Supporting Information

Controllable Chemoselectivity in Coupling of Bromoalkynes with Alcohols under Visible-Light Irradiation without Additives: Synthesis of Propargyl Alcohols and α-Ketoesters

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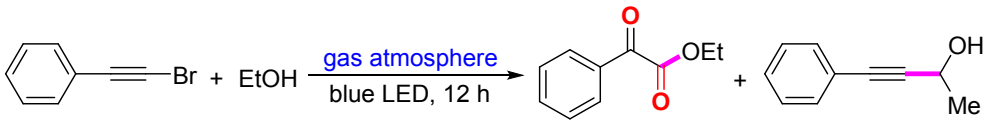
Table of Contents

1. General remarks

All reactions were conducted in clean glassware with magnetic stirring. Chromatographic purification was performed on silica gel (400~500 mesh) and analytical thin layer chromatography (TLC) on silica gel 60-F_{254} (Qindao), which was detected by fluorescence. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were measured with a Bruker AC 400 spectrometer with $CDCl_3$ as solvent and recorded in ppm relative to internal tetramethylsilane standard. NMR data are reported as follows: δ, chemical shift; coupling constants (*J* are given in Hertz, Hz) and integration. Abbreviations to denote the multiplicity of a particular signal were s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broad singlet). High resolution mass spectra were obtained with a Micromass GCT-TOF mass spectrometer. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. GC-MS spectra were measured with GCMS-QP2010 Plus. All light sources are purchased from the market without any particularity.

2. Optimization of reaction conditions for coupling of bromoalkynes with alcohols



1a **2a** **3aa** **4aa**

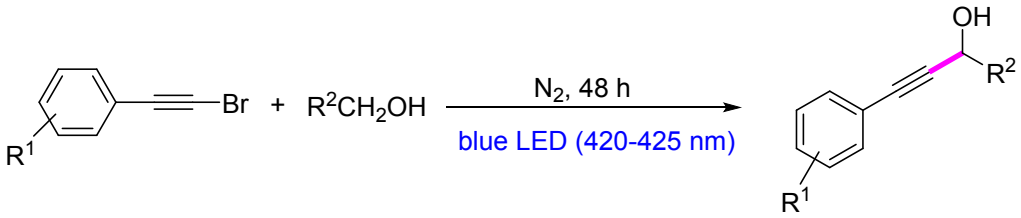
Entry	Light source (nm)	Gas atmosphere	Yield of **3aa** (%)[a]	Yield of **4aa** (%)[a]
1	Blue LED (420–470)	Air	57	Trace
2	*Blue LED (420–470)*	*O_2*	*73*	*Trace*
3	Blue LED (420–425)	O_2	12	Trace
4	Blue LED (450–455)	O_2	53	Trace
5	—	O_2	Trace	Trace
6	Red LED (610–650)	O_2	NR	NR
7	Yellow LED (570–610)	O_2	NR	NR
8	Green LED (480–570)	O_2	Trace	Trace
9	Blue LED (420–470)	N_2	Trace	15[b]
10	Blue LED (420–425)	N_2	Trace	37[b]
11	Blue LED (450–455)	N_2	Trace	18[b]
12	Blue LED (420–425)	N_2	Trace	45[c]
13	Blue LED (420–425)	N_2	Trace	51[c,d]
14	*Blue LED (420–425)*	*N_2*	*Trace*	*63[c,e]*
15	Blue LED (420–425)	N_2	Trace	54[c,f]

Reaction conditions: **1a** (0.30 mmol), **2a** (2 mL), light source, room temperature for 12 h. [a]Isolated yield. [b]For 36 h. [c]For 48 h. [d]**2a** (4 mL) was used. [e]**2a** (6 mL) was used. [f]**2a** (10 mL) was used.

3. General procedure for the synthesis of α-ketoesters

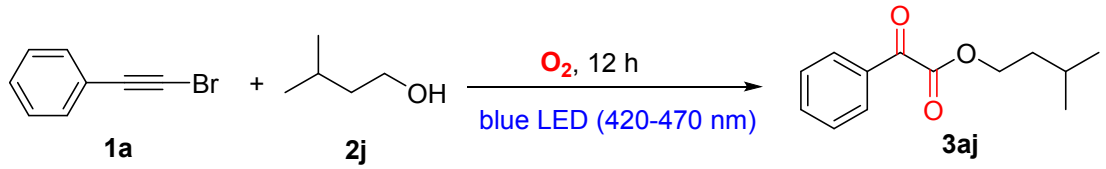
Bromoalkyne (0.20 mmol) was dissolved in ethanol or methanol (2.0 mL). The mixture was stirred tightly with the blue LED (420–470 nm) light source in O_2 for 12 h. Then, the residue was purified by column chromatography on silica gel (20:1 petroleum ether/EtOAc) to give the pure product [Note: CH_3CN was used as solvent when bromoalkynes were reacted with other alcohols (containing C atoms ⩾ 3, 2.0 mmol)].

4. General procedure for the synthesis of propargyl alcohols



Bromoalkyne (0.20 mmol) was dissolved in alcohol (6.0 mL). The mixture was stirred tightly with the blue LED (420–425 nm) light source in N_2 for 48 h. Then, the residue was purified by column chromatography on silica gel (1:2 petroleum ether/CH_2Cl_2) to give the pure product.

5. Optimization of the solvent on the reaction (For alcohol: C atoms ≥3)



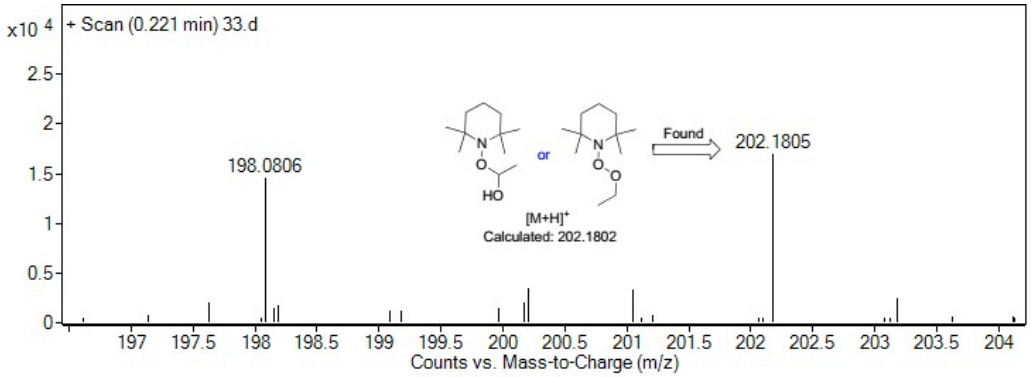
1a **2j** **3aj**

Entry	Solvent	Yield[b] (%)
1	CH_3CN	51
2	EtOAc	40
3	Ether	39
4	THF	35
5	1,4-Dioxane	33
6	CH_2Cl_2	< 10
7	DCE	< 10
8	Toluene	< 10
9	DMF	< 10
10	DMSO	< 10
11	CH_3CN	39[c]
12	CH_3CN	62[d]
13	*CH_3CN*	*76[e]*
14	CH_3CN	68[f]

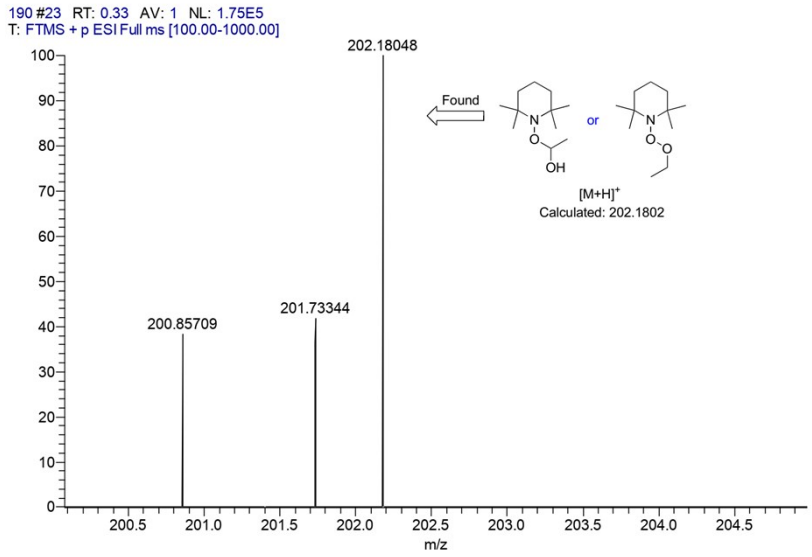
[a]Reaction conditions: **1a** (0.30 mmol), **2j** (0.60 mmol), blue LED (420–470 nm), solvent (2.0 mL), in O_2 atmosphere, room temperature for 12 h. [b]Isolated yield. [c]**2j** (0.30 mmol) was used. [d]**2j** (1.0 mmol) was used. [e]**2j** (2.0 mmol) was used. [f]**2j** (3.0 mmol) was used.

6. HRMS analysis for the intermediate C (or E), possible oxidation product of 1a, and the coupling product of 1a with 1g

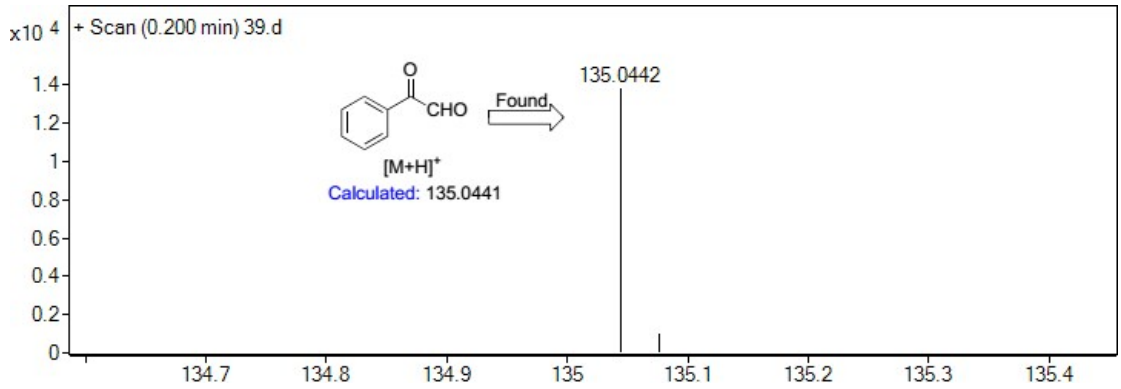
The HRMS studies (Schemes 4b and 4c) were tested to prove the formation of possible key intermediate **C** (or **E**), and which could be detected when 2,2,6,6-tetramethylpiperidinyl-1-oxy (TEMPO) was added under different conditions (one condition is formation of α-ketoesters, and another condition is formation of propargyl alcohol), but we could not be sure which one was coupled with TEMPO (one or both of them have). Further possible generation of byproducts (oxidation product of **1a**) and the different dimer products of **1a** with **1g** were also observed by HRMS studies, which imply that the initiation of the reaction might be started from the homolysis of bromoalkynes.



HRMS analysis of **C** or **E** for Scheme 4b of control experiment



HRMS analysis of **C** or **E** for Scheme 4c of control experiment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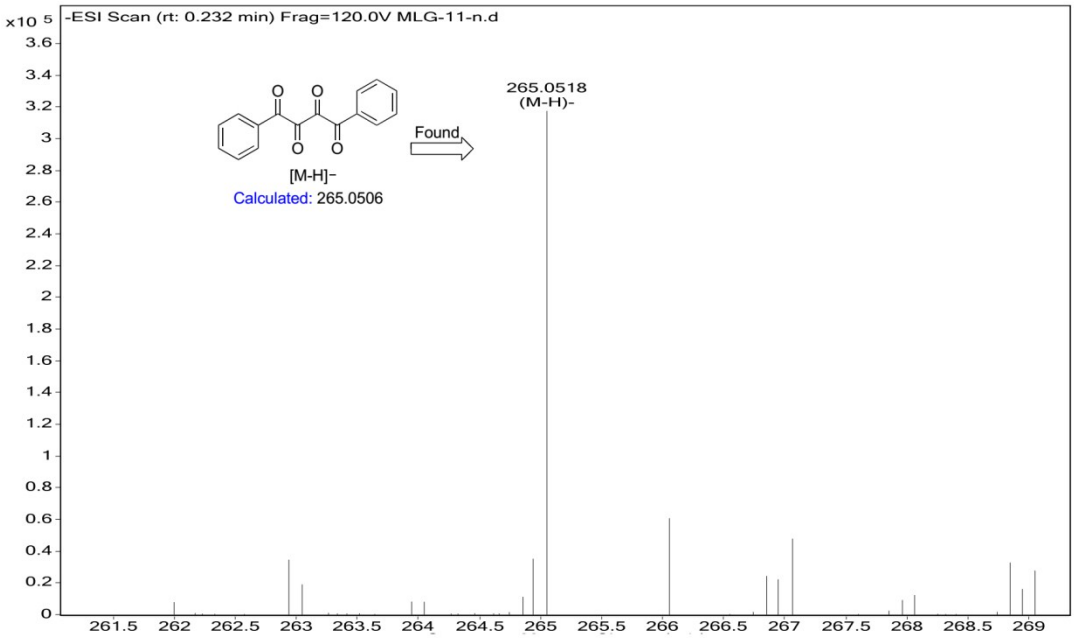
+ Scan (0.200 min) 39.d
O
CHO
Found
135.0442
[M+H]+
Calculated: 135.0441
1.4
1.2
1
0.8
0.6
0.4
0.2
0
134.7
134.8
134.9
135
135.1
135.2
135.3
135.4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O
O
O
Found
265.0518
(M-H)-
[M-H]−
Calculated: 265.0506
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
261.5
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266.5
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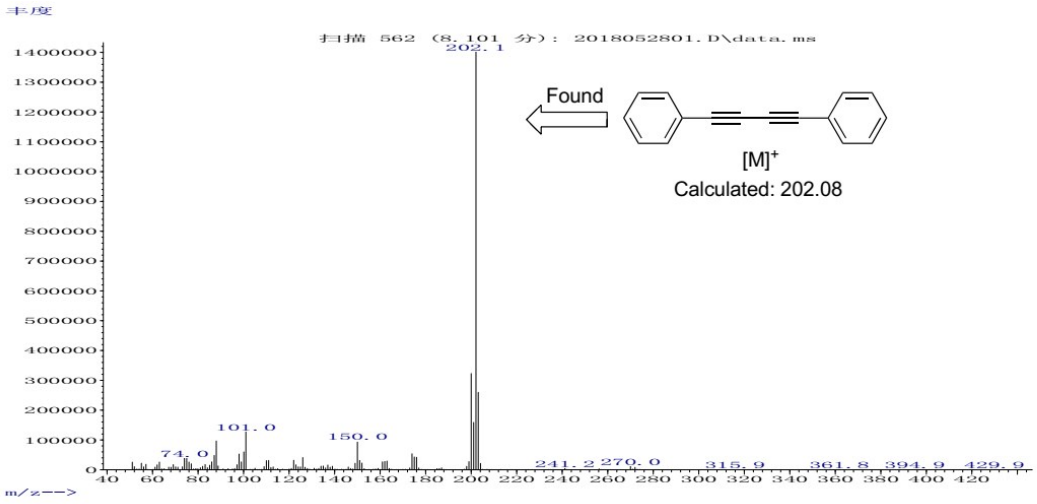
267.5
268
268.5
269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[M]+
Calculated: 202.08
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1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
101.0
150.0
74.0
241.2
270.0
315.9
361.8
394.9
429.9
40
60
80
100
120
140
160
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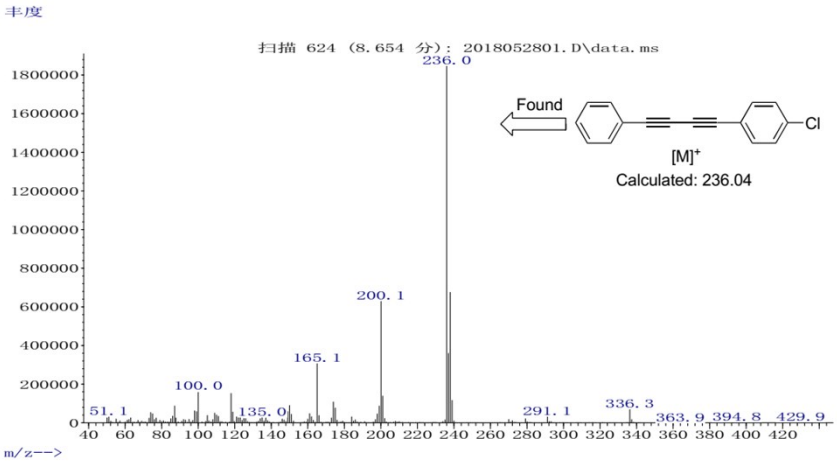
280
300
320
340
360
380
400
420
m/z-->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100.0
51.1
135.0
291.1
336.3
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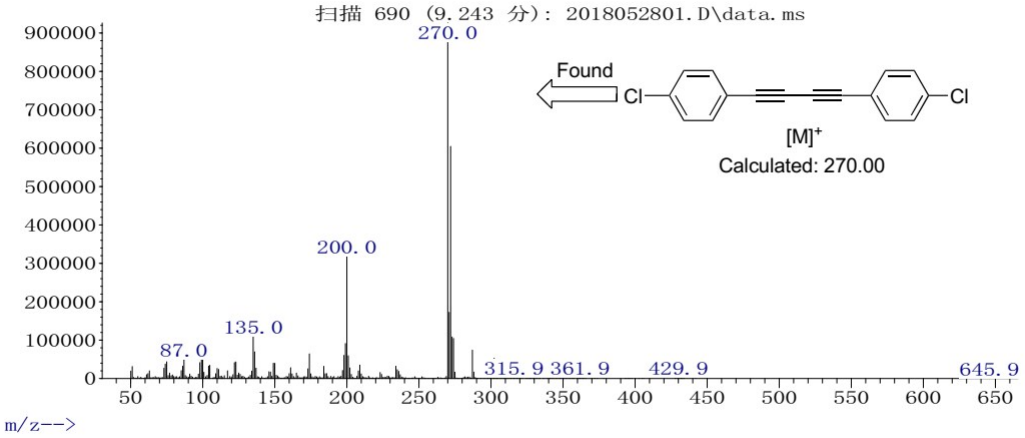
[M]+
Calculated: 236.04
m/z-->

丰度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Cl
[M]+
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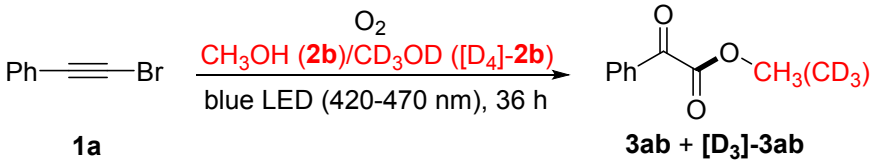
m/z-->

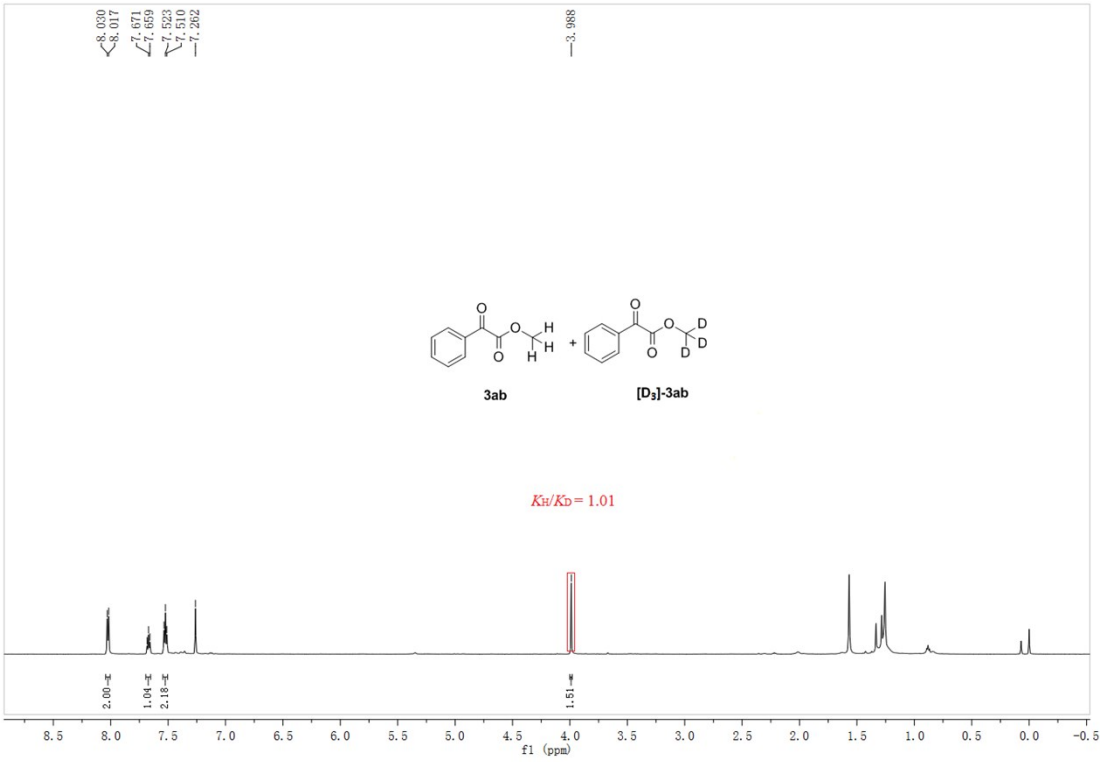
7. Kinetic isotope effect (KIE) experiments

7.1 KIE experiment (I)

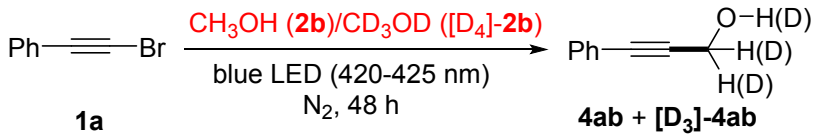


1a **3ab + [D$_3$]-3ab**

Phenylethynyl bromide (**1a**, 0.20 mmol) was dissolved in mixture of methanol (25 mmol) and D_4-methanol (25 mmol). The mixture was stirred tightly with the blue LED (420–470 nm) irradiation in O_2 for 36 h. Then, the residue was purified by column chromatography on silica gel (20:1 petroleum ether/EtOAc) to give the pure product (6 mg, ~19% total yield). The KIE value (k_H/k_D = 1) was determined by ^{1}H NMR (600 MHz) of **3ab** and **[D$_3$]-3ab**.

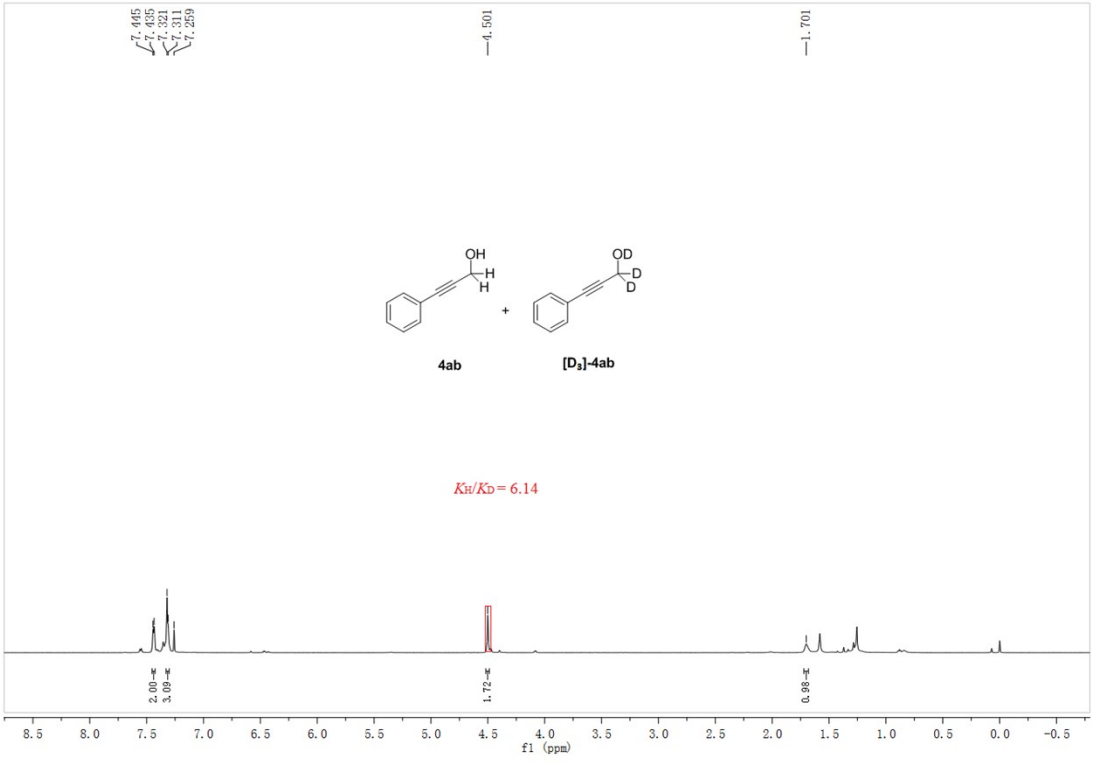


7.2 KIE experiment (II)



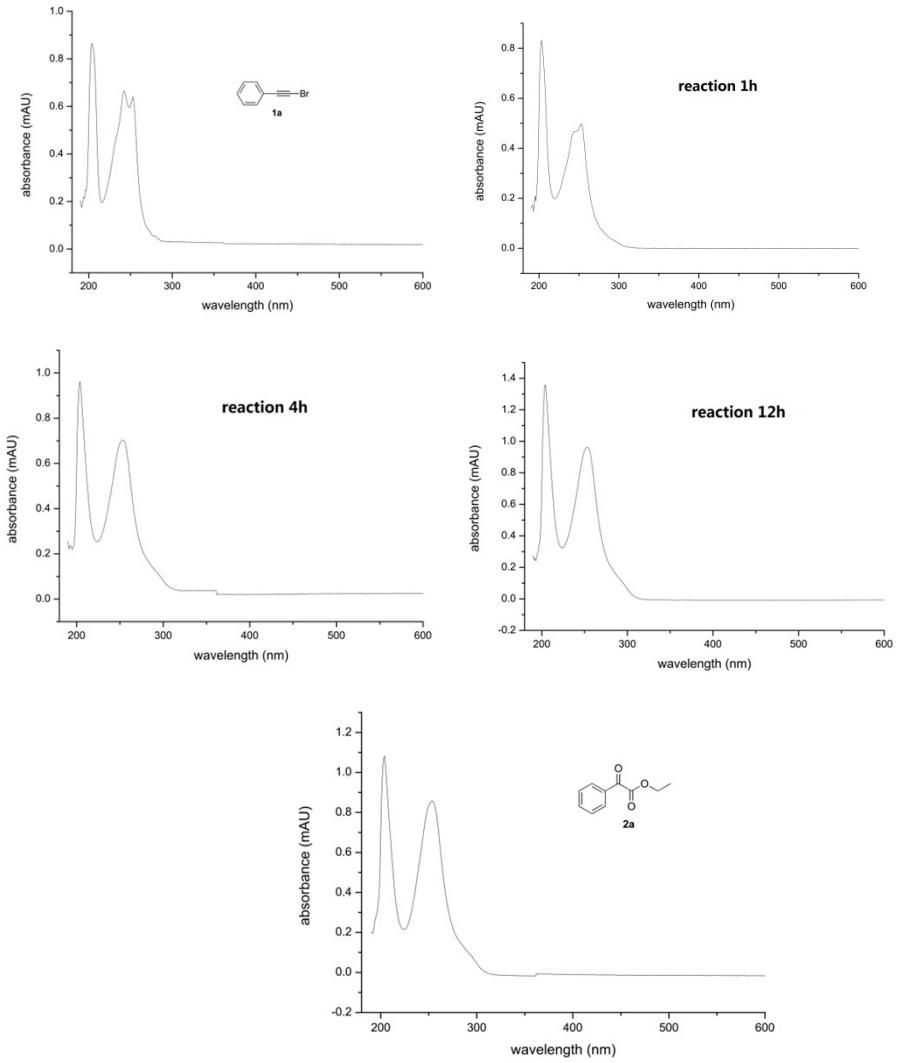
1a **4ab** + **[D_3]-4ab**

Phenylethynyl bromide (**1a**, 0.20 mmol) was dissolved in in mixture of methanol (36 mmol) and D_4-methanol (36 mmol). The mixture was stirred tightly with the blue LED (420–425 nm) irradiation in N_2 for 48 h. Then, the residue was purified by column chromatography on silica gel (1:2 petroleum ether/CH_2Cl_2) to give the pure product (4 mg, ~16% total yield). The KIE value (k_H/k_D = 6.14) was determined by ^{1}H NMR (600 MHz) of **4ab** and **[D_3]-4ab**.



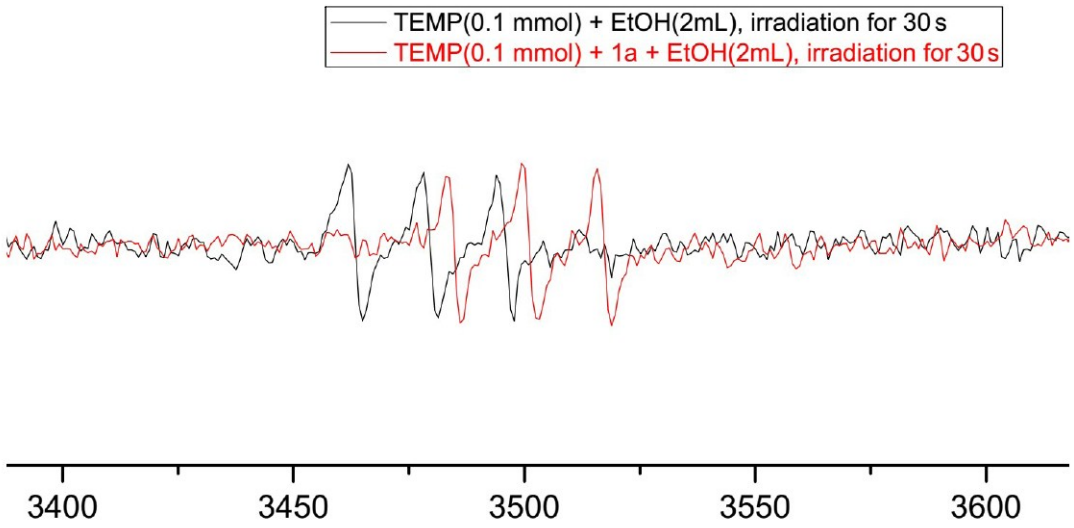
8. UV-Vis experiments

The UV-Vis measurement was performed with an ethanol solution of **1a**, indicating that an electron-donor acceptor (EDA) complex was not formed.



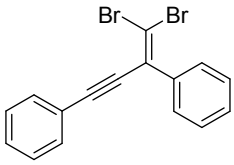
9. EPR experiments

The EPR were investigated under following conditions, which proved the non-existence of $^1O_2$ during the formation of α-ketoesters.

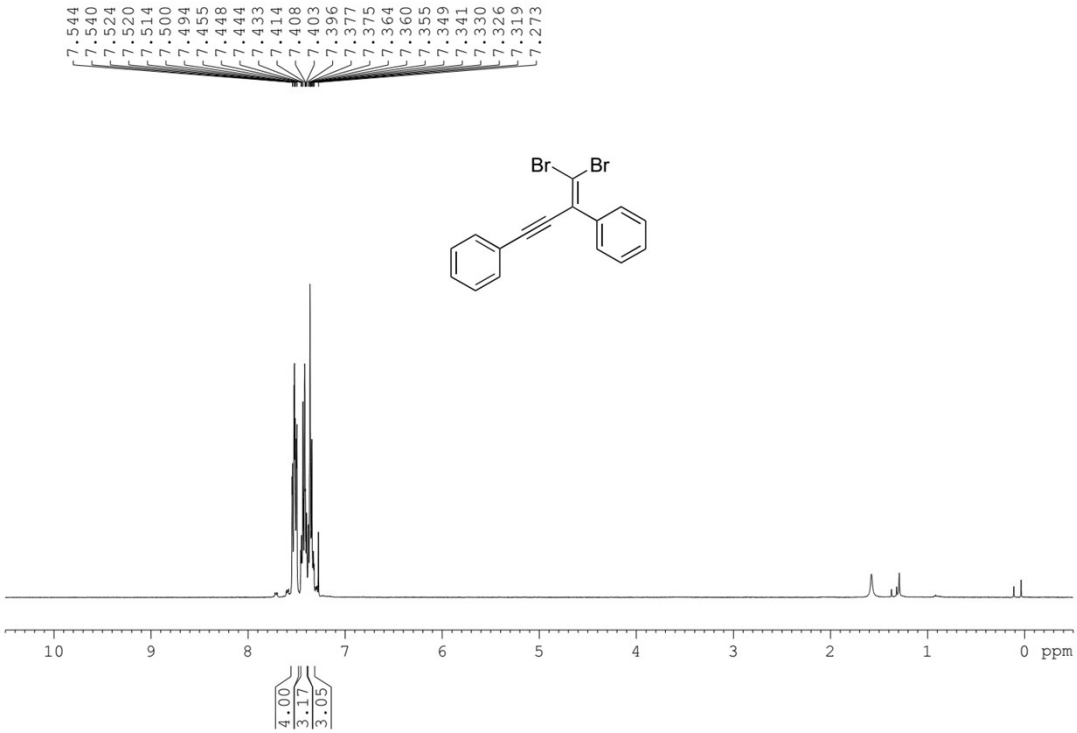


10. Characterization data for 4,4-dibromobut-3-en-1-yne-1,3-diyl)dibenzene

Known compound, see: V. K. Karapala, H.-P. Shih and C.-C. Han, *Org. Lett*., 2018, **20**, 1550.



Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54–7.49 (m, 4H), 7.45–7.39 (m, 3H), 7.37–7.31 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.0, 131.5, 130.9, 128.9, 128.5, 128.5, 128.3, 128.3, 122.5, 98.9, 97.5, 88.9.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7.524
7.520
7.514
7.500
7.494
7.455
7.448
7.444
7.433
7.414
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7.396
7.377
7.375
7.364
7.360
7.355
7.349
7.341
7.330
7.326
7.319
7.273
Br
Br
10
9
8
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2
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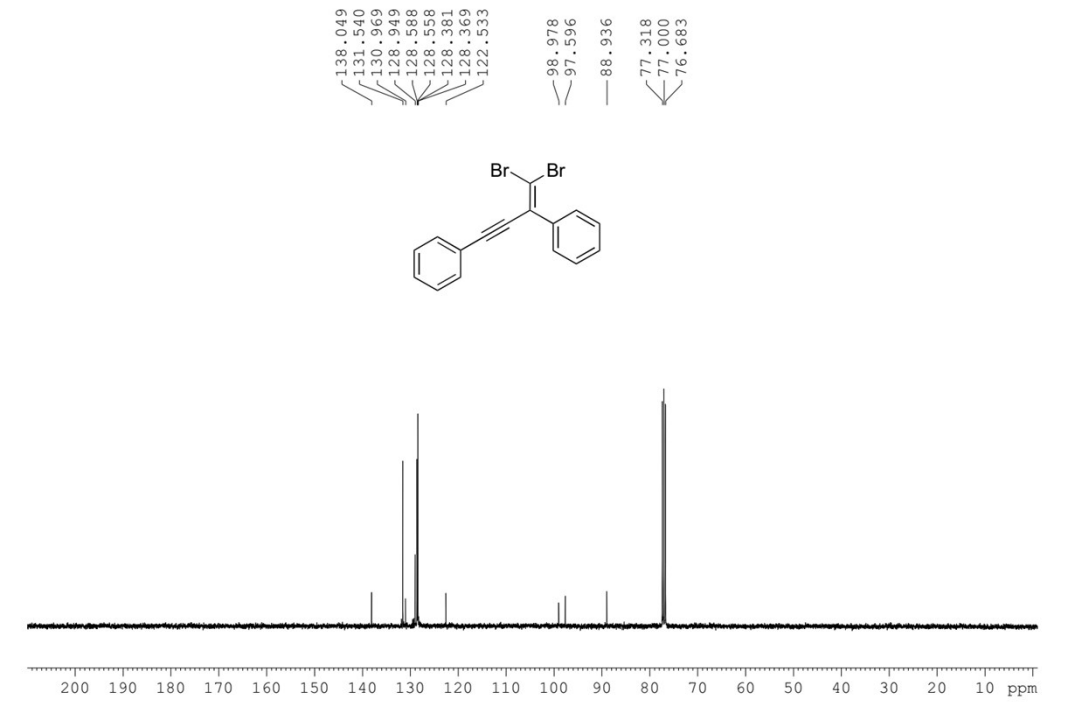
3.17
3.05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Br
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
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40
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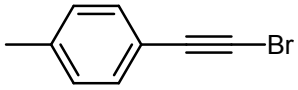
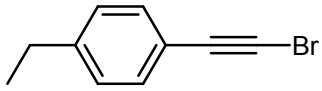
20
10 ppm

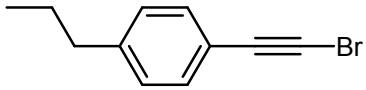
11. Characterization data for the bromoalkynes (1b–1n)



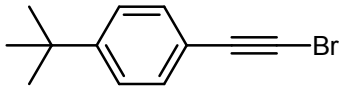
1-(Bromoethynyl)-4-methylbenzene (1b).[1] Yellow oil (163 mg, 84% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 2.36 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.8, 131.8, 129.0, 119.6, 80.1, 48.7, 21.4.



1-(Bromoethynyl)-4-ethylbenzene (1c).[2] Yellow oil (170 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.1, 131.9, 127.8, 119.8, 80.1, 48.6, 28.8, 15.2.

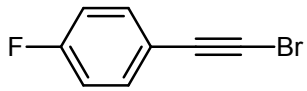


1-(Bromoethynyl)-4-propylbenzene (1d).[3] Yellow oil (180 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.39 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 2.61 (t, J = 7.2 Hz, 2H), 1.69 (sextet, J = 7.2 Hz, 2H), 0.97 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.6, 131.8, 128.4, 119.8, 80.2, 48.7, 37.9, 24.2, 13.7.

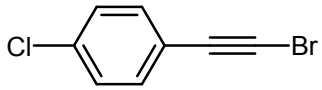


1-(Bromoethynyl)-4-(*tert*-butyl)benzene (1e).[3] Colorless oil (185 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31–7.39 (m, 2H), 7.35–7.33 (m, 2H), 1.32 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.9, 131.7, 125.3, 119.6, 80.1,

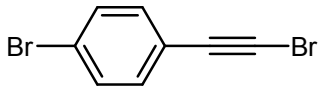
48.6, 34.8, 31.3.



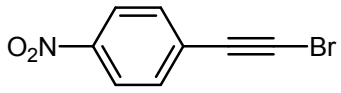
1-(Bromoethynyl)-4-fluorobenzene (1f).[2] Yellow oil (155 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46–7.41 (m, 2H), 7.04–6.99 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.9 (d, J = 248.7 Hz), 133.9 (d, J = 8.5 Hz), 118.8 (d, J = 3.5 Hz), 115.7 (d, J = 22.0 Hz), 79.0, 49.5.



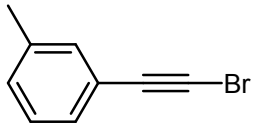
1-(Bromoethynyl)-4-chlorobenzene (1g).[1] White solid (174 mg, 81% yield). Mp: 88–90 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40–7.37 (m, 2H), 7.31–7.28 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.8, 133.2, 128.7, 121.1, 79.0, 51.0.



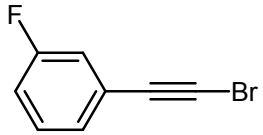
1-Bromo-4-(bromoethynyl)benzene (1h).[1] White solid (207 mg, 80% yield). Mp: 100–101 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47–7.44 (m, 2H), 7.33–7.29 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.4, 131.6, 123.0, 121.6, 79.0, 51.2.



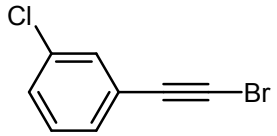
1-(Bromoethynyl)-4-nitrobenzene (1i).[1] Yellow solid (171 mg, 76% yield). Mp: 170–172 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21–8.18 (m, 2H), 7.62–7.58 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 147.3, 132.8, 129.4, 123.6, 78.4, 56.3.



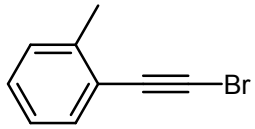
1-(Bromoethynyl)-3-methylbenzene (1j).[2] Yellow oil (144 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30–7.27 (m, 2H), 7.24–7.16 (m, 2H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.0, 132.5, 129.5, 129.0, 128.2, 122.5, 80.2, 49.2, 21.7.



1-(Bromoethynyl)-3-fluorobenzene (1k).[4] Yellow oil (149 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31–7.22 (m, 2H), 7.17–7.13 (m, 1H), 7.09–7.04 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.4 (d, J = 245.5 Hz), 129.9 (d, J = 8.4 Hz), 127.9 (d, J = 3.0 Hz), 124.5 (d, J = 9.5 Hz), 118.9 (d, J = 23.0 Hz), 116.2 (d, J = 21.1 Hz), 78.8, 51.2.

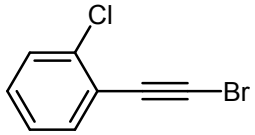


1-(Bromoethynyl)-3-chlorobenzene (1l).[1] Yellow oil (169 mg, 79% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 (t, J = 1.6 Hz, 1H), 7.34–7.32 (m, 2H), 7.27–7.23 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.1, 131.8, 130.1, 129.5, 129.0, 124.3, 78.7, 51.4.



