Supporting Information

I. General Procedures

All reactions were carried out under an atmosphere of N_2 using glassware that was either oven- or flame-dried prior to use. Hexanes, tetrahydrofuran (THF), diethyl ether (Et_2O), and toluene (PhMe), were degassed with argon and then passed through two 4 x 36 inch columns of anhydrous neutral A-2 alumina (8 x 14 mesh; LaRoche Chemicals; activated under a flow of argon at 350 ºC for 12 h) to remove H_2O. All other solvents utilized were purchased "anhydrous" commercially, or purified as described (vide infra). ^{1}H NMR spectra were recorded on Bruker GN-500 (500 MHz ^{1}H, 125.7 MHz ^{13}C), CRYO-500 (500 MHz ^{1}H, 125.7 MHz ^{13}C) or DRX-400 (400 MHz ^{1}H, 100 MHz ^{13}C) spectrometers. Proton chemical shifts are reported in ppm (δ) relative to internal tetramethylsilane (TMS, δ 0.00). Data are reported as follows: chemical shift (multiplicity [singlet (s), broad singlet (br s), doublet (d), doublet of doublets (dd), triplet (t), doublet of triplets (dt), doublet of doublet of triplets (ddt), triplet of triplets (tt), quartet (q), quintet (quint), multiplet (m), apparent singlet (ap s), apparent doublet (ap d), apparent quartet (ap q), broad doublet (br d) and broad multiplet (br m)], coupling constants [Hz], integration). Carbon chemical shifts are reported in ppm (δ) relative to TMS with the respective solvent resonance as the internal standard ($CDCl_3$, δ 77.16 ppm). Unless otherwise indicated, NMR data were collected at 25 ºC. Analytical thin-layer chromatography (TLC) was performed using Silica Gel 60 F_{254} pre-coated plates (0.25 mm thickness). Visualization was accomplished by irradiation with a UV lamp and/or staining with $KMnO_4$ solution. Flash chromatography was performed using Silica Gel 60Å (170-400 mesh) from Fisher Scientific. Preparatory HPLC was performed on an Agilent 1100 using an Alltima Silica 5 μm, 250 x 22 mm column. Melting points (m.p.) were obtained using a Mel-Temp melting point apparatus and are uncorrected. Infrared spectra were obtained on a Mattson Instruments *Galaxy 5000* (thin film) and Perkin-Elmer Spectrum 1000 FT-IR Systems and are reported in terms of frequency of absorption (cm^{-1}). High resolution mass spectrometry was performed by the University of California, Irvine Mass Spectrometry Center. Optical rotations were measured with a Rudolph Research Analytical Autopol IV Automatic Polarimeter or a Jasco P-1010 digital polarimeter. SFC determinations of enantiopurity were performed on a Berger Analytical instrument using a Daicel™ Chiralpak® column (OD-H, OJ-H, or AD-H; 100 bar, 50 °C, 215 nm).

$Ni(cod)_2$ was purchased from Strem, stored in a glovebox freezer (–20 °C) under an atmosphere of N_2, and used as received. $Ni(PPh_3)_4$ was purchased from Aldrich and used as received. $Ni(acac)_2$ was purchased from Strem, stored in a glovebox under an atmosphere of N_2, and used as received. 1,2-Bis(diphenylphosphino)ethane (dppe) was purchased from Alfa Aesar, stored in a glovebox under an atmosphere of N_2, and used as received. 1,2-Bis(diphenylphosphino)ethane nickel (II) chloride ($Ni(dppe)Cl_2$) was purchased from Strem and used as received.

Organomagnesium reagents for substrate synthesis were freshly prepared from the halide precursor in THF and molarities were determined by titration with I_2.[1] Activated MnO_2 was prepared according to a procedure reported by Attenburrow and co-workers.[2] All other chemicals were purchased commercially and used as received.

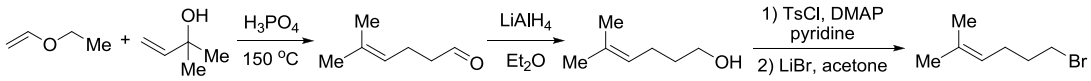
II. Preparation of Organomagnesium Reagents for Cross-Coupling Reactions

For satisfactory yields and enantiospecificities in the cross-coupling reactions, the Grignard reagent must be prepared from the alkyl bromide in diethyl ether.

General Procedure: Magnesium turnings (1.08 g, 45.0 mmol) were added to a round-bottom flask equipped with a stir bar and condenser. The reaction apparatus was flame-dried under vacuum and cooled under N_2. Et_2O (5.0 mL) was added to the reaction apparatus, followed by a single crystal of I_2 (ca. 2 mg). The organohalide[3] (15.0 mmol) was added portion-wise over 30 min. The reaction was stirred at ambient temperature for an additional two hours. The resulting Grignard reagents was typically between 2.0 and 3.0 M as titrated using Knochel's method,[1] and could be stored (sealed, under nitrogen) for at least 4 weeks without detrimental effects.

***p*-(*N*,*N*-Dimethylamino)phenylmagnesium bromide** was prepared according to a procedure reported by Jarvo and co-workers.[4]

(5-methylhex-4-enyl)magnesium bromide was prepared from 5-methylhex-4-enylbromide. The latter has been prepared via the following synthetic route:

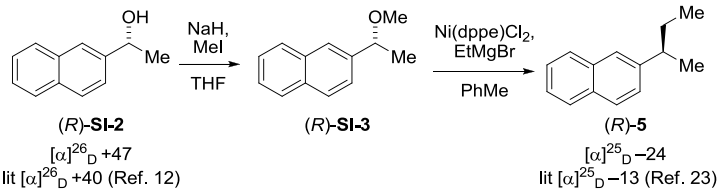


5-methylhex-4-enal was prepared according to a modified procedure reported by Saucy and co-workers.[5] A sealed tube was charged with ethoxyethane (11.6 mL, 121 mmol), 2-methylbut-3-en-2-ol (6.40 mL, 60 mmol), and 85% phosphoric acid (59 µL, 0.60 mmol). The tube was sealed, heated to 150 °C, and allowed to stir for 2.5 h. The reaction mixture was cooled to room temp, opened, and neutralized with triethylamine. Purification by fractional distillation (120 °C, 50 torr) afforded the title compound as a clear, colorless oil (2.41 g, 21.5 mmol, 36%). Analytical data is consistent with literature values.[6]

5-methylhex-4-ene-1-ol was prepared according to the procedure reported by Heathcock and co-workers.[7] Analytical data was consistent with literature values.[8]

6-Bromo-2-methylhex-2-ene was prepared according to the procedure reported by Boyer.[9] Analytical data was consistent with literature values.[9]

III. Demonstration of Cross-Coupling Stereochemical Course

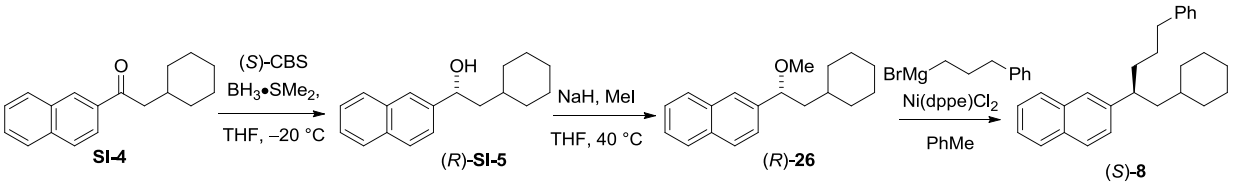


(*R*)-**SI-2**
$[\alpha]^{26}_{D}$ +47
lit $[\alpha]^{26}_{D}$ +40 (Ref. 12)

(*R*)-**SI-3**

(*R*)-**5**
$[\alpha]^{25}_{D}$ –24
lit $[\alpha]^{25}_{D}$ –13 (Ref. 23)

Enantioenriched alcohol (*R*)-**SI-2** was prepared by CBS reduction using (*S*)-2-methyl-CBS-oxazaborolidine (vide infra), and the stereochemistry was verified by comparison of the optical rotation to the literature value. Conversion to ether (*R*)-**SI-3** followed by stereospecific cross-coupling produced (*R*)-**5**, the stereochemistry of which was determined by comparison of the optical rotation to the literature value. This product corresponds to net inversion in the cross-coupling reaction.

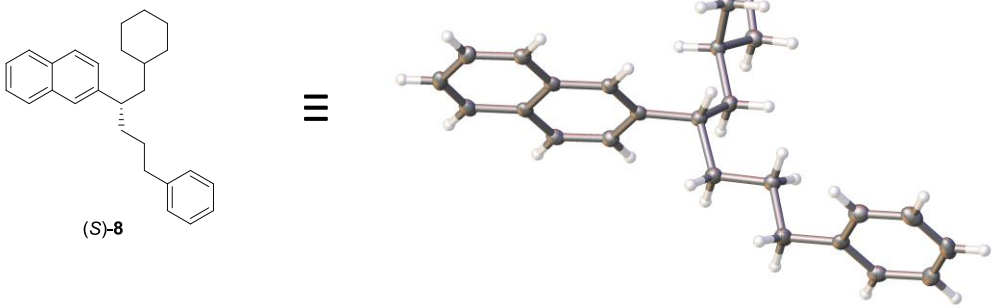


SI-4

(*R*)-**SI-5**

(*R*)-**26**

(*S*)-**8**

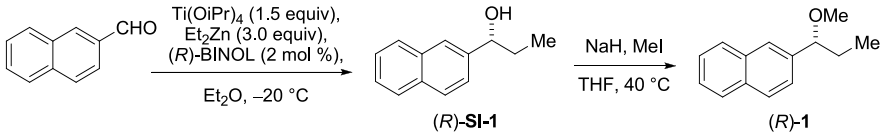


(*S*)-**8**

Enantioenriched alcohol (*R*)-**SI-5** was prepared by CBS reduction of **SI-4** using (*S*)-2-methyl-CBS-oxazaborolidine. Absolute configuration was assigned as *R* based on the accepted model for selectivity in CBS reduction[10] and confirmed by Competing Enantioselective Conversion (CEC).[11] Conversion to ether (*R*)-**26** followed by stereospecific cross-coupling produced (*S*)-**8**, the stereochemistry of which was determined by X-ray crystallographic analysis (vide infra). This product corresponds to net inversion in the cross-coupling reaction. See SI section X for crystallographic data.

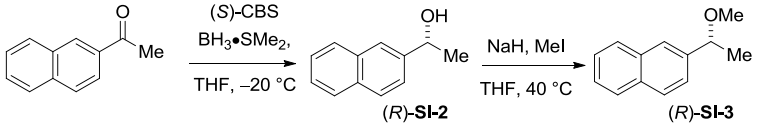
The absolute configurations of all other products were assigned based on the assumption that the cross-coupling reaction proceeds with inversion.

IV. Synthesis and Characterization of Substrates



(*R*)-1-(naphthalen-2-yl)propan-1-ol ((*R*)-SI-1). Prepared according to the procedure reported by Jarvo and co-workers.[12] Analytical data is consistent with literature values:[12] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.80 (m, 3H), 7.73 (s, 1H), 7.45 (m, 3H), 4.72 (t, *J* = 6.8 Hz, 1 H), 2.17 (s, 1H), 1.79–1.90 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.0, 133.3, 133.1, 128.3, 128.0, 127.8, 126.2, 125.9, 124.8, 124.2, 76.2, 31.8, 10.3; **$[\alpha]^{24}_D$** +39.5 (*c* 1.01, $CHCl_3$, 98% ee), lit. $[\alpha]^{23}_D$ +41.9 (*c* 1.02, $CHCl_3$, 96% ee);[12] **SFC** analysis (OD-H, 10% IPA, 2.5 mL/min) indicated 95% ee: t_R (minor) = 9.1 minutes, t_R (major) = 9.9 minutes.

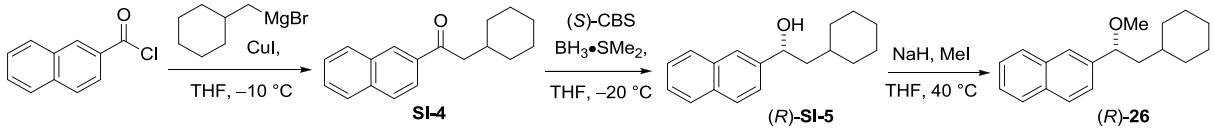
(*R*)-2-(1-methoxypropyl)naphthalene ((*R*)-1). Prepared according to the procedure reported by Jarvo and co-workers.[12] Analytical data is consistent with literature values:[12] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (m, 3H), 7.70 (s, 1H), 7.45 (m, 3H), 4.17 (t, *J* = 6.6 Hz, 1 H), 3.24 (s, 3H), 1.92 (m, 1H), 1.75 (m, 1H), 0.89 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 139.8, 133.3, 133.2, 128.4, 128.0, 127.8, 126.17, 126.16, 125.8, 124.7, 85.8, 56.9, 30.9, 10.4; **$[\alpha]^{24}_D$** +110.5 (*c* 1.07, $CHCl_3$), lit. $[\alpha]^{23}_D$ +92.2 (*c* 1.82, $CHCl_3$, 96% ee);[12] **SFC** analysis (OD-H, 1% IPA, 2.5 mL/min) indicated 95% ee: t_R (minor) = 5.8 minutes, t_R (major) = 6.2 minutes.



(*R*)-1-(naphthalen-2-yl)ethanol ((*R*)-SI-2). Prepared according to a modified procedure by Panek and co-workers.[13] To a cooled (–30 °C) solution (*S*)-2-methyl-CBS-oxazaborolidine (0.083 g, 0.30 mmol) in THF (10 mL) was added borane dimethyl sulfide (0.60 mL, 6.0 mmol) and the reaction mixture was stirred for 45 min. Naphthylmethylketone (0.510 g, 3.0 mmol) in THF (5 mL) was added drop-wise and the reaction was further stirred at –30 °C for 12 h. The reaction was quenched by slow addition of MeOH (5 mL), warmed to room temperature and diluted with water. The product was extracted with Et_2O (2 x 20 mL) and the combined organics were washed with brine, dried over $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (30% EtOAc in hexanes) afforded the title compound as a white solid (0.48 g, 2.8 mmol, 92%). The product was recrystallized from hexanes to yield higher enantiopurity. Analytical data is consistent with literature values:[14] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76 (m, 4H), 7.42 (m, 3H), 4.95 (q, *J* = 6.0 Hz, 1H), 2.59 (s, 1H), 1.51 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.3, 133.4, 133.0, 128.4, 128.0, 127.8, 126.2, 125.9, 123.93, 123.93; **$[\alpha]^{26}_D$** +46.6 (*c* 0.86, $CHCl_3$), lit. $[\alpha]^{25}_D$ +40.0 (*c* 1.00, $CHCl_3$, 92% ee);[14] **SFC** analysis (OD-H, 10% IPA, 2.5 mL/min) indicated 92% ee: t_R (minor) = 8.8 minutes, t_R (major) = 9.5 minutes.

(*R*)-2-(1-methoxyethyl)naphthalene ((*R*)-SI-3). To a solution of NaH (0.081 g, 3.4 mmol) in THF (10 mL) was added a solution of (*R*)-**SI-2** (0.291 g, 1.68 mmol) in THF (2 mL) and the mixture was stirred at 40 °C for 30 min. MeI (0.31 mL, 5.1 mmol) was added and stirring was continued for 8 h. Reaction was quenched with MeOH and the solvent was removed in vacuo. The crude mixture was taken up in CH_2Cl_2 (100 mL), filtered through Celite, and concentrated in vacuo. Purification by flash chromatography (5% EtOAc in hexanes) afforded the title compound as a colorless oil (0.305 g, 1.64 mmol, 97%). Analytical data is consistent with literature values:[15] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (m, 3H), 7.71 (s, 1H), 7.44

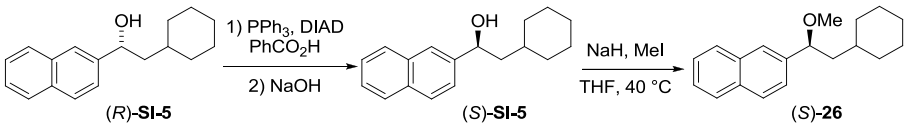
(m, 3H), 4.42 (q, *J* = 6.4 Hz, 1H), 3.23 (s, 3H), 1.50 (d, *J* = 6.4 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 141.0, 133.4, 133.1, 128.5, 127.9, 127.8, 126.2, 125.8, 125.2, 124.2, 79.8, 56.6, 24.0; **$[\alpha]^{26}_D$** +105.0 (*c* 0.85, $CHCl_3$); **SFC** analysis (OD-H, 1% IPA, 2.5 mL/min) indicated 92% ee: t_R (minor) = 7.6 minutes, t_R (major) = 8.3 minutes.



2-cyclohexyl-1-(naphthalen-2-yl)ethanone (SI-4). Prepared according to the procedure reported by Jarvo and co-workers.[16] Analytical data is consistent with literature values:[16] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.45 (s, 1H), 8.03 (d, *J* = 9.0 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.88 (t, *J* = 9.0 Hz, 2H), 7.46–7.61 (m, 2H), 2.95 (d, *J* = 6.5 Hz, 2H), 2.10–1.97 (m, 1H), 1.85–1.75 (m, 2H), 1.70–1.65 (m, 3H), 1.31–1.26 (m, 2H), 1.22–1.17 (m, 1H), 1.15–1.02 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 200.4, 135.7, 135.0, 132.7, 129.9, 129.7, 128.52, 128.47, 127.9, 126.8, 124.2, 46.4, 34.9, 33.7, 26.4, 26.3.

(*R*)-2-cyclohexyl-1-(naphthalen-2-yl)ethanol ((*R*)-SI-5). Prepared according to the procedure reported by Jarvo and co-workers.[16] Analytical data is consistent with literature values:[16] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 (m, 3H), 7.78 (s, 1H), 7.49–7.45 (m, 3H), 4.96 (m, 1H), 1.85–1.77 (m, 4H), 1.71–1.60 (m, 4H), 1.51–1.40 (m, 1H), 1.29–1.13 (m, 3H), 1.04–0.92 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.8, 133.5, 133.1, 128.4, 128.1, 127.8, 126.3, 125.9, 124.6, 124.3, 72.4, 47.1, 34.4, 34.1, 33.1, 26.7, 26.4, 26.3; **$[\alpha]^{25}_D$** +33.3 (*c* 0.17, $CHCl_3$), lit. $[\alpha]^{28}_D$ +23.8 (*c* 1.0, $CHCl_3$, 87% ee);[16] **SFC analysis** (AS-H, 3% IPA, 3 mL/min) indicated 96% ee; t_R (minor) = 12.2 minutes, t_R (major) = 12.8 minutes. Absolute configuration was assigned as *R* based on the accepted model for selectivity in CBS reduction[10] and confirmed by Competing Enantioselective Conversion (CEC).[11]

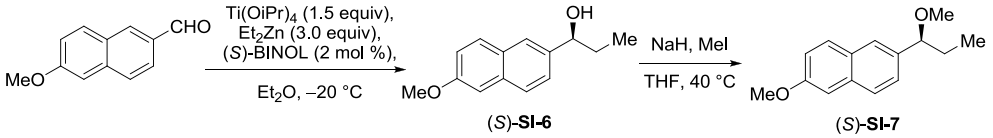
(*R*)-2-(2-cyclohexyl-1-methoxyethyl)naphthalene ((*R*)-26). To a solution of NaH (0.514 g, 21.4 mmol) in THF (100 mL) was added (*R*)-**SI-5** (2.72 g, 10.7 mmol) and mixture was stirred at 40 °C for 30 min. MeI (2.00 mL, 32.1 mL) was added and stirring was continued for 8 h. The reaction was quenched with MeOH and the solvent was removed in vacuo. The crude mixture was taken up in CH_2Cl_2 (100 mL), washed with sat. $NaCO_3$, brine, dried over $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (5% EtOAc in hexanes) afforded the title compound as a white solid (2.85 g, 10.6 mmol, 99%): **TLC R_f** = 0.4 (5% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (m, 3H), 7.70 (s, 1H), 7.49–7.43 (m, 3H), 4.36 (dd, *J* = 8.6, 5.7 Hz, 1H), 3.21 (s, 3H), 1.84–1.76 (m, 3H), 1.69–1.62 (m, 3H), 1.54–1.49 (m, 1H), 1.42–1.37 (m, 1H), 1.25–1.10 (m, 3H), 0.99–0.90 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.5, 133.4, 133.2, 128.4, 127.9, 127.8, 126.2, 125.9, 125.8, 124.6, 81.9, 56.8, 46.2, 34.3, 34.0, 33.3, 26.7, 26.4, 26.3; **$[\alpha]^{25}_D$** +63.2 (*c* 1.06, $CHCl_3$); **SFC analysis** (OJ-H, 3% IPA, 2.5 mL/min) indicated 97% ee t_R (minor) = 7.1 minutes, t_R (major) = 8.8 minutes.



(*S*)-2-cyclohexyl-1-(naphthalen-2-yl)ethanol ((*S*)-SI-5). Prepared according to a modified procedure reported by Presnell and co-workers.[17] To a cooled (brine ice bath) solution of (*R*)-**SI-5** (0.15 g, 0.59 mmol), benzoic acid (0.29 g, 2.4 mmol), and PPh_3 (0.62 g, 2.4 mmol) in THF (5 mL) was added DIAD (0.46 mL, 2.4 mmol) drop-wise over 30 min. After the addition was complete the reaction was allowed to

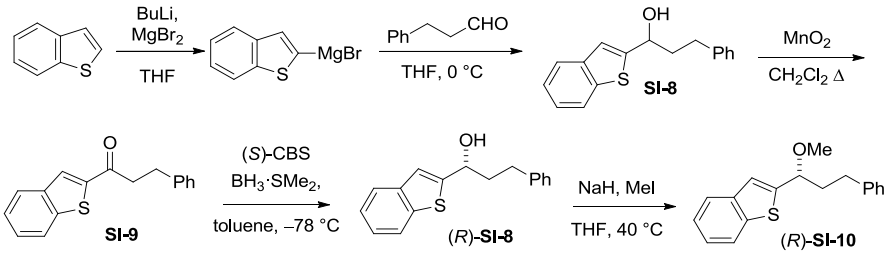
warm to room temperature and stir for 12 h then heated up to 40 °C and stirred for an additional 3 h. The reaction mixture was diluted with Et_2O (10 mL), washed with sat. $NaHCO_3$, dried over $NaSO_4$, and concentrated in vacuo. Trituration with hexanes removed the PPh_3 by-products and purification by flash chromatography (10% EtOAc in hexanes) afforded the title compound as a white solid (0.112 g, 0.43 mmol, 73%). The product was recrystallized from hexanes to yield higher enantiopurity. Analytical data is consistent with literature values:[16] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84 (m, 3H), 7.78 (s, 1H), 7.49–7.45 (m, 3H), 4.96 (m, 1H), 1.85–1.79 (m, 4H), 1.71–1.60 (m, 4H), 1.51–1.40 (m, 1H), 1.29–1.13 (m, 3H), 1.04–0.92 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.8, 133.5, 133.1, 128.4, 128.1, 127.8, 126.3, 125.9, 124.6, 124.3, 72.4, 47.1, 34.4, 34.1, 33.1, 26.7, 26.4, 26.3; **$[\alpha]^{26}_D$** –27.4 (*c* 1.02, $CHCl_3$); **SFC analysis** (AS-H, 3% IPA, 3 mL/min) indicated 94% ee; t_R (major) = 11.8 minutes, t_R (minor) = 12.7 minutes.

(*S*)-2-(2-cyclohexyl-1-methoxyethyl)naphthalene ((*S*)-26). Prepared according to the procedure reported above for (*R*)-**26**. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.83 (m, 3H), 7.70 (s, 1H), 7.49–7.43 (m, 3H), 4.36 (dd, *J* = 8.6, 5.7 Hz, 1H), 3.21 (s, 3H), 1.84–1.76 (m, 3H), 1.69–1.62 (m, 3H), 1.54–1.49 (m, 1H), 1.42–1.37 (m, 1H), 1.25–1.10 (m, 3H), 0.99–0.90 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.5, 133.4, 133.2, 128.4, 127.9, 127.8, 126.2, 125.9, 125.8, 124.6, 81.9, 56.8, 46.2, 34.3, 34.0, 33.3, 26.7, 26.4, 26.3; **$[\alpha]^{25}_D$** –58.1 (*c* 1.30, $CHCl_3$); **SFC analysis** (OJ-H, 3% IPA, 2.5 mL/min) indicated 92% ee t_R (major) = 7.0 minutes, t_R (minor) = 8.9 minutes.



(*S*)-1-(6-methoxynaphthalen-2-yl)propan-1-ol ((*S*)-SI-6) Prepared according to the procedure reported by Jarvo and co-workers.[12] Analytical data is consistent with literature values:[12] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (m, 3H), 7.44 (d, *J* = 8.5 Hz, 1H), 7.14 (d, *J* = 11.5 Hz, 2H), 4.72 (t, *J* = 6.5 Hz, 1 H), 3.92 (s, 3H), 1.92–1.82 (m, 3H), 0.93 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.8, 139.8, 134.2, 129.5, 128.8, 127.2, 124.83, 124.80, 119.1, 105.8, 76.3, 55.5, 31.9, 10.3; **$[\alpha]^{28}_D$** –37.3 (*c* 0.44, $CHCl_3$), lit. $[\alpha]^{23}_D$ –28.9 (*c* 0.97, $CHCl_3$, 90% ee);[12] **SFC** analysis (OD-H, 12.5% IPA, 3 mL/min) indicated 94% ee: t_R (major) = 5.3 minutes, t_R (minor) = 6.5 minutes. Absolute configuration was assigned as *S* based on analogy with the titanium-catalyzed ethylation of aldehydes with Et_2Zn[18] and confirmed by Competing Enantioselective Conversion (CEC).[11]

(*S*)-2-methoxy-6-(1-methoxypropyl)naphthalene ((*S*)-SI-7). Prepared according to the procedure reported by Jarvo and co-workers.[12] Analytical data is consistent with literature values:[12] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 5.0, 8.0 Hz, 2H), 7.63 (s, 1H), 7.39 (d, *J* = 8.5 Hz, 1H), 7.14 (m, 2H), 4.14 (t, *J* = 6.8 Hz, 1 H), 3.92 (s, 3H), 3.23 (s, 3H), 1.91 (p, *J* = 7.0 Hz, 1H), 1.74 (quint, *J* = 7.0 Hz, 1H), 0.88 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.7, 137.4, 134.3, 129.4, 128.8, 127.2, 126.1, 125.2, 119.0, 105.8, 85.8, 56.8, 55.5, 30.9, 10.4; **$[\alpha]^{24}_D$** –82.3 (*c* 0.86, $CHCl_3$), lit. $[\alpha]^{23}_D$ –81.9 (*c* 1.09, $CHCl_3$, 90% ee);[12] **SFC** analysis (OD-H, 4% IPA, 2.5 mL/min) indicated 93% ee: t_R (major) = 5.4 minutes, t_R (minor) = 5.9 minutes.



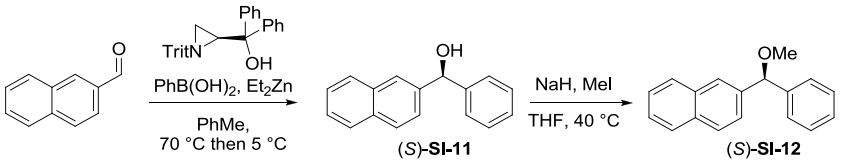
(*rac*)-1-(benzo[*b*]thiophen-2-yl)-3-phenylpropan-1-ol ((*rac*)-SI-8). Prepared according to a modified procedure reported by Guinchard and co-workers.[19] To a cooled (ice bath) solution of benzothiophene (3.35 g, 25.0 mmol) in Et_2O (15 mL) was added *n*-BuLi (21 mL, 28 mmol, 1.3 M in hexane) and the reaction was stirred for two hours allowing it to warm to room temperature. The solution was then cooled to –78 °C and hydrocinnamaldehyde (2.57 mL, 20.0 mmol) was slowly added. The reaction was stirred overnight allowing it to warm up to room temperature. The reaction was quenched with MeOH (10 mL) and diluted with Et_2O (100 mL). The solution was washed with water, brine, dried over $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (10–15% EtOAc in hexanes) afforded the title compound as a white solid (3.42 g, 12.7 mmol, 64%). **m.p.** 95–97 °C; **TLC R_f** = 0.5 (20% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 7.2 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.36–7.19 (m, 8H), 5.00 (dd, *J* = 10.8, 5.6 Hz, 1H), 2.84–2.71 (m, 2H), 2.31–2.15 (m, 2H), 2.13 (d, *J* = 4.0 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.2, 141.4, 139.6, 139.5, 128.63, 128.62, 126.2, 124.5, 124.4, 123.6, 122.7, 120.5, 70.2, 40.5, 32.0; **I.R.** (neat) 2929, 1181, 1085, 1054, 873 cm^{-1}; **HRMS** (TOF MS EI+) *m / z* calcd for $C_{17}H_{16}OS$ $[M]^+$ 268.0922, found 268.0912.

1-(benzo[*b*]thiophen-2-yl)-3-phenylpropan-1-one (SI-9). To a solution of *rac*-**SI-8** (2.83 g, 10.5 mmol) in CH_2Cl_2 (10 mL) was added MnO_2 (4.58 g, 52.7 mmol) and the reaction mixture was stirred overnight. Upon completion as judged by TLC, the reaction mixture was cooled to room temperature, passed through a plug of Celite, and the solvent was removed in vacuo. The resulting solid was purified by flash chromatography (10–30% EtOAc in hexanes) followed by recrystallization from EtOAc/hexanes to afford the title compound as an colorless crystalline solid (2.03 g, 7.62 mmol, 73% yield): **m.p.** 118–120 °C; **TLC R_f** = 0.6 (20% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.85 (d, *J* = 9.2 Hz, 2H), 7.45 (m, 1H), 7.39 (m, 1H), 7.32–7.19 (m, 5H), 3.33 (t, *J* = 4.0 Hz, 2H), 3.10 (t, *J* = 7.8 Hz, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 193.8, 143.6, 142.6, 141.0, 139.2, 129.1, 128.7, 128.6, 127.5, 126.4, 126.0, 125.1, 123.1, 41.2, 30.5; **I.R.** (neat) 3052, 3024, 2920, 1665, 1162, 752, 698 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{17}H_{14}OS$ $[M+Na]^+$ 289.0663, found 289.0663.

(*R*)-1-(benzo[*b*]thiophen-2-yl)-3-phenylpropan-1-ol ((*R*)-SI-8). Prepared according to a modified procedure by Panek and co-workers.[13] To a cooled (–78 °C) solution (*S*)-2-methyl-CBS-oxazaborolidine (0.211 g, 0.762 mmol) and **SI-9** (2.03 g, 7.62 mmol) in toluene (50 mL) was added dropwise $BH_3{\cdot}Me_2S$ (1.56 mL, 15.2 mmol) and the reaction mixture was stirred for 20 h. The reaction was quenched by slow addition of water (5 mL), warmed to room temperature and extracted with Et_2O (3 x 50 mL). The compbined organics were washed with brine, dried over $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (3% EtOAc in hexanes) afforded the title compound as a white solid (1.92 g, 7.15 mmol, 94%). The product was recrystallized from EtOAc and hexanes to yield higher enantiopurity. **$[\alpha]^{27}_D$** +99.2 (*c* 0.89, $CHCl_3$); **SFC analysis** (AD-H, 15% MeOH, 3 mL/min) indicated 99% ee t_R (major) = 10.8 minutes, t_R (minor) = 13.6 minutes. Absolute configuration was assigned as *R* based on the accepted model for selectivity in CBS reductions.[10]

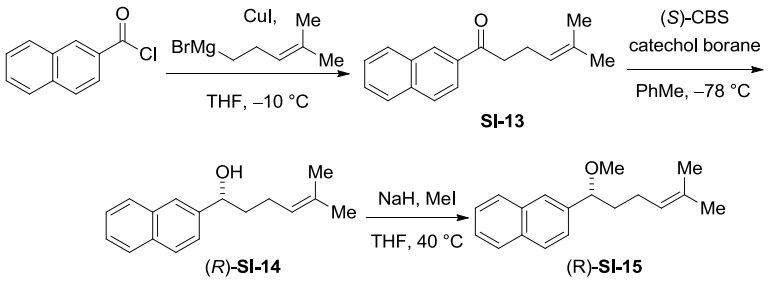
(*R*)-2-(1-methoxy-3-phenylpropyl)benzo[*b*]thiophene ((*R*)-SI-10). To a solution of NaH (0.291 g, 12.1 mmol) in THF (30 mL) was added a solution of (*R*)-**SI-8** (1.63 g, 6.07 mmol) in THF (10 mL) and the mixture was stirred at 40 °C for 30 min. MeI (1.13 mL, 18.22 mmol) was added and stirring was

continued for 8 h. Reaction was quenched with MeOH and the solvent was removed in vacuo. The crude mixture was taken up in CH_2Cl_2 (100 mL), filtered, and concentrated in vacuo. Purification by flash chromatography (5% EtOAc in hexanes) afforded the title compound as a white solid (1.63 g, 5.77 mmol, 95%). **m.p.** 52–54 °C; **TLC R_f** = 0.7 (15% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.35–7.26 (m, 4H), 7.21–7.17 (m, 4H), 4.40 (t, *J* = 6.8 Hz, 1H), 3.30 (s, 3H), 2.72 (m, 2H), 2.29 (m, 1H), 2.10 (m, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 147.1, 141.6, 139.8, 139.5, 128.6, 128.5, 126.0, 124.3 (2C), 123.5, 122.7, 122.3, 79.1, 56.8, 39.6, 32.0; **IR** (neat) 3022, 2930, 2860, 1456, 1099, 839, 750 cm^{-1}; **HRMS** (TOF MS EI$^+$) *m / z* cacld for $C_{18}H_{18}OS$ $[M]^+$ 282.1078 found 282.1074; **$[\alpha]^{27}_D$** +16.6 (*c* 1.20, $CHCl_3$); **SFC analysis** (AD-H, 10% IPA, 3 mL/min) indicated 99% ee t_R (major) = 6.2 minutes, t_R (minor) = 7.4 minutes.



(*S*)-naphthalen-2-yl(phenyl)methanol ((*S*)-SI-11). Prepared according to the procedure reported by Jarvo and co-workers.[12] Analytical data is consistent with literature values:[12] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.83–7.78 (m, 3H), 7.49–7.41 (m, 5H), 7.35 (m, 2H), 7.27 (m, 1H), 6.00 (d, *J* = 3.5 Hz, 1H), 2.33 (d, *J* = 3.5 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.8, 141.2, 133.4, 133.0, 128.7, 128.5, 128.2, 127.83, 127.81, 126.8, 126.3, 126.1, 125.1, 124.9, 76.5; **$[\alpha]^{29}_D$** –4.1 (*c* 1.22, benzene), lit. $[\alpha]^{19}_D$ –3.8 (*c* 1.70, benzene, >98% ee);[20] **SFC** analysis (OD-H, 20% IPA, 3 mL/min) indicated 99% ee: t_R (major) = 6.6 minutes, t_R (minor) = 7.6 minutes.

(*S*)-2-(methoxy(phenyl)methyl)naphthalene ((*S*)-SI-12). Prepared according to the procedure reported by Jarvo and co-workers.[12] Analytical data is consistent with literature values:[12] **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84–7.78 (m, 4H), 7.48–7.39 (m, 5H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.25 (m, 1H), 5.40 (s, 1H), 3.43 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 142.1, 139.6, 133.4, 133.0, 128.6, 128.4, 128.1, 127.8, 127.7, 127.1, 126.2, 126.0, 125.9, 125.1, 85.6, 57.2; **$[\alpha]^{25}_D$** –29.1 (*c* 1.20, $CHCl_3$), lit. $[\alpha]^{23}_D$ –32.0 (*c* 1.11, $CHCl_3$, >99% ee);[12] **SFC** analysis (OD-H, 5% IPA, 3 mL/min, 110 psi) indicated >99% ee: t_R (major) = 5.3 minutes, t_R (minor) = 6.4 minutes.

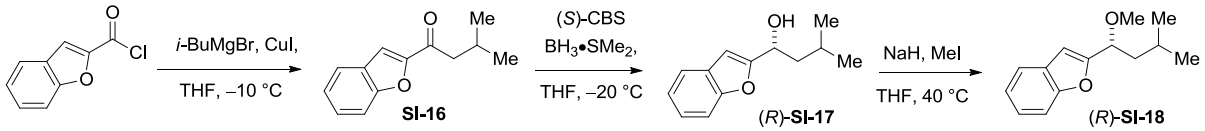


5-methyl-1-(naphthalen-2-yl)hex-4-en-1-one (SI-13). Prepared according to a modified procedure reported by Hultzsch and co-workers.[21] To a cooled (brine/ice bath) solution of CuI (0.059 g, 0.31 mmol) and 2-naphthoyl chloride (1.19 g, 6.25 mmol) in THF (7 mL) was slowly added (4-methylpent-3-enyl)magnesium bromide (10.9 mL, 6.25 mmol, 0.574 M in THF) and the reaction mixture was stirred for 1 h. The reaction was quenched by the addition of MeOH and the solvent was removed in vacuo. The crude reaction mixture was taken up in EtOAc (30 mL), washed with 1 N HCl (10 mL), sat. $NaHCO_3$ (10 mL), brine (10 mL), dried with $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (4% EtOAc in hexanes) afforded the title compound as a colorless oil (1.01 g, 4.22 mmol, 68% yield).

This compound has been previously reported.[22] Our spectral data is not fully consistent with the reported literature values, therefore we provide full characterization data to support our structural assignment: **TLC R_f** = 0.4 (10% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.03 (d, *J* = 8.8 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.86 (t, *J* = 7.4 Hz, 2H), 7.56 (m, 2H), 5.22 (t, *J* = 7.2 Hz, 1H), 3.12 (t, *J* = 7.4 Hz, 2H), 2.48 (q, *J* = 7.4 Hz, 2H), 1.70 (s, 3H), 1.65 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.0, 135.6, 134.4, 132.8, 132.6, 129.7, 129.6, 128.43, 128.39, 127.8, 126.8, 124.0, 123.1, 38.9, 25.8, 23.2, 17.8; **IR** (neat) 3058, 2967, 2913, 1678, 1277, 1180, 1123 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{17}H_{18}O$ $[M+H]^+$ 239.1436, found 239.1429.

(*R*)-5-methyl-1-(naphthalen-2-yl)hex-4-en-1-ol ((*R*)-SI-14). Prepared according to a modified procedure by Okamura and co-workers.[23] To a cooled (–78 °C) solution (*S*)-2-methyl-CBS-oxazaborolidine (0.12 g, 0.42 mmol) and ketone **SI-13** (1.01 g, 4.22 mmol) in toluene (20 mL) was added dropwise catecholborane (0.90 mL, 8.4 mmol) and the reaction mixture was stirred for 20 h. The reaction was quenched by slow addition of MeOH (2 mL) followed by sat. NH_4Cl (10 mL), warmed to room temperature and extracted with Et_2O (3 x 20 mL). The combined organics were washed with sat. $NaCO_3$, brine, dried over $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (10–20% EtOAc in hexanes) afforded the title compound as a white solid (0.703 g, 2.91 mmol, 69%). The product was recrystallized from hexanes to yield higher enantiopurity. **m.p.** 53–55 °C; **TLC R_f** = 0.5 (20% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.0 Hz, 3H), 7.76 (s, 1H), 7.46 (m, 3H), 5.16 (t, *J* = 7.0 Hz, 1H), 4.83 (t, *J* = 5.8 Hz, 1H), 2.12–2.04 (m, 3H), 1.94–1.82 (m, 2H), 1.69 (s, 3H), 1.58 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 142.3, 133.4, 133.1, 132.5, 128.4, 128.1, 127.8, 126.2, 125.9, 124.7, 124.3, 123.9, 74.5, 39.0, 25.9, 24.6, 17.9; **IR** (neat) 3263, 2924, 2856, 1059, 1016 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{17}H_{20}O$ $[M+NH_4]^+$ 258.1858, found 258.1847. **$[\alpha]^{26}_D$** +4.9 (*c* 1.16, $CHCl_3$); **SFC analysis** (OD-H, 15% IPA, 3 mL/min) indicated 93% ee t_R (minor) = 4.9 minutes, t_R (major) = 5.3 minutes. Absolute configuration was assigned as *R* based on the accepted model for selectivity in CBS reductions.[10]

(*R*)-2-(1-methoxy-5-methylhex-4-enyl)naphthalene ((*R*)-SI-15). To a solution of NaH (0.032 g, 1.3 mmol) in THF (3 mL) was added a solution of (*R*)-**SI-14** (0.160 g, 0.67 mmol) in THF (3 mL) and the mixture was stirred at 40 °C for 30 min. MeI (0.124 mL, 2.00 mmol) was added and stirring was continued for 5 h. Reaction was quenched with MeOH and the solvent was removed in vacuo. The crude mixture was taken up in CH_2Cl_2 (10 mL), filtered, and concentrated in vacuo. Purification by flash chromatography (5% EtOAc in hexanes) afforded the title compound as a colorless oil (0.164 g, 0.64 mmol, 96%). **TLC R_f** = 0.5 (10% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (app d, *J* = 8.0 Hz, 3H), 7.70 (s, 1H), 7.46 (m, 3H), 5.12 (t, *J* = 6.8 Hz, 1H), 4.24 (t, *J* = 6.6 Hz, 1H), 3.23 (s, 3H), 2.04 (m, 2H), 1.93 (m, 1H), 1.73 (m, 4H), 1.56 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 140.0, 133.4, 133.2, 132.2, 128.4, 128.0, 127.9, 126.2, 126.1, 125.8, 124.6, 124.0, 83.6, 56.8, 38.1, 25.9, 24.5, 17.9; **IR** (neat) 3055, 2966, 2926, 1445, 1099, 745 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{18}H_{22}O$ $[M]^+$ 254.1671, found 254.1652; **$[\alpha]^{27}_D$** +30.2 (*c* 1.11, $CHCl_3$); **SFC analysis** (OD-H, 5% IPA, 2.5 mL/min) indicated 94% ee t_R (minor) = 4.2 minutes, t_R (major) = 4.6 minutes.



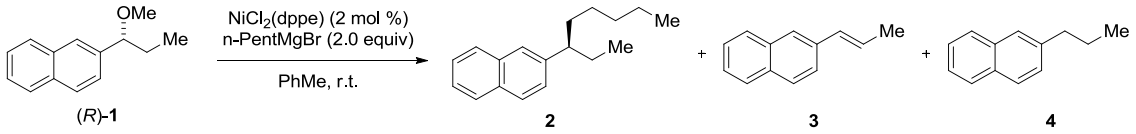
1-(benzofuran-2-yl)-3-methylbutan-1-one (SI-16). Prepared according to a modified procedure reported by Hultzsch and co-workers.[21] To a cooled (brine/ice bath) solution of CuI (0.050 g, 0.260 mmol) and benzofuran-2-carbonyl chloride (0.944 g, 5.23 mmol) in THF (15 mL) was slowly added isobutylmagnesium bromide (7.47 mL, 5.23 mmol, 0.700 M in THF) and the reaction mixture was stirred for 1 h. The reaction was quenched by the addition of MeOH and the solvent was removed in vacuo. The

crude reaction mixture was taken up in EtOAc (30 mL), washed with 1 N HCl (10 mL), sat. $NaHCO_3$ (10 mL), brine (10 mL), dried with $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (4% EtOAc in hexanes) afforded the title compound as a colorless oil (0.833 g, 4.12 mmol, 79% yield): **TLC R_f** = 0.4 (10% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.50–7.46 (m, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 2.83 (d, *J* = 6.8 Hz, 2H), 2.35 (sept, *J* = 6.6 Hz, 1H), 1.03 (d, *J* = 6.4 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 191.5, 155.8, 153.1, 128.3, 127.2, 124.0, 123.4, 112.9, 112.6, 47.9, 25.6, 22.9; **IR** (neat) 2957, 2871, 1678, 1556, 1298, 1161, 1143 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{13}H_{14}O_2$ $[M+H]^+$ 203.1072, found 203.1069.

(*R*)-1-(benzofuran-2-yl)-3-methylbutan-1-ol ((*R*)-SI-17). Prepared according to a modified procedure by Panek and co-workers.[13] To a cooled (–20 °C) solution (***S***)-2-methyl-CBS-oxazaborolidine (0.114 g, 0.41 mmol) in THF (30 mL) was added $BH_3{\cdot}Me_2S$ (0.800 mL, 8.43 mmol) and the reaction mixture was stirred for 30 min. A solution of **SI-16** (0.700 g, 3.46 mmol) in THF (5 mL) was added and the reaction mixture was stirred for 17 h. at –20 °C. The reaction was quenched by slow addition of MeOH (5 mL) followed by sat. NH_4Cl (30 mL), warmed to room temperature and extracted with EtOAc (3 x 30 mL). The combined organics were washed with sat. $NaCO_3$, brine, dried over $NaSO_4$, and concentrated in vacuo. Purification by flash chromatography (5–10% EtOAc in hexanes) followed by recrystallization from hexanes afforded the title compound as white needles (0.461 g, 2.25 mmol, 65%). **m.p.** 72–73 °C; **TLC R_f** = 0.5 (20% EtOAc in hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.5 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.26 (m, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 6.60 (s, 1H), 4.88 (d, *J* = 4.0 Hz, 1H), 2.05 (d, *J* = 4.0 Hz, 1H), 1.87–1.75 (m, 3H), 0.98 (t, *J* = 5.5 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.8, 154.9, 128.3, 124.2, 122.9, 121.1, 111.4, 102.5, 66.7, 44.6, 24.7, 23.2, 22.3; **IR** (neat) 3339, 2955, 2869, 1454, 1253 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{13}H_{16}O_2$ $[M]^+$ 204.1150, found 204.1155. **$[\alpha]^{24}_D$** +25.3 (*c* 1.17, $CHCl_3$); **SFC analysis** (AD-H, 5% MeOH, 3 mL/min) indicated 95% ee t_R (minor) = 4.9 minutes, t_R (major) = 5.2 minutes. Absolute configuration was assigned as *R* based on the accepted model for selectivity in CBS reductions.[10]

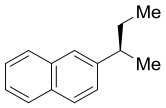
(*R*)-2-(1-methoxy-3-methylbutyl)benzofuran ((*R*)-SI-18). To a solution of NaH (0.103 g, 4.30 mmol) in THF (5 mL) was added a solution of (*R*)-**SI-17** (0.439 g, 2.15 mmol) in THF (3 mL) and the mixture was stirred at 40 °C for 30 min. MeI (0.402 mL, 6.44 mmol) was added and stirring was continued for 8 h. Reaction was quenched with MeOH and the solvent was removed in vacuo. The crude mixture was taken up in CH_2Cl_2 (100 mL), filtered, and concentrated in vacuo. Purification by flash chromatography (5% EtOAc in hexanes) afforded the title compound as a colorless oil (0.467 g, 2.14 mmol, 99%): **TLC R_f** = 0.5 (10% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.28–7.19 (m, 2H), 6.64 (s, 1H), 4.35 (t, *J* = 7.2 Hz, 1H), 3.32 (s, 3H), 1.90 (m, 1H), 1.75–1.68 (m, 2H), 0.94 (t, *J* = 6.8 Hz, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.5, 155.1, 128.2, 124.2, 122.8, 121.0, 111.5, 104.6, 75.7, 56.9, 43.3, 24.8, 23.0, 22.5; **IR** (neat) 2955, 2931, 2869, 1454, 1252, 1093 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{14}H_{18}O_2$ $[M]^+$ 218.1307, found 218.1302; **$[\alpha]^{24}_D$** +100.3 (*c* 1.05, $CHCl_3$); **SFC analysis** (AD-H, 3% IPA, 3 mL/min) indicated 97% ee t_R (major) = 2.0 minutes, t_R (minor) = 2.2 minutes.

V. Representative Procedure for Cross-Coupling Reactions



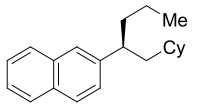
(–)-2-(octan-3-yl)naphthalene (2, Table 1, entry 16): A vial was charged with (*R*)-**1** (0.100 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), flushed with nitrogen and capped. Toluene (3.0 mL) was added, followed by *n*-pentylmagnesium bromide (0.60 mL, 1.0 mmol, 1.7 M in Et_2O) and the reaction was allowed to stir at room temperature for 24 h. The reaction was quenched by the addition of EtOAc (1 mL) and the entire reaction mixture was adsorbed onto silica gel (1 g). The solvents were removed in vacuo and the crude was purified by flash column chromatography (100% hexanes). The resulting colorless oil (0.118 g) was a mixture of the title compound (96% calculated yield), the product of reduction (2% calculated yield), and the product of elimination (1% calculated yield). Further purification (100% heptanes) afforded a pure sample of (*R*)-**2**: **TLC** $\mathbf{R_f}$ = 0.6 (100% hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80–7.76 (m, 3H), 7.56 (s, 1H), 7.46–7.38 (m, 2H), 7.30 (dd, *J* = 8.4, 0.8 Hz, 1H), 2.56 (m, 1H), 1.78–1.60 (m, 4H), 1.26–1.10 (m, 6H), 0.82 (m, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.7, 133.7, 132.2, 127.9, 127.7, 127.6, 126.5, 126.2, 125.8, 125.1, 48.2, 36.6, 32.2, 29.8, 27.5, 22.7, 14.2, 12.4; **IR** (neat) 3056, 2981, 2918, 2850, 1107, 1067 cm^{-1}; **HRMS** (TOF MS CI^+) *m / z* cacld for $C_{18}H_{24}$ $[M]^+$ 240.1878, found 240.1871; $\mathbf{[\alpha]^{27}_D}$ –1.6 (*c* 1.83, $CHCl_3$); **SFC** analysis (OJ-H, 2% hexanes, 2 mL/min) indicated 96% ee: t_R (minor) = 10.0 minutes, t_R (major) = 10.6 minutes.

VI. Characterization Data for Products



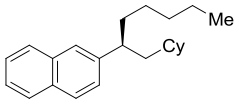
(*R*)-5

(*R*)-2-sec-butylnaphthalene ((*R*)-5, table 2, entry 1): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**SI-3** (0.093 g, 0.50 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), ethylmagnesium bromide (0.36 mL, 1.0 mmol, 2.8 M in Et_2O) and toluene (3.0 mL). Purification by flash column chromatography (100% hexanes) afforded the title compound as a colorless oil (0.73 g, 80%). Analytical data is consistent with literature values:[12] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81–7.76 (m, 3H), 7.60 (s, 1H), 7.46–7.34 (m, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 2.76 (sextet, *J* = 7.2 Hz, 1H), 1.73–1.65 (m, 2H), 1.32 (d, *J* = 6.8 Hz, 3H), 0.85 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.3, 133.8, 132.3, 128.0, 127.71, 127.68, 126.0, 125.9, 125.3, 125.1, 42.0, 31.2, 22.0, 12.4; $\mathbf{[\alpha]^{27}_D}$ –26.5 (*c* 1.17, $CHCl_3$), $\mathbf{[\alpha]^{25}_D}$ –24.4 (*c* 1.00, heptane), lit. $[\alpha]^{25}_D$ –12.7 (*c* 2.4, heptane, 42% ee);[24] **SFC** analysis (OD-H, 1% hexanes, 2.0 mL/min) indicated 91% ee t_R (minor) = 9.9 minutes, t_R (major) = 10.4 minutes.



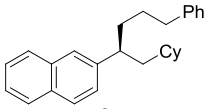
6

(+)-2-(1-cyclohexylpentan-2-yl)naphthalene (6, table 2, entry 2): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.134 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), *n*-propylmagnesium bromide (0.44 mL, 1.0 mmol, 2.3 M in Et_2O) and toluene (3.0 mL). Purification by flash column chromatography (100% hexanes) afforded a colorless oil (0.137 g) as a mixture of the title compound (calculated yield 93%) and the product of elimination (5% calculated yield). Further purification (100% heptanes) afforded a sample of analytically pure material: $\mathbf{R_f}$ = 0.7 (100% hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.80–7.76 (m, 3H), 7.55 (s, 1H), 7.45–7.39 (dquint, *J* = 5.5, 1.2 Hz, 2H), 7.32 (dd, *J* = 8.5, 1.5 Hz, 1H), 2.84–2.79 (dq *J* = 9.3, 5.5 Hz, 1H), 1.84 (d, *J* = 12.8 Hz, 1H), 1.85–1.47 (m, 8H), 1.26–1.05 (m, 6H), 0.91–0.86 (m, 5H); **^{13}C NMR** (500 MHz, $CDCl_3$) δ 144.1, 133.7, 132.3, 128.0, 127.73, 127.65, 126.4, 126.2, 125.8, 125.1, 44.9, 42.7, 39.9, 35.0, 34.4, 33.0, 26.8, 26.4, 26.3, 20.9, 14.3; **IR** (thin film) 3052, 2661, 1915, 1633, 1600 cm^{-1}; **HRMS** (TOF MS Cl+) *m / z* cacld for $C_{21}H_{28}$ [M]$^+$ 280.2191, found 280.2187; $\mathbf{[\alpha]^{29}_D}$ +17.8 (*c* 1.11, $CHCl_3$); **SFC** analysis (OJ-H, 2% hexanes, 2.0 mL/min) indicated 97% ee t_R (major) = 11.4 minutes, t_R (minor) = 12.3 minutes.



7

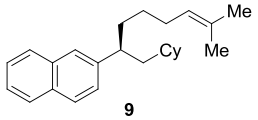
(+)-2-(1-cyclohexylheptan-2-yl)naphthalene (7, table 2, entry 3): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.134 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), *n*-pentylmagnesium bromide (0.50 mL, 1.0 mmol, 2.0 M in Et_2O), and toluene (3.0 mL). Purification by flash column chromatography (100% hexanes) afforded a colorless oil (0.147 g) as a mixture of the title compound (91% calculated yield) and the product of elimination (6% calculated yield). Further purification (100% heptanes) afforded a sample of analytically pure material: $\mathbf{R_f}$ = 0.3 (100% hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80–7.75 (m, 3H), 7.55 (s, 1H), 7.44–7.37 (m, 2H), 7.31 (dd, *J* = 8.4, 1.2 Hz, 1H), 2.79 (m, 1H), 1.84 (d, *J* = 12.8 Hz, 1H), 1.63–1.44 (m, 8H), 1.21–1.04 (m, 10H), 0.89–0.81 (m, 5H); **^{13}C NMR** (500 MHz, $CDCl_3$) δ 144.2, 133.7, 132.3, 128.0, 127.74, 127.67, 126.4, 126.1, 125.8, 125.1, 45.0, 43.0, 37.6, 35.0, 34.4, 33.0, 32.2, 27.5, 26.8, 26.4, 26.3, 22.7, 14.3; **IR** (neat) 3020, 2920, 2850, 815, 744, 697 cm^{-1}; **HRMS** (TOF MS CI+) *m / z* cacld for $C_{23}H_{32}$ [M]$^+$ 308.2504, found 308.2507; $\mathbf{[\alpha]^{27}_D}$ +9.4 (*c* 1.20, $CHCl_3$); **SFC** analysis (OJ-H, 2% hexanes, 2.0 mL/min) indicated 97% ee t_R (minor) = 11.4 minutes, t_R (major) = 12.3 minutes.



8

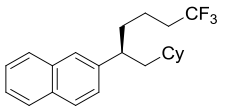
(*S*)-2-(1-cyclohexyl-5-phenylpentan-2-yl)naphthalene (8, table 2, entry 4): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.401 g, 1.50 mmol), $NiCl_2$(dppe) (15.8 mg, 0.030 mmol), (3-phenylpropyl)magnesium bromide (1.59 mL, 1.89 mmol, 1.9 M in Et_2O), and toluene (22 mL). Purification by flash column chromatography (0–5% EtOAc in hexanes) afforded a colorless oil (0.522 g) as a mixture of the title compound (88% calculated yield) and the product of Wurtz coupling of the organomagnesium reagent (1,6-diphenylhexane). Further purification by flash chromatography (100% pentane) afforded a sample of analytically pure material: **TLC** $\mathbf{R_f}$ = 0.3 (100% hexanes); **m.p.** 81–81 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.0 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 2H), 7.54 (s, 1H), 7.46–7.39 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.22 (m, 2H), 7.13 (t, *J*

= 7.5 Hz, 1H), 7.08 (d, *J* = 7.0 Hz, 2H), 2.82 (p, *J* = 5.0 Hz, 1H), 2.54 (m, 2H), 1.82 (d, *J* = 12.5 Hz, 1H), 1.69–1.43 (br m, 10H), 1.11–1.00 (m, 4H), 0.85 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.7, 142.7, 133.7, 132.3, 128.5, 128.3, 128.0, 127.73, 127.68, 126.4, 126.1, 125.9, 125.7, 125.1, 44.9, 42.9, 37.2, 36.1, 34.9, 34.4, 32.9, 29.6, 26.8, 26.4, 26.3; **IR** (neat) 2918, 2850, 1442, 822, 745, 696 cm^{-1}; **HRMS** (TOF MS CI+) *m / z* cacld for $C_{27}H_{32}$ $[M]^+$ 356.2504, found 356.2509; **$[\alpha]^{20}_D$** +1.0 (*c* 1.03, $CHCl_3$); **SFC** analysis (OJ-H, 20% IPA, 2.5 mL/min) indicated 97% ee t_R (minor) = 4.2 minutes, t_R (major) = 5.2 minutes. Crystals suitable for X-ray diffraction (vide infra) were grown by slow evaporation of solvent from a solution of the title compound in a mixture of methanol and pentane.



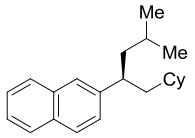
9

(+)-2-(1-cyclohexyl-7-methyloct-6-en-2-yl)naphthalene (9, table 2, entry 5): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.0537 g, 0.200 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), (5-methylhex-4-enyl)magnesium bromide (0.48 mL, 0.40 mmol, 0.83 M in Et_2O), and toluene (3.0 mL) for 48 h. Purification by flash column chromatography (100% pentane) afforded a colorless oil (0.054 g) as a mixture of the title compound (81% calculated yield) and the product of elimination (12% calculated yield). Further purification by flash chromatography on silver-impregnated silica (0–3% Et_2O in pentane) afforded a sample of analytically pure material: **TLC R_f** = 0.4 (100% pentane); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.81–7.76 (m, 3H), 7.55 (s, 1H), 7.46–7.39 (dp, *J* = 8.4, 1.2 Hz, 2H), 7.31 (dd, *J* = 8.5, 1.5 Hz, 1H), 5.01 (t, *J* = 7.1 Hz 1H), 2.80 (dq *J* = 14.8, 5.3 Hz, 1H), 1.96–1.82 (m, 3H), 1.68–1.47 (m, 14H), 1.36–1.18 (m, 2H), 1.16–1.01 (m, 4H), 0.94–0.80 (m, 2H); **^{13}C NMR** (500 MHz, $CDCl_3$) δ 144.0, 133.7, 132.3, 131.3, 128.0, 127.7, 127.6, 126.4, 126.1, 125.8, 125.1, 124.9, 44.9, 42.9, 37.2, 35.0, 34.4, 32.9, 28.2, 28.0, 26.8, 26.4, 26.3, 25.8, 17.8; **IR** (neat) 2919, 2850, 1447, 853, 815, 743 cm^{-1}; **HRMS** (TOF MS EI+) *m / z* cacld for $C_{25}H_{34}$ $[M]^+$ 334.2661, found 334.2660; **$[\alpha]^{24}_D$** +11.8 (*c* 5.33, $CHCl_3$) ; **SFC** analysis (OJ-H, 3% IPA, 2.5 mL/min) indicated 97% ee t_R (minor) = 6.5 minutes, t_R (major) = 6.9 minutes.



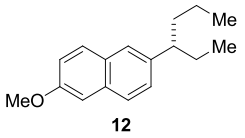
10

(+)-2-(1-cyclohexyl-6,6,6-trifluorohexan-2-yl)naphthalene (10, table 2, entry 6): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.0537 g, 0.200 mmol) and $NiCl_2$(dppe) (10.6 mg, 0.0200 mmol), (4,4,4-trifluorobutyl)magnesium bromide (0.20 mL, 0.40 mmol, 2.0 M in Et_2O), and toluene (3.0 mL) for a period of 48 h. Purification by flash column chromatography (100% pentane) afforded a colorless oil (0.054 g) as a mixture of the title compound (67% calculated yield) and the product of elimination (15% calculated yield). Further purification by flash chromatography on silver-impregnated silica (100% pentane) afforded a sample of analytically pure material: **TLC R_f** = 0.4 (100% pentane); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82–7.78 (m, 3H), 7.55 (s, 1H), 7.48–7.40 (dp, *J* = 6.9, 1.3 Hz, 2H), 7.29 (dd, *J* = 8.5, 1.5 Hz, 1H), 2.81 (dq *J* = 14.8, 4.9 Hz, 1H), 2.11–1.90 (m, 2H), 1.83 (d, *J* = 12.9 Hz, 1H), 1.75–1.25 (m, 10H), 1.15–1.01 (m, 4H), 0.93–0.81 (m, 2H); **^{13}C NMR** (500 MHz, $CDCl_3$) δ 142.9, 133.7, 132.4, 128.3, 127.8, 127.7, 126.4, 126.0, 125.7,125.3, 44.8, 42.8, 36.5, 34.9, 34.3, 33.9 (q, *J* = 28.3 Hz, 1C), 32.9, 26.7, 26.7, 26.3, 26.2, 20.3 (q, *J* = 2.8 Hz, 1C); **IR** (neat) 2920, 2850, 1448, 1253, 1131, 816, 744 cm^{-1}; **HRMS** (TOF MS EI+) *m / z* cacld for $C_{22}H_{27}F_3$ $[M]^+$ 348.2065, found 348.2065; **$[\alpha]^{26}_D$** +19.7 (*c* 1.2, $CHCl_3$); **SFC** analysis (OJ-H, 10% hexanes, 2.5 mL/min) indicated 97% ee t_R (major) = 4.7 minutes, t_R (minor) = 5.3 minutes.



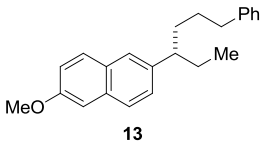
11

(+)-2-(1-cyclohexyl-4-methylpentan-2-yl)naphthalene (11, table 2, entry 7): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*S*)-**26** (0.134 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), *i*-butylmagnesium bromide (0.40 mL, 1.0 mmol, 2.5 M in Et_2O), and toluene (3.0 mL). Purification by flash column chromatography (100% hexanes) afforded a colorless oil (0.067 g) as a mixture of the title compound (40% calculated yield), the product of reduction (8% calculated yield), and the product of elimination (7% calculated yield). Further purification (100% heptanes) afforded a sample of analytically pure material: **TLC R_f** = 0.7 (100% hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 (q, *J* = 7.5 Hz, 3H), 7.56 (s, 1H), 7.43 (m, 2H), 7.32 (d, *J* = 9.0 Hz, 1H), 2.92 (hept, *J* = 5.0 Hz, 1H), 1.85 (d, *J* = 12.5 Hz, 1H), 1.66–1.54 (m, 6H), 1.49–1.39 (m, 2H), 1.33 (m, 1H), 1.14–1.03 (m, 4H), 0.92–0.84 (m, 5H), 0.80 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 144.2, 133.7, 132.3, 128.0, 127.7, 127.6, 126.3, 126.1, 125.8, 125.1, 46.9, 45.4, 40.5, 34.9, 34.3, 33.0, 26.8, 26.4, 26.3, 25.5, 23.7, 22.0; **IR** (neat) 2919, 2849, 1447, 853, 813, 743 cm^{-1}; **HRMS** (TOF MS EI^+) *m / z* cacld for $C_{22}H_{30}$ $[M]^+$ 294.2347, found 294.2350; **$[\alpha]^{27}_D$** +14.9 (*c* 0.80, $CHCl_3$); **SFC** analysis (OJ-H, 2% hexanes, 2.0 mL/min) indicated 90% ee: t_R (major) = 7.0 minutes, t_R (minor) = 8.4 minutes.



12

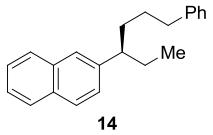
(–)-2-(hexan-3-yl)-6-methoxynaphthalene (12, table 2, entry 8): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*S*)-**SI-7** (0.115 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), *n*-propylmagnesium bromide (0.44 mL, 1.0 mmol, 2.3 M in Et_2O), and toluene (3.0 mL). Purification by flash column chromatography (3% EtOAc in hexanes) afforded a white solid (0.108 g) as a mixture of the title compound (80% calculated yield), the product of reduction (6% calculated yield), and the product of elimination (5% calculated yield). Further purification (100% hexanes) afforded a sample of analytically pure material: **TLC R_f** = 0.4 (5% EtOAc in hexanes); **m.p.** 57–58 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.68 (m, 2H), 7.49 (s, 1H), 7.28 (m, 1H), 7.12 (dd, *J* = 6.0, 2.8 Hz, 2H), 3.91 (s, 3H), 2.54 (m, 1H), 1.73–1.60 (m, 4H), 1.21–1.14 (m, 2H), 0.84 (t, *J* = 7.2, 3H), 0.78 (t, *J* = 7.4, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.2, 141.3, 133.2, 129.1 (2C), 126.8, 126.7, 126.4, 118.6, 105.8, 55.5, 47.7, 39.0, 29.8, 20.9, 14.3, 12.4; **IR** (neat) 2953, 2920, 2856, 816, 744, 697 cm^{-1}; **HRMS** (TOF MS CI^+) *m / z* cacld for $C_{17}H_{22}O$ $[M+H]^+$ 243.1749, found 243.1741; **$[\alpha]^{28}_D$** –8.2 (*c* 0.97, $CHCl_3$); **SFC** analysis (OD-H, 10% hexanes, 3.5 mL/min) indicated 92% ee: t_R (minor) = 4.4 minutes, t_R (major) = 4.6 minutes.



13

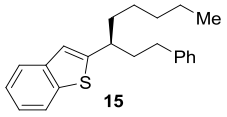
(+)-2-methoxy-6-(6-phenylhexan-3-yl)naphthalene (13, table 2, entry 9): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*S*)-**SI-7** (0.115 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), (3-phenylpropyl)magnesium bromide (0.50 mL, 1.0 mmol, 2.0 M in Et_2O), and toluene (3.0 mL). Purification by flash column chromatography (3% Et_2O in heptanes) afforded a colorless oil (0.145 g) as a mixture of the title compound (88% calculated yield), the

product of reduction (4% calculated yield), and the product of elimination (1% calculated yield). Further purification (preparatory TLC, 2% Et_2O in heptanes) afforded a sample of analytically pure material: **TLC R_f** = 0.4 (5% EtOAc in hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.5 Hz, 2H), 7.47 (s, 1H), 7.22 (m, 3H), 7.14–7.07 (m, 5H), 3.90 (s, 3H), 2.61–2.49 (m, 3H), 1.74–1.57 (m, 4H), 1.52–1.46 (m, 2H), 0.76 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.2, 142.8, 140.9, 133.3, 129.1 (2C), 128.5, 128.3, 126.9, 126.6, 126.4, 125.7, 118.6, 105.7, 55.4, 47.9, 36.3, 36.1, 29.9, 29.6, 12.4; **IR** (neat) 3025, 2930, 2856, 1605, 1264, 1032, 850 cm^{-1}; **HRMS** (TOF MS CI$^+$) *m / z* cacld for $C_{23}H_{26}O$ $[M]^+$ 318.1984, found 318.1994; **$[\alpha]^{26}_D$** +12.1 (*c* 0.50, $CHCl_3$); **SFC** analysis (OJ-H, 15% IPA, 2.0 mL/min) indicated 93% ee: t_R (minor) = 6.9 minutes, t_R (major) = 8.5 minutes.



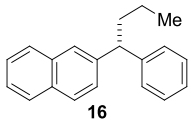
14

(–)-2-(6-phenylhexan-3-yl)naphthalene (14, table 2, entry 10): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**1** (0.040 g, 0.20 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), (3-phenylpropyl)magnesium bromide (0.24 mL, 0.40 mmol, 1.7 M in Et_2O), and toluene (3.0 mL). Purification by flash column chromatography (100% heptanes) afforded a colorless oil (0.054 g) as a mixture of the title compound (93% calculated yield) and the product of Wurtz coupling of the organomagnesium reagent (1,6-diphenylhexane). Further purification (flash column chromatography in 100% pentanes) afforded a sample of analytically pure material: **TLC R_f** = 0.6 (100% hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.1 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.54 (s, 1H), 7.42 (dt, J = 17.4, 6.7 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 1H), 7.22 (m, 2H), 7.12 (m, 1H), 7.08 (d, *J* = 7.3 Hz, 2H), 2.61–2.49 (m, 3H), 1.79–1.59 (m, 4H), 1.57–1.41 (m, 2H), 0.77 (t, *J* = 7.3Hz, 3H) **^{13}C NMR** (125 MHz, $CDCl_3$) δ 143.3, 142.7, 133.7, 132.4, 128.5, 128.5, 128.3, 128.3, 128.0, 127.7, 127.7, 126.6, 126.1, 125.9, 125.7, 125.2, 48.1, 36.2, 36.2, 29.8, 29.6, 12.4; **IR** (neat) 3024, 2928, 2856, 815, 743 cm^{-1}; **HRMS** (TOF MS CI$^+$) *m / z* cacld for $C_{22}H_{24}$ $[M]^+$ 288.1878, found 288.1880; **$[\alpha]^{24}_D$** –15.1 (*c* 1.08, $CHCl_3$); **SFC** analysis (OJ-H, 15% IPA, 2.0 mL/min) indicated 97% ee: t_R (minor) = 6.3 minutes, t_R (major) = 7.8 minutes.



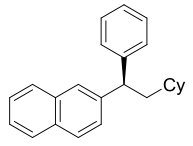
15

(+)-2-(1-phenyloctan-3-yl)benzo[*b*]thiophene (15, table 2, entry 11): A 7 mL vial was charged with (*R*)-**SI-10** (0.056 g, 0.200 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), flushed with nitrogen and capped. Toluene (3 mL) was added, followed by *n*-pentylmagnesium bromide (0.18 mL, 0.40 mmol, 2.3 M in Et_2O) and the reaction was allowed to stir at room temperature for 10 h. The vial was cracked open and another batch of $NiCl_2$(dppe) (5.3 mg, 0.010 mmol) was added. After further stirring for 14 h, the reaction was quenched by the addition of EtOAc (1 mL) and the entire reaction mixture was adsorbed onto silica gel (1 g). The solvents were removed in vacuo and the crude was purified by flash column chromatography (100% hexanes) to afford **15** as a colorless oil (0.035 g, 0.11 mmol, 54%): **TLC R_f** = 0.4 (100% hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 7.3 Hz, 1H), 7.26 (m, 3H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 2H), 7.03 (s, 1H), 2.93 (hept, *J* = 5.0 Hz, 1H), 2.60 (m, 1H), 2.54 (m, 1H), 2.03 (m, 1H), 1.94 (m, 1H), 1.55–1.70 (m, 2H), 1.26–1.13 (m, 6H), 0.82 (t, *J* = 6.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 151.2, 142.3, 140.1, 139.2, 128.6, 128.5, 125.9, 124.1, 123.5, 122.9, 122.5, 120.9, 42.0, 39.4, 37.8, 33.8, 31.9, 27.2, 22.7, 14.2; **IR** (neat) 3060, 2925, 2854, 1455, 1436, 821 cm^{-1}; **HRMS** (TOF MS CI$^+$) *m / z* cacld for $C_{22}H_{26}S$ $[M+H]^+$ 323.1833, found 323.1833; **$[\alpha]^{26}_D$** +13.4 (*c* 0.95, $CHCl_3$); **SFC** analysis (OD-H, 3% IPA, 2.5 mL/min) indicated 96% ee: t_R (major) = 20.0 minutes, t_R (minor) = 21.4 minutes.



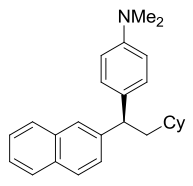
16

(–)-2-(1-phenylbutyl)naphthalene (16, table 2, entry 12): A 7 mL vial was charged with (*S*)-**SI-12** (0.124 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), flushed with nitrogen and capped. Toluene (3 mL) was added and the reaction was cooled to 0 °C. *n*-Propylmagnesium bromide (0.18 mL, 0.40 mmol, 2.3 M in Et_2O) was added and the reaction was allowed to stir at 0 °C for 48 h. The reaction was quenched by the addition of EtOAc (1 mL) and the entire reaction mixture was adsorbed onto silica gel (1 g). The solvents were removed in vacuo and the crude was purified by flash column chromatography (100% hexanes). The resulting colorless oil (0.104 g) was an inseparable mixture of the title compound (67% calculated yield) and the product of reduction[25] (15% calculated yield). Purification by preparatory HPLC (100 hexanes) afforded a small sample of analytically pure **16**: **TLC** $\mathbf{R_f}$ = 0.5 (100% hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (t, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.70 (s, 1H), 7.42 (m, 2H), 7.34 (d, *J* = 8.4 Hz, 1H), 7.28 (m, 4H), 7.17 (m, 1H), 4.02 (t, *J* = 8.2 Hz, 1H), 2.13 (hept, *J* = 5.6 Hz, 2H), 1.32 (sextet, *J* = 7.6 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 145.3, 142.9, 133.7, 132.2, 128.5, 128.13, 128.12, 127.8, 127.7, 127.0, 126.2, 126.02, 125.99, 125.4, 51.2, 37.8, 21.3, 14.3; **IR** (neat) 3055, 3024, 2954, 2928, 1599, 1506, 1493 cm^{-1}; **HRMS** (TOF MS CI^+) *m / z* cacld for $C_{20}H_{20}$ $[M]^+$ 260.1565, found 260.1567; $\mathbf{[\alpha]^{24}_D}$ –25.2 (*c* 0.54, $CHCl_3$); **SFC** analysis (OD-H, 2% IPA, 2.5 mL/min) indicated 91% ee: t_R (minor) = 5.9 minutes, t_R (major) = 7.5 minutes.



17

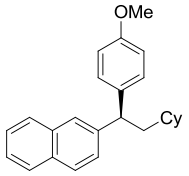
(–)-2-(2-cyclohexyl-1-phenylethyl)naphthalene (17, table 3, entry 1): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.134 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), phenylmagnesium bromide (0.37 mL, 1.0 mmol, 2.7 M in Et_2O), and toluene (7.5 mL) for a period of 24 h. Purification by flash column chromatography (100% pentane) afforded the title compound as a colorless oil (0.105 g, 0.33 mmol, 67%): **TLC** $\mathbf{R_f}$ = 0.2 (100% pentane); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (t, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.69 (s, 1H), 7.41 (quintd, *J* = 6.9, 1.3 Hz, 2H), 7.34 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.29–7.24 (m, 4H), 7.15 (m, 1H), 4.23 (t, *J* = 7.9 Hz, 1H), 2.08–1.95 (m, 2H), 1.80 (t, *J* = 11.7 Hz, 2H), 1.66–1.58 (m, 3H), 1.26–1.05 (m, 4H), 1.01–0.93 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 145.5, 143.0, 133.7, 132.3, 128.5, 128.1, 127.9, 127.7, 127.0, 126.2, 126.0, 125.4, 48.2, 43.5, 35.0, 33.7, 33.5, 26.8, 26.3 **IR** (neat) 2919, 2849, 1448, 3055, 1490, 743, 698 cm^{-1}; **HRMS** (TOF MS ES^+) *m / z* cacld for $C_{24}H_{26}$ $[M]^+$ 314.2035, found 314.2030; $\mathbf{[\alpha]^{25}_D}$ –10.8 (*c* 1.99, $CHCl_3$); **SFC** analysis (OJ-H, 15% IPA, 2.5 mL/min) indicated 92% ee: t_R (major) = 6.1 minutes, t_R (minor) = 6.9 minutes.



18

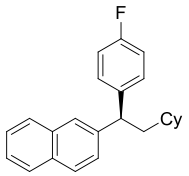
(–)-4-(2-cyclohexyl-1-(naphthalen-2-yl)ethyl)-*N*,*N*-dimethylaniline (18, table 3, entry 2): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26**

(0.054 g, 0.20 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), 4-(*N*,*N*-dimethylamino) phenylmagnesium bromide (0.133 g, 0.40 mmol), and toluene (3.0 mL) for a period of 48 h. Purification by flash column chromatography (1% Et_3N, 5% Et_2O in pentane) afforded the title compound as a yellow oil (0.057 g, 0.16 mmol, 79%): **TLC R_f** = 0.3 (1% Et_3N, 5% Et_2O in pentane); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.67 (t, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.67 (s, 1H), 7.44–7.32 (m, 3H), 7.13 (d, *J* = 8.6 Hz, 2H), 6.66 (d, *J* = 8.7 Hz), 4.14 (t, *J* = 7.9 Hz), 2.88 (s, 6H), 2.04–1.91 (m, 2H), 1.80 (t, *J* = 12.6, 2H), 1.66 (m, 3H), 1.25–1.05 (m, 4H), 1.01–0.92 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.1, 143.9, 133.7, 133.5, 132.1, 128.7, 128.0, 127.8, 127.7, 127.1, 125.8, 125.7, 125.2, 112.9, 47.1, 43.7. 40.9, 35.0, 33.7, 33.6, 26.8, 26.3; **IR** (neat) 2918, 2848, 1614, 1519, 1446, 1345, 813, 731 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{26}H_{31}N$ $[M+H]^+$ 358.2535, found 358.2529; **$[\alpha]^{26}_D$** –1.55 (*c* 2.59, $CHCl_3$).



19

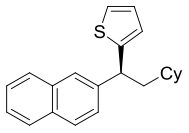
(–)-2-(2-cyclohexyl-1-(4-methoxyphenyl)ethyl)naphthalene (19, table 3, entry 3): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.134 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), 4-methoxyphenylmagnesium bromide (0.53 mL, 1.0 mmol, 1.9 M in Et_2O), and toluene (7.5 mL) for a period of 24 h. Purification by flash column chromatography (5% Et_2O in pentane) afforded a colorless oil (0.157 g) as a mixture of the title compound (86% calculated yield) and the starting material (15% calculated yiled). Further purification by column chromatography (1–15% benzene in hexanes) afforded a pure sample of **17**: **TLC R_f** = 0.7 (5% EtOAc in hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (t, *J* = 9.3 Hz, 2H), 7.72 (d, *J* = 8.5 Hz, 1H), 7.66 (s, 1H), 7.41 (m, 2H), 7.32 (d, *J* = 8.5 Hz, 1H), 7.18 (d, *J* = 8.5 Hz, 2H), 6.83 (d, *J* = 9.0 Hz, 2H), 4.18 (t, *J* = 7.3 Hz, 1H), 3.74 (s, 3H), 1.98 (m, 2H), 1.79 (m, 2H), 1.70–1.55 (m, 3H), 1.23–1.04 (m, 4H), 1.02–0.91 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 157.9, 143.4, 137.6, 133.7, 132.2, 129.0, 128.5, 128.1, 127.8, 127.7, 127.0, 126.0, 125.8, 125.4, 113.9, 55.3, 47.2, 43.7, 35.0, 33.62, 33.57, 26.8, 26.3; **IR** (neat) 2919, 2848, 1509, 1447, 1245, 1177, 1037 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{25}H_{28}O$ $[M]^+$ 344.2140, found 344.2131; **$[\alpha]^{24}_D$** –6.3 (*c* 1.17, $CHCl_3$); **SFC** analysis (AD-H, 15% IPA, 3.0 mL/min) indicated 97% ee: t_R (major) = 9.0 minutes, t_R (minor) = 9.6 minutes.



20

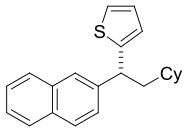
(–)-2-(2-cyclohexyl-1-(4-fluorophenyl)ethyl)naphthalene (20, table 3, entry 4): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.134 g, 0.500 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), 4-flourophenylmagnesium bromide (0.46 mL, 1.0 mmol, 2.2 M in Et_2O), and toluene (7.5 mL) for a period of 48 h. Purification by flash column chromatography (100% hexanes) afforded a colorless oil (0.147 g) as a mixture of the title compound (82% calculated yield) and the product of Wurtz coupling of the organomagnesium reagent. Further purification by column chromatography (100% pentane) afforded a pure sample of **18**: **TLC R_f** = 0.8 (5% EtOAc in hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (t, *J* = 7.5 Hz, 2H), 7.74 (d, *J* = 8.5 Hz, 1H), 7.66 (s, 1H), 7.43 (m, 2H), 7.31 (d, *J* = 8.5 Hz, 1H), 7.22 (dd, *J* = 8.5, 6.0 Hz, 2H), 6.95 (app t, *J* = 8.5 Hz, 2H), 4.21 (t, *J* = 8.0 Hz, 1H), 2.02 (quint, *J* = 7.1 Hz, 1H), 1.94 (quint, *J* = 7.0 Hz, 1H), 1.79 (t, *J* = 12.3

Hz, 2H), 1.70–1.56 (m, 3H), 1.22–1.04 (m, 4H), 0.99 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.4 (d, *J* = 242.5 Hz, 1C), 142.8, 141.1 (d, *J* = 3.3 Hz, 1C), 133.7, 132.2, 129.5 (d, *J* = 7.8 Hz, 2C), 128.2, 127.8, 127.7, 126.8, 126.1, 125.9, 125.5, 115.3 (d, *J* = 84.0 Hz, 2C), 47.3, 43.6, 35.0, 33.6, 33.5, 26.7, 26.2 (2C); **IR** (neat) 3053, 2920, 2850, 1506, 1222, 793 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{24}H_{25}F$ $[M]^+$ 332.1940, found 332.1930; **$[\alpha]^{20}_D$** –11.1 (*c* 0.91, $CHCl_3$); **SFC** analysis (OJ-H, 15% IPA, 2.5 mL/min) indicated 87% ee: t_R (major) = 4.3 minutes, t_R (minor) = 5.6 minutes.



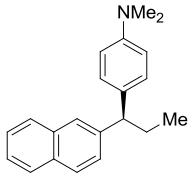
21

(+)-2-(2-cyclohexyl-1-(naphthalen-2-yl)ethyl)thiophene ((+)-21, table 3, entry 5): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**26** (0.054 g, 0.20 mmol) and $NiCl_2$(dppe) (10.6 mg, 0.0200 mmol), 2-thienylmagnesium bromide (0.15 mL, 0.40 mmol, 2.6 M in Et_2O), and toluene (3.0 mL) for a period of 48 h. Purification by flash column chromatography (2% Et_2O in pentane) afforded the title compound as a yellow oil (0.049 g, 0.15 mmol, 76%): **TLC R_f** = 0.5 (100% hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (t, *J* = 9.0 Hz, 3H), 7.70 (s, 1H), 7.42 (m, 3H), 7.12 (d, *J* = 4.4 Hz, 1H), 6.91 (dd, *J* = 5.2, 3.2 Hz, 1H), 6.83 (d, *J* = 3.2 Hz, 1H), 4.45 (t, *J* = 8.0 Hz, 1H), 2.05 (t, *J* = 7.4 Hz, 2H), 1.85 (d, *J* = 12.4 Hz, 1H), 1.73 (d, *J* = 12.4 Hz, 1H), 1.64–1.50 (m, 3H), 1.30–0.96 (m, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.2, 142.5, 133.7, 132.5, 128.4, 127.9, 127.8, 126.7, 126.3, 126.2, 126.1, 125.6, 123.9, 123.6, 45.1, 43.9, 35.1, 33.8, 33.1, 26.7, 26.3, 26.2; **IR** (neat) 3026, 2922, 2853, 1453, 743, 697 cm^{-1}; **HRMS** (TOF MS Cl^+) *m / z* cacld for $C_{22}H_{24}S$ $[M+H]^+$ 321.1677, found 321.1672; **$[\alpha]^{24}_D$** +42.4 (*c* 1.20, $CHCl_3$); **SFC** analysis (OD-H, 20% hexanes, 3.0 mL/min) indicated 93% ee: t_R (minor) = 14.9 minutes, t_R (major) = 17.5 minutes.



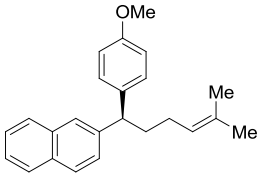
21

(–)-2-(2-cyclohexyl-1-(naphthalen-2-yl)ethyl)thiophene ((–)-21). Prepared according to the representative procedure outlined above using the following amounts of reagents: (*S*)-**26** (0.039 g, 0.15 mmol) and $NiCl_2$(dppe) (7.7 mg, 0.015 mmol), 2-thienylmagnesium bromide (0.17 mL, 0.29 mmol, 2.0 M in Et_2O), and toluene (2.2 mL) for a period of 48 h. Purification by flash column chromatography (2% Et_2O in pentane) afforded the title compound as a yellow oil (0.033 g, 0.10 mmol, 70%): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (t, *J* = 8.6 Hz, 3H), 7.70 (s, 1H), 7.42 (m, 3H), 7.13 (d, *J* = 5.2 Hz, 1H), 6.91 (dd, *J* = 5.2, 3.6 Hz, 1H), 6.84 (d, *J* = 3.6 Hz, 1H), 4.45 (t, *J* = 8.0 Hz, 1H), 2.05 (t, *J* = 7.4 Hz, 2H), 1.86 (d, *J* = 12.8 Hz, 1H), 1.73 (d, *J* = 12.4 Hz, 1H), 1.64–1.54 (m, 3H), 1.26–0.96 (m, 6H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.2, 142.5, 133.7, 132.5, 128.4, 127.9, 127.8, 126.7, 126.3, 126.14, 126.09, 125.6, 123.9, 123.6, 45.1, 43.8, 35.1, 33.8, 33.1, 26.7, 26.25, 26.21; **$[\alpha]^{24}_D$** –42.9 (*c* 0.98, $CHCl_3$); **SFC** analysis (OD-H, 20% hexanes, 3.0 mL/min) indicated 92% ee: t_R (major) = 14.3 minutes, t_R (minor) = 17.5 minutes.



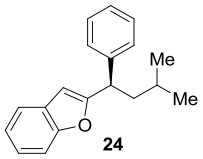
22

(–)-*N*,*N*-dimethyl-4-(1-(naphthalen-2-yl)propyl)aniline (22, table 3, entry 7): A 7 mL vial was equipped with a stir bar, flame dried, and pumped into a glove box while still warm. (*R*)-**1** (0.040 g, 0.20 mmol), $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), and 4-(*N*,*N*-dimethylamino) phenylmagnesium bromide (0.133 g, 0.400 mmol) were added. The vial was capped, removed from the glove box and put under a nitrogen atmosphere. Toluene (3 mL) was added and the reaction mixture was stirred for 24 h at which point the reaction was quenched with methanol. The crude mixture was eluted through a silica plug (100% Et_2O) and concentrated in vacuo. Purification by flash column chromatography (1% Et_3N, 5% Et_2O in pentane) afforded the title compound as a yellow oil (0.047 g, 0.16 mmol, 80% yield). Trace amounts (<5%) of Wurtz coupling product of the organomagnesium reagent could not be separated from the product: **TLC** $\mathbf{R_f}$ = 0.2 (1% Et_3N, 5% EtOAc in hexanes) **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.77 (t, *J* = 8.0 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.68 (s, 1H), 7.40 (quint, *J* = 8.0 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 6.75 (d, *J* = 8.4 Hz, 2H), 3.87 (t, *J* = 7.6 Hz, 1H), 2.89 (s, 6H), 2.17–2.08 (quint, *J* = 7.2 Hz, 2H), 0.93 (t, *J* = 7.4 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 149.2, 143.6, 133.7, 133.3, 132.2, 128.7, 128.0, 127.8, 127.7, 127.1, 125.9, 125.8, 125.2, 112.9, 52.4, 40.9, 28.6, 13.0; $\mathbf{[\alpha]^{26}_D}$ –3.4 (*c* 1.17, $CHCl_3$); **IR** (neat) 2958, 2928, 2871, 2797, 1613, 1564, 1818, 1345, 811, 780, 747; **HRMS** (TOF MS ES$^+$) *m* / *z* cacld for $C_{21}H_{23}N$ $[M+H]^+$ 290.1909, found 290.1903; $\mathbf{[\alpha]^{25}_D}$ –3.4 (*c* 1.16, $CHCl_3$) **SFC** analysis (AD-H, 20% IPA, 2.5 mL/min) indicated 95% ee: t_R (major) = 6.1 minutes, t_R (minor) = 7.4 minutes.



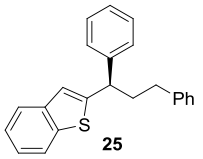
23

(–)-2-(1-(4-methoxyphenyl)-5-methylhex-4-enyl)naphthalene (23, table 3, entry 8): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**SI-15** (0.071 g, 0.28 mmol) and $NiCl_2$(dppe) (5.3 mg, 0.010 mmol), (4-methoxy)phenylmagnesium bromide (0.32 mL, 0.56 mmol, 1.8 M in Et_2O), and toluene (4.2 mL) for a period of 48 h. Purification by flash column chromatography (2% Et_2O in pentane) afforded an oil (0.091 g) as a mixture of the title compound (94% calculated yield) and the product of Wurtz coupling of the organomagnesium reagent. Further purification by column chromatography (1% Et_2O in pentane) afforded a pure sample of **21**: **TLC** $\mathbf{R_f}$ = 0.7 (2% EtOAc in hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (t, *J* = 8.3 Hz, 2H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.68 (s, 1H), 7.41 (m, 2H), 7.31 (d, *J* = 8.5 Hz, 1H), 7.19 (d, *J* = 9.0 Hz, 2H), 6.81 (d, *J* = 9.0 Hz, 2H), 5.17 (t, *J* = 7.0 Hz, 1H), 4.02 (t, *J* = 7.8 Hz, 1H), 3.75 (s, 3H), 2.14 (m, 2H), 1.97 (app q, *J* = 7.5 Hz, 2H), 1.69 (s, 3H), 1.48 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 158.0, 143.1, 137.3, 133.7, 132.22, 132.16, 129.1, 128.1, 127.8, 127.7, 126.9, 126.0, 125.9, 125.4, 124.3, 113.9, 55.3, 49.9, 35.8, 26.5, 25.9, 17.9; **IR** (neat) 2925, 1608, 1509, 1440, 1245 cm^{-1}; **HRMS** (TOF MS Cl$^+$) *m* / *z* cacld for $C_{24}H_{26}O$ $[M]^+$ 330.1984, found 330.1986; $\mathbf{[\alpha]^{20}_D}$ –2.7 (*c* 1.06, $CHCl_3$); **SFC** analysis (AD-H, 10% IPA, 3.0 mL/min) indicated 78% ee: t_R (major) = 8.5 minutes, t_R (minor) = 9.2 minutes.



24

(–)-2-(3-methyl-1-phenylbutyl)benzofuran (24, table 3, entry 9): Prepared according to the representative procedure outlined above using the following amounts of reagents: (*R*)-**SI-18** (0.044 g, 0.20 mmol) and $NiCl_2$(dppe) (10.6 mg, 0.020 mmol), phenylmagnesium bromide (0.13 mL, 0.40 mmol, 3.1 M in Et_2O), and toluene (3.0 mL) for a period of 48 h. Purification by flash column chromatography (100% hexanes) afforded the title compound as a colorless oil (0.037 g, 0.14 mmol, 71%): **TLC R_f** = 0.6 (5% EtOAc in hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.0 Hz, 1H), 7.39 (d, *J* = 7.5 Hz, 1H), 7.30 (m, 4H), 7.23–7.14 (m, 3H), 6.43 (s, 1H), 4.16 (t, *J* = 8.0 Hz, 1H) 2.08 (m, 1H), 1.89 (m, 1H), 1.51 (m, 1H), 0.95 (d, *J* = 6.5 Hz, 3H), 0.93 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 161.6, 154.9, 142.3, 128.8, 128.7, 128.1, 126.8, 123.4, 122.6, 120.5, 111.1, 102.4, 43.7, 43.6, 25.6, 23.0, 22.4; **IR** (neat) 3028, 2954, 2926, 2867, 1453, 1253 cm^{-1}; **HRMS** (TOF MS CI^+) *m / z* cacld for $C_{19}H_{20}O$ $[M+H]^+$ 265.1592, found 265.1594; **$[\alpha]^{24}_D$** –45.5 (*c* 1.05, $CHCl_3$); **SFC** analysis (OD-H, 2% IPA, 3.0 mL/min) indicated 95% ee: t_R (minor) = 5.2 minutes, t_R (major) = 5.7 minutes.



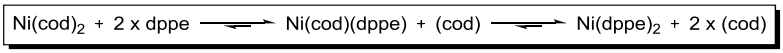
25

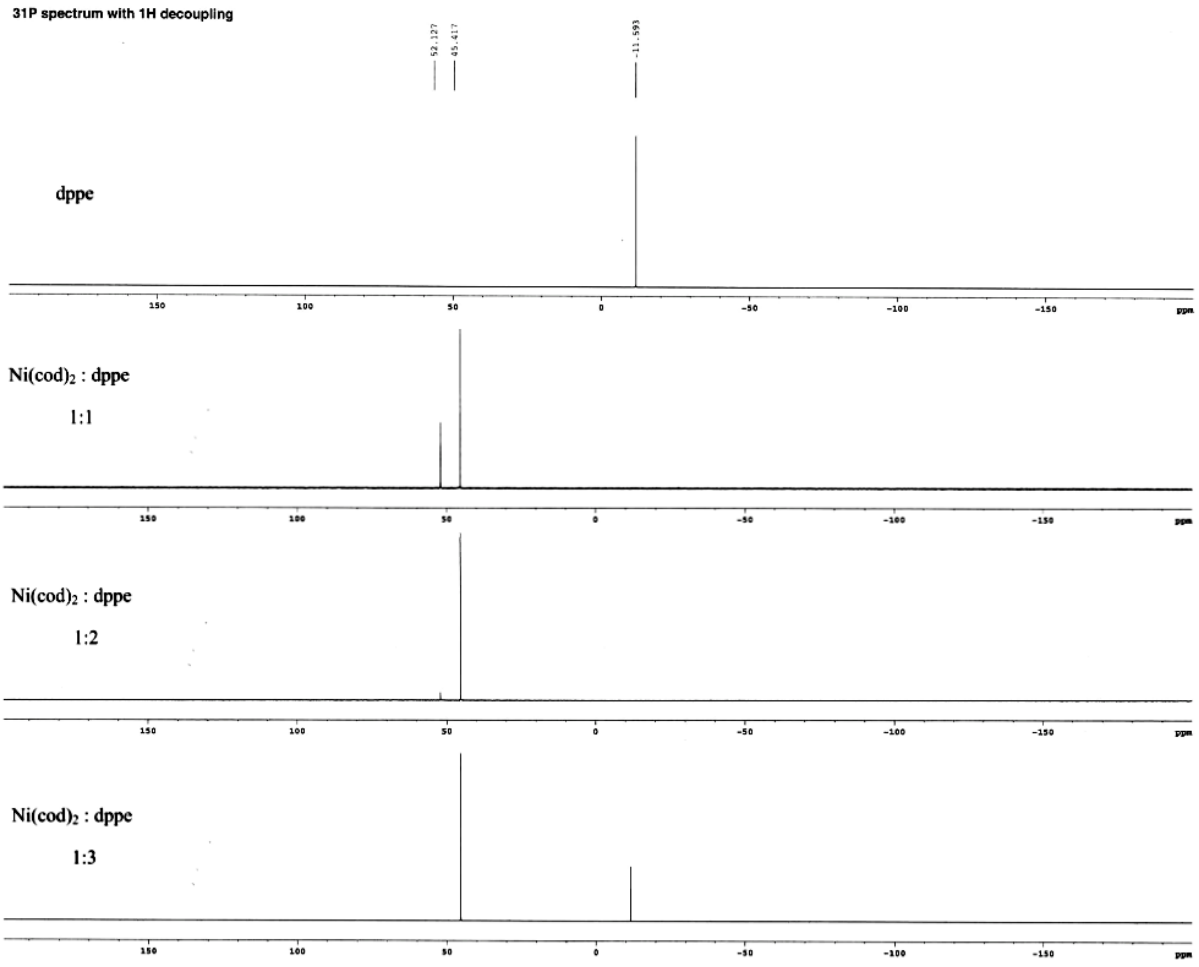
(–)-2-(1,3-diphenylpropyl)benzo[*b*]thiophene (25, table 3, entry 10): A 7 mL vial was charged with (*R*)-**SI-10** (0.056 g, 0.20 mmol) and $NiCl_2$(dppe) (10.6 mg, 0.0200 mmol), flushed with nitrogen and capped. Toluene (3 mL) was added, followed by phenylmagnesium bromide (0.13 mL, 0.40 mmol, 3.1 M in Et_2O) and the reaction was allowed to stir at room temperature for 12 h. The vial was cracked open and another batch of $NiCl_2$(dppe) (10.6 mg, 0.0200 mmol) was added. After further stirring for 14 h, the reaction was quenched by the addition of EtOAc (1 mL) and the entire reaction mixture was adsorbed onto silica gel (1 g). The solvents were removed in vacuo and the crude was purified by flash column chromatography (2% EtOAc in hexanes) to afford the title compound as a colorless oil (0.050 g, 0.15 mmol, 76%): **TLC R_f** = 0.4 (5% EtOAc in hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.35–7.16 (m, 12H), 7.08 (s, 1H), 4.20 (t, *J* = 7.6 Hz, 1H), 2.66 (m, 2H), 2.56–2.40 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ 150.3, 143.7, 141.8, 140.0, 139.5, 128.8, 128.63, 128.56, 128.0, 127.0, 126.1, 124.3, 123.8, 123.2, 122.3, 120.5, 47.0, 38.4, 34.0; **IR** (neat) 3026, 2922, 2853, 1453 cm^{-1}; **HRMS** (TOF MS CI^+) *m / z* cacld for $C_{23}H_{20}S$ $[M+H]^+$ 329.1364, found 329.1362; **$[\alpha]^{24}_D$** –8.4 (*c* 1.00, $CHCl_3$); **SFC** analysis (OD-H, 5% IPA, 3.0 mL/min) indicated 93% ee: t_R (minor) = 16.6 minutes, t_R (major) = 17.7 minutes.

VII. Mechanistic Studies

Activity of Ni^0 Complexes

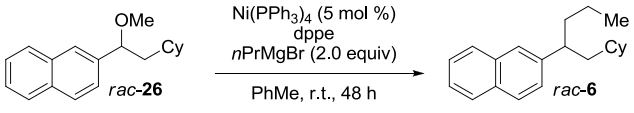
Procedure for NMR studies: In a glovebox, a vial was charged with $Ni(cod)_2$ (11 mg, 0.040 mmol), dppe (16 mg, 0.040 mmol) and toluene (3.0 mL). The solution was transferred to a NMR tube and a ^{31}P NMR spectrum was collected. Experiment was repeated with 2 and 3 equiv of dppe, (32 mg, 0.080 mmol) and (48 mg, 0.012 mmol) respectively, as well as a control experiment without $Ni(cod)_2$.





^{31}P NMR analysis revealed that the thermodynamically favorable $Ni(dppe)_2$ complex (45.4 ppm) is the major observed product. At equimolar ratio of Ni and dppe, we observed a peak at 51.1 ppm, which is attributed to a Ni(dppe)(cod) complex. Over time (20 min) this peak disappears and only a signal due to $Ni(dppe)_2$ is observed.

Procedure for $Ni(PPh_3)_4$ studies: In a glovebox, a vial was charged with $Ni(PPh_3)_4$ (11 mg, 0.010 mmol), dppe (4.0 mg, 0.010 mmol), *rac*-**26** (0.054 g, 0.20 mmol) and toluene (3.0 mL). The vial was capped, taken out of the glovebox and placed under N_2 atmosphere. *n*-PrMgBr (0.17 mL, 0.40 mmol, 2.3 M in Et_2O) was added and the mixture was stirred for 48 h. The reaction was quenched by the addition of EtOAc (1 mL), passed through a silica plug (100% Et_2O), the organics were removed under reduced pressure, and the crude was analyzed by ^1H NMR spectroscopy with $PhSiMe_3$ as internal standard. Experiment was repeated with 12 mol % dppe (9.6 mg), as well as in the absence of dppe.



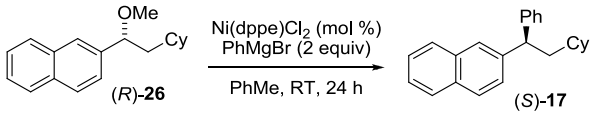
Entry	dppe (mol %)	Recovered **26** (%)[a]	Yield **6** (%)[a]
1	0	91	0
2	5	0	73
3	11	101	0

[a] Determined by ^1H NMR analysis using internal standard ($PhSiMe_3$).

We postulated that the ligand exchange rate between dppe and PPh_3 will be slower than in the case with cod. This difference in rates could preclude the swift formation of the $Ni(dppe)_2$ complex, thus restoring reactivity in the system. The cross-coupling reaction of *n*-propylmagnesium bromide employing $Ni(PPh_3)_4$ as the nickel source afforded **6** in 73% yield. Notably, in the absence of dppe as well as when there is an excess of dppe (>2:1 dppe:Ni) no desired reactivity is observed.

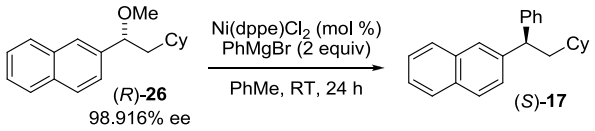
Effect of Catalyst Loading on Enantiospecificity

Procedure: Experiments were performed following the general procedure outlined in Section V. For consistency purposes, only two amounts of $NiCl_2$(dppe) were weighed out, while the amounts of other reagents were varied to achieve the desired catalyst loading. Benzylic ether (*R*)-**26** was dispensed as a 0.100 M solution in toluene. Phenylmagnesium bromide was dispensed as a 2.8 M solution in Et_2O. For precise amounts of reagents used see Table SI-1 below.



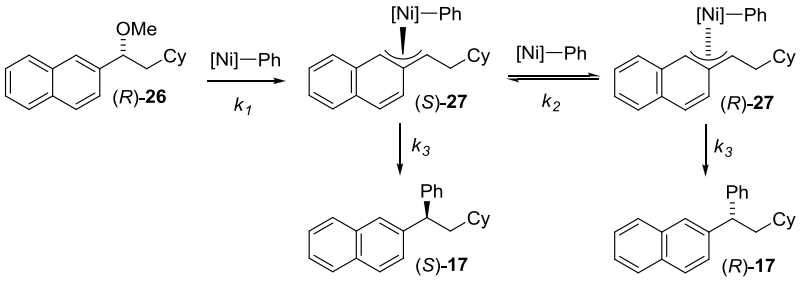
Entry	$Ni(dppe)Cl_2$ [mol %]	$Ni(dppe)Cl_2$ [mmol]	$Ni(dppe)Cl_2$ [mg]	(*S*)-**26** [mmol]	(*R*)-**26** [mL]	PhMe [mL]	Total volume [mL]	PhMgBr [mmol]	PhMgBr [µL]
1	4.0	0.010	5.3	0.25	2.50	1.25	3.75	0.50	185
2	6.0	0.012	6.3	0.20	2.00	1.00	3.00	0.40	148
3	8.0	0.012	6.3	0.15	1.50	0.75	2.25	0.30	111
4	10.0	0.010	5.3	0.10	1.00	0.50	1.50	0.20	74
5	12.0	0.012	6.3	0.10	1.00	0.50	1.50	0.20	74

Results:



Entry	$Ni(dppe)Cl_2$ [mol %]	ee [%]	es [%]
1	4.0	92.918	93.936
2	6.0	85.178	86.111
3	8.0	81.158	82.047
4	10.0	77.298	78.145
5	12.0	74.358	75.173

Derivation:



We reasoned that one could use a steady state approximation to describe intermediate (*R*)-**27** and express it in terms of concentration of Ni (Eq. 1 and 2). There are a few key assumptions that have to be made: (1) the complex that undergoes oxidative addition and the nucleophilic nickel species responsible for racemization are one and the same or in a fast equilibrium with each other and (2) the above complexes also need to be in fast equilibrium with the precatalyst. Thus, the ratio of the two enantiomers of product formed in the reaction should be inversely proportional to the concentration of nickel (Eq. 3).

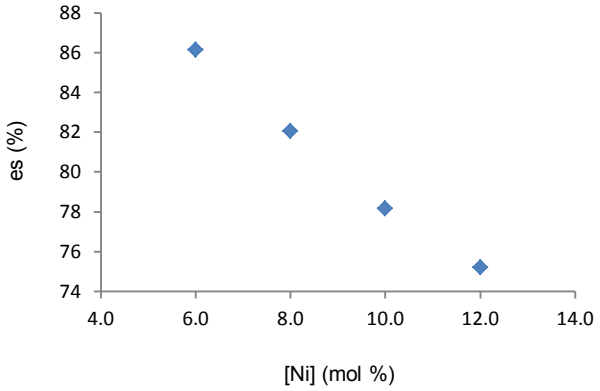
$$\frac{d[(R)\text{-}\mathbf{27}]}{dt} = k_2*[(S)\text{-}\mathbf{27}]*[\mathrm{Ni}] - k_3*[(R)\text{-}\mathbf{17}] - k_2*[(R)\text{-}\mathbf{27}]*[\mathrm{Ni}] = 0 \qquad (1)$$

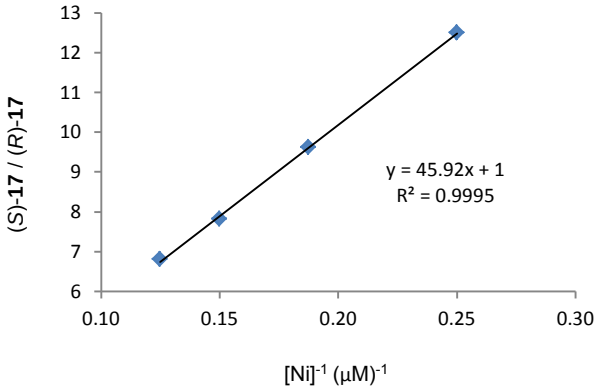
$$[(R)\text{-}\mathbf{27}] = \frac{k_2*[(S)\text{-}\mathbf{27}]*[\mathrm{Ni}]}{k_3 + k_2*[\mathrm{Ni}]} \qquad (2)$$

$$\frac{(S)\text{-}\mathbf{17}}{(R)\text{-}\mathbf{17}} = \frac{k_3*[(S)\text{-}\mathbf{27}]}{k_3*[(R)\text{-}\mathbf{27}]} = \frac{[(S)\text{-}\mathbf{27}]}{\frac{k_2*[(S)\text{-}\mathbf{27}]*[\mathrm{Ni}]}{k_3 + k_2*[\mathrm{Ni}]}} = \frac{k_3 + k_2*[\mathrm{Ni}]}{k_2*[\mathrm{Ni}]} = \frac{k_3}{k_2*[\mathrm{Ni}]} + 1 = \frac{k_{obs}}{[\mathrm{Ni}]} + 1 \qquad (3)$$

Plots:

Entry	$Ni(dppe)Cl_2$ [mol %]	[Ni] [μM]	$[Ni]^{-1}$ $[\mu M^{-1}]$	(*S*)-**17** [%]	(*R*)-**17** [%]	(*S*)-**17** / (*R*)-**17**
1	6.0	4.00	0.250	92.589	7.411	12.493
2	8.0	5.33	0.188	90.579	9.421	9.615
3	10.0	6.67	0.150	88.649	11.351	7.810
4	12.0	8.00	0.125	87.179	12.821	6.800





VIII. Biological Experiments

General Information

Biological experiments were performed according to a modified procedure by Sigman et al.[26]

Materials: The following reagents were obtained from commercial sources as indicated: Dulbecco's Modified Eagle's Medium (DMEM)/high glucose containing 4.5 g/L glucose and 4.0 mM L-glutamine (HyClone); fetal bovine serum (FBS), heat-inactivated (Omega Scientific); L-glutamine, 200 mM (Gibco); penicillin/streptomycin solution 50X (Mediatech); DMEM/Ham's Nutrient Mixture F12 containing 2.5 mM L-glutamine, 3151 mg/L dextrose, and 55 mg/L sodium pyruvate (Sigma-Aldrich); horse serum (Sigma-Aldrich); 50 μM hydrocortisone solution (Sigma-Aldrich); human insulin solution (Sigma-Aldrich); cholera toxin (Sigma-Aldrich); human Epidermal Growth Factor (EGF), recombinant (Sigma-Aldrich); 0.25% Trypsin-EDTA (Gibco); nuclease-free sterile water (Fisher Scientific); molecular biology grade DMSO (Sigma-Aldrich); ICI 182,780 (faslodex) (Tocris Bioscience).

Cell Lines and Culture Conditions: MCF-7 cells were maintained in DMEM/high glucose supplemented with 10% FBS, L-glutamine, and penicillin/streptomycin. Experiments with MCF-7 cells were performed in DMEM/high glucose supplemented with 2% FBS, L-glutamine, and penicillin/streptomycin.

MCF-10A cells were maintained in standard medium according to a modified recipe by Brugge et al.[27]: DMEM/F12 supplemented with 5% horse serum, 10 μg/mL human insulin, 0.5 μg/mL hydrocortisone, 10 ng/mL EGF, 100 ng/mL cholera toxin, and penicillin/streptomycin. Experiments with MCF-10A cells were performed in the same medium.

Evaluation of Compounds Against MCF-7 Cells

Procedure: MCF-7 cells were centrifuged in 1X PBS for 20 min, then the pellet was resuspended in DMEM supplemented with 10% FBS and filtered through a 40 μm nylon cell strainer (Fisher Scientific) to prevent clumping. The cells were seeded at 1,500 cells per well in 96-well flat bottom plates suitable for fluorimetry, using 175 μL per well DMEM supplemented with 10% FBS, and incubated with 5% CO_2 at 37 °C for 24 h. The compounds (including the faslodex positive control) were dissolved in molecular biology grade DMSO to achieve a 3.5 mM stock, then sterile filtered through a 0.45 μm PVDF syringe filter unit (Fisher Scientific). The 3.5 mM stock solutions were subsequently diluted to a final concentration of 10 μM in DMEM supplemented with 2% FBS. Additionally, the corresponding DMSO vehicle control was diluted using the same medium.

The medium was aspirated from the 96-well plates containing the MCF-7 cells using a multichannel pipettor and the medium containing the compounds and controls was added (day 0). The outer row of wells contained medium only to negate edge effects due to the evaporation of the medium. The cells were incubated with compound for 48 h then treated again by aspirating the medium and adding fresh medium containing the compounds and controls (day 2). This procedure was repeated after an additional 48 h (day 4). After incubating a final 24 h, the 96-well plates were flicked dry of medium, rinsed with 1X PBS, blotted dry, and then frozen at –78 °C overnight (day 5). On day 6, cell proliferation was measured using the fluorescence-based CyQUANT Cell Proliferation Assay Kit (Invitrogen).

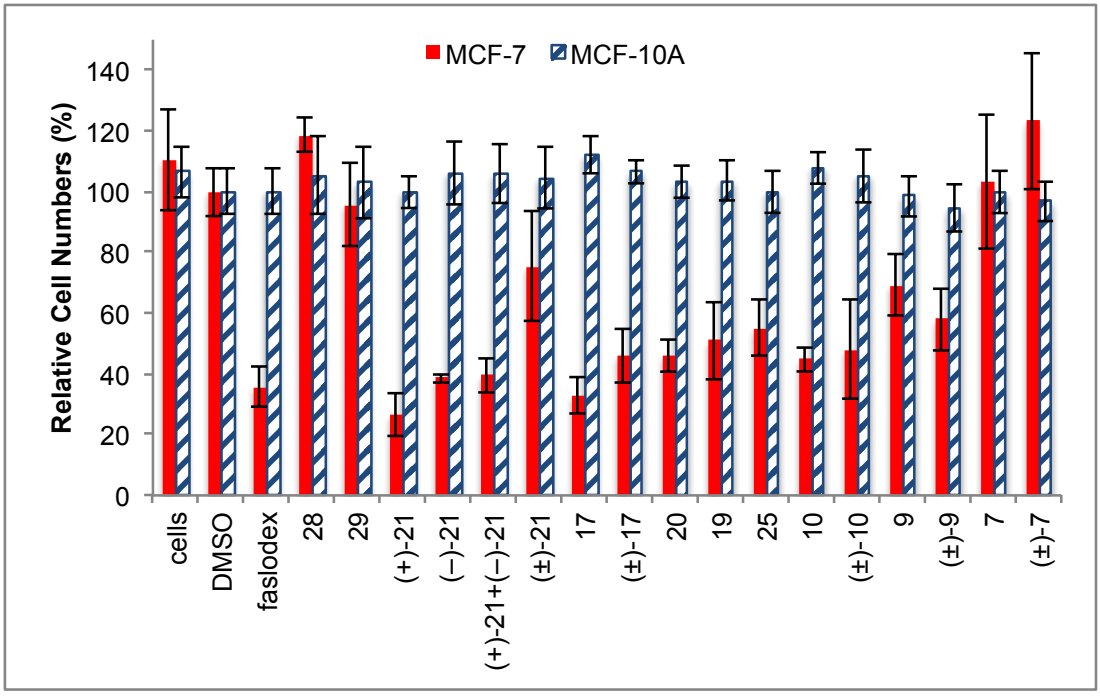
Fluorimetry analysis was performed according to a modified procedure by McGowan et al.[28] Cells were stained with 200 μL/well of 1X CyQUANT GR dye in cell lysis buffer for 10 min in the dark at RT and quantified by fluorimetry at 535 nm with 485 nm excitation, measured using a PerkinElmer VICTOR^3 1420 Multilabel Counter. The fluorescence values were normalized to the DMSO vehicle control. The normalized values were plotted as an average ± standard deviation of 4 wells per compound.

Evaluation of Compounds Against MCF-10A Cells

Procedure: MCF-10A cells were centrifuged in 1X PBS for 20 min, then the pellet was resuspended in DMEM/F12 and filtered through a 40 μm nylon cell strainer (Fisher Scientific) to prevent clumping. The cells were seeded at 9,000 cells per well in 96-well flat bottom plates suitable for fluorimetry, using 175 μL per well DMEM/F12, and incubated with 5% CO_2 at 37 °C for 24 h. The 3.5 mM stock solutions of compound in DMSO were subsequently diluted to a final concentration of 10 μM in DMEM/F12. Additionally, the corresponding DMSO vehicle control was diluted using the same medium.

Addition of compounds was performed as specified above for days 0 through 6. Fluorimetry analysis was performed as specified above for MCF-7 cells, with the exception of staining MCF-10A cells with 200 μL/well of 5X CyQUANT GR dye in cell lysis buffer for 10 min in the dark at RT before quantification by fluorimetry. The fluorescence values were normalized to the DMSO vehicle control. The normalized values were plotted as an average ± standard deviation of 6 wells per compound.

Results:

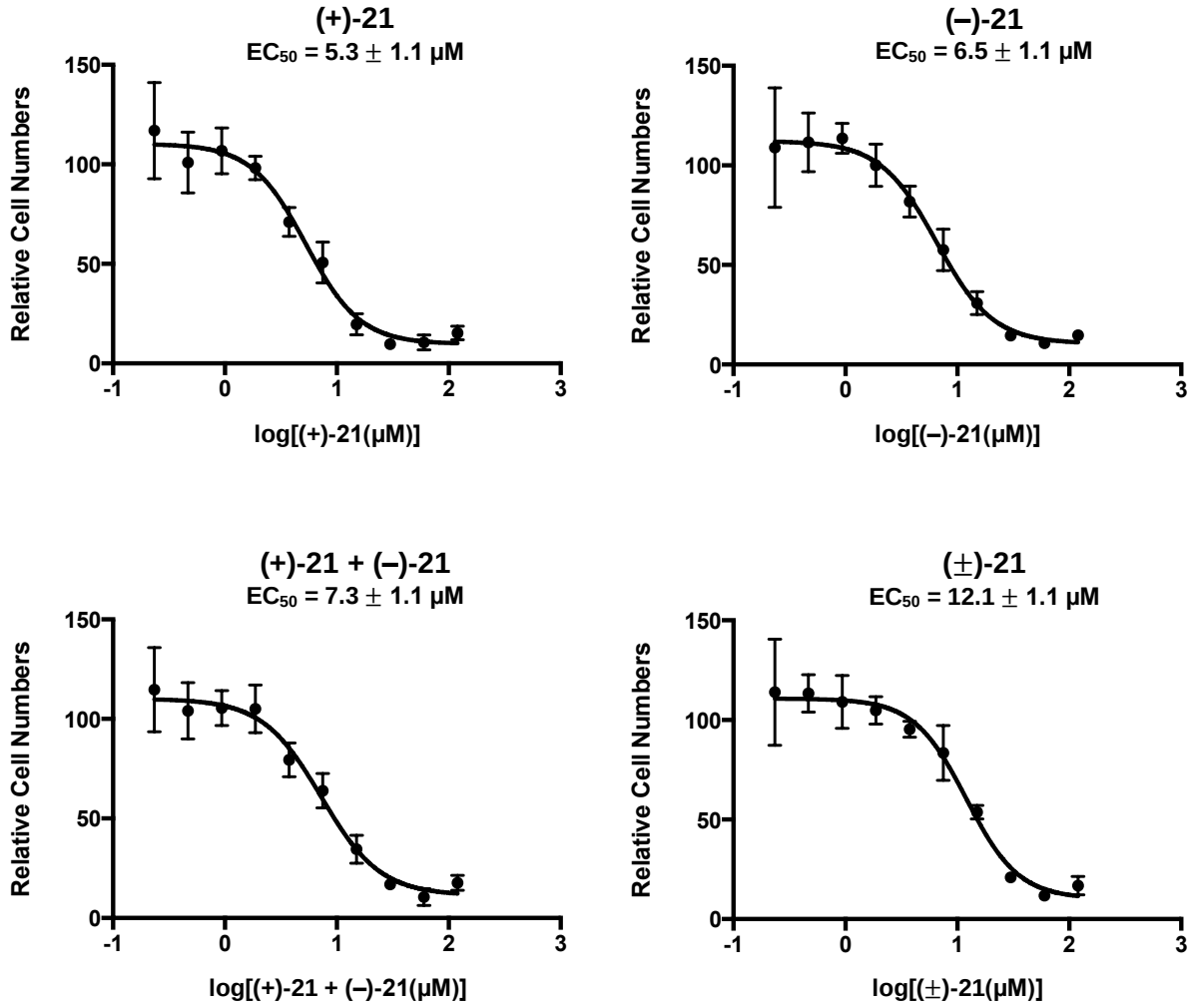


Dose Response of Compounds (+)-21, (–)-21, (+)-21 + (–)-21, and (±)-21

Procedure: MCF-7 cells were centrifuged in 1X PBS for 20 min, then the pellet was resuspended in DMEM supplemented with 10% FBS and filtered through a 40 μm nylon cell strainer (Fisher Scientific) to prevent clumping. The cells were seeded at 1,500 cells per well in 96-well flat bottom plates suitable for fluorimetry, using 175 μL per well DMEM supplemented with 10% FBS, and incubated with 5% CO_2 at 37 °C for 24 h. The compounds (+)-**21**, (–)-**21**, (+)-**21** + (–)-**21**, and (±)-**21**[29] were dissolved in molecular biology grade DMSO to achieve a 42 mM stock, then sterile filtered through a 0.45 μm PVDF syringe filter unit (Fisher Scientific). The 42 mM stock solutions in DMSO were subsequently diluted to 120 μM in DMEM supplemented with 2% FBS, and then serially diluted to achieve 10 different concentrations. Additionally, the corresponding DMSO vehicle controls for each concentration were serially diluted using the same medium.

Addition of compounds was performed as specified above for days 0 through 6. Fluorimetry analysis was performed as specified above for the evaluation of compounds against MCF-7 cells. The fluorescence values were normalized to the DMSO vehicle controls corresponding to each concentration. The normalized values were plotted as an average ± standard deviation of 4 wells per concentration and these data were analyzed using the dose response nonlinear regression fitting function (log[inhibitor] vs. response with variable slope (four parameters)) with GraphPad Prism 6.

Dose Response Curves:



IX. References

[1] Krasovskiy, A.; Knochel, P. *Synthesis* **2006**, *5*, 890–891.
[2] Attenburrow, J.; Cameron, A. F. B.; Chapman, J. H.; Evans, R. M.; Hems, B. A.; Jansen, A. B. A.; Walker, T. *J. Chem. Soc.* **1952**, 1094–1111.
[3] All alkyl and arylhalides were commercially available and used as received without any purification unless otherwise noted.
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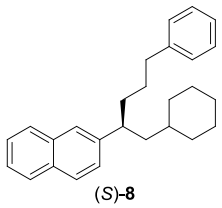
[29] (+)-**21** and (–)-**21** are samples of each single enantiomer with 93% ee and 92% ee, respectively; (±)-**21** is a sample of the racemic standard; (+)-**21** + (–)-**21** is a sample containing an equimolar ratio of the two enantiomers, combined in DMSO prior to biological testing.

X. Crystallographic Data

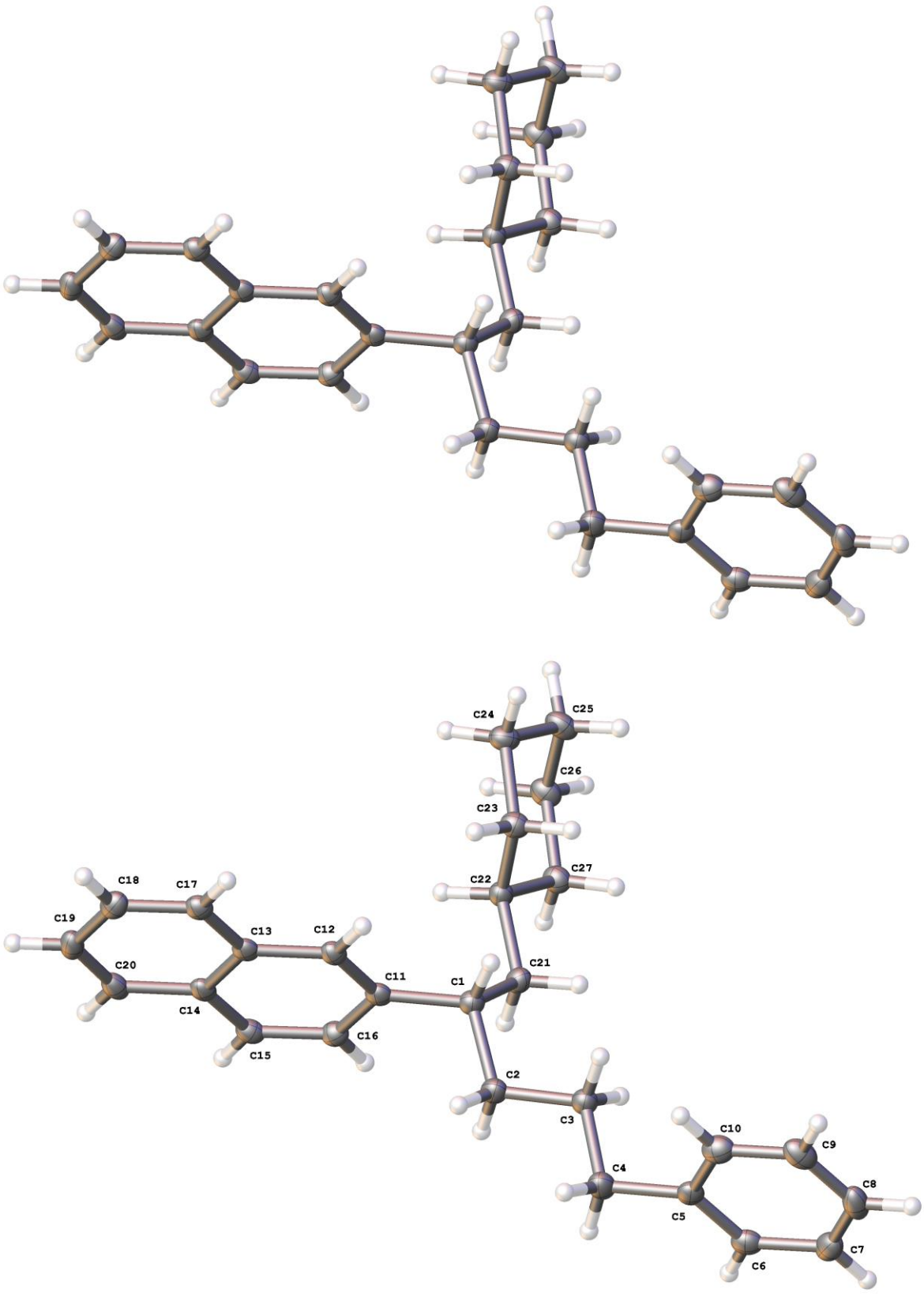


(*S*)-**8**

X-ray Data Collection, Structure Solution and Refinement for (*S*)-**8** (Table 2, entry 4).

The single crystal X-ray diffraction studies were carried out on a Bruker Kappa APEX CCD diffractometer equipped with Cu K_α radiation (λ = 1.5478). Crystals of the subject compound were grown by slow evaporation of solvent from a solution of the title compound in a mixture of methanol and pentane. A 0.217 x 0.095 x 0.053 mm colorless needle was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 90(2) K using ϕ and ϖ scans. Data was collected at two crystal-to-detector distances, 45mm or 60mm, using variable exposure time (2s-10s) depending on θ with a scan width of 1.0°. Data collection was 98.7% complete to 68.00° in θ. A total of 57312 reflections were collected covering the indices, --7<=h<=7, -16<=k<=16, -17<=l<=17. 7355 reflections were found to be symmetry independent, with a R_{int} of 0.0524. Indexing and unit cell refinement indicated a primitive, triclinic lattice. The space group was found to be *P*1. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model consistent with the proposed structure.

All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2013). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2013. Crystallographic data are summarized in Table 1.


C24
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C8
C5
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C6

Table 1. Crystal data and structure refinement for Jarvo02.

Identification code	ERJ-14	
Empirical formula	C27 H32	
Molecular formula	C27 H32	
Formula weight	356.52	
Temperature	90 K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	a = 5.9031(2) Å	α= 106.3499(15)°.
	b = 13.8552(5) Å	β= 98.3273(14)°.
	c = 14.0936(5) Å	γ = 101.5540(15)°.
Volume	1058.56(7) $Å^3$	
Z	2	
Density (calculated)	1.119 Mg/m^3	
Absorption coefficient	0.463 mm^{-1}	
F(000)	388	
Crystal size	0.217 x 0.095 x 0.053 mm^3	
Crystal color, habit	Colorless Needle	
Theta range for data collection	3.345 to 69.358°.	
Index ranges	-7<=h<=7, -16<=k<=16, -17<=l<=17	
Reflections collected	57312	
Independent reflections	7355 [R(int) = 0.0524]	
Completeness to theta = 68.000°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7532 and 0.7017	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7355 / 3 / 487	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0787	
R indices (all data)	R1 = 0.0324, wR2 = 0.0799	
Absolute structure parameter	0.065(347)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.120 and -0.172 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Jarvo02. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8627(3)	2712(2)	9759(1)	20(1)
C(2)	8982(4)	1839(2)	10204(2)	23(1)
C(3)	9335(3)	883(2)	9445(1)	21(1)
C(4)	10054(4)	108(2)	9944(2)	27(1)
C(5)	10507(3)	-808(2)	9186(1)	21(1)
C(6)	8896(3)	-1776(2)	8845(2)	23(1)
C(7)	9312(4)	-2603(2)	8126(2)	27(1)
C(8)	11349(4)	-2473(2)	7748(2)	29(1)
C(9)	12964(4)	-1513(2)	8083(2)	28(1)
C(10)	12546(4)	-689(2)	8797(2)	26(1)
C(11)	8776(3)	3692(2)	10609(1)	18(1)
C(12)	10775(3)	4502(2)	10932(1)	18(1)
C(13)	11023(3)	5399(2)	11773(1)	18(1)
C(14)	9133(3)	5458(2)	12292(1)	19(1)
C(15)	7078(3)	4622(2)	11945(1)	21(1)
C(16)	6901(3)	3768(2)	11136(1)	20(1)
C(17)	13086(3)	6234(2)	12111(1)	20(1)
C(18)	13267(3)	7090(2)	12923(2)	23(1)
C(19)	11385(4)	7148(2)	13438(2)	24(1)
C(20)	9373(4)	6355(2)	13131(2)	22(1)
C(21)	6322(3)	2349(2)	8940(2)	21(1)
C(22)	5748(3)	3152(2)	8446(1)	19(1)
C(23)	7800(3)	3596(2)	8012(2)	22(1)
C(24)	7172(4)	4332(2)	7439(2)	24(1)
C(25)	4963(4)	3801(2)	6602(2)	27(1)
C(26)	2893(3)	3389(2)	7036(2)	25(1)
C(27)	3503(3)	2646(2)	7602(2)	22(1)
C(1')	9460(3)	671(2)	3372(1)	21(1)
C(2')	10172(4)	1568(2)	2946(2)	24(1)
C(3')	11922(4)	2533(2)	3706(2)	23(1)
C(4')	12998(4)	3309(2)	3205(2)	28(1)

C(5')	14500(4)	4307(2)	3977(2)	23(1)
C(6')	13548(4)	5157(2)	4278(2)	25(1)
C(7')	14867(4)	6067(2)	5020(2)	28(1)
C(8')	17162(4)	6145(2)	5474(2)	29(1)
C(9')	18138(4)	5304(2)	5183(2)	28(1)
C(10')	16815(4)	4395(2)	4438(2)	26(1)
C(11')	7920(3)	-281(2)	2526(1)	19(1)
C(12')	8759(3)	-1134(2)	2159(1)	19(1)
C(13')	7410(3)	-2009(2)	1326(1)	18(1)
C(14')	5111(3)	-1999(2)	863(1)	19(1)
C(15')	4255(3)	-1114(2)	1263(2)	21(1)
C(16')	5600(3)	-288(2)	2066(2)	21(1)
C(17')	8279(3)	-2891(2)	942(1)	20(1)
C(18')	6937(4)	-3720(2)	136(2)	23(1)
C(19')	4663(3)	-3706(2)	-327(2)	23(1)
C(20')	3773(3)	-2862(2)	29(2)	22(1)
C(21')	8305(3)	988(2)	4284(2)	22(1)
C(22')	7554(3)	139(2)	4758(1)	19(1)
C(23')	9615(3)	-298(2)	5085(2)	23(1)
C(24')	8856(4)	-1122(2)	5585(2)	26(1)
C(25')	7787(4)	-692(2)	6486(2)	28(1)
C(26')	5719(4)	-262(2)	6172(2)	27(1)
C(27')	6475(3)	559(2)	5667(2)	24(1)

Table 3. Bond lengths [Å] and angles [°] for Jarvo02.

C(1)-H(1)	1.0000	C(16)-H(16)	0.9500
C(1)-C(2)	1.546(3)	C(17)-H(17)	0.9500
C(1)-C(11)	1.514(3)	C(17)-C(18)	1.370(3)
C(1)-C(21)	1.542(3)	C(18)-H(18)	0.9500
C(2)-H(2A)	0.9900	C(18)-C(19)	1.415(3)
C(2)-H(2B)	0.9900	C(19)-H(19)	0.9500
C(2)-C(3)	1.523(3)	C(19)-C(20)	1.366(3)
C(3)-H(3A)	0.9900	C(20)-H(20)	0.9500
C(3)-H(3B)	0.9900	C(21)-H(21A)	0.9900
C(3)-C(4)	1.533(3)	C(21)-H(21B)	0.9900
C(4)-H(4A)	0.9900	C(21)-C(22)	1.536(3)
C(4)-H(4B)	0.9900	C(22)-H(22)	1.0000
C(4)-C(5)	1.510(3)	C(22)-C(23)	1.533(3)
C(5)-C(6)	1.388(3)	C(22)-C(27)	1.538(3)
C(5)-C(10)	1.392(3)	C(23)-H(23A)	0.9900
C(6)-H(6)	0.9500	C(23)-H(23B)	0.9900
C(6)-C(7)	1.389(3)	C(23)-C(24)	1.534(3)
C(7)-H(7)	0.9500	C(24)-H(24A)	0.9900
C(7)-C(8)	1.384(3)	C(24)-H(24B)	0.9900
C(8)-H(8)	0.9500	C(24)-C(25)	1.522(3)
C(8)-C(9)	1.382(3)	C(25)-H(25A)	0.9900
C(9)-H(9)	0.9500	C(25)-H(25B)	0.9900
C(9)-C(10)	1.384(3)	C(25)-C(26)	1.526(3)
C(10)-H(10)	0.9500	C(26)-H(26A)	0.9900
C(11)-C(12)	1.373(3)	C(26)-H(26B)	0.9900
C(11)-C(16)	1.424(3)	C(26)-C(27)	1.533(3)
C(12)-H(12)	0.9500	C(27)-H(27A)	0.9900
C(12)-C(13)	1.421(3)	C(27)-H(27B)	0.9900
C(13)-C(14)	1.423(3)	C(1')-H(1')	1.0000
C(13)-C(17)	1.416(3)	C(1')-C(2')	1.539(3)
C(14)-C(15)	1.415(3)	C(1')-C(11')	1.519(3)
C(14)-C(20)	1.420(3)	C(1')-C(21')	1.538(3)
C(15)-H(15)	0.9500	C(2')-H(2'A)	0.9900
C(15)-C(16)	1.366(3)	C(2')-H(2'B)	0.9900

C(2')-C(3')	1.524(3)	C(21')-H(21C)	0.9900
C(3')-H(3'A)	0.9900	C(21')-H(21D)	0.9900
C(3')-H(3'B)	0.9900	C(21')-C(22')	1.531(3)
C(3')-C(4')	1.531(3)	C(22')-H(22')	1.0000
C(4')-H(4'A)	0.9900	C(22')-C(23')	1.533(3)
C(4')-H(4'B)	0.9900	C(22')-C(27')	1.533(3)
C(4')-C(5')	1.505(3)	C(23')-H(23C)	0.9900
C(5')-C(6')	1.391(3)	C(23')-H(23D)	0.9900
C(5')-C(10')	1.392(3)	C(23')-C(24')	1.530(3)
C(6')-H(6')	0.9500	C(24')-H(24C)	0.9900
C(6')-C(7')	1.385(3)	C(24')-H(24D)	0.9900
C(7')-H(7')	0.9500	C(24')-C(25')	1.524(3)
C(7')-C(8')	1.381(3)	C(25')-H(25C)	0.9900
C(8')-H(8')	0.9500	C(25')-H(25D)	0.9900
C(8')-C(9')	1.388(3)	C(25')-C(26')	1.524(3)
C(9')-H(9')	0.9500	C(26')-H(26C)	0.9900
C(9')-C(10')	1.386(3)	C(26')-H(26D)	0.9900
C(10')-H(10')	0.9500	C(26')-C(27')	1.531(3)
C(11')-C(12')	1.369(3)	C(27')-H(27C)	0.9900
C(11')-C(16')	1.425(3)	C(27')-H(27D)	0.9900
C(12')-H(12')	0.9500		
C(12')-C(13')	1.422(3)	C(2)-C(1)-H(1)	107.4
C(13')-C(14')	1.423(2)	C(11)-C(1)-H(1)	107.4
C(13')-C(17')	1.417(3)	C(11)-C(1)-C(2)	109.61(15)
C(14')-C(15')	1.421(3)	C(11)-C(1)-C(21)	113.87(16)
C(14')-C(20')	1.413(3)	C(21)-C(1)-H(1)	107.4
C(15')-H(15')	0.9500	C(21)-C(1)-C(2)	110.96(16)
C(15')-C(16')	1.366(3)	C(1)-C(2)-H(2A)	108.7
C(16')-H(16')	0.9500	C(1)-C(2)-H(2B)	108.7
C(17')-H(17')	0.9500	H(2A)-C(2)-H(2B)	107.6
C(17')-C(18')	1.369(3)	C(3)-C(2)-C(1)	114.19(16)
C(18')-H(18')	0.9500	C(3)-C(2)-H(2A)	108.7
C(18')-C(19')	1.411(3)	C(3)-C(2)-H(2B)	108.7
C(19')-H(19')	0.9500	C(2)-C(3)-H(3A)	109.1
C(19')-C(20')	1.373(3)	C(2)-C(3)-H(3B)	109.1
C(20')-H(20')	0.9500	C(2)-C(3)-C(4)	112.66(16)

H(3A)-C(3)-H(3B)	107.8	C(15)-C(14)-C(13)	118.46(18)
C(4)-C(3)-H(3A)	109.1	C(15)-C(14)-C(20)	122.61(18)
C(4)-C(3)-H(3B)	109.1	C(20)-C(14)-C(13)	118.94(18)
C(3)-C(4)-H(4A)	109.3	C(14)-C(15)-H(15)	119.4
C(3)-C(4)-H(4B)	109.3	C(16)-C(15)-C(14)	121.24(18)
H(4A)-C(4)-H(4B)	107.9	C(16)-C(15)-H(15)	119.4
C(5)-C(4)-C(3)	111.74(16)	C(11)-C(16)-H(16)	119.4
C(5)-C(4)-H(4A)	109.3	C(15)-C(16)-C(11)	121.12(18)
C(5)-C(4)-H(4B)	109.3	C(15)-C(16)-H(16)	119.4
C(6)-C(5)-C(4)	121.28(18)	C(13)-C(17)-H(17)	119.6
C(6)-C(5)-C(10)	118.54(19)	C(18)-C(17)-C(13)	120.76(18)
C(10)-C(5)-C(4)	120.17(19)	C(18)-C(17)-H(17)	119.6
C(5)-C(6)-H(6)	119.8	C(17)-C(18)-H(18)	119.9
C(5)-C(6)-C(7)	120.47(19)	C(17)-C(18)-C(19)	120.16(19)
C(7)-C(6)-H(6)	119.8	C(19)-C(18)-H(18)	119.9
C(6)-C(7)-H(7)	119.8	C(18)-C(19)-H(19)	119.8
C(8)-C(7)-C(6)	120.3(2)	C(20)-C(19)-C(18)	120.5(2)
C(8)-C(7)-H(7)	119.8	C(20)-C(19)-H(19)	119.8
C(7)-C(8)-H(8)	120.2	C(14)-C(20)-H(20)	119.7
C(9)-C(8)-C(7)	119.6(2)	C(19)-C(20)-C(14)	120.66(19)
C(9)-C(8)-H(8)	120.2	C(19)-C(20)-H(20)	119.7
C(8)-C(9)-H(9)	120.0	C(1)-C(21)-H(21A)	108.3
C(8)-C(9)-C(10)	120.0(2)	C(1)-C(21)-H(21B)	108.3
C(10)-C(9)-H(9)	120.0	H(21A)-C(21)-H(21B)	107.4
C(5)-C(10)-H(10)	119.5	C(22)-C(21)-C(1)	116.10(16)
C(9)-C(10)-C(5)	121.0(2)	C(22)-C(21)-H(21A)	108.3
C(9)-C(10)-H(10)	119.5	C(22)-C(21)-H(21B)	108.3
C(12)-C(11)-C(1)	120.95(17)	C(21)-C(22)-H(22)	108.5
C(12)-C(11)-C(16)	118.36(18)	C(21)-C(22)-C(27)	109.54(16)
C(16)-C(11)-C(1)	120.57(18)	C(23)-C(22)-C(21)	111.91(15)
C(11)-C(12)-H(12)	119.0	C(23)-C(22)-H(22)	108.5
C(11)-C(12)-C(13)	121.99(17)	C(23)-C(22)-C(27)	109.80(15)
C(13)-C(12)-H(12)	119.0	C(27)-C(22)-H(22)	108.5
C(12)-C(13)-C(14)	118.84(17)	C(22)-C(23)-H(23A)	109.1
C(17)-C(13)-C(12)	122.18(17)	C(22)-C(23)-H(23B)	109.1
C(17)-C(13)-C(14)	118.98(18)	C(22)-C(23)-C(24)	112.37(15)

H(23A)-C(23)-H(23B)	107.9	C(3')-C(2')-C(1')	114.09(16)
C(24)-C(23)-H(23A)	109.1	C(3')-C(2')-H(2'A)	108.7
C(24)-C(23)-H(23B)	109.1	C(3')-C(2')-H(2'B)	108.7
C(23)-C(24)-H(24A)	109.3	C(2')-C(3')-H(3'A)	109.1
C(23)-C(24)-H(24B)	109.3	C(2')-C(3')-H(3'B)	109.1
H(24A)-C(24)-H(24B)	108.0	C(2')-C(3')-C(4')	112.48(16)
C(25)-C(24)-C(23)	111.43(17)	H(3'A)-C(3')-H(3'B)	107.8
C(25)-C(24)-H(24A)	109.3	C(4')-C(3')-H(3'A)	109.1
C(25)-C(24)-H(24B)	109.3	C(4')-C(3')-H(3'B)	109.1
C(24)-C(25)-H(25A)	109.6	C(3')-C(4')-H(4'A)	109.3
C(24)-C(25)-H(25B)	109.6	C(3')-C(4')-H(4'B)	109.3
C(24)-C(25)-C(26)	110.29(16)	H(4'A)-C(4')-H(4'B)	107.9
H(25A)-C(25)-H(25B)	108.1	C(5')-C(4')-C(3')	111.69(16)
C(26)-C(25)-H(25A)	109.6	C(5')-C(4')-H(4'A)	109.3
C(26)-C(25)-H(25B)	109.6	C(5')-C(4')-H(4'B)	109.3
C(25)-C(26)-H(26A)	109.4	C(6')-C(5')-C(4')	120.02(19)
C(25)-C(26)-H(26B)	109.4	C(6')-C(5')-C(10')	118.34(19)
C(25)-C(26)-C(27)	110.99(16)	C(10')-C(5')-C(4')	121.6(2)
H(26A)-C(26)-H(26B)	108.0	C(5')-C(6')-H(6')	119.5
C(27)-C(26)-H(26A)	109.4	C(7')-C(6')-C(5')	120.91(19)
C(27)-C(26)-H(26B)	109.4	C(7')-C(6')-H(6')	119.5
C(22)-C(27)-H(27A)	109.1	C(6')-C(7')-H(7')	119.9
C(22)-C(27)-H(27B)	109.1	C(8')-C(7')-C(6')	120.3(2)
C(26)-C(27)-C(22)	112.43(17)	C(8')-C(7')-H(7')	119.9
C(26)-C(27)-H(27A)	109.1	C(7')-C(8')-H(8')	120.2
C(26)-C(27)-H(27B)	109.1	C(7')-C(8')-C(9')	119.6(2)
H(27A)-C(27)-H(27B)	107.9	C(9')-C(8')-H(8')	120.2
C(2')-C(1')-H(1')	107.3	C(8')-C(9')-H(9')	120.0
C(11')-C(1')-H(1')	107.3	C(10')-C(9')-C(8')	119.99(19)
C(11')-C(1')-C(2')	109.48(15)	C(10')-C(9')-H(9')	120.0
C(11')-C(1')-C(21')	113.10(16)	C(5')-C(10')-H(10')	119.5
C(21')-C(1')-H(1')	107.3	C(9')-C(10')-C(5')	120.9(2)
C(21')-C(1')-C(2')	112.20(17)	C(9')-C(10')-H(10')	119.5
C(1')-C(2')-H(2'A)	108.7	C(12')-C(11')-C(1')	120.97(17)
C(1')-C(2')-H(2'B)	108.7	C(12')-C(11')-C(16')	118.38(18)
H(2'A)-C(2')-H(2'B)	107.6	C(16')-C(11')-C(1')	120.59(18)

C(11')-C(12')-H(12')	118.9	C(21')-C(22')-C(27')	110.28(16)
C(11')-C(12')-C(13')	122.11(17)	C(23')-C(22')-H(22')	108.1
C(13')-C(12')-H(12')	118.9	C(23')-C(22')-C(27')	109.76(15)
C(12')-C(13')-C(14')	118.90(18)	C(27')-C(22')-H(22')	108.1
C(17')-C(13')-C(12')	122.20(17)	C(22')-C(23')-H(23C)	109.3
C(17')-C(13')-C(14')	118.90(18)	C(22')-C(23')-H(23D)	109.3
C(15')-C(14')-C(13')	118.23(18)	H(23C)-C(23')-H(23D)	107.9
C(20')-C(14')-C(13')	119.09(18)	C(24')-C(23')-C(22')	111.76(15)
C(20')-C(14')-C(15')	122.68(17)	C(24')-C(23')-H(23C)	109.3
C(14')-C(15')-H(15')	119.4	C(24')-C(23')-H(23D)	109.3
C(16')-C(15')-C(14')	121.23(17)	C(23')-C(24')-H(24C)	109.4
C(16')-C(15')-H(15')	119.4	C(23')-C(24')-H(24D)	109.4
C(11')-C(16')-H(16')	119.4	H(24C)-C(24')-H(24D)	108.0
C(15')-C(16')-C(11')	121.13(18)	C(25')-C(24')-C(23')	111.14(18)
C(15')-C(16')-H(16')	119.4	C(25')-C(24')-H(24C)	109.4
C(13')-C(17')-H(17')	119.6	C(25')-C(24')-H(24D)	109.4
C(18')-C(17')-C(13')	120.72(18)	C(24')-C(25')-H(25C)	109.4
C(18')-C(17')-H(17')	119.6	C(24')-C(25')-H(25D)	109.4
C(17')-C(18')-H(18')	119.8	C(24')-C(25')-C(26')	110.98(17)
C(17')-C(18')-C(19')	120.34(19)	H(25C)-C(25')-H(25D)	108.0
C(19')-C(18')-H(18')	119.8	C(26')-C(25')-H(25C)	109.4
C(18')-C(19')-H(19')	119.9	C(26')-C(25')-H(25D)	109.4
C(20')-C(19')-C(18')	120.27(19)	C(25')-C(26')-H(26C)	109.5
C(20')-C(19')-H(19')	119.9	C(25')-C(26')-H(26D)	109.5
C(14')-C(20')-H(20')	119.7	C(25')-C(26')-C(27')	110.94(17)
C(19')-C(20')-C(14')	120.68(18)	H(26C)-C(26')-H(26D)	108.0
C(19')-C(20')-H(20')	119.7	C(27')-C(26')-H(26C)	109.5
C(1')-C(21')-H(21C)	108.4	C(27')-C(26')-H(26D)	109.5
C(1')-C(21')-H(21D)	108.4	C(22')-C(27')-H(27C)	109.2
H(21C)-C(21')-H(21D)	107.5	C(22')-C(27')-H(27D)	109.2
C(22')-C(21')-C(1')	115.48(16)	C(26')-C(27')-C(22')	112.16(17)
C(22')-C(21')-H(21C)	108.4	C(26')-C(27')-H(27C)	109.2
C(22')-C(21')-H(21D)	108.4	C(26')-C(27')-H(27D)	109.2
C(21')-C(22')-H(22')	108.1	H(27C)-C(27')-H(27D)	107.9
C(21')-C(22')-C(23')	112.32(15)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Jarvo02. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(1)	19(1)	18(1)	7(1)	3(1)	6(1)
C(2)	30(1)	20(1)	18(1)	7(1)	2(1)	7(1)
C(3)	24(1)	20(1)	19(1)	7(1)	3(1)	7(1)
C(4)	38(1)	24(1)	21(1)	9(1)	6(1)	13(1)
C(5)	26(1)	20(1)	17(1)	9(1)	1(1)	9(1)
C(6)	22(1)	27(1)	22(1)	13(1)	2(1)	8(1)
C(7)	34(1)	22(1)	20(1)	6(1)	-4(1)	5(1)
C(8)	41(1)	31(1)	18(1)	5(1)	2(1)	20(1)
C(9)	27(1)	39(1)	24(1)	14(1)	7(1)	16(1)
C(10)	24(1)	28(1)	26(1)	12(1)	1(1)	4(1)
C(11)	21(1)	21(1)	16(1)	9(1)	1(1)	8(1)
C(12)	20(1)	21(1)	16(1)	8(1)	3(1)	9(1)
C(13)	22(1)	21(1)	16(1)	10(1)	2(1)	9(1)
C(14)	24(1)	22(1)	15(1)	10(1)	3(1)	11(1)
C(15)	21(1)	26(1)	20(1)	11(1)	6(1)	9(1)
C(16)	20(1)	21(1)	19(1)	8(1)	1(1)	4(1)
C(17)	21(1)	23(1)	18(1)	10(1)	2(1)	8(1)
C(18)	24(1)	21(1)	21(1)	7(1)	-3(1)	5(1)
C(19)	32(1)	21(1)	16(1)	4(1)	-1(1)	12(1)
C(20)	28(1)	28(1)	16(1)	10(1)	6(1)	15(1)
C(21)	25(1)	18(1)	19(1)	6(1)	1(1)	5(1)
C(22)	22(1)	18(1)	16(1)	6(1)	3(1)	7(1)
C(23)	22(1)	25(1)	21(1)	9(1)	4(1)	7(1)
C(24)	28(1)	26(1)	24(1)	13(1)	7(1)	9(1)
C(25)	30(1)	36(1)	19(1)	13(1)	5(1)	12(1)
C(26)	23(1)	31(1)	21(1)	10(1)	1(1)	9(1)
C(27)	22(1)	25(1)	19(1)	7(1)	2(1)	5(1)
C(1')	24(1)	21(1)	18(1)	8(1)	4(1)	5(1)
C(2')	30(1)	22(1)	18(1)	7(1)	3(1)	4(1)
C(3')	28(1)	22(1)	20(1)	8(1)	4(1)	3(1)
C(4')	36(1)	25(1)	21(1)	9(1)	5(1)	2(1)

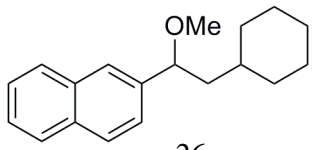
C(5')	28(1)	24(1)	19(1)	12(1)	6(1)	3(1)
C(6')	26(1)	29(1)	21(1)	12(1)	2(1)	6(1)
C(7')	37(1)	25(1)	24(1)	10(1)	5(1)	9(1)
C(8')	36(1)	26(1)	19(1)	9(1)	0(1)	-2(1)
C(9')	22(1)	39(1)	22(1)	14(1)	1(1)	2(1)
C(10')	29(1)	30(1)	24(1)	13(1)	10(1)	9(1)
C(11')	21(1)	21(1)	16(1)	10(1)	4(1)	4(1)
C(12')	18(1)	23(1)	17(1)	10(1)	3(1)	4(1)
C(13')	21(1)	21(1)	15(1)	10(1)	5(1)	5(1)
C(14')	19(1)	24(1)	17(1)	11(1)	4(1)	5(1)
C(15')	18(1)	27(1)	20(1)	12(1)	3(1)	8(1)
C(16')	24(1)	21(1)	22(1)	9(1)	7(1)	10(1)
C(17')	20(1)	23(1)	19(1)	9(1)	3(1)	7(1)
C(18')	28(1)	22(1)	21(1)	8(1)	7(1)	8(1)
C(19')	24(1)	24(1)	16(1)	4(1)	0(1)	2(1)
C(20')	20(1)	27(1)	18(1)	9(1)	2(1)	6(1)
C(21')	28(1)	18(1)	19(1)	6(1)	4(1)	6(1)
C(22')	22(1)	18(1)	17(1)	5(1)	4(1)	4(1)
C(23')	23(1)	27(1)	23(1)	11(1)	7(1)	9(1)
C(24')	27(1)	29(1)	26(1)	15(1)	7(1)	10(1)
C(25')	30(1)	36(1)	23(1)	15(1)	8(1)	11(1)
C(26')	27(1)	33(1)	25(1)	12(1)	11(1)	9(1)
C(27')	27(1)	23(1)	22(1)	6(1)	7(1)	8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Jarvo02.

	x	y	z	U(eq)
H(1)	9972	2865	9422	24
H(2A)	10378	2122	10774	27
H(2B)	7583	1624	10479	27
H(3A)	10576	1106	9092	25
H(3B)	7846	532	8931	25
H(4A)	11504	466	10479	32
H(4B)	8780	-144	10268	32
H(6)	7500	-1873	9104	27
H(7)	8192	-3260	7893	32
H(8)	11636	-3041	7260	35
H(9)	14362	-1419	7824	33
H(10)	13667	-32	9025	31
H(12)	12031	4461	10582	22
H(15)	5797	4654	12280	25
H(16)	5504	3215	10921	24
H(17)	14359	6200	11771	24
H(18)	14659	7645	13142	27
H(19)	11522	7743	14001	28
H(20)	8121	6405	13482	27
H(21A)	6416	1730	8401	25
H(21B)	4988	2127	9248	25
H(22)	5437	3736	8972	23
H(23A)	8240	3016	7546	26
H(23B)	9192	3979	8572	26
H(24A)	6906	4953	7920	29
H(24B)	8515	4567	7142	29
H(25A)	5272	3218	6086	32
H(25B)	4559	4303	6268	32
H(26A)	1488	3019	6480	30
H(26B)	2496	3980	7506	30

H(27A)	3735	2022	7114	27
H(27B)	2157	2418	7901	27
H(1')	10945	490	3617	25
H(2'A)	10880	1318	2357	29
H(2'B)	8727	1763	2700	29
H(3'A)	13209	2320	4063	28
H(3'B)	11102	2878	4216	28
H(4'A)	13979	2994	2755	33
H(4'B)	11710	3462	2783	33
H(6')	11971	5113	3971	30
H(7')	14190	6640	5217	34
H(8')	18067	6770	5981	34
H(9')	19713	5351	5495	34
H(10')	17498	3824	4239	31
H(12')	10291	-1142	2470	22
H(15')	2720	-1095	966	25
H(16')	4978	291	2321	25
H(17')	9809	-2908	1246	24
H(18')	7540	-4306	-113	27
H(19')	3744	-4283	-886	27
H(20')	2243	-2859	-289	26
H(21C)	9433	1592	4813	26
H(21D)	6892	1219	4068	26
H(22')	6310	-444	4239	23
H(23C)	10234	-608	4486	28
H(23D)	10908	277	5567	28
H(24C)	7677	-1729	5083	31
H(24D)	10247	-1361	5815	31
H(25C)	9015	-132	7019	34
H(25D)	7232	-1251	6771	34
H(26C)	5121	53	6777	32
H(26D)	4417	-837	5696	32
H(27C)	7651	1167	6169	28
H(27D)	5081	796	5439	28

1H spectrum



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Current Data Parameters
USER                aaron
NAME              AGJ_1_90
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20120423
Time                 18.09
INSTRUM              drx400
PROBHD  5 mm QNP H/P/P
PULPROG              zg30
TD                  65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1118579 sec
RG                      32
DW                 78.000 usec
DE                  4.50 usec
TE                 298.1 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                  12.00 usec
PL1                 -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300372 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    2.00
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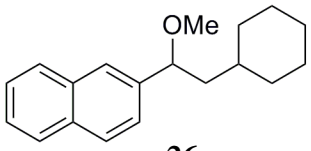
13C spectrum with 1H decoupling



26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Current Data Parameters
USER                aaron
NAME             AGJ_1_190
EXPNO                    2
PROCNO                   1

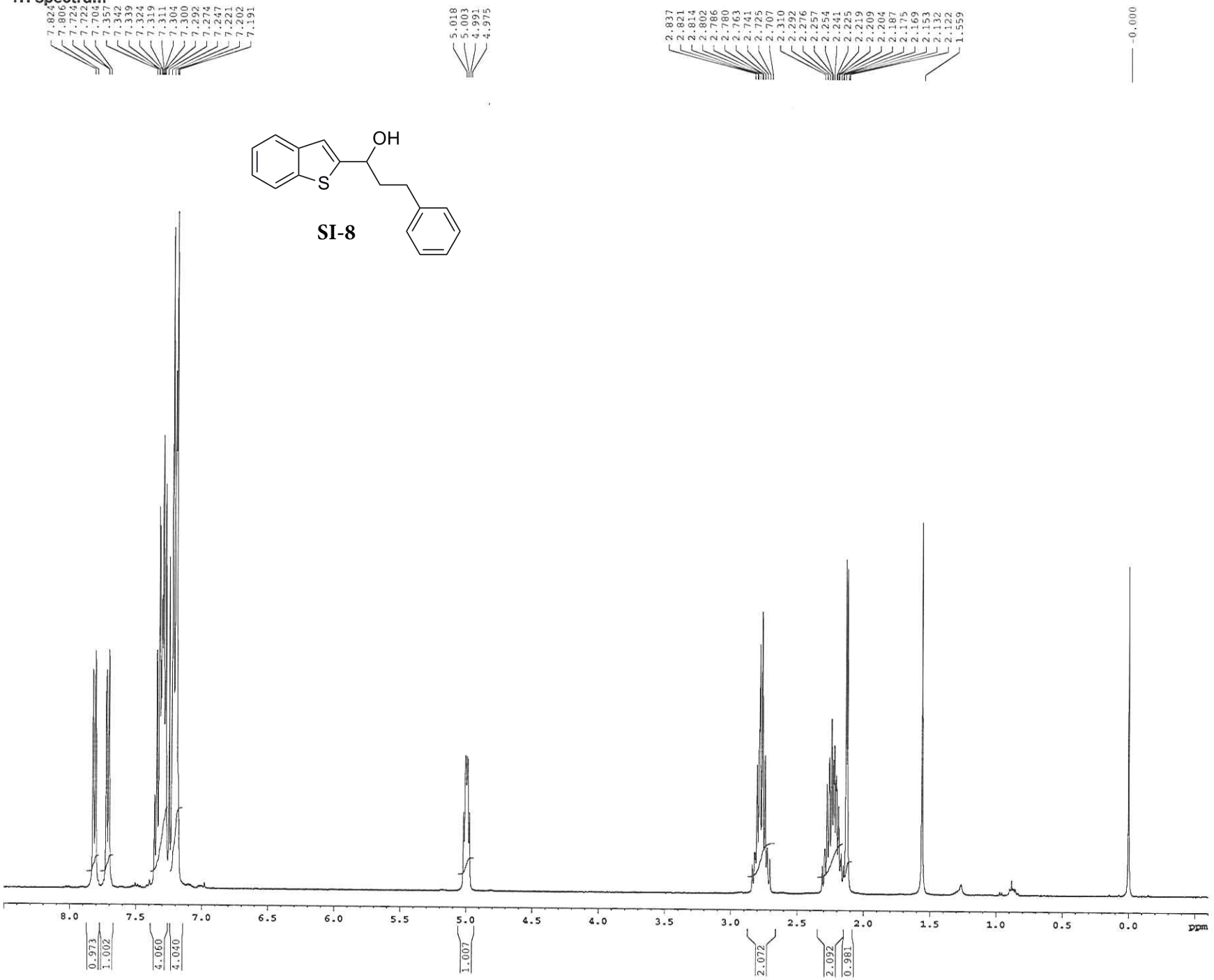
F2 - Acquisition Parameters
Date_             20120423
Time                 17.52
INSTRUM              drx400
PROBHD   5 mm QNP H/F/P
PULPROG             zgdc30
TD                   65536
SOLVENT              CDCl3
NS                     614
DS                       4
SWH              24154.590 Hz
FIDRES           0.368570 Hz
AQ               1.3566452 sec
RG                  9195.2
DW                 20.700 usec
DE                 20.39 usec
TE                 298.0 K
D1              0.10000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                  11.00 usec
PL1                  0.00 dB
SFO1          100.6237964 MHz

======== CHANNEL f2 ========
CPDPRG2             mlev16
NUC2                   1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                16.20 dB
SFO2          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            100.6127635 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.00
```

1H spectrum

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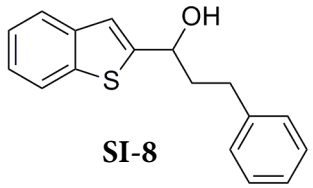
Current Data Parameters
USER                yonova
NAME              IMY5 - 10C
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20121201
Time                 21.27
INSTRUM            drx400
PROBHD   5 mm QNP H/F/P
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1118579 sec
RG                  287.4
DW                 78.000 usec
DE                  4.50 usec
TE                 298.1 K
D1              0.10000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                  65536
SF            400.1300265 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling



SI-8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Current Data Parameters
USER                ygnova
NAME              IMY5 - 150
EXPNO                  111
PROCNO                   1

F2 - Acquisition Parameters
Date_            20121203
Time                14.29
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchop180gp.prd
TD                  65536
SOLVENT              CDCl3
NS                     272
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0814105 sec
RG                  2896.3
DW                 16.500 usec
DE                  6.00 usec
TE                 298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                 31.00 usec

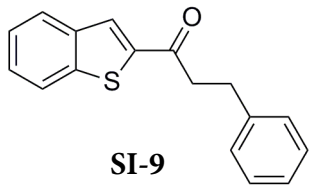
======== CHANNEL f1 ========
NUC1                 13C
P1                 15.50 usec
P11               500.00 usec
PL2              2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SF1                 3.20 dB
SP2                 3.20 dB
SPNAM1    Crp50,0.5,20.1
SPNAM2      Crp60comp.4
SPOFS1               0.00 Hz
SPOFS2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                   65536
SF            125.7800094 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00
```

1H spectrum



SI-9

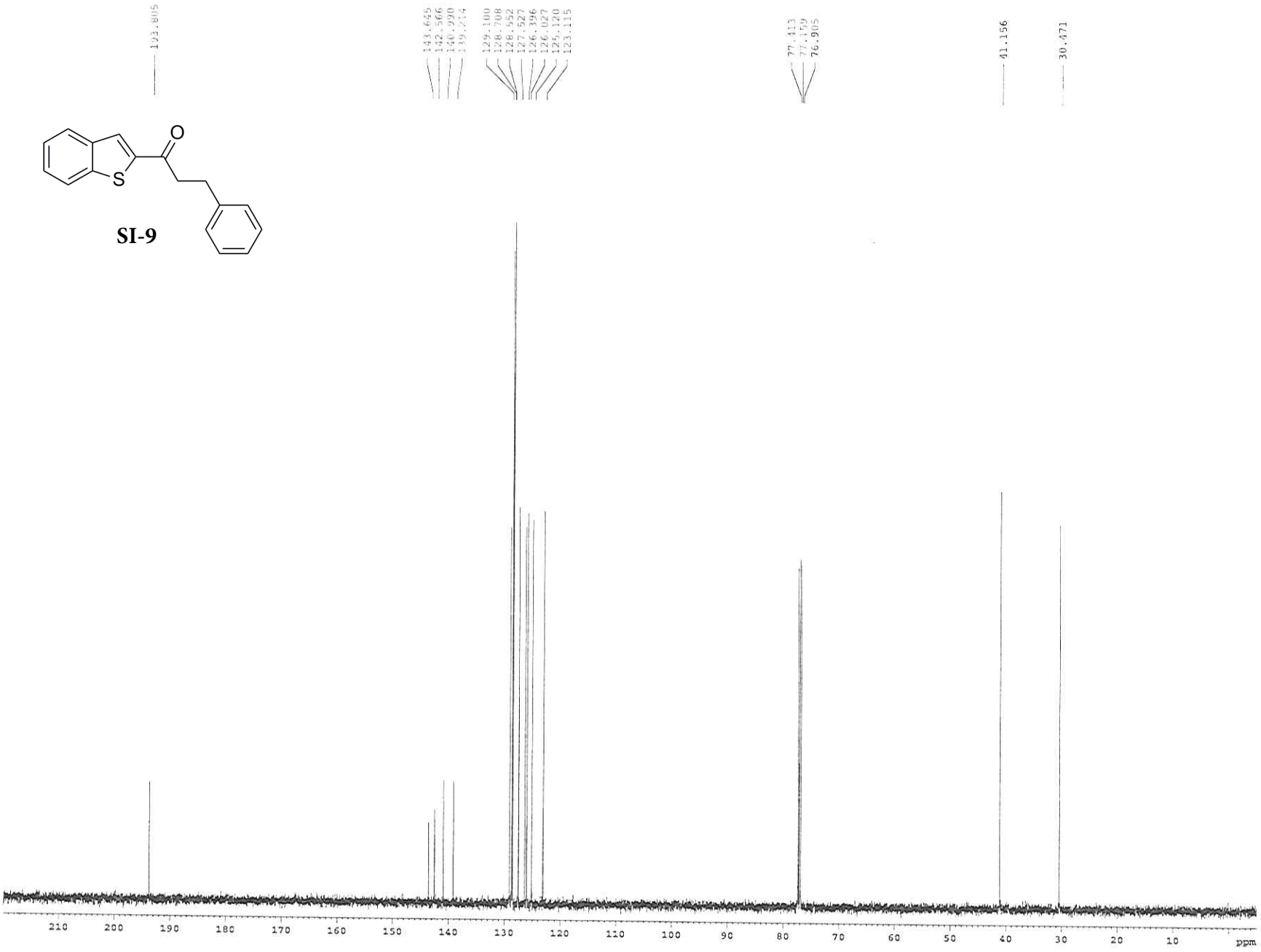

```
Current Data Parameters
USER                yonova
NAME              IMY5 - 080
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20121121
Time                 18.13
INSTRUM             drx400
PROBHD   5 mm QNP H/F/P
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1118579 sec
RG                     181
DW                  78.000 usec
DE                   4.50 usec
TE                  298.1 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.00 usec
PL1                  -0.60 dB
SFO1            400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF              400.1300279 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                yonova
NAME            IMY5 - 060
EXPNO                  222
PROCNO                   1

F2 - Acquisition Parameters
Date_            20121124
Time                16.56
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchop13Cqp.prd
TD                  65536
SOLVENT             CDCl3
NS                     72
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0814105 sec
RG                   5502
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
PS                31.00 usec

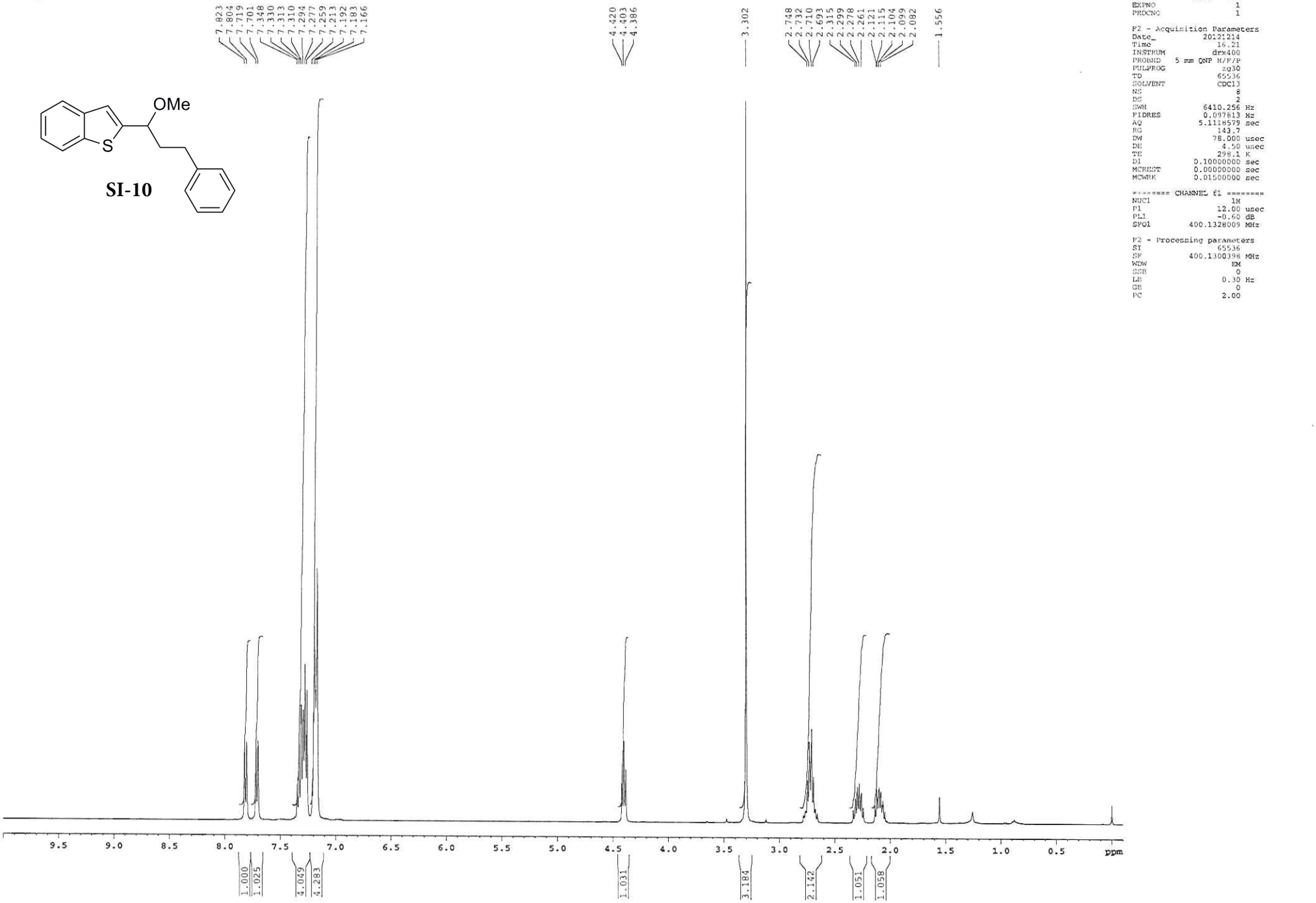
======== CHANNEL f1 ========
NUC1                  13C
P1                  15.50 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7842548 MHz
SP1                 3.20 dB
SP2                 3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12               24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
P15               500.00 usec
P16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF            125.7804131 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 2.00
```

1H spectrum



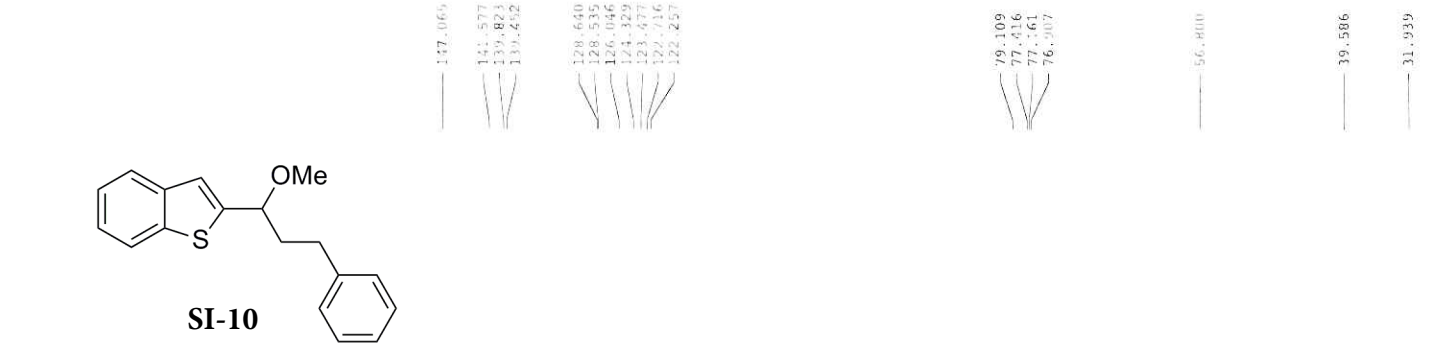

```
Current Data Parameters
USER                yonova
NAME              IMY5 - 128
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20121214
Time                  16.21
INSTRUM              drx400
PROBHD   5 mm QNP H/P/D
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                6410.256 Hz
FIDRES             0.097813 Hz
AQ                 5.1118579 sec
RG                     143.7
DW                  78.000 usec
DE                   4.50 usec
TE                  298.1 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

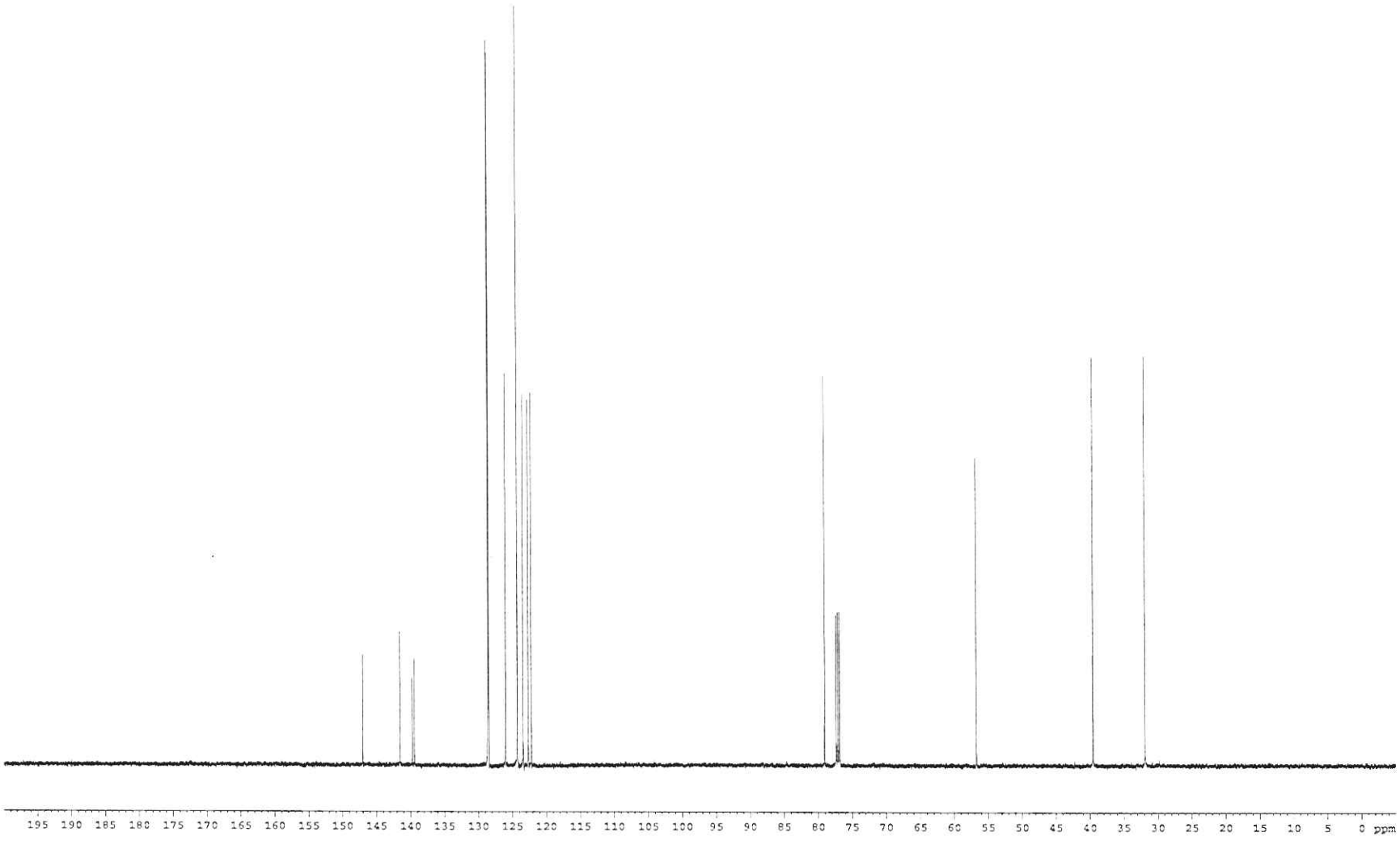
======== CHANNEL f1 ========
NUC1                      1H
P1                   12.00 usec
PL1                  -0.60 dB
SFO1           400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF             400.1300000 MHz
WDW                       EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                    2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling



SI-10




```
Current Data Parameters
USER                ycmbvo
NAME              IMYS - 128
EXPNO                  222
PROCNO                   1

F2 - Acquisition Parameters
Date_           20121214
Time                17:17
INSTRUM           dryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30up.prd
TD                  65536
SOLVENT             CDCl3
NS                    223
DS                     16
SWH               30303.031 Hz
FIDRES            0.462388 Hz
AQ                1.0614105 sec
RG                   3251
DW                 16.500 usec
DE                  6.00 usec
TE                 298.0 K
D1                0.25000000 sec
d11               0.03000000 sec
D12               0.00020000 sec
d17               0.00019600 sec
MCWEST            0.00000000 sec
MCWRK             0.01500000 sec
P2                 31.00 usec

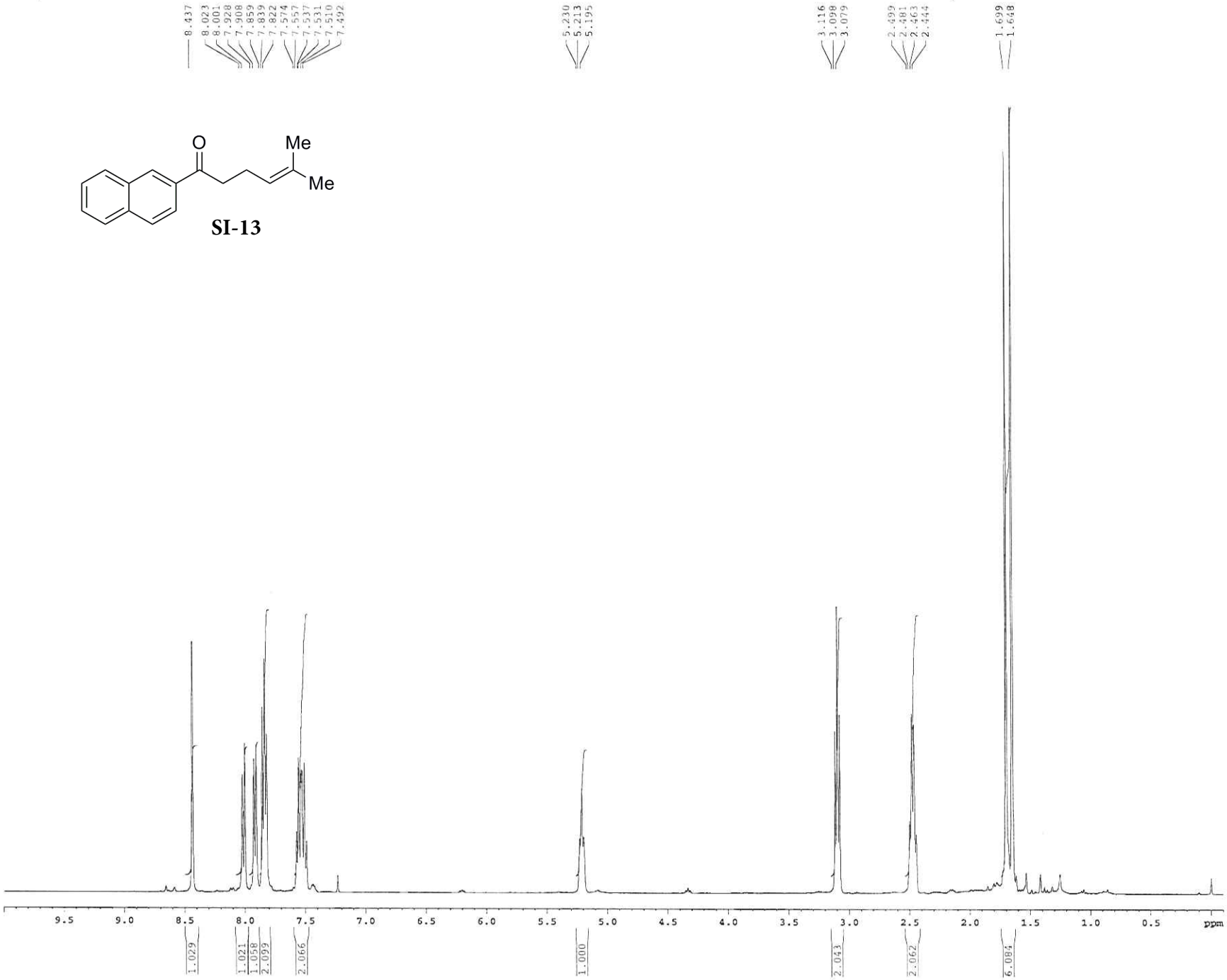
======== CHANNEL f1 ========
NUC1                  13C
P1                  15.50 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                 3.20 dB
SP2                 3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2          500.2225011 MHz

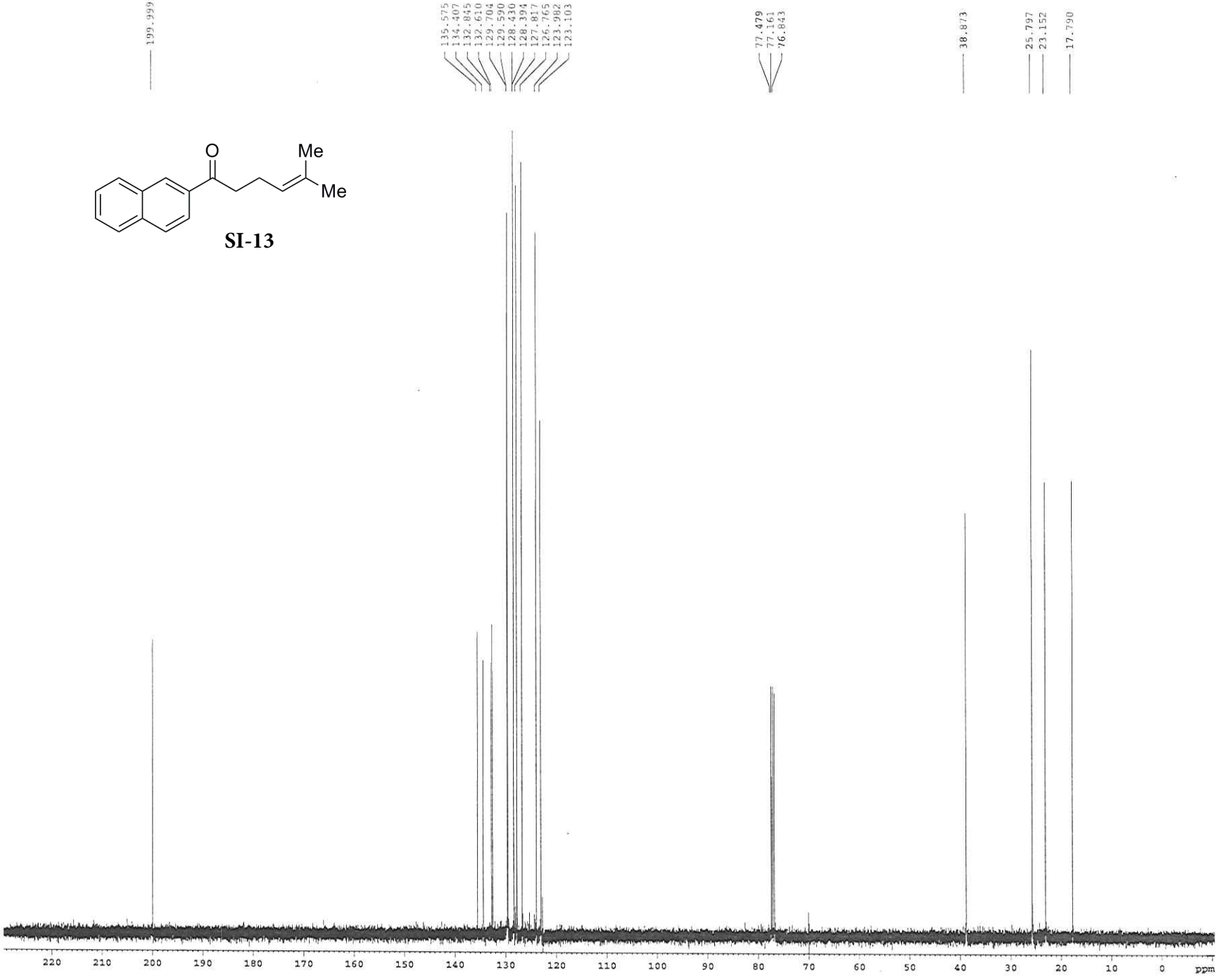
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
P15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF            125.7804154 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  2.00
```

1H spectrum


8.437
8.023
8.001
7.928
7.908
7.859
7.839
7.822
7.574
7.557
7.537
7.531
7.510
7.492
5.230
5.213
5.195
3.116
3.098
3.079
2.499
2.481
2.463
2.444
1.699
1.648
O
Me
Me
SI-13
Current Data Parameters
USER yonova
NAME imy5 - AGJ-3-45
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130615
Time 16.33
INSTRUM drx400
PROBHD 5 mm QNP H/P/F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1118579 sec
RG 32
DW 78.000 usec
DE 4.50 usec
TE 298.1 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -0.60 dB
SFO1 400.1328009 MHz
F2 - Processing parameters
SI 65536
SF 400.1300312 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.029
1.021
1.058
2.099
2.066
1.000
2.043
2.062
6.084

13C spectrum with 1H decoupling



SI-13

```
Current Data Parameters
USER                yonova
NAME       imy5 - AGJ-3-45
EXPNO                    2
PROCNO                   1

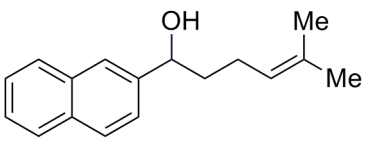
F2 - Acquisition Parameters
Date_             20130615
Time                 18.38
INSTRUM              drx400
PROBHD   5 mm QNP H/F/P
PULPROG              zgdc30
TD                    65536
SOLVENT               CDCl3
NS                      339
DS                        4
SWH               24154.590 Hz
FIDRES            0.368570 Hz
AQ                1.3566452 sec
RG                   1149.4
DW                  20.700 usec
DE                   20.39 usec
TE                   298.0 K
D1              0.10000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                   11.00 usec
PL1                   0.00 dB
SFO1          100.6237964 MHz

======== CHANNEL f2 ========
CPDPRG2              mlev16
NUC2                    1H
PCPD2                80.00 usec
PL2                   0.00 dB
PL12                 16.20 dB
SFO2          400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF            100.6127683 MHz
WDW                      no
SSB                       0
LB                    0.00 Hz
GB                        0
PC                     2.00
```

1H spectrum



SI-14

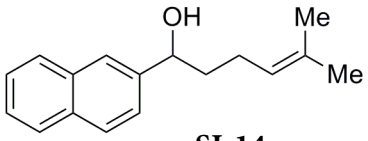

```
Current Data Parameters
USER                aaronj
NAME          AGJ_3_33_c1
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130511
Time                 18.58
INSTRUM             drx400
PROBHD   5 mm QNP H/F/P
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       8
DS                       2
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1118579 sec
RG                   101.6
DW                78.000 usec
DE                 4.50 usec
TE                298.2 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300296 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    2.00
```

11B spectrum with 1H decoupling, using composite pulse for background suppression



SI-14

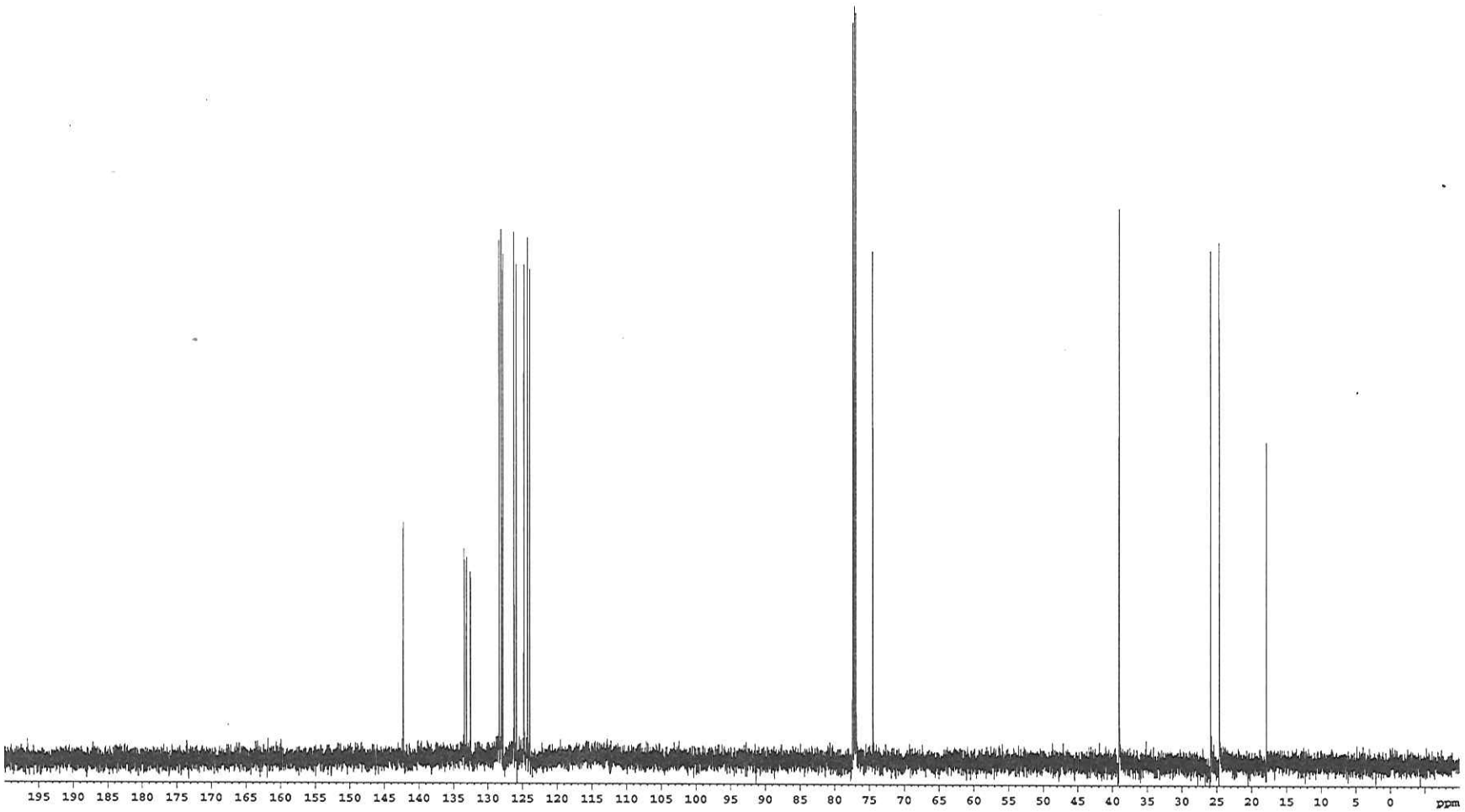
142.264
133.437
133.105
132.524
128.370
128.056
127.809
126.227
125.888
124.741
124.260
123.934
77.370
77.159
76.947
74.502
39.031
25.872
24.639
17.891

```
Current Data Parameters
USER                aaronj
NAME              AGJ_3_33
EXPNO                    5
PROCNO                   1

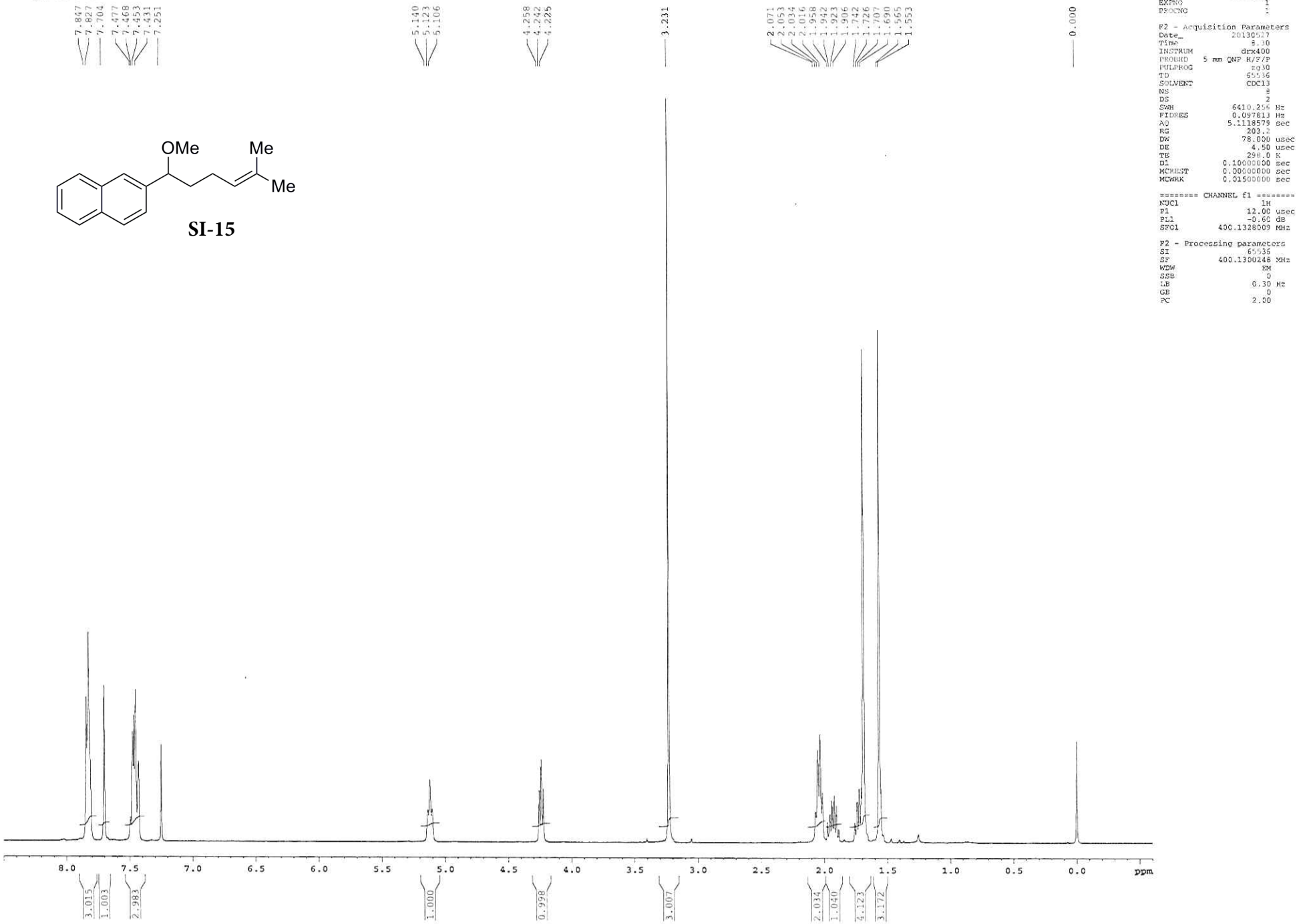
F2 - Acquisition Parameters
Date_             20130511
Time                 19.24
INSTRUM              av600
PROBHD    5 mm TBI 1H/13
PULPROG           zgdc30
TD                 65400
SOLVENT             CDCl3
NS                    550
DS                      4
SWH           36231.883 Hz
FIDRES        0.554004 Hz
AQ            0.9025700 sec
RG                   1010
DW               13.800 usec
DE                6.00 usec
TE                298.1 K
D1            0.40000001 sec
D11           0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                  13C
P1                15.00 usec

F2 - Processing parameters
SI                   65536
SF            150.9027969 MHz
WDW                     EM
SSB                      0
LB                1.00 Hz
GB                       0
PC                1.00
```



1H spectrum



SI-15

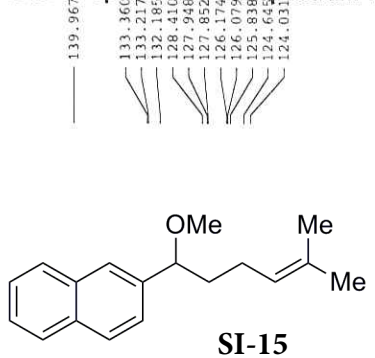
```
Current Data Parameters
USER                aaronj
NAME              AGG_3_39
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130527
Time                   8.30
INSTRUM              drx400
PROBHD  5 mm QNP H/F/P
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       8
DS                       2
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1118579 sec
RG                   203.2
DW                78.000 usec
DE                 4.50 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF          400.1300246 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 2.00
```

Z–restored spin–echo 13C spectrum with 1H decoupling



SI-15


```
Current Data Parameters
USER                aaron
NAME              AGJ_3_39
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20130527
Time                 8.48
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     400
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0814105 sec
RG                     8192
DW                 16.500 usec
DE                  6.00 usec
TE                 298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                 31.00 usec

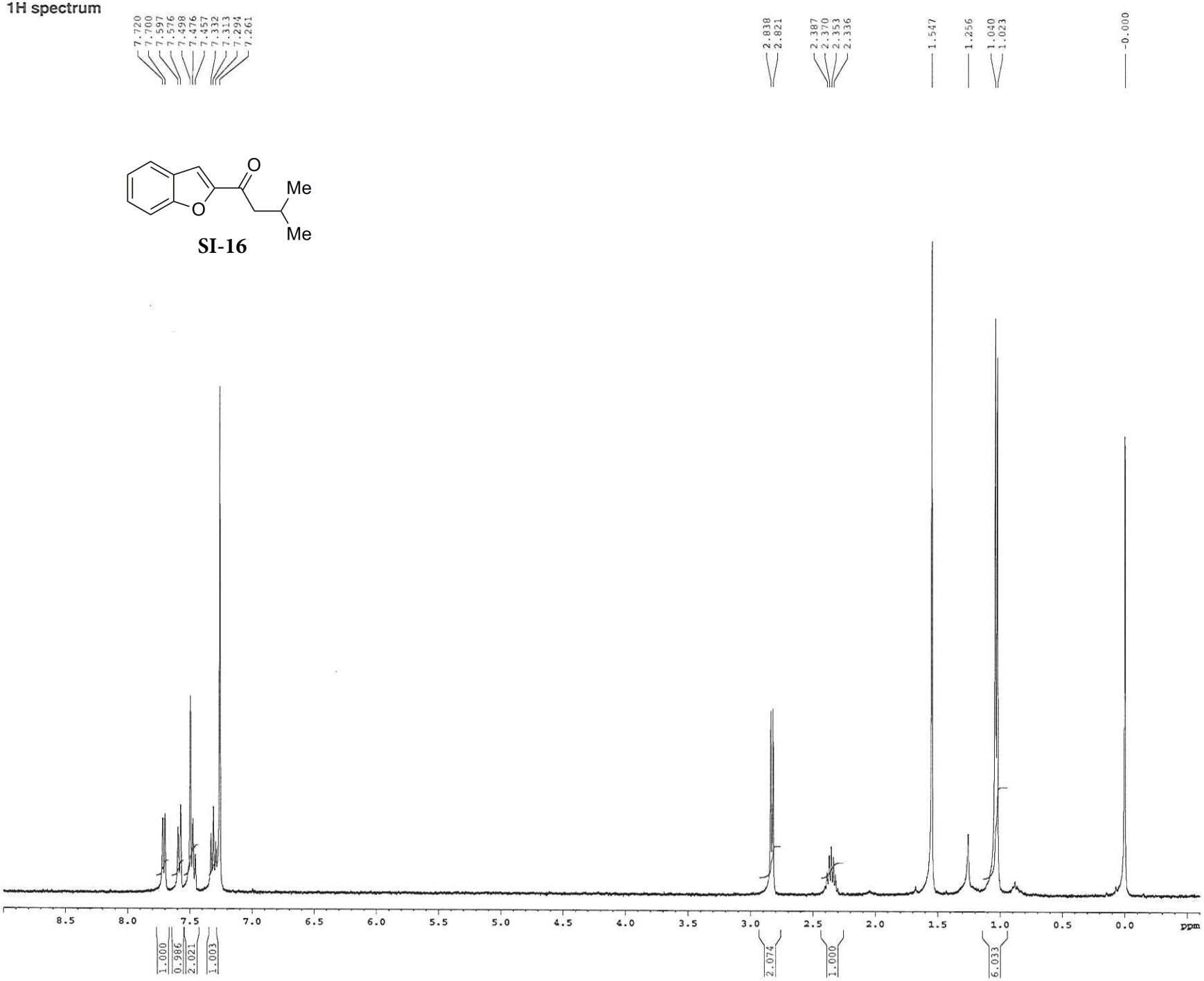
======== CHANNEL f1 ========
NUC1                   13C
P1                   15.50 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1         125.7942548 MHz
SP1                  3.20 dB
SP2                  3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               100.00 usec
PL2                   1.60 dB
PL12                 24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

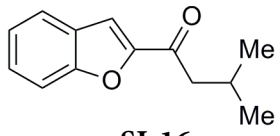
F2 - Processing parameters
SI                   65536
SF           125.7804085 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00
```

1H spectrum



SI-16

Z–restored spin–echo 13C spectrum with 1H decoupling



SI-16


```
Current Data Parameters
USER                yonova
NAME             imy5 - 261
EXPNO                 222
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130616
Time                19.02
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                   3000
DS                     16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0814105 sec
RG                 4597.6
DW                 16.500 usec
DE                  6.00 usec
TE                 298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                 31.00 usec

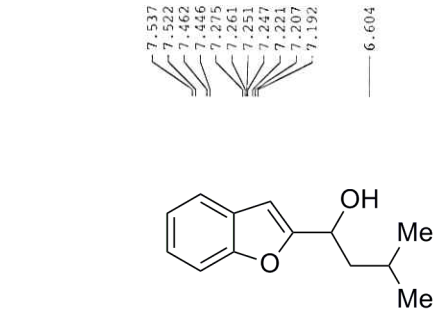
======== CHANNEL f1 ========
NUC1                 13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804076 MHz
WDW                 EM
SSB                 0
LB                 1.00 Hz
GB                  0
PC                 2.00
```

1H spectrum



S-17

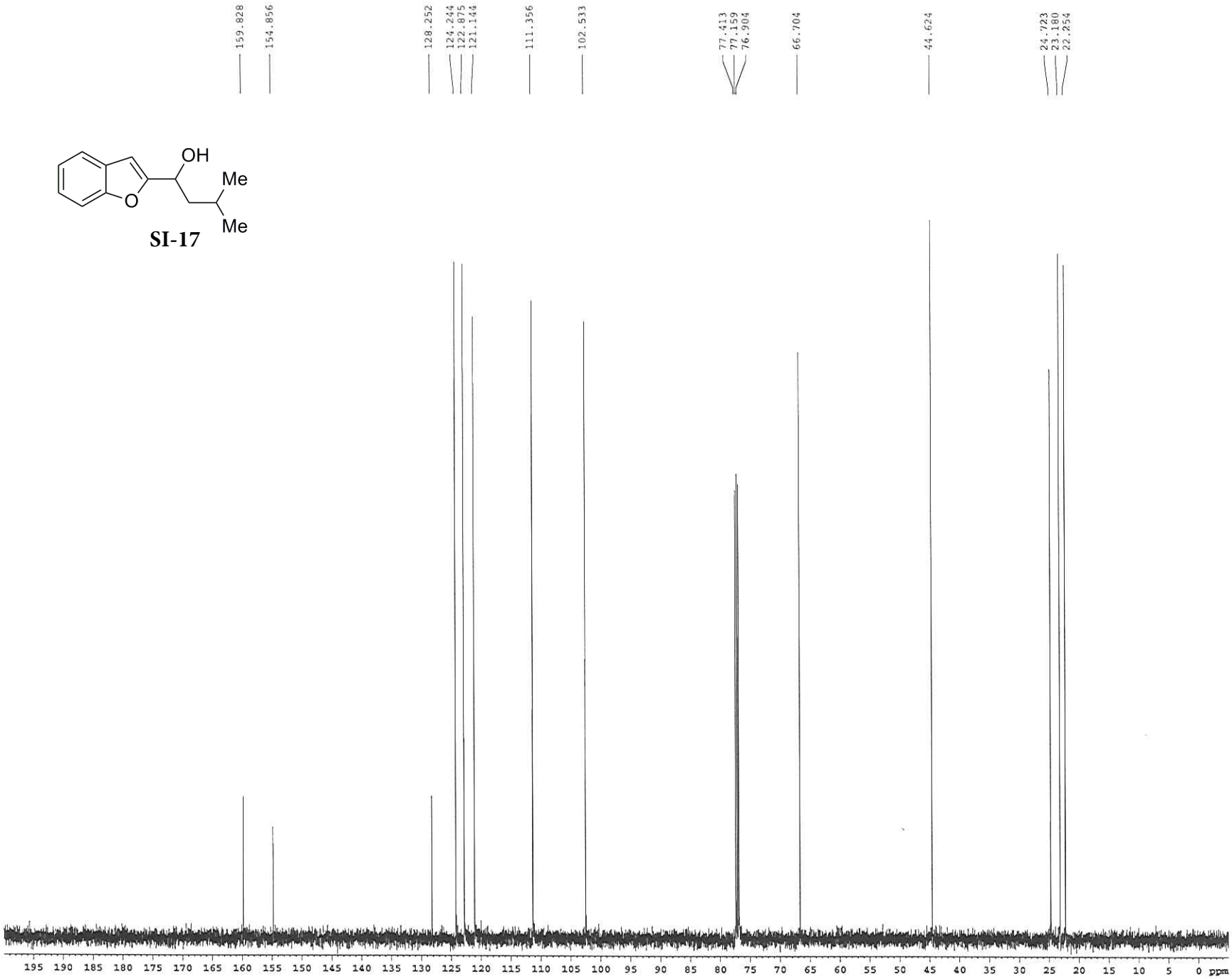

```
Current Data Parameters
USER                yonova
NAME              agjj - 32
EXPNO                   111
PROCNO                    1

F2 - Acquisition Parameters
Date_            20130519
Time                 18.37
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    81728
SOLVENT             CDCl3
NS                        8
DS                        2
SWH                8012.820 Hz
FIDRES                0.098043 Hz
AQ                 5.0998774 sec
RG                        9
DW                   62.400 usec
DE                    6.00 usec
TE                  298.0 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    7.50 usec
PL1                   1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameters
SI                       65536
SF            500.2200358 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    4.00
```

Z–restored spin–echo 13C spectrum with 1H decoupling



SI-17

```
Current Data Parameters
USER                yonova
NAME              agj3 - 32
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_            20130519
Time                18.39
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT              CDCl3
NS                      89
DS                      16
SWH              30303.031 Hz
FIDRES           0.462398 Hz
AQ               1.0814105 sec
RG                  5160.6
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1            0.25000000 sec
d11           0.03000000 sec
D16           0.00020000 sec
d17           0.00019600 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
P2                31.00 usec

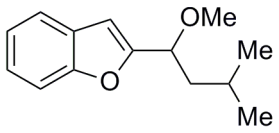
======== CHANNEL f1 ========
NUC1                 13C
P1                15.50 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1         125.7942546 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.60 dB
PL12              24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
pl5               500.00 usec
pl6              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804108 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00
```

1H spectrum



SI-18

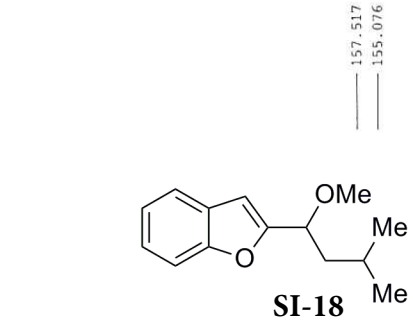

```
Current Data Parameters
USER                yonova
NAME              lmy5 - 250
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130520
Time               17.24
INSTRUM            drx400
PROBHD   5 mm QNP H/P/F
PULPROG            zg30
TD                 65536
SOLVENT            CDCl3
NS                 8
DS                 2
SWH             6410.256 Hz
FIDRES          0.097813 Hz
AQ              5.1118579 sec
RG                 143.7
DW                78.000 usec
DE                 4.50 usec
TE                 298.1 K
D1              0.10000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300249 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  2.00
```

Z–restored spin–echo 13C spectrum with 1H decoupling



SI-18


```
Current Data Parameters
USER                yonova
NAME               imy5 - 239
EXPNO                  222
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130519
Time                 18.32
INSTRUM             cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT                CDCl3
NS                       134
DS                        16
SWH                30303.031 Hz
FIDRES             0.462388 Hz
AQ                 1.0814105 sec
RG                    7298.2
DW                    16.500 usec
DE                     6.00 usec
TE                    298.0 K
D1                 0.25000000 sec
d11                0.03000000 sec
D16                0.00020000 sec
d17                0.00019600 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec
P2                    31.00 usec

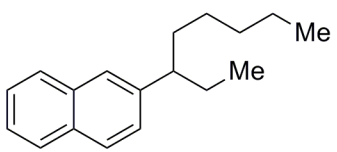
======== CHANNEL f1 ========
NUC1                     13C
P1                    15.50 usec
P11                  500.00 usec
P12                 2000.00 usec
PL0                  120.00 dB
PL1                   -1.00 dB
SFO1            125.7942548 MHz
SP1                    3.20 dB
SP2                    3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                100.00 usec
PL2                    1.60 dB
PL12                  24.60 dB
SFO2            500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPX1                   0.00 %
GPX2                   0.00 %
GPY1                   0.00 %
GPY2                   0.00 %
GPZ1                  30.00 %
GPZ2                  50.00 %
p15                  500.00 usec
p16                 1000.00 usec

F2 - Processing parameters
SI                    65536
SF              125.7804094 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     2.00
```

1H spectrum



2

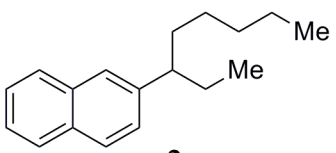

```
Current Data Parameters
USER                yonova
NAME             IMY5 - 054
EXPNO                   111
PROCNO                    1

F2 - Acquisition Parameters
Date_            20121204
Time                 0.12
INSTRUM            drx400
PROBHD   5 mm QNP H/F/P
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1118579 sec
RG                  228.1
DW                 78.000 usec
DE                  4.50 usec
TE                 298.1 K
D1            0.10000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                  65536
SF           400.1300255 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling



2


```
Current Data Parameters
USER                yonova
NAME             IMY5 - 055
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_            20121129
Time                 5.35
INSTRUM           cryo500
PROBHD     5 mm CPTCI 1H-
PULPROG    SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    192
DS                     16
SWH              30303.031 Hz
FIDRES           0.462186 Hz
AQ               1.0814105 sec
RG                  7298.2
DW                 16.500 usec
DE                  6.00 usec
TE                 298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                 31.00 usec

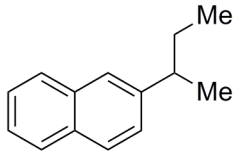
======== CHANNEL f1 ========
NUC1                  13C
P1                  15.50 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                 3.20 dB
SW2                 3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12               24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                 65536
SF           125.7804090 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  2.00
```

1H spectrum



5

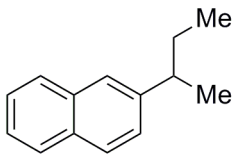

```
Current Data Parameters
USER                yonova
NAME              lmy5 - 2-2
EXPNO                   111
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130622
Time                  15.14
INSTRUM             drx400
PROBHD   5 mm QNP H/P/F
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1118579 sec
RG                    161.3
DW                 78.000 usec
DE                  4.50 usec
TE                  298.1 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                  12.00 usec
PL1                 -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300000 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    2.00
```

13C spectrum with 1H decoupling



5


```
Current Data Parameters
USER                yonova
NAME              lmy5 - 232
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130622
Time                  15.18
INSTRUM             drx400
PROBHD   5 mm QNP H/F/P
PULPROG             zgdc30
TD                   65536
SOLVENT              CDCl3
NS                     307
DS                       4
SWH              24154.590 Hz
FIDRES           0.368570 Hz
AQ               1.3566452 sec
RG                  9195.2
DW                 20.700 usec
DE                 20.39 usec
TE                 298.1 K
D1              0.10000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 11.00 usec
PL1                0.00 dB
SFO1          100.6237964 MHz

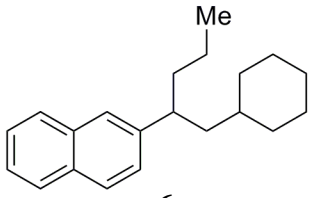
======== CHANNEL f2 ========
CPDPRG2             mlev16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              16.20 dB
SFO2          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            100.6127595 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                  1.00
```

1H spectrum

7.804 7.788 7.775 7.758 7.554 7.453 7.451 7.439 7.438 7.424 7.421 7.416 7.413 7.399 7.386 7.320 7.317 7.303 7.300 7.221

2.844 2.833 2.825 2.814 2.804 2.796 2.785 1.852 1.827 1.645 1.635 1.626 1.620 1.617 1.608 1.597 1.590 1.579 1.570 1.564 1.522 1.510 1.504 1.494 1.483 1.477 1.466 1.255 1.217 1.203 1.190 1.176 1.173 1.158 1.150 1.144 1.138 1.136 1.131 1.124 1.119 1.109 1.105 1.091 1.073 1.052 0.912 0.894 0.884 0.871 0.861



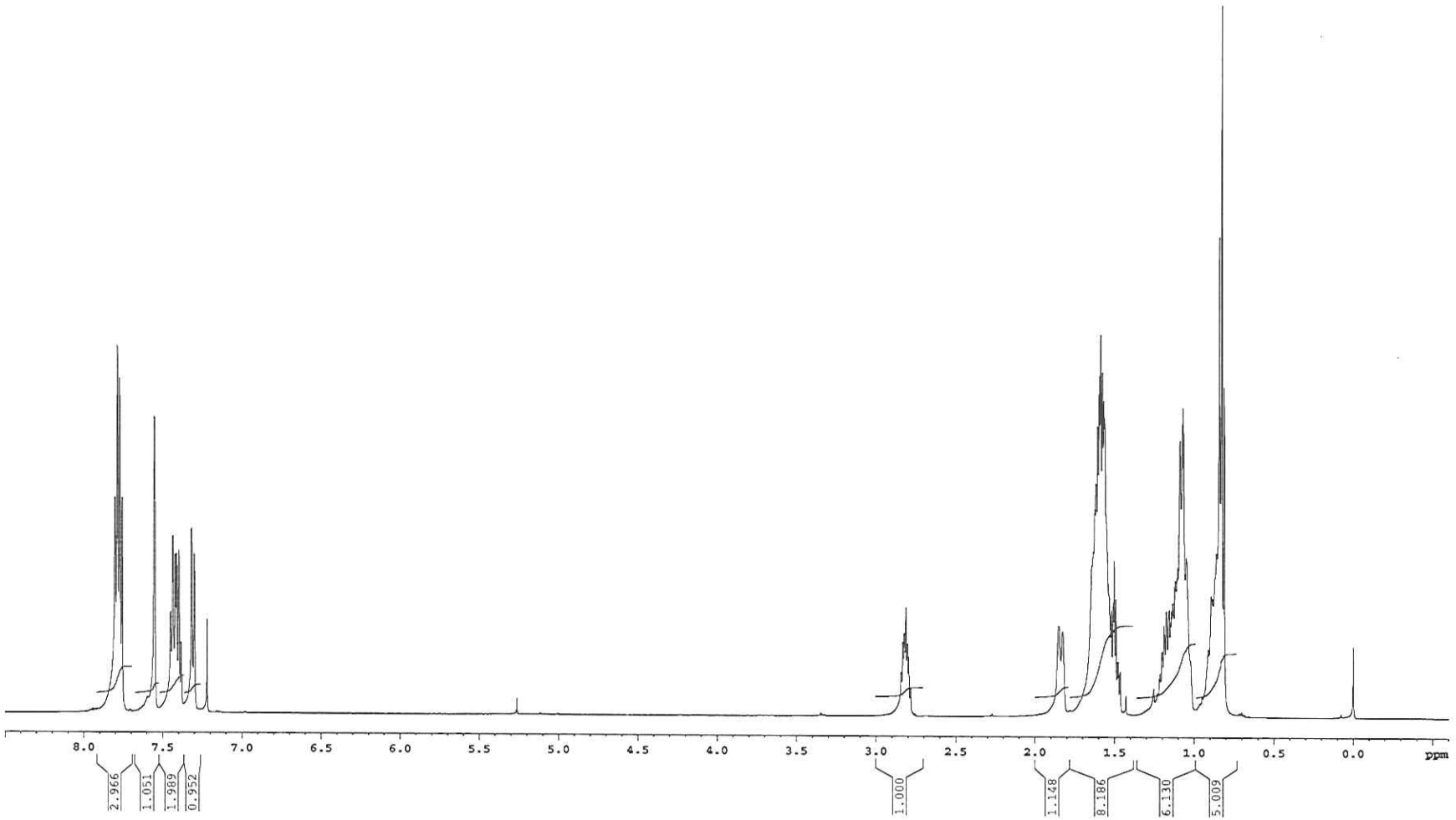
6

```
Current Data Parameters
USER                aaronj
NAME              AGJ_1_160
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120502
Time                 23.25
INSTRUM             cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    81728
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8012.820 Hz
FIDRES             0.098043 Hz
AQ                 5.0998774 sec
RG                        5
DW                   62.400 usec
DE                    6.00 usec
TE                   298.0 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    7.50 usec
PL1                   1.60 dB
SFO1           500.2235015 MHz

F2 - Processing parameters
SI                        65536
SF             500.2200512 MHz
WDW                       EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    4.00
```



Z–restored spin–echo 13C spectrum with 1H decoupling


```
Current Data Parameters
USER                aaronj
NAME              AGJ_1_160
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_            20120502
Time                23.32
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30qp.prd
TD                  65536
SOLVENT             CDCl3
NS                    412
DS                     16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                 5792.6
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.25000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                31.00 usec

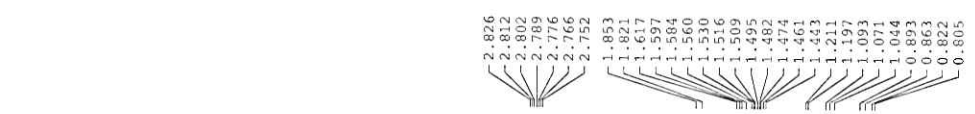
======== CHANNEL f1 ========
NUC1                  13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1          125.7942548 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

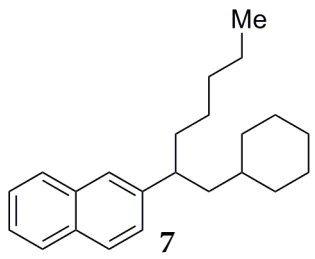
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804122 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                 2.00
```

1H spectrum



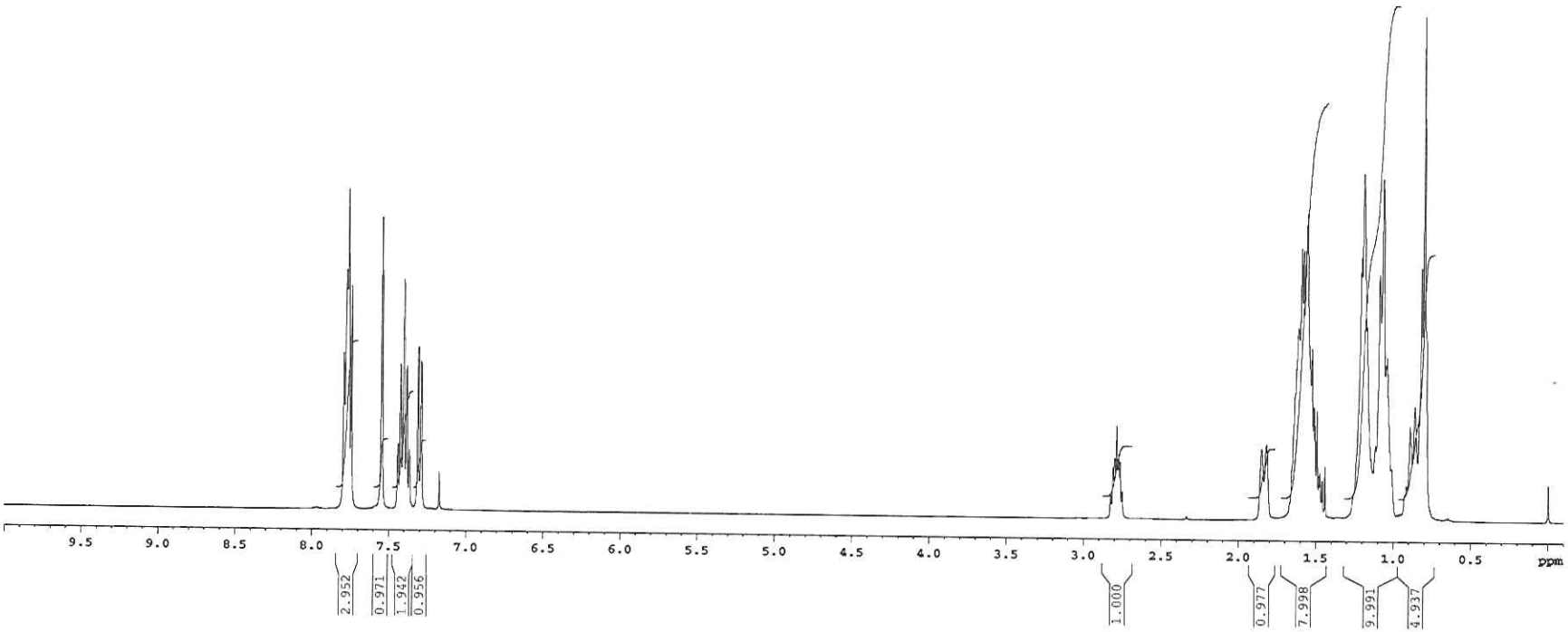



```
Current Data Parameters
USER                yonova
NAME              IMY5 - 117
EXPNO                     11
PROCNO                     1

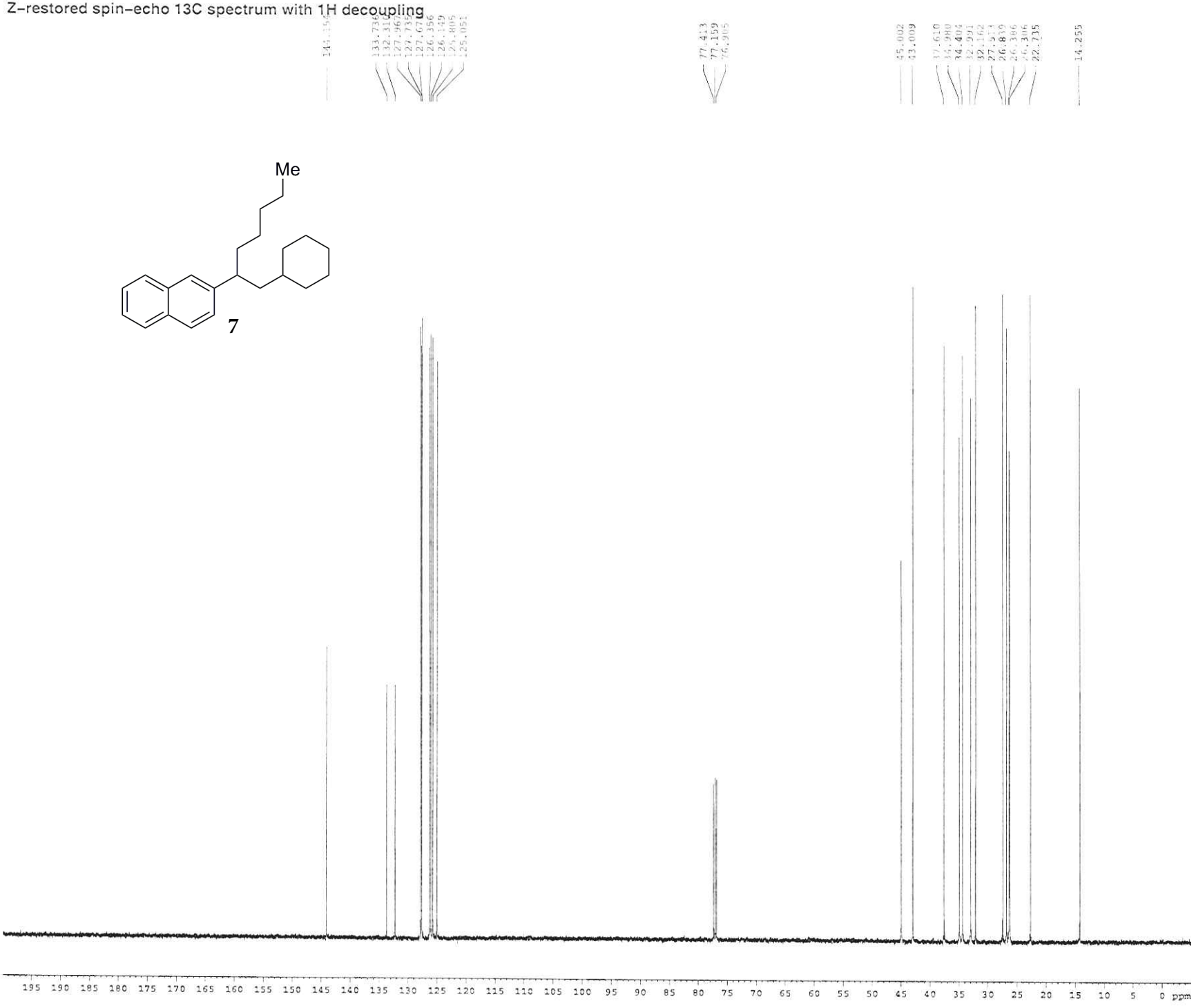
F2 - Acquisition Parameters
Date_              20121209
Time                  15.41
INSTRUM             drx400
PROBHD   5 mm QNP H/P/P
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1118579 sec
RG                      32
DW                78.000 usec
DE                 4.50 usec
TE                 298.1 K
D1              0.10000000 sec
MCREST          0.00000000 sec
MCWRK           0.02500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300549 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    2.00
```



Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                    yongda
NAME                  IMYS   117
EXPNO                      222
PROCNO                       1

P2   Acquisition Parameters
Date_              20131209
Time                  15.53
INSTRUM             cryo600
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30qp.prd
TD                     65536
SOLVENT                CDCl3
NS                        93
DS                        16
SWH                30303.031 Hz
FIDRES             0.462398 Hz
AQ                 1.0814105 sec
RG                      8192
DW                   16.500 usec
DE                    6.00 usec
TE                   298.2 K
D1                   0.25000000 sec
d11                  0.03000000 sec
D16                  0.00020000 sec
d17                  0.00019600 sec
MCREST               0.00000000 sec
MCWRK                0.01500000 sec
P2                     31.00 usec

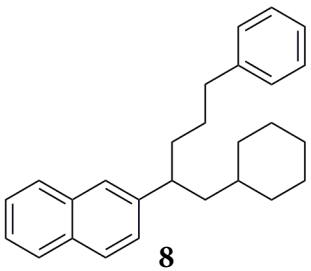
======== CHANNEL f1 ========
NUC1                      13C
P1                     15.50 usec
P11                   500.00 usec
P12                  2000.00 usec
PL6                   120.00 dB
PL1                    -1.00 dB
SFO1           125.7942048 MHz
SP1                    3.20 dB
SP2                    3.20 dB
SPNAM1     Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SFOFF1                 0.00 Hz
SFOFF2                 0.00 Hz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                100.00 usec
PL2                    1.60 dB
PL12                  24.60 dB
SFO2           500.2225011 MHz

====== GRADIENT CHANNEL =====
GNAM1               SINE.100
GNAM2               SINE.100
GPX1                   0.00 %
GPX2                   0.00 %
GPY1                   0.00 %
GPY2                   0.00 %
GPZ1                  30.00 %
GPZ2                  50.00 %
p15                  500.00 usec
p16                  1000.00 usec

F2 - Processing parameters
SI                        65536
SF             125.7804168 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                       2.00
```

1H spectrum



8

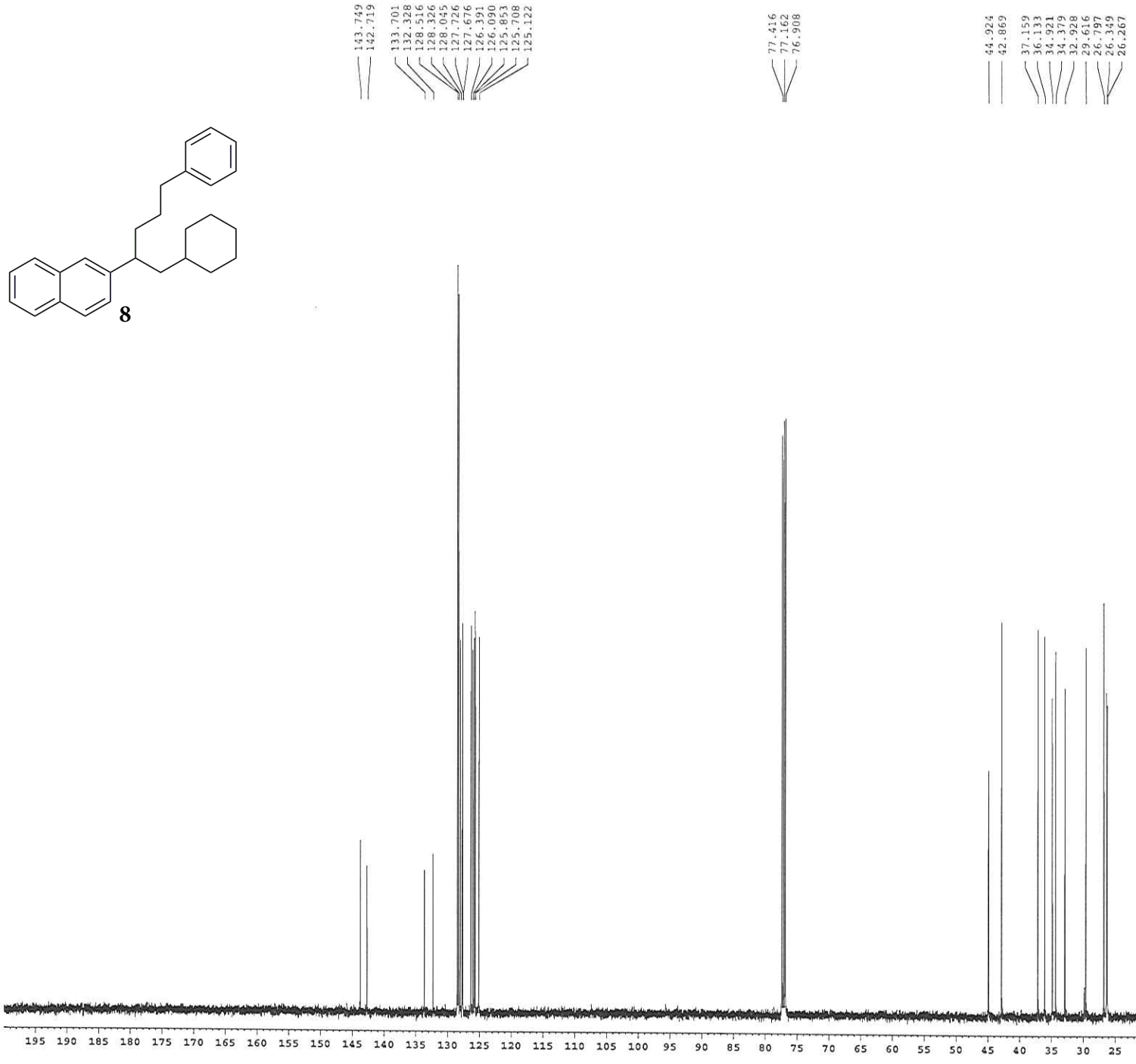

```
Current Data Parameters
USER                yonova
NAME           imy5 - 109
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20130620
Time                20.57
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 Hz
AQ              5.0999398 sec
RG                   7.1
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 7.50 usec
PL1                1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameters
SI                 65536
SF          500.2200000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  4.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                yonova
NAME              imy5 - 109
EXPNO                    222
PROCNO                     1

F2 - Acquisition Parameters
Date_              20130620
Time                 21.03
INSTRUM              cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                     65536
SOLVENT                CDCl3
NS                       520
DS                        16
SWH                30303.031 Hz
FIDRES             0.462388 Hz
AQ                 1.0814105 sec
RG                   10321.3
DW                    16.500 usec
DE                     6.00 usec
TE                    298.0 K
D1                 0.25000000 sec
d11                0.03000000 sec
D16                0.00020000 sec
d17                0.00019600 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec
P2                    31.00 usec

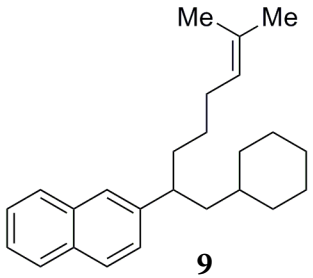
======== CHANNEL f1 ========
NUC1                      13C
P1                      15.50 usec
P11                    500.00 usec
P12                   2000.00 usec
PL0                    120.00 dB
PL1                     -1.00 dB
SFO1               125.7942548 MHz
SP1                      3.20 dB
SP2                      3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                   0.00 Hz
SPOFF2                   0.00 Hz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  100.00 usec
PL2                      1.60 dB
PL12                    24.66 dB
SFO2               500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1               SINE.100
GPNAM2               SINE.100
GPX1                     0.00 %
GPX2                     0.00 %
GPY1                     0.00 %
GPY2                     0.00 %
GPZ1                    30.00 %
GPZ2                    50.00 %
p15                    500.00 usec
p16                   1000.00 usec

F2 - Processing parameters
SI                       65536
SF                 125.7804090 MHz
WDW                         EM
SSB                          0
LB                       1.00 Hz
GB                           0
PC                       2.00
```

1H spectrum



9

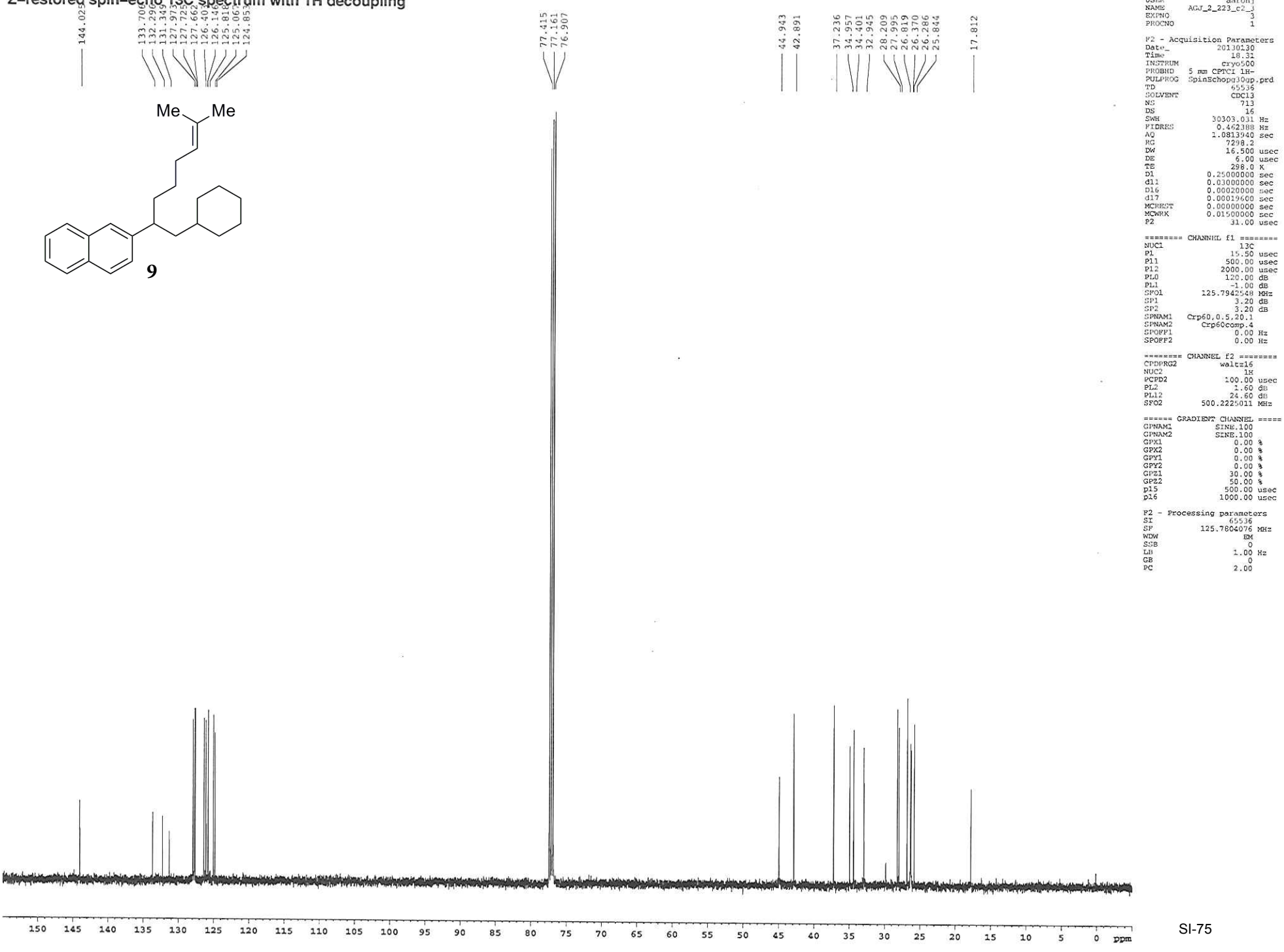
```
Current Data Parameters
USER                aaronj
NAME       AGJ_2_223_c2_1
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20130130
Time                18.25
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES             0.098043 Hz
AQ              5.0998774 sec
RG                   5.7
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  7.50 usec
PL1                 1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameters
SI                  65536
SF            500.2200330 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00
```

Z–restored spin–echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                aaronj
NAME          AGJ_2_223_c2_1
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130130
Time                 18.31
INSTRUM             cryo600
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     713
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                  7298.2
DW                 16.500 usec
DE                  6.00 usec
TE                298.0 K
D1             0.25000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                 31.00 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                 3.20 dB
SP2                 3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1              0.00 Hz
SPOFF2              0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12               24.60 dB
SFO2         500.2225011 MHz

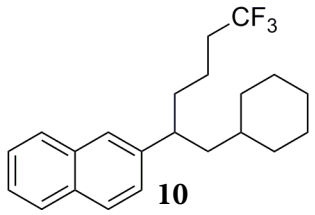
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                   65536
SF           125.7804076 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00
```

1H spectrum

7.823
7.802
7.781
7.552
7.482
7.479
7.465
7.463
7.447
7.442
7.427
7.424
7.410
7.304
7.300
7.282
7.279
7.243

2.842
2.829
2.818
2.805
2.793
2.782
2.768
2.056
2.044
2.029
2.017
2.002
1.992
1.976
1.964
1.949
1.937
1.928
1.922
1.845
1.814
1.744
1.725
1.709
1.701
1.683
1.665
1.651
1.644
1.628
1.617
1.604
1.592
1.559
1.530
1.517
1.513
1.496
1.483
1.474
1.468
1.462
1.453
1.444
1.438
1.428
1.420
1.413
1.405
1.393
1.382
1.368
1.354
1.343
1.334
1.328
1.319
1.309
1.256
1.120



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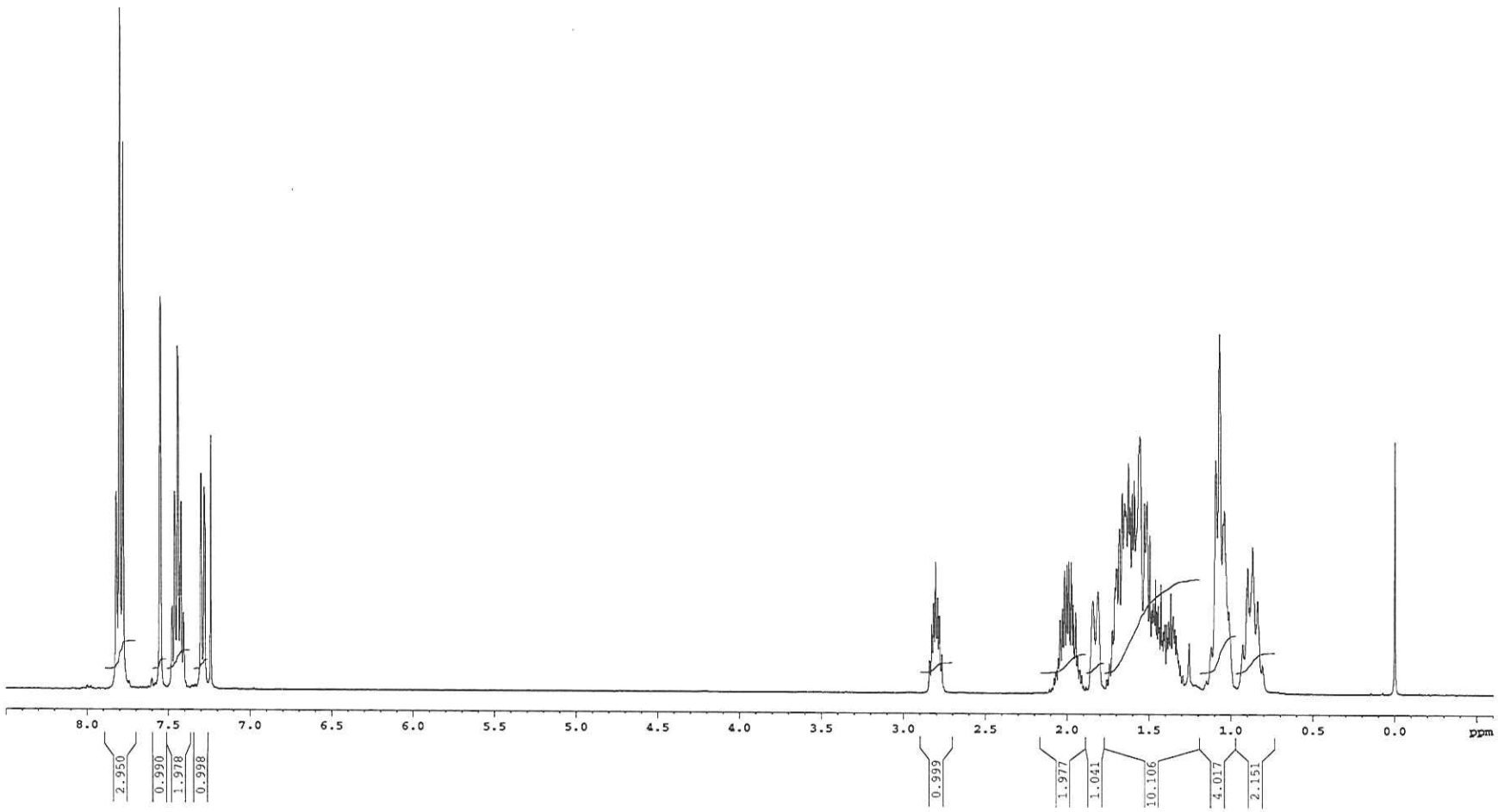
```
Current Data Parameters
USER            aaronj
NAME        AGJ_2_235_c1
EXPNO                  1
PROCNO                 1

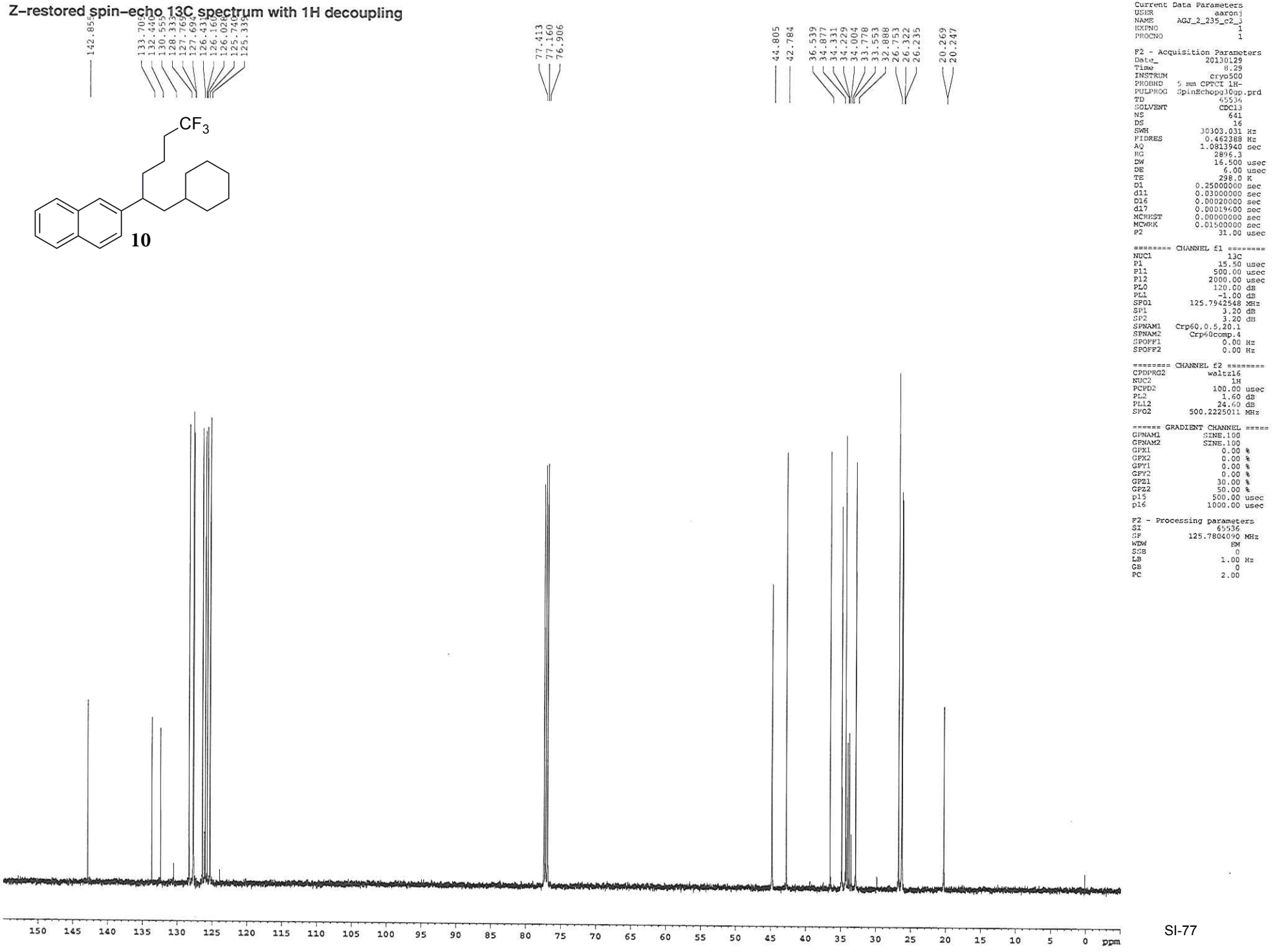
F2 - Acquisition Parameters
Date_           20110128
Time              11.08
INSTRUM         drx400
PROBHD   5 mm QNP H/F/P
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           6410.256 Hz
FIDRES        0.097813 Hz
AQ            5.1118579 sec
RG                143.7
DW               78.000 usec
DE                4.50 usec
TE               298.1 K
D1            0.10000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                12.00 usec
PL1               -0.60 dB
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300280 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 2.00
```



Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                aaronj
NAME          AGJ_2_235_c2_3
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130129
Time                   8.29
INSTRUM              cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                    65536
SOLVENT               CDCl3
NS                      641
DS                       16
SWH                30303.031 Hz
FIDRES             0.462388 Hz
AQ                 1.0813940 sec
RG                    2896.3
DW                   16.500 usec
DE                    6.00 usec
TE                   298.0 K
D1                0.25000000 sec
d11               0.03000000 sec
D16               0.00020000 sec
d17               0.00019600 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec
P2                   31.00 usec

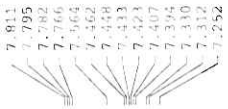
======== CHANNEL f1 ========
NUC1                    13C
P1                    15.50 usec
P11                  500.00 usec
P12                 2000.00 usec
PL0                  120.00 dB
PL1                   -1.00 dB
SFO1          125.7942548 MHz
SP1                   3.20 dB
SP2                   3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

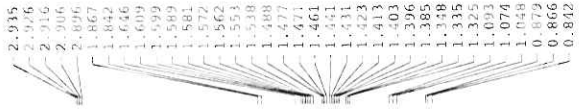
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                100.00 usec
PL2                   1.60 dB
PL12                 24.60 dB
SFO2          500.2225011 MHz

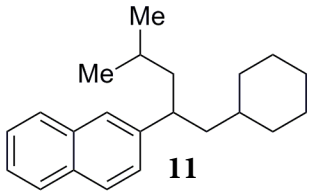
====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                    65536
SF            125.7804090 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00
```

1H spectrum







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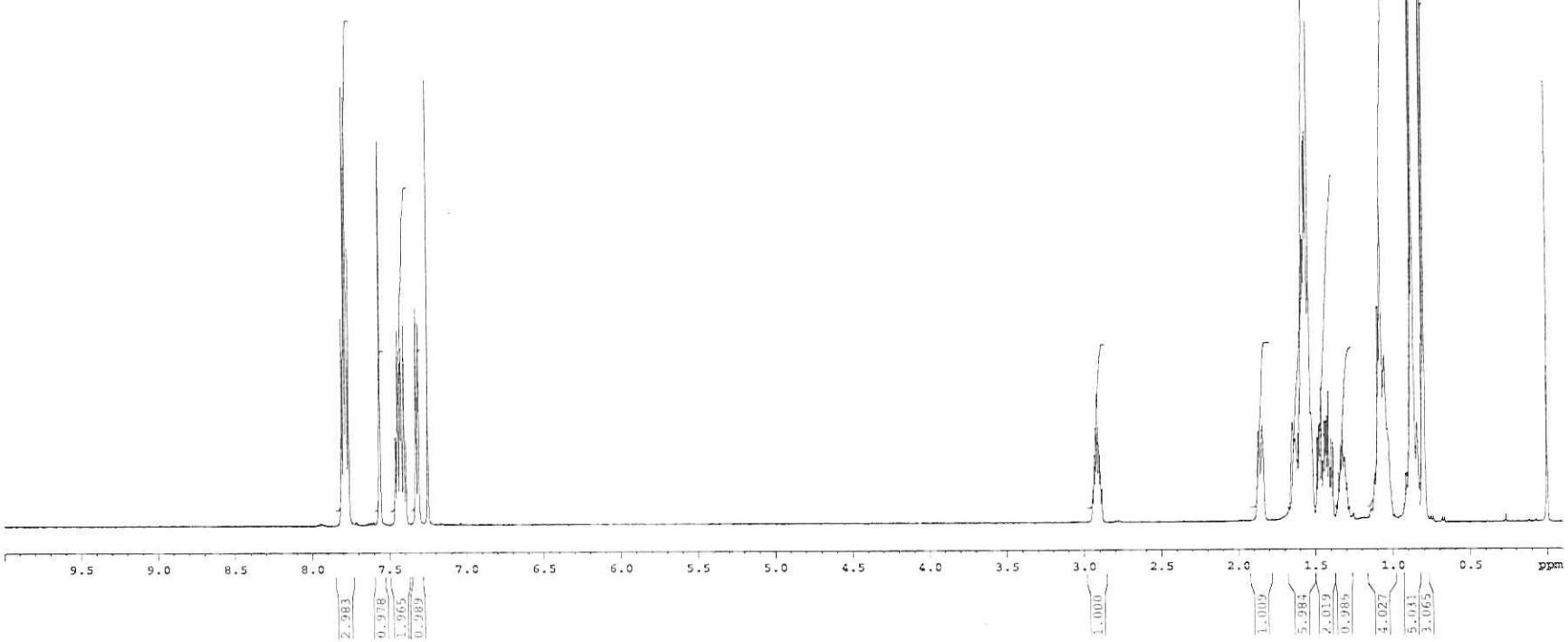
```
Current Data Parameters
USER            yonova
NAME            DEVS - 126
EXPNO               111
PROCNO                1

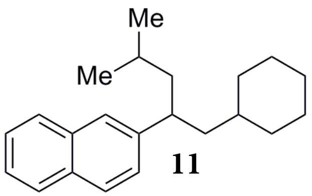
F2 - Acquisition Parameters
Date_          20121114
Time              12.55
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               81728
SOLVENT           CDCl3
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.098043 Hz
AQ            5.0999398 sec
RG                 5.7
DW               62.400 usec
DE                6.05 usec
TE               298.0 K
D1            0.10000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                7.50 usec
PL1               1.60 dB
SFO1        500.2235015 MHz

F2 - Processing parameters
SI                65536
SF          500.2200344 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                4.00
```



Z-restored spin-echo 13C spectrum with 1H decoupling



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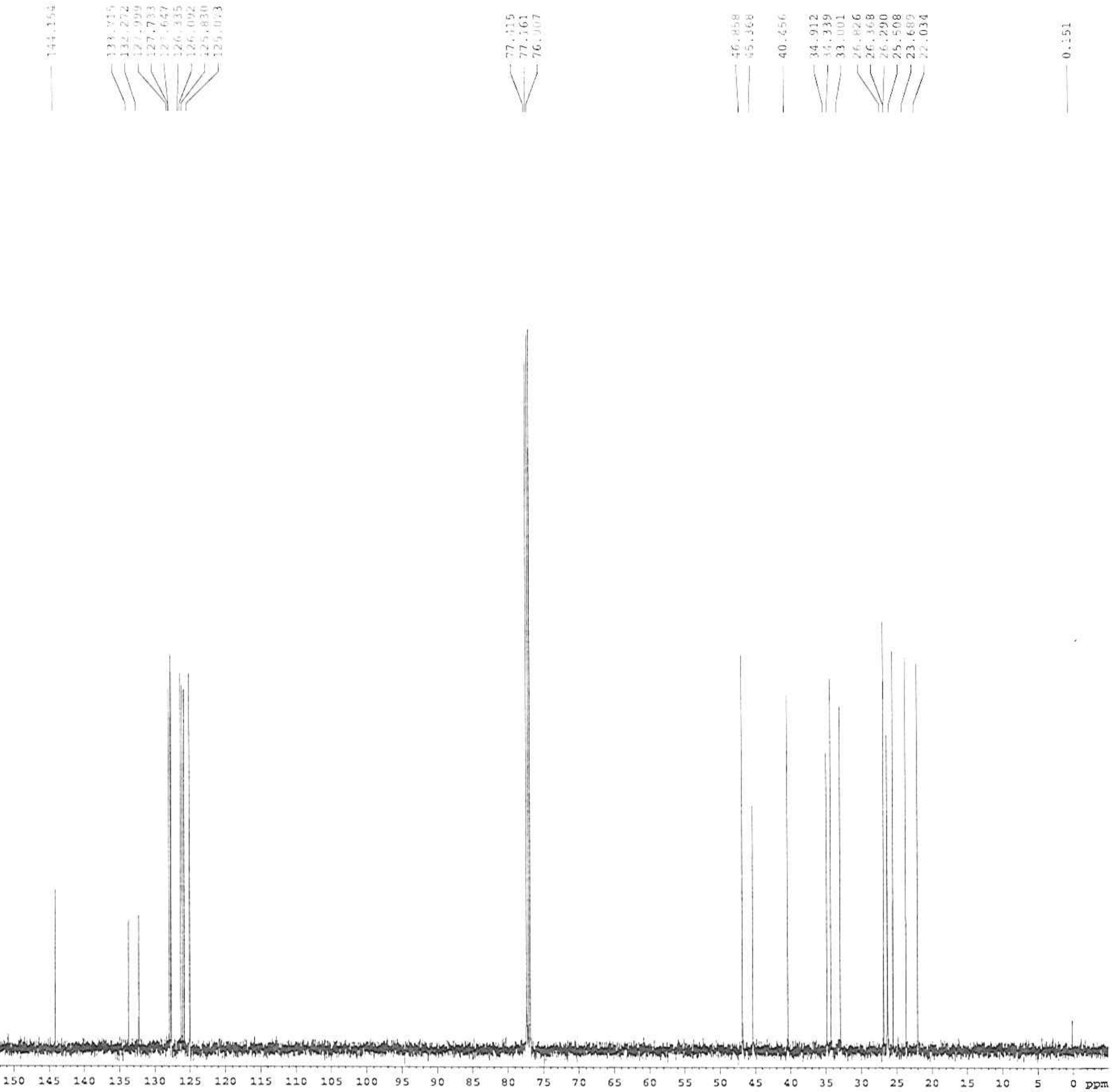



```
Current Data Parameters
USER            yonova
NAME         DMY5 - 135
EXPNO              222
PROCNO               1

F2 - Acquisition Parameters
Date_         20121214
Time             13.31
INSTRUM        cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD               65536
SOLVENT          CDCl3
NS                 275
DS                  16
SWH          30303.031 Hz
FIDRES        0.462388 Hz
AQ           1.0814105 sec
RG              5160.6
DW              16.500 usec
DE                6.00 usec
TE               298.0 K
D1          0.25000000 sec
d11         0.03000000 sec
D16         0.00020000 sec
d17         0.00019600 sec
MCREST      0.00000000 sec
MCWRK       0.01500000 sec
P2               31.00 usec

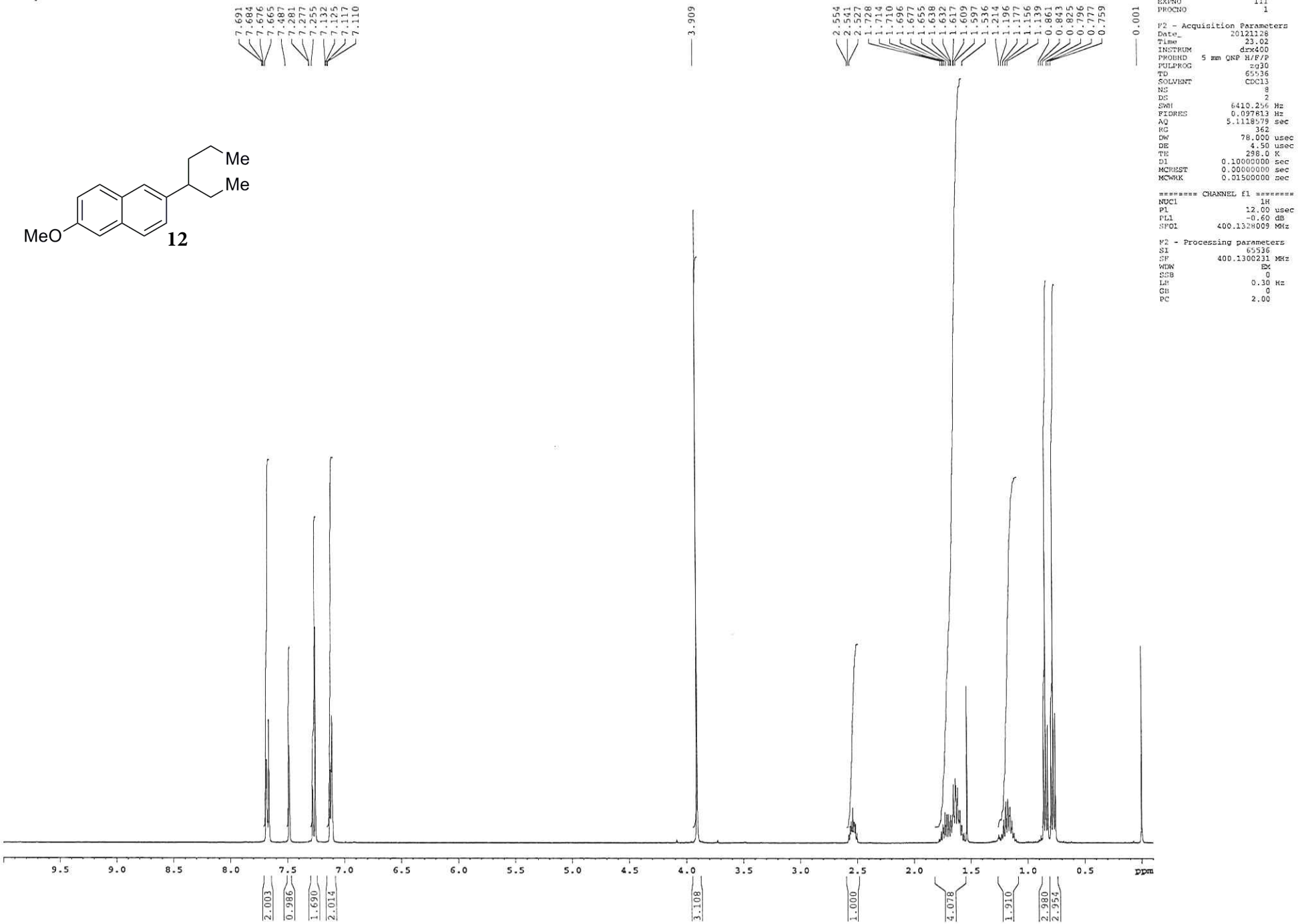
======== CHANNEL f1 ========
NUC1               13C
P1               15.50 usec
P11             500.00 usec
P12            2000.00 usec
PL0             120.00 dB
PL1              -1.00 dB
SFO1       125.7942548 MHz
SP1               3.20 dB
SP2               3.20 dB
SPNAM1   Crp60,0.5,20.1
SPNAM2     Crp60comp.4
SPOFF1            0.00 Hz
SPOFF2            0.00 Hz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2                1H
PCPD2           100.00 usec
PL2               1.60 dB
PL12             24.60 dB
SFO2       500.2225011 MHz

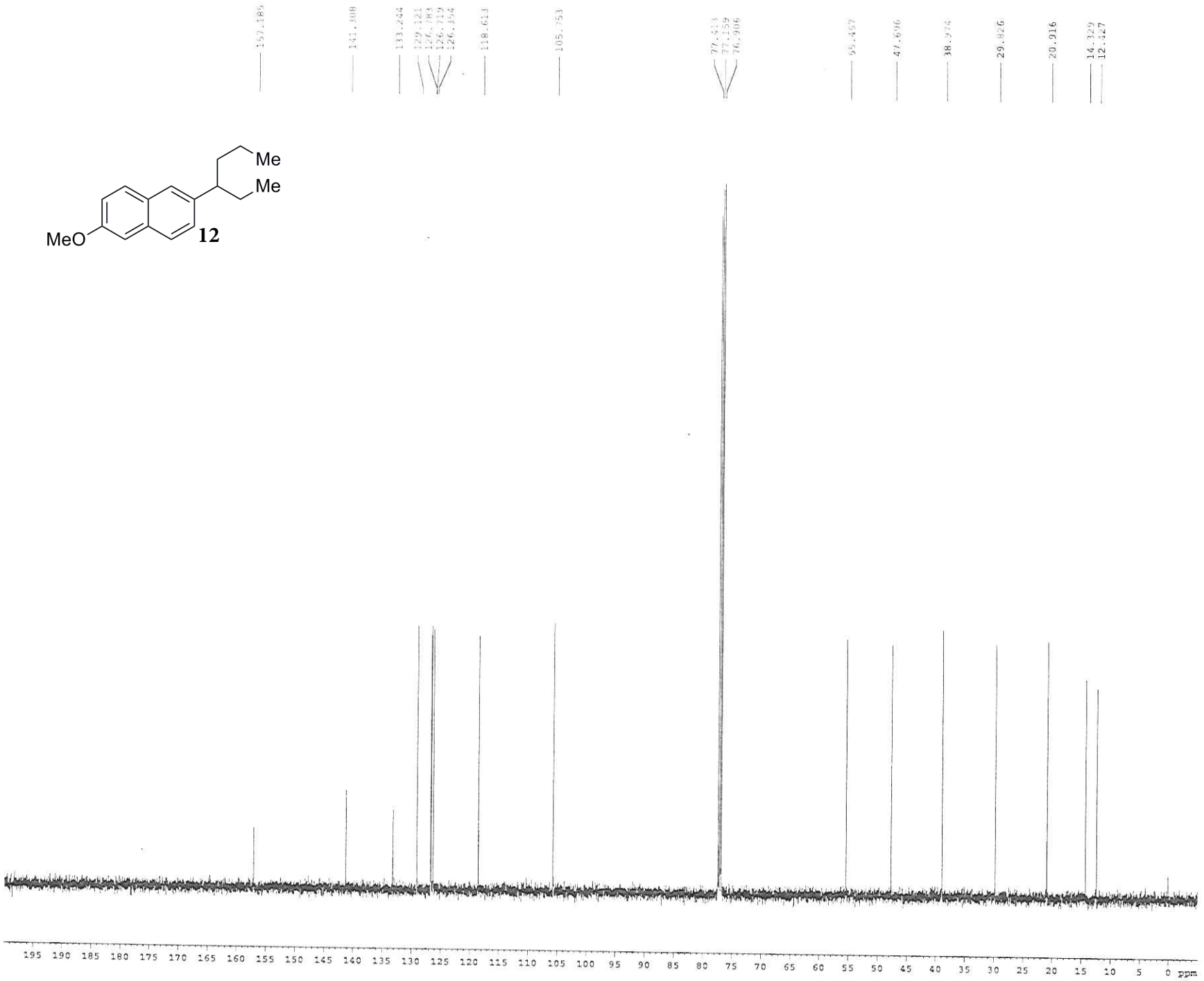
====== GRADIENT CHANNEL =====
GPNAM1        SINE.100
GPNAM2        SINE.100
GPX1              0.00 %
GPX2              0.00 %
GPY1              0.00 %
GPY2              0.00 %
GPZ1             30.00 %
GPZ2             50.00 %
p15             500.00 usec
p16            1000.00 usec

F2 - Processing parameters
SI               65536
SF         125.7804076 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                2.00
```

1H spectrum


7.691
7.684
7.676
7.665
7.487
7.281
7.277
7.255
7.132
7.125
7.117
7.110
3.909
2.554
2.541
2.527
1.728
1.714
1.710
1.696
1.677
1.655
1.638
1.632
1.617
1.609
1.597
1.536
1.214
1.196
1.177
1.156
1.139
0.861
0.843
0.825
0.796
0.777
0.759
0.001
Me
Me
MeO
12
Current Data Parameters
USER yonova
NAME IMY5 - 60MeNapKtDP
EXPNO 111
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121128
Time 23.02
INSTRUM drx400
PHODND 5 mm QNP H/F/P
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1118579 sec
RG 362
DW 78.000 usec
DE 4.50 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -0.60 dB
SFO1 400.1328009 MHz
F2 - Processing parameters
SI 65536
SF 400.1300231 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.003
0.986
1.690
2.014
3.108
1.000
4.078
1.910
2.980
2.954

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
NAME                 yqmova
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_           20121129
Time                 5.07
INSTRUM           cryo500
PROBHD     5 mm CPTCI 1H-
PULPROG   SpinEchopu10gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     378
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0814105 sec
RG                  2580.3
DW                 16.500 usec
DE                  6.00 usec
TE                298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                 31.00 usec

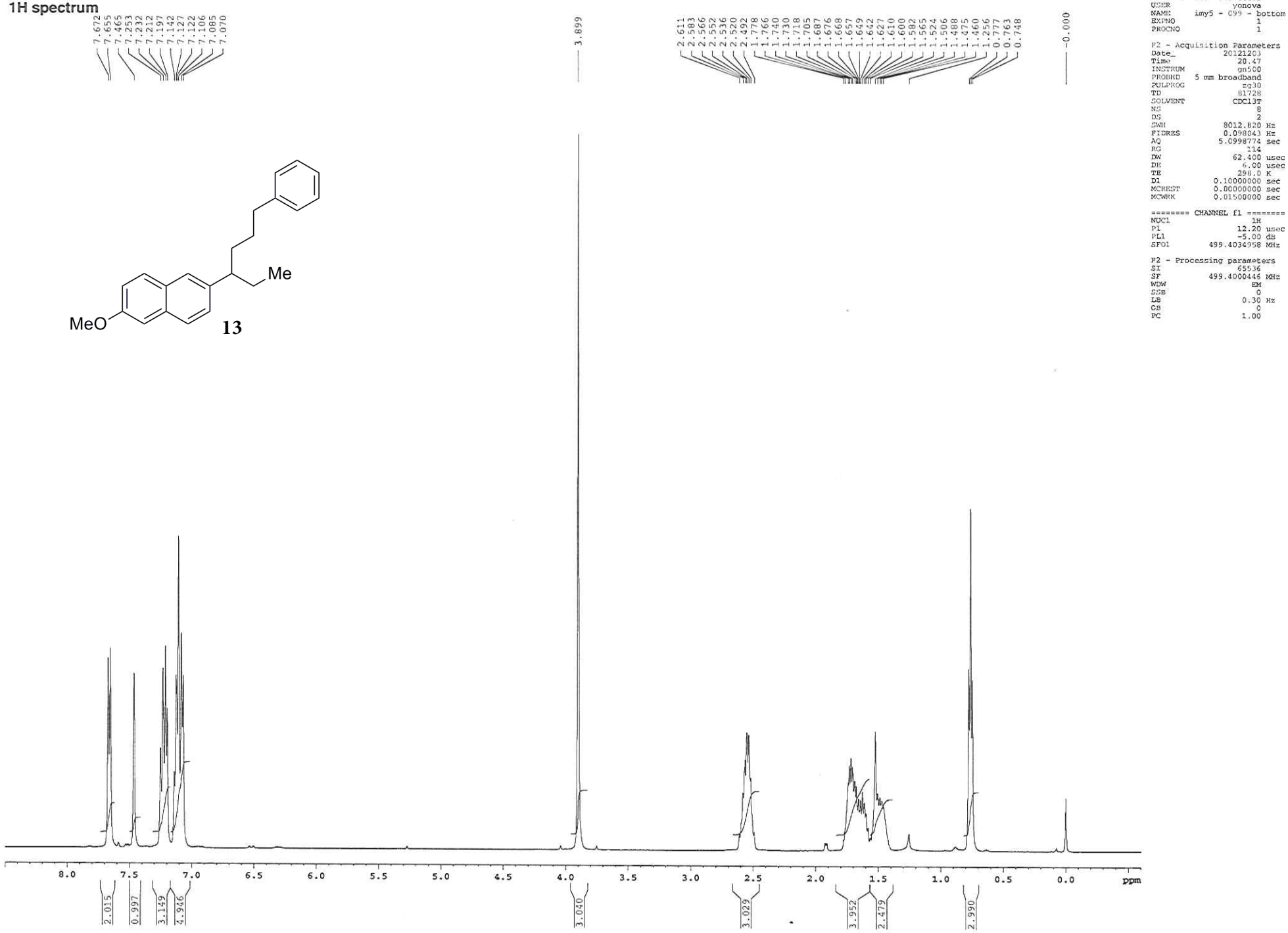
======== CHANNEL f1 ========
NUC1                  13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SF1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1             0.00 Hz
SPOFF2             0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1               0.00 %
GPX2               0.00 %
GPY1               0.00 %
GPY2               0.00 %
GPZ1              30.00 %
GPZ2              50.00 %
P15              500.00 usec
P16             1000.00 usec

F2 - Processing parameters
SI                  65536
SF          125.7804071 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00
```

1H spectrum



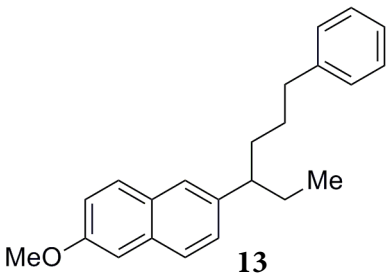

```
Current Data Parameters
USER                yonova
NAME      imy5 - 099 - bottom
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20121203
Time            20.47
INSTRUM         qn500
PROBHD   5 mm broadband
PULPROG         zg30
TD              81728
SOLVENT         CDCl3T
NS              8
DS              2
SWH             8012.820 Hz
FIDRES          0.098043 Hz
AQ              5.0998774 sec
RG              114
DW              62.400 usec
DE              6.00 usec
TE              298.0 K
D1              0.10000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  12.20 usec
PL1                 -5.00 dB
SFO1          499.4034958 MHz

F2 - Processing parameters
SI                     65536
SF            499.4000446 MHz
WDW                    EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling



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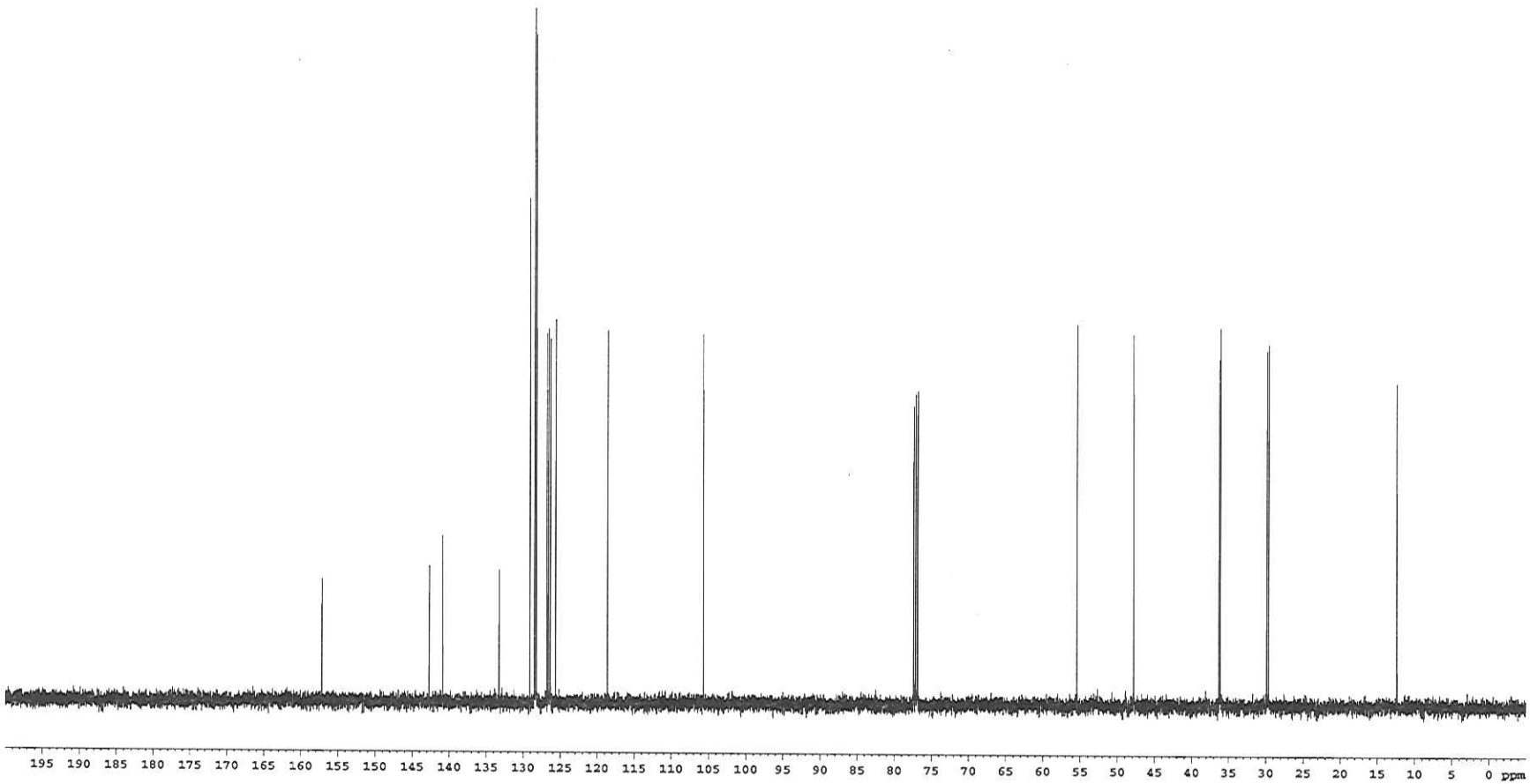



```
Current Data Parameters
USER                yonova
NAME             IMY5 - 099
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_              20121203
Time                 21.04
INSTRUM              cryo600
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                    65536
SOLVENT               CDCl3
NS                       56
DS                       16
SWH               30303.031 Hz
FIDRES            0.462388 Hz
AQ                2.0813940 sec
RG                     4096
DW                  16.500 usec
DE                   6.00 usec
TE                  298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCRSST          0.00000000 sec
MCWRK           0.01500000 sec
P2                  31.00 usec

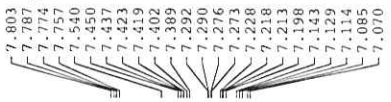
======== CHANNEL f1 ========
NUC1                   13C
P1                   15.50 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1          125.7942548 MHz
SP1                  3.20 dB
SP2                  3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

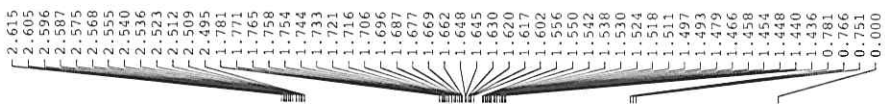
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2          500.2225011 MHz

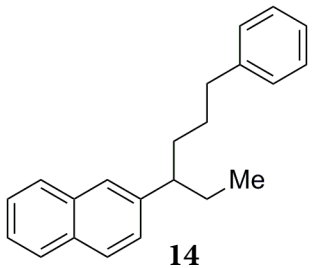
====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                    65536
SF            125.7804113 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00
```

1H spectrum







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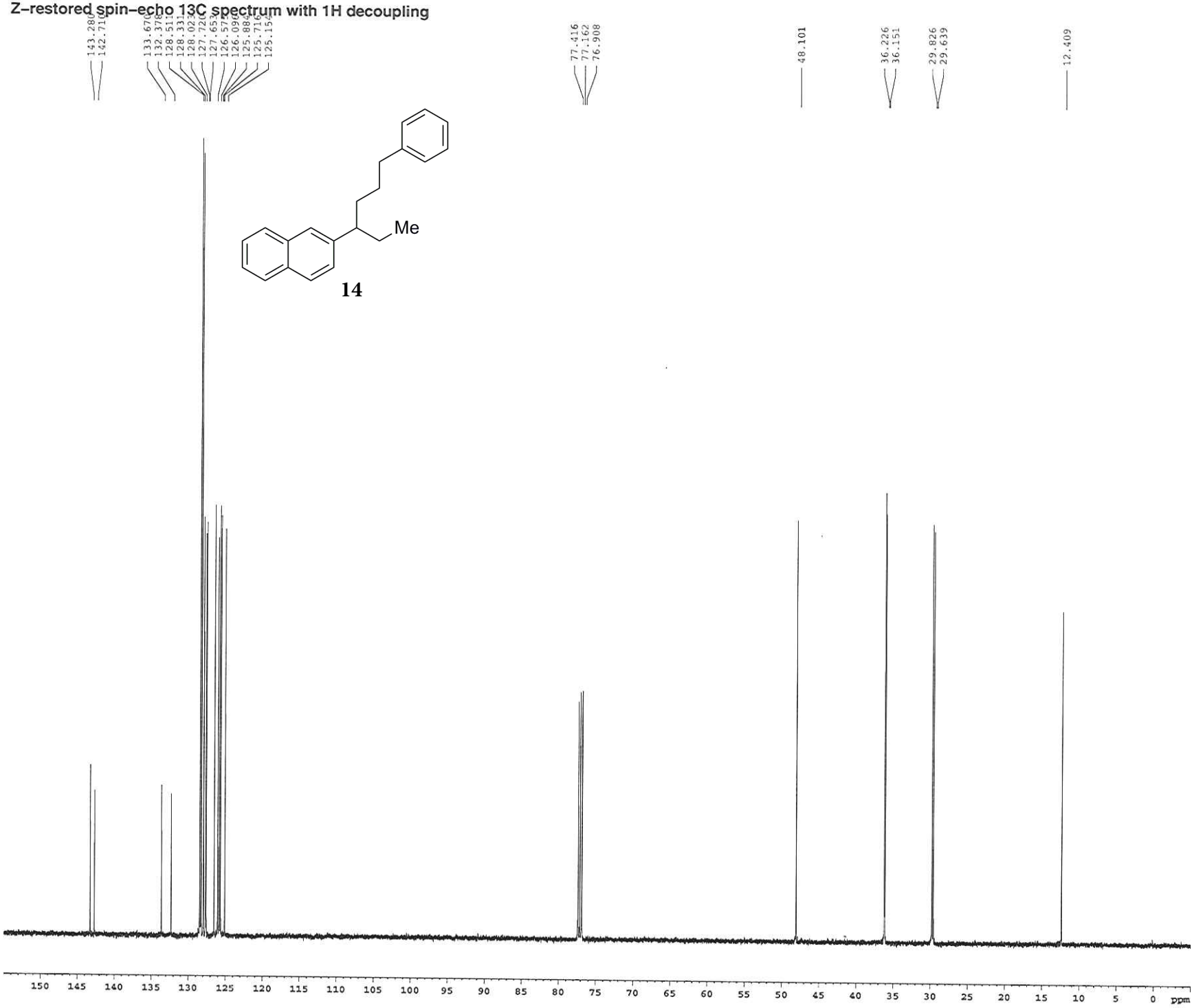
```
Current Data Parameters
USER                aaronj
NAME          AGJ_2_142_c2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130523
Time                 11.50
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    81728
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8012.820 Hz
FIDRES                0.098043 Hz
AQ                 5.0998774 sec
RG                        6.3
DW                   62.400 usec
DE                    6.00 usec
TE                   298.0 K
D1                 0.10000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    7.50 usec
PL1                   1.60 dB
SFO1           500.2235015 MHz

F2 - Processing parameters
SI                       65536
SF             500.2200519 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    4.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                aaronj
NAME          AGJ_2_142_c2
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130523
Time                 11.54
INSTRUM              cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     332
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                  4597.6
DW                 16.500 usec
DE                  6.00 usec
TE                298.0 K
D1             0.25000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                 31.00 usec

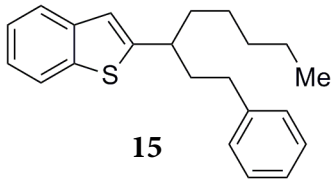
======== CHANNEL f1 ========
NUC1                 13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1             0.00 Hz
SPOFF2             0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1               0.00 %
GPX2               0.00 %
GPY1               0.00 %
GPY2               0.00 %
GPZ1              30.00 %
GPZ2              50.00 %
p15              500.00 usec
p16             1000.00 usec

F2 - Processing parameters
SI                   65536
SF           125.7804122 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   2.00
```

1H spectrum



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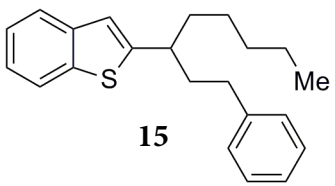
```
Current Data Parameters
USER                yonova
NAME           imy5 - 210
EXPNO                 111
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130329
Time                21.59
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 Hz
AQ              5.0999398 sec
RG                    6.3
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 7.50 usec
PL1                1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameters
SI                 65536
SF            500.2200403 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling



15


```
Current Data Parameters
USER                yonova
NAME              imy5 - 210
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130329
Time                  22.08
INSTRUM             cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                    65536
SOLVENT               CDCl3
NS                      304
DS                       16
SWH               30303.031 Hz
FIDRES            0.462388 Hz
AQ                1.0814105 sec
RG                   7298.2
DW                 16.500 usec
DE                  6.00 usec
TE                  298.0 K
D1                0.25000000 sec
d11               0.03000000 sec
D16               0.00020000 sec
d17               0.00019600 sec
MCHEST            0.00000000 sec
MCWRK             0.01500000 sec
P2                  31.00 usec

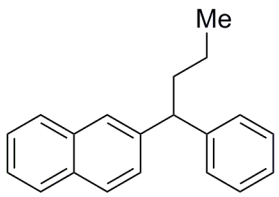
======== CHANNEL f1 ========
NUC1                    13C
P1                    15.50 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1           125.7942548 MHz
SP1                   3.20 dB
SP2                   3.20 dB
SPNAM1     Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               100.00 usec
PL2                   1.60 dB
PL12                 24.60 dB
SFO2           500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                    65536
SF             125.7804099 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     2.00
```

1H spectrum



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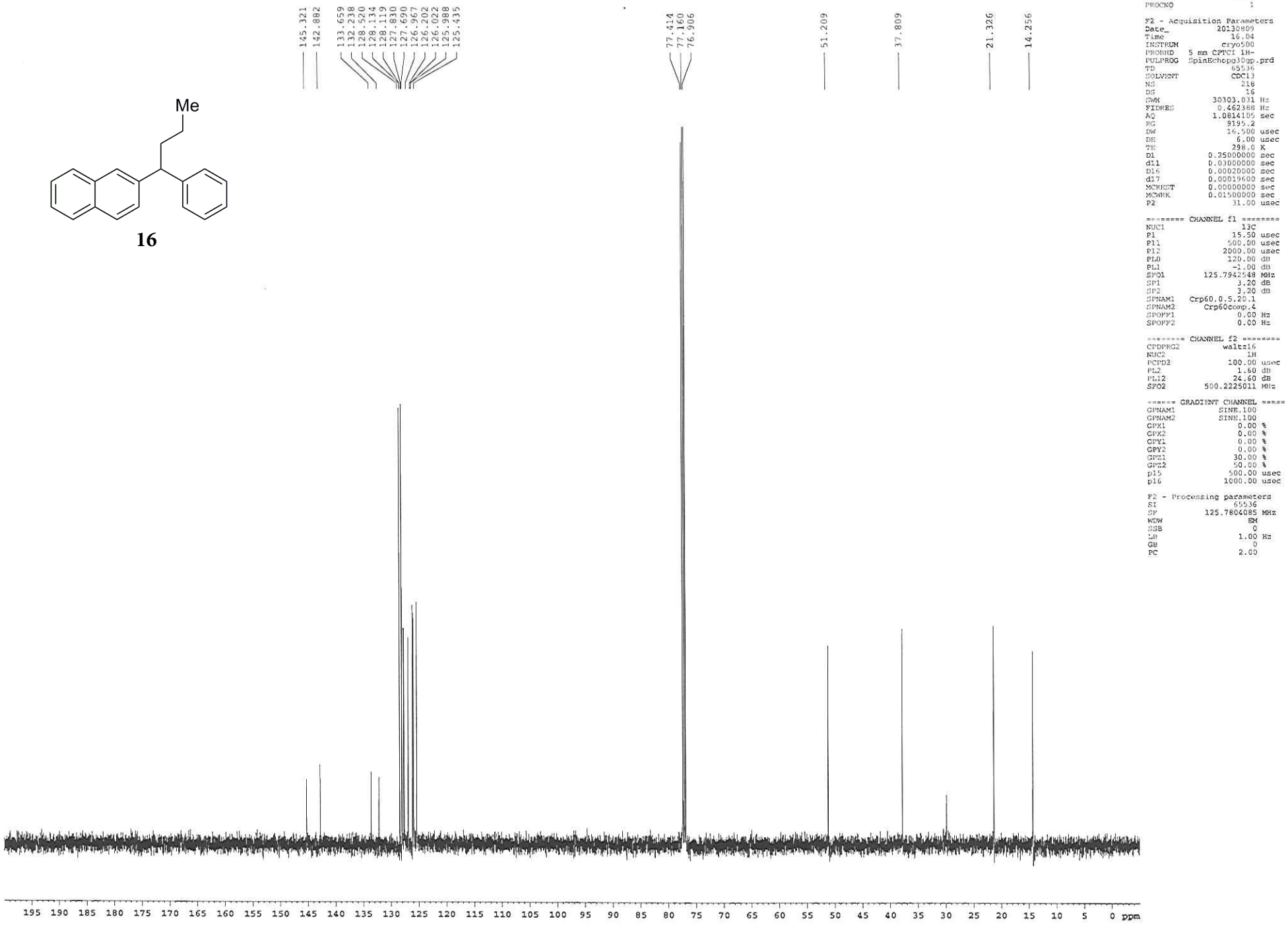
Current Data Parameters
USER yonova
NAME imy5 - 143
EXPNO 91
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130807
Time 19.11
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1118579 sec
RG 406.4
DW 78.000 usec
DE 4.50 usec
TE 298.1 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -0.60 dB
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 400.1300227 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                yonova
NAME              imy5 - 141
EXPNO                 22222
PROCNO                    1

F2 - Acquisition Parameters
Date_           20130809
Time                 16.04
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT               CDCl3
NS                      218
DS                       16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0814105 sec
RG                  9195.2
DW                  16.500 usec
DE                   6.00 usec
TE                  298.0 K
D1               0.25000000 sec
d11              0.03000000 sec
D16              0.00020000 sec
d17              0.00019600 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec
P2                  31.00 usec

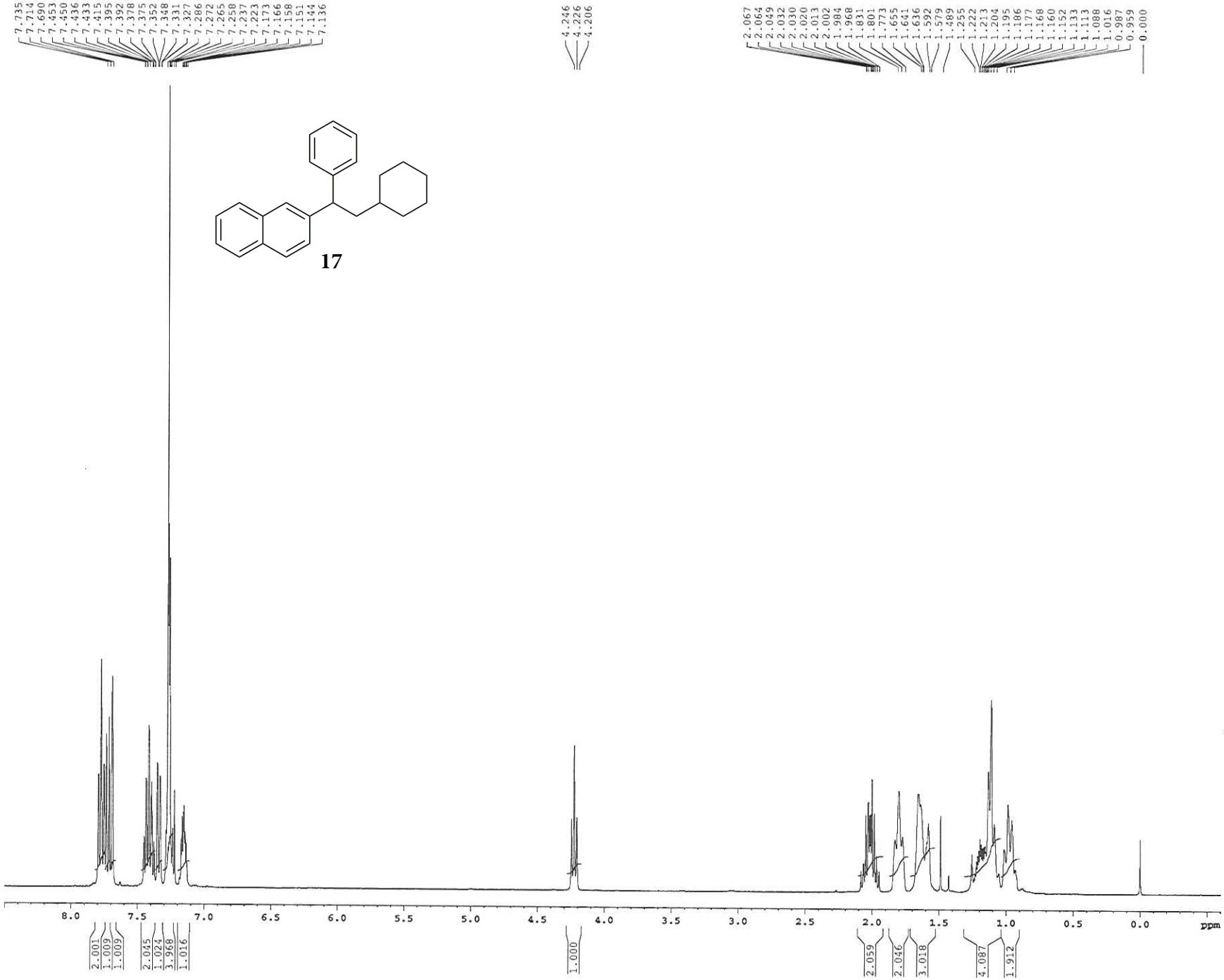
======== CHANNEL f1 ========
NUC1                   13C
P1                   15.50 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1          125.7942548 MHz
SP1                  3.20 dB
SP2                  3.20 dB
SPNAM1     Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                    65536
SF           125.7804085 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00
```

1H spectrum



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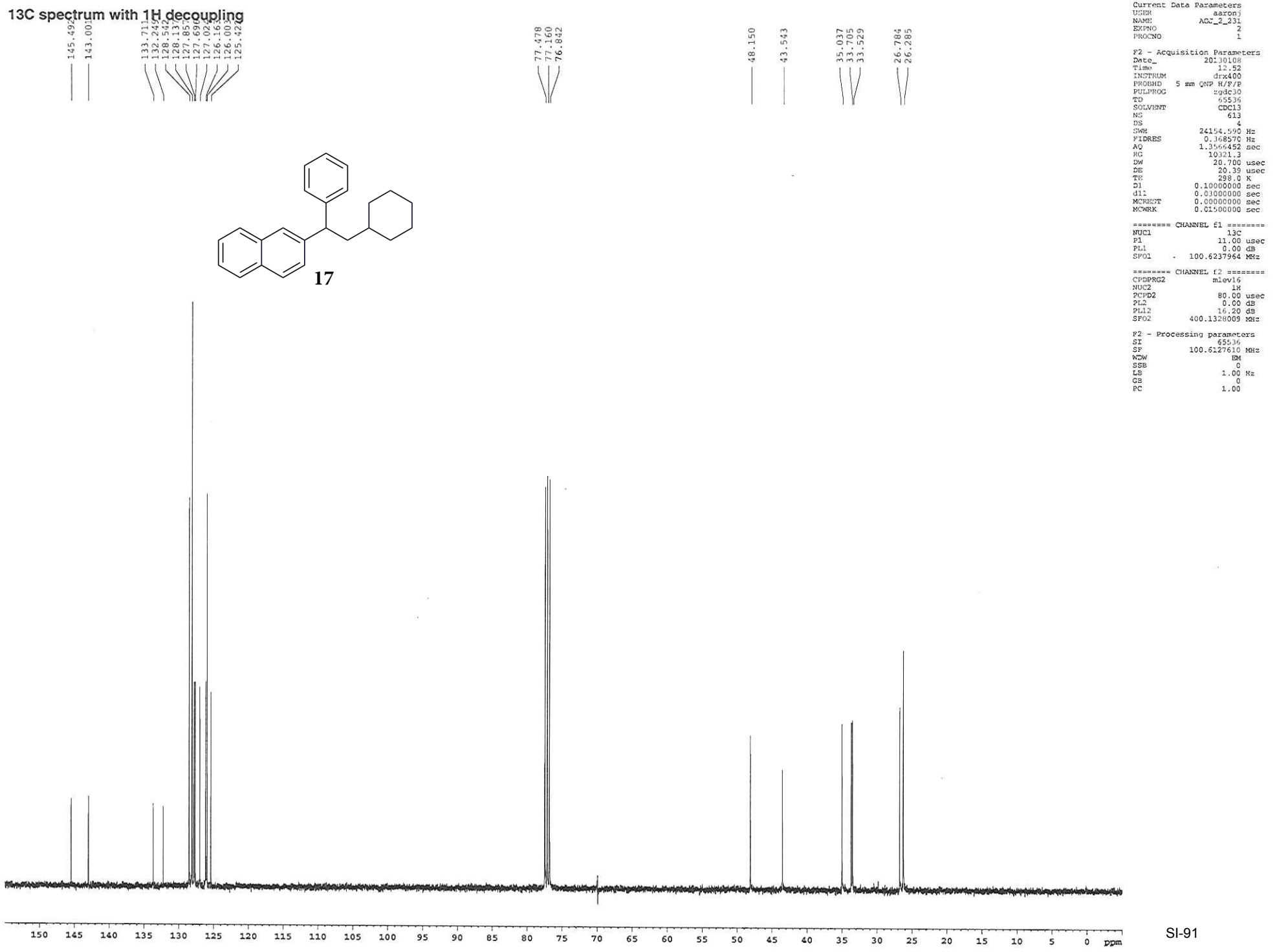
```
Current Data Parameters
USER                aaronj
NAME              AGJ_2_231
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130108
Time                 11.57
INSTRUM              drx400
PROBHD  5 mm QNP H/F/P
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1118579 sec
RG                     114
DW                78.000 usec
DE                 4.50 usec
TE                 298.0 K
D1              0.10000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300361 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 2.00
```

13C spectrum with 1H decoupling




```
Current Data Parameters
USER                aaronj
NAME              AGJ_2_231
EXPNO                     2
PROCNO                    1

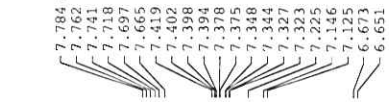
F2 - Acquisition Parameters
Date_              20130108
Time                  12.52
INSTRUM              drx400
PROBHD   5 mm QNP H/F/P
PULPROG              zgdc30
TD                    65536
SOLVENT               CDCl3
NS                      613
DS                        4
SWH                24154.590 Hz
FIDRES             0.368570 Hz
AQ                 1.3566452 sec
RG                   10321.3
DW                    20.700 usec
DE                    20.39 usec
TE                   298.0 K
D1                0.10000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

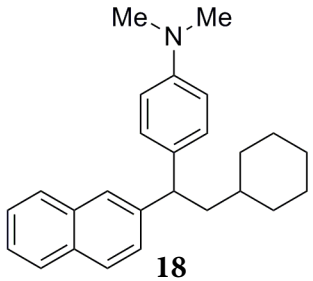
======== CHANNEL f1 ========
NUC1                     13C
P1                     11.00 usec
PL1                     0.00 dB
SFO1          100.6237964 MHz

======== CHANNEL f2 ========
CPDPRG2                mlev16
NUC2                       1H
PCPD2                  80.00 usec
PL2                     0.00 dB
PL12                   16.20 dB
SFO2          400.1328009 MHz

F2 - Processing parameters
SI                        65536
SF                100.6127610 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.00
```

1H spectrum





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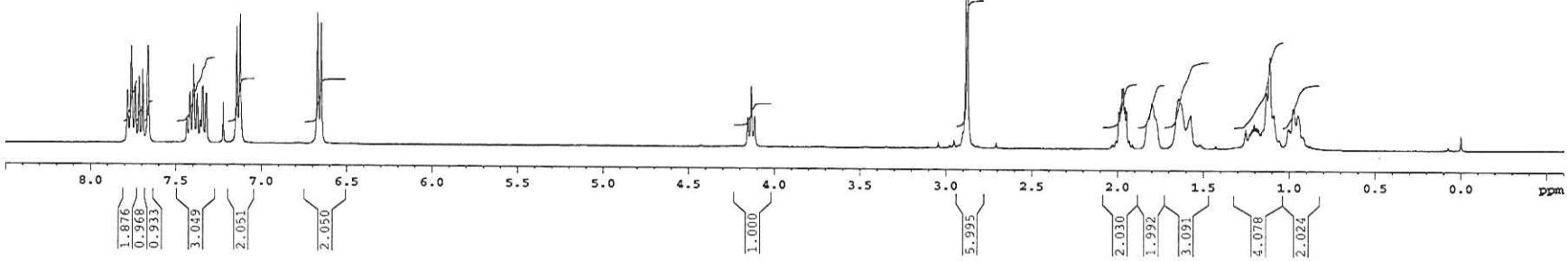
```
Current Data Parameters
USER            aaronj
NAME        AGJ_2_251_c1
EXPNO                  1
PROCNO                 1

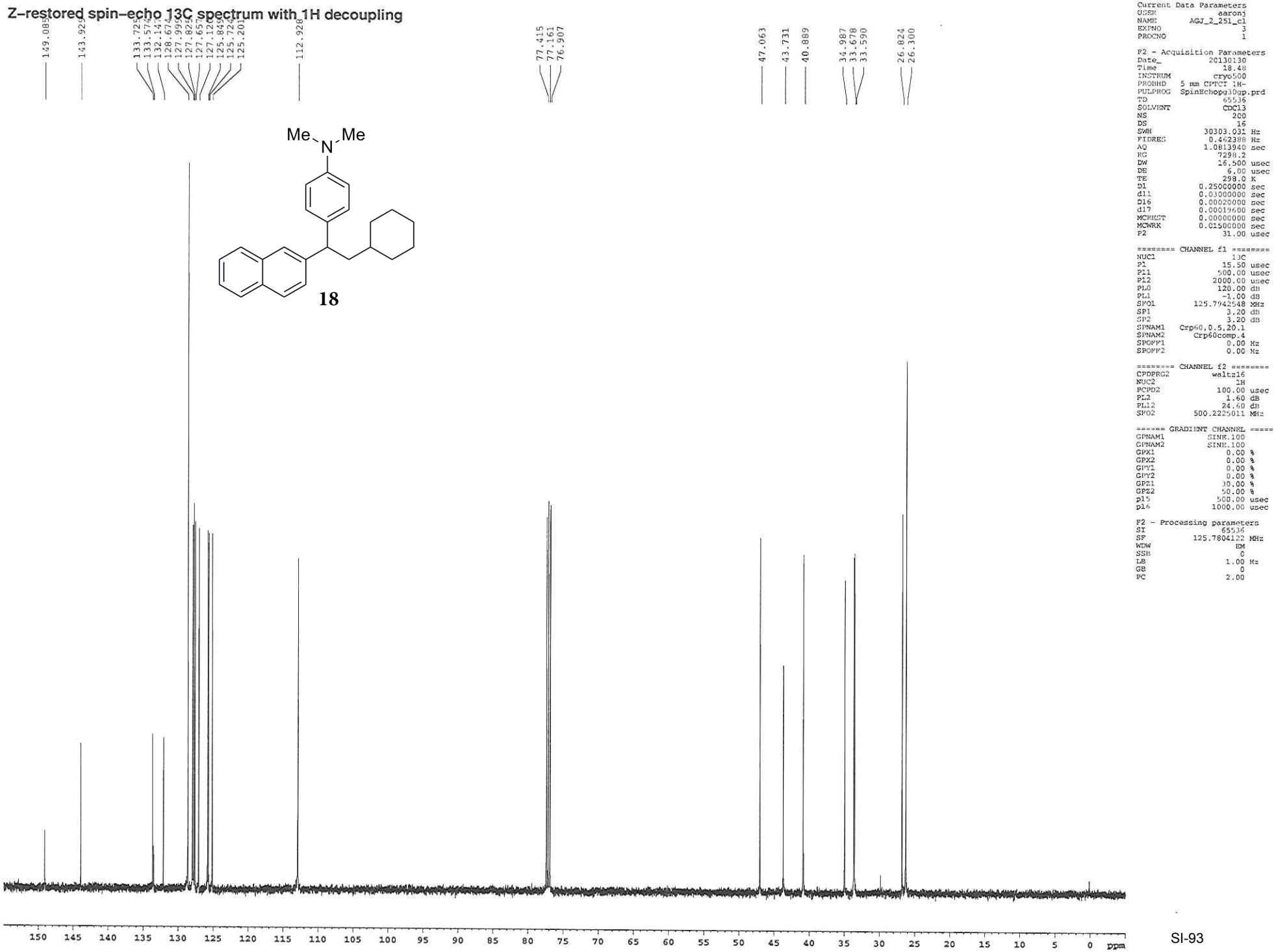
F2 - Acquisition Parameters
Date_           20130122
Time              21.02
INSTRUM         drx400
PROBHD   5 mm QNP H/F/P
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           6410.256 Hz
FIDRES        0.097813 Hz
AQ            5.1118579 sec
RG                 114
DW              78.000 usec
DE               4.50 usec
TE              298.0 K
D1            0.10000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1               1H
P1              12.00 usec
PL1             -0.60 dB
SFO1       400.1328009 MHz

F2 - Processing parameters
SI               65536
SF         400.1300353 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               2.00
```



Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                aaronj
NAME          AGJ_2_251_c1
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_            20130130
Time                18.48
INSTRUM           cryo500
PROBHD  5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    200
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                 7298.2
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                31.00 usec

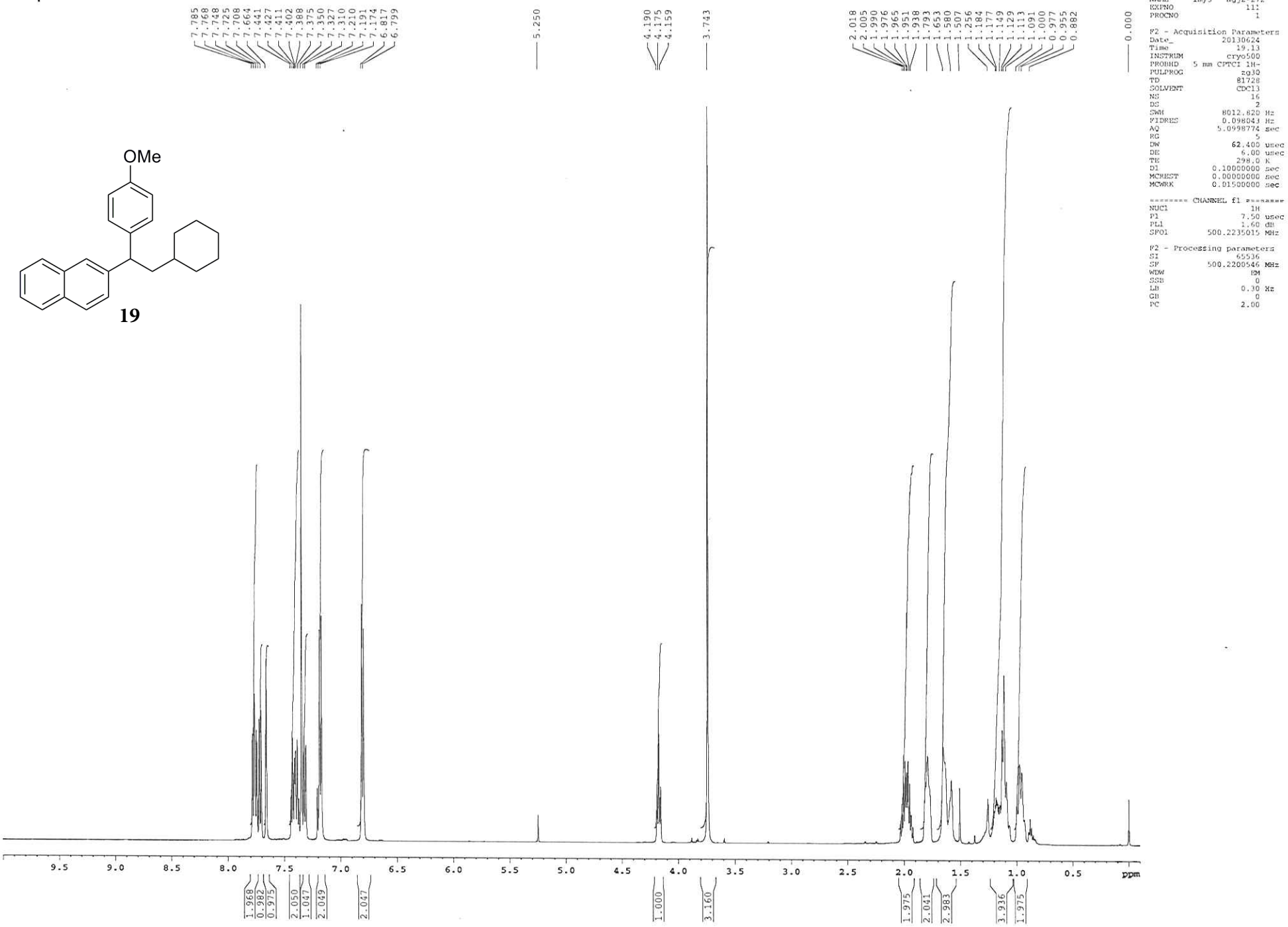
======== CHANNEL f1 ========
NUC1                  13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1            0.00 Hz
SPOFF2            0.00 Hz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2               1.60 dB
PL12             24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1              0.00 %
GPX2              0.00 %
GPY1              0.00 %
GPY2              0.00 %
GPZ1             30.00 %
GPZ2             50.00 %
p15             500.00 usec
p16            1000.00 usec

F2 - Processing parameters
SI                65536
SF          125.7804122 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 2.00
```

1H spectrum



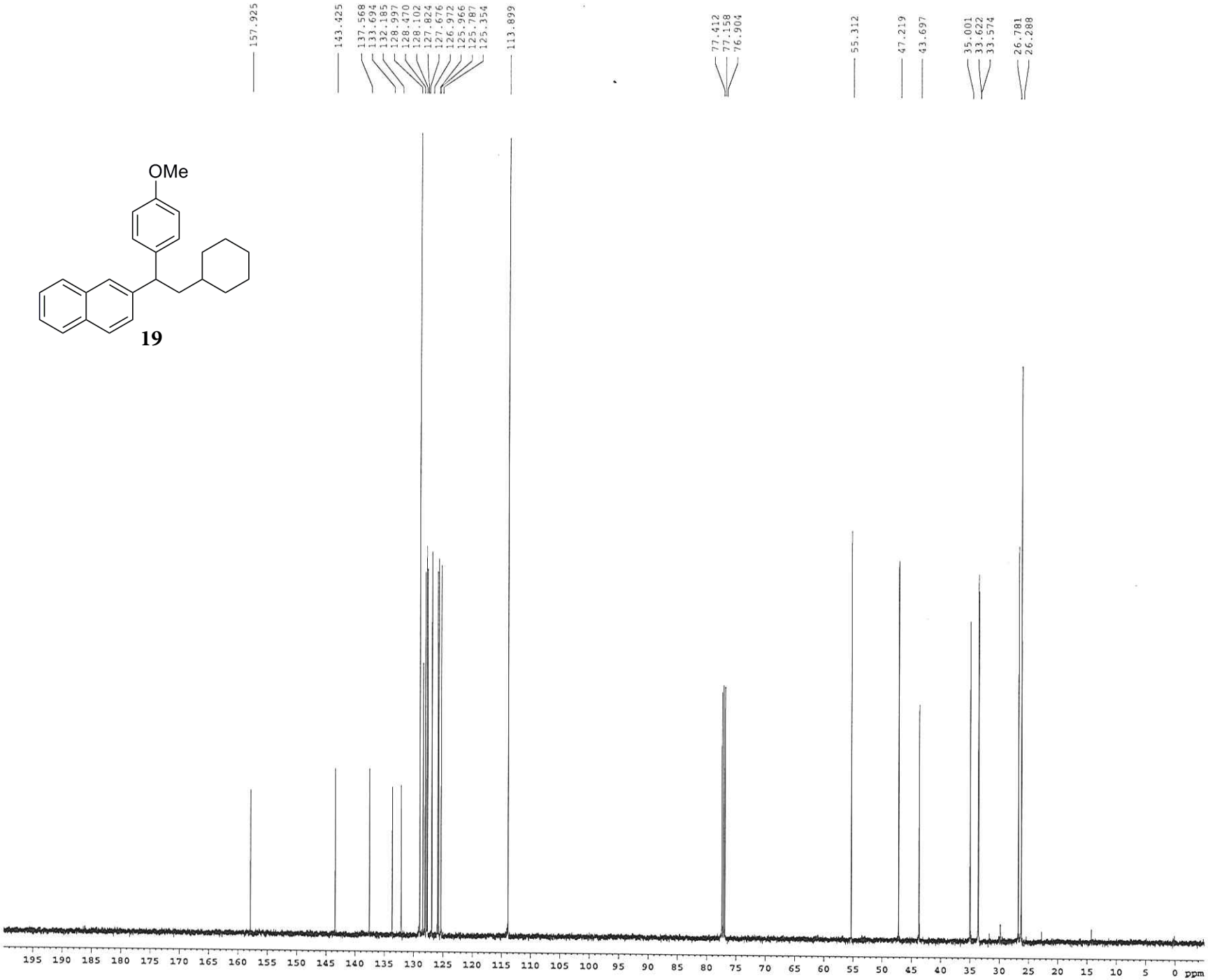

```
Current Data Parameters
USER                yonova
NAME          imy5 - agj2-272
EXPNO                   111
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130624
Time                  19.13
INSTRUM             cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG               zg30
TD                   81728
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8012.820 Hz
FIDRES            0.098043 Hz
AQ                5.0998774 sec
RG                       5
DW                  62.400 usec
DE                   6.00 usec
TE                  298.0 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   7.50 usec
PL1                  1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameters
SI                   65536
SF            500.2200546 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    2.00
```

Z–restored spin–echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                yonova
NAME          imy5 - agj2-272
EXPNO                    222
PROCNO                     1

F2 - Acquisition Parameters
Date_            20130624
Time                19.20
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    207
DS                     16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                  7298.2
DW                 16.500 usec
DE                  6.00 usec
TE                298.0 K
D1               0.25000000 sec
d11              0.03000000 sec
D16              0.00020000 sec
d17              0.00019600 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec
P2                 31.00 usec

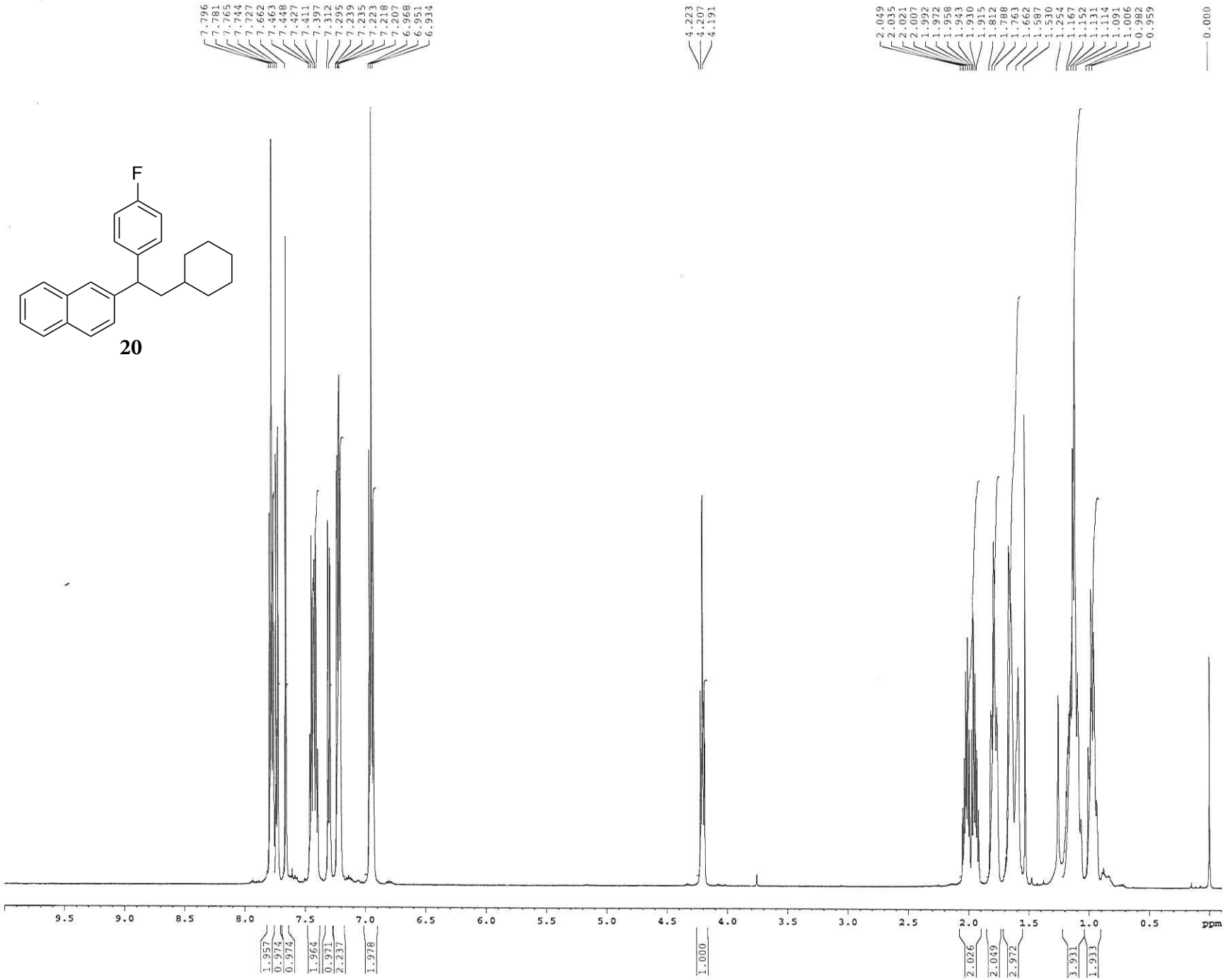
======== CHANNEL f1 ========
NUC1                    13C
P1                   15.50 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1          125.7942548 MHz
SP1                  3.20 dB
SP2                  3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF            125.7804140 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   4.00
```

1H spectrum



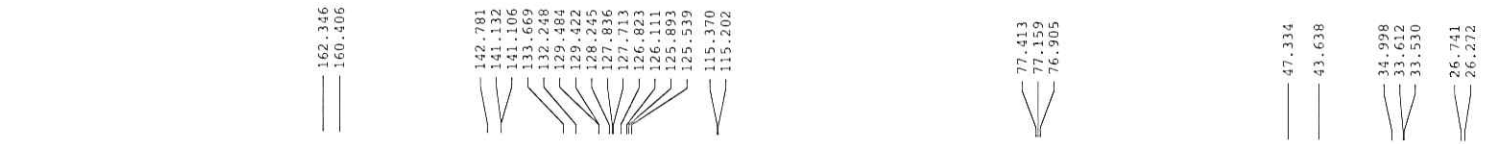

```
Current Data Parameters
USER                yonova
NAME          lmy5 - agj2-281
EXPNO                   111
PROCNO                    1

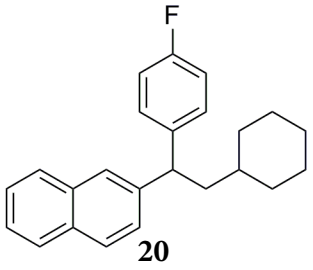
F2 - Acquisition Parameters
Date_              20130621
Time                  21.01
INSTRUM             cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    81728
SOLVENT               cdcl3
NS                        8
DS                        2
SWH                8012.820 Hz
FIDRES             0.098043 Hz
AQ                 5.0999398 sec
RG                        5
DW                   62.400 usec
DE                    6.00 usec
TE                   298.0 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    7.50 usec
PL1                   1.60 dB
SFO1           500.2235015 MHz

F2 - Processing parameters
SI                        65536
SF             500.2200399 MHz
WDW                       EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling





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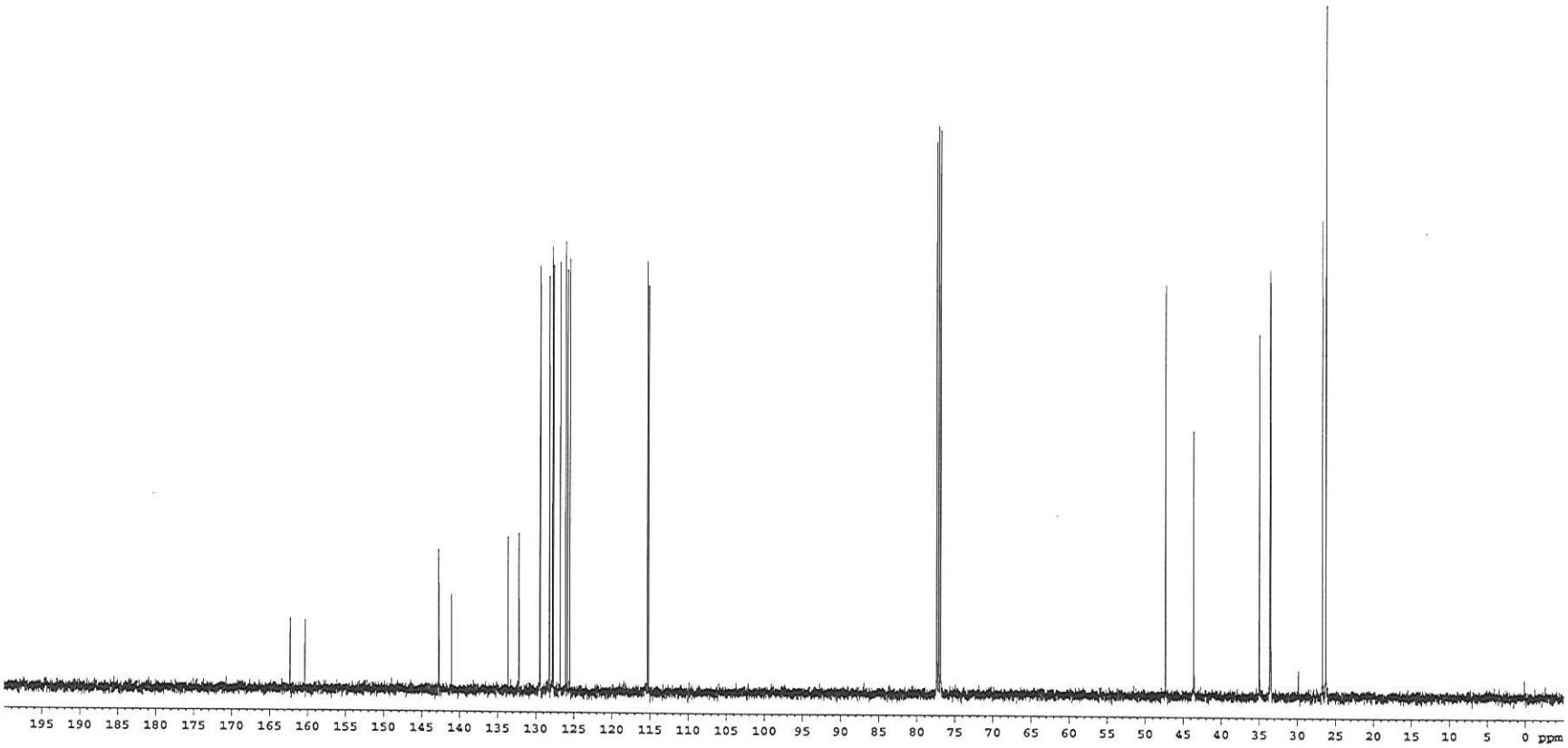



```
Current Data Parameters
USER                yonova
NAME        imy5 - agj2-281
EXPNO                  222
PROCNO                   1

F2 - Acquisition Parameters
Date_            20130621
Time                21.07
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    238
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0814105 sec
RG                 7298.2
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.25000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                31.00 usec

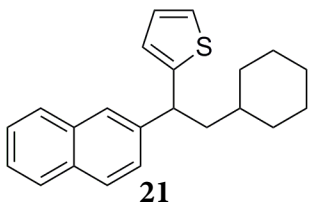
======== CHANNEL f1 ========
NUC1                 13C
P1                 15.50 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                3.20 dB
SP2                3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804094 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00
```

1H spectrum



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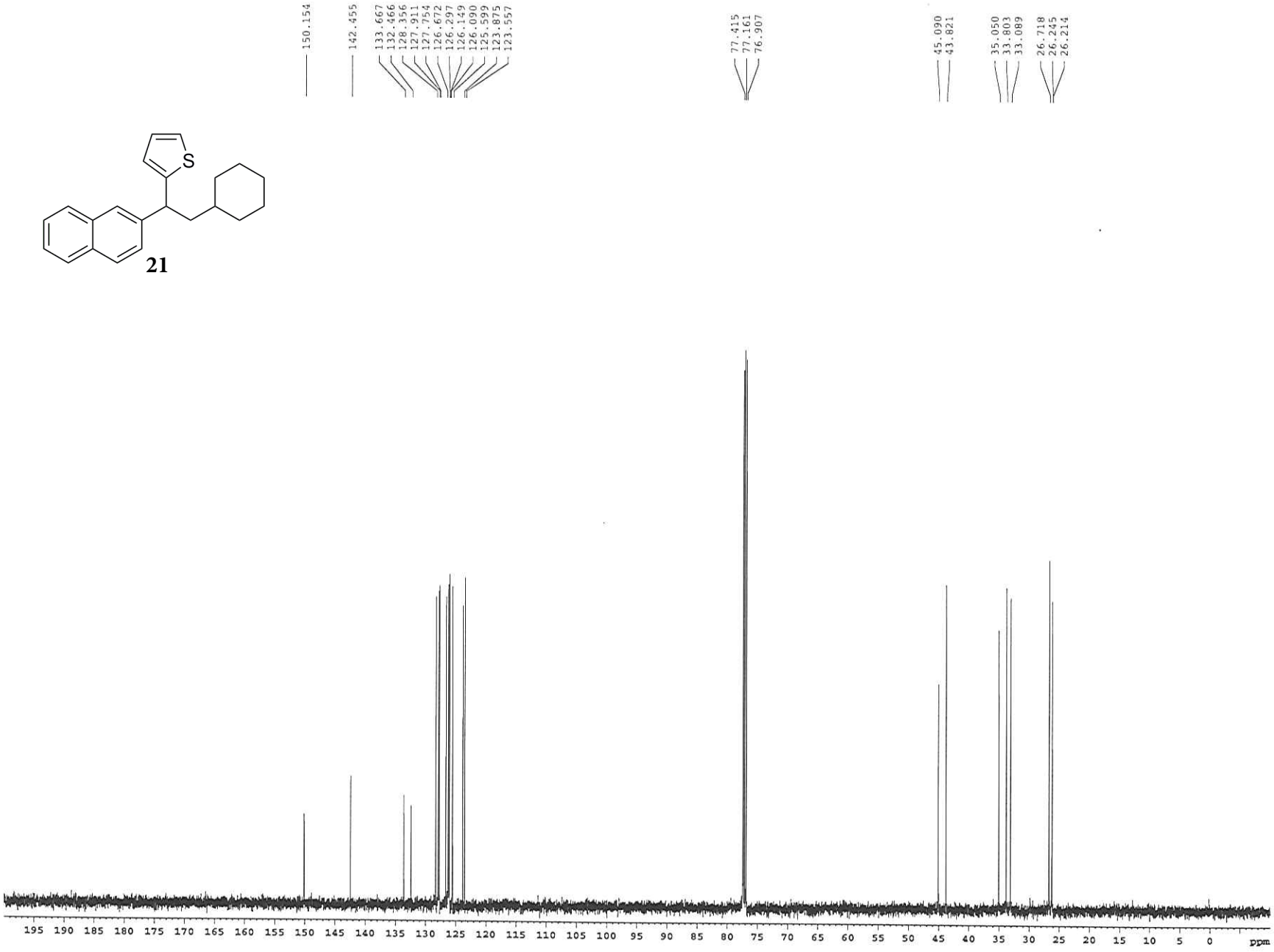
```
Current Data Parameters
USER                yoncva
NAME              imy5 - 243
EXPNO                    17
PROCNO                    1

F2 - Acquisition Parameters
Date_             20130509
Time                 13.57
INSTRUM              drx400
PROBHD    5 mm QNP H/F/P
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                       8
DS                       2
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1118579 sec
RG                   287.4
DW                78.000 usec
DE                 4.50 usec
TE                 298.1 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF          400.1300249 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                 2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                yonova
NAME              imy5 - 243
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130510
Time                  14.26
INSTRUM             cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                    65536
SOLVENT                CDCl3
NS                       325
DS                        16
SWH                30303.031 Hz
FIDRES             0.462388 Hz
AQ                 1.0814105 sec
RG                    5792.6
DW                   16.500 usec
DE                    6.00 usec
TE                   298.0 K
D1                0.25000000 sec
d11               0.03000000 sec
D16               0.00020000 sec
d17               0.00019600 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec
P2                   31.00 usec

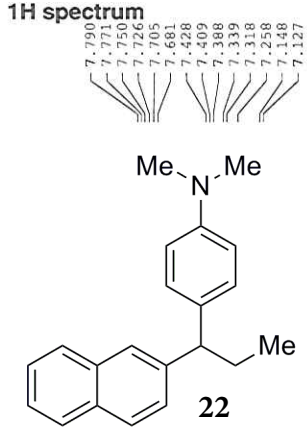
======== CHANNEL f1 ========
NUC1                     13C
P1                     15.50 usec
P11                   500.00 usec
P12                  2000.00 usec
PL0                   120.00 dB
PL1                    -1.00 dB
SFO1           125.7942548 MHz
SP1                    3.20 dB
SP2                    3.20 dB
SPNAM1     Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                 0.00 Hz
SPOFF2                 0.00 Hz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                100.00 usec
PL2                    1.60 dB
PL12                  24.60 dB
SFO2           500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPX1                   0.00 %
GPX2                   0.00 %
GPY1                   0.00 %
GPY2                   0.00 %
GPZ1                  30.00 %
GPZ2                  50.00 %
p15                  500.00 usec
p16                 1000.00 usec

F2 - Processing parameters
SI                    65536
SF             125.7804094 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     2.00
```

1H spectrum



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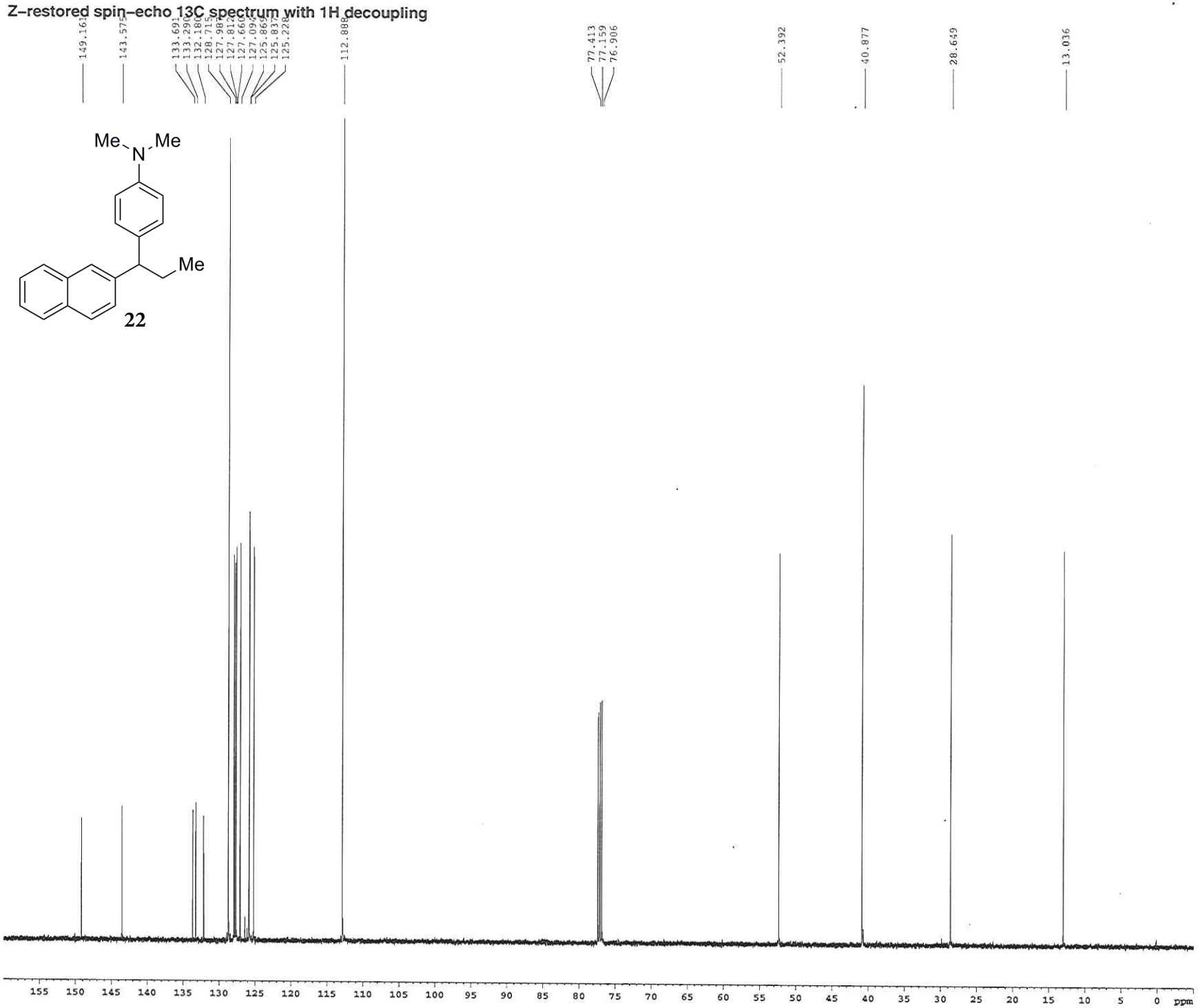
```
Current Data Parameters
USER                aaronj
NAME          AGJ_3_11_c2
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20130625
Time                17.41
INSTRUM          drx400
PROBHD    5 mm QNP H/P/P
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             6410.256 Hz
FIDRES          0.097813 Hz
AQ              5.1118579 sec
RG                 724.1
DW                78.000 usec
DE                 4.50 usec
TE                297.9 K
D1             0.10000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 12.00 usec
PL1                -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                 65536
SF            400.1300221 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                aaronj
NAME              AGJ_3_11
EXPNO                    5
PROCNO                   1

F2 - Acquisition Parameters
Date_            20130625
Time               18.40
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                 65536
SOLVENT            CDCl3
NS                   440
DS                    16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                 7298.2
DW                16.500 usec
DE                 6.00 usec
TE                298.0 K
D1             0.25000000 sec
d11            0.03000000 sec
D16            0.00020000 sec
d17            0.00019600 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec
P2                31.00 usec

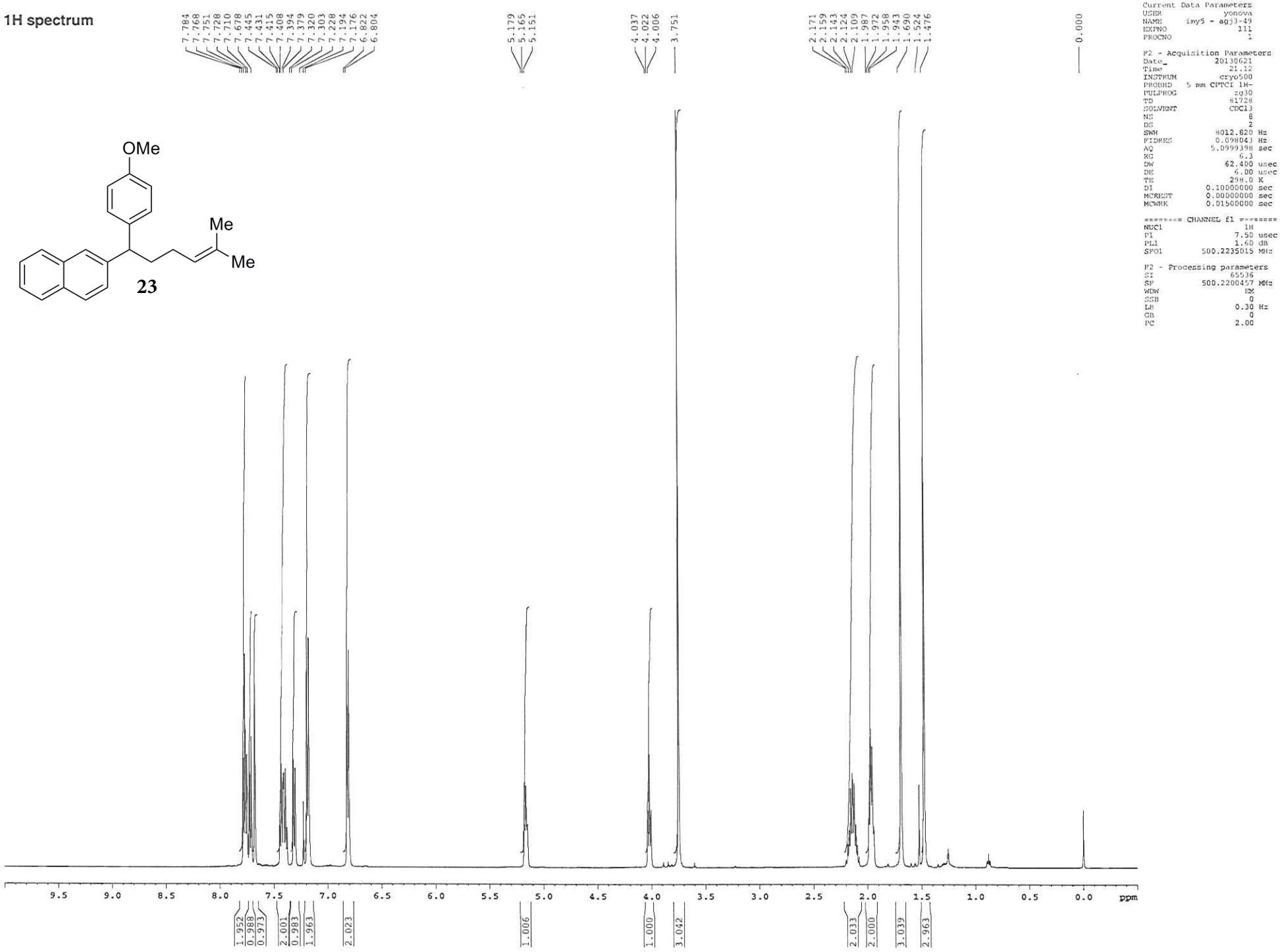
======== CHANNEL f1 ========
NUC1                 13C
P1                15.50 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1         125.7942548 MHz
SP1               3.20 dB
SP2               3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1             0.00 Hz
SPOFF2             0.00 Hz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2               1.60 dB
PL12             24.60 dB
SFO2         500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1               0.00 %
GPX2               0.00 %
GPY1               0.00 %
GPY2               0.00 %
GPZ1              30.00 %
GPZ2              50.00 %
p15             500.00 usec
p16            1000.00 usec

F2 - Processing parameters
SI                 65536
SF           125.7804127 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 2.00
```

1H spectrum



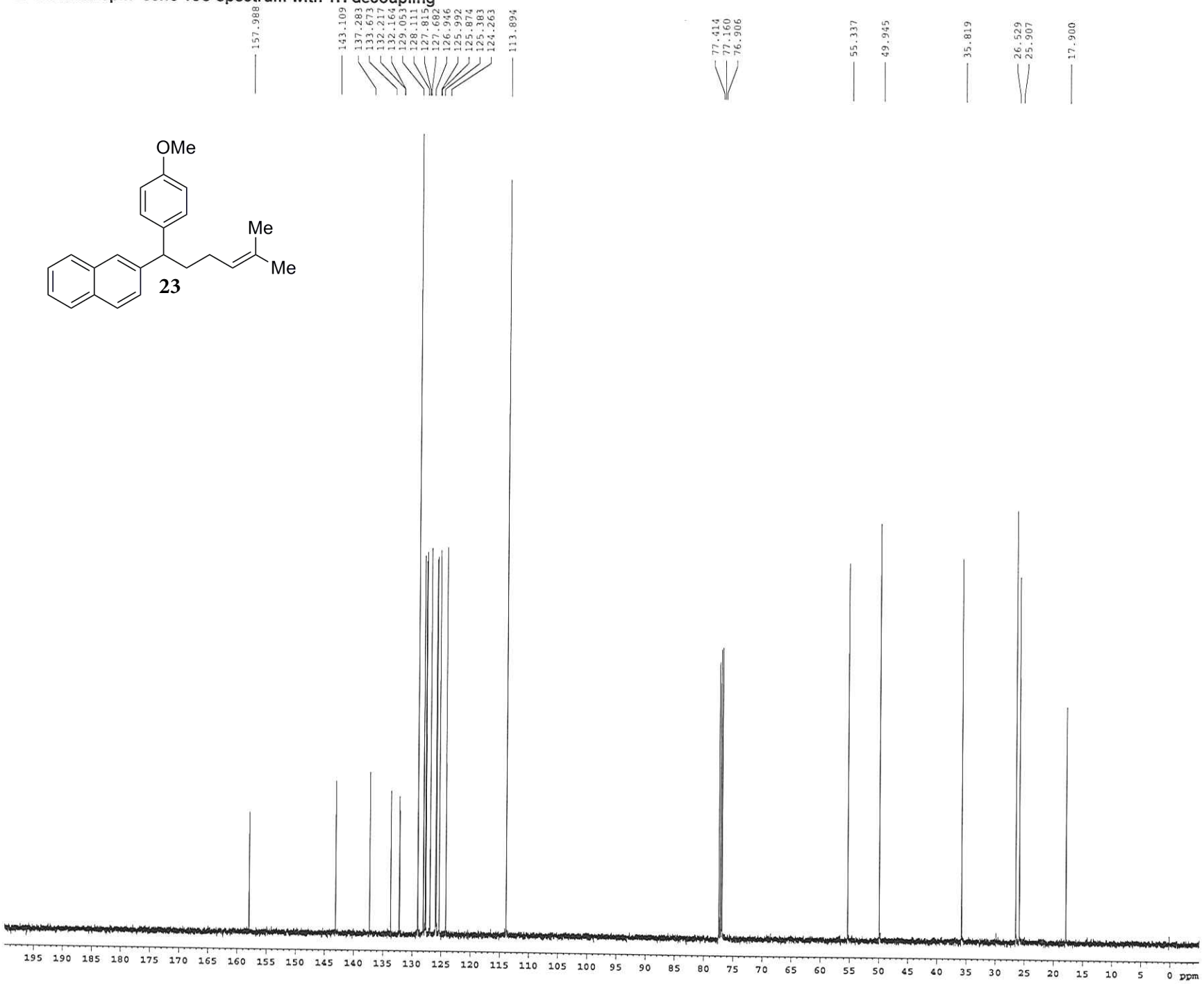

```
Current Data Parameters
USER                yonova
NAME          imy5 - agj3-49
EXPNO                  111
PROCNO                   1

F2 - Acquisition Parameters
Date_           20130621
Time              21.12
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               81728
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.098041 Hz
AQ            5.0999398 sec
RG                 6.3
DW              62.400 usec
DE               6.00 usec
TE              298.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                1H
P1               7.50 usec
PL1              1.60 dB
SFO1        500.2235015 MHz

F2 - Processing parameters
SI                65536
SF          500.2200457 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling




```
Current Data Parameters
USER                yonova
NAME          imy5 - agj3-49
EXPNO                   222
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130621
Time                  21.20
INSTRUM             cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                     65536
SOLVENT                CDCl3
NS                       276
DS                        16
SWH                30303.031 Hz
FIDRES             0.462388 Hz
AQ                 1.0814105 sec
RG                    5792.6
DW                   16.500 usec
DE                    6.00 usec
TE                   298.0 K
D1                0.25000000 sec
d11               0.03000000 sec
D16               0.00020000 sec
d17               0.00019600 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec
P2                   31.00 usec

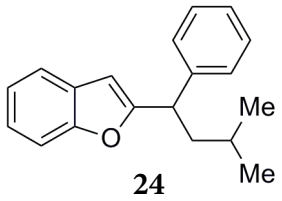
======== CHANNEL f1 ========
NUC1                    13C
P1                    15.50 usec
P11                  500.00 usec
PL2                 2000.00 usec
PL0                  120.00 dB
PL1                   -1.00 dB
SFO1           125.7942548 MHz
SP1                   3.20 dB
SP2                   1.20 dB
SPNAM1     Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                100.00 usec
PL2                   1.60 dB
PL12                 24.60 dB
SFO2           500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1              SINE.100
GPNAM2              SINE.100
GPX1                  0.00 %
GPX2                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPZ1                 30.00 %
GPZ2                 50.00 %
p15                 500.00 usec
p16                1000.00 usec

F2 - Processing parameters
SI                     65536
SF             125.7804113 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      4.00
```

1H spectrum



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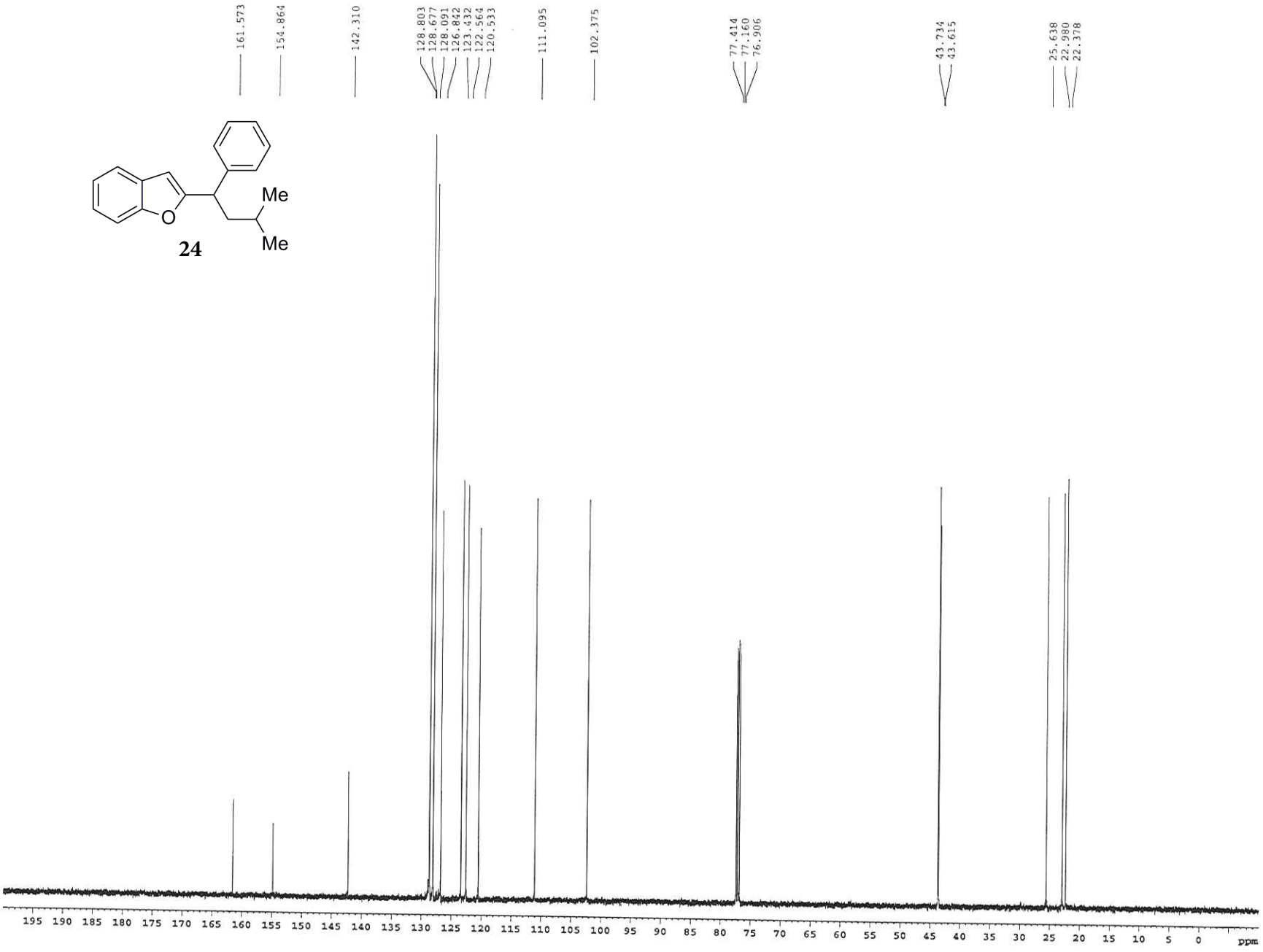
```
Current Data Parameters
USER                yonova
NAME              imy5 - 240
EXPNO                   111
PROCNO                    1

F2 - Acquisition Parameters
Date_            20130510
Time                14.16
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                   81728
SOLVENT              CDCl3
NS                       8
DS                       2
SWH                8012.820 Hz
FIDRES             0.098043 Hz
AQ                 5.0999398 sec
RG                       4.5
DW                    62.400 usec
DE                     6.00 usec
TE                   298.0 K
D1                 0.10000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                     7.50 usec
PL1                    1.60 dB
SFO1          500.2235015 MHz

F2 - Processing parameters
SI                     65536
SF            500.2200474 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     2.00
```

Z–restored spin–echo 13C spectrum with 1H decoupling



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```
Current Data Parameters
USER                ygnova
NAME            imy5 - 240
EXPNO                  222
PROCNO                   1

F2 - Acquisition Parameters
Date_            20130510
Time                14.24
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT               CDCl3
NS                      274
DS                       16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0814105 sec
RG                  5792.6
DW                  16.500 usec
DE                   6.00 usec
TE                  298.0 K
D1              0.25000000 sec
d11             0.03000000 sec
D16             0.00020000 sec
d17             0.00019600 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                  31.00 usec

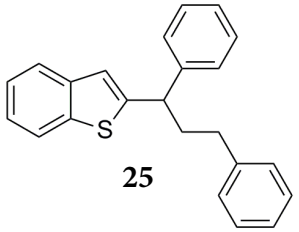
======== CHANNEL f1 ========
NUC1                   13C
P1                  15.50 usec
P11                500.00 usec
P12               2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1          125.7942548 MHz
SP1                  3.20 dB
SP2                  3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2          500.2225011 MHz

====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF           125.7804117 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   4.00
```

1H spectrum



25

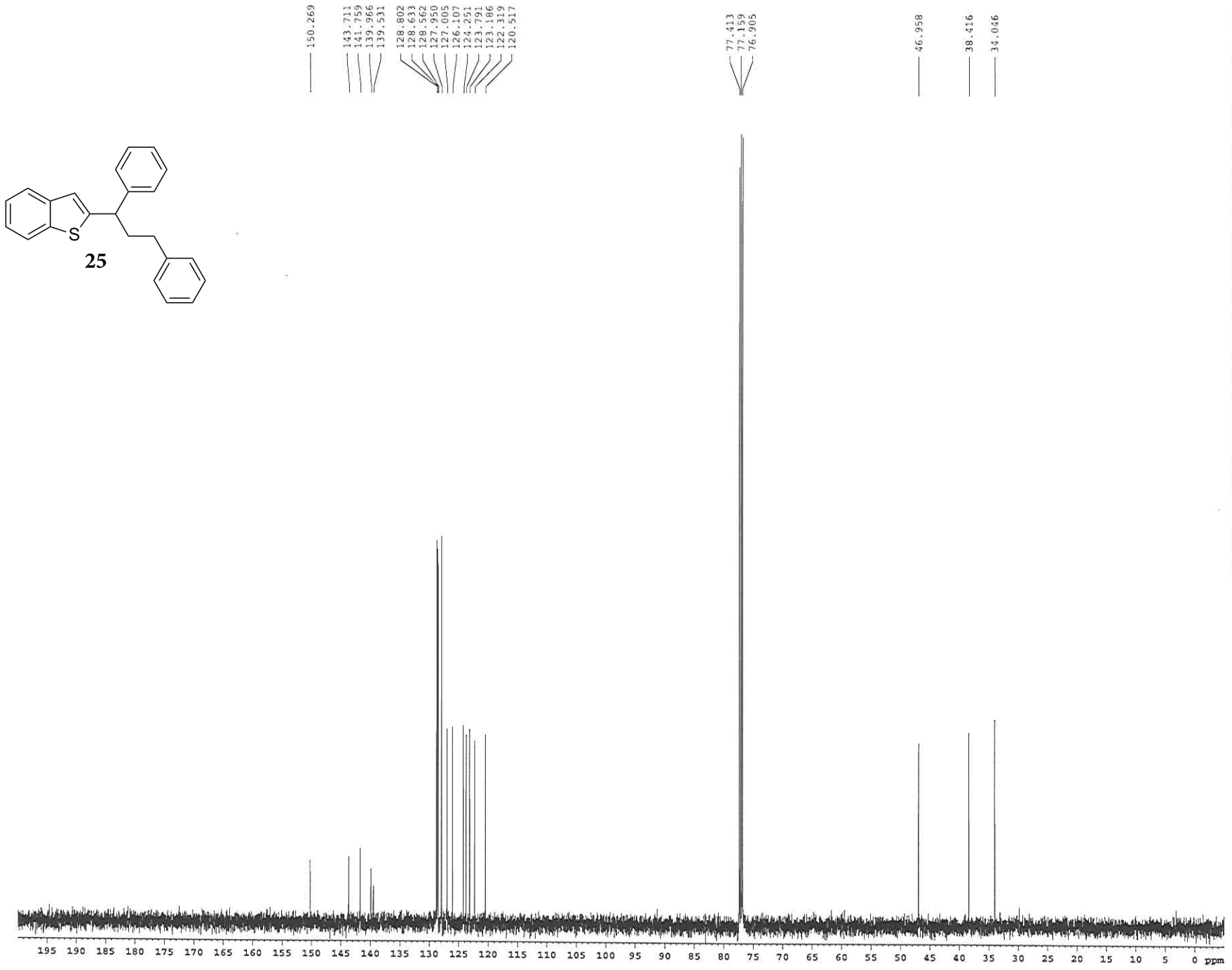

```
Current Data Parameters
USER                yonova
NAME              imy5 - 233
EXPNO                    20
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130516
Time                  14.52
INSTRUM              drx400
PROBHD   5 mm QNP H/F/P
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        8
DS                        2
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1118579 sec
RG                    456.1
DW                 78.000 usec
DE                  4.50 usec
TE                  297.9 K
D1                0.10000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    12.00 usec
PL1                   -0.60 dB
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF            400.1300212 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     2.00
```

Z-restored spin-echo 13C spectrum with 1H decoupling



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```
Current Data Parameters
USER                yonova
NAME            imy5 - 133
EXPNO                  222
PROCNO                   1

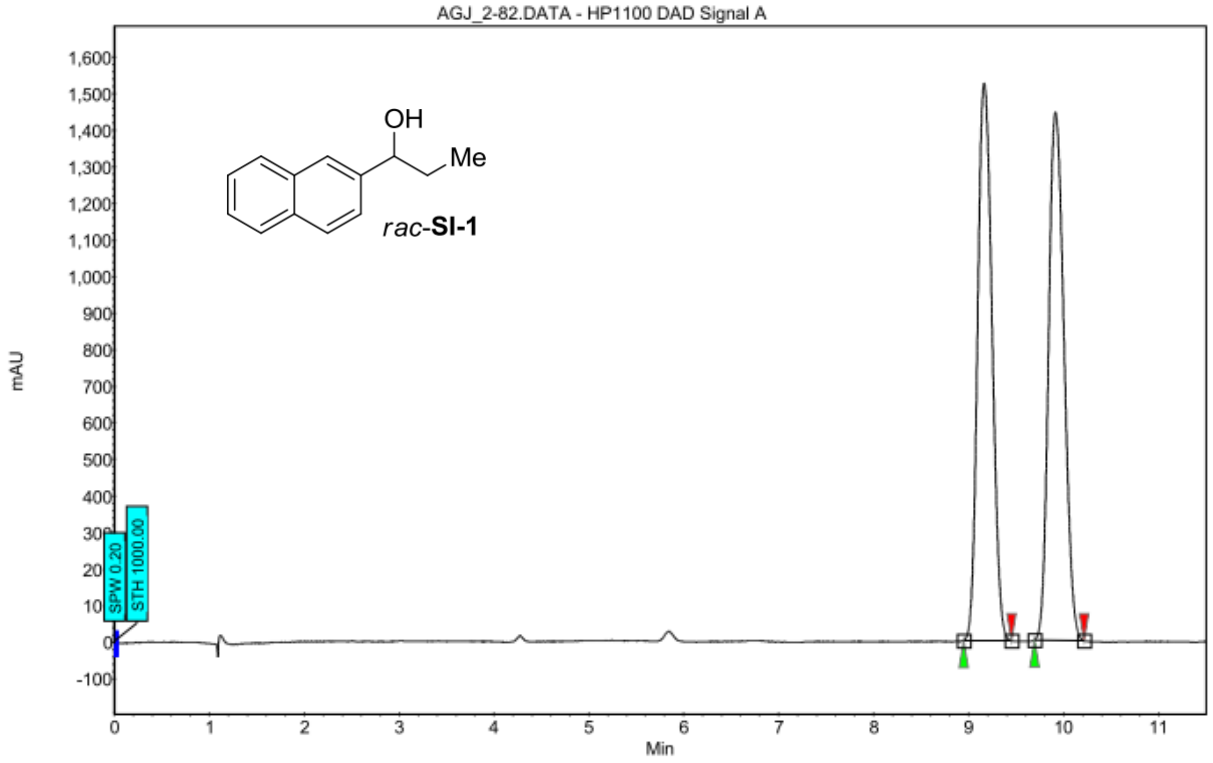
F2 - Acquisition Parameters
Date_            20130519
Time               18.26
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30qp.prd
TD                  65536
SOLVENT             CDCl3
NS                    288
DS                     16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0814105 sec
RG                  5160.6
DW                  16.500 usec
DE                   6.00 usec
TE                  298.0 K
D1               0.25000000 sec
d11              0.03000000 sec
D16              0.00020000 sec
d17              0.00019600 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec
P2                  31.00 usec

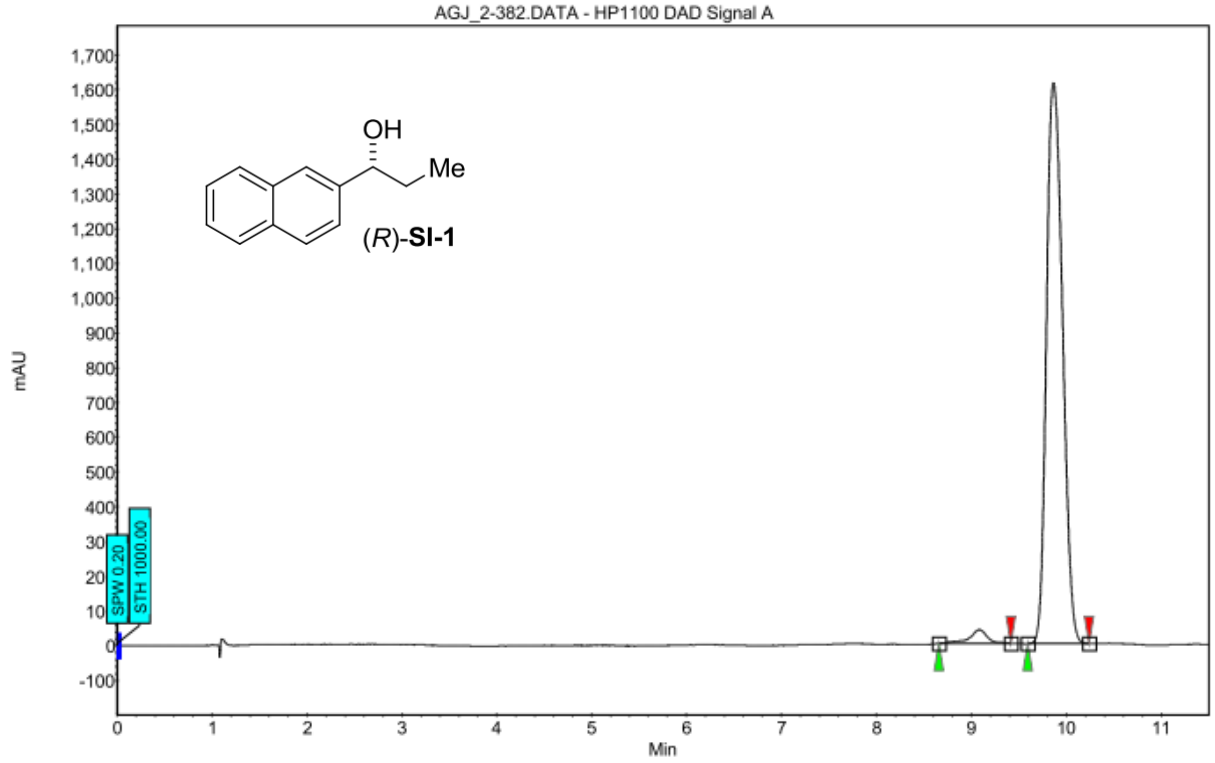
======== CHANNEL f1 ========
NUC1                   13C
P1                  15.50 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                  3.20 dB
SP2                  3.20 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2          500.2225011 MHz

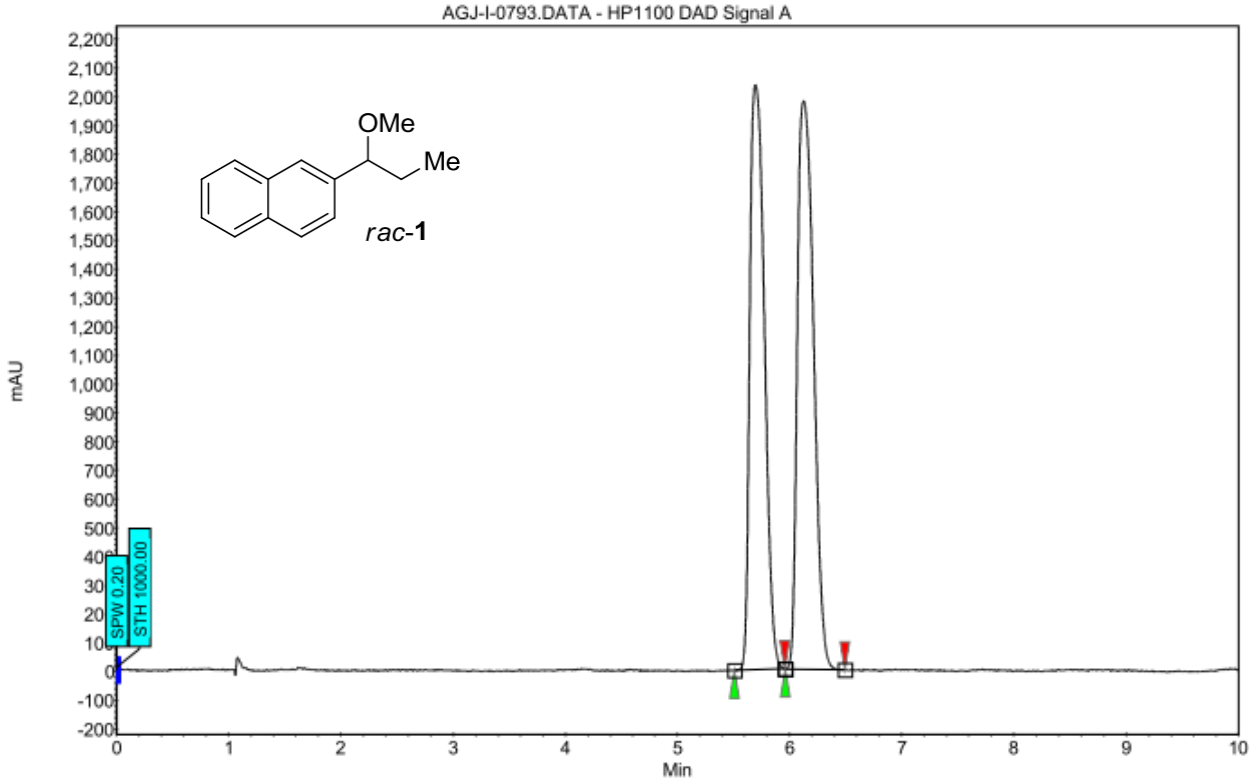
====== GRADIENT CHANNEL =====
GPNAM1           SINE.100
GPNAM2           SINE.100
GPX1                 0.00 %
GPX2                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPZ1                30.00 %
GPZ2                50.00 %
p15                500.00 usec
p16               1000.00 usec

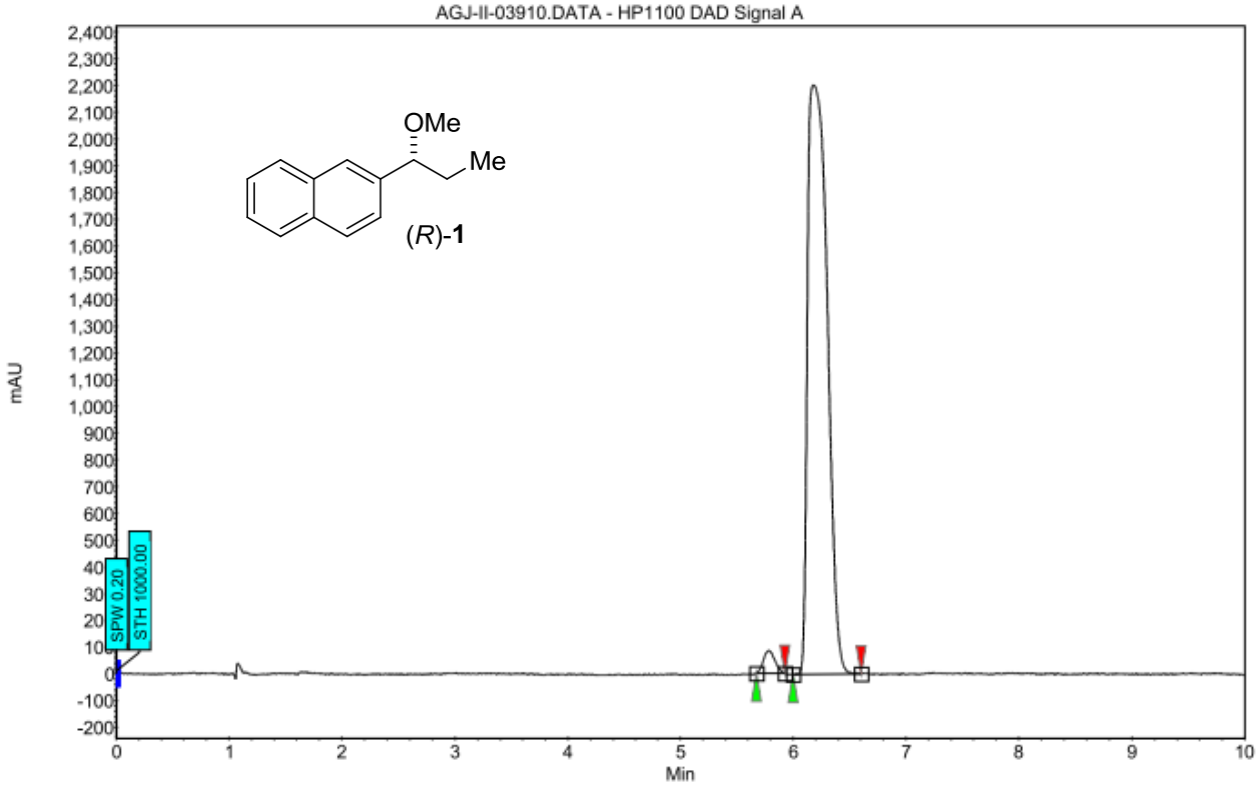
F2 - Processing parameters
SI                   65536
SF            125.7804085 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   4.00
```



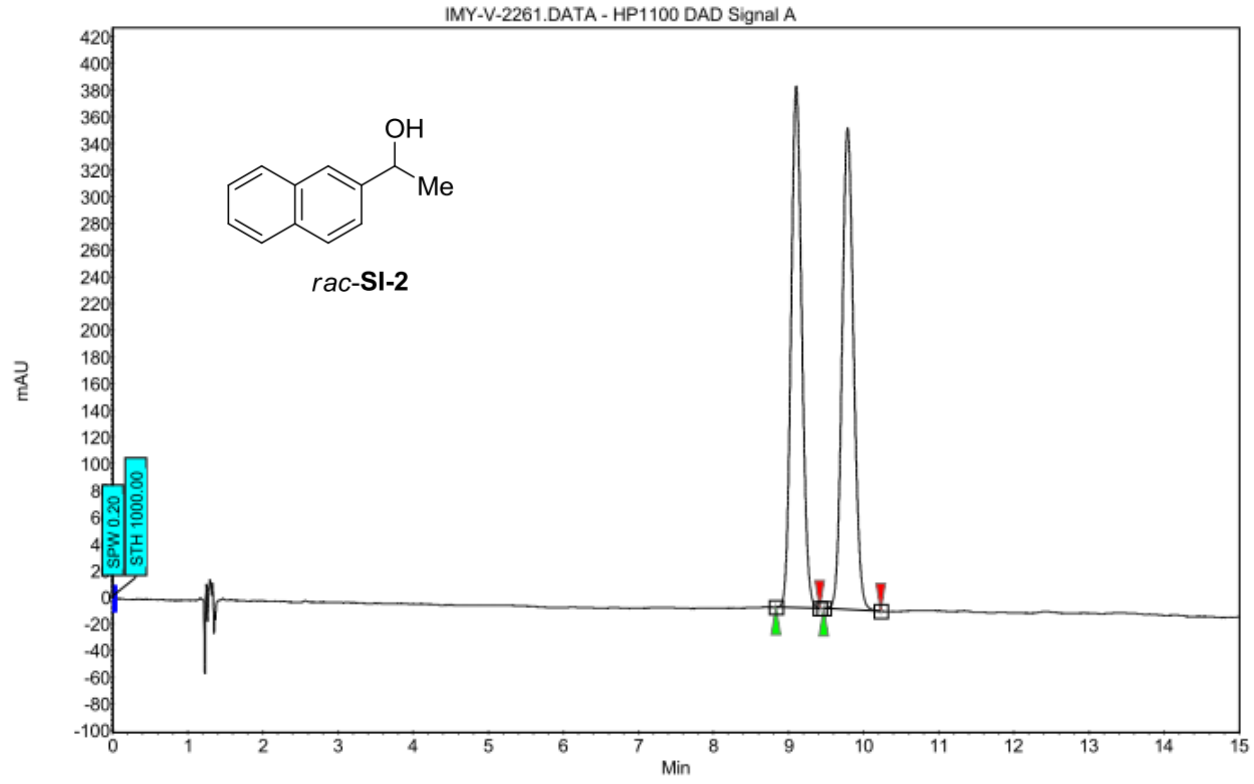


Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	8.66	9.08	9.42	0.00	2.69	39.6	8.8	2.691
1	UNKNOWN	9.60	9.86	10.24	0.00	97.31	1613.2	316.9	97.309
Total						100.00	1652.8	325.7	100.000

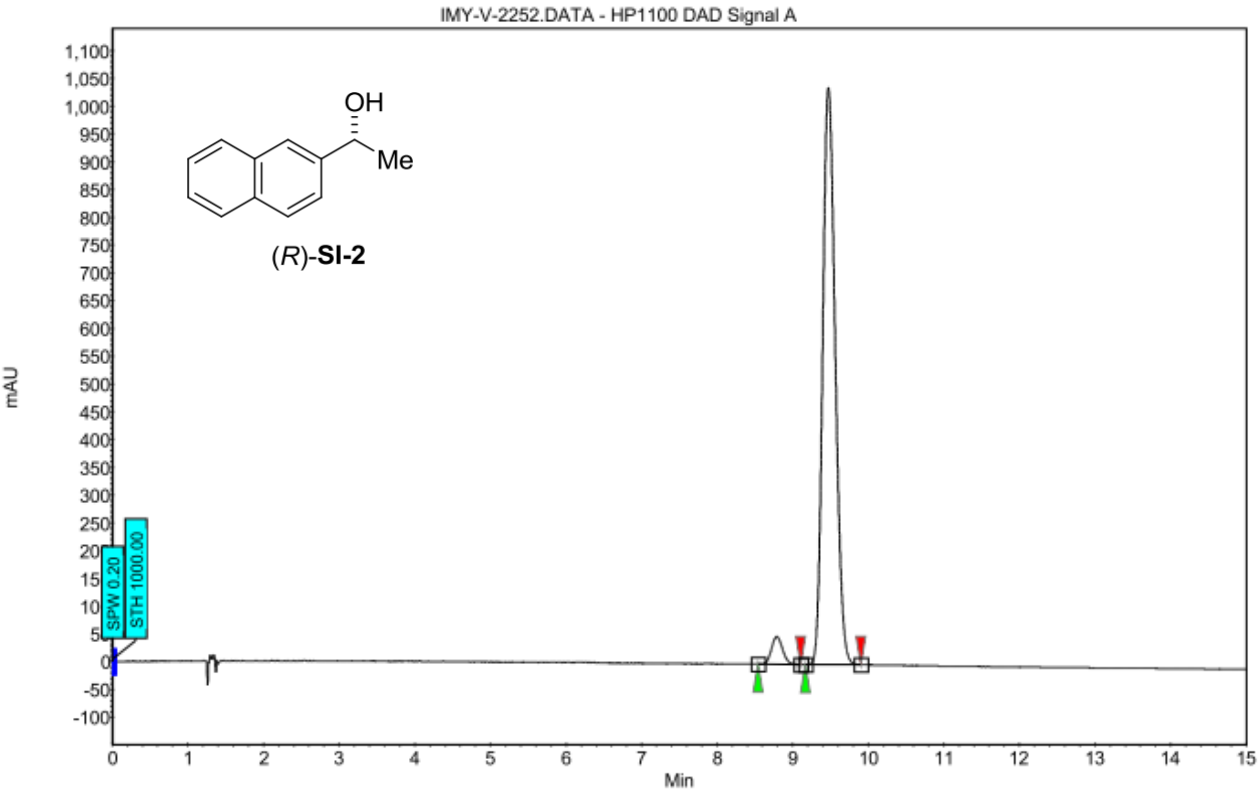




Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	5.67	5.78	5.93	0.00	2.19	84.6	10.0	2.186
1	UNKNOWN	6.00	6.18	6.60	0.00	97.81	2204.3	445.6	97.814
Total						100.00	2288.8	455.6	100.000

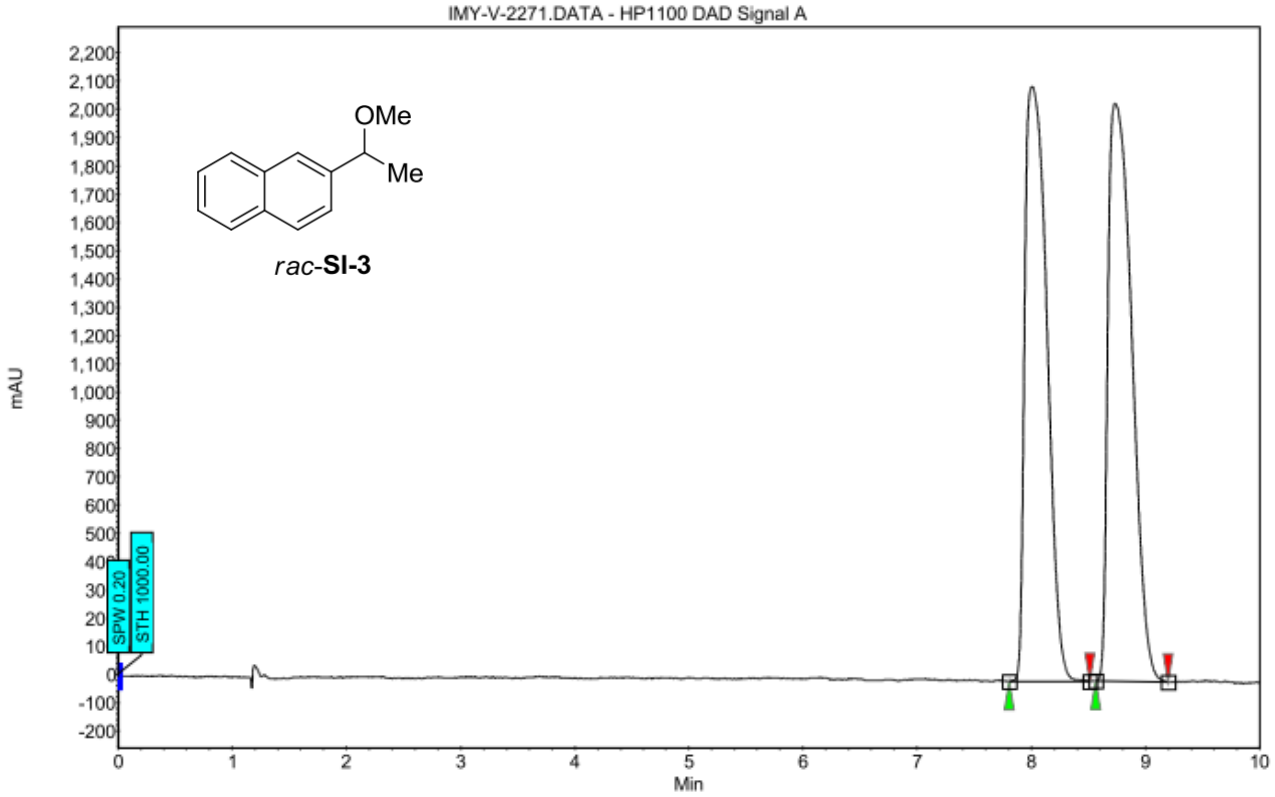


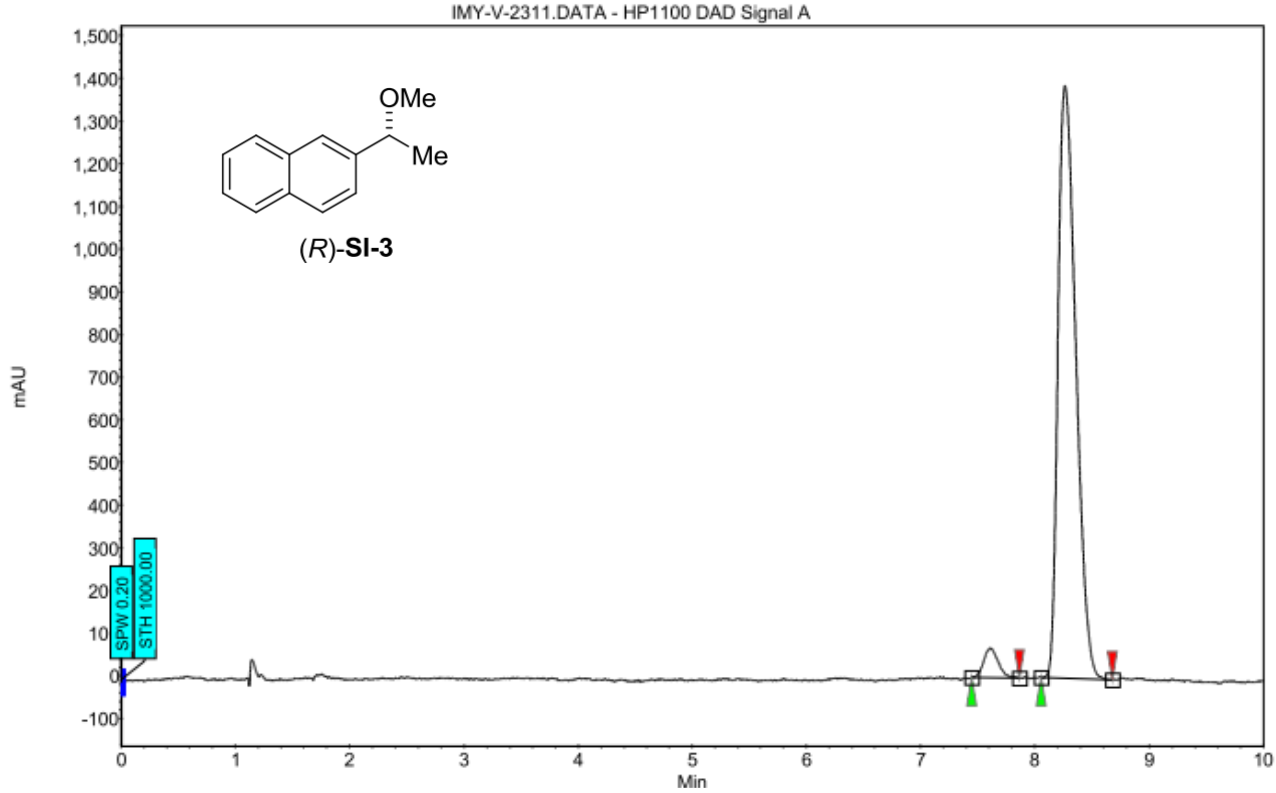
rac-**SI-2**



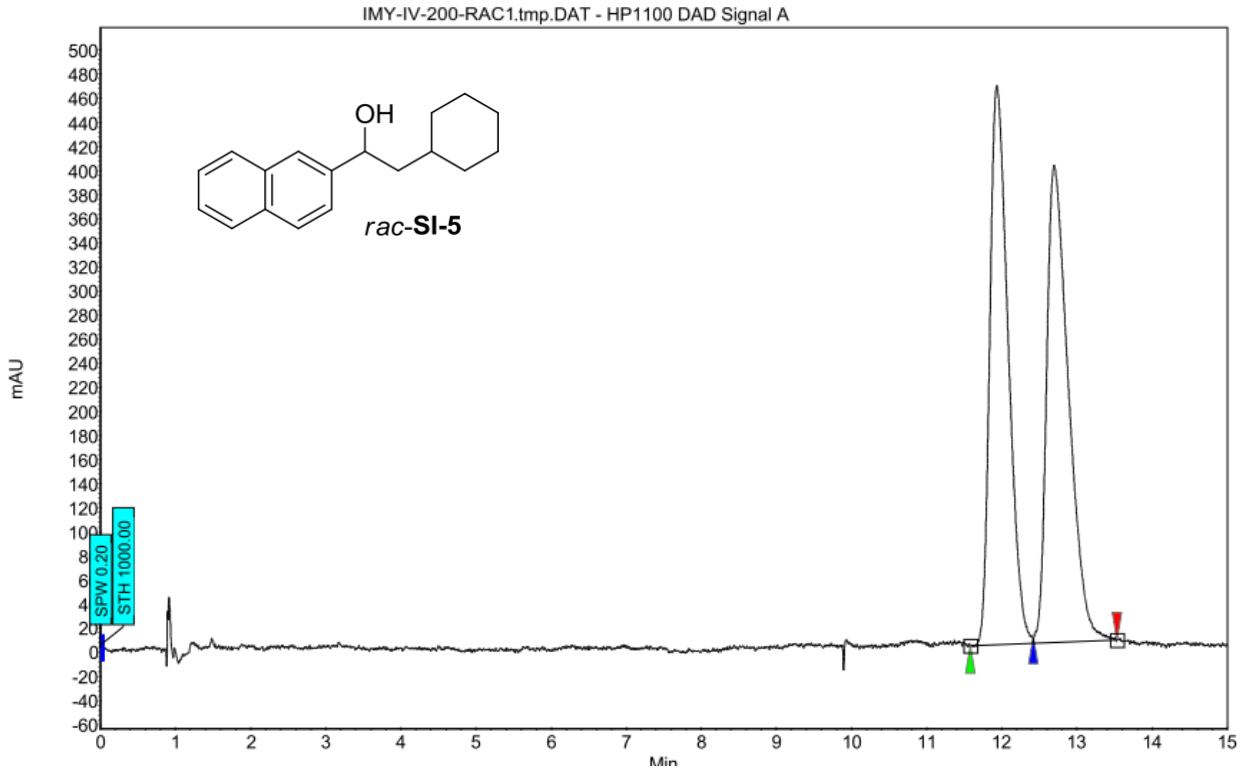
(*R*)-**SI-2**

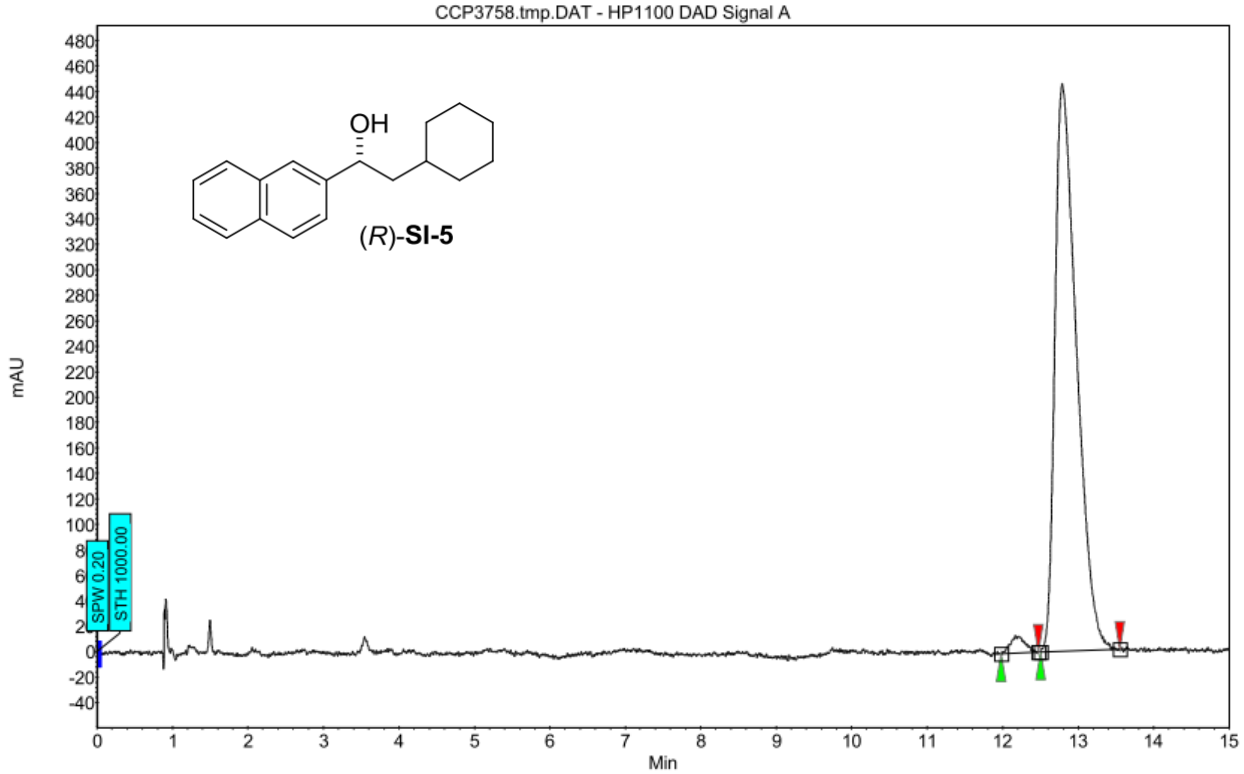
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	8.54	8.79	9.10	0.00	4.06	49.8	8.4	4.057
2	UNKNOWN	9.17	9.48	9.91	0.00	95.94	1038.5	198.9	95.943
Total						100.00	1088.3	207.3	100.000



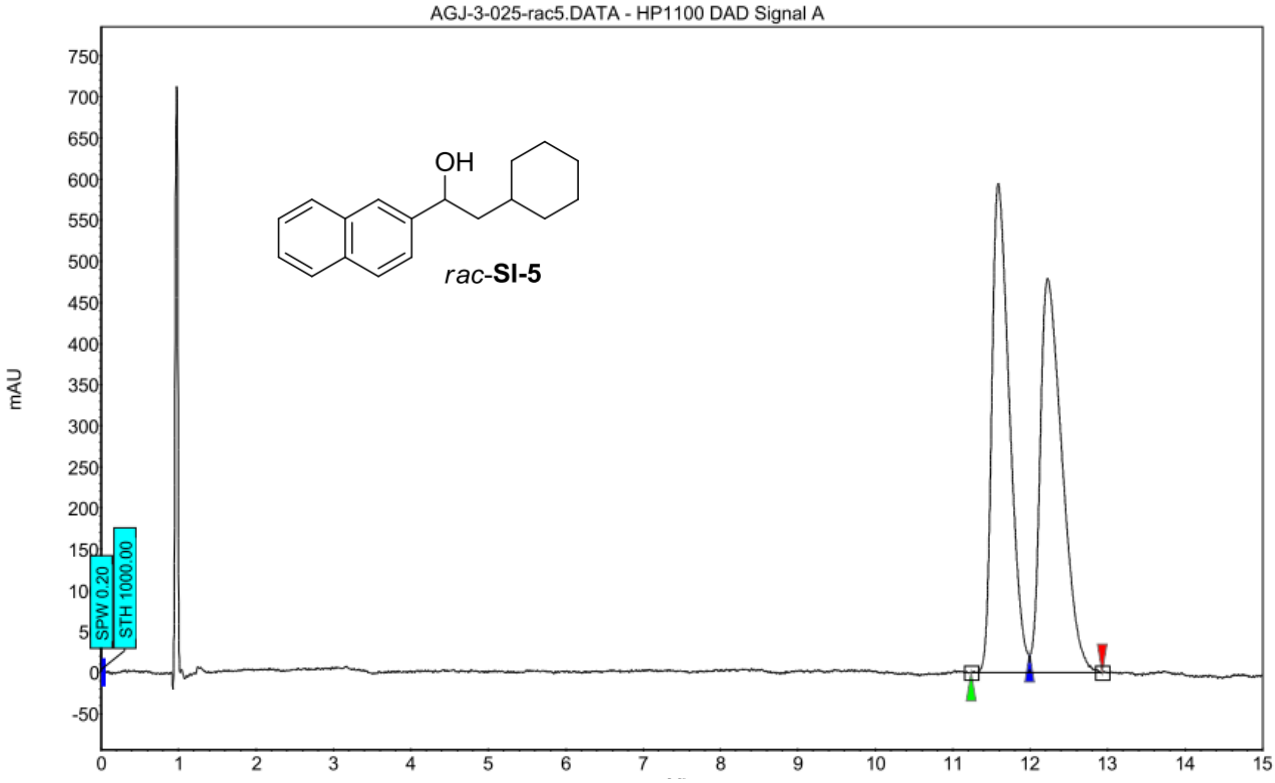


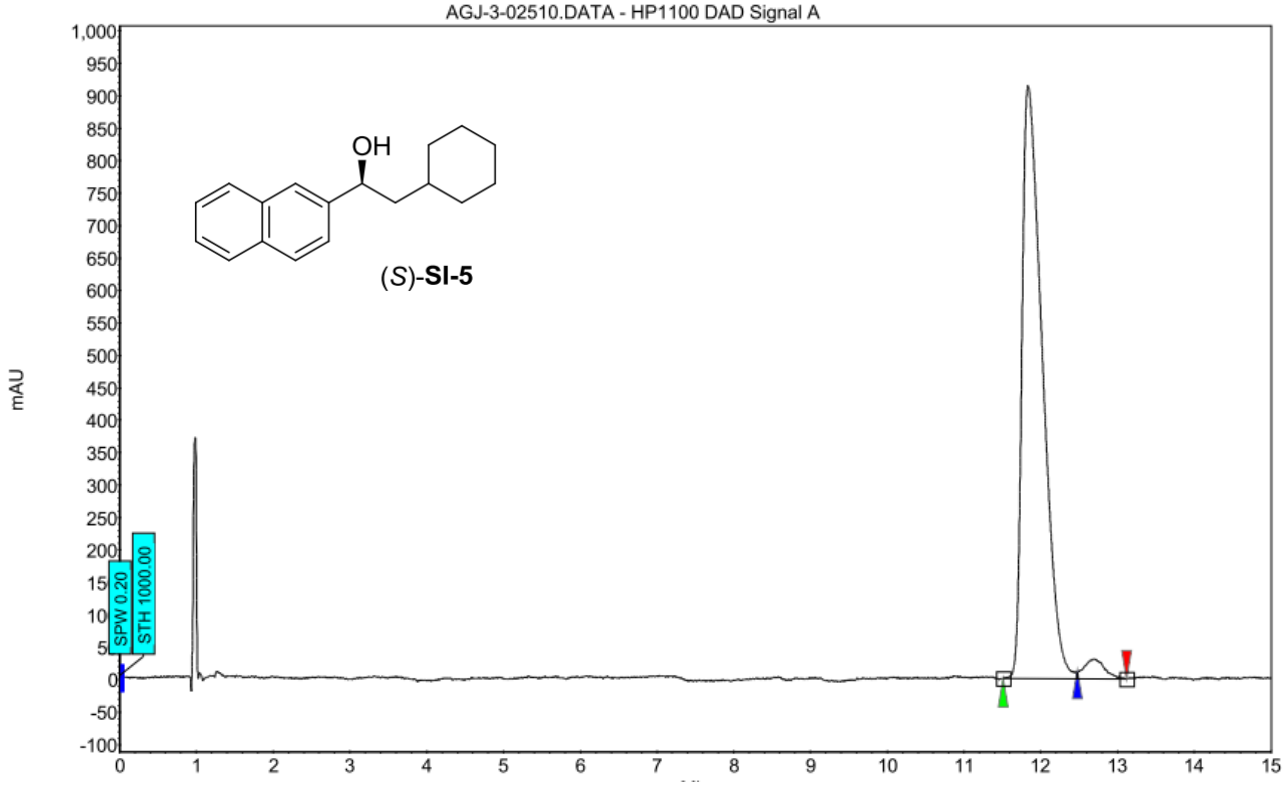
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	7.45	7.61	7.86	0.00	3.88	69.8	10.1	3.884
2	UNKNOWN	8.06	8.26	8.68	0.00	96.12	1389.0	250.7	96.116
Total						100.00	1458.8	260.8	100.000



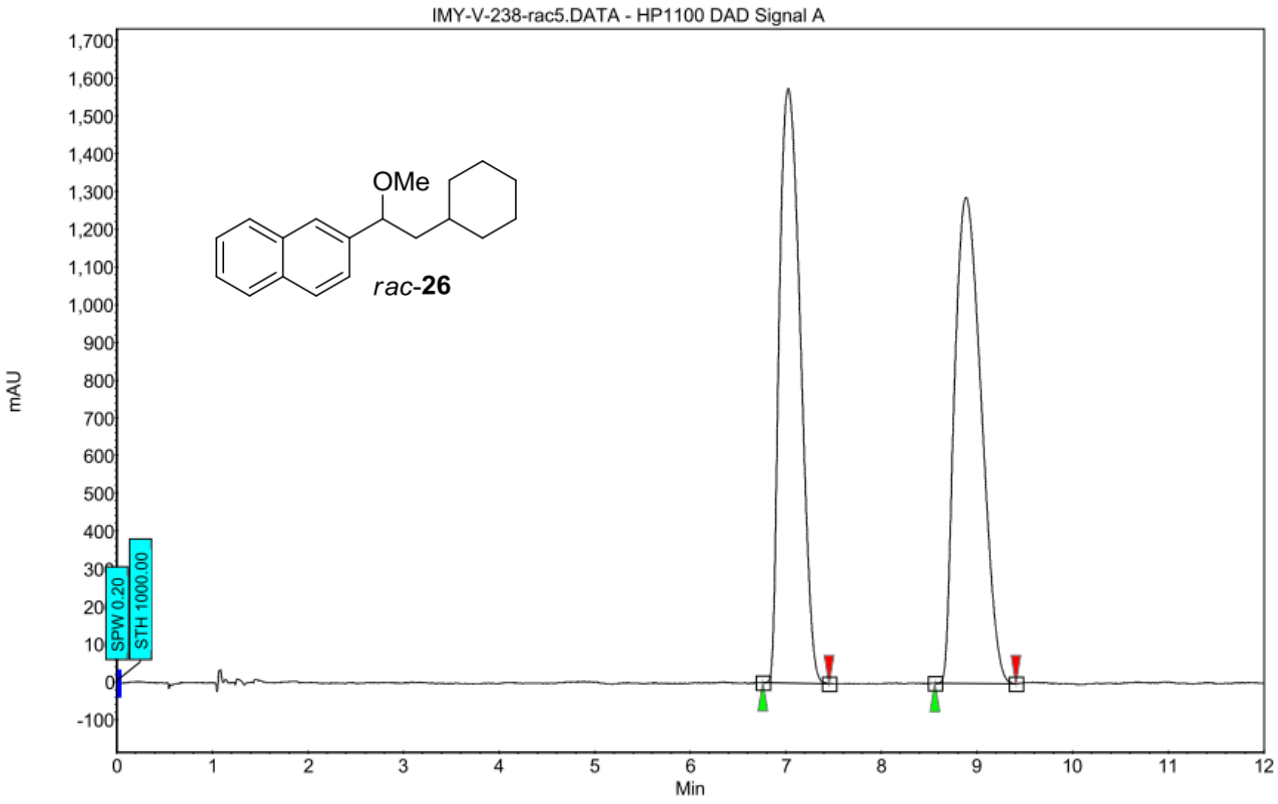


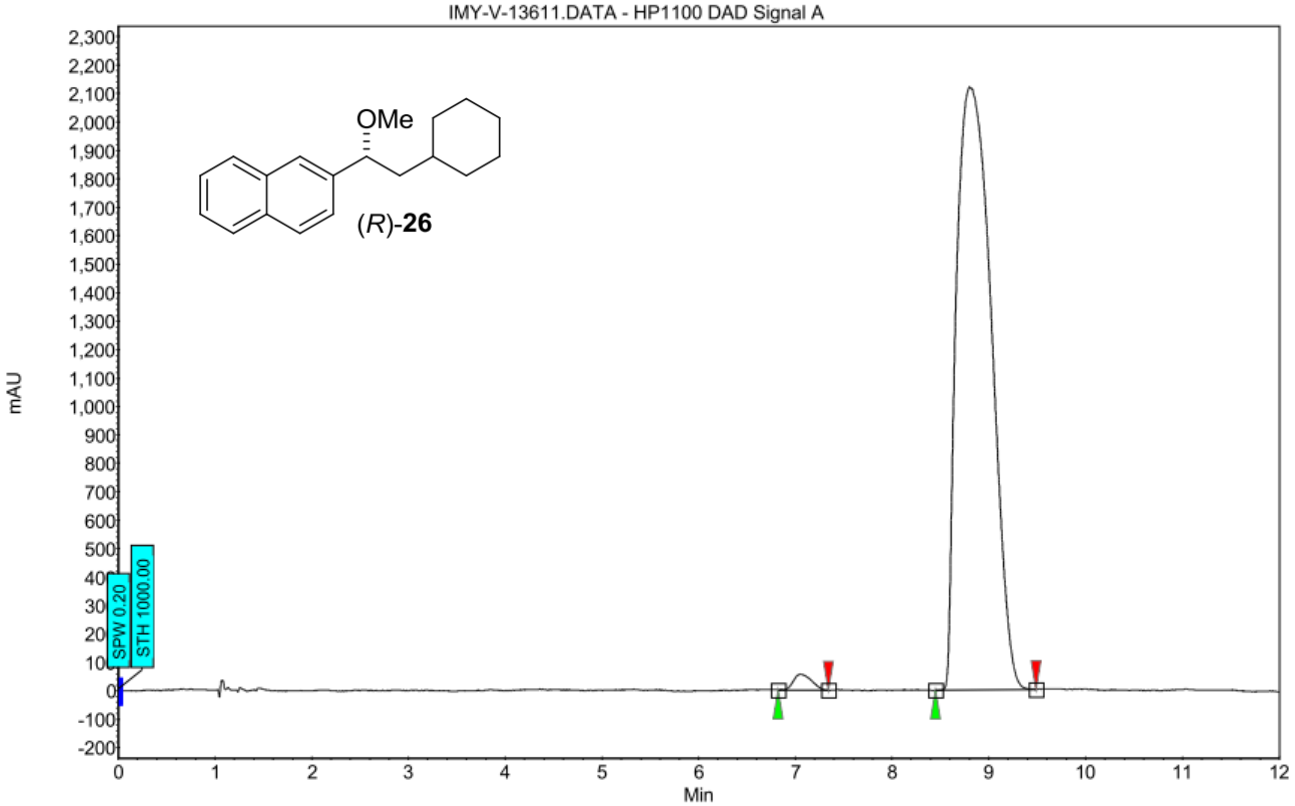
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	11.98	12.17	12.47	0.00	2.01	13.9	3.0	2.010
2	UNKNOWN	12.50	12.79	13.55	0.00	97.99	445.8	147.3	97.990
Total						100.00	459.7	150.3	100.000



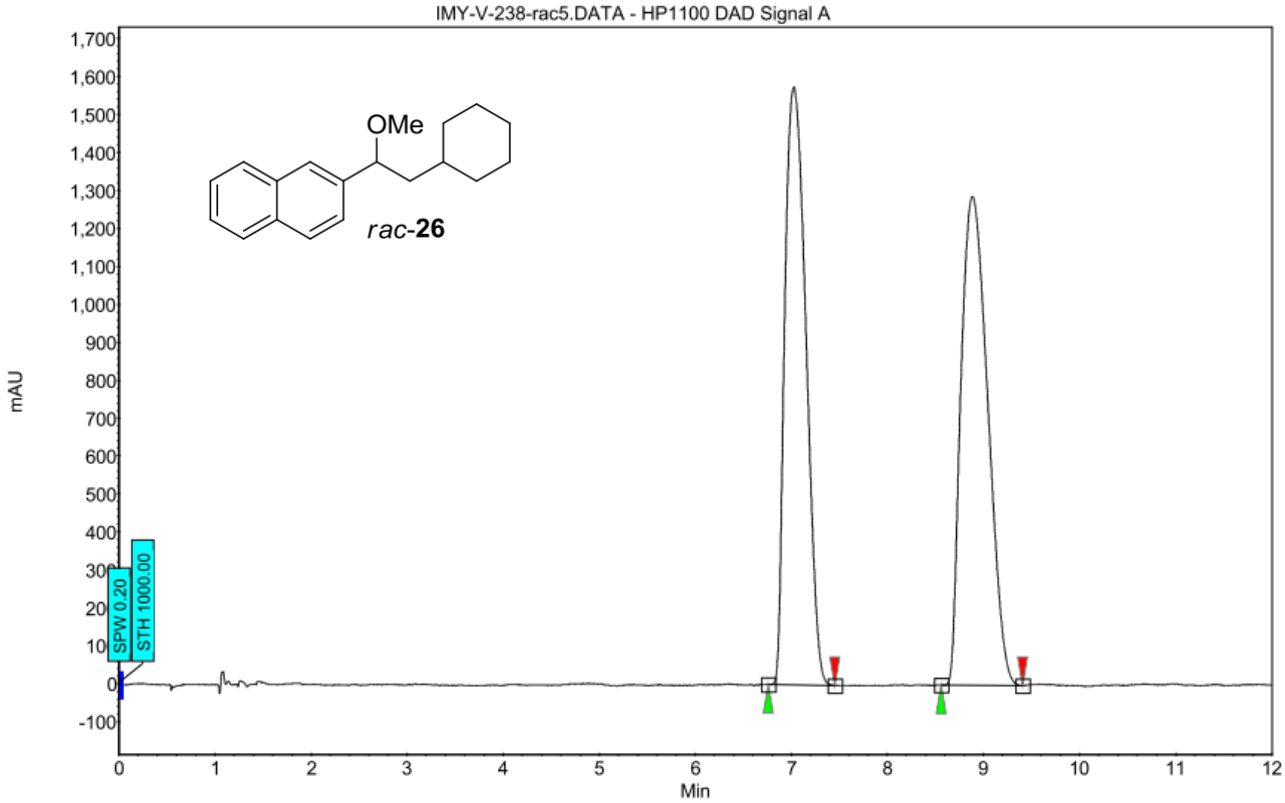


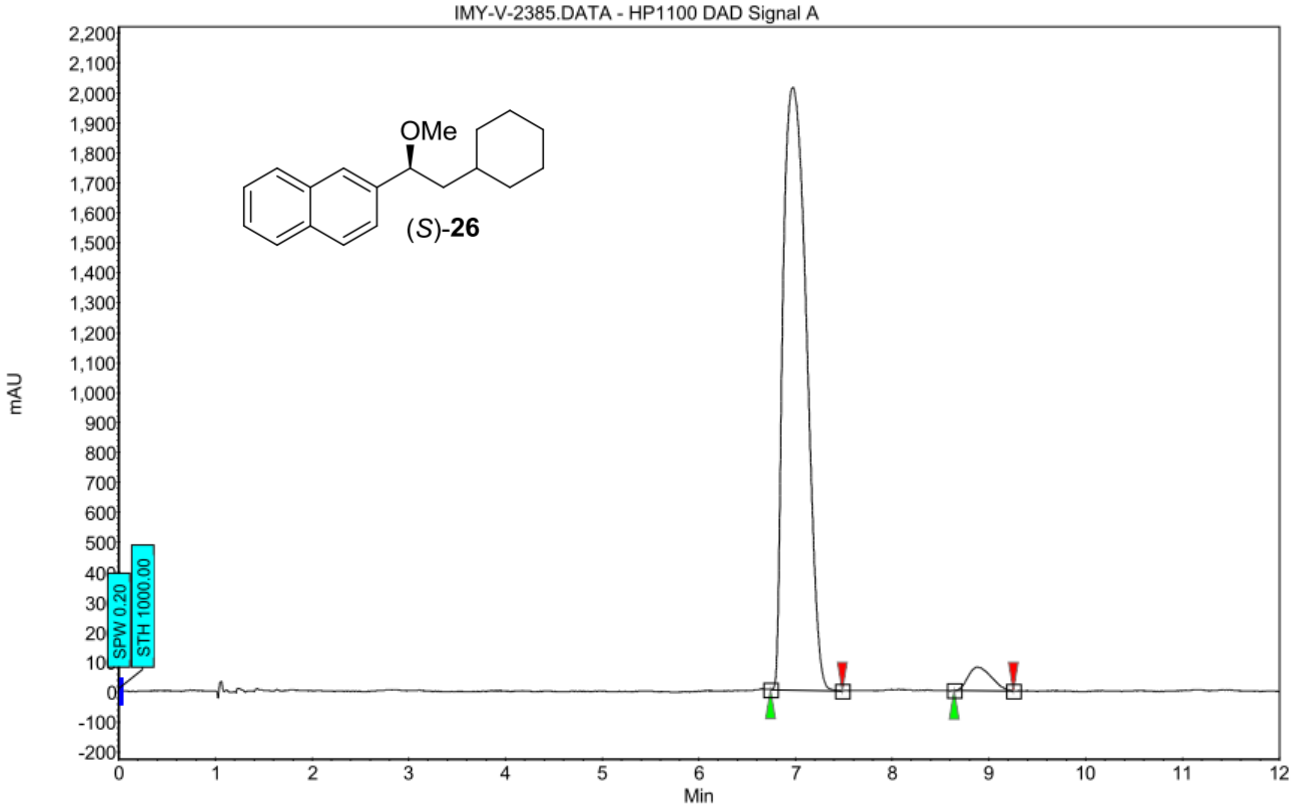
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	11.51	11.83	12.47	0.00	96.72	913.1	279.8	96.723
2	UNKNOWN	12.47	12.70	13.11	0.00	3.28	30.9	9.5	3.277
Total						100.00	944.0	289.3	100.000



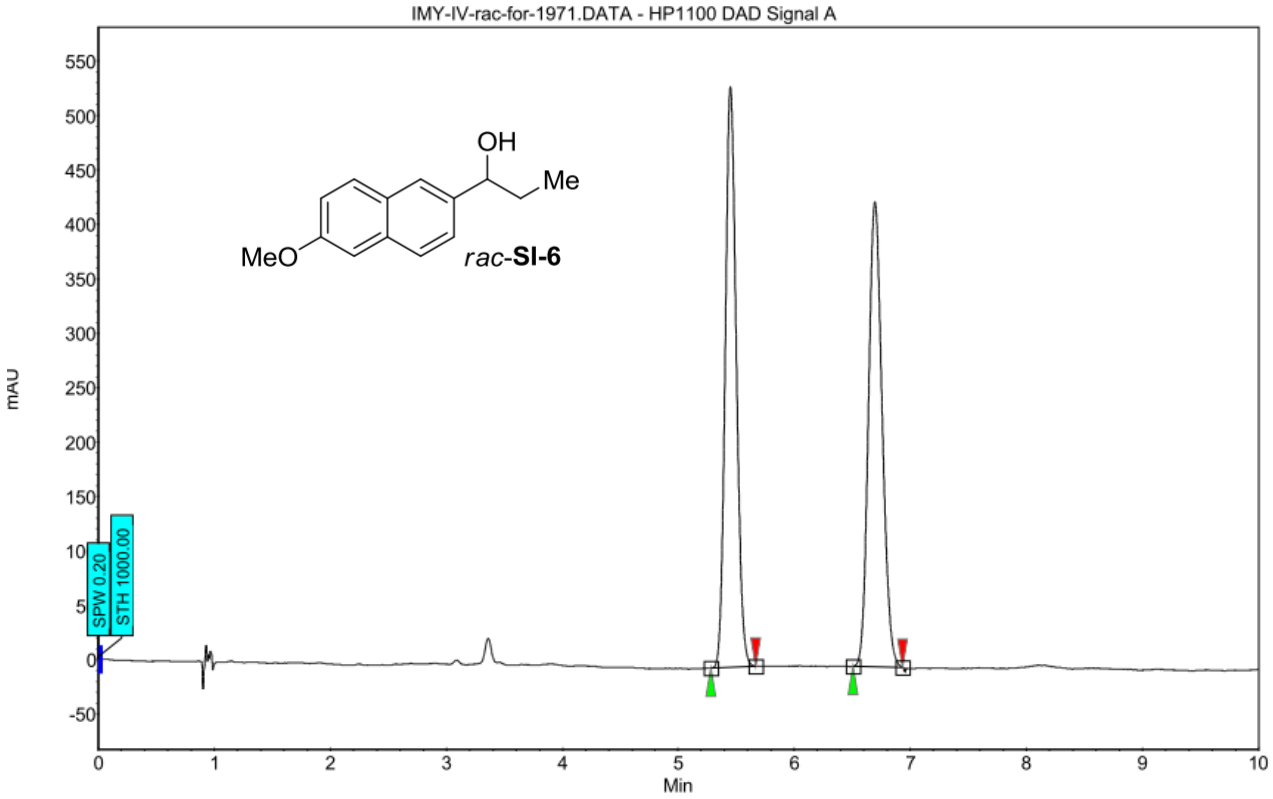


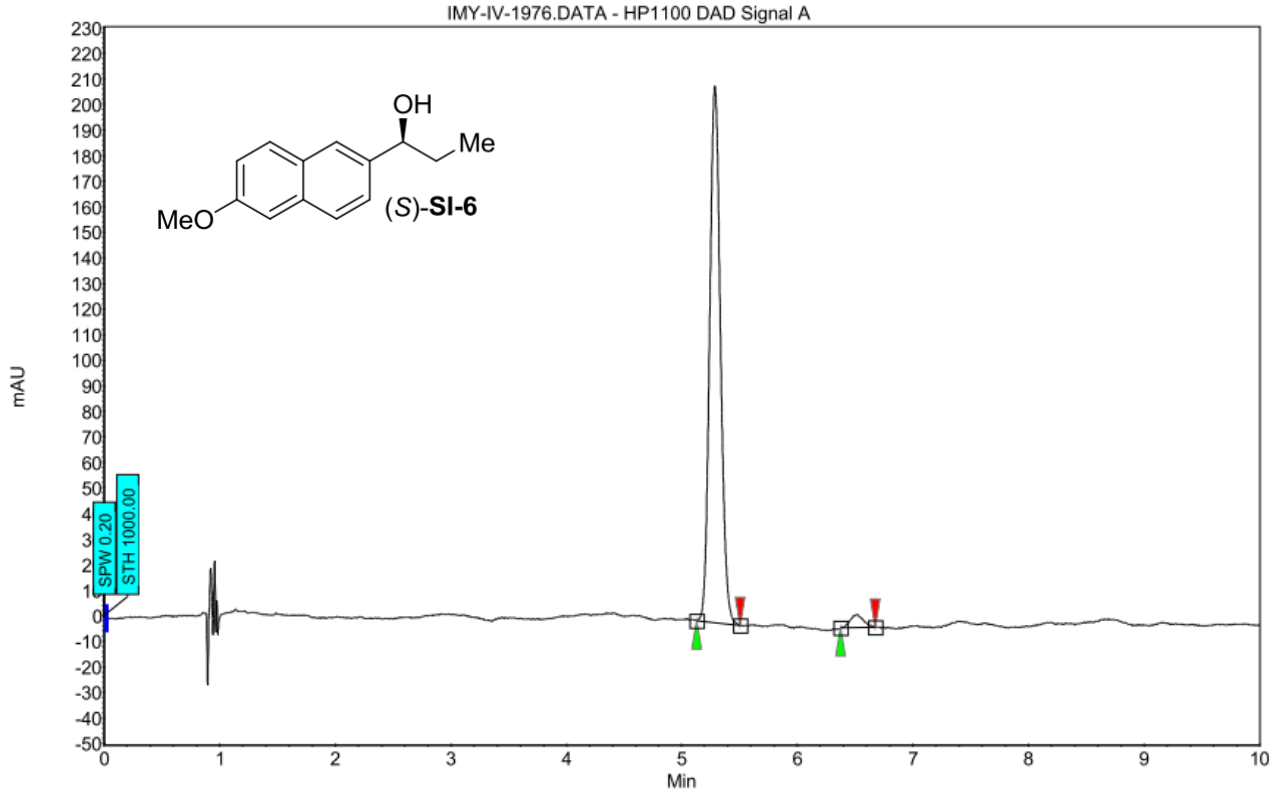
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	6.82	7.05	7.34	0.00	1.35	56.2	12.1	1.352
1	UNKNOWN	8.45	8.80	9.49	0.00	98.65	2120.6	879.3	98.648
Total						100.00	2176.8	891.4	100.000



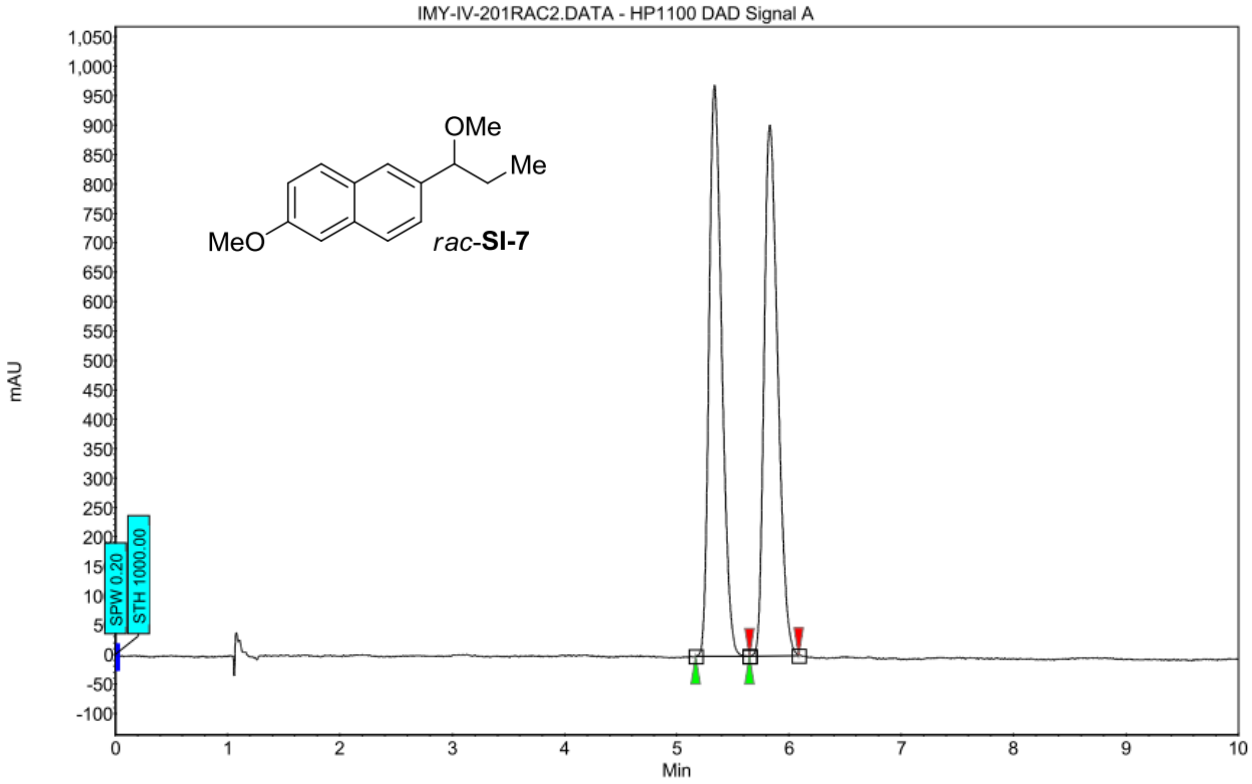


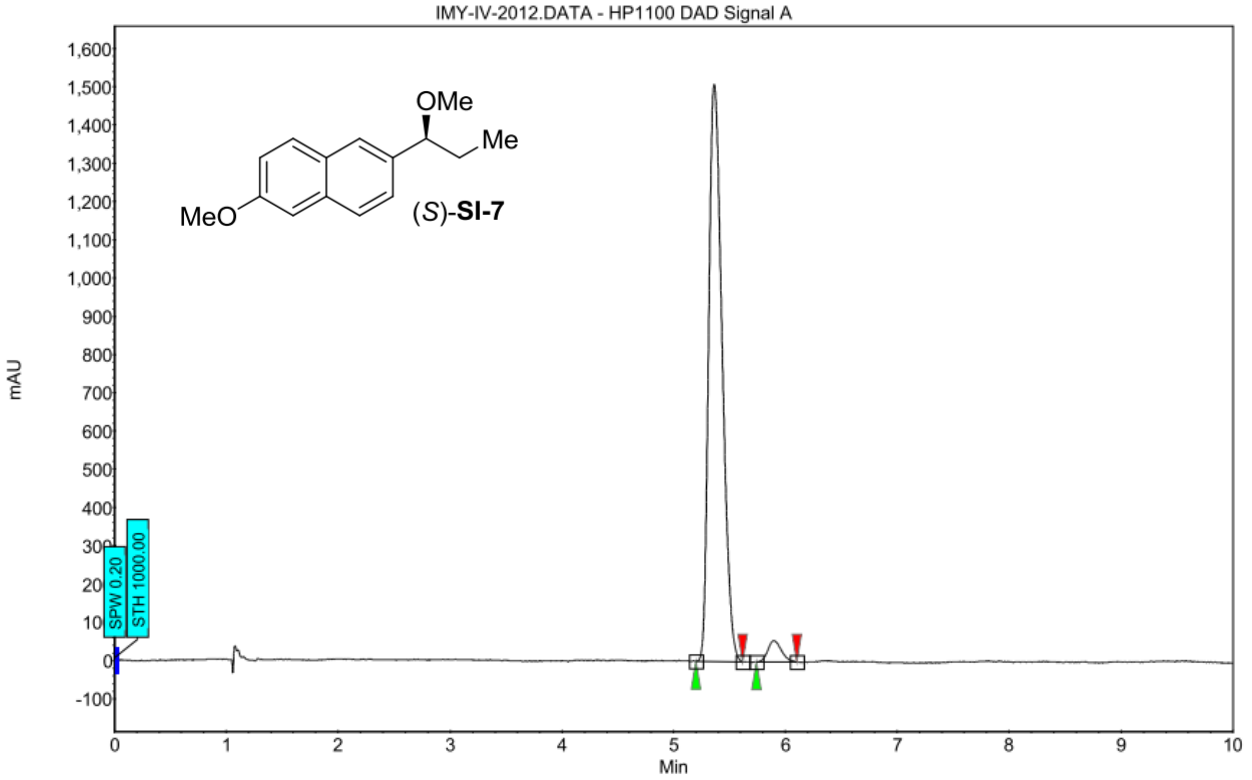
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.75	6.98	7.49	0.00	96.23	2011.3	558.6	96.229
2	UNKNOWN	8.64	8.87	9.25	0.00	3.77	78.5	21.9	3.771
Total						100.00	2089.9	580.5	100.000



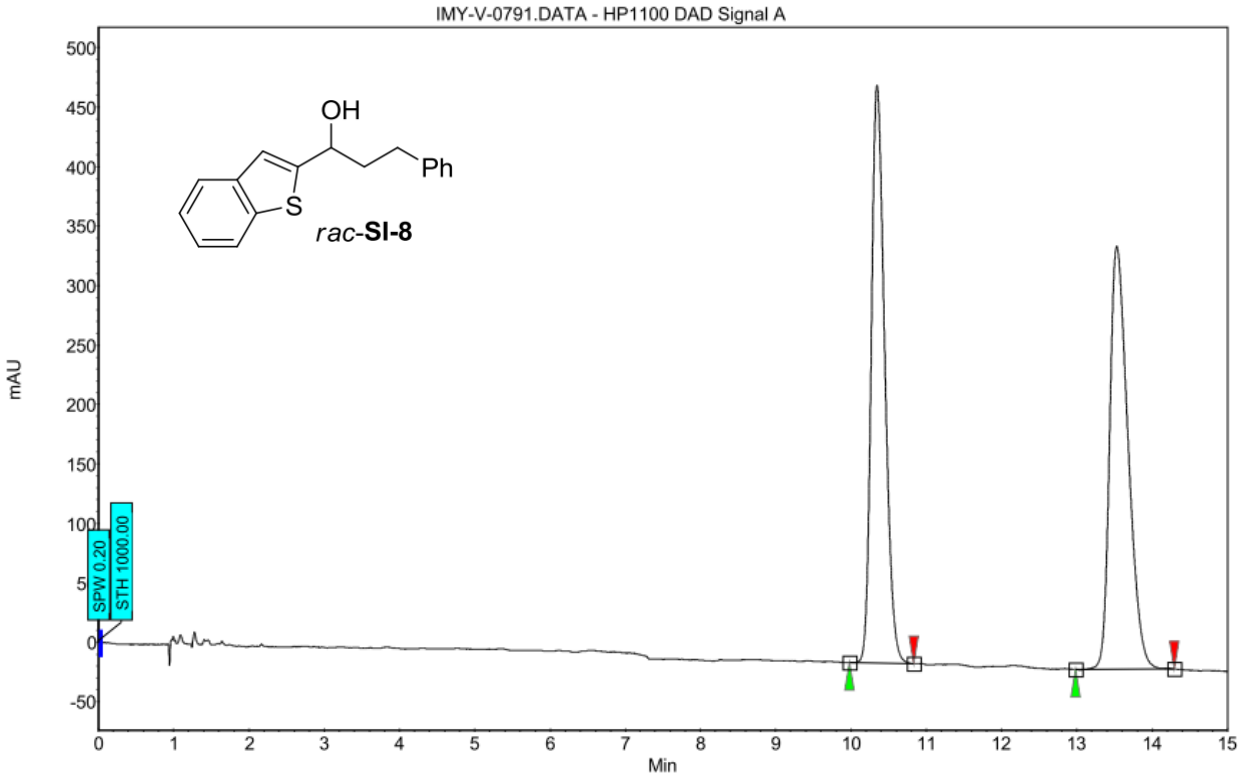


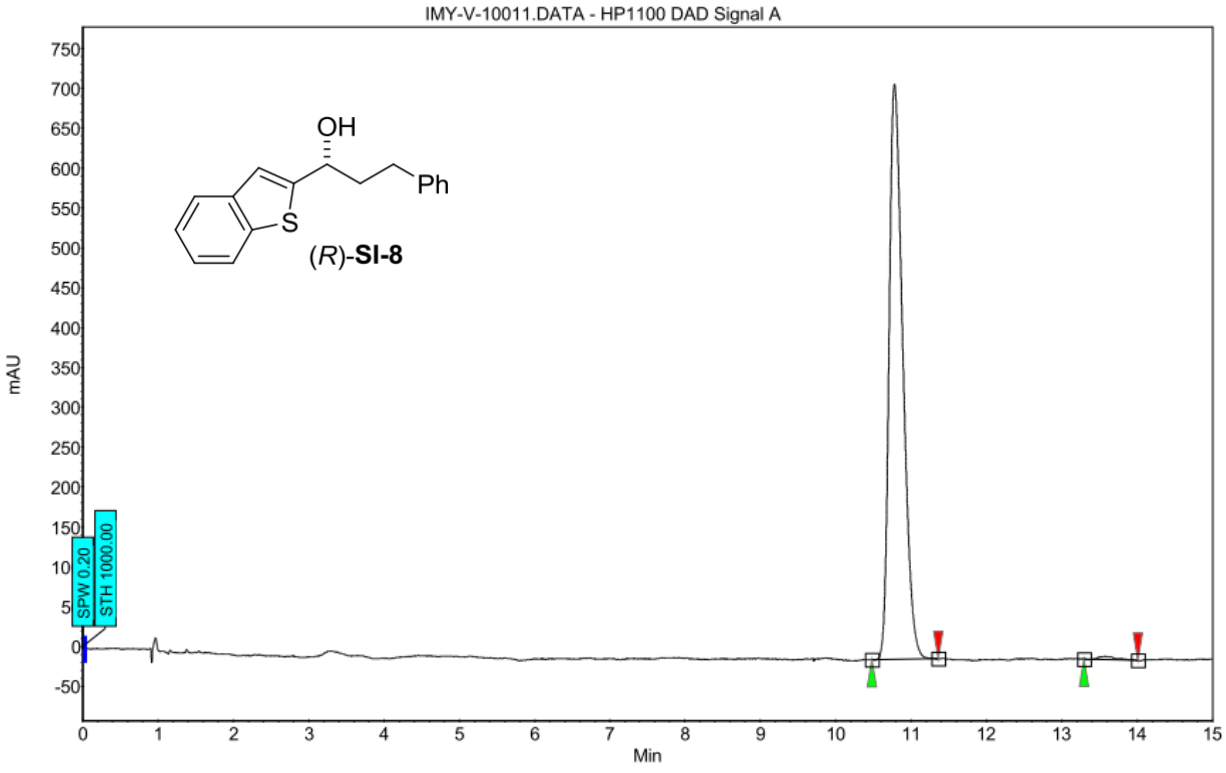
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	5.13	5.29	5.51	0.00	97.12	209.9	22.7	97.119
2	UNKNOWN	6.38	6.52	6.67	0.00	2.88	5.2	0.7	2.881
Total						100.00	215.0	23.4	100.000



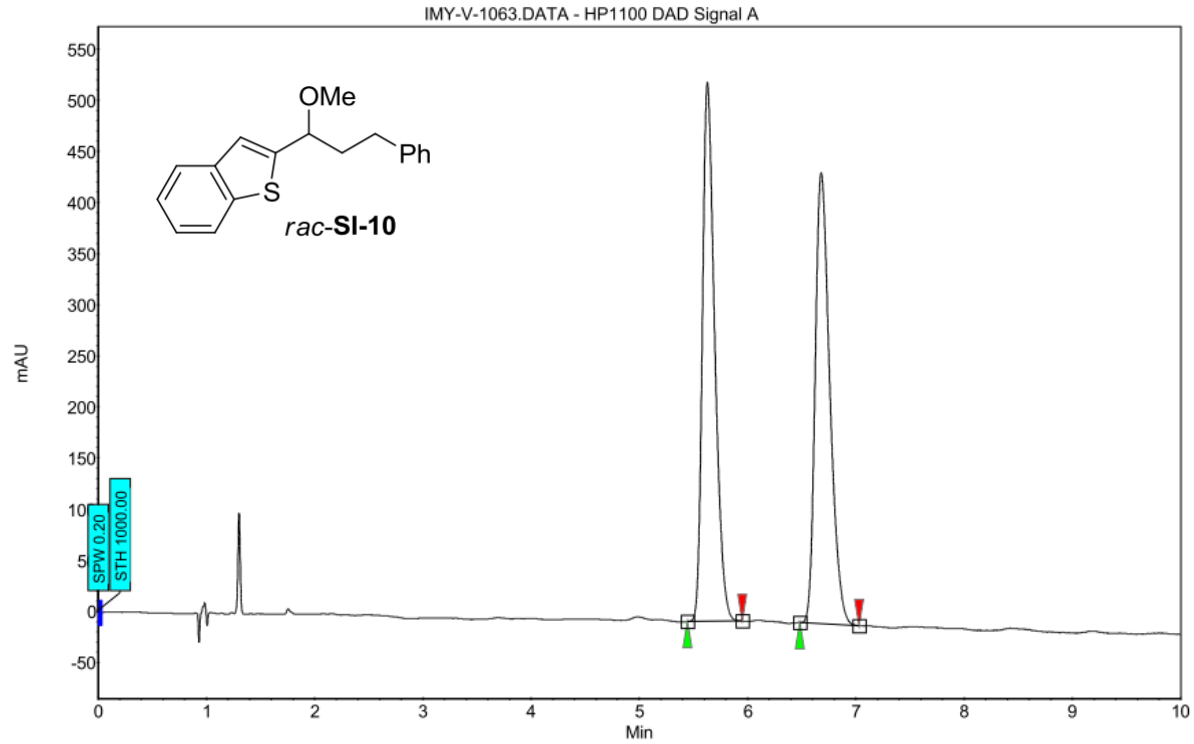


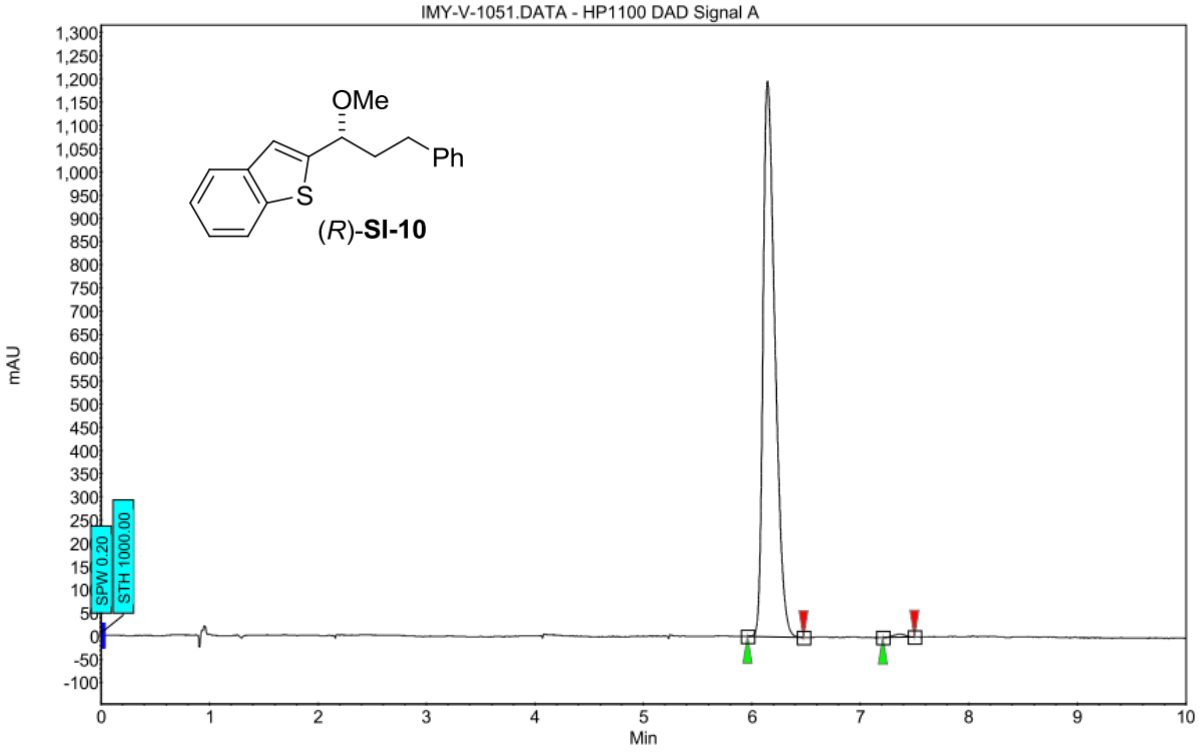
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	5.20	5.37	5.62	0.00	96.49	1508.6	209.6	96.491
2	UNKNOWN	5.74	5.90	6.10	0.00	3.51	55.5	7.6	3.509
Total						100.00	1564.1	217.3	100.000



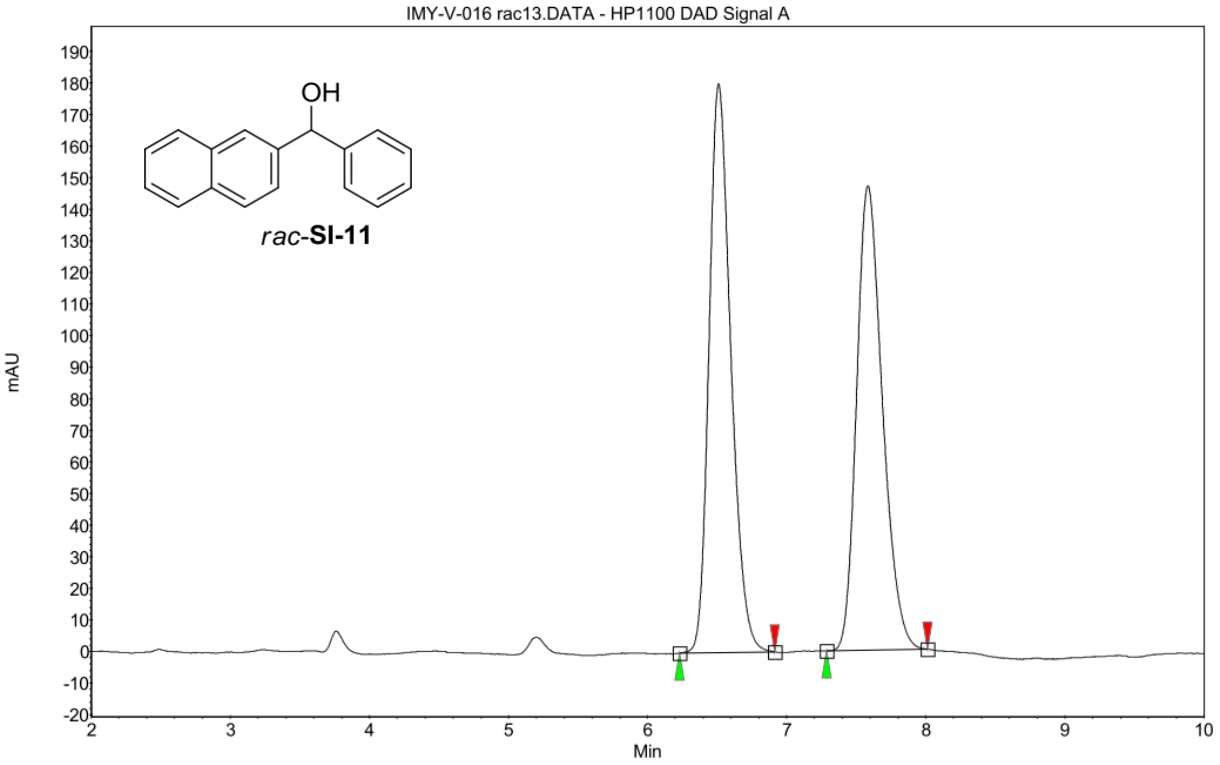


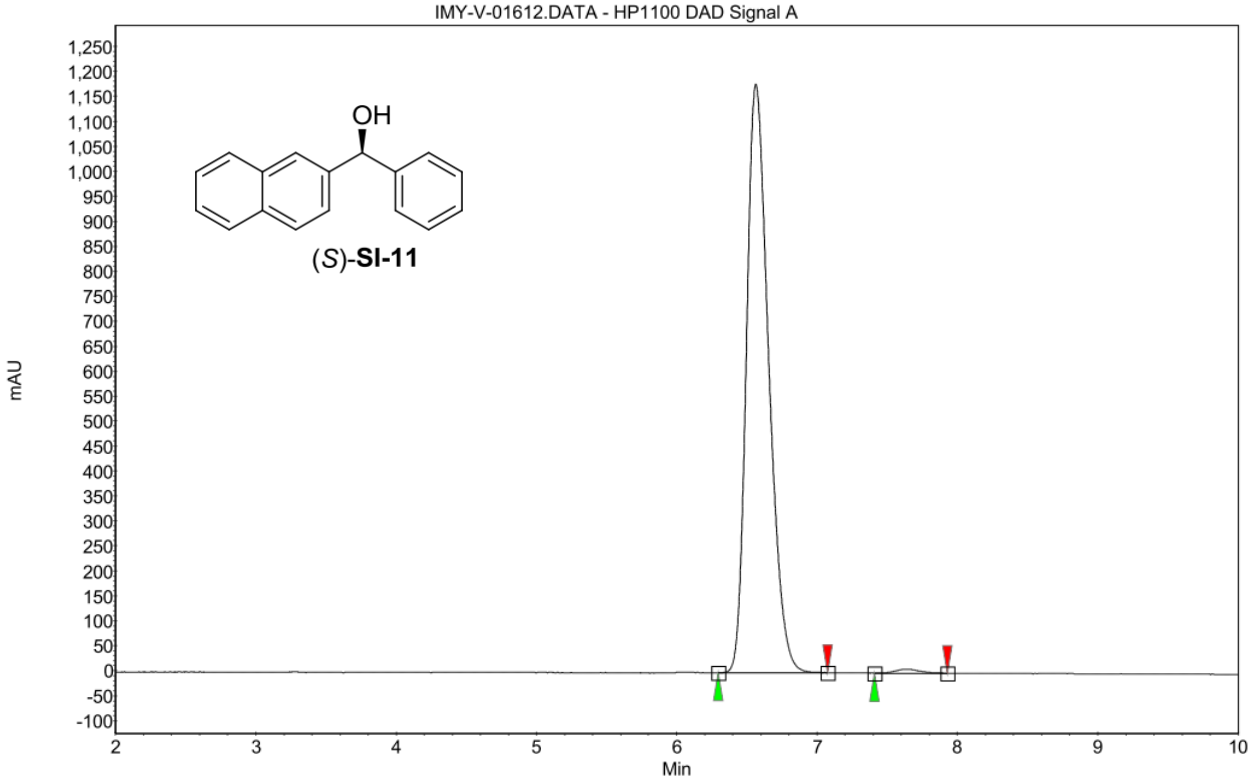
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	10.48	10.78	11.36	0.00	99.34	720.8	151.9	99.336
2	UNKNOWN	13.30	13.59	14.01	0.00	0.66	4.2	1.0	0.664
Total						100.00	725.0	153.0	100.000



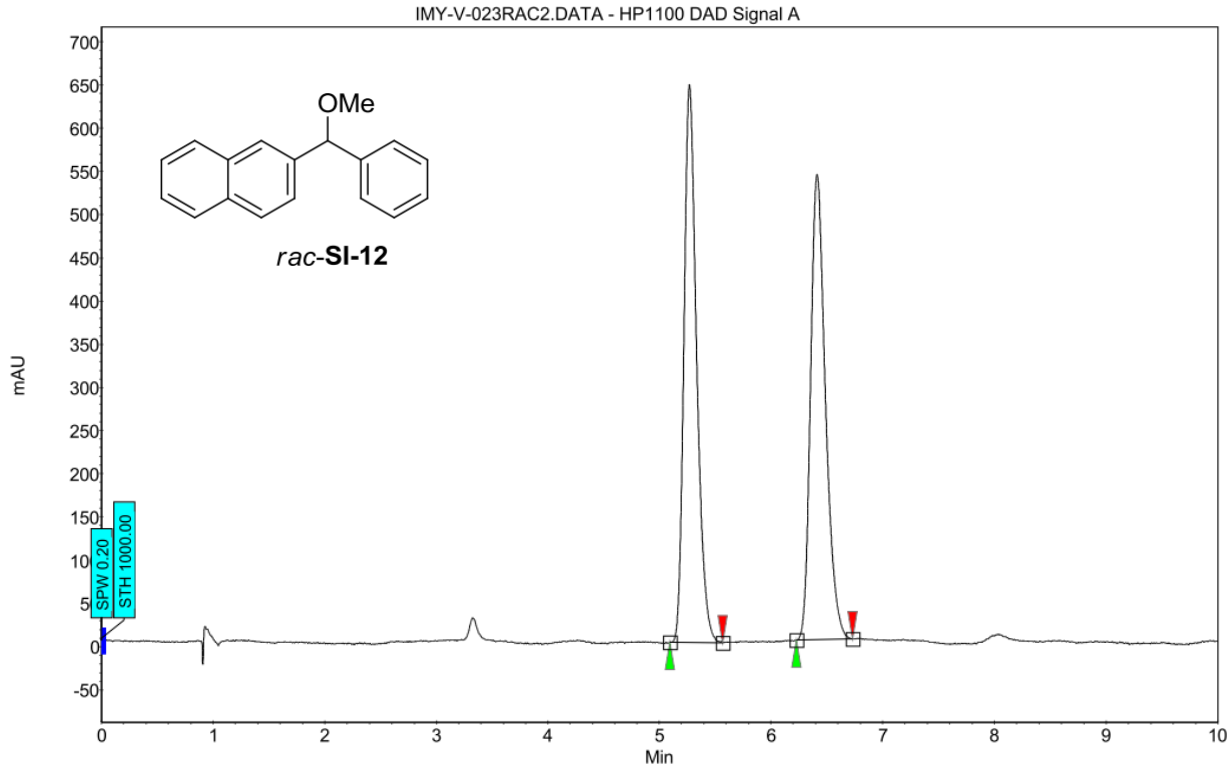


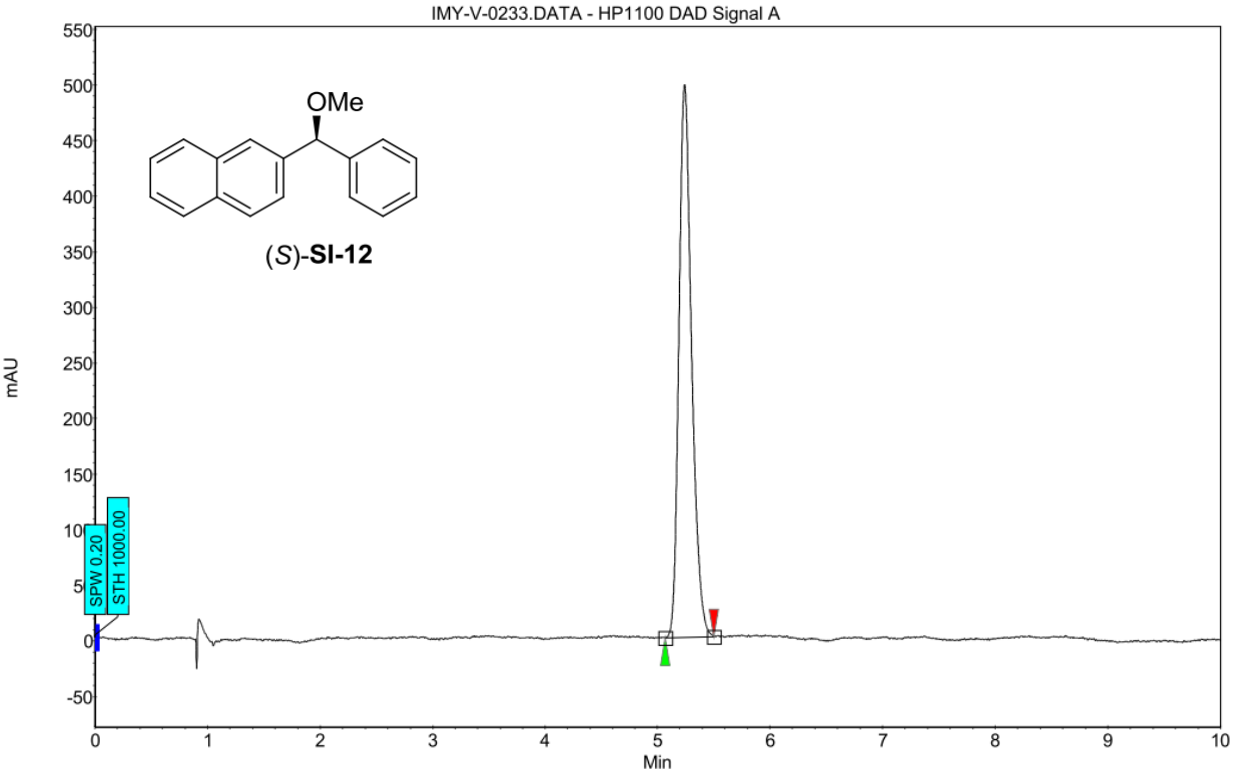
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	5.96	6.15	6.48	0.00	99.49	1196.1	152.3	99.490
2	UNKNOWN	7.21	7.37	7.50	0.00	0.51	6.6	0.8	0.510
Total						100.00	1202.7	153.0	100.000



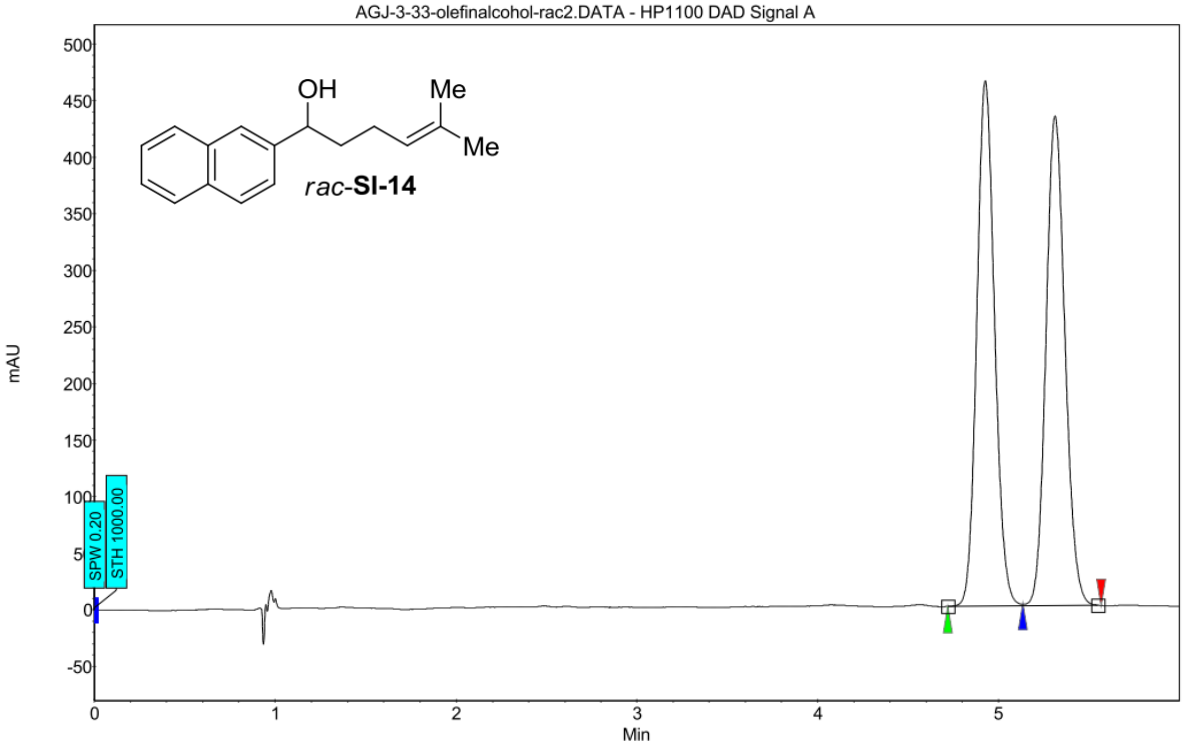


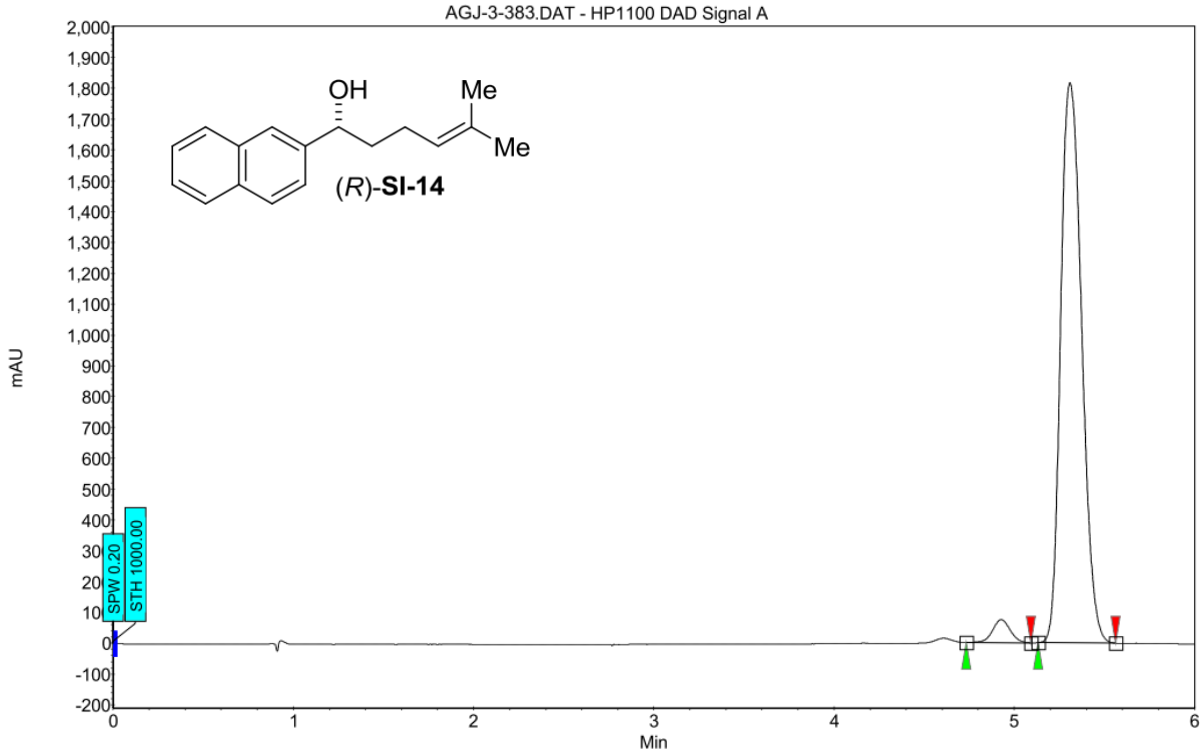
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.30	6.56	7.07	0.00	99.26	1178.6	215.7	99.260
2	UNKNOWN	7.41	7.64	7.93	0.00	0.74	8.1	1.6	0.740
Total						100.00	1186.7	217.3	100.000



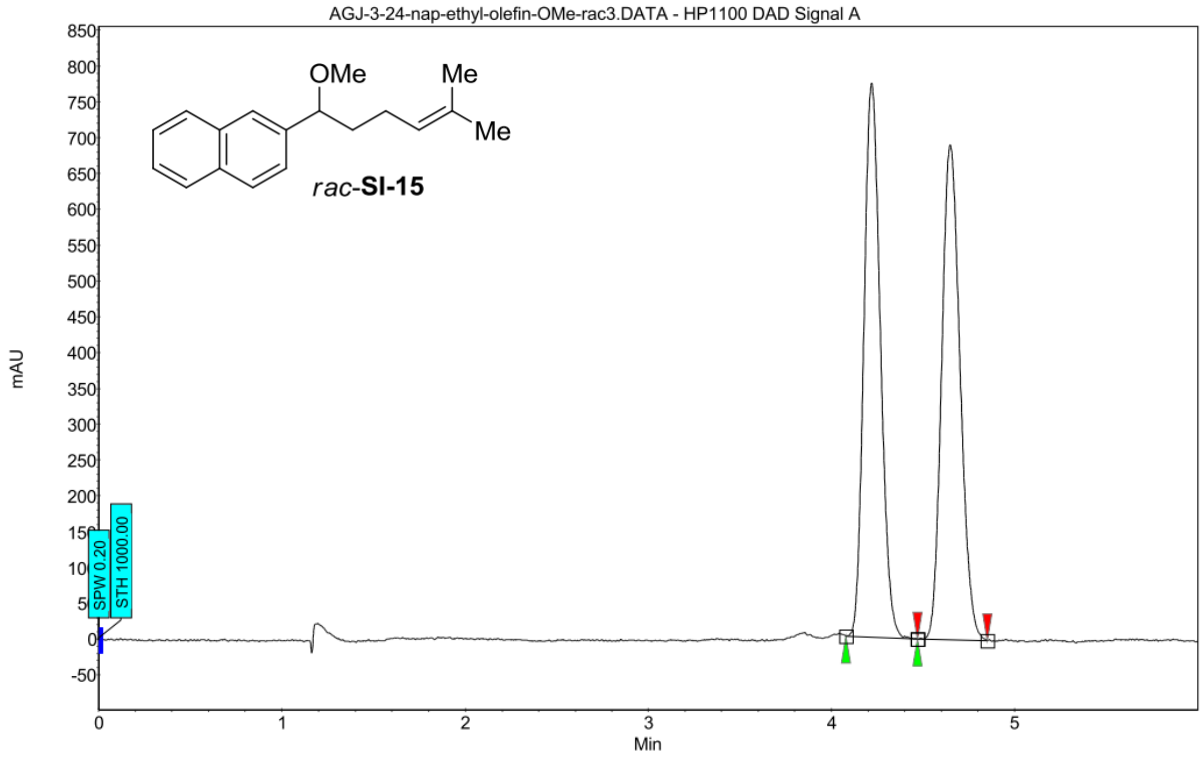


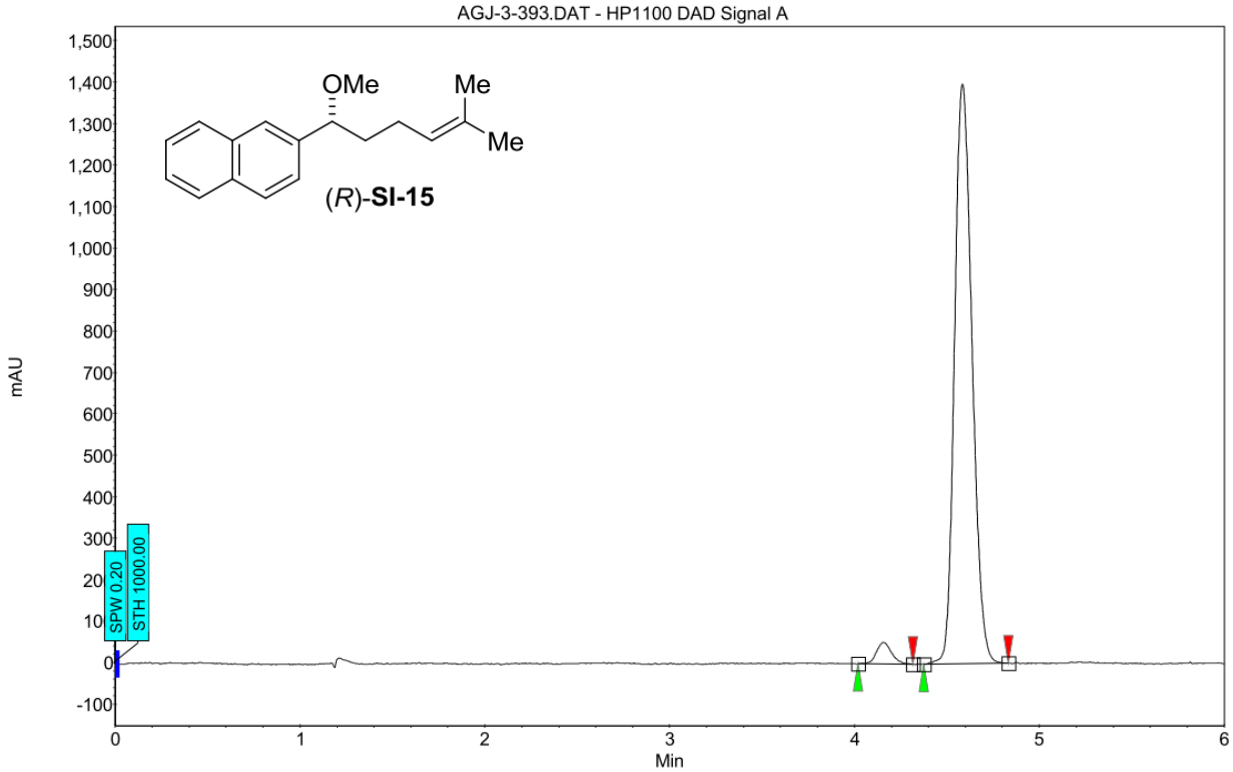
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	5.07	5.24	5.50	0.00	100.00	497.0	64.9	100.000
Total						100.00	497.0	64.9	100.000



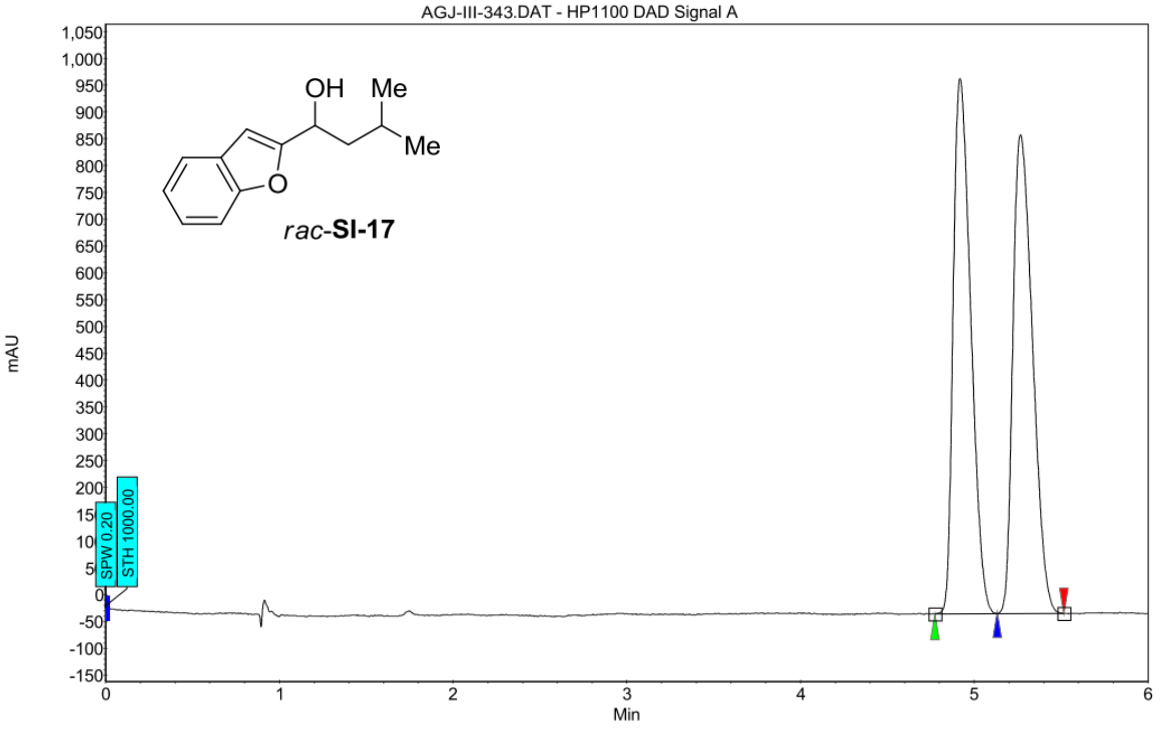


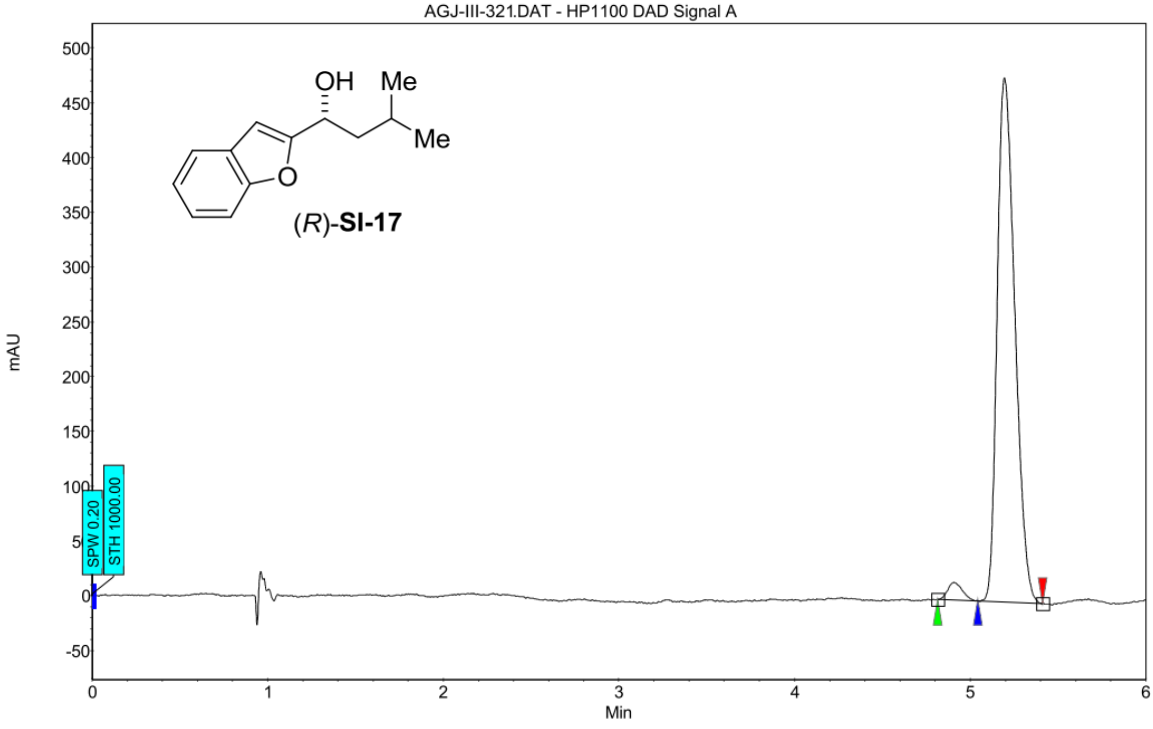
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	4.73	4.93	5.09	0.00	3.37	75.0	8.6	3.373
1	UNKNOWN	5.13	5.31	5.56	0.00	96.63	1816.9	245.2	96.627
Total						100.00	1891.9	253.8	100.000



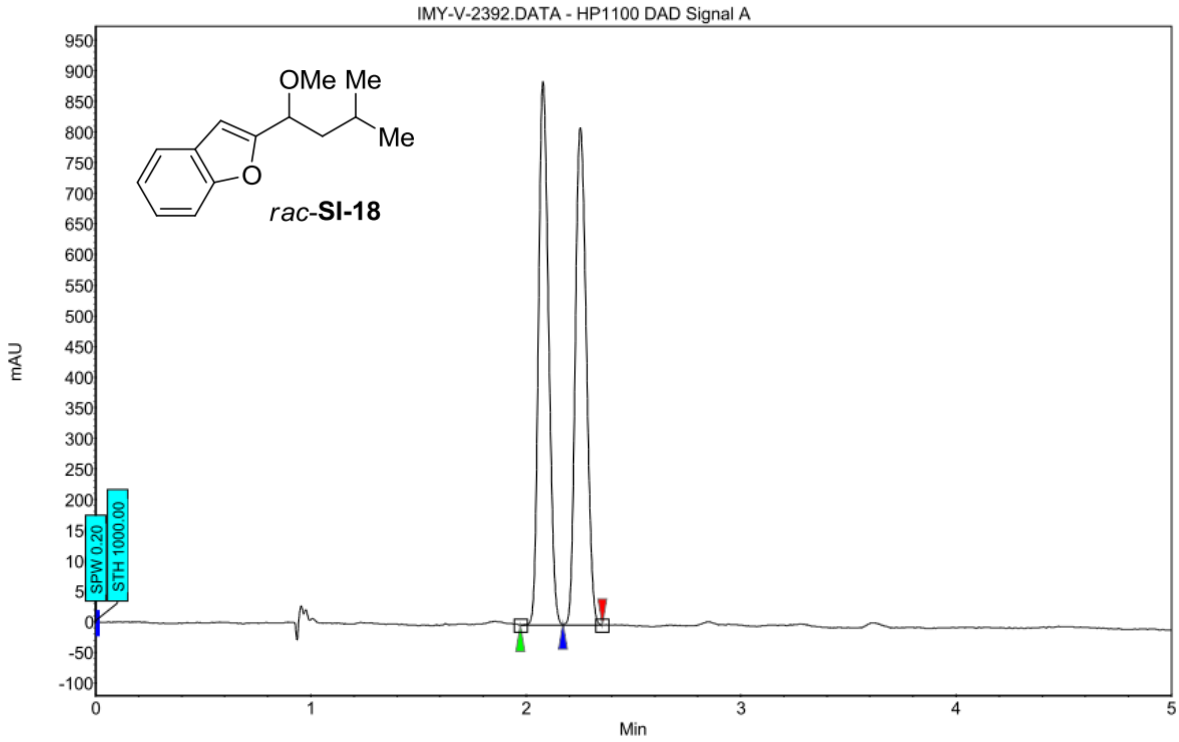


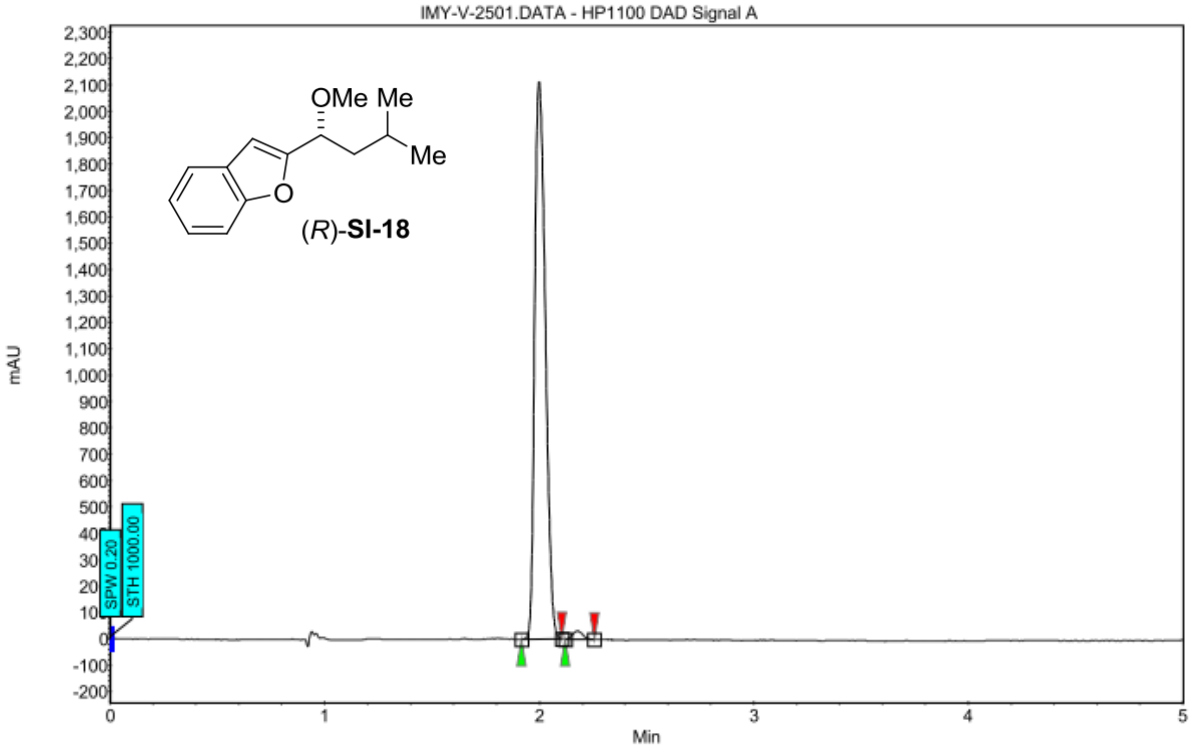
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	4.02	4.16	4.32	0.00	3.08	51.8	4.9	3.080
1	UNKNOWN	4.37	4.58	4.83	0.00	96.92	1396.8	153.4	96.920
Total						100.00	1448.6	158.2	100.000



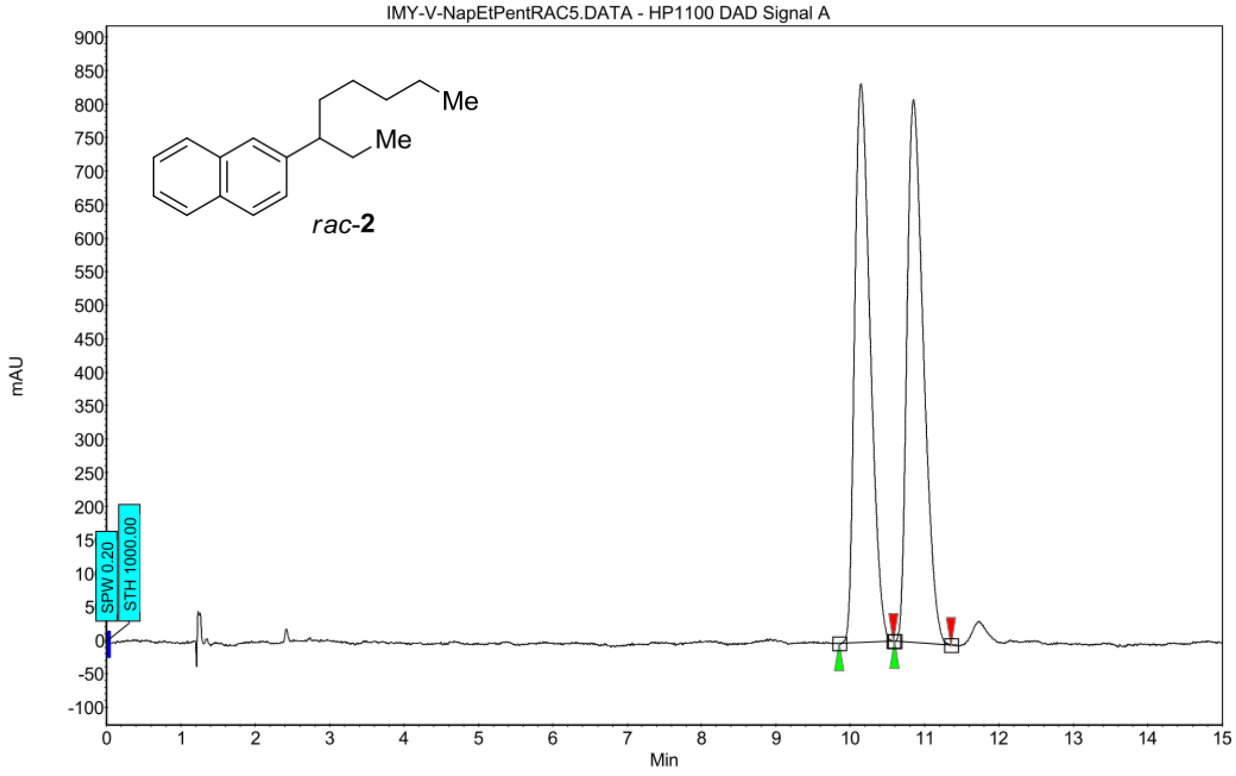


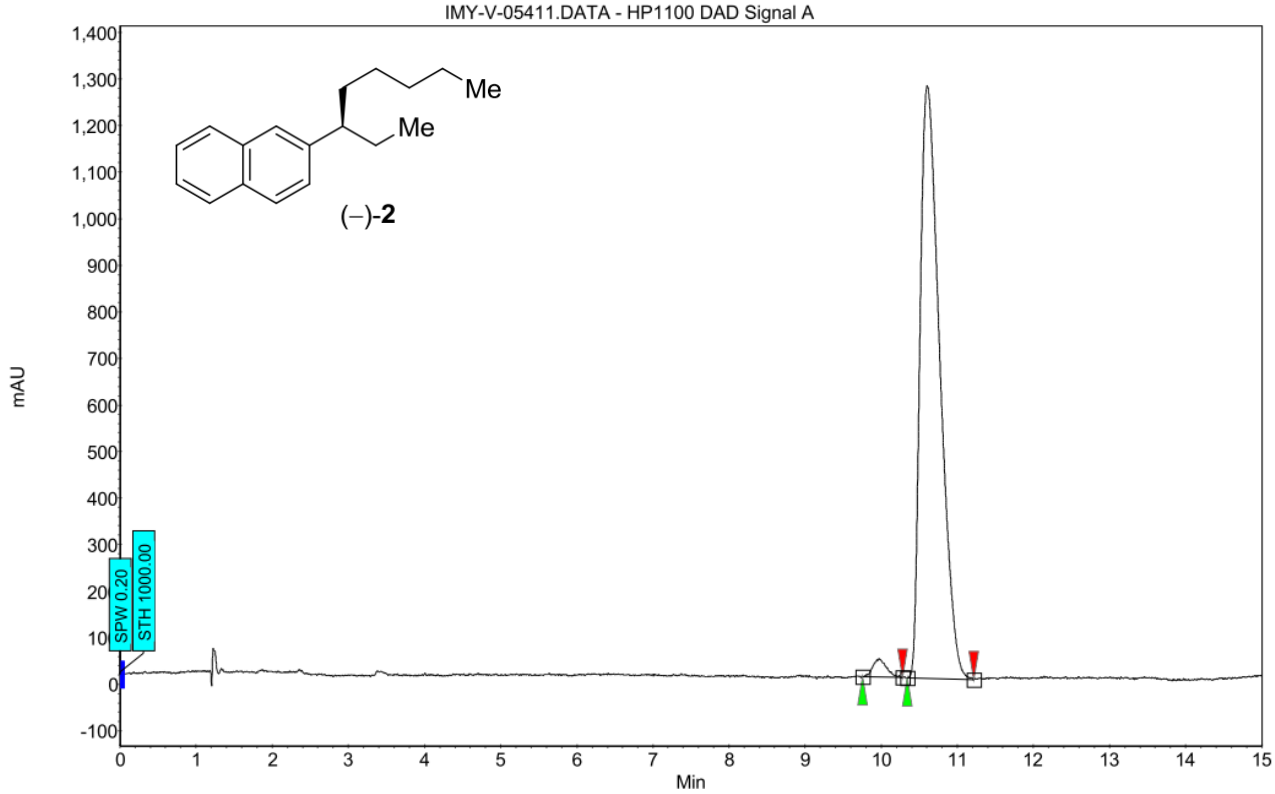
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.81	4.91	5.04	0.00	2.72	16.2	1.6	2.724
2	UNKNOWN	5.04	5.20	5.41	0.00	97.28	478.6	55.8	97.276
Total						100.00	494.7	57.4	100.000



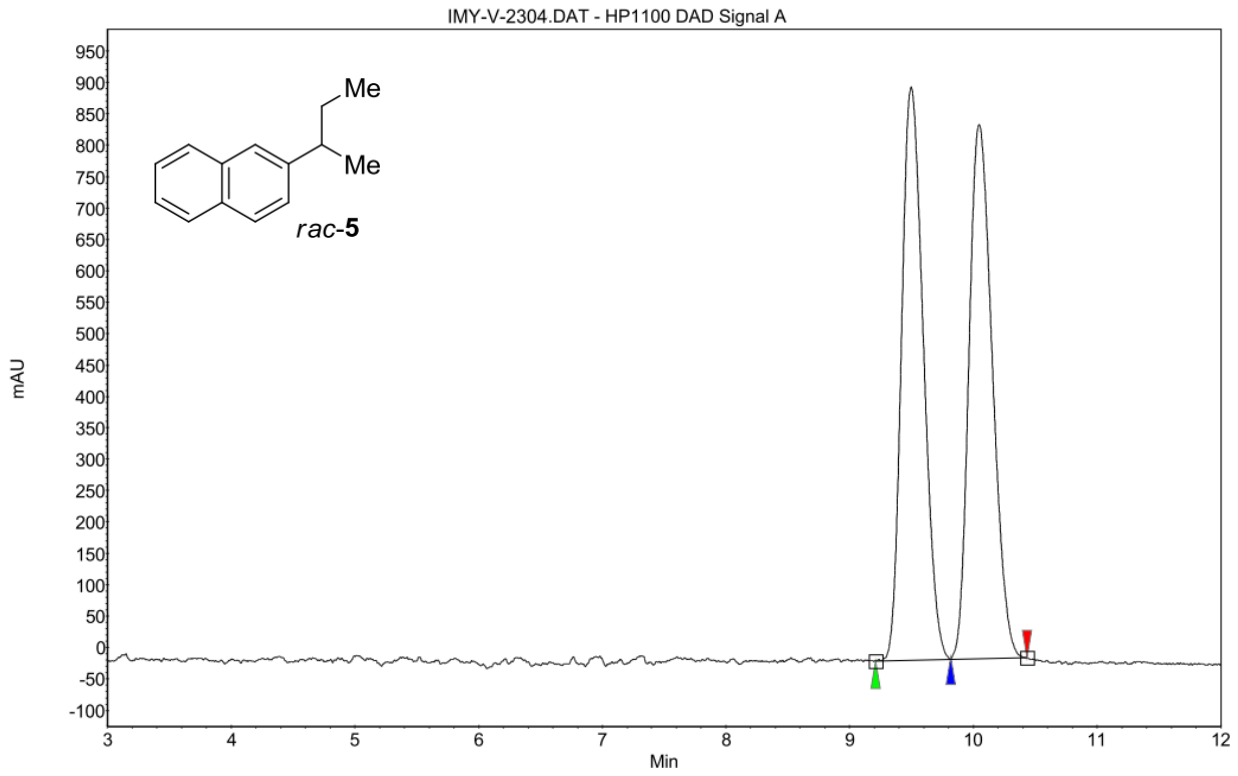


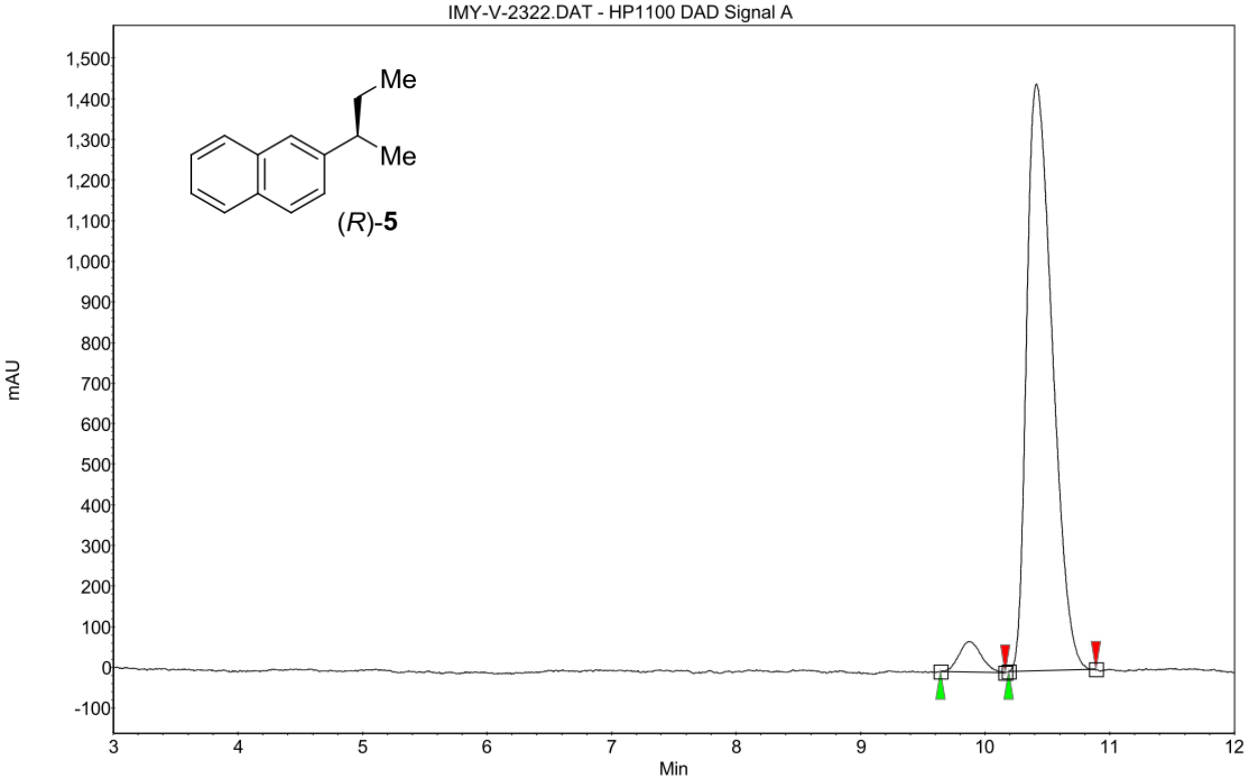
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	1.92	2.00	2.10	0.00	98.61	2113.6	121.9	98.613
2	UNKNOWN	2.12	2.18	2.26	0.00	1.39	31.1	1.7	1.387
Total						100.00	2144.6	123.6	100.000



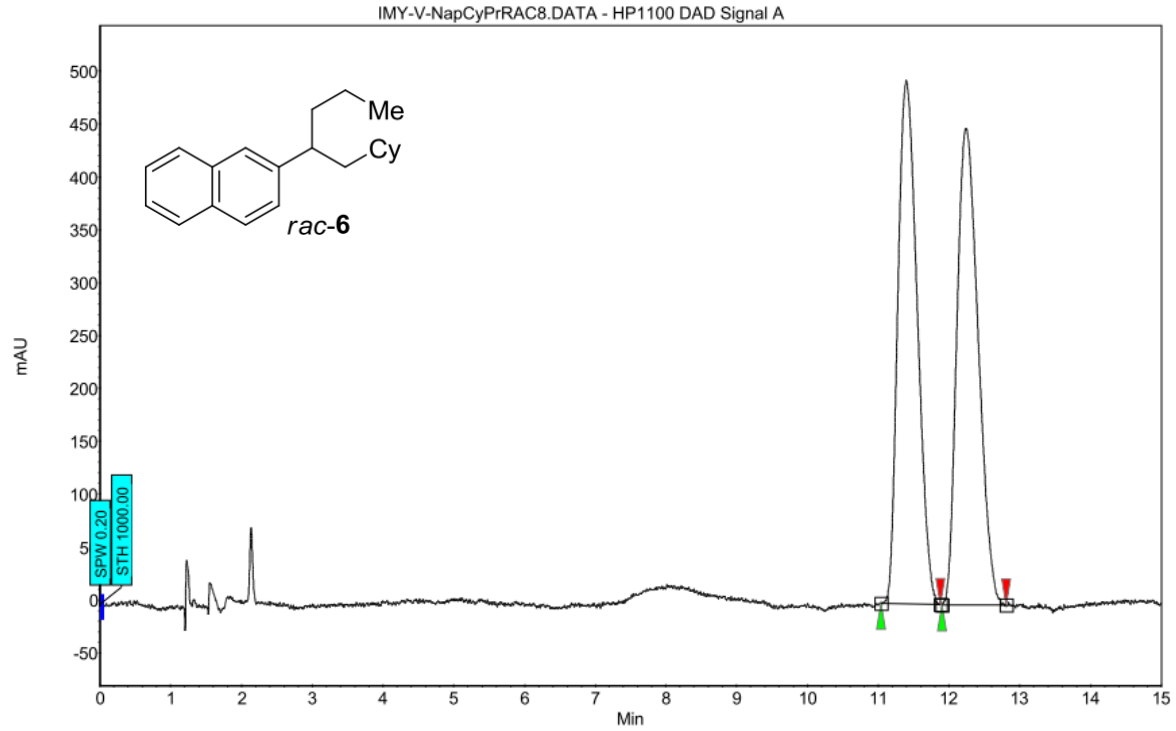


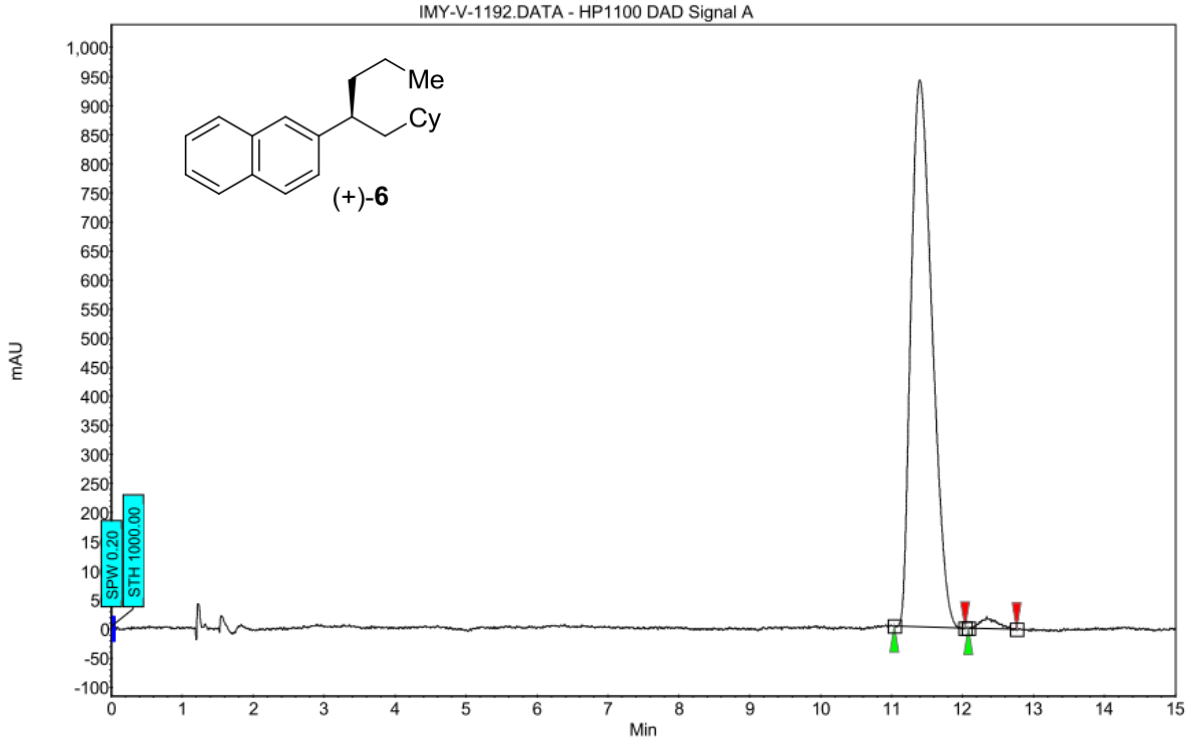
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	9.76	9.97	10.28	0.00	1.97	38.7	7.7	1.972
2	UNKNOWN	10.34	10.61	11.22	0.00	98.03	1272.5	380.8	98.028
Total						100.00	1311.2	388.5	100.000



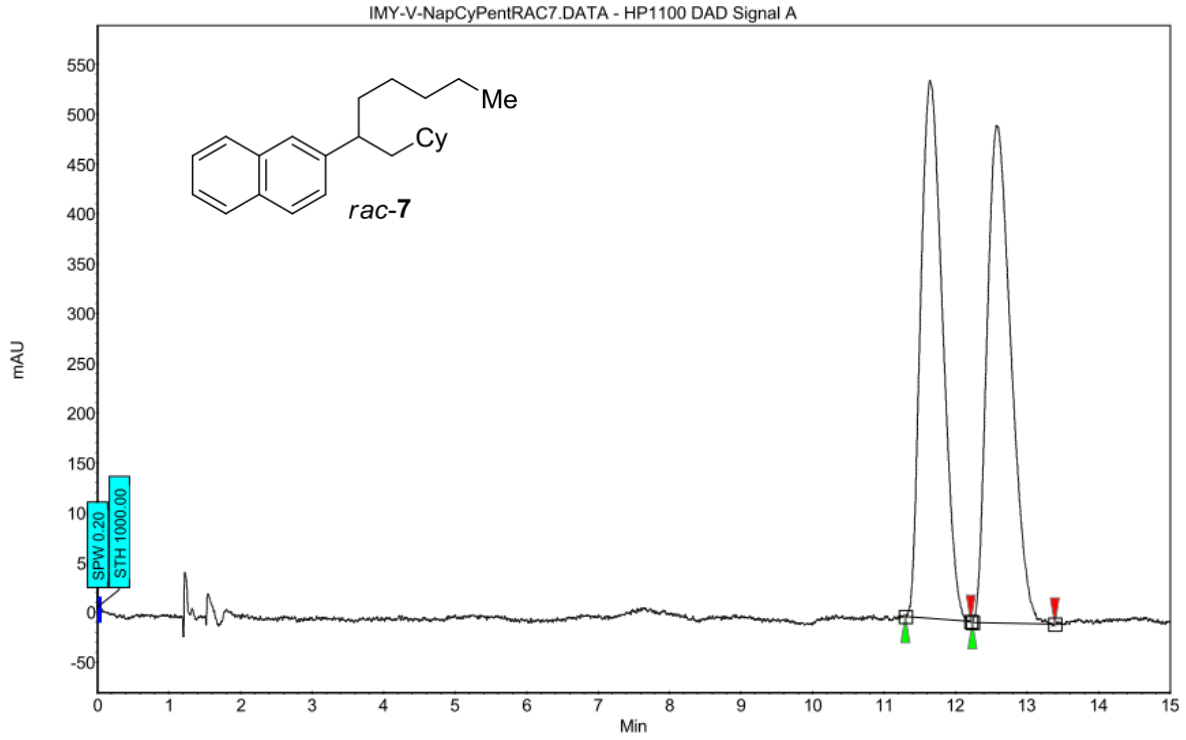


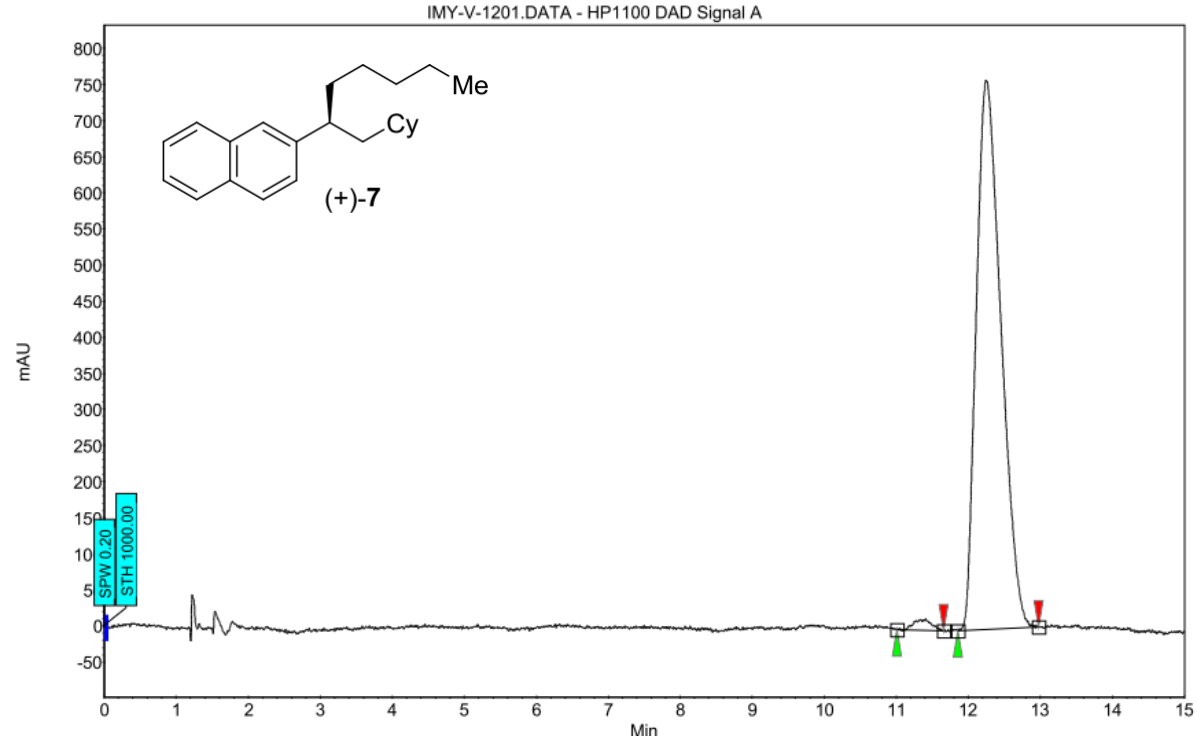
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	9.64	9.88	10.16	0.00	4.29	75.2	15.4	4.287
2	UNKNOWN	10.19	10.41	10.89	0.00	95.71	1445.1	344.9	95.713
Total						100.00	1520.4	360.4	100.000



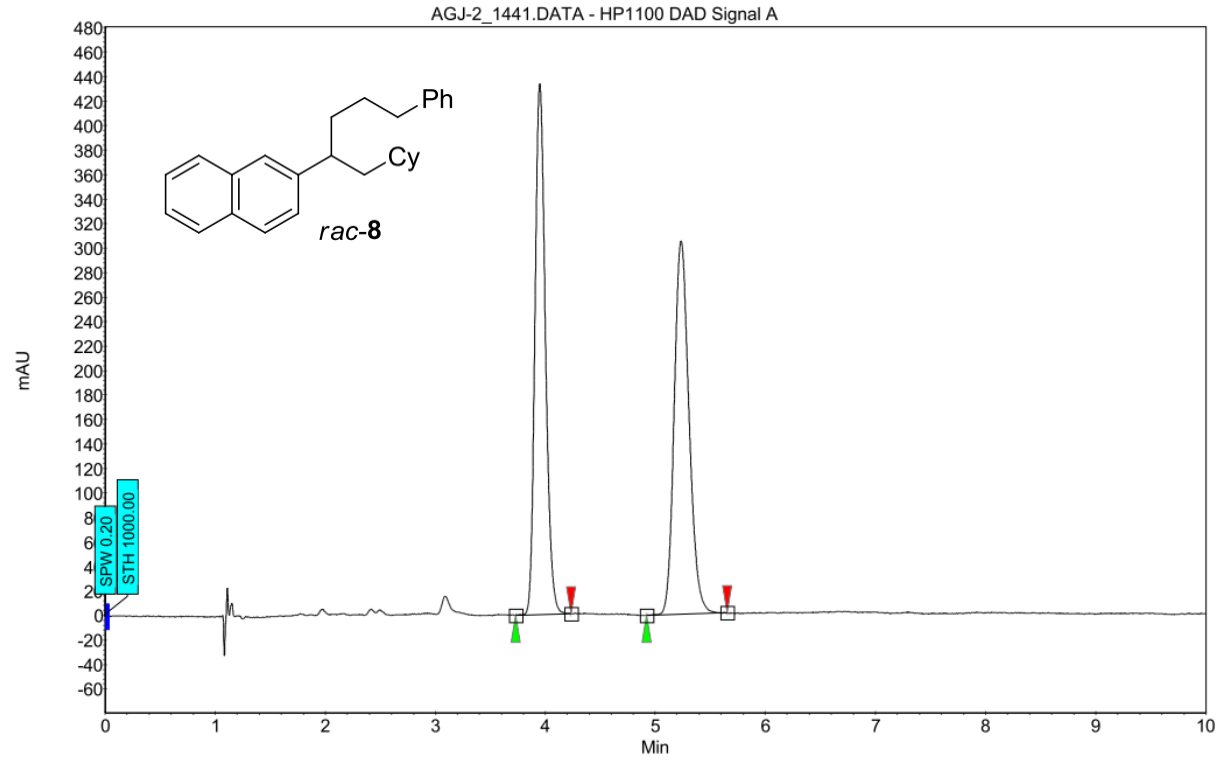


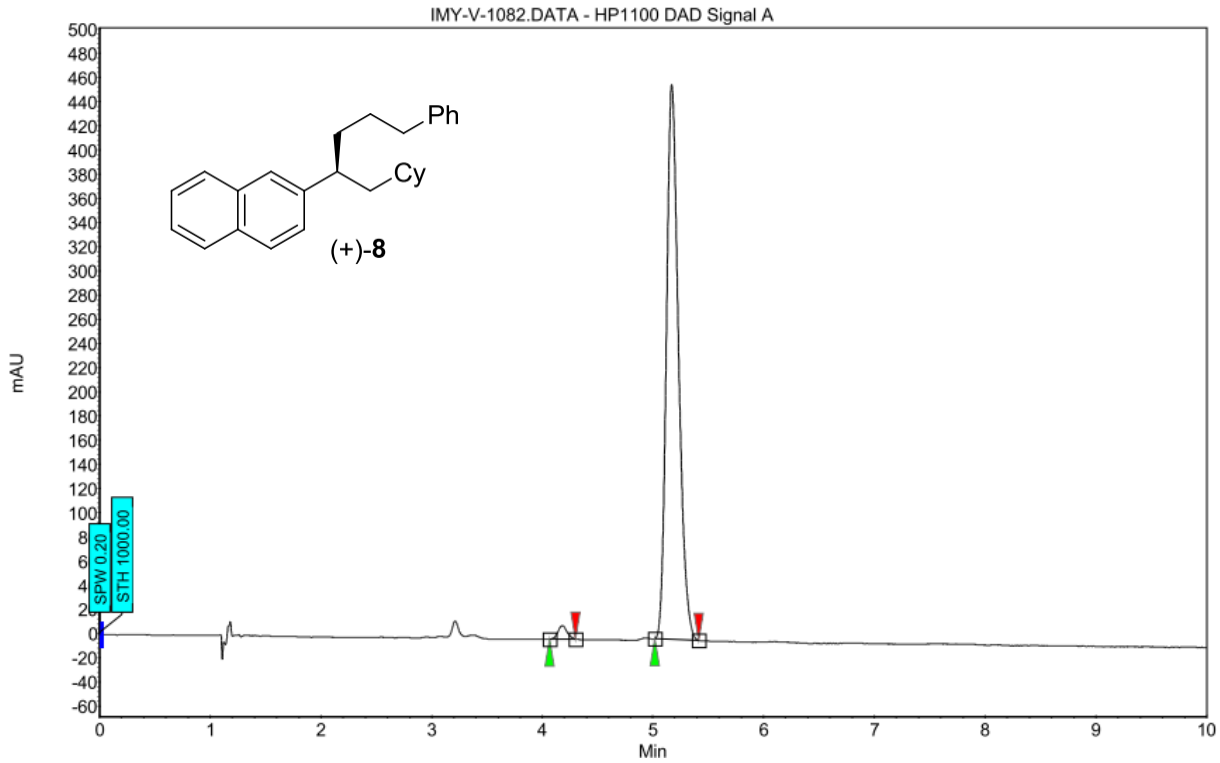
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	11.04	11.40	12.03	0.00	98.37	939.8	323.2	98.367
2	UNKNOWN	12.08	12.34	12.76	0.00	1.63	20.8	5.4	1.633
Total						100.00	960.6	328.6	100.000



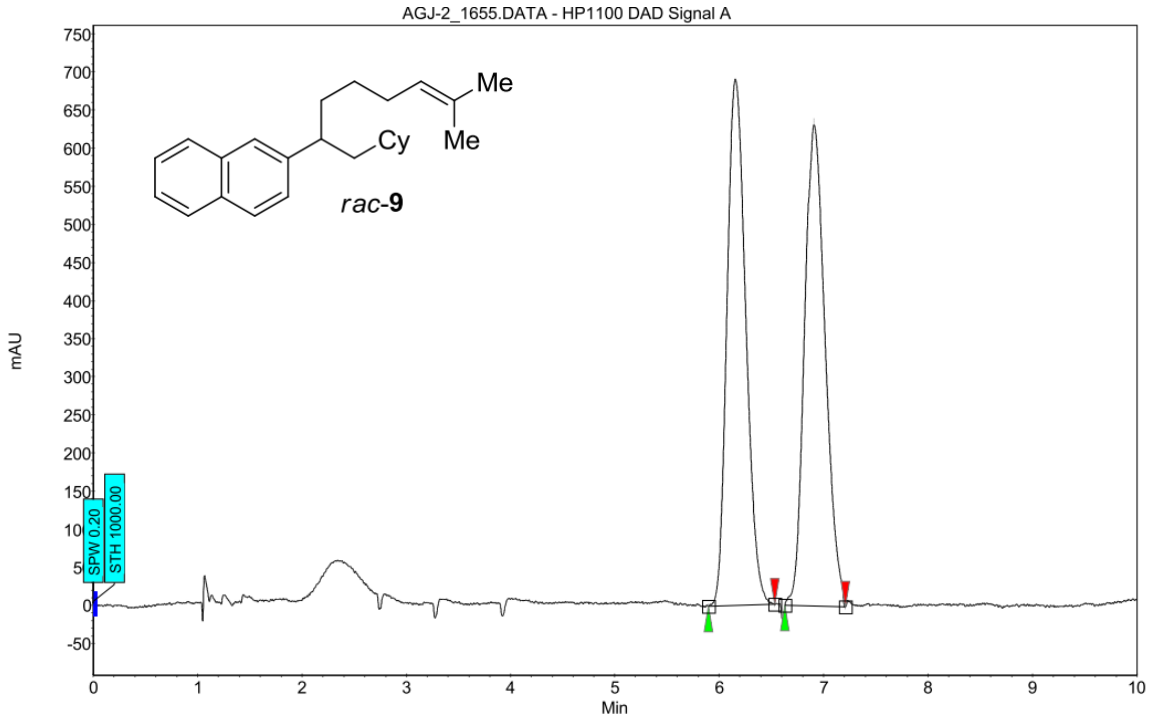


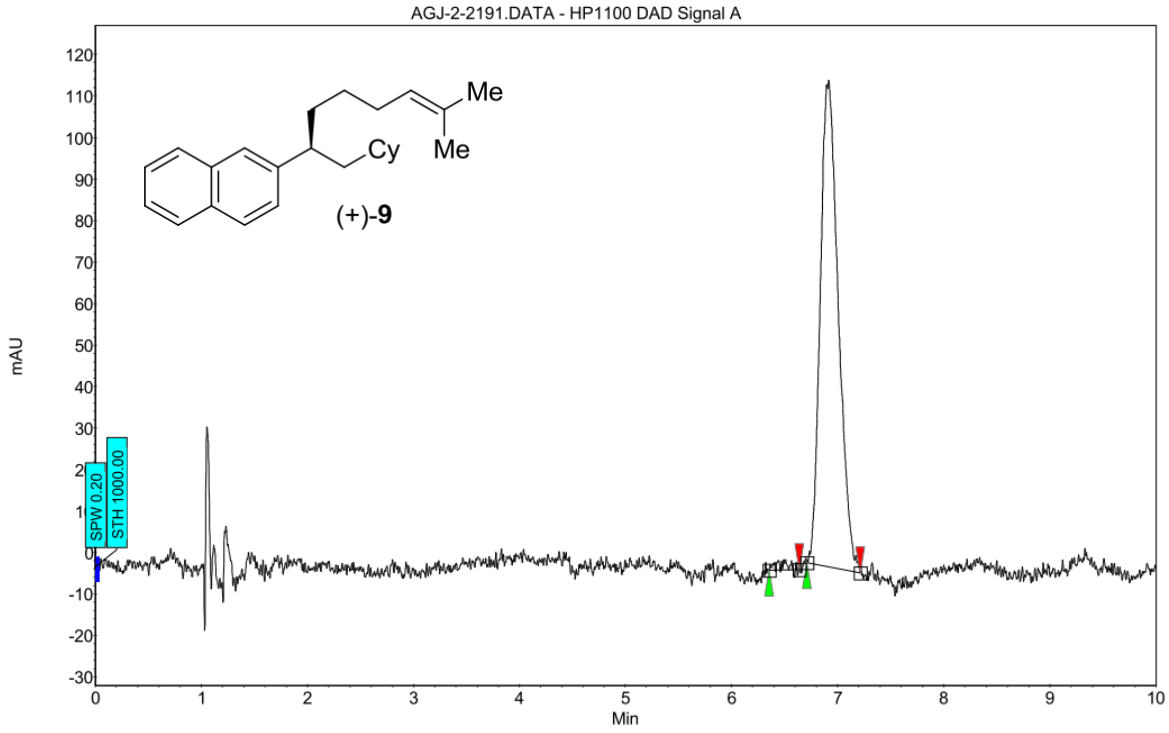
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	11.01	11.41	11.66	0.00	1.44	16.2	4.4	1.435
1	UNKNOWN	11.85	12.25	12.98	0.00	98.56	759.8	301.9	98.565
Total						100.00	776.0	306.3	100.000



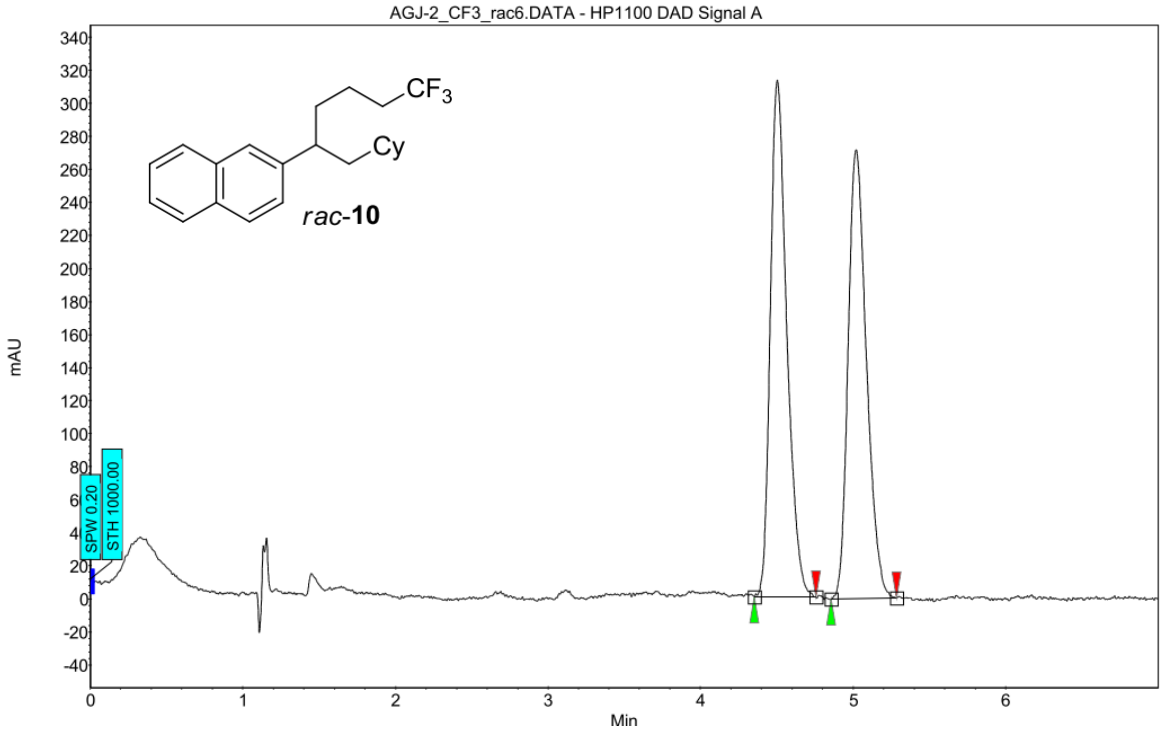


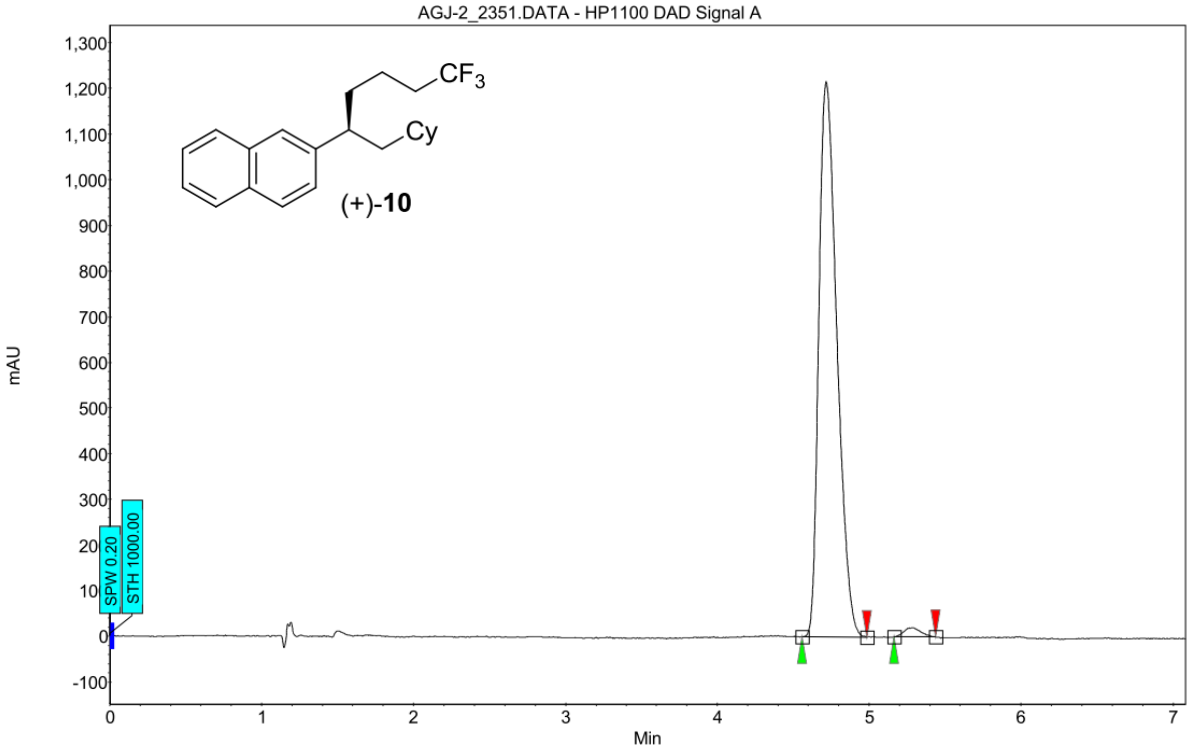
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.07	4.18	4.30	0.00	1.74	11.2	1.0	1.735
2	UNKNOWN	5.02	5.17	5.42	0.00	98.26	458.7	58.1	98.265
Total						100.00	469.9	59.1	100.000



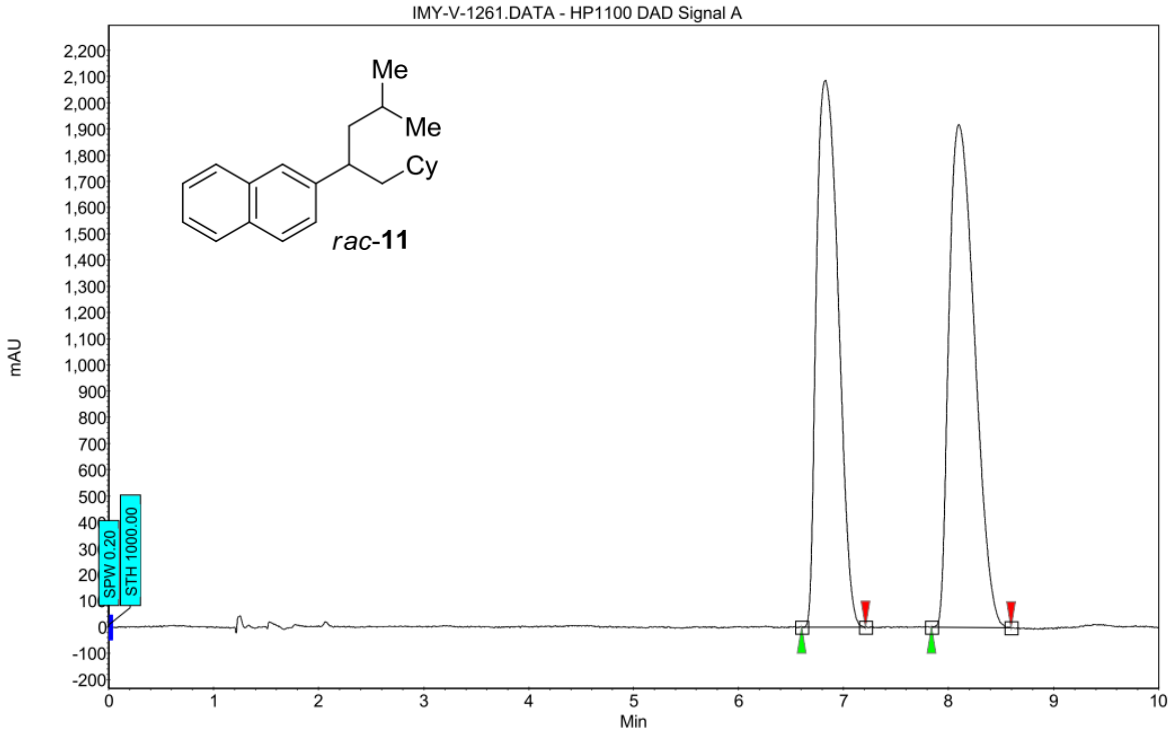


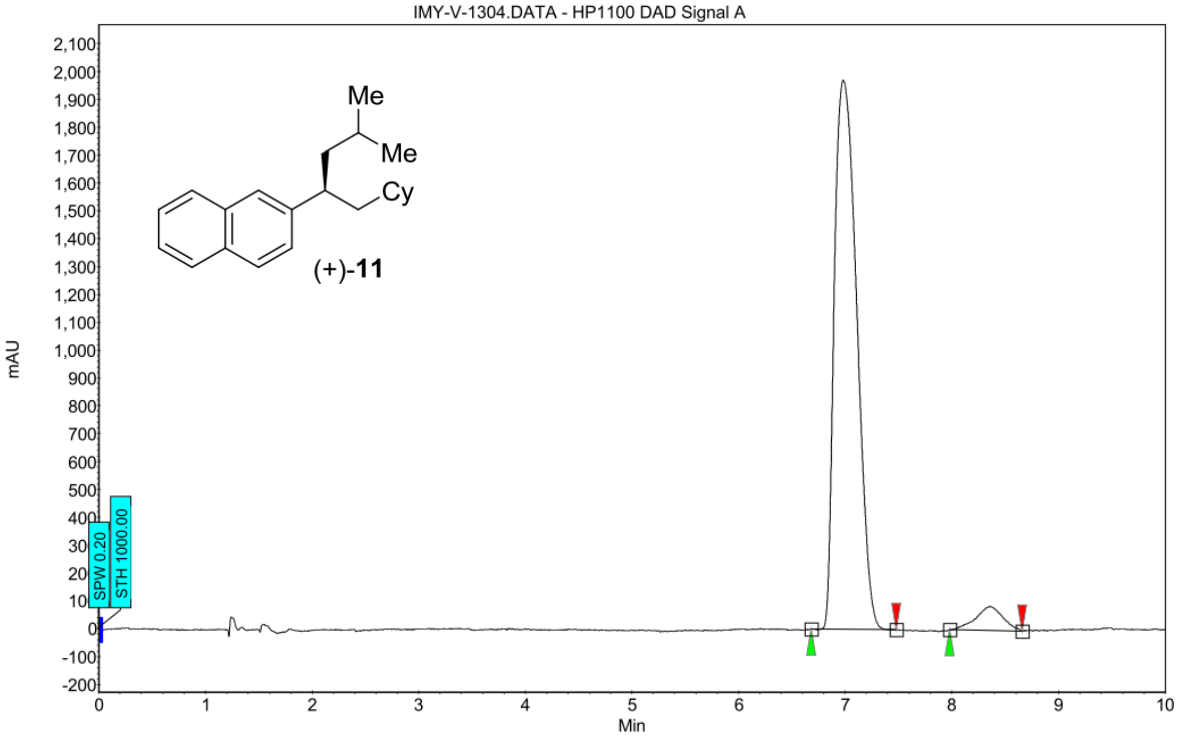
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	6.35	6.49	6.64	0.00	1.12	2.2	0.3	1.119
1	UNKNOWN	6.71	6.92	7.21	0.00	98.88	117.2	23.0	98.881
Total						100.00	119.4	23.3	100.000



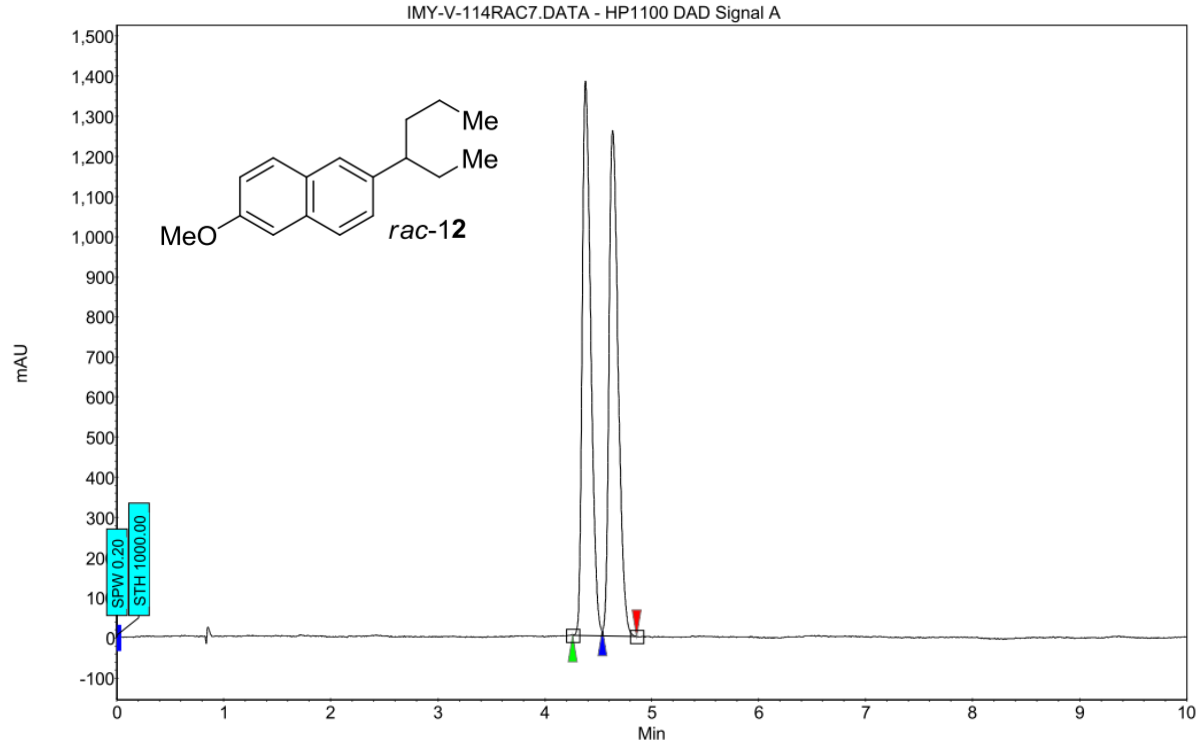


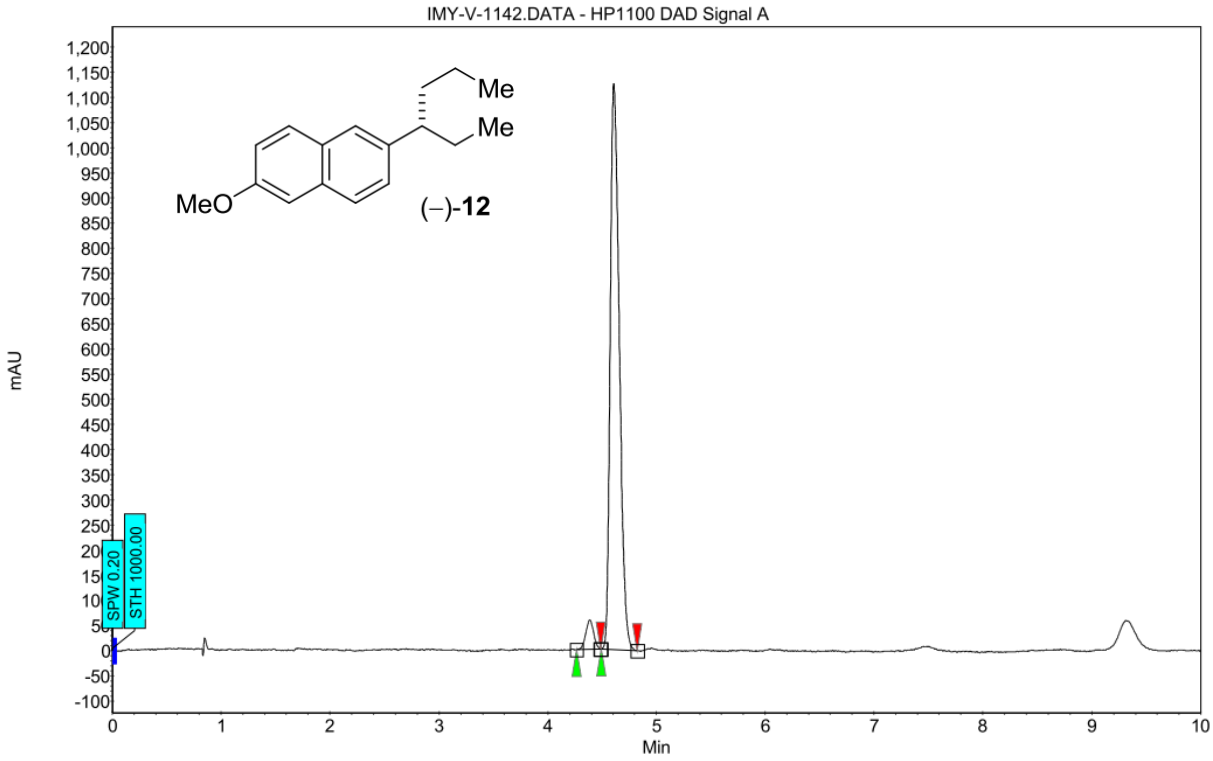
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.56	4.72	4.99	0.00	98.50	1215.7	167.4	98.504
2	UNKNOWN	5.16	5.29	5.44	0.00	1.50	20.2	2.5	1.496
Total						100.00	1235.9	169.9	100.000



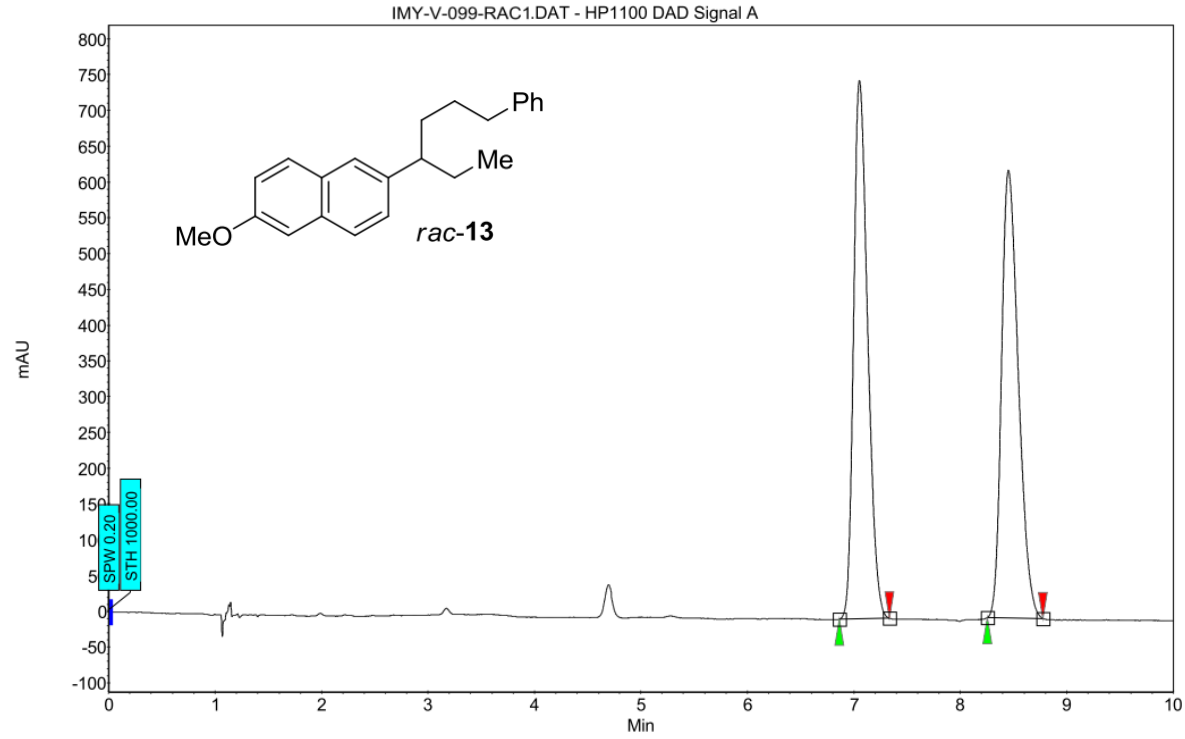


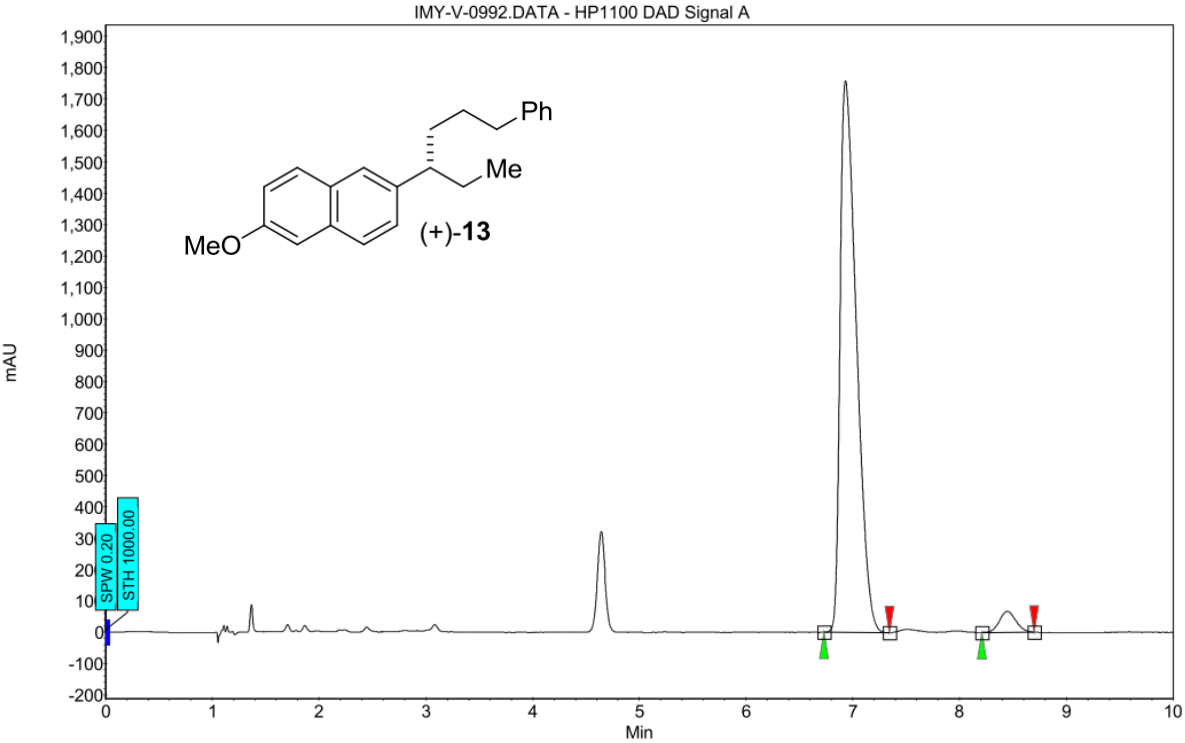
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.68	6.98	7.48	0.00	94.98	1972.0	477.3	94.985
2	UNKNOWN	7.98	8.36	8.66	0.00	5.02	86.7	25.2	5.015
Total						100.00	2058.6	502.5	100.000



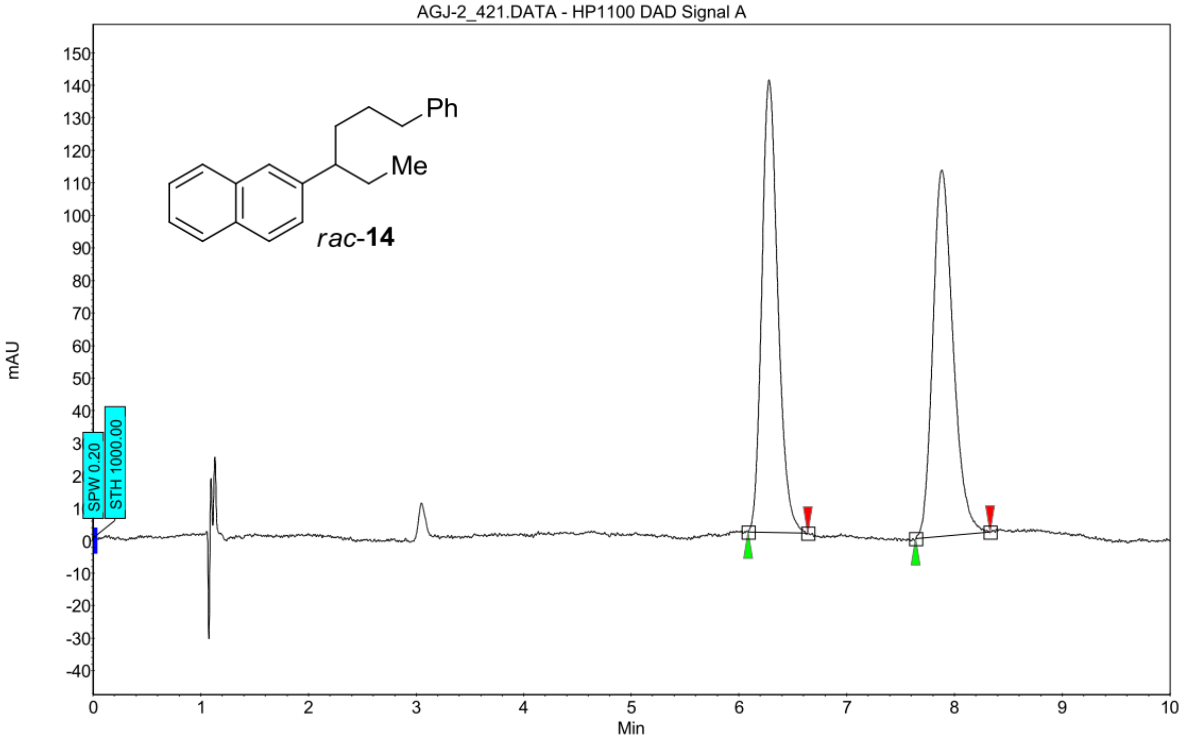


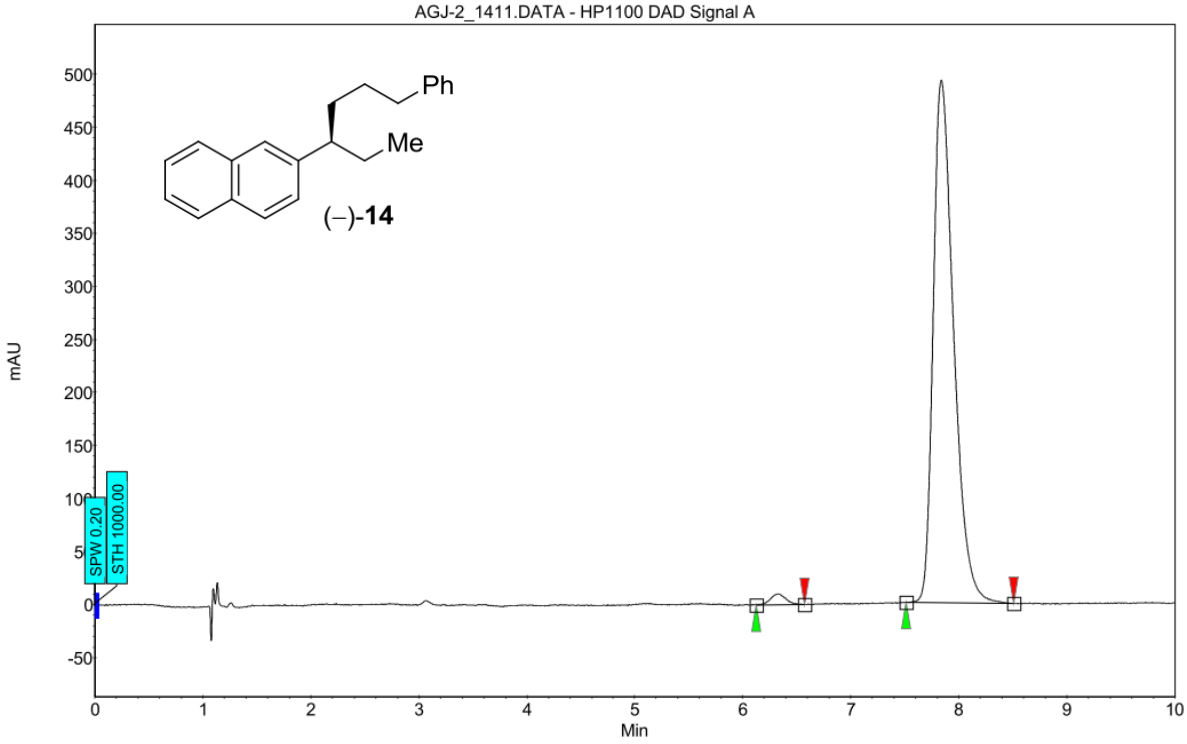
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.27	4.39	4.48	0.00	4.24	58.1	4.9	4.239
2	UNKNOWN	4.49	4.61	4.83	0.00	95.76	1124.7	110.8	95.761
Total						100.00	1182.8	115.7	100.000



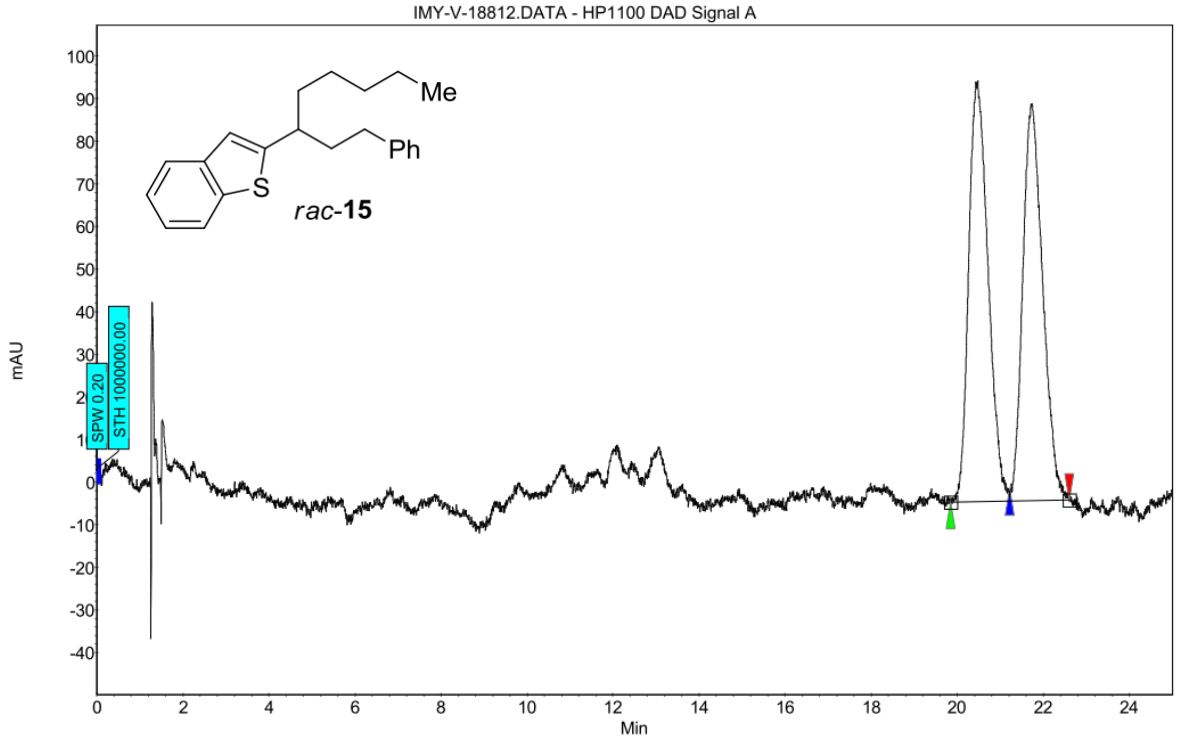


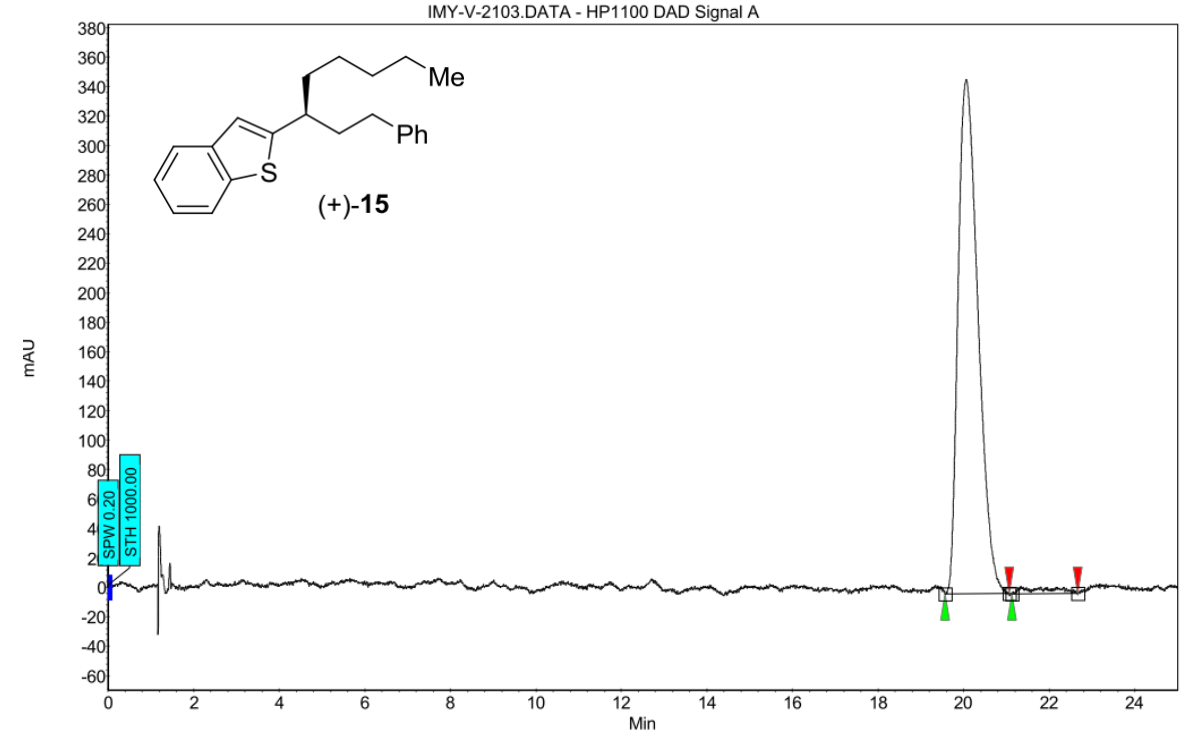
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.73	6.93	7.34	0.00	96.27	1758.4	310.2	96.265
2	UNKNOWN	8.21	8.45	8.70	0.00	3.73	67.1	12.0	3.735
Total						100.00	1825.5	322.3	100.000



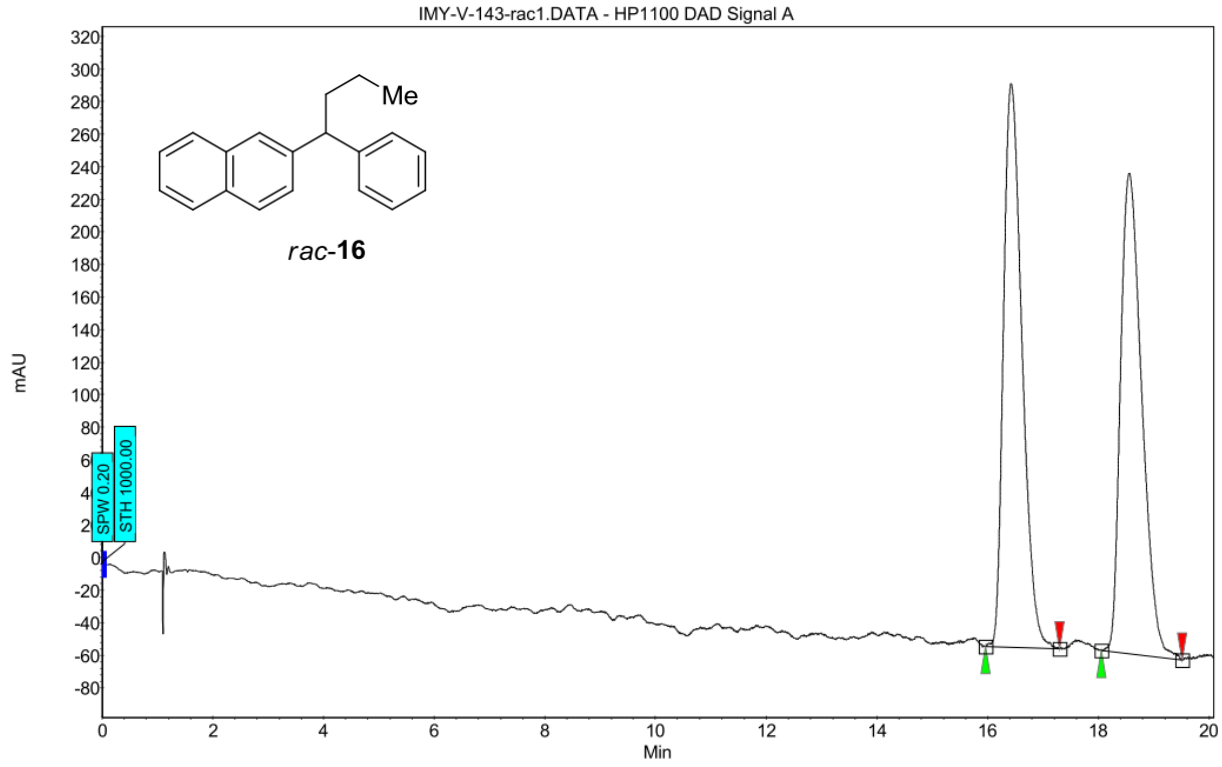


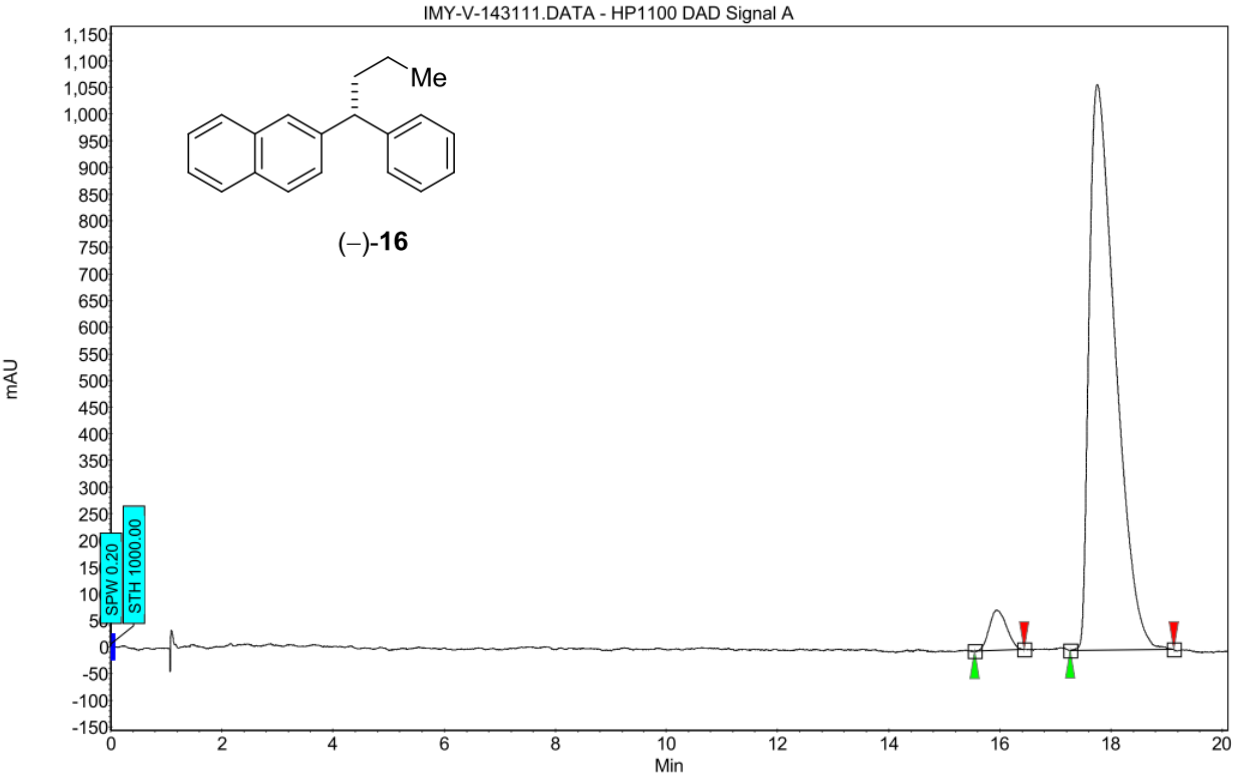
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.12	6.32	6.57	0.00	1.49	10.0	1.6	1.489
2	UNKNOWN	7.51	7.84	8.51	0.00	98.51	492.5	107.7	98.511
Total						100.00	502.5	109.3	100.000



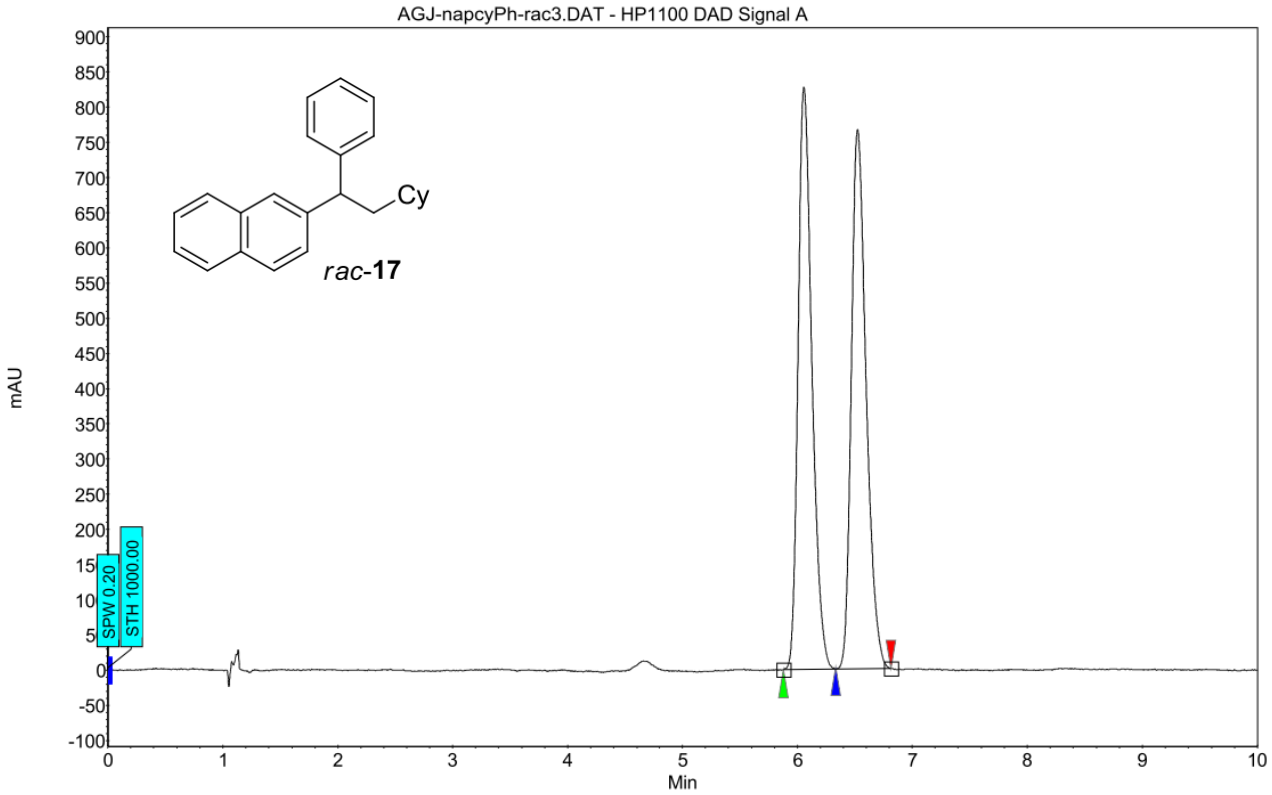


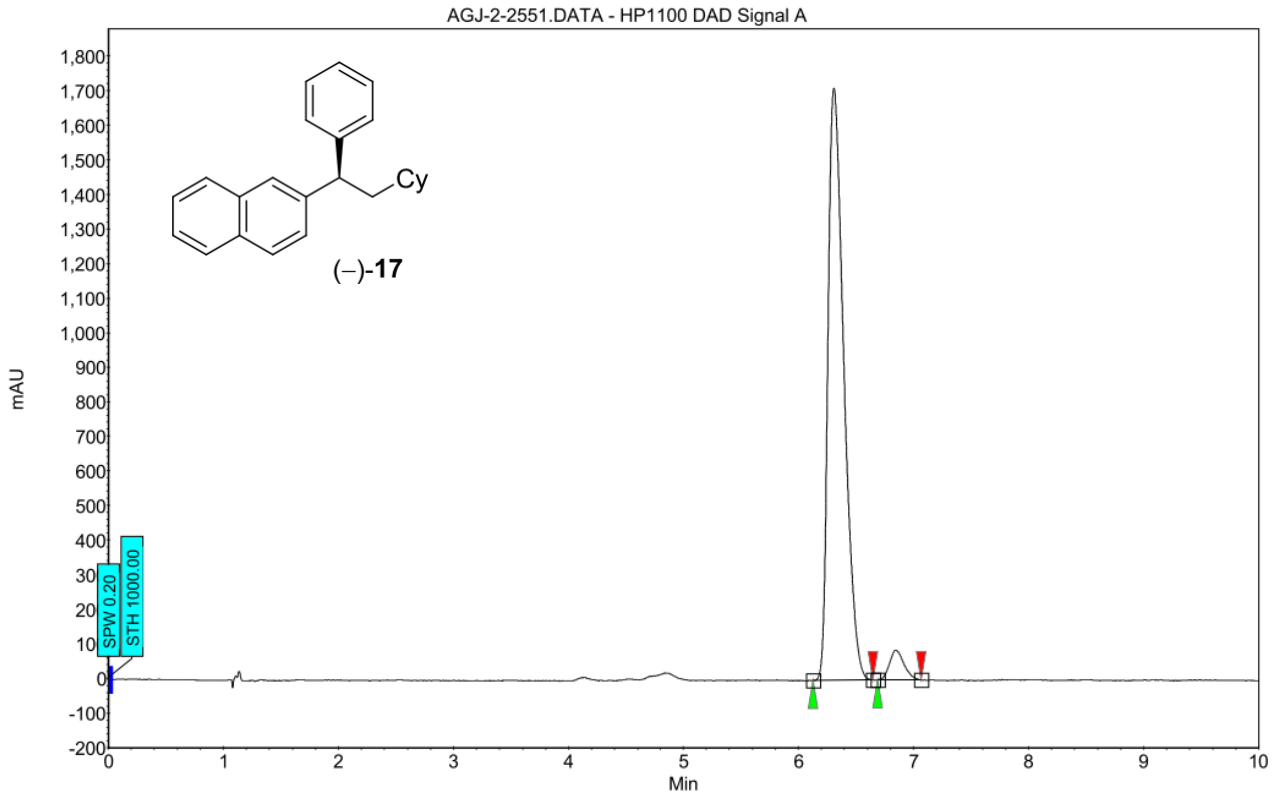
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	19.56	20.06	21.06	0.00	97.88	349.2	188.1	97.876
2	UNKNOWN	21.13	21.35	22.66	0.00	2.12	5.3	4.1	2.124
Total						100.00	354.5	192.2	100.000



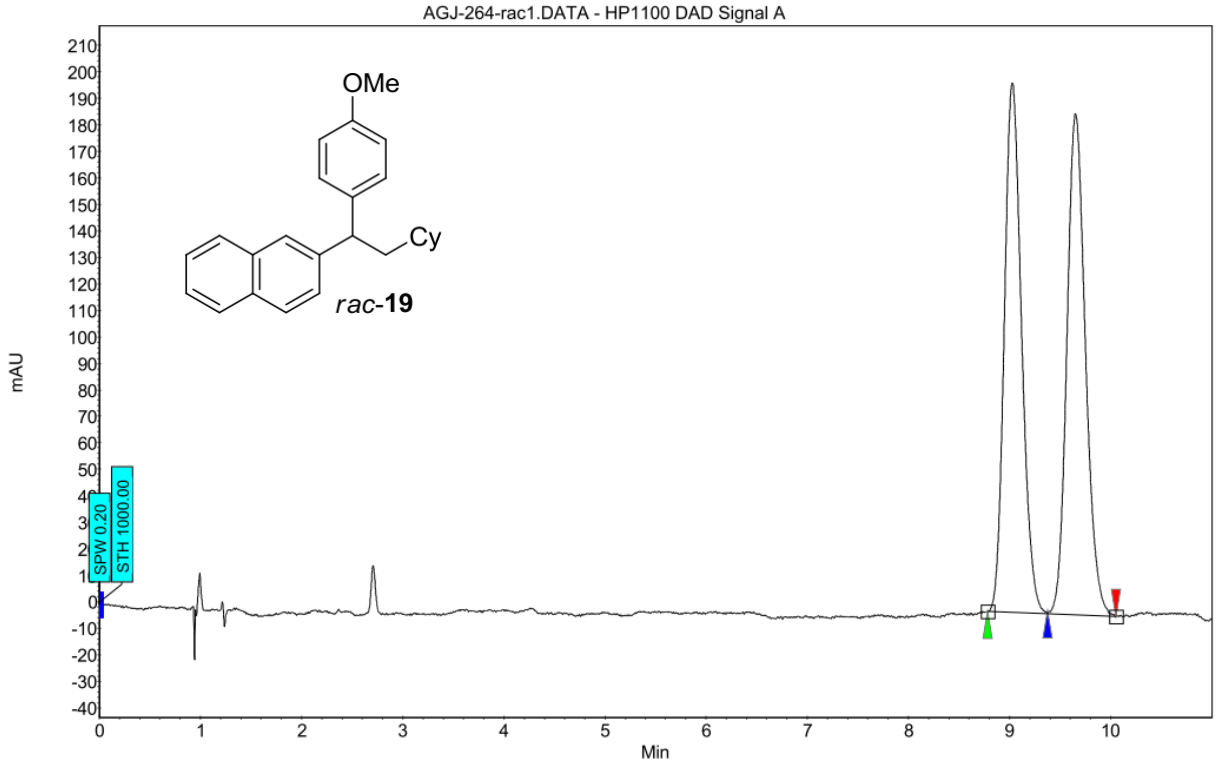


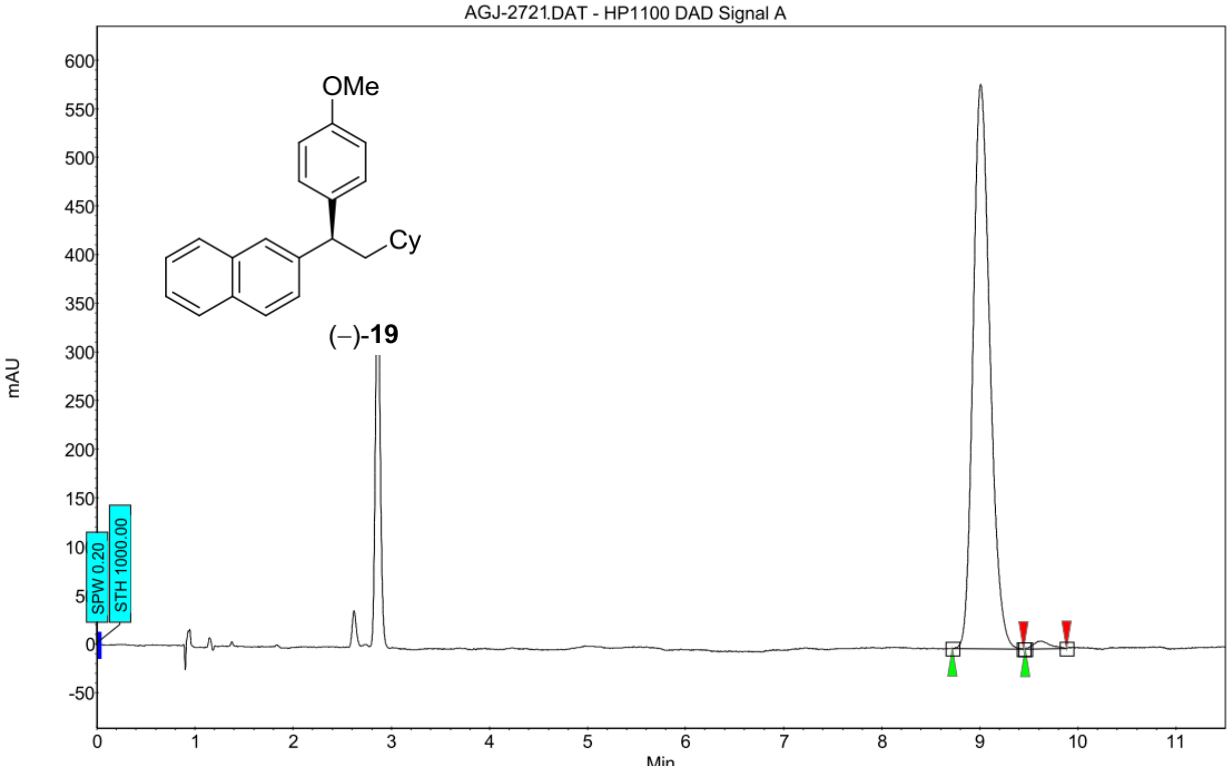
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	15.55	15.95	16.44	0.00	4.46	75.3	27.0	4.458
2	UNKNOWN	17.27	17.75	19.13	0.00	95.54	1061.4	578.6	95.542
Total						100.00	1136.7	605.5	100.000



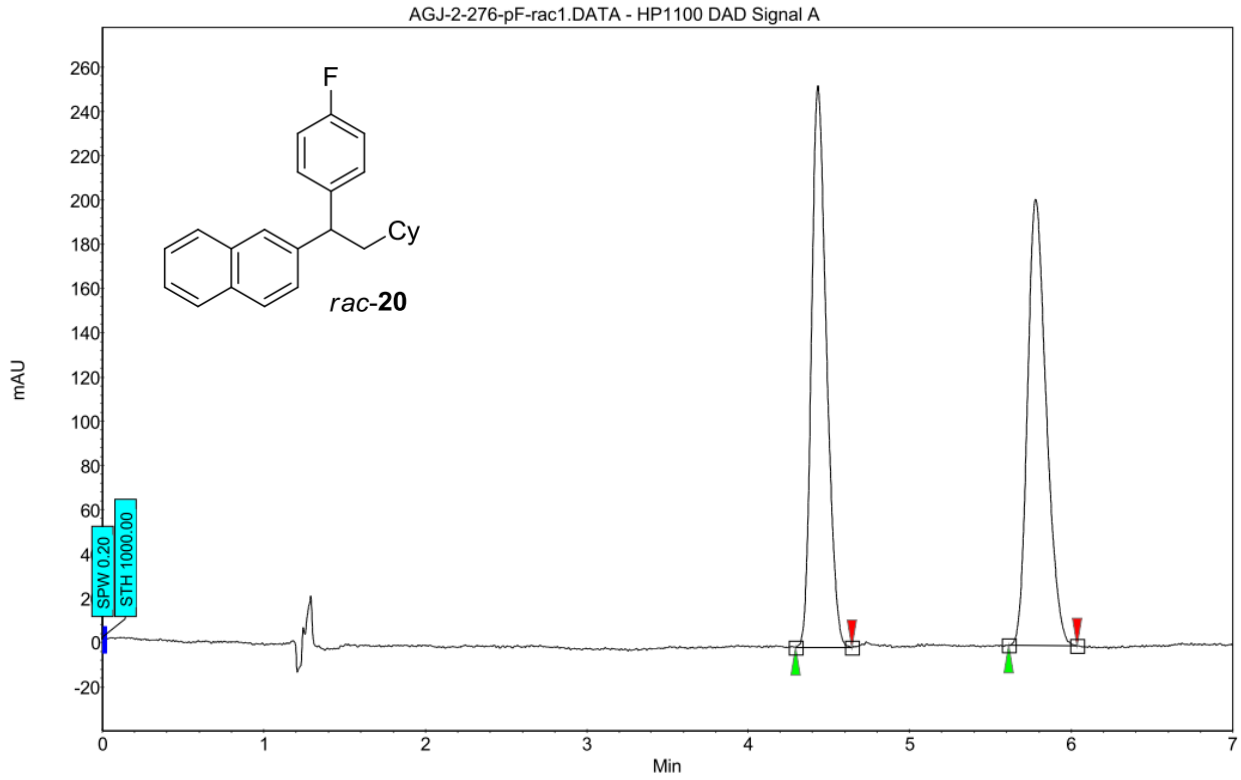


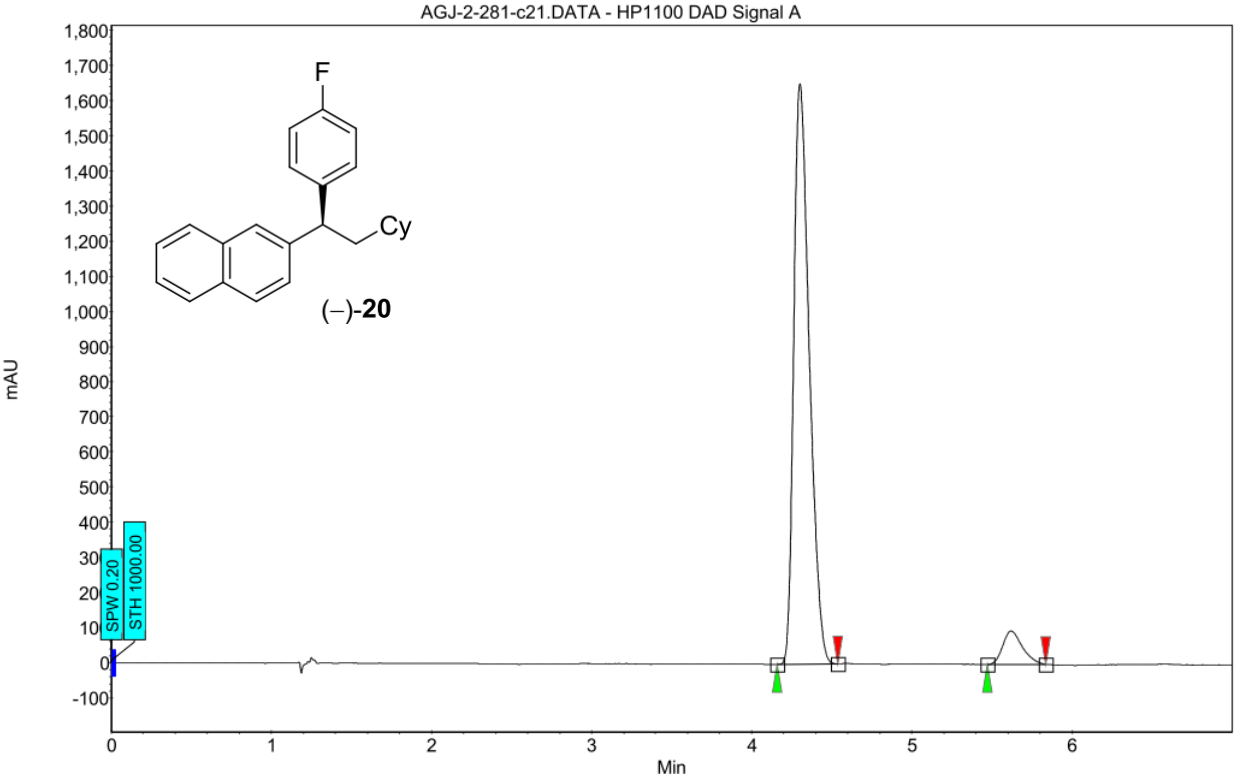
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.13	6.31	6.65	0.00	95.60	1711.1	272.1	95.596
2	UNKNOWN	6.69	6.85	7.07	0.00	4.40	85.5	12.5	4.404
Total						100.00	1796.6	284.6	100.000



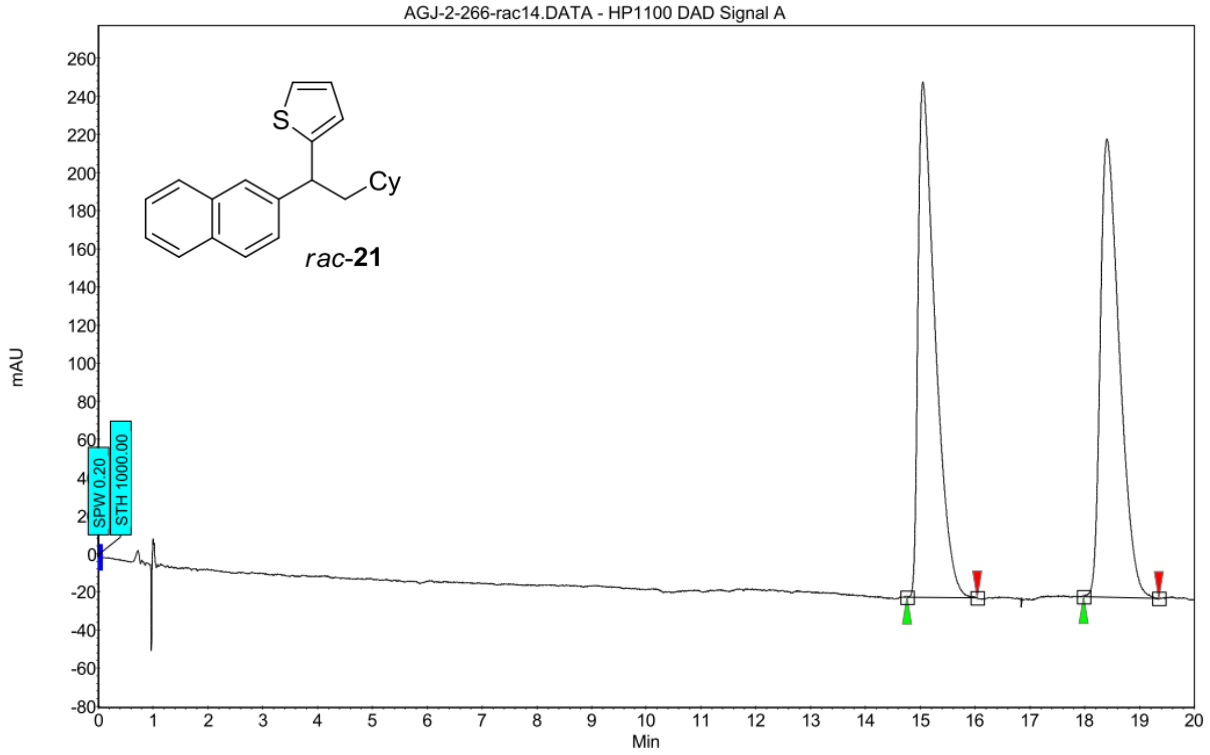


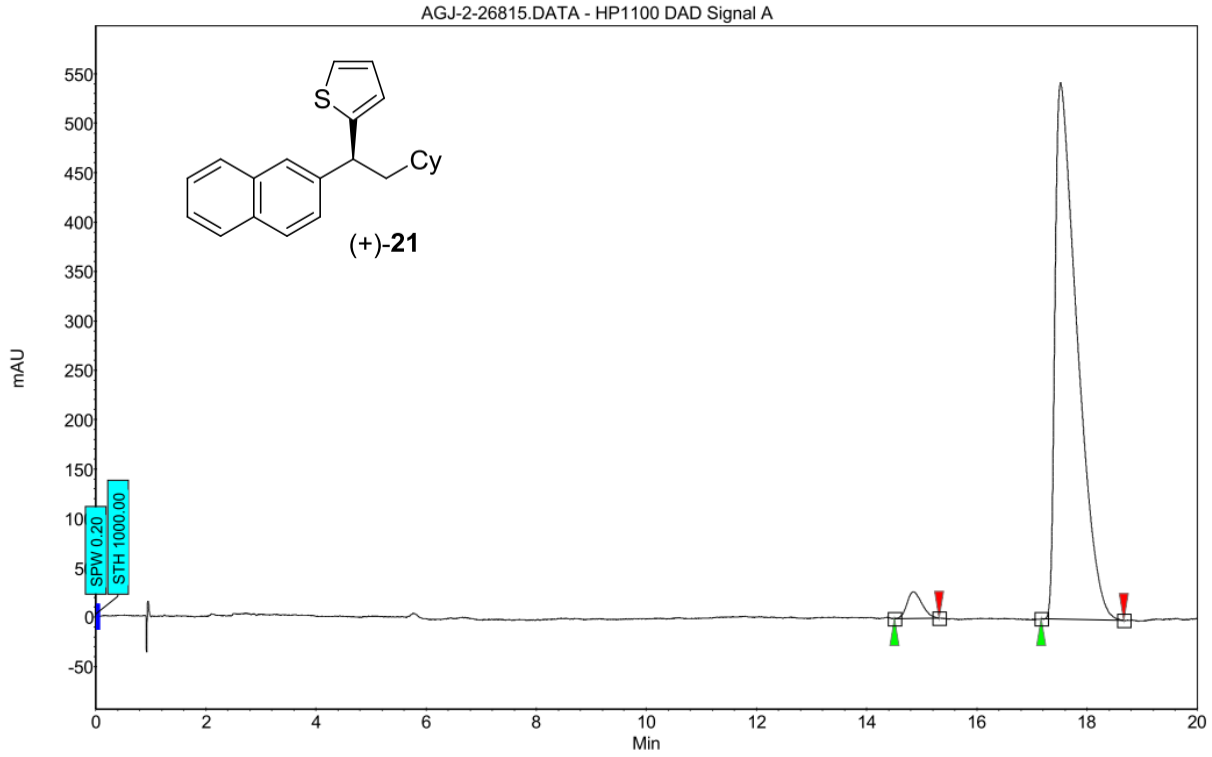
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	8.72	9.01	9.44	0.00	98.68	579.9	115.5	98.681
2	UNKNOWN	9.46	9.63	9.88	0.00	1.32	8.0	1.5	1.319
Total						100.00	587.9	117.0	100.000



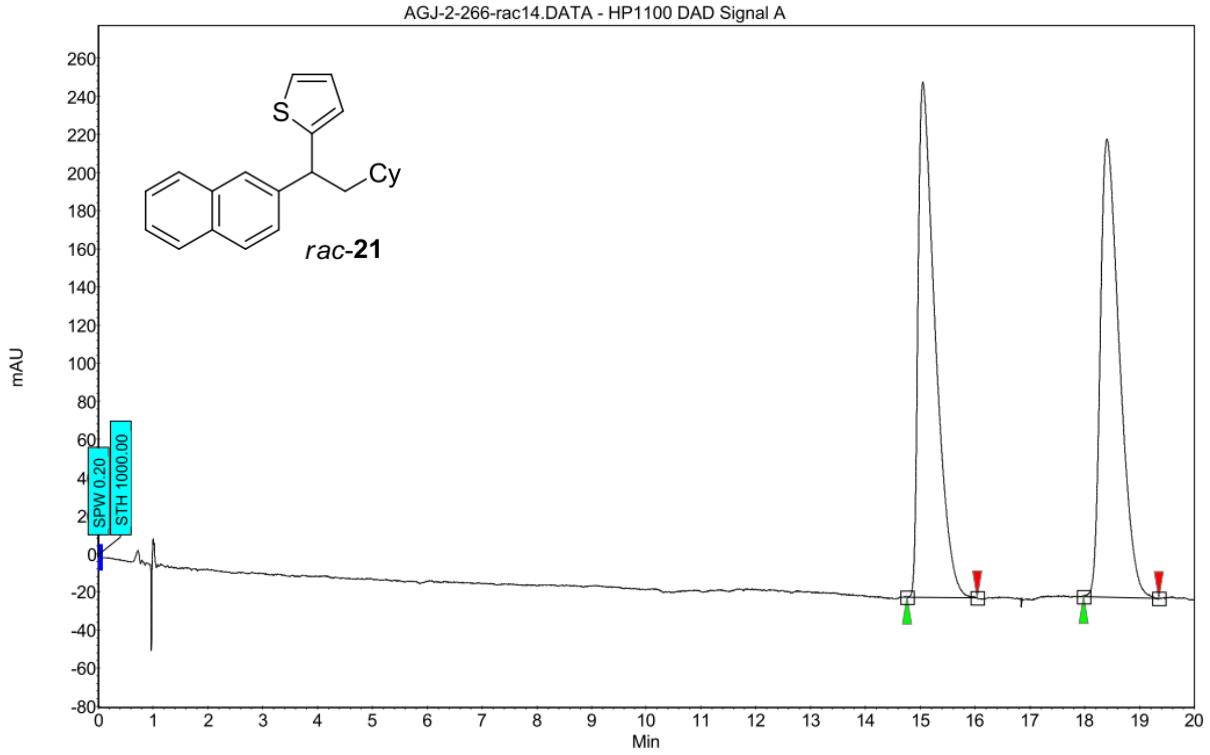


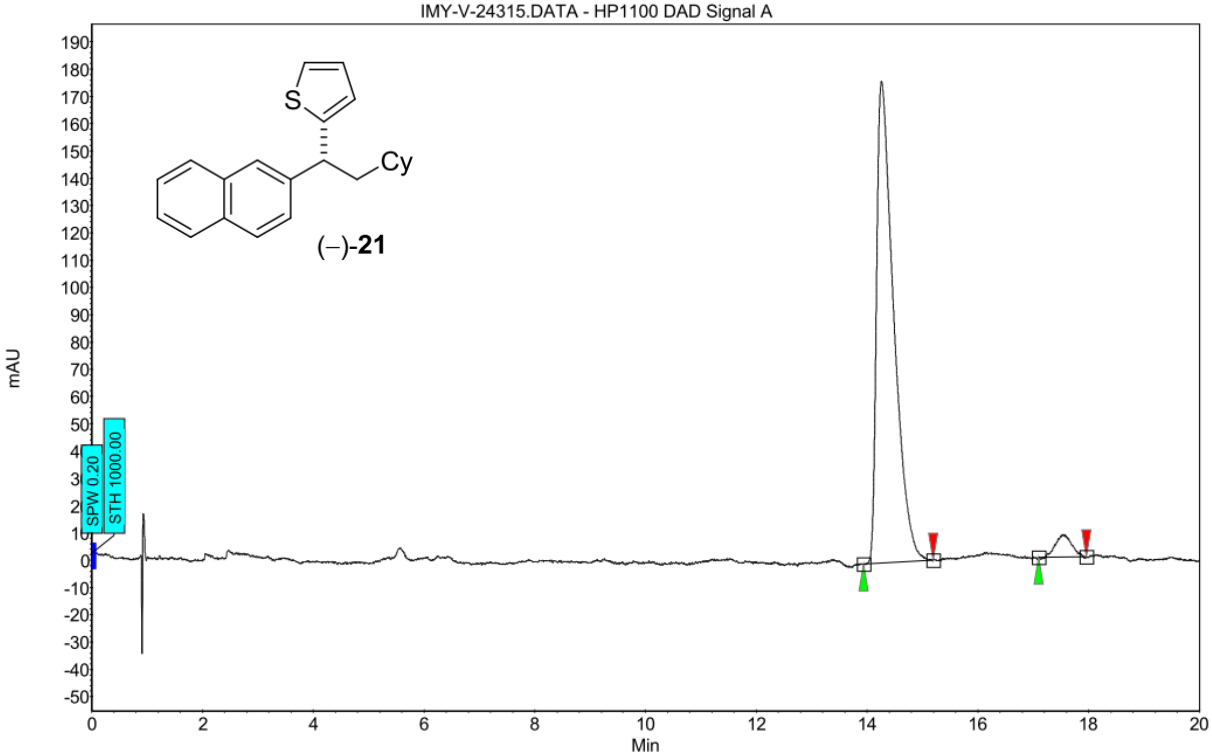
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	4.16	4.30	4.54	0.00	93.26	1651.3	185.9	93.264
2	UNKNOWN	5.47	5.62	5.84	0.00	6.74	94.7	13.4	6.736
Total						100.00	1746.0	199.4	100.000



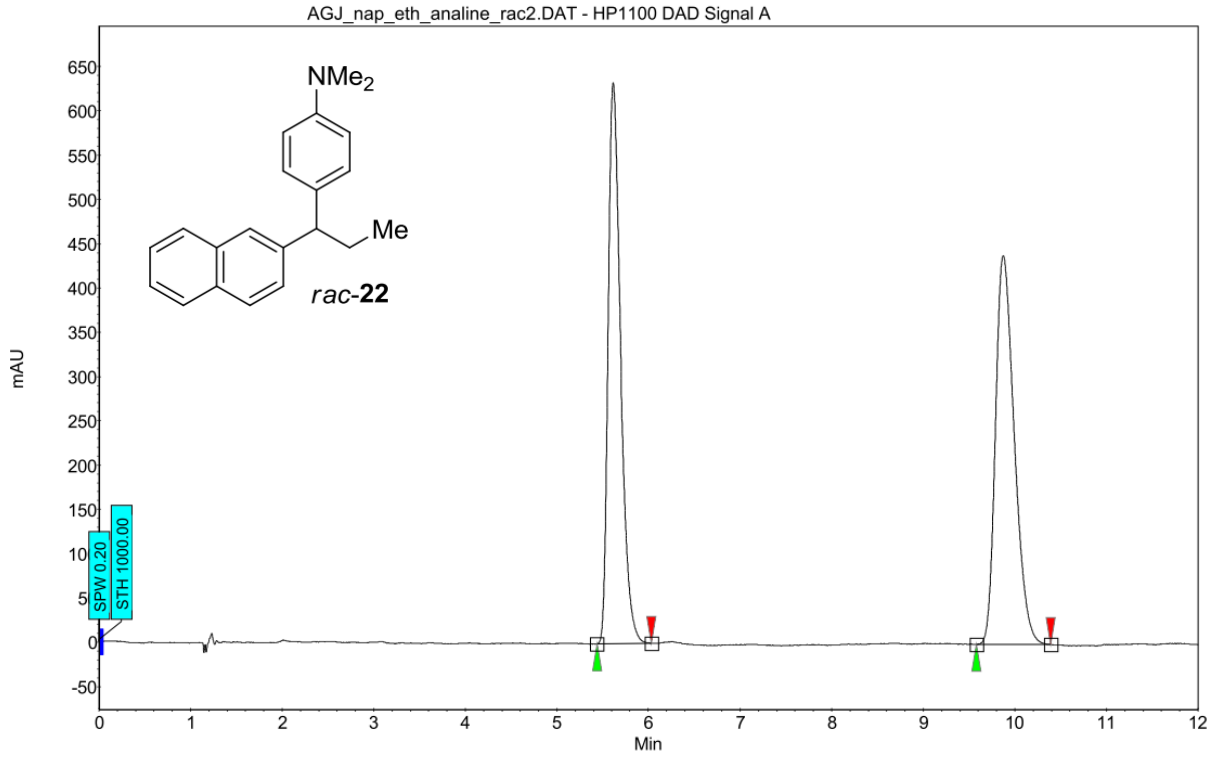


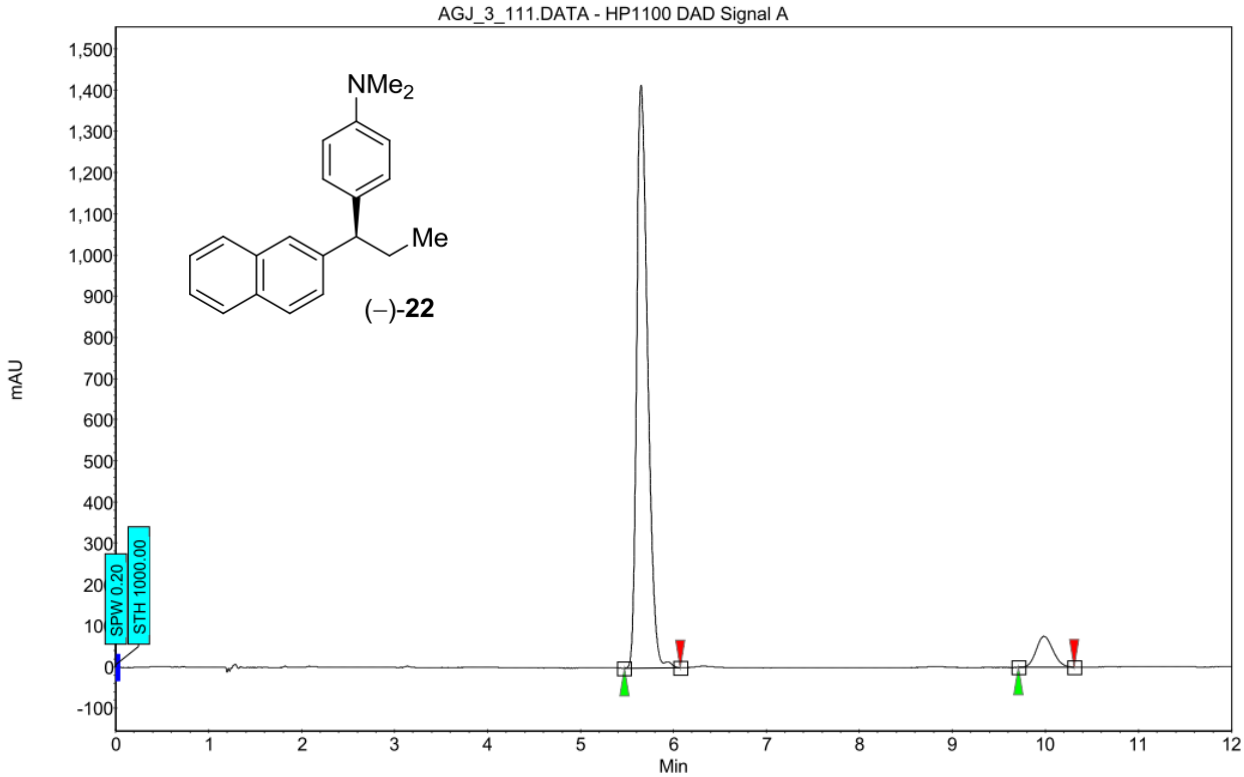
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	14.50	14.85	15.31	0.00	3.24	26.9	8.4	3.236
1	UNKNOWN	17.17	17.52	18.67	0.00	96.76	543.4	252.1	96.764
Total						100.00	570.3	260.5	100.000



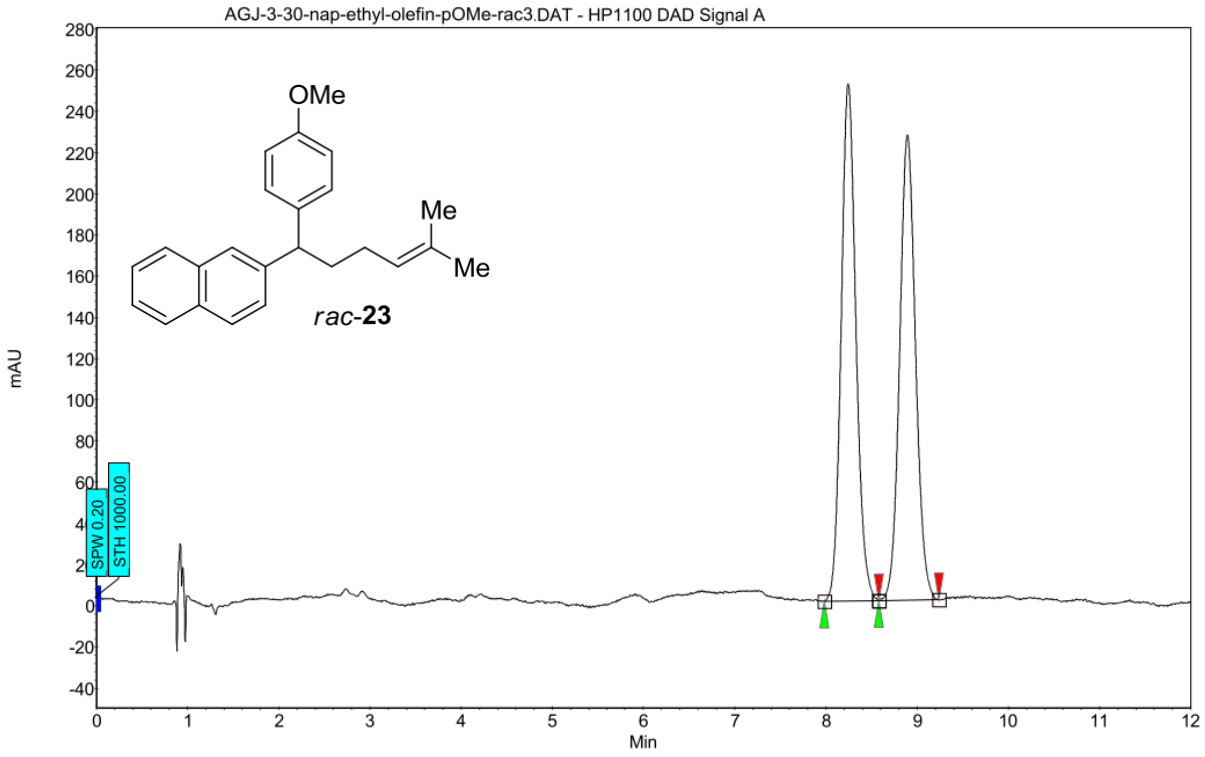


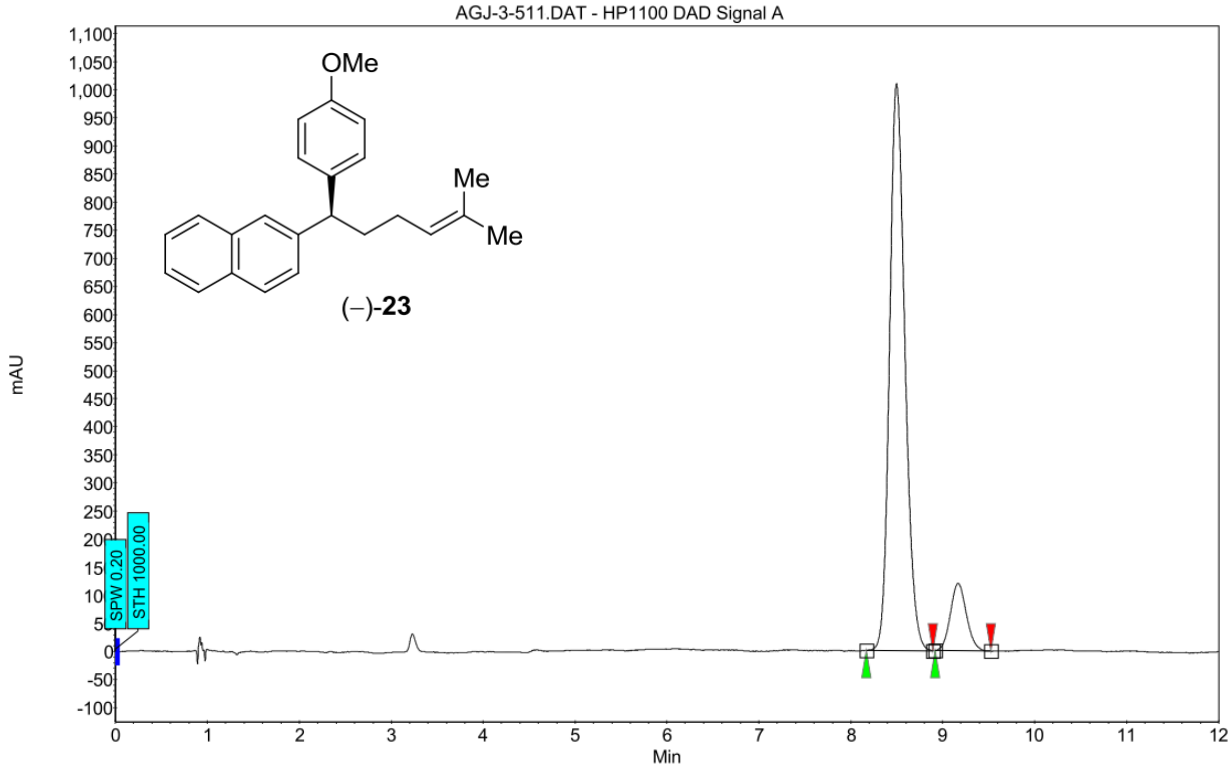
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	13.94	14.26	15.20	0.00	95.79	176.7	62.8	95.788
2	UNKNOWN	17.10	17.53	17.96	0.00	4.21	8.4	2.8	4.212
Total						100.00	185.2	65.6	100.000



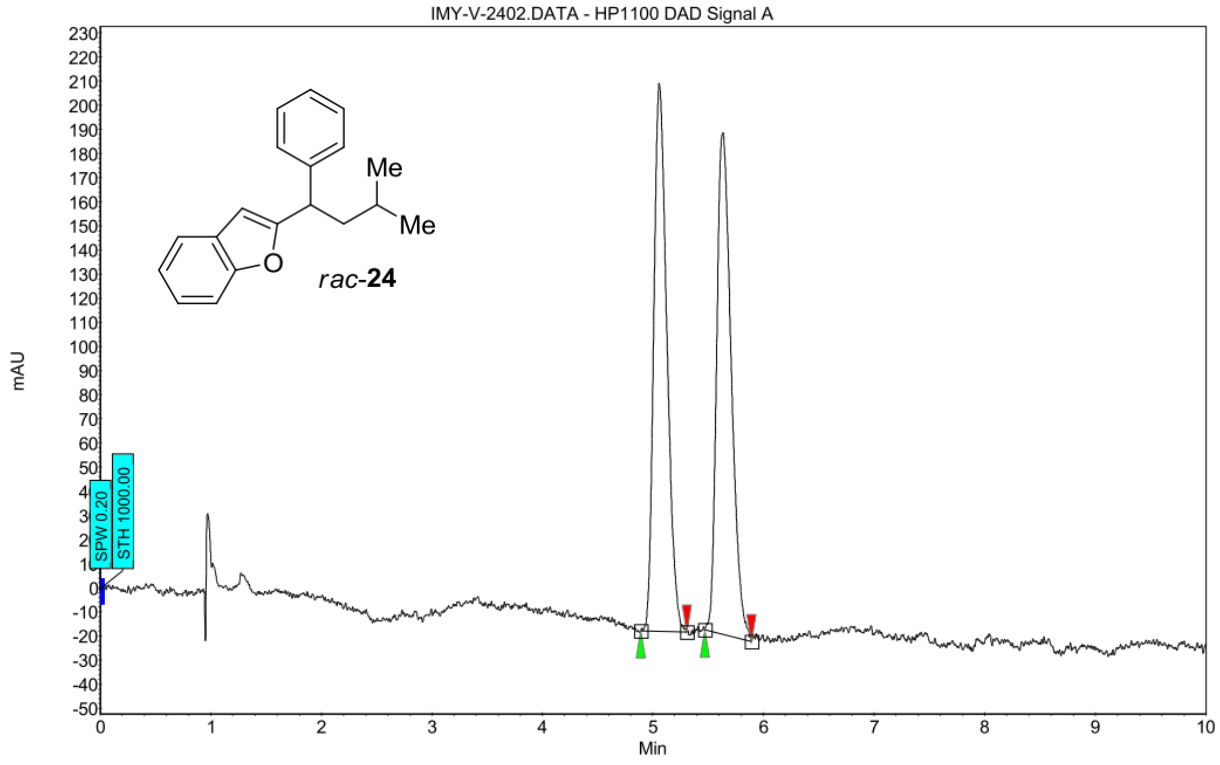


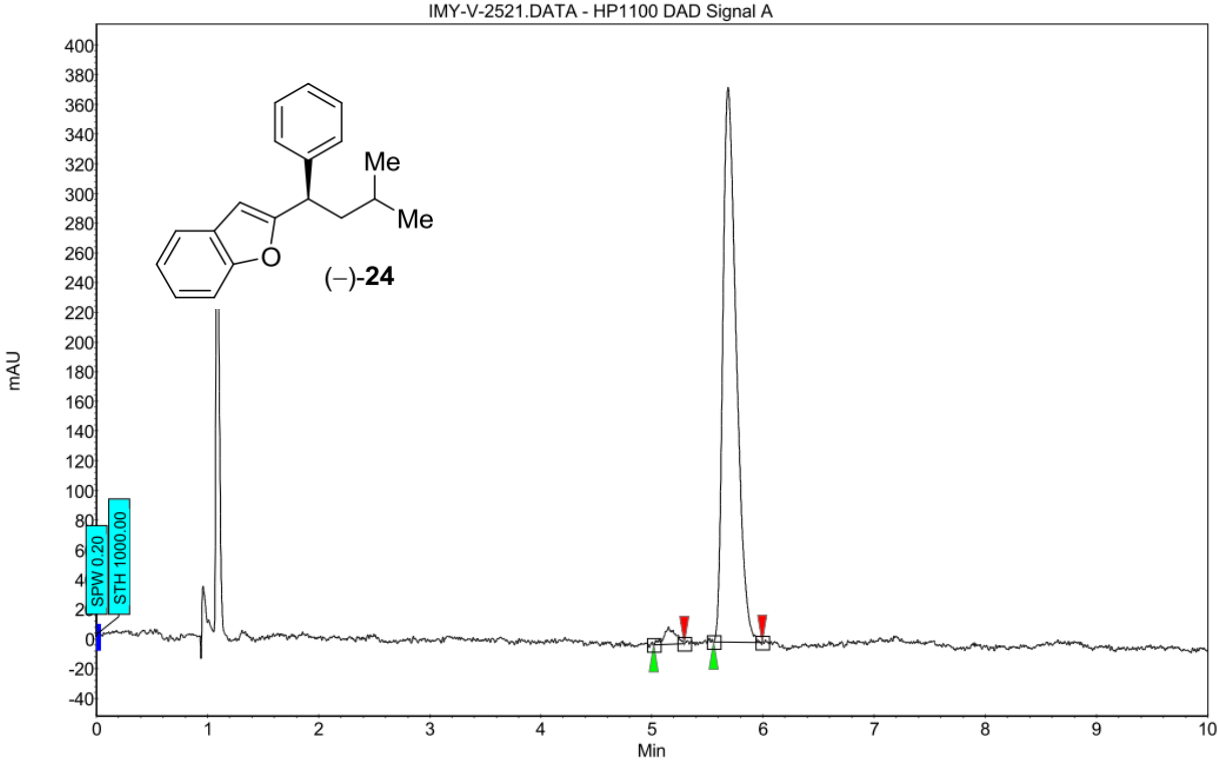
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	5.47	5.65	6.08	0.00	92.72	1414.5	200.0	92.717
2	UNKNOWN	9.71	9.98	10.31	0.00	7.28	75.1	15.7	7.283
Total						100.00	1489.6	215.7	100.000



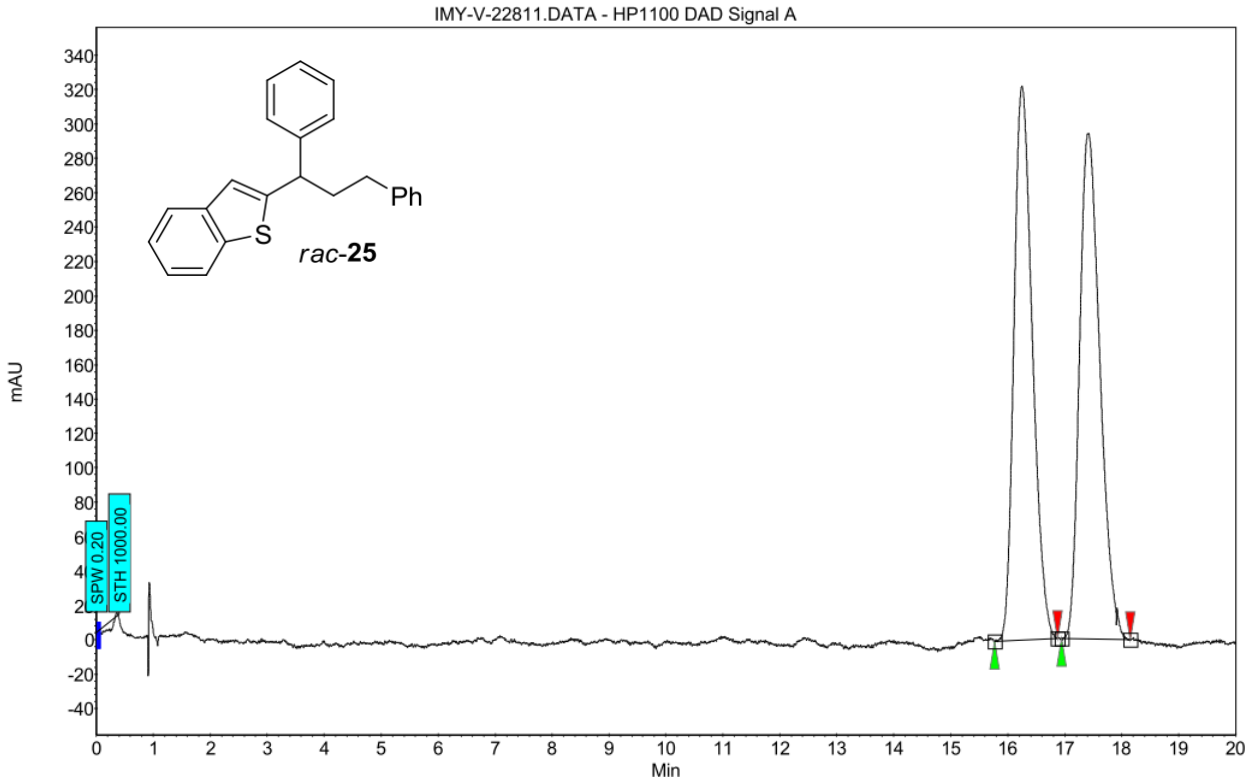


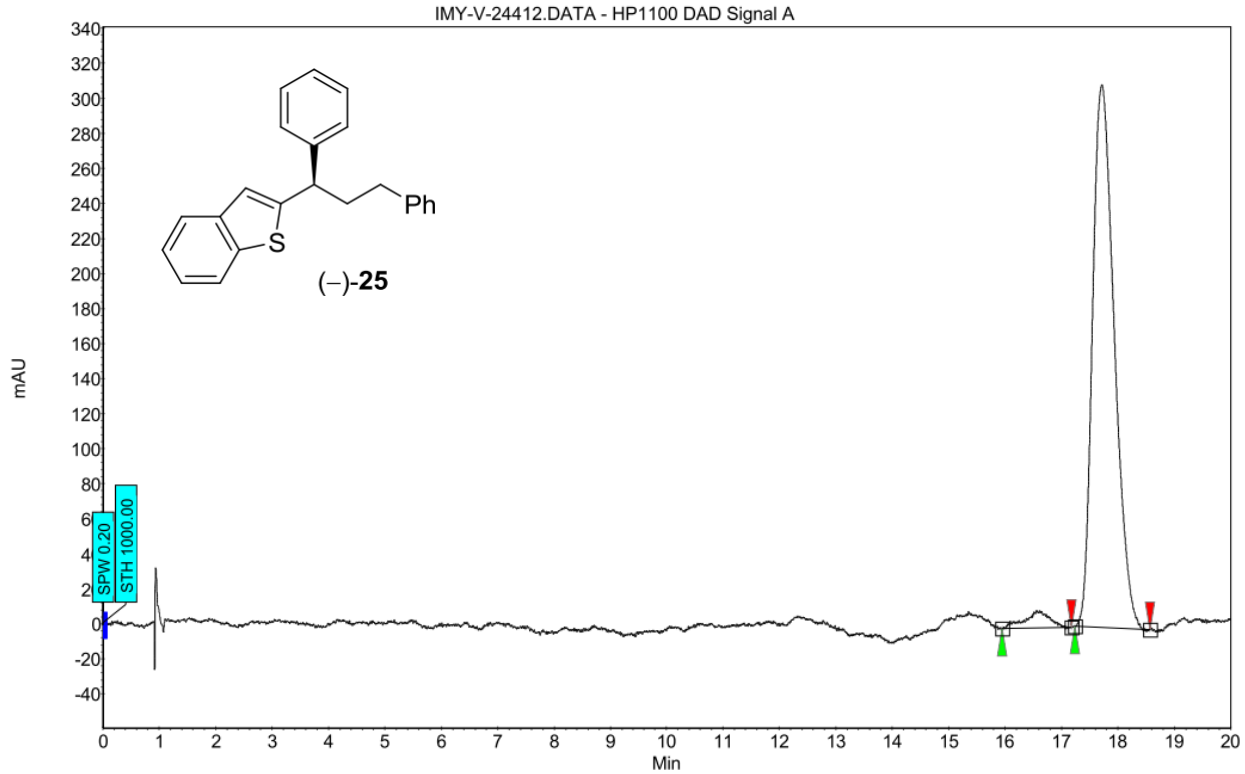
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	8.17	8.50	8.89	0.00	89.04	1009.3	195.4	89.036
2	UNKNOWN	8.91	9.17	9.52	0.00	10.96	119.6	24.1	10.964
Total						100.00	1128.9	219.5	100.000





Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	5.02	5.15	5.29	0.00	2.50	11.5	1.3	2.499
1	UNKNOWN	5.55	5.69	5.99	0.00	97.50	373.5	52.3	97.501
Total						100.00	385.0	53.6	100.000





Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	15.95	16.57	17.17	0.00	3.31	9.8	4.7	3.313
2	UNKNOWN	17.24	17.72	18.57	0.00	96.69	309.8	138.2	96.687
Total						100.00	319.6	142.9	100.000