

Supplementary Information

for

Continuous flow hydrogenation of olefins and nitrobenzenes catalysed by platinum nanoparticles dispersed in an amphiphilic polymer

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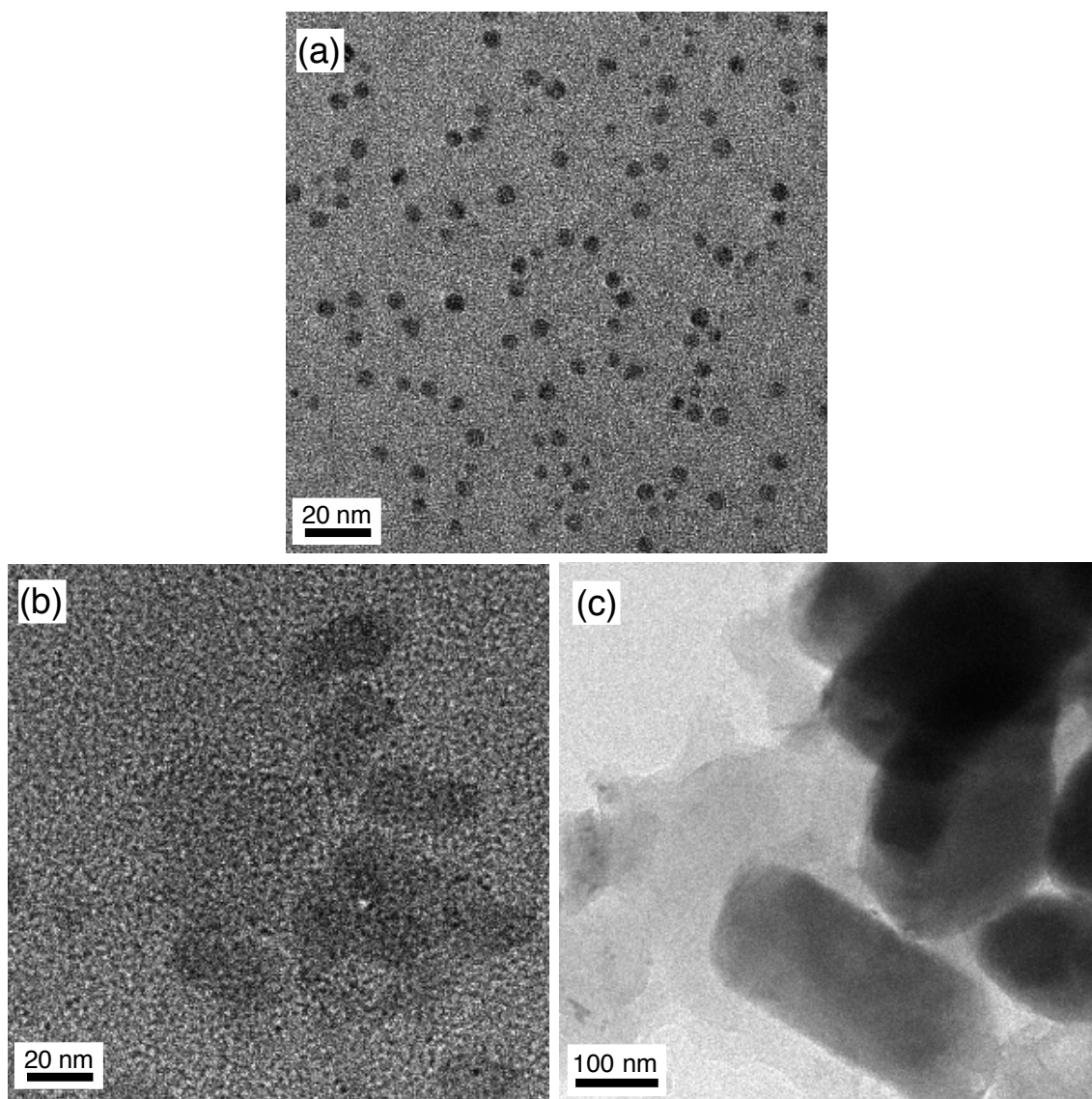


Fig. S1 TEM Images for the used catalysts. (a) Fresh ARP-Pt. (b) After the hydrogenation of styrene for 63 h. (c) After the hydrogenation of nitrobenzene for 70 h.

Characterization of products.

Ethylbenzene (**2a**) [CAS: 98-86-2]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.31\text{-}7.16$ (m, 5H, Ph), 2.65 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 1.24 (t, $J = 7.5$ Hz, 2H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 144.25$ (Ph), 128.28 (Ph), 127.84 (Ph), 125.57 (Ph), 28.87 ($-\text{CH}_2-$), 15.63 ($-\text{CH}_3$). MS (EI) $m/z = 106$ (M).

4-Ethylanisole (**2b**) [CAS: 1515-95-3]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.12$ (d, $J = 7.9$ Hz, 2H, $\text{Ar}_{\text{H}2}$ and $\text{Ar}_{\text{H}6}$), 6.83 (d, $J = 7.9$ Hz, 2H, $\text{Ar}_{\text{H}3}$ and $\text{Ar}_{\text{H}5}$), 2.59 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 1.21 (t, $J = 7.5$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (99.55 MHz, CDCl_3): $\delta = 157.56$ (Ar), 136.36 (Ar), 128.68 (Ar), 113.68 (Ar), 55.23 (OCH_3), 27.94 ($-\text{CH}_2-$), 15.90 ($-\text{CH}_3$). MS (EI) $m/z = 136$ (M).

4-Ethyltoluene (**2c**) [CAS: 622-96-8]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.10$ (s, 4H, Ar), 2.61 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 2.32 (s, 3H, $-\text{CH}_3$), 1.22 (t, 3H, $J = 7.5$ Hz, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 141.19$ (Ar), 134.97 (Ar), 128.97 (Ar), 127.71 (Ar), 28.41 ($-\text{CH}_2-$), 20.96 ($-\text{CH}_3$), 15.78 ($-\text{CH}_3$). MS (EI) $m/z = 120$ (M).

2-Ethyltoluene (**2d**) [CAS: 611-14-3]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.16\text{-}7.08$ (m, 4H, Ar), 2.63 (q, $J = 7.9$ Hz, 2H, $-\text{CH}_2-$), 2.31 (s, 3H, $-\text{CH}_3$), 1.21 (t, $J = 7.9$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (99.55 MHz, CDCl_3): $\delta = 142.28$ (Ar), 135.74 (Ar), 129.98 (Ar), 127.85 (Ar), 125.98 (Ar), 125.70 (Ar), 26.16 ($-\text{CH}_2-$), 19.15 (CH_3), 14.35 (CH_3). MS (EI) $m/z = 120$ (M).

3-Ethyltoluene (**2e**) [CAS: 620-14-4]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.18$ (t, $J = 7.9$ Hz, 1H, $\text{Ar}_{\text{H}5}$), 7.02-6.99 (m, 3H, Ar), 2.61 (q, $J = 7.9$ Hz, 2H, $-\text{CH}_2-$), 2.33 (s, 3H, $-\text{CH}_3$), 1.23 (t, $J = 7.9$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 144.20$ (Ar), 137.82 (Ar), 128.69 (Ar), 128.20 (Ar), 126.30 (Ar), 124.83 (Ar), 28.78 ($-\text{CH}_2-$), 21.40 ($-\text{CH}_3$), 15.65 ($-\text{CH}_3$). MS (EI) $m/z = 120$ (M).

1-Chloro-4-ethylbenzene (**2f**) [CAS: 622-98-0]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.24$ (d, $J = 8.7$ Hz, 2H, $\text{Ar}_{\text{H}2}$ and $\text{Ar}_{\text{H}6}$), 7.12 (d, $J = 8.3$ Hz, 2H, $\text{Ar}_{\text{H}3}$ and $\text{Ar}_{\text{H}5}$), 2.61 (q, $J = 7.9$ Hz, 2H, $-\text{CH}_2-$), 1.22 (t, $J = 7.9$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 142.61$ (Ar), 131.22 (Ar), 129.18 (Ar), 128.34 (Ar), 28.24 ($-\text{CH}_2-$), 15.53 ($-\text{CH}_3$). MS (EI) $m/z = 140$ (M).

4-Ethylbenzenetrifluoride (**2g**) [CAS: 27190-69-8]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.53$ (d, $J = 7.9$ Hz, 2H, $\text{Ar}_{\text{H}2}$ and $\text{Ar}_{\text{H}6}$), 7.30 (d, $J = 7.9$ Hz, 2H, $\text{Ar}_{\text{H}3}$ and $\text{Ar}_{\text{H}5}$), 2.71 (q, $J = 7.9$ Hz, 2H, $-\text{CH}_2-$), 1.26 (t, $J = 7.9$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 148.28$ (Ar), 128.51 (Ar), 125.24 (q, $J = 3.8$ Hz, Ar), 124.42 (q, $J = 271$ Hz, $-\text{CF}_3$), 28.77 ($-\text{CH}_2-$), 15.33 ($-\text{CH}_3$). MS (EI) $m/z = 174$ (M).

4-Ethylbenzonitrile (**2h**) [CAS: 25309-65-3]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.57$ (d, $J = 7.5$ Hz, 2H, $\text{Ar}_{\text{H}2}$ and $\text{Ar}_{\text{H}6}$), 7.30 (d, $J = 7.1$ Hz, 2H, $\text{Ar}_{\text{H}3}$ and $\text{Ar}_{\text{H}5}$), 2.71 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 1.26 (t, $J = 7.5$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 149.81$ (Ar), 132.19 (Ar), 128.68 (Ar), 119.22 (CN), 109.47 (Ar), 29.08 ($-\text{CH}_2-$), 15.05 ($-\text{CH}_3$). MS (EI) $m/z = 131$ (M).

4-Ethylacetophenone (**2i**) [CAS: 937-30-4]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.89$ (dt, $J = 8.7$ and 2.0 Hz, 2H, $\text{Ar}_{\text{H}2}$ and $\text{Ar}_{\text{H}6}$), 7.29 (d, $J = 8.3$ Hz, 2H, $\text{Ar}_{\text{H}3}$ and $\text{Ar}_{\text{H}5}$), 2.71 (q, $J = 7.9$ Hz, 2H, $-\text{CH}_2-$), 2.59 (s, 3H, $-\text{CH}_3$), 1.26 (t, $J = 7.9$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 197.93$ (CO), 150.05 (Ar), 134.86 (Ar), 128.52 (Ar), 128.04 (Ar), 28.91 ($-\text{CH}_2-$), 26.55 ($-\text{CH}_3$), 15.21 ($-\text{CH}_3$). MS (EI) $m/z = 148$ (M).

Methyl 4-ethylbenzoate (**2j**) [CAS: 6908-41-4]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.96$ (d, $J = 7.5$ Hz, 2H, $\text{Ar}_{\text{H}2}$ and $\text{Ar}_{\text{H}6}$), 7.26 (d, $J = 7.9$ Hz, 2H, $\text{Ar}_{\text{H}3}$ and $\text{Ar}_{\text{H}5}$), 3.90 (s, 3H, OCH_3), 2.70 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 1.26 (t, $J = 7.9$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 167.17$ (CO), 149.71 (Ar), 129.65 (Ar), 127.84 (Ar), 127.57 (Ar), 51.92 (OCH_3), 28.91 ($-\text{CH}_2-$), 15.20 ($-\text{CH}_3$). MS (EI) $m/z = 164$ (M).

Benzyl (4-ethylphenyl)carbamate (**2k**) [CAS: 957783-10-7]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.42$ -7.28 (m, 7H, Ar), 7.13 (d, $J = 8.7$ Hz, 2H, Ar), 6.61 (brs, 1H, NH), 5.19 (s, 2H, $-\text{CH}_2\text{Ph}$), 2.60 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 1.21 (t, 3H, $J = 7.5$ Hz, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 153.48$ (CO), 139.57 (Ar), 136.12 (Ar), 135.32 (Ar), 128.59 (Ar), 128.37 (Ar), 128.29 (Ar), 118.87 (Ar), 66.92 (CH_2Ph), 28.19 ($-\text{CH}_2-$), 15.69 ($-\text{CH}_3$). MS (EI) $m/z = 255$ (M).

2-Ethyl-naphthalene (**2l**) [CAS: 939-27-5]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.81\text{-}7.76$ (m, 3H, Ar), 7.62 (s, 1H, $\text{Ar}_{\text{H}1}$), 7.46-7.38 (m, 2H, Ar), 7.35 (d, $J = 8.3$ Hz, 1H, Ar), 2.81 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 1.33 (t, $J = 7.5$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 141.73$ (Ar), 133.65 (Ar), 131.88 (Ar), 127.76 (Ar), 127.57 (Ar), 127.37 (Ar), 127.06 (Ar), 125.79 (Ar), 125.50 (Ar), 124.97 (Ar), 29.01 ($-\text{CH}_2-$), 15.52 ($-\text{CH}_3$). MS (EI) $m/z = 156$ (M).

2-Ethylpyridine (**2m**) [CAS: 100-71-0]: ^1H NMR (396 MHz, CDCl_3): $\delta = 8.53$ (d, $J = 4.5$ Hz, 1H, $\text{Py}_{\text{H}6}$), 7.59 (td, $J = 7.5$ Hz, 1H, $\text{Py}_{\text{H}4}$), 7.16 (d, $J = 7.5$ Hz, 1H, $\text{Py}_{\text{H}3}$), 7.10 (t, $J = 7.5$ Hz, 1H, $\text{Py}_{\text{H}5}$), 2.83 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), 1.31 (t, $J = 7.5$ Hz, 3H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 163.43$ (Py), 149.08 (Py), 136.33 (Py), 121.99 (Py), 120.83 (Py), 31.32 ($-\text{CH}_2-$), 13.87 ($-\text{CH}_3$). MS (EI) $m/z = 107$ (M).

2-Ethylthiophene (**2n**) [CAS: 872-55-9]: The flow hydrogenation of 2-vinylthiophene gave a mixture of 2-ethylthiophene and unreacted 2-vinylthiophene. Therefore the yield of **2n** was determined with ^1H NMR using an internal standard (1,1,2,2-tetrachloroethane: $\delta = 5.79$). ^1H NMR (396 MHz, CDCl_3): $\delta = 6.96$ (dd, $J = 5.1$ and 1.2 Hz, 1H, Ar), 6.79-6.77 (m, 1H, Ar), 6.67-6.66 (m, 1H, Ar), 2.76 (q, $J = 7.5$ Hz, 2H, $-\text{CH}_2-$), The peak (near 1.3 ppm) derived from protons of the methyl group was overlapped with the solvent peak. MS (EI) $m/z = 112$ (M).

Cumene (**2o**) [CAS: 98-82-8]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.31\text{-}7.16$ (m, 5H, Ar), 2.91 (sep, $J = 7.5$ Hz, 1H, $-\text{CH}-$), 1.25 (d, $J = 7.5$ Hz, 6H, $-\text{CH}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 148.99$ (Ar), 128.43 (Ar), 126.55 (Ar), 34.25 ($-\text{CH}-$), 24.15 ($-\text{CH}_3$). MS (EI) $m/z = 120$ (M).

1,2-Diphenylethane (**2p**) [CAS: 103-29-7]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.31\text{-}7.26$ (m, 5H, Ar), 7.21-7.15 (m, 5H, Ar), 2.92 (s, 4H, $-\text{CH}_2-$). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 141.75$ (Ar), 128.42 (Ar), 128.30 (Ar), 125.89 (Ar), 37.93 ($-\text{CH}_2-$). MS (EI) $m/z = 182$ (M).

3-Phenylpropan-1-ol (**2q**) [CAS: 122-97-4]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.30\text{-}7.27$ (m, 2H, Ph), 7.21-7.16 (m, 3H, Ph), 3.66 (t, $J = 6.7$ Hz, 2H, $-\text{CH}_2\text{OH}$), 2.70 (t, $J = 7.5$ Hz, 2H, PhCH_2-),

1.93-1.85 (m, 2H, -CH₂-). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 141.77 (Ar), 128.38 (Ar), 128.35 (Ar), 125.81 (Ar), 62.19 (-CH₂-), 34.16 (-CH₂-), 32.01 (-CH₂-). MS (EI) *m/z* = 136 (M).

N-Benzylaniline (**2r**) [CAS: 103-32-2]: ¹H NMR (396 MHz, CDCl₃): δ = 7.39-7.25 (m, 5H, Ph), 7.18 (t, *J* = 7.5 Hz, 2H, Ph), 6.72 (t, *J* = 7.5 Hz, 1H, Ph), 6.64 (t, *J* = 7.5 Hz, 2H, Ph), 4.33 (s, 2H, -CH₂-), 4.03 (brs, 1H, NH). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 148.12 (Ar), 139.39 (Ar), 129.25 (Ar), 128.62 (Ar), 127.49 (Ar), 127.21 (Ar), 117.53 (Ar), 112.79 (Ar), 48.29 (-CH₂-). MS (EI) *m/z* = 183 (M).

Octane (**2s**) [CAS: 111-65-9]: ¹H NMR (396 MHz, CDCl₃): δ = 1.35-1.26 (m, 12H, CH₂), 0.88 (t, *J* = 6.3 Hz, 6H, -CH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 31.91 (-CH₂-), 29.32 (-CH₂-), 22.69 (-CH₂-), 14.12 (-CH₃). MS (EI) *m/z* = 114 (M).

Decane (**2t**) [CAS: 124-18-5]: ¹H NMR (396 MHz, CDCl₃): δ = 1.34-1.26 (m, 16H, CH₂), 0.88 (t, *J* = 6.7 Hz, 6H, -CH₃). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 31.93 (-CH₂-), 29.67 (-CH₂-), 29.38 (-CH₂-), 22.70 (-CH₂-), 14.12 (-CH₃). MS (EI) *m/z* = 142 (M).

Cyclooctane (**2v**) [CAS: 292-64-8]: ¹H NMR (396 MHz, CDCl₃): δ = 1.53 (s, 16H, -CH₂-). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 26.67 (-CH₂-). MS (EI) *m/z* = 112 (M).

4-Isopropyl-1-methylcyclohex-1-ene (**2w**) [CAS: 1195-31-9]: ¹H NMR (396 MHz, CDCl₃): δ = 5.39-5.35 (m, 1H), 2.02-1.93 (m, 3H), 1.77-1.64 (m, 5H), 1.50-1.42 (m, 1H), 1.25-1.18 (m, 2H), 0.88 (dd, *J* = 6.7 and 5.9 Hz, 6H). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 133.95 (C=C), 121.00 (C=C), 39.99, 32.28, 30.80, 28.94, 26.47, 23.47, 20.00, 19.68. MS (EI) *m/z* = 138 (M).

[(3,7-Dimethyloctyl)oxy]methyl]benzene (**2x**) [CAS: 215942-19-1]: ¹H NMR (396 MHz, CDCl₃): δ = 7.35-7.26 (m, 5H, Ar), 4.50 (s, 2H, CH₂Ph), 3.55-3.45 (m, 2H, -CH₂O-), 1.70-1.37 (m, 4H, -CH₂-), 1.36-1.20 (m, 3H), 1.16-1.06 (m, 3H), 0.88-0.85 (m, 9H). ¹³C{¹H} NMR (100 MHz, CDCl₃): δ = 138.68 (Ar), 128.32 (Ar), 127.60 (Ar), 127.44 (Ar), 72.87 (CH₂), 68.76 (CH₂), 39.25 (CH₂), 37.32 (CH₂), 36.77 (CH₂), 29.86 (CH₂), 27.94 (CH₂), 24.65 (CH₂), 22.70 (CH₃), 22.59 (CH₃), 19.66 (CH₃). MS (EI) *m/z* = 248 (M), 157 (M-Bn).

Aniline hydrochloride (**4a**) [CAS: 142-04-1]: ^1H NMR (396 MHz, CD_3OD): $\delta = 7.57\text{-}7.46$ (m, 3H, Ar), 7.42 (dd, $J = 7.2$ and 1.4 Hz, 2H, Ar). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CD_3OD): $\delta = 131.97$ (Ar), 131.28 (Ar), 130.22 (Ar), 124.29 (Ar). After neutralization, Mass analysis was performed. MS (EI) $m/z = 93$ (M) for aniline.

p-Anisidine (**4b**) [CAS: 104-94-9]: ^1H NMR (396 MHz, CDCl_3): $\delta = 6.75$ (ddd, $J = 9.1, 3.2,$ and 2.3 Hz, 2H, Ar), 6.65 (ddd, $J = 9.1, 3.2$ and 2.3 Hz, 2H, Ar), 3.75 (s, 3H, OCH_3), 3.41 (brs, 2H, NH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 152.78$ (Ar), 139.84 (Ar), 116.41 (Ar), 114.77 (Ar), 55.71 (OCH_3). MS (EI) $m/z = 123$ (M).

p-Toluidine (**4c**) [CAS: 106-49-0]: ^1H NMR (396 MHz, CDCl_3): $\delta = 6.96$ (d, $J = 7.7$ Hz, 2H, Ar), 6.61 (dt, $J = 8.2$ and 2.3 Hz, 2H, Ar), 3.52 (brs, 2H, NH_2), 2.24 (s, 3H, CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 134.75$ (Ar), 129.71 (Ar), 127.76 (Ar), 115.22 (Ar), 20.42 (CH_3). MS (EI) $m/z = 107$ (M).

o-Toluidine hydrochloride (**4d**) [CAS: 636-21-5]: ^1H NMR (396 MHz, CD_3OD): $\delta = 7.39\text{-}7.33$ (m, 4H, Ar), 2.41 (t, $J = 2.4$ Hz, 3H, CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CD_3OD): $\delta = 132.95$ (Ar), 130.65 (Ar), 130.46 (Ar), 128.68 (Ar), 124.26 (Ar), 124.21 (Ar), 17.02 (CH_3). After neutralization, Mass analysis was performed. MS (EI) $m/z = 107$ (M) for *o*-toluidine.

m-Toluidine hydrochloride (**4e**) [CAS: 638-03-9]: ^1H NMR (396 MHz, CD_3OD): $\delta = 7.32$ (t, $J = 7.9$ Hz, 1H, Ar), 7.22 (d, $J = 7.9$ Hz, 1H, Ar), 7.13-7.07 (m, 2H, Ar), 2.31 (s, 3H, CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CD_3OD): $\delta = 141.97$ (Ar), 131.81 (Ar), 131.11 (Ar), 130.90 (Ar), 142.47 (Ar), 121.03 (Ar), 21.25 (CH_3). After neutralization, Mass analysis was performed. MS (EI) $m/z = 107$ (M).

4-Chloroaniline hydrochloride (**4f**) [CAS: 20265-96-7]: The resulting product was obtained as mixture of 4-chloroaniline and aniline hydrochlorides (3:1). ^1H NMR (396 MHz, CD_3OD): $\delta = 7.54$ (d, $J = 7.7$ Hz, 2H, Ar), 7.41-7.37 (m, 2H, Ar). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CD_3OD): $\delta = 135.88$ (Ar), 131.35 (Ar), 130.28 (Ar), 125.77 (Ar). MS (EI) $m/z = 127$ (M).

4-Trifluoromethylaniline (**4g**) [CAS: 455-14-1]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.39$ (d, $J = 8.2$ Hz, 2H, Ar), 6.68 (d, $J = 8.2$ Hz, 2H, Ar), 3.94 (brs, 2H, NH_2). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 149.34$ (Ar), 126.70 (q, $J = 3.8$ Hz, Ar), 124.81 (q, $J = 268.9$ Hz, CF_3), 120.16 (q, $J = 32.4$ Hz, Ar), 114.18 (Ar). MS (EI) $m/z = 161$ (M).

4-Aminoacetophene (**4h**) [CAS: 99-92-3]: In the flow reaction, a mixture of 4-aminoacetophene **4h** and the polymeric imine derived from **4h** was obtained (the ratio = 2:3 in ^1H NMR). Therefore the yield of **4h** was determined with GC-MS using an internal standard.

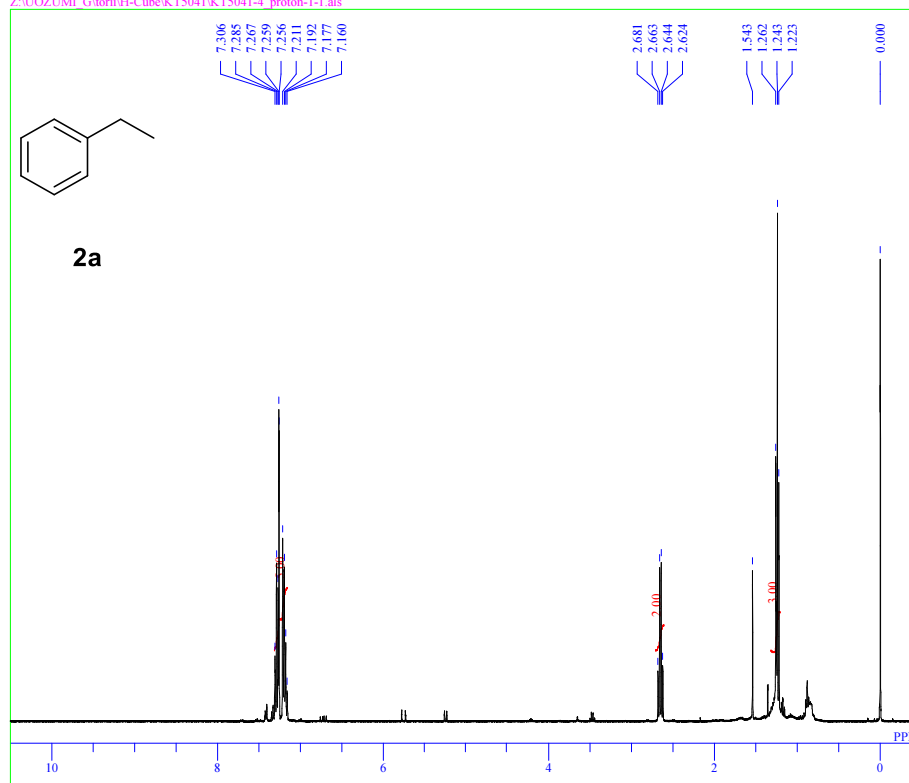
^1H NMR for **4h** (396 MHz, CDCl_3): $\delta = 7.81$ (ddd, $J = 8.3, 2.8,$ and 1.6 Hz, 2H, Ar), 6.65 (ddd, $J = 8.7, 2.8,$ and 1.6 Hz, 2H, Ar), 4.13 (brs, 2H, NH_2), 2.51 (s, 3H, CH_3). MS (EI) $m/z = 135$ (M).

Methyl 4-aminobenzoate (**4i**) [CAS: 619-45-4]: ^1H NMR (396 MHz, CDCl_3): $\delta = 7.85$ (ddd, $J = 8.6, 2.7,$ and 1.8 Hz, 2H, Ar), 6.64 (ddd, $J = 8.6, 2.7,$ and 1.8 Hz, 2H, Ar), 4.07 (brs, 2H, NH_2), 3.85 (s, 3H, CH_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): $\delta = 167.13$ (C=O), 150.76 (Ar), 131.56 (Ar), 119.66 (Ar), 113.75 (Ar), 51.59 (CH_3). MS (EI) $m/z = 151$ (M).

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of ethylbenzene (**2a**).

single_pulse

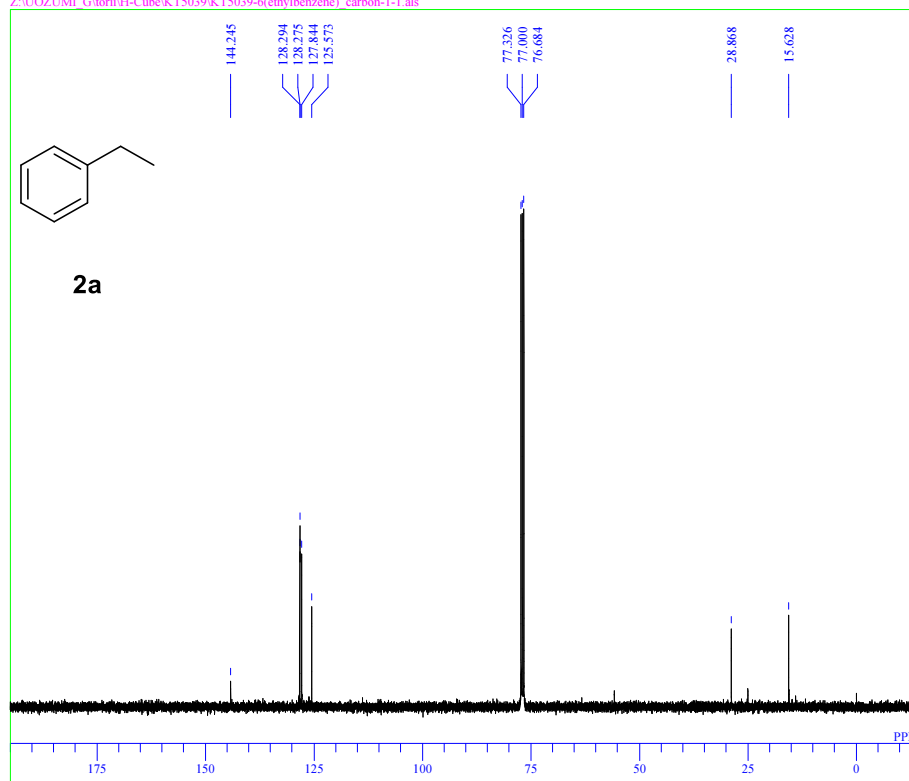
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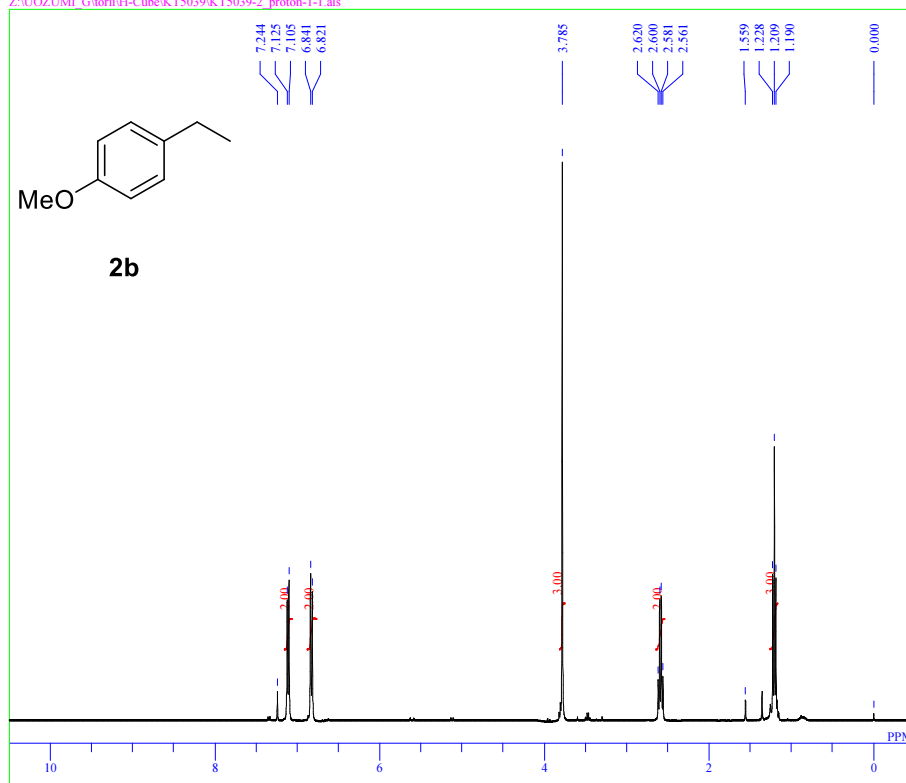


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 BF 0.40 Hz
 RGAIN 58

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

single_pulse

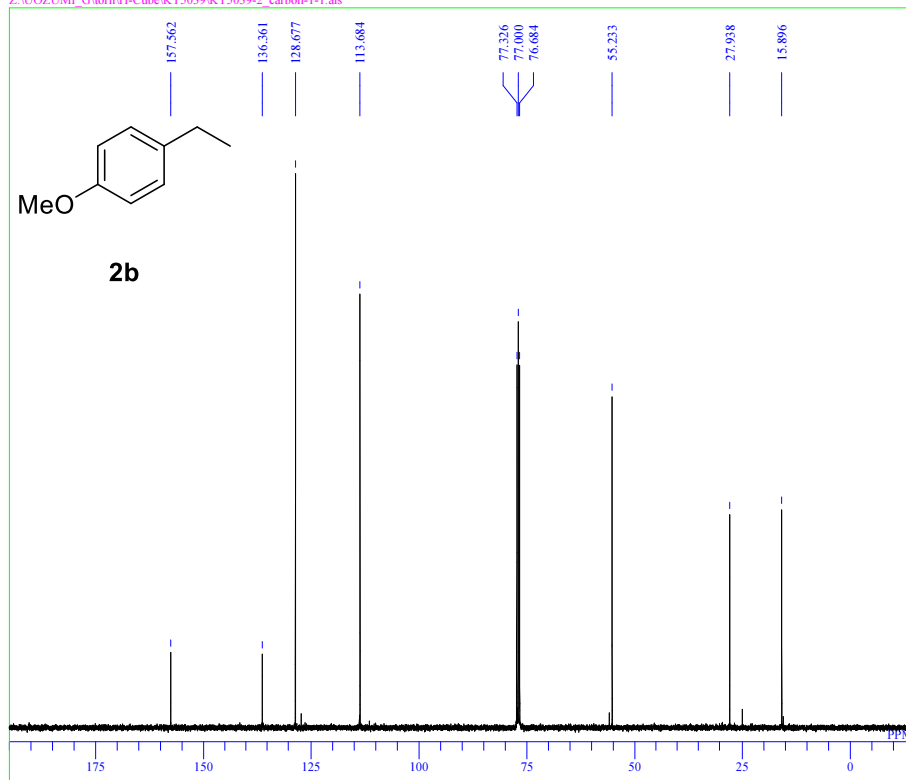
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DFILE KT5039-2_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-03-07 14:30:35
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 20.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.80 Hz
 RGAIN 30

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5039\KT5039-2_carbon-1-1.als

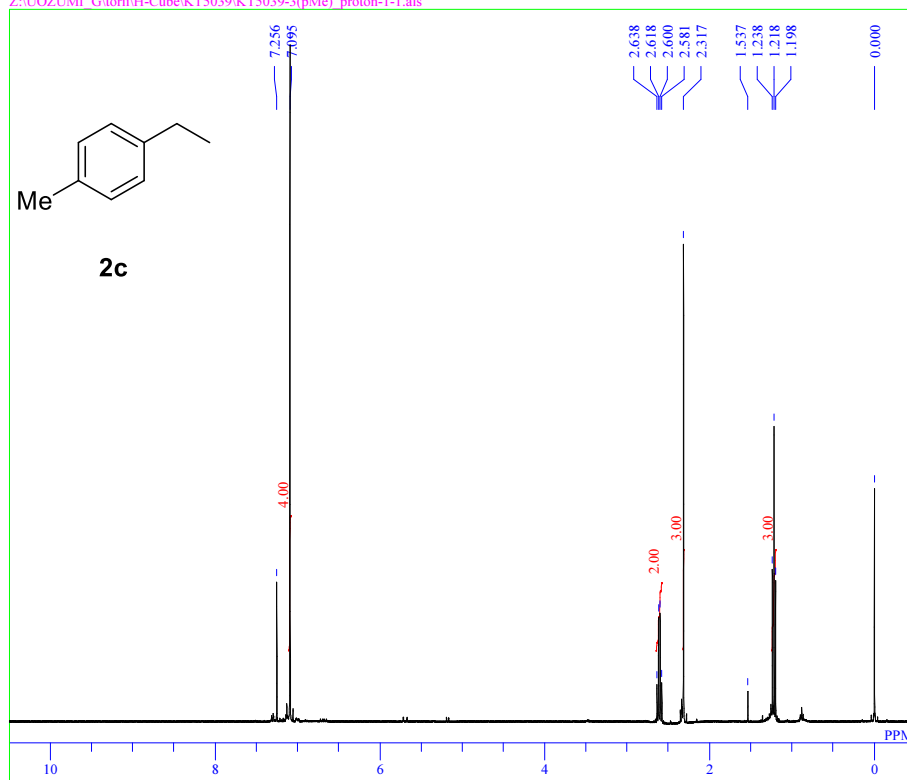


DFILE KT5039-2_carbon-1-1.als
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 DATIM 2014-03-07 14:31:60
 OBNUC 13C
 EXMOD carbon.jsp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 26214
 FREQU 25000.00 Hz
 SCANS 842
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.80 Hz
 RGAIN 60

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

single_pulse

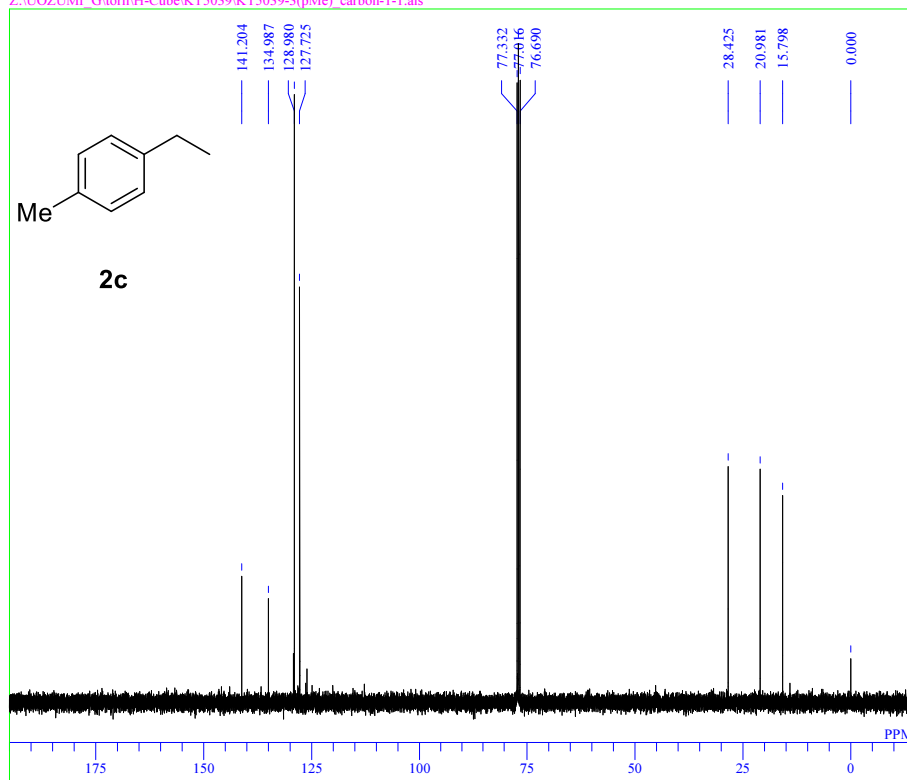
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DFILE KT5039-3(pMe)_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-03-10 14:19:05
 OBNUC ^1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 16384
 FREQU 7422.80 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC ^1H
 CTEMP 20.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 40

single pulse decoupled gated NOE

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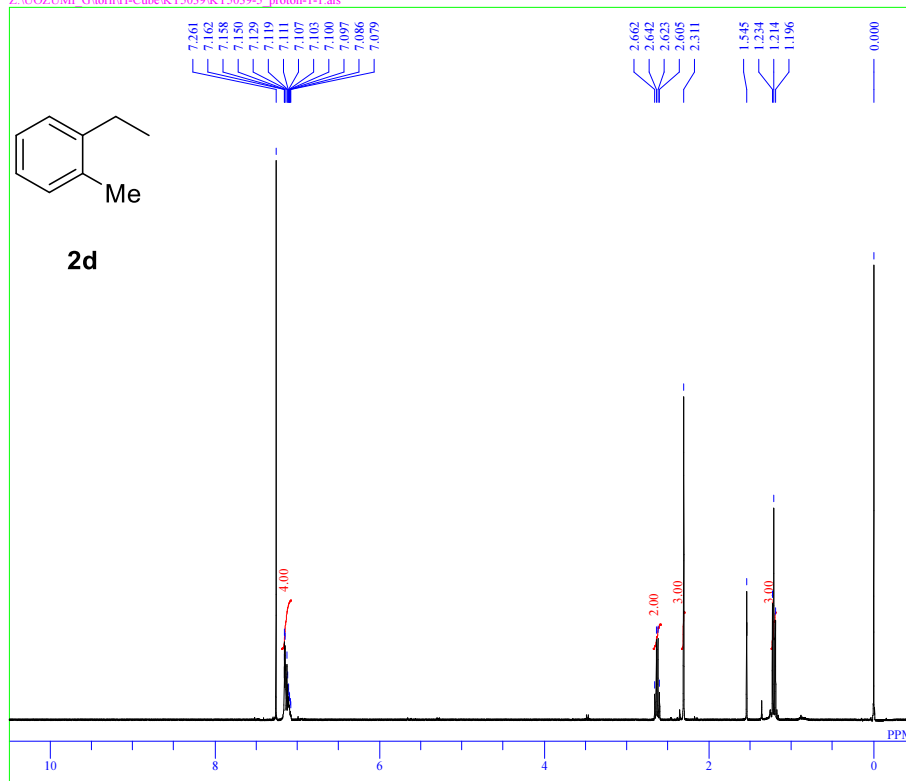


DFILE KT5039-3(pMe)_carbon-1-1.als
 COMNT single pulse decoupled gated NOE
 DATIM 2014-03-10 12:58:05
 OBNUC ^{13}C
 EXMOD carbon.jxp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 496
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC ^1H
 CTEMP 20.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 2-ethyltoluene (**2d**).

single_pulse

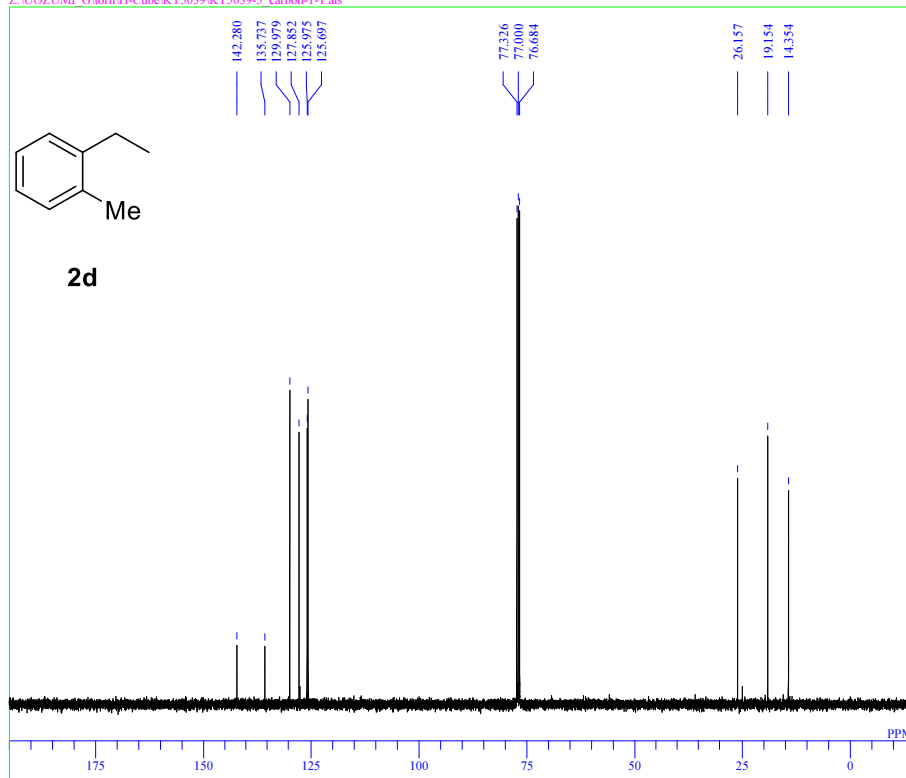
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DFILE KT5039-5_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-03-14 14:25:34
 OBNUC 1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 20.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 44

single_pulse decoupled gated NOE

Z:\UOZUMI_GitoriiH-Cube\KT5039\KT5039-5_carbon-1-1.als

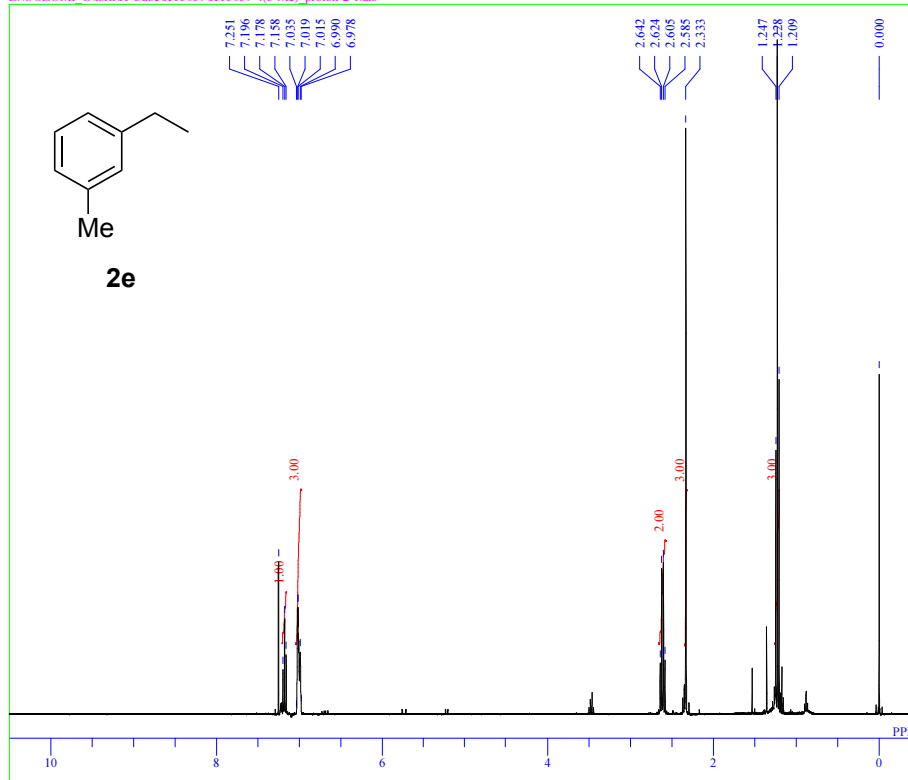


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 DATIM 2014-03-14 14:52:19
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 EXMOD carbon.jxp
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 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 377
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.8 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.40 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 3-ethyltoluene (**2e**).

single_pulse

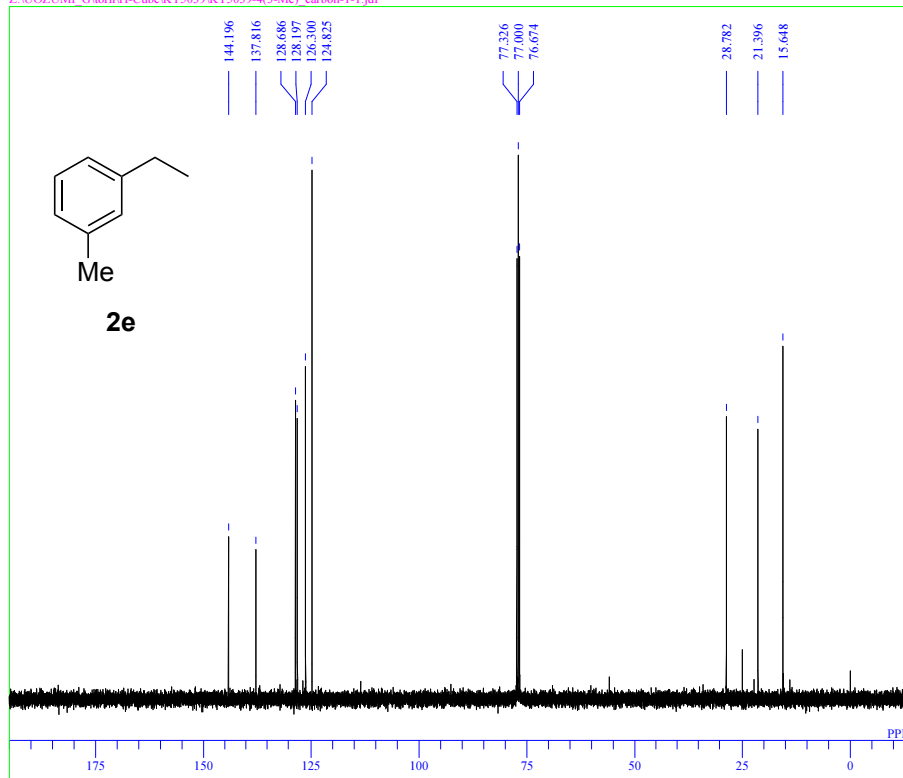
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DFILE KT5039-4(3-Me)_proton-2-1.als
COMNT single_pulse
DATIM 2014-03-10 15:50:17
OBNUC ^1H
EXMOD proton.jxp
OBFRQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC ^1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 36

single_pulse decoupled gated NOE

Z:\UOZUMI Gitorii\H-Cube\KT5039\KT5039-4(3-Me) carbon-1-1.jdf

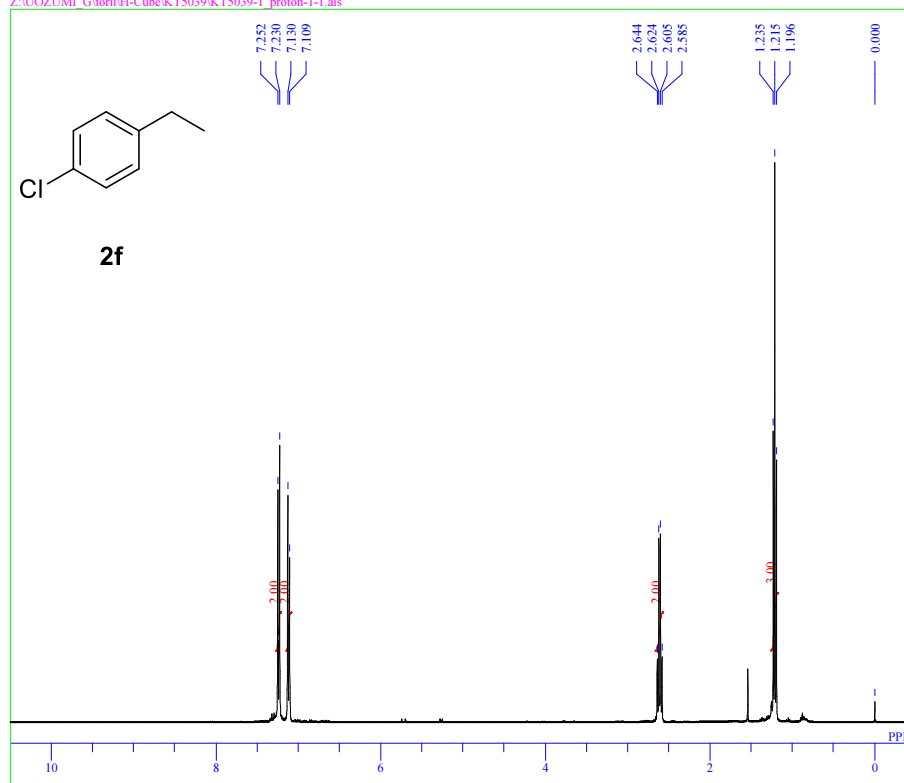


DFILE KT5039-4(3-Me)_carbon-1-1.jdf
COMNT single_pulse decoupled gated NOE
DATIM 2014-03-10 15:32:45
OBNUC ^{13}C
EXMOD carbon.jxp
OBFRQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 187
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC ^1H
CTEMP 20.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.30 Hz
RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 1-chloro-4-ethylbenzene (**2f**).

single_pulse

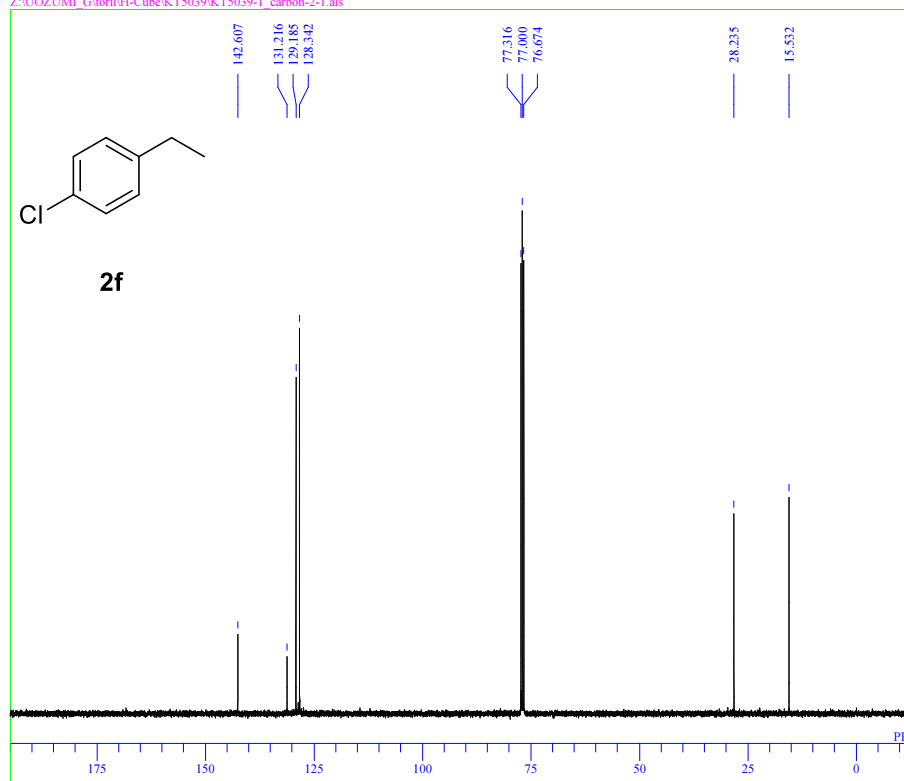
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DFILE KT5039-1_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-03-07 11:53:34
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.80 Hz
 RGAIN 34

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5039\KT5039-1_carbon-2-1.als

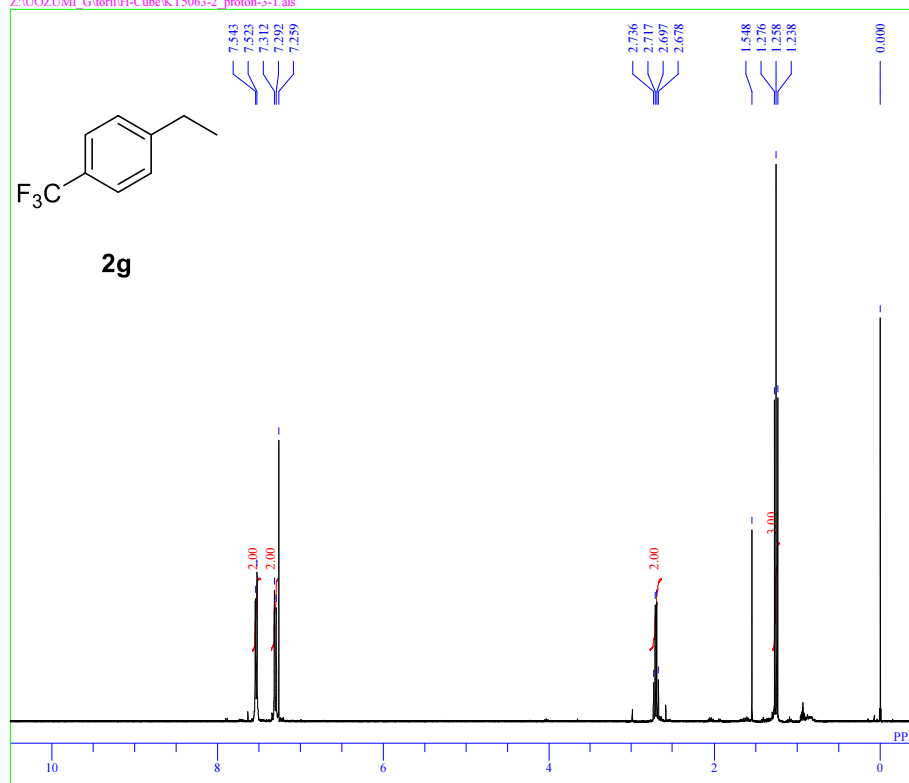


DFILE KT5039-1_carbon-2-1.als
 COMNT single_pulse decoupled gated NOE
 DATIM 2014-03-07 12:30:27
 OBNUC 13C
 EXMOD carbon.jsp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 26214
 FREQU 25000.00 Hz
 SCANS 989
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 20.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.80 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 4-ethylbenzenetrifluoride (**2g**).

single_pulse

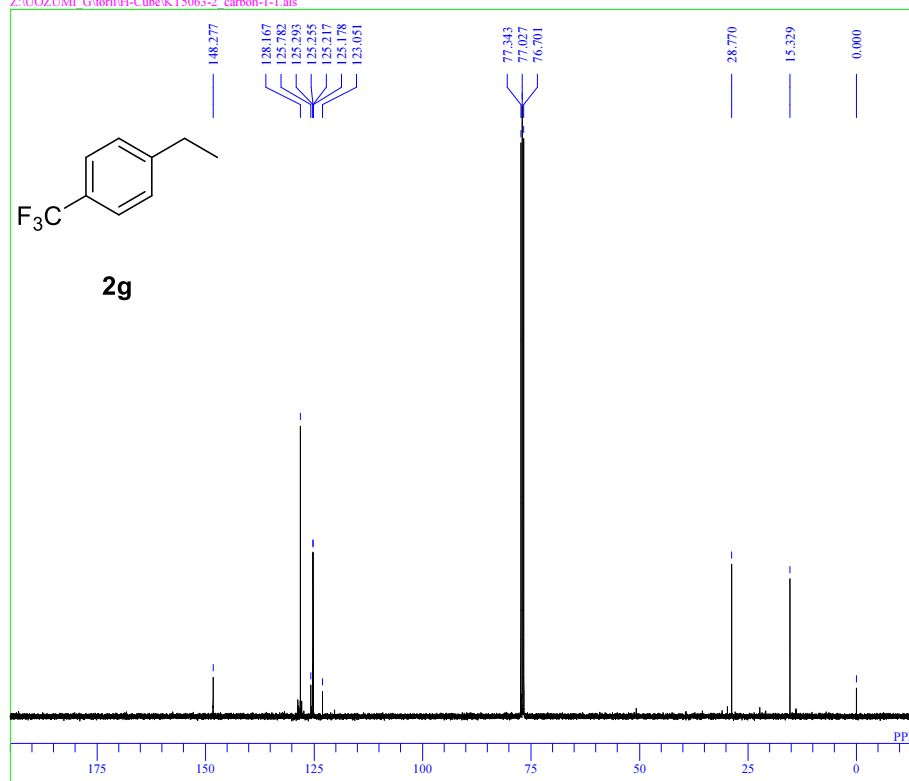
Z:\UOZUMI GitoriiH-Cube\KT5063-2 proton-3-1.als



DFILE KT5063-2 proton-3-1.als
COMNT single_pulse
DATIM 2014-06-03 16:25:54
OBNUC ^1H
EXMOD proton.jsp
OBFRQ 395.88 MHz
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 19.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 40

single pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5063-2 carbon-1-1.als

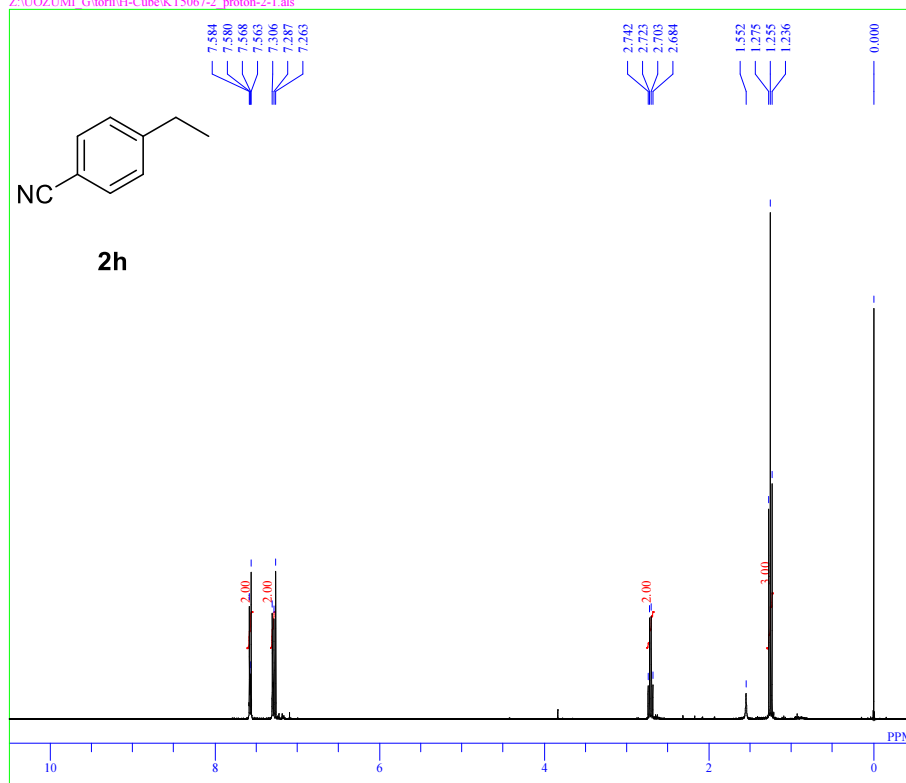


DFILE KT5063-2 carbon-1-1.als
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DATIM 2014-06-03 16:55:59
OBNUC ^{13}C
EXMOD carbon.jsp
OBFRQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 2500
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC ^1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.20 Hz
RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 4-ethylbenzonitrile (**2h**).

single_pulse

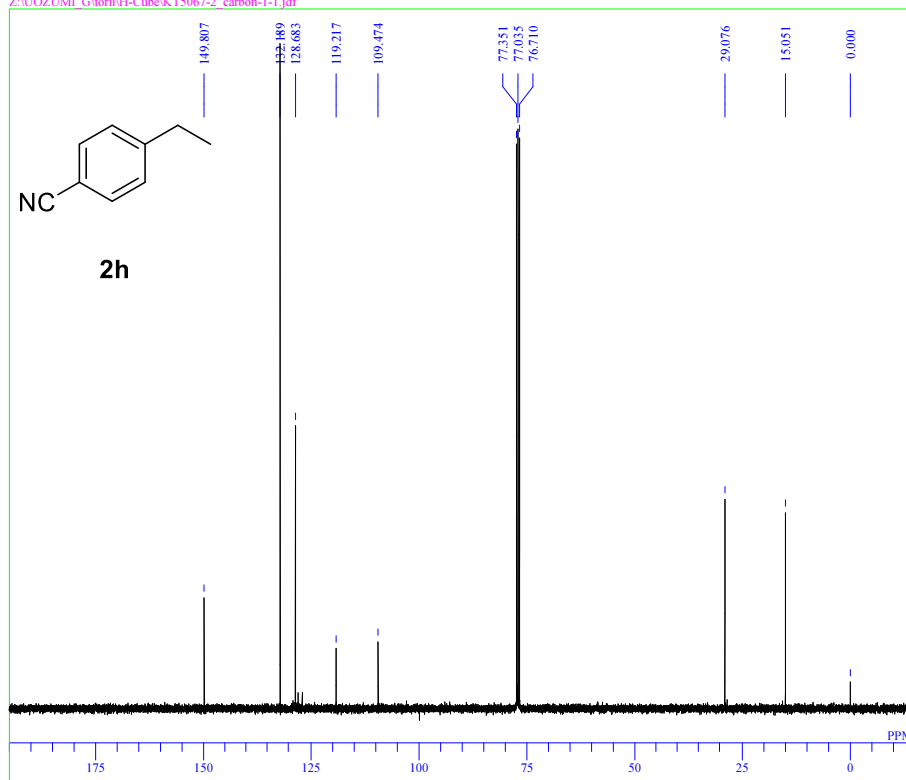
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DFILE KT5067-2 proton-2-1.als
COMNT single_pulse
DATIM 2014-05-27 10:19:07
OBNUC 1H
EXMOD proton.jsp
OBFRQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 13107
FREQU 5938.24 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PW1 3.12 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 42

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5067-2 carbon-1-1.jdf

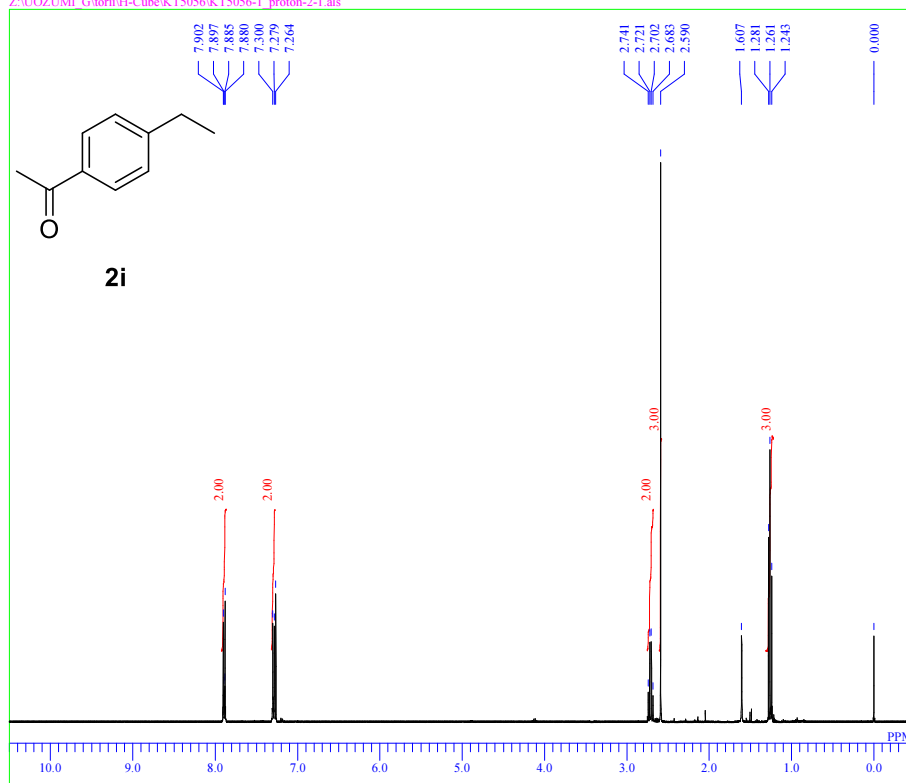


DFILE KT5067-2 carbon-1-1.jdf
COMNT single_pulse decoupled gated NOE
DATIM 2014-05-27 11:00:57
OBNUC ^{13}C
EXMOD carbon.jsp
OBFRQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 1343
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC 1H
CTEMP 19.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.30 Hz
RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 4-ethylacetophenone (**2i**).

single_pulse

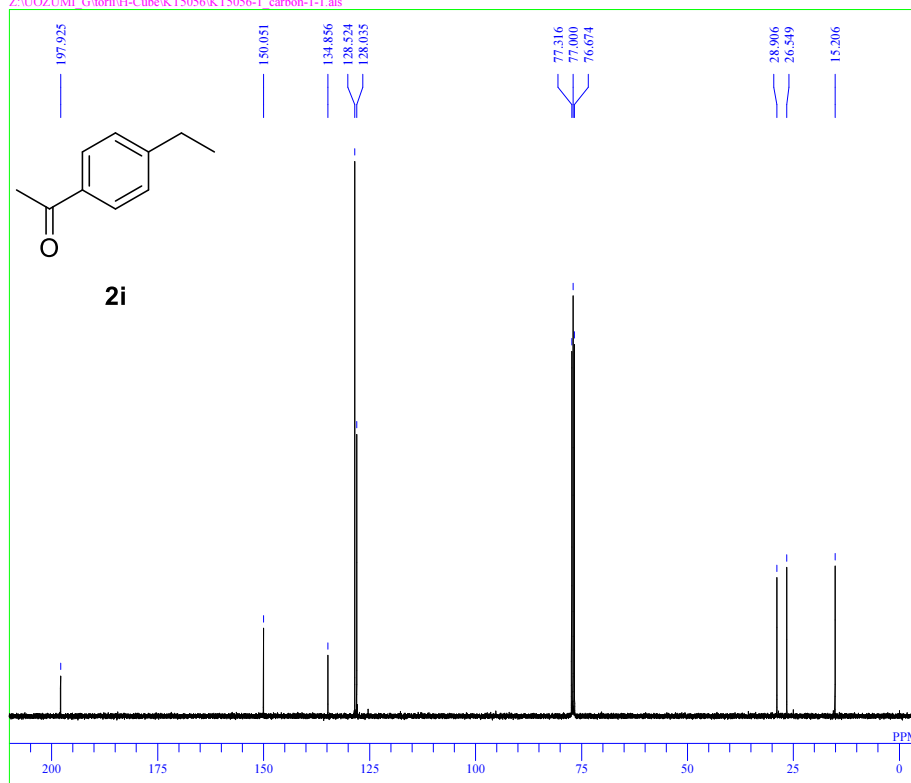
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DFILE KT5056-1 proton-2-1.als
 COMNT single_pulse
 DATIM 2014-05-02 10:41:26
 OBNUC 1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 40

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5056\KT5056-1 carbon-1-1.als

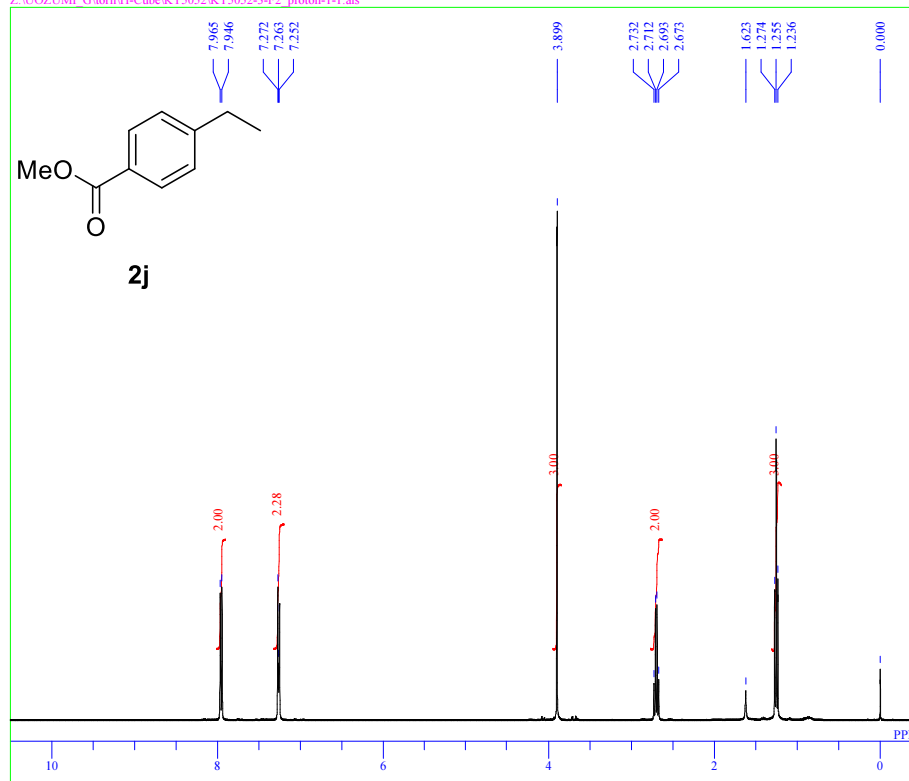


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 DATIM 2014-05-02 11:45:03
 OBNUC 13C
 EXMOD carbon.jxp
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 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 26214
 FREQU 25000.00 Hz
 SCANS 1489
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.4 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.40 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of methyl 4-ethylbenzoate (**2j**).

single_pulse

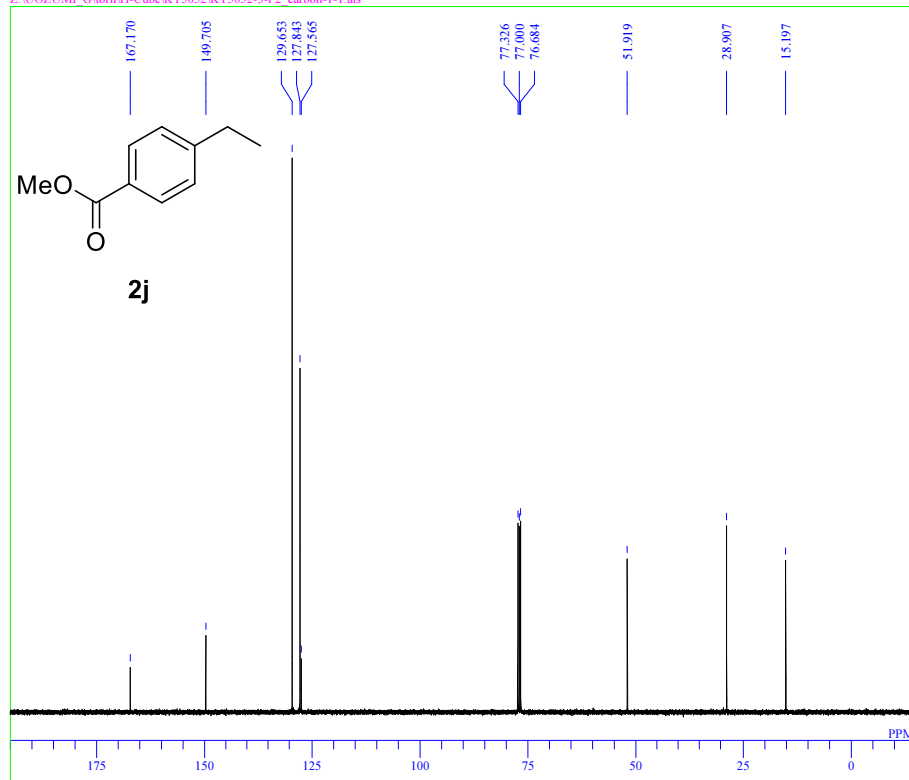
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DFILE KT5052-3-F2_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-04-21 13:08:25
 OBNUC ^1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC ^1H
 CTEMP 19.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 34

single_pulse decoupled gated NOE

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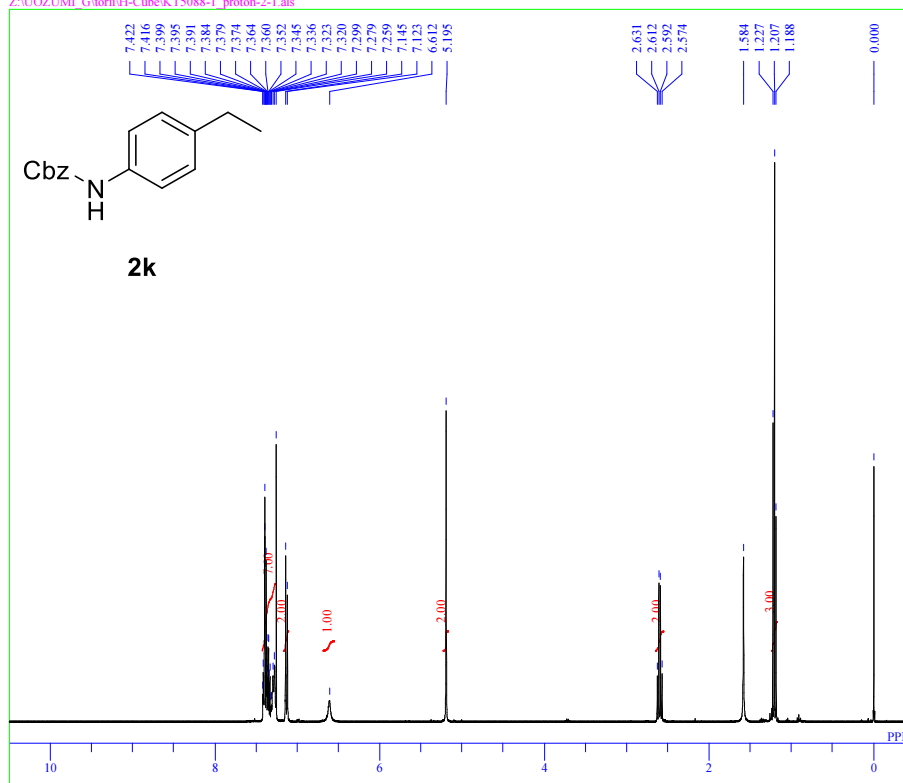


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 COMNT single_pulse decoupled gated NOE
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 OBNUC ^{13}C
 EXMOD carbon.jxp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 421
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC ^1H
 CTEMP 19.6 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.30 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of benzyl (4-ethyl)carbamate (**2k**).

single_pulse

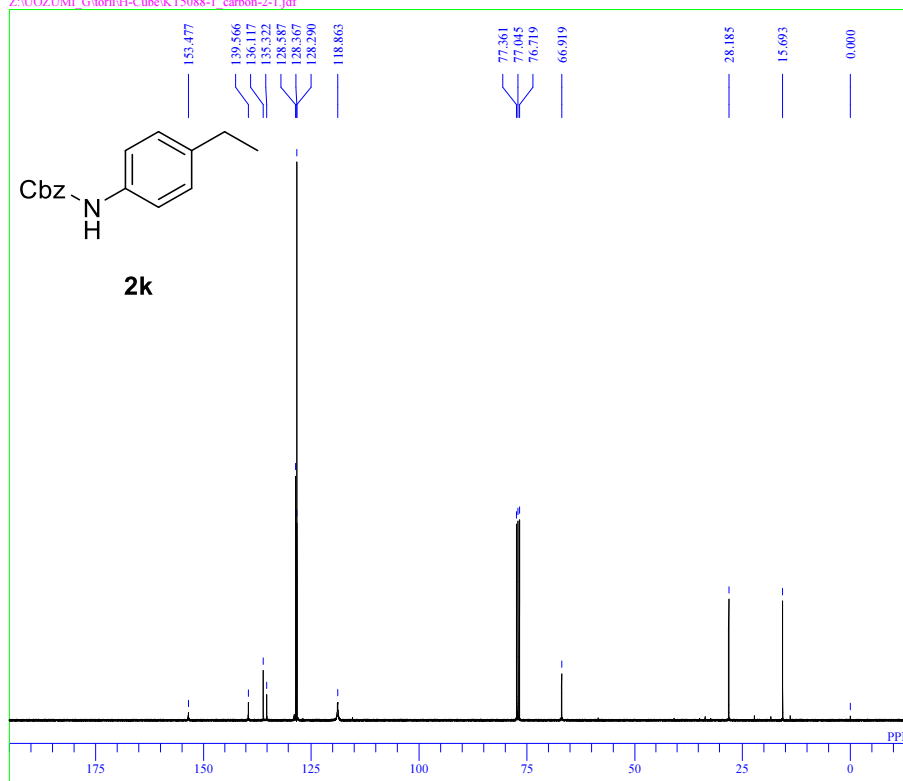
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DFILE KT5088-1 proton-2-1.als
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 DATIM 2014-07-01 14:04:38
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.05 Hz
 RGAIN 40

single_pulse decoupled gated NOE

Z:\UOZUMI Gitorii\H-Cube\KT5088-1 carbon-2-1.jdf

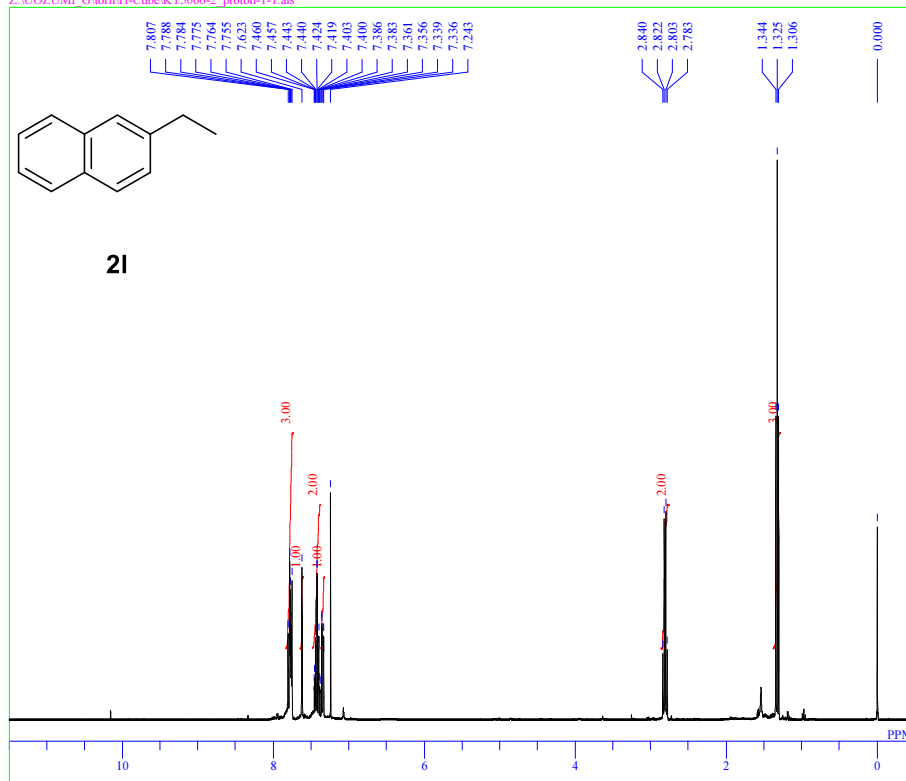


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 EXMOD carbon.jsp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 12000
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.15 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 2-ethylnaphthalene (**21**).

single_pulse

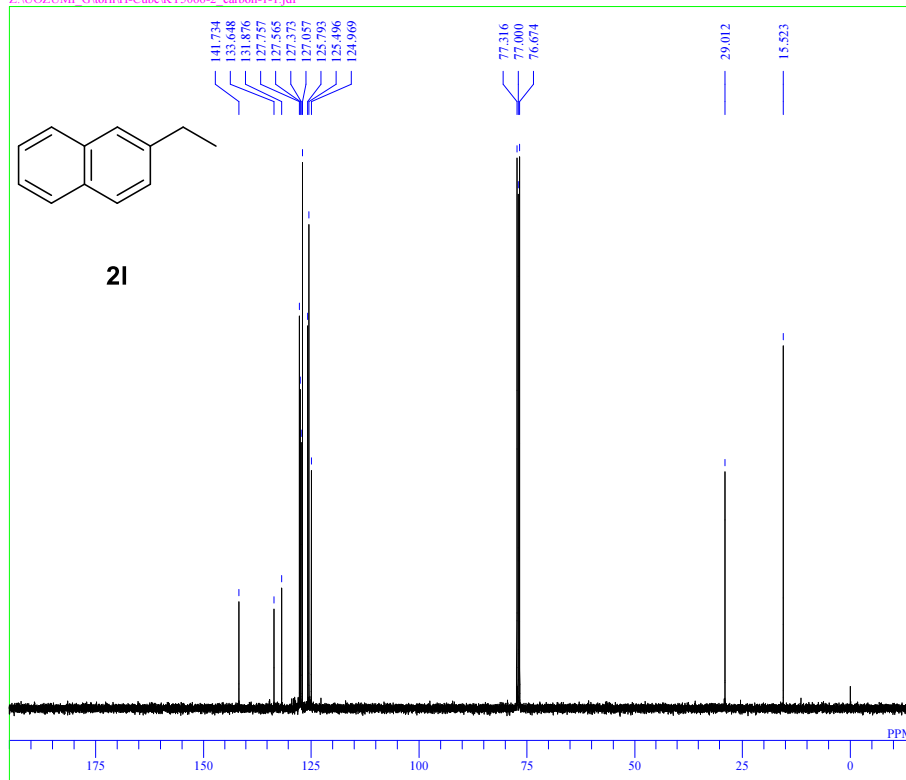
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DFILE KT5066-2_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-09-09 12:24:45
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.8 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 34

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5066-2_carbon-1-1.jdf

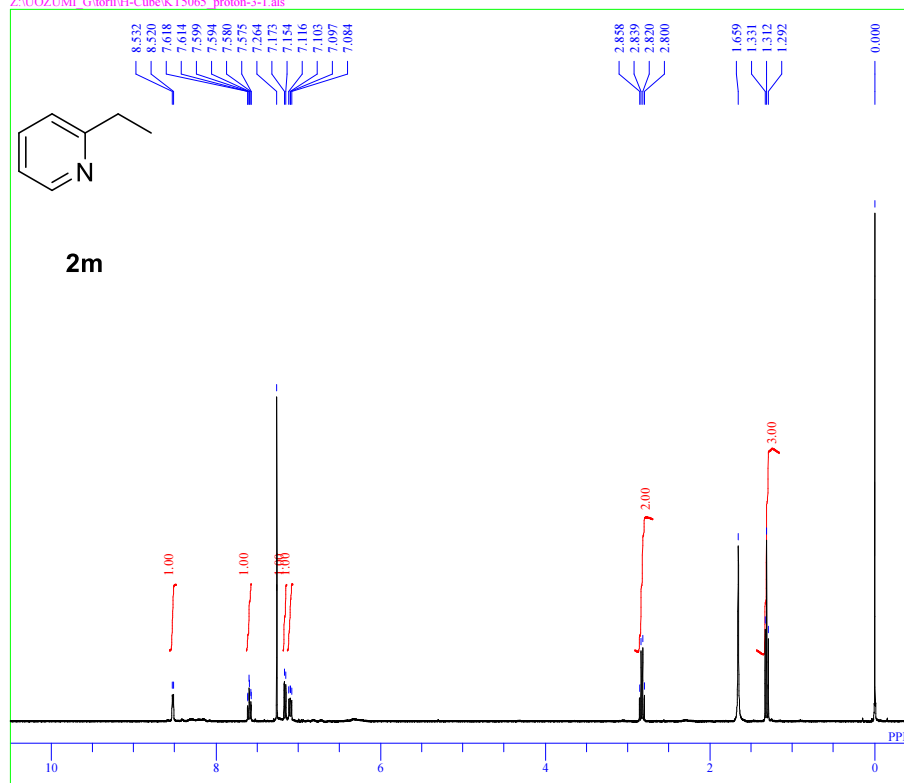


DFILE KT5066-2_carbon-1-1.jdf
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 EXMOD carbon.jsp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 746
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.20 Hz
 RGAIN 60

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

single_pulse

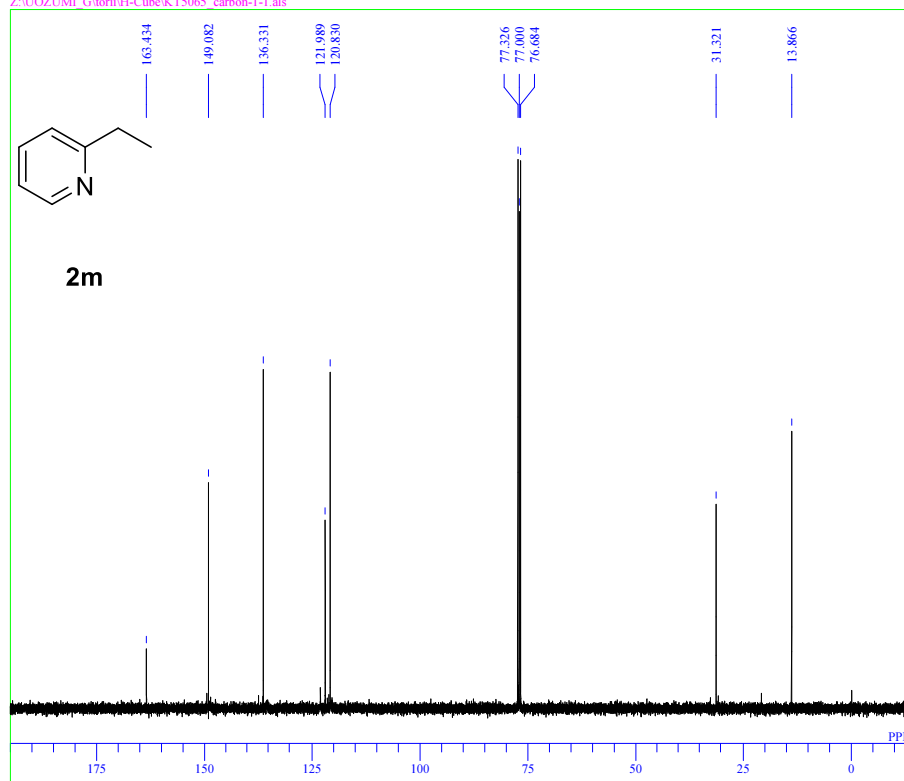
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DFILE KT5065 proton-3-1.als
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 DATIM 2014-06-05 14:30:45
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.2 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 44

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5065 carbon-1-1.als

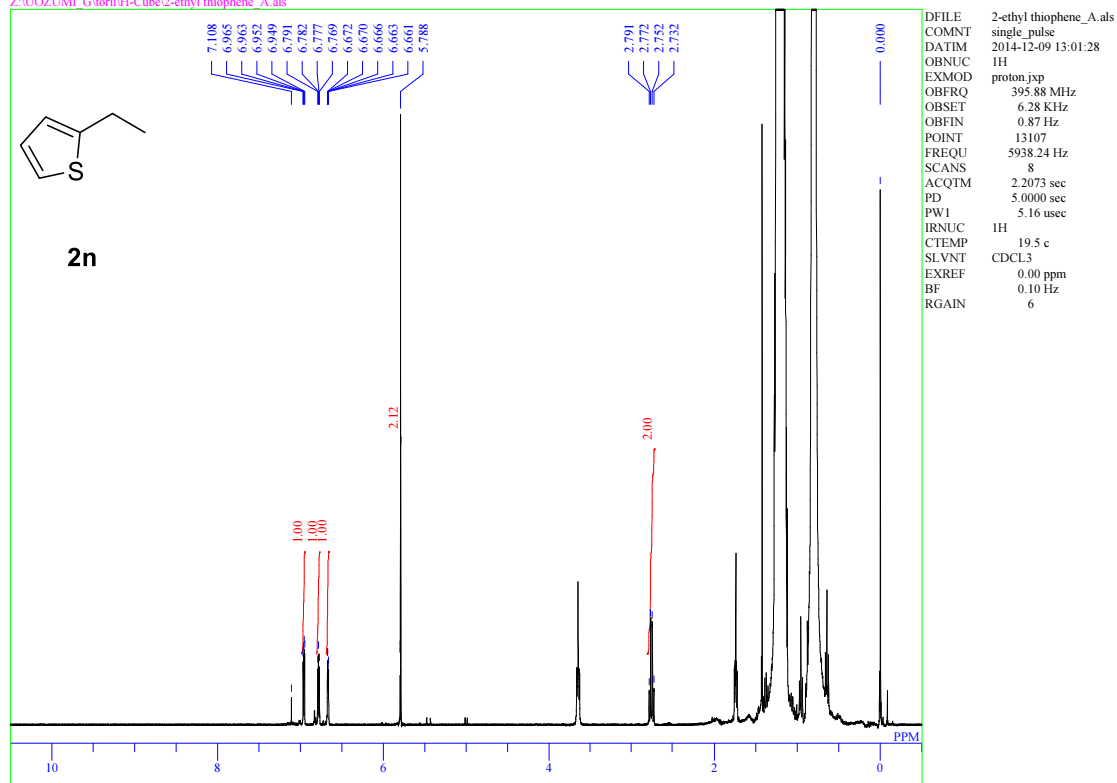


DFILE KT5065 carbon-1-1.als
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 DATIM 2014-06-05 14:51:39
 OBNUC ^{13}C
 EXMOD carbon.jsp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 722
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.00 Hz
 RGAIN 60

¹H NMR spectra of 2-ethylthiophene (**2n**).

single_pulse

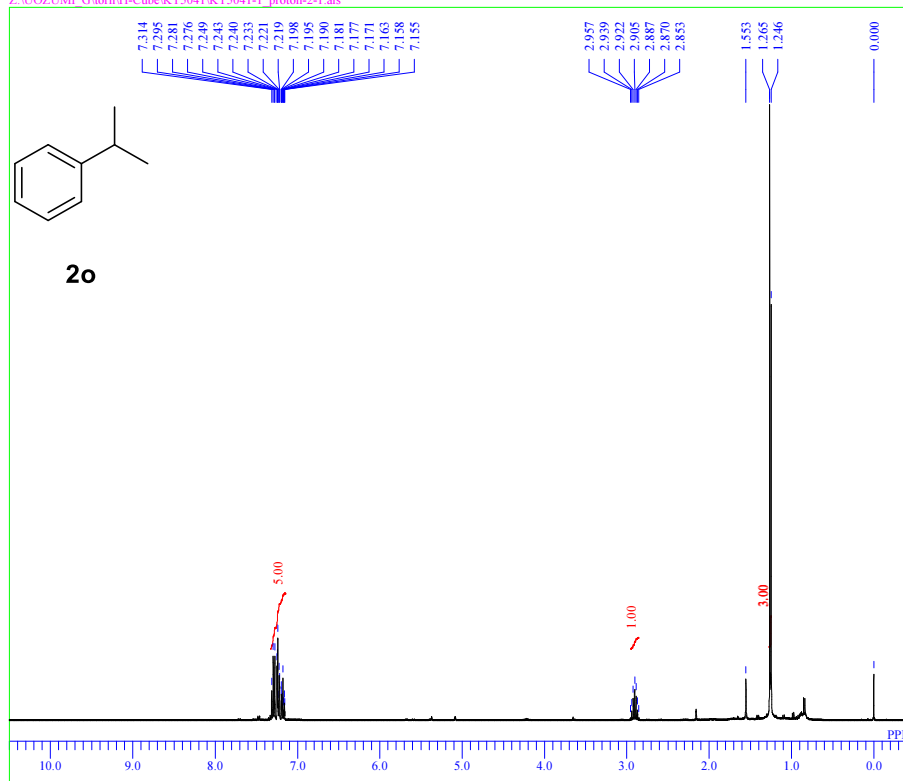
Z:\UOZUMI Gitorii\H-Cube\2-ethyl thiophene_A.als



^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of cumene (**2o**).

single_pulse

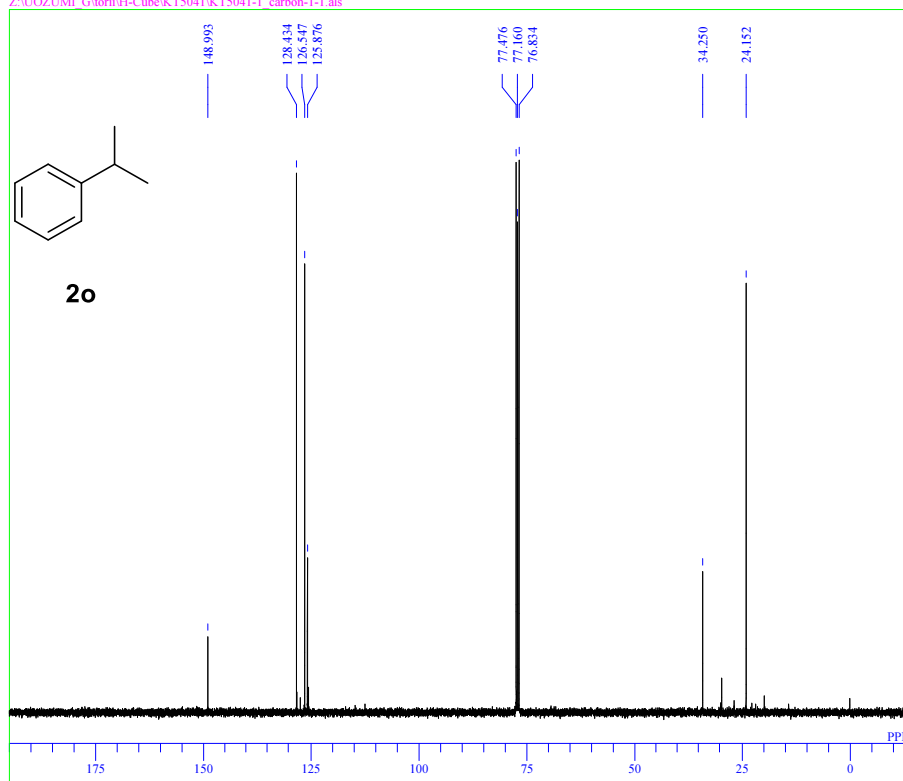
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DFILE KT5041-1_proton-2-1.als
 COMNT single_pulse
 DATIM 2014-05-02 10:25:59
 OBNUC 1H
 EXMOD proton.jsp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 30

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5041\KT5041-1_carbon-1-1.als

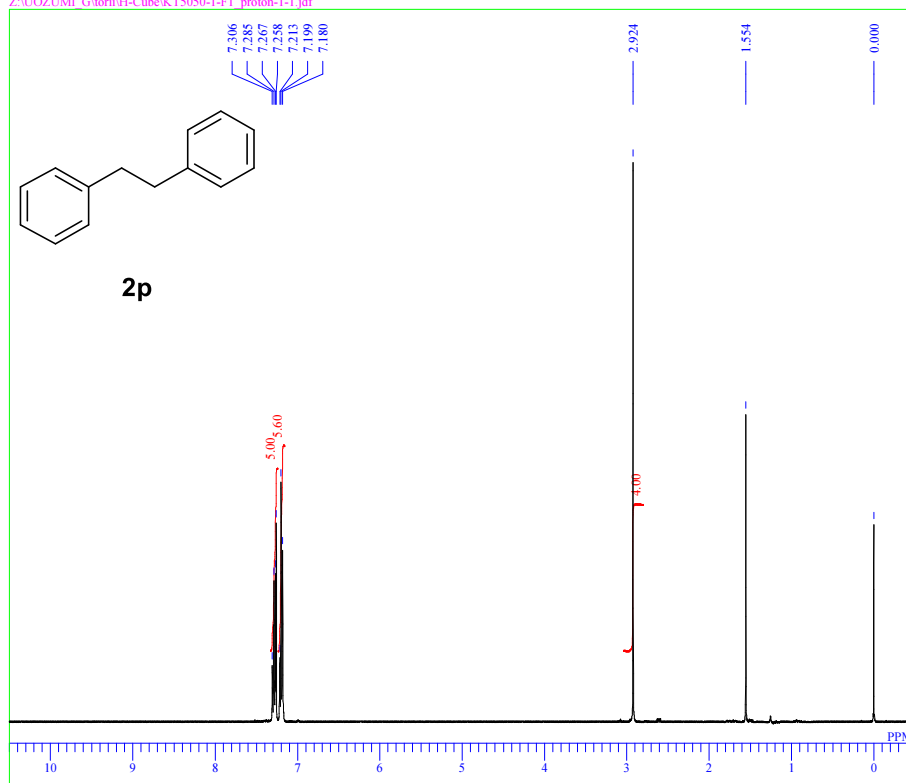


DFILE KT5041-1_carbon-1-1.als
 COMNT single_pulse decoupled gated NOE
 DATIM 2014-05-02 13:04:34
 OBNUC ^{13}C
 EXMOD carbon.jsp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 806
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 18.9 c
 SLVNT NONE
 EXREF 77.16 ppm
 BF 0.40 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 1,2-diphenylethane (**2p**).

single_pulse

Z:\UOZUMI GitoriiH-Cube\KT5050-1-F1_proton-1-1.jdf



```

DFILE  KT5050-1-F1_proton-1-1.jdf
COMNT  single_pulse
DATIM  2014-04-22 09:46:20
OBNUC  1H
EXMOD  proton.jxp
OBFRQ  395.88 MHz
OBSET  6.28 KHz
OBFIN  0.87 Hz
POINT  16384
FREQU  7422.80 Hz
SCANS  8
ACQTM  2.2073 sec
PD      5.0000 sec
PWI     3.12 usec
IRNUC  1H
CTEMP  19.3 c
SLVNT  CDCL3
EXREF  0.00 ppm
BF      0.10 Hz
RGAIN  42
    
```

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5050-1-F1_carbon-1-1.als



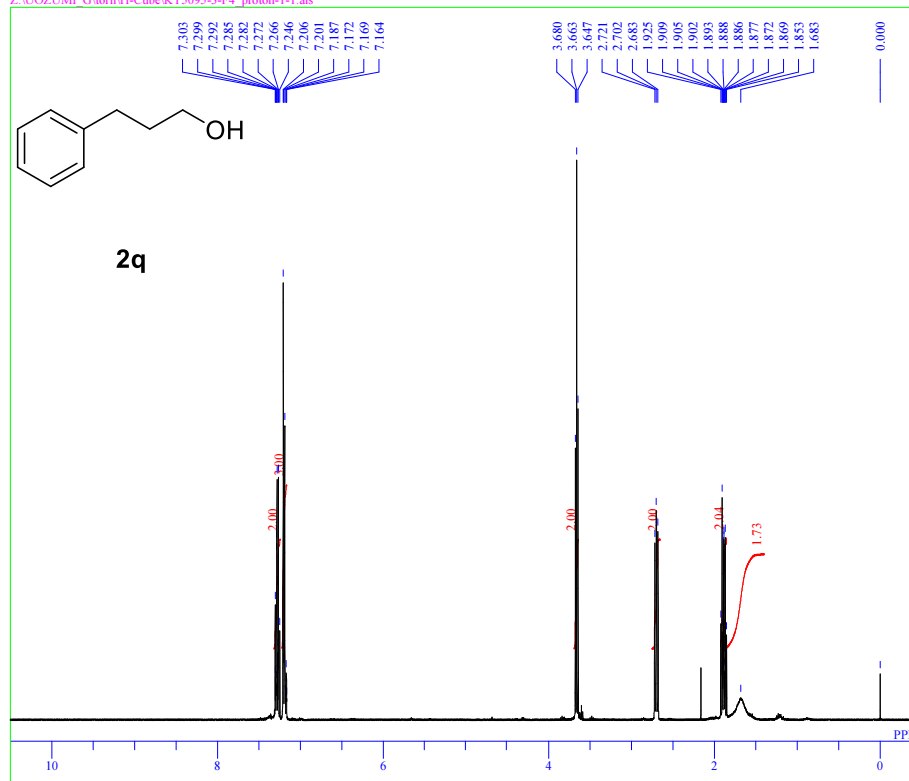
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DFILE  KT5050-1-F1_carbon-1-1.als
COMNT  single_pulse decoupled gated NOE
DATIM  2014-04-22 10:06:29
OBNUC  13C
EXMOD  carbon.jxp
OBFRQ  99.55 MHz
OBSET  5.13 KHz
OBFIN  0.98 Hz
POINT  32767
FREQU  31250.00 Hz
SCANS  602
ACQTM  1.0486 sec
PD      2.0000 sec
PWI     3.42 usec
IRNUC  1H
CTEMP  19.0 c
SLVNT  CDCL3
EXREF  77.00 ppm
BF      0.20 Hz
RGAIN  60
    
```


^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 3-phenylpropan-1-ol (**2q**).

single_pulse

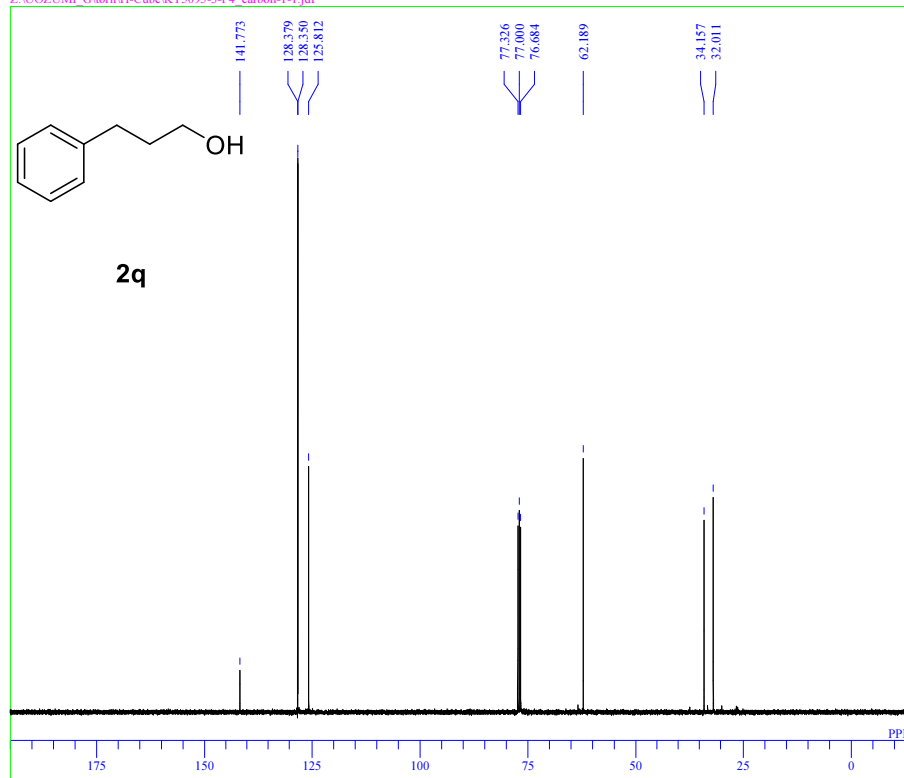
Z:\UOZUMI GitoriiH-Cube\KT5095-3-F4 proton-1-1.als



DFILE KT5095-3-F4 proton-1-1.als
 COMNT single_pulse
 DATIM 2014-07-22 11:37:53
 OBNUC 1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 OBSETE 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 20.4 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 26

single_pulse decoupled gated NOE

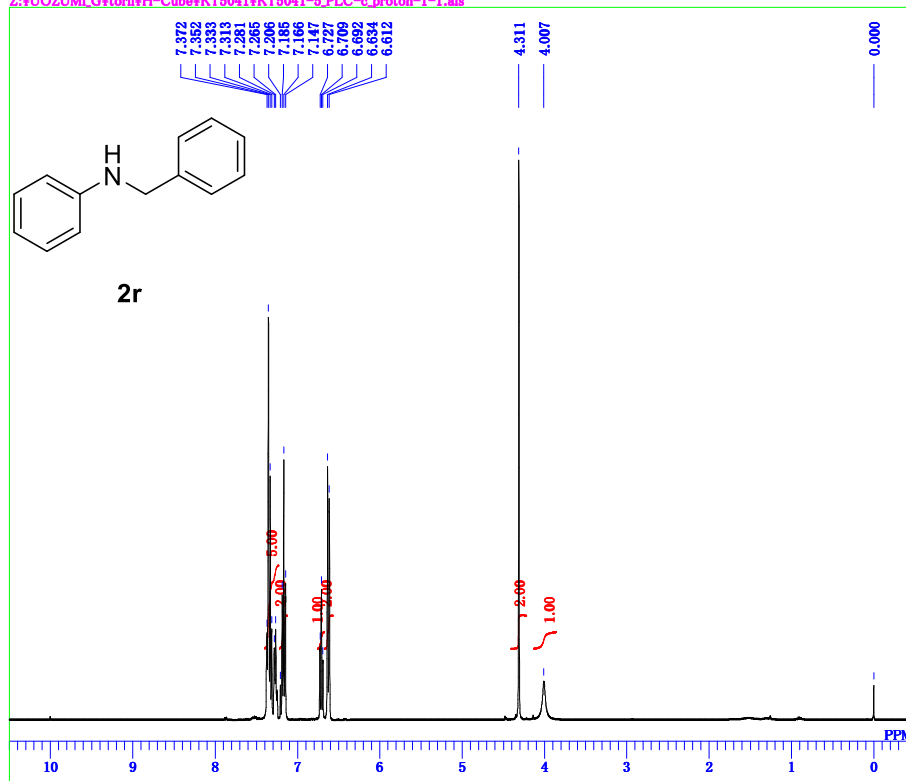
Z:\UOZUMI GitoriiH-Cube\KT5095-3-F4 carbon-1-1.jdf



DFILE KT5095-3-F4 carbon-1-1.jdf
 COMNT single_pulse decoupled gated NOE
 DATIM 2014-07-22 11:40:17
 OBNUC ^{13}C
 EXMOD carbon.jxp
 OBFREQ 99.55 MHz
 OBSETE 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 344
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 20.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.40 Hz
 RGAIN 60

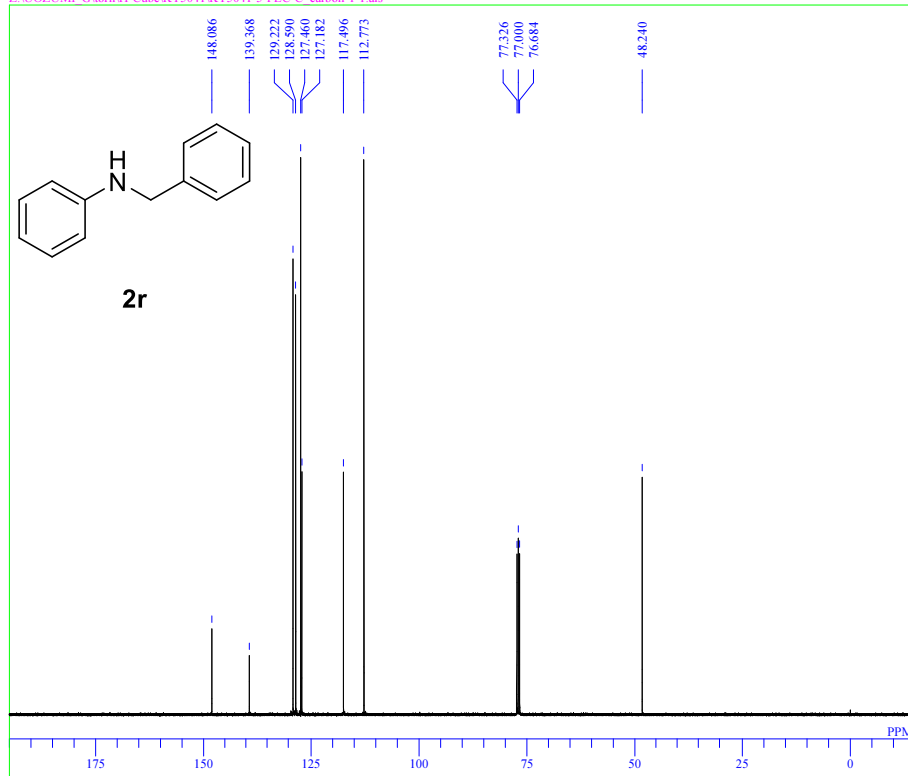
^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of *N*-benzylaniline (**2r**).

Z:\UOZUMI_G\Iori\H-Cube\KT5041\KT5041-5-PLC-c_proton-1-1.als



DFILE KT5041-5-PLC-c_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-03-26 15:31:37
 OBNUC ^1H
 EXMOD proton_jxp
 OBFREQ 395.88 MHz
 OBSET 6.28 KHz
 OBFIN 0.67 Hz
 POINT 16384
 FREQU 7422.80 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC ^1H
 CTEMP 19.5 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.10 Hz
 RGAIN 26

Z:\UOZUMI_G\Iori\H-Cube\KT5041\KT5041-5-PLC-C_carbon-1-1.als

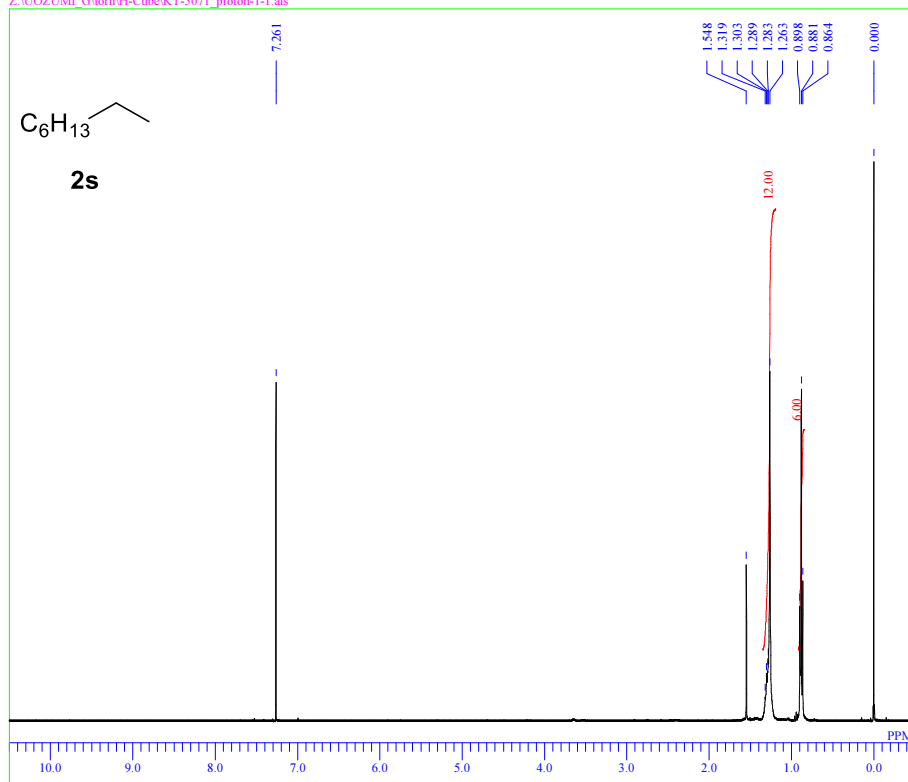


DFILE KT5041-5-PLC-C_carbon-1-1.als
 COMNT single_pulse_decoupled_gated_NOE
 DATIM 2014-03-26 15:52:49
 OBNUC ^{13}C
 EXMOD carbon_jxp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 1761
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC ^{13}C
 CTEMP 19.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.30 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of octane (**2s**).

single_pulse

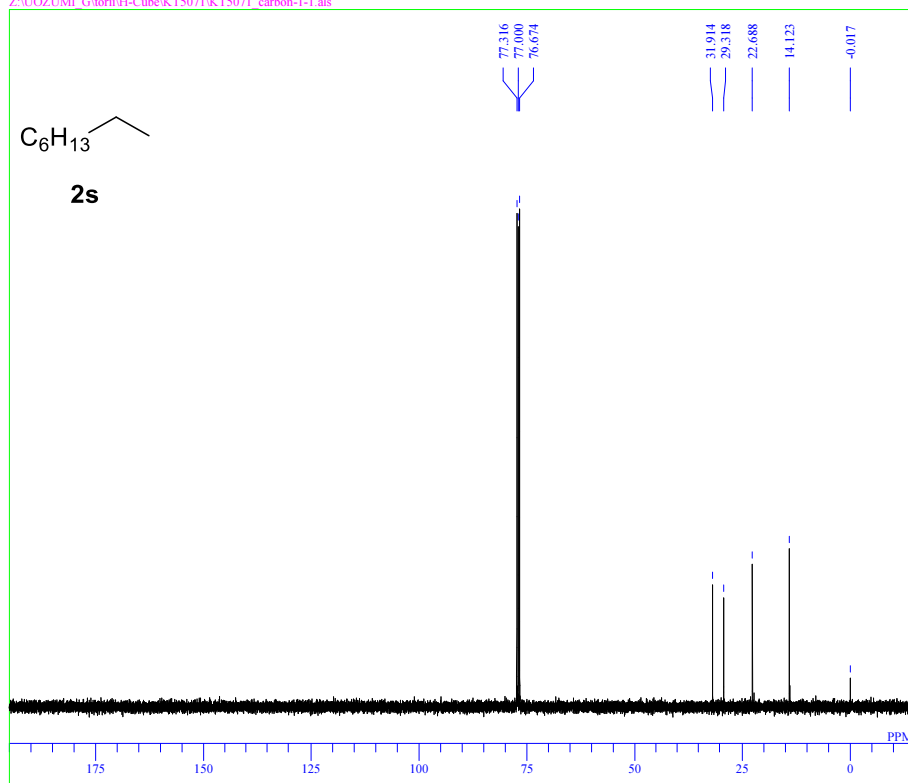
Z:\UOZUMI_Gitorii\H-Cube\KT-5071_proton-1-1.als



DFILE KT-5071_proton-1-1.als
COMNT single_pulse
DATIM 2014-05-28 13:23:41
OBNUC ^1H
EXMOD proton.jxp
OBFREQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 16384
FREQU 7422.80 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PW1 3.12 usec
IRNUC ^1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 42

single pulse decoupled gated NOE

Z:\UOZUMI_Gitorii\H-Cube\KT5071\KT5071_carbon-1-1.als

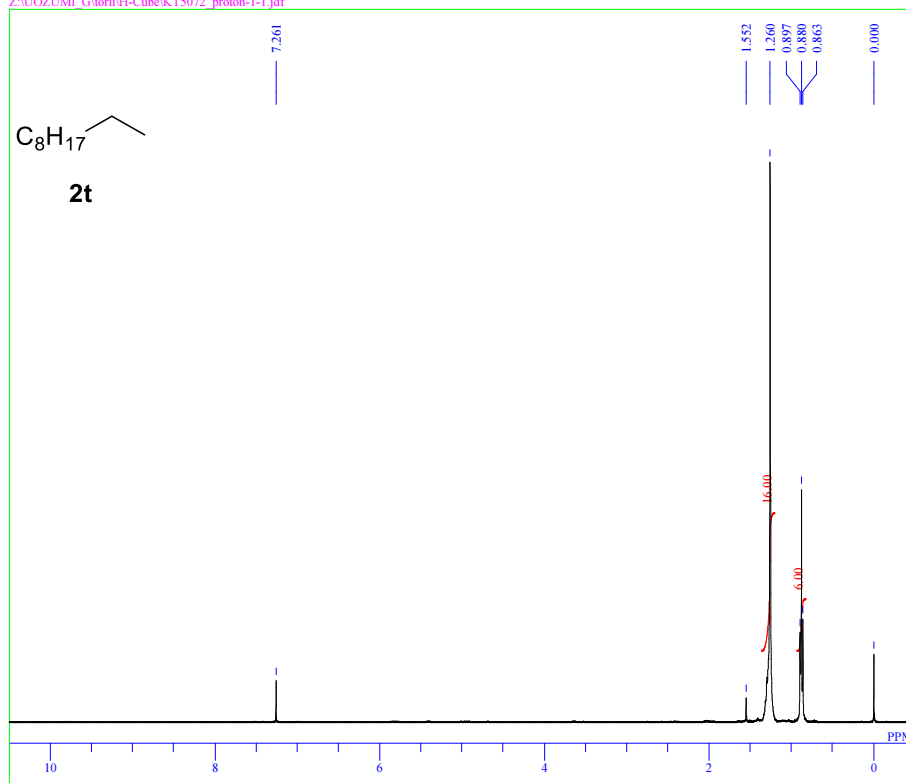


DFILE KT5071_carbon-1-1.als
COMNT single pulse decoupled gated NOE
DATIM 2014-05-28 14:05:51
OBNUC ^{13}C
EXMOD carbon.jxp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 26214
FREQU 25000.00 Hz
SCANS 408
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC ^1H
CTEMP 19.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.10 Hz
RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of decane (**2t**).

single_pulse

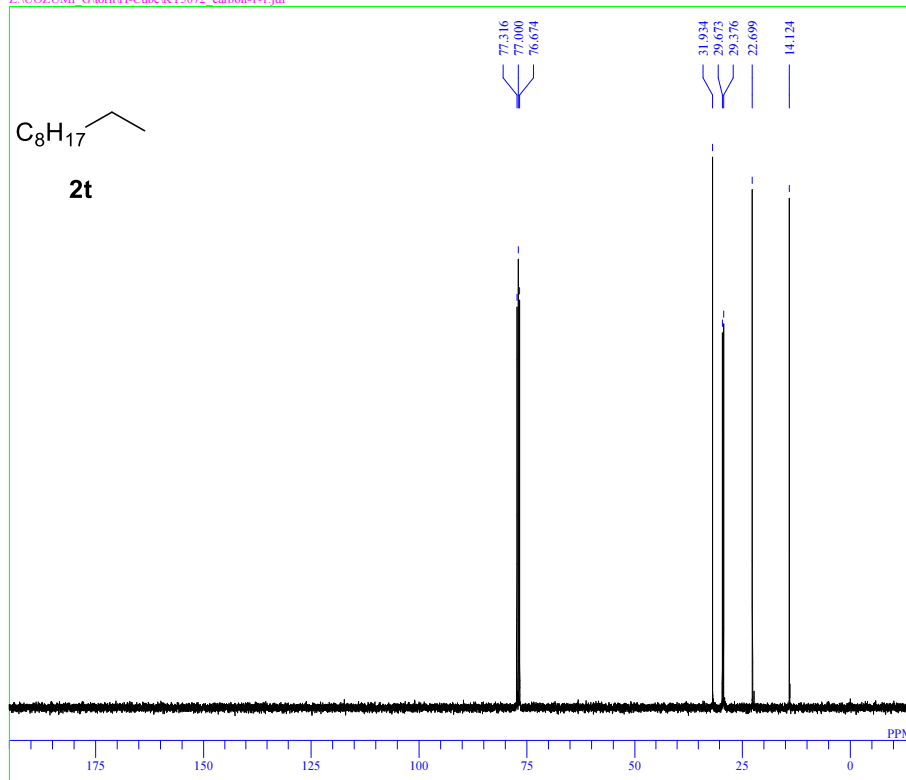
Z:\UOZUMI GitoriiH-Cube\KT5072_proton-1-1.jdf



DFILE KT5072_proton-1-1.jdf
COMNT single_pulse
DATIM 2014-05-29 13:52:19
OBNUC 1H
EXMOD proton.jsp
OBFRQ 395.88 MHz
OBSET 6.28 KHz
OBFIN 0.87 Hz
POINT 16384
FREQU 7422.80 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PWI 3.12 usec
IRNUC 1H
CTEMP 19.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.80 Hz
RGAIN 30

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5072_carbon-1-1.jdf

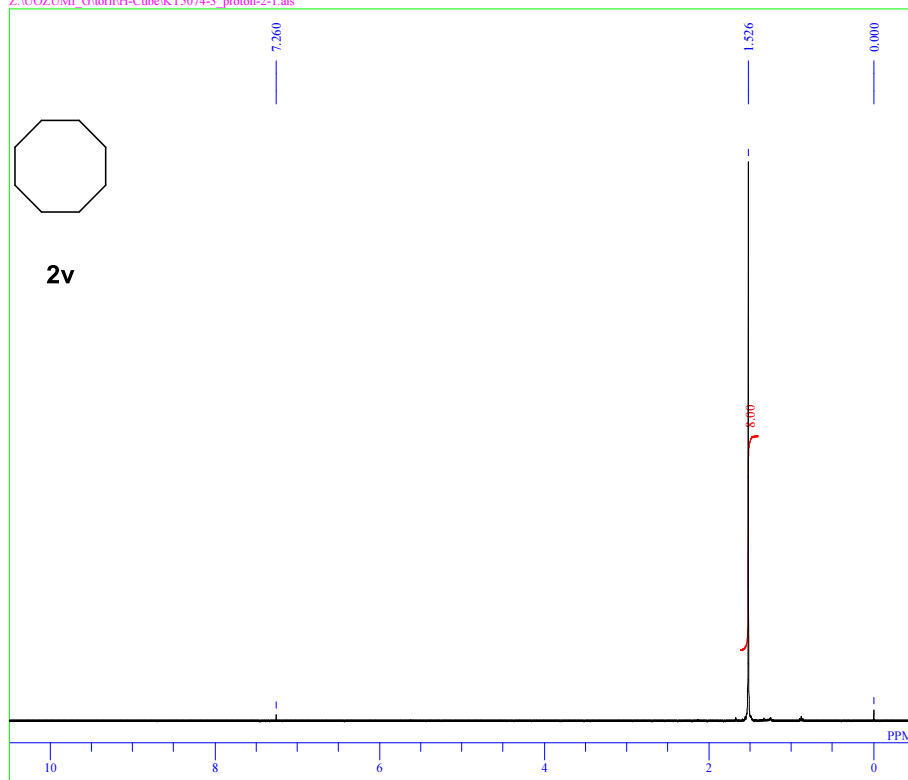


DFILE KT5072_carbon-1-1.jdf
COMNT single_pulse decoupled gated NOE
DATIM 2014-05-29 14:04:24
OBNUC 13C
EXMOD carbon.jsp
OBFRQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 321
ACQTM 1.0486 sec
PD 2.0000 sec
PWI 3.42 usec
IRNUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.80 Hz
RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of cyclooctane (**2v**).

single_pulse

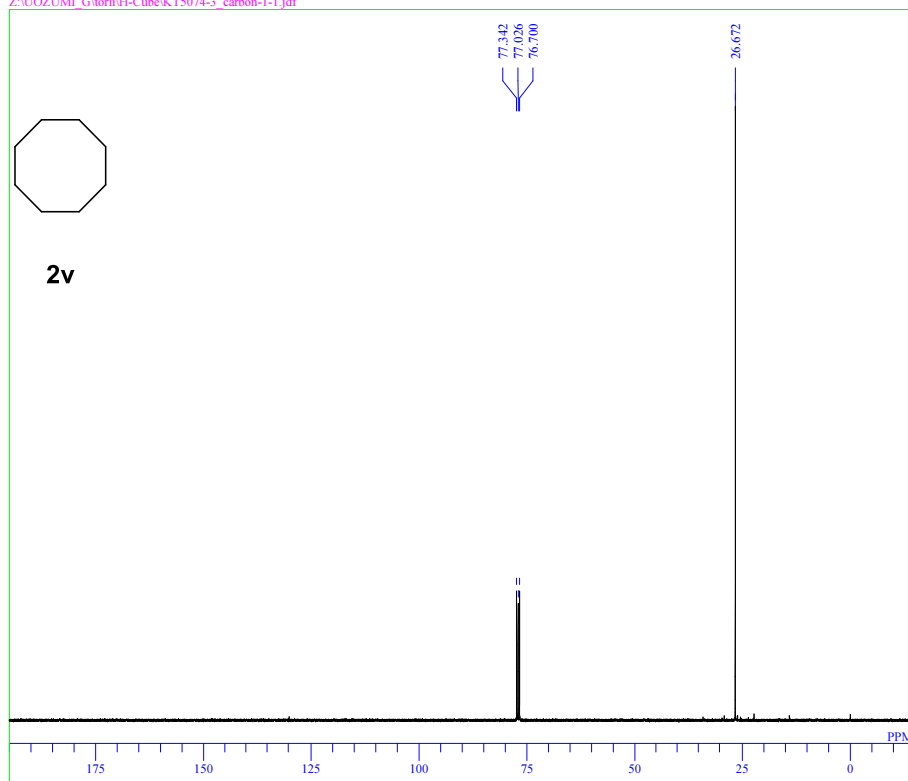
Z:\UOZUMI_Gitorii\H-Cube\KT5074-3_proton-2-1.als



DFILE KT5074-3_proton-2-1.als
COMNT single_pulse
DATIM 2014-05-29 12:28:32
OBNUC 1H
EXMOD proton.jxp
OBFREQ 395.88 MHz
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 19.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.80 Hz
RGAIN 26

single pulse decoupled gated NOE

Z:\UOZUMI_Gitorii\H-Cube\KT5074-3_carbon-1-1.jdf

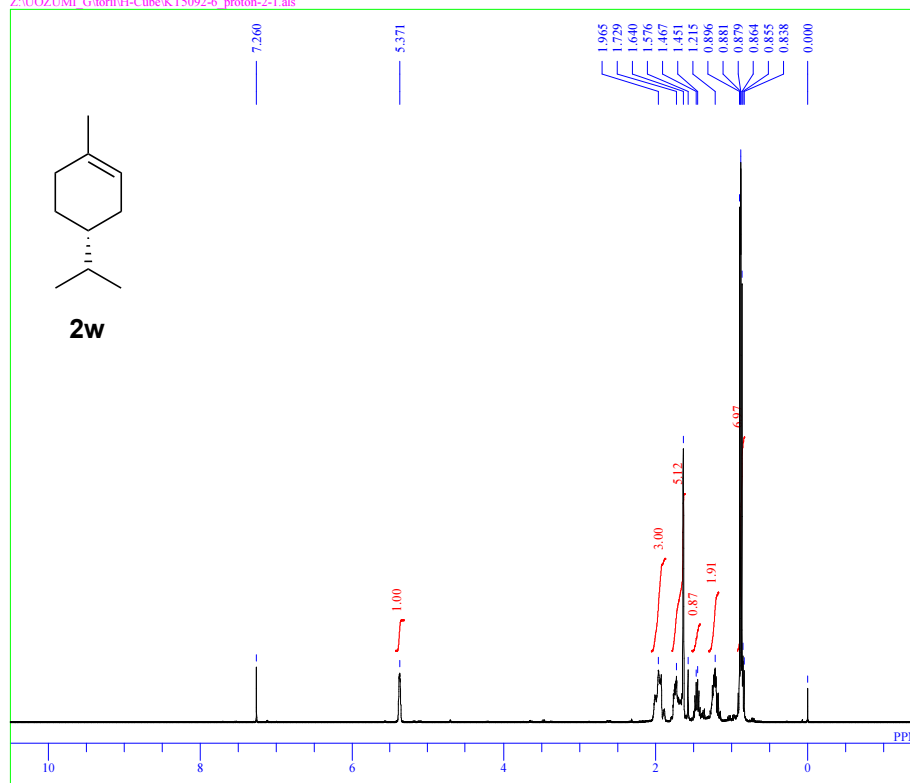


DFILE KT5074-3_carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2014-05-29 12:29:58
OBNUC ^{13}C
EXMOD carbon.jxp
OBFREQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 703
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC 1H
CTEMP 19.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.80 Hz
RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 4-isopropyl-1-methylcyclohex-1-ene (**2w**).

single_pulse

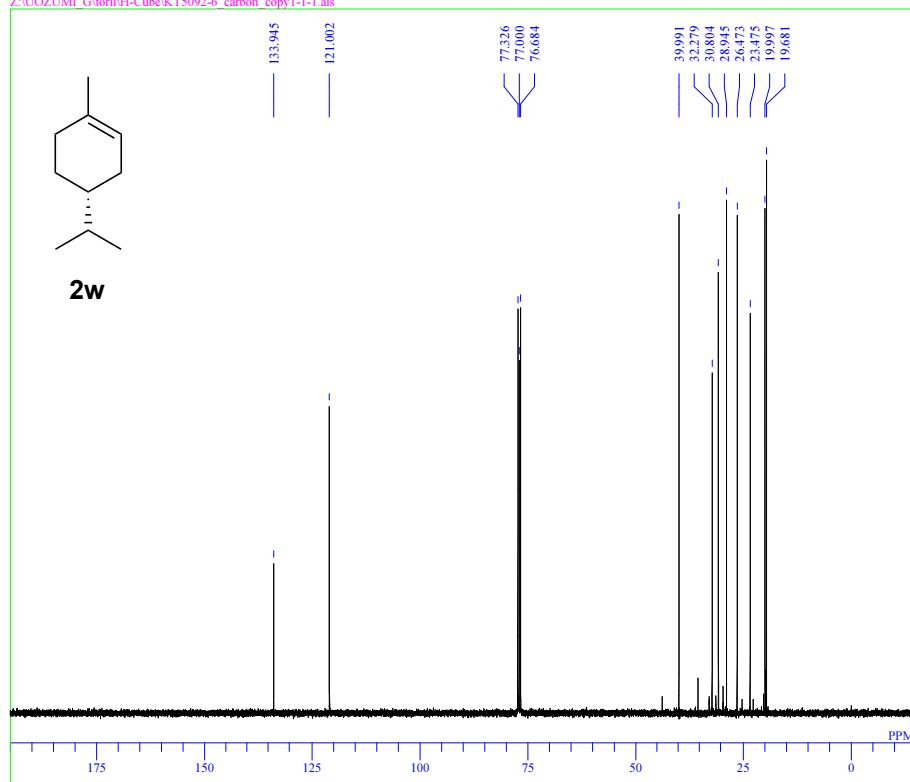
Z:\UOZUMI GitoriiH-Cube\KT5092-6 proton-2-1.als



DFILE KT5092-6 proton-2-1.als
 COMNT single_pulse
 DATIM 2014-07-09 13:12:13
 OBNUC ^1H
 EXMOD proton.jpg
 OBFREQ 395.88 MHz
 OBSETE 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 20.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.40 Hz
 RGAIN 24

single pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5092-6 carbon_copy1-1-1.als

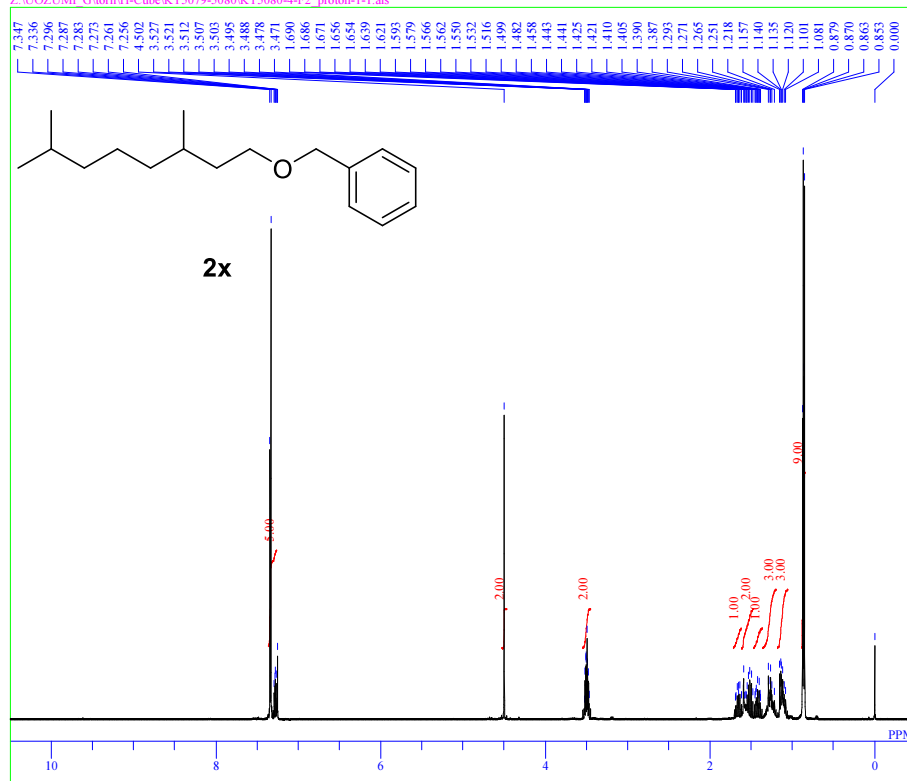


DFILE KT5092-6 carbon_copy1-1-1.als
 COMNT single pulse decoupled gated NOE
 DATIM 2014-07-09 13:13:39
 OBNUC ^{13}C
 EXMOD carbon.jpg
 OBFREQ 99.55 MHz
 OBSETE 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 631
 ACQTM 0.0000 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC ^1H
 CTEMP 20.0 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.40 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of [[(3,7-dimethylcylo)oxy]methyl]benzene (**2x**).

single_pulse

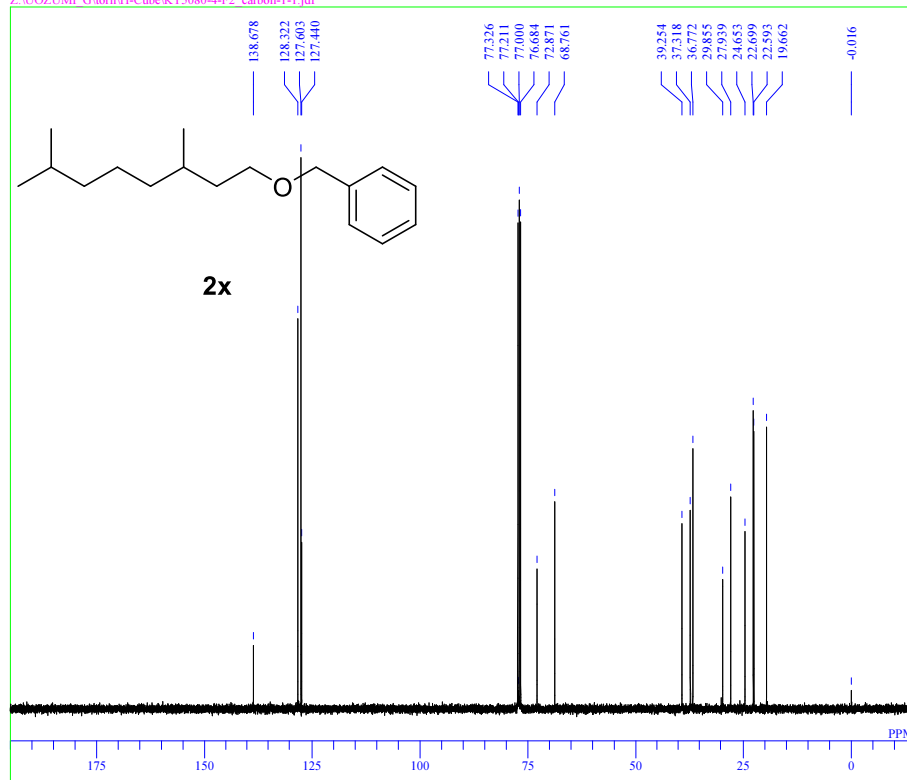
Z:\UOZUMI_GitoriiH-Cube\KT5079-5080\KT5080-4-F2_proton-1-1.als



DFILE KT5080-4-F2_proton-1-1.als
 COMNT single_pulse
 DATIM 2014-06-19 11:46:55
 OBNUC 1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 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 19.3 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 28

single pulse decoupled gated NOE

Z:\UOZUMI_GitoriiH-Cube\KT5080-4-F2_carbon-1-1.jdf

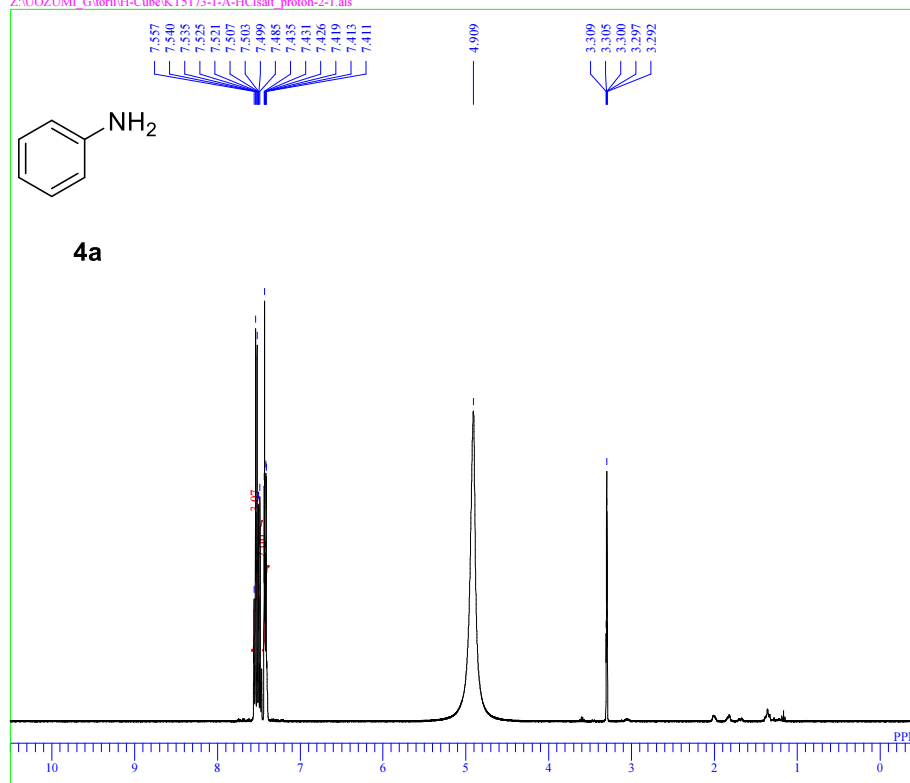


DFILE KT5080-4-F2_carbon-1-1.jdf
 COMNT single pulse decoupled gated NOE
 DATIM 2014-06-19 12:58:45
 OBNUC 13C
 EXMOD carbon.jxp
 OBFREQ 99.55 MHz
 OBSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 578
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.6 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.40 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of aniline hydrochloride (**4a**).

single_pulse

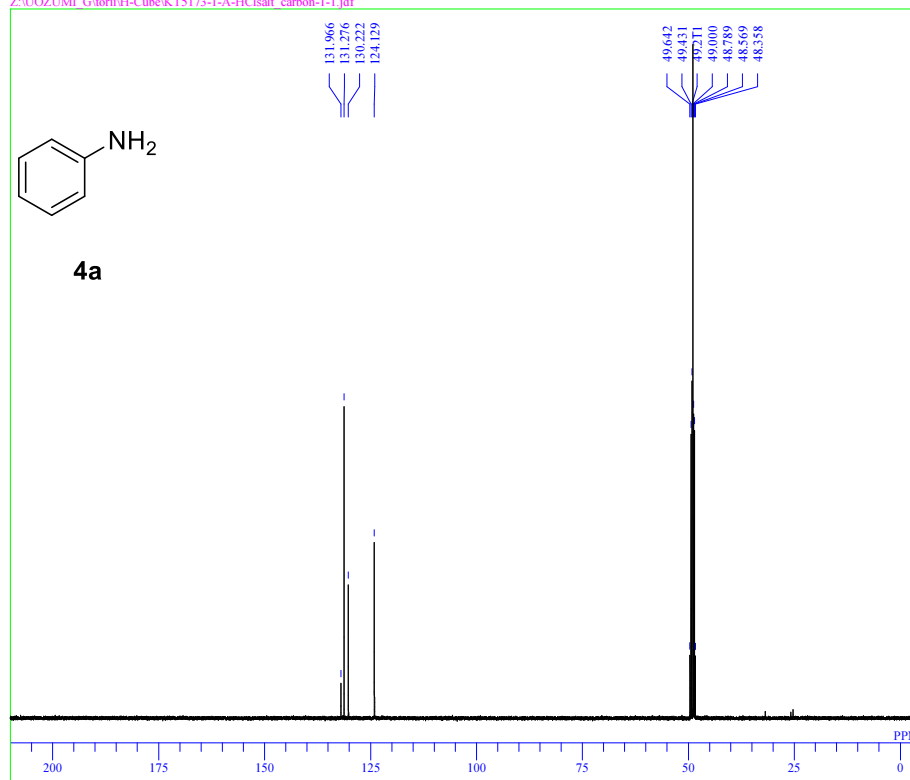
Z:\UOZUMI_GitoriiH-Cube\KT5173-1-A-HClSalt_proton-2-1.als



DFILE KT5173-1-A-HClSalt_proton-2-1.als
COMNT single_pulse
DATIM 2015-02-16 09:58:21
OBNUC ^1H
EXMOD proton.jsp
OBFREQ 395.88 MHz
OBSETE 6.28 KHz
OBFIN 0.87 Hz
POINT 16384
FREQU 7422.80 Hz
SCANS 8
ACQTM 2.2073 sec
PD 5.0000 sec
PW1 3.12 usec
IRNUC ^1H
CTEMP 19.0 c
SLVNT CD3OD
EXREF 3.30 ppm
BF 0.00 Hz
RGAIN 30

single pulse decoupled gated NOE

Z:\UOZUMI_GitoriiH-Cube\KT5173-1-A-HClSalt_carbon-1-1.jdf

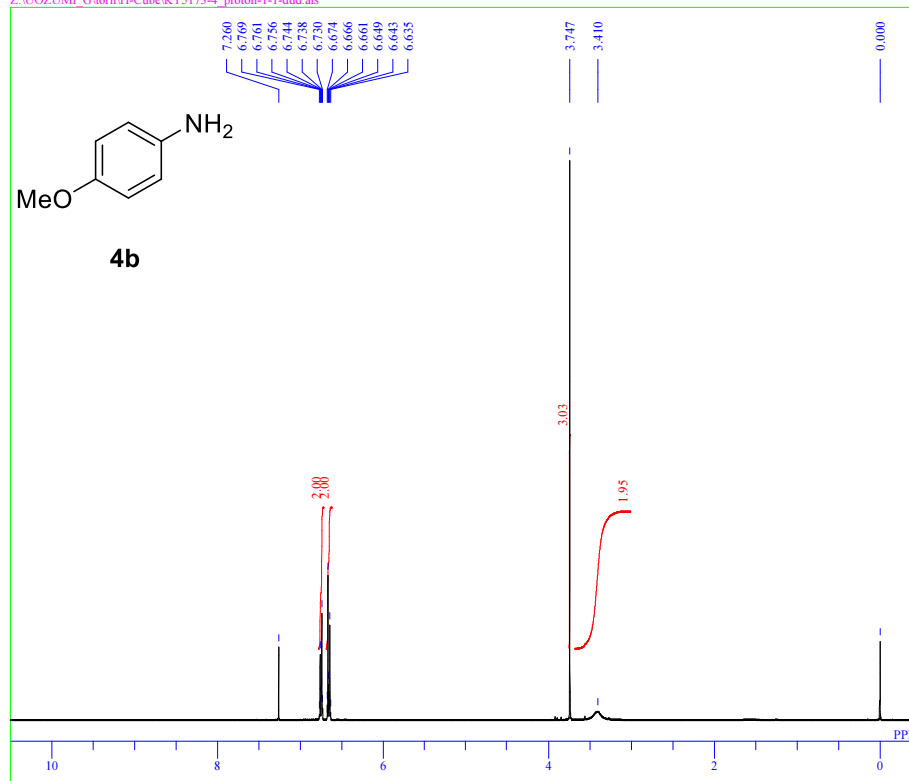


DFILE KT5173-1-A-HClSalt_carbon-1-1.jdf
COMNT single pulse decoupled gated NOE
DATIM 2015-02-16 10:00:35
OBNUC ^{13}C
EXMOD carbon.jsp
OBFREQ 99.55 MHz
OBSETE 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 1024
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC ^1H
CTEMP 19.8 c
SLVNT CD3OD
EXREF 49.00 ppm
BF 0.40 Hz
RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of *p*-anisidine (**4b**).

single_pulse

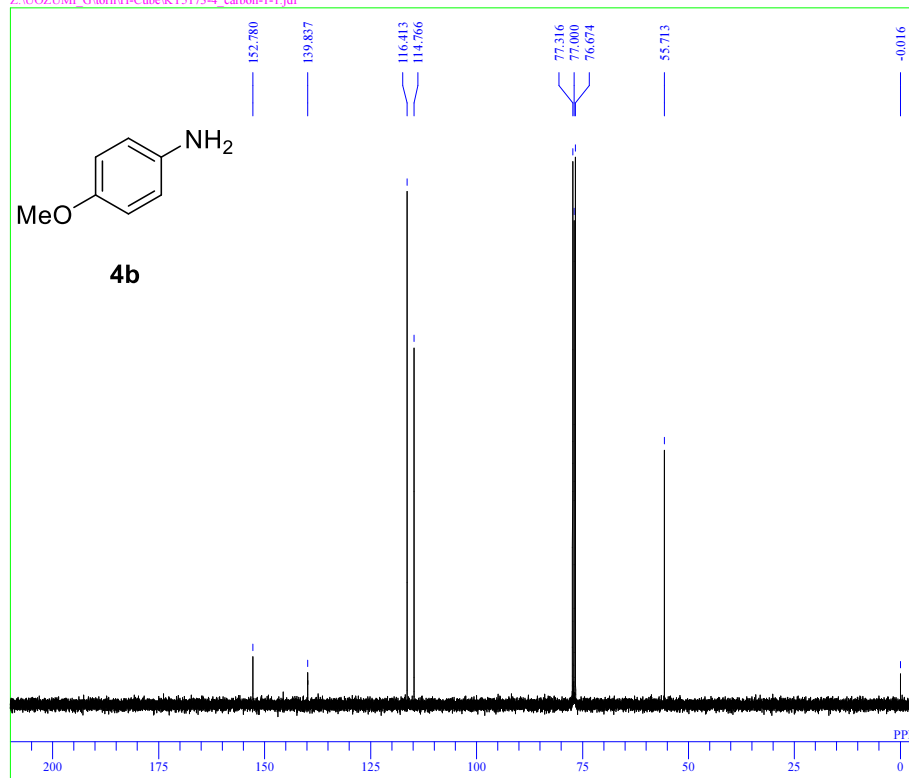
Z:\UOZUMI GitoriiH-Cube\KT5173-4 proton-1-1-ddd.als



DFILE KT5173-4 proton-1-1-ddd.als
COMNT single_pulse
DATIM 2015-02-10 14:28:59
OBNUC ^1H
EXMOD proton.jxp
OBFRQ 395.88 MHz
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 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.00 Hz
RGAIN 38

single_pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5173-4 carbon-1-1.jdf

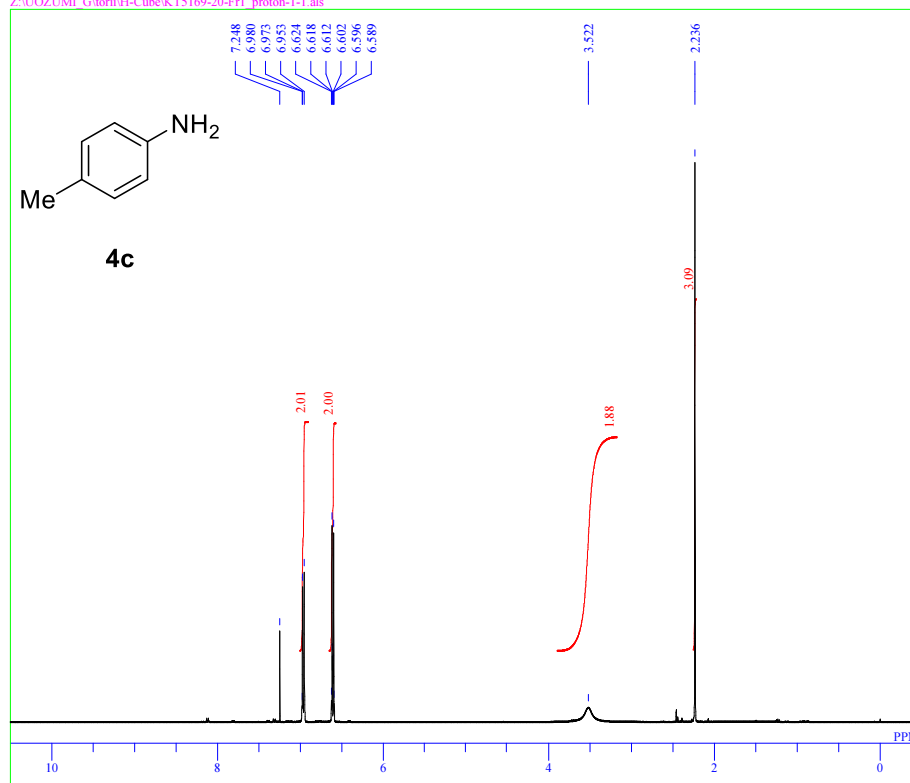


DFILE KT5173-4_carbon-1-1.jdf
COMNT single_pulse decoupled gated NOE
DATIM 2015-02-10 14:30:25
OBNUC ^{13}C
EXMOD carbon.jxp
OBFRQ 99.55 MHz
OBSET 5.13 KHz
OBFIN 0.98 Hz
POINT 32767
FREQU 31250.00 Hz
SCANS 1024
ACQTM 1.0486 sec
PD 2.0000 sec
PW1 3.42 usec
IRNUC ^1H
CTEMP 19.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.10 Hz
RGAIN 60

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

single_pulse

Z:\UOZUMI GitoriiH-Cube\KT5169-20-Fr1_proton-1-1.als

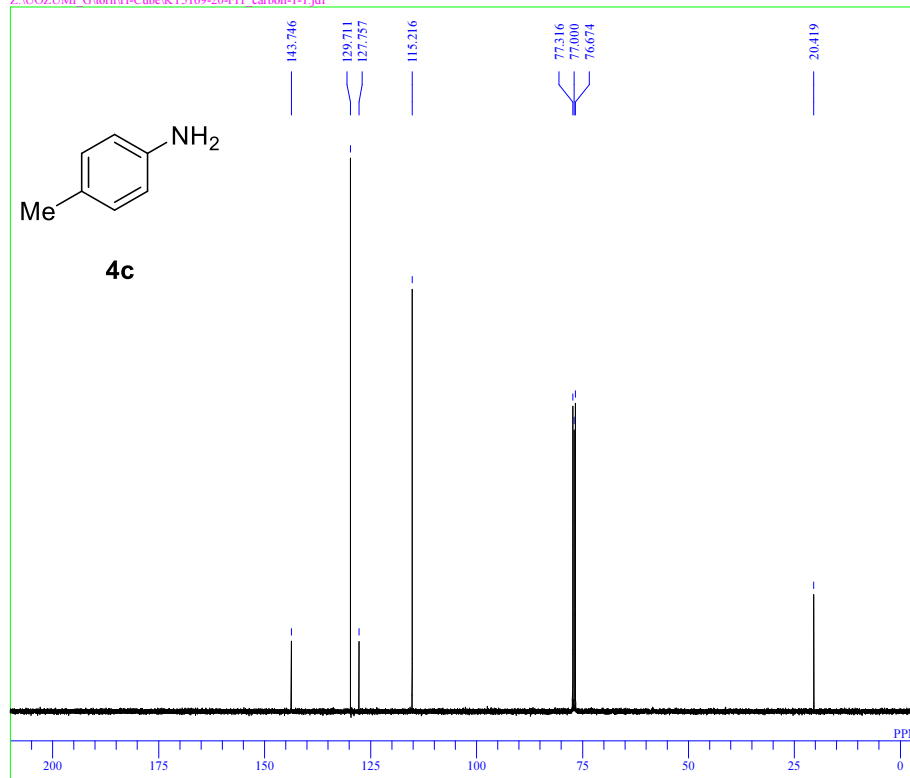


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DFILE  KT5169-20-Fr1_proton-1-1.als
COMNT  single_pulse
DATIM  2015-02-05 11:11:45
OBNUC  1H
EXMOD  proton.jsp
OBFRQ  395.88 MHz
OBSET  6.28 KHz
OBFIN  0.87 Hz
POINT  16384
FREQU  7422.80 Hz
SCANS  8
ACQTM  2.2073 sec
PD      5.0000 sec
PW1     3.12 usec
IRNUC  1H
CTEMP  20.0 c
SLVNT  CDCL3
EXREF  0.00 ppm
BF      0.00 Hz
RGAIN  34
    
```

single pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5169-20-Fr1_carbon-1-1.jdf



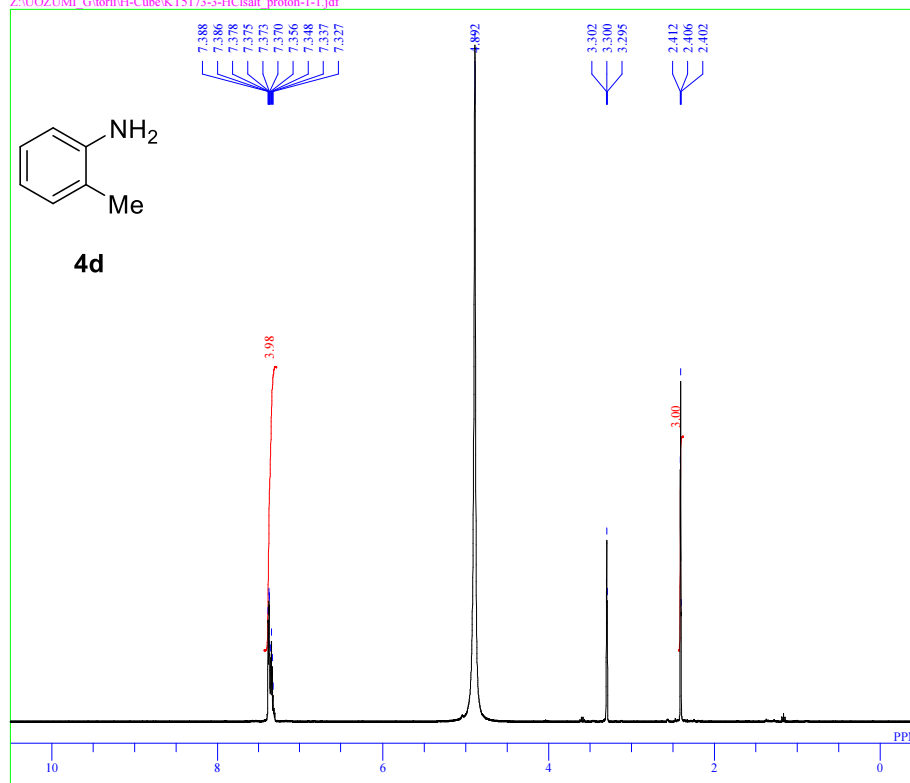
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DFILE  KT5169-20-Fr1_carbon-1-1.jdf
COMNT  single pulse decoupled gated NOE
DATIM  2015-02-05 11:13:11
OBNUC  13C
EXMOD  carbon.jsp
OBFRQ  99.55 MHz
OBSET  5.13 KHz
OBFIN  0.98 Hz
POINT  32767
FREQU  31250.00 Hz
SCANS  1008
ACQTM  1.0486 sec
PD      2.0000 sec
PW1     3.42 usec
IRNUC  1H
CTEMP  19.5 c
SLVNT  CDCL3
EXREF  77.00 ppm
BF      0.20 Hz
RGAIN  60
    
```

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of *o*-toluidine hydrochloride (**4d**).

single_pulse

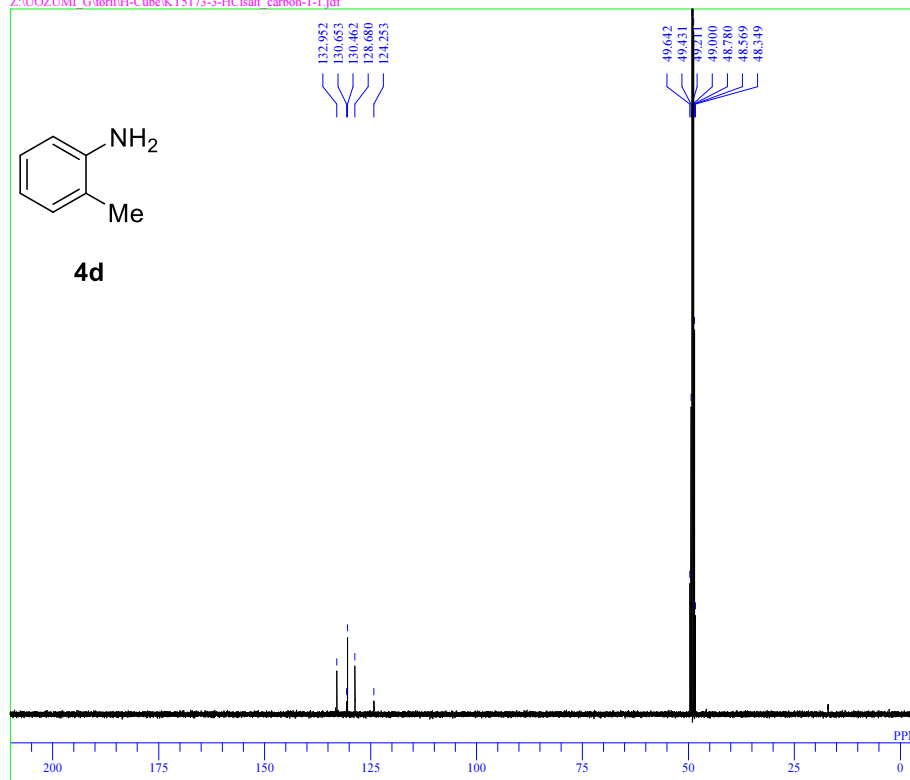
Z:\UOZUMI_GitoriiH-Cube\KT5173-3-HClSalt_proton-1-1.jdf



DFILE KT5173-3-HClSalt_proton-1-1.jdf
 COMNT single_pulse
 DATIM 2015-02-16 11:11:49
 OBNUC ^1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 OBSSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 16384
 FREQU 7422.80 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC ^1H
 CTEMP 18.8 c
 SLVNT CD3OD
 EXREF 3.30 ppm
 BF 0.00 Hz
 RGAIN 32

single pulse decoupled gated NOE

Z:\UOZUMI_GitoriiH-Cube\KT5173-3-HClSalt_carbon-1-1.jdf

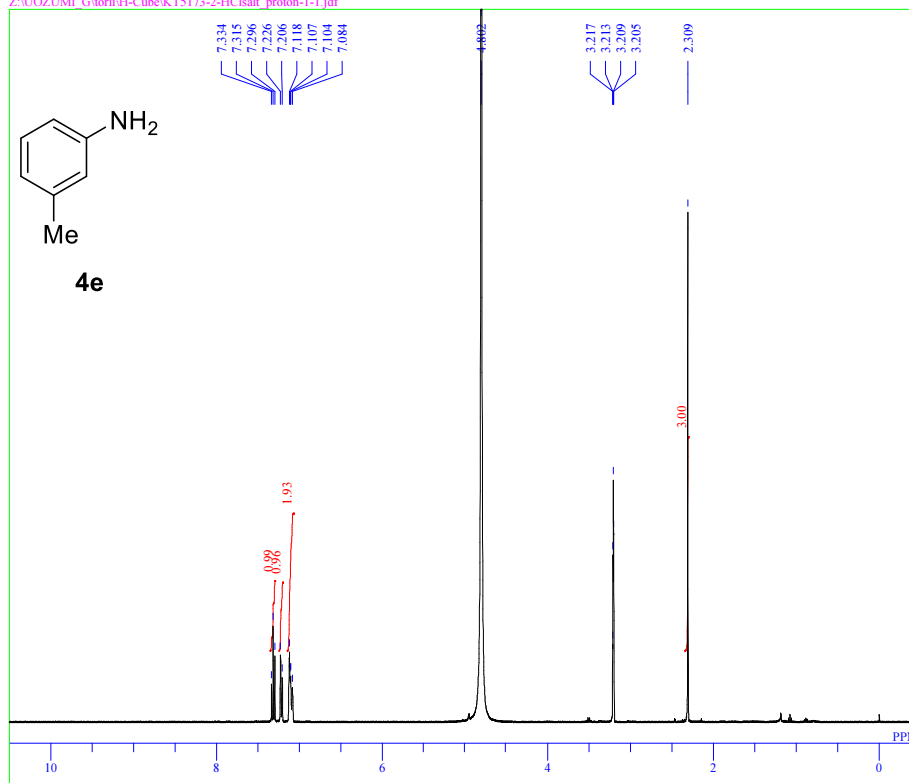


DFILE KT5173-3-HClSalt_carbon-1-1.jdf
 COMNT single pulse decoupled gated NOE
 DATIM 2015-02-16 11:13:20
 OBNUC ^{13}C
 EXMOD carbon.jxp
 OBFREQ 99.55 MHz
 OBSSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 1024
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC ^1H
 CTEMP 19.7 c
 SLVNT CD3OD
 EXREF 49.00 ppm
 BF 0.00 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of *m*-toluidine hydrochloride (**4e**).

single_pulse

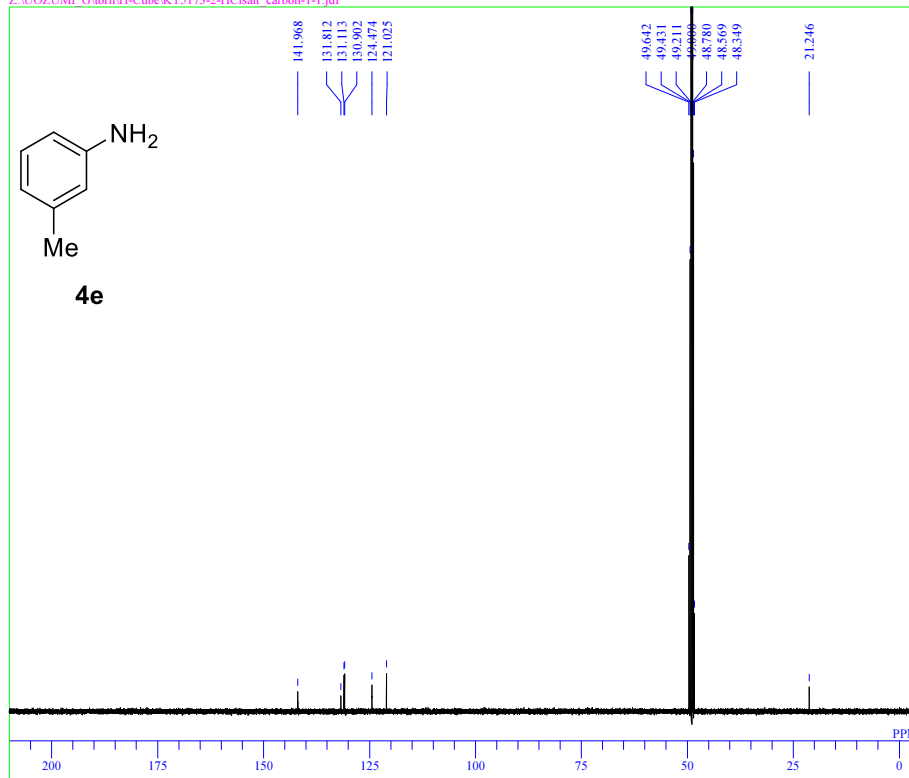
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DFILE KT5173-2-HClSalt_proton-1-1.jdf
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 DATIM 2015-02-16 12:10:30
 OBNUC 1H
 EXMOD proton.jxp
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 OBSETE 6.28 KHz
 OBFIN 0.87 Hz
 POINT 16384
 FREQU 7422.80 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.4 c
 SLVNT CD3OD
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 32

single pulse decoupled gated NOE

Z:\UOZUMI GitoriiH-Cube\KT5173-2-HClSalt_carbon-1-1.jdf

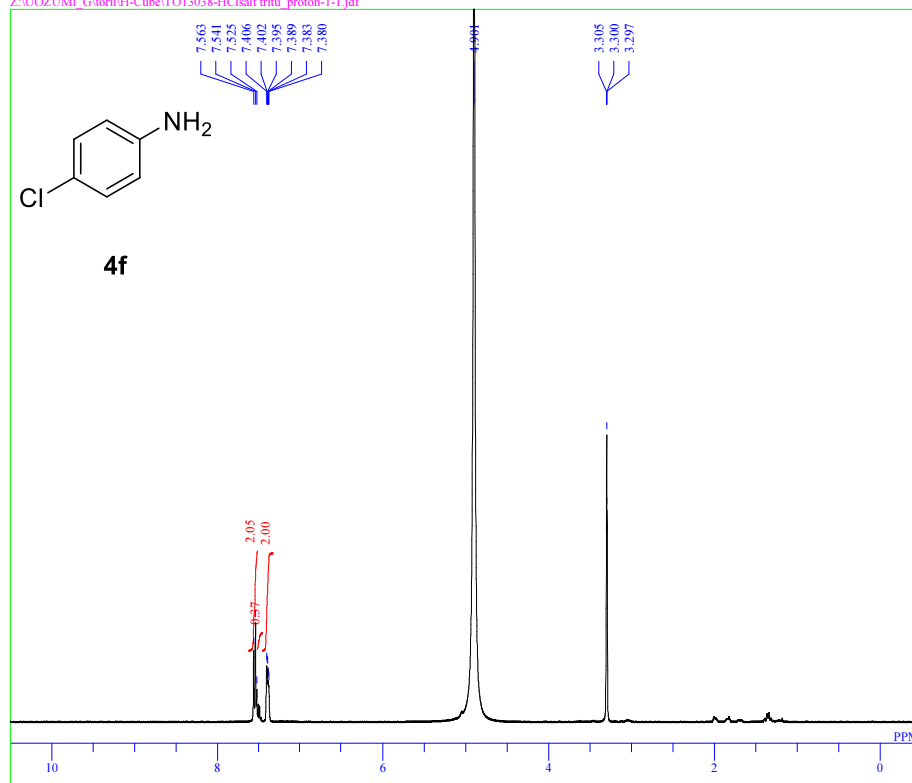


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 EXMOD carbon.jxp
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 OBSETE 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 1024
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.7 c
 SLVNT CD3OD
 EXREF 49.00 ppm
 BF 0.00 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 4-chloroaniline hydrochloride (**4f**).

single_pulse

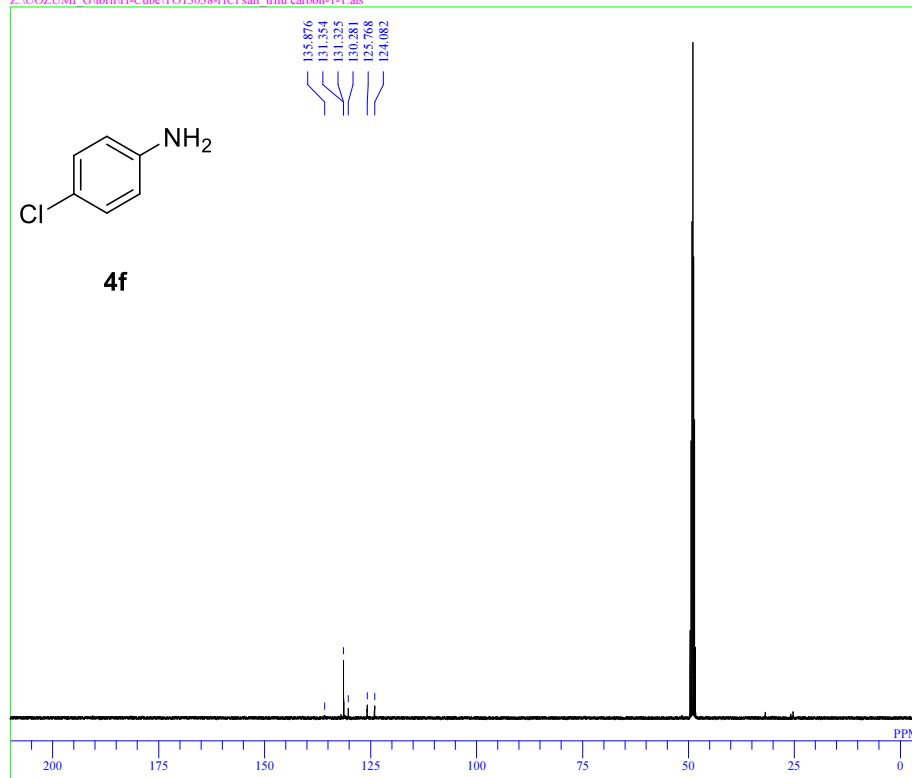
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DFILE TO13038-HCl salt tritu_proton-1-1.jdf
 COMNT single_pulse
 DATIM 2015-02-17 14:03:58
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 EXMOD proton.jxp
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 OBSETE 6.28 KHz
 OBFIN 0.87 Hz
 POINT 16384
 FREQU 7422.80 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC ^1H
 CTEMP 18.9 c
 SLVNT CD3OD
 EXREF 3.30 ppm
 BF 0.80 Hz
 RGAIN 36

single pulse decoupled gated NOE

Z:\UOZUMI_GitoriiH-Cube\TO13038-HCl salt tritu carbon-1-1.als

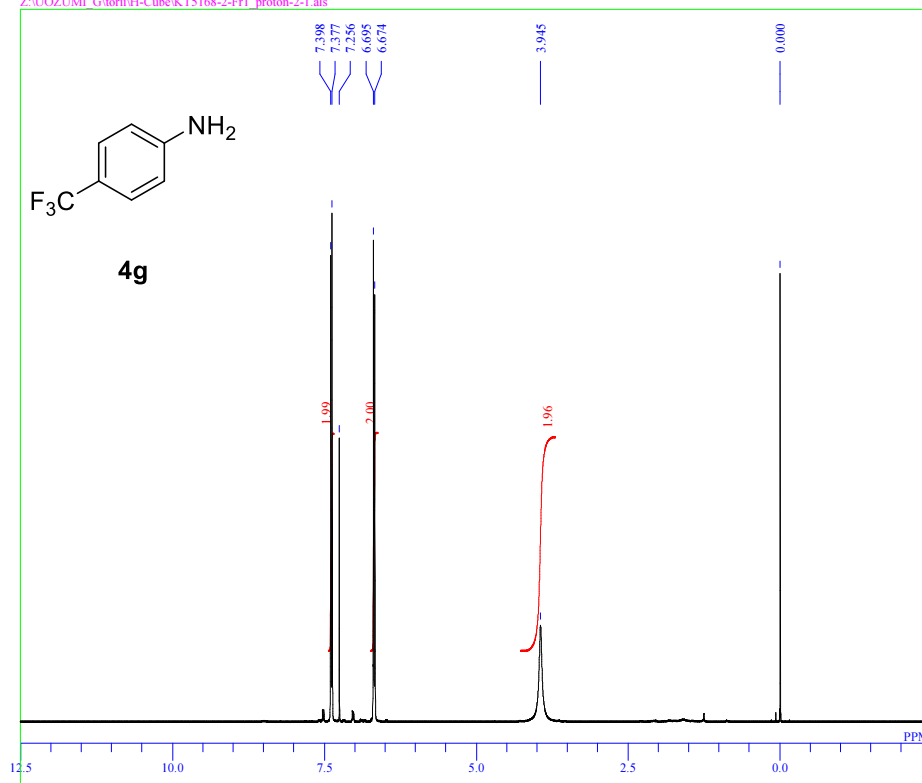


DFILE TO13038-HCl salt tritu carbon-1-1.als
 COMNT single pulse decoupled gated NOE
 DATIM 2015-02-23 13:05:36
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 EXMOD carbon.jxp
 OBFREQ 99.55 MHz
 OBSETE 5.13 KHz
 OBFIN 0.98 Hz
 POINT 26214
 FREQU 25000.00 Hz
 SCANS 2048
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC ^1H
 CTEMP 18.8 c
 SLVNT CD3OD
 EXREF 49.00 ppm
 BF 0.80 Hz
 RGAIN 60

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of 4-(trifluoromethyl)aniline (**4g**).

single_pulse

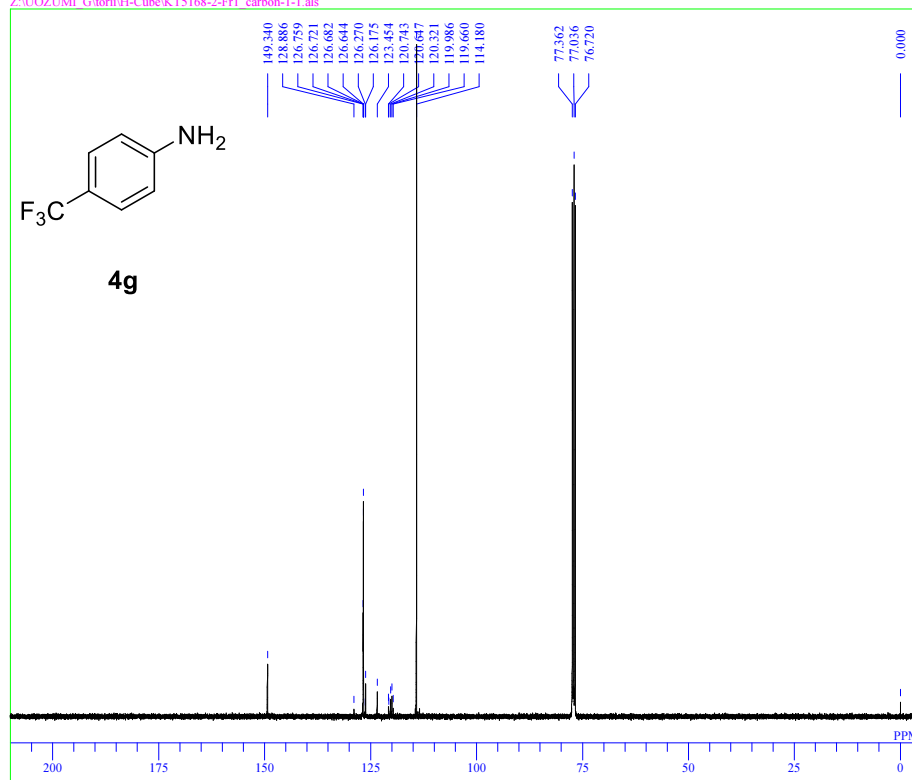
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 EXMOD proton.jsp
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 OBSSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC ^1H
 CTEMP 19.6 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 36

single pulse decoupled gated NOE

Z:\UOZUMI_Gitorii\H-Cube\KT5168-2-Fr1_carbon-1-1.als

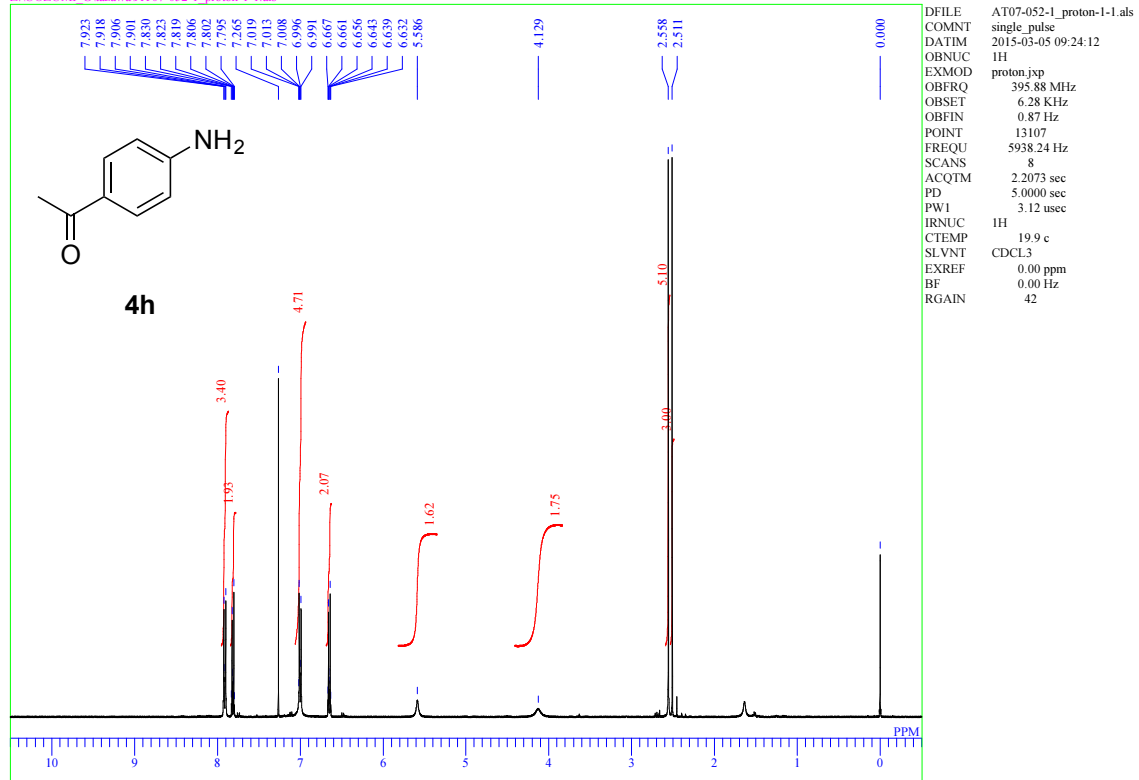


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 OBFIN 0.98 Hz
 POINT 26214
 FREQU 25000.00 Hz
 SCANS 11854
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC ^1H
 CTEMP 19.1 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 60

¹H NMR spectra of 4-aminoacetophenone (4h).

single_pulse

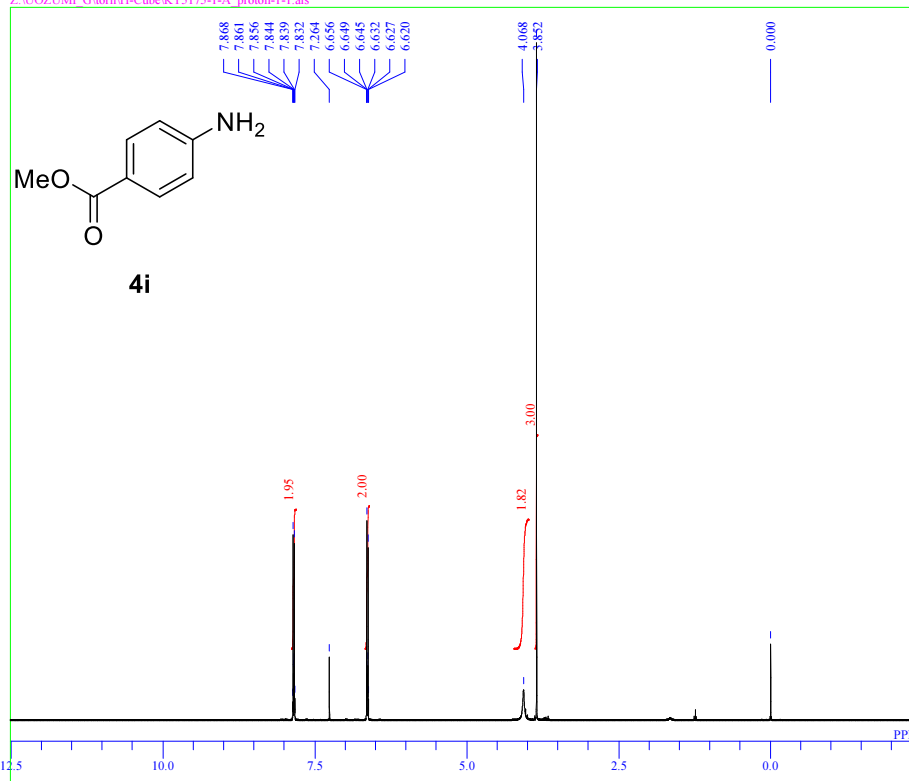
Z:\UOZUMI Gitazawa\AT07-052-1_proton-1-1.als



^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of methyl 4-aminobenzoate (**4i**).

single_pulse

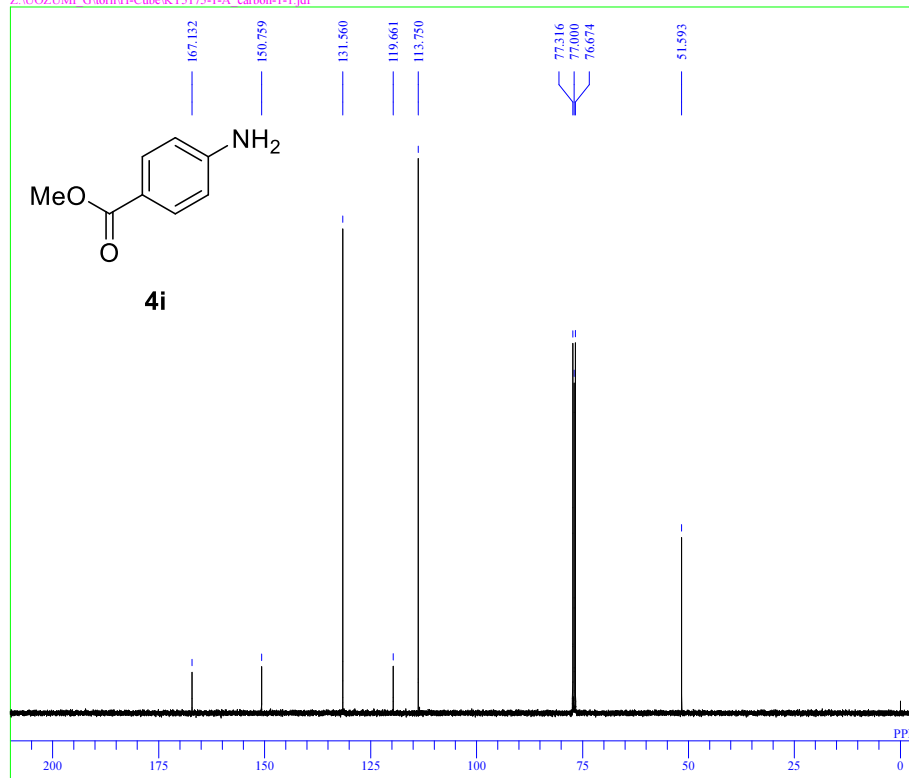
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DFILE KT5175-1-A_proton-1-1.als
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 OBNUC 1H
 EXMOD proton.jxp
 OBFREQ 395.88 MHz
 OBSSET 6.28 KHz
 OBFIN 0.87 Hz
 POINT 13107
 FREQU 5938.24 Hz
 SCANS 8
 ACQTM 2.2073 sec
 PD 5.0000 sec
 PW1 3.12 usec
 IRNUC 1H
 CTEMP 19.7 c
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 0.00 Hz
 RGAIN 34

single pulse decoupled gated NOE

Z:\UOZUMI_GitoriiH-Cube\KT5175-1-A_carbon-1-1.jdf



DFILE KT5175-1-A_carbon-1-1.jdf
 COMNT single pulse decoupled gated NOE
 DATIM 2015-02-13 15:29:42
 OBNUC 13C
 EXMOD carbon.jxp
 OBFREQ 99.55 MHz
 OBSSET 5.13 KHz
 OBFIN 0.98 Hz
 POINT 32767
 FREQU 31250.00 Hz
 SCANS 1024
 ACQTM 1.0486 sec
 PD 2.0000 sec
 PW1 3.42 usec
 IRNUC 1H
 CTEMP 19.7 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 0.30 Hz
 RGAIN 60