Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for

Chemoselective hydrogen peroxide oxidation of primary alcohols to aldehydes by a water-soluble and reusable iron(III) catalyst in pure water at room temperature

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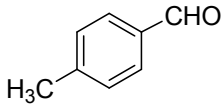
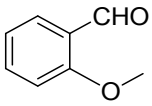
1. Characterization data

4-Methylbenzaldehyde[1] (2a)



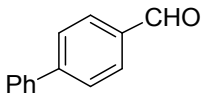
Colorless oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.00 (s, 1H), 7.81 (d, J = 8.1 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 2.48 (s, 3H).

2-Methoxybenzaldehyde[2] (2b, Table 2, entry 1)



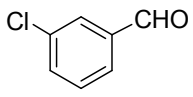
Yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.52 (s, 1H), 7.89 (s, 1H), 7.63-7.58 (m, 1H), 7.08 (d, J = 7.5 Hz, 1H), 7.05 (t, J = 11.8 Hz, 1H), 3.98 (s, 3H).

4-Phenylbenzaldehyde[3] (2c, Table 2, entry 2)



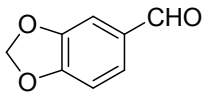
White solid, m.p. 56.8-57.1 ^{o}C (lit. 57-59 ^{o}C). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.06 (s, 1H), 7.95 (d, J = 8.3 Hz, 2H), 7.76 (d, J = 8.2 Hz, 2H), 7.64 (d, J = 7.9 Hz, 2H), 7.49 (t, J = 8.2 Hz, 2H), 7.47-7.42 (m, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ 191.94, 147.17, 139.68, 135.17, 130.26, 129.00, 128.47, 127.66, 127.35.

3-Chlorobenzaldehyde[4] (2d, Table 2, entry 3)



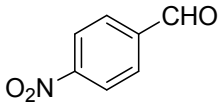
Light yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.02 (s, 1H), 7.90 (s, 1H), 8.45 (d, J = 7.6 Hz, 1H), 7.66-7.63 (m, 1H), 7.53 (t, J = 15.6 Hz, 1H).

3,4-(Methylenedioxy)benzaldehyde[5] (2e, Table 2, entry 4)



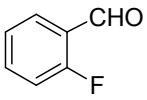
White crystalline solid, m.p. 82.0-83.4 °C (lit. 83-84 °C). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.86 (s, 1H), 7.46 (q, J = 9.4 Hz, 1H), 7.38 (s, 1H), 6.97 (d, J = 8.0 Hz, 1H), 6.13 (s, 2H).

4-Nitrobenzaldehyde[5] (2f, Table 2, entry 5)



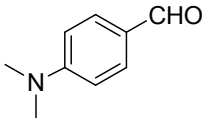
Light yellow solid, m.p. 103.1-104.7 °C (lit. 104-105 °C). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.21 (s, 1H), 8.45 (q, J = 8.7 Hz, 2H), 8.13 (q, J = 8.8 Hz, 2H).

2-Fluorobenzaldehyde[6] (2g, Table 2, entry 6)



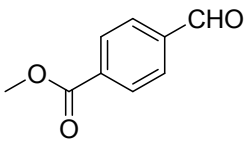
Light yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.39 (s, 1H), 7.91-7.87 (m, 1H), 7.67-7.61 (m, 1H), 7.31 (d, J = 7.6 Hz, 1H), 7.22-7.18 (m, 1H).

4-(Dimethylamino)benzaldehyde[4] (2h, Table 2, entry 7)



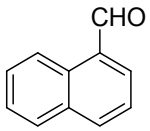
Light yellow solid, m.p. 72.1-72.6 °C (lit. 72-75 °C). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.79 (s, 1H), 7.81-7.77 (m, 2H), 6.76 (d, J = 9.0 Hz, 2H), 3.14 (s, 6H).

Methyl 4-formylbenzoate[2] (2i, Table 2, entry 8)



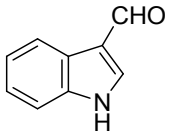
Light yellow solid, m.p. 58.7-58.9 °C (lit. 59-63 °C). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.09 (s, 1H), 8.19 (d, J = 8.2 Hz, 2H), 7.94 (d, J = 8.3 Hz, 2H), 3.95 (s, 3H).

1-Naphthaldehyde[2] (2j, Table 2, entry 9)



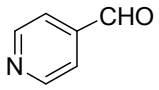
Light yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.45 (s, 1H), 9.31 (d, J = 8.7 Hz, 1H), 8.15 (d, J = 8.2 Hz, 1H), 8.04 (q, J = 8.2 Hz, 1H), 7.97 (d, J = 8.1 Hz, 1H), 7.77-7.73 (m, 1H), 7.70-7.63 (m, 2H).

1*H*-indole-3-carbaldehyde[7] (2k, Table 2, entry 10)



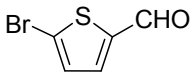
Light yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.12 (s, 1H), 8.89 (s, br, 1H), 8.37 (t, J = 9.2 Hz, 1H), 7.91 (d, J = 3.1 Hz, 1H), 7.52-7.49 (m, 1H), 7.40-7.37 (m, 2H).

4-Pyridinealdehyde[8] (2l, Table 2, entry 11)



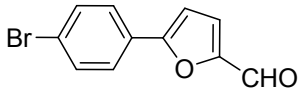
Light yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 10.06 (s, 1H), 8.86 (q, J = 5.9 Hz, 2H), 7.68 (q, J = 5.9 Hz, 2H).

5-Bromothiophene-2-carbaldehyde[9] (2m, Table 2, entry 12)



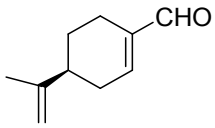
Colorless oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.81 (s, 1H), 7.57 (d, J = 4.0 Hz, 1H), 7.23 (d, J = 4.0 Hz, 1H).

5-(4-Bromophenyl)furan-2-carbaldehyde[10] (2n, Table 2, entry 13)



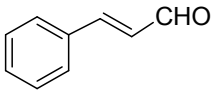
Light yellow solid, m.p. 152.4-153.4 ^{o}C (lit. 152-155 ^{o}C). ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.66 (s, 1H), 7.68 (d, J = 8.6 Hz, 2H), 7.58 (d, J = 8.6 Hz, 2H), 7.31 (d, J = 3.7 Hz, 1H), 6.84 (d, J = 3.7 Hz, 1H).

(S)-Perillaldehyde[11] (4a, Table 3, entry 1)



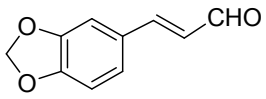
Colorless oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.42 (s, 1H), 6.81 (q, J = 5.6 Hz, 1H), 4.73 (q, J = 20.0 Hz, 2H), 2.46-2.41 (m, 2H), 2.26-2.21 (m, 2H), 2.11-2.10 (m, 1H), 1.93-1.87 (m, 1H), 1.75 (s, 3H), 1.46-1.41 (m, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ 194.40, 151.11, 148.88, 141.80, 110.05, 41.23, 32.26, 26.88, 22.10, 21.22.

Cinnamaldehyde[4] (4b, Table 3, entry 2)



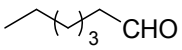
Light yellow oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.76 (d, J = 7.7 Hz, 1H), 7.62 (q, J = 9.6 Hz, 2H), 7.55 (s, 1H), 7.49 (q, J = 6.9 Hz, 3H), 6.77 (q, J = 23.6 Hz, 1H).

(*E*)-3',4'-(Methylenedioxy)cinnamaldehyde [12] (4c, Table 3, entry 3)



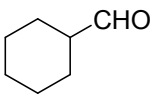
Light yellow solid, m.p. 90.6-91.1 ^{o}C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.69 (d, J = 7.7 Hz, 1H), 7.42 (d, J = 15.8 Hz, 1H), 7.11 (t, J = 5.9 Hz, 2H), 6.90 (d, J = 8.5 Hz, 1H), 6.60 (q, J = 23.5 Hz, 1H), 6.09 (s, 2H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ 194.01, 153.02, 151.03, 149.13, 129.07, 127.42, 125.76, 109.28, 107.33, 102.34.

Heptanal[4] (4d, Table 3, entry 4)



Colorless oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.66 (s, 1H), 2.36-2.28 (m, 2H), 1.65-1.59 (m, 2H), 1.29 (d, J = 3.1 Hz, 6H), 0.87 (d, J = 5.6 Hz, 3H).

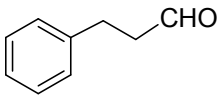
Cyclohexanecarbaldehyde[13] (4e, Table 3, entry 5)



Colorless oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.61 (s, 1H), 2.23 (t, J = 14.6 Hz, 1H), 1.89 (d, J = 10.3

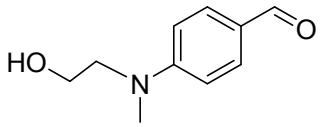
Hz, 2H), 1.73 (t, J = 9.6 Hz, 2H), 1.65 (t, J = 11.6 Hz, 1H), 1.41-1.23 (m, 5H).

3-Phenylpropanal[4] (4f, Table 3, entry 6)



Colorless oil. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.87 (s, 1H), 7.37 (q, J = 7.4 Hz, 2H), 7.29-7.25 (m, 3H), 3.02 (t, J = 15.1 Hz, 2H), 2.86-2.82 (m, 2H).

4-((2-hydroxyethyl)(methyl)amino)benzaldehyde[14] (4g)



Yellow solid, m.p. 72.1-72.6 ^{o}C. ^{1}H-NMR (400 MHz, $CDCl_3$): δ 9.71 (s, 1H), 7.70 (t, J = 8.8 Hz, 2H), 6.76 (t, J = 8.7 Hz, 2H), 3.87 (t, J = 11.3 Hz, 2H), 3.62 (t, J = 11.6 Hz, 2H), 3.12 (s, 3H), 1.07 (s, br, 1H). ^{13}C-NMR (100 MHz, $CDCl_3$): δ 190.94, 154.48, 132.67, 125.81, 111.72, 60.54, 54.89, 39.70.

2 Reference

[1] A. Dijksman, A. Marino-González, A. M. i Payeras, I. W. C. E. Arends, R. A. Sheldon, *J. Am. Chem. Soc.*, 2001, **123***,* 6826-6833.

[2] Y. Zhu, B. Zhao, Y. Shi, *Org. Lett.*, 2013, **15**, 992-995.

[3] G. A. Molander, L. Iannazzo, *J. Org. Chem.*, 2011, **76**, 9182-9187.

[4] N. Jiang, A. J. Ragauskas, *Org. Lett.*, 2005, **7**, 3689-3692.

[5] K. Surendra, K.N. Srilakshmi, R.M. Arjun, M. Nageswar, R.K. Rama, *J. Org. Chem.*, 2003, **68**, 2058-2059.

[6] J. Wu, Y. Liu, X. Ma, P. Liu, C. Gu, B. Dai, *Appl. Organometal. Chem.*, 2016, **30**, 577-580.

[7] D. Baruah, U. P. Saikia, P. Pahari, D. Konwar, *Tetrahedron Lett.*, 2015, **56**, 2543-2547.

[8] R. Prebil, G. Stavber, S. Stavber, *Eur. J. Org. Chem.*, 2014, 395-402.

[9] J. D. M. Muñoz, J. Alcázar, A. D. L. Hoz, A. Díaz-Ortiz, *Eur. J. Org. Chem.*, 2012, 260-263.

[10] S. H. Kim, R. D. Rieke, *J. Org. Chem.*, 2013, **78**, 1984

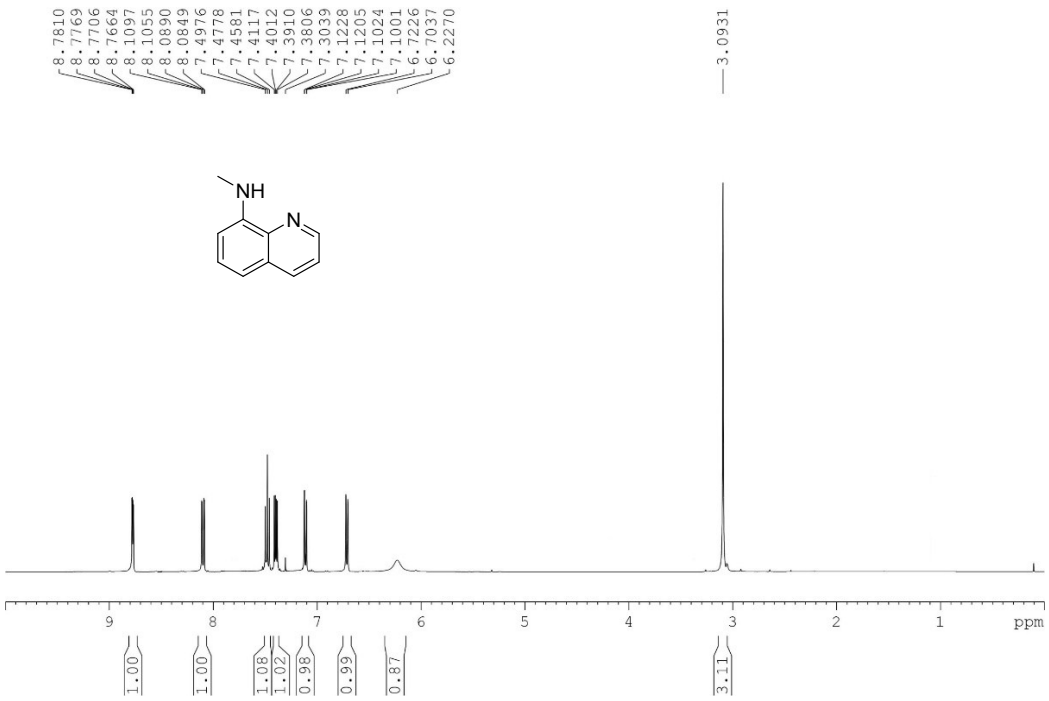
[11] K. Ishihara, H. Kurihara, H. Yamamoto, *J. Org. Chem.*, 1997, **62***,* 5664-5665.

