Electronic supplementary information for

Transfer of axial chirality through the nickel-catalyzed hydrocyanation of chiral allenes

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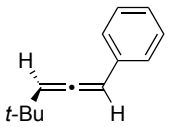
A. General remarks

All reactions were performed with dry solvents and reagents were purified by the usual methods. Reactions were monitored by thin-layer chromatography carried out on 0.25 mm Merck silica gel plates (60F-254). Column chromatography was performed with silica gel (Fuji Silysia, PSQ-60B). IR spectra were recorded on a JASCO FT/IR-230 Fourier transform spectrophotometer. NMR spectra were recorded on JEOL JMN-ECS-400, ECP-400, ECA-600 and ECP-600 at 400 and 600 MHz for ^{1}H NMR and at 100 and 150 MHz for ^{13}C NMR, with calibration using residual undeuterated solvent as an internal reference. Mass spectra were recorded using ESI mode with JEOL JMS-T100LP and APPI mode with Thermo Fisher Exactive. The enantiomeric excess was determined by HPLC analysis using JASCO HPLC LC-2000Plus series (PU-2089, CO-2065, UV-2075). Optical rotations were measured using JASCO P-1020 and P-2200 Polarimeter. X-ray crystal data were collected with Rigaku VariMax with RAPID diffractometer at –180±1 °C using filtered Cu-Kα radiation.

B. Synthesis of optically active allenes

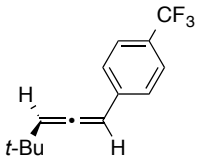
Optically active allenes were synthesized according to the reported procedure[1]. Spectral data of (*R*)-**3a,3d-g** and **3k** were identical to the literature data. [2]

(*R*)-(4,4-dimethylpenta-1,2-dien-1-yl)benzene ((*R*)-**3a**) [3]



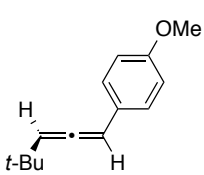
HPLC conditions: Chiralcel OJ-H, hexane (100%), f: 0.5mL/min, tR: 10.2, 10.7 min (99% ee).

(*R*)-1-(4,4-dimethylpenta-1,2-dien-1-yl)-4-(trifluoromethyl)benzene ((*R*)-**3b**)



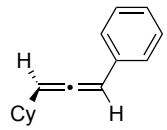
Colorless oil. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 1.13 (s, 9H), 5.64 (d, 1H, *J* = 6.0 Hz), 6.21 (d, 1H, *J* = 6.0 Hz), 7.37 (d, 2H, *J* = 7.8 Hz), 7.53 (d, 2H, *J* = 7.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 30.2, 32.9, 95.4, 107.4, 124.3 (q, *J* = 270.0 Hz), 125.5 (q, *J* = 4.4 Hz), 126.4, 128.5 (q, *J* = 31.7 Hz), 139.2, 203.5; IR (ATR) ν: 2961, 1949 cm^{-1}; HRMS (APPI) m/z calcd for $C_{14}H_{15}F_3$ $[M]^+$ 240.1120, found 240.1116; $[\alpha]_D^{25}$ = -234.30 (*c* = 1.24, $CHCl_3$, 98% ee); HPLC conditions: Chiralcel OJ-H, hexane (100%), f: 0.5 mL/min, tR: 9.1, 9.4 min (98% ee).

(*R*)-1-(4,4-dimethylpenta-1,2-dien-1-yl)-4-methoxybenzene ((*R*)-**3c**)



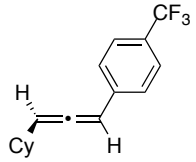
Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.11 (s, 9H), 3.79 (s, 3H), 5.55 (d, 1H, *J* = 5.6 Hz), 6.15 (d, 1H, *J* = 5.6 Hz), 6.84 (d, 2H, *J* = 8.4 Hz), 7.21 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 30.3, 32.7, 55.3, 95.6, 106.9, 114.1, 127.4, 127.6, 158.5, 201.7; IR (ATR) n: 2057, 1947 cm^{-1}; HRMS (APPI) m/z calcd for $C_{14}H_{19}O$ $[M+H]^+$ 203.1430, found 240.1425; $[\alpha]_D^{25}$ = -248.2 (*c* = 1.02, $CHCl_3$, 88% ee); HPLC conditions: Chiralcel OJ-H, hexane/*i*-PrOH = 99:1, f: 0.5 mL/min, tR: 12.7, 14.5 min (88% ee).

(*R*)-(3-cyclohexylpropa-1,2-dien-1-yl)benzene ((*R*)-**3d**)[1]



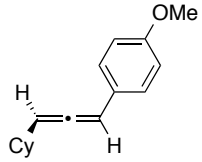
HPLC conditions: Chiralcel IB, hexane (100%), f: 0.5 mL/min, 9.6, 10.6 min (97% ee).

(*R*)-1-(3-cyclohexylpropa-1,2-dien-1-yl)-4-(trifluoromethyl)benzene ((*R*)-**3e**)



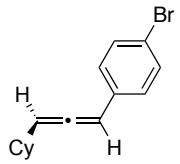
$[\alpha]_D^{24}$ = -300.1 (*c* = 1.12, $CHCl_3$, 98% ee); HPLC conditions: Chiralcel OD-H, hexane (100%), f: 1.0 mL/min, tR: 5.4, 6.0 min (97% ee)

(*R*)-1-(3-cyclohexylpropa-1,2-dien-1-yl)-4-methoxybenzene ((*R*)-**3f**)



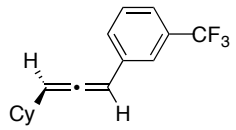
$[\alpha]_D^{26}$ = -268.4 (*c* = 1.26, $CHCl_3$, 85% ee); HPLC conditions: Chiralcel OD-H, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 4.7, 5.1 min (85% ee).

(*R*)-1-bromo-4-(3-cyclohexylpropa-1,2-dien-1-yl)benzene ((*R*)-**3g**)



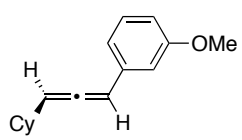
$[\alpha]_D^{24}$ = -306.9 (*c* = 1.28, $CHCl_3$, 98% ee); HPLC conditions: Chiralpak IB, hexane (100%), f: 0.5 mL/min, tR: 9.1, 11.4 min (98% ee)

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



Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.16-1.36 (m, 5H), 1.63-1.67 (m, 1H), 1.73-1.76 (m, 2H), 1.83-1.86 (m, 2H), 2.12-2.21 (m, 1H), 5.63 (dd, 1H, *J* = 6.4, 6.4 Hz), 6.18 (dd, 1H, *J* = 6.4, 3.2 Hz), 7.37-7.47 (m, 3H), 7.52 (s, 1H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 25.97, 26.04, 33.1, 37.5, 94.6, 101.8, 123.0 (*J* = 2.9 Hz), 123.1 (*J* = 2.9 Hz), 124.2 (*J* = 271.4 Hz), 128.9, 129.5, 131.0 (*J* = 33.0 Hz), 136.3, 204.6; IR (ATR) ν: 2925, 2852, 1948 cm^{-1}; HRMS (APPI) m/z calcd for $C_{16}H_{17}F_3$ $[M]^+$ 266.1277, found 266.1269; $[\alpha]_D^{24}$ = -286.5 (*c* = 1.12, $CHCl_3$, 97% ee); HPLC conditions: Chiralcel OD-H, hexane (100%), f: 0.5 mL/min, tR: 9.1, 9.8 min (97% ee).

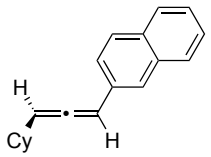
(*R*)-1-(3-cyclohexylpropa-1,2-dien-1-yl)-3-methoxybenzene ((*R*)-**3i**)



Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.13-1.35 (m, 5H), 1.62-1.65 (m, 1H), 1.71-1.76 (m, 2H), 1.82-1.85 (m, 2H), 2.09-2.17 (m, 1H), 3.80 (s, 3H), 5.65 (dd, 1H, *J* = 6.4, 6.4 Hz), 6.12 (dd, 1H, *J* = 6.4, 2.8 Hz), 6.73 (dd, 1H, *J* = 8.0, 2.4 Hz), 6.85-6.89 (m, 2H), 7.20 (dd, 1H, *J* = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 26.0, 26.0, 26.1, 33.05, 33.15, 37.5, 55.0, 95.3, 101.0, 111.6, 112.3, 119.1, 129.4, 136.7, 159.8, 204.1; IR (ATR) ν: 2921, 2849, 1946 cm^{-1}; HRMS (APPI) m/z calcd for

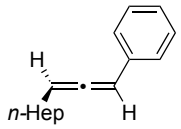
$C_{16}H_{20}O$ $[M]^+$ 228.1509, found 228.1503; $[\alpha]_D^{24}$ = -327.7 (*c* = 0.97, $CHCl_3$, 94% ee); HPLC conditions: Chiralcel OJ-H, hexane/*i*-PrOH = 99:1, f: 0.5 mL/min, tR: 11.5, 12.4 min (94% ee)

(*R*)-2-(3-cyclohexylpropa-1,2-dien-1-yl)naphthalene ((*R*)-**3j**)



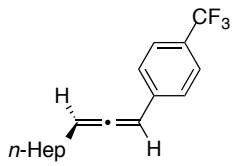
Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.16-1.37 (m, 5H), 1.63-1.66 (m, 1H), 1.73-1.1.78 (m, 2H), 1.86-1.89 (m, 2H), 2.13-2.22 (m, 1H), 5.64 (dd, 1H, *J* = 6.4 Hz), 6.34 (dd, 1H, *J* = 6.4, 4.8 Hz), 7.26-7.46 (m, 2H), 7.50 (dd, 1H, *J* = 8.8, 2.0 Hz), 7.64 (s, 1H), 7.75-7.79 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 26.0, 26.1, 33.1, 33.2, 37.6, 95.8, 101.3, 124.5, 125.1, 125.4, 126.1, 127.6, 127.7, 128.1, 132.5, 132.7, 133.7, 204.7; IR (ATR) ν: 2922, 2849, 1946 cm^{-1}; HRMS (APPI) m/z calcd for $C_{19}H_{20}$ $[M]^+$ 248.1560, found 248.1554; mp. 42-43 °C; $[\alpha]_D^{26}$ = -323.8 (*c* = 1.03, $CHCl_3$, 96% ee) ; HPLC conditions: Chiralcel AS-H, hexane (100%), f: 0.5 mL/min, tR: 9.9, 10.2 min, (96% ee).

(*R*)-deca-1,2-dien-1-ylbenzene ((*R*)-**3k**)



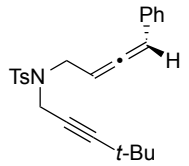
$[\alpha]_D^{24}$ = -237.9 (*c* = 1.28, $CHCl_3$, 97% ee); HPLC conditions: Chiralcel OD-H, hexane (100%), f: 0.5 mL/min, tR: 10.2, 10.7 min (97% ee).

(*R*)-1-(deca-1,2-dien-1-yl)-4-(trifluoromethyl)benzene ((*R*)-**3l**)



Colorless oil. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 0.87 (t, 3H, *J* = 7.2 Hz), 1.24-1.38 (m, 8H), 1.45-1.51 (m, 2H), 2.14 (ddt, 2H, *J* = 7.2, 7.2, 3.0 Hz), 5.63 (dt, 1H, *J* = 7.2, 7.2 Hz), 6.14 (dt, 1H, *J* = 7.2, 3.0 Hz), 7.37 (d, 2H, *J* = 7.8 Hz), 7.53 (d, 2H, *J* = 7.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.0, 22.6, 28.5, 29.09, 29.09, 29.14, 31.9, 93.8, 95.7, 124.3 (q, *J* = 270 Hz), 125.4 (q, *J* = 3.8 Hz), 126.6, 128.5 (q, *J* = 32 Hz), 139.2, 206.1; IR (ATR) ν: 2925, 2855, 1949 cm^{-1}; HRMS (APPI) m/z calcd for $C_{17}H_{21}F_3$ $[M]^+$ 282.1590, found 282.1590; $[\alpha]_D^{26}$ = -190.6 (*c* = 1.22, $CHCl_3$, 96% ee); HPLC conditions: Chiralcel OD-H, hexane (100%), f: 0.5 mL/min, tR: 8.0, 8.6 min (96% ee).

(*R*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-4-methyl-*N*-(4-phenylbuta-2,3-dien-1-yl)benzenesulfonamide ((*R*)-**6**)

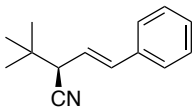


Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.87 (s, 9H), 2.41 (s, 3H), 3.92 (ddd, 1H, *J* = 14.0, 7.2, 2.0 Hz), 4.01 (dd, 1H, *J* = 14.0, 6.8, 2.8 Hz), 4.21 (s, 2H), 5.49 (ddd, 1H, *J* = 7.2, 6.8, 6.8 Hz), 6.21 (ddd, 1H *J* = 6.8, 2.8, 2.0 Hz), 7.18-7.21 (m, 1H), 7.25-7.31 (m, 6H), 7.74 (d, 2H, *J* = 7.6 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 21.4, 27.0, 30.4, 36.6, 45.5, 70.4, 90.4, 94.9, 96.1, 126.9, 127.3, 127.7, 128.6, 129.6, 133.5, 136.2, 143.3, 206.7; IR (ATR) ν: 2969, 1952, 1348, 1160 cm^{-1}; HRMS (ESI) m/z calcd for $C_{24}H_{27}NNaO_2S$ $[M+Na]^+$ 416.1660, found 416.1663; mp. 60-61 °C; $[\alpha]_D^{25}$ = -171.2 (*c* = 0.99, $CHCl_3$, 70% ee); HPLC conditions: Chiralpak IA, hexane/*i*-PrOH = 90:10, f: 1.0 mL/min, tR: 6.0, 6.5 min (92% ee).

C. General Procedure for Hydrocyanation

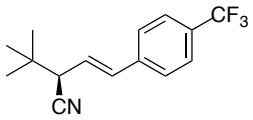
A solution of $PMePh_2$ (14 μL, 0.075 mmol) and $Ni[P(OPh)_3]_4$ (24.4 mg, 0.019 mmol) in toluene (190 μL) was heated under Ar atmosphere at 100 °C for 10 min. After cooling to room temperature, a solution of allene (0.19 mmol) and acetonecyanohydrin (84 μL, 0.94 mmol) in toluene (280 μL) were added and heated until the allene was disappeared. The reaction mixture was filtrated through Celite®, concentrated under vacuo and purified by column chromatography. Spectral data of (*R*)-**3a,** (*S*)-**3d-g** and **3k** were identical to the literature data.[2]

(*R*,*E*)-2-(*tert*-butyl)-4-phenylbut-3-enenitrile ((*R*)-**4a**)



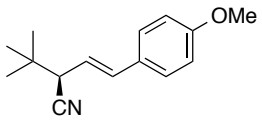
$[\alpha]_D^{25}$ = +28.6 (*c* = 1.67, $CHCl_3$, 94% ee); HPLC conditions: Chiralcel OD-H, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 9.4, 10.1 min (97% ee).

(*R*,*E*)-2-(*tert*-butyl)-4-(4-(trifluoromethyl)phenyl)but-3-enenitrile ((*R*)-**4b**)



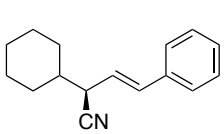
Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.13 (s, 9H), 3.22 (dd, 1H, *J* = 7.2, 1.2 Hz), 6.22 (dd, 1H, *J* = 16.0, 7.2 Hz), 6.76 (d, 1H, *J* = 16.0 Hz), 7.49 (d, 2H, *J* = 8.4 Hz), 7.60 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 27.3, 34.8, 46.7, 119.0, 123.5, 124.0 (q, *J* = 270.2 Hz), 125.6, (q, *J* = 3.8 Hz), 126.7, 130.0 (q, *J* = 33.5 Hz), 133.7, 139.2; IR (ATR) ν: 2968, 2309 cm^{-1}; HRMS (APPI) m/z calcd for $C_{15}H_{17}NF_3$ $[M+H]^+$ 268.1308, found 268.1300; mp. 50-52 °C; $[\alpha]_D^{25}$ = +27.0 (*c* = 1.0 , $CHCl_3$, 94% ee); HPLC conditions; Chiralcel OJ-H, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 15.2, 18.8 min (94% ee).

(*R*,*E*)-2-(*tert*-butyl)-4-(4-methoxyphenyl)but-3-enenitrile ((*R*)-**4c**)



Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.10 (s, 9H), 3.15 (d, 1H, *J* = 7.2 Hz), 3.82 (s, 3H), 5.97 (dd, 1H, *J* = 15.6, 7.2 Hz), 6.63 (d, 1H, *J* = 16.0 Hz), 6.87 (d, 2H, *J* = 8.0 Hz), 7.33 (d, 2H, *J* = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 27.3, 34.6, 46.7, 55.3, 114.0, 118.4, 119.5, 127.7, 128.6, 134.4, 159.6; IR (ATR) ν: 2964, 2235 cm^{-1}; HRMS (APPI) m/z calcd for $C_{15}H_{20}ON$ $[M+H]^+$ 230.1539, found 250.2539; mp. 72-73 °C; $[\alpha]_D^{25}$ = +22.7 (*c* = 1.0, $CHCl_3$, 84% ee); HPLC conditions: Chiralpak IA, hexane/*i*-PrOH = 98:2, f: 1.0 mL/min, tR: 9.1, 9.8 min (84% ee).

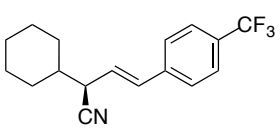
(*S*,*E*)-2-cyclohexyl-4-phenylbut-3-enenitrile ((*S*)-**4d**)



$[\alpha]_D^{25}$ = +19.0 (*c* = 1.09, $CHCl_3$, 97% ee)*; HPLC conditions: Chiralcel OD-H, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 11.7, 13.1 min (78% ee).

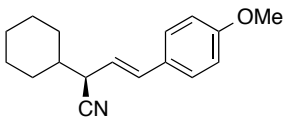
*Measured after recrystallization from hexane.

(*S*,*E*)-2-cyclohexyl-4-(4-(trifluoromethyl)phenyl)but-3-enenitrile ((*S*)-**4e**)



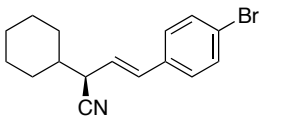
$[\alpha]_D^{25}$ = +9.55 (*c* = 1.43, $CHCl_3$, 82% ee); HPLC conditions: Chiralpak IB, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 8.4, 8.8 min (82% ee).

(*S*,*E*)-2-cyclohexyl-4-(4-methoxyphenyl)but-3-enenitrile ((*S*)-**4f**)



$[\alpha]_D^{25}$ = +10.73 (*c* = 1.12, $CHCl_3$, 65% ee)**;** HPLC conditions: Chiralpak IB, hexane/*i*-PrOH = 98:2, f: 1.0 mL/min, tR: 8.1, 8.5 min (65% ee).

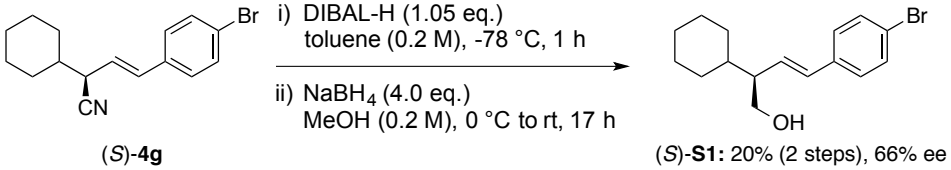
(*S*,*E*)-4-(4-bromophenyl)-2-cyclohexylbut-3-enenitrile ((*S*)-**4g**)



$[\alpha]_D^{25}$ = +6.84 (*c* = 0.51, $CHCl_3$)

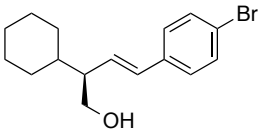
Ee was determined after converted to (*S*)-**S1** (Scheme S1)**.**

Scheme S1. **Reduction of** (*S*)-**4g**



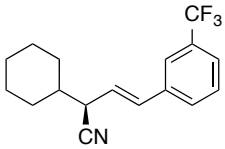
(*S*)-**4g** (*S*)-**S1:** 20% (2 steps), 66% ee

(*S*,*E*)-4-(4-bromophenyl)-2-cyclohexylbut-3-en-1-ol ((*S*)-**S1**)



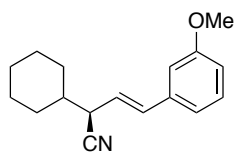
Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.94-1.35 (m, 6H), 1.40-1.49 (m, 1H), 1.63-1.72 (m, 5H), 2.17-2.24 (m, 1H), 3.57 (dd, 1H, *J* = 10.0, 9.2 Hz), 3.75-3.80 (m, 1H), 6.05 (dd, 1H, *J* = 16.0, 10.0 Hz), 6.40 (d, 1H, *J* = 16.0 Hz), 7.24 (d, 2H, *J* = 8.4 Hz), 7.43 (d, 2H, *J* = 8.4 Hz) ; ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 26.37, 26.40, 26.5, 30.4, 31.2, 38.9, 52.2, 63.8, 120.9, 127.6, 131.2, 131.6, 131.8, 136.0; IR (ATR) ν: 3289, 2922, 2849 cm^{-1}; HRMS (APPI) m/z calcd for $C_{16}H_{22}OBr$ $[M+H]^+$ 309.0849, found 309.0861; mp. 97-98 °C; $[\alpha]_D^{23}$ = +8.81 (*c* = 0.71, $CHCl_3$, 66% ee); HPLC conditions: Chiralcel OJ-H, hexane/*i*-PrOH = 95:5, f: 1.0 mL/min, tR: 9.4, 10.6 min (66% ee).

(*S*,*E*)-2-cyclohexyl-4-(3-(trifluoromethyl)phenyl)but-3-enenitrile ((*S*)-**4h**)



Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.13-1.29 (m, 5H), 1.68-1.90 (m, 6H), 3.33 (dd, 1H, *J* = 6.4, 6.4 Hz), 6.11 (dd, 1H, *J* = 16.0, 6.4 Hz), 6.74 (d, 1H, *J* = 16.0 Hz), 7.45 (dd, 1H, *J* = 7.6, 7.6 Hz), 7.51-7.54 (m, 2H,), 7.61 (s, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 25.77, 25.79, 25.9, 29.6, 31.0, 40.8, 41.1, 118.0, 123.0 (q, *J* = 2.9 Hz), 124.0 (q, *J* = 271.2 Hz), 124.2, 124.7 (q, *J* = 2.7 Hz), 129.2, 129.8, 131.1 (q, 32.6 Hz), 132.5, 136.5; IR (ATR) ν: 2928, 2855, 2241 cm^{-1}; HRMS (APPI) m/z calcd for $C_{17}H_{18}F_3N$ $[M]^+$ 293.1386, found 293.1379; $[\alpha]_D^{25}$ = +7.85 (*c* = 0.94, $CHCl_3$, 80% ee); HPLC conditions: Chiralpak IB, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 9.0, 10.0 min (80% ee).

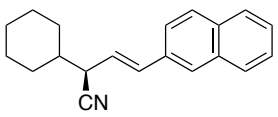
(*S*,*E*)-2-cyclohexyl-4-(3-methoxyphenyl)but-3-enenitrile ((*S*)-**4i**)



Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.13-1.29 (m, 5H), 1.67-1.81 (m, 2H), 1.78-1.91 (m, 4H), 3.30 (dd, 1H, *J* = 6.4, 6.4 Hz), 3.82 (s, 3H), 6.03 (dd, 1H, *J* = 16.0, 6.4 Hz), 6.67 (d, 1H, *J* = 16.0 Hz), 6.83 (d, 1H, *J* = 8.0 Hz), 6.91 (s, 1H), 6.97 (d, 1H, *J* = 8.0

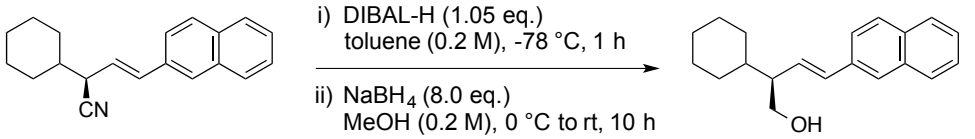
Hz), 7.25 (dd, 1H, *J* = 8.0, 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 25.8, 25.8, 25.9, 29.6, 30.9, 40.8, 41.1, 55.2, 111.9, 113.7, 119.0, 119.3, 122.4, 129.6, 133.8, 137.2, 159.8; IR (ATR) ν: 2926, 2853, 2239 cm^{-1}; HRMS (APPI) m/z calcd for $C_{17}H_{21}NO$ $[M]^+$ 255.1618, found 255.1611; $[\alpha]_D^{25}$ = +6.24 (*c* = 0.79, $CHCl_3$, 74% ee); HPLC conditions: Chiralpak IB, hexane/*i*-PrOH = 98:2, f: 1.0 mL/min, tR: 9.3, 15.9 min (74% ee).

(*S*,*E*)-2-cyclohexyl-4-(naphthalen-2-yl)but-3-enenitrile ((*S*)-**4j**)



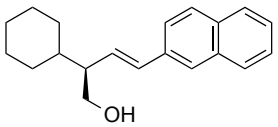
Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.18-1.32 (m, 5H), 1.69-1.95 (m, 6H), 3.36 (ddd, 1H, *J* = 6.8, 2.4 Hz), 6.17 (dd, 1H, *J* = 16.0, 6.8 Hz), 6.86 (d, 1H, *J* = 16 Hz), 7.44-7.50 (m, 2H), 7.57 (d, 1H, *J* = 8.8 Hz), 7.79 (s, 1H), 7.80-7.85 (m, 3H); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 25.8, 25.8, 26.0, 29.6, 31.0, 40.9, 41.2, 119.4, 122.4, 123.3, 126.2, 126.4, 126.8, 127.7, 128.0, 128.4, 133.16, 133.21, 133.5, 134.0; IR (ATR) ν: 2927, 2853, 2237 cm^{-1}; HRMS (APPI) m/z calcd for $C_{20}H_{22}N$ $[M+H]^+$ 276.1747, found 276.1742; mp. 123-124 °C; $[\alpha]_D^{25}$ = +16.7 (*c* = 0.91, $CHCl_3$).
Ee was determined after converted to the corresponding alcohol (*S*)-**S2** (Scheme S2)**.**

Scheme S2. Reduction of (*S*)-**4j**



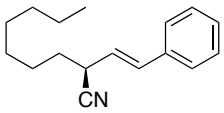
(*S*)-**4j** (*S*)-**S2:** 40% (2 steps), 72% ee

(*S*,*E*)-2-cyclohexyl-4-(naphthalen-2-yl)but-3-en-1-ol ((*S*)-**S2**)



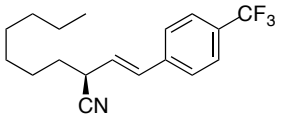
Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.04-1.29 (m, 5H), 1.40-1.54 (m, 2H), 1.64-1.75 (m, 5H), 2.24-2.31 (m, 1H), 3.61 (dd, 1H, *J* = 10.4, 8.4 Hz), 3.80-3.84 (m, 1H), 6.18 (dd, 1H, *J* = 15.6, 10.0 Hz), 6.63 (d, 1H, *J* = 15.6 Hz), 7.41-7.47 (m, 2H), 7.60 (dd, 2H, *J* = 8.0, 1.2 Hz), 7.72 (s, 1H), 7.77-7.80 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 26.4, 26.4, 26.5, 30.5, 31.3, 39.1, 52.5, 64.9, 123.5, 125.7, 125.8, 126.2, 127.6, 127.9, 128.1, 130.7, 132.8, 133.3, 133.6, 134.5; IR (ATR) ν: 3242, 2921, 2849 cm^{-1}; HRMS (APPI) m/z calcd for $C_{20}H_{24}N$ $[M]^+$ 280.1822, found 280.1817; mp. 97-98 °C; $[\alpha]_D^{23}$ = +8.8 (*c* = 0.71, $CHCl_3$, 72% ee); HPLC Conditions: Chiralcel IA, hexane/*i*-PrOH = 95:5, f: 1.0 mL/min, tR: 12.5, 15.9 min (72% ee).

(*S*,*E*)-2-styryloctanenitrile ((*S*)-**4k**)



$[\alpha]_D^{25}$ = +8.1 (*c* = 1.14, $CHCl_3$, 47% ee); HPLC cconditions: Chiralpak IB, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 9.5, 9.7 min (47% ee).

(*S*,*E*)-2-(4-(trifluoromethyl)styryl)nonanenitrile ((*S*)-**4l**)

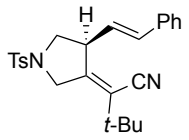


Colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 0.89 (t, 3H, *J* = 7.2 Hz), 1.29-1.37 (m, 9H), 1.43-1.60 (m, 1H), 1.79 (dt, 2H, *J* = 7.2, 7.2 Hz), 3.46 (dt, 1H, *J* = 6.4, 6.4 Hz), 6.14 (dd,

1H, *J* = 16.0, 6.4 Hz), 6.78 (d, 1H, *J* = 16.0 Hz), 7.48 (d, 2H, 8.0 Hz), 7.59 (d, 2H, *J* = 8.0 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 14.0, 22.5, 26.8, 28.91, 28.93, 31.6, 33.1, 34.4, 199.8, 124.0 (q, *J* = 270.2), 125.6 (q, *J* = 3.8 Hz), 126.0, 126.7, 130.0 (q, *J* = 32.6 Hz), 131.8, 139.2; IR (ATR) ν: 2928, 2858, 2242 cm^{-1}; HRMS (APPI) m/z calcd for $C_{18}H_{22}F_3N$ $[M]^+$ 309.1699, found 309.1694; $[\alpha]_D^{25}$ = +6.8 (*c* = 1.15, $CHCl_3$, 63% ee); HPLC conditions*: Chiralcel AD-H, hexane/*i*-PrOH = 99:1, f: 1.0 mL/min, tR: 10.3, 11.3 min (63% ee).

*Racemic sample was separated by using Chiralcpak IA better than Chiralcel AD-H, however chiral sample could not be separated very well by using Chiralcpak IA. Both charts are shown in page xx.

(*E*)-3,3-dimethyl-2-((*S*)-4-((*E*)-styryl)-1-tosylpyrrolidin-3-ylidene)butanenitrile ((*S*)-**7**)

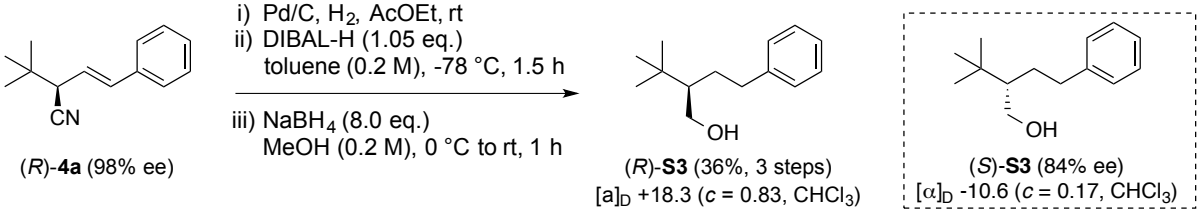


Colorless solid. ^{1}H NMR ($CDCl_3$, 600 MHz) δ: 1.21 (s, 9H), 2.45 (s, 3H), 3.16 (dd, 1H, *J* = 11.4, 6.0 Hz), 3.51 (d, 1H, *J* = 9.6 Hz), 3.78 (dd, 1H, 7.8, 6.0 Hz), 3.96 (d, 1H, *J* = 16.2 Hz), 4.33 (d, 1H, *J* = 16.2 Hz), 5.99 (dd, 1H, *J* = 16.2, 7.8 Hz), 6.57 (d, 1H, *J* = 16.2 Hz), 7.23-7.25 (m, 1H), 7.30-7.31 (m, 4H), 7.37 (d, 2H, *J* = 7.8 Hz), 7.73 (d, 2H, *J* = 7.8 Hz); ^{13}C NMR ($CDCl_3$, 100 MHz) δ: 21.6, 29.6, 35.4, 49.5, 50.0, 51.8, 117.1, 120.0, 125.9, 126.6, 127.8, 128.5, 129.9, 130.0, 132.0, 132.4, 136.3, 144.3, 153.3; IR (ATR) ν: 2968, 2212, 1348, 1161 cm^{-1}; HRMS (ESI) m/z calcd for $C_{25}H_{28}N_2NaO_2S$ $[M+Na]^+$ 443.1769, found 443.1771; mp. 123-124 °C; $[\alpha]_D^{25}$ = -59.6 (*c* = 0.51, $CHCl_3$, 42% ee); HPLC conditions: Chiralpak IB, hexane/*i*-PrOH = 75:25, f: 1.0 mL/min, tR: 6.6, 8.1 min (64% ee).

D. Determination of absolute stereochemistry of (*R*)-**4a and** (*S*)-**4d**

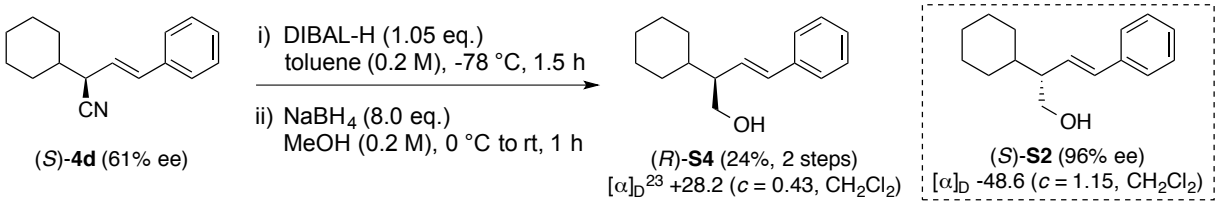
Absolute stereochemistry of (*R*)-**4a** was determined after conversion to (*R*)-**S3** and comparing specific optical rotation with that of reported (*S*)-**S3**[4] (Scheme S3).

Scheme S3. Reduction of (*R*)-**4a**



Absolute stereochemistry of (*S*)-**4d** was determined after conversion to (*S*)-**S4** and comparing specific optical rotation with that of reported (*R*)-**S4**[5] (Scheme S4).

Scheme S4. Reduction of (*S*)-**4d**



E. Examination of time course

A solution of phosphorous ligand and $Ni[P(OPh)_3]_4$ (33.7 mg, 0.028 mmol) in toluene (285 μL) was heated under Ar atmosphere at 100 °C for 10 min. After cooling to room temperature, a solution of allene (0.28 mmol), acetonecyanohydrin (52 μL, 0.56 mmol) and 4-methoxybiphenyl (10.4 mg, 0.056 mmol) as an internal standard in toluene (420 μL) were added and heated. The sample was taken from the reaction mixture via syringe in a specific time, filtrated through Celite® and concentrated under vacuo. The yield was calculated according to the ^{1}H NMR spectra and the ee was determined by HPLC after purification by preparative TLC.

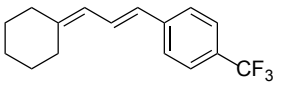
Table S1. Time course profiling

time (min)	(*R*)-**3a** y. (%) (ee %)	(*R*)-**4a** y. (%) (ee %)	(*R*)-**3d** y. (%) (ee %)	(*S*)-**4d** y. (%) (ee %)	(*R*)-**3k** y. (%) (ee %)	(*S*)-**4k** y. (%) (ee %)
0	100 (99)	0 (-)	100 (96)	0 (-)	100 (97)	0 (-)
2	-	-	90 (94)	2 (78)	71 (92)	15 (52)
5	55 (96)	28 (98)	69 (91)	18 (78)	0 (-)	74 (48)
15	41 (92)	44 (98)	37 (80)	47 (74)	-	-
20	20 (92)	59 (98)	9 (80)	67 (74)	-	-
30	4 (80)	84 (97)	0 (-)	76 (72)	-	-
45	0 (-)	91 (97)	-	-	-	-

F. Examination of racemization

A solution of phosphorous ligand and $Ni[P(OPh)_3]_4$ (12.2 mg, 0.0094 mmol) in toluene (100 μL) was heated under Ar atmosphere at 100 °C for 10 min. After cooling to room temperature, a solution of (*R*)-**3e** (25.0 mg, 0.094 mmol) in toluene (135 μL) were added and heated for 6 h. The reaction mixture was filtrated through Celite®, concentrated under vacuo and purified by column chromatography to provide **3e** (6.0 mg, 0.023 mmol, 24%, 2% ee) and **8** (3.8 mg, 0.014 mmol, 15%).

(*E*)-1-(3-cyclohexylideneprop-1-en-1-yl)-4-(trifluoromethyl)benzene (8)



Colorless solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ: 1.61 (bs, 6H), 2.22 (bs, 2 H), 2.41 (bs, 2H), 5.97 (d, 1H, *J* = 10.8 Hz), 6.46 (d, 1H, *J* = 15.6 Hz), 7.14 (dd, 1H, *J* = 15.6, 10.8 Hz), 7.46 (d, 2H, *J* = 8.4 Hz), 7.53 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR ($CDCl_3$, 150 MHz) δ: 26.7, 27.9, 28.6, 29.7, 37.6, 122.0, 123.3 (*J* = 270 Hz), 125.5 (*J* = 4.2 Hz), 126.0, 127.3, 128.2, 128.5 (*J* = 30.3 Hz), 141.7, 147.0; IR (ATR) ν: 2927, 2852, 1638, 1608, 1321 cm^{-1}; HRMS (APPI) m/z calcd for $C_{16}H_{17}F_3$ $[M]^+$ 266.1277, found 266.1277; mp. 63-64 °C.

G. References

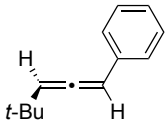
1) Lu, R., Ye, J. Cao, T., Chen, B., Fan, W. Lin, W., Liu, J., Luo, H., Miao, B., Ni, S., Tang, X., Wang, N., Wang, Y., Xie, X., Yu, Q., Yuan, W., Zhang, W., Zhu, C., Ma, S. *Org. Lett.* **2013**, 15, 2254-2257.
2) Arai, S., Hori, H., Amako, Y., Nishida, A. **2015**, *Chem. Commun*. *51*, 7493-7496.
3) Elsevier, C. J., Vermeer, P. *J. Org. Chem.* **1989**, *54* , 3726–3730.

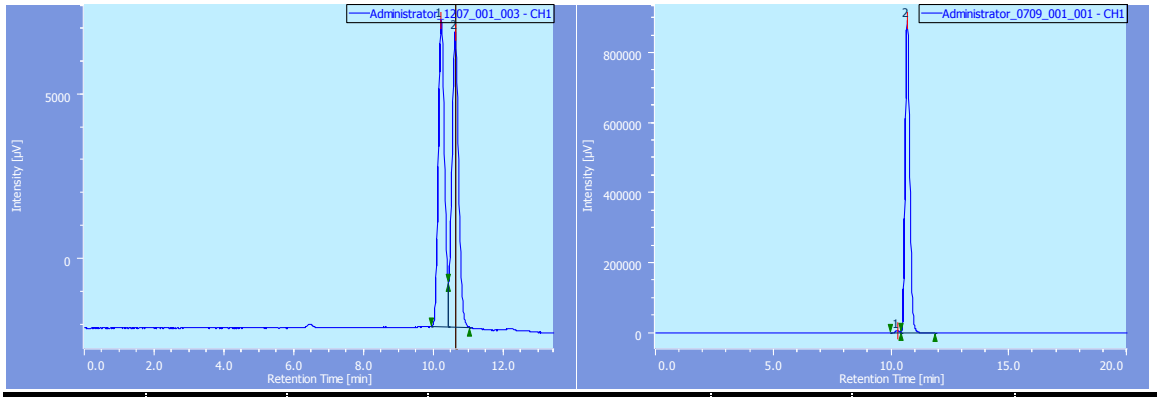
4) Spino, C., Gund, V. G., Nadeau, S. *J. Comb. Chem.* **2005,** 7, 345-352.

5) Kim, H., MacMillan, D. W. C. *J. Am. Chem. Soc.* **2008**, 130, 398-399.

H. HPLC Charts

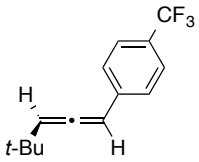
(*R*)-(4,4-dimethylpenta-1,2-dien-1-yl)benzene ((*R*)-**3a**)

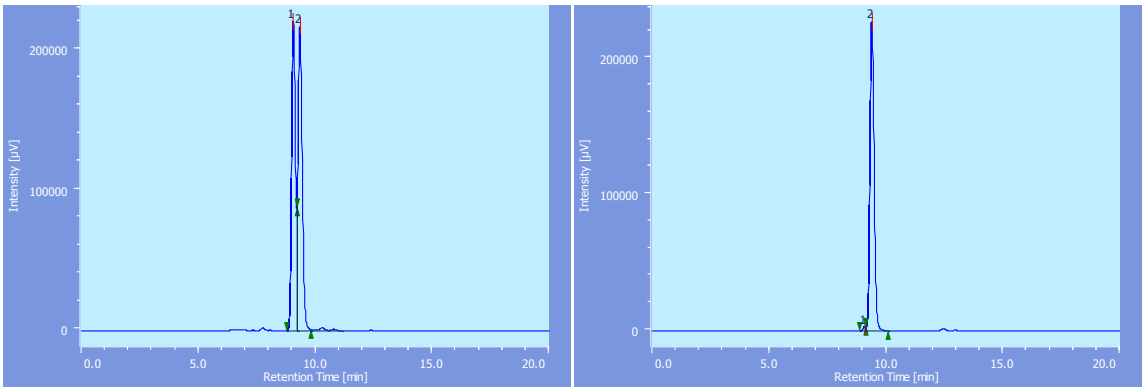




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	10.208	116539	49.457	1	10.258	77294	0.641
2	10.608	119098	50.543	2	10.657	11988380	99.359

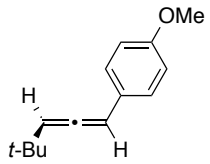
(*R*)-1-(4,4-dimethylpenta-1,2-dien-1-yl)-4-(trifluoromethyl)benzene ((*R*)-**3b**)

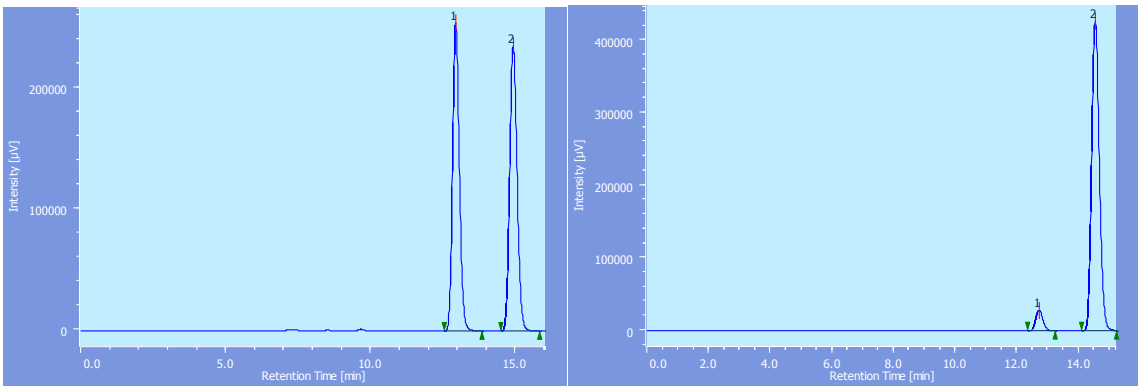




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.067	2515360	48.043	1	9.108	26240	0.944
2	9.350	2720324	51.957	2	9.400	2753971	99.056

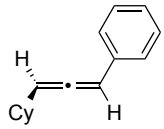
(*R*)-1-(4,4-dimethylpenta-1,2-dien-1-yl)-4-methoxybenzene ((*R*)-**3c**)

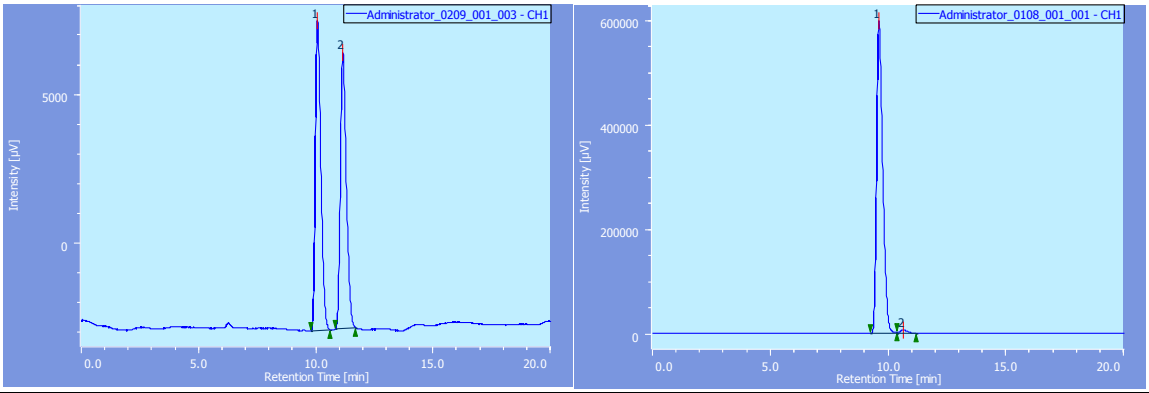




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	12.925	4160965	49.964	1	12.708	463934	5.945
2	14.908	4166903	50.036	2	14.525	7339823	94.055

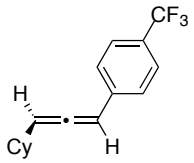
(*R*)-(3-cyclohexylpropa-1,2-dien-1-yl)benzene ((*R*)-**3d**)

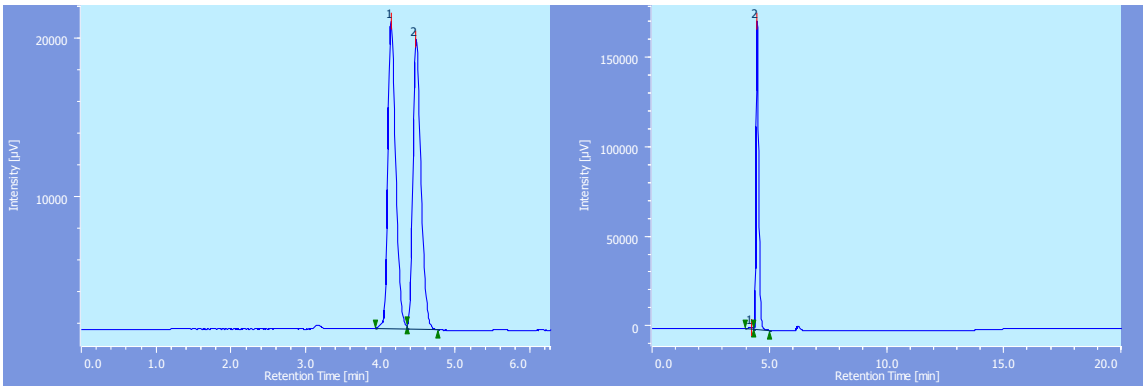




#	tR	面積	面積%	#	tR	面積	面積%
1	10.067	168862	50.756	1	9.600	10874658	98.672
2	11.133	163830	49.244	2	10.633	146395	1.328

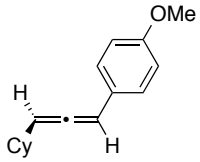
(*R*)-1-(3-cyclohexylpropa-1,2-dien-1-yl)-4-(trifluoromethyl)benzene ((*R*)-**3e**)

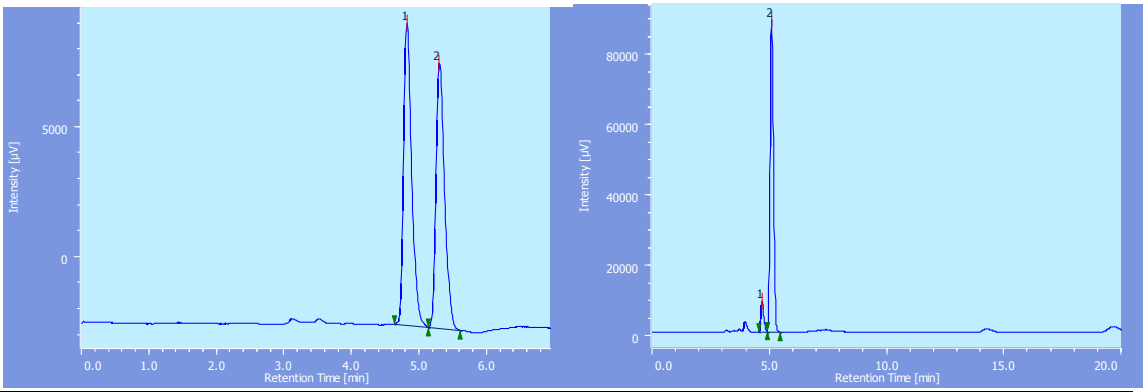




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	4.133	140906	50.655	1	4.217	13800	1.009
2	4.467	137263	49.345	2	4.475	1354521	98.991

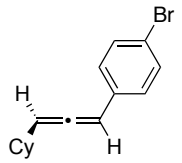
(*R*)-1-(3-cyclohexylpropa-1,2-dien-1-yl)-4-methoxybenzene ((*R*)-**3f**)

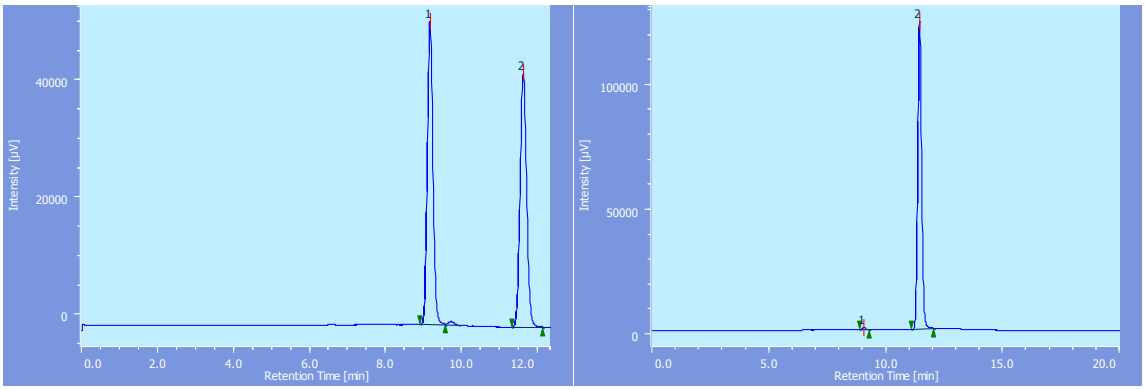




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	4.808	96076	51.637	1	4.683	70987	7.397
2	5.292	89986	48.363	2	5.083	888631	92.603

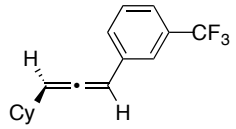
(*R*)-1-bromo-4-(3-cyclohexylpropa-1,2-dien-1-yl)benzene ((*R*)-**3g**)

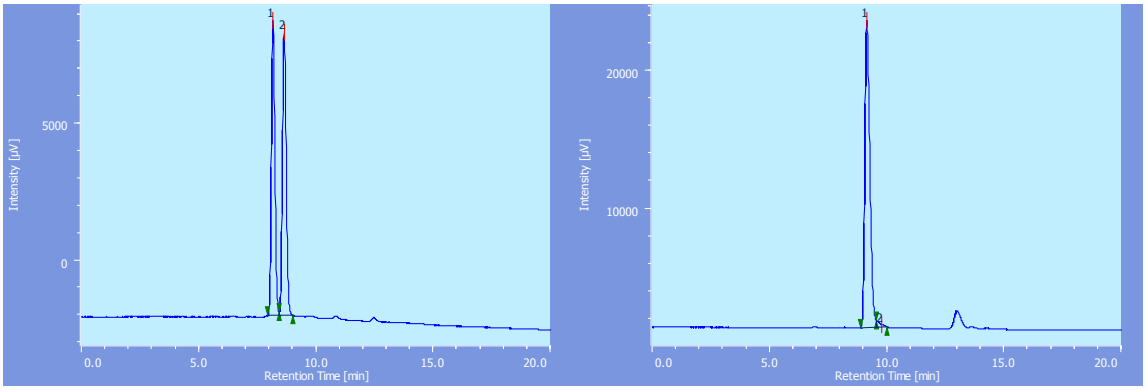




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.158	519146	50.222	1	9.058	11288	0.766
2	11.600	514558	49.778	2	11.433	1461677	99.234

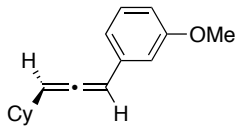
(*R*)-1-(3-cyclohexylpropa-1,2-dien-1-yl)-3-(trifluoromethyl)benzene ((*R*)-**3h**)

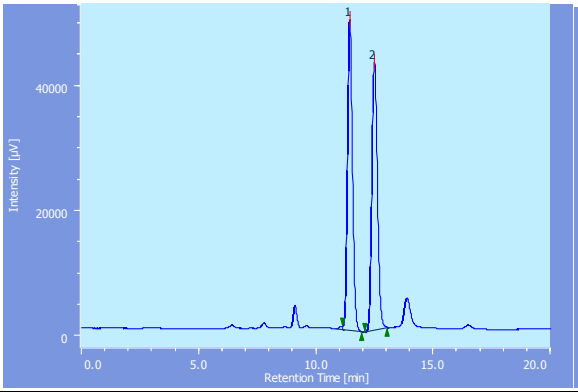


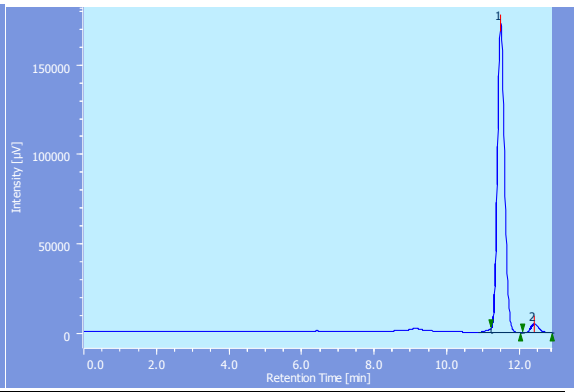


#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	8.158	113154	49.820	1	9.142	334070	98.504
2	8.642	113971	50.180	2	9.767	5073	1.496

(*R*)-1-(3-cyclohexylpropa-1,2-dien-1-yl)-3-methoxybenzene ((*R*)-**3i**)

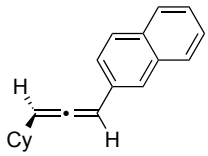


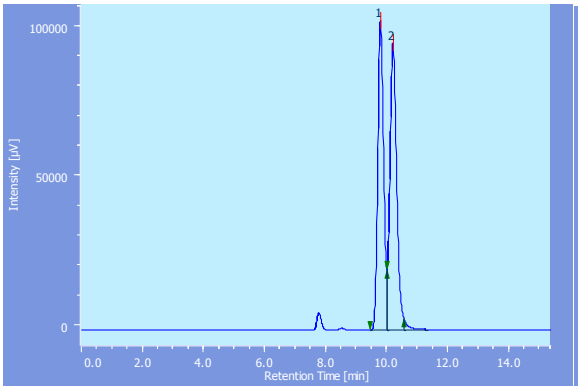


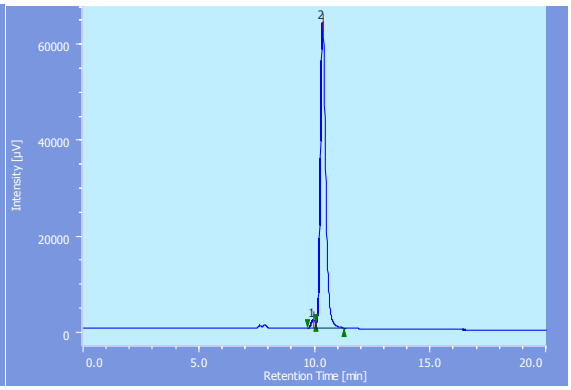


#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	11.433	738457	51.554	1	11.467	2360718	96.908
2	12.483	693931	48.446	2	12.400	75313	3.092

(*R*)-2-(3-cyclohexylpropa-1,2-dien-1-yl)naphthalene ((*R*)-**3j**)

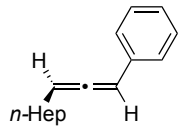


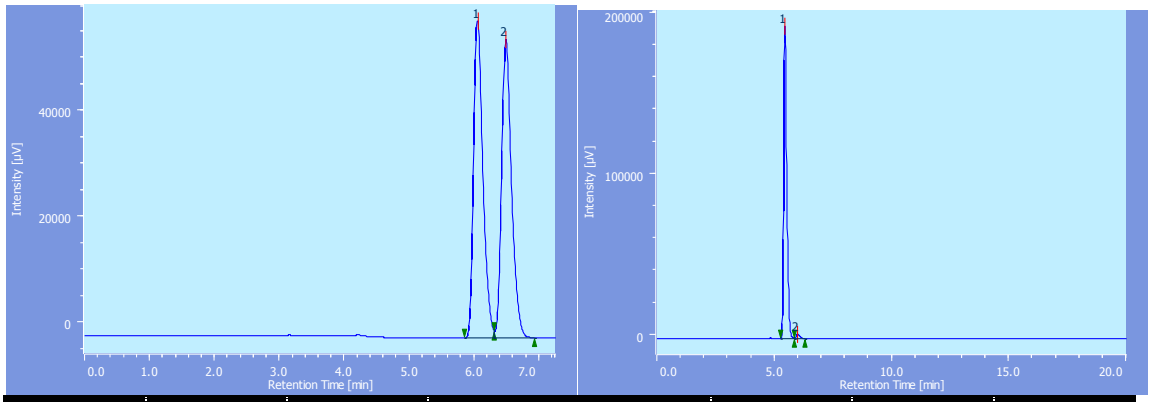




#	tR	面積	面積%	#	tR	面積	面積%
1	9.783	1382910	48.441	1	9.933	22318	2.160
2	10.200	1471900	51.559	2	10.342	1011019	97.840

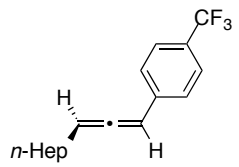
(*R*)-deca-1,2-dien-1-ylbenzene ((*R*)-3k)

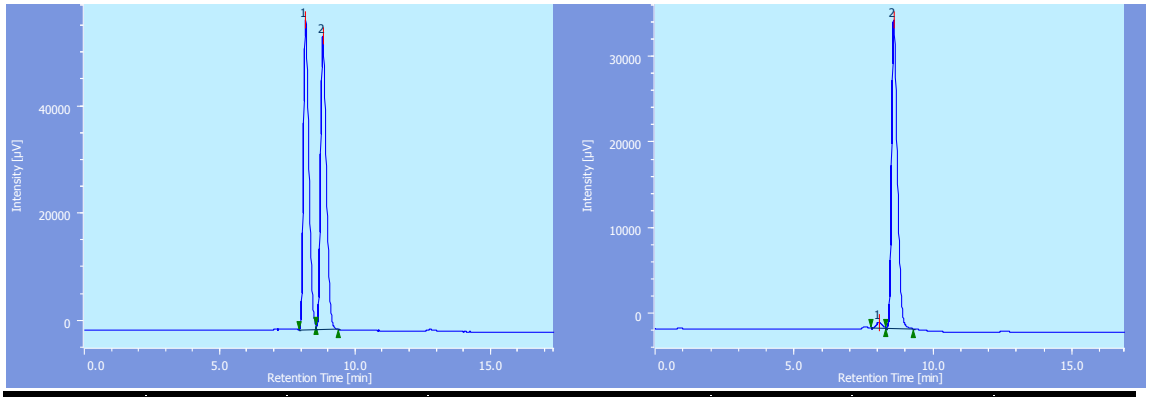




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	6.050	584762	49.946	1	5.450	1828575	98.488
2	6.483	586021	50.054	2	6.000	28071	1.512

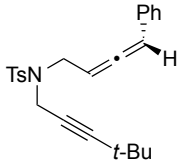
(*R*)-1-(deca-1,2-dien-1-yl)-4-(trifluoromethyl)benzene ((*R*)-3l)

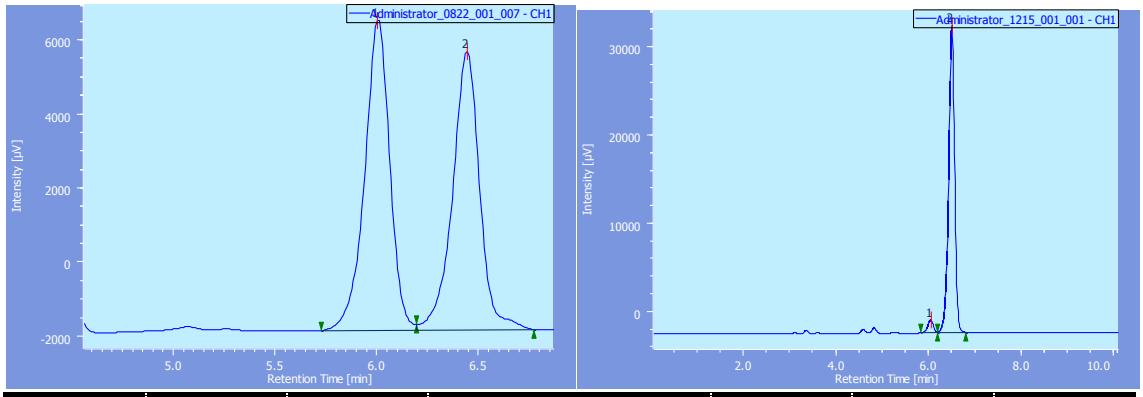




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	8.158	797619	50.049	1	8.042	10438	1.977
2	8.800	796053	49.951	2	8.575	517630	98.023

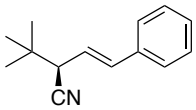
(*R*)-*N*-(4,4-dimethylpent-2-yn-1-yl)-4-methyl-*N*-(4-phenylbuta-2,3-dien-1-yl)benzenesulfonamide ((*R*)-**6**)

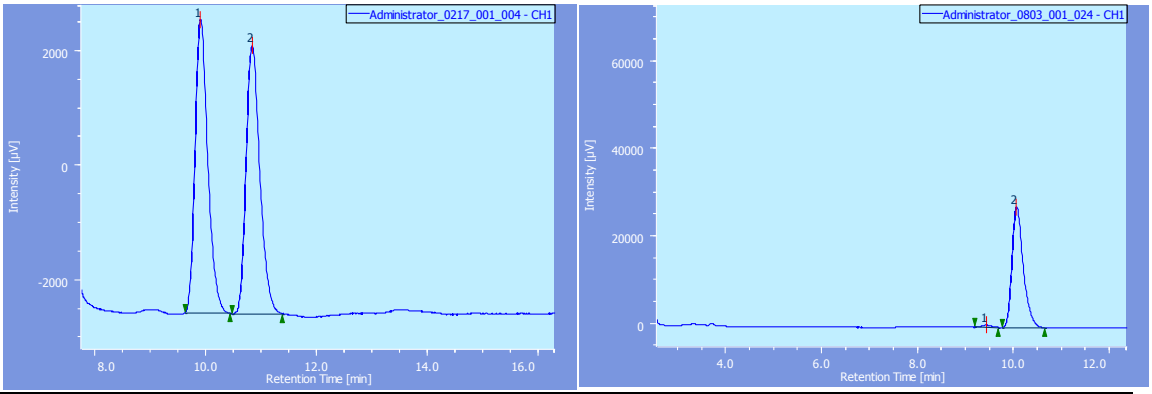




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	6.000	71568	50.937	1	6.042	12209	3.780
2	6.442	68935	49.063	2	6.492	310814	96.220

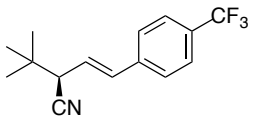
(*R*,*E*)-2-(*tert*-butyl)-4-phenylbut-3-enenitrile ((*R*)-**4a**)

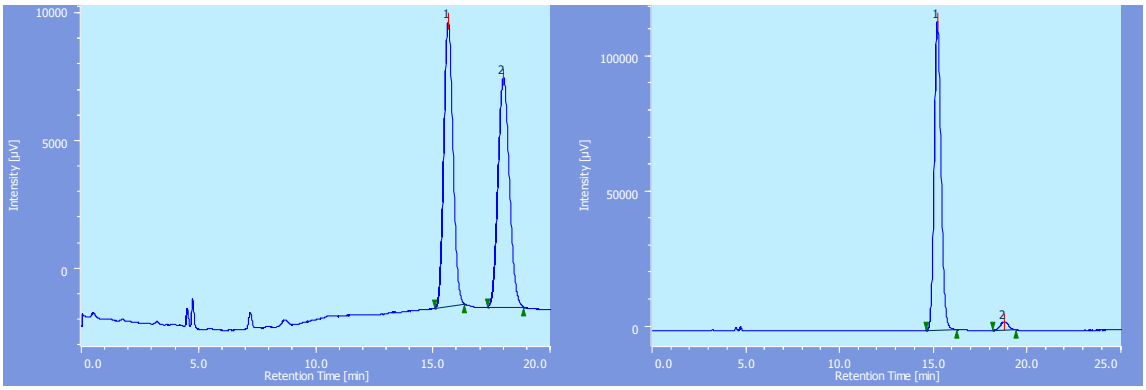




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.900	81652	50.342	1	9.417	6681	1.462
2	10.833	80542	49.658	2	10.050	450198	98.538

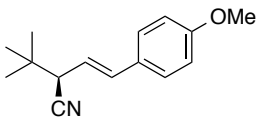
(*R*,*E*)-2-(*tert*-butyl)-4-(4-(trifluoromethyl)phenyl)but-3-enenitrile ((*R*)-4b)

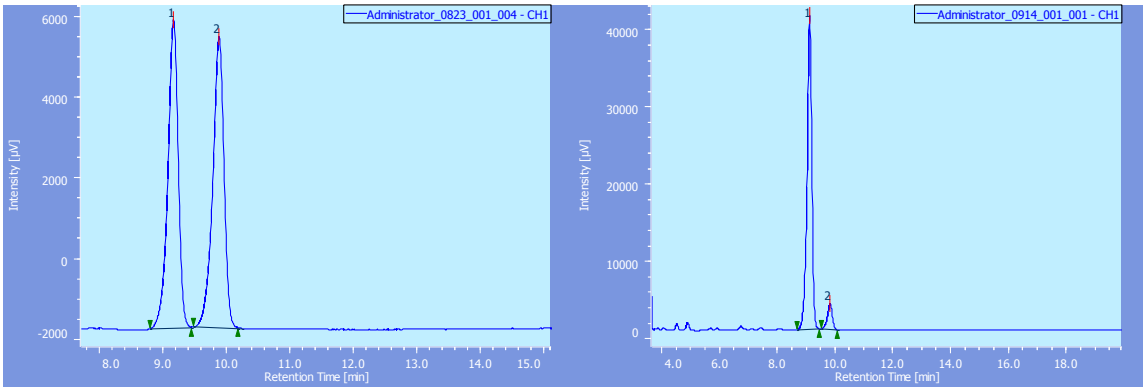




#	tR	面積	面積%	#	tR	面積	面積%
1	15.625	299721	50.014	1	15.200	2897462	96.821
2	17.983	299557	49.986	2	18.775	95140	3.179

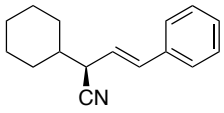
(*R*,*E*)-2-(*tert*-butyl)-4-(4-methoxyphenyl)but-3-enenitrile ((*R*)-4c)

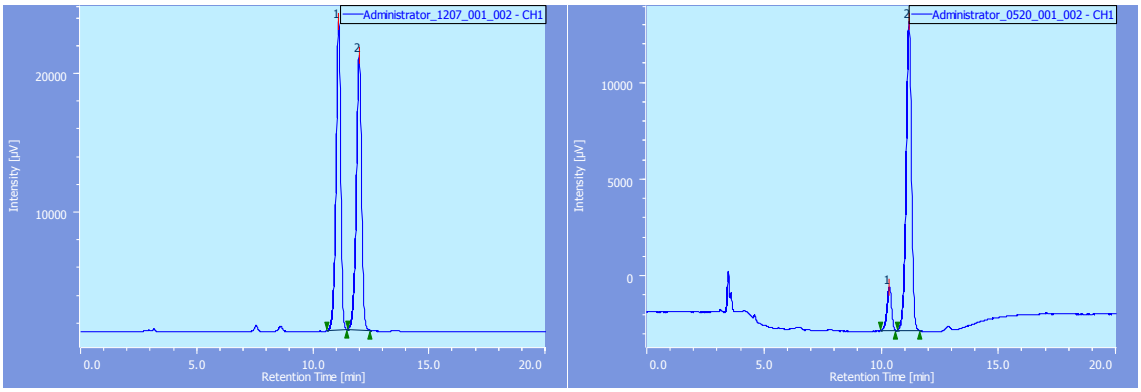




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.167	86087	49.281	1	9.117	468366	92.137
2	9.883	88600	50.719	2	9.817	39971	7.863

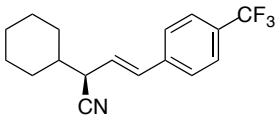
(*S*,*E*)-2-cyclohexyl-4-phenylbut-3-enenitrile ((*S*)-**4d**)

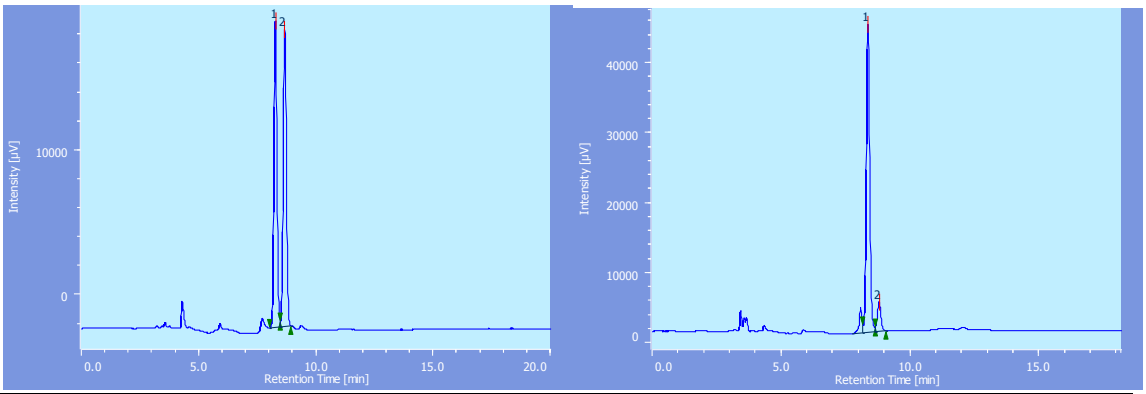




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	11.092	304346	50.188	1	10.333	30546	10.788
2	11.975	302069	49.812	2	11.167	252609	89.212

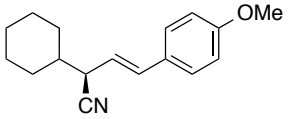
(*S*,*E*)-2-cyclohexyl-4-(4-(trifluoromethyl)phenyl)but-3-enenitrile ((*R*)-**4e**)

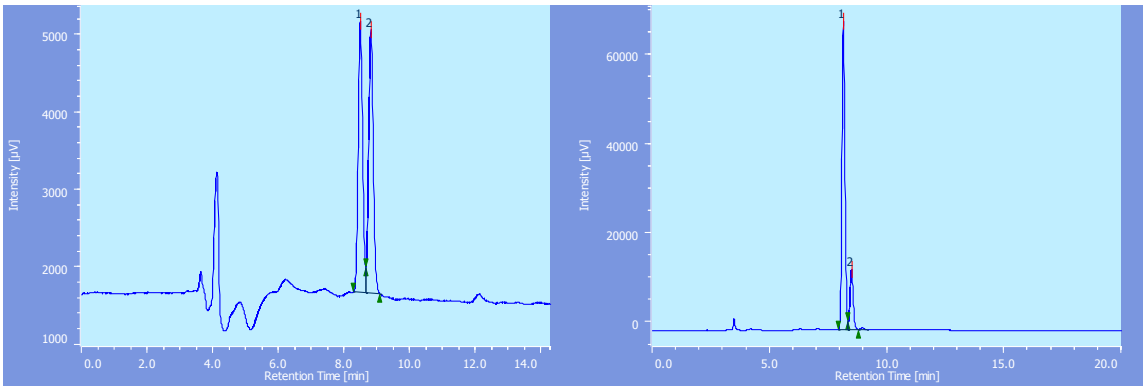




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	8.267	190719	50.214	1	8.358	414668	90.782
2	8.667	189094	49.786	2	8.792	42106	9.218

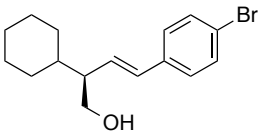
(*S*,*E*)-2-cyclohexyl-4-(4-methoxyphenyl)but-3-enenitrile ((*S*)-**4f**)

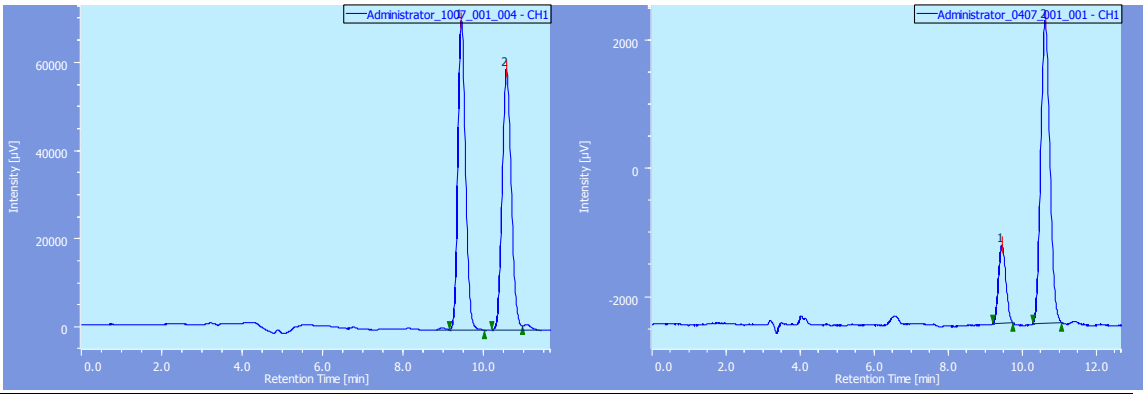




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	8.483	32362	49.540	1	8.142	613972	82.734
2	8.808	32963	50.460	2	8.492	128132	17.266

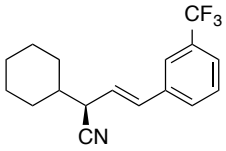
(*S*,*E*)-4-(4-bromophenyl)-2-cyclohexylbut-3-en-1-ol ((*S*)-**S1**)

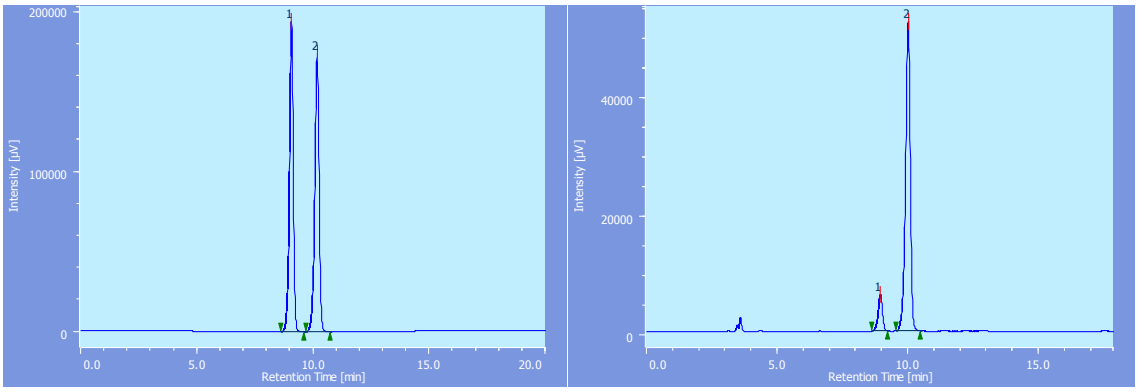




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.433	925379	50.261	1	9.442	16612	17.189
2	10.550	915767	49.739	2	10.600	80028	82.811

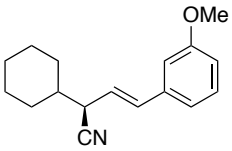
(*S*,*E*)-2-cyclohexyl-4-(3-(trifluoromethyl)phenyl)but-3-enenitrile ((*S*)-**4h**)

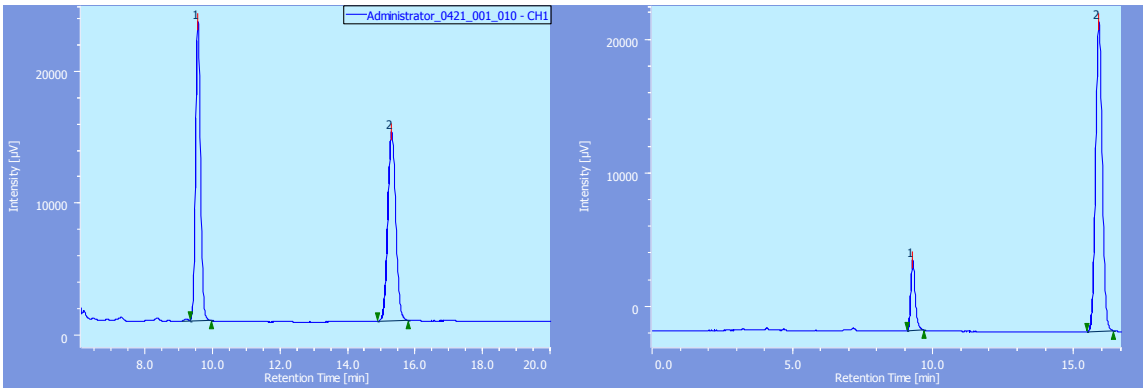




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.067	2195016	50.015	1	8.950	69742	9.683
2	10.167	2193729	49.985	2	10.000	650499	90.317

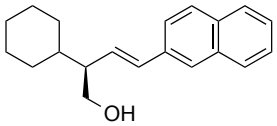
(*S*,*E*)-2-cyclohexyl-4-(3-methoxyphenyl)but-3-enenitrile ((*S*)-**4i**)

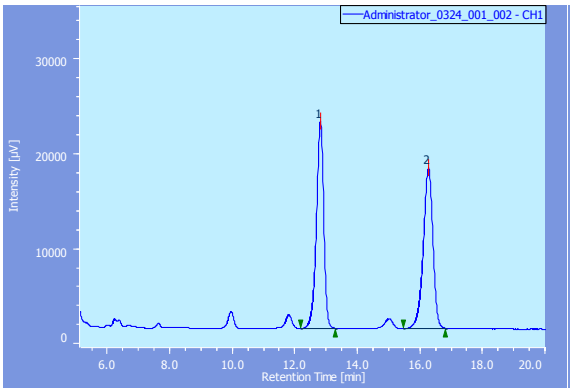


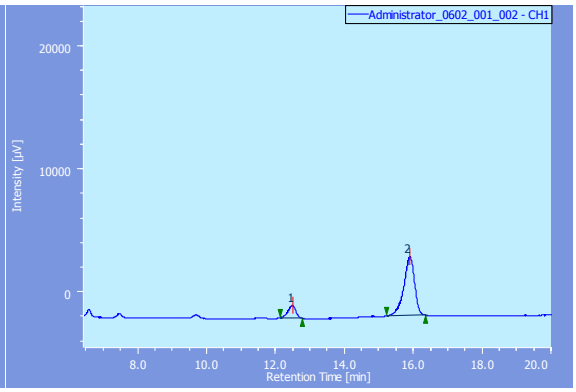


#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.567	231967	50.007	1	9.267	56560	12.859
2	15.292	231906	49.993	2	15.875	383276	87.141

(*S*,*E*)-2-cyclohexyl-4-(naphthalen-2-yl)but-3-en-1-ol ((*S*)-**S2**)

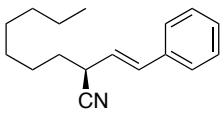


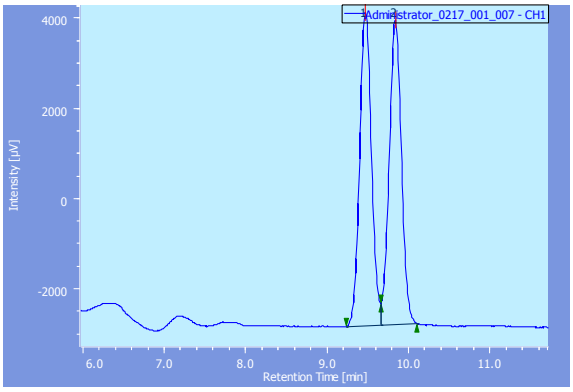


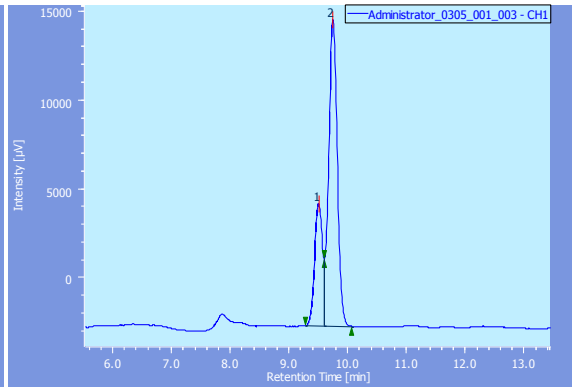


#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	12.800	355799	50.161	1	12.483	16634	13.962
2	16.250	353519	49.839	2	15.883	102500	86.038

(*S*,*E*)-2-styryloctanenitrile ((*S*)-**4k**)

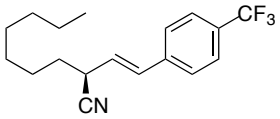




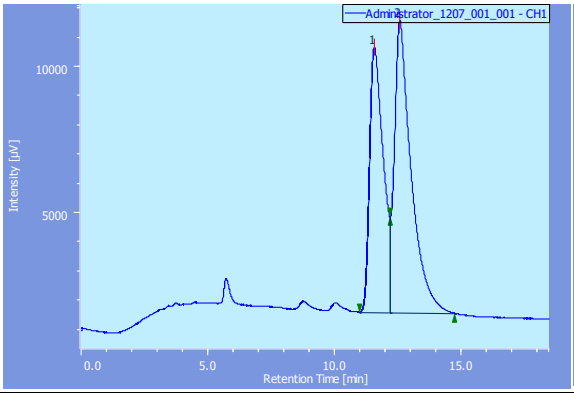


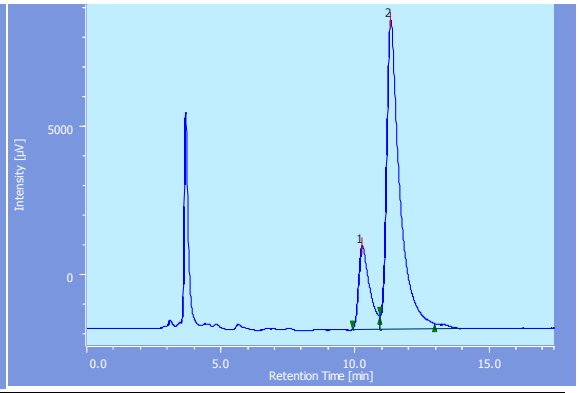
#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.467	70132	49.967	1	9.500	63612	26.459
2	9.833	70224	50.033	2	9.742	176805	73.541

(*S*,*E*)-2-(4-(trifluoromethyl)styryl)nonanenitrile ((*S*)-4l)



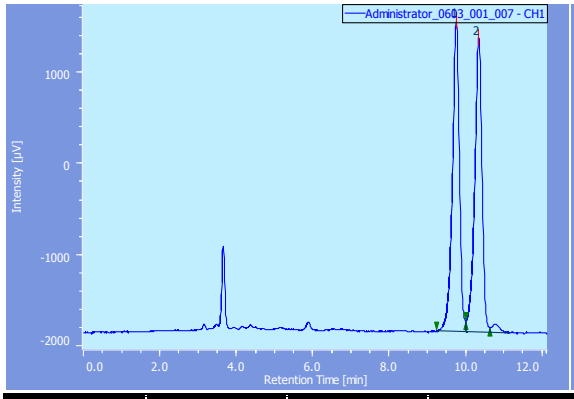
Chiralcel AD-H

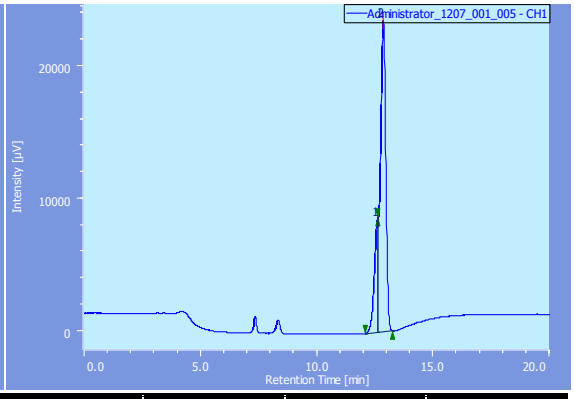




#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	11.567	339592	42.502	1	10.250	79367	18.376
2	12.567	459407	57.498	2	11.317	352547	81.624

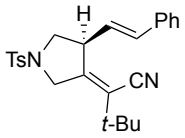
Chiralpak IA

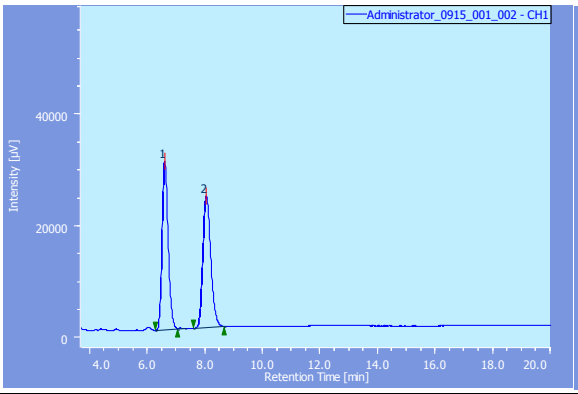


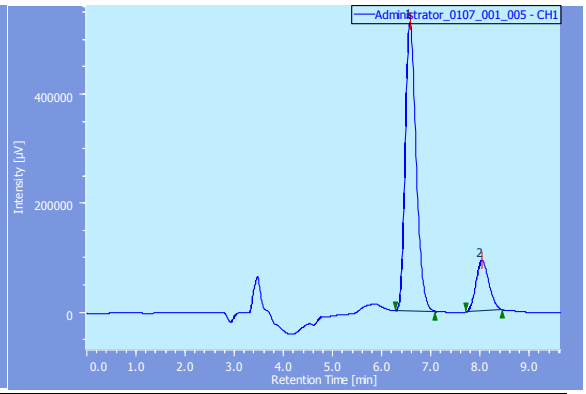


#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	9.742	43051	50.169	1	12.600	43051	20.530
2	10.325	42762	49.831	2	12.850	372721	79.470

(*E*)-3,3-dimethyl-2-((*S*)-4-((*E*)-styryl)-1-tosylpyrrolidin-3-ylidene)butanenitrile ((*S*)-**7**)

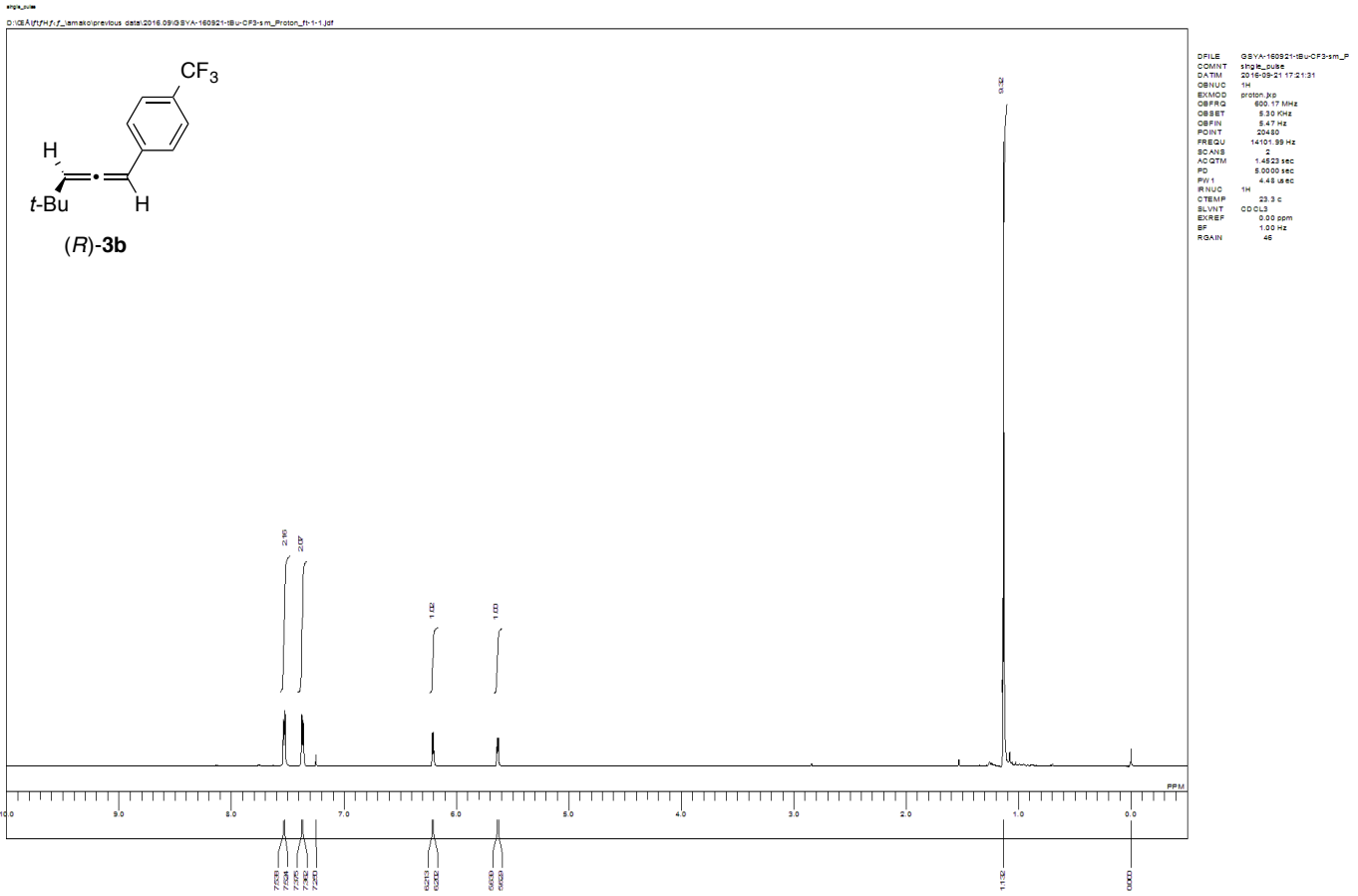


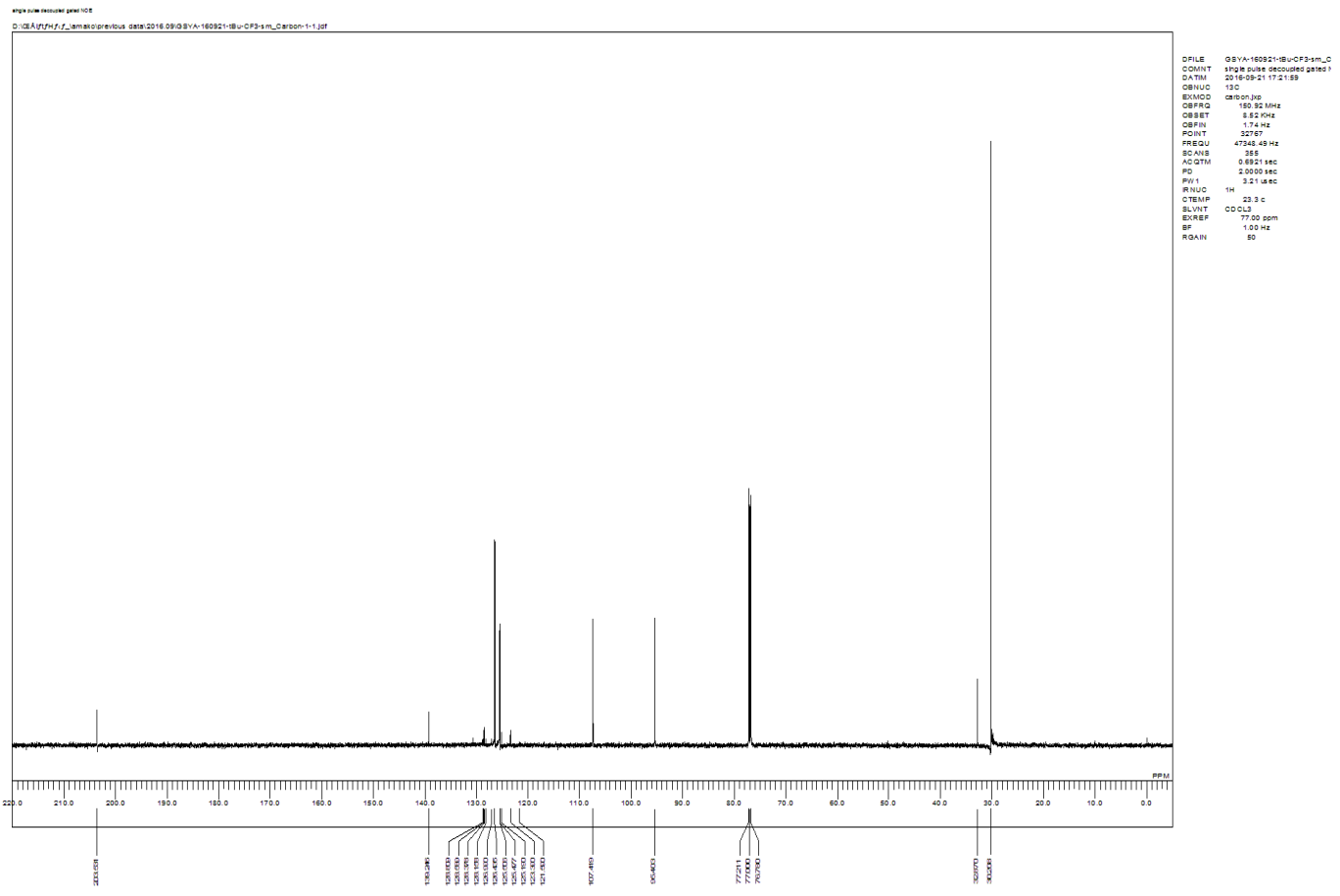


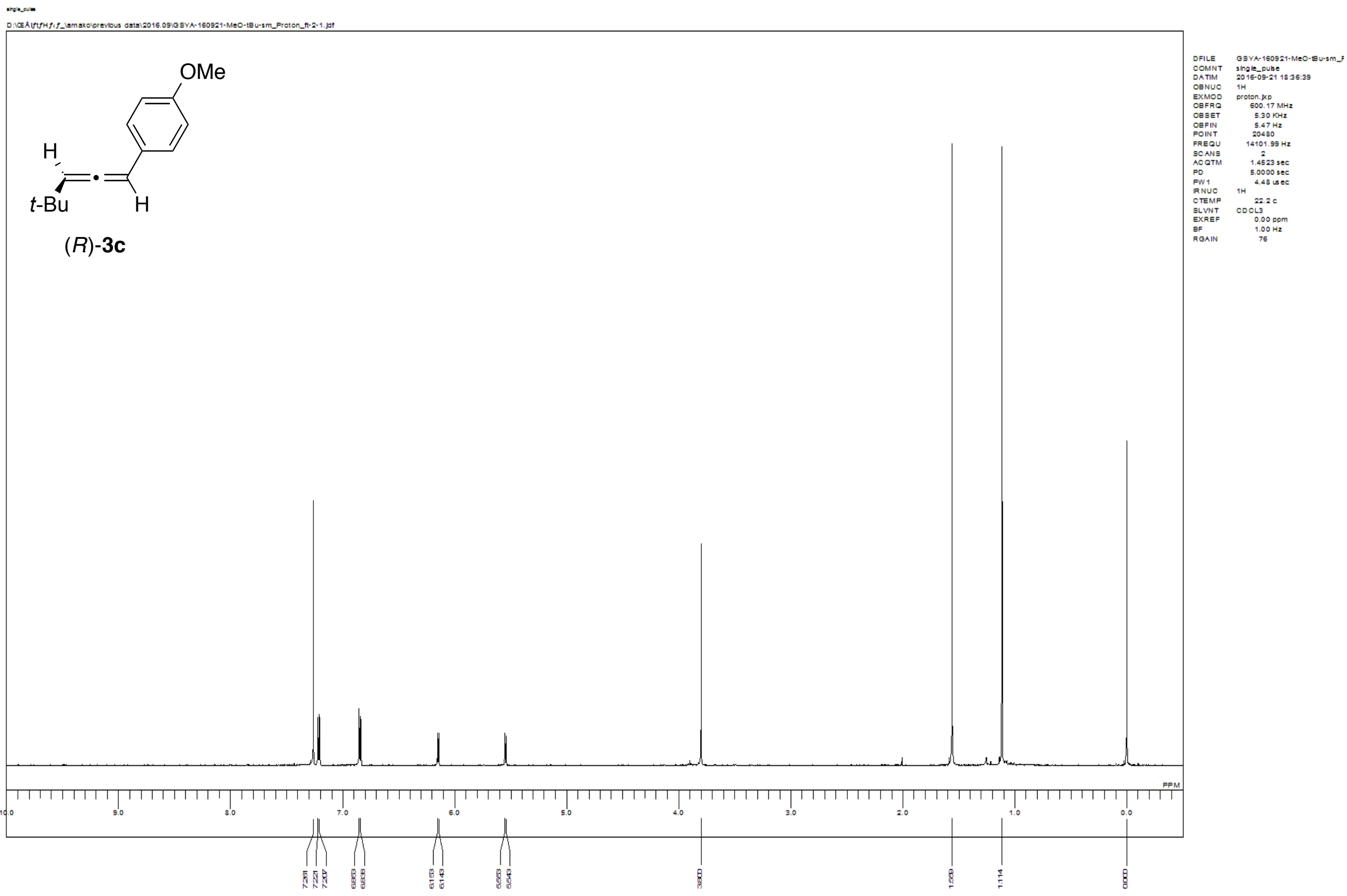


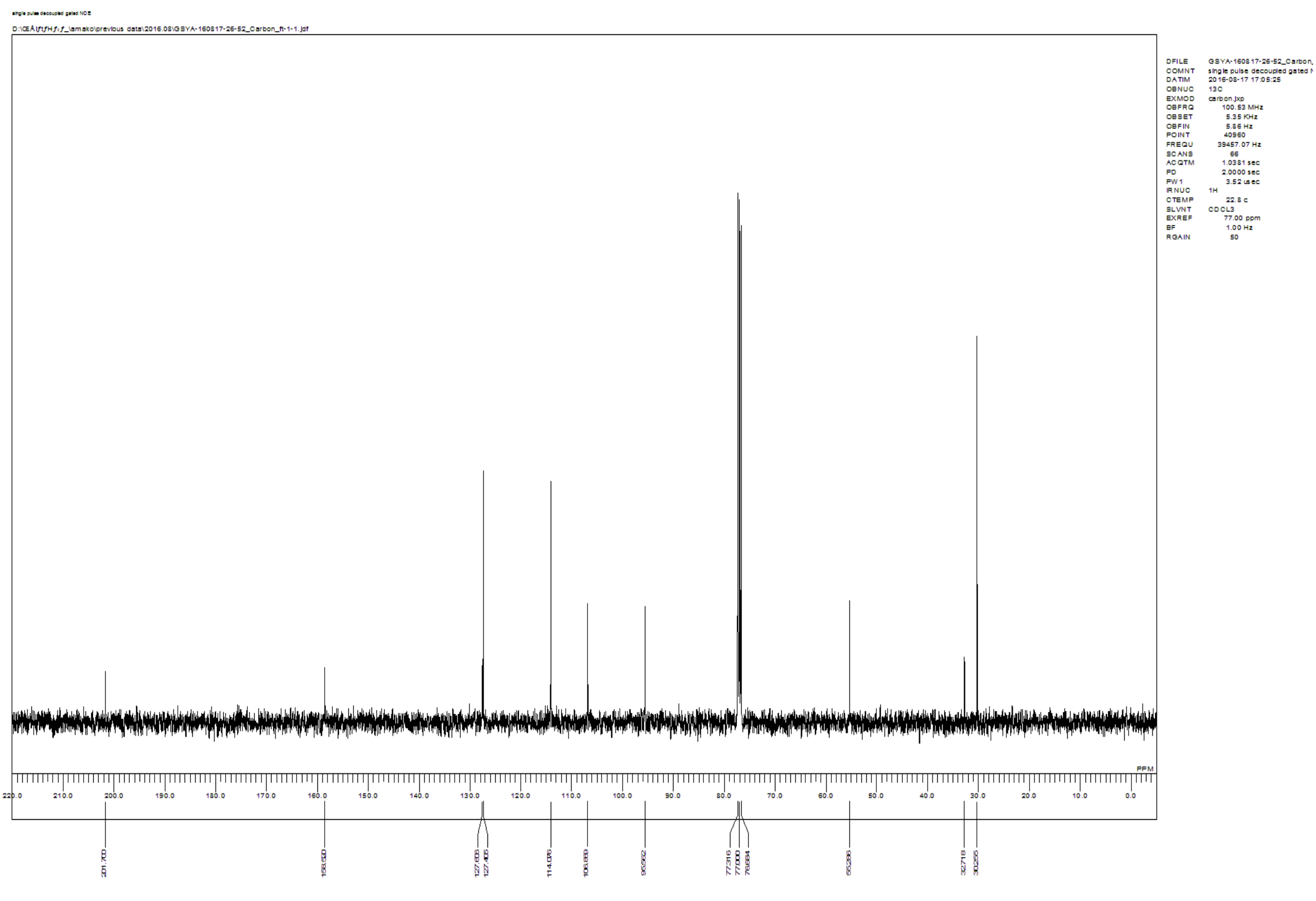
#	tR (min)	面積	面積%	#	tR (min)	面積	面積%
1	6.608	446340	49.869	1	6.558	8132999	82.694
2	8.050	448681	50.131	2	8.107	1702068	17.306

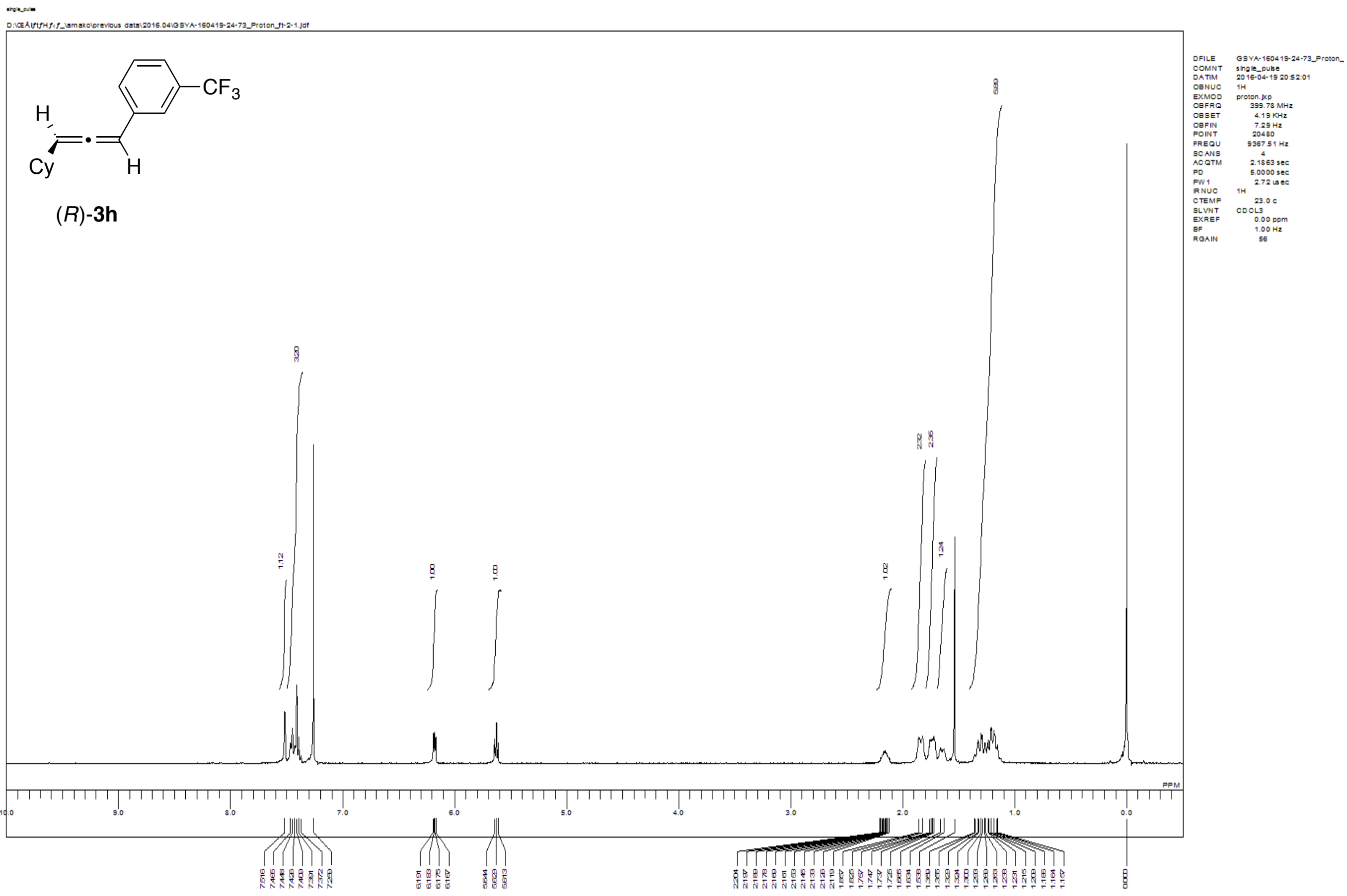
I. 1H and 13C NMR charts for all new compounds

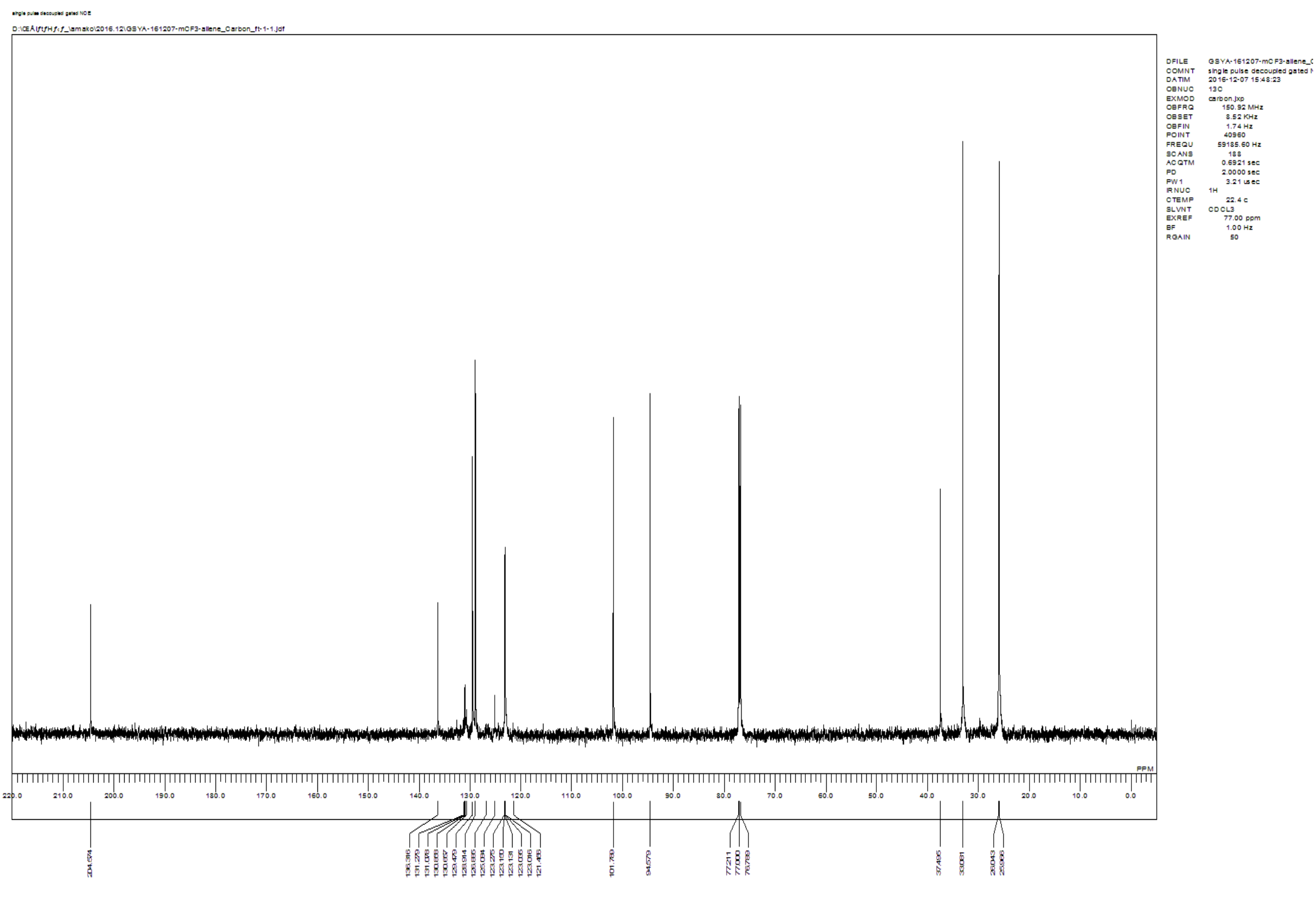


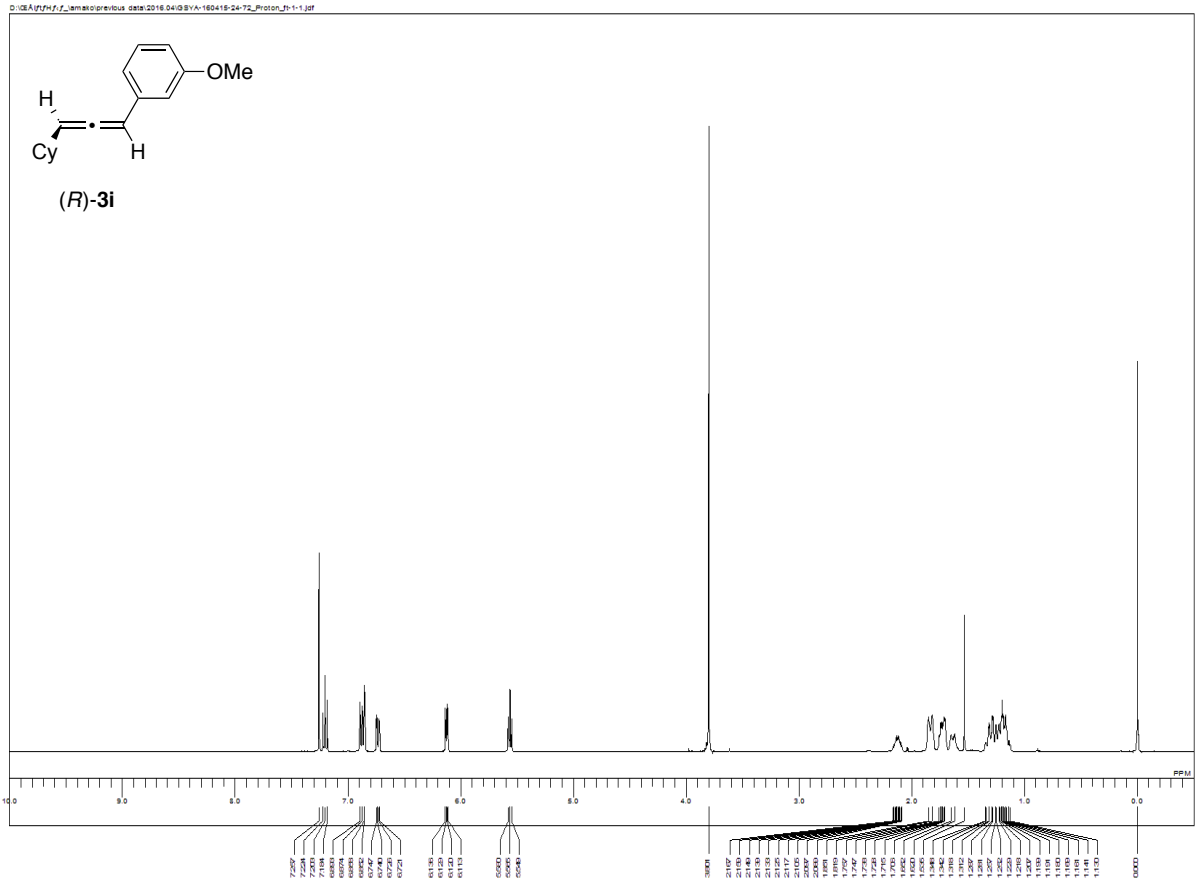


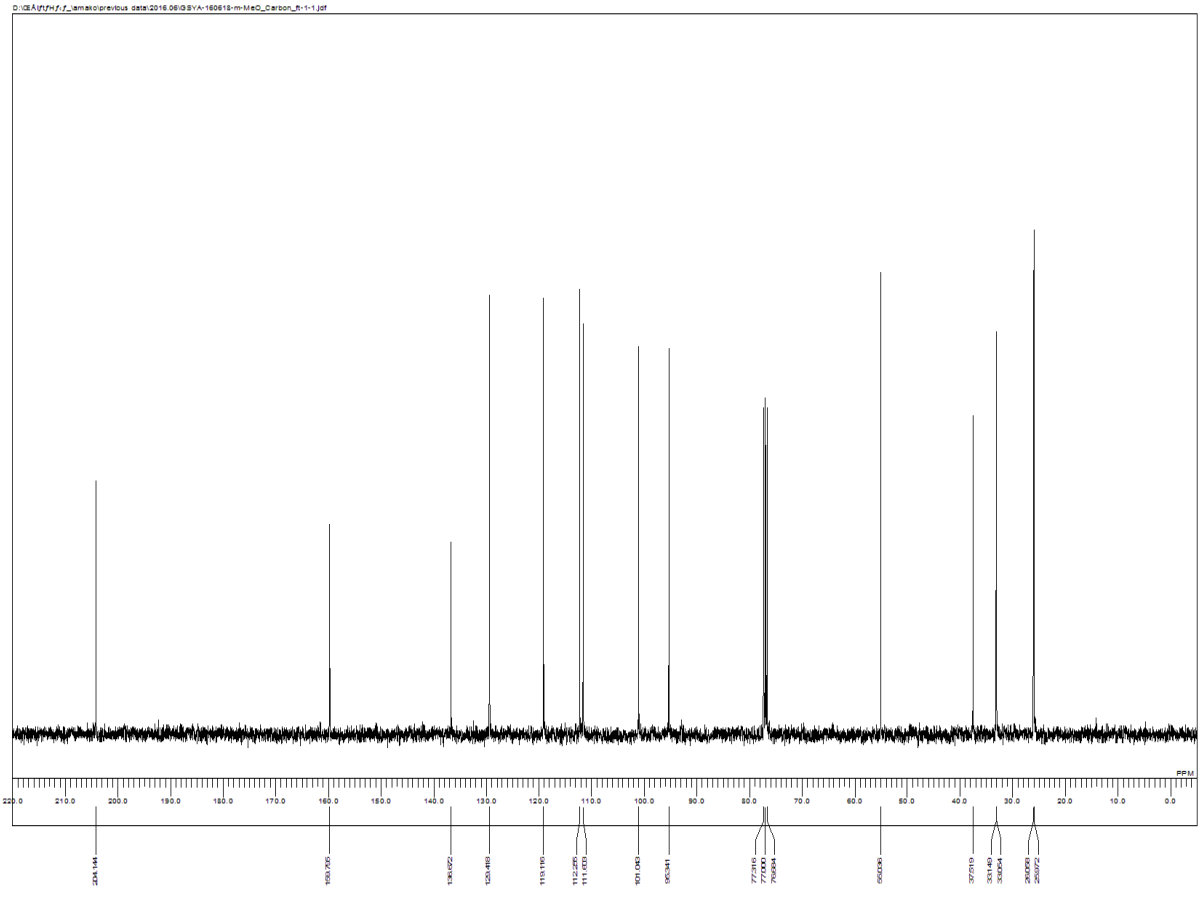

single_pulse
D:\ŒÅ\ƒtƒHƒ‹ƒ_\amako\previous data\2016.09\GSYA-160921-MeO-tBu-sm_Proton_ft-2-1.jdf
OMe
H
t-Bu
H
(R)-3c
DFILE GSYA-160921-MeO-tBu-sm_F
COMNT single_pulse
DATIM 2016-09-21 18:36:39
OBNUC 1H
EXMOD proton.jxp
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 20480
FREQU 14101.99 Hz
SCANS 2
ACQTM 1.4523 sec
PD 5.0000 sec
PW1 4.48 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 76
PPM
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
7.261 7.221 7.207 6.853 6.838 6.153 6.143 5.553 5.543 3.800 1.559 1.114 0.000

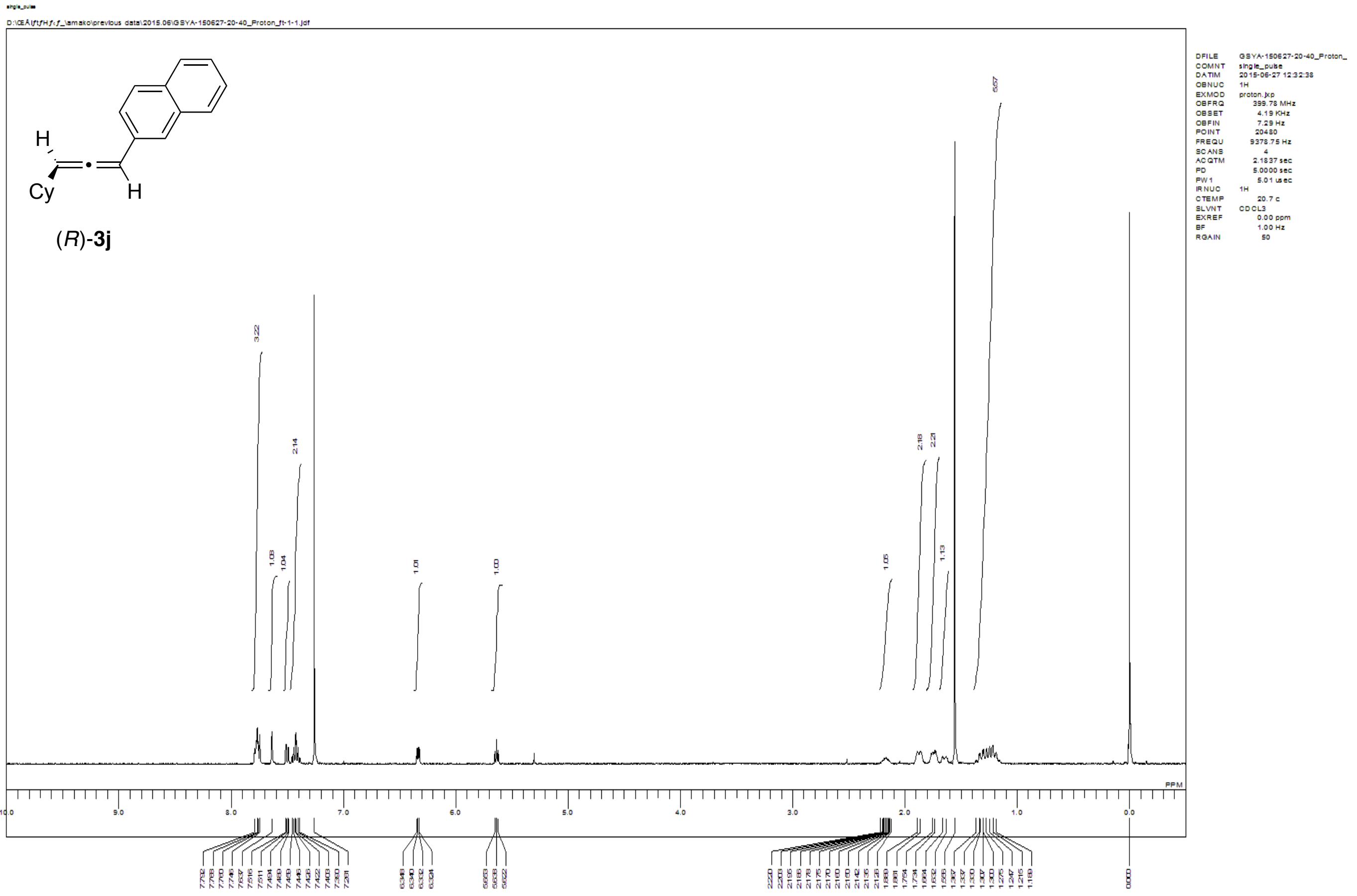

single pulse decoupled gated NOE
D:\ŒÅ\ƒtƒHƒ‹ƒ_\amako\previous data\2016.08\GSYA-160817-26-52_Carbon_ft-1-1.jdf
DFILE GSYA-160817-26-52_Carbon_
COMNT single pulse decoupled gated N
DATIM 2016-08-17 17:05:25
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39457.07 Hz
SCANS 66
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 22.8 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50
PPM
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0.0
201.700 158.520 127.606 127.405 114.076 106.889 95.562 77.316 77.000 76.684 55.286 32.718 30.255

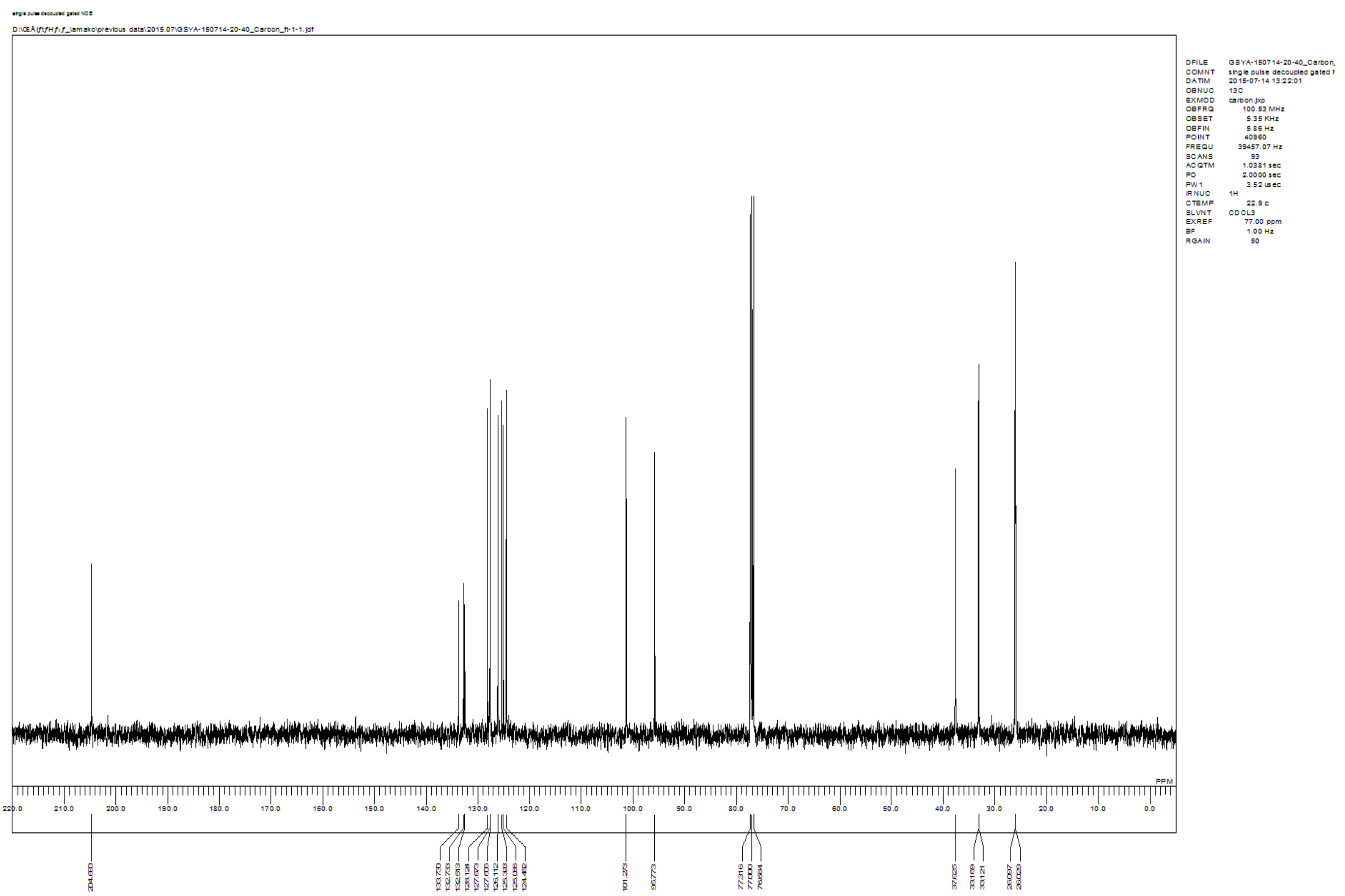

H
CF3
Cy
H
(R)-3h

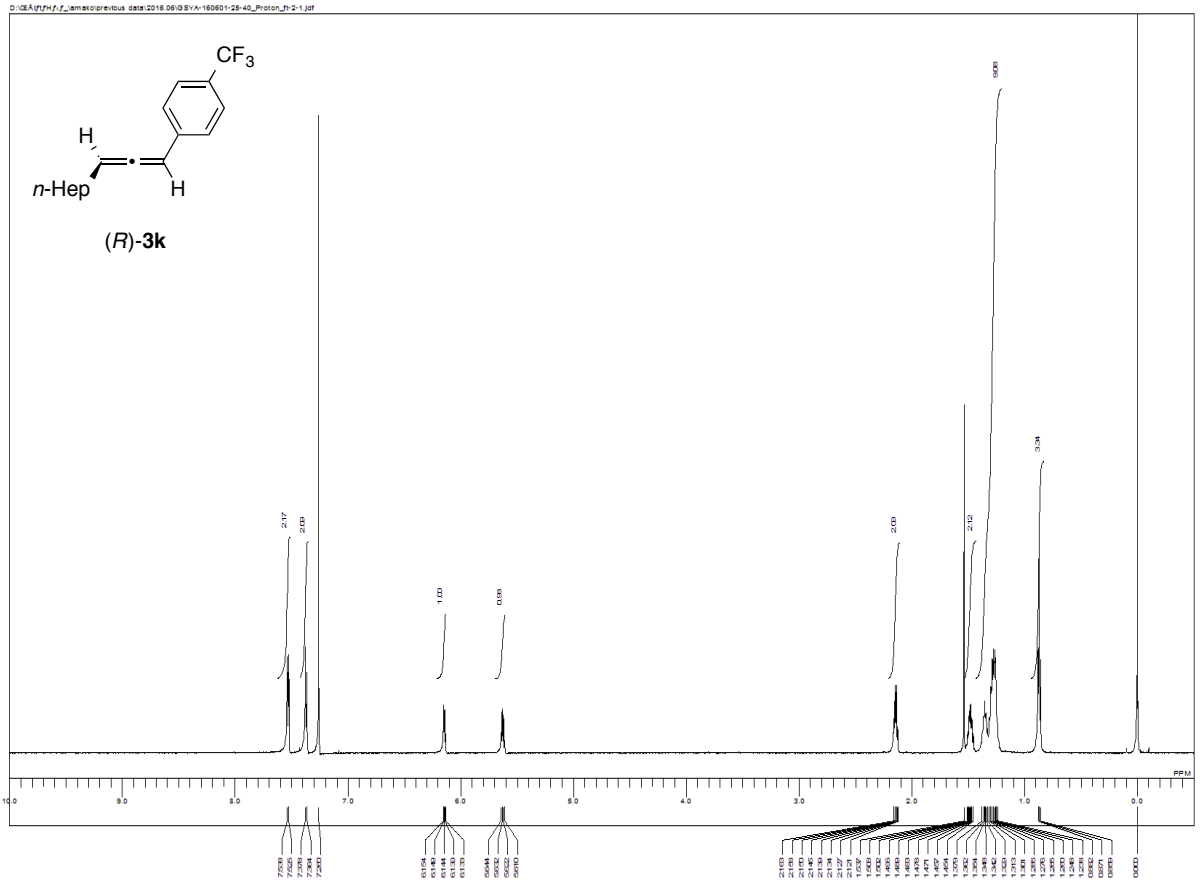


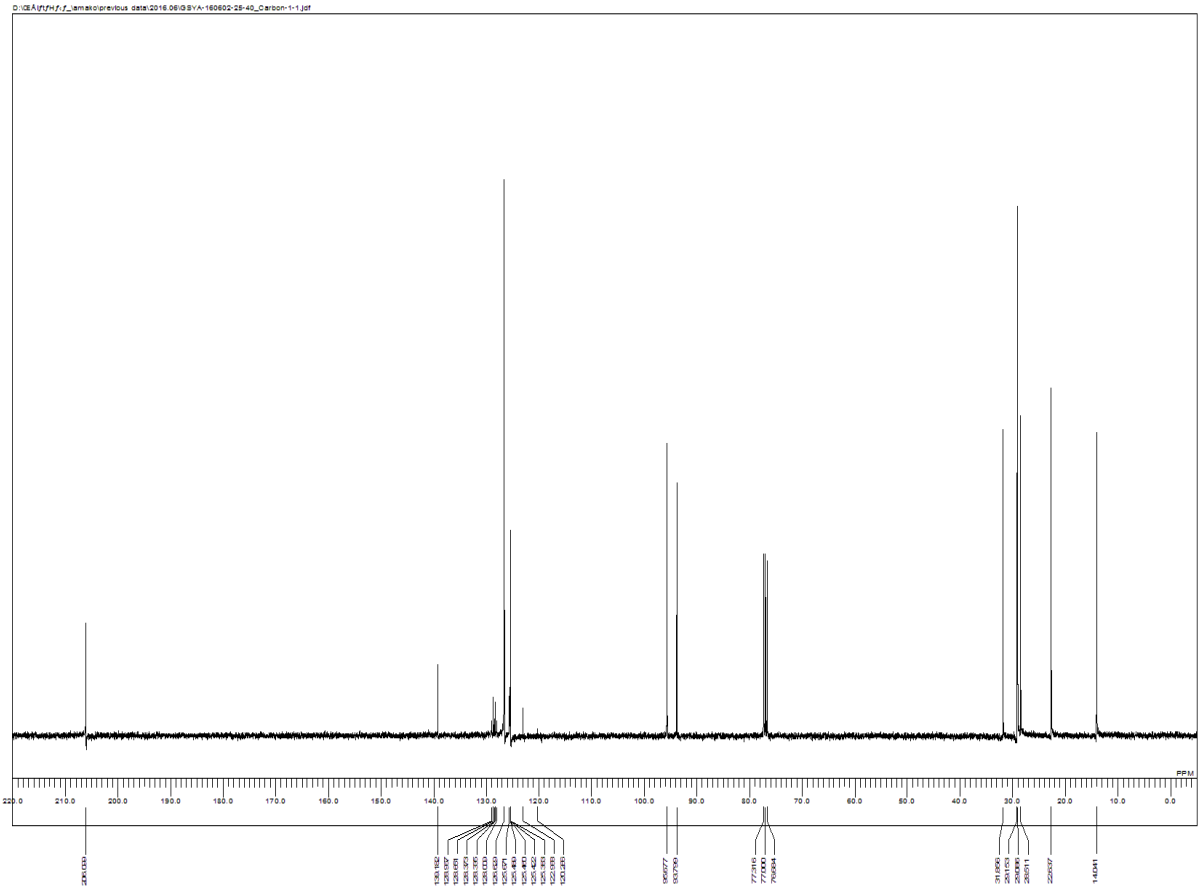

OMe
H
Cy
H
(R)-3i
PPM

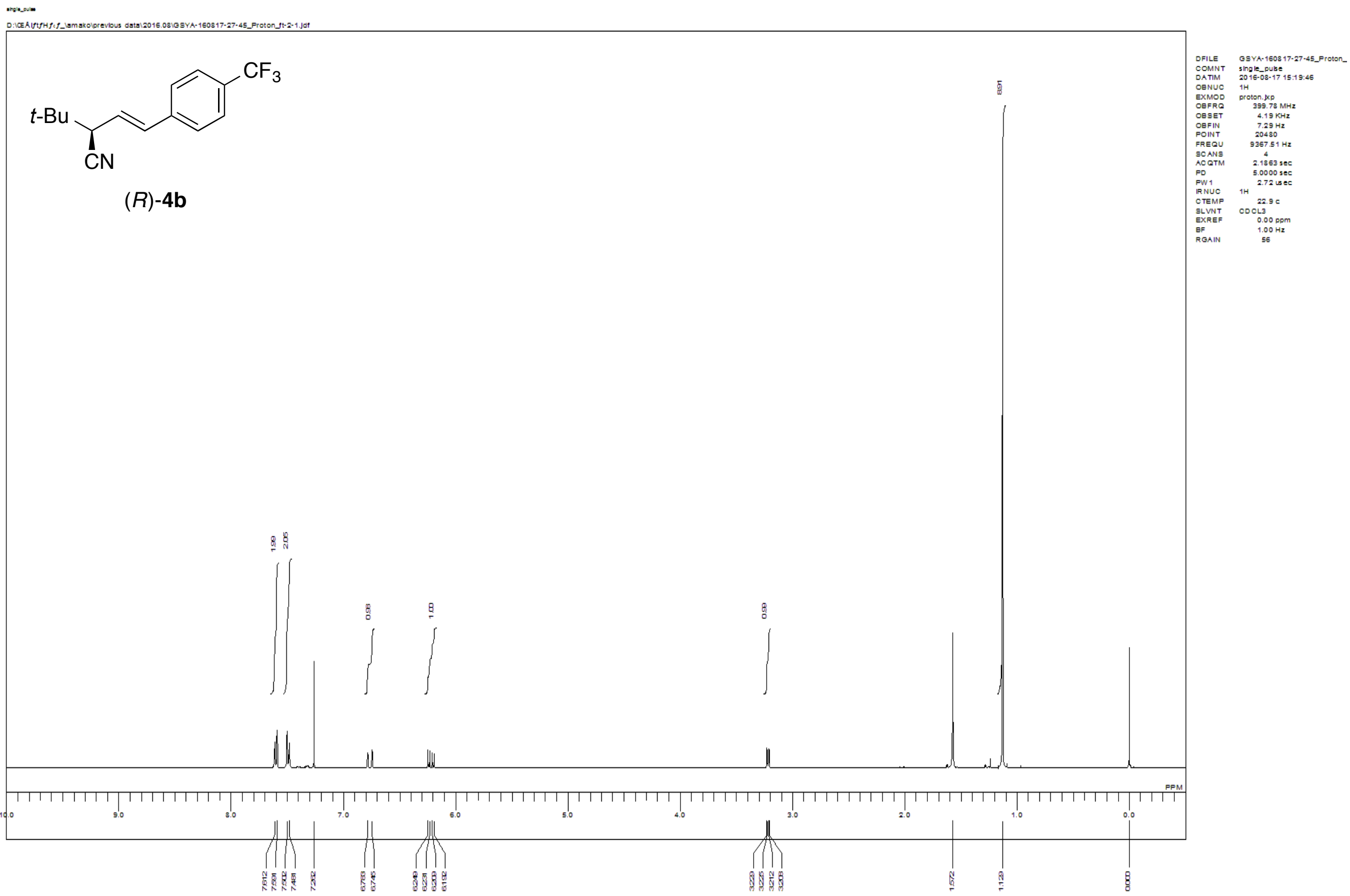

PPM


H
Cy
H
(*R*)-**3j**
PPM

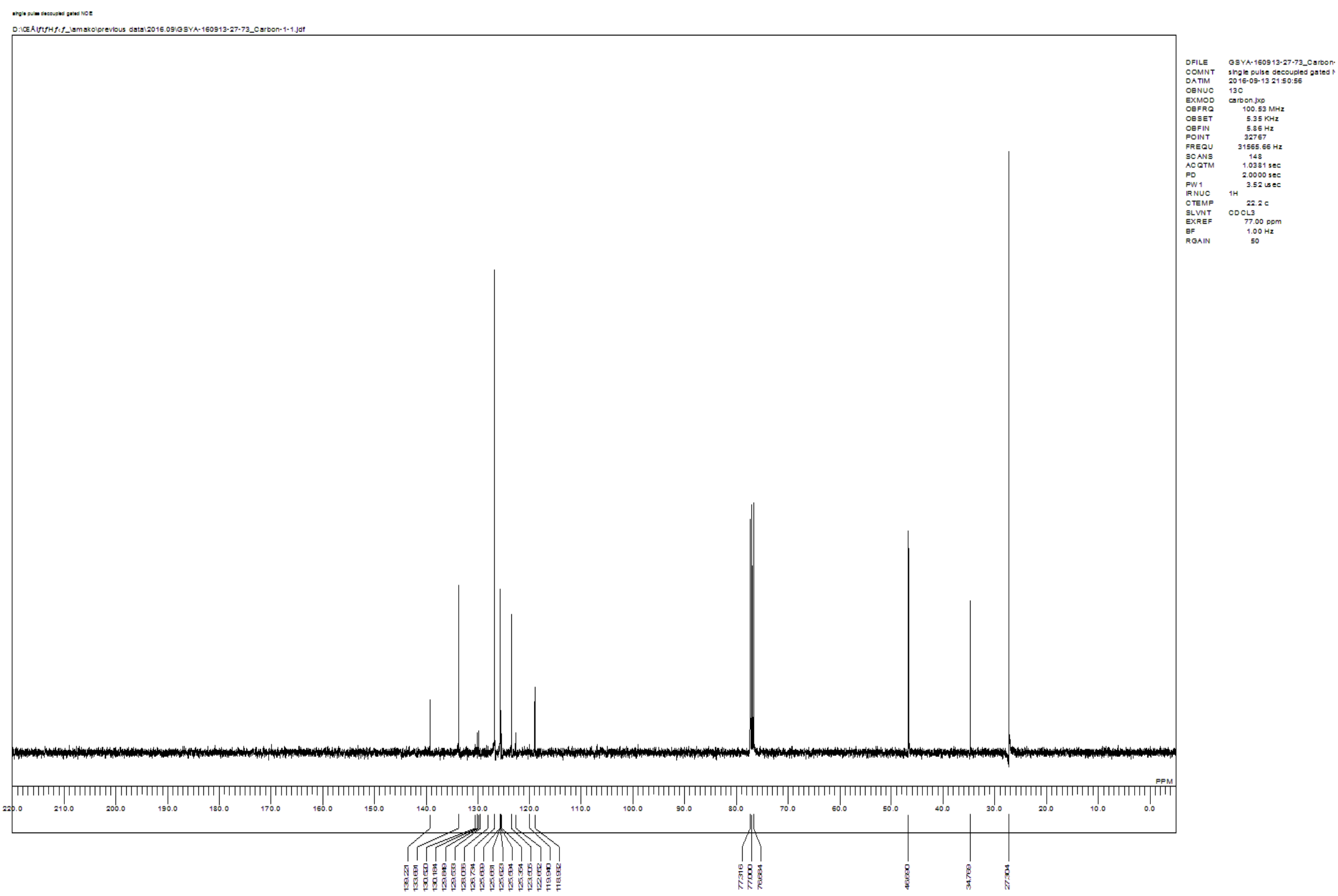

PPM


CF3
H
n-Hep
H
(R)-3k
2.17
2.09
1.03
0.98
2.00
2.12
9.08
3.34
PPM

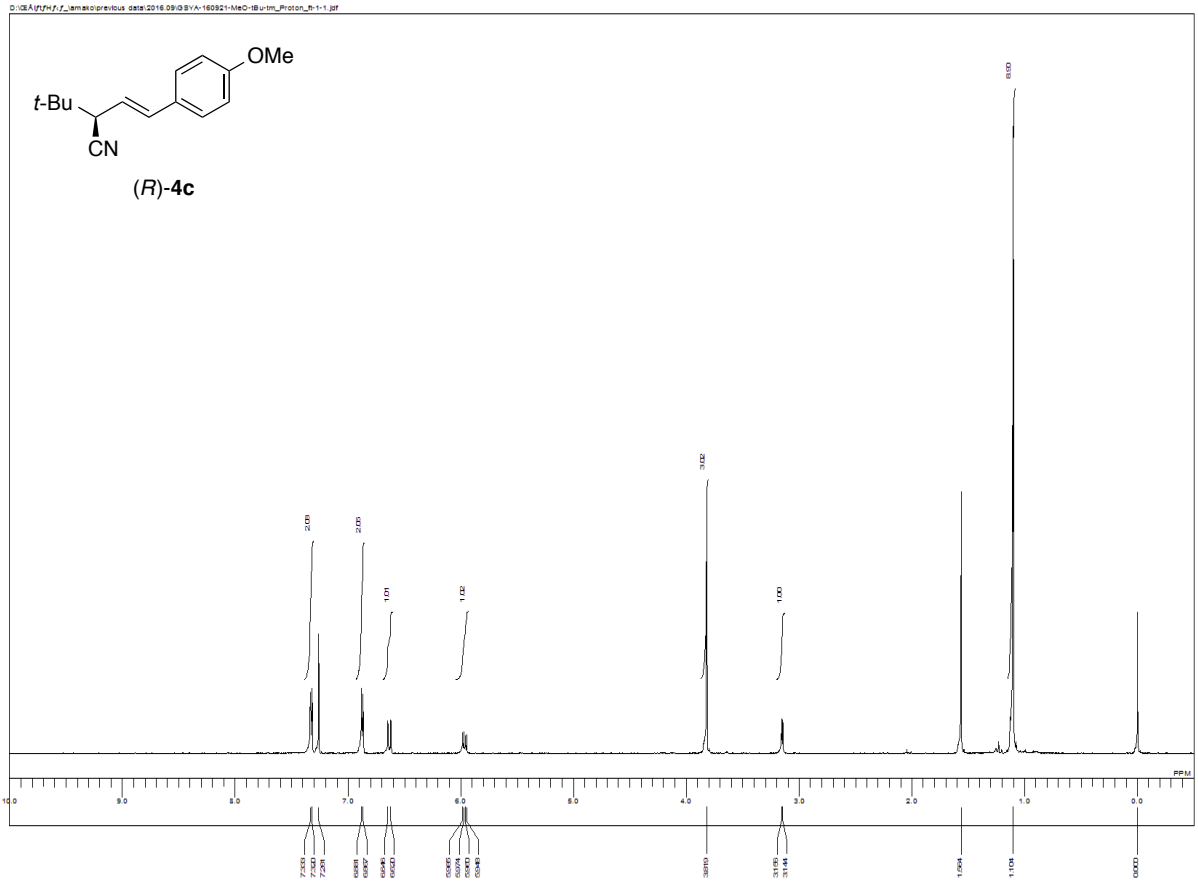

PPM

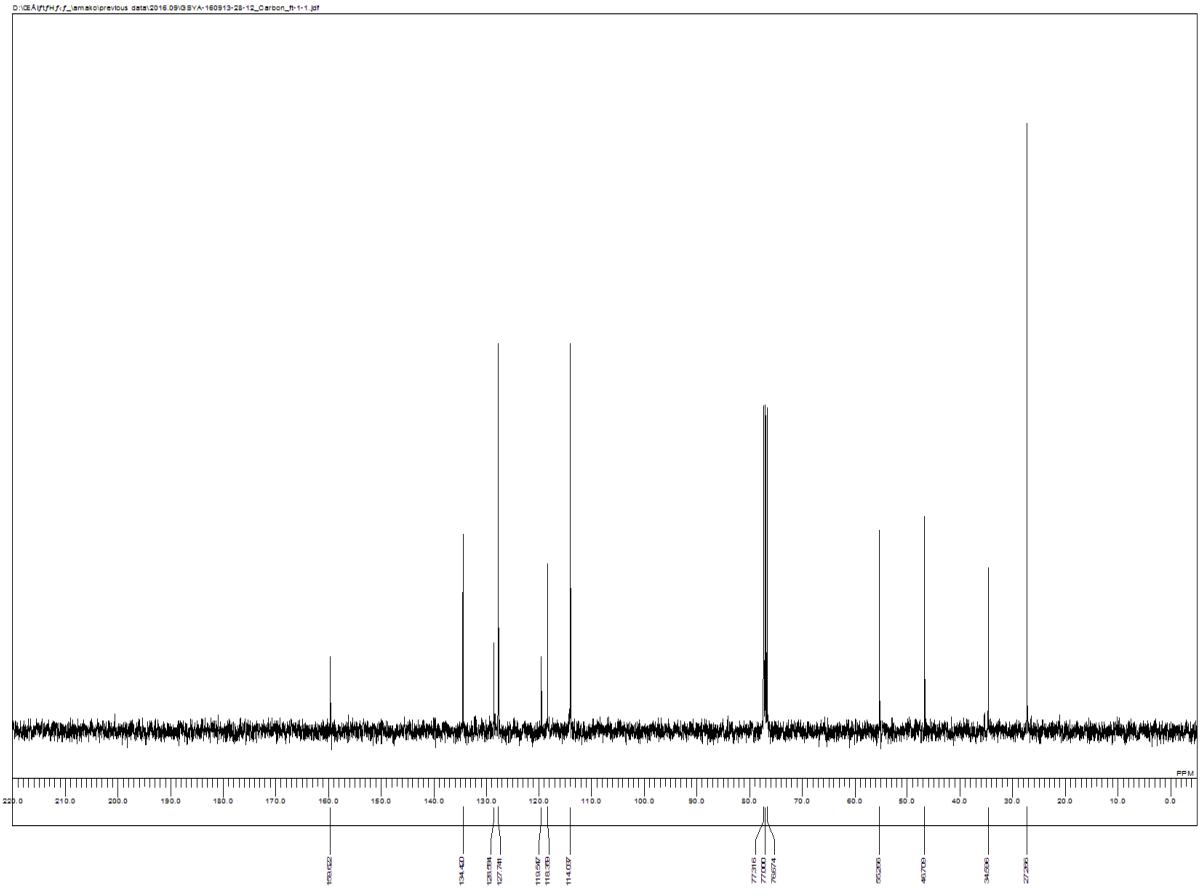


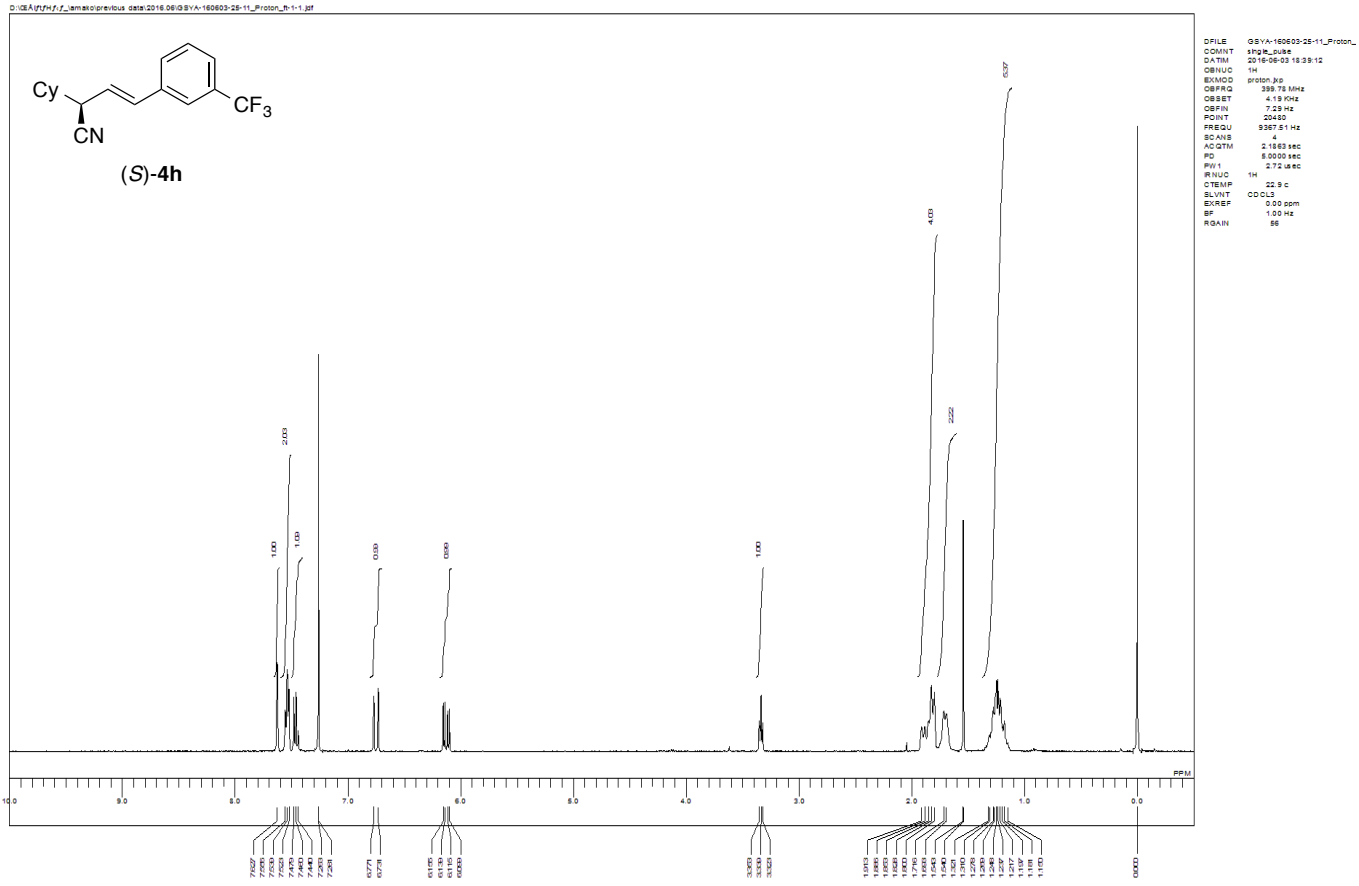
t-Bu
CN
CF3
(R)-4b
DFILE GSYA-160817-27-45_Proton_
COMNT single_pulse
DATIM 2016-08-17 15:19:46
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9367.51 Hz
SCANS 4
ACQTM 2.1863 sec
PD 5.0000 sec
PW1 2.72 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 56
PPM

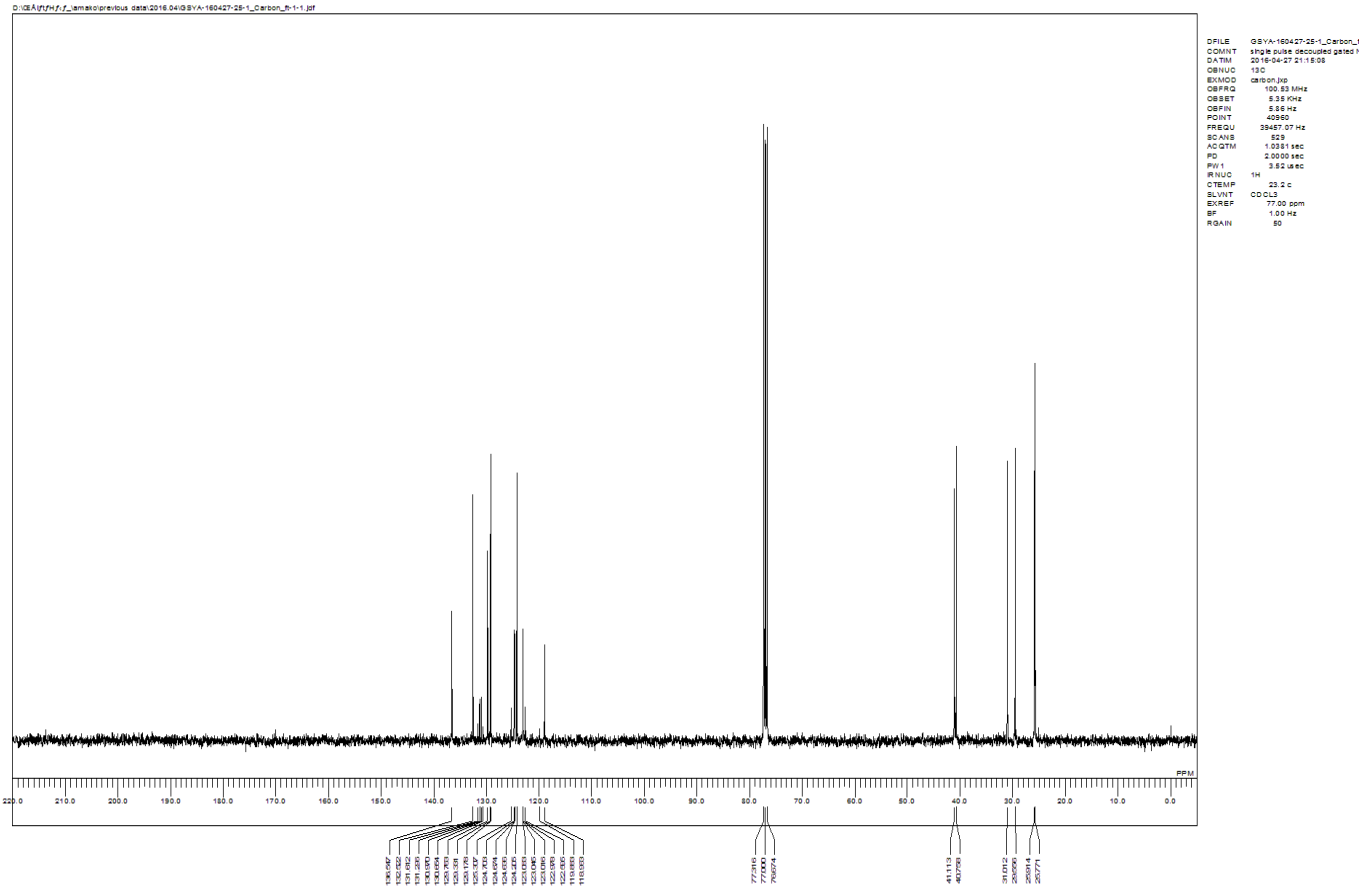


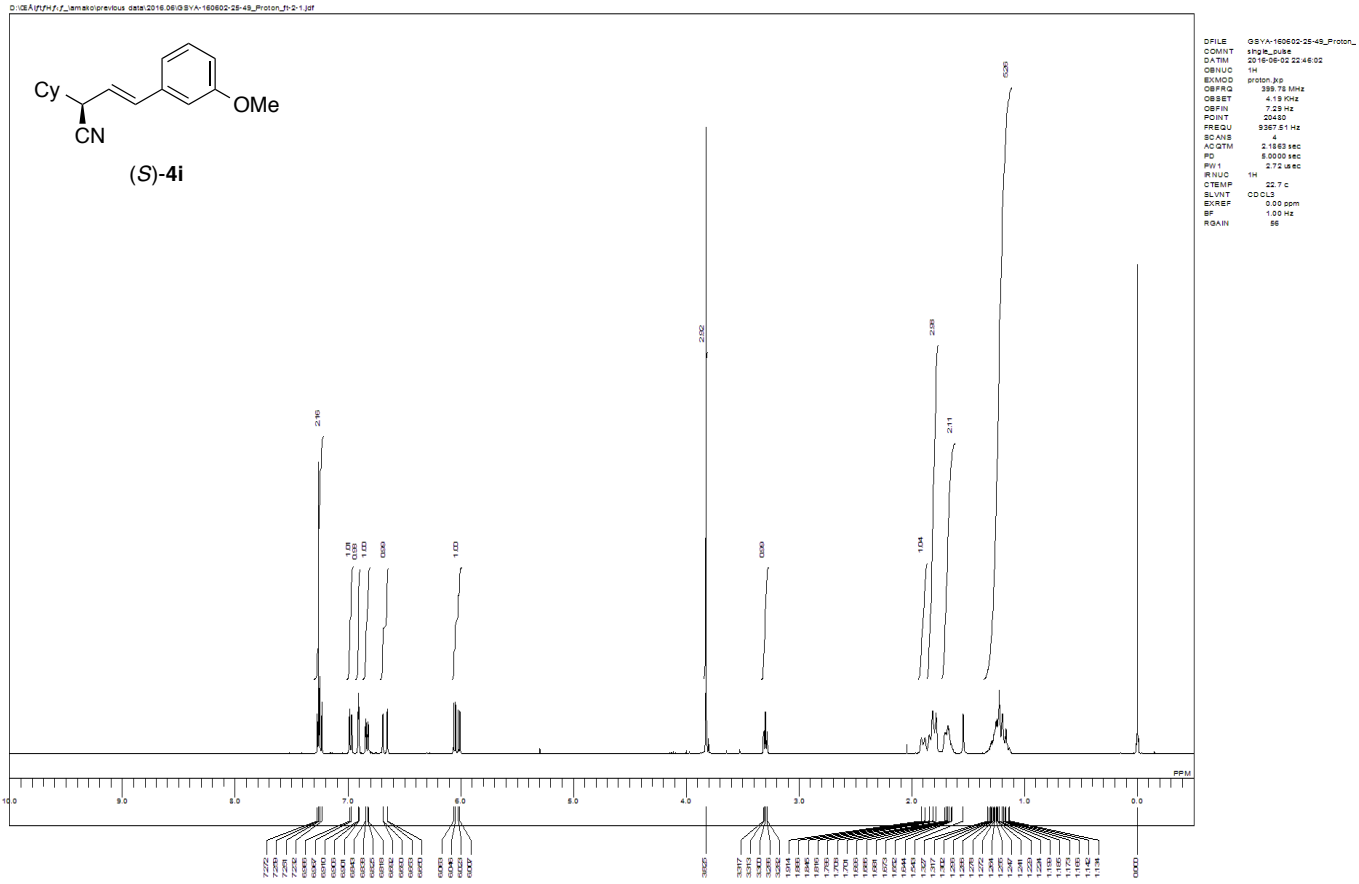
DFILE GSYA-160913-27-73_Carbon-
COMNT single pulse decoupled gated
DATIM 2016-09-13 21:50:56
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 32767
FREQU 31565.66 Hz
SCANS 148
ACQTM 1.0381 sec
PD 2.0000 sec
PW1 3.52 usec
IRNUC 1H
CTEMP 22.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50
PPM

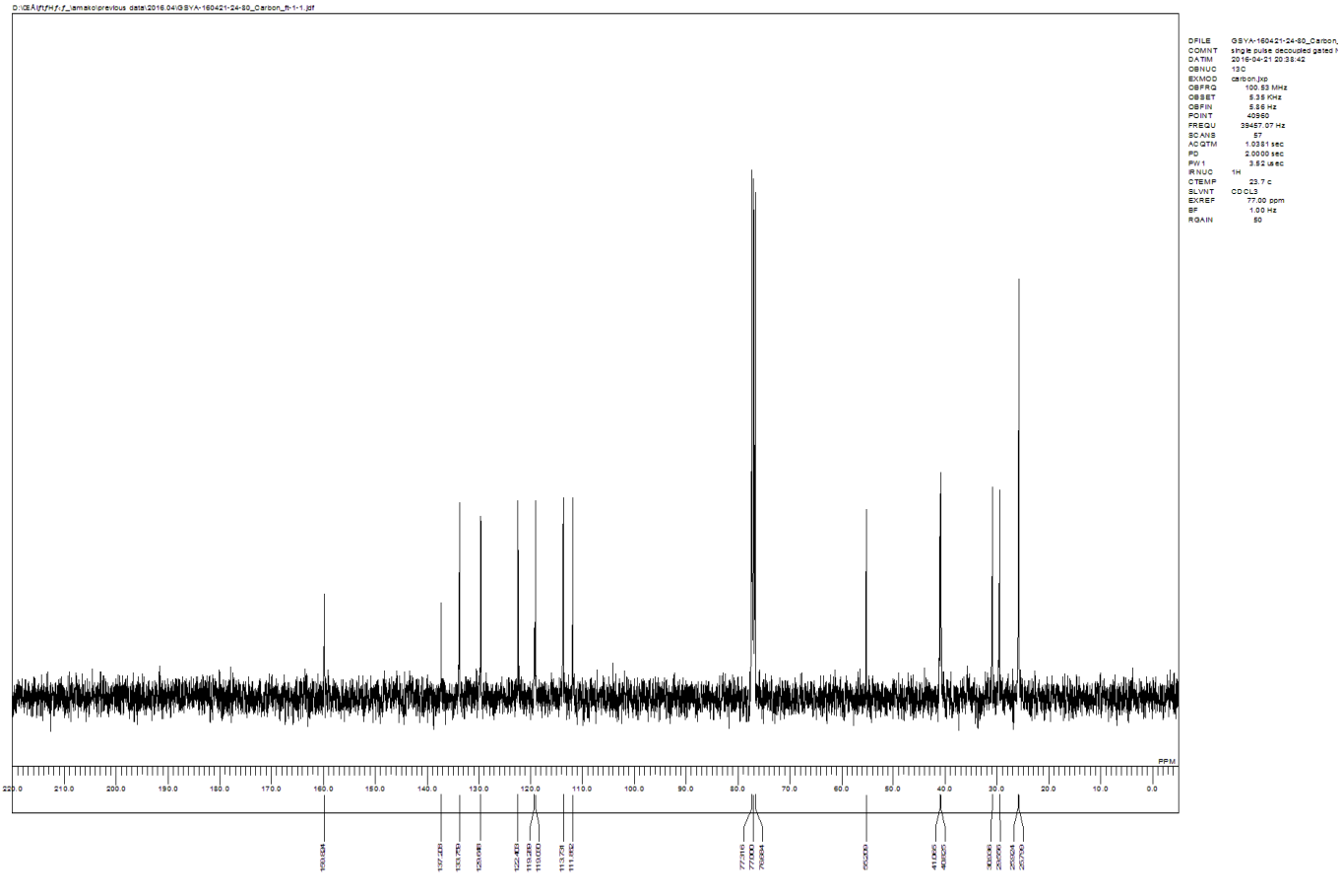

OMe
t-Bu
CN
(R)-4c
PPM

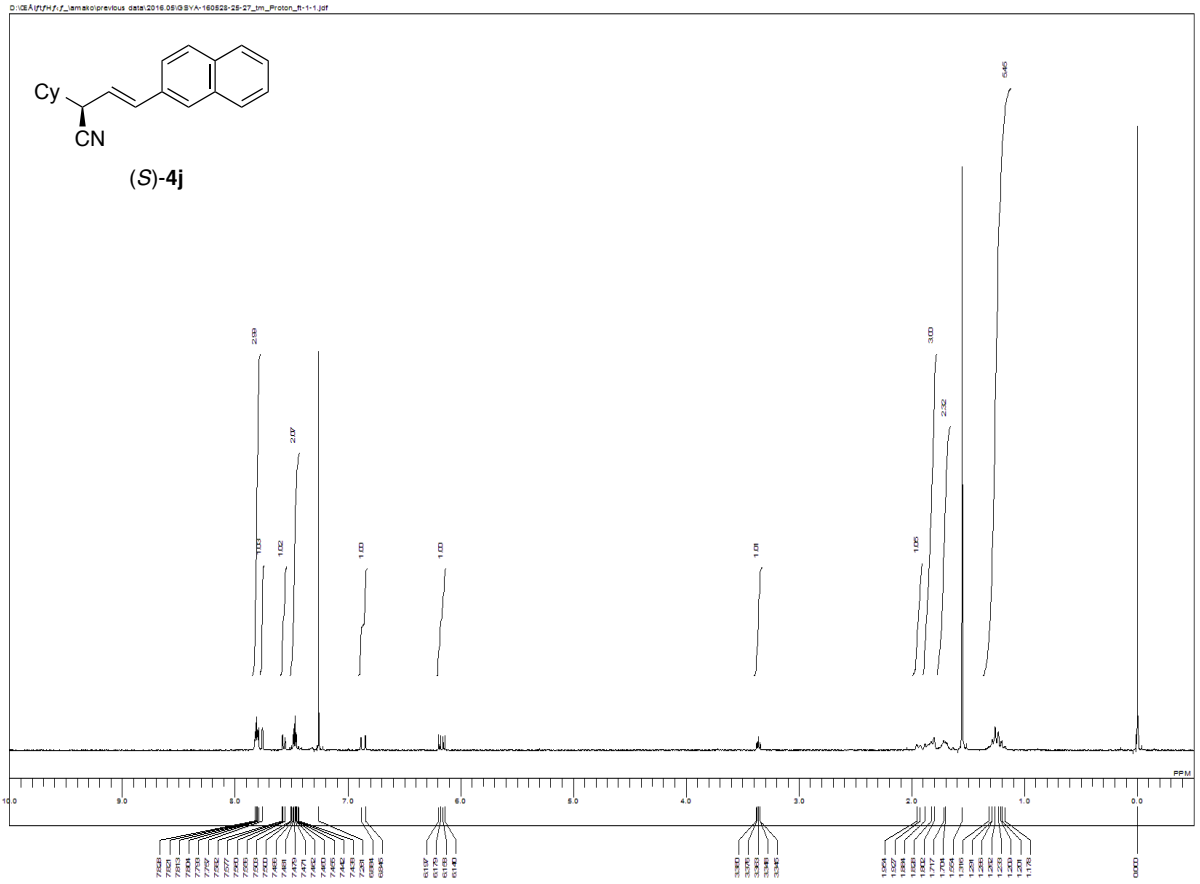

PPM

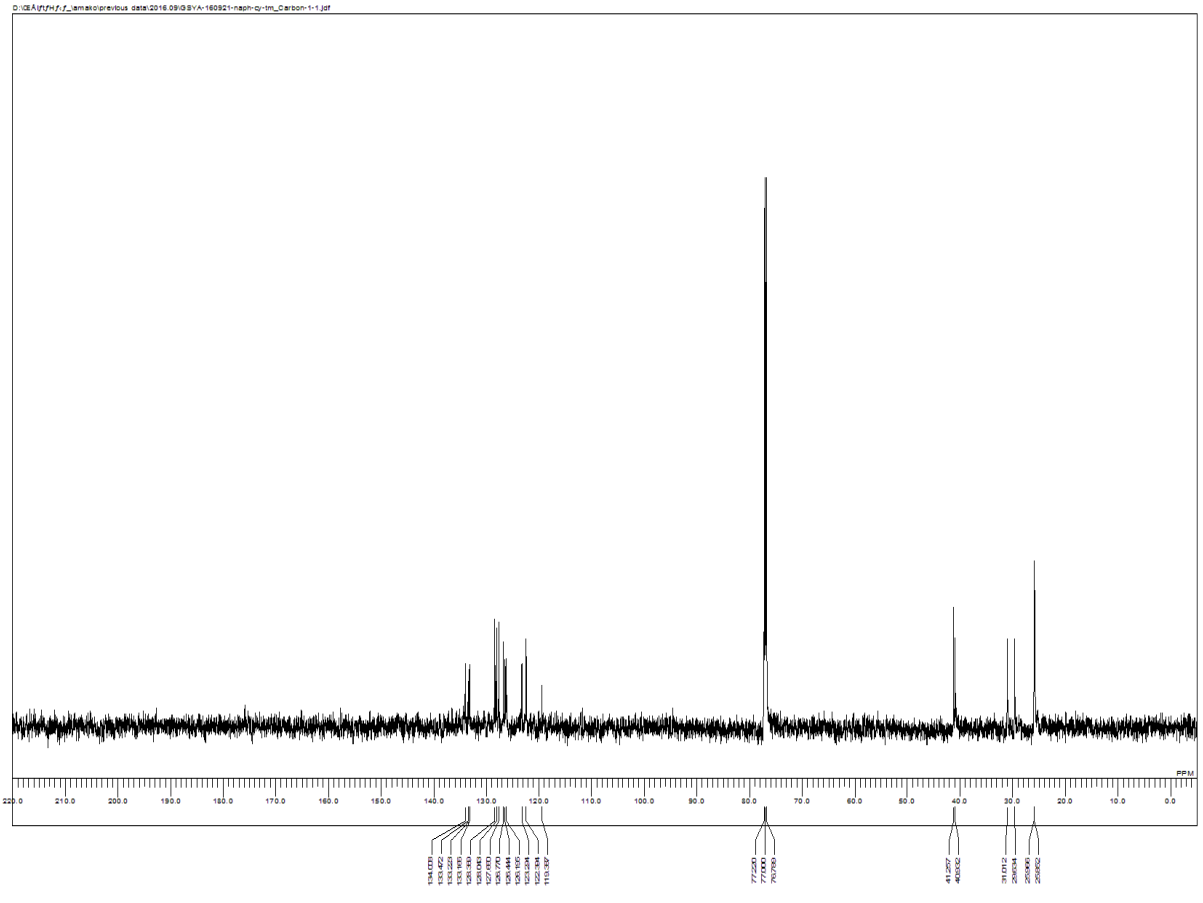

single_pulse
Cy
CN
CF3
(S)-4h
DFILE GSYA-160603-25-11_Proton_
COMNT single_pulse
DATIM 2016-06-03 18:39:12
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9367.51 Hz
SCANS 4
ACQTM 2.1863 sec
PD 8.0000 sec
PW1 2.72 usec
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 56
PPM


single pulse decoupled gated NOE
DFILE GSYA-160427-25-1_Carbon_
COMNT single pulse decoupled gated N
DATIM 2016-04-27 21:15:08
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 100.63 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 40960
FREQU 39457.07 Hz
SCANS 629
ACQTM 1.0351 sec
PD 2.0000 sec
PW1 3.62 usec
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50
PPM


Cy
CN
OMe
(S)-4i

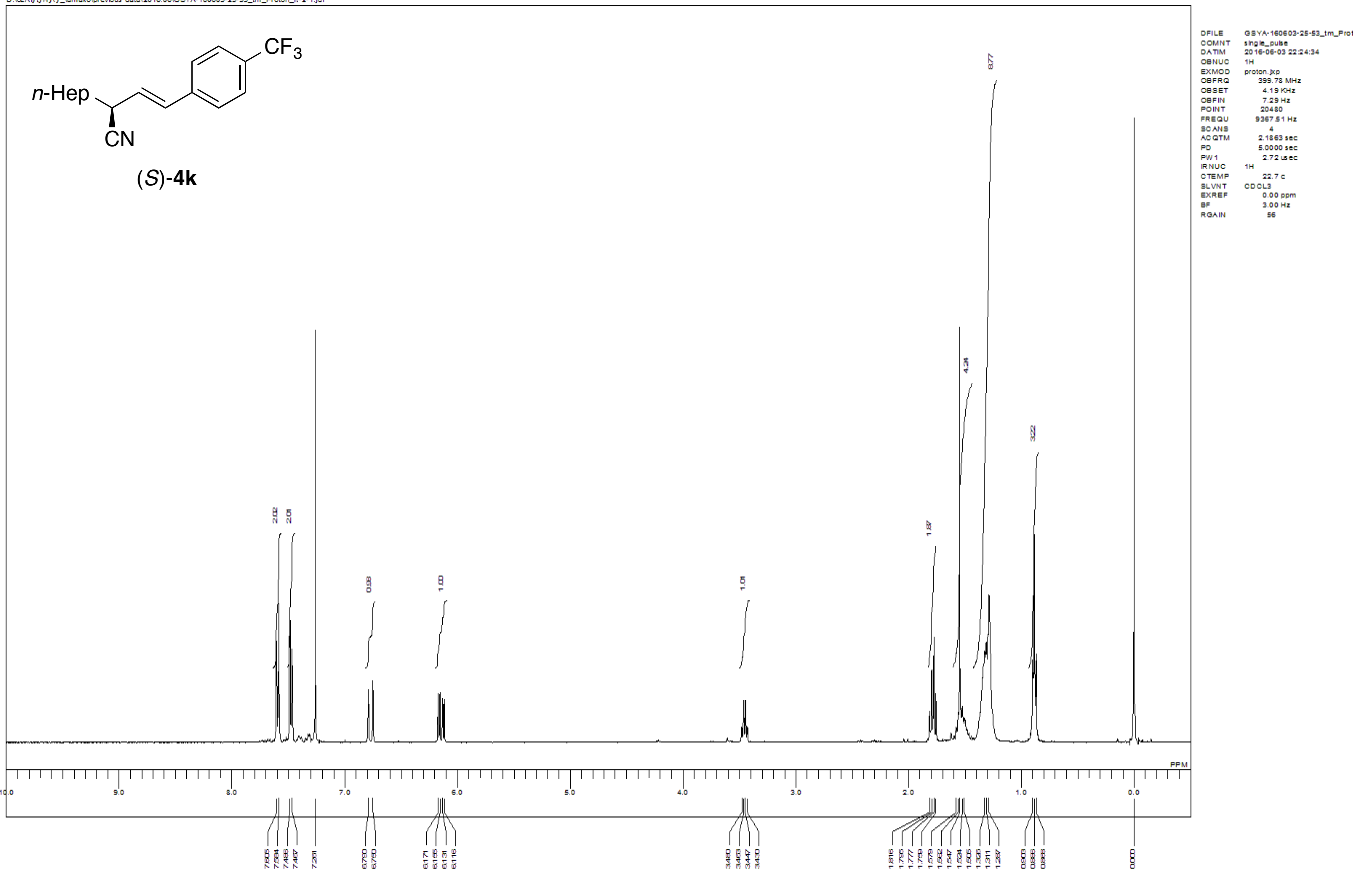



Cy
CN
(S)-4j



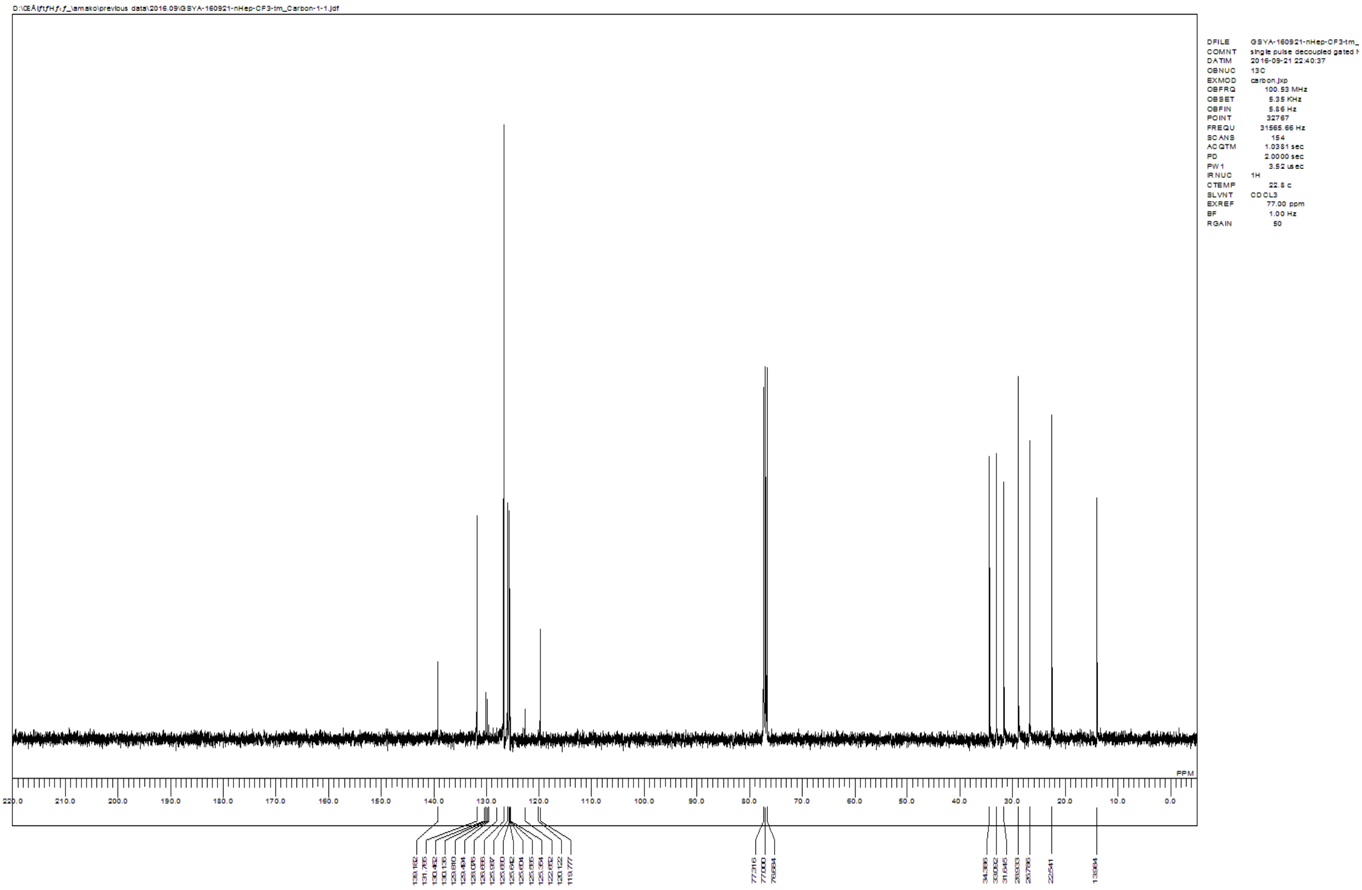
single_pulse

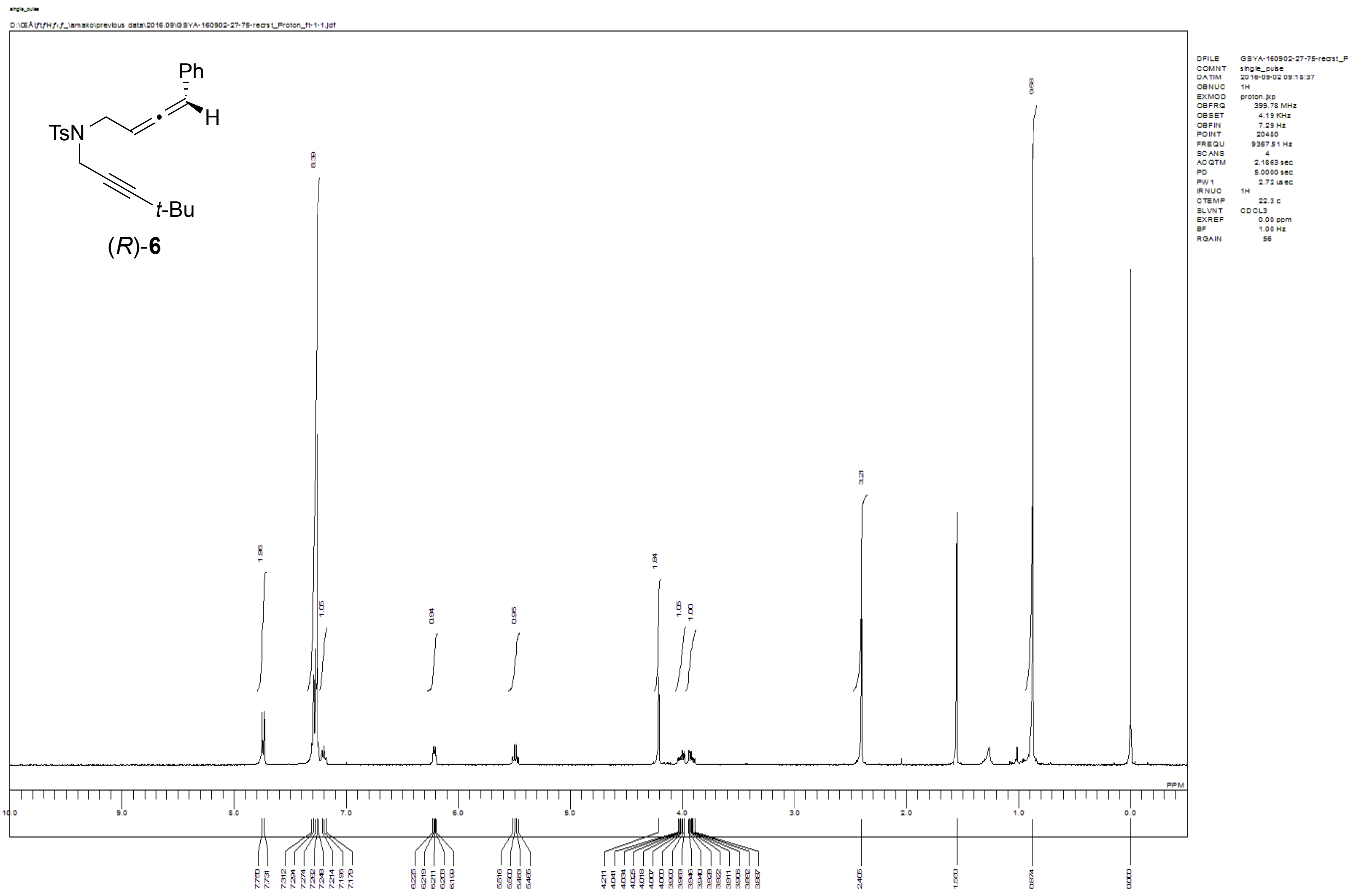
D:\ŒÅlƒtƒHƒ‹ƒ_\amako\previous data\2016.06\GSYA-160603-25-53_tm_Proton_ft-2-1.jdf

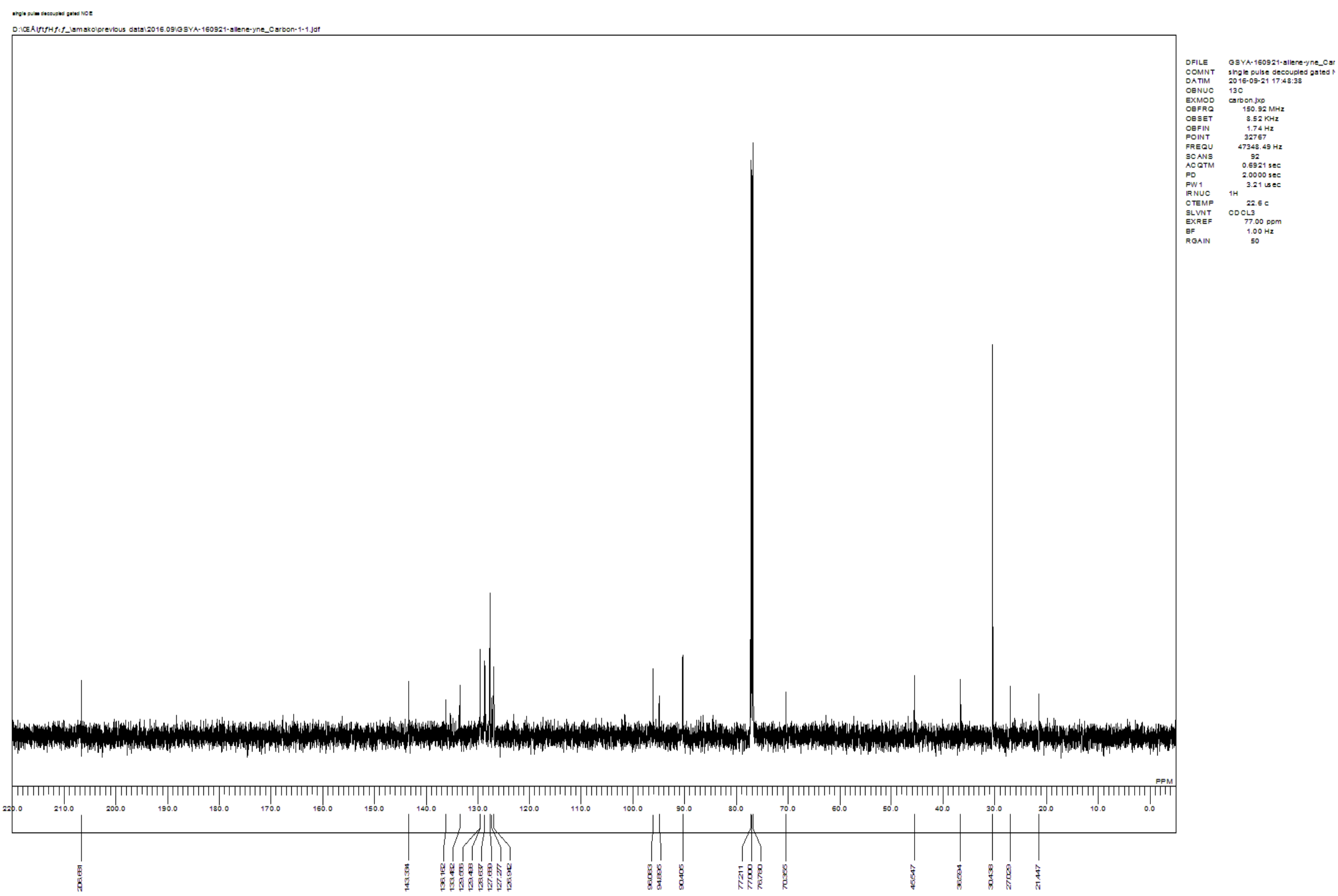


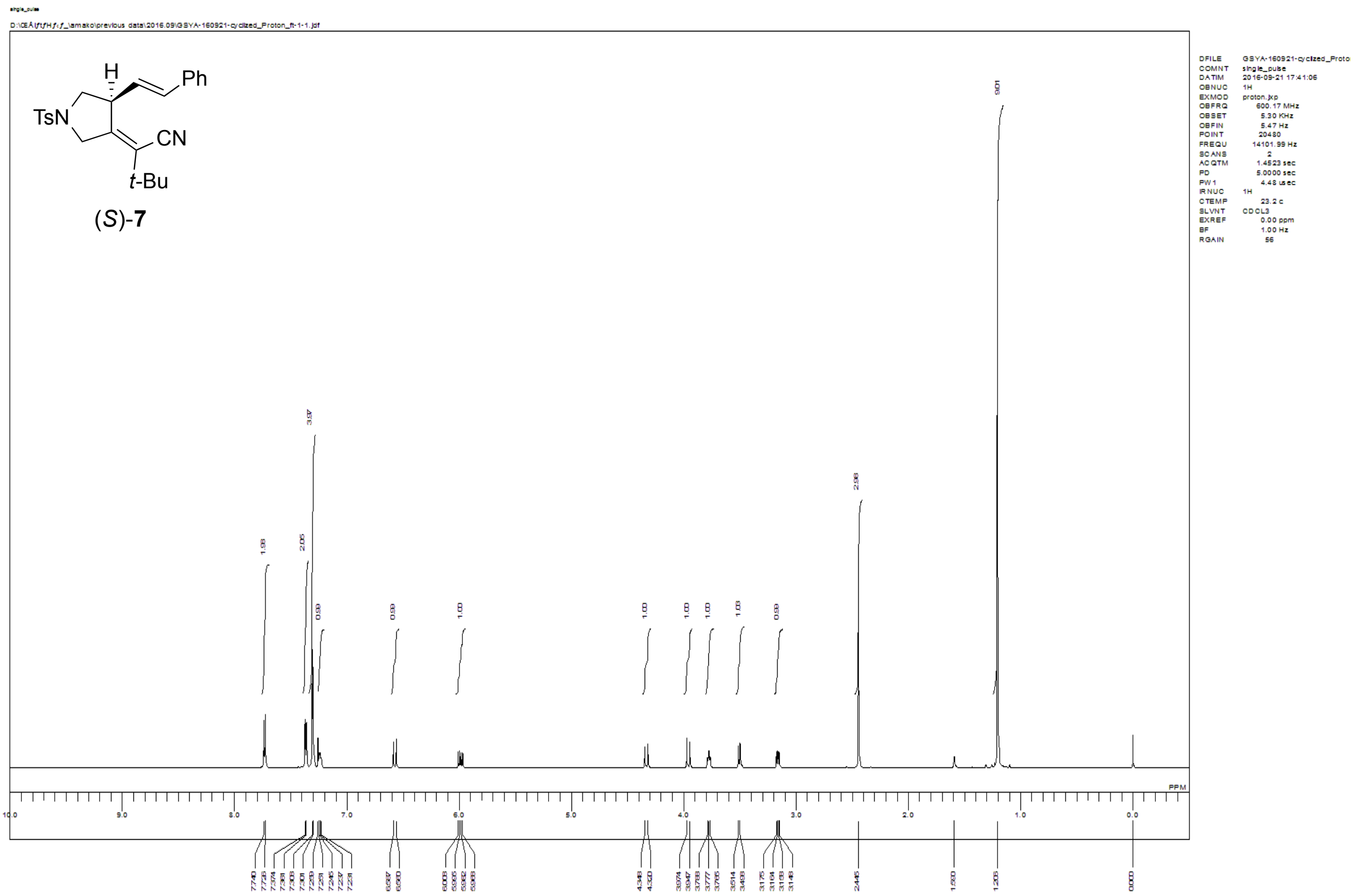
single pulse decoupled gated NOE

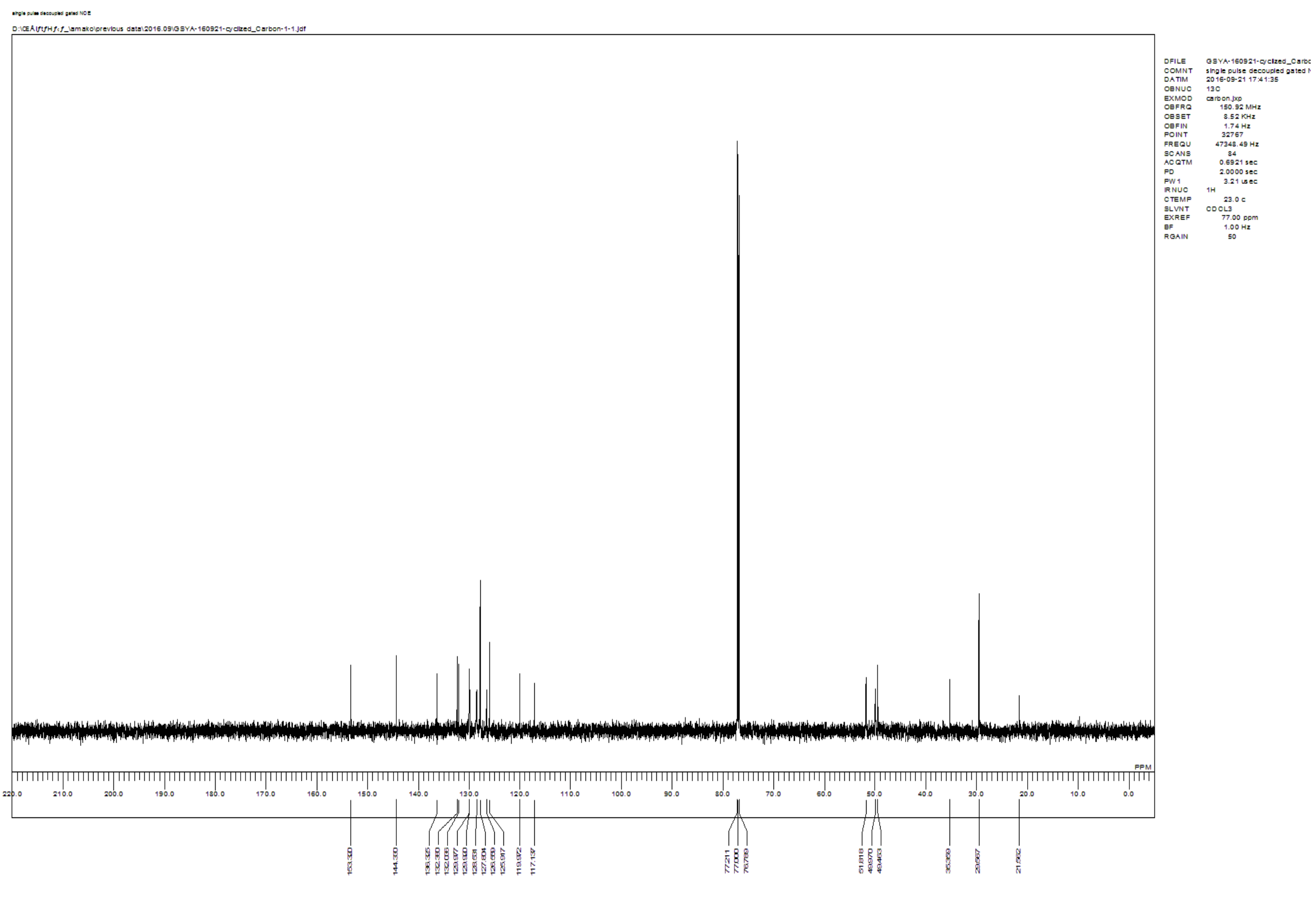
D:\ŒÅlƒtƒHƒ‹ƒ_\amako\previous data\2016.09\GSYA-160921-nHep-CF3-tm_Carbon-1-1.jdf




Ph
TsN
H
t-Bu
(R)-6

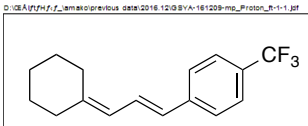



single_pulse
TsN
H
Ph
CN
t-Bu
(S)-7
DFILE GSYA-160921-cyclized_Proto
COMNT single_pulse
DATIM 2016-09-21 17:41:06
OBNUC 1H
EXMOD proton.jxp
OBFRQ 600.17 MHz
OBSET 5.30 KHz
OBFIN 5.47 Hz
POINT 20480
FREQU 14101.99 Hz
SCANS 2
ACQTM 1.4523 sec
PD 5.0000 sec
PW1 4.48 usec
IRNUC 1H
CTEMP 23.2 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 56
PPM


DFILE GSYA-160921-cyclized_Carbo
COMNT single pulse decoupled gated N
DATIM 2016-09-21 17:41:35
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 32767
FREQU 47348.49 Hz
SCANS 84
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.21 usec
IRNUC 1H
CTEMP 23.0 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.00 Hz
RGAIN 50
PPM

single_pulse

D:\CEA\IT\HY_lamako\previous data\2016.12\GSYA-161209-mp_Proton_ft-1-1.jdf

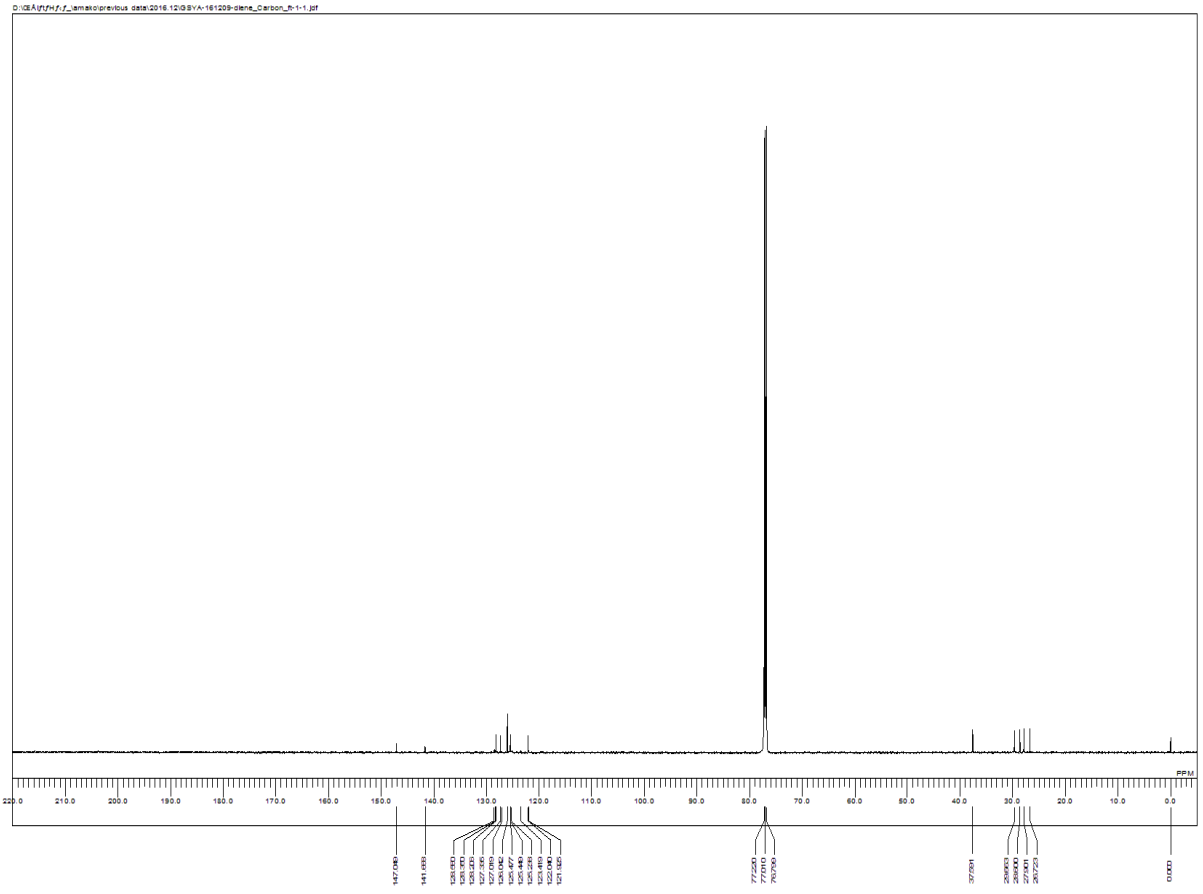


8

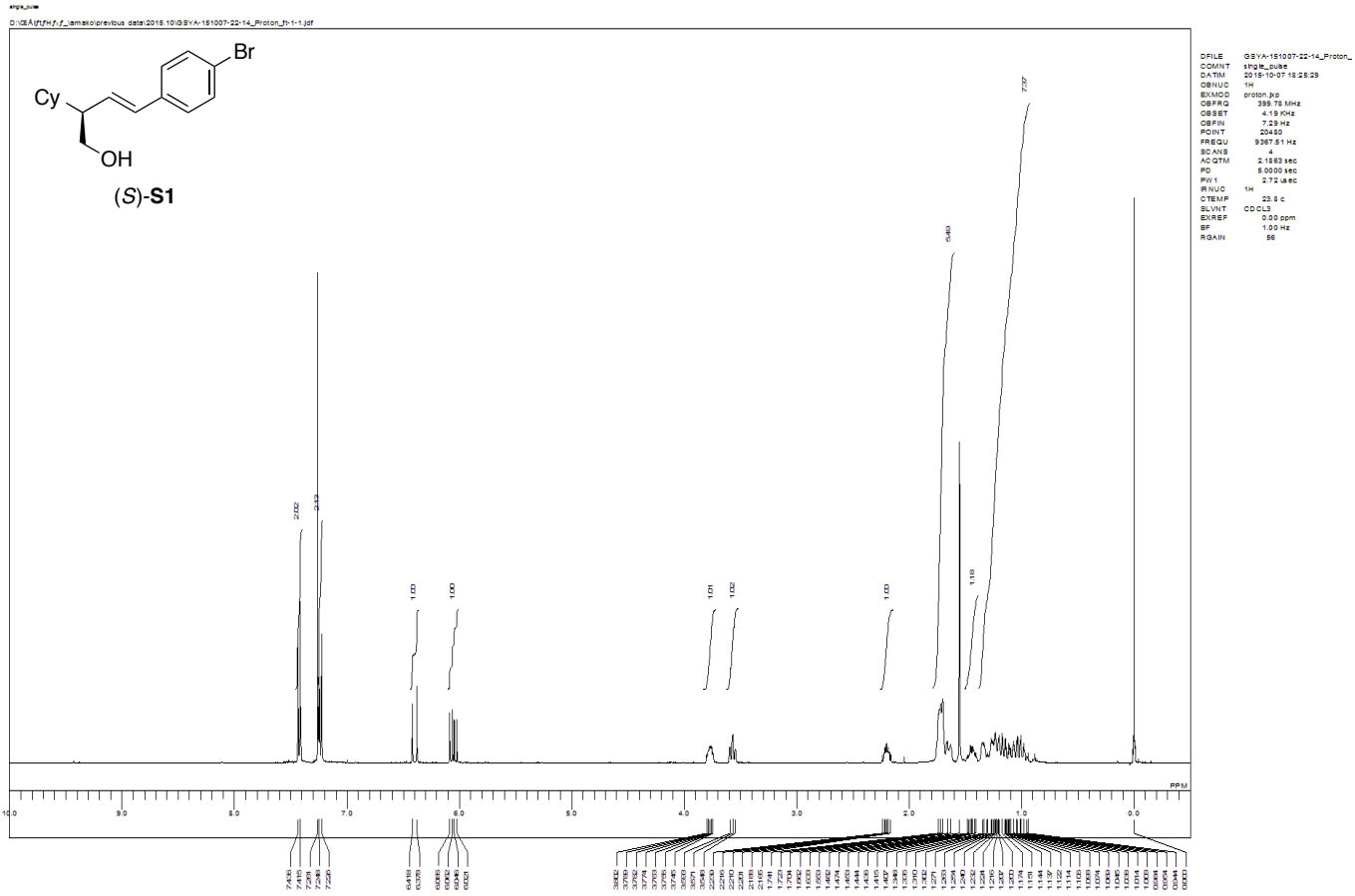
DFILE GSYA-161209-mp_Proton_ft-
COMNT single_pulse
DATIM 2016-12-08 10:25:21
OBNUC 1H
EXMOD proton.jxp
OBFRQ 399.78 MHz
OBSET 4.19 KHz
OBFIN 7.29 Hz
POINT 20480
FREQU 9367.51 Hz
SCANS 8
ACQTM 2.1863 sec
PD 8.0000 sec
PW1 2.72 usec
IRNUC 1H
CTEMP 21.0 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 66

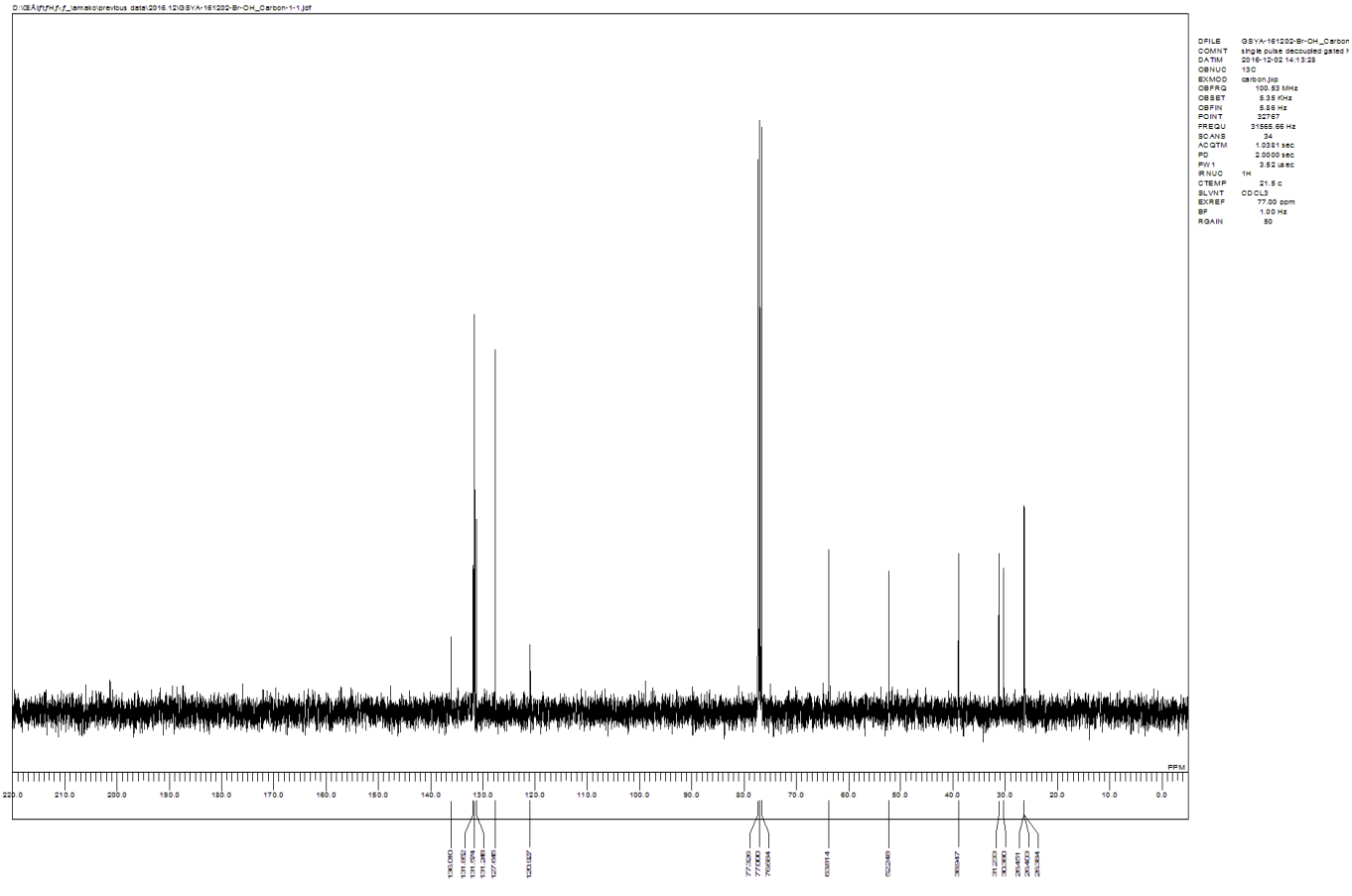
single pulse decoupled gated NOE

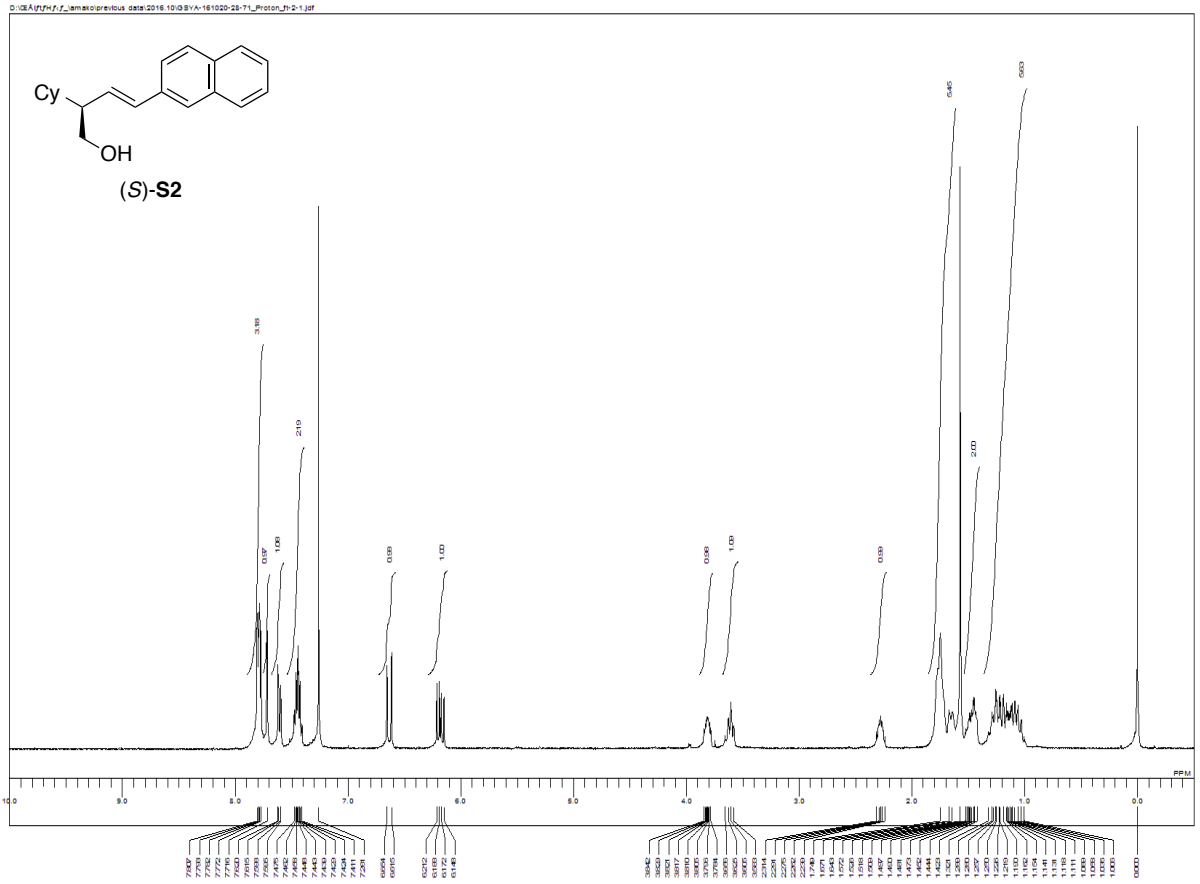
D:\CEA\IT\HY_lamako\previous data\2016.12\GSYA-161209-diene_Carbon_ft-1-1.jdf

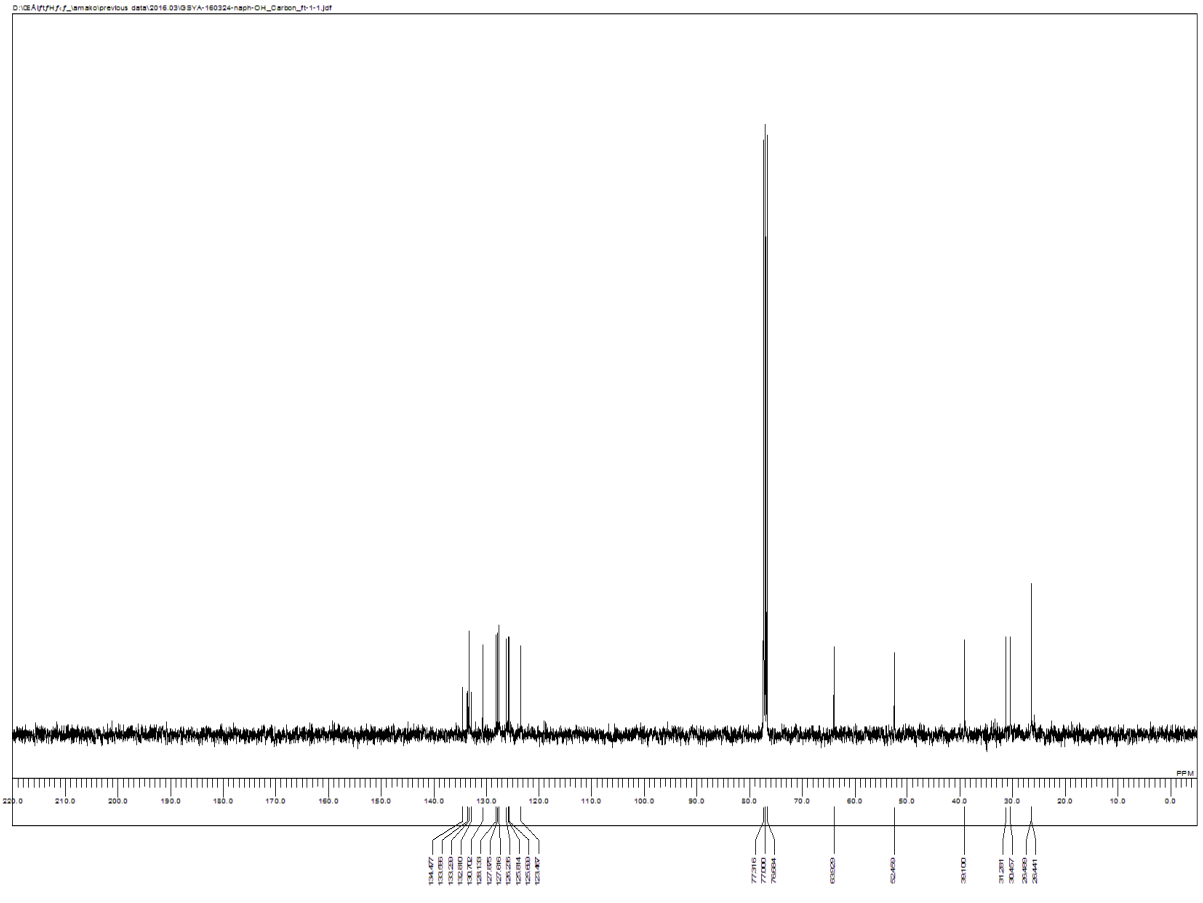


DFILE GSYA-161209-diene_Carbon_
COMNT single pulse decoupled gated N
DATIM 2016-12-09 00:58:15
OBNUC 13C
EXMOD carbon.jxp
OBFRQ 150.92 MHz
OBSET 8.52 KHz
OBFIN 1.74 Hz
POINT 40960
FREQU 59155.60 Hz
SCANS 5905
ACQTM 0.6921 sec
PD 2.0000 sec
PW1 3.33 usec
IRNUC 1H
CTEMP 25.1 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.00 Hz
RGAIN 50


Br
Cy
OH
(S)-S1
2.02
2.13
1.00
1.00
1.01
1.02
1.00
5.49
1.18
7.37
PPM


PPM


Cy
OH
(S)-S2
3.89
0.97
1.00
2.10
0.99
1.00
0.99
1.00
0.99
5.45
5.63
2.00
PPM


PPM