Supplementary Material (ESI) for Green Chemistry
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An Eco-Sustainable Erbium(III)-Catalyzed Method for Formation/Cleavage of *O*-Boc-esters

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Supplementary Informations

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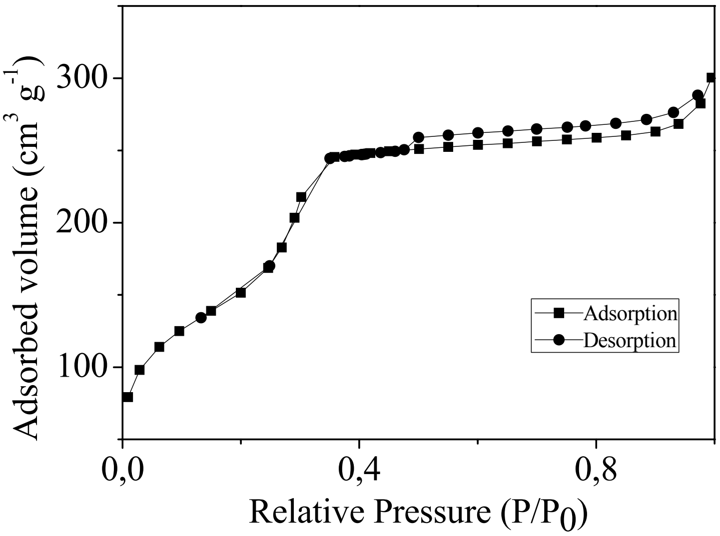
Experimental

^{1}H spectra were recorded on a Bruker WM 300 instrument on samples dissolved in $CDCl_3$ Chemical shifts are given in parts per million (ppm) from tetramethylsilane as the internal standard (0.0 ppm). Coupling constants (J) are given in Hertz. Reactions were monitored by a GC–MS Agilent workstation, formed by a GC-6890N (30-m RESTEK-5SIL capillary column, working on spitless mode, 1 mL/min He as carrier gas) and by an 5973N mass detector. The characterization of the porous structure was obtained by N_2 adsorption/desorption isotherms, measured at 77 K on a Micromeritics ASAP 2010 volumetric adsorption analyser. Before measurements, samples were outgassed at 393 K for 6 hours. These isotherms were used to evaluate BET specific surface area, pore volume and pore size distributions. The pore size distribution has been calculated using an algorithm based on the BJH theory. ICP-MS measures were performed in a quadrupole-based ICP-MS system XSERIES 2 ICP-MS, from Thermo Fisher Scientific, working in standard mode. Samples were introduced in a quartz concentric nebulizer by a peristaltic pump (selected speed of 30 rpm). The element concentration was determined against external calibration using a synthetic acid multielement calibration standard. MW-assisted reactions were performed in Synthos 3000 instrument from Anton Paar, equipped with a 64MG5 rotor and an IR probe as external control of the temperature. Using a temperature controlled program the instrument is able to tune the power magnetron in order to reach and to maintain the fixed temperature throughout the experiment. For each run 16 positions of the rotor were occupied by 0.3-3 ml glass vials sealed with a dedicated PEEK screw-cup together with a reliable PTFE seal. US reaction were performed in an ultrasound bath ULTRASONIC 06 from Falc (Power 40W, frequency out 45/55 KHz). TLC were performed using silica plates 60-F264 on alumina, commercially available from Merk. Liquid Flash chromatography was performed on a Supelco VERSA FLASH HTFP station on silica cartridges commercially available from Supelco. All solvents were distilled before using by standard methods. All chemicals were used as commercially available.

N_2 absorption /desorption curves

Er^{III}-MCM-41 before US exposure



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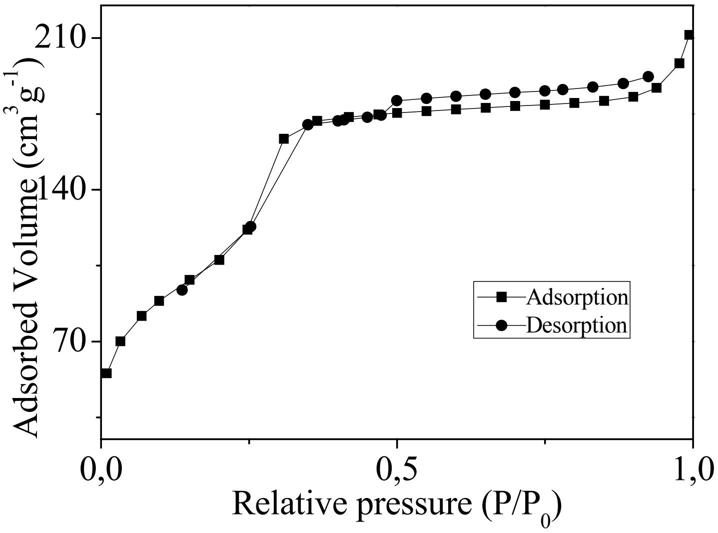

Synthesis of *tert*-Butyl Carbonates

Room temperature synthesis of terz-butyl Carbonates

In a general procedure 2.0 mmol of alcohol were dissolved in 2.3 eq of di-*tert*-butyl dicarbonate under soft heating (T < 40°C). 20 mg of MCM-43 (1%mol of Er(III)) were added to the mixture under N_2 atmosphere and the mixture was stirred at room temperature for 24 hours. The reaction was monitored by TLC or GC/MS. On completion, the mixture was diluted with diethyl ether, the catalyst was filtered off and the solvent was evaporated under vacuum. 3 ml of trifluoroethanol were then added and the solution was put in a ultrasound bath for 30 minutes in order to decompose the excess of di-*tert*-butyl dicarbonate . The solvent was evaporated under vacuum and desired pure product was separated from the crude by flash chromatography. The catalyst was washed for three times with ether, dried under vacuum and reused for the next run.

US-assisted synthesis of terz-butyl Carbonates

In a general procedure 2.0 mmol of alcohol were dissolved in 2.3 eq of di-*tert*-butyl dicarbonate under soft heating (T < 40°C). 20 mg of MCM-43 (1%mol of Er(III)) were added to the mixture under N_2 atmosphere and the mixture was stirred in an ultrasound bath for 1 up to 5 hours. The reaction was monitored by TLC or GC/MS. On completion, the mixture was diluted with diethyl ether, the catalyst was filtered off and the solvent was evaporated under vacuum. 3 ml of trifluoroethanol were then added and the solution was put in a ultrasound bath for 30 minutes in order to decompose the excess of di-*tert*-butyl dicarbonate . The solvent was evaporated under vacuum and desired pure product was separated from the crude by flash chromatography. The catalyst was washed for three times with ether, dried under vacuum and reused for the next run.

tert-butyl 4-methoxyphenyl carbonate (1). Yield 99%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.50;δ (ppm)(300MHz, $CDCl_3$): 1.55 (s, 9H, OtBut), 3.78 (s, 3H, OCH_3), 6.87 (ddd, 2H, H_C, H_B, J_{orto}=8 Hz, J_{meta}=1.99 Hz, J_{para}=1.80 Hz), 7.06 (ddd, 2H, H_A, H_D, J_{orto}=8.Hz, J_{meta}=1.99 Hz, J_{para}=1.80 Hz); m/z: 224 $[M]^+$, 209 $[M-CH_3]^+$, 124 $[M-COOtBut+H]^+$, 109 $[M-CH_3-COOtBut+H]^+$, 57 $[tBut]^+$.

tert-butyl octyl carbonate (2). Yield 71%; Rf (Petroleum Ether-Diethylic Ether 97.5:2.5) 0.66; δ (ppm)(300MHz, $CDCl_3$): 0.88 (t, 3H, CH_3, J_{CH3CH2}=6.5 Hz), 1.17-1.44 (m,8H, 2 x CH_2),1.48 (s, 9H, OtBut), 1.58 – 1.71 (m, 4H, 2 x CH_2), 4. 05(t, 2H, CH_2OBoc, J_{CH2CH2}=6.86Hz); m/z: 113 $[M-CO_2-OtBut]^+$, 112 $[M-CO_2-HOtBut]^+$, 57 $[t\text{-}but]^+$

sec-butyl tert-butyl carbonate (3). Yield 50%; volatile compound; m/z= 119 [M-isobutene]$^+$, 57 [t-but]$^+$.

tert-butyl pent-4-enyl carbonate (4). Yield 99%; Rf (Petroleum Ether-Diethylic Ether 8:2) 0.72; δ (ppm)(300MHz, $CDCl_3$): 1.38 (s, 9H, -OtBut), 1.67-1.81 (m, 2H, H_2), 2.09-2.19 (m, 2H, H_3), 4.07 (t, 2H, H_1, J_{H1H2}=6.83 Hz), 4.96-5.10 (m, 2H, H_5, $H_{5'}$); 5.73-5.88 (m, 1H, H_4) m/z=: 130 [M-tBut]$^+$, 69 [M-COOtBut]$^+$, 57 [tBut]$^+$.

tert-butyl cyclohexyl carbonate (5). Yield 92%; δ (ppm)(300MHz, $CDCl_3$): 1.48 (s, 9H, OtBut), 1.22-1.62 (m, 6H, 2 x H_3, 2 x H_4, 2 x H_5), 1.74-1.78 (m, 2H, H_2, $H_{2'}$), 1.93-1.96 (m, 2H, H_6, $H_{6'}$), 4.48-4.57 (m, 1H, H_1); m/z: 145 [M-isobutene]$^+$, 99 [M-COOtBut]$^+$, 83 [M-CO_2-OtBut]$^+$, 57 [tBut]$^+$.

tert-butyl phenyl carbonate (6). Yield 99%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.64; δ (ppm)(300MHz, $CDCl_3$): 1.56 (s, 9H, -OtBut), 7.08-7.44 (m, 5H, Ar) m/z=: 194 [M]$^+$, 179 [M-CH_3]$^+$, 94 [M-COOtBut]$^+$, 57 [tBut]$^+$.

4-bromophenyl tert-butyl carbonate (7). Yield 99%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.64; δ (ppm)(300MHz, $CDCl_3$): 1.55 (s, 9H, OtBut), 7.06 (ddd, 2H, H_C, H_B, J_{orto}=8 Hz, J_{meta}=1.99 Hz, J_{para}=1.80 Hz), 7.48 (ddd, 2H, H_A, H_D, J_{orto}=8.Hz, J_{meta}=1.99 Hz, J_{para}=1.80 Hz); m/z: 272 [M]$^+$, 274 (90%) [M+2]$^+$,253 [M-CH_3]$^+$, 259 (90%) [M+2-CH_3]$^+$,199 [M-tBut]$^+$, 201 (90%) [M+2-tBut]$^+$. 172 [M-OtBut]$^+$, 174 (90%) [M+2-tBut]$^+$, 57 [tBut]$^+$.

tert-butyl 4-ethylphenyl carbonate (8). Yield 99%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.66; δ (ppm)(300MHz, $CDCl_3$): 1.22 (t, 3H, -$C\underline{H}_3CH_2$, J_{CH3CH2}=7.67 Hz), 1.55 (s, 9H, OtBut), 2.63 (q, 2H, -$CH_3C\underline{H}_2$, J_{CH3CH2}=7.67 Hz), 7.06 (ddd, 2H, H_C, H_B, J_{orto}=8.Hz, J_{meta}=1.99 Hz, J_{para}=1.80 Hz), 7.19 (ddd, 2H, H_A, H_D, J_{orto}=8.Hz, J_{meta}=1.99 Hz, J_{para}=1.80 Hz); m/z: 122 [M]$^+$, 207 [M-CH_3]$^+$, 122 [M-CO_2-isobutene]$^+$, 107 [122- CH_3]$^+$, 57 [tBut]$^+$.

tert-butyl 4-nitrophenyl carbonate (9). Yield 99%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.46; δ (ppm)(300MHz, $CDCl_3$): 1.58 (s, 9H, OtBut), 7.33 (ddd, 2H, H_A, H_D, J_{orto}=8 Hz), 8.25 (ddd, 2H, H_C, H_B, J_{orto}=8) m/z:224 [M-CH_3]$^+$, 176 [M-OtBut]$^+$, 139 [M-COOtBut+H]$^+$, 57 [tBut]$^+$.

methyl 2-(tert-butoxycarbonylamino)-3-(4-(tert-butoxycarbonyloxy)phenyl)propanoate (10). Yield 99%; Rf (CH_2Cl_2-MeOH 98:2) 0.68; δ (ppm)(300MHz, $CDCl_3$): 1.42 (s, 9H, NHBoc), 1.55 (s, 9H, PhOtBut), 3.00-3.150 (m, 1H, H_1), 3.71 (s, 3H, $COOCH_3$), 4.50-4.65 (m, 1H,H_2), 4.9-5.1 (m, 1H, $H_{2'}$), 7.05-7.20 (m, 4H, Ar), ; m/z: 280 [M-NHBoc]$^+$, 178 [M-NHBoc-COOMe]$^+$,107 [Boc]$^+$, 57 [tBut]$^+$.

tert-butyl 4-(2-hydroxyethyl)-2-methoxyphenyl carbonate (11a). Yield 73%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.60; δ (ppm)(300MHz, $CDCl_3$): 1.55 (s, 9H, OtBut), 2.83 (t, 2H, -C$\underline{H}_2$CH$_2$OtBut, J_{CH2CH2}=6.59 Hz), 3.77-3.91 (m, 2H, -CH$_2$C$\underline{H}_2$OtBut), 3.84 (s, 3H, OCH$_3$), 6.78 (dd, 1H, H$_B$, J_{orto}=8.07 Hz, J_{meta}=1.89 Hz), 6.82 (d, 1H, H$_C$, J_{meta}=1.85 Hz), 7.05 (d, 1H, H$_D$, J_{orto}=8.07 Hz); m/z: 195 [M-OtBut]$^+$, 168 [M-COOtBut-H]$^+$, 137 [M-COOtBut- OCH$_3$]$^+$.