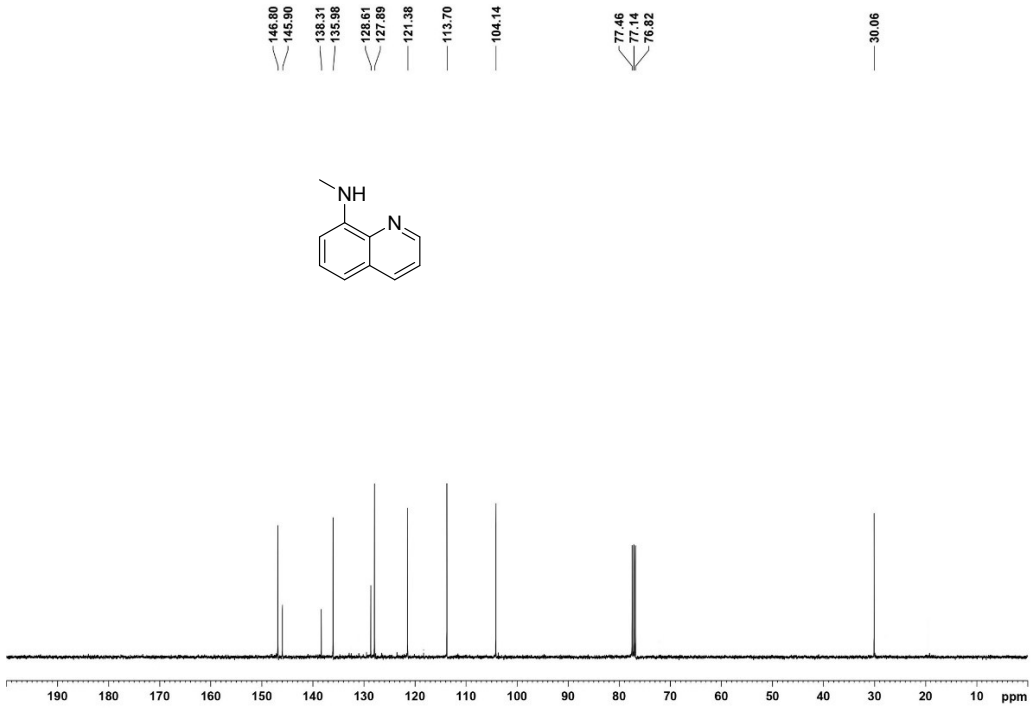
[12] P. S.-W. Leung, Y. Teng, P. H. Toy, *Org. Lett.*, 2010, **12**, 4996-4999.

[13] J. M. Hoover, S. S. Stahl, *J. Am. Chem. Soc.*, 2011, **133**, 16901-16910.

[14] P. W. Hickmott, *J. Chem. Soc.*, 1964, 883-887.

3 NMR Spectra

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138.31
135.98
128.61
127.89
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30.06
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N
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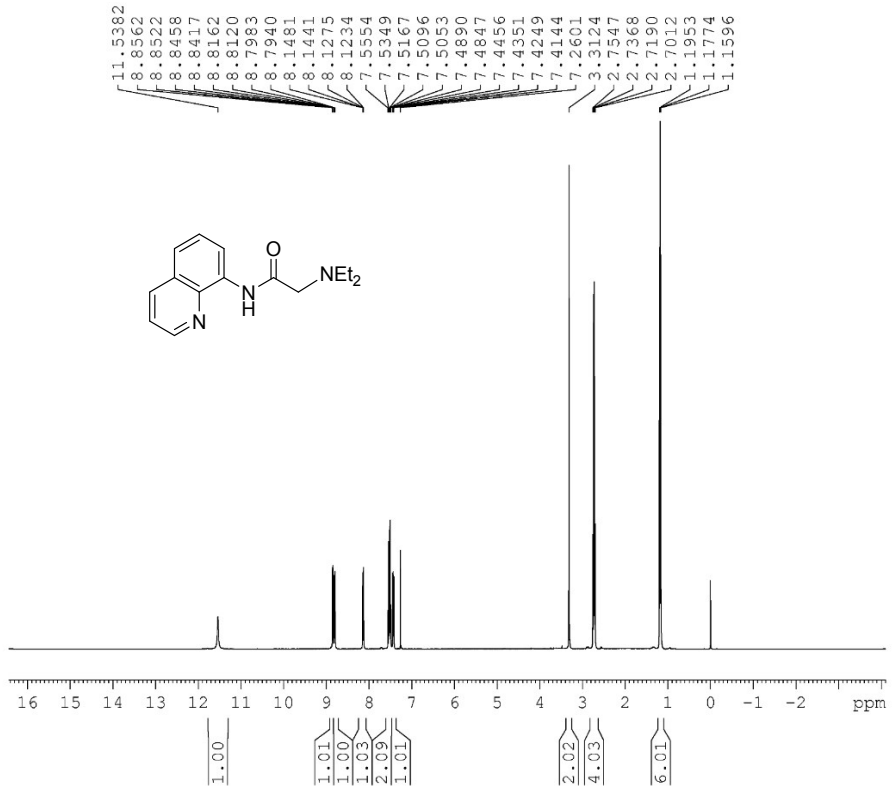
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8.8562
8.8522
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8.1275
8.1234
7.5554
7.5349
7.5167
7.5096
7.5053
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7.4847
7.4456
7.4351
7.4249
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2.7012
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1.1774
1.1596
O
NEt2
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H
N
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 ppm
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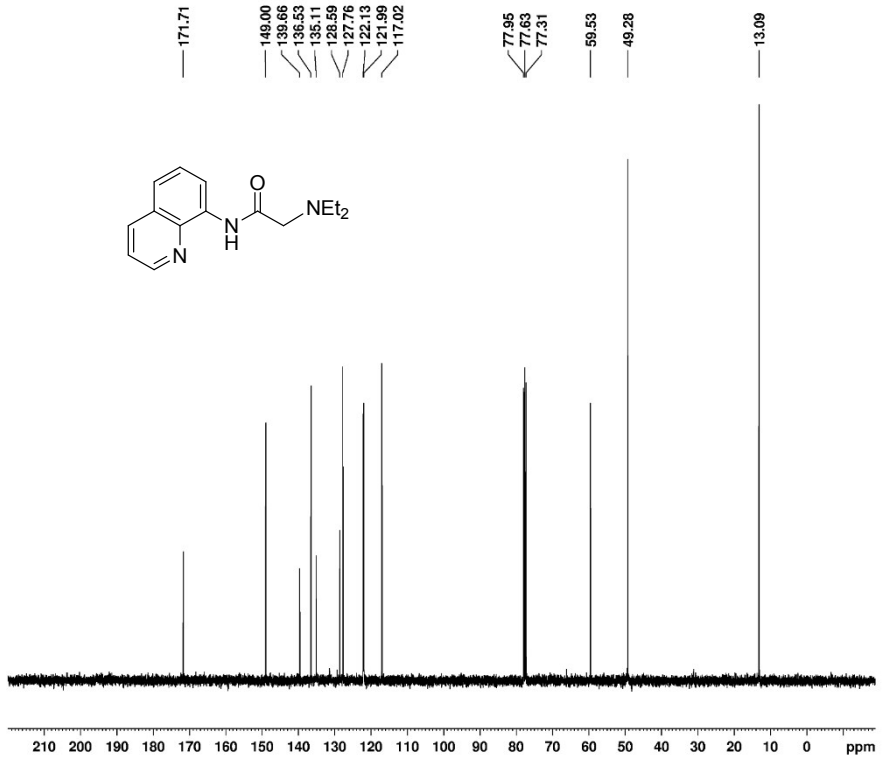
1.03
2.09
1.01
2.02
4.03
6.01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136.53
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122.13
121.99
117.02
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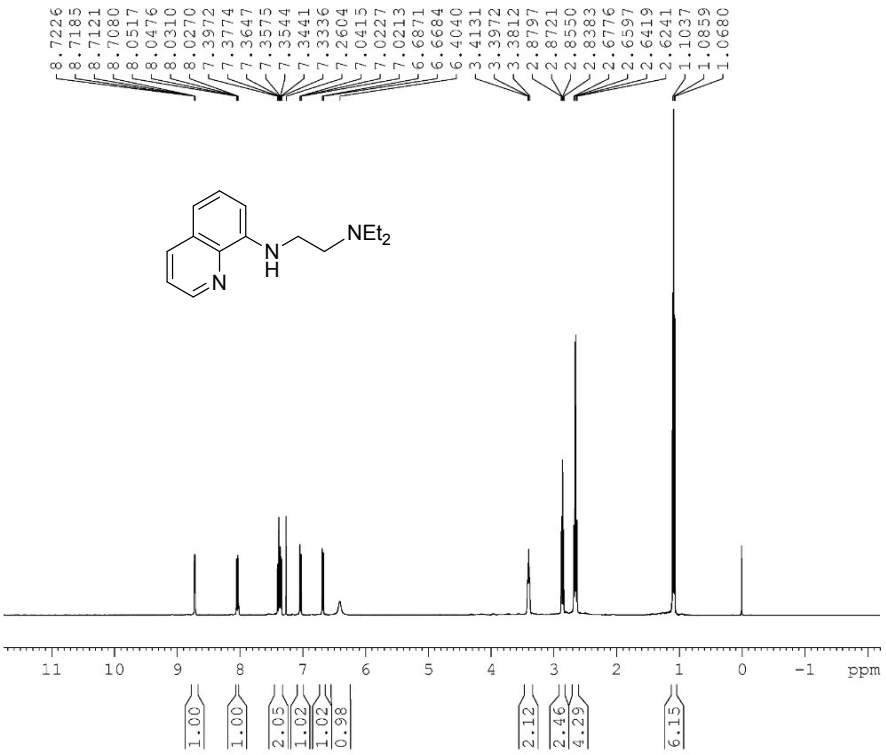
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7.3647
7.3575
7.3544
7.3441
7.3336
7.2604
7.0415
7.0227
7.0213
6.6871
6.6684
6.4040
3.4131
3.3972
3.3812
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2.6776
2.6597
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N
H
NEt2
N
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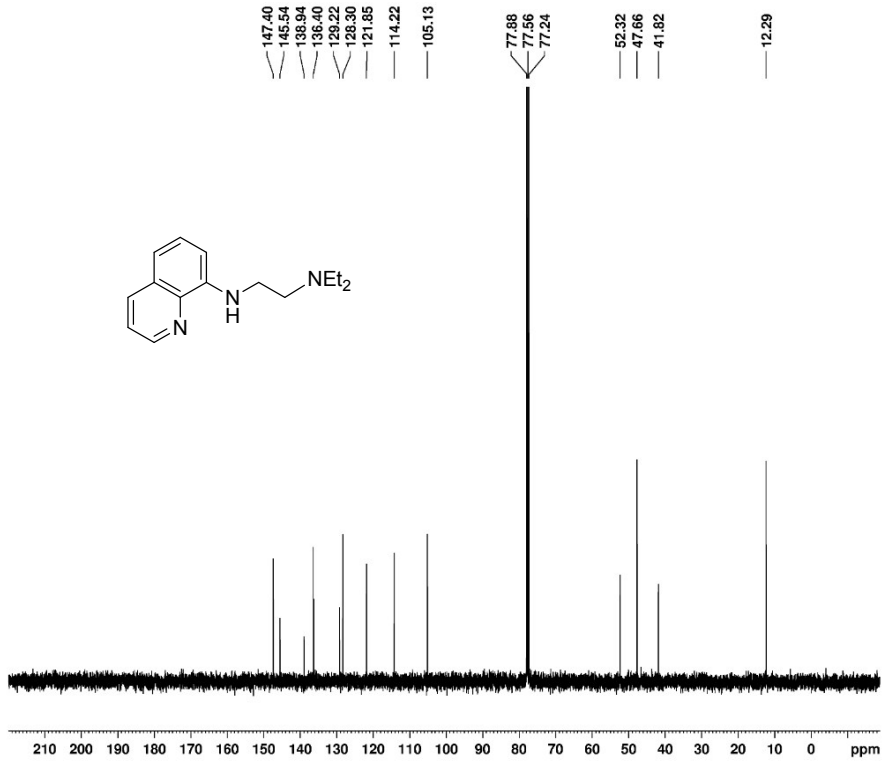
6.15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128.30
121.85
114.22
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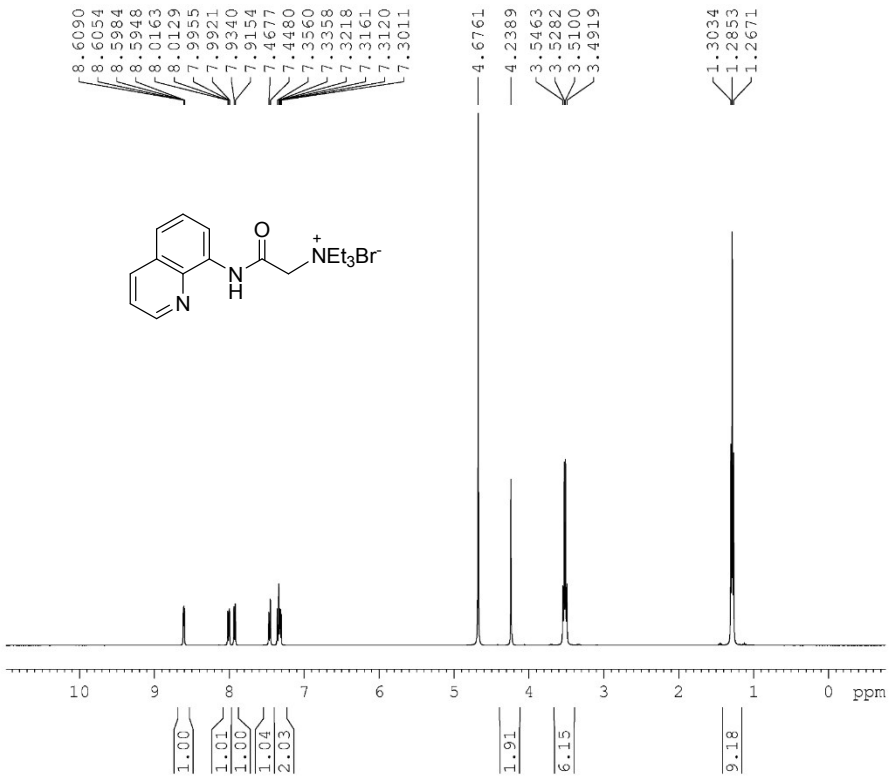
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3.5463
3.5282
3.5100
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1.3034
1.2853
1.2671
O
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NEt3Br-
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H
N
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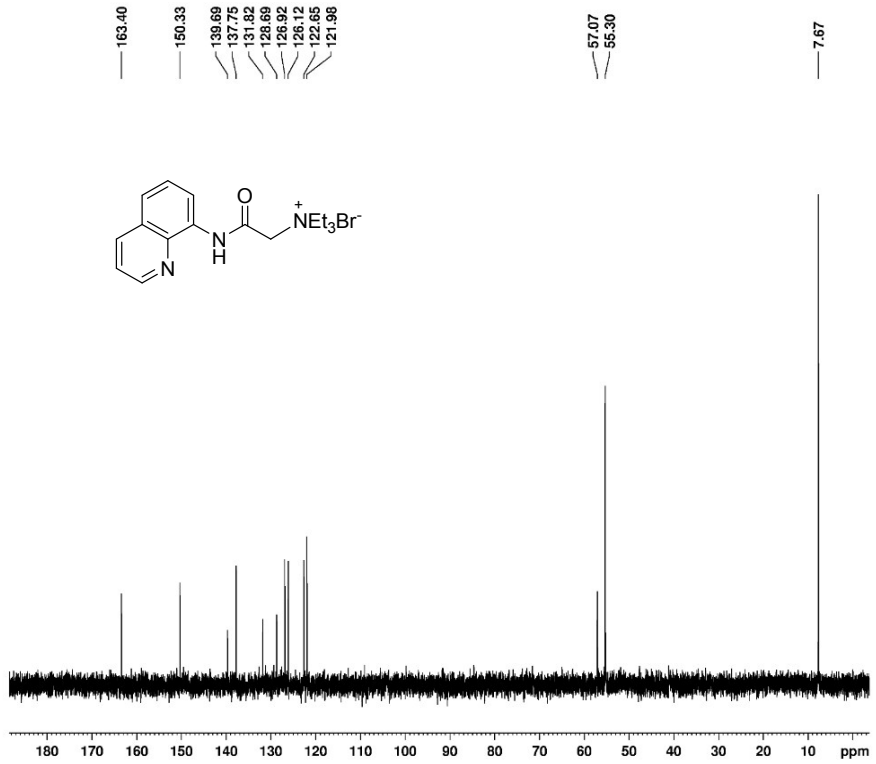
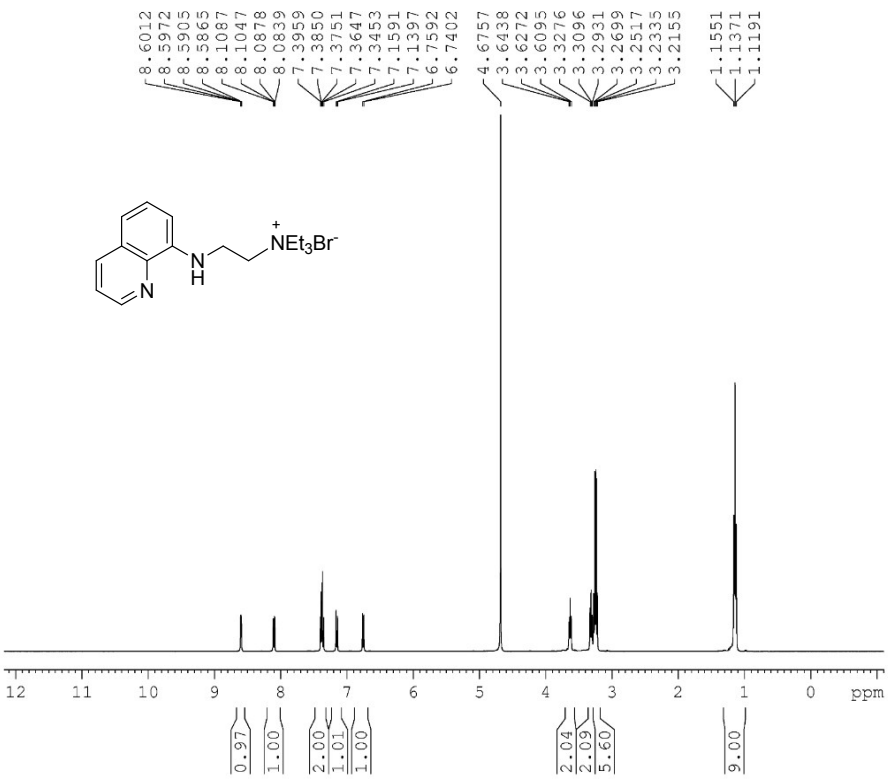
1.00
1.01
1.00
1.04
2.03
1.91
6.15
9.18


163.40
150.33
139.69
137.75
131.82
128.69
126.92
126.12
122.65
121.98
57.07
55.30
7.67
O
N
H
N
+
NEt3Br-
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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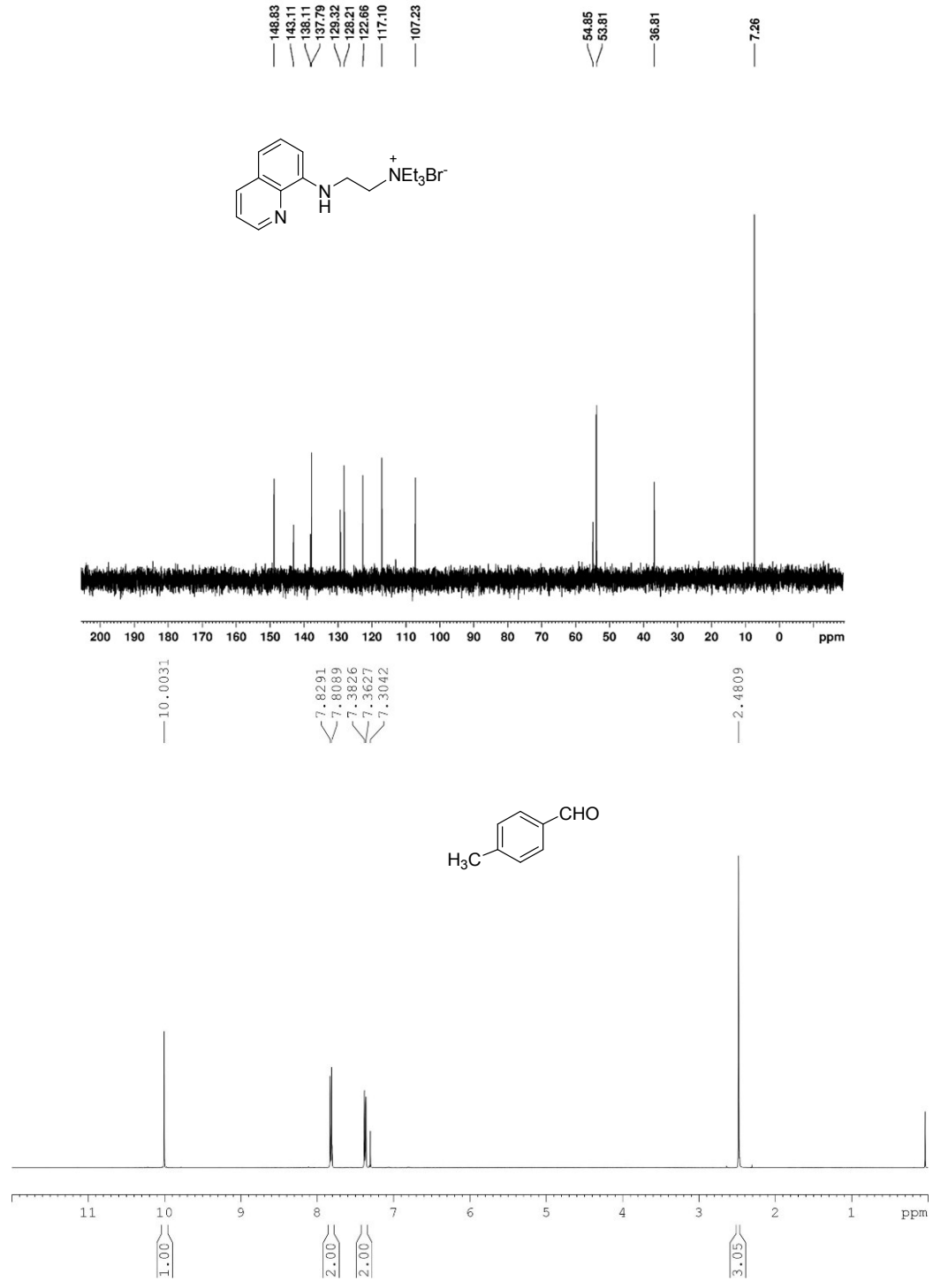
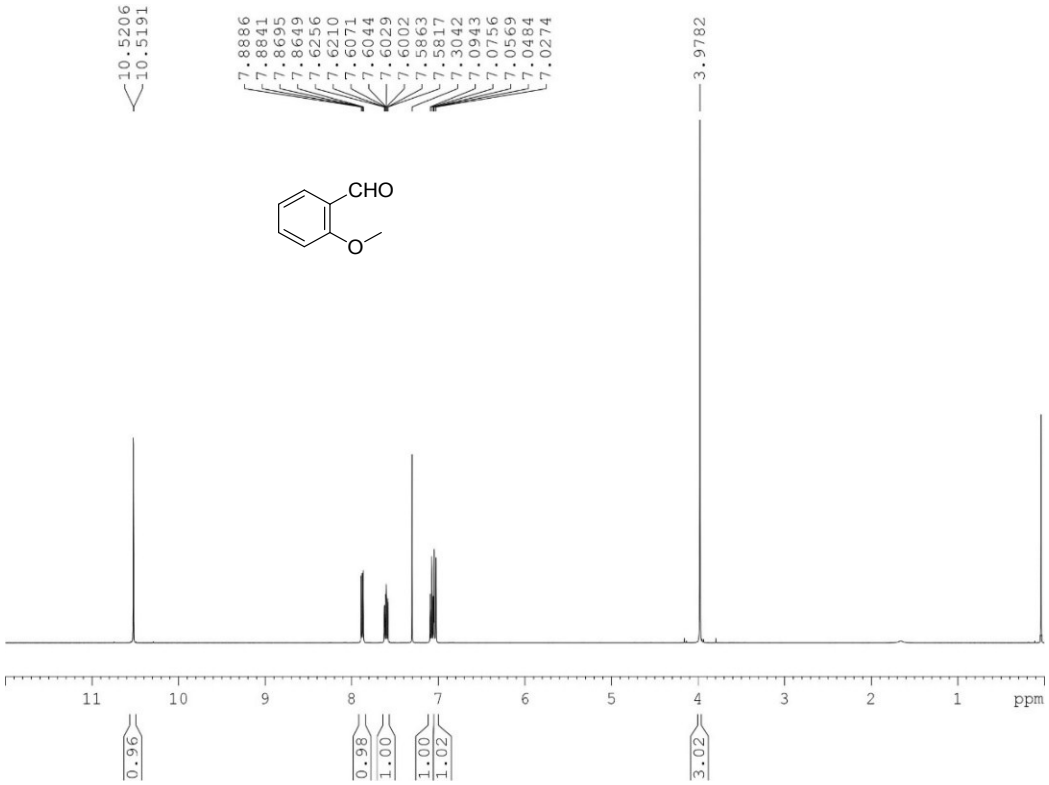
8.5972
8.5905
8.5865
8.1087
8.1047
8.0878
8.0839
7.3959
7.3850
7.3751
7.3647
7.3453
7.1591
7.1397
6.7592
6.7402
4.6757
3.6438
3.6272
3.6095
3.3276
3.3096
3.2931
3.2699
3.2517
3.2335
3.2155
1.1551
1.1371
1.1191
N
H
N
+
NEt3Br-
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.97
1.00
2.00
1.01
1.00
2.04
2.09
5.60
9.00


148.83
143.11
138.11
137.79
129.32
128.21
122.66
117.10
107.23
54.85
53.81
36.81
7.26
NEt3Br-
N
H
N
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
10.0031
7.8291
7.8089
7.3826
7.3627
7.3042
2.4809
CHO
H3C
11 10 9 8 7 6 5 4 3 2 1 ppm
1.00
2.00
2.00
3.05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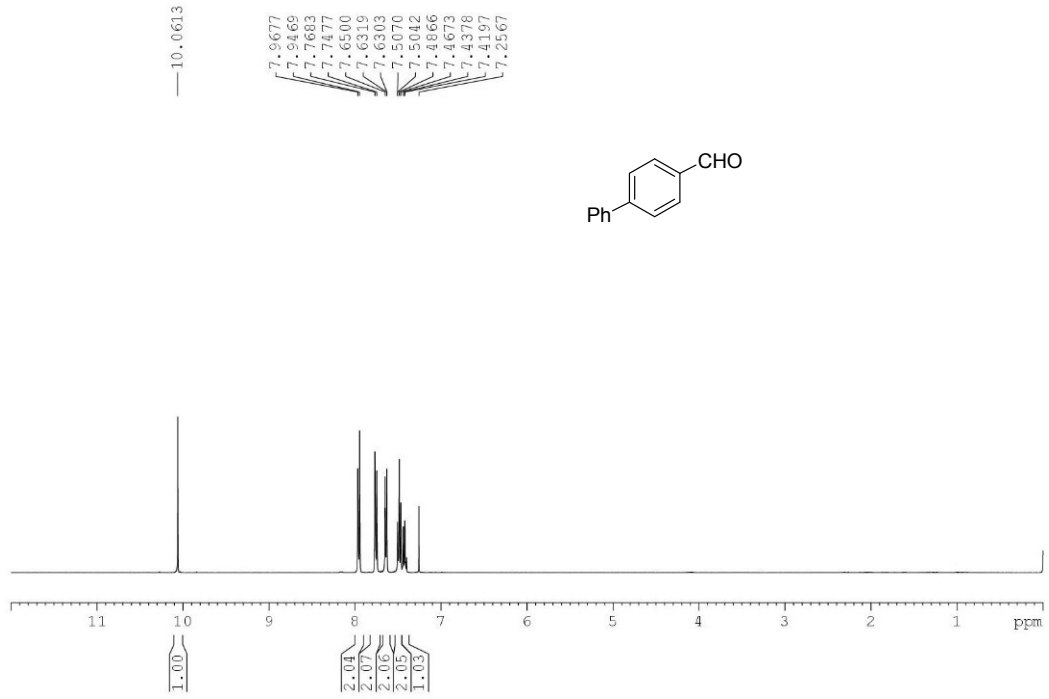
10.5191
7.8886
7.8841
7.8695
7.8649
7.6256
7.6210
7.6071
7.6044
7.6029
7.6002
7.5863
7.5817
7.3042
7.0943
7.0756
7.0569
7.0484
7.0274
3.9782
CHO
O
11
10
9
8
7
6
5
4
3
2
1
ppm
0.96
0.98
1.00
1.00
1.02
3.02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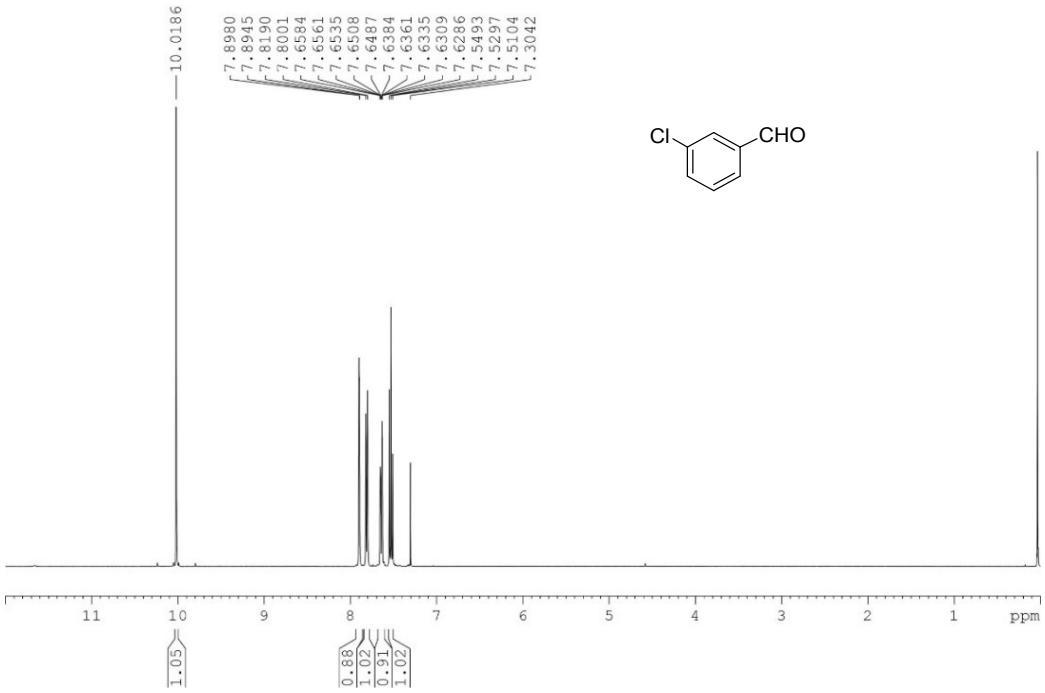
7.9677
7.9469
7.7683
7.7477
7.6500
7.6319
7.6303
7.5070
7.5042
7.4866
7.4673
7.4378
7.4197
7.2567
CHO
Ph
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.04
2.07
2.06
2.05
1.03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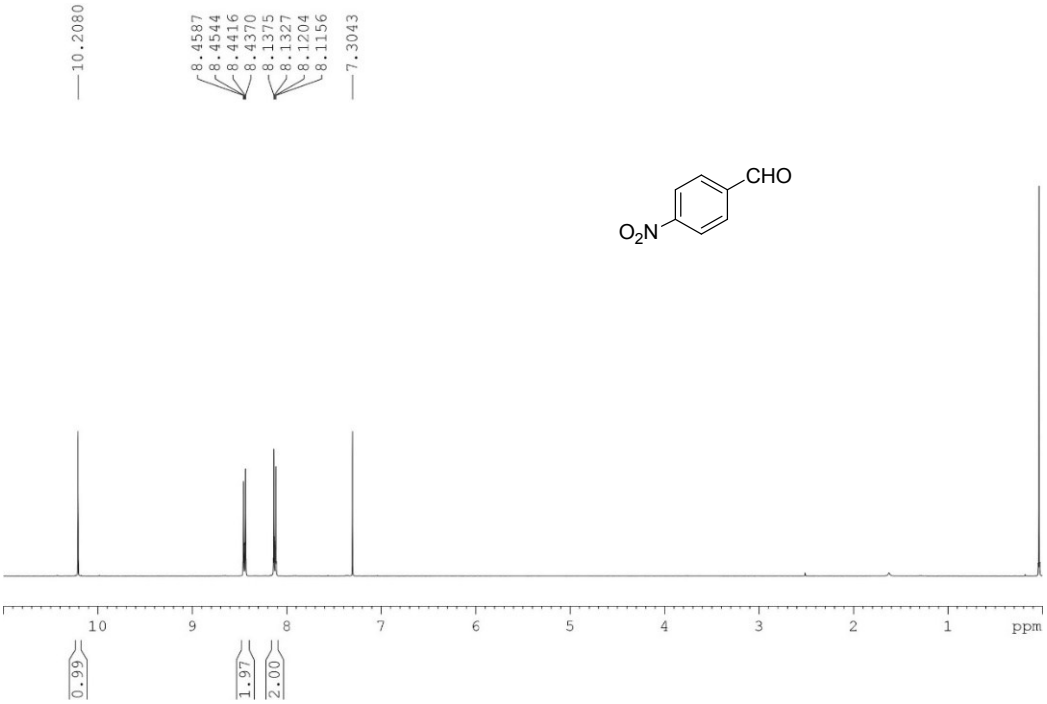
7.8980
7.8945
7.8190
7.8001
7.6584
7.6561
7.6535
7.6508
7.6487
7.6384
7.6361
7.6335
7.6309
7.6286
7.5493
7.5297
7.5104
7.3042
Cl
CHO
11
10
9
8
7
6
5
4
3
2
1
ppm
1.05
0.88
1.02
0.91
1.02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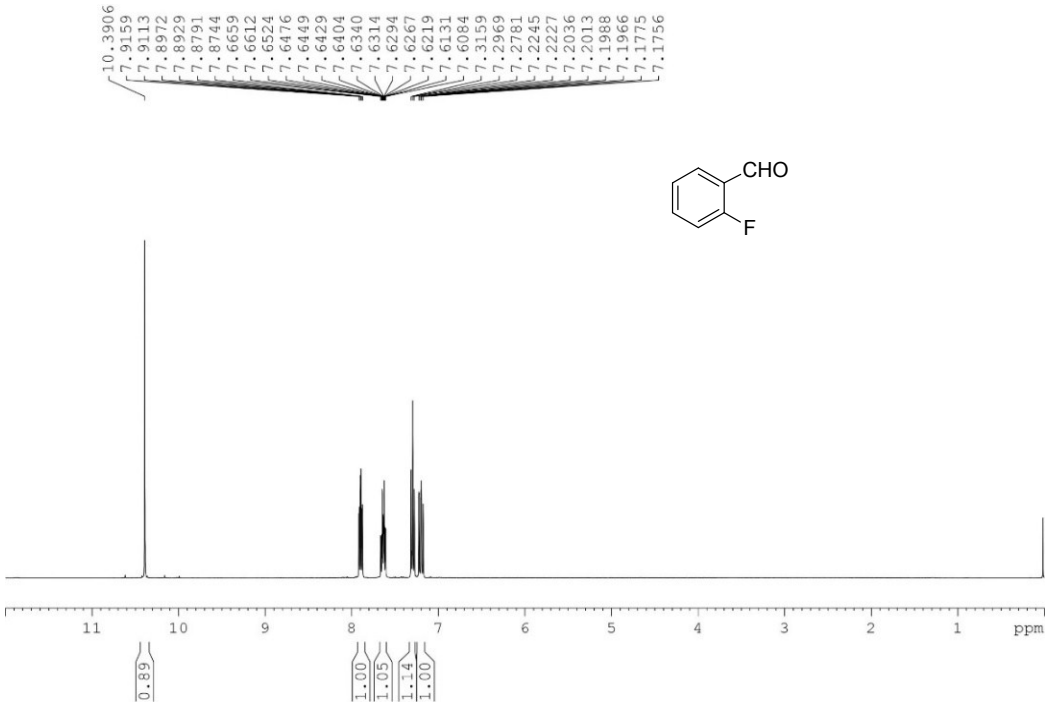
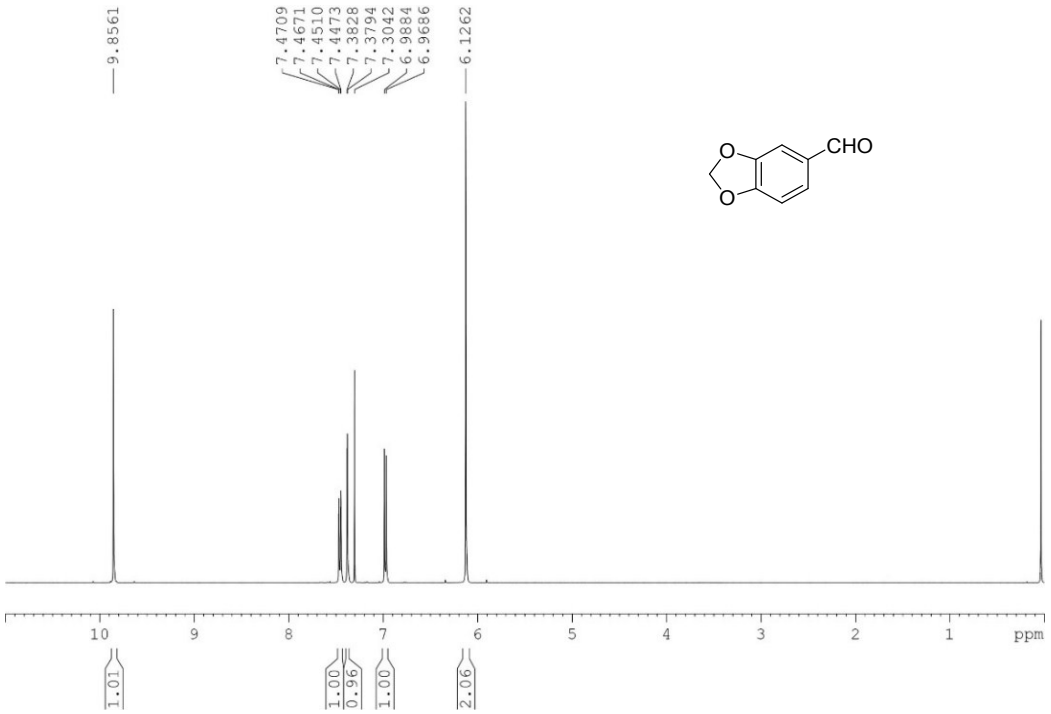
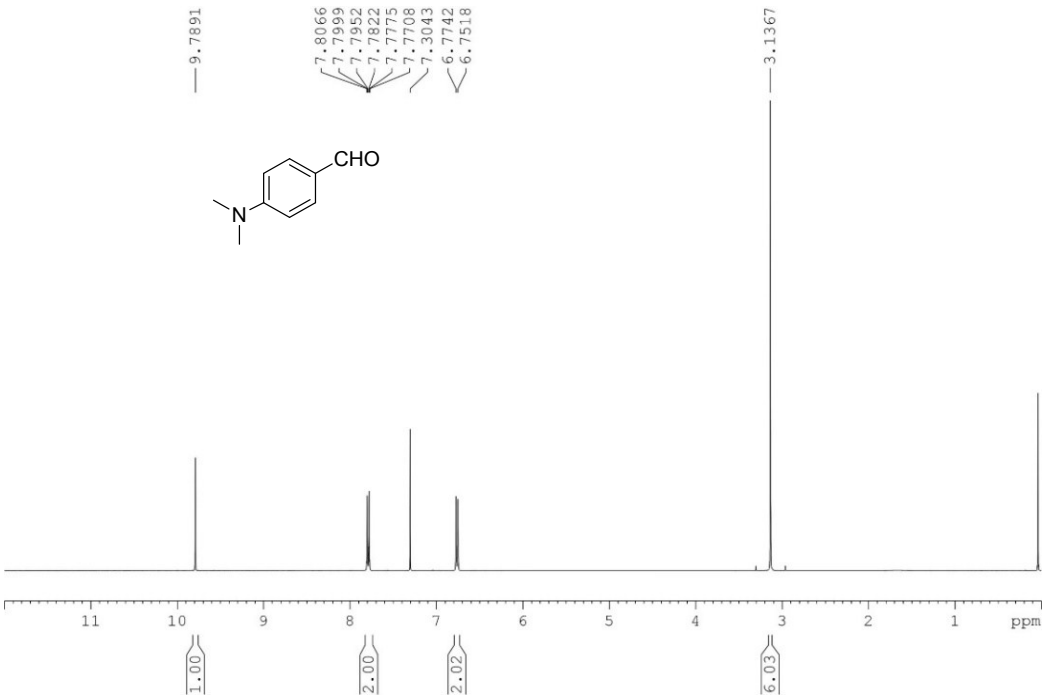
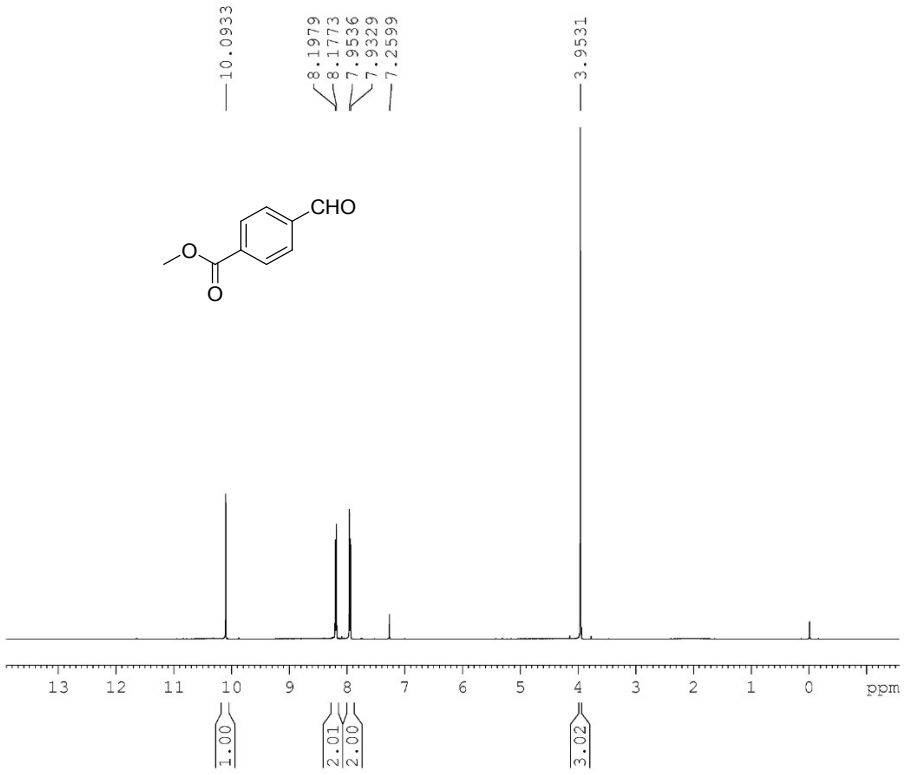
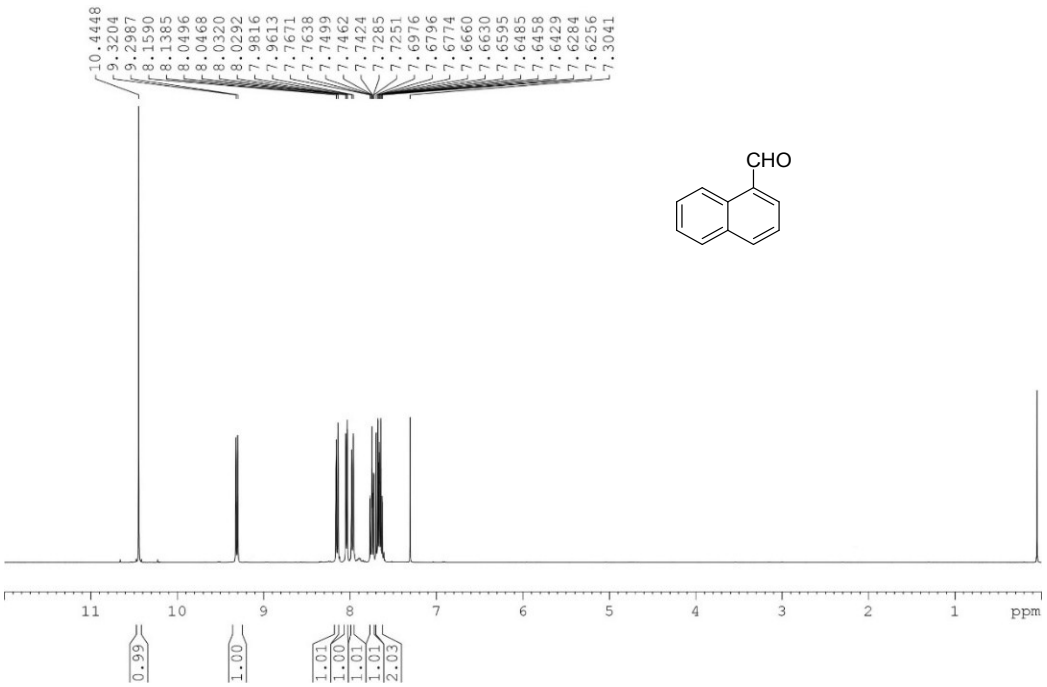
8.4587
8.4544
8.4416
8.4370
8.1375
8.1327
8.1204
8.1156
7.3043
CHO
O2N
10
9
8
7
6
5
4
3
2
1
ppm
0.99
1.97
2.00

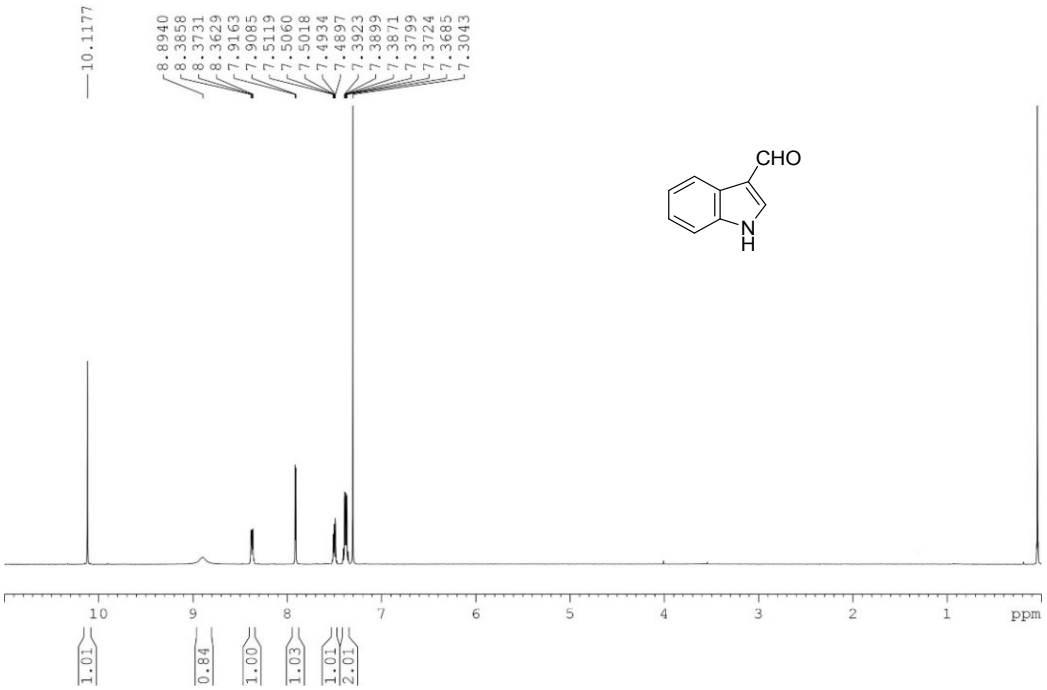

10.3906
7.9159
7.9113
7.8972
7.8929
7.8791
7.8744
7.6659
7.6612
7.6524
7.6476
7.6449
7.6429
7.6404
7.6340
7.6314
7.6294
7.6267
7.6219
7.6131
7.6084
7.3159
7.2969
7.2781
7.2245
7.2227
7.2036
7.2013
7.1988
7.1966
7.1775
7.1756
CHO
F
11
10
9
8
7
6
5
4
3
2
1
ppm
0.89
1.00
1.05
1.14
1.00

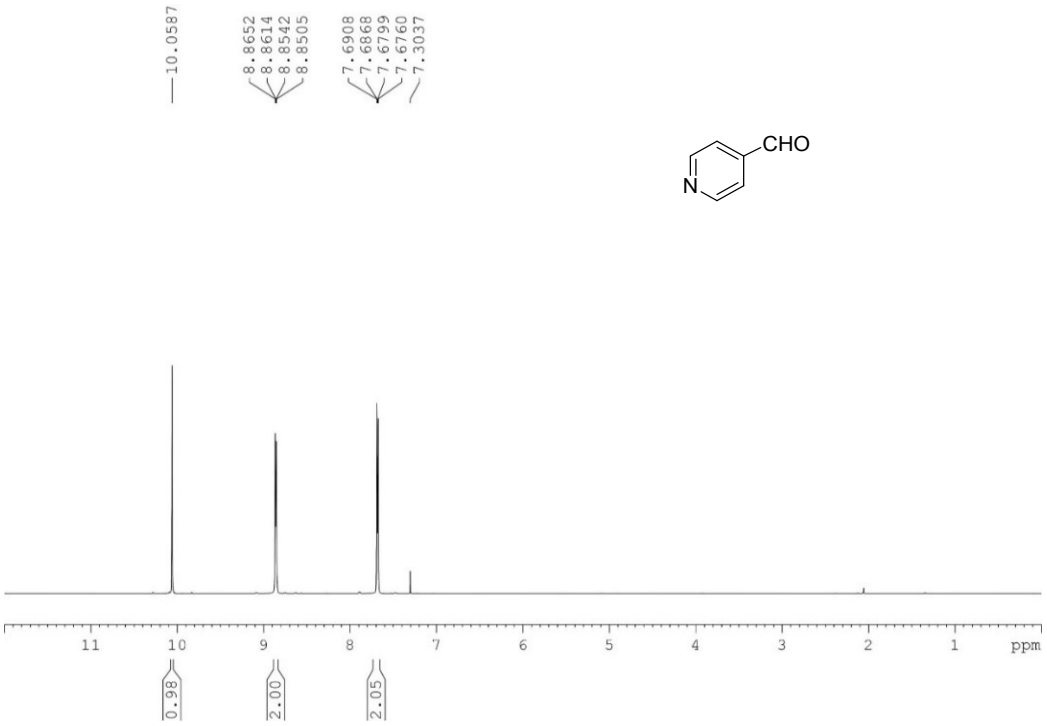

9.8561
7.4709
7.4671
7.4510
7.4473
7.3828
7.3794
7.3042
6.9884
6.9686
6.1262
CHO
O
O
10
9
8
7
6
5
4
3
2
1
ppm
1.01
1.00
0.96
1.00
2.06

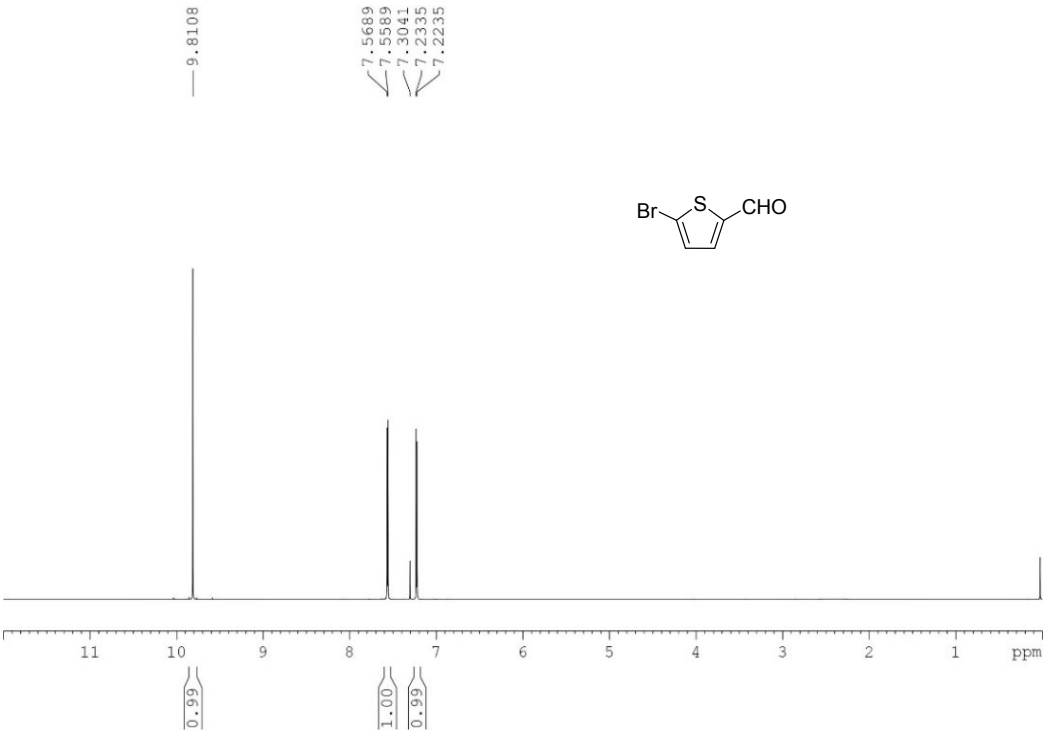

9.7891
7.8066
7.7999
7.7952
7.7822
7.7775
7.7708
7.3043
6.7742
6.7518
3.1367
CHO
N
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
2.00
2.02
6.03

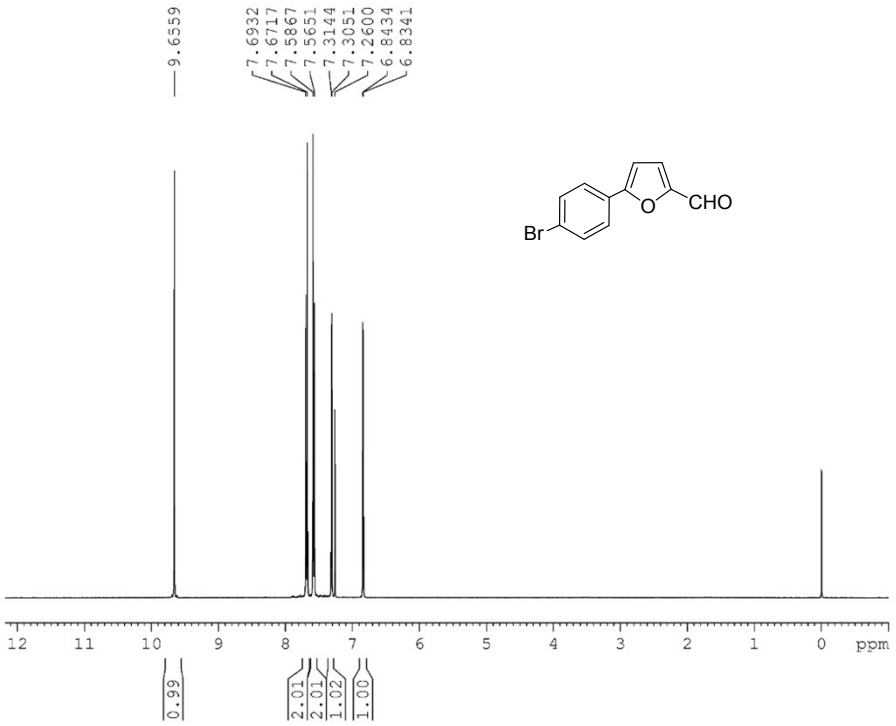

10.0933
8.1979
8.1773
7.9536
7.9329
7.2599
3.9531
CHO
O
O
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.01
2.00
3.02


10.4448
9.3204
9.2987
8.1590
8.1385
8.0496
8.0468
8.0320
8.0292
7.9816
7.9613
7.7671
7.7638
7.7499
7.7462
7.7424
7.7285
7.7251
7.6976
7.6796
7.6774
7.6660
7.6630
7.6595
7.6485
7.6458
7.6429
7.6284
7.6256
7.3041
CHO
11
10
9
8
7
6
5
4
3
2
1
ppm
0.99
1.00
1.01
1.00
1.01
1.01
2.03


10.1177
8.8940
8.3858
8.3731
8.3629
7.9163
7.9085
7.5119
7.5060
7.5018
7.4934
7.4897
7.3923
7.3899
7.3871
7.3799
7.3724
7.3685
7.3043
CHO
N
H
10
9
8
7
6
5
4
3
2
1
ppm
1.01
0.84
1.00
1.03
1.01
2.01


10.0587
8.8652
8.8614
8.8542
8.8505
7.6908
7.6868
7.6799
7.6760
7.3037
CHO
N
11
10
9
8
7
6
5
4
3
2
1
ppm
0.98
2.00
2.05


9.8108
7.5689
7.5589
7.3041
7.2335
7.2235
Br
S
CHO
11
10
9
8
7
6
5
4
3
2
1
ppm
0.99
1.00
0.99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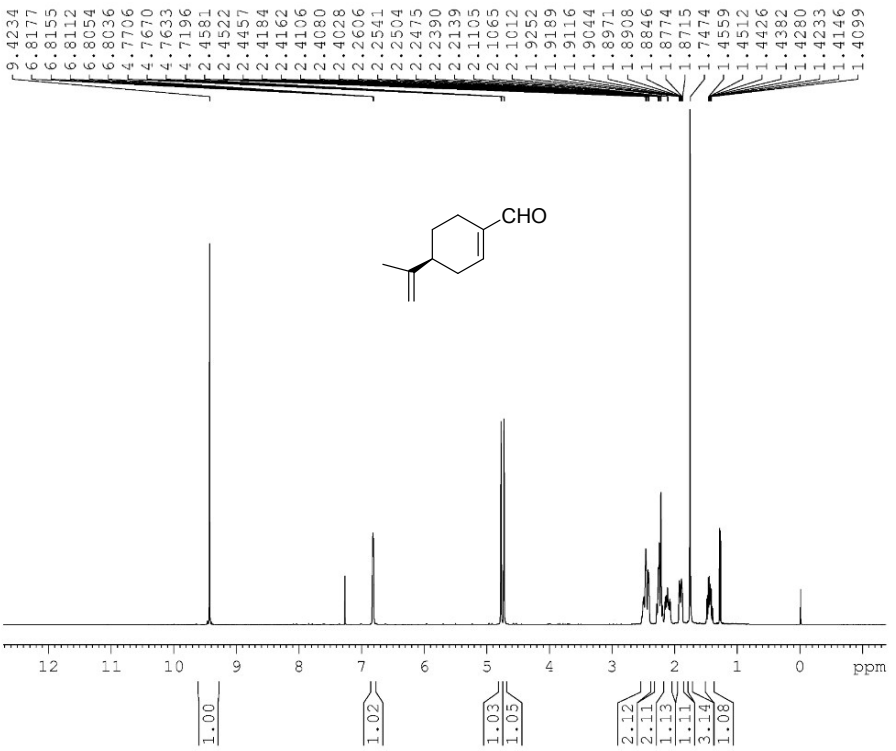
7.6932
7.6717
7.5867
7.5651
7.3144
7.3051
7.2600
6.8434
6.8341
Br
O
CHO
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.99
2.01
2.01
1.02
1.00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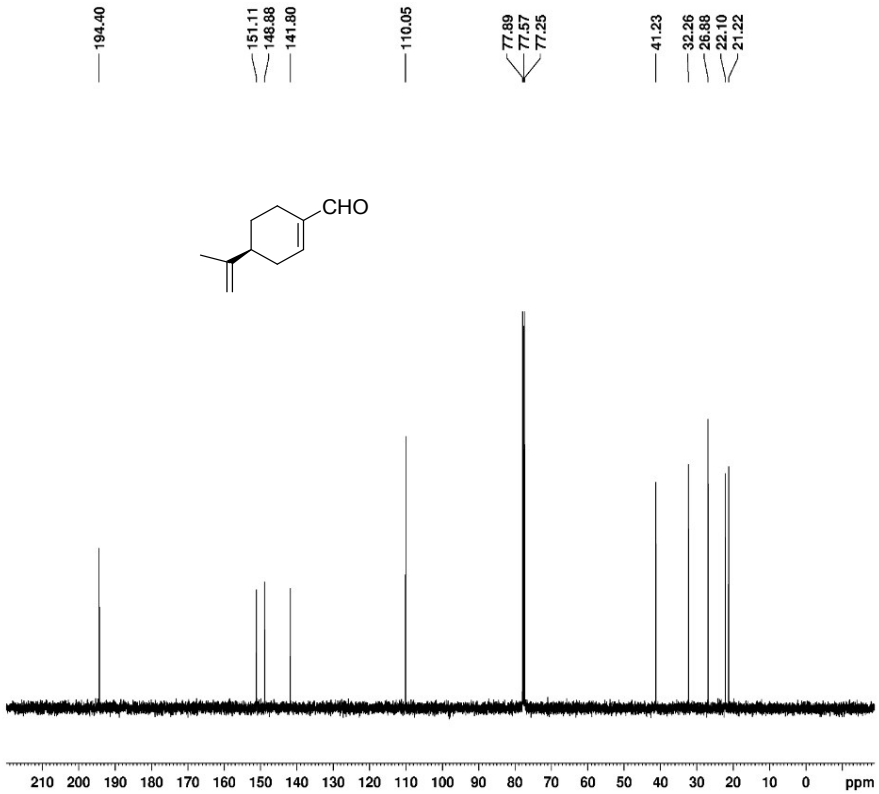
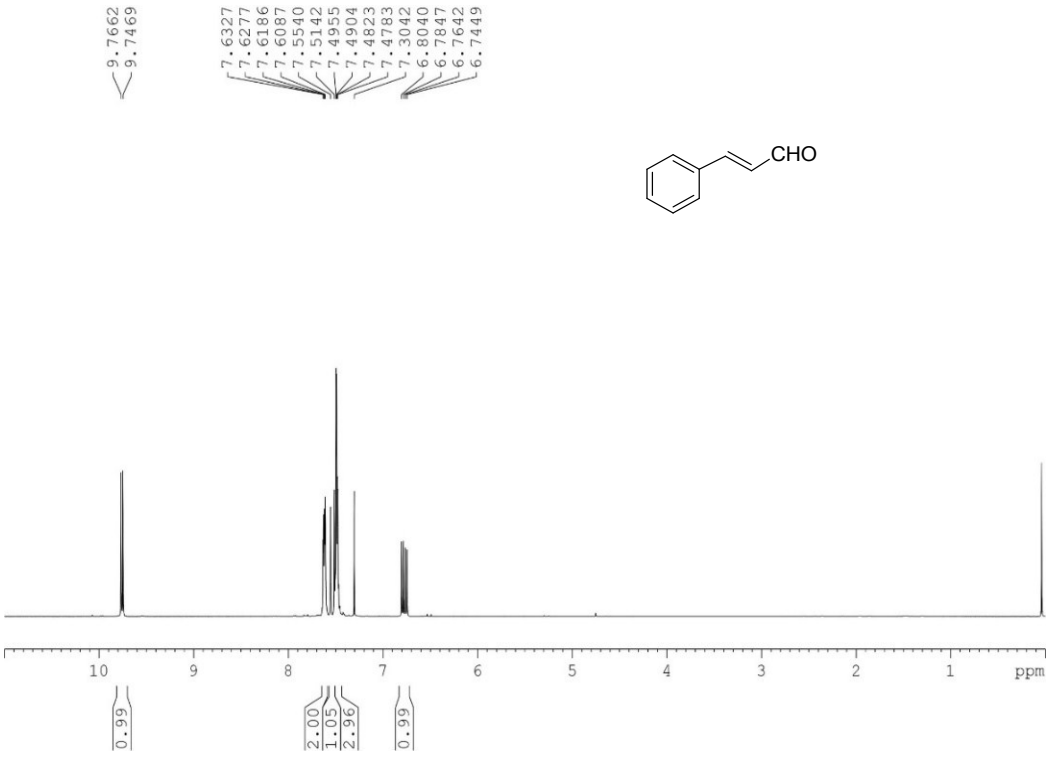
6.8155
6.8112
6.8054
6.8036
4.7706
4.7670
4.7633
4.7196
2.4581
2.4522
2.4457
2.4184
2.4162
2.4106
2.4080
2.4028
2.2606
2.2541
2.2504
2.2475
2.2390
2.2139
2.1105
2.1065
2.1012
1.9252
1.9189
1.9116
1.9044
1.8971
1.8908
1.8846
1.8774
1.8715
1.7474
1.4559
1.4512
1.4426
1.4382
1.4280
1.4233
1.4146
1.4099
CHO
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.02
1.03
1.05
2.12
2.11
1.13
1.11
3.14
1.08


194.40
151.11
148.88
141.80
110.05
77.89
77.57
77.25
41.23
32.26
26.88
22.10
21.22
CHO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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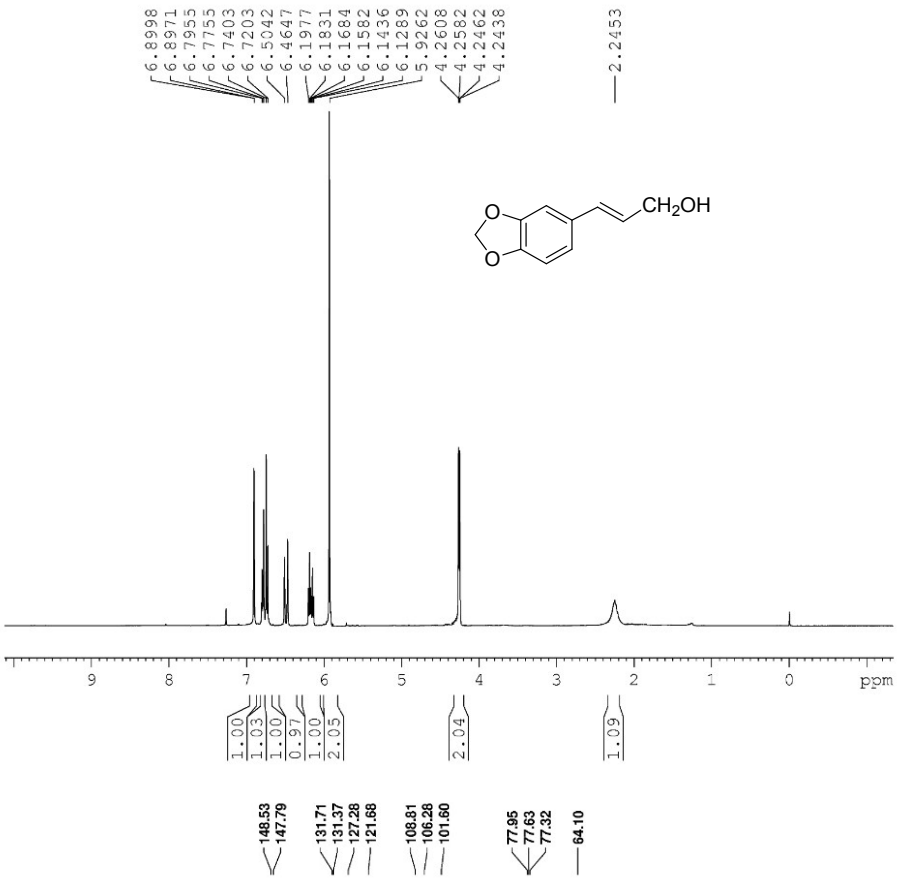
9.7469
7.6327
7.6277
7.6186
7.6087
7.5540
7.5142
7.4955
7.4904
7.4823
7.4783
7.3042
6.8040
6.7847
6.7642
6.7449
CHO
10 9 8 7 6 5 4 3 2 1 ppm
0.99
2.00
1.05
2.96
0.99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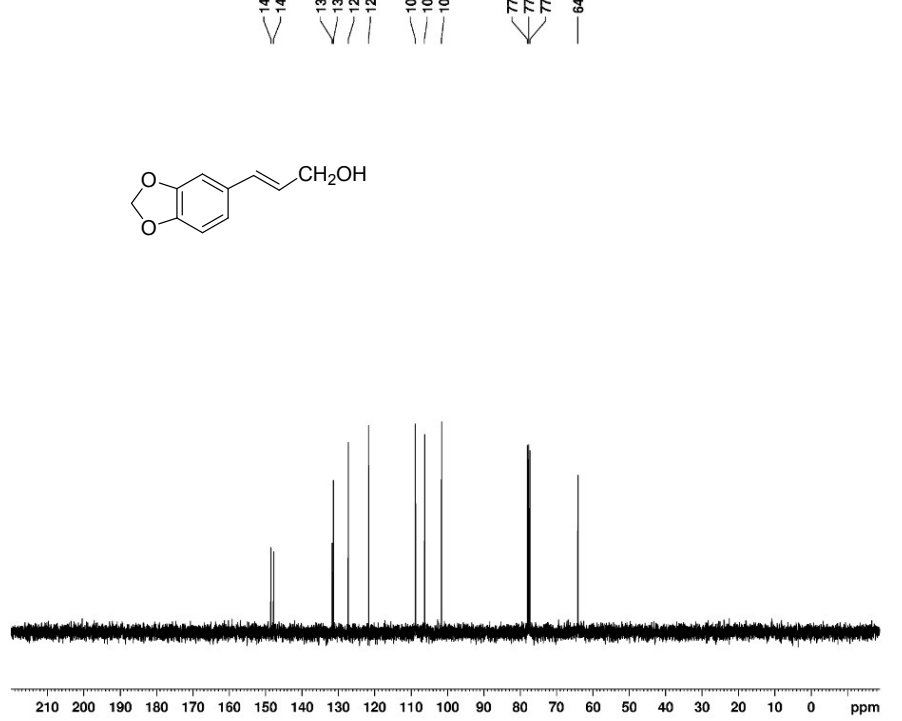
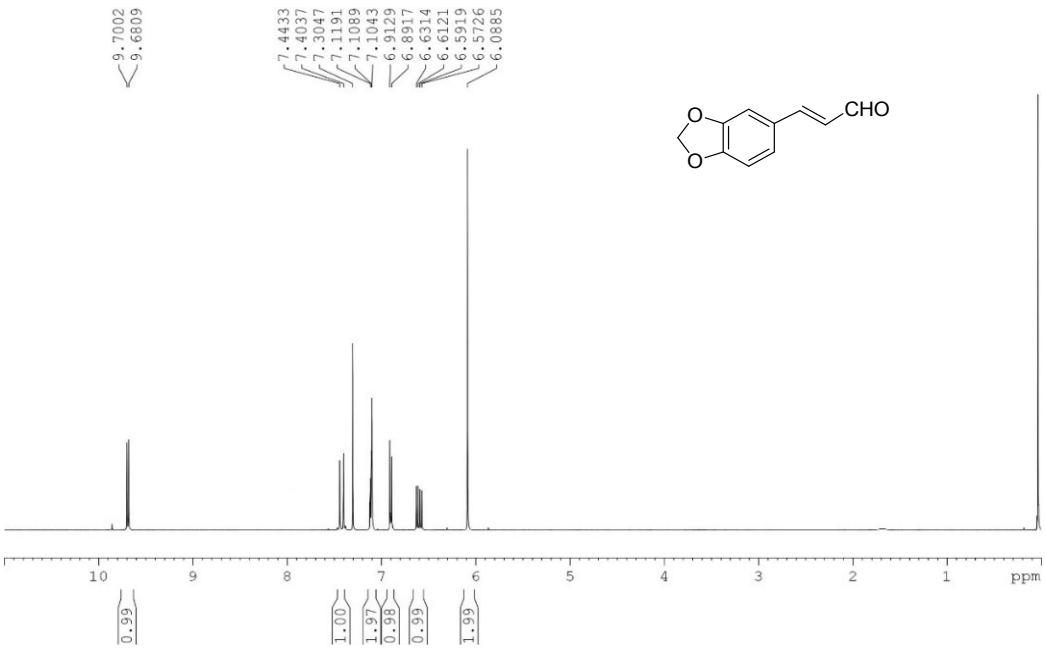
6.8971
6.7955
6.7755
6.7403
6.7203
6.5042
6.4647
6.1977
6.1831
6.1684
6.1582
6.1436
6.1289
5.9262
4.2608
4.2582
4.2462
4.2438
2.2453
CH2OH
O
O
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
1.00
0.97
1.00
2.05
2.04
1.09


148.53
147.79
131.71
131.37
127.28
121.68
108.81
106.28
101.60
77.95
77.63
77.32
64.10
CH2OH
O
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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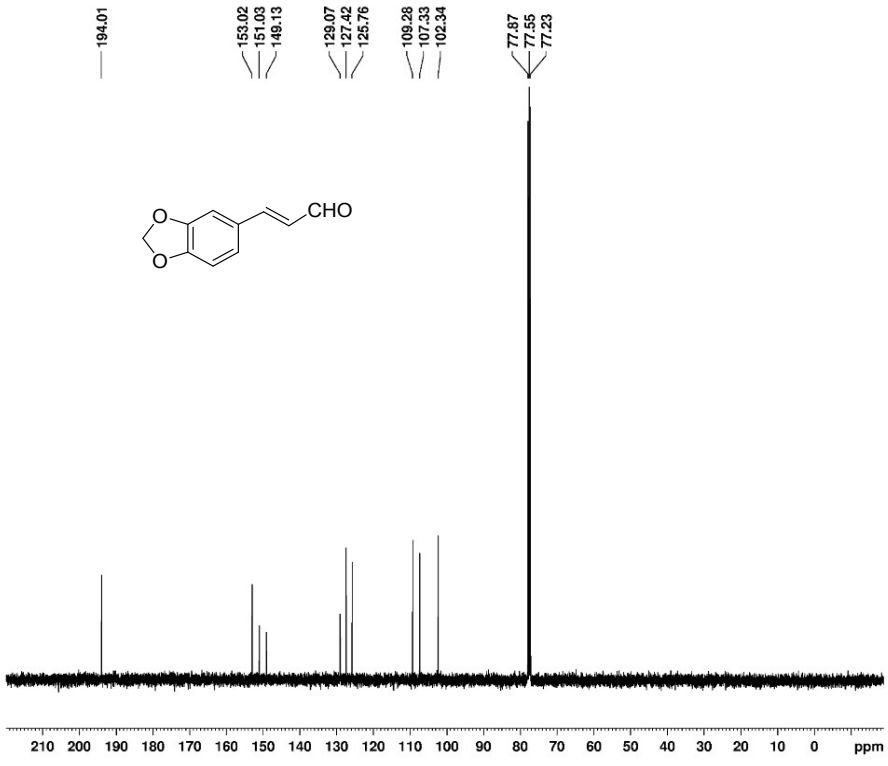
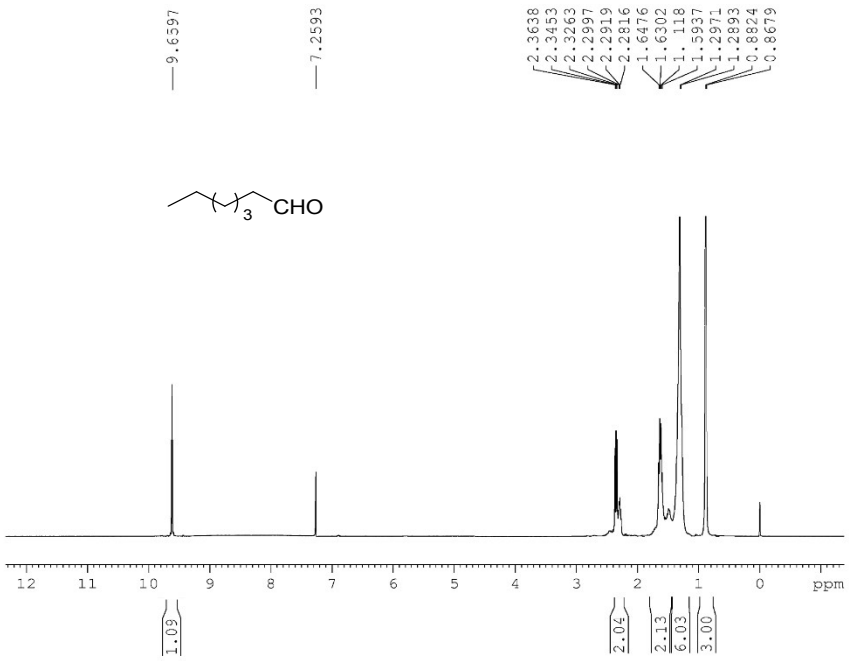
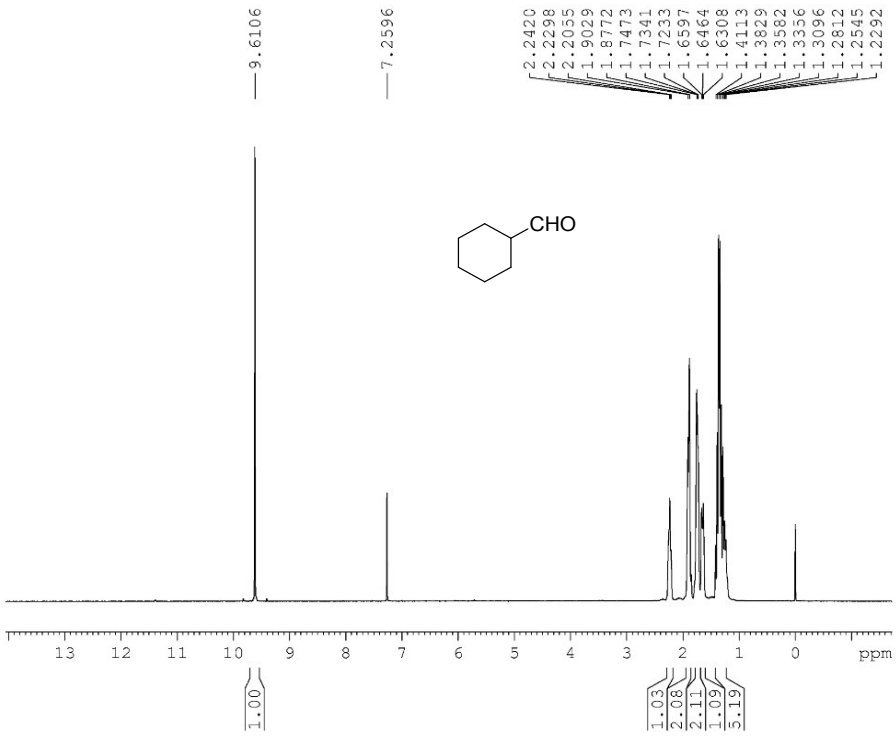
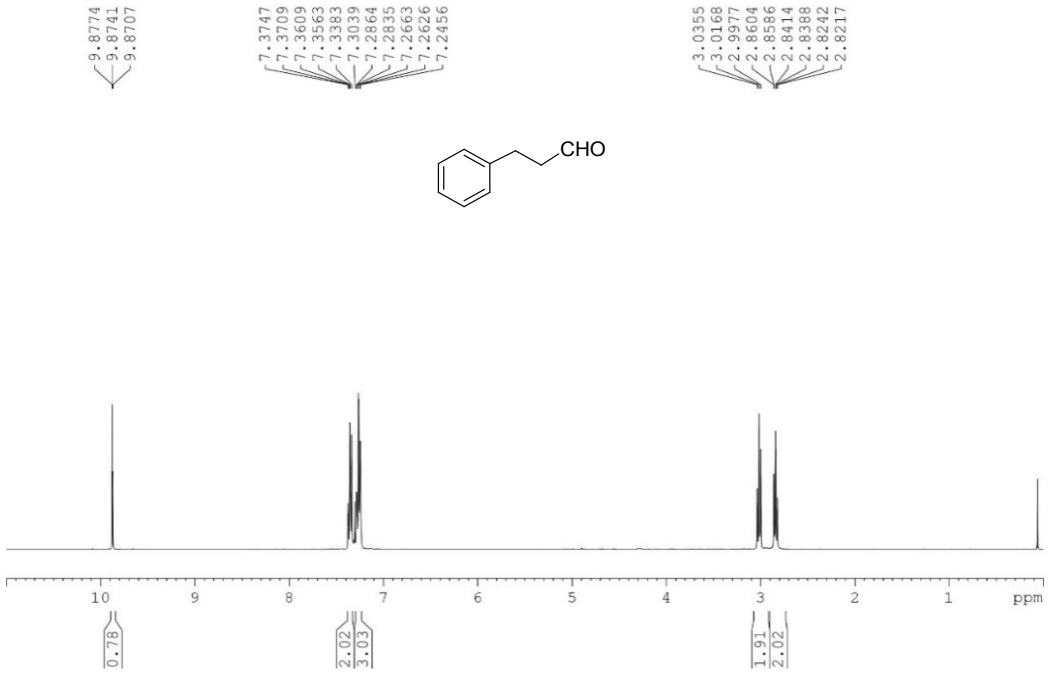
9.6809
7.4433
7.4037
7.3047
7.1191
7.1089
7.1043
6.9129
6.8917
6.6314
6.6121
6.5919
6.5726
6.0885
O
O
CHO
10
9
8
7
6
5
4
3
2
1
ppm
0.99
1.00
1.97
0.98
0.99
1.99


194.01
153.02
151.03
149.13
129.07
127.42
125.76
109.28
107.33
102.34
77.87
77.55
77.23
O
O
CHO
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


9.6597
7.2593
2.3638
2.3453
2.3263
2.2997
2.2919
2.2816
1.6476
1.6302
1.118
1.5937
1.2971
1.2893
0.8824
0.8679
3
CHO
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.09
2.04
2.13
6.03
3.00


9.6106
7.2596
2.2420
2.2298
2.2055
1.9029
1.8772
1.7473
1.7341
1.7233
1.6597
1.6464
1.6308
1.4113
1.3829
1.3582
1.3356
1.3096
1.2812
1.2545
1.2292
CHO
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.03
2.08
2.11
1.09
5.19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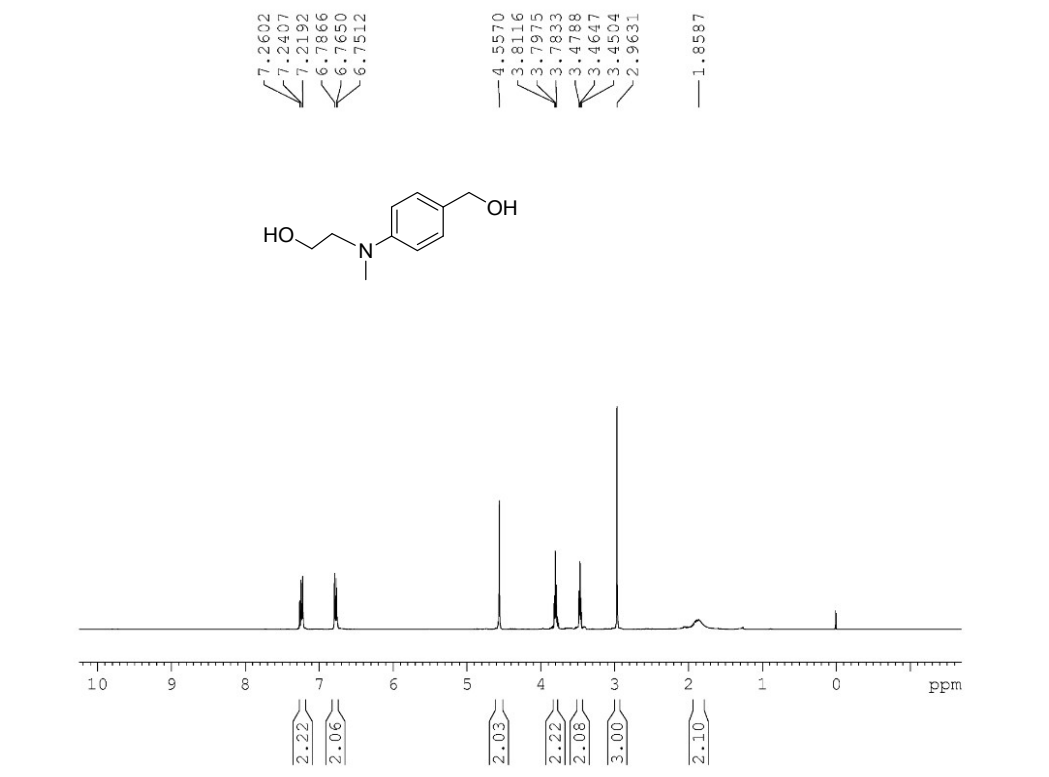
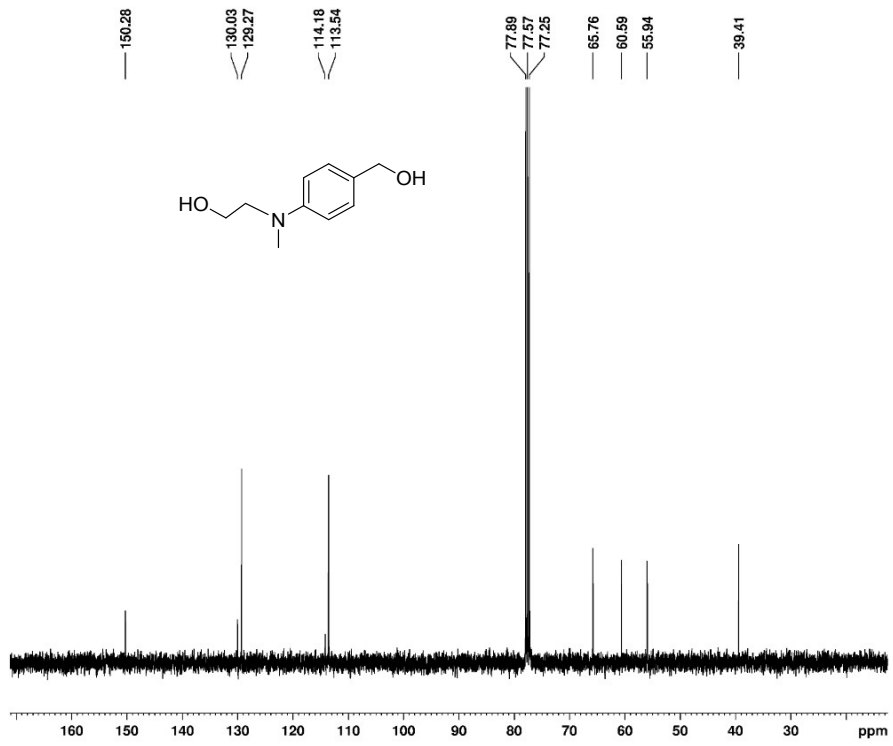
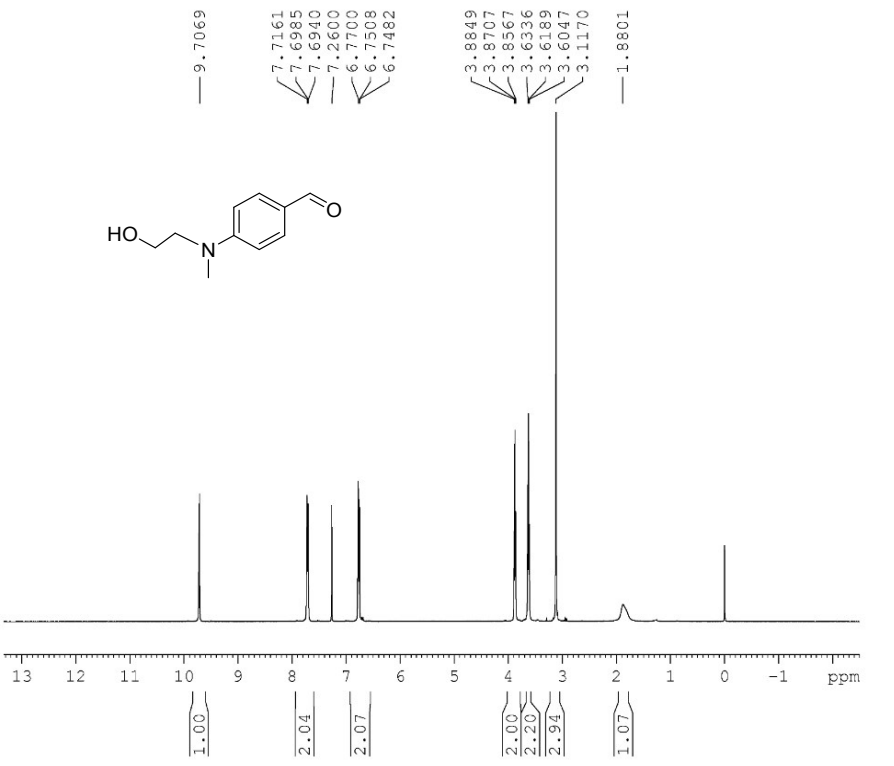
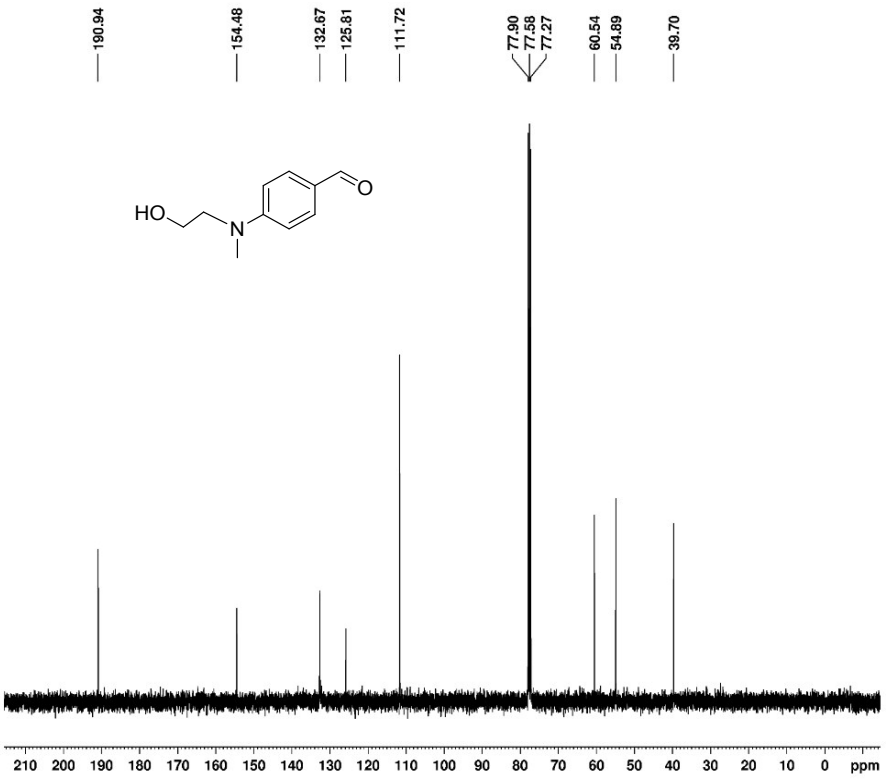
9.8741
9.8707
7.3747
7.3709
7.3609
7.3563
7.3383
7.3039
7.2864
7.2835
7.2663
7.2626
7.2456
3.0355
3.0168
2.9977
2.8604
2.8586
2.8414
2.8388
2.8242
2.8217
CHO
10
9
8
7
6
5
4
3
2
1
ppm
0.78
2.02
3.03
1.91
2.02


7.2602
7.2407
7.2192
6.7866
6.7650
6.7512
4.5570
3.8116
3.7975
3.7833
3.4788
3.4647
3.4504
2.9631
1.8587
HO
N
OH
10
9
8
7
6
5
4
3
2
1
0
ppm
2.22
2.06
2.03
2.22
2.08
3.00
2.10


150.28
130.03
129.27
114.18
113.54
77.89
77.57
77.25
65.76
60.59
55.94
39.41
HO
N
OH
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


9.7069
7.7161
7.6985
7.6940
7.2600
6.7700
6.7508
6.7482
3.8849
3.8707
3.8567
3.6336
3.6189
3.6047
3.1170
1.8801
HO
N
O
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.00
2.04
2.07
2.00
2.20
2.94
1.07


190.94
154.48
132.67
125.81
111.72
77.90
77.58
77.27
60.54
54.89
39.70
HO
N
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm