Supporting Information

for

A New and Versatile One-Pot Strategy to synthesize alpha-Bromoketones from Secondary Alcohols Using Ammonium Bromide and Oxone

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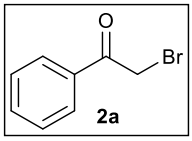
Table of contents

1. Spectroscopic data of all products:

2-Bromo-1-(1-phenyl)ethanone (2a)[1]

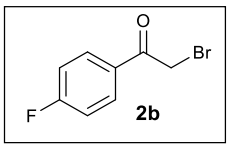


m.p.49-50°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.01-7.97 (m, 2H), 7.64-7.59 (m, 1H), 7.53-7.48 (m, 2H), 4.46 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 191.20, 133.89, 128.86, 128.80, 30.90.

2-Bromo-1-(4-fluorophenyl)ethanone (2b)[10]

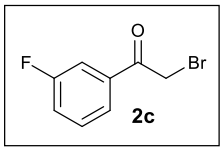


m.p.46-47°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.06-8.01 (m, 2H), 7.20-7.14 (m, 2H), 4.41 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 189.80, 166.14 (d, J = 256 Hz), 131.71 (d, J = 9.54 Hz), 130.33 (d, J = 3.70 Hz), 116.08 (d, J = 22.74 Hz), 30.39.

2-Bromo-1-(3-fluorophenyl)ethanone (2c)[4a]



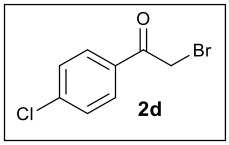
Yellow liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.79-7.76 (m, 2H), 7.70-7.66 (m, 1H), 7.52-7.46 (m, 1H), 7.35-7.29 (m, 1H), 4.42 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 190.10, 162.84 (d, J = 248.85 Hz), 135.93 (d, J = 6.35 Hz), 130.54 (d, J = 7.26 Hz), 124.70 (d, J = 2.72 Hz), 121.04 (d, J = 21.79 Hz), 115.68 (d, J = 22.70 Hz), 30.44.

IR (KBr): ν_{Max} 3075, 2944, 1688, 1588, 1485, 1443, 1394, 1278, 1233, 1197, 1147, 1108, 1025, 999, 876, 793, 750, 700, 676, 619 and 527 cm^{-1}.

2-Bromo-1-(4-chlorophenyl)ethanone (2d)[3]

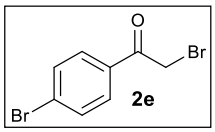


m.p.94-95°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.93 (d, J = 8.6 Hz, 2H), 7.47 (d, J = 8.6 Hz, 2H), 4.41 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 190.17, 140.51, 132.21, 130.34, 129.21, 30.33.

2-Bromo-1-(4-bromophenyl)ethanone (2e)[2]

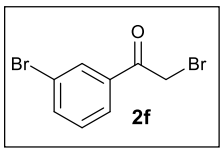


m.p.108-109°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.85-7.82 (m, 2H), 7.66-7.60 (m, 2H), 4.41 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 190.29, 132.52, 132.10, 130.31, 129.18, 30.40.

2-Bromo-1-(3-bromophenyl)ethanone (2f)[5]

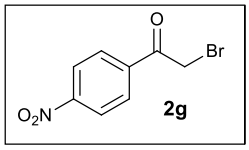


m.p.49-50°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.12 (t, J = 1.83 Hz, 1H), 7.92-7.89 (m, 1H), 7.75-7.72 (m, 1H), 7.38 (t, J = 7.9 Hz, 1H), 4.42 (s, 2H).

^{13}CNMR (75 MHz, $CDCl_3$): δ (ppm) = 189.97, 136.77, 135.62, 131.88, 130.38, 127.43, 123.16, 30.35.

2-Bromo-1-(4-nitrophenyl)ethanone (2g)[5]

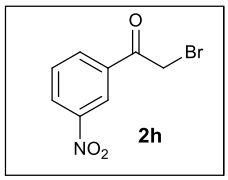


m.p.91-92°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.37-8.33 (m, 2H), 8.18-8.14 (m, 2H), 4.46 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 189.85, 150.71, 138.34, 130.05, 124.03, 30.04.

2-Bromo-1-(3-nitrophenyl)ethanone (2h)[5]

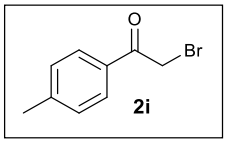


m.p.94-95°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 8.82 (t, J = 1.95 Hz, 1H), 8.49-8.46 (m, 1H), 8.34-8.31 (m, 1H), 7.74 (t, J = 8.06 Hz, 1H), 4.48 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 189.31, 148.51, 135.12, 134.43, 130.17, 128.11, 123.83, 29.84.

2-Bromo-1-(4-methylphenyl)ethanone (2i)[3]

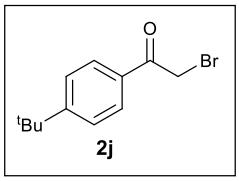


m.p.50-51°C

^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.88 (d, J = 8.08 Hz, 2H), 7.29 (d, J = 7.79 Hz, 2H), 4.43 (s, 2H), 2.43 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 190.91, 144.97, 131.44, 129.52, 129.02, 30.89, 21.73.

2-Bromo-1-(4-*tert*-phenyl)ethanone (2j)[3]

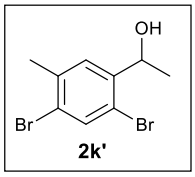


m.p.52-53°C

^{1}H NMR (300 MHz, $CDCl_3$): δ (ppm) = 7.93 (d, J = 8.52 Hz, 2H), 7.51 (d, J = 8.52 Hz, 2H), 4.44 (s, 2H), 1.35 (s, 9H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 190.90, 157.89, 131.35, 128.90, 125.82, 35.23, 31.00, 30.86.

1-(2,4-dibromo-5-methylphenyl)ethanol (2k')

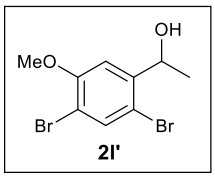


^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.66 (s, 1H), 7.18 (s, 1H), 5.18-5.14 (m, 1H), 3.91 (s, 3H), 2.04 (s, 1H), 1.46 (d, J = 6.4 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 155.77, 145.21, 135.99, 111.53, 110.79, 109.70, 69.10, 56.43, 23.70.

HR-MS (EI) m/z calcd for $C_9H_{10}Br_2O_1$, 291.90984; Found 291.90784.

1-(2,4-dibromo-5-methoxyphenyl)ethanol (2l')

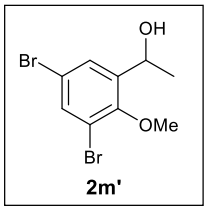


^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.66 (s, 1H), 7.18 (s, 1H), 5.18-5.15 (m, 1H), 3.91 (s, 3H), 2.07 (brs, 1H), 1.46 (d, J = 6.40 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 155.75, 145.22, 135.99, 111.53, 110.79, 109.70, 69.10, 56.43, 23.70.

HR-MS (EI) m/z calcd for $C_9H_{10}Br_2O_2$, 307.90476; Found 307.90299.

1-(3,5-dibromo-2-metoxyphenyl)ethanol (2m')

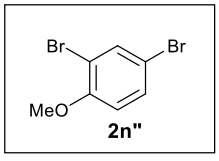


^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 7.61 (d, J = 2.4 Hz, 1H), 7.56 (d, J = 2.4 Hz, 1H), 5.18-5.13 (m, 1H), 3.87 (s, 3H), 1.62 (s, 1H), 1.49 (d, J = 6.40 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 153.24, 142.28, 134.69, 128.88, 117.87, 117.72, 65.15, 61.44, 24.17.

HR-MS (EI) m/z calcd for $C_9H_{10}Br_2O_2$, 307.90476; Found 307.90376.

2,4-dibromo-1-methoxybenzene (2n")[6]

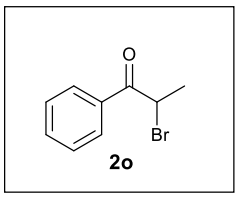


m.p.62-63°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.66 (d, J = 2.44 Hz, 1H), 7.37 (dd, J = 8.80, 2.44 Hz, 1H), 6.76 (d, J = 8.80 Hz, 1H), 3.87 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 155.18, 135.41. 131.18, 113.07, 112.84, 112.50, 56.36.

2-Bromo-1-phenyl-1-propanone (2o)[3]

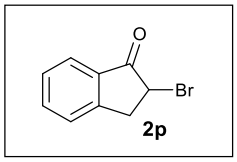


m.p.109-110°C

^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.04-8.01 (m, 2H), 7.61-7.57 (m, 1H), 7.51-7.47 (m, 2H), 5.30 (q, J = 6.5 Hz, 1H), 1.91 (d, J = 6.7 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 193.29, 134.00, 133.63, 128.87, 128.70, 41.42, 20.10.

2-Bromo-1-indanone (2p)[3]

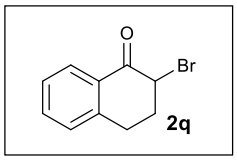


m.p.37-38°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.83 (d, J = 7.58 Hz, 1H), 7.67 (t, J = 7.94 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 4.66 (dd, J = 3.17, 7.45 Hz, 1H), 3.84 (dd, J = 7.45, 18.09 Hz, 1H), 3.44 (dd, J = 3.17, 18.09 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 199.52, 151.04, 135.90, 133.46, 128.21, 126.37, 124.98, 44.03, 37.91.

2-Bromo-1-tetralone (2q)[9]

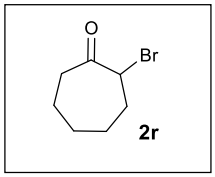


m.p.40-41°C

^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 8.08 (d, J = 7.93 Hz, 1H), 7.54-7.50 (td, 1.52, 7.62 Hz 1H), 7.36-7.27 (m, 2H), 4.73 (t, J = 4.42 Hz, 1H), 3.34-3.27 (m, 1H), 2.92 (dt, J = 4.42, 17.09 Hz,1H), 2.56-2.42 (m, 2H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 190.47, 142.92, 134.05, 129.83, 128.69, 128.56, 127.02, 50.41, 31.85, 26.06.

2-Bromocycloheptanone (2r)[7]

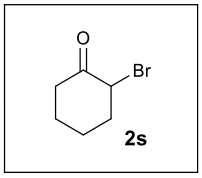


m.p.36-37°C

^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 4.38 (dd, J = 5.03, 9.46 Hz, 1H), 2.89-2.83 (m, 1H), 2.52-2.47 (m, 1H), 2.39-2.33 (m, 1H), 2.05-1.91 (m, 3H), 1.80-1.74 (m, 1H), 1.62-1.52 (m, 2H), 1.48-1.34 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$): δ (ppm) = 206.27, 53.69, 39.38, 35.00, 29.56, 26.80, 24.95.

2-Bromocyclohexanone (2s)[7]

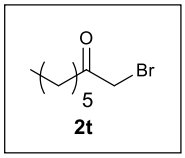


m.p.74-75°C

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.46-4.42 (m, 1H), 3.03-2.95 (m, 1H), 2.37-2.19 (m, 3H), 2.04-1.70 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 202.07, 53.35, 37.87, 36.74, 26.78, 22.06.

1-Bromo-2-octanone (2t)[8]

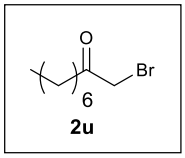


^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 3.88 (s, 2H), 2.64 (t, J = 7.47 Hz, 2H), 1.64-1.58 (m, 2H), 1.33-1.26 (m, 6H), 0.89 (t, J = 6.71 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 202.25, 39.84, 34.26, 31.47, 28.69, 23.81, 22.43, 13.98.

IR (KBr): ν_{Max} 2926, 2855, 1719, 1461, 1375, 1282, 1125, 1072 and 725 cm^{-1}.

1-Bromo-2-nonanone (2u)[4a,7b]



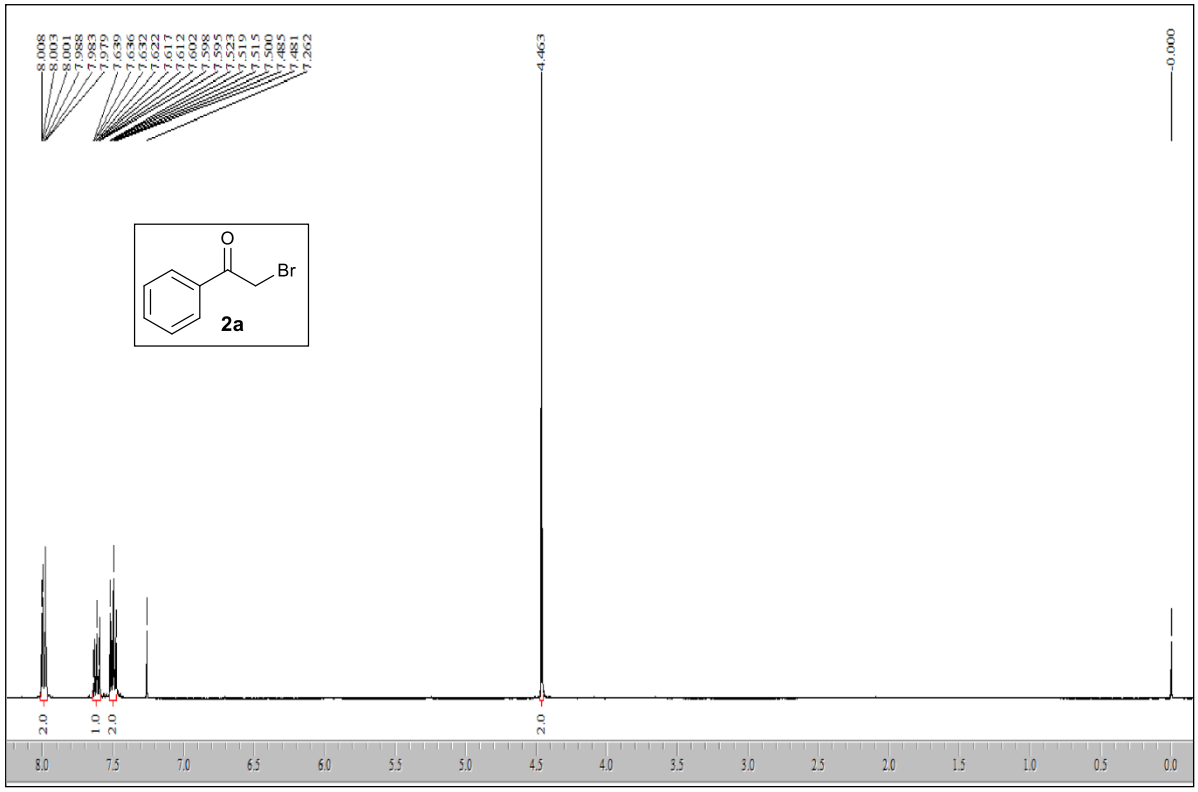
2u

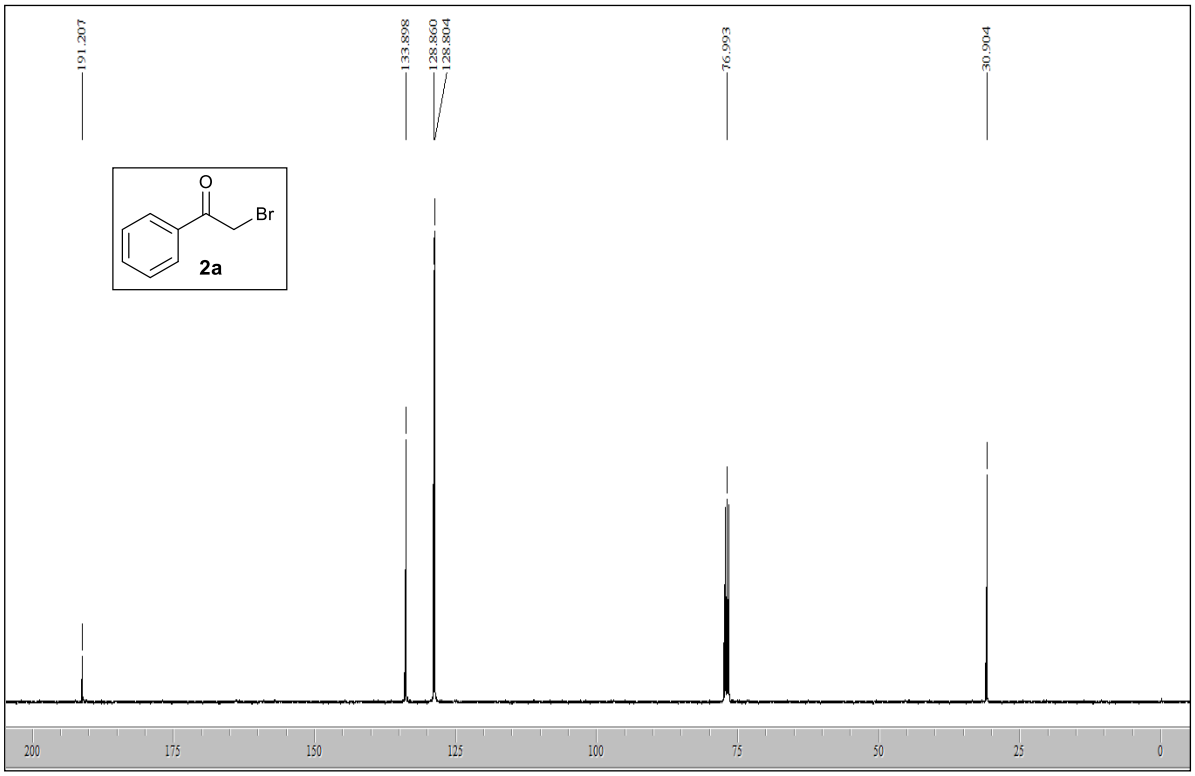
^{1}H NMR (500 MHz, $CDCl_3$): δ (ppm) = 3.88 (s, 2H), 2.65 (t, J = 7.32 Hz, 2H), 1.65-1.58 (m, 2H), 1.31-1.24 (m, 8H), 0.90-0.86 (m, 3H).

