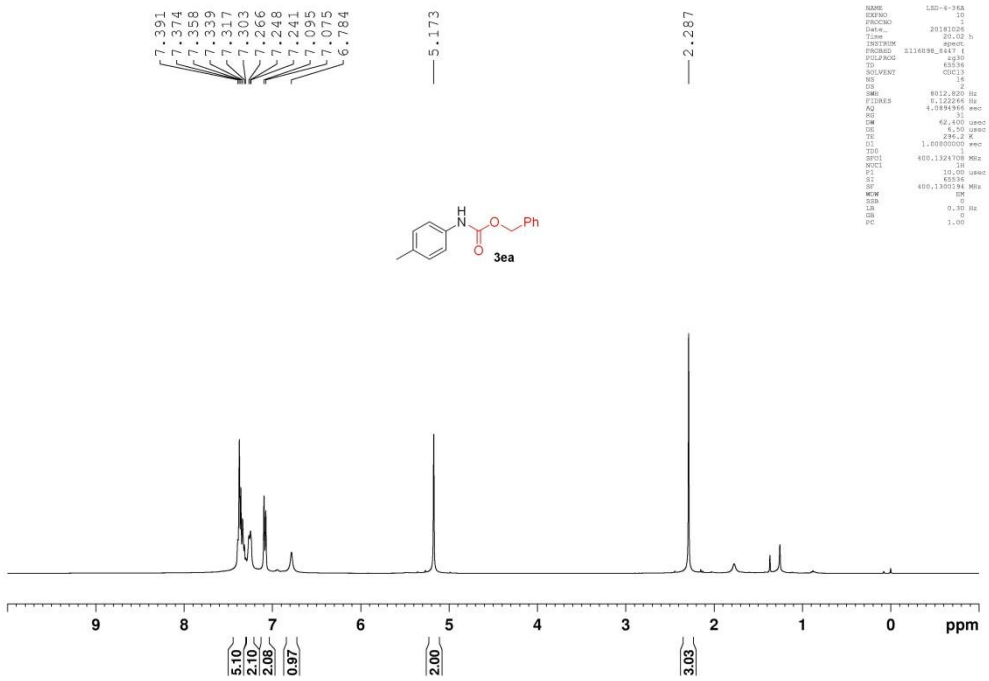
50
40
30
20
10
ppm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7.374
7.358
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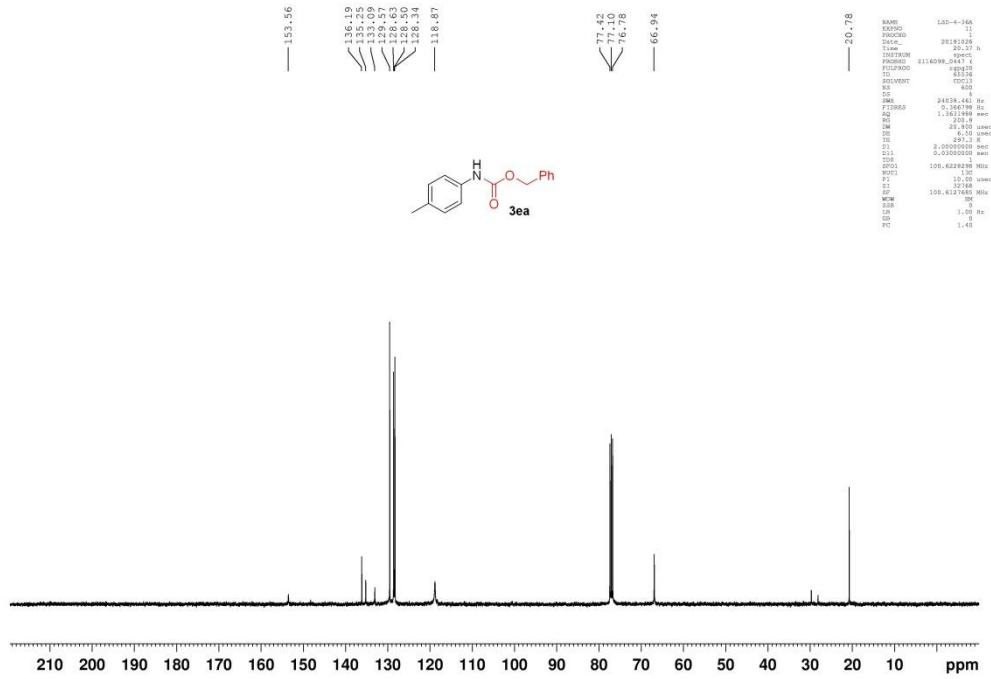
7.317
7.303
7.266
7.248
7.241
7.095
7.075
6.784
5.173
2.287
3ea
9
8
7
6
5
4
3
2
1
0
ppm
5.10
2.10
2.08
0.97
2.00
3.03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133.09
129.57
128.63
128.50
128.34
118.87
77.42
77.10
76.78
66.94
20.78
3ea
210
200
190
180
170
160
150
140
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120
110
100
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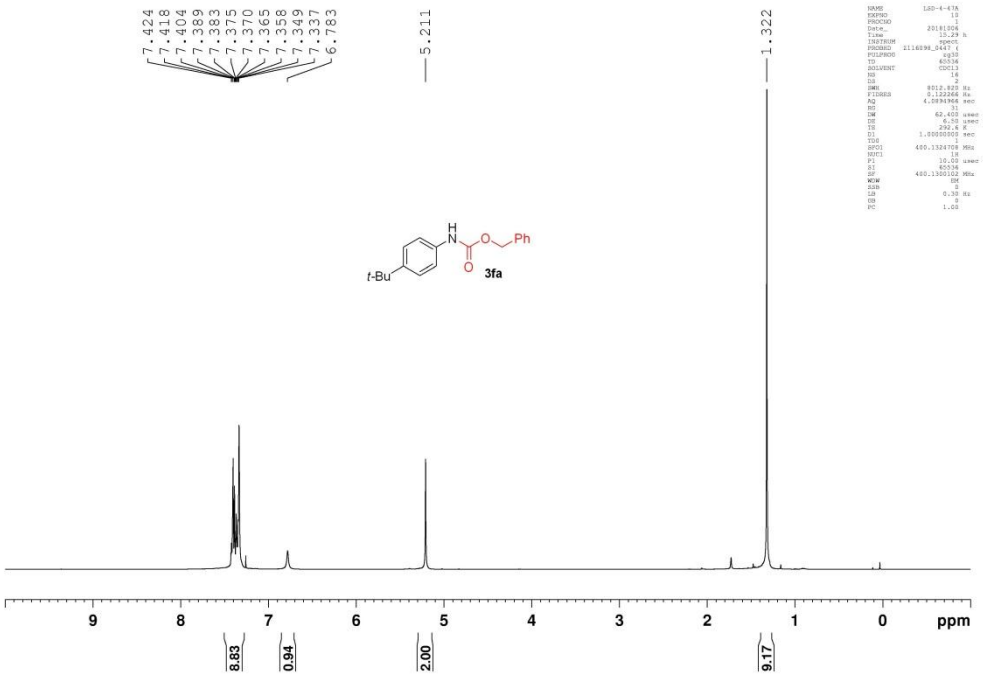
70
60
50
40
30
20
10
ppm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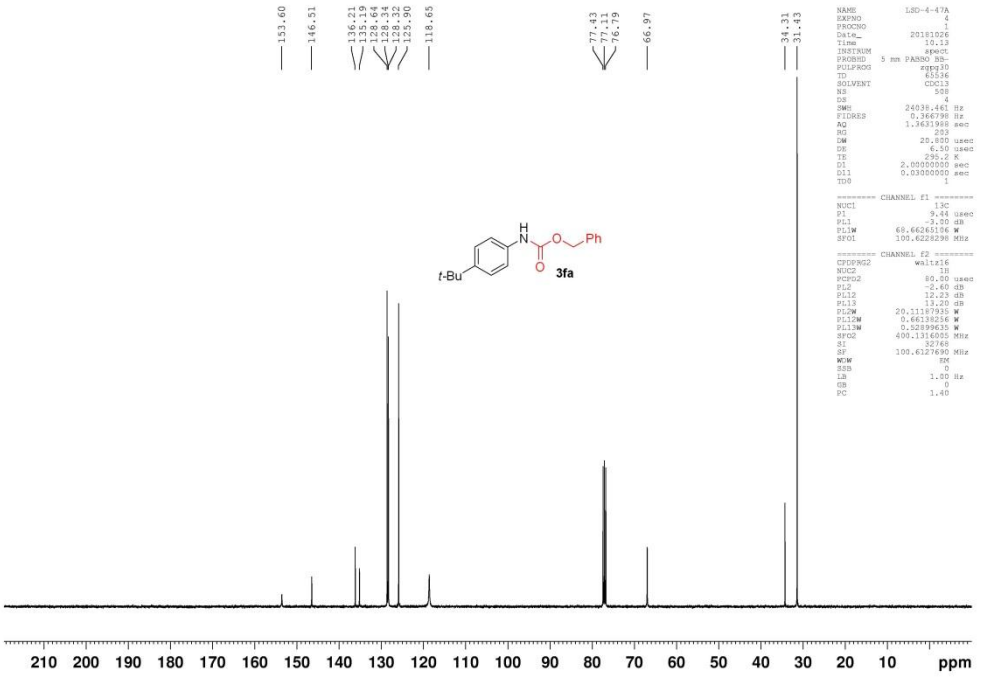
7.418
7.404
7.389
7.383
7.375
7.370
7.365
7.358
7.349
7.337
6.783
5.211
1.322
t-Bu
Ph
3fa
9
8
7
6
5
4
3
2
1
0
ppm
8.83
0.94
2.00
9.17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146.51
136.21
135.19
128.64
128.34
128.32
125.90
118.65
77.43
77.11
76.79
66.97
34.31
31.43
t-Bu
Ph
3fa
210
200
190
180
170
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150
140
130
120
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100
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80
70
60
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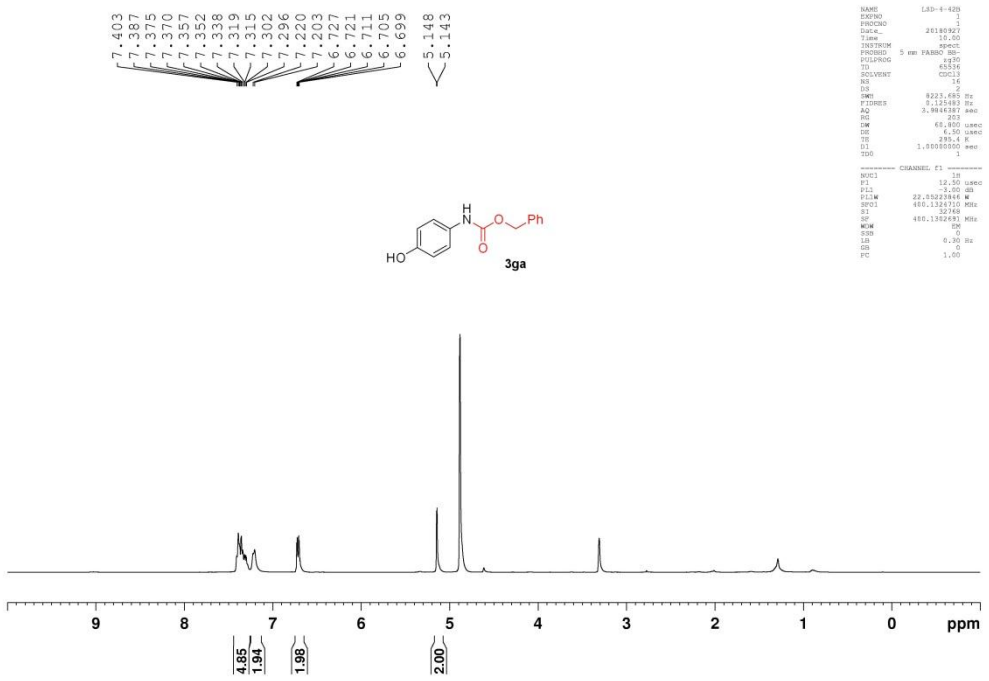
40
30
20
10
ppm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7.375
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7.357
7.352
7.338
7.319
7.315
7.302
7.296
7.220
7.203
6.727
6.721
6.711
6.705
6.699
5.148
5.143
HO
Ph
3ga
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7
6
5
4
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ppm
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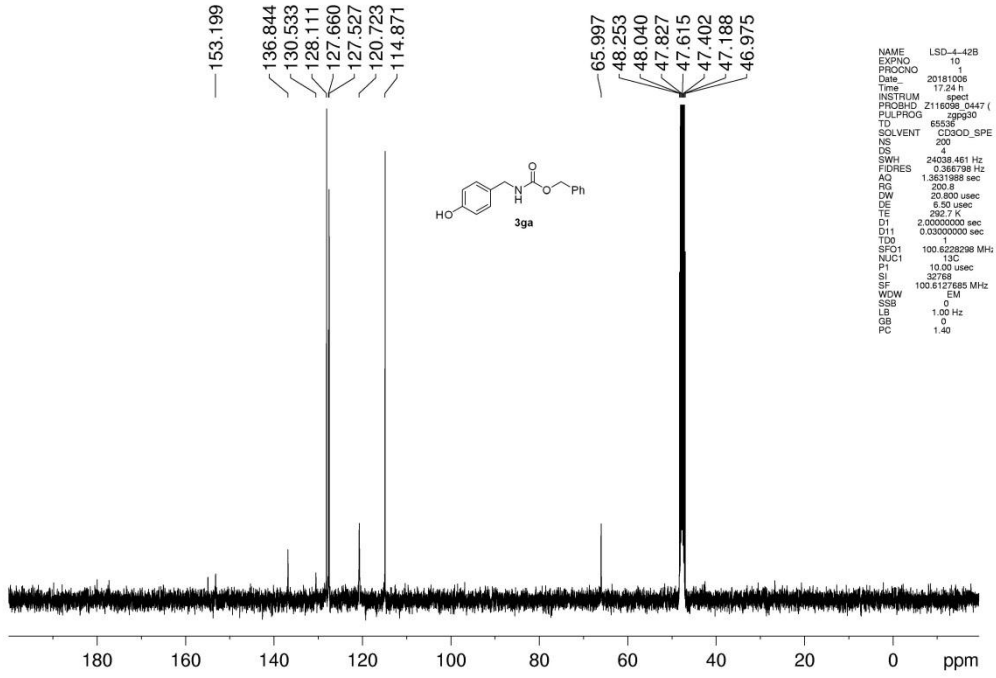
1.94
1.98
2.00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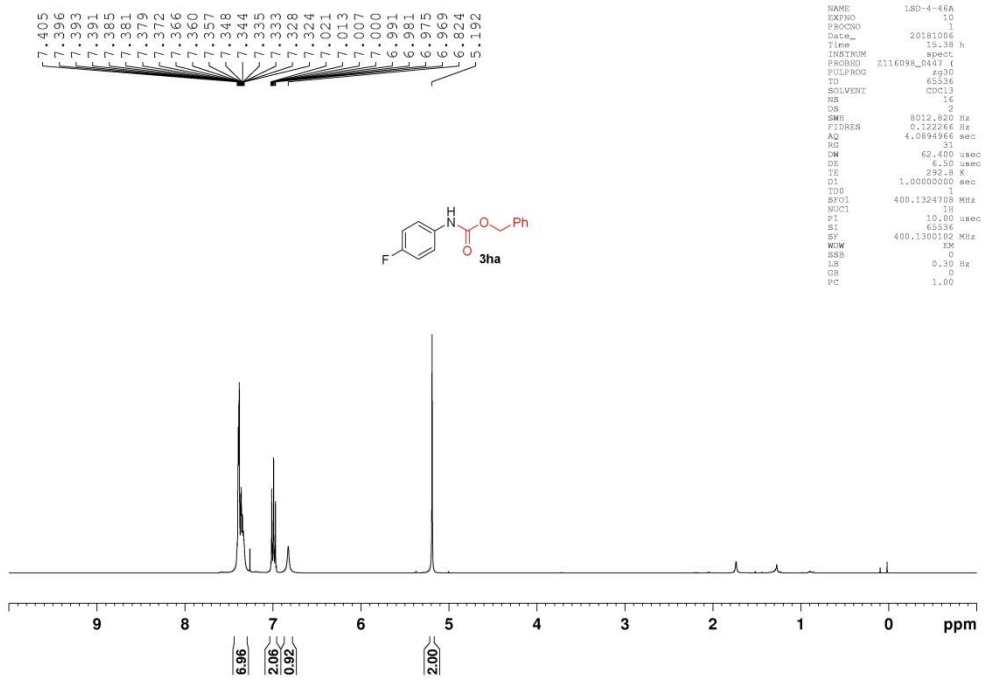
127.527
120.723
114.871
65.997
48.253
48.040
47.827
47.615
47.402
47.188
46.975
HO
Ph
3ga
180
160
140
120
100
80
60
40
20
0
ppm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7.372
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7.360
7.357
7.348
7.344
7.335
7.333
7.328
7.324
7.021
7.013
7.007
7.000
6.991
6.981
6.975
6.969
6.824
5.192
3ha
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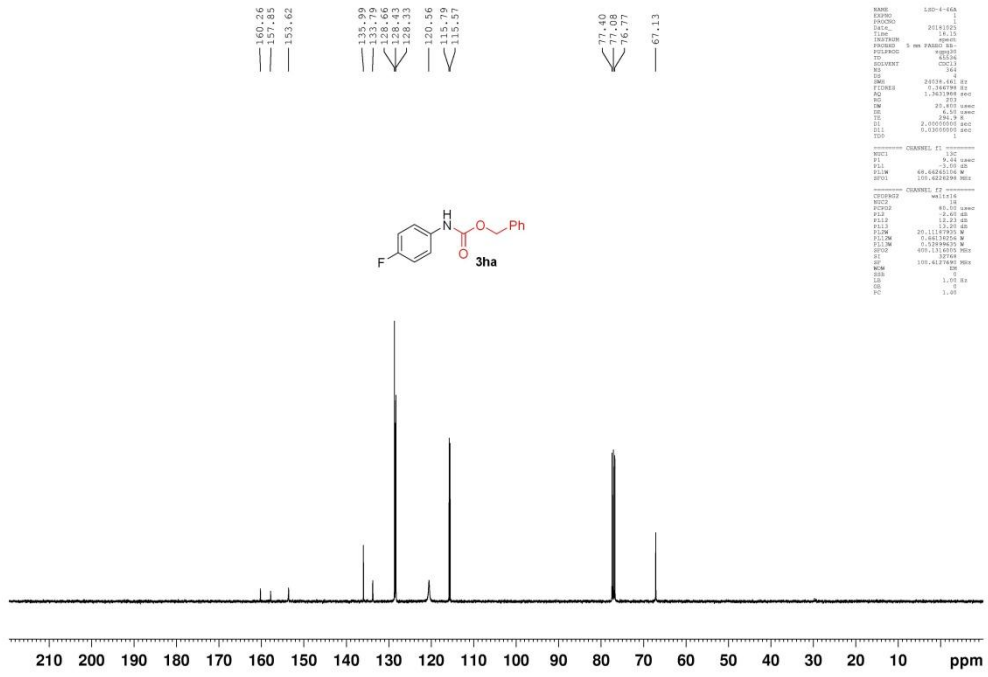
2.06
0.92
2.00
9
8
7
6
5
4
3
2
1
0
ppm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157.85
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133.79
128.66
128.43
128.33
120.56
115.79
115.57
77.40
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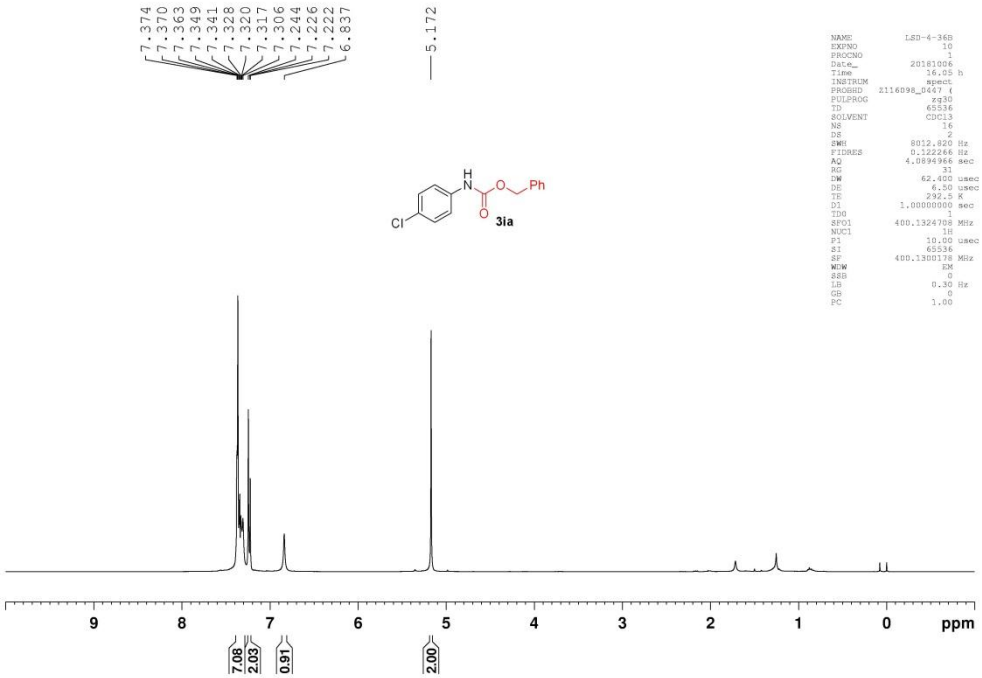
76.77
67.13
3ha
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.370
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7.328
7.320
7.317
7.306
7.244
7.226
7.222
6.837
5.172
3ia
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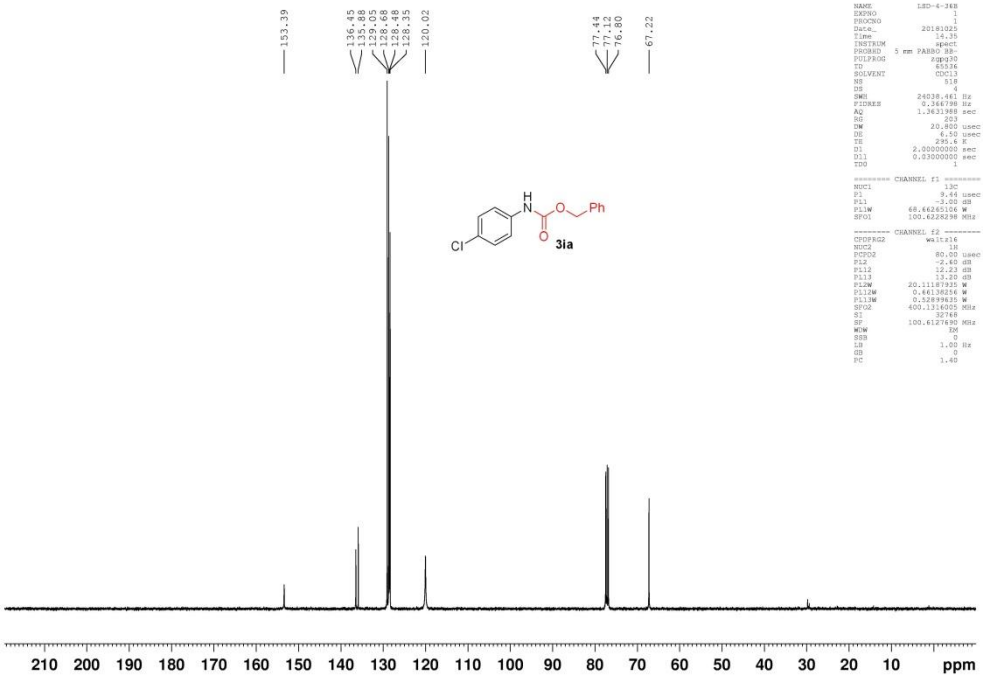
8
7
6
5
4
3
2
1
0
ppm
7.08
2.03
0.91
2.00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135.88
129.05
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124.48
120.02
77.44
77.12
76.80
67.22
3ia
210
200
190
180
170
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140
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120
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100
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80
70
60
50
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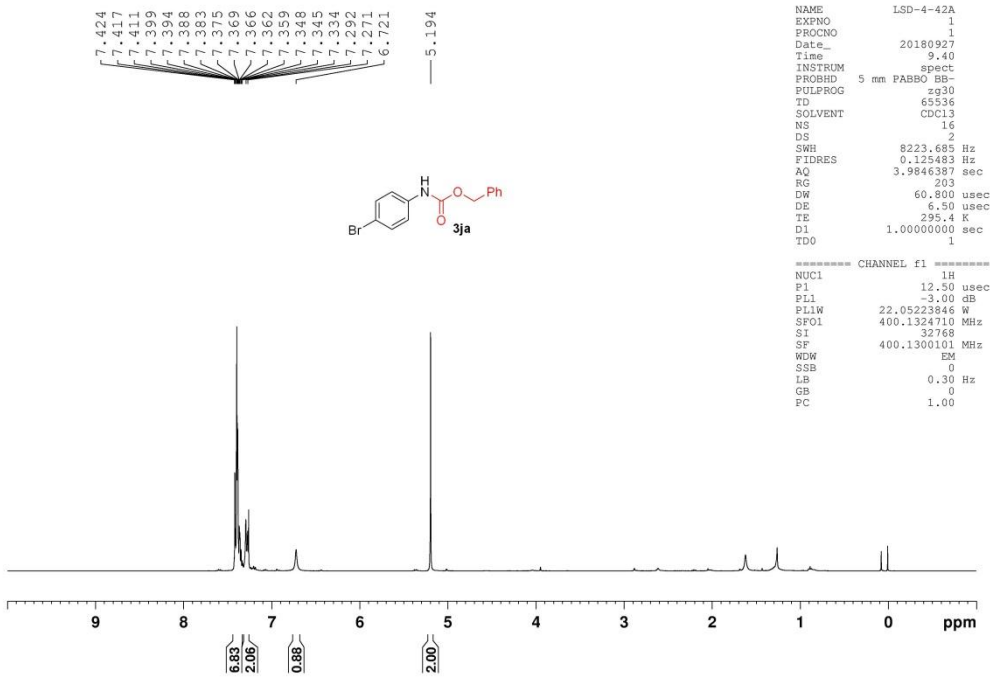
30
20
10
ppm


7.424
7.417
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7.399
7.394
7.388
7.383
7.375
7.369
7.366
7.362
7.359
7.348
7.345
7.334
7.292
7.271
6.721
5.194
NAME LSD-4-42A
EXPNO 1
PROCNO 1
Date_ 20180927
Time 9.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -3.00 dB
PL1W 22.05223846 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
Ph
3ja
9
8
7
6
5
4
3
2
1
0
ppm
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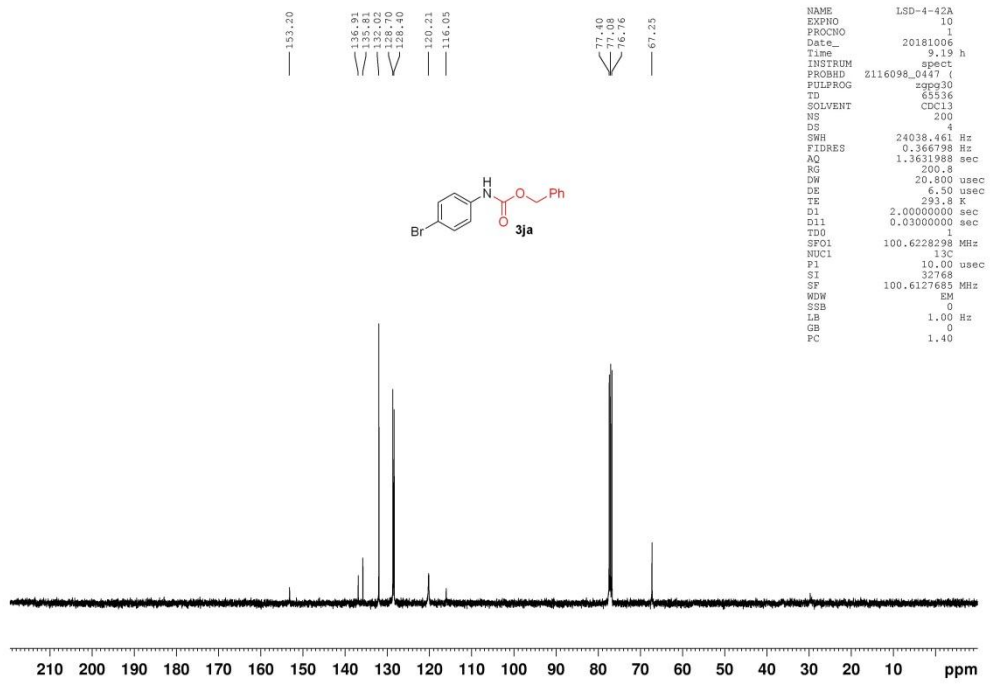
2.06
0.88
2.00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136.91
135.81
132.02
128.70
128.40
120.21
116.05
77.40
77.08
76.76
67.25
NAME LSD-4-42A
EXPNO 10
PROCNO 1
Date_ 20181006
Time 9.19 h
INSTRUM spect
PROBHD Z116098_0447 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 200.8
DW 20.800 usec
DE 6.50 usec
TE 293.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Br
Ph
3ja
210
200
190
180
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140
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110
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70
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50
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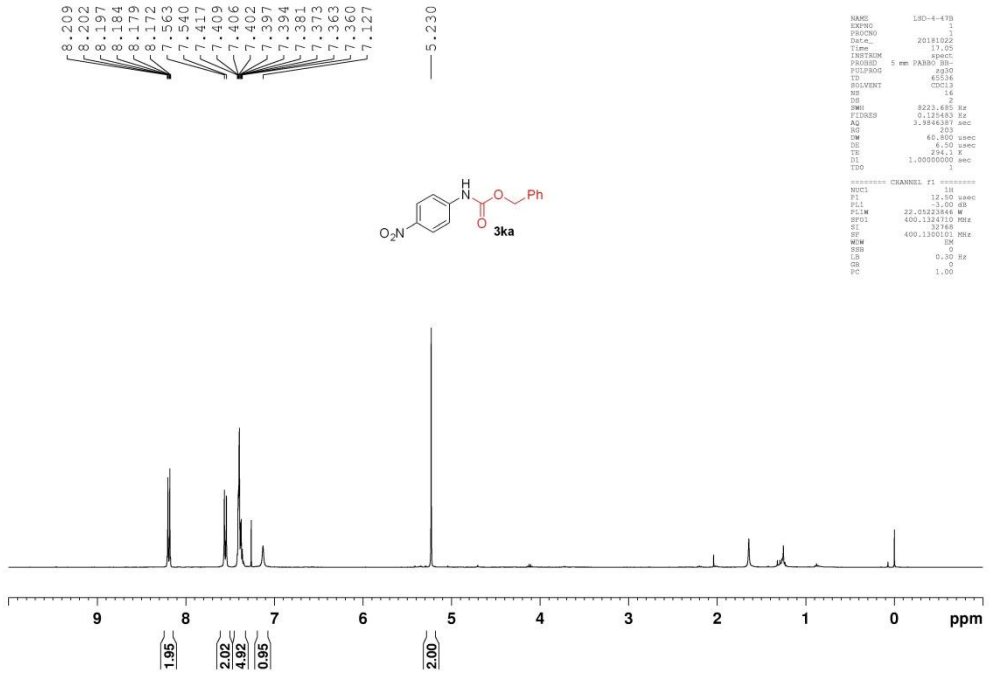
30
20
10
ppm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8.179
8.172
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7.540
7.417
7.409
7.406
7.402
7.397
7.394
7.381
7.373
7.363
7.360
7.127
5.230
3ka
9
8
7
6
5
4
3
2
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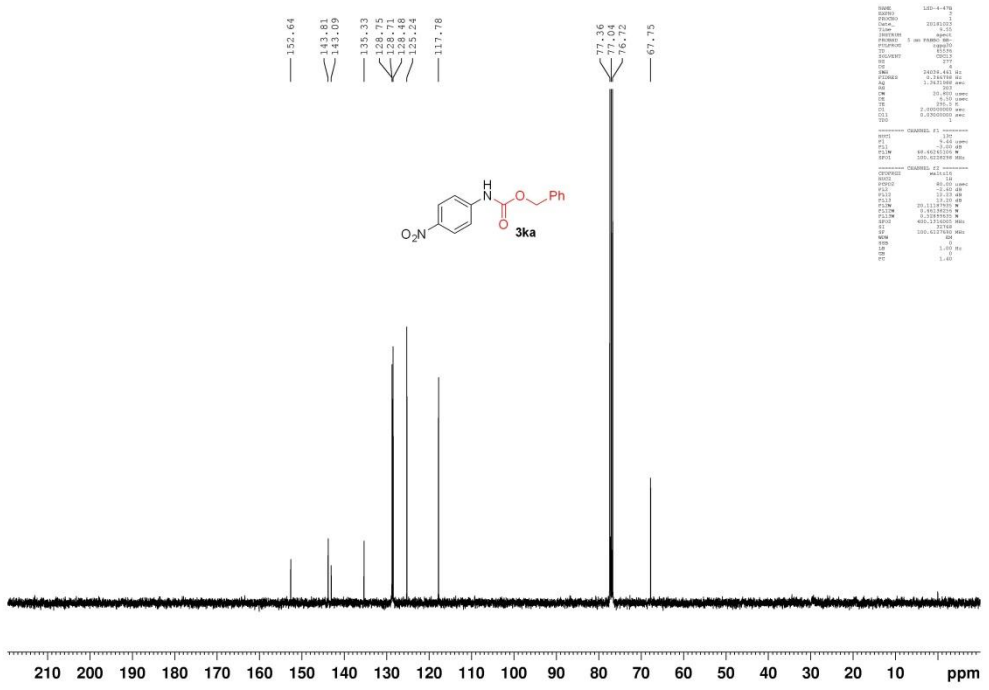
0
ppm
1.95
2.02
4.92
0.95
2.00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125.24
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77.36
77.04
76.72
67.75
3ka
210
200
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180
170
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150
140
130
120
110
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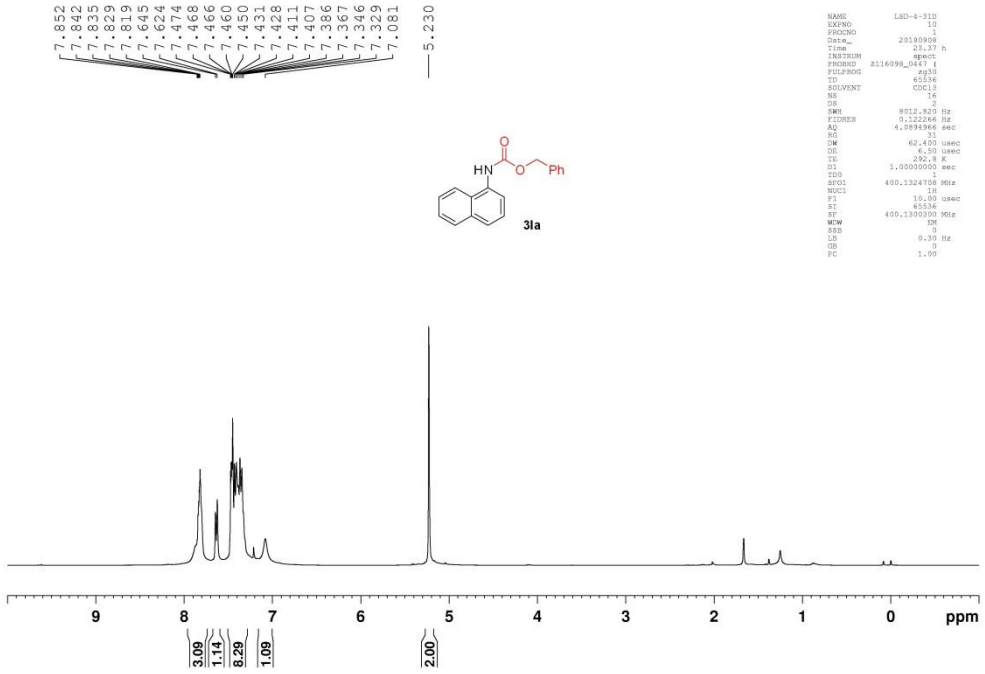
90
80
70
60
50
40
30
20
10
ppm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7.468
7.466
7.460
7.450
7.431
7.428
7.411
7.407
7.386
7.367
7.346
7.329
7.081
5.230
HN
O
O
Ph
3Ia
NAME LSD-4-31D
EXPNO 10
PROCNO 1
Date_ 20180908
Time 23.37 h
INSTRUM spect
PROBHD Z116098_0447 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 31
DW 62.400 usec
DE 6.50 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
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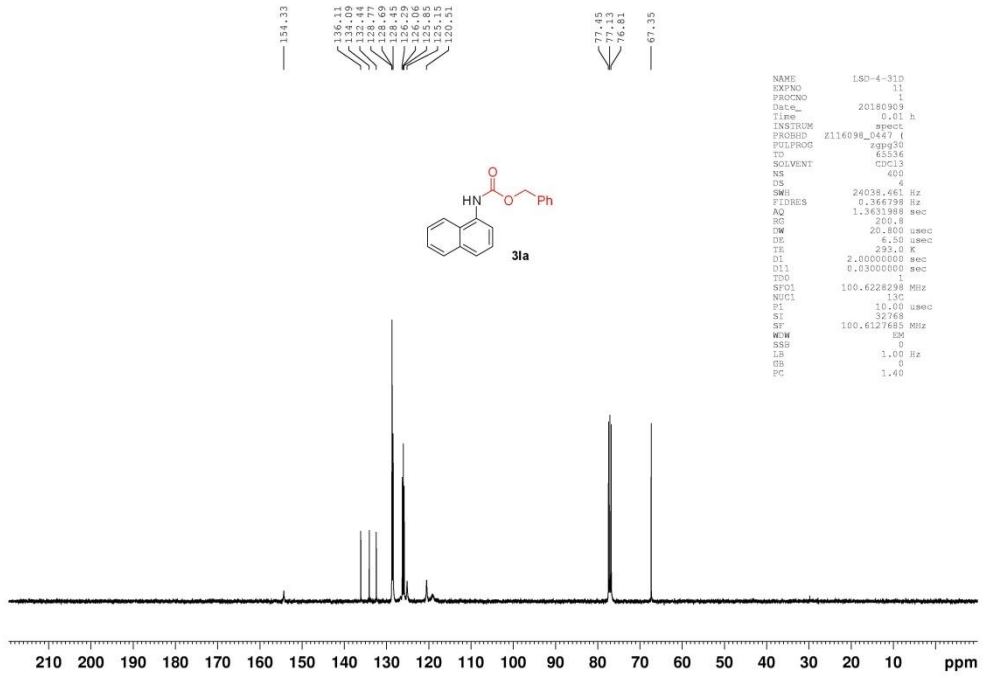
3.09
1.14
8.29
1.09
2.00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132.44
128.77
128.69
128.45
126.29
126.06
125.65
125.15
120.51
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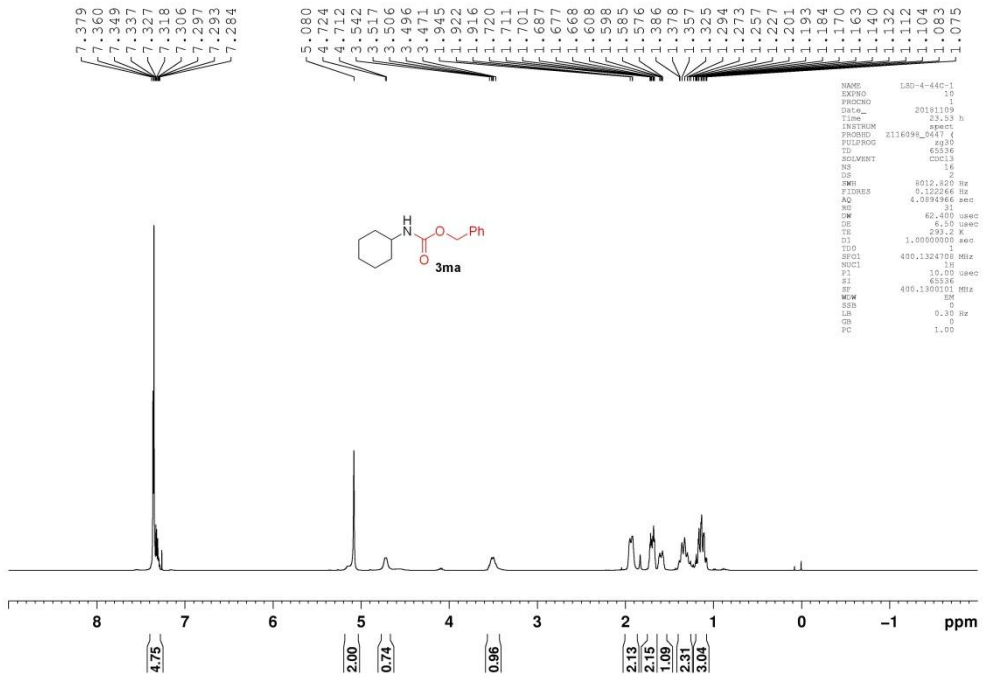
77.13
76.81
67.35
HN
O
O
Ph
3Ia
NAME LSD-4-31D
EXPNO 11
PROCNO 1
Date_ 20180909
Time 0.01 h
INSTRUM spect
PROBHD Z116098_0447 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203.8
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.306
7.297
7.293
7.284
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4.724
4.712
3.542
3.517
3.506
3.496
3.471
1.945
1.922
1.916
1.720
1.711
1.701
1.687
1.677
1.668
1.608
1.598
1.585
1.576
1.386
1.378
1.357
1.325
1.294
1.273
1.257
1.227
1.201
1.193
1.184
1.170
1.163
1.140
1.132
1.112
1.104
1.083
1.075
3ma
8
7
6
5
4
3
2
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−1
ppm
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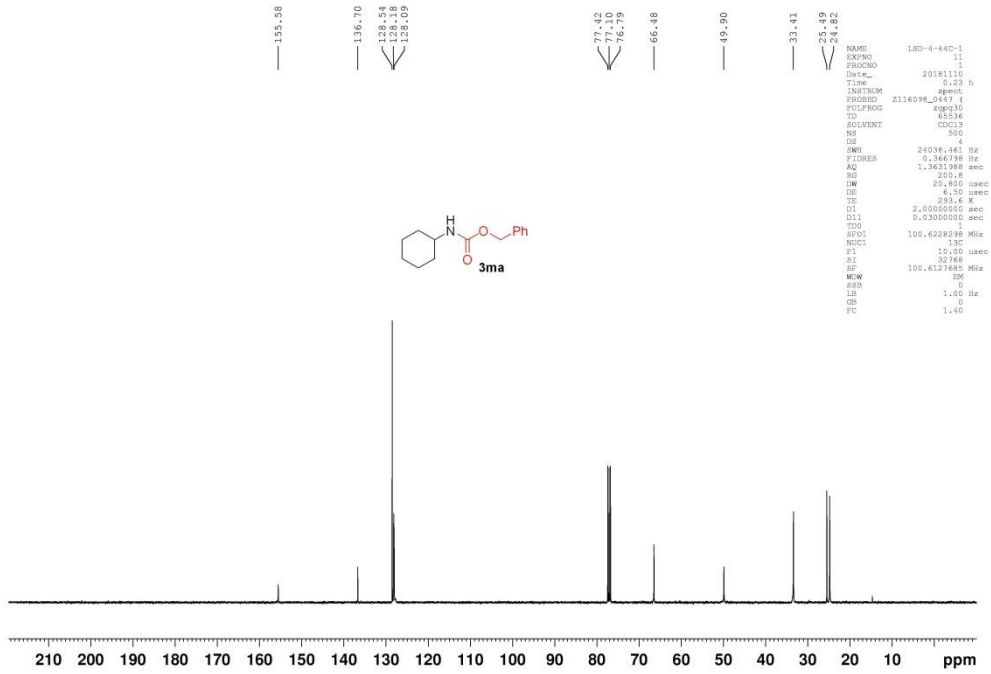
2.13
2.15
1.09
2.31
3.04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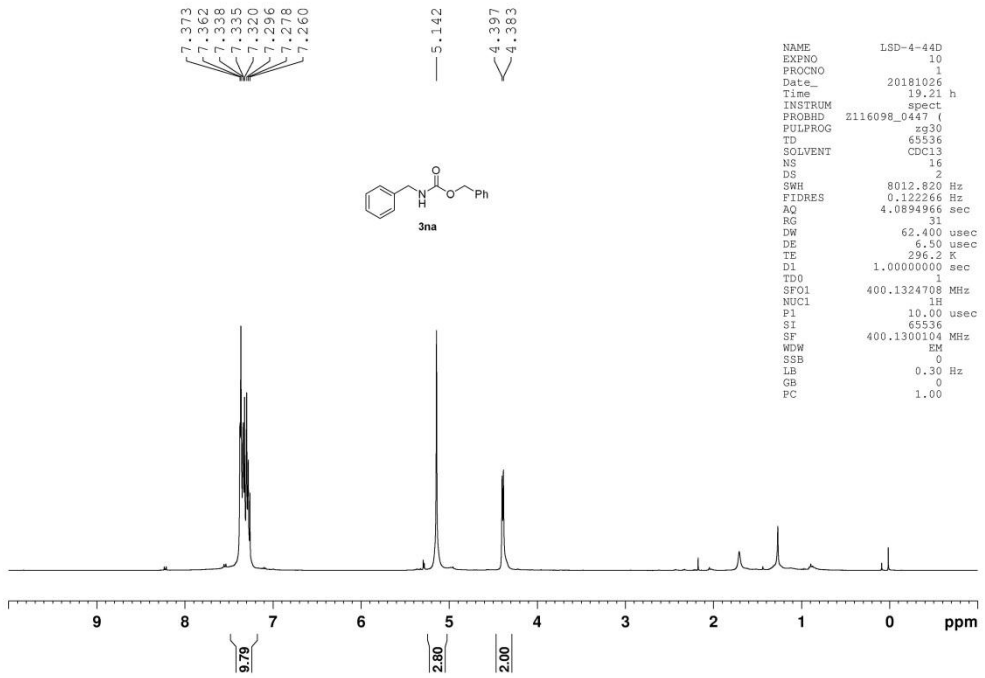
128.54
128.18
128.09
77.42
77.00
76.79
66.48
49.90
33.41
25.49
24.82
3ma
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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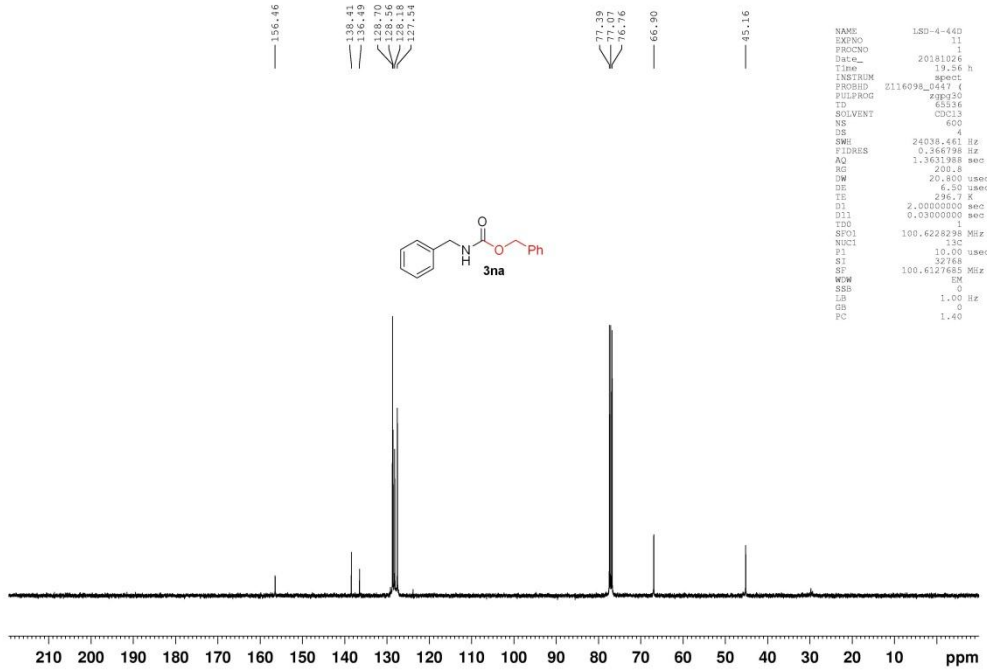
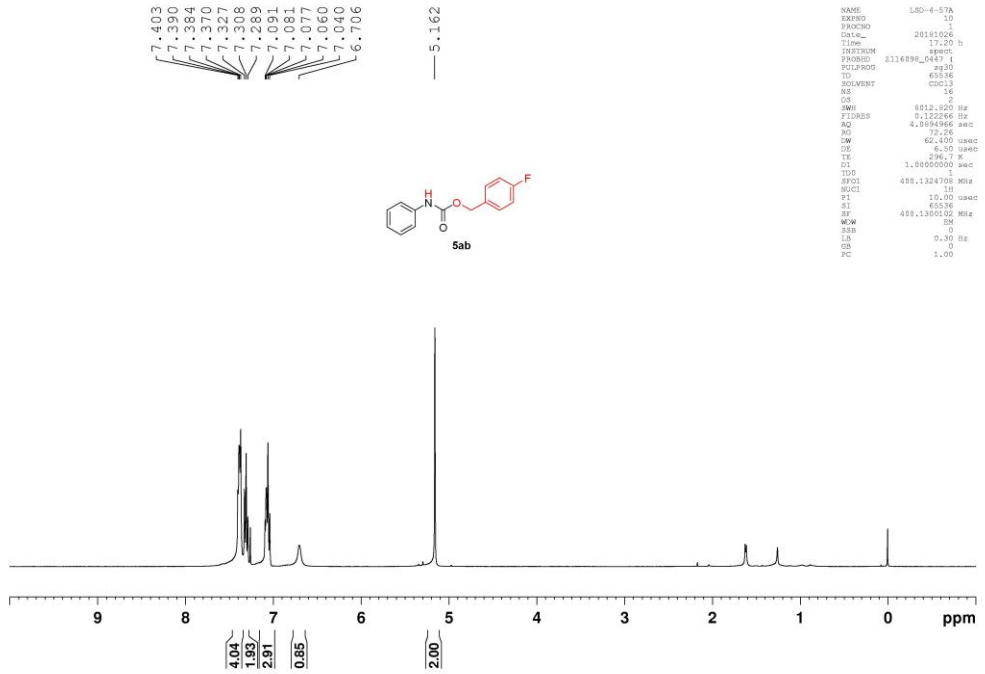
7.320
7.296
7.278
7.260
5.142
4.397
4.383
3na
NAME LSD-4-44D
EXPNO 10
PROCNO 1
Date_ 20181026
Time 19.21 h
INSTRUM spect
PROBHD Z116098_0447 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 31
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 0 ppm
9.79
2.80
2.00


156.46
138.41
136.49
128.70
128.56
128.18
127.54
77.39
77.07
76.76
66.90
45.16
3na
NAME LSD-4-44D
EXPNO 11
PROCNO 1
Date_ 20181026
Time 19.56 h
INSTRUM spect
PROBHD Z116098_0447 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 200.8
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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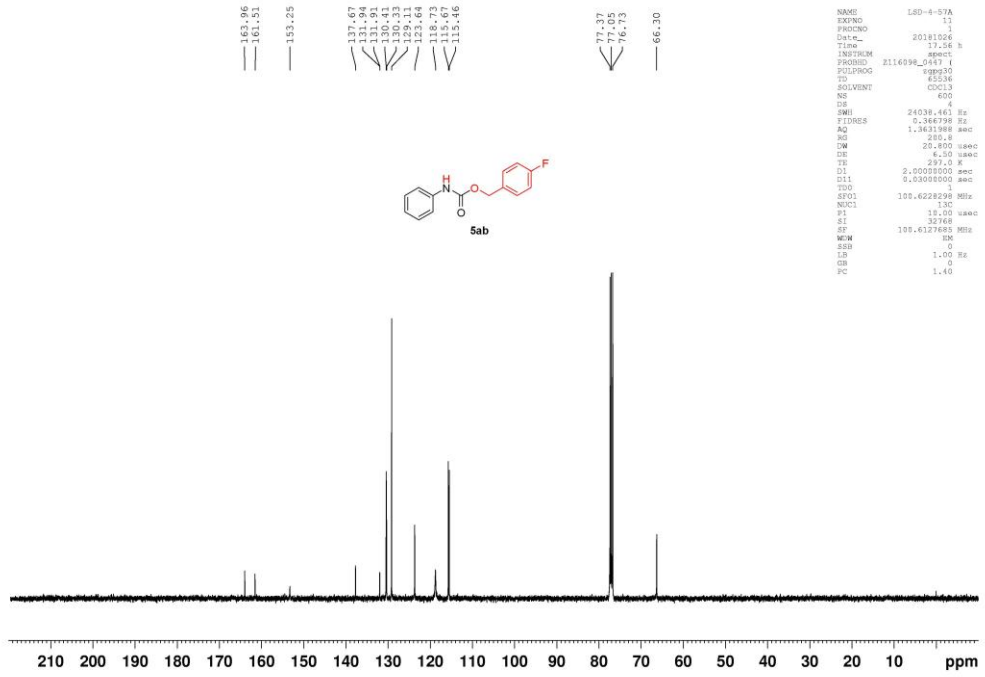
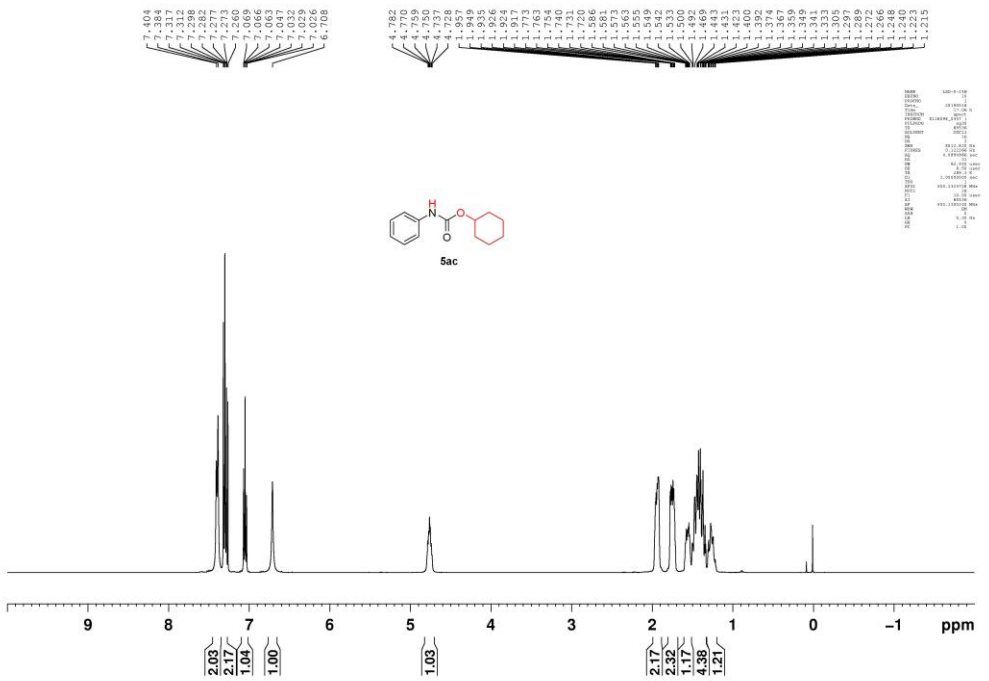
7.390
7.384
7.370
7.327
7.308
7.289
7.091
7.081
7.077
7.060
7.040
6.706
5.162
5ab
9
8
7
6
5
4
3
2
1
0
ppm
4.04
1.93
2.91
0.85
2.00


163.96
161.51
153.25
137.67
131.94
131.91
130.11
130.33
129.11
123.64
118.73
115.67
115.46
77.37
77.05
76.73
66.30
5ab
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.404
7.384
7.317
7.312
7.298
7.282
7.277
7.273
7.260
7.069
7.066
7.063
7.047
7.032
7.029
7.026
6.708
4.782
4.770
4.759
4.750
4.737
4.728
1.957
1.948
1.935
1.926
1.924
1.917
1.773
1.763
1.754
1.740
1.731
1.720
1.586
1.581
1.573
1.563
1.555
1.549
1.542
1.533
1.490
1.482
1.469
1.443
1.431
1.423
1.403
1.392
1.374
1.367
1.357
1.349
1.341
1.333
1.305
1.297
1.289
1.272
1.266
1.248
1.240
1.223
1.215
5ac
9
8
7
6
5
4
3
2
1
0
−1
ppm
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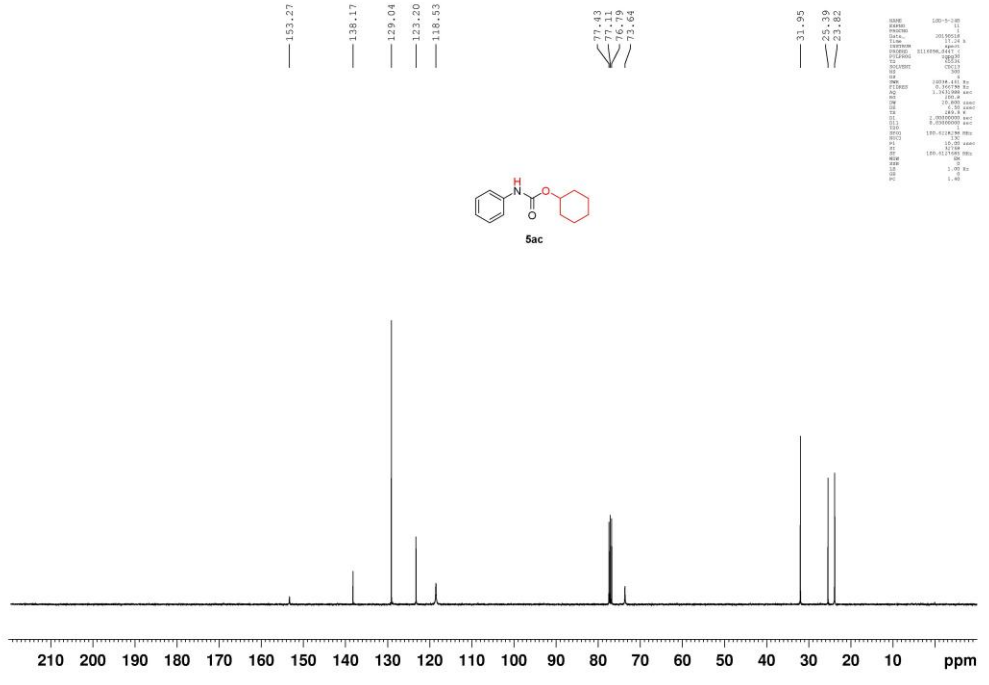
2.17
1.04
1.00
1.03
2.17
2.32
1.17
4.38
1.21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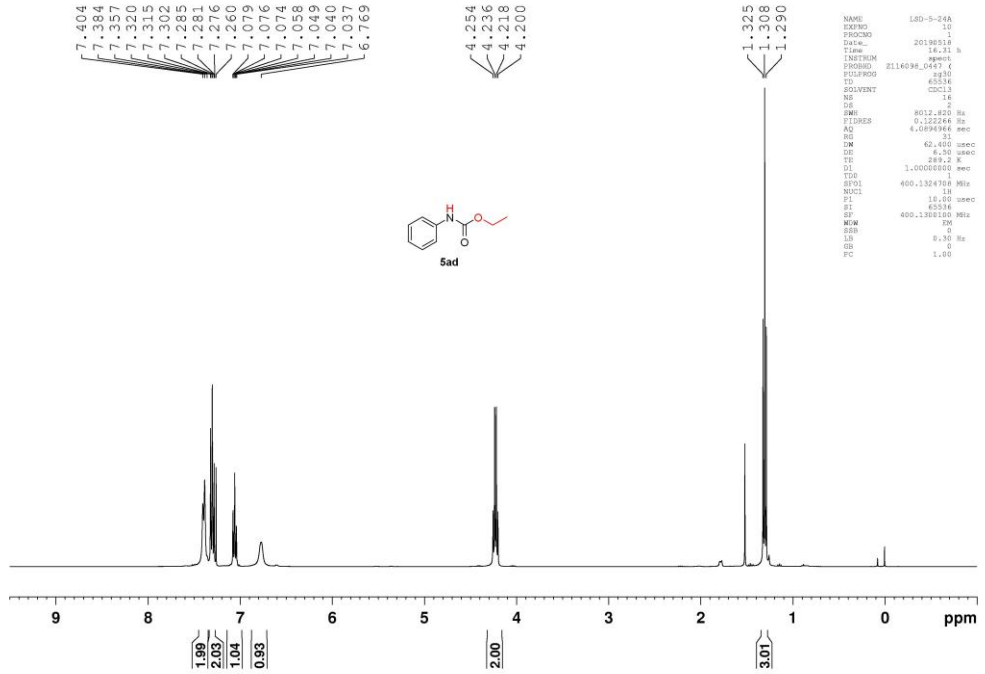
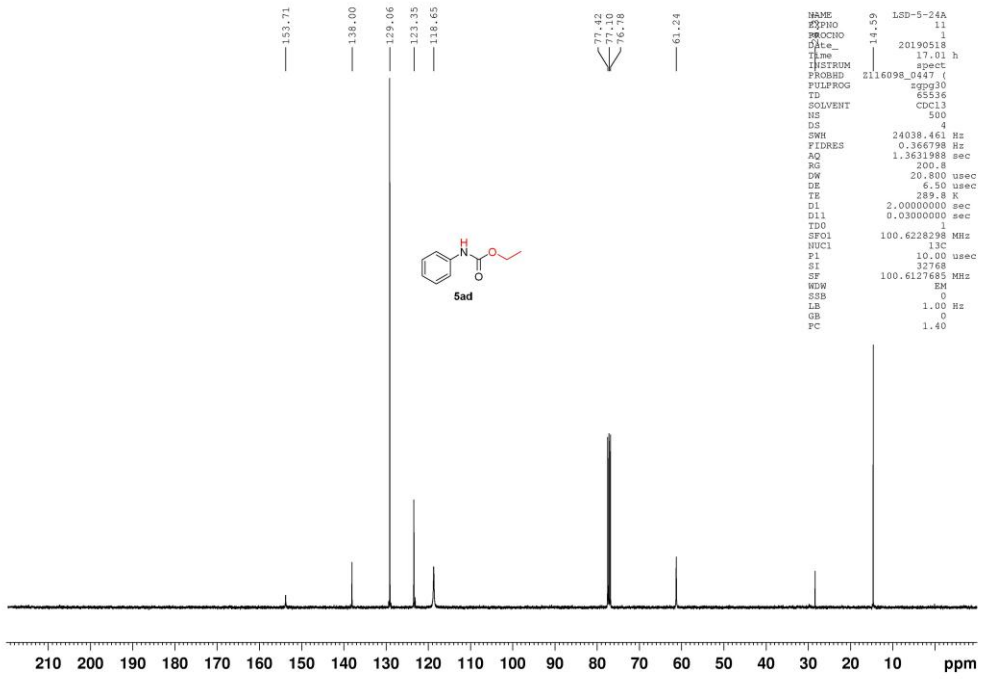
129.04
123.20
118.53
77.43
77.11
76.79
73.64
31.95
25.39
23.82
5ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.404
7.384
7.357
7.320
7.315
7.302
7.285
7.281
7.276
7.260
7.079
7.076
7.074
7.058
7.049
7.040
7.037
6.769
4.254
4.236
4.218
4.200
1.325
1.308
1.290
5ad
9
8
7
6
5
4
3
2
1
0
ppm
1.99
2.03
1.04
0.93
2.00
3.01


153.71
138.00
129.06
123.35
118.65
77.42
77.10
76.78
61.24
14.59
5ad
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm