Supplementary Information

for

Aerobic flow oxidation of alcohols in water catalyzed by an amphiphilic polymer-dispersion of platinum nanoparticles

Takao Osako,[a] Kaoru Torii[a] and Yasuhiro Uozumi*[a,b]

[a] *Institute for Molecular Science (IMS), Myodaiji, Okazaki, Aichi, 444-8787, Japan.*

[b] *RIKEN, 2-1 Hirosawa, Wako, Saitama, 351-0198, Japan.*

E-mail: uo@ims.ac.jp

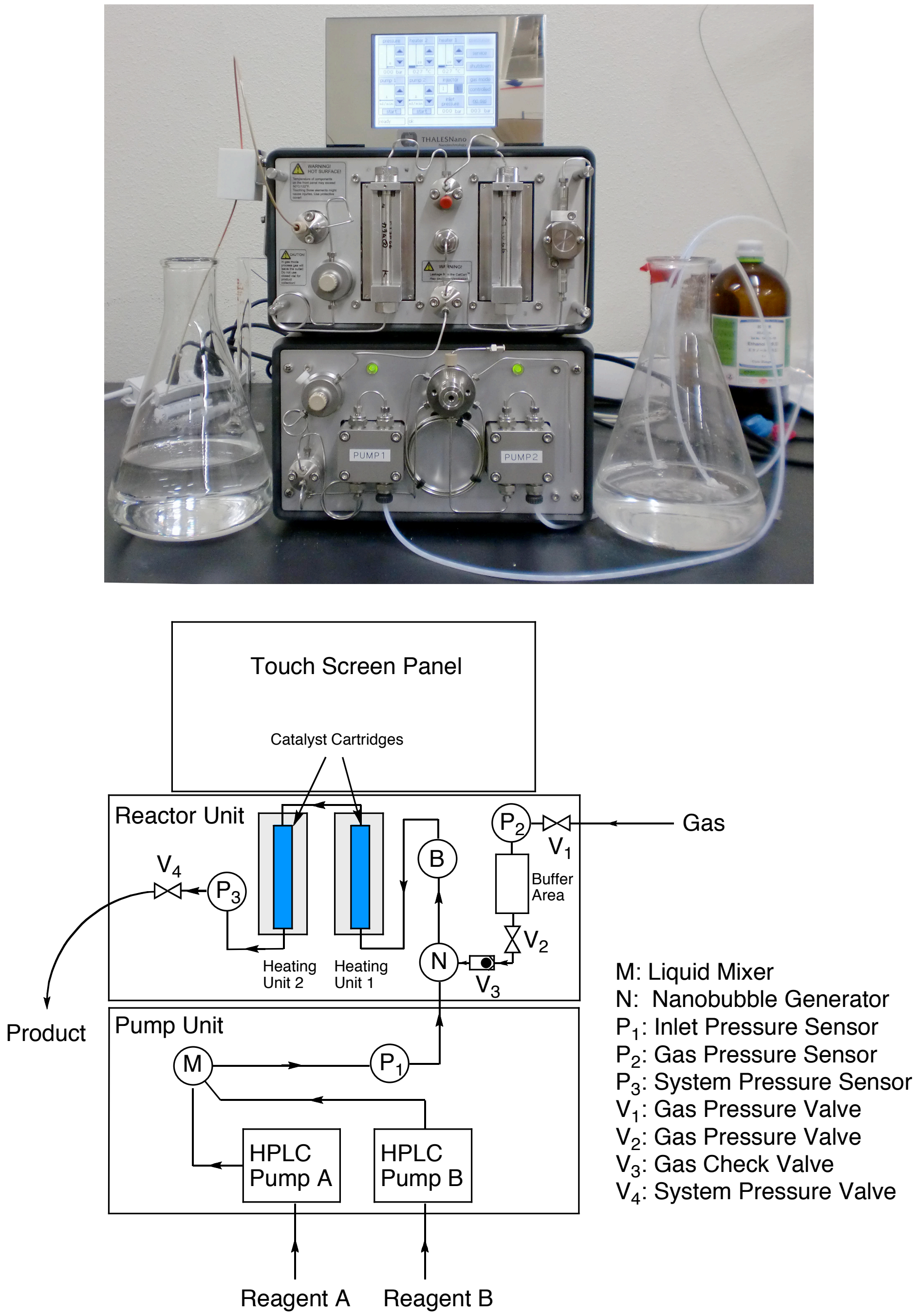


Fig. S1 The picture (top) and the schematic diagram (bottom) of the X-Cube reactor.

Characterization of products.

Acetophenone (**2a**) [CAS: 98-86-2]: ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.96 (dd, J = 8.5 and 1.0 Hz, 2H, Ph_{H-2} and Ph_{H-6}), 7.57 (t, J = 8.0 Hz, 1H, Ph_{H-4}), 7.47 (t, J= 8.0 Hz, 2H, Ph_{H-3} and Ph_{H-5}), 2.61 (s, 3H, $-CH_3$). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 198.10 (C=O), 137.06 (Ph), 133.04 (Ph), 128.50 (Ph), 128.24 (Ph), 26.54 (CH_3). EI-TOF-MS m/z = 120 (M).

4'-Methoxyacetophenone (**2b**) [CAS: 100-06-1]: ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.93 (d, J = 9.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 6.92 (d, J = 9.5 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 3.86 (s, 3H, $-OCH_3$), 2.55 (s, 3H, -CH_3). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 196.72 (C=O), 163.44 (Ar), 130.54 (Ar), 130.30 (Ar), 113.63 (Ar), 55.42 (OCH_3), 26.29 (CH_3). EI-TOF-MS m/z = 150 (M).

4'-Methylacetophenone (**2c**) [CAS: 122-00-9]: ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.85 (d, J = 10.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.26 (d, J =10.0 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 2.56 (s, 3H, $-CH_3$), 2.40 (s, 3H, -CH_3). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 197.74 (C=O), 143.75 (Ar), 134.59 (Ar), 129.12 (Ar), 128.32 (Ar), 26.38 (CH_3), 21.49 (CH_3). EI-TOF-MS m/z = 134 (M).

4'-Chloroacetophenone (**2d**) [CAS: 99-91-2]: ^{1}H NMR (396 MHz, $CDCl_3$): δ = 7.90 (dt, J = 8.7 and 2.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.44 (dt, J = 8.7 and 2.0 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 2.59 (s, 3H, -CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 196.81 (C=O), 139.50 (Ar), 135.34 (Ar), 129.67 (Ar), 128.83 (Ar), 26.53 (CH_3). EI-TOF-MS m/z = 154 (M).

4'-(Trifluoromethyl)acetophenone (**2e**) [CAS: 709-63-7]: ^{1}H NMR (396 MHz, $CDCl_3$): δ = 8.07 (d, J = 7.9 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.74 (d, J = 7.9 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 2.66 (s, 3H, $-CH_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 197.00 (C=O), 139.61 (Ar), 134.38 (q, J = 32.5 Hz, Ar), 128.60 (Ar), 125.65 (q, J = 3.8 Hz Ar), 123.56 (q, J = 272.8 Hz, Ar), 26.78 (CH_3). EI-TOF-MS m/z = 188 (M).

Cyclopropyl phenyl ketone (**2f**) [CAS: 3481-02-5]: ^{1}H NMR (396 MHz, $CDCl_3$): δ = 8.02 (d, J = 7.5 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.57 (tt, J = 7.5 and 1.2 Hz, 1H, Ar_{H-4}), 7.48 (t, J = 7.5 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 2.69 (sept, J = 4.5 Hz, 1H, CH), 1.27-1.24 (m, 2H, CH_2), 1.07-1.03 (m, 2H, CH_2).

$^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 200.58 (C=O), 137.85 (Ar), 132.63 (Ar), 128.39 (Ar), 127.89 (Ar), 17.02 (CH), 11.60 (CH_2). EI-TOF-MS m/z = 146 (M).

2-Pentanone (**2g**) [CAS: 107-87-9]: ^1H NMR (500 MHz, $CDCl_3$): δ = 2.41 (t, J = 7.5 Hz, 2H, -$C\underline{H}_2COCH_3$), 2.14 (s, 3H, $C\underline{H}_3CO$-), 1.61 (sext, J = 7.5 Hz, 2H, $CH_3C\underline{H}_2CH_2$-), 0.92 (t, J = 7.5 Hz, 3H, $C\underline{H}_3CH_2$-). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 209.18 (C=O), 45.63 (-$\underline{C}H_2COCH_3$), 29.79 (-$CO\underline{C}H_3$), 17.24 ($CH_3\underline{C}H_2$-), 13.62 ($\underline{C}H_3CH_2$-). EI-TOF-MS m/z = 86 (M).

2-Hexanone (**2h**) [CAS: 591-78-6]: ^1H NMR (500 MHz, $CDCl_3$): δ = 2.43 (t, J = 7.5 Hz, 2H, -$C\underline{H}_2COCH_3$), 2.14 (s, 3H, $C\underline{H}_3CO$-), 1.56 (quint, J = 7.5 Hz, 2H, -$C\underline{H}_2CH_2COCH_3$), 1.32 (sext, J = 7.5 Hz, 2H, $CH_3C\underline{H}_2CH_2$-), 0.91 (t, J = 7.5 Hz, 3H, $C\underline{H}_3CH_2$-). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 209.35 (C=O), 43.48 (-$\underline{C}H_2COCH_3$), 29.80 (-$CO\underline{C}H_3$), 25.93 ($CH_3CH_2\underline{C}H_2$-), 22.25 ($CH_3\underline{C}H_2CH_2$-), 13.80 ($\underline{C}H_3CH_2$-). EI-TOF-MS m/z = 100 (M).

2-Octanone (**2i**) [CAS: 111-13-7]: ^1H NMR (396 MHz, $CDCl_3$): δ = 2.43 (t, J = 7.1 Hz, 2H, -$C\underline{H}_2COCH_3$), 2.14 (s, 3H, $C\underline{H}_3CO$-), 1.57 (quint, J = 7.1 Hz, 2H, $CH_3C\underline{H}_2CH_2$-), 1.33-1.25 (m, 6H, -CH_2-), 0.88 (t, J = 7.1 Hz, 3H, $C\underline{H}_3CH_2$-). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 209.40 (C=O), 43.73 (-$\underline{C}H_2COCH_3$), 31.52 (-CH_2-), 29.77 (-CH_2-), 28.77 (-$CO\underline{C}H_3$), 23.74 (-CH_2-), 22.42 ($CH_3\underline{C}H_2$-), 13.95 ($\underline{C}H_3CH_2$-). EI-TOF-MS m/z = 128 (M).

2-Decanone (**2j**) [CAS: 693-54-9]: ^1H NMR (396 MHz, $CDCl_3$): δ = 2.42 (t, J = 7.5 Hz, 2H, -$C\underline{H}_2COCH_3$), 2.14 (s, 3H, $C\underline{H}_3CO$-), 1.57 (quint, J = 7.5 Hz, 2H, $CH_3C\underline{H}_2CH_2$-), 1.28 (br-s, 10H, -CH_2-), 0.88 (t, J = 6.7 Hz, 3H, $C\underline{H}_3CH_2$-). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 209.49 (C=O), 43.80 (-$\underline{C}H_2COCH_3$), 31.78 (-CH_2-), 29.84, 29.33, 29.15, 29.11, 23.83, 22.61 ($CH_3\underline{C}H_2$-), 14.07 ($\underline{C}H_3CH_2$-). EI-TOF-MS m/z = 156 (M).

Cyclopentanone (**2k**) [CAS: 120-92-3]: ^1H NMR (500 MHz, $CDCl_3$): δ = 2.18-2.15 (m, 4H, $C\underline{H}_2COC\underline{H}_2$-), 1.98-1.95 (m, 4H, -$C\underline{H}_2C\underline{H}_2$-). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 220.60 (C=O), 38.25 (-$\underline{C}H_2CO\underline{C}H_2$-), 23.13 (-$\underline{C}H_2\underline{C}H_2$-). EI-TOF-MS m/z = 84 (M).

Cyclohexanone (**2l**) [CAS: 108-94-1]: ^1H NMR (500 MHz, $CDCl_3$): δ = 2.34 (t, J = 7.0 Hz, 4H, -$C\underline{H}_2COC\underline{H}_2$-), 1.87 (quint, J = 7.0 Hz, 4H, -$C\underline{H}_2CH_2COCH_2C\underline{H}_2$-), 1.75-1.70 (m, 2H, -

$CH_2CH_2C\underline{H}_2CH_2CH_2$-). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 212.05 (C=O), 41.88 (-$\underline{C}H_2CO\underline{C}H_2$-), 26.92 (-$\underline{C}H_2CH_2COCH_2\underline{C}H_2$-), 24.89 (-$CH_2CH_2\underline{C}H_2CH_2CH_2$-). EI-TOF-MS *m*/*z* = 98 (M).

Cycloheptanone (**2m**) [CAS: 502-42-1]: ^1H NMR (500 MHz, $CDCl_3$): δ = 2.50 (t, *J* = 6.0 Hz, 4H, -$C\underline{H}_2COC\underline{H}_2$-), 1.72-1.68 (m, 8H, -$CH_2(C\underline{H}_2)_4CH_2$-). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 215.31 (C=O), 43.79 (-$\underline{C}H_2CO\underline{C}H_2$-), 30.34 (-$\underline{C}H_2CH_2COCH_2\underline{C}H_2$-), 24.26 (-$CH_2CH_2(\underline{C}H_2)_2CH_2CH_2$-). EI-TOF-MS *m*/*z* = 112 (M).

2-Adamantanone (**2n**) [CAS: 700-58-3]: ^1H NMR (500 MHz, $CDCl_3$): δ = 2.55 (s, 2H, -$C\underline{H}C(O)$-), 2.10-1.94 (m, 12H, alkyl). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 218.47 (C=O), 46.91 (-$\underline{C}HC(O)$-), 39.20 (-CH_2-), 36.23 (-CH_2-), 27.39 (-CH-). EI-TOF-MS *m*/*z* = 150 (M).

(+)-Camphor (**2o**) [CAS: 464-49-3]: The yield of the ketone (82%) was determined by ^1H-NMR with an internal standard ($CHCl_2CHCl_2$: δ = 6.01). The starting alcohol was also observed (13%). ^1H NMR (396 MHz, $CDCl_3$): δ = 2.36 (dt, *J* = 18.2 and 3.6 Hz, 1H, $COC\underline{H}H$), 2.10 (t, *J* = 4.4 Hz, 1H, CH), 2.00-1.90 (m, 1H, CH_2), 1.85 (d, *J* = 18.2 Hz, 1H, $COCH\underline{H}$), 1.69 (td, *J* = 13.1 and 3.6 Hz, 1H, CH_3), 1.44-1.31 (m, 2H, CH_2), 0.96 (s, 3H, CH_3), 0.91 (s, 3H, CH_3), 0.84 (s, 2H, CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 219.71 (C=O), 57.62, 46.71, 43.21, 42.93, 29.81, 26.95, 19.70, 19.06, 9.18. EI-TOF-MS *m*/*z* = 152 (M).

Benzoic acid (**4a**) [CAS: 65-85-0]. ^1H NMR (500 MHz, $CDCl_3$): δ = 8.14 (dd, *J* = 8.0 and 1.0 Hz, 2H, Ph_{H-2} and Ph_{H-6}), 7.62 (td, *J* = 7.5 and 1.0 Hz, 1H, Ph_{H-4}), 7.49 (t, *J* = 8.0 Hz, 2H, Ph_{H-3} and Ph_{H-5}). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 172.34 (C=O), 133.82 (Ph), 130.21 (Ph), 129.30 (Ph), 128.48 (Ph). EI-TOF-MS *m*/*z* = 122 (M).

p-Anisic acid (**4b**) [CAS: 100-09-4]. ^1H NMR (500 MHz, DMSO-d_6): δ = 12.63 (s, 1H, COOH), 7.89 (dt, *J* = 9.5 and 2.5 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.02 (dt, *J* = 8.5 and 2.0 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 3.82 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6): δ = 167.06 (C=O), 162.87 (Ar), 131.39 (Ar), 122.99 (Ar), 113.84 (Ar), 55.47 (CH_3). EI-TOF-MS *m*/*z* = 152 (M).

p-Toluic acid (**4c**) [CAS: 99-94-5]. ^1H NMR (500 MHz, DMSO-d_6): δ = 12.84 (br-s, 1H, COOH), 7.88 (d, *J* = 8.5 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.34 (d, *J* = 8.5 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 2.41 (s, 3H, -CH_3).

$^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6): δ = 167.33 (C=O), 143.04 (Ar), 129.35 (Ar), 129.13 (Ar), 128.04 (Ar), 21.13 (CH_3). EI-TOF-MS m/z = 136 (M).

4-Chlorobenzoic acid (**4d**) [CAS: 74-11-3]. ^1H NMR (500 MHz, DMSO-d_6): δ = 13.19 (br-s, 1H, COOH), 7.95 (dt, J = 9.0 and 2.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.58 (dt, J = 8.5 and 2.0 Hz, 2H, Ar_{H-3} and Ar_{H-5}). $^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6): δ = 166.46 (C=O), 137.80 (Ar), 131.14 (Ar), 129.64 (Ar), 128.73 (Ar). EI-TOF-MS m/z = 156 (M).

4-Nitrobenzoic acid (**4e**) [CAS: 62-23-7]. ^1H NMR (500 MHz, DMSO-d_6): δ = 13.69 (br-s, 1H, COOH), 8.33 (dt, J = 9.0 and 2.5 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 8.17 (dt, J = 9.0 and 2.5 Hz, 2H, Ar_{H-3} and Ar_{H-5}). $^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6): δ = 165.77 (C=O), 150.02 (Ar), 136.37 (Ar), 130.66 (Ar), 123.71 (Ar). EI-MS m/z = 167 (M).

4-(Trifluoromethyl)benzoic acid (**4f**) [CAS: 455-24-3]. ^1H NMR (500 MHz, DMSO-d_6): δ = 13.48 (br-s, 1H, COOH), 8.17 (d, J = 8.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.88 (d, J = 8.5 Hz, 2H, Ar_{H-3} and Ar_{H-5}). $^{13}C\{^1H\}$ NMR (126 MHz, DMSO-d_6): δ = 166.26 (C=O), 134.64 (Ar), 132.56 (q, J = 32.1 Hz, Ar), 130.13 (Ar), 123.841 (q, J = 272.7 Hz, CF_3). EI-TOF-MS m/z = 190 (M).

Terephthalic acid (**4g**) [CAS: 100-21-0]. ^1H NMR (500 MHz, DMSO-d_6): δ = 13.28 (br-s, 2H, COOH), 8.04 (s, 4H, Ar). $^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6): δ = 166.79 (C=O), 134.54 (Ar), 129.57 (Ar). EI-MS m/z = 166 (M).

o-Toluic acid (**4h**) [CAS: 118-90-1]. ^1H NMR (500 MHz, $CDCl_3$): δ = 12.52 (br-s, 1H, COOH), 8.08 (d, J = 7.5 Hz, 1H, Ar_{H-6}), 7.45 (td, J = 7.5 and 1.5 Hz, 1H, Ar_{H-4}), 7.28-7.25 (m, 2H, Ar_{H-3} and Ar_{H-5}). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 173.47 (C=O), (Ar), 141.37 (Ar), 132.96 (Ar), 131.92 (Ar), 131.59 (Ar), 128.32 (Ar), 125.85 (Ar), 22.11 (CH_3). EI-TOF-MS m/z = 136 (M).

m-Toluic acid (**4i**) [CAS: 99-04-7]. ^1H NMR (396 MHz, $CDCl_3$): δ = 11.31 (br-s, 1H, COOH), 7.93 (s, 1H, Ar_{H-2}), 7.92 (d, J = 7.9 Hz, 1H, Ar_{H-6}), 7.42-7.33 (m, 2H, Ar_{H-4} and Ar_{H-5}), 2.41 (s, 3H, CH_3). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 172.60 (C=O), 138.30 (Ar), 134.59 (Ar), 130.71 (Ar), 129.24 (Ar), 128.37 (Ar), 127.37 (Ar), 21.24 (CH_3). EI-TOF-MS m/z = 136 (M).

2-Chrolobenzoic acid (**4j**) [CAS: 118-91-2]. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 13.38 (br-s, 1H, COOH), 7.78 (d, J = 8.0 Hz, 1H, $Ar_{H\text{-}6}$), 7.56-7.52 (m, 2H, $Ar_{H\text{-}3}$ and $Ar_{H\text{-}4}$), 7.43 (ddd, J = 7.8, 5.5 and 2.5 Hz, 1H, $Ar_{H\text{-}5}$). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ = 166.72 (C=O), 132.56 (Ar), 131.54 (Ar), 131.47 (Ar), 130.77 (Ar), 130.59 (Ar), 127.22 (Ar). EI-TOF-MS m/z = 156 (M).

3-Chrolobenzoic acid (**4k**) [CAS: 535-80-8]. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 13.34 (br-s, 1H, COOH), 7.91-7.90 (m, 2H, $Ar_{H\text{-}2}$ and $Ar_{H\text{-}6}$), 7.71 (d, J = 8.5 Hz, 1H, $Ar_{H\text{-}4}$), 7.55 (t, J = 8.5 Hz, 1H, $Ar_{H\text{-}5}$). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 166.11 (C=O), 133.37 (Ar), 132.91 (Ar), 132.76 (Ar), 130.71 (Ar), 128.86 (Ar), 127.96 (Ar). EI-TOF-MS m/z = 156 (M).

Methyl terephthalate (**4l**) [CAS: 39379-10-7]. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 13.36 (br-s, 1H, COOH), 8.09-8.06 (m, 4H, Ar), 3.90 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ = 166.56 (COOH), 165.62 ($\underline{C}OOCH_3$), 134.82 (Ar), 133.17 (Ar), 129.59 (Ar), 129.34 (Ar), 52.45 (CH_3). EI-TOF-MS m/z = 180 (M).

Piperonylic acid (**4m**) [CAS: 94-53-1]. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 12.81 (br-s, 1H, COOH), 7.59 (dd, J = 8.0 and 2.0 Hz, 1H, $Ar_{H\text{-}6}$), 7.41 (d, J = 2.0 Hz, 1H, $Ar_{H\text{-}2}$), 7.04 (d, J = 8.0 Hz, 1H, $Ar_{H\text{-}5}$), 6.17 (s, 2H, CH_2). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ = 166.64 (COOH), 151.14 (Ar), 147.48 (Ar), 124.97 (Ar), 124.66 (Ar), 108.80 (Ar), 108.06 (Ar), 101.95 (CH_2). EI-TOF-MS m/z = 166 (M).

4-(Methylthio)benzoic acid (**4n**) [CAS: 13205-48-6]. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 12.86 (br-s, 1H, COOH), 7.87 (d, J = 8.5 Hz, 2H, $Ar_{H\text{-}2}$ and $Ar_{H\text{-}6}$), 7.35 (d, J = 8.5 Hz, 2H, $Ar_{H\text{-}3}$ and $Ar_{H\text{-}5}$), 2.53 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ = 167.04 (COOH), 144.77 (Ar), 129.70 (Ar), 126.72 (Ar), 124.87 (Ar), 13.95 (CH_3). EI-TOF-MS m/z = 168 (M).

4-Aminobenzaldehyde (**5o**) [CAS: 556-23-8]. The yield (94%) was determined by ^{1}H-NMR with an internal standard ($CHCl_2CHCl_2$: δ = 6.14) due to instability of product **5o**. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 9.71 (s, 1H, CHO), 7.65 (dt, J = 8.5 and 2.5 Hz, 2H, $Ar_{H\text{-}2}$ and $Ar_{H\text{-}6}$), 6.70 (d, J = 9.0 Hz, 2H, $Ar_{H\text{-}3}$ and $Ar_{H\text{-}5}$). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ = 190.18 (C=O), 153.29 (Ar), 132.19 (Ar), 126.40 (Ar), 113.60 (Ar). EI-MS m/z = 135 (M).

4-Hydroxybenzaldehyde (**5p**) [CAS: 123-08-0]. ^{1}H NMR (396 MHz, DMSO-d_6): δ = 10.60 (br-s, 1H, phenolic OH), 9.79 (s, 1H, CHO), 7.76 (dt, J = 8.7 and 2.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 6.93 (dt, J = 8.7 and 2.4 Hz, 2H, Ar_{H-3} and Ar_{H-5}). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6)): δ = 191.01 (C=O), 163.32 (Ar), 132.13 (Ar), 128.42 (Ar), 115.85 (Ar). EI-TOF-MS m/z = 121(M-1), 122 (M).

4-(*tert*-Butoxycarbonylamino)benzoic acid (**4q**) [CAS: 66493-39-8]. ^{1}H NMR (500 MHz, DMSO-d_6): δ = 12.61 (br-s, 1H, COOH), 9.74 (s, 1H, NH), 7.83 (dt, J = 9.0 and 2.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.55 (d, J = 8.5 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 1.49 (s, 9H, -C(CH_3)$_3$). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ = 166.99 (C=O), 152.52 (NHCO), 143.76 (Ar), 130.34 (Ar), 123.93 (Ar), 117.19 (Ar), 79.64 ($\underline{C}$(CH_3)$_3$), 28.04(C($\underline{C}H_3$)$_3$). EI-MS m/z = 237 (M).

4-Acetoxybenzoic acid (**4r**) [CAS: 2345-34-8]. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.15 (dt, J = 9.0 and 2.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.22 (dt, J = 8.5 and 2.0 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 2.34 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 171.13 (COOH), 168.89 (O$\underline{C}$(O)CH_3), 154.91 (Ar), 131.84 (Ar), 126.84 (Ar), 121.74 (Ar), 21.16 (CH_3). EI-TOF-MS m/z = 180 (M).

2-Picolinic acid (**4s**) [CAS: 98-98-6]. ^{1}H NMR (396 MHz, DMSO-d_6): δ = 13.16 (br-s, 1H, COOH), 8.72 (d, J = 4.0 Hz, 1H, Ar_{H-6}), 8.06 (d, J = 8.0 Hz, 1H, Ar_{H-3}), 7.99 (td, J = 8.0 and 1.2 Hz, 1H, Ar_{H-5}), 7.64 (ddd, J = 8.0, 4.6 and 1.2 Hz, 1H, Ar_{H-4}). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 166.21 (C=O), 149.46 (Ar), 148.34 (Ar), 137.55 (Ar), 127.12 (Ar), 124.69 (Ar). EI-TOF-MS m/z = 123 (M).

2-Thiophenecarboxylic acid (**4t**) [CAS: 527-72-0]. ^{1}H NMR (396 MHz, DMSO-d_6): δ = 13.09 (br-s, 1H, COOH), 7.89 (dd, J = 4.8 and 1.2 Hz, 1H, Ar_{H-5}), 7.74 (d, J = 3.6 Hz, 1H, Ar_{H-3}), 7.20 (dd, J = 5.0 and 3.6 Hz, 1H, Ar_{H-4}). ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6): δ = 162.96 (C=O), 134.66 (Ar), 133.32 (Ar), 133.25 (Ar), 128.27 (Ar). EI-TOF-MS m/z = 128 (M).

2-Furancarboxylic acid (**4u**) [CAS: 88-14-2]. ^{1}H NMR (396 MHz, $CDCl_3$): δ = 7.68 (d, J = 2.0 Hz, 1H, Ar_{H-5}), 7.35 (d, J = 3.6 Hz, 1H, Ar_{H-3}), 6.57 (dd, J = 3.6 and 2.0 Hz, 1H, Ar_{H-4}). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 163.40 (C=O), 147.44 (Ar), 143.76 (Ar), 120.15 (Ar), 112.29 (Ar). EI-TOF-MS m/z = 112 (M).

Cinnamic acid (**4v**) [CAS: 140-10-3]. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 11.84 (br-s, 1H, COOH), 7.80 (d, J = 16.0 Hz, 1H, -$C\underline{H}$=CHCOOH), 7.57-7.55 (m, 2H, $Ar_{H\text{-}2}$ and $Ar_{H\text{-}6}$), 7.42-7.39 (m, 3H, $Ar_{H\text{-}3}$, $Ar_{H\text{-}4}$, and $Ar_{H\text{-}5}$), 6.46 (d, J = 15.5, 1H, -CH=$C\underline{H}$COOH). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$): δ = 172.61 (C=O), 147.12 (-$\underline{C}$H=CHCOOH), 134.01 (Ar), 130.75 (Ar), 128.95 (Ar), 128.37 (Ar), 117.31 (-CH=$\underline{C}$HCOOH). EI-TOF-MS m/z = 147 (M-1), 148 (M).

Pentanoic acid (**4w**) [CAS: 109-52-4]. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.36 (t, J = 7.5 Hz, 2H, $CH_3(CH_2)_2C\underline{H}_2COOH$), 1.62 (quint, J = 7.5 Hz, 2H, $CH_3CH_2C\underline{H}_2CH_2COOH$), 1.37 (sext, J = 7.5 Hz, 2H, $CH_3C\underline{H}_2(CH_2)_2COOH$), 0.92 (t, J = 6.5, 3H, CH_3-). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 180.22 (C=O), 33.78 ($CH_3(CH_2)_2\underline{C}H_2COOH$), 26.71 ($CH_3CH_2\underline{C}H_2CH_2COOH$), 22.15 ($CH_3\underline{C}H_2(CH_2)_2COOH$), 13.65 ($\underline{C}H_3$-). EI-TOF-MS m/z = 87 (M-15).

Hexanoic acid (**4x**) [CAS: 142-62-1]. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.35 (t, J = 7.5 Hz, 2H, -$C\underline{H}_2COOH$), 1.64 (quint, J = 7.5 Hz, 2H, -$C\underline{H}_2CH_2COOH$), 1.36-1.31 (m, 4H, -$(CH_2)_2$-), 0.90 (t, J = 6.5, 3H, CH_3-). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 180.08 (C=O), 34.01 ($CH_3(CH_2)_3\underline{C}H_2COOH$), 31.19 ($CH_3CH_2\underline{C}H_2(CH_2)_2COOH$), 24.35 ($CH_3(CH_2)_2\underline{C}H_2CH_2COOH$), 22.28 ($CH_3\underline{C}H_2(CH_2)_3COOH$), 13.85 ($CH_3$-). EI-TOF-MS m/z = 87 (M-29).

Octanoic acid (**4y**) [CAS: 124-07-2]. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.35 (t, J = 7.5 Hz, 2H, -$C\underline{H}_2COOH$), 1.64 (quint, J = 7.5 Hz, 2H, -$C\underline{H}_2CH_2COOH$), 1.33-1.28 (m, 8H, -$(CH_2)_4$-), 0.88 (t, J = 7.0 Hz, 3H, CH_3-). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 180.35 (C=O), 34.09 ($CH_3(CH_2)_5\underline{C}H_2COOH$), 31.61 ($CH_3CH_2\underline{C}H_2(CH_2)_4COOH$), 29.00 ($CH_3(CH_2)_2\underline{C}H_2(CH_2)_3COOH$), 28.87 ($CH_3(CH_2)_3\underline{C}H_2(CH_2)_2COOH$), 24.66 ($CH_3(CH_2)_4\underline{C}H_2CH_2COOH$), 22.56 ($CH_3\underline{C}H_2(CH_2)_5COOH$), 14.01 ($CH_3$-). EI-TOF-MS m/z = 144 (M).

Decanoic acid (**4z**) [CAS: 334-48-5]. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.36 (t, J = 7.5 Hz, 2H, -$C\underline{H}_2COOH$), 1.63 (quint, J = 7.5 Hz, 2H, -$C\underline{H}_2CH_2COOH$), 1.33-1.27 (m, 12H, -$(CH_2)_6$-), 0.88 (t, J = 7.0 Hz, 3H, CH_3-). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 179.62 (C=O), 33.99 ($CH_3(CH_2)_7\underline{C}H_2COOH$), 31.87 ($CH_3CH_2\underline{C}H_2(CH_2)_6COOH$), 29.40 ($CH_3(CH_2)_3\underline{C}H_2(CH_2)_4COOH$), 29.25 ($CH_3(CH_2)_2\underline{C}H_2CH_2\underline{C}H_2(CH_2)_3COOH$), 29.07 ($CH_3(CH_2)_5\underline{C}H_2(CH_2)_2COOH$) , 24.70 ($CH_3(CH_2)_6\underline{C}H_2CH_2COOH$), 22.67 ($CH_3\underline{C}H_2(CH_2)_7COOH$), 14.10 (CH_3-). EI-TOF-MS *m*/*z* = 172 (M).

Adipic acid (**4aa**) [CAS : 124-04-9]. ^{1}H NMR(500 MHz, DMSO-d_6) : δ =12.00 (br-s, 2H, COOH), 2.23-2.18 (m, 4H, -$C\underline{H}_2COOH$), 1.50 (quint, J = 3.5 Hz, 4H, -$\underline{C}H_2CH_2COOH$). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6): δ = 174.28 (C=O), 33.35 (-$\underline{C}H_2COOH$), 24.00 (-$\underline{C}H_2CH_2COOH$). EI-MS *m*/*z* = 128 (M-18).

Benzaldehyde (**5a**) [CAS: 100-52-7]. ^{1}H NMR (396 MHz, $CDCl_3$): δ = 10.02 (s, 1H, CHO), 7.89 (d, J = 7.2 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.64 (tt, J = 7.6 and 1.2 Hz, 1H, Ar_{H-4}), 7.53 (t, J = 7.6 Hz, 2H, Ar_{H-3} and Ar_{H-5}). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 192.35 (C=O), 136.35 (Ar), 134.42 (Ar), 129.68 (Ar), 128.94 (Ar). EI-TOF-MS *m*/*z* = 105 (M-1), 106 (M).

p-Anisaldehyde (**5b**) [CAS: 123-11-5]. ^{1}H NMR (396 MHz, $CDCl_3$): δ = 9.89 (s, 1H, CHO), 7.84 (dt, J = 8.8 and 2.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.01 (dt, J = 8.8 and 2.0 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 3.89 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 190.76 (C=O), 164.54 (Ar), 131.91 (Ar), 129.87 (Ar), 114.24 (Ar), 55.51 (CH_3). EI-TOF-MS *m*/*z* = 135 (M-1), 136 (M).

p-Tolualdehyde (**5c**) [CAS: 104-87-0]. ^{1}H NMR (396 MHz, $CDCl_3$): δ = 9.89 (s, 1H, CHO), 7.70 (d, J = 7.6 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.26 (d, J = 7.6 Hz, 2H, Ar_{H-3} and Ar_{H-5}), 2.37 (s, 3H, CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 192.02 (C=O), 145.54 (Ar), 134.13 (Ar), 129.83 (Ar), 129.67 (Ar), 21.87 (CH_3). EI-TOF-MS *m*/*z* = 119 (M-1), 120 (M).

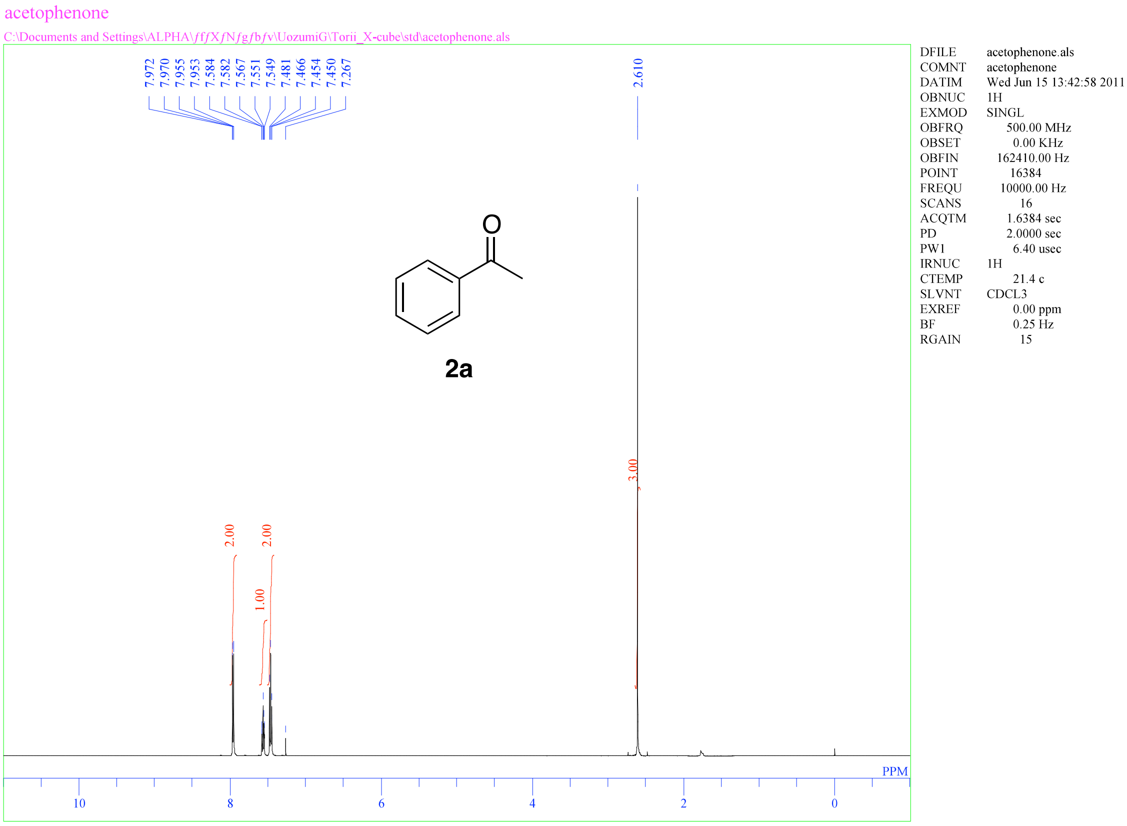
p-Chlorobenzaldehyde (**5d**) [CAS: 104-88-1]. The yield of the aldehyde (62%) was determined by ^{1}H-NMR with an internal standard ($CHCl_2CHCl_2$: δ = 6.88). The starting alcohol and the carboxylic acid were also obtained in 22% and 14% yield, respectively. ^{1}H NMR (396 MHz, DMSO-d_6): δ = 10.01 (s, 1H, CHO), 7.92 (dt, J = 8.4 and 2.0 Hz, 2H, Ar_{H-2} and Ar_{H-6}), 7.64 (dt, J = 8.8 and 2.0 Hz, 2H, Ar_{H-3} and Ar_{H-5}). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ = 191.90 (C=O), 139.49 (Ar), 134.91 (Ar), 131.18 (Ar), 129.33 (Ar). EI-TOF-MS (EI) *m*/*z* = 139 (M-1), 140 (M).

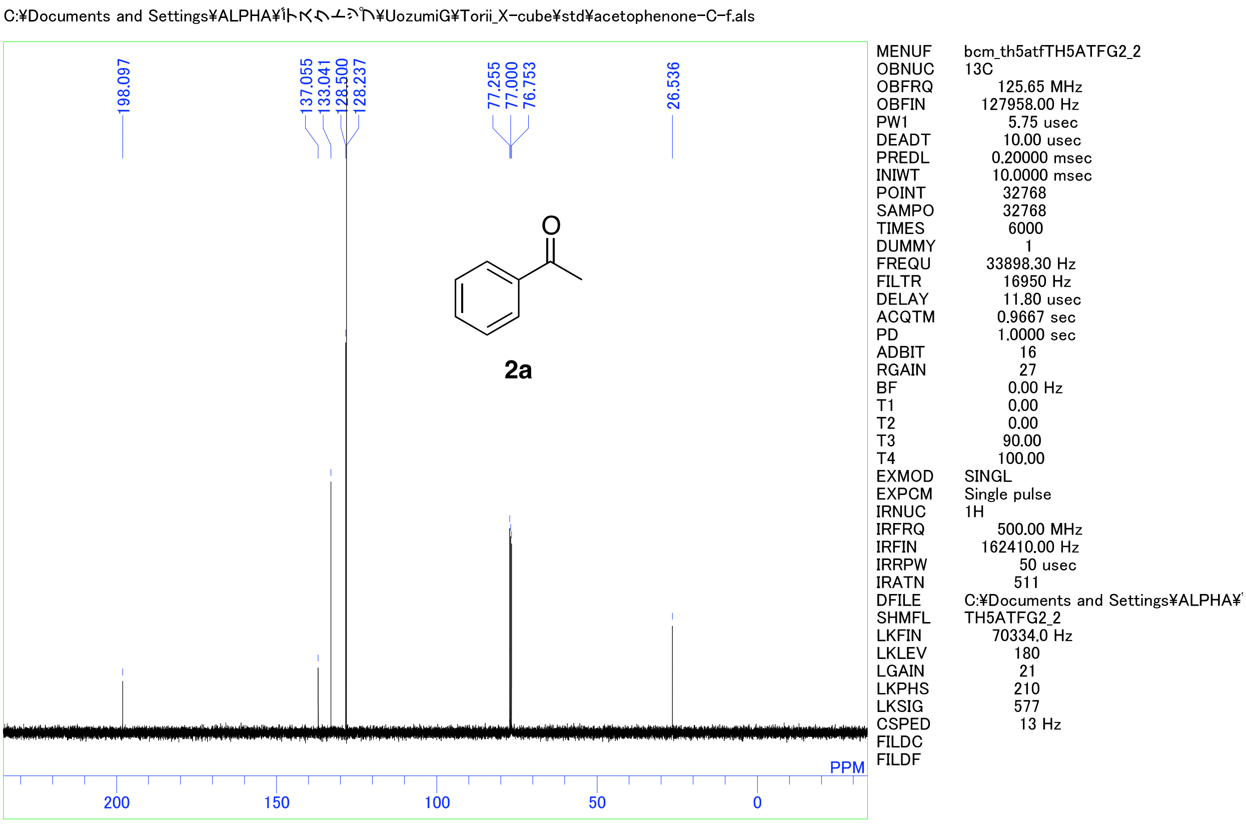
Cinnamaldehyde (**5v**) [CAS: 140-55-2]. ^{1}H NMR (396 MHz, $CDCl_3$): δ = 9.71 (d, J = 8.0 Hz, 1H, CHO), 7.59-7.57 (m, 2H, Ar_{H-2} and Ar_{H-6}), 7.49 (d, J = 16.0 Hz, 2H, -$C\underline{H}$=CHCOOH), 7.46-7.43 (m, 3H, $Ar_{H\text{-}3}$, $Ar_{H\text{-}4}$, and $Ar_{H\text{-}5}$), 6.73 (dd, J = 16.0 and 7.6 Hz, 1H, -CH=C$\underline{H}$COOH). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ = 193.77 (C=O), 152.85 (-$\underline{C}$H=CHCOOH), 133.95 (Ar), 131.27 (-CH=C$\underline{H}$COOH), 129.09 (Ar), 128.55 (Ar), 128.48 (Ar). EI-TOF-MS m/z = 131 (M-1), 132 (M).

3,6,9,12-Tetraoxatetracosanoic acid (**8a**) [CAS: 20858-25-7]: ^1H NMR (500 MHz, $CDCl_3$): δ = 4.15 (s, 2H, -OC$\underline{H}_2$COOH), 3.78-3.77 (m, 2H, -OCH_2C$\underline{H}_2$OCH_2COOH), 3.70-3.60 (m, 8H, -OC$\underline{H}_2$CH_2O-), 3.47 (t, J = 7.0 Hz, 2H, $C_{12}H_{25}$OC$\underline{H}_2$CH_2O-), 1.62-1.58 (m, 2H, $C_{11}H_{23}$C$\underline{H}_2$O-), 1.33-1.21 (m, 20H, -$C_{10}\underline{H}_{20}$-), 0.88 (t, J = 7.0 Hz, 3H, CH_3-). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$): δ = 172.20 (C=O), 71.61 (-$\underline{C}H_2$COOH), 71.42 (-O$\underline{C}H_2CH_2$O-), 70.62 (-O$\underline{C}H_2CH_2$O-), 70.39 (-O$\underline{C}H_2CH_2$O-), 70.37 (-O$\underline{C}H_2CH_2$O-), 70.29 (-O$\underline{C}H_2CH_2$O-), 70.06 (-O$\underline{C}H_2CH_2$O-), 69.10 (-O$\underline{C}H_2CH_2$), 31.88 (-OC$H_2\underline{C}H_2CH_2$-), 29.63 (-C$H_2\underline{C}H_2CH_2$-), 29.60 (-C$H_2\underline{C}H_2CH_2$-), 29.57 (-C$H_2\underline{C}H_2CH_2$-), 29.42 (-C$H_2\underline{C}H_2CH_2$-), 29.40 (-C$H_2\underline{C}H_2CH_2$-), 29.32 (-C$H_2\underline{C}H_2CH_2$-), 25.99 (-C$H_2\underline{C}H_2CH_2$-), 22.65 (-C$H_2\underline{C}H_2CH_2$-), 22.65 (C$H_3\underline{C}H_2$-), 14.08 (CH_3-). ESI-TOF-MS (neg) m/z = 375 (M^-).

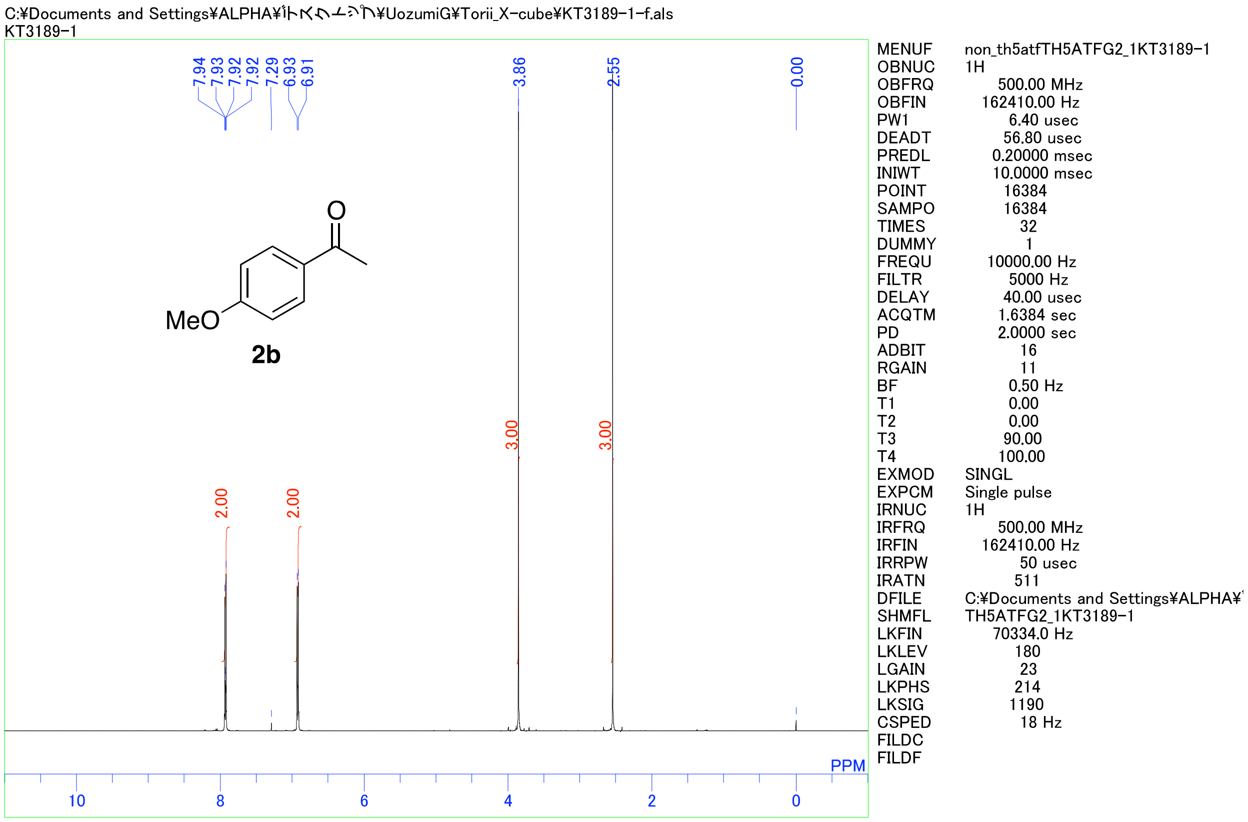
Detergent **8b** ^1H NMR (500 MHz, $CDCl_3$): δ = 4.17-4.15 (s x 4), 3.77-3.73 (m), 3.71-3.63 (m), 3.61-3.58 (m), 348-3.44 (m), 1.57 (quint, J = 7.0 Hz, CH_3C$\underline{H}_2$CH_2-), 1.32-1.26 (m), 0.88 (t, J = 7.0 Hz, CH_3). $^{13}C\{^1H\}$ NMR (100MHz, $CDCl_3$) : δ = 172.02 (C=O), 170.49 (C=O), 71.71, 71.64, 71.60, 71.58, 71.55, 71.50, 71.34, 70.98, 70.92, 70.88, 70.71, 70.58, 70.55, 70.53, 70.50, 70.46, 70.44, 70.33, 70.30, 70.20, 70.18, 70.14, 70.04, 70.00, 69.95, 69.81, 69.32, 69.24, 68.95, 68.79, 68.49, 63.79, 33.83, 91.92, 29.68, 29.65, 29.61, 29.59, 29.50, 29.43, 29.36, 29.32, 29.27, 29.10, 26.08, 26.04, 25.99, 25.84, 24.76, 22.70, 14 (pos) m/z = 333 ($[M_{(n = 3)} + 1]^+$), 377 ($[M_{(n = 4)} + 1]^+$), 421 ($[M_{(n = 5)} + 1]^+$), 465 ($[M_{(n = 5)}$ + 1] .14. FAB-MS $^+$).

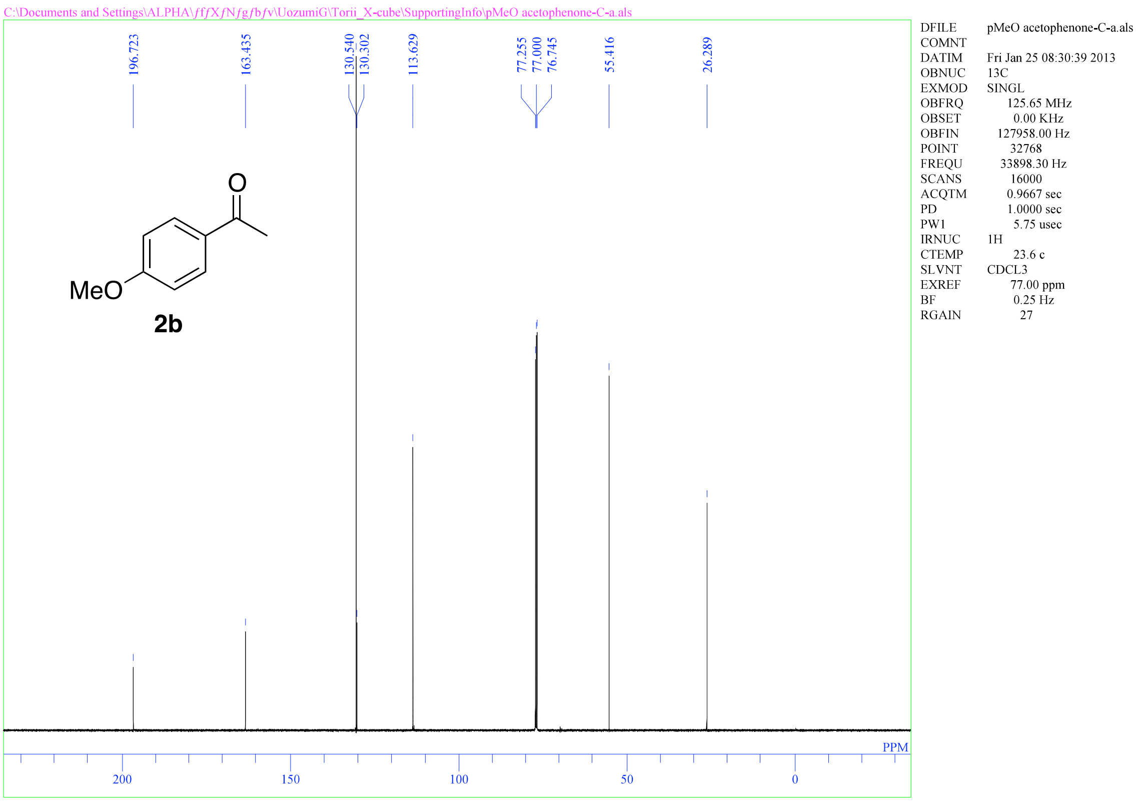
[1]H and [13]C{[1]H} NMR spectra of acetophenone (**2a**).



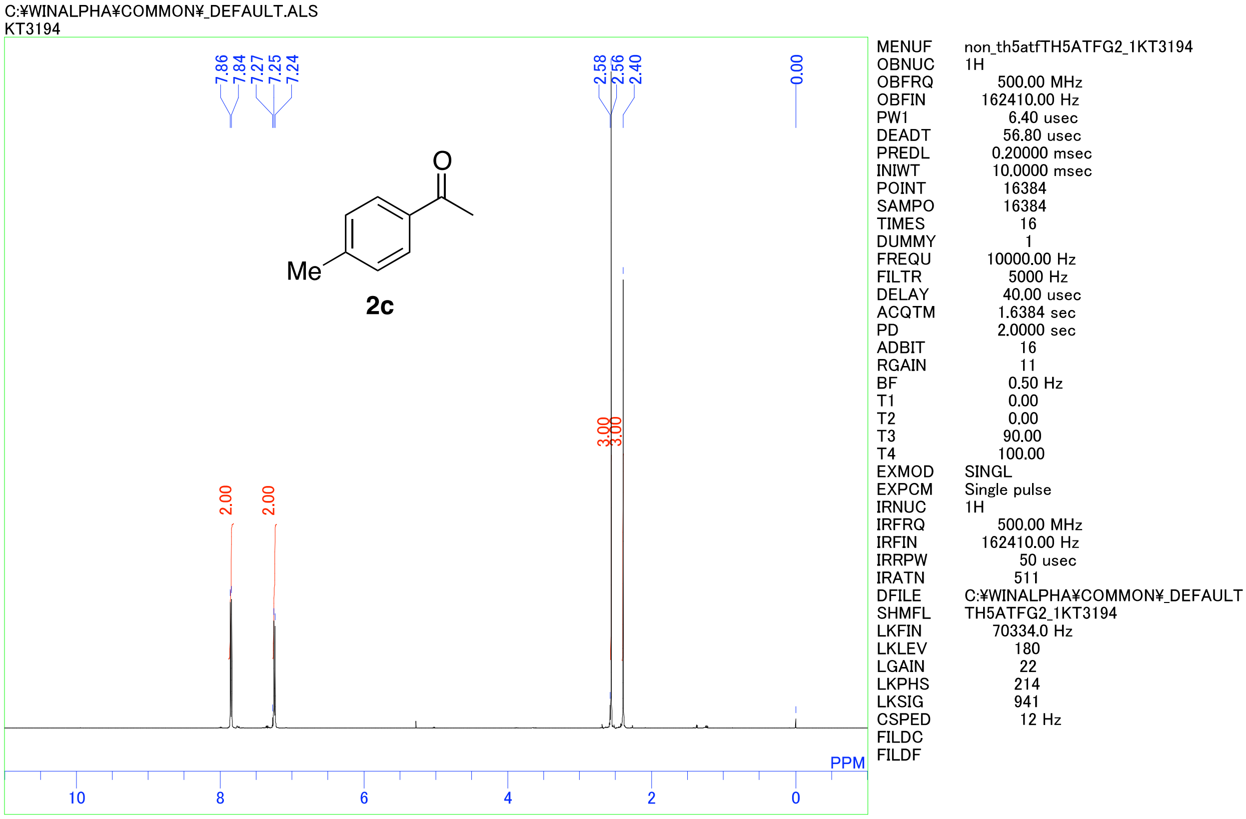


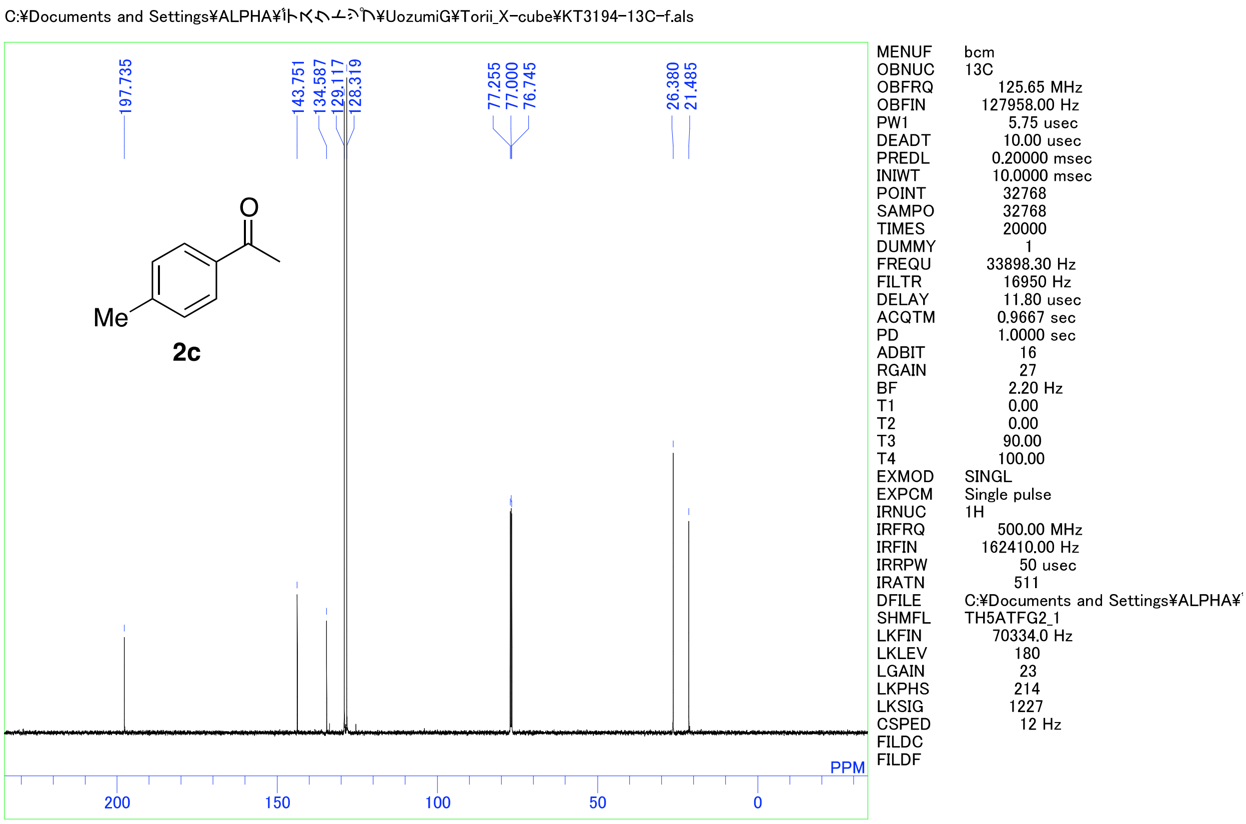
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 4’-methoxyacetophenone (**2b**).





^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 4'-methylacetophenone (**2c**).





[1]H and [13]C{[1]H} NMR spectra of 4’-chloroacetophenone (**2d**).

single_pulse

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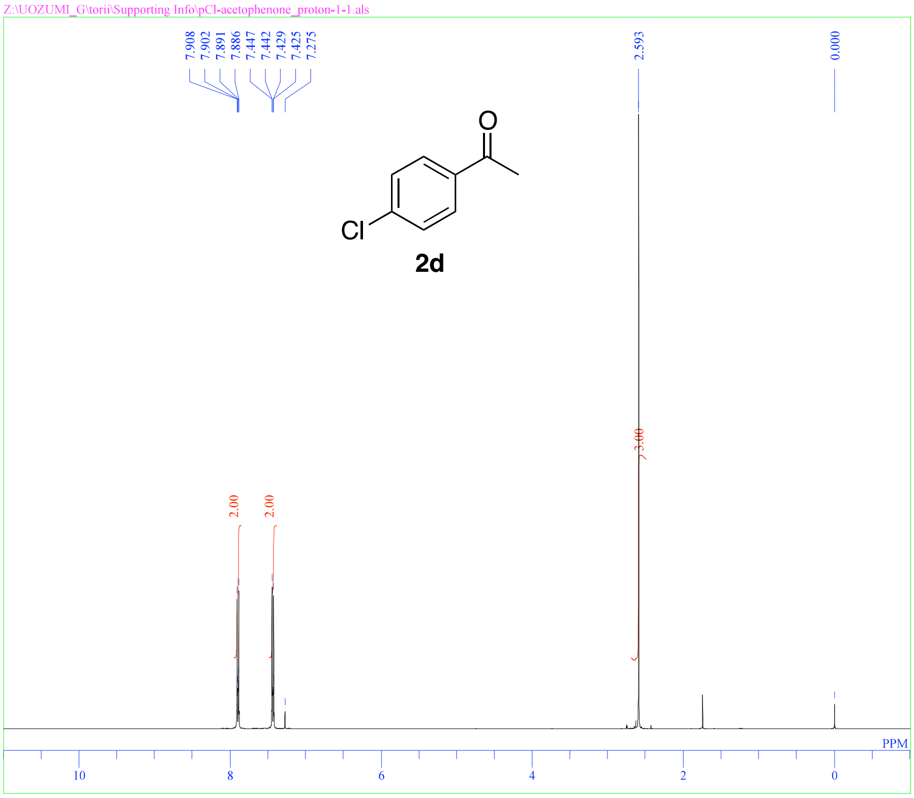

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PD	5.0000 sec
PW1	3.12 usec
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CTEMP	19.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.40 Hz
RGAIN	30

single pulse decoupled gated NOE

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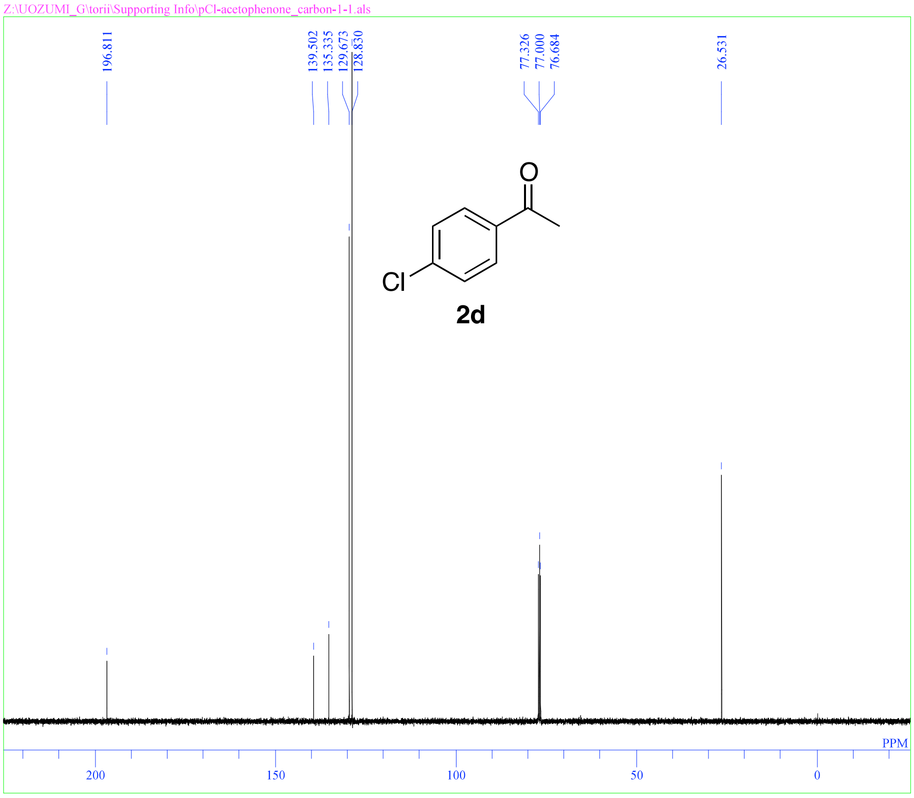

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OBFIN	0.98 Hz
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PD	2.0000 sec
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SLVNT	CDCL3
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BF	0.40 Hz
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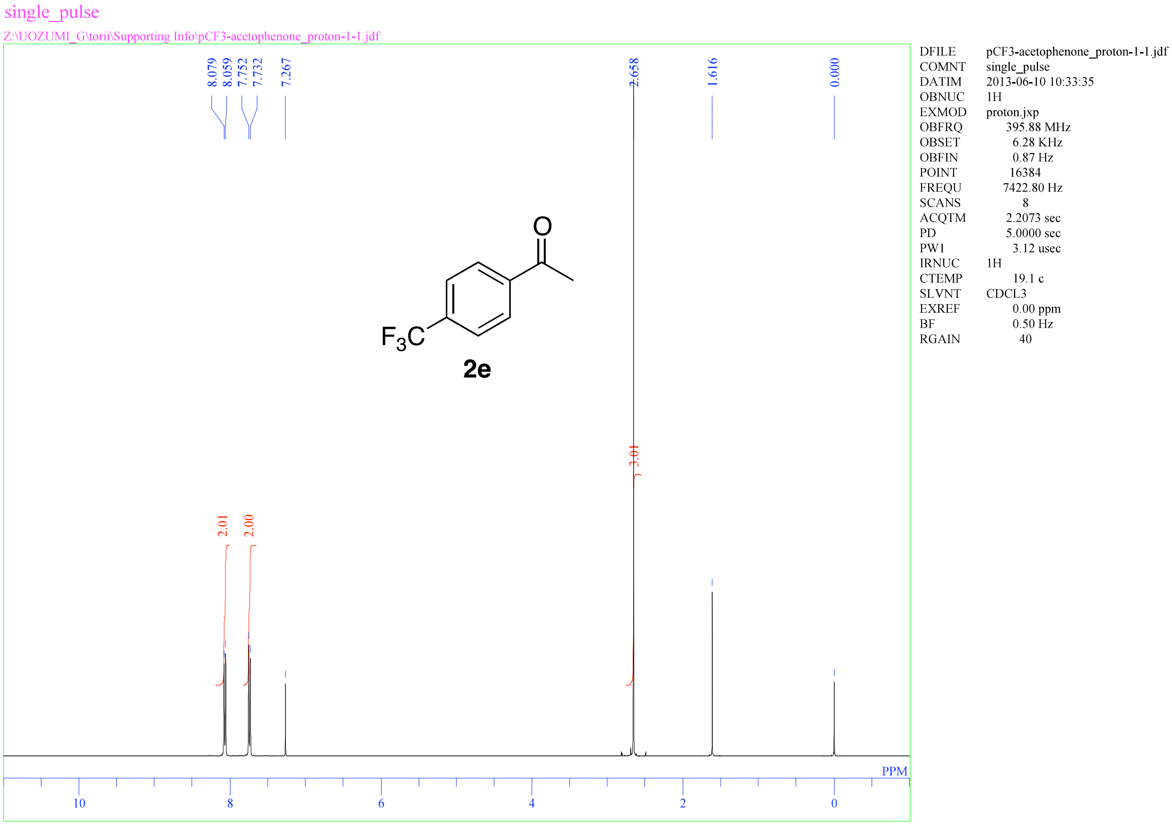
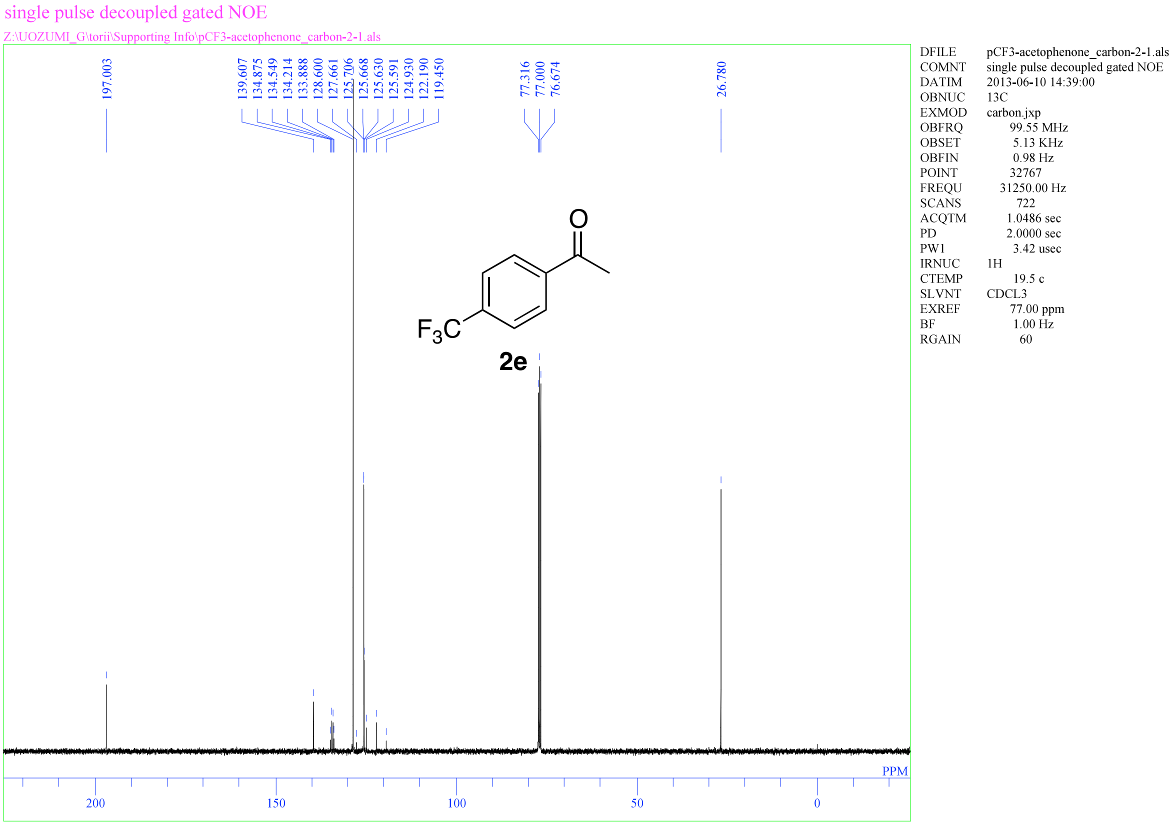
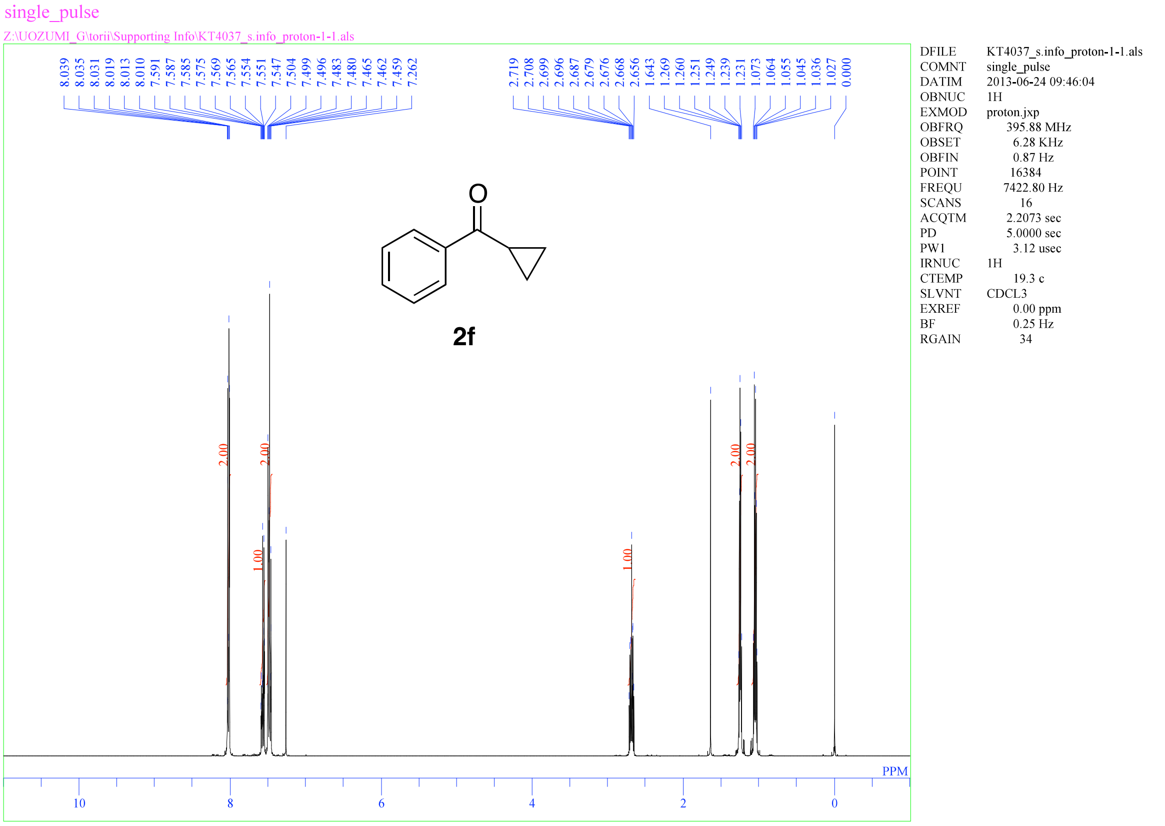
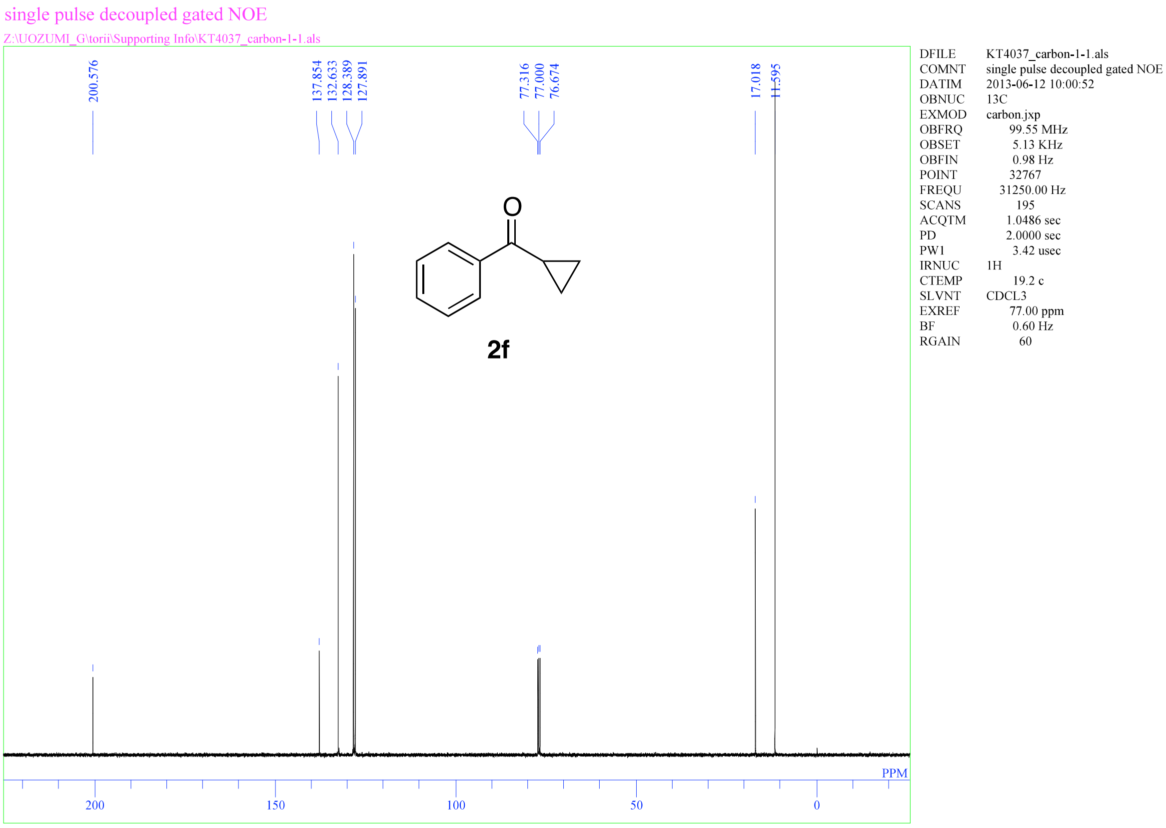
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 4'-(trifluoromethyl)acetophenone (**2e**).



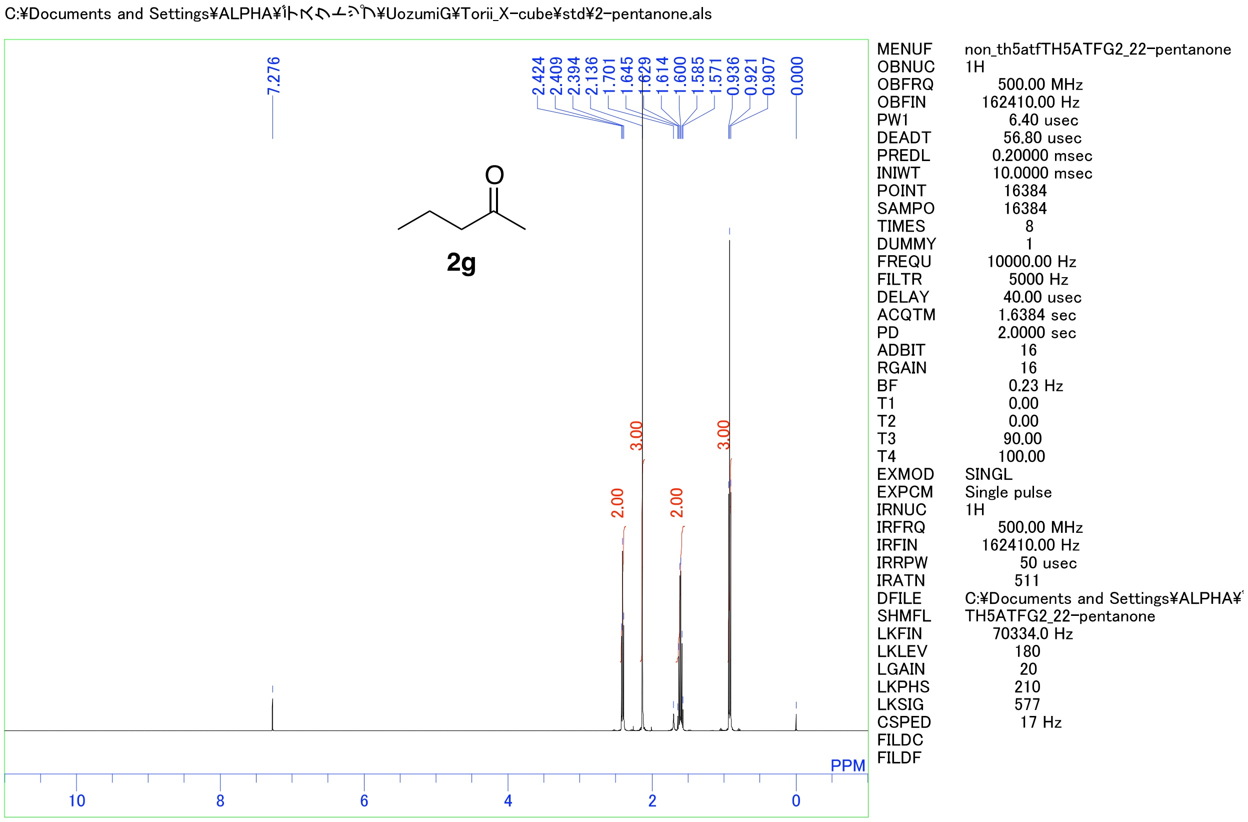


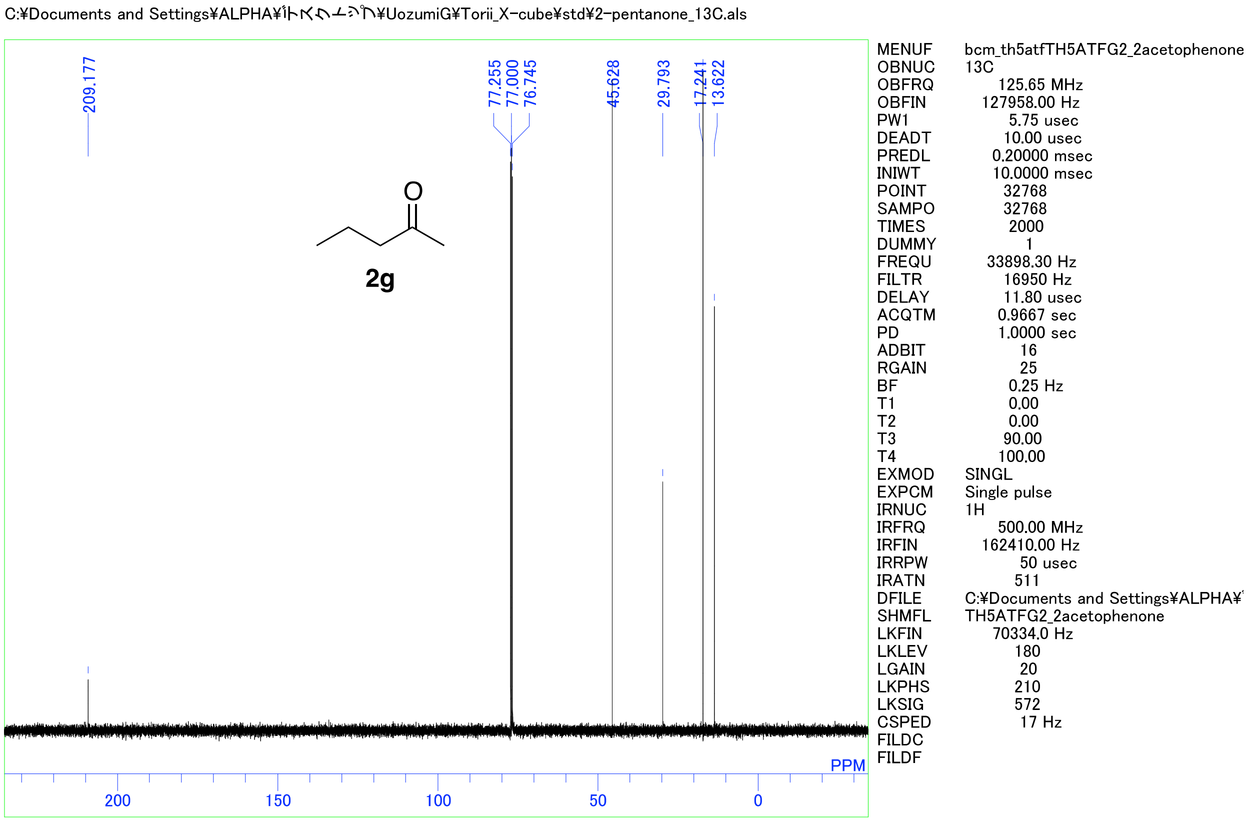
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of cyclopropyl phenyl ketone (**2f**).



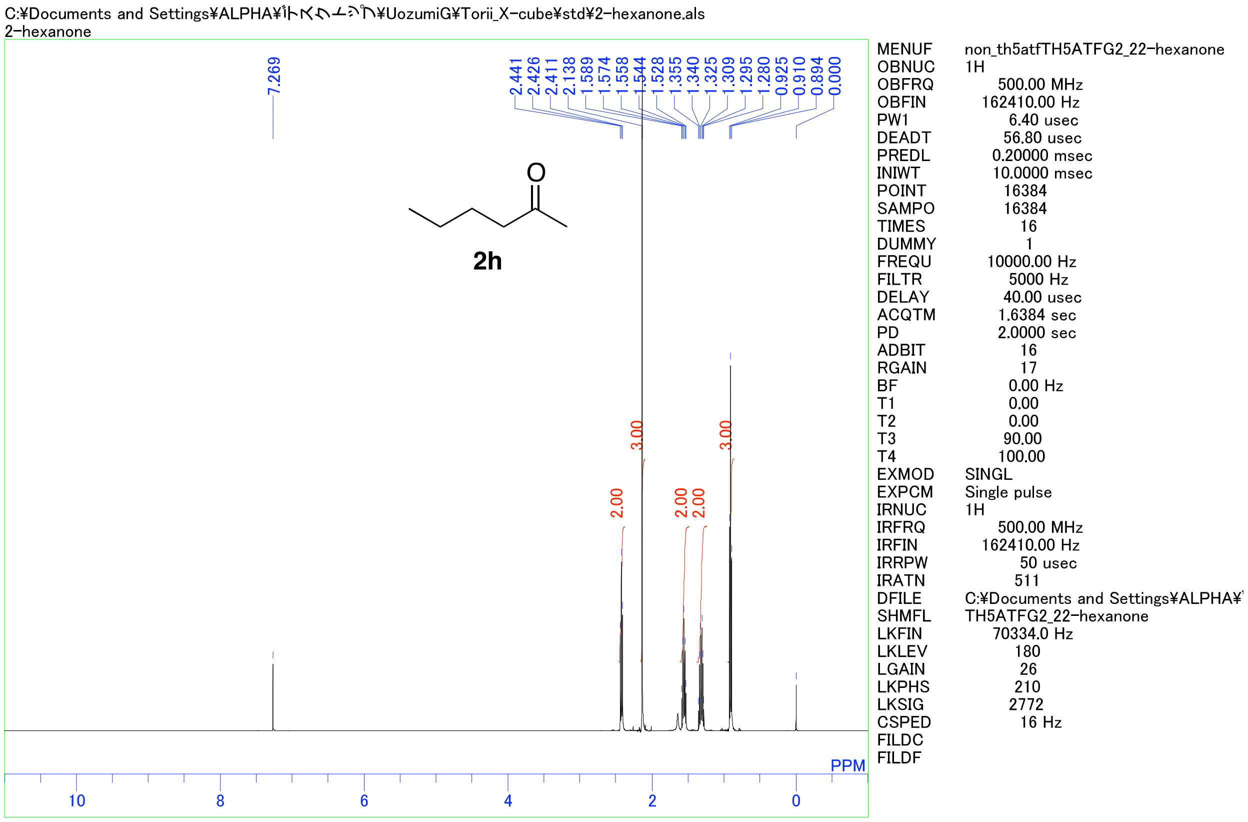


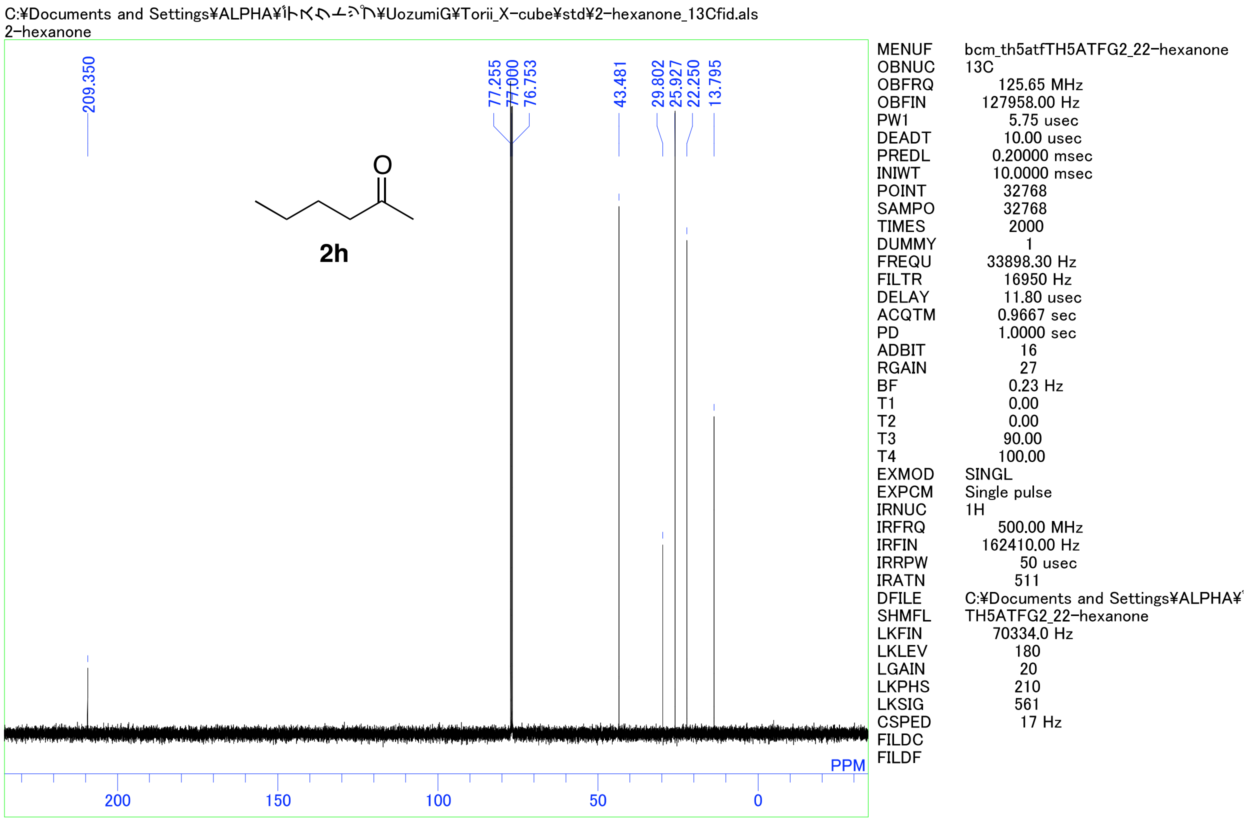
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-pentanone (**2g**).



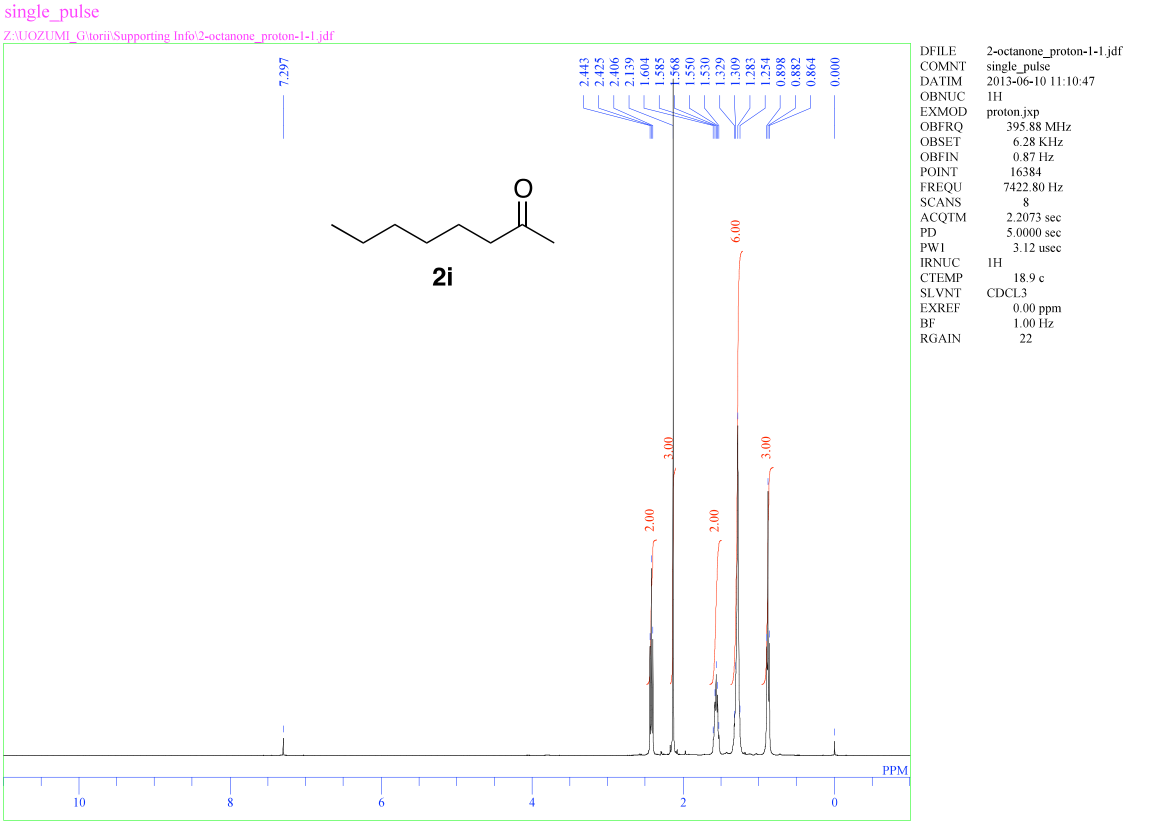


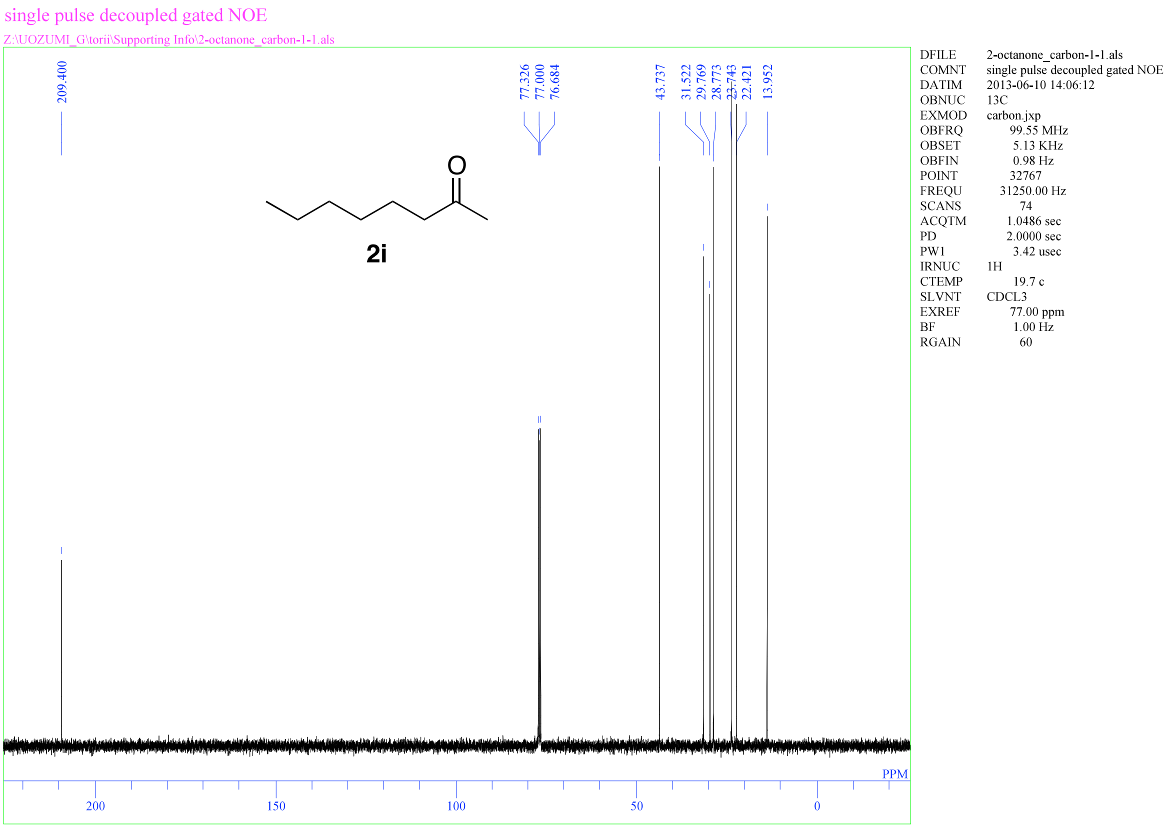
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-hexanone (**2h**).



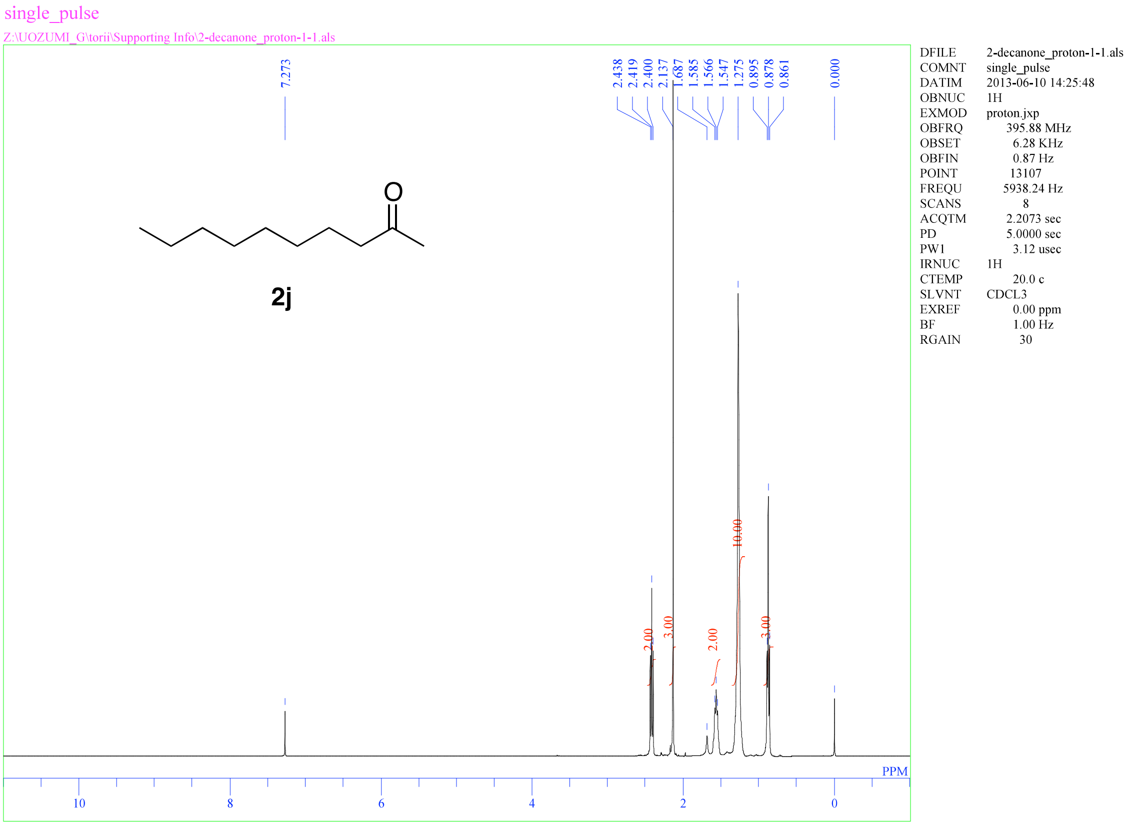


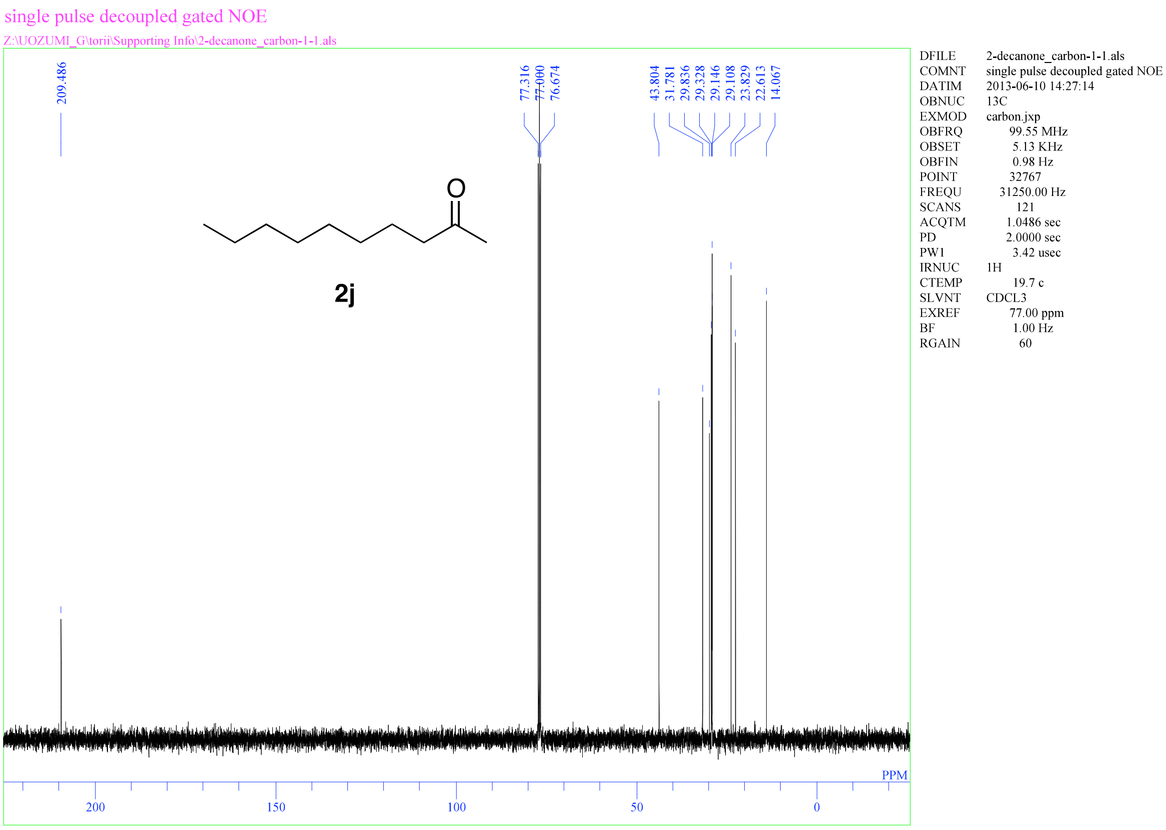
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-octanone (**2i**).



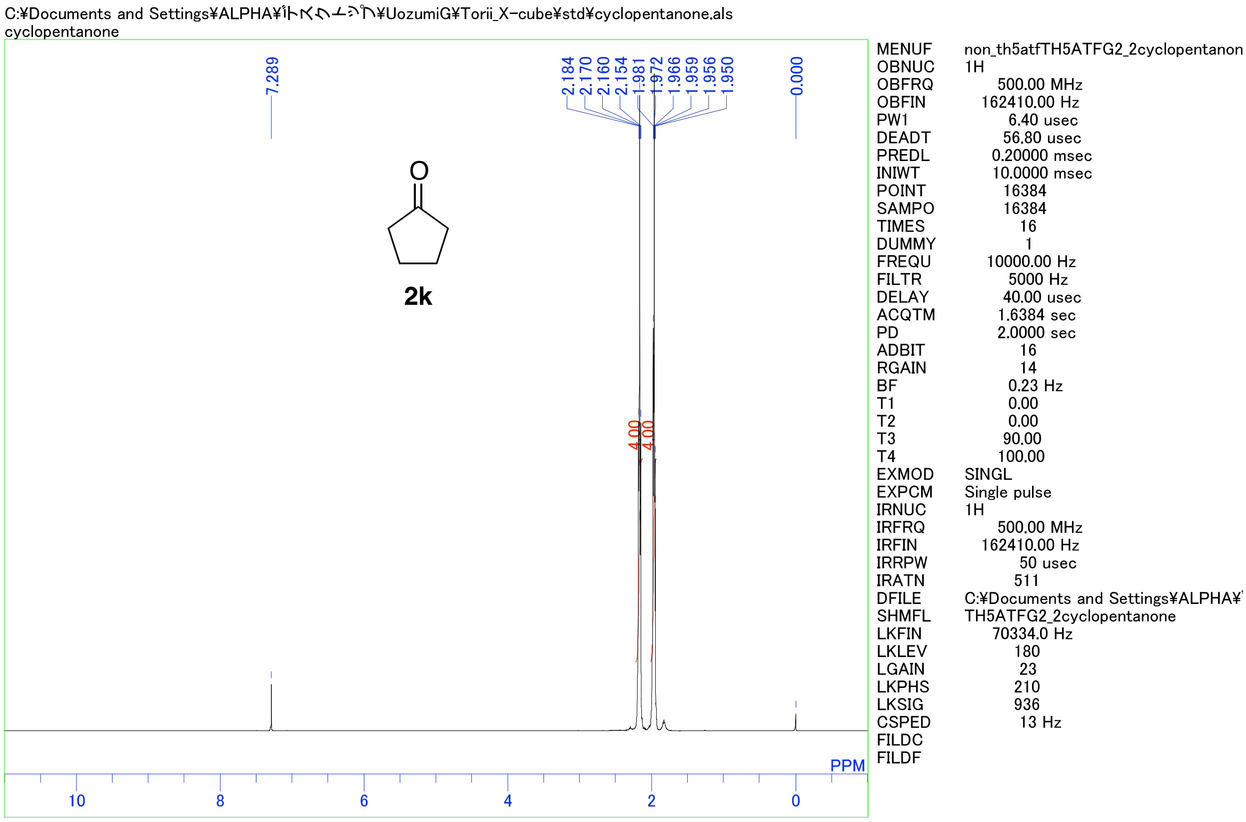


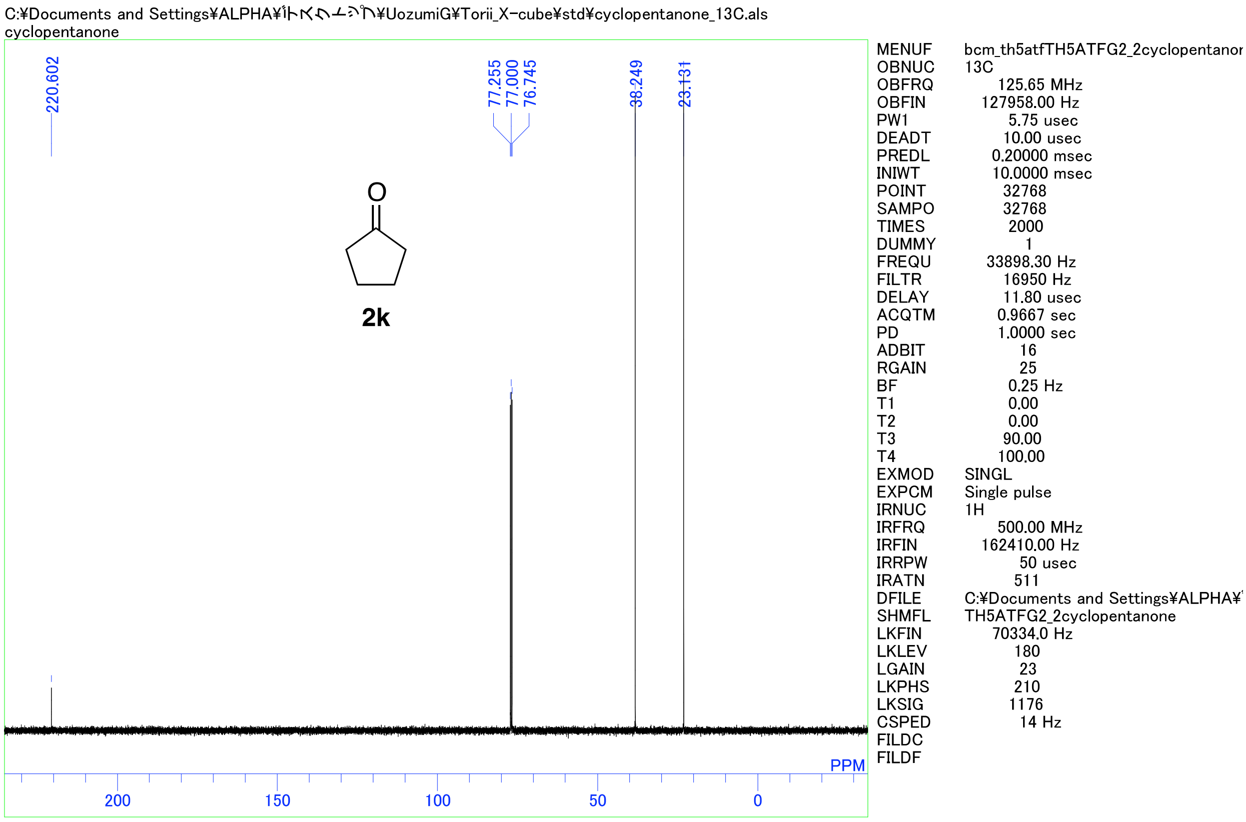
[1]H and [13]C{[1]H} NMR spectra of 2-decanone (**2j**).



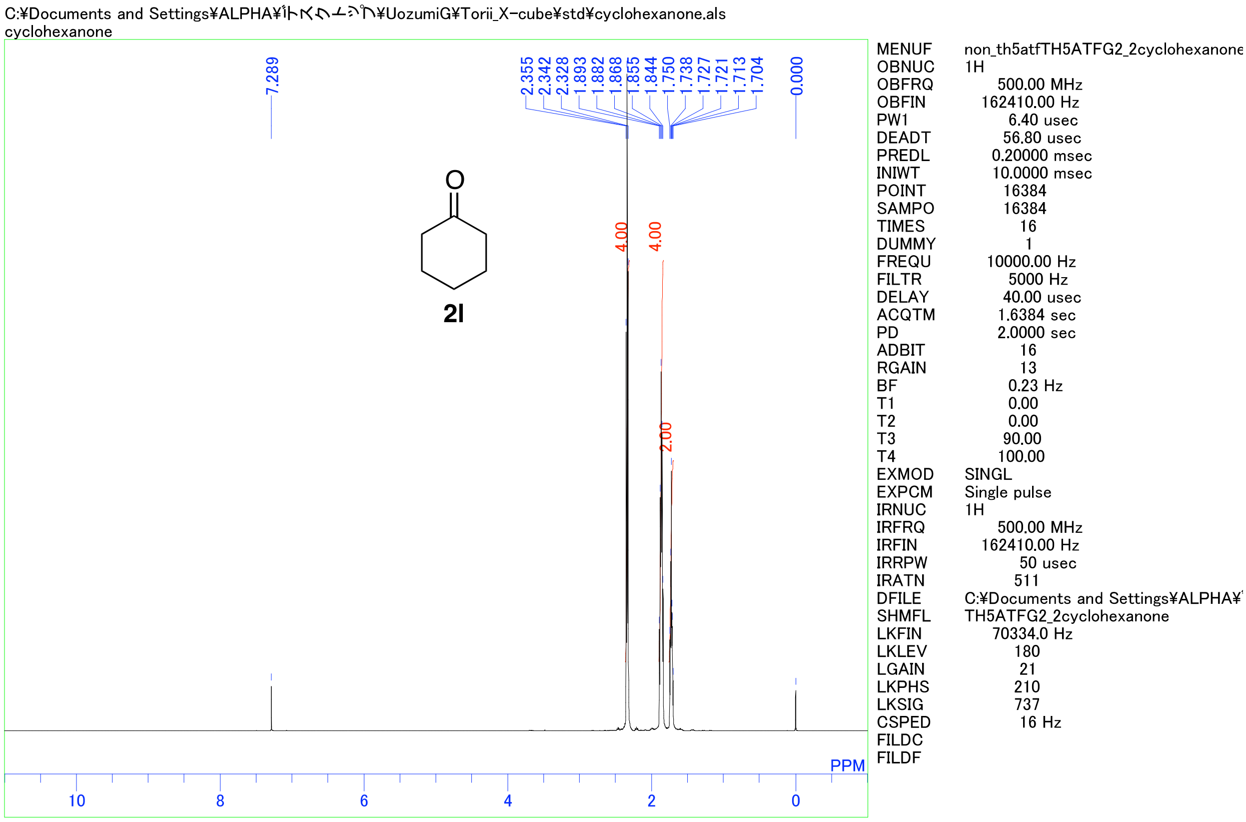


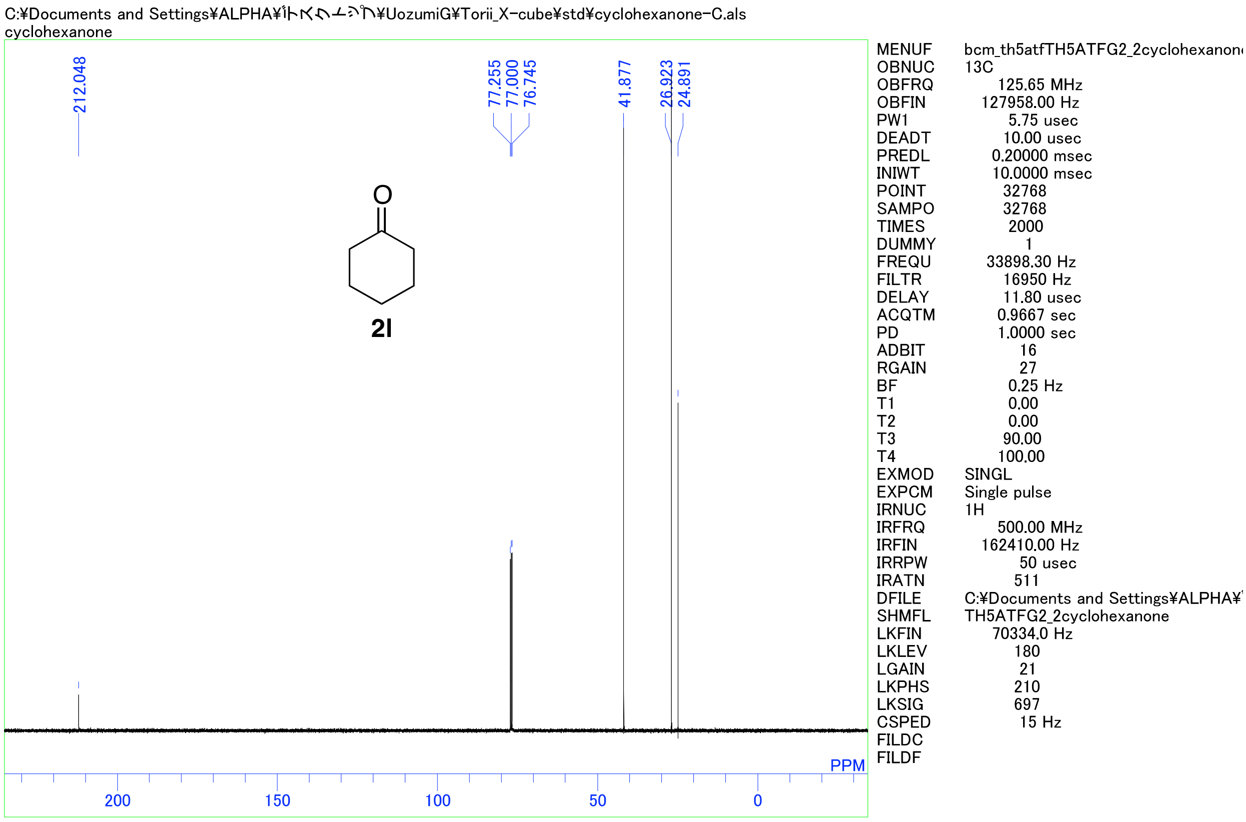
^{1}H and ^{13}C{^{1}H} NMR spectra of cyclopentanone (**2k**).



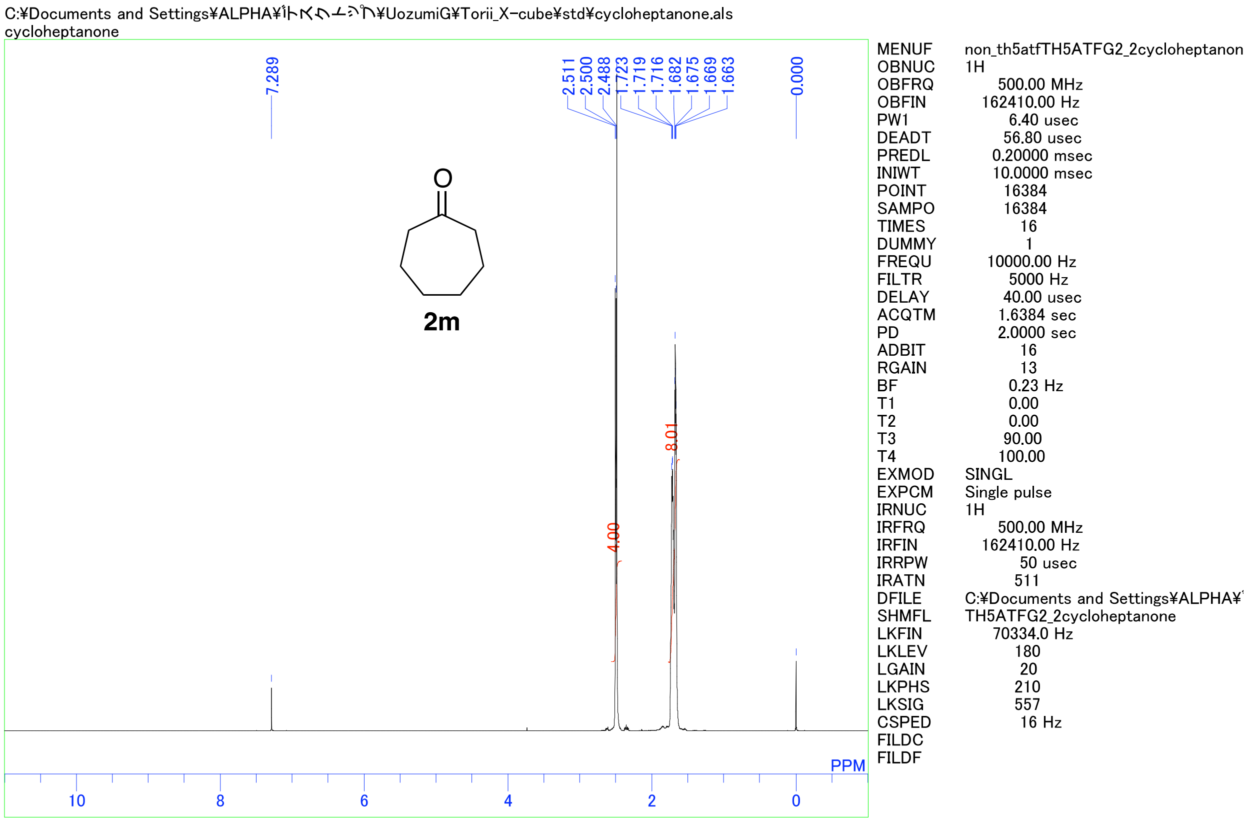


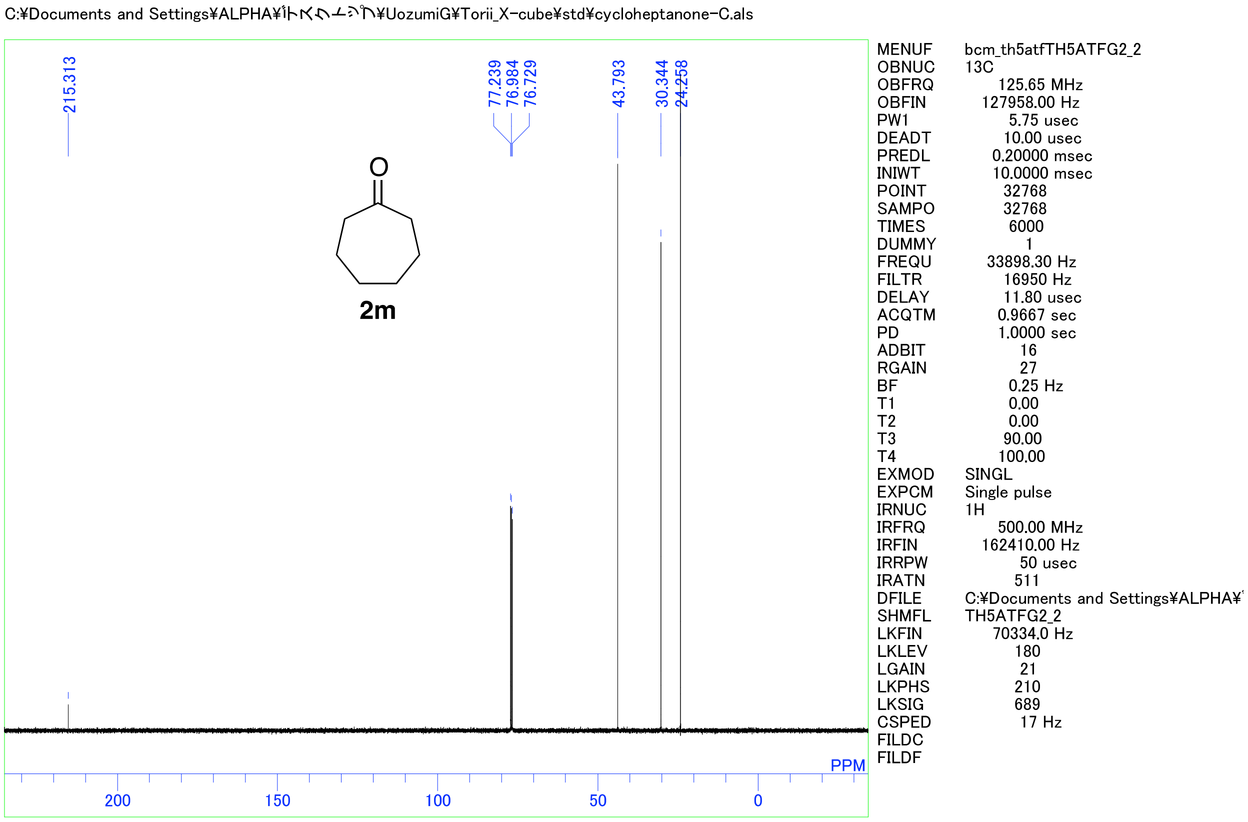
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of cyclohexanone (**2l**).



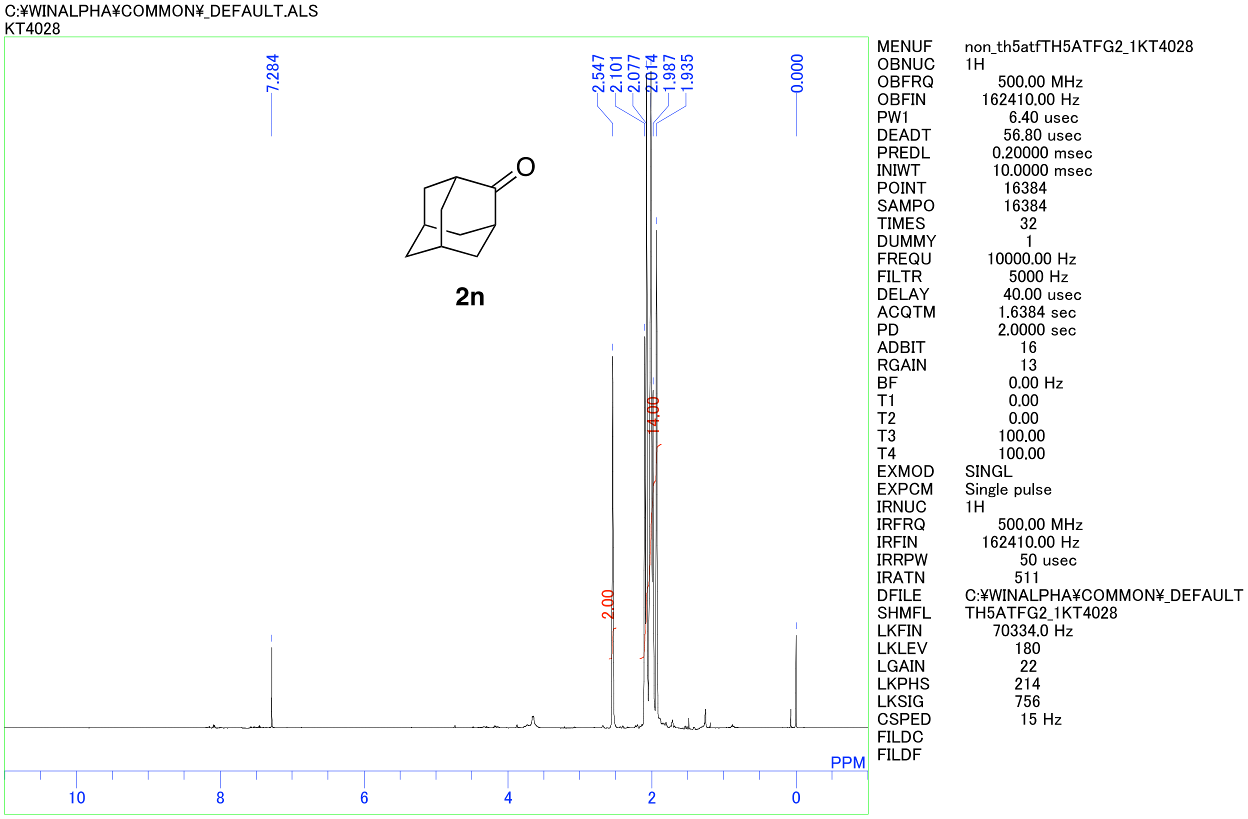


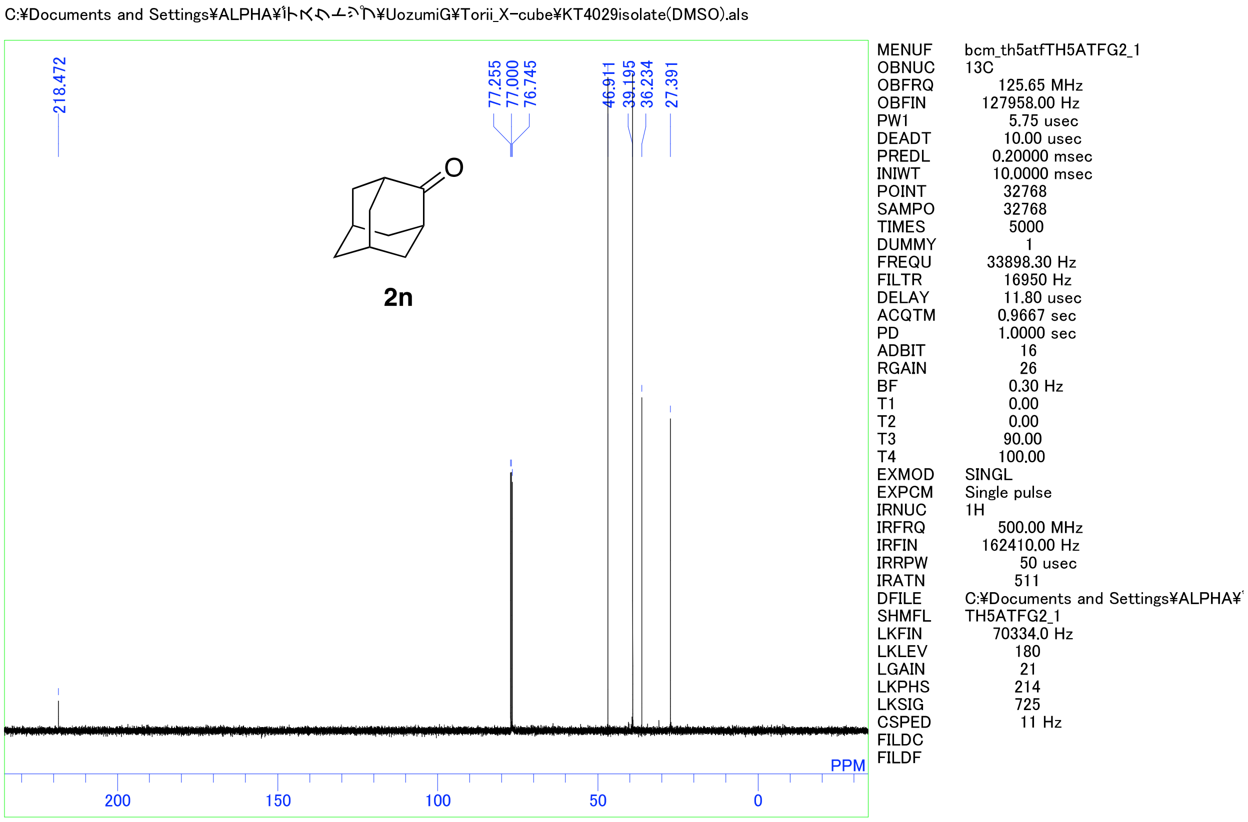
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of cycloheptanone (**2m**).



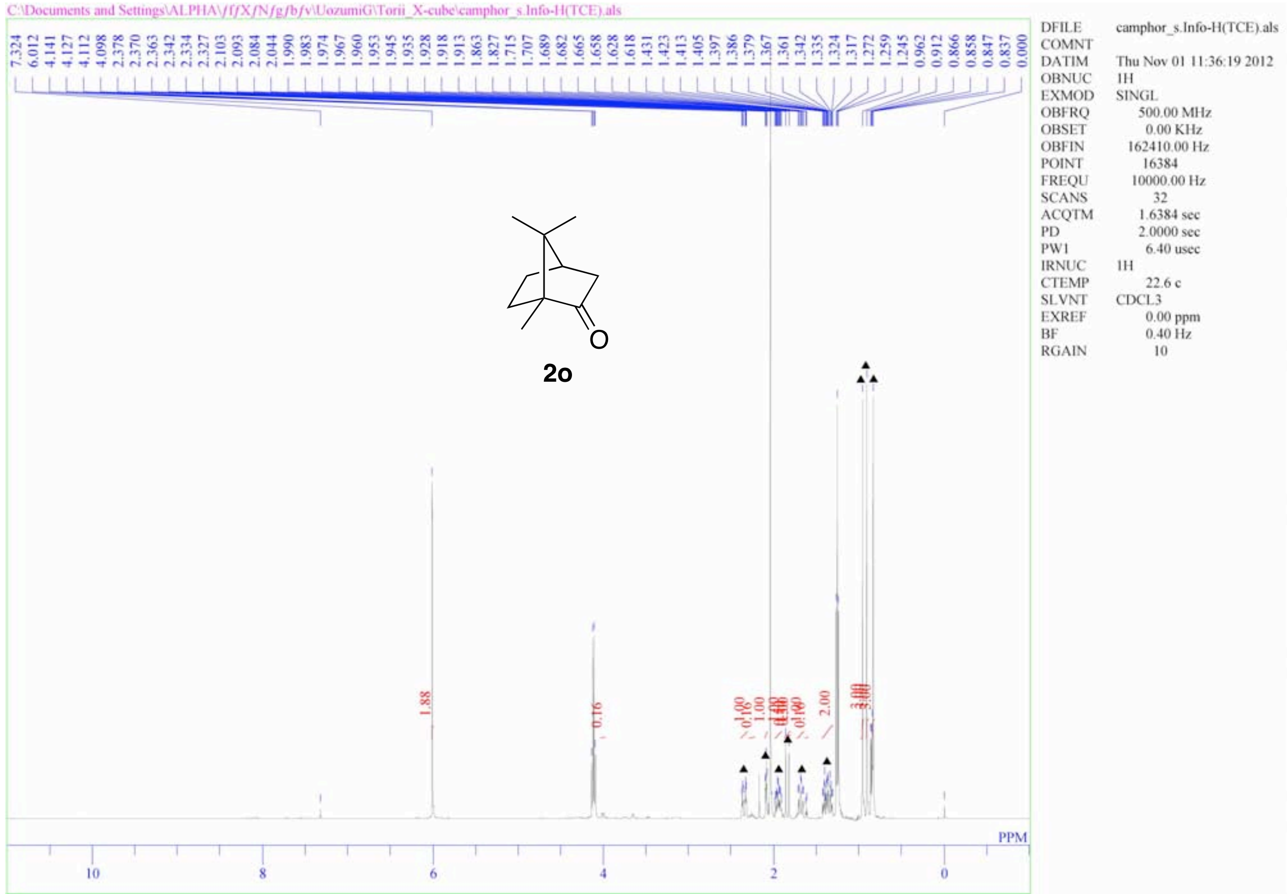


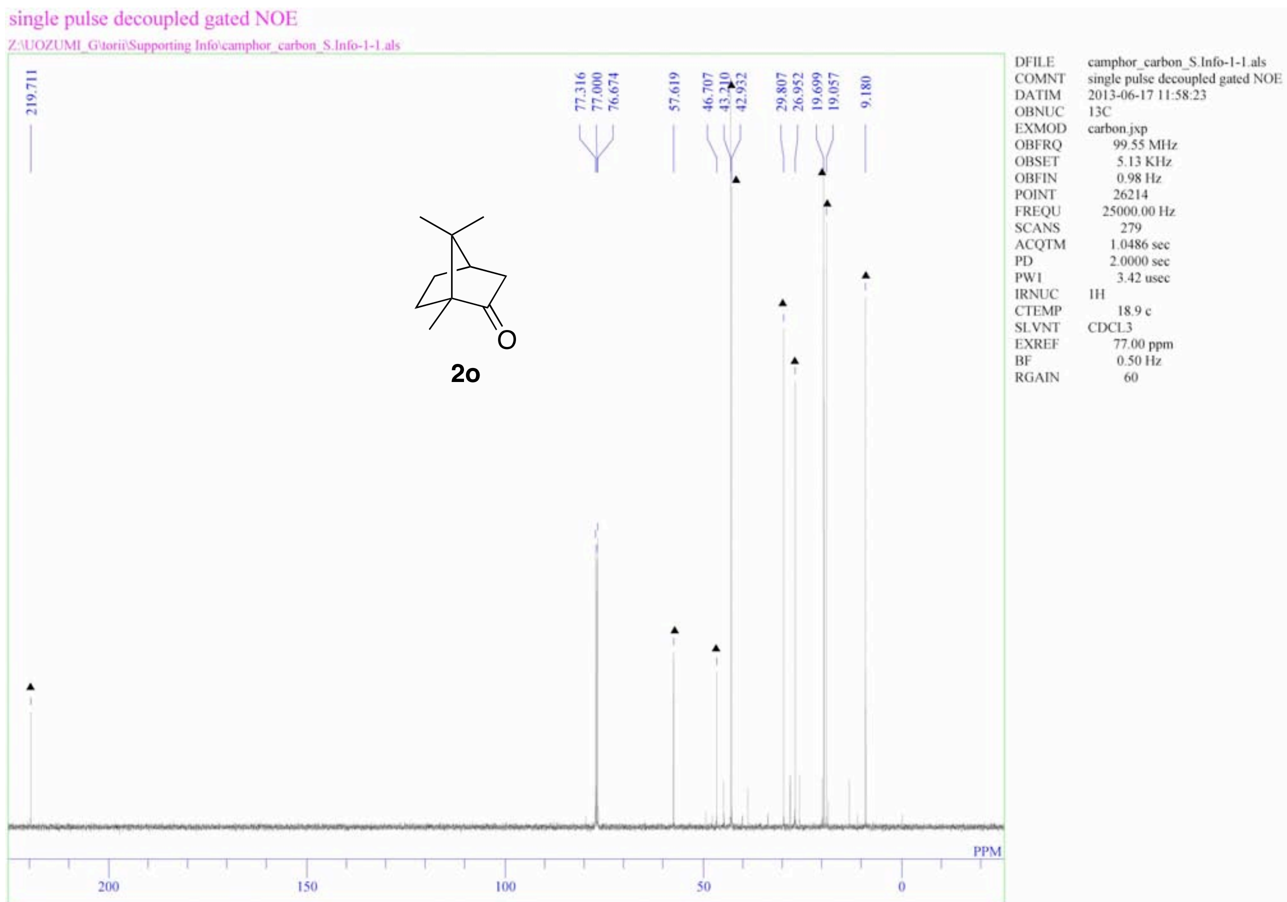
[1]H and [13]C{[1]H} NMR spectra of 2-adamantanone (**2n**).



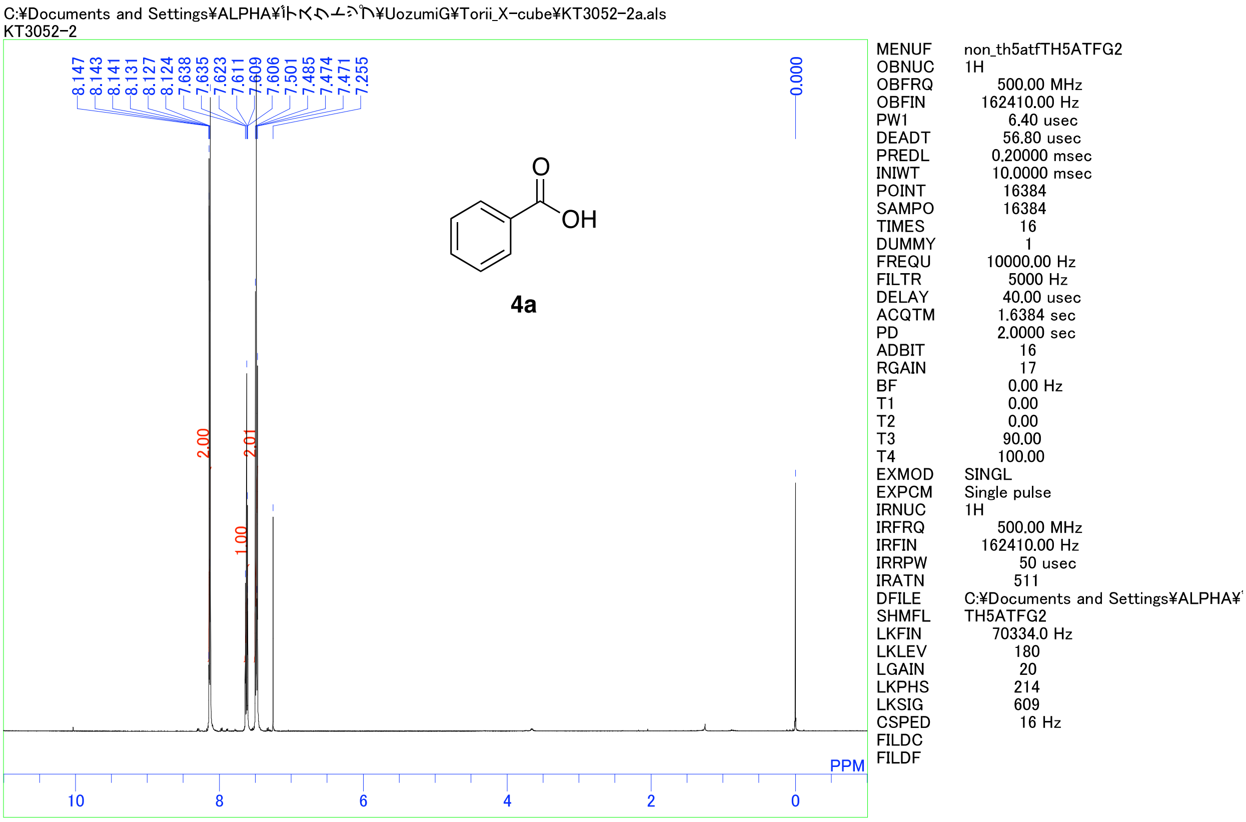


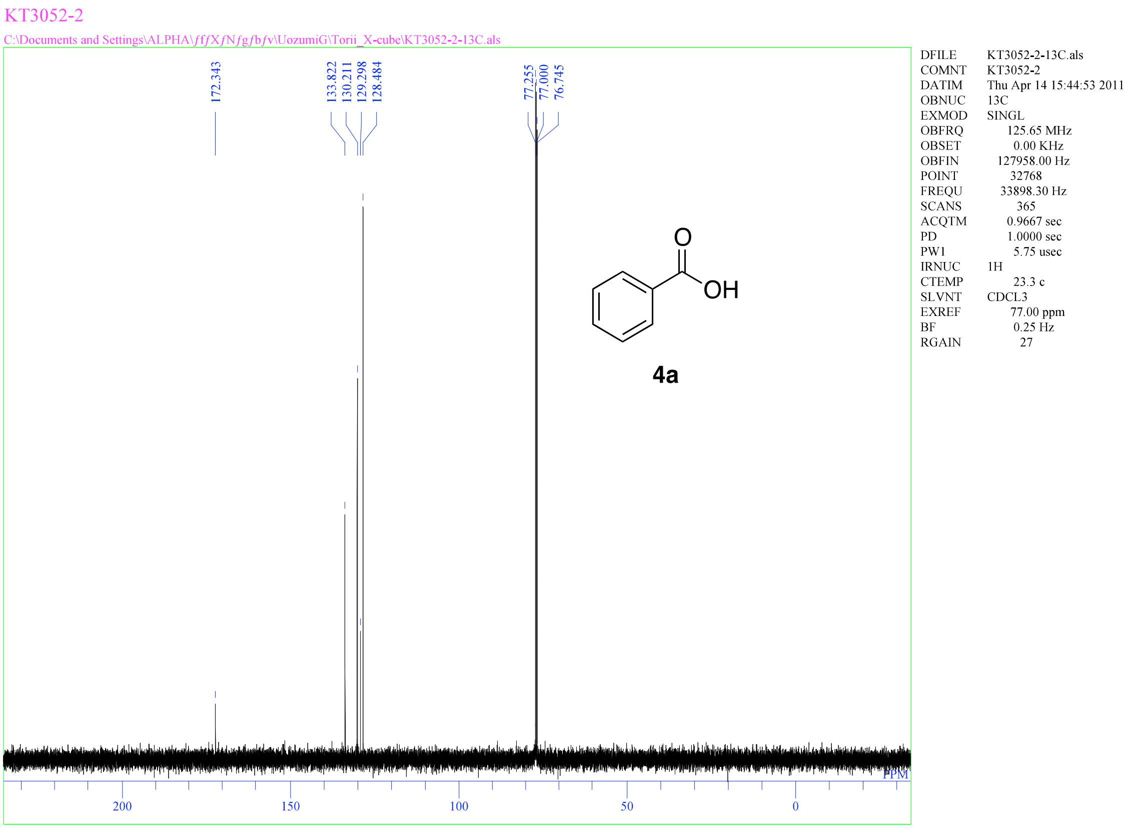
[1]H and [13]C{[1]H} NMR spectra of camphor (**2o**).



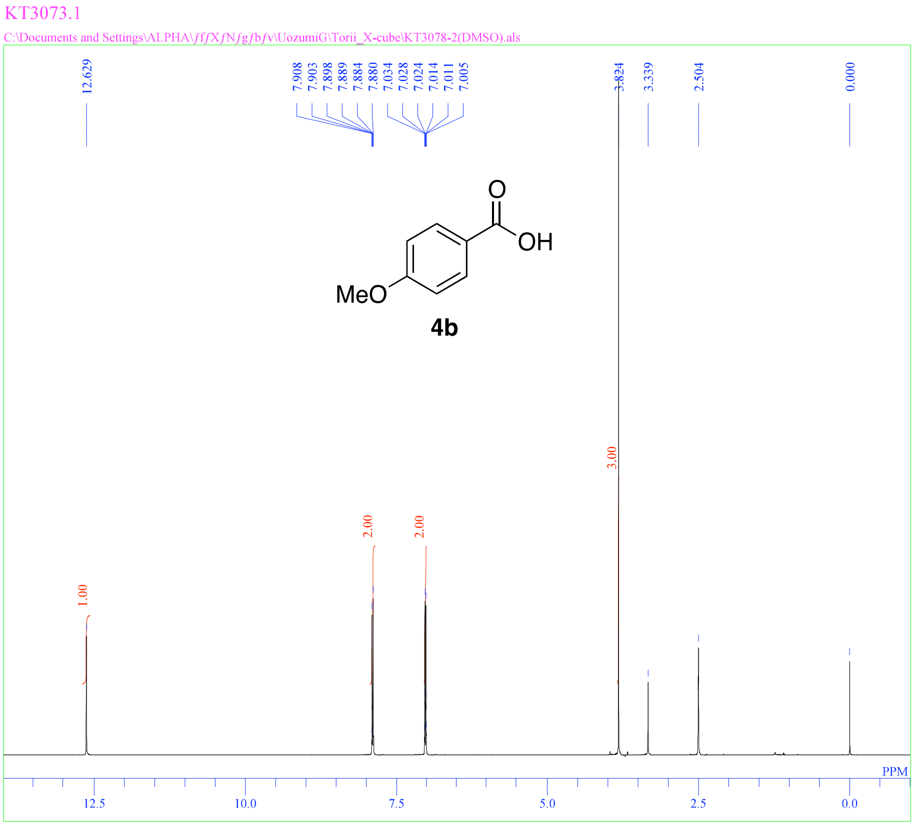


^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of benzoic acid (**4a**).





[1]H and [13]C{[1]H} NMR spectra of *p*-anisic acid (**4b**).



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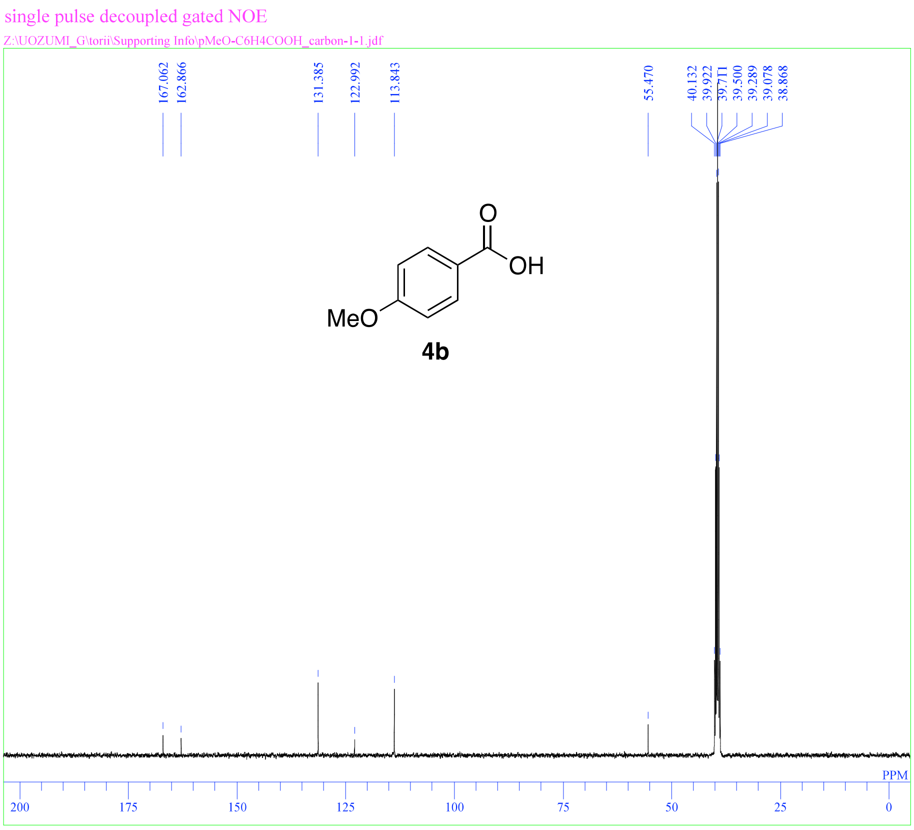
OBSET 0.00 KHz
OBFIN 162410.00 Hz
POINT 16384
FREQU 10000.00 Hz
SCANS 16
ACQTM 1.6384 sec
PD 2.0000 sec
PW1 6.40 usec
IRNUC 1H
CTEMP 21.6 c
SLVNT DMSO
EXREF 0.00 ppm
BF 0.23 Hz
RGAIN 21



DFILE pMeO-C6H4COOH_carbon-1-1.jdf
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EXMOD carbon.jxp
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OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 456
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC 1H
CTEMP 20.0 c
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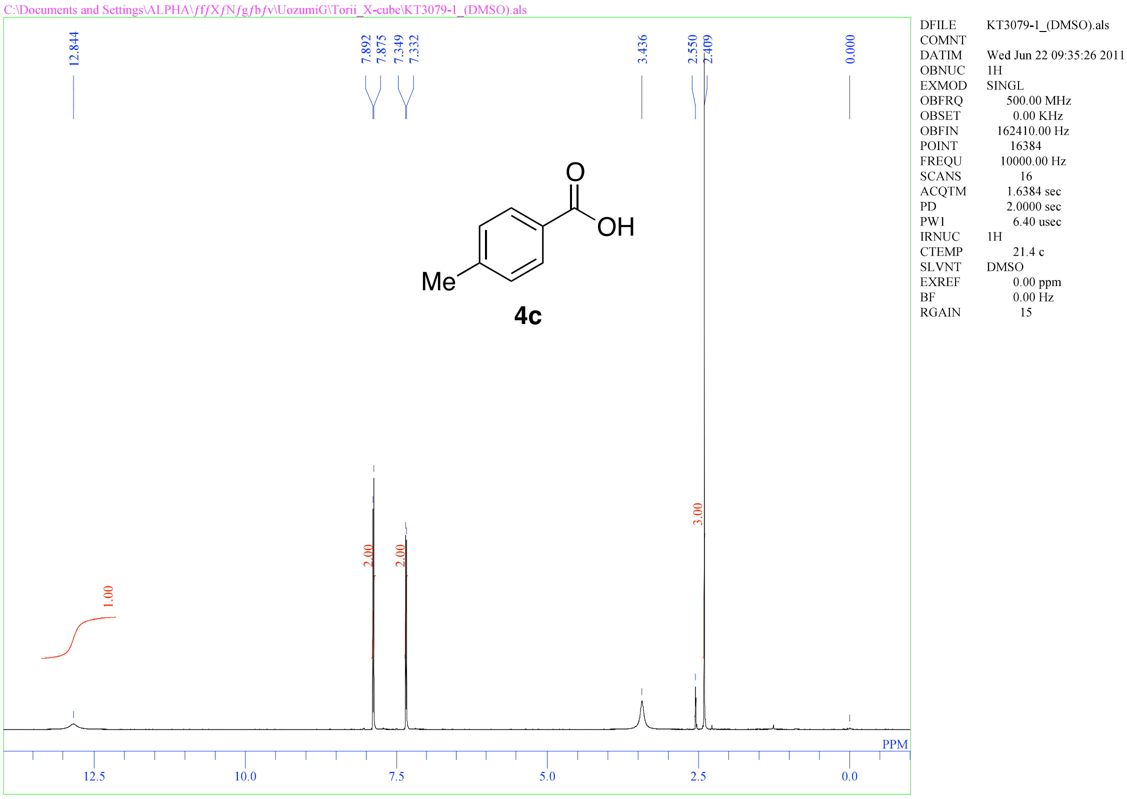
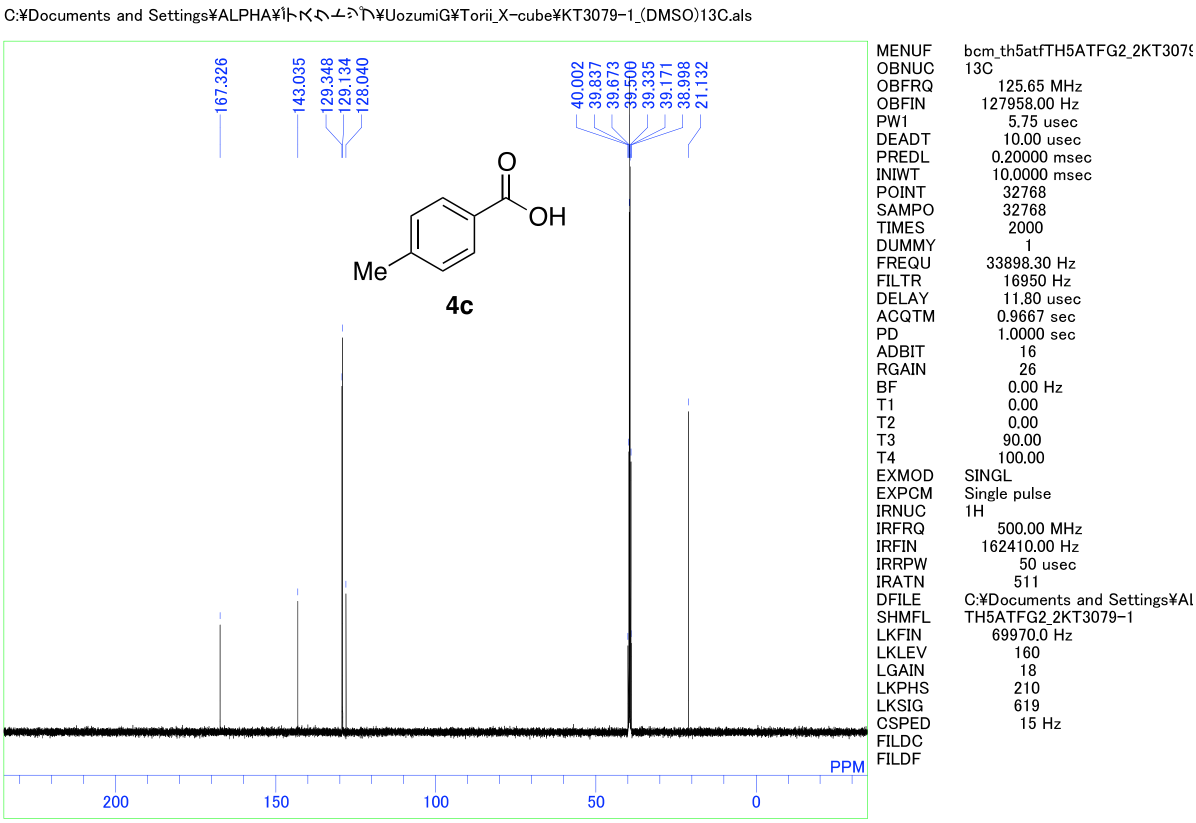
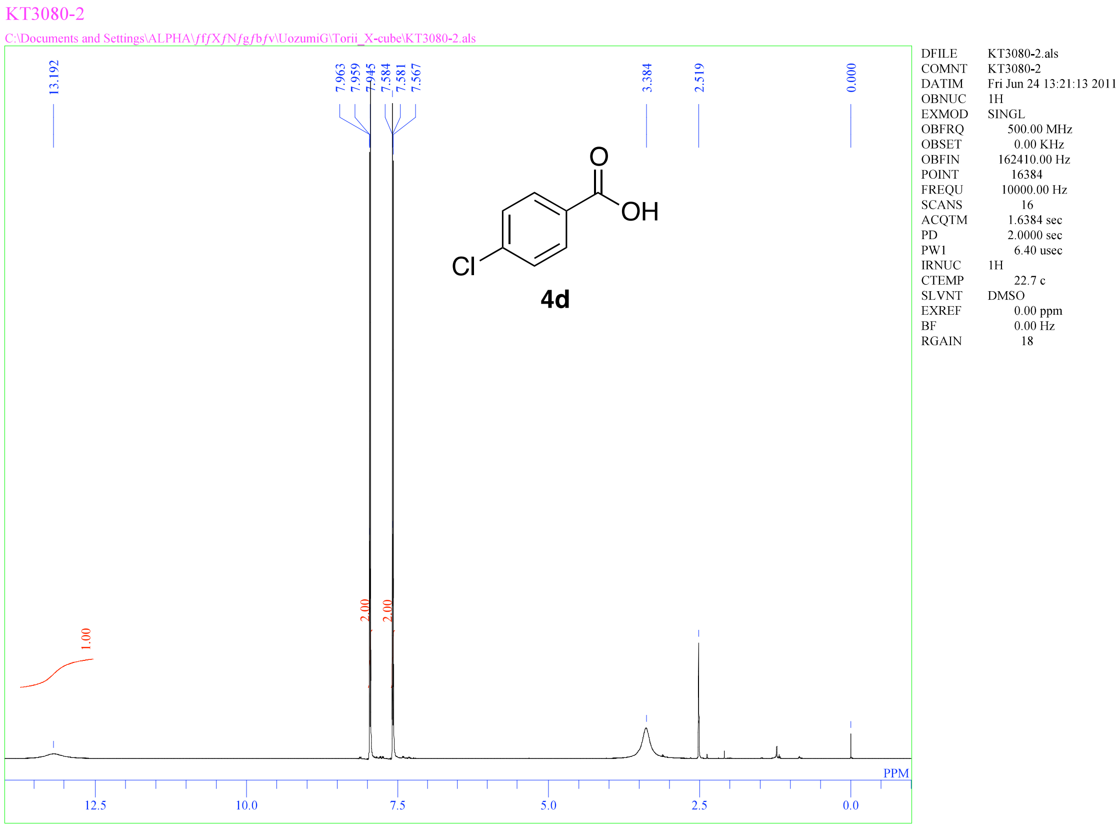
BF 2.80 Hz
RGAIN 60

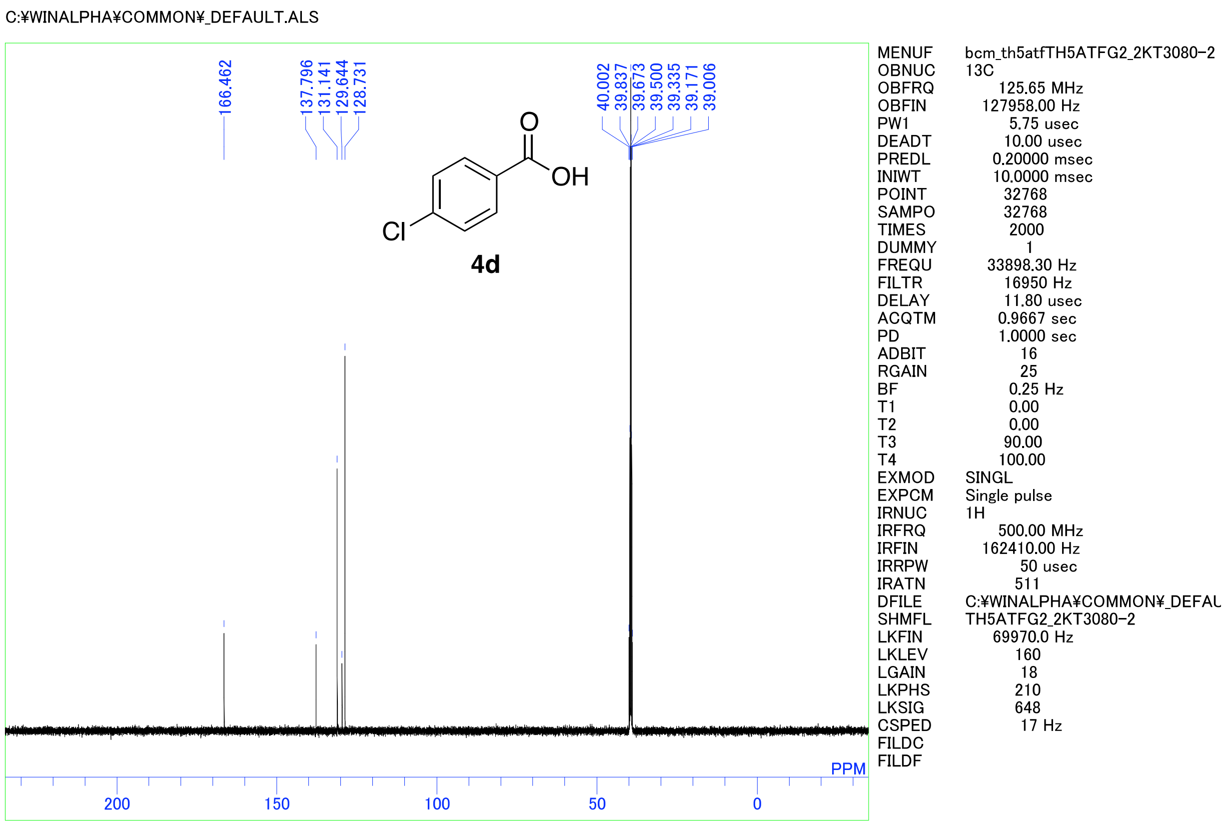
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of *p*-toluic acid (**4c**).



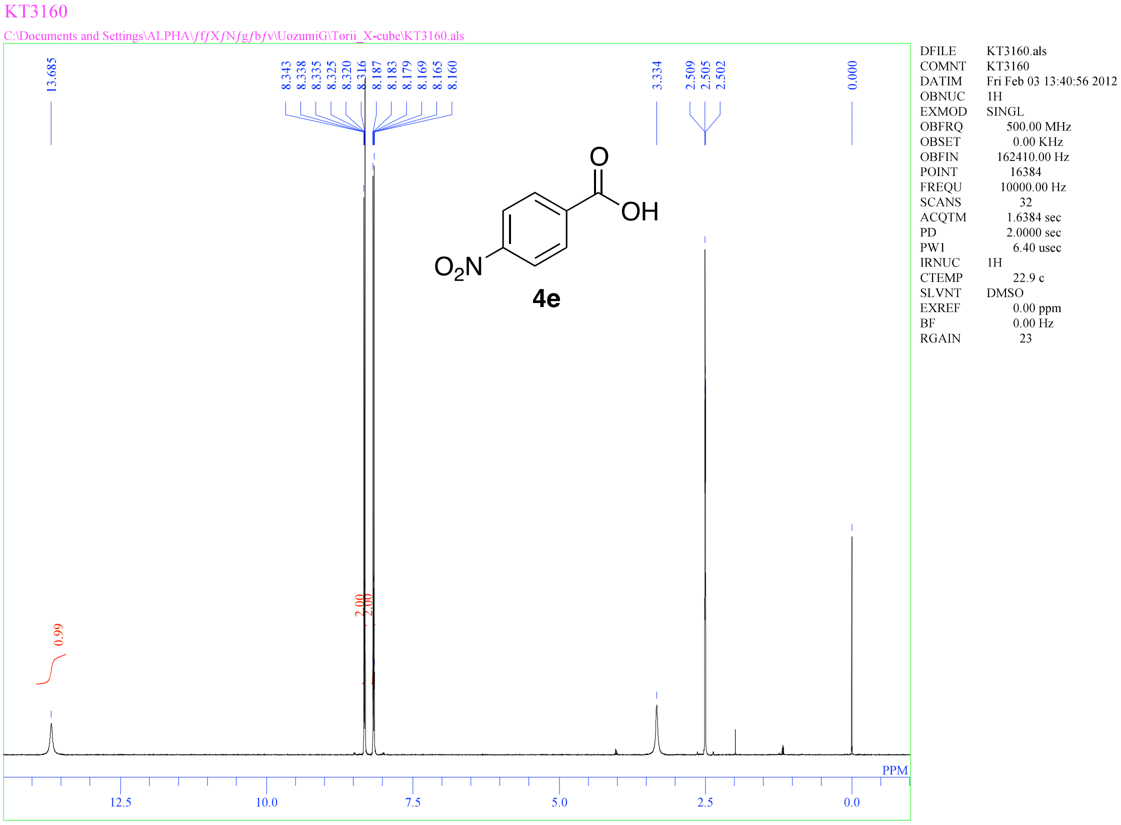


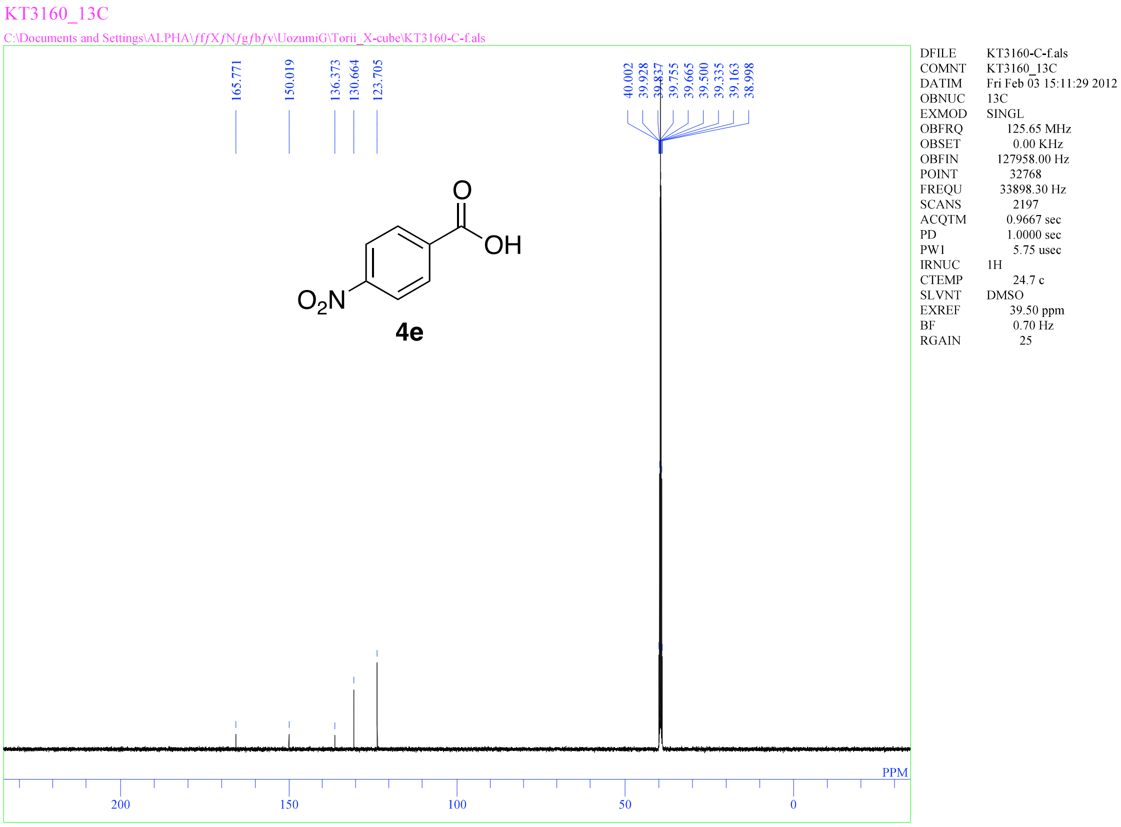
[1]H and [13]C{[1]H} NMR spectra of 4-chlorobenzoic acid (**4d**).



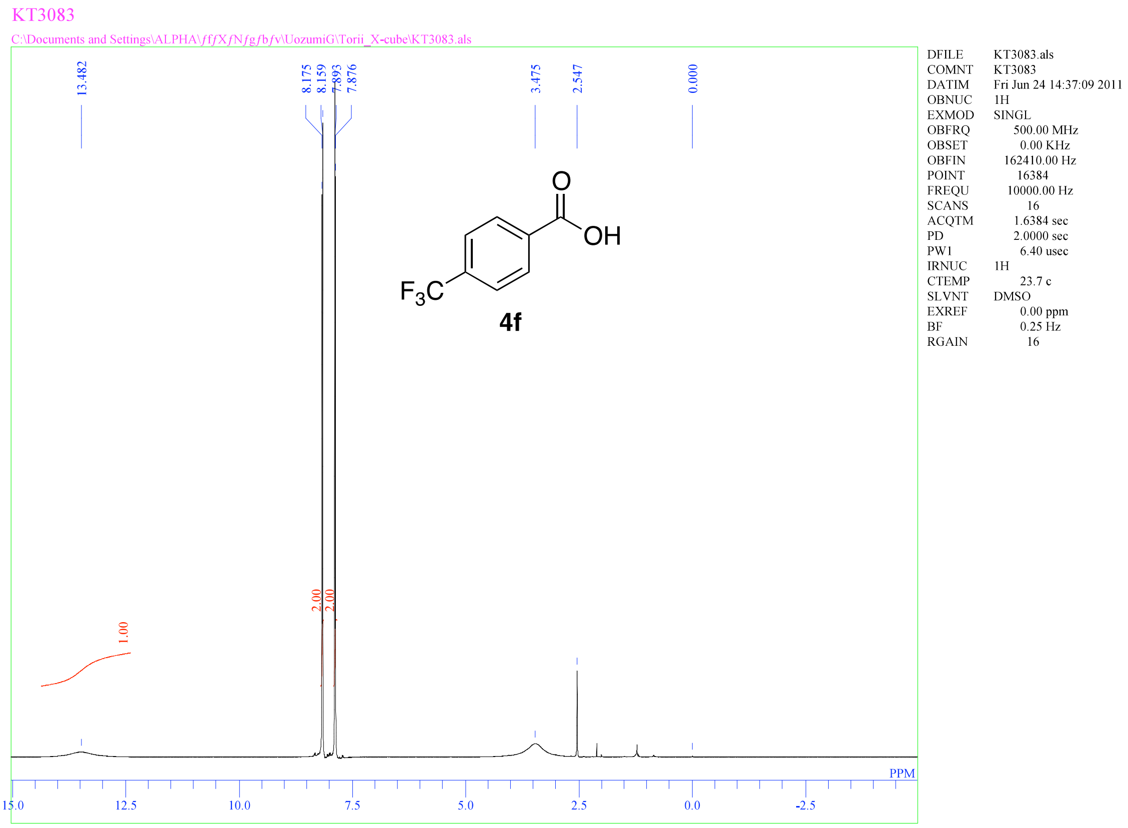


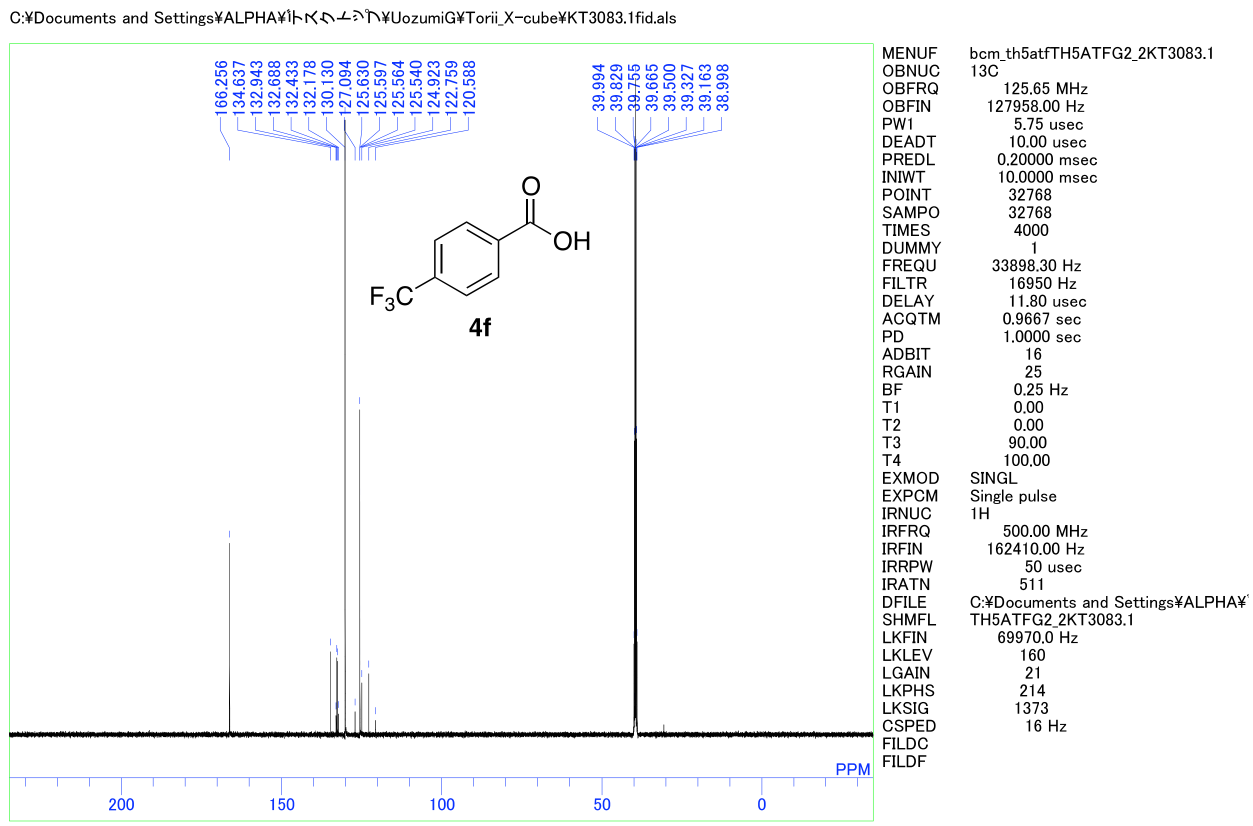
^{1}H and ^{13}C{^{1}H} NMR spectra of *p*-nitrobenzoic acid (**4e**).



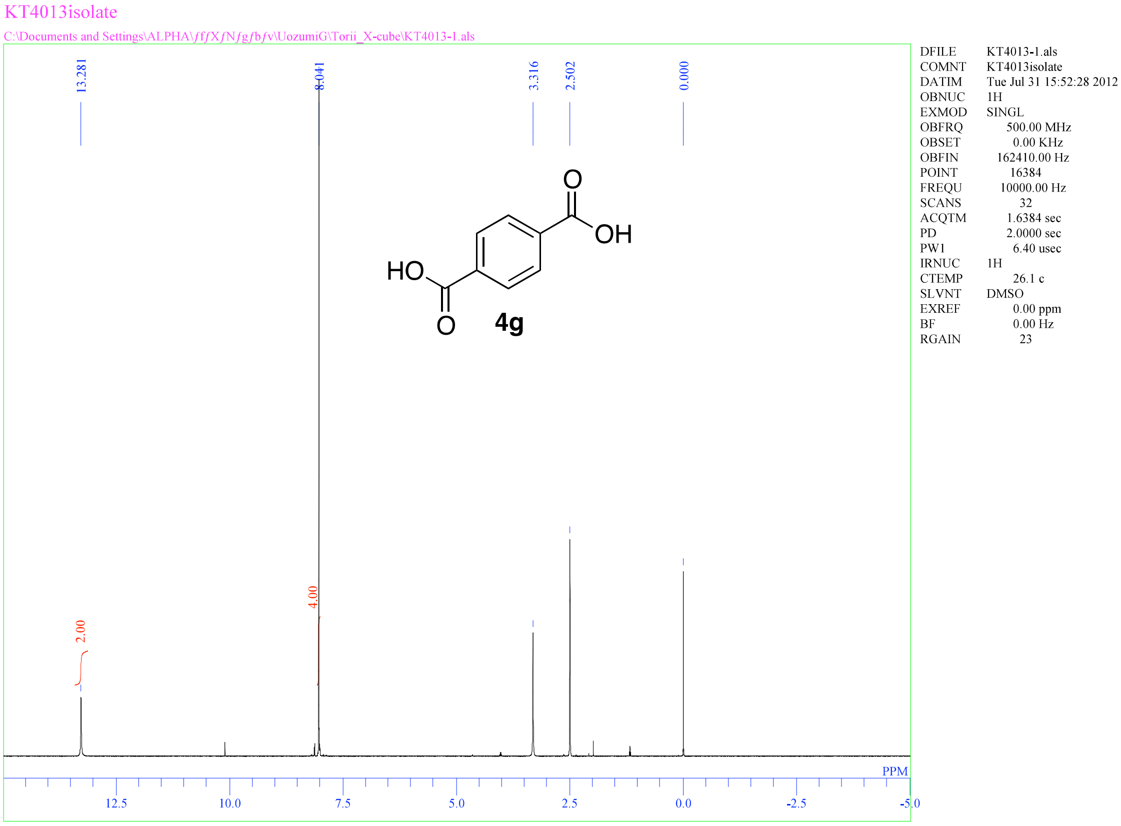


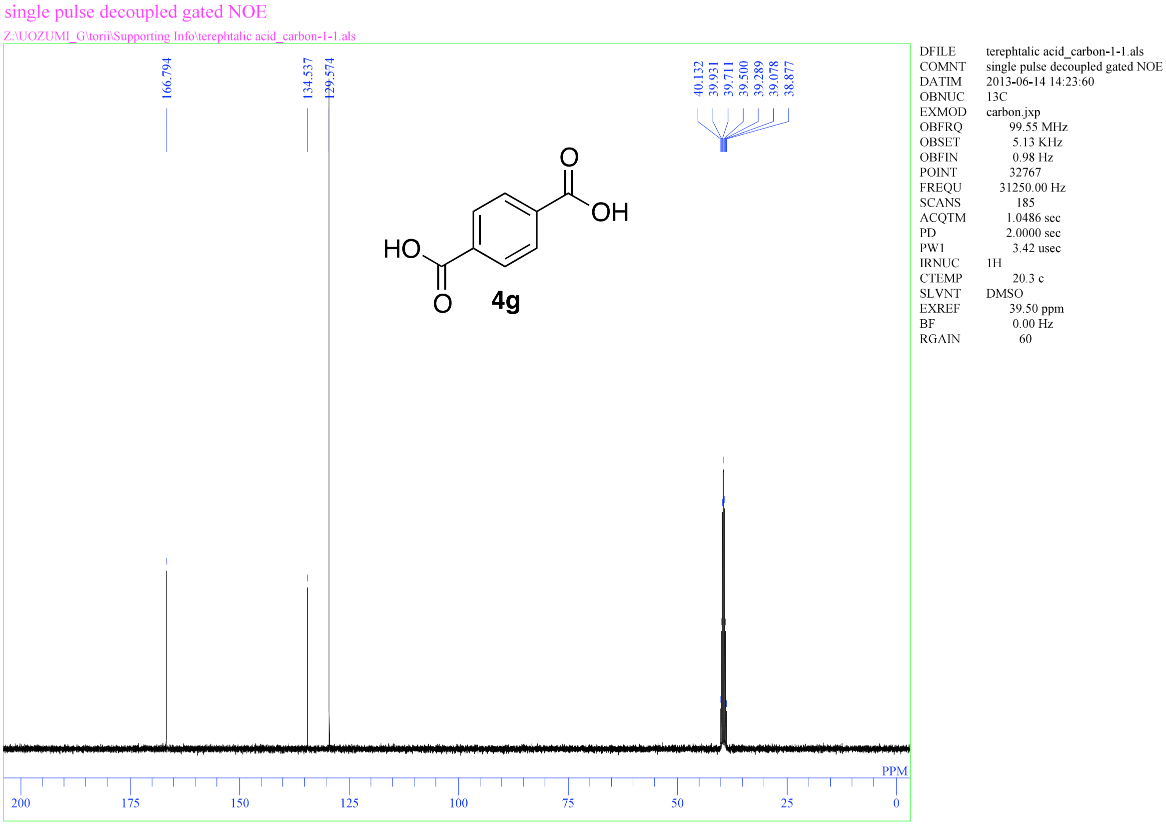
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 4-(trifluoromethyl)benzoic acid (**4f**).



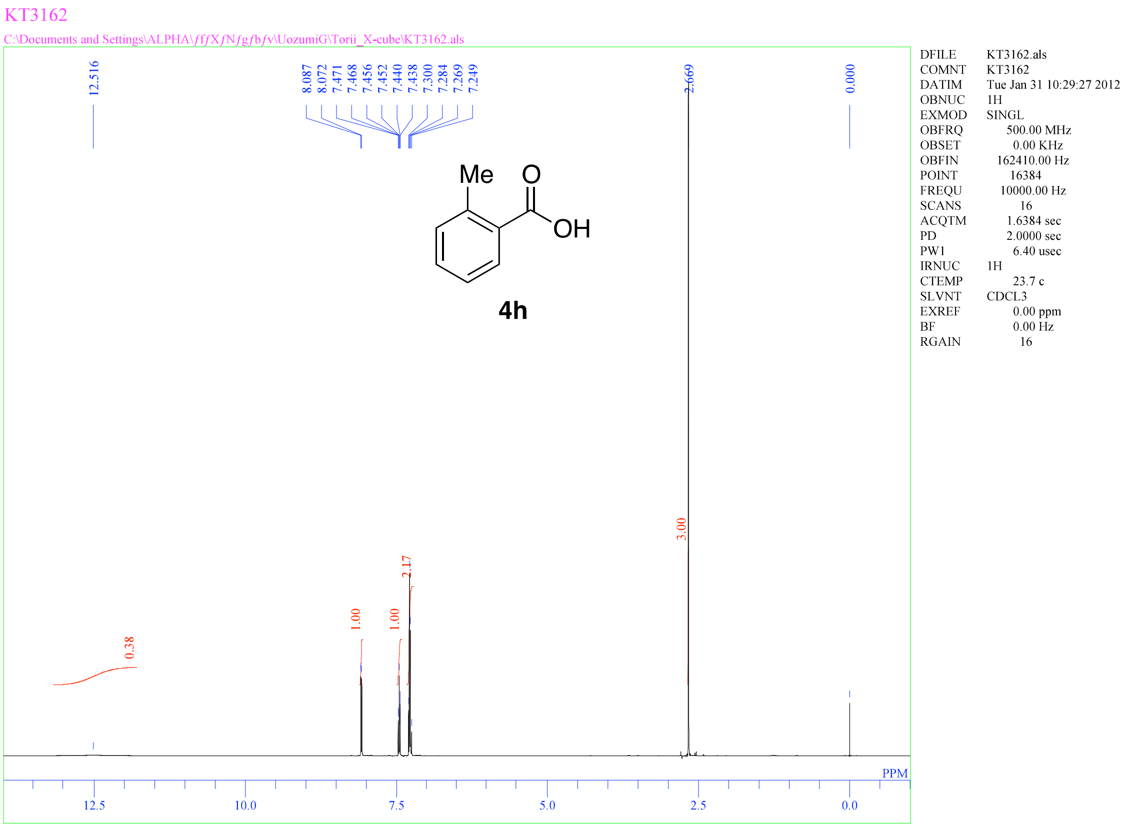


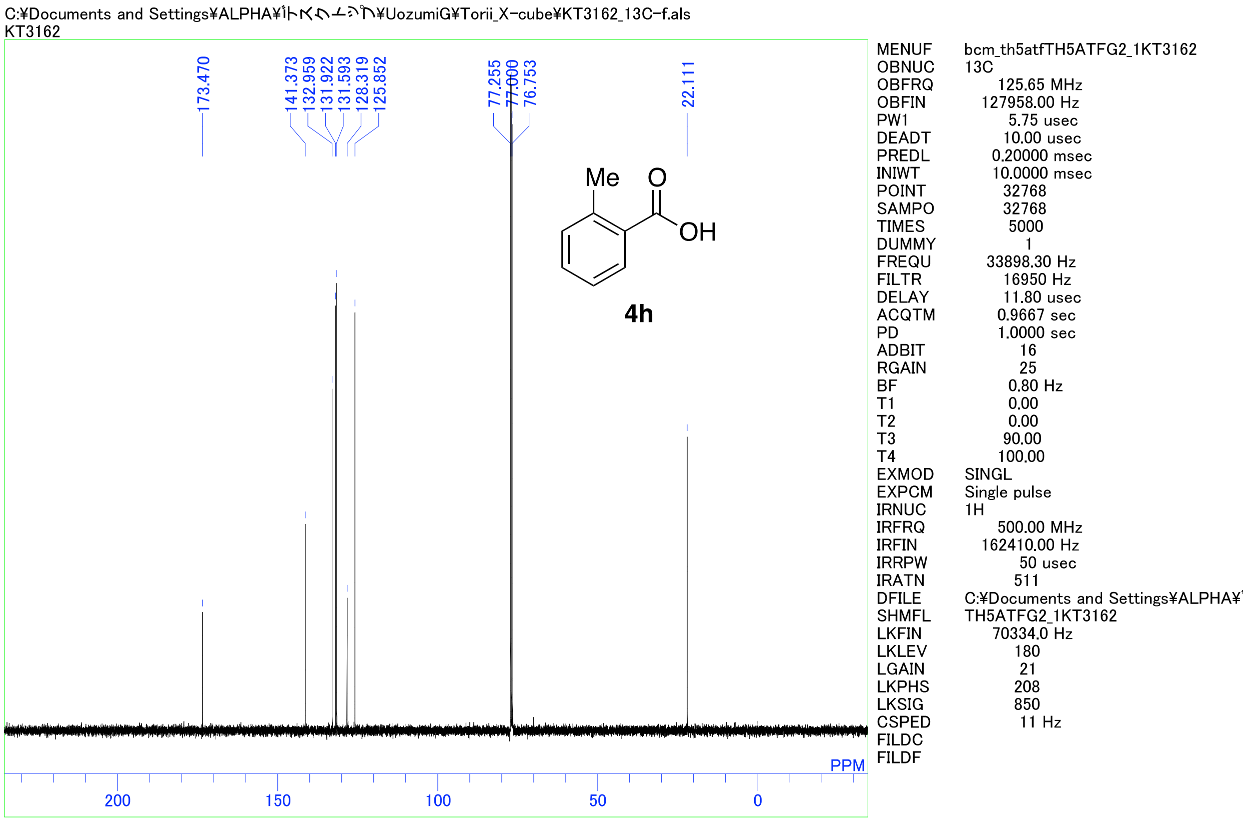
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of terephthalic acid (**4g**).



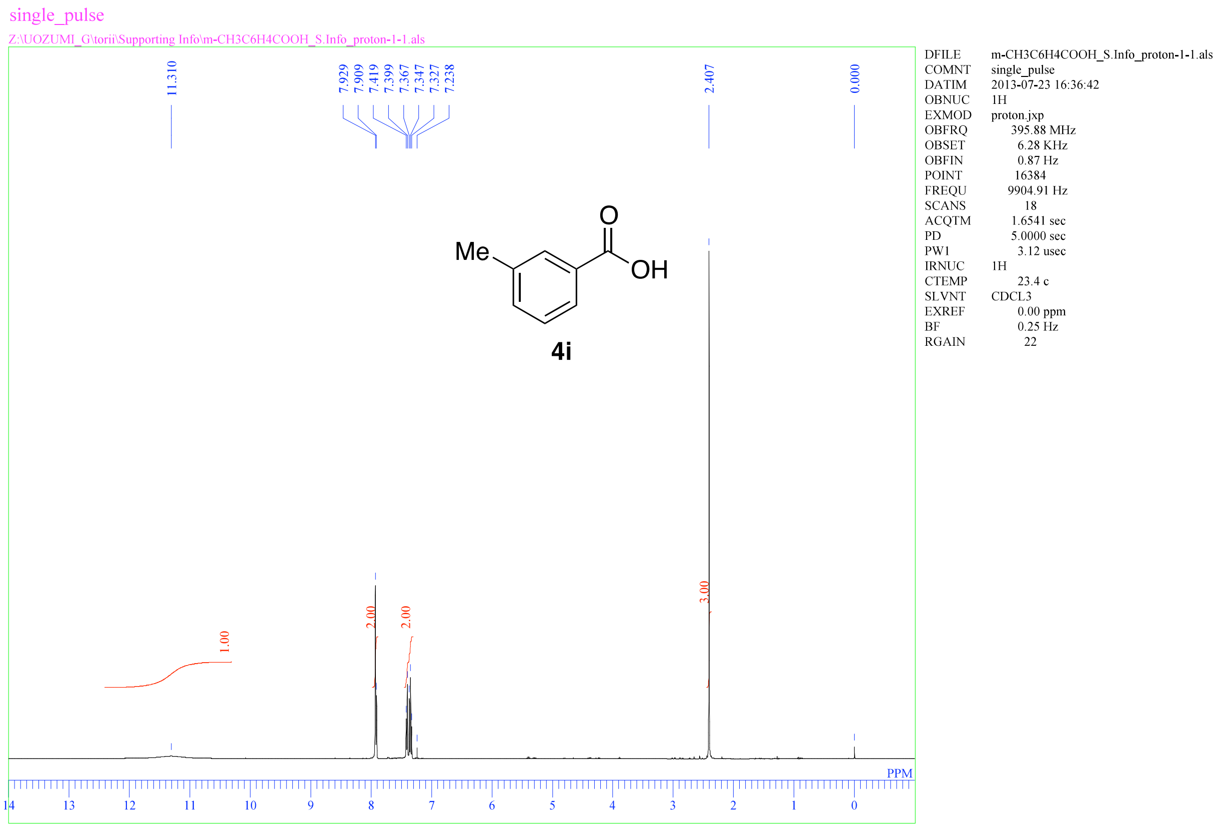


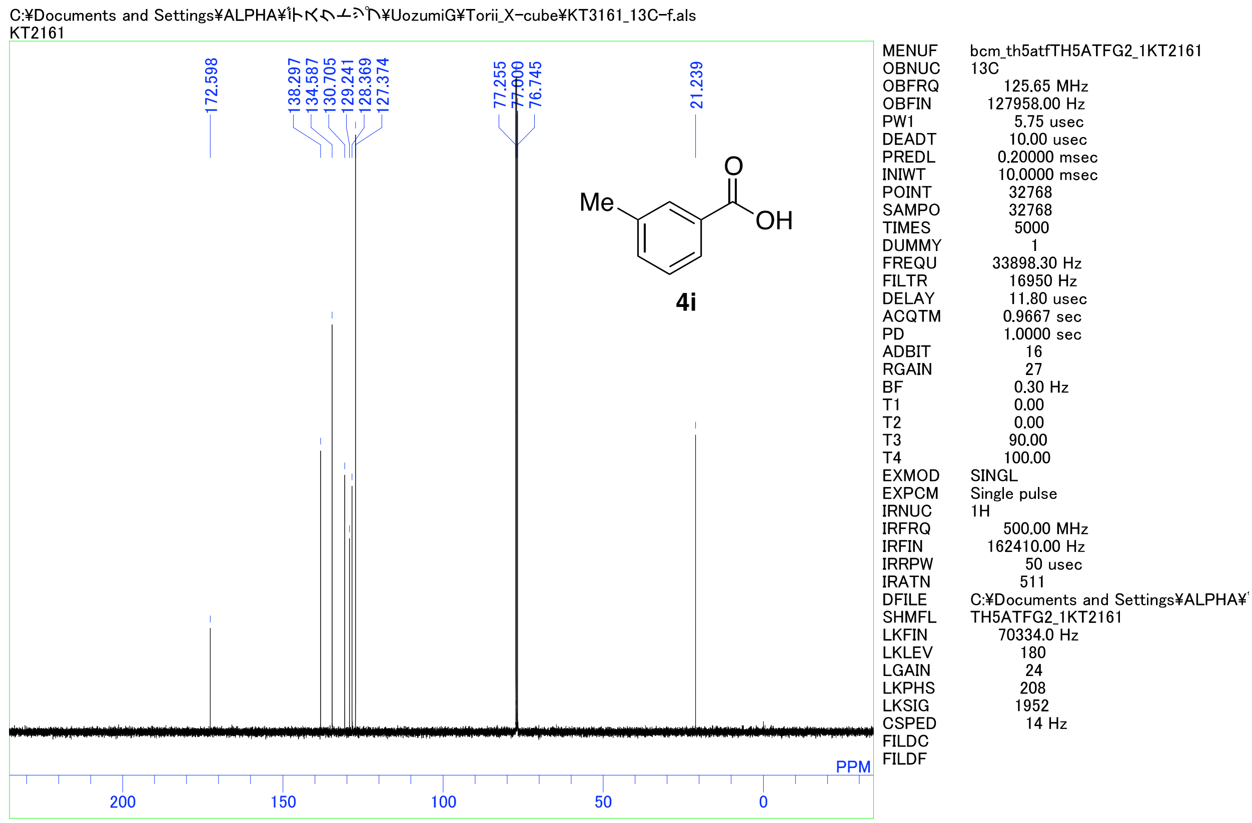
^{1}H and ^{13}C{^{1}H} NMR spectra of *o*-toluic acid (**4h**).



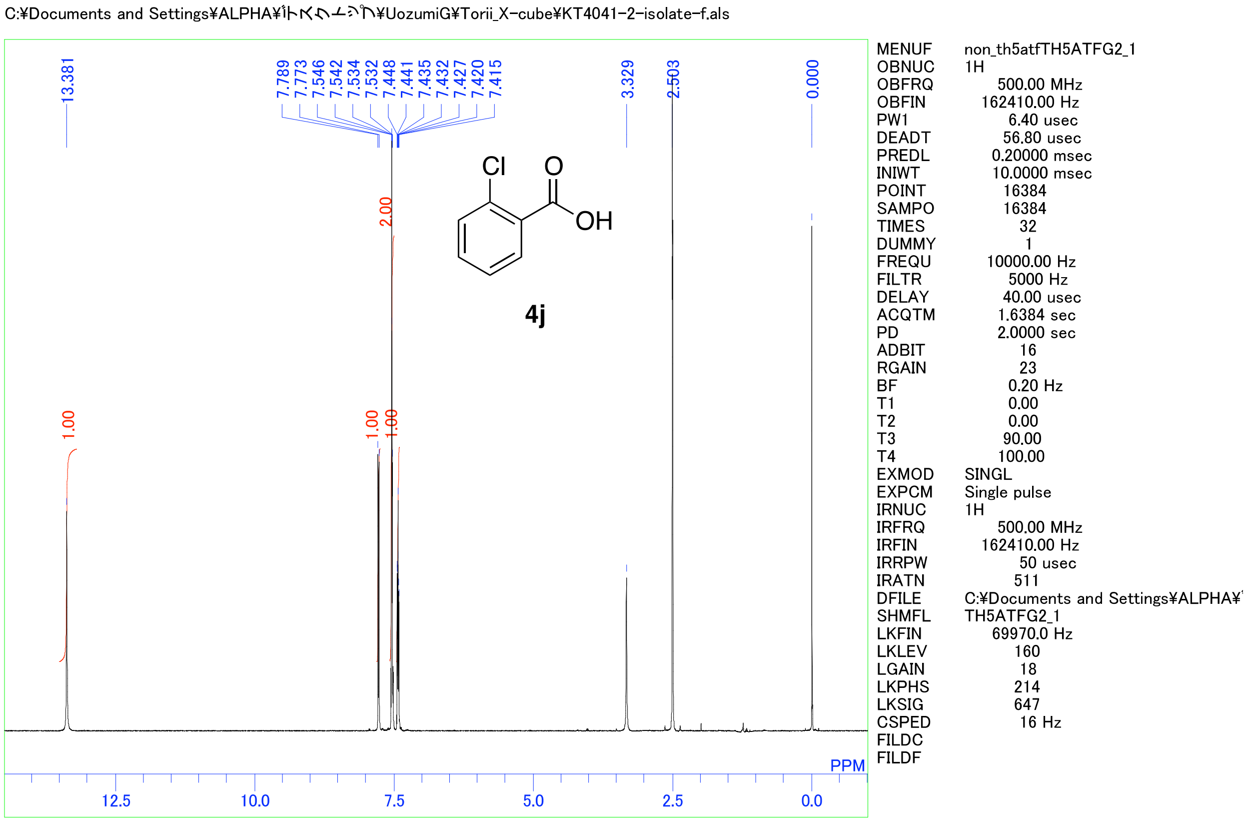


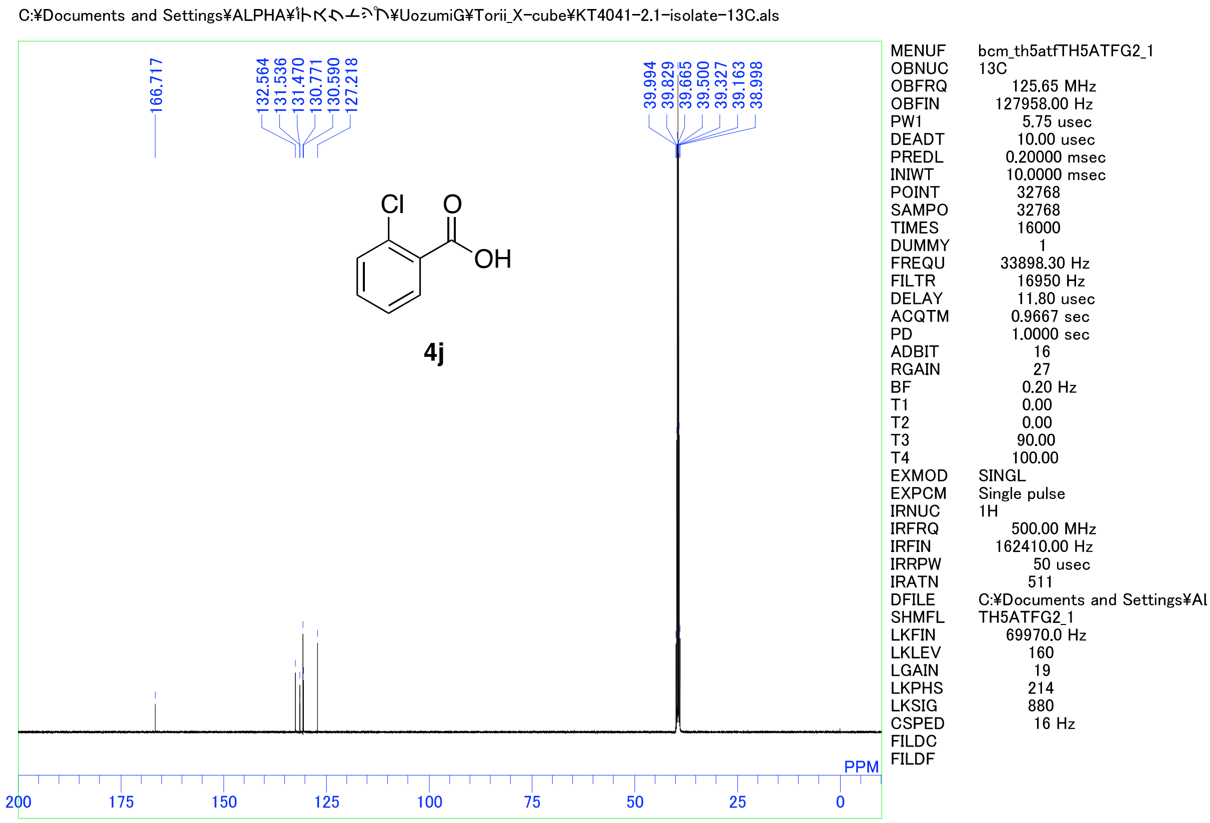
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of *m*-toluic acid (**4i**).



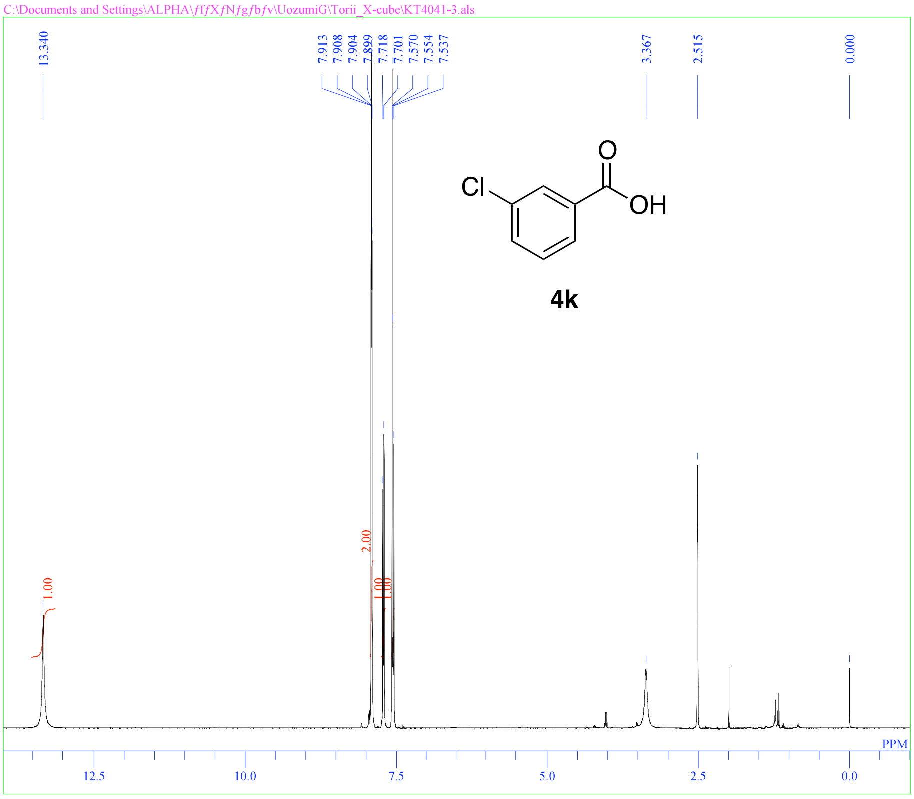


[1]H and [13]C{[1]H} NMR spectra of 2-chlorobenzoic acid (**4j**).





[1]H and [13]C{[1]H} NMR spectra of 3-chlorobenzoic acid (**4k**).



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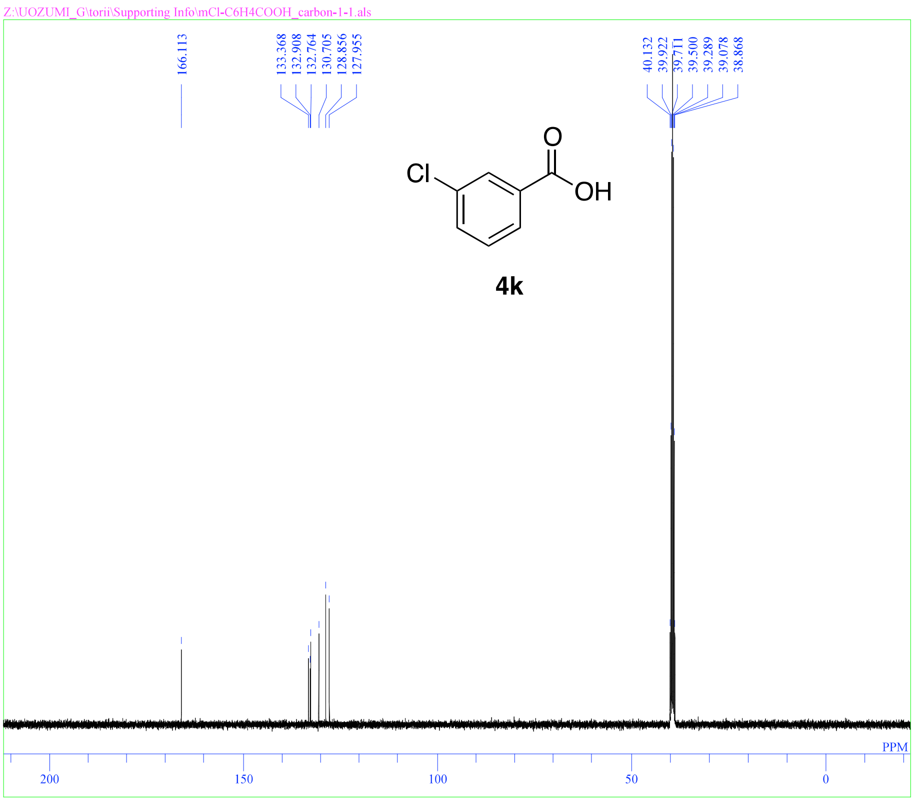
OBSET	0.00 KHz
OBFIN	162410.00 Hz
POINT	16384
FREQU	10000.00 Hz
SCANS	32
ACQTM	1.6384 sec
PD	2.0000 sec
PW1	6.40 usec
IRNUC	1H
CTEMP	22.8 c
SLVNT	DMSO
EXREF	0.00 ppm
BF	0.00 Hz
RGAIN	19

single pulse decoupled gated NOE



DFILE	mCl-C6H4COOH_carbon-1-1.als
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EXMOD	carbon.jxp
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OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	32767
FREQU	31250.00 Hz
SCANS	299
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	3.42 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	DMSO
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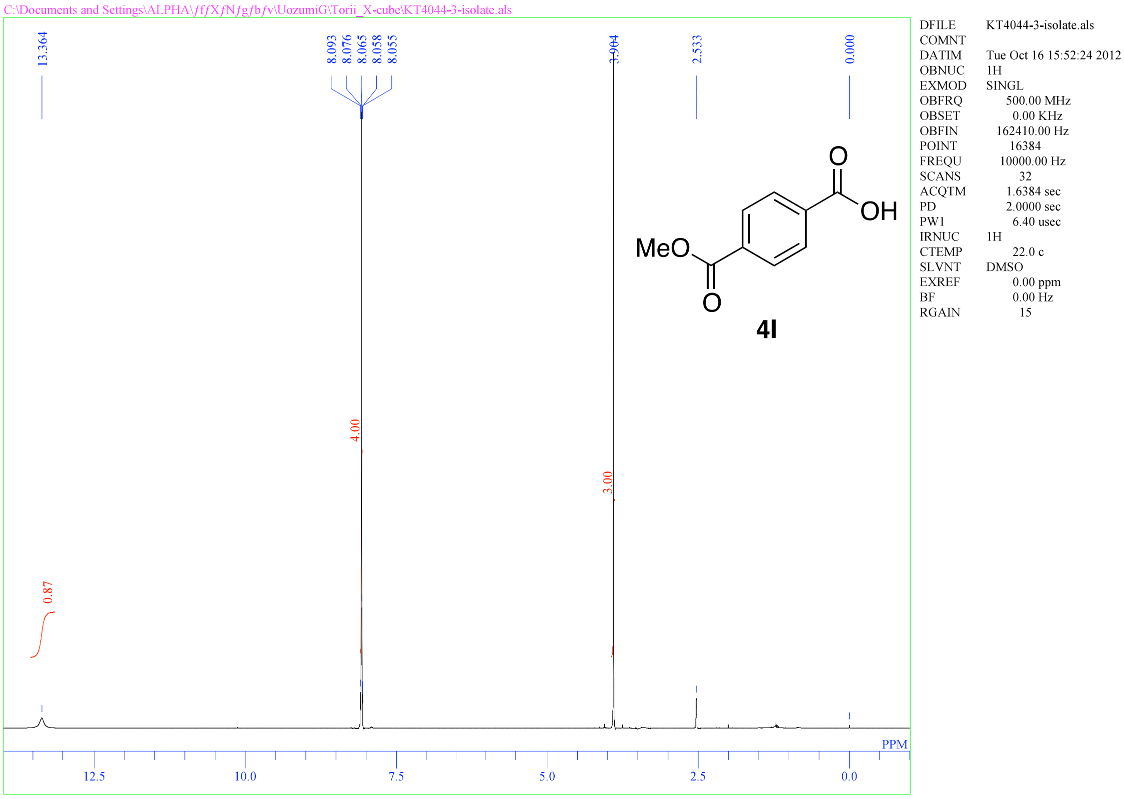
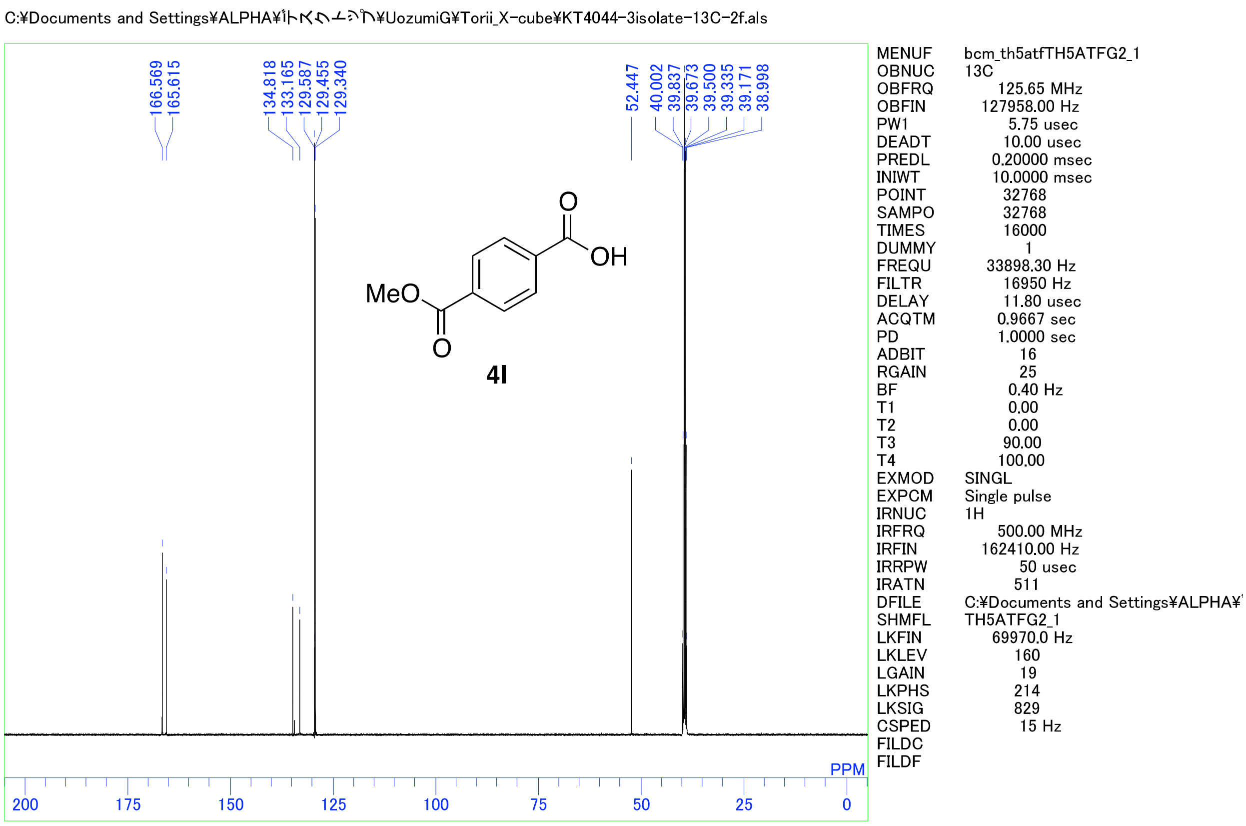
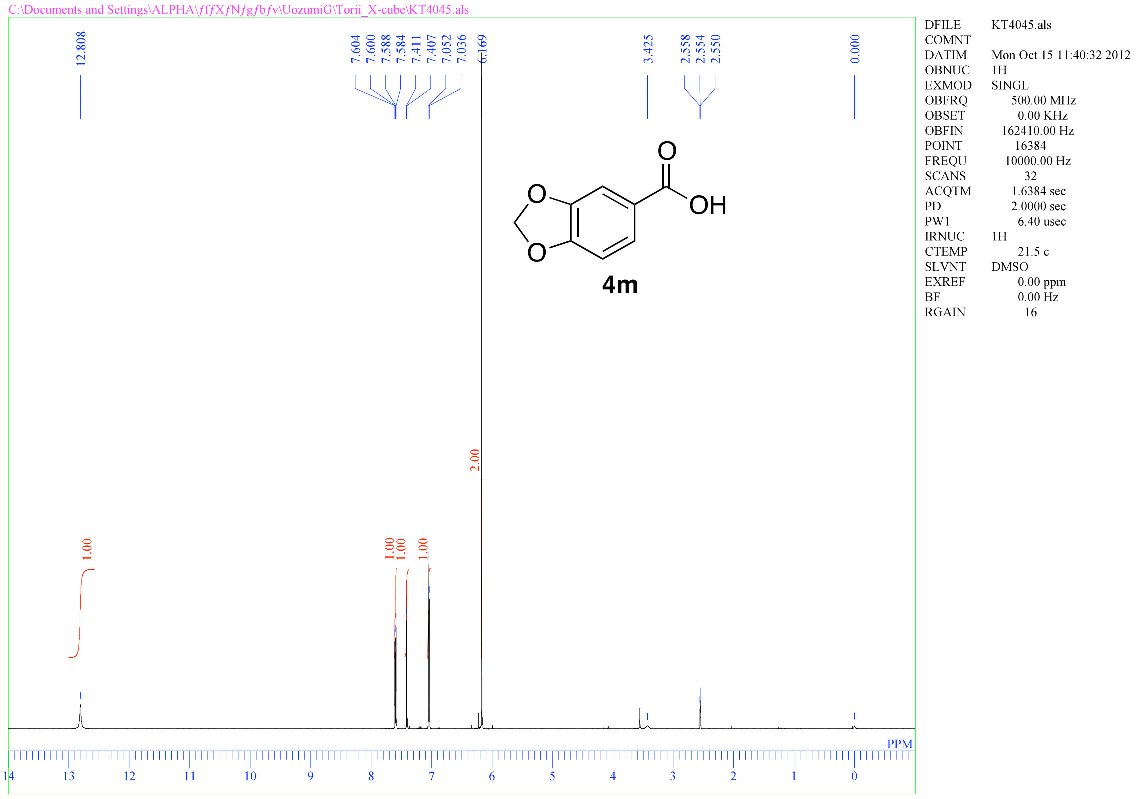
BF	0.50 Hz
RGAIN	60

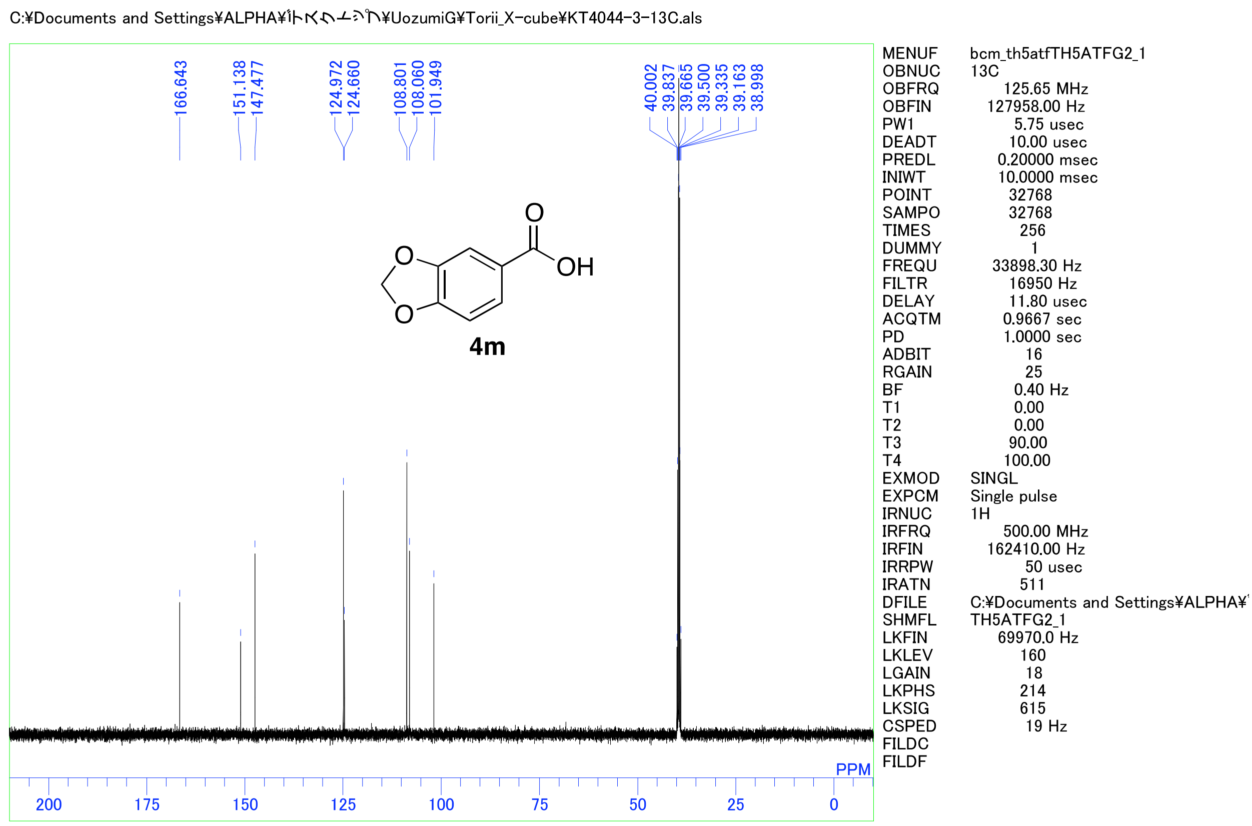
[1]H and [13]C{[1]H} NMR spectra of methyl terephthalate (**4l**).



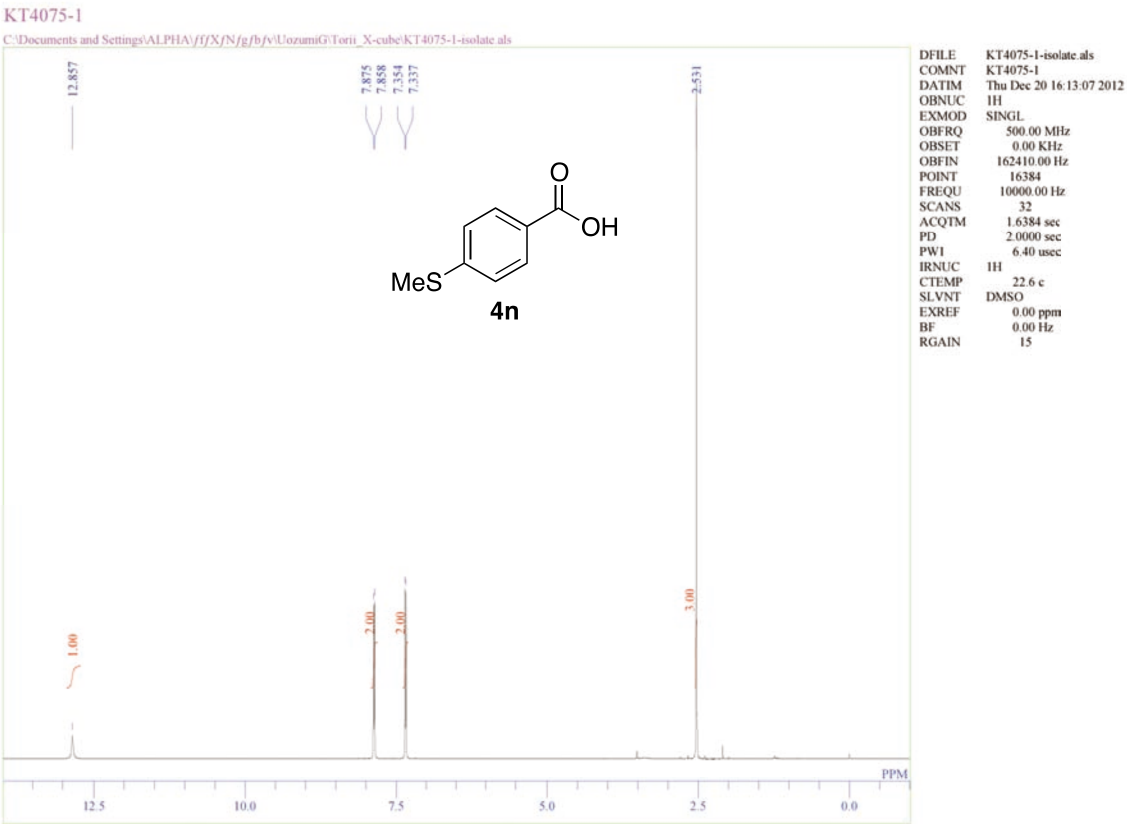


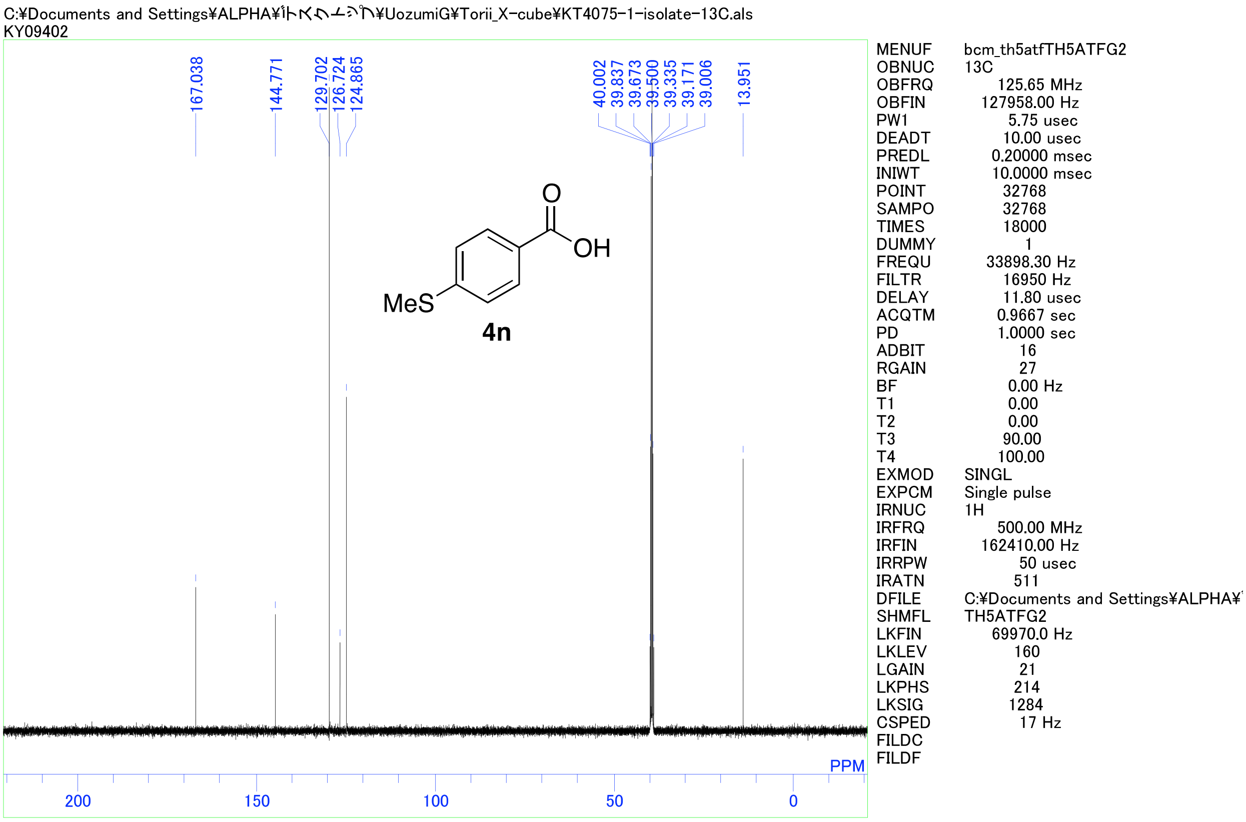
[1]H and [13]C{[1]H} NMR spectra of piperonylic acid (**4m**).



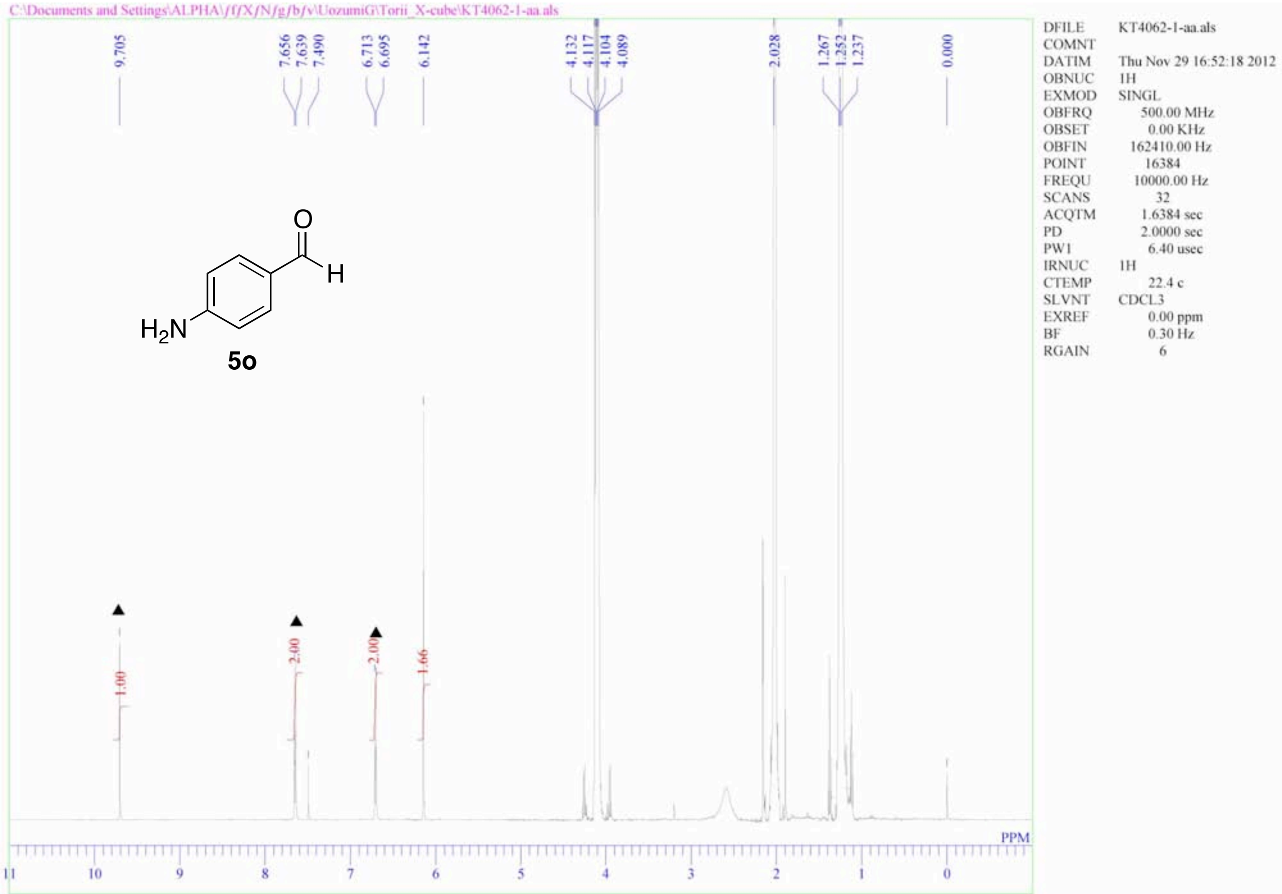


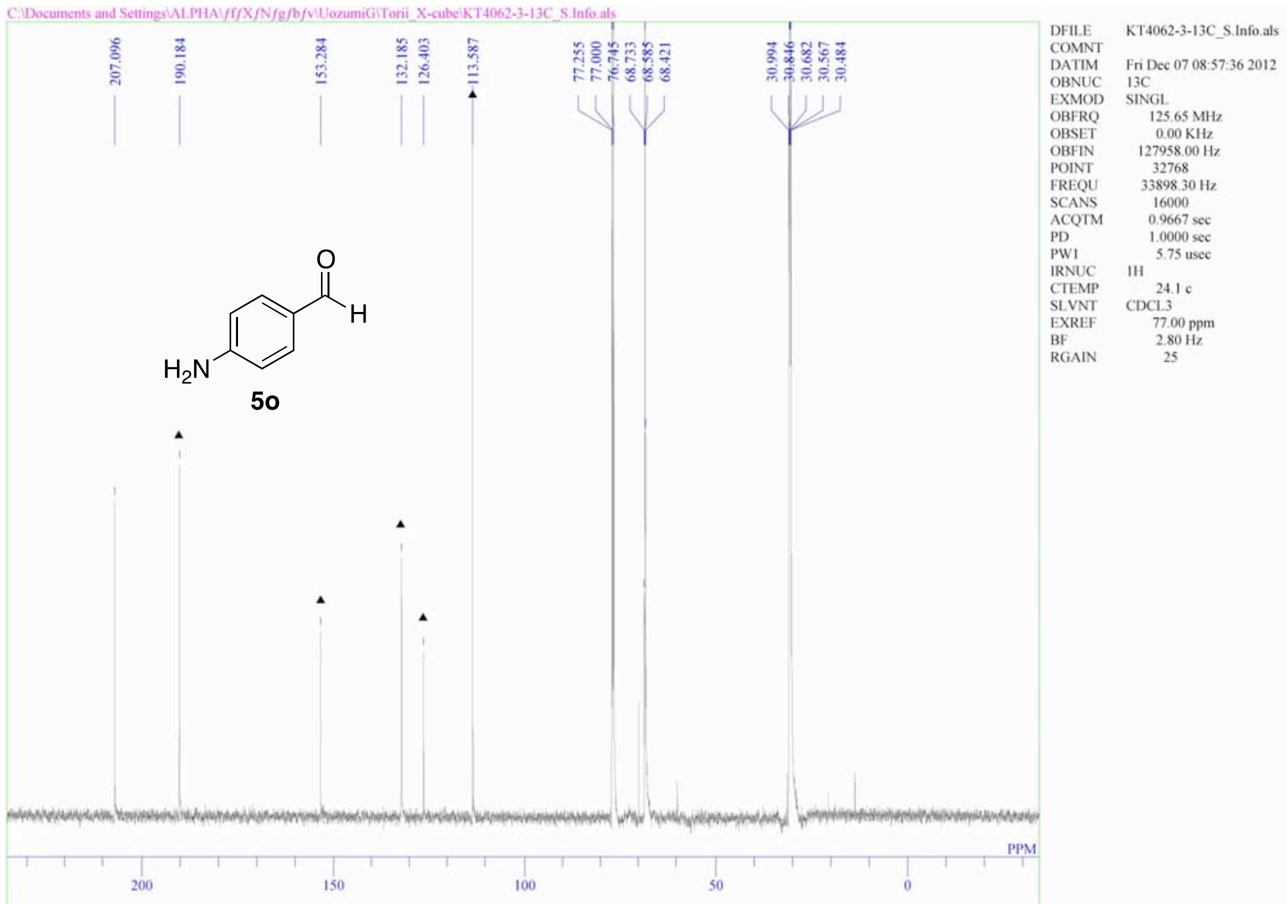
^{1}H and ^{13}C{^{1}H} NMR spectra of 4-(methylthio)benzoic acid (**4n**).



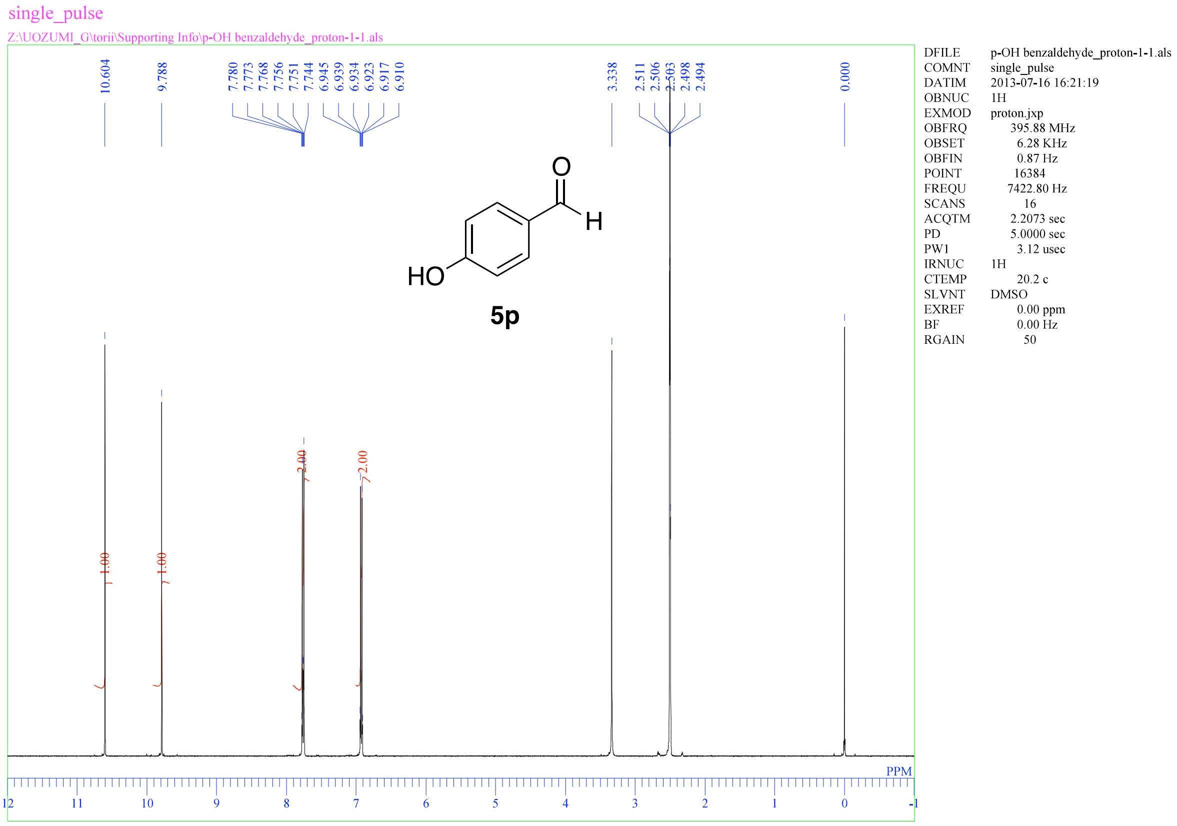


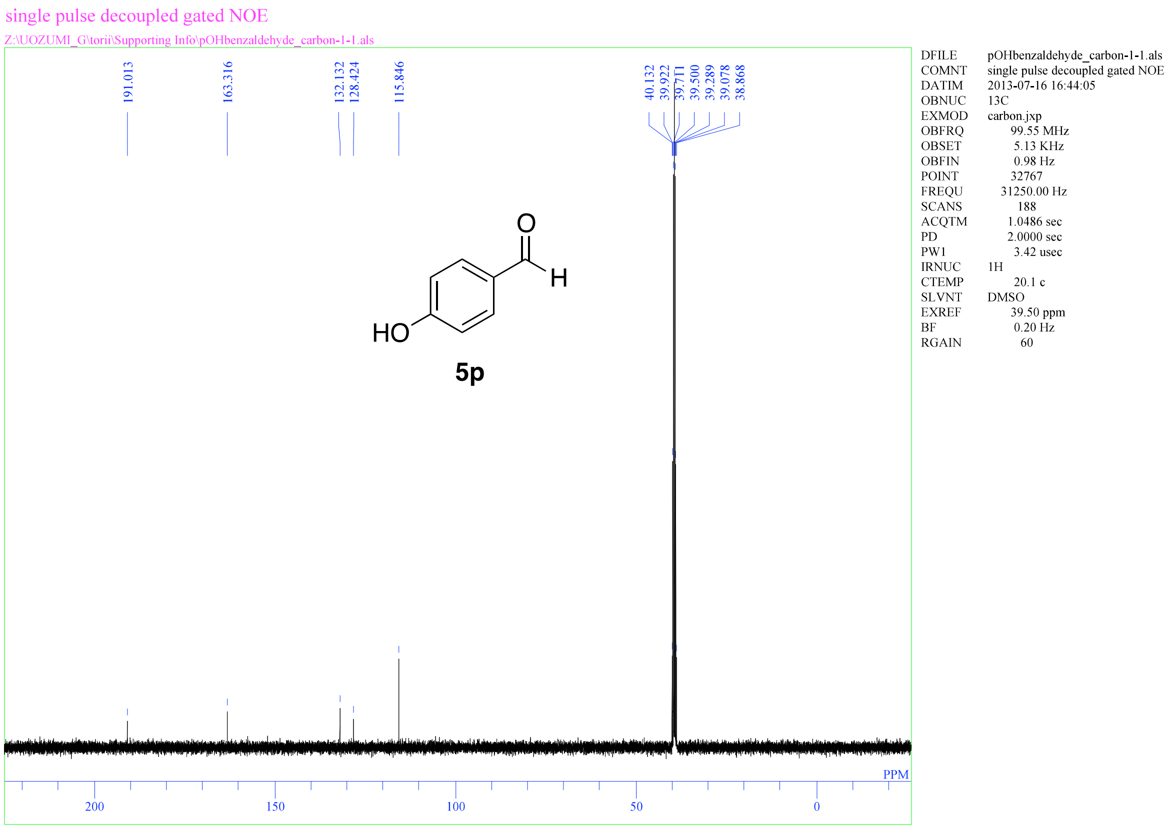
^{1}H and ^{13}C{^{1}H} NMR spectra of 4-aminobenzaldehyde (**5o**).





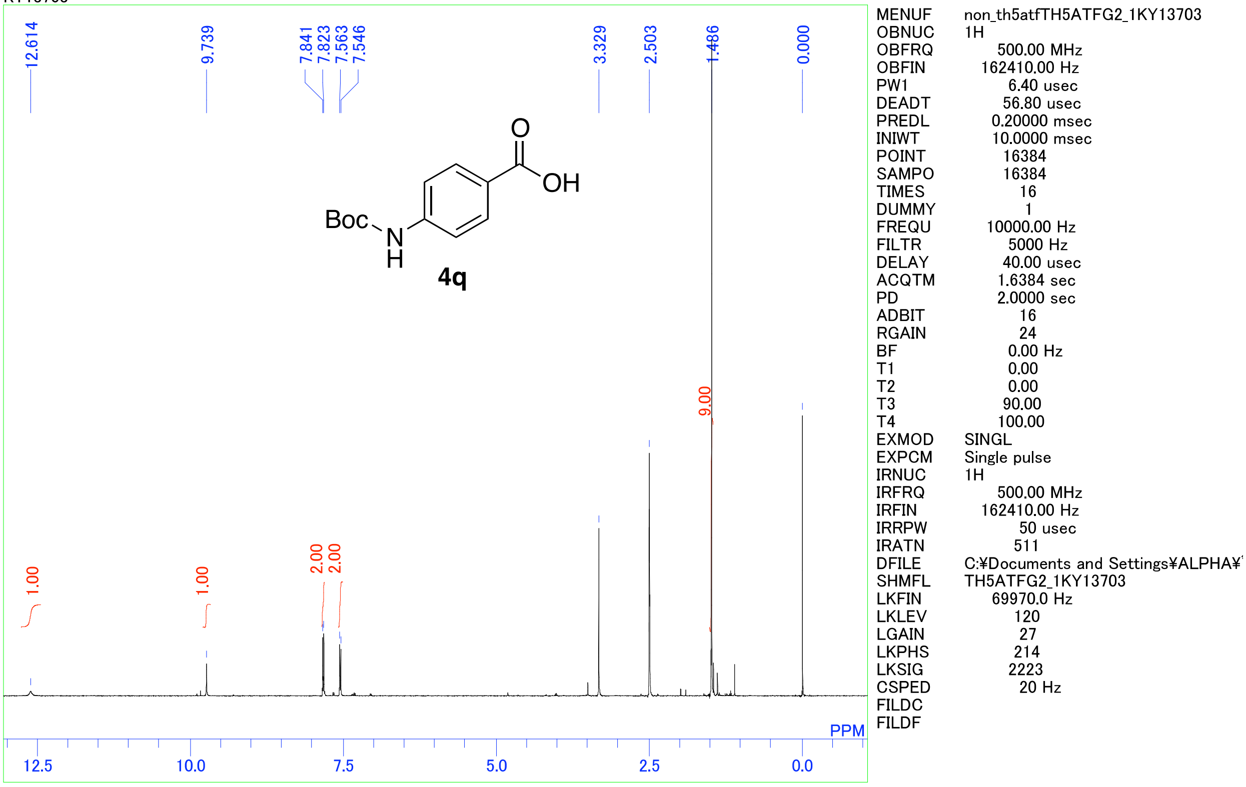
[1]H and [13]C{[1]H} NMR spectra of 4-hydroxybenzaldehyde (**5p**).



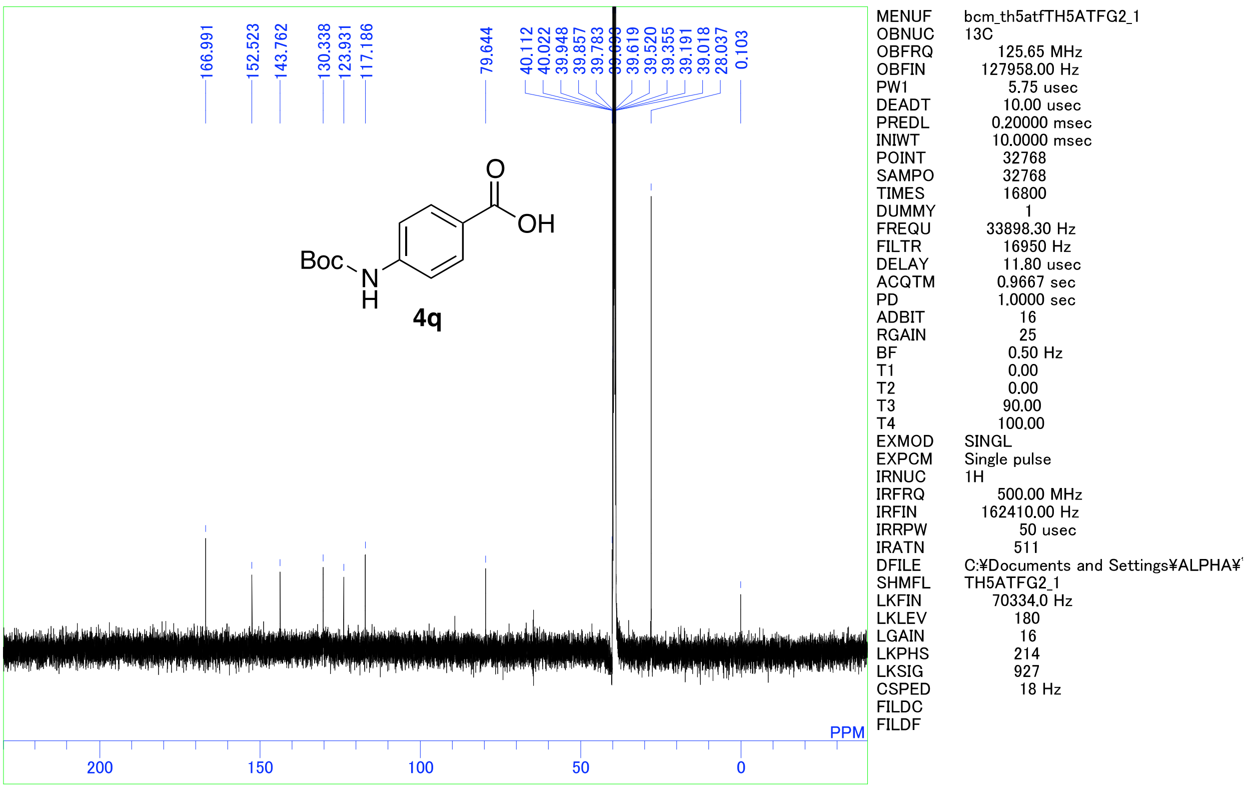


[1]H and [13]C{[1]H} NMR spectra of 4-(*tert*-butoxycarbonylamino)benzoic acid (**4q**).

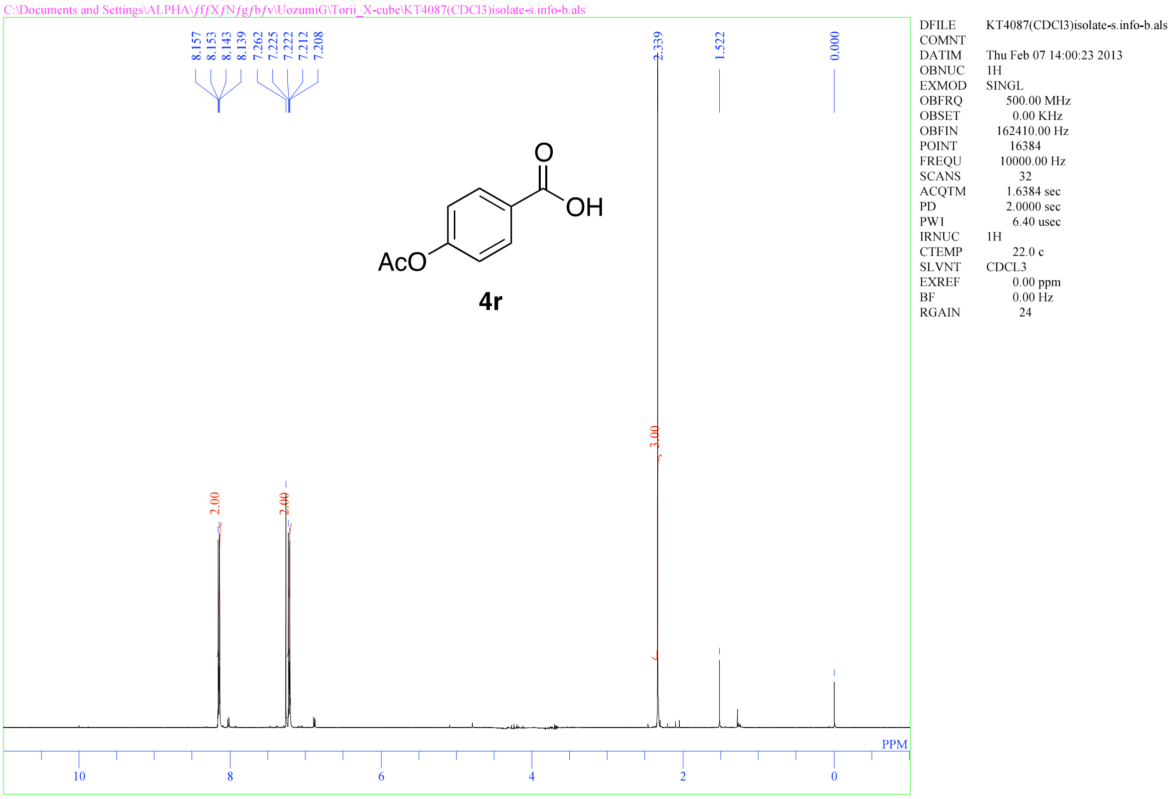
C:¥Documents and Settings¥ALPHA¥ｲﾄｸﾗﾑﾃﾞｰﾀ¥UozumiG¥Torii_X-cube¥KT4074-2isolate.als
KY13703

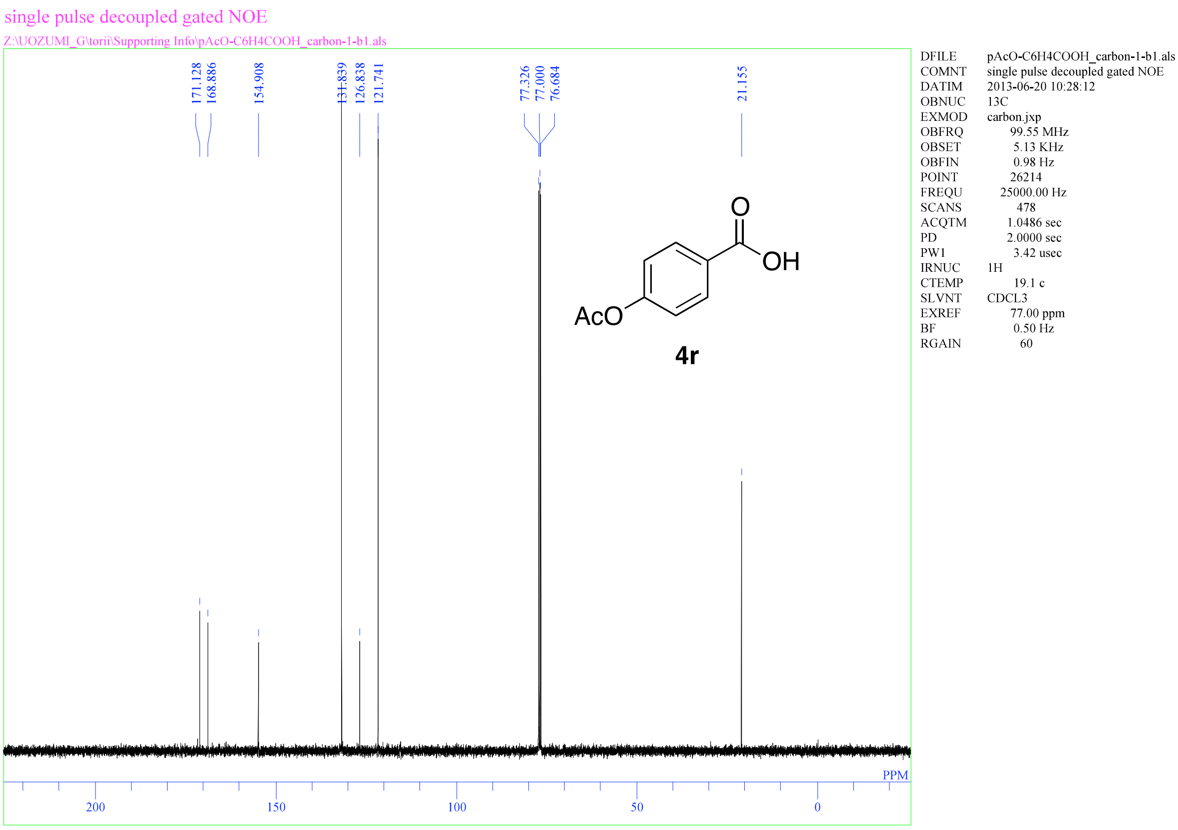


C:¥Documents and Settings¥ALPHA¥ｲﾄｸﾗﾑﾃﾞｰﾀ¥UozumiG¥Torii_X-cube¥KT4074-2isolate-C.als

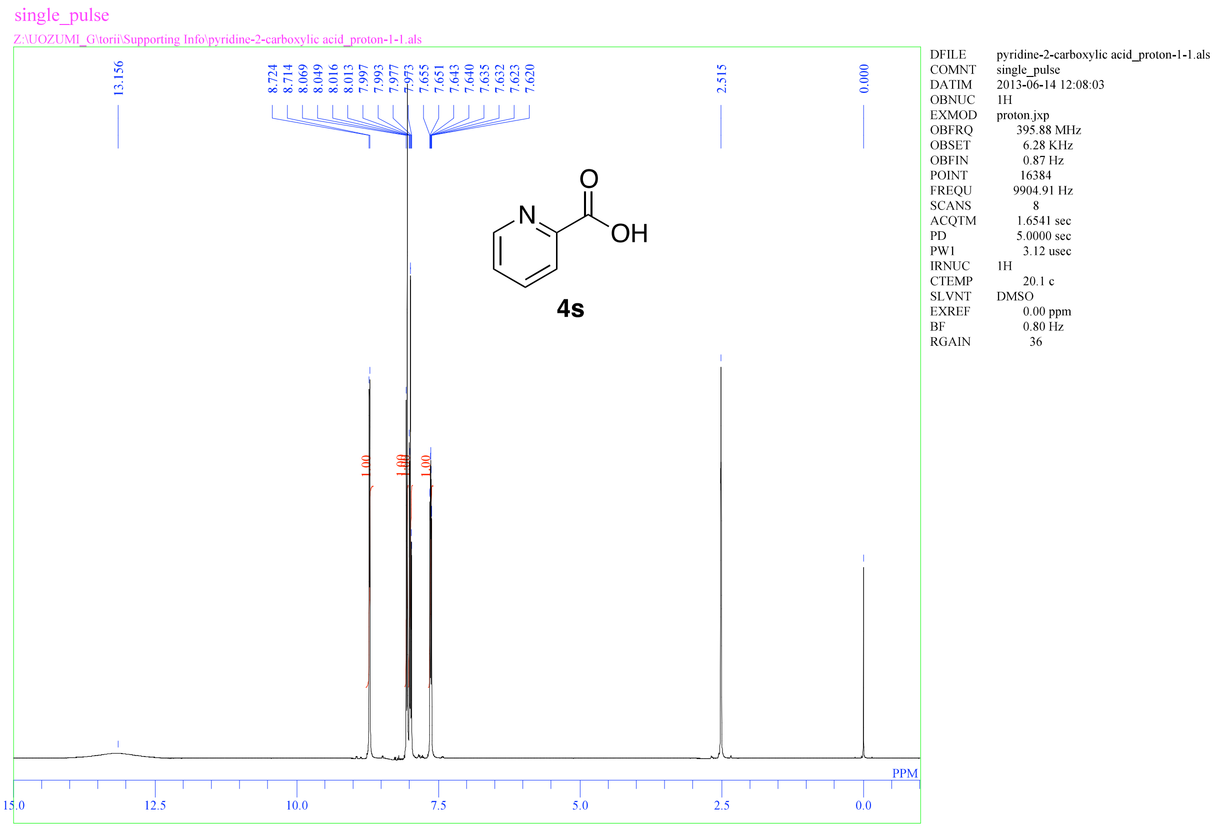


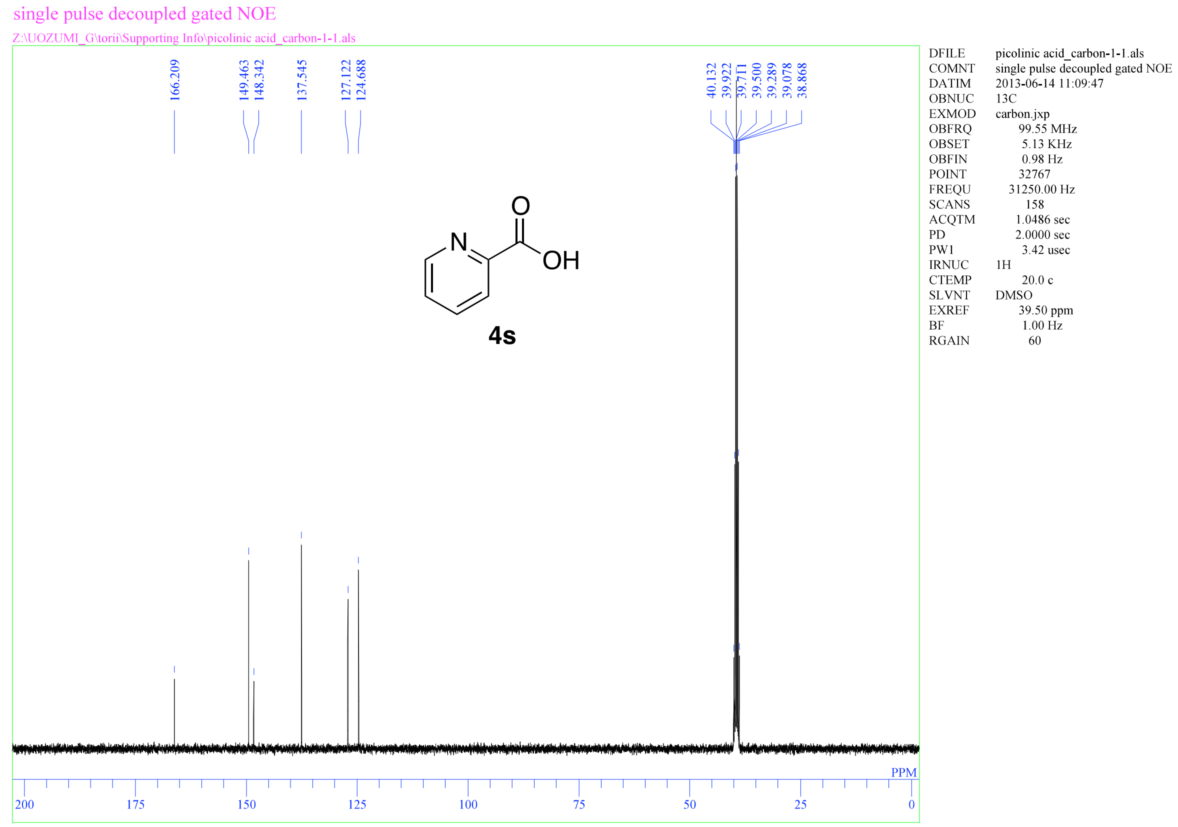
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 4-acetoxybenzoic acid (**4r**).



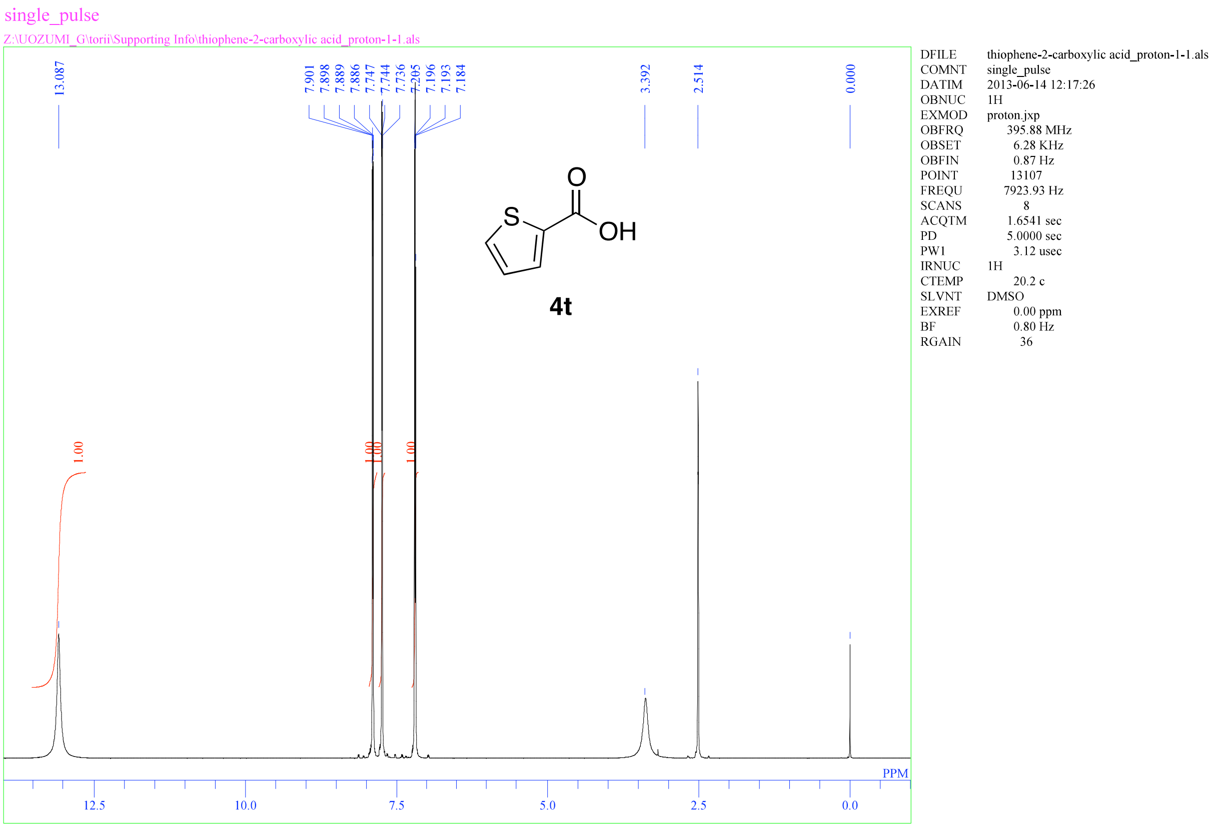


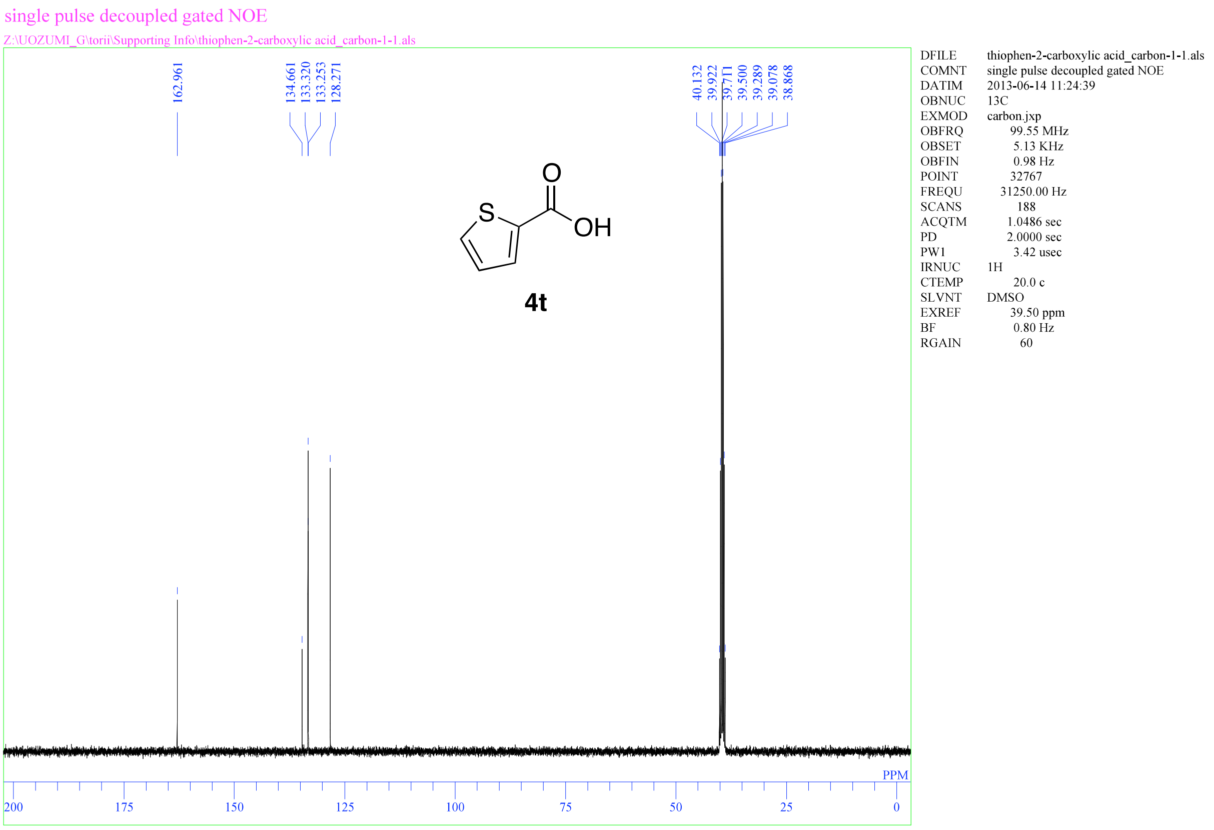
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-picolinic acid (**4s**).



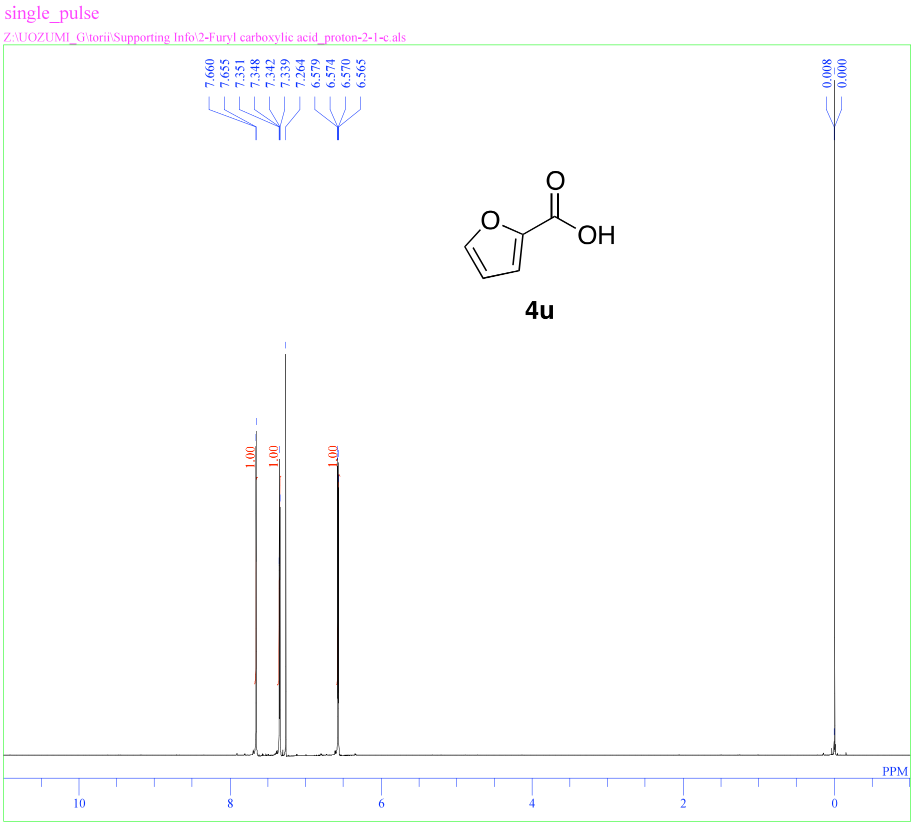


^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-thiophenecarboxylic acid (**4t**).





^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of 2-furancarboxylic acid (**4u**).



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OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 7923.93 Hz
SCANS 8
ACQTM 1.6541 sec
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IRNUC 1H
CTEMP 20.1 c
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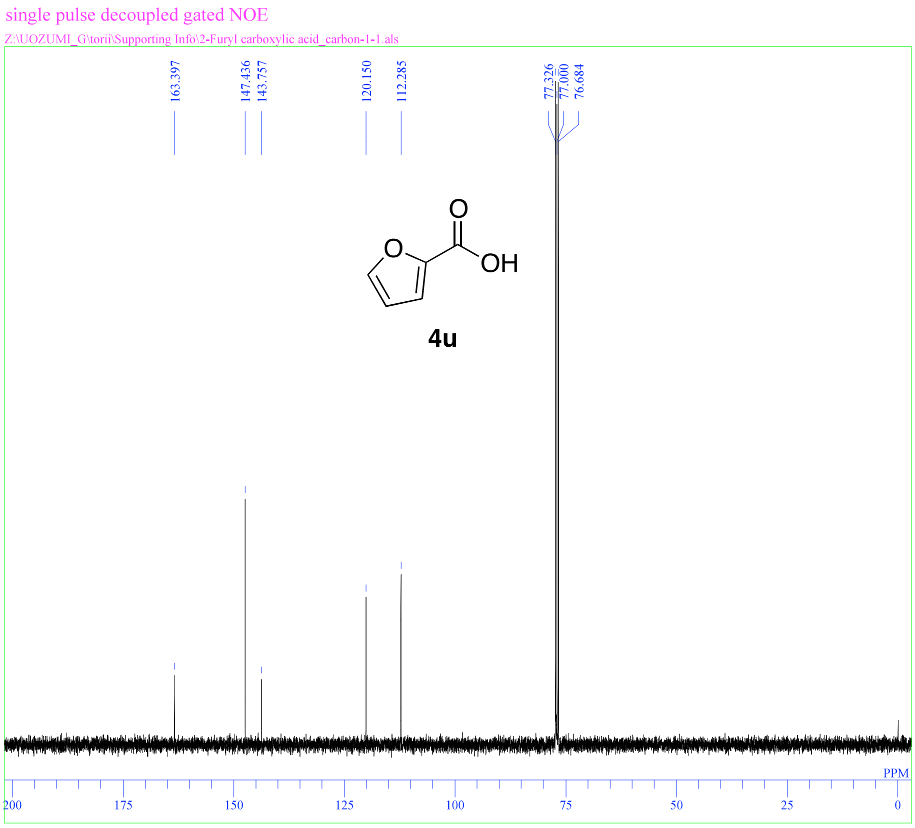
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 42



DFILE 2-Furyl carboxylic acid_carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2013-06-14 11:41:44
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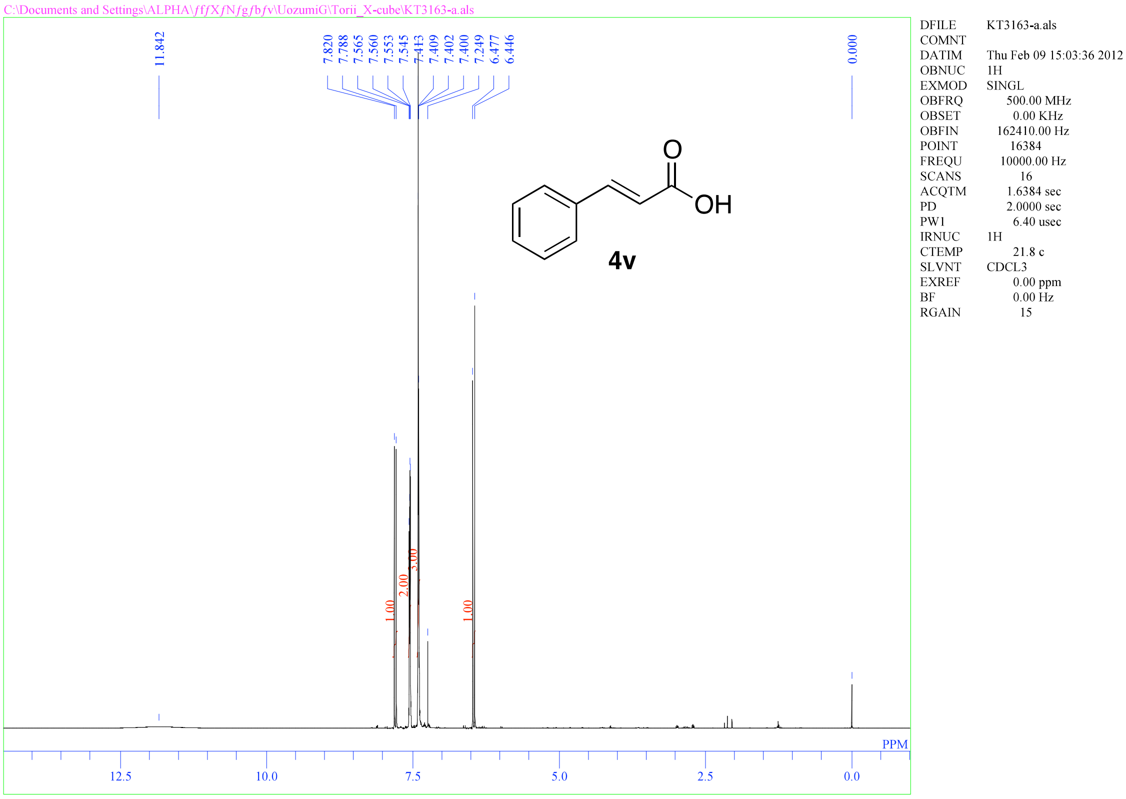
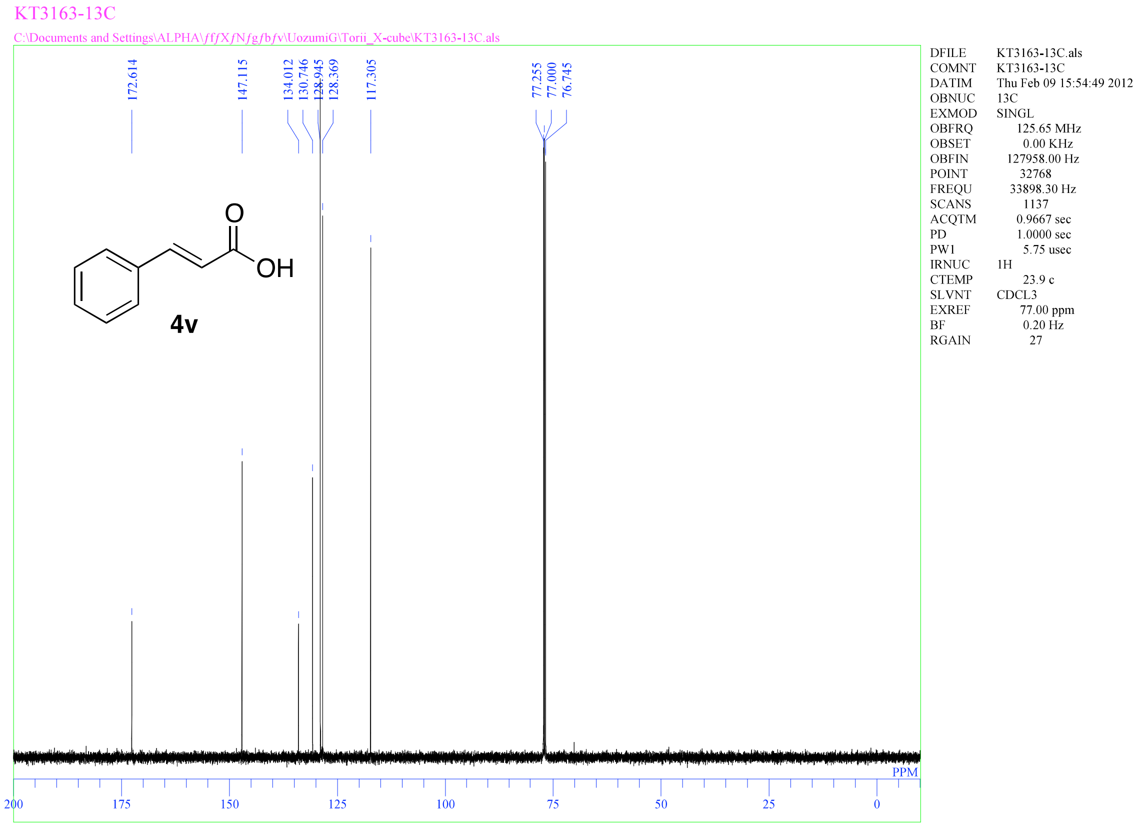
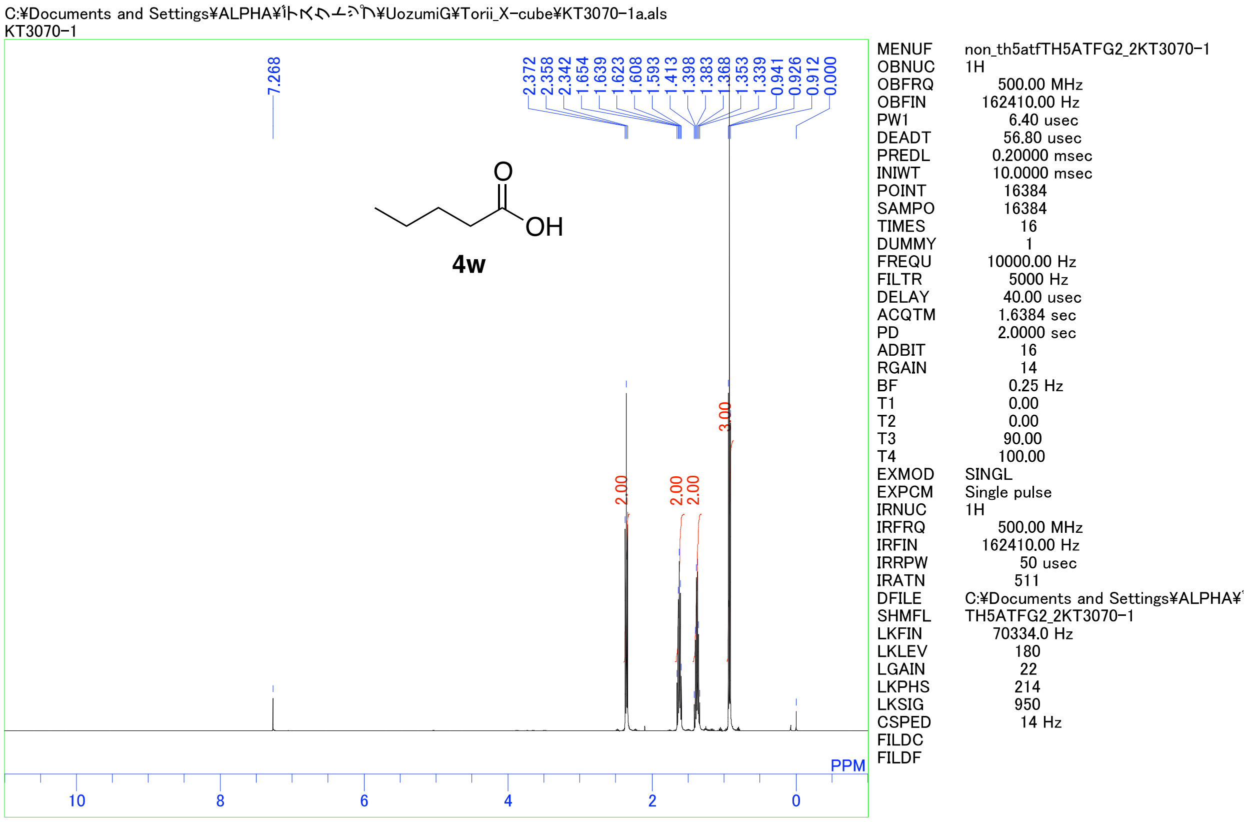
EXMOD carbon.jxp
OBFRQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 245
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC 1H
CTEMP 20.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.80 Hz
RGAIN 60

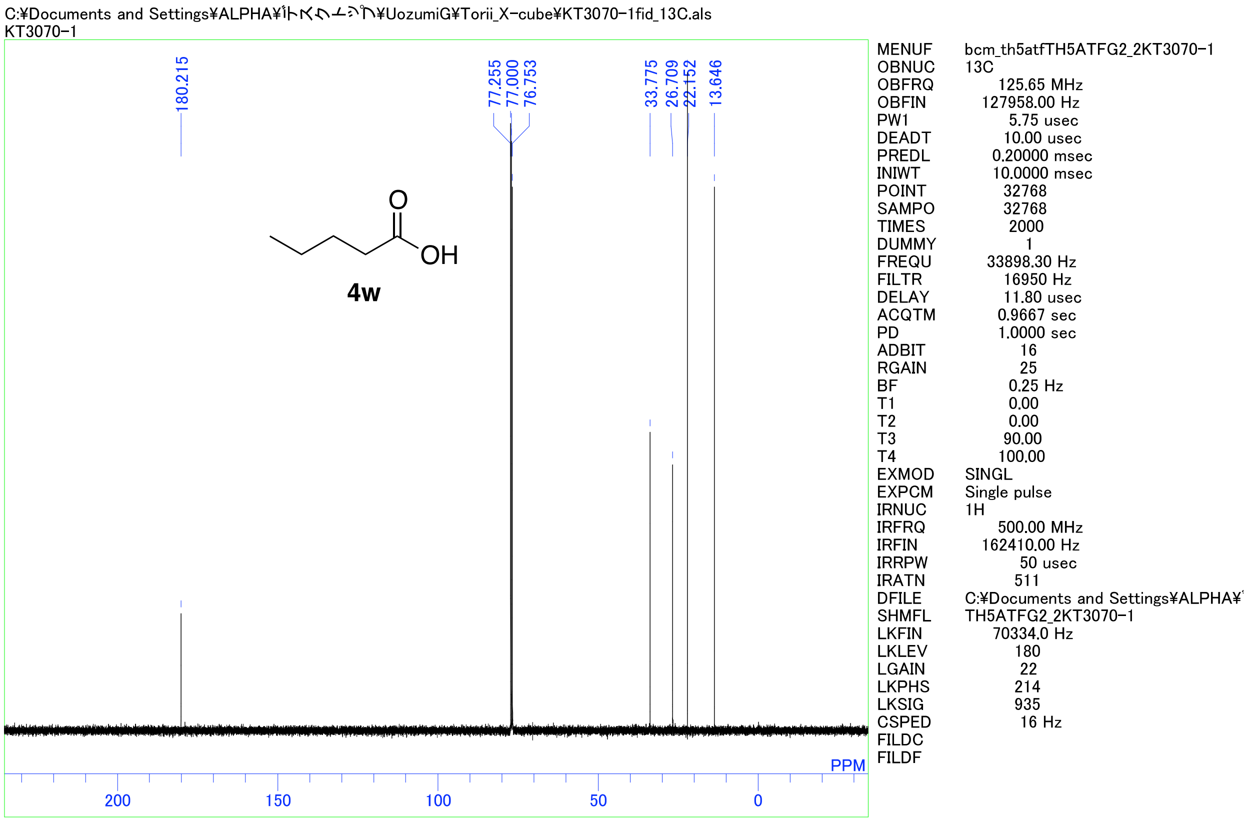
[1]H and [13]C{[1]H} NMR spectra of cinnamic acid (**4v**).



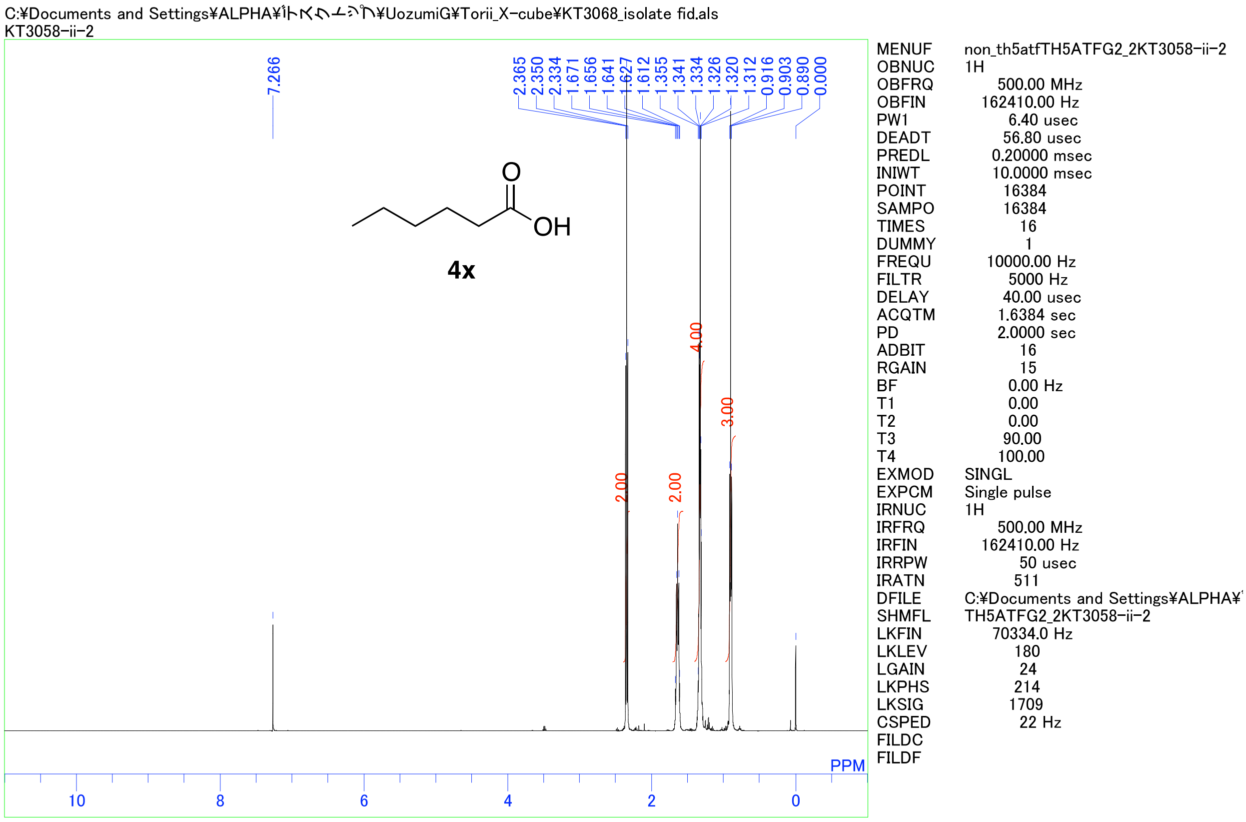


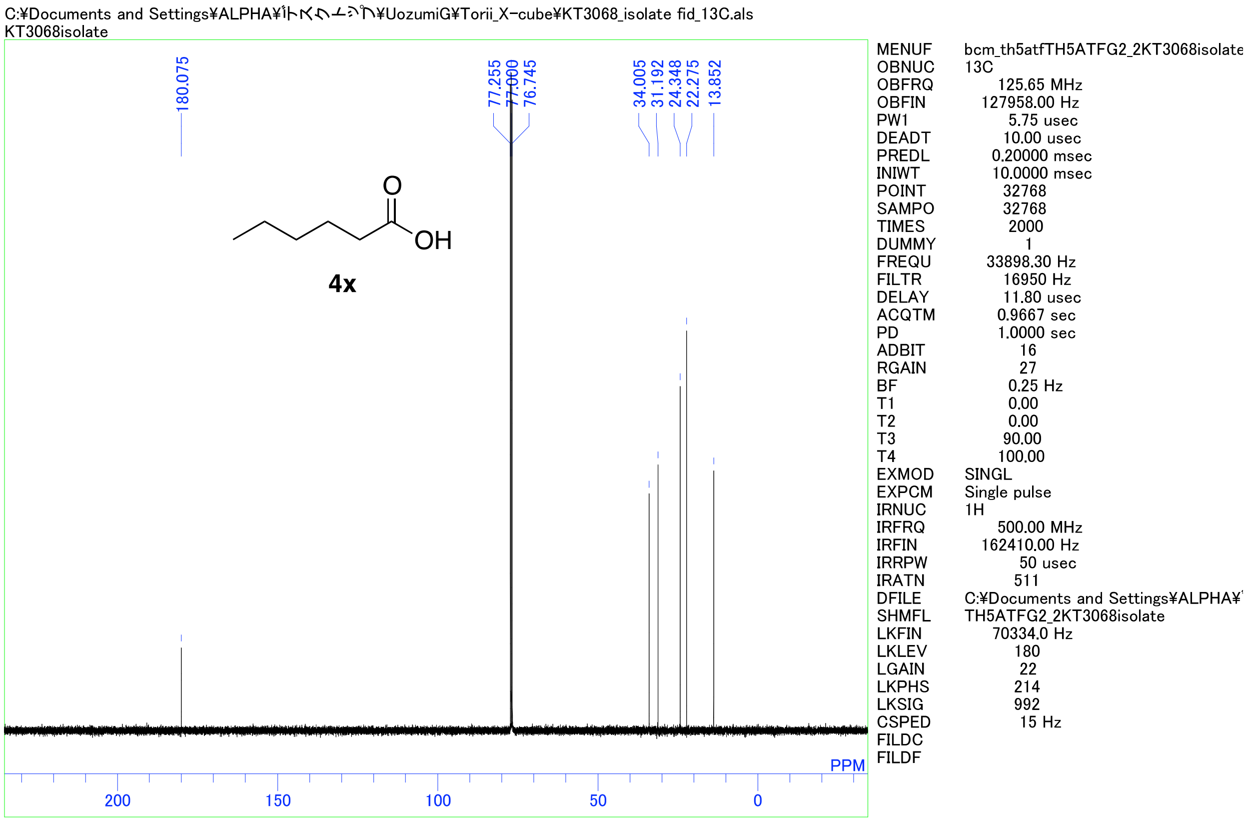
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of pentanoic acid (**4w**).



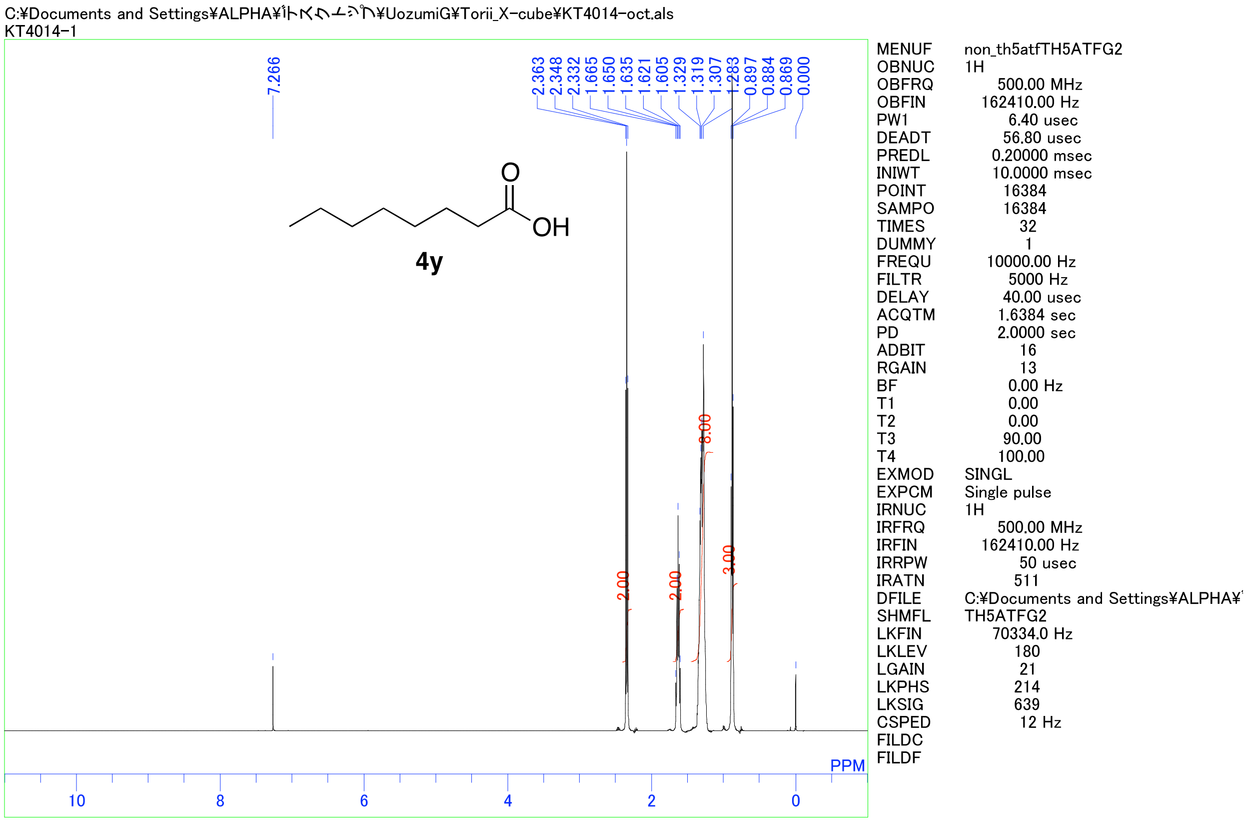


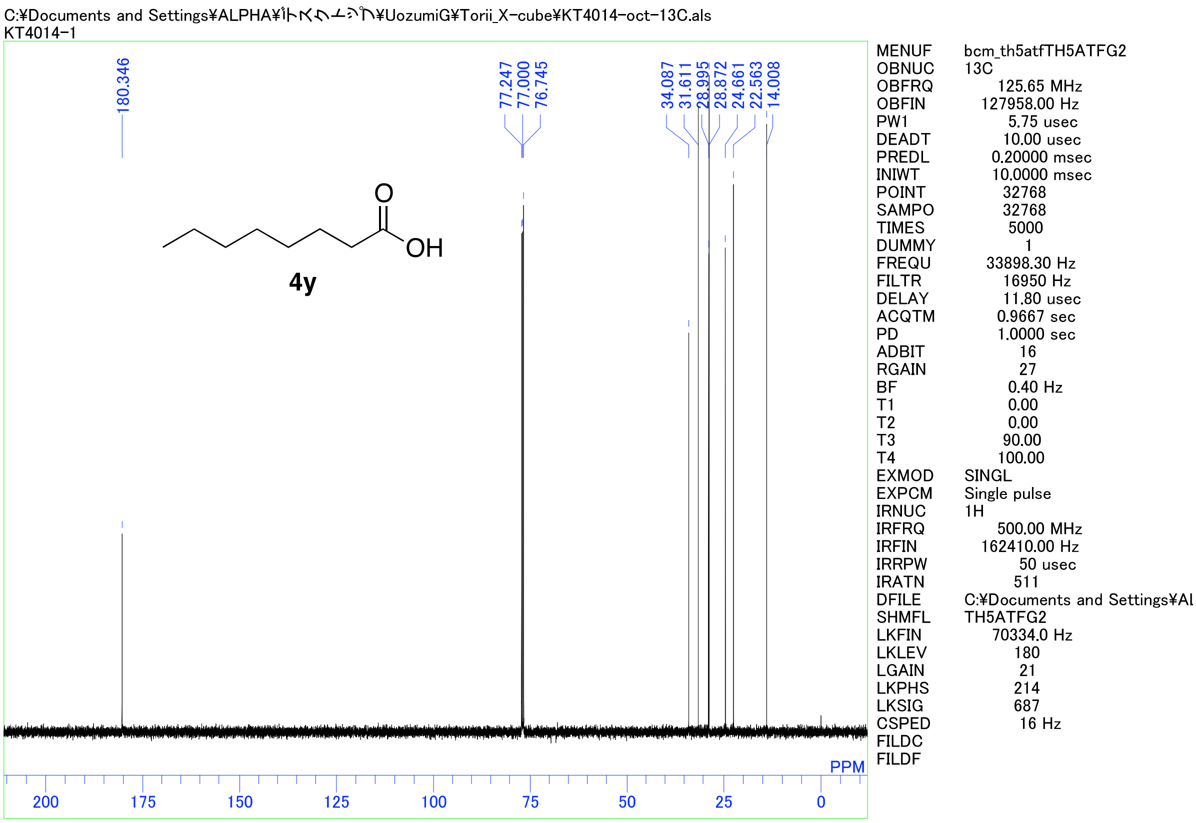
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of hexanoic acid (**4x**).



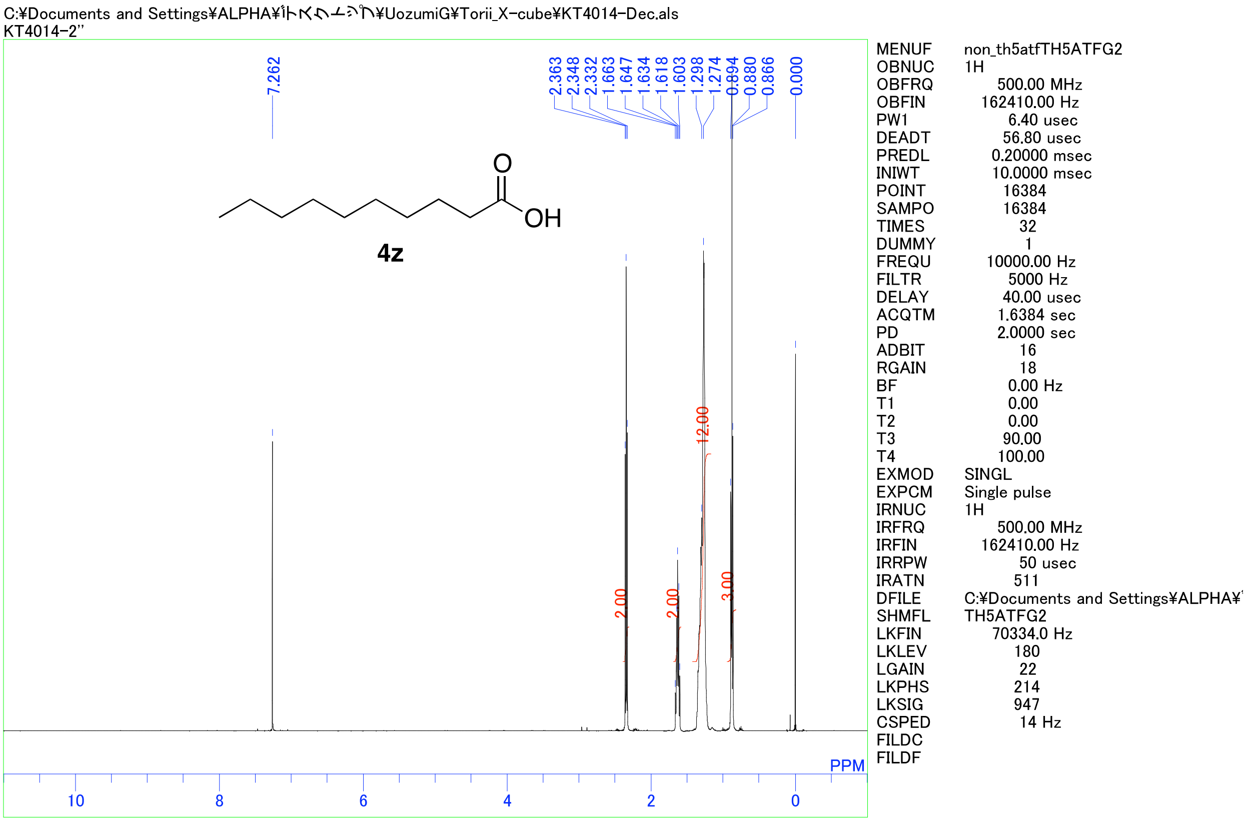


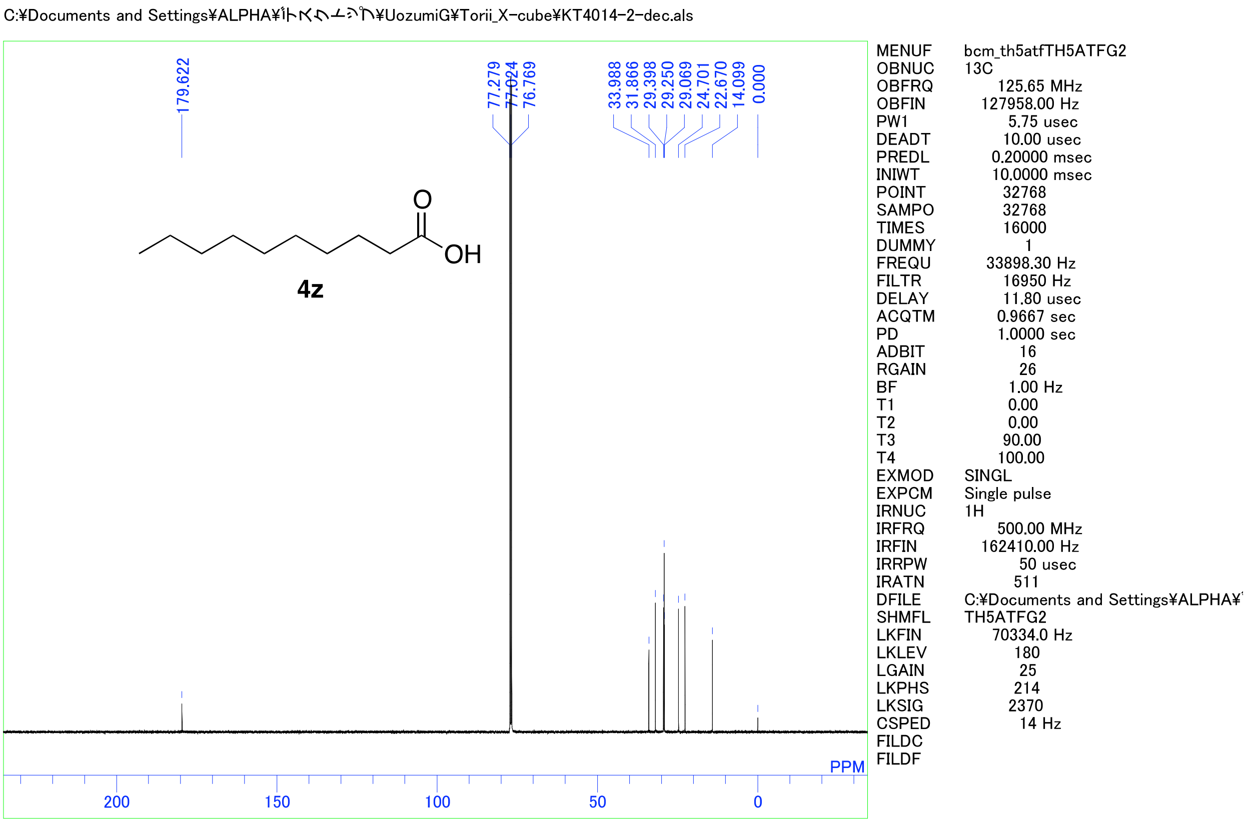
^{1}H and ^{13}C{^{1}H} NMR spectra of octanoic acid (**4y**).



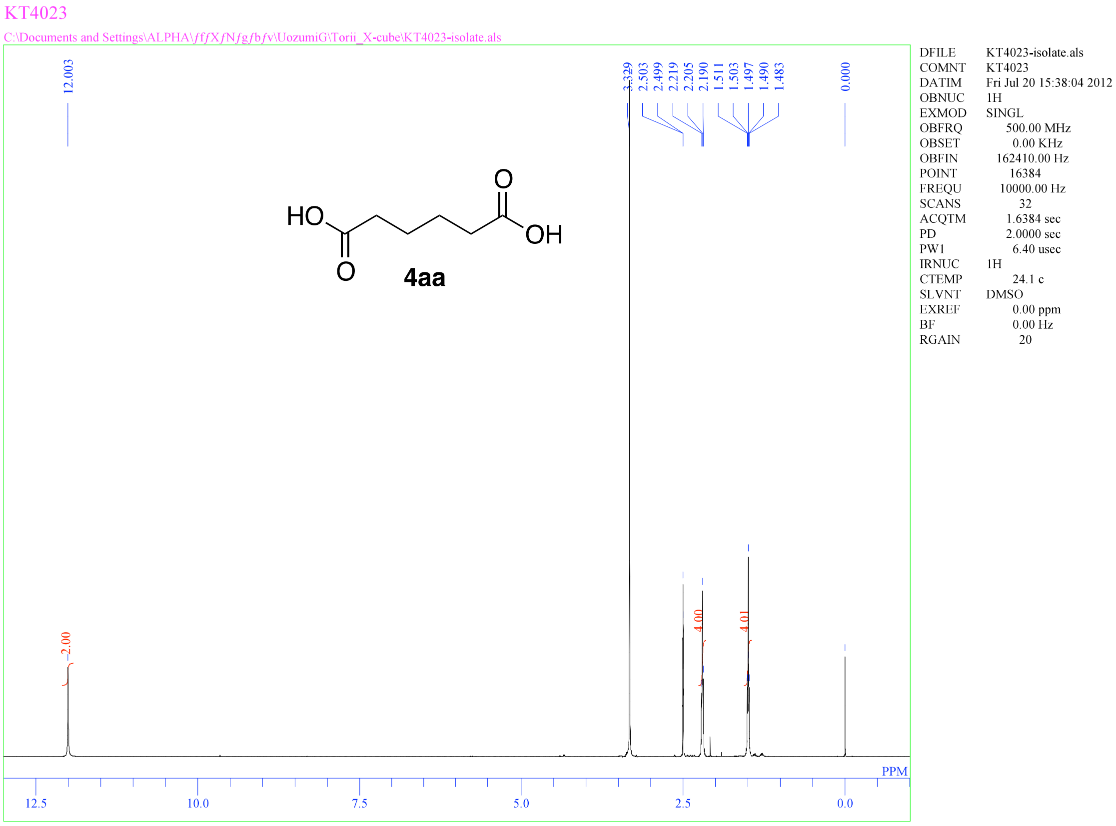


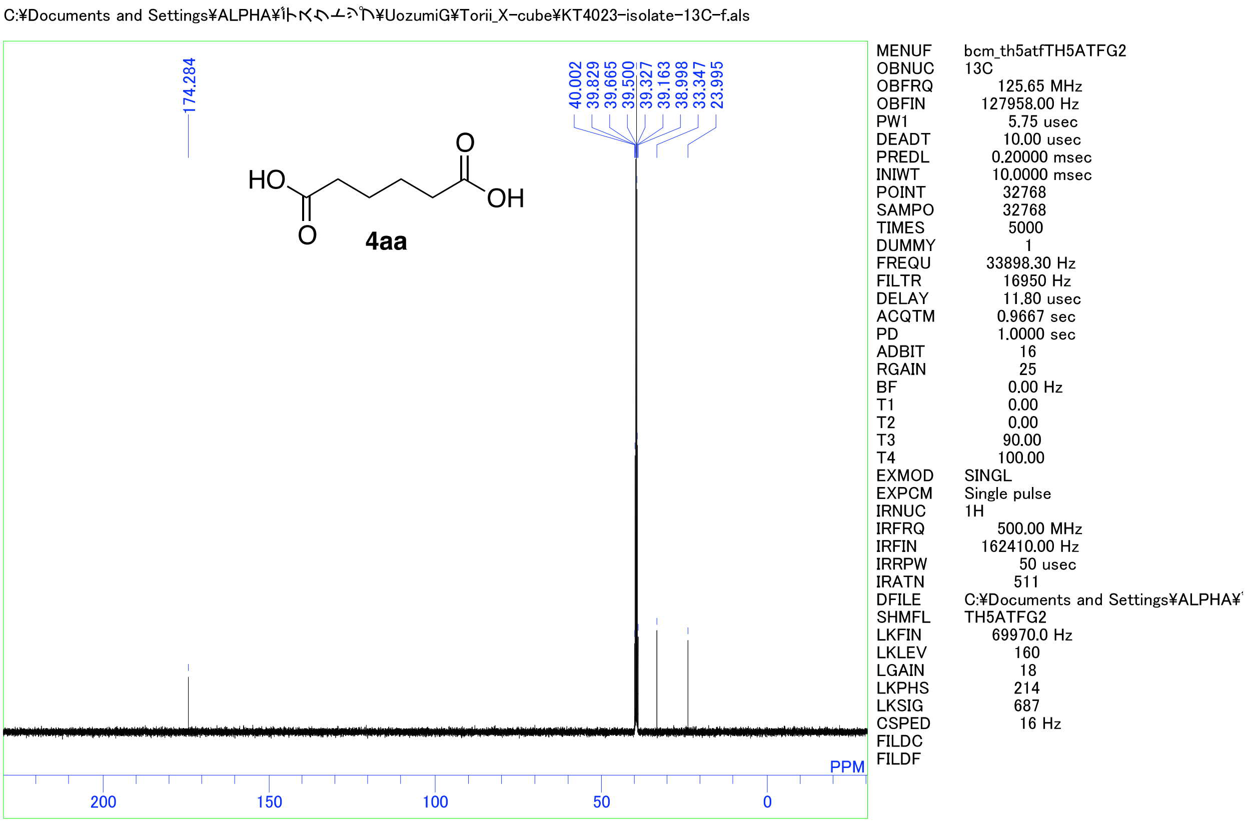
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of decanoic acid (**4z**).





^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of adipic acid (**4aa**).

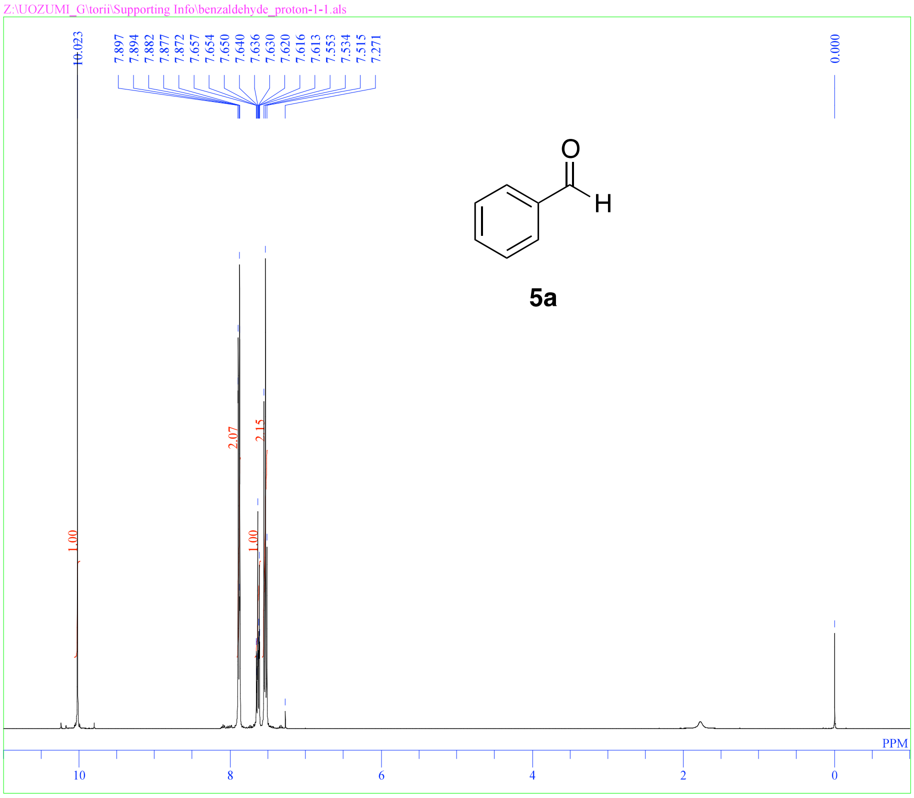




[1]H and [13]C{[1]H} NMR spectra of benzaldehyde (**5a**).

single_pulse

Z:\UOZUMI_G\torii\Supporting Info\benzaldehyde_proton-1-1.als



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COMNT	single_pulse
DATIM	2013-07-11 11:38:22
OBNUC	1H
EXMOD	proton.jxp
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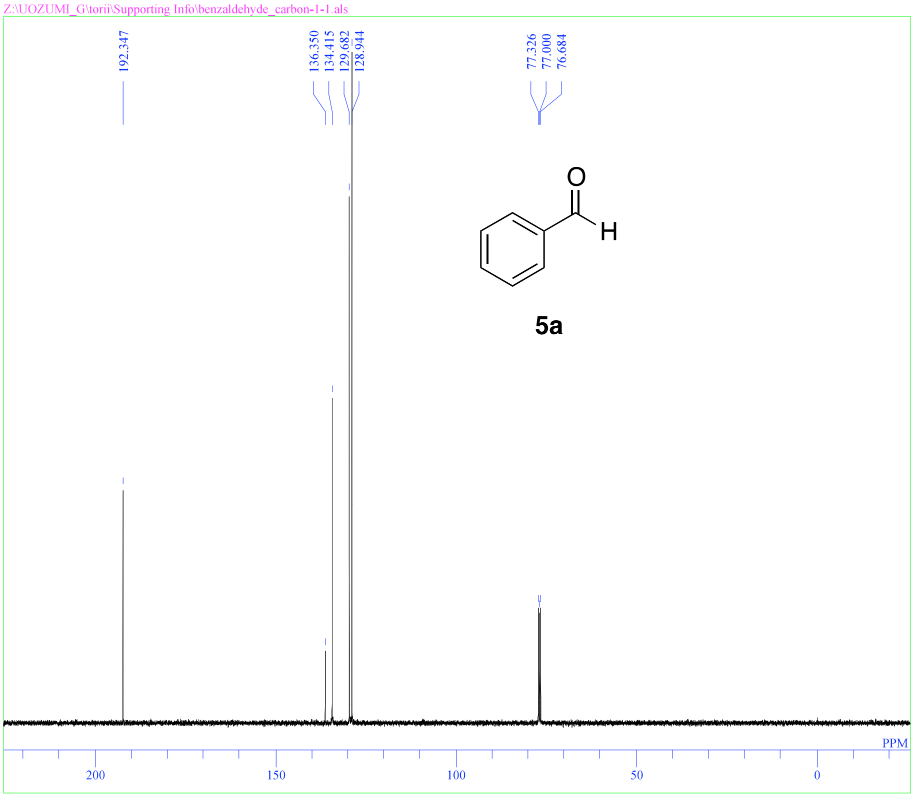
OBSET	6.28 KHz
OBFIN	0.87 Hz
POINT	13107
FREQU	5938.24 Hz
SCANS	8
ACQTM	2.2073 sec
PD	5.0000 sec
PW1	3.12 usec
IRNUC	1H
CTEMP	22.9 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.30 Hz
RGAIN	32

single pulse decoupled gated NOE

Z:\UOZUMI_G\torii\Supporting Info\benzaldehyde_carbon-1-1.als



DFILE	benzaldehyde_carbon-1-1.als
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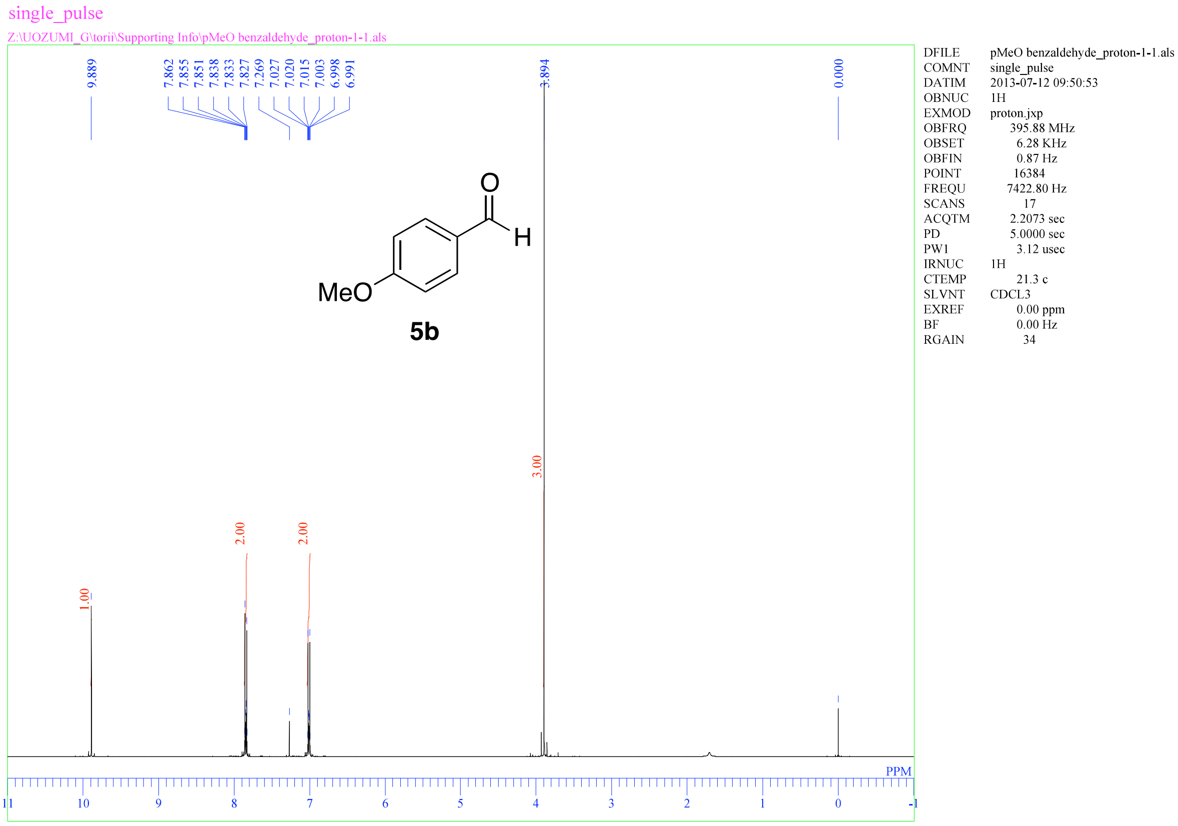
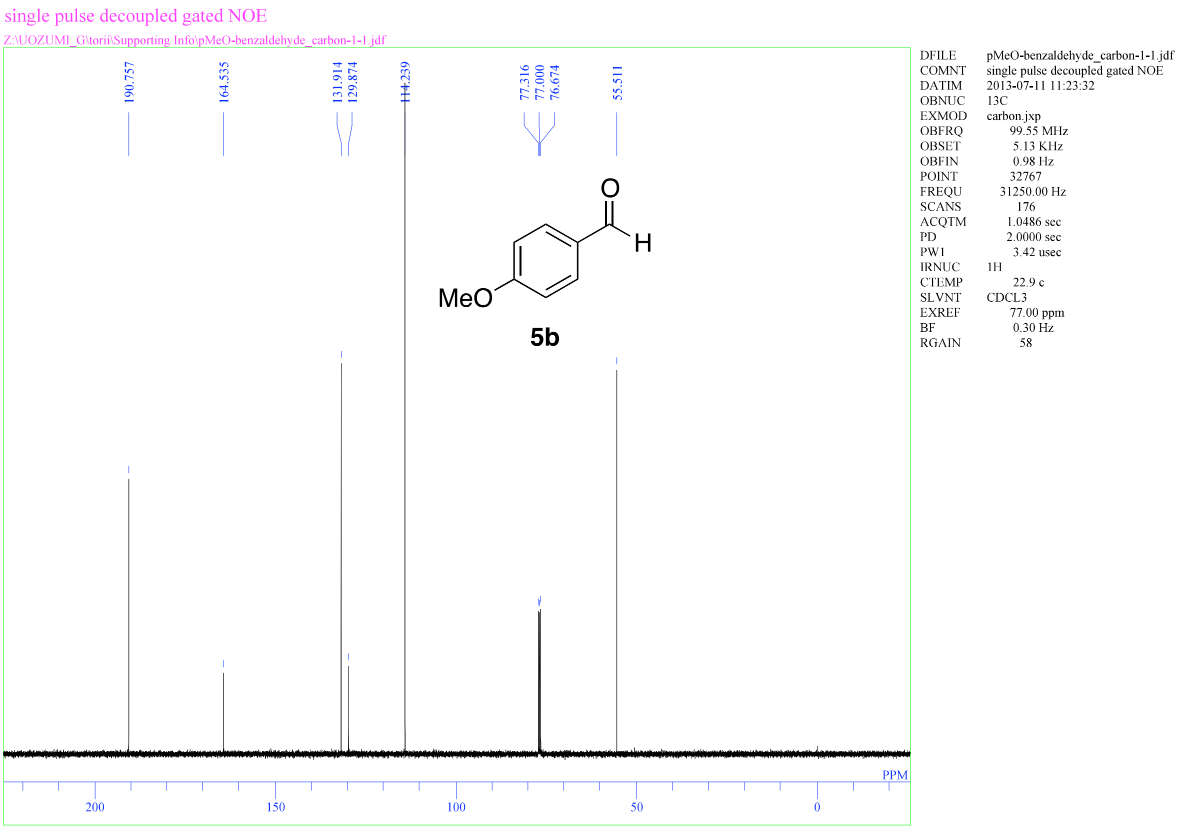
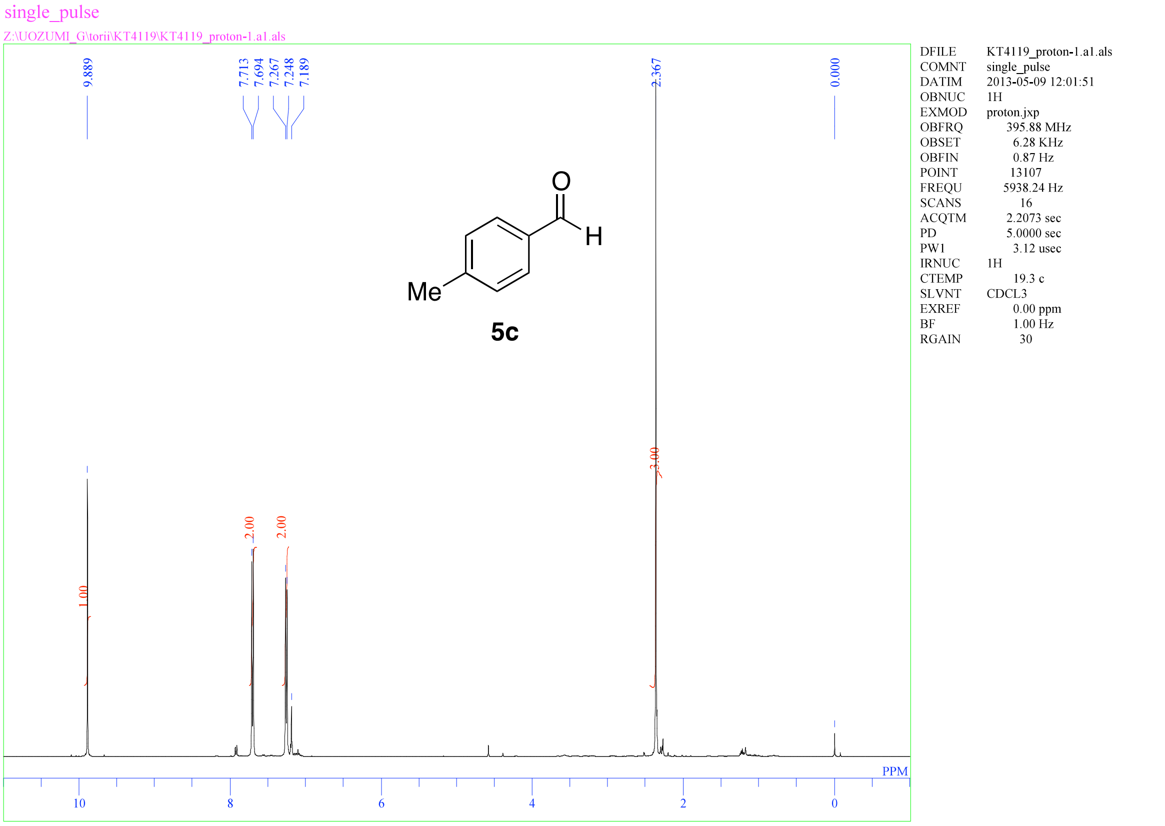
EXMOD	carbon.jxp
OBFRQ	99.55 MHz
OBSET	5.13 KHz
OBFIN	0.98 Hz
POINT	32767
FREQU	31250.00 Hz
SCANS	237
ACQTM	1.0486 sec
PD	2.0000 sec
PW1	3.42 usec
IRNUC	1H
CTEMP	22.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.30 Hz
RGAIN	60

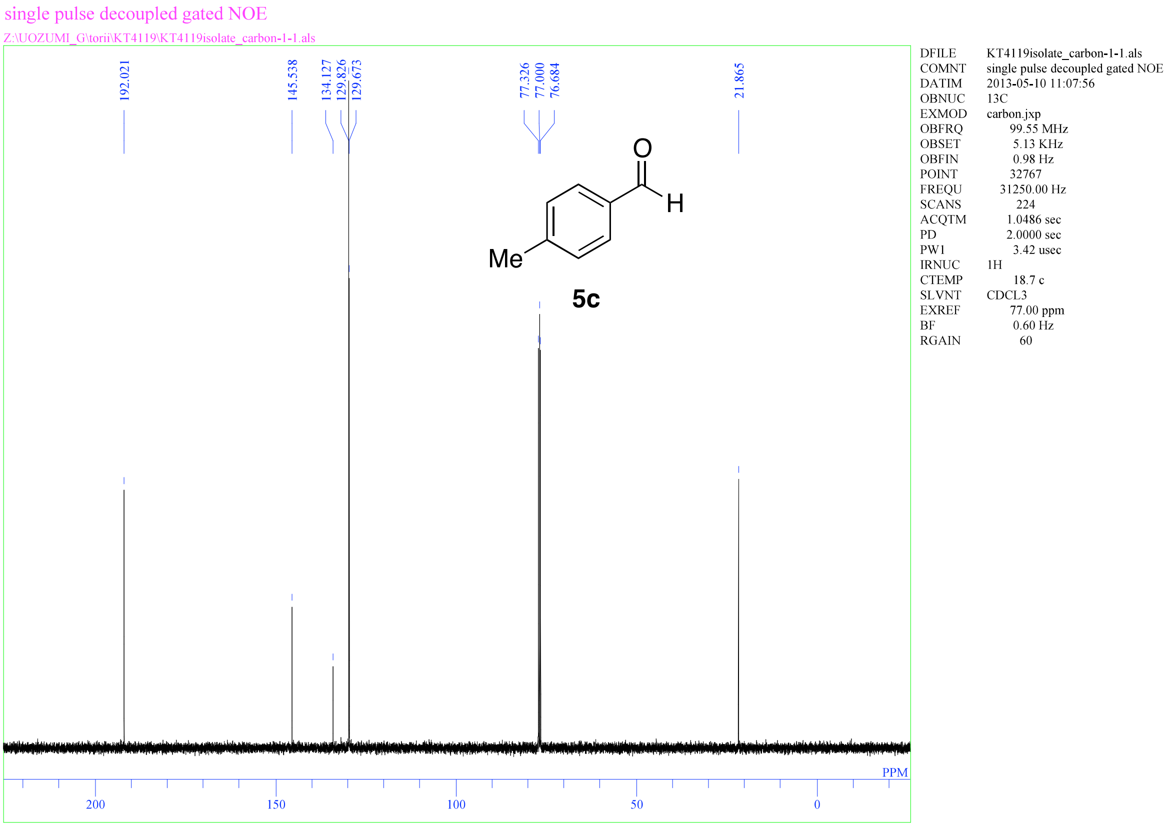
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of *p*-anisaldehyde (**5b**).



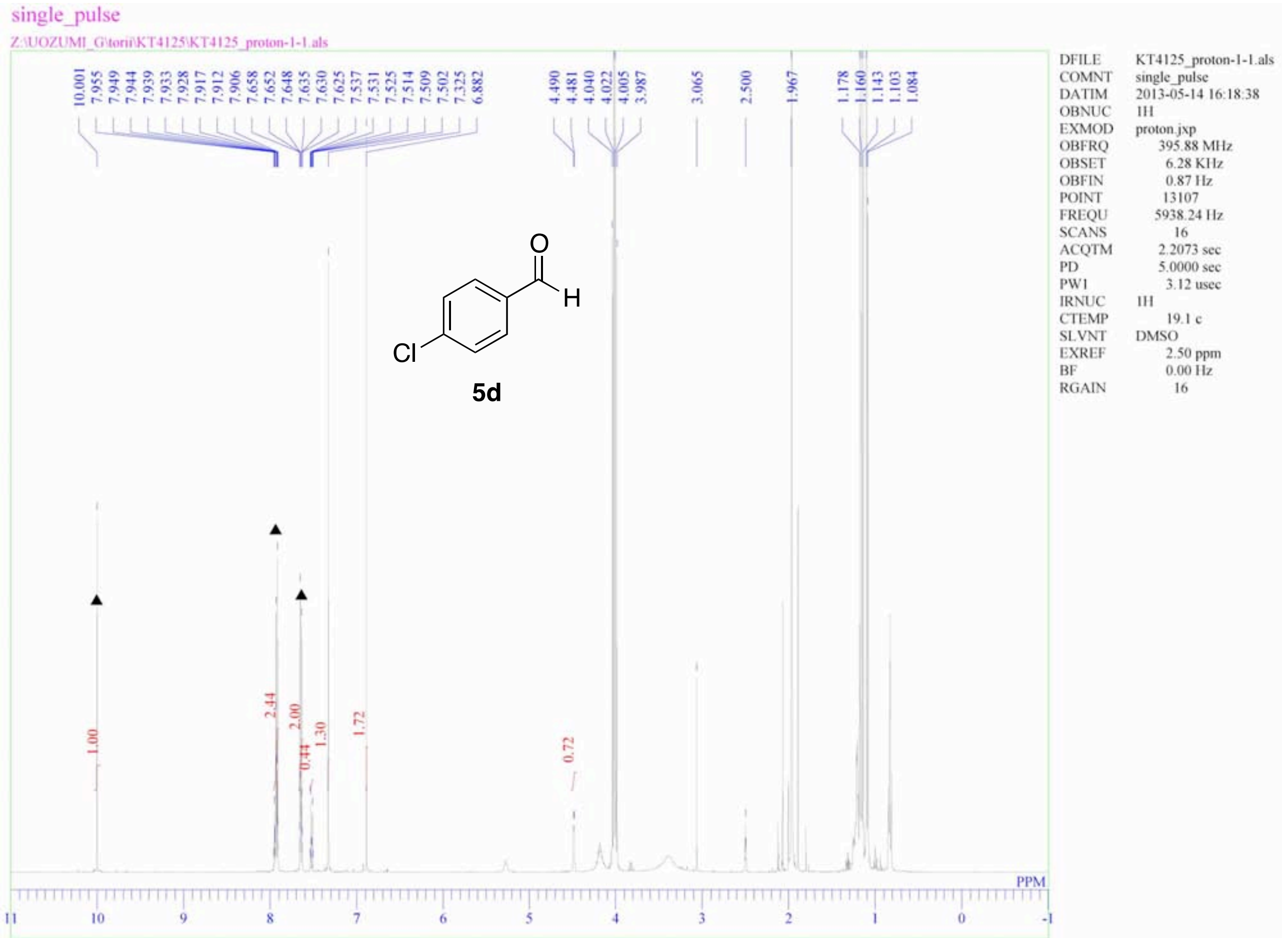


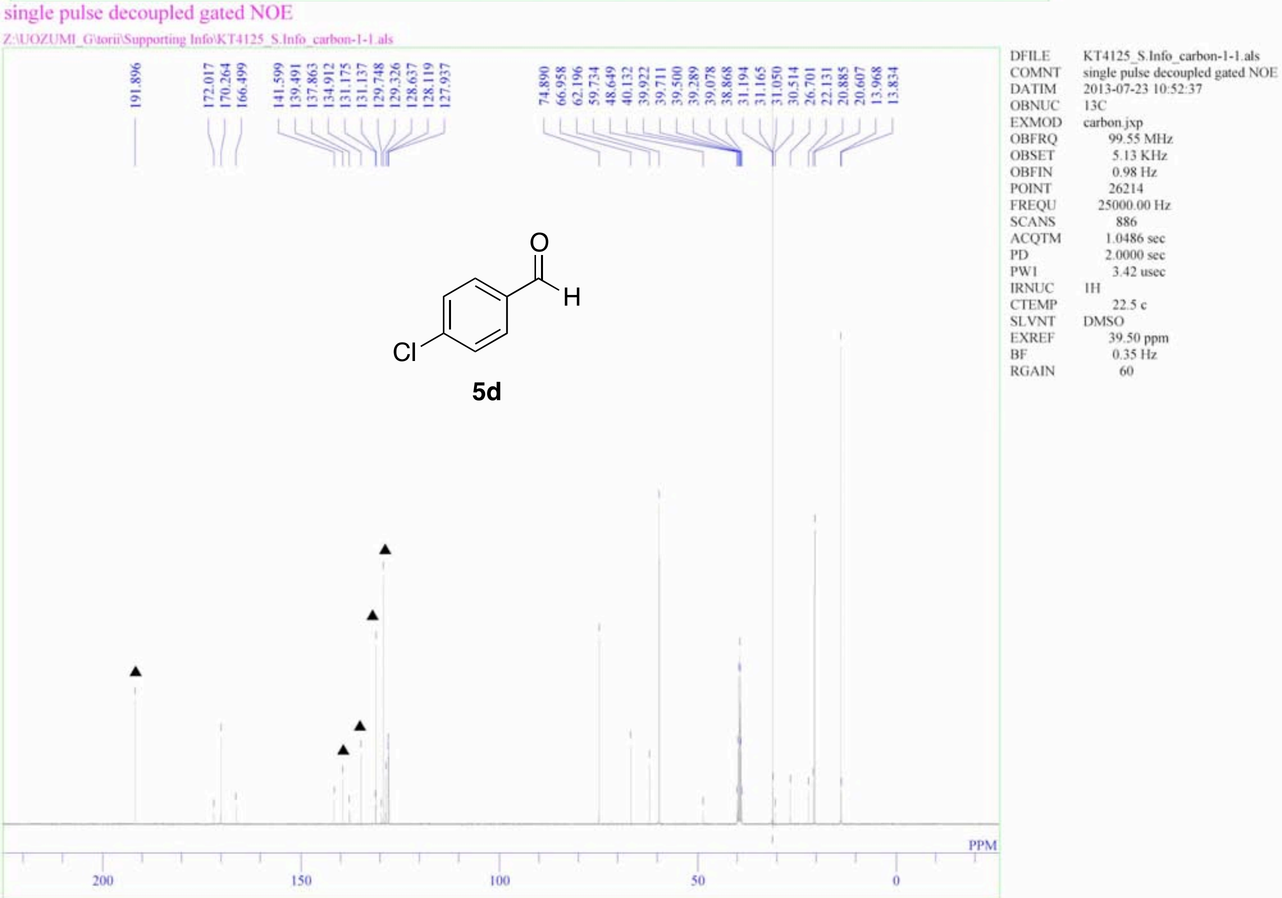
^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of *p*-tolualdehyde (**5c**).



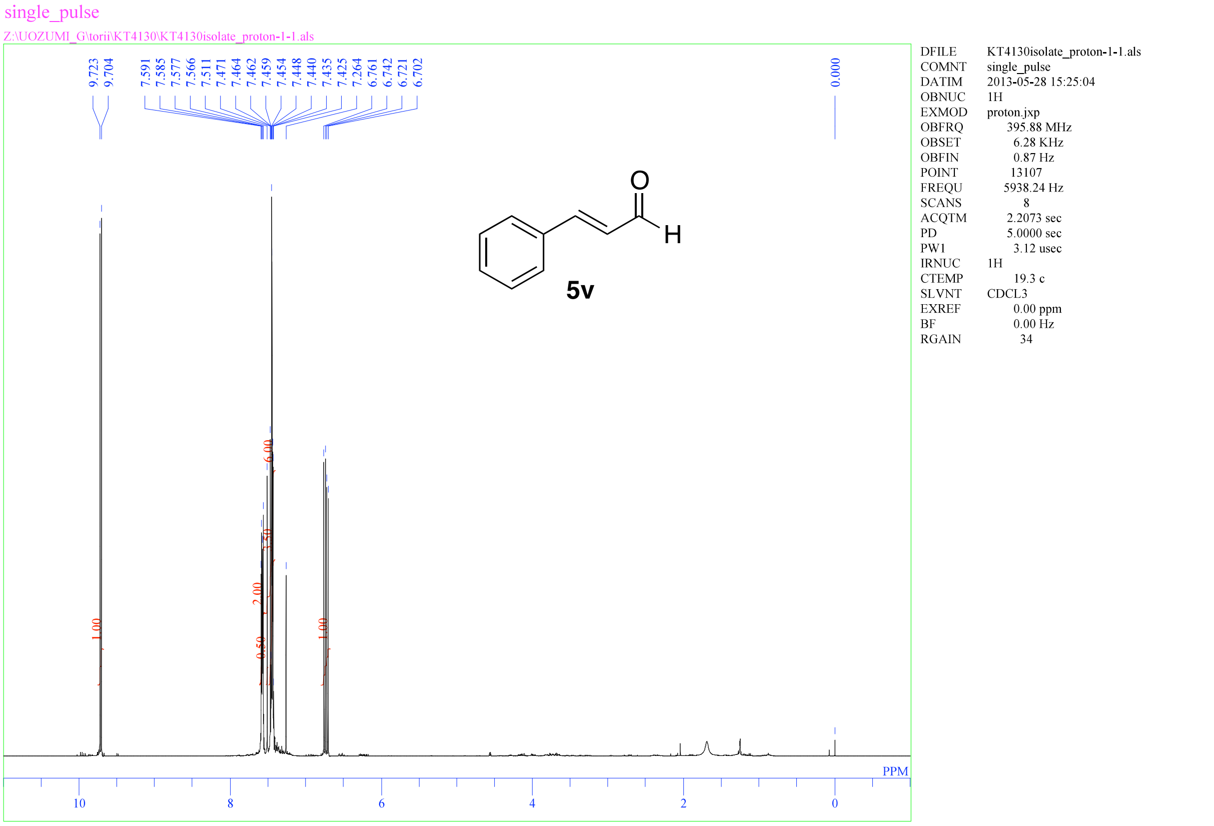


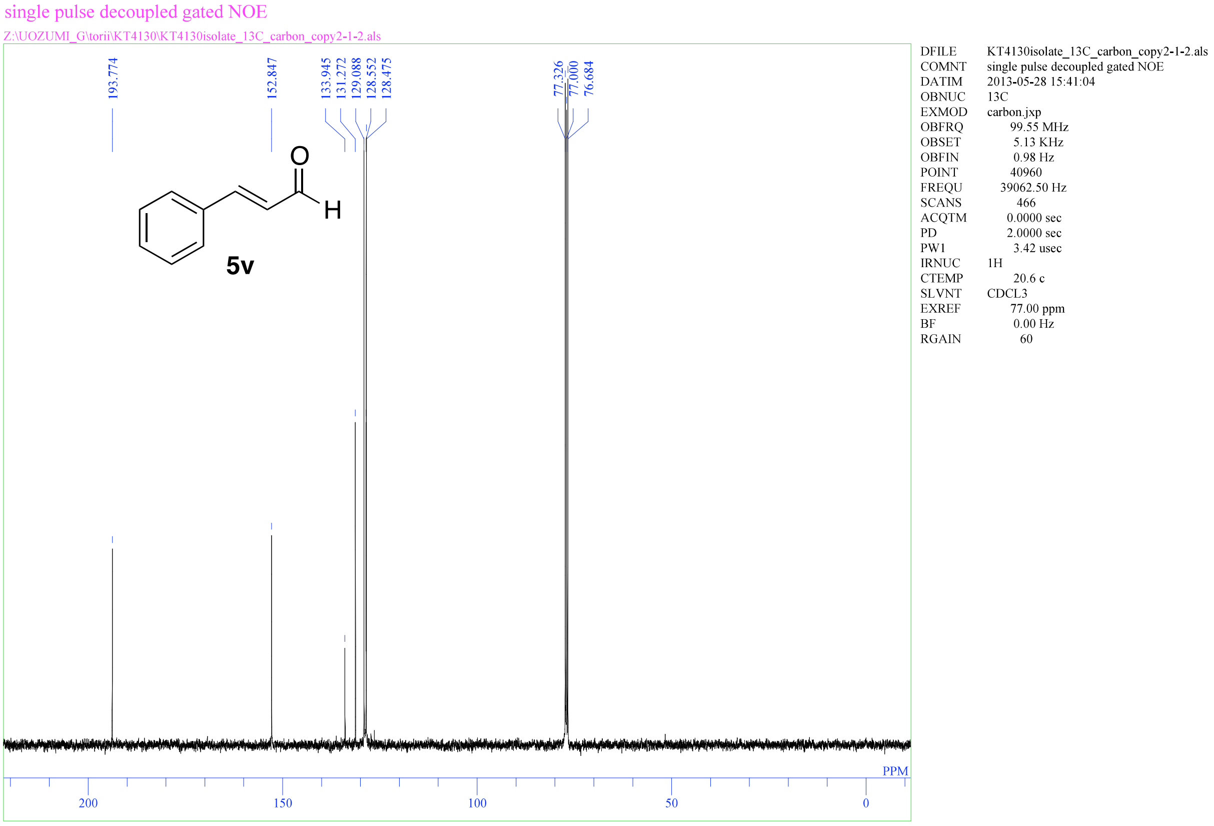
[1]H NMR spectra of *p*-chlorobenzaldehyde (**5d**).



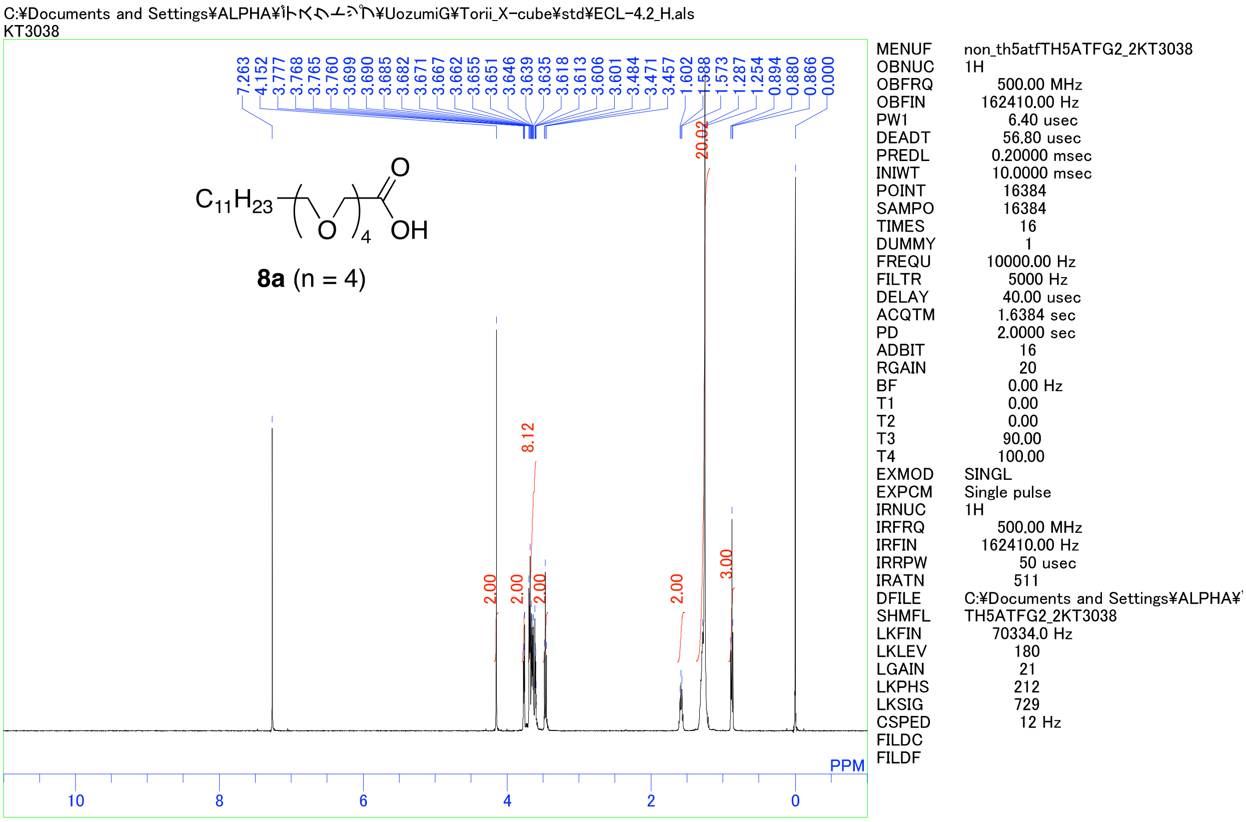


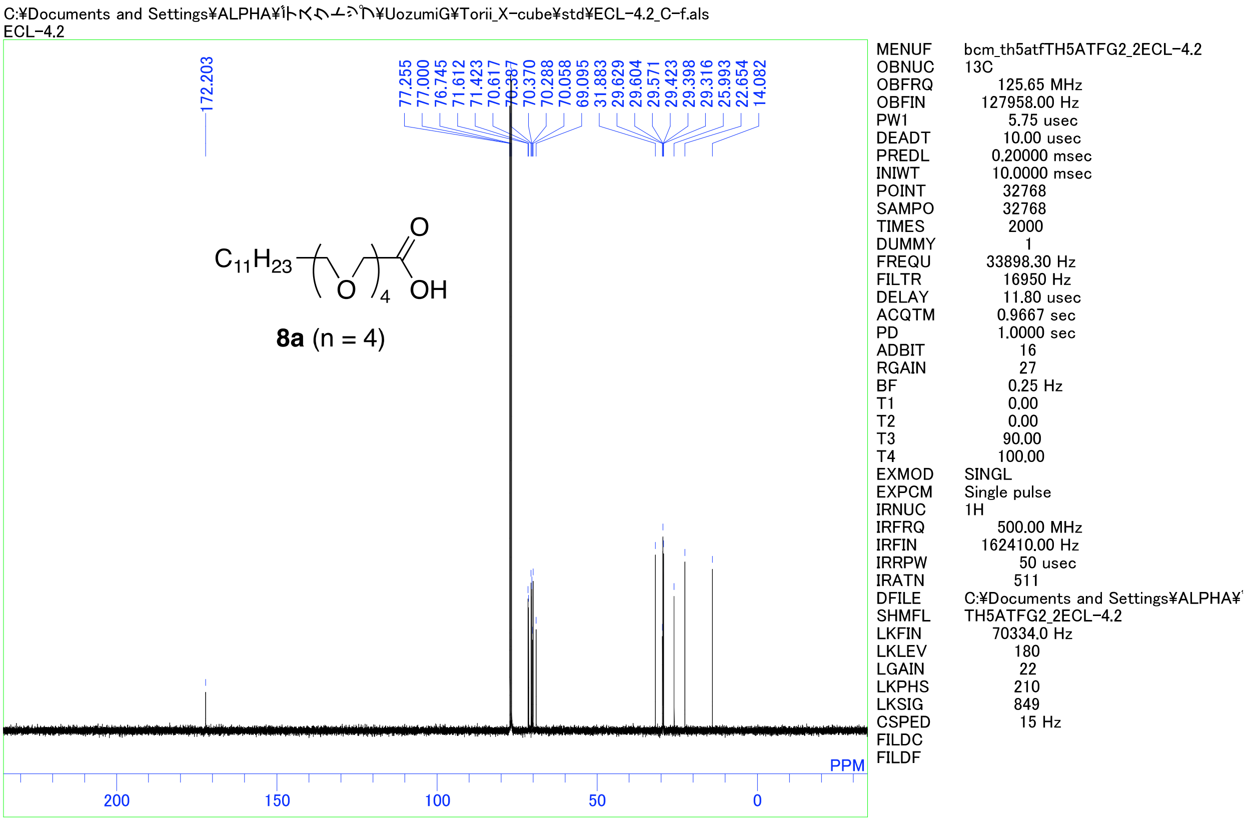
^{1}H and ^{13}C{^{1}H} NMR spectra of cinnamaldehyde (**5v**).





[1]H and [13]C{[1]H} NMR spectra of ECL-4.2(3,6,9,12-tetraoxatetracosanoic acid) (**8a**).





[1]H and [13]C{[1]H} NMR spectra of detergent **8b**.