tert-butyl 4-(2-tert-butoxyethyl)-2-methoxyphenyl carbonate (11b). Yield 86%; Rf (CH$_2$Cl$_2$-MeOH 9:1) 0.8; δ (ppm)(300MHz, CDCl$_3$): 1.48 (s, 9H, OtBoc), 1.55 (s, 9H, PhOtBut), 2.99 (t, 2H, -C$\underline{H}_2$CH$_2$OtBut, J_{CH2CH2}=7.3 Hz), 3.84 (s, 3H, OCH$_3$), 4.25 (t, 2H, -CH$_2$C$\underline{H}_2$OPh, J_{CH2CH2}=7.3 Hz), 6.79 (dd, 1H, H$_B$, J_{orto}=8.07 Hz, J_{meta}=1.89 Hz), 6.8 (d, 1H, H$_C$, J_{meta}=1.85 Hz), 7.04 (d, 1H, H$_D$, J_{orto}=8.07 Hz) m/z: 295 [M-OtBut]$^+$, 168 [M-2 x COOtBut]$^+$, 150 [M-2 x COOtBut -2 x CO$_2$]$^+$,137 [M-2 x COOtBut-OCH$_3$]$^+$.

tert-butyl 2-methoxyphenyl carbonate (12). Yield 98%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.38; δ (ppm)(300MHz, CDCl$_3$): 1.55 (s, 9H, OtBut), 3.85 (s, 3H, -OCH$_3$), 6.90-7.19 (m, 4H, Ar); m/z: 224 [M]$^+$, 151[M-OtBut]$^+$, 124 [M-COOtBut]$^+$, 109 [M-OCOOtBut]$^+$, 92 [M-OCOOtBut-CH$_3$]$^+$, 77 [Ph]$^+$.

tert-butyl 4-methylphenyl carbonate (13) . Yield 99%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.7; δ (ppm)(300MHz, CDCl$_3$): 1.55 (s, 9H, OtBut), 2.33 (s, 3H, -CH$_3$), 7.04 (ddd, 2H, H$_C$, H$_B$, J_{orto}=7.30 Hz, J_{meta}=3.01 Hz, J_{para}=1.00 Hz), 7.15 (ddd, 2H, H$_A$, H$_D$, J_{orto}=7.30 Hz, J_{meta}=3.01 Hz, J_{para}=1.00 Hz); m/z: 208 [M]$^+$, 193 [M-CH$_3$]$^+$, 108 [M-CO$_2$-isobutene]$^+$, 91 [M-COOtBut]$^+$, 77 [Ph]$^+$.

tert-butyl 2-methylphenyl carbonate (14). Yield 97%; Rf (Petroleum Ether-Diethylic Ether 9:1) 0.7; δ (ppm)(300MHz, CDCl$_3$): 1.55 (s, 9H, OtBut), 2.33 (s, 3H, -CH$_3$), 7.06-7.22 (m, 4H, Ar); m/z: 208 [M]$^+$, 193 [M-CH$_3$]$^+$, 108 [M-CO$_2$-isobutene]$^+$, 91 [M-COOtBut]$^+$, 77 [Ph]$^+$.

Cleavage of *tert*-Butyl Carbonatess

Oil Bath Heating Cleavage of tert-Butyl Ethers

In a general procedure 1.0 mmol of tert-butyl ether was solved in 2.0 ml of EtOH and, after addition of 5%mol of Er $(OTf)_3$ (0.50 mmol, 30.70 mg), the mixture was heated until reflux temperature (70°C) in an oil bath. The reaction was monitored by TLC or GC/MS. On completion, the mixture was diluted with ether, then extracted for three times with water. The organic phases collected were dried on Na_2SO_4, filtered and then evaporated under vacuum giving rise to the pure product.

MW-Assisted Cleavage of tert-Butyl Ethers

In a general procedure 1.0 mmol of tert-butyl ether was solved in 2.0 ml of EtOH and 1%mol of Er $(OTf)_3$ (0.O10 mmol, 6.140 mg) were added in a 0.3-3 ml glass vials from Anton Paar sealed with a dedicated PEEK screw-cup together with a reliable PTFE seal. The mixture was reacted for 25 min. in a Synthos 3000 instrument from Anton Paar, equipped with a 64MG5 rotor and an IR probe as external control of the temperature, fixed on the temperature value of 80°C. On completion, the mixture was diluted with ether, then extracted for three times with water. The organic phases collected were dried on Na_2SO_4, filtered and then evaporated under vacuum giving rise to the pure product.

EI/MS Spectra

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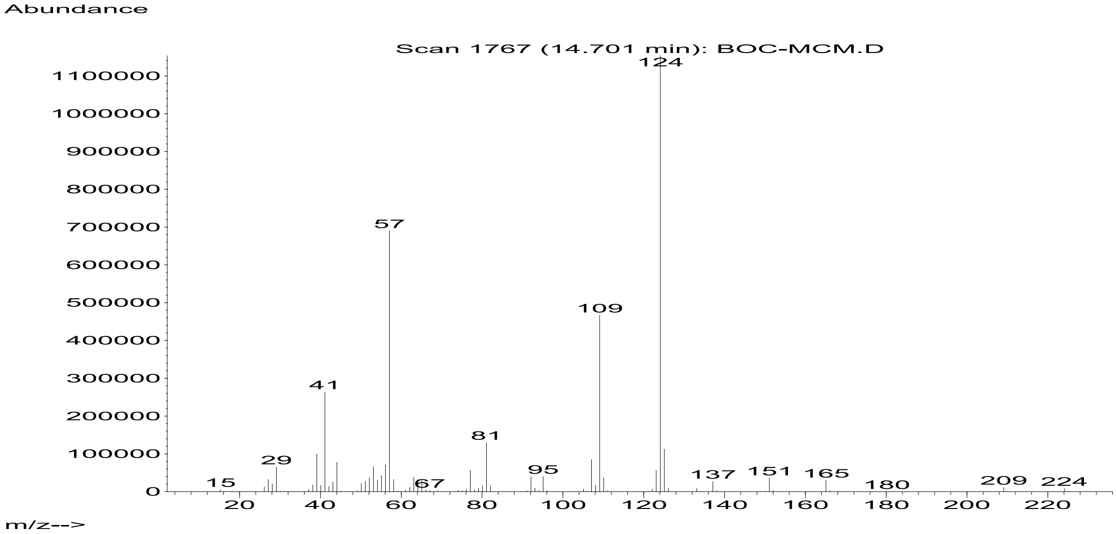

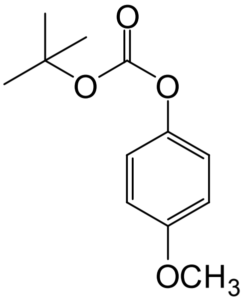

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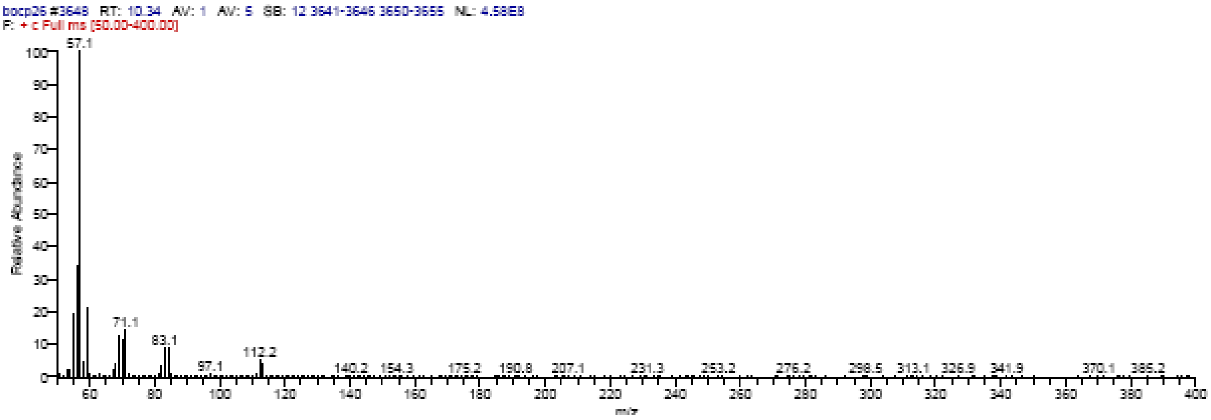
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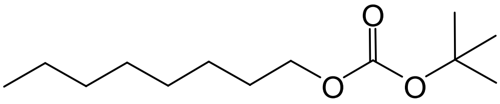
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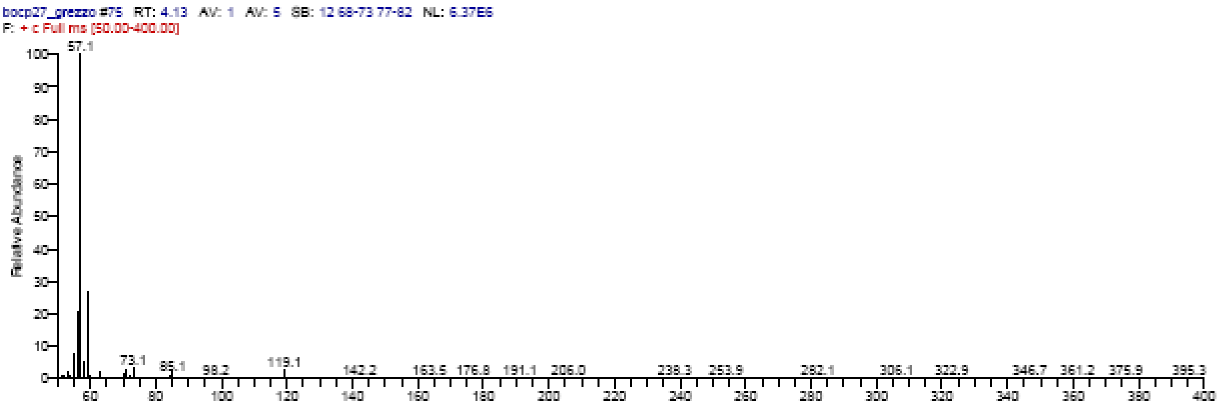
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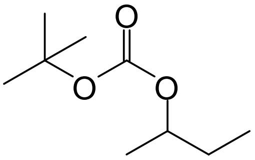
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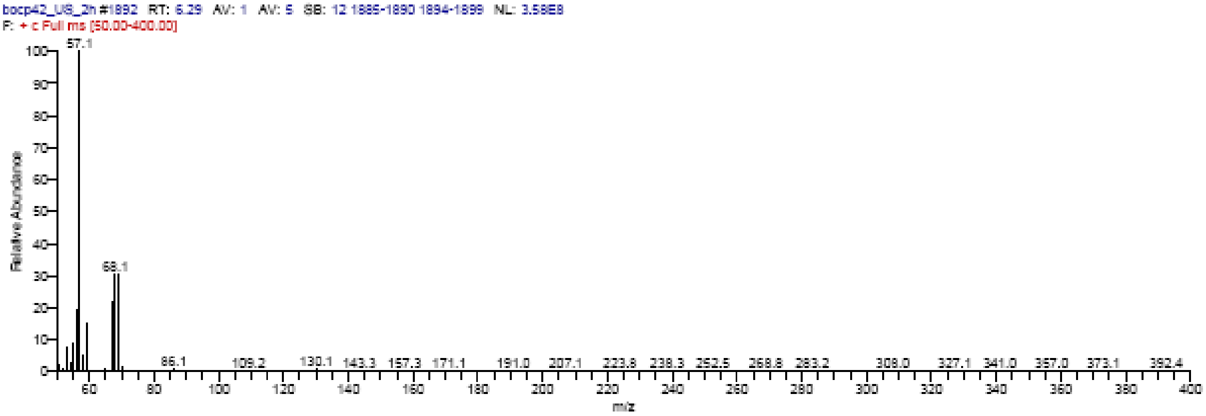
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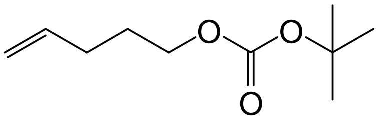
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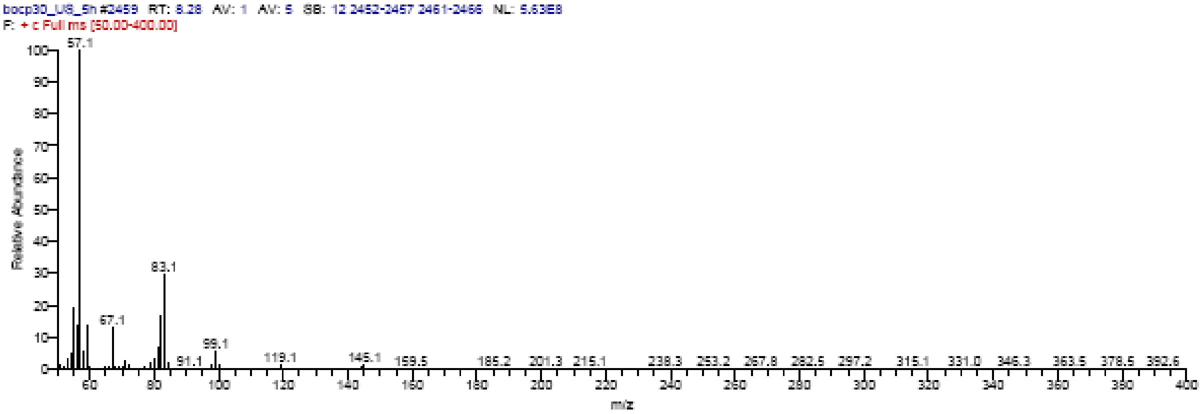
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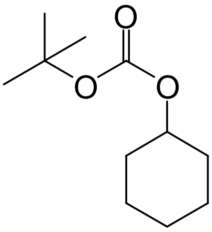
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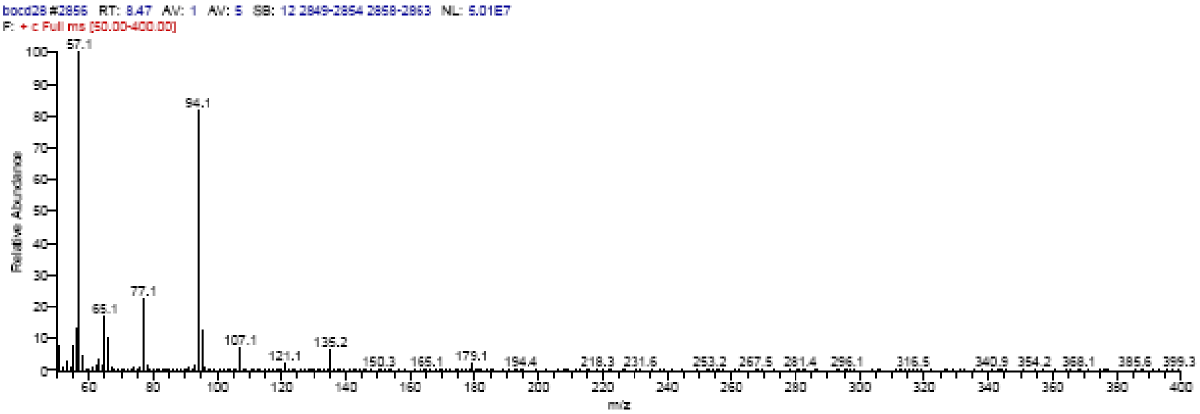
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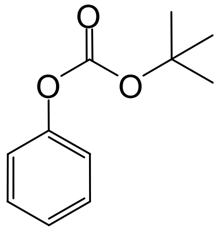
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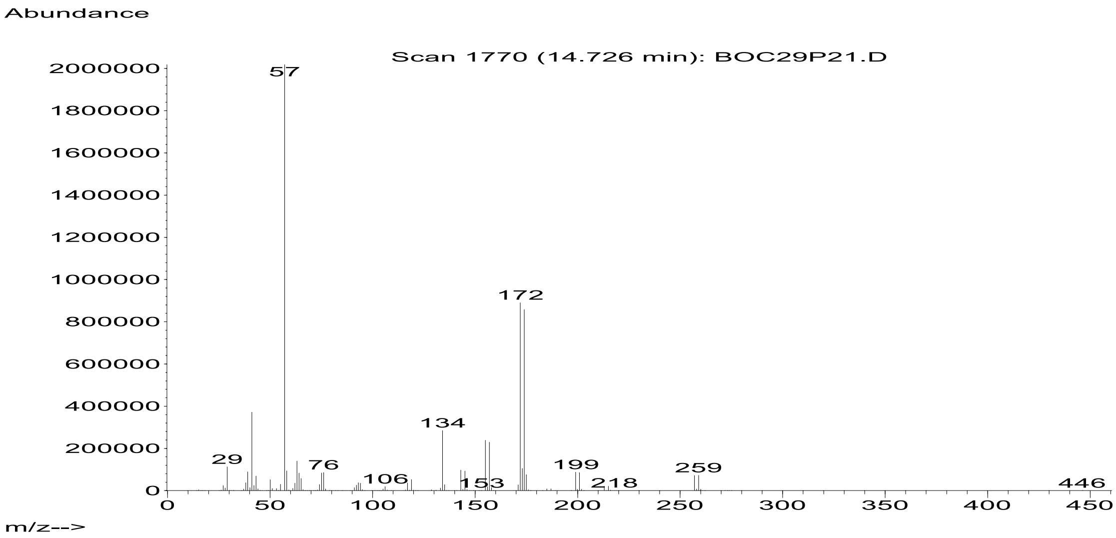
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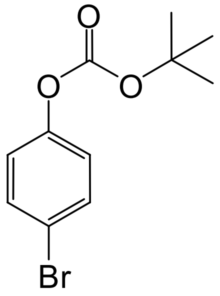
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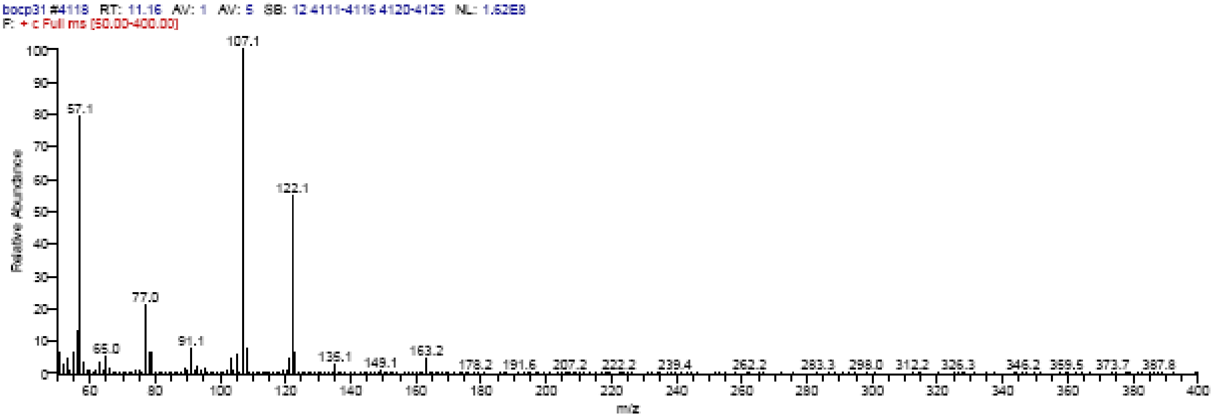
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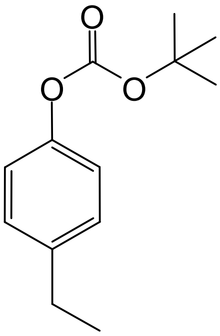
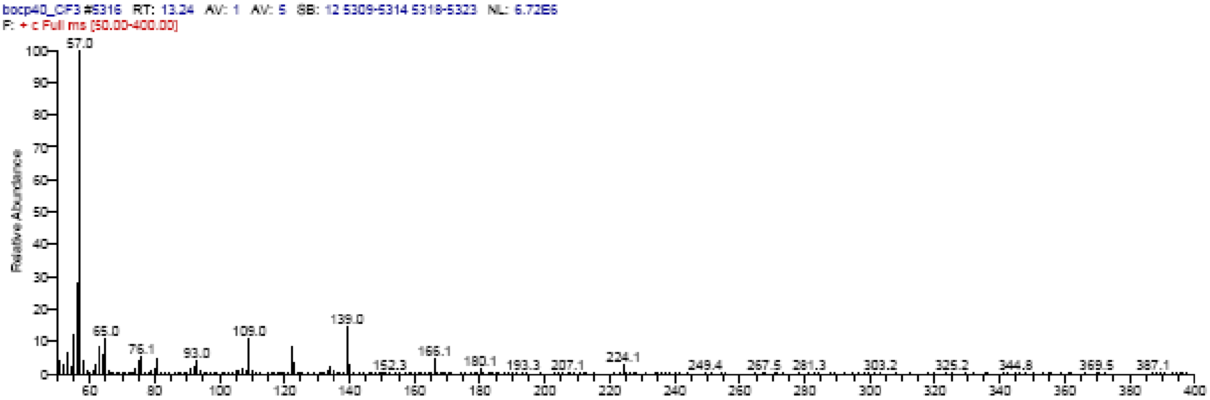
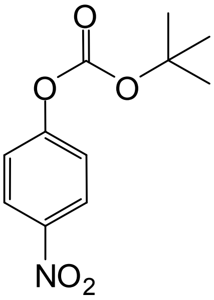
380
400
m/z

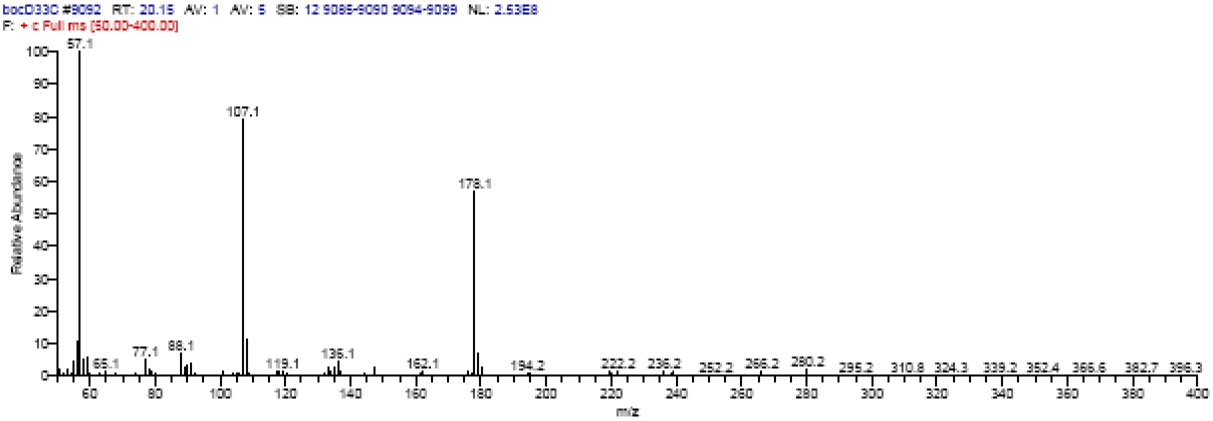

O
O
O

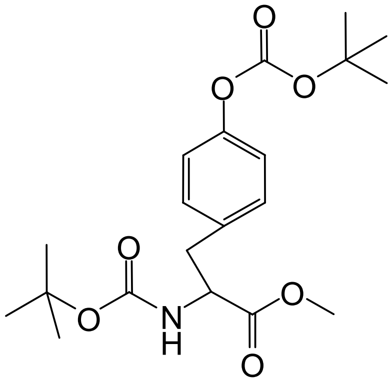
Sample **9**


bocp40_CF3 #5316 RT: 13.24 AV: 1 AV: 5 SB: 12 5309-5314 5318-5323 NL: 6.72E6
F: + c Full ms [50.00-400.00]
Relative Abundance
0
10
20
30
40
50
60
70
80
90
100
57.0
65.0
76.1
93.0
109.0
139.0
152.3
166.1
180.1
193.3
207.1
224.1
249.4
267.5
281.3
303.2
325.2
344.8
369.5
387.1
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400

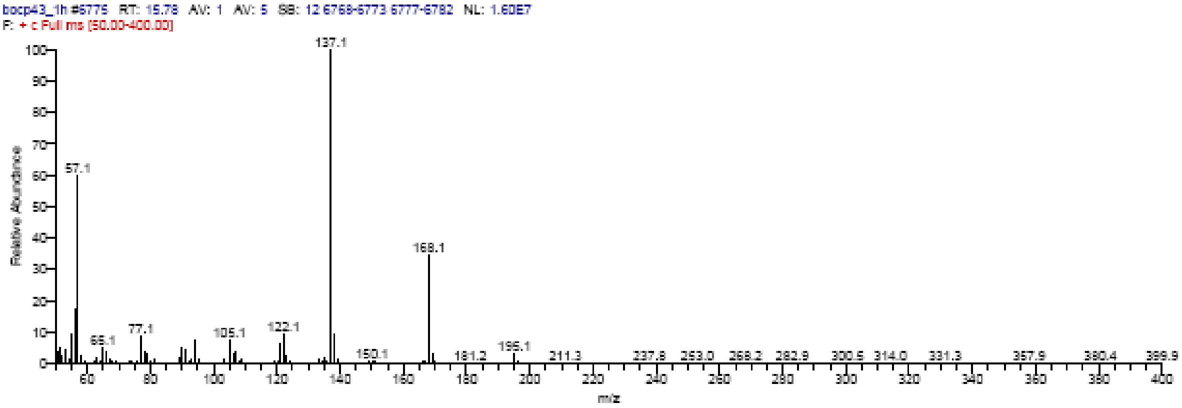

O
O
O
NO2

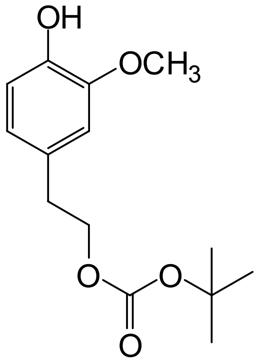
Sample **10**


bocD33C #9092 RT: 20.15 AV: 1 AV: 5 SB: 12 9085-9090 9094-9099 NL: 2.53E8
F: + c Full ms [50.00-400.00]
Relative Abundance
0
10
20
30
40
50
60
70
80
90
100
57.1
65.1
77.1
88.1
107.1
119.1
136.1
162.1
178.1
194.2
222.2
236.2
252.2
266.2
280.2
295.2
310.8
324.3
339.2
352.4
366.6
382.7
396.3
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
m/z

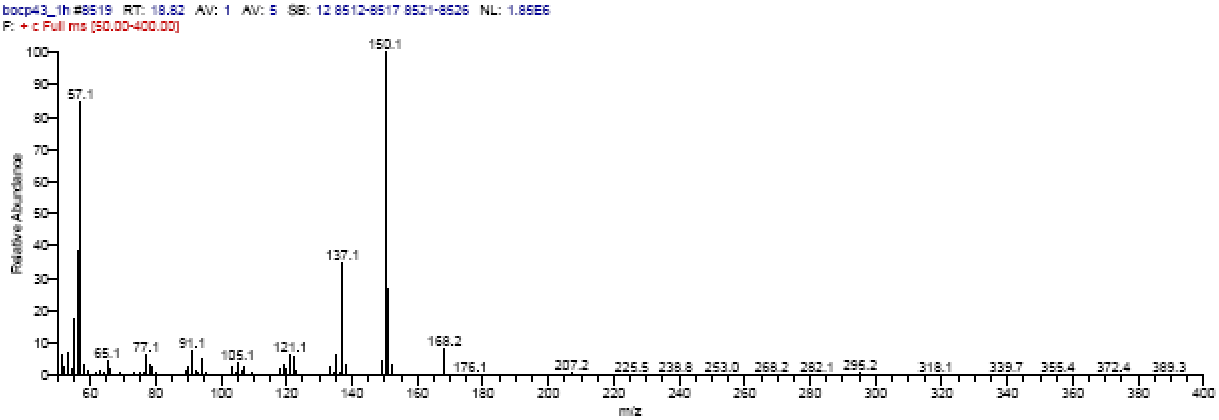

O
O
O
O
N
H
O
O
O

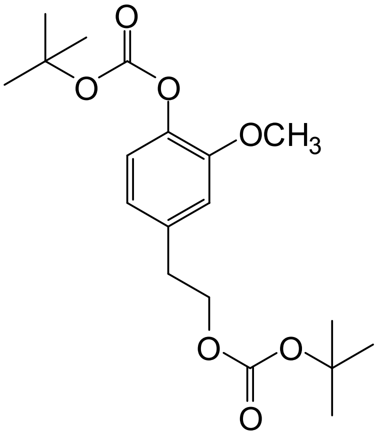
Sample **11a**


bocp43_1h #6775 RT: 15.78 AV: 1 AV: 5 SB: 12 6768-6773 6777-6782 NL: 1.60E7
F: + c Full ms [50.00-400.00]
Relative Abundance
0
10
20
30
40
50
60
70
80
90
100
57.1
65.1
77.1
105.1
122.1
137.1
150.1
168.1
181.2
196.1
211.3
237.8
253.0
268.2
282.9
300.5
314.0
331.3
357.9
380.4
399.9
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
m/z

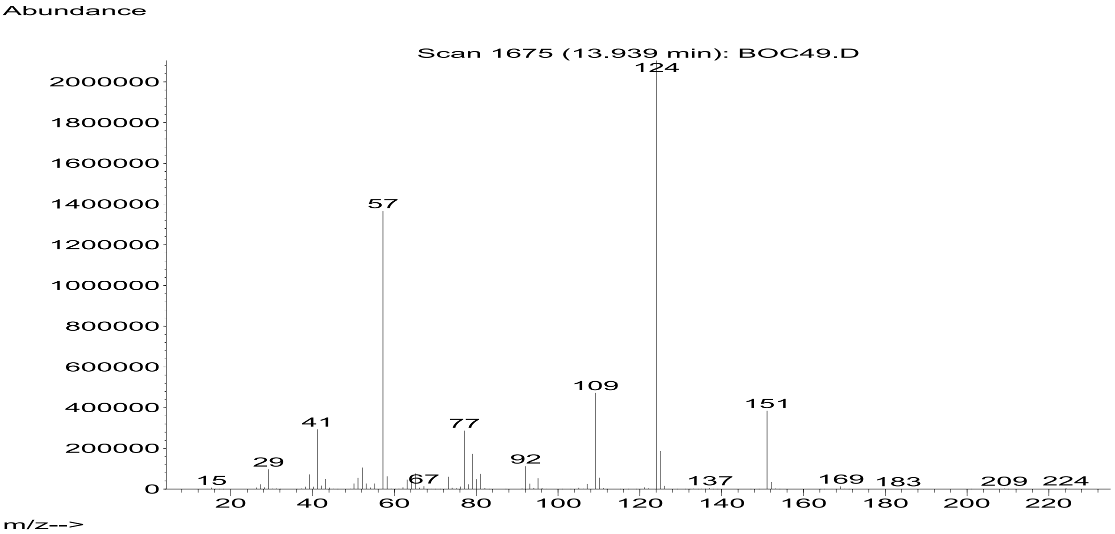

OH
OCH3
O
O
O

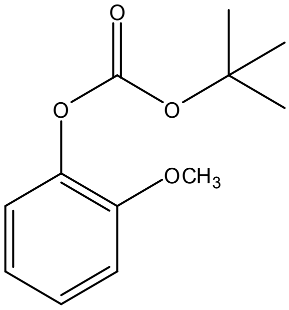
Sample **11b**


bocp43_1h #8519 RT: 18.82 AV: 1 AV: 5 SB: 12 8512-8517 8521-8526 NL: 1.85E6
F: + c Full ms [50.00-400.00]
Relative Abundance
0
10
20
30
40
50
60
70
80
90
100
57.1
65.1
77.1
91.1
105.1
121.1
137.1
150.1
168.2
176.1
207.2
225.5
238.8
253.0
268.2
282.1
295.2
318.1
339.7
355.4
372.4
389.3
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
m/z

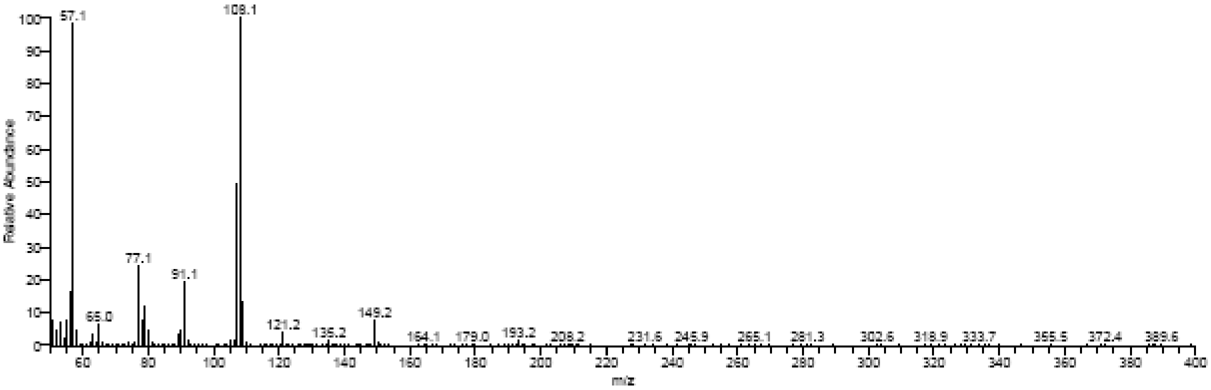

O
O
O
OCH3
O
O
O

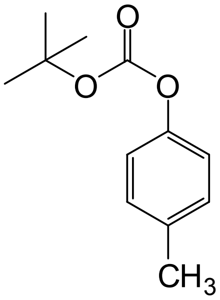
Sample **12**


Abundance
Scan 1675 (13.939 min): BOC49.D
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
124
57
109
151
41
77
92
29
15
67
137
169
183
209
224
20
40
60
80
100
120
140
160
180
200
220
m/z-->

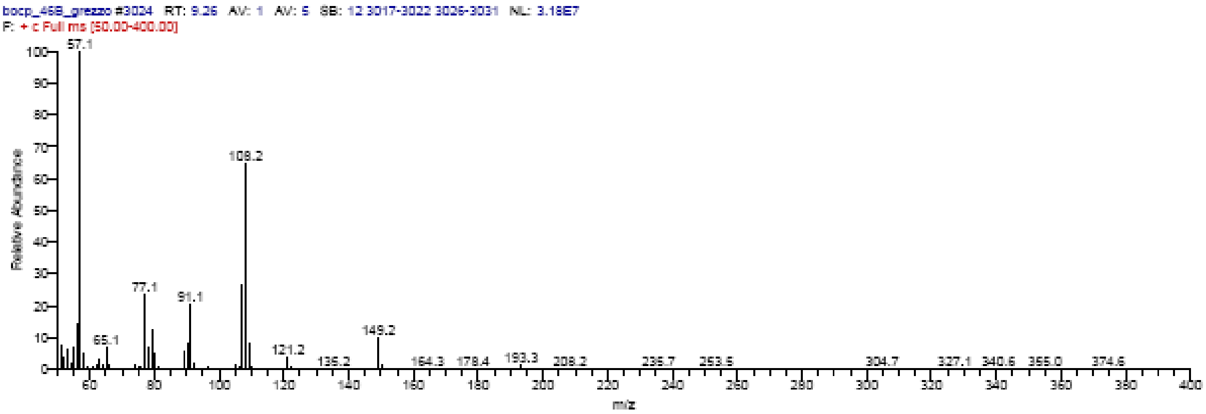

O
O
O
OCH3

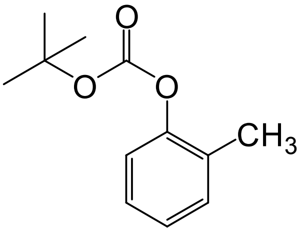
Sample **13**


Relative Abundance
100
90
80
70
60
50
40
30
20
10
0
57.1
108.1
77.1
91.1
65.0
121.2
135.2
149.2
164.1
179.0
193.2
208.2
231.6
245.9
265.1
281.3
302.6
318.9
333.7
355.5
372.4
389.6
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
m/z


O
O
O
CH3

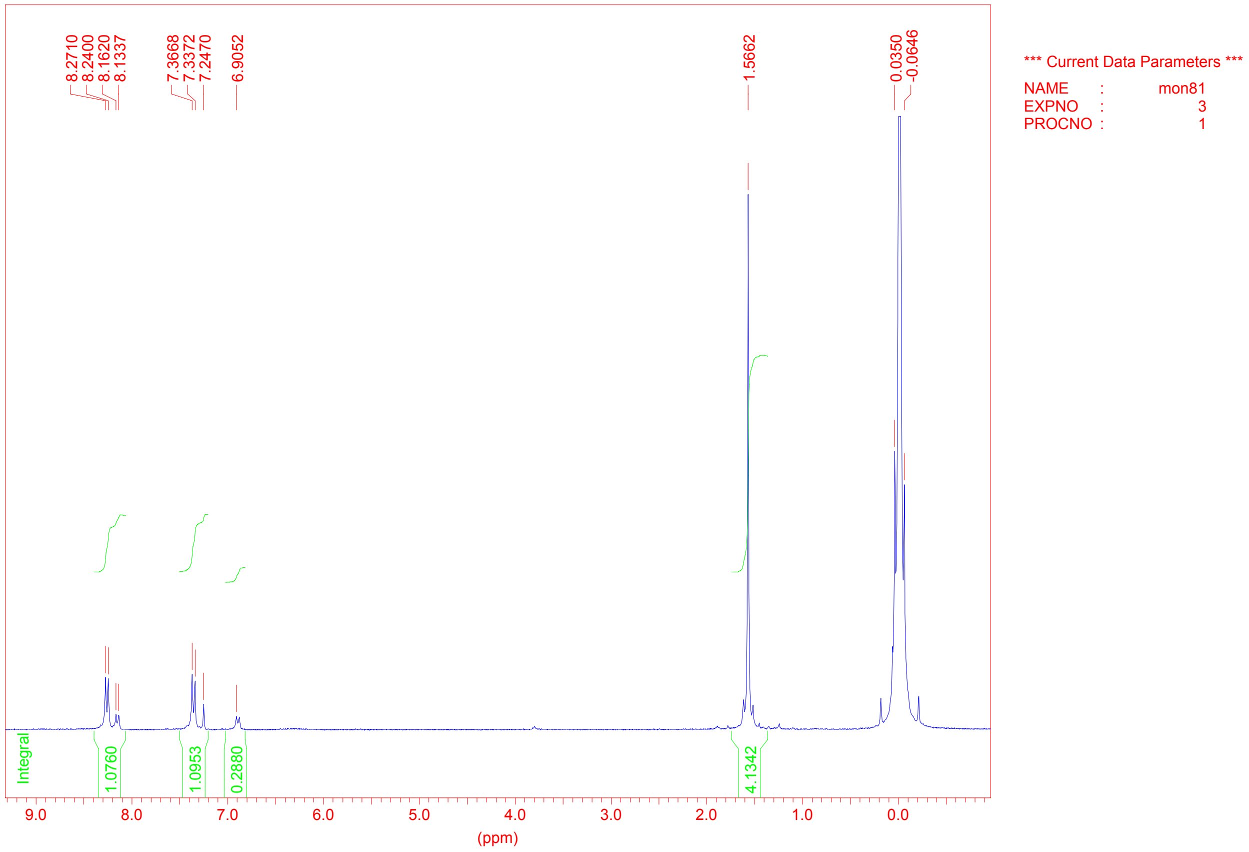
Sample **14**

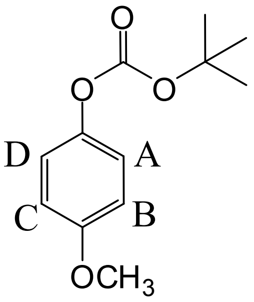

bocp_46B_grezzo #3024 RT: 9.26 AV: 1 AV: 5 SB: 12 3017-3022 3026-3031 NL: 3.18E7
F: + c Full ms [50.00-400.00]
Relative Abundance
100
90
80
70
60
50
40
30
20
10
0
57.1
108.2
77.1
91.1
65.1
149.2
121.2
136.2
164.3
178.4
193.3
208.2
235.7
253.5
304.7
327.1
340.6
355.0
374.6
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
400
m/z


O
O
O
CH3

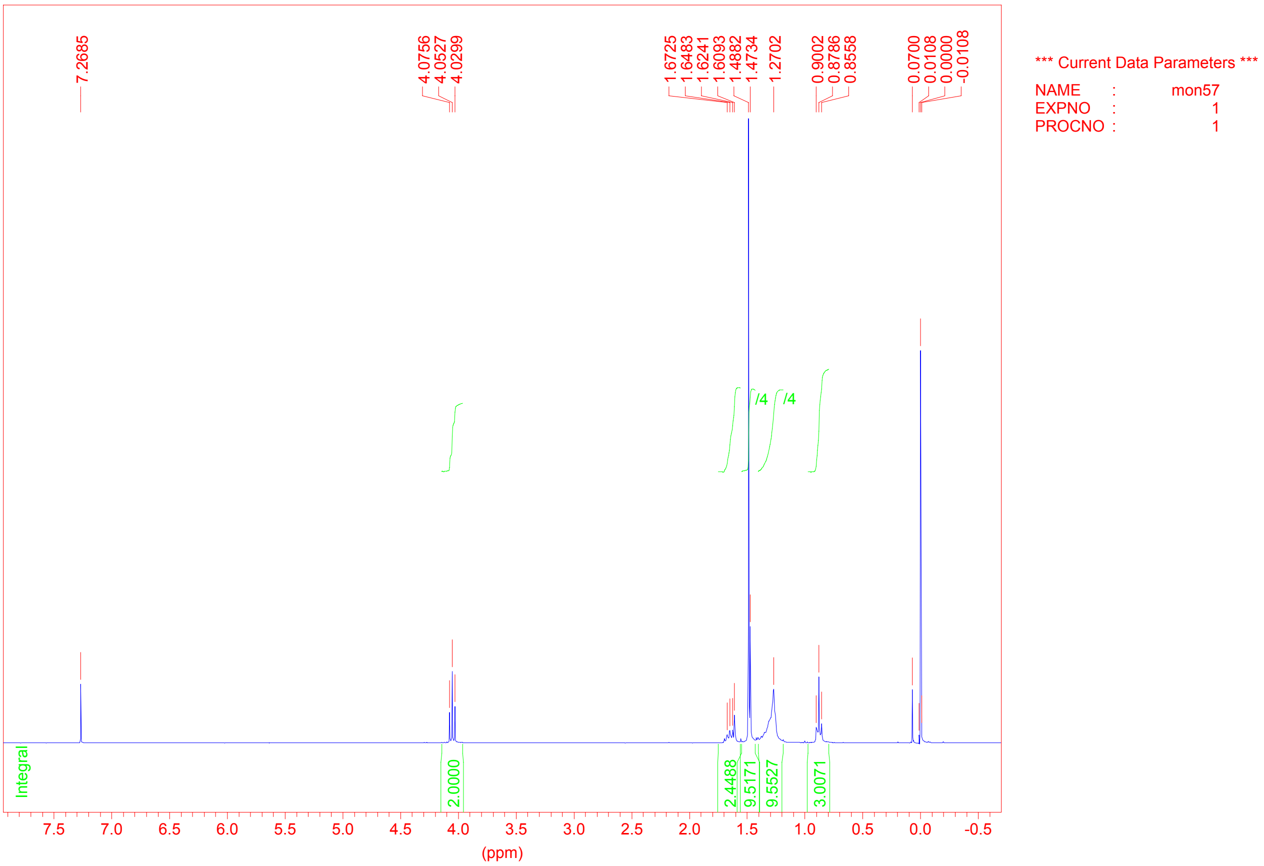
^{1}H-NMR Spectra

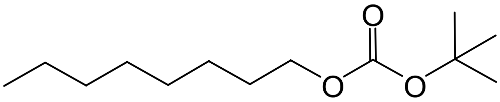
Sample **1**



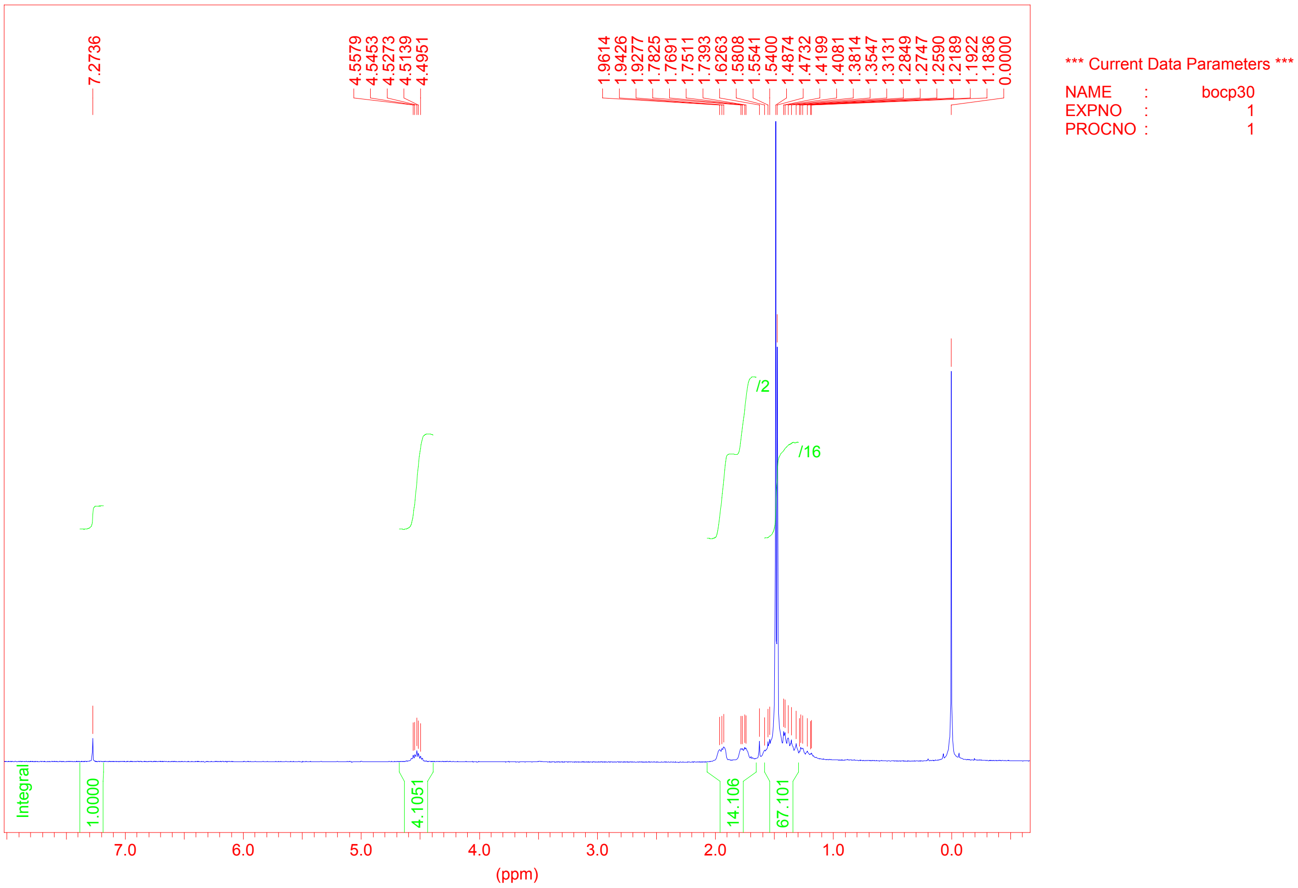


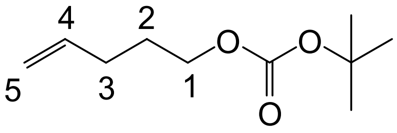
Sample **2**


7.2685
4.0756
4.0527
4.0299
1.6725
1.6483
1.6241
1.6093
1.4882
1.4734
1.2702
0.9002
0.8786
0.8558
0.0700
0.0108
0.0000
-0.0108
*** Current Data Parameters ***
NAME : mon57
EXPNO : 1
PROCNO : 1
/4
/4
Integral
2.0000
2.4488
9.5171
9.5527
3.0071
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
(ppm)

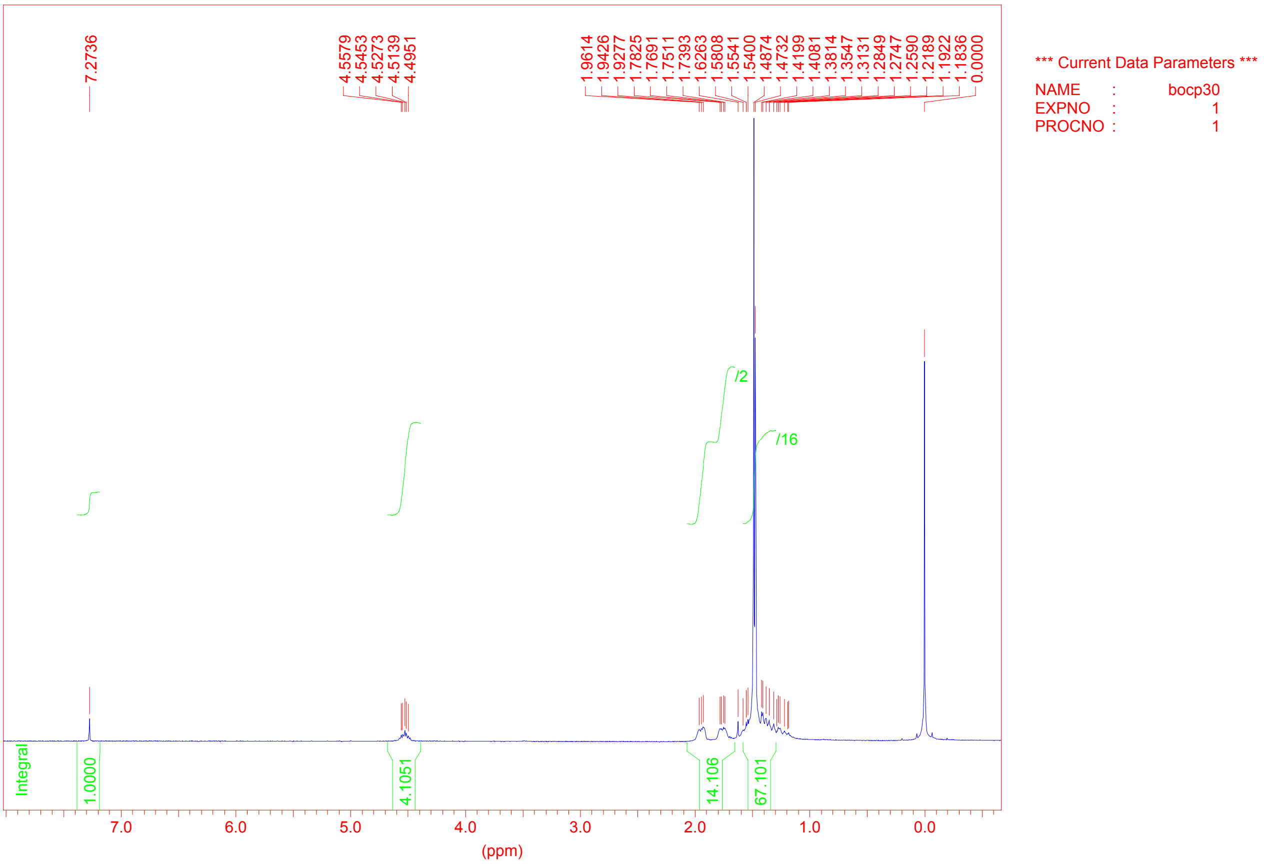

O
O
O

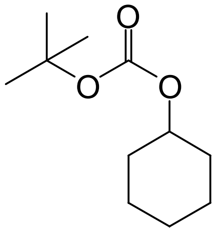
Sample **4**


7.2736
4.5579
4.5453
4.5273
4.5139
4.4951
1.9614
1.9426
1.9277
1.7825
1.7691
1.7511
1.7393
1.6263
1.5808
1.5541
1.5400
1.4874
1.4732
1.4199
1.4081
1.3814
1.3547
1.3131
1.2849
1.2747
1.2590
1.2189
1.1922
1.1836
0.0000
/2
/16
Integral
1.0000
4.1051
14.106
67.101
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
*** Current Data Parameters ***
NAME : bocp30
EXPNO : 1
PROCNO : 1

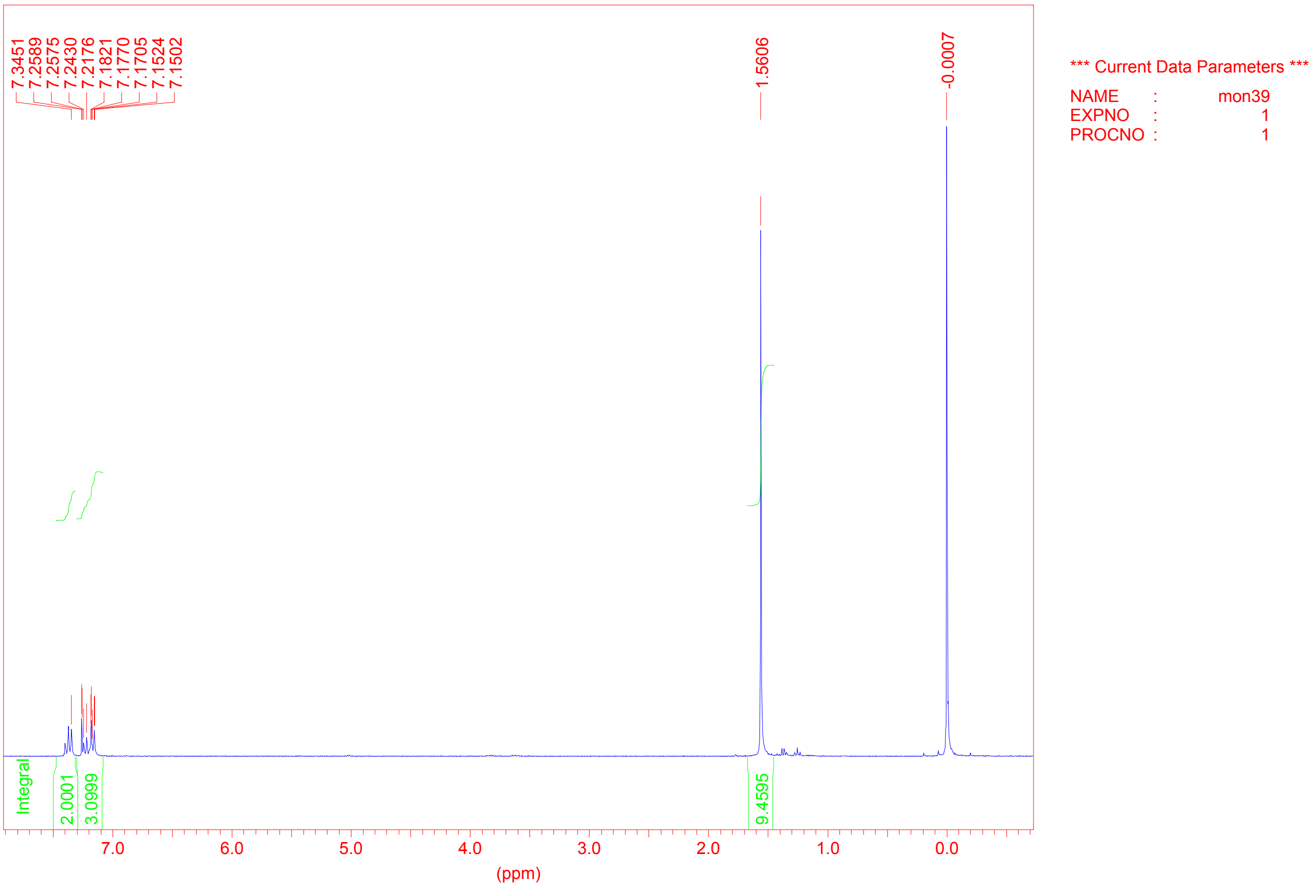

4
2
5
3
1
O
O
O

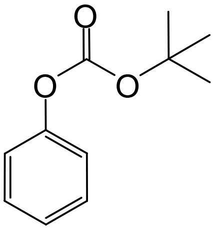
Sample **5**


7.2736
4.5579
4.5453
4.5273
4.5139
4.4951
1.9614
1.9426
1.9277
1.7825
1.7691
1.7511
1.7393
1.6263
1.5808
1.5541
1.5400
1.4874
1.4732
1.4199
1.4081
1.3814
1.3547
1.3131
1.2849
1.2747
1.2590
1.2189
1.1922
1.1836
0.0000
*** Current Data Parameters ***
NAME : bocp30
EXPNO : 1
PROCNO : 1
/2
/16
Integral
1.0000
4.1051
14.106
67.101
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

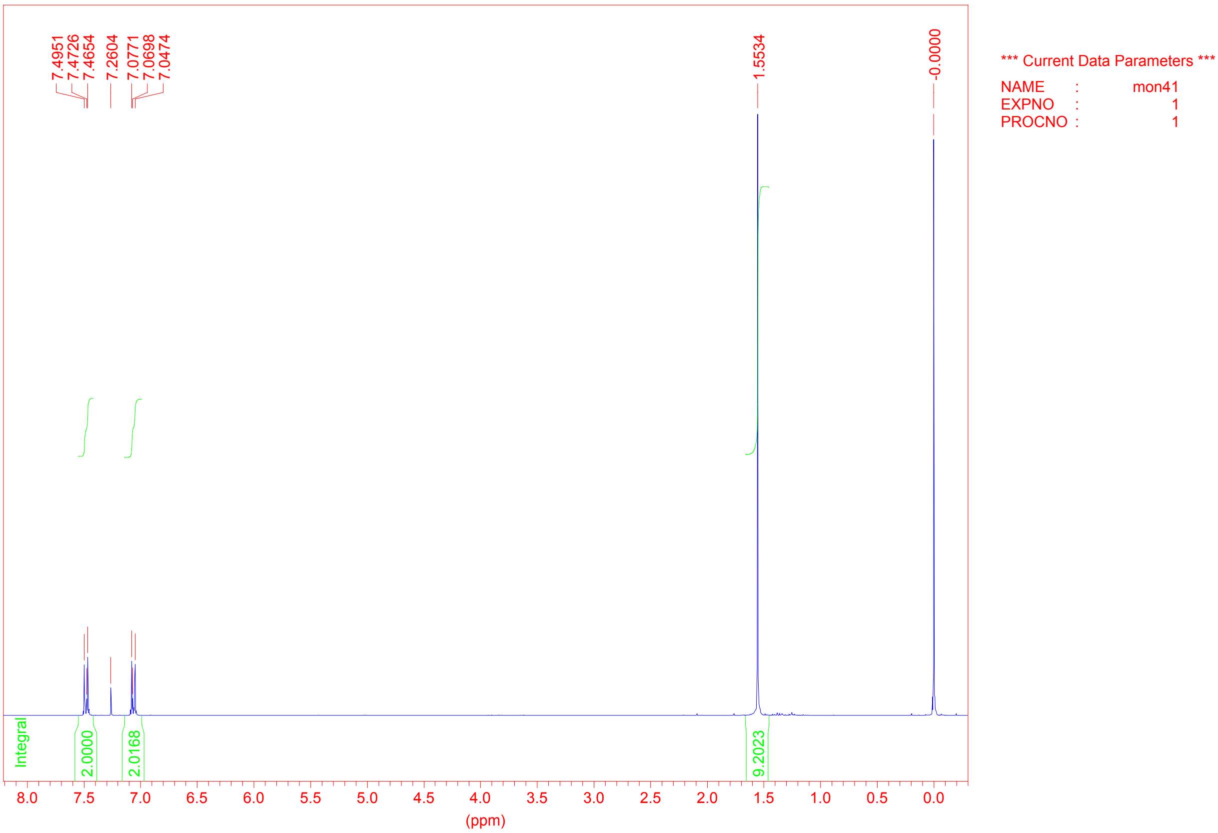

O
O
O

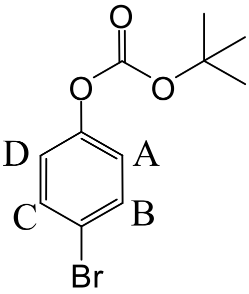
Sample **6**


7.3451
7.2589
7.2575
7.2430
7.2176
7.1821
7.1770
7.1705
7.1524
7.1502
1.5606
-0.0007
*** Current Data Parameters ***
NAME : mon39
EXPNO : 1
PROCNO : 1
Integral
2.0001
3.0999
9.4595
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

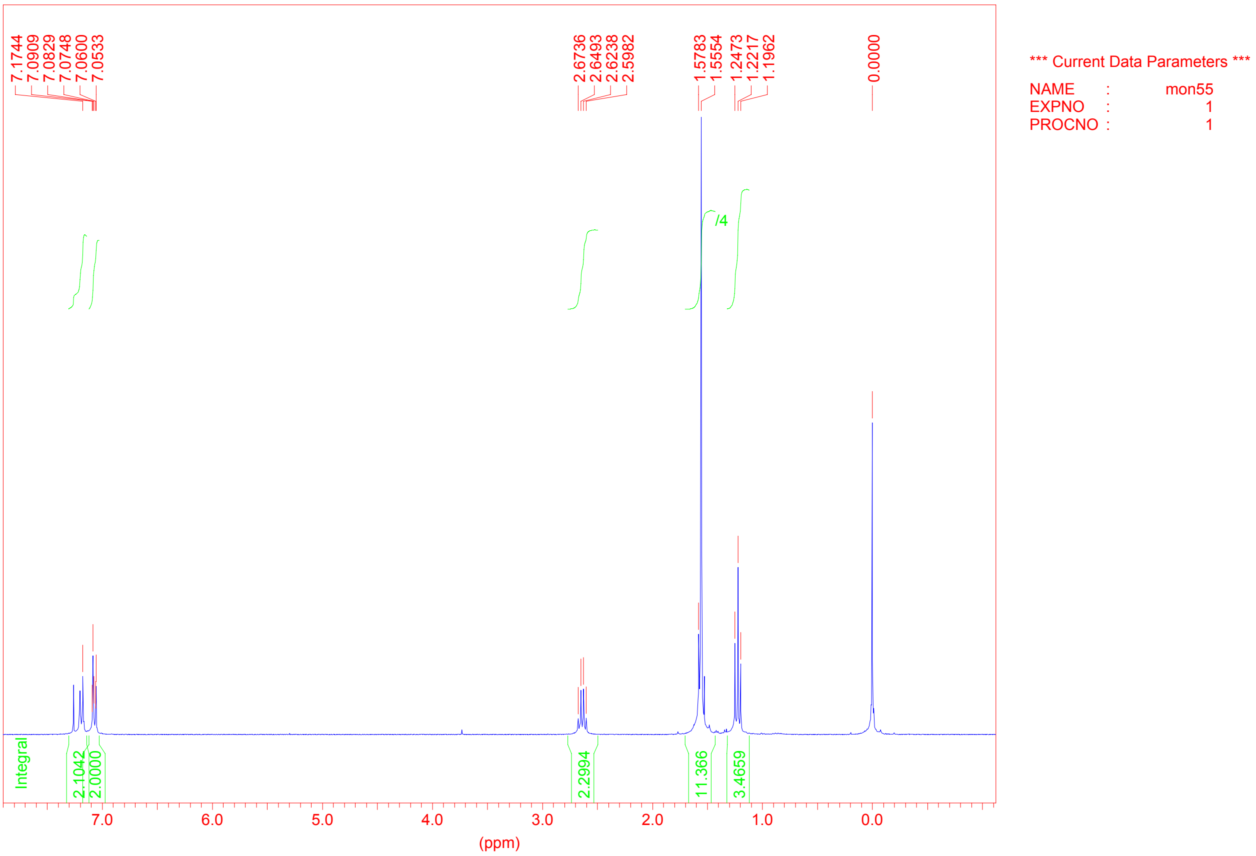

O
O
O

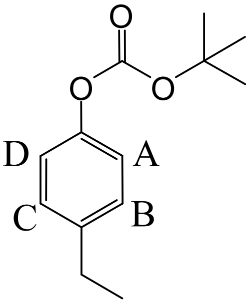
Sample **7**


7.4951
7.4726
7.4654
7.2604
7.0771
7.0698
7.0474
1.5534
-0.0000
*** Current Data Parameters ***
NAME : mon41
EXPNO : 1
PROCNO : 1
Integral
2.0000
2.0168
9.2023
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

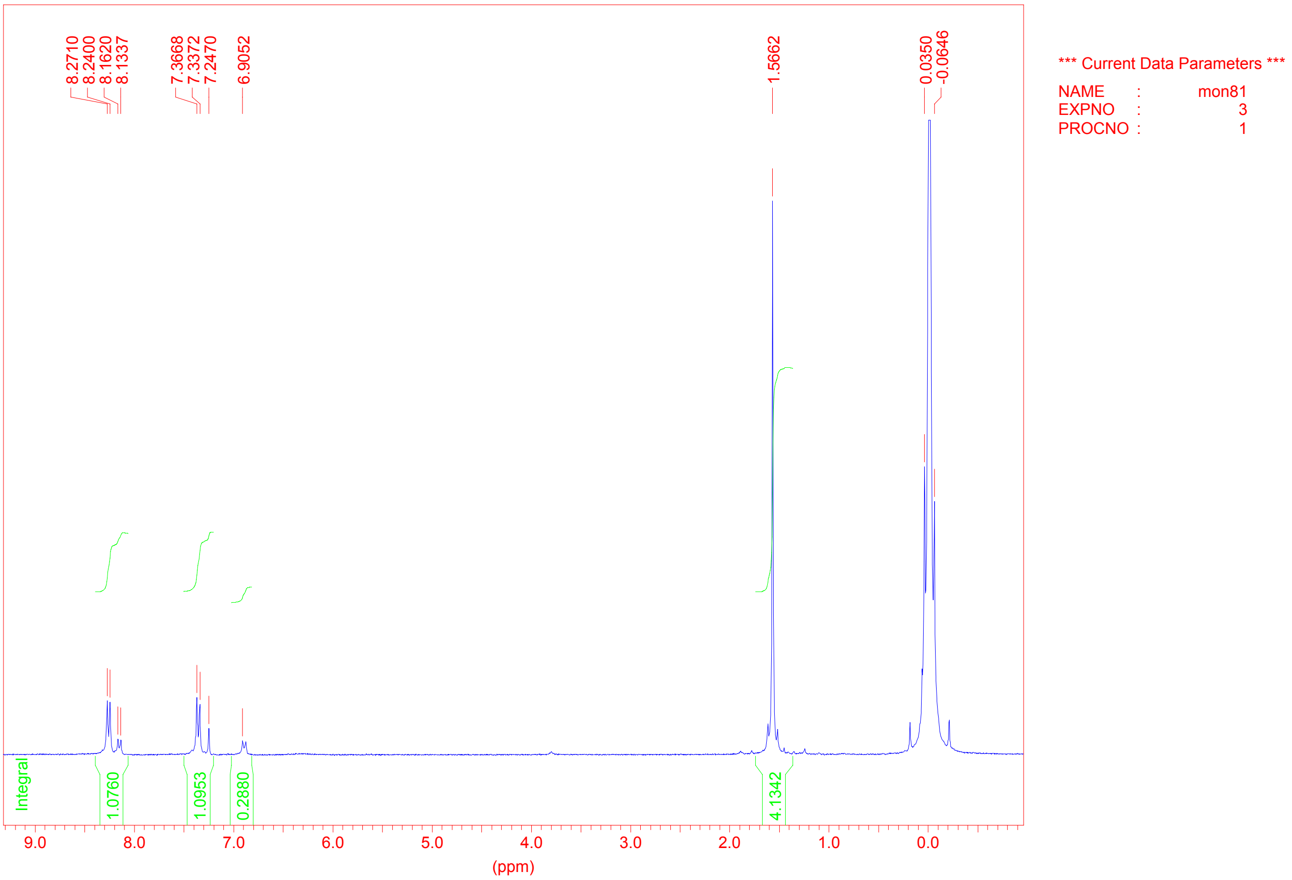

O
O
O
D
A
C
B
Br

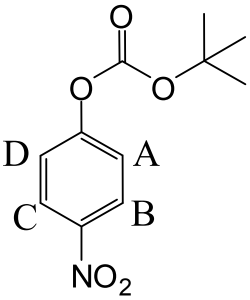
Sample **8**


7.1744
7.0909
7.0829
7.0748
7.0600
7.0533
2.6736
2.6493
2.6238
2.5982
1.5783
1.5554
1.2473
1.2217
1.1962
0.0000
/4
Integral
2.1042
2.0000
2.2994
11.366
3.4659
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
*** Current Data Parameters ***
NAME : mon55
EXPNO : 1
PROCNO : 1

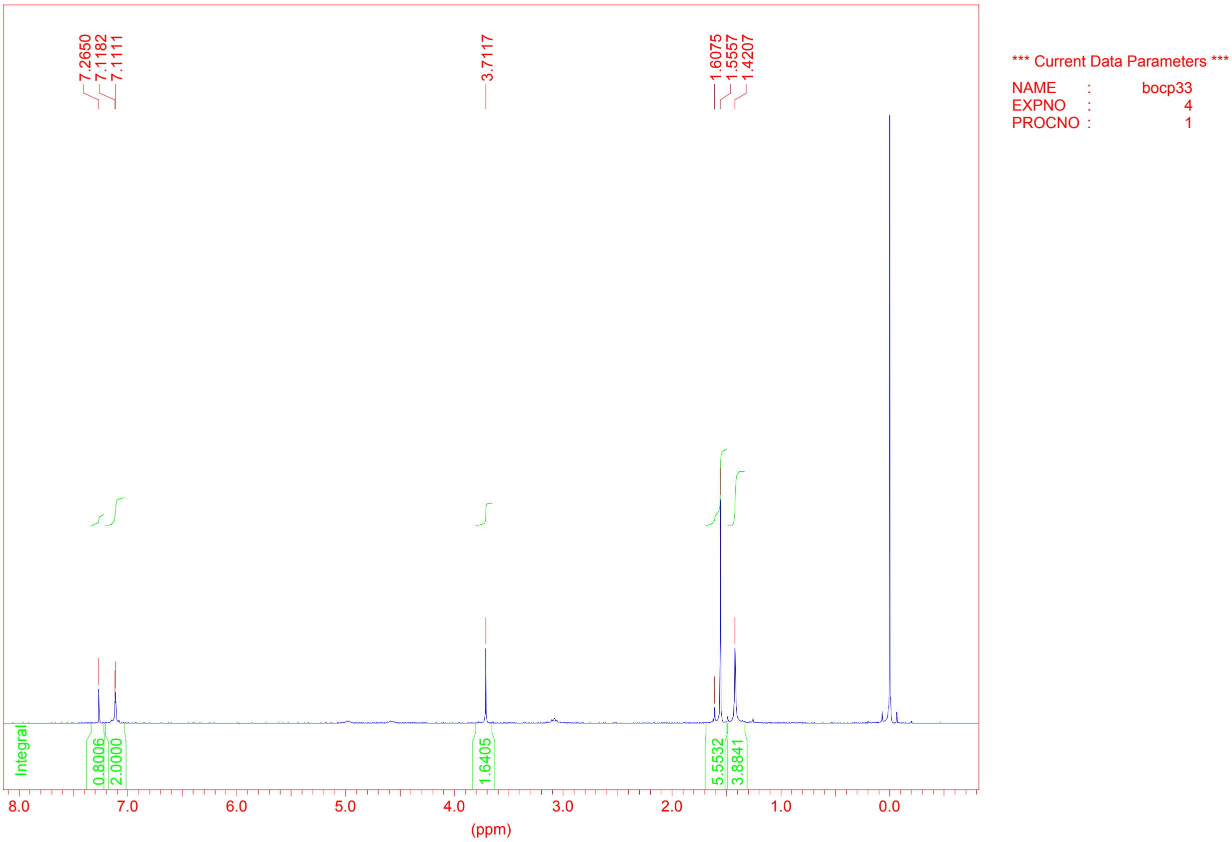

O
O
O
D
A
C
B

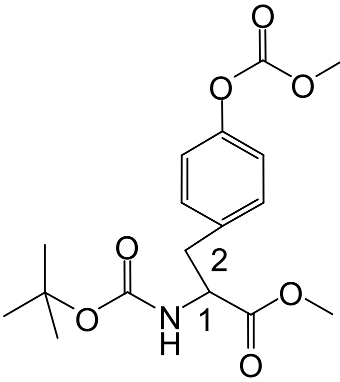
Sample **9**


8.2710
8.2400
8.1620
8.1337
7.3668
7.3372
7.2470
6.9052
1.5662
0.0350
-0.0646
*** Current Data Parameters ***
NAME : mon81
EXPNO : 3
PROCNO : 1
Integral
1.0760
1.0953
0.2880
4.1342
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

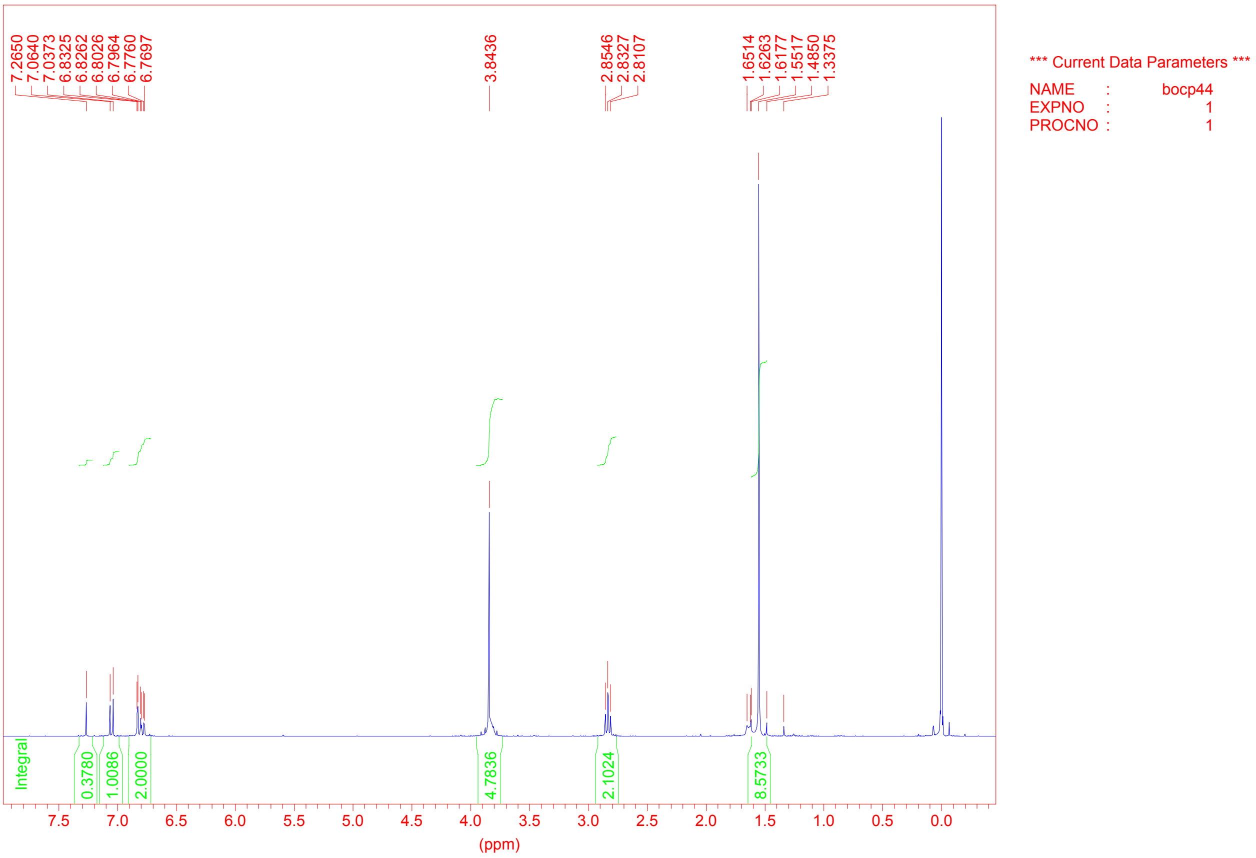

O
O
O
D
A
C
B
NO2

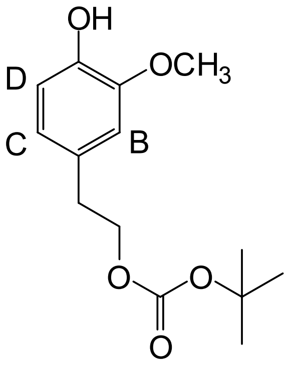
Sample **10**


7.2650
7.1182
7.1111
3.7117
1.6075
1.5557
1.4207
*** Current Data Parameters ***
NAME : bocp33
EXPNO : 4
PROCNO : 1
Integral
0.8006
2.0000
1.6405
5.5532
3.8841
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

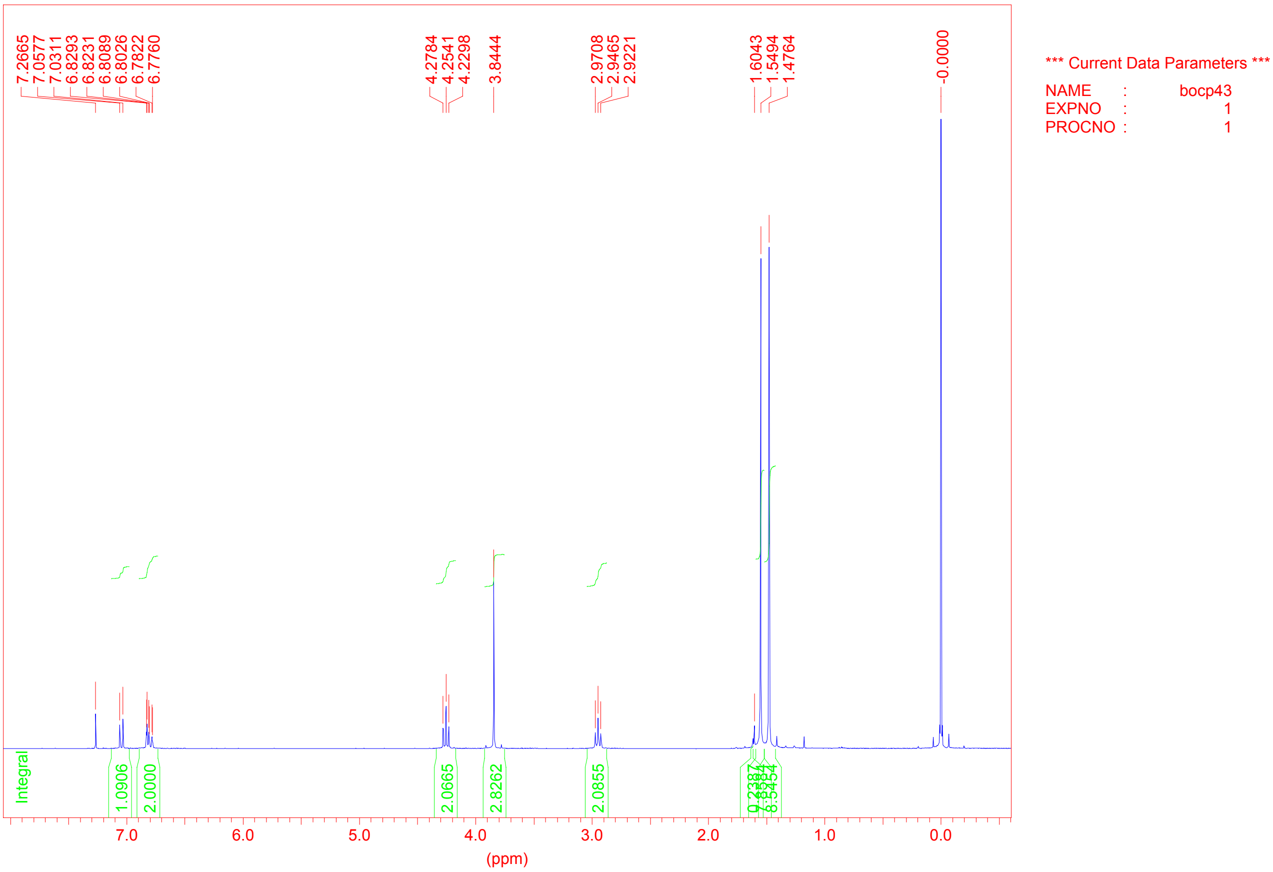

O
O
O
O
N
H
1
2
O
O
O

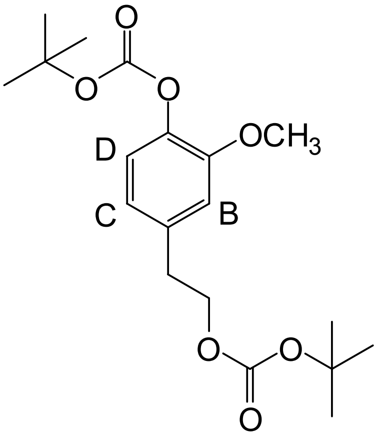
Sample **11a**


7.2650
7.0640
7.0373
6.8325
6.8262
6.8026
6.7964
6.7760
6.7697
3.8436
2.8546
2.8327
2.8107
1.6514
1.6263
1.6177
1.5517
1.4850
1.3375
*** Current Data Parameters ***
NAME : bocp44
EXPNO : 1
PROCNO : 1
Integral
0.3780
1.0086
2.0000
4.7836
2.1024
8.5733
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

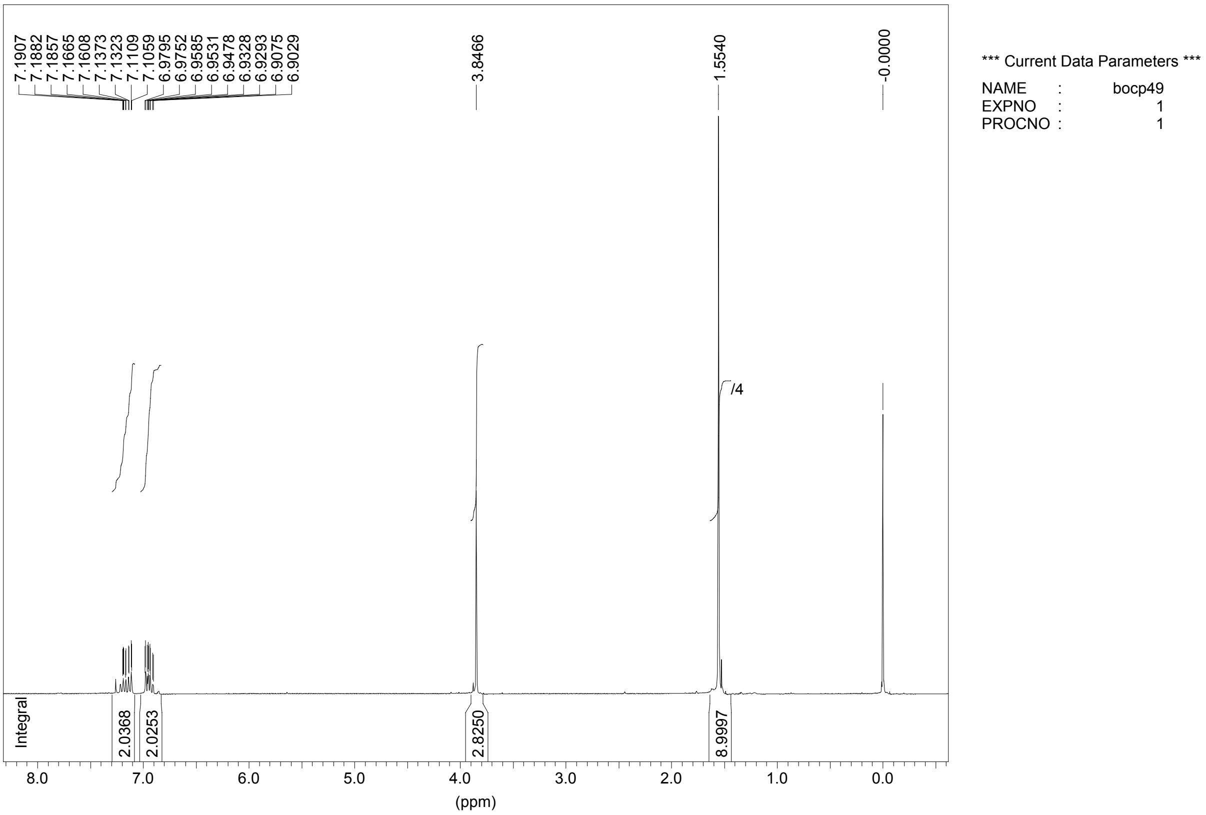

OH
OCH3
D
C
B
O
O
O

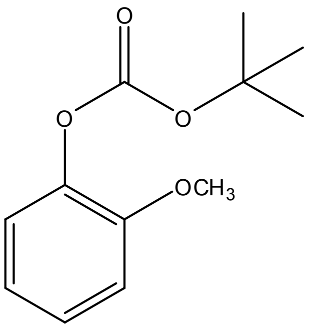
Sample **11b**


7.2665
7.0577
7.0311
6.8293
6.8231
6.8089
6.8026
6.7822
6.7760
4.2784
4.2541
4.2298
3.8444
2.9708
2.9465
2.9221
1.6043
1.5494
1.4764
-0.0000
*** Current Data Parameters ***
NAME : bocp43
EXPNO : 1
PROCNO : 1
Integral
1.0906
2.0000
2.0665
2.8262
2.0855
0.2387
8.5454
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)

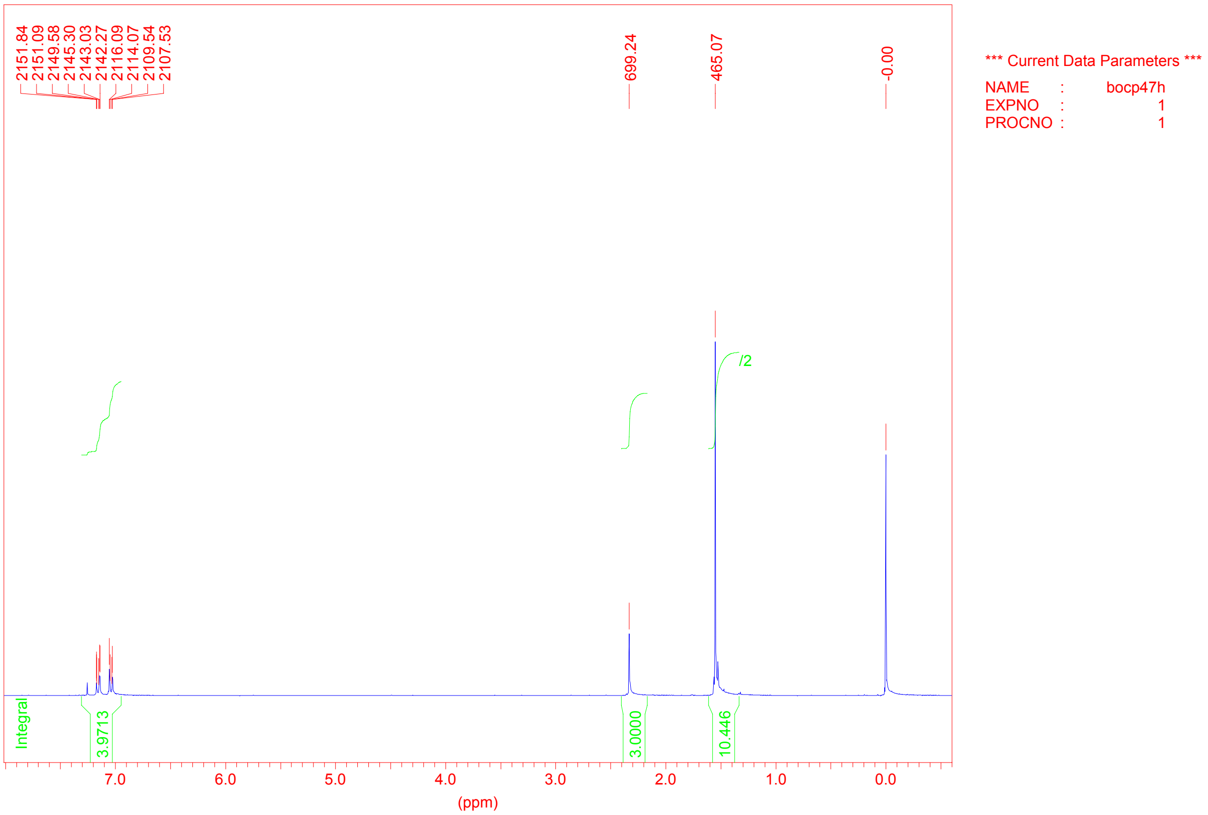

O
O
O
D
OCH3
C
B
O
O
O

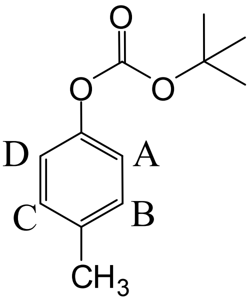
Sample **12**


7.1907
7.1882
7.1857
7.1665
7.1608
7.1373
7.1323
7.1109
7.1059
6.9795
6.9752
6.9585
6.9531
6.9478
6.9328
6.9293
6.9075
6.9029
3.8466
1.5540
-0.0000
/4
Integral
2.0368
2.0253
2.8250
8.9997
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
*** Current Data Parameters ***
NAME : bocp49
EXPNO : 1
PROCNO : 1

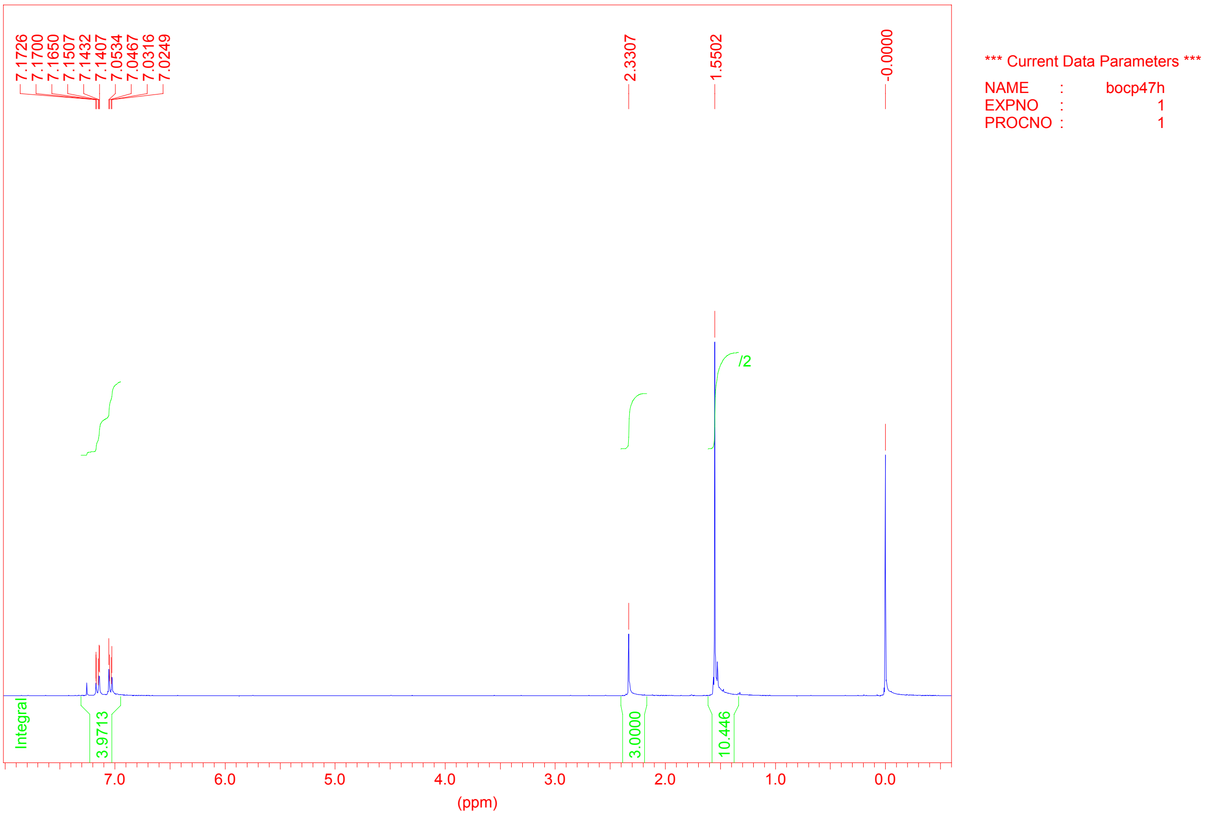

O
O
O
OCH3

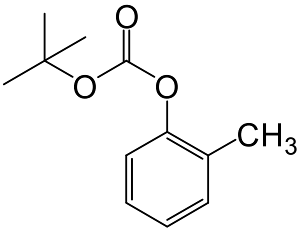
Sample **13**


2151.84
2151.09
2149.58
2145.30
2143.03
2142.27
2116.09
2114.07
2109.54
2107.53
699.24
465.07
-0.00
/2
Integral
3.9713
3.0000
10.446
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)
*** Current Data Parameters ***
NAME : bocp47h
EXPNO : 1
PROCNO : 1


O
O
O
D
A
C
B
CH3

Sample **14**


7.1726
7.1700
7.1650
7.1507
7.1432
7.1407
7.0534
7.0467
7.0316
7.0249
2.3307
1.5502
-0.0000
*** Current Data Parameters ***
NAME : bocp47h
EXPNO : 1
PROCNO : 1
/2
Integral
3.9713
3.0000
10.446
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)


O
O
O
CH3