Electronic supplementary information for

A new protocol for nickel-catalyzed regio- and stereoselective hydrocyanation of allene and its derivatives

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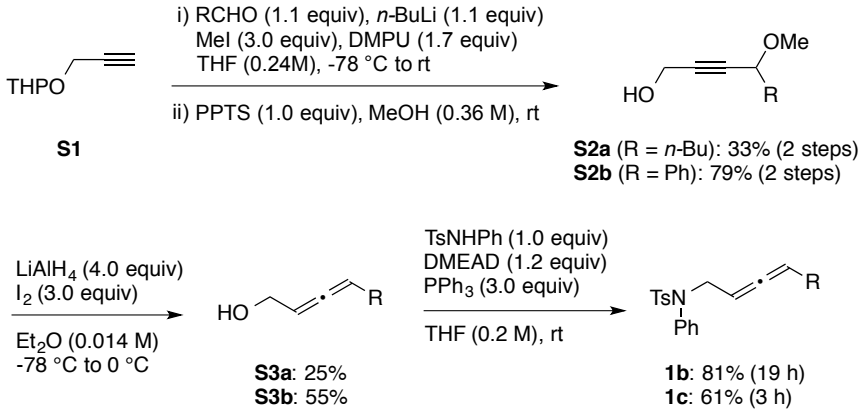
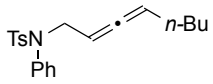
Scheme S1. Syntheses of 1b and 1c



S3a, S3b were synthesized by the reported procedure[1].

4-methyl-*N*-(octa-2,3-dien-1-yl)-*N*-phenylbenzenesulfonamide (1b)

To a solution of TsNHPh (216 mg, 0.87 mmol) in THF (3.0 mL) was added PPh_3 (274 mg, 1.04 mmol) and the mixture was cooled to 0 °C. Then DMEAD (azodicarboxylic acid bis(2-methoxyethyl) ester, 245 mg, 0.87 mmol) and a solution of **S3a** in THF (1.4 mL) was slowly added and the reaction was warmed to room temperature. After stirring 19 h, the solvent was removed under reduced pressure and the residue was filtrated through a short pad of silica and concentrated in vacuo. The crude product was purified by column chromatography (Hex/AcOEt = 15/1) to afford **1b** as a colorless solid (250 mg, 81%).

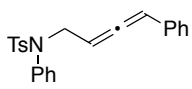


Colorless solid. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 0.81 (t, 3H, J = 7.2 Hz), 1.08-1.23 (m, 4H), 1.70-1.76 (m, 2H), 2.42 (s, 3H), 4.06 (ddd, 1H, J = 13.8, 7.2, 2.4 Hz), 4.25 (ddd, 1H, J = 13.8, 6.6, 3.0 Hz), 4.99-5.05 (m, 2H), 7.04-7.06 (m, 2H), 7.24-7.31 (m, 5H), 7.49 (d, 2H, J = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 13.8, 21.5, 22.0, 27.9, 30.9, 50.6, 86.8, 92.5, 127.67, 127.70, 128.7, 129.0, 129.4, 135.6, 139.0, 143.3, 205.5; IR (ATR) ν: 3058, 2952, 2922, 2850, 1964, 1340, 1157 cm^{-1}; HRMS (ESI) m/z calcd for $C_{21}H_{25}NNaO_2S$ $[M+Na]^+$ 378.1504, found 378.1510; mp. 66-67 °C.

4-methyl-*N*-phenyl-*N*-(4-phenylbuta-2,3-dien-1-yl)benzenesulfonamide (1c)

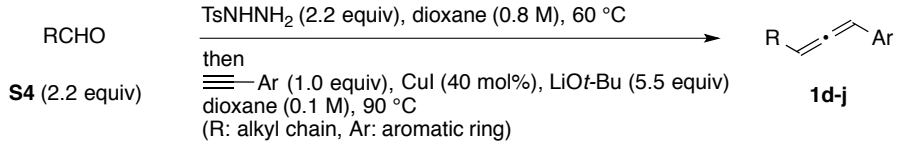
To a solution of TsNHPh (694 mg, 2.8 mmol) in THF (12 mL) was added PPh_3 (881 mg, 3.4 mmol) and the mixture was cooled to 0 °C. Then DMEAD (azodicarboxylic acid bis(2-methoxyethyl) ester, 787 mg, 3.4 mmol) and a solution of **S3b** in THF (2 mL) was slowly added and the reaction was warmed to room temperature. After stirring 3 h, the solvent was removed under reduced pressure and the residue was filtrated through a pad column and concentrated in vacuo. The crude solid was dissolved in small amount of CH_2Cl_2, and then hexane was added to the solution. The precipitation was filtrated

and dried under reduced pressure to afford **1c** as a colorless solid (664 mg, 61%).

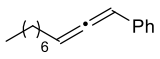


Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 2.41 (s, 3H), 4.13 (ddd, 1H, J = 14.4, 7.6, 2.0 Hz), 4.46 (ddd, 1H, J = 14.4, 6.0, 2.8 Hz), 5.52 (ddd, 1H, J = 7.6, 7.2, 6.0 Hz), 6.04 (ddd, 1H, J = 7.2, 2.8, 2.0 Hz), 6.82-6.85 (m, 2H), 7.07-7.09 (m, 2H), 7.12-7.16 (m, 3H), 7.24 (d, 2H, J = 8.0 Hz), 7.29-7.32 (m, 3H), 7.50 (d, 2H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 21.5, 50.3, 91.2, 96.0, 126.8, 127.1, 127.7, 127.9, 128.4, 129.0, 129.1, 129.4, 133.2, 135.3, 138.9, 143.5, 206.5; IR (ATR) ν: 3031, 1951, 1343, 1213 cm^{-1}; HRMS (ESI) m/z calcd for $C_{23}H_{21}NNaO_2S$ $[M+Na]^+$ 398.1191, found 398.1200; mp. 94-96 °C.

Scheme S2. Syntheses of 1d-j[2]

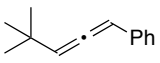


deca-1,2-dien-1-ylbenzene (1d)



Colorless oil. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 0.87 (t, 3H, J = 7.2 Hz), 1.24-1.31 (m, 6H), 1.33-1.38 (m, 2H), 1.45-1.51 (m, 2H), 2.12 (ddt, 2H, J = 6.6, 6.6, 3.6 Hz), 5.56 (dt, 1H, J = 6.6, 6.6 Hz), 6.12 (dt, 1H, J = 6.6, 3.6 Hz), 7.16-7.20 (m, 1H), 7.29-7.31 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.1, 22.6, 28.8, 29.1, 29.2, 29.2, 31.8, 94.5, 95.1, 126.55, 126.57, 128.5, 135.2, 205.1; IR (ATR) ν: 2954, 2924, 2853, 1949 cm^{-1}; HRMS (APPI) m/z calcd for $C_{26}H_{22}$ $[M]^+$ 214.1716, found 214.1712. (49%, 127 mg)

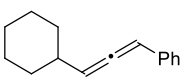
(4,4-dimethylpenta-1,2-dien-1-yl)benzene (1e)



(CAS-Reg# 69248-81-3) Spectral data were identical to the literature data.[2]

^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.13 (s, 9H), 5.57 (d, 1H, J = 6.4 Hz), 6.18 (d, 1H, J = 6.4 Hz), 7.16-7.21 (m, 1H), 7.29-7.32 (m, 4H). (88%, 181 mg)

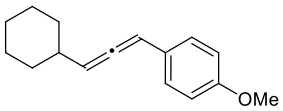
(3-cyclohexylpropa-1,2-dien-1-yl)benzene (1f)



(CAS-Reg# 67647-93-2) Spectral data were identical to the literature data.[2]

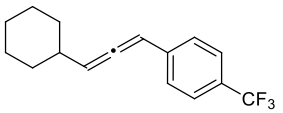
^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.15-1.33 (m, 5H), 1.61-1.65 (m, 1H), 1.71-1.76 (m, 2H), 1.82-1.86 (m, 2H), 2.10-2.14 (m, 1H), 5.56 (dd, 1H, J = 6.4 Hz), 6.15 (dd, 1H, J = 6.4, 3.2 Hz), 7.15-7.19 (m, 1H), 7.29-7.31 (m, 4H). (28%, 96 mg)

1-(3-cyclohexylpropa-1,2-dien-1-yl)-4-methoxybenzene (1g)



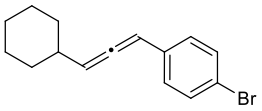
Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.11-1.35 (m, 5H), 1.61-1.67 (m, 1H), 1.70-1.76 (m, 2H), 1.81-1.86 (m, 2H), 2.06-2.15 (m, 1H), 3.80 (s, 3H), 5.54 (dd, 1H, J = 6.4, 6.4 Hz), 6.12 (dd, 1H, J = 6.4, 2.4 Hz), 6.85 (d, 2H, J = 9.2 Hz), 7.22 (d, 2H, J = 9.2 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 26.00, 26.02, 26.1, 33.1, 33.2, 37.7, 55.2, 94.7, 101.0, 114.0, 127.4, 127.5, 158.8, 203.3; IR (ATR) ν: 2923, 2850, 1244 cm^{-1}; HRMS (APPI) m/z calcd for $C_{16}H_{20}O$ $[M]^+$ 228.1509, found 228.1502. (41%, 112 mg)

1-(3-cyclohexylpropa-1,2-dien-1-yl)-4-(trifluoromethyl)benzene (1h)



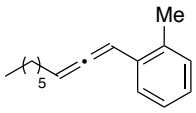
Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.14-1.26 (m, 3H), 1.27-1.34 (m, 2H), 1.64-1.66 (m, 1H), 1.71-1.76 (m, 2H), 1.83-1.85 (m, 2H), 2.12-2.18 (m, 1H), 5.63 (dd, 1H, J = 6.6, 6.6 Hz), 6.18 (dd, 1H, J = 6.6, 3.0 Hz), 7.37 (d, 2H, J = 8.4 Hz), 7.53 (m, 2H, J = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 25.99, 26.01, 26.04, 33.07, 33.15, 37.5, 94.7, 101.6, 124.3, (q, J = 270 Hz), 125.5 (q, J = 2.7 Hz), 126.5, 128.4 (q, J = 31.7 Hz), 139.2, 205.1; IR (ATR) ν: 2925, 2852, 1947, 1321 cm^{-1}; HRMS (APPI) m/z calcd for $C_{16}H_{17}F_3$ $[M]^+$ 266.1277, found 266.1277;. (69%, 221 mg)

1-bromo-4-(3-cyclohexylpropa-1,2-dien-1-yl)benzene (1i)



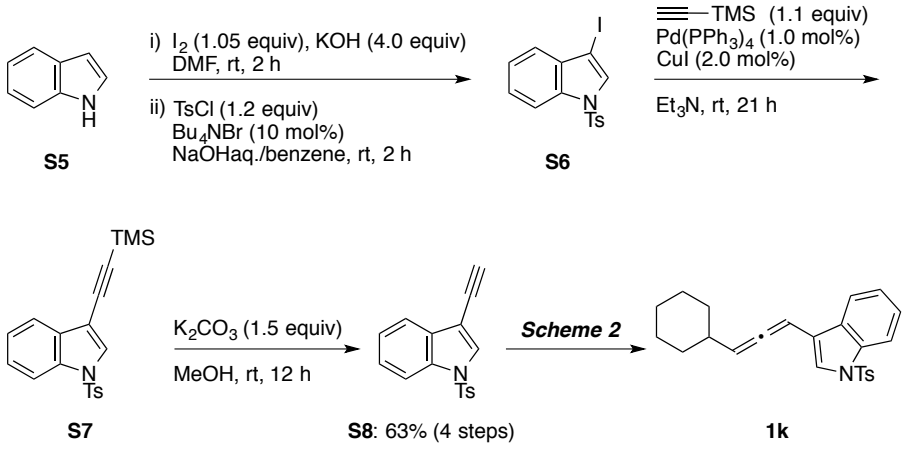
Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.11-1.36 (m, 5H), 1.63-1.66 (m, 1H), 1.71-1.76 (m, 2H), 1.81-1.84 (m, 2H), 2.08-2.17 (m, 1H), 5.26 (dd, 1H, J = 6.4, 6.4 Hz), 6.09 (dd, 1H, J = 6.4, 2.8 Hz), 7.15 (dt, 1H, J = 8.4, 2.0 Hz), 7.40 (dt, 1H, J = 8.4, 2.0 Hz) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 25.96, 25.98, 26.0, 33.05, 33.11, 37.5, 94.6, 101.5, 120.1, 127.9, 131.6, 134.3, 204.2; IR (ATR) ν: 2922, 2849, 1946, 1487, 829 cm^{-1}; HRMS (APPI) m/z calcd for $C_{15}H_{17}Br$ $[M]^+$ 276.0508, found 276.0499. (40%, 135 mg)

1-methyl-2-(nona-1,2-dien-1-yl)benzene (1j)

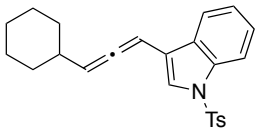


Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.88 (t, 3H, J = 6.8 Hz), 1.27-1.39 (m, 6H), 1.44-1.50 (m, 2H), 2.12 (ddt, 2H, J = 6.8, 6.8, 3.2 Hz), 2.36 (s, 3H), 5.52 (dt, 1H, J = 6.8, 6.8 Hz), 6.30 (dt, 1H, J = 6.8, 3.2 Hz), 7.06-7.16 (m, 3H), 7.37 (d, 1H, J = 7.6 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.1, 19.8, 22.6, 28.8, 28.9, 29.2, 31.7, 91.7, 94.2, 126.0, 126.5, 127.0, 130.4, 133.2, 134.7, 205.8; IR (ATR) ν: 2955, 2924, 2854, 1946 cm^{-1}; HRMS (APPI) m/z calcd for $C_{16}H_{23}$ $[M+H]^+$ 215.1794, found 215.1791. (39%, 100 mg)

Scheme S3. Synthesis of 1k[3]

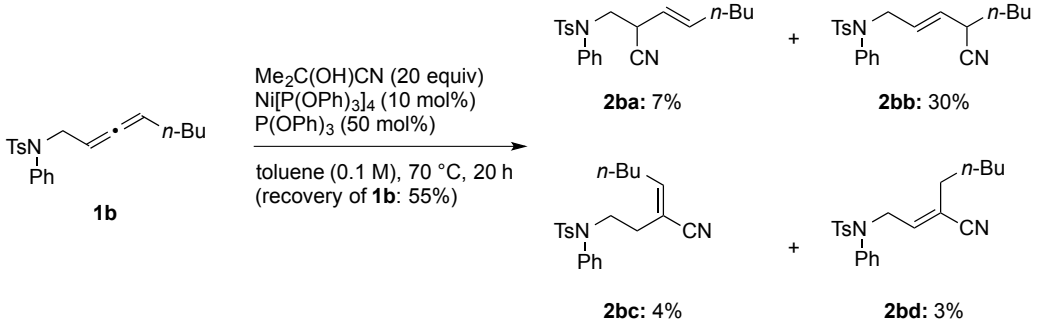


3-(3-cyclohexylpropa-1,2-dien-1-yl)-1-tosyl-1*H*-indole (1k)



Yellow amorphous. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.16-1.28 (m, 5H), 1.62-1.65 (m, 1H), 1.71-1.76 (m, 2H), 1.81-1.89 (m, 2H), 2.11-2.18 (m, 1H), 2.34 (s, 3H), 5.57 (dd, 1H, J = 6.0, 6.0 Hz), 6.32 (dd, 1H, J = 6.0, 3.2 Hz), 7.20-7.24 (m, 3H), 7.32 (dd, 1H, J = 8.0 Hz), 7.46 (s, 1H), 7.76 (d, 2H, J = 8.4 Hz), 7.89 (d, 1H, J = 8.0 Hz), 7.97 (d, 1H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.6, 26.0, 26.0, 26.1, 32.77, 32.83, 37.7, 86.3, 100.3, 113.6, 116.7, 120.8, 123.1, 123.3, 124.9, 126.8, 129.3, 129.9, 135.1, 135.6, 144.9, 205.2; IR (ATR) ν: 2923, 2850, 1957, 1371, 1172 cm^{-1}; HRMS (ESI) m/z calcd for $C_{24}H_{26}NO_2S$ $[M+H]^+$ 392.1684, found 392.1696. (69%, 150 mg)

Scheme S4. Hydrocyanation of 1b



(*E*)-*N*-(2-cyanooct-3-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (2ba)

(*E*)-*N*-(4-cyanooct-2-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (2bb)

(*E*)-*N*-(3-cyanooct-3-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (2bc)

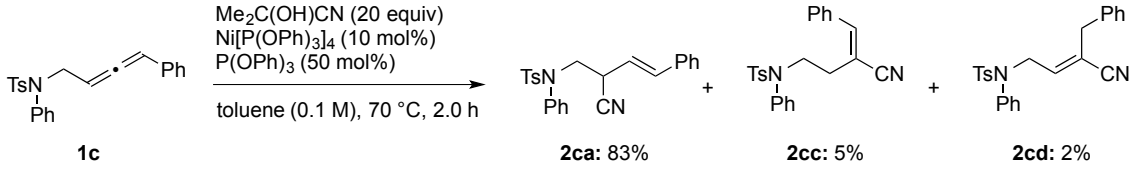
(*E*)-*N*-(3-cyanooct-2-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (2bd)

Above products were obtained as an inseparable mixture.

(**2ba**:**2bb**:**2bc**:**2bd**=0.24:1.00:0.12:0.084). The yields were estimated by ^{1}H NMR.

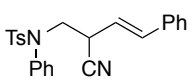
^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.82-0.92 (m, (1.0 + 0.24 + 0.12 + 0.084) x 3H), 1.15-1.41 (m, (1.0 + 0.24 + 0.12 + 0.084) x 4H), 1.44-1.51 (m, (1.0 + 0.084) x 2H), 2.02-2.08 (m, (0.24 + 0.084) x 2H), 2.13 (dt, 0.12 x 2H, *J* = 7.2, 7.2 Hz), 2.43-2.48 (m, 0.12 x 2H), 2.43 (s, (1.0 + 0.24 + 0.12 + 0.084) x 3H), 3.11 (dt, 1.0 x 1H, *J* = 6.4, 6.4 Hz), 3.47 (dt, 0.24 x 1H, *J* = 8.0, 6.8 Hz), 3.68 (t, 0.12 x 2H, *J* = 7.2 Hz), 3.72 (dd, 0.24 x 2H, *J* = 13.6, 8.0 Hz), 3.77 (dd, 0.24 x 2H, *J* = 13.6, 8.0 Hz), 4.16 (dd, 1.0 x 1H, *J* = 14.8, 6.8 Hz), 4.21 (dd, 1.0 x 1H, *J* = 14.8, 6.4 Hz), 4.30 (d, 0.084 x 2H, *J* = 6.4 Hz), 5.31 (dd, 0.24 x 1H, *J* = 15.2, 6.8 Hz), 5.39 (dd, 1.0 x 1H, *J* = 15.2, 6.4 Hz), 5.73 (dddd, 1.0 x 1H, *J* = 15.2, 6.8, 6.4, 1.2 Hz), 5.84 (dt, 0.24 x 1H, *J* = 15.2, 6.8 Hz), 6.24 (t, 0.084 x 1H, *J* = 6.4 Hz), 6.39 (t, 0.12 x 1H, *J* = 7.2 Hz), 7.00-7.13 (m, (1.0 + 0.24 + 0.12 + 0.084) x 2H), 7.19-7.37 (m, (1.0 + 0.24 + 0.12 + 0.084) x 5H), 7.35-7.52 (m, (1.0 + 0.24 + 0.12 + 0.084) x 2H)

Scheme S5. Hydrocyanation of 1c



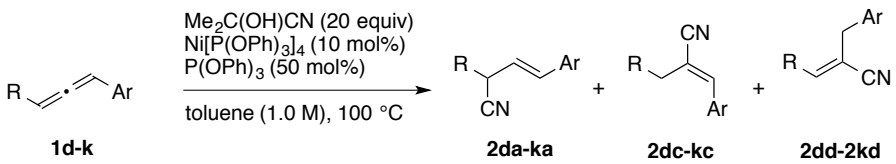
(*E*)-*N*-(2-cyano-4-phenylbut-3-en-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (2ca)

2ca was obtained together with **2cc** and **2cd.** The yield was estimated by ^{1}H NMR. Then **2ca** was partially separated by recrystallization from hexane/CH_2Cl_2.



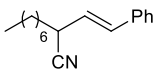
Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 2.43 (s, 3H), 3.73 (dt, 1H, *J* = 8.0, 7.2 Hz), 3.85 (dd, 1H, *J* = 13.6, 7.2 Hz), 3.89 (dd, 1H, *J* = 13.6, 8.0 Hz), 6.03 (dd, 1H, *J* = 16.0, 7.2 Hz), 6.74 (dd, 16.0, 1.2 Hz), 7.06-7.09 (m, 2H), 7.25 (d, 2H, *J* = 8.0 Hz), 7.29-7.34 (m, 8H), 7.47 (d, 2H, *J* = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.6, 35.2, 53.1, 118.1, 119.5, 126.7, 127.8, 128.6, 128.68, 128.72, 129.1, 129.4, 129.6, 134.6, 135.3, 135.5, 139.0, 144.1; IR (ATR) ν: 3057, 2246, 1350, 1161 cm^{-1}; HRMS (ESI) m/z calcd for $C_{24}H_{22}N_2NaO_2S$ $[M+Na]^+$ 425.1300, found 425.1311; mp. 108-110 °C. (91%, 58 mg)

Scheme S6. Hydrocyanation of 1d-k



(*E*)-2-styryloctanenitrile (2da)

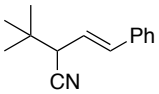
This reaction was performed with 0.24 mmol of **1d** and **2da** was obtained as inseparable mixture with **2dc** (8%) and **2dd** (3%). The yield was estimated by ^{1}H NMR.



Colorless oil. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 0.88 (t, 3H, *J* = 6.6 Hz), 1.21-1.38 (m, 8H), 1.43-1.58 (m, 2H), 1.75-1.79 (m, 2H), 3.42 (dt, 1H, *J* = 7.2, 7.2 Hz), 6.04 (dd, 1H, *J* = 16.2, 6.6 Hz), 6.72 (d, 1H, *J* = 16.2 Hz), 7.27-7.29 (m, 1H), 7.34 (dd, 2H, *J* = 7.2, 7.2 Hz), 7.37-7.39 (m, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 14.1, 22.6, 26.8, 29.0, 29.0, 31.7, 33.3, 34.4, 120.2, 123.3, 126.5, 128.2, 128.7, 133.1, 135.8; IR (ATR) ν: 2925, 2856, 2240, 1449 cm^{-1}; HRMS (APPI) m/z calcd for $C_{17}H_{23}N$ $[M]^+$ 241.1825, found 241.1820. (69%, 40.2 mg)

(*E*)-2-(*tert*-butyl)-4-phenylbut-3-enenitrile (2ea)

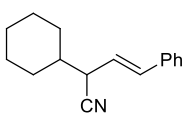
This reaction was performed with 0.24 mmol of **1e** using sealed tube and **2ea** was obtained together with **2ed** (6%). These yields were calculated by ^{1}H NMR. Then **2ea** was partially separated by recrystallization from *n*-pentane.



Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.12 (s, 9H), 3.18 (dd, 1H, *J* = 7.2, 0.8 Hz), 6.12 (dd, 1H, *J* = 15.6, 7.6 Hz), 6.71 (d, 1H, *J* = 15.6 Hz), 7.26-7.30 (m, 1H), 7.35 (dd, 2H, *J* = 7.2 Hz), 7.39-7.40 (m, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 27.3, 34.7, 46.7, 119.4, 120.7, 126.5, 128.2, 128.7, 130.0, 135.8; IR (ATR) ν: 2962, 2867, 2232 cm^{-1}; HRMS (ESI) m/z calcd for $C_{14}H_{19}NNa$ $[M+Na]^+$ 222.1253, found 222.1251; mp. 56 °C. (79%, 37.8 mg)

(*E*)-2-cyclohexyl-4-phenylbut-3-enenitrile (2fa)

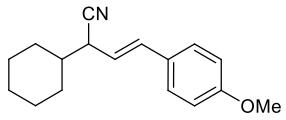
This reaction was performed with 0.24 mmol of **1f** and **2fa** was obtained together with **2fc** (6%) and **2fd** (5%). These yields were estimated by ^{1}H NMR. Then **2fa** was partially purofied by recrystallization from *n*-hexane.



Colorless solid. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 1.15-1.31 (m, 5H), 1.65-1.70 (m, 2H), 1.79-1.85 (m, 3H), 1.89-1.91 (m, 1H), 3.30 (dd, 1H, *J* = 6.0, 6.0 Hz), 6.40 (dd, 1H, *J* = 15.6, 6.6 Hz), 6.70 (d, 1H, *J* = 15.6 Hz), 7.26-7.29 (m, 1H), 7.34 (dd, 2H, *J* = 7.2, 7.2 Hz), 7.38-7.39 (m, 2H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 25.8, 25.8, 25.9, 29.4, 31.0, 40.9, 41.1, 119.3, 122.1, 126.5, 128.1, 128.7, 133.9, 135.8; IR (ATR) ν: 2923, 2854, 2233, 1449 cm^{-1}; HRMS (APPI) m/z calcd for $C_{16}H_{19}N$ $[M]^+$ 225.1512, found 225.1507; mp. 77-78 °C. (74%, 40.1 mg)

(*E*)-2-cyclohexyl-4-(4-methoxyphenyl)but-3-enenitrile (2ga)

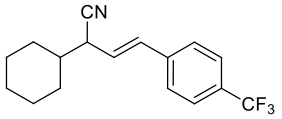
This reaction was performed with 0.29 mmol of **1g** and **2ga** was obtained together with **2gc** (5%) and **2gd** (6%). The yield was estimated by ^{1}H NMR. Then **2ga** was partially separated by recrystallization from *n*-pentane.



Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.15-1.29 (m, 5H), 1.63-1.70 (m, 2H), 1.78-1.84 (m, 3H), 1.89-1.91 (m, 1H), 3.27 (dd, 1H, *J* = 6.0, 6.0 Hz), 3.82 (s, 3H), 5.90 (dd, 1H, *J* = 15.6, 7.2 Hz), 6.63 (d, 1H, *J* = 15.6 Hz), 6.87 (d, 2H, *J* = 9.0 Hz), 7.31 (d, 2H, *J* = 9.0 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 25.9, 26.0, 29.6, 31.0, 40.9, 41.2, 55.3, 114.1, 119.6, 119.8, 127.7, 128.6, 133.3, 159.6; IR (ATR) ν: 2954, 2929, 2853, 2234 cm^{-1}; HRMS (APPI) m/z calcd for $C_{17}H_{21}NO$ $[M]^+$ 255.1618, found 255.1608; mp. 60-61 °C. (77%, 57.4 mg)

(*E*)-2-cyclohexyl-4-(4-(trifluoromethyl)phenyl)but-3-enenitrile (2ha)

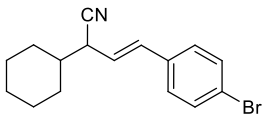
This reaction was performed with 0.24 mmol of **1h** and **2ha** was obtained together with **2hc** (6%) and **2hd** (4%). The yield was estimated by ^{1}H NMR. Then **2ha** was partially separated by recrystallization from *n*-pentane.



Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.15-1.34 (m, 5H), 1.70-1.72 (m, 2H), 1.80-1.90 (m, 4H), 3.35 (dd, 1H, *J* = 6.0, 6.0 Hz), 6.15 (dd, 1H, *J* = 15.6, 9.6 Hz), 6.75 (d, 1H, *J* = 15.6 Hz), 7.48 (d, 2H, *J* = 8.0 Hz), 7.59 (d, 2H, *J* = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 25.77, 25.79, 25.9, 29.5, 31.0, 40.8, 41.1, 118.9, 124.0 (q, *J* = 270 Hz), 124.9, 125.6 (q, *J* = 3.9 Hz), 126.7, 130.0 (q, *J* = 18 Hz), 132.6, 139.2; IR (ATR) ν: 2925, 2855, 2243 cm^{-1}; HRMS (APPI) m/z calcd for $C_{17}H_{18}F_3N$ $[M]^+$ 293.1386, found 293.1376; mp. 60-61 °C. (76%, 53.6 mg)

(*E*)-4-(4-bromophenyl)-2-cyclohexylbut-3-enenitrile (2ia)

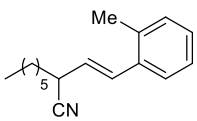
This reaction was performed with 0.34 mmol of **1i** and **2ia** was obtained together with **2ic** (6%) and **2id** (4%). The yield was estimated by ^{1}H NMR. Then **2ia** was partially separated by recrystallization from pentane.



Colorless solid. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 1.15-1.31 (m, 5H), 1.66-1.71 (m, 2H), 1.79-1.84 (m, 3H), 1.88-1.90 (m, 1H), 3.30 (ddd, 1H, *J* = 6.0, 6.0, 1.2 Hz), 6.04 (dd, 1H, *J* = 16.2, 6.0 Hz), 6.65 (d, 1H, *J* = 16.2 Hz), 7.25 (d, 2H, *J* = 8.4 Hz), 7.46 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 25.8, 25.8, 25.9, 29.6, 31.0, 40.8, 41.1, 119.1, 122.0, 122.9, 128.0, 131.8, 132.7, 134.7; IR (ATR) ν: 2929, 2854, 2234 cm^{-1}; HRMS (ESI) m/z calcd for $C_{16}H_{17}BrNNa$ $[M+Na]^+$ 326.0515, found 326.0506; mp. 80-82 °C. (75%, 77.8 mg)

(*E*)-2-(2-methylstyryl)octanenitrile (2ja)

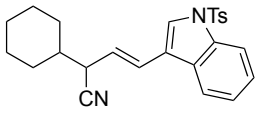
This reaction was performed with 0.20 mmol of **1j** and **2ja** was obtained as inseparable mixture with **2jc** (8%) and **2jd** (4%). The yield was estimated by ^{1}H NMR. Then **2ja** was partially separated by column chromatography.



Colorless oil. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 0.89 (t, 3H, J = 7.2 Hz), 1.24-1.39 (m, 6H), 1.43-1.61 (m, 2H), 1.75-1.81 (m, 2H), 2.36 (s, 3H), 3.44 (dt, 1H, J = 7.6, 6.8 Hz), 5.91 (dd, 1H, J = 16.0, 6.8 Hz), 6.93 (d, 1H, J = 16.0 Hz), 7.15-7.20 (m, 3H), 7.37-7.39 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.0, 19.7, 22.5, 26.7, 26.7, 31.5, 33.3, 34.6, 120.3, 124.7, 125.7, 126.1, 128.1, 130.4, 131.1, 135.0, 135.7; IR (ATR) ν: 2926, 2858, 2239 cm^{-1}; HRMS (APPI) m/z calcd for $C_{17}H_{23}N$ $[M]^+$ 241.1825, found 241.1822. (78%, 36.9 mg)

(*E*)-2-cyclohexyl-4-(1-tosyl-1*H*-indol-3-yl)but-3-enenitrile (2ka)

This reaction was performed with 0.29 mmol of **1k** and **2ka** was obtained together with **2kc** (8%) and **2kd** (5%). The yield was estimated by ^{1}H NMR. Then **2ka** was partially separated by column chromatography.

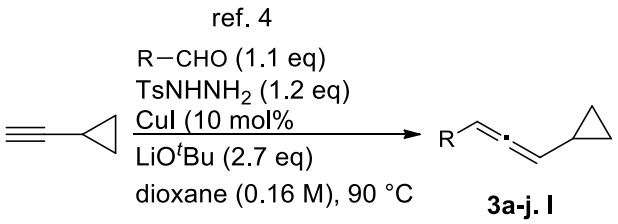


Colorless amorphous. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.15-1.33 (m, 5H), 1.64-1.93 (m, 6H), 2.34 (s, 3H), 3.33 (dd, 1H, J = 6.0, 6.8 Hz), 6.11 (dd, 1H, J = 16.0, 6.8 Hz), 6.28 (d, 1H, J = 16.0 Hz), 7.20-7.25 (m, 3H), 7.27-7.31 (m, 1H), 7.62 (s, 1H), 7.68 (d, 1H, J = 7.2 Hz), 7.78 (d, 2H, 8.4 Hz), 8.00 (d, 2H, J = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 21.5, 25.8, 25.8, 25.9, 29.6, 31.0, 40.8, 41.5, 113.8, 119.0, 119.2, 120.1, 123.2, 123.6, 124.4, 124.6, 125.1, 126.8, 128.6, 129.9, 134.9, 135.4, 145.2; IR (ATR) ν: 2026, 2853, 2238, 1370, 1172 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{27}N_2O_2S$ $[M+H]^+$ 419.1793, found 419.1796. (78%, 95.4 mg)

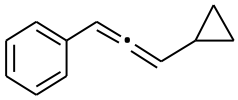
References

1) a) Y. Imada, M. Nishida, K. Kutsuwa, S. Murahashi, T. Naota, *Org. Lett.* **2005**, *7*, 5837. b) G. E. Keck, R. R. Webb, *Tetrahedron Lett.*, **1982**, *23*, 3051.
2) M. L. Hosain, F. Ye, Y. Zhang, J. Wang, *J. Org. Chem.*, **2013**, *78*, 1236.
3) K. Tanaka, T. Kobayashi, H. Mori, S. Katsumura, *J. Org. Chem.*, **2004**, *69,* 5906.

Scheme S7. Synthesis of cyclopropylallenes (3a–j, l) [4]

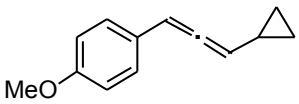


(3-cyclopropylpropa-1,2-dien-1-yl)benzene (3a) (CAS-Reg# 200417-79-4)



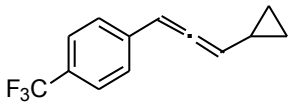
(37%, 1.84 g)

1-(3-cyclopropylproopa-1,2-dien-1-yl)-4-methoxybenzene (3b)



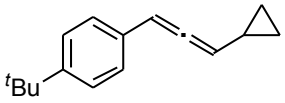
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.40-0.50 (m, 2H), 0.69-0.79 (m, 2H), 1.30-1.38 (m, 1H), 3.80 (s. 3H), 5.41 (dd, 1H, J = 6.8, 6.8 Hz), 6.16 (d, 1H, J = 6.8 Hz), 6.84 (d, 2H, J = 8.8 Hz), 7.20 (d, 2H, J = 8.8 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.8, 7.0, 9.6, 55.3, 95.6, 99.4, 114.1, 127.2, 127.7, 158.7, 204.0 ; IR (ATR) ν: 2928, 1717, 1599, 1510, 1253, 1161, 1023 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{15}O$, $[M+H]^+$ 187.1117, found 187.1117; yellow oil (25%, 250 mg)

1-(3-cyclopropylpropa-1,2-dien-1-yl)-4-(trifluoromethyl)benzene (3c)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.42-0.52 (m, 2H), 0.78 (dd, 2H, J = 8.4, 2.4 Hz), 1.33-1.41 (m, 1H), 5.50 (dd, 1H, J = 6.4, 6.4 Hz), 6.22 (d, 2H, J = 6.4 Hz), 7.37 (d, 2H, J = 8.0 Hz), 7.53 (d, 2H, J = 8.0 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 7.0, 7.0, 9.2, 95.4, 100.2, 125.5, 126.7, 128.5, 138.9, 205.9 ; IR (ATR) ν: 3007, 1948, 1615, 1321, 1119, 1106, 1065, 844 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{11}F_3$, $[M]^+$ 224.0807, found 224.0803; Yellow oil (23%, 225 mg)

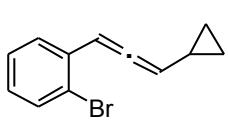
1-(*tert*-butyl)-4-(3-cyclopropylpropa-1,2-dien-1-yl)benzene (3d)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.42-0.44 (m, 2H), 0.70-0.74 (m, 2H), 1.29-1.30 (m, 10H), 5.42 (dd, 1H, J = 6.4, 6.4 Hz), 6.17 (d, 1H, J = 6.4 Hz), 7.21 (d, 2H, J = 8.4 Hz), 7.30 (d, 2H, J = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.8, 7.1, 31.3, 34.5, 95.9, 99.2, 125.5, 126.3, 131.9, 149.8, 204.6; IR (ATR) ν: 2961, 1947, 1514, 1268, 1018, 875, 836 cm^{-1}; HRMS (APPI) Calcd for $C_{16}H_{20}$, $[M]^+$ 212.1560, found 212.1556; Yellow oil (23%, 228.9 mg)

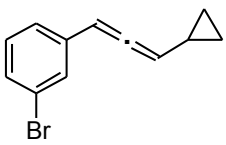
1-bromo-2-(3-cyclopropylpropa-1,2-dien-1-yl)benzene (3e)

^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.39-0.50 (m, 2H), 0.69-0.82 (m, 2H), 1.31-1.39 (m, 1H),



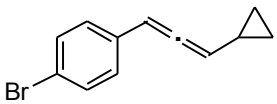
5.45 (dd, 1H, J = 6.8, 6.8 Hz), 6.64 (d, 1H, J = 6.8 Hz), 7.00 (dd, 1H, J = 7.6, 7.6 Hz), 7.21 (dd, 1H, J = 7.6, 7.6 Hz), 7.42 (d, 1H, J = 7.6 Hz), 7.48 (d, 1H, J = 7.6 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.9, 7.0, 9.3, 95.2, 99.7, 122.4, 127.3, 128.0, 128.2, 132.9, 134.2, 205.9; IR (ATR) ν: 3003, 1947, 1473, 1019, 740 cm^{-1}; HRMS (APPI) Calcd for $C_{12}H_{11}Br$, [M]$^+$ 234.0039, found 234.0036; Yellow oil (11%, 108.4 mg)

1-bromo-3-(3-cyclopropylpropa-1,2-dien-1-yl)benzene (3f)



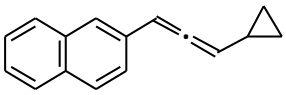
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.36-0.49 (m, 2H), 0.70-0.80 (m, 2H), 1.30-1.36 (m, 1H), 5.43 (dd, 1H, J = 6.4, 6.4 Hz), 6.10 (d, 1H, J = 6.4 Hz), 7.09-7.17 (m, 2H), 7.26 (d, 1H, J = 7.6 Hz), 7.41 (s, 1H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 7.0, 9.4, 95.1, 100.0, 122.7, 125.2, 129.3, 129.6, 129.9, 137.2, 205.1; IR (ATR) ν: 3080, 3003, 1947, 1588, 1564, 1474, 883, 784, 679 cm^{-1}; HRMS (APPI) Calcd for $C_{12}H_{11}Br$, [M]$^+$ 234.0039, found 234.0036; Yellow oil (20%, 201.2 mg)

1-bromo-4-(3-cyclopropylpropa-1,2-dien-1-yl)benzene (3g)



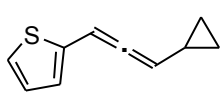
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.38-0.50 (m, 2H), 0.72-0.81 (m, 2H), 1.30-1.39 (m, 1H), 5.43 (dd, 1H, J = 6.8, 6.8 Hz), 6.13 (d, 1H, J = 6.8 Hz), 7.14 (d, 2H, J = 8.4 Hz), 7.40 (d, 2H, J = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 7.0, 7.1, 9.3, 95.3, 99.9, 120.3, 128.1, 131.5, 133.9, 204.9; IR (ATR) ν: 3079, 3003, 1946, 1487, 1068, 1009, 828 cm^{-1}; HRMS (APPI) Calcd for $C_{12}H_{12}Br$, [M+H]$^+$ 235.0117, found 235.0111; Yellow oil (41%, 823.6 mg)

2-(3-cyclopropylpropa-1,2-dien-1-yl)naphthalene (3h)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.45-0.53 (m, 2H), 0.72-0.81 (m, 2H), 1.36-1.43 (m, 1H), 5.51 (dd, 1H, J = 6.8, 6.8 Hz), 6.38 (d, 1H, J = 6.8 Hz), 7.40-7.50 (m, 3H), 7.65 (s, 1H), 7.75-7.80 (m, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.9, 7.1, 9.5, 96.6, 99.7, 124.6, 125.4, 125.5, 126.1, 127.6, 127.7, 128.1, 132.4, 132.6, 133.7, 205.4 ; IR (ATR) ν: 3054, 3003, 1944, 1629, 1597, 1508, 1248 cm^{-1}; HRMS (APPI) Calcd for $C_{16}H_{14}$, [M]$^+$ 206.1090, found 206.1085; Colorless solid (mp: 45-48 °C, 27%, 269 mg)

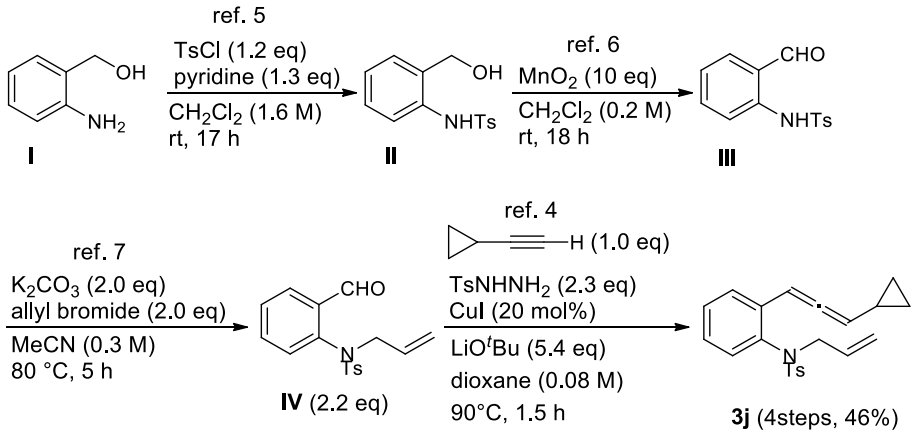
2-(3-cyclopropylpropa-1,2-dien-1-yl)thiophene (3i)



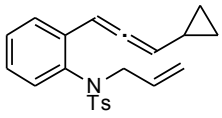
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.43-0.51 (m, 2H), 0.74-0.78 (m, 2H), 1.30-1.38 (m, 1H), 5.47 (dd, 1H, J = 6.4, 6.4 Hz), 6.41 (d, 1H, J = 6.4 Hz), 6.89 (d, 1H, J = 3.6 Hz), 6.94 (dd, 1H, J = 4.8, 3.6 Hz), 7.13 (d, 1H, J = 4.8 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.8, 7.4, 9.5, 90.6, 99.9, 124.2, 124.4,

127.4, 139.5, 204.0; IR (ATR) ν: 3079, 3002, 1653, 1428, 1256 cm^{-1}; HRMS (APPI) Calcd for $C_{10}H_{10}S$, $[M]^+$ 162.0498, found 162.0494; Yellow oil (14%, 143.4 mg)

Scheme S8. Synthesis of 3j[1, 2, 3, 4]

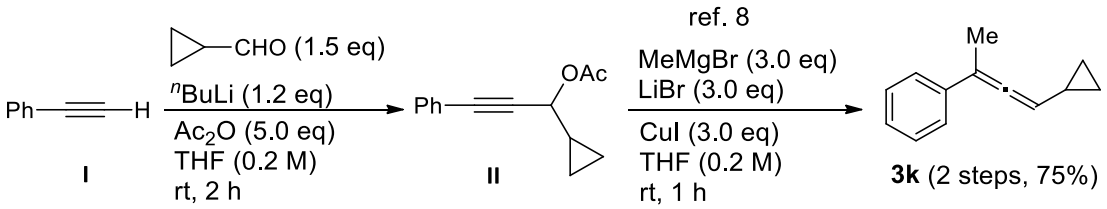


N-allyl-N-(2-(3-cyclopropylpropa-1,2-dien-1-yl)phenyl)-4-methylbenzenesulfonamide (3j)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.42-0.75 (m, 4H), 1.25-1.34 (m, 1H), 2.44 (s, 3H), 3.89-4.02 (m, 1H), 4.21-4.41 (m, 1H), 4.99 (d, 2H, J = 10.4 Hz), 5.42)dd, 1H, J = 6.8, 6.8 Hz), 5.68-5.82 (m, 1H), 6.50-6.70 (m, 2H), 7.00-7.11 (m, 1H), 7.21-7.31 (m, 3H), 7.49-7.67 (m, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 7.2, 7.4, 8.4, 9.6, 9.7, 21.9, 55.2, 73.1, 86.1, 92.5, 99.7, 119.6, 120.0, 127.2, 127.2, 128.2, 128.4, 128.8, 129.0, 129.3, 129.6, 129.9, 130.1, 132.5, 132.8, 135.8, 136.2, 136.3, 137.4, 139.7, 143.9, 144.0, 206.0; IR (ATR) ν: 3429, 3067, 3012, 2250, 1944, 1697, 1597, 1490, 1343, 1161, 1090 cm^{-1}; HRMS (ESI) Calcd for $C_{22}H_{23}NNaO_2S$, $[M+Na]^+$ 388.1347, found 388.1348; Yellow oil (2.12 g)

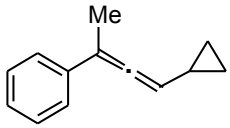
Scheme S9. Synthesis of 3k[8]



I to **II** : To a THF (23.4 mL) solution of ethynylbenzene (0.51 mL 4.7 mmol) was added n-buthyllithium (3.6 ml, 1.55 M in THF, 5.6 mmol) at -78 °C under argon. The resulting solution was allowed to stir for an additional 30 min at same temperature. To this solution was added cyclopropanecarboxaldehyde (0.2 mL, 7.0 mmol) at -78 °C. The mixture was stirred for an additional 30 min, then warmed to 0 °C over 2 h. After acetic anhydride (2.2 mL, 23.4 mmol) was added, the mixture was allowed to be stirred

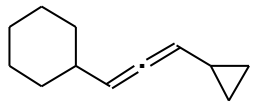
for 1 h at 0 °C. The reaction was quenched with saturated aqueous ammonium chloride, and the mixture was extracted with AcOEt. The combined organic layers were washed with brine and dried over anhydrous sodium sulfate. After removal of the solvent under reduced pressure, the residue (1.24 g) was used directly in the next step without further purification.

(4-cyclopropylbuta-2,3-dien-2-yl)benzene (3k)



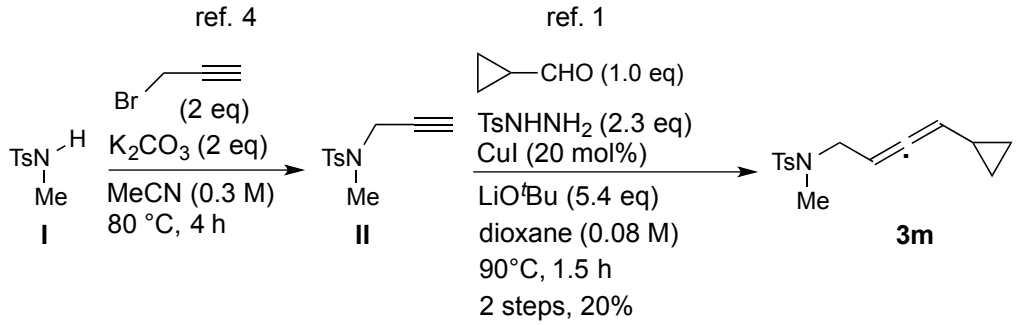
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.39-0.43 (m, 2H), 0.69-0.73 (m, 2H), 1.27-1.36 (m, 1H), 2.08 (dd, 3H, J = 2.8, 0.8 Hz), 5.29 (dd, 1H, J = 6.8, 2.8 Hz), 7.17 (dd, 1H, J = 8.4, 8.4 Hz), 7.30 (dd, 2H, J = 8.4, 8.4 Hz), 7.39 (dd, 2H, J = 8.4, 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.9, 6.9, 9.7, 17.3, 97.4, 102.0, 125.6, 126.4, 128.2, 137.5, 203.6; IR (ATR) ν: 3734, 3669, 3081, 3003, 1943, 1597, 1492, 1442, 1370, 1258 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{14}$, $[M]^+$ 170.1090, found 170.1088: Yellow oil (597.5 mg)

(3-cyclopropylpropa-1,2-dien-1-yl)cyclohexane (3l)

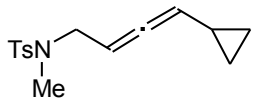


^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.27-0.41 (m, 2H), 0.62-0.70 (m, 2H), 1.01-1.11 (m, 2H), 1.13-1.32 (m, 4H), 1.60-1.64 (m, 1H), 1.69-1.76 (m, 4H), 1.89-1.98 (m, 1H), 5.04 (ddd, 1H, J = 6.4, 6.4, 2.8 Hz), 5.16 (ddd, 1H, J = 6.4, 6.4, 1.2 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.4, 6.9, 9.5, 26.0, 26.2, 33.1, 37.4, 95.9, 99.0, 201.8 ; IR (ATR) ν: 2922, 2850, 1447, 1017, 889 cm^{-1}; HRMS (APPI) Calcd for $C_{12}H_{19}$, $[M+H]^+$ 163.1481, found 163.1479; Colorless oil (23%, 180 mg)

Scheme S10. Synthesis of 3m[4, 7]



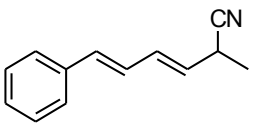
N-(4-cyclopropylbuta-2,3-dien-1-yl)-N,4-dimethylbenzenesulfonamide (3m)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 0.26-0.34 (m, 2H), 0.66-0.73 (m, 2H), 1.14-1.23 (m, 1H), 2.42 (s, 3H), 2.73 (s, 3H), 3.63 (d, 2H, J = 6.0 Hz), 5.00-5.06 (m, 2H), 7.31 (d, 2H, J = 8.0 Hz), 7.66 (d, 2H, J = 8.0 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 6.6, 6.7, 9.2, 34.0, 50.0, 88.0, 97.0, 127.3, 129.6, 134.6,

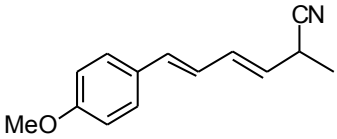
143.3, 204.9; IR (ATR) ν: 3004, 1597, 1451, 1338, 1158, 1089, 1019 cm^{-1}; HRMS (ESI) Calcd for $C_{15}H_{20}N1O_2S$, $[M+H]^+$ 278.1215, found 278.1220; Colorless oil (20%, 133.4 mg)

(3*E*,5*E*)-2-methyl-6-phenylhexa-3,5-dienenitrile (4a)



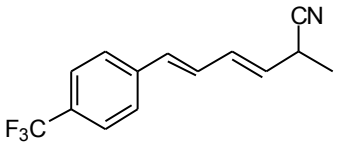
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.46 (d, 3H, *J* = 6.8 Hz), 3.44 (qd, 1H, *J* = 6.8, 6.0 Hz), 5.67 (dd, 1H, *J* = 10.4, 6.4 Hz), 6.52 (dd, 1H, *J* = 15.2, 10.4 Hz), 6.60 (d, 1H, *J* = 15.6 Hz), 6.74 (dd, 1H, *J* = 15.6, 10.4 Hz), 7.23-7.27 (m, 1H), 7.33 (dd, 2H, *J* = 7.2, 7.2 Hz), 7.40 (d, 2H, *J* = 7.2 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 19.0, 28.1, 120.8, 126.5, 126.9, 127.6, 127.9, 128.6, 132.8, 134.1, 136.7; IR (ATR) ν: 3025, 2984, 2937, 2240, 2216, 985, 747, 691 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{13}NNa$, $[M+H]^+$ 184.1121, found 184.1115; Colorless oil (72%, 28.4 mg)

(3*E*,5*E*)-6-(4-methoxyphenyl)-2-methylhexa-3,5-dienenitrile (4b)



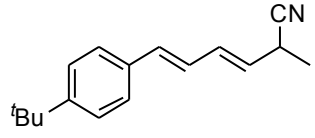
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.45 (d, 3H, *J* = 6.8 Hz), 3.43 (dq, 1H, *J* = 6.8, 6.0 Hz), 3.82 (s, 3H), 5.61 (dd, 1H, *J* = 14.8, 6.0 Hz), 6.48 (dd, 1H, *J* = 15.2, 9.6 Hz), 6.54 (d, 1H, *J* = 15.2 Hz), 6.61 (dd, 1H, *J* = 15.2, 9.6 Hz), 6.86 (d, 2H, *J* = 8.4 Hz), 7.33 (d, 2H, *J* = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 19.0, 28.1, 55.3, 114.1, 120.9, 124.9, 126.4, 127.7, 129.5, 133.0, 133.6, 159.5; IR (ATR) ν: 2935, 2240, 1603, 1509, 1247, 1174, 1030, 984, 831 cm^{-1}; HRMS (APPI) Calcd for $C_{14}H_{15}ON$, $[M]^+$ 213.1148, found 213.1141; Colorless solid (mp: 52-55 °C; 49%, 17.6 mg)

(3*E*,5*E*)-2-methyl-6-(4-(trifluoromethyl)phenyl)hexa-3,5-dienenitrile (4c)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.47 (d, 3H, *J* = 6.8 Hz), 3.43-3.50 (m, 1H), 5.74 (dd, 1H, *J* = 15.6, 6.4 Hz), 6.51-6.58 (m, 1H), 6.62 (d, 1H, *J* = 15.6 Hz), 6.81 (dd, 1H, *J* = 15.6, 10.4 Hz), 7.48 (d, 2H, *J* = 8.4 Hz), 7.57 (d, 2H, *J* = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.1, 120.6, 125.6, 125.6, 126.6, 129.3, 129.4, 132.2, 132.4, 140.1; IR (ATR) ν: 2989, 2243, 1613, 1415, 1321, 1163, 1118, 1106, 1065, 985, 839 cm^{-1}; HRMS (APPI) Calcd for $C_{14}H_{12}NF_3$, $[M]^+$251.0916, found 251.0908; Yellow oil (65%, 49.0 mg)

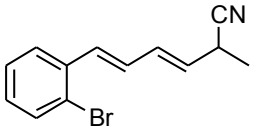
(3*E*,5*E*)-6-(4-(*tert*-butyl)phenyl)-2-methylhexa-3,5-dienenitrile (4d)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.31 (s, 9H), 1.44 (d, 3H, *J* = 7.2 Hz), 3.38-3.45 (m, 1H), 5.62 (dd, 1H, *J* = 15.2, 6.4 Hz), 6.49 (dd, 1H, *J* = 15.2, 10.4 Hz), 6.57 (d, 1H, *J* = 15.2 Hz), 6.70 (dd, 1H,

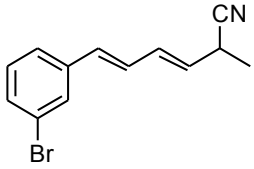
J = 15.2, 10.4 Hz), 7.28-7.38 (m, 4H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.1, 31.2, 34.6, 120.8, 125.6, 126.1, 126.2, 127.1, 132.9, 133.9, 151.1; IR (ATR) ν: 2961, 2242, 1459, 1363, 1269, 985, 835, 732 cm^{-1}; HRMS (APPI) Calcd for $C_{17}H_{21}N$, [M]$^+$ 239.1169, found 239.1660; Yellow oil (74%, 41.7 mg)

(3*E*,5*E*)-6-(2-bromophenyl)-2-methylhexa-3,5-dienenitrile (4e)



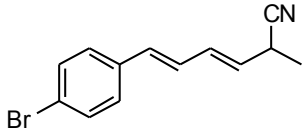
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.47-1.48 (d, 3H, J = 7.6 Hz), 3.45 (dq, 1H, J = 7.6, 6.0 Hz), 5.72 (dd, 1H, J = 15.2, 6.0 Hz), 6.58 (dd, 1H, J = 15.2, 10.4 Hz), 6.69 (dd, 1H, J = 10.4, 15.2 Hz), 6.96 (d, 1H, J = 15.2 Hz), 7.10 (dd, 1H, J = 7.2, 7.2 Hz), 7.22-7.29 (m, 1H), 7,55 (dd, 2H, J = 7.2, 7.2 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.8, 28.1, 120.7, 124.0, 126.5, 127.5, 128.9, 129.1, 129.5, 132.6, 132.6, 133.1, 136.4; IR (ATR) ν: 2934, 2242, 1465, 1437, 984, 747 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{12}NBr$, [M]$^+$ 261.0148, found 261.0138; Colorless oil (60%, 25.0 mg)

(3*E*,5*E*)-6-(3-bromophenyl)-2-methylhexa-3,5-dienenitrile (4f)



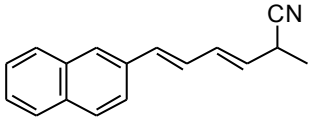
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.45 (d, 3H, J = 7.2 Hz), 3.44 (dq, 1H, J = 7.2, 6.4 Hz), 5.69 (dd, 1H, J = 16.0, 6.4 Hz), 6..46-6.54 (m, 2H), 6.72 (dd, 1H, J = 16.0, 10.8 Hz), 7.18 (dd, 1H, J = 7.6, 7.6 Hz), 7.29 (d, 1H, J = 7.6 Hz), 7.35-7.38 (m, 1H), 7.54 (dd, 1H, J = 1.6, 1.6 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.1, 120.6, 122.8, 125.1, 128.3, 128.8, 129.1, 130.1, 130.7, 132.3, 132.3, 138.8; IR (ATR) ν: 2985, 2243, 1588, 1471, 984, 731 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{12}NBr$, [M]$^+$ 261.0148, found 261.0142; Colorless oil (67%, 33.6 mg)

(3*E*,5*E*)-6-(4-bromophenyl)-2-methylhexa-3,5-dienenitrile (4g)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.45 (d, 3H, J = 6.8 Hz), 3.43 (dq, 1H, J = 6.8, 6.4 Hz), 5.68 (dd, 1H, J = 15.2, 6.4 Hz), 6.46-6.55 (m, 2H), 6.71 (dd, 1H, J = 15.2, 10.8 Hz), 7.24 (d, 2H, J = 8.4 Hz), 7.43 (d, 2H, J = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.1, 120.6, 121.7, 127.6, 127.9, 128.3, 131.7, 132.4, 132.7, 135.6; IR (ATR) ν: 2986, 2241, 1486, 1071, 984, 827, 731 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{12}NBr$, [M+H]$^+$ 261.0148, found 261.0140; Colorless solid (mp: 35-39 °C, 68%, 61.8 mg)

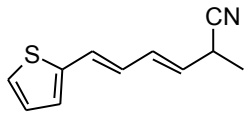
(3*E*,5*E*)-2-methyl-6-(naphthalen-2-yl)hexa-3,5-dienenitrile (4h)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.46 (d, 3H, J = 7.2 Hz), 3.42-3.48 (m, 1H), 5.69 (dd, 1H, J =15.2, 6.4 Hz), 6.56 (dd, 1H, J = 15.2, 9.6 Hz), 6.75 (d, 1H, J = 15.2, 9.6 Hz), 7.42-7.49 (m,

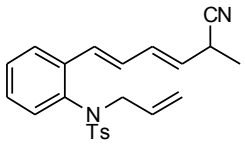
2H), 7.59 (dd, 1H, *J* = 8.4, 1.6 Hz), 7.74 (s, 1H), 7.77-7.83 (m, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 19.0, 28.2, 120.8, 123.3, 126.1, 126.4, 126.8, 127.2, 127.7, 127.8, 128.0, 128.3, 132.8, 133.1, 133.5, 134.2; IR (ATR) ν: 2996, 2239, 2215, 1507, 1454 cm^{-1}; HRMS (APPI) Calcd for $C_{17}H_{15}N$, $[M]^+$ 233.1199, found 233.1190; Colorless solid (mp: 117-122 °C, 76%, 51.1 mg)

(3*E*,5*E*)-2-methyl-6-(thiophen-2-yl)hexa-3,5-dienenitrile (4i)



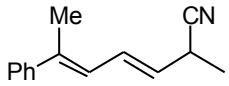
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.45 (d, 3H, *J* = 6.8 Hz), 3.40-3.46 (m, 1H), 5.63 (dd, 1H, *J* = 15.2, 6.0 Hz), 6.45 (dd, 1H, *J* = 15.2, 10.4 Hz), 6.73 (d, 1H, *J* = 15.2 Hz), 6.97-7.00 (m, 2H), 7.18 (d, 1H, *J* = 5.2 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.1, 120.7, 124.9, 126.5, 126.8, 127.4, 127.6, 129.7, 132.2, 142.0; IR (ATR) ν: 3022, 2984, 2936, 2241, 1593, 1452, 1210 cm^{-1}; HRMS (APPI) Calcd for $C_{11}H_{11}NS$, $[M]^+$ 189.0607, found 189.0601; Yellow oil (50%, 38.1 mg)

N-allyl-N-(2-((1*E*,3*E*)-5-cyanohexa-1,3-dien-1-yl)phenyl)-4-methylbenzenesulfonamide (4j)



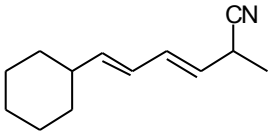
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.47 (d, 3H, *J* = 7.6 Hz), 2.44 (s, 3H), 3.44 (qd, 1H, *J* = 7.6, 6.4 Hz), 3.91-4.10 (brs, 1H), 4.17-4.33 (m, 1H), 4.95 (dd, 1H, *J* = 15.6, 1.2 Hz), 4.99 (dd, 1H, *J* = 9.6, 1.2 Hz), 5.65-5.79 (m, 2H), 6.40 (dd, 1H, *J* = 15.6, 9.6 Hz), 6.64-6.86 (m, 3H), 7.13 (dd, 1H, *J* = 7.6, 7.6 Hz), 7.28 (d, 2H, *J* = 8.8 Hz), 7.30 (d, 1H, *J* = 8.8 Hz), 7.58 (d, 2H, *J* = 8.8 Hz), 7.62 (d, 1H, *J* = 8.8 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 21.6, 28.1, 54.8, 119.4, 120.8, 125.9, 127.8, 128.1, 128.3, 128.5, 128.5, 129.5, 129.6, 132.3, 133.1, 136.0, 136.9, 137.6, 143.6; IR (ATR) ν: 3024, 2242, 1597, 1481, 1450, 1343, 1162, 1091, 989 cm^{-1}; HRMS (ESI) Calcd for $C_{23}H_{24}N_2NaO_2S$, $[M+Na]^+$ 415.1456, found 415.1449; Yellow oil (44%, 112 mg)

(3*E*,5*E*)-2-methyl-6-phenylhepta-3,5-dienenitrile (4k)



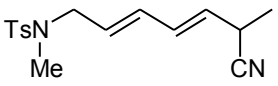
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.42 (d, 3H, *J* = 7.2 Hz), 2.17 (s, 3H), 3.41 (qd, 1H, *J* = 7.2, 6.4 Hz), 5.61 (dd, 1H, *J* = 14.8, 6.4 Hz), 6.38 (d, 1H, *J* = 11.2 Hz), 6.73 (ddd, 1H, *J* = 14.8, 11.2, 1.6 Hz), 7.29-7.34 (m, 3H), 7.42 (d, 2H, *J* = 7.6 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 16.1, 19.0, 28.2, 120.9, 124.9, 125.6, 127.3, 127.8, 128.2, 129.1, 138.1, 142.5; IR (ATR) ν: 3065, 2985, 2937, 2237, 1467, 1437, 1024, 963 cm^{-1}; HRMS (APPI) Calcd for $C_{14}H_{16}N$, $[M+H]^+$ 198.1277, found 198.1273; Colorless oil (97%, 104.0 mg)

(3*E*,5*E*)-6-cyclohexyl-2-methylhexa-3,5-dienenitrile (4l)



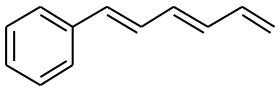
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.04-1.33 (m, 6H), 1.40 (d, 3H, *J* = 7.2 Hz), 1.68-1.75 (m, 4H), 1.96-2.05 (m, 1H), 3.31-3.39 (m, 1H), 5.43 (dd, 1H, *J* = 15.6, 6.4 Hz), 5.72 (dd, 1H, *J* = 15.6, 6.4 Hz), 5.94 (dd, 1H, *J* = 15.2, 10.8 Hz), 6.29 (ddd, 1H, *J* = 15.2, 10.4, 0.8 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 19.0, 25.9, 26.2, 28.0, 32.7, 40.7, 120.9, 125.1, 126.0, 133.3, 142.7; IR (ATR) ν: 2923, 2850, 2241, 1655, 1448, 986 cm^{-1}; HRMS (APPI) Calcd for $C_{13}H_{20}N$, $[M+H]^+$ 190.1590, found 190.1584; Colorless oil (52%, 73.4 mg)

N-((2*E*,4*E*)-6-cyanohepta-2,4-dien-1-yl)-N,4-dimethylbenzenesulfonamide (4m)

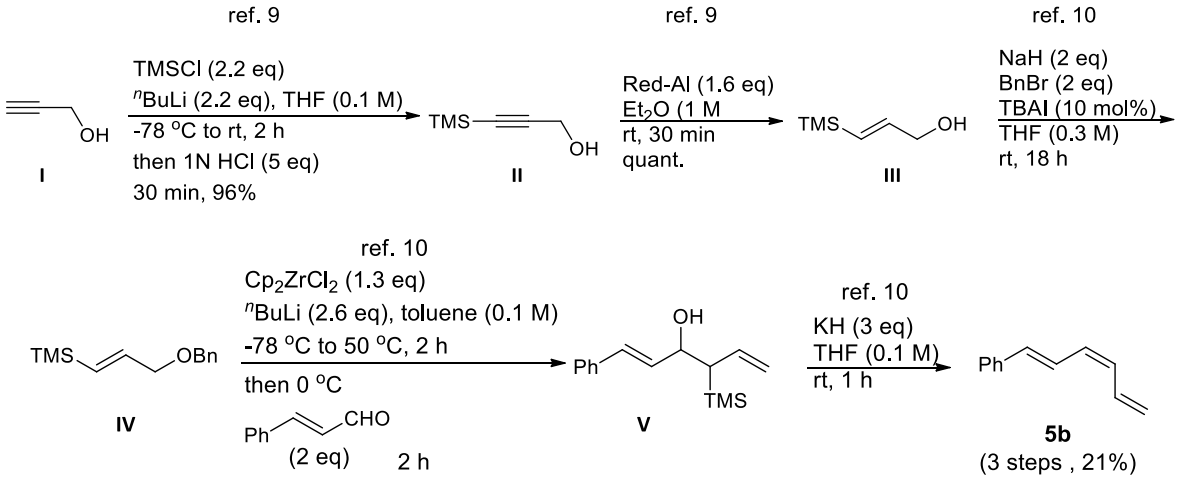


^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.41 (d, 3H, *J* = 7.2 Hz), 2.44 (s, 3H), 2.67 (s, 3H), 3.34-3.42 (m, 1H), 3.67 (d ,2H, *J* = 6.0 Hz), 5.51-5.64 (m, 2H), 6.13 (dd, 1H, *J* = 15.2, 6.4 Hz), 6.31 (dd, 1H, *J* = 15.2, 6.4 Hz), 7.32 (d, 2H, *J* = 8.0 Hz), 7.67 (d, 2H, *J* = 8.0 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.7, 21.5, 27.9, 34.4, 51.9, 120.6, 127.4, 128.3, 129.0, 129.7, 131.3, 132.1, 134.3, 143.5; IR (ATR) ν: 2934, 1598, 1452, 1335, 1157, 1089 cm^{-1}; HRMS (ESI) Calcd for $C_{16}H_{20}N_2NaO_2S$, $[M+Na]^+$ 327.1143, found 327.1154; Yellow oil (50%, 21.7 mg)

(1*E*,3*E*)-hexa-1,3,5-trien-1-ylbenzene (5a) (CAS-Reg# 35008-84-5)

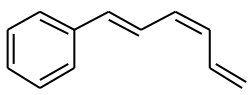


(10%, 3.3 mg)



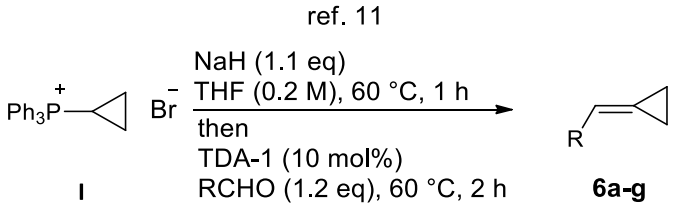
Scheme S11. Synthesis of 5b[9, 10]

(1*E*,3*Z*)-hexa-1,3,5-trien-1-ylbenzene (5b) (CAS-Reg# 3864-19-5)

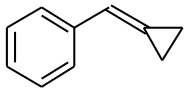


(54 mg)

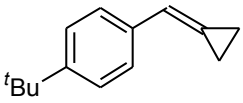
Scheme S12. Synthesis of 6a-g[11]



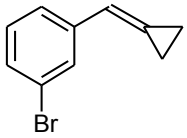
(cyclopropylidenemethyl)benzene (6a) (CAS-Reg# 7555-67-1)
(58%, 755.0 mg)



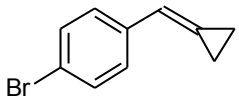
1-(*tert*-butyl)-4-(cyclopropylidenemethyl)benzene (6b)
(CAS-Reg# 918831-65-9)
(75%, 1.49 g)



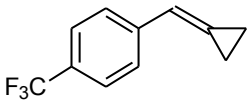
1-bromo-3-(cyclopropylidenemethyl)benzene (6c) (CAS-Reg# 888505-25-7)
(25%, 42.8 mg)



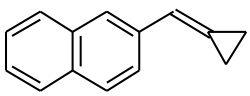
1-bromo-4-(cyclopropylidenemethyl)benzene (6d)
(CAS-Reg# 179251-27-5)
(84%, 1.68 g)



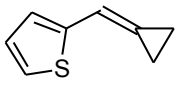
1-(cyclopropylidenemethyl)-4-(trifluoromethyl)benzene (6e) (CAS-Reg# 243449-23-2)
(33%, 660 mg)



2-(cyclopropylidenemethyl)naphthalene (6f) (CAS-Reg# 68854-50-2)
(41%, 325.8 mg)

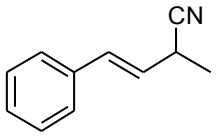


2-(cyclopropylidenemethyl)thiophene (6g)



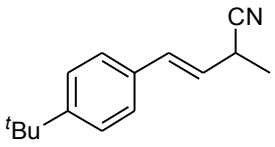
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.29-1.33 (m, 4H), 6.94 (dd, 1H, J = 1.6, 1.6 Hz), 6.98-7.00 (m, 2H), 7.15 (d, 1H, J = 4.8 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 2.9, 4.4, 112.7, 123.9, 124.1, 124.4, 127.2, 144.1; IR (ATR) ν: 3069, 3046, 2975, 1786, 1660, 1523, 1411, 1215, 1040 cm^{-1}; HRMS (APPI) Calcd for C_8H_9S, $[M+H]^+$137.0419, found137.0418; Yellow oil (48%, 964.3 mg)

(*E*)-2-methyl-4-phenylbut-3-enenitrile (7a) (CAS-Reg# 112528-98-0)



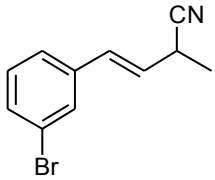
(63%, 28.4 mg)

(*E*)-4-(4-(*tert*-butyl)phenyl)-2-methylbut-3-enenitrile (7b)



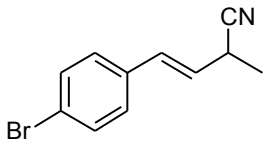
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.32 (s, 9H), 1.49 (d, 3H, J = 7.2 Hz), 3.49 (qd, 1H, *J*=7.2, 6.4 Hz), 6.02 (dd, 1H, *J*= 16.0, 6.4 Hz), 6.67 (d, 1H, *J* = 16.0 Hz), 7.30 (d, 2H, *J* = 8.0 Hz), 7.35 (d, 2H, *J* = 8.0 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 19.1, 28.4, 31.2, 34.6, 121.0, 123.5, 125.6, 126.2, 132.2, 132.9, 151.4; IR (ATR) ν: 3734, 2962, 2242, 1783, 1509, 1456, 1363, 1269, 1109, 966, 814 cm^{-1}; HRMS (APPI) Calcd for $C_{15}H_{19}N$, [M] $^+$213.1512, found 213.1507; Colorless oil (67%, 28.8 mg)

(*E*)-4-(3-bromophenyl)-2-methylbut-3-enenitrile (7c)



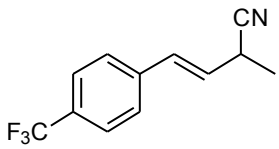
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.50 (d, 3H, *J* = 6.8 Hz), 3.47-3.54 (m, 1H), 6.03-6.10 (m, 1H), 6.64 (dd, 1H, *J* = 15.6, 6.8 Hz), 7.21 (dd, 1H, *J* = 8.0, 8.0 Hz), 7.27 (dd, 1H, *J* = 7.2, 7.2 Hz), 7.39 (dd, 1H, *J* = 7.2, 7.2 Hz), 7.51 (d, 1H, *J* =7.2 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.3, 120.5, 122.8, 125.3, 125.8, 129.3, 130.2, 131.1, 137.7; IR (ATR) ν: 2985, 2242, 1561, 1473, 1072, 961, 883 cm^{-1}; HRMS (APPI) Calcd for $C_{11}H_{10}NBr$, [M] $^+$234.9991, found 234.9986; Colorless oil (72%, 31.2 mg)

(*E*)-4-(4-bromophenyl)-2-methylbut-3-enenitrile (7d)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.50 (d, 3H, *J* = 7.2 Hz), 3.50 (qd, 1H, *J* = 7.2, 6.4 Hz), 6.05 (dd, 1H, *J* = 16.0, 6.4 Hz), 6.64 (d, 1H, *J* =16.0 Hz), 7.23 (d, 2H, *J* = 8.0 Hz), 7.45 (d, 2H, *J* = 8.0 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.3, 120.6, 122.1, 125.0, 128.0, 131.3, 131.8, 134.5; IR (ATR) ν: 2991, 2939, 2243, 1487, 1072, 1008, 965, 807 cm^{-1}; HRMS (APPI) Calcd for $C_{11}H_{10}NBr$, [M] $^+$234.9991, found 234.9987; Colorless solid (mp: 36-40 °C, 76%, 34.1 mg)

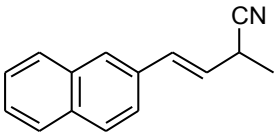
(*E*)-2-methyl-4-(4-(trifluoromethyl)phenyl)but-3-enenitrile (7e)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.53 (d, 3H, *J* = 7.2 Hz), 3.54 (qd, *J* = 7.2, 5.6 Hz), 6.16 (dd, 1H, *J* = 16.0, 5.6 Hz), 6.75 (d, 1H, *J* = 16.0 Hz), 7.47 (d, 2H, *J* = 8.0 Hz), 7.59 (d, 2H, *J* = 8.0 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ:18.8, 28.3, 120.4, 125.6, 125.6, 126.7, 126.9, 131.1, 139.1; IR (ATR) ν: 2991, 2245, 1617, 1416, 1263, 1164, 1119, 1107,

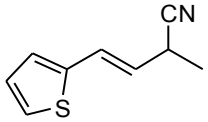
1065, 1016 cm^{-1}; HRMS (APPI) Calcd for $C_{12}H_{10}NF_3$, [M] $^+$225.0760, found 225.0755; Colorless oil (79%, 47.3 mg)

(*E*)-2-methyl-4-(naphthalen-2-yl)but-3-enenitrile (7f)

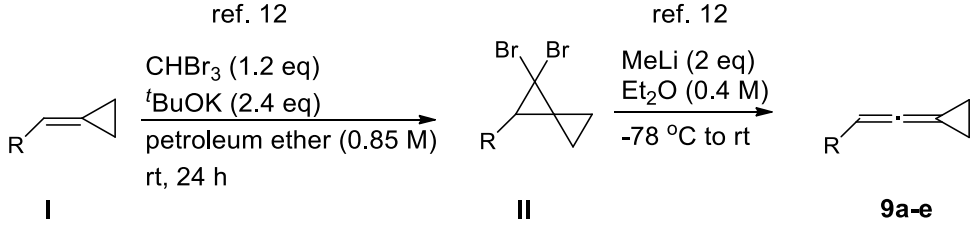


^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.53 (d, 3H, *J* = 6.8 Hz), 3.52-3.59 (qd, 1H, *J* = 6.8, 6.0 Hz), 6.16 (dd, 1H, *J* = 15.6, 6.0 Hz), 6.86 (d, 1H, *J* = 15.6 Hz), 7.44-7.50 (m, 2H), 7.55 (d, 1H, *J* = 8.4 Hz), 7.75 (s, 1H), 7.79-7.82 (m, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 19.1, 28.5, 120.9, 123.2, 124.5, 126.2, 126.4, 126.9, 127.7, 128.0, 128.4, 132.6, 133.0, 133.2, 133.4; IR (ATR) ν: 2994, 2237, 1964, 1709, 1508, 1460 cm^{-1}; HRMS (APPI) Calcd for $C_{15}H_{13}N$, [M] $^+$207.1043, found 207.1037; Colorless solid (mp: 85-88 °C, 93%, 38.3 mg)

(*E*)-2-methyl-4-(thiophen-2-yl)but-3-enenitrile (7g)

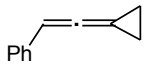


^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.48 (d, 3H, *J* = 7.2 Hz), 3.44 (qd, 1H, *J* = 7.2, 6.0 Hz), 5.89 (d, 1H, *J* = 16.0, 6.0 Hz), 6.82 (d, 1H, *J* = 16.0 Hz), 6.96-7.00 (m, 2H), 7.19 (d, 1H, *J* = 4.8 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 18.9, 28.1, 120.6, 123.5, 125.0, 125.6, 126.7, 127.5, 140.3; IR (ATR) ν: 2986, 2938, 2242, 1783, 1645, 1591, 1487, 1452, 1433, 1205, 1040 cm^{-1}; HRMS (APPI) Calcd for C_9H_9NS, [M] $^+$163.0450, found163.0445; Colorless oil (75%, 35.2 mg)

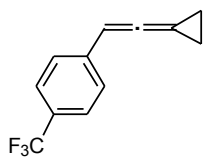


Scheme S13. Synthesis of 9a-e[12]

(2-cyclopropylidenevinyl)benzene (9a) (CAS-Reg# 42311-14-8) (12%, 16.4 mg)

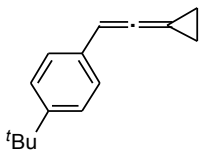


1-(2-cyclopropylidenevinyl)-4-(trifluoromethyl)benzene (9b)



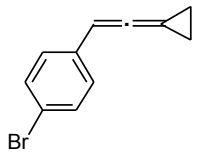
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.70-1.82 (m, 4H), 6.29 (ddd, 1H, *J* = 6.8, 3.6, 3.6 Hz), 7.35 (d, 2H, *J* = 8.4 Hz), 7.51 (d, 2H, *J* = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 9.3, 80.2, 95.6, 125.4, 125.4, 126.5, 131.7, 140.0, 190.7; IR (ATR) ν: 2993, 2009, 1613, 1320, 1161, 1104, 1064, 846 cm^{-1}; HRMS (ESI) Calcd for $C_{12}H_9CsF_3$, $[M+Cs]^+$342.9711, found 342.9700; Colorless oil (25%, 89.0 mg)

1-(*tert*-butyl)-4-(2-cyclopropylidenevinyl)benzene (9c)



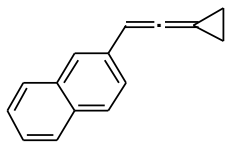
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.30 (s, 9H), 1.61-1.74 (m, 4H), 6.23 (ddd, 1H, J = 6.8, 3.6, 3.6 Hz), 7.21 (d, 2H, J = 8.4 Hz), 7.30 (d, 2H, J = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 8.7, 31.4, 34.6, 80.0, 96.4, 125.6, 126.3, 133.0, 149.6, 189.9; IR (ATR) ν: 2961, 2009, 1699, 1514, 1362, 1268, 841 cm^{-1}; HRMS (ESI) Calcd for $C_{15}H_{18}Cs$, $[M+Cs]^+$331.0463, found 331.0466; Yellow oil (5%, 9.5 mg)

1-bromo-4-(2-cyclopropylidenevinyl)benzene (9d)



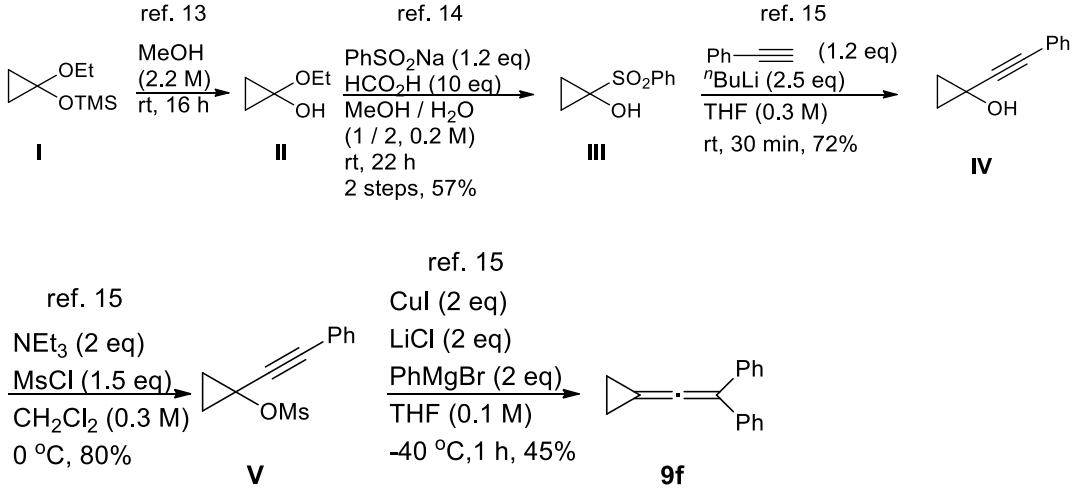
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.66-1.78 (m, 4H), 6.22 (ddd, 1H, J = 6.8, 3.6, 3.6 Hz), 7.13 (d, 2H, J = 8.4 Hz), 7.38 (d, 2H, J = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 8.9, 80.3, 95.7, 119.8, 128.0, 131.5, 133.0, 189.9; IR (ATR) ν: 2985, 2008, 1475, 1008, 831 cm^{-1}; HRMS (ESI) Calcd for $C_{11}H_9BrCs$, $[M+Cs]^+$352.8942, found 352.8947; yellow oil (5%, 25.6 mg)

2-(2-cyclopropylidenevinyl)naphthalene (9e)

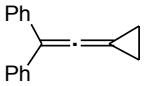


^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.69-1.82 (m, 4H), 6.46 (ddd, 1H, J = 7.2, 3.6, 3.6 Hz), 7.38-7.48 (m, 3H), 7.76 (s, 1H), 7.73-7.82 (m, 3H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 8.9, 80.2, 96.9, 124.8, 124.9, 125.3, 126.1, 127.6, 127.7, 128.0, 132.4, 133.4, 133.7, 190.3; IR (ATR) ν: 3045, 2006, 1597, 1508, 902, 822 cm^{-1}; HRMS (ESI) Calcd for $C_{15}H_{12}Cs$, $[M+Cs]^+$324.9994, found 324.9981; Colorless solid (mp: 63-65 °C, 13%, 124.1 mg)

Scheme S14. Synthesis of 9f[13-15]

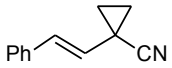


(2-cyclopropylideneethene-1,1-diyl)dibenzene (9f) (CAS-Reg# 1403484-23-0)



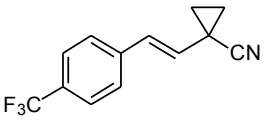
(40%, 187.6 mg)

(*E*)-1-styrylcyclopropanecarbonitrile (10a)



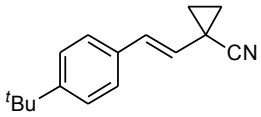
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.15-1.25 (m, 2H), 1.55-1.65 (m, 2H), 5.51 (d, 1H, *J* = 15.6 Hz), 6.80 (d, 1H, *J* = 15.6 Hz), 7.25-7.33 (m, 5H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 12.5, 16.8, 121.3, 126.1, 126.2, 127.9, 128.7, 130.8, 135.8; IR (ATR) ν: 3025, 2234, 1448, 1071, 963, 806 cm^{-1}; HRMS (ESI) Calcd for $C_{12}H_{11}CsN$, $[M+Cs]^+$ 301.9946, found 301.9939; Colorless oil (63%, 12.2 mg)

(*E*)-1-(4-(trifluoromethyl)styryl)cyclopropanecarbonitrile (10b)



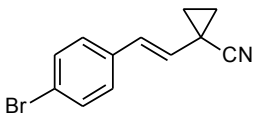
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.26 (dd, 2H, *J* = 7.2, 5.6 Hz), 1.66 (dd, 2H, *J* = 7.2, 5.6 Hz), 5.59 (d, 1H, *J* = 15.6 Hz), 6.84 (d, 1H, *J* = 15.6 Hz), 7.42 (d, 2H, *J* = 8.4 Hz), 7.56 (d, 2H, *J* = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 12.7, 17.1, 120.9, 125.6, 125.7, 126.3, 129.1, 129.4, 139.2; IR (ATR) ν: 3016, 2240, 1326, 1103, 1067, 967 cm^{-1}; HRMS (ESI) Calcd for $C_{13}H_{10}CsF_3N$, $[M+Cs]^+$369.9820, found 369.9826; Colorless solid (mp: 91-93 °C, 76%, 35.9 mg)

(*E*)-1-(4-(*tert*-butyl)styryl)cyclopropanecarbonitrile (10c)



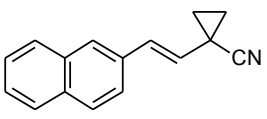
^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.15-1.21 (m, 2H), 1.31 (s, 9H), 1.58-1.62 (m, 2H), 5.48 (d, 1H, *J* = 16.0 Hz), 6.78 (d, 1H, *J* = 16.0 Hz), 7.26 (d, 2H, *J* = 8.4 Hz), 7.33 (d, 2H, *J* = 8.4 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 12.5, 16.8, 31.2, 34.6, 121.5, 125.4, 125.6, 125.8, 129.7, 130.6, 133.0; IR (ATR) ν: 2961, 2235, 963, 828 cm^{-1}; HRMS (ESI) Calcd for $C_{16}H_{19}CsN$, $[M+Cs]^+$358.0572, found 358.0562; Colorless solid (mp: 65-69 °C, 65%, 4.6 mg)

(*E*)-1-(4-bromostyryl)cyclopropanecarbonitrile (10d)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.20-1.23 (m, 2H), 1.61-1.65 (m, 2H), 5.50 (d, 1H, *J* = 16.0 Hz), 6.74 (d, 1H, *J* = 16.0 Hz), 7.19 (d, 2H, *J* = 8.0 Hz), 7.43 (d, 2H, *J* = 8.0 Hz); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 12.6,16.9, 121.1, 121.7, 127.1, 127.6, 129.7, 131.8, 134.8; IR (ATR) ν: 3016, 2237, 1488, 1068, 957 cm^{-1}; HRMS (ESI) Calcd for $C_{12}H_{10}BrCsN$, $[M+Cs]^+$379.9051, found 379.9043; Colorless solid (mp: 105-107 °C, 82%, 23.6 mg)

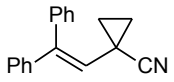
(*E*)-1-(2-(naphthalen-2-yl)vinyl)cyclopropanecarbonitrile (10e)



^{1}H-NMR ($CDCl_3$, 400 MHz) δ: 1.24 (dd, 2H, *J* = 6.8, 5.2 Hz), 1.63

(dd, 2H, J = 6.8, 5.2 Hz), 5.63 (d, 1H, J = 15.6 Hz), 6.96 (d, 1H, J = 15.6 Hz), 7.43-7.50 (m, 3H), 7.72-7.80 (m, 4H); ^{13}C-NMR ($CDCl_3$, 100 MHz) δ: 12.7, 16.9, 121.3, 123.0, 126.0, 126.2, 126.4, 126.5, 127.6, 128.0, 128.3, 130.8, 133.0, 133.2, 133.5; IR (ATR) ν: 3054, 2236, 969, 954, 818 cm^{-1}; HRMS (ESI) Calcd for $C_{16}H_{13}CsN$, $[M+Cs]^+$352.0102, found 352.0092; Colorless solid (mp: 93-95 °C, quant, 31.6 mg)

1-(2,2-diphenylvinyl)cyclopropanecarbonitrile (10f)



(CAS-Reg# 260261-08-3)

(17%, 7.9 mg)

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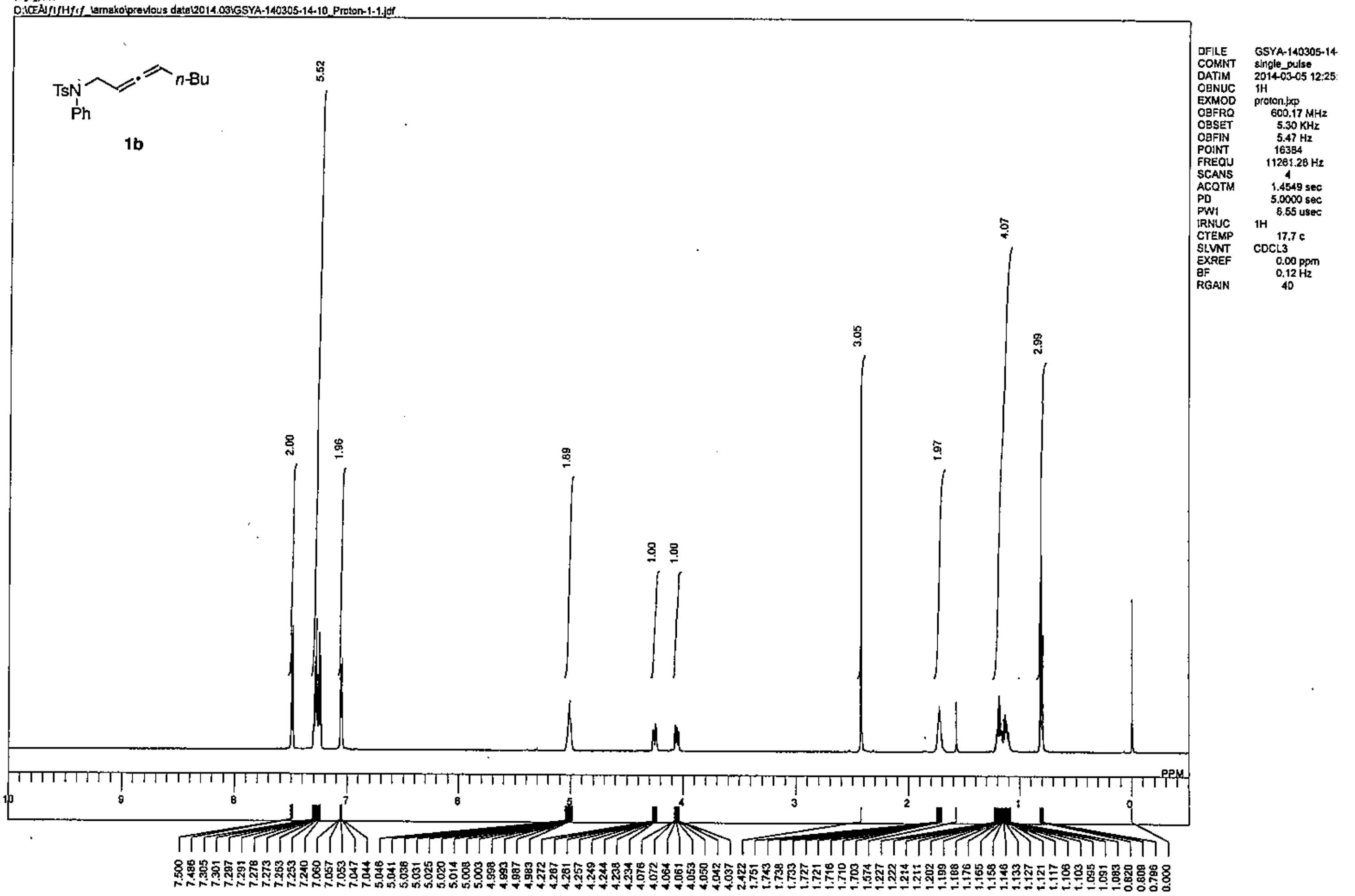
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PD 5.0000 sec
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1.00
1.00
3.05
1.97
4.07
2.99
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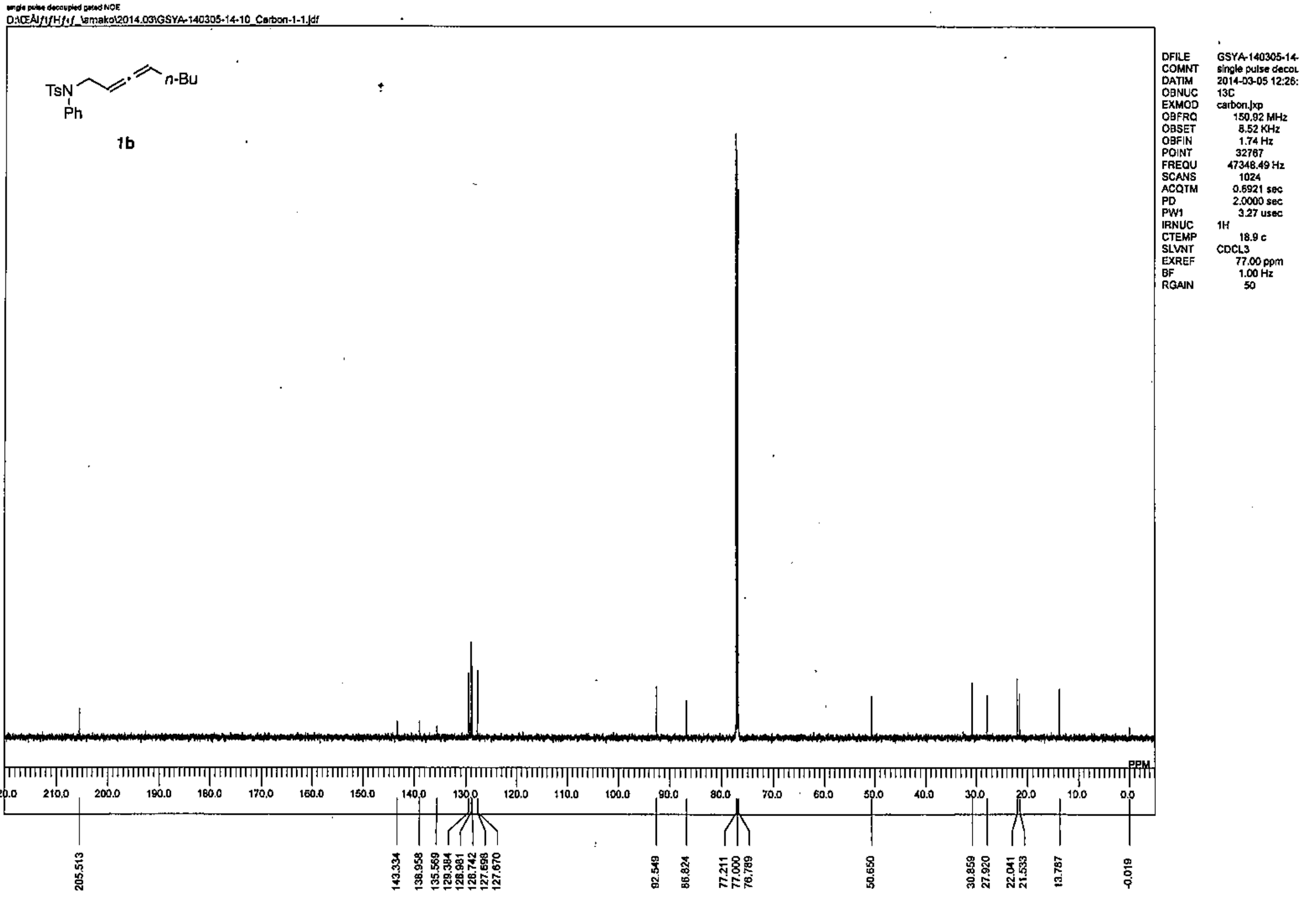
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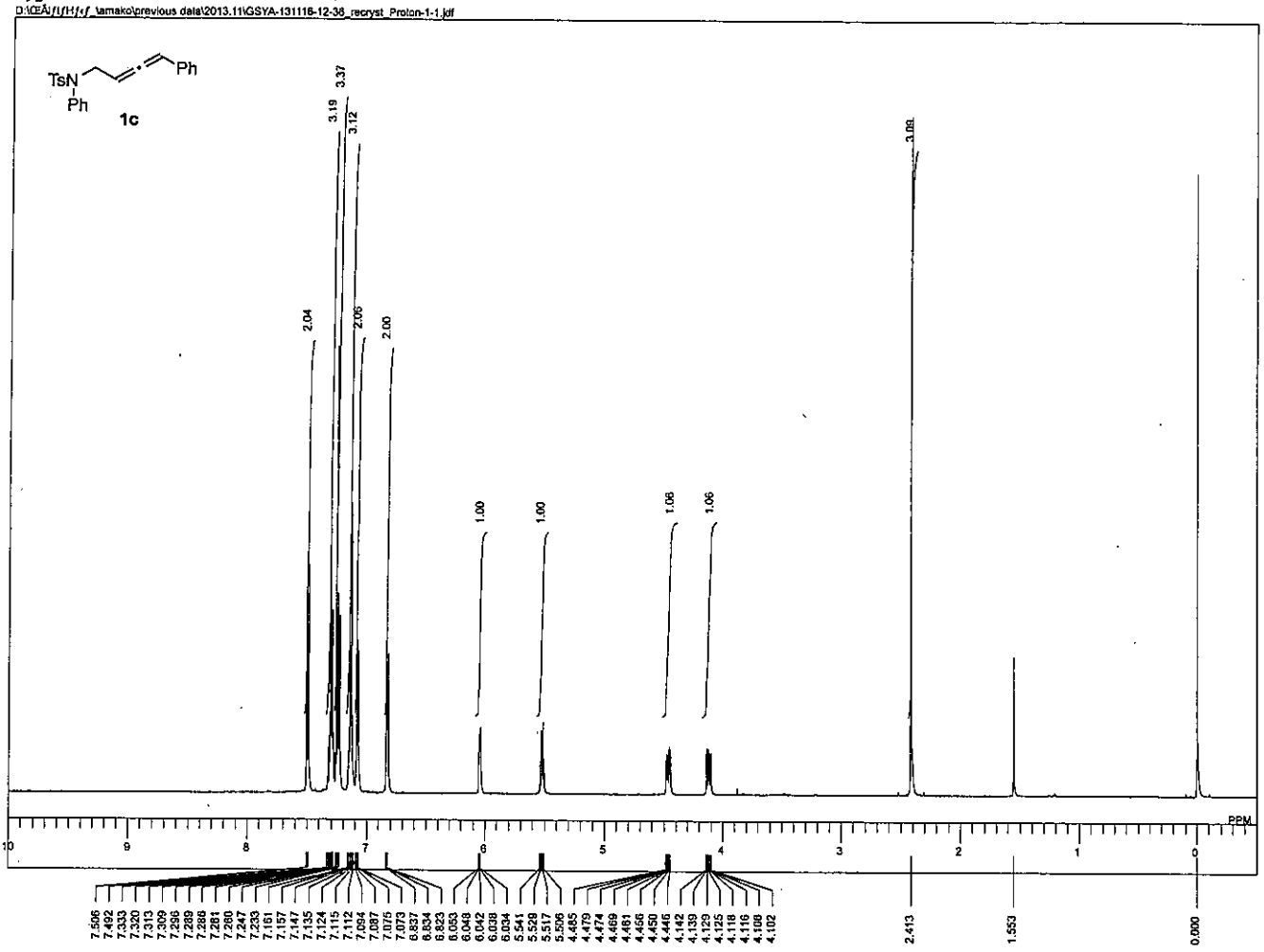

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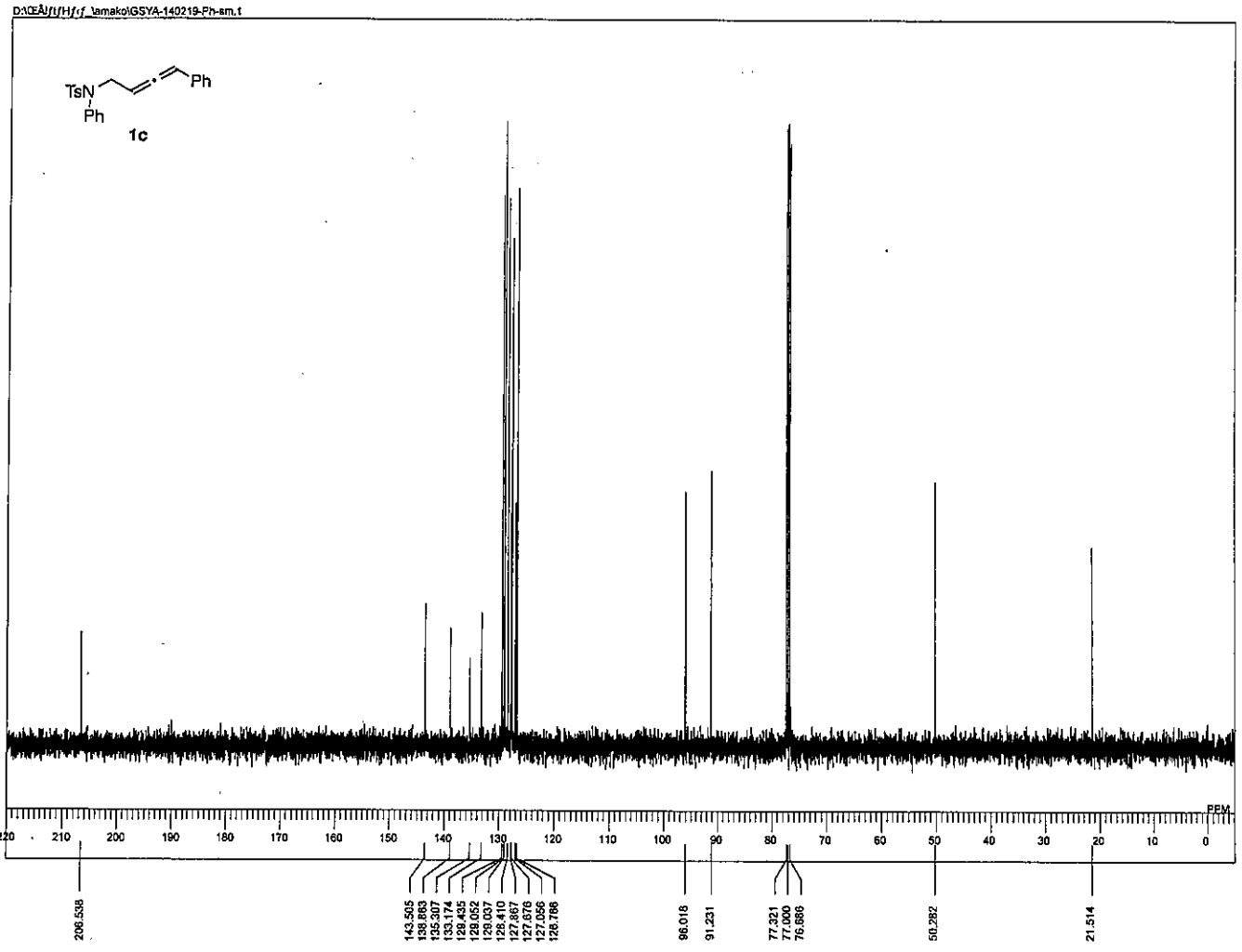

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PD 1.0000 sec
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CTEMP 21.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 23

single_pulse

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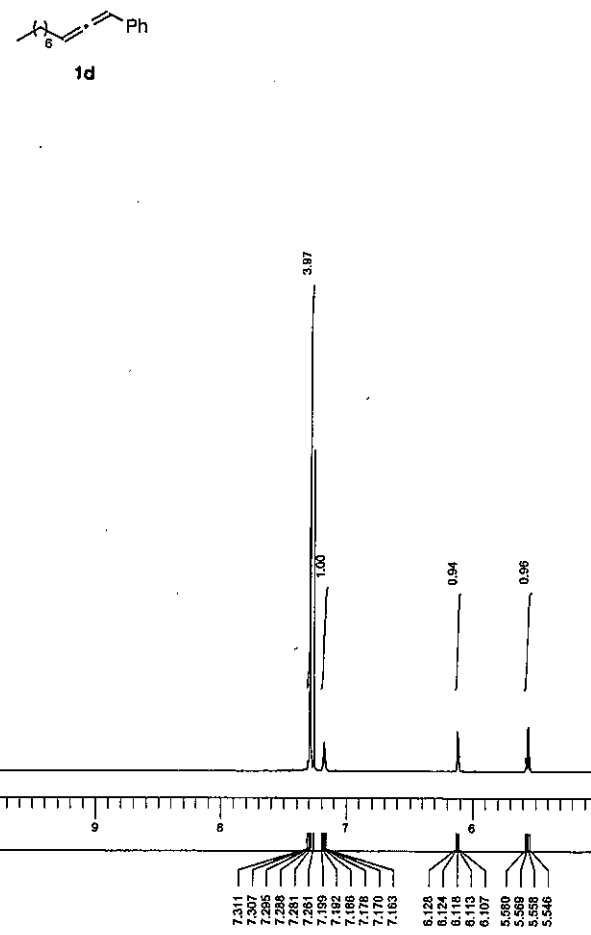

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POINT 16384
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SCANS 4
ACQTM 1.4549 sec
PD 5.0000 sec
PW1 6.55 usec
IRNUC 1H
CTEMP 18.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 48

D:\CEA\f1\H\cf_\amako\GSYA-131204-12-50.2

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PD 1.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 24

single_pulse
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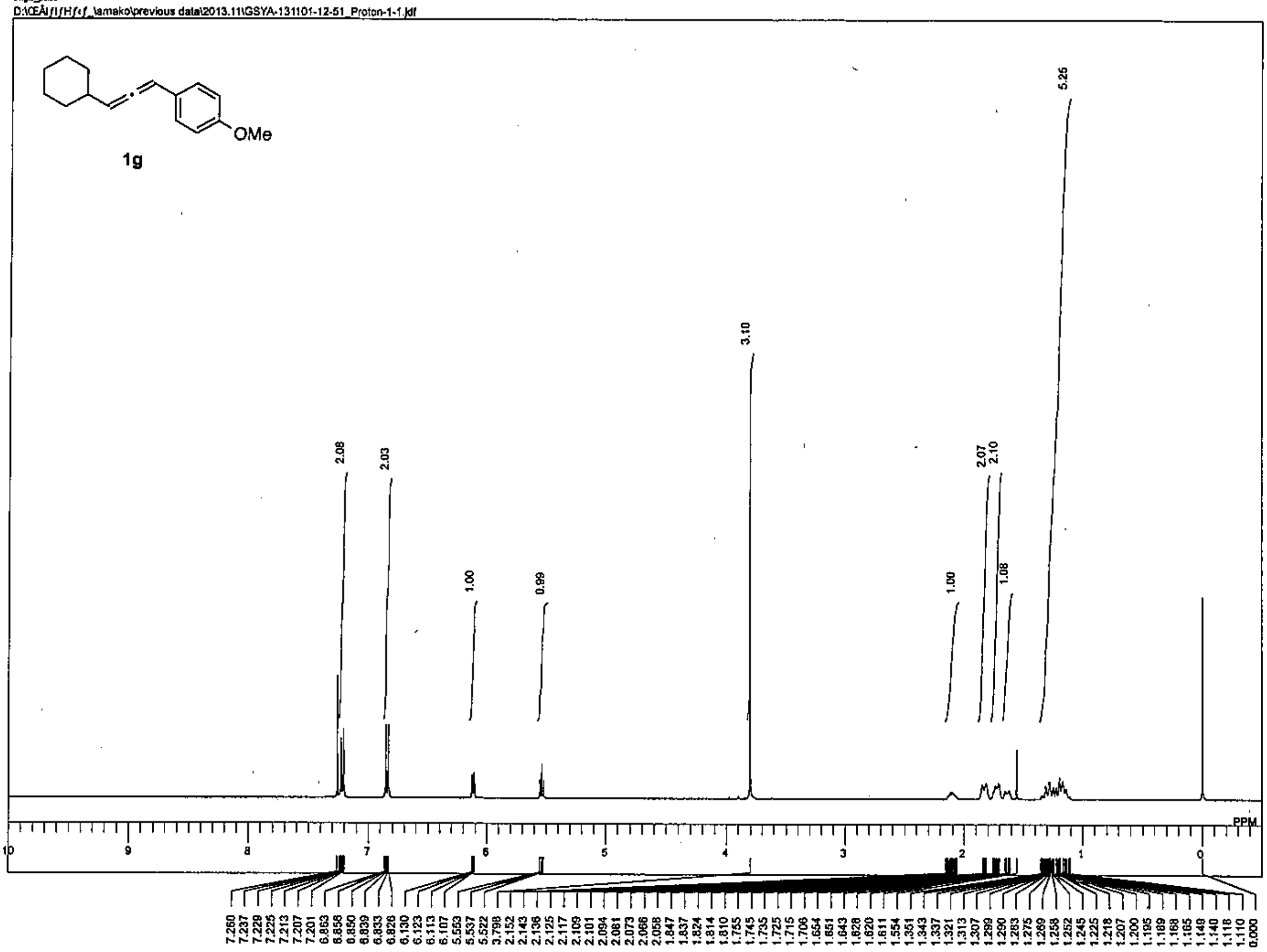

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0.99
3.10
1.00
2.07
2.10
1.08
5.25
PPM
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7.260 7.237 7.229 7.225 7.213 7.207 7.201 6.863 6.858 6.850 6.839 6.833 6.826 6.130 6.123 6.113 6.107 5.553 5.537 5.522 3.798 2.152 2.143 2.136 2.125 2.117 2.109 2.101 2.094 2.081 2.073 2.066 2.058 1.847 1.837 1.824 1.814 1.810 1.755 1.745 1.735 1.725 1.715 1.706 1.654 1.651 1.643 1.628 1.620 1.611 1.554 1.351 1.343 1.337 1.321 1.313 1.307 1.299 1.290 1.283 1.275 1.269 1.258 1.252 1.245 1.225 1.218 1.207 1.200 1.195 1.189 1.168 1.165 1.148 1.140 1.118 1.110 0.000

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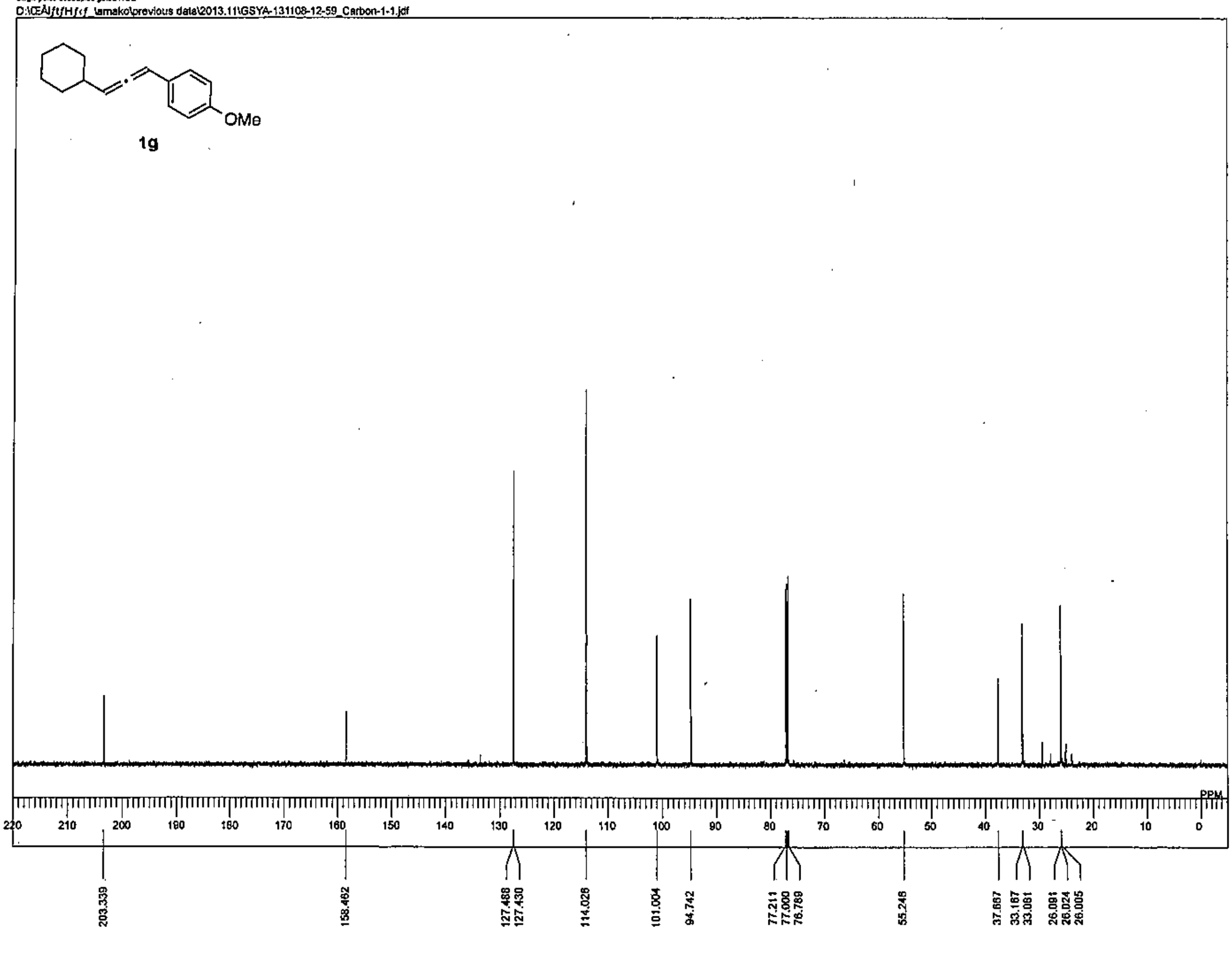

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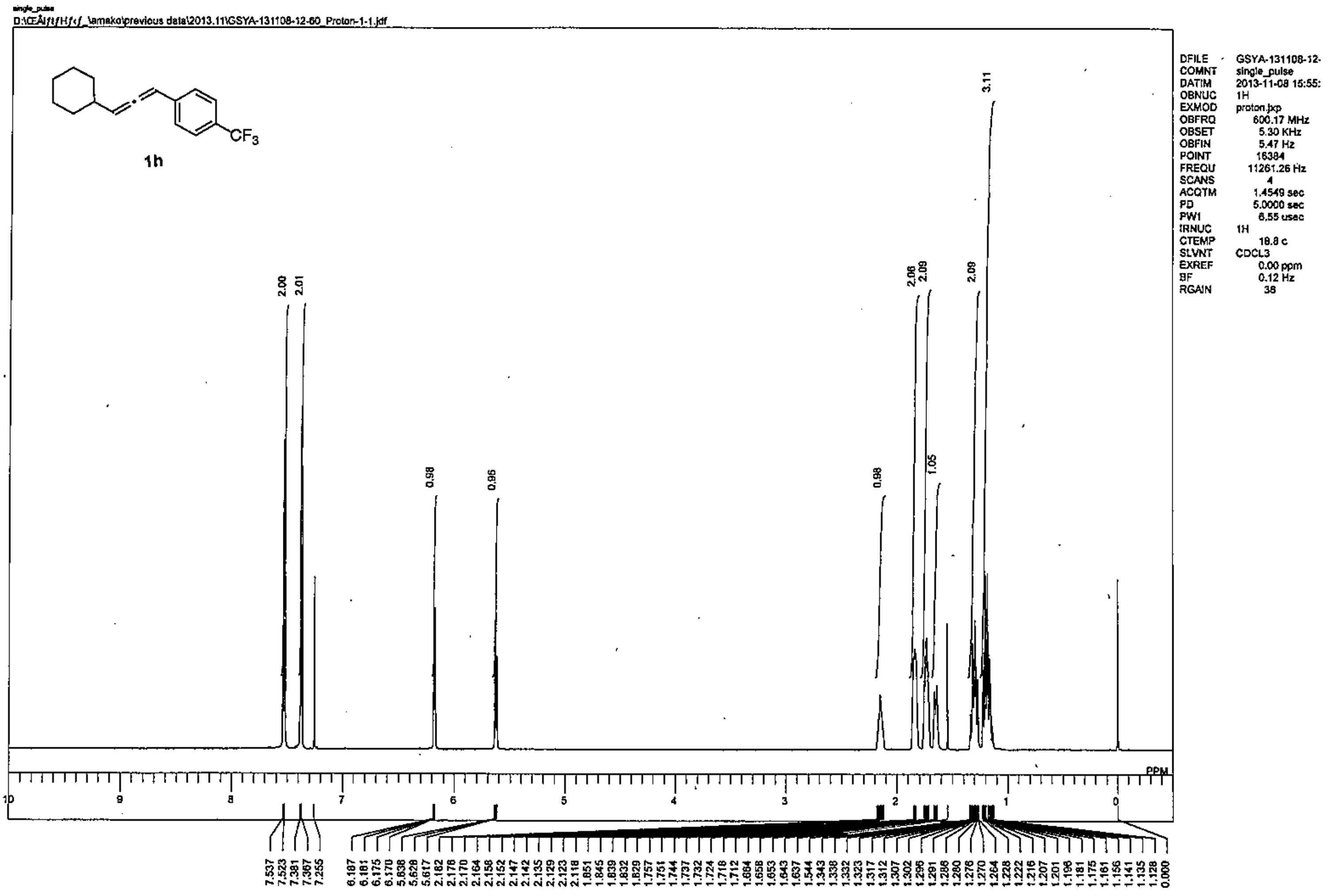

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POINT 16384
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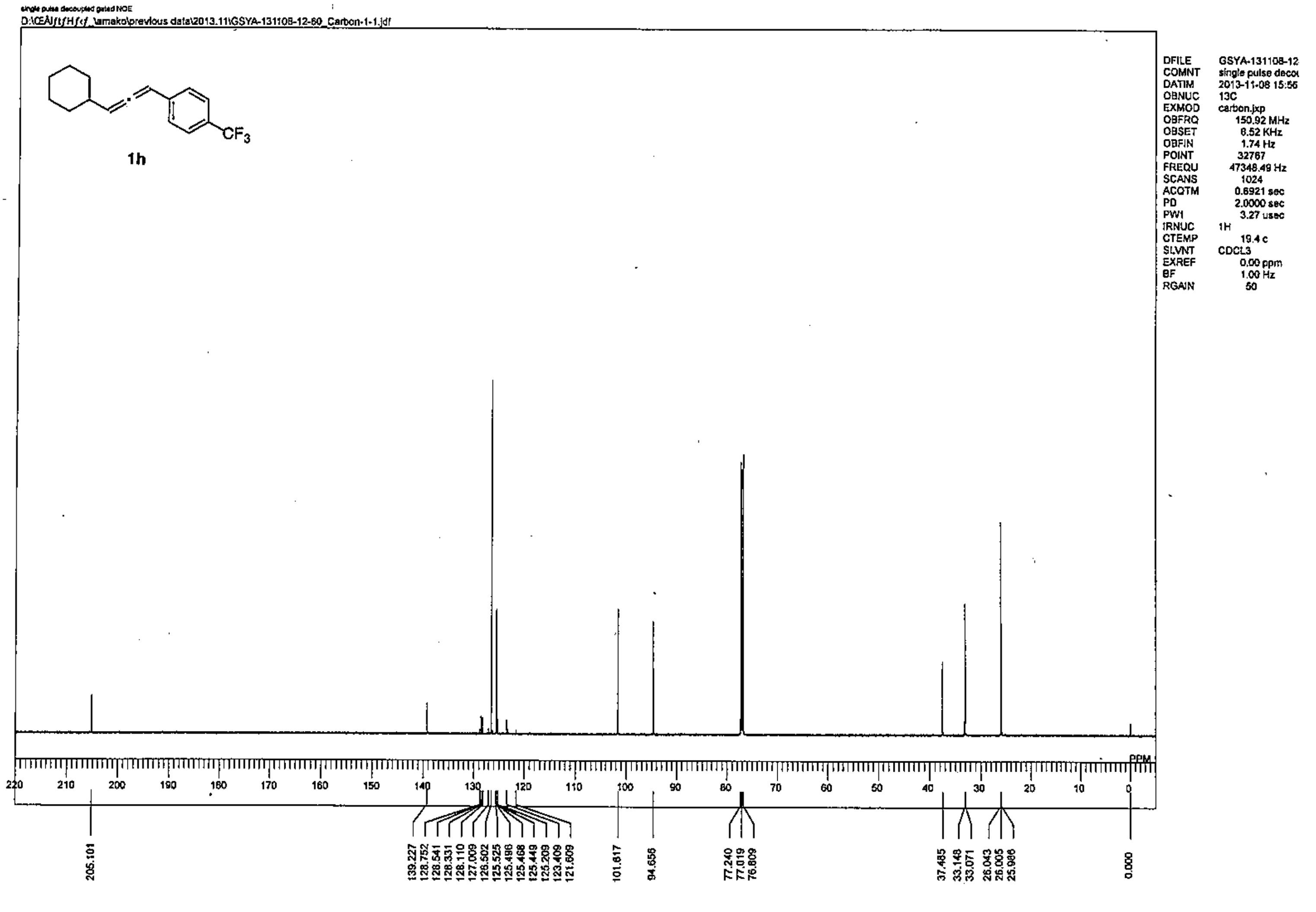
PD 5.0000 sec
PW1 6.55 usec
IRNUC 1H
CTEMP 18.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 38
2.00 2.01 0.98 0.96 0.98 2.06 2.09 1.05 2.09 3.11
PPM
10 9 8 7 6 5 4 3 2 1 0
7.537 7.523 7.381 7.367 7.255 6.187 6.181 6.175 6.170 5.638 5.628 5.617 2.182 2.176 2.170 2.164 2.158 2.152 2.142 2.135 2.129 2.123 2.118 1.851 1.845 1.839 1.832 1.829 1.757 1.751 1.744 1.737 1.732 1.724 1.718 1.712 1.664 1.658 1.653 1.643 1.637 1.544 1.343 1.338 1.332 1.323 1.317 1.312 1.307 1.302 1.296 1.291 1.288 1.280 1.276 1.270 1.264 1.228 1.222 1.216 1.207 1.201 1.196 1.181 1.175 1.161 1.156 1.141 1.135 1.128 0.000



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CTEMP 19.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
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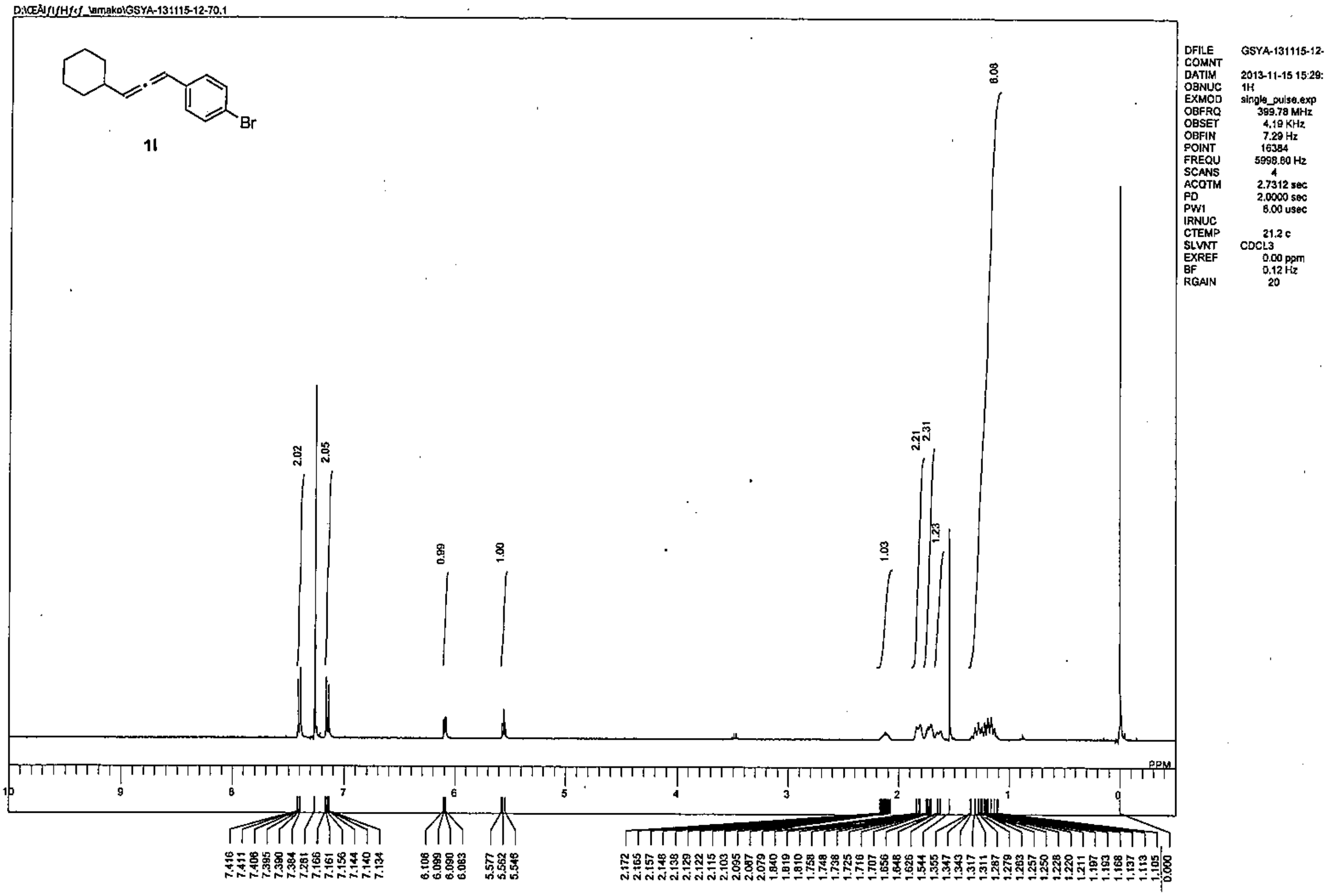
205.101 139.227 128.752 128.541 128.331 128.110 127.009 126.502 125.525 125.496 125.468 125.449 125.209 123.409 121.609 101.617 94.656 77.240 77.019 76.809 37.485 33.148 33.071 26.043 26.005 25.986 0.000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CTEMP 21.2 c
SLVNT CDCL3
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BF 0.12 Hz
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2.05
0.99
1.00
1.03
2.21
2.31
1.23
6.08
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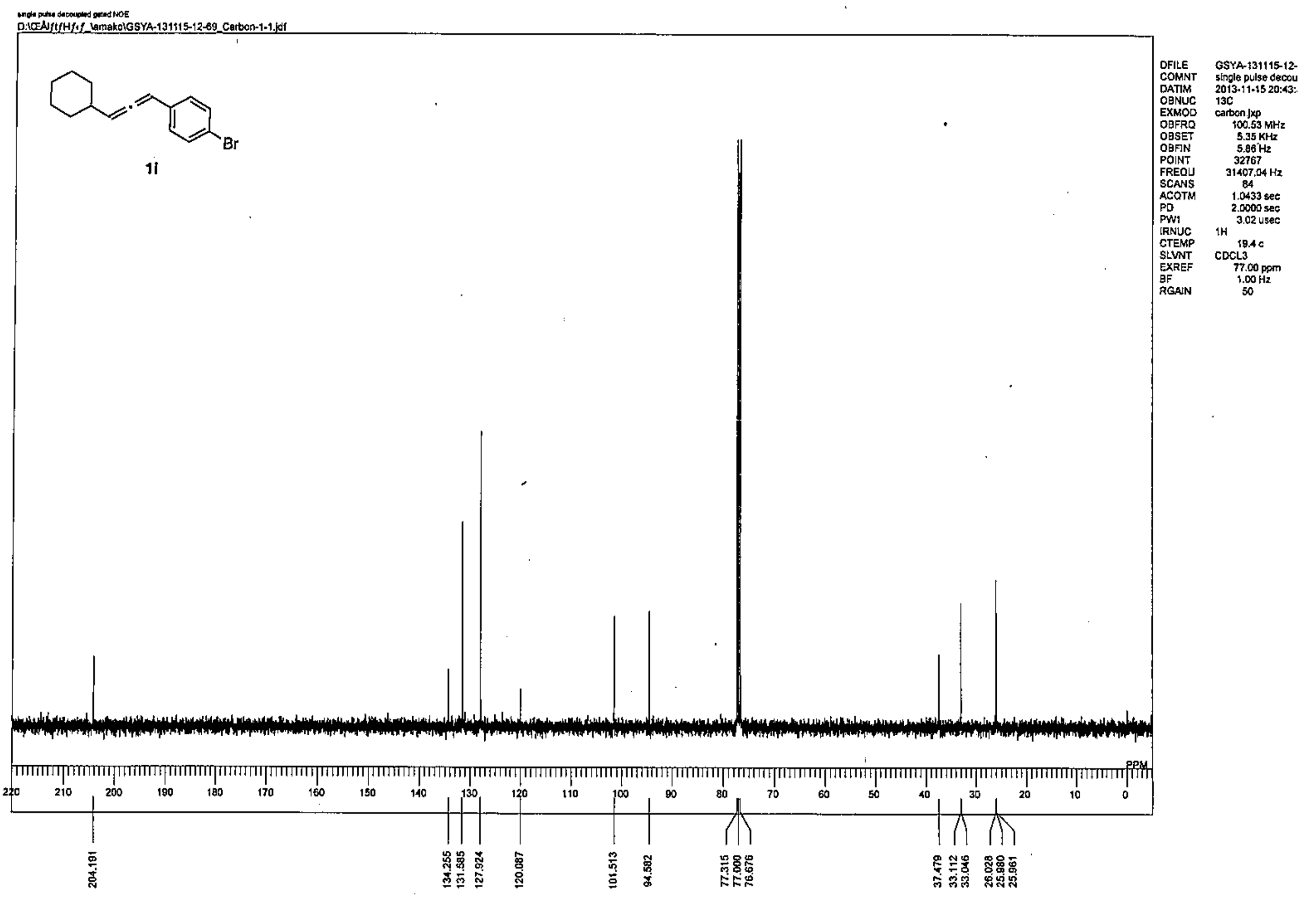
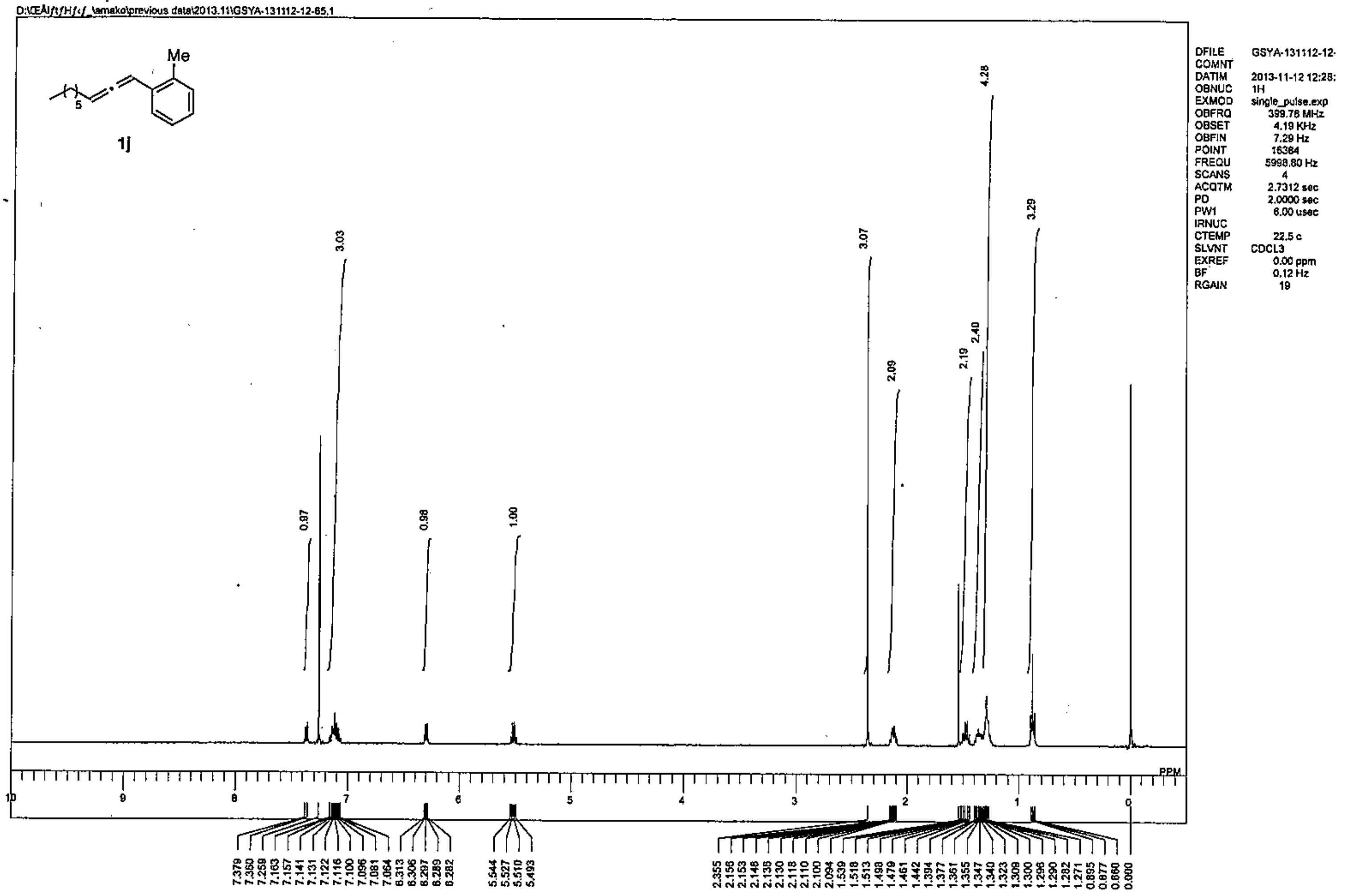
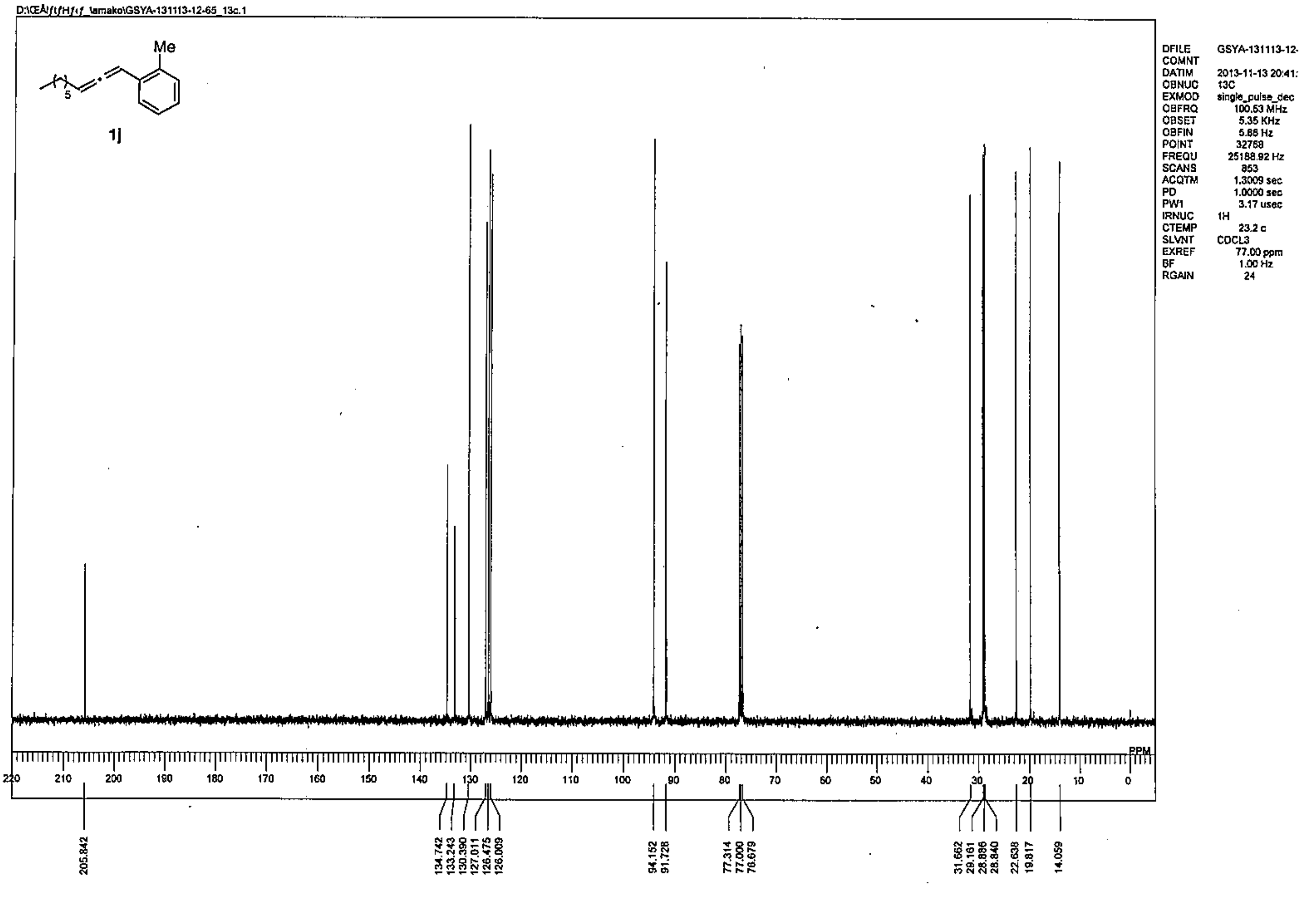
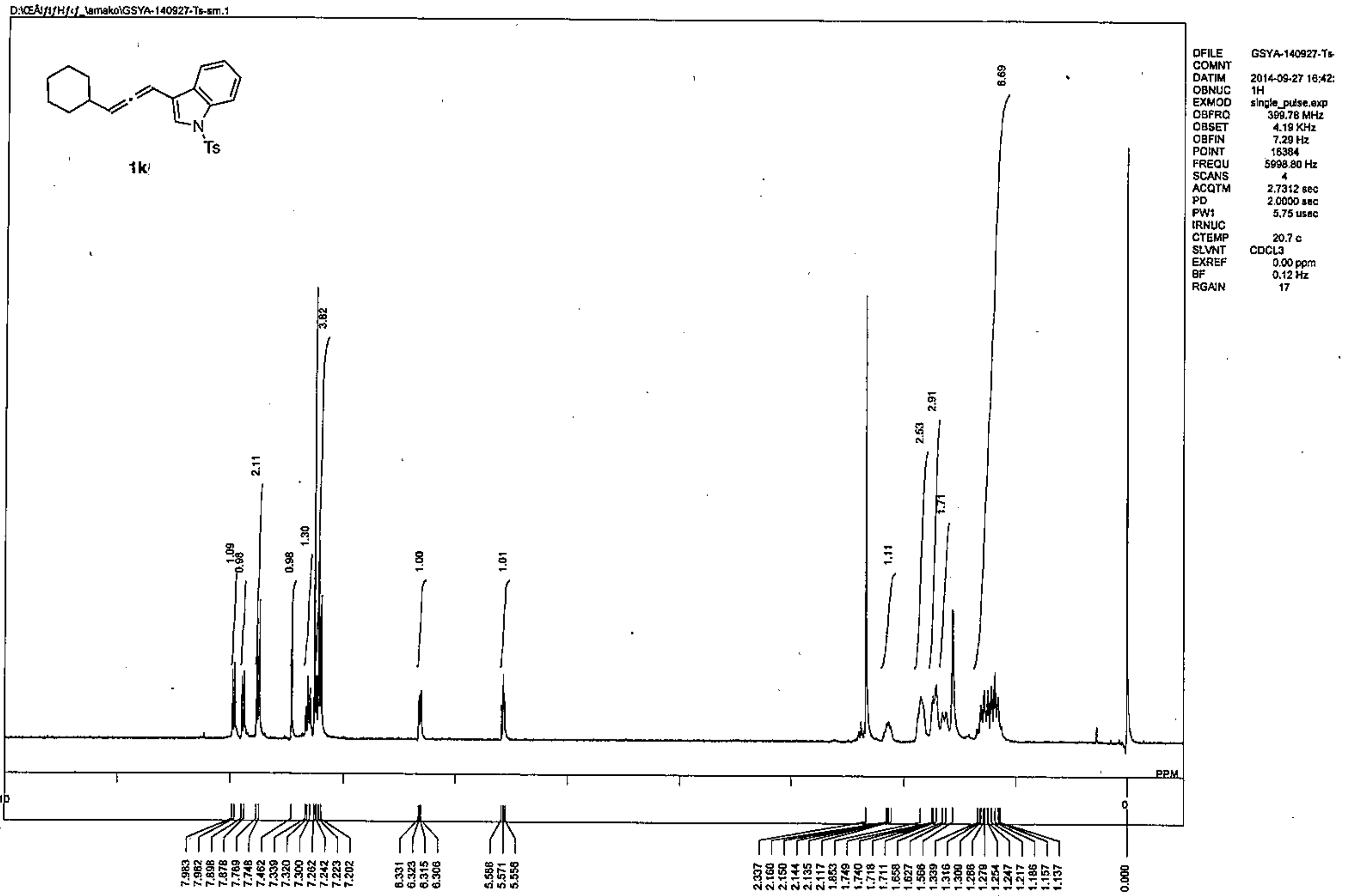
6.108 6.099 6.090 6.083
5.577 5.562 5.546
2.172 2.165 2.157 2.148 2.138 2.129 2.122 2.115 2.103 2.095 2.087 2.079 1.840 1.819 1.810 1.758 1.748 1.738 1.725 1.716 1.707 1.656 1.648 1.626 1.544 1.355 1.347 1.343 1.317 1.311 1.287 1.279 1.263 1.257 1.250 1.228 1.220 1.211 1.197 1.193 1.168 1.137 1.113 1.105 0.000


single pulse decoupled gated NOE
Br
1l
DFILE GSYA-131115-12-
COMNT single pulse decou
DATIM 2013-11-15 20:43:
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31407.04 Hz
SCANS 84
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50
PPM
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
204.191
134.255 131.585 127.924
120.087
101.513
94.582
77.315 77.000 76.676
37.479 33.112 33.046
26.028 25.980 25.961

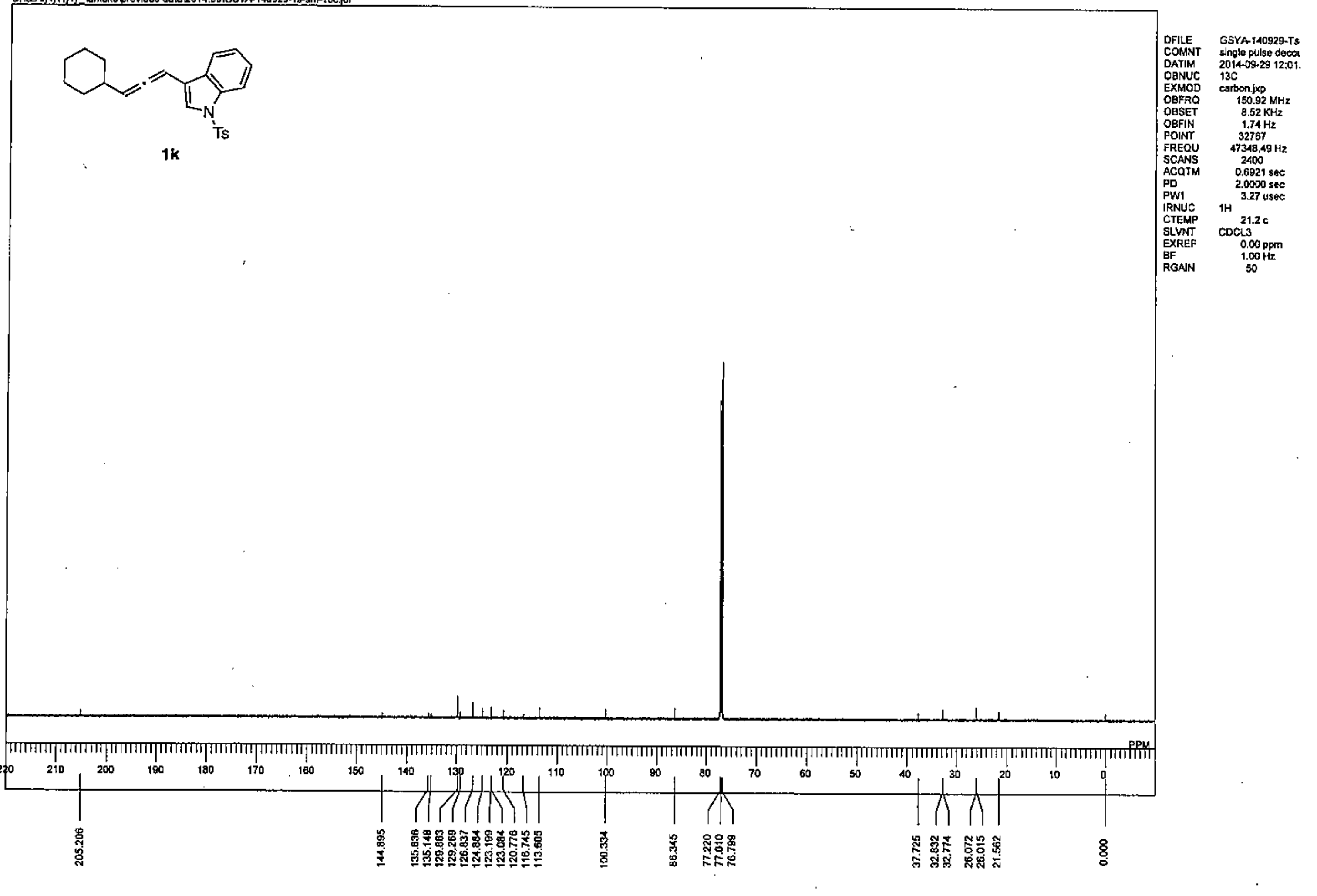

D:\ŒÃÌƒtƒHƒ‹ƒ_\amako\previous data\2013.11\GSYA-131112-12-65.1
Me
5
1j
DFILE GSYA-131112-12-
COMNT
DATIM 2013-11-12 12:28:
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 4
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.00 usec
IRNUC
CTEMP 22.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 19
0.97
3.03
0.98
1.00
3.07
2.09
2.19
2.40
4.28
3.29
PPM
7.379 7.360 7.259 7.163 7.157 7.141 7.131 7.122 7.116 7.100 7.096 7.081 7.064 6.313 6.306 6.297 6.289 6.282
5.544 5.527 5.510 5.493
2.355 2.158 2.153 2.146 2.135 2.130 2.118 2.110 2.100 2.094 1.539 1.518 1.513 1.498 1.479 1.461 1.442 1.394 1.377 1.361 1.355 1.347 1.340 1.323 1.309 1.300 1.296 1.290 1.282 1.271 0.895 0.877 0.860 0.000


D:\ŒÃÌƒtƒHƒ‹ƒ_\amako\GSYA-131113-12-65_13c.1
Me
5
1j
DFILE GSYA-131113-12-
COMNT
DATIM 2013-11-13 20:41:
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.88 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 853
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.17 usec
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 24
PPM
205.842
134.742 133.243 130.390 127.011 126.475 126.009
94.152 91.728
77.314 77.000 76.679
31.662 29.161 28.886 28.840 22.638 19.817 14.059

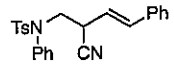
D:\ŒÂl ƒtƒHƒ_\amako\GSYA-140927-Ts-sm.1


N
Ts
1k
DFILE GSYA-140927-Ts-
COMNT
DATIM 2014-09-27 16:42:
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 4
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 5.75 usec
IRNUC
CTEMP 20.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17
1.09
0.98
2.11
0.98
1.30
3.82
1.00
1.01
1.11
2.53
2.91
1.71
8.69
PPM
10
0
7.983
7.982
7.898
7.878
7.769
7.748
7.462
7.339
7.320
7.300
7.262
7.242
7.223
7.202
6.331
6.323
6.315
6.306
5.588
5.571
5.558
2.337
2.160
2.144
2.135
2.117
1.853
1.749
1.740
1.718
1.711
1.658
1.627
1.566
1.339
1.316
1.300
1.288
1.279
1.254
1.247
1.217
1.185
1.157
1.137
0.000

single pulse decoupled gated NOE
D:\ŒÂl ƒtƒHƒ_\amako\previous data\2014.09\GSYA-140929-Ts-sm-13c.jdf


N
Ts
1k
DFILE GSYA-140929-Ts
COMNT single pulse decou
DATIM 2014-09-29 12:01
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 2400
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 21.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50
PPM
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
205.206
144.895
135.836
135.148
129.863
129.269
126.837
124.884
123.199
123.084
120.778
116.745
113.605
100.334
88.345
77.220
77.010
76.799
37.725
32.832
32.774
26.072
26.015
21.562
0.000

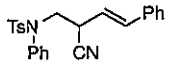
D:\CEÅ/tfH/cf_\amako\previous data\2014.02\GSYA-140205-tm.1



2ca

DFILE	GSYA-140205-tm.
COMNT	
DATIM	2014-02-05 11:00:
OBNUC	1H
EXMOD	single_pulse.exp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.20 Hz
POINT	16384
FREQU	5998.80 Hz
SCANS	4
ACQTM	2.7312 sec
PD	2.0000 sec
PW1	6.00 usec
IRNUC	
CTEMP	20.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	21

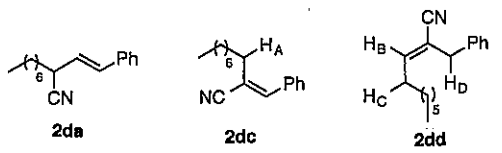
D:\CEÅ/tfH/cf_\amako\previous data\2014.02\GSYA-140211-Ph-tm.1



2ca

DFILE	GSYA-140211-Ph-
COMNT	
DATIM	2014-02-11 12:42:
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	25188.92 Hz
SCANS	675
ACQTM	1.3009 sec
PD	1.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	22.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	24

single_pulse
D:\CEA\f\f\Hf\f_\amako\previous data\2013.11\GSYA-131105-12-53_Proton-1-1.jdf



2da

2dc

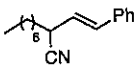
2dd

DFILE	GSYA-131105-12
COMNT	single_pulse
DATIM	2013-11-05 12:39
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	600.17 MHz
OBSET	5.30 KHz
OBFIN	5.47 Hz
POINT	16384
FREQU	11261.26 Hz
SCANS	4
ACQTM	1.4549 sec
PD	5.0000 sec
PW1	6.55 usec
IRNUC	1H
CTEMP	18.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.00 Hz
RGAIN	44

7.433 7.421 7.410 7.396 7.387 7.374 7.352 7.340 7.327 7.300 7.292 7.280 7.268 7.261 7.220 6.732 6.705 6.463 6.411 6.458 6.062 6.050 6.035 6.024

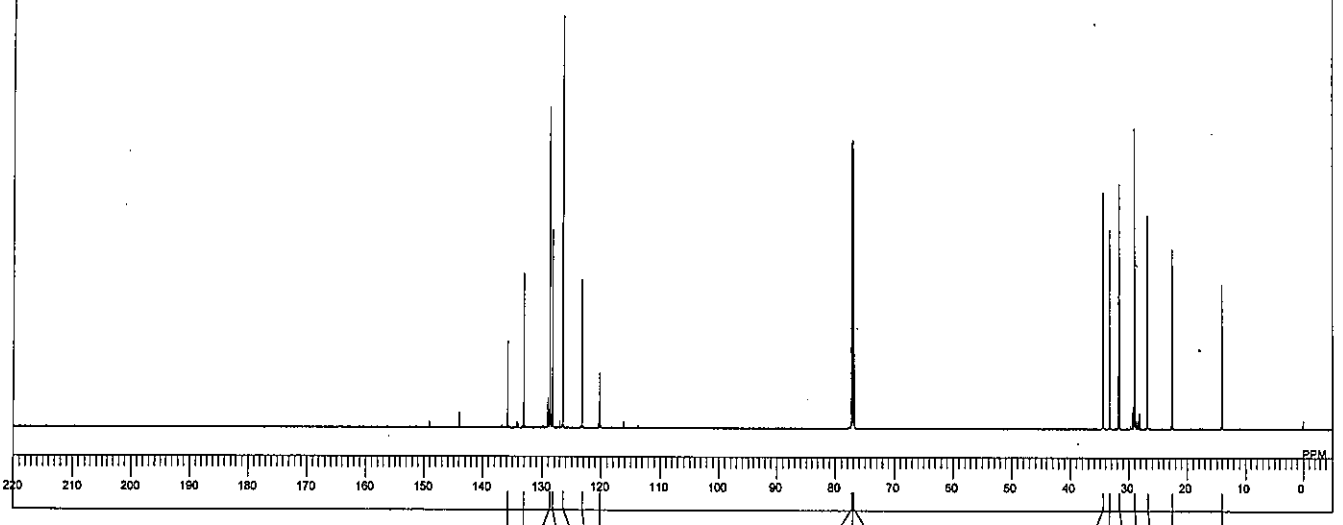
3.547 3.439 3.428 3.416 3.406 2.469 2.457 2.443 2.316 2.304 2.292 2.278 1.813 1.803 1.790 1.784 1.774 1.768 1.763 1.758 1.751 1.746 1.736 1.725 1.672 1.659 1.647 1.560 1.551 1.537 1.525 1.522 1.511 1.504 1.493 1.482 1.469 1.454 1.441 1.433 1.359 1.349 1.331 1.316 1.306 1.294 1.283 1.278 0.896 0.884 0.873 0.864 0.071 0.000

single pulse decoupled gated NOE
D:\CEA\f\f\Hf\f_\amako\previous data\2013.11\GSYA-131105-12-53_Carbon-1-2.jdf



2da

DFILE	GSYA-131105-12-
COMNT	single pulse decou
DATIM	2013-11-06 05:07:
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	150.92 MHz
OBSET	8.52 KHz
OBFIN	1.74 Hz
POINT	32767
FREQU	47348.49 Hz
SCANS	4800
ACQTM	0.6921 sec
PD	2.0000 sec
PW1	3.27 usec
IRNUC	1H
CTEMP	19.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.00 Hz
RGAIN	50



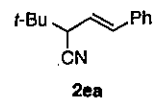
135.770 133.108 128.694 128.206 128.511 123.256 120.240

77.259 77.048 76.838

34.402 33.301 31.702 28.992 28.689 22.586 14.075

single_pulse

D:\CEÅ\ƒ1\H\ƒ±ƒ_\amako\previous data\2013.11\GSYA-131121-12-63_Proton-1-1.jdf

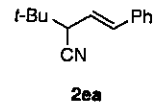


2ea

DFILE	GSYA-131121-12-
COMNT	single_pulse
DATIM	2013-11-21 19:00:
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	15384
FREQU	7503.00 Hz
SCANS	4
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	20.4 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	50

single pulse decoupled gated NOE

D:\CEÅ\ƒ1\H\ƒ±ƒ_\amako\previous data\2013.12\GSYA-131202-tBu-Im_Carbon-1-1.jdf



2ea

DFILE	GSYA-131202-tBu
COMNT	single pulse deco
DATIM	2013-12-02 17:02
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	150.92 MHz
OBSET	8.52 KHz
OBFIN	1.74 Hz
POINT	32767
FREQU	47348.49 Hz
SCANS	1024
ACQTM	0.6921 sec
PD	2.0000 sec
PW1	3.27 usec
IRNUC	1H
CTEMP	19.5 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	50

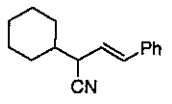
single_pulse

D:\CEÅ/ƒ‡H/ƒ‹_\amako\previous data\2013.10\GSYA-131010-12-9_Proton-1-1.jdf

2fa

DFILE GSYA-131010-12-
COMNT single_pulse
DATIM 2013-10-10 12:17:
OBNUC 1H
EXMOD proton.jxp
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 16384
FREQU 11261.26 Hz
SCANS 4
ACQTM 1.4549 sec
PD 5.0000 sec
PW1 6.55 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 40

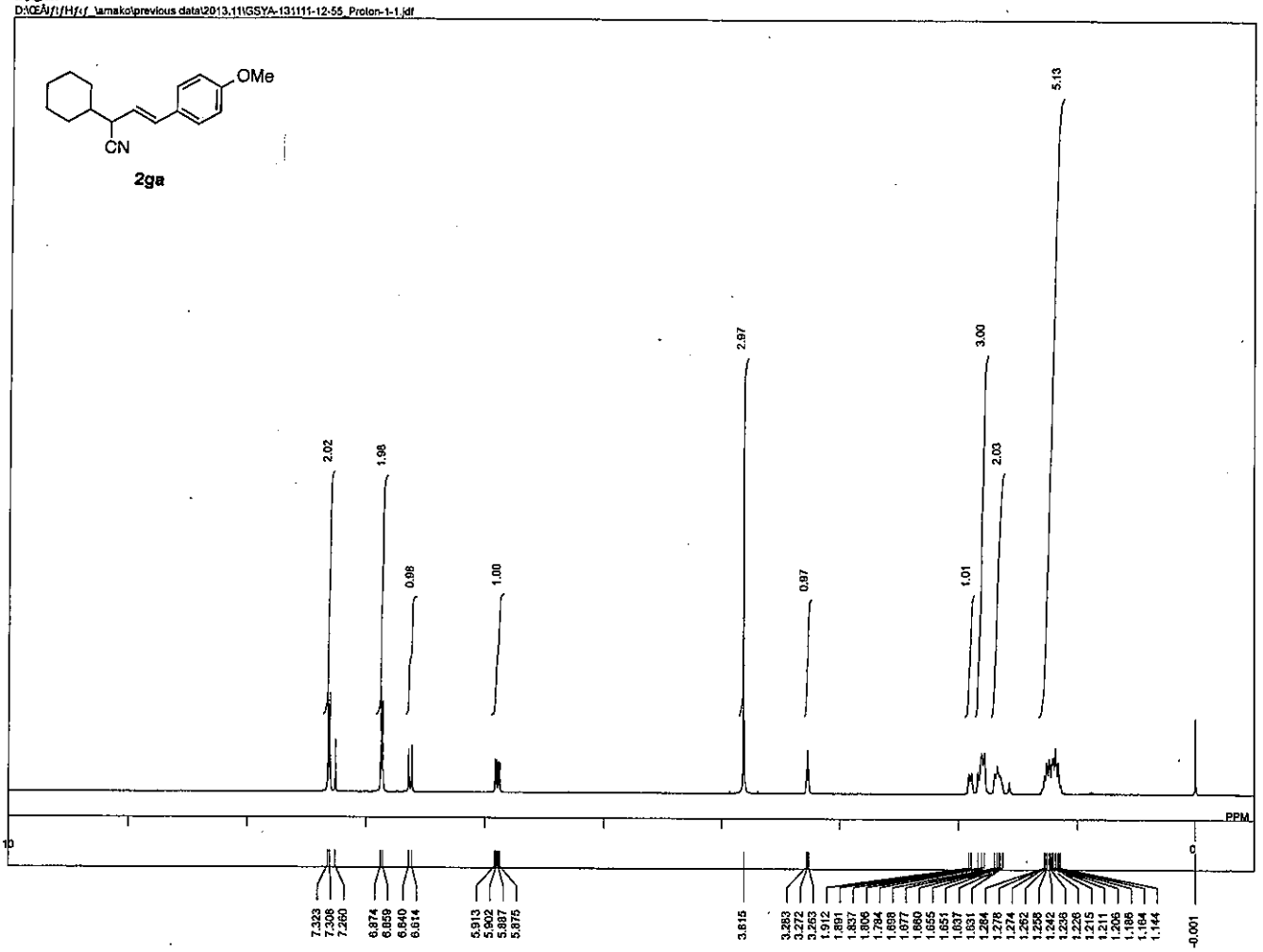
D:\CEÅ/ƒ‡H/ƒ‹_\amako\previous data\2013.10\GSYA-131004-12-9.1



2fa

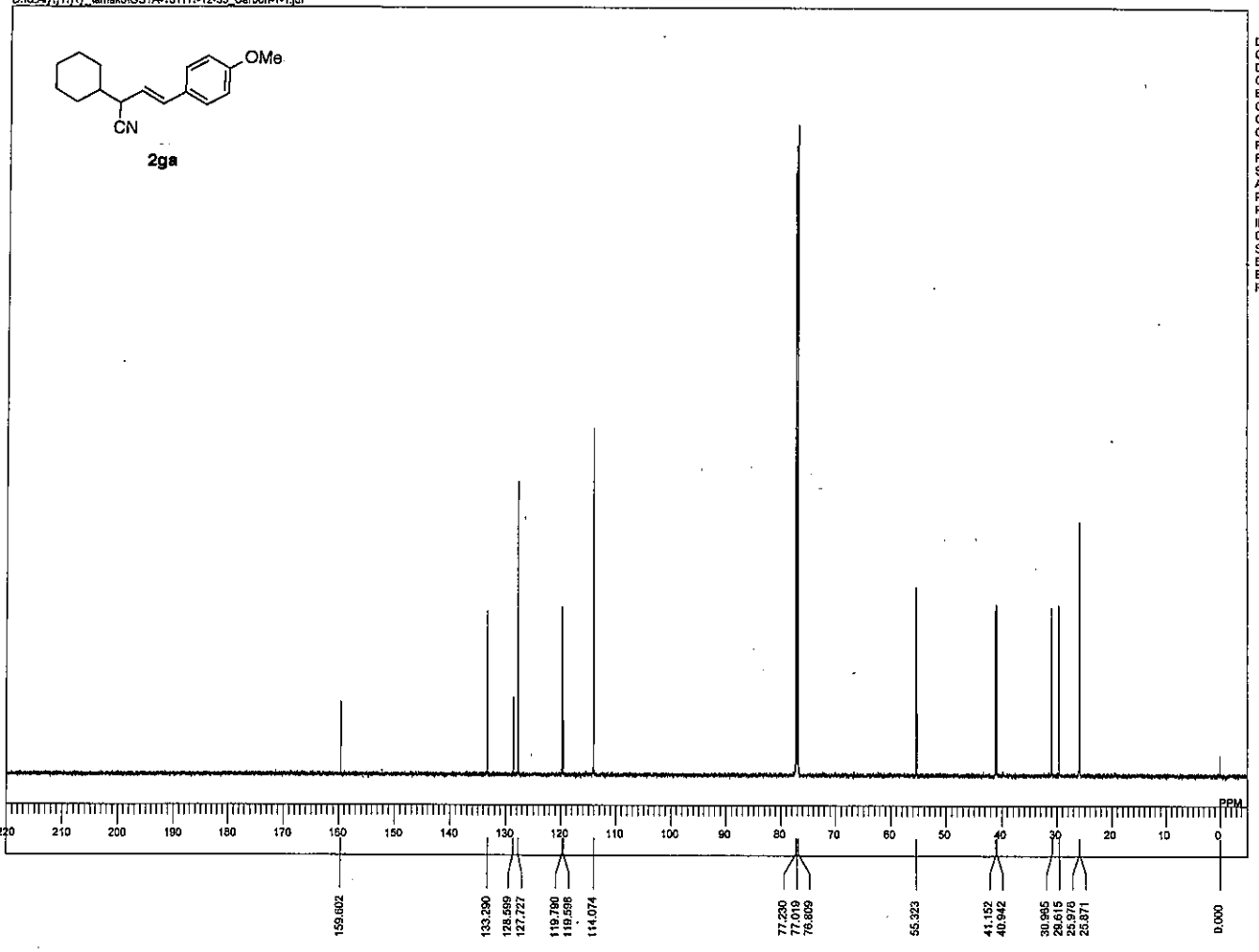
DFILE GSYA-131004-12-
COMNT
DATIM 2013-10-04 11:12:
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 1000
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.17 usec
IRNUC 1H
CTEMP 24.1 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 24

single_pulse
D:\CEÂ\f1\H\ƒ‹f_\amako\previous data\2013.11\GSYA-131111-12-55_Proton-1-1.jdf



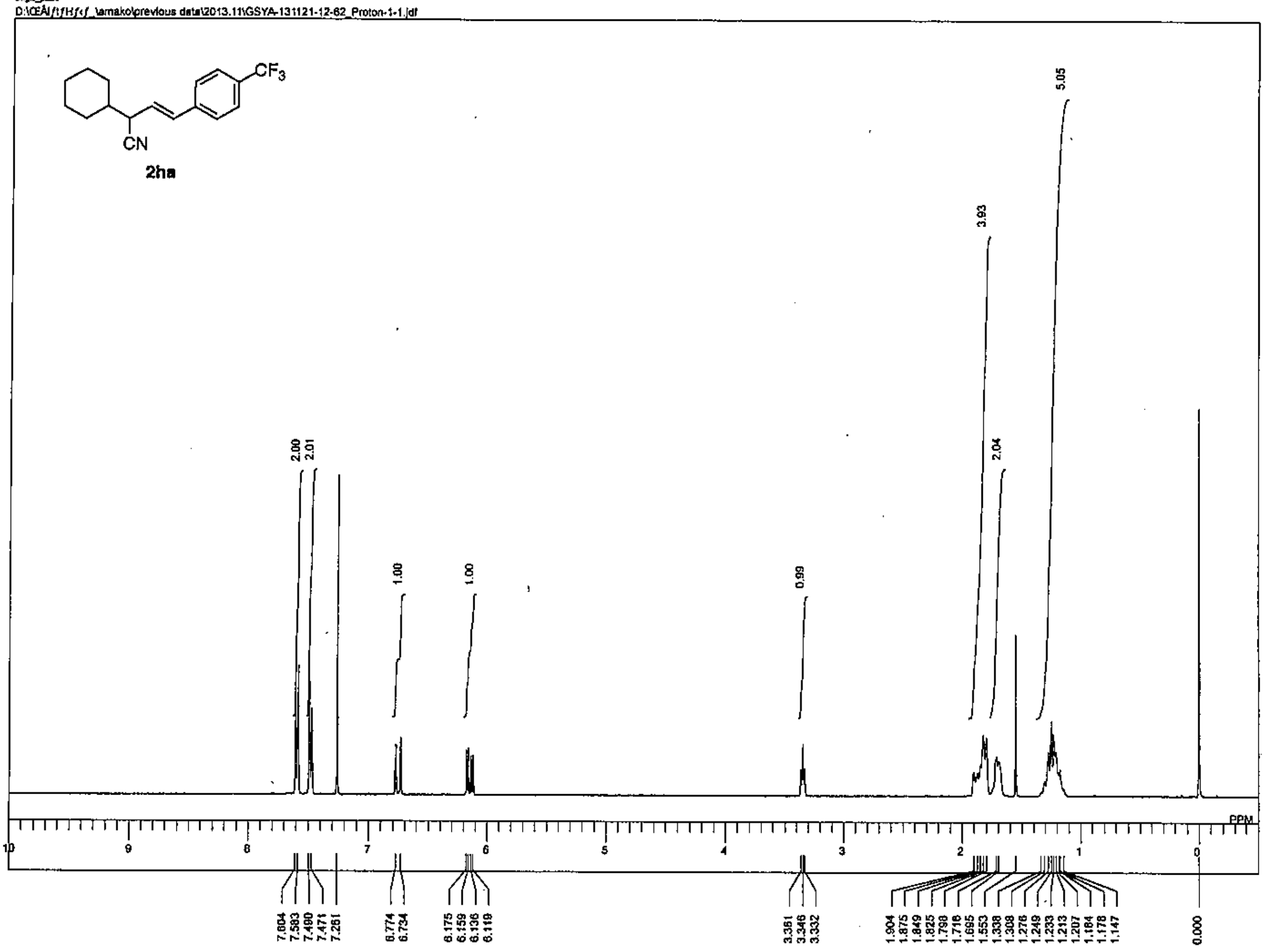
DFILE GSYA-131111-12-
COMNT single_pulse
DATIM 2013-11-11 15:12:
OBNUC 1H
EXMOD proton.jxp
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 15384
FREQU 11261.26 Hz
SCANS 4
ACQTM 1.4548 sec
PD 5.0000 sec
PW1 6.55 usec
IRNUC 1H
CTEMP 18.5 c
SLVNT CDCL3
EXREF 7.26 ppm
BF 0.12 Hz
RGAIN 40

single pulse decoupled gated NOE
D:\CEÂ\f1\H\ƒ‹f_\amako\GSYA-131111-12-55_Carbon-1-1.jdf



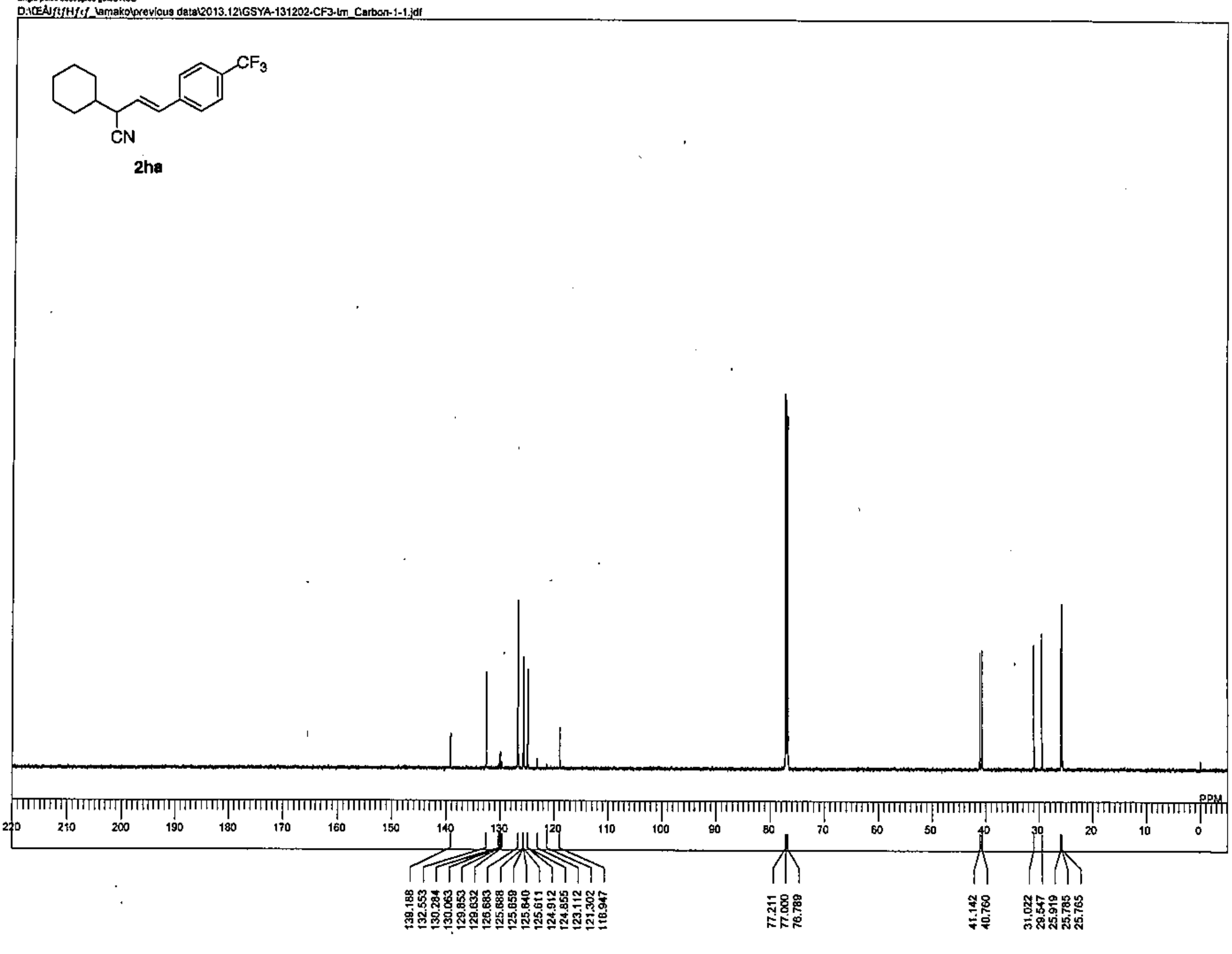
DFILE GSYA-131111-12-
COMNT single pulse decou
DATIM 2013-11-11 15:13:
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 819
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50

single_pulse
D:\ŒÂl\ƒtƒHƒ‹ƒ_\amako\previous data\2013.11\GSYA-131121-12-62_Proton-1-1.jdf

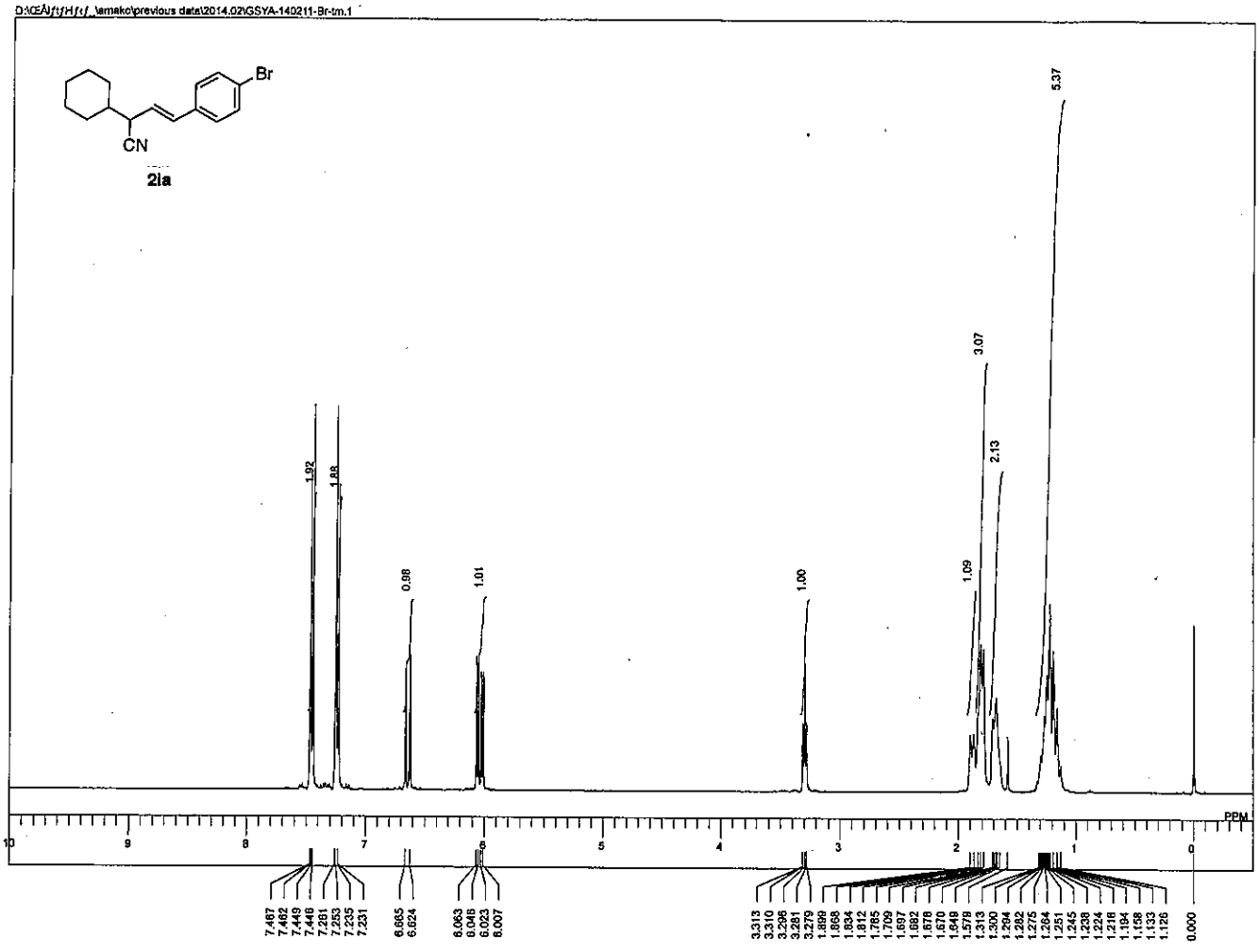


DFILE GSYA-131121-12-
COMNT single_pulse
DATIM 2013-11-21 19:05:
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 4
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 50

single pulse decoupled gated NOE
D:\ŒÂl\ƒtƒHƒ‹ƒ_\amako\previous data\2013.12\GSYA-131202-CF3-tm_Carbon-1-1.jdf



DFILE GSYA-131202-CF
COMNT single pulse decou
DATIM 2013-12-02 17:54:
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 1024
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 19.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50


D:\CEA\ft\H\ft_\amako\previous data\2014.02\GSYA-140211-Br-1m.1
Br
CN
2ia
DFILE GSYA-140211-Br
COMNT
DATIM 2014-02-11 14:58
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 4
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.00 usec
IRNUC
CTEMP 19.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 11
1.92
1.88
0.98
1.01
1.00
1.09
3.07
2.13
5.37
PPM
7.467
7.462
7.449
7.446
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7.253
7.235
7.231
6.665
6.624
6.063
6.046
6.023
6.007
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3.310
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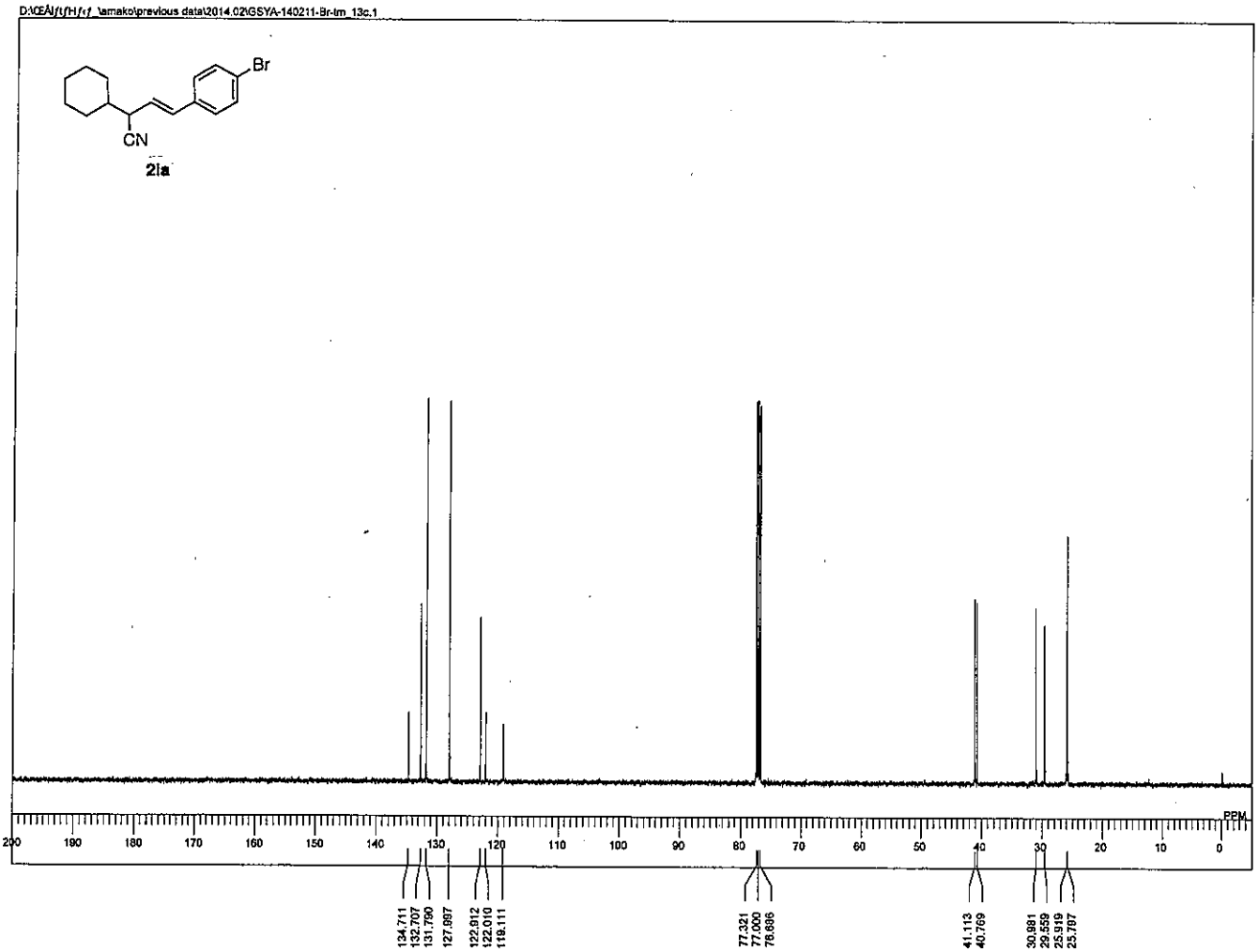
0.000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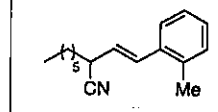
Br
CN
2ia
DFILE GSYA-140211-Br
COMNT
DATIM 2014-02-11 15:50
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 1328
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.17 usec
IRNUC 1H
CTEMP 20.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 23
PPM
134.711
132.707
131.790
127.997
122.912
122.010
119.111
77.321
77.000
76.686
41.113
40.769
30.981
29.559
25.919
25.787

D:\ŒÀ¡f¦H¦c¦_\amako\2015.01\GSYA-150123-18-23_tm.1



2ja

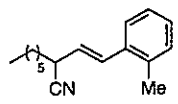
DFILE	GSYA-150123-18
COMNT	
DATIM	2015-01-23 12:15
OBNUC	1H
EXMOD	single_pulse.exp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	5998.80 Hz
SCANS	4
ACQTM	2.7312 sec
PD	2.0000 sec
PW1	5.75 usec
IRNUC	
CTEMP	21.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	18

7.393 7.380 7.370 7.290 7.201 7.195 7.187 7.179 7.171 7.164 7.159 7.148 6.852 6.848 6.813 6.810 5.939 5.923 5.900 5.883

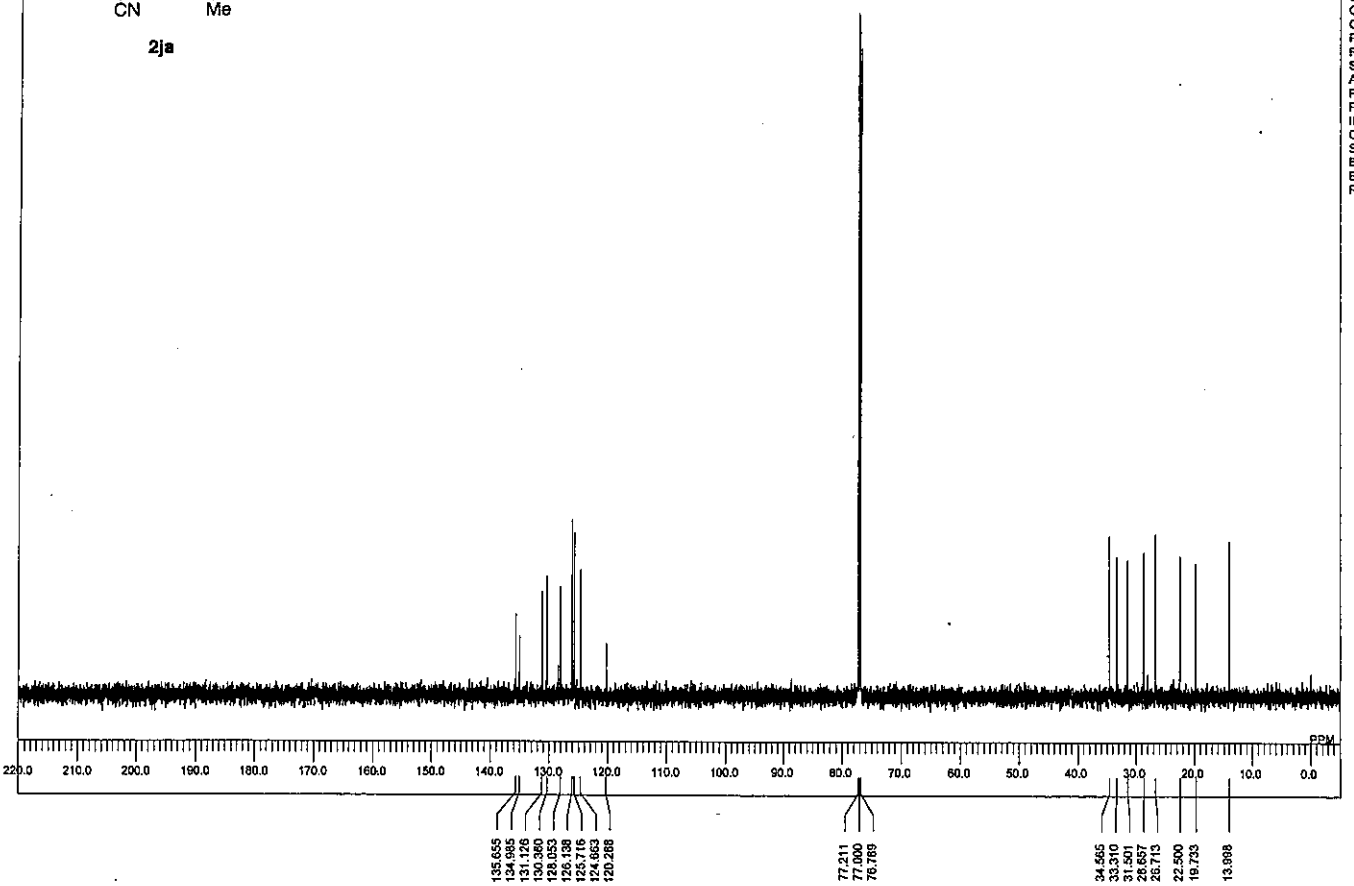
3.466 3.462 3.446 3.430 3.414 3.411 2.362 1.828 1.811 1.803 1.795 1.792 1.787 1.781 1.776 1.769 1.765 1.751 1.748 1.732 1.595 1.579 1.559 1.553 1.545 1.520 1.503 1.493 1.477 1.466 1.461 1.444 1.391 1.372 1.355 1.342 1.317 1.310 1.283 1.234 0.911 0.894 0.876 0.000

single pulse decoupled gated NOE

D:\ŒÀ¡f¦H¦c¦_\amako\GSYA-140215-12-68_tm_Carbon-1-1.jdf



2ja



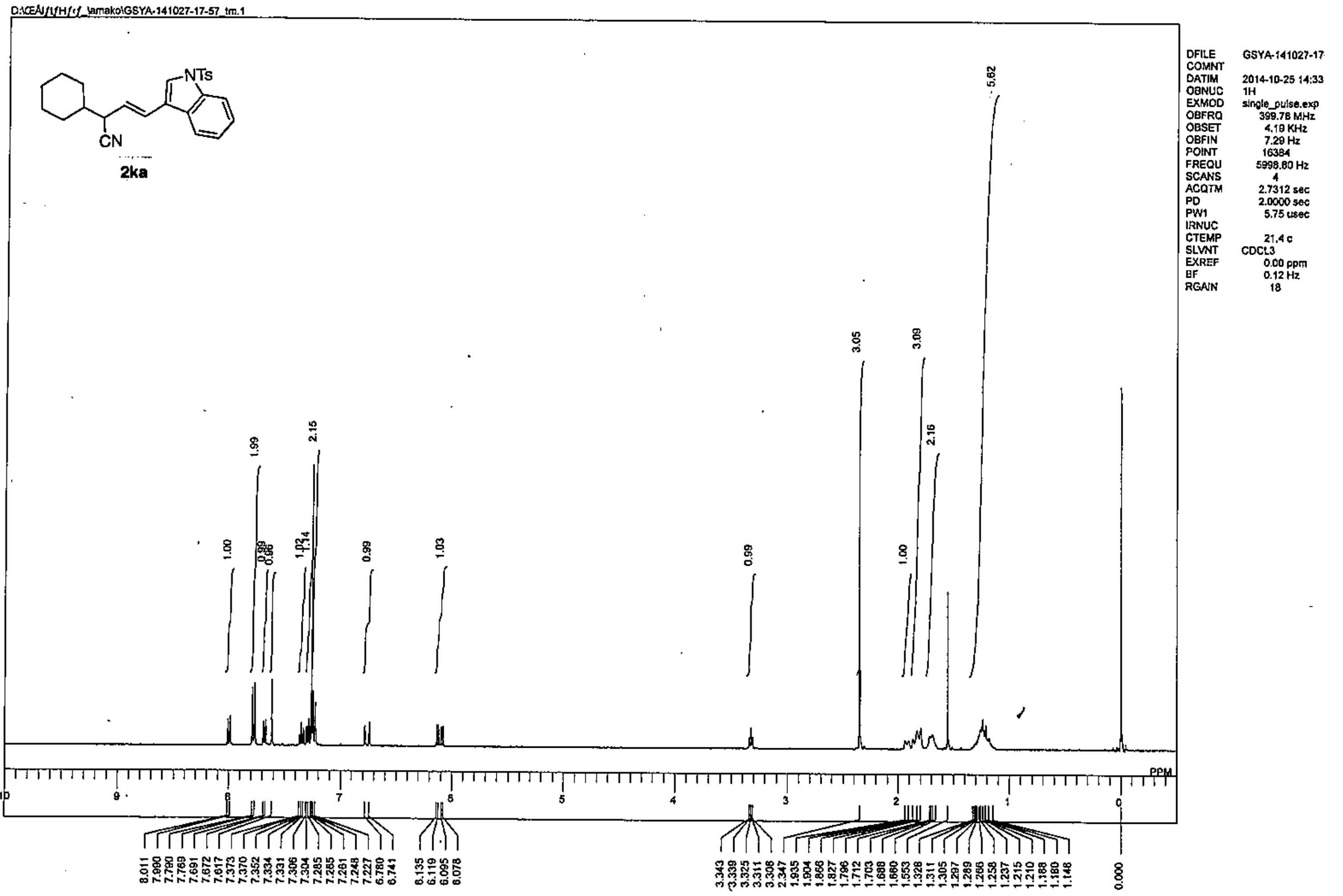
DFILE	GSYA-140215-12-
COMNT	single pulse decou
DATIM	2014-02-15 14:37:
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	150.92 MHz
OBSET	8.52 KHz
OBFIN	1.74 Hz
POINT	32767
FREQU	47348.49 Hz
SCANS	43
ACQTM	0.6921 sec
PD	2.0000 sec
PW1	3.27 usec
IRNUC	1H
CTEMP	18.2 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	50

135.655 134.985 131.126 130.360 128.053 126.138 125.716 124.663 120.288

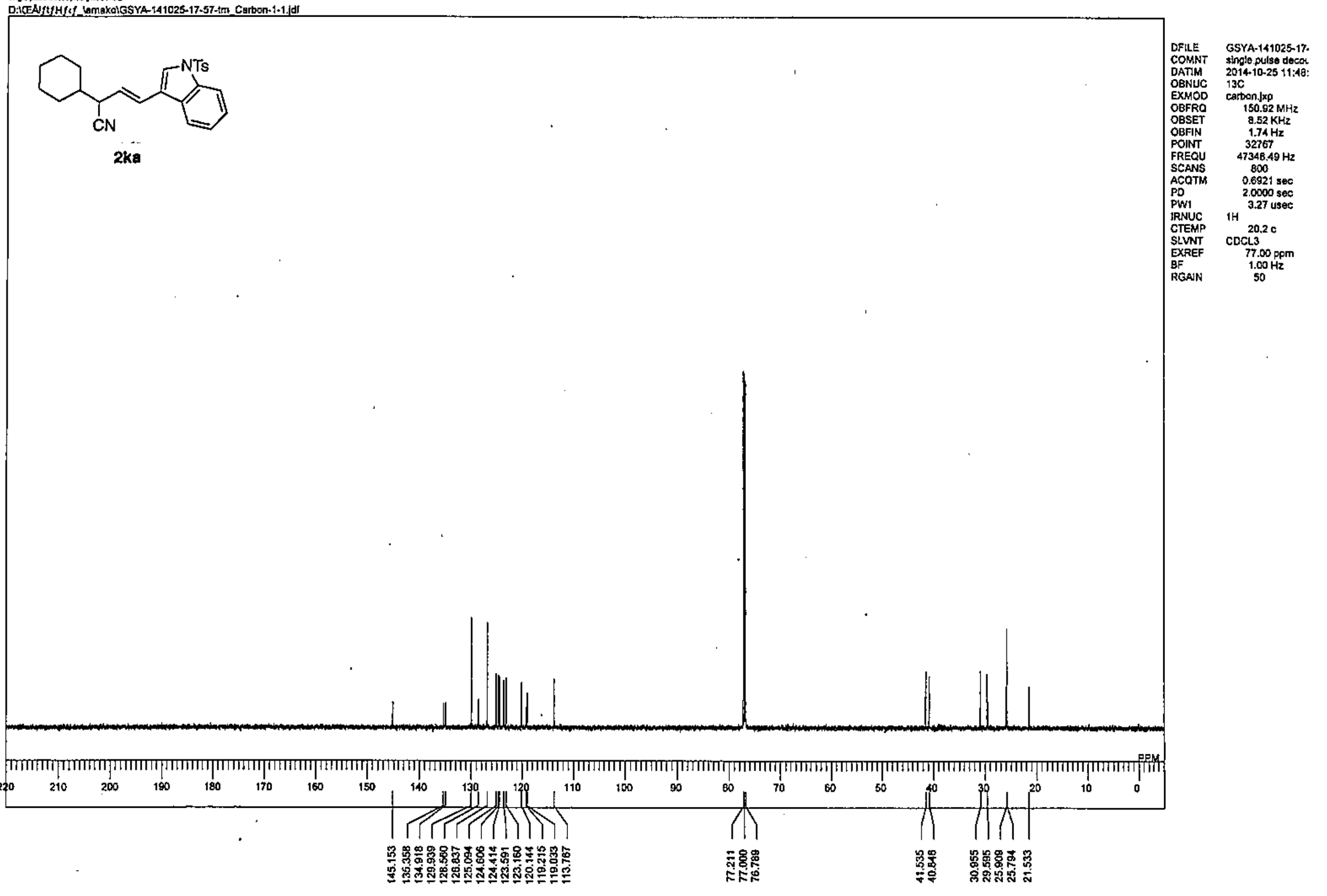
77.211 77.000 76.789

34.565 33.310 31.501 28.857 28.713 22.500 19.733 13.998

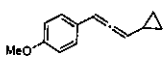
D:\ŒÄÌ/ƒƒHƒcƒ_\amako\GSYA-141027-17-57_tm.1


NTs
CN
2ka
DFILE GSYA-141027-17
COMNT
DATIM 2014-10-25 14:33
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 4
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 5.75 usec
IRNUC
CTEMP 21.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
PPM
8.011 7.990 7.790 7.769 7.691 7.672 7.617 7.373 7.370 7.352 7.334 7.331 7.306 7.304 7.285 7.281 7.248 7.227 6.780 6.741
6.135 6.119 6.095 6.078
3.343 3.339 3.325 3.311 3.308 2.347 1.935 1.904 1.866 1.827 1.796 1.712 1.703 1.688 1.660 1.553 1.328 1.311 1.305 1.297 1.289 1.266 1.258 1.237 1.215 1.210 1.188 1.180 1.148
0.000

single pulse decoupled gated NOE
D:\ŒÄÌ/ƒƒHƒcƒ_\amako\GSYA-141025-17-57-tm_Carbon-1-1.jdf

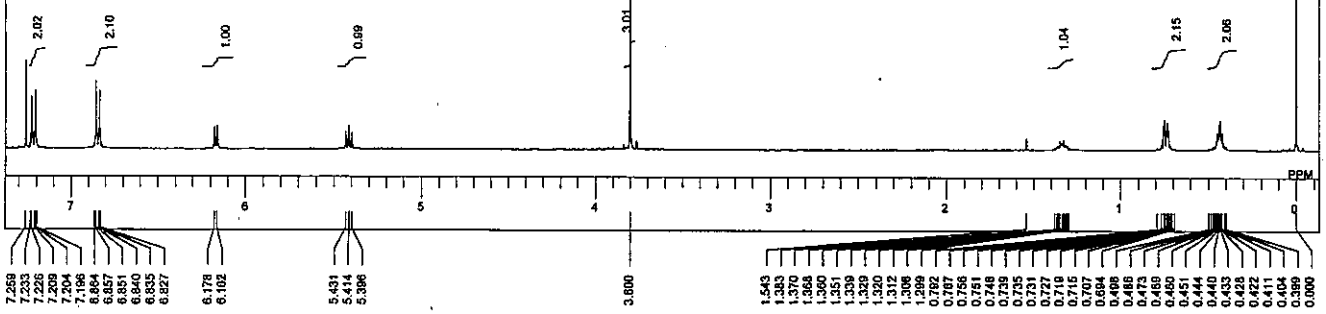

NTs
CN
2ka
DFILE GSYA-141025-17-
COMNT single pulse decou
DATIM 2014-10-25 11:48
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 800
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.27 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50
PPM
145.153 135.358 134.918 129.939 128.560 126.837 125.094 124.606 124.414 123.591 123.160 120.144 119.215 119.033 113.767
77.211 77.000 76.789
41.535 40.848
30.955 29.595 25.909 25.794 21.533

single_pulse
D:\CEA\f1\H\f1_1hori\12\1201~1220\GSHH 1201 2nd_Proton_ft-1-1.jdf



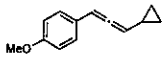
3b

DFILE	GSHH 1201 2nd_P
COMNT	single_pulse
DATIM	2014-04-11 13:43:4
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	9378.75 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	21.0 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	46



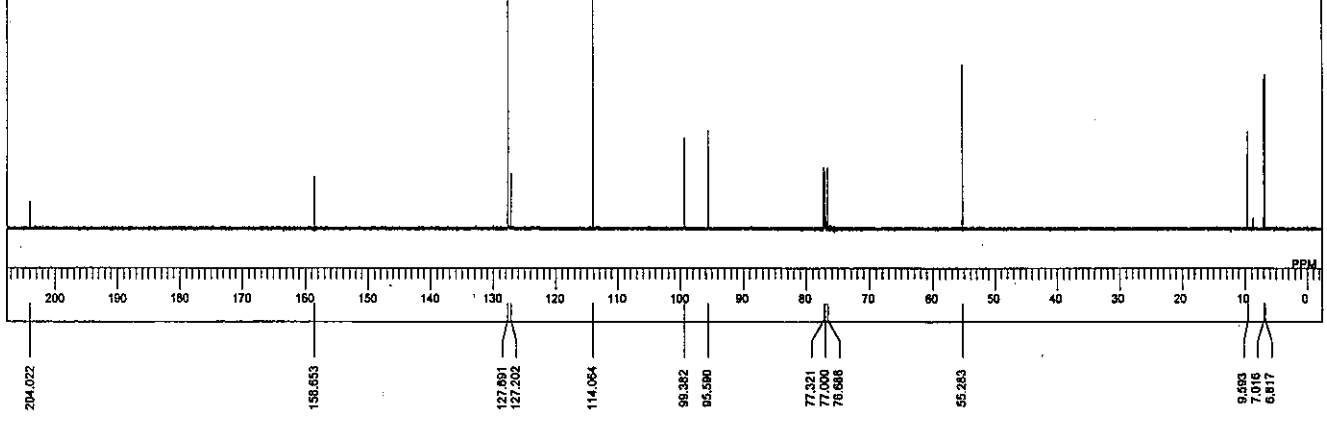
7.259, 7.233, 7.226, 7.209, 7.204, 7.196, 6.864, 6.857, 6.851, 6.840, 6.835, 6.827, 6.179, 6.102, 5.431, 5.414, 5.396, 3.800, 1.543, 1.383, 1.370, 1.368, 1.360, 1.351, 1.339, 1.329, 1.320, 1.312, 1.306, 1.299, 0.782, 0.767, 0.756, 0.751, 0.748, 0.739, 0.735, 0.731, 0.727, 0.718, 0.715, 0.707, 0.694, 0.466, 0.466, 0.473, 0.469, 0.450, 0.451, 0.444, 0.440, 0.433, 0.428, 0.422, 0.411, 0.404, 0.389, 0.000

D:\CEA\f1\H\f1_1hori\12\1201~1220\GSHH_1201_c.1



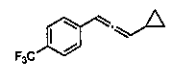
3b

DFILE	GSHH_1201_c.1
COMNT	
DATIM	2014-04-09 15:28:6
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.85 Hz
POINT	32768
FREQU	25188.92 Hz
SCANS	500
ACQTM	1.3009 sec
PD	1.0000 sec
PW1	3.17 usec
IRNUC	1H
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	24



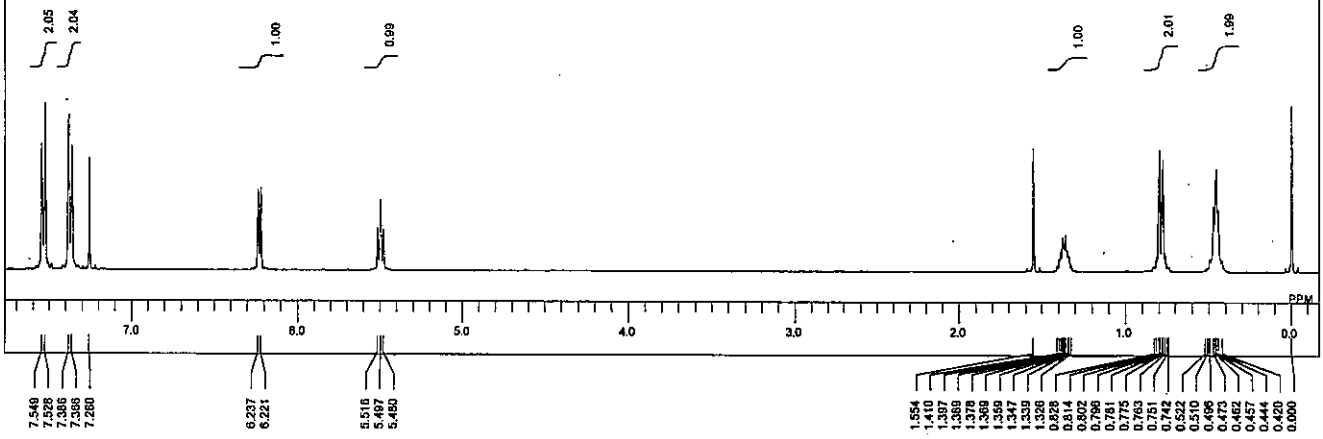
204.022, 158.653, 127.691, 127.202, 114.064, 99.382, 95.590, 77.321, 77.000, 76.688, 55.283, 9.593, 7.016, 6.817

single_pulse
D:\CEA\f\H\f_\hori\11\1161~1180\GSHH 11 66_Proton_ft-1-1.jdf

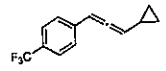


3c

DFILE	GSHH 11 66_Proto
COMNT	single_pulse
DATIM	2014-03-19 17:41:3
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	9378.75 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	19.2 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	50

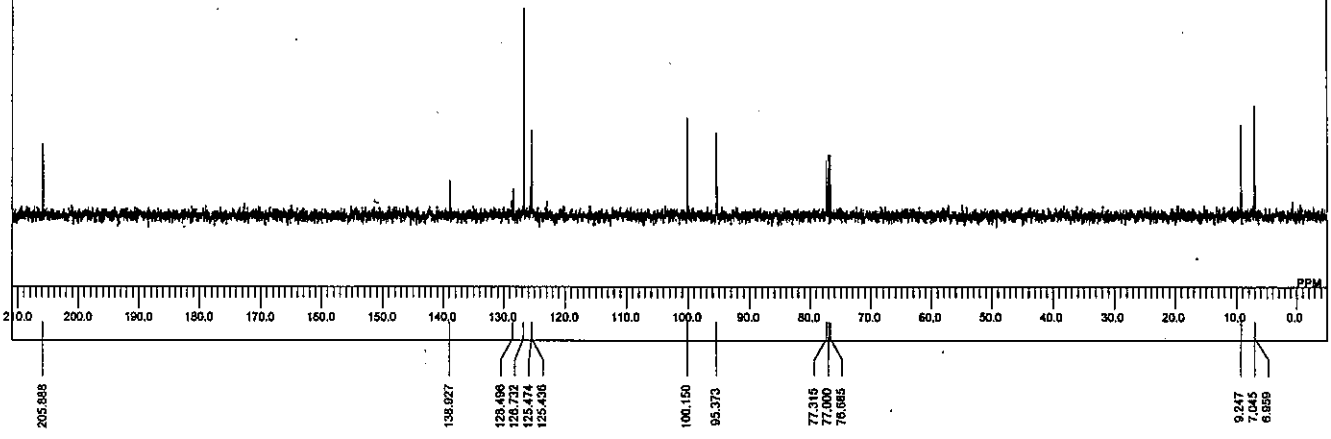


single pulse decoupled gated NOE
D:\CEA\f\H\f_\hori\11\1161~1180\GSHH 11 66 c_Carbon_ft-1-1.als

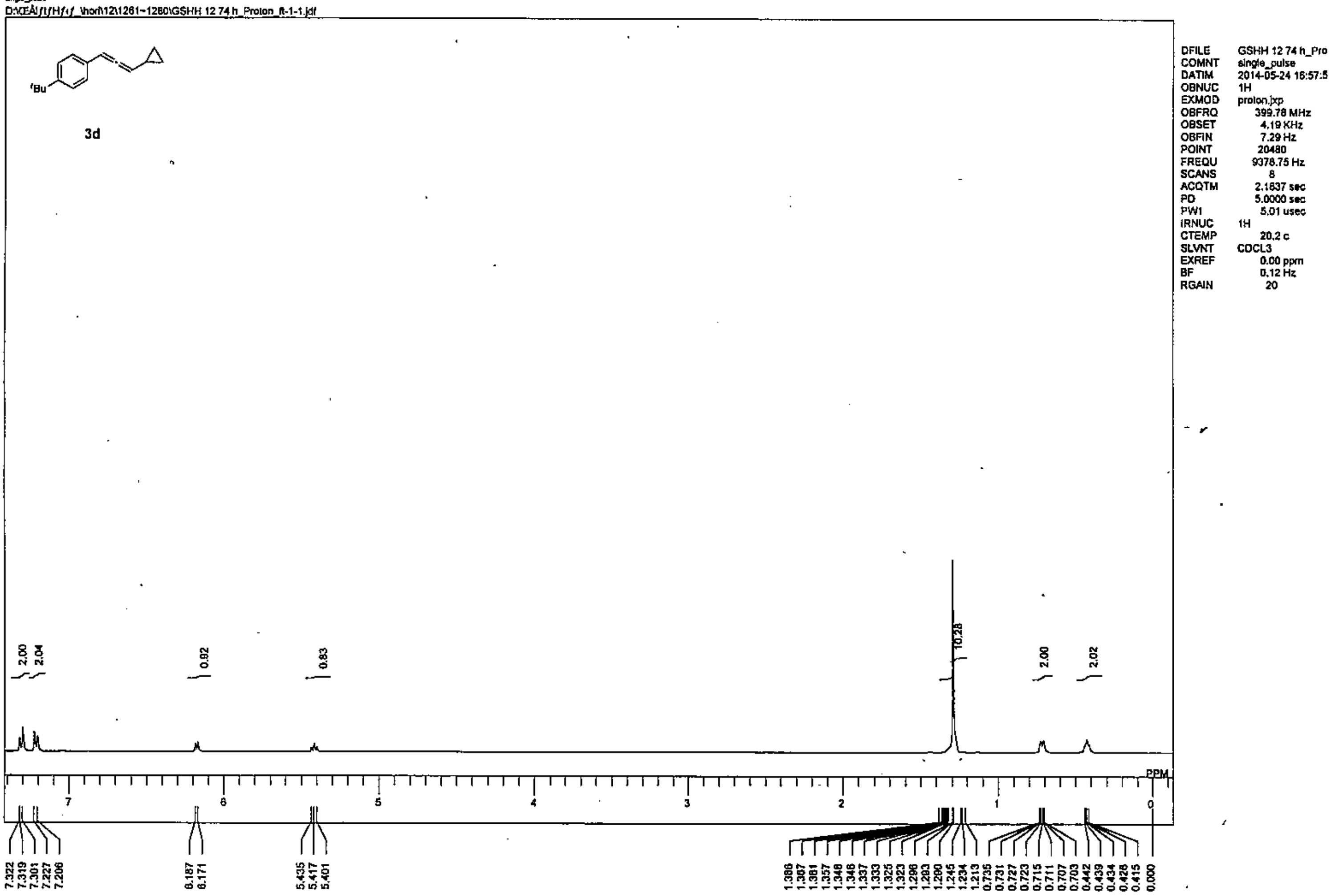


3c

DFILE	GSHH 11 66 c_Car
COMNT	single pulse decoup
DATIM	2014-03-19 18:38:5
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.66 Hz
POINT	32768
FREQU	31407.04 Hz
SCANS	50
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	19.8 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50

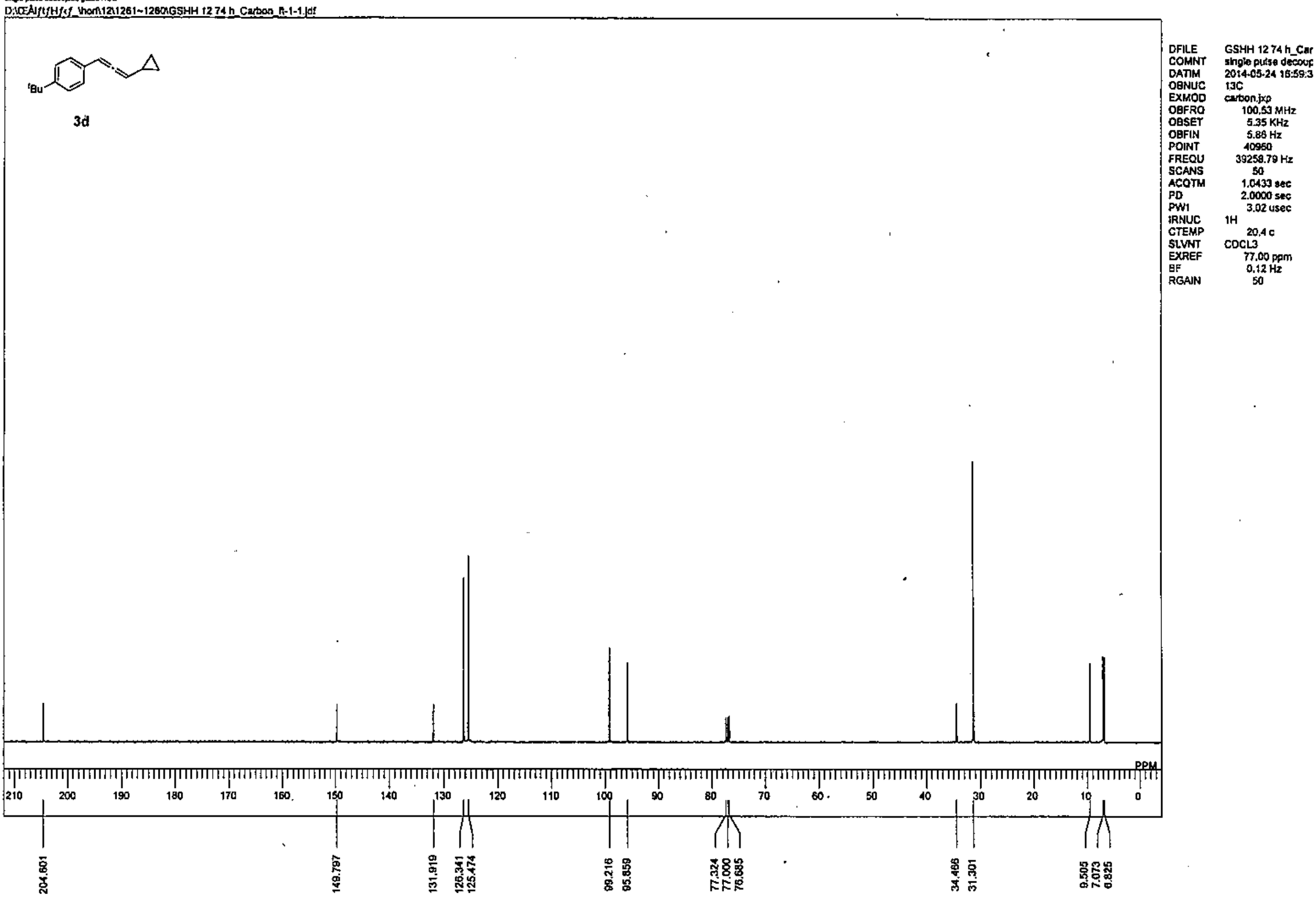


single_pulse
D:\ŒÂ\ƒ!ƒHƒ‹ƒ_\hori\12\1261~1280\GSHH 12 74 h_Proton_ft-1-1.jdf

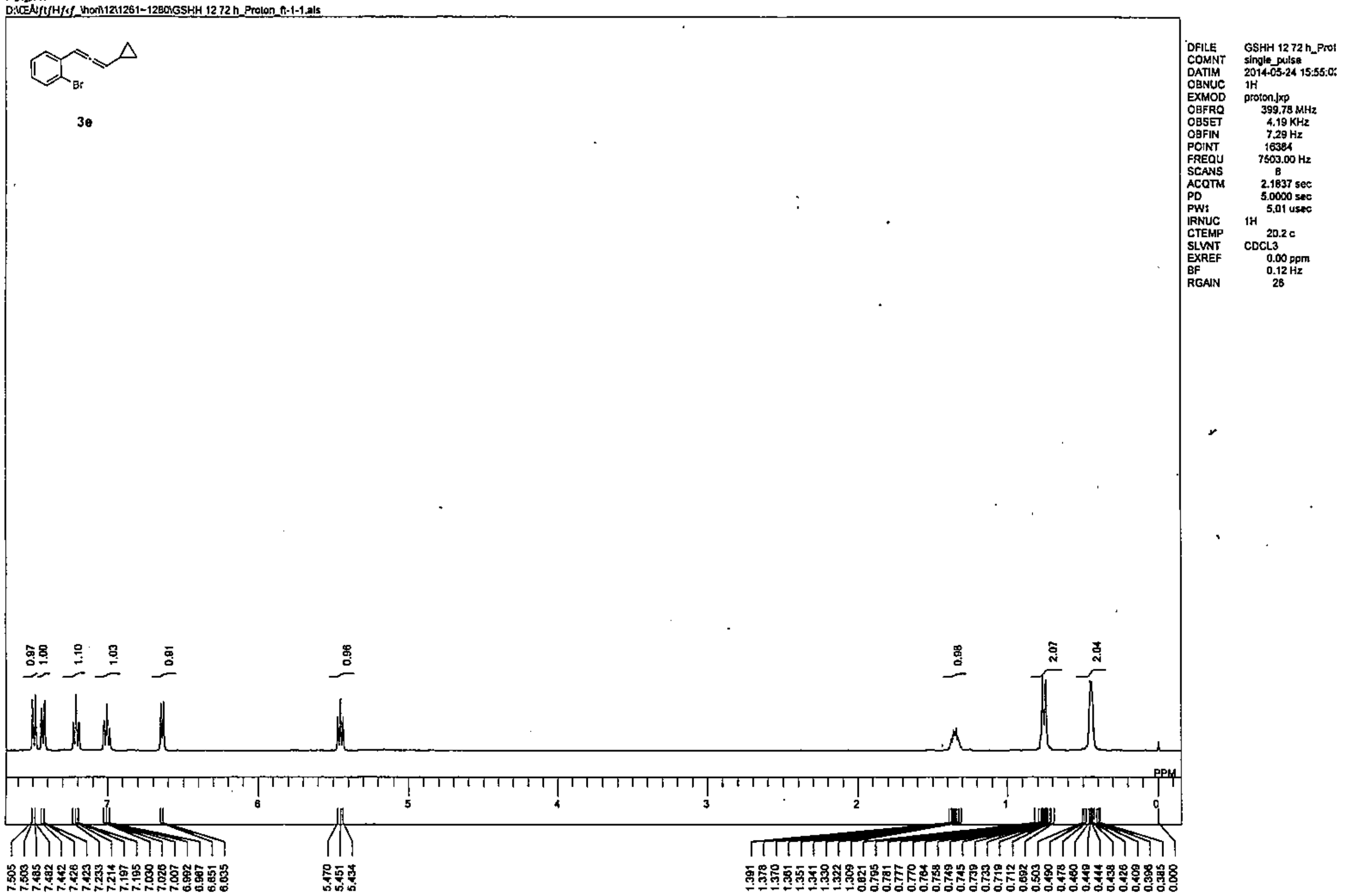


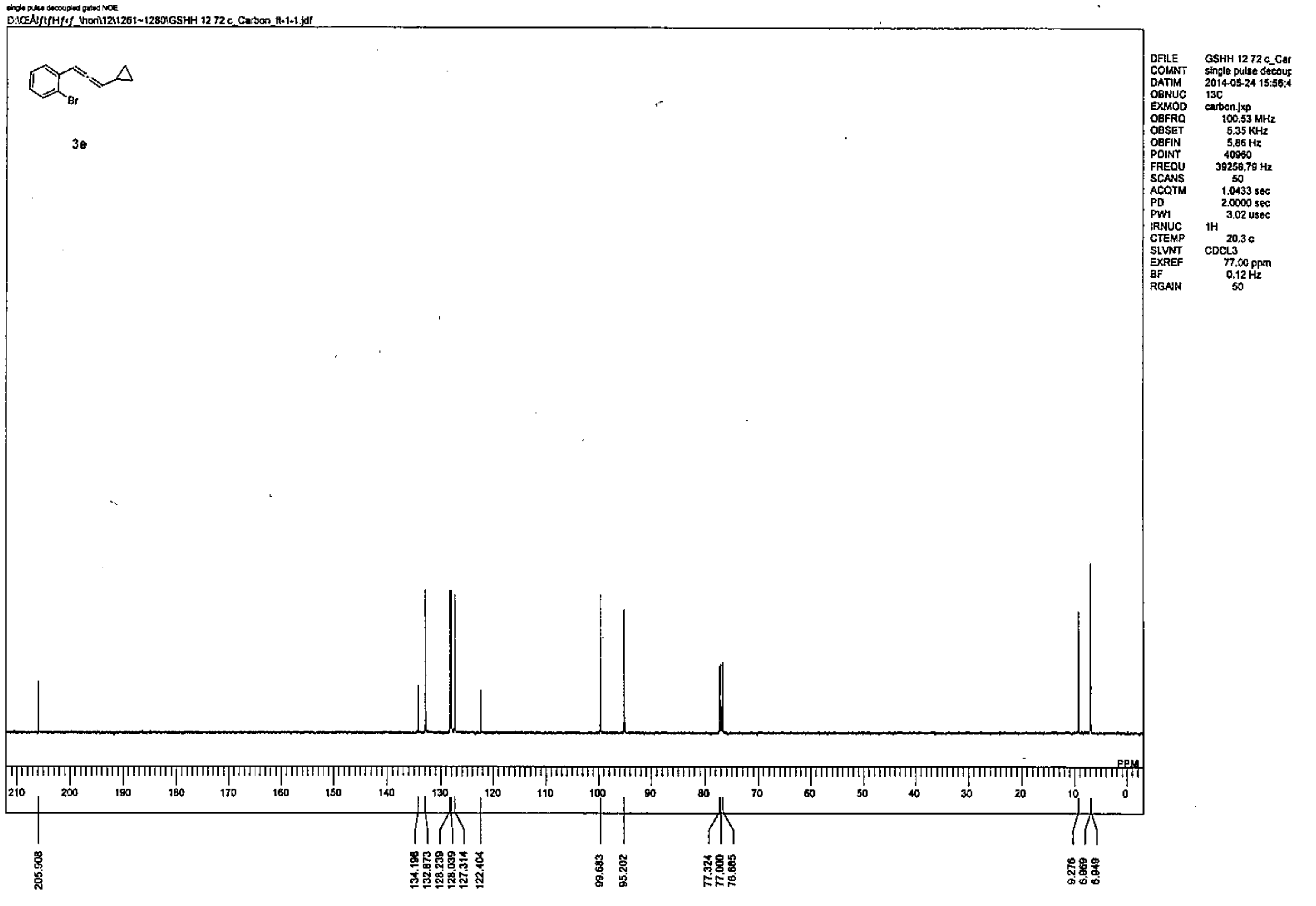
ᵗBu
3d
2.00
2.04
0.92
0.83
10.28
2.00
2.02
PPM
7.322
7.319
7.301
7.227
7.206
6.187
6.171
5.435
5.417
5.401
1.386
1.367
1.381
1.357
1.348
1.337
1.332
1.325
1.323
1.298
1.293
1.260
1.245
1.234
1.213
0.735
0.731
0.727
0.723
0.715
0.711
0.707
0.703
0.442
0.439
0.434
0.428
0.415
0.000
DFILE GSHH 12 74 h_Pro
COMNT single_pulse
DATIM 2014-05-24 16:57:5
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 20

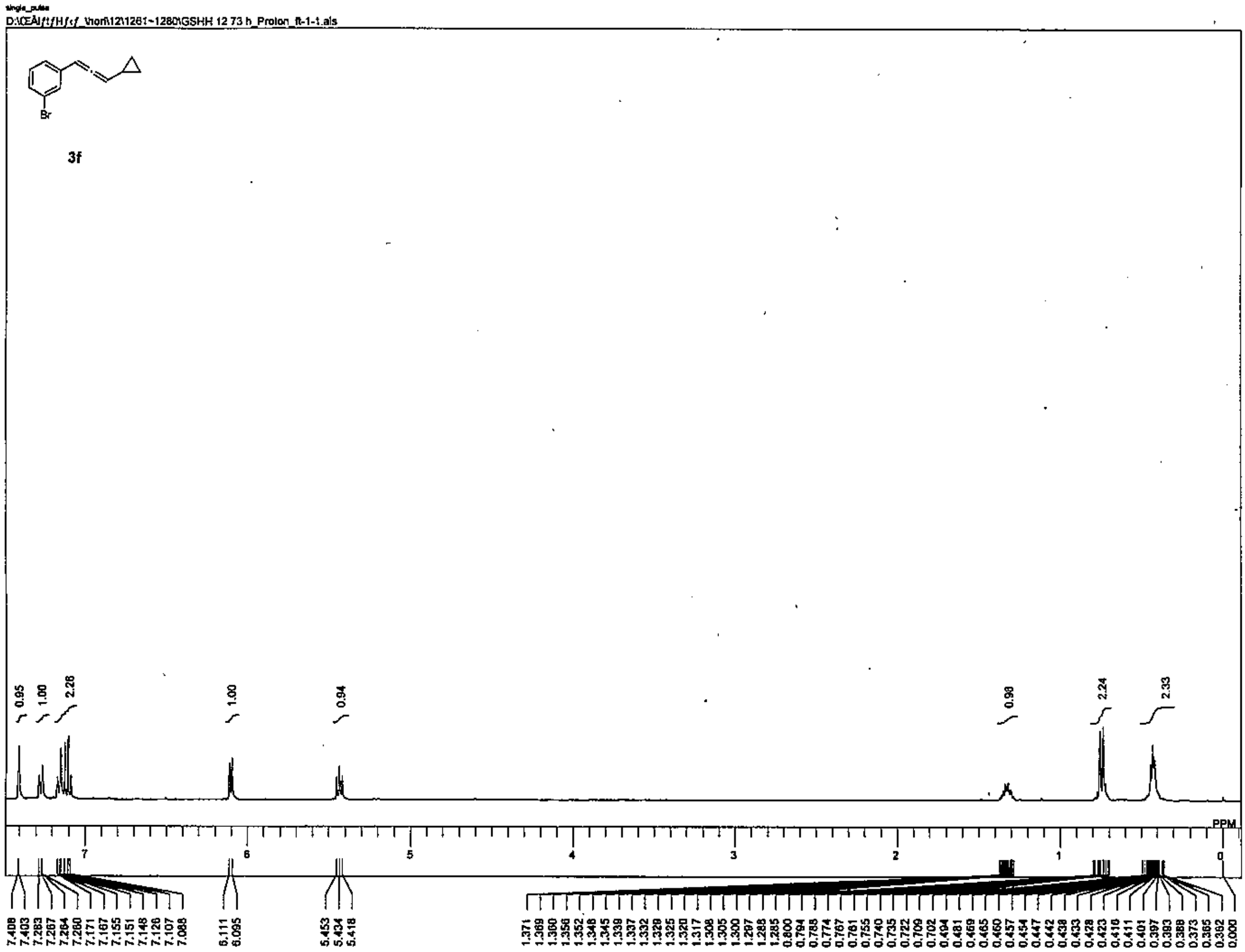
single pulse decoupled gated NOE
D:\ŒÂ\ƒ!ƒHƒ‹ƒ_\hori\12\1261~1280\GSHH 12 74 h_Carbon_ft-1-1.jdf



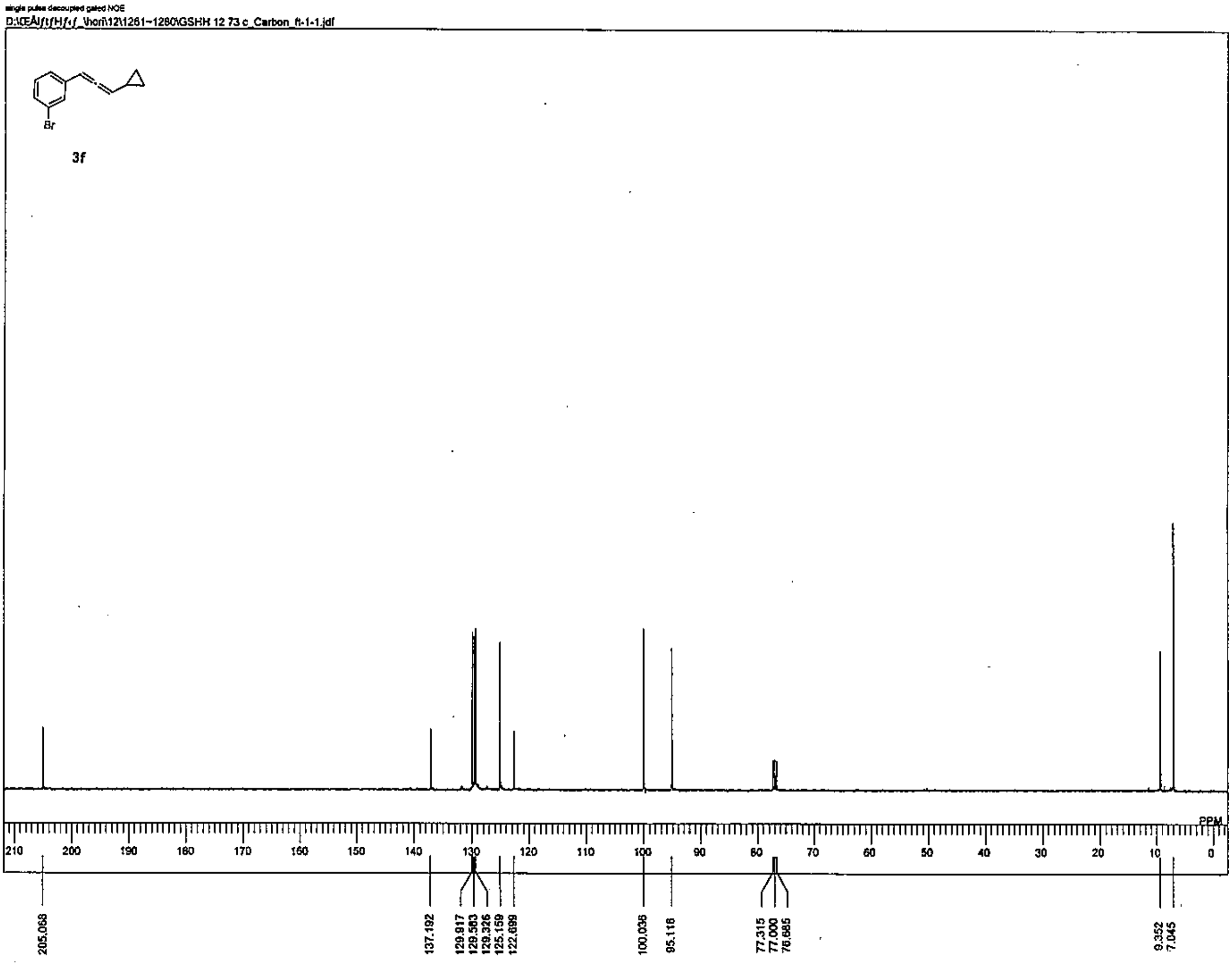
ᵗBu
3d
PPM
204.601
149.797
131.919
126.341
125.474
99.216
95.859
77.324
77.000
76.685
34.466
31.301
9.505
7.073
6.825
DFILE GSHH 12 74 h_Car
COMNT single pulse decoup
DATIM 2014-05-24 16:59:3
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 50
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50


single_pulse
D:\CEÄ\ƒtƒHƒ‹ƒ_\hori\12\1261~1280\GSHH 12 72 h_Proton_ft-1-1.als
3e
Br
DFILE GSHH 12 72 h_Prot
COMNT single_pulse
DATIM 2014-05-24 15:55:0
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 26
0.97 1.00 1.10 1.03 0.91 0.96 0.98 2.07 2.04
PPM
7 6 5 4 3 2 1 0
7.505 7.503 7.485 7.482 7.442 7.426 7.423 7.233 7.214 7.197 7.195 7.030 7.026 7.007 6.992 6.987 6.851 6.835
5.470 5.451 5.434
1.391 1.378 1.370 1.361 1.351 1.341 1.330 1.322 1.309 0.821 0.795 0.781 0.777 0.770 0.764 0.758 0.749 0.745 0.739 0.733 0.719 0.712 0.692 0.503 0.490 0.478 0.460 0.449 0.444 0.438 0.426 0.409 0.396 0.385 0.000


single pulse decoupled gated NOE
D:\CEÄ\ƒtƒHƒ‹ƒ_\hori\12\1261~1280\GSHH 12 72 c_Carbon_ft-1-1.jdf
3e
Br
DFILE GSHH 12 72 c_Car
COMNT single pulse decoup
DATIM 2014-05-24 15:56:4
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 50
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
205.908
134.198 132.873 128.239 128.039 127.314 122.404
99.683
95.202
77.324 77.000 76.685
9.276 6.869 6.849

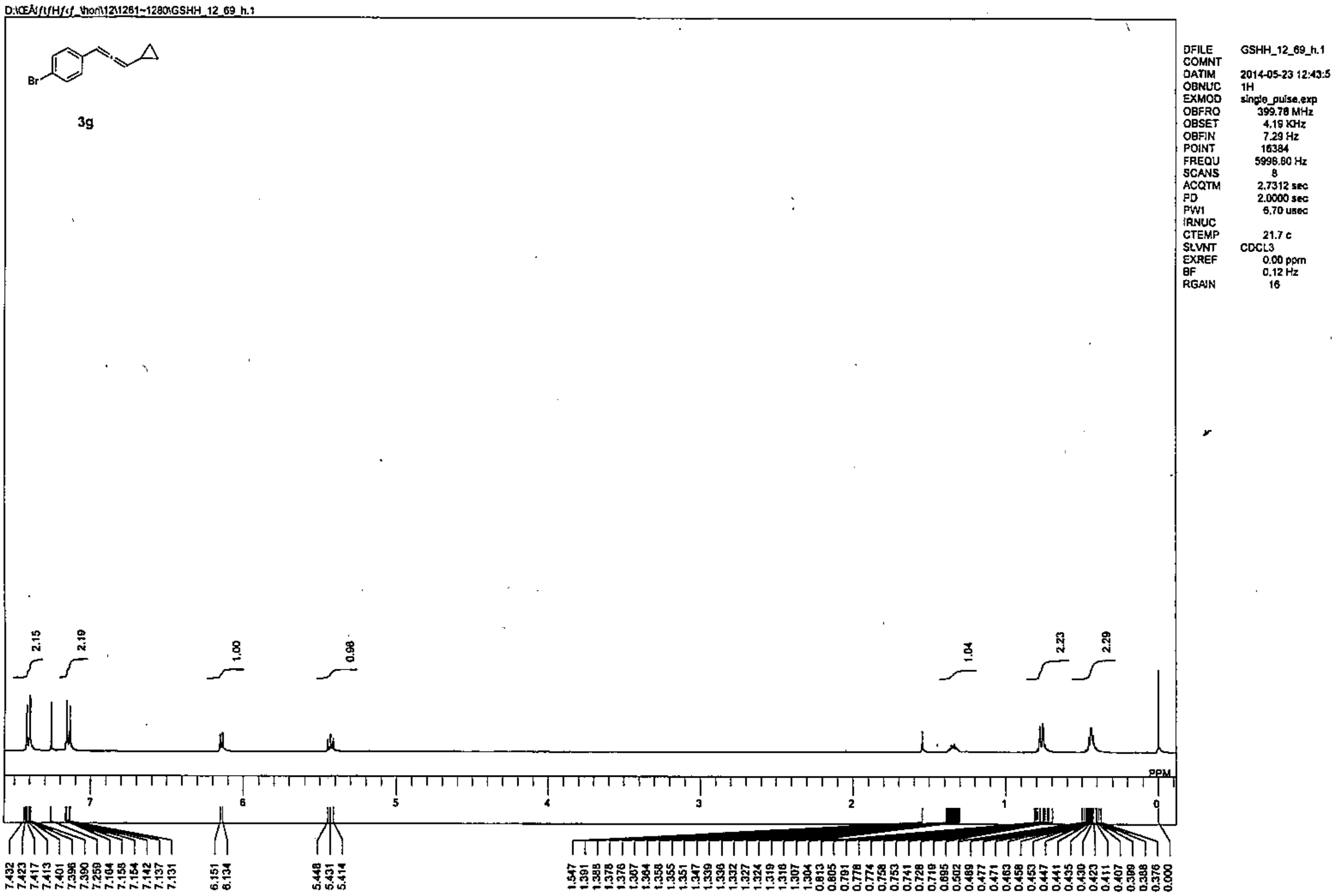

single_pulse
D:\CEÂ\ƒtƒHƒ‹ƒ_\hori\12\1261~1280\GSHH 12 73 h_Proton_ft-1-1.als
Br
3f
0.95
1.00
2.28
1.00
0.94
0.98
2.24
2.33
PPM
7.408
7.403
7.283
7.267
7.264
7.260
7.171
7.167
7.155
7.151
7.148
7.126
7.107
7.088
6.111
6.095
5.453
5.434
5.418
1.371
1.369
1.356
1.352
1.348
1.345
1.339
1.337
1.332
1.329
1.325
1.320
1.317
1.308
1.305
1.300
1.297
1.288
1.285
0.800
0.794
0.785
0.774
0.767
0.761
0.755
0.740
0.735
0.722
0.709
0.702
0.494
0.481
0.469
0.465
0.460
0.457
0.454
0.447
0.442
0.438
0.433
0.428
0.423
0.416
0.411
0.401
0.397
0.393
0.388
0.373
0.365
0.362
0.000

DFILE	GSHH 12 73 h_Prot
COMNT	single_pulse
DATIM	2014-05-24 16:02:3
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	7503.00 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	20.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	22



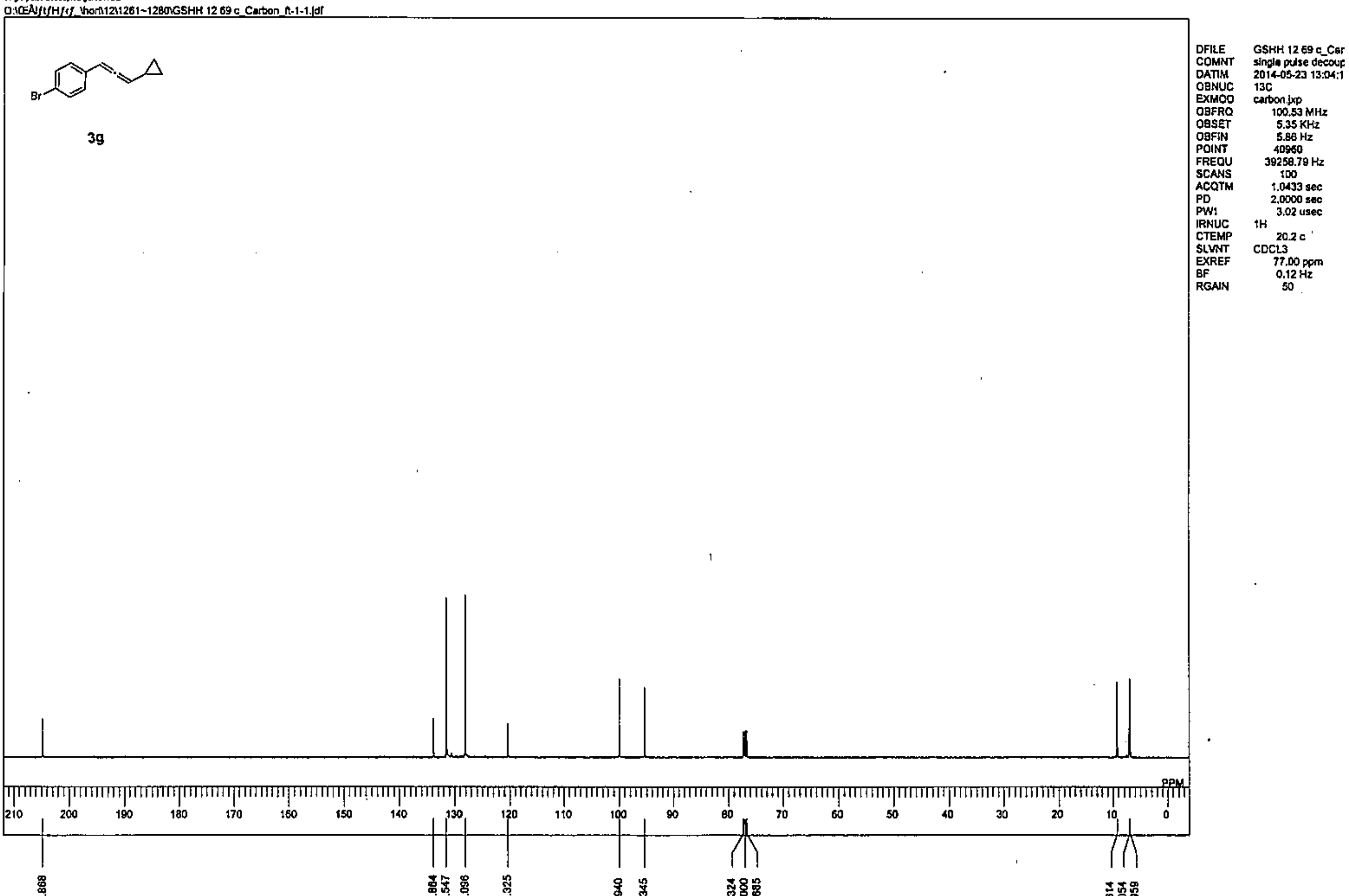
DFILE	GSHH 12 73 c_Car
COMNT	single pulse decoup
DATIM	2014-05-24 16:04:0
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	50
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	20.3 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50

D:\ŒÂ\ƒ\ƒHƒcƒ_\hori\12\1261~1280\GSHH_12_69_h.1



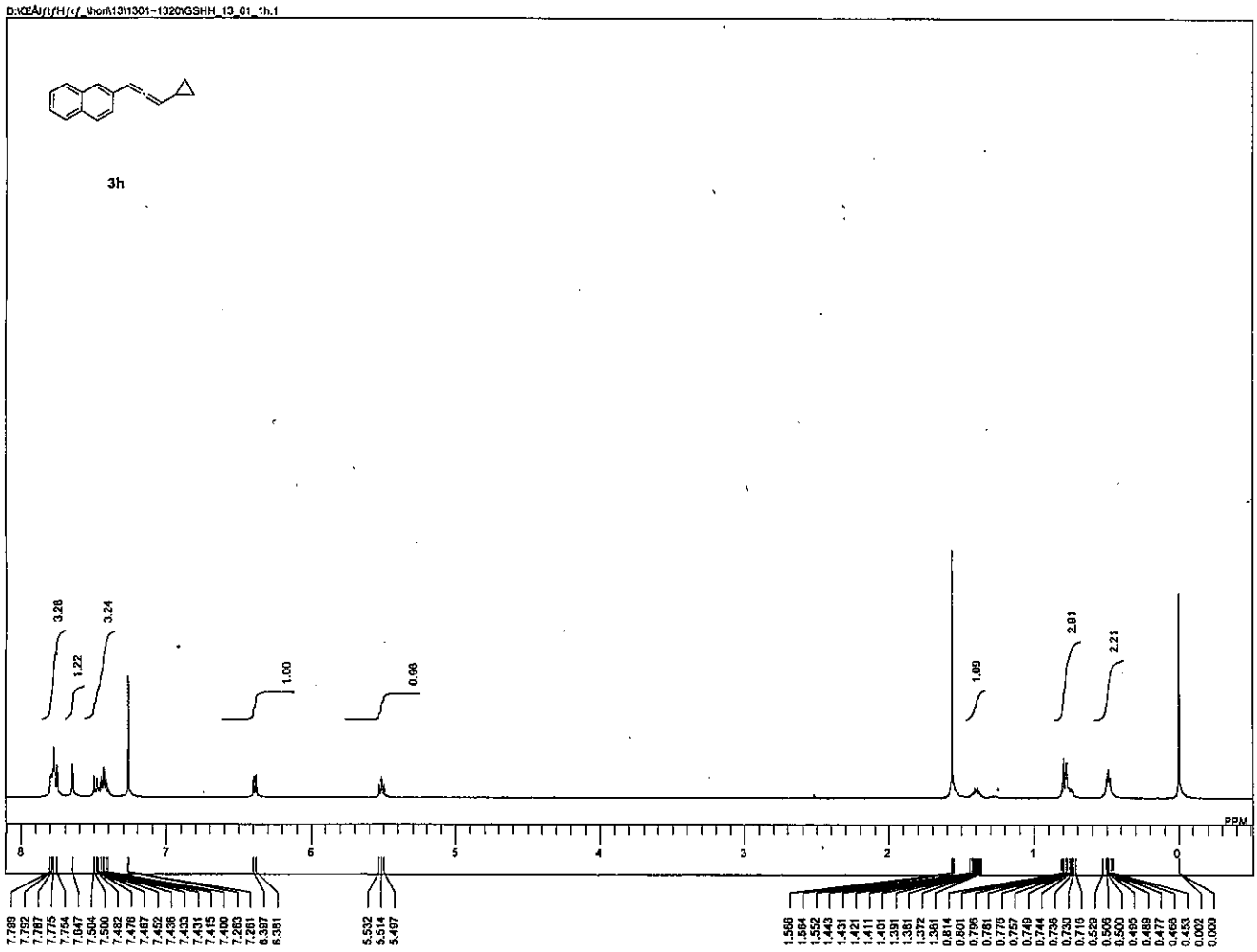
Br
3g
DFILE GSHH_12_69_h.1
COMNT
DATIM 2014-05-23 12:43:5
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.70 usec
IRNUC
CTEMP 21.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 16
2.15
2.19
1.00
0.98
1.04
2.23
2.29
PPM
7.432 7.423 7.417 7.413 7.401 7.396 7.390 7.259 7.164 7.158 7.154 7.142 7.137 7.131
6.151 6.134
5.448 5.431 5.414
1.547 1.391 1.388 1.376 1.367 1.364 1.358 1.355 1.351 1.347 1.339 1.336 1.332 1.327 1.324 1.319 1.316 1.307 1.304 0.813 0.805 0.791 0.778 0.774 0.758 0.753 0.741 0.728 0.719 0.695 0.502 0.489 0.477 0.471 0.463 0.458 0.453 0.447 0.441 0.435 0.430 0.423 0.411 0.407 0.399 0.388 0.376 0.000

single pulse decoupled gated NOE
D:\ŒÂ\ƒ\ƒHƒcƒ_\hori\12\1261~1280\GSHH 12 69 c_Carbon_ft-1-1.jdf



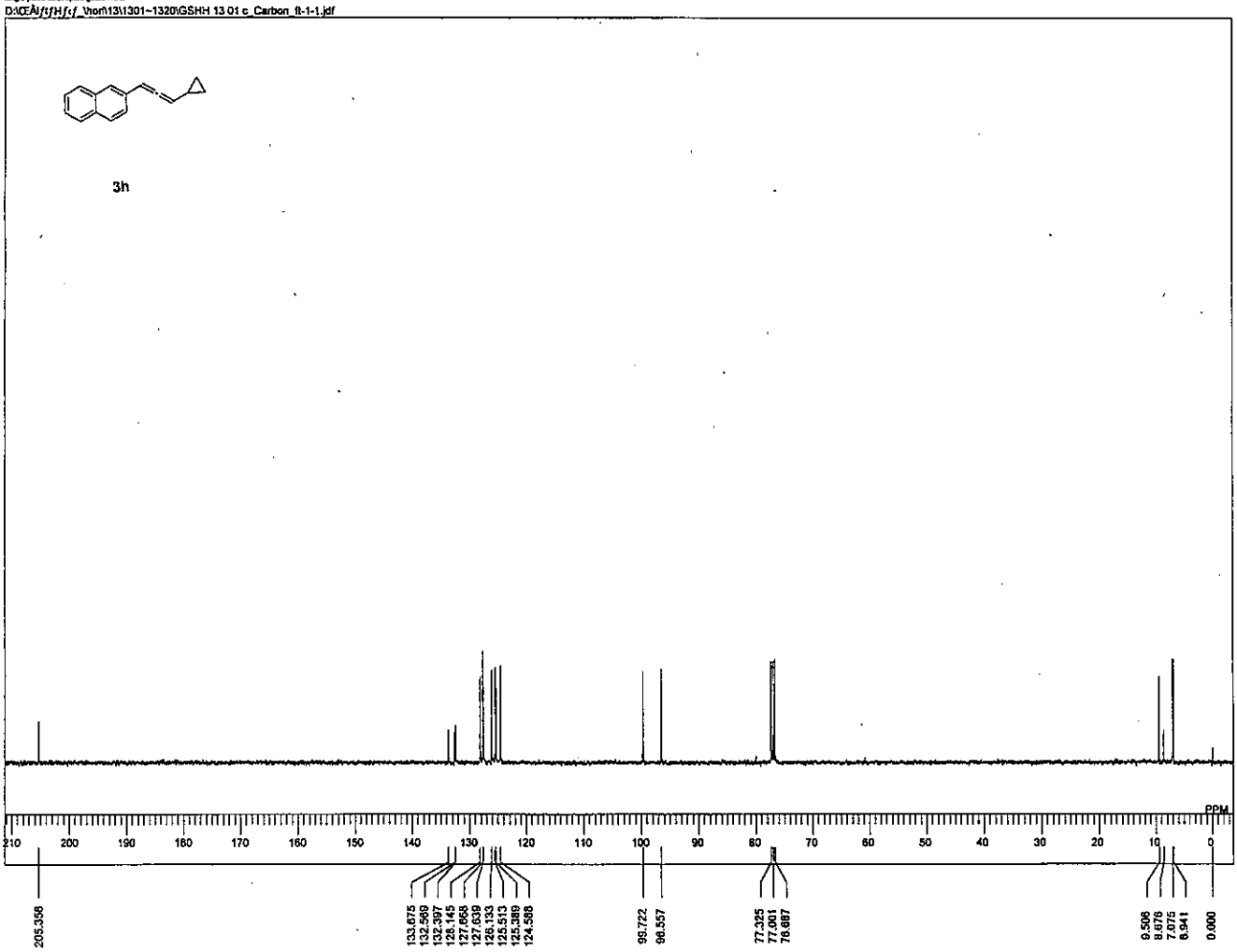
Br
3g
DFILE GSHH 12 69 c_Car
COMNT single pulse decoup
DATIM 2014-05-23 13:04:1
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 100
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM
204.868
133.884 131.547 128.096
120.325
99.940
95.345
77.324 77.000 76.685
9.314 7.054 6.959

D:\CEÀ¡t¡H¡c¡_\hori\13\1301~1320\GSHH_13_01_1h.1



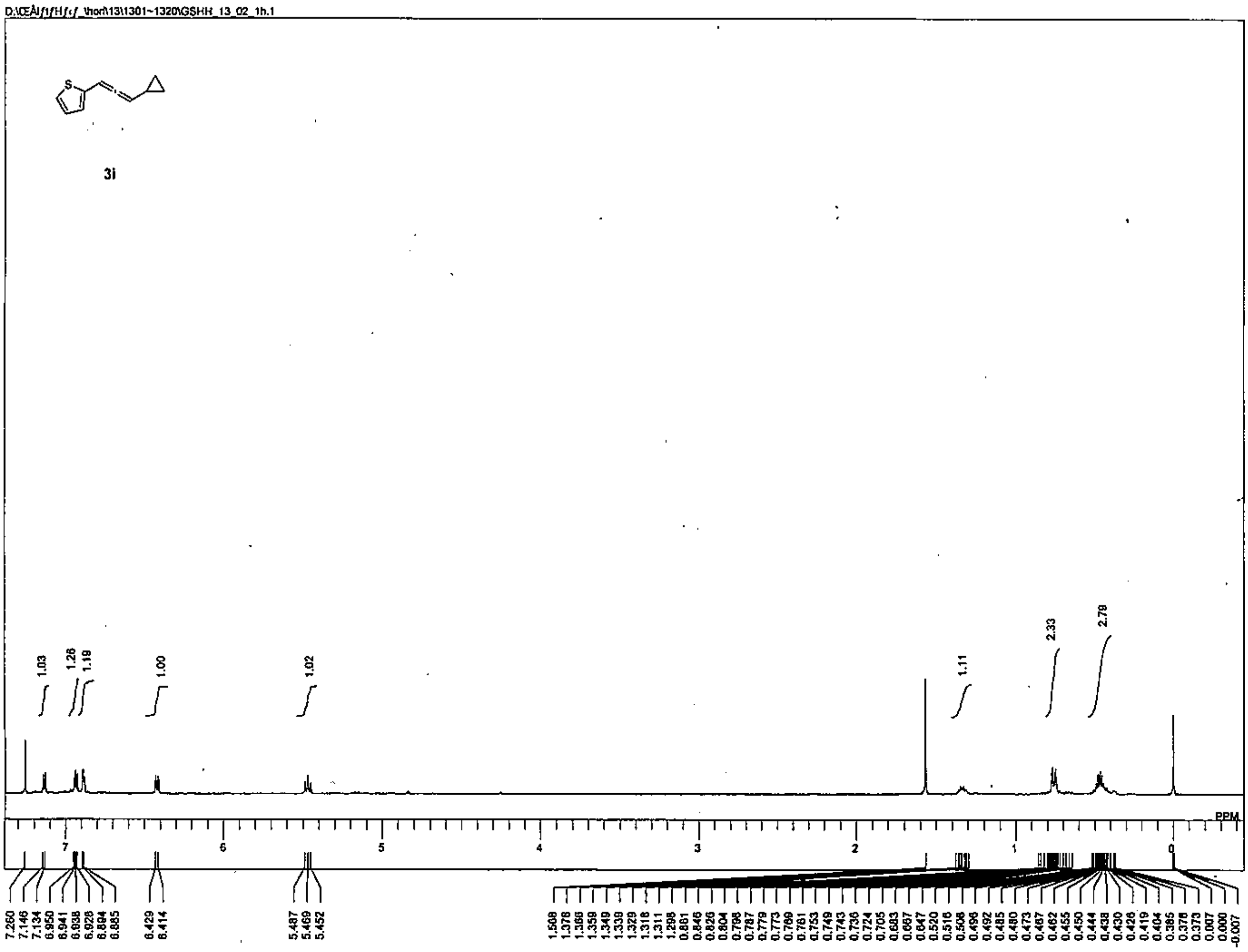
DFILE GSHH_13_01_1h.1
COMNT
DATIM 2014-05-28 08:25:3
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.70 usec
IRNUC
CTEMP 19.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18

single pulse decoupled gated NOE
D:\CEÀ¡t¡H¡c¡_\hori\13\1301~1320\GSHH 13 01 c_Carbon_ft-1-1.jdf



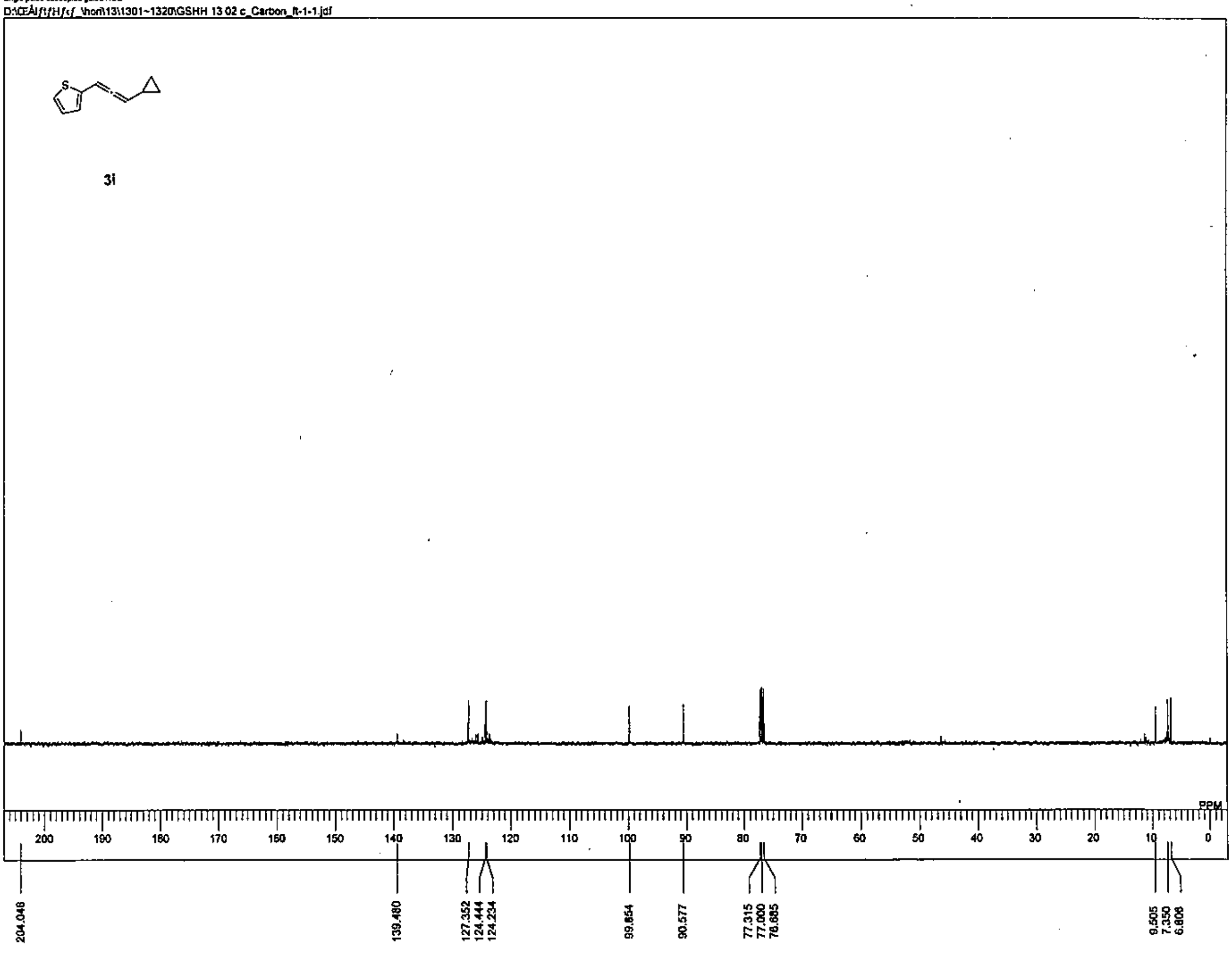
DFILE GSHH 13 01 c_Carl
COMNT single pulse decoup
DATIM 2014-05-28 10:37:3
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 50
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 50

D:\ŒÀ\ƒ\ƒHƒ‹ƒ_\hori\13\1301~1320\GSHH_13_02_1h.1


3i
1.03
1.26
1.18
1.00
1.02
1.11
2.33
2.79
PPM
7
6
5
4
3
2
1
0
7.260
7.146
7.134
6.950
6.941
6.938
6.928
6.894
6.885
6.429
6.414
5.487
5.469
5.452
1.508
1.376
1.368
1.358
1.349
1.338
1.329
1.318
1.311
1.298
0.861
0.846
0.826
0.804
0.798
0.787
0.779
0.773
0.769
0.761
0.753
0.749
0.743
0.736
0.724
0.705
0.683
0.667
0.647
0.520
0.516
0.508
0.496
0.492
0.485
0.480
0.473
0.467
0.462
0.455
0.450
0.444
0.438
0.430
0.426
0.419
0.404
0.385
0.378
0.373
0.000
0.007
-0.007

DFILE GSHH_13_02_1h.1
COMNT
DATIM 2014-05-28 08:29:0
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.70 usec
IRNUC
CTEMP 19.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 17

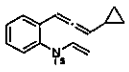
single pulse decoupled gated NOE
D:\ŒÀ\ƒ\ƒHƒ‹ƒ_\hori\13\1301~1320\GSHH 13 02 c_Carbon_ft-1-1.jdf



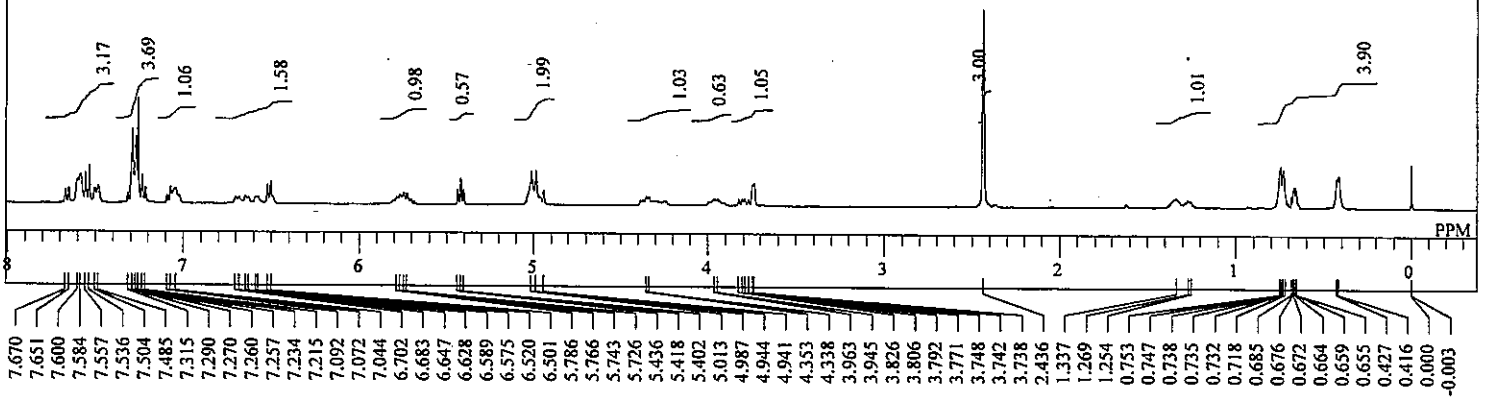
DFILE GSHH 13 02 c_Car
COMNT single pulse decoup
DATIM 2014-05-28 10:42:3
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 50
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50

single pulse

D:\...\...\...\hori\others\GSHH NTs sm_Proton_ft-1-1.jdf



3j

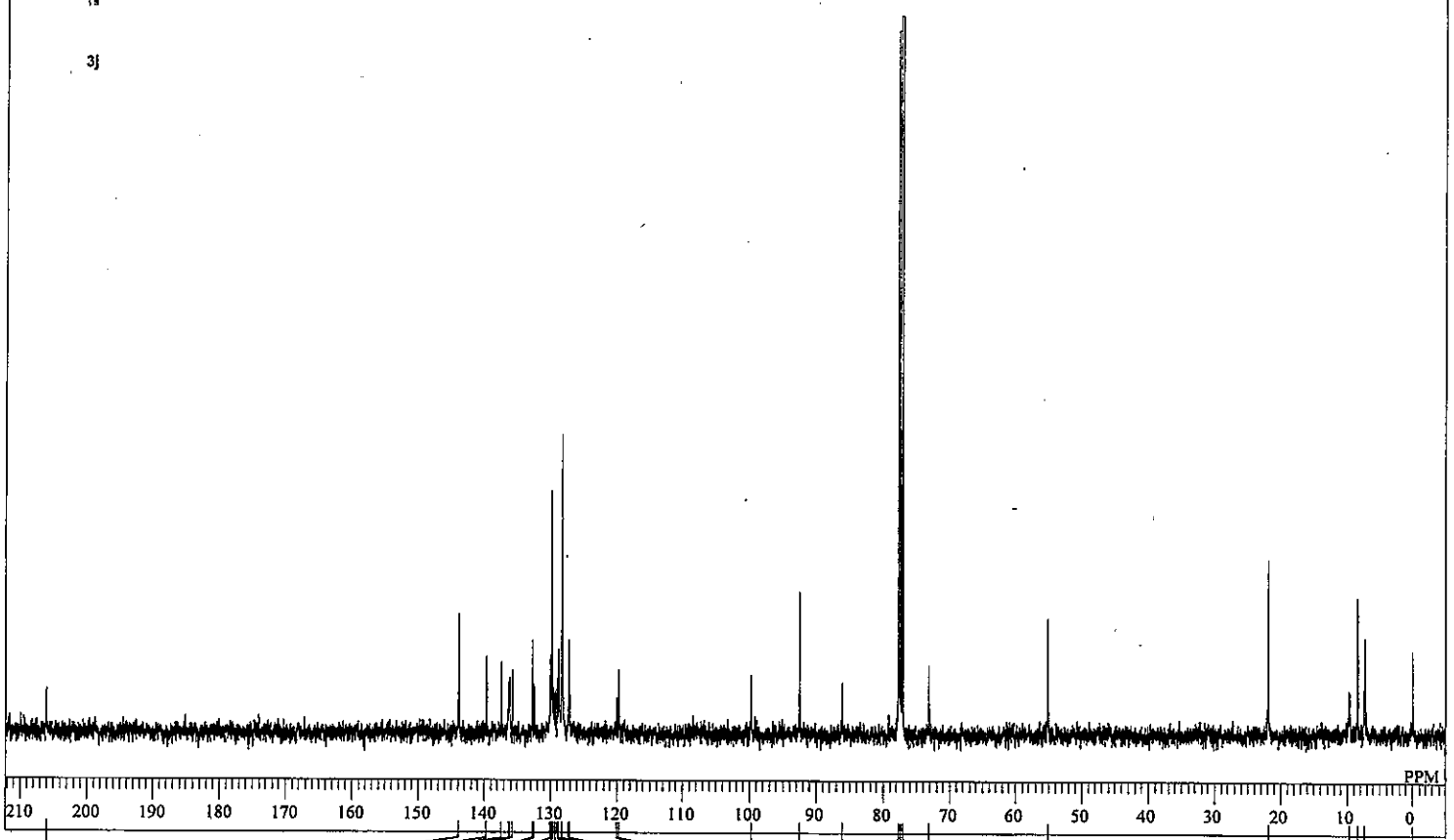


7.670 7.651 7.600 7.584 7.557 7.536 7.504 7.485 7.315 7.290 7.270 7.260 7.257 7.234 7.215 7.092 7.072 7.044 6.702 6.683 6.647 6.628 6.589 6.575 6.520 6.501 5.786 5.766 5.743 5.726 5.436 5.418 5.402 5.013 4.987 4.944 4.941 4.353 4.338 3.963 3.945 3.826 3.806 3.792 3.771 3.748 3.742 3.738 2.436 1.337 1.269 1.254 0.753 0.747 0.738 0.735 0.732 0.718 0.685 0.676 0.672 0.664 0.659 0.655 0.427 0.416 0.000 -0.003

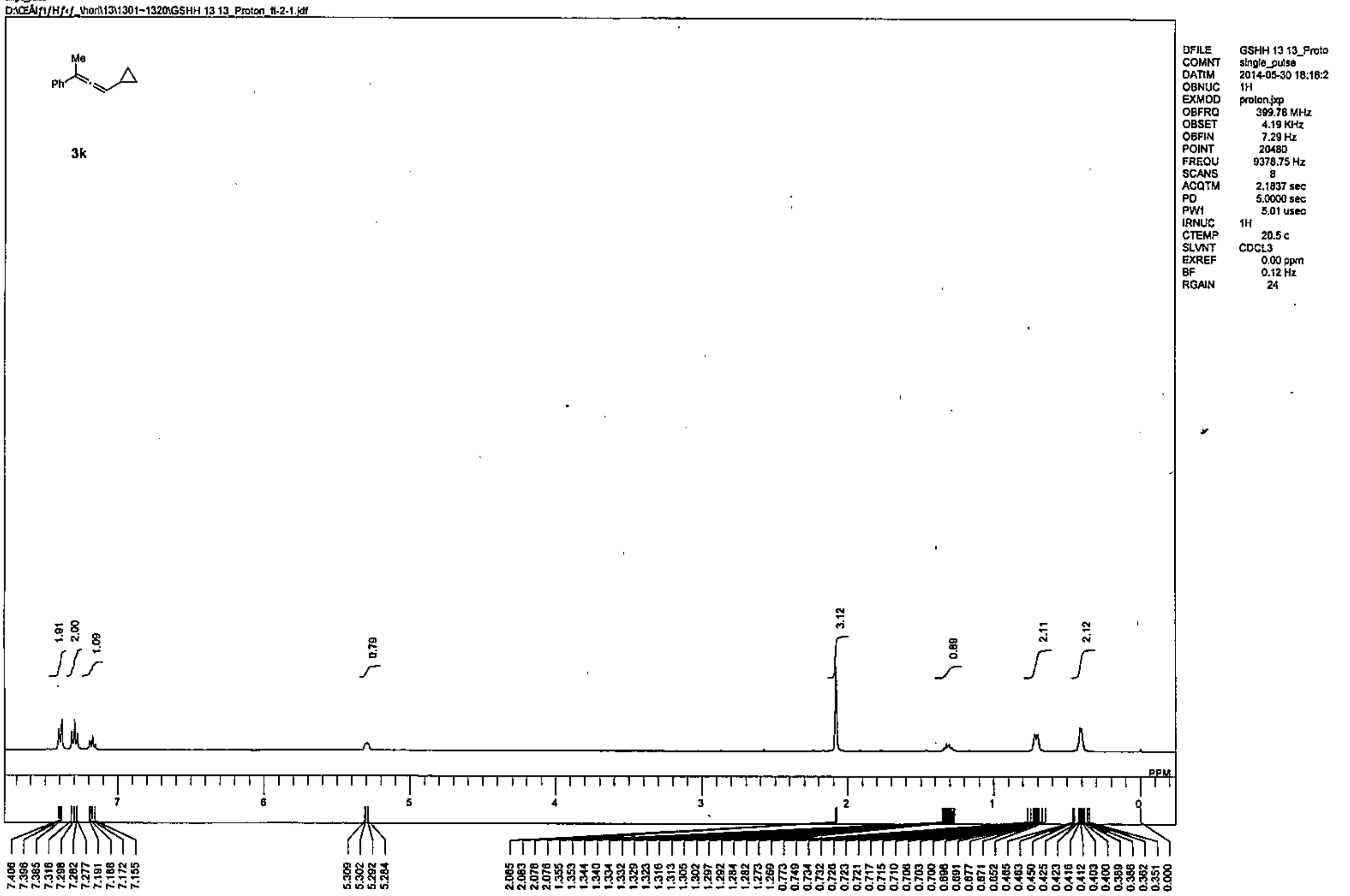
single pulse decoupled gated NOE

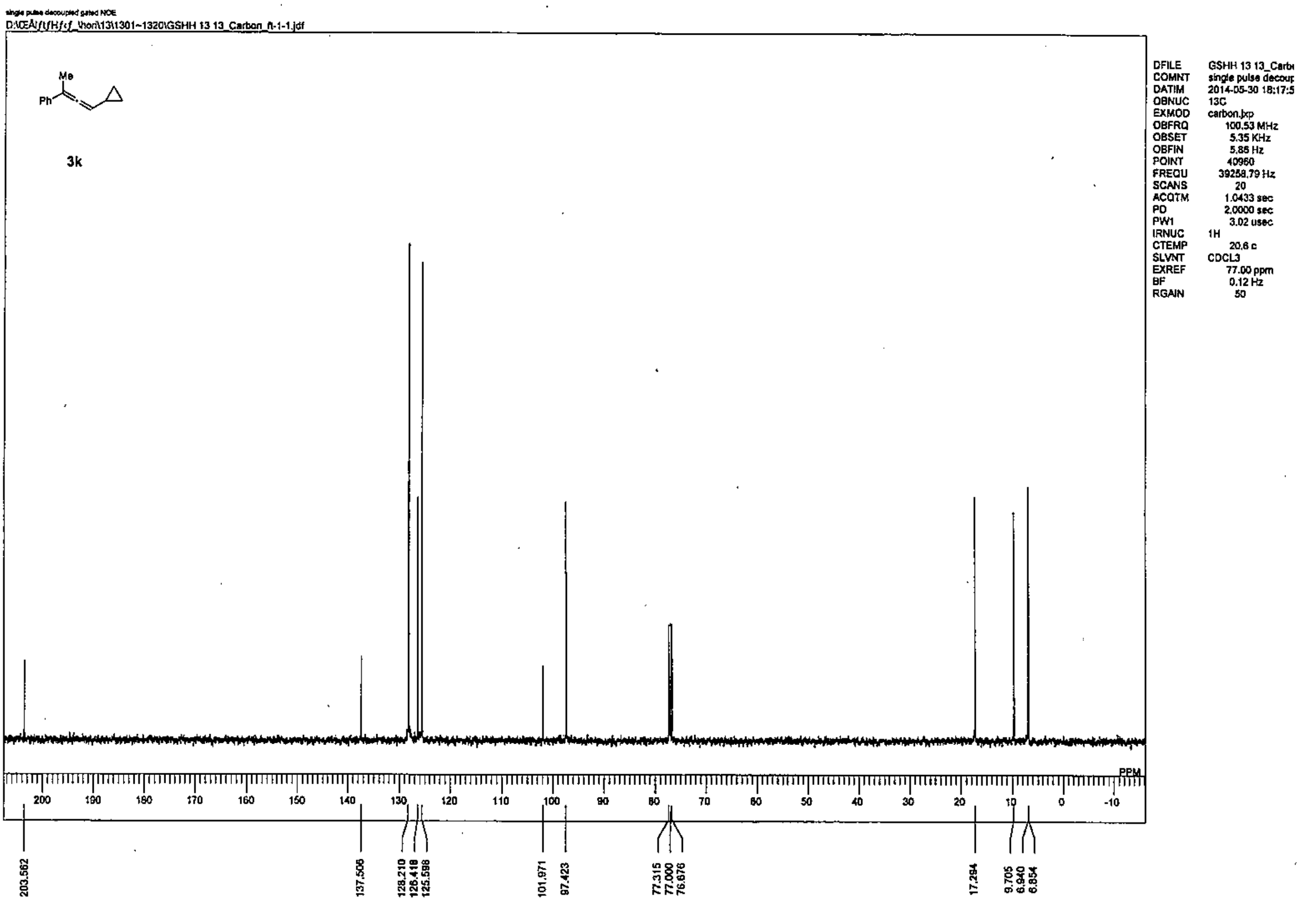
D:\...\...\...\hori\others\GSHH NTs sm_Carbon_ft-2-1.jdf

3j

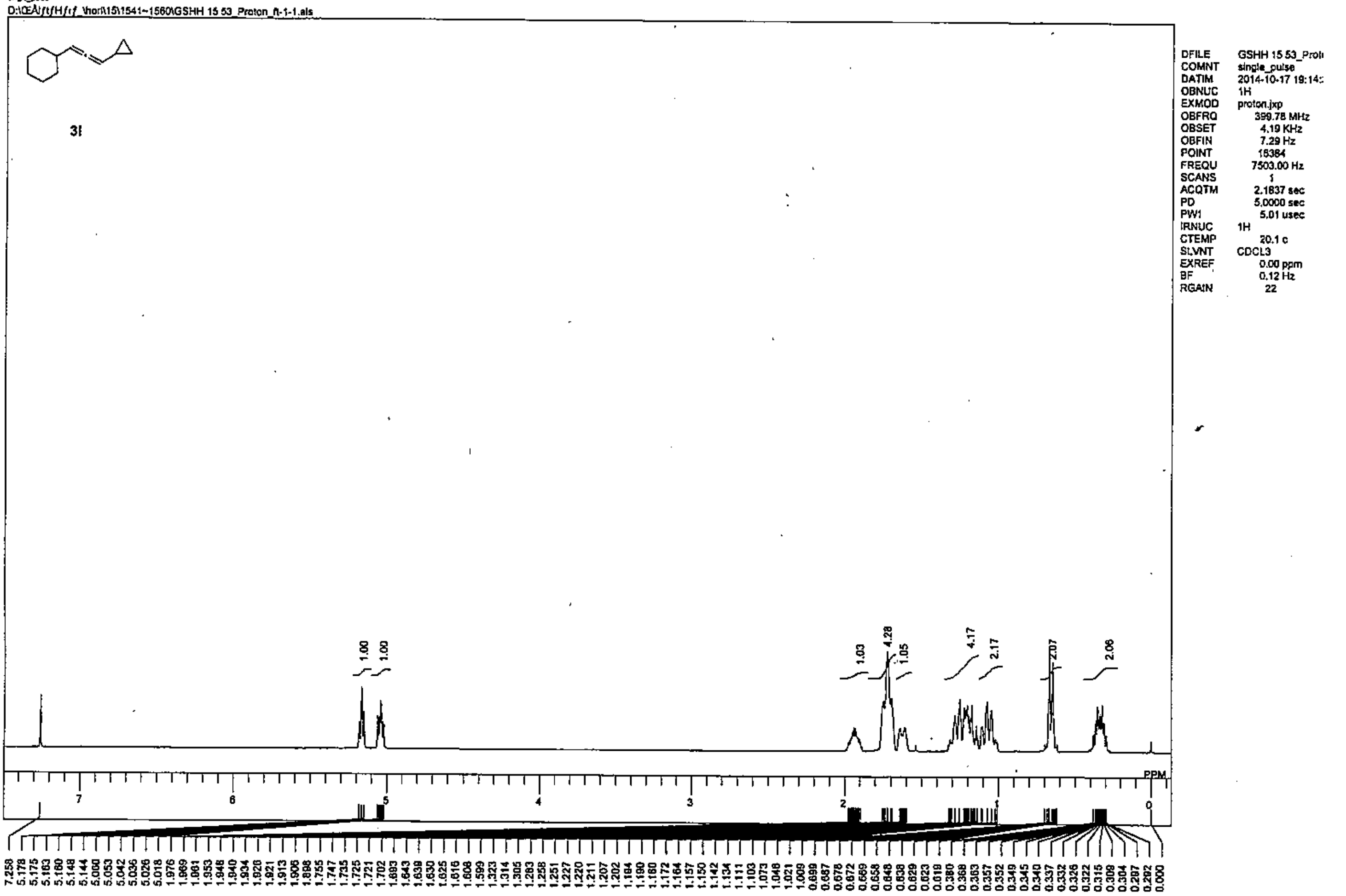


205.985 143.982 143.858 139.672 137.412 136.287 136.182 135.753 132.769 132.502 130.052 129.851 129.623 129.308 128.993 128.774 128.355 128.240 127.229 127.153 120.002 119.649 99.741 92.495 86.135 77.707 77.383 77.068 73.111 55.167 21.901 9.735 9.582 8.352 7.418 7.246 0.000

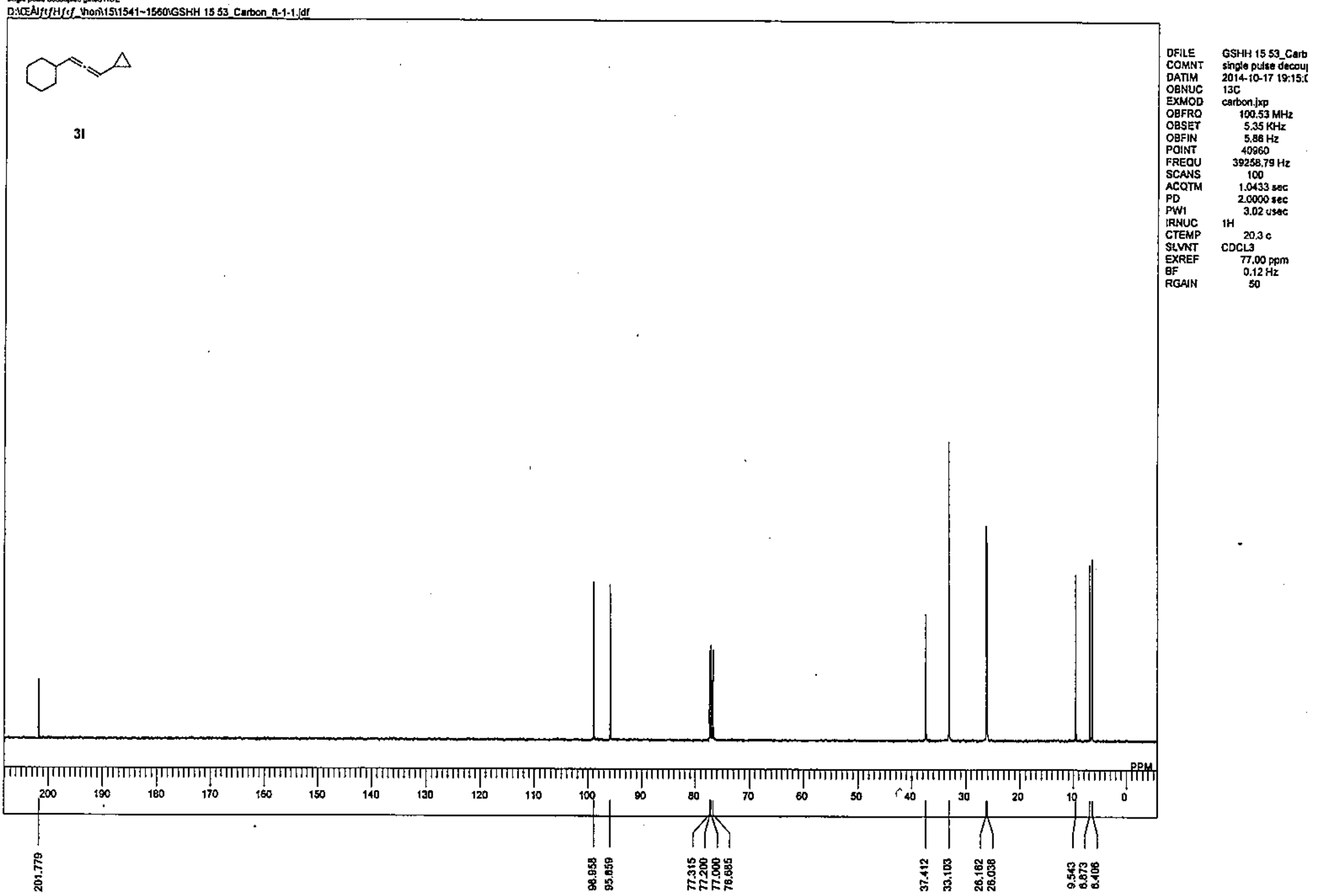

single_pulse
GSHH 13 13_Proton_ft-2-1.jdf
Me
Ph
3k
DFILE GSHH 13 13_Proto
COMNT single_pulse
DATIM 2014-05-30 18:18:2
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 24
1.91
2.00
1.09
0.79
3.12
0.89
2.11
2.12
PPM


single pulse decoupled gated NOE
GSHH 13 13_Carbon_ft-1-1.jdf
Me
Ph
3k
DFILE GSHH 13 13_Carb
COMNT single pulse decoup
DATIM 2014-05-30 18:17:5
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 20
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM
203.562
137.506
128.210
126.418
125.598
101.971
97.423
77.315
77.000
76.676
17.294
9.705
6.940
6.854

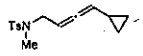
single_pulse
D:\ŒÀƒtƒHƒ‹ƒ_\hori\15\1541~1560\GSHH 15 53_Proton_ft-1-1.als


3l
DFILE GSHH 15 53_Prot
COMNT single_pulse
DATIM 2014-10-17 19:14:
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 1
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 22
1.00
1.00
1.03
4.28
1.05
4.17
2.17
2.07
2.06
7
6
5
4
3
2
1
0
PPM
7.258
5.178
5.175
5.163
5.160
5.148
5.144
5.060
5.053
5.042
5.036
5.026
5.018
1.976
1.969
1.961
1.953
1.948
1.940
1.934
1.926
1.921
1.913
1.906
1.898
1.755
1.747
1.735
1.725
1.721
1.702
1.693
1.643
1.639
1.630
1.625
1.616
1.608
1.599
1.323
1.314
1.305
1.283
1.258
1.251
1.227
1.220
1.211
1.207
1.202
1.194
1.190
1.180
1.172
1.164
1.157
1.150
1.142
1.134
1.111
1.103
1.073
1.048
1.021
1.009
0.699
0.687
0.676
0.672
0.669
0.658
0.648
0.638
0.629
0.623
0.619
0.380
0.368
0.363
0.357
0.352
0.349
0.345
0.340
0.337
0.332
0.326
0.322
0.315
0.309
0.304
0.297
0.292
0.000

single pulse decoupled gated NOE
D:\ŒÀƒtƒHƒ‹ƒ_\hori\15\1541~1560\GSHH 15 53_Carbon_ft-1-1.jdf

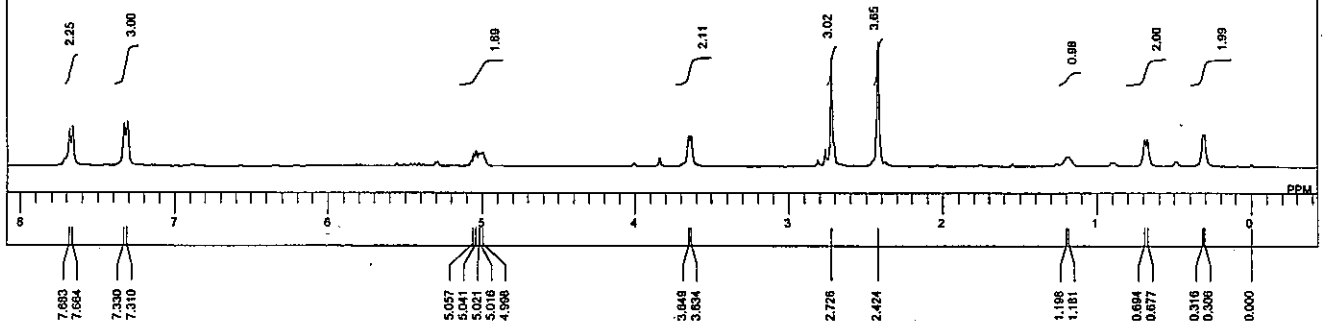

3l
DFILE GSHH 15 53_Carb
COMNT single pulse decou
DATIM 2014-10-17 19:15:
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 100
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
PPM
201.779
98.958
95.859
77.315
77.200
77.000
76.685
37.412
33.103
26.162
26.038
9.543
6.873
6.406

D:\CEA\f\f\H\r_\hori\14\1401-1420\GSHH_14_03_h.als



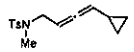
3m

DFILE GSHH_14_03_h.als
COMNT
DATIM 2014-07-07 15:12:5
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 5.75 usec
IRNUC
CTEMP 21.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 3.00 Hz
RGAIN 6



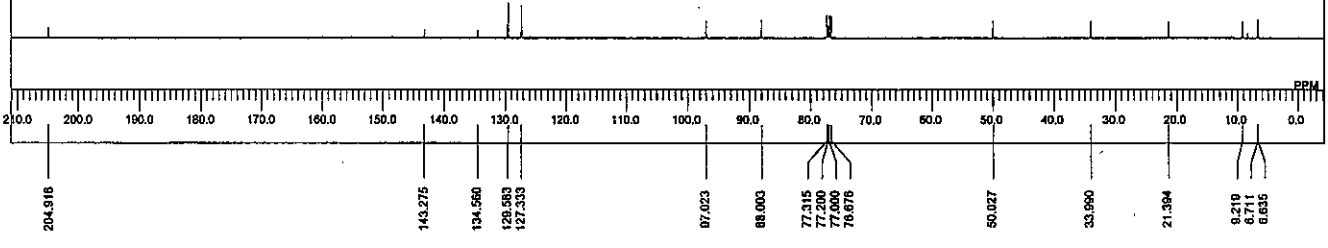
single pulse decoupled gated NOE

D:\CEA\f\f\H\r_\hori\14\1401-1420\GSHH 14 03 2nd_Carbon_ft-1-1.jdf

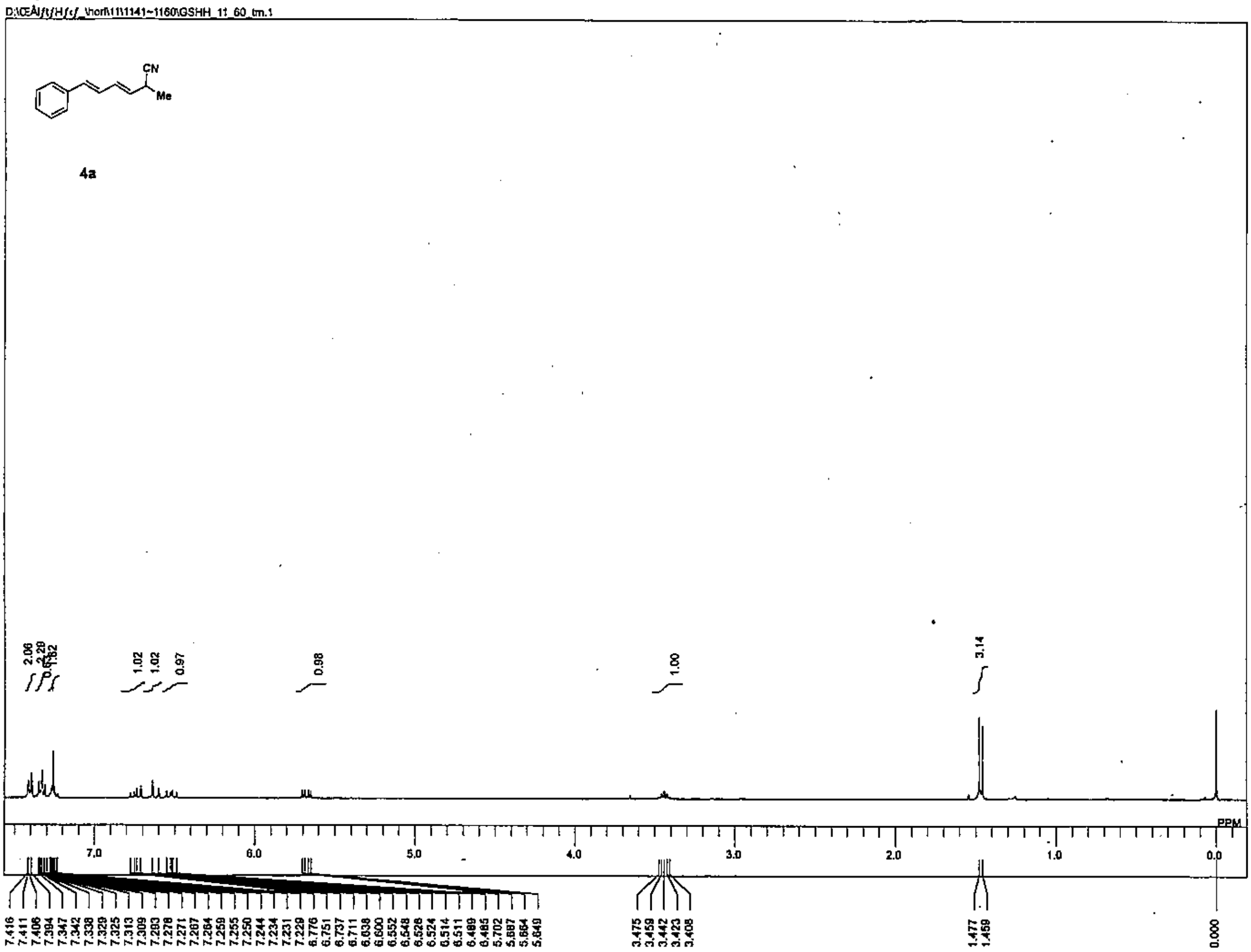


3m

DFILE GSHH 14 03 2nd_C
COMNT single pulse decou
DATIM 2014-08-15 17:08:4
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 30
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 23.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50



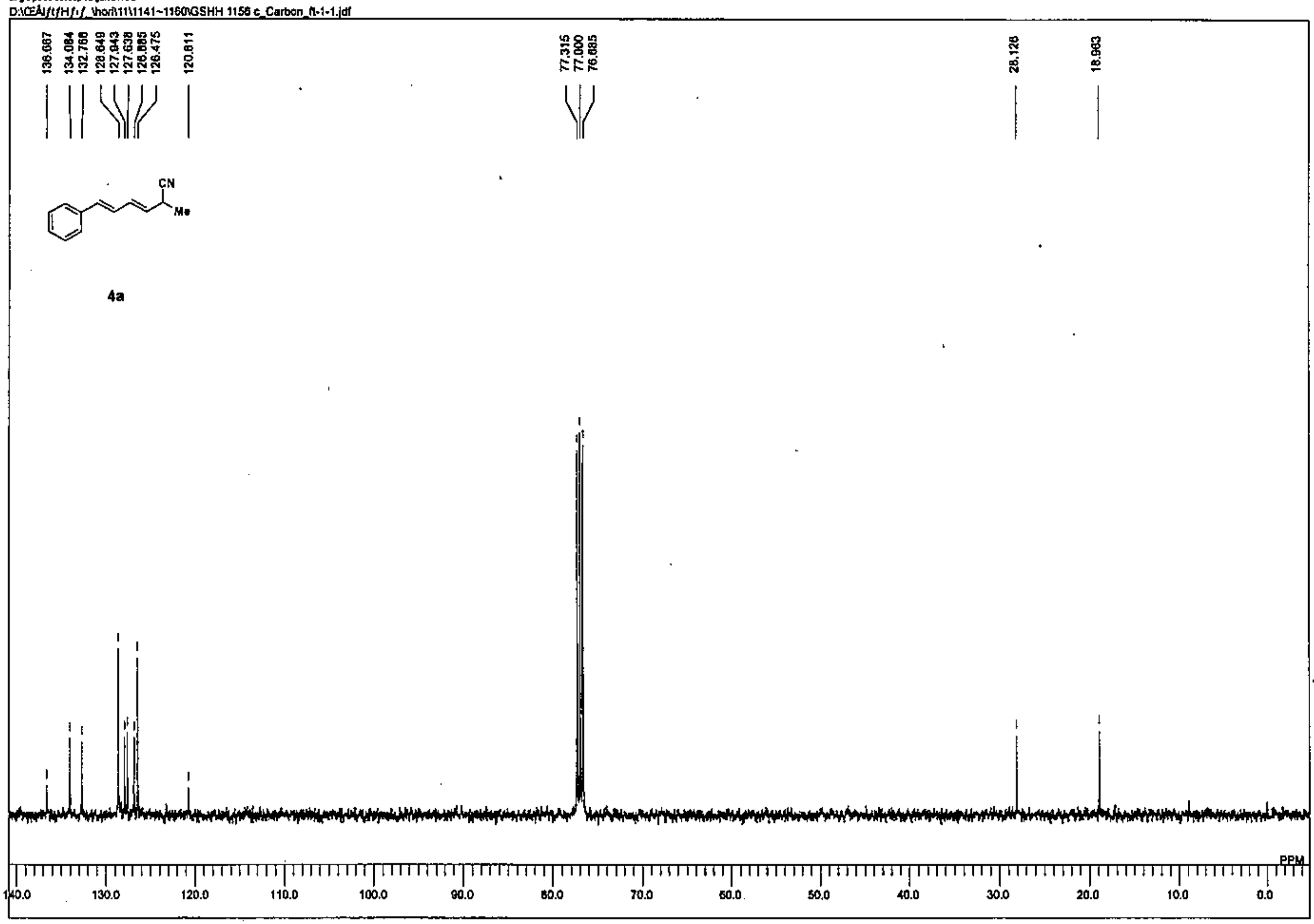
D:\ŒÂlƒtƒHƒ‹ƒ_\hori\11\1141~1160\GSHH_11_60_tm.1



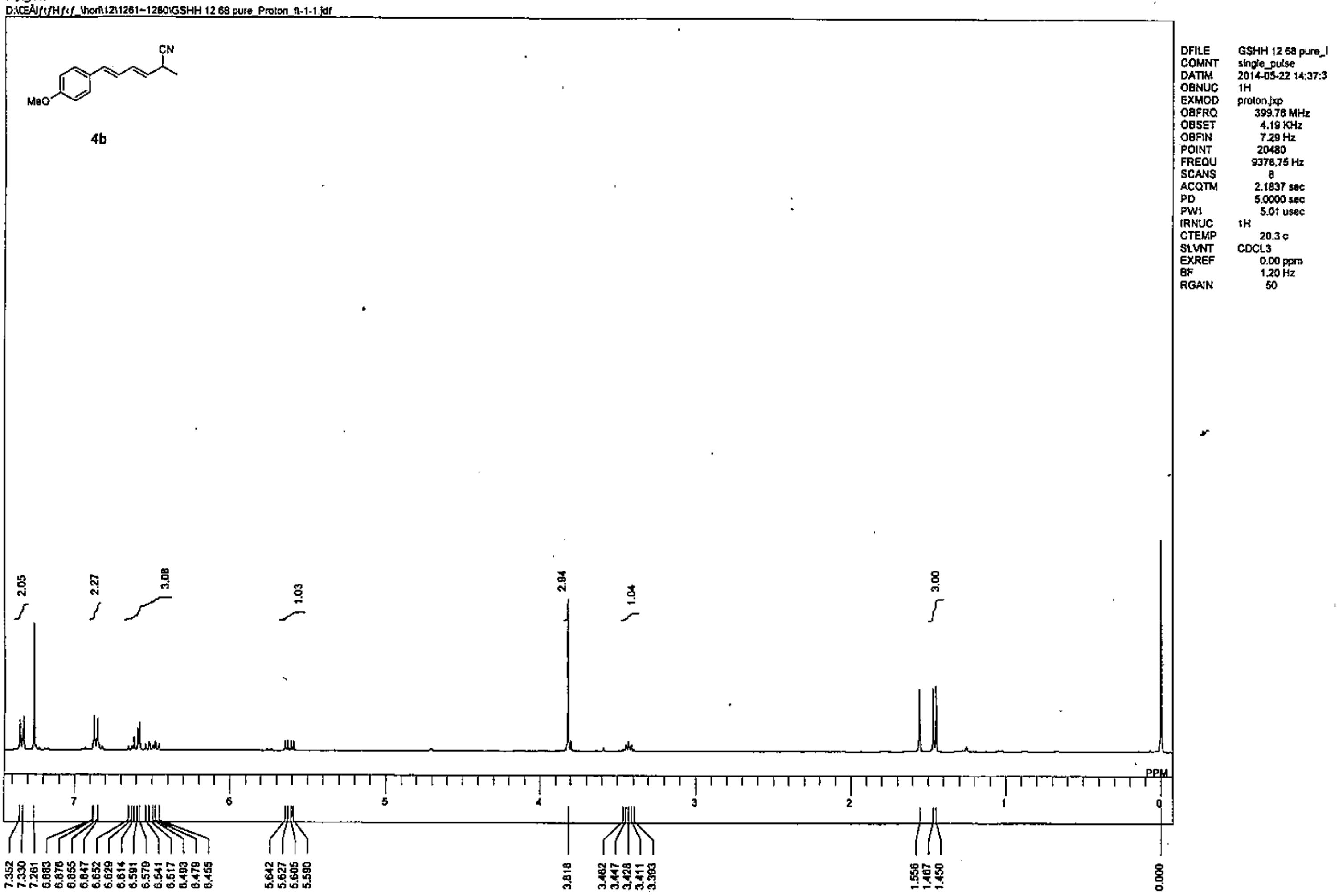
CN
Me
4a
2.06
2.29
1.52
1.02
1.02
0.97
0.98
1.00
3.14
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM
7.416
7.411
7.406
7.394
7.347
7.342
7.338
7.329
7.325
7.313
7.309
7.293
7.278
7.271
7.267
7.264
7.259
7.255
7.250
7.244
7.234
7.231
7.229
6.776
6.751
6.737
6.711
6.638
6.600
6.552
6.548
6.526
6.524
6.514
6.511
6.489
6.485
5.702
5.687
5.664
5.649
3.475
3.459
3.442
3.423
3.408
1.477
1.459
0.000

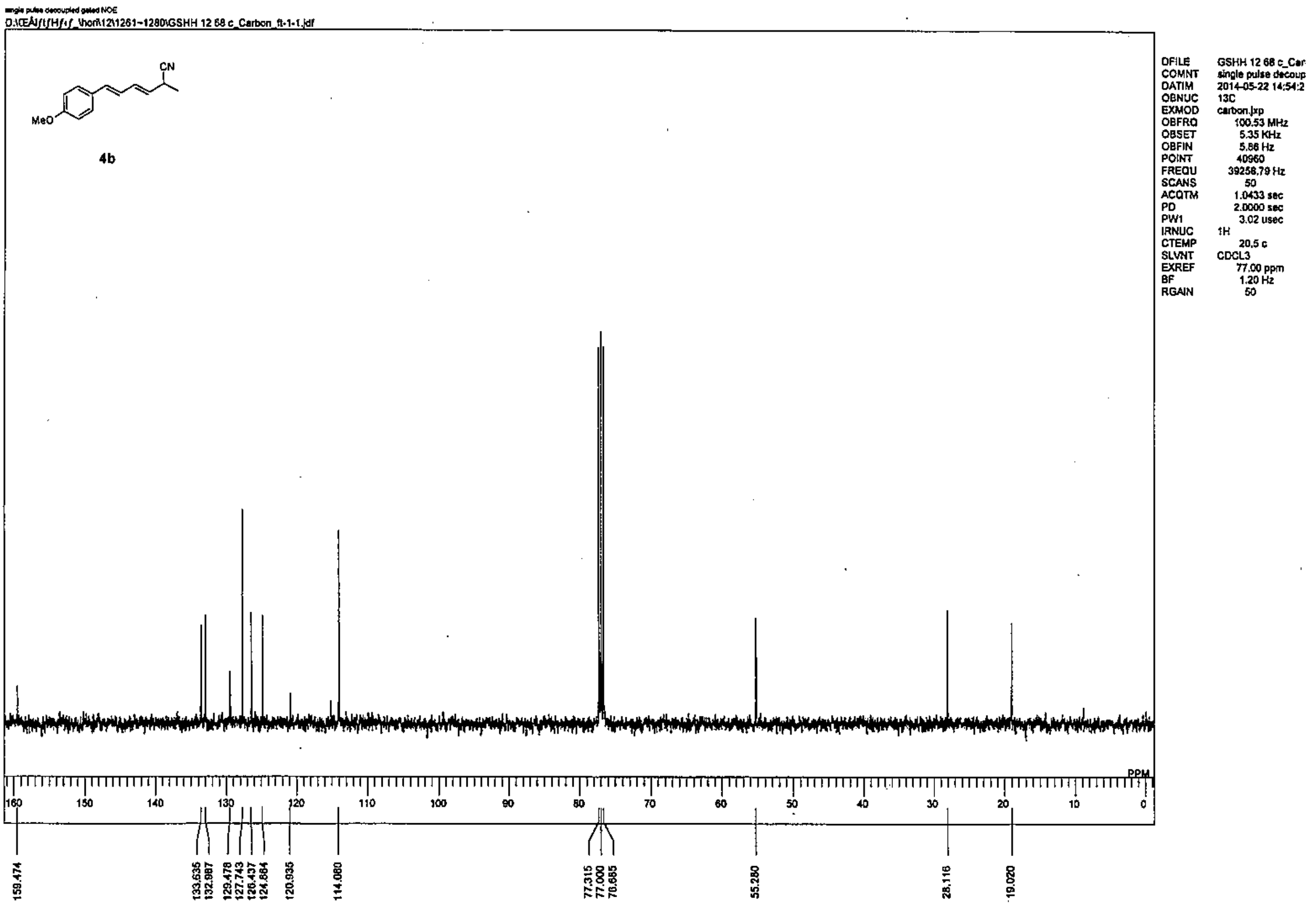
DFILE	GSHH_11_60_tm.1
COMNT	
DATIM	2014-03-15 14:27:5
OBNUC	1H
EXMOD	single_pulse.exp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	5996.80 Hz
SCANS	8
ACQTM	2.7312 sec
PD	2.0000 sec
PW1	6.00 usec
IRNUC	
CTEMP	21.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	17

single pulse decoupled gated NOE
D:\ŒÂlƒtƒHƒ‹ƒ_\hori\11\1141~1160\GSHH 1156 c_Carbon_ft-1-1.jdf

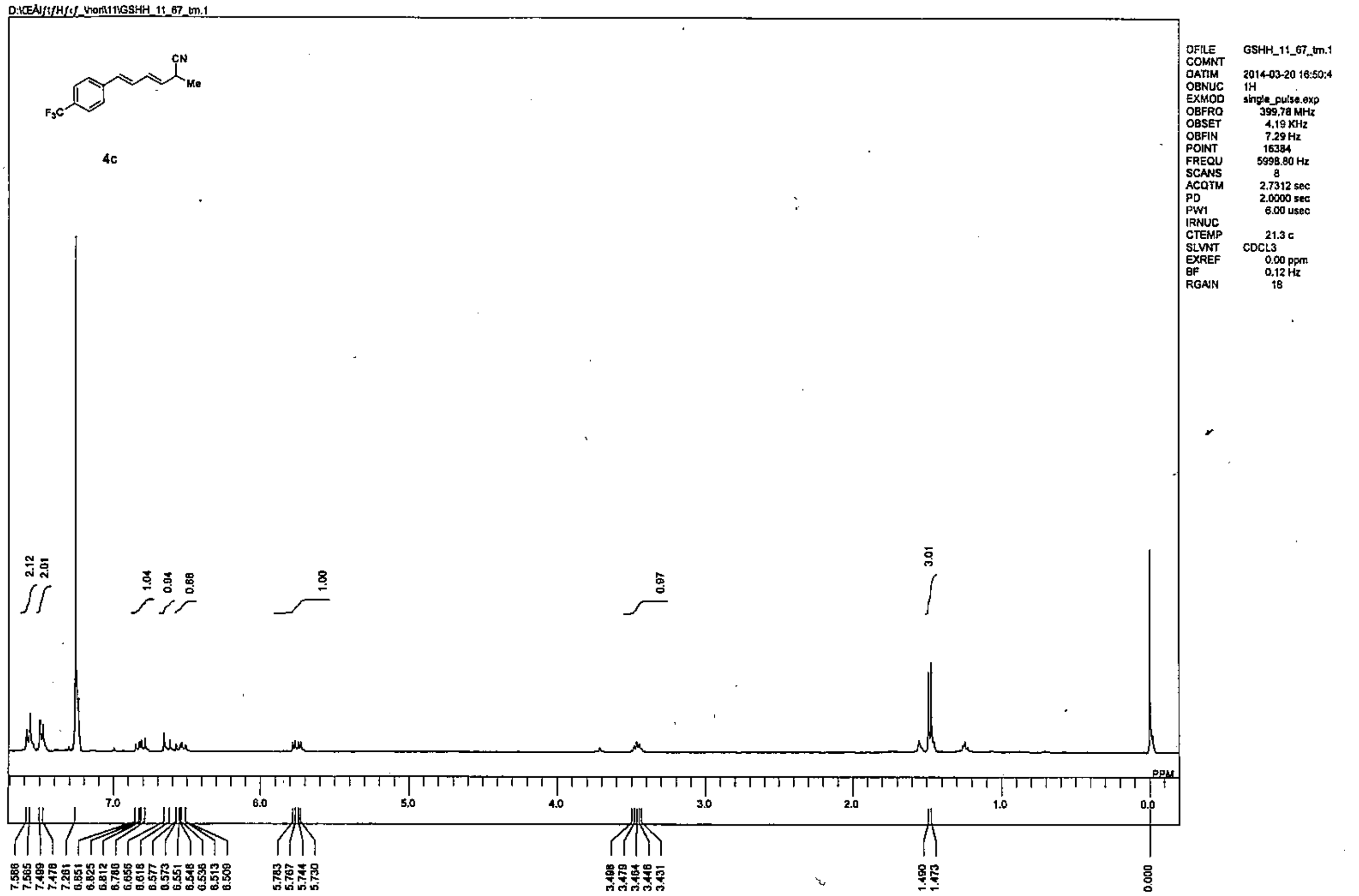


DFILE	GSHH 1156 c_Carl
COMNT	single pulse decour
DATIM	2014-03-13 13:08:5
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	100
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	19.1 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50

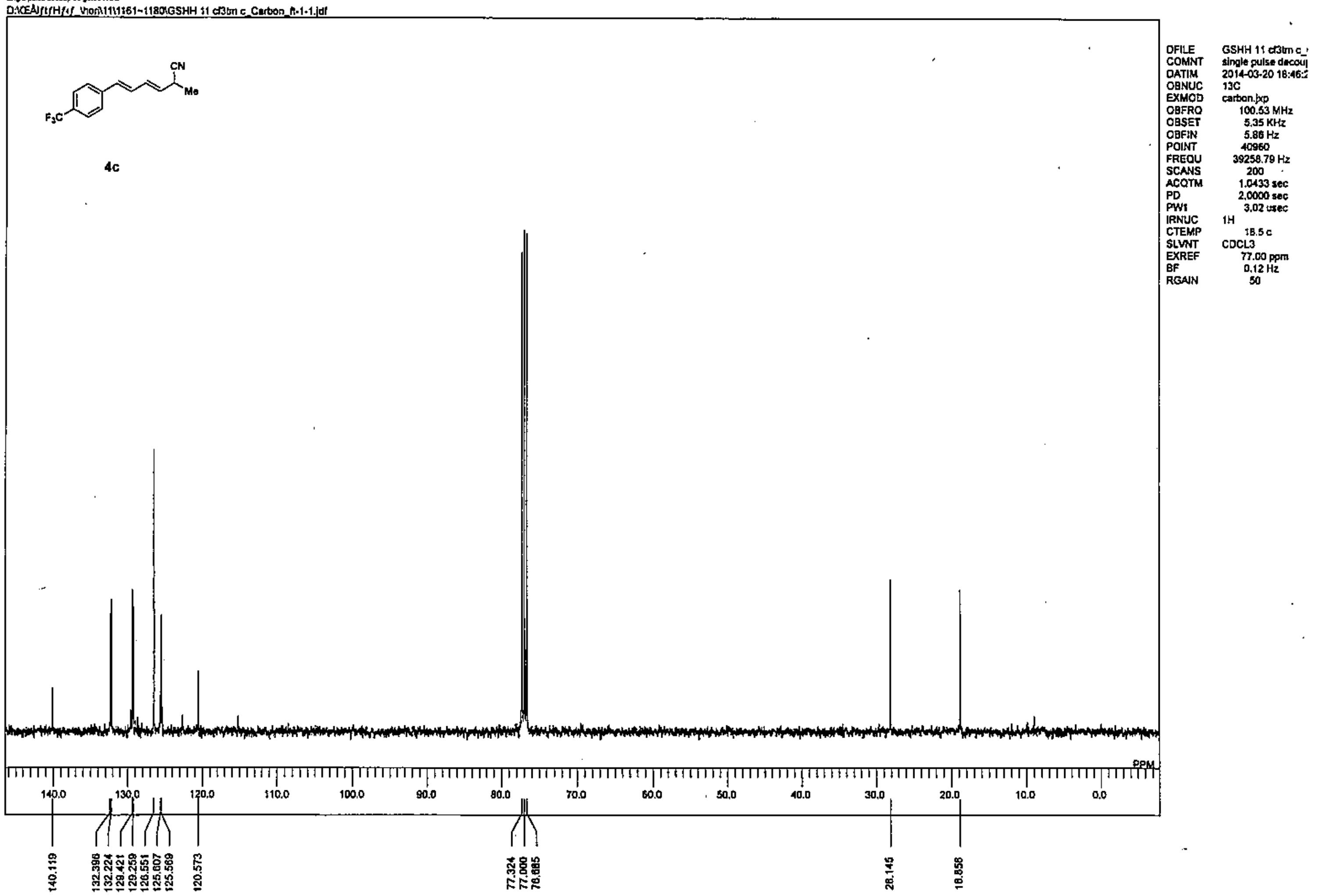

single_pulse
D:\CEÄƒtƒHƒcƒ_\hori\12\1261~1280\GSHH 12 68 pure_Proton_ft-1-1.jdf
CN
MeO
4b
DFILE GSHH 12 68 pure_I
COMNT single_pulse
DATIM 2014-05-22 14:37:3
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9376.75 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 50
2.05
2.27
3.08
1.03
2.94
1.04
3.00
PPM
7.352 7.330 7.261 6.883 6.876 6.855 6.847 6.852 6.629 6.614 6.591 6.579 6.541 6.517 6.493 6.479 6.455
5.642 5.627 5.605 5.590
3.818
3.462 3.447 3.428 3.411 3.393
1.556 1.467 1.450
0.000

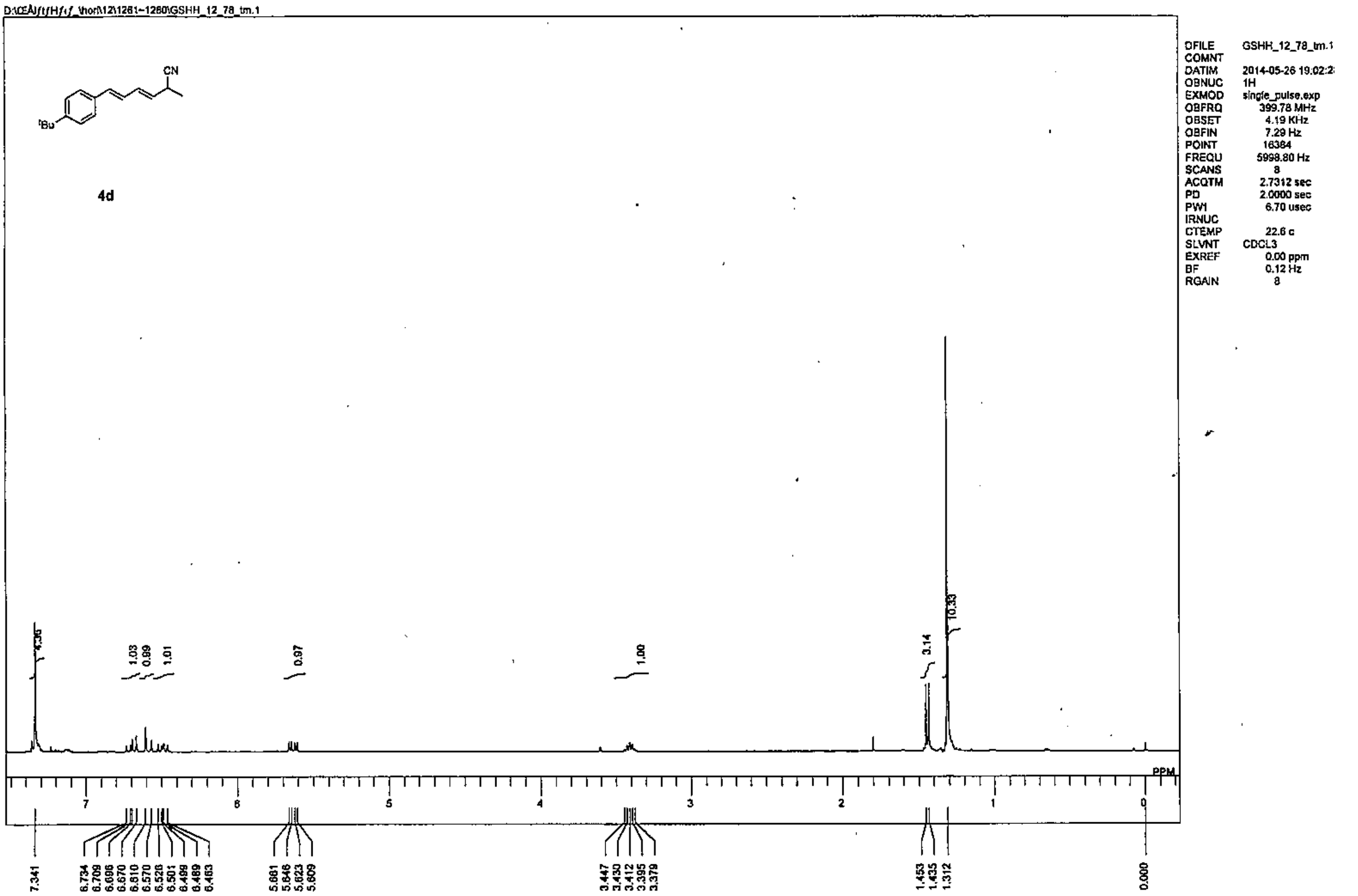

single pulse decoupled gated NOE
D:\CEÄƒtƒHƒcƒ_\hori\12\1261~1280\GSHH 12 68 c_Carbon_ft-1-1.jdf
CN
MeO
4b
DFILE GSHH 12 68 c_Car
COMNT single pulse decoup
DATIM 2014-05-22 14:54:2
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 50
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 50
PPM
159.474
133.635 132.987 129.478 127.743 126.437 124.884
120.935
114.080
77.315 77.000 76.685
55.280
28.116
19.020

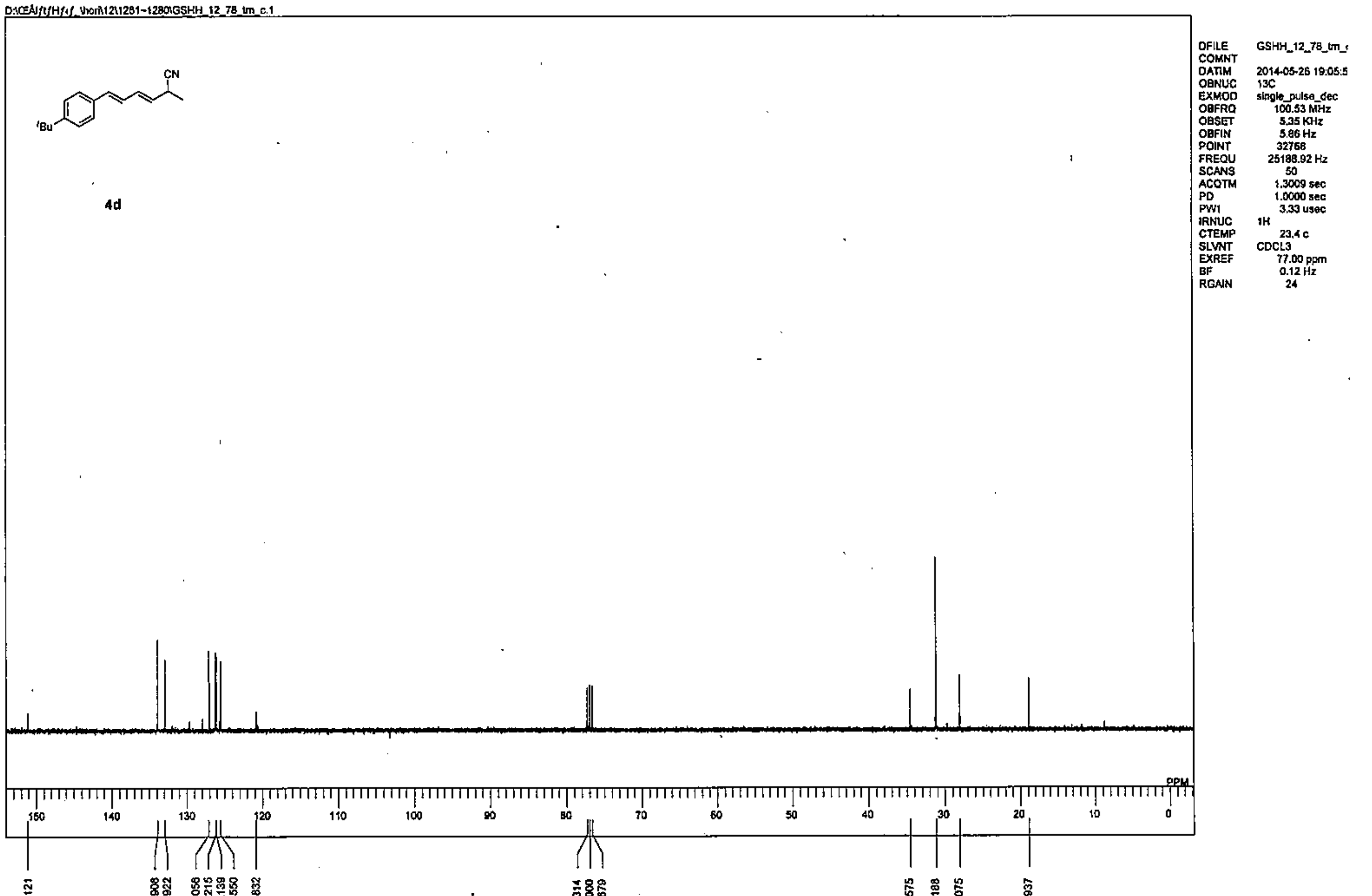
D:\ŒÊÀ\ƒ‡ƒHƒ‹ƒ_\hori\11\GSHH_11_67_tm.1

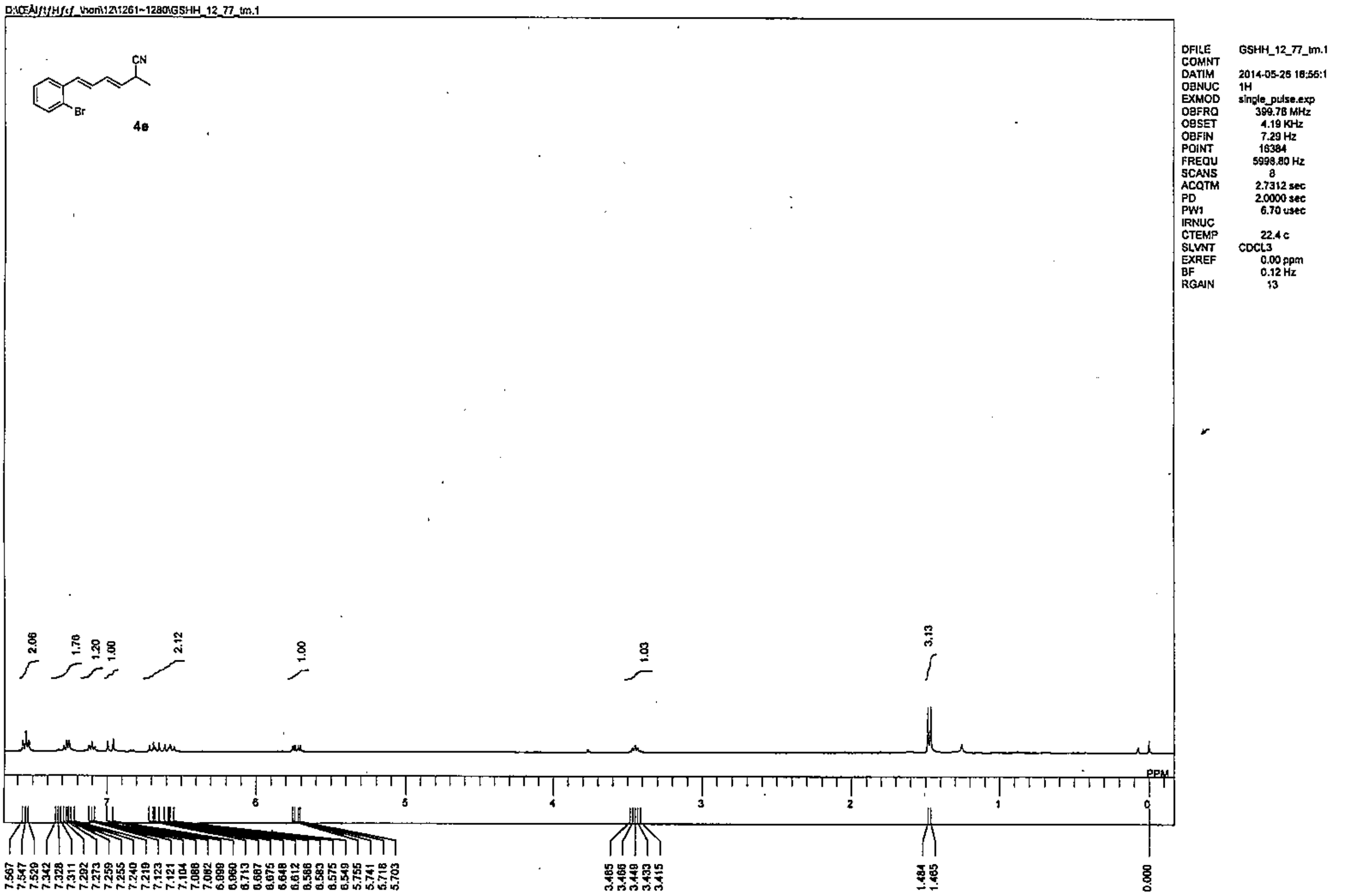

CN
Me
F3C
4c
DFILE GSHH_11_67_tm.1
COMNT
DATIM 2014-03-20 16:50:4
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.00 usec
IRNUC
CTEMP 21.3 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 18
2.12
2.01
1.04
0.94
0.88
1.00
0.97
3.01
PPM
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
7.586
7.565
7.499
7.478
7.281
6.851
6.825
6.812
6.780
6.656
6.618
6.577
6.573
6.551
6.548
6.536
6.513
6.509
5.783
5.767
5.744
5.730
3.498
3.479
3.464
3.446
3.431
1.490
1.473
0.000

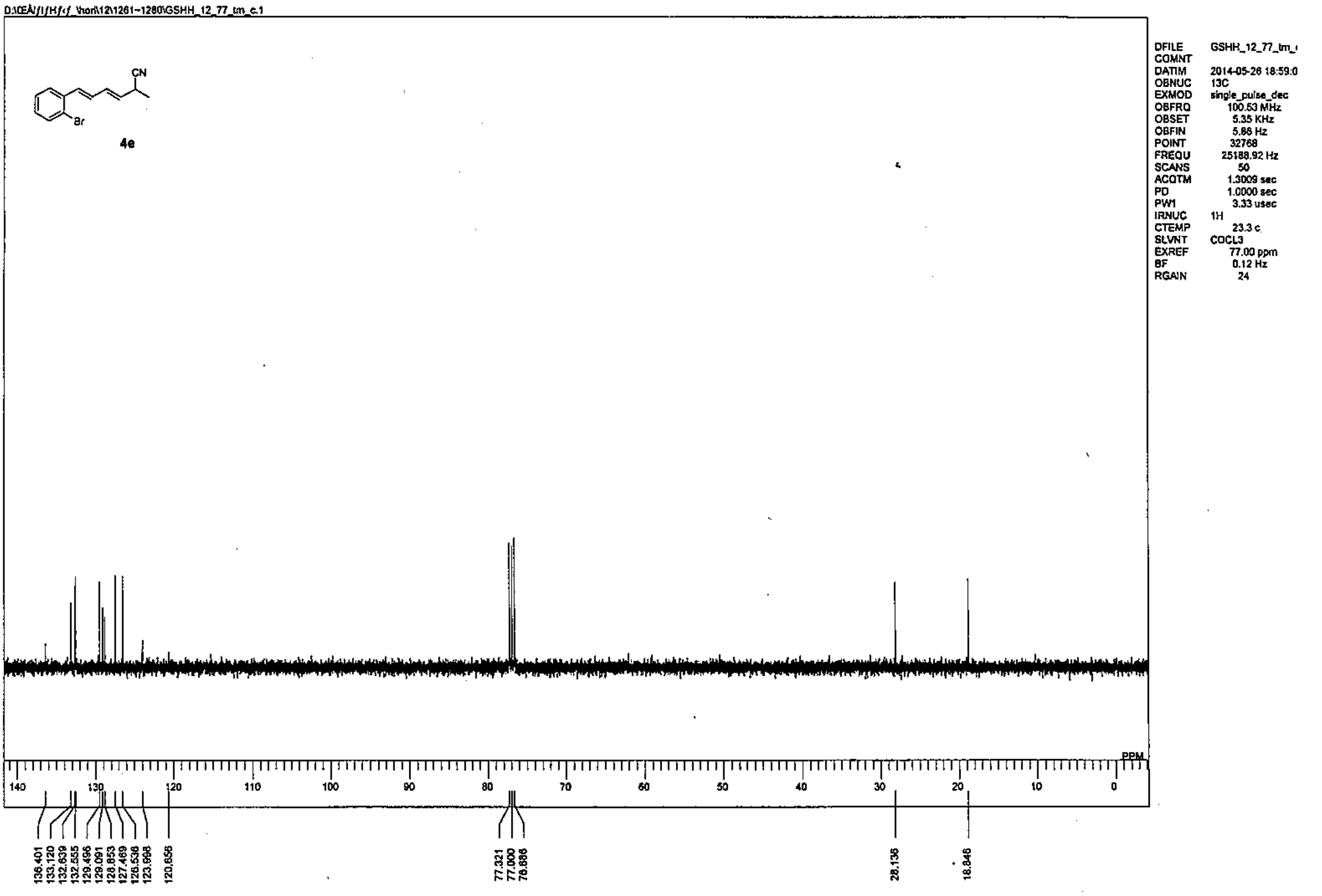
single pulse decoupled gated NOE
D:\ŒÊÀ\ƒ‡ƒHƒ‹ƒ_\hori\11\1161~1180\GSHH 11 cf3tm c_Carbon_ñ-1-1.jdf


CN
Me
F3C
4c
DFILE GSHH 11 cf3tm c_
COMNT single pulse decou
DATIM 2014-03-20 16:46:2
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 200
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 18.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
140.119
132.386
132.224
129.421
129.259
126.551
125.607
125.569
120.573
77.324
77.000
76.685
28.145
18.858

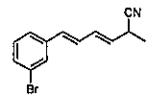

D:\CEÂ\ƒt\ƒHƒ\ƒ_\hori\12\1261~1280\GSHH_12_78_tm.1
CN
tBu
4d
DFILE GSHH_12_78_tm.1
COMNT
DATIM 2014-05-26 19:02:2
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.70 usec
IRNUC
CTEMP 22.6 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 8
4.36
1.03
0.99
1.01
0.97
1.00
3.14
10.33
PPM
7.341
6.734
6.709
6.698
6.670
6.610
6.570
6.526
6.501
6.499
6.489
6.463
5.661
5.646
5.623
5.609
3.447
3.430
3.412
3.395
3.379
1.453
1.435
1.312
0.000


D:\CEÂ\ƒt\ƒHƒ\ƒ_\hori\12\1261~1280\GSHH_12_78_tm_c.1
CN
tBu
4d
DFILE GSHH_12_78_tm_
COMNT
DATIM 2014-05-26 19:05:5
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 50
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 23.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24
PPM
151.121
133.906
132.922
127.056
126.215
126.139
125.550
120.832
77.314
77.000
76.679
34.575
31.188
28.075
18.937


D:\ŒÂ\f\Hƒcf_\hori\12\1261~1280\GSHH_12_77_tm.1
CN
Br
4e
DFILE GSHH_12_77_tm.1
COMNT
DATIM 2014-05-26 18:56:1
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.70 usec
IRNUC
CTEMP 22.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13
2.06
1.76
1.20
1.00
2.12
1.00
1.03
3.13
PPM
7.567 7.547 7.529 7.342 7.328 7.311 7.292 7.273 7.259 7.255 7.240 7.219 7.123 7.121 7.104 7.088 7.082 6.899 6.960 6.713 6.687 6.675 6.648 6.612 6.586 6.583 6.575 6.549 5.755 5.741 5.718 5.703
3.465 3.466 3.449 3.433 3.415
1.484 1.465
0.000


D:\ŒÂ\f\Hƒcf_\hori\12\1261~1280\GSHH_12_77_tm_c.1
CN
Br
4e
DFILE GSHH_12_77_tm_
COMNT
DATIM 2014-05-26 18:59:0
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 50
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 23.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24
PPM
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
136.401 133.120 132.639 132.555 129.496 129.091 128.853 127.469 126.536 123.998 120.656
77.321 77.000 76.686
28.136
18.846

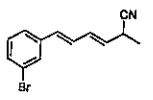
D:\CEA\ft\H\cf_\hom\12\1261~1280\GSHH_12_76_tm.1



4f

DFILE	GSHH_12_76_tm.1
COMNT	
DATIM	2014-05-26 18:50:0
OBNUC	1H
EXMOD	single_pulse.exp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	5998.80 Hz
SCANS	8
ACQTM	2.7312 sec
PD	2.0000 sec
PW1	6.70 usec
IRNUC	
CTEMP	22.3 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	12

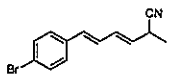
D:\CEA\ft\H\cf_\hom\12\1261~1280\GSHH_12_76_tm_c.1



4f

DFILE	GSHH_12_76_tm_c
COMNT	
DATIM	2014-05-26 18:53:0
OBNUC	13C
EXMOD	single_pulse_dec
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	25188.92 Hz
SCANS	50
ACQTM	1.3009 sec
PD	1.0000 sec
PW1	3.33 usec
IRNUC	1H
CTEMP	23.2 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	24

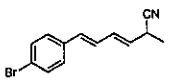
D:\CEÅ/t/tH/ɾ/_\hon\12\1261~1280\GSHH_12_75_tm.1



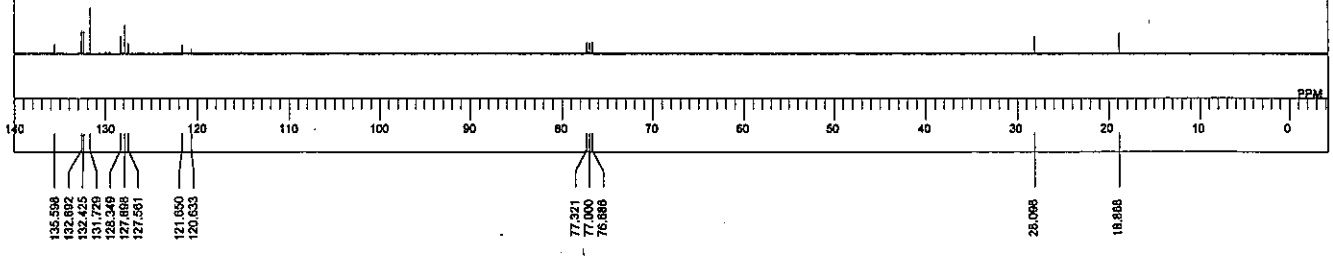
4g

DFILE GSHH_12_75_tm.1
COMNT
DATIM 2014-05-26 16:44:0
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 8.70 usec
IRNUC
CTEMP 21.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 11

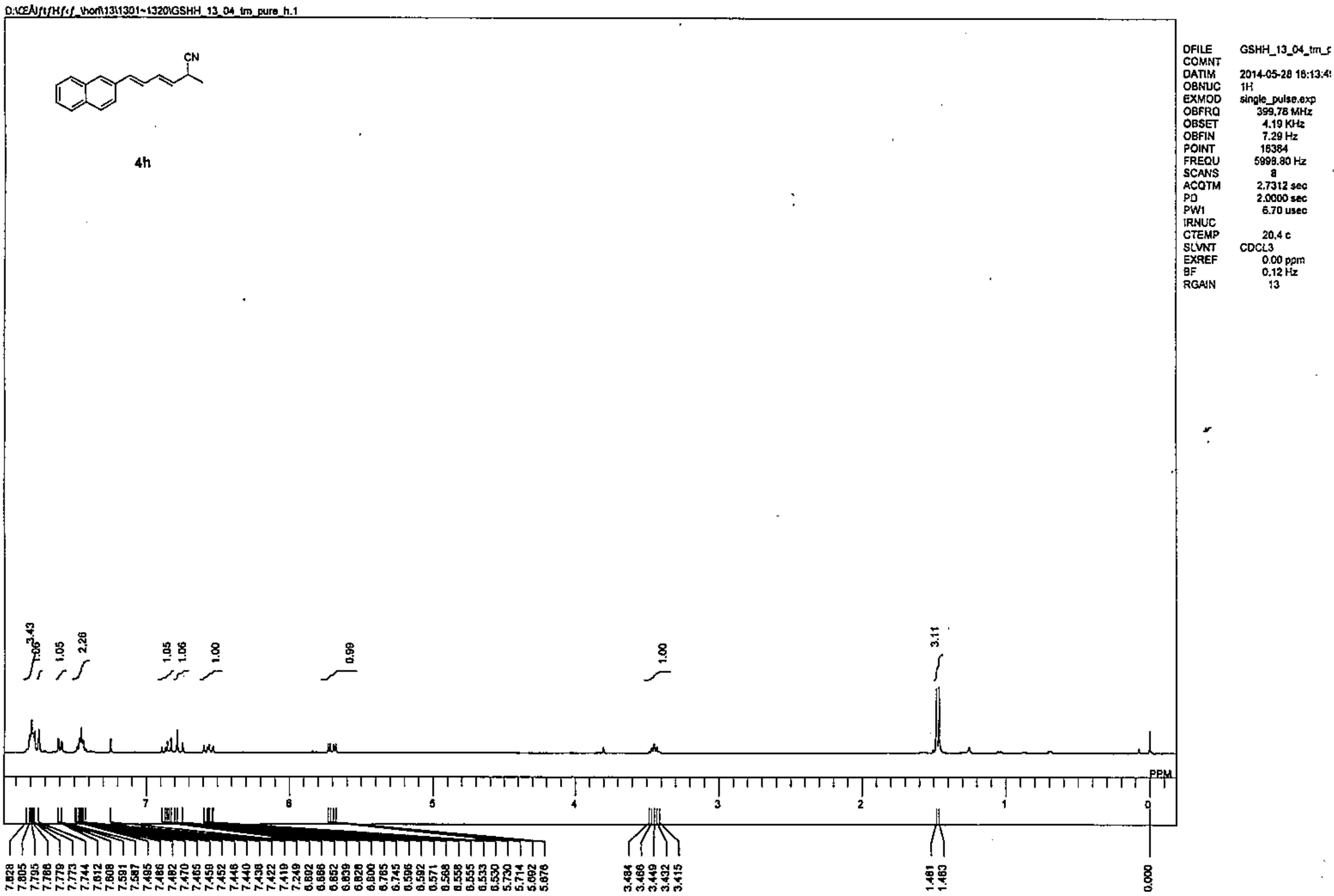
D:\CEÅ/t/tH/ɾ/_\hon\12\1261~1280\GSHH_12_75_tm_c.1



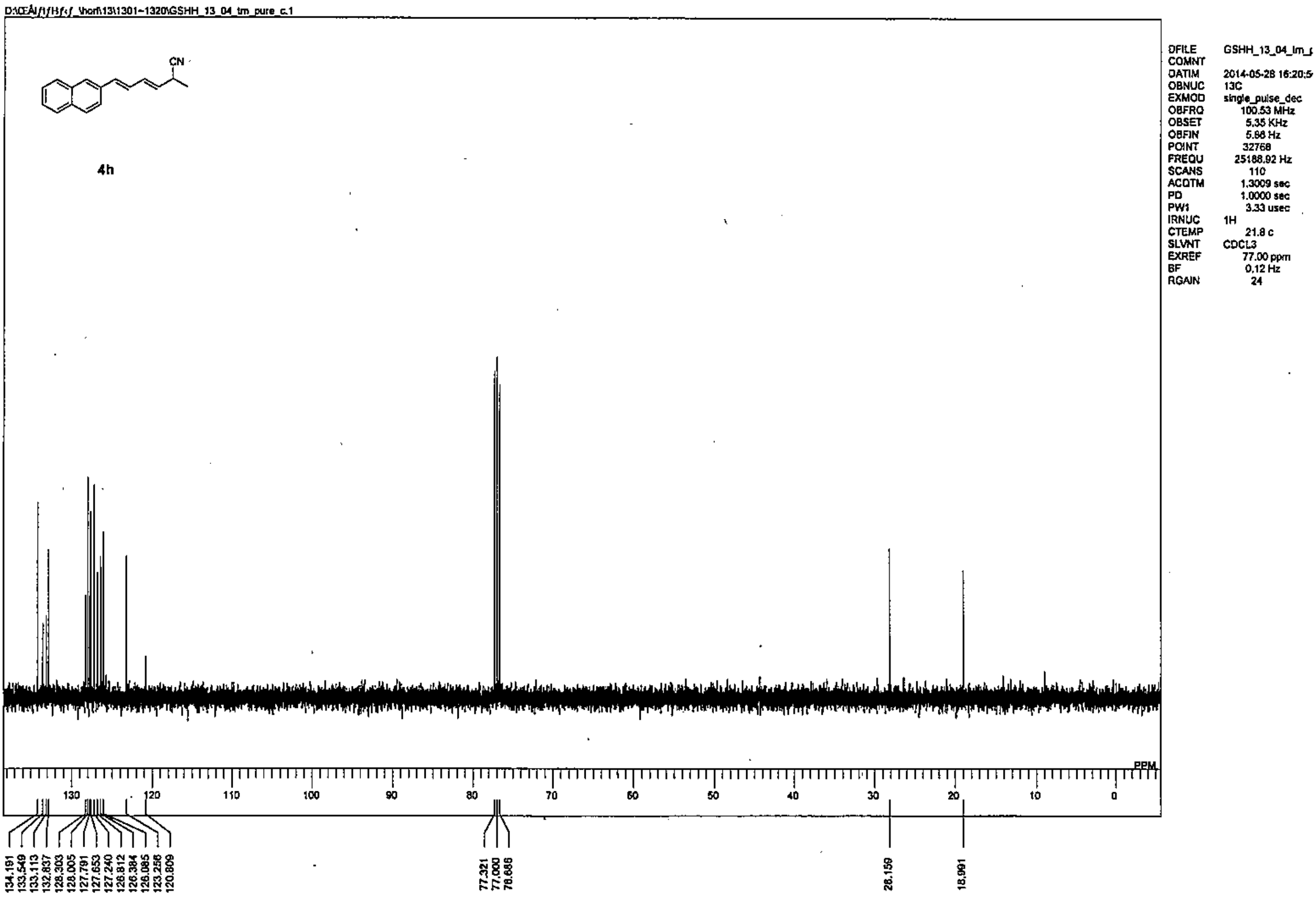
4g



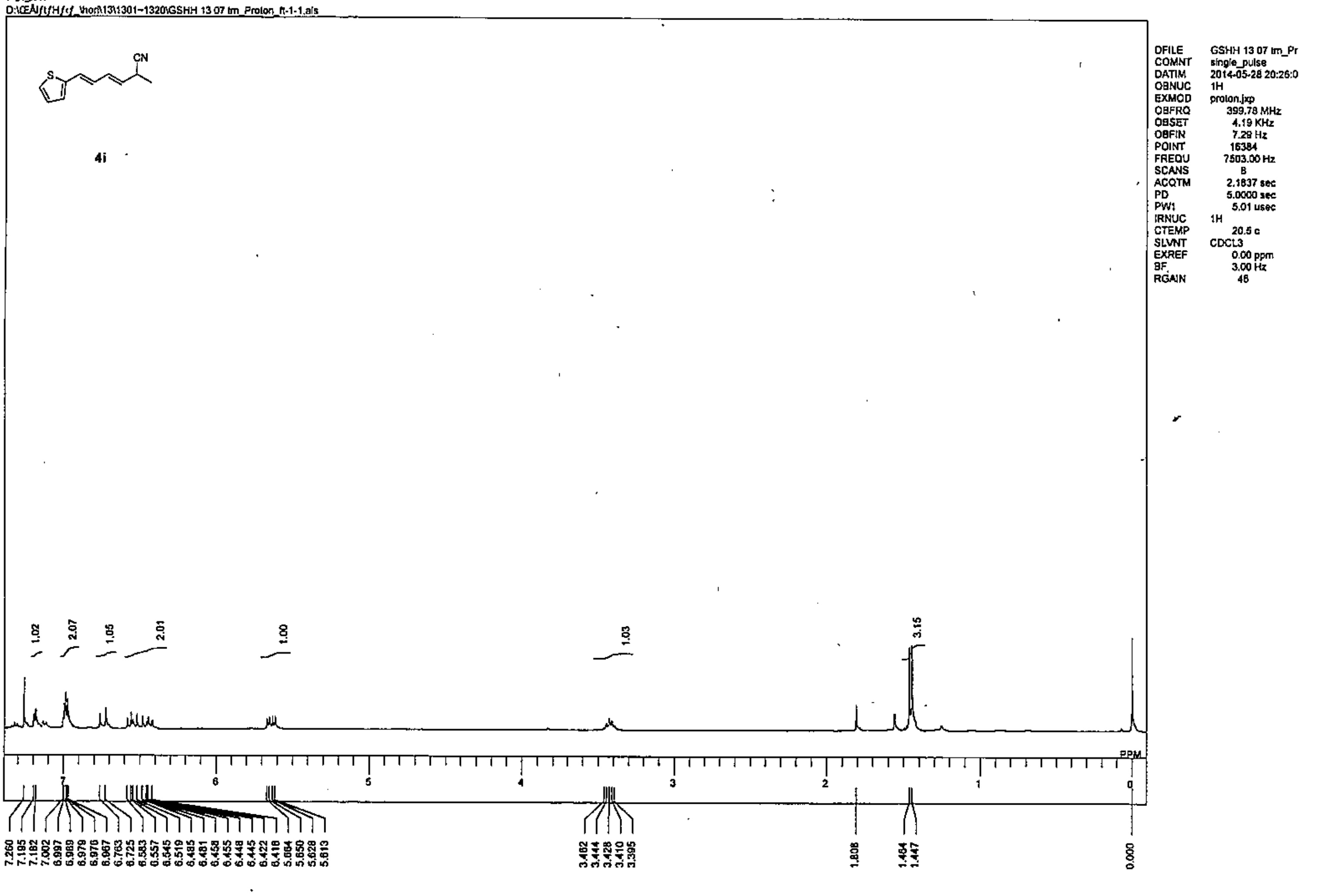
DFILE GSHH_12_75_tm_c
COMNT
DATIM 2014-05-26 16:47:0
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.68 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 50
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24



D:\ŒÅ\ƒ†ƒHƒ‹ƒ_\hori\13\1301~1320\GSHH_13_04_tm_pure_h.1
CN
4h
DFILE GSHH_13_04_tm_
COMNT
DATIM 2014-05-28 16:13:4
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 6.70 usec
IRNUC
CTEMP 20.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 13
3.43 1.06 1.05 2.26 1.05 1.06 1.00 0.99 1.00 3.11
PPM
7 6 5 4 3 2 1 0
7.828 7.805 7.795 7.788 7.779 7.773 7.744 7.612 7.608 7.591 7.587 7.495 7.486 7.482 7.470 7.465 7.458 7.452 7.446 7.440 7.438 7.422 7.419 7.249 6.892 6.866 6.852 6.839 6.826 6.800 6.765 6.745 6.596 6.592 6.571 6.568 6.558 6.555 6.533 6.530 5.730 5.714 5.692 5.676
3.484 3.466 3.449 3.432 3.415
1.481 1.463
0.000



D:\ŒÅ\ƒ†ƒHƒ‹ƒ_\hori\13\1301~1320\GSHH_13_04_tm_pure_c.1
CN
4h
DFILE GSHH_13_04_tm_
COMNT
DATIM 2014-05-28 16:20:5
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 110
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 21.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 24
PPM
130 120 110 100 90 80 70 60 50 40 30 20 10 0
134.181 133.549 133.113 132.837 128.303 128.005 127.791 127.653 127.240 126.812 126.384 126.085 123.256 120.809
77.321 77.000 76.686
28.159
18.991


single_pulse
D:\ŒÀ\ƒ\ƒH\ƒ\ƒ\hori\13\1301~1320\GSHH 13 07 tm_Proton_ft-1-1.als
CN
S
4i
DFILE GSHH 13 07 tm_Pr
COMNT single_pulse
DATIM 2014-05-28 20:26:0
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 3.00 Hz
RGAIN 46
1.02
2.07
1.05
2.01
1.00
1.03
3.15
PPM
7
6
5
4
3
2
1
0
7.260
7.185
7.182
7.002
6.997
6.989
6.978
6.976
6.967
6.763
6.725
6.583
6.557
6.545
6.519
6.485
6.481
6.458
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6.445
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5.664
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3.410
3.395
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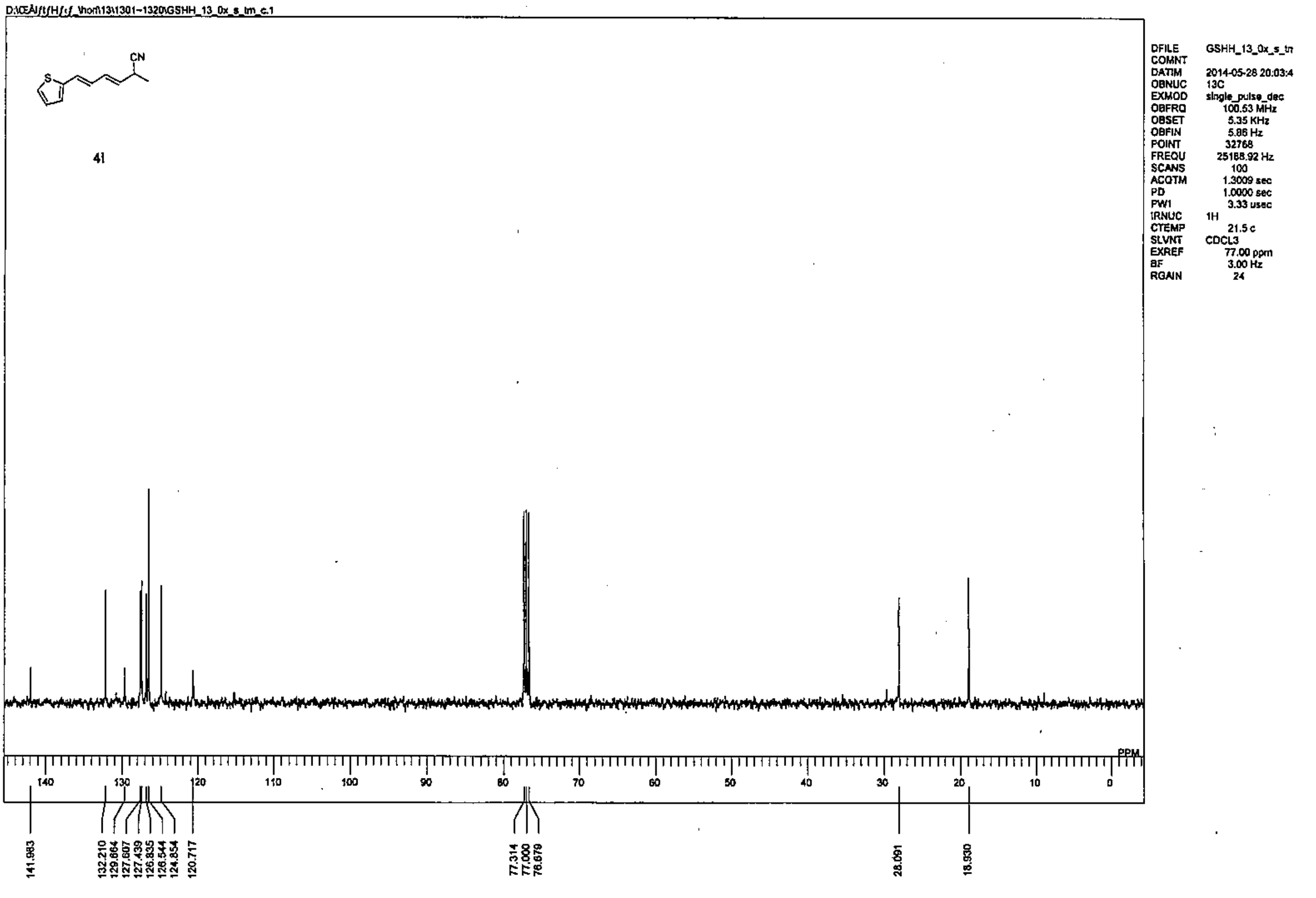
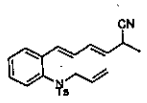
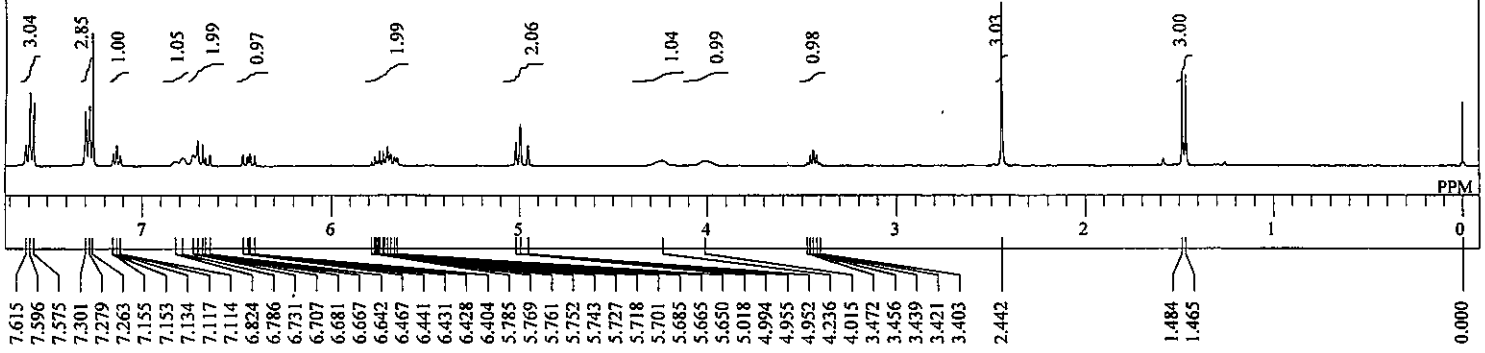
0.000


D:\ŒÀ\ƒ\ƒH\ƒ\ƒ\hori\13\1301~1320\GSHH_13_0x_s_tm_c.1
CN
S
4i
DFILE GSHH_13_0x_s_tm
COMNT
DATIM 2014-05-28 20:03:4
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 25188.92 Hz
SCANS 100
ACQTM 1.3009 sec
PD 1.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 21.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 3.00 Hz
RGAIN 24
PPM
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
141.983
132.210
129.664
127.607
127.439
126.835
126.544
124.854
120.717
77.314
77.000
76.679
28.091
18.930

D:\ŒÂl/t/Hƒ‹f_\hori\others\GSHH_NTs_TM_pure_h.als

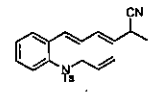


4j



7.615 7.596 7.575 7.301 7.279 7.263 7.155 7.153 7.134 7.117 7.114 6.824 6.786 6.731 6.707 6.681 6.667 6.642 6.467 6.441 6.431 6.428 6.404 5.785 5.769 5.761 5.752 5.743 5.727 5.718 5.701 5.685 5.665 5.650 5.018 4.994 4.955 4.952 4.236 4.015 3.472 3.456 3.439 3.421 3.403 2.442 1.484 1.465 0.000

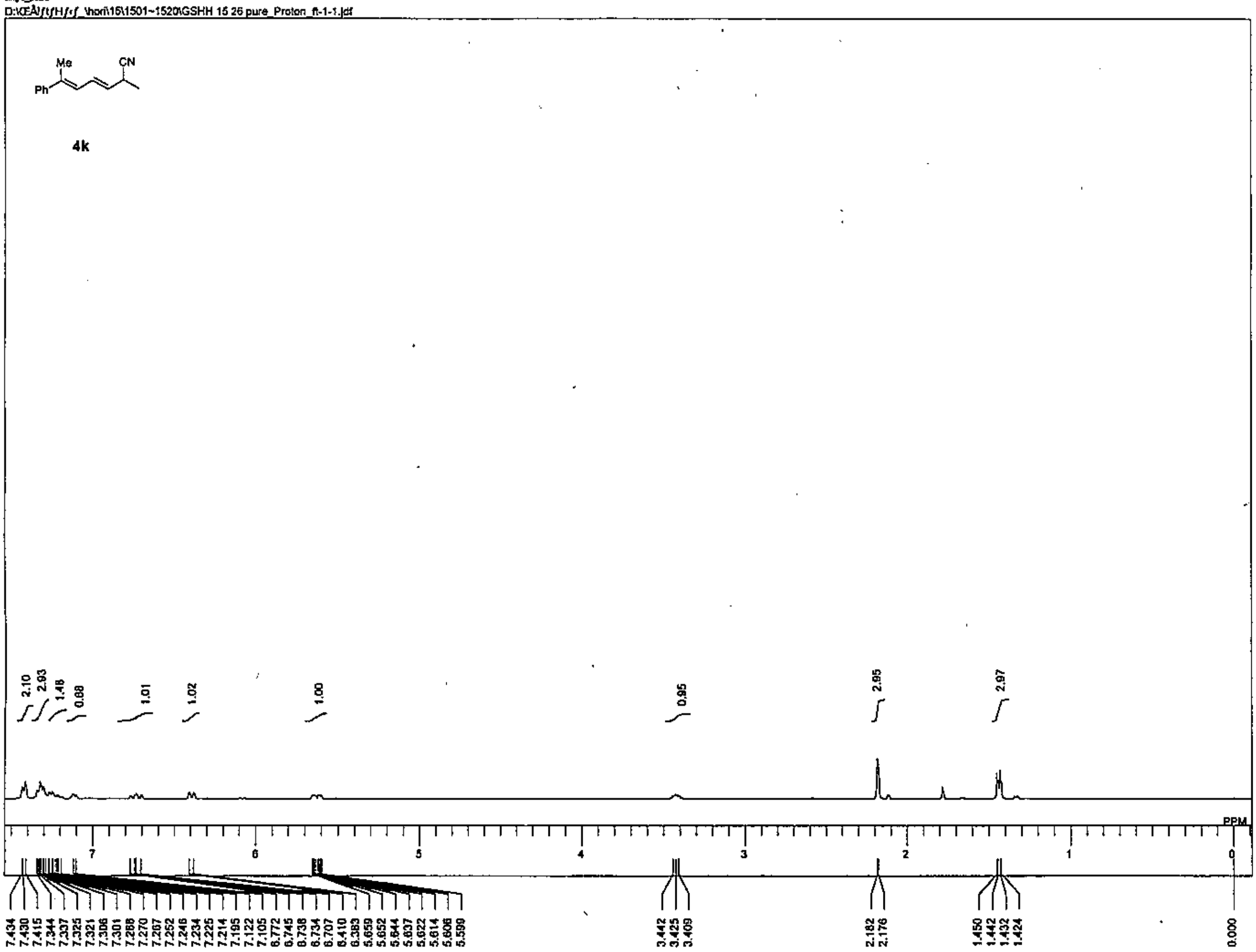
D:\ŒÂl/t/Hƒ‹f_\hori\others\GSHH_Br_TM_13C.als



4j

43.627 37.571 36.867 35.980 33.082 32.310 29.618 29.542 28.517 28.502 28.280 28.058 27.844 25.886 20.755 19.402 77.321 77.206 77.000 76.686 54.839 28.136 21.552 18.853

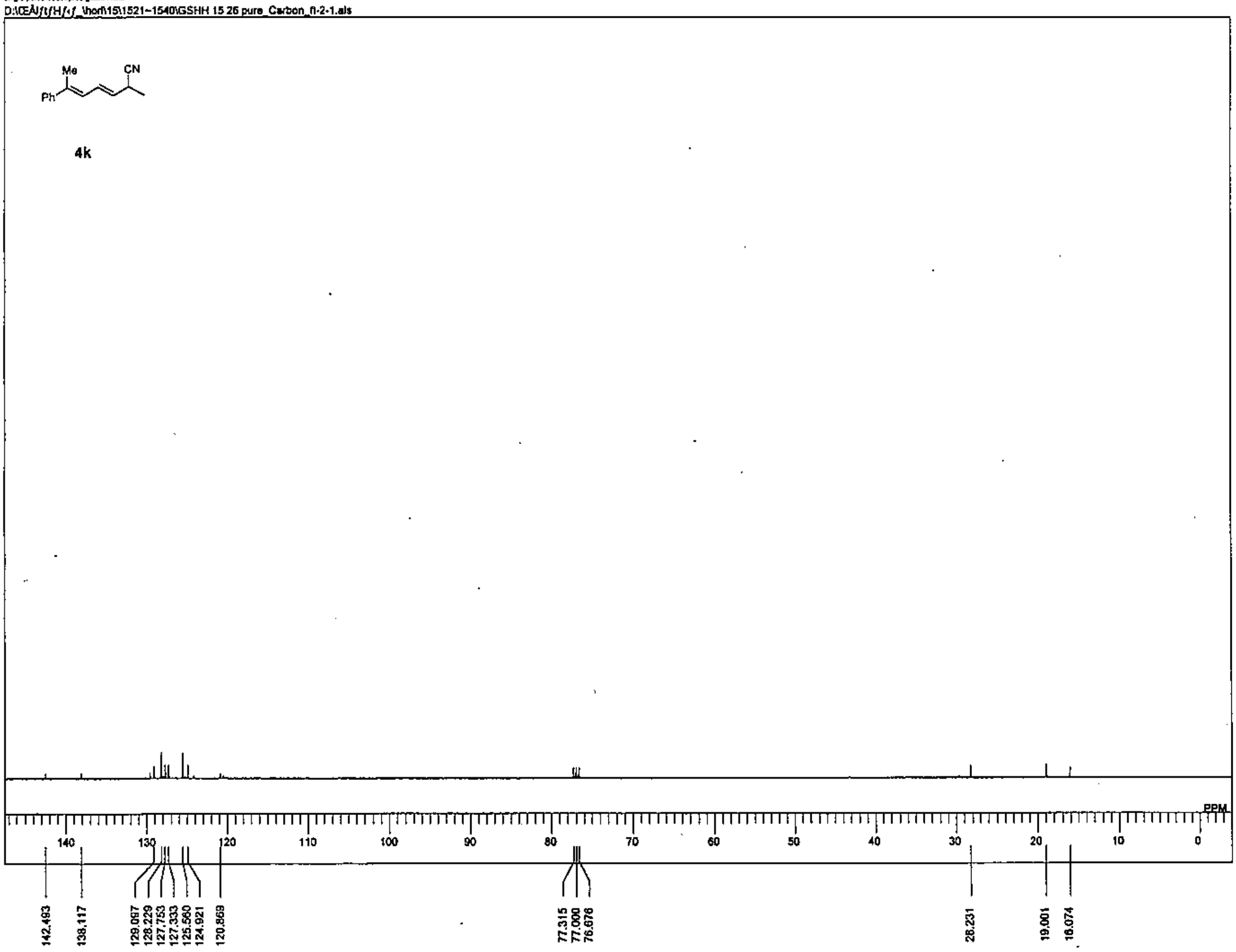
single_pulse
D:\ŒÃÌƒtƒHƒ‹ƒ_\hori\15\1501~1520\GSHH 15 26 pure_Proton_ft-1-1.jdf



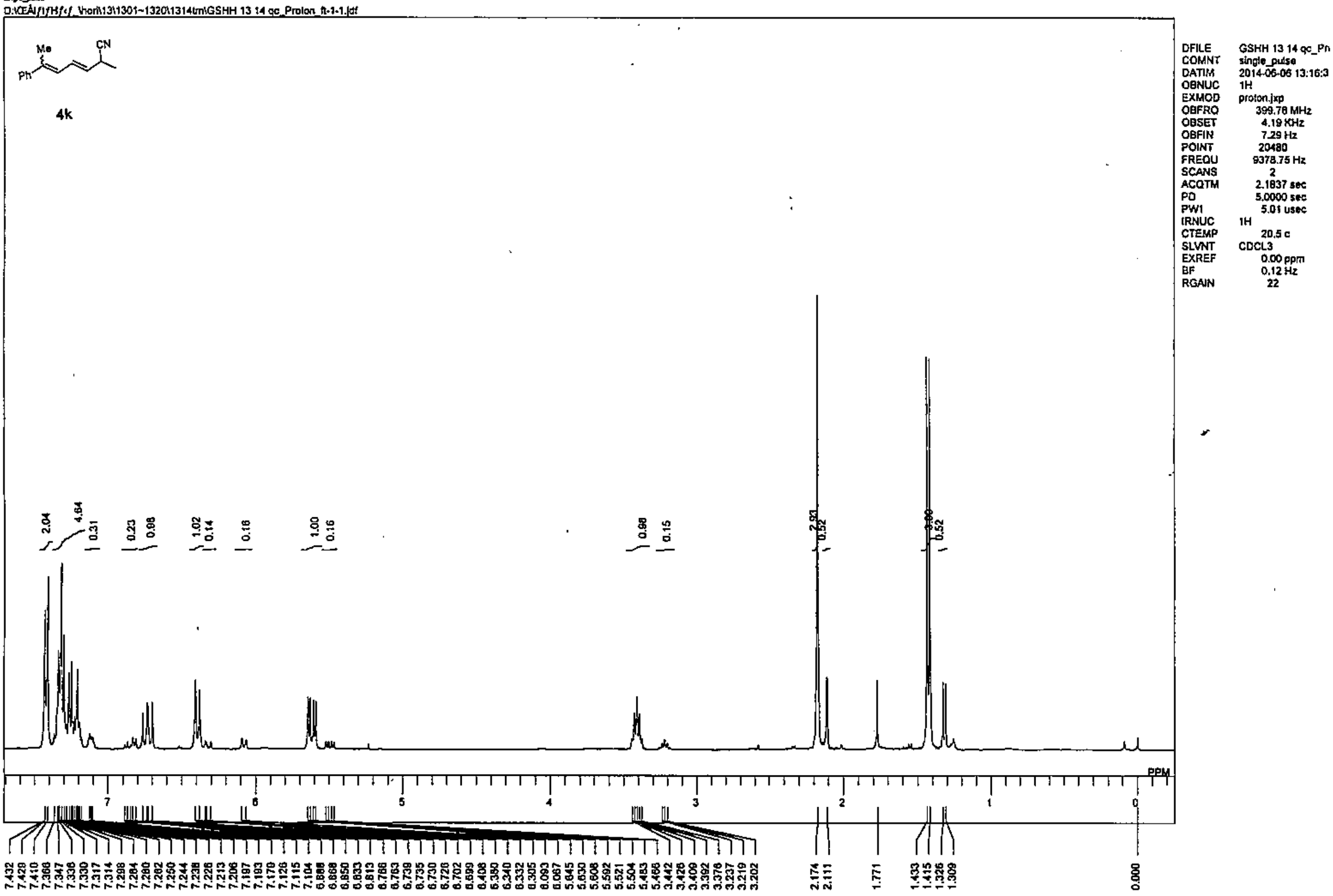
Me
CN
Ph
4k
2.10
2.93
1.48
0.88
1.01
1.02
1.00
0.95
2.95
2.97
PPM
7
6
5
4
3
2
1
0
7.434
7.430
7.415
7.344
7.337
7.325
7.321
7.306
7.301
7.288
7.270
7.267
7.252
7.246
7.234
7.225
7.214
7.195
7.122
7.105
6.772
6.745
6.738
6.734
6.707
6.410
6.383
5.659
5.652
5.644
5.637
5.622
5.614
5.606
5.599
3.442
3.425
3.409
2.182
2.176
1.450
1.442
1.432
1.424
0.000

DFILE GSHH 15 26 pure_I
COMNT single_pulse
DATIM 2014-09-30 11:24:2
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 1
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.8 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 24

single pulse decoupled gated NOE
D:\ŒÃÌƒtƒHƒ‹ƒ_\hori\15\1521~1540\GSHH 15 26 pure_Carbon_ft-2-1.als



DFILE GSHH 15 26 pure_(
COMNT single pulse decoup
DATIM 2014-09-30 11:25:1
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32768
FREQU 31407.04 Hz
SCANS 100
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50


single_pulse
GSHH 13 14 qc_Proton_ft-1-1.jdf
Me
CN
Ph
4k
DFILE GSHH 13 14 qc_Pr
COMNT single_pulse
DATIM 2014-06-06 13:16:3
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 2
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 22
PPM
2.04
4.64
0.31
0.23
0.98
1.02
0.14
0.16
1.00
0.16
0.98
0.15
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0.52
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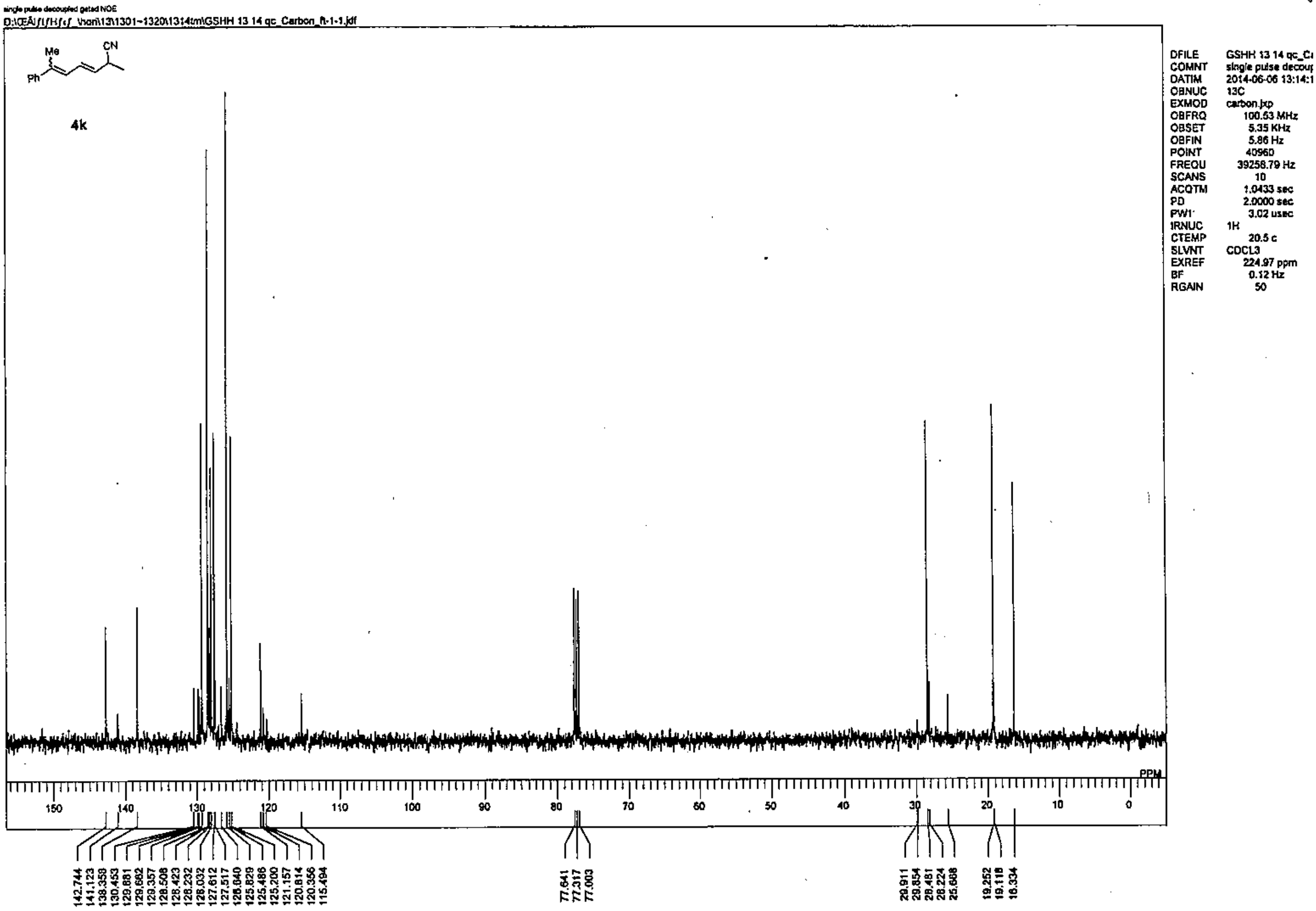
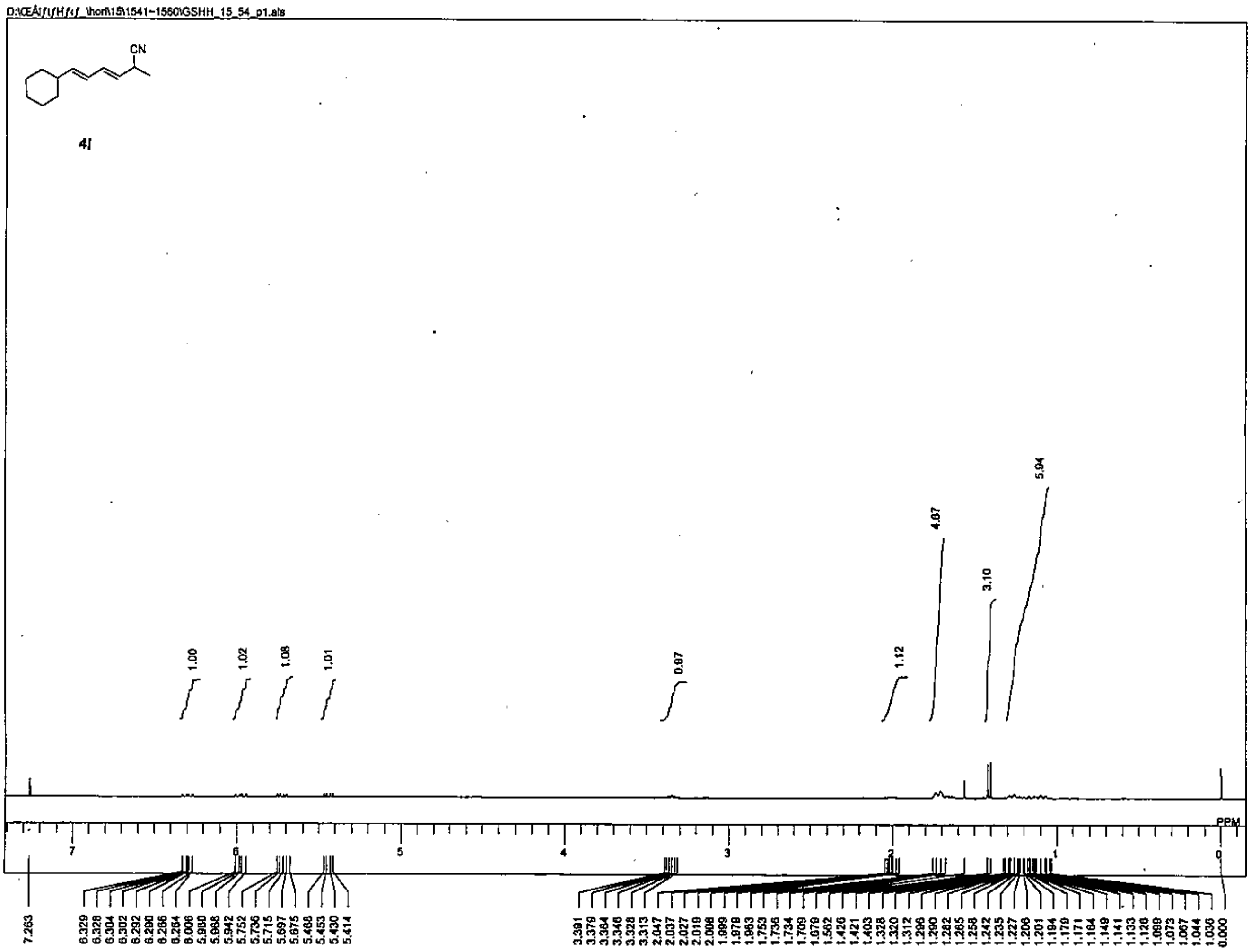
0.000

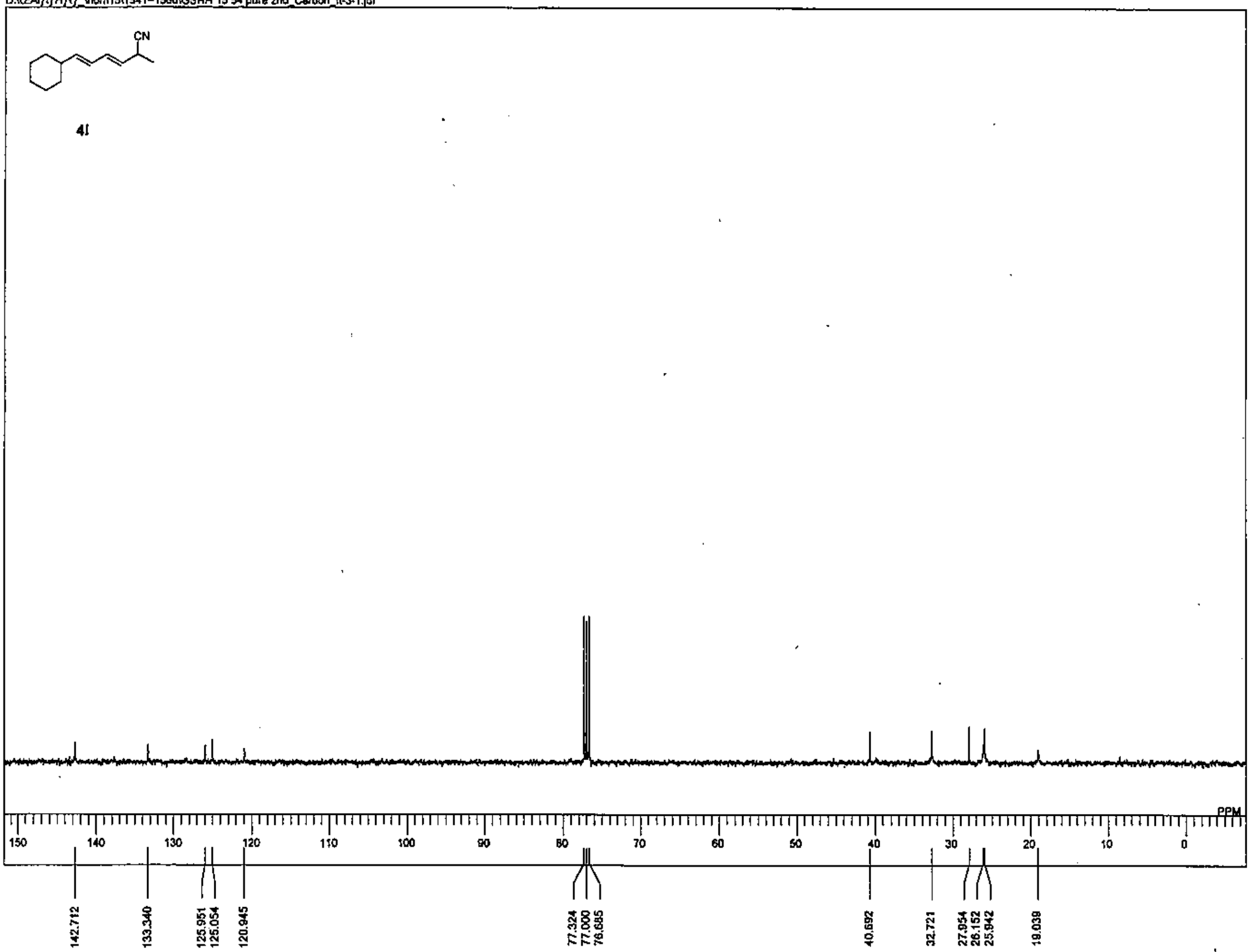

single pulse decoupled gated NOE
GSHH 13 14 qc_Carbon_ft-1-1.jdf
Me
CN
Ph
4k
DFILE GSHH 13 14 qc_C
COMNT single pulse decoup
DATIM 2014-06-06 13:14:1
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 10
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 224.97 ppm
BF 0.12 Hz
RGAIN 50
PPM
142.744
141.123
138.358
130.453
129.881
129.662
129.357
128.508
128.423
128.232
128.032
127.612
127.517
126.840
125.829
125.486
125.200
121.157
120.814
120.356
115.494
77.641
77.317
77.003
29.911
29.854
28.481
28.224
25.608
19.252
19.118
16.334

D:\ŒÅ\ƒtƒHƒ‹ƒ_\hori\15\1541~1560\GSHH_15_54_p1.als


CN
4l
1.00
1.02
1.08
1.01
0.97
1.12
4.87
3.10
5.94
PPM
7.263
6.329
6.328
6.304
6.302
6.292
6.290
6.288
6.264
6.008
5.980
5.968
5.942
5.752
5.736
5.715
5.697
5.675
5.468
5.453
5.430
5.414
3.391
3.379
3.364
3.346
3.328
3.313
2.047
2.037
2.027
2.019
2.008
1.999
1.978
1.963
1.753
1.736
1.734
1.709
1.679
1.562
1.426
1.421
1.403
1.328
1.320
1.312
1.296
1.290
1.282
1.265
1.258
1.242
1.235
1.227
1.206
1.201
1.194
1.179
1.171
1.164
1.149
1.141
1.133
1.126
1.099
1.073
1.067
1.044
1.036
0.000

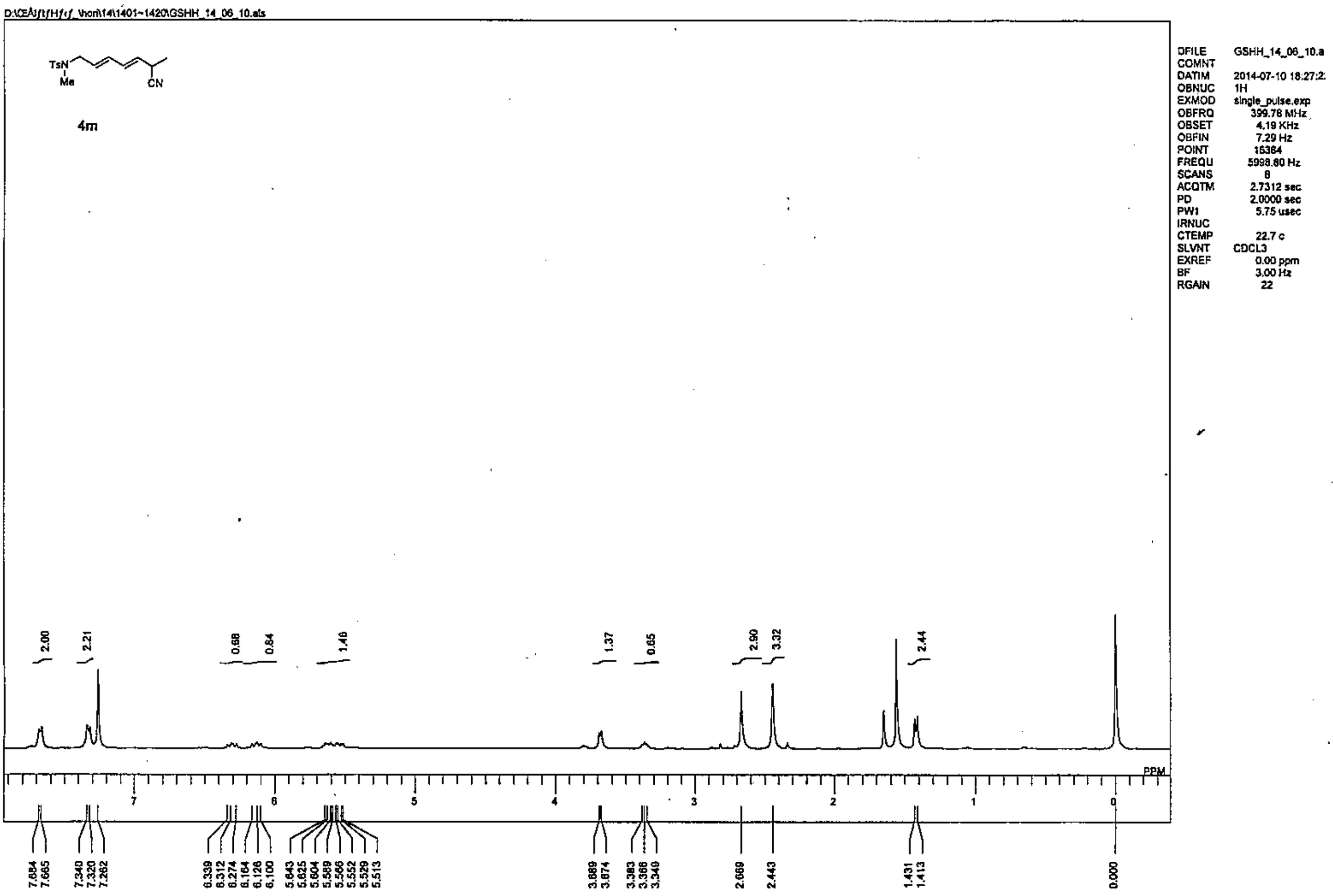
DFILE	GSHH_15_54_p1.a
COMNT	
DATIM	2014-10-20 14:32:
OBNUC	1H
EXMOD	single_pulse.exp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	16384
FREQU	5998.80 Hz
SCANS	8
ACQTM	2.7312 sec
PD	2.0000 sec
PW1	5.75 usec
IRNUC	
CTEMP	22.1 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	15

single pulse decoupled gated NOE
D:\ŒÅ\ƒtƒHƒ‹ƒ_\hori\15\1541~1560\GSHH 15 54 pure 2nd_Carbon_ft-3-1.jdf



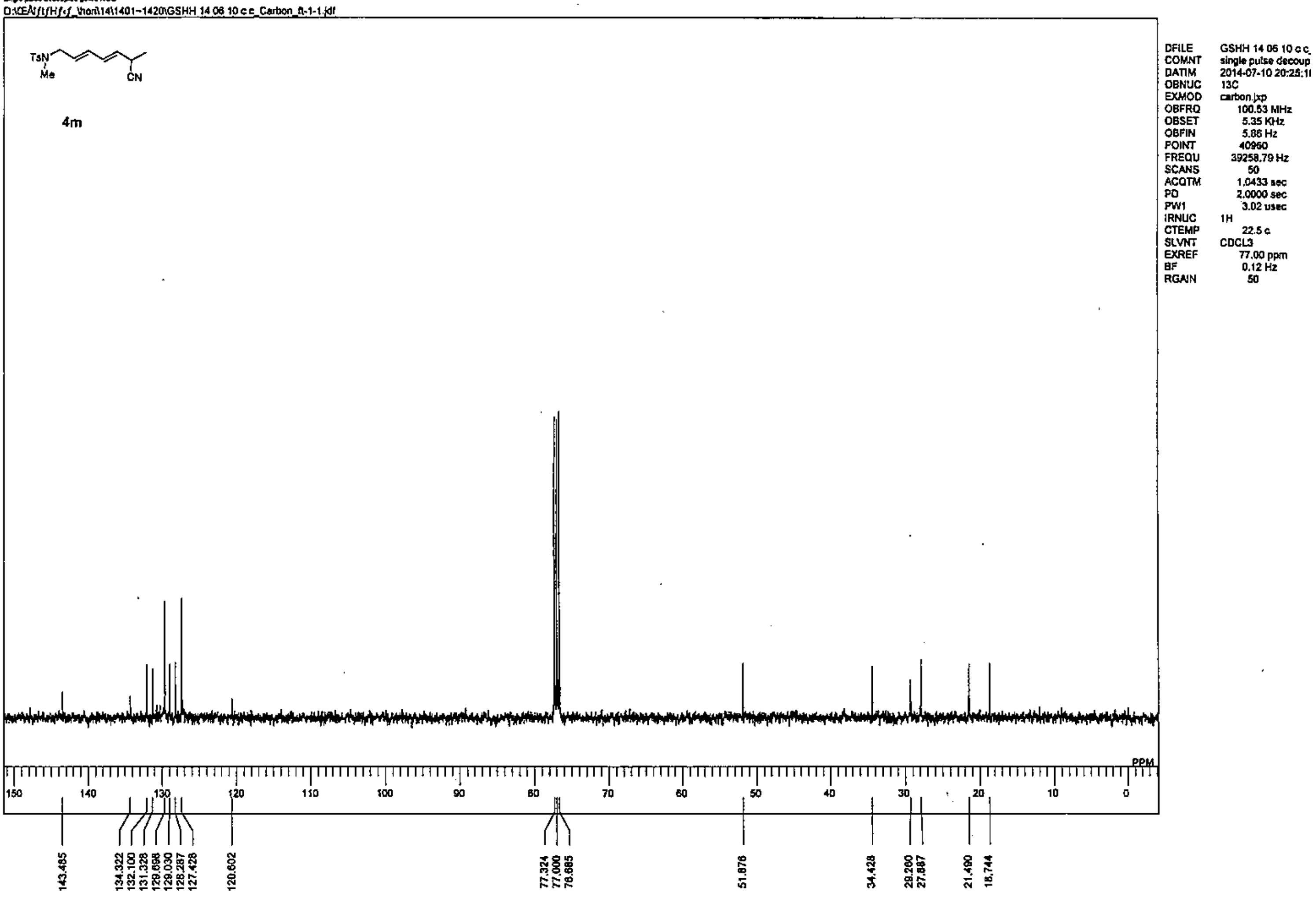
DFILE	GSHH 15 54 pure 2
COMNT	single pulse decou
DATIM	2014-10-20 17:02:
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	70
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	55.0 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	50

D:\ŒÄ\ƒtƒ@ƒCƒ‹_\nori\14\1401~1420\GSHH_14_06_10.als



TsN
Me
CN
4m
DFILE GSHH_14_06_10.a
COMNT
DATIM 2014-07-10 18:27:2
OBNUC 1H
EXMOD single_pulse.exp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 5998.80 Hz
SCANS 8
ACQTM 2.7312 sec
PD 2.0000 sec
PW1 5.75 usec
IRNUC
CTEMP 22.7 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 3.00 Hz
RGAIN 22
2.00
2.21
0.68
0.84
1.46
1.37
0.65
2.90
3.32
2.44
PPM
7.684 7.665
7.340 7.320 7.262
6.339 6.312 6.274 6.164 6.126 6.100
5.643 5.625 5.604 5.589 5.566 5.552 5.529 5.513
3.689 3.674
3.383 3.366 3.349
2.669
2.443
1.431 1.413
0.000

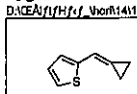
single pulse decoupled gated NOE
D:\ŒÄ\ƒtƒ@ƒCƒ‹_\nori\14\1401~1420\GSHH_14 06 10 c c_Carbon_ft-1-1.jdf



TsN
Me
CN
4m
DFILE GSHH 14 06 10 c c
COMNT single pulse decoup
DATIM 2014-07-10 20:25:1
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 50
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 22.5 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50
PPM
143.485
134.322 132.100 131.328 129.698 128.030 128.287 127.428
120.602
77.324 77.000 76.685
51.876
34.428
29.260 27.887
21.490 18.744

single_pulse

D:\CEA\f1fH\f_\hori\14\1461~1480\GSHH 14 70 pure_Proton_ft-1-1.jdf

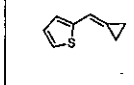


6g

DFILE	GSHH 14 70 pure_F
COMNT	single_pulse
DATIM	2014-09-09 20:56:1
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	8376.75 Hz
SCANS	1
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	20.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	44

single pulse decoupled gated NOE

D:\CEA\f1fH\f_\hori\14\1461~1480\GSHH 1470h_Carbon_ft-1-1.jdf

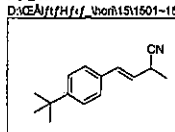


6g

DFILE	GSHH 1470h_Carb
COMNT	single pulse decoup
DATIM	2014-09-09 19:11:3
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	30
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	20.9 c
SLVNT	CDCL3
EXREF	224.97 ppm
BF	0.12 Hz
RGAIN	50

single_pulse

D:\CEA\ft\HF-f_\hori\15\1501~1520\GSHH tbu pure_Proton_ft-1-1.jdf

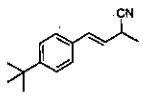


7b

DFILE	GSHH tbu pure_Pro
COMNT	single_pulse
DATIM	2014-09-13 14:50:3
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	9378.75 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	20.8 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.00 Hz
RGAIN	46

single pulse decoupled gated NOE

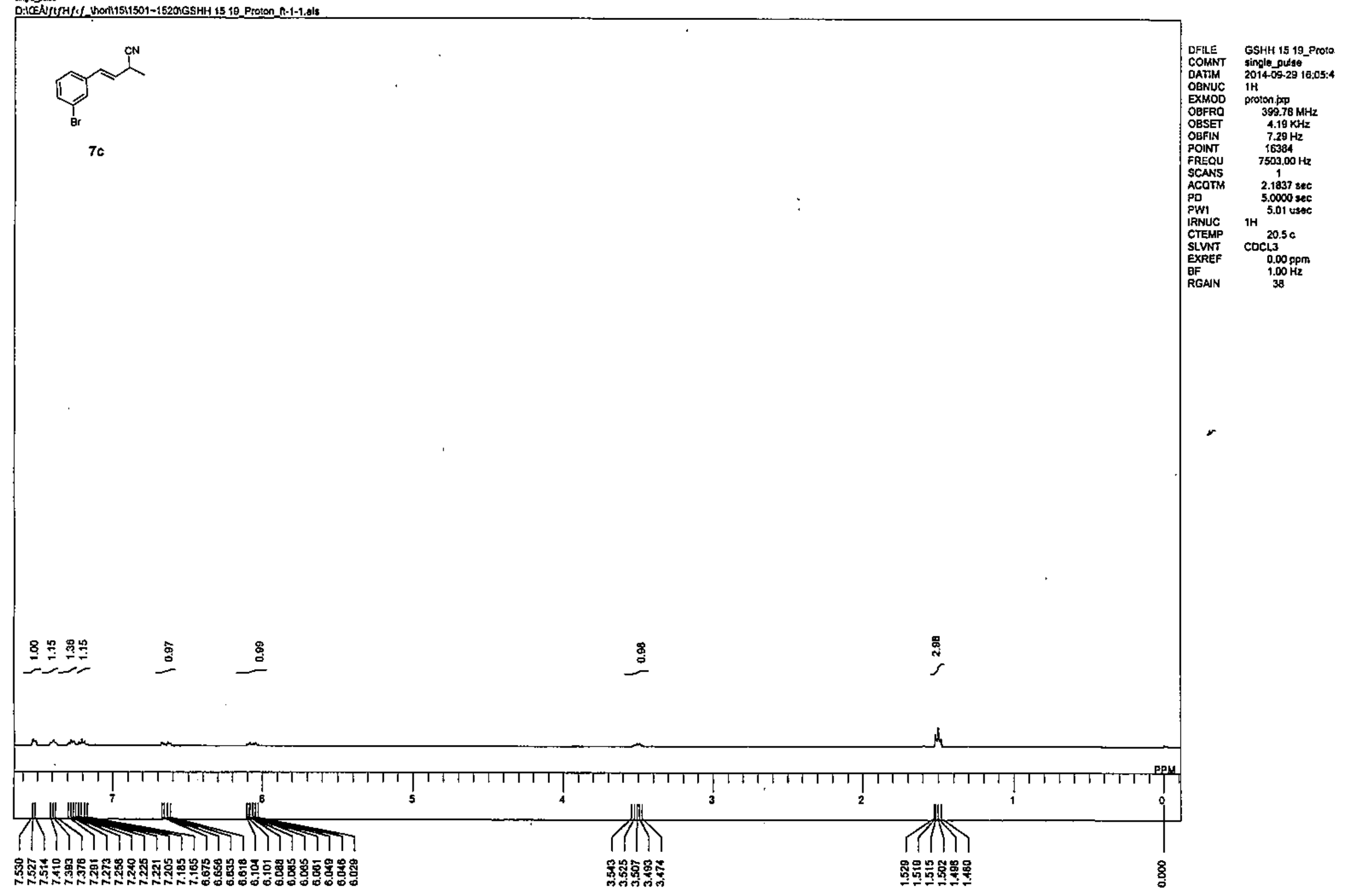
D:\CEA\ft\HF-f_\hori\15\1501~1520\GSHH tbu pure_Carbon_ft-1-1.jdf



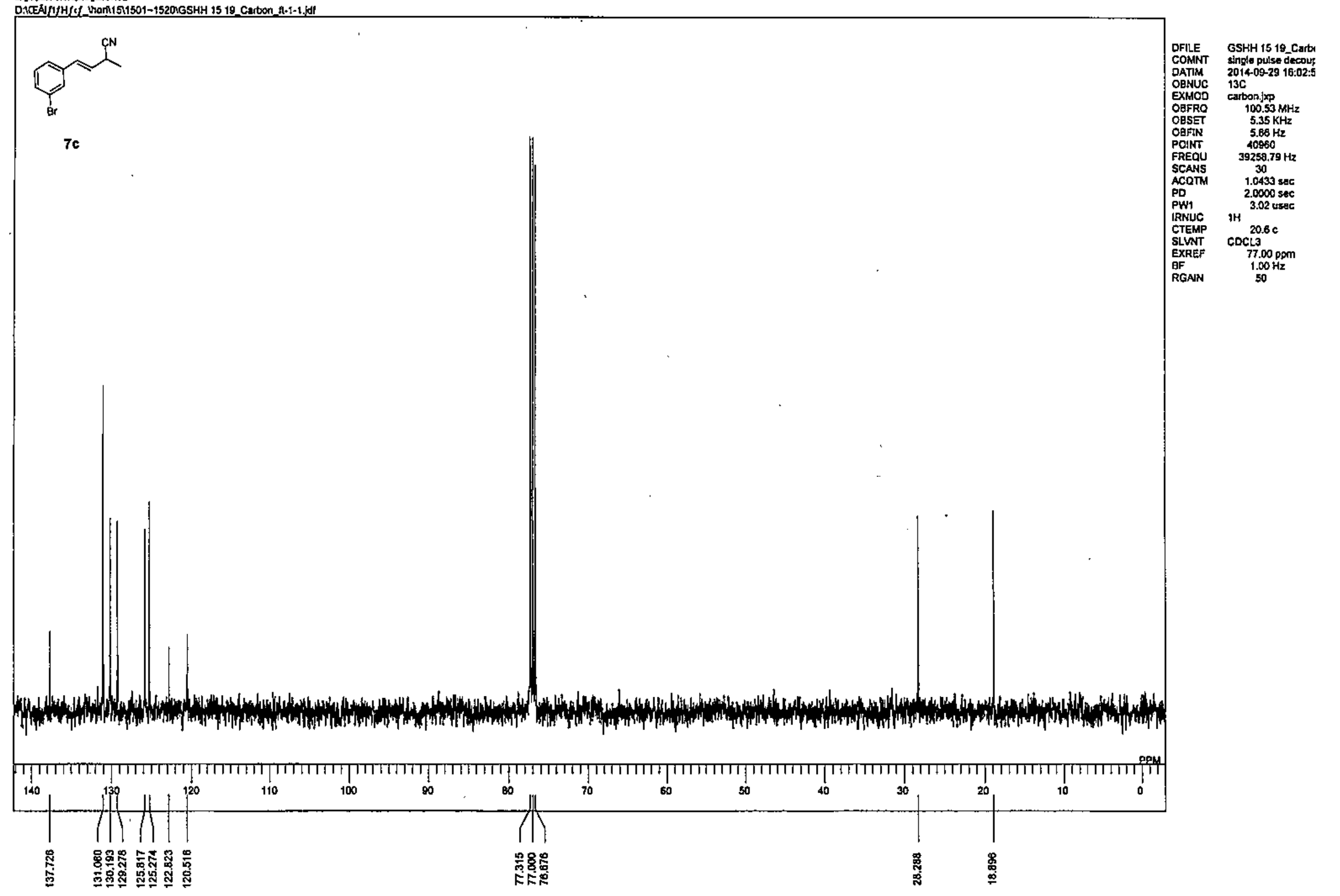
7b

DFILE	GSHH tbu pure_Ca
COMNT	single pulse decou
DATIM	2014-09-13 14:52:0
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.85 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	50
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	20.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.00 Hz
RGAIN	50

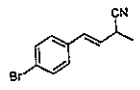
single_pulse
D:\ŒÄ\ƒtƒHƒ‹ƒ_\hori\15\1501~1520\GSHH 15 19_Proton_ft-1-1.als


CN
Br
7c
1.00
1.15
1.38
1.15
0.97
0.99
0.98
2.98
PPM
7
6
5
4
3
2
1
0
7.530 7.527 7.514 7.410 7.393 7.376 7.291 7.273 7.258 7.240 7.225 7.221 7.205 7.185 6.675 6.656 6.635 6.618 6.104 6.101 6.088 6.085 6.065 6.061 6.049 6.046 6.029
3.543 3.525 3.507 3.493 3.474
1.529 1.518 1.515 1.502 1.498 1.480
0.000
DFILE GSHH 15 19_Proto
COMNT single_pulse
DATIM 2014-09-29 16:05:4
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 1
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 20.5 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 38

single pulse decoupled gated NOE
D:\ŒÄ\ƒtƒHƒ‹ƒ_\hori\15\1501~1520\GSHH 15 19_Carbon_ft-1-1.jdf

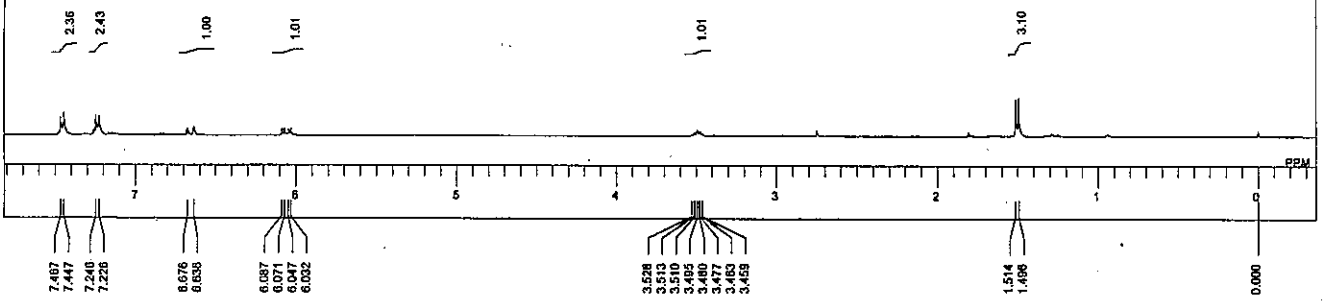

CN
Br
7c
PPM
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
137.726
131.060 130.193 129.278 125.817 125.274 122.823 120.518
77.315 77.000 76.676
28.288
18.896
DFILE GSHH 15 19_Carb
COMNT single pulse decoup
DATIM 2014-09-29 16:02:5
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 30
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50

single_pulse
D:\CEA\ft\H\ｃｆ_\hori\15\1501~1520\GSHH 15 02 lm_Proton_ft-1-1.jdf

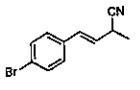


7d

DFILE	GSHH 15 02 lm_Pr
COMNT	single_pulse
DATIM	2014-09-12 17:08:1
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	9378.75 Hz
SCANS	1
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	20.7 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	36

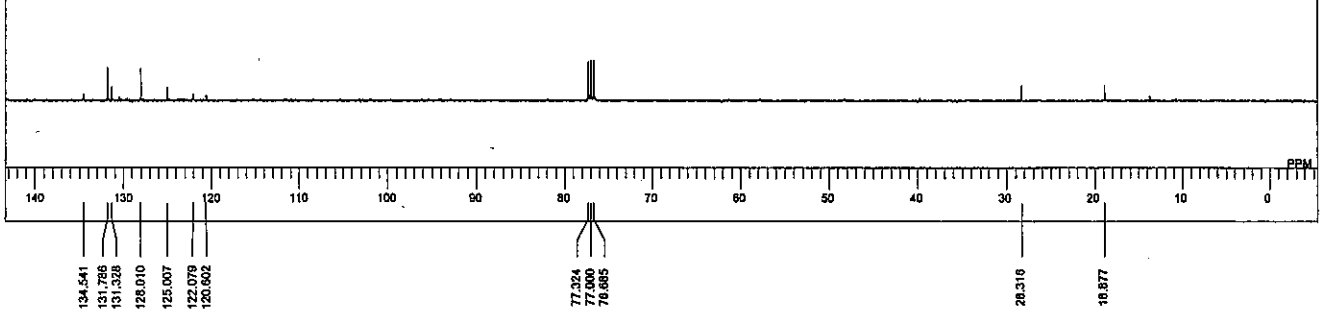


single pulse decoupled gated NOE
D:\CEA\ft\H\ｃｆ_\hori\15\1501~1520\GSHH 15 02 lm_Carbon_ft-1-1.jdf

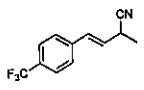


7d

DFILE	GSHH 15 02 lm_C
COMNT	single pulse decoup
DATIM	2014-09-12 17:08:4
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40950
FREQU	39258.79 Hz
SCANS	30
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	20.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50

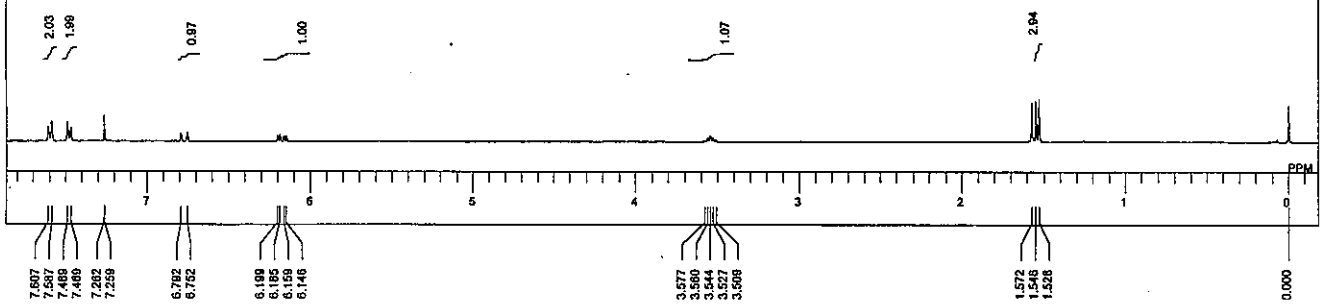


single_pulse
D:\CEA\f1\H\1_Vhom\14\1481~1480\GSHH 14 65_Proton_ft-1-1.als

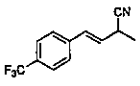


7e

DFILE GSHH 14 65_Proto
COMNT single_pulse
DATIM 2014-09-08 14:45:2
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 16384
FREQU 7503.00 Hz
SCANS 8
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 21.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 48

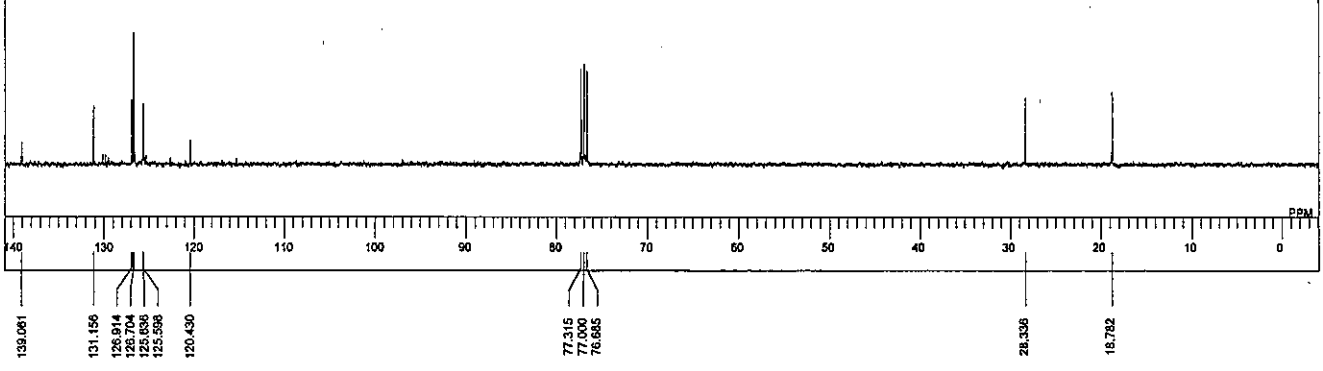


single pulse decoupled gated NOE
D:\CEA\f1\H\1_Vhom\14\1481~1480\GSHH 1465c_Carbon_ft-1-1.jdf



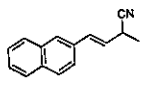
7e

DFILE GSHH 1465c_Carb
COMNT single pulse decoup
DATIM 2014-09-09 19:14:5
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 30
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 20.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50



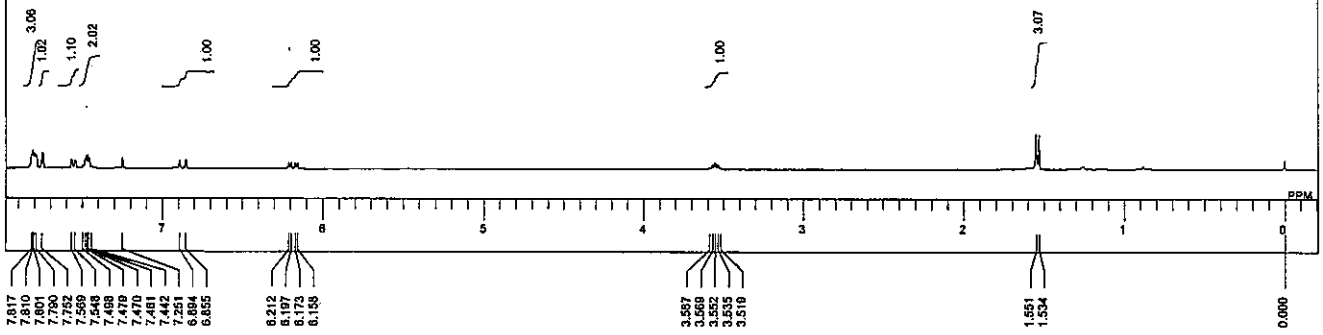
single_pulse

D:\CEA\1\H\r_Vion\141461~1480\GSHH 14 75 tm pure_Proton_fi-1-1.jdf



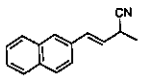
7f

DFILE	GSHH 14 75 tm pur
COMNT	single_pulse
DATIM	2014-09-11 11:22:5
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	9378.75 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	20.7 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	40



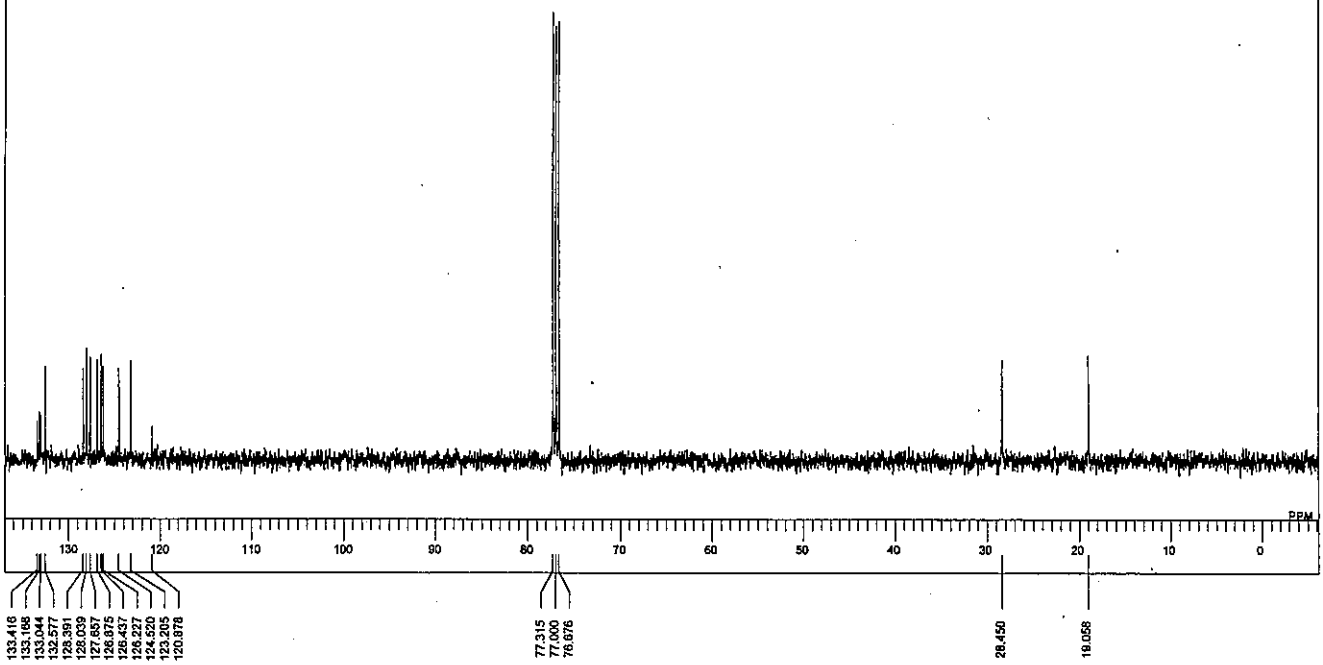
single pulse decoupled gated NOE

D:\CEA\1\H\r_Vion\141461~1480\GSHH 14 75 tm pure_Carbon_fi-1-1.jdf



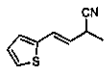
7f

DFILE	GSHH 14 75 tm pur
COMNT	single pulse decoup
DATIM	2014-09-11 11:24:2
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	40
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	20.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50



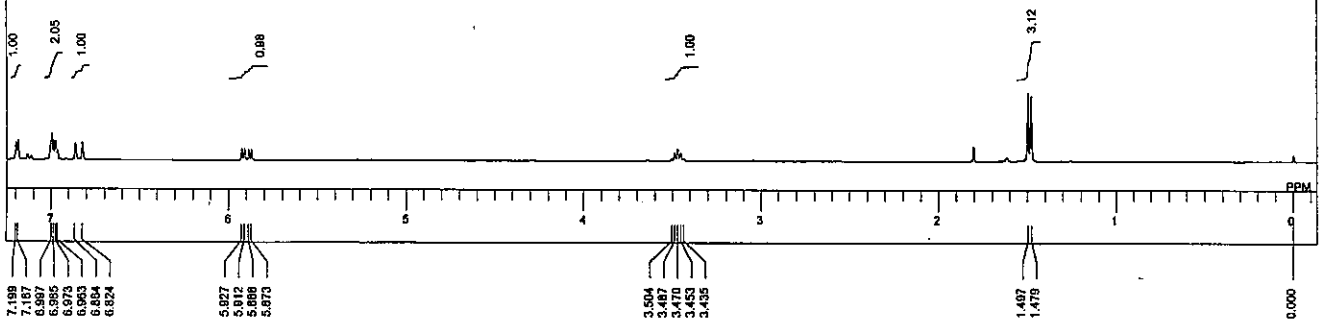
single_pulse

D:\CEAJt\HJt_Vhom\14\1461~1480\GSHH 14 76 tm pure_Proton_ft-1-1.jdf



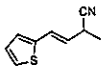
7g

DFILE	GSHH 14 76 tm pur
COMNT	single_pulse
DATIM	2014-09-11 11:15:4
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	9378.75 Hz
SCANS	8
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	20.7 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	36



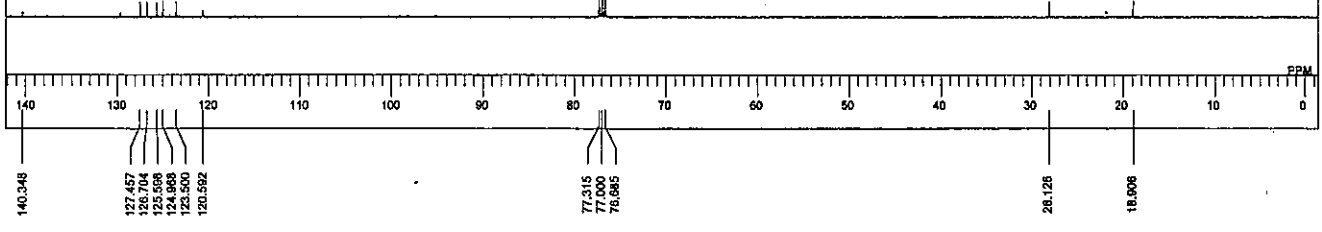
single pulse decoupled gated NOE

D:\CEAJt\HJt_Vhom\14\1461~1480\GSHH 14 75 tm pure_Carbon_ft-1-1.jdf



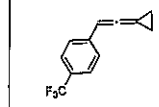
7g

DFILE	GSHH 14 76 tm pur
COMNT	single pulse decoup
DATIM	2014-09-11 11:17:1
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	40
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	20.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50



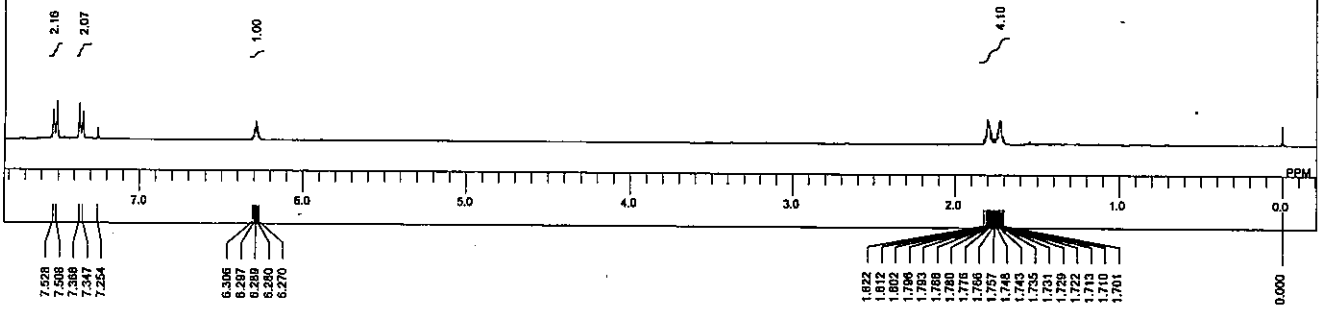
single_pulse

D:\CEA\1\1H\r_thorl\16\GSHH 8_Proton_ft-1-1.jdf



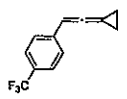
9b

DFILE GSHH 8_Proton_ft
COMNT single_pulse
DATIM 2015-01-26 10:20:3
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 1
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 18.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 38



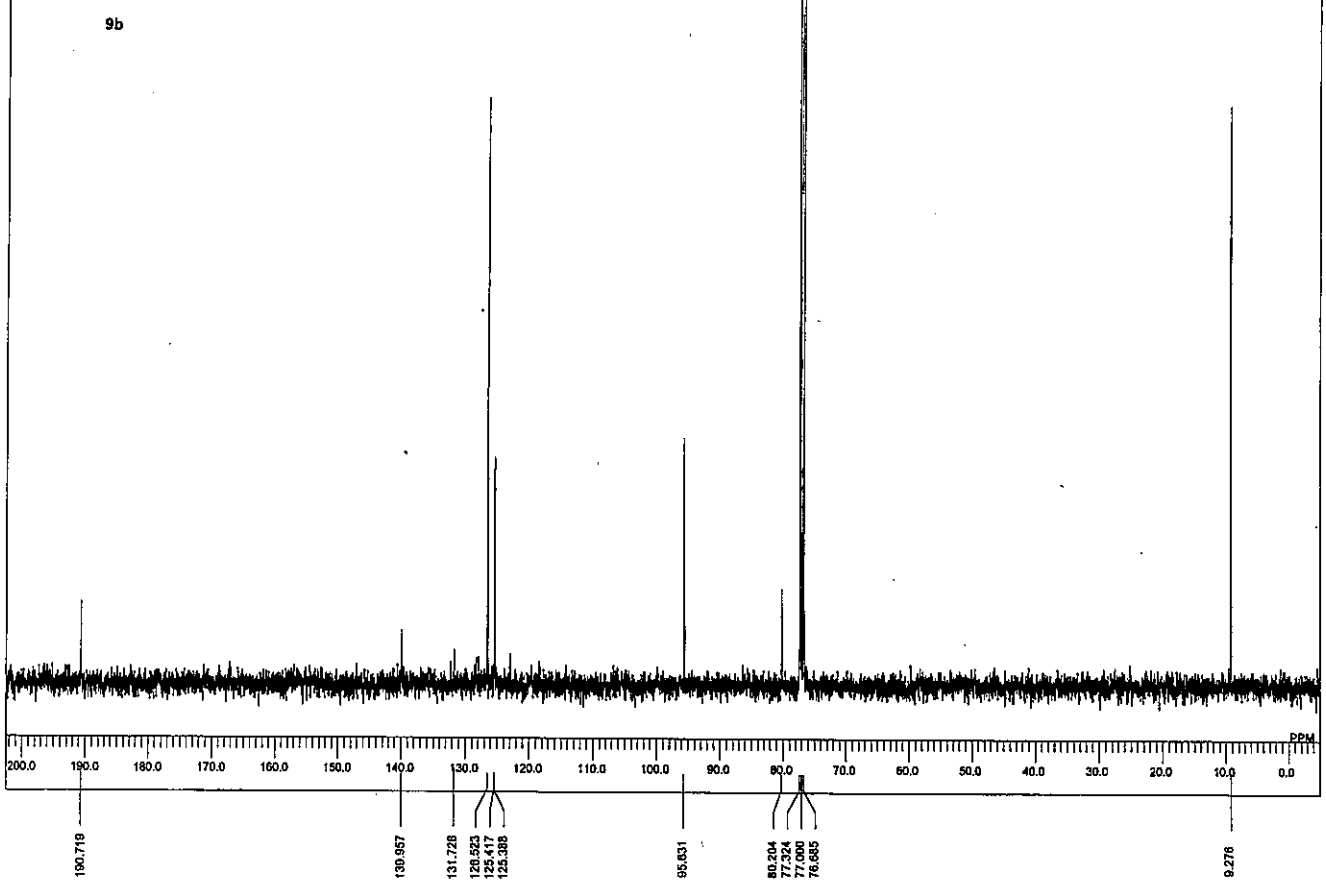
single pulse decoupled gated NOE

D:\CEA\1\1H\r_thorl\16\GSHH 8_Carbon_ft-1-1.jdf



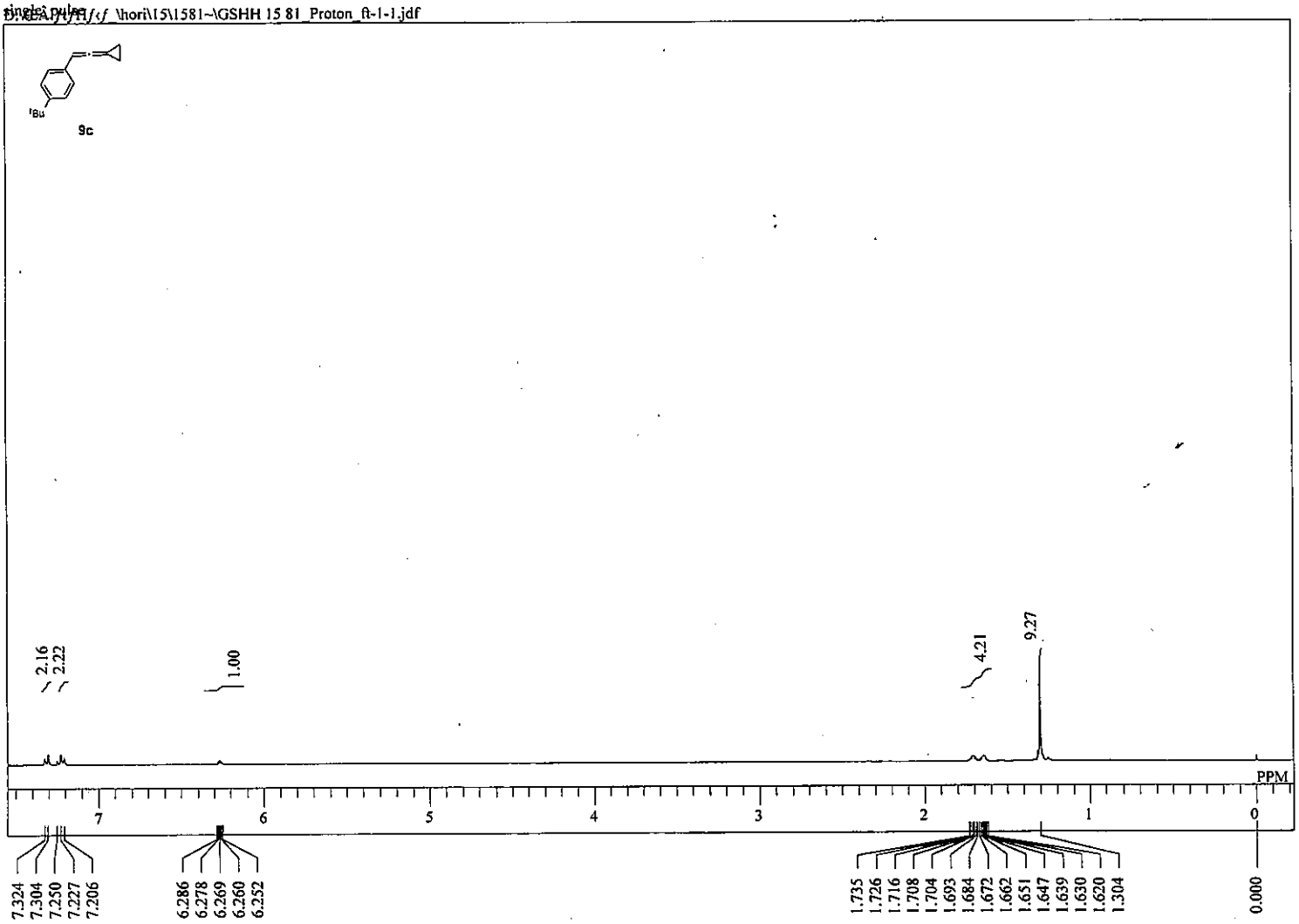
9b

DFILE GSHH 8_Carbon_f
COMNT single pulse decou
DATIM 2015-01-26 10:21:
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 30
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 18.7 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50



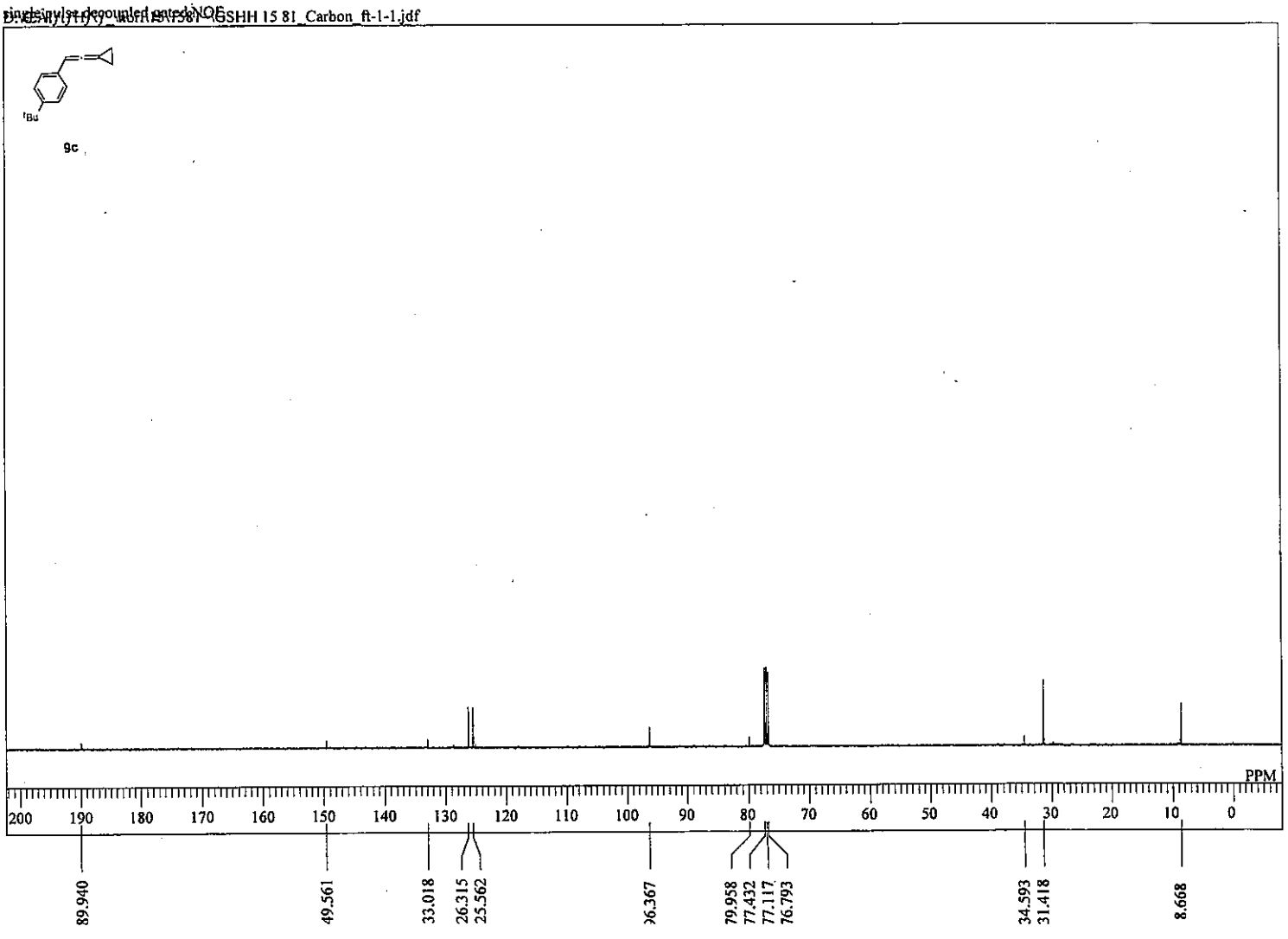
single pulse

D:\GSHH\nmr\ \hori\15\1581~\GSHH 15 81_Proton_ft-1-1.jdf

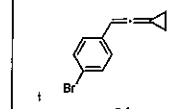


single pulse decoupled gated NOE

D:\GSHH\nmr\ \hori\15\1581~\GSHH 15 81_Carbon_ft-1-1.jdf



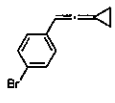
D:\CÂl/t/fH/c/f_\hori\others\GSHH_vdcp_mo4.1



9d

single pulse decoupled gated NOE

D:\CÂl/t/fH/c/f_\hori\others\GSHH vdcp mo4 13c_Carbon_ft-1-1.als

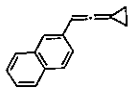


9d

DFILE	GSHH vdcp mo4 1
COMNT	single pulse decou
DATIM	2015-02-06 13:03:!
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	32768
FREQU	31407.04 Hz
SCANS	50
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	17.9 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50

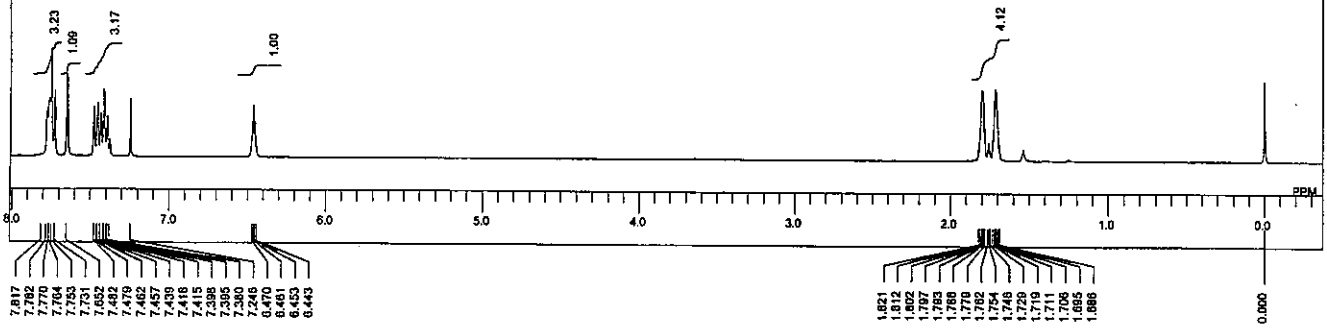
single_pulse

D:\CEA\1\H\1_thom16\GSHH 10_Proton_ft-1-1.jdf



9e

DFILE	GSHH 10_Proton_
COMNT	single_pulse
DATIM	2015-01-26 10:25:
OBNUC	1H
EXMOD	proton.jxp
OBFRQ	399.78 MHz
OBSET	4.19 KHz
OBFIN	7.29 Hz
POINT	20480
FREQU	9378.75 Hz
SCANS	1
ACQTM	2.1837 sec
PD	5.0000 sec
PW1	5.01 usec
IRNUC	1H
CTEMP	18.2 c
SLVNT	CDCL3
EXREF	0.00 ppm
BF	0.12 Hz
RGAIN	42



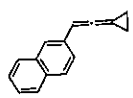
7.817 7.782 7.770 7.764 7.753 7.731 7.652 7.482 7.479 7.462 7.457 7.439 7.418 7.415 7.398 7.395 7.380 7.246 6.461 6.453 6.443

1.821 1.812 1.802 1.797 1.783 1.768 1.770 1.762 1.754 1.746 1.729 1.719 1.711 1.706 1.695 1.686

0.000

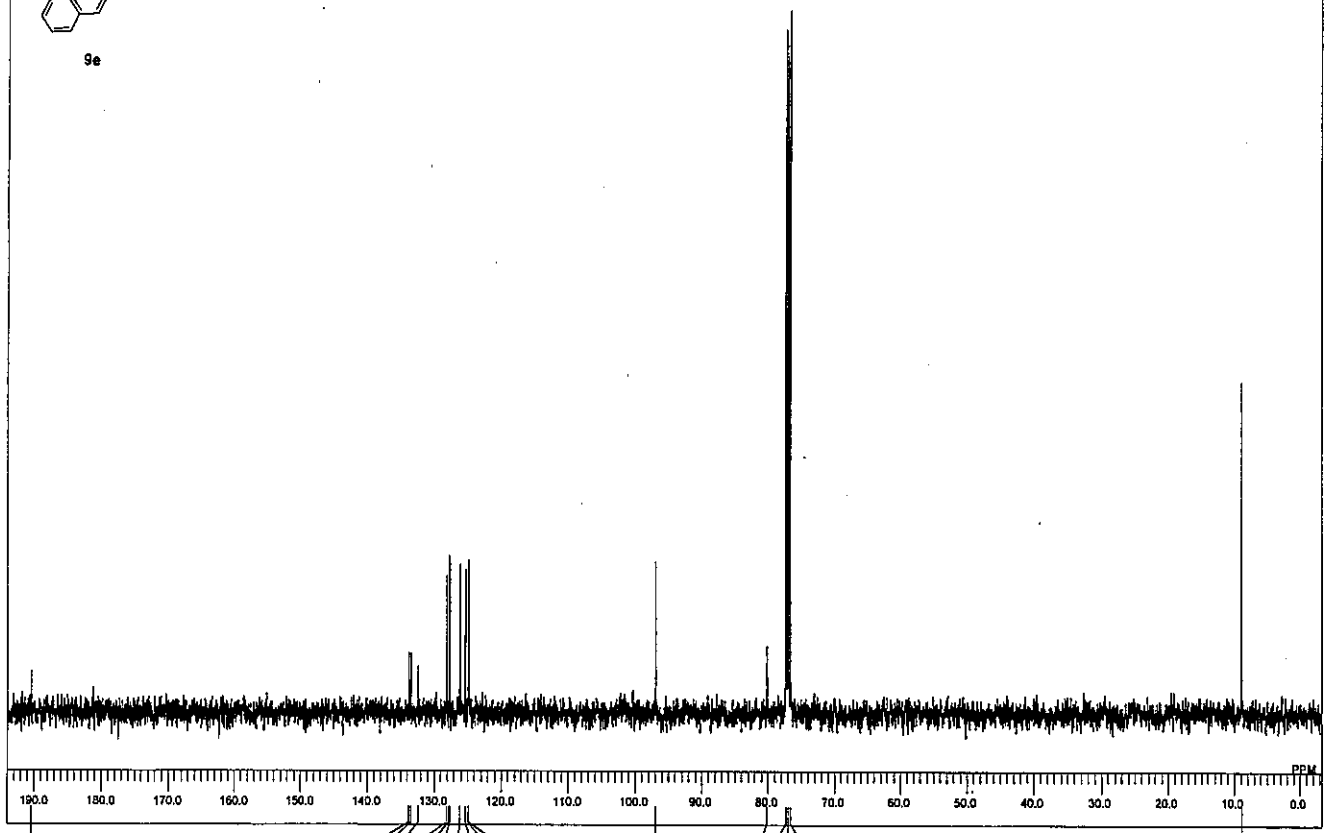
single pulse decoupled gated nOE

D:\CEA\1\H\1_thom16\GSHH 10_Carbon_ft-1-1.jdf



9e

DFILE	GSHH 10_Carbon_
COMNT	single pulse decou
DATIM	2015-01-26 10:26:
OBNUC	13C
EXMOD	carbon.jxp
OBFRQ	100.53 MHz
OBSET	5.35 KHz
OBFIN	5.86 Hz
POINT	40960
FREQU	39258.79 Hz
SCANS	30
ACQTM	1.0433 sec
PD	2.0000 sec
PW1	3.02 usec
IRNUC	1H
CTEMP	18.2 c
SLVNT	CDCL3
EXREF	77.00 ppm
BF	0.12 Hz
RGAIN	50



190.347

133.731 133.445 132.377 128.048 127.676 127.590 126.103 125.331 124.911 124.797

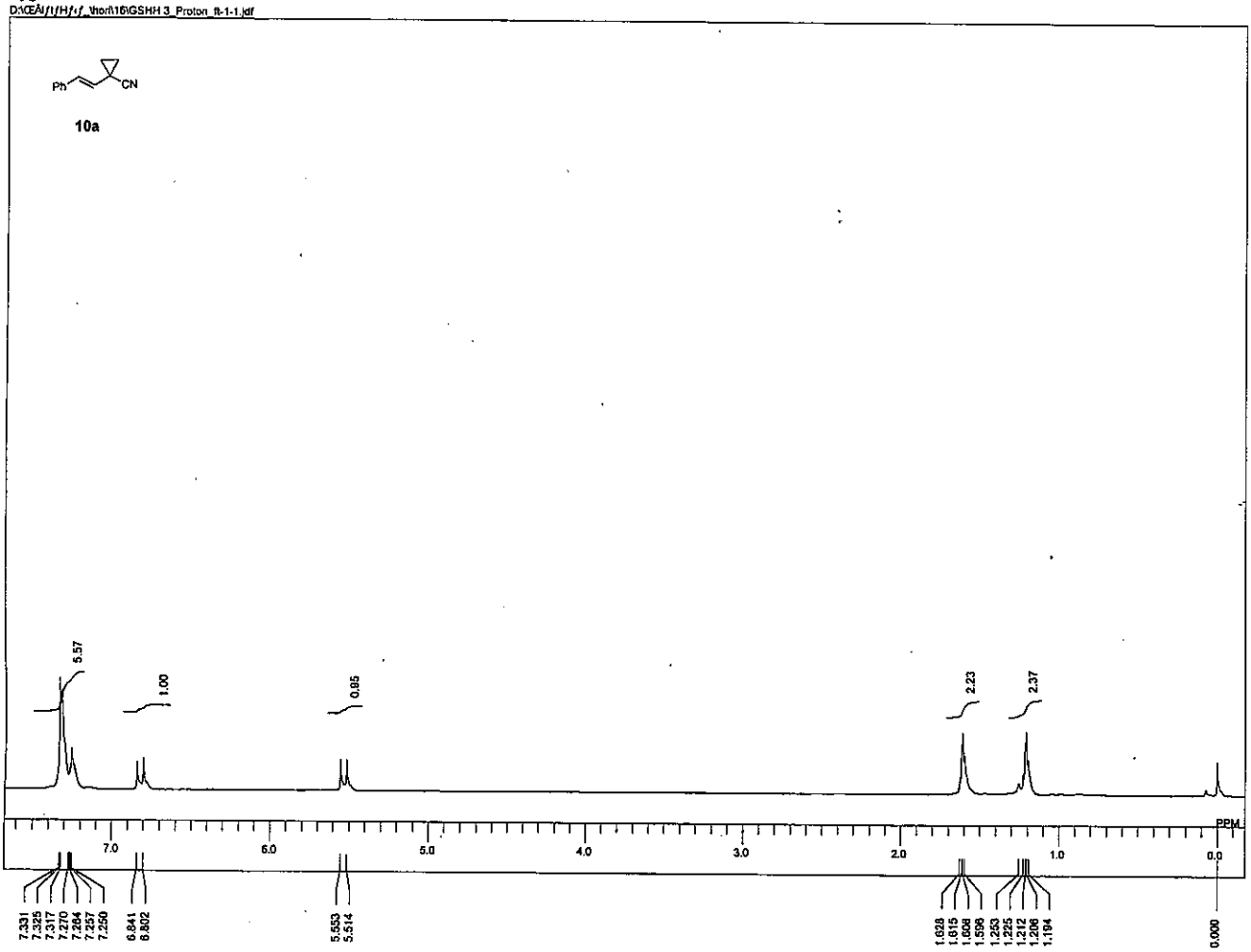
96.846

80.175 77.324 77.000 76.685

8.933

single_pulse

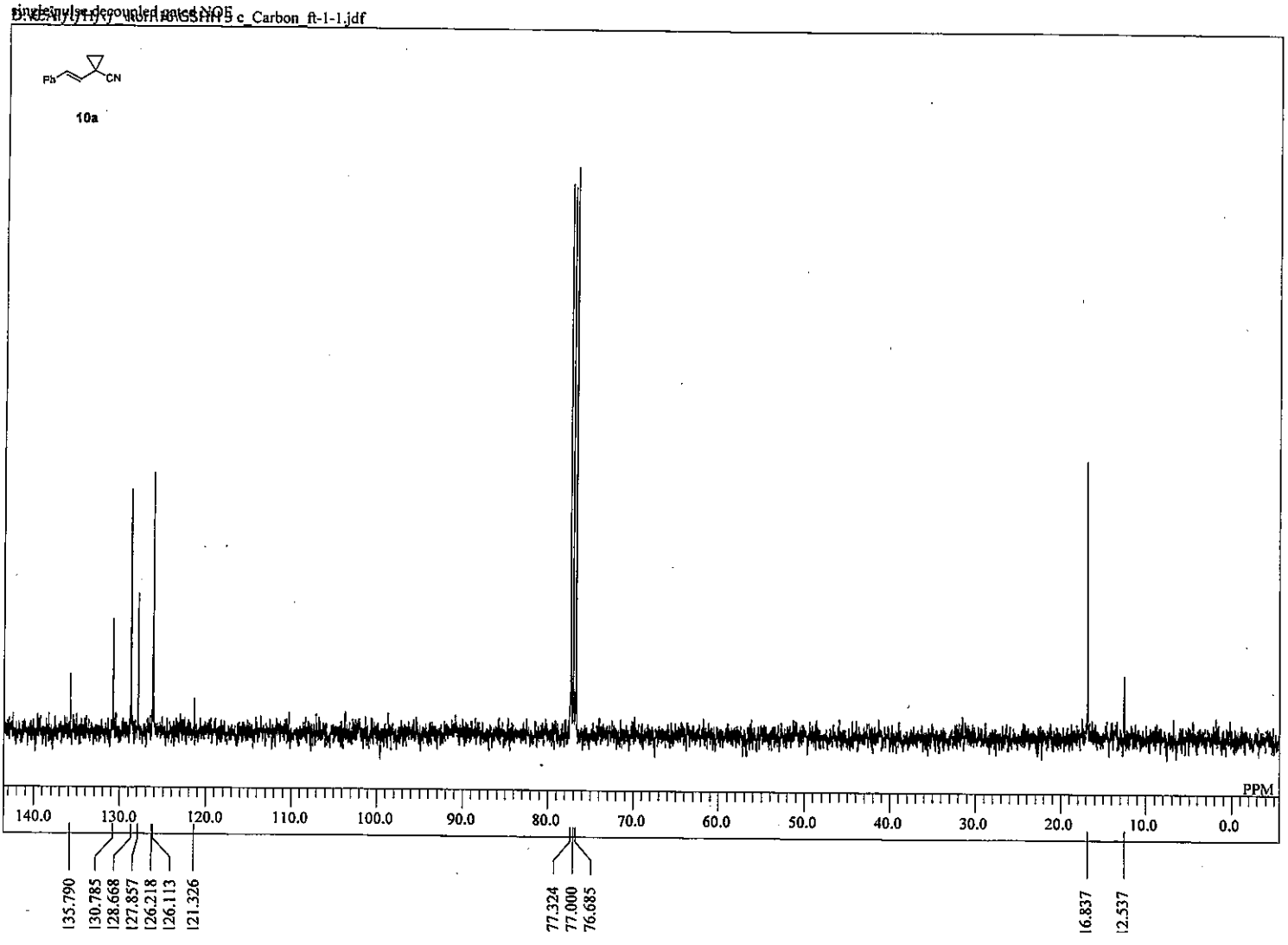
D:\CEA\1\H\/_thor\16\GSHH 3_Proton_ft-1-1.jdf



DFILE GSHH 3_Proton_ft-
COMNT single_pulse
DATIM 2015-01-26 10:45:3
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 1
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 18.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 40

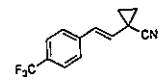
single_pulse_decoupled_gated_NOE

D:\CEA\1\H\/_thor\16\GSHH 5 c_Carbon_ft-1-1.jdf



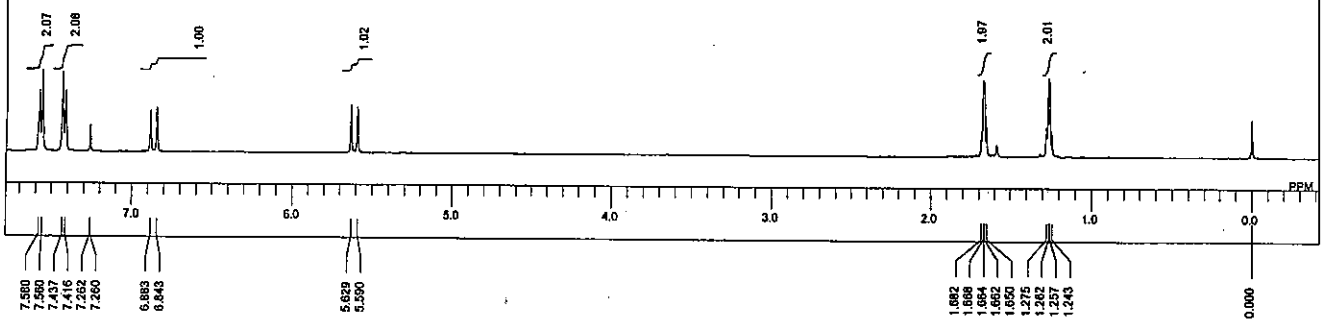
single_pulse

D:\CEA\1\H\r_thom16\GSHH 9_Proton_ft-1-1.jdf



10b

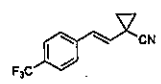
DFILE GSHH 9_Proton_ft
COMNT single_pulse
DATIM 2015-01-26 10:30:
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 1
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 18.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 40



7.580 7.580 7.437 7.416 7.262 7.260 6.863 6.843 5.629 5.590 1.882 1.868 1.864 1.662 1.650 1.275 1.262 1.257 1.243 0.000

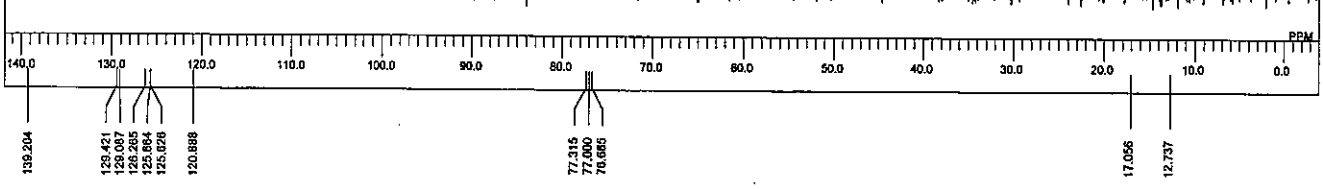
single pulse decoupled gated NOE

D:\CEA\1\H\r_thom16\GSHH 9_Carbon_ft-1-1.jdf



10b

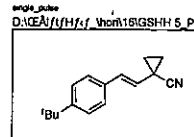
DFILE GSHH 9_Carbon_f
COMNT single pulse decou
DATIM 2015-01-26 10:31:
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39258.79 Hz
SCANS 30
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.02 usec
IRNUC 1H
CTEMP 18.4 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 50



139.204 129.421 129.087 126.265 125.864 125.626 120.888 77.315 77.000 76.685 17.056 12.737

single_pulse

D:\CEA\fjfHf\sf_thom16\GSHH 5_Proton_ft-1-1.jdf



10c

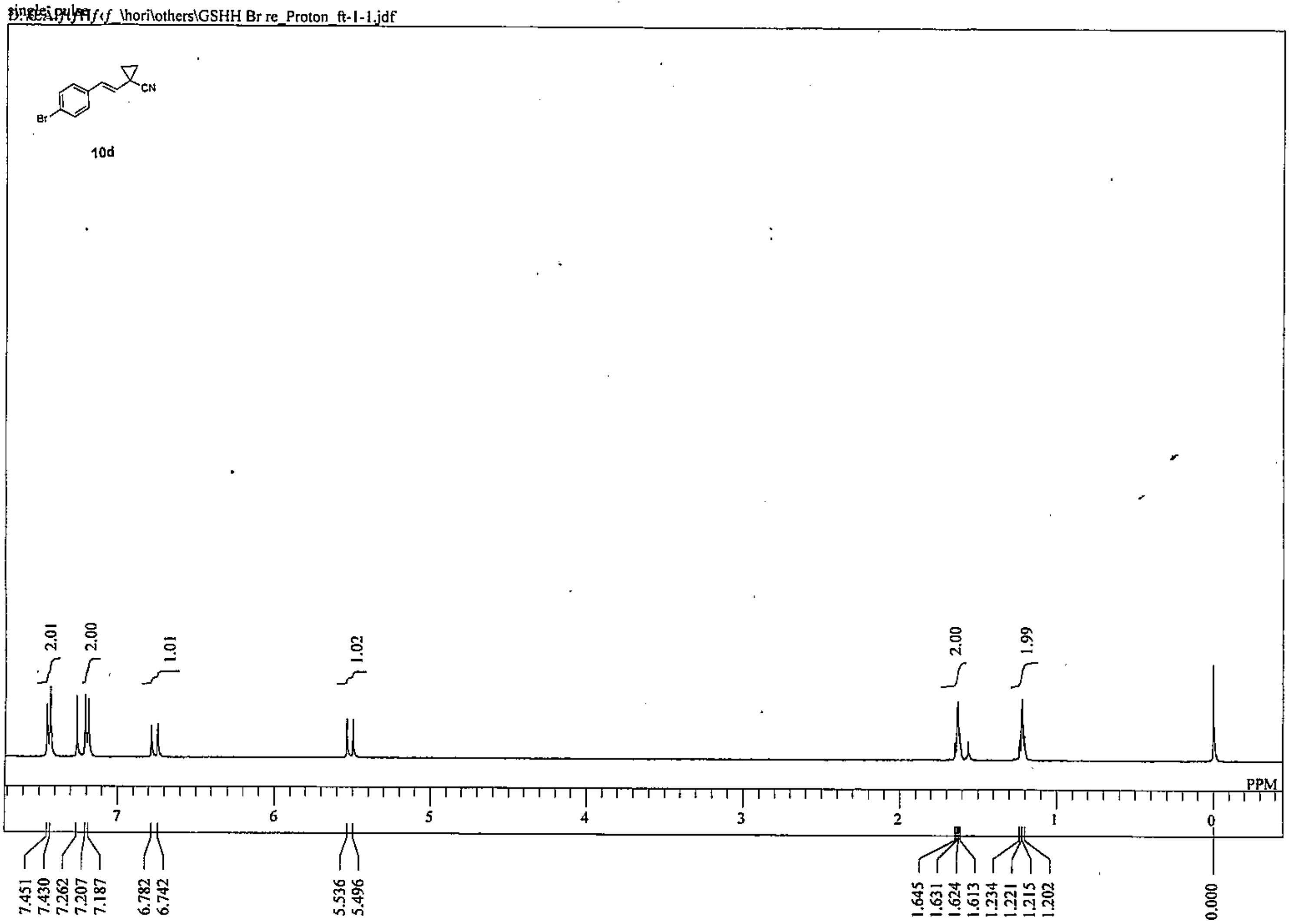
DFILE GSHH 5_Proton_ft
COMNT single_pulse
DATIM 2015-01-26 10:39:5
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9378.75 Hz
SCANS 1
ACQTM 2.1837 sec
PD 5.0000 sec
PW1 5.01 usec
IRNUC 1H
CTEMP 18.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 0.12 Hz
RGAIN 44

single pulse decoupled gated NOE

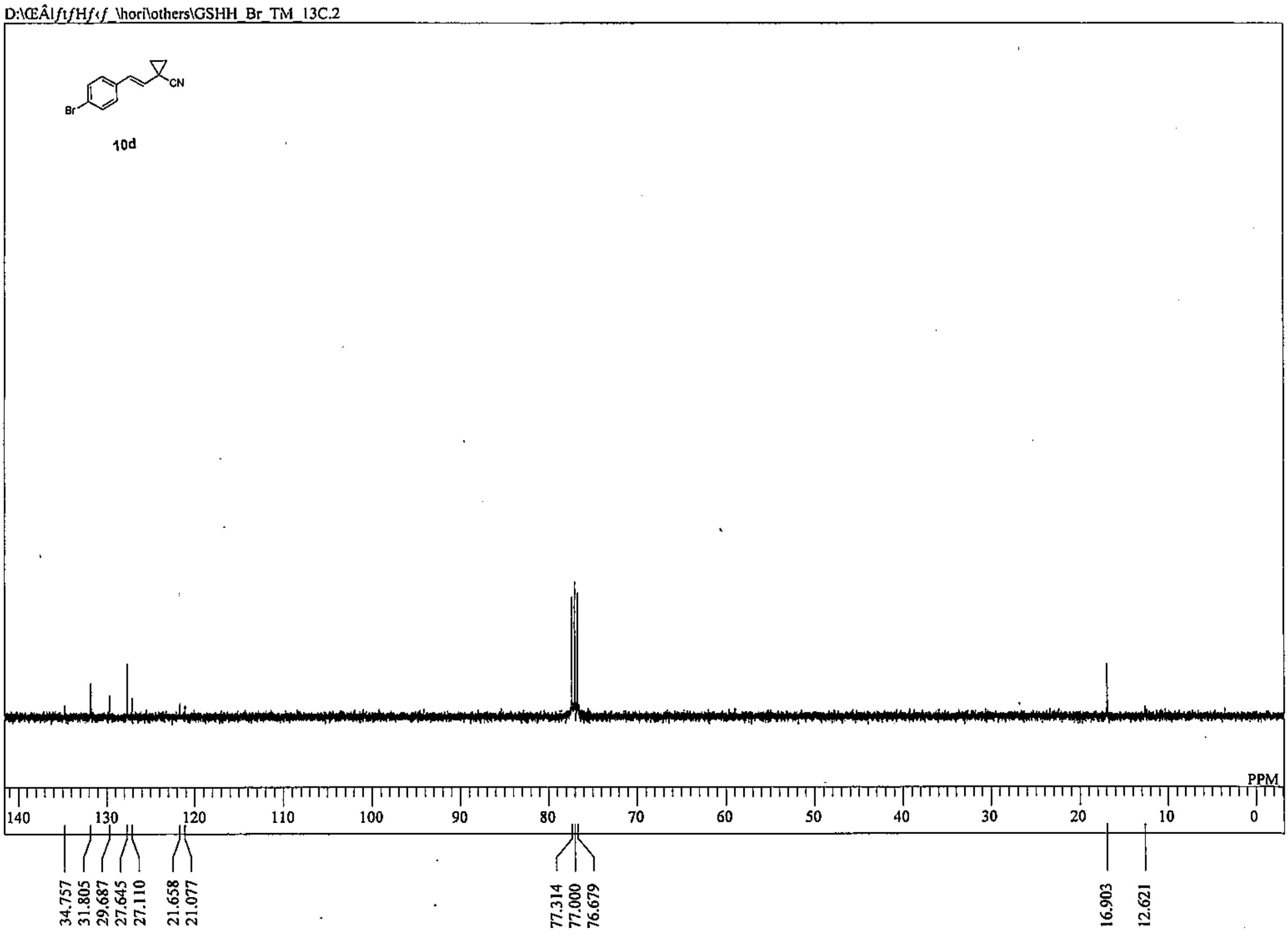
D:\CEA\fjfHf\sf_thom16\GSHH 5 c_Carbon_ft-1-1.jdf

10c

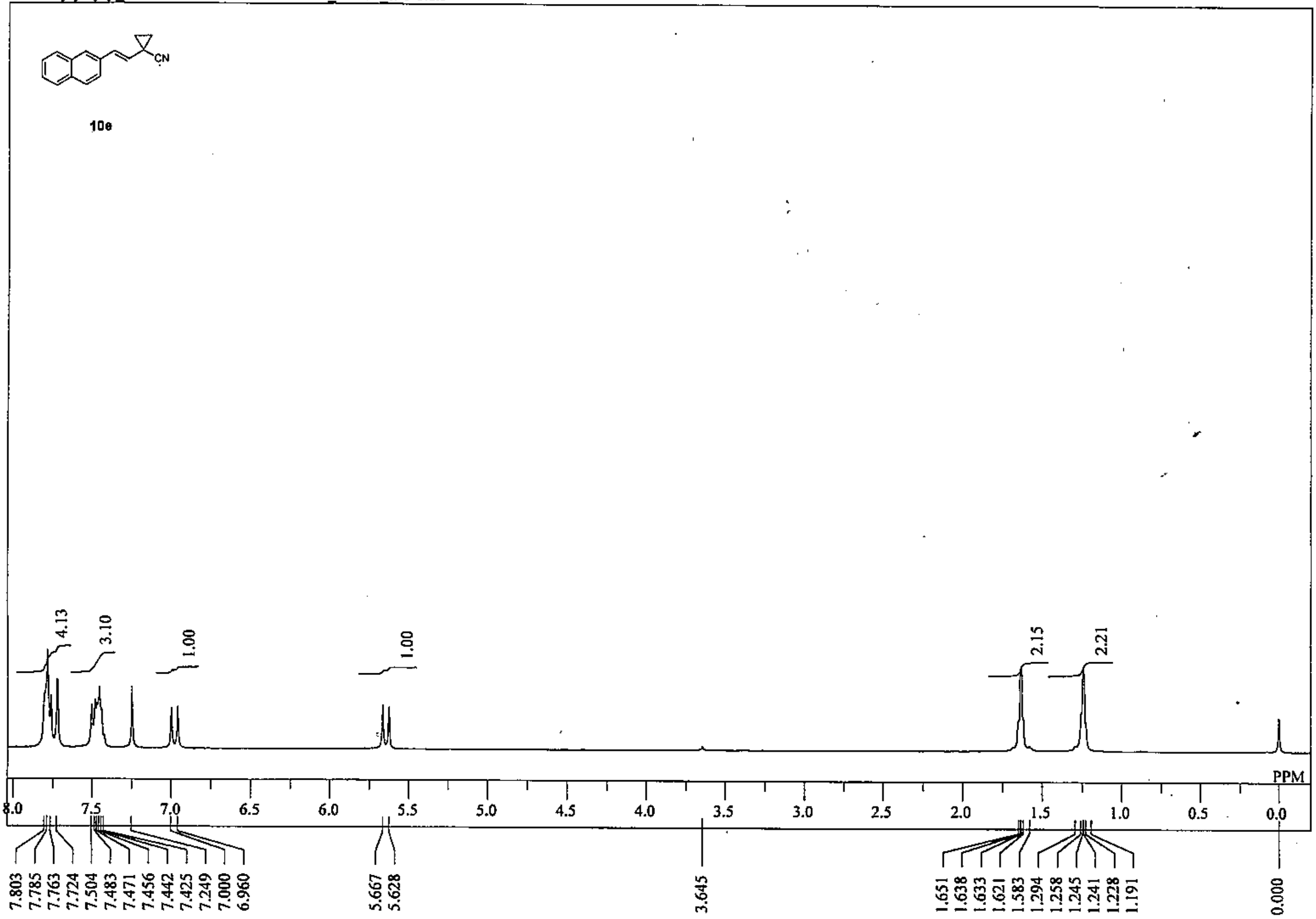
single pulse
D:\ŒÂÌƒtƒHƒ‹ƒ_\hori\others\GSHH Br re_Proton_ft-1-1.jdf



D:\ŒÂÌƒtƒHƒ‹ƒ_\hori\others\GSHH_Br_TM_13C.2



single pulse
D:\...\hori\15\1581~\GSHH 15 88 re_Proton_ft-1-1.als



single pulse decoupled gated NOE
D:\...\hori\15\1581~\GSHH 15 88 re_Carbon_ft-1-1.jdf