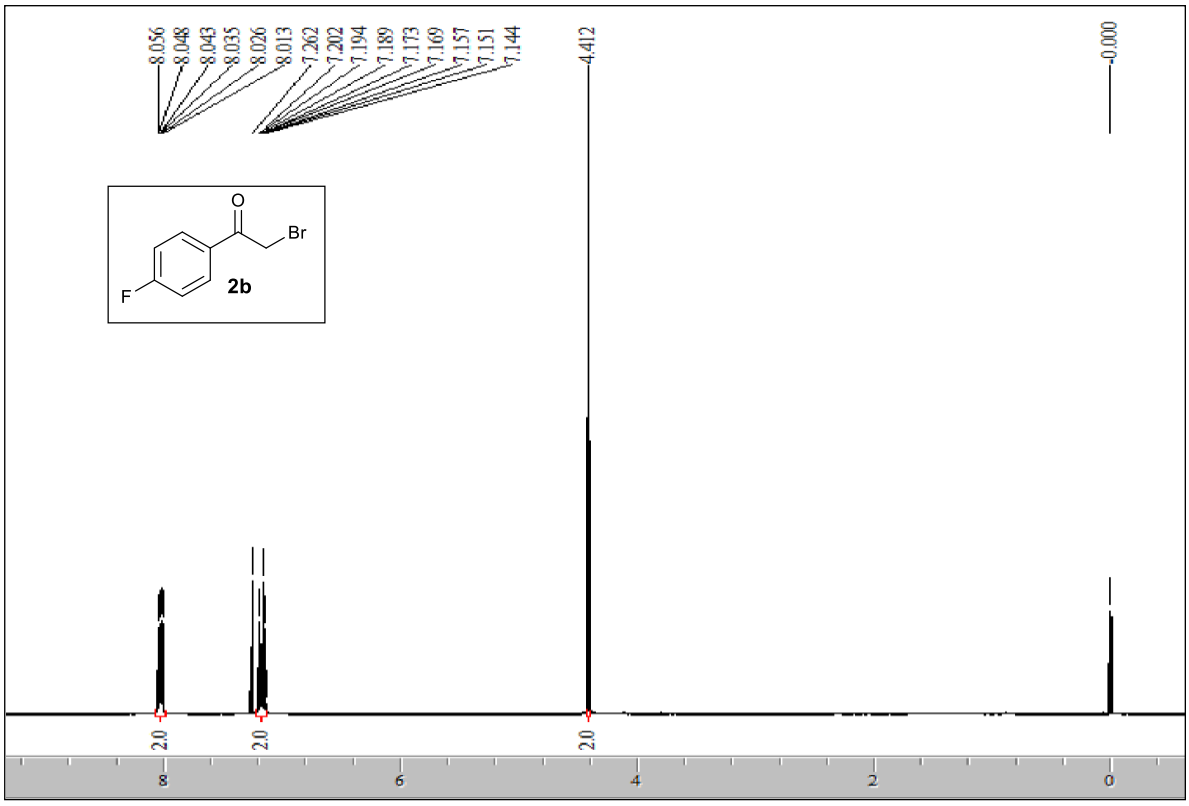
^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 202.26, 39.83, 34.27, 31.60, 28.95, 27.21, 23.84, 22.56, 14.03.

IR (KBr): ν_{Max} 2927, 2857, 1717, 1460, 1401, 1175, 1059 and 629 cm^{-1}.

2.Copies of ^{1}H and ^{13}C NMR spectra of all products:



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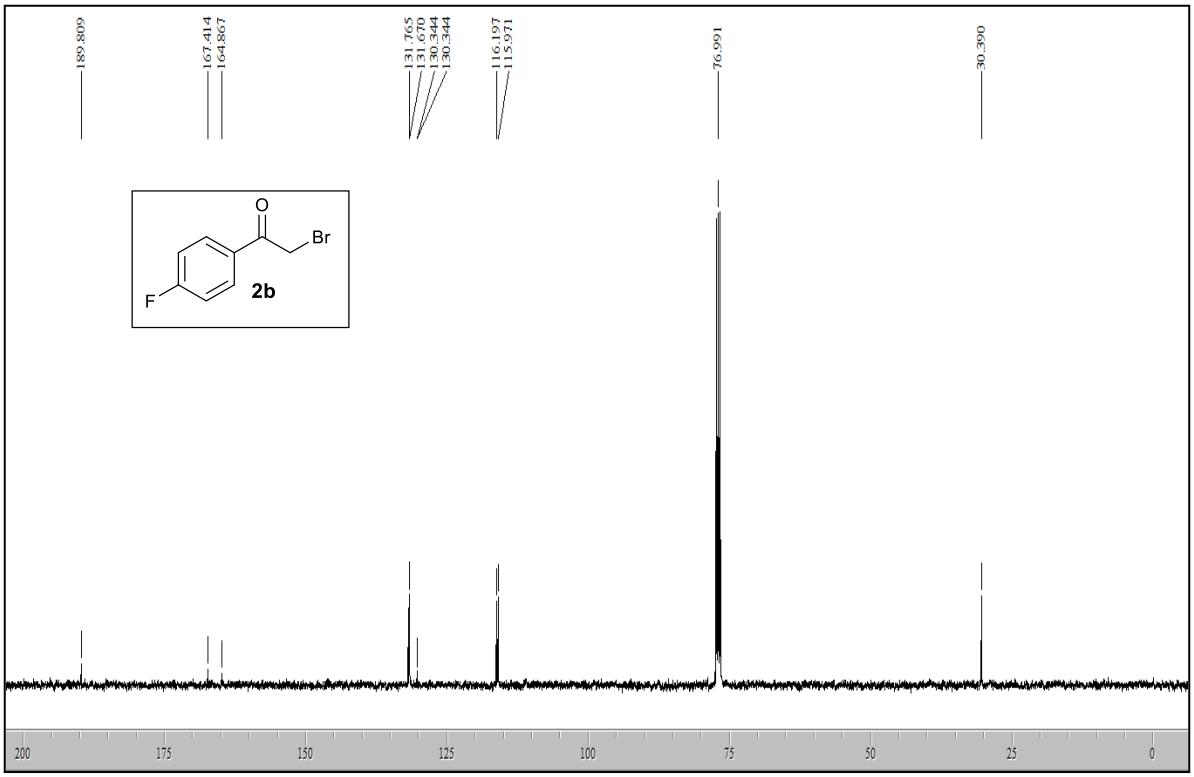
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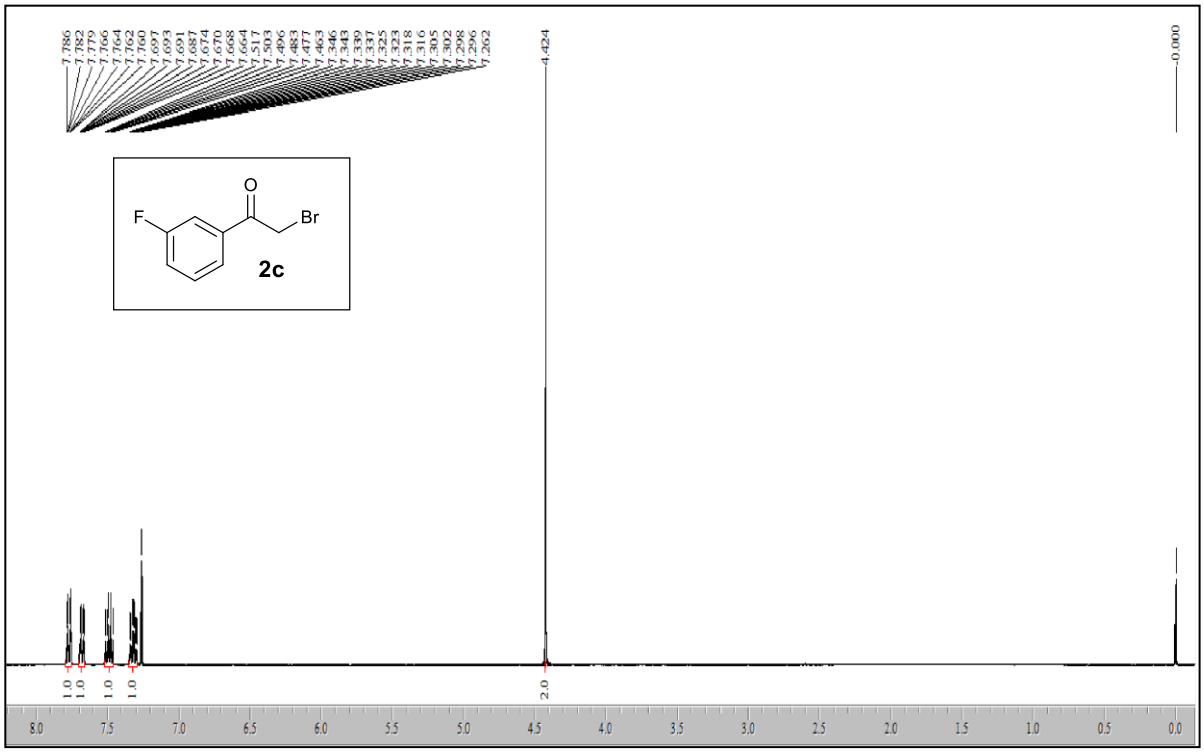
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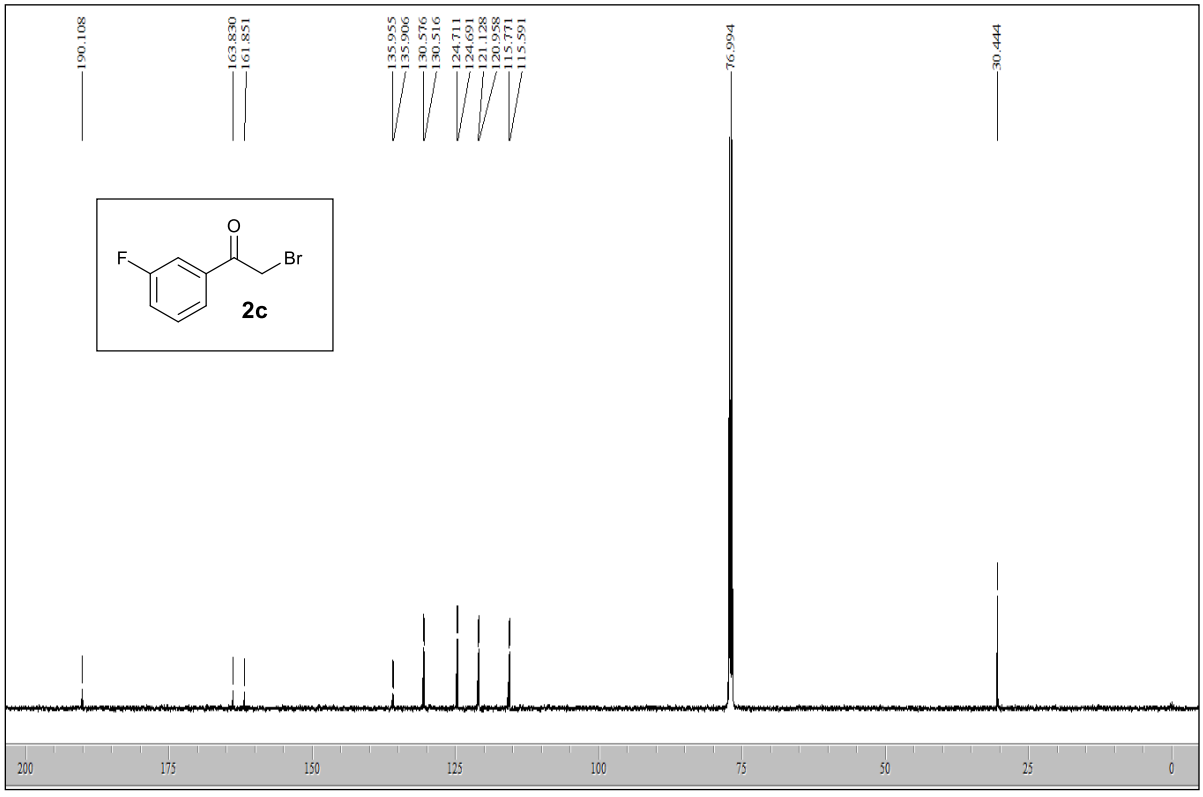
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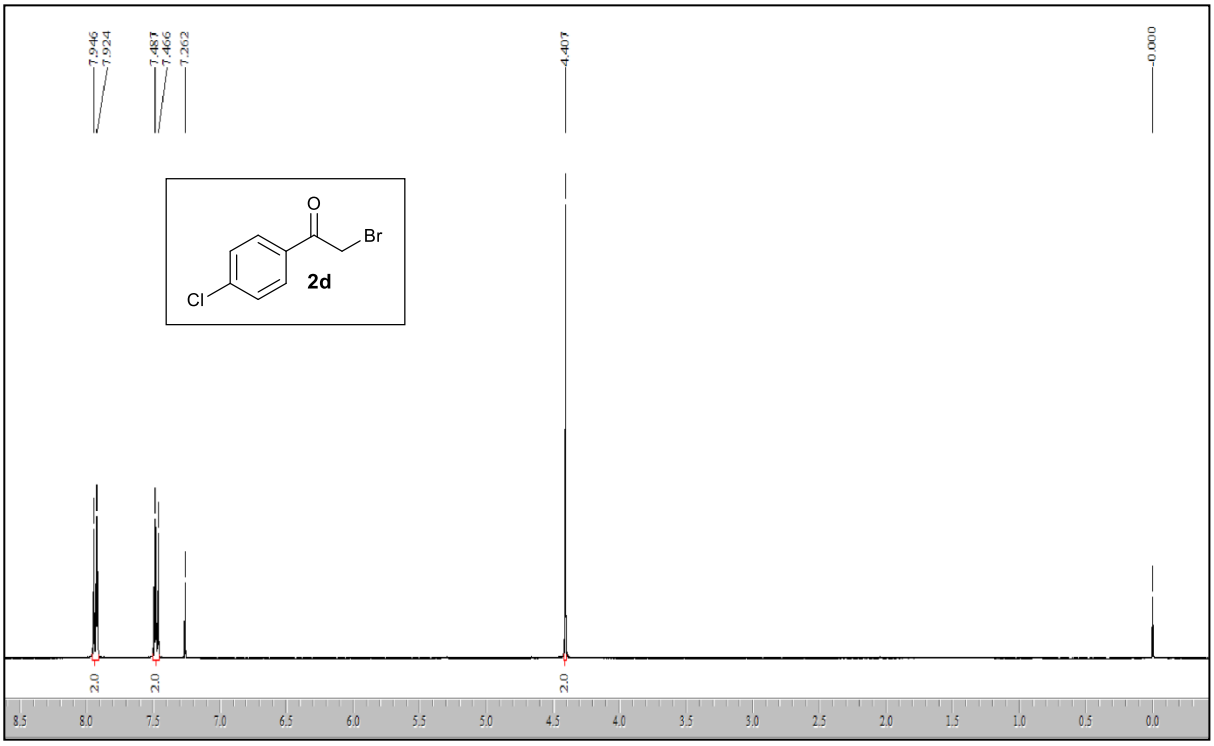
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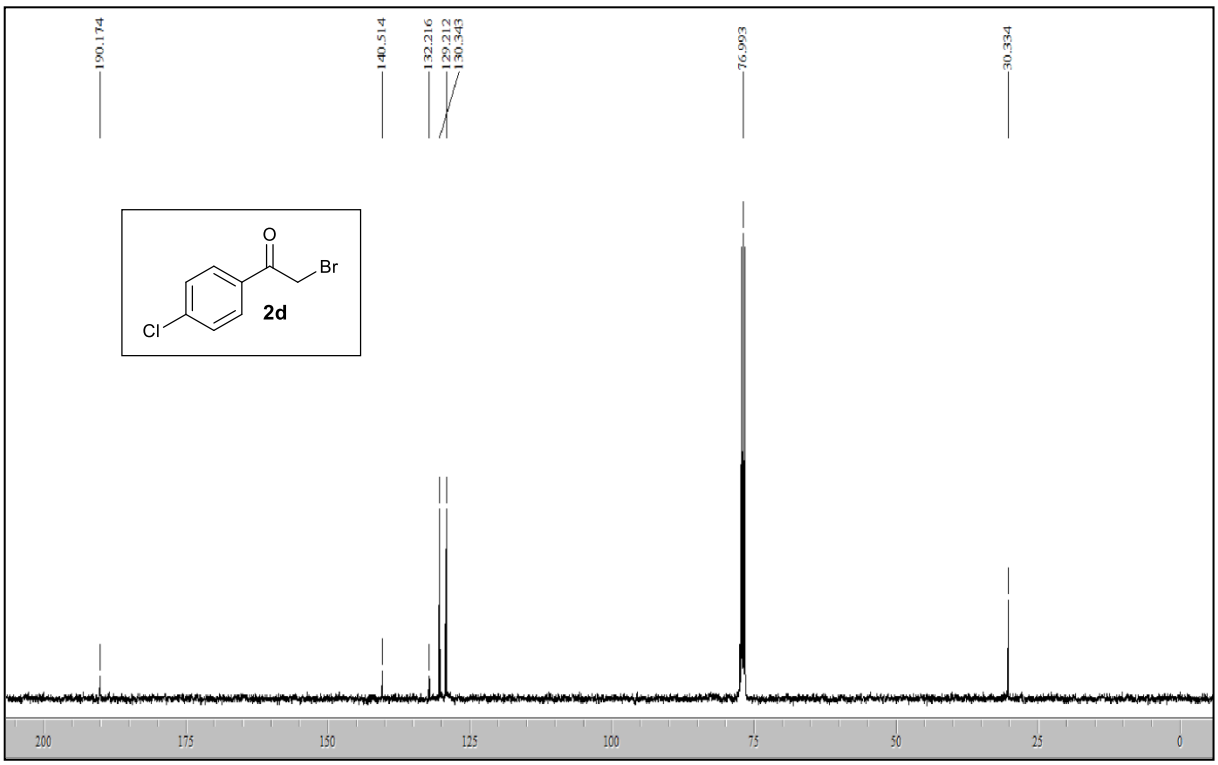
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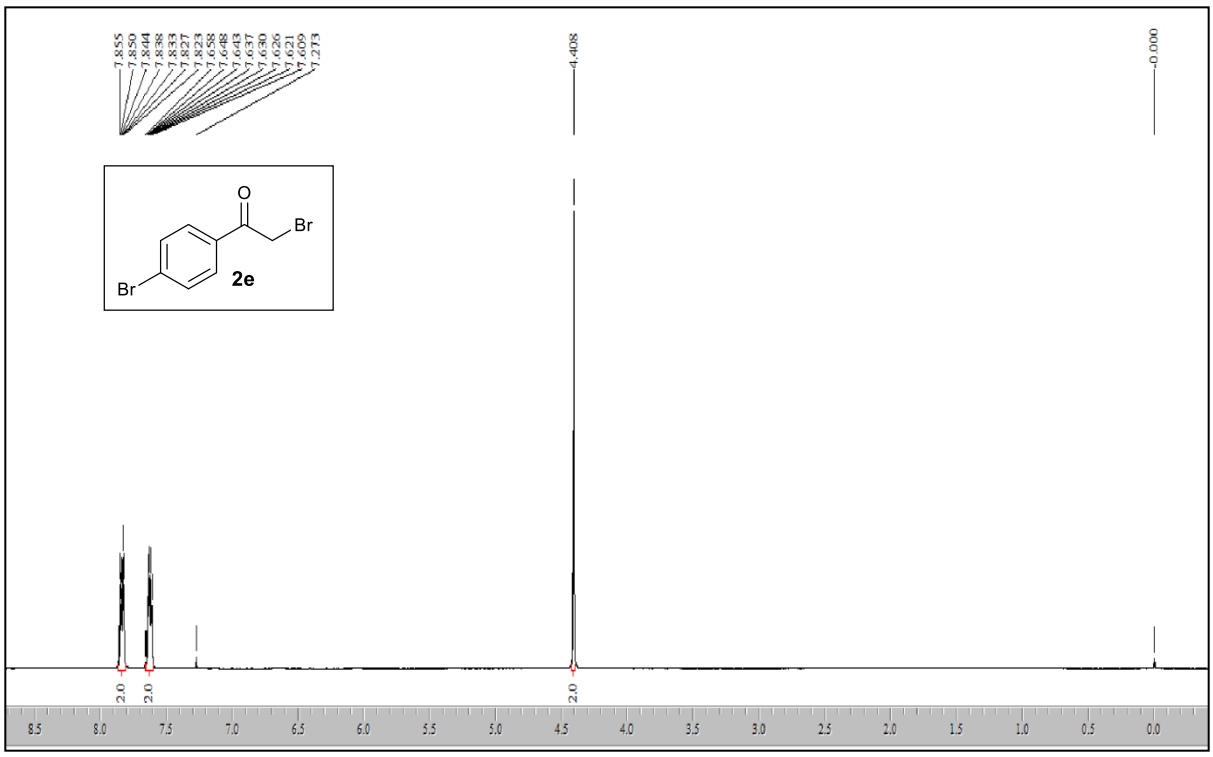
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Br
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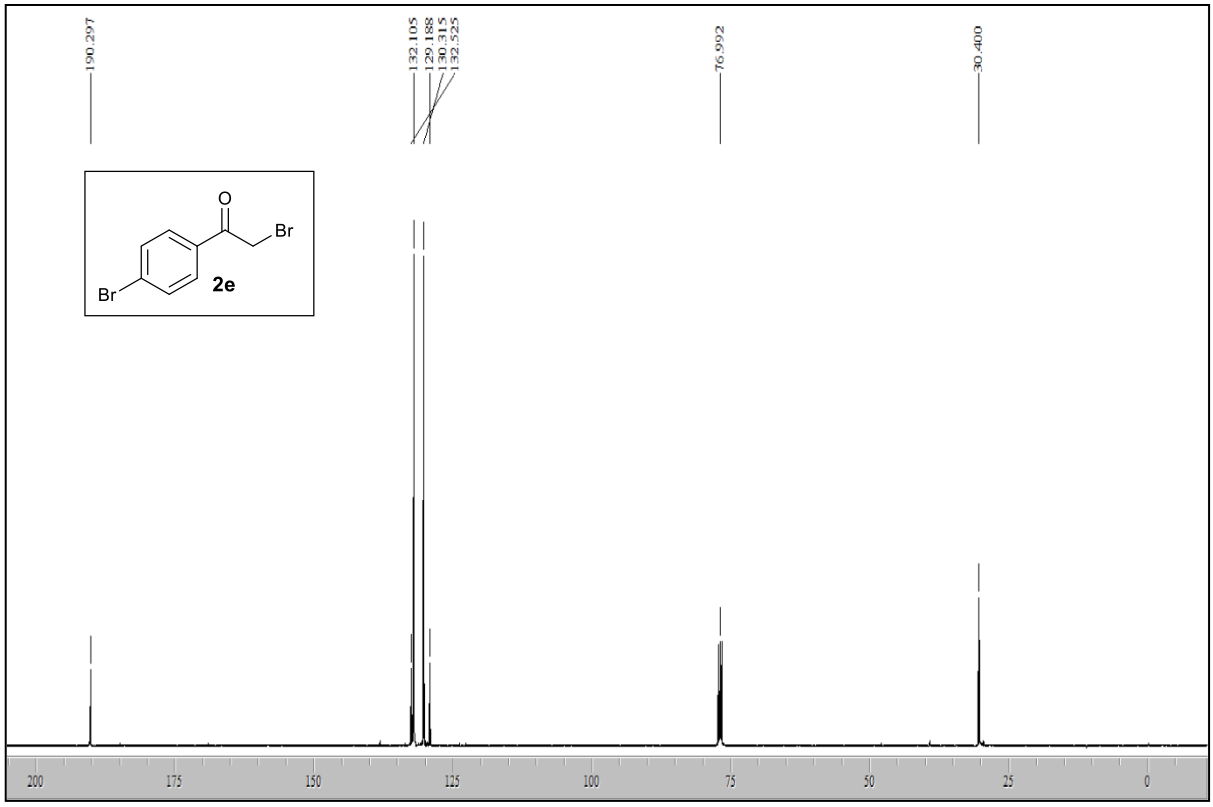
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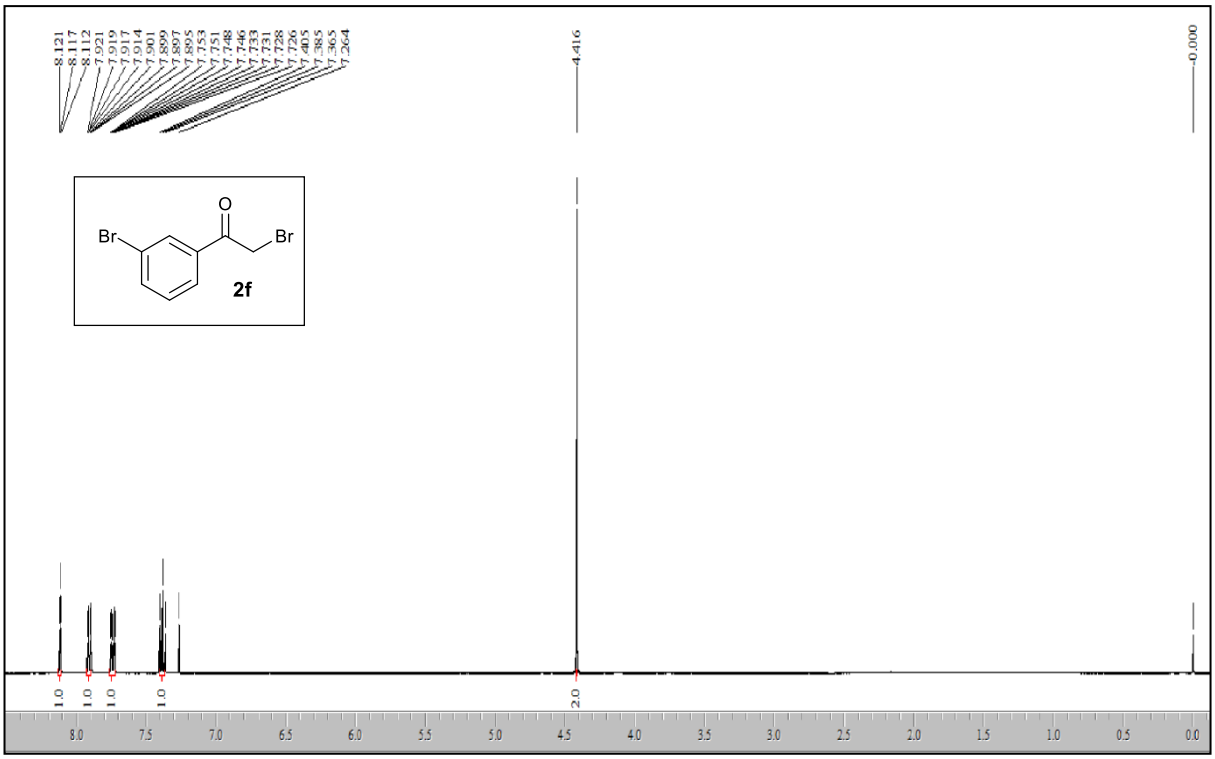
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7.728
7.726
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O
Br
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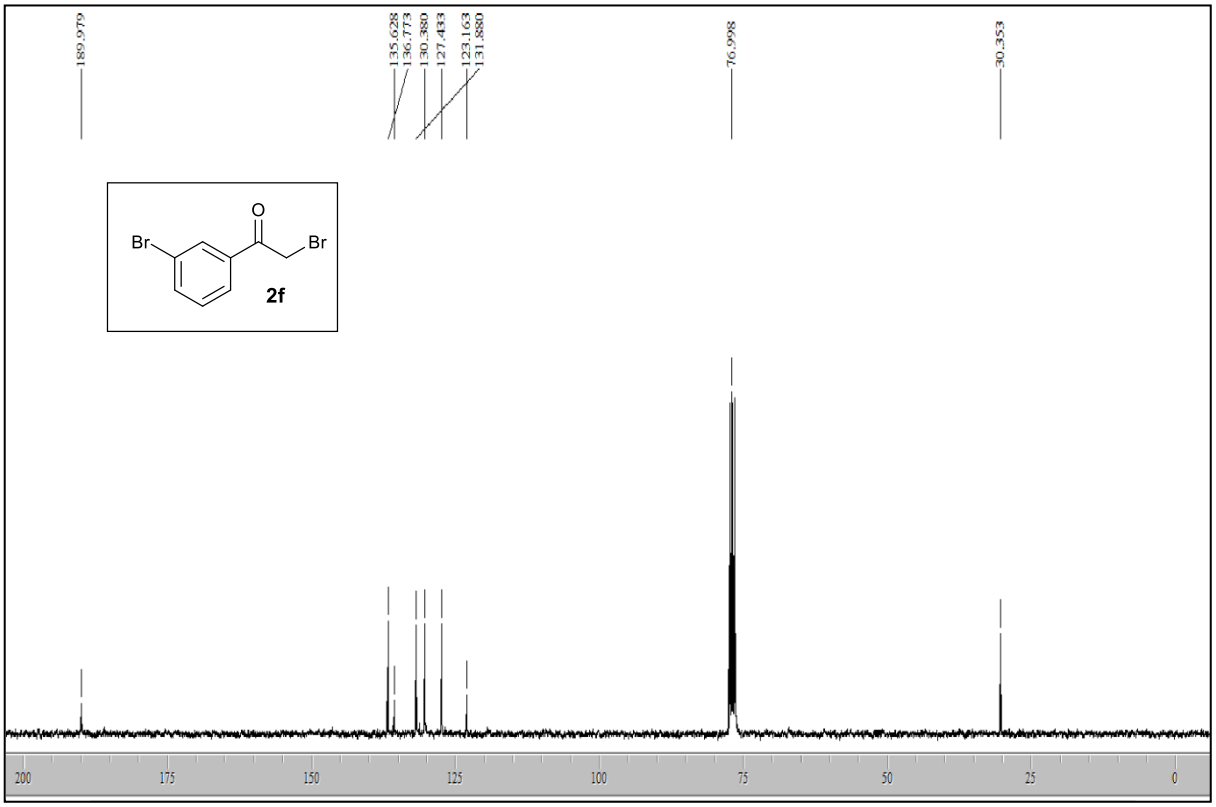
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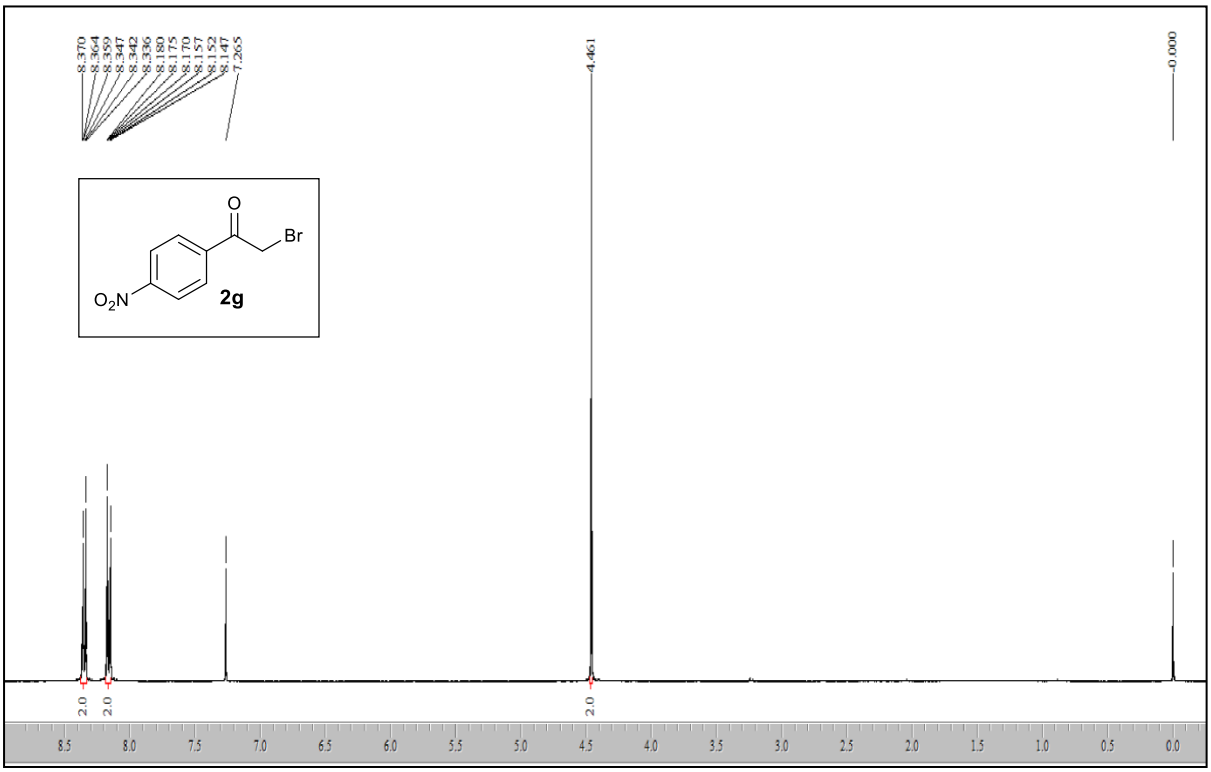
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2g
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2.0
2.0
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8.0
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7.0
6.5
6.0
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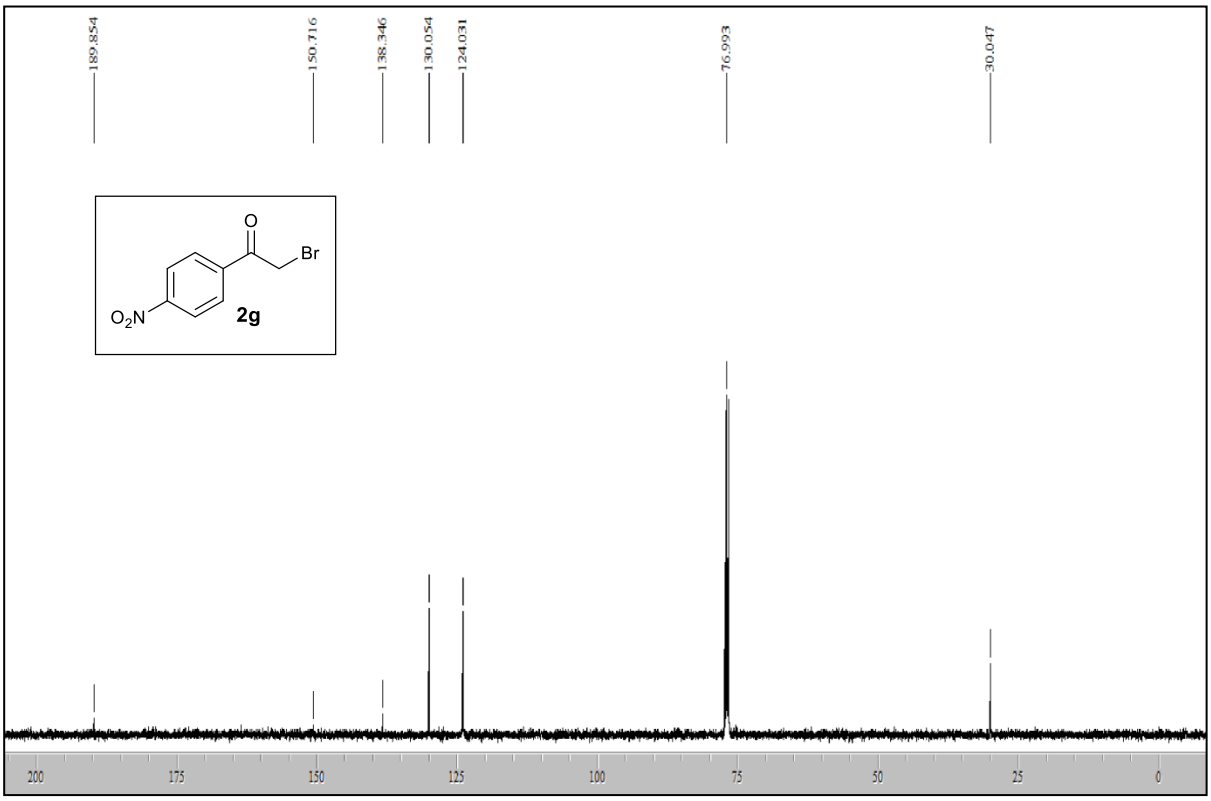
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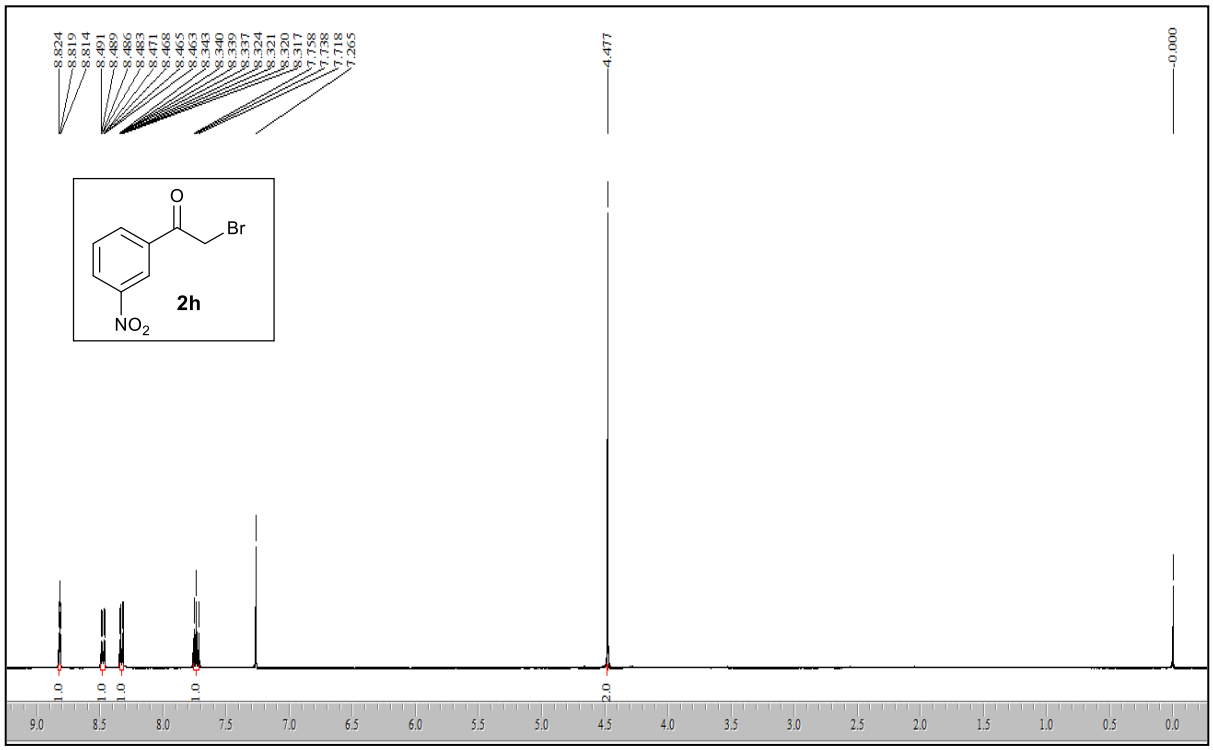
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7.718
7.265
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NO2
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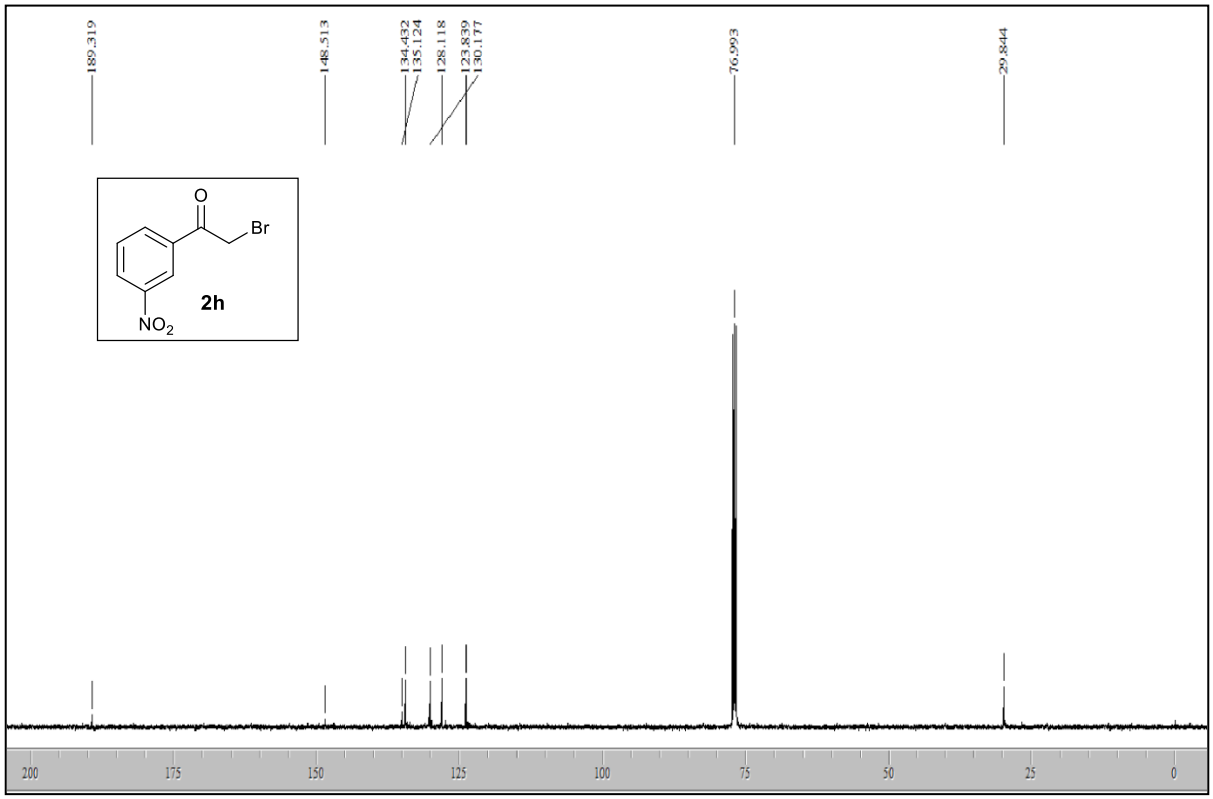
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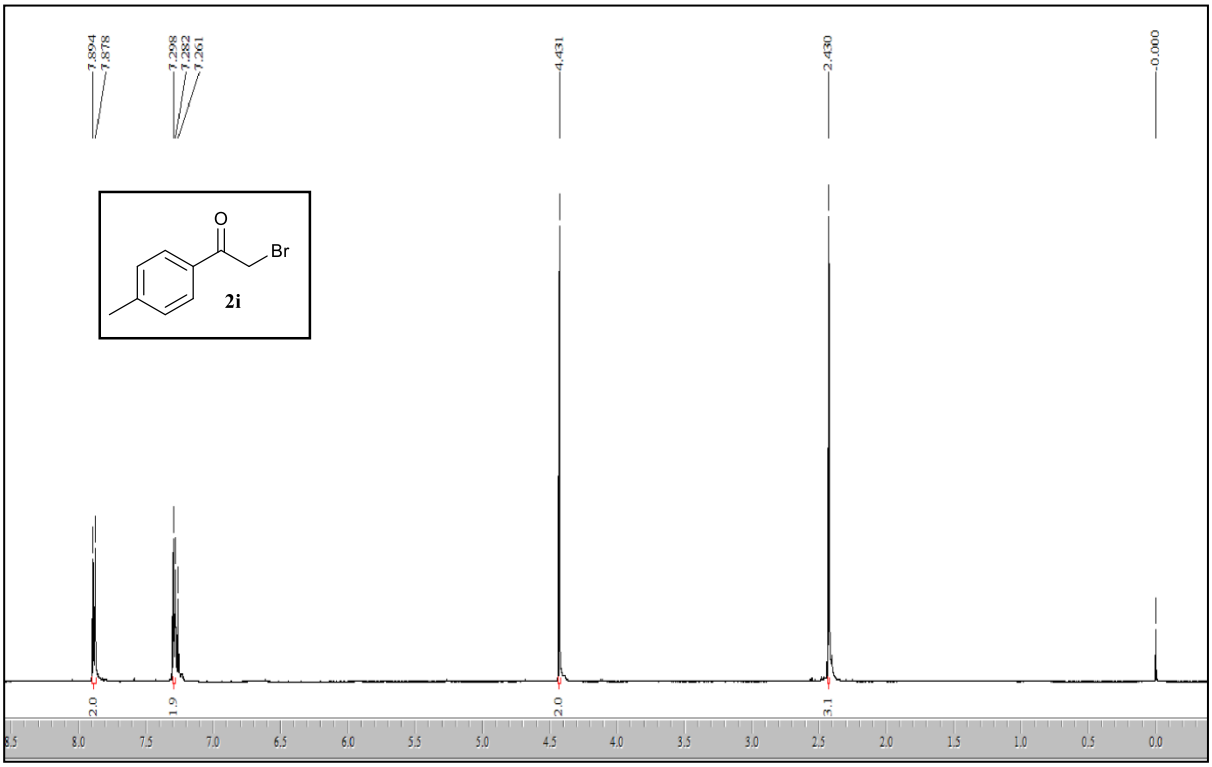
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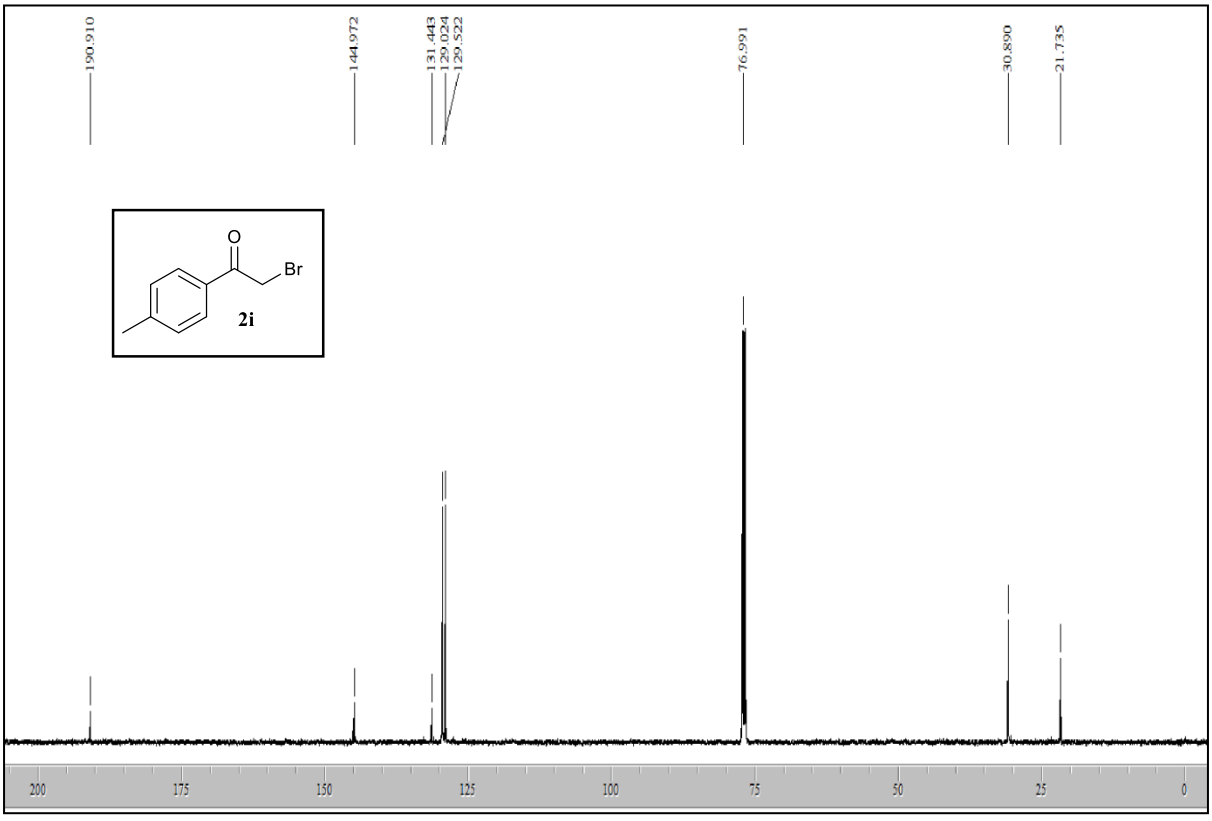
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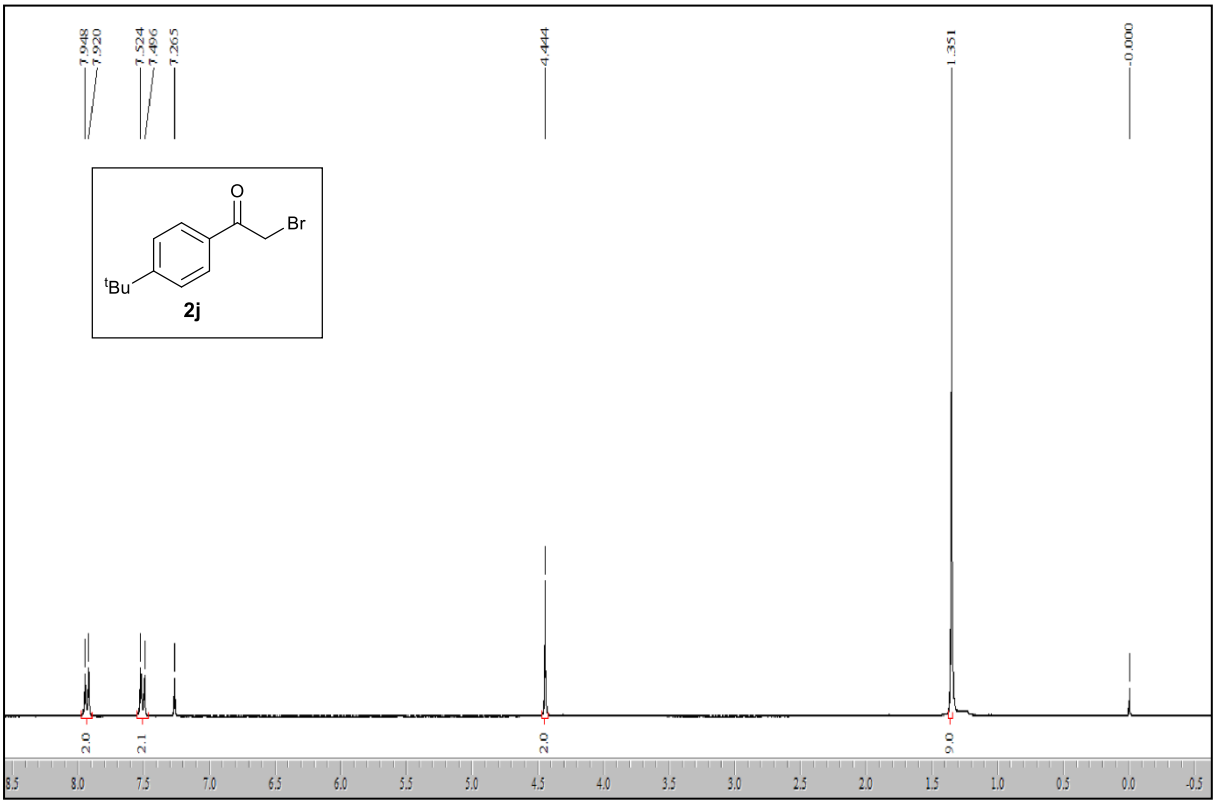
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tBu
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2.0
9.0
8.5
8.0
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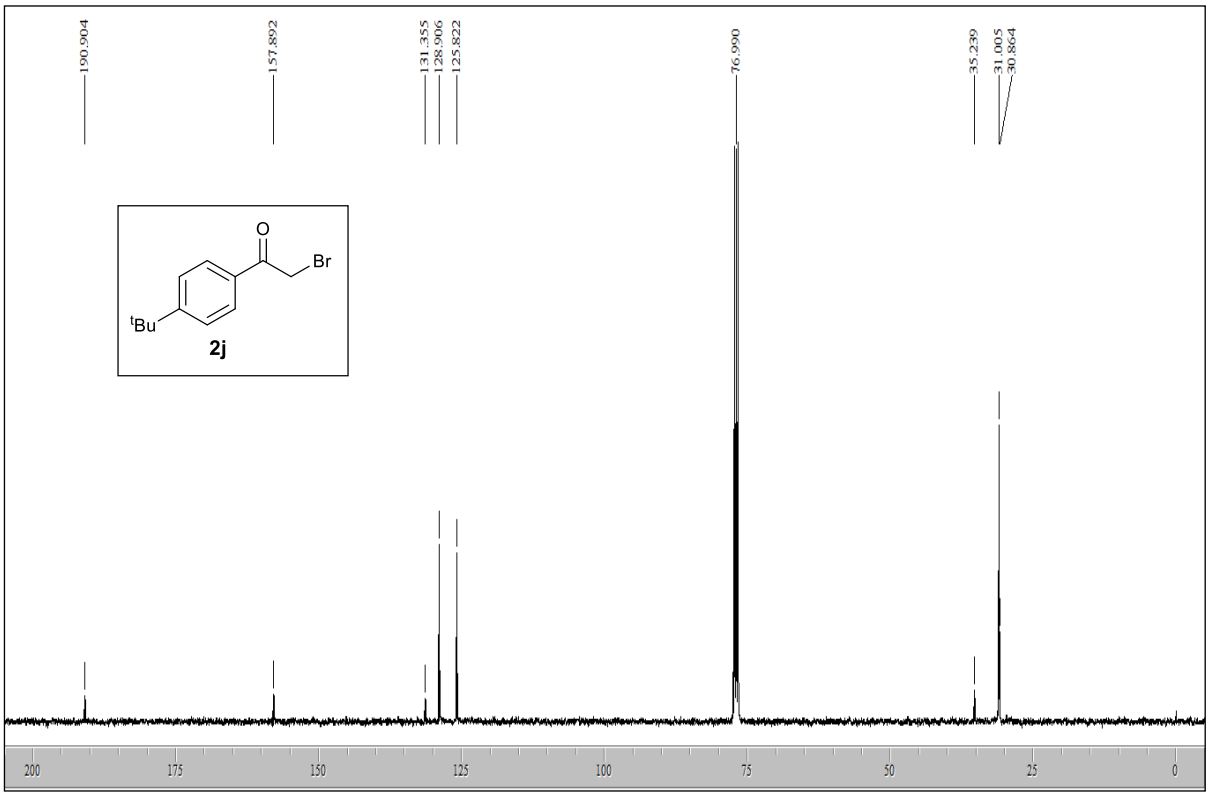
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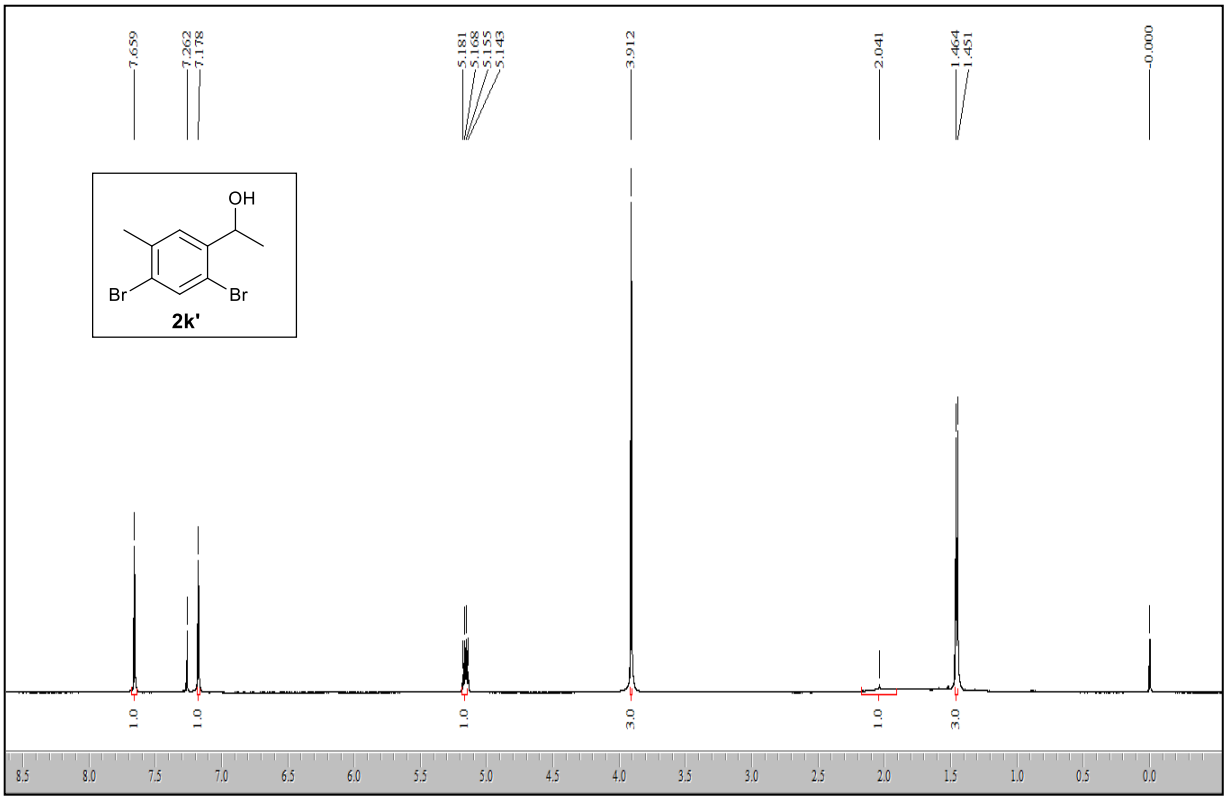
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Br