1-(Bromoethynyl)-2-methylbenzene (1m).[1] Yellow oil (146 mg, 75% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 (d, J = 7.6 Hz, 1H), 7.28–7.20 (m, 2H),

7.17–7.13 (m, 1H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.8, 132.3, 129.4, 128.6, 125.5, 122.5, 79.1, 52.7, 20.5.



1-(Bromoethynyl)-2-chlorobenzene (1n).[1] Colorless oil (159 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (dd, *J* = 1.2, 7.6 Hz 1H), 7.41 (dd, *J* = 0.8, 8.0 Hz, 1H), 7.30 (td, *J* = 1.2, 7.6 Hz, 1H), 7.23 (td, *J* = 1.2, 7.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 136.3, 133.8, 129.6, 129.3, 126.4, 122.6, 76.9, 55.2.

Reference:

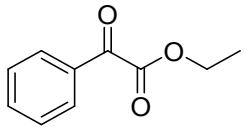
1. X. Y. Chen, L. Wang, M. Frings and C. Bolm, *Org. Lett*., 2014, **16**, 3796.

2. Y.-S. Feng, Z.-Q. Xu, L. Mao, F.-F. Zhang and H.-J. Xu, *Org. Lett*., 2013, **15**, 1472.

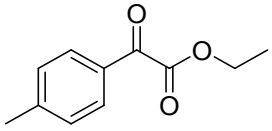
3. K. K. Rajbongshi, D. Hazarika and P. Phukan, *Tetrahedron,* 2016, **72**, 4151.

4. K. Villeneuve, N. Riddell, R. W. Jordan, G. C. Tsui and W. Tam, *Org. Lett*., 2004, **6**, 4543.

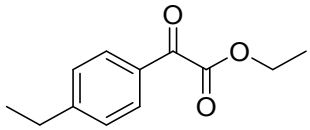
12. Characterization data for all products



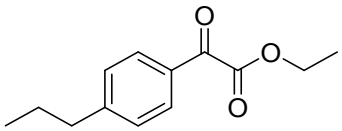
Ethyl 2-oxo-2-phenylacetate1 (3aa).[1] Colorless oil (39 mg, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02–8.00 (m, 2H), 7.68–7.64 (m, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 4.48 (q, *J* = 7.2 Hz, 2H), 1.44 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.4, 163.8, 134.8, 132.4, 130.0, 128.8, 62.3, 14.1.



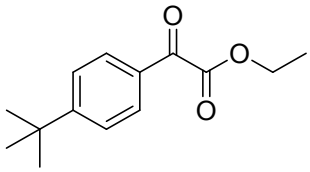
Ethyl 2-oxo-2-(*p*-tolyl)acetate (3ba).[2] Pale yellow oil (44 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.4, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 4.46 (q, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 1.43 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.0, 164.0, 146.1, 130.1, 130.0, 129.6, 62.1, 21.8, 14.0.



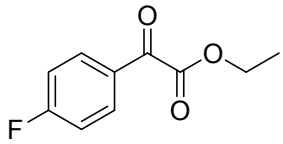
Ethyl 2-(4-ethylphenyl)-2-oxoacetate (3ca).[3] Pale yellow oil (43 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 7.6 Hz, 2H), 4.40 (q, *J* = 7.2 Hz, 2H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.21 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.1, 164.0, 152.3, 130.3, 130.2, 128.4, 62.2, 29.1, 15.0, 14.1.



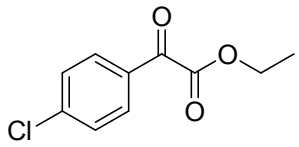
Ethyl 2-oxo-2-(4-propylphenyl)acetate (3da).[4] Pale yellow oil (47 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7,93 (d, *J* = 8.0 Hz, 2H), 7.32 (d, *J* = 8.0 Hz, 2H), 4.47 (q, *J* = 7.2 Hz, 2H), 2.68 (t, *J* = 7.2 Hz, 2H), 1.71 (sextet, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H), 0.96 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.1, 164.0, 150.8, 130.2, 130.1, 129.0, 62.1, 38.1, 24.0, 14.1, 13.7.



Ethyl 2-(4-(*tert*-butyl)phenyl)-2-oxoacetate (3ea).[5] Pale yellow oil (54 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96–7.93 (m, 2H), 7.53–7.51 (m, 2H), 4.47 (q, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H), 1.34 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.0, 164.0, 159.0, 130.0, 129.9, 125.9, 62.2, 35.3, 30.9, 14.1.

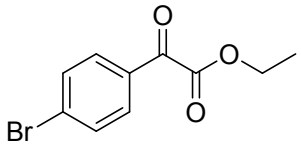


Ethyl 2-(4-fluorophenyl)-2-oxoacetate (3fa).[2] Pale yellow oil (46 mg, 78% yield). ^{1}H NMR (400 MHz, DMSO-d_6): 8.08–8.03 (m, 2H), 7.46 (m, 2H), 4.43 (q, *J* = 7.2 Hz, 2H), 1.33 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 185.4, 167.9 (*J* = 253.9 Hz), 163.7, 133.5 (*J* = 10.1 Hz), 129.1 (*J* = 2.7 Hz), 117.1 (*J* = 22.4 Hz), 62.8, 14.2.

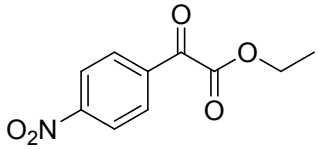


Ethyl 2-(4-chlorophenyl)-2-oxoacetate (3ga).[2] Pale yellow oil (47 mg, 74% yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.00–7.97 (m, 2H), 7.50–7.47 (m, 2H),

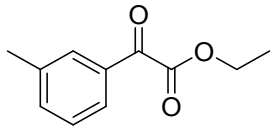
4.47 (q, J = 7.2 Hz, 2H), 1.44 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.8, 163.2, 141.6, 131.4, 130.9, 129.2, 62.5, 14.0



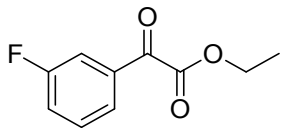
Ethyl 2-(4-bromophenyl)-2-oxoacetate (3ha).[1] Pale yellow oil (58 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.90–7.88 (m, 2H), 7.66–7.64 (m, 2H), 4.47 (q, J = 7.2 Hz, 2H), 1.43 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 185.0, 163.1, 132.2, 131.4, 131.3, 130.4, 62.5, 14.0.



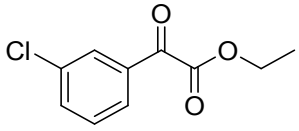
Ethyl 2-(4-nitrophenyl)-2-oxoacetate (3ia).[6] Pale yellow oil (35 mg, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 8.4 Hz, 2H), 8.25 (d, J = 8.4 Hz, 2H), 4.51 (q, J = 7.2 Hz, 2H), 1.47 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.1, 162.2, 151.1, 137.0, 131.2, 123.9, 63.0, 14.0.



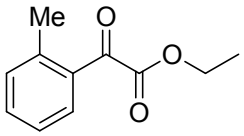
Ethyl 2-oxo-2-(*m*-tolyl)acetate (3ja).[2] Pale yellow oil (42 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (d, J = 7.2 Hz, 2H), 7.47 (d, J = 7.6 Hz, 1H), 7.41 (t, J = 8.0 Hz, 1H), 4.47 (q, J = 7.2 Hz, 2H), 2.42 (s, 3H), 1.44 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.6, 164.0, 138.8, 135.7, 132.4, 130.2, 128.7, 127.3, 62.2, 21.2, 14.1.



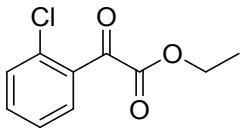
Ethyl 2-(3-fluorophenyl)-2-oxoacetate (3ka).[7] Pale yellow oil (41 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.83 (d, J = 7.6 Hz, 1H), 7.75 (dt, J = 2.4, 9.2 Hz, 1H), 7.53–7.48 (m, 1H), 7.38 (td, J = 2.8, 8.4 Hz, 1H), 4.48 (q, J = 7.2 Hz, 2H), 1.45 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.9 (d, J = 2.5 Hz), 163.9 (d, J = 247.6 Hz), 163.0, 134.5 (d, J = 6.6 Hz), 130.6 (d, J = 7.7 Hz), 126.0 (d, J = 3.1 Hz), 122.1 (d, J = 21.4 Hz), 116.5 (d, J = 22.7 Hz), 62.5, 14.0.



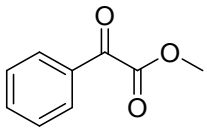
Ethyl 2-(3-chlorophenyl)-2-oxoacetate (3la).[1] Pale yellow oil (43 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (t, J = 1.6 Hz, 1H), 7.92 (dt, J = 1.2, 7.6 Hz, 1H), 7.64 (ddd, J = 1.2, 2.0, 8.0 Hz, 1H), 7.48 (t, J = 8.0 Hz, 1H), 4.88 (q, J = 7.2 Hz, 2H), 1.45 (d, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 184.8, 162.9, 135.2, 134,7, 134.0, 130.2, 129.8, 128.2, 62.6, 14.0.



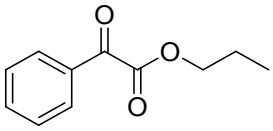
Ethyl 2-oxo-2-(*o*-tolyl)acetate (3ma).[2] Pale yellow oil (39 mg, 68% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, J = 8.0 Hz, 1H), 7.51 (td, J = 1.2, 7.6 Hz, 1H), 7.33 (t, J = 8.0 Hz, 2H), 4.46 (q, J = 7.2 Hz, 2H), 2.61 (s, 3H), 1.43 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 188.7, 164.6, 141.3, 133.6, 132.3, 132.2, 131.2, 125.9, 62.2, 21.4, 14.0.



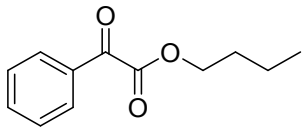
Ethyl 2-(2-chlorophenyl)-2-oxoacetate (3na).[1] Pale yellow oil (40 mg, 63% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.77 (dd, *J* = 2.0, 7.6 Hz, 1H), 7.54–7.50 (m, 1H), 7.45–7.38 (m, 2H), 4.45 (q, *J* = 7.2 Hz, 1H), 1.41 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.5, 163.0, 134.2, 133.8, 133.3, 131.6, 130.5, 127.2, 62.8, 13.8.



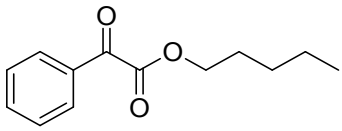
Methyl 2-oxo-2-phenylacetate (3ab).[8] Colorless oil (32 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02–8.00 (m, 2H), 7.68–7.64 (m, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 3.98 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.0, 164.0, 135.0, 132.4, 130.0, 128.9, 52.7.



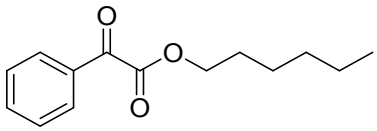
Propyl 2-oxo-2-phenylacetate (3ac).[8] Colorless oil (38 mg, 66% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.99 (m, 2H), 7.68–7.64 (m, 1H), 7.53–7.49 (m, 2H), 4.37 (t, *J* = 6.8 Hz, 2H), 1.82 (sextet, *J* = 7.6 Hz, 2H), 1.03 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.5, 164.0, 134.8, 132.5, 129.9, 128.8, 67.7, 21.8, 10.2.



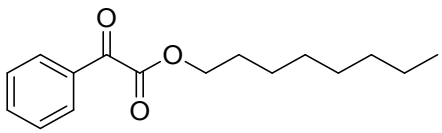
Butyl 2-oxo-2-phenylacetate (3ad).[8] Colorless oil (44 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.99 (m, 2H), 7.68–7.64 (m, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 4.41 (t, *J* = 6.8 Hz, 2H), 1.80 (quintet, *J* = 6.8 Hz, 2H), 1.50 (sextet, *J* = 7.6 Hz, 2H), 0.98 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.4, 164.0, 134.8, 132.5, 129.9, 128.8, 66.0, 30.4, 19.0, 13.6.



Pentyl 2-oxo-2-phenylacetate (3ae).[8] Colorless oil (45 mg, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.99 (m, 2H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 8.0 Hz, 2H), 4.40 (t, *J* = 7.2 Hz, 2H), 1.82 (quintet, *J* = 7.2Hz, 2H), 1.42–1.33 (m, 4H), 0.93 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.4, 164.0, 134.8, 132.5, 130.0, 128.8, 66.3, 28.1, 27.8, 22.2, 13.8.

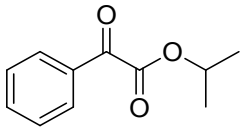


Hexyl 2-oxo-2-phenylacetate (3af).[8] Colorless oil (50 mg, 72% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (dd, *J* = 0.8, 8.0 Hz, 2H), 7.67–7.63 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 4.40 (t, *J* = 7.2 Hz, 2H), 1.81 (quintet, *J* = 7.2 Hz, 2H), 1.45–1.37 (m, 2H), 1.34–1.30 (m, 4H), 0.91 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.4, 164.0, 134.8, 132.5, 130.0, 128.8, 66.3, 31.3, 28.4, 25.4, 22.4, 13.9.

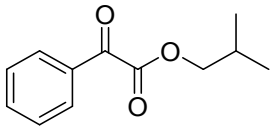


Octyl 2-oxo-2-phenylacetate (3ag).[9] Colorless oil (58 mg, 74% yield). ^{1}H

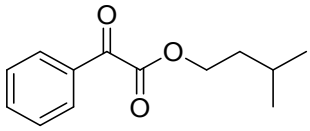
NMR (400 MHz, $CDCl_3$): δ 8.01 (dd, *J* = 1.2, 8.0 Hz, 2H), 7.68–7.63 (m, 1H), 7.53–7.49 (m, 2H), 4.40 (t, *J* = 7.2 Hz, 2H), 1.81 (quintet, *J* = 7.2 Hz, 1H), 1.44–1.27 (m, 12H), 0.89 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.4, 163.9, 134.8, 132.5, 129.9, 128.8, 66.3, 31.7, 29.0, 28.4, 25.7, 22.5, 14.0.



***iso*-Propyl 2-oxo-2-phenylacetate (3ah).[8]** Colorless oil (28 mg, 48% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00–7.98 (m, 2H), 7.68–7.73 (m, 1H), 7.53–7.49 (m, 2H), 5.37 (septet, *J* = 6.4 Hz, 1H), 1.42 (d, *J* = 6.4 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.7, 163.6, 134.7, 132.5, 129.9, 128.8, 70.6, 21.7

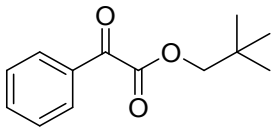


***iso*-Butyl 2-oxo-2-phenylacetate (3ai).[8]** Colorless oil (47 mg, 77% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93–7.90 (m, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 4.10 (d, *J* = 6.8 Hz, 2H), 2.05 (septet, *J* = 6.8 Hz, 1H), 0.93 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.5, 164.0, 134.8, 132.5, 129.9, 128.9, 72.0, 27.7, 18.9.

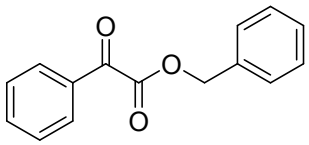


***iso*-Pentyl 2-oxo-2-phenylacetate (3aj).[8]** Colorless oil (50 mg, 76% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.95–7.93 (m, 2H), 7.80 (t, *J* = 7.6 Hz, 2H),

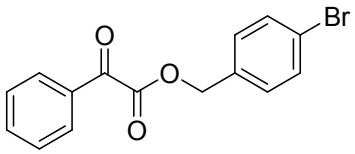
7.63 (t, J = 7.6 Hz, 2H), 4.38 (t, J = 6.8 Hz, 2H), 1.72 (quintet, J = 6.4 Hz, 2H), 1.33–1.28 (m, 4H), 0.87 (t, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 187.2, 164.2, 135.9, 132.1, 130.1, 129.7, 66.5, 27.9, 27.8, 22.0, 14.2.



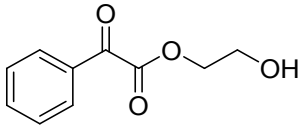
Neopentyl 2-oxo-2-phenylacetate (3ak).[10] Colorless oil (47 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01–7.99 (m, 2H), 7.68–7.64 (m, 1H), 7.53 (t, J = 8.0 Hz, 2H), 4.10 (s, 2H), 1.01 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.5, 164.1, 134.8, 132.5, 129.9, 128.9, 75.2, 31.5, 26.3.



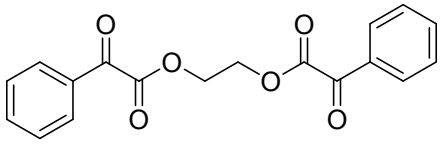
Benzyl 2-oxo-2-phenylacetate (3al).[11] Colorless oil (43 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96–7.94 (m, 2H), 7.64 (t, J = 7.6 Hz, 1H), 7.48–7.42 (m, 4H), 7.40–7.34 (m, 3H), 5.40 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 186.0, 163.6, 134.9, 134.5, 132.4, 130.0, 128.9, 128.8, 128.7, 128.6, 67.7.



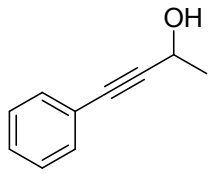
4-Bromobenzyl 2-oxo-2-phenylacetate (3am).[11] Yellow soild (56 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (dd, J = 0.8, 8.0 Hz, 2H), 7.67–7.63 (m, 1H), 7.53–7.47 (m, 4H), 7.33 (d, J = 8.4 Hz, 2H), 5.35 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 185.7, 163.4, 135.0, 133.5, 132.3, 131.9, 130.2, 130.0, 128.9, 122.9, 66.9.



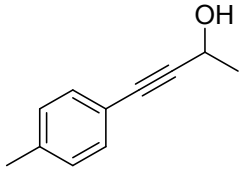
2-Hydroxyethyl 2-oxo-2-phenylacetate (3an). Pale yellow oil (36 mg, 62% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.99–7.97 (m, 2H), 7.81–7.76 (m, 1H), 7.64–7.60 (m, 2H), 4.42 (t, J = 4.8 Hz, 2H), 3.71 (t, J = 4.8 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 187.3, 164.3, 135.9, 132.2, 130.2, 129.7, 68.1, 59.1. HRMS (ESI) calcd for $C_{10}H_{11}O_4$ $(M+H)^+$: 195.0652; Found: 195.0643.



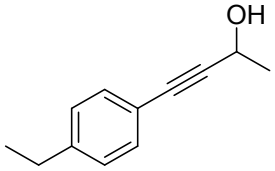
Ethane-1,2-diyl bis(2-oxo-2-phenylacetate) (3ao). Pale yellow oil (28 mg, 29% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02–8.00 (m, 4H), 7.67–7.63 (m, 2H), 7.51 (t, J = 7.6 Hz, 4H), 4.74 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 185.5, 163.2, 135.1, 132.1, 130.1, 128.9, 62.9. HRMS (ESI) calcd for $C_{18}H_{15}O_6$ $(M+H)^+$: 327.0863; Found: 327.0866.



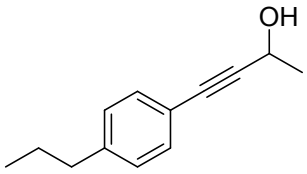
4-Phenylbut-3-yn-2-ol (4aa).[12] Colorless oil (18.1 mg, 63% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7,45–7.43 (m, 2H), 7.33–7.31 (m, 3H), 4.80–4.74 (m, 1H), 1.99 (d, J = 5.3 Hz, 1H), 1.57 (d, J = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.6, 128.3, 128.2, 122.5, 90.9, 84.0, 58.8, 24.4.



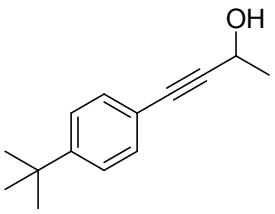
4-(*p*-Tolyl)but-3-yn-2-ol (4ba).[13] Pale yellow oil (16.3 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.32 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 4.77 (q, *J* = 6.5 Hz, 1H), 2.34 (s, 3H), 2.01 (s, 1H). 1.55 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.4, 131.5, 129.0, 119.5, 90.2, 84.1, 58.8, 24.3, 21.4.



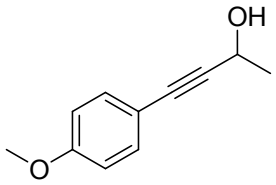
4-(4-Ethylphenyl)but-3-yn-2-ol (4ca). Pale yellow oil (17 mg, 49% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (d, *J* = 8.1 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 4.77 (q, *J* = 6.5 Hz, 1H), 2.66 (q, *J* = 7.6 Hz, 2H), 2.05 (s, 1H), 1.55 (d, *J* = 6.5 Hz, 3H), 1.23 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.7, 131.6, 127.8, 119.7, 90.3, 84.1, 58.8, 28.7, 24.4, 15.2. HRMS (ESI) calcd for $C_{12}H_{15}O$ $(M+H)^+$: 175.1117; Found: 175.1118.



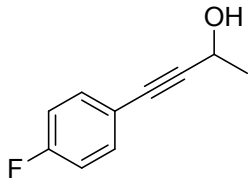
4-(4-Propylphenyl)but-3-yn-2-ol (4da). Pale yellow oil (20 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 4.79–4.72 (m 1H), 2.60 (t, *J* = 7.4 Hz, 2H), 1.95–1.94 (m, 1H), 1.62–1.61 (m, 2H), 1.56 (d, *J* = 6.6 Hz, 3H), 0.95 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.2, 131.5, 128.4, 119.7, 90.2, 84.1, 58.9, 37.8, 24.4, 24.2, 13.6. HRMS (ESI) calcd for $C_{12}H_{15}O$ $(M+H)^+$: 189.1274; Found: 189.1274.



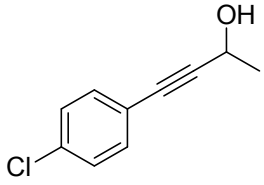
4-(4-(*tert*-Butyl)phenyl)but-3-yn-2-ol (4ea).[14] Pale yellow oil (24.6 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37–7.35 (m, 2H), 7.33–7.30 (m, 2H), 4.77 (q, *J* = 6.5 Hz, 1H), 2.01 (s, 1H), 1.55 (d, *J* = 6.5 Hz, 3H), 1.30 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.1, 131.3, 125.2, 119.5, 90.2, 84.1, 58.9, 34.7, 31.1, 24.4.



4-(4-Methoxyphenyl)but-3-yn-2-ol (4fa).[13] Pale yellow oil (10.5 mg, 30% yield). ^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.33 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 5.37 (d, *J* = 5.3 Hz, 1H), 4.58–4.52 (m, 1H), 3.75 (s, 3H), 1.36 (d, *J* = 6.5 Hz, 2H). ^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 159.6, 133.1, 114.9, 114.6, 92.2, 82.5, 57.1, 55.6, 25.1.

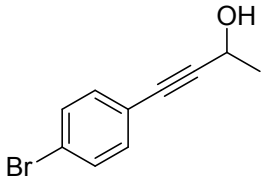


4-(4-Fluorophenyl)but-3-yn-2-ol (4ga).[13] Pale yellow oil (18.6 mg, 57% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43–7.38 (m, 2H), 7.03–6.97 (m, 2H), 4.78–4.72 (m, 1H), 2.01 (d, *J* = 5.1 Hz, 1H), 1.56 (d, *J* = 6.6 Hz, 3H), 1.31 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.7 (*J* = 248.0 Hz), 133.5 (*J* = 8.3 Hz), 118.6 (*J* = 3.5 Hz), 115.6 (*J* = 21.9 Hz), 90.6, 82.9, 58.8, 24.3.

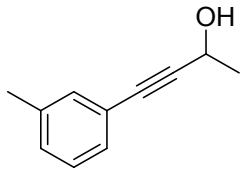


4-(4-Chlorophenyl)but-3-yn-2-ol (4ha).[15] Pale yellow oil (22 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36–7.32 (m, 2H), 7.29–7.27 (m, 2H), 4.78–4.72 (m, 1H), 2.12 (d, *J* = 5.1 Hz, 1H), 1.56 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$):

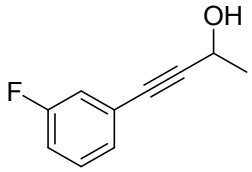
δ 134.4, 132.8, 128.6, 121.0, 91.9, 82.9, 58.7, 24.3.



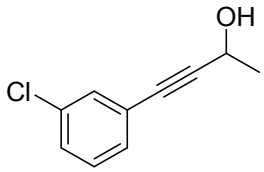
4-(4-Bromophenyl)but-3-yn-2-ol (4ia).[13] Pale yellow oil (26.9 mg, 60% yield). ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.56–7.53 (m, 2H), 7.35–7.31 (m, 2H), 5.47 (d, *J* = 5.2 Hz, 1H), 4.60–4.53 (m, 1H), 1.37 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ 133.5, 132.1, 122.2, 122.1, 95.1, 81.5, 57.1, 24.9.



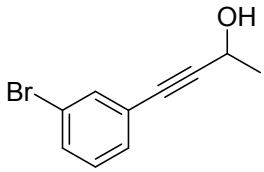
4-(*m*-Tolyl)but-3-yn-2-ol (4ja).[13] Pale yellow oil (15.5 mg, 48% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25–7.21 (m, 2H), 7.20–7.16(m, 1H), 7.13–7.11(m, 1H), 4.77 (q, *J* = 6.5 Hz, 1H), 2.31 (s, 3H), 2.03 (s, 1H),1.55 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 137.9, 132.2, 129.2, 128.7, 128.1, 122.3, 90.6, 84.1, 58.8, 24.4, 21.1.



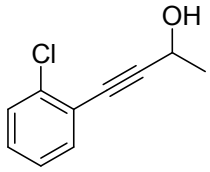
4-(3-Fluorophenyl)but-3-yn-2-ol (4ka).[13] Pale yellow oil (20.3 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.30–7.26 (m, 1H), 7.21-7.19(m, 1H), 7.14–7.11(m, 1H), 7.05–7.00(m, 1H), 4.79–4.72 (m, 1H), 2.05 (s, 1H), 1.57 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.5 (*J* = 245.0 Hz), 129.8 (*J* = 8.5 Hz), 127.5 (*J* = 3.0 Hz), 124.5 (*J* = 9.3 Hz), 118.5 (*J* = 22.7 Hz), 115.8 (*J* = 21.0 Hz), 91.8, 82.8 (*J* = 3.4 Hz), 58.7, 24.2.



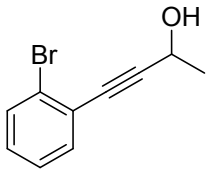
4-(3-Chlorophenyl)but-3-yn-2-ol (4la).[14] Pale yellow oil (22.3 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.41–7.40 (m, 1H), 7.30–7.28 (m, 2H), 7.24–7.20 (m, 1H), 4.75–4.73 (m, 1H), 2.00 (s, 1H), 1.55 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.1, 131.5, 129.7, 129.4, 128.6, 124.3, 92.1, 82.6, 58.7, 24.2.



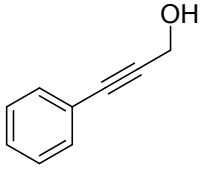
4-(3-Bromophenyl)but-3-yn-2-ol (4ma).[15] Pale yellow oil (28.6 mg, 64% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (t, *J* = 1.6 Hz, 3H), 7.45 (dq, *J* = 0.96, 8.0 Hz, 1H), 7.35 (dt, *J* = 1.1, 7.7 Hz, 1H), 7.18 (t, *J* = 7.8 Hz, 1H), 4.78–4.72 (m, 1H), 2.28 (s, 1H), 1.56 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 134.4, 131.5, 130.1, 129.7, 124.6, 122.0, 92.3, 82.5, 58.7, 24.2.



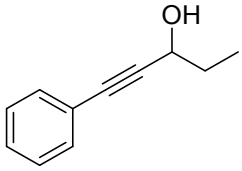
4-(2-Chlorophenyl)but-3-yn-2-ol (4na).[16] Pale yellow oil (22.3 mg, 62% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.47 (dd, *J* = 1.8, 7.4 Hz, 1H), 7.40 (dd, *J* = 1.3, 7.9 Hz, 1H), 7.25–7.18 (m, 2H), 4.84–4.77 (m, 1H), 2.01 (d, *J* = 5.2 Hz, 1H),1.59 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.9, 133.3, 129.4, 129.2, 126.4, 122.5, 96.2, 80.8, 58.9, 24.2.



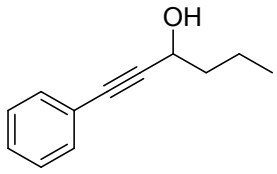
4-(2-Bromophenyl)but-3-yn-2-ol (4oa).[15] Pale yellow oil (26.4 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (dd, *J* = 1.0, 8.0 Hz, 1H), 7.40 (dd, *J* = 1.6, 7.6 Hz, 1H) 7.27–7.23(m, 1H), 7.18–7.14 (m, 1H), 4.84–4.77 (m, 1H), 2.18 (d, *J* = 5.2 Hz, 1H), 1.60 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 133.3, 132.3, 129.5, 126.9, 125.5, 124.7, 95.6, 82.6, 58.9, 24.2.



3-Phenylprop-2-yn-1-ol (4ab).[12] Colorless oil (10.3 mg, 39% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46–7.44 (m, 2H), 7.34–7.31 (m, 3H), 4.51 (d, *J* = 4.4 Hz, 1H), 1.77 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.6, 128.4, 128.3, 122.5, 87.1, 85.7, 51.6.

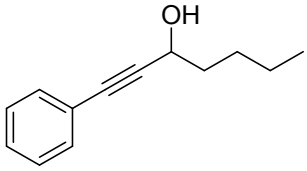


1-Phenylpent-1-yn-3-ol (4ac).[17] Pale yellow oil (16.4 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45–7.43 (m, 2H), 7.34–7.30 (m, 3H), 4.59 (q, *J* = 6.2 Hz, 1H), 2.01–2.00 (m, 1H), 1.87–1.80 (m, 2H), 1.11 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.6, 128.3, 128.2, 122.6, 89.9, 84.9, 64.2, 30.9, 9.4.

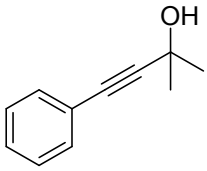


1-Phenylhex-1-yn-3-ol (4ad).[18] Pale yellow oil (12.5 mg, 36% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45–7.43 (m, 2H), 7.33–7.31 (m, 3H), 4.64 (q, *J* = 6.4 Hz, 1H), 1.93

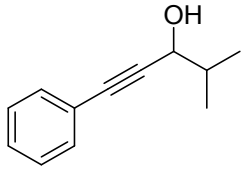
(d, J = 6.4 Hz, 1H), 1.83–1.77 (m, 2H), 1.59–1.52 (m, 2H), 1.02 (t, J = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.6, 128.3, 128.2, 122.6, 90.2, 84.2, 62.7, 40.0, 18.4, 13.7.



1-Phenylhept-1-yn-3-ol (4ae).[19] Pale yellow oil (11.6 mg, 31% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45–7.43 (m, 2H), 7.33–7.31 (m, 3H), 4.63 (q, J = 6.4 Hz, 1H), 1.93–1.91 (m, 1H), 1.85–1.79 (m, 2H), 1.56–1.48 (m, 2H), 1.45–1.38 (m, 2H), 0.97 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.6, 128.3, 128.2, 122.7, 90.2, 84.8, 63.0, 37.6, 27.3, 22.3, 13.9.



2-Methyl-4-phenylbut-3-yn-2-ol (4af).[20] Pale yellow oil (9.6 mg, 30% yield). ^{1}H NMR (400 MHz, CDCl3): δ 7.44–7.41 (m, 2H), 7.32–7.29 (m, 3H), 2.13 (s, 1H), 1.63 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.6, 128.2, 122.7, 93.7, 82.1, 65.6, 31.4.



4-Methyl-1-phenylpent-1-yn-3-ol (4ag).[21] Pale yellow oil (12.1 mg, 35% yield). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46–7.43 (m, 2H), 7.32–7.30 (m, 3H), 4.42 (t, J = 5.6 Hz, 1H), 1.99–1.96 (m, 1H), 1.31 (s, 1H), 1.10 (d, J = 6.7 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 131.6, 128.3, 128.2, 122.7, 88.9, 85.5, 68.4, 34.7, 18.1, 17.5.

References:

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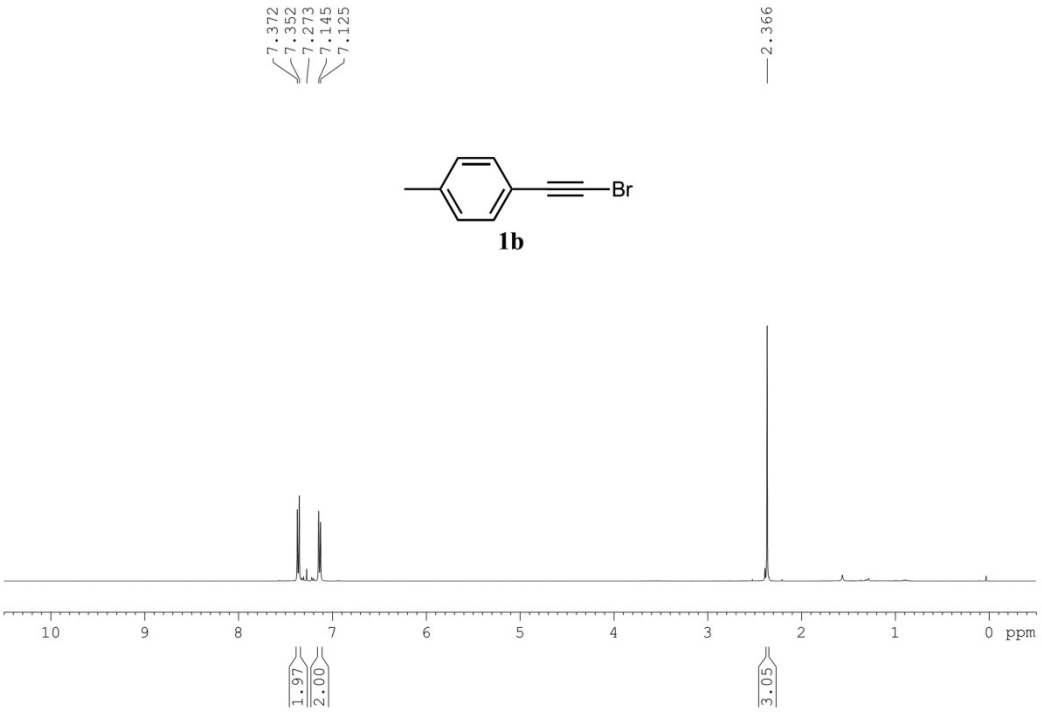
13. ^{1}H and ^{13}C NMR spectra of bromoalkynes (1b–1n) and all products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7.145
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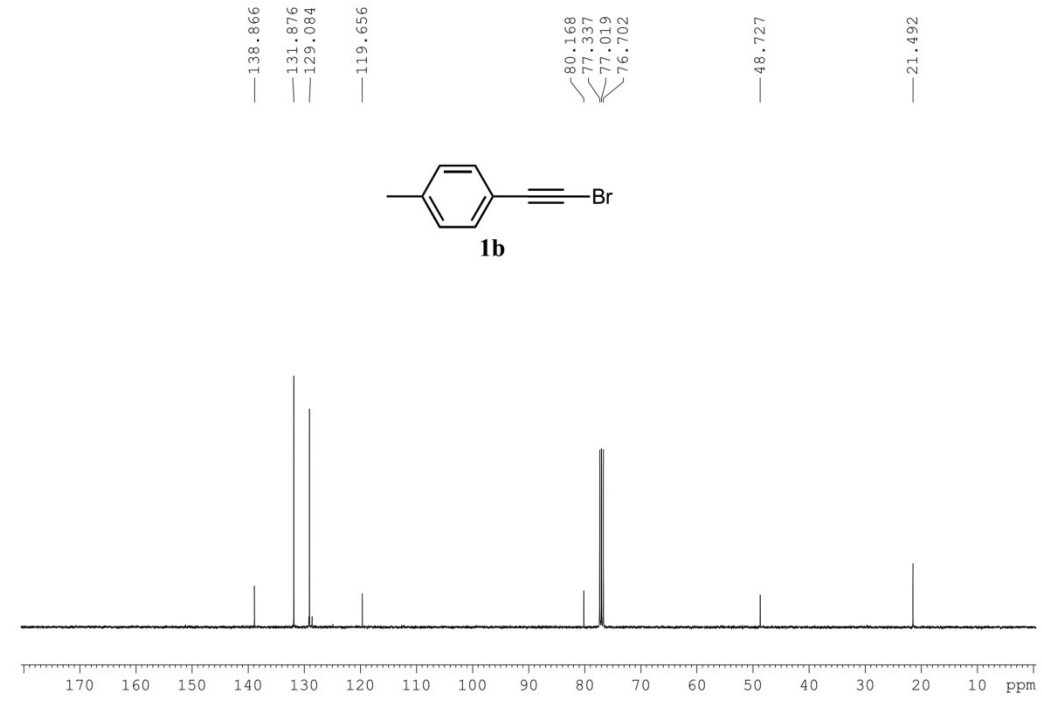
8
7
6
5
4
3
2
1
0 ppm
1.97
2.00
3.05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150
140
130
120
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100
90
80
70
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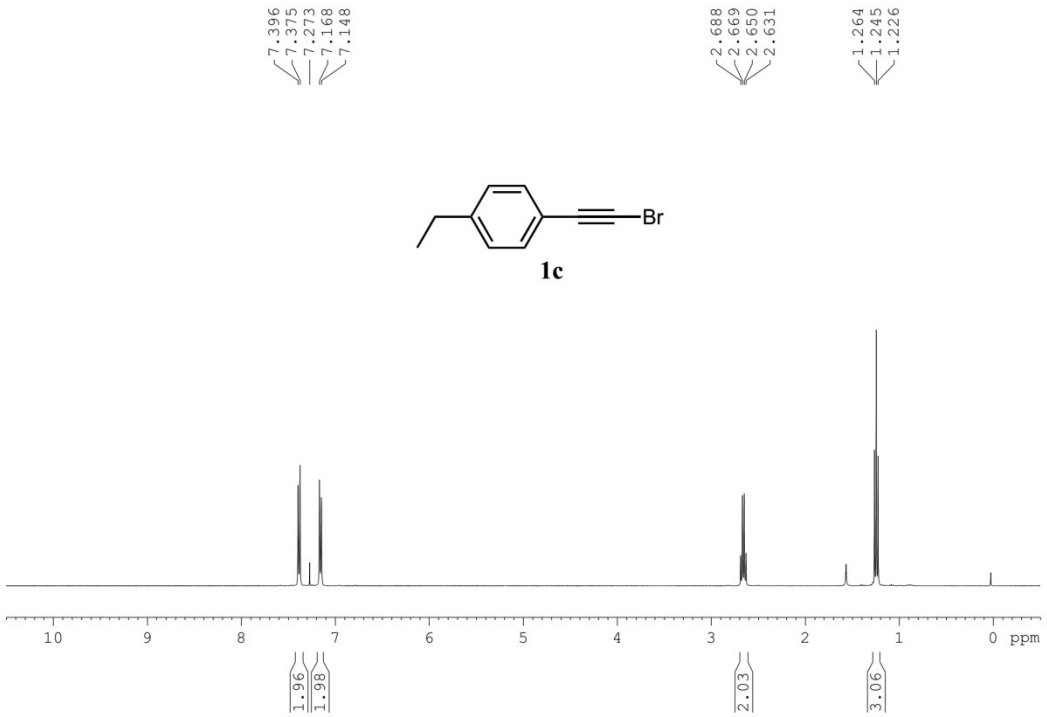
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7.375
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7.168
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2.669
2.650
2.631
1.264
1.245
1.226
Br
1c
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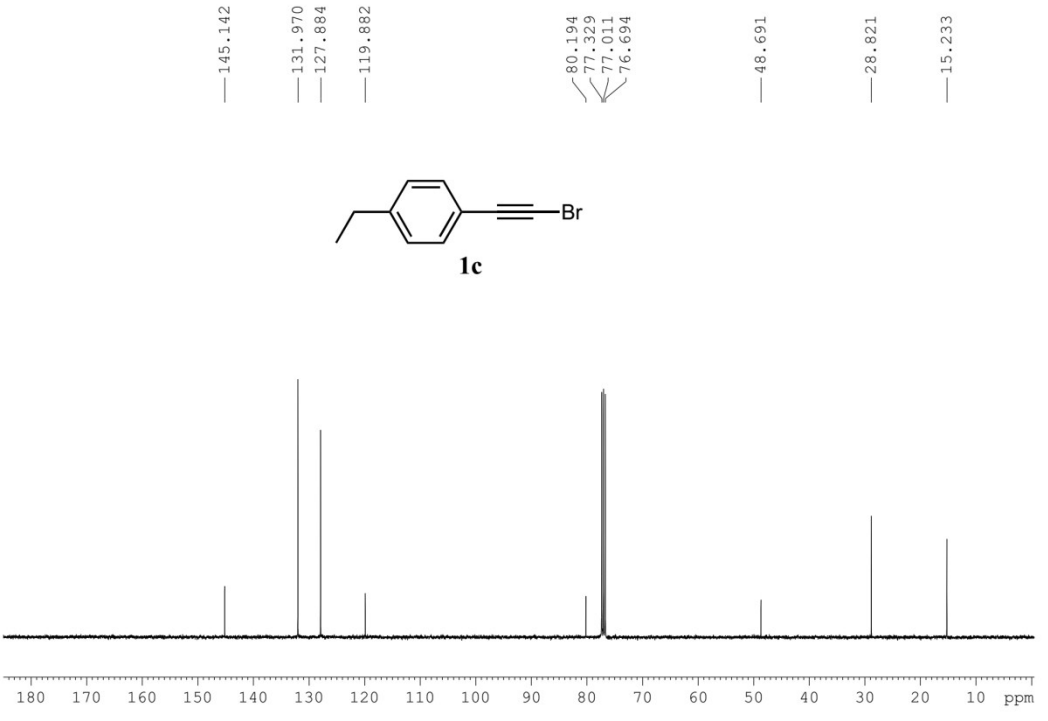
9
8
7
6
5
4
3
2
1
0 ppm
1.96
1.98
2.03
3.06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170
160
150
140
130
120
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100
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80
70
60
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40
30
20
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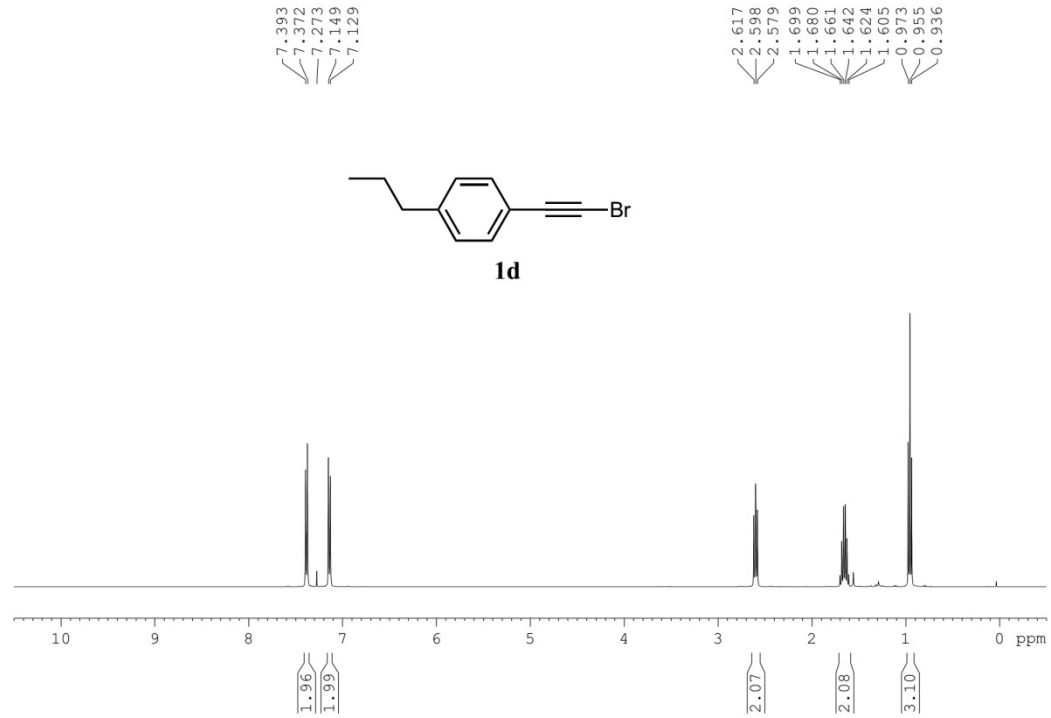
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7.129
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1.624
1.605
0.973
0.955
0.936
Br
1d
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9
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7
6
5
4
3
2
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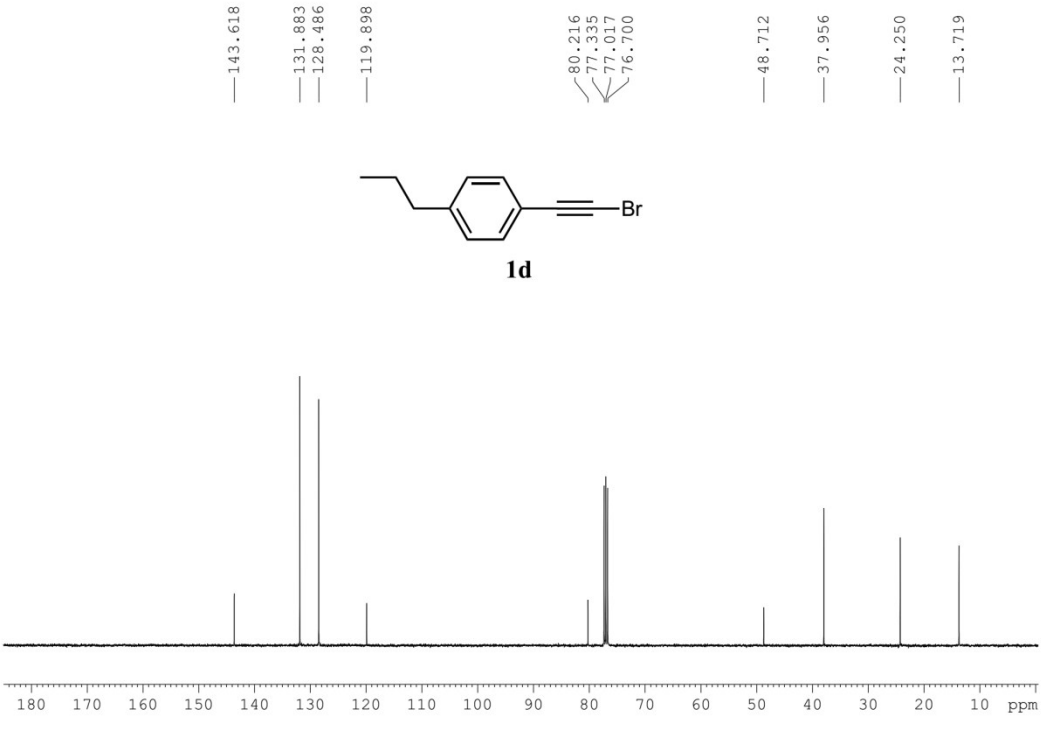
1.96
1.99
2.07
2.08
3.10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20
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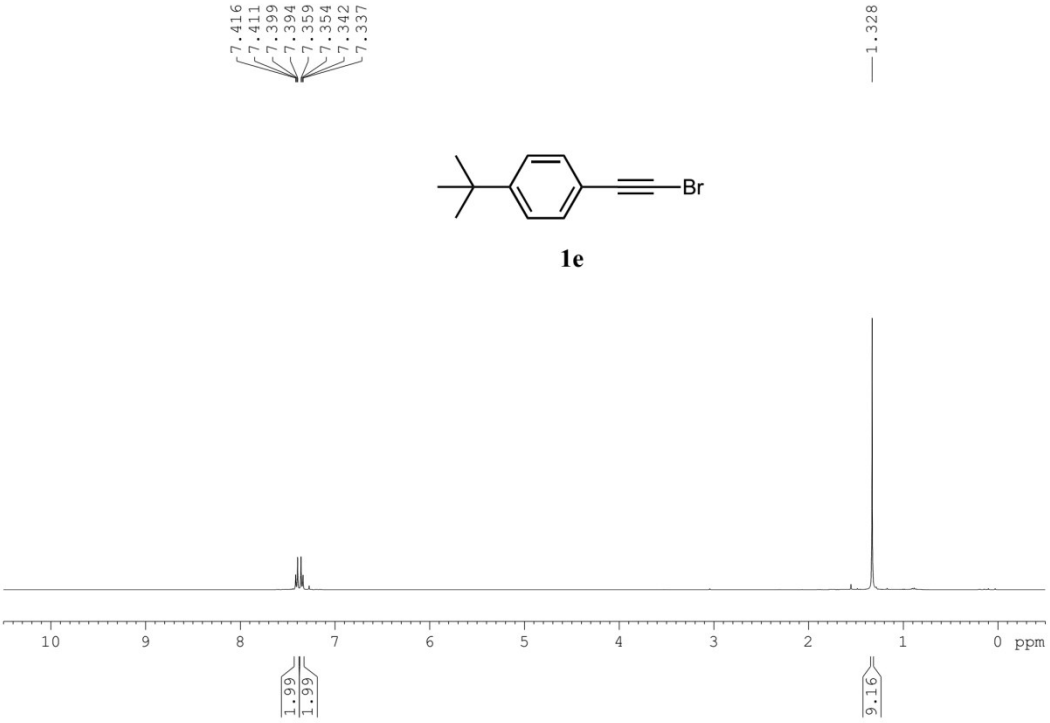
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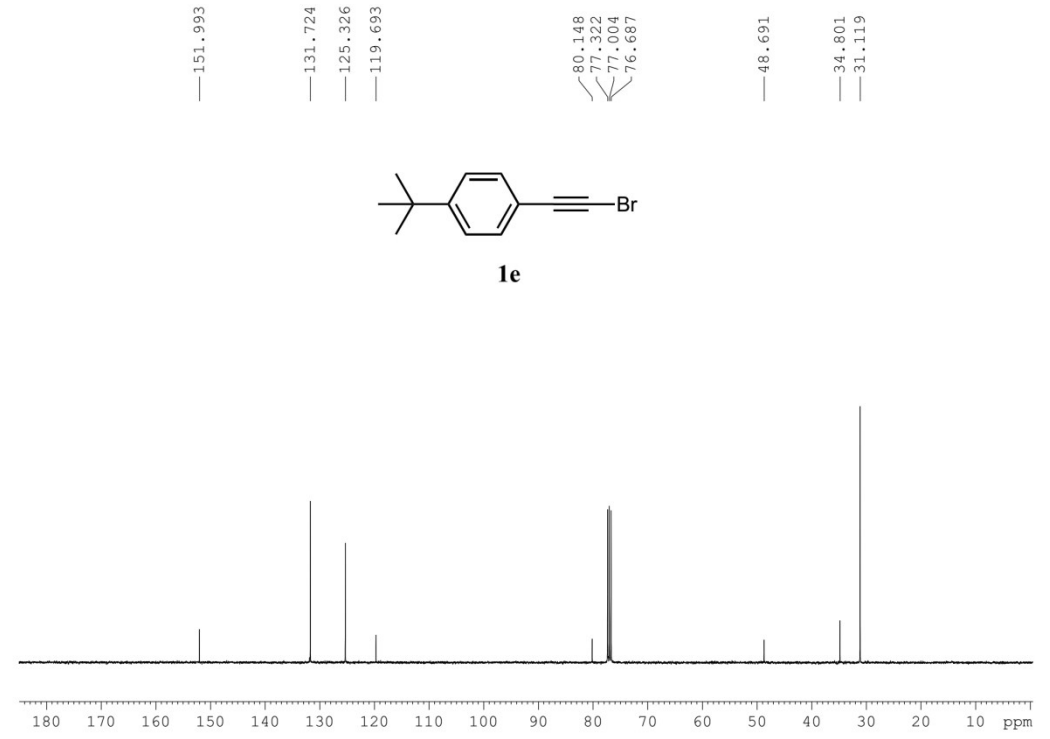
1.99
9.16

1e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20
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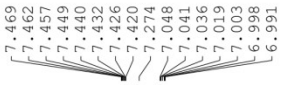
1e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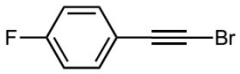
6.991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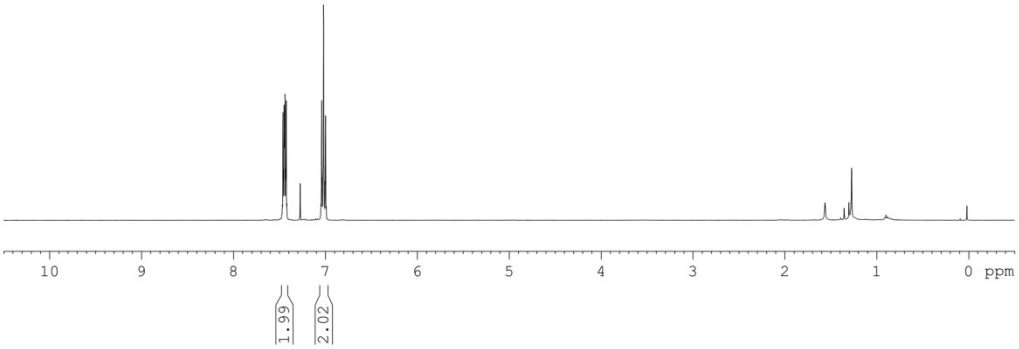
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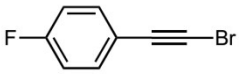
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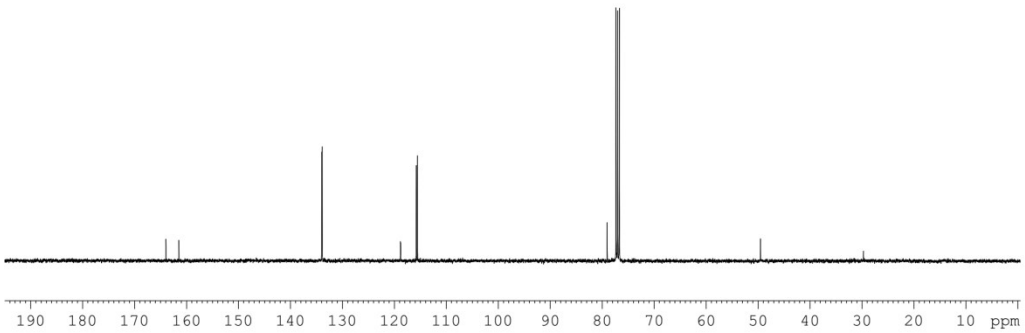
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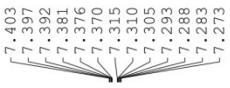
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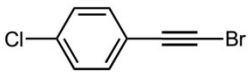
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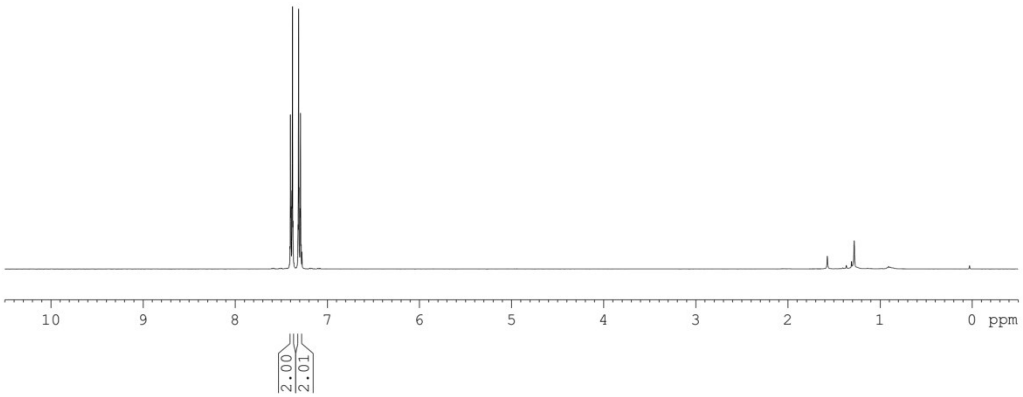
1g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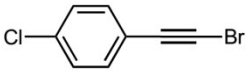
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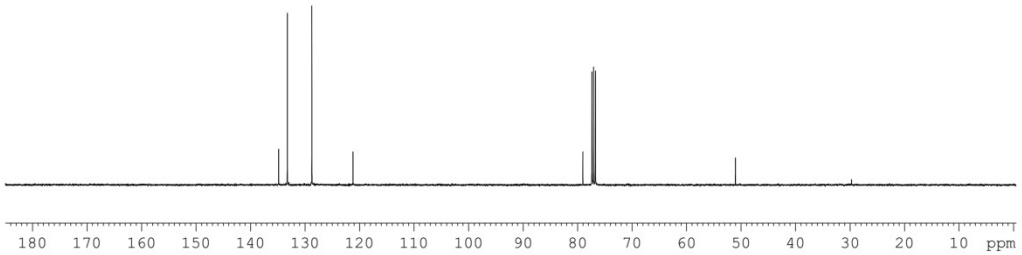
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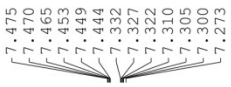
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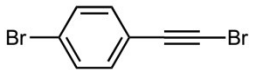
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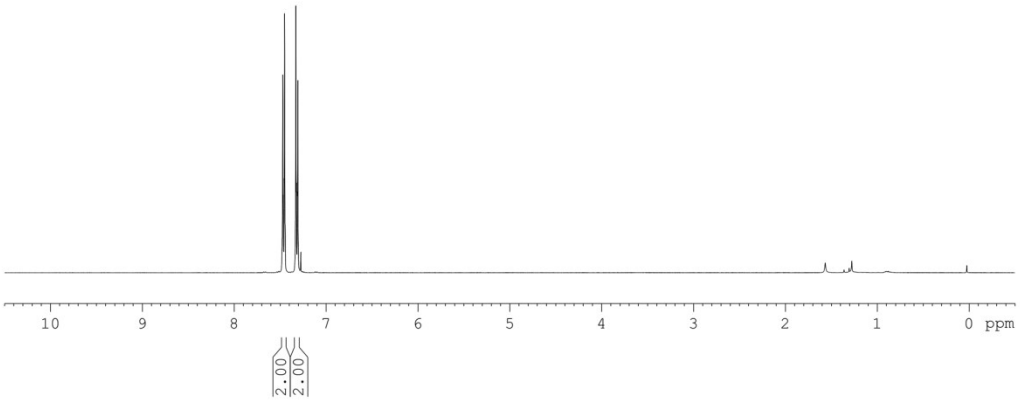
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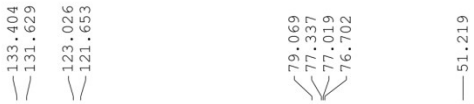
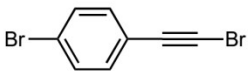
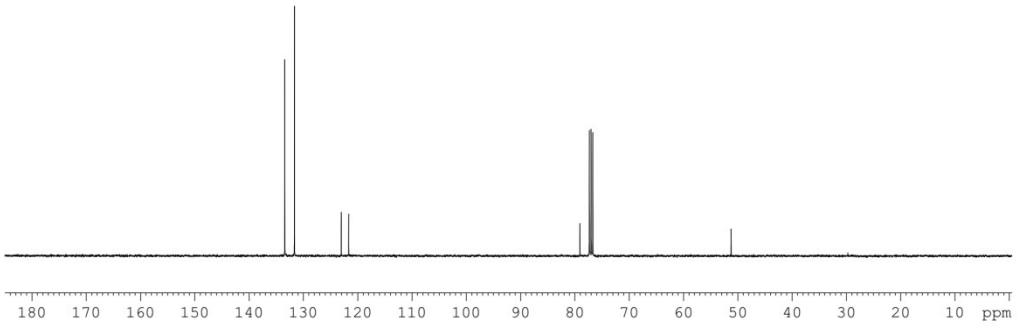
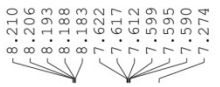
2.00

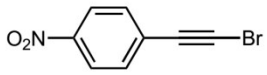

133.404
131.629
123.026
121.653
79.069
77.337
77.019
76.702
51.219


Br
Br

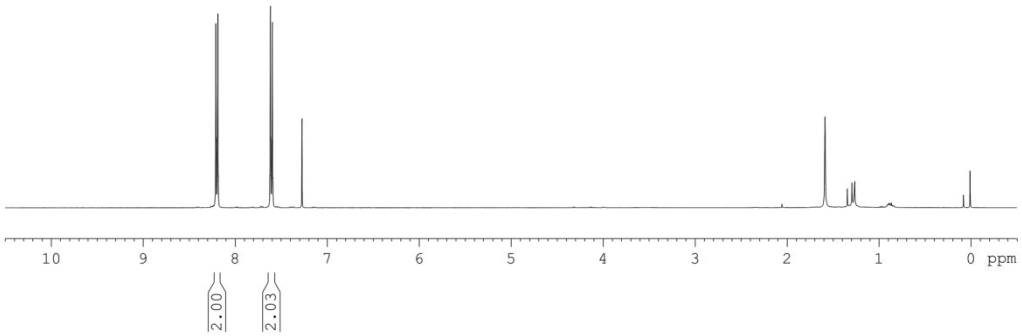
1h


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

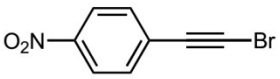

8.210
8.206
8.193
8.188
8.183
7.622
7.617
7.612
7.599
7.595
7.590
7.274


O2N
Br

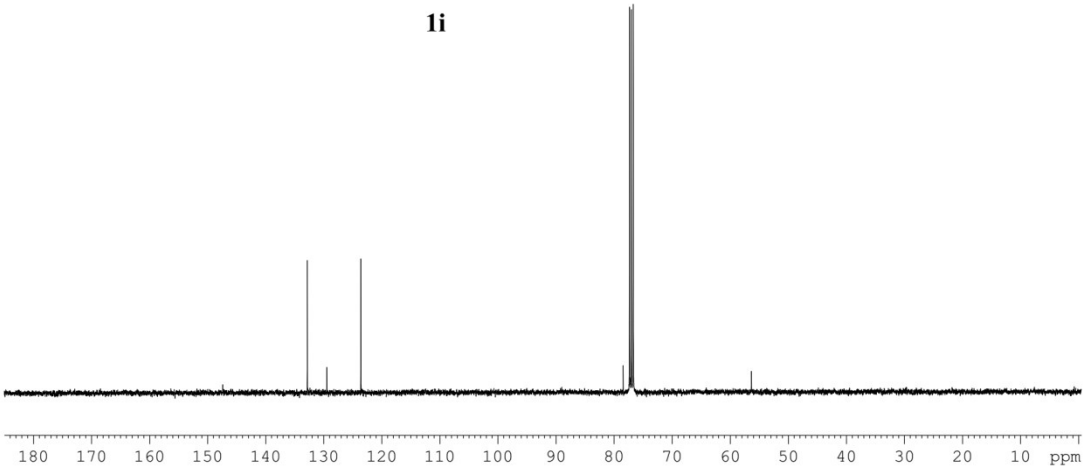
1i

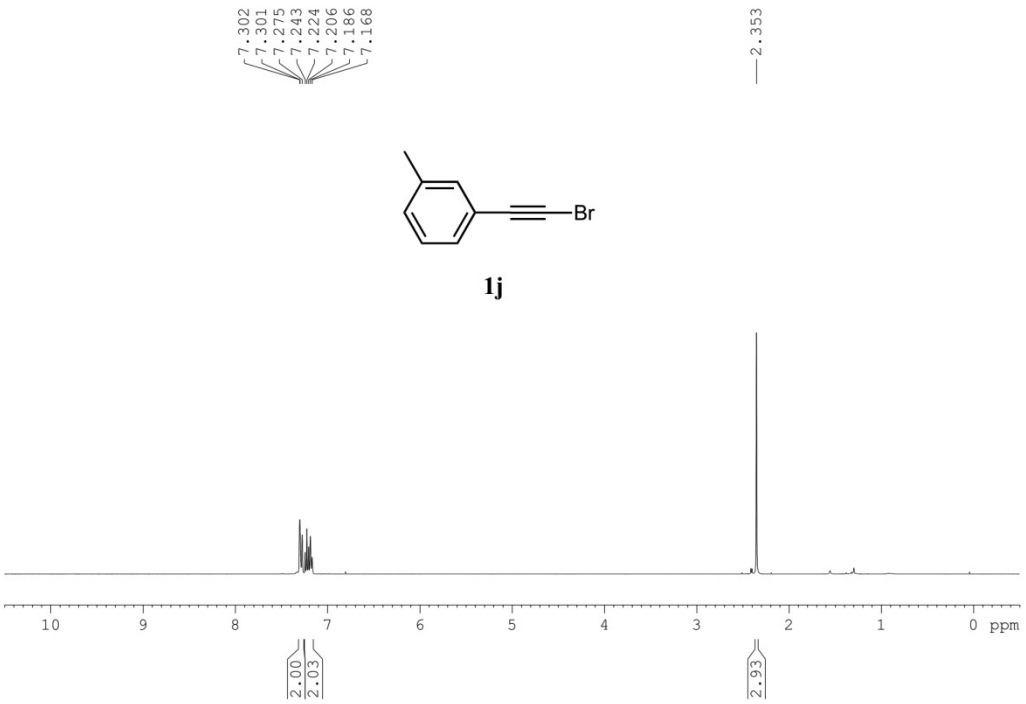

10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.03


147.356
132.817
129.465
123.601
78.416
77.317
77.000
76.682
56.331

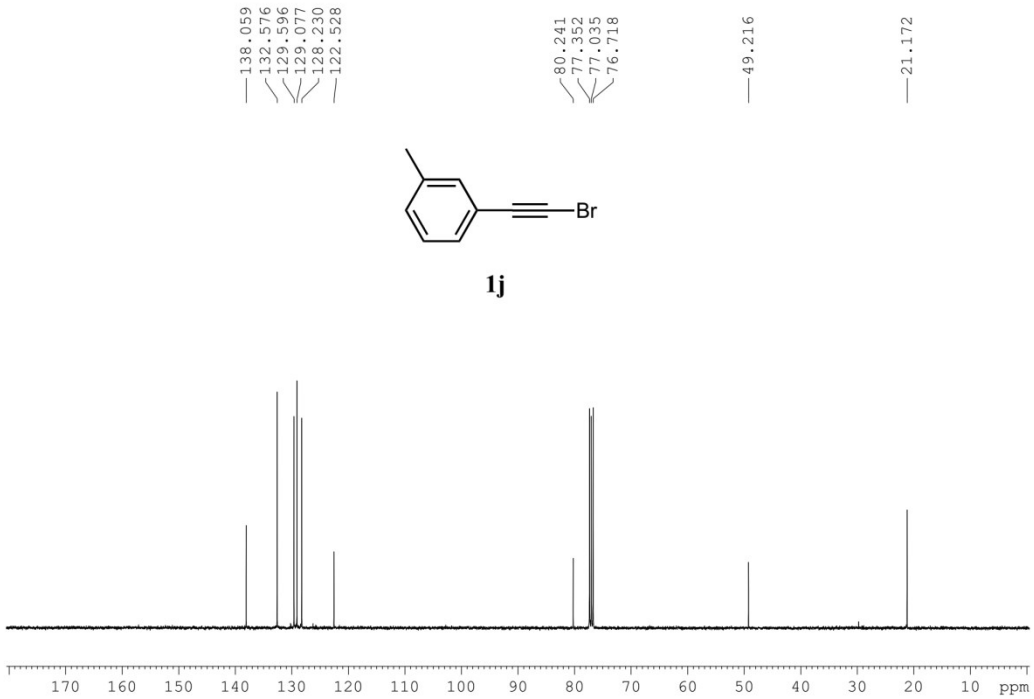

O2N
Br

1i


180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

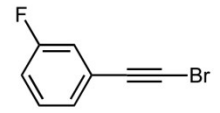

7.302
7.301
7.275
7.243
7.224
7.206
7.186
7.168
2.353
Br
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.03
2.93

1j

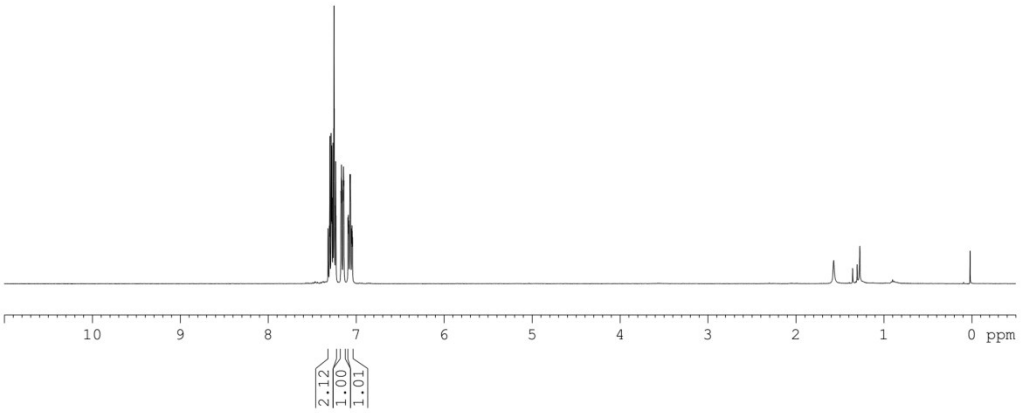

138.059
132.576
129.596
129.077
128.230
122.528
80.241
77.352
77.035
76.718
49.216
21.172
Br
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

1j


7.317
7.303
7.298
7.284
7.278
7.273
7.264
7.254
7.250
7.248
7.234
7.231
7.229
7.171
7.165
7.162
7.148
7.142
7.139
7.091
7.088
7.085
7.082
7.070
7.066
7.064
7.050
7.046
7.044
7.040


F
Br

1k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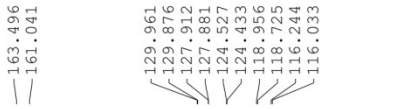
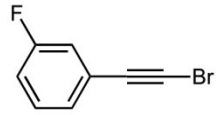
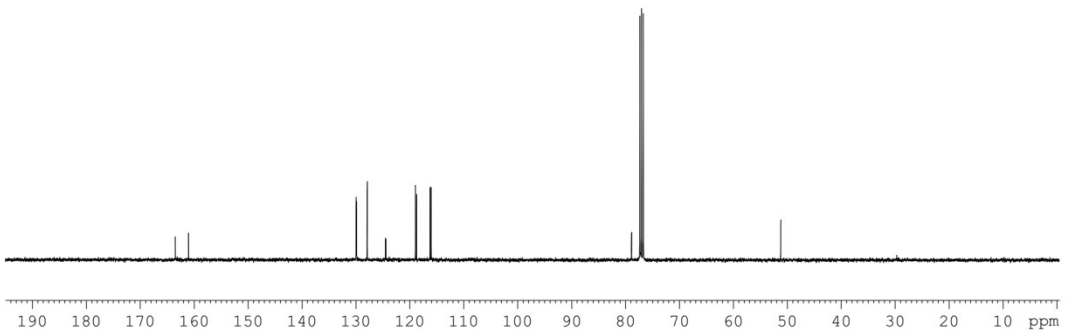
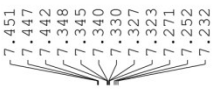
9
8
7
6
5
4
3
2
1
0 ppm
2.12
1.00
1.01

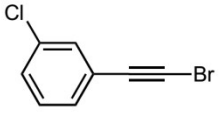

163.496
161.041
129.961
129.876
127.912
127.881
124.527
124.433
118.956
118.725
116.244
116.033
78.890
78.855
77.318
77.001
76.683
51.200


F
Br

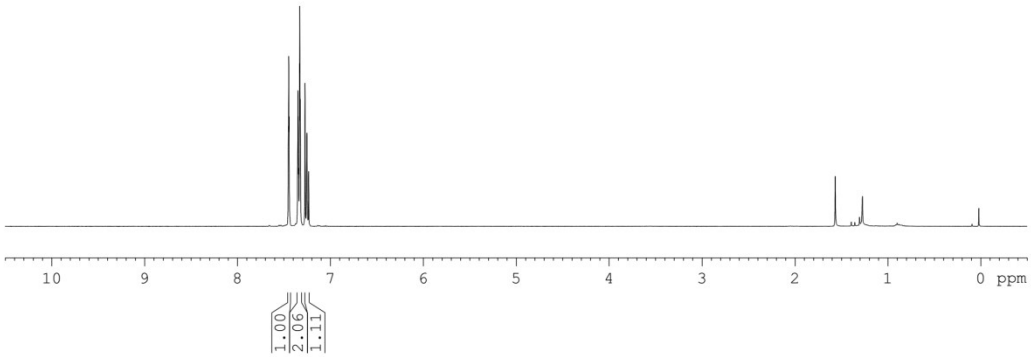
1k


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

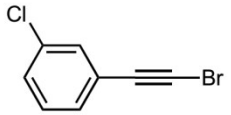

7.451
7.447
7.442
7.348
7.345
7.340
7.330
7.327
7.323
7.271
7.252
7.232


Cl
Br

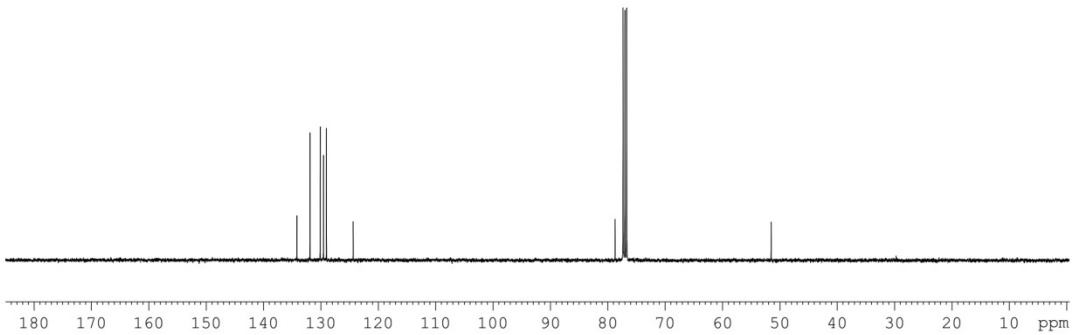
1l

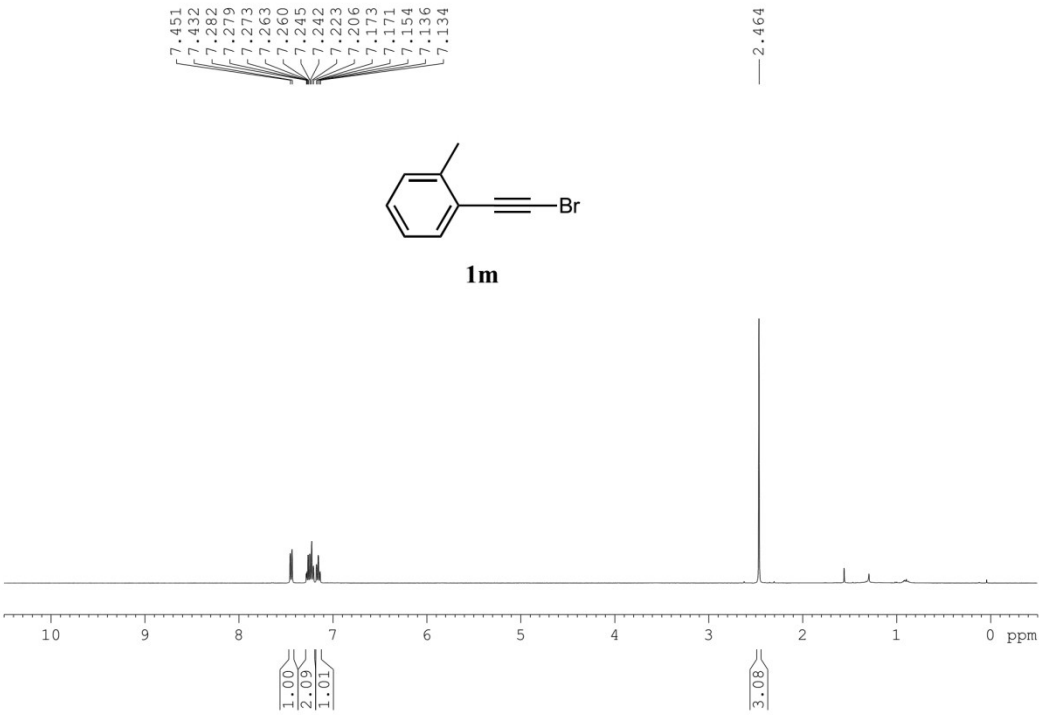

10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.06
1.11


134.188
131.892
130.120
129.546
129.025
124.372
78.710
77.323
77.005
76.688
51.499

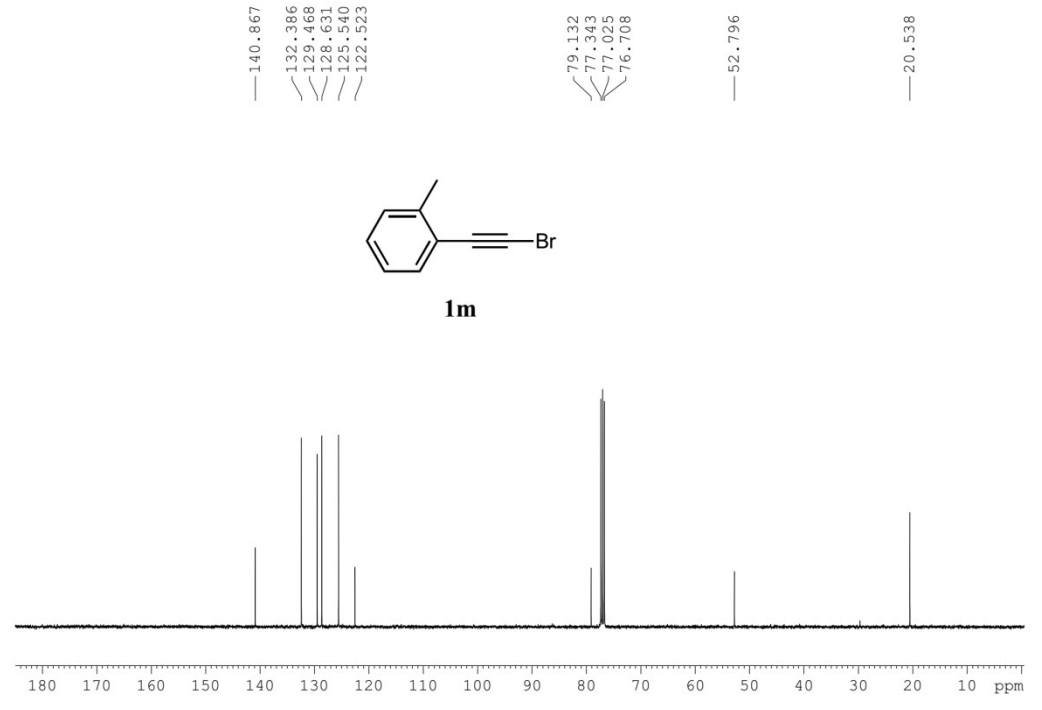

Cl
Br

1l

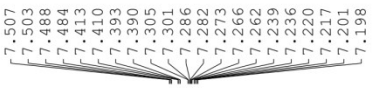

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

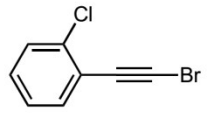

7.451
7.432
7.282
7.279
7.273
7.263
7.260
7.245
7.242
7.223
7.206
7.173
7.171
7.154
7.136
7.134
2.464
Br
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.09
1.01
3.08

1m

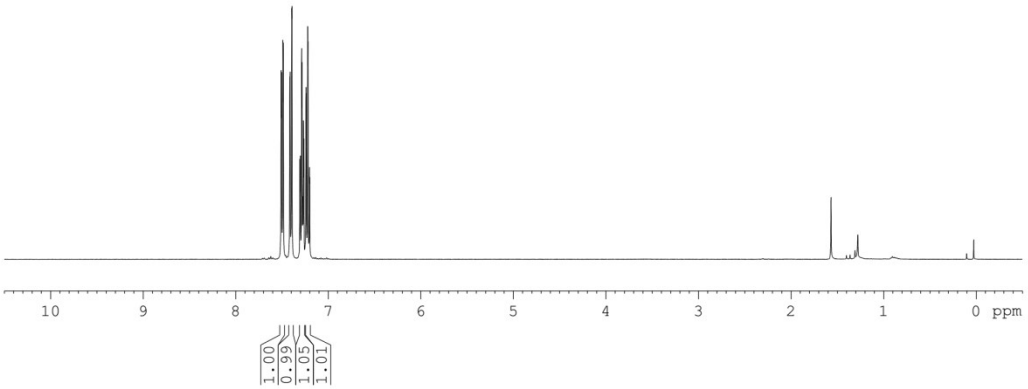

140.867
132.386
129.468
128.631
125.540
122.523
79.132
77.343
77.025
76.708
52.796
20.538
Br
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

1m


7.507
7.503
7.488
7.484
7.413
7.410
7.393
7.390
7.305
7.301
7.286
7.282
7.273
7.266
7.262
7.239
7.236
7.220
7.217
7.201
7.198


Cl
Br

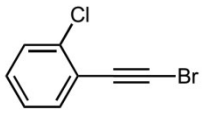
1n


10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
0.99
1.05
1.01

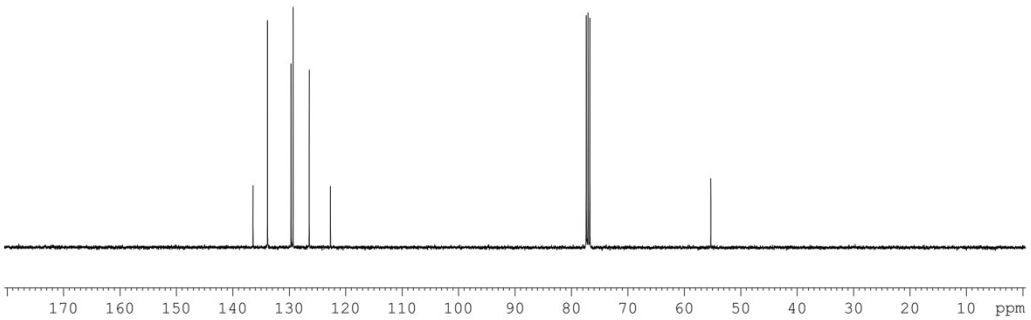

136.388
133.817
129.657
129.303
126.435
122.653

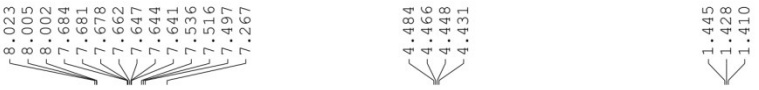

77.344
77.026
76.998
76.709

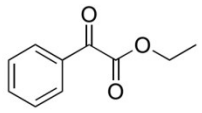
55.259


Cl
Br

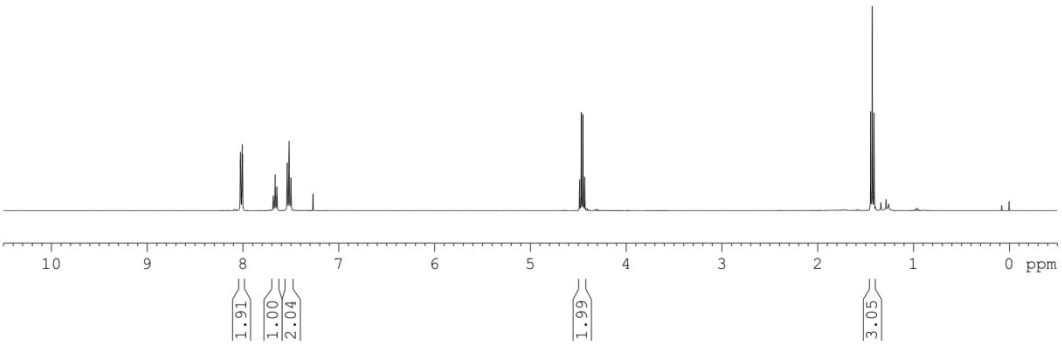
1n


170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

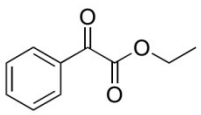

8.023
8.005
8.002
7.684
7.681
7.678
7.662
7.647
7.644
7.641
7.536
7.516
7.497
7.267
4.484
4.466
4.448
4.431
1.445
1.428
1.410



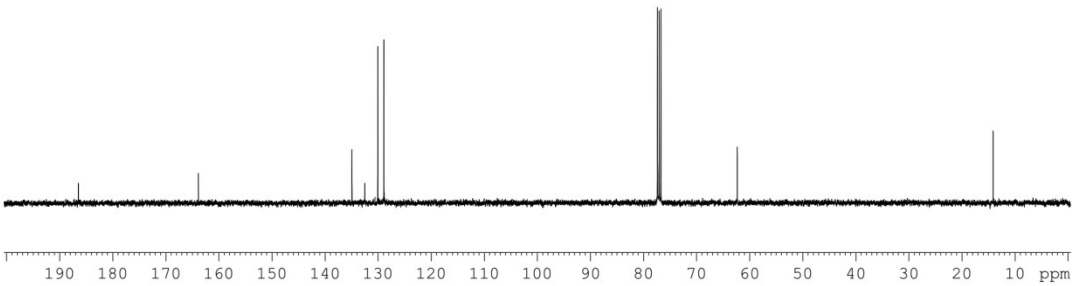
3aa

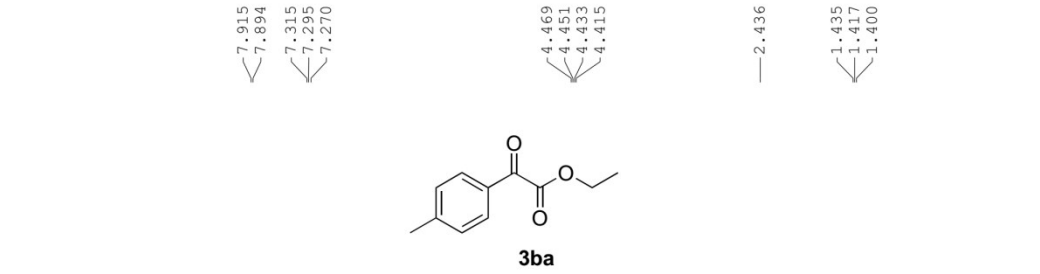

10
9
8
7
6
5
4
3
2
1
0 ppm
1.91
1.00
2.04
1.99
3.05

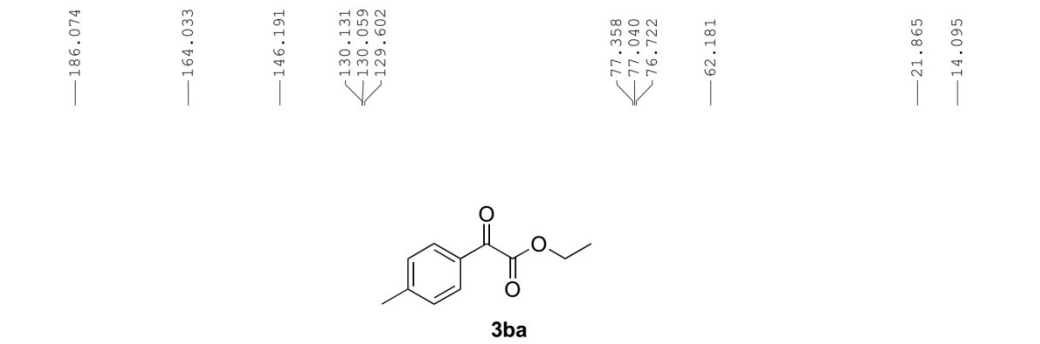

186.418
163.827
134.879
132.484
130.017
128.880
77.346
77.029
76.711
62.325
14.104

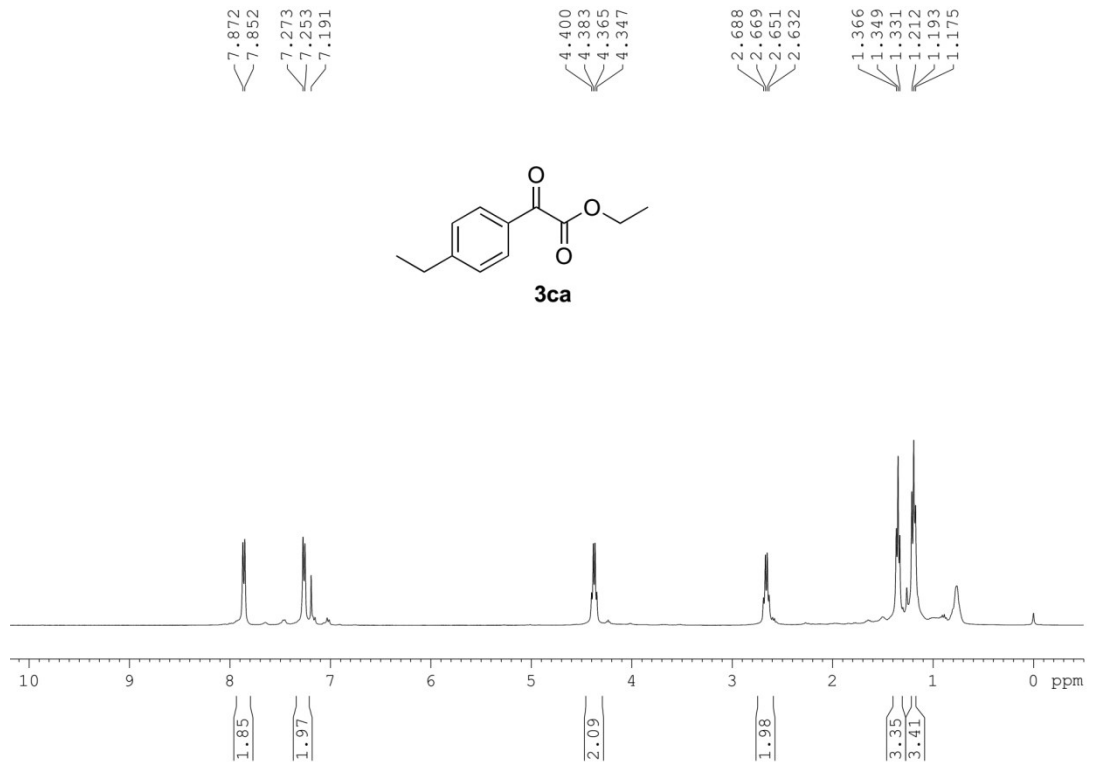


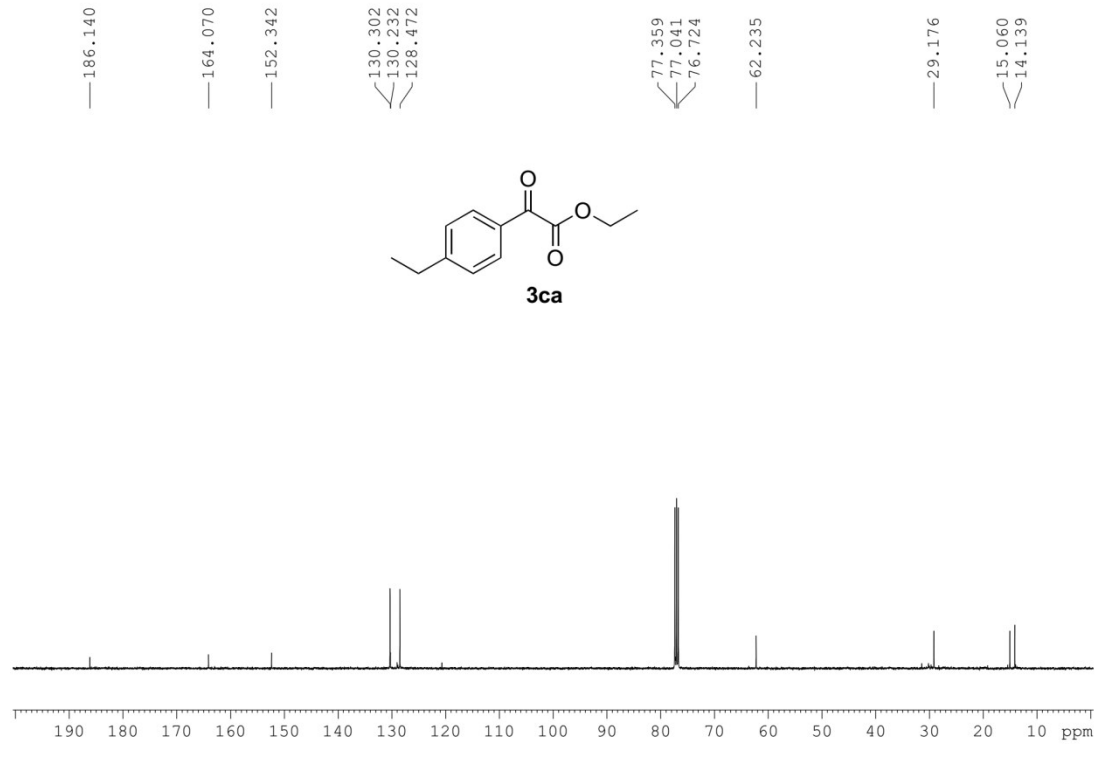
3aa

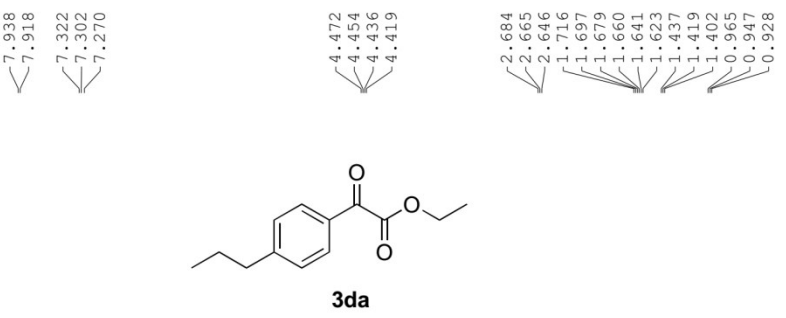

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.915
7.894
7.315
7.295
7.270
4.469
4.451
4.433
4.415
2.436
1.435
1.417
1.400
O
O
O
3ba
10
9
8
7
6
5
4
3
2
1
0 ppm
1.96
1.94
2.00
3.00
3.10

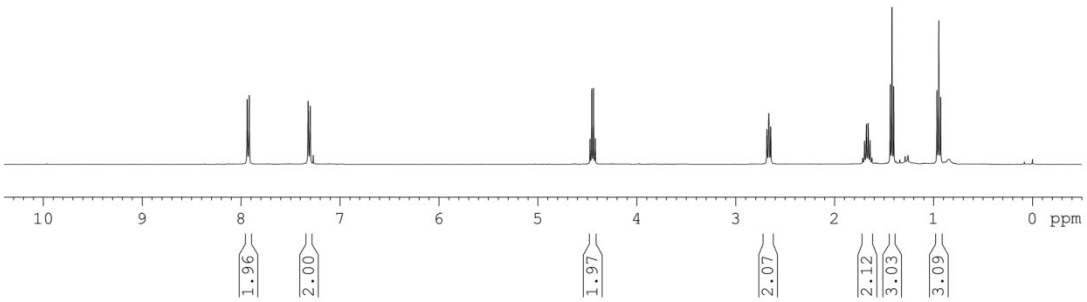

186.074
164.033
146.191
130.131
130.059
129.602
77.358
77.040
76.722
62.181
21.865
14.095
O
O
O
3ba
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.872
7.852
7.273
7.253
7.191
4.400
4.383
4.365
4.347
2.688
2.669
2.651
2.632
1.366
1.349
1.331
1.212
1.193
1.175
O
O
O
3ca
10 9 8 7 6 5 4 3 2 1 0 ppm
1.85
1.97
2.09
1.98
3.35
3.41

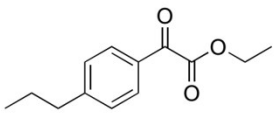

186.140
164.070
152.342
130.302
130.232
128.472
77.359
77.041
76.724
62.235
29.176
15.060
14.139
O
O
O
3ca
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.938
7.918
7.322
7.302
7.270
4.472
4.454
4.436
4.419
2.684
2.665
2.646
1.716
1.697
1.679
1.660
1.641
1.623
1.437
1.419
1.402
0.965
0.947
0.928
O
O
O

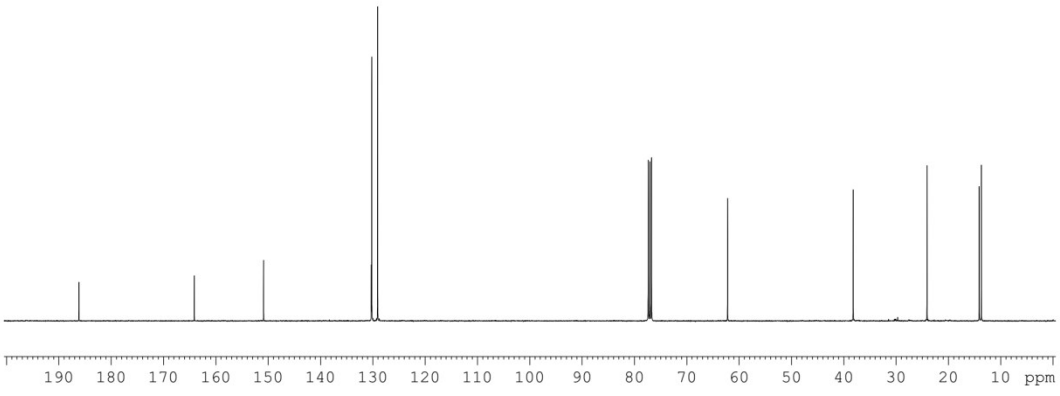
3da

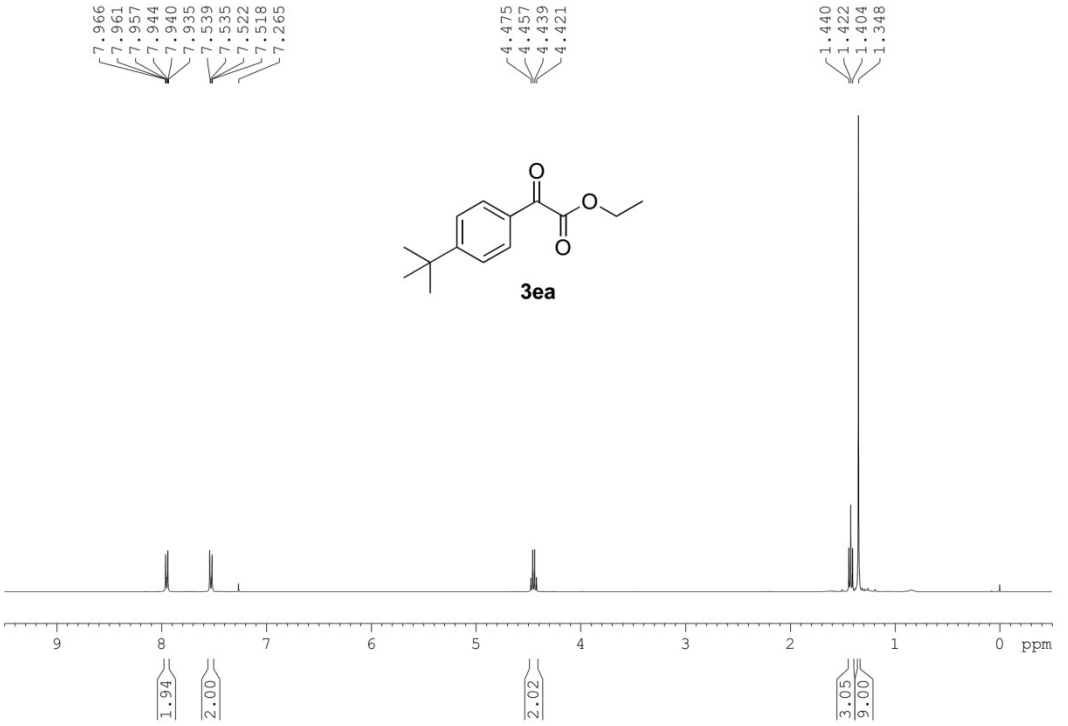

10
9
8
7
6
5
4
3
2
1
0 ppm
1.96
2.00
1.97
2.07
2.12
3.03
3.09

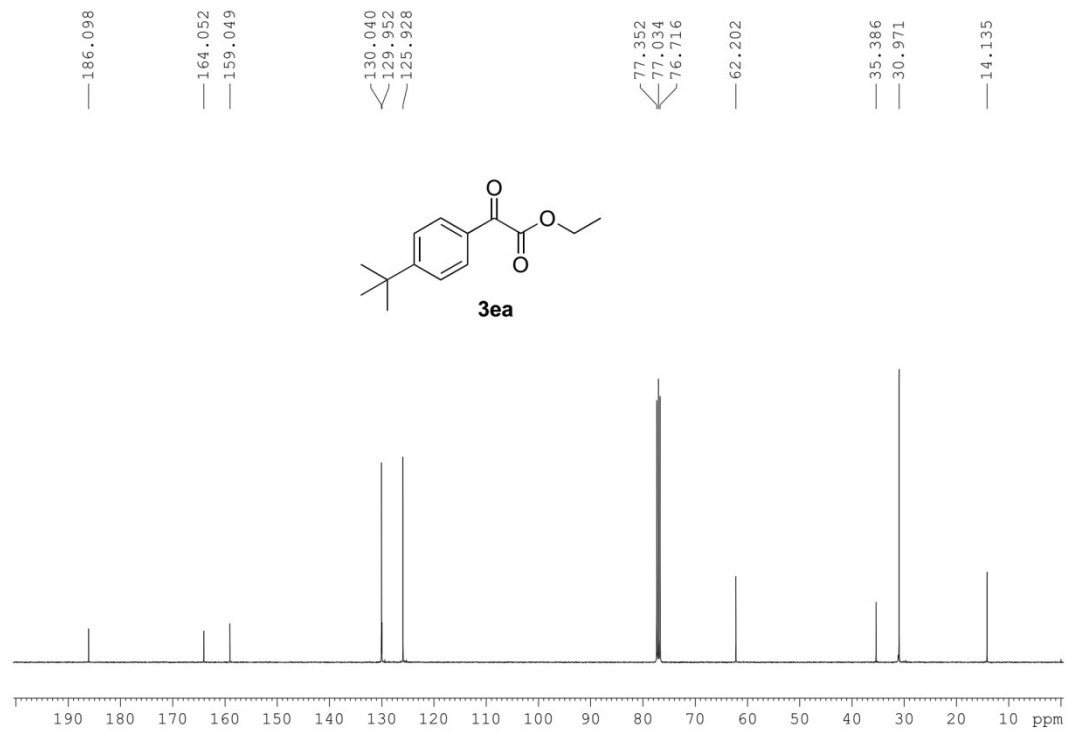

186.129
164.083
150.841
130.255
130.168
129.043
77.371
77.053
76.735
62.196
38.197
24.085
14.116
13.702


O
O
O

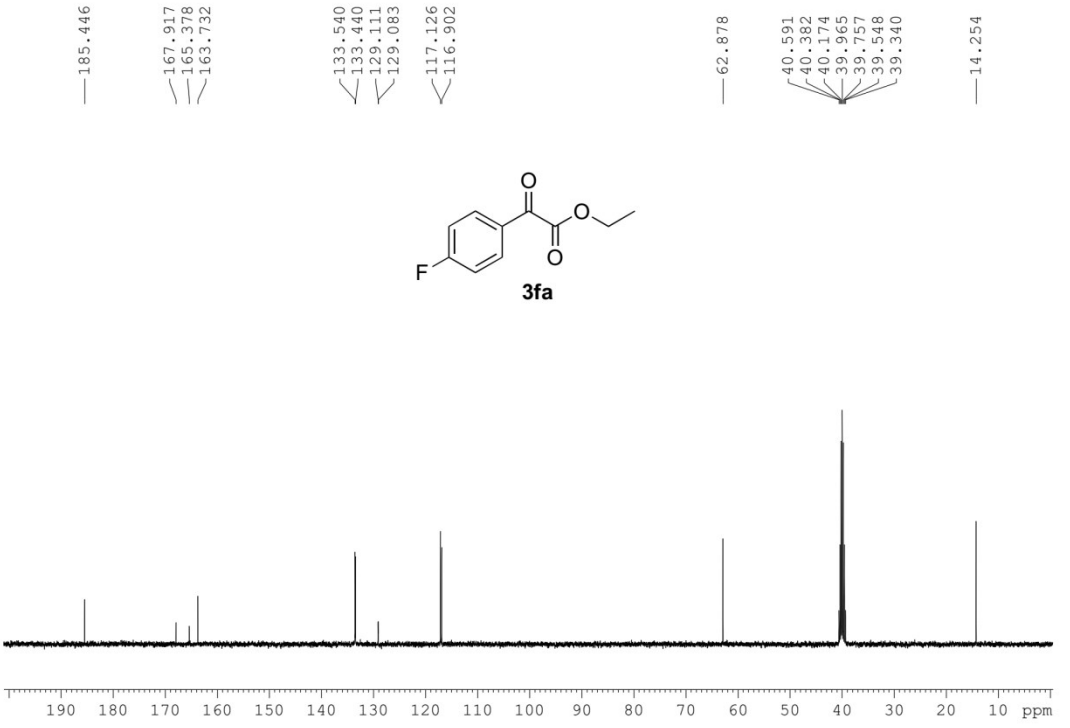
3da


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

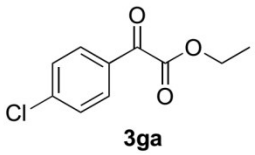

7.966
7.961
7.957
7.944
7.940
7.935
7.539
7.535
7.522
7.518
7.265
4.475
4.457
4.439
4.421
1.440
1.422
1.404
1.348
O
O
O
3ea
9
8
7
6
5
4
3
2
1
0 ppm
1.94
2.00
2.02
3.05
9.00


186.098
164.052
159.049
130.040
129.952
125.928
77.352
77.034
76.716
62.202
35.386
30.971
14.135
O
O
O
3ea
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

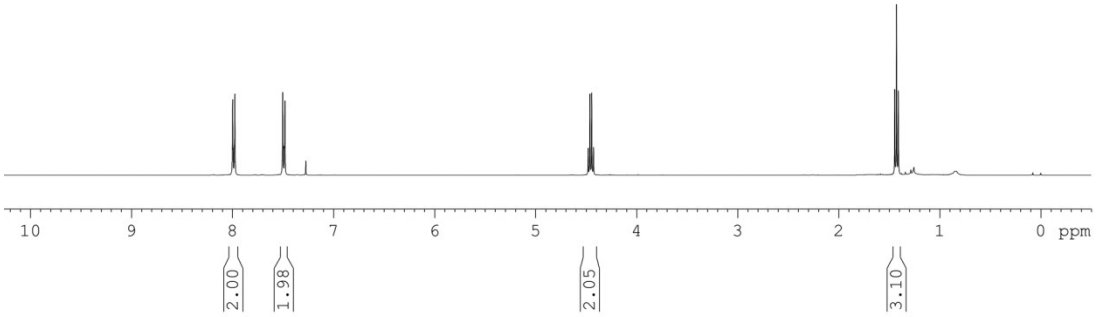

8.088
8.081
8.075
8.067
8.064
8.062
8.059
8.050
8.045
8.037
7.468
7.461
7.456
7.444
7.439
7.434
7.422
7.417
7.409
4.433
4.415
4.397
4.379
3.343
2.497
2.492
2.488
1.336
1.319
1.301
O
O
O
F
3fa
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
2.03
2.07
3.10


185.446
167.917
165.378
163.732
133.540
133.440
129.111
129.083
117.126
116.902
62.878
40.591
40.382
40.174
39.965
39.757
39.548
39.340
14.254
O
O
O
F
3fa
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

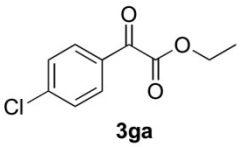

8.003
7.998
7.993
7.981
7.976
7.970
7.508
7.502
7.497
7.485
7.481
7.475
7.274
4.479
4.462
4.444
4.426
1.445
1.427
1.409


O
O
O
Cl

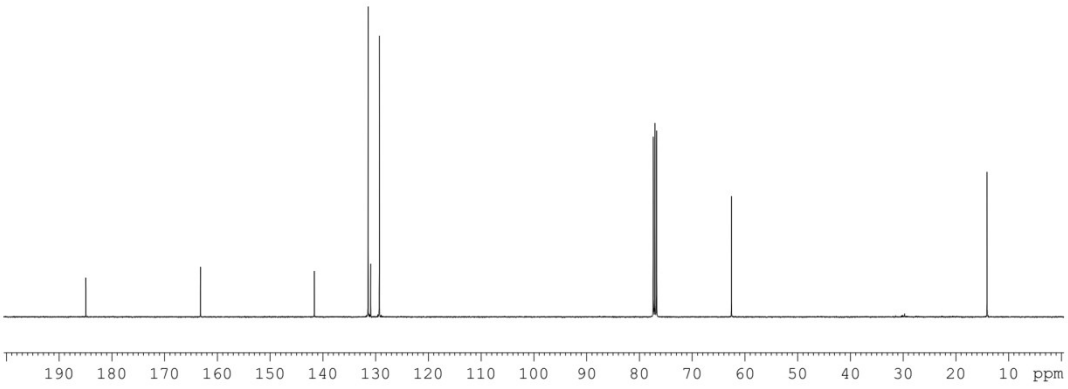
3ga

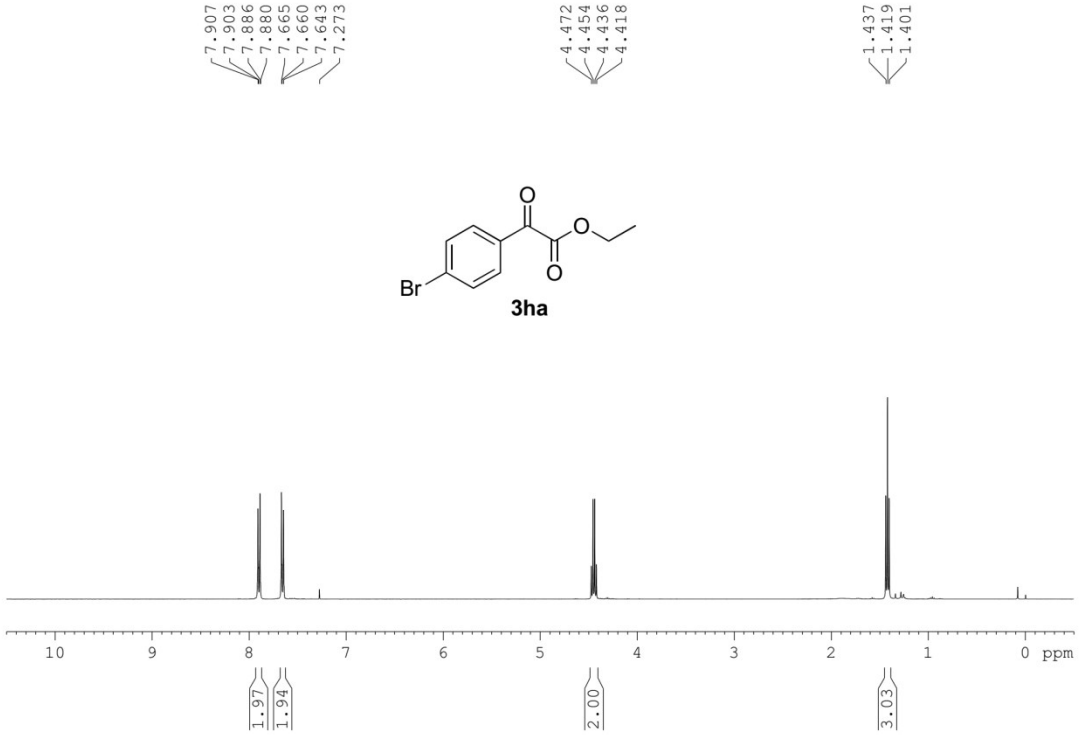

10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.98
2.05
3.10


184.878
163.203
141.609
131.426
130.938
129.295
77.358
77.040
76.722
62.533
14.080

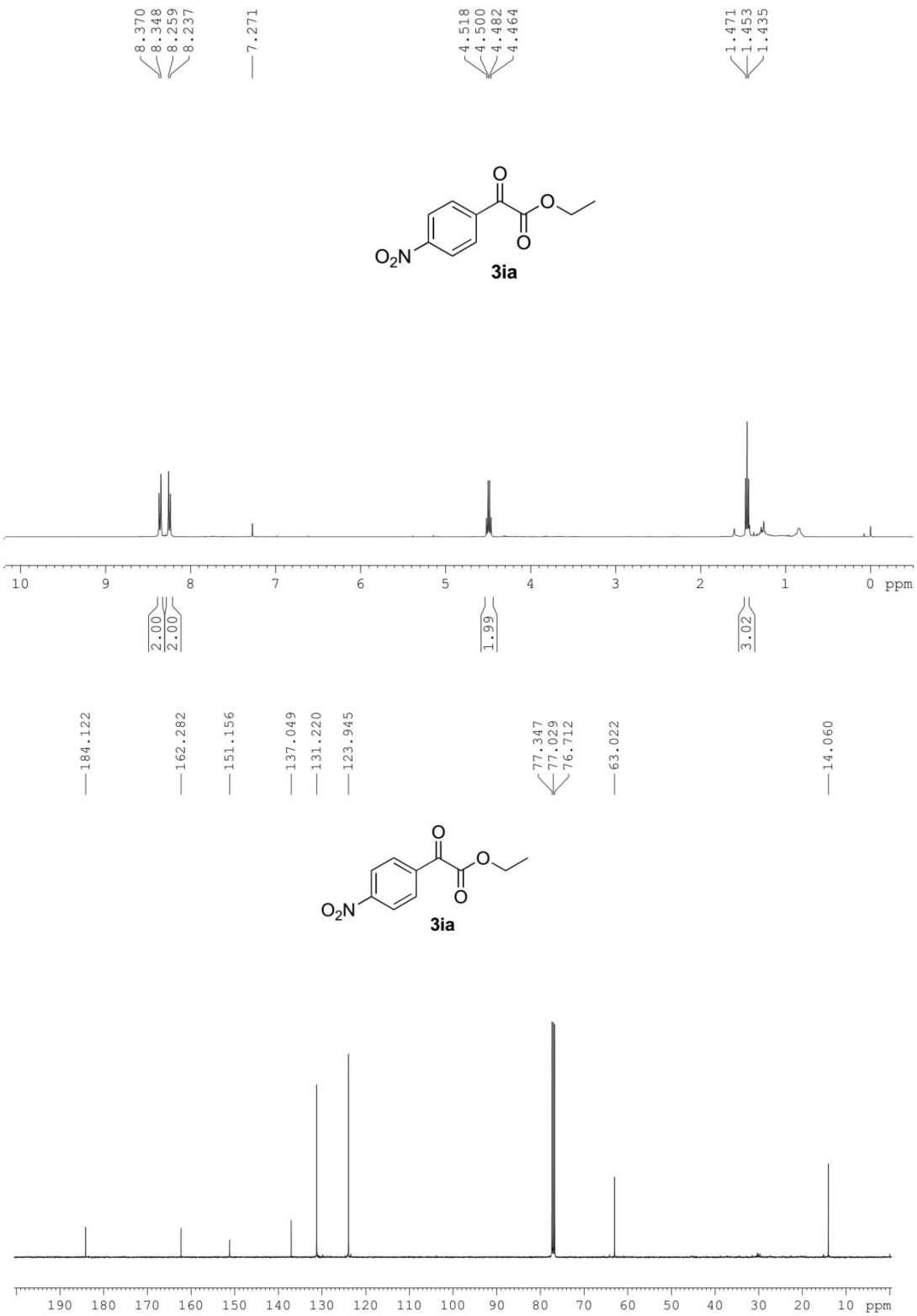

O
O
O
Cl

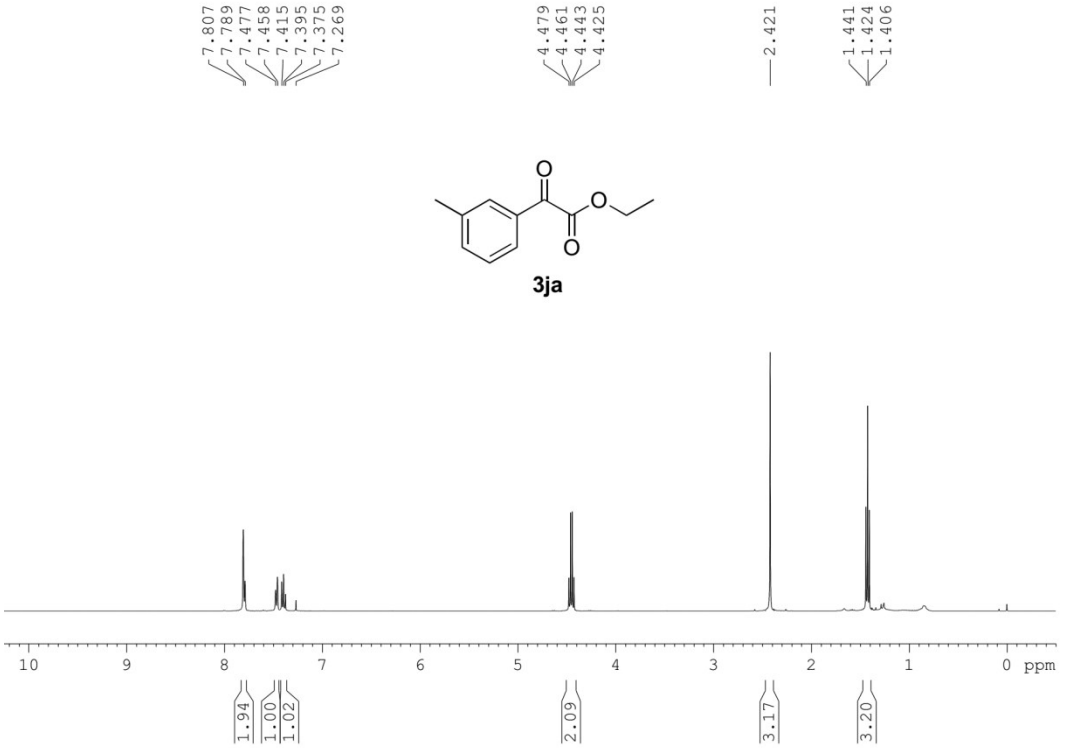
3ga

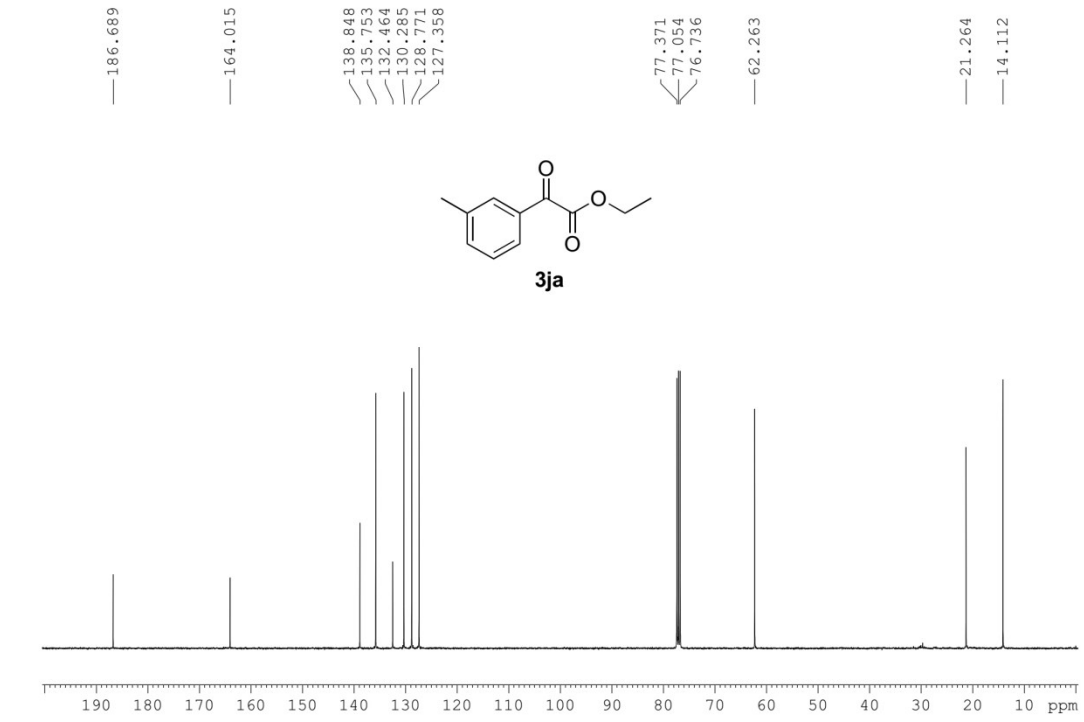

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.907
7.903
7.886
7.880
7.665
7.660
7.643
7.273
4.472
4.454
4.436
4.418
1.437
1.419
1.401
Br
3ha
10
9
8
7
6
5
4
3
2
1
0 ppm
1.97
1.94
2.00
3.03

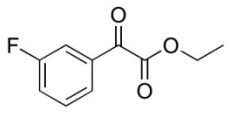

185.069
163.148
132.274
131.418
131.342
130.476
77.362
77.044
76.726
62.523
14.066
Br
3ha
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


8.370
8.348
8.259
8.237
7.271
4.518
4.500
4.482
4.464
1.471
1.453
1.435
O
O
O
O
O2N
3ia
10 9 8 7 6 5 4 3 2 1 0 ppm
2.00
2.00
1.99
3.02
184.122
162.282
151.156
137.049
131.220
123.945
77.347
77.029
76.712
63.022
14.060
O
O
O
O
O2N
3ia
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

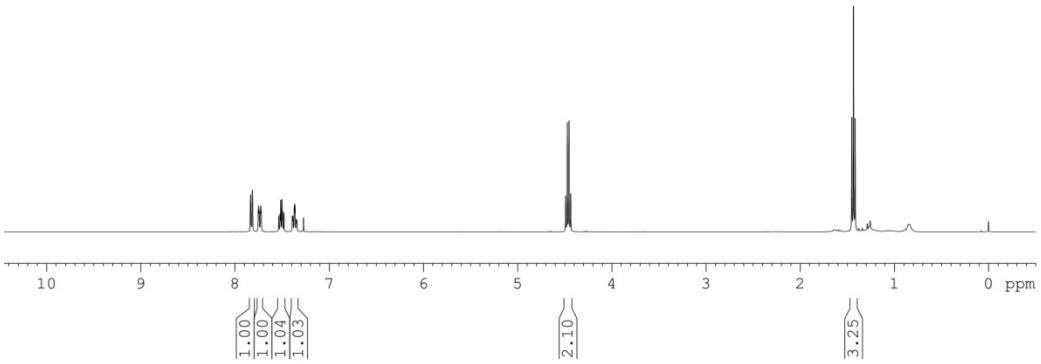

7.807
7.789
7.477
7.458
7.415
7.395
7.375
7.269
4.479
4.461
4.443
4.425
2.421
1.441
1.424
1.406
3ja
10
9
8
7
6
5
4
3
2
1
0 ppm
1.94
1.00
1.02
2.09
3.17
3.20


186.689
164.015
138.848
135.753
132.464
130.285
128.771
127.358
77.371
77.054
76.736
62.263
21.264
14.112
3ja
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

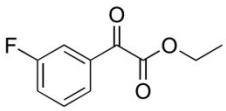

7.834
7.814
7.752
7.747
7.742
7.729
7.724
7.719
7.534
7.520
7.513
7.500
7.494
7.480
7.389
7.383
7.369
7.363
7.348
7.342
7.271
4.489
4.471
4.453
4.435
1.451
1.433
1.415


O
F
O
O

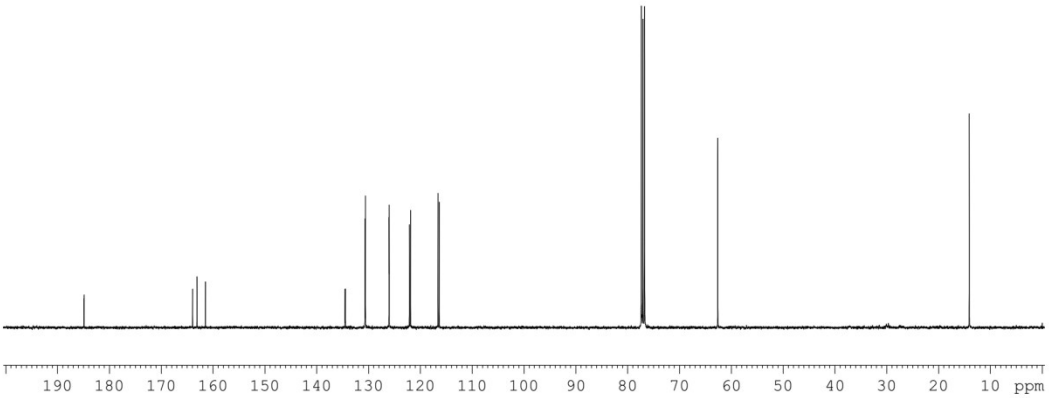
3ka


10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.00
1.04
1.03
2.10
3.25

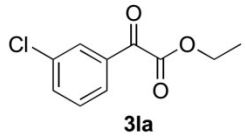

184.912
184.888
163.957
163.094
161.482
134.534
134.468
130.680
130.604
126.042
126.011
122.112
121.898
116.597
116.370
77.348
77.030
76.713
62.600
14.071


O
F
O
O

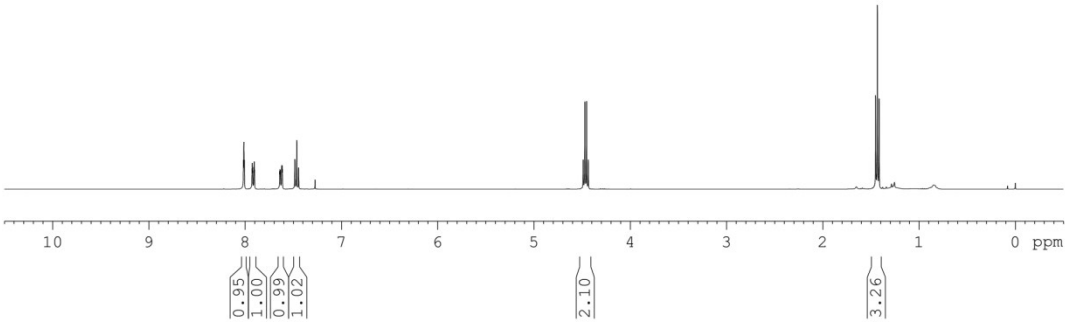
3ka


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

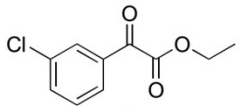

8.018
8.013
8.009
7.928
7.926
7.922
7.909
7.906
7.902
7.641
7.639
7.636
7.633
7.621
7.619
7.616
7.613
7.484
7.464
7.445
7.274
4.489
4.471
4.453
4.435
1.451
1.433
1.415


Cl
O
O
O

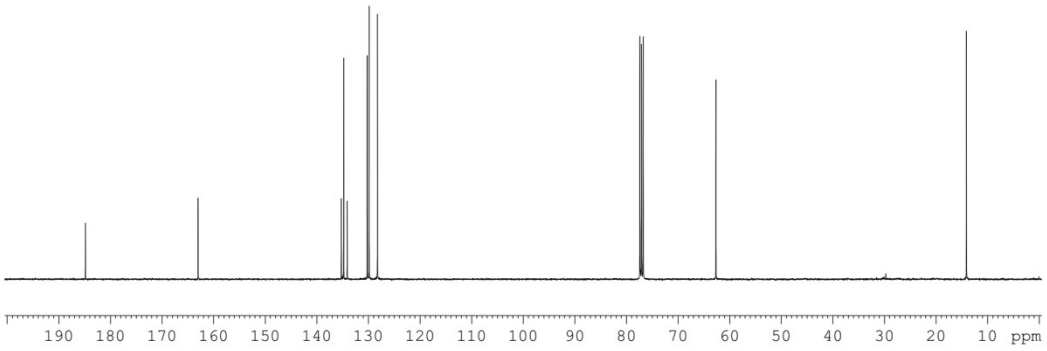
3la

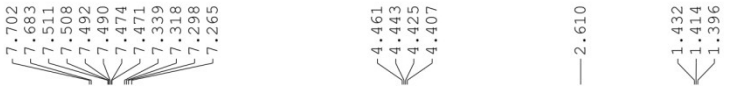

10
9
8
7
6
5
4
3
2
1
0 ppm
0.95
1.00
0.99
1.02
2.10
3.26

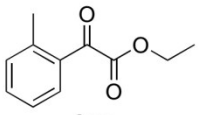

184.832
162.998
135.236
134.770
134.079
130.206
129.845
128.226
77.362
77.044
76.727
62.632
14.074


Cl
O
O
O

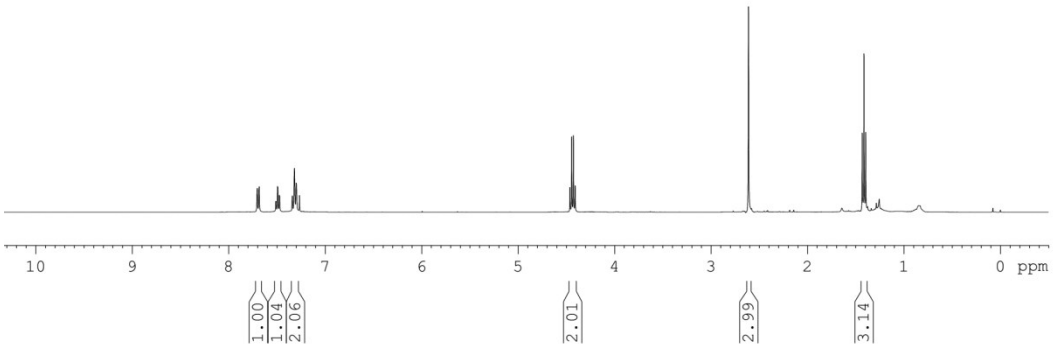
3la


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

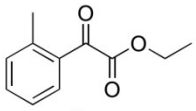

7.702
7.683
7.511
7.508
7.492
7.490
7.474
7.471
7.339
7.318
7.298
7.265
4.461
4.443
4.425
4.407
2.610
1.432
1.414
1.396



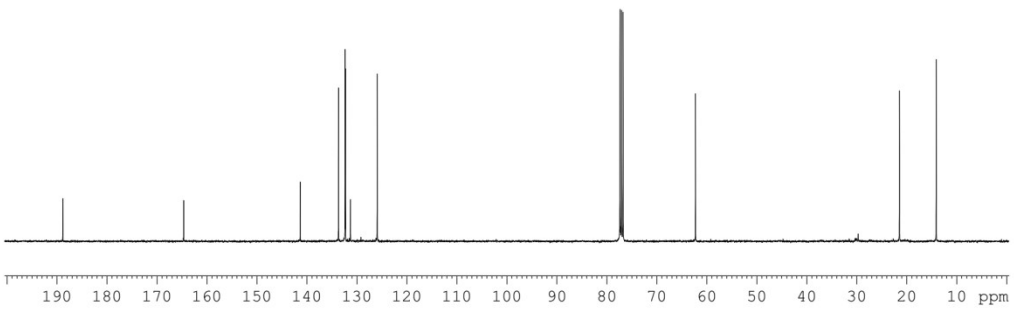
3ma

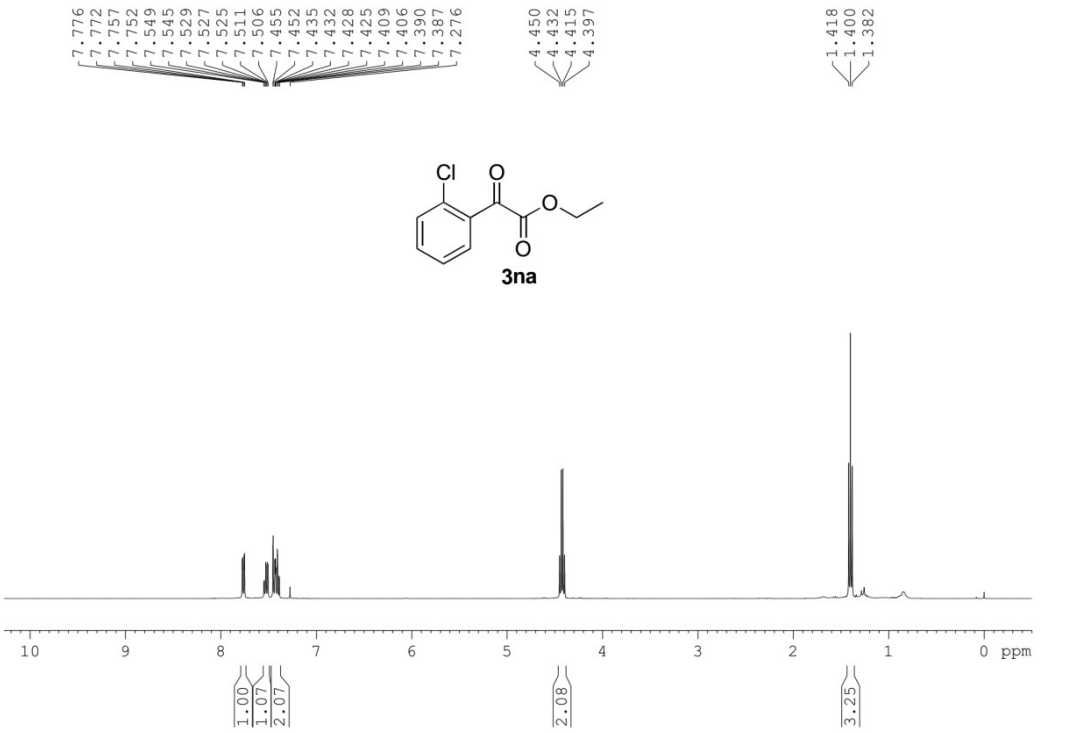

10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.04
2.06
2.01
2.99
3.14

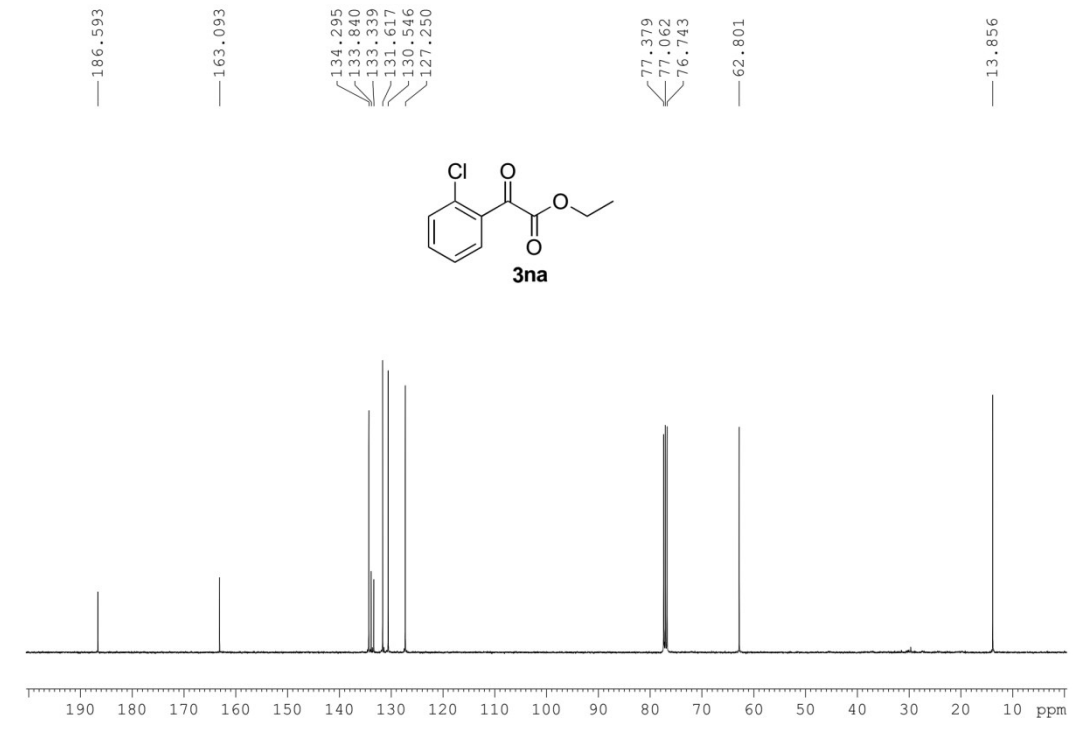

188.794
164.635
141.323
133.662
132.354
132.258
131.271
125.918
77.362
77.043
76.726
62.253
21.439
14.088

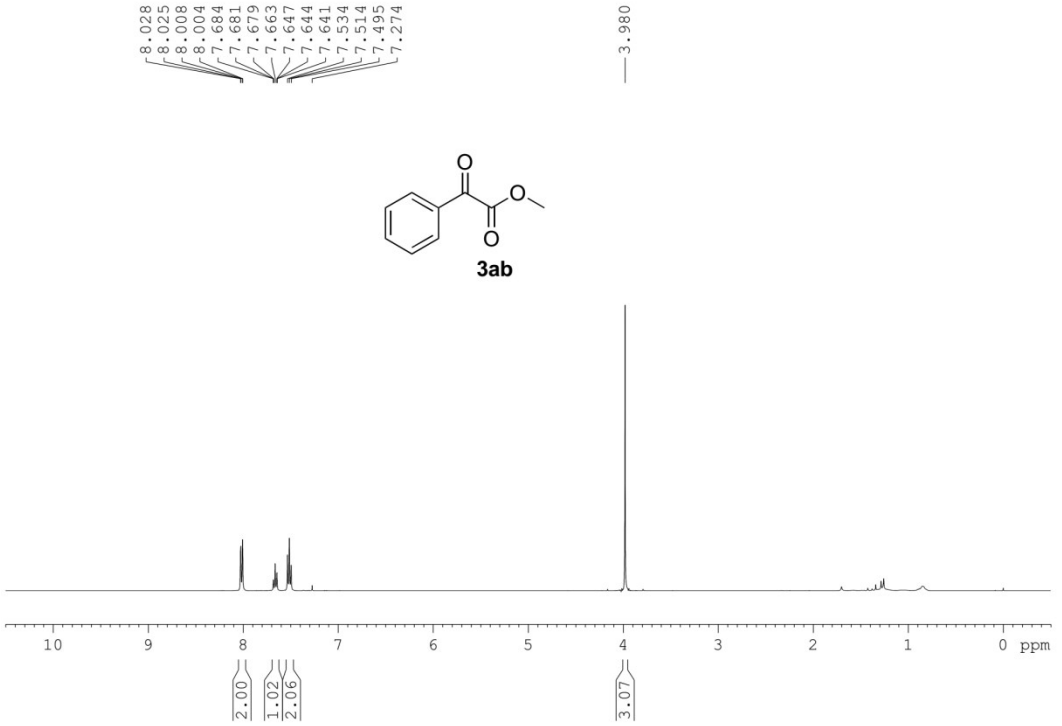


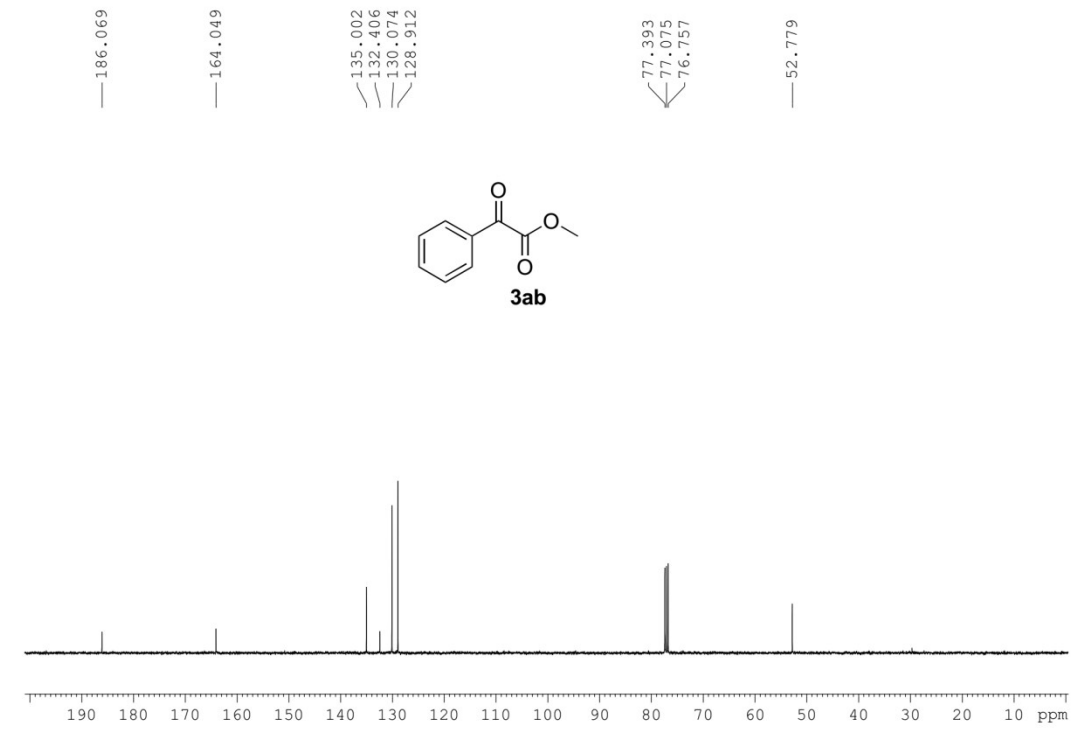
3ma


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

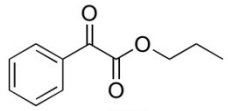

7.776
7.772
7.757
7.752
7.549
7.545
7.529
7.527
7.525
7.511
7.506
7.455
7.452
7.435
7.432
7.428
7.425
7.409
7.406
7.390
7.387
7.276
4.450
4.432
4.415
4.397
1.418
1.400
1.382
Cl
O
O
O
3na
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.07
2.07
2.08
3.25


186.593
163.093
134.295
133.840
133.339
131.617
130.546
127.250
77.379
77.062
76.743
62.801
13.856
Cl
O
O
O
3na
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

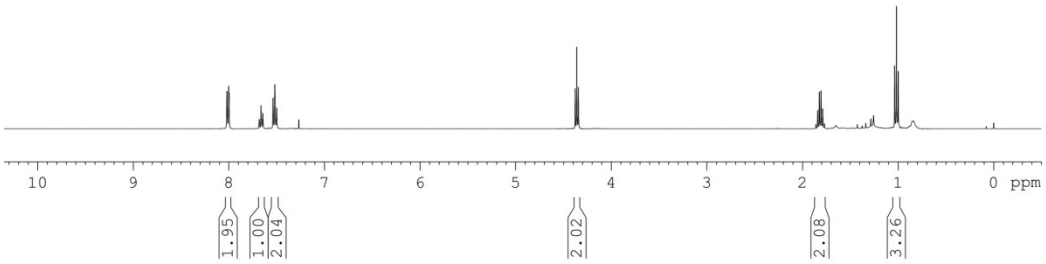

8.028
8.025
8.008
8.004
7.684
7.681
7.679
7.663
7.647
7.644
7.641
7.534
7.514
7.495
7.274
3.980
3ab
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.02
2.06
3.07


186.069
164.049
135.002
132.406
130.074
128.912
77.393
77.075
76.757
52.779
3ab
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

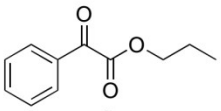

8.020
8.017
8.004
8.000
7.996
7.684
7.681
7.678
7.662
7.646
7.643
7.640
7.537
7.517
7.502
7.498
7.267
4.376
4.359
4.342
1.858
1.840
1.822
1.804
1.787
1.769
1.036
1.017
0.999



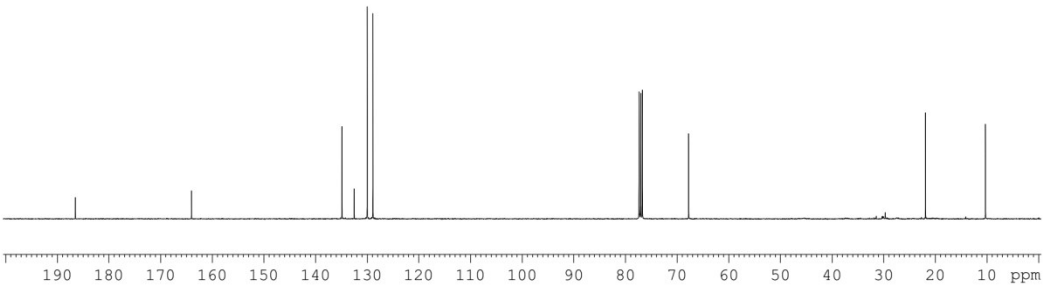
3ac

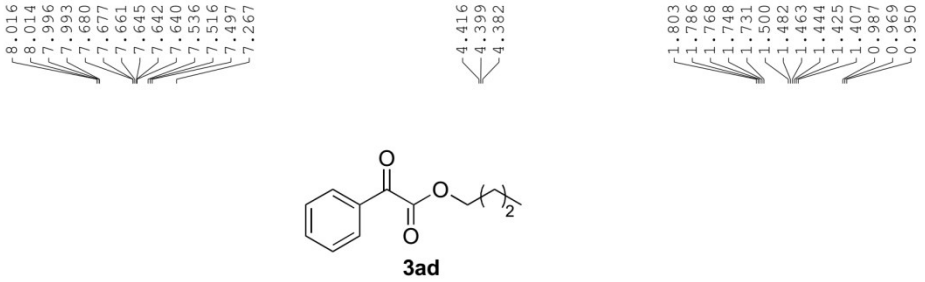

10
9
8
7
6
5
4
3
2
1
0 ppm
1.95
1.00
2.04
2.02
2.08
3.26


186.500
164.018
134.877
132.514
129.998
128.896
77.356
77.039
76.721
67.765
21.891
10.296

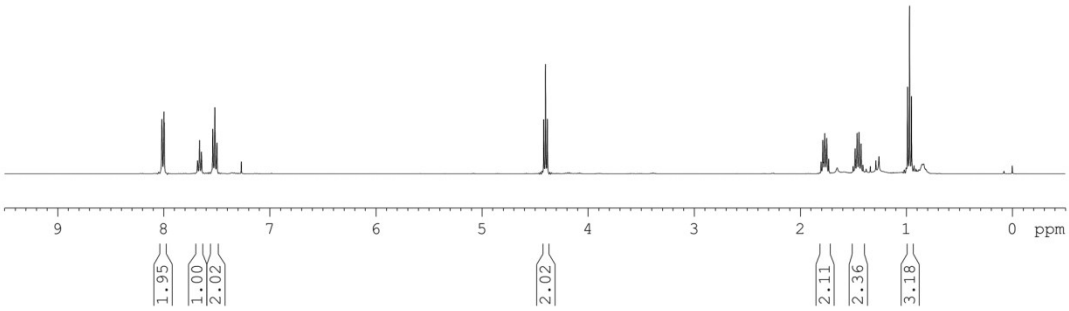


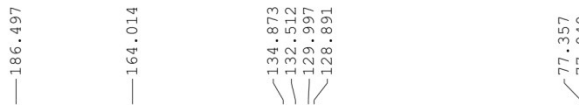
3ac


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


8.016
8.014
7.996
7.993
7.680
7.677
7.661
7.645
7.642
7.640
7.536
7.516
7.497
7.267
4.416
4.399
4.382
1.803
1.786
1.768
1.748
1.731
1.500
1.482
1.463
1.444
1.425
1.407
0.987
0.969
0.950

3ad


9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.00
2.02
2.02
2.11
2.36
3.18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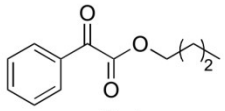
164.014
134.873
132.512
129.997
128.891
77.357
77.040
76.722
66.094
30.469
19.031
13.615



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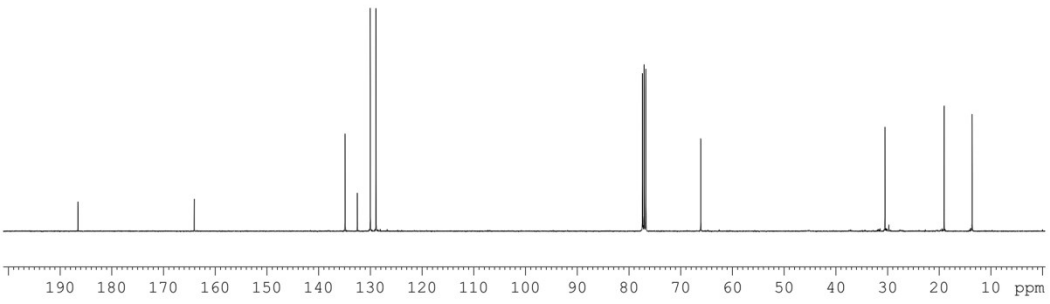
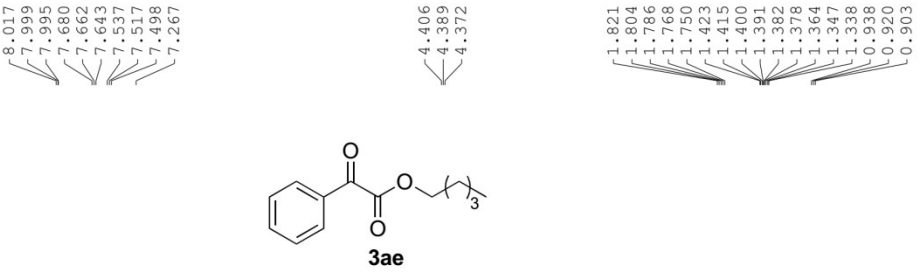
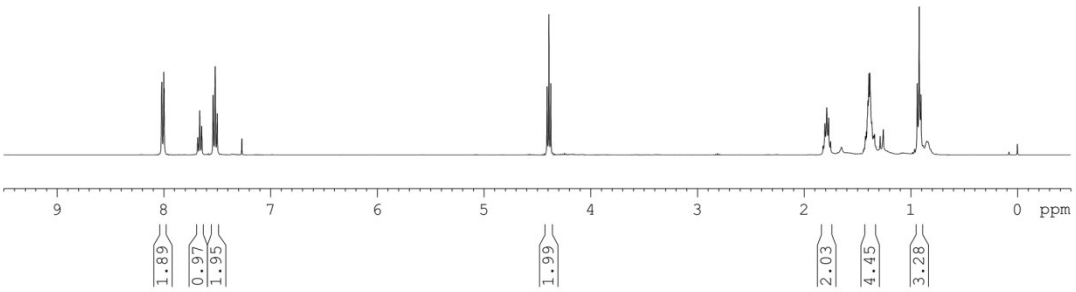
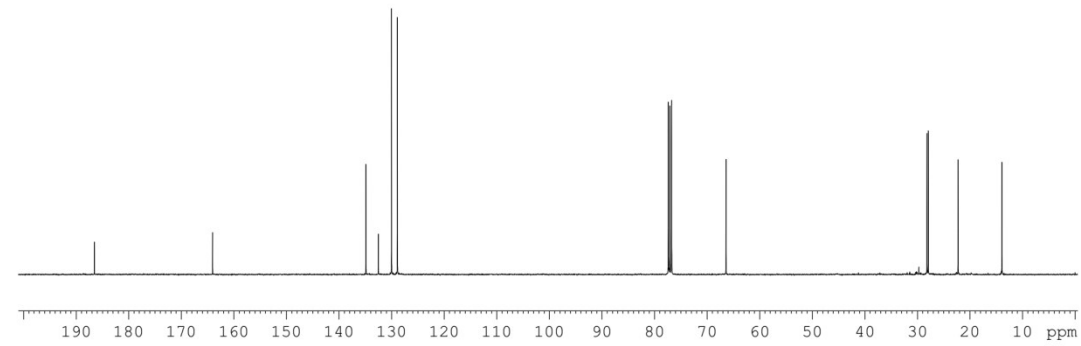

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

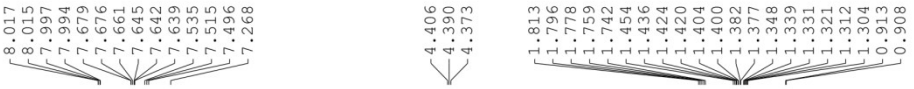

8.017
7.999
7.995
7.680
7.662
7.643
7.537
7.517
7.498
7.267
4.406
4.389
4.372
1.821
1.804
1.786
1.768
1.750
1.423
1.415
1.400
1.391
1.382
1.378
1.364
1.347
1.338
0.938
0.920
0.903
O
O
O
3
3ae


9
8
7
6
5
4
3
2
1
0
ppm
1.89
0.97
1.95
1.99
2.03
4.45
3.28


186.497
164.005
134.874
132.515
130.005
128.889
77.356
77.038
76.720
66.376
28.153
27.898
22.235
13.894

O
O
O
3
3ae


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.017
8.015
7.997
7.994
7.679
7.676
7.661
7.645
7.642
7.639
7.535
7.515
7.496
7.268
4.406
4.390
4.373
1.813
1.796
1.778
1.759
1.742
1.454
1.436
1.424
1.420
1.404
1.400
1.382
1.377
1.348
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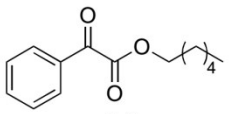
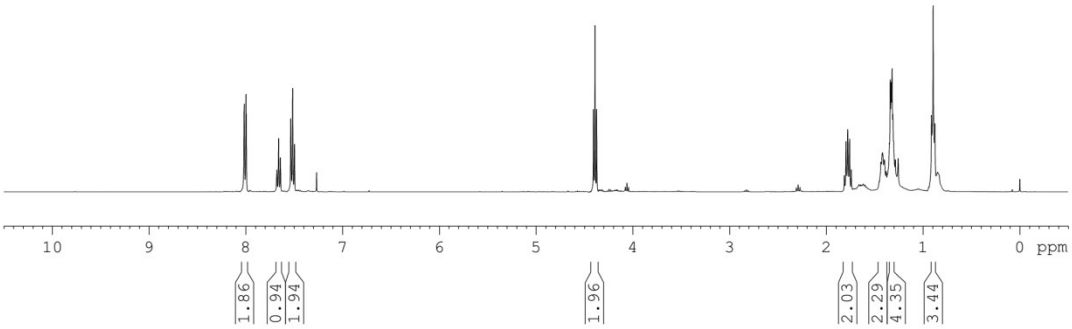
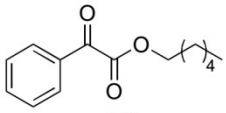
1.321
1.312
1.304
0.913
0.908


O
O
O
4

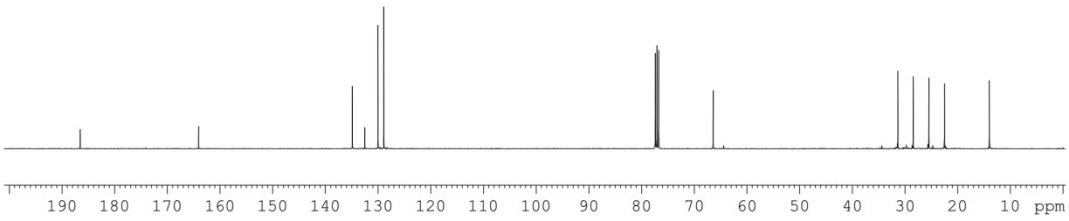
3af

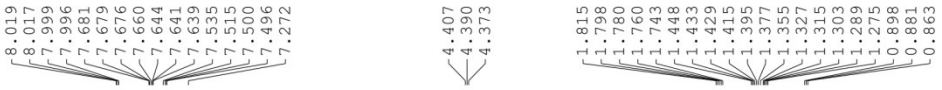

10
9
8
7
6
5
4
3
2
1
0 ppm
1.86
0.94
1.94
1.96
2.03
2.29
4.35
3.44


186.497
164.011
134.868
132.516
130.000
128.883
77.358
77.041
76.722
66.386
31.318
28.424
25.442
22.479
13.949


O
O
O
4

3af


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


8.019
8.017
7.999
7.996
7.681
7.679
7.676
7.660
7.644
7.641
7.639
7.535
7.515
7.500
7.496
7.272
4.407
4.390
4.373
1.815
1.798
1.780
1.760
1.743
1.448
1.433
1.429
1.415
1.395
1.377
1.355
1.327
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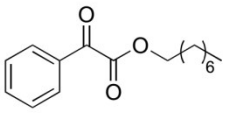
1.303
1.289
1.275
0.898
0.881
0.863



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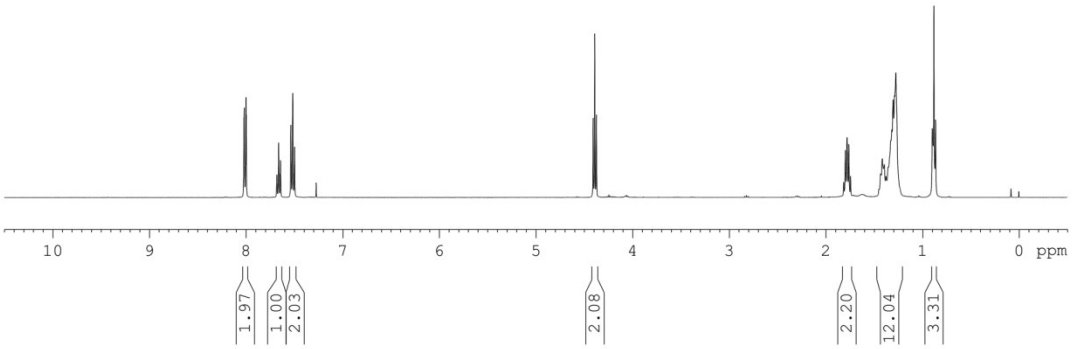
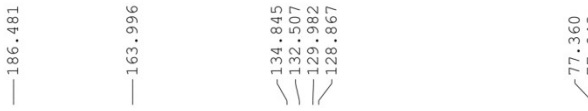
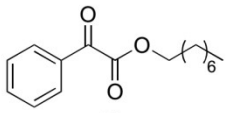
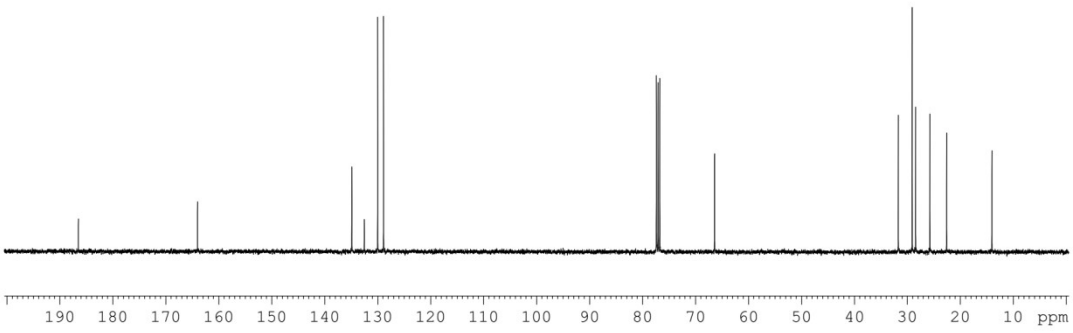
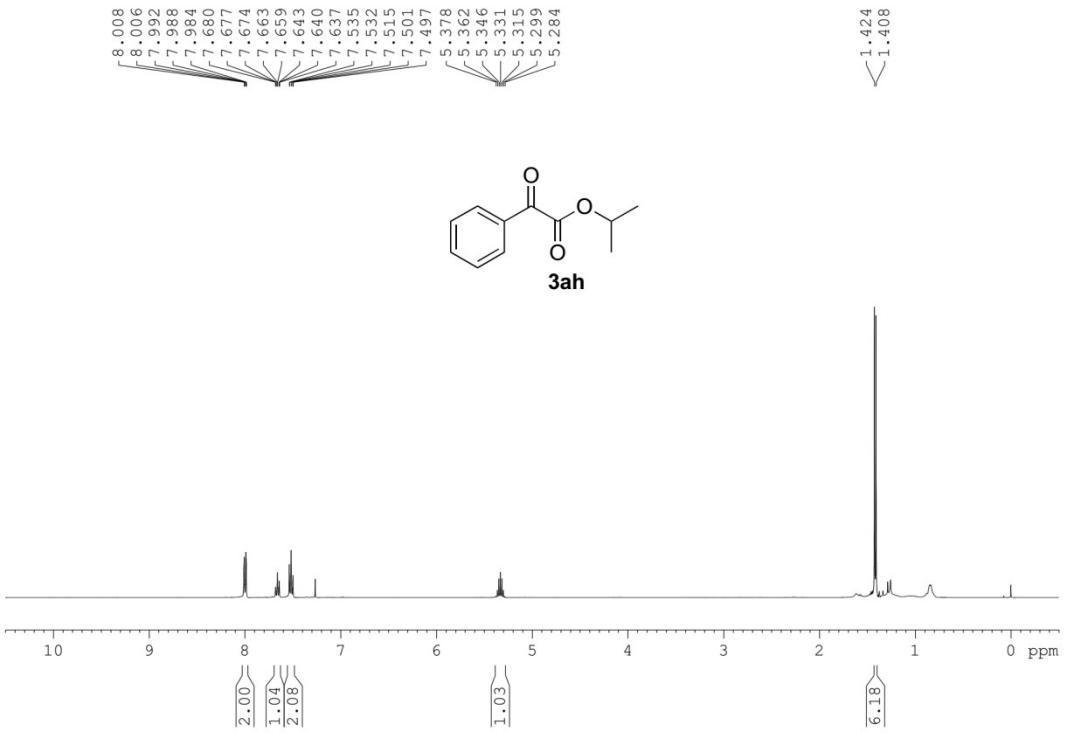

10
9
8
7
6
5
4
3
2
1
0 ppm
1.97
1.00
2.03
2.08
2.20
12.04
3.31

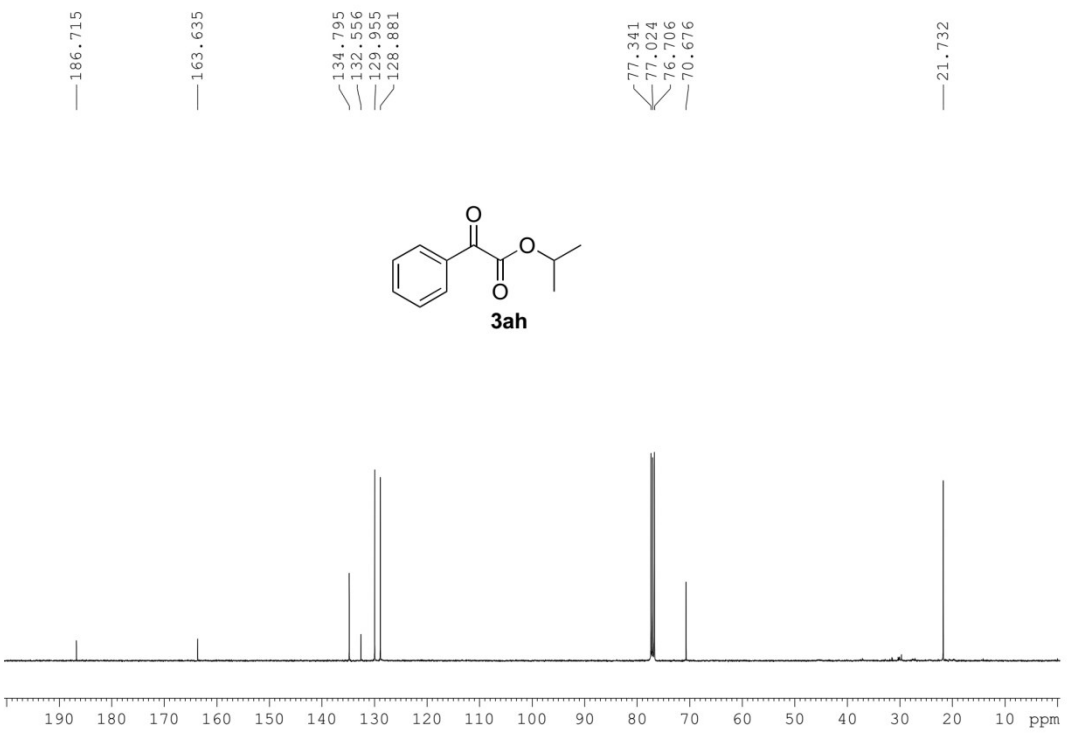

186.481
163.996
134.845
132.507
129.982
128.867
77.360
77.043
76.725
66.367
31.717
29.098
28.448
25.764
22.597
14.043

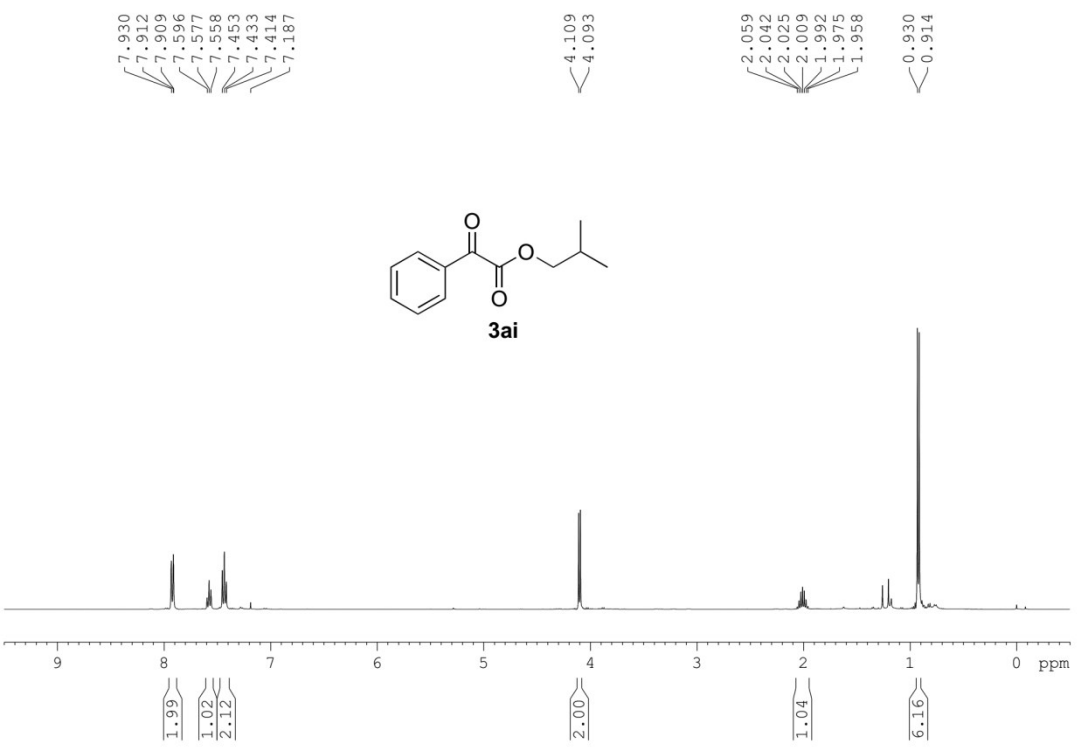


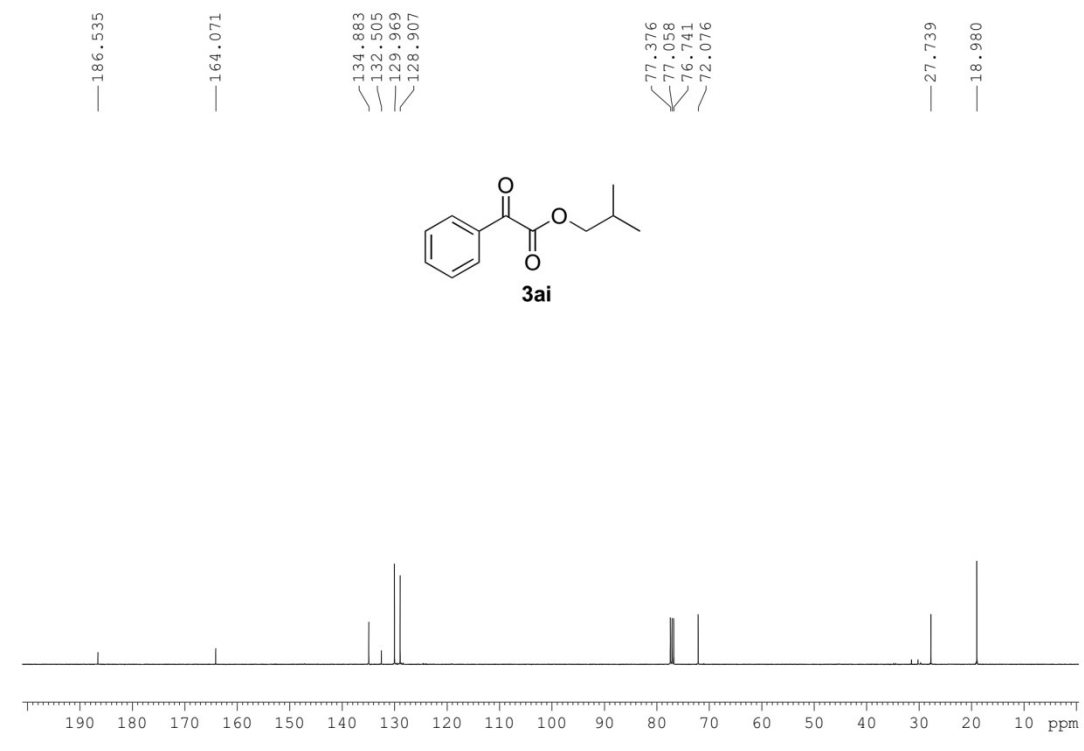
3ag

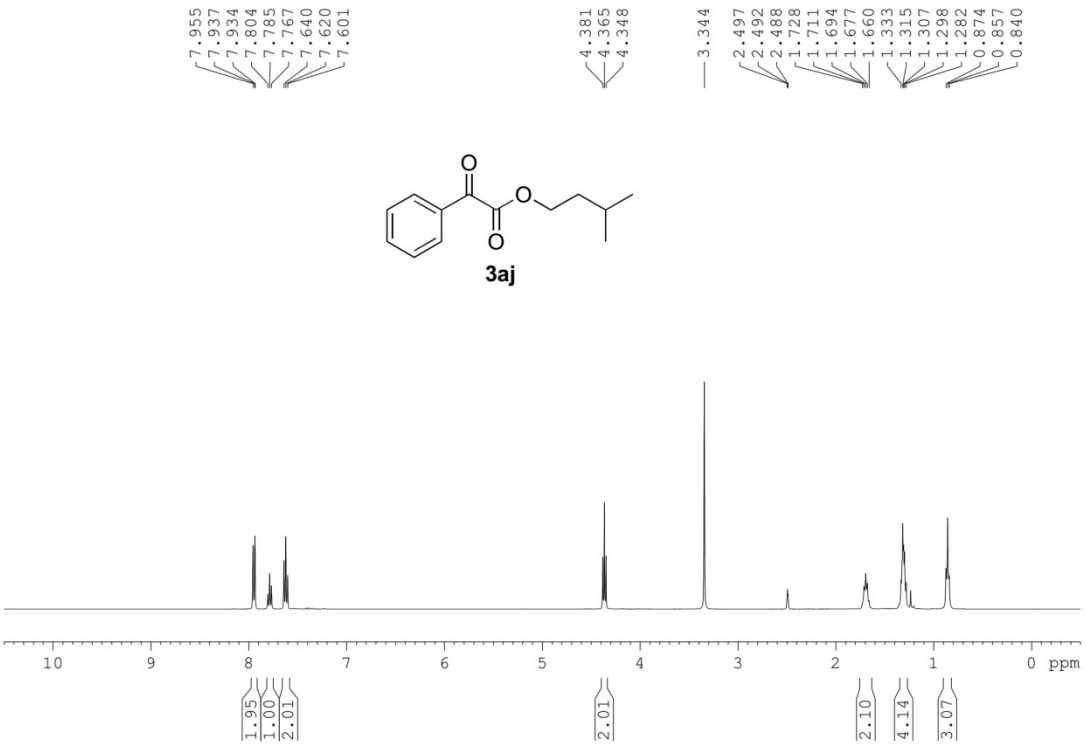

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


8.008
8.006
7.992
7.988
7.984
7.680
7.677
7.674
7.663
7.659
7.643
7.640
7.637
7.535
7.532
7.515
7.501
7.497
5.378
5.362
5.346
5.331
5.315
5.299
5.284
1.424
1.408
3ah
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.04
2.08
1.03
6.18


186.715
163.635
134.795
132.556
129.955
128.881
77.341
77.024
76.706
70.676
21.732
3ah
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm


7.930
7.912
7.909
7.596
7.577
7.558
7.453
7.433
7.414
7.187
4.109
4.093
2.059
2.042
2.025
2.009
1.992
1.975
1.958
0.930
0.914
3ai
9
8
7
6
5
4
3
2
1
0 ppm
1.99
1.02
2.12
2.00
1.04
6.16


186.535
164.071
134.883
132.505
129.969
128.907
77.376
77.058
76.741
72.076
27.739
18.980
3ai
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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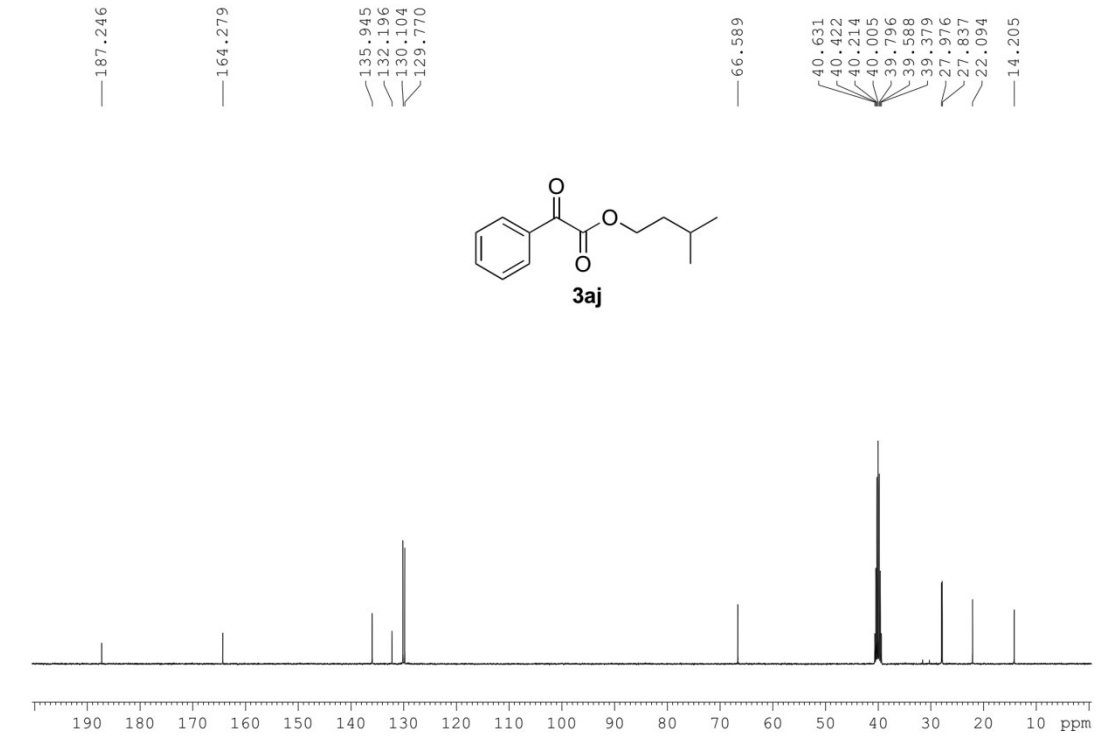
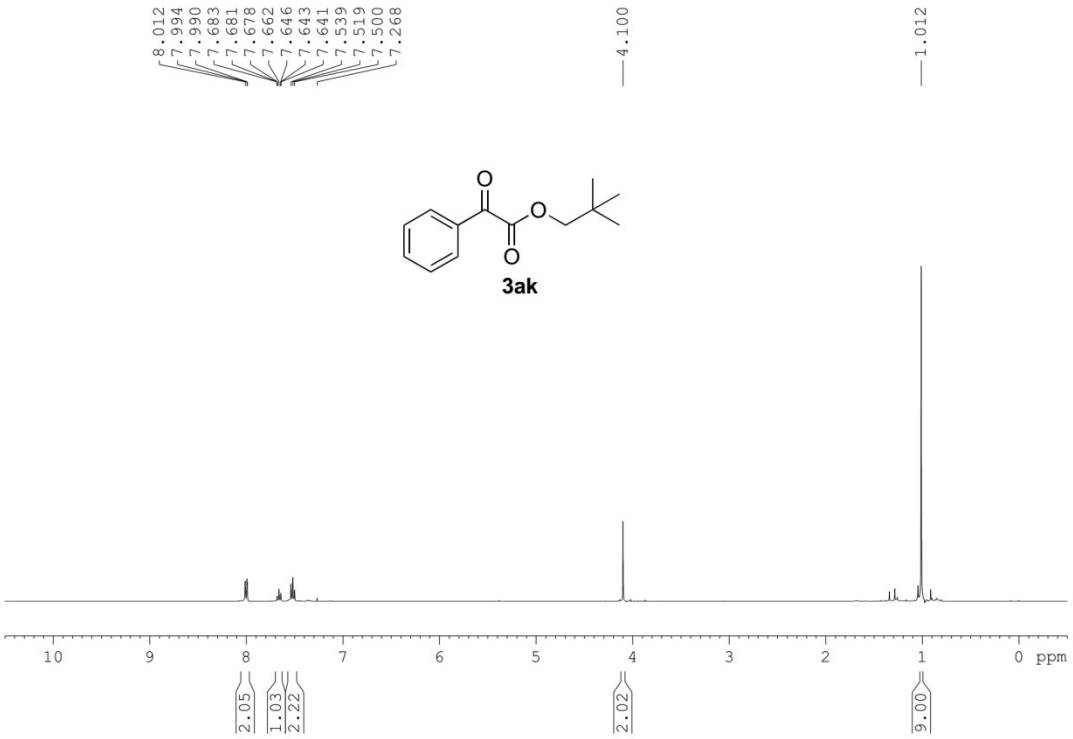
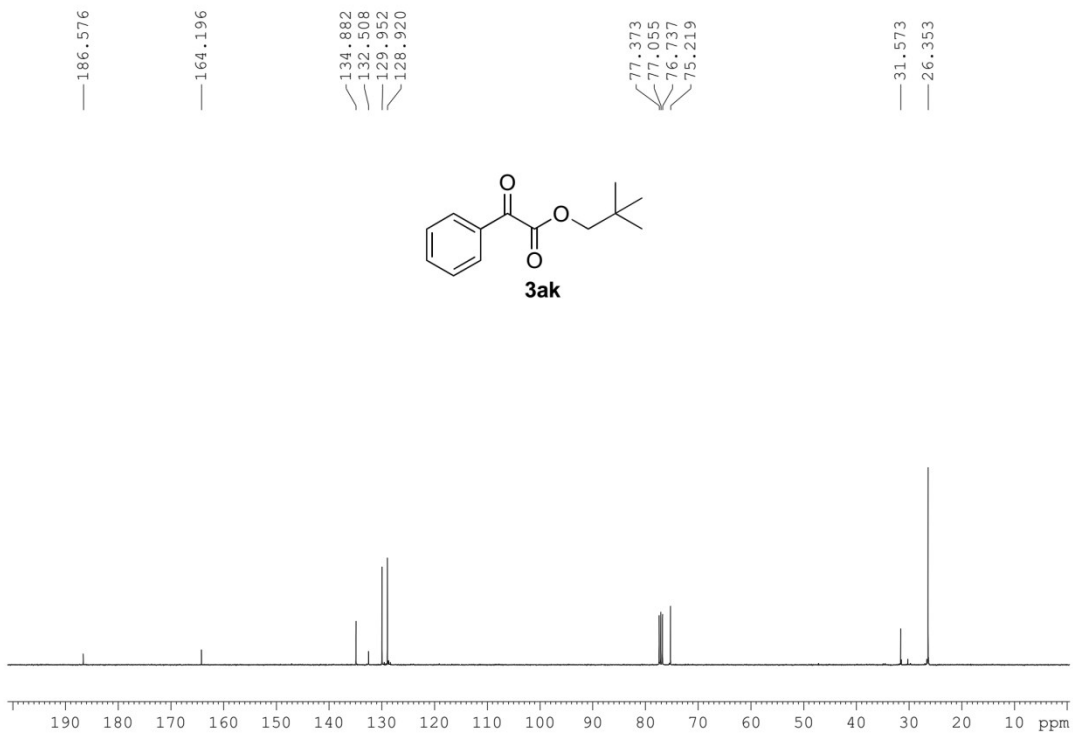
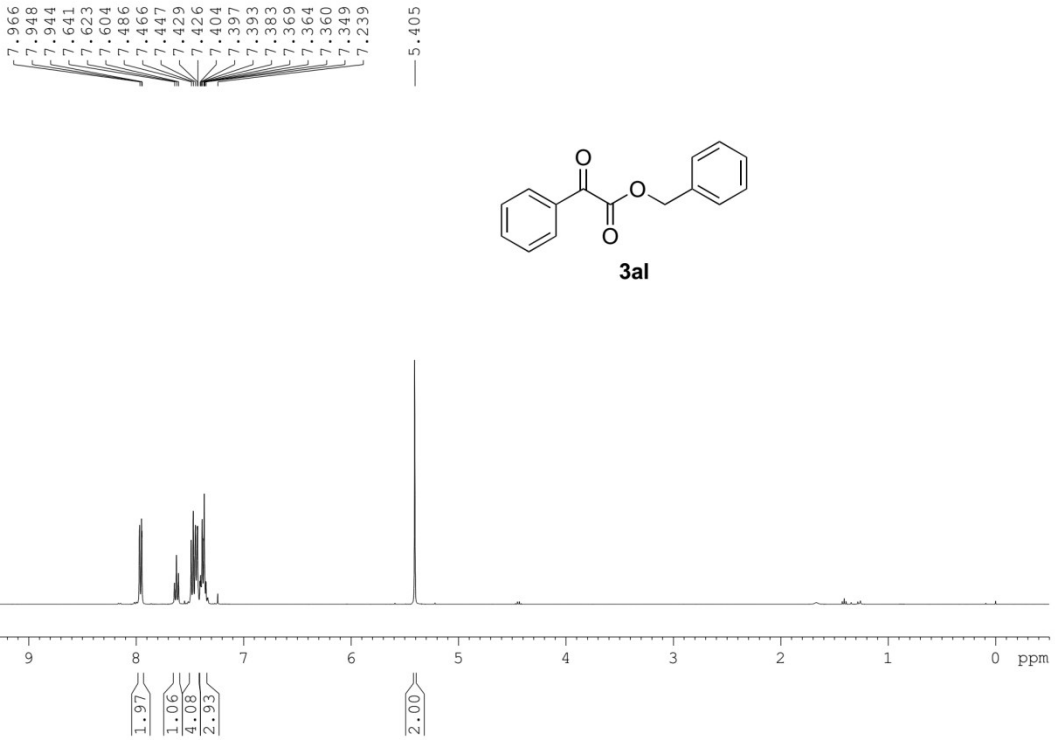
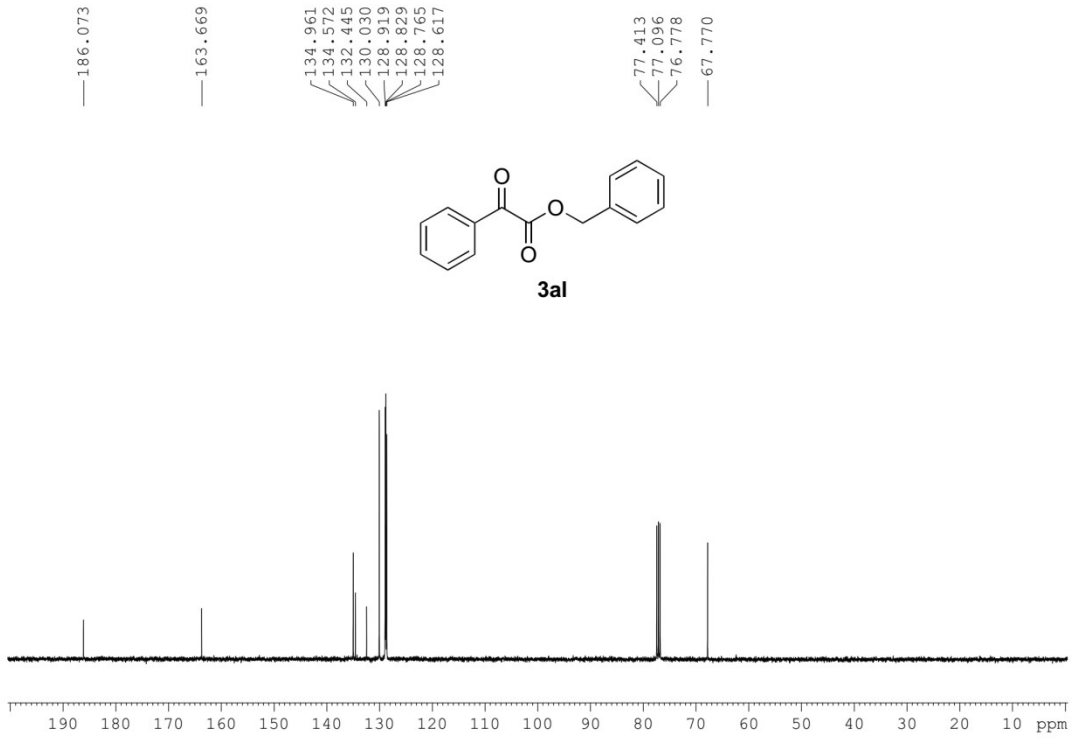
7.937
7.934
7.804
7.785
7.767
7.640
7.620
7.601
4.381
4.365
4.348
3.344
2.497
2.492
2.488
1.728
1.711
1.694
1.677
1.660
1.333
1.315
1.307
1.298
1.282
0.874
0.857
0.840
3aj
10 9 8 7 6 5 4 3 2 1 0 ppm
1.95
1.00
2.01
2.01
2.10
4.14
3.07

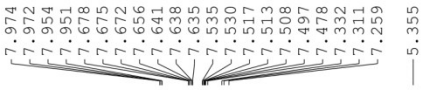

187.246
164.279
135.945
132.196
130.104
129.770
66.589
40.631
40.422
40.214
40.005
39.796
39.588
39.379
27.976
27.837
22.094
14.205
3aj
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

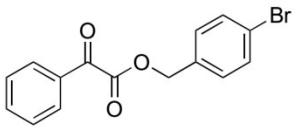

8.012
7.994
7.990
7.683
7.681
7.678
7.662
7.646
7.643
7.641
7.539
7.519
7.500
7.268
4.100
1.012
3ak
10
9
8
7
6
5
4
3
2
1
0 ppm
2.05
1.03
2.22
2.02
9.00


186.576
164.196
134.882
132.508
129.952
128.920
77.373
77.055
76.737
75.219
31.573
26.353
3ak
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

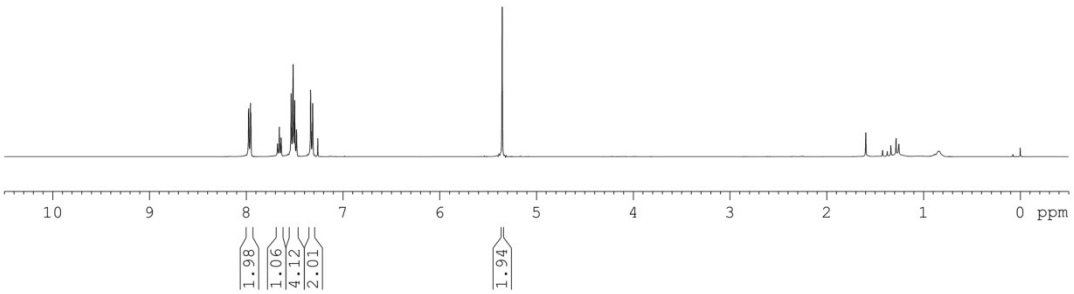

7.966
7.948
7.944
7.641
7.623
7.604
7.486
7.466
7.447
7.429
7.426
7.404
7.397
7.393
7.383
7.369
7.364
7.360
7.349
7.239
5.405
O
O
O
3al
9
8
7
6
5
4
3
2
1
0 ppm
1.97
1.06
4.08
2.93
2.00

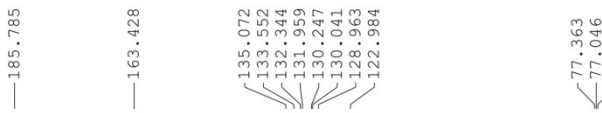

186.073
163.669
134.961
134.572
132.445
130.030
128.919
128.829
128.765
128.617
77.413
77.096
76.778
67.770
O
O
O
3al
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

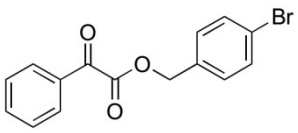

7.974
7.972
7.954
7.951
7.678
7.675
7.672
7.656
7.641
7.638
7.635
7.535
7.530
7.517
7.513
7.508
7.497
7.478
7.332
7.311
7.259
5.355


Br
O
O
O

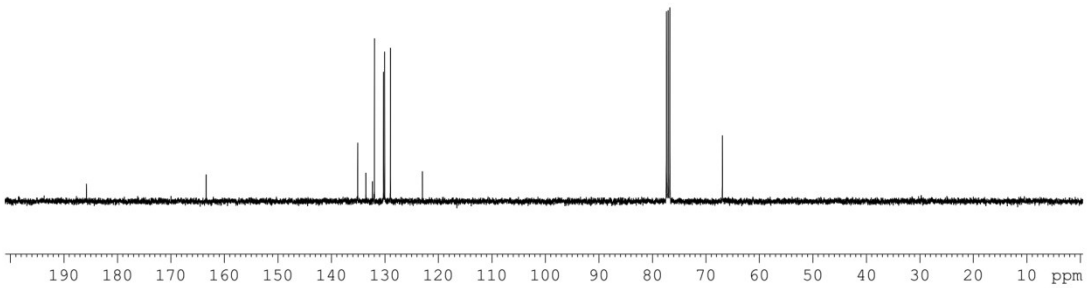
3am


10
9
8
7
6
5
4
3
2
1
0 ppm
1.98
1.06
4.12
2.01
1.94

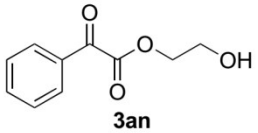

185.785
163.428
135.072
133.552
132.344
131.959
130.247
130.041
128.963
122.984
77.363
77.046
76.728
66.903


Br
O
O
O

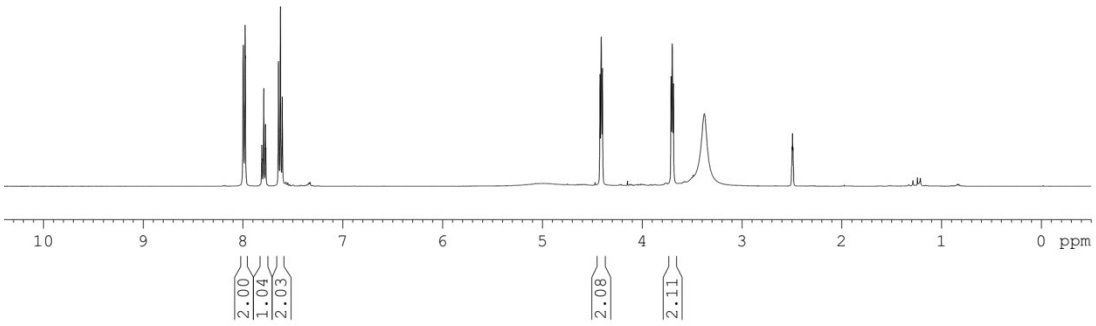
3am


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

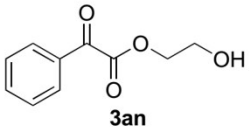

7.995
7.977
7.974
7.813
7.809
7.807
7.791
7.775
7.772
7.769
7.643
7.623
7.608
7.604
4.422
4.410
4.398
3.710
3.698
3.686
3.377
2.498
2.493
2.489


O
O
O
OH

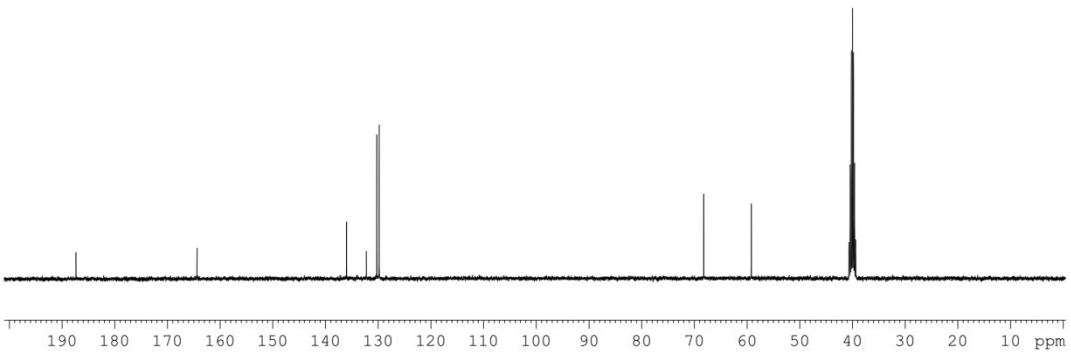
3an

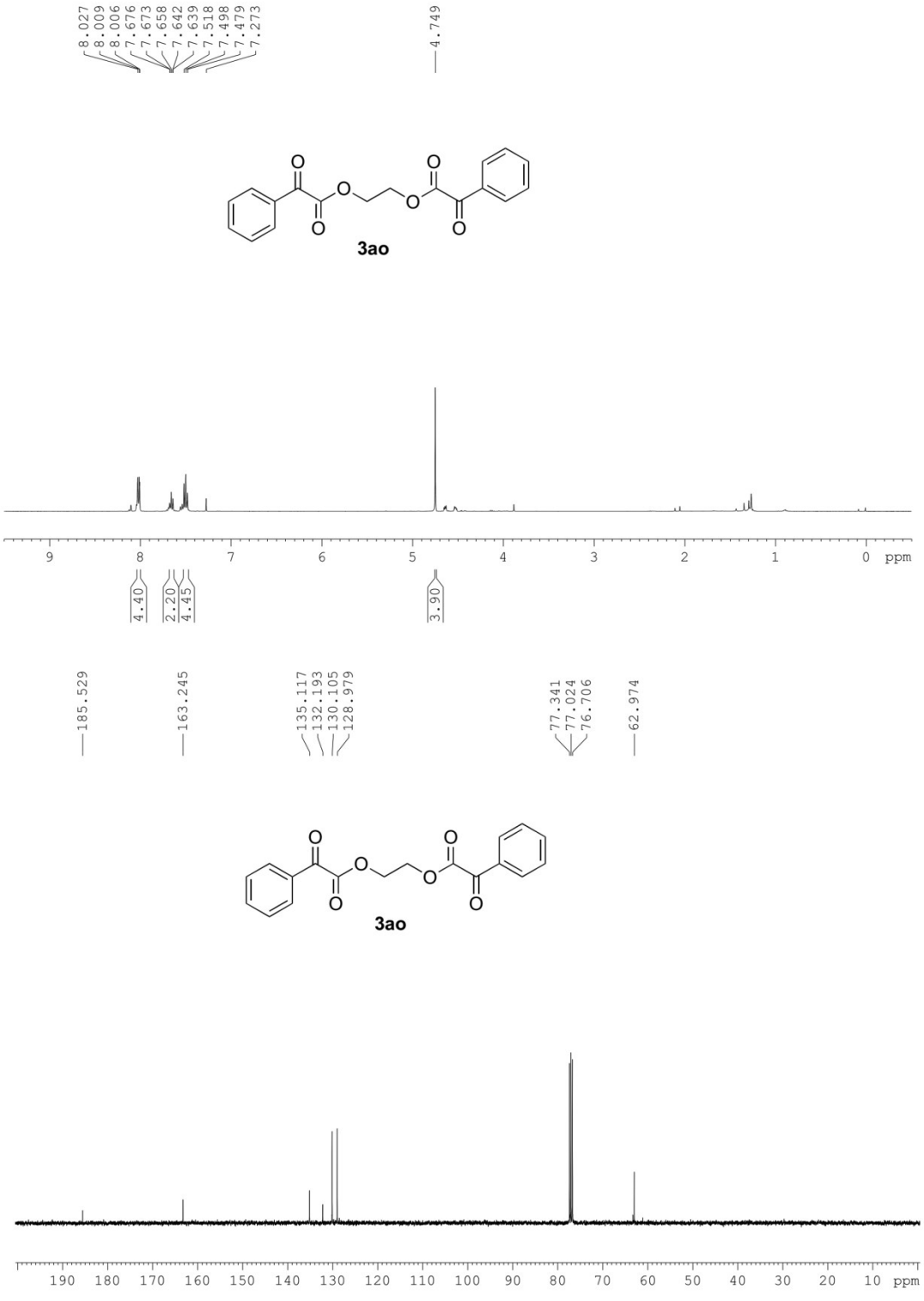

10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
1.04
2.03
2.08
2.11

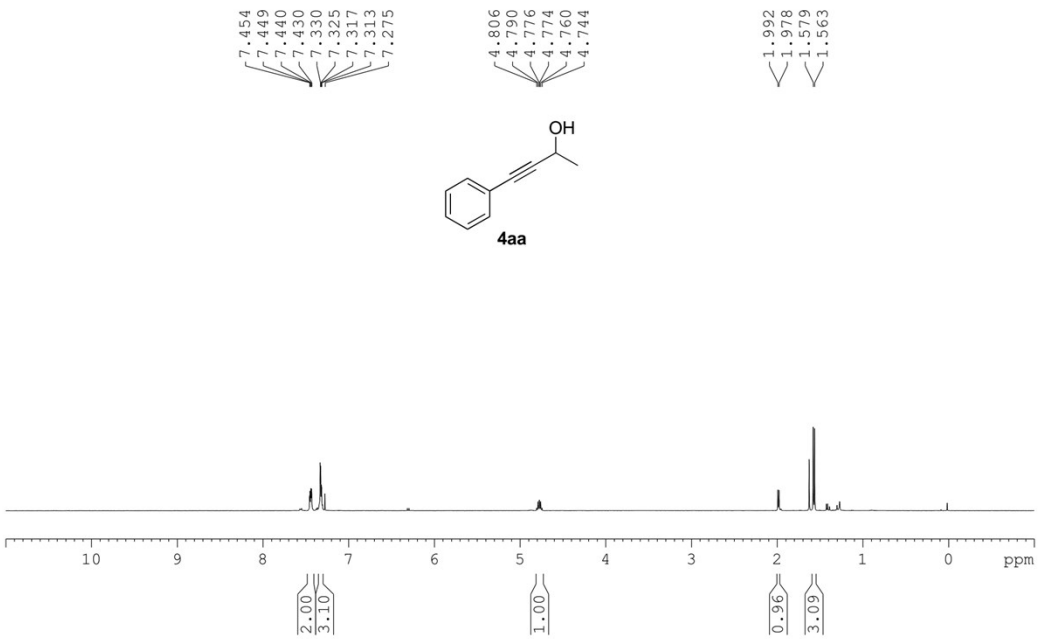

187.311
164.362
135.970
132.219
130.213
129.770
68.174
59.144
40.589
40.380
40.172
39.963
39.754
39.545
39.336

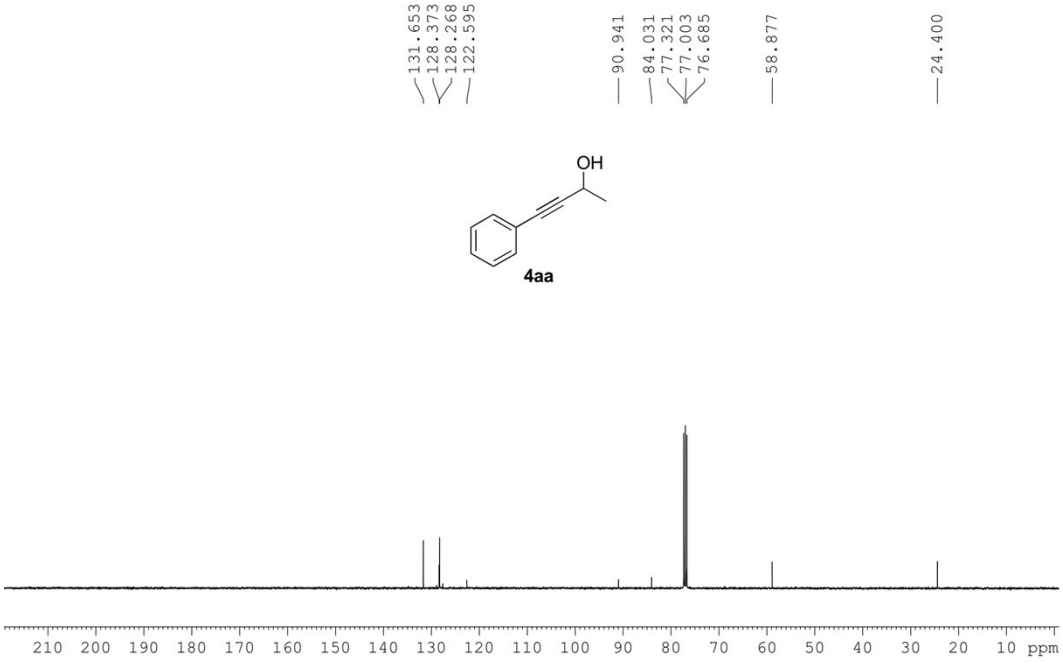

O
O
O
OH

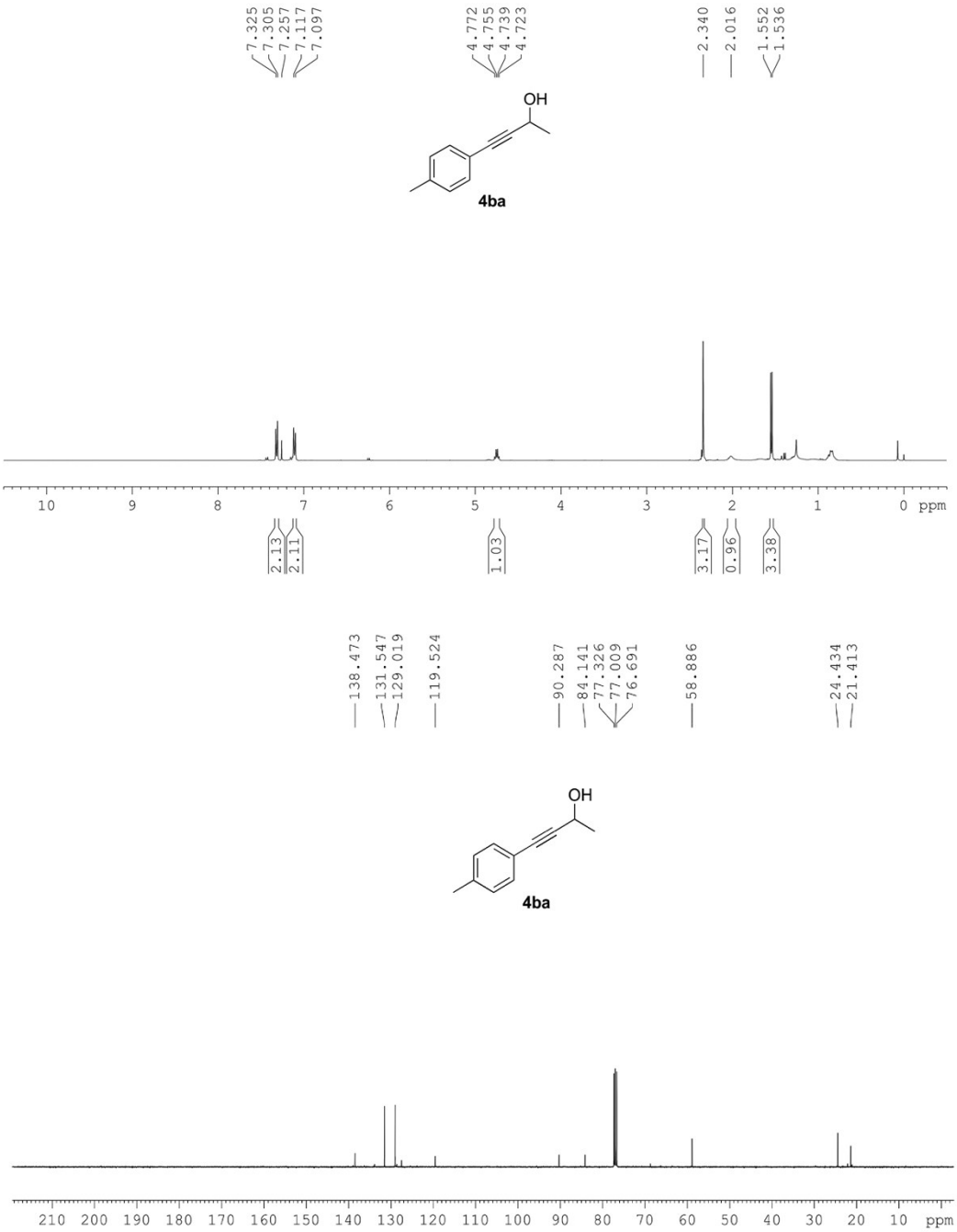
3an

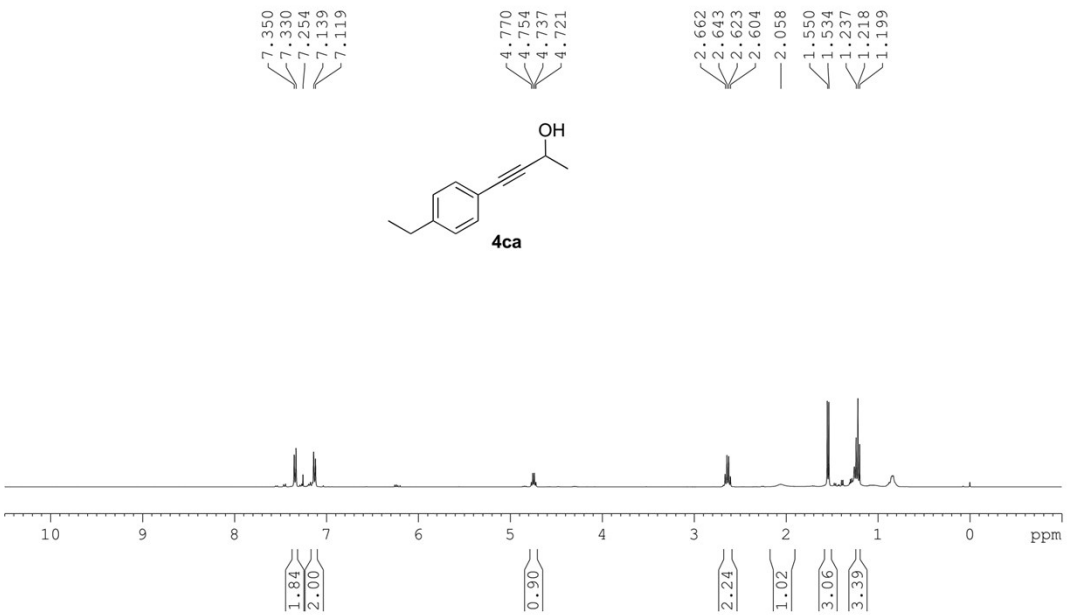

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm

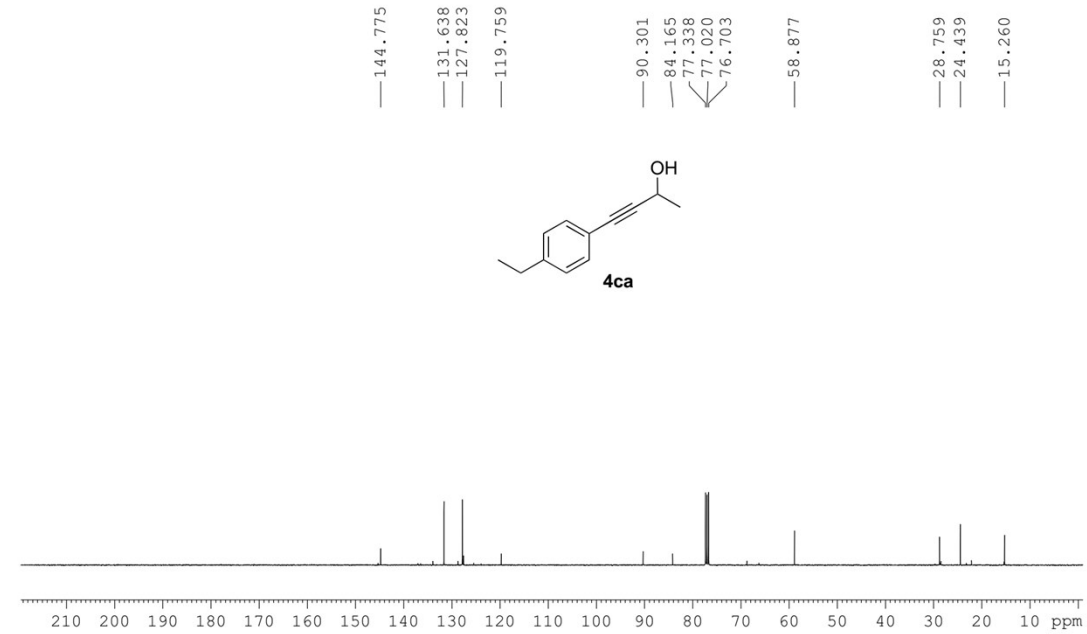

8.027
8.009
8.006
7.676
7.673
7.658
7.642
7.639
7.518
7.498
7.479
7.273
4.749
3ao
9
8
7
6
5
4
3
2
1
0 ppm
4.40
2.20
4.45
3.90
185.529
163.245
135.117
132.193
130.105
128.979
77.341
77.024
76.706
62.974
3ao
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

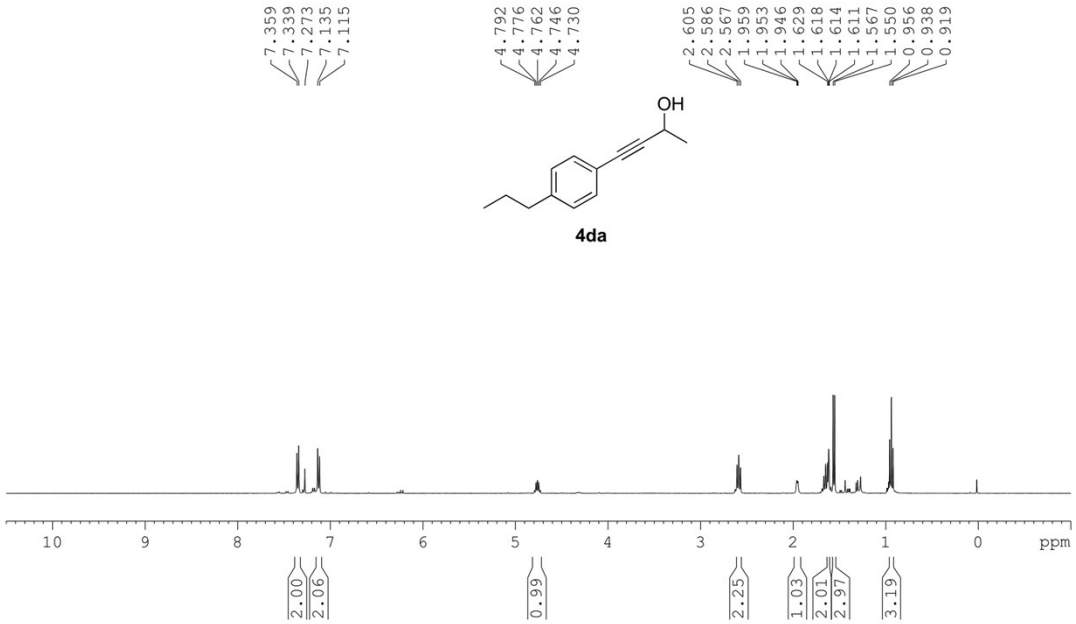

7.454
7.449
7.440
7.430
7.330
7.325
7.317
7.313
7.275
4.806
4.790
4.776
4.774
4.760
4.744
1.992
1.978
1.579
1.563
OH
4aa
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.10
1.00
0.96
3.09

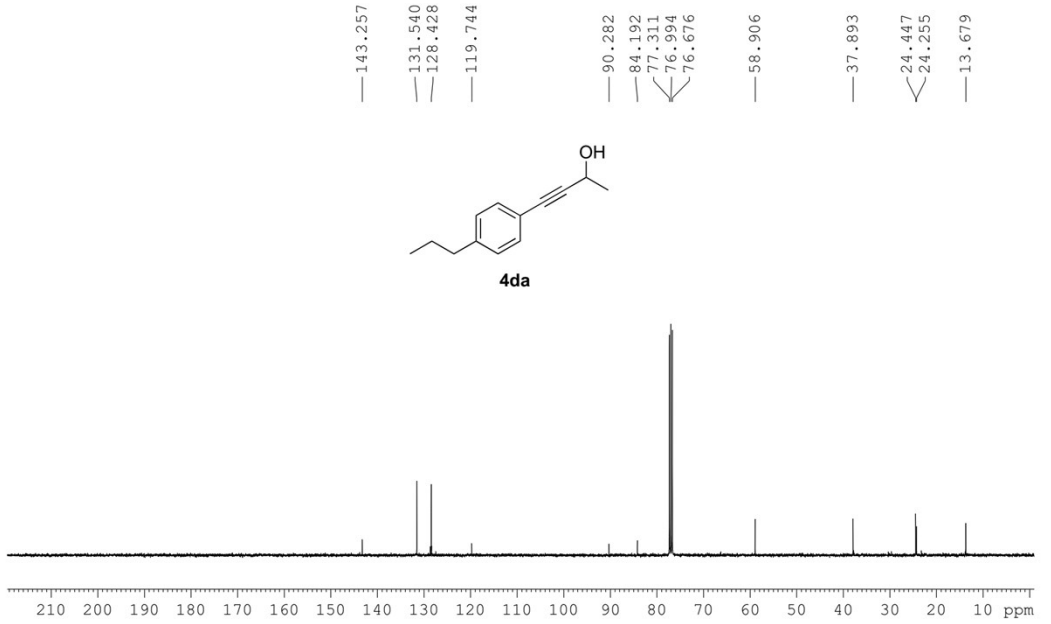

131.653
128.373
128.268
122.595
90.941
84.031
77.321
77.003
76.685
58.877
24.400
OH
4aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

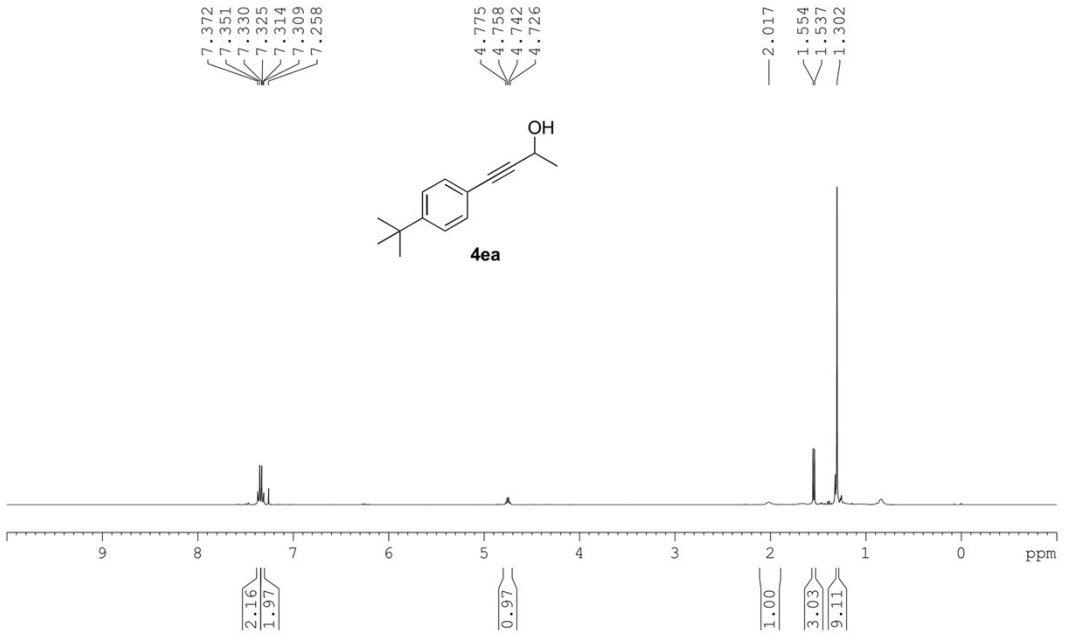

7.325
7.305
7.257
7.117
7.097
4.772
4.755
4.739
4.723
2.340
2.016
1.552
1.536
OH
4ba
10 9 8 7 6 5 4 3 2 1 0 ppm
2.13
2.11
1.03
3.17
0.96
3.38
138.473
131.547
129.019
119.524
90.287
84.141
77.326
77.009
76.691
58.886
24.434
21.413
OH
4ba
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

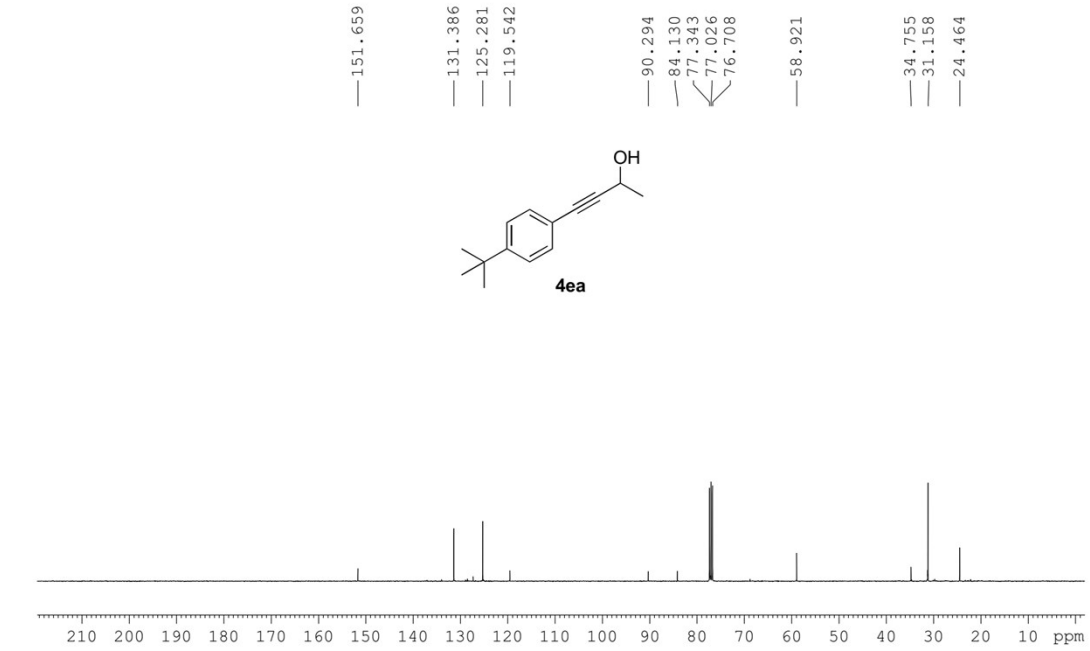

7.350
7.330
7.254
7.139
7.119
4.770
4.754
4.737
4.721
2.662
2.643
2.623
2.604
2.058
1.550
1.534
1.237
1.218
1.199
OH
4ca
10
9
8
7
6
5
4
3
2
1
0
ppm
1.84
2.00
0.90
2.24
1.02
3.06
3.39

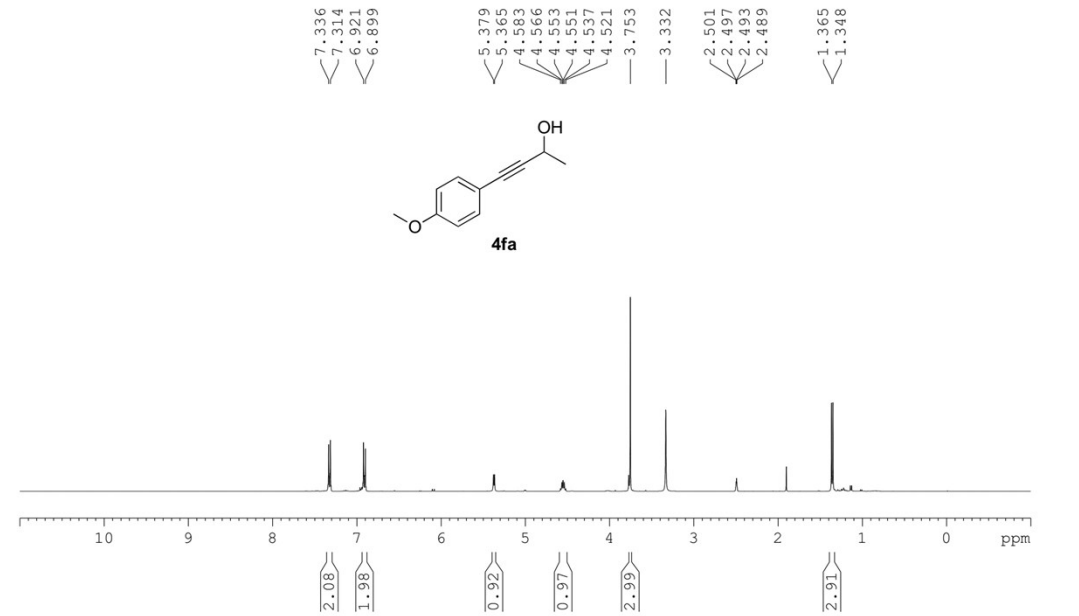

144.775
131.638
127.823
119.759
90.301
84.165
77.338
77.020
76.703
58.877
28.759
24.439
15.260
OH
4ca
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

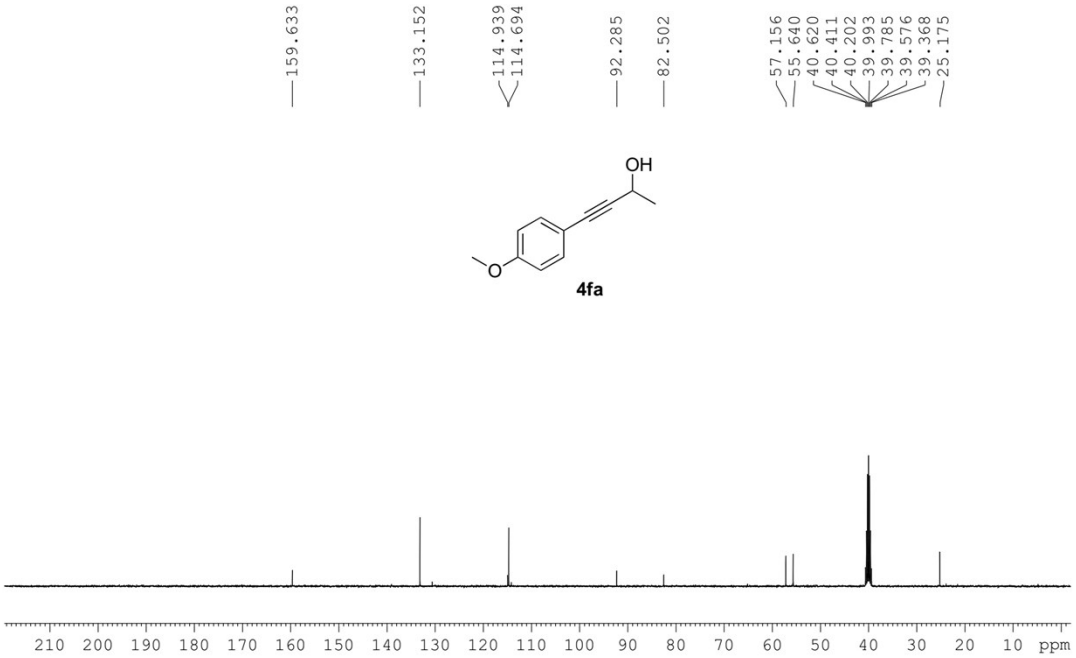

7.359
7.339
7.273
7.135
7.115
4.792
4.776
4.762
4.746
4.730
2.605
2.586
2.567
1.959
1.953
1.946
1.629
1.618
1.614
1.611
1.567
1.550
0.956
0.938
0.919
OH
4da
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.06
0.99
2.25
1.03
2.01
2.97
3.19

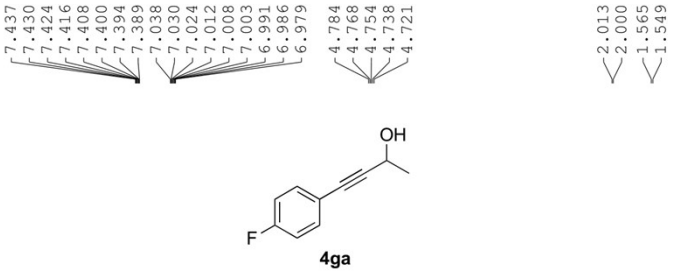

143.257
131.540
128.428
119.744
90.282
84.192
77.311
76.994
76.676
58.906
37.893
24.447
24.255
13.679
OH
4da
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.372
7.351
7.330
7.325
7.314
7.309
7.258
4.775
4.758
4.742
4.726
2.017
1.554
1.537
1.302
OH
4ea
9
8
7
6
5
4
3
2
1
0
ppm
2.16
1.97
0.97
1.00
3.03
9.11

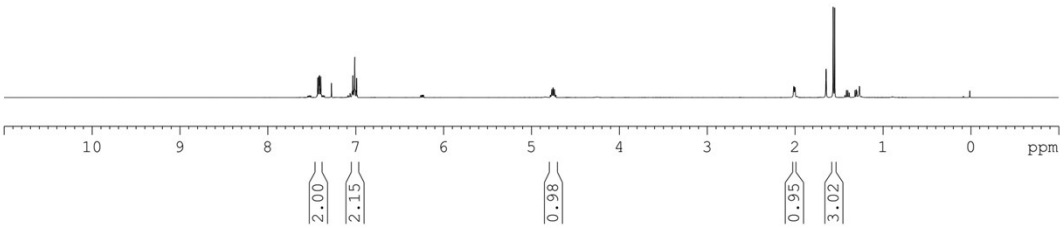

151.659
131.386
125.281
119.542
90.294
84.130
77.343
77.026
76.708
58.921
34.755
31.158
24.464
OH
4ea
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.336
7.314
6.921
6.899
5.379
5.365
4.583
4.566
4.553
4.551
4.537
4.521
3.753
3.332
2.501
2.497
2.493
2.489
1.365
1.348
OH
O
4fa
10
9
8
7
6
5
4
3
2
1
0
ppm
2.08
1.98
0.92
0.97
2.99
2.91

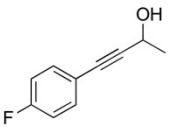

159.633
133.152
114.939
114.694
92.285
82.502
57.156
55.640
40.620
40.411
40.202
39.993
39.785
39.576
39.368
25.175
OH
O
4fa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.437
7.430
7.424
7.416
7.408
7.400
7.394
7.389
7.038
7.030
7.024
7.012
7.008
7.003
6.991
6.986
6.979
4.784
4.768
4.754
4.738
4.721
2.013
2.000
1.565
1.549
OH
F

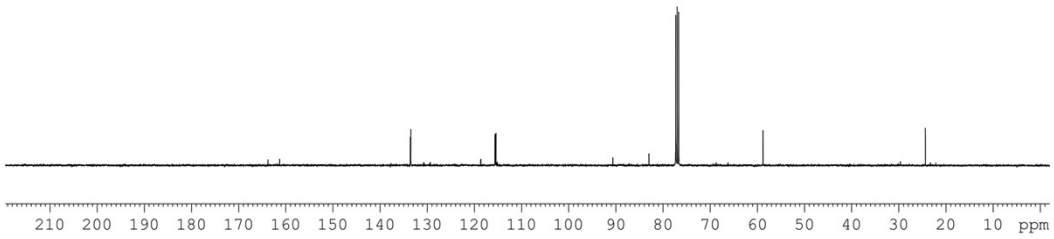
4ga

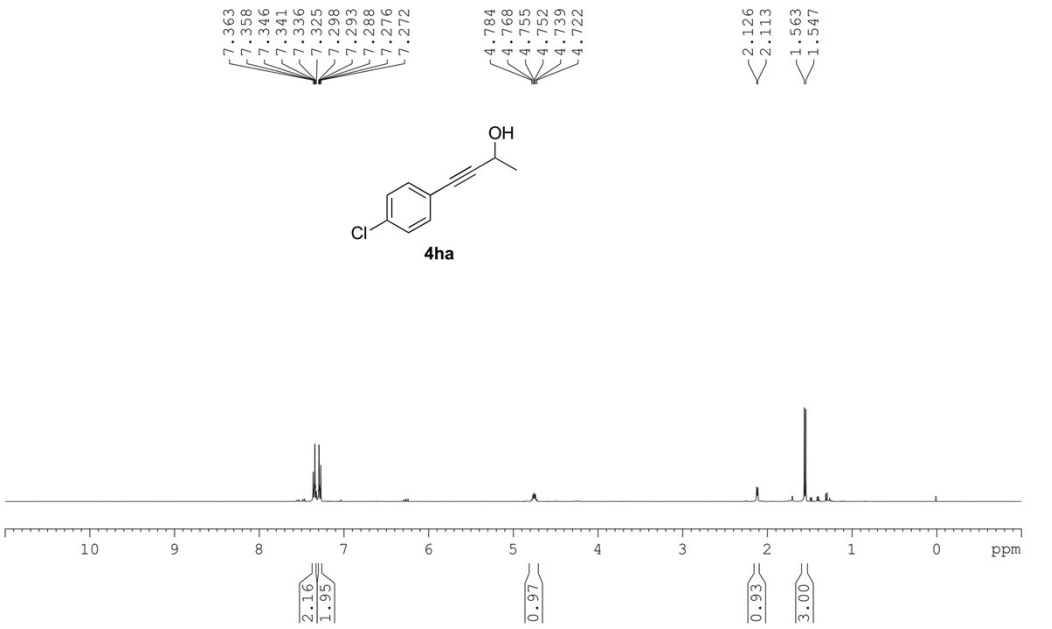

10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
2.15
0.98
0.95
3.02

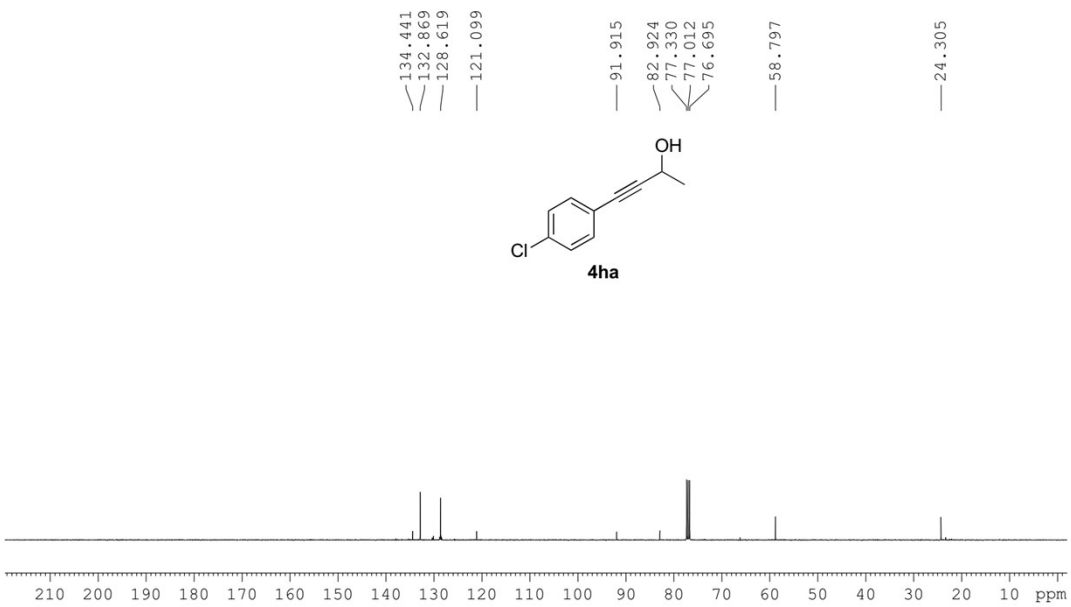

163.793
161.313
133.587
133.503
118.693
118.658
115.655
115.435
90.642
82.980
77.311
76.994
76.676
58.811
24.365

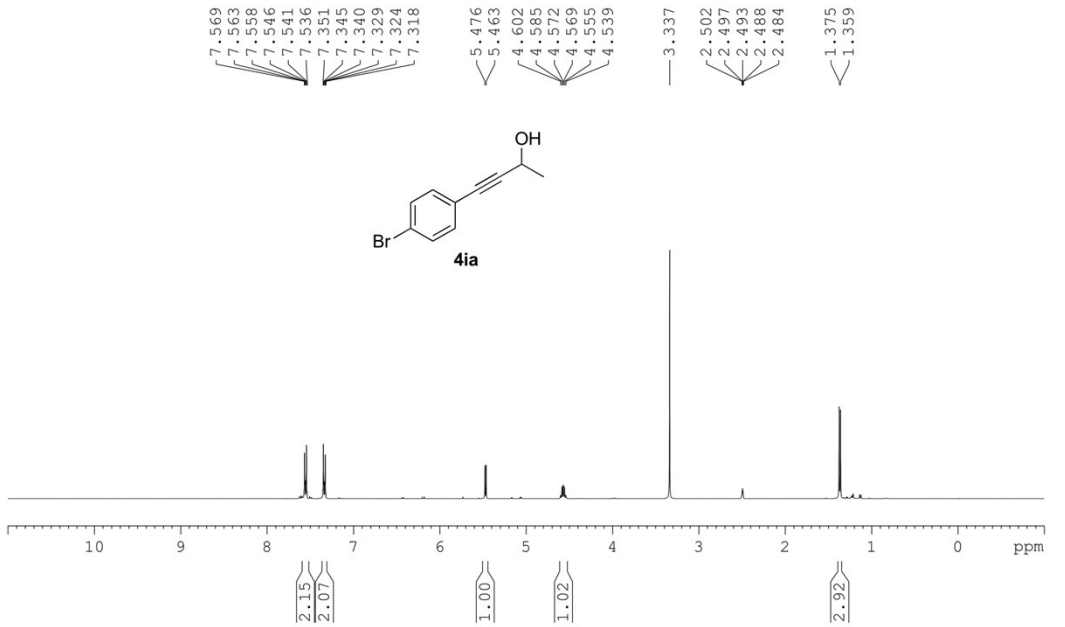

OH
F

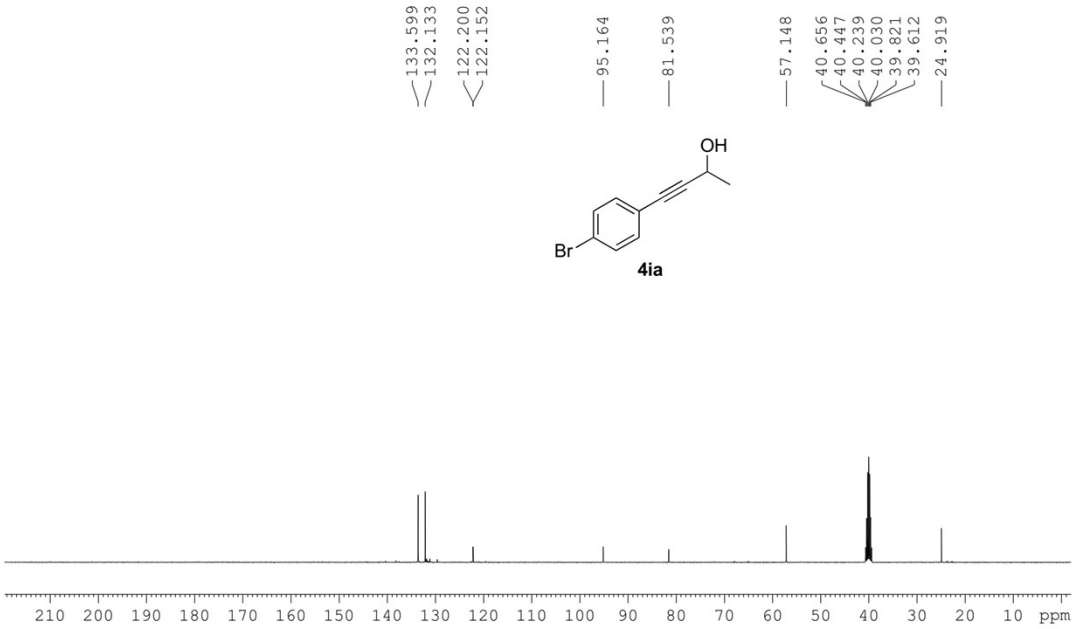
4ga

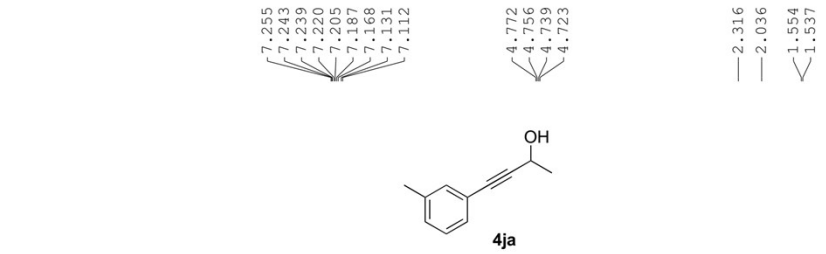

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.363
7.358
7.346
7.341
7.336
7.325
7.298
7.293
7.288
7.276
7.272
4.784
4.768
4.755
4.752
4.739
4.722
2.126
2.113
1.563
1.547
OH
Cl
4ha
10
9
8
7
6
5
4
3
2
1
0
ppm
2.16
1.95
0.97
0.93
3.00

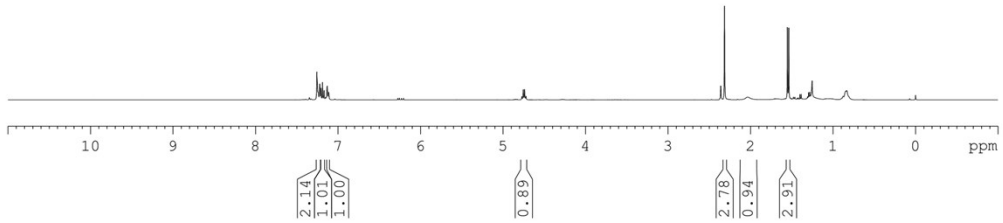

134.441
132.869
128.619
121.099
91.915
82.924
77.330
77.012
76.695
58.797
24.305
OH
Cl
4ha
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

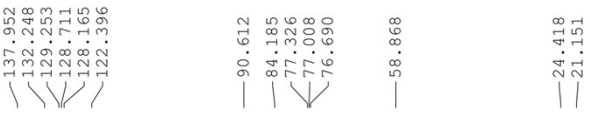

7.569
7.563
7.558
7.546
7.541
7.536
7.351
7.345
7.340
7.329
7.324
7.318
5.476
5.463
4.602
4.585
4.572
4.569
4.555
4.539
3.337
2.502
2.497
2.493
2.488
2.484
1.375
1.359
OH
Br
4ia
10
9
8
7
6
5
4
3
2
1
0
ppm
2.15
2.07
1.00
1.02
2.92


133.599
132.133
122.200
122.152
95.164
81.539
57.148
40.656
40.447
40.239
40.030
39.821
39.612
24.919
OH
Br
4ia
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

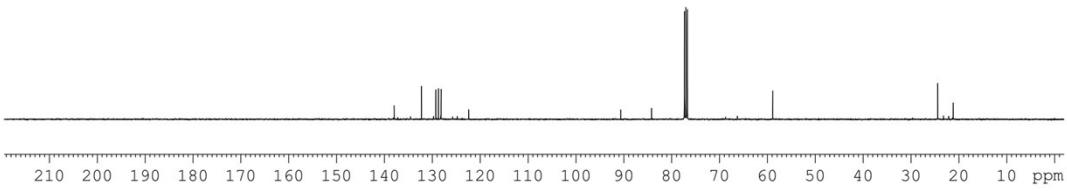

7.255
7.243
7.239
7.220
7.205
7.187
7.168
7.131
7.112
4.772
4.756
4.739
4.723
2.316
2.036
1.554
1.537
OH

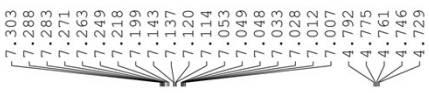
4ja

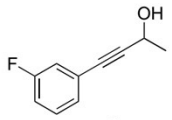

10
9
8
7
6
5
4
3
2
1
0
ppm
2.14
1.01
1.00
0.89
2.78
0.94
2.91


137.952
132.248
129.253
128.711
128.165
122.396
90.612
84.185
77.326
77.008
76.690
58.868
24.418
21.151
OH

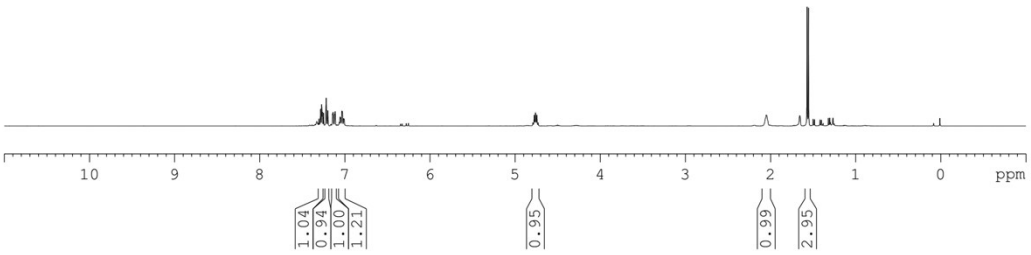
4ja

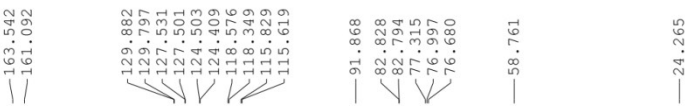

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

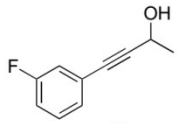

7.303
7.288
7.283
7.271
7.263
7.249
7.218
7.199
7.143
7.137
7.120
7.114
7.053
7.049
7.048
7.033
7.028
7.012
7.007
4.792
4.775
4.761
4.746
4.729
2.051
1.571
1.554


OH
F

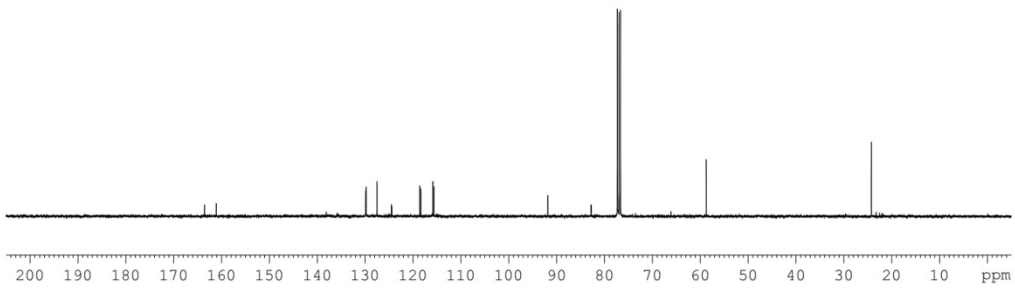
4ka


10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
0.94
1.00
1.21
0.95
0.99
2.95


163.542
161.092
129.882
129.797
127.531
127.501
124.503
124.409
118.576
118.349
115.829
115.619
91.868
82.828
82.794
77.315
76.997
76.680
58.761
24.265


OH
F

4ka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180
170
160
150
140
130
120
110
100
90
80
70
60
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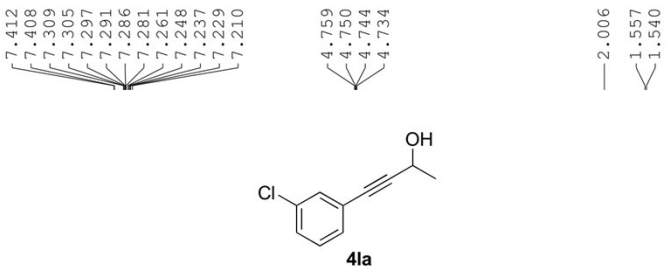
40
30
20
10
ppm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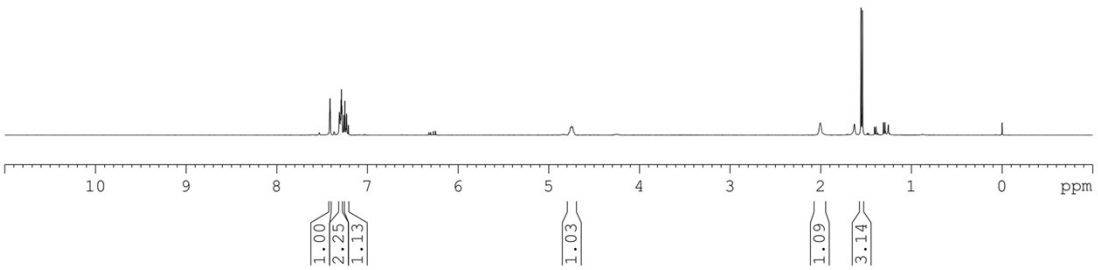
7.408
7.309
7.305
7.297
7.291
7.286
7.281
7.261
7.248
7.237
7.229
7.210
4.759
4.750
4.744
4.734
2.006
1.557
1.540
OH
Cl

4la


10
9
8
7
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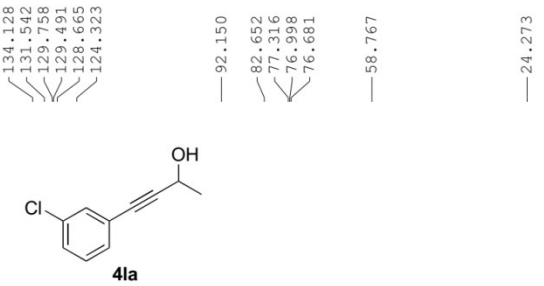
5
4
3
2
1
0
ppm
1.00
2.25
1.13
1.03
1.09
3.14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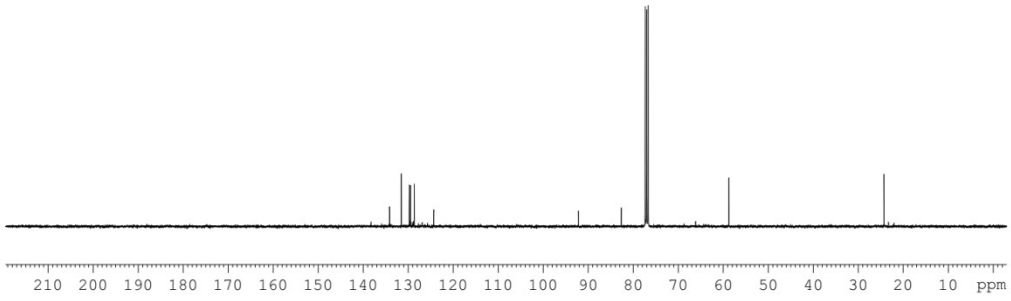
131.542
129.758
129.491
128.665
124.323
92.150
82.652
77.316
76.998
76.681
58.767
24.273
OH
Cl

4la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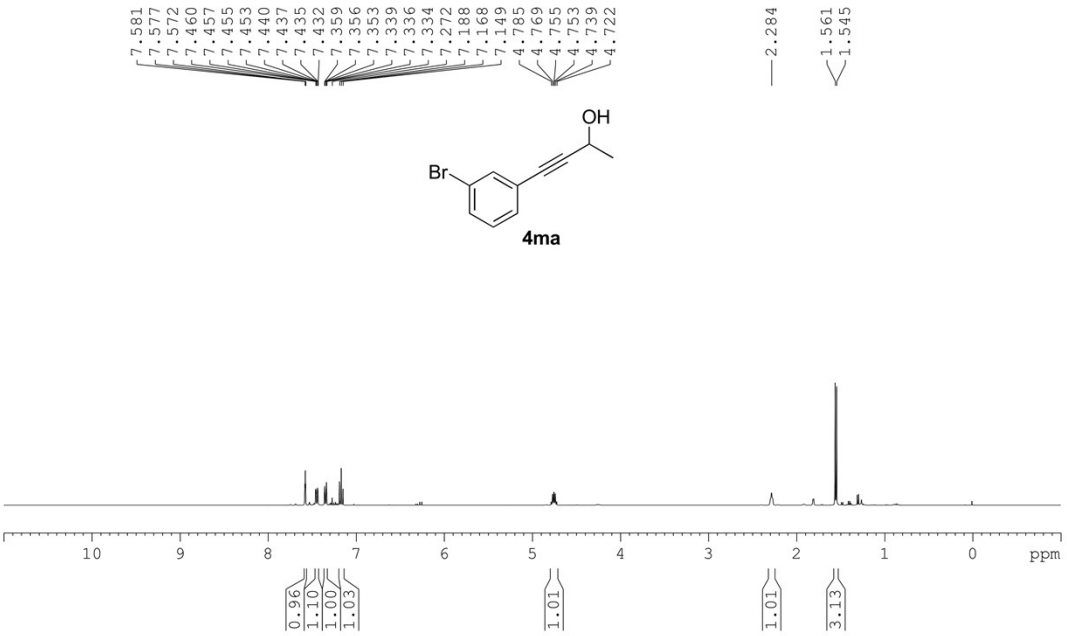
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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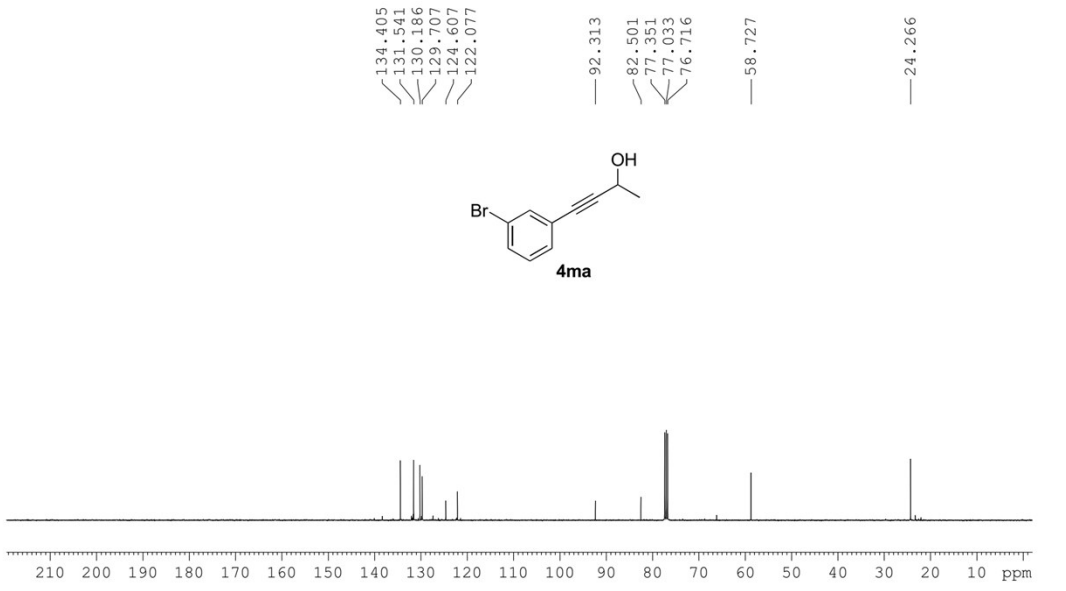
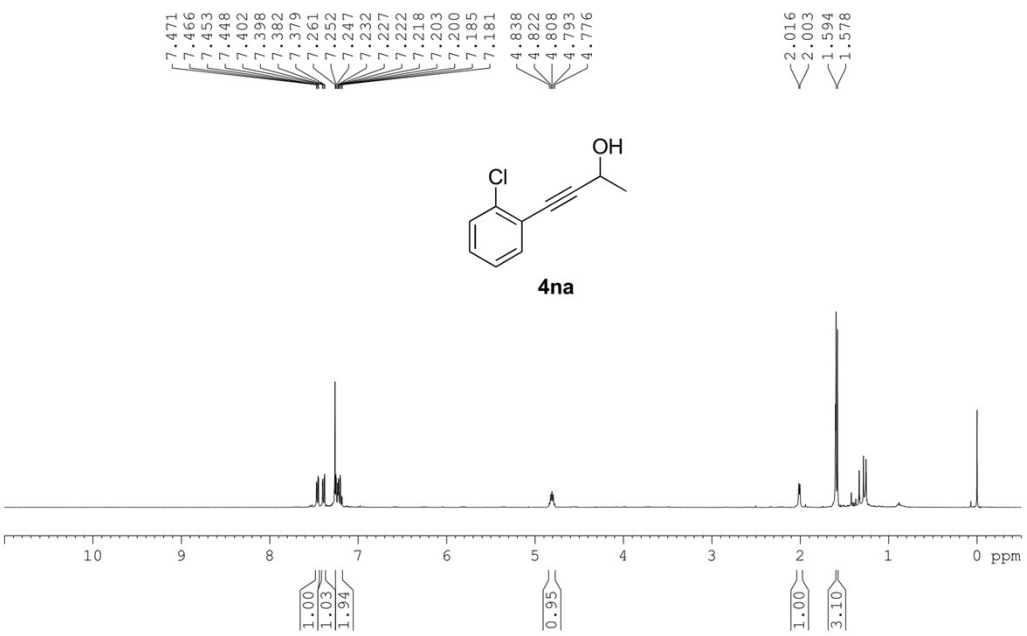
7.577
7.572
7.460
7.457
7.455
7.453
7.440
7.437
7.435
7.432
7.359
7.356
7.353
7.339
7.336
7.334
7.272
7.188
7.168
7.149
4.785
4.769
4.755
4.753
4.739
4.722
2.284
1.561
1.545
OH
Br
4ma
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.10
1.00
1.03
1.01
1.01
3.13


134.405
131.541
130.186
129.707
124.607
122.077
92.313
82.501
77.351
77.033
76.716
58.727
24.266
OH
Br
4ma
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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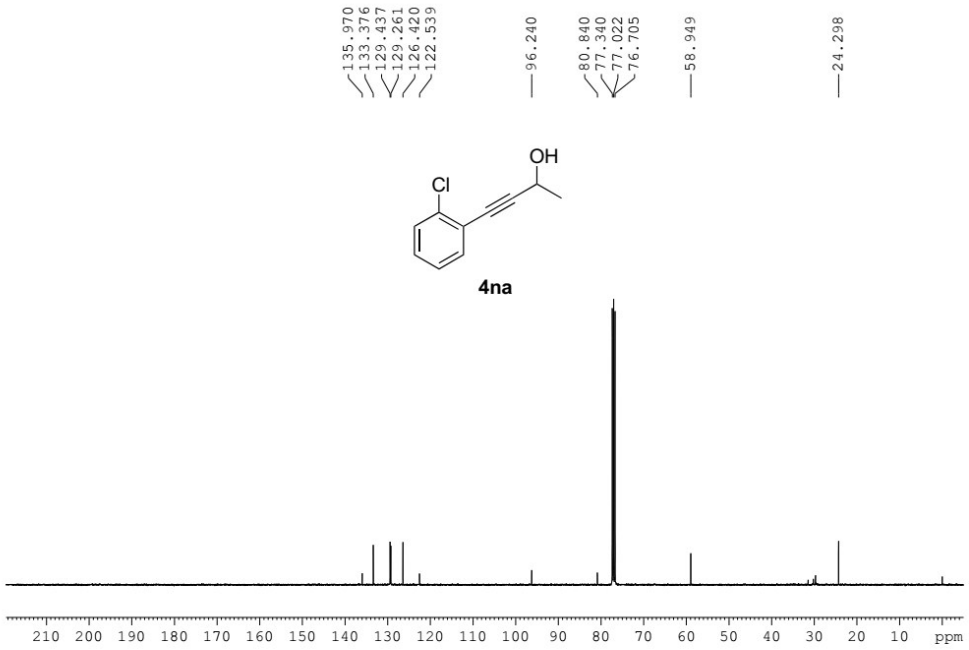
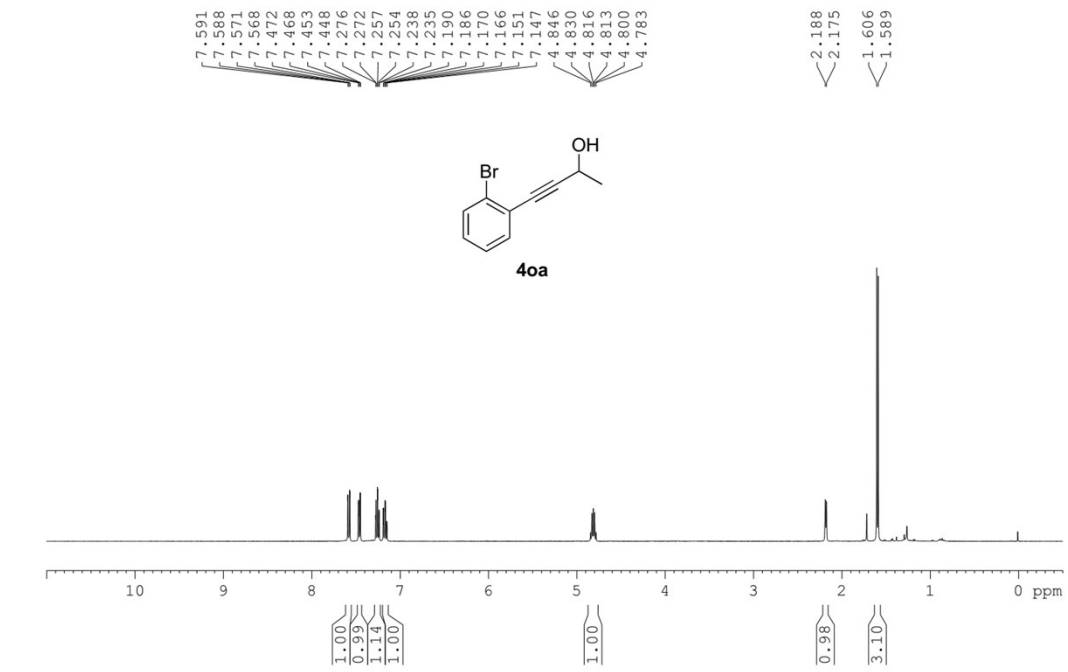
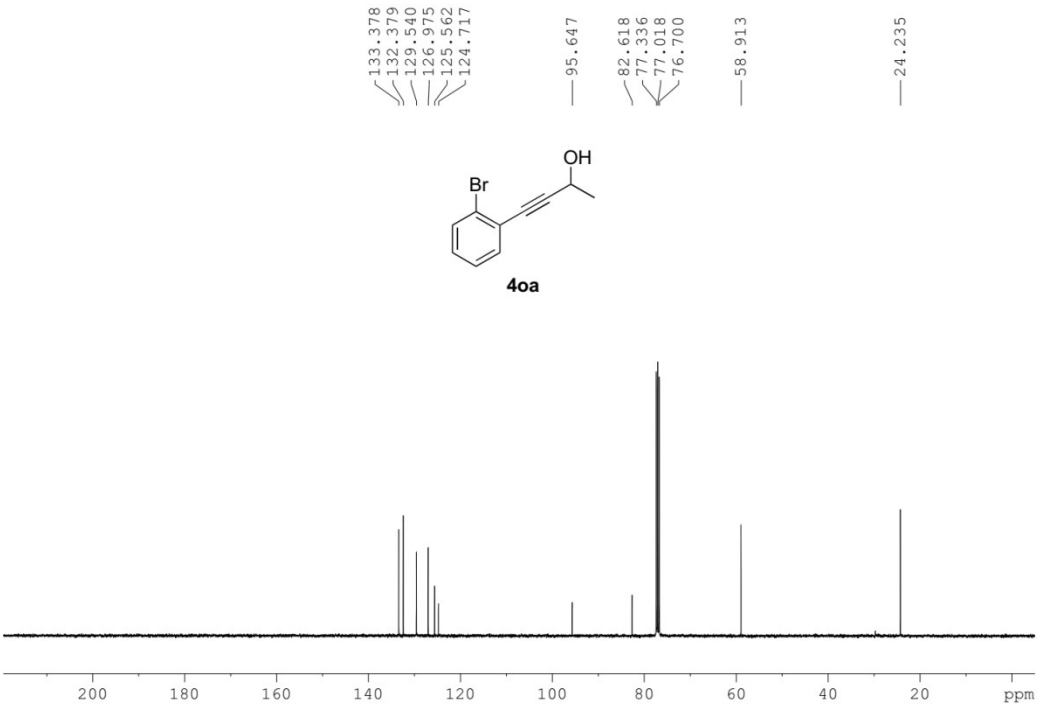
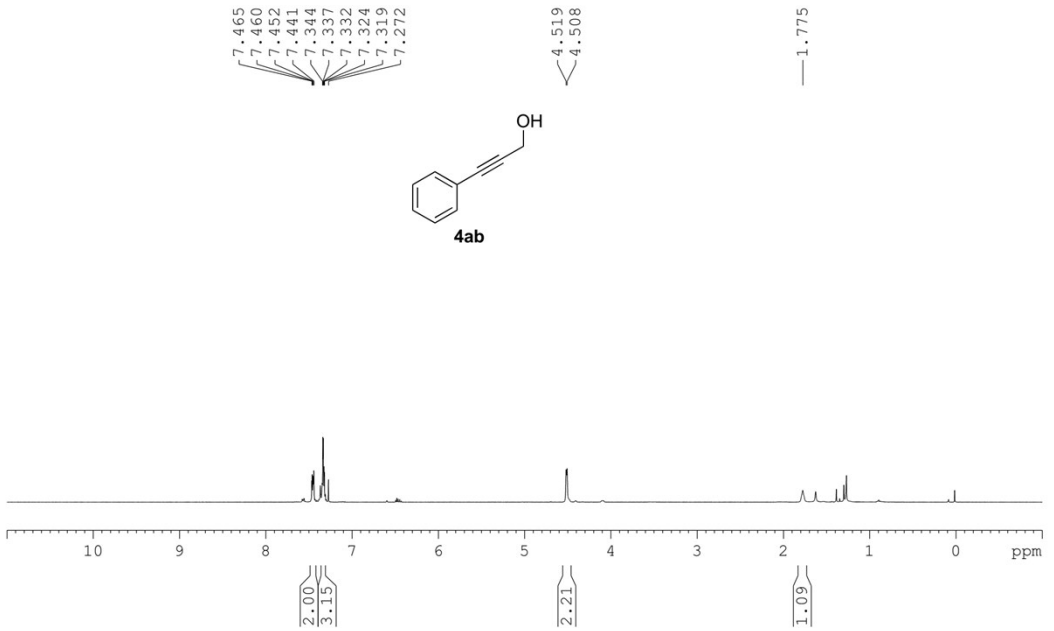
7.466
7.453
7.448
7.402
7.398
7.382
7.379
7.261
7.252
7.247
7.232
7.227
7.222
7.218
7.203
7.200
7.185
7.181
4.838
4.822
4.808
4.793
4.776
2.016
2.003
1.594
1.578
OH
Cl
4na
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
1.03
1.94
0.95
1.00
3.10


135.970
133.376
129.437
129.261
126.420
122.539
96.240
80.840
77.340
77.022
76.705
58.949
24.298
OH
Cl
4na
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.591
7.588
7.571
7.568
7.472
7.468
7.453
7.448
7.276
7.272
7.257
7.254
7.238
7.235
7.190
7.186
7.170
7.166
7.151
7.147
4.846
4.830
4.816
4.813
4.800
4.783
2.188
2.175
1.606
1.589
OH
Br
4oa
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
0.99
1.14
1.00
1.00
0.98
3.10


133.378
132.379
129.540
126.975
125.562
124.717
95.647
82.618
77.336
77.018
76.700
58.913
24.235
OH
Br
4oa
200
180
160
140
120
100
80
60
40
20
ppm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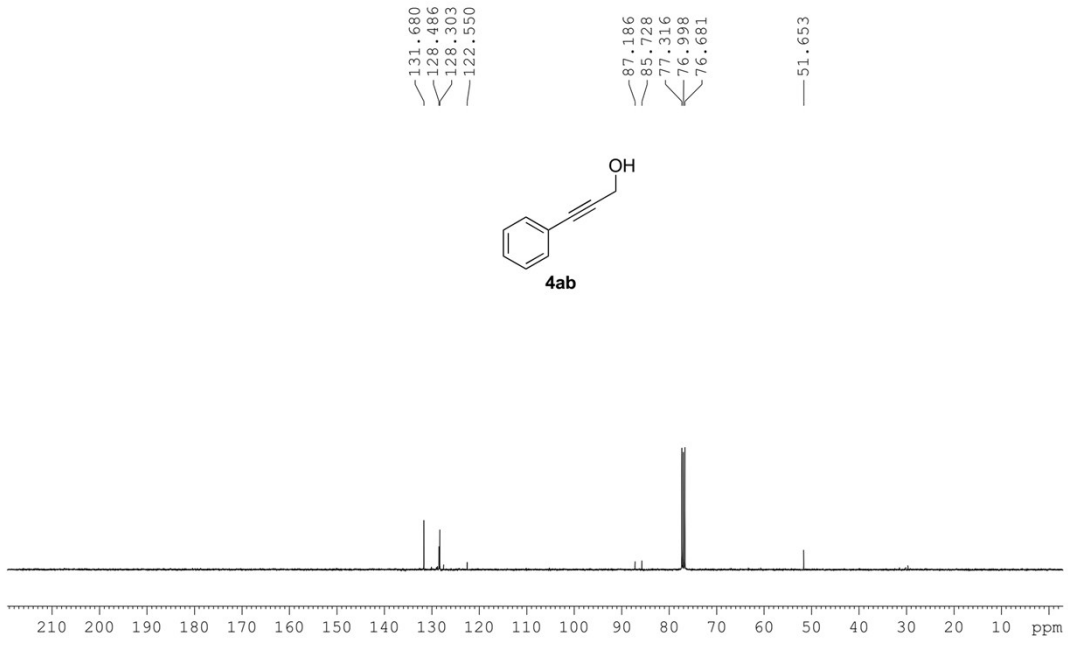
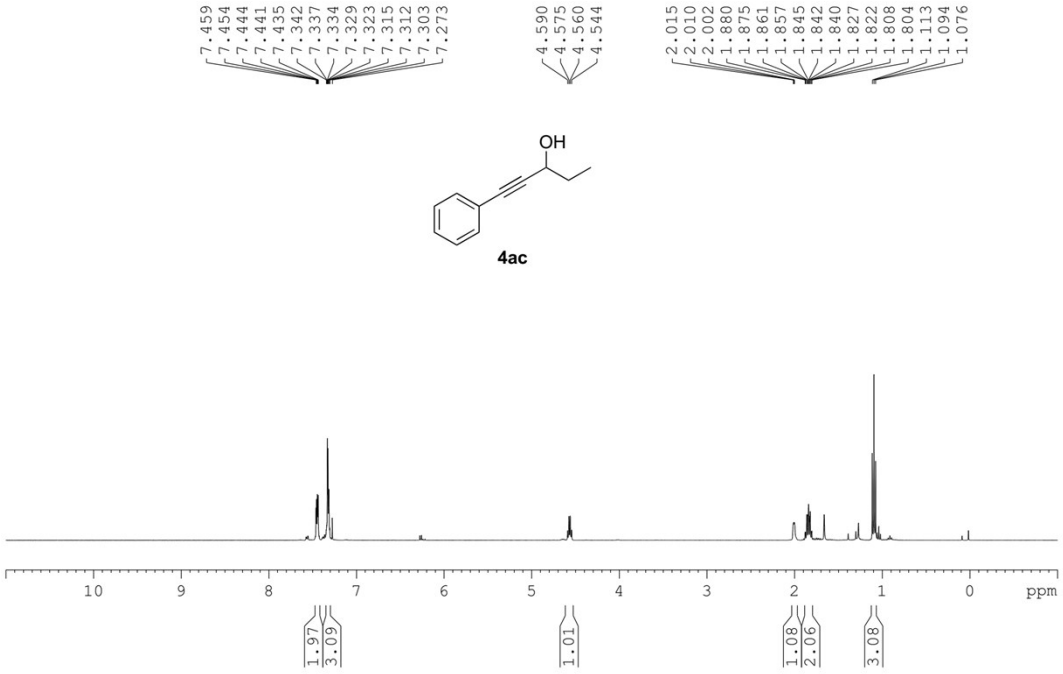
7.460
7.452
7.441
7.344
7.337
7.332
7.324
7.319
7.272
4.519
4.508
1.775
OH
4ab
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.15
2.21
1.09


131.680
128.486
128.303
122.550
87.186
85.728
77.316
76.998
76.681
51.653
OH
4ab
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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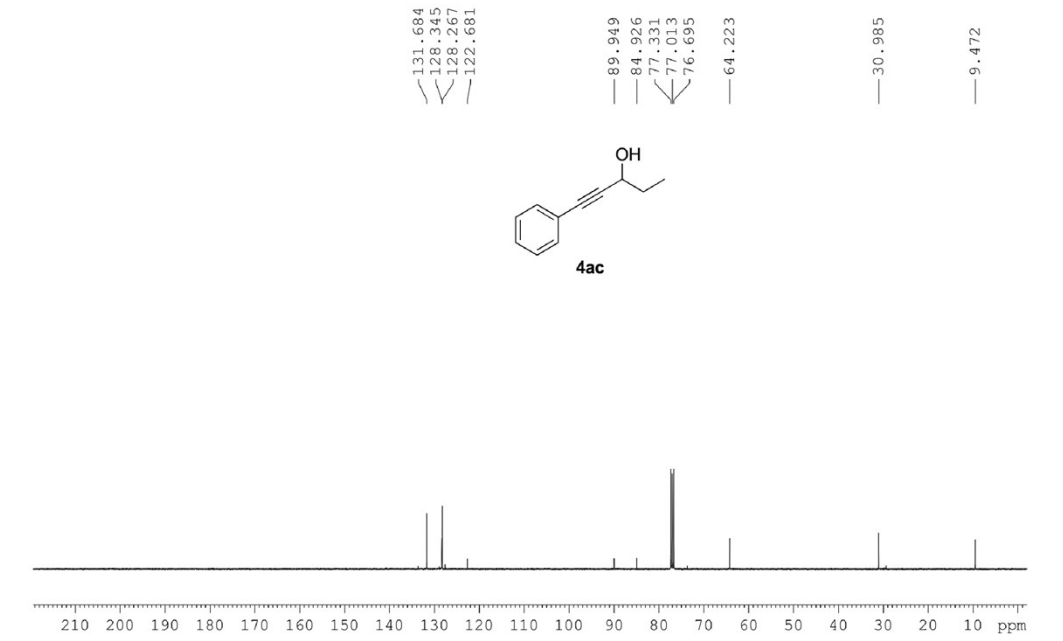
7.454
7.444
7.441
7.435
7.342
7.337
7.334
7.329
7.323
7.315
7.312
7.303
7.273
4.590
4.575
4.560
4.544
2.015
2.010
2.002
1.880
1.875
1.861
1.857
1.845
1.842
1.840
1.827
1.822
1.808
1.804
1.113
1.094
1.076
OH
4ac
10
9
8
7
6
5
4
3
2
1
0
ppm
1.97
3.09
1.01
1.08
2.06
3.08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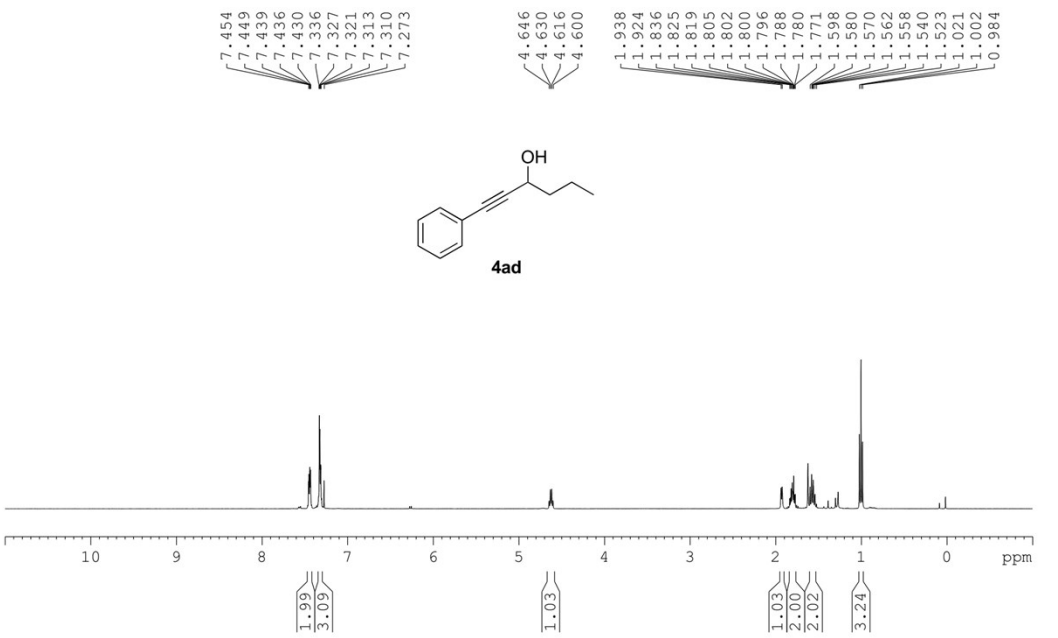
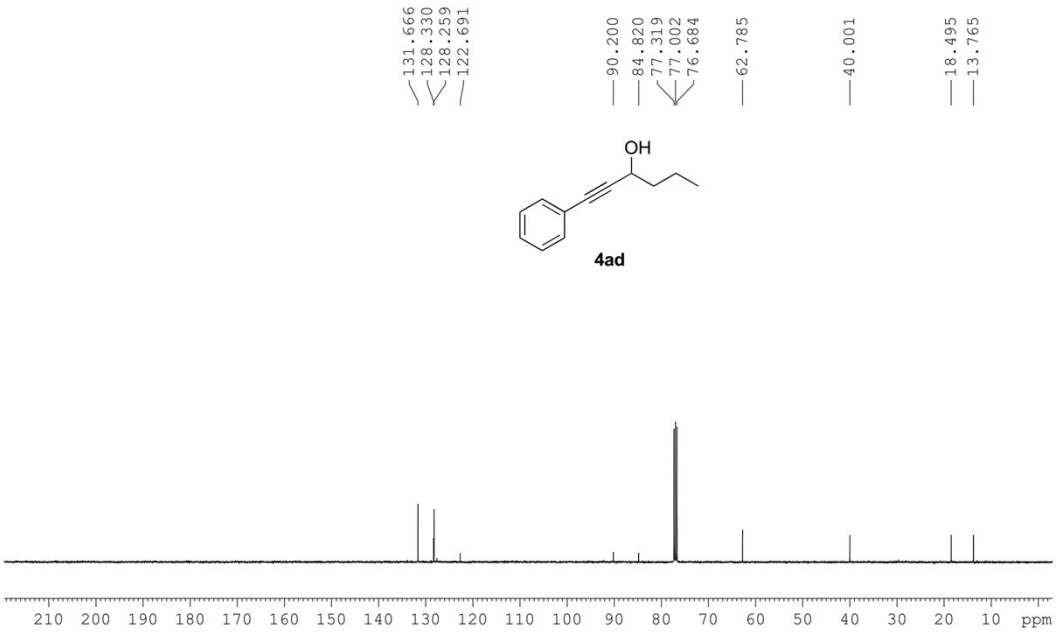
128.345
128.267
122.681
89.949
84.926
77.331
77.013
76.695
64.223
30.985
9.472
OH
4ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


7.454
7.449
7.439
7.436
7.430
7.336
7.327
7.321
7.313
7.310
7.273
4.646
4.630
4.616
4.600
1.938
1.924
1.836
1.825
1.819
1.805
1.802
1.800
1.796
1.788
1.780
1.771
1.598
1.580
1.570
1.562
1.558
1.540
1.523
1.021
1.002
0.984
OH
4ad
ppm
1.99
3.09
1.03
1.03
2.00
2.02
3.24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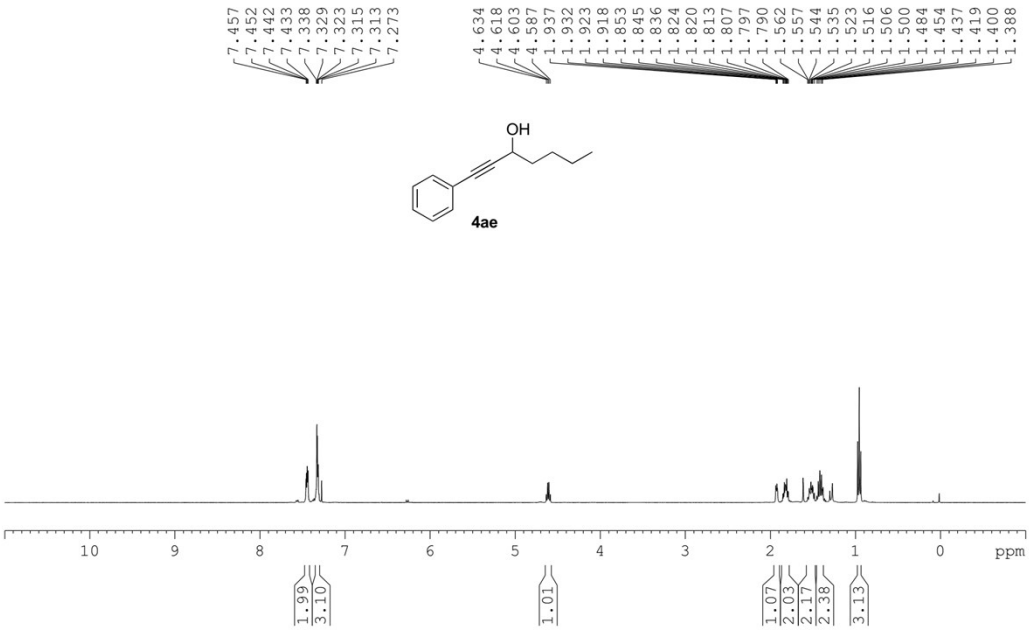
128.330
128.259
122.691
90.200
84.820
77.319
77.002
76.684
62.785
40.001
18.495
13.765
OH
4ad
ppm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7.452
7.442
7.433
7.338
7.329
7.323
7.315
7.313
7.273
4.634
4.618
4.603
4.587
1.937
1.932
1.923
1.918
1.853
1.845
1.836
1.824
1.820
1.813
1.807
1.797
1.790
1.562
1.557
1.544
1.535
1.523
1.516
1.506
1.500
1.484
1.454
1.437
1.419
1.400
1.388
OH
4ae
10
9
8
7
6
5
4
3
2
1
0
ppm
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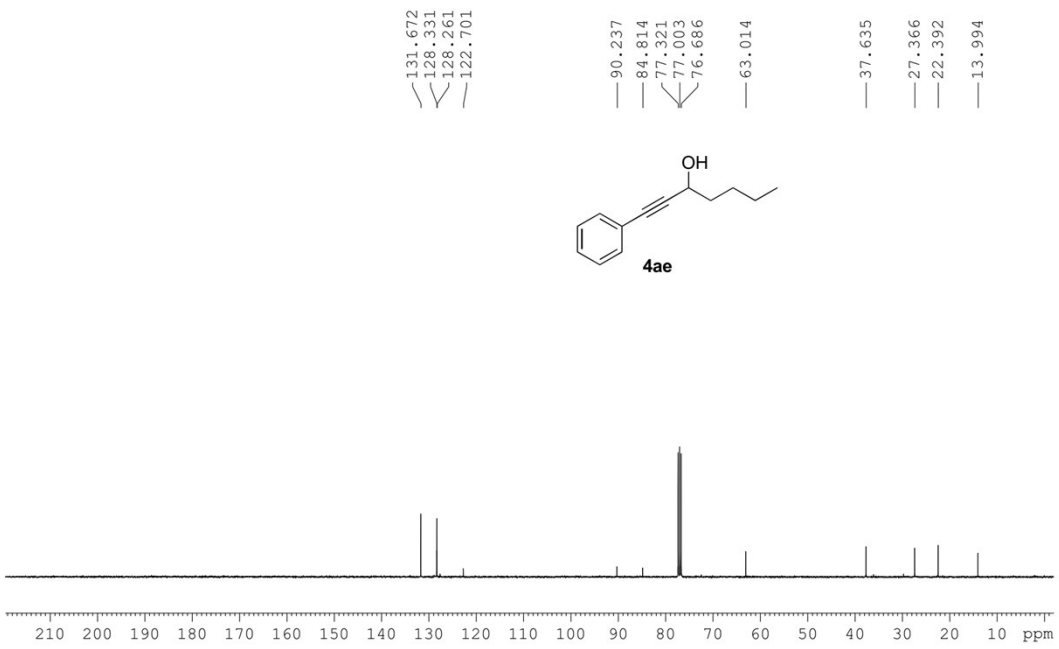
3.10
1.01
1.07
2.03
2.17
2.38
3.13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128.261
122.701
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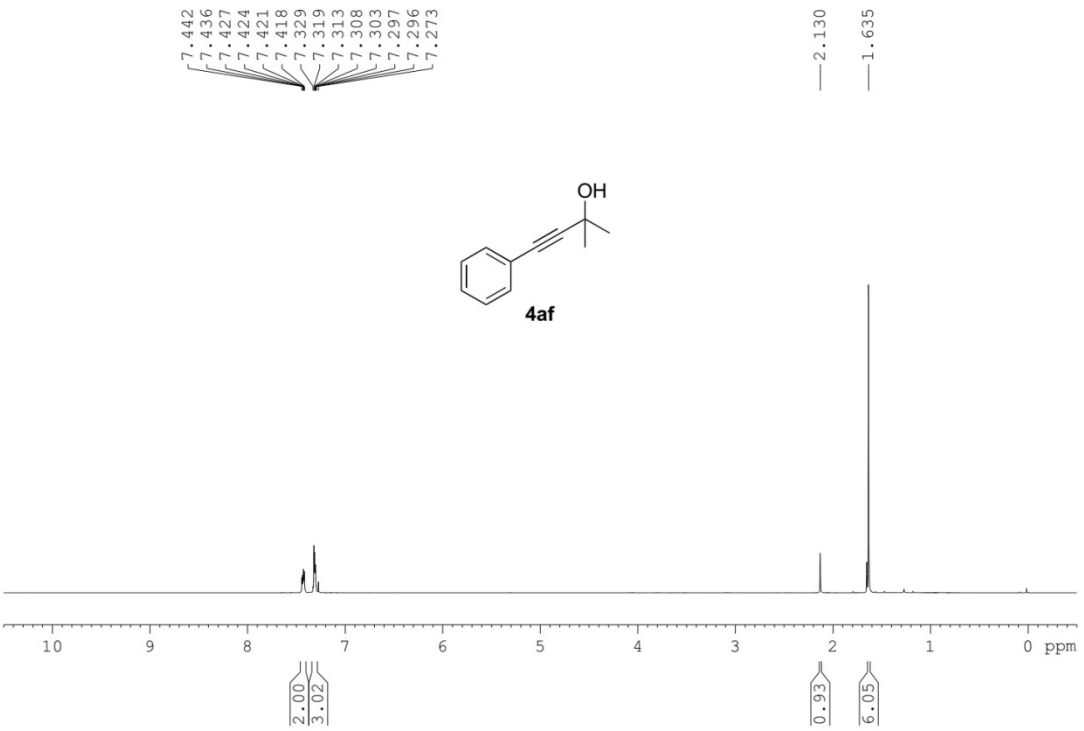
84.814
77.321
77.003
76.686
63.014
37.635
27.366
22.392
13.994
OH
4ae
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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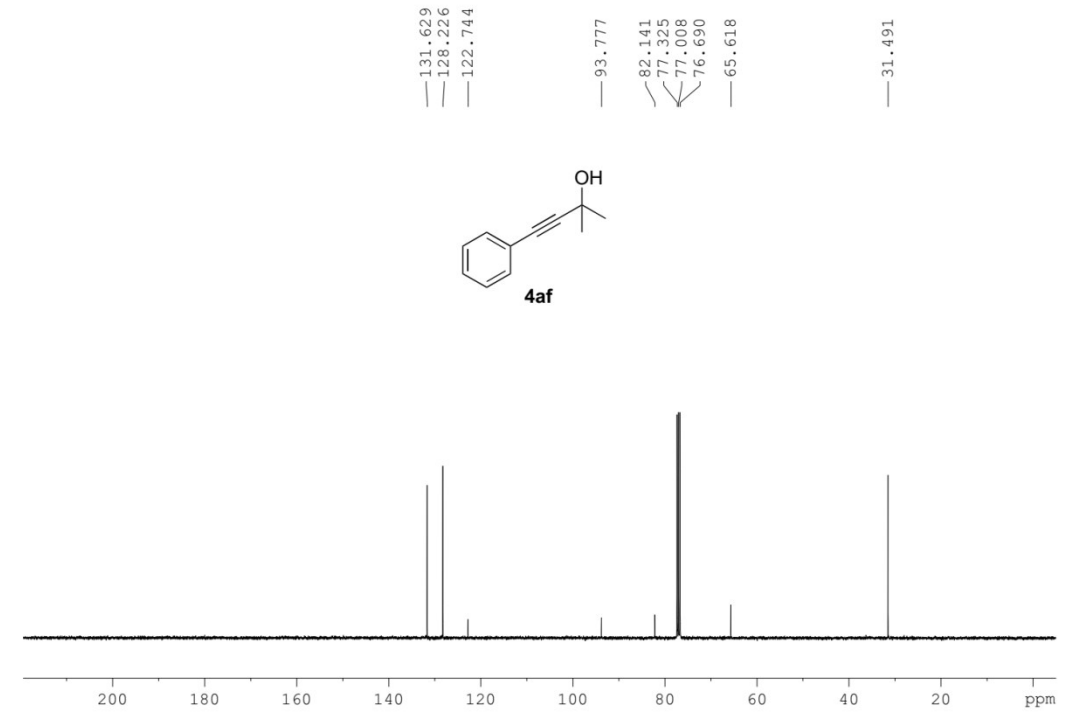
7.436
7.427
7.424
7.421
7.418
7.329
7.319
7.313
7.308
7.303
7.297
7.296
7.273
2.130
1.635
OH
4af
10
9
8
7
6
5
4
3
2
1
0 ppm
2.00
3.02
0.93
6.05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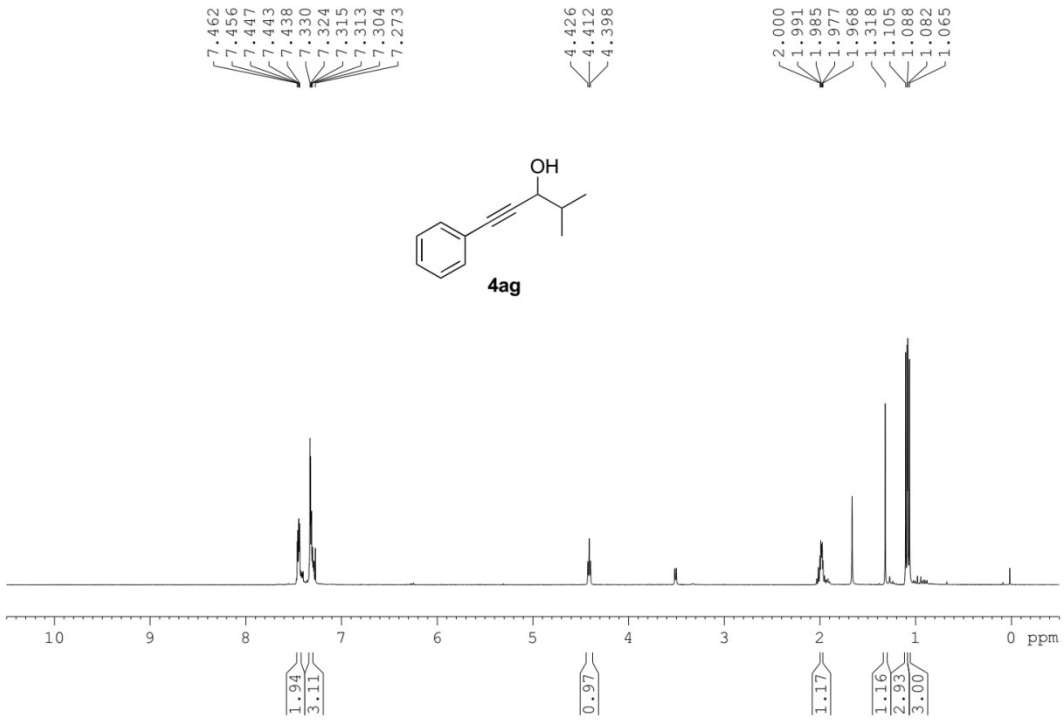
128.226
122.744
93.777
82.141
77.325
77.008
76.690
65.618
31.491
OH
4af
200
180
160
140
120
100
80
60
40
20
ppm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7.456
7.447
7.443
7.438
7.330
7.324
7.315
7.313
7.304
7.273
4.426
4.412
4.398
2.000
1.991
1.985
1.977
1.968
1.318
1.105
1.088
1.082
1.065
OH
4ag
10
9
8
7
6
5
4
3
2
1
0 ppm
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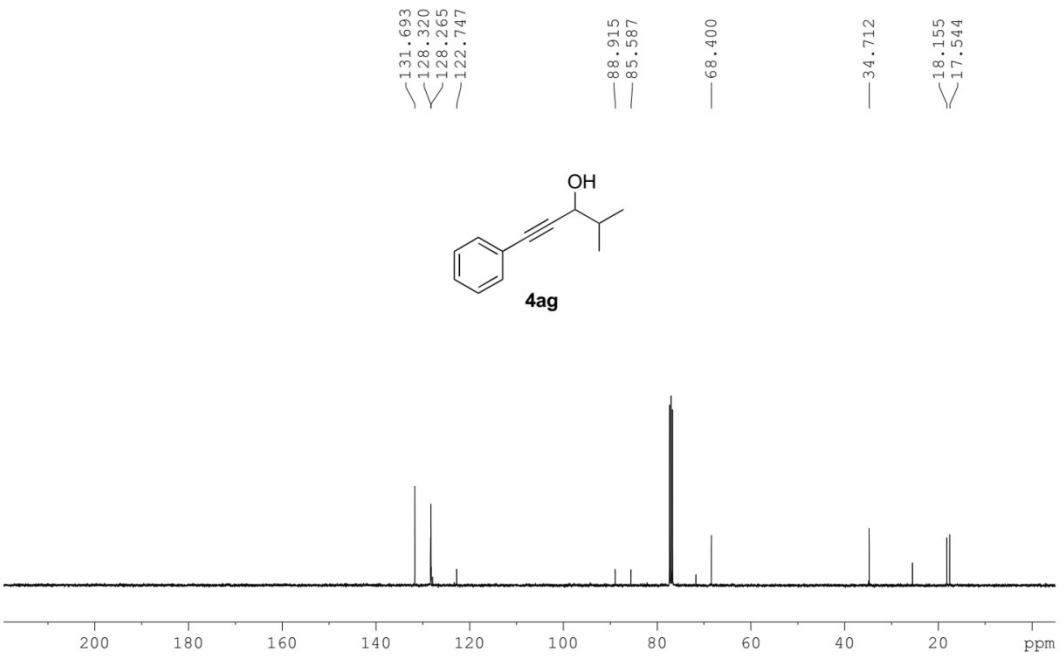
3.11
0.97
1.17
1.16
2.93
3.00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88.915
85.587
68.400
34.712
18.155
17.544
OH
4ag
200
180
160
140
120
100
80
60
40
20
ppm