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1.0
1.0
3.0
1.0
3.0
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8.0
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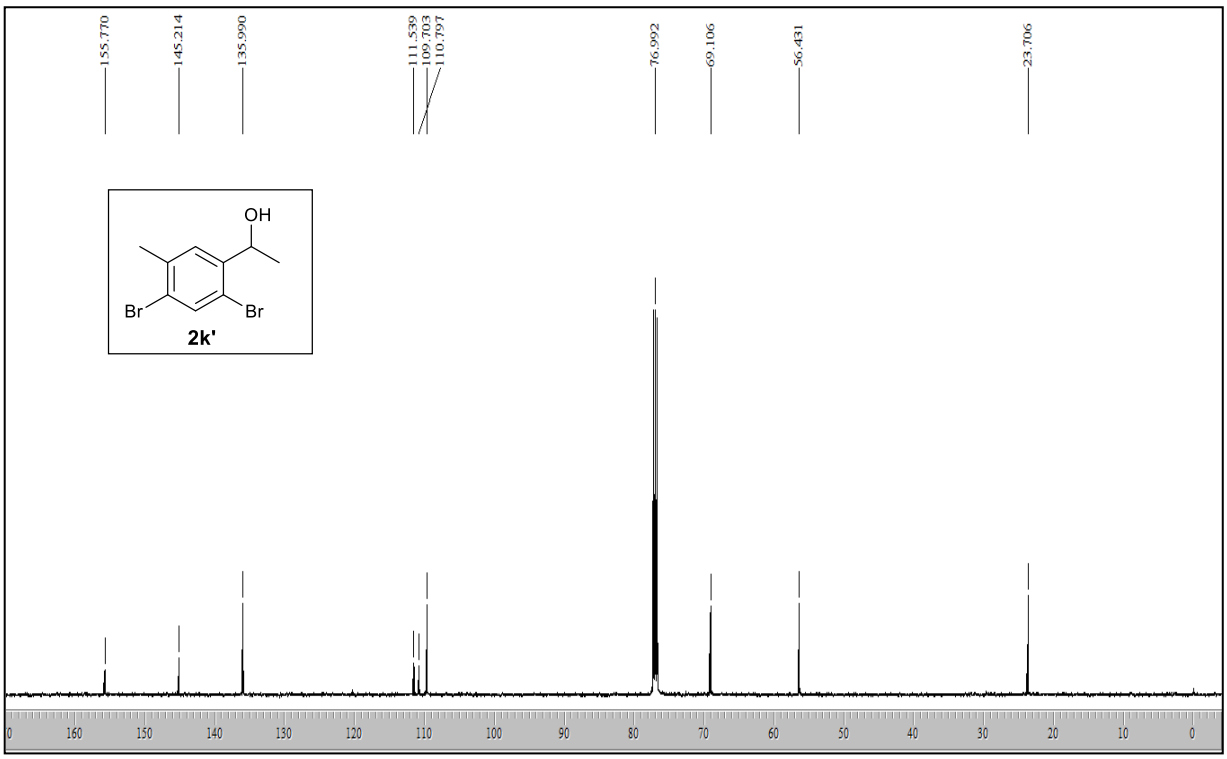
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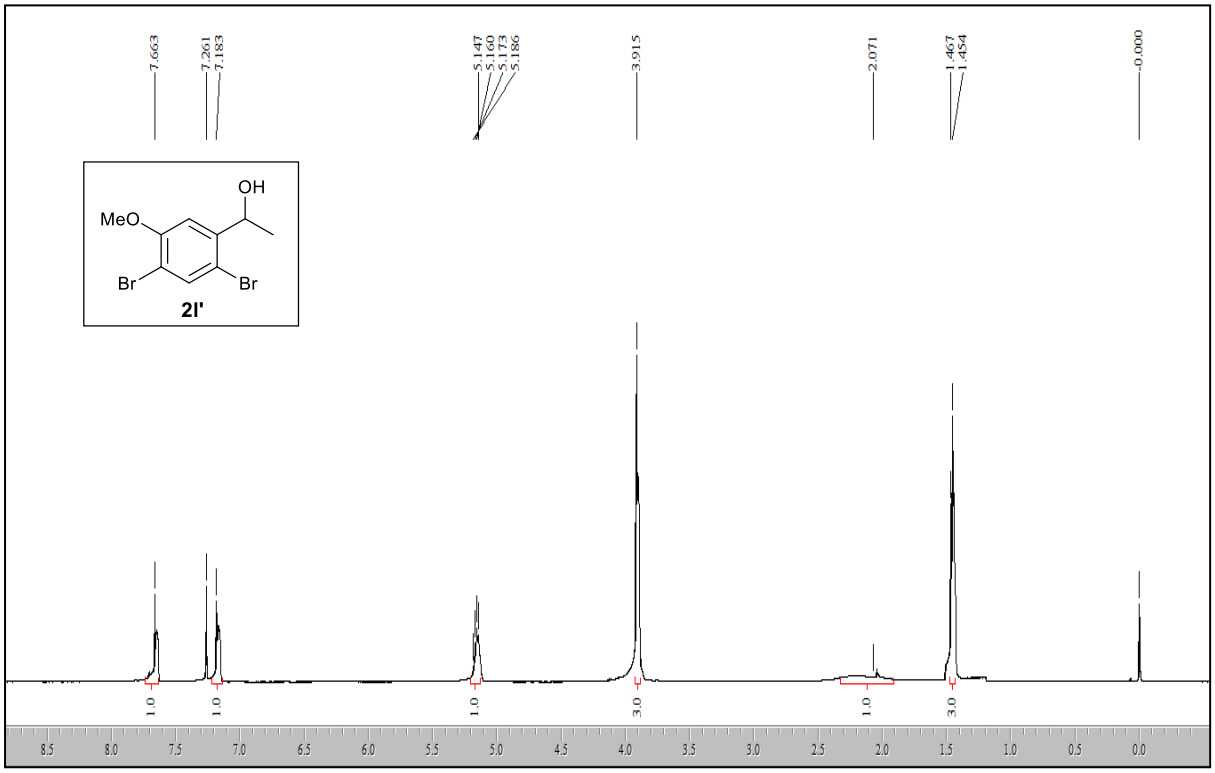
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MeO
Br
Br
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1.0
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6.0
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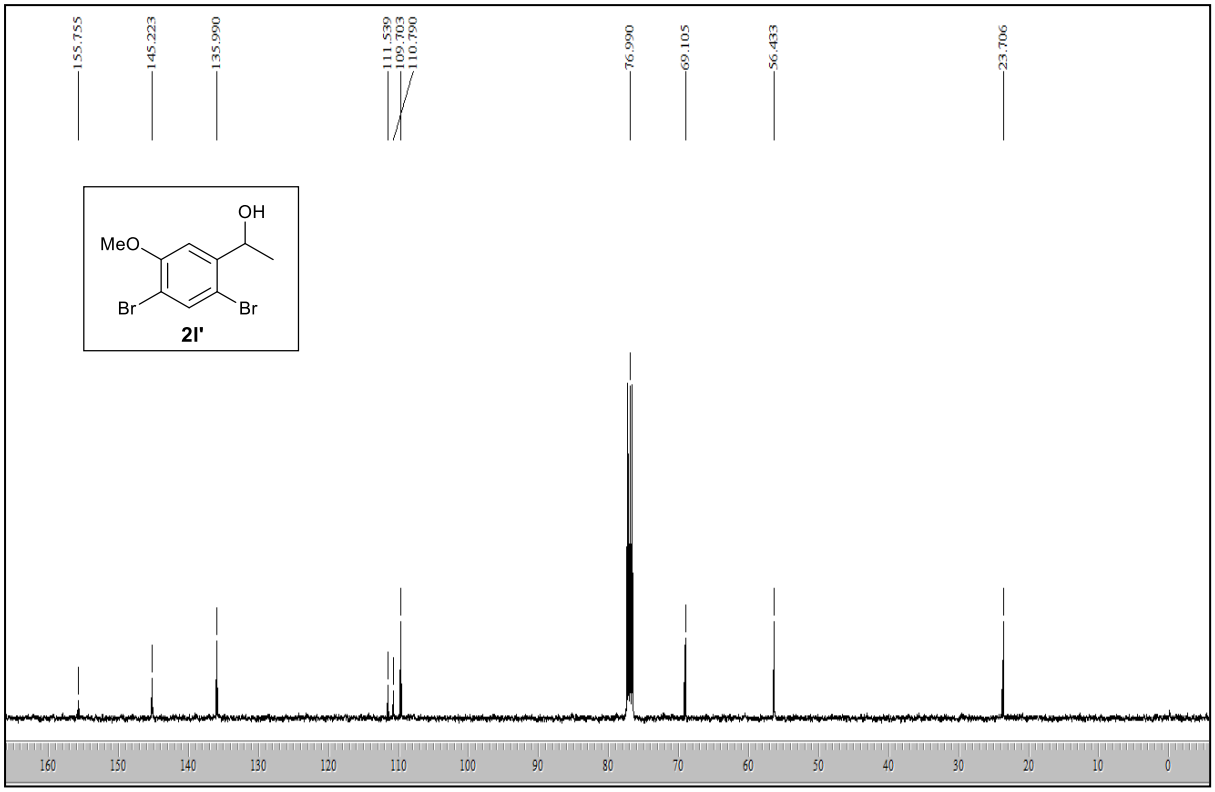
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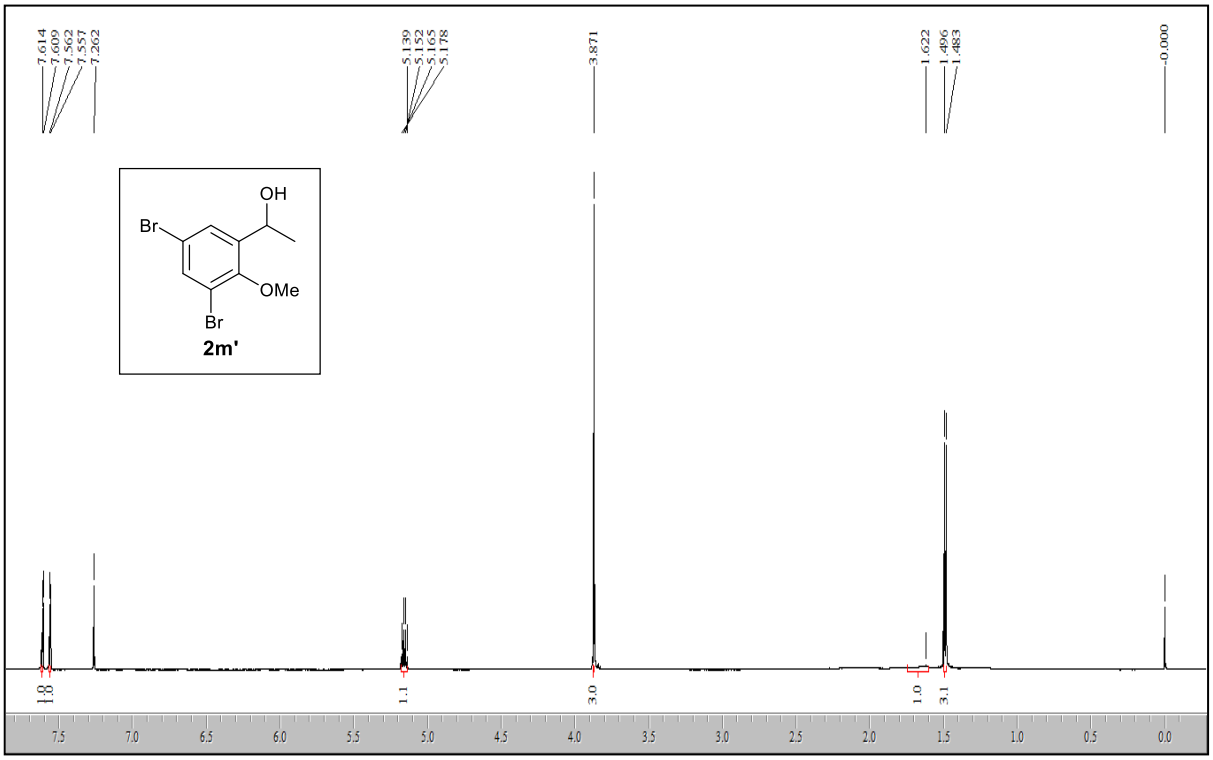
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OMe
Br
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1.0
3.1
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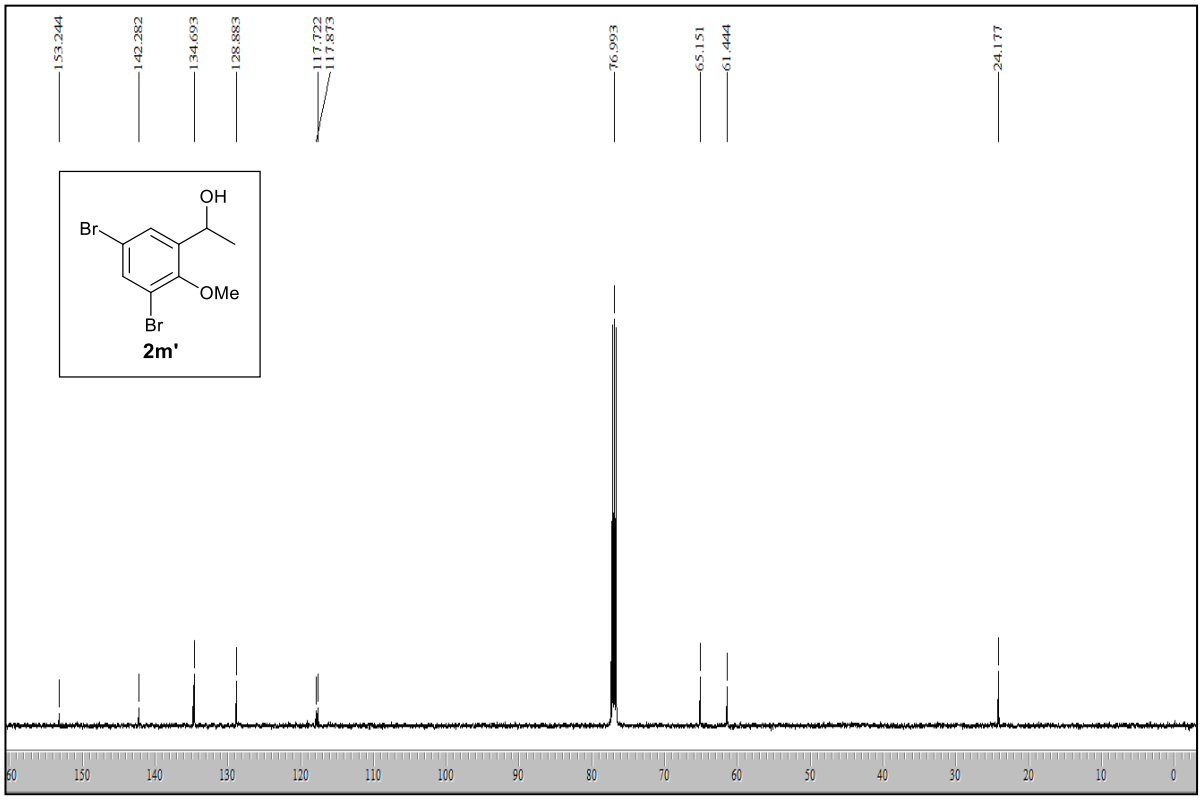
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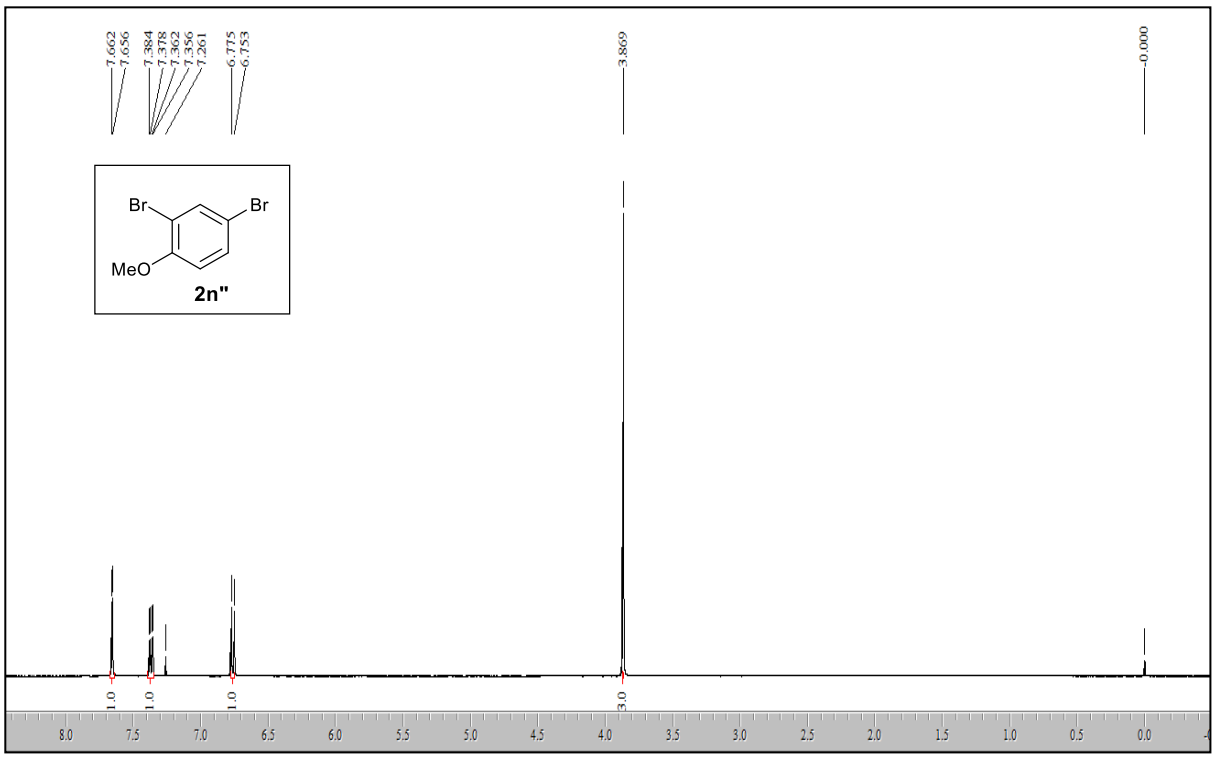
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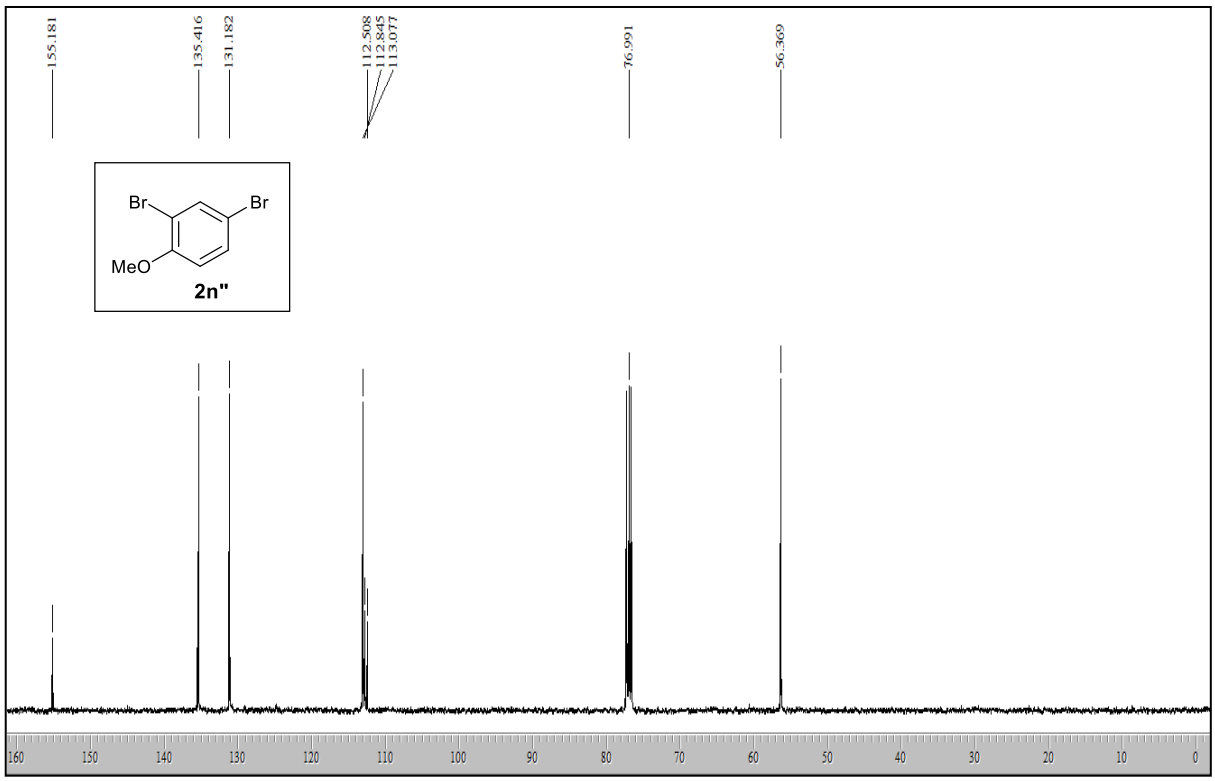
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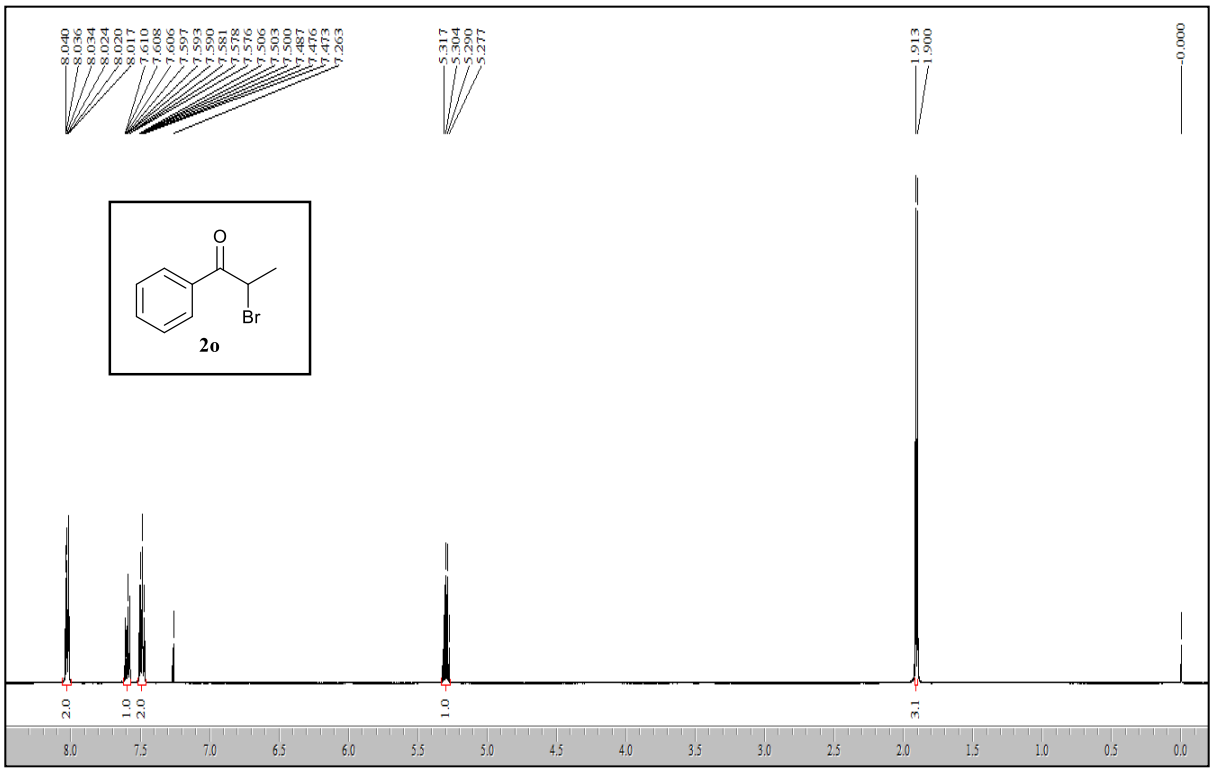
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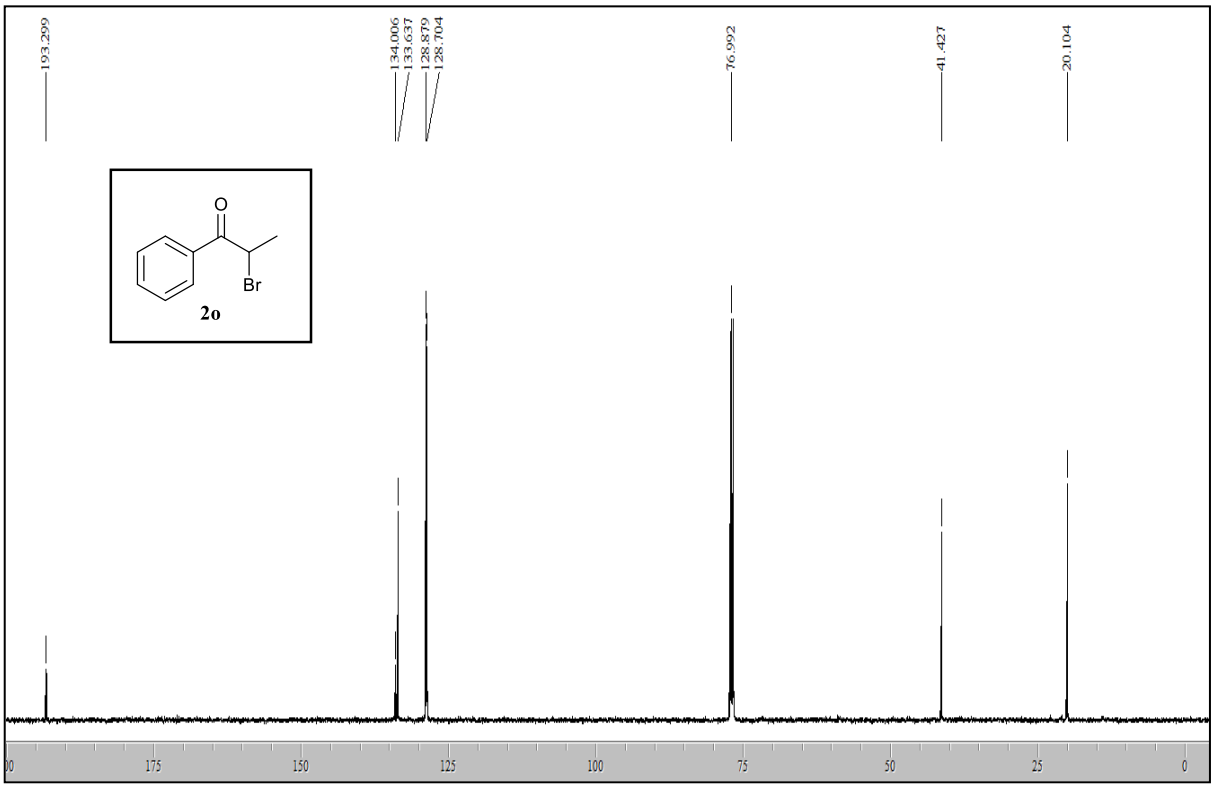
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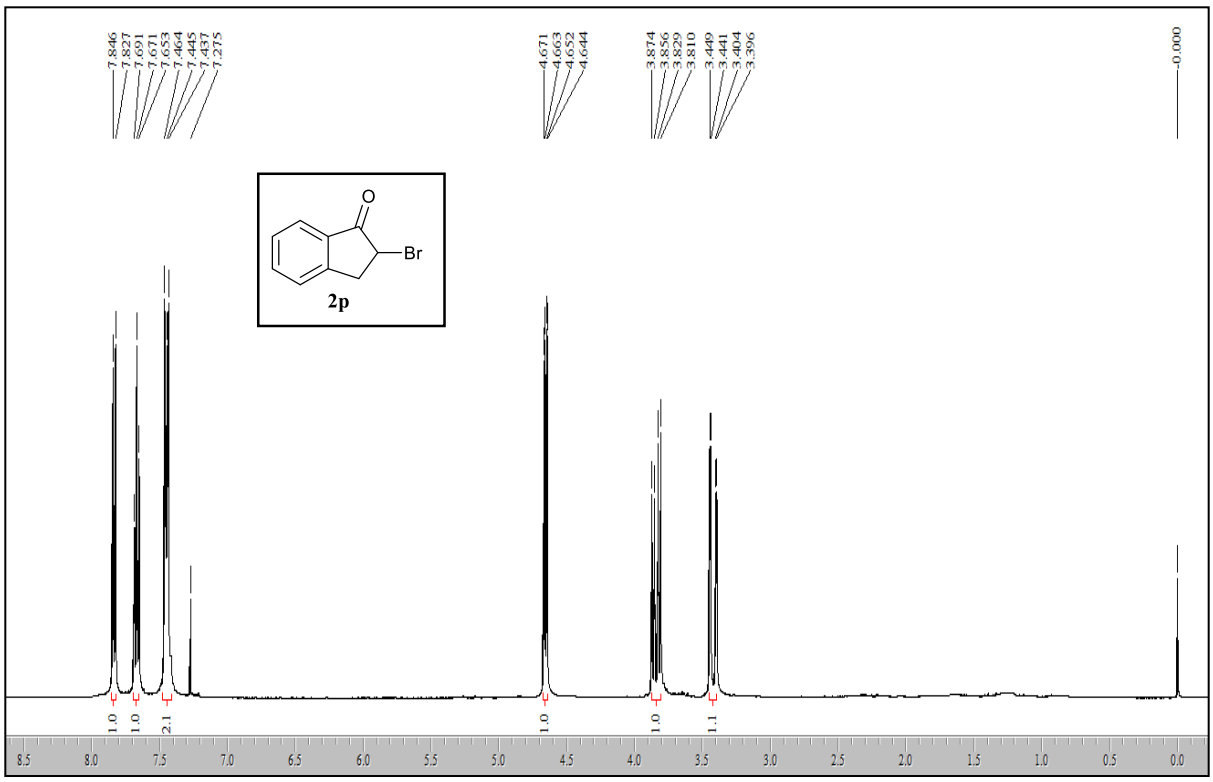
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1.0
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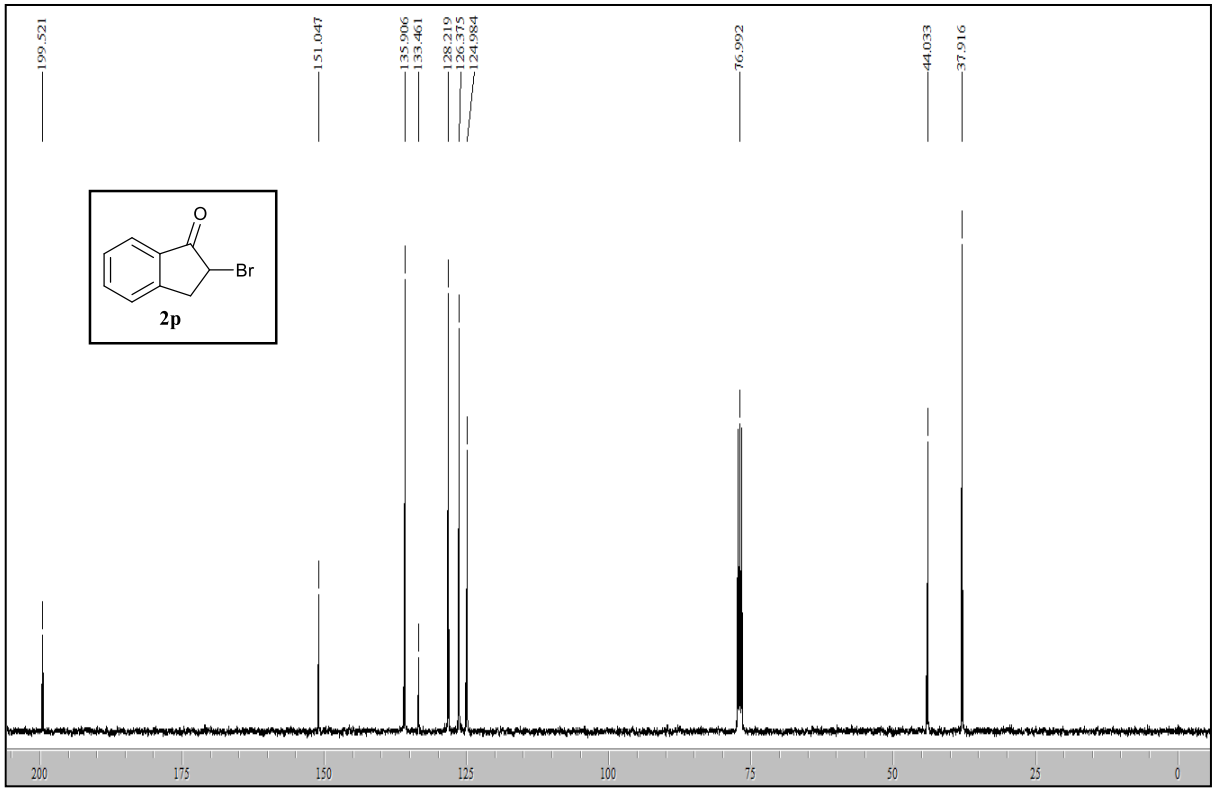
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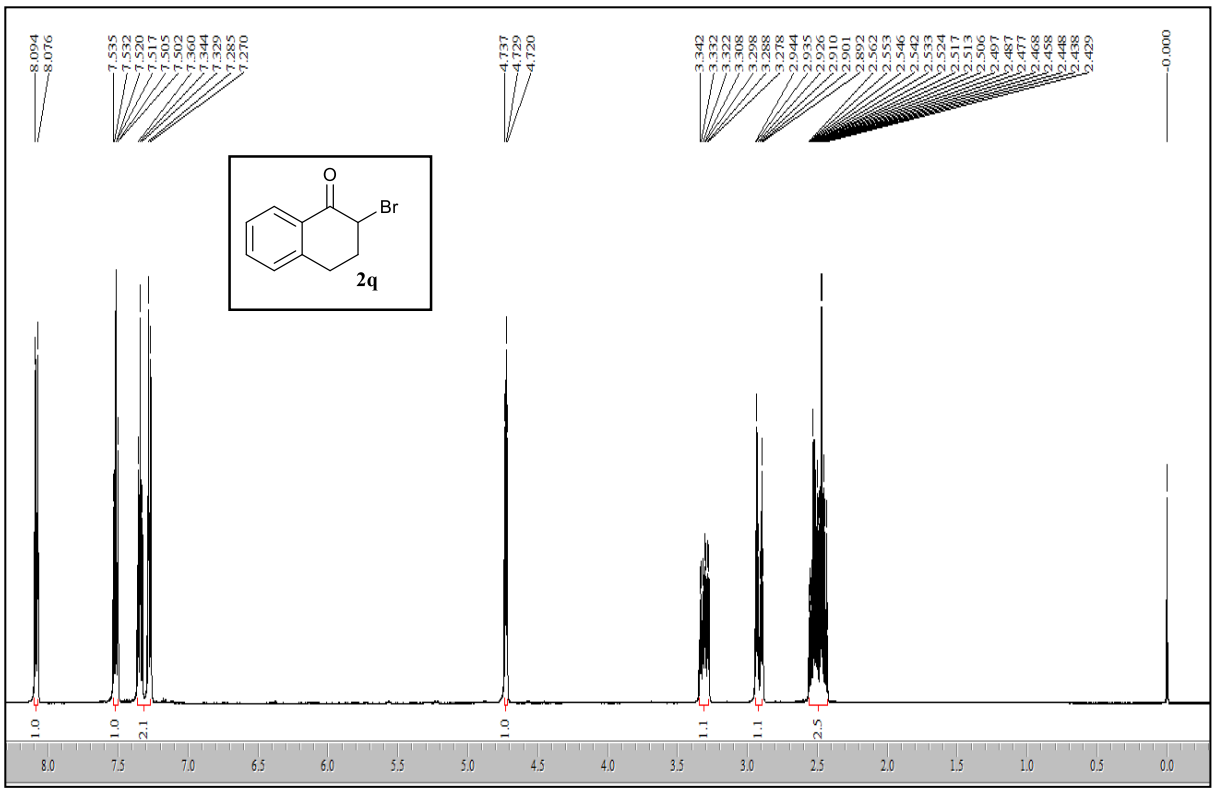
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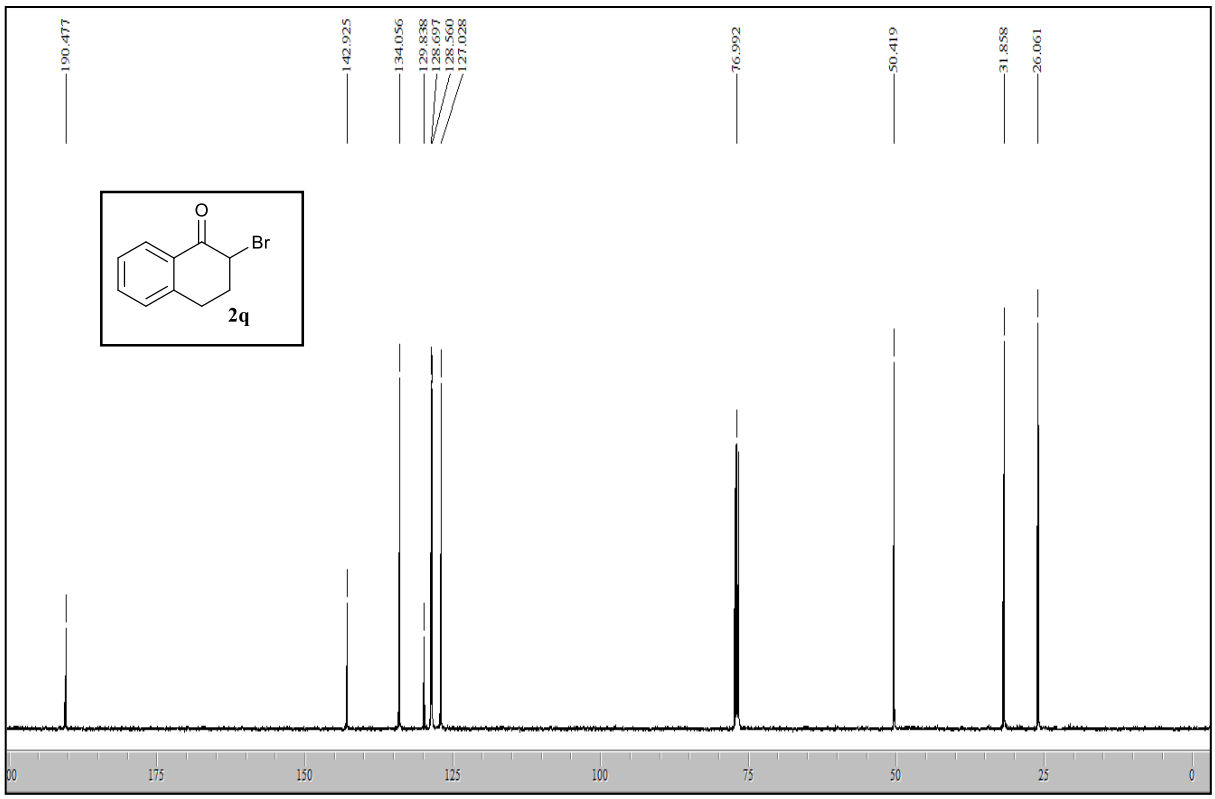
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2q
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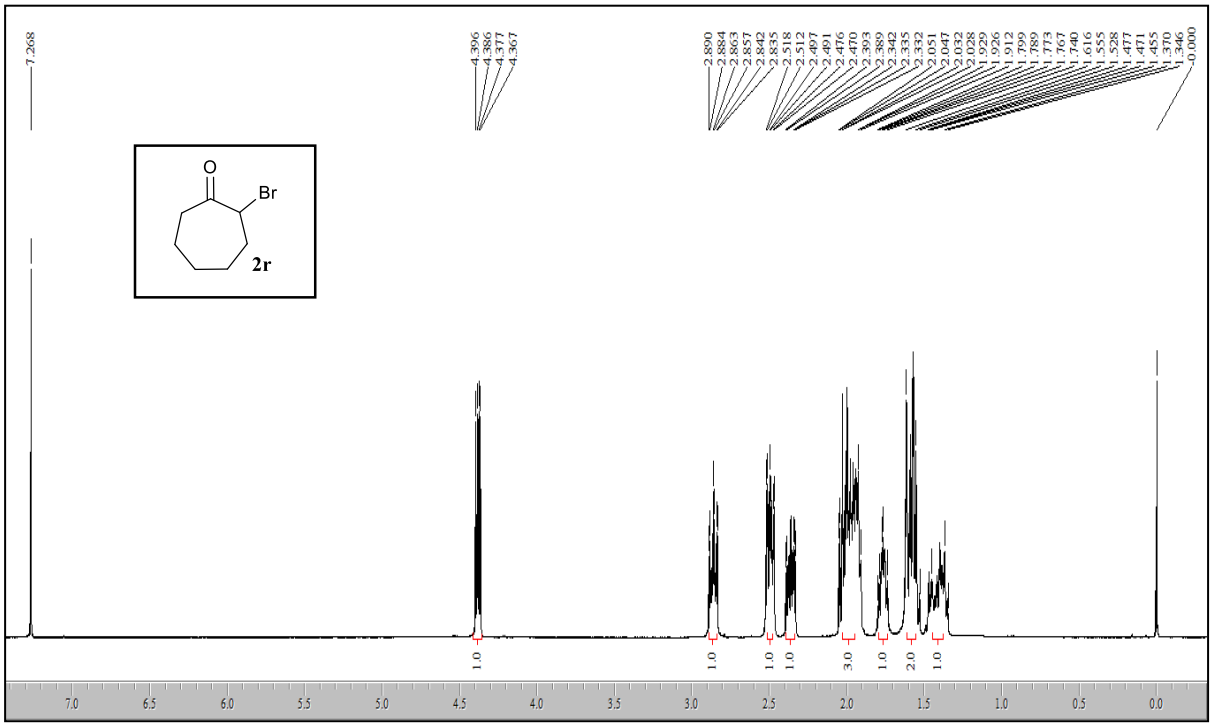
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2.332
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2.047
2.032
2.028
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1.926
1.912
1.799
1.789
1.773
1.767
1.740
1.616
1.555
1.528
1.477
1.471
1.455
1.370
1.346
0.000
O
Br
2r
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1.0
1.0
1.0
3.0
1.0
2.0
1.0
7.0
6.5
6.0
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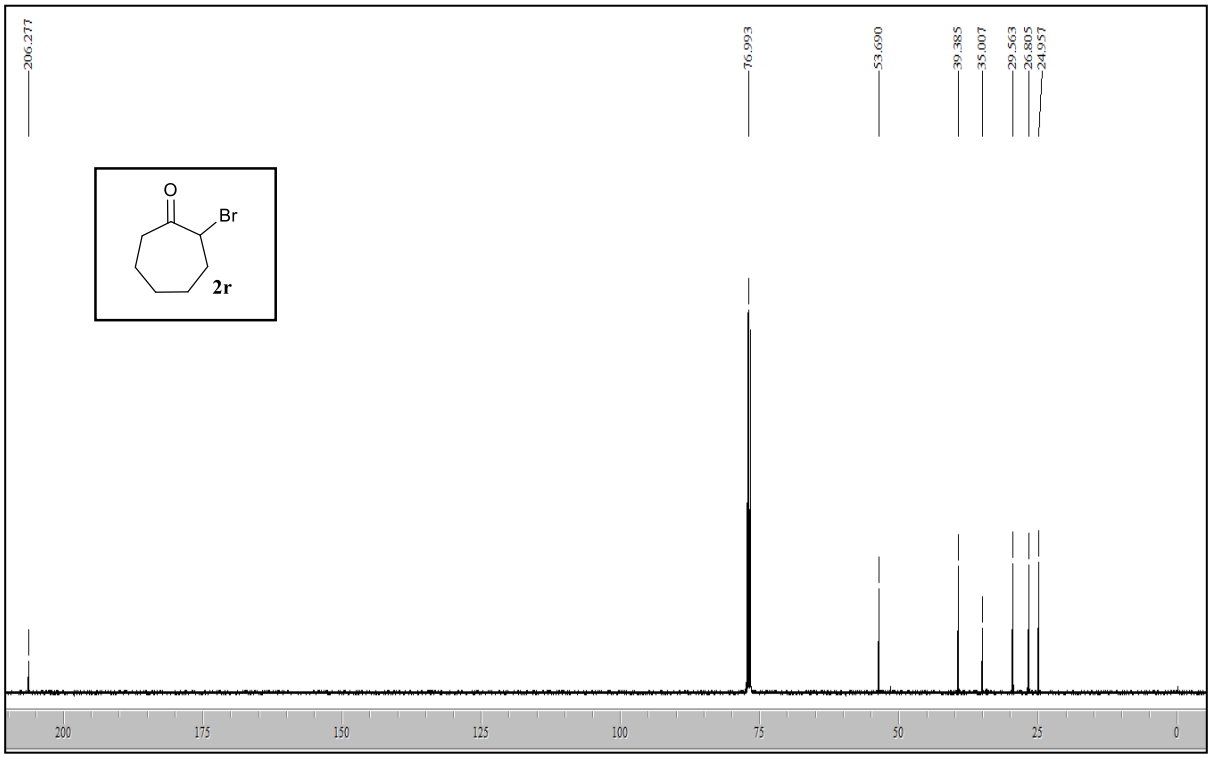
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25
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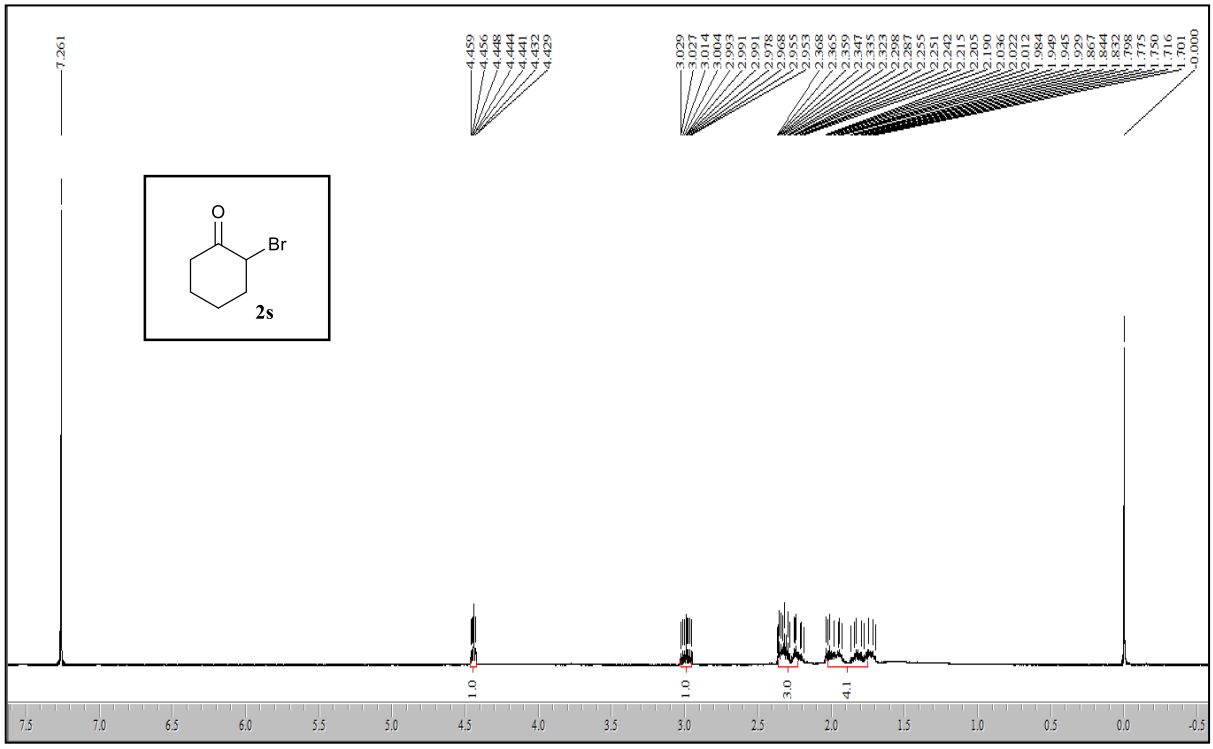
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2.991
2.978
2.968
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2.368
2.365
2.359
2.347
2.335
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1.929
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1.832
1.798
1.775
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1.701
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Br
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1.0
3.0
4.1
7.5
7.0
6.5
6.0
5.5
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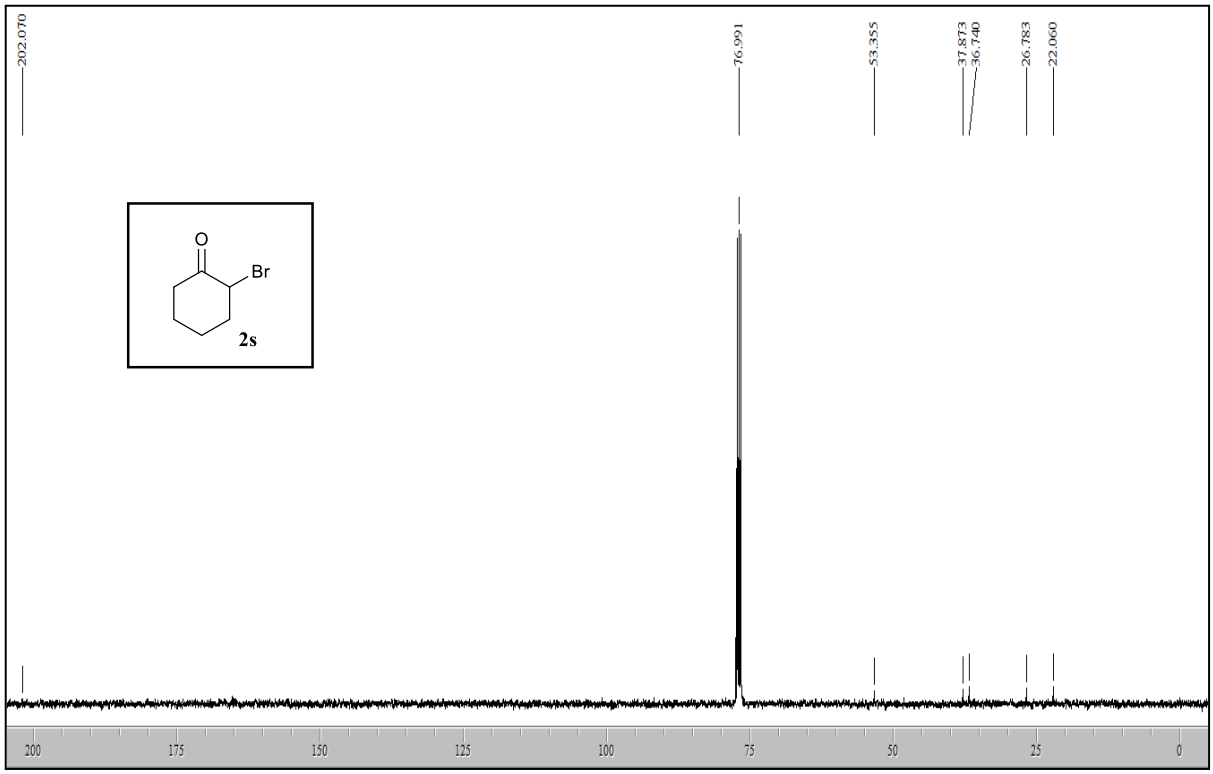
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150
125
100
75
50
25
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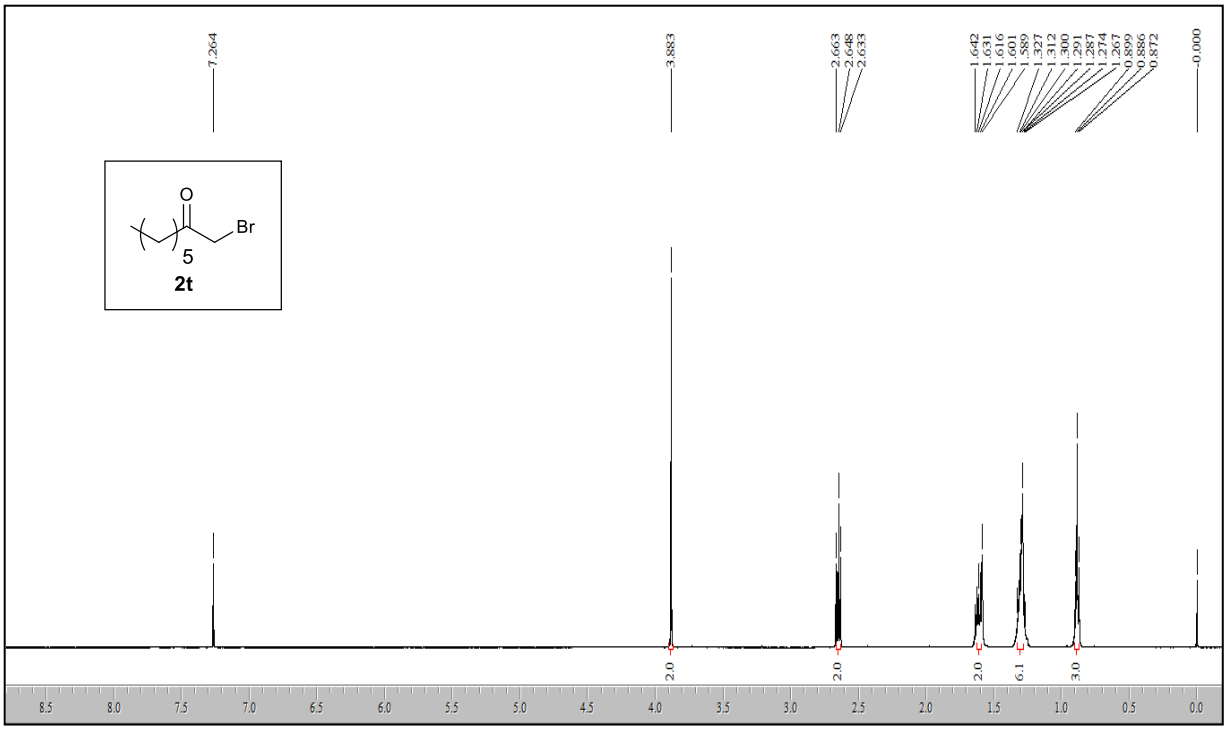
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1.291
1.287
1.274
1.267
0.897
0.886
0.872
0.000
O
Br
5
2t
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2.0
2.0
6.1
3.0
8.5
8.0
7.5
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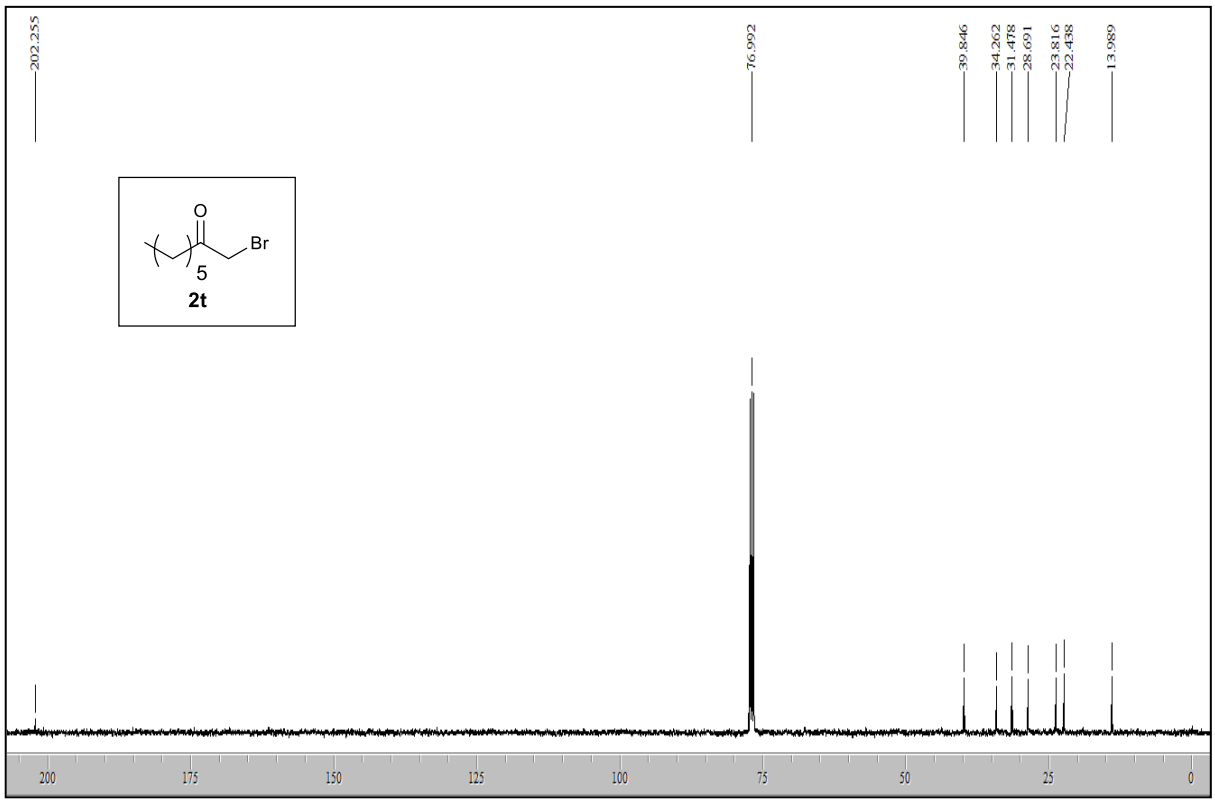
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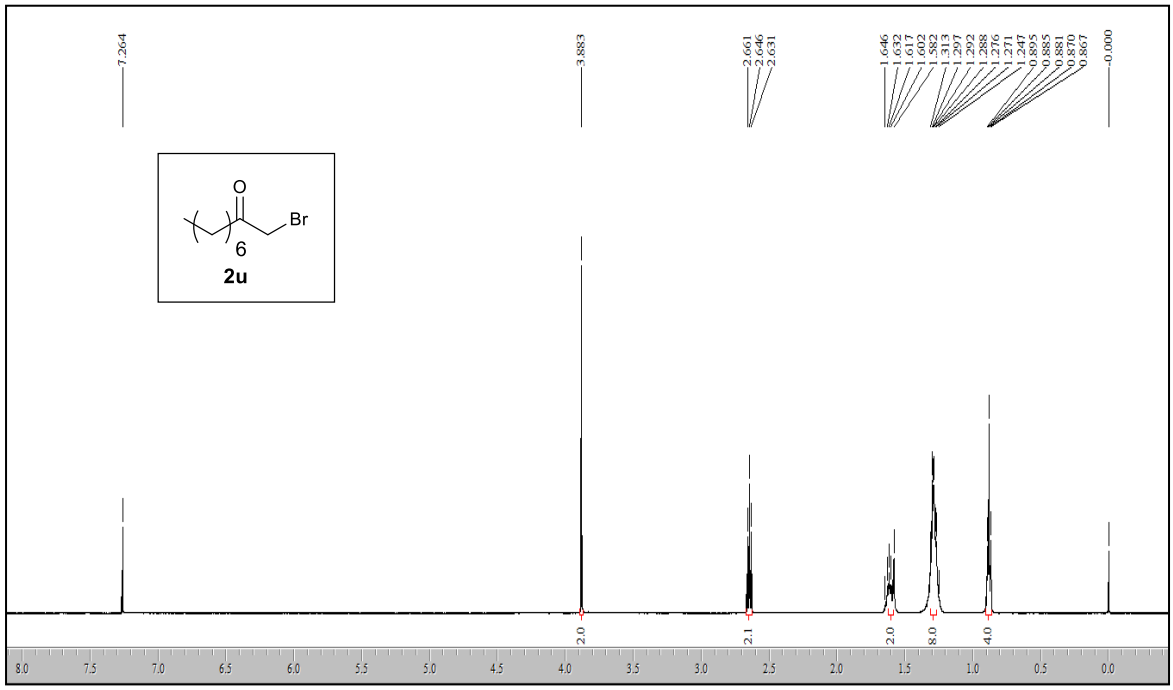
Br
5
2t
200
175
150
125
100
75
50
25
0


7.264
3.883
2.661
2.646
2.631
1.646
1.632
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1.582
1.313
1.297
1.292
1.288
1.276
1.271
1.247
0.895
0.885
0.881
0.870
0.867
0.000
O
Br
6
2u
2.0
2.1
2.0
8.0
4.0
8.0
7.5
7.0
6.5
6.0
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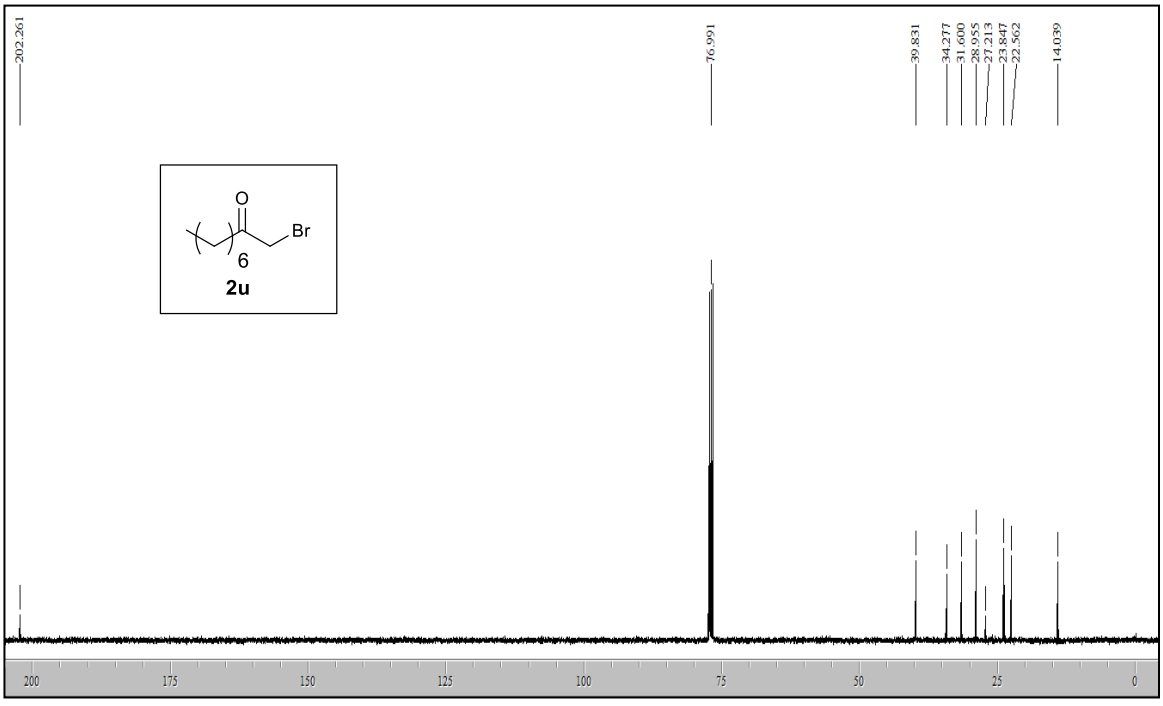
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23.847
22.562
14.039
O
Br
6
2u
200
175
150
125
100
75
50
25
0

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