SUPPORTING INFORMATION

STEREOSPECIFIC INTRAMOLECULAR REDUCTIVE CROSS-ELECTROPHILE COUPLING REACTIONS FOR CYCLOPROPANE SYNTHESIS

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I. GENERAL PROCEDURES

All reactions were carried out under a N_2 atmosphere, unless otherwise stated. All glassware was either oven dried or flame-dried prior to use. Toluene (PhMe), diethyl ether (Et_2O), dichloromethane (CH_2Cl_2), benzene (C_6H_6), and tetrahyrdofuran (THF) 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 °C for 12 hours) to remove H_2O. Other solvents were purchased "anhydrous" commercially, or were purified as described. ^{1}H NMR were recorded on Bruker DRX-400 (400 MHz ^{1}H, 100 MHz ^{13}C), GN-500 (500 MHz ^{1}H, 125.7 MHz ^{13}C), or CRYO-500 (500 MHz ^{1}H, 125.7 MHz ^{13}C) spectrometers. Proton chemical shifts are reported in ppm (δ) relative to internal trimethylsilane (TMS, δ 0.00). Data are reported as follows: chemical shift (multiplicity [singlet (s), broad singlet (br s), doublet (d), doublet of doublets (dd), doublet of doublet of doublets (ddd), triplet (t), doublet of triplets (dt), triplet of doublets (td), doublet of doublet of triplets (ddt), quartet (q), quintet (quint), quintet of triplets (quintt), quintet of doublets (quintd), sextet (sext), septet (sept), multiplet (m), apparent doublet (ad), apparent triplet (at), apparent quartet (aq), apparent quintet (aquint)], coupling constants [Hz], integration). Carbon chemical shifts are reported in ppm (δ) relative to TMS with the solvent resonance as the internal standard ($CDCl_3$, δ 77.16 ppm). NMR data were collected at 25 °C. Infrared spectra were obtained on a Thermo Scientific Nicolet iS5 spectrometer with an iD5 ATR tip (neat) and are reported in terms of frequency of absorption (cm^{-1}). Analytical thin-layer chromatography (TLC) was performed using Silica Gel 60Å F254 precoated plates (0.25 mm thickness). Visualization was accomplished by irradiation with a UV lamp and/or staining with *p*-anisaldehyde (PAA), cerium ammonium molybdate (CAM), or potassium permanganate ($KMnO_4$) solutions. Flash chromatography was performed using Silica Gel 60 (170-400 mesh) from Fisher Scientific. Melting points (m.p.) were obtained using a Mel-Temp melting point apparatus and are uncorrected. Optical rotations were measured with a Rudolph Research Analytical Autopol III Automatic Polarimeter. SFC determinations of enantiopurity were performed on a Berger Analytical instrument using a Daicel™ Chiralpak® column (OD-H; 100 bar, 215 nm, 50 °C). High resolution mass spectrometry was performed by the University of California, Irvine Mass Spectrometry Center.

Bis(1,5-cyclooctadiene)nickel was purchased from Strem, stored in a glove box freezer (–20 °C) under an atmosphere of N_2 and used as received. Zinc (II) chloride was purchased from Strem and stored under an atmosphere of N_2. All ligands were purchased from Strem or Sigma Aldrich and were stored under N_2 atmosphere and used as received. The methyl Grignard reagent was titrated with iodine prior to use.[1] All other chemicals were purchased commercially and used as received, unless otherwise noted.

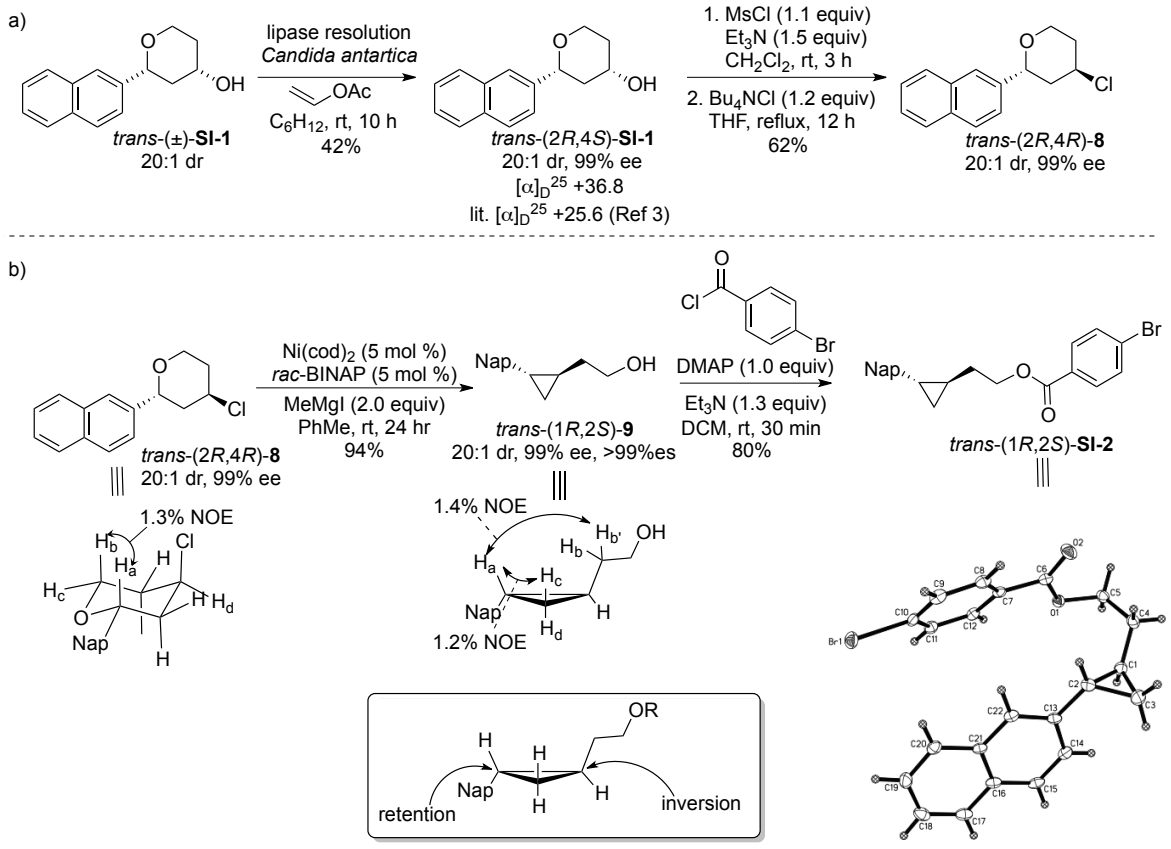
II. EXPERIMENTAL

A. STEREOCHEMICAL PROOFS

Absolute configuration. To determine the stereochemical outcome of the reductive cross-coupling reaction, the absolute configuration of the starting material and product were assigned for two examples. In both examples, the reaction proceeds with retention of stereochemistry at the benzylic carbon and with inversion of stereochemistry at the alkylic chloride. The full experimental details of the synthesis of the starting material, reductive cross-electrophile coupling reaction, and derivatization of the product, including full characterization for all compounds, can be found in the following sections of this document.

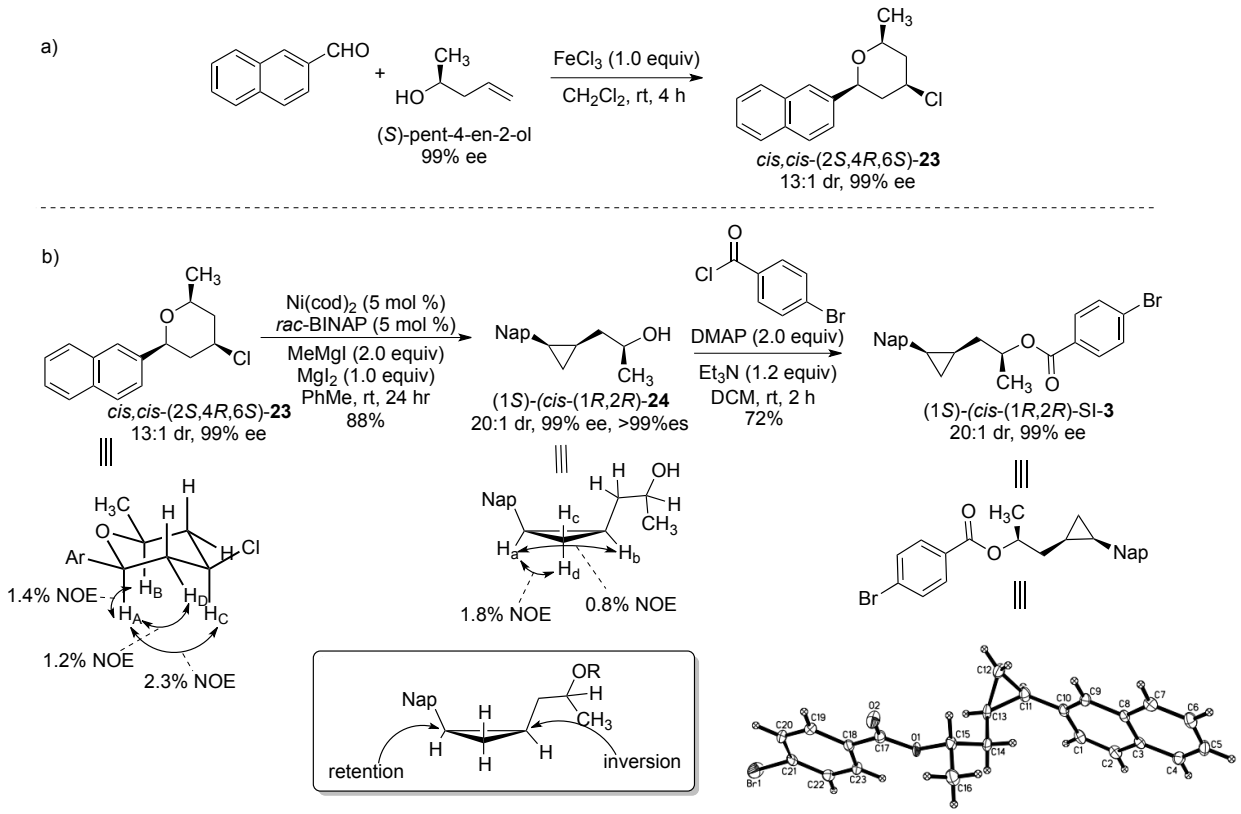
Example 1. The absolute configurations of *trans*-**8** and *trans*-**9** were assigned. The absolute configuration of tetrahydropyran *trans*-**8** was assigned as 2*R*,4*R* by comparison of optical rotations of **SI-1** to the literature from a lipase resolution (Scheme SI 1a).[2,3] The absolute configuration of cyclopropane *trans*-**9** was assigned as 1*R*,2*S* by derivatization to **SI-2** and single crystal X-ray crystallographic analysis (Scheme SI 1b). These absolute configurations are consistent with retention at the benzylic center and inversion of stereochemistry at the alkyl chloride.

Scheme SI 1: Determination of Absolute Configuration of the Reductive Cross-Coupling Reaction of *trans*-8



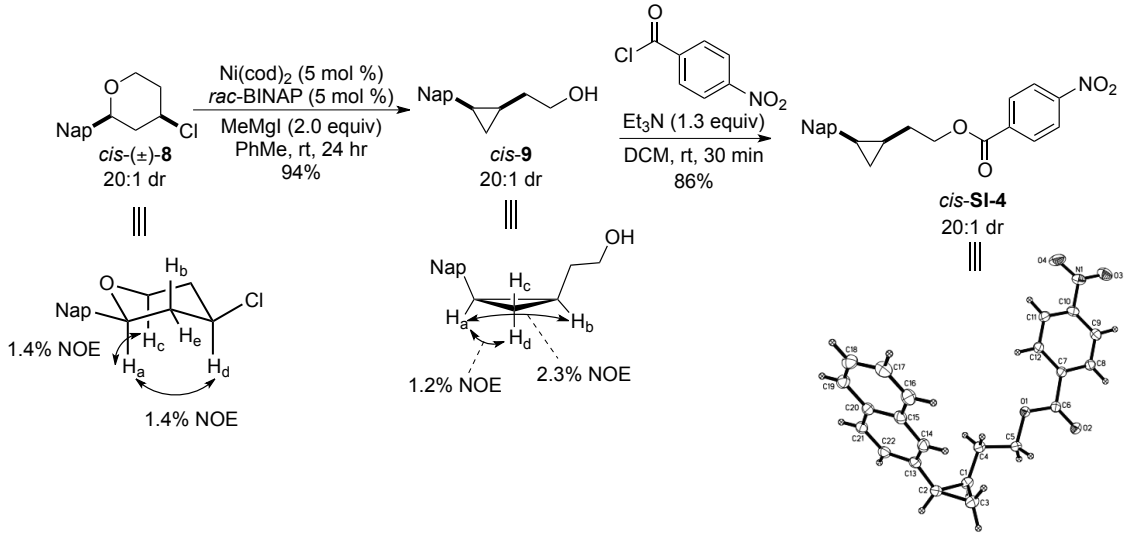
Example 2. To determine the stereochemical outcome of the reductive cross-coupling reaction of *cis*,*cis*-**23** to afford *cis*-**24**, the absolute configurations of the starting material and product were assigned. Tetrahydropyran *cis*,*cis*-**23** was prepared from commercial (*S*)-pent-4-en-2-ol and was therefore assigned as 2*S*,4*R*,6*S* (Scheme SI 2a). The absolute configuration of cyclopropane *cis*-**24** was assigned by derivatization to **SI-3** and single crystal X-ray crystallographic analysis (Scheme SI 2b). These absolute configurations are consistent with retention at the benzylic center and inversion of stereochemistry at the alkyl chloride.

Scheme SI 2: Determination of Absolute Configuration of the Reductive Cross-Coupling Reaction of *cis,cis*-23



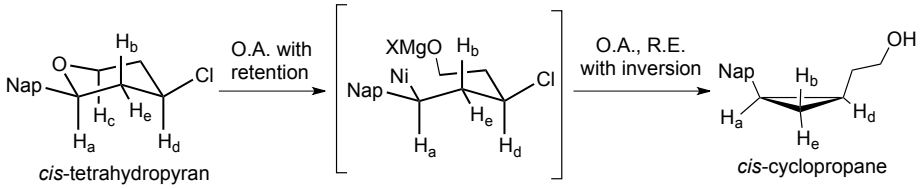
Relative configuration. The relative configuration of tetrahydropyran *cis*-**8** and cyclopropane *cis*-**9** were assigned by NOE experiments. The assignment of *cis*-**9** was confirmed by derivitization to *cis*-**SI-4** and single crystal X-ray crystallographic analysis (Scheme SI 3). For all other reductive coupling reactions, relative configurations were assigned by NOE analysis of starting materials and products (Table SI 1). In all cases, *cis*-tetrahydropyrans afford only *cis*-cyclopropanes and *trans*-tetrahydropyrans afford only *trans*-cyclopropanes. By analogy with the preceding examples, these results are consistent with retention at the benzylic center and inversion at the alkyl chloride.

Scheme SI 3: Stereochemical Course of the Reductive Cross-Coupling Reaction



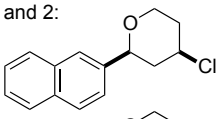
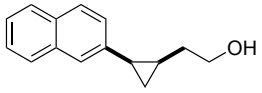
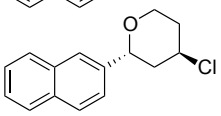
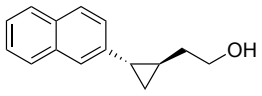
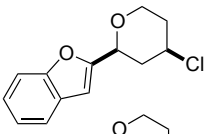
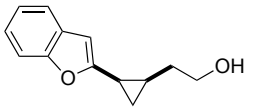
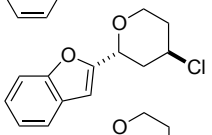
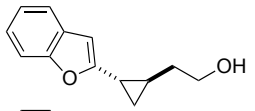
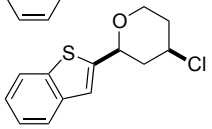
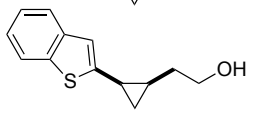
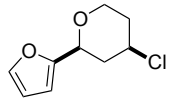
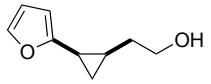
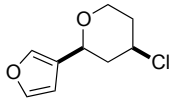
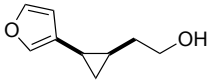
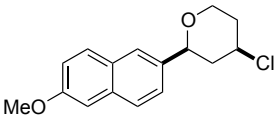
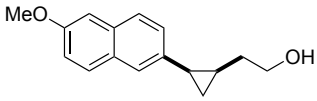
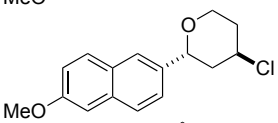
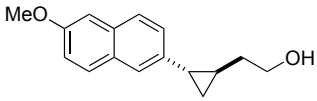
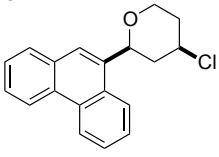
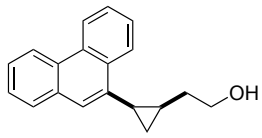
Based on the observation that *cis*-tetrahydropyrans afford only *cis*-cyclopropanes and *trans*-tetrahydropyrans afford only *trans*-cyclopropanes, we propose a model that accounts for this stereospecific outcome (Scheme SI 4). This is purely a simplified working model, and additional mechanistic experiments will be required to determine the order of events and mechanisms of oxidative addition.

Scheme SI 4: Proposed Working Model for Stereospecificity



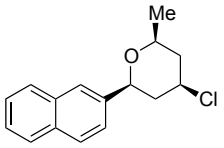
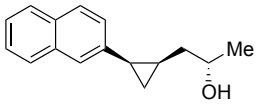
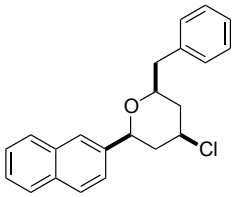
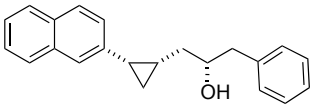
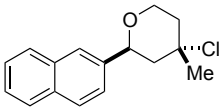
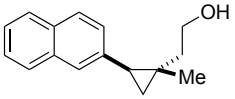
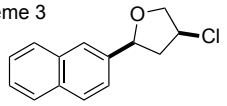
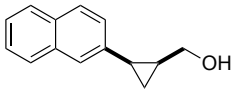
The relative configurations of all other starting materials and reductive cross-coupling products were assigned based on NOE or X-ray crystallographic data. These stereochemical assignments are summarized in Table SI 1. Table SI 1 also summarizes how the configuration of each compound was assigned. We assume that the reactions proceed with retention of stereochemistry at the benzylic position and inversion of stereochemistry at the alkylic chloride.

Table SI 1. Configuration of Starting Material and Products

Tetrahydropyran		Configuration[a] Assigned by:	Product		Configuration[a] Assigned by:
Tables 1 and 2: 	**8**	*cis* NOE		**9**	*cis* NOE X-Ray of derivative
	**8**	*trans* 2*R*,4*R* (–) lit $[\alpha]_D$ of precursor		**9**	*trans* 1*R*,2*S* (+) X-Ray of derivative
Table 3 	**11**	*cis* NOE		**12**	*cis* NOE
	**11**	*trans* NOE		**12**	*trans* NOE
	**13**	*cis* NOE		**14**	*cis* NOE
	**15**	*cis* NOE		**16**	*cis* NOE of derivative
	**17**	*cis* NOE		**18**	*cis* NOE
	**19**	*cis* NOE		**20**	*cis* NOE
	**19**	*trans* NOE		**20**	*cis* NOE
	**21**	*cis* NOE		**22**	*cis* NOE

[a]For NOE values see the characterization data for each compound. For optical rotation values see the characterization data for the compound.

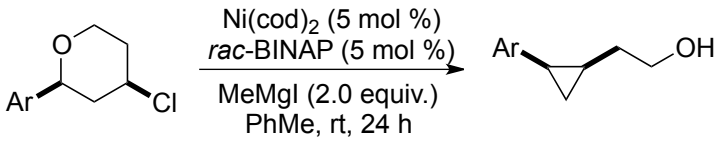
Table SI 1. Continued

Tetrahydropyran		Configuration[a] Assigned by:	Product		Configuration[a] Assigned by:
Table 4 	**23**	*cis,cis* NOE *2S,4R,6S* (–) Prepared from commercial *S* homoallylic alcohol		**24**	*cis* NOE *1S*-(*cis*-(1*R*,2*R*)) (+) X-Ray of derivative
	**25**	*cis,cis* NOE		**26**	*cis* NOE
	**27**	*trans* NOE		**28**	*trans* NOE
Scheme 3 	**29**	*cis* NOE		**30**	*cis* NOE

[a]For NOE values see the characterization data for each compound. For optical rotation values see the characterization data for the compound.

B. General Reductive Coupling Procedures

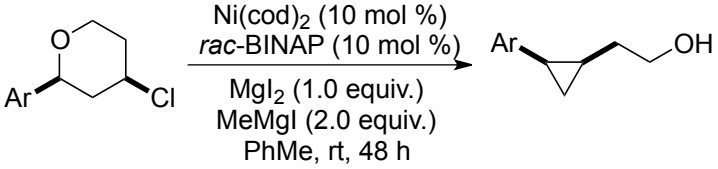
Method A: Reductive Couplings with Methyl Grignard



(1)

In a glovebox, a flame-dried 7 mL vial equipped with a stir bar was charged with substrate (1.0 equiv.), $Ni(cod)_2$ (0.05 equiv.), *rac*-BINAP (0.05 equiv.), and PhMe (1 M in substrate). MeMgI (2.0 equiv.) was then added dropwise over a minute. After 24 h the reaction was removed from the glovebox, quenched with isopropyl alcohol, filtered through a plug of silica gel (neat Et_2O), and concentrated in vacuo. Phenyltrimethylsilane (PhTMS) was added as internal standard and a ^1H NMR yield was obtained before purification by flash column chromatography.

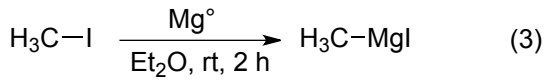
Method B: Reductive Couplings with Methyl Grignard and MgI_2



(2)

In a glovebox, a flame-dried 7 mL vial equipped with a stir bar was charged with substrate (1.0 equiv.), $Ni(cod)_2$ (0.10 equiv.), *rac*-BINAP (0.10 equiv.), MgI_2 (1.0 equiv.), and PhMe (1 M). MeMgI (2.0 equiv.) was then added dropwise. After 48 h the reaction was removed from the glovebox, quenched with isopropyl alcohol, filtered through a plug of silica gel (neat Et_2O), and concentrated in vacuo. Phenyltrimethylsilane (PhTMS) was added as internal standard and a ^1H NMR yield was obtained before purification by flash column chromatography.

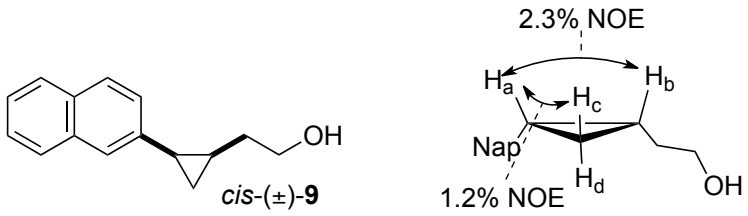
1) Preparation of Methyl Grignard Reagent



(3)

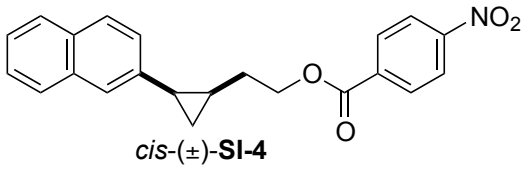
Under a N_2 atmsophere, a 3-necked flask equipped with a stir bar, reflux condenser, and Schlenk filtration apparatus was charged with magnesium turnings (1.1 g, 45 mmol). The flask and magnesium turnings were then flame-dried under vacuum and the flask was back-filled with N_2. Anhydrous Et_2O (7 mL) and a crystal of iodine (ca. 2 mg) were added to the flask. Freshly distilled iodomethane (1.9 mL, 31 mmol) was slowly added over 30 min to maintain a gentle reflux. The mixture was stirred for 2 h at room temperature then filtered through the fritted Schlenk filter into the Schlenk bomb under N_2 atmosphere. The magnesium turnings were washed with Et_2O (2 x 1.0 mL) then the Schlenk bomb was sealed, removed, and placed under an argon atmosphere. The resulting methyl Grignard reagent was typically between 2.4 and 3.0 M as titrated by Knochel's method1 and could be stored (sealed under argon atmosphere or in a glovebox) for up to 4 weeks.

C. CHARACTERIZATION DATA FOR TABLE 2 PRODUCTS



cis-(±)-**9**

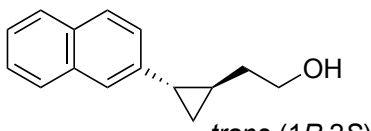
2-(*cis*-(±)-2-(Naphthalen-2-yl)cyclopropyl)ethan-1-ol (*cis*-9) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.8 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (6.9 mg, 0.011 mmol, 0.055 equiv.), substrate *cis*-**8** (49 mg, 0.20 mmol, 1.0 equiv., >20:1 cis:trans dr), PhMe (1.8 mL), and methylmagnesium iodide (0.16 mL, 0.42 mmol, 2.6 M in Et_2O, 2.1 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as a pale tan oil (40 mg, 0.19 mmol, 94%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.80–7.73 (m, 3H), 7.56 (s, 1H), 7.46–7.36 (m, 3H), 3.57–3.52 (m, 2H), 2.30 (aq, *J* = 8.3, 1H), 1.43–1.38 (m, 1H), 1.27–1.19 (m, 3H), 1.12–1.07 (m, 1H), 0.90–0.86 (m, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 136.9, 133.5, 132.2, 128.3, 127.7, 127.60, 127.57, 126.8, 126.1, 125.3, 63.0, 31.8, 20.9, 16.0, 9.4; **IR** (neat) 3328, 3052, 2999, 2928, 1721, 1631, 1600, 1505 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{15}H_{16}ONa$ $(M + Na)^+$ 235.1099, found 235.1098.



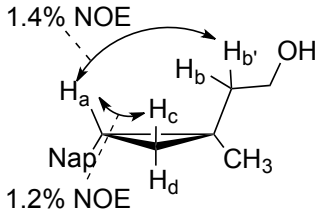
cis-(±)-**SI-4**

2-(*cis*-(±)-(2-Naphthyl)cyclopropyl)ethyl-4-nitrobenzoate (*cis*-SI-4) To a flame dried 250 mL round bottom flask equipped with a stir bar was added substrate *cis*-**9** (330 mg, 1.6 mmol, 1.0 equiv.) and anhydrous CH_2Cl_2 (60 mL). The flask was capped with a rubber septum, evacuated, and backfilled with N_2. Anhydrous NEt_3 (0.30 mL, 2.2 mmol, 1.3 equiv.) was added via syringe and the mixture was set to stir in an ice bath. To a separate 50 mL flame dried round bottom flask equipped with a stir bar was added 4-nitrobenzoyl chloride (330 mg, 1.8 mmol, 1.1 equiv.) and anhydrous CH_2Cl_2 (15 mL). The flask was set to stir until complete dissolution. The solution was slowly added to the reaction mixture over 5 min, then the reaction flask was allowed to warm to ambient temperature. After stirring at ambient temperature for 45 min, the reaction mixture was concentrated in vacuo, and H_2O (50 mL) was added. The solution was extracted with EtOAc (3 x 40 mL) and the combined organic extracts were washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. The product was purified by flash column chromatography (20% EtOAc in hexanes) to afford compound **SI-4** as a yellow solid (480 mg, 1.3 mmol, 86%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 81–84 °C, **TLC R_f** = 0.6 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 8.5, 2H), 8.09 (d, *J* = 8.5, 2H), 7.80 (d, *J* = 7.9, 1H), 7.75 (d, *J* = 8.4, 2H), 7.59 (s, 1H), 7.47–7.37 (m, 3H), 4.36–4.24 (m, 2H), 2.37 (td, *J* = 8.4, 6.5, 1H), 1.70 (sext, *J* = 7.0. 1H). 1.43

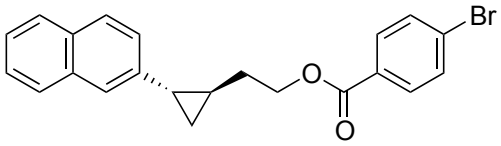
(sext, J = 7.1, 1H), 1.36–1.27 (m, 1H), 1.18–1.11 (m, 1H), 0.92 (q, J = 5.6, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 164.8, 150.5, 136.6, 135.8, 133.5, 132.2, 130.74, 130.73, 128.1, 127.75, 127.73, 127.6, 126.9, 126.7, 125.5, 123.6 (2C), 66.0, 28.0, 21.1, 16.1, 9.7; **IR** (neat) 3060, 3012, 1709, 1631, 1600, 1520, 1504, 1474 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{22}H_{19}NO_4$ $(M + NH_4)^+$ 379.1658, found 379.1664.



trans-(1*R*,2*S*)-**9**



2-(*trans*-(1*R*,2*S*)-2-(Naphthalen-2-yl)cyclopropyl)ethan-1-ol (*trans*-9) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (8.5 mg, 0.030 mmol, 0.050 equiv.), *rac*-BINAP (20 mg, 0.03 mmol, 0.05 equiv.), substrate *trans*-**8** (150 mg, 0.60 mmol, 1.0 equiv., 20:1 trans:cis dr, 99% ee), PhMe (6.0 mL), and methylmagnesium iodide (0.51 mL, 1.2 mmol, 2.4 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as a white solid (120 mg, 0.58 mmol, 96%, 20:1 trans:cis dr, 99% ee). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 58–60 °C; **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, J = 8.1, 1H), 7.73 (d, J = 8.3, 2H), 7.50 (s, 1H), 7.45–7.35 (m, 2H), 7.17 (dd, J = 8.6, 1.7, 1H), 3.78 (t, J = 6.5, 2H), 1.87–1.81 (m, 1H), 1.70 (sept, J = 6.6, 2H), 1.50 (br s, 1H), 1.24–1.16 (m, 1H), 1.05 (dt, J = 8.6, 4.9, 1H), 0.89 (dt, J = 8.6, 4.9, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 141.0, 133.7, 132.0, 128.0, 127.7, 127.3, 126.2, 125.0, 124.8, 123.7, 63.0, 37.5, 23.2, 20.5, 15.8; **IR** (neat) 3315, 3054, 3007, 2929, 2857 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{15}H_{16}ONa$ $(M + Na)^+$ 235.1099, found 235.1098; **$[\alpha]_D^{24}$** +70.7 (*c* 1.0, $CHCl_3$); **SFC analysis** (AD-H, 10% IPA, 2.5 mL/min, 215 nm) indicated >99% ee: t_R (major) = 18.1 minutes; t_R (minor) = 19.7 minutes.

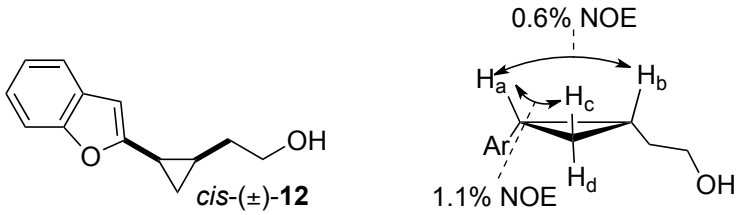


trans-(1*R*,2*S*)-**SI-2**

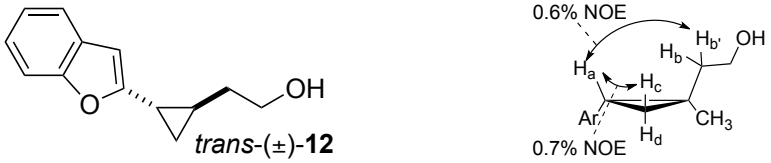
2-((1*R*,2*S*)-2-(Naphthalen-2-yl)cyclopropyl)ethyl 4-bromobenzoate (*cis*-SI-2). To a flame-dried round bottom flask was added *trans*-**9** (0.104 g, 0.490 mmol, 1.00 equiv.), Et_3N (0.11 mL, 0.79 mmol, 1.6 equiv.), 4-dimethylaminopyridine (0.115 g, 0.941 mmol, 2.00 equiv.) and CH_2Cl_2 (10 mL). The solution was cooled to 0 °C and *p*-bromobenzoyl chloride was added dropwise over 5 min. The reaction was allowed to warm to room temperature and the mixture was stirred for 2 hours. The reaction was quenched with DI H_2O (10 mL) and the aqueous layer was extracted with CH_2Cl_2 (3 x 10 mL). The combined organics were washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated in vacuo. The product was purified by flash column chromatography (5–10% EtOAc/hexanes) to afford **SI-2** as a white solid (0.155 g, 0.392 mmol, 80% yield, 20:1 trans:cis dr, 99% ee). **TLC R_f** = 0.8 (20%

EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88–7.84 (m, 2H), 7.76 (d, *J* = 8.0, 1H), 7.69 (t, *J* = 8.0, 2H), 7.54–7.50 (m, 2H), 7.47–7.35 (m, 3H), 7.14 (dd, *J* = 8.7, 1.8, 1H), 4.46 (t, *J* = 6.5, 2H), 1.94–1.83 (m, 3H), 1.30–1.19 (m, 1H), 1.08 (dt, *J* = 8.4, 5.0, 1H), 0.91 (dt, *J* = 8.8, 5.2, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 166.03, 140.6, 133.6, 132.0, 131.8, 131.2, 129.4, 128.1, 128.0, 127.7, 127.3, 126.2, 125.1, 124.7, 124.0, 65.2, 33.6, 23.5, 20.5, 15.6; **IR** (neat) 3016, 1716, 1270, 754 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{22}H_{19}BrO_2Na$ $(M + Na)^+$ 417.0466, found 417.0486; **$[\alpha]_D^{24}$** +55.7 (*c* 1.0, $CHCl_3$); **SFC analysis** (OD-H, 20% IPA, 2.5 mL/min, 215 nm) indicated >99% ee: t_R (major) = 33.5 minutes; t_R (minor) = 11.8 minutes.

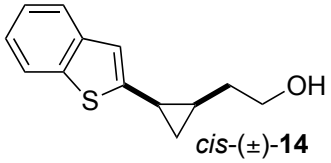
D. CHARACTERIZATION DATA FOR TABLE 3 PRODUCTS



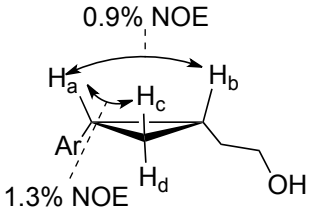
2-(*cis*-(±)-2-(Benzofuran-2-yl)cyclopropyl)ethan-1-ol (*cis*-12) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.7 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (7.0 mg, 0.011 mmol, 0.055 equiv.), substrate *cis*-**11** (47 mg, 0.20 mmol, 1.0 equiv., 20:1 cis:trans dr), PhMe (1.8 mL), and methylmagnesium iodide (0.20 mL, 0.40 mmol, 2.0 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (25% Et_2O/pentane) to yield the title compound as a colorless oil (31 mg, 0.15 mmol, 68%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.3, 1H), 7.39 (d, *J* = 7.7, 1H), 7.18 (qd, *J* = 8.1, 1.1, 2H), 6.38 (s, 1H), 3.61 (td, *J* = 6.2, 2.2, 2H), 2.16 (q, *J* = 6.2, 1H), 1.53 (qd, *J* = 6.5, 2.8, 2H), 1.43 (br s, 1H), 1.30 (q, *J* = 7.2, 1H) 1.19 (m, 1H), 0.85 (q, *J* = 5.4, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 158.0, 154.7, 128.9, 123.3, 122.6, 120.2, 110.8, 103.4, 62.8, 31.8, 16.7, 14.1, 10.6; **IR** (neat) 3331, 2925, 1601, 1455 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{14}O_2H$ $(M + H)^+$ 203.1072, found 203.1073.



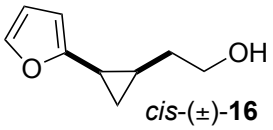
2-(*trans*-(±)-2-(Benzofuran-2-yl)cyclopropyl)ethan-1-ol (*trans*-12) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.7 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (6.2 mg, 0.010 mmol, 0.050 equiv.), substrate *trans*-**11** (47 mg, 0.20 mmol, 1.0 equiv., 8:1 trans:cis dr), PhMe (1.0 mL), and methylmagnesium iodide (0.17 mL, 0.40 mmol, 2.4 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (25% Et_2O/pentane) to yield the title compound as a colorless oil (23 mg, 0.11 mmol, 55%, 8:1 trans:cis dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.2 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.43 (dd, *J* = 6.4, 2.1, 1H), 7.35 (d, *J* = 7.2, 1H), 7.19–7.12 (m, 2H), 6.33 (s, 1H), 3.78 (t, *J* = 6.5, 2H), 1.85–1.80 (m, 1H), 1.66 (q, *J* = 6.5, 2H), 1.61–1.49 (m, 1H), 1.36 (sext, *J* = 6.9, 1H), 1.21–1.15 (m, 1H), 0.86 (dt, *J* = 8.1, 5.0, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 160.0, 154.4, 129.2, 123.1, 122.6, 120.0, 110.7, 100.3, 62.8, 36.8, 18.6, 16.4, 13.8; **IR** (neat) 3350, 2929, 1601, 1455, 1253 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{14}O_2H$ $(M + H)^+$ 203.1072, found 203.1069.



cis-(±)-**14**

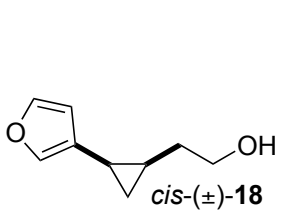


2-(*cis*-(±)-2-(Benzo[b]thiophen-2-yl)cyclopropyl)ethan-1-ol (*cis*-14) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.7 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (7.0 mg, 0.011 mmol, 0.055 equiv.), substrate *cis*-**13** (51 mg, 0.20 mmol, 1.0 equiv., 16:1 cis:trans dr), PhMe (1.8 mL), and methylmagnesium iodide (0.20 mL, 0.40 mmol, 2.0 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (25% Et_2O/pentane) to yield the title compound as a colorless oil (35 mg, 0.16 mmol, 80%, 10:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes; stained with $KMnO_4$); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.0, 1H), 7.64 (d, *J* = 7.8, 1H), 7.29 (atd, *J* = 7.2, 1.1, 1H), 7.24 (atd, *J* = 5.5, 1.34, 1H), 6.95 (s, 1H), 3.64 (t, *J* = 6.3, 2H), 2.28 (q, *J* = 8.3, 1H), 1.57 (sext, *J* = 7.0, 1H), 1.40 (sext, *J* = 7.0, 1H), 1.33–1.19 (m, 3H), 0.80 (q, *J* = 5.5, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 145.0, 140.4, 139.7, 124.4, 123.9, 123.0, 122.3, 121.8, 63.0, 32.0, 17.2, 16.5, 12.5; **IR** (neat) 3327, 3059, 2999, 2927, 2873, 1457, 1437 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{14}OSH$ $(M + H)^+$ 219.0844, found 219.0838.

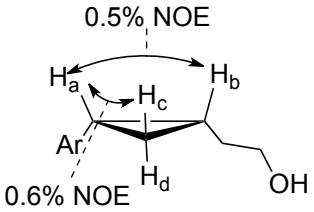


cis-(±)-**16**

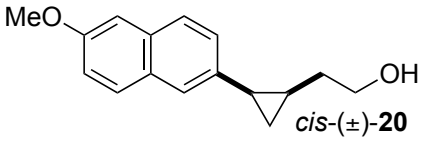
2-(*cis*-(±)-2-(Furan-2-yl)cyclopropyl)ethan-1-ol (*cis*-16) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.7 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (7.0 mg, 0.011 mmol, 0.055 equiv.), substrate *cis*-**15** (37 mg, 0.20 mmol, 1.0 equiv., 20:1 cis:trans dr), PhMe (1.8 mL), and methylmagnesium iodide (0.16 mL, 0.42 mmol, 2.6 M in Et_2O, 2.1 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as a colorless oil (28 mg, 0.18 mmol, 91%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes; stained with $KMnO_4$); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.29 (s, 1H), 6.29 (d, *J* = 2.0, 1H), 5.99 (d, *J* = 2.9, 1H), 3.61 (t, *J* = 6.6, 2H), 2.03 (q, *J* = 8.6, 1H), 1.53–1.37 (m, 3H), 1.16 (sext, *J* = 7.3, 1H), 1.08 (td, *J* = 8.6, 4.8, 1H), 0.68 (q, *J* = 5.3, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 154.8, 141.2, 110.3, 103.5, 62.9, 31.9, 16.0, 13.6, 10.0; **IR** (neat) 3336 (br) 3004, 2931, 1507 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_9H_{12}O_2H$ $(M + H)^+$ 153.0916, found 153.0910.



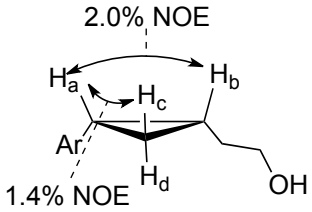
cis-(±)-**18**



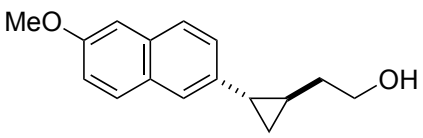
2-(*cis*-(±)-2-(Furan-3-yl)cyclopropyl)ethan-1-ol (*cis*-18) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.7 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (7.0 mg, 0.011 mmol, 0.055 equiv.), substrate *cis*-**17** (37 mg, 0.20 mmol, 1.0 equiv., 20:1 cis:trans dr), PhMe (1.8 mL), and methylmagnesium iodide (0.20 mL, 0.40 mmol, 2.0 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (25% Et_2O/pentane) to yield the title compound as a colorless oil (34 mg, 0.22 mmol, 96%, 15:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes; stained with $KMnO_4$); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.33 (s, 1H), 7.18 (s, 1H), 6.26 (s, 1H), 3.62 (t, *J* = 6.5, 2H), 1.81 (q, *J* = 8.6, 1H), 1.46 (sext, *J* = 7.1, 2H), 1.38 (sext, *J* = 6.8, 1H), 1.06 (sext, *J* = 8.3, 1H), 0.99 (td, *J* = 8.6, 4.6, 1H), 0.40 (q, *J* = 5.1, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 143.0, 140.4, 123.8, 112.1, 63.2, 32.1, 14.8, 11.1, 10.4; **IR** (neat) 3329, 2999, 2927, 2873, 1504 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_9H_{12}OH$ $(M + H)^+$ 153.0916, found 153.0915.



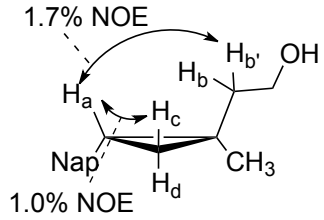
cis-(±)-**20**



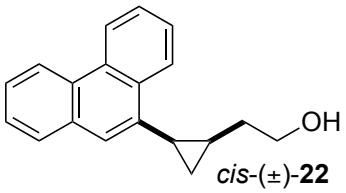
2-(*cis*-(±)-2-(6-Methoxynaphthalen-2-yl)cyclopropyl)ethan-1-ol (*cis*-20) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.9 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (6.9 mg, 0.011 mmol, 0.055 equiv.), substrate *cis*-**19** (56 mg, 0.20 mmol, 1.0 equiv., 20:1 cis:trans dr), PhMe (1.8 mL), and methylmagnesium iodide (0.16 mL, 0.42 mmol, 2.6 M in Et_2O, 2.1 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as an off-white solid (48 mg, 0.19 mmol, 97%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 87–89 °C; **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (t, *J* = 7.6, 2H), 7.49 (s, 1H), 7.34 (dd, *J* = 8.4, 1.3, 1H), 7.17–7.08 (m, 2H), 3.90 (s, 3H), 3.59–3.51 (m, 2H), 2.27 (q, *J* = 6.2, 1H), 1.45–1.36 (m, 1H), 1.30 (br s, 1H), 1.24–1.15 (m, 2H), 1.09–1.03 (m, 1H), 0.83 (q, *J* = 5.5, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 157.3, 134.5, 133.1, 129.1, 129.0, 128.8, 126.7, 126.5, 118.8, 105.7, 63.0, 55.4, 31.9, 20.6, 15.8, 9.3; **IR** (neat) 3283 (br), 3070, 2995, 2931 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{18}O_2NH_4$ $(M + NH_4)^+$ 260.1650, found 260.1648.



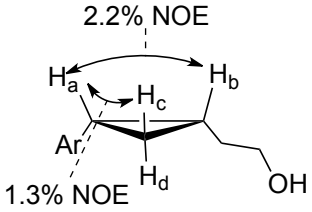
trans-(±)-**20**



2-(*trans*-(±)-2-(6-Methoxynaphthalen-2-yl)cyclopropyl)ethan-1-ol (*trans*-20) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.9 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (6.8 mg, 0.011 mmol, 0.055 equiv.), substrate *trans*-**19** (55 mg, 0.20 mmol, 1.0 equiv., 20:1 trans:cis dr), PhMe (1.8 mL), and methylmagnesium iodide (0.20 mL, 0.40 mmol, 2.0 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as a white solid (47 mg, 0.19 mmol, 97%, 20:1 trans:cis dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 105–107 °C; **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.8, 2H), 7.43 (s, 1H), 7.14 (dd, *J* = 8.3, 1.7, 1H), 7.12–7.06 (m, 2H), 3.90 (s, 3H), 3.80 (t, *J* = 6.5, 2H), 1.82 (dt, *J* = 8.7, 4.5, 1H), 1.70 (sept, *J* = 6.7, 2H), 1.43 (br s, 1H), 1.20–1.13 (m, 1H), 1.02 (dt, *J* = 8.4, 5.0, 1H), 0.87 (*J* = 8.4, 5.1, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.1, 138.6, 133.0, 129.2, 128.9, 126.9, 125.3, 123.7, 119.0, 105.7, 63.1, 55.4, 37.5, 23.0, 20.2, 15.5; **IR** (neat) 3325 (br s), 3005, 2930, 1605, 1240 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{18}O_2NH_4$ $(M + NH_4)^+$ 260.1650, found 260.1648.

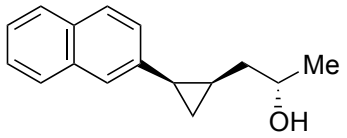


cis-(±)-**22**

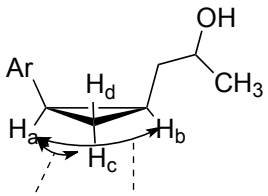


2-(*cis*-(±)-2-(Phenanthren-9-yl)cyclopropyl)ethan-1-ol (*cis*-22) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.9 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (7.0 mg, 0.011 mmol, 0.055 equiv.), substrate *cis*-**21** (60 mg, 0.20 mmol, 1.0 equiv., 20:1 cis:trans dr), PhMe (1.8 mL), and methylmagnesium iodide (0.16 mL, 0.42 mmol, 2.6 M in Et_2O, 2.1 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as a clear oil (52 mg, 0.19 mmol, 98%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.72–8.66 (m, 1H), 8.62 (d, *J* = 8.0, 1H), 8.42–8.36 (m, 1H), 7.80 (d, *J* = 7.5, 1H), 7.68–7.61 (m, 2H), 7.61–7.52 (m, 2H), 7.52 (s, 1H) 3.51–3.40 (m, 2H), 2.49 (q, *J* = 6.7, 1H), 1.53–1.37 (m, 2H), 1.31 (br s, 1H), 1.23–1.14 (m, 1H), 0.95 (q, *J* = 5.4, 1H), 0.88–0.77 (m, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 134.1, 133.0, 131.9, 130.4, 129.8, 128.3, 126.8, 126.73, 126.69, 126.5, 126.3, 125.2, 123.1, 122.6, 63.0, 31.8, 19.1, 15.4, 9.2; **IR** (neat) 3335, 3095, 2927, 1044, 907 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{19}H_{18}ONH_4$ $(M + NH_4)^+$ 280.1701, found 280.1701.

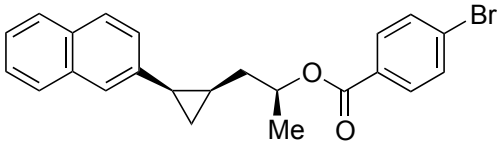
E. CHARACTERIZATION DATA FOR TABLE 4 PRODUCTS



(1*S*)-(*cis*-(1*R*,2*R*)-**24**



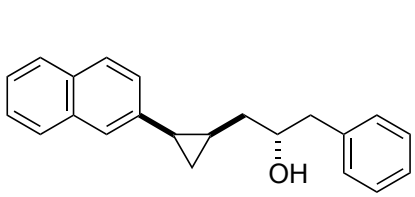
(*S*)-1-((1*R*,2*R*)-2-(Naphthalen-2-yl)cyclopropyl)propan-2-ol (*cis*-24) was prepared according to Method B. The following amounts of reagents were used: $Ni(cod)_2$ (5.5 mg, 0.020 mmol, 0.10 equiv.), *rac*-BINAP (12.5 mg, 0.02 mmol, 0.10 equiv.), substrate *cis*-**23** (52 mg, 0.20 mmol, 1.0 equiv., 13:1 cis:trans dr, 94% ee), MgI_2 (56 mg, 0.20 mmol, 1.0 equiv.), PhMe (1.0 mL), and methylmagnesium iodide (0.16 mL, 0.50 mmol, 3.2 M in Et_2O, 2.5 equiv.). The compound was purified by flash column chromatography (25% Et_2O/pentane) to yield the title compound as a colorless oil (40 mg, 0.18 mmol, 88%, 20:1 cis:trans dr, 96% ee). The dr was determined based on the integration of the benzylic methines in the ^1H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^1H NMR** (500 MHz, $CDCl_3$) δ 7.77 (q, *J* = 8.0, 2H), 7.74 (d, *J* = 8.5, 1H), 7.55 (s, 1H), 7.42 (dt, *J* = 18.7, 7.0, 2H), 7.36 (dd, *J* = 8.4, 1.5, 1H), 3.74 (sext, *J* = 6.4, 1H), 2.30 (aq, *J* = 8.7, 1H), 1.43–1.35 (m, 2H), 1.29–1.22 (m, 1H), 1.11–1.06 (m, 1H), 1.08 (d, *J* = 6.4, 3H), 0.93 (ddd, *J* = 14.0, 8.3, 5.6, 1H), 0.83 (q, *J* = 5.6, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 137.2, 133.6, 132.3, 128.5, 127.9, 127.79, 127.76, 127.0, 126.2, 125.5, 68.6, 38.4, 23.6, 21.2, 16.2, 9.9; **IR** (neat) 3353, 3053, 2965, 2925, 1632, 1601, 1506 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{18}ONH_4$ $(M + NH_4)^+$ 244.1701, found 244.1694; **$[\alpha]_D^{28}$** +16.5 (*c* 0.8, $CHCl_3$); **SFC analysis** (OD-H, 20% IPA, 2.5 mL/min, 215 nm) indicated 99% ee: t_R (major) = 3.6 minutes; t_R (minor) = 3.4 minutes.



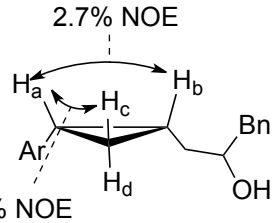
(1*S*)-(*cis*-(1*R*,2*R*))-**SI-3**

(*S*)-1-((1*R*,2*R*)-2-(Naphthalen-2-yl)cyclopropyl)propan-2-yl 4-bromobenzoate (*cis*-SI-3). To a flame-dried round bottom flask was added **24** (0.204 g, 0.901 mmol, 1.00 equiv.), Et_3N (0.151 mL, 1.08 mmol, 1.20 equiv.), 4-dimethylaminopyridine (0.220 g, 1.80 mmol, 2.00 equiv.) and CH_2Cl_2 (15 mL). The solution was cooled to 0 °C and *p*-bromobenzoyl chloride (0.237g, 1.08 mmol, 1.20 equiv.) in CH_2Cl_2 (5 mL) was added dropwise over 5 min. The reaction was allowed to warm to room temperature and the mixture was stirred for 2 hours. The reaction was quenched with DI H_2O (20 mL) and the aqueous layer was extracted with DCM (3 x 15 mL). The combined organics were washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated in vacuo. The product was purified by flash column chromatography (5% EtOAc/hexanes) to afford **SI-3** as a white solid (0.264 g, 0.644 mmol, 72% yield, 20:1 cis:trans dr, 99% ee). **TLC R_f** = 0.8 (20% EtOAc/hexanes); **^1H NMR** (500 MHz, $CDCl_3$) δ 7.80 (at, *J* = 8.6, 3H), 7.74 (at, *J* = 5.8, 2H), 7.55 (s, 1H), 7.51 (d, *J* = 8.6, 2H), 7.43 (aquint, *J* =8.6, 2H), 7.34 (ad, *J* =8.1, 1H), 5.19 (q, *J* = 6.2, 1H), 2.30 (q, *J* = 6.2, 1H), 1.77 (ddd, *J* =

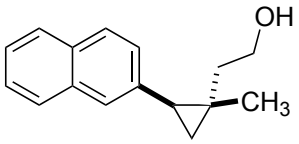
12.3, 7.2, 5.1, 1H), 1.26 (d, J = 6.5, 3H), 1.30–1.20 (m, 1H), 1.11 (aq, J = 8.6, 1H), 1.00 (ddd, 14.3, 8.8, 5.0, 1H), 0.86 (q, J = 5.9, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 165.4, 136.8, 133.4, 132.1, 131.6(2C), 131.1(2C), 129.7, 128.2, 127.8, 127.6, 127.56, 127.53, 126.9, 126.0, 125.3, 72.5, 35.2, 21.0, 20.2, 15.7, 10.0; **IR** (neat) 2927, 1715, 1590, 1270 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{23}H_{21}BrO_2Na$ $(M + Na)^+$ 431.0623, found 431.0622; **$[\alpha]_D^{25}$** -36.2 (*c* 1.0, $CHCl_3$); **SFC analysis** (OD-H, 20% IPA, 2.5 mL/min, 215 nm) indicated 99% ee: t_R (major) = 7.5 minutes; t_R (minor) = 6.7 minutes.



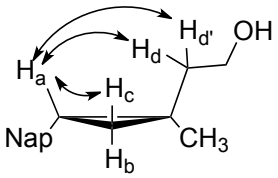
cis-(±)-**26**



(±)-1-(*cis*-2-(Naphthalen-2-yl)cyclopropyl)-3-phenylpropan-2-ol (*cis*-26) was prepared according to Method B. The following amounts of reagents were used: $Ni(cod)_2$ (5.7 mg, 0.020 mmol, 0.10 equiv.), *rac*-BINAP (13 mg, 0.020 mmol, 0.10 equiv.), substrate *cis,cis*-**25** (68 mg, 0.20 mmol, 1.0 equiv., 20:1 cis:trans dr), MgI_2 (56 mg, 0.20 mmol, 1.0 equiv.), PhMe (1.8 mL), and methylmagnesium iodide (0.12 mL, 0.40 mmol, 3.5 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as a white solid (51 mg, 0.17 mmol, 85%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 41–43 °C; **TLC R_f** = 0.4 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82–7.70 (m, 3H), 7.54 (s, 1H), 7.43 (quintd, J = 7.8, 2.0, 2H), 7.36 (dd, J = 8.6, 1.8, 1H), 7.28–7.21 (m, 2H), 7.20–7.16 (m, 1H), 7.14–7.10 (m, 2H), 3.86–3.75 (m, 1H), 2.73 (dd, J = 13.7, 4.0, 1H), 2.53 (dd, J = 13.7, 8.9, 1H), 2.38–2.30 (m, 1H), 1.55–1.44 (m, 1H), 1.42–1.34 (m, 2H), 1.15–1.02 (m, 2H), 0.85 (q, J = 5.5, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 138.8, 137.1, 133.5, 132.2, 129.5, 128.6, 128.3, 127.72, 127.66, 127.63, 126.8, 126.5, 126.1, 125.3, 73.0, 43.9, 35.9, 21.2, 16.1, 9.8; **IR** (neat) 3422 (br s), 3059, 3025, 2921, 1601 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{22}H_{22}ONH_4$ $(M + NH_4)^+$ 320.2014, found 320.2011.



trans-(±)-**28**

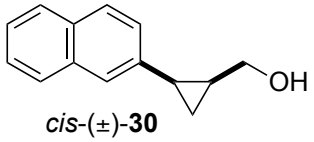


	NOE
H_a–H_d	1.0%
H_a–$H_{d'}$	0.9%
H_a–H_c	1.0%

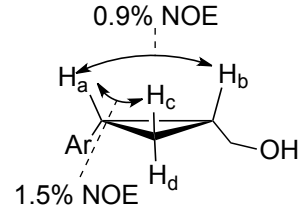
2-((±)-1-Methyl-2-(naphthalen-2-yl)cyclopropyl)ethan-1-ol (*trans*-28) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (2.7 mg, 0.010 mmol, 0.050 equiv.), *rac*-BINAP (7.0 mg, 0.011 mmol, 0.055 equiv.), substrate *trans*-**27** (52 mg, 0.20 mmol, 1.0 equiv., 9:1 trans:cis dr), PhMe (1.8 mL), and methylmagnesium iodide (0.20 mL, 0.40 mmol, 2.0 M in Et_2O, 2.0 equiv.). The compound was purified by flash column chromatography (25% Et_2O/pentane) to yield the title compound as a colorless oil (28 mg, 0.12 mmol, 62%, 8:1 trans:cis dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. Further isolation gave a single diastereomer

reported here. **TLC** $\mathbf{R_f}$ = 0.35 (minor), 0.30 (major) (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (dd, *J* = 14.4, 8.0, 2H), 7.75 (d, *J* = 8.4, 1H), 7.55 (s, 1H), 7.43 (dtd, *J* = 19.2, 7.0, 1.1, 2H), 7.35 (dd, *J* = 8.4, 1.8, 1H), 3.89 (t, *J* = 6.85, 2H), 2.11 (dd, *J* = 8.2, 6.1, 1H), 1.82 (quint, *J* = 7.0, 1H), 1.69 (quint, *J* = 7.0, 1H), 1.25 (br, 1H), 0.98 (t, *J* = 5.3, 1H), 0.93 (dd, *J* = 8.3, 4.8, 1H), 0.80 (s, 3H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 137.4, 133.5, 132.1, 128.4, 127.7, 127.58, 127.53, 126.8, 126.0, 125.3, 61.6, 43.9, 29.0, 20.6, 18.0, 17.6; **IR** (neat) 3345, 3054, 2924, 1631, 1600, 1506 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{18}ONH_4$ $(M + NH_4)^+$ 244.1701, found 244.1694.

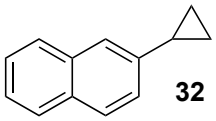
F. CHARACTERIZATION DATA FOR SCHEME 3 PRODUCTS



cis-(±)-**30**



(*cis*-(±)-2-(Naphthalen-2-yl)cyclopropyl)methanol (*cis*-30) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (1.4 mg, 0.0050 mmol, 0.050 equiv.), *rac*-BINAP (3.9 mg, 0.0050 mmol, 0.050 equiv.), substrate *cis*-**29** (23 mg, 0.10 mmol, 1.0 equiv., 20:1 cis:trans dr), PhMe (0.90 mL), and methylmagnesium iodide (0.06 mL, 0.2 mmol, 3.5 M in Et_2O, 2.1 equiv.). The compound was purified by flash column chromatography (20% EtOAc/hexanes) to yield the title compound as a colorless oil (17.2 mg, 0.087 mmol, 87%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.1, 1H), 7.77 (d, *J* = 8.0, 2H), 7.63 (s, 1H), 7.48–7.39 (m, 3H), 3.53–3.43 (m, 1H), 3.27 (t, *J* = 9.8, 1H), 2.44 (q, *J* = 7.7, 1H), 1.63–1.52 (m, 1H), 1.16–1.09 (m, 1H), 1.07 (br s, 1H), 1.02 (q, *J* = 5.7, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 136.0, 133.5, 132.3, 128.0, 127.9, 127.8, 127.6, 126.9, 126.3, 125.6, 63.0, 21.3, 21.1, 7.9; **IR** (neat) 3367 (br s), 3053, 3006, 2878, 1019 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{14}H_{14}ONH_4$ $(M + NH_4)^+$ 216.1388, 216.1389 found.

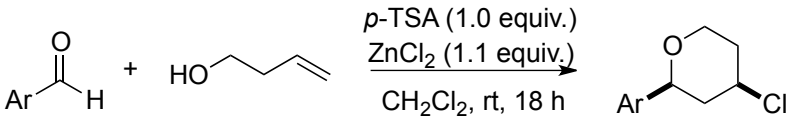


32

2-Cyclopropylnaphthalene (32) was prepared according to Method A. The following amounts of reagents were used: $Ni(cod)_2$ (8.3 mg, 0.030 mmol, 0.17 equiv.), *rac*-BINAP (18.7 mg, 0.030 mmol, 0.17 equiv.), substrate **31** (40 mg, 0.17 mmol, 1.0 equiv.), PhMe (1.8 mL), and methylmagnesium iodide (0.12 mL, 0.43 mmol, 3.6 M in Et_2O, 2.5 equiv.). The compound was purified by flash column chromatography (5% Et_2O/pentane) to yield the title compound as a colorless oil (20 mg, 0.12 mmol, 71%) **TLC R_f** = 0.3 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.0, 1H), 7.73 (dd, *J* = 8.4 3.5, 2H), 7.52 (s, 1H), 7.42 (td, *J* = 8.4, 1.2, 1H), 7.37 (td, *J* = 8.0, 1.1, 1H), 7.18 (dd, *J* = 8.4, 1.5, 1H), 2.05 (tt, *J* = 5.3, 3.6, 1H), 1.02 (qd, *J* = 8.4, 1.8, 2H), 0.80 (qd, *J* = 4.8, 1.6, 2H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 141.8, 133.9, 132.2, 128.2, 127.9, 127.5, 126.3, 125.2, 124.9, 124.0, 16.0, 9.5 (2C); **IR** (neat) 3080, 3052, 3010, 2925, 2853, 1633, 1601 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{12}$ $(M)^+$ 168.0939, 168.0940 found.

G. General Procedures for Cis Tetrahydropyran Synthesis

Method C: Prins Cyclization with $ZnCl_2$



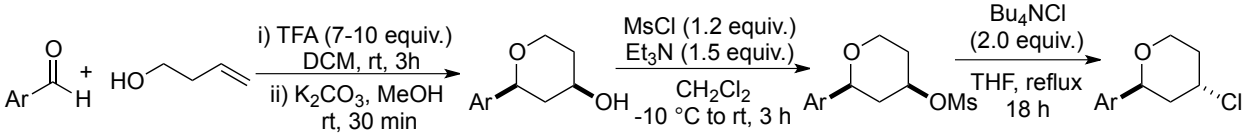
(4)

Modified from a procedure reported by Grée.[4] Zinc dichloride ($ZnCl_2$, 1.1 equiv.) was added to a flame-dried flask equipped with a stir bar and then flame dried again under vacuum. *p*-Toluene sulfonic acid monohydrate (1.0 equiv.) and anhydrous CH_2Cl_2 were added and the reaction mixture was set to stir at ambient temperature. To a separate flame dried flask was added aldehyde (1.0 equiv.). Anhydrous CH_2Cl_2 and homoallylic alcohol (1.1 equiv.) were added and the mixture was stirred for 5 min at room temperature. The aldehyde solution was added to the $ZnCl_2$ solution and the reaction mixture was allowed to stir at room temperature for 18 h. The reaction was quenched with saturated aqueous $NaHCO_3$ (20 mL) and was extracted with CH_2Cl_2 (x 3). The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo.

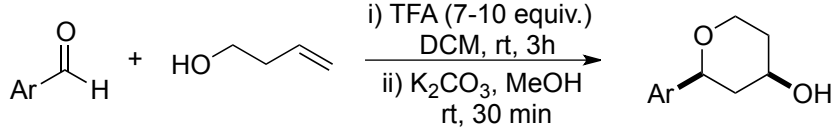
To remove unreacted aldehyde that was difficult to separate from the desired product, the crude mixture was subjected to $NaBH_4$ reduction by a modified procedure reported by Franzén.[5] The crude mixture was dissolved in 1:1 MeOH/CH_2Cl_2 and the reaction cooled to 0 °C. $NaBH_4$ (1.6 equiv. relative to 1.0 equiv of aldehyde as determined by ^1H NMR integration) was added in one portion and the reaction stirred 30 min at 0 °C, then 30 min at room temperature. The reaction was quenched with water and extracted with CH_2Cl_2 (x 3). The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo.

H. General Procedures for Trans Tetrahydropyran Synthesis

Scheme SI 4: Synthesis of trans 2-aryl-4-chlorotetrahydropyrans



Method D: Prins Cyclization with TFA

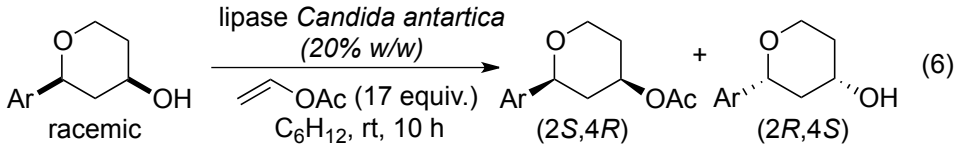


(5)

Modified from a procedure reported by Sabitha.[6] To a stirring solution of aldehyde (1.0 equiv.) in anhydrous CH_2Cl_2 under N_2 was added 3-buten-1-ol (1.1 equiv.). Trifluoroacetic acid (TFA, 7–10 equiv.) was slowly added via syringe. After stirring for 3 h at ambient temperature sat. aq.

$NaHCO_3$ was slowly added and the pH was adjusted to >7 by addition of Et_3N. The aqueous layer was extracted with CH_2Cl_2 (x 3). The combined organics were washed with brine, dried over $MgSO_4$, filtered and concentrated in vacuo. The residue was then redissolved in MeOH, K_2CO_3 (3.5 equiv.) was added, and the reaction was stirred for 30 min at room temperature. The MeOH was removed under reduced pressure, H_2O was added to the residue, and the mixture was extracted with CH_2Cl_2 (x 3). The combined organics were washed with brine, dried over $MgSO_4$, filtered and concentrated in vacuo.

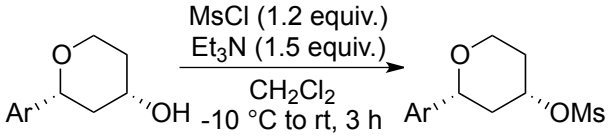
METHOD E: CHIRAL RESOLUTION OF 4-HYDROXY THPS VIA LIPASE *CANDIDA ANTARTICA*



(6)

Modified from a procedure reported by Yadav.[2] To a solution of 4-hydroxy THP from Method D (1.0 equiv.) in cyclohexane (0.1M) was added vinyl acetate (17 equiv.) and lipase *Candida antartica* (20% w/w, Sigma Aldrich). The reaction was allowed to stir at room temperature open to air for 10 h. The mixture was then passed through a plug of Celite with EtOAc and concentrated in vacuo.

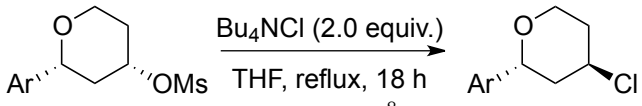
METHOD F: MESYLATION OF 4-HYDROXY THPS



(7)

Modified from a procedure reported by Wallace.[7] To a solution of anhydrous Et_3N (1.5 equiv.) in anhydrous CH_2Cl_2 (2 M in substrate) was added the 4-hydroxy THP from Method D or E (1.0 equiv.) at –10 °C under N_2. After stirring for 10 min, methanesulfonyl chloride (MsCl, 1.2 equiv.) was added slowly via syringe. After stirring for 3 h at ambient temperature and monitoring by TLC, the reaction was quenched with sat. aq. $NaHCO_3$, washed with H_2O, and extracted with CH_2Cl_2 (x 3). The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo.

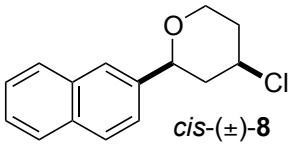
METHOD G: DISPLACEMENT FOR TRANS TETRAHYDROPYRANS



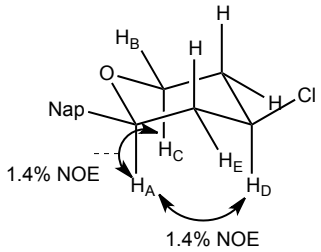
(8)

Modified from a procedure reported by Cahiez.[8] To a flame dried round bottom flask equipped with a stir bar was added the mesylate from Method E (1.0 equiv.) in anhydrous THF. The solution was allowed to stir at 70 °C until complete dissolution and then tetrabutylammonium chloride (Bu_4NCl, 2.0 equiv.) was added. The reaction was stirred at 70 °C for 18 h before it was quenched with H_2O. The mixture was extracted EtOAc (x 3), washed with brine, dried over $MgSO_4$, filtered and concentrated in vacuo.

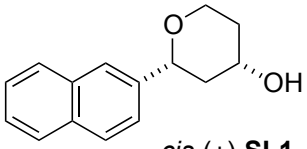
I. Synthesis and Characterization of Substrates For Tables 1 and 2



cis-(±)-**8**

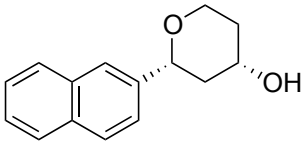


***cis*-(±)-4-Chloro-2-(2-naphthyl)-tetrahydro-*2H*-pyran (*cis*-8)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (1.9 g, 14 mmol, 1.1 equiv.), *p*-toluene sulfonic acid monohydrate (2.5 g, 13 mmol, 1.0 equiv.), 2-naphthaldehyde (2.1 g, 13 mmol, 1.0 equiv.), 3-buten-1-ol (1.3 mL, 15 mmol, 1.1 equiv.), and anhydrous CH_2Cl_2 (120 mL). The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a white solid (2.6 g, 16 mmol, 80%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 62–64 °C; **TLC R_f** = 0.6 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85–7.80 (m, 4H), 7.49–7.44 (m, 3H), 4.50 (dd, *J* = 11.3, 2.0, 1H), 4.26–4.18 (m, 2H), 3.66 (td, *J* = 12.2, 2.1, 1H), 2.49–2.45 (m, 1H), 2.23–2.18 (m, 1H), 2.09–1.95 (m, 2H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 138.8, 133.4, 133.1, 128.4, 128.1, 127.8, 126.3, 126.1, 124.7, 124.0, 79.5, 67.6, 55.9, 44.7, 37.0; **IR** (neat) 3059, 2956, 2927, 2853, 1601, 1505, 1445 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{15}H_{15}ClO$ $(M + Na)^+$ 253.1205, found 253.1205.



cis-(±)-**SI-1**

***cis*-(±)-2-(2-Naphthyl)-tetrahydro-*2H*-pyran-4-ol (*cis*-SI-1)** was prepared according to Method D. The following amounts of reagents were used: 2-naphthaldehyde (4.7 g, 30 mmol, 1.0 equiv.), 3-buten-1-ol (3.0 mL, 15 mmol, 1.1 equiv.), trifluoroacetic acid (15 mL, 0.20 mol, 6.5 equiv.), anhydrous CH_2Cl_2 (120 mL), K_2CO_3 (14 g, 0.10 mol, 3.4 equiv.), and MeOH (80 mL). The product was purified by flash column chromatography (50% EtOAc/hexanes) to afford the title compound as a white solid (2.7 g, 12 mmol, 40%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. Analytical data is consistent with *cis*-(2*R*,4*S*)-**SI-1** below.

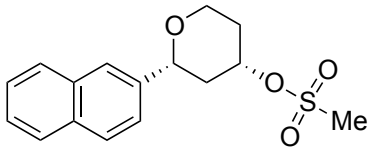


cis-(2*R*,4*S*)-**SI-1**

$[\alpha]_D^{25}$ +36.8
lit. $[\alpha]_D^{25}$ +25.6 (Ref 3)

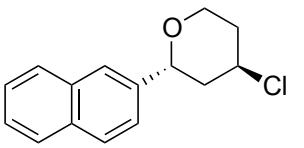
***cis*-(2*R*,4*S*)-2-(2-Naphthyl)-tetrahydro-*2H*-pyran-4-ol (*cis*-SI-1)** was prepared according to Method E. The following amounts of reagents were used: *cis*-(±)-**SI-1** (1.3 g, 5.7 mmol, 1.0 equiv.), vinyl acetate (9.0 mL, 98 mmol, 17 equiv.), lipase *Candida antartica* (0.26 g,

20% w/w), and cyclohexane (60 mL). The product was purified by flash column chromatography (30–50% EtOAc/hexanes) to afford the title compound as a white solid (0.552 g, 2.39 mmol, 42%, 20:1 dr, 99% ee). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 84–86 °C; **TLC R_f** = 0.4 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85–7.45 (m, 4H), 7.49–7.40 (m, 3H), 4.45 (d, *J* = 11.3, 1H), 4.21 (d, *J* = 11.7, 1H), 4.00–3.89 (m, 1H), 3.61 (t, *J* = 12.6, 1H), 2.34 (d, *J* = 11.5, 1H), 1.98 (d, *J* = 12.5, 1H), 1.77 (s, 1H), 1.71–1.54 (m, 2H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 139.5, 133.4, 133.1, 128.3, 128.1, 127.8, 126.2, 126.0, 124.6, 124.2, 78.6, 68.6, 66.6, 43.5, 35.7; **IR** (neat) 3272 (br) 2948, 2919, 2852, 1358 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{15}H_{16}O_2NH_4$ $(M + NH_4)^+$ 246.1494, found 246.1492; **$[\alpha]_D^{25}$** +36.8 (*c* 1.0, $CHCl_3$); **SFC analysis** (OD-H, 5% IPA, 2.5 mL/min, 215 nm) indicated 99% ee: t_R (major) = 29.3 minutes; t_R (minor) = 30.3 minutes.

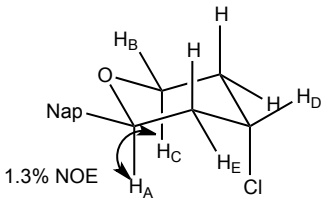


cis-(2*R*,4*S*)-**SI-5**

***cis*-(2*R*,4*S*)-2-(Naphthalen-2-yl)tetrahydro-*2H*-pyran-4-yl methanesulfonate (*cis*-SI-5)** was prepared according to Method F. The following amounts of reagents were used: substrate *cis*-**SI-1** (0.500 g, 2.19 mmol, 1.00 equiv., 99% ee), methanesulfonyl chloride (0.25 mL, 3.2 mmol, 1.5 equiv.), anhydrous Et_3N (0.80 mL, 5.7 mmol, 2.6 equiv.), anhydrous CH_2Cl_2 (25 mL). The product was purified by flash column chromatography (30–50% EtOAc/hexanes) to afford the title compound as a white solid (0.518 g, 1.69 mmol, 77%, 20:1 cis:trans dr, 99% ee). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 63–65 °C; **TLC R_f** = 0.6 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.87–7.74 (m, 4H), 7.51–7.39 (m, 3H), 5.08–4.96 (m, 1H), 4.55 (d, *J* = 11.7, 1H), 4.27 (d, *J* = 11.6, 1H), 3.69 (t, *J* = 12.6, 1H), 3.04 (s, 3H), 2.47 (d, *J* = 12.6, 1H), 2.20 (d, *J* = 12.6, 1H), 2.05–1.86 (m, 2H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 138.4, 133.4, 133.2, 128.5, 128.2, 127.8, 126.4, 126.2, 124.7, 123.9, 78.3, 77.8, 66.0, 40.8, 39.2, 33.2; **IR** (neat) 2936, 2854, 1349, 1173 1080 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{18}O_4SNa$ $(M + Na)^+$ 329.0823, found 329.0818; **$[\alpha]_D^{24}$** –14.0 (*c* 1.0, $CHCl_3$); **SFC analysis** (OD-H, 20% IPA, 2.5 mL/min, 215 nm) indicated 99% ee: t_R (major) = 10.0 minutes; t_R (minor) = 9.2 minutes.



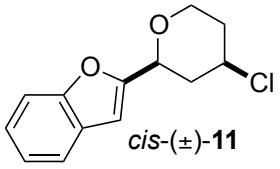
trans-(2*R*,4*R*)-**8**



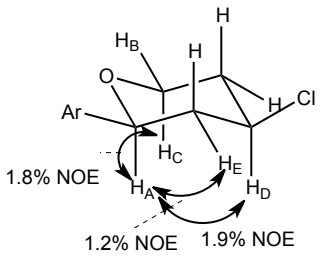
***trans*-(2*R*,4*R*)-4-Chloro-2-(2-naphthyl)-tetrahydro-*2H*-pyran (*trans*-8)** was prepared according to Method G. The following amounts of reagents were used: substrate *cis*-**SI-5** (0.477 g, 1.56 mmol, 1.00 equiv.), Bu_4NCl (0.91 g, 3.3 mmol, 2.1 equiv.), and anhydrous THF (40 mL). The product was purified by flash column chromatography (5–10%

EtOAc/hexanes) to afford the title compound as a white solid (0.31 g, 1.2 mmol, 80%, 20:1 trans:cis dr, 99% ee). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. Irradiation of the benzylic proton (H_A) gave no NOE enhancement of the proton geminal to the chloride (H_D), indicating a trans relationship. **m.p.** 81–83 °C; **TLC R_f** = 0.5 (5% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85–7.79 (m, 4H), 7.49–7.43 (m, 3H), 5.06 (dd, *J* = 10.6, 2.2, 1H), 4.69 (aquint, *J* = 3.1, 1H), 4.20 (td, *J* = 12.0, 2.0, 1H), 4.06 (dd, *J* = 12.0, 4.8, 1H), 2.29–2.10 (m, 3H), 1.92 (ad, *J* = 14.6, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 139.5, 133.5, 133.1, 128.3, 128.1, 127.8, 126.2, 126.0, 124.7, 124.2, 73.9, 63.0, 56.6, 41.5, 33.6; **IR** (neat) 3057 (br), 2957, 2923, 2864, 1267 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{15}H_{15}ClONH_4$ $(M + NH_4)^+$ 264.1155, found 264.1146; **$[\alpha]_D^{24}$** +3.3 (*c* 1.0, $CHCl_3$); **SFC analysis** (OD-H, 20% IPA, 2.5 mL/min, 215 nm) indicated 99% ee: t_R (major) = 6.8 minutes; t_R (minor) = 6.3 minutes.

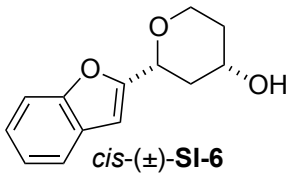
J. SYNTHESIS AND CHARACTERIZATION OF SUBSTRATES FOR TABLE 3



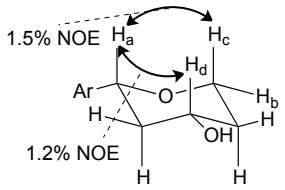
cis-(±)-**11**



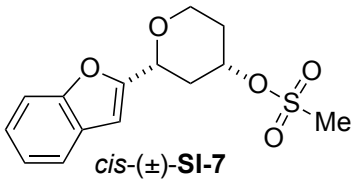
***2*-(*cis*-(±)-4-Chlorotetrahydro-*2H*-pyran-2-yl)benzofuran (*cis*-11)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (0.30 g, 2.2 mmol, 1.1 equiv.), *p*-toluene sulfonic acid monohydrate (0.38 g, 2.0 mmol, 1.0 equiv.), benzofuran-2-carbaldehyde (0.27 mL, 2.2 mmol, 1.1 equiv.), 3-buten-1-ol (0.17 mL, 2.0 mmol, 1.0 equiv.), and anhydrous CH_2Cl_2 (20 mL). The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a white solid (0.28 g, 1.2 mmol, 61%, 7:1 cis:trans dr), purified to increase dr (cis:trans 20:1). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 44–47 °C; **TLC R_f** = 0.7 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0, 1H), 7.47 (d, *J* = 8.0, 1H), 7.27 (t, *J* = 7.4, 1H), 7.22 (q, *J* = 7.0, 1H), 6.65 (s, 1H), 4.52 (d, *J* = 11.3, 1H), 4.22–4.11 (m, 2H), 3.62 (td, *J* = 12.2, 1.8, 1H), 2.52 (dt, *J* = 12.9, 2.2, 1H), 2.23–2.15 (m, 2H), 2.02 (qd, *J* = 12.6. 4.9, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 155.8, 154.9, 127.9, 124.6, 123.0, 121.3, 111.5, 103.6, 73.0, 67.6, 54.9, 40.6, 36.8; **IR** (neat) 2962, 2929, 2851, 1454, 1370, 1344 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{13}ClO_2NH_4$ $(M + NH_4)^+$ 254.0948, found 254.0951.



cis-(±)-**SI-6**

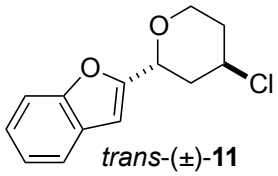


***cis*-(±)-2-(Benzofuran-2-yl)tetrahydro-2*H*-pyran-4-ol (*cis*-SI-6)** was prepared according to Method D. The following amounts of reagents were used: benzofuran-2-carbaldehyde (1.7 g, 12 mmol, 1.0 equiv.), 3-buten-1-ol (1.3 mL, 14 mmol, 1.2 equiv.), trifluoroacetic acid (8.9 mL, 81 mol, 10 equiv.), anhydrous CH_2Cl_2 (50 mL), K_2CO_3 (5.6 g, 40 mmol, 3.4 equiv.), and MeOH (40 mL). The product was purified by flash column chromatography (30–50% EtOAc/hexanes) to afford the title compound as an off-white solid (0.875 g, 4.01 mmol, 34%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 112–114 °C; **TLC R_f** = 0.5 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.7, 1H), 7.47 (d, *J* = 8.2, 1H), 7.27 (t, *J* = 7.7, 1H), 7.21 (t, *J* = 7.5, 1H), 6.65 (s, 1H), 4.53 (dd, *J* = 11.6, 1.3, 1H), 4.18 (dd, *J* = 11.9, 4.4, 1H), 4.00–3.90 (m, 1H), 3.63 (td, *J* = 12.1, 1.6, 1H), 2.36–2.30 (m, 1H), 2.02–1.95 (m, 1H), 1.85 (q, *J* = 11.6, 1H), 1.76 (s, 1H), 1.69 (qd, *J* = 12.1, 5.0, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 156.6, 154.9, 128.0, 124.5, 122.9, 121.3, 111.5, 103.4, 72.1, 67.9, 66.6, 39.3, 35.5; **IR** (neat) 3456 (br), 3123, 2962, 2856, 1452 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{14}O_3NH_4$ $(M + NH_4)^+$ 236.1287, found 236.1295.

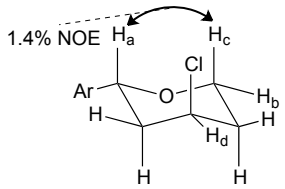


cis-(±)-**SI-7**

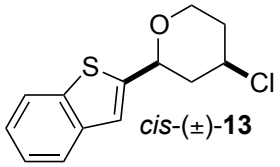
***cis*-(±)-2-(Benzofuran-2-yl)tetrahydro-*2H*-pyran-4-yl methanesulfonate (*cis*-SI-7)** was prepared according to Method F. The following amounts of reagents were used: substrate *cis*-**SI-6** (0.208 g, 0.954 mmol, 1.00 equiv.), methanesulfonyl chloride (0.10 mL, 1.1 mmol, 1.2 equiv.), anhydrous Et_3N (0.20 mL, 1.4 mmol, 1.5 equiv.), anhydrous CH_2Cl_2 (15 mL). The product was purified by flash column chromatography (30–50% EtOAc/hexanes) to afford the title compound as a yellow oil (0.263 g, 0.887 mmol, 93%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. The product was directly used in the next reaction without further purification. **TLC R_f** = 0.3 (30% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.7, 1H). 7.47 (d, *J* = 8.3, 1H), 7.27 (t, *J* = 7.7, 1H), 7.21 (t, *J* = 7.7, 1H), 6.66 (s, 1H), 5.00–4.91 (m, 1H), 4.58 (dd, *J* = 11.7, 1.6, 1H), 4.20 (dd, *J* = 12.1, 1.2, 1H), 3.66 (td, *J* = 12.5, 1.8, 1H), 3.05 (s, 3H), 2.55–2.48 (m, 1H), 2.19–2.11 (m, 2H), 1.97 (qd, *J* = 12.5, 5.0, 1H); **IR** (neat) 2938, 1455, 1351, 1172 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{14}H_{16}O_5SNH_4$ $(M + NH_4)^+$ 314.1062, found 314.1050.



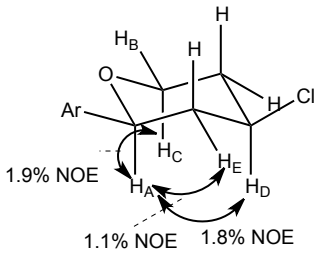
trans-(±)-**11**



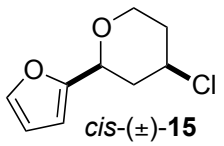
***2*-(*trans*-(±)-4-Chlorotetrahydro-*2H*-pyran-2-yl)benzofuran (*trans*-11)** was prepared according to Method G. The following amounts of reagents were used: substrate *cis*-**SI-7** (0.24 g, 0.82 mmol, 1.0 equiv.), Bu_4NCl (0.46 g, 1.6 mmol, 2.0 equiv.), and anhydrous THF (20 mL). The product was purified by flash column chromatography (5–10% EtOAc/hexanes) to afford the title compound as a white solid (0.11 g, 56%, 8:1 trans:cis dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. Irradiation of the benzylic proton (H_A) gave no NOE enhancement of the proton geminal to the chloride (H_D), indicating a trans relationship. **m.p.** 70–72 °C; **TLC R_f** = 0.5 (5% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.7, 1H), 7.47 (d, *J* = 8.2, 1H), 7.27 (t, *J* = 7.6, 1H), 7.21 (t, *J* = 7.6, 1H), 6.65 (s, 1H), 5.10 (dd, *J* = 10.8, 2.3, 1H), 4.69 (quint, *J* = 3.6, 1H), 4.16 (td, *J* = 11.7, 2.2, 1H), 4.02–3.96 (m, 1H), 2.48–2.39 (m, 1H), 2.28–2.18 (m, 2H), 1.94–1.88 (m, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 156.1, 155.0, 128.0, 124.5, 122.9, 121.3, 111.5, 103.8, 68.1, 63.0, 55.6, 37.6, 33.7; **IR** (neat) 2959, 2865, 1606, 1454, 1253 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{13}ClO_2NH_4$ $(M + NH_4)^+$ 254.0948, found 254.0936.



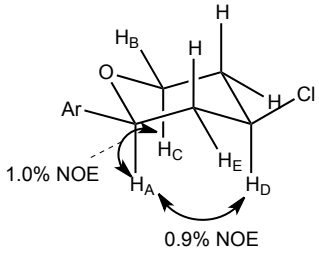
cis-(±)-**13**



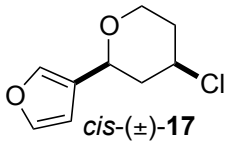
***cis*-(±)-2-(Benzo[b]thiophen-2-yl)-4-chlorotetrahydro-*2H*-pyran (*cis*-13)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (0.30 g, 2.2 mmol, 1.1 equiv.), *p*-toluene sulfonic acid monohydrate (0.38 g, 2.0 mmol, 1.0 equiv.), benzo[b]thiophene-2-carbaldehyde (0.36 g, 2.2 mmol, 1.1 equiv.), 3-buten-1-ol (0.17 mL, 2.0 mmol, 1.0 equiv.), and anhydrous CH_2Cl_2 (20 mL). The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a white solid (0.33 g, 1.3 mmol, 65%, 16:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 64–66 °C; **TLC R_f** = 0.7 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.0, 1H), 7.69 (d, *J* = 8.0, 1H), 7.28 (dt, *J* = 18.3, 7.4, 2H), 7.12 (s, 1H), 4.55 (d, *J* = 11.6, 1H), 4.12 (dd, *J* = 12.2, 4.9, 1H), 4.05 (tt, *J* = 11.7, 4.4, 1H), 3.52 (t, *J* = 12.5, 1H), 2.49 (d, *J* = 12.5, 1H), 2.12–2.00 (m, 2H), 1.95 (qd, *J* = 12.3, 4.7, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 145.1, 139.51, 139.48, 124.5 (2C), 123.8, 122.6, 120.3, 75.6, 67.6, 55.2, 44.2, 36.8; **IR** (neat) 2960, 2926, 2850, 1458, 1438 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{13}H_{13}ClOSNH_4$ $(M + NH_4)^+$ 270.0719, found 270.0725.



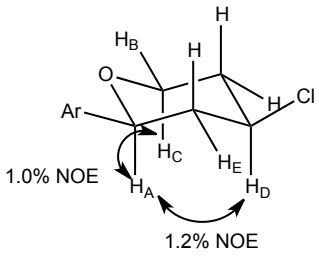
cis-(±)-**15**



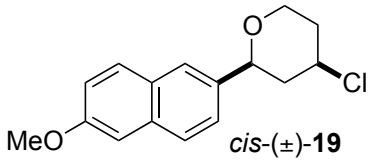
***cis*-(±)-4-Chloro-2-(furan-2-yl)-tetrahydro-*2H*-pyran (*cis*-15)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (2.73 g, 20.0 mmol, 1.00 equiv.), *p*-toluene sulfonic acid monohydrate (3.80 g, 20.0 mmol, 1.00 equiv.), distilled furfural (1.65 mL, 20.0 mmol, 1.00 equiv.), 3-buten-1-ol (2.0 mL, 22 mmol, 1.1 equiv.), and anhydrous CH_2Cl_2 (100 mL). The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a clear oil (1.8 g, 9.6 mmol, 48%, 1.5:1 cis:trans dr). The cis diastereomer was separated via slow column chromatography (2% Et_2O/pentane) to afford the title compound as a clear oil and as a single diastereomer (0.72 g, 3.8 mmol, 19%, 20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.2 (2% Et_2O/pentane); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 1.9, 0.9, 1H), 6.34 (dd, *J* = 3.3, 1.9, 1H), 6.30 (dt, *J* = 3.3, 0.9, 1H), 4.39 (dd, *J* = 11.7, 2.0, 1H), 4.15–4.05 (m, 2H), 3.58 (td, *J* = 12.4, 2.0, 1H), 2.44–2.38 (m, 1H), 2.19–2.09 (m, 2H), 1.97 (qd, *J* = 12.4, 4.8, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 153.3, 142.6, 110.3, 107.0, 72.5, 67.3, 55.1, 40.4, 36.8; **IR** (neat) 2960, 2862, 1504, 1061, 1019 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_9H_{11}ClO_2H$ $(M + H)^+$ 187.0526, found 187.0531.



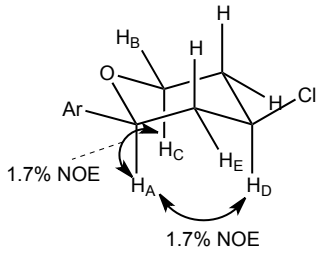
cis-(±)-**17**



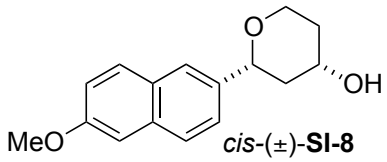
***cis*-(±)-4-Chloro-2-(furan-3-yl)tetrahydro-*2H*-pyran (*cis*-17)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (0.30 g, 2.2 mmol, 1.1 equiv.), *p*-toluene sulfonic acid monohydrate (0.38 g, 2.0 mmol, 1.0 equiv.), furan-2-carbaldehyde (0.19 mL, 2.2 mmol, 1.1 equiv.), 3-buten-1-ol (0.17 mL, 2.0 mmol, 1.0 equiv.), and anhydrous CH_2Cl_2 (20 mL). The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a yellow oil (0.22 g, 1.2 mmol, 60%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.7 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.3, 2H), 6.40 (s, 1H), 4.31 (d, *J* = 11.4, 1H), 4.13–4.06 (m, 2H), 3.55 (td, *J* = 12.4, 1.8, 1H), 2.37 (dt, J = 12.96, 2.4, 1H), 2.13 (dq, *J* = 13.1, 2.2, 1H), 2.00–1.89 (m, 2H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 143.5, 139.4, 126.2, 108.8, 72.4, 67.4, 55.5, 43.3, 37.0; **IR** (neat) 2960, 2928, 2850, 1502 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_9H_{11}ClO_2$ $(M)^+$ 186.0448, found 186.0450.



cis-(±)-**19**

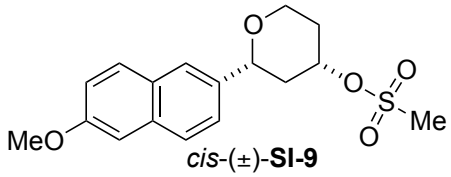


***cis*-(±)-4-Chloro-2-(6-methoxynaphthalen-2-yl)tetrahydro-*2H*-pyran (*cis*-19)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (1.95 g, 14.3 mmol, 1.1 equiv.), *p*-toluene sulfonic acid monohydrate (2.1 g, 11 mmol, 0.80 equiv.), 6-methoxy-2-naphthaldehyde (2.52 g, 13.5 mmol, 1.00 equiv.), 3-buten-1-ol (1.35 mL, 14.7 mmol, 1.10 equiv.), and anhydrous CH_2Cl_2 (120 mL). The product was purified by flash column chromatography (5–10% EtOAc/hexanes) to afford the title compound as a white solid (2.07 g, 55%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 97–98 °C; **TLC R_f** = 0.5 (5% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75–7.69 (m, 3H), 7.41 (dd, *J* = 8.7, 1.5, 1H), 7.14 (dd, *J* = 8.8, 2.5, 1H), 7.12 (d, *J* = 2.5, 1H), 4.46 (dd, *J* = 11.4, 2.1, 1H), 4.26–4.16 (m, 2H), 3.91 (s, 3H), 3.65 (td, *J* = 12.2, 2.1, 1H), 2.48–2.41 (m, 1H), 2.23–2.17 (m, 1H), 2.09–1.95 (m, 2H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 157.9, 136.5, 134.3, 129.6, 128.8, 127.3, 124.7, 124.6, 119.2, 105.8, 79.6, 67.6, 56.0, 55.4, 44.7, 37.1; **IR** (neat) 3315 (br), 3054, 3007, 2929, 2857 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{17}ClO_2H$ $(M + H)^+$ 277.0995, found 277.0997.



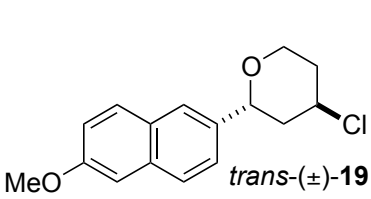
cis-(±)-**SI-8**

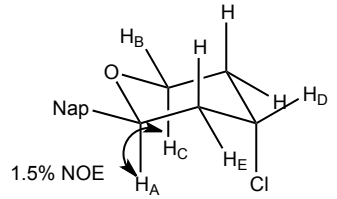
***cis*-(±)-2-(6-Methoxynaphthalen-2-yl)-tetrahydro-*2H*-pyran-4-ol (*cis*-SI-8)** was prepared according to Method D. The following amounts of reagents were used: 6-methoxy-2-naphthaldehyde (1.86 g, 10.0 mmol, 1.00 equiv.), 3-buten-1-ol (1.1 mL, 12 mmol, 1.1 equiv.), trifluoroacetic acid (5.5 mL, 72 mmol, 7.2 equiv.), anhydrous CH_2Cl_2 (40 mL), K_2CO_3 (4.7 g, 34 mmol, 3.4 equiv.), and MeOH (27 mL). The product was purified by flash column chromatography (50% EtOAc/hexanes) to afford the title compound as a white solid (0.447 g, 1.7 mmol, 17%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 132–134 °C; **TLC R_f** = 0.3 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.72 (d, *J* = 9.0, 3H), 7.43 (d, *J* = 8.8, 1H), 7.14 (d, *J* = 9.0, 2H), 4.46 (d, *J* = 11.4, 1H), 4.22 (dd, *J* = 12.0, 4.6, 1H), 4.00 (sept, *J* = 4.6, 1H), 3.91 (s, 3H), 3.65 (td, *J* = 12.0, 2.0, 1H), 2.30–2.22 (m, 1H), 2.05–1.97 (m, 1H), 1.74–1.58 (m, 2H); 1.59 (br s, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.8, 137.2, 134.2, 129.6, 128.9, 127.2, 124.8, 124.6, 119.0, 105.8, 78.6, 68.7, 66.6, 55.4, 43.4, 35.7; **IR** (neat) 3393 (br), 2942, 2845, 1609 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{18}O_3NH_4$ $(M + NH_4)^+$ 276.1600, found 276.1603.



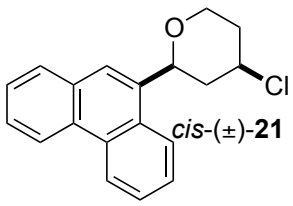
cis-(±)-**SI-9**

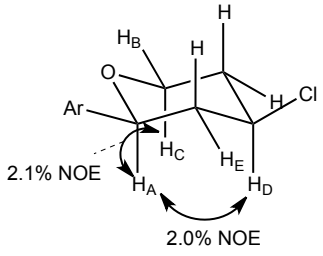
***cis*-(±)-2-(6-Methoxynaphthalen-2-yl)tetrahydro-*2H*-pyran-4-yl methanesulfonate (*cis*-SI-9)** was prepared according to Method F. The following amounts of reagents were used: substrate *cis*-**SI-8** (0.269 g, 1.04 mmol, 1.00 equiv.), methanesulfonyl chloride (0.10 mL, 1.2 mmol, 1.2 equiv.), anhydrous Et_3N (0.25 mL, 1.5 mmol, 1.5 equiv.), anhydrous CH_2Cl_2 (20 mL). The product was purified by flash column chromatography (30–50% EtOAc/hexanes) to afford the title compound as a pale yellow solid (0.31 g, 0.91 mmol, 88%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 98–100 °C; **TLC R_f** = 0.5 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.75–7.68 (m, 3H), 7.41 (dd, *J* = 8.5, 1.5, 1H), 7.17–7.09 (m, 2H), 5.06–4.96 (m, 1H), 4.50 (dd, *J* = 11.4, 2.0, 1H), 4.25 (ddd, *J* =12.2, 5.2, 1.8, 1H), 3.91 (s, 3H), 3.67 (td, *J* = 12.2, 2.1, 1H), 3.04 (s, 3H), 2.45 (ddt, *J* = 12.7, 4.8, 2.1, 1H), 2.23–2.14 (m, 1H), 2.04–1.87 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 157.9, 136.1, 134.4, 129.6, 128.8, 127.3, 124.7, 124.5, 119.2, 105.8, 76.3, 77.9, 66.0, 55.4, 40.7, 39.2, 33.1; **IR** (neat) 2961, 2859, 1354, 1175 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{17}H_{20}O_5SNa$ $(M + Na)^+$ 359.0929, found 359.0931.





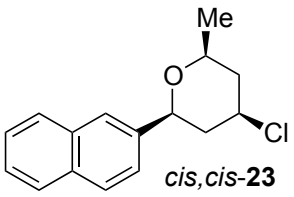
***trans*-(±)-4-Chloro-2-(6-methoxynaphthalen-2-yl)-tetrahydro-*2H*-pyran (*trans*-19)** was prepared according to Method G. The following amounts of reagents were used: substrate *cis*-**SI-5** (0.26 g, 0.76 mmol, 1.0 equiv.), Bu_4NCl (0.51 g, 1.8 mmol, 2.4 equiv.), and anhydrous THF (25 mL). The product was purified by flash column chromatography (5–10% EtOAc/hexanes) to afford the title compound as a white solid (0.17 g, 0.63 mmol, 82%, >20:1 trans:cis dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. Irradiation of the benzylic proton (H_A) gave no NOE enhancement of the proton germinal to the chloride, indicating a trans relationship. **m.p.** 124–126 °C; **TLC** $\mathbf{R_f}$ = 0.3 (5% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.76–7.69 (m, 3H), 7.43 (d, *J* = 8.6, 1H), 7.16–7.10 (m, 2H), 5.02 (dd, *J* = 10.0, 3.2, 1H), 4.72–4.67 (m, 1H), 4.20 (td, *J* = 12.1, 2.0, 1H), 4.05 (dd, *J* = 11.7, 5.0, 1H), 3.91 (s, 3H), 2.29–2.11 (m, 3H), 1.92 (d, *J* = 14.7, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 157.8, 137.2, 134.2, 129.6, 128.9, 127.2, 124.8, 124.6, 119.1, 105.7, 73.9, 63.0, 56.7, 55.4, 41.4, 33.6; **IR** (neat) 2955, 2862, 1608, 1485, 1268 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{17}ClO_2H$ $(M + H)^+$ 277.0995, found 277.0995.



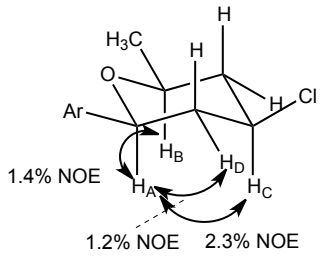


***cis*-(±)-4-Chloro-2-(phenanthren-9-yl)tetrahydro-*2H*-pyran (*cis*-21)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (0.79 g, 5.8 mmol, 1.2 equiv.), *p*-toluene sulfonic acid monohydrate (1.1 g, 5.5 mmol, 1.1 equiv.), 9-phenanthrenecarboxaldehyde (1.0 g, 5.0 mmol, 1.0 equiv.), 3-buten-1-ol (0.55 mL, 6.0 mmol, 1.2 equiv.), and anhydrous CH_2Cl_2 (50 mL). The product was purified by recrystallization from boiling hexanes and EtOAc to afford the title compound as a white solid (0.81 g, 2.7 mmol, 55%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 127–129 °C; **TLC** $\mathbf{R_f}$ = 0.4 (5% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.2, 1H), 8.66 (d, *J* = 8.2, 1H), 8.02 (d, *J* = 7.7, 1H), 7.92–7.87 (m, 2H), 7.64 (quintd, *J* = 7.6, 2.1, 3H), 7.59 (q, *J* = 7.7, 1H), 5.06 (d, *J* = 11.1, 1H), 4.36–4.28 (m, 2H), 3.79 (td, *J* = 12.2, 1.7, 1H), 2.71–2.65 (m, 1H), 2.31–2.25 (m, 1H), 2.18–2.07 (m, 2H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 135.0, 131.5, 130.9, 130.2, 129.4, 129.1, 126.94, 126.91, 126.8, 126.5, 124.3, 123.7, 123.5, 122.6, 76.5, 67.8, 56.0, 43.6, 37.3; **IR** (neat) 3076, 2966, 2855, 1079 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{19}H_{17}ClONH_4$ $(M + NH_4)^+$ 314.1312, found 314.1308.

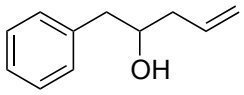
K. Synthesis and Characterization of Starting Materials For Table 4



cis,cis-**23**



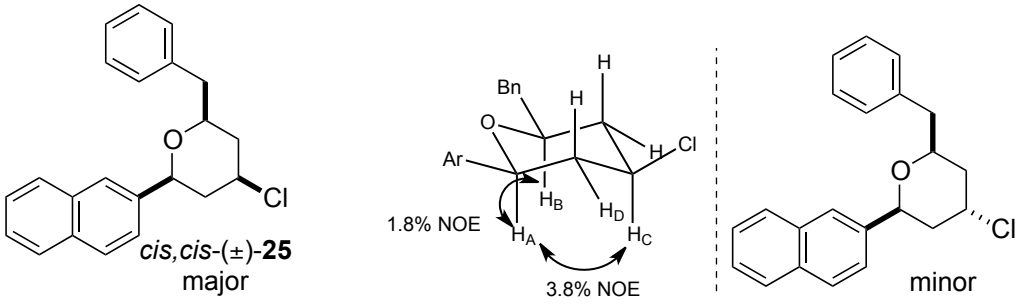
(2S,4R,6S)-4-chloro-2-methyl-6-(naphthalen-2-yl)tetrahydro-2H-pyran (*cis*-23) was prepared according to a procedure reported by Martín.[9] A flame-dried 50 mL round bottom flask equipped with a stir bar was charged with $FeCl_3$ (0.49 g, 0.0030 mol, 1.0 equiv.) and flame dried again. A second flame dried round bottom flask equipped with a stir bar was charged with 2-naphthaldehyde (0.47 g, 0.0030 mol, 1.0 equiv.), (*S*)-(+)-4-penten-2-ol (0.31 mL, 0.0030 mol, 1.0 equiv.), and anhydrous CH_2Cl_2 (10 mL). Anhydrous CH_2Cl_2 (5 mL) was added to the first round bottom flask, then the contents of the second flask were added drop wise to the first flask. After 4 h, the reaction was quenched with $NaHCO_3$ (10 mL) and the reaction mixture was extracted with CH_2Cl_2 (3 x 10 mL). The combined organics were washed with saturate brine solution (30 mL), dried over $MgSO_4$, filtered, and concentrated in vacuo. The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a white solid (0.30 g, 1.2 mmol, 38%, >20:1 cis:trans dr, 46% ee). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. The product was recrystallized 3 times (100% hexanes) which saw a decrease in dr but an increase in ee (13:1 cis:trans dr, 99% ee). **TLC R_f** = 0.7 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84–7.79 (m, 4H), 7.48–7.43 (m, 3H), 4.52 (d, *J* = 11.3, 1H), 4.20 (tt, *J* = 12.1, 4.7, 1H), 3.69 (sextd, *J* = 6.4, 1.7, 1H), 2.42 (dt, *J* = 13.0, 2.1, 1H), 2.23 (dt, *J* = 12.9, 2.2, 1H), 1.90 (q, *J* = 11.7, 1H), 1.68 (q, *J* = 11.6, 1H), 1.34 (d, *J* = 6.0, 3H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 139.0, 133.6, 133.3, 128.6, 128.3, 128.0, 126.4, 126.2, 125.0, 124.4, 79.1, 73.6, 56.0, 44.3, 44.2, 22.0; **IR** (neat) 2928, 2851, 2359, 1309, 1144 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{17}ClONH_4$ $(M + NH_4)^+$ 278.1312, found 278.1312; **$[\alpha]_D^{28}$** –39.9 (*c* 0.8, $CHCl_3$); **SFC analysis** (OD-H, 20% IPA, 2.5 mL/min, 215 nm) indicated 99% ee: t_R (major) = 1.3 minutes; t_R (minor) = 1.5 minutes.



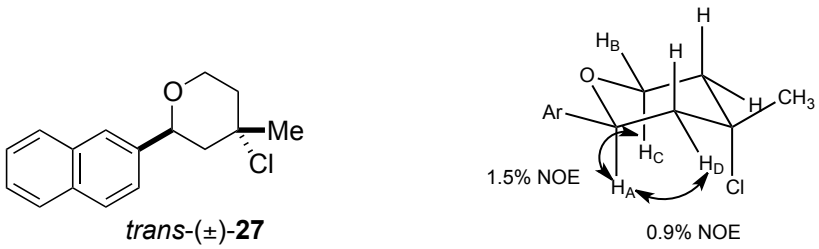
SI-10

1-Phenylpent-4-en-2-ol (SI-10) To a flame dried 100 mL round bottom flask was added allylmagnesium bromide (30 mL, 0.61 M in Et_2O, 18 mmol, 1.1 equiv.) under an atmosphere of N_2. The flask was cooled to 0 °C in an ice bath and a solution of phenylacetaldehyde (1.90 mL, 16.4 mmol, 1.00 equiv.) in anhydrous Et_2O (10 mL) was added drop wise. The reaction was allowed to stir at ambient temperature for 1 h. The reaction was quenched with sat. aq. NH_4Cl (20 mL), extracted with EtOAc (3 x 10 mL), washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. The product was purified by flash column chromatography (5% EtOAc/hexanes) to afford the title compound as a clear oil (2.19 g, 13.5 mmol, 82%). Analytical data is consistent with literature values.[10] **TLC R_f** = 0.3 (5%

EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.8, 2H), 7.24–7.19 (m, 3H), 5.90–5.80 (m, 1H), 5.17–5.13 (m, 1H), 5.13 (t, *J* = 1.4, 1H), 3.89–3.83 (m, 1H), 2.80 (dd, *J* = 13.6, 4.9, 1H), 2.71 (dd, *J* = 13.6, 7.8, 1H), 2.35–2.28 (m, 1H), 2.24–2.17 (m, 1H), 1.81 (br s, 1H).



***cis,cis*-(±)-2-Benzyl-4-chloro-6-(naphthalen-2-yl)tetrahydro-*2H*-pyran** ***(cis,cis*-25)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (1.26 g, 9.24 mmol, 1.10 equiv.), *p*-toluene sulfonic acid monohydrate (1.6 g, 8.4 mmol, 1.0 equiv.), 2-naphthaldehyde (1.31 g, 8.40 mmol, 1.00 equiv.), **SI-10** (1.50 g, 9.25 mmol, 1.10 equiv.), and anhydrous CH_2Cl_2 (100 mL). Before purification, the dr of the product was found to be 8:1 major:minor by ^{1}H NMR. The minor trans diastereomer eluted before the major diastereomer. The product was purified by flash column chromatography (2% Et_2O/pentane) to afford the title compound as a pale yellow oil (0.53 g, 1.6 mmol, 19%, 20:1 major:minor dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.5 (5% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85–7.74 (m, 4H), 7.49–7.38 (m, 3H), 7.32–7.18 (m, 5H), 4.48 (dd, *J* = 11.6, 2.0, 1H), 4.09 (tt, *J* = 11.8, 4.5, 1H), 3.75–3.66 (m, 1H), 3.07 (dd, *J* = 13.6, 6.0, 1H), 2.80 (dd, *J* = 13.6, 6.9, 1H), 2.45–2.38 (m, 1H), 2.21–2.13 (m, 1H), 1.87 (q, *J* = 12.0, 1H), 1.66 (q, *J* = 12.0, 1H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 138.9, 137.9, 133.4, 133.1, 129.8 (2C), 128.5 (2C), 128.3, 128.1, 127.8, 126.6, 126.2, 126.0, 124.6, 124.1, 78.7, 78.1, 55.9, 44.2, 42.5, 41.6; **IR** (neat) 3027, 2924, 2849, 1076 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{22}H_{21}ClONH_4$ $(M + NH_4)^+$ 354.1625, found 354.1612.

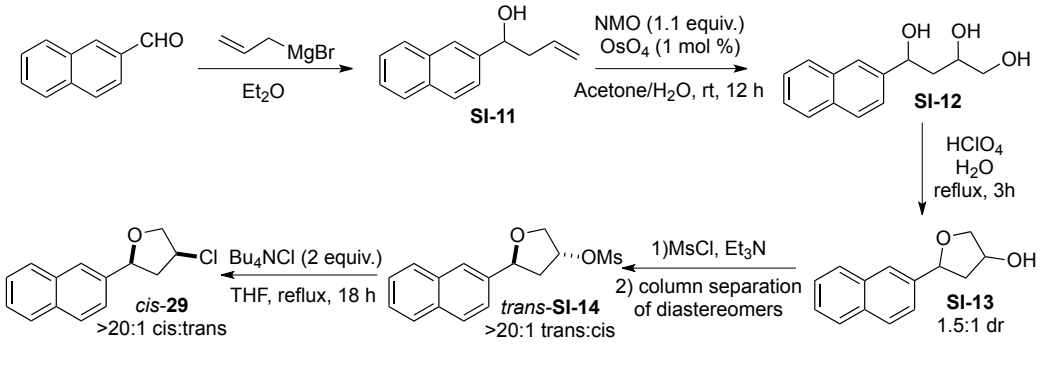


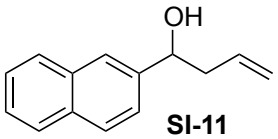
***cis*-(±)-4-Chloro-4-methyl-2-(naphthalen-2-yl)tetrahydro-*2H*-pyran** **(*trans*-27)** was prepared according to Method C. The following amounts of reagents were used: Zinc chloride (0.30 g, 2.2 mmol, 1.1 equiv.), *p*-toluene sulfonic acid monohydrate (0.38 g, 2.0 mmol, 1.0 equiv.), 2-naphthaldehyde (0.34 g, 2.2 mmol, 1.1 equiv.), 3-methyl-3-buten-1-ol (0.20 mL, 2.0 mmol, 1.0 equiv.), and anhydrous CH_2Cl_2 (20 mL). The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a white solid (0.26 g, 1.0 mmol, 51%, 9:1 trans:cis dr). The dr was determined based on the

integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 57–60 °C **TLC** $\mathbf{R_f}$ = 0.6 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.90–7.86 (m, 4H), 7.54–7.49 (m, 3H), 5.02 (d, *J* = 11.0, 1H), 4.20–4.17 (m, 2H), 2.28 (d, *J* = 14.1, 1H) 2.00 (at, *J* = 6.5, 2H), 1.89 (aq, *J* = 13.8, 1H) 1.76 (s, 3H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 139.7, 133.7, 133.3, 128.5, 128.3, 128.0, 126.4, 126.1, 124.8, 124.4, 75.9, 69.6, 64.8, 48.8, 40.8, 34.5; **IR** (neat) 2968, 2924, 2865, 1509, 1445, 1265 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{16}H_{17}ClO$ $(M)^+$ 260.0968, found 260.0961.

L. Synthesis and Characterization of Starting Materials For Scheme 3

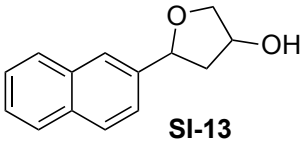
Scheme SI 5: Synthesis of *cis*-29





SI-11

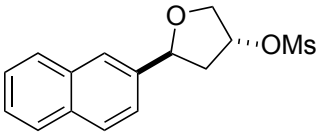
1-(Naphthalen-2-yl)but-3-en-1-ol (SI-11) A solution of allylmagnesium bromide (30 mL, 18 mmol, 0.61 M in Et_2O, 1.1 equiv.) at 0 °C was treated in a dropwise manner with a solution of 2-naphthaldehyde (2.6 g, 16 mmol, 1.0 equiv.) in anhydrous Et_2O to maintain a gentle reflux. The reaction mixture was warmed to room temperature and allowed to stir for 1 h. The reaction was quenched with saturated aqueous NH_4Cl (20 mL) and extracted with EtOAc (20 mL x 3). The organic extracts were washed with brine, dried over $MgSO_4$, and concentrated in vacuo. The compound was purified by flash column chromatography (10% EtOAC in hexanes) to afford the title compound as a pale yellow oil (2.70 g, 13.8 mmol, 84%). Analytical data is consistent with literature values.[11] **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87–7.77 (m, 4H), 7.52–7.42 (m, 3H), 5.84 (ddt, *J* = 16.8, 10.5, 6.8, 1H), 5.18 (d, *J* = 17.3, 1H), 5.14 (d, *J* = 9.9, 1H), 4.95–4.88 (m, 1H), 2.68–2.52 (m, 2H), 2.15 (d, *J* = 3.0, 1H).



SI-13

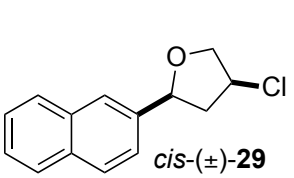
5-(Naphthalene-2-yl)tetrahydrofuran-3-ol (SI-13) was prepared in two steps. To a stirring solution of substrate **SI-11** (2.41 g, 12.4 mmol, 1.00 equiv.) in acetone (25 mL) and H_2O (5 mL) was added N-methylmorpholine-N-oxide (NMO, 1.60 g, 13.7 mmol, 1.10 equiv.) and osmium tetroxide (4% w/w in H_2O, 0.80 mL, 0.12 mmol, 0.010 equiv.). After stirring for 18 h at room temperature, saturated aqueous $NaHCO_3$ (30 mL) was added and the mixture was filtered over celite. The mixture was extracted with EtOAc (3 x 25 mL) and the combined organic extracts were washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. The intermediate triol **SI-12** was isolated by flash column chromatography (70% EtOAc/hexanes) to afford a white solid (1.42 g, 6.09 mmol, 49%).

Substrate **SI-12** (1.24 g, 5.3 mmol, 1.0 equiv.) was added to a flask with H_2O (40 mL). To this stirring solution was added $HClO_4$ (1.70 mL, 4.8 mmol, 0.90 equiv.). The reaction was stirred at reflux for 3 h before it was cooled to room temperature and extracted with EtOAc (3 x 25 mL), washed with brine, dried with $MgSO_4$, and concentrated in vacuo. The product was purified by flash column chromatography to afford the title compound as a pale yellow solid as a mixture of diastereomers (1.0 g, 4.7 mmol, 87%, 43% from SI-7, 1.5:1 dr). The substrate was used as a mixture of diastereomers in the next step. NMR data is reported as a 1.5:1 dr mixture. The diastereomers were not assigned. **m.p.** 54–55 °C; **TLC** $\mathbf{R_f}$ = 0.4 (50% EtOAc/hexanes); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88–7.74 (m, 4H), 7.54–7.37 (m, 3H), 5.32 (dd, *J* = 9.9, 5.8, 0.6H), 5.06 (t, *J* = 7.6, 0.4H), 4.66–4.61 (m, 0.6H), 4,61–4.55 (m, 0.4H), 4.29 (dd, *J* = 9.8, 4.4, 0.6H), 4.10 (d, *J* = 10.0, 0.4H), 3.96–3.92 (m, 1H), 2.75–2.67 (m, 0.4H), 2.37 (dd, *J* = 13.5, 5.9, 0.6H), 2.05–1.95 (m, 1.6H), 1.86 (d, *J* = 5.6, 0.4H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 140.0, 139.7, 133.4, 133.0, 128.5, 128.4, 128.1, 128.02, 128.01, 127.80, 126.29, 126.26, 126.0, 125.9, 124.5, 124.38, 124.37, 124.2, 124.0, 80.5, 79.8, 76.6, 76.5, 76.4, 72.99, 72.97, 44.7, 44.0; **IR** (neat) 3383 (br) 3055, 2938, 2870, 1064 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{14}H_{14}O_2Na$ $(M + Na)^+$ 237.0892, found 237.0898.

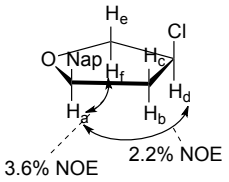


trans-(±)-**SI-14**

***trans*-(±)-5-(Naphthalen-2-yl)tetrahydrofuran-3-yl methanesulfonate (*trans*-SI-14)** was prepared according to Method E. The following amounts of reagents were used: substrate **SI-13** (0.939 g, 4.38 mmol, 1.00 equiv.), methanesulfonyl chloride (0.42 mL, 5.4 mmol, 1.2 equiv.), anhydrous Et_3N (0.95 mL, 6.9 mmol, 1.5 equiv.), anhydrous CH_2Cl_2 (40 mL). TLC analysis of the crude mixture (50% EtOAc/hexanes) had two spots, corresponding to the trans and cis diastereomers (trans R_f = 0.65, cis R_f = 0.55). The product was purified by flash column chromatography (20–40% EtOAc/hexanes) to afford the title compound as an off-white solid (0.426 g, 1.46 mmol, 33%, >20:1 trans:cis dr). The remainder was recovered as a mixture with the cis diastereomer (0.565 g, 1.93 mmol, 44%). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. **m.p.** 108–110 °C; **TLC** $\mathbf{R_f}$ = 0.7 (50% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86–7.78 (m, 4H), 7.51–7.44 (m, 2H), 7.41 (d, *J* = 8.4, 1H), 5.45 (t, *J* = 5.1, 1H), 5.30 (dd, *J* = 10.5, 5.8, 1H), 4.42 (dd, *J* = 11.0, 4.8, 1H), 4.21 (d, *J* = 11.0, 1H), 3.10 (s, 3H), 2.73 (dd, *J* = 14.2, 5.5, 1H), 2.22–2.14 (m, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 138.2, 133.3, 133.2, 128.6, 128.0, 127.8, 126.4, 126.2, 124.6, 123.7, 81.3, 79.9, 73.7, 42.1, 38.8; **IR** (neat) 3034, 2939, 1327, 1170 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{15}H_{16}O_4SNa$ $(M + Na)^+$ 315.0667, found 315.0659.

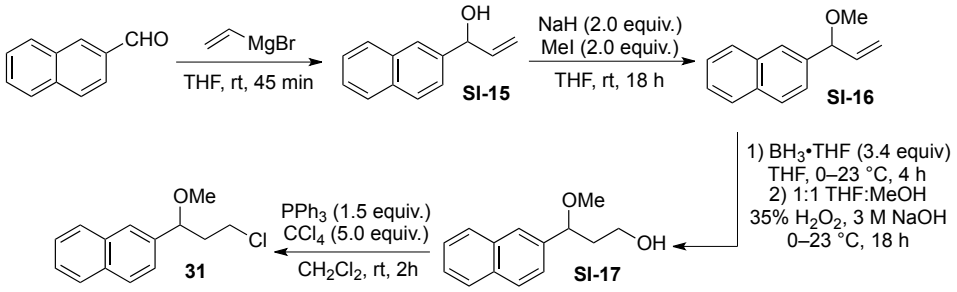


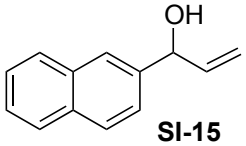
cis-(±)-**29**



***cis*-(±)-4-Chloro-2-(naphthalen-2-yl)tetrahydrofuran (*cis*-29)** was prepared according to Method F. The following amounts of reagents were used: substrate *trans*-**SI-10** (0.38 g, 1.3 mmol, 1.0 equiv.), Bu_4NCl (0.75 g, 2.6 mmol, 2.0 equiv.), and anhydrous THF (30 mL). The product was purified by flash column chromatography (5–10% EtOAc/hexanes) to afford the title compound as an off-white solid (0.300 g, 1.29 mmol, 99%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^{1}H NMR spectrum. Irradiation of the benzylic proton (H_A) gave an NOE enhancement of the proton germinal to the chloride, indicating a cis relationship. **m.p.** 54–56 °C; **TLC R_f** = 0.4 (5% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88–7.78 (m, 4H), 7.53 (dd, *J* = 8.6, 1.5, 1H), 7.49–7.43 (m, 2H), 5.05 (t, *J* = 8.0, 1H), 4.57–4.51 (m, 1H), 4.22 (dd, *J* = 10.2, 3.9, 1H), 4.19 (dd, *J* = 10.0, 5.5, 1H), 2.93 (dt, *J* = 13.9, 7.3, 1H), 2.25 (ddd, *J* = 13.9, 8.2, 5.1, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 138.9, 133.3, 133.2, 128.6, 128.1, 127.8, 126.3, 126.1, 125.0, 124.1, 81.0, 76.3, 56.6, 44.9; **IR** (neat) 3056, 2986, 2854, 1062 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{14}H_{13}ClONH_4$ $(M + NH_4)^+$ 250.0999, found 250.1001.

Scheme SI 6: Synthesis of 31

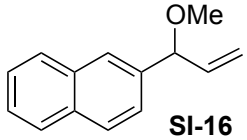




SI-15

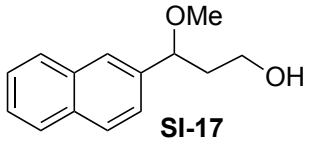
1-(Naphthalen-2-yl)prop-2-en-1-ol (SI-15) A flame-dried 50 mL round bottom flask equipped with a stir bar was charged with 2-naphthaldehyde (0.78 g, 0.0050 mol, 1.0 equiv.) and THF (15 mL). Next, vinylmagnesium bromide (7.3 mL, 0.0060 mol, 0.82 M in Et_2O, 1.2 equiv.) was slowly added to the reaction flask. After 45 min, the reaction was quenched with 1 M HCl (5 mL) and diluted with DI water (10 mL). The reaction mixture was extracted with Et_2O (3 x 10 mL). The combined organics were washed with saturate brine solution (20 mL), then dried over $MgSO_4$. The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a white powder (0.74 g, 4.0 mmol, 80%). **m.p.** 60–65°C; **TLC R_f** = 0.5 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 (t, *J* = 4.5, 2H), 7.76 (d, *J* = 5.0, 2H), 7.46–7.41 (m, 3H), 6.06 (ddd, *J* = 16.6, 10.4, 6.1, 1H),

5.35 (ad, J = 17.1, 1H), 5.28 (d, J = 5.9, 1H), 5.18 (ad, J = 10.5, 1H), 2.40 (br s, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 140.2, 140.0, 133.4, 133.0, 128.4, 128.1, 127.8, 126.2, 126.0, 125.0, 124.6, 115.5, 75.5; **IR** (neat) 3334, 3055, 1601, 1508 cm^{-1}; **HRMS** (TOF MS ES+) m/z calcd for $C_{13}H_{12}ONH_4$ $(M)^+$ 184.0888, found 184.0884.



SI-16

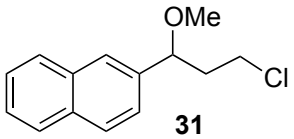
2-(1-Methoxyallyl)naphthalene (SI-16) A flame-dried 50 mL round bottom flask equipped with a stir bar was taken into a glove-box and charged with sodium hydride (0.19 g, 0.0080 mol, 2.0 equiv.). The reaction flask was removed from the glove box and charged with THF (15 mL) and substrate **SI-15** (0.74 g, 0.0040 mol, 1.0 equiv.). The reaction mixture was stirred for 30 min, then iodomethane (0.50 mL, 0.0080 mol, 2.0 equiv.) was added dropwise. The reaction mixture was stirred overnight then quenched with $NaHCO_3$ (15 mL) and extracted with Et_2O (3 x 10 mL). The combined organics were washed with brine (20 mL), then dried over $MgSO_4$. The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a clear, colorless oil (0.53 g, 2.6 mmol, 67%). **TLC R_f** = 0.9 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.85–7.77 (m, 4H), 7.48–7.43 (m, 3H), 6.05–5.96 (m, 1H), 5.33 (ad, J = 17.2, 1H), 5.23 (ad, J = 10.2, 1H), 4.78 (d, J = 5.9, 1H), 3.38−3.35 (m, 3H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 138.8, 138.3, 133.4, 133.2, 128.4, 128.0, 127.8, 126.2, 126.0, 125.8, 124.9, 116.6, 84.8, 56.6; **IR** (neat) 3056, 2981, 2930, 2820, 1601, 1508 cm^{-1}; **HRMS** (TOF MS ES+) m/z calcd for $C_{14}H_{14}O$ $(M)^+$ 198.1045, found 198.1044.



SI-17

3-Methoxy-3-(naphthalen-2-yl)propan-1-ol (SI-17) A flame-dried 250 mL round bottom flask equipped with a stir bar and a reflux condenser was charged with substrate **SI-16** (0.53 g, 0.0027 mol, 1.0 equiv.) and THF (50 ml).The reaction was cooled to 0 ^oC, then BH_3•THF (9.0 mL, 0.0090 mol, 3.4 equiv.) was added slowly to the reaction mixture over 15 min. The reaction mixture was warmed to room temperature and stirred for 3 h. H_2O_2 (11 ml, 30% in H_2O), NaOH (25 ml, 0.75 mol, 3 M in H_2O), and MeOH (21 mL) were added and the reaction mixture was stirred overnight. The reaction was diluted with H_2O (20 mL) and extracted with EtOAc (3 X 25 mL). The combined organics were washed with brine (60 mL) and then dried over $MgSO_4$. The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a clear, colorless oil (0.40 g, 1.8 mmol, 70%). **TLC R_f** = 0.4 (20% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.84–7.77 (m, 3H), 7.72 (s, 1H), 7.48–7.40 (m, 3H), 4.52 (dd, J = 8.6, 4.8, 1H), 3.76 (aq, J = 5.7, 2H), 3.23 (s, 3H), 3.05 (br s, 1H), 2.13 (asext, J = 7.3, 1H), 1.90 (dq, J = 14.8, 4.7 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 139.1, 133.4, 133.3, 128.6, 128.0, 127.8, 126.3, 126.0, 125.8, 124.3,

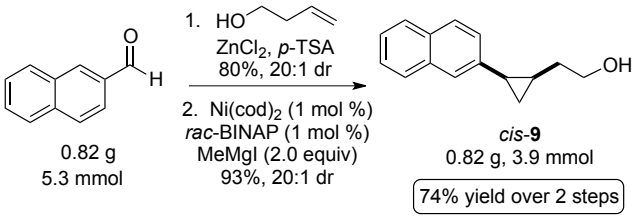
83.4, 60.8, 56.8, 40.5; **IR** (neat) 3370 (br), 3054, 2931, 2822, 1601, 1508 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{14}H_{16}O_2$ $(M)^+$ 216.1150, found 216.1143.



31

2-(3-Chloro-1-methoxypropyl)naphthalene (31). To a flame-dried round bottom flask was added **SI-13** (0.201 g, 0.93 mmol, 1.0 equiv.), triphenylphosphine (0.365 g, 1.40 mmol, 1.5 equiv.) and CH_2Cl_2 (5 mL). Carbon tetrachloride (0.45 mL, 4.65 mmol, 5.0 equiv.) was added drop wise, then the reaction mixture was stirred for 2 h. The reaction was quenched with $NaHCO_3$ (5 mL), then extracted with CH_2Cl2 (3 x 5 mL). The combined organics were washed with saturated brine solution (10 mL) then dried over $MgSO_4$. The product was purified by flash column chromatography (10% EtOAc/hexanes) to afford the title compound as a clear, colorless oil (0.10 g, 0.43 mmol, 46%). **TLC** $\mathbf{R_f}$ = 0.8 (10% EtOAc/hexanes); $^{\mathbf{1}}$**H NMR** (500 MHz, $CDCl_3$) δ 7.84 (at, *J* = 8.2, 3H), 7.76 (s, 1H), 7.51–7.45 (m, 2H), 7.44 (dd, *J* = 8.4, 1.5, 1H), 4.53 (dd, *J* = 8.3, 4.9, 1H), 3.73 (ddd, *J* = 11.0, 8.2, 5.8, 1H), 3.51 (dt, *J* = 11.4, 6.0, 1H), 3.26 (s, 3H), 2.32 (ddt, *J* = 14.5, 8.4, 6.0, 1H), 2.08 (ddt, *J* = 14.0, 8.3, 5.7, 1H); $^{\mathbf{13}}$**C NMR** (125.7 MHz, $CDCl_3$) δ 138.6, 133.31, 133.29, 128.7, 127.9, 127.8, 126.3, 126.1, 126.0, 124.2, 80.6, 57.0, 41.8, 40.8; **IR** (neat) 3056, 2927, 2821, 1508, 1373 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{14}H_{15}ClONH_4$ $(M)^+$ 234.0811, found 234.0816.

M. EXPERIMENTAL DATA FOR GRAM SCALE SYNTHESIS (SCHEME 2)

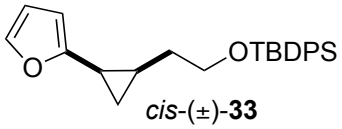


(9)

To a flame dried 250 mL round bottom flask was added $ZnCl_2$ (0.71 g, 5.2 mmol, 1.0 equiv.), *p*-toluenesulfonic acid (1.0 g, 5.2 mmol, 1.0 equiv.), and anhydrous CH_2Cl_2 (30 mL). The mixture was allowed to stir under N_2 for 15 min at ambient temperature. To a separate flame dried flask was added 2-naphthaldehyde (0.82 g, 5.2 mmol, 1.0 equiv.). Anhydrous CH_2Cl_2 (20 mL) and 3-buten-1-ol (0.49 mL, 5.7 mmol, 1.1 equiv.) were added and the mixture was stirred for 5 min at room temperature. The aldehyde solution was added to the $ZnCl_2$ solution and the reaction mixture was allowed to stir at room temperature for 18 h. The reaction was quenched with saturated aqueous $NaHCO_3$ (20 mL) and was extracted with CH_2Cl_2 (3 x 20 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. To remove unreacted aldehyde, the crude mixture was dissolved in 1:1 MeOH/CH_2Cl_2 (50 mL) and cooled to 0 °C. $NaBH_4$ (0.11 g, 3.0 mmol 0.58 equiv.) was added in one portion and the reaction stirred 30 min at 0 °C, then 30 min at room temperature. The reaction was quenched with water and extracted with CH_2Cl_2 (20 mL x 3). The combined organic layers were washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. Flash column chromatography (5–10% EtOAc/hexanes) was used to isolate *cis*-**8** as a white solid (1.03 g, 4.18 mmol, 80%, >20:1 cis:trans dr). The dr was determined based on the integration of the benzylic methines in the ^1H NMR spectrum.

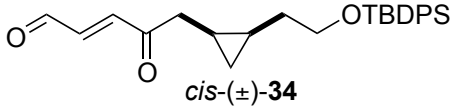
In a glove box, *cis*-**8** (1.02 g, 4.11 mmol, >20:1 dr) was added to a flame dried 100 mL round bottom flask equipped with a stir bar. $Ni(cod)_2$ (12 mg, 0.043 mmol, 0.010 equiv.) *rac*-BINAP (29 mg, 0.047 mmol, 0.010 equiv.), and anhydrous PhMe (40 mL) were added and the reaction was stirred for 5 min. Then methyl magnesium iodide (3.30 mL, 8.25 mmol, 2.50 M in Et_2O, 2.00 equiv.) was added drop wise over three min at room temperature without notable evolution of heat. Upon addition of the Grignard reagent a color change from orange to dark brown was observed. The reaction was stirred in the glove box at room temperature for 48 h before it was removed from the glove box and quenched with isopropyl alcohol (5.0 mL). The crude mixture was passed through a silica gel plug (neat Et_2O) and concentrated in vacuo. Flash column chromatography (20% EtOAc/hexanes) was used to isolate *cis*-**9** as a pale tan oil (0.82 g, 0.39 mmol, 93%, >20:1 cis:trans dr), corresponding to a total yield of 74% over 2 steps. The dr was determined based on the integration of the benzylic methines in the ^1H NMR spectrum.

N. SYNTHESIS OF 34 (SCHEME 4)

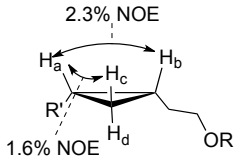


cis-(±)-**33**

***cis*-(±)-*tert*-Butyl(2-(2-(furan-2-yl)cyclopropyl)ethyoxy)diphenylsilane (*cis*-33)** A flame dried round bottom flask was charged with *cis*-**18** (99 mg, 0.65 mmol, 1.0 equiv.), imidazole (53 mg, 0.78 mmol, 1.2 equiv.), and anhydrous CH_2Cl_2 (10 mL). After stirring under N_2 for 15 min, *tert*-butyl(chloro)diphenylsilane (TBDPSCl, 0.20 mL, 0.77 mmol, 1.2 equiv.) was added drop wise. The reaction was stirred for 4 h at room temperature before sat. aq. NH_4Cl (10 mL) was added. The mixture was extracted with CH_2Cl_2 (3 x 10 mL), washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. The product was purified by flash column chromatography (5% EtOAc/hexanes) to afford the title compound as a clear oil (0.224 g, 0.573 mmol, 88%, >20:1 cis:trans dr). The dr was determined based on integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.7 (5% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69–7.62 (m, 4H), 7.44–7.33 (m, 6H), 7.23 (s, 1H), 6.24 (t, *J* = 2.3, 1H), 5.91 (d, *J* = 3.2, 1H), 3.64 (t, *J* = 6.6, 2H), 1.96 (q, *J* = 8.8, 1H), 1.55–1.46 (m, 1H), 1.41–1.32 (m, 1H), 1.28–1.19 (m, 1H), 1.03 (s, 9H), 1.05–0.99 (m, 1H), 0.62 (q, *J* = 5.8, 1H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 155.1, 141.0, 135.73 (2C), 135.71 (2C), 134.2 (2C), 129.61, 129.60, 127.7 (4C), 110.1, 106.2, 63.8, 32.0, 27.0 (3C), 19.4, 16.1, 13.6, 10.4; **IR** (neat) 3071, 2930, 2857, 1106 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{25}H_{30}O_2SiNa$ $(M + Na)^+$ 413.1913, found 413.1921.



cis-(±)-**34**

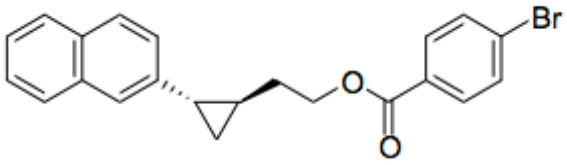


5-(*cis*-(±)-2-(2-((*tert*-Butyldiphenylsilyl)oxy)ethyl)cyclopropyl)-4-oxopent-2-enal (*cis*-34) was prepared according to a procedure reported by Kobayashi.[12] To a 10 mL round bottom flask was added N-bromosuccinamide (NBS, 41 mg, 0.23 mmol, 1.1 equiv.), $NaHCO_3$ (37 mg, 0.44 mmol, 2.2 equiv.) and a 10:1 mixture of acetone: H_2O (1.5 mL). The mixture was set to stir under N_2 at –15 °C for 5 min. A solution of *cis*-**33** (78 mg, 0.20 mmol, 1.0 equiv.) in acetone (0.5 mL) was added drop wise and a color change to bright yellow was observed. After stirring for 45 min at –15 °C, pyridine (0.10 mL, 1.2 mmol, 6.2 equiv.) was added via syringe and the reaction was stirred for 2 h at ambient temperature. The reaction was diluted with EtOAc (2 mL) and quenched with a 3.5 pH HCl solution (20 mL). The mixture was extracted with EtOAc (3 x 20 mL), washed with brine, dried over $MgSO_4$, filtered, and concentrated in vacuo. The product was isolated by flash column chromatography (10% EtOAc/hexane) to afford the title compound as a yellow oil (55 mg, 0.13 mmol, 66%, >20:1 cis:trans dr). The dr was determined based on integration of the benzylic methines in the ^{1}H NMR spectrum. **TLC R_f** = 0.3 (10% EtOAc/hexanes); **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.67 (d, *J* = 7.5, 1H), 7.63 (td, *J* = 7.6, 1.6, 4H), 7.44–7.34 (m, 6H), 6.82 (d, *J* = 16.1, 1H), 6.69 (dd, *J* = 16.1, 7.5, 1H), 3.66–3.60 (m, 1H), 3.55–3.48 (m, 1H), 2.31 (q, *J* = 7.1, 1H), 1.85–1.76 (m, 2H), 1.66–1.56 (m, 1H), 1.31–1.24 (m, 1H), 1.18 (td, *J* = 7.6, 4.2, 1H), 1.04 (s, 9H); **^{13}C NMR** (125.7 MHz, $CDCl_3$) δ 198.0, 193.6, 146.4, 136.6, 135.7 (4C), 134.0, 133.8, 129.8 (2C), 127.8 (4C), 63.9, 29.4, 27.0 (3C), 25.7, 25.2, 19.4, 15.9; **IR** (neat) 2930, 2857, 1696, 1678, 1109, 1082 cm^{-1}; **HRMS** (TOF MS ES+) *m / z* calcd for $C_{25}H_{30}O_3SiNa$ $(M + Na)^+$ 429.1862, found 429.1870.

III. CRYSTALLOGRAPHIC DATA

A. X-ray Data Collection, Structure Solution, and Refinement for *trans*-(1*R*,2*S*)-SI-2:

CCDC Number: 1414041



trans-(1*R*,2*S*)-**SI-2**

A colorless crystal of approximate dimensions 0.126 x 0.279 x 0.528 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[13] program package was used to determine the unit-cell parameters and for data collection (15 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[14] and SADABS[15] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[16] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space groups $P2_1$ and $P2_1/m$. It was later determined that the noncentrosymmetric space group $P2_1$ was correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[17] for neutral atoms were used throughout the analysis. Hydrogen atoms were located from a difference-Fourier map and refined (x,y,z and fixed U_{iso}). There were two molecules of the formula-unit present (Z = 4).

At convergence, wR2 = 0.0514 and Goof = 1.051 for 565 variables refined against 8341 data (0.74Å), R1 = 0.0230 for those 7989 data with $I > 2.0\sigma(I)$. The absolute structure was assigned by refinement of the Flack parameter.[18]

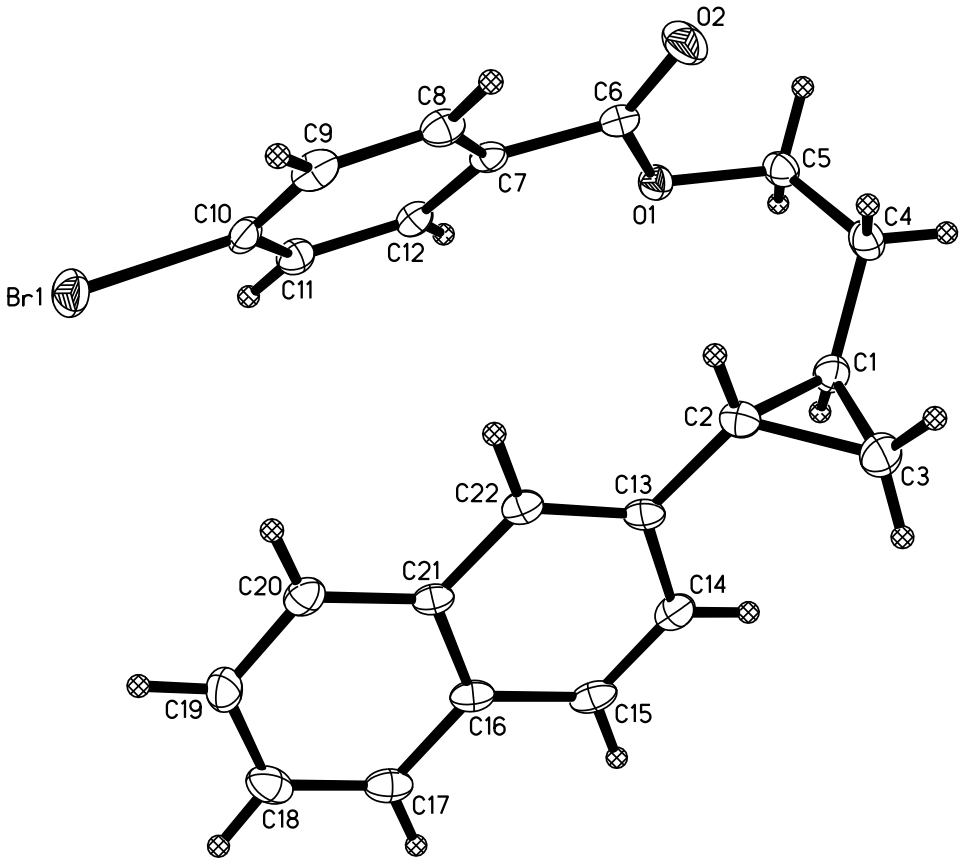
Definitions:

$wR2 = [\Sigma[w(F_o^2-F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$

$Goof = S = [\Sigma[w(F_o^2-F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.


O2
C6
C8
C9
C7
C5
C10
O1
C4
C12
Br1
C11
C1
C2
C3
C22
C13
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C16
C15
C18
C17

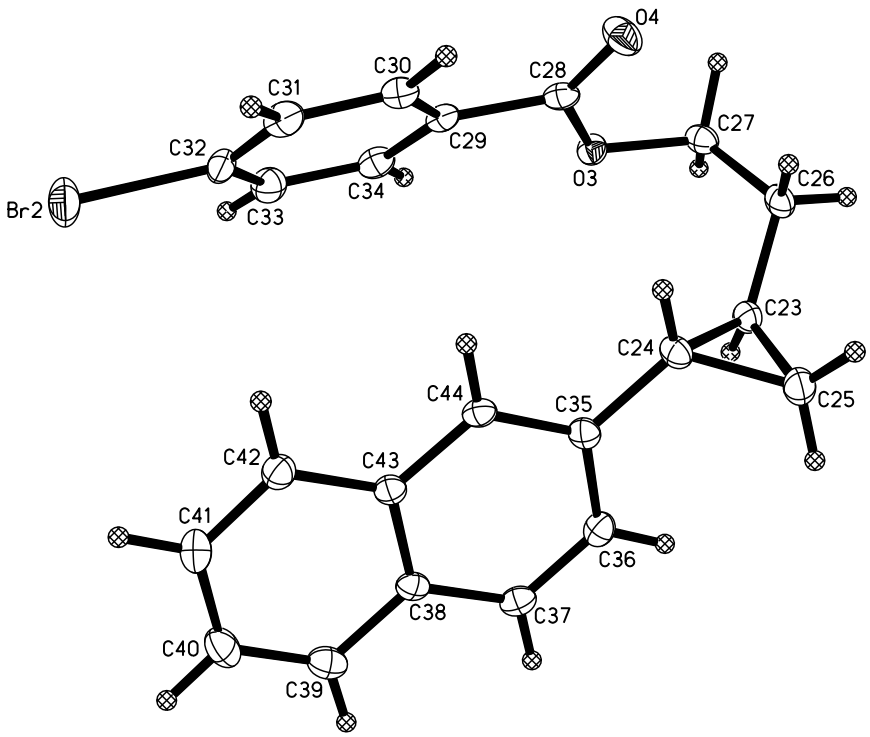


Table 1. Crystal data and structure refinement for erj27.

Identification code	erj27 (Emily Tollefson)	
Empirical formula	C_{22} H_{19} Br O_2	
Formula weight	395.28	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 14.6894(8) Å	α= 90°.
	b = 5.9472(3) Å	β= 98.8906(7)°.
	c = 20.3256(11) Å	γ = 90°.
Volume	1754.33(16) Å^3	
Z	4	

Density (calculated)	1.497 Mg/m^3
Absorption coefficient	2.355 mm^{-1}
F(000)	808
Crystal color	colorless
Crystal size	0.528 x 0.279 x 0.126 mm^3
Theta range for data collection	1.403 to 28.748°
Index ranges	$-19 \leq h \leq 19$, $-8 \leq k \leq 7$, $-27 \leq l \leq 27$
Reflections collected	21151
Independent reflections	8341 [R(int) = 0.0181]
Completeness to theta = 25.500°	100.0 %
Absorption correction	Numerical
Max. and min. transmission	0.5922 and 0.3438
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8341 / 1 / 565
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I) = 7989 data]	R1 = 0.0230, wR2 = 0.0507
R indices (all data, 0.74Å)	R1 = 0.0250, wR2 = 0.0514
Absolute structure parameter	-0.012(2)
Largest diff. peak and hole	0.419 and -0.195 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for erj27. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-2448(1)	9730(1)	1825(1)	22(1)
O(1)	-4555(1)	5098(3)	-1056(1)	16(1)
O(2)	-4742(1)	8715(3)	-1378(1)	26(1)
C(1)	-3193(2)	3610(4)	-1868(1)	18(1)
C(2)	-2504(2)	4903(5)	-1374(1)	18(1)
C(3)	-2310(2)	4428(6)	-2074(1)	25(1)
C(4)	-4086(2)	4720(5)	-2160(1)	19(1)
C(5)	-4850(2)	4374(4)	-1743(1)	17(1)
C(6)	-4487(2)	7317(4)	-957(1)	16(1)
C(7)	-4036(2)	7871(4)	-266(1)	14(1)
C(8)	-3673(2)	10027(4)	-146(1)	17(1)
C(9)	-3193(2)	10558(5)	478(1)	18(1)
C(10)	-3111(2)	8951(4)	977(1)	16(1)
C(11)	-3486(2)	6833(4)	874(1)	16(1)
C(12)	-3945(2)	6290(4)	244(1)	15(1)
C(13)	-1966(2)	3771(4)	-787(1)	16(1)
C(14)	-1599(2)	1573(4)	-837(1)	18(1)
C(15)	-1067(2)	584(5)	-310(1)	18(1)
C(16)	-861(2)	1701(4)	311(1)	16(1)
C(17)	-275(2)	759(5)	860(1)	20(1)
C(18)	-73(2)	1913(5)	1445(1)	24(1)
C(19)	-464(2)	4047(5)	1515(1)	23(1)
C(20)	-1034(2)	5008(4)	995(1)	18(1)
C(21)	-1240(2)	3884(4)	375(1)	15(1)
C(22)	-1795(1)	4860(4)	-186(1)	15(1)
Br(2)	3128(1)	5460(1)	-6724(1)	29(1)
O(3)	4237(1)	146(3)	-3756(1)	15(1)
O(4)	4178(1)	3666(3)	-3356(1)	24(1)
C(23)	2669(2)	-1634(4)	-3178(1)	16(1)
C(24)	2051(2)	-102(5)	-3656(1)	16(1)
C(25)	1728(2)	-1015(5)	-3032(1)	21(1)
C(26)	3506(2)	-637(4)	-2757(1)	17(1)
C(27)	4375(2)	-745(4)	-3077(1)	17(1)
C(28)	4138(2)	2375(4)	-3818(1)	16(1)
C(29)	3942(2)	3087(4)	-4531(1)	15(1)
C(30)	3562(2)	5208(4)	-4670(1)	17(1)
C(31)	3314(2)	5905(4)	-5326(1)	20(1)
C(32)	3476(2)	4479(5)	-5833(1)	19(1)
C(33)	3876(2)	2384(5)	-5705(1)	21(1)
C(34)	4100(2)	1680(4)	-5048(1)	18(1)
C(35)	1633(2)	-833(4)	-4335(1)	15(1)
C(36)	1196(2)	-2954(4)	-4459(1)	17(1)
C(37)	787(2)	-3551(4)	-5084(1)	16(1)

C(38)	786(2)	-2081(4)	-5632(1)	15(1)
C(39)	326(2)	-2594(5)	-6284(1)	21(1)
C(40)	322(2)	-1093(5)	-6793(1)	23(1)
C(41)	781(2)	983(5)	-6682(1)	22(1)
C(42)	1230(2)	1536(4)	-6063(1)	18(1)
C(43)	1236(1)	40(4)	-5522(1)	15(1)
C(44)	1655(2)	611(4)	-4865(1)	15(1)

Table 3. Bond lengths [Å] and angles [°] for erj27.

Br(1)-C(10)	1.902(2)
O(1)-C(6)	1.337(3)
O(1)-C(5)	1.461(3)
O(2)-C(6)	1.210(3)
C(1)-C(3)	1.504(3)
C(1)-C(4)	1.506(3)
C(1)-C(2)	1.520(3)
C(2)-C(13)	1.486(3)
C(2)-C(3)	1.519(4)
C(4)-C(5)	1.520(3)
C(6)-C(7)	1.494(3)
C(7)-C(12)	1.390(3)
C(7)-C(8)	1.395(3)
C(8)-C(9)	1.389(3)
C(9)-C(10)	1.385(4)
C(10)-C(11)	1.378(4)
C(11)-C(12)	1.390(3)
C(13)-C(22)	1.372(3)
C(13)-C(14)	1.424(4)
C(14)-C(15)	1.359(4)
C(15)-C(16)	1.418(4)
C(16)-C(17)	1.415(3)
C(16)-C(21)	1.426(3)
C(17)-C(18)	1.364(4)
C(18)-C(19)	1.409(4)
C(19)-C(20)	1.368(4)
C(20)-C(21)	1.417(3)
C(21)-C(22)	1.419(3)
Br(2)-C(32)	1.897(2)
O(3)-C(28)	1.337(3)
O(3)-C(27)	1.463(3)
O(4)-C(28)	1.208(3)
C(23)-C(25)	1.504(3)
C(23)-C(26)	1.507(3)
C(23)-C(24)	1.524(3)
C(24)-C(35)	1.486(3)
C(24)-C(25)	1.522(4)
C(26)-C(27)	1.521(3)
C(28)-C(29)	1.494(3)
C(29)-C(34)	1.391(4)
C(29)-C(30)	1.391(3)
C(30)-C(31)	1.390(3)
C(31)-C(32)	1.383(4)
C(32)-C(33)	1.385(4)
C(33)-C(34)	1.388(4)
C(35)-C(44)	1.382(3)

C(35)-C(36)	1.420(3)
C(36)-C(37)	1.366(4)
C(37)-C(38)	1.416(3)
C(38)-C(39)	1.424(3)
C(38)-C(43)	1.426(3)
C(39)-C(40)	1.366(4)
C(40)-C(41)	1.408(4)
C(41)-C(42)	1.367(4)
C(42)-C(43)	1.414(3)
C(43)-C(44)	1.421(3)

C(6)-O(1)-C(5)	116.07(19)
C(3)-C(1)-C(4)	119.1(2)
C(3)-C(1)-C(2)	60.33(16)
C(4)-C(1)-C(2)	119.3(2)
C(13)-C(2)-C(3)	120.9(2)
C(13)-C(2)-C(1)	121.2(2)
C(3)-C(2)-C(1)	59.33(16)
C(1)-C(3)-C(2)	60.34(16)
C(1)-C(4)-C(5)	113.3(2)
O(1)-C(5)-C(4)	110.91(19)
O(2)-C(6)-O(1)	124.3(2)
O(2)-C(6)-C(7)	123.8(2)
O(1)-C(6)-C(7)	111.8(2)
C(12)-C(7)-C(8)	120.1(2)
C(12)-C(7)-C(6)	121.9(2)
C(8)-C(7)-C(6)	117.9(2)
C(9)-C(8)-C(7)	119.6(2)
C(10)-C(9)-C(8)	119.1(2)
C(11)-C(10)-C(9)	122.2(2)
C(11)-C(10)-Br(1)	119.80(19)
C(9)-C(10)-Br(1)	118.04(19)
C(10)-C(11)-C(12)	118.5(2)
C(11)-C(12)-C(7)	120.5(2)
C(22)-C(13)-C(14)	118.5(2)
C(22)-C(13)-C(2)	120.2(2)
C(14)-C(13)-C(2)	121.2(2)
C(15)-C(14)-C(13)	121.3(2)
C(14)-C(15)-C(16)	121.1(2)
C(17)-C(16)-C(15)	122.5(2)
C(17)-C(16)-C(21)	119.2(2)
C(15)-C(16)-C(21)	118.4(2)
C(18)-C(17)-C(16)	120.7(3)
C(17)-C(18)-C(19)	120.3(3)
C(20)-C(19)-C(18)	120.6(3)
C(19)-C(20)-C(21)	120.7(2)
C(20)-C(21)-C(22)	122.5(2)
C(20)-C(21)-C(16)	118.5(2)

C(22)-C(21)-C(16)	118.9(2)
C(13)-C(22)-C(21)	121.7(2)
C(28)-O(3)-C(27)	116.48(19)
C(25)-C(23)-C(26)	119.0(2)
C(25)-C(23)-C(24)	60.34(16)
C(26)-C(23)-C(24)	118.7(2)
C(35)-C(24)-C(25)	122.2(2)
C(35)-C(24)-C(23)	122.5(2)
C(25)-C(24)-C(23)	59.18(16)
C(23)-C(25)-C(24)	60.47(16)
C(23)-C(26)-C(27)	113.9(2)
O(3)-C(27)-C(26)	112.62(19)
O(4)-C(28)-O(3)	124.4(2)
O(4)-C(28)-C(29)	123.6(2)
O(3)-C(28)-C(29)	112.0(2)
C(34)-C(29)-C(30)	120.1(2)
C(34)-C(29)-C(28)	122.2(2)
C(30)-C(29)-C(28)	117.7(2)
C(31)-C(30)-C(29)	120.1(2)
C(32)-C(31)-C(30)	118.8(2)
C(31)-C(32)-C(33)	121.9(2)
C(31)-C(32)-Br(2)	118.1(2)
C(33)-C(32)-Br(2)	120.0(2)
C(32)-C(33)-C(34)	118.9(2)
C(33)-C(34)-C(29)	120.2(2)
C(44)-C(35)-C(36)	118.5(2)
C(44)-C(35)-C(24)	119.1(2)
C(36)-C(35)-C(24)	122.4(2)
C(37)-C(36)-C(35)	121.2(2)
C(36)-C(37)-C(38)	121.2(2)
C(37)-C(38)-C(39)	122.8(2)
C(37)-C(38)-C(43)	118.6(2)
C(39)-C(38)-C(43)	118.5(2)
C(40)-C(39)-C(38)	120.7(2)
C(39)-C(40)-C(41)	120.3(2)
C(42)-C(41)-C(40)	120.7(2)
C(41)-C(42)-C(43)	120.6(2)
C(42)-C(43)-C(44)	122.0(2)
C(42)-C(43)-C(38)	119.2(2)
C(44)-C(43)-C(38)	118.8(2)
C(35)-C(44)-C(43)	121.6(2)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for erj27. 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}
Br(1)	22(1)	25(1)	19(1)	-8(1)	2(1)	-3(1)
O(1)	17(1)	16(1)	15(1)	-1(1)	2(1)	0(1)
O(2)	34(1)	18(1)	22(1)	2(1)	-4(1)	6(1)
C(1)	16(1)	20(1)	17(1)	-2(1)	3(1)	-1(1)
C(2)	15(1)	19(1)	20(1)	0(1)	1(1)	1(1)
C(3)	17(1)	37(2)	21(1)	1(1)	6(1)	-1(1)
C(4)	17(1)	22(1)	16(1)	0(1)	0(1)	-2(1)
C(5)	16(1)	17(1)	17(1)	-2(1)	-2(1)	0(1)
C(6)	14(1)	16(1)	20(1)	0(1)	4(1)	3(1)
C(7)	10(1)	15(1)	18(1)	-2(1)	2(1)	1(1)
C(8)	18(1)	13(1)	22(1)	2(1)	6(1)	1(1)
C(9)	16(1)	13(1)	26(1)	-3(1)	7(1)	-3(1)
C(10)	13(1)	21(1)	16(1)	-7(1)	4(1)	1(1)
C(11)	16(1)	16(1)	18(1)	1(1)	5(1)	1(1)
C(12)	15(1)	14(1)	18(1)	-2(1)	6(1)	-1(1)
C(13)	8(1)	18(1)	21(1)	0(1)	2(1)	-1(1)
C(14)	14(1)	19(1)	23(1)	-7(1)	4(1)	-3(1)
C(15)	13(1)	13(1)	31(1)	-3(1)	7(1)	-1(1)
C(16)	10(1)	15(1)	25(1)	3(1)	6(1)	-2(1)
C(17)	15(1)	19(1)	29(1)	7(1)	7(1)	1(1)
C(18)	16(1)	33(2)	22(1)	10(1)	3(1)	1(1)
C(19)	21(1)	34(2)	15(1)	-2(1)	4(1)	-2(1)
C(20)	15(1)	20(1)	21(1)	-2(1)	6(1)	-2(1)

C(21)	9(1)	15(1)	21(1)	1(1)	5(1)	-2(1)
C(22)	12(1)	13(1)	21(1)	-1(1)	4(1)	-2(1)
Br(2)	30(1)	38(1)	19(1)	11(1)	3(1)	1(1)
O(3)	18(1)	12(1)	16(1)	1(1)	3(1)	0(1)
O(4)	33(1)	16(1)	19(1)	-1(1)	-4(1)	0(1)
C(23)	16(1)	19(1)	14(1)	2(1)	1(1)	0(1)
C(24)	16(1)	17(1)	15(1)	1(1)	-1(1)	1(1)
C(25)	16(1)	31(1)	16(1)	2(1)	2(1)	1(1)
C(26)	19(1)	18(1)	13(1)	2(1)	-1(1)	1(1)
C(27)	17(1)	14(1)	17(1)	1(1)	-2(1)	0(1)
C(28)	11(1)	15(1)	21(1)	1(1)	0(1)	-1(1)
C(29)	13(1)	15(1)	19(1)	1(1)	3(1)	-3(1)
C(30)	15(1)	14(1)	20(1)	-1(1)	2(1)	-1(1)
C(31)	15(1)	17(1)	26(1)	6(1)	1(1)	1(1)
C(32)	17(1)	24(1)	17(1)	7(1)	2(1)	-4(1)
C(33)	21(1)	22(1)	21(1)	-2(1)	6(1)	-2(1)
C(34)	15(1)	17(1)	24(1)	1(1)	4(1)	0(1)
C(35)	12(1)	18(1)	16(1)	1(1)	1(1)	3(1)
C(36)	16(1)	16(1)	18(1)	5(1)	3(1)	3(1)
C(37)	13(1)	14(1)	23(1)	1(1)	3(1)	1(1)
C(38)	10(1)	16(1)	17(1)	-2(1)	2(1)	1(1)
C(39)	19(1)	20(1)	23(1)	-5(1)	1(1)	-1(1)
C(40)	24(1)	29(1)	15(1)	-4(1)	1(1)	2(1)
C(41)	27(1)	24(2)	16(1)	3(1)	5(1)	2(1)
C(42)	17(1)	19(1)	18(1)	1(1)	4(1)	0(1)
C(43)	11(1)	18(1)	16(1)	0(1)	2(1)	1(1)
C(44)	11(1)	14(1)	18(1)	1(1)	1(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)for erj27.

	x	y	z	U(eq)
H(1A)	-3231(19)	2040(50)	-1766(14)	21
H(2A)	-2680(20)	6410(60)	-1312(14)	22
H(3A)	-2320(20)	5670(60)	-2375(15)	30
H(3B)	-1880(20)	3310(60)	-2125(15)	30
H(4A)	-4301(19)	4100(50)	-2593(14)	22
H(4B)	-3965(19)	6290(60)	-2192(14)	22
H(5A)	-5398(18)	5120(50)	-1928(13)	21
H(5B)	-4960(20)	2820(50)	-1686(14)	21
H(8A)	-3733(19)	11080(50)	-458(14)	20
H(9A)	-2940(20)	11870(50)	566(14)	22
H(11A)	-3420(18)	5760(50)	1226(13)	20
H(12A)	-4211(17)	4790(60)	171(13)	19
H(14A)	-1731(19)	910(50)	-1223(14)	22
H(15A)	-810(19)	-850(60)	-359(14)	22
H(17A)	-20(20)	-690(60)	809(14)	24
H(18A)	320(20)	1250(60)	1790(15)	28
H(19A)	-340(19)	4860(60)	1910(14)	28
H(20A)	-1280(20)	6410(60)	1054(14)	22
H(22A)	-2049(18)	6430(50)	-137(13)	18
H(23A)	2758(19)	-3160(50)	-3341(14)	19
H(24A)	2256(19)	1430(50)	-3611(14)	20
H(25A)	1686(18)	20(50)	-2676(14)	25
H(25B)	1270(20)	-2110(60)	-3084(15)	25

H(26A)	3661(19)	-1510(50)	-2342(14)	20
H(26B)	3391(19)	910(50)	-2660(13)	20
H(27A)	4868(18)	210(50)	-2828(13)	20
H(27B)	4520(20)	-2190(50)	-3144(14)	20
H(30A)	3460(19)	6230(50)	-4329(14)	20
H(31A)	3010(20)	7300(50)	-5413(14)	24
H(33A)	4000(20)	1480(50)	-6059(15)	25
H(34A)	4371(18)	180(50)	-4960(13)	22
H(36A)	1167(19)	-3960(50)	-4115(14)	20
H(37A)	505(18)	-5010(50)	-5149(13)	20
H(39A)	10(20)	-3930(60)	-6331(14)	25
H(40A)	20(20)	-1530(50)	-7229(15)	28
H(41A)	800(20)	2010(50)	-7036(15)	26
H(42A)	1540(20)	2990(50)	-5984(14)	21
H(44A)	1953(19)	2030(50)	-4786(13)	18

Table 6. Torsion angles [°] for erj27.

C(3)-C(1)-C(2)-C(13)	-109.8(3)
C(4)-C(1)-C(2)-C(13)	141.4(2)
C(4)-C(1)-C(2)-C(3)	-108.7(3)
C(4)-C(1)-C(3)-C(2)	109.1(3)
C(13)-C(2)-C(3)-C(1)	110.3(3)
C(3)-C(1)-C(4)-C(5)	-158.9(2)
C(2)-C(1)-C(4)-C(5)	-88.6(3)
C(6)-O(1)-C(5)-C(4)	72.7(3)
C(1)-C(4)-C(5)-O(1)	54.4(3)
C(5)-O(1)-C(6)-O(2)	8.0(3)
C(5)-O(1)-C(6)-C(7)	-170.55(18)
O(2)-C(6)-C(7)-C(12)	165.0(2)
O(1)-C(6)-C(7)-C(12)	-16.5(3)
O(2)-C(6)-C(7)-C(8)	-17.2(4)
O(1)-C(6)-C(7)-C(8)	161.3(2)
C(12)-C(7)-C(8)-C(9)	2.2(3)
C(6)-C(7)-C(8)-C(9)	-175.6(2)
C(7)-C(8)-C(9)-C(10)	-2.1(3)
C(8)-C(9)-C(10)-C(11)	0.3(4)
C(8)-C(9)-C(10)-Br(1)	179.87(17)
C(9)-C(10)-C(11)-C(12)	1.3(4)
Br(1)-C(10)-C(11)-C(12)	-178.20(18)
C(10)-C(11)-C(12)-C(7)	-1.2(4)
C(8)-C(7)-C(12)-C(11)	-0.5(4)
C(6)-C(7)-C(12)-C(11)	177.2(2)
C(3)-C(2)-C(13)-C(22)	147.9(2)

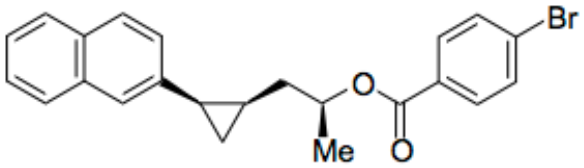
C(1)-C(2)-C(13)-C(22)	-141.5(2)
C(3)-C(2)-C(13)-C(14)	-30.6(3)
C(1)-C(2)-C(13)-C(14)	40.0(3)
C(22)-C(13)-C(14)-C(15)	-2.1(3)
C(2)-C(13)-C(14)-C(15)	176.4(2)
C(13)-C(14)-C(15)-C(16)	0.4(4)
C(14)-C(15)-C(16)-C(17)	-177.1(2)
C(14)-C(15)-C(16)-C(21)	1.0(3)
C(15)-C(16)-C(17)-C(18)	178.2(2)
C(21)-C(16)-C(17)-C(18)	0.1(3)
C(16)-C(17)-C(18)-C(19)	1.4(4)
C(17)-C(18)-C(19)-C(20)	-1.3(4)
C(18)-C(19)-C(20)-C(21)	-0.3(4)
C(19)-C(20)-C(21)-C(22)	-177.2(2)
C(19)-C(20)-C(21)-C(16)	1.7(3)
C(17)-C(16)-C(21)-C(20)	-1.6(3)
C(15)-C(16)-C(21)-C(20)	-179.8(2)
C(17)-C(16)-C(21)-C(22)	177.3(2)
C(15)-C(16)-C(21)-C(22)	-0.9(3)
C(14)-C(13)-C(22)-C(21)	2.2(3)
C(2)-C(13)-C(22)-C(21)	-176.3(2)
C(20)-C(21)-C(22)-C(13)	178.1(2)
C(16)-C(21)-C(22)-C(13)	-0.8(3)
C(25)-C(23)-C(24)-C(35)	-110.8(3)
C(26)-C(23)-C(24)-C(35)	140.2(2)
C(26)-C(23)-C(24)-C(25)	-109.0(3)
C(26)-C(23)-C(25)-C(24)	108.4(3)
C(35)-C(24)-C(25)-C(23)	111.3(3)

C(25)-C(23)-C(26)-C(27)	-161.1(2)
C(24)-C(23)-C(26)-C(27)	-91.1(3)
C(28)-O(3)-C(27)-C(26)	71.7(3)
C(23)-C(26)-C(27)-O(3)	50.9(3)
C(27)-O(3)-C(28)-O(4)	1.9(3)
C(27)-O(3)-C(28)-C(29)	-176.43(18)
O(4)-C(28)-C(29)-C(34)	165.3(2)
O(3)-C(28)-C(29)-C(34)	-16.4(3)
O(4)-C(28)-C(29)-C(30)	-16.8(4)
O(3)-C(28)-C(29)-C(30)	161.5(2)
C(34)-C(29)-C(30)-C(31)	1.9(3)
C(28)-C(29)-C(30)-C(31)	-176.1(2)
C(29)-C(30)-C(31)-C(32)	-1.7(3)
C(30)-C(31)-C(32)-C(33)	0.0(4)
C(30)-C(31)-C(32)-Br(2)	179.76(17)
C(31)-C(32)-C(33)-C(34)	1.6(4)
Br(2)-C(32)-C(33)-C(34)	-178.14(19)
C(32)-C(33)-C(34)-C(29)	-1.5(4)
C(30)-C(29)-C(34)-C(33)	-0.2(4)
C(28)-C(29)-C(34)-C(33)	177.6(2)
C(25)-C(24)-C(35)-C(44)	153.2(2)
C(23)-C(24)-C(35)-C(44)	-135.3(2)
C(25)-C(24)-C(35)-C(36)	-25.7(3)
C(23)-C(24)-C(35)-C(36)	45.8(3)
C(44)-C(35)-C(36)-C(37)	-1.4(3)
C(24)-C(35)-C(36)-C(37)	177.5(2)
C(35)-C(36)-C(37)-C(38)	0.3(4)
C(36)-C(37)-C(38)-C(39)	-176.7(2)

C(36)-C(37)-C(38)-C(43)	0.9(3)
C(37)-C(38)-C(39)-C(40)	178.1(2)
C(43)-C(38)-C(39)-C(40)	0.5(4)
C(38)-C(39)-C(40)-C(41)	0.5(4)
C(39)-C(40)-C(41)-C(42)	-0.5(4)
C(40)-C(41)-C(42)-C(43)	-0.5(4)
C(41)-C(42)-C(43)-C(44)	-176.6(2)
C(41)-C(42)-C(43)-C(38)	1.5(4)
C(37)-C(38)-C(43)-C(42)	-179.2(2)
C(39)-C(38)-C(43)-C(42)	-1.5(3)
C(37)-C(38)-C(43)-C(44)	-1.0(3)
C(39)-C(38)-C(43)-C(44)	176.8(2)
C(36)-C(35)-C(44)-C(43)	1.4(3)
C(24)-C(35)-C(44)-C(43)	-177.6(2)
C(42)-C(43)-C(44)-C(35)	178.0(2)
C(38)-C(43)-C(44)-C(35)	-0.2(3)

B. X-ray Data Collection, Structure Solution, and Refinement for (1*S*)-(*cis*-(1*R*,2*R*)-SI-3:

CCDC Number: 1413565



(1*S*)-(*cis*-(1*R*,2*R*))-**SI-3**

A colorless crystal of approximate dimensions 0.116 x 0.258 x 0.438 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2[13] program package was used to determine the unit-cell parameters and for data collection (10 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[14] and SADABS[15] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[16] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space groups $P2_1$ and $P2_1/m$. It was later determined that space group $P2_1$ was correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[17] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

At convergence, wR2 = 0.0918 and Goof = 1.041 for 344 variables refined against 5777 data (0.74Å), R1 = 0.0373 for those 5215 data with $I > 2.0\sigma(I)$. The absolute structure was assigned by refinement of the Flack[18] parameter.

Definitions:

$wR2 = [\Sigma[w(F_o^2-F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$

$Goof = S = [\Sigma[w(F_o^2-F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.

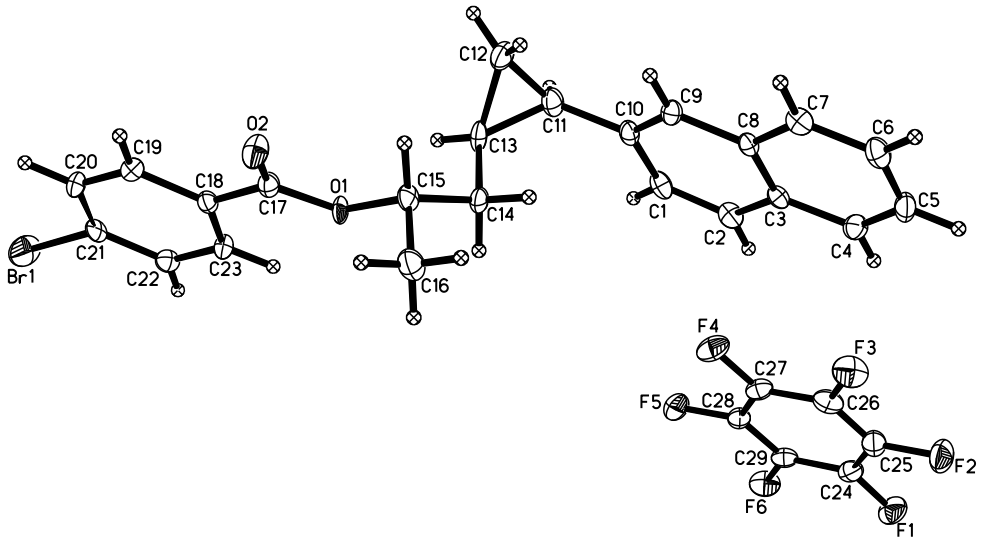


Table 1. Crystal data and structure refinement for erj25.

Identification code	erj25 (Lucas Erickson)	
Empirical formula	$C_{29}\ H_{21}\ Br\ F_6\ O_2$	
Formula weight	595.37	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 7.4814(5) Å	α= 90°.
	b = 6.0033(4) Å	β= 97.0064(8)°.
	c = 27.9363(18) Å	γ = 90°.
Volume	1245.34(14) Å^3	
Z	2	
Density (calculated)	1.588 Mg/m^3	

Absorption coefficient	1.722 mm^{-1}
F(000)	600
Crystal color	colorless
Crystal size	0.438 x 0.258 x 0.116 mm^3
Theta range for data collection	1.469 to 28.803°
Index ranges	$-9 \le h \le 10$, $-8 \le k \le 8$, $-37 \le l \le 37$
Reflections collected	15060
Independent reflections	5777 [R(int) = 0.0276]
Completeness to theta = 25.500°	99.7 %
Absorption correction	Numerical
Max. and min. transmission	0.8040 and 0.5925
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5777 / 1 / 344
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I) = 5215 data]	R1 = 0.0373, wR2 = 0.0888
R indices (all data, 0.74Å)	R1 = 0.0434, wR2 = 0.0918
Absolute structure parameter	0.005(4)
Largest diff. peak and hole	0.633 and -0.422 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for erj25. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	859(1)	10016(1)	3940(1)	38(1)
O(1)	3911(3)	12042(4)	6286(1)	16(1)
O(2)	4370(4)	15463(5)	5998(1)	24(1)
C(1)	7127(5)	6005(6)	7883(1)	20(1)
C(2)	6917(5)	5593(6)	8350(1)	20(1)
C(3)	7460(5)	7183(6)	8715(1)	16(1)
C(4)	7310(5)	6792(7)	9209(1)	20(1)
C(5)	7863(5)	8354(7)	9551(1)	22(1)
C(6)	8609(5)	10392(7)	9416(1)	22(1)
C(7)	8780(5)	10811(6)	8939(1)	19(1)
C(8)	8197(5)	9238(6)	8576(1)	14(1)
C(9)	8400(5)	9603(6)	8082(1)	16(1)
C(10)	7890(5)	8024(6)	7736(1)	17(1)
C(11)	8088(5)	8269(7)	7213(1)	21(1)
C(12)	8553(5)	10392(7)	6984(1)	25(1)
C(13)	6683(5)	9479(6)	6866(1)	20(1)
C(14)	5138(5)	10664(6)	7051(1)	17(1)
C(15)	4558(5)	12775(6)	6772(1)	17(1)
C(16)	3067(5)	13995(7)	6985(2)	25(1)
C(17)	3888(5)	13583(6)	5935(1)	16(1)
C(18)	3169(5)	12625(6)	5456(1)	15(1)
C(19)	3303(5)	13939(7)	5048(1)	18(1)
C(20)	2634(5)	13171(7)	4595(1)	20(1)
C(21)	1824(5)	11092(7)	4556(1)	18(1)
C(22)	1689(5)	9758(7)	4954(1)	18(1)
C(23)	2385(5)	10526(6)	5407(1)	16(1)
C(24)	2249(5)	-3261(7)	9060(2)	23(1)
C(25)	3032(6)	-1329(7)	9258(2)	24(1)
C(26)	3622(5)	268(8)	8964(1)	24(1)
C(27)	3425(5)	-24(8)	8470(1)	21(1)
C(28)	2650(5)	-1950(7)	8271(1)	20(1)
C(29)	2075(5)	-3556(7)	8567(2)	21(1)
F(1)	1647(3)	-4812(5)	9342(1)	33(1)
F(2)	3216(4)	-1036(5)	9732(1)	37(1)
F(3)	4374(4)	2148(4)	9151(1)	34(1)
F(4)	3986(3)	1536(4)	8181(1)	30(1)
F(5)	2452(3)	-2235(4)	7796(1)	29(1)
F(6)	1305(3)	-5431(4)	8374(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for erj25.

Br(1)-C(21)	1.896(3)
O(1)-C(17)	1.347(5)
O(1)-C(15)	1.453(4)
O(2)-C(17)	1.191(5)
C(1)-C(2)	1.356(5)
C(1)-C(10)	1.421(6)
C(2)-C(3)	1.420(5)
C(3)-C(4)	1.418(5)
C(3)-C(8)	1.425(5)
C(4)-C(5)	1.366(6)
C(5)-C(6)	1.414(6)
C(6)-C(7)	1.376(5)
C(7)-C(8)	1.416(5)
C(8)-C(9)	1.424(5)
C(9)-C(10)	1.372(5)
C(10)-C(11)	1.496(5)
C(11)-C(12)	1.486(6)
C(11)-C(13)	1.523(5)
C(12)-C(13)	1.501(6)
C(13)-C(14)	1.502(5)
C(14)-C(15)	1.522(5)
C(15)-C(16)	1.516(5)
C(17)-C(18)	1.496(5)
C(18)-C(23)	1.390(5)
C(18)-C(19)	1.401(5)
C(19)-C(20)	1.381(5)
C(20)-C(21)	1.386(6)
C(21)-C(22)	1.384(5)
C(22)-C(23)	1.388(5)
C(24)-F(1)	1.333(5)
C(24)-C(29)	1.378(6)
C(24)-C(25)	1.384(6)
C(25)-F(2)	1.327(5)
C(25)-C(26)	1.370(6)
C(26)-F(3)	1.339(5)
C(26)-C(27)	1.380(5)
C(27)-F(4)	1.337(5)
C(27)-C(28)	1.379(6)
C(28)-F(5)	1.331(4)
C(28)-C(29)	1.372(6)
C(29)-F(6)	1.346(5)
C(17)-O(1)-C(15)	116.5(3)
C(2)-C(1)-C(10)	122.0(3)
C(1)-C(2)-C(3)	120.8(3)
C(4)-C(3)-C(2)	122.6(3)

C(4)-C(3)-C(8)	119.2(3)
C(2)-C(3)-C(8)	118.2(3)
C(5)-C(4)-C(3)	120.9(4)
C(4)-C(5)-C(6)	120.2(3)
C(7)-C(6)-C(5)	120.2(4)
C(6)-C(7)-C(8)	121.0(4)
C(7)-C(8)-C(9)	122.2(3)
C(7)-C(8)-C(3)	118.5(3)
C(9)-C(8)-C(3)	119.2(3)
C(10)-C(9)-C(8)	121.4(3)
C(9)-C(10)-C(1)	118.3(3)
C(9)-C(10)-C(11)	124.6(4)
C(1)-C(10)-C(11)	117.1(3)
C(12)-C(11)-C(10)	124.1(3)
C(12)-C(11)-C(13)	59.8(3)
C(10)-C(11)-C(13)	121.7(3)
C(11)-C(12)-C(13)	61.3(3)
C(12)-C(13)-C(14)	119.2(3)
C(12)-C(13)-C(11)	58.9(3)
C(14)-C(13)-C(11)	120.5(3)
C(13)-C(14)-C(15)	113.7(3)
O(1)-C(15)-C(16)	109.6(3)
O(1)-C(15)-C(14)	105.5(3)
C(16)-C(15)-C(14)	112.3(3)
O(2)-C(17)-O(1)	124.6(4)
O(2)-C(17)-C(18)	124.4(4)
O(1)-C(17)-C(18)	111.0(3)
C(23)-C(18)-C(19)	120.1(3)
C(23)-C(18)-C(17)	122.6(3)
C(19)-C(18)-C(17)	117.3(3)
C(20)-C(19)-C(18)	120.3(4)
C(19)-C(20)-C(21)	118.6(4)
C(22)-C(21)-C(20)	122.1(3)
C(22)-C(21)-Br(1)	118.4(3)
C(20)-C(21)-Br(1)	119.5(3)
C(21)-C(22)-C(23)	119.0(4)
C(22)-C(23)-C(18)	119.9(3)
F(1)-C(24)-C(29)	120.2(4)
F(1)-C(24)-C(25)	120.4(4)
C(29)-C(24)-C(25)	119.4(4)
F(2)-C(25)-C(26)	120.3(4)
F(2)-C(25)-C(24)	119.8(4)
C(26)-C(25)-C(24)	119.9(4)
F(3)-C(26)-C(25)	120.4(4)
F(3)-C(26)-C(27)	119.1(4)
C(25)-C(26)-C(27)	120.5(4)
F(4)-C(27)-C(28)	119.5(3)
F(4)-C(27)-C(26)	120.7(4)

C(28)-C(27)-C(26)	119.8(4)
F(5)-C(28)-C(29)	120.4(4)
F(5)-C(28)-C(27)	120.0(4)
C(29)-C(28)-C(27)	119.6(4)
F(6)-C(29)-C(28)	119.8(4)
F(6)-C(29)-C(24)	119.4(4)
C(28)-C(29)-C(24)	120.8(4)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for erj25. 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}
Br(1)	38(1)	60(1)	16(1)	-7(1)	1(1)	-18(1)
O(1)	23(1)	17(1)	8(1)	2(1)	-3(1)	-3(1)
O(2)	37(2)	17(2)	18(1)	0(1)	-1(1)	-9(1)
C(1)	21(2)	17(2)	18(2)	-3(1)	-5(2)	2(1)
C(2)	20(2)	15(2)	23(2)	1(1)	-2(1)	-1(1)
C(3)	13(2)	17(2)	17(2)	1(1)	-2(1)	3(1)
C(4)	20(2)	19(2)	20(2)	3(2)	3(2)	0(2)
C(5)	23(2)	28(2)	14(2)	3(2)	1(2)	6(2)
C(6)	23(2)	23(2)	18(2)	-4(2)	-2(1)	3(2)
C(7)	19(2)	14(2)	22(2)	0(1)	0(2)	1(1)
C(8)	13(2)	16(2)	14(2)	0(1)	-1(1)	2(1)
C(9)	18(2)	14(2)	15(2)	2(1)	2(1)	2(1)
C(10)	16(2)	21(2)	14(2)	1(1)	0(1)	6(1)
C(11)	24(2)	26(2)	14(2)	-2(2)	1(2)	5(2)
C(12)	26(2)	34(2)	16(2)	5(2)	7(1)	4(2)
C(13)	29(2)	22(2)	8(2)	2(1)	0(1)	4(2)
C(14)	21(2)	22(2)	9(2)	1(1)	1(1)	-1(1)
C(15)	21(2)	19(2)	11(2)	-3(1)	-2(1)	-3(2)
C(16)	24(2)	31(2)	19(2)	-2(2)	0(2)	7(2)
C(17)	18(2)	18(2)	13(2)	0(1)	1(1)	2(2)
C(18)	14(2)	17(2)	12(2)	0(1)	0(1)	1(1)
C(19)	17(2)	19(2)	17(2)	2(1)	3(1)	-1(1)
C(20)	21(2)	28(2)	12(2)	6(2)	3(1)	1(2)

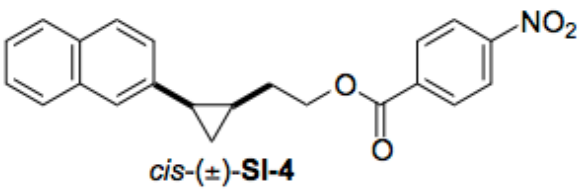
C(21)	15(2)	31(2)	7(2)	-5(1)	-2(1)	0(2)
C(22)	17(2)	19(2)	18(2)	-2(2)	2(1)	-1(2)
C(23)	20(2)	17(2)	12(2)	2(1)	1(1)	0(1)
C(24)	19(2)	23(2)	27(2)	9(2)	7(2)	6(2)
C(25)	23(2)	29(2)	21(2)	-1(2)	3(2)	10(2)
C(26)	19(2)	21(2)	34(2)	-5(2)	3(2)	4(2)
C(27)	19(2)	18(2)	27(2)	1(2)	8(1)	1(2)
C(28)	17(2)	24(2)	20(2)	0(2)	5(2)	5(2)
C(29)	16(2)	19(2)	28(2)	-2(2)	6(2)	2(2)
F(1)	34(1)	31(1)	35(1)	15(1)	11(1)	4(1)
F(2)	41(2)	51(2)	19(1)	-2(1)	4(1)	8(1)
F(3)	34(1)	28(1)	42(2)	-12(1)	5(1)	-4(1)
F(4)	32(1)	23(1)	38(2)	6(1)	14(1)	-5(1)
F(5)	32(1)	35(1)	21(1)	-3(1)	8(1)	1(1)
F(6)	28(1)	20(1)	40(1)	-2(1)	6(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for erj25.

	x	y	z	U(eq)
H(1A)	6753	4911	7646	23
H(2A)	6401	4223	8434	24
H(4A)	6818	5425	9304	24
H(5A)	7747	8072	9880	26
H(6A)	8992	11473	9655	26
H(7A)	9296	12177	8853	22
H(9A)	8898	10969	7989	19
H(11A)	8601	6921	7069	26
H(12A)	9366	10314	6730	30
H(12B)	8706	11734	7191	30
H(13A)	6412	8792	6539	24
H(14A)	5486	11056	7394	21
H(14B)	4098	9636	7035	21
H(15A)	5617	13785	6765	21
H(16A)	3494	14444	7317	38
H(16B)	2023	13010	6985	38
H(16C)	2721	15321	6791	38
H(19A)	3858	15363	5082	21
H(20A)	2726	14051	4316	24
H(22A)	1127	8339	4917	21
H(23A)	2326	9618	5683	20

C. X-ray Data Collection, Structure Solution, and Refinement for *cis*-(±)-SI-4:

CCDC Number: 1059382



cis-(±)-**SI-4**

A colorless crystal of approximate dimensions 0.365 x 0.343 x 0.256 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX[19] program package was used to determine the unit-cell parameters and for data collection (10 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT[20] and SADABS[21] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[22] program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/c$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques.[23] The analytical scattering factors[17] for neutral atoms were used throughout the analysis. Hydrogen atoms were located from a difference-Fourier map and refined (x,y,z and U_{iso}).

At convergence, wR2 = 0.1290 and Goof = 1.084 for 320 variables refined against 4355 data (0.74 Å), R1 = 0.0477 for those 3714 data with $I > 2.0\sigma(I)$.

Definitions:

$wR2 = [\Sigma[w(F_o^2-F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$

$Goof = S = [\Sigma[w(F_o^2-F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.

The thermal ellipsoid plot is shown at the 50% probability level.

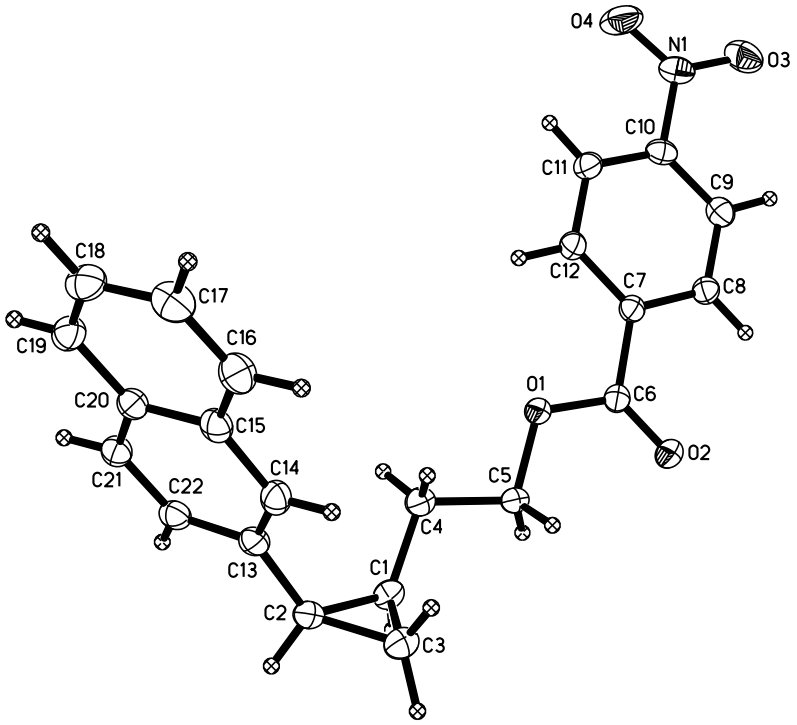


Table 1. Crystal data and structure refinement for erj12.

Identification code	erj12 (Emily Tollefson)	
Empirical formula	$C_{22}\ H_{19}\ N\ O_4$	
Formula weight	361.38	
Temperature	88(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 16.4673(7) Å	α= 90°.
	b = 8.7330(4) Å	β= 93.6709(5)°.
	c = 12.2472(5) Å	γ = 90°.
Volume	1757.64(13) $Å^3$	
Z	4	

Density (calculated)	1.366 Mg/m^3
Absorption coefficient	0.094 mm^{-1}
F(000)	760
Crystal color	colorless
Crystal size	0.365 x 0.343 x 0.256 mm^3
Theta range for data collection	2.479 to 28.842°
Index ranges	$-22 \le h \le 21$, $-11 \le k \le 11$, $-16 \le l \le 16$
Reflections collected	20431
Independent reflections	4355 [R(int) = 0.0321]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8621 and 0.8109
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4355 / 0 / 320
Goodness-of-fit on F^2	1.084
Final R indices [I>2sigma(I) = 3714 data]	R1 = 0.0477, wR2 = 0.1244
R indices (all data, 0.74 Å)	R1 = 0.0548, wR2 = 0.1290
Largest diff. peak and hole	0.740 and -0.282 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for erj12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	81(1)	-346(2)	-2322(1)	26(1)
O(1)	3011(1)	3589(1)	-162(1)	21(1)
O(2)	3327(1)	3775(1)	-1919(1)	25(1)
O(3)	-84(1)	-627(2)	-3292(1)	37(1)
O(4)	-316(1)	-824(2)	-1580(1)	42(1)
C(1)	4575(1)	5314(2)	1830(1)	23(1)
C(2)	4598(1)	6173(2)	2911(1)	23(1)
C(3)	4611(1)	7033(2)	1851(1)	26(1)
C(4)	3801(1)	4523(2)	1409(1)	23(1)
C(5)	3763(1)	4394(2)	171(1)	21(1)
C(6)	2882(1)	3331(2)	-1238(1)	19(1)
C(7)	2128(1)	2411(2)	-1497(1)	19(1)
C(8)	1975(1)	1913(2)	-2572(1)	21(1)
C(9)	1305(1)	1005(2)	-2852(1)	23(1)
C(10)	796(1)	621(2)	-2034(1)	22(1)
C(11)	924(1)	1115(2)	-964(1)	23(1)
C(12)	1599(1)	2017(2)	-697(1)	22(1)
C(13)	3890(1)	6183(2)	3624(1)	22(1)
C(14)	3230(1)	7133(2)	3471(1)	25(1)
C(15)	2588(1)	7131(2)	4203(1)	24(1)
C(16)	1900(1)	8103(2)	4058(1)	29(1)
C(17)	1311(1)	8106(2)	4800(1)	32(1)
C(18)	1379(1)	7129(2)	5725(1)	30(1)

C(19)	2028(1)	6165(2)	5881(1)	26(1)
C(20)	2648(1)	6137(2)	5124(1)	22(1)
C(21)	3327(1)	5140(2)	5256(1)	23(1)
C(22)	3921(1)	5154(2)	4525(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for erj12.

N(1)-O(4)	1.2260(18)
N(1)-O(3)	1.2266(18)
N(1)-C(10)	1.4730(18)
O(1)-C(6)	1.3398(16)
O(1)-C(5)	1.4592(16)
O(2)-C(6)	1.2089(17)
C(1)-C(3)	1.503(2)
C(1)-C(4)	1.511(2)
C(1)-C(2)	1.520(2)
C(2)-C(13)	1.5004(19)
C(2)-C(3)	1.501(2)
C(4)-C(5)	1.5175(19)
C(6)-C(7)	1.4957(18)
C(7)-C(8)	1.3943(18)
C(7)-C(12)	1.3959(18)
C(8)-C(9)	1.383(2)
C(9)-C(10)	1.388(2)
C(10)-C(11)	1.383(2)
C(11)-C(12)	1.385(2)
C(13)-C(14)	1.370(2)
C(13)-C(22)	1.421(2)
C(14)-C(15)	1.429(2)
C(15)-C(16)	1.418(2)
C(15)-C(20)	1.422(2)
C(16)-C(17)	1.371(2)
C(17)-C(18)	1.417(2)

C(18)-C(19)	1.366(2)
C(19)-C(20)	1.423(2)
C(20)-C(21)	1.418(2)
C(21)-C(22)	1.368(2)

O(4)-N(1)-O(3)	123.64(13)
O(4)-N(1)-C(10)	118.29(12)
O(3)-N(1)-C(10)	118.07(13)
C(6)-O(1)-C(5)	115.70(10)
C(3)-C(1)-C(4)	119.61(13)
C(3)-C(1)-C(2)	59.55(10)
C(4)-C(1)-C(2)	119.79(12)
C(13)-C(2)-C(3)	123.68(13)
C(13)-C(2)-C(1)	122.18(12)
C(3)-C(2)-C(1)	59.67(10)
C(2)-C(3)-C(1)	60.77(10)
C(1)-C(4)-C(5)	110.82(11)
O(1)-C(5)-C(4)	107.16(10)
O(2)-C(6)-O(1)	124.05(12)
O(2)-C(6)-C(7)	123.86(12)
O(1)-C(6)-C(7)	112.08(11)
C(8)-C(7)-C(12)	120.20(13)
C(8)-C(7)-C(6)	117.77(12)
C(12)-C(7)-C(6)	122.01(12)
C(9)-C(8)-C(7)	120.36(13)
C(8)-C(9)-C(10)	118.00(13)
C(11)-C(10)-C(9)	123.06(13)
C(11)-C(10)-N(1)	118.46(13)

C(9)-C(10)-N(1)	118.48(13)
C(10)-C(11)-C(12)	118.23(13)
C(11)-C(12)-C(7)	120.14(13)
C(14)-C(13)-C(22)	118.53(13)
C(14)-C(13)-C(2)	124.28(13)
C(22)-C(13)-C(2)	117.18(13)
C(13)-C(14)-C(15)	121.73(13)
C(16)-C(15)-C(20)	118.67(14)
C(16)-C(15)-C(14)	122.57(14)
C(20)-C(15)-C(14)	118.74(13)
C(17)-C(16)-C(15)	120.77(15)
C(16)-C(17)-C(18)	120.42(15)
C(19)-C(18)-C(17)	120.29(14)
C(18)-C(19)-C(20)	120.52(14)
C(21)-C(20)-C(15)	118.68(13)
C(21)-C(20)-C(19)	122.00(13)
C(15)-C(20)-C(19)	119.32(13)
C(22)-C(21)-C(20)	120.77(13)
C(21)-C(22)-C(13)	121.47(14)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for erj12. 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}
N(1)	20(1)	24(1)	36(1)	-5(1)	1(1)	0(1)
O(1)	20(1)	25(1)	17(1)	-1(1)	2(1)	-4(1)
O(2)	24(1)	31(1)	20(1)	1(1)	4(1)	-5(1)
O(3)	31(1)	40(1)	39(1)	-9(1)	-5(1)	-6(1)
O(4)	33(1)	47(1)	47(1)	-7(1)	12(1)	-18(1)
C(1)	22(1)	25(1)	23(1)	1(1)	5(1)	-1(1)
C(2)	20(1)	27(1)	23(1)	-2(1)	1(1)	-5(1)
C(3)	26(1)	25(1)	29(1)	3(1)	4(1)	-2(1)
C(4)	22(1)	26(1)	23(1)	-1(1)	3(1)	-3(1)
C(5)	19(1)	24(1)	20(1)	0(1)	2(1)	-5(1)
C(6)	18(1)	20(1)	18(1)	1(1)	2(1)	3(1)
C(7)	17(1)	20(1)	19(1)	2(1)	1(1)	3(1)
C(8)	19(1)	24(1)	19(1)	0(1)	3(1)	2(1)
C(9)	22(1)	24(1)	21(1)	-4(1)	0(1)	3(1)
C(10)	17(1)	20(1)	28(1)	-1(1)	0(1)	2(1)
C(11)	20(1)	26(1)	23(1)	3(1)	4(1)	0(1)
C(12)	20(1)	26(1)	19(1)	1(1)	2(1)	1(1)
C(13)	24(1)	23(1)	21(1)	-6(1)	2(1)	-6(1)
C(14)	31(1)	23(1)	20(1)	-1(1)	1(1)	-5(1)
C(15)	27(1)	22(1)	22(1)	-4(1)	-1(1)	-3(1)
C(16)	32(1)	28(1)	28(1)	-2(1)	-1(1)	2(1)
C(17)	27(1)	31(1)	36(1)	-7(1)	0(1)	5(1)
C(18)	26(1)	32(1)	32(1)	-9(1)	8(1)	-1(1)

C(19)	28(1)	27(1)	24(1)	-3(1)	5(1)	-4(1)
C(20)	24(1)	21(1)	21(1)	-4(1)	1(1)	-4(1)
C(21)	26(1)	21(1)	22(1)	-2(1)	1(1)	-4(1)
C(22)	21(1)	23(1)	24(1)	-4(1)	0(1)	-3(1)

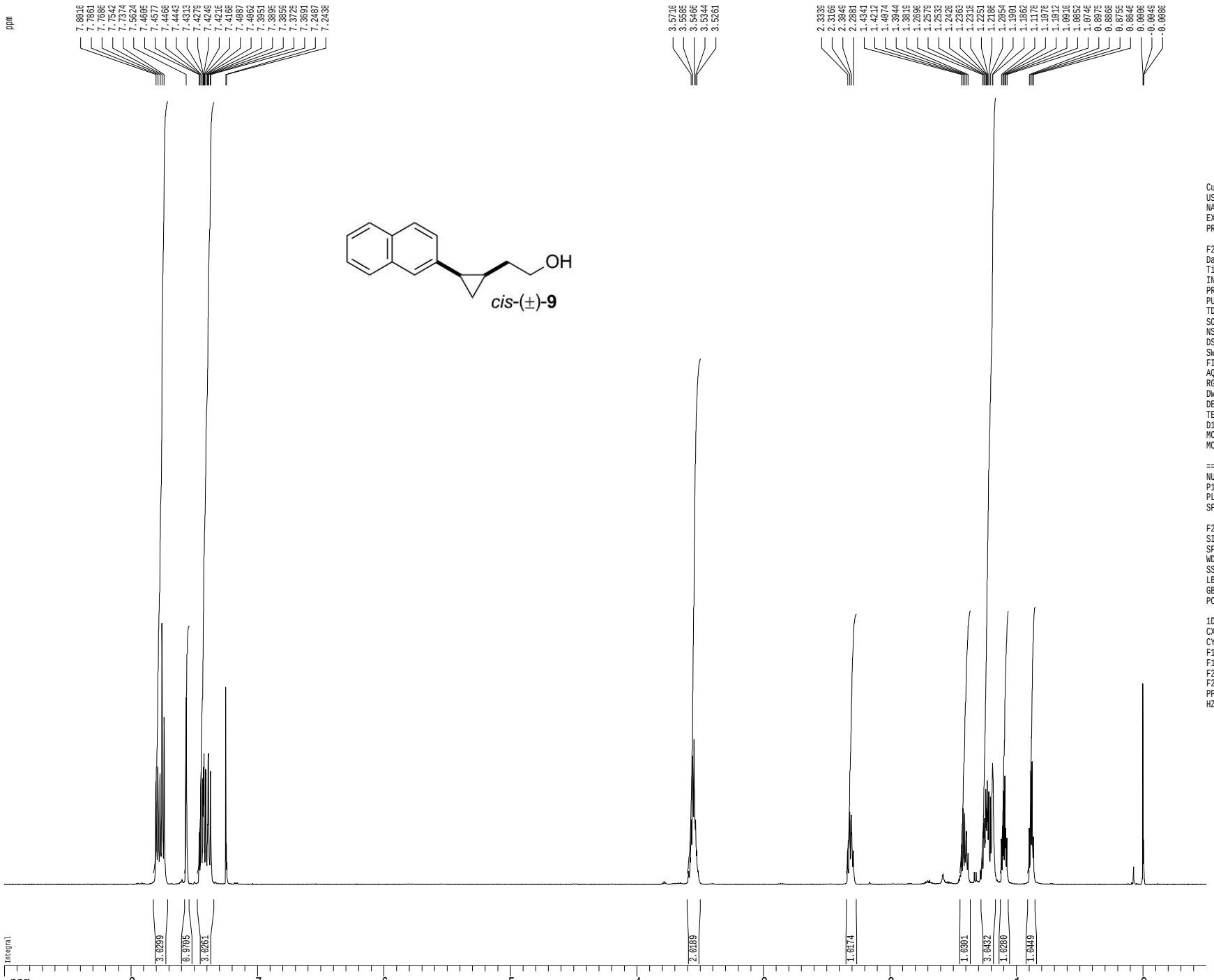
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for erj12.

	x	y	z	U(eq)
H(1A)	5084(11)	4750(20)	1682(14)	27(4)
H(2A)	5150(12)	6110(20)	3334(15)	31(5)
H(3A)	5140(12)	7560(20)	1666(16)	36(5)
H(3B)	4104(12)	7570(20)	1594(16)	37(5)
H(4A)	3369(10)	5239(19)	1441(13)	17(4)
H(4B)	3762(12)	3430(20)	1775(16)	37(5)
H(5A)	3761(10)	5400(20)	-171(14)	22(4)
H(5B)	4234(10)	3806(19)	-62(13)	18(4)
H(8A)	2335(11)	2190(20)	-3118(14)	26(4)
H(9A)	1182(11)	640(20)	-3595(14)	24(4)
H(11A)	571(12)	800(20)	-450(15)	31(5)
H(12A)	1705(11)	2360(20)	59(15)	27(4)
H(14A)	3178(10)	7800(20)	2877(14)	21(4)
H(16A)	1856(12)	8760(20)	3397(16)	31(5)
H(17A)	837(13)	8760(20)	4695(17)	41(6)
H(18A)	971(12)	7130(20)	6233(15)	30(5)
H(19A)	2071(11)	5450(20)	6495(14)	24(4)
H(21A)	3375(11)	4470(20)	5872(15)	26(4)
H(22A)	4373(11)	4440(20)	4631(15)	29(5)

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1H spectrum




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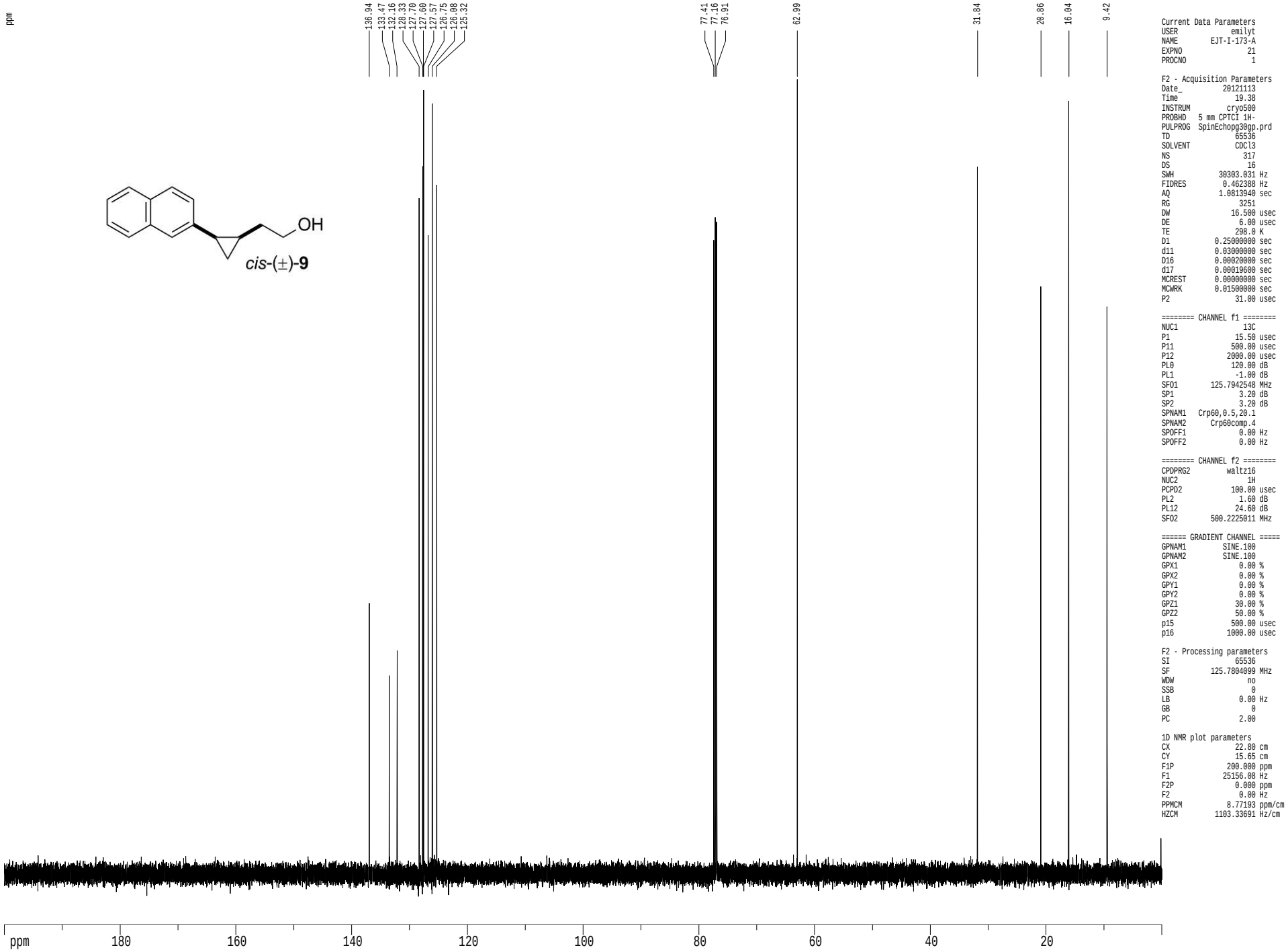
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RG                   5.7
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TE                298.0 K
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Z-restored spin-echo 13C spectrum with 1H decoupling




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MCWRK          0.01500000 sec
P2                31.00 usec

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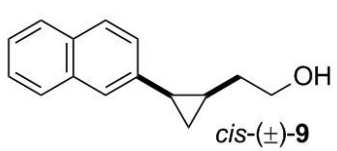
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GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15              500.00 usec
p16             1000.00 usec

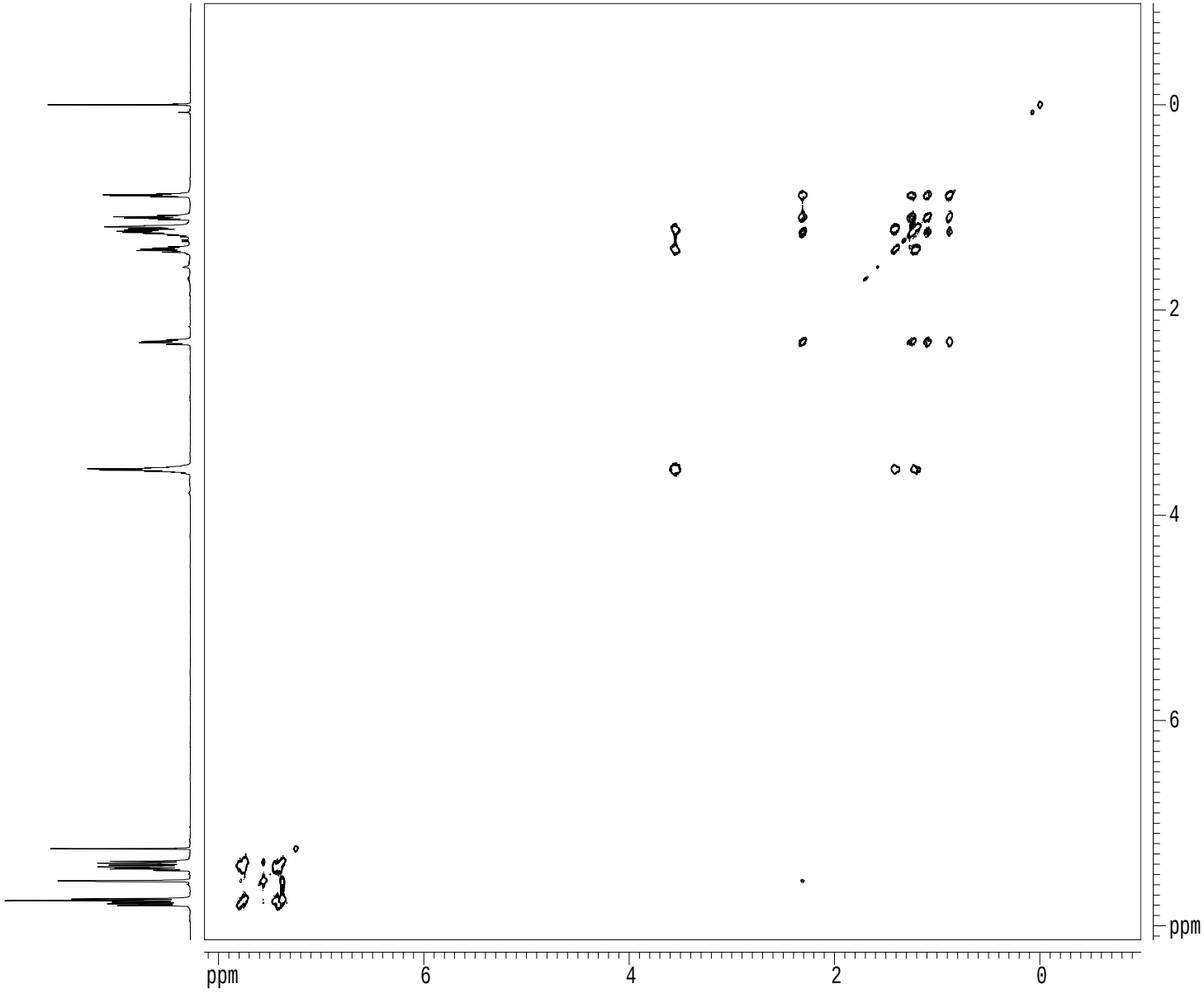
F2 - Processing parameters
SI                 65536
SF           125.7804099 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.65 cm
F1P              200.000 ppm
F1             25156.08 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           8.77193 ppm/cm
HZCM          1103.33691 Hz/cm
```

gcosy60



cis-(±)-**9**



Current Data Parameters

USER	emilyt
NAME	EJT-I-173-A
EXPNO	20
PROCNO	1

F2 - Acquisition Parameters

Date_	20121113
Time	19.19
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4562.044 Hz
FIDRES	2.227561 Hz
AQ	0.2245108 sec
RG	161.3
DW	109.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00021920 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2218248 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	257
SFO1	500.2218 MHz
FIDRES	17.751143 Hz
SW	9.120 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200365 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

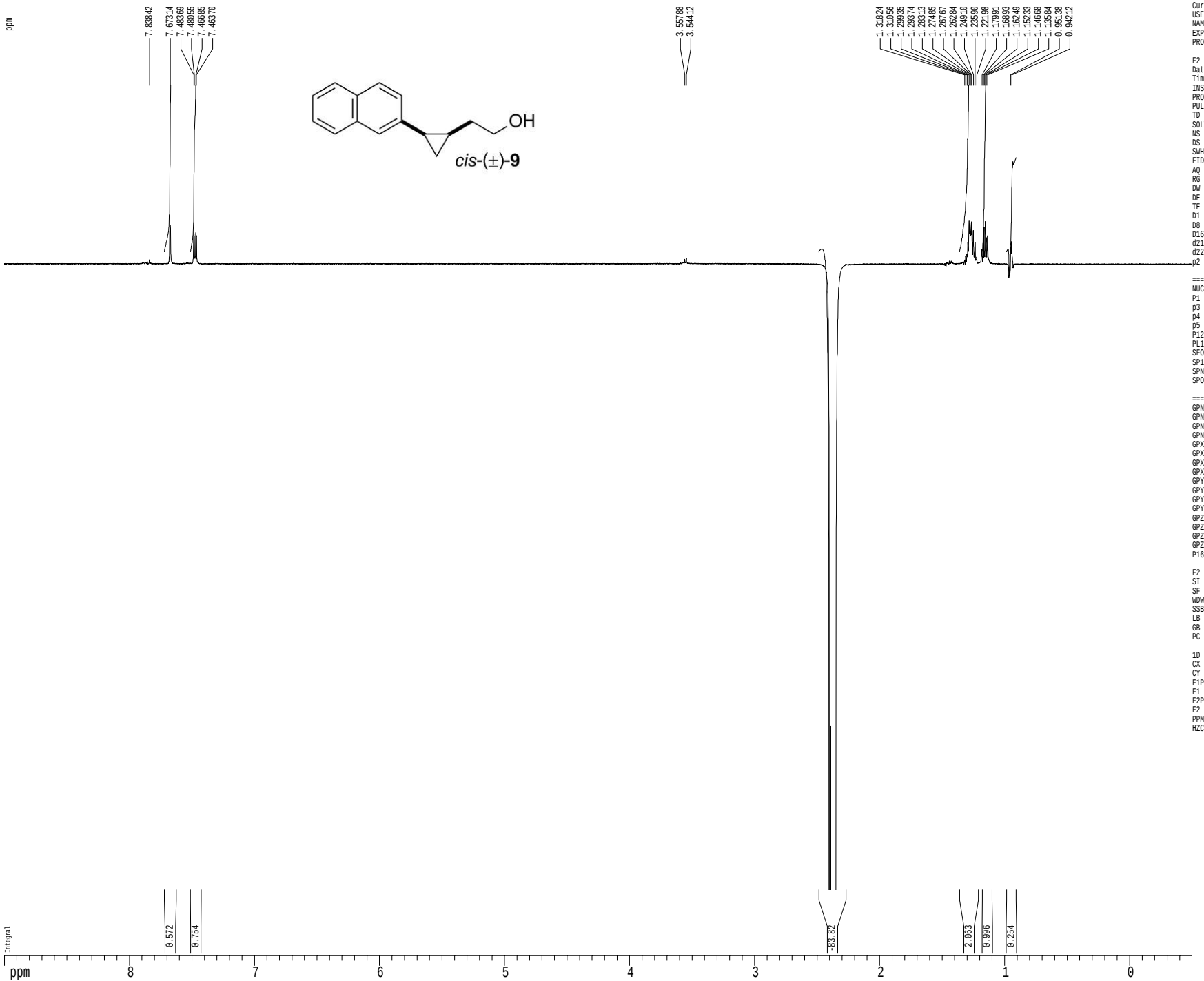
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200365 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.135 ppm
F2LO	4069.30 Hz
F2PHI	-0.985 ppm
F2HI	-492.74 Hz
F1PLO	8.135 ppm
F1LO	4069.30 Hz
F1PHI	-0.985 ppm
F1HI	-492.74 Hz
F2PPMCM	0.60800 ppm/cm
F2HZCM	304.13623 Hz/cm
F1PPMCM	0.60800 ppm/cm
F1HZCM	304.13623 Hz/cm

gnoe



Current Data Parameters
USER emilyt
NAME EJT-V-nap cyc cis noe
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 20.24
INSTRUM gn500
PROBHD 5 mm broadband
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 114
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33374399 sec
d22 0.16399699 sec
p2 24.00 usec

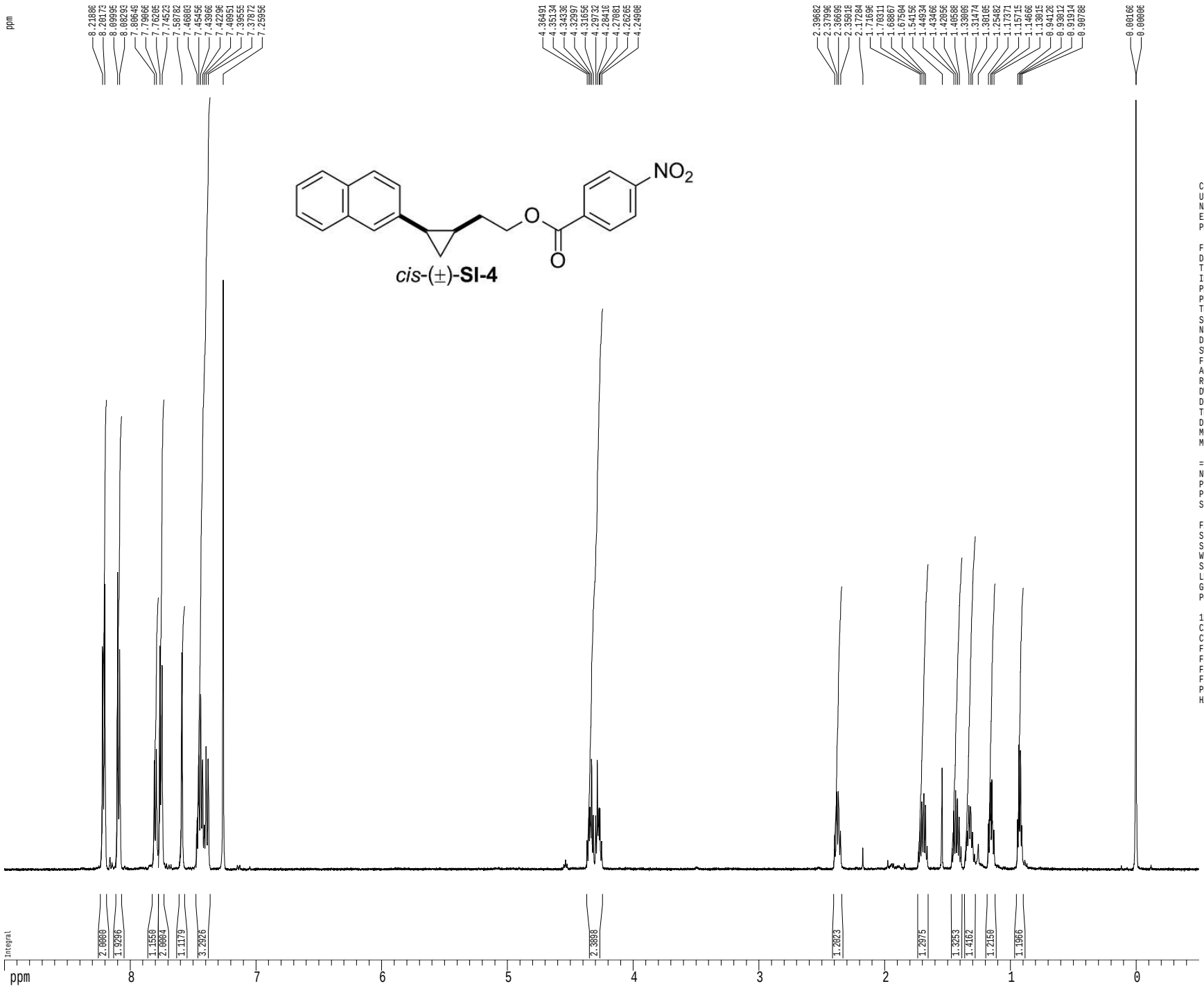
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
p3 36.00 usec
p4 48.00 usec
p5 32.00 usec
P12 40000.00 usec
PL1 -5.80 dB
SFO1 499.1811856 MHz
SP1 53.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 499.1800000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4492.62 Hz
F2P -0.500 ppm
F2 -249.59 Hz
PPMCM 0.41667 ppm/cm
HZCM 207.99167 Hz/cm

1H spectrum




```
Current Data Parameters
USER                emilyt
NAME       EJT-II-122-AA
EXPNO                  1
PROCNO                 1

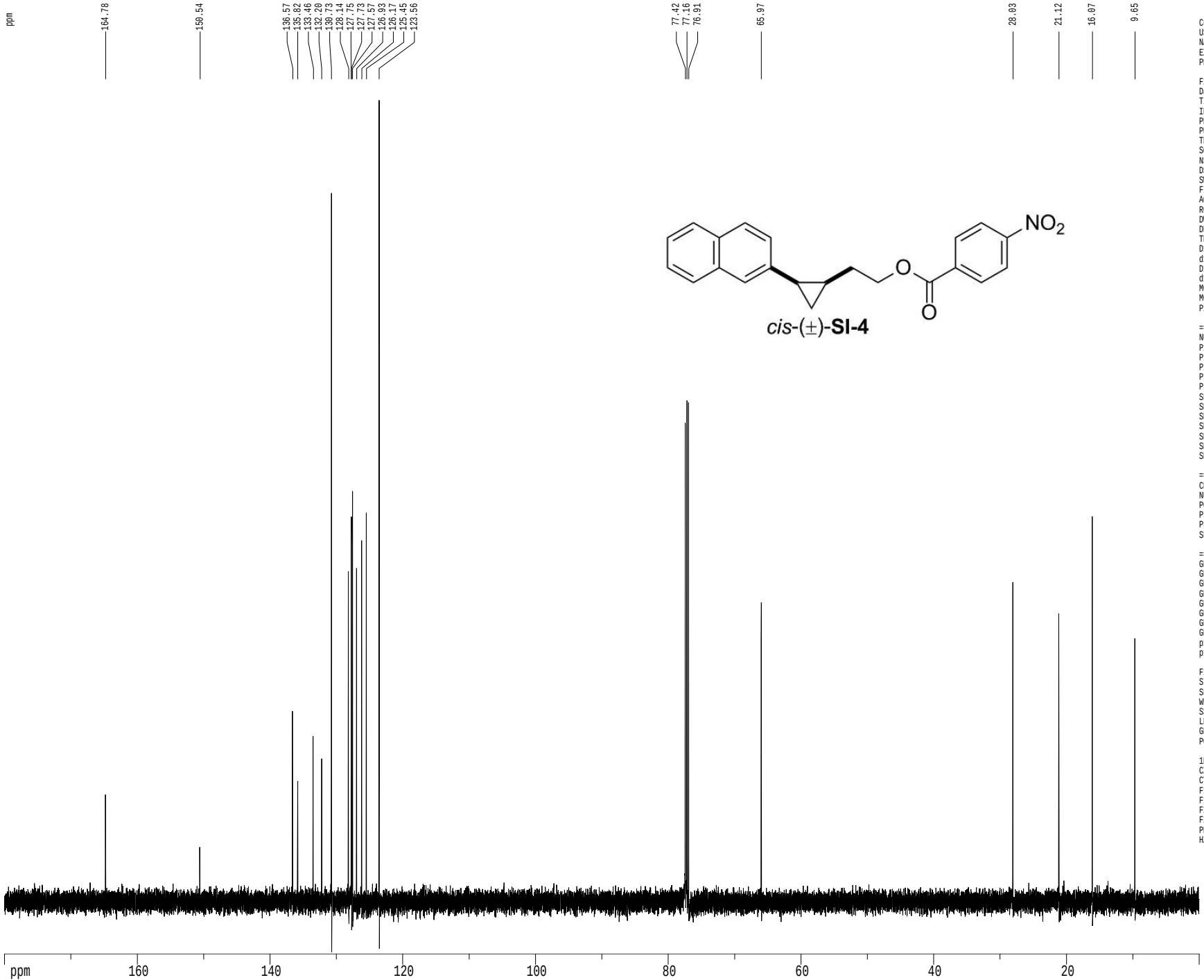
F2 - Acquisition Parameters
Date_           20130415
Time              19.04
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 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           500.2200311 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              4501.98 Hz
F2P              -0.500 ppm
F2              -250.11 Hz
PPMCM           0.41667 ppm/cm
HZCM          208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME            EJT-II-122-A
EXPNO                      6
PROCNO                     1

F2 - Acquisition Parameters
Date_               20130412
Time                   19.45
INSTRUM              cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                     65536
SOLVENT                CDCl3
NS                       172
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

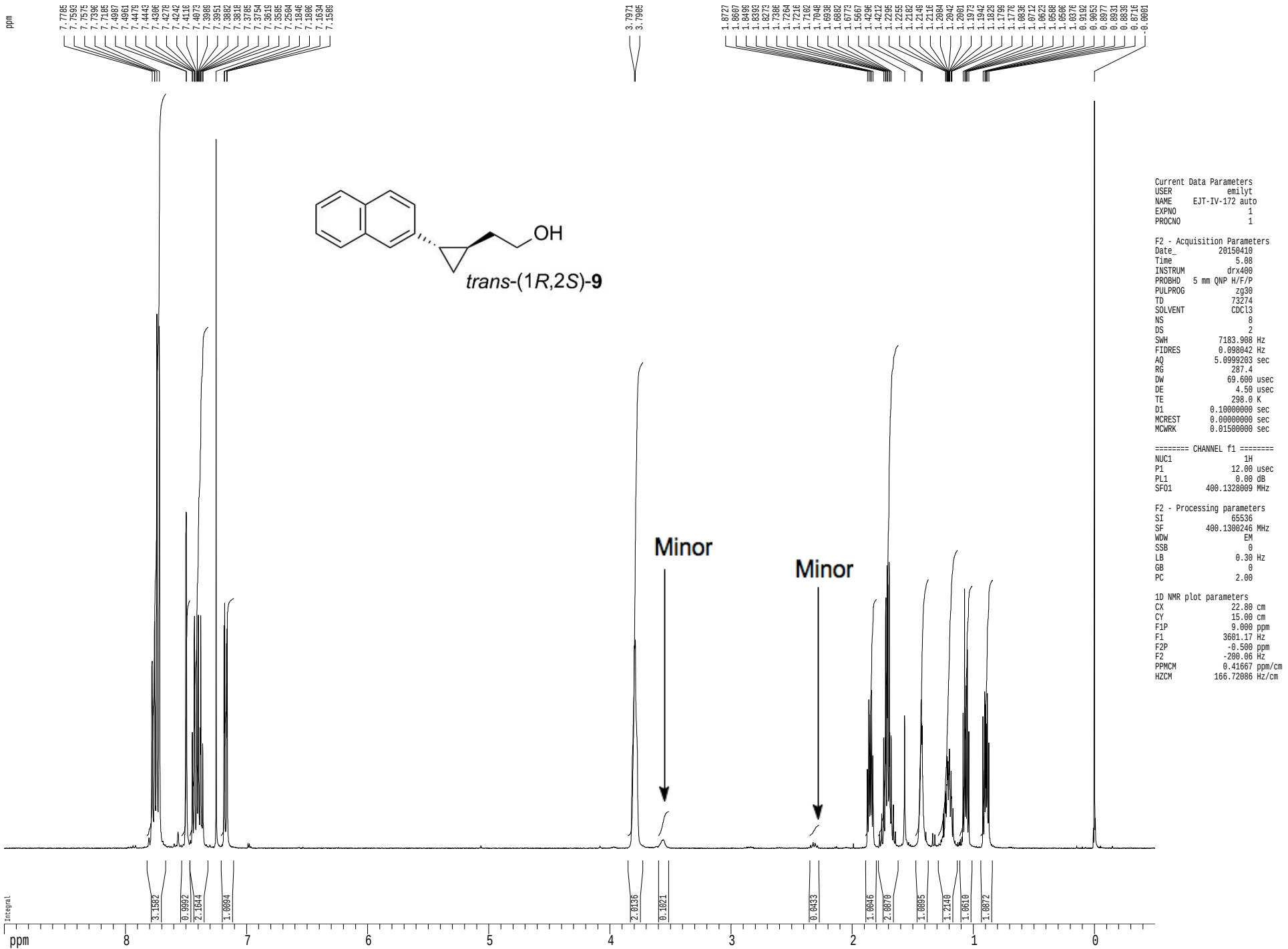
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                100.00 usec
PL2                    1.60 dB
PL12                  24.60 dB
SFO2              500.2225011 MHz

====== 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                125.7804094 MHz
WDW                       no
SSB                        0
LB                     0.00 Hz
GB                         0
PC                     2.00

1D NMR plot parameters
CX                     22.80 cm
CY                     15.65 cm
F1P                  180.000 ppm
F1                 22640.47 Hz
F2P                    0.000 ppm
F2                     0.00 Hz
PPMCM                7.89474 ppm/cm
HZCM               993.00330 Hz/cm
```

PI Jarvo
h1 CDCl3 v emilyt 109




```
Current Data Parameters
USER              emilyt
NAME      EJT-IV-172 auto
EXPNO                  1
PROCNO                 1

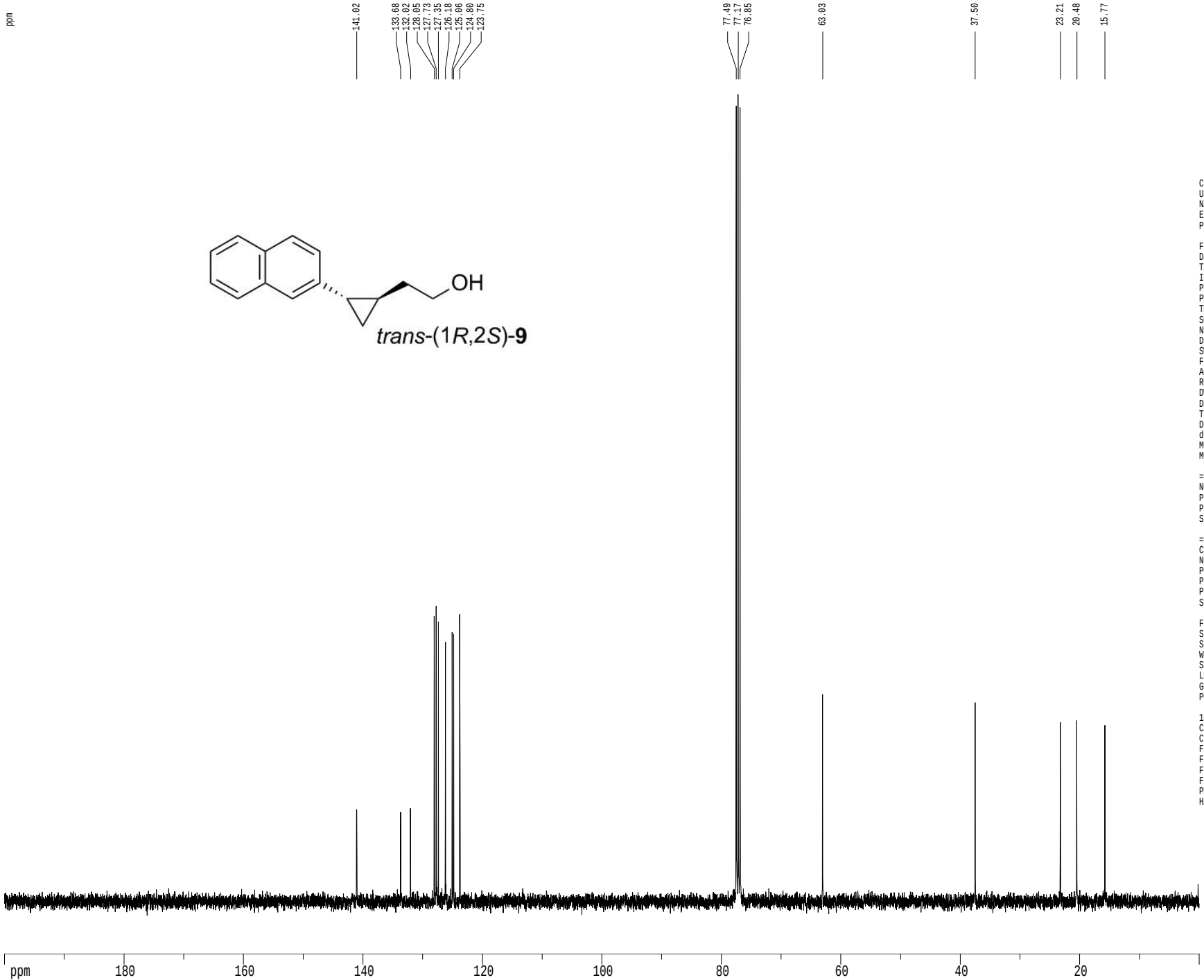
F2 - Acquisition Parameters
Date_          20150410
Time               5.08
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG             zg30
TD                 73274
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             7183.908 Hz
FIDRES          0.098042 Hz
AQ              5.0999203 sec
RG                 287.4
DW                69.600 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                 0.00 dB
SFO1         400.1328009 MHz

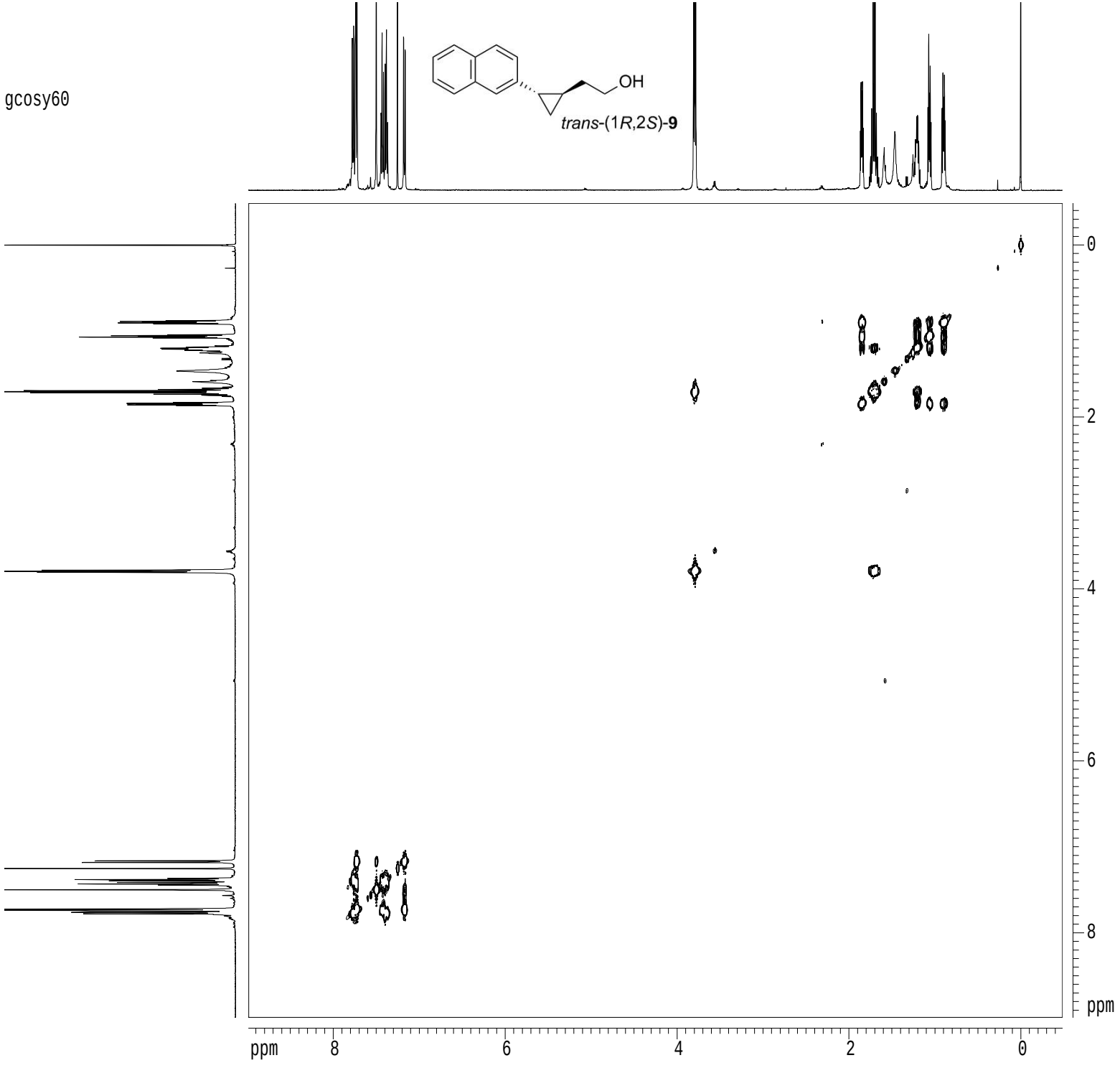
F2 - Processing parameters
SI                 65536
SF           400.1300246 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P                9.000 ppm
F1               3601.17 Hz
F2P                -0.500 ppm
F2               -200.06 Hz
PPMCM           0.41667 ppm/cm
HZCM          166.72086 Hz/cm
```

PI Jarvo
c13 CDCl3 v emilyt 109



gcosy60



Current Data Parameters

USER	emilyt
NAME	EJT-IV-172 noe
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20150206
Time	20.45
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4734.849 Hz
FIDRES	2.311938 Hz
AQ	0.2163188 sec
RG	203.2
DW	105.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00021120 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2221618 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2222 MHz
FIDRES	36.991005 Hz
SW	9.465 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200359 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

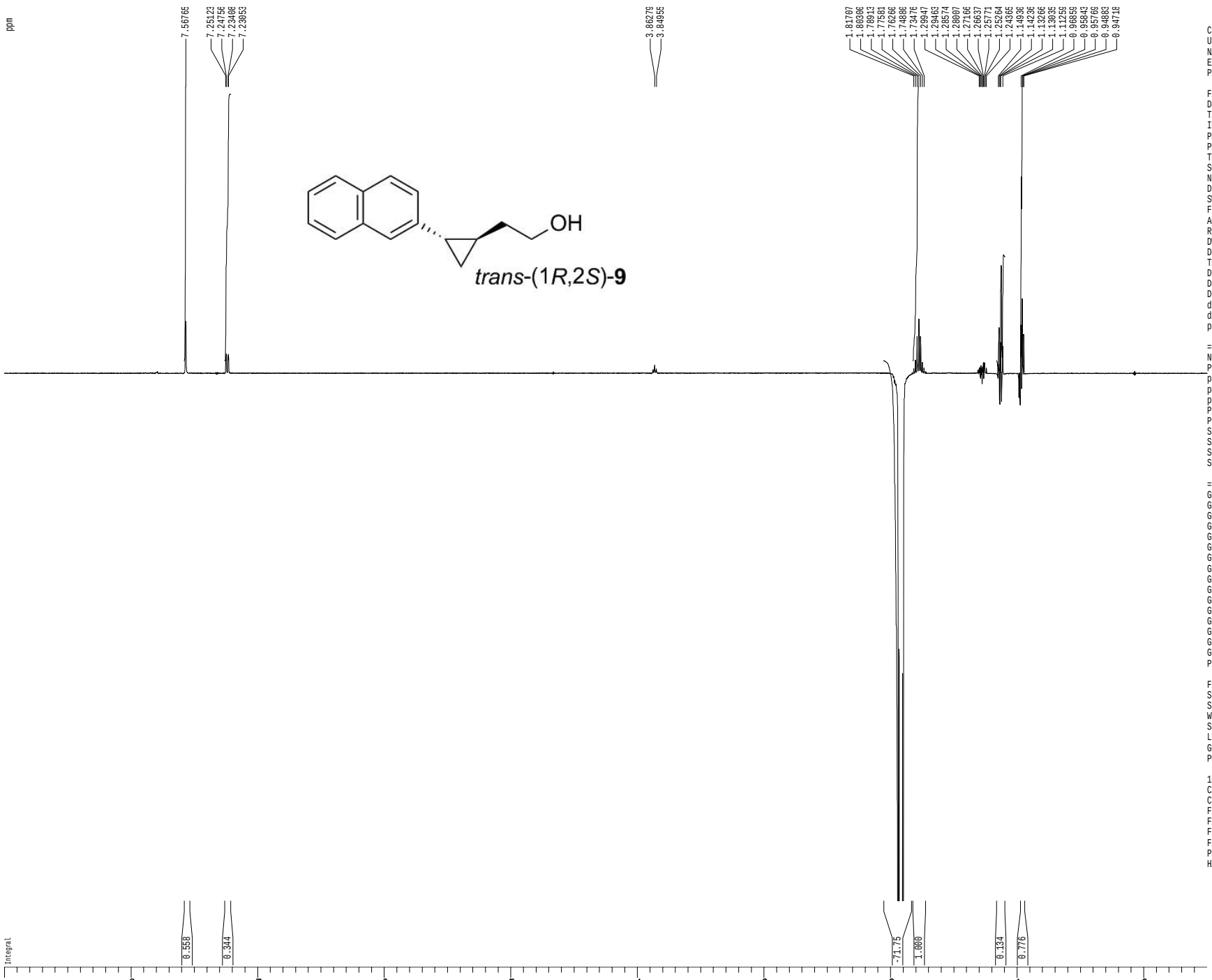
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200359 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.983 ppm
F2LO	4493.36 Hz
F2PHI	-0.483 ppm
F2HI	-241.49 Hz
F1PLO	8.983 ppm
F1LO	4493.36 Hz
F1PHI	-0.483 ppm
F1HI	-241.49 Hz
F2PPMCM	0.63104 ppm/cm
F2HZCM	315.65656 Hz/cm
F1PPMCM	0.63104 ppm/cm
F1HZCM	315.65656 Hz/cm

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-172 noe
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150206
Time 21.05
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.8
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

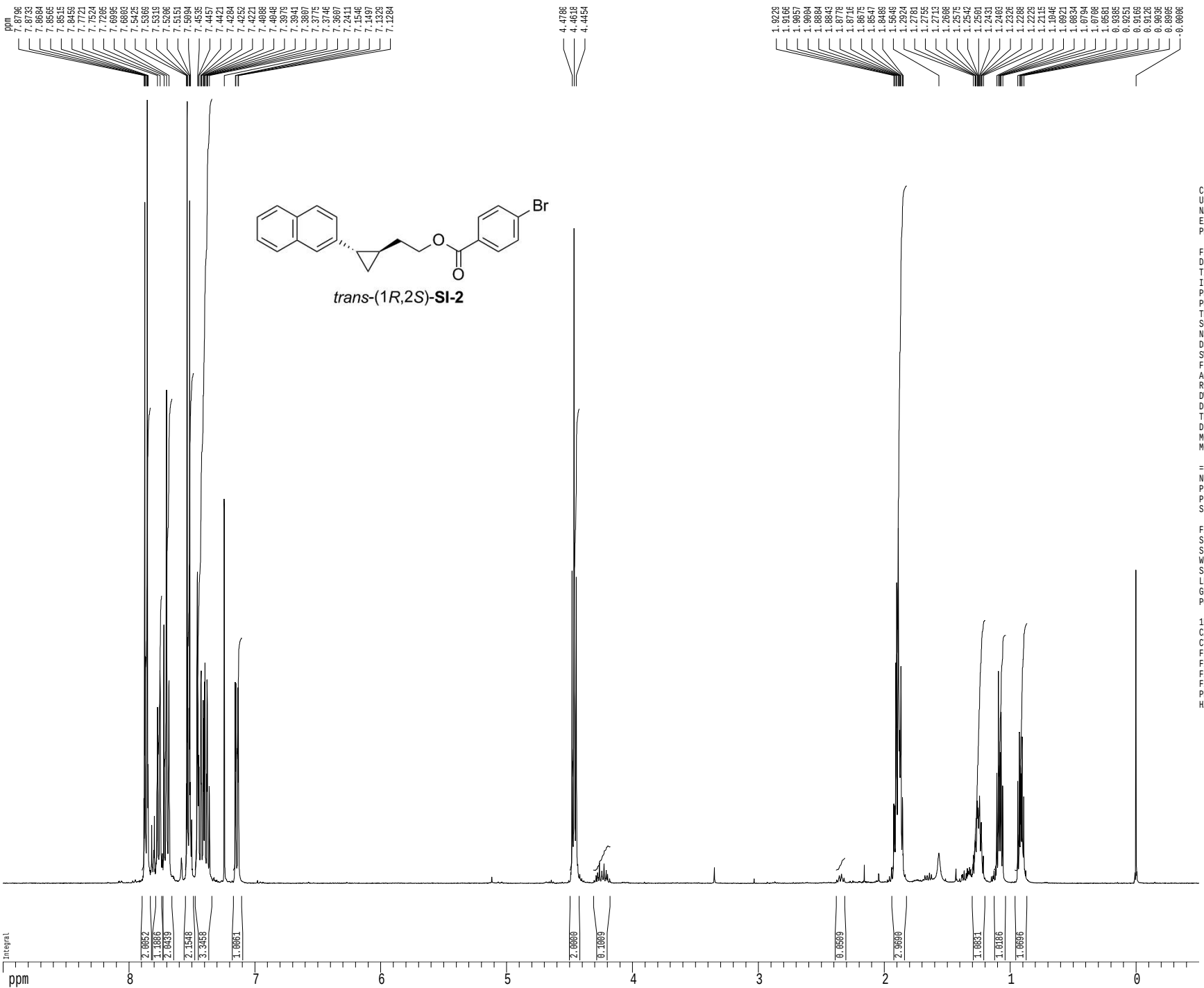
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2209604 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

PI Jarvo
h1 CDCl3 v emilyt 14



Current Data Parameters
USER emilyt
NAME EJT-V-093-A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150717
Time 0.35
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zg30
TD 73274
SOLVENT CDCl3
NS 8
DS 2
SWH 7183.908 Hz
FIDRES 0.098042 Hz
AQ 5.0999203 sec
RG 181
DW 69.600 usec
DE 4.50 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

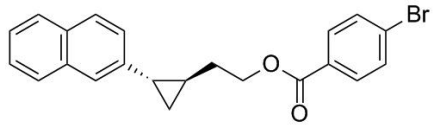
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 400.1300291 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.41667 ppm/cm
HZCM 166.72086 Hz/cm

PI Jarvo
c13 CDCl3 v emilyt 14





trans-(1*R*,2*S*)-**SI-2**


```
Current Data Parameters
USER              emilyt
NAME         EJT-V-093-A
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20150717
Time               1.02
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG          zgdc30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24154.590 Hz
FIDRES         0.368570 Hz
AQ             1.3566452 sec
RG               14596.5
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

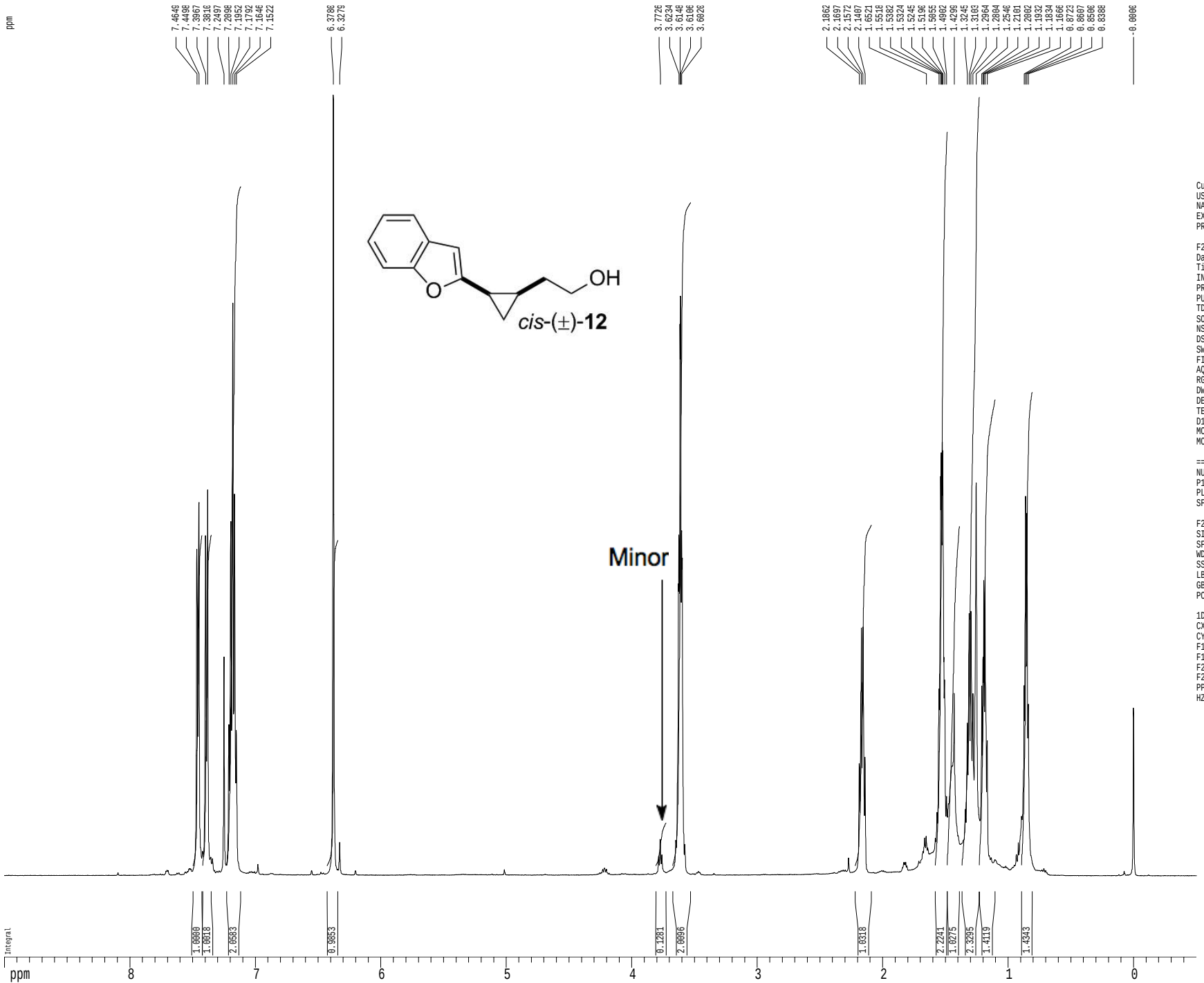
======== CHANNEL f1 ========
NUC1               13C
P1                7.75 usec
PL1               -3.00 dB
SFO1        100.6237964 MHz

======== CHANNEL f2 ========
CPDPRG2          mlev16
NUC2                1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              17.70 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

1D NMR plot parameters
CX                22.80 cm
CY                15.50 cm
F1P              200.000 ppm
F1             20122.55 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           8.77193 ppm/cm
HZCM          882.56812 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-260-cryo
EXPNO                    1
PROCNO                   1

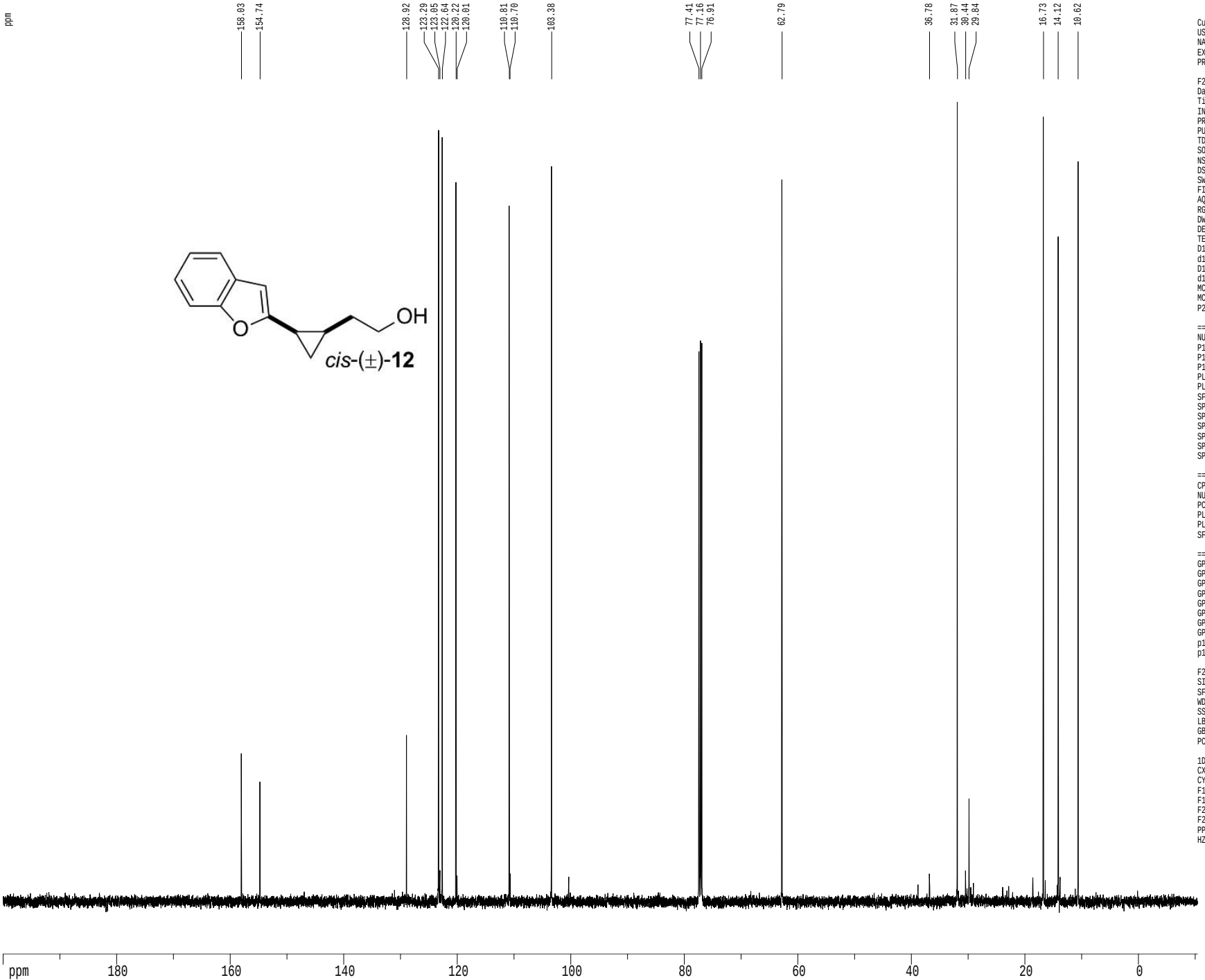
F2 - Acquisition Parameters
Date_             20150310
Time                 19.51
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  48074
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.166677 Hz
AQ               2.9998677 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            500.2200360 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-260-cryo
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150310
Time                20.19
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    303
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 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
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                  33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

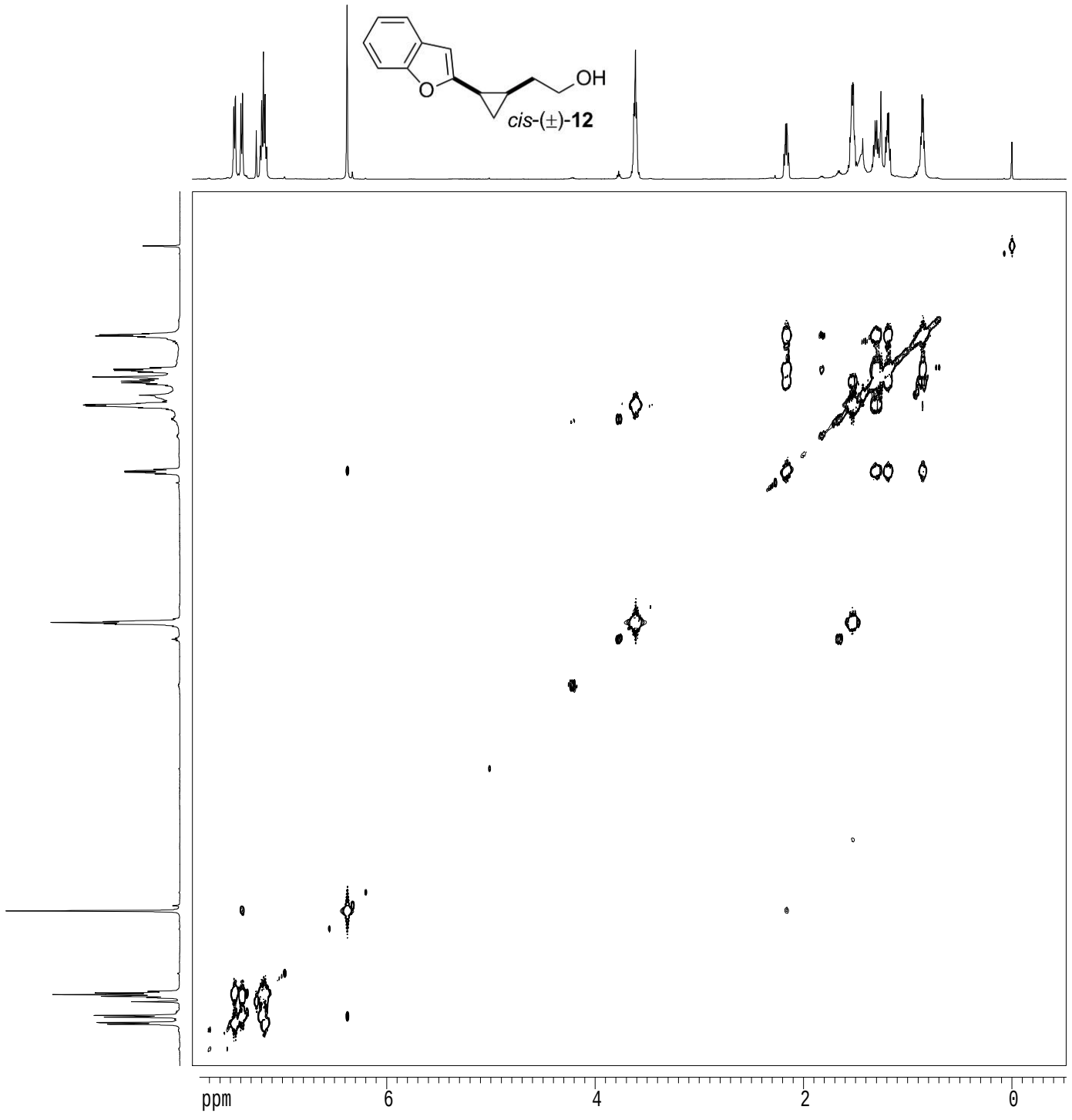
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7804113 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1              25156.08 Hz
F2P                -10.399 ppm
F2              -1307.93 Hz
PPMCM             9.22801 ppm/cm
HZCM           1160.70227 Hz/cm
```

gcosy60



Current Data Parameters

USER	lucase
NAME	LWE-II-260-cryo
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20150310
Time	20.08
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4194.631 Hz
FIDRES	2.048160 Hz
AQ	0.2441716 sec
RG	114
DW	119.200 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00023840 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2218368 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2218 MHz
FIDRES	32.770554 Hz
SW	8.386 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200360 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

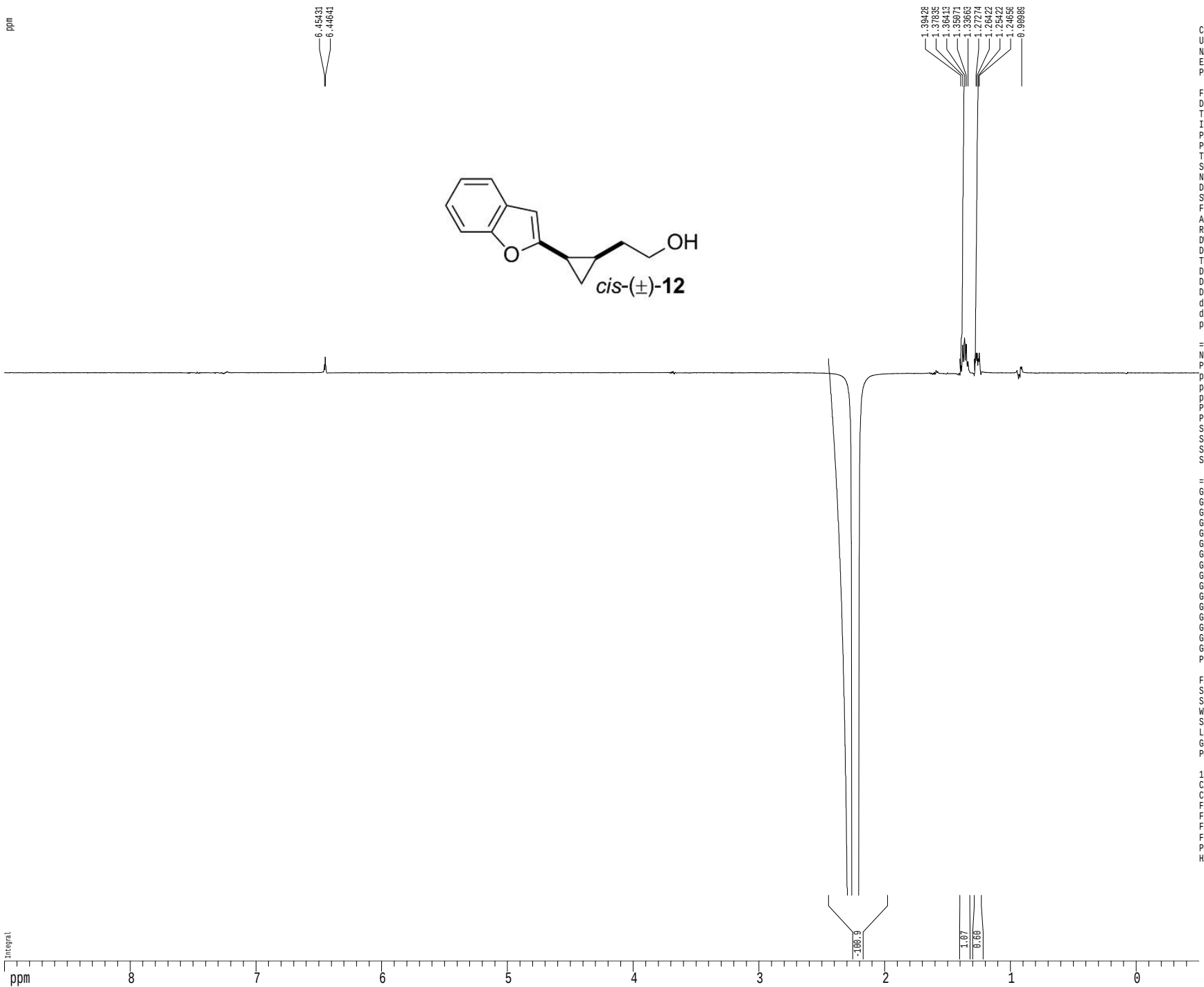
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200360 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	7.865 ppm
F2LO	3934.14 Hz
F2PHI	-0.521 ppm
F2HI	-260.49 Hz
F1PLO	7.865 ppm
F1LO	3934.14 Hz
F1PHI	-0.521 ppm
F1HI	-260.49 Hz
F2PPMCM	0.55904 ppm/cm
F2HZCM	279.64206 Hz/cm
F1PPMCM	0.55904 ppm/cm
F1HZCM	279.64206 Hz/cm

gnoe




```
Current Data Parameters
USER                lucase
NAME      LWE-II-260-cryo
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150310
Time                20.06
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   80.6
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
D8             0.50000000 sec
D16            0.00020000 sec
d21            0.33376500 sec
d22            0.16399699 sec
p2                 15.00 usec

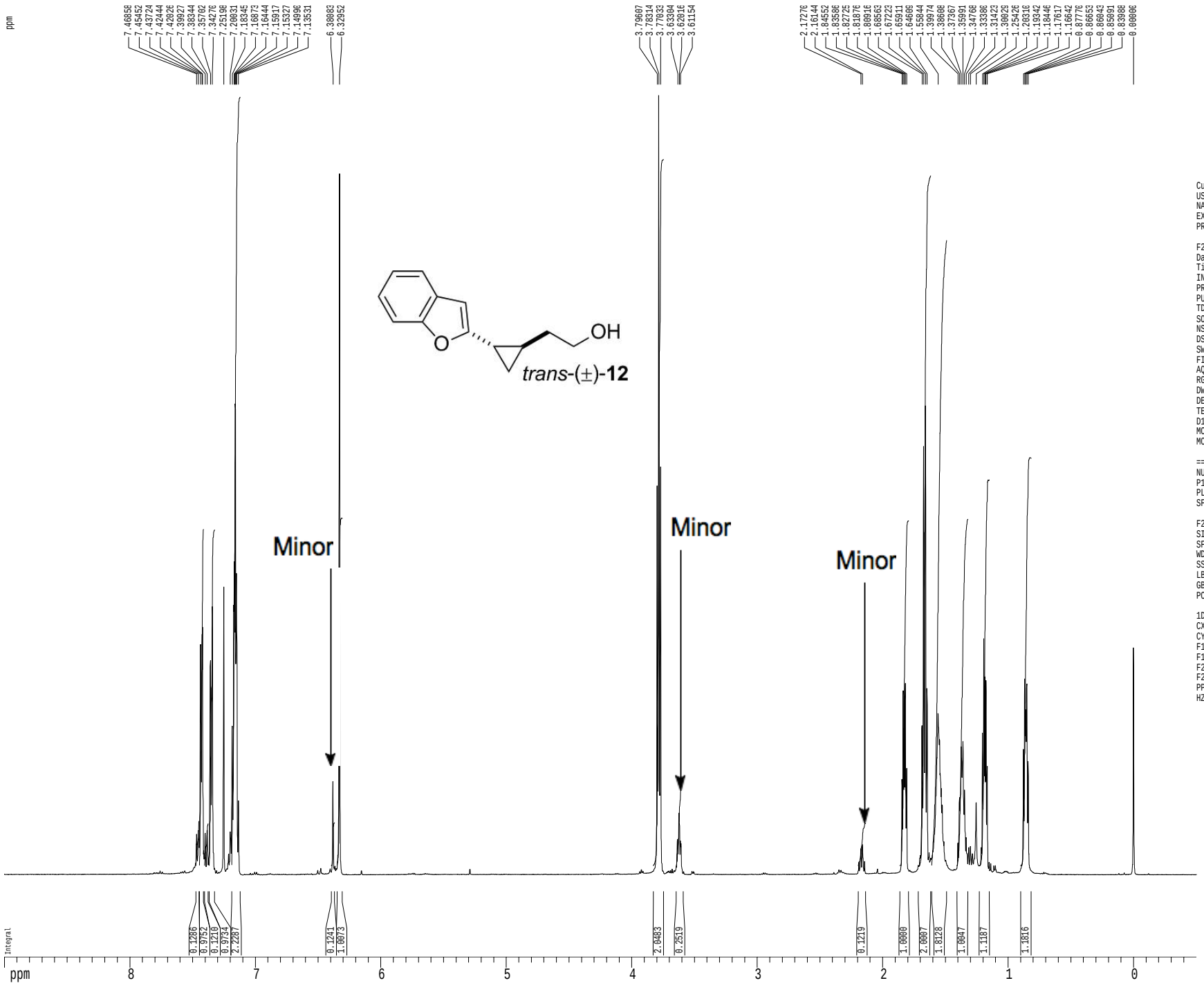
======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
p3                  22.50 usec
p4                  30.00 usec
p5                  20.00 usec
P12               40000.00 usec
PL1                  1.60 dB
SFO1          500.2211181 MHz
SP1                 61.60 dB
SPNAM1         gauss1.512
SPOFF1               0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1           sine.100
GPNAM2           sine.100
GPNAM3           sine.100
GPNAM4           sine.100
GPX1                 0.00 %
GPX2                 0.00 %
GPX3                 0.00 %
GPX4                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPY3                 0.00 %
GPY4                 0.00 %
GPZ1                 7.00 %
GPZ2                 3.00 %
GPZ3                 2.30 %
GPZ4                -2.30 %
P16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF            500.2200000 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  22.80 cm
CY                  50.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2               -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42500 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER                emilyt
NAME      LWE-III-024 prod
EXPNO                   10
PROCNO                   1

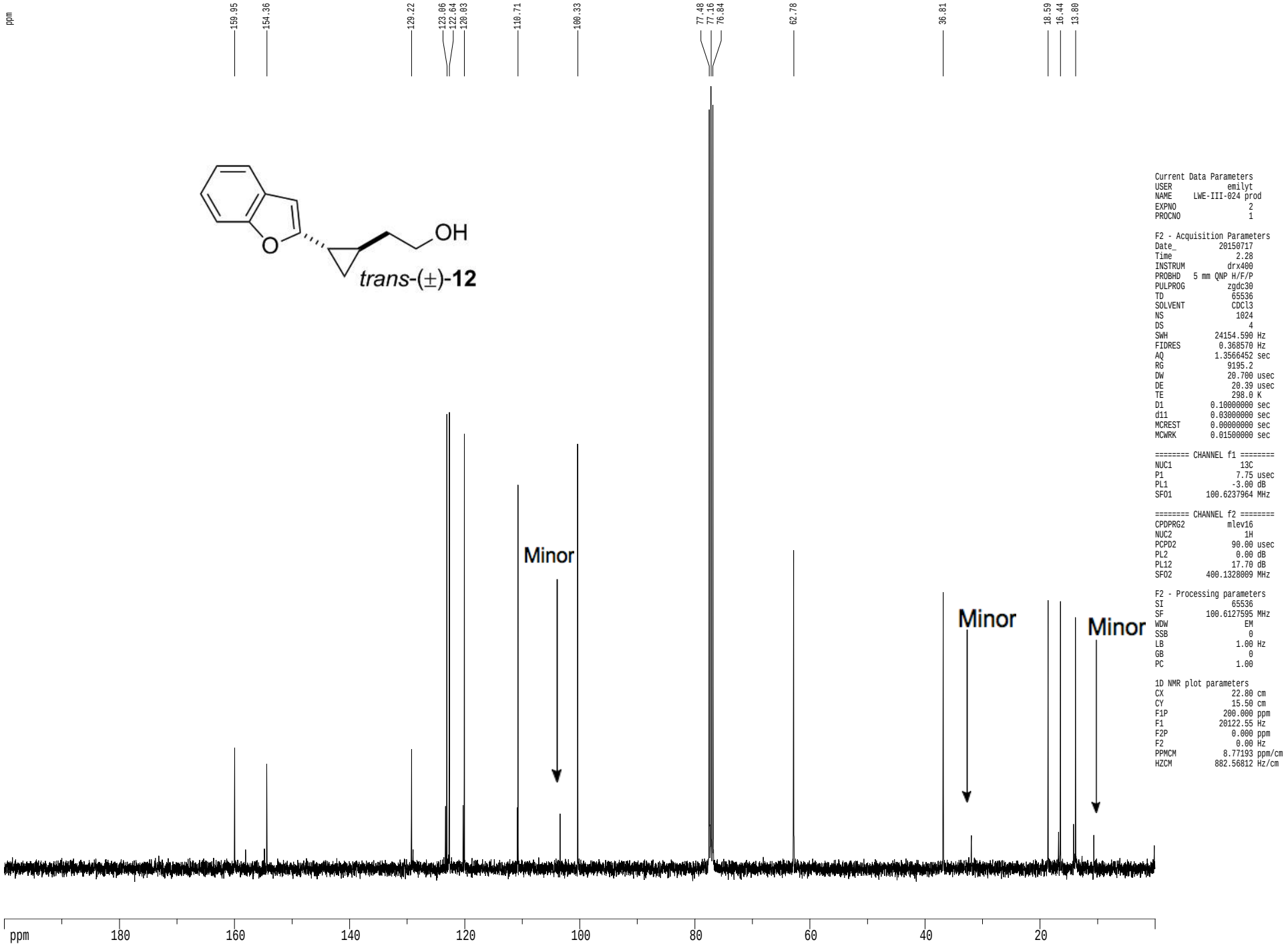
F2 - Acquisition Parameters
Date_             20150717
Time                 14.21
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  81728
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0999398 sec
RG                   10.1
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

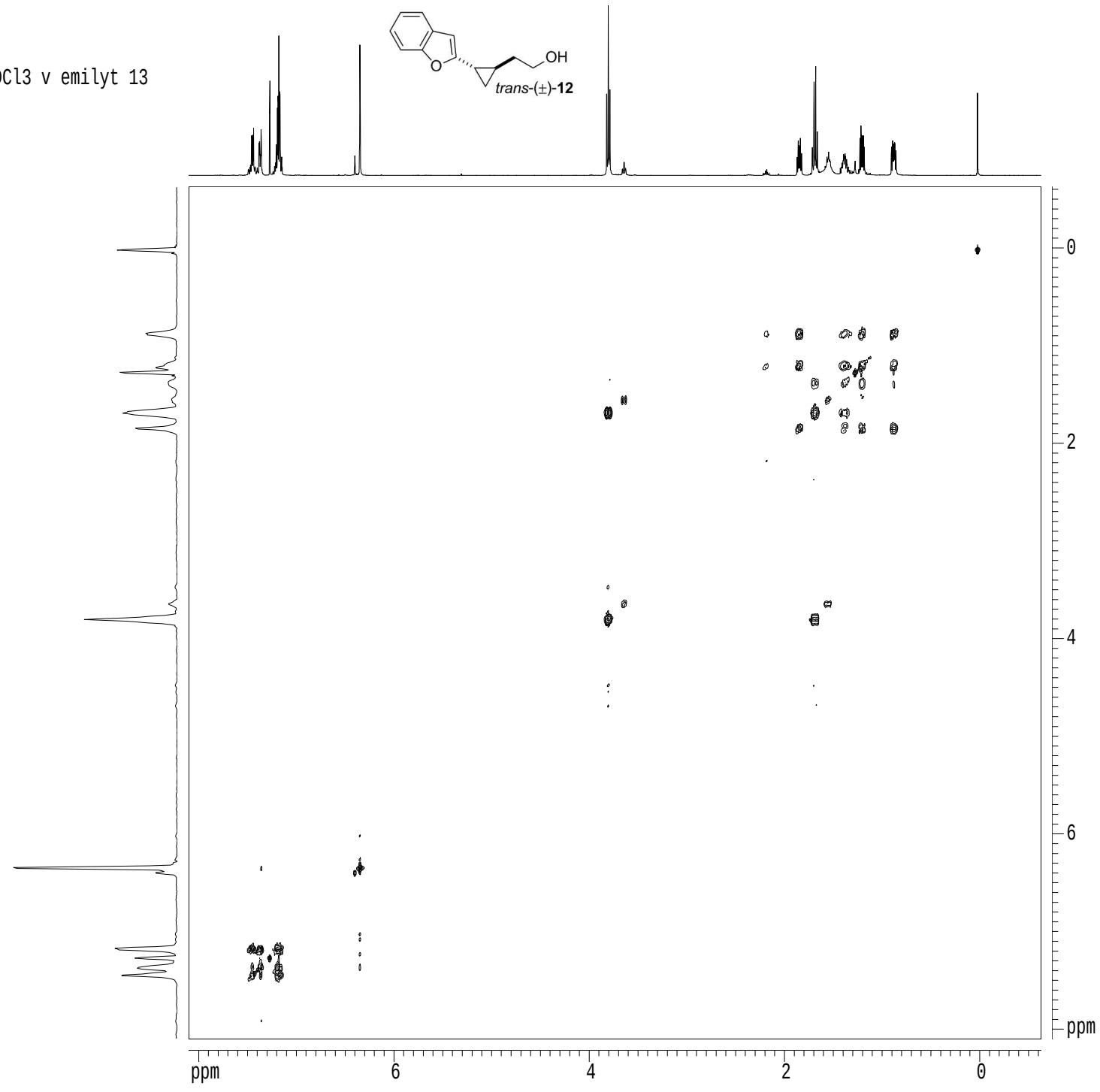
F2 - Processing parameters
SI                    65536
SF            500.2200353 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                   4.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.00 cm
F1P                  9.000 ppm
F1                 4501.98 Hz
F2P                 -0.500 ppm
F2                 -250.11 Hz
PPMCM             0.41667 ppm/cm
HZCM            208.42502 Hz/cm
```

PI Jarvo
c13 CDCl3 v emilyt 13



PI Jarvo
gcosy.q CDCl3 v emilyt 13



Current Data Parameters

USER	emilyt
NAME	LWE-III-024 prod
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20150717
Time	2.30
INSTRUM	drx400
PROBHD	5 mm QNP H/F/P
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	3491.620 Hz
FIDRES	1.704893 Hz
AQ	0.2933236 sec
RG	1448.2
DW	143.200 usec
DE	4.50 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00028640 sec

======== CHANNEL f1 ========

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1315124 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	256
SFO1	400.1315 MHz
FIDRES	13.639141 Hz
SW	8.726 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	400.1300176 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

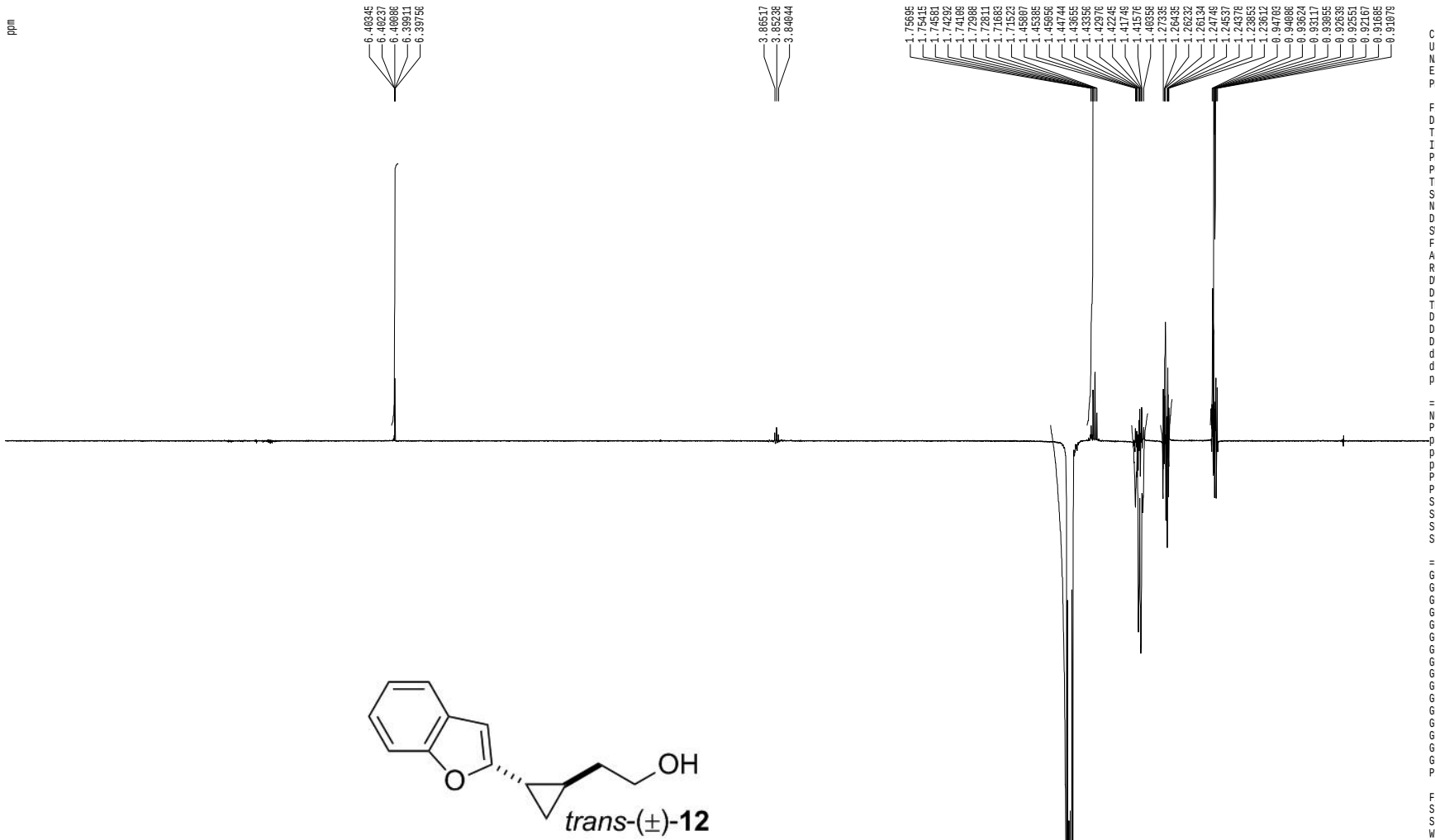
F1 - Processing parameters

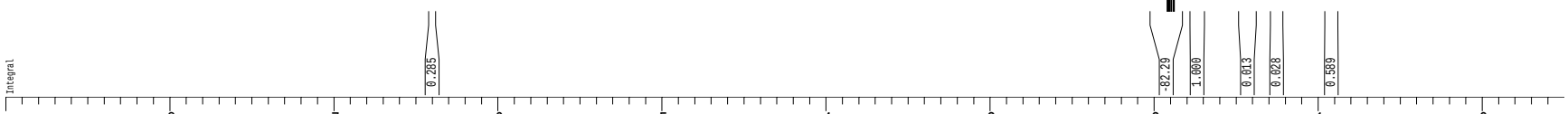
SI	1024
MC2	QF
SF	400.1300176 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.099 ppm
F2LO	3240.66 Hz
F2PHI	-0.627 ppm
F2HI	-250.96 Hz
F1PLO	8.099 ppm
F1LO	3240.66 Hz
F1PHI	-0.627 ppm
F1HI	-250.96 Hz
F2PPMCM	0.58175 ppm/cm
F2HZCM	232.77467 Hz/cm
F1PPMCM	0.58175 ppm/cm
F1HZCM	232.77467 Hz/cm

gnoe





Current Data Parameters
USER emilyt
NAME LWE-III-024 prod
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150718
Time 11.57
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

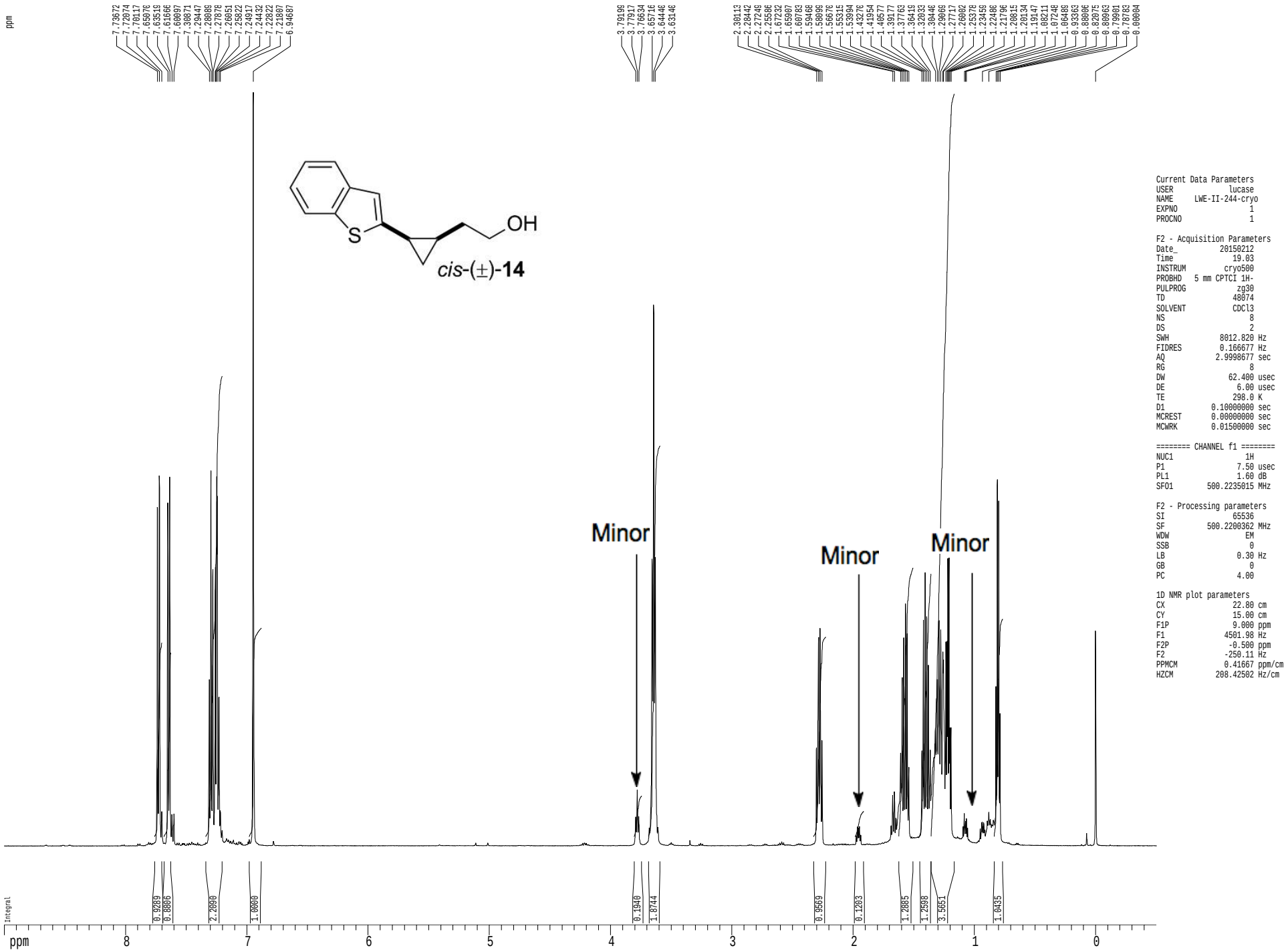
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2209495 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-244-cryo
EXPNO                    1
PROCNO                   1

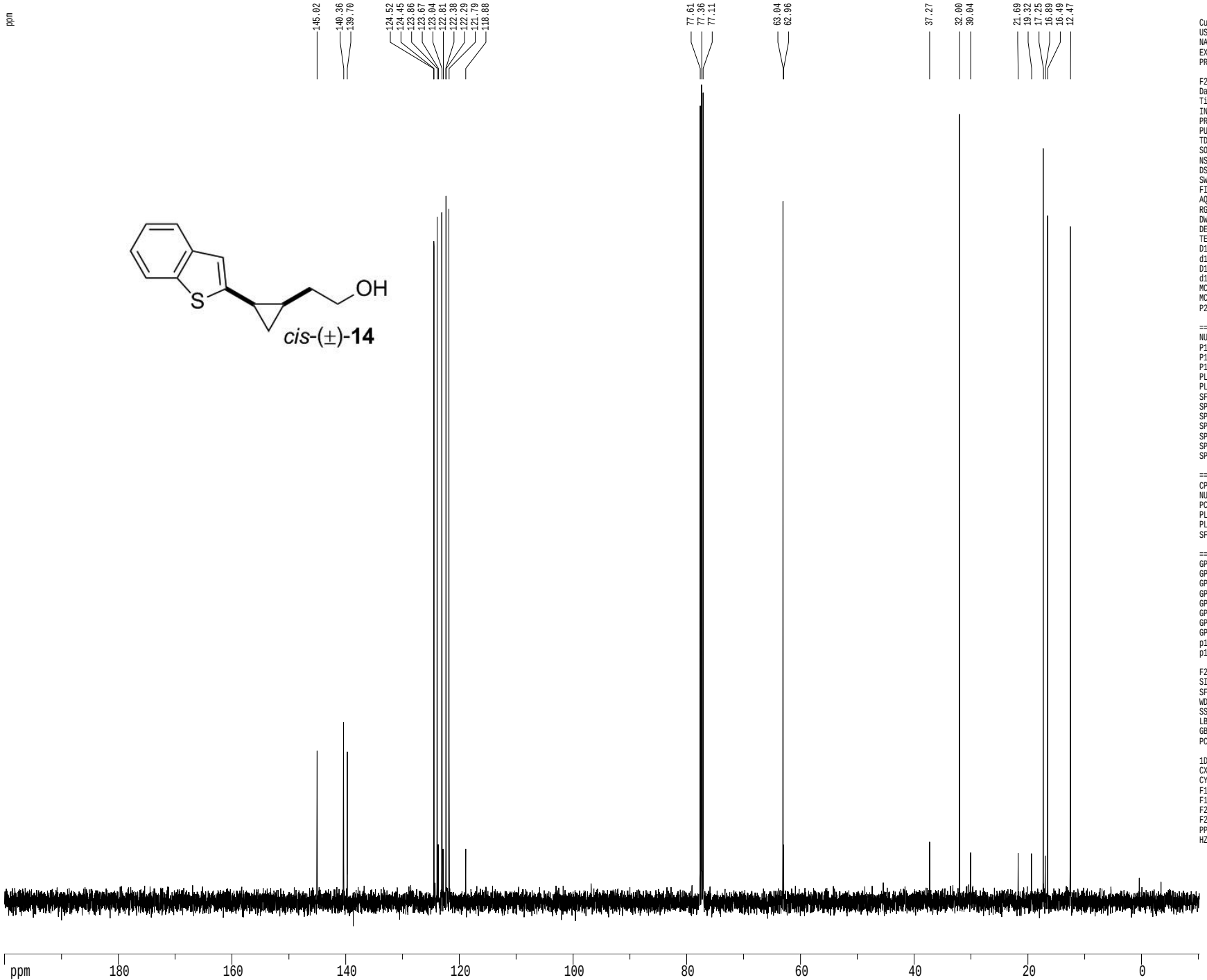
F2 - Acquisition Parameters
Date_             20150212
Time                 19.03
INSTRUM            cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG                zg30
TD                    48074
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8012.820 Hz
FIDRES                0.166677 Hz
AQ                 2.9998677 sec
RG                        8
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              500.2200362 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    4.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.00 cm
F1P                   9.000 ppm
F1                 4501.98 Hz
F2P                  -0.500 ppm
F2                 -250.11 Hz
PPMCM              0.41667 ppm/cm
HZCM             208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-244-cryo
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150212
Time                 19.05
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     122
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                    6502
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

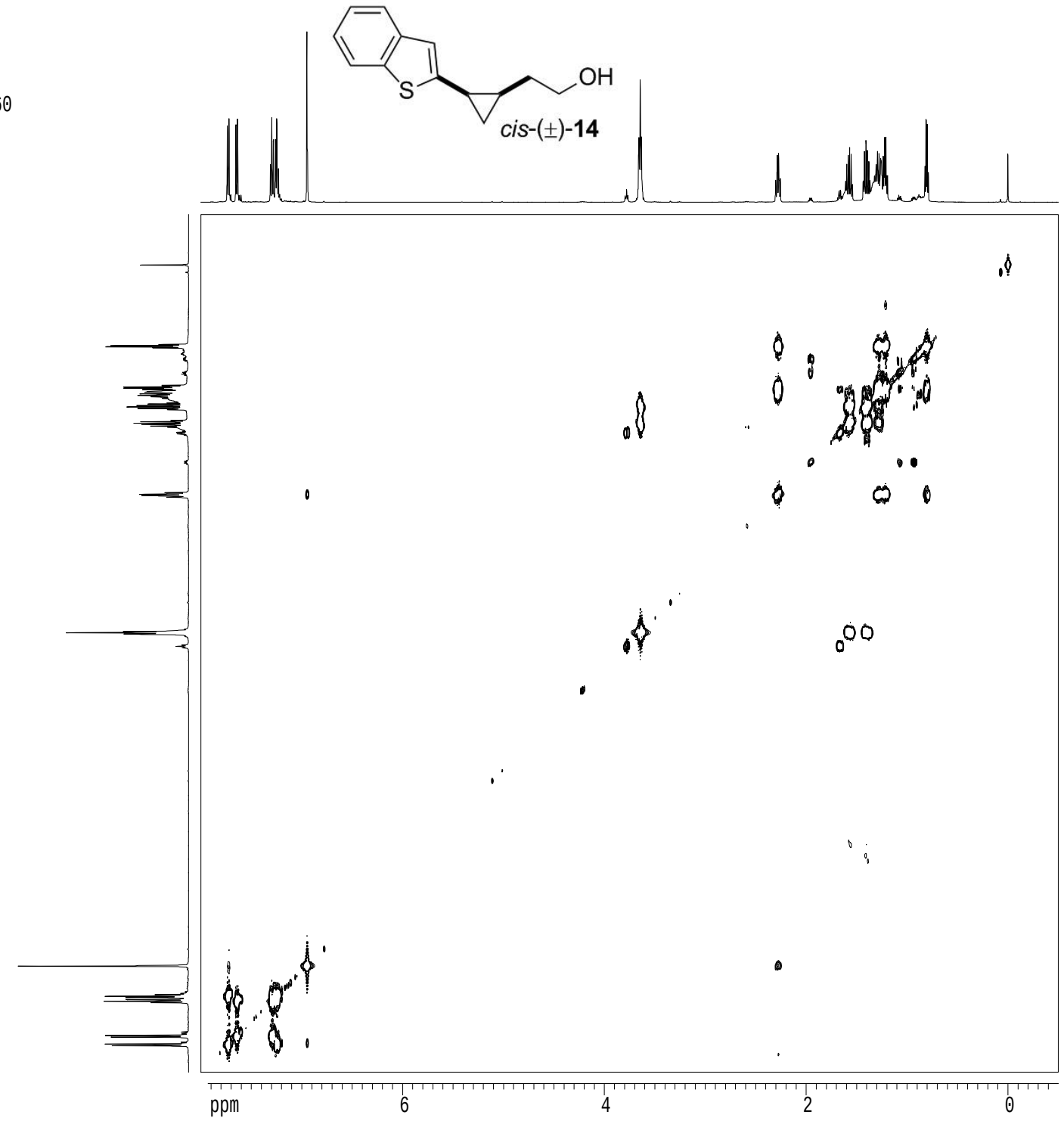
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7803857 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1               25156.08 Hz
F2P                -10.195 ppm
F2               -1282.31 Hz
PPMCM              9.21907 ppm/cm
HZCM            1159.57861 Hz/cm
```

gcosy60




```
        Current Data Parameters
USER              lucase
NAME      LWE-II-244-cryo
EXPNO                  3
PROCNO                 1

      F2 - Acquisition Parameters
Date_           20150212
Time              19.09
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG    cosygp60.prd
TD                2048
SOLVENT           CDCl3
NS                   2
DS                  16
SWH            4251.701 Hz
FIDRES         2.076026 Hz
AQ             0.2408948 sec
RG                161.3
DW              117.600 usec
DE                6.00 usec
TE                298.0 K
d0           0.00000300 sec
D1           1.00000000 sec
d13          0.00000300 sec
D16          0.00020000 sec
IN0          0.00023520 sec

     ======== CHANNEL f1 ========
NUC1                  1H
P1                  7.50 usec
PL1                 1.60 dB
SFO1         500.2218758 MHz

     ====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               17.00 %
GPZ2               17.00 %
P16              1000.00 usec

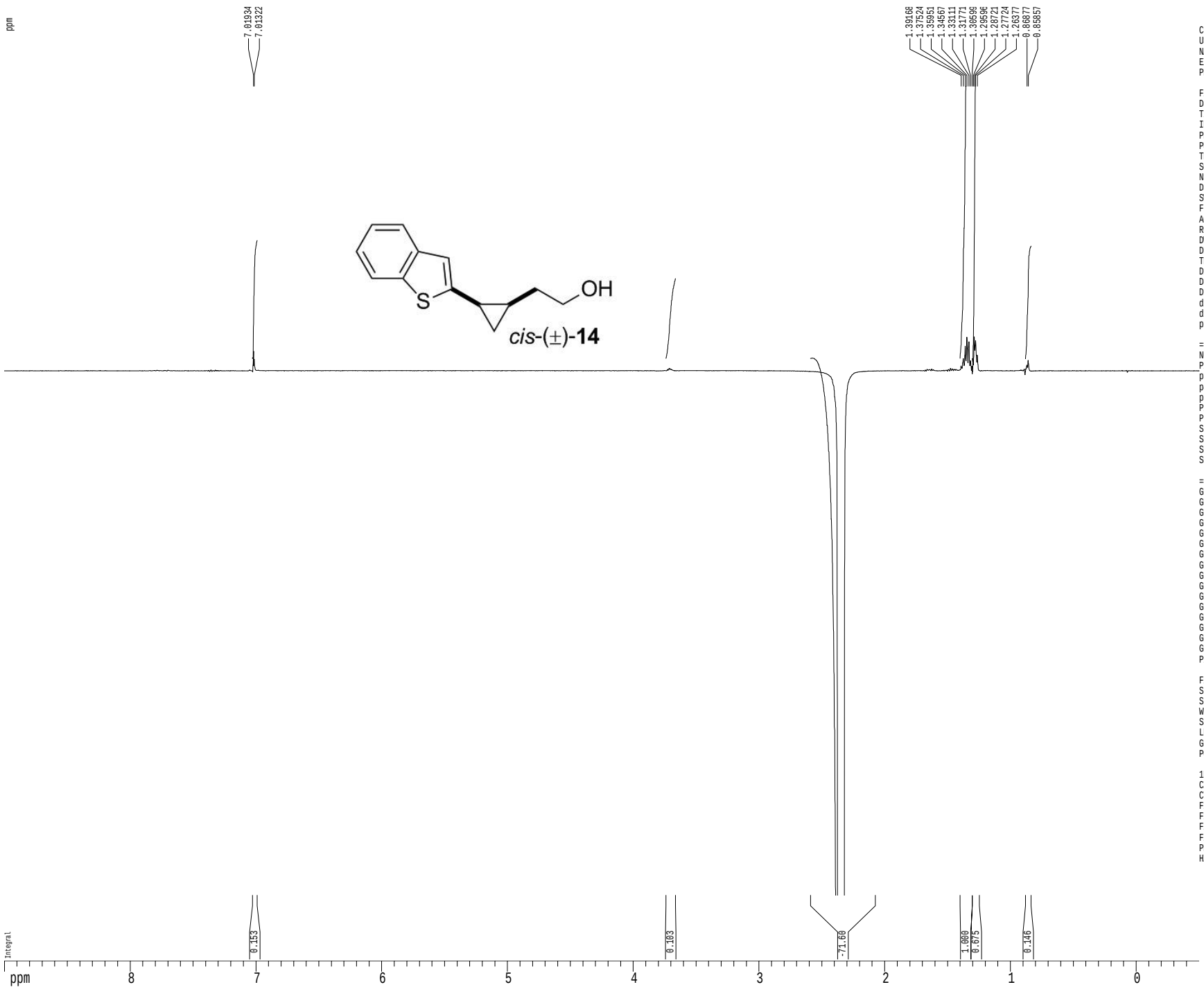
      F1 - Acquisition parameters
ND0                   1
TD                  128
SFO1          500.2219 MHz
FIDRES        33.216412 Hz
SW                8.500 ppm
FnMODE        undefined

      F2 - Processing parameters
SI                 1024
SF           500.2200362 MHz
WDW                SINE
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 2.00

      F1 - Processing parameters
SI                 1024
MC2                  QF
SF           500.2200362 MHz
WDW                SINE
SSB                   0
LB                 0.00 Hz
GB                    0

        2D NMR plot parameters
CX2               15.00 cm
CX1               15.00 cm
F2PLO             8.000 ppm
F2LO            4001.67 Hz
F2PHI            -0.500 ppm
F2HI             -250.03 Hz
F1PLO             8.000 ppm
F1LO            4001.67 Hz
F1PHI            -0.500 ppm
F1HI             -250.03 Hz
F2PPMCM          0.56664 ppm/cm
F2HZCM         283.44672 Hz/cm
F1PPMCM          0.56664 ppm/cm
F1HZCM         283.44672 Hz/cm
```

gnoe




```
Current Data Parameters
USER                lucase
NAME      LWE-II-244-cryo
EXPNO                    5
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150212
Time                19.30
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                  101.6
DW                62.400 usec
DE                 6.00 usec
TE                 298.0 K
D1              1.00000000 sec
D8              0.50000000 sec
D16             0.00020000 sec
d21             0.33376500 sec
d22             0.16399699 sec
p2                15.00 usec

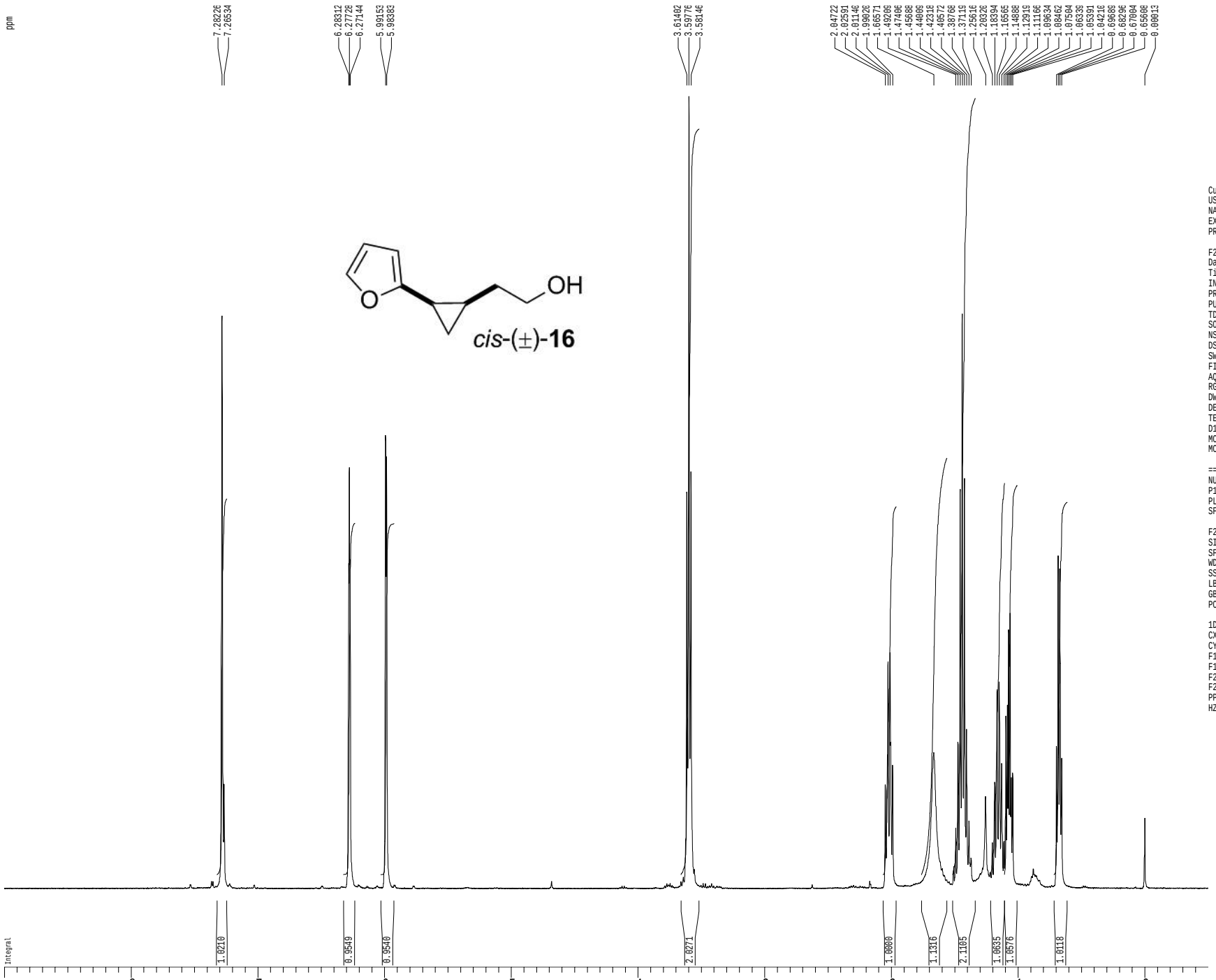
======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
p3                  22.50 usec
p4                  30.00 usec
p5                  20.00 usec
P12               40000.00 usec
PL1                  1.60 dB
SFO1          500.2211758 MHz
SP1                 61.60 dB
SPNAM1         gauss1.512
SPOFF1               0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1           sine.100
GPNAM2           sine.100
GPNAM3           sine.100
GPNAM4           sine.100
GPX1                 0.00 %
GPX2                 0.00 %
GPX3                 0.00 %
GPX4                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPY3                 0.00 %
GPY4                 0.00 %
GPZ1                 7.00 %
GPZ2                 3.00 %
GPZ3                 2.30 %
GPZ4                -2.30 %
P16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF            500.2200000 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  22.80 cm
CY                  50.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42500 Hz/cm
```

1H spectrum



Current Data Parameters
USER emilyt
NAME EJT-V-043
EXPNO 10
PROCNO 1

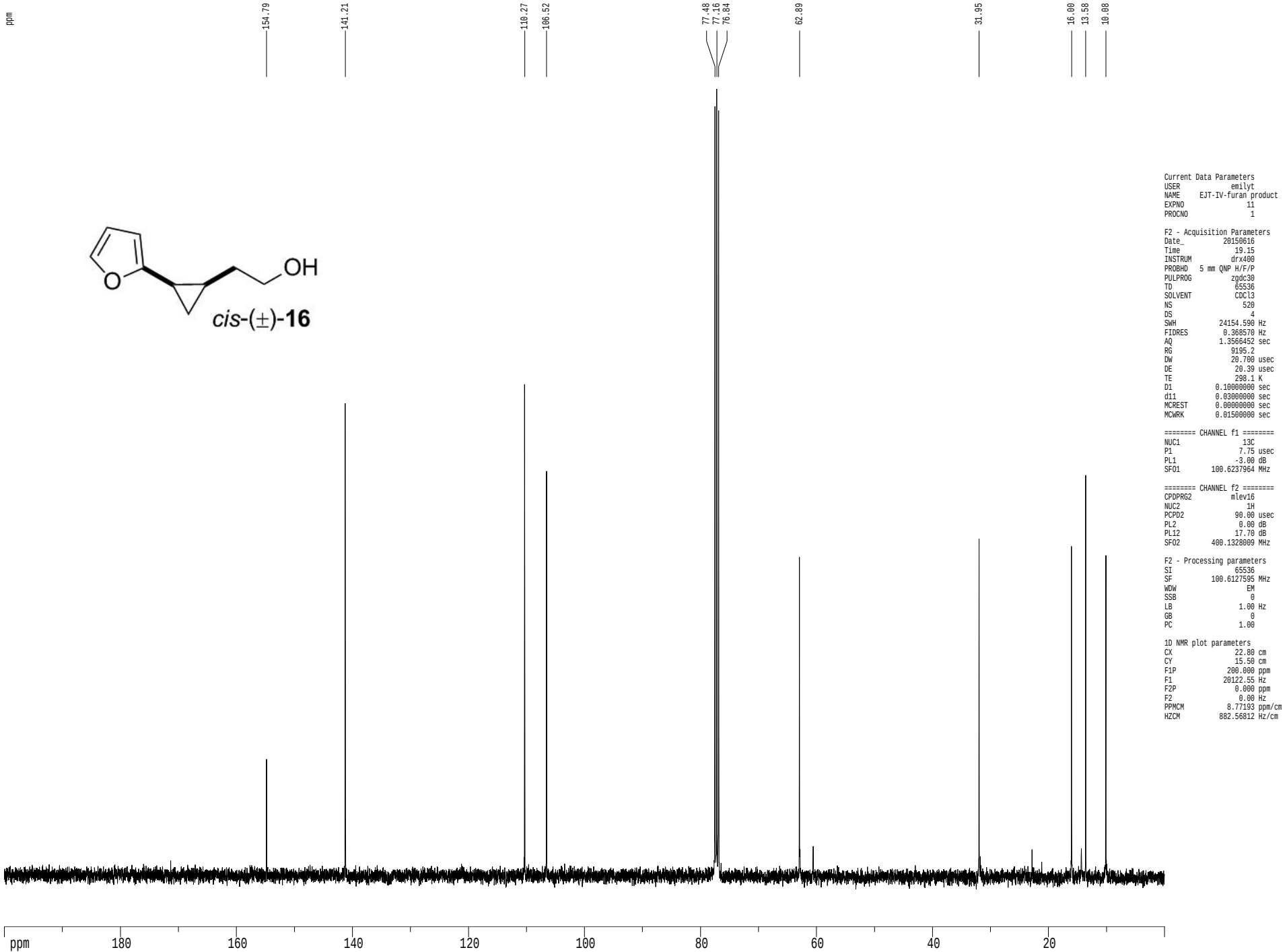
F2 - Acquisition Parameters
Date_ 20150226
Time 15.08
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1118579 sec
RG 80.6
DW 78.000 usec
DE 4.50 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1328009 MHz

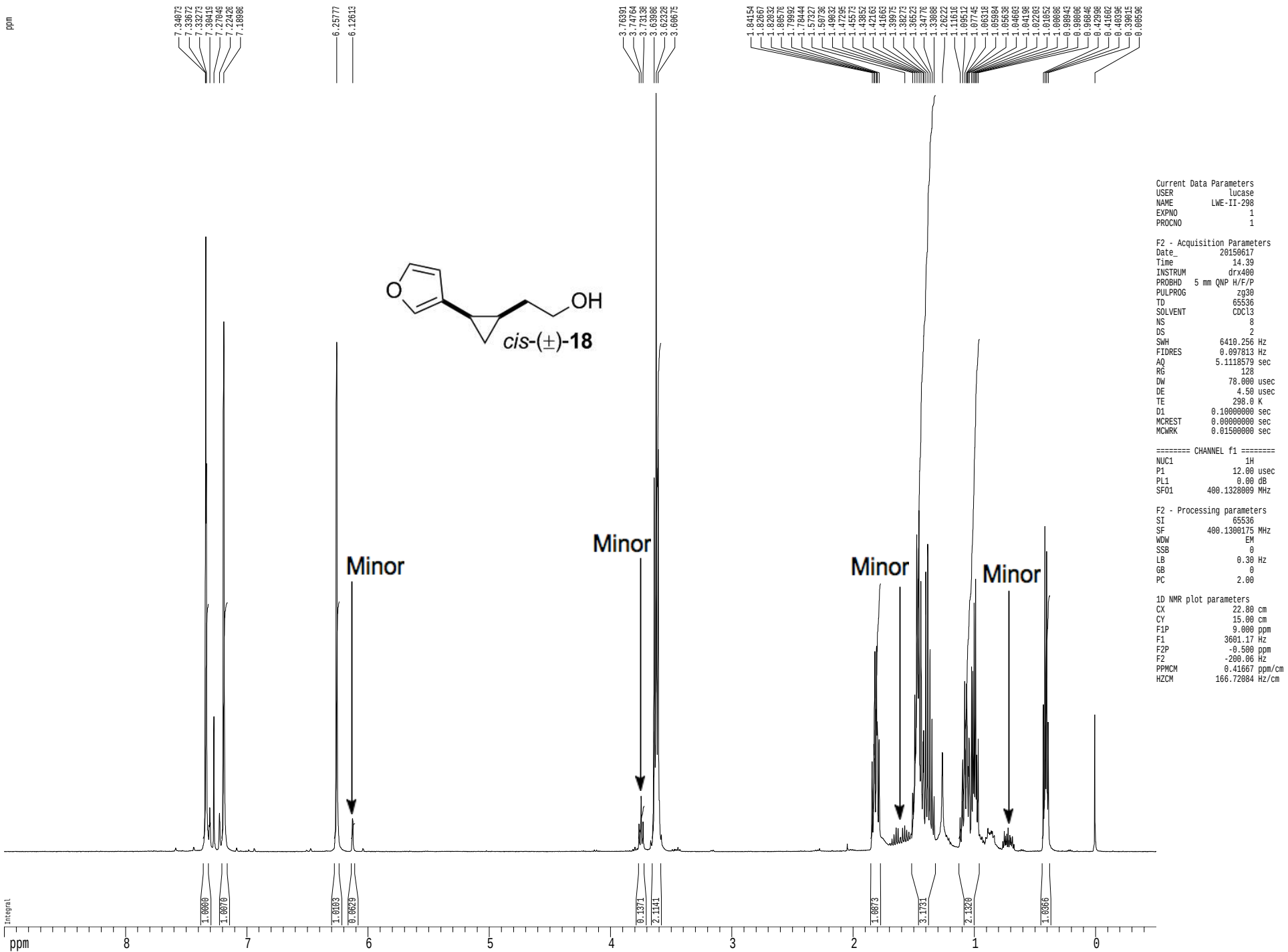
F2 - Processing parameters
SI 65536
SF 400.1300181 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.41667 ppm/cm
HZCM 166.72084 Hz/cm

13C spectrum with 1H decoupling



1H spectrum




```
Current Data Parameters
USER                lucase
NAME           LWE-II-298
EXPNO                   1
PROCNO                  1

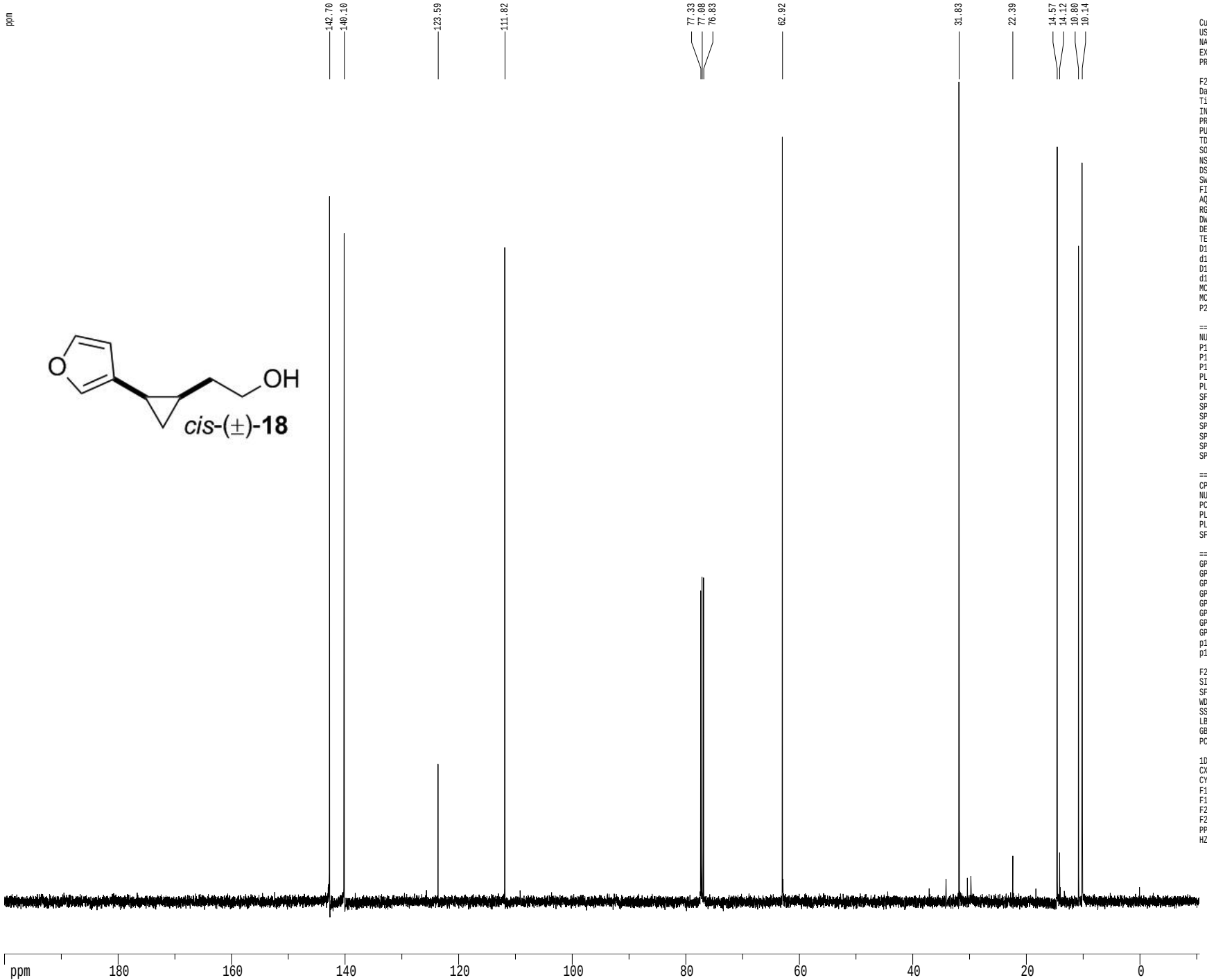
F2 - Acquisition Parameters
Date_            20150617
Time                14.39
INSTRUM           drx400
PROBHD   5 mm QNP H/F/P
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1118579 sec
RG                    128
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                 0.00 dB
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF           400.1300175 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.00 cm
F1P                  9.000 ppm
F1                3601.17 Hz
F2P                 -0.500 ppm
F2                -200.06 Hz
PPMCM             0.41667 ppm/cm
HZCM            166.72084 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-242-cryo7
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150403
Time                17.45
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    129
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                   3251
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

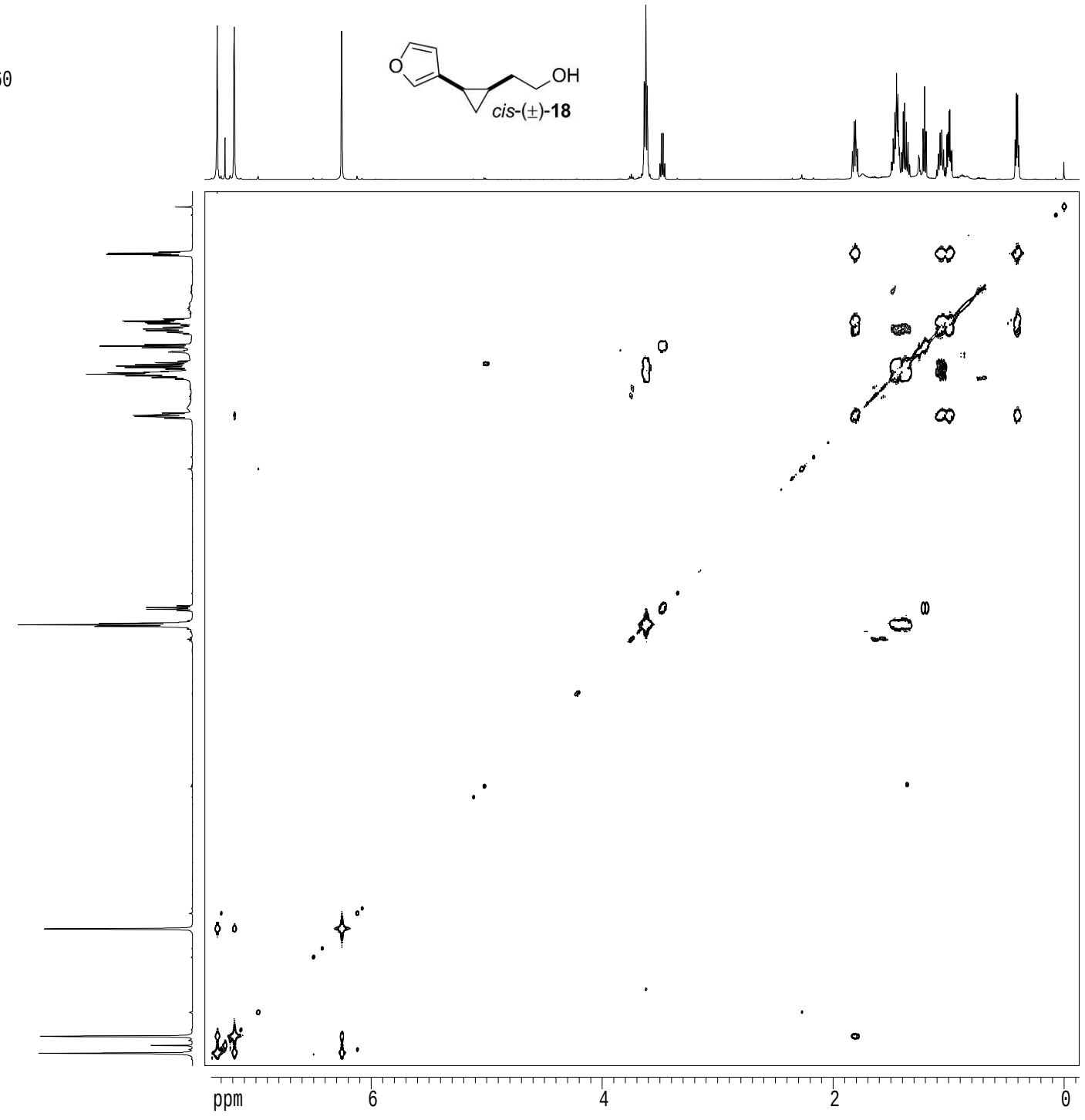
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7804190 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1               25156.09 Hz
F2P                -10.460 ppm
F2               -1315.66 Hz
PPMCM              9.23070 ppm/cm
HZCM            1161.04163 Hz/cm
```

gcosy60



Current Data Parameters

USER	lucase
NAME	LWE-II-242-cryo
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20150129
Time	15.36
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	3787.879 Hz
FIDRES	1.849550 Hz
AQ	0.2703860 sec
RG	35.9
DW	132.000 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00026400 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2218289 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	256
SFO1	500.2218 MHz
FIDRES	14.796402 Hz
SW	7.572 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200281 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

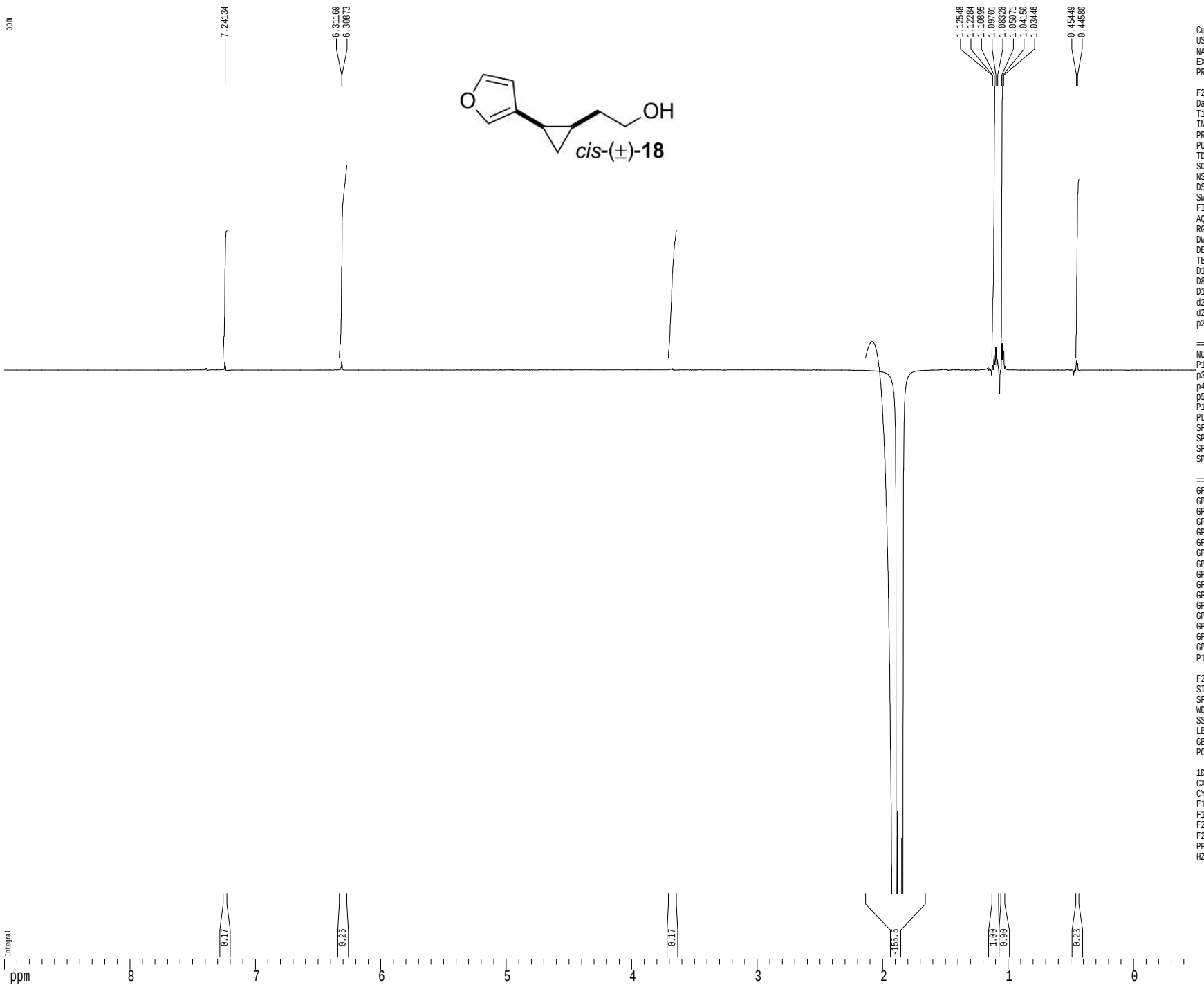
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200281 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	7.442 ppm
F2LO	3722.82 Hz
F2PHI	-0.130 ppm
F2HI	-65.06 Hz
F1PLO	7.442 ppm
F1LO	3722.82 Hz
F1PHI	-0.130 ppm
F1HI	-65.06 Hz
F2PPMCM	0.50483 ppm/cm
F2HZCM	252.52527 Hz/cm
F1PPMCM	0.50483 ppm/cm
F1HZCM	252.52527 Hz/cm

gnoe




```
Current Data Parameters
USER                lucase
NAME      LWE-II-242-cryo
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150129
Time                16.17
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   71.8
DW                 62.400 usec
DE                  6.00 usec
TE                298.0 K
D1              1.00000000 sec
D8              0.50000000 sec
D16             0.00020000 sec
d21             0.33376500 sec
d22             0.16399699 sec
p2                  15.00 usec

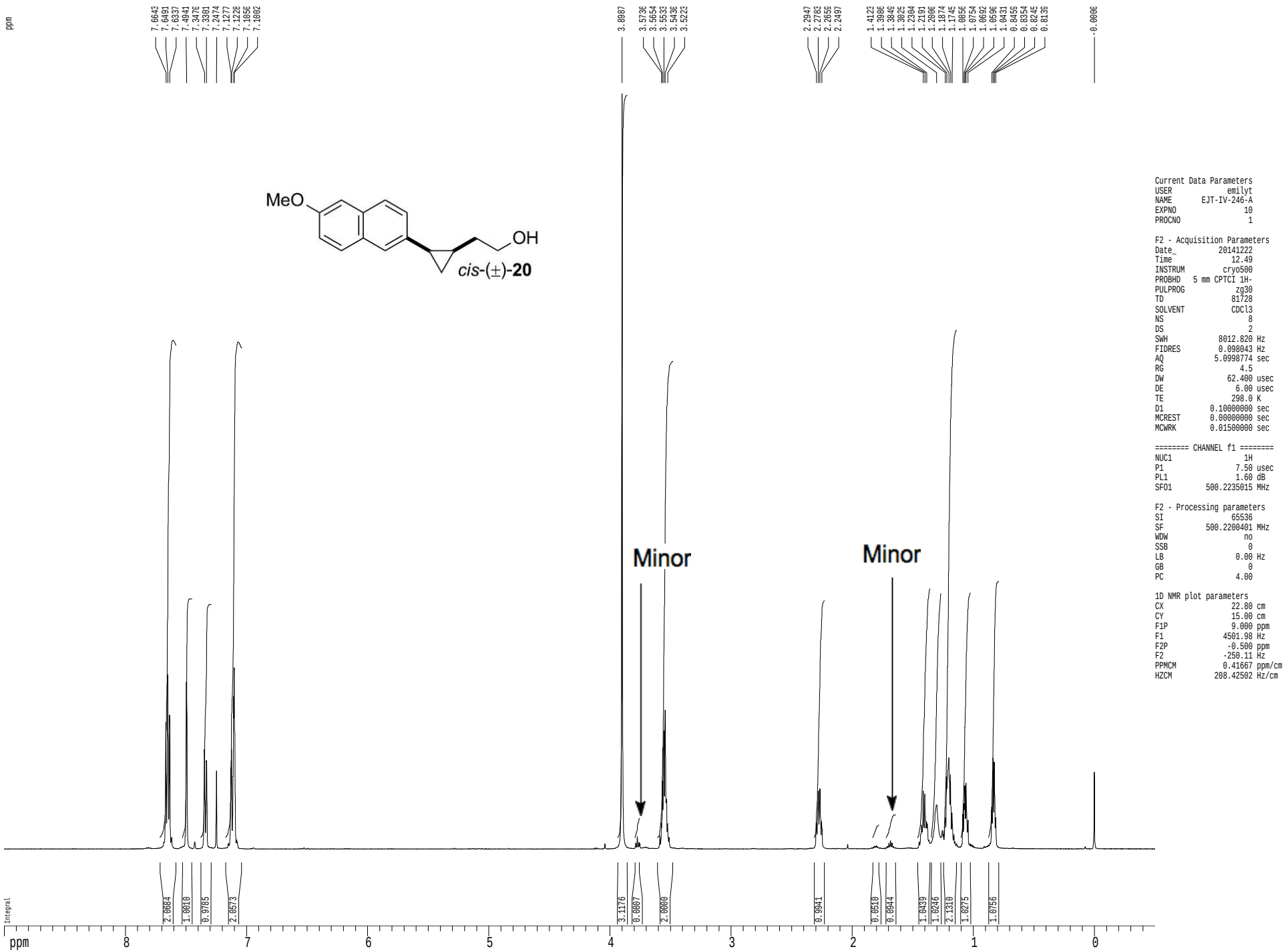
======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
p3                  22.50 usec
p4                  30.00 usec
p5                  20.00 usec
P12                40000.00 usec
PL1                    1.60 dB
SFO1           500.2209337 MHz
SP1                   61.60 dB
SPNAM1          gauss1.512
SPOFF1                 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1            sine.100
GPNAM2            sine.100
GPNAM3            sine.100
GPNAM4            sine.100
GPX1                  0.00 %
GPX2                  0.00 %
GPX3                  0.00 %
GPX4                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPY3                  0.00 %
GPY4                  0.00 %
GPZ1                  7.00 %
GPZ2                  3.00 %
GPZ3                  2.30 %
GPZ4                 -2.30 %
P16                1000.00 usec

F2 - Processing parameters
SI                    65536
SF             500.2200000 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    22.80 cm
CY                    50.00 cm
F1P                    9.000 ppm
F1                  4501.98 Hz
F2P                   -0.500 ppm
F2                  -250.11 Hz
PPMCM              0.41667 ppm/cm
HZCM             208.42500 Hz/cm
```

1H spectrum



Current Data Parameters
USER emilyt
NAME EJT-IV-246-A
EXPNO 10
PROCNO 1

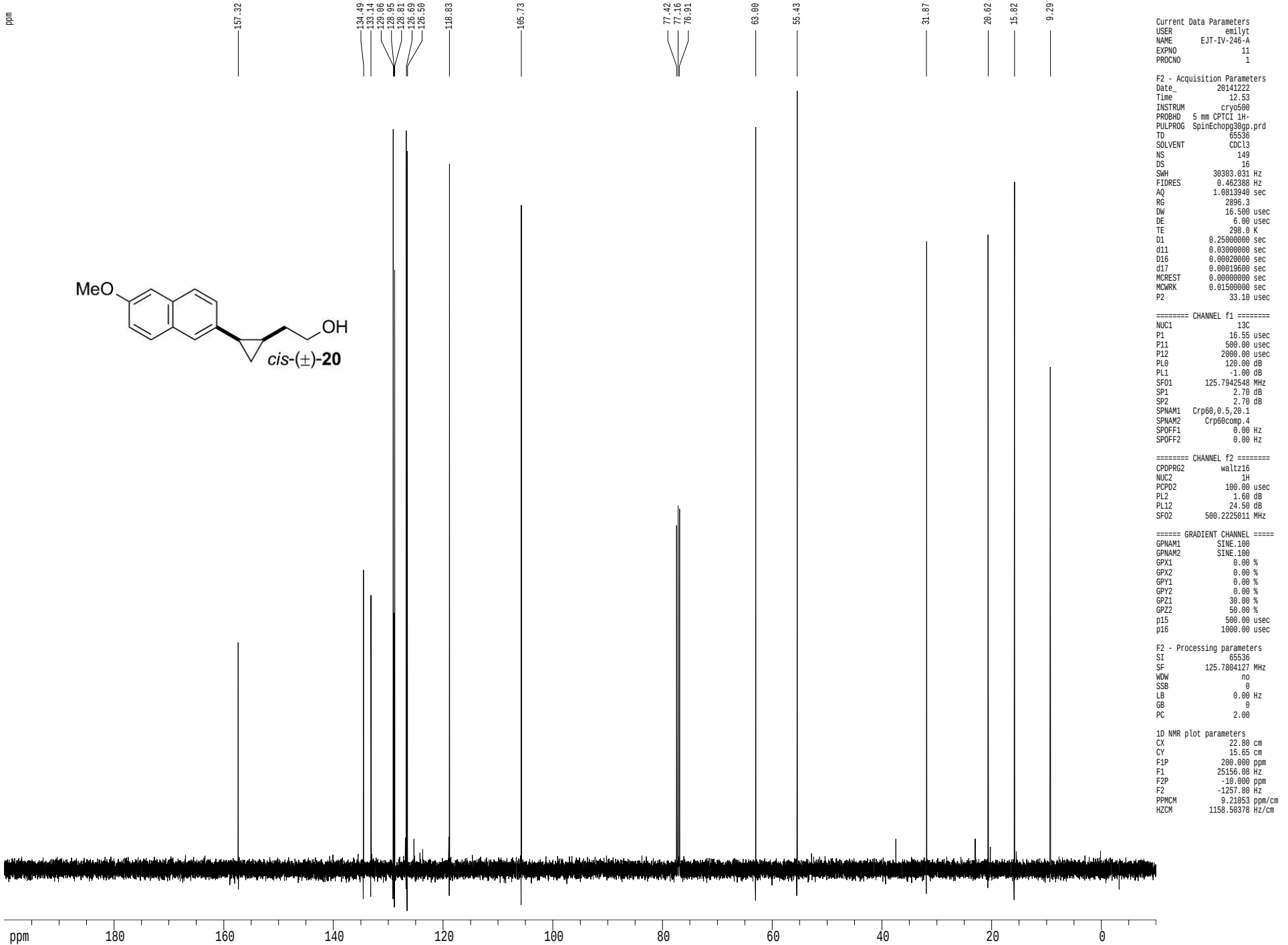
F2 - Acquisition Parameters
Date_ 20141222
Time 12.49
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 4.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200401 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42502 Hz/cm

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



Current Data Parameters
USER emilyt
NAME EJT-IV-246-A
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141222
Time 12.53
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT CDCl3
NS 149
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 33.10 usec

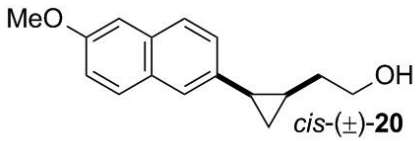
======== CHANNEL f1 ========
NUC1 13C
P1 16.55 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7942548 MHz
SP1 2.70 dB
SP2 2.70 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

======== 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 125.7804127 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -10.000 ppm
F2 -1257.80 Hz
PPMCM 9.21053 ppm/cm
HZCM 1158.50378 Hz/cm



cis-(±)-**20**

gcosy60


```
       Current Data Parameters
USER            emilyt
NAME     EJT-IV-260 noe
EXPNO                2
PROCNO               1

      F2 - Acquisition Parameters
Date_          20150204
Time              22.37
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG    cosygp60.prd
TD                2048
SOLVENT           CDCl3
NS                   2
DS                  16
SWH            4734.849 Hz
FIDRES         2.311938 Hz
AQ             0.2163188 sec
RG                228.1
DW              105.600 usec
DE                6.00 usec
TE               298.0 K
d0            0.00000300 sec
D1            1.00000000 sec
d13           0.00000300 sec
D16           0.00020000 sec
IN0           0.00021120 sec

     ======== CHANNEL f1 ========
NUC1                 1H
P1                 7.50 usec
PL1                1.60 dB
SFO1        500.2221588 MHz

     ====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               17.00 %
GPZ2               17.00 %
P16              1000.00 usec

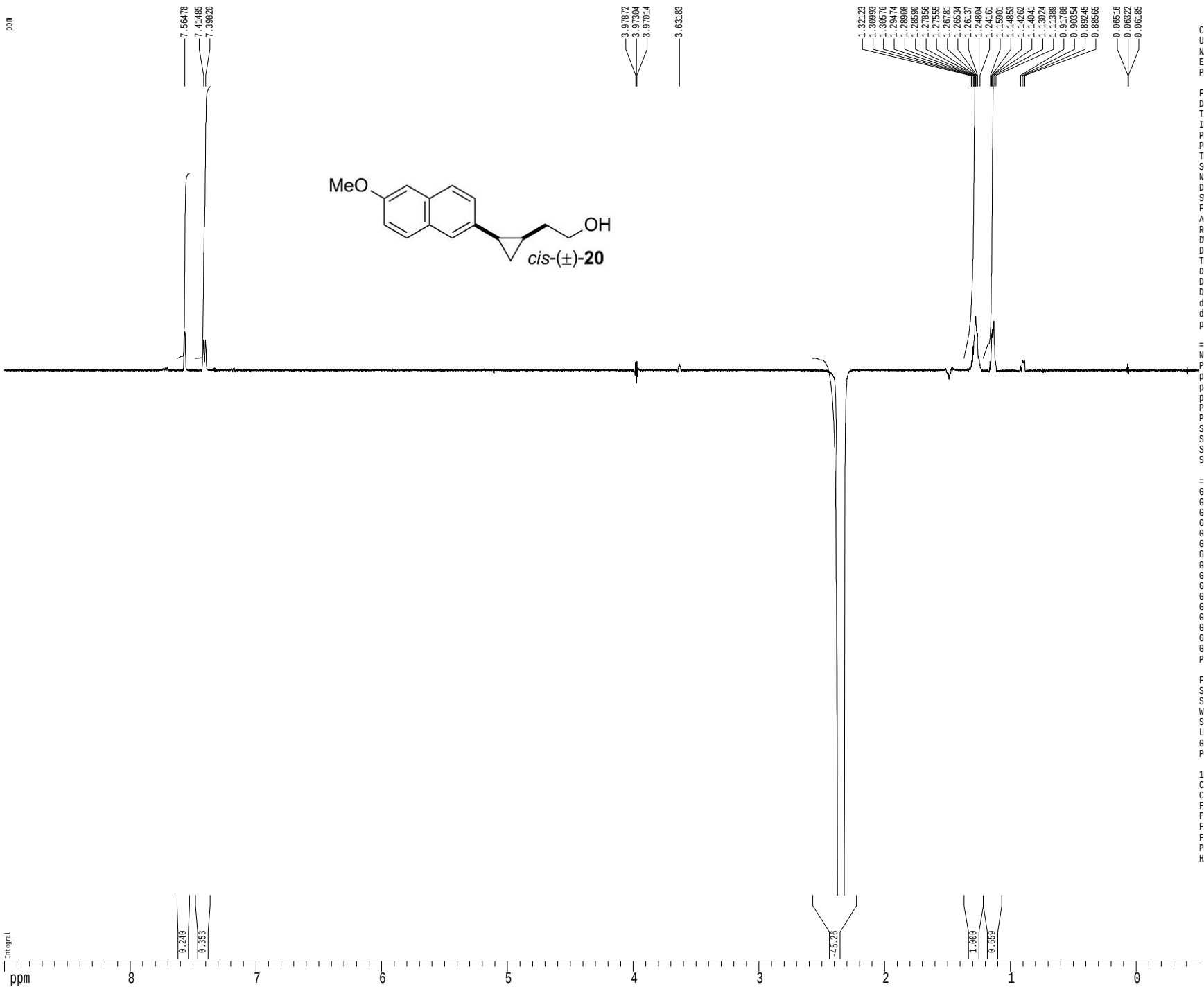
      F1 - Acquisition parameters
ND0                  1
TD                 128
SFO1          500.2222 MHz
FIDRES        36.991005 Hz
SW                9.465 ppm
FnMODE        undefined

      F2 - Processing parameters
SI                1024
SF          500.2200329 MHz
WDW               SINE
SSB                  0
LB                0.00 Hz
GB                   0
PC                4.00

      F1 - Processing parameters
SI                1024
MC2                 QF
SF          500.2200329 MHz
WDW               SINE
SSB                  0
LB                0.00 Hz
GB                   0

       2D NMR plot parameters
CX2              15.00 cm
CX1              15.00 cm
F2PLO             8.983 ppm
F2LO           4493.36 Hz
F2PHI            -0.483 ppm
F2HI           -241.49 Hz
F1PLO             8.983 ppm
F1LO           4493.36 Hz
F1PHI            -0.483 ppm
F1HI           -241.49 Hz
F2PPMCM         0.63104 ppm/cm
F2HZCM        315.65659 Hz/cm
F1PPMCM         0.63104 ppm/cm
F1HZCM        315.65659 Hz/cm
```

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-260 noe
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150204
Time 23.12
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 101.6
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

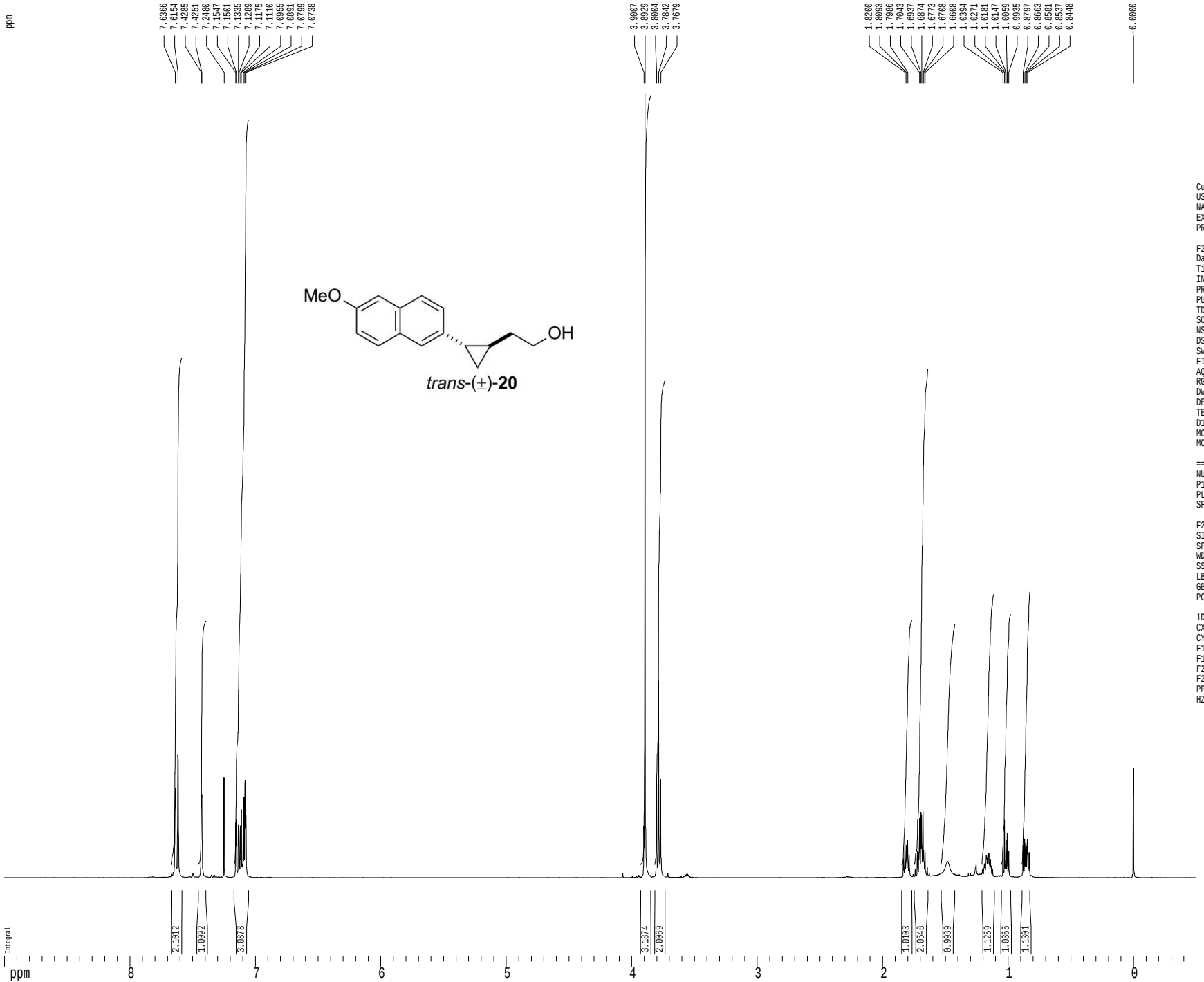
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2211752 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

PI Jarvo
h1 CDCl3 v emilyt 108



Current Data Parameters
USER emilyt
NAME EJT-V-031-A
EXPNO 4
PROCNO 1

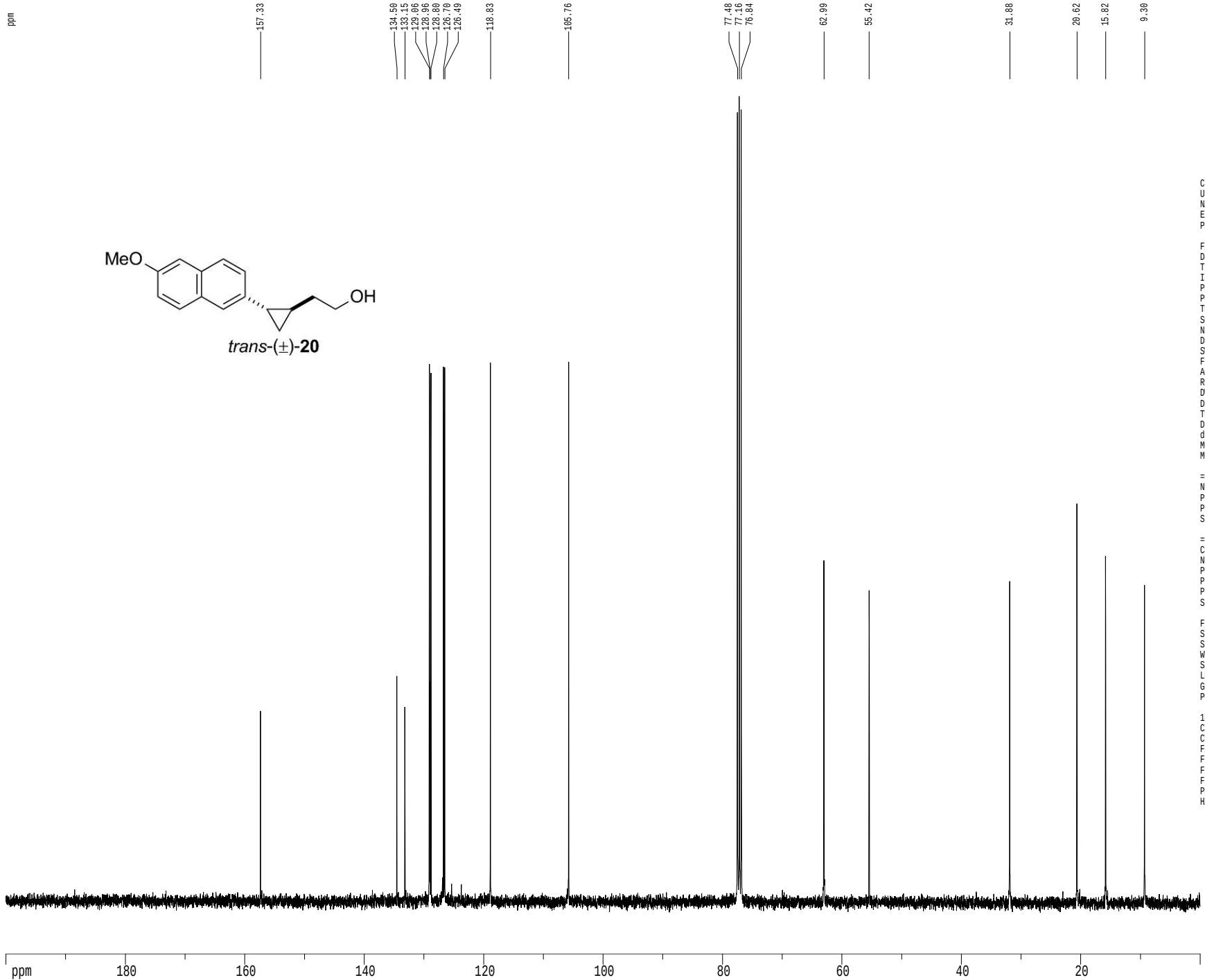
F2 - Acquisition Parameters
Date_ 20150408
Time 4.24
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zg30
TD 73274
SOLVENT CDCl3
NS 8
DS 2
SWH 7183.908 Hz
FIDRES 0.098042 Hz
AQ 5.0999203 sec
RG 203.2
DW 69.600 usec
DE 4.50 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1328009 MHz

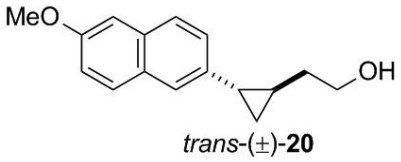
F2 - Processing parameters
SI 65536
SF 400.1300255 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.41667 ppm/cm
HZCM 166.72086 Hz/cm

PI Jarvo
c13 CDCl3 v emilyt 20



gcosy60



trans-(±)-**20**

Current Data Parameters

USER	emilyt
NAME	EJT-V-031-A
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20150204
Time	22.10
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4734.849 Hz
FIDRES	2.311938 Hz
AQ	0.2163188 sec
RG	161.3
DW	105.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00021120 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2221571 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2222 MHz
FIDRES	36.991005 Hz
SW	9.465 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200255 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

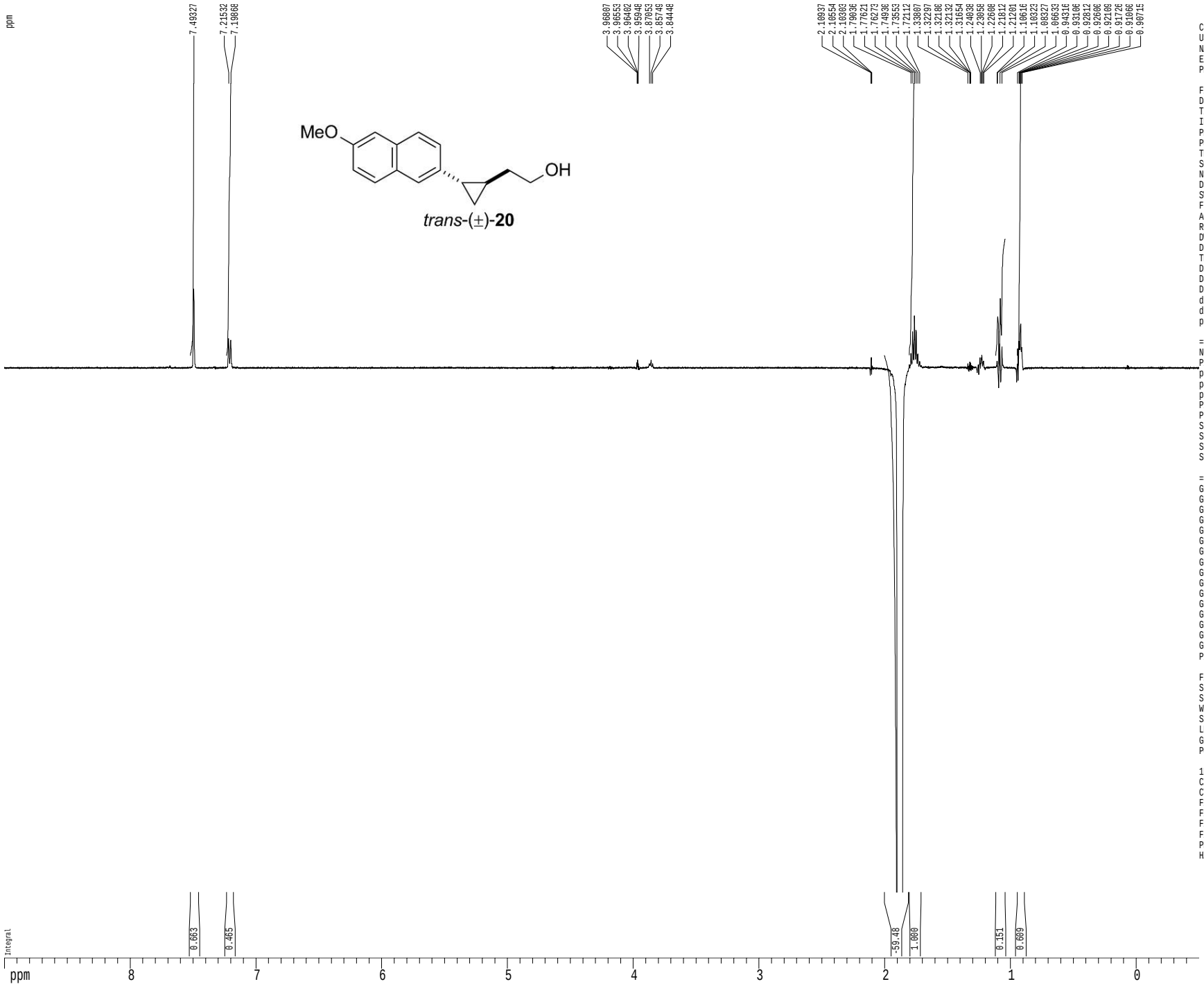
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200255 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.983 ppm
F2LO	4493.35 Hz
F2PHI	-0.483 ppm
F2HI	-241.50 Hz
F1PLO	8.983 ppm
F1LO	4493.35 Hz
F1PHI	-0.483 ppm
F1HI	-241.50 Hz
F2PPMCM	0.63104 ppm/cm
F2HZCM	315.65659 Hz/cm
F1PPMCM	0.63104 ppm/cm
F1HZCM	315.65659 Hz/cm

gnoe



Current Data Parameters
USER emilyt
NAME EJT-V-031-A
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150204
Time 22.29
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 90.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

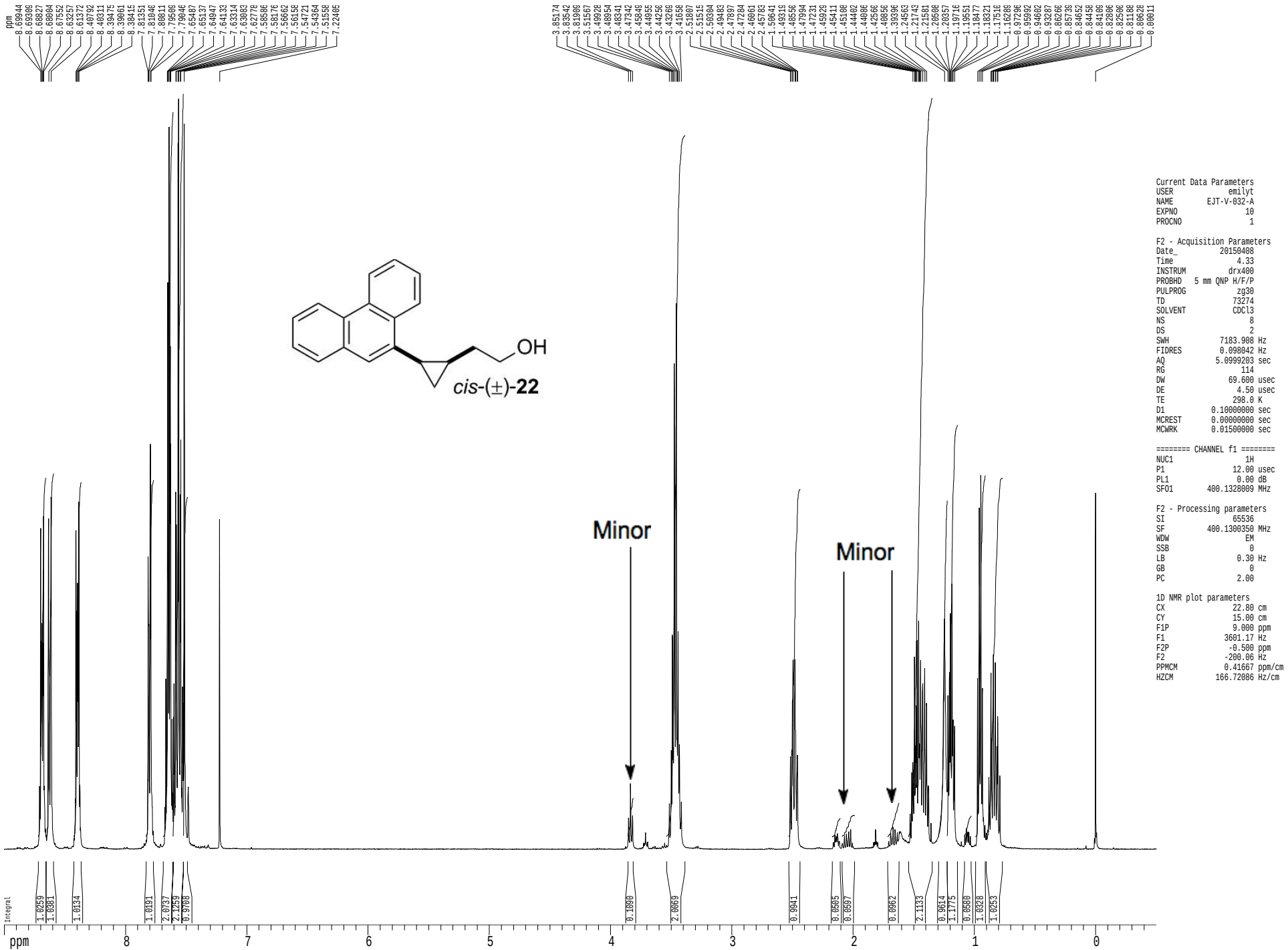
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2209408 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

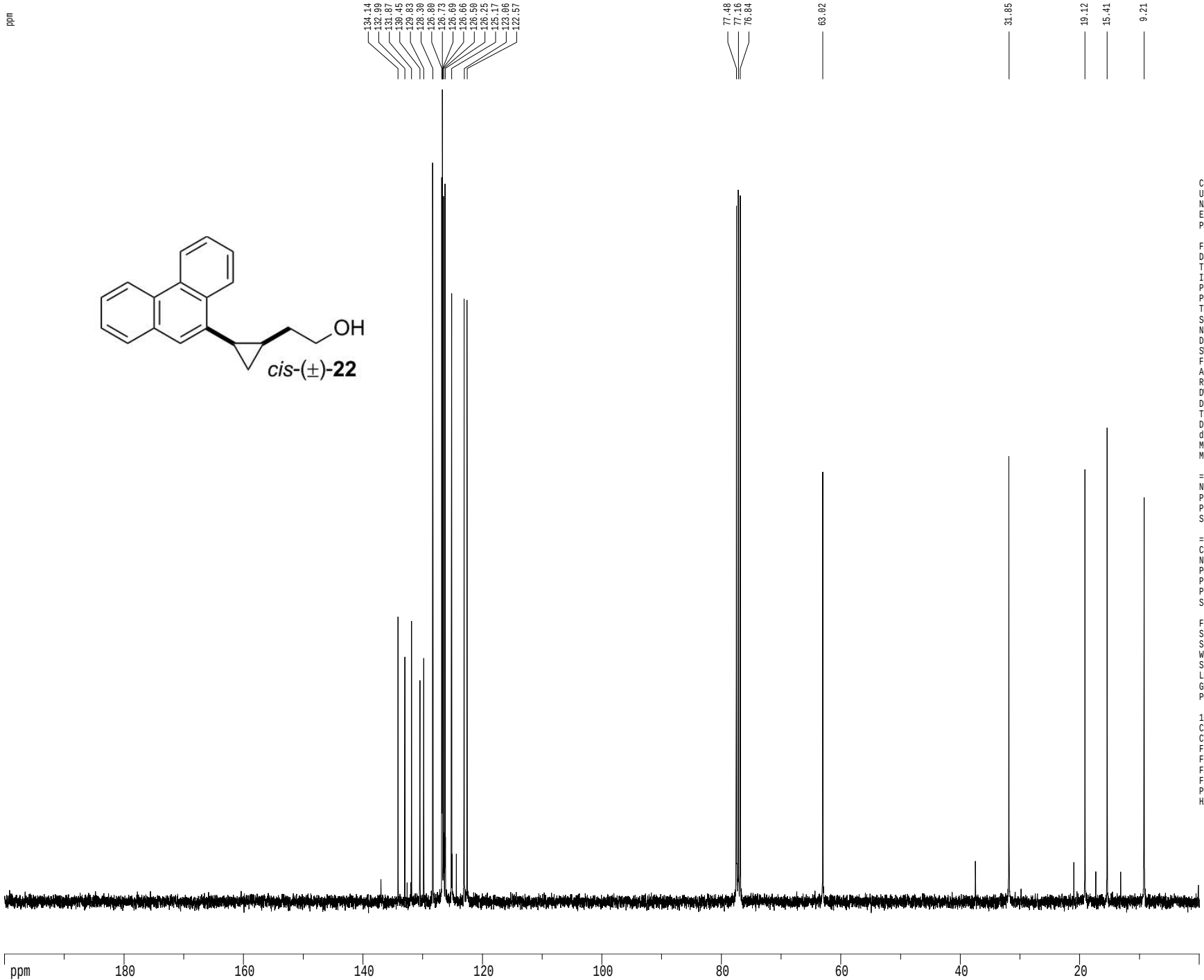
F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

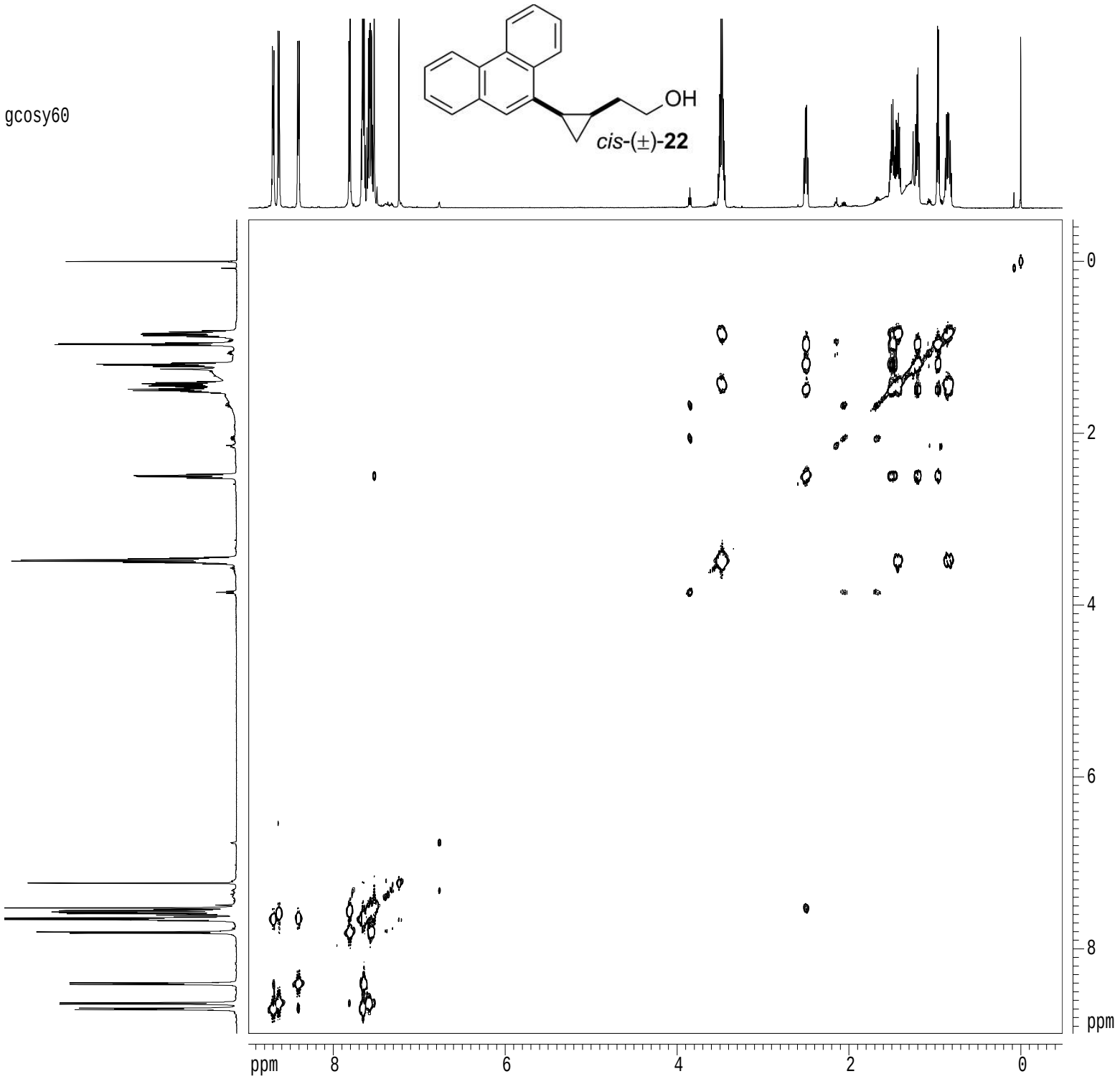
PI Jarvo
h1 CDCl3 v emilyt 103



PI Jarvo
c13 CDCl3 v emilyt 103



gcosy60



Current Data Parameters

USER	emilyt
NAME	EJT-IV-247 noe
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20150206
Time	21.47
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4734.849 Hz
FIDRES	2.311938 Hz
AQ	0.2163188 sec
RG	35.9
DW	105.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00021120 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2221697 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2222 MHz
FIDRES	36.991005 Hz
SW	9.465 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200437 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

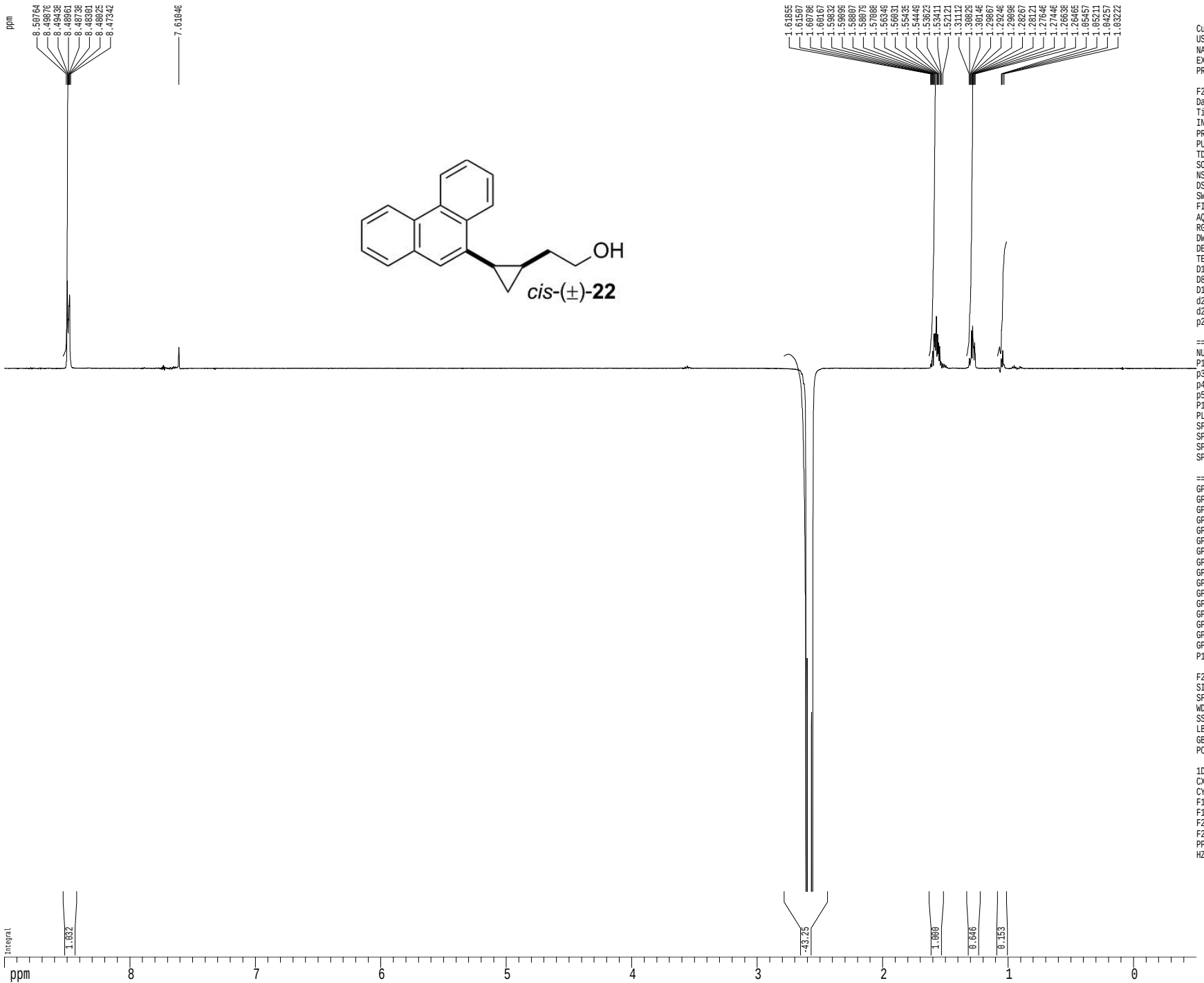
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200437 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.983 ppm
F2LO	4493.36 Hz
F2PHI	-0.483 ppm
F2HI	-241.49 Hz
F1PLO	8.983 ppm
F1LO	4493.36 Hz
F1PHI	-0.483 ppm
F1HI	-241.49 Hz
F2PPMCM	0.63104 ppm/cm
F2HZCM	315.65656 Hz/cm
F1PPMCM	0.63104 ppm/cm
F1HZCM	315.65656 Hz/cm

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-247 noe
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150206
Time 22.06
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 101.6
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

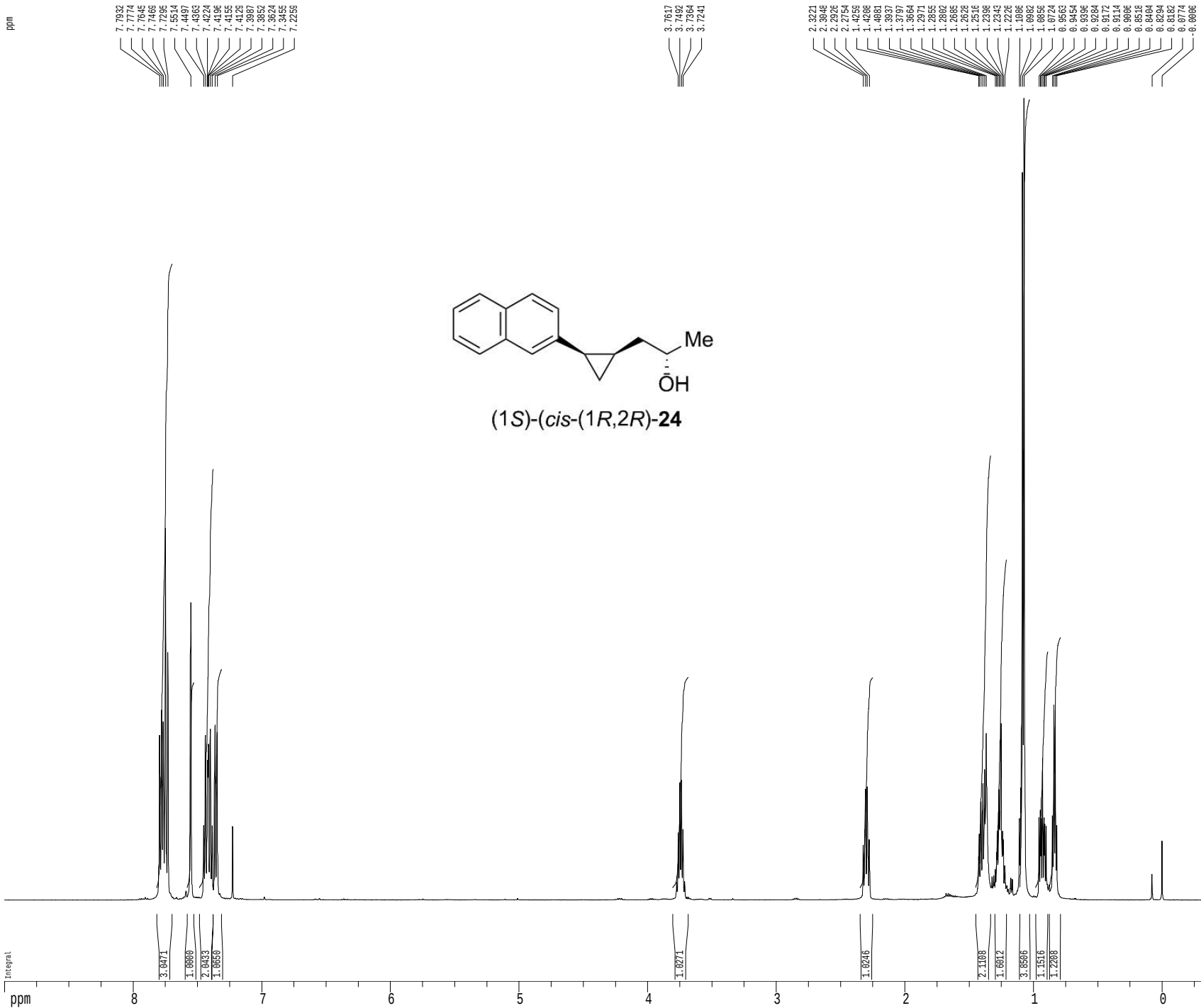
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2212933 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-261-cryo
EXPNO                    5
PROCNO                   1

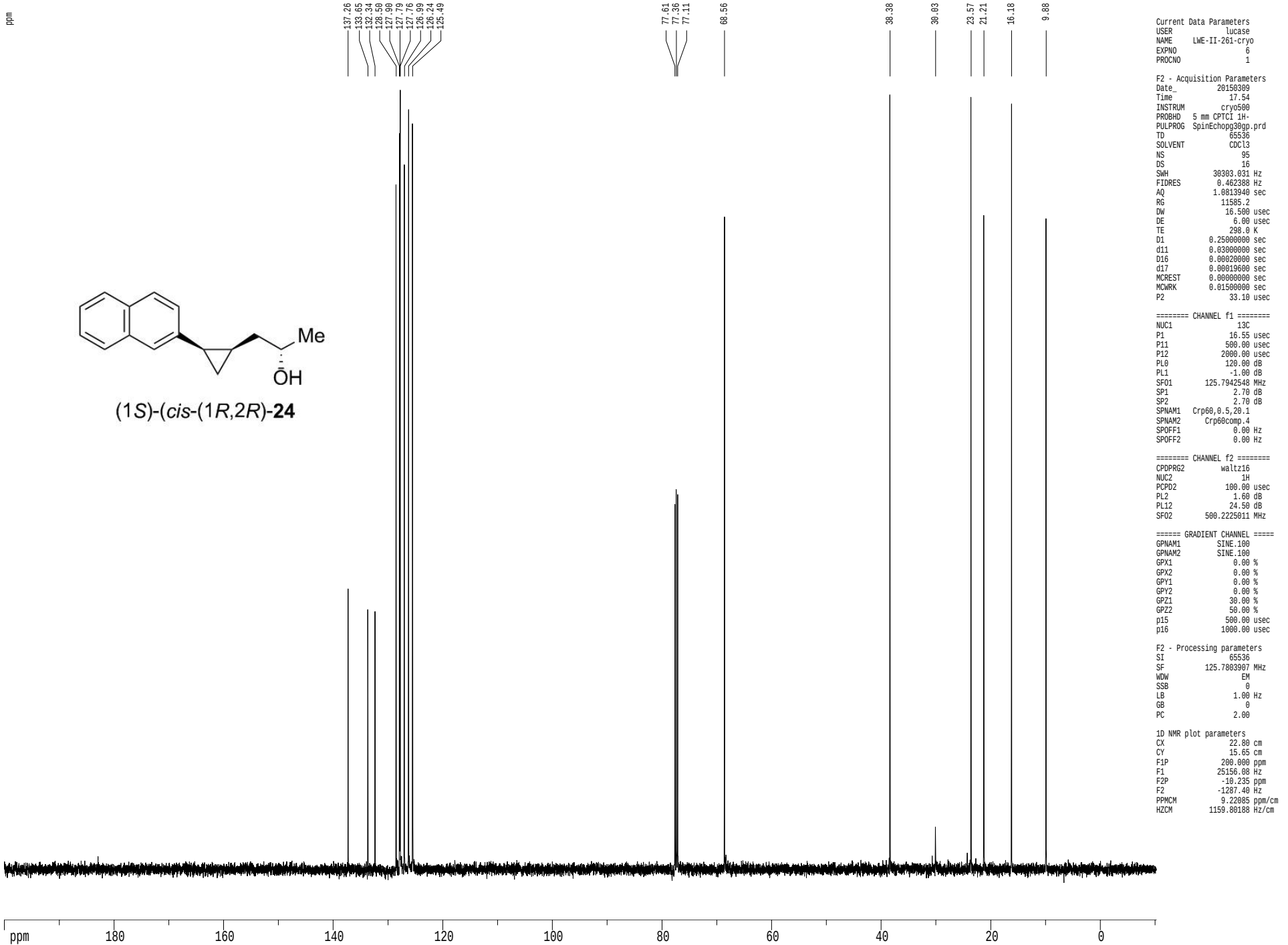
F2 - Acquisition Parameters
Date_             20150309
Time                 17.51
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG                zg30
TD                    48074
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8012.820 Hz
FIDRES                0.166677 Hz
AQ                 2.9998677 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

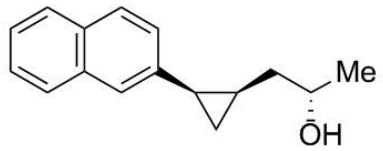
F2 - Processing parameters
SI                    65536
SF                500.2200479 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                    4.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.00 cm
F1P                   9.000 ppm
F1                 4501.98 Hz
F2P                  -0.500 ppm
F2                 -250.11 Hz
PPMCM                0.41667 ppm/cm
HZCM               208.42503 Hz/cm
```

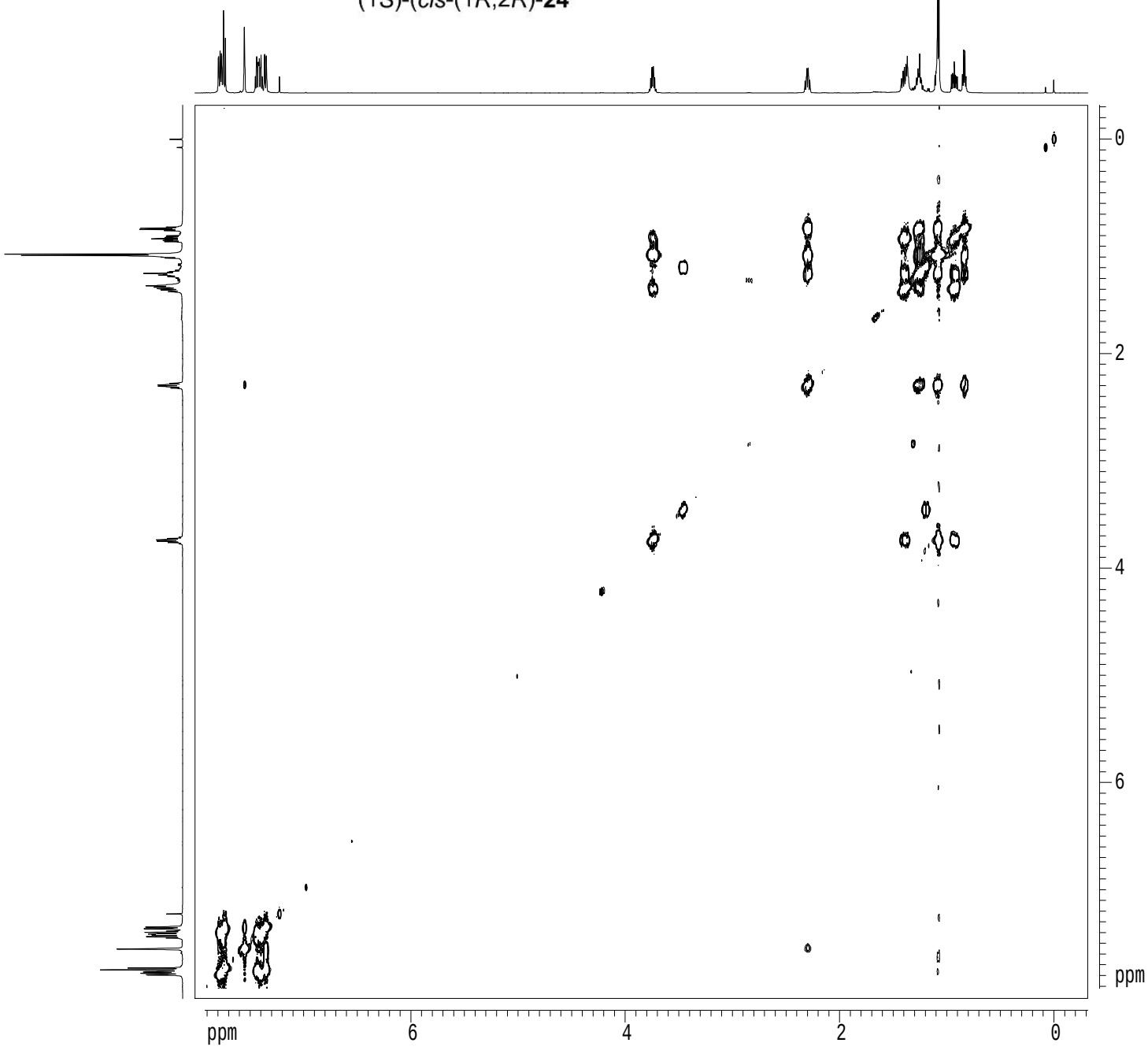
Z-restored spin-echo 13C spectrum with 1H decoupling



gcosy60



(1*S*)-(*cis*-(1*R*,2*R*)-**24**




```
        Current Data Parameters
USER              lucase
NAME      LWE-II-261-cryo
EXPNO                  4
PROCNO                 1

      F2 - Acquisition Parameters
Date_           20150309
Time               11.53
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG     cosygp60.prd
TD                  2048
SOLVENT            CDCl3
NS                     2
DS                    16
SWH             4166.667 Hz
FIDRES             2.034505 Hz
AQ              0.2458100 sec
RG                  35.9
DW               120.000 usec
DE                 6.00 usec
TE                298.0 K
d0             0.00000300 sec
D1             1.00000000 sec
d13            0.00000300 sec
D16            0.00020000 sec
IN0            0.00024000 sec

     ======== CHANNEL f1 ========
NUC1                  1H
P1                 7.50 usec
PL1                1.60 dB
SFO1         500.2219258 MHz

     ====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPX1               0.00 %
GPX2               0.00 %
GPY1               0.00 %
GPY2               0.00 %
GPZ1              17.00 %
GPZ2              17.00 %
P16             1000.00 usec

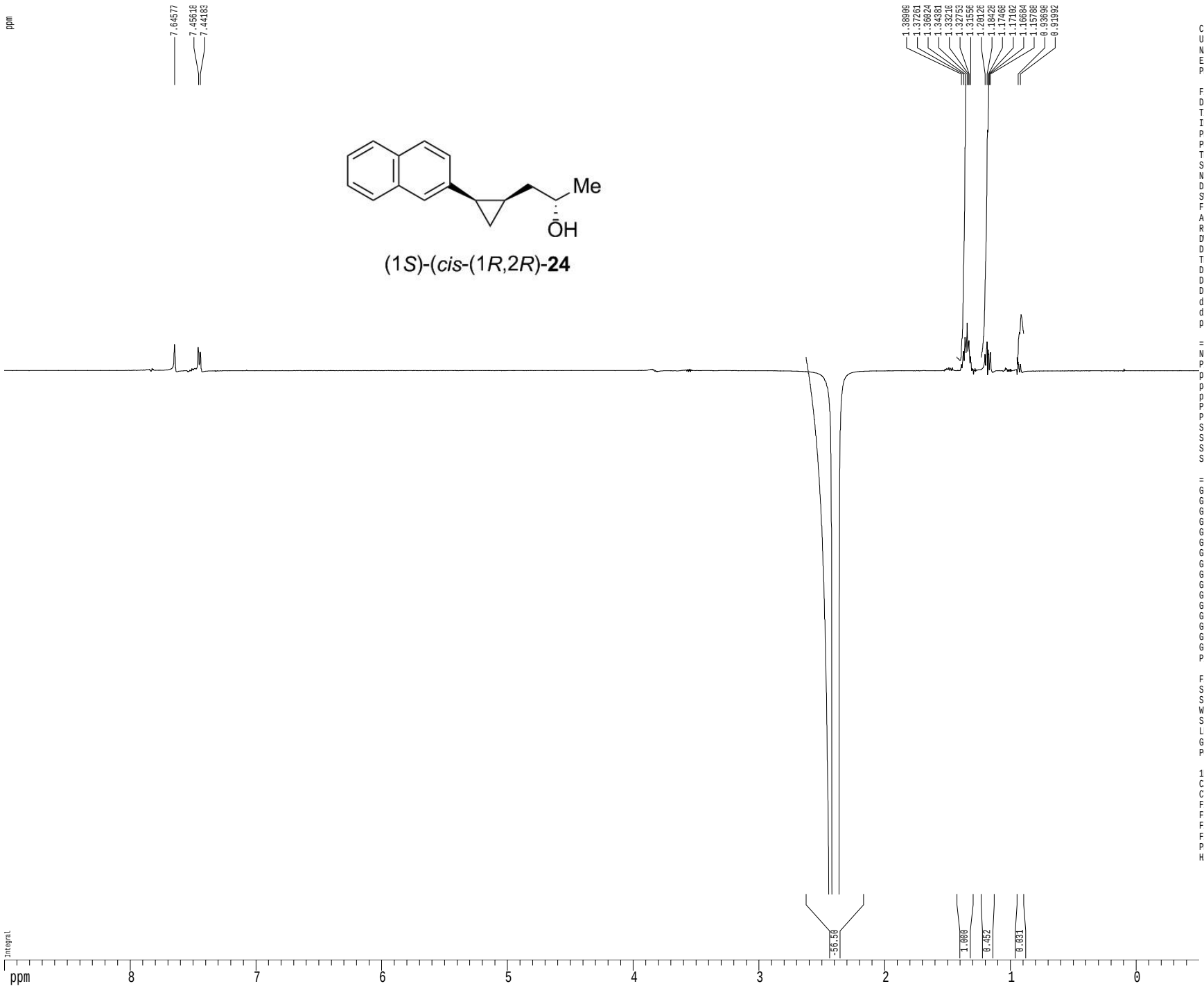
      F1 - Acquisition parameters
ND0                    1
TD                   128
SFO1           500.2219 MHz
FIDRES         32.552082 Hz
SW                 8.330 ppm
FnMODE         undefined

      F2 - Processing parameters
SI                  1024
SF           500.2200479 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00

      F1 - Processing parameters
SI                  1024
MC2                   QF
SF           500.2200479 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0

        2D NMR plot parameters
CX2                15.00 cm
CX1                15.00 cm
F2PLO              8.015 ppm
F2LO             4009.18 Hz
F2PHI             -0.315 ppm
F2HI             -157.49 Hz
F1PLO              8.015 ppm
F1LO             4009.18 Hz
F1PHI             -0.315 ppm
F1HI             -157.49 Hz
F2PPMCM          0.55531 ppm/cm
F2HZCM         277.77780 Hz/cm
F1PPMCM          0.55531 ppm/cm
F1HZCM         277.77780 Hz/cm
```

gnoe




```
Current Data Parameters
USER                lucase
NAME      LWE-II-261-cryo
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150309
Time                 11.52
INSTRUM            cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG         gnoe1cc.wu
TD                    65536
SOLVENT               CDCl3
NS                      128
DS                        8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                     50.8
DW                  62.400 usec
DE                   6.00 usec
TE                  298.0 K
D1               1.00000000 sec
D8               0.50000000 sec
D16              0.00020000 sec
d21              0.33376500 sec
d22              0.16399699 sec
p2                  15.00 usec

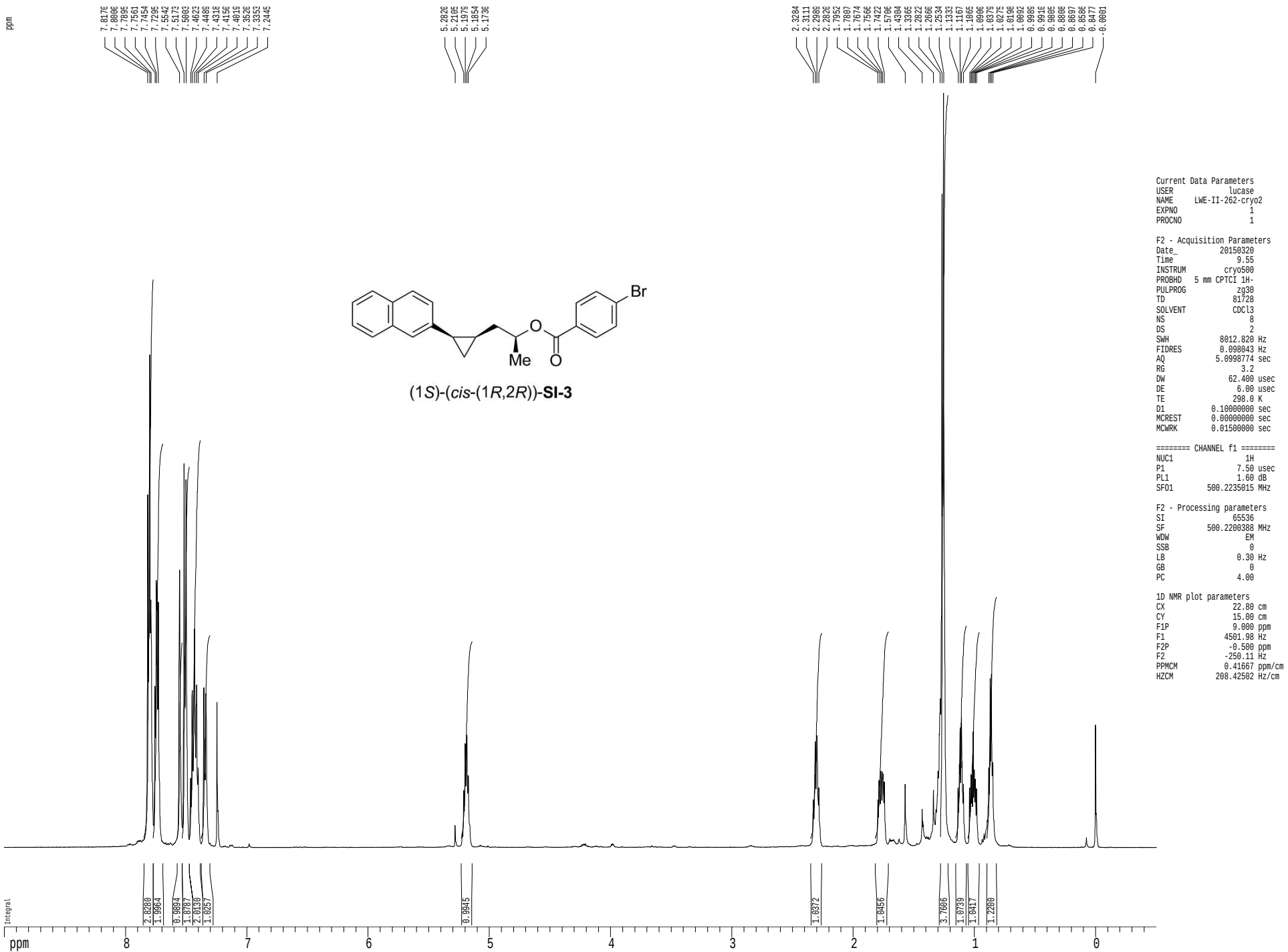
======== CHANNEL f1 ========
NUC1                    1H
P1                   7.50 usec
p3                  22.50 usec
p4                  30.00 usec
p5                  20.00 usec
P12                40000.00 usec
PL1                    1.60 dB
SFO1           500.2211982 MHz
SP1                   61.60 dB
SPNAM1          gauss1.512
SPOFF1                 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1            sine.100
GPNAM2            sine.100
GPNAM3            sine.100
GPNAM4            sine.100
GPX1                  0.00 %
GPX2                  0.00 %
GPX3                  0.00 %
GPX4                  0.00 %
GPY1                  0.00 %
GPY2                  0.00 %
GPY3                  0.00 %
GPY4                  0.00 %
GPZ1                  7.00 %
GPZ2                  3.00 %
GPZ3                  2.30 %
GPZ4                 -2.30 %
P16                1000.00 usec

F2 - Processing parameters
SI                    65536
SF             500.2200000 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                    1.00

1D NMR plot parameters
CX                   22.80 cm
CY                   50.00 cm
F1P                   9.000 ppm
F1                 4501.98 Hz
F2P                  -0.500 ppm
F2                 -250.11 Hz
PPMCM             0.41667 ppm/cm
HZCM            208.42500 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-262-cryo2
EXPNO                    1
PROCNO                   1

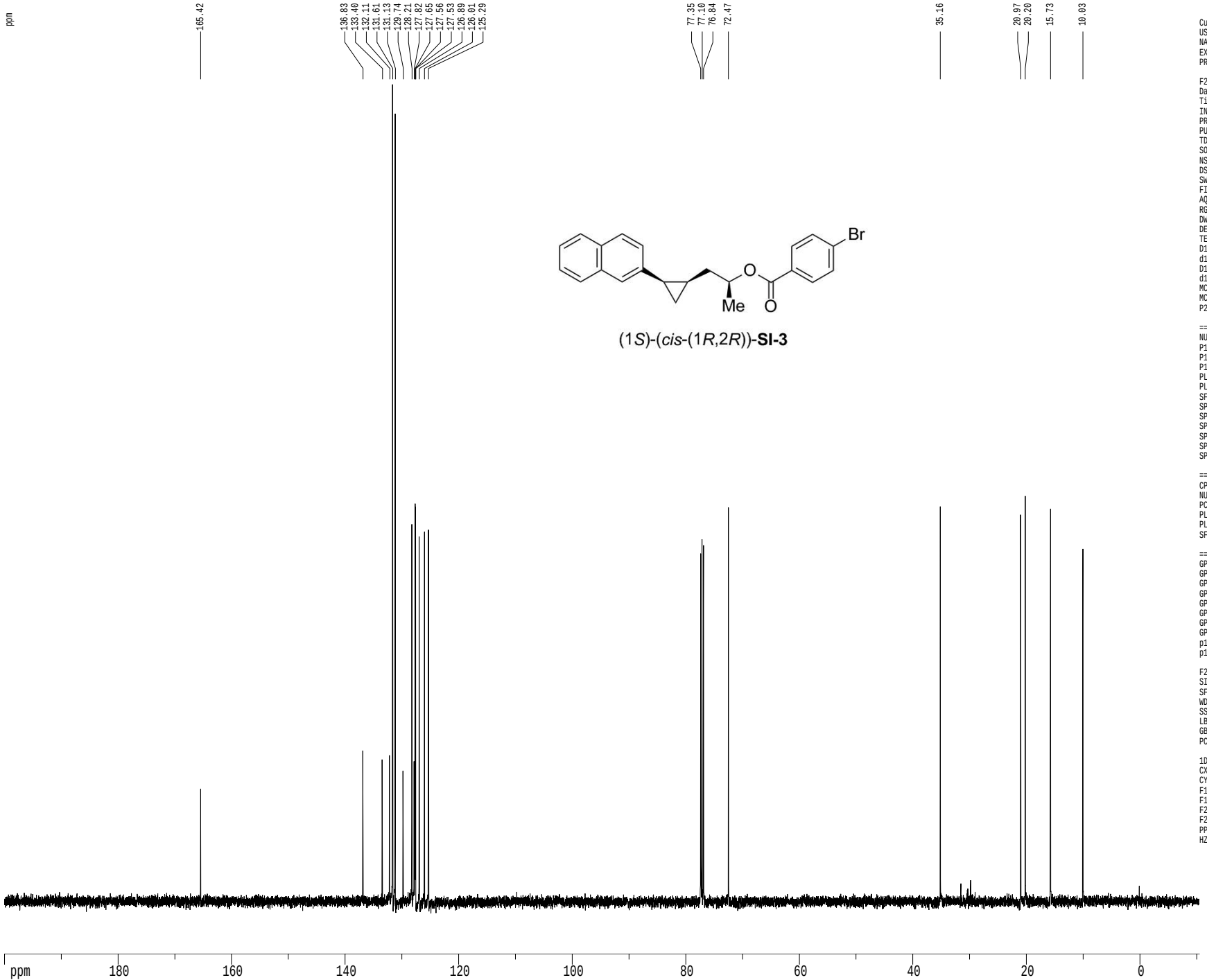
F2 - Acquisition Parameters
Date_            20150320
Time                 9.55
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  81728
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                    3.2
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            500.2200388 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                    4.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.00 cm
F1P                   9.000 ppm
F1                 4501.98 Hz
F2P                  -0.500 ppm
F2                 -250.11 Hz
PPMCM             0.41667 ppm/cm
HZCM            208.42502 Hz/cm
```

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



(1*S*)-(*cis*-(1*R*,2*R*))-**SI-3**

```
Current Data Parameters
USER                lucase
NAME      LWE-II-262-cryo2
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150320
Time                  9.58
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     186
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                  2.70 dB
SP2                  2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

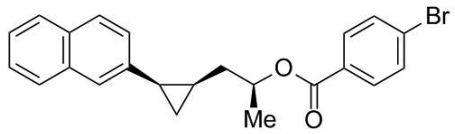
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7804190 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1               25156.09 Hz
F2P                -10.460 ppm
F2               -1315.66 Hz
PPMCM             9.23070 ppm/cm
HZCM           1161.04138 Hz/cm
```

gcosy60



(1*S*)-(*cis*-(1*R*,2*R*))-**SI-3**

Current Data Parameters

USER	lucase
NAME	LWE-II-262-cryo
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20150314
Time	15.53
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	5208.333 Hz
FIDRES	2.543132 Hz
AQ	0.1966580 sec
RG	32
DW	96.000 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00019200 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2226476 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2226 MHz
FIDRES	40.690105 Hz
SW	10.412 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200464 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

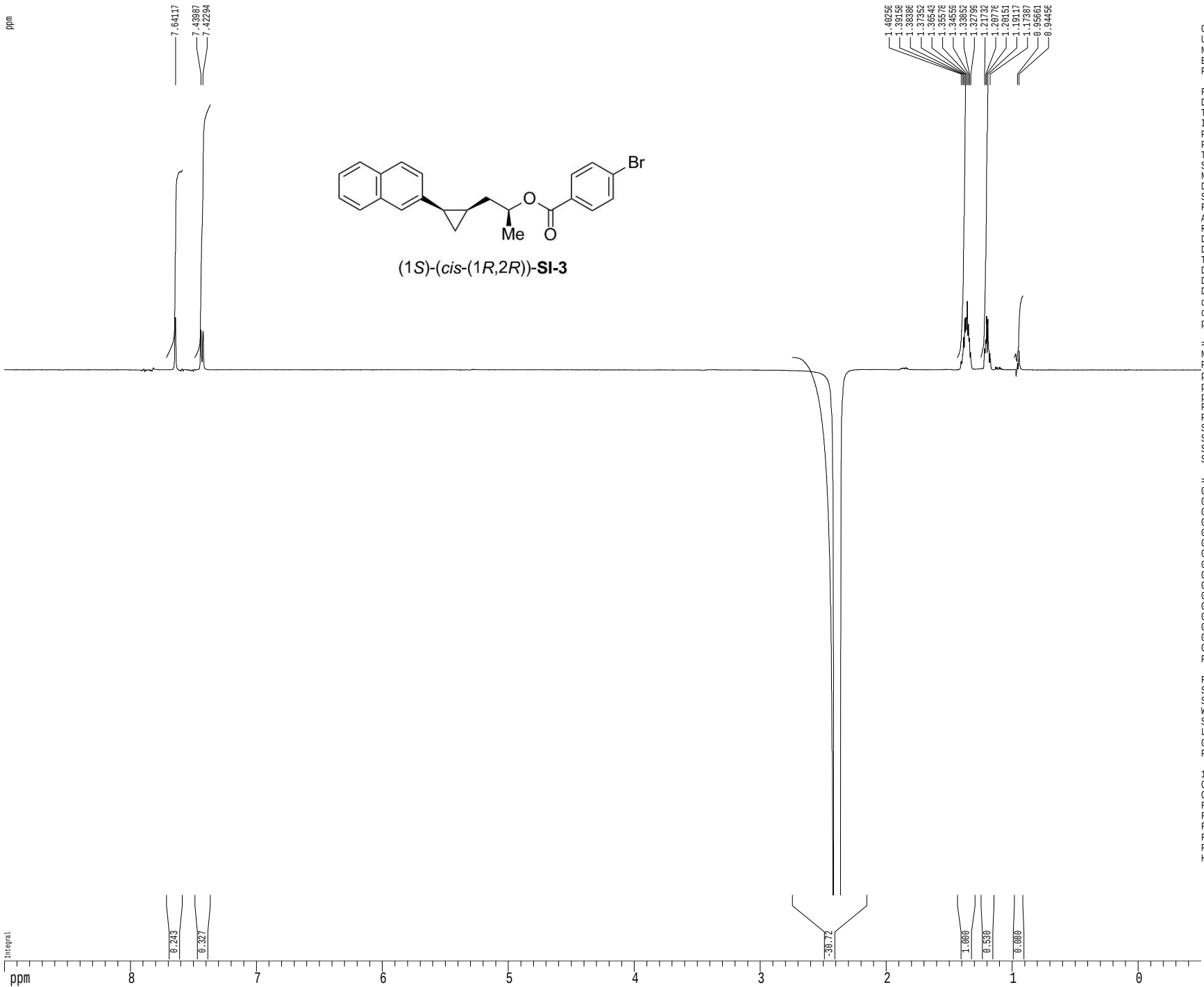
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200464 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	9.000 ppm
F2LO	4501.98 Hz
F2PHI	0.087 ppm
F2HI	43.41 Hz
F1PLO	9.000 ppm
F1LO	4501.98 Hz
F1PHI	0.087 ppm
F1HI	43.41 Hz
F2PPMCM	0.59422 ppm/cm
F2HZCM	297.23825 Hz/cm
F1PPMCM	0.59422 ppm/cm
F1HZCM	297.23825 Hz/cm

gnoe



Current Data Parameters
USER lucase
NAME LWE-II-262-cryo
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150314
Time 15.49
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

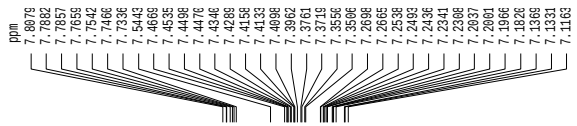
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2211963 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

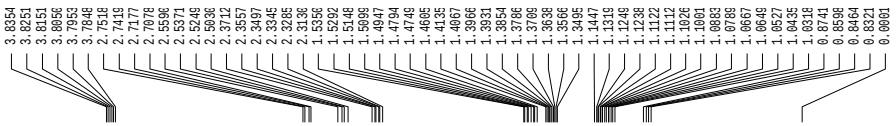
====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

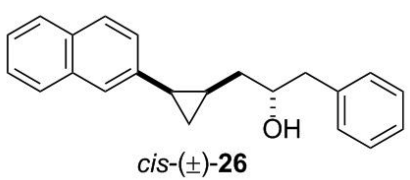
F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

PI Jarvo
h1 CDCl3 v emilyt 101







cis-(±)-**26**

Minor

Minor

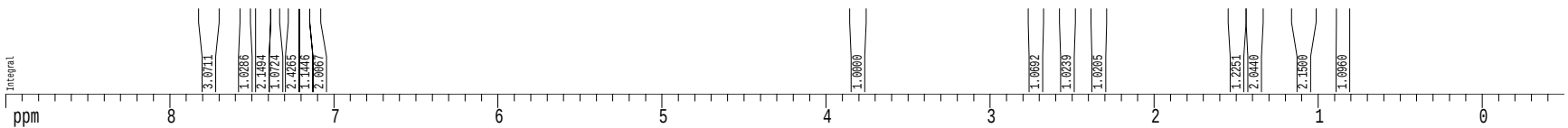
Current Data Parameters
USER emilyt
NAME EJT-V-023-A
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150408
Time 0.26
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zg30
TD 73274
SOLVENT CDCl3
NS 8
DS 2
SWH 7183.908 Hz
FIDRES 0.098042 Hz
AQ 5.0999203 sec
RG 228.1
DW 69.600 usec
DE 4.50 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

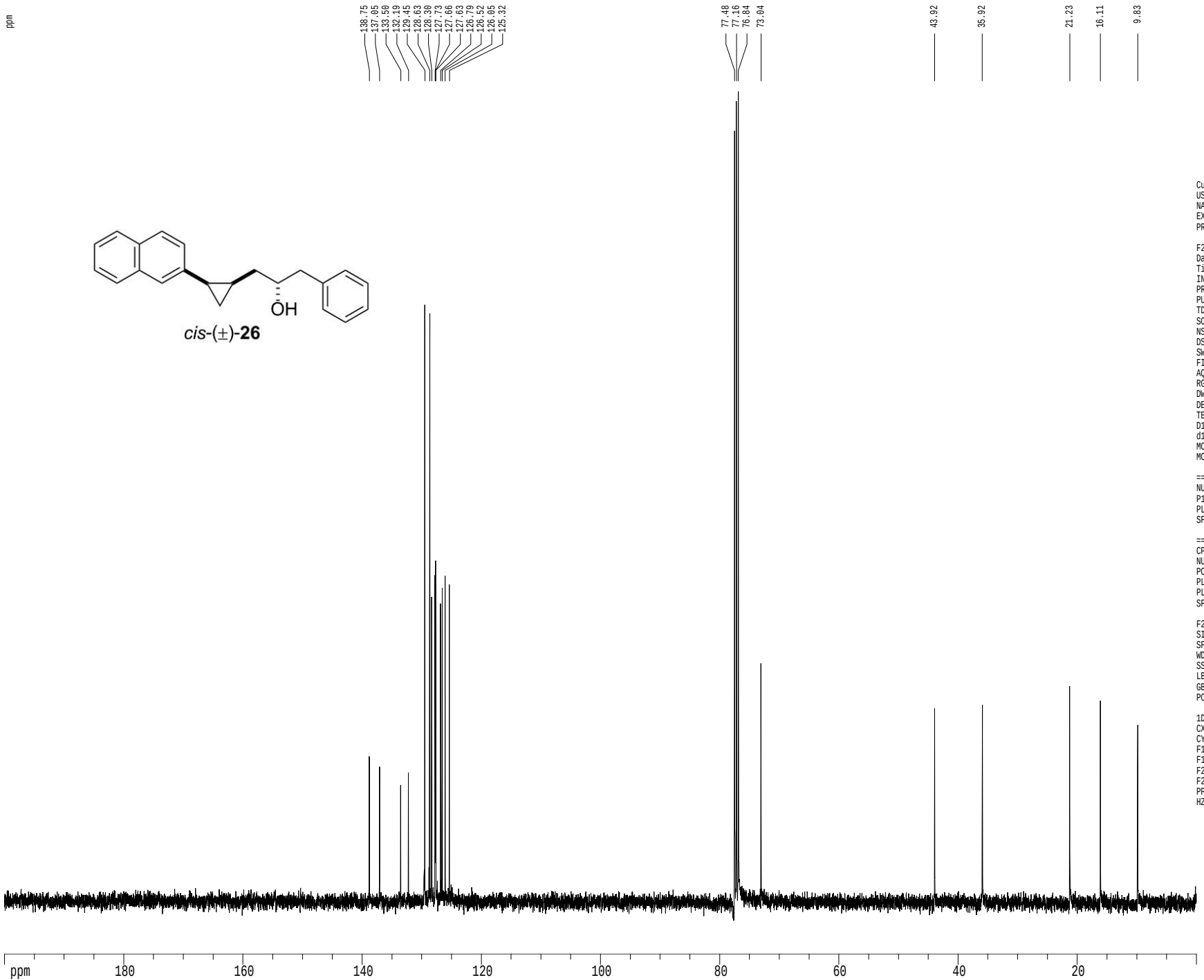
======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 400.1300274 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

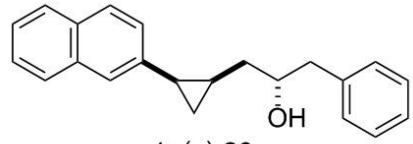
1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.41667 ppm/cm
HZCM 166.72086 Hz/cm



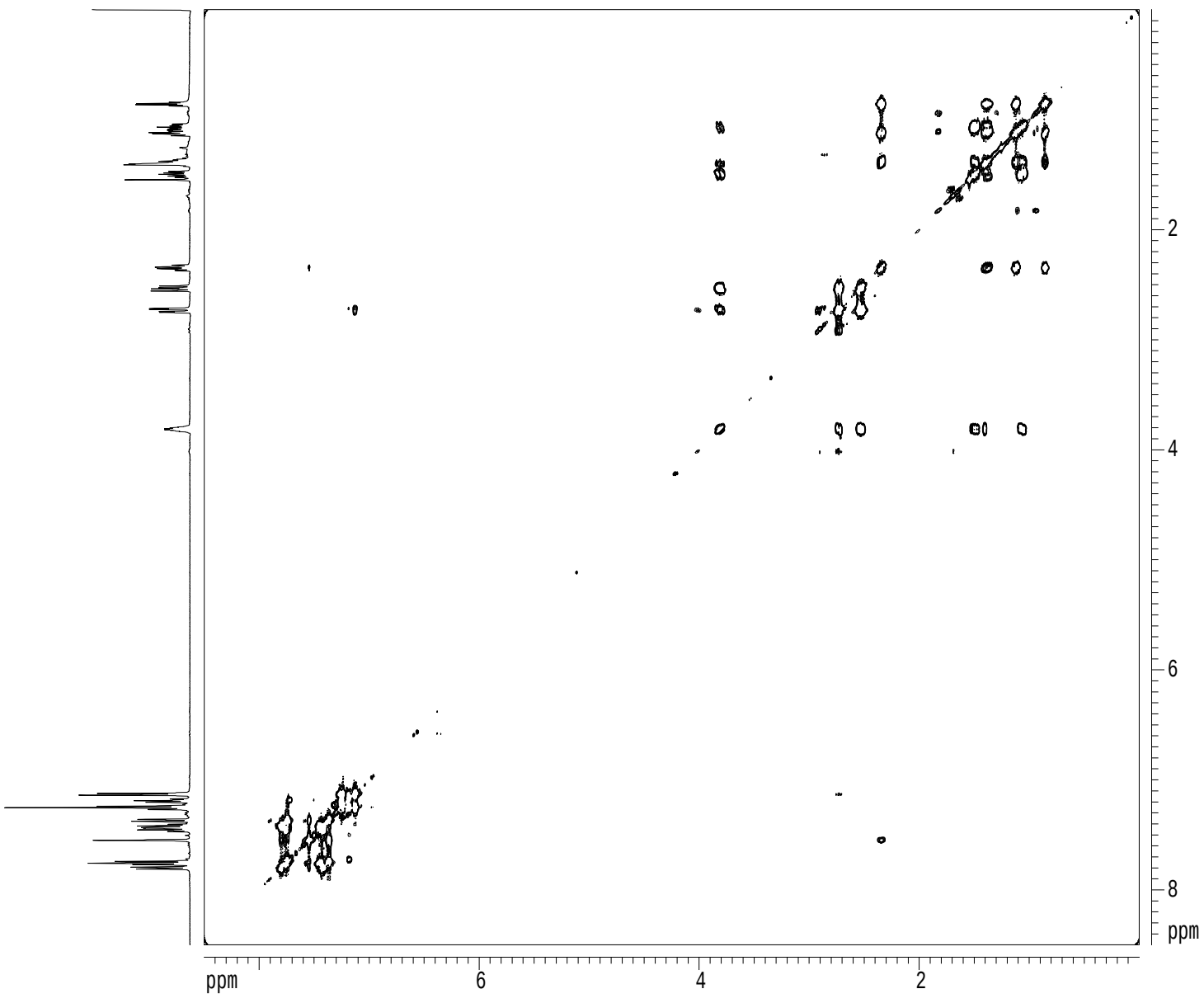
PI Jarvo
c13 CDCl3 v emilyt 101



gcosy60



cis-(±)-**26**



Current Data Parameters

USER	emilyt
NAME	EJT-V-023
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20150130
Time	21.09
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4251.701 Hz
FIDRES	2.076026 Hz
AQ	0.2408948 sec
RG	203.2
DW	117.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00023520 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2221616 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	256
SFO1	500.2222 MHz
FIDRES	16.608206 Hz
SW	8.500 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200357 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

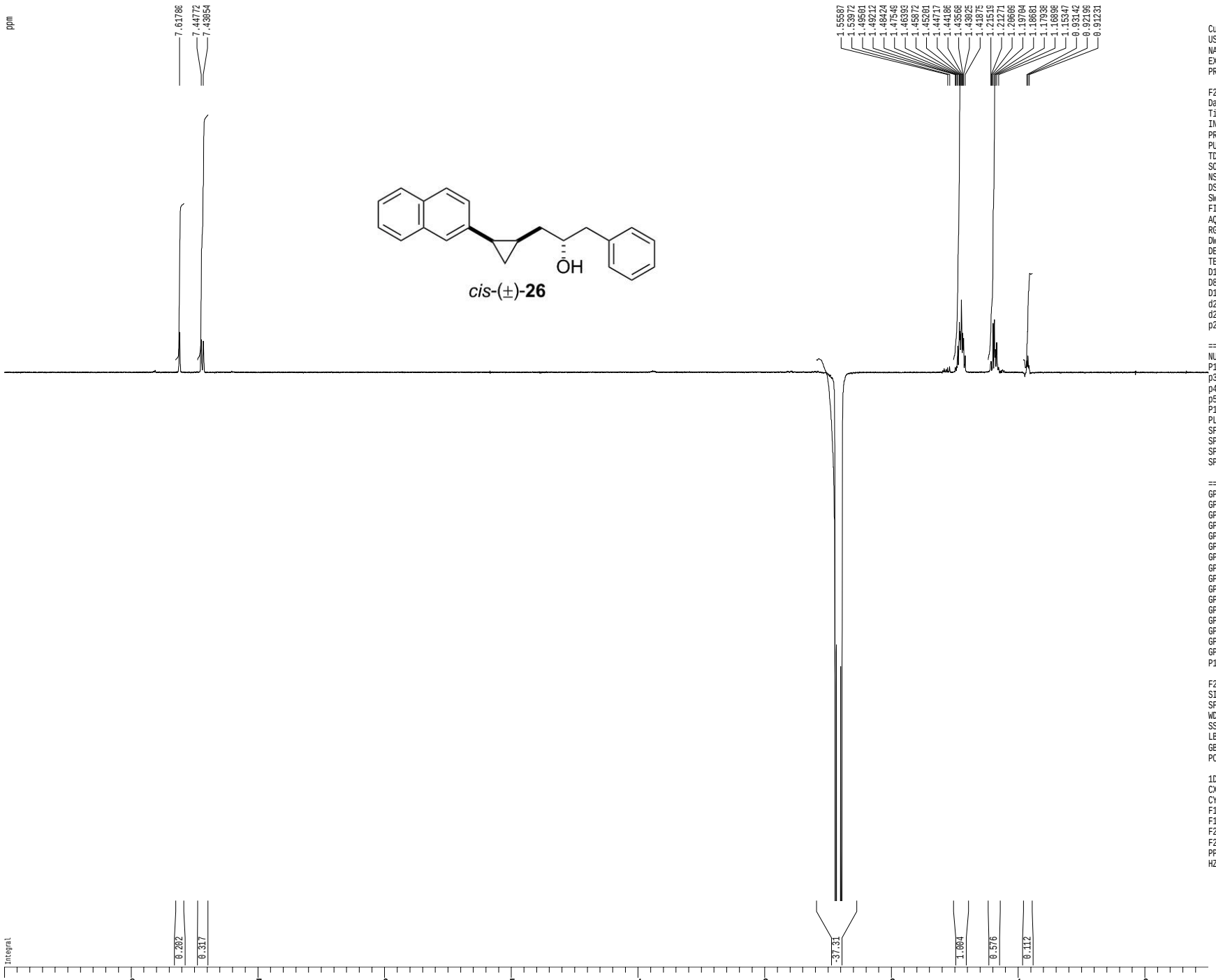
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200357 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.500 ppm
F2LO	4251.78 Hz
F2PHI	0.000 ppm
F2HI	0.08 Hz
F1PLO	8.500 ppm
F1LO	4251.78 Hz
F1PHI	0.000 ppm
F1HI	0.08 Hz
F2PPMCM	0.56664 ppm/cm
F2HZCM	283.44672 Hz/cm
F1PPMCM	0.56664 ppm/cm
F1HZCM	283.44672 Hz/cm

gnoe



Current Data Parameters
USER emilyt
NAME EJT-V-023
EXPNO 13
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150130
Time 21.46
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 101.6
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

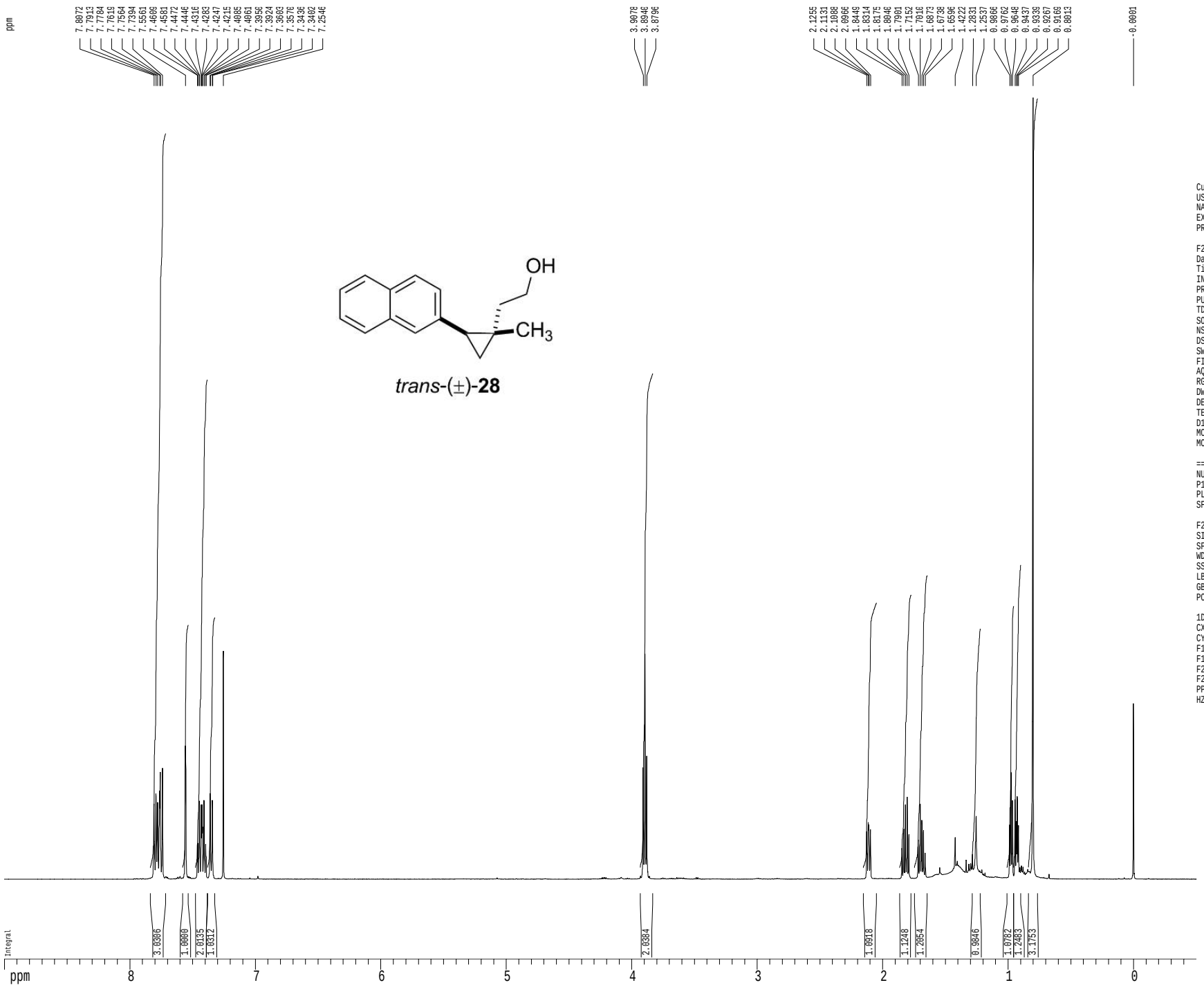
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2212100 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-251-cryo7
EXPNO                   1
PROCNO                  1

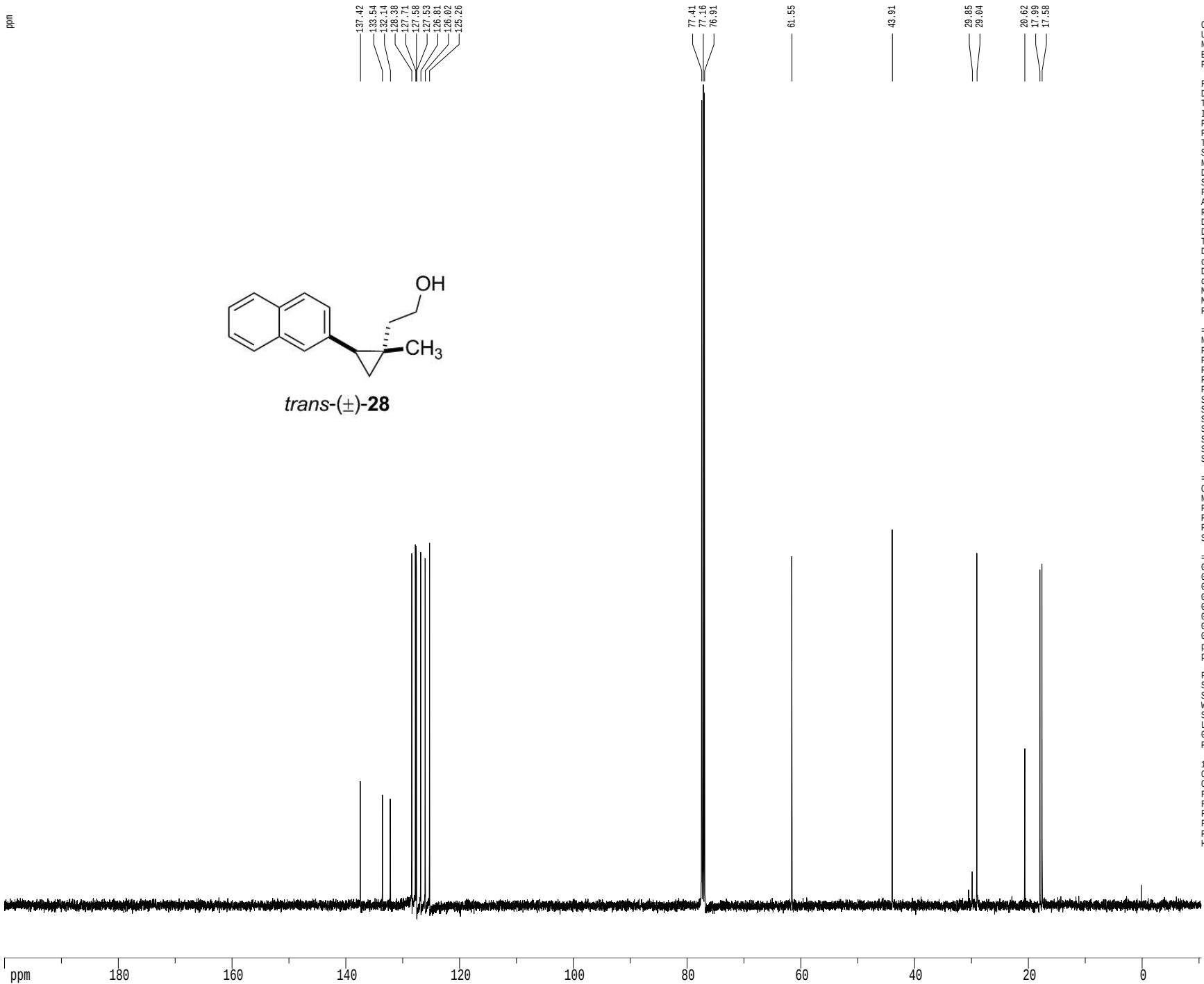
F2 - Acquisition Parameters
Date_            20150403
Time                17.48
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG             zg30
TD                 48074
SOLVENT            CDCl3
NS                     8
DS                     2
SWH              8012.820 Hz
FIDRES           0.166677 Hz
AQ               2.9998677 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            500.2200336 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  4.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P                9.000 ppm
F1               4501.98 Hz
F2P               -0.500 ppm
F2               -250.11 Hz
PPMCM           0.41667 ppm/cm
HZCM          208.42502 Hz/cm
```

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



trans-(±)-**28**

```
Current Data Parameters
USER                lucase
NAME      LWE-II-251-cryo7
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150403
Time                 17.55
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     458
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                    3251
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1          125.7942548 MHz
SP1                   2.70 dB
SP2                   2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

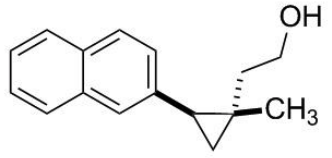
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2              100.00 usec
PL2                   1.60 dB
PL12                 24.50 dB
SFO2          500.2225011 MHz

====== 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

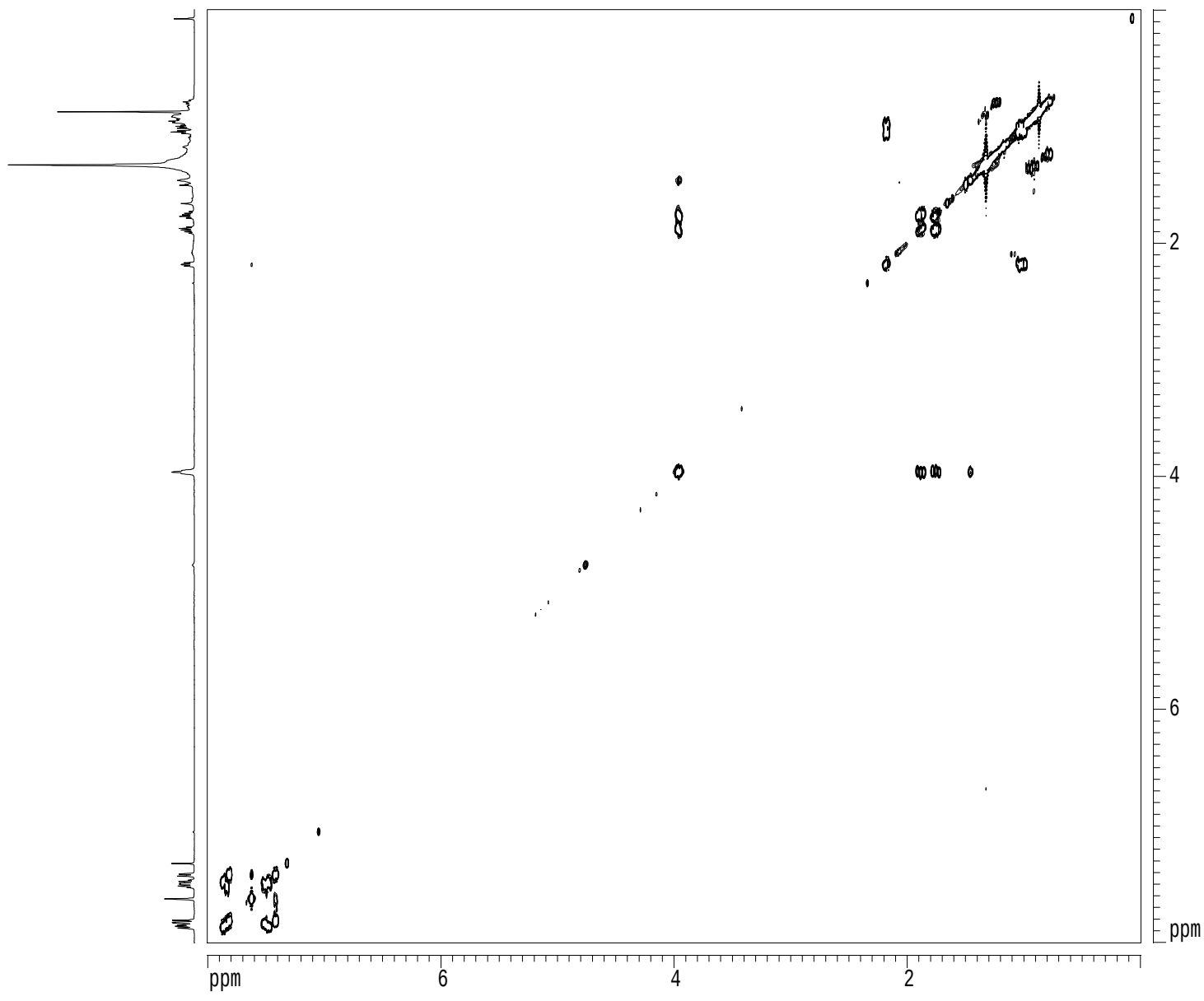
F2 - Processing parameters
SI                   65536
SF            125.7804085 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1               25156.08 Hz
F2P                -10.376 ppm
F2               -1305.15 Hz
PPMCM             9.22704 ppm/cm
HZCM           1160.58032 Hz/cm
```

gcosy60



trans-(±)-**28**




```
        Current Data Parameters
USER              lucase
NAME      LWE-II-251-cryo
EXPNO                  2
PROCNO                 1

      F2 - Acquisition Parameters
Date_           20150323
Time              17.28
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG    cosygp60.prd
TD                2048
SOLVENT           CDCl3
NS                   2
DS                  16
SWH            4006.410 Hz
FIDRES         1.956255 Hz
AQ             0.2556404 sec
RG                35.9
DW              124.800 usec
DE                6.00 usec
TE               298.0 K
d0            0.00000300 sec
D1            1.00000000 sec
d13           0.00000300 sec
D16           0.00020000 sec
IN0           0.00024960 sec

     ======== CHANNEL f1 ========
NUC1                  1H
P1                 7.50 usec
PL1                1.60 dB
SFO1         500.2220009 MHz

    ====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               17.00 %
GPZ2               17.00 %
P16              1000.00 usec

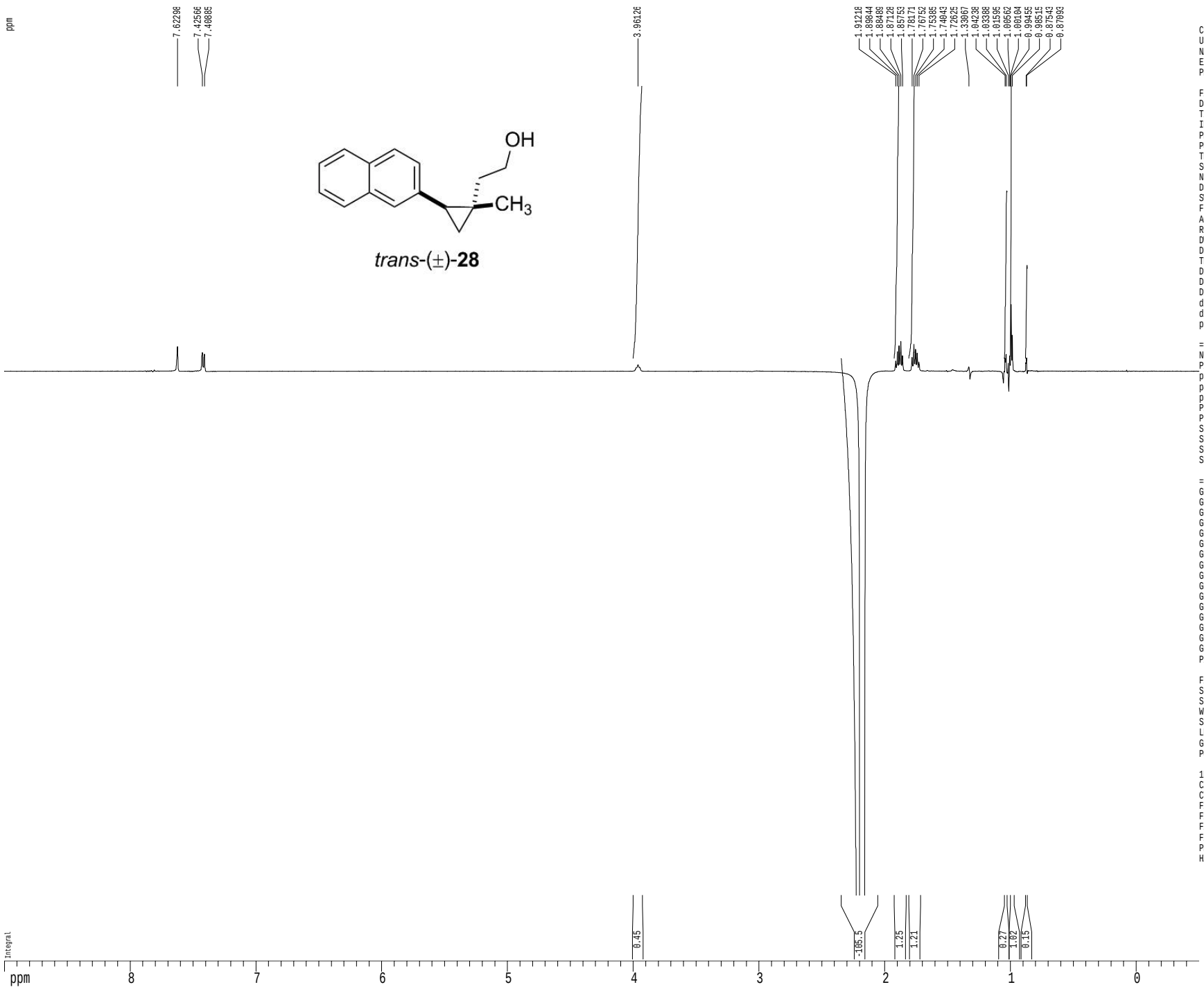
      F1 - Acquisition parameters
ND0                    1
TD                   128
SFO1           500.222 MHz
FIDRES        31.300079 Hz
SW                 8.009 ppm
FnMODE         undefined

      F2 - Processing parameters
SI                  1024
SF           500.2200000 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  4.00

      F1 - Processing parameters
SI                  1024
MC2                   QF
SF           500.2200000 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0

       2D NMR plot parameters
CX2                15.00 cm
CX1                15.00 cm
F2PLO              8.005 ppm
F2LO             4004.08 Hz
F2PHI             -0.005 ppm
F2HI               -2.33 Hz
F1PLO              8.005 ppm
F1LO             4004.08 Hz
F1PHI             -0.005 ppm
F1HI               -2.33 Hz
F2PPMCM          0.53395 ppm/cm
F2HZCM         267.09402 Hz/cm
F1PPMCM          0.53395 ppm/cm
F1HZCM         267.09402 Hz/cm
```

gnoe



Current Data Parameters
USER lucase
NAME LWE-II-251-cryo
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150323
Time 17.48
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 101.6
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

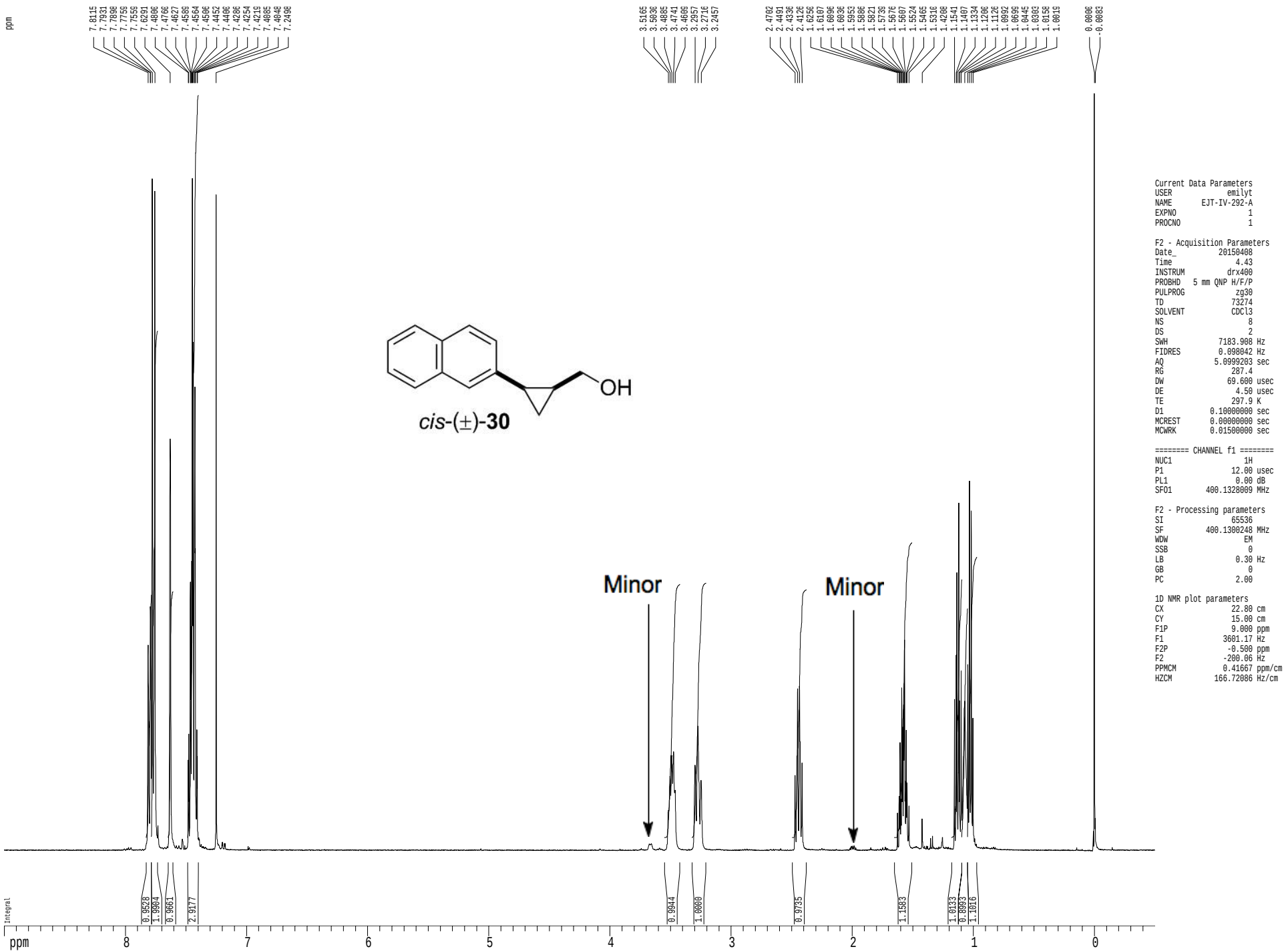
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2210909 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

PI Jarvo
h1 CDCl3 v emilyt 104



Current Data Parameters
USER emilyt
NAME EJT-IV-292-A
EXPNO 1
PROCNO 1

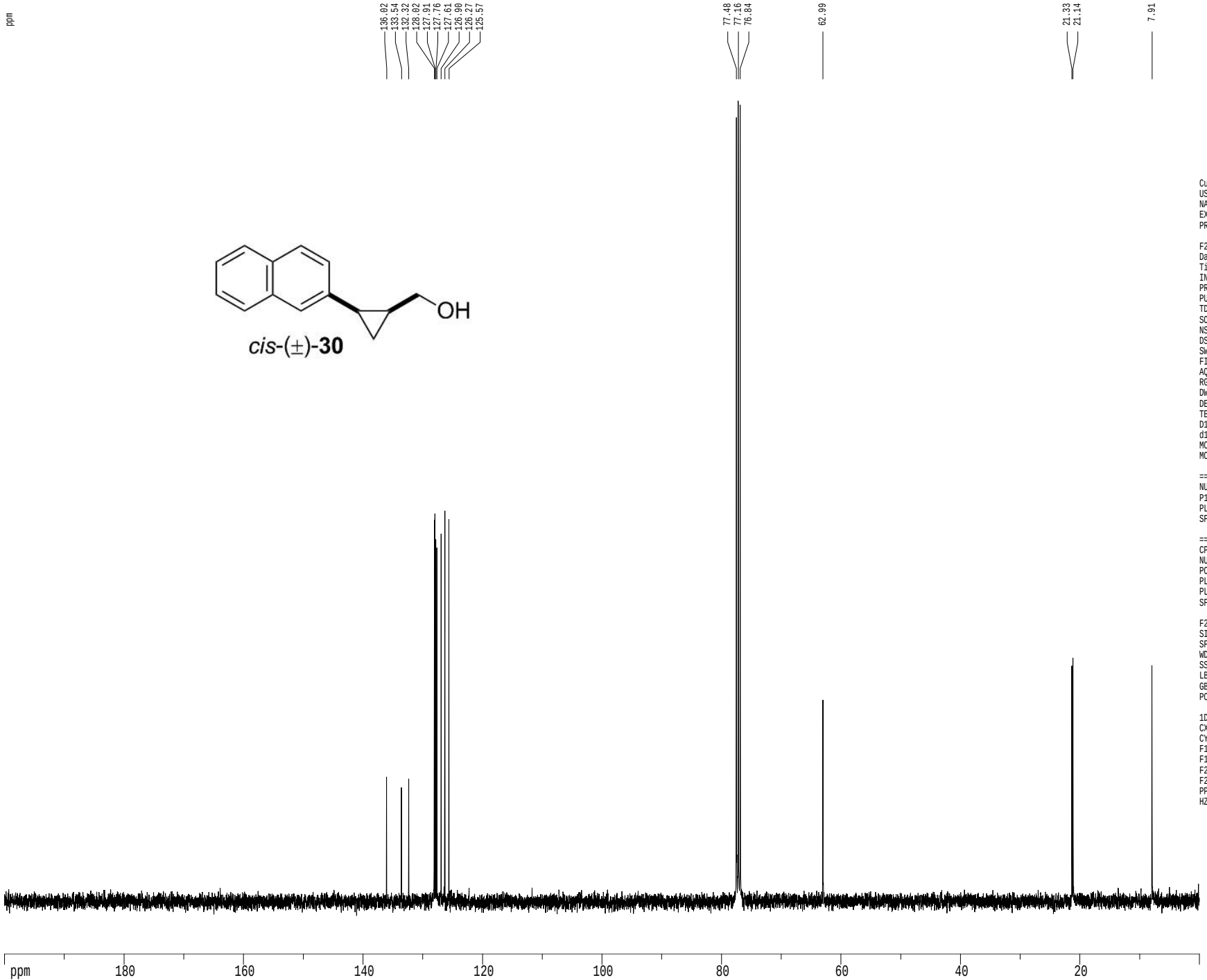
F2 - Acquisition Parameters
Date_ 20150408
Time 4.43
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zg30
TD 73274
SOLVENT CDCl3
NS 8
DS 2
SWH 7183.908 Hz
FIDRES 0.098042 Hz
AQ 5.0999203 sec
RG 287.4
DW 69.600 usec
DE 4.50 usec
TE 297.9 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1328009 MHz

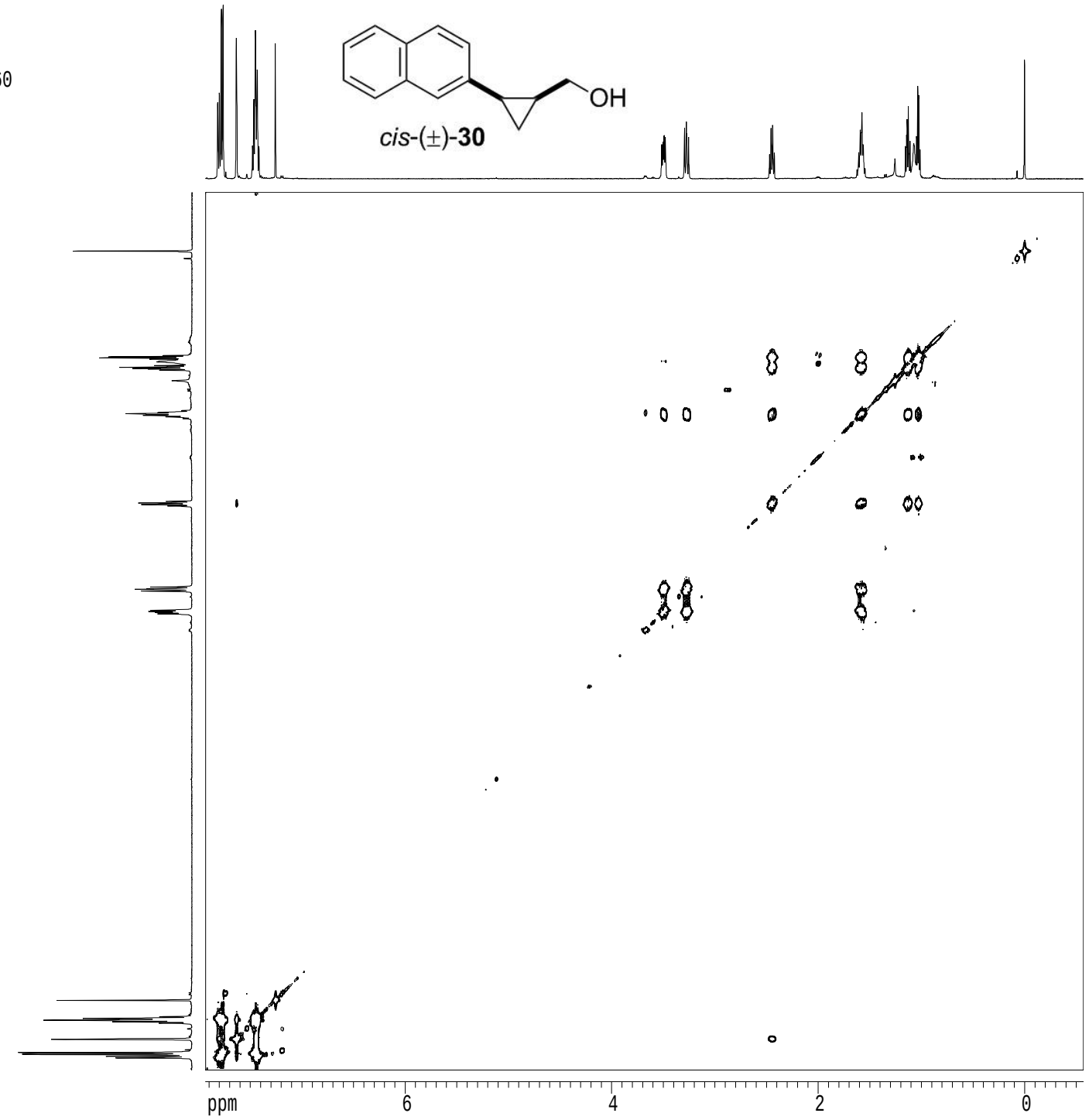
F2 - Processing parameters
SI 65536
SF 400.1300248 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.41667 ppm/cm
HZCM 166.72086 Hz/cm

PI Jarvo
c13 CDCl3 v emilyt 104



gcosy60



Current Data Parameters

USER	emilyt
NAME	EJT-IV-294-A
EXPNO	11
PROCNO	1

F2 - Acquisition Parameters

Date_	20150130
Time	20.17
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4251.701 Hz
FIDRES	2.076026 Hz
AQ	0.2408948 sec
RG	287.4
DW	117.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00023520 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2218758 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	256
SFO1	500.2219 MHz
FIDRES	16.608206 Hz
SW	8.500 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200338 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

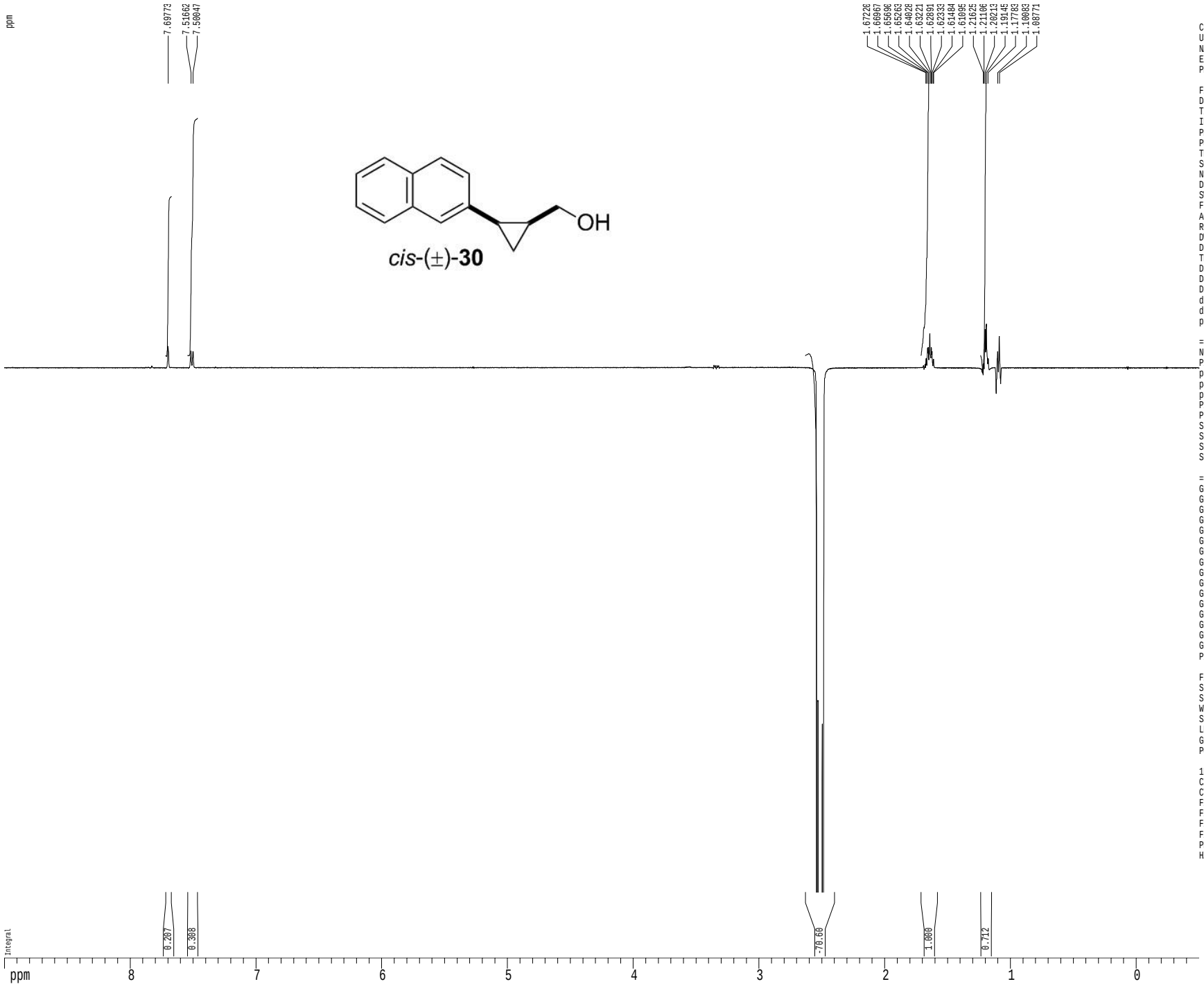
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200338 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	7.932 ppm
F2LO	3967.83 Hz
F2PHI	-0.567 ppm
F2HI	-283.87 Hz
F1PLO	7.932 ppm
F1LO	3967.83 Hz
F1PHI	-0.567 ppm
F1HI	-283.87 Hz
F2PPMCM	0.56664 ppm/cm
F2HZCM	283.44672 Hz/cm
F1PPMCM	0.56664 ppm/cm
F1HZCM	283.44672 Hz/cm

gnoe




```
Current Data Parameters
USER              emilyt
NAME        EJT-IV-294-A
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20150130
Time              21.02
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG       gnoe1cc.wu
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    8
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894966 sec
RG                  114
DW               62.400 usec
DE                6.00 usec
TE                298.0 K
D1           1.00000000 sec
D8           0.50000000 sec
D16          0.00020000 sec
d21          0.33376500 sec
d22          0.16399699 sec
p2               15.00 usec

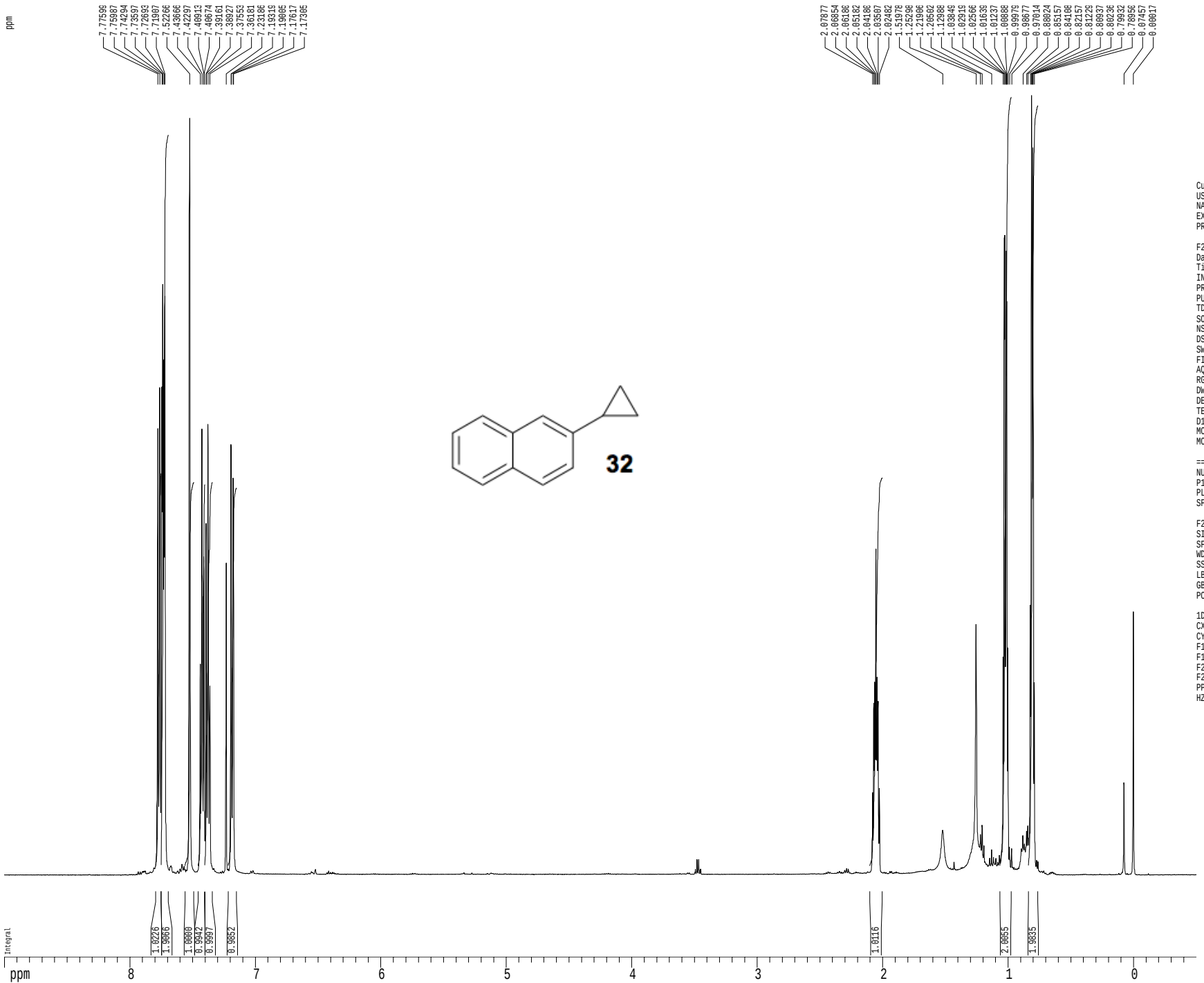
======== CHANNEL f1 ========
NUC1                 1H
P1                 7.50 usec
p3                22.50 usec
p4                30.00 usec
p5                20.00 usec
P12            40000.00 usec
PL1                1.60 dB
SFO1         500.2212578 MHz
SP1                61.60 dB
SPNAM1        gauss1.512
SPOFF1             0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPNAM3          sine.100
GPNAM4          sine.100
GPX1               0.00 %
GPX2               0.00 %
GPX3               0.00 %
GPX4               0.00 %
GPY1               0.00 %
GPY2               0.00 %
GPY3               0.00 %
GPY4               0.00 %
GPZ1               7.00 %
GPZ2               3.00 %
GPZ3               2.30 %
GPZ4              -2.30 %
P16             1000.00 usec

F2 - Processing parameters
SI                65536
SF           500.2200000 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.80 cm
CY                50.00 cm
F1P                9.000 ppm
F1              4501.98 Hz
F2P               -0.500 ppm
F2              -250.11 Hz
PPMCM           0.41667 ppm/cm
HZCM          208.42500 Hz/cm
```

1H spectrum



Current Data Parameters
USER lucase
NAME LWE-II-112-final
EXPNO 1
PROCNO 1

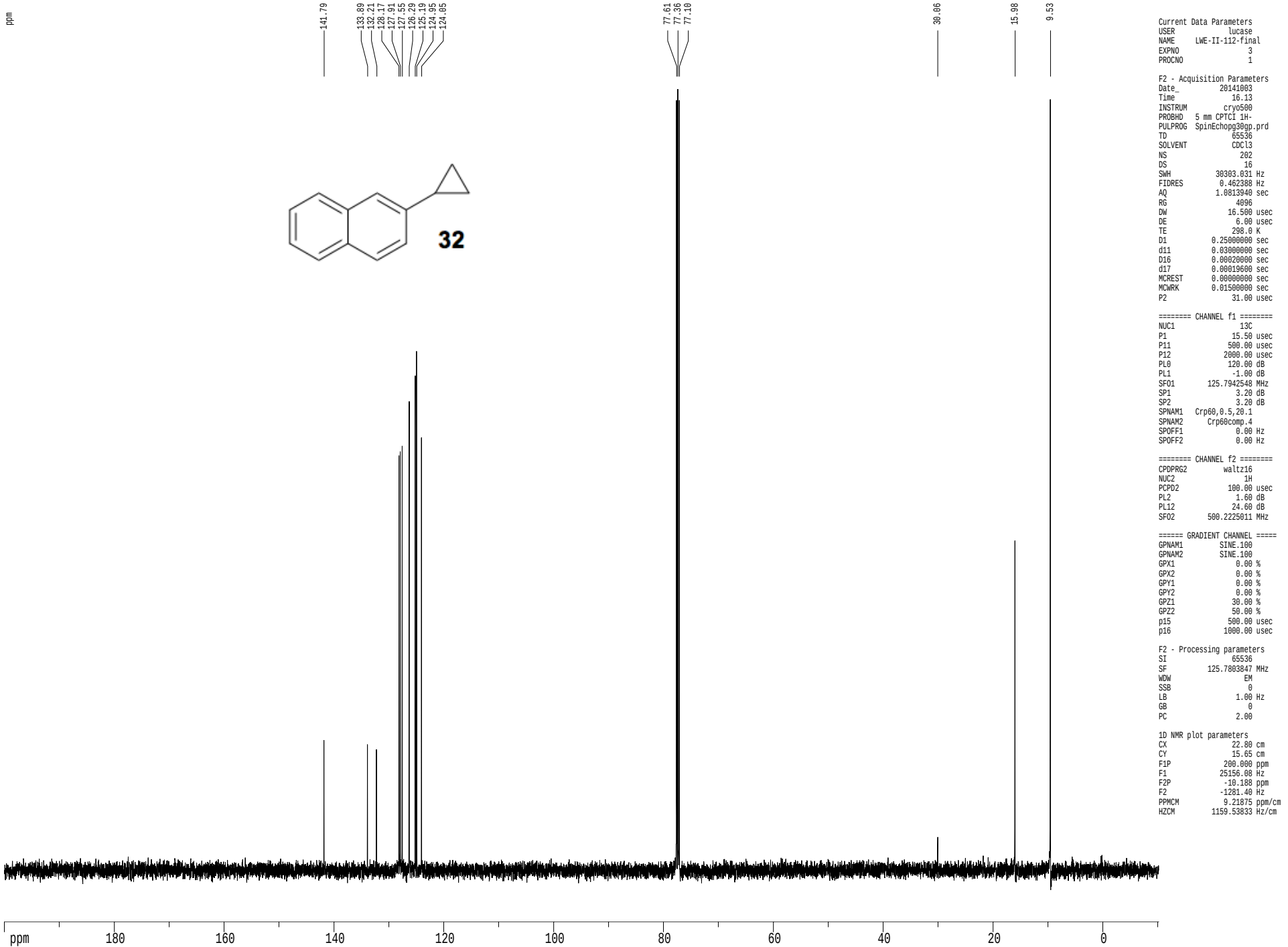
F2 - Acquisition Parameters
Date_ 20140924
Time 11.35
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 4.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200456 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42502 Hz/cm

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-112-final
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141003
Time                16.13
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    202
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 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
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

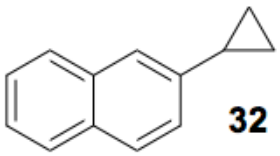
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              100.00 usec
PL2                 1.60 dB
PL12               24.60 dB
SFO2          500.2225011 MHz

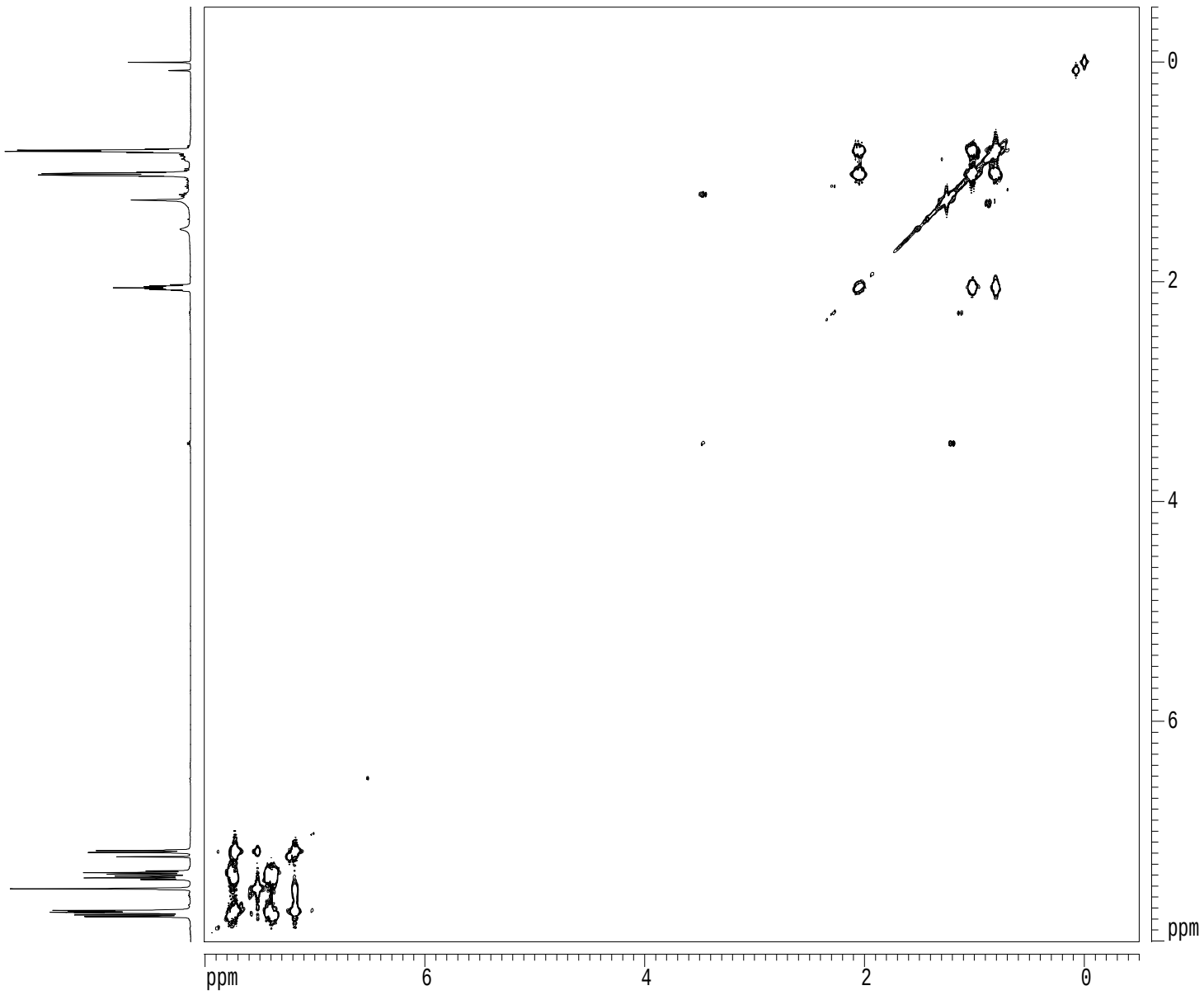
====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPNAM2          SINE.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               30.00 %
GPZ2               50.00 %
p15               500.00 usec
p16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF            125.7803847 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               200.000 ppm
F1              25156.08 Hz
F2P               -10.188 ppm
F2              -1281.40 Hz
PPMCM            9.21875 ppm/cm
HZCM          1159.53833 Hz/cm
```

gcosy60






```
        Current Data Parameters
 USER             lucase
NAME      LWE-II-112-final
 EXPNO                 2
 PROCNO                1

      F2 - Acquisition Parameters
 Date_          20140924
 Time              11.39
 INSTRUM         cryo500
 PROBHD   5 mm CPTCI 1H-
 PULPROG    cosygp60.prd
 TD                2048
 SOLVENT           CDCl3
 NS                   2
 DS                  16
 SWH            6009.615 Hz
 FIDRES         2.934382 Hz
 AQ            0.1704436 sec
 RG                161.3
 DW               83.200 usec
 DE                6.00 usec
 TE               298.0 K
 d0           0.00000300 sec
 D1           1.00000000 sec
 d13          0.00000300 sec
 D16          0.00020000 sec
 IN0          0.00016640 sec

     ======== CHANNEL f1 ========
 NUC1                 1H
 P1                 7.50 usec
 PL1                1.60 dB
 SFO1        500.2210460 MHz

     ====== GRADIENT CHANNEL =====
 GPNAM1          sine.100
 GPNAM2          sine.100
 GPX1               0.00 %
 GPX2               0.00 %
 GPY1               0.00 %
 GPY2               0.00 %
 GPZ1              17.00 %
 GPZ2              17.00 %
 P16             1000.00 usec

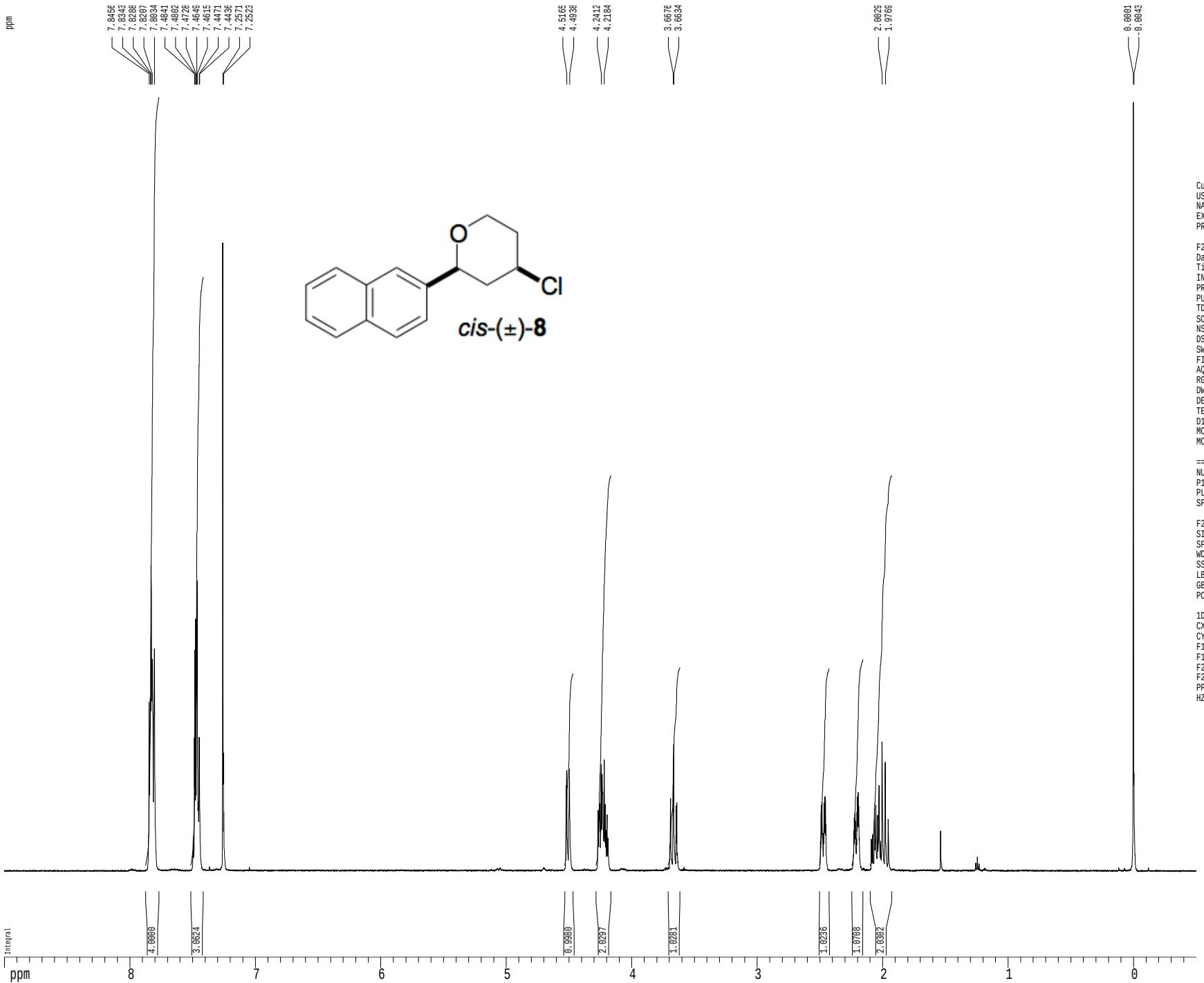
      F1 - Acquisition parameters
 ND0                  1
 TD                 256
 SFO1           500.221 MHz
 FIDRES        23.475060 Hz
 SW               12.014 ppm
 FnMODE        undefined

      F2 - Processing parameters
 SI                1024
 SF          500.2200456 MHz
 WDW               SINE
 SSB                  0
 LB                0.00 Hz
 GB                   0
 PC                4.00

      F1 - Processing parameters
 SI                1024
 MC2                 QF
 SF          500.2200456 MHz
 WDW               SINE
 SSB                  0
 LB                0.00 Hz
 GB                   0

        2D NMR plot parameters
 CX2              15.00 cm
 CX1              15.00 cm
 F2PLO             8.007 ppm
 F2LO           4005.35 Hz
 F2PHI            -0.500 ppm
 F2HI           -250.11 Hz
 F1PLO             8.007 ppm
 F1LO           4005.35 Hz
 F1PHI            -0.500 ppm
 F1HI           -250.11 Hz
 F2PPMCM         0.56715 ppm/cm
 F2HZCM        283.69736 Hz/cm
 F1PPMCM         0.56715 ppm/cm
 F1HZCM        283.69736 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME         EJT-I-265-C
EXPNO                1
PROCNO               1

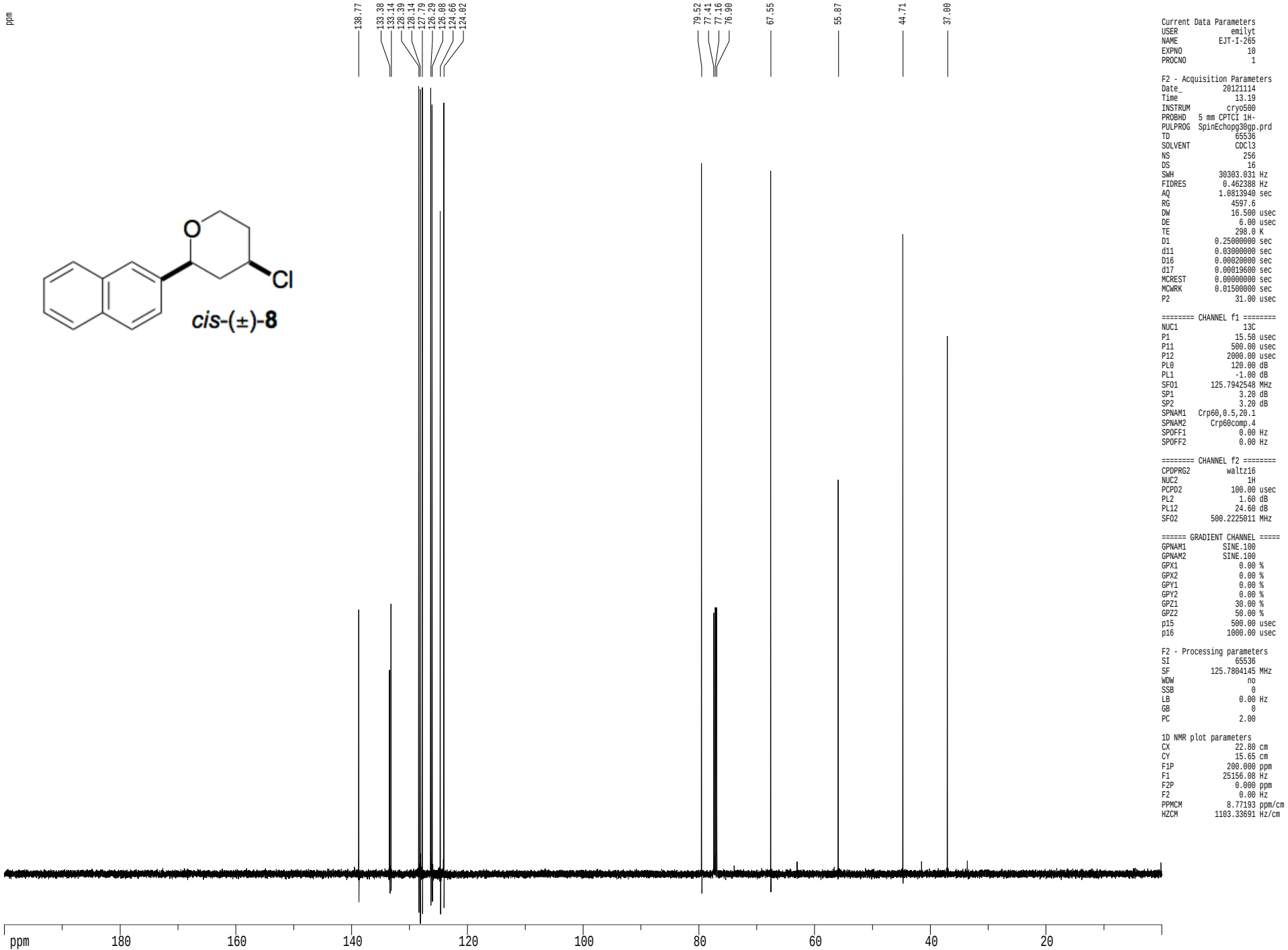
F2 - Acquisition Parameters
Date_          20121113
Time              18.28
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                81728
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8012.820 Hz
FIDRES         0.098043 Hz
AQ             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           500.2200324 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              4501.98 Hz
F2P              -0.500 ppm
F2             -250.11 Hz
PPMCM          0.41667 ppm/cm
HZCM         208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME             EJT-I-265
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_             20121114
Time                 13.19
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     256
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

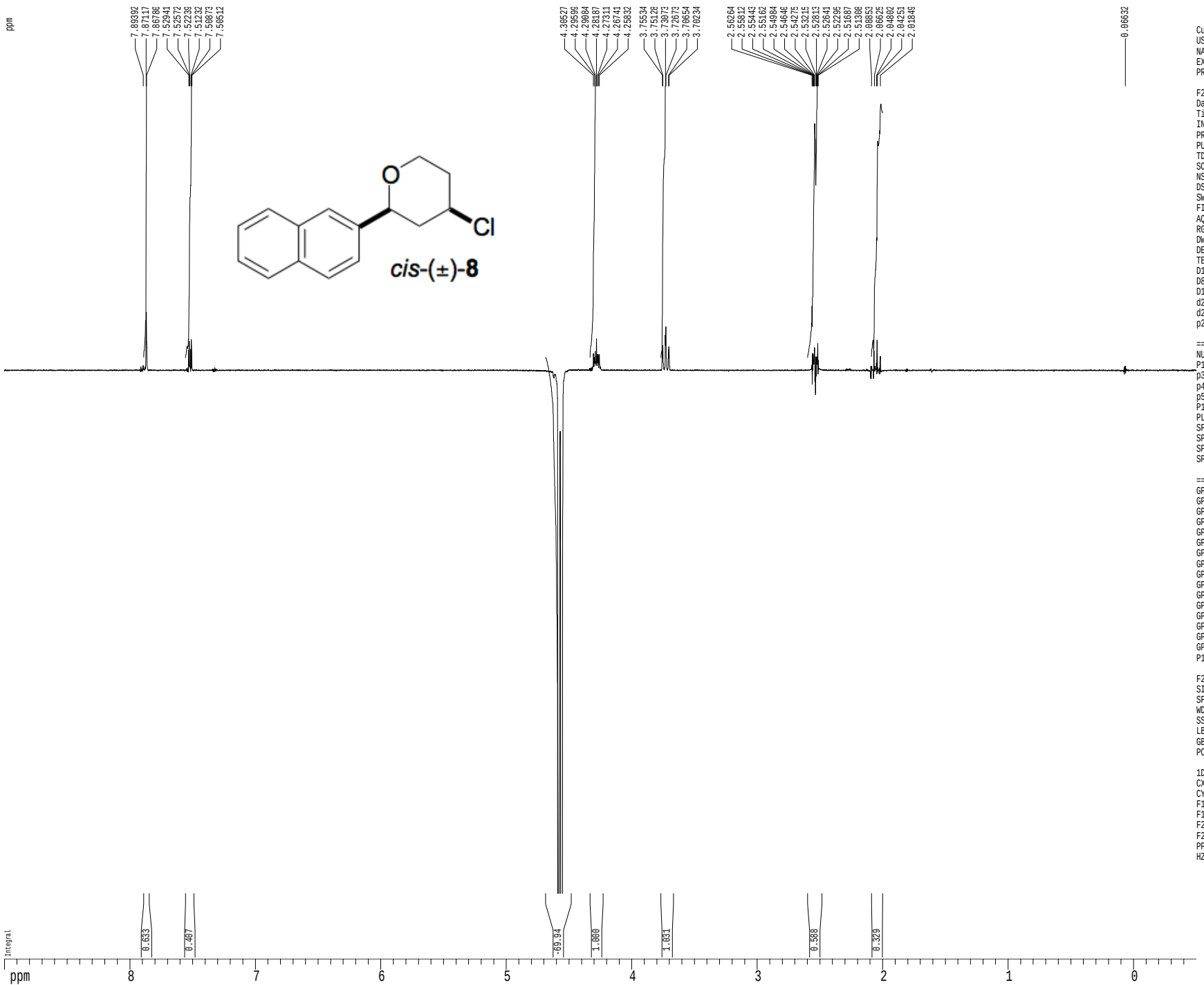
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.60 dB
SFO2           500.2225011 MHz

====== 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             125.7804145 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1                25156.08 Hz
F2P                  0.000 ppm
F2                    0.00 Hz
PPMCM             8.77193 ppm/cm
HZCM           1103.33691 Hz/cm
```

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-100 noe
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150206
Time 21.41
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

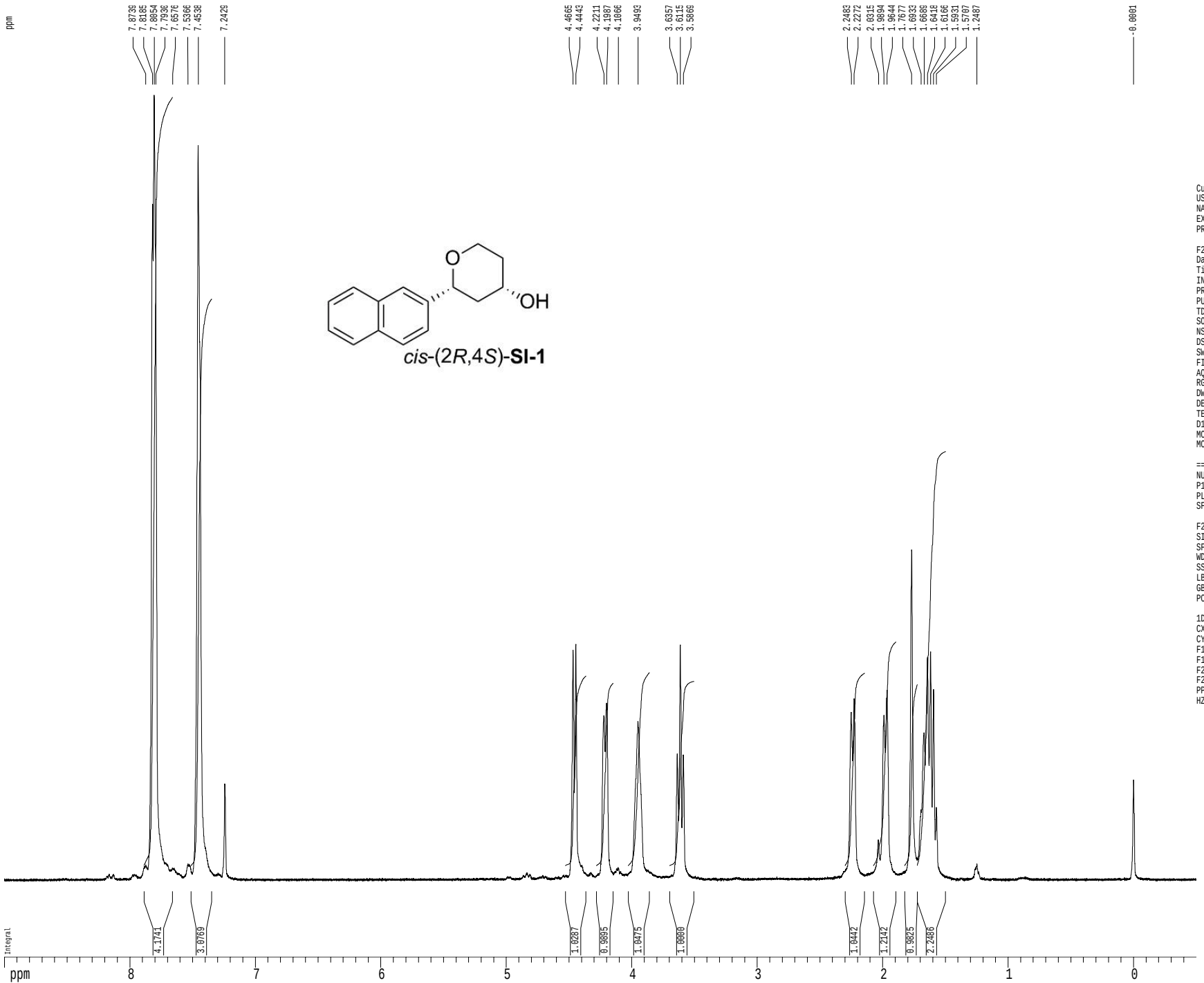
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2222865 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum



Current Data Parameters
USER emilyt
NAME EJT-IV-160 char
EXPNO 1
PROCNO 1

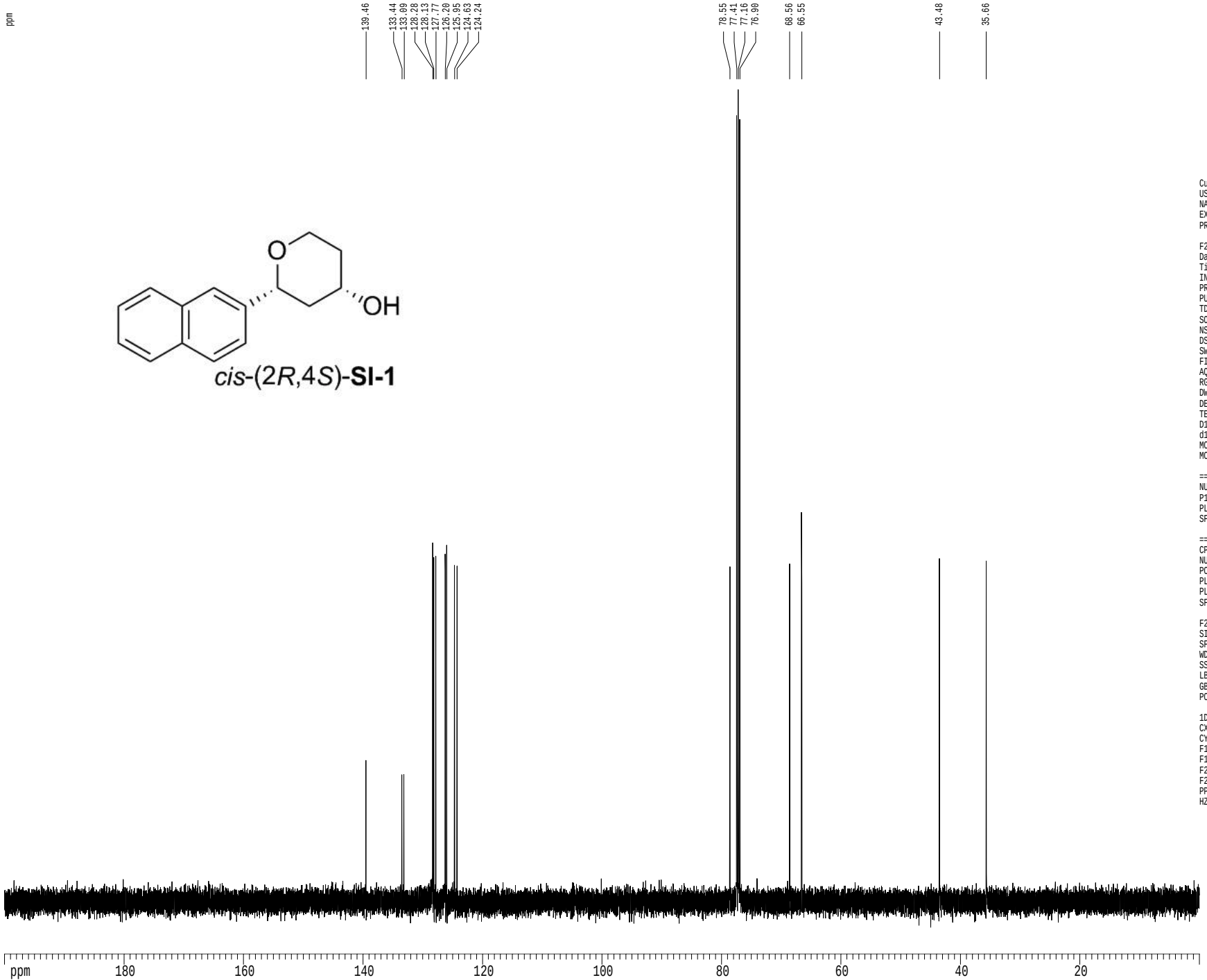
F2 - Acquisition Parameters
Date_ 20141221
Time 23.56
INSTRUM gn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 114
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 -5.80 dB
SFO1 499.1834943 MHz

F2 - Processing parameters
SI 65536
SF 499.1800361 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 4492.62 Hz
F2P -0.500 ppm
F2 -249.59 Hz
PPMCM 0.41667 ppm/cm
HZCM 207.99168 Hz/cm

13C spectrum with 1H decoupling




```
Current Data Parameters
USER              emilyt
NAME      EJT-IV-160 char
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20141222
Time               0.02
INSTRUM           gn500
PROBHD   5 mm broadband
PULPROG          zgdc30
TD                65536
SOLVENT           CDCl3
NS                  409
DS                    4
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.0813940 sec
RG                3649.1
DW               16.500 usec
DE                4.50 usec
TE                298.0 K
D1            0.25000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

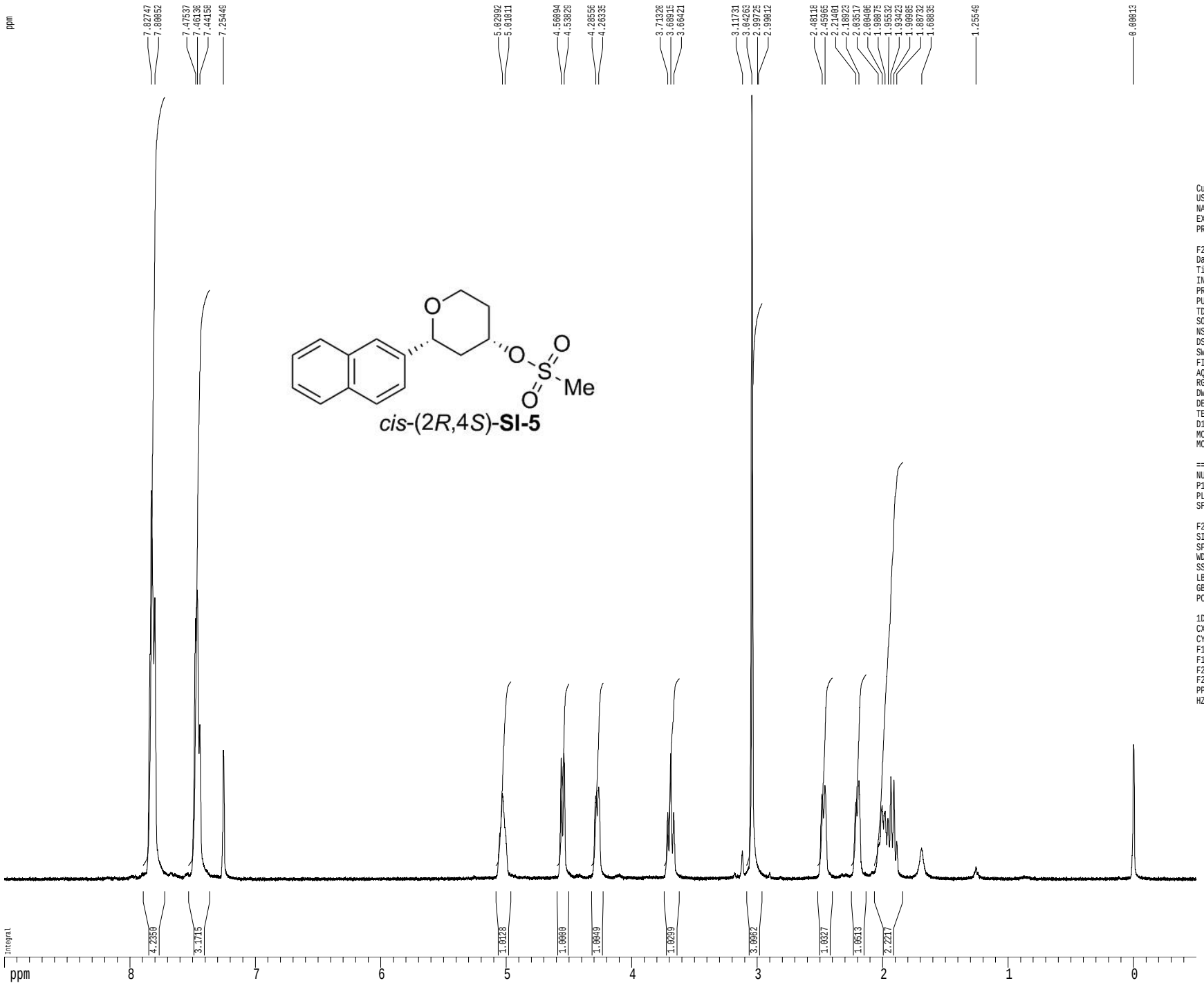
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.00 usec
PL1                -0.60 dB
SFO1        125.5327181 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -3.00 dB
PL12               12.80 dB
SFO2        499.1824959 MHz

F2 - Processing parameters
SI                65536
SF           125.5189025 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.80 cm
CY                15.65 cm
F1P              200.000 ppm
F1             25103.78 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM          8.77193 ppm/cm
HZCM        1101.04309 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME      EJT-IV-151 char
EXPNO                  1
PROCNO                 1

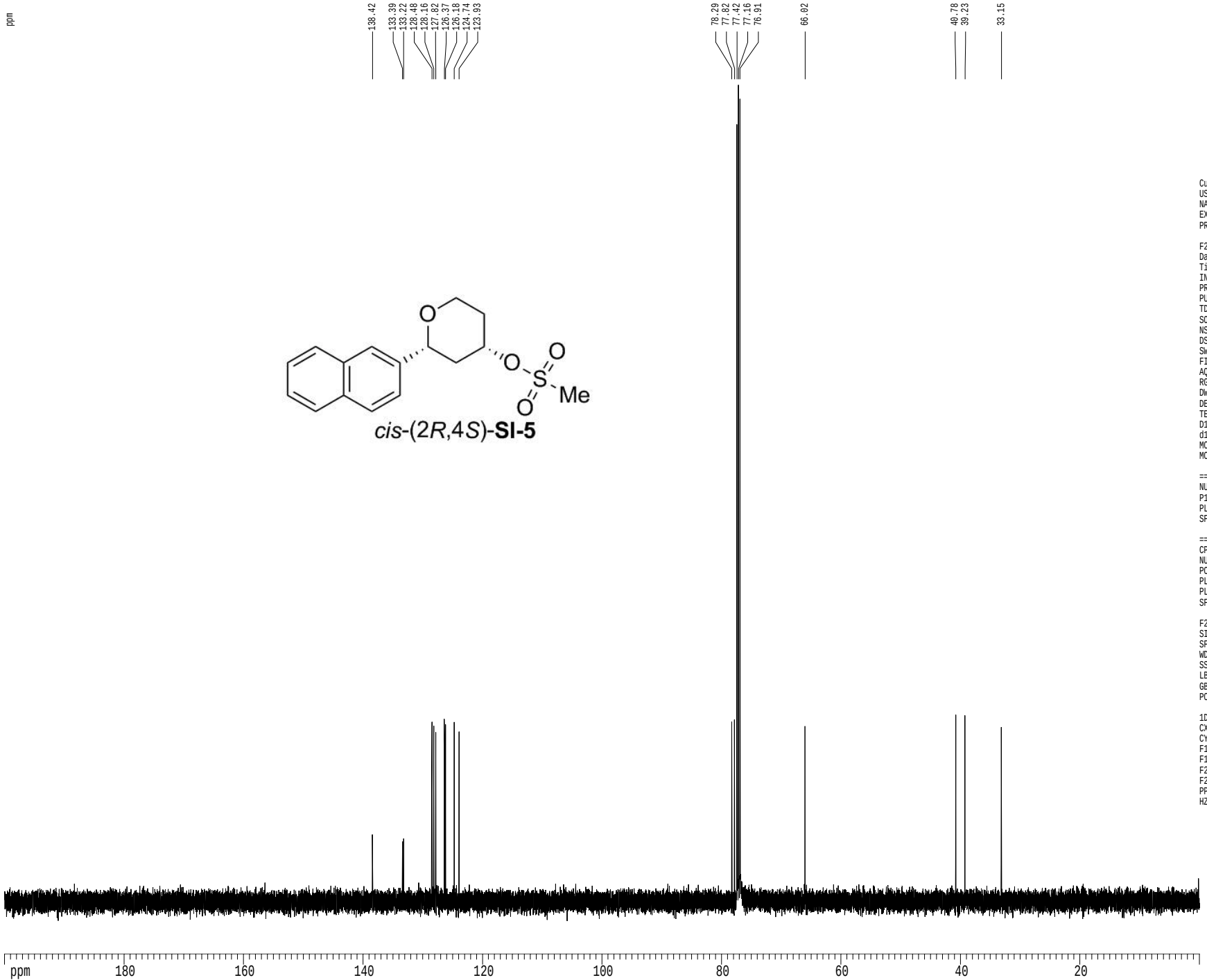
F2 - Acquisition Parameters
Date_           20141222
Time                0.11
INSTRUM            gn500
PROBHD   5 mm broadband
PULPROG             zg30
TD                 81728
SOLVENT           CDCl3T
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 Hz
AQ              5.0998774 sec
RG                 724.1
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                12.00 usec
PL1                -5.80 dB
SFO1         499.1834943 MHz

F2 - Processing parameters
SI                 65536
SF           499.1800305 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              4492.62 Hz
F2P              -0.500 ppm
F2              -249.59 Hz
PPMCM           0.41667 ppm/cm
HZCM          207.99168 Hz/cm
```

13C spectrum with 1H decoupling




```
Current Data Parameters
USER              emilyt
NAME      EJT-IV-151 char
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20141222
Time               0.24
INSTRUM           gn500
PROBHD   5 mm broadband
PULPROG          zgdc30
TD                65536
SOLVENT           CDCl3
NS                  964
DS                    4
SWH           30303.031 Hz
FIDRES         0.462388 Hz
AQ             1.0813940 sec
RG                9195.2
DW                16.500 usec
DE                 4.50 usec
TE                298.0 K
D1           0.25000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

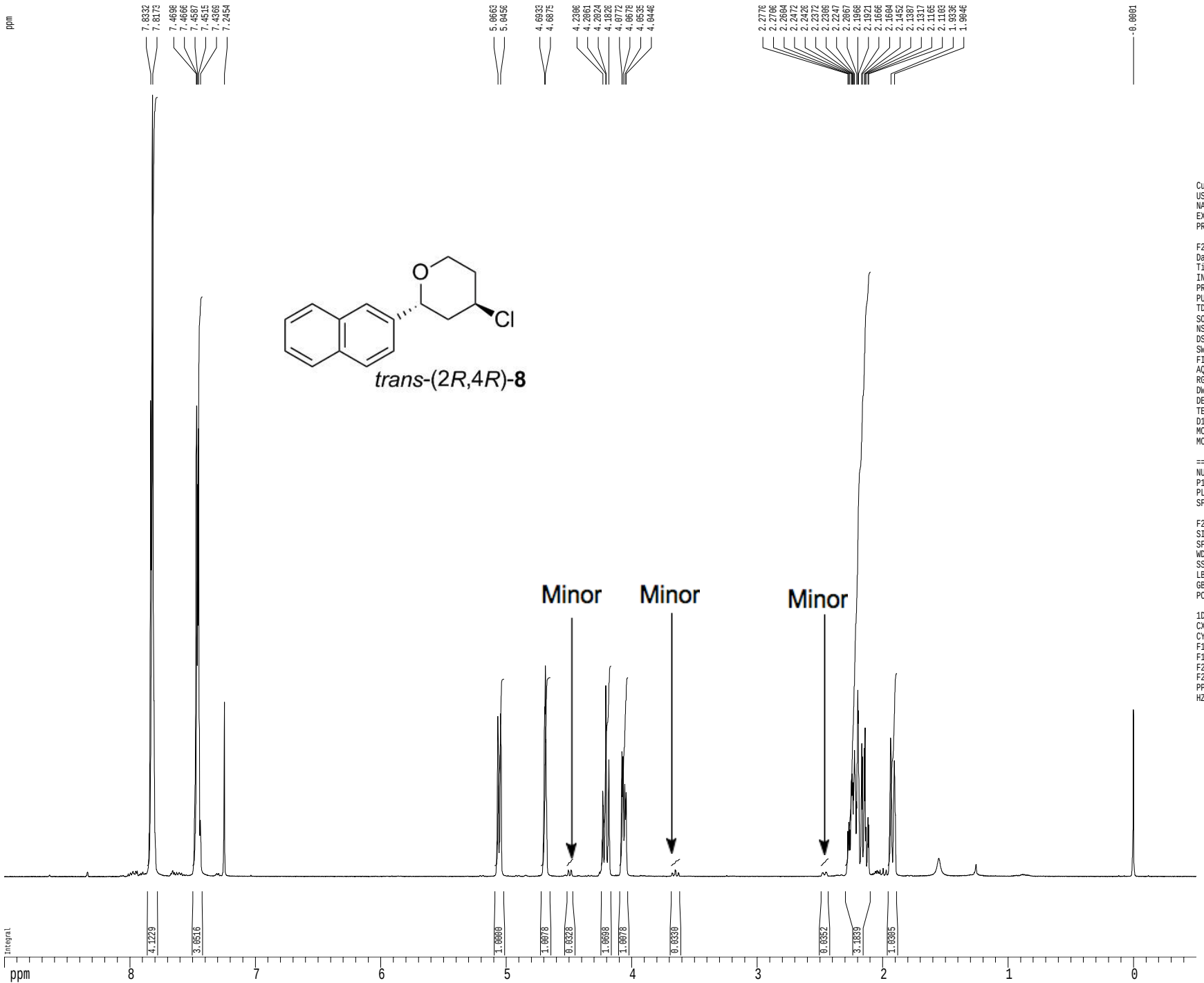
======== CHANNEL f1 ========
NUC1                13C
P1                 9.00 usec
PL1               -0.60 dB
SFO1        125.5327181 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              12.80 dB
SFO2        499.1824959 MHz

F2 - Processing parameters
SI                 65536
SF           125.5188988 MHz
WDW                   no
SSB                    0
LB                0.00 Hz
GB                     0
PC                2.00

1D NMR plot parameters
CX                22.80 cm
CY                15.65 cm
F1P              200.000 ppm
F1             25103.78 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM          8.77193 ppm/cm
HZCM         1101.04297 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER                emilyt
NAME      EJT-IV-169 trans
EXPNO                   1
PROCNO                  1

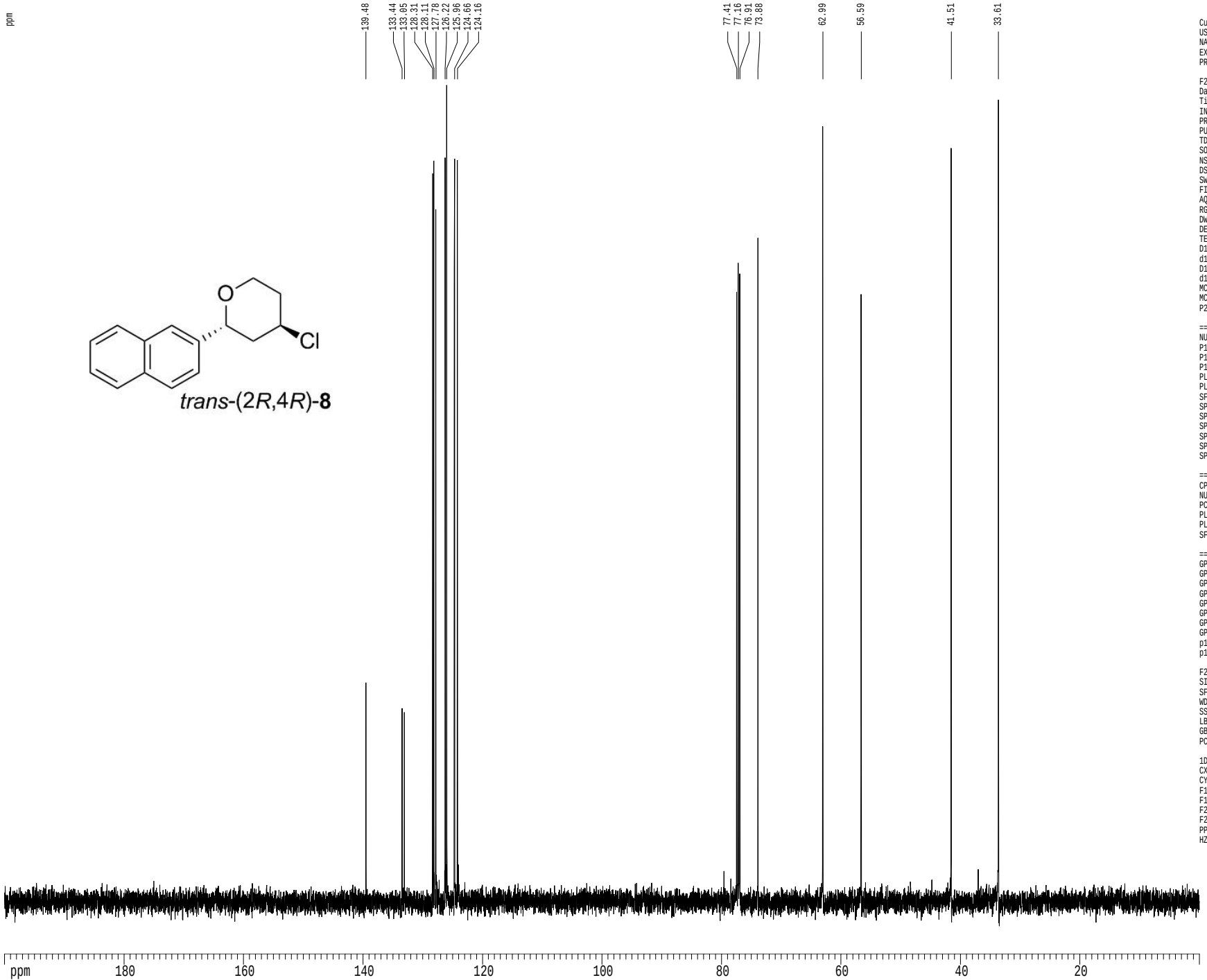
F2 - Acquisition Parameters
Date_            20141222
Time                13.02
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  81728
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                      8
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            500.2200409 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME      EJT-IV-169 trans
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20141222
Time                13.05
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    114
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 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
MCREST          0.00000000 sec
MCWRK           0.01500000 sec
P2                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                  2.70 dB
SP2                  2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

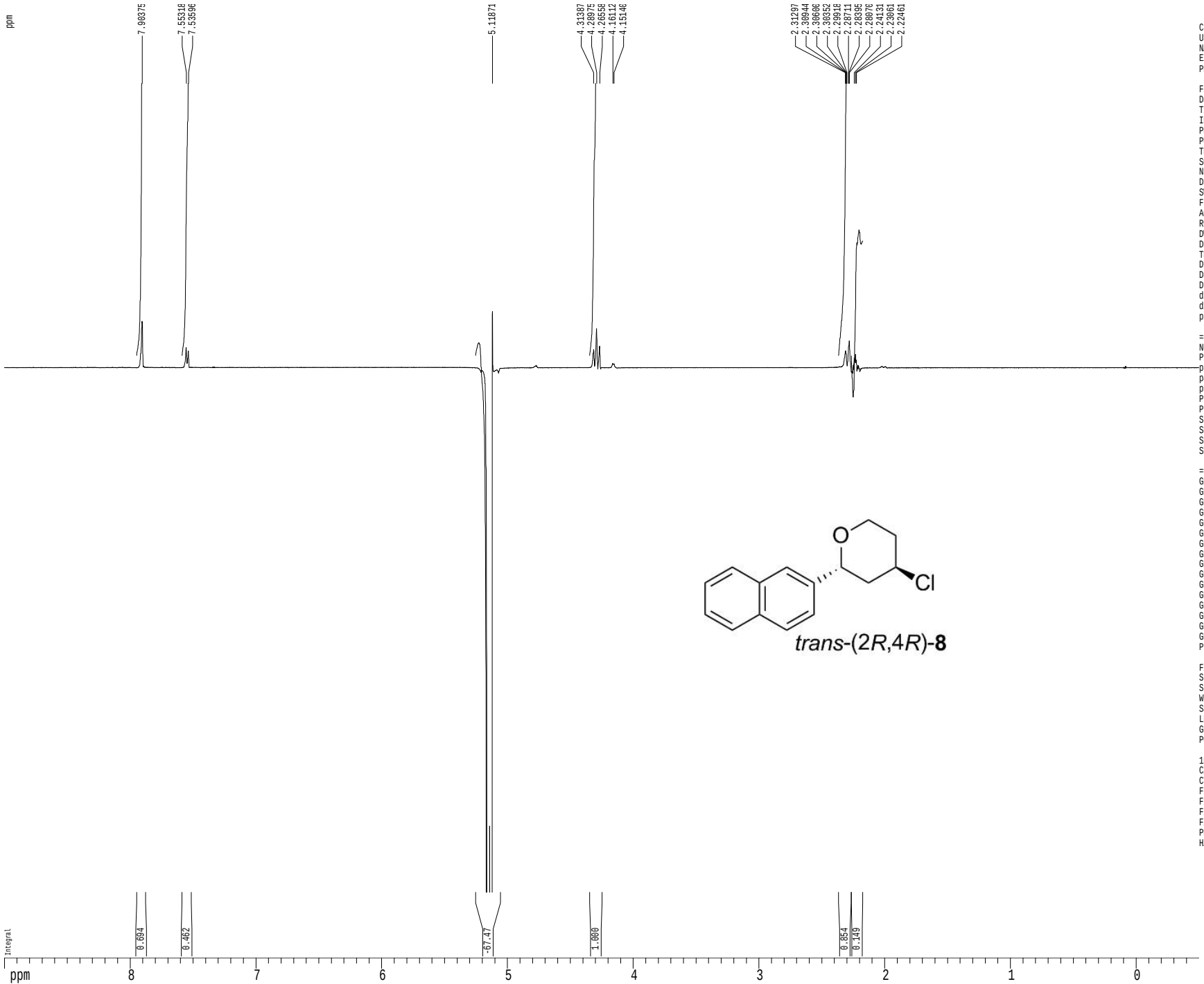
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7804122 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               200.000 ppm
F1              25156.08 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            8.77193 ppm/cm
HZCM          1103.33691 Hz/cm
```

gnoe



trans-(2*R*,4*R*)-**8**

Current Data Parameters
USER emilyt
NAME EJT-IV-169 trans
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141222
Time 13.32
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

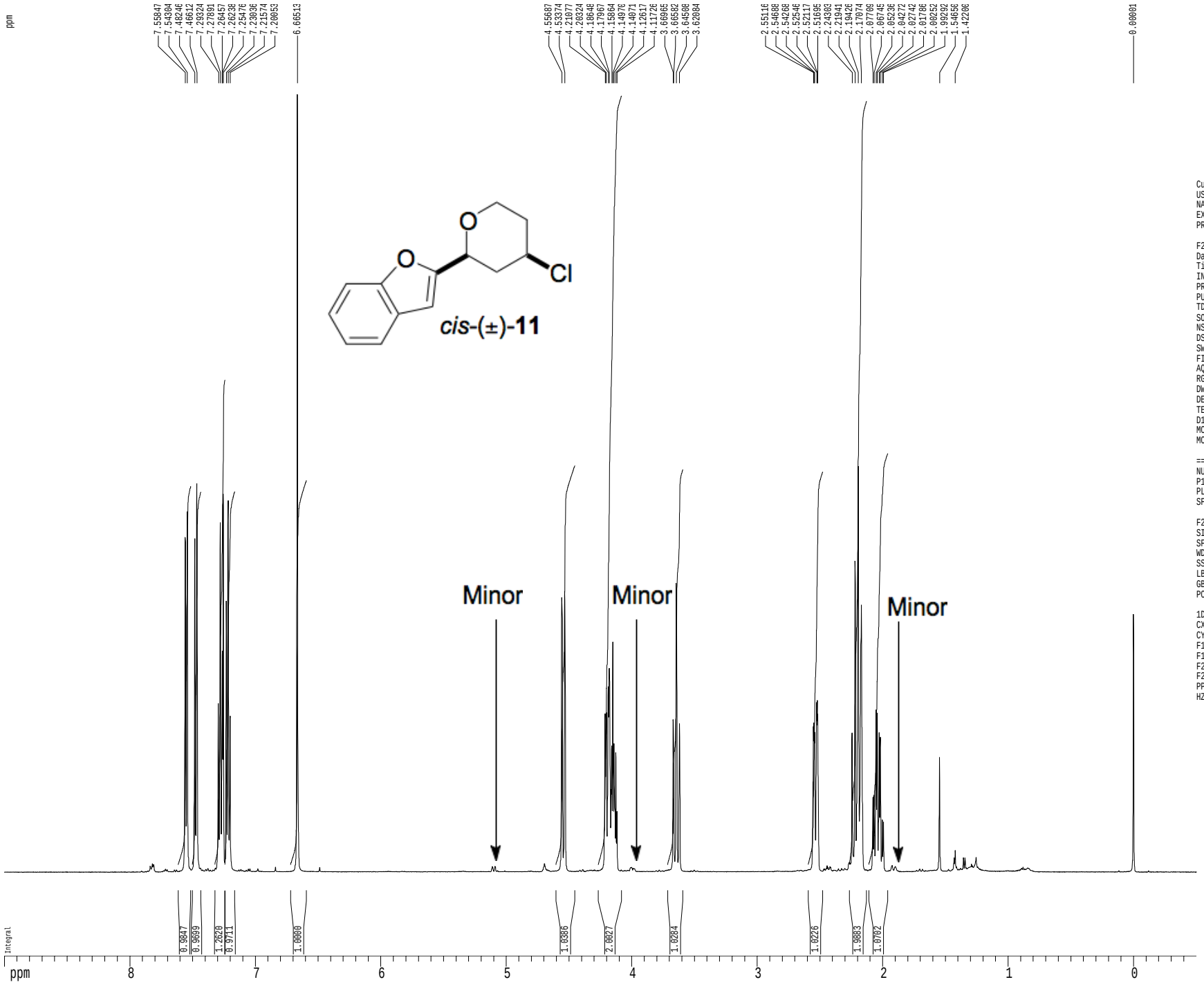
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2225704 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-212-cryo8
EXPNO                    1
PROCNO                   1

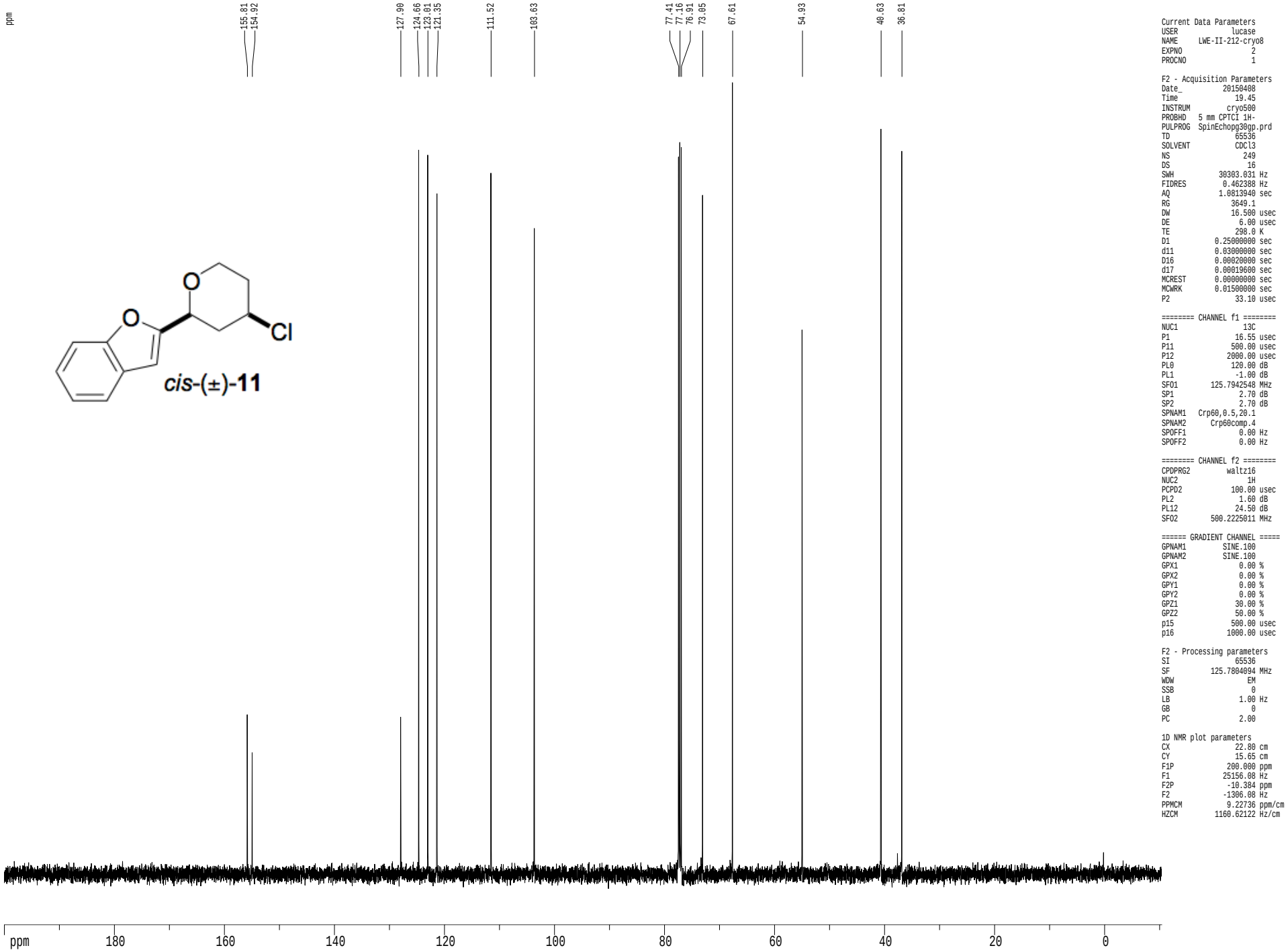
F2 - Acquisition Parameters
Date_            20150408
Time                19.41
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  81728
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                    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            500.2200335 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                    4.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.00 cm
F1P                   9.000 ppm
F1                 4501.98 Hz
F2P                  -0.500 ppm
F2                 -250.11 Hz
PPMCM             0.41667 ppm/cm
HZCM            208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-212-cryo8
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150408
Time                19.45
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    249
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                3649.1
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                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

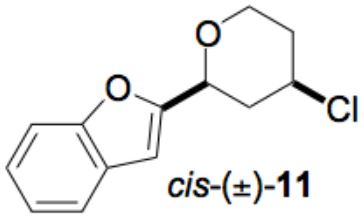
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2         500.2225011 MHz

====== 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

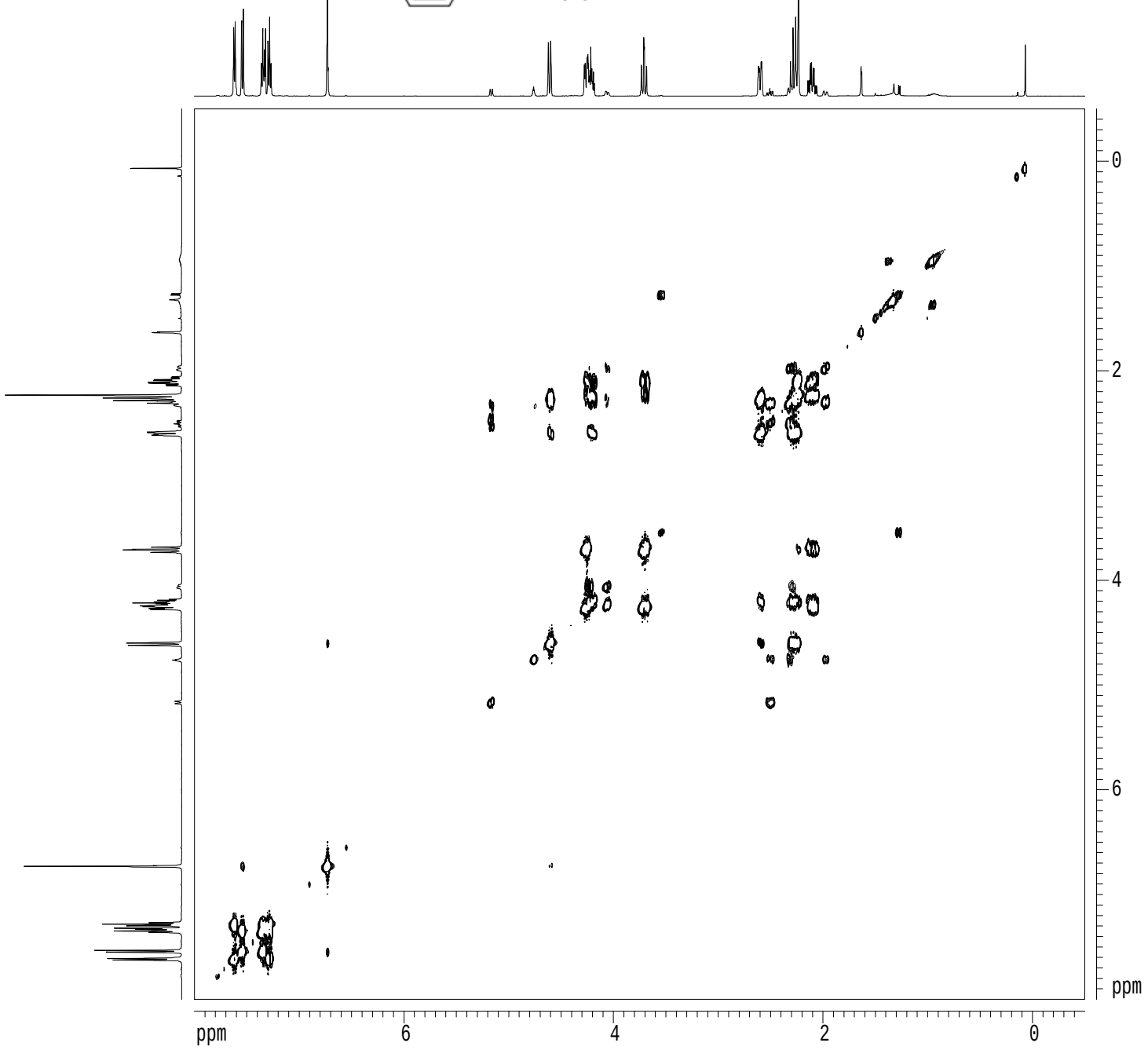
F2 - Processing parameters
SI                  65536
SF           125.7804094 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               200.000 ppm
F1              25156.08 Hz
F2P               -10.384 ppm
F2              -1306.08 Hz
PPMCM             9.22736 ppm/cm
HZCM           1160.62122 Hz/cm
```

gcosy60



cis-(±)-**11**



Current Data Parameters

USER	lucase
NAME	LWE-II-212-cryo2
EXPNO	4
PROCNO	1

F2 - Acquisition Parameters

Date_	20150211
Time	19.22
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4251.701 Hz
FIDRES	2.076026 Hz
AQ	0.2408948 sec
RG	35.9
DW	117.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00023520 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2218758 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2219 MHz
FIDRES	33.216412 Hz
SW	8.500 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

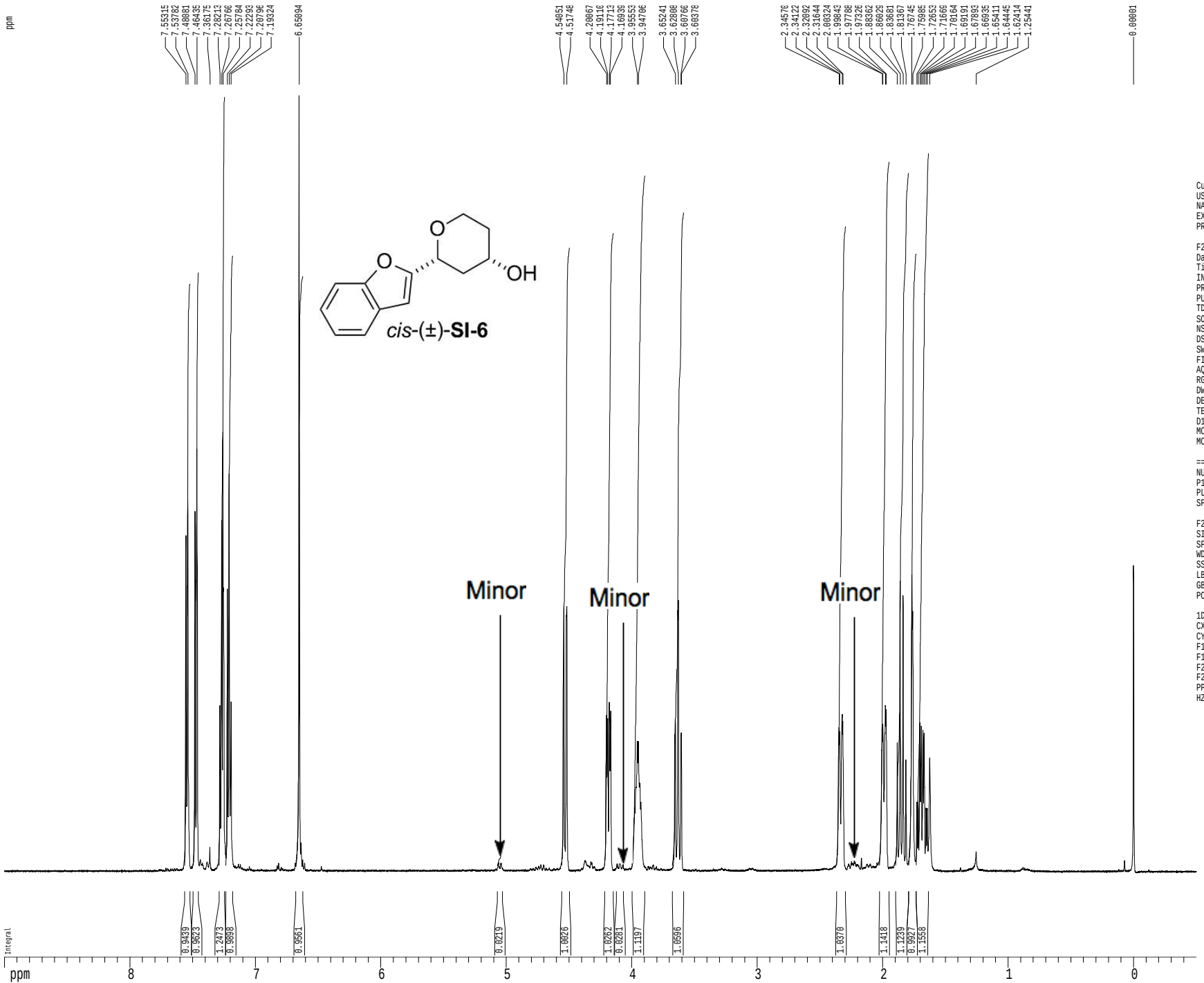
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.000 ppm
F2LO	4001.67 Hz
F2PHI	-0.500 ppm
F2HI	-250.03 Hz
F1PLO	8.000 ppm
F1LO	4001.67 Hz
F1PHI	-0.500 ppm
F1HI	-250.03 Hz
F2PPMCM	0.56664 ppm/cm
F2HZCM	283.44672 Hz/cm
F1PPMCM	0.56664 ppm/cm
F1HZCM	283.44672 Hz/cm

1H spectrum




```
Current Data Parameters
USER                emilyt
NAME      LWE-III-019 OH
EXPNO                 10
PROCNO                 1

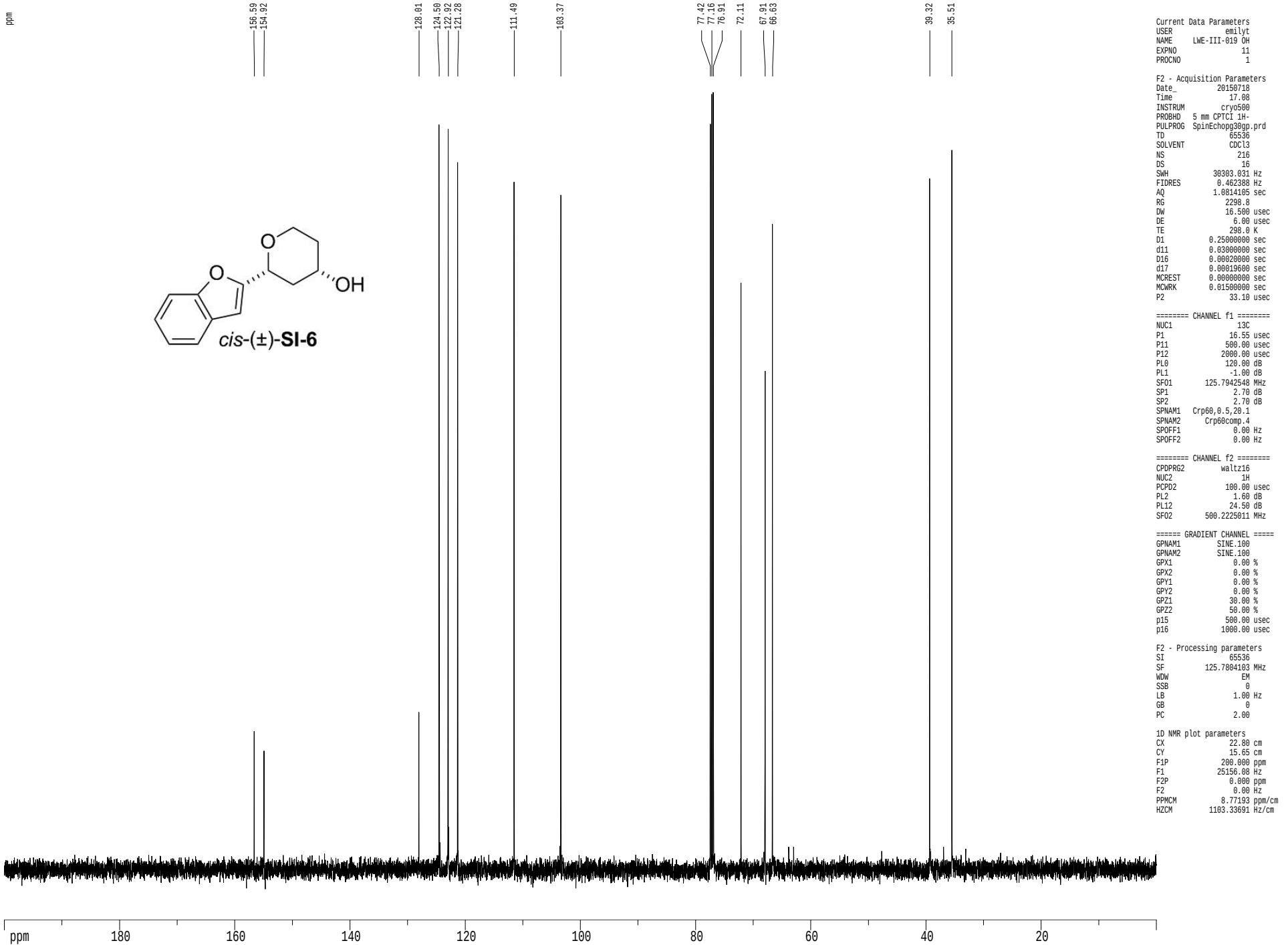
F2 - Acquisition Parameters
Date_           20150718
Time              17.04
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 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           500.2200326 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P                9.000 ppm
F1               4501.98 Hz
F2P               -0.500 ppm
F2               -250.11 Hz
PPMCM          0.41667 ppm/cm
HZCM          208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME      LWE-III-019 OH
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150718
Time                17.08
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    216
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0814105 sec
RG                 2298.8
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                 33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

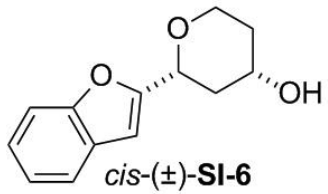
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2         500.2225011 MHz

====== 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           125.7804103 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.65 cm
F1P              200.000 ppm
F1             25156.08 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           8.77193 ppm/cm
HZCM         1103.33691 Hz/cm
```

gcosy60



cis-(±)-**SI-6**

Current Data Parameters

USER	emilyt
NAME	LWE-III-019 OH
EXPNO	12
PROCNO	1

F2 - Acquisition Parameters

Date_	20150718
Time	17.12
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4734.849 Hz
FIDRES	2.311938 Hz
AQ	0.2164244 sec
RG	406.4
DW	105.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00021120 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2221585 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2222 MHz
FIDRES	36.991005 Hz
SW	9.465 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200326 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

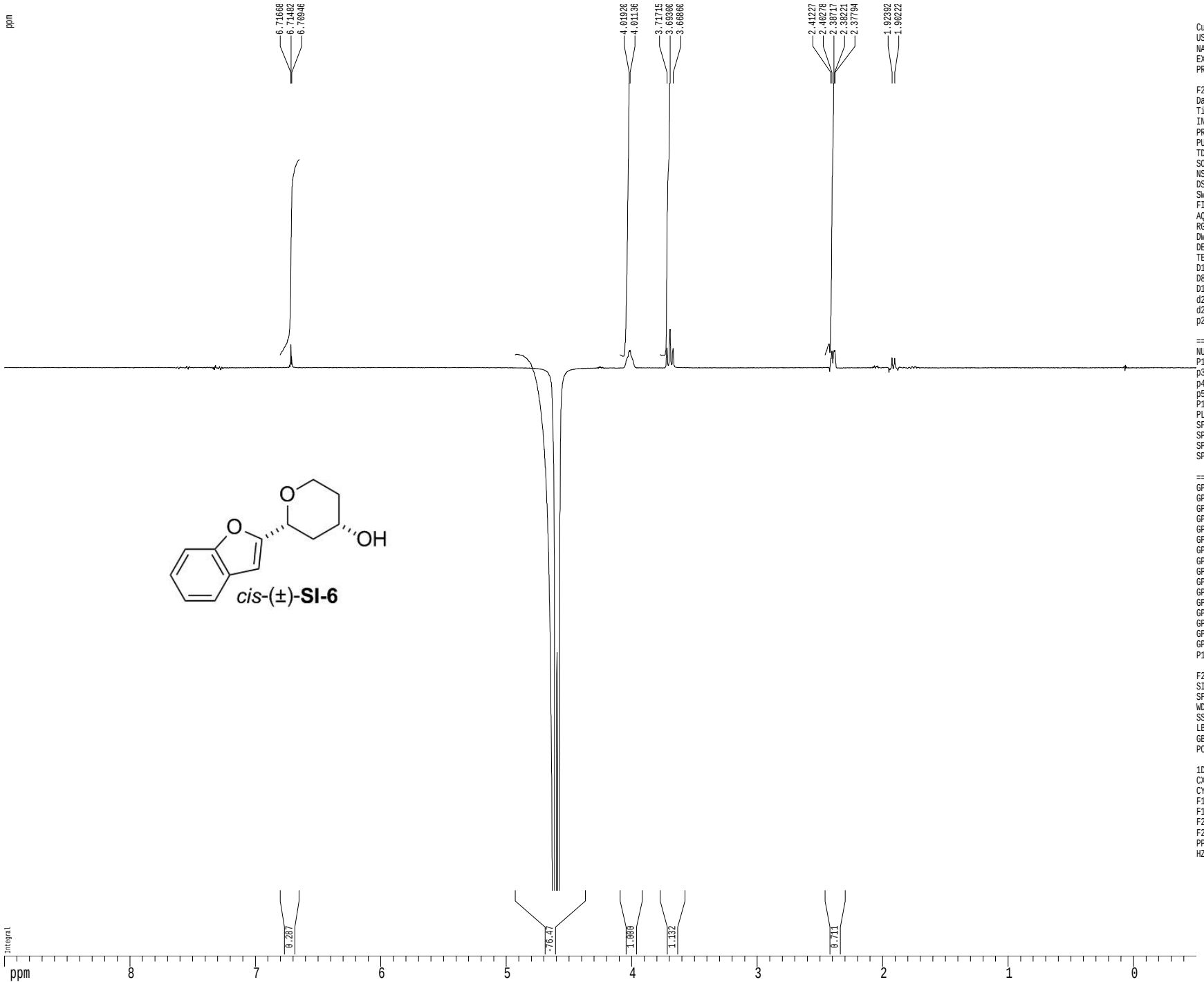
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200326 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	9.048 ppm
F2LO	4525.97 Hz
F2PHI	-0.418 ppm
F2HI	-208.88 Hz
F1PLO	9.048 ppm
F1LO	4525.97 Hz
F1PHI	-0.418 ppm
F1HI	-208.88 Hz
F2PPMCM	0.63104 ppm/cm
F2HZCM	315.65659 Hz/cm
F1PPMCM	0.63104 ppm/cm
F1HZCM	315.65659 Hz/cm

gnoe




```
Current Data Parameters
USER                emilyt
NAME      LWE-III-019 OH
EXPNO                  13
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150718
Time                17.33
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                  161.3
DW                62.400 usec
DE                 6.00 usec
TE                 298.0 K
D1              1.00000000 sec
D8              0.50000000 sec
D16             0.00020000 sec
d21             0.33376500 sec
d22             0.16399699 sec
p2                 15.00 usec

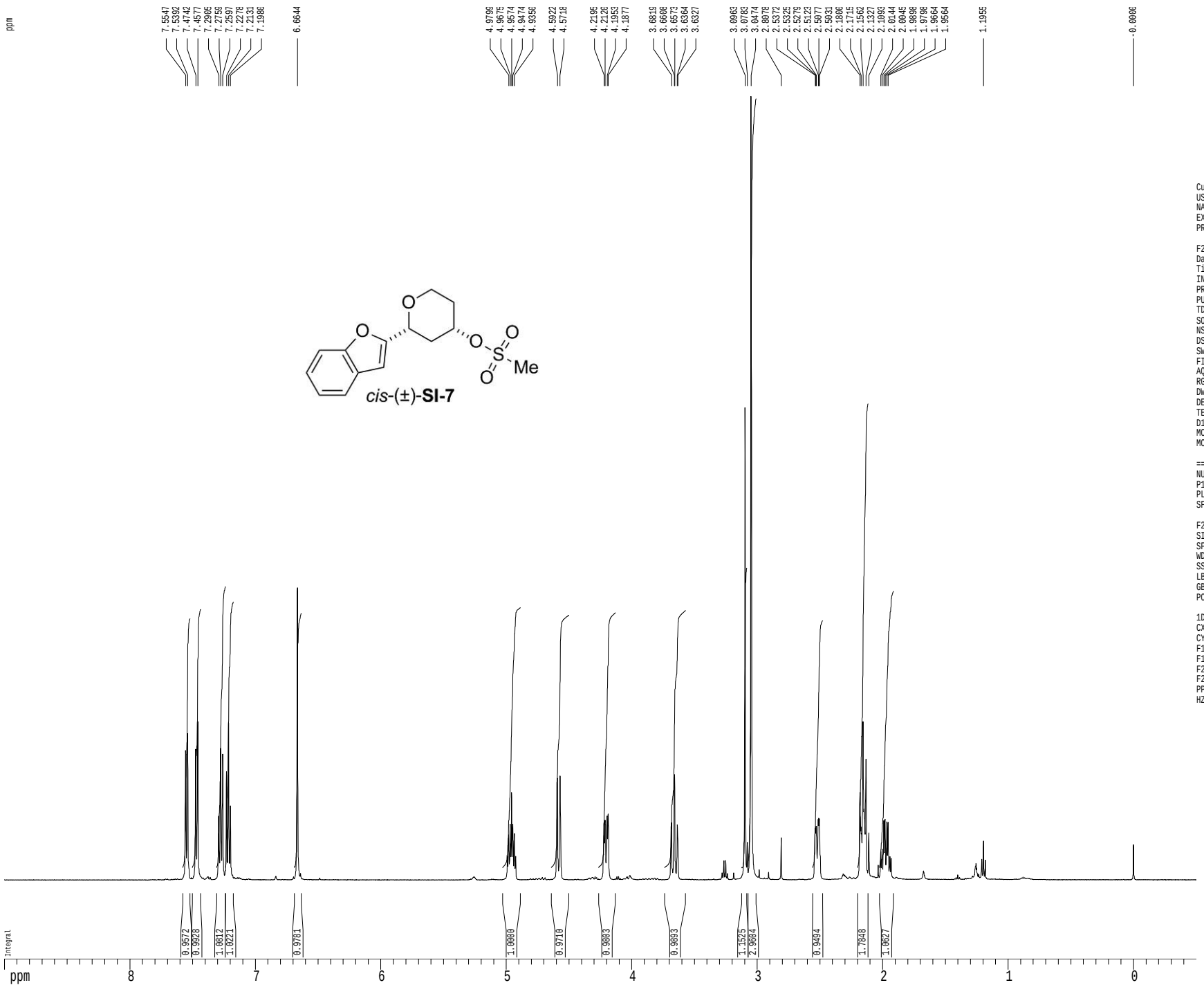
======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
p3                  22.50 usec
p4                  30.00 usec
p5                  20.00 usec
P12              40000.00 usec
PL1                  1.60 dB
SFO1          500.2222993 MHz
SP1                 61.60 dB
SPNAM1         gauss1.512
SPOFF1               0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1           sine.100
GPNAM2           sine.100
GPNAM3           sine.100
GPNAM4           sine.100
GPX1                 0.00 %
GPX2                 0.00 %
GPX3                 0.00 %
GPX4                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPY3                 0.00 %
GPY4                 0.00 %
GPZ1                 7.00 %
GPZ2                 3.00 %
GPZ3                 2.30 %
GPZ4                -2.30 %
P16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF            500.2200000 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  22.80 cm
CY                  50.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42500 Hz/cm
```

1H spectrum



Current Data Parameters
USER emilyt
NAME LWE-III-022 OMs
EXPNO 10
PROCNO 1

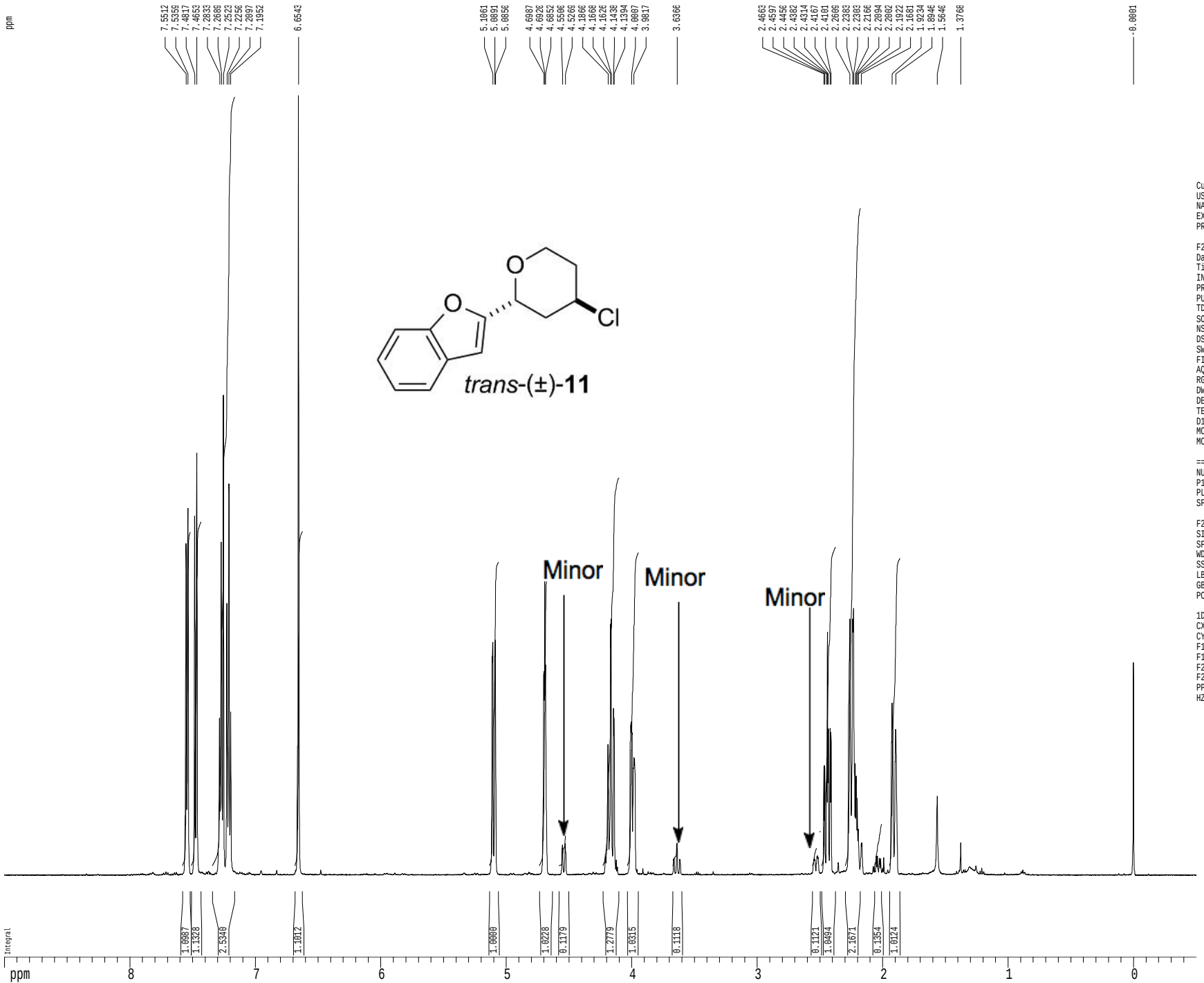
F2 - Acquisition Parameters
Date_ 20150719
Time 11.18
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 4
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200310 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42502 Hz/cm

1H spectrum




```
Current Data Parameters
USER                emilyt
NAME      LWE-III-023 Cl
EXPNO                 15
PROCNO                 1

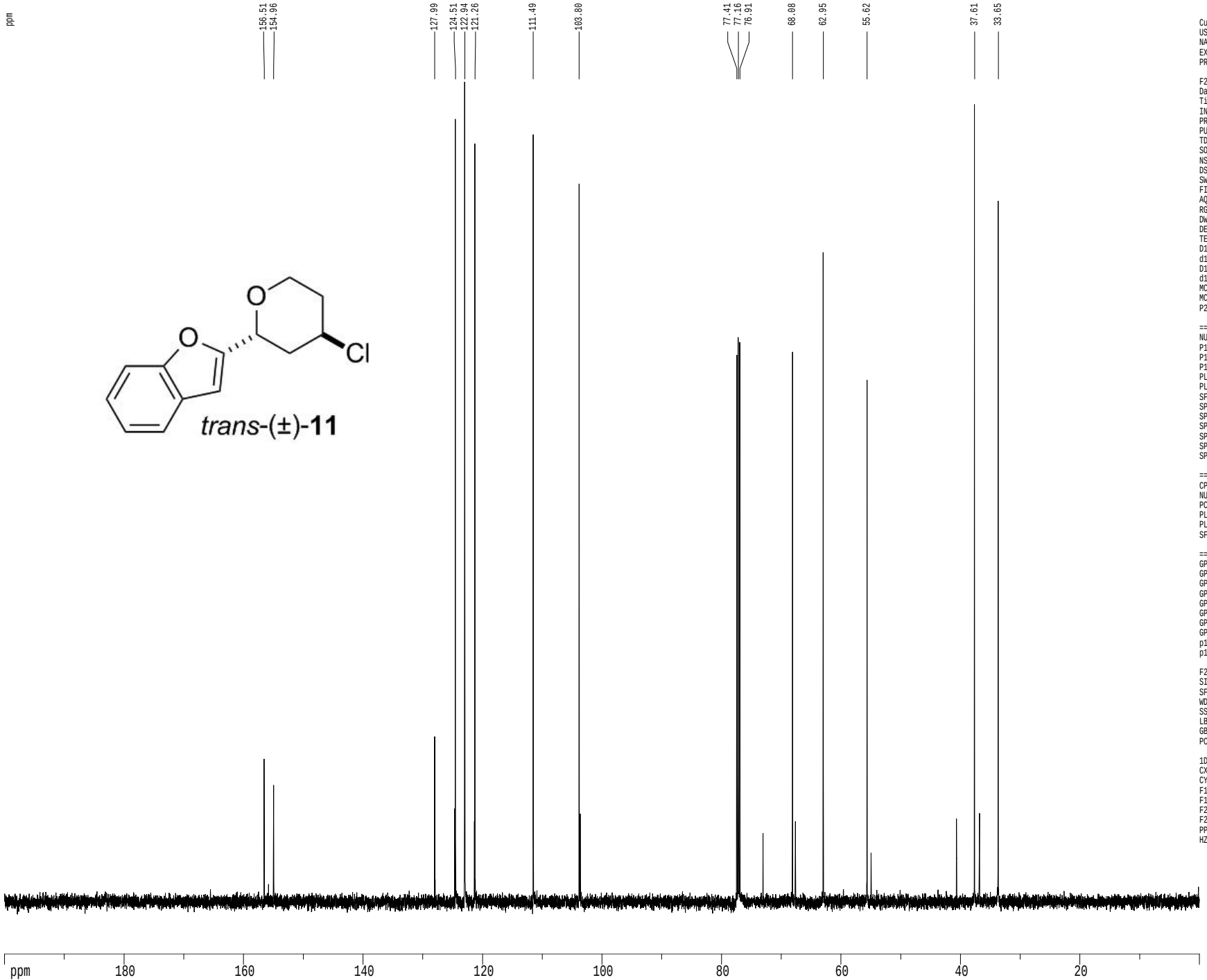
F2 - Acquisition Parameters
Date_           20150719
Time                11.26
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 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           500.2200349 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  4.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P                 9.000 ppm
F1               4501.98 Hz
F2P                -0.500 ppm
F2               -250.11 Hz
PPMCM           0.41667 ppm/cm
HZCM          208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME      LWE-III-023 Cl
EXPNO                 16
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150719
Time                11.29
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    221
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0814105 sec
RG                   3251
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                 2.70 dB
SP2                 2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

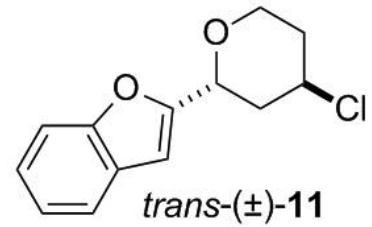
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7804108 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1                25156.08 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM             8.77193 ppm/cm
HZCM           1103.33691 Hz/cm
```

PI Jarvo
gcosy.q CDCl3 v emilyt 12



trans-(±)-**11**

Current Data Parameters

USER	emilyt
NAME	LWE-III-023 Cl
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20150717
Time	1.41
INSTRUM	drx400
PROBHD	5 mm QNP H/F/P
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	3472.222 Hz
FIDRES	1.695421 Hz
AQ	0.2949620 sec
RG	912.3
DW	144.000 usec
DE	4.50 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00028800 sec

======== CHANNEL f1 ========

NUC1	1H
P1	12.00 usec
PL1	0.00 dB
SFO1	400.1315432 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	256
SFO1	400.1315 MHz
FIDRES	13.563368 Hz
SW	8.678 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	400.1300177 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

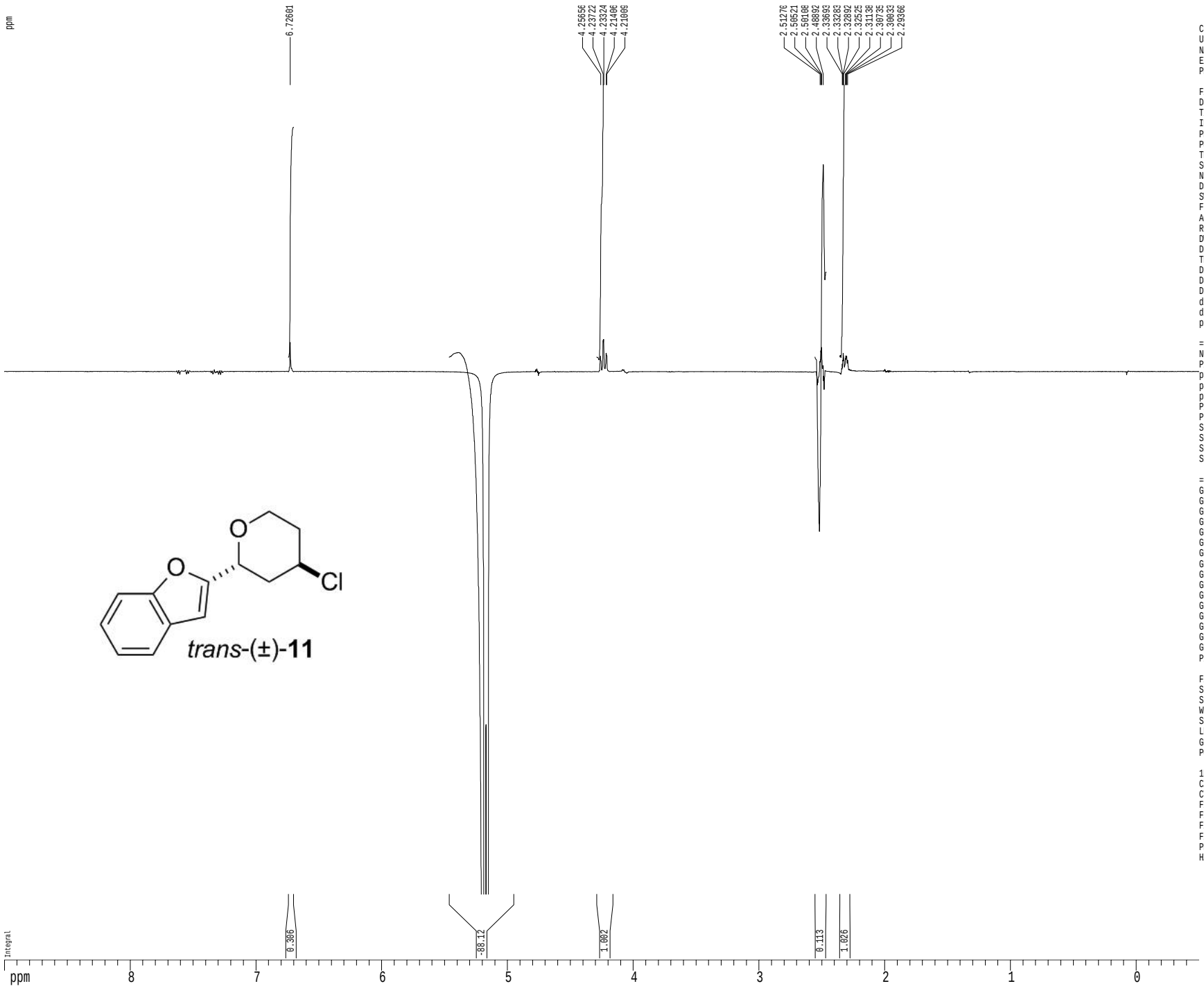
F1 - Processing parameters

SI	1024
MC2	QF
SF	400.1300177 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.152 ppm
F2LO	3261.66 Hz
F2PHI	-0.526 ppm
F2HI	-210.56 Hz
F1PLO	8.152 ppm
F1LO	3261.66 Hz
F1PHI	-0.526 ppm
F1HI	-210.56 Hz
F2PPMCM	0.57852 ppm/cm
F2HZCM	231.48149 Hz/cm
F1PPMCM	0.57852 ppm/cm
F1HZCM	231.48149 Hz/cm

gnoe




```
Current Data Parameters
USER                emilyt
NAME      LWE-III-023 Cl
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150717
Time                14.18
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                    128
DW                 62.400 usec
DE                  6.00 usec
TE                298.0 K
D1              1.00000000 sec
D8              0.50000000 sec
D16             0.00020000 sec
d21             0.33376500 sec
d22             0.16399699 sec
p2                 15.00 usec

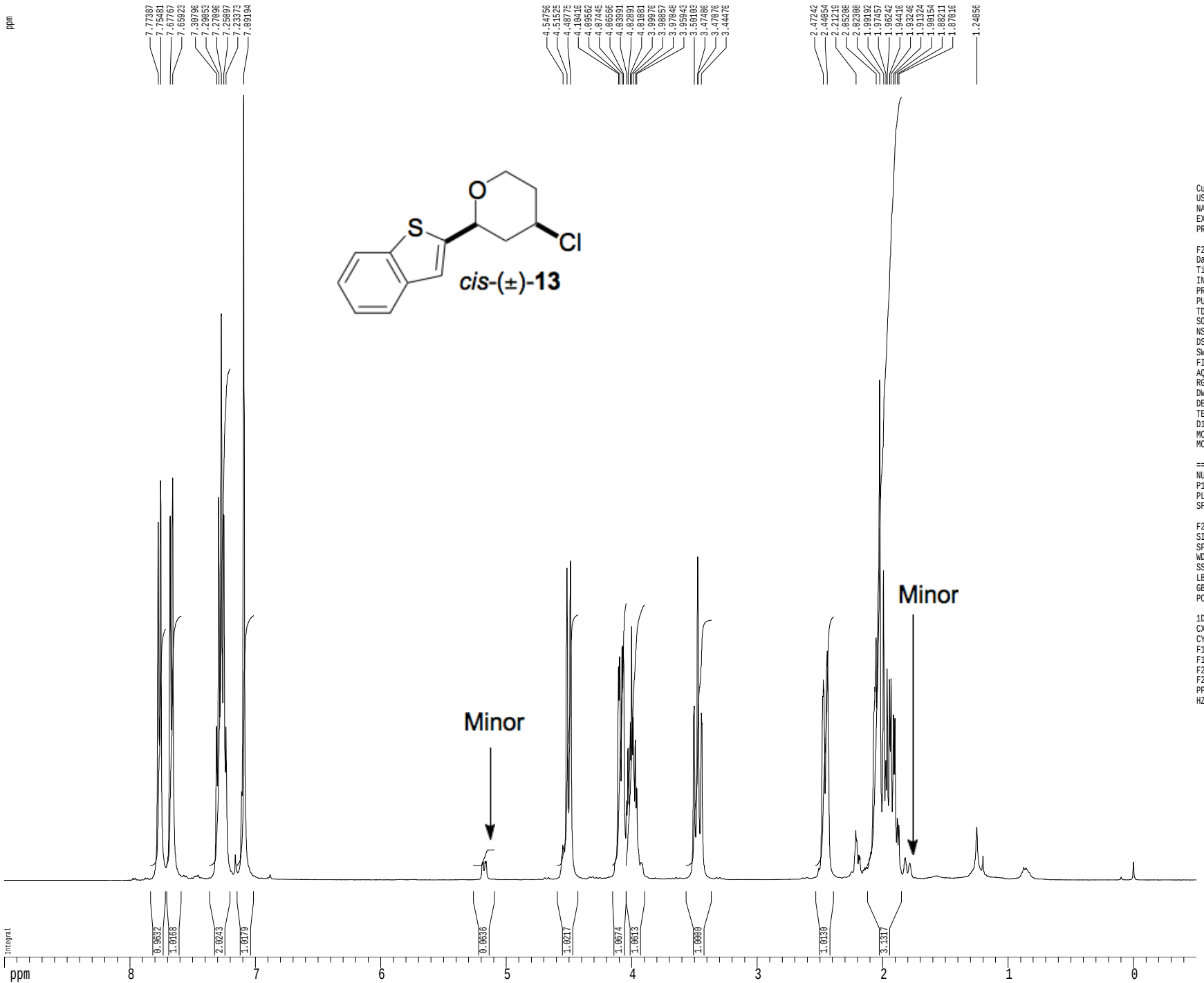
======== CHANNEL f1 ========
NUC1                   1H
P1                  7.50 usec
p3                 22.50 usec
p4                 30.00 usec
p5                 20.00 usec
P12               40000.00 usec
PL1                 1.60 dB
SFO1          500.2225869 MHz
SP1                61.60 dB
SPNAM1         gauss1.512
SPOFF1              0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1           sine.100
GPNAM2           sine.100
GPNAM3           sine.100
GPNAM4           sine.100
GPX1                0.00 %
GPX2                0.00 %
GPX3                0.00 %
GPX4                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPY3                0.00 %
GPY4                0.00 %
GPZ1                7.00 %
GPZ2                3.00 %
GPZ3                2.30 %
GPZ4               -2.30 %
P16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF            500.2200000 MHz
WDW                    EM
SSB                     0
LB                  1.00 Hz
GB                      0
PC                  1.00

1D NMR plot parameters
CX                 22.80 cm
CY                 50.00 cm
F1P                 9.000 ppm
F1               4501.98 Hz
F2P                -0.500 ppm
F2               -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42500 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              lucase
NAME      LWE-II-239-D1
EXPNO                1
PROCNO               1

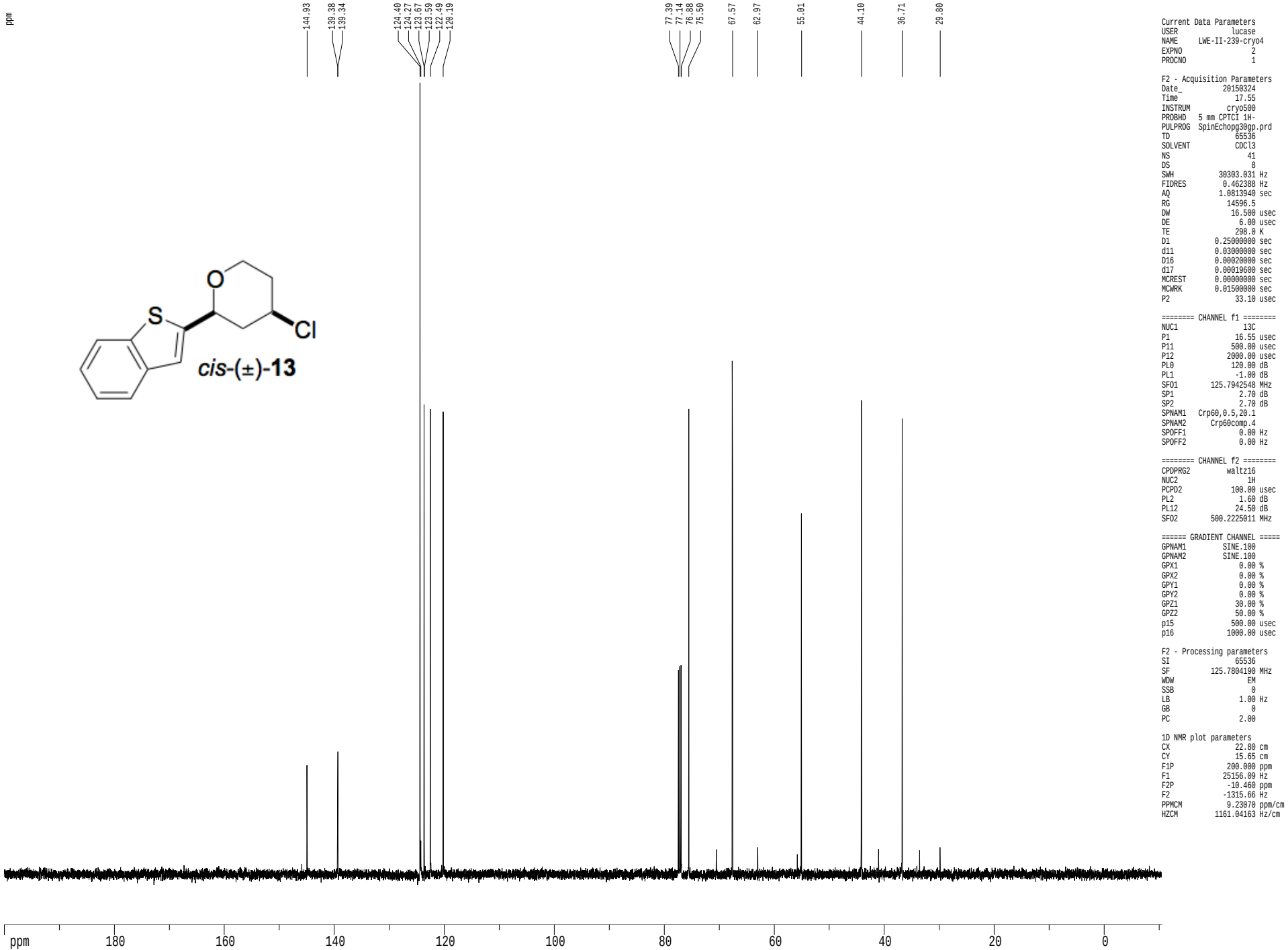
F2 - Acquisition Parameters
Date_          20150126
Time               8.59
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG            zg30
TD                25640
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            6410.256 Hz
FIDRES         0.250010 Hz
AQ             1.9999700 sec
RG                   32
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                0.00 dB
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300605 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              3601.17 Hz
F2P              -0.500 ppm
F2             -200.06 Hz
PPMCM          0.41667 ppm/cm
HZCM          166.72087 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-239-cryo4
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150324
Time                17.55
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                     41
DS                      8
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                14596.5
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                 33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

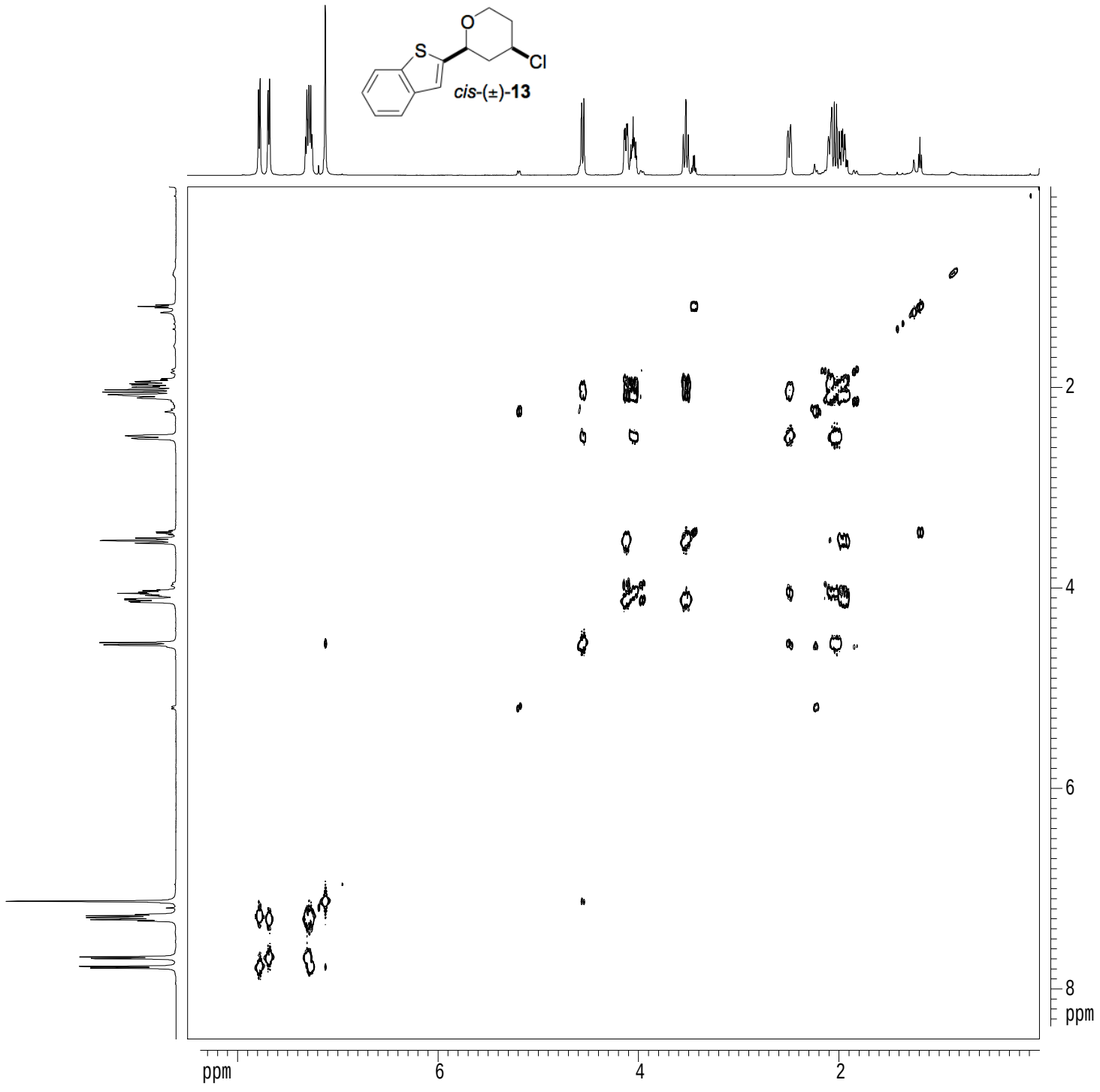
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== 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           125.7804190 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.65 cm
F1P              200.000 ppm
F1             25156.09 Hz
F2P              -10.460 ppm
F2             -1315.66 Hz
PPMCM            9.23070 ppm/cm
HZCM          1161.04163 Hz/cm
```

gcosy60




```
        Current Data Parameters
 USER             lucase
NAME      LWE-II-239-cryo2
 EXPNO                4
 PROCNO               1

      F2 - Acquisition Parameters
 Date_          20150310
 Time              19.12
 INSTRUM         cryo500
 PROBHD   5 mm CPTCI 1H-
 PULPROG    cosygp60.prd
 TD                2048
 SOLVENT           CDCl3
 NS                   2
 DS                  16
 SWH           4251.701 Hz
 FIDRES        2.076026 Hz
 AQ            0.2408948 sec
 RG                25.4
 DW             117.600 usec
 DE               6.00 usec
 TE               298.0 K
 d0           0.00000300 sec
 D1           1.00000000 sec
 d13          0.00000300 sec
 D16          0.00020000 sec
 IN0          0.00023520 sec

     ======== CHANNEL f1 ========
 NUC1                1H
 P1                7.50 usec
 PL1               1.60 dB
 SFO1       500.2221259 MHz

     ====== GRADIENT CHANNEL =====
 GPNAM1         sine.100
 GPNAM2         sine.100
 GPX1              0.00 %
 GPX2              0.00 %
 GPY1              0.00 %
 GPY2              0.00 %
 GPZ1             17.00 %
 GPZ2             17.00 %
 P16            1000.00 usec

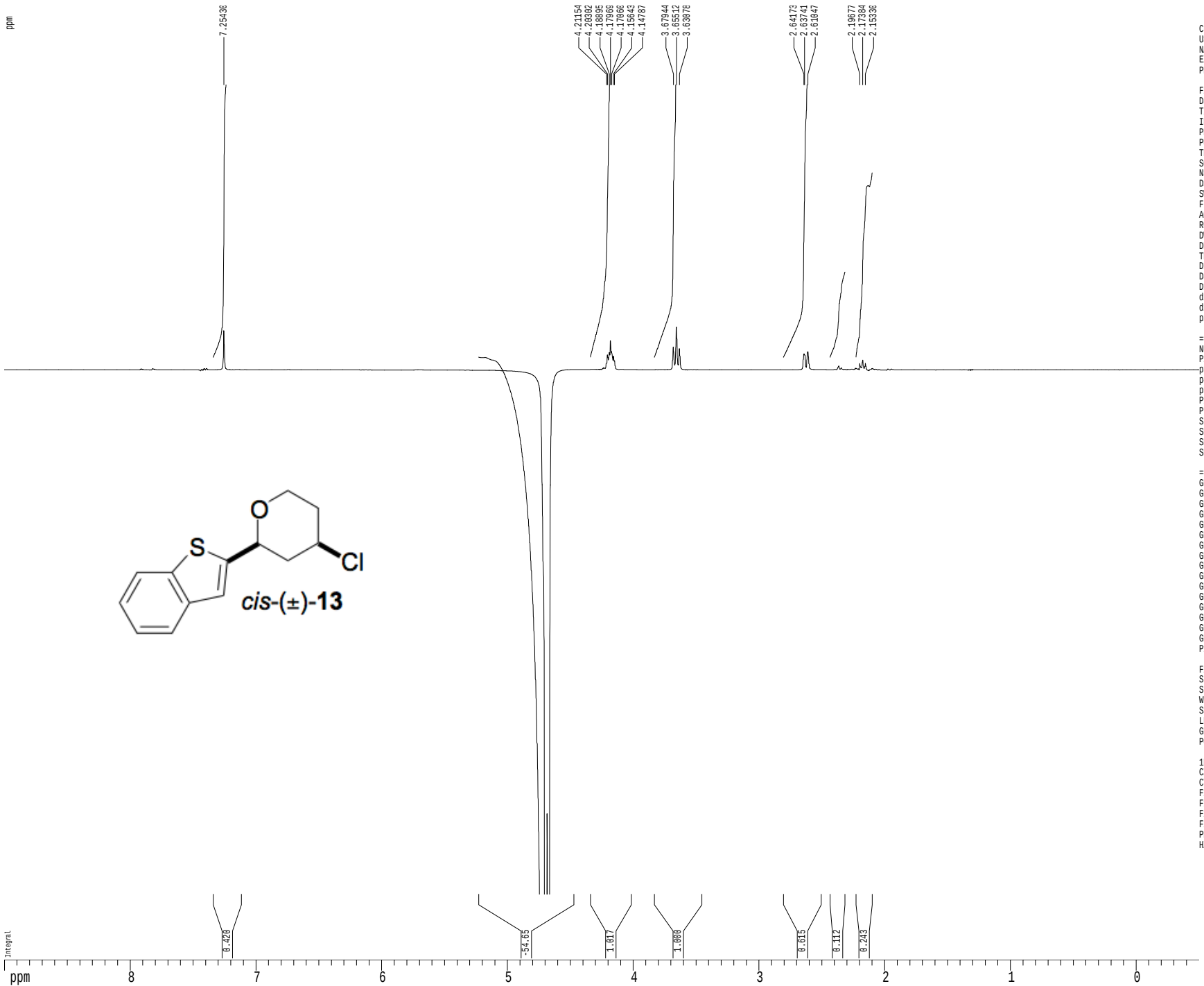
      F1 - Acquisition parameters
 ND0                  1
 TD                 128
 SFO1          500.2221 MHz
 FIDRES        33.216412 Hz
 SW                8.500 ppm
 FnMODE        undefined

      F2 - Processing parameters
 SI                1024
 SF          500.2200653 MHz
 WDW               SINE
 SSB                  0
 LB                0.00 Hz
 GB                   0
 PC                2.00

      F1 - Processing parameters
 SI                1024
 MC2                 QF
 SF          500.2200653 MHz
 WDW               SINE
 SSB                  0
 LB                0.00 Hz
 GB                   0

       2D NMR plot parameters
 CX2              15.00 cm
 CX1              15.00 cm
 F2PLO             8.500 ppm
 F2LO           4251.78 Hz
 F2PHI             0.000 ppm
 F2HI              0.08 Hz
 F1PLO             8.500 ppm
 F1LO           4251.78 Hz
 F1PHI             0.000 ppm
 F1HI              0.08 Hz
 F2PPMCM         0.56664 ppm/cm
 F2HZCM        283.44675 Hz/cm
 F1PPMCM         0.56664 ppm/cm
 F1HZCM        283.44675 Hz/cm
```

gnoe



Current Data Parameters
USER lucase
NAME LWE-II-239-cryo2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150310
Time 19.10
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 40.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

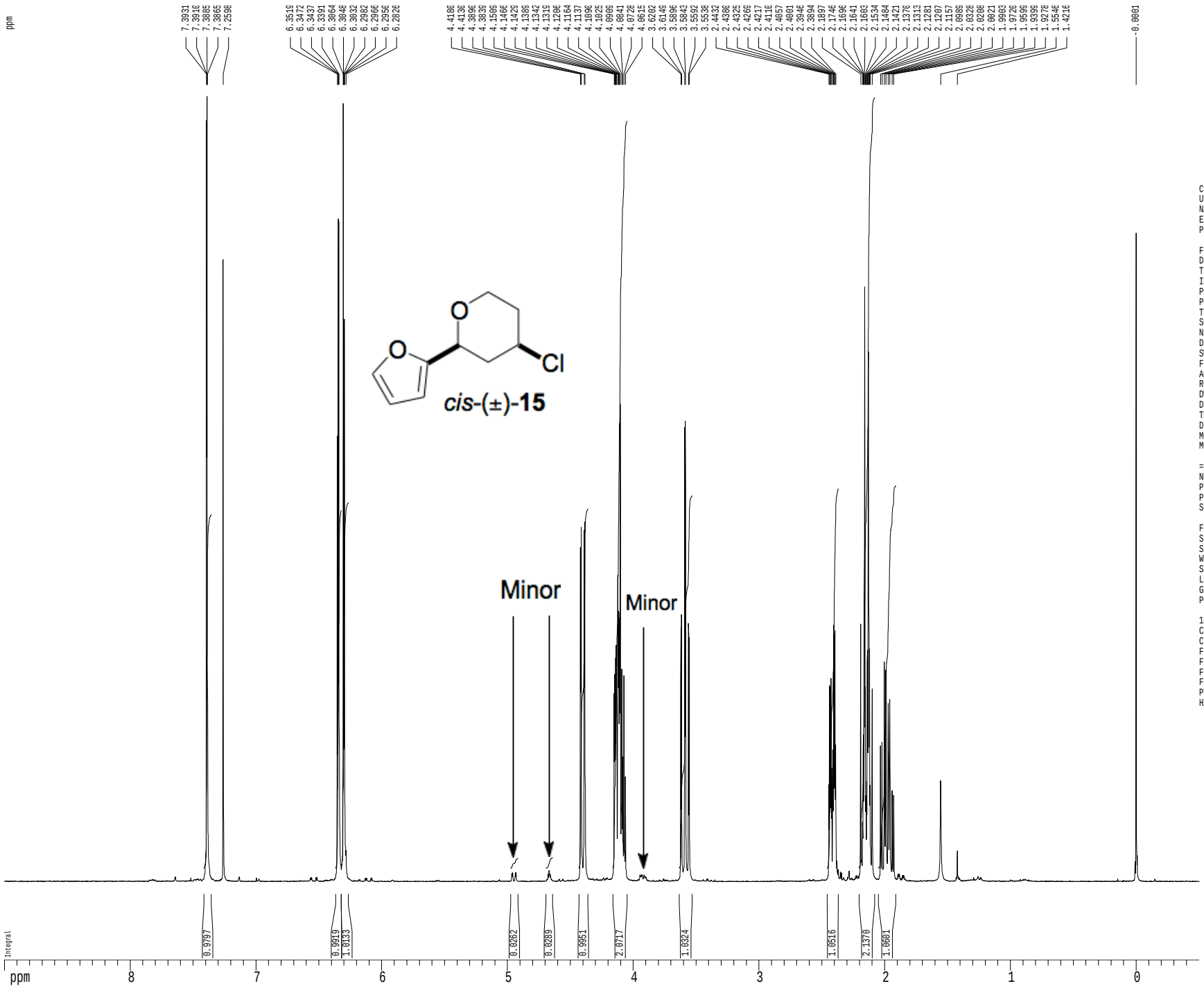
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2223454 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

PI Jarvo
h1 CDCl3 v emilyt 108




```
Current Data Parameters
USER              emilyt
NAME      EJT-V-040-A auto
EXPNO                1
PROCNO               1

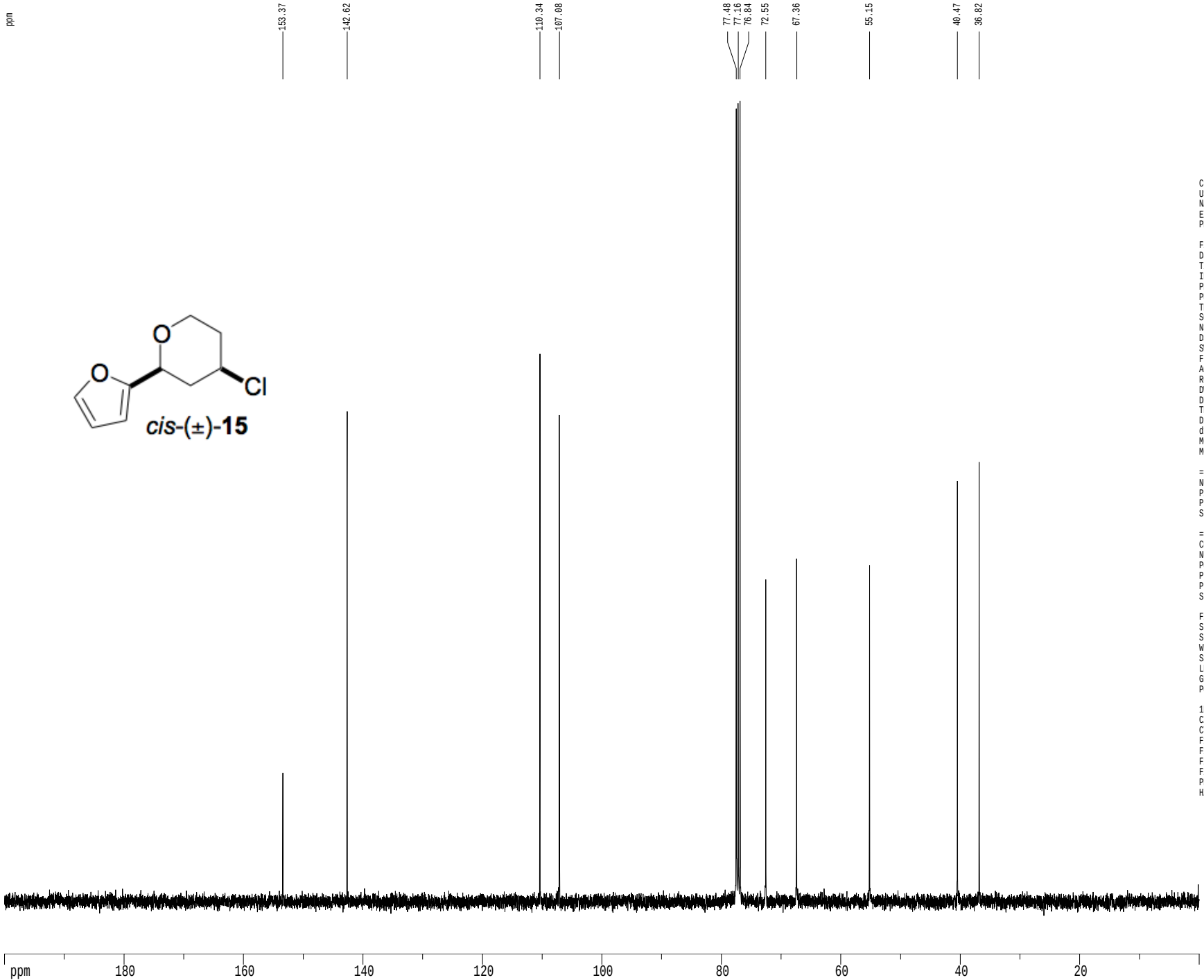
F2 - Acquisition Parameters
Date_          20150410
Time               4.32
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG            zg30
TD                73274
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            7183.908 Hz
FIDRES        0.098042 Hz
AQ            5.0999203 sec
RG                  256
DW               69.600 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                0.00 dB
SFO1         400.1328009 MHz

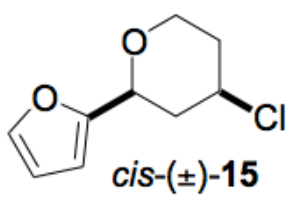
F2 - Processing parameters
SI                65536
SF          400.1300209 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              3601.17 Hz
F2P              -0.500 ppm
F2              -200.06 Hz
PPMCM          0.41667 ppm/cm
HZCM          166.72086 Hz/cm
```

PI Jarvo
c13 CDCl3 v emilyt 108



gcosy60



cis-(±)-**15**


```
        Current Data Parameters
 USER            emilyt
NAME     EJT-IV-266-A char
 EXPNO                3
 PROCNO               1

      F2 - Acquisition Parameters
 Date_          20141222
 Time               0.19
 INSTRUM         cryo500
 PROBHD   5 mm CPTCI 1H-
 PULPROG    cosygp60.prd
 TD                 2048
 SOLVENT           CDCl3
 NS                    2
 DS                   16
 SWH            4734.849 Hz
 FIDRES         2.311938 Hz
 AQ             0.2163188 sec
 RG                35.9
 DW              105.600 usec
 DE                6.00 usec
 TE               298.0 K
 d0            0.00000300 sec
 D1            1.00000000 sec
 d13           0.00000300 sec
 D16           0.00020000 sec
 IN0           0.00021120 sec

     ======== CHANNEL f1 ========
 NUC1                 1H
 P1                 7.50 usec
 PL1                1.60 dB
 SFO1        500.2221588 MHz

     ====== GRADIENT CHANNEL =====
 GPNAM1          sine.100
 GPNAM2          sine.100
 GPX1               0.00 %
 GPX2               0.00 %
 GPY1               0.00 %
 GPY2               0.00 %
 GPZ1              17.00 %
 GPZ2              17.00 %
 P16             1000.00 usec

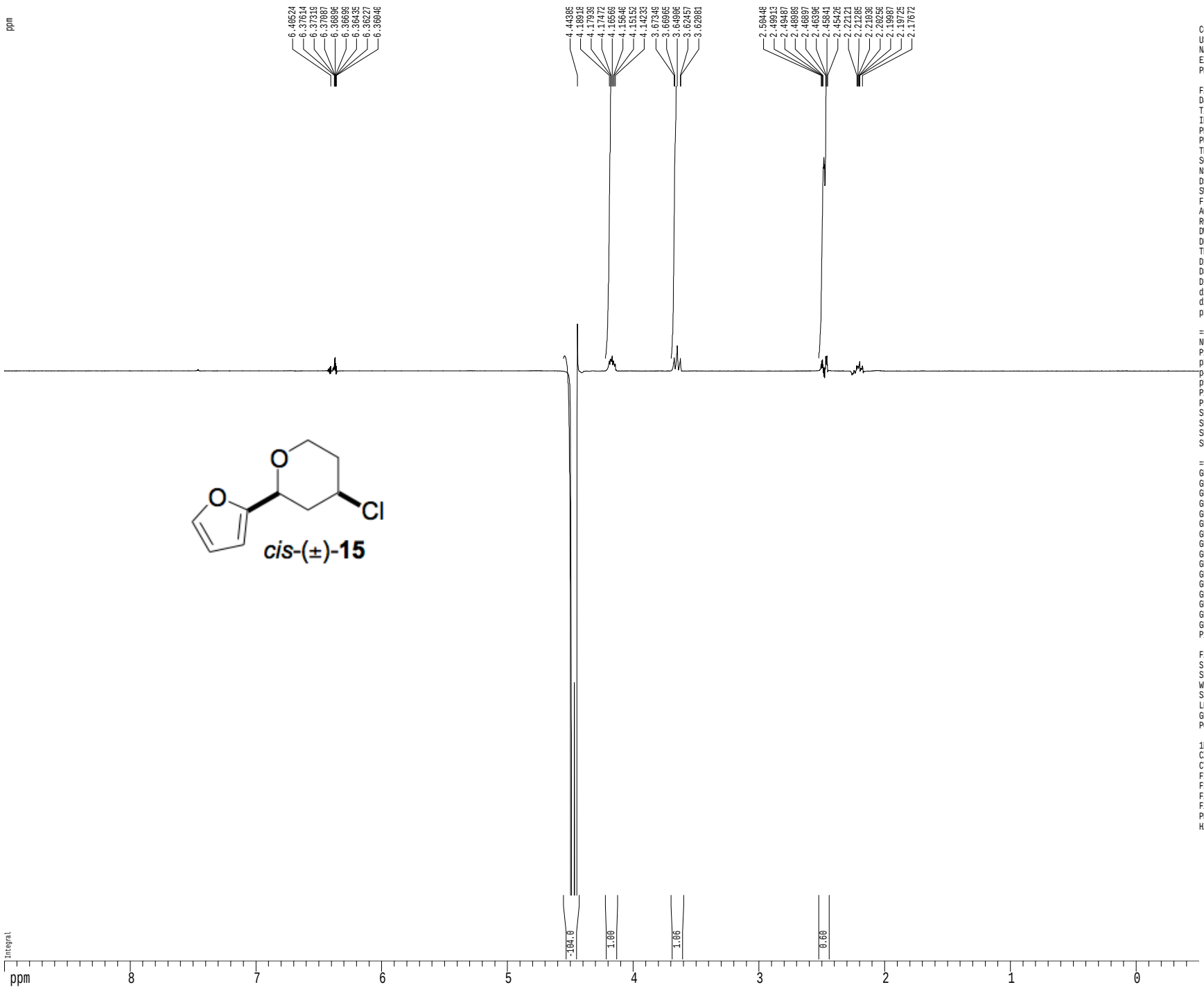
      F1 - Acquisition parameters
 ND0                  1
 TD                 256
 SFO1          500.2222 MHz
 FIDRES        18.495502 Hz
 SW                9.465 ppm
 FnMODE        undefined

      F2 - Processing parameters
 SI                 1024
 SF          500.2200329 MHz
 WDW                SINE
 SSB                   0
 LB                 0.00 Hz
 GB                    0
 PC                 2.00

      F1 - Processing parameters
 SI                 1024
 MC2                  QF
 SF          500.2200329 MHz
 WDW                SINE
 SSB                   0
 LB                 0.00 Hz
 GB                    0

       2D NMR plot parameters
 CX2               15.00 cm
 CX1               15.00 cm
 F2PLO              8.983 ppm
 F2LO            4493.36 Hz
 F2PHI             -0.483 ppm
 F2HI            -241.49 Hz
 F1PLO              8.983 ppm
 F1LO            4493.36 Hz
 F1PHI             -0.483 ppm
 F1HI            -241.49 Hz
 F2PPMCM          0.63104 ppm/cm
 F2HZCM         315.65659 Hz/cm
 F1PPMCM          0.63104 ppm/cm
 F1HZCM         315.65659 Hz/cm
```

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-266-A char
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141222
Time 0.55
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

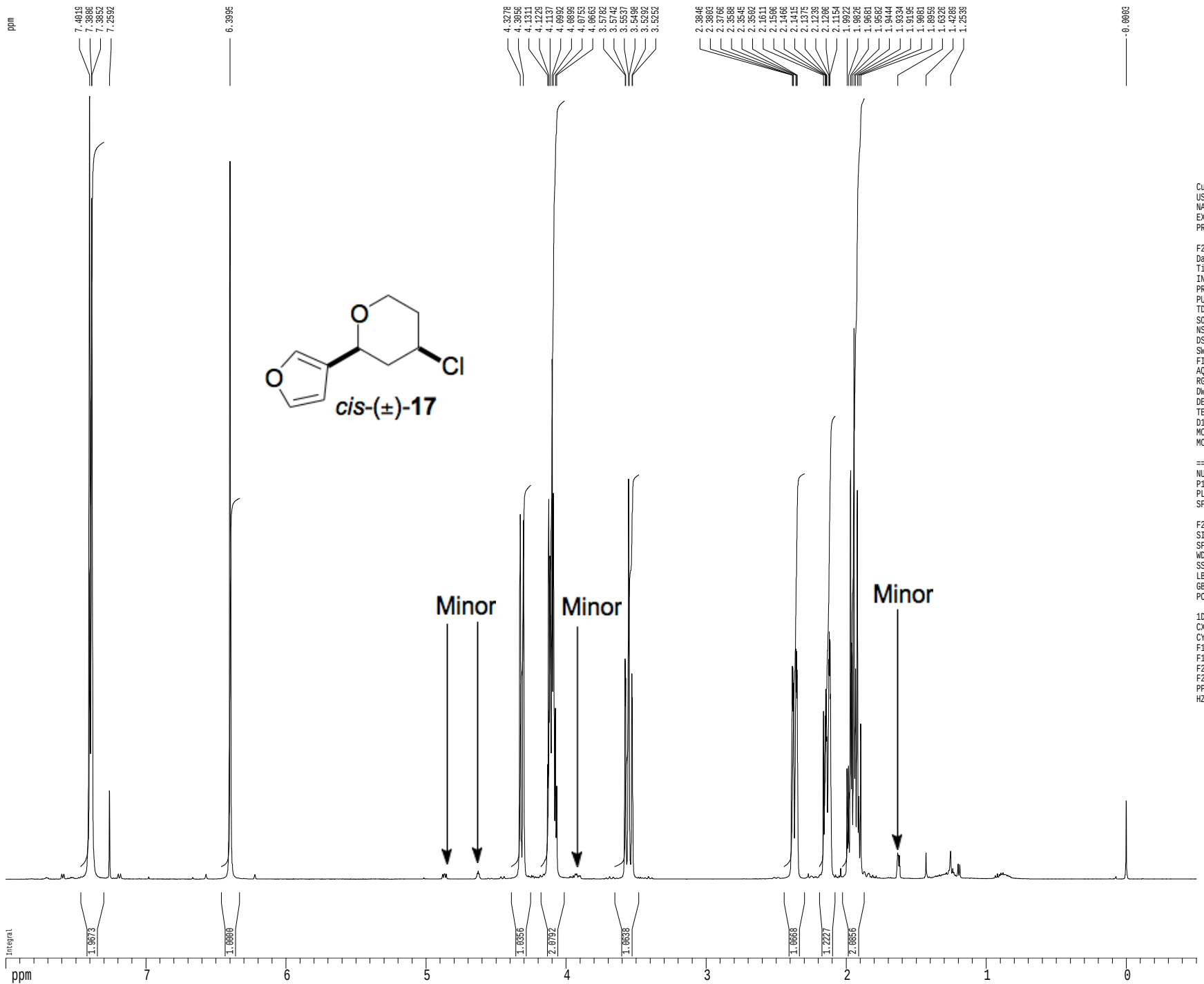
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2222317 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-237-cryo
EXPNO                    5
PROCNO                   1

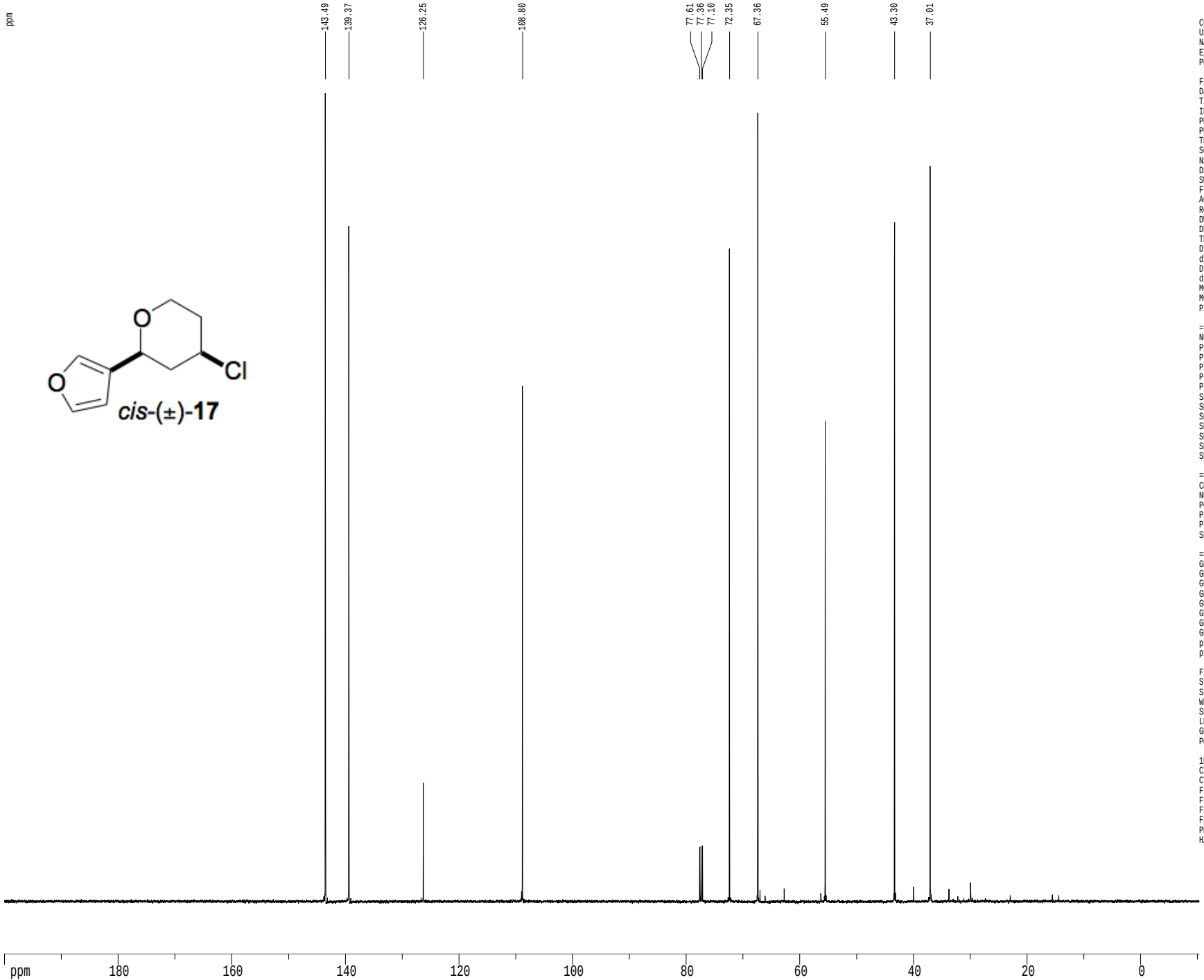
F2 - Acquisition Parameters
Date_            20150212
Time                17.58
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  48074
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.166677 Hz
AQ               2.9998677 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           500.2200311 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 8.000 ppm
F1                4001.76 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.37281 ppm/cm
HZCM           186.48555 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-237-cryo
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150128
Time                 19.57
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                      89
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                  2.70 dB
SP2                  2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

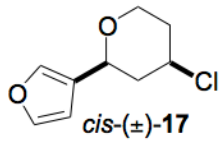
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12               24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7803995 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               200.000 ppm
F1              25156.08 Hz
F2P               -10.305 ppm
F2              -1296.19 Hz
PPMCM             9.22391 ppm/cm
HZCM          1160.18762 Hz/cm
```

gcosy60



cis-(±)-**17**


```
        Current Data Parameters
USER              lucase
NAME      LWE-II-237-cryo
EXPNO                  2
PROCNO                 1

      F2 - Acquisition Parameters
Date_           20150128
Time              19.10
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG    cosygp60.prd
TD                2048
SOLVENT           CDCl3
NS                   2
DS                  16
SWH            3591.954 Hz
FIDRES         1.753884 Hz
AQ             0.2851316 sec
RG                25.4
DW              139.200 usec
DE                6.00 usec
TE               298.0 K
d0            0.00000300 sec
D1            1.00000000 sec
d13           0.00000300 sec
D16           0.00020000 sec
IN0           0.00027840 sec

     ======== CHANNEL f1 ========
NUC1                 1H
P1                 7.50 usec
PL1                1.60 dB
SFO1         500.2218008 MHz

     ====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPX1               0.00 %
GPX2               0.00 %
GPY1               0.00 %
GPY2               0.00 %
GPZ1              17.00 %
GPZ2              17.00 %
P16             1000.00 usec

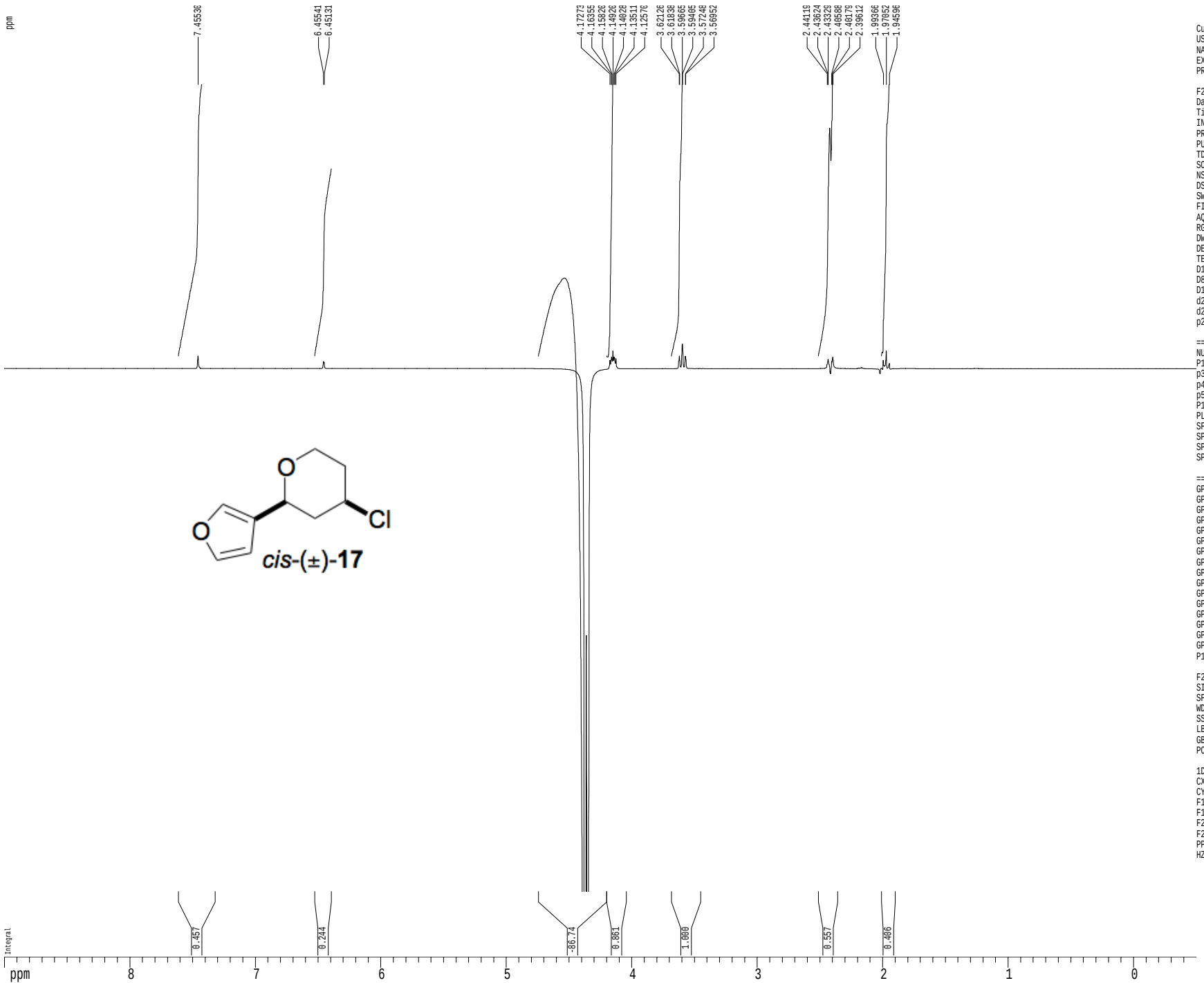
      F1 - Acquisition parameters
ND0                  1
TD                 256
SFO1          500.2218 MHz
FIDRES        14.031071 Hz
SW                7.181 ppm
FnMODE        undefined

      F2 - Processing parameters
SI                1024
SF          500.2200312 MHz
WDW               SINE
SSB                  0
LB                0.00 Hz
GB                   0
PC                4.00

      F1 - Processing parameters
SI                1024
MC2                 QF
SF          500.2200312 MHz
WDW               SINE
SSB                  0
LB                0.00 Hz
GB                   0

        2D NMR plot parameters
CX2              15.00 cm
CX1              15.00 cm
F2PLO             7.190 ppm
F2LO           3596.77 Hz
F2PHI             0.010 ppm
F2HI              4.81 Hz
F1PLO             7.190 ppm
F1LO           3596.77 Hz
F1PHI             0.010 ppm
F1HI              4.81 Hz
F2PPMCM         0.47872 ppm/cm
F2HZCM        239.46361 Hz/cm
F1PPMCM         0.47872 ppm/cm
F1HZCM        239.46361 Hz/cm
```

gnoe




```
Current Data Parameters
USER                lucase
NAME      LWE-II-237-cryo
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150128
Time                19.54
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    256
DS                      8
SWH              6009.615 Hz
FIDRES           0.091699 Hz
AQ               5.4526453 sec
RG                   45.3
DW                 83.200 usec
DE                  6.00 usec
TE                298.0 K
D1              1.00000000 sec
D8              0.50000000 sec
D16             0.00020000 sec
d21             0.33376500 sec
d22             0.16399699 sec
p2                 15.00 usec

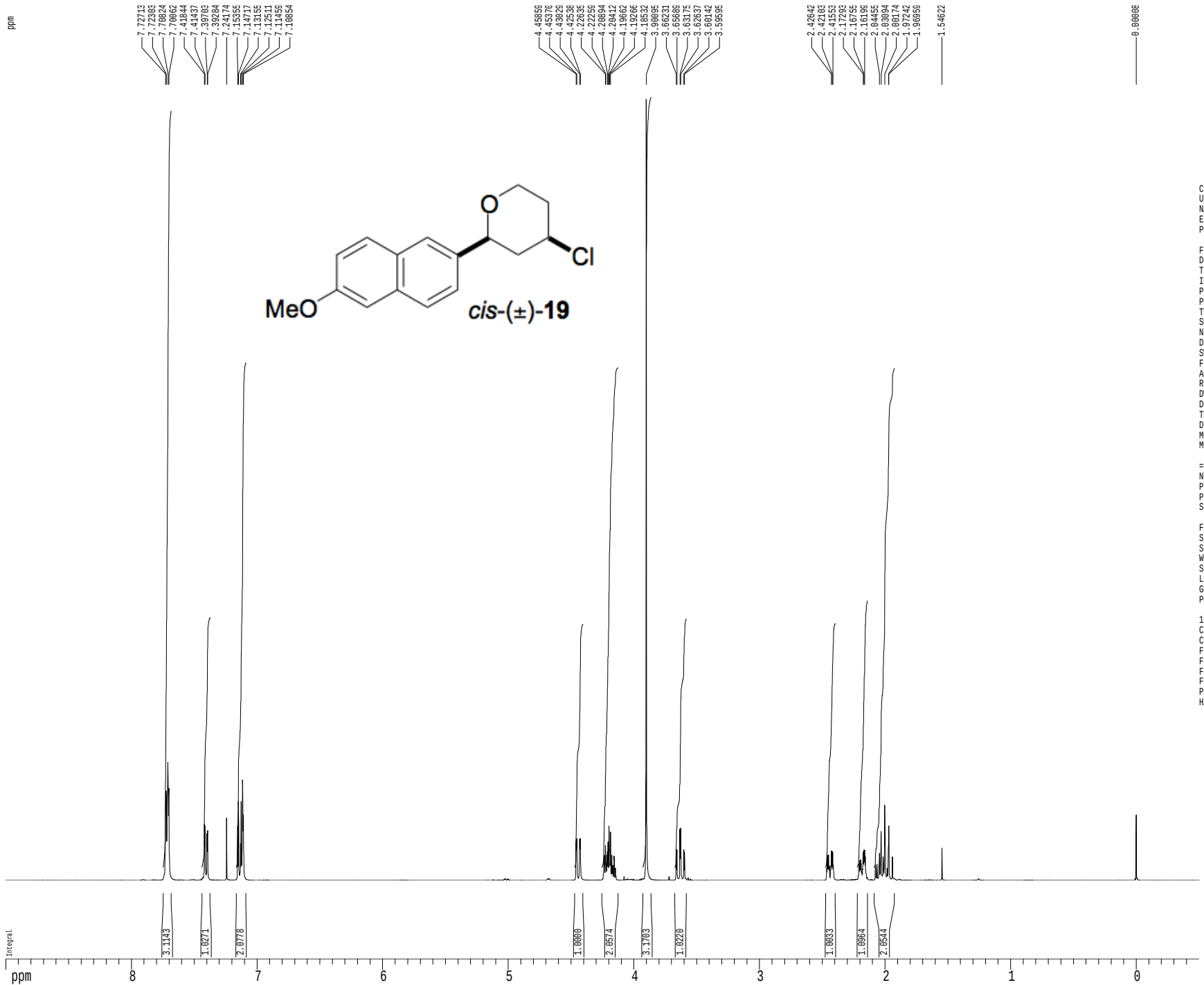
======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
p3                  22.50 usec
p4                  30.00 usec
p5                  20.00 usec
P12               40000.00 usec
PL1                  1.60 dB
SFO1          500.2221824 MHz
SP1                 61.60 dB
SPNAM1         gauss1.512
SPOFF1               0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1           sine.100
GPNAM2           sine.100
GPNAM3           sine.100
GPNAM4           sine.100
GPX1                 0.00 %
GPX2                 0.00 %
GPX3                 0.00 %
GPX4                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPY3                 0.00 %
GPY4                 0.00 %
GPZ1                 7.00 %
GPZ2                 3.00 %
GPZ3                 2.30 %
GPZ4                -2.30 %
P16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF            500.2200000 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  22.80 cm
CY                  50.00 cm
F1P                 9.000 ppm
F1               4501.98 Hz
F2P                -0.500 ppm
F2               -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42500 Hz/cm
```

PI Jarvo
h1 CDCl3 v emilyt 107




```
Current Data Parameters
USER              emilyt
NAME      EJT-IV-232 auto
EXPNO                  1
PROCNO                 1

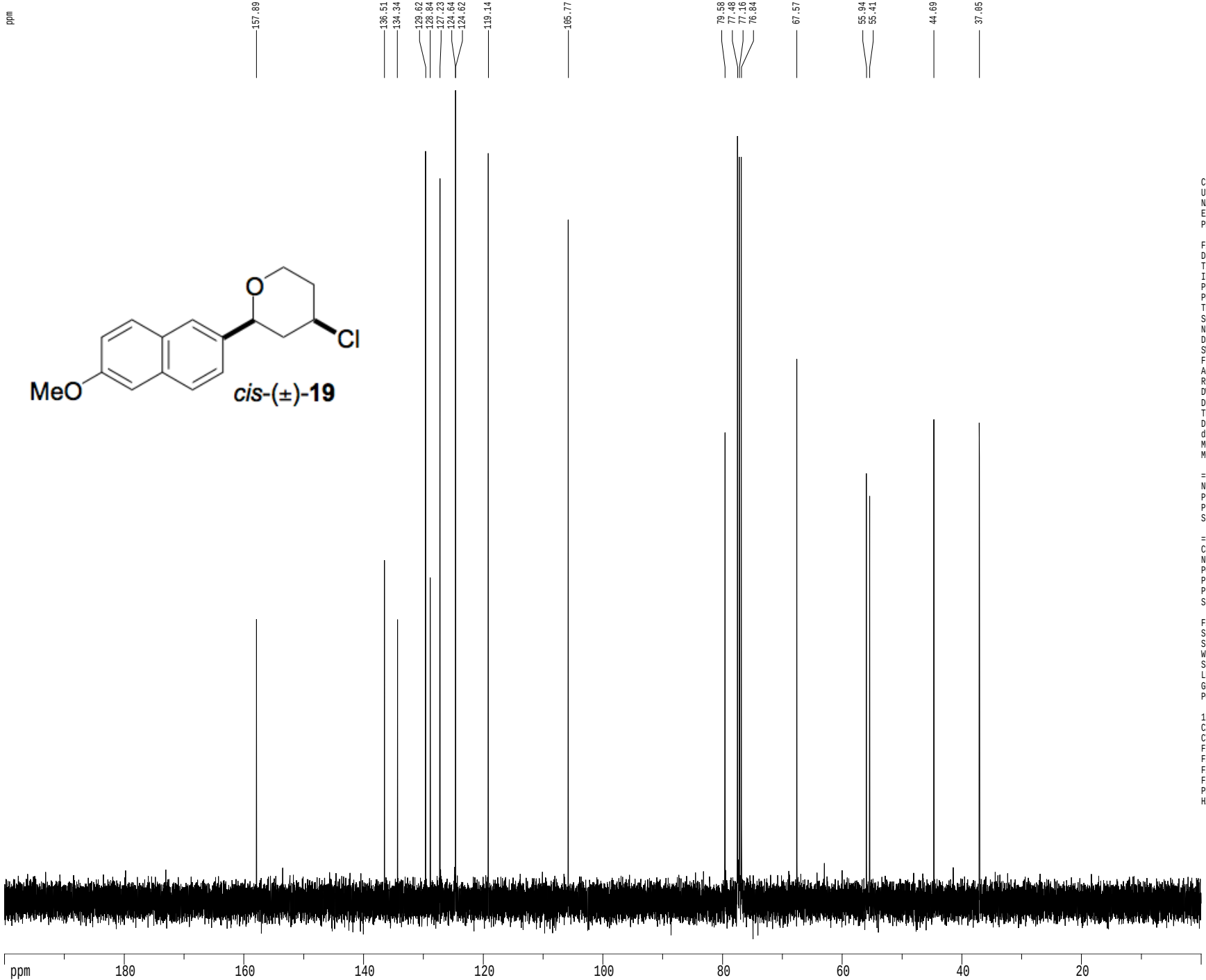
F2 - Acquisition Parameters
Date_          20150410
Time               4.23
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG            zg30
TD                73274
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            7183.908 Hz
FIDRES        0.098042 Hz
AQ            5.0999203 sec
RG                143.7
DW               69.600 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                0.00 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

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              3601.17 Hz
F2P              -0.500 ppm
F2             -200.06 Hz
PPMCM          0.41667 ppm/cm
HZCM          166.72086 Hz/cm
```

13C spectrum with 1H decoupling




```
Current Data Parameters
USER              emilyt
NAME      EJT-IV-232 auto
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150410
Time               21.09
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG          zgdc30
TD                65536
SOLVENT           CDCl3
NS                  294
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

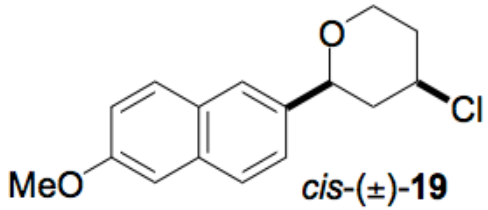
======== CHANNEL f1 ========
NUC1                13C
P1                 7.75 usec
PL1                -3.00 dB
SFO1        100.6237964 MHz

======== CHANNEL f2 ========
CPDPRG2          mlev16
NUC2                1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              17.70 dB
SFO2        400.1328009 MHz

F2 - Processing parameters
SI                 65536
SF           100.6127613 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00

1D NMR plot parameters
CX                22.80 cm
CY                15.50 cm
F1P              200.000 ppm
F1             20122.55 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           8.77193 ppm/cm
HZCM          882.56812 Hz/cm
```

gcosy60



cis-(±)-**19**

Current Data Parameters

USER	emilyt
NAME	EJT-IV-232-noe
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20150131
Time	17.56
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4734.849 Hz
FIDRES	2.311938 Hz
AQ	0.2163188 sec
RG	287.4
DW	105.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00021120 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2221259 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	128
SFO1	500.2221 MHz
FIDRES	36.991005 Hz
SW	9.465 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00

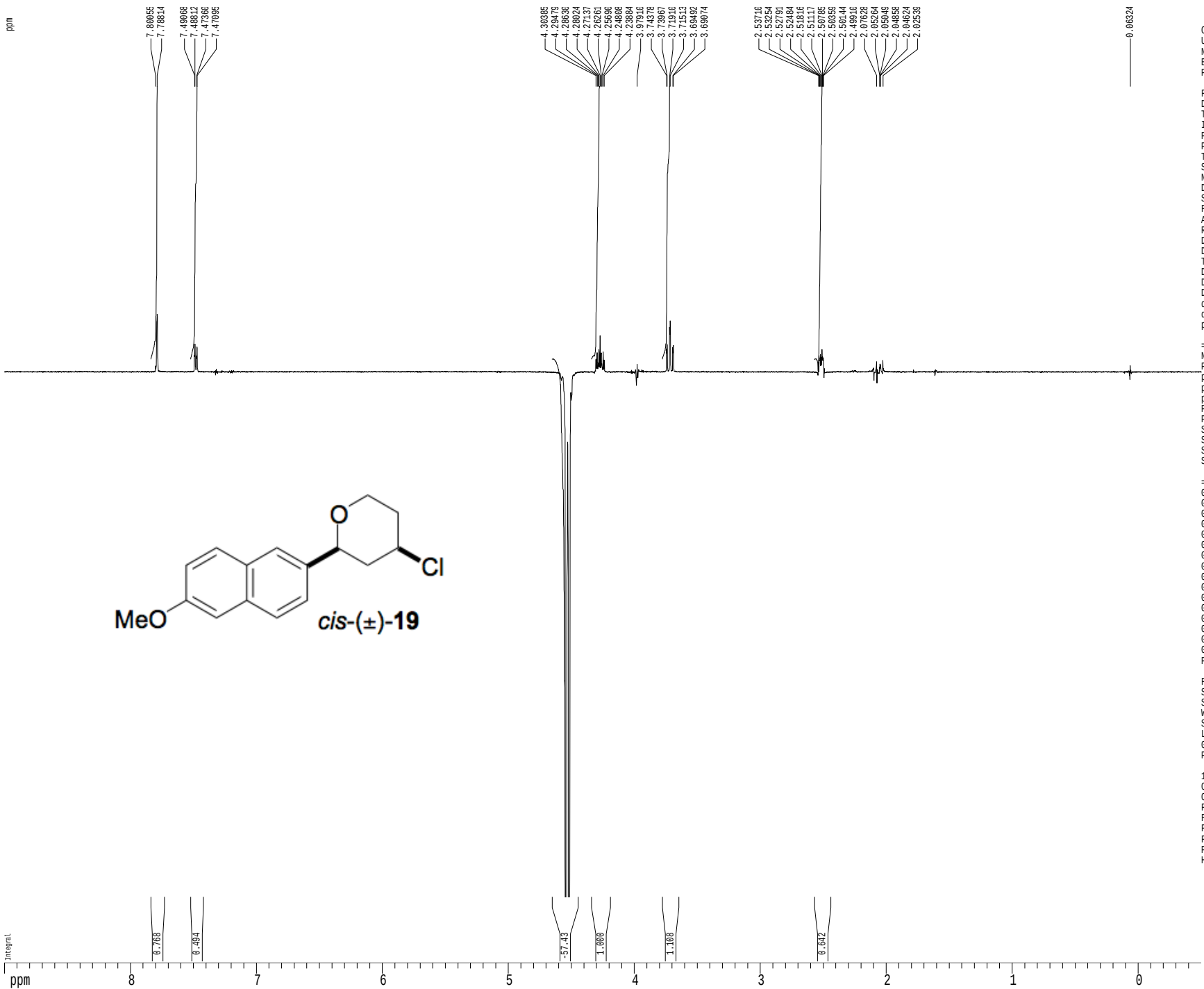
F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.983 ppm
F2LO	4493.36 Hz
F2PHI	-0.483 ppm
F2HI	-241.49 Hz
F1PLO	8.983 ppm
F1LO	4493.36 Hz
F1PHI	-0.483 ppm
F1HI	-241.49 Hz
F2PPMCM	0.63104 ppm/cm
F2HZCM	315.65659 Hz/cm
F1PPMCM	0.63104 ppm/cm
F1HZCM	315.65659 Hz/cm

gnoe




```
Current Data Parameters
USER                emilyt
NAME      EJT-IV-232-noe
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150131
Time                18.15
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                   90.5
DW                 62.400 usec
DE                  6.00 usec
TE                298.0 K
D1              1.00000000 sec
D8              0.50000000 sec
D16             0.00020000 sec
d21             0.33376500 sec
d22             0.16399699 sec
p2                 15.00 usec

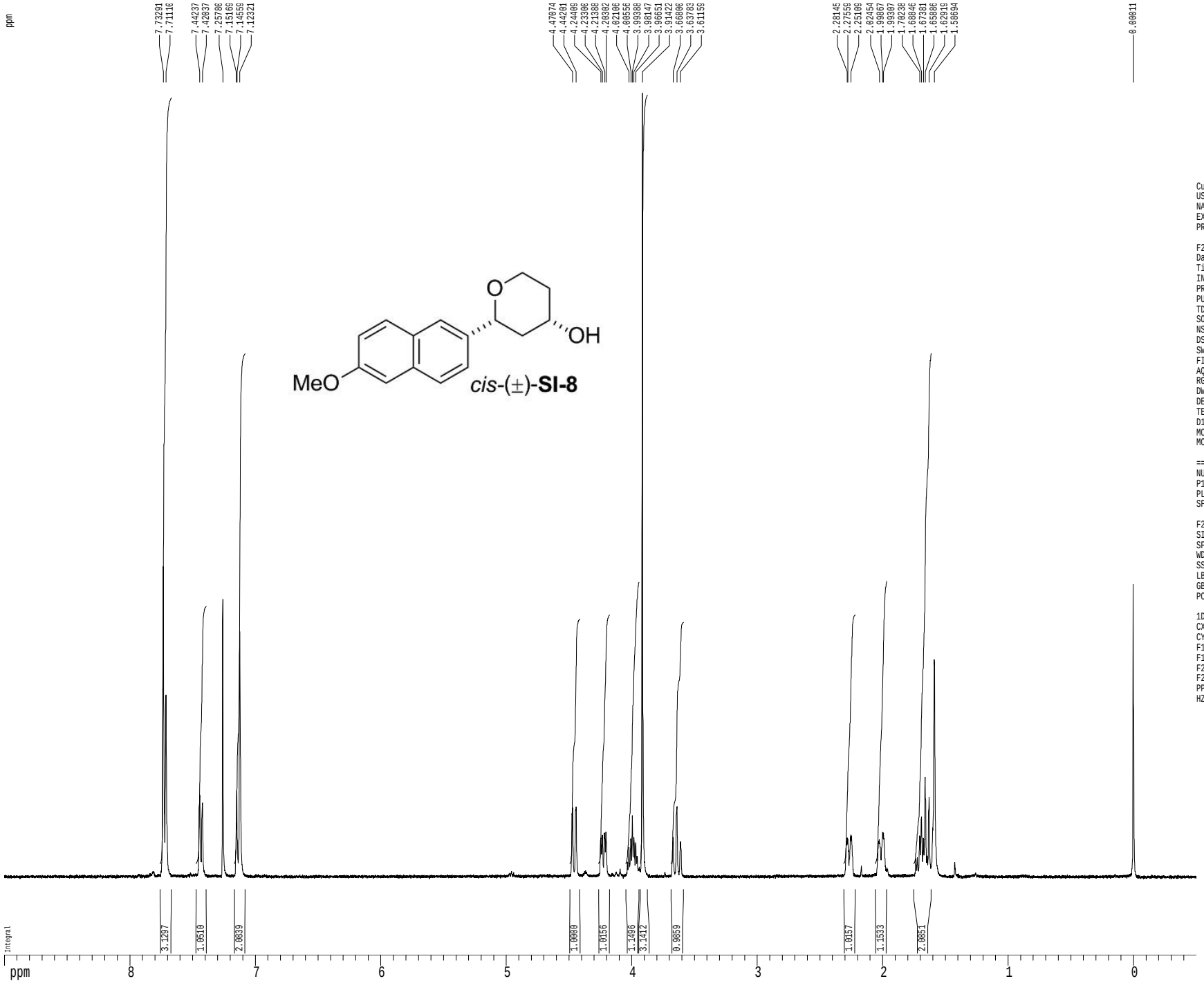
======== CHANNEL f1 ========
NUC1                   1H
P1                   7.50 usec
p3                  22.50 usec
p4                  30.00 usec
p5                  20.00 usec
P12               40000.00 usec
PL1                  1.60 dB
SFO1          500.2222656 MHz
SP1                 61.60 dB
SPNAM1         gauss1.512
SPOFF1               0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1           sine.100
GPNAM2           sine.100
GPNAM3           sine.100
GPNAM4           sine.100
GPX1                 0.00 %
GPX2                 0.00 %
GPX3                 0.00 %
GPX4                 0.00 %
GPY1                 0.00 %
GPY2                 0.00 %
GPY3                 0.00 %
GPY4                 0.00 %
GPZ1                 7.00 %
GPZ2                 3.00 %
GPZ3                 2.30 %
GPZ4                -2.30 %
P16               1000.00 usec

F2 - Processing parameters
SI                  65536
SF            500.2200000 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  22.80 cm
CY                  50.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2               -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42500 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME        EJT-IV-270-A
EXPNO                20
PROCNO                1

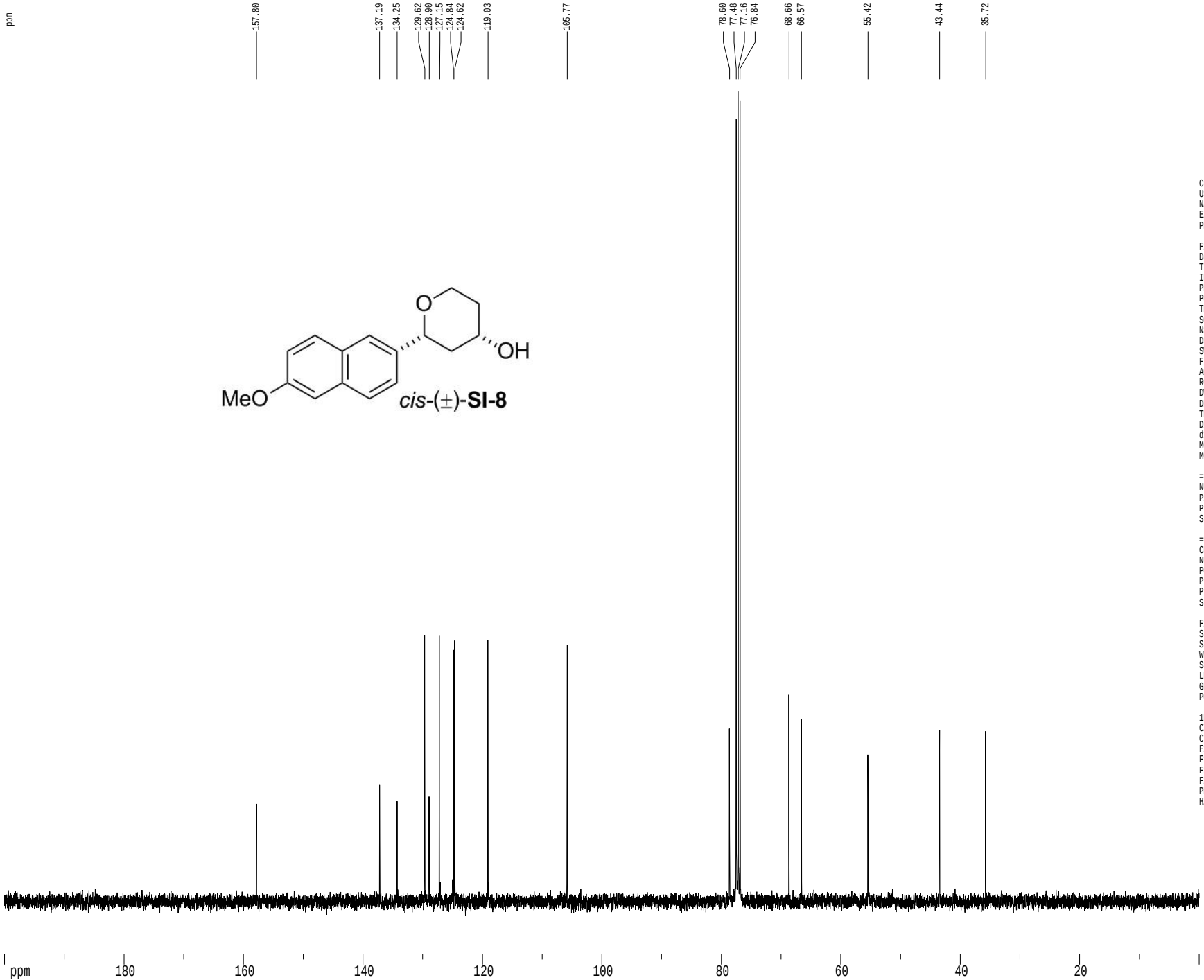
F2 - Acquisition Parameters
Date_          20150410
Time              18.50
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            6410.256 Hz
FIDRES        0.097813 Hz
AQ            5.1118579 sec
RG                456.1
DW               78.000 usec
DE                4.50 usec
TE                298.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                12.00 usec
PL1                0.00 dB
SFO1         400.1328009 MHz

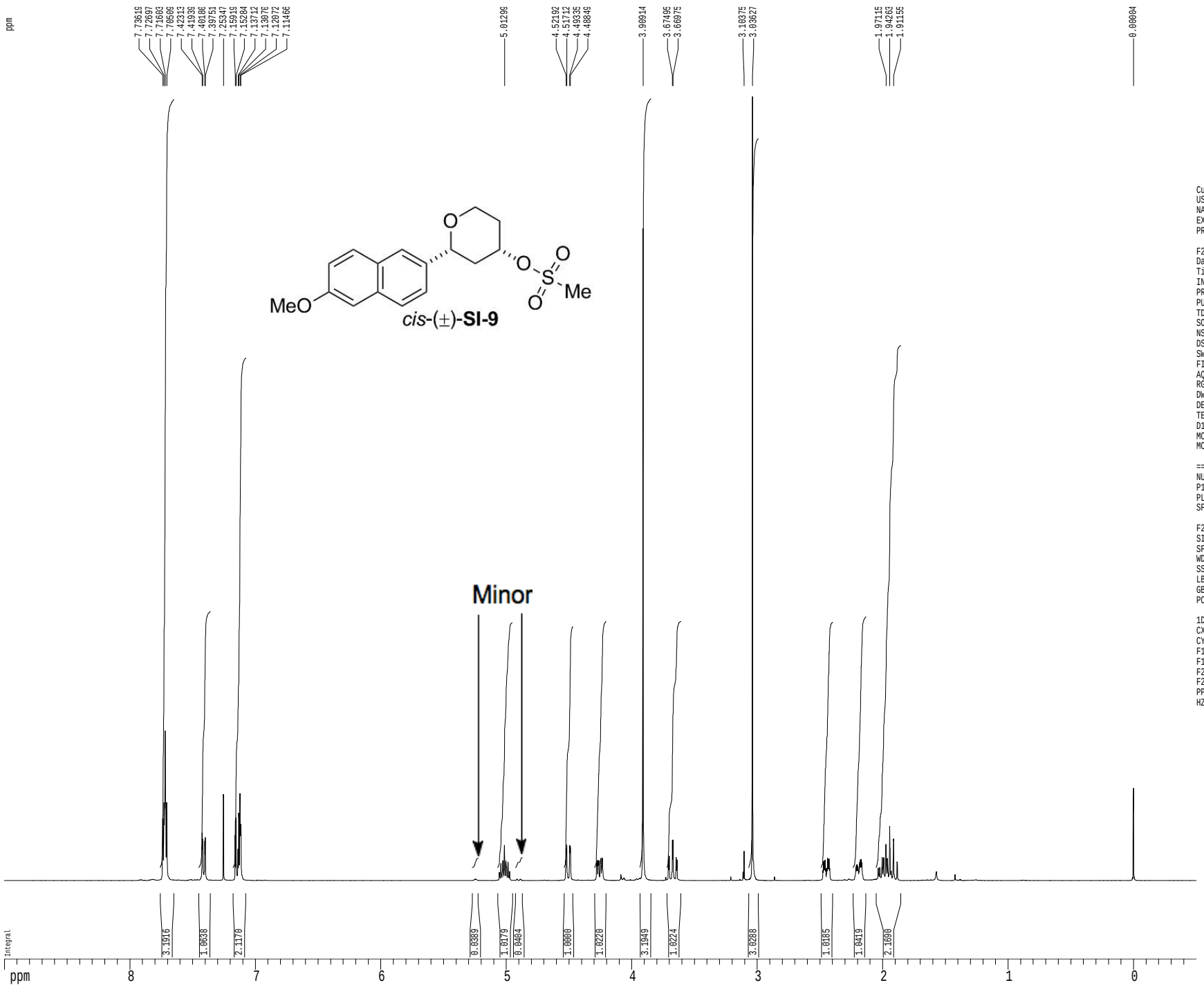
F2 - Processing parameters
SI                65536
SF           400.1300213 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              3601.17 Hz
F2P              -0.500 ppm
F2              -200.06 Hz
PPMCM          0.41667 ppm/cm
HZCM          166.72086 Hz/cm
```

PI Jarvo
c13 CDCl3 v emilyt 106



PI Jarvo
h1 CDCl3 v emilyt 106




```
Current Data Parameters
USER              emilyt
NAME      EJT-IV-271 auto
EXPNO                  1
PROCNO                 1

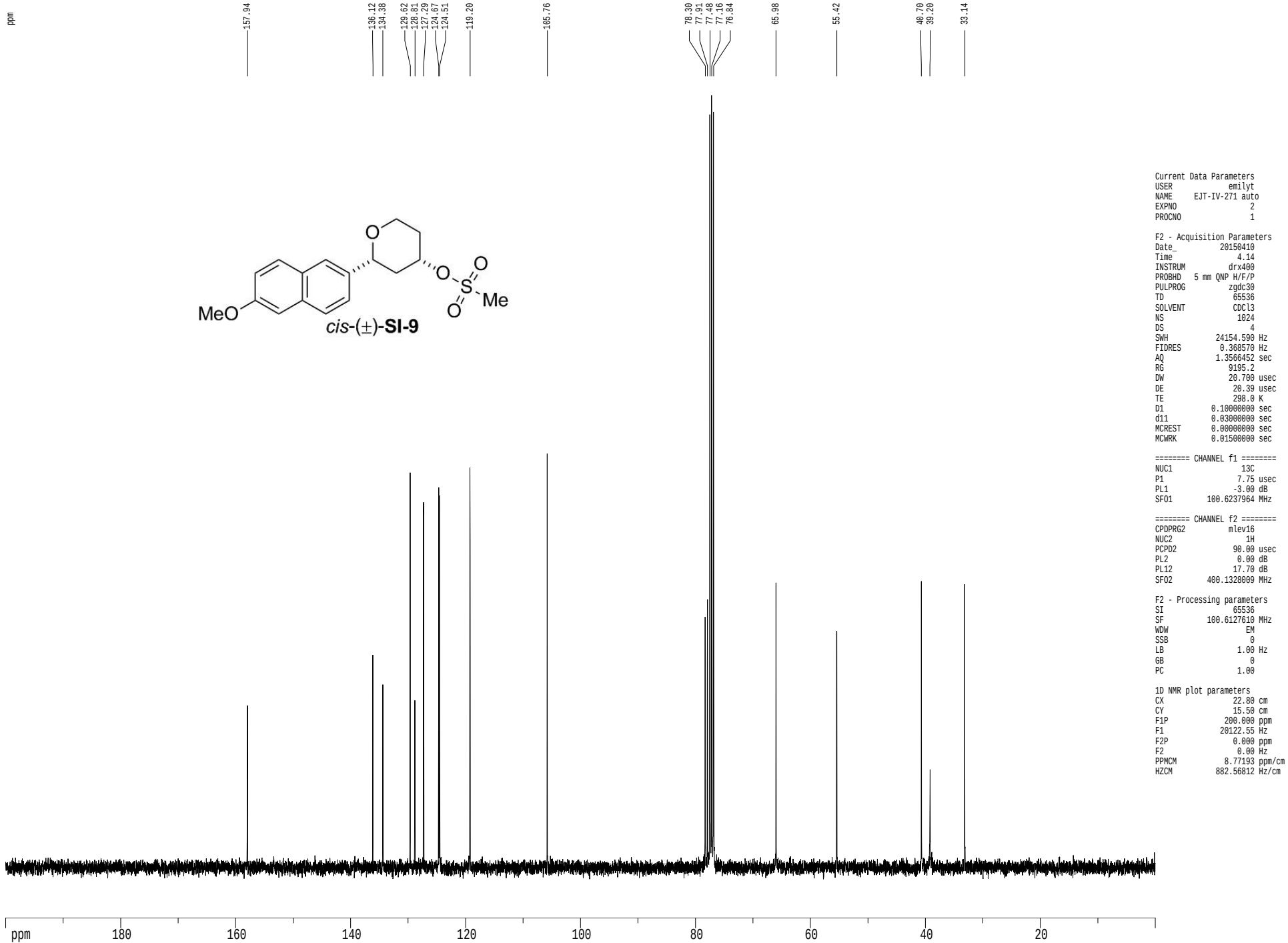
F2 - Acquisition Parameters
Date_          20150410
Time               3.48
INSTRUM          drx400
PROBHD   5 mm QNP H/F/P
PULPROG            zg30
TD                73274
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           7183.908 Hz
FIDRES         0.098042 Hz
AQ            5.0999203 sec
RG                203.2
DW               69.600 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                0.00 dB
SFO1        400.1328009 MHz

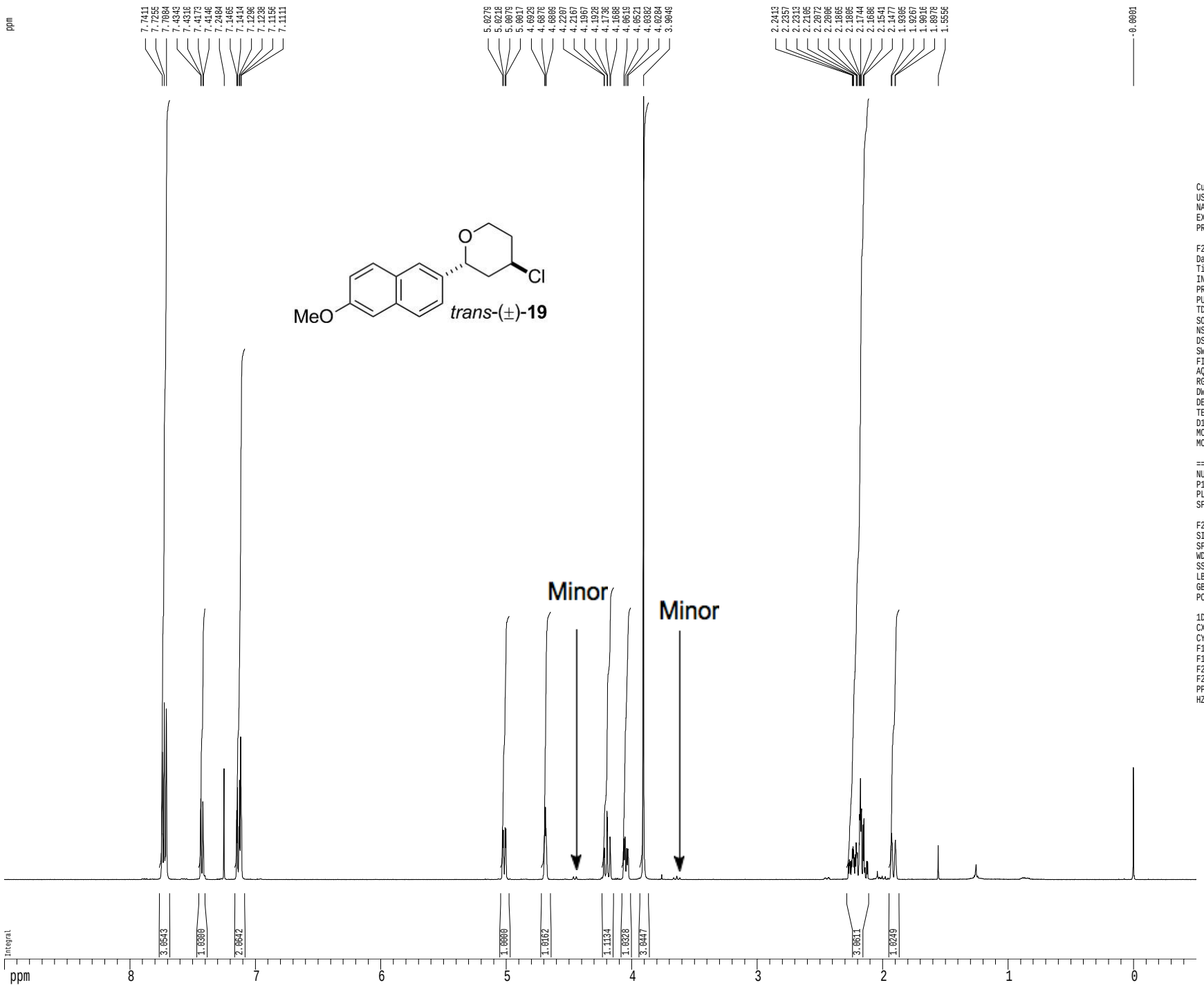
F2 - Processing parameters
SI                 65536
SF          400.1300233 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 2.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1             3601.17 Hz
F2P              -0.500 ppm
F2             -200.06 Hz
PPMCM          0.41667 ppm/cm
HZCM          166.72086 Hz/cm
```

PI Jarvo
c13 CDCl3 v emilyt 106



1H spectrum




```
Current Data Parameters
USER              emilyt
NAME          EJT-IV-273
EXPNO                 20
PROCNO                 1

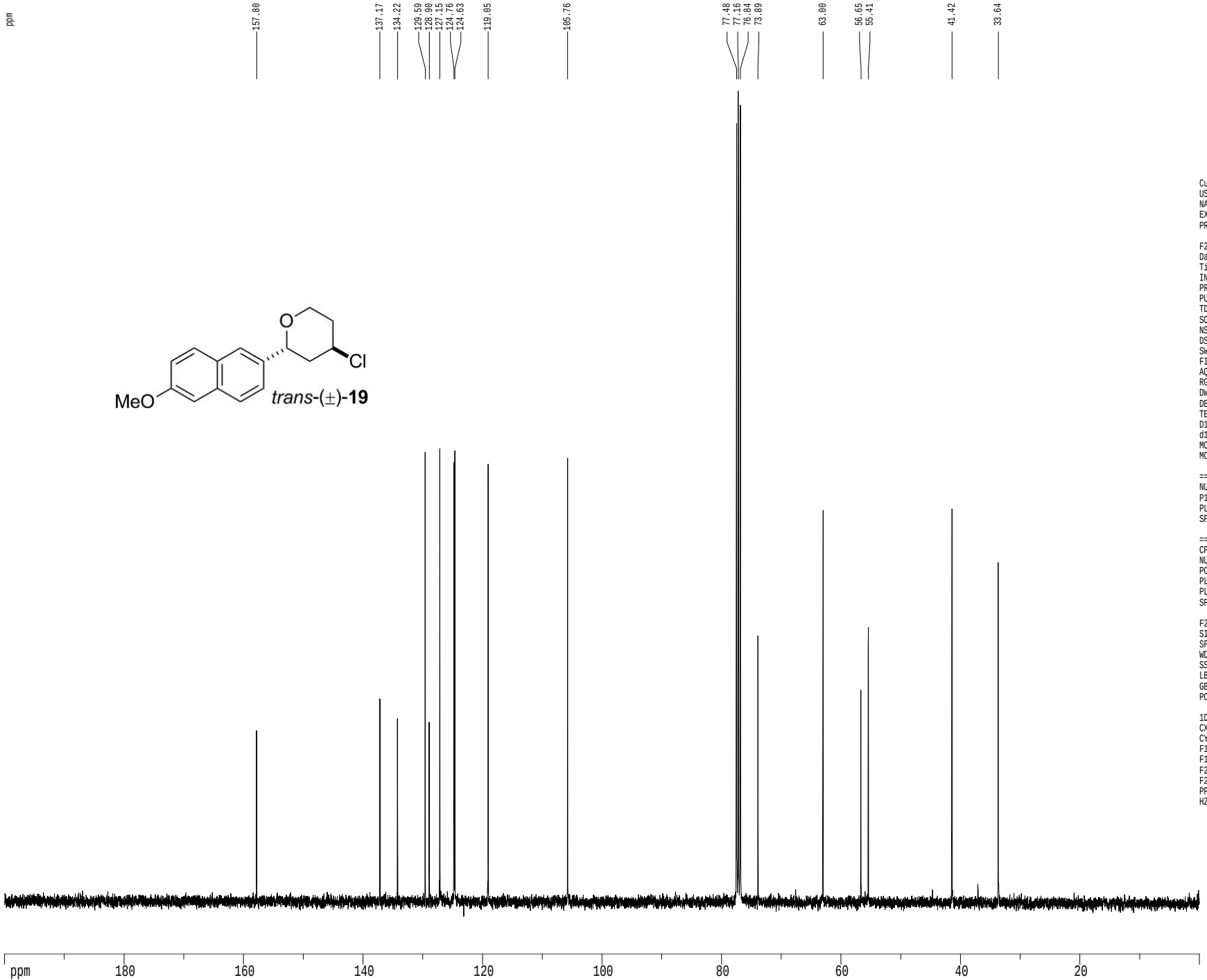
F2 - Acquisition Parameters
Date_           20150406
Time               20.34
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  81728
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           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           500.2200364 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42502 Hz/cm
```

PI Jarvo
c13 CDCl3 v emilyt 19



Current Data Parameters
USER emilyt
NAME EJT-IV-trans-19
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150616
Time 0.41
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1024
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

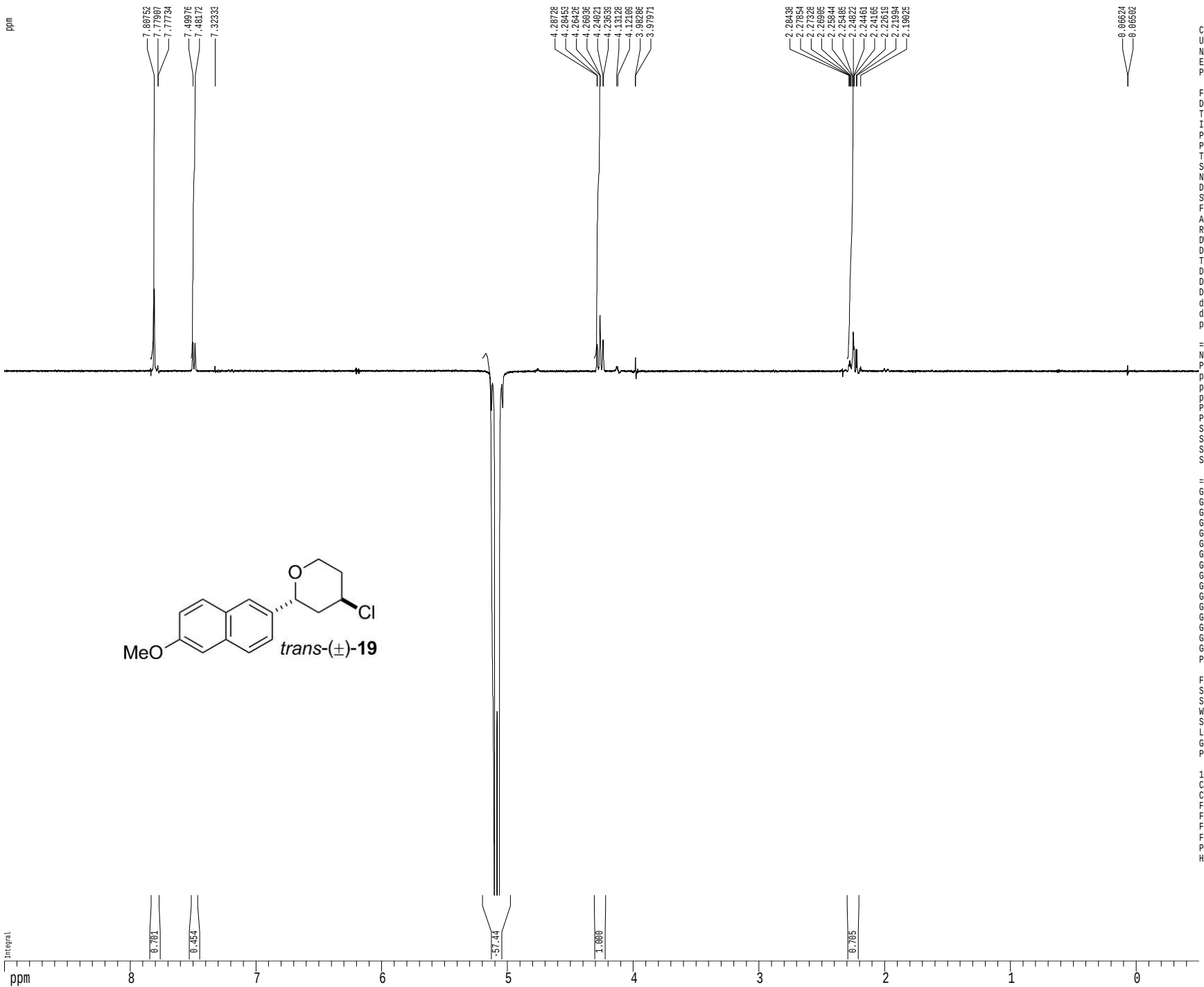
======== CHANNEL f1 ========
NUC1 13C
P1 7.75 usec
PL1 -3.00 dB
SFO1 100.6237964 MHz

======== CHANNEL f2 ========
CPDPRG2 mlev16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 17.70 dB
SFO2 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 100.6127606 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 15.50 cm
F1P 200.000 ppm
F1 20122.55 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 8.77193 ppm/cm
HZCM 882.56812 Hz/cm

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-273 noe
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150204
Time 23.39
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 80.6
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

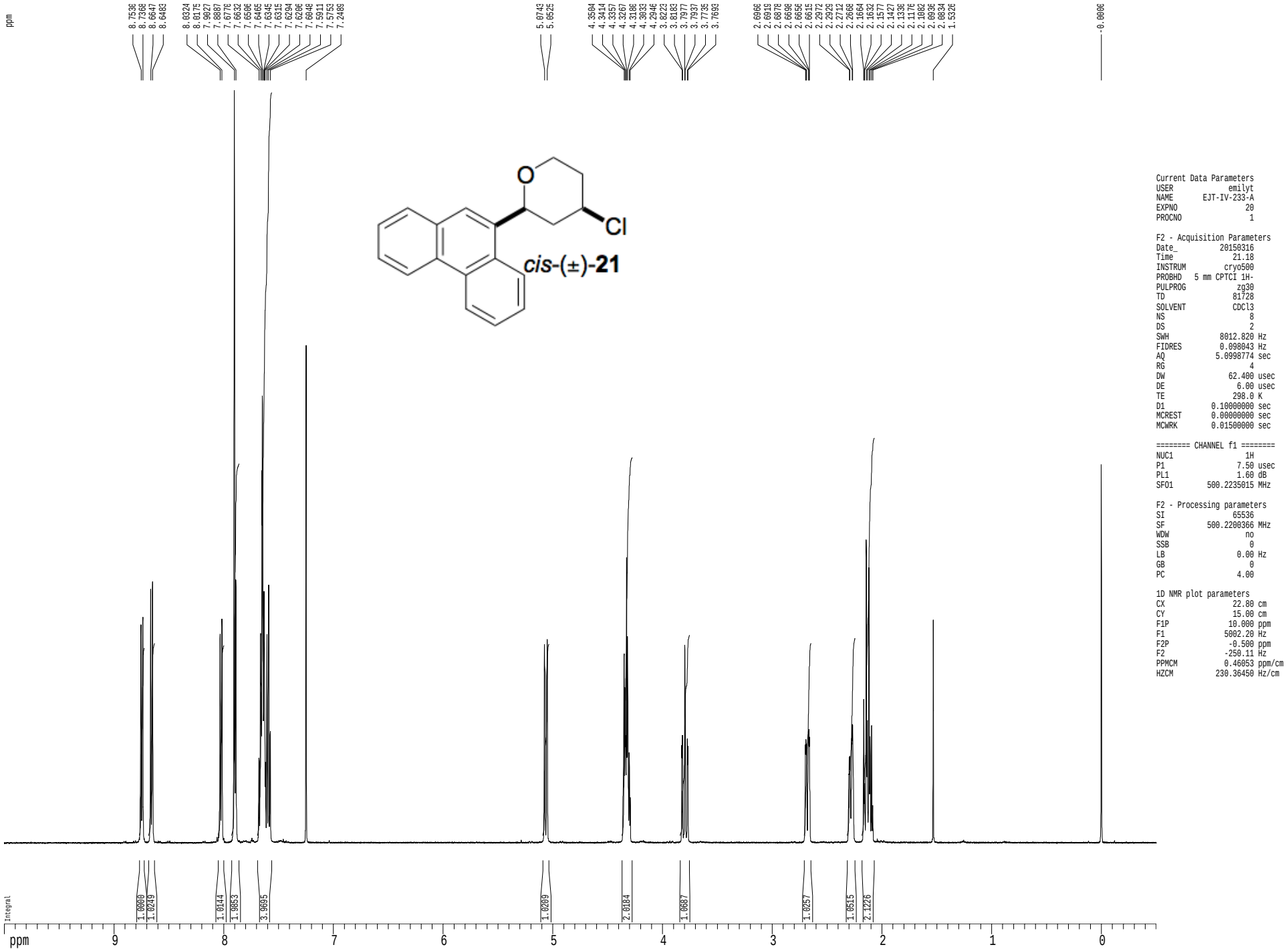
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2225429 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME        EJT-IV-233-A
EXPNO                20
PROCNO                1

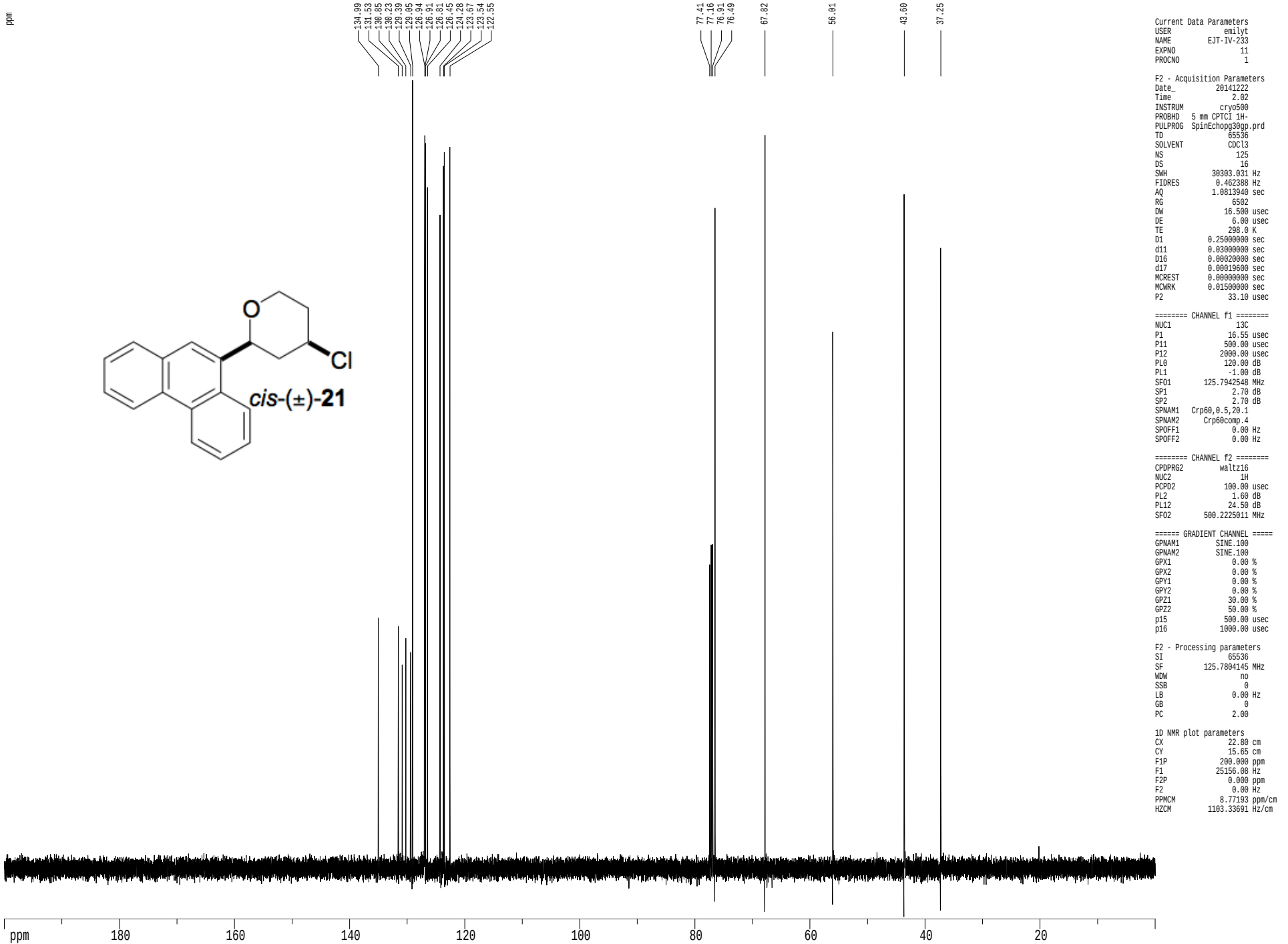
F2 - Acquisition Parameters
Date_          20150316
Time              21.18
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                81728
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8012.820 Hz
FIDRES         0.098043 Hz
AQ             5.0998774 sec
RG                    4
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           500.2200366 MHz
WDW                  no
SSB                   0
LB                0.00 Hz
GB                    0
PC                4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P              10.000 ppm
F1             5002.20 Hz
F2P              -0.500 ppm
F2             -250.11 Hz
PPMCM          0.46053 ppm/cm
HZCM         230.36450 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME            EJT-IV-233
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20141222
Time                  2.02
INSTRUM             cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                    65536
SOLVENT               CDCl3
NS                      125
DS                       16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                    6502
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                    13C
P1                   16.55 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1           125.7942548 MHz
SP1                   2.70 dB
SP2                   2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

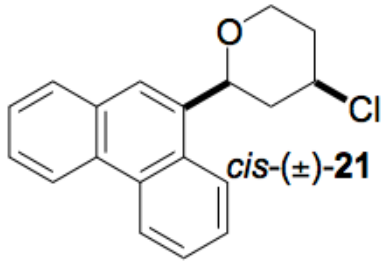
======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               100.00 usec
PL2                   1.60 dB
PL12                 24.50 dB
SFO2           500.2225011 MHz

====== 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             125.7804145 MHz
WDW                      no
SSB                       0
LB                    0.00 Hz
GB                        0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1                25156.08 Hz
F2P                  0.000 ppm
F2                    0.00 Hz
PPMCM             8.77193 ppm/cm
HZCM           1103.33691 Hz/cm
```

gcosy60



cis-(±)-**21**


```
        Current Data Parameters
USER              emilyt
NAME      EJT-IV-233-noe
EXPNO                 2
PROCNO                1

      F2 - Acquisition Parameters
Date_           20150131
Time               18.19
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG    cosygp60.prd
TD                 2048
SOLVENT           CDCl3
NS                    2
DS                   16
SWH            4734.849 Hz
FIDRES         2.311938 Hz
AQ             0.2163188 sec
RG                 724.1
DW              105.600 usec
DE                6.00 usec
TE                298.0 K
d0            0.00000300 sec
D1            1.00000000 sec
d13           0.00000300 sec
D16           0.00020000 sec
IN0           0.00021120 sec

     ======== CHANNEL f1 ========
NUC1                  1H
P1                  7.50 usec
PL1                 1.60 dB
SF01         500.2221259 MHz

     ====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               17.00 %
GPZ2               17.00 %
P16              1000.00 usec

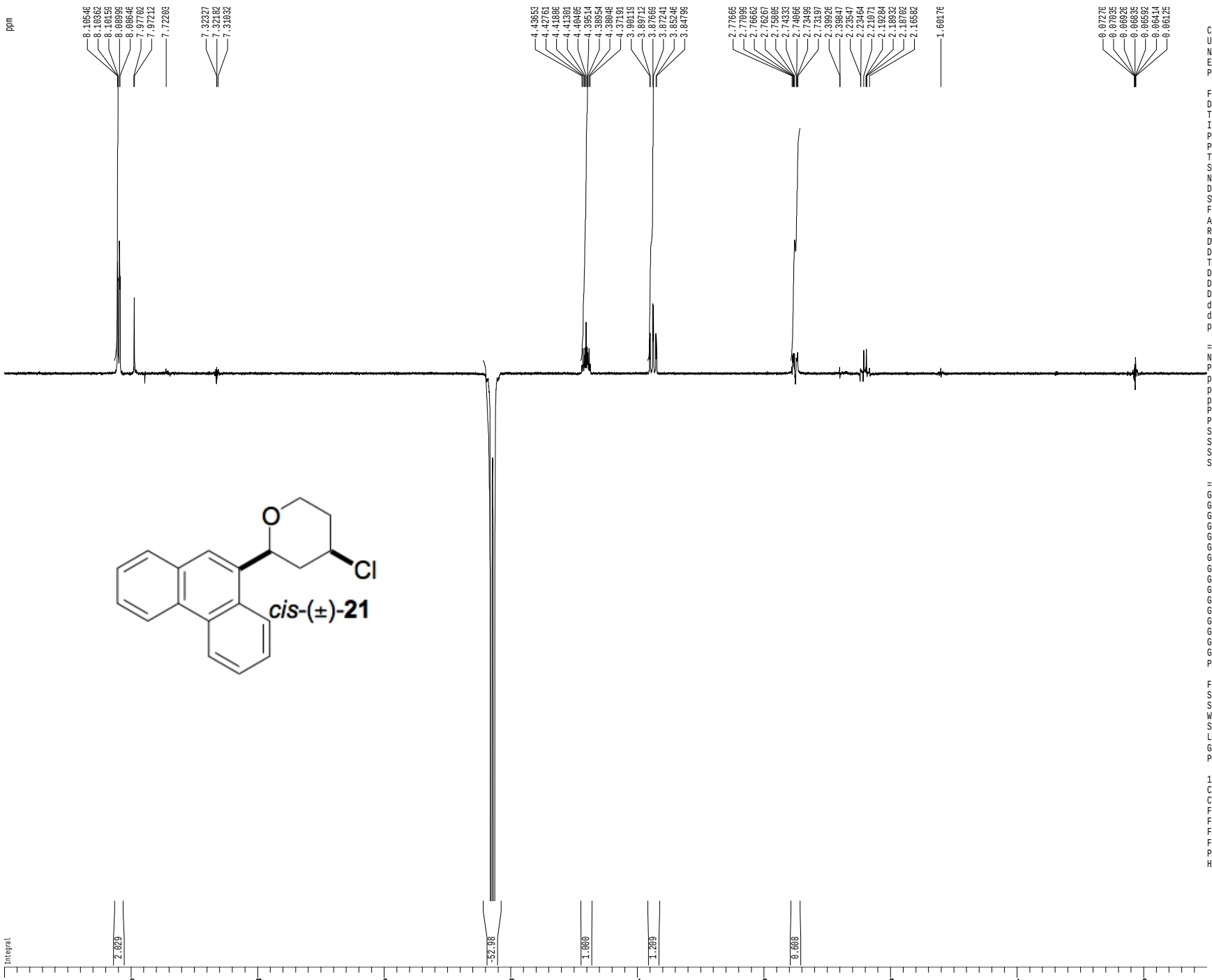
      F1 - Acquisition parameters
ND0                   1
TD                  128
SFO1           500.2221 MHz
FIDRES         36.991005 Hz
SW                 9.465 ppm
FnMODE         undefined

      F2 - Processing parameters
SI                  1024
SF           500.2200000 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  4.00

      F1 - Processing parameters
SI                  1024
MC2                   QF
SF           500.2200000 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0

        2D NMR plot parameters
CX2                15.00 cm
CX1                15.00 cm
F2PLO               8.983 ppm
F2LO             4493.36 Hz
F2PHI               1.000 ppm
F2HI              500.22 Hz
F1PLO               8.983 ppm
F1LO             4493.36 Hz
F1PHI               1.000 ppm
F1HI              500.22 Hz
F2PPMCM          0.53218 ppm/cm
F2HZCM         266.20917 Hz/cm
F1PPMCM          0.53218 ppm/cm
F1HZCM         266.20917 Hz/cm
```

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-233-noe
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150131
Time 18.39
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 128
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 80.6
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 0.50000000 sec
D16 0.00020000 sec
d21 0.33376500 sec
d22 0.16399699 sec
p2 15.00 usec

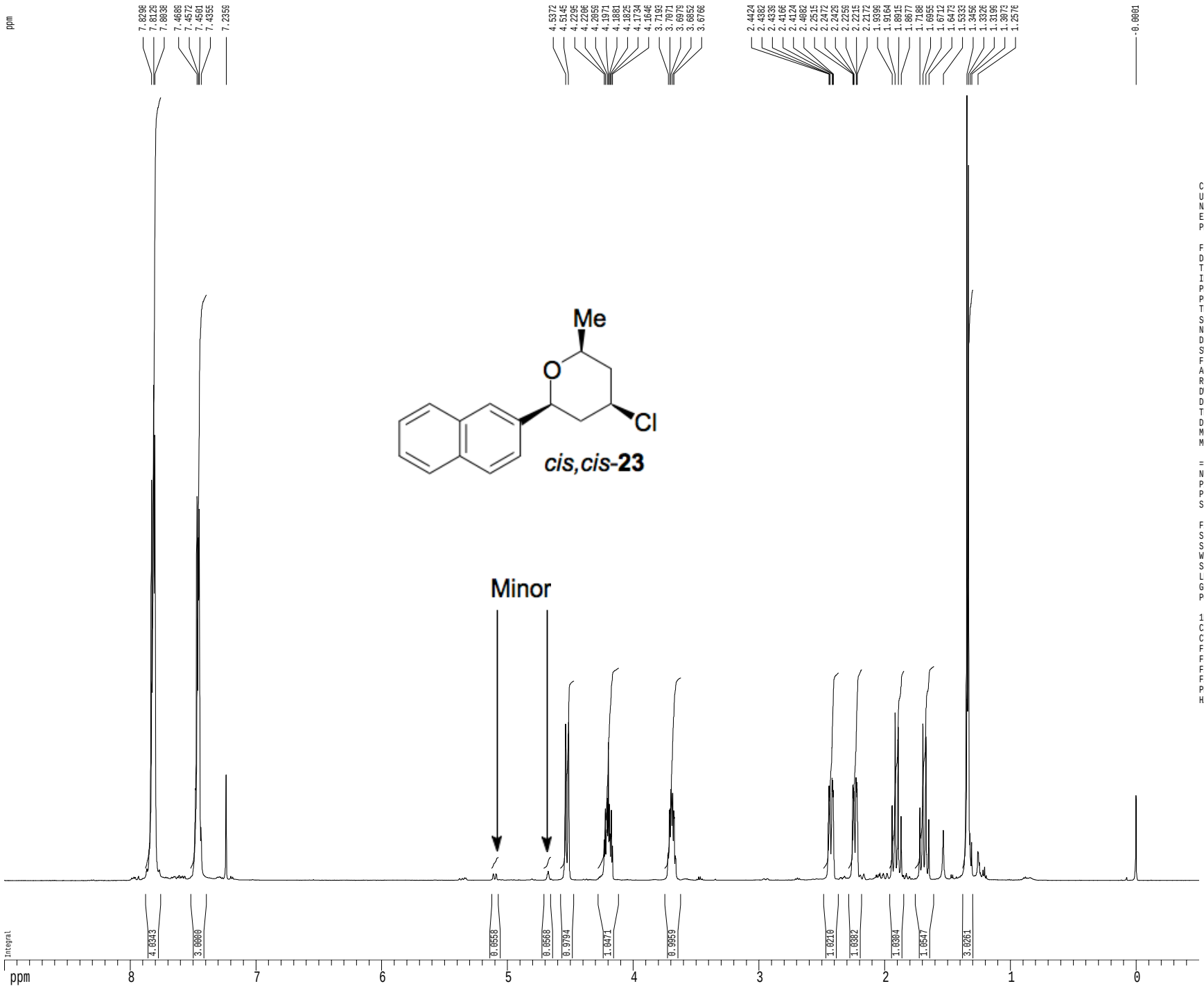
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2225728 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-228-cryo2
EXPNO                   1
PROCNO                  1

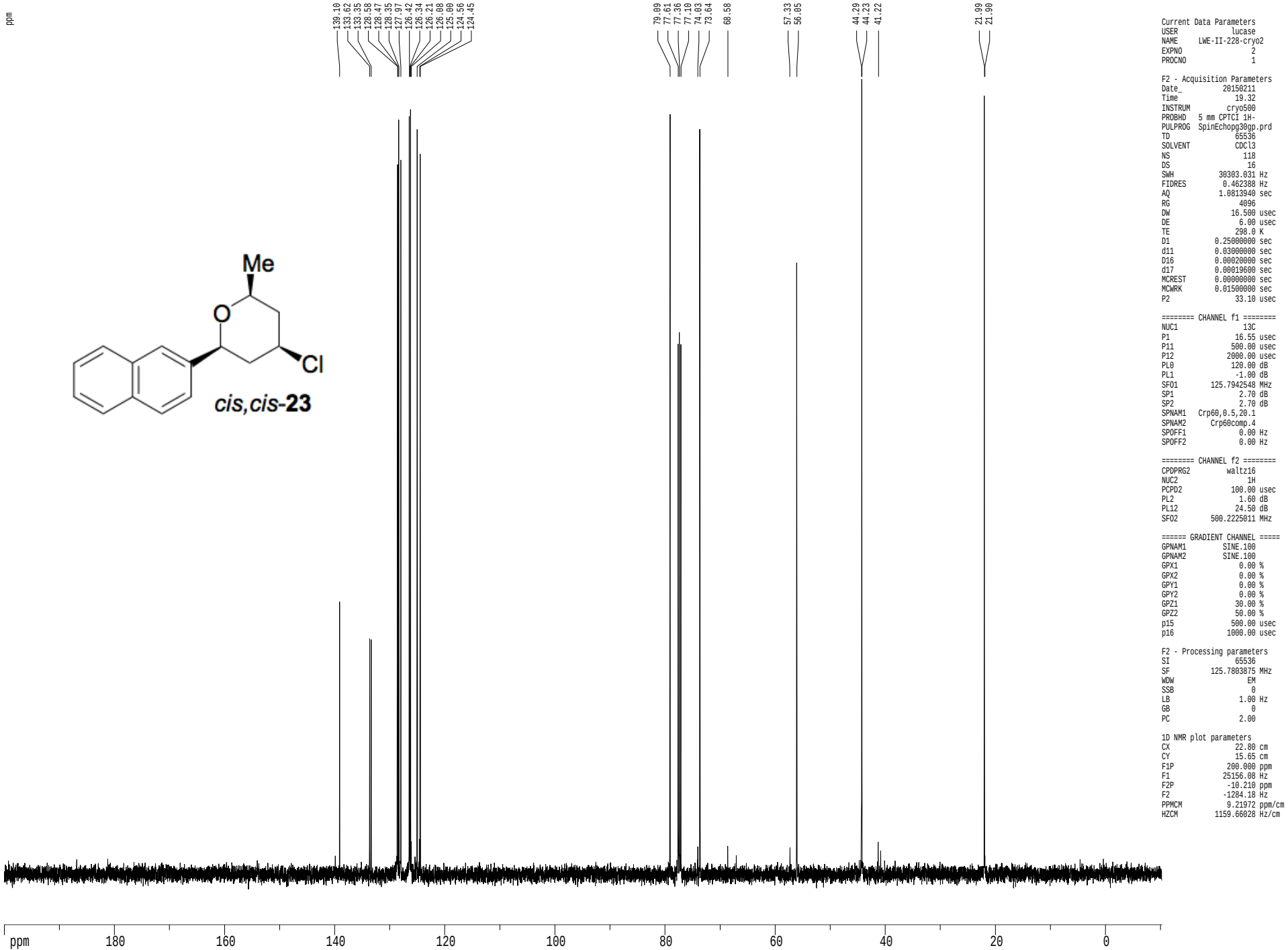
F2 - Acquisition Parameters
Date_            20150211
Time                19.29
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG             zg30
TD                 48074
SOLVENT            CDCl3
NS                     8
DS                     2
SWH              8012.820 Hz
FIDRES           0.166677 Hz
AQ               2.9998677 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            500.2200426 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P                9.000 ppm
F1               4501.98 Hz
F2P               -0.500 ppm
F2               -250.11 Hz
PPMCM           0.41667 ppm/cm
HZCM          208.42502 Hz/cm
```

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



Current Data Parameters
USER lucase
NAME LWE-II-228-cryo2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150211
Time 19.32
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT CDCl3
NS 118
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813940 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
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 33.10 usec

======== CHANNEL f1 ========
NUC1 13C
P1 16.55 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7942548 MHz
SP1 2.70 dB
SP2 2.70 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

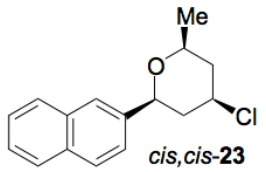
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.50 dB
SFO2 500.2225011 MHz

====== 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

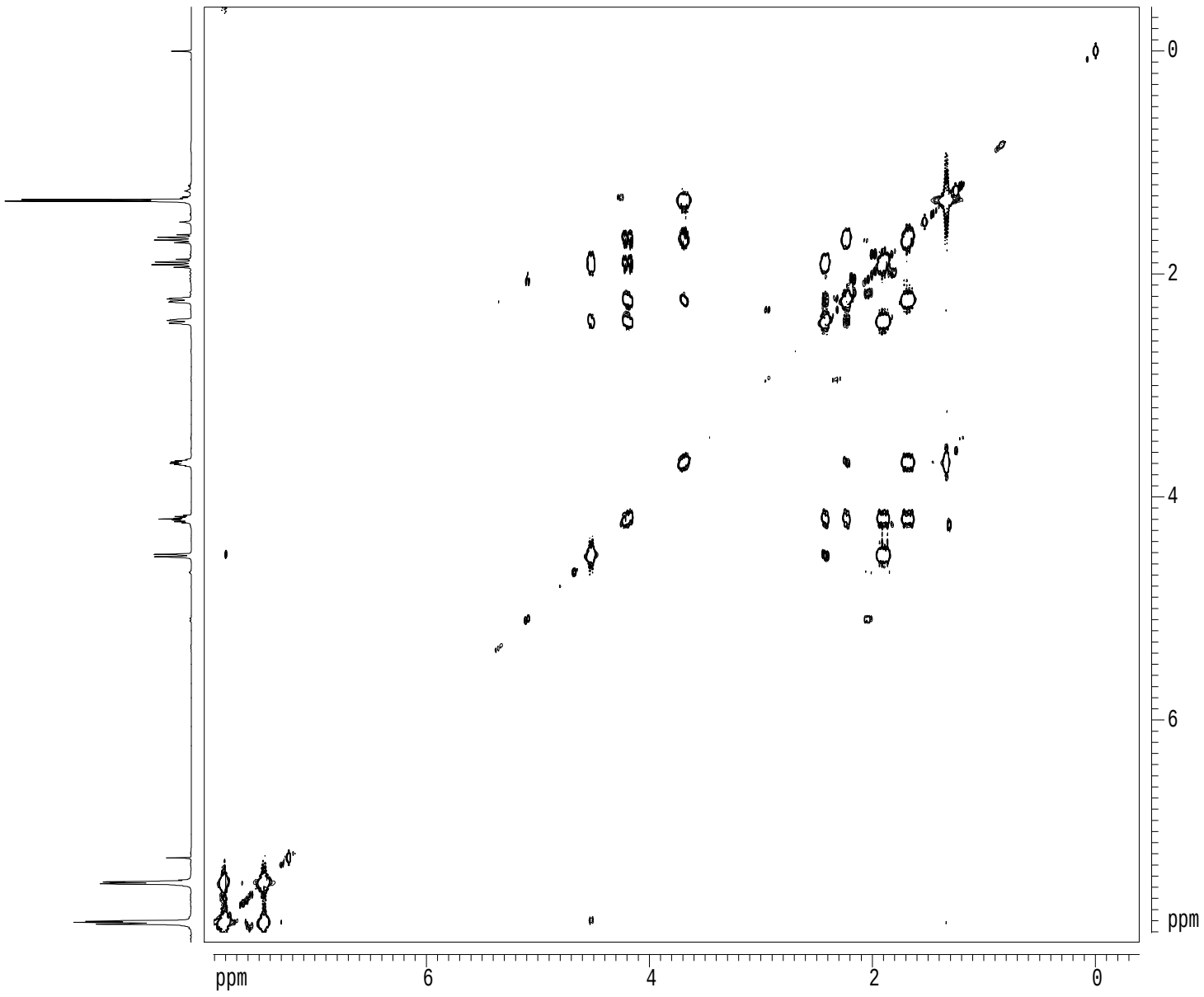
F2 - Processing parameters
SI 65536
SF 125.7803875 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -10.210 ppm
F2 -1284.18 Hz
PPMCM 9.21972 ppm/cm
HZCM 1159.66028 Hz/cm

gcosy60



cis,cis-**23**




```
        Current Data Parameters
 USER             lucase
NAME      LWE-II-228-cryo2
 EXPNO                4
 PROCNO               1

      F2 - Acquisition Parameters
 Date_          20150211
 Time             19.48
 INSTRUM         cryo500
 PROBHD   5 mm CPTCI 1H-
 PULPROG    cosygp60.prd
 TD                2048
 SOLVENT           CDCl3
 NS                   2
 DS                  16
 SWH           4194.631 Hz
 FIDRES          2.048160 Hz
 AQ            0.2441716 sec
 RG                35.9
 DW             119.200 usec
 DE               6.00 usec
 TE              298.0 K
 d0           0.00000300 sec
 D1           1.00000000 sec
 d13          0.00000300 sec
 D16          0.00020000 sec
 IN0          0.00023840 sec

     ======== CHANNEL f1 ========
 NUC1                1H
 P1                7.50 usec
 PL1               1.60 dB
 SFO1        500.2219008 MHz

     ====== GRADIENT CHANNEL =====
 GPNAM1          sine.100
 GPNAM2          sine.100
 GPX1              0.00 %
 GPX2              0.00 %
 GPY1              0.00 %
 GPY2              0.00 %
 GPZ1             17.00 %
 GPZ2             17.00 %
 P16            1000.00 usec

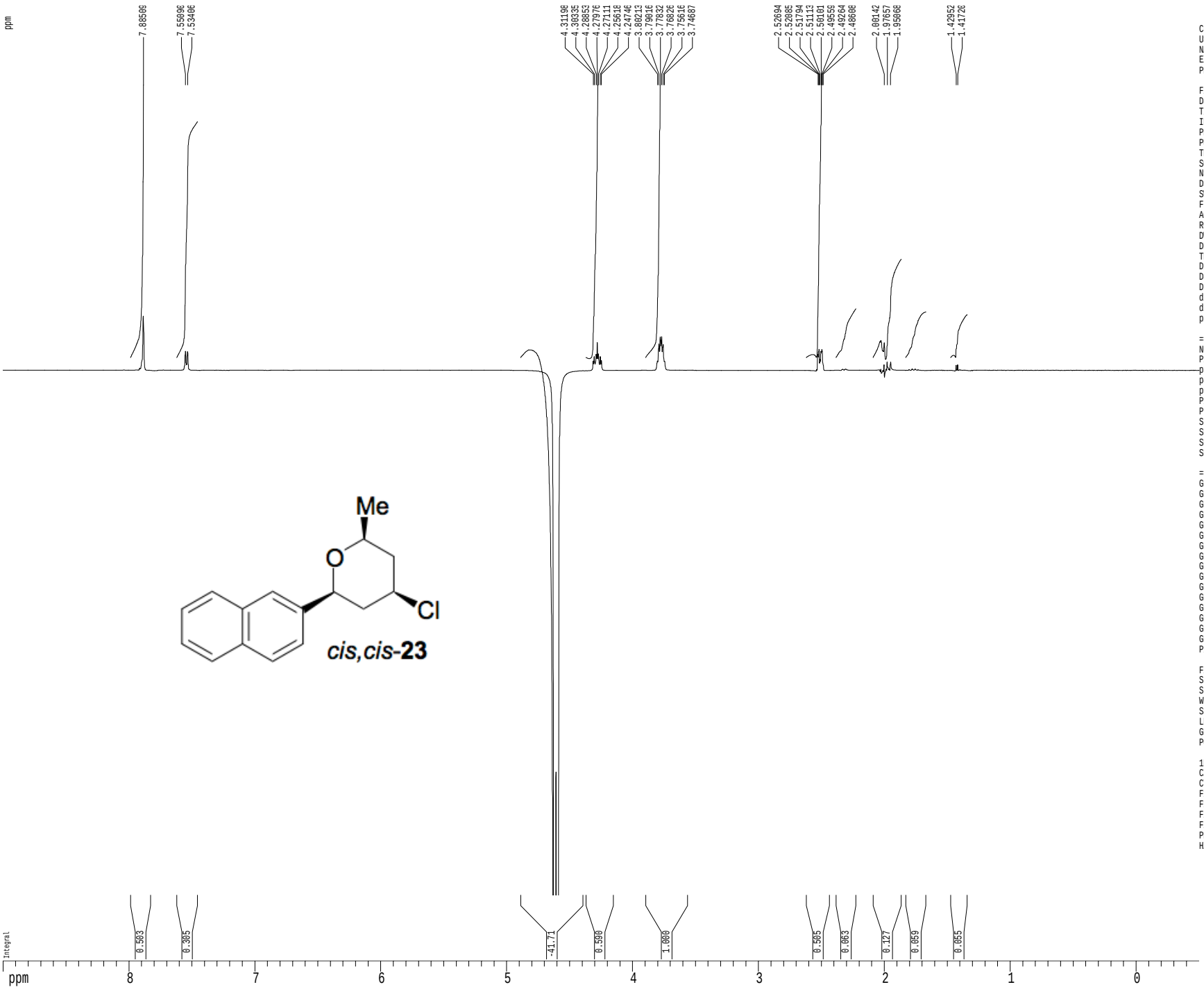
      F1 - Acquisition parameters
 ND0                  1
 TD                 128
 SFO1          500.2219 MHz
 FIDRES        32.770554 Hz
 SW                8.386 ppm
 FnMODE        undefined

      F2 - Processing parameters
 SI                1024
 SF          500.2200426 MHz
 WDW               SINE
 SSB                  0
 LB                0.00 Hz
 GB                   0
 PC                1.00

      F1 - Processing parameters
 SI                1024
 MC2                 QF
 SF          500.2200426 MHz
 WDW               SINE
 SSB                  0
 LB                0.00 Hz
 GB                   0

       2D NMR plot parameters
 CX2              15.00 cm
 CX1              15.00 cm
 F2PLO             7.993 ppm
 F2LO           3998.15 Hz
 F2PHI            -0.393 ppm
 F2HI           -196.48 Hz
 F1PLO             7.993 ppm
 F1LO           3998.15 Hz
 F1PHI            -0.393 ppm
 F1HI           -196.48 Hz
 F2PPMCM         0.55904 ppm/cm
 F2HZCM        279.64206 Hz/cm
 F1PPMCM         0.55904 ppm/cm
 F1HZCM        279.64206 Hz/cm
```

gnoe




```
Current Data Parameters
USER                lucase
NAME      LWE-II-228-cryo2
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150211
Time                19.47
INSTRUM           cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG        gnoe1cc.wu
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      8
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894966 sec
RG                  161.3
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
D8             0.50000000 sec
D16            0.00020000 sec
d21            0.33376500 sec
d22            0.16399699 sec
p2                15.00 usec

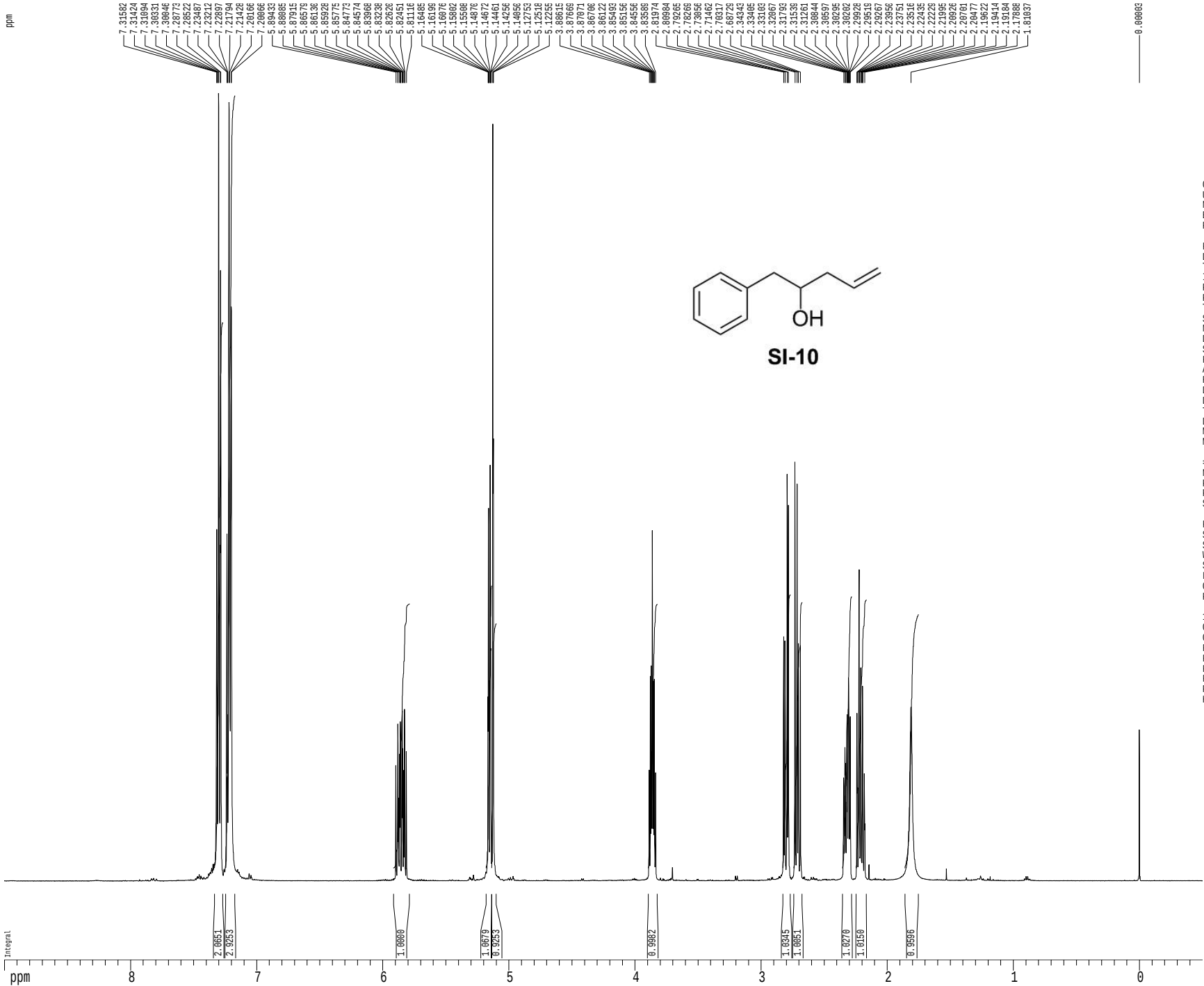
======== CHANNEL f1 ========
NUC1                   1H
P1                  7.50 usec
p3                 22.50 usec
p4                 30.00 usec
p5                 20.00 usec
P12             40000.00 usec
PL1                 1.60 dB
SFO1          500.2223060 MHz
SP1                61.60 dB
SPNAM1         gauss1.512
SPOFF1              0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1           sine.100
GPNAM2           sine.100
GPNAM3           sine.100
GPNAM4           sine.100
GPX1                0.00 %
GPX2                0.00 %
GPX3                0.00 %
GPX4                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPY3                0.00 %
GPY4                0.00 %
GPZ1                7.00 %
GPZ2                3.00 %
GPZ3                2.30 %
GPZ4               -2.30 %
P16              1000.00 usec

F2 - Processing parameters
SI                  65536
SF            500.2200000 MHz
WDW                    EM
SSB                     0
LB                  1.00 Hz
GB                      0
PC                  1.00

1D NMR plot parameters
CX                 22.80 cm
CY                 50.00 cm
F1P                9.000 ppm
F1               4501.98 Hz
F2P                -0.500 ppm
F2               -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42500 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME          EJT-IV-250
EXPNO                 12
PROCNO                 1

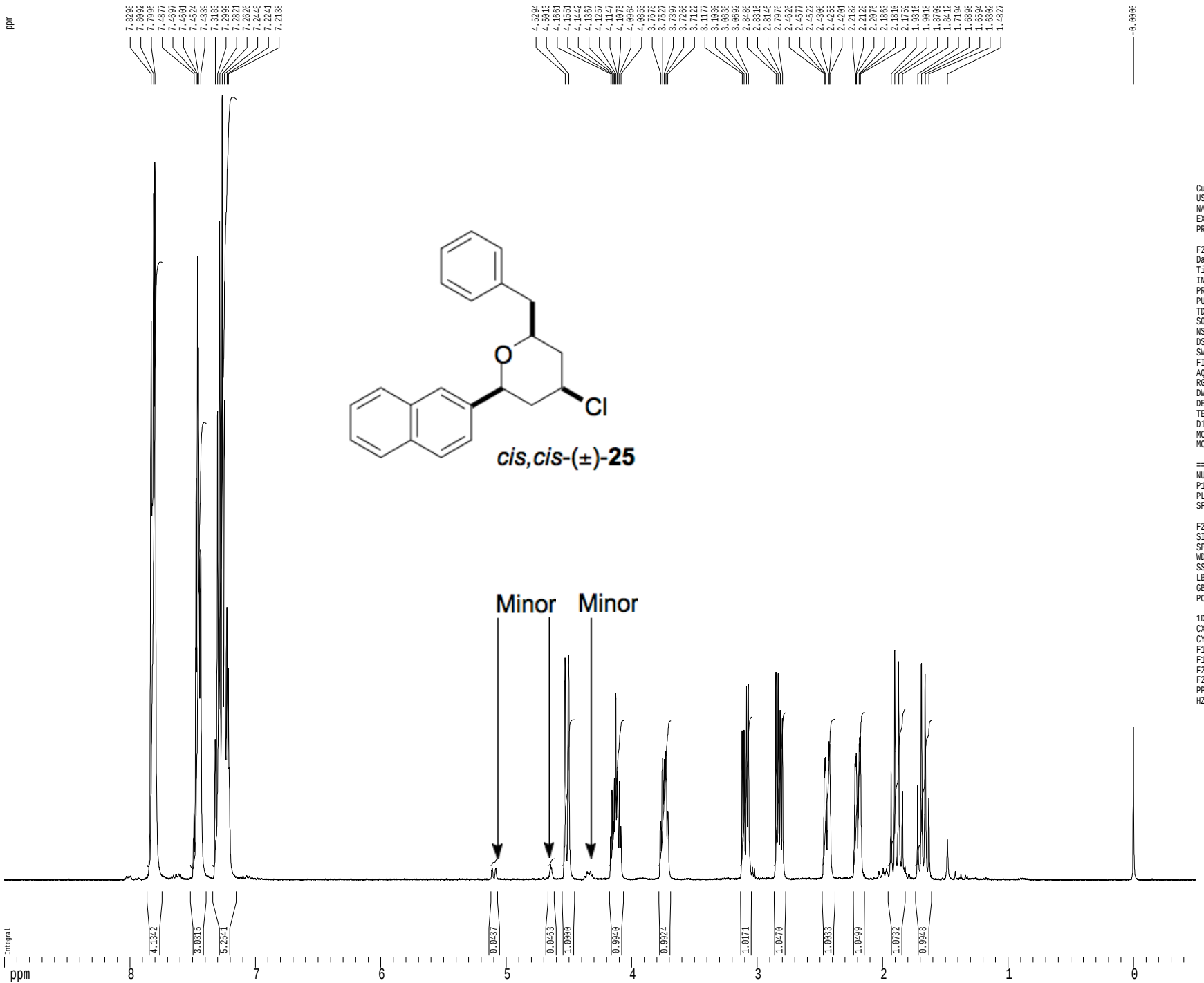
F2 - Acquisition Parameters
Date_           20150404
Time               22.52
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  81728
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.098043 Hz
AQ               5.0998774 sec
RG                      4
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            500.2200462 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42502 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME        EJT-IV-277-A
EXPNO               50
PROCNO               1

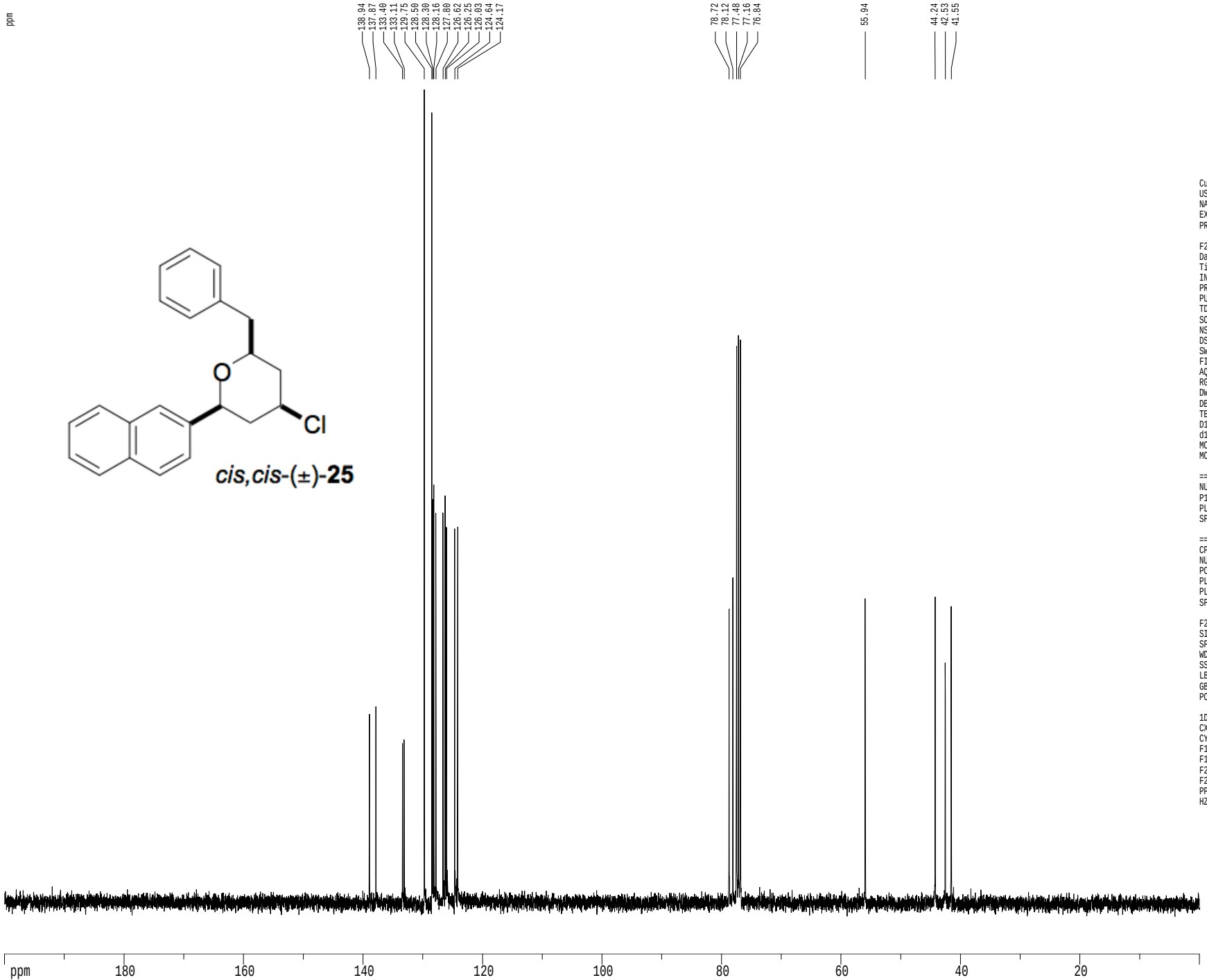
F2 - Acquisition Parameters
Date_          20150410
Time              18.37
INSTRUM           drx400
PROBHD   5 mm QNP H/F/P
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            6410.256 Hz
FIDRES         0.097813 Hz
AQ             5.1118579 sec
RG                101.6
DW               78.000 usec
DE                4.50 usec
TE                298.0 K
D1           0.10000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                12.00 usec
PL1                0.00 dB
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300389 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              3601.17 Hz
F2P              -0.500 ppm
F2              -200.06 Hz
PPMCM          0.41667 ppm/cm
HZCM          166.72086 Hz/cm
```

13C spectrum with 1H decoupling




```
Current Data Parameters
USER             emilyt
NAME       EJT-IV-277-A
EXPNO              51
PROCNO              1

F2 - Acquisition Parameters
Date_          20150410
Time              18.42
INSTRUM         drx400
PROBHD   5 mm QNP H/F/P
PULPROG         zgdc30
TD              65536
SOLVENT          CDCl3
NS                 263
DS                   4
SWH          24154.590 Hz
FIDRES        0.368570 Hz
AQ            1.3566452 sec
RG               4597.6
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

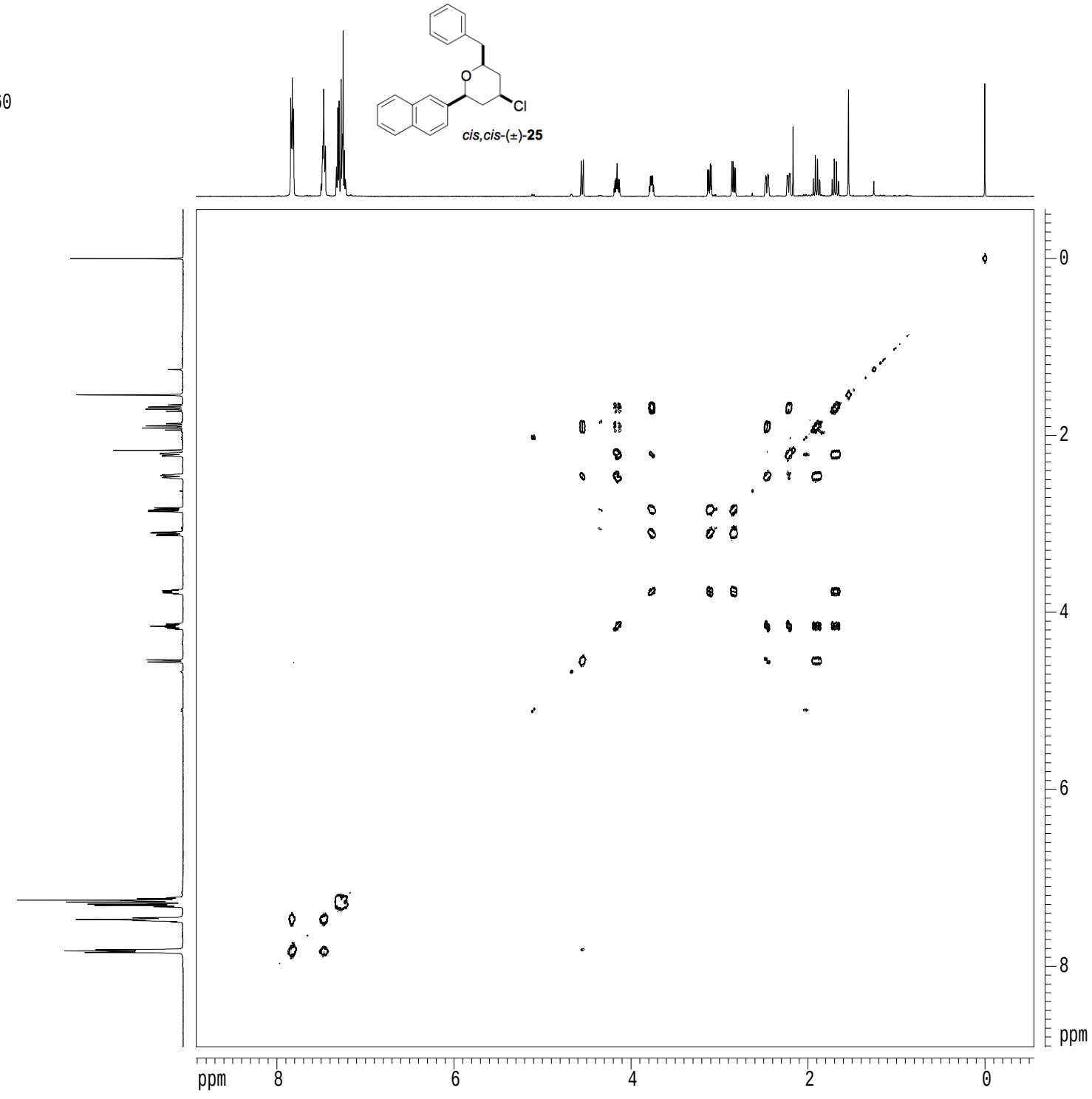
======== CHANNEL f1 ========
NUC1               13C
P1                7.75 usec
PL1               -3.00 dB
SFO1        100.6237964 MHz

======== CHANNEL f2 ========
CPDPRG2          mlev16
NUC2               1H
PCPD2             90.00 usec
PL2                0.00 dB
PL12              17.70 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

1D NMR plot parameters
CX                22.80 cm
CY                15.50 cm
F1P              200.000 ppm
F1             20122.55 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM          8.77193 ppm/cm
HZCM         882.56812 Hz/cm
```

gcosy60



Current Data Parameters

USER	emilyt
NAME	EJT-V-026
EXPNO	13
PROCNO	1

F2 - Acquisition Parameters

Date_	20150131
Time	13.05
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	cosygp60.prd
TD	2048
SOLVENT	CDCl3
NS	2
DS	16
SWH	4734.849 Hz
FIDRES	2.311938 Hz
AQ	0.2163188 sec
RG	228.1
DW	105.600 usec
DE	6.00 usec
TE	298.0 K
d0	0.00000300 sec
D1	1.00000000 sec
d13	0.00000300 sec
D16	0.00020000 sec
IN0	0.00021120 sec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
PL1	1.60 dB
SFO1	500.2221259 MHz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	17.00 %
GPZ2	17.00 %
P16	1000.00 usec

F1 - Acquisition parameters

ND0	1
TD	256
SFO1	500.2221 MHz
FIDRES	18.495502 Hz
SW	9.465 ppm
FnMODE	undefined

F2 - Processing parameters

SI	1024
SF	500.2200351 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40

F1 - Processing parameters

SI	1024
MC2	QF
SF	500.2200351 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

2D NMR plot parameters

CX2	15.00 cm
CX1	15.00 cm
F2PLO	8.913 ppm
F2LO	4458.30 Hz
F2PHI	-0.553 ppm
F2HI	-276.55 Hz
F1PLO	8.913 ppm
F1LO	4458.30 Hz
F1PHI	-0.553 ppm
F1HI	-276.55 Hz
F2PPMCM	0.63104 ppm/cm
F2HZCM	315.65656 Hz/cm
F1PPMCM	0.63104 ppm/cm
F1HZCM	315.65656 Hz/cm

gnoe



Current Data Parameters

USER	emilyt
NAME	EJT-V-026
EXPNO	14
PROCNO	1

F2 - Acquisition Parameters

Date_	20150131
Time	13.30
INSTRUM	cryo500
PROBHD	5 mm CPTCI 1H-
PULPROG	gnoe1cc.wu
TD	65536
SOLVENT	CDCl3
NS	128
DS	8
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	90.5
DW	62.400 usec
DE	6.00 usec
TE	298.0 K
D1	1.00000000 sec
D8	0.50000000 sec
D16	0.00020000 sec
d21	0.33376500 sec
d22	0.16399699 sec
p2	15.00 usec

======== CHANNEL f1 ========

NUC1	1H
P1	7.50 usec
p3	22.50 usec
p4	30.00 usec
p5	20.00 usec
P12	40000.00 usec
PL1	1.60 dB
SFO1	500.2223121 MHz
SP1	61.60 dB
SPNAM1	gauss1.512
SPOFF1	0.00 Hz

====== GRADIENT CHANNEL =====

GPNAM1	sine.100
GPNAM2	sine.100
GPNAM3	sine.100
GPNAM4	sine.100
GPX1	0.00 %
GPX2	0.00 %
GPX3	0.00 %
GPX4	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPY3	0.00 %
GPY4	0.00 %
GPZ1	7.00 %
GPZ2	3.00 %
GPZ3	2.30 %
GPZ4	-2.30 %
P16	1000.00 usec

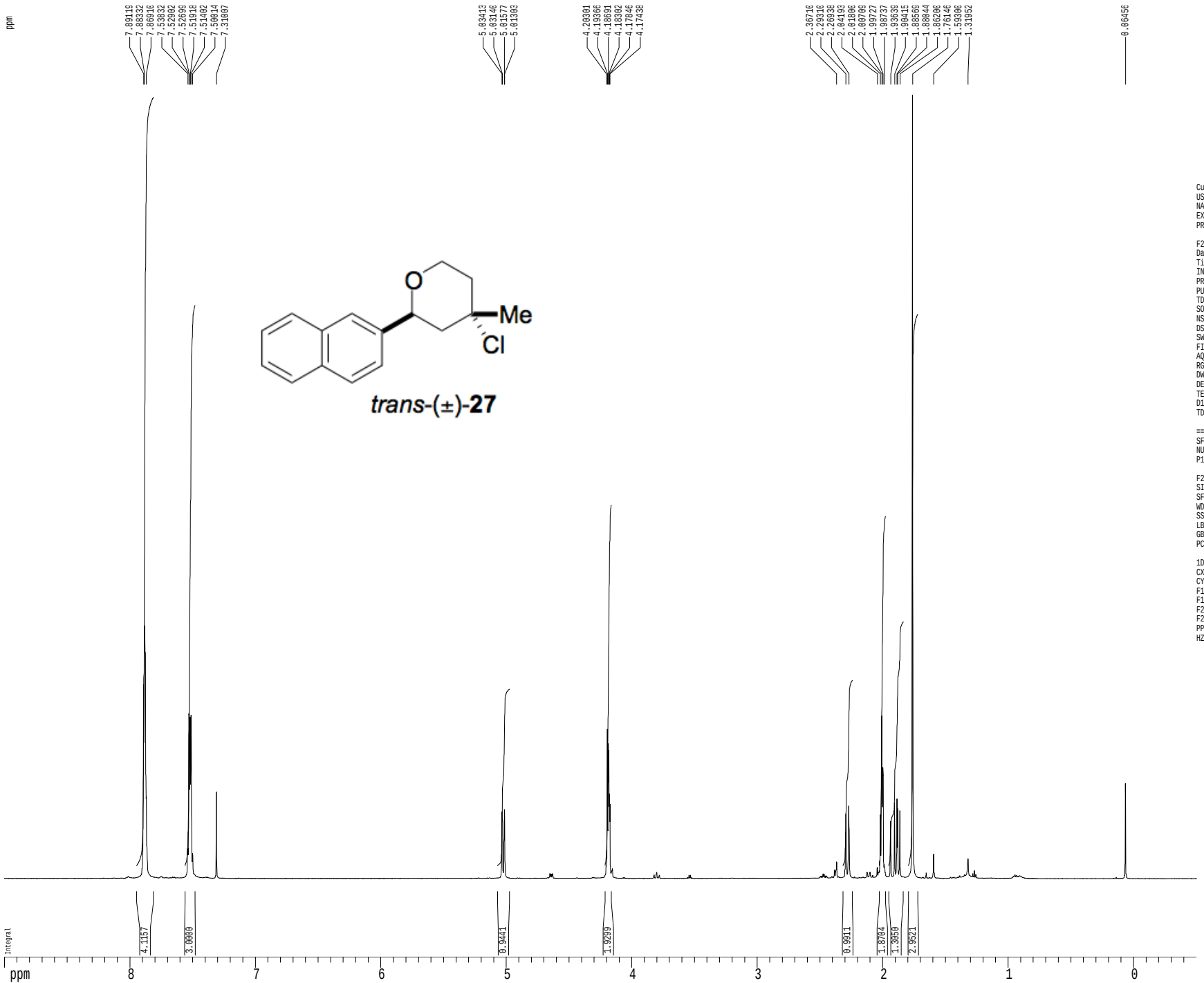
F2 - Processing parameters

SI	65536
SF	500.2200000 MHz
WDW	no
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.80 cm
CY	50.00 cm
F1P	9.000 ppm
F1	4501.98 Hz
F2P	-0.500 ppm
F2	-250.11 Hz
PPMCM	0.41667 ppm/cm
HZCM	208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-248-avance600
EXPNO                    1
PROCNO                   1

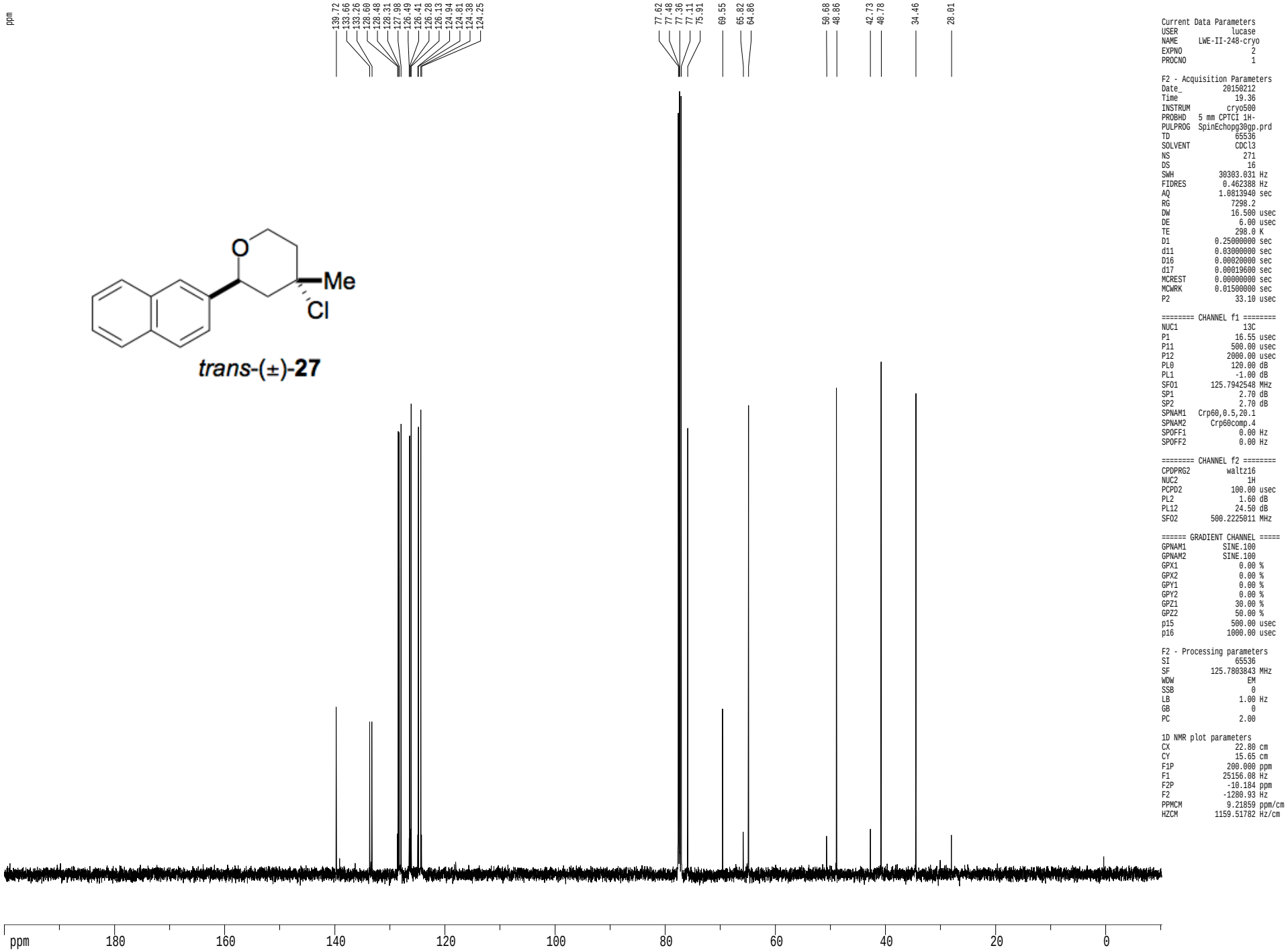
F2 - Acquisition Parameters
Date_            20150412
Time                19.20
INSTRUM             av600
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 57690
SOLVENT            CDCl3
NS                     8
DS                     2
SWH              9615.385 Hz
FIDRES           0.166673 Hz
AQ               2.9999299 sec
RG                   228
DW                 52.000 usec
DE                 14.33 usec
TE                 298.5 K
D1             0.10000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          600.1342009 MHz
NUC1                  1H
P1                  9.00 usec

F2 - Processing parameters
SI                 65536
SF            600.1300040 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P                9.000 ppm
F1              5401.17 Hz
F2P                -0.500 ppm
F2              -300.06 Hz
PPMCM           0.41667 ppm/cm
HZCM           250.05418 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-248-cryo
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150212
Time                 19.36
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     271
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1          125.7942548 MHz
SP1                   2.70 dB
SP2                   2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

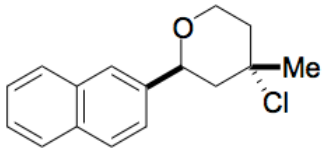
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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

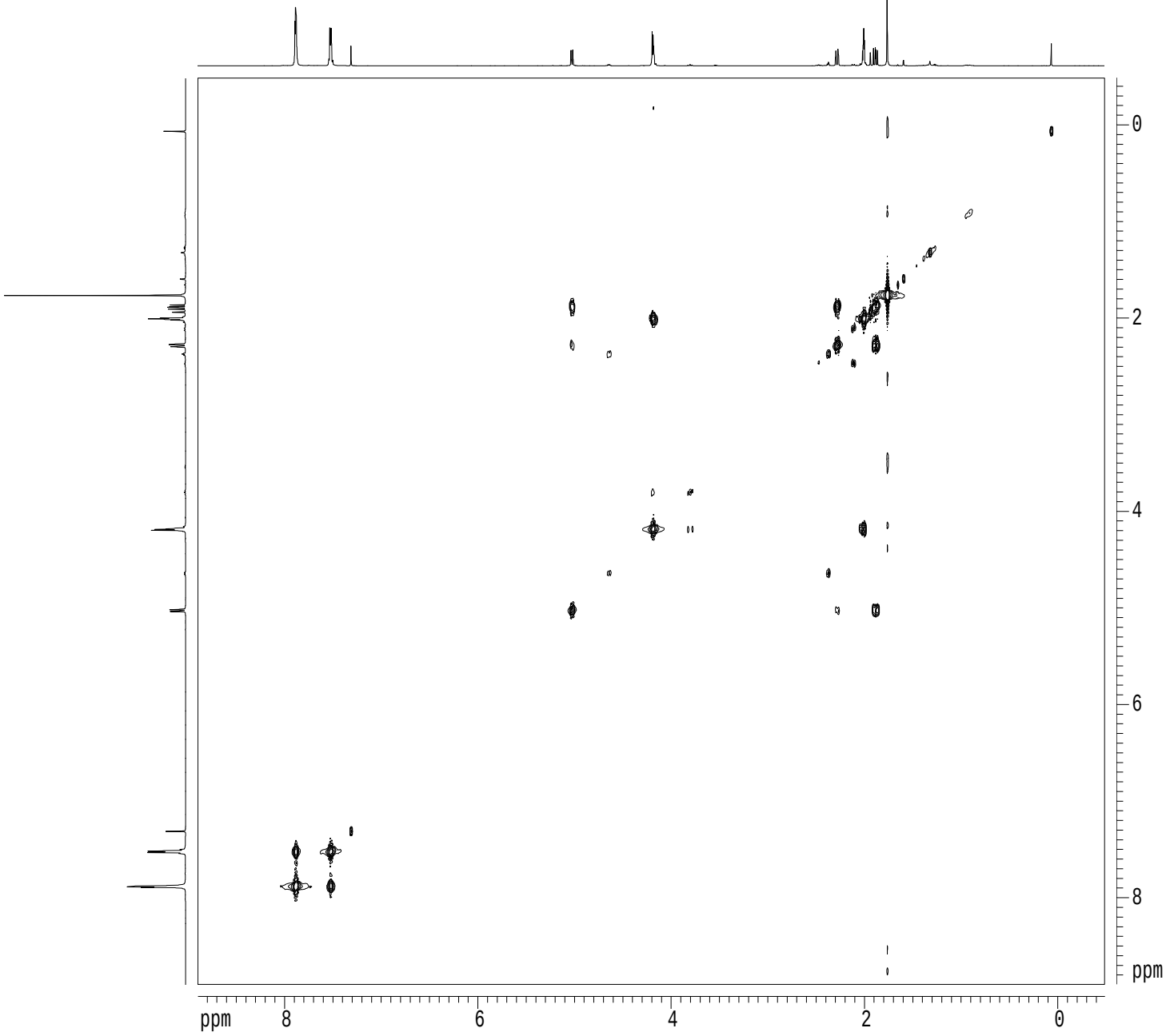
F2 - Processing parameters
SI                    65536
SF            125.7803843 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1                25156.08 Hz
F2P                -10.184 ppm
F2                -1280.93 Hz
PPMCM              9.21859 ppm/cm
HZCM            1159.51782 Hz/cm
```

gcosy



trans-(±)-**27**




```
        Current Data Parameters
   USER            lucase
NAME     LWE-II-248-avance600
   EXPNO                3
   PROCNO               1

      F2 - Acquisition Parameters
   Date_          20150412
   Time              19.42
   INSTRUM           av600
   PROBHD   5 mm BBO BB-1H
   PULPROG        cosygpqf
   TD                2048
   SOLVENT           CDCl3
   NS                   2
   DS                  16
   SWH            5630.631 Hz
   FIDRES         2.749331 Hz
   AQ             0.1819124 sec
   RG                 575
   DW                88.800 usec
   DE                 6.50 usec
   TE                298.5 K
   D0             0.00000300 sec
   D1             1.48689198 sec
   D13            0.00000400 sec
   D16            0.00020000 sec
   IN0            0.00017760 sec

     ======== CHANNEL f1 ========
   SFO1         600.1325245 MHz
   NUC1               1H
   P0                6.00 usec
   P1                9.00 usec

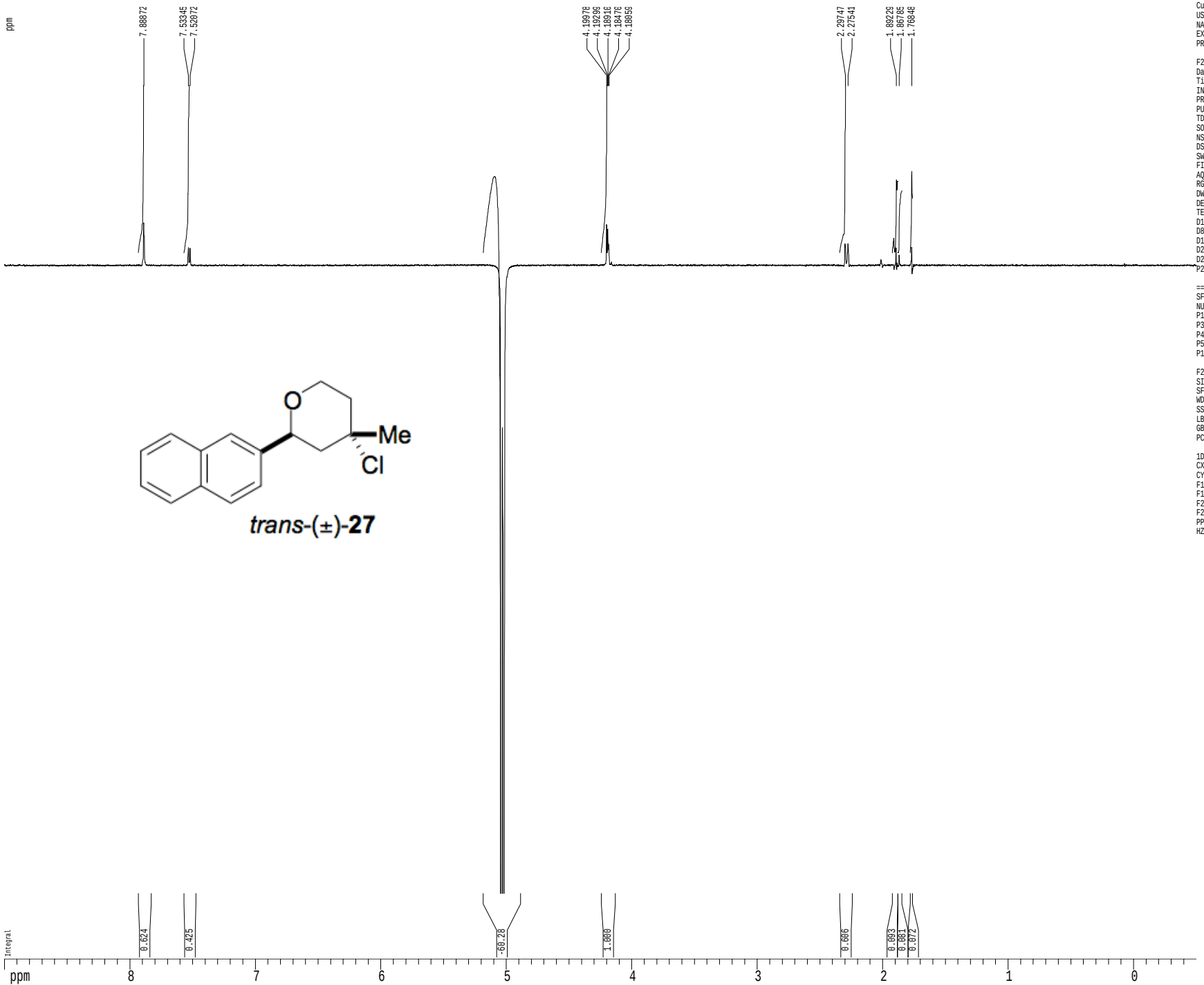
      F1 - Acquisition parameters
   ND0                  1
   TD                 128
   SFO1           600.1325 MHz
   FIDRES         43.989304 Hz
   SW                9.382 ppm
   FnMODE               QF

      F2 - Processing parameters
   SI                 1024
   SF          600.1300040 MHz
   WDW                SINE
   SSB                   0
   LB                 0.00 Hz
   GB                    0
   PC                 1.00

      F1 - Processing parameters
   SI                 1024
   MC2                  QF
   SF          600.1300040 MHz
   WDW                SINE
   SSB                   0
   LB                 0.00 Hz
   GB                    0

        2D NMR plot parameters
   CX2               15.00 cm
   CX1               15.00 cm
   F2PLO              8.898 ppm
   F2LO            5339.86 Hz
   F2PHI             -0.485 ppm
   F2HI            -290.77 Hz
   F1PLO              8.898 ppm
   F1LO            5339.86 Hz
   F1PHI             -0.485 ppm
   F1HI            -290.77 Hz
   F2PPMCM         0.62549 ppm/cm
   F2HZCM        375.37540 Hz/cm
   F1PPMCM         0.62549 ppm/cm
   F1HZCM        375.37540 Hz/cm
```

gnoe




```
Current Data Parameters
USER                lucase
NAME      LWE-II-248-avance600
EXPNO                   2
PROCNO                  1

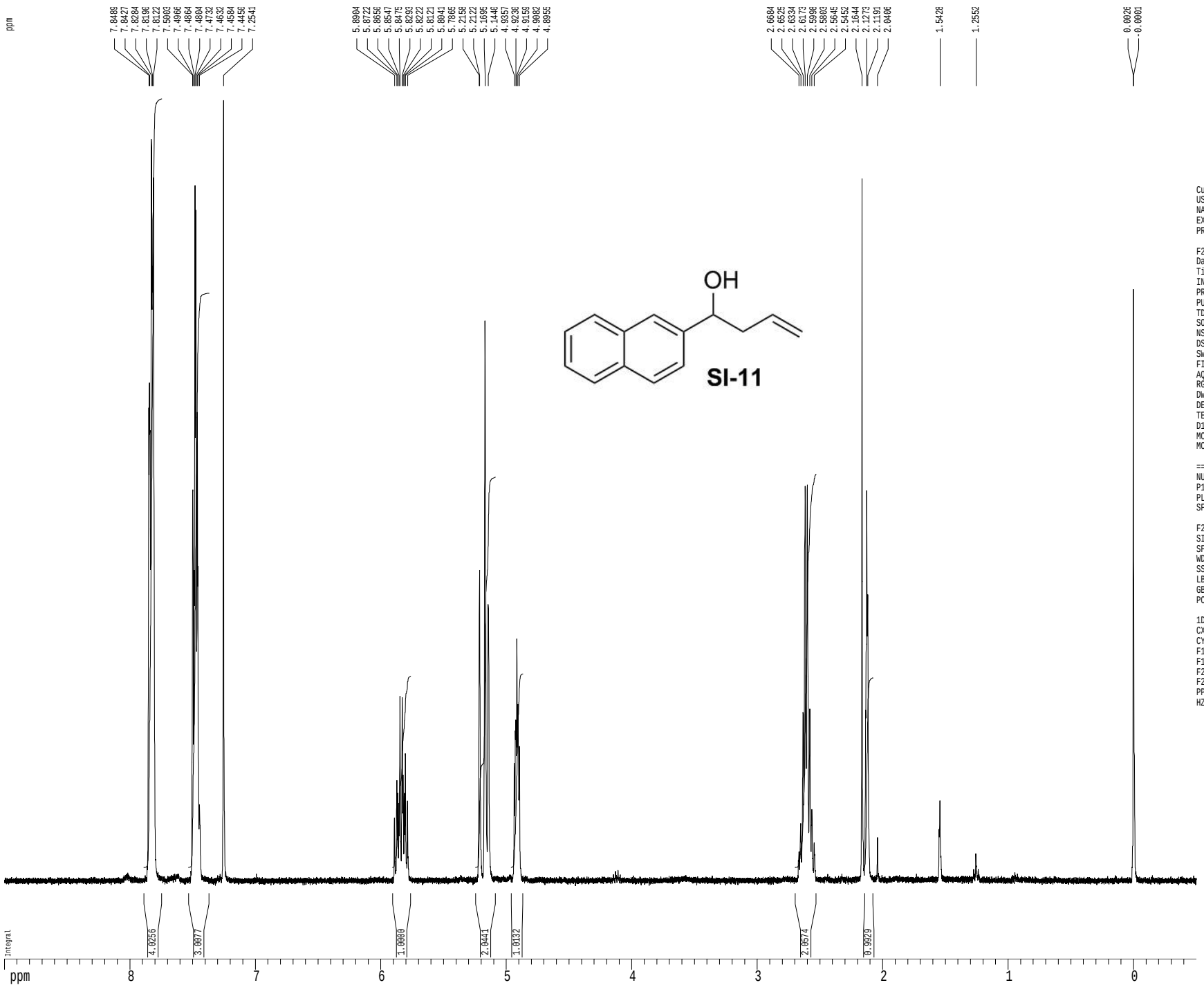
F2 - Acquisition Parameters
Date_           20150412
Time              19.39
INSTRUM           av600
PROBHD   5 mm BBO BB-1H
PULPROG       gnoe1cc.wu
TD                98074
SOLVENT           CDCl3
NS                  128
DS                    8
SWH            9615.385 Hz
FIDRES         0.098042 Hz
AQ             5.0998979 sec
RG                 1290
DW               52.000 usec
DE                6.50 usec
TE                298.0 K
D1           1.00000000 sec
D8           0.50000000 sec
D16          0.00020000 sec
D21          0.33375800 sec
D22          0.16399699 sec
P2               18.00 usec

======== CHANNEL f1 ========
SFO1         600.1330186 MHz
NUC1                1H
P1                9.00 usec
P3               27.00 usec
P4               36.00 usec
P5               24.00 usec
P12           40000.00 usec

F2 - Processing parameters
SI                65536
SF           600.1300000 MHz
WDW                 EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.80 cm
CY                50.00 cm
F1P               9.000 ppm
F1             5401.17 Hz
F2P              -0.500 ppm
F2             -300.06 Hz
PPMCM          0.41667 ppm/cm
HZCM         250.05418 Hz/cm
```

1H spectrum



Current Data Parameters
USER emilyt
NAME EJT-III-098
EXPNO 1
PROCNO 1

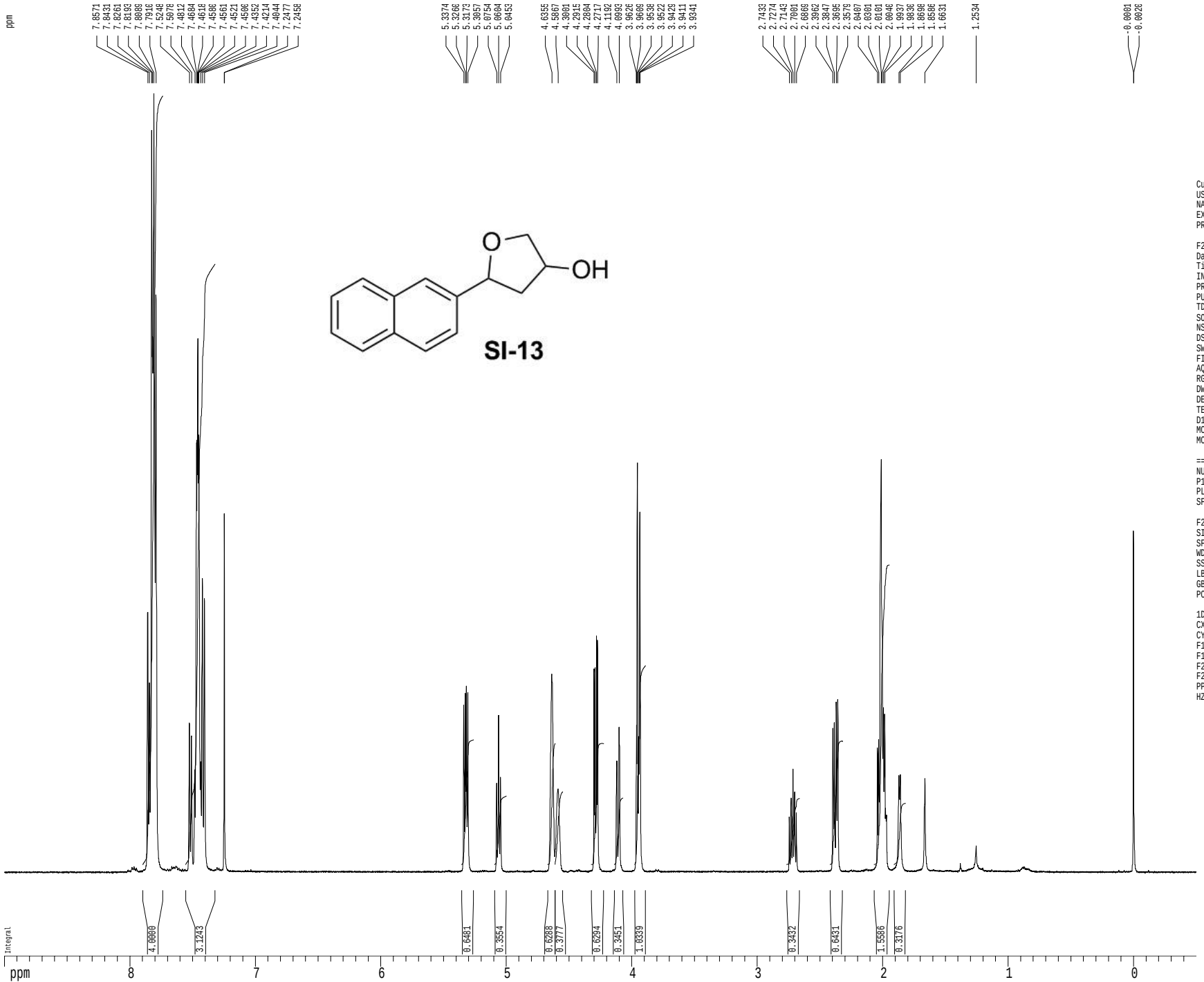
F2 - Acquisition Parameters
Date_ 20131202
Time 18.43
INSTRUM drx400
PROBHD 5 mm QNP H/F/P
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1118579 sec
RG 456.1
DW 78.000 usec
DE 4.50 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 400.1300243 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 3601.17 Hz
F2P -0.500 ppm
F2 -200.06 Hz
PPMCM 0.41667 ppm/cm
HZCM 166.72086 Hz/cm

1H spectrum



Current Data Parameters
USER emilyt
NAME EJT-IV-281
EXPNO 20
PROCNO 1

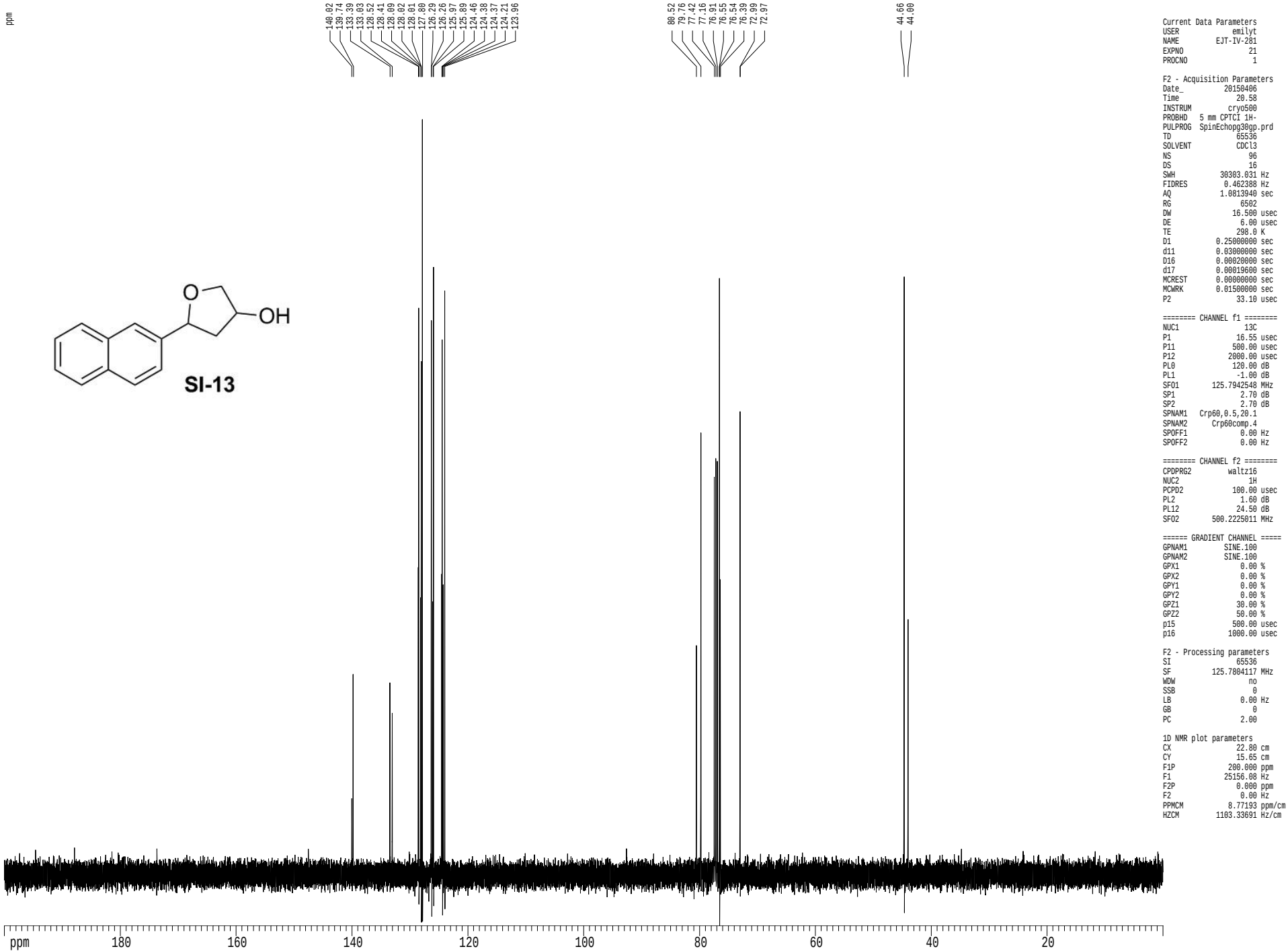
F2 - Acquisition Parameters
Date_ 20150406
Time 20.55
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200373 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42502 Hz/cm

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




```
Current Data Parameters
USER                emilyt
NAME           EJT-IV-281
EXPNO                  21
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150406
Time               20.58
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                 65536
SOLVENT            CDCl3
NS                    96
DS                    16
SWH            30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                  6502
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                33.10 usec

======== CHANNEL f1 ========
NUC1                 13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1   Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

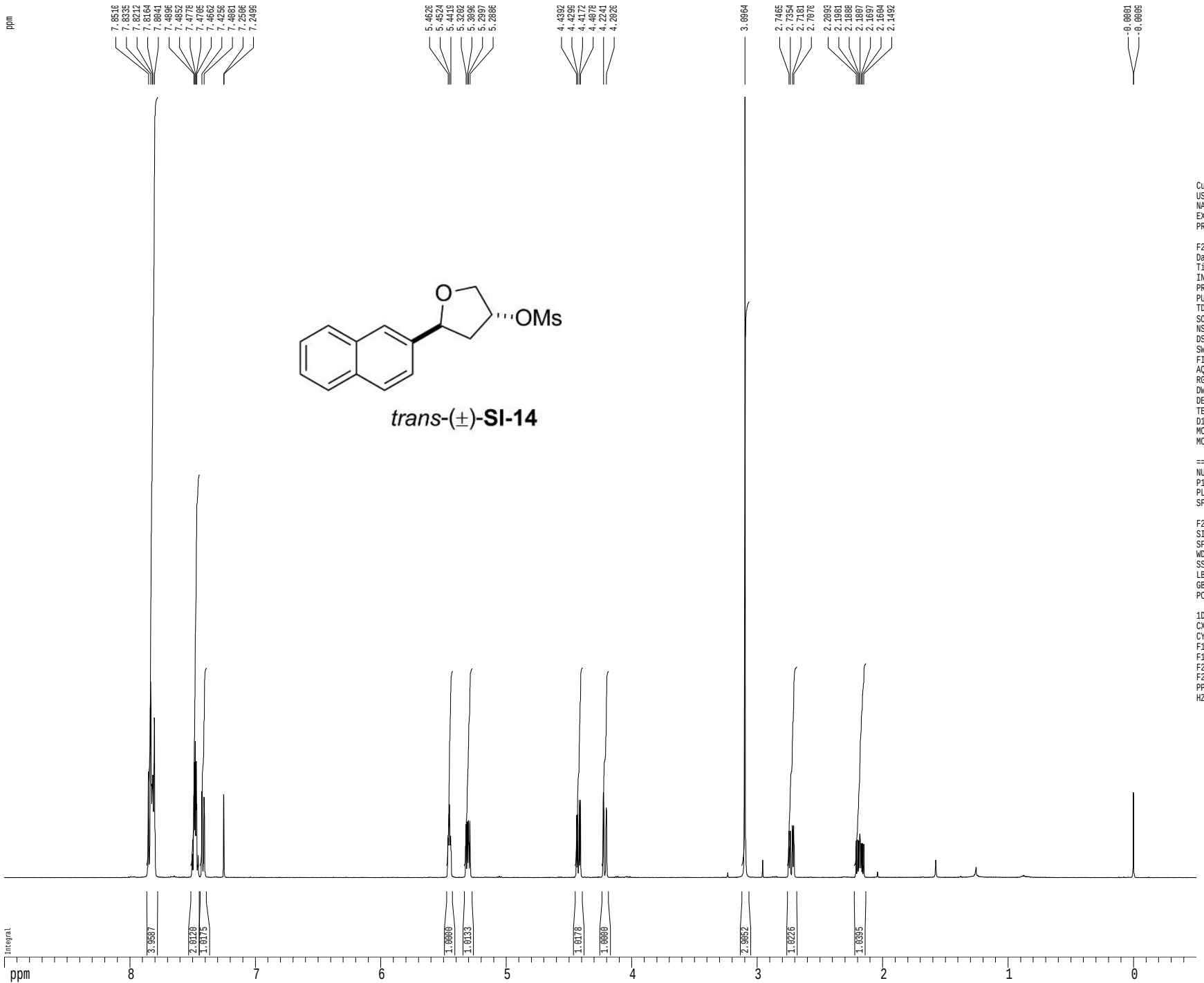
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2         500.2225011 MHz

====== 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           125.7804117 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  2.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.65 cm
F1P              200.000 ppm
F1             25156.08 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           8.77193 ppm/cm
HZCM         1103.33691 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME          EJT-IV-282
EXPNO                 20
PROCNO                 1

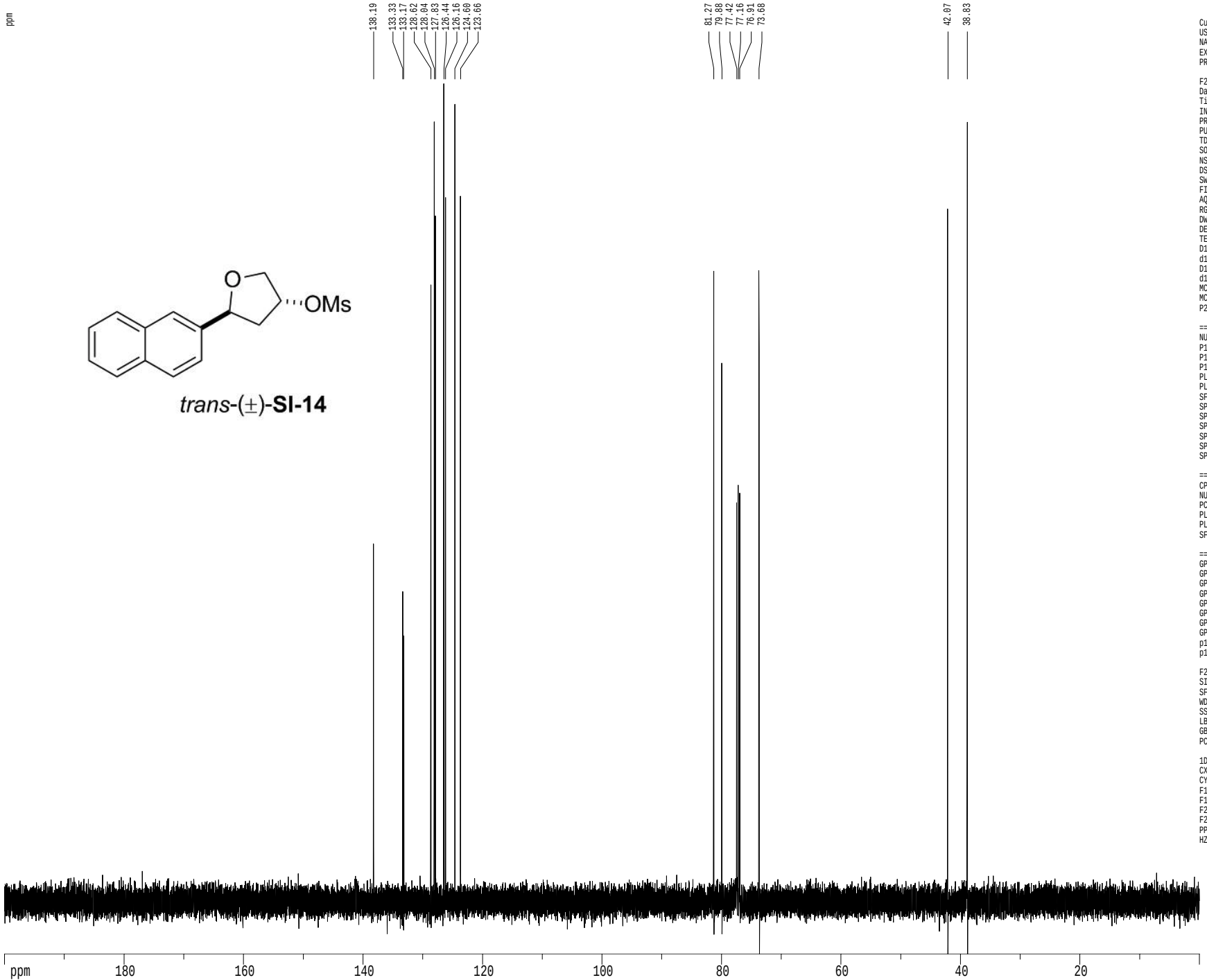
F2 - Acquisition Parameters
Date_          20150406
Time              21.03
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 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           500.2200355 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P                9.000 ppm
F1               4501.98 Hz
F2P               -0.500 ppm
F2               -250.11 Hz
PPMCM          0.41667 ppm/cm
HZCM         208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME            EJT-IV-282
EXPNO                   21
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150406
Time                 21.06
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                      55
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                  2.70 dB
SP2                  2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

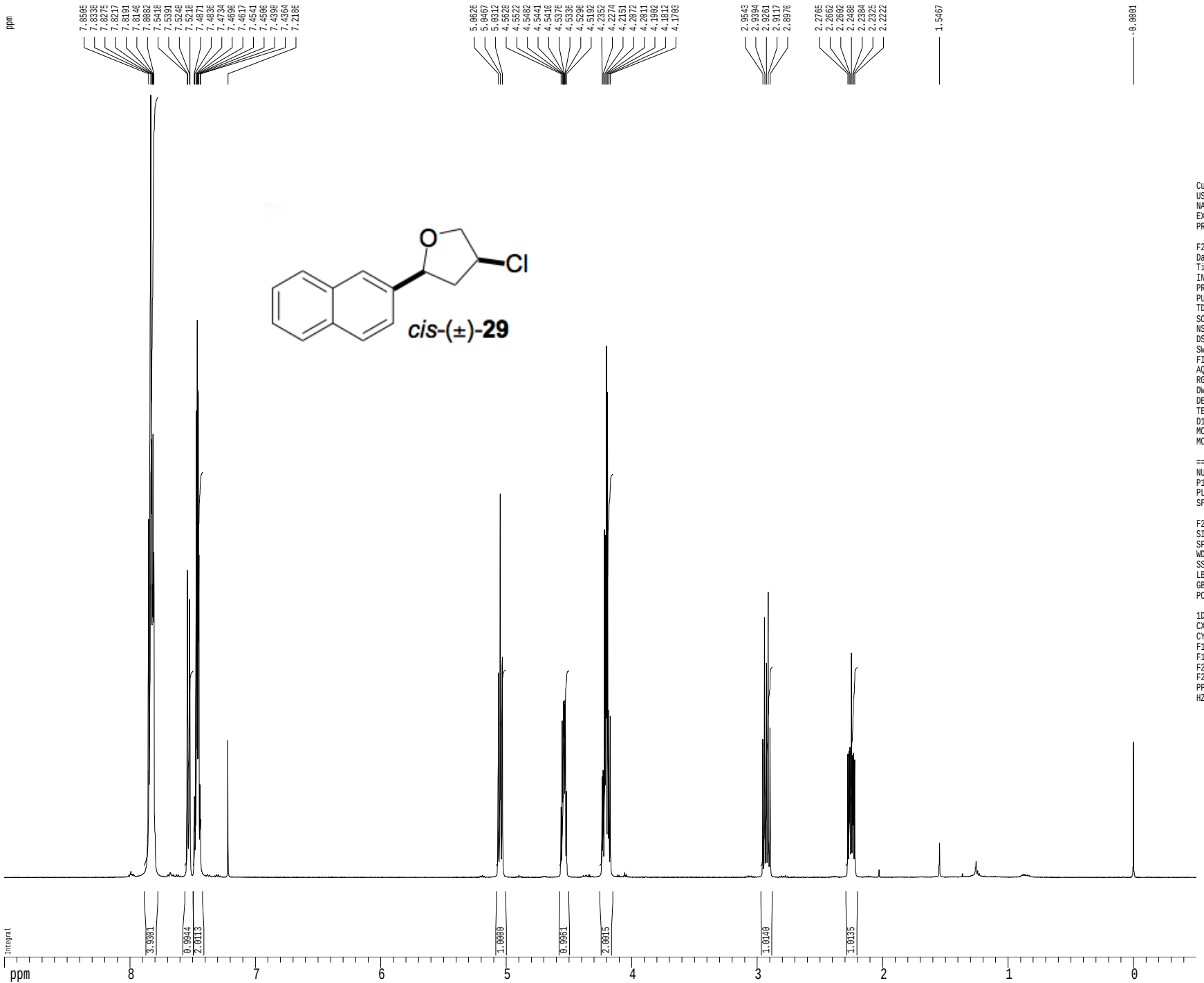
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              100.00 usec
PL2                  1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7804122 MHz
WDW                     no
SSB                      0
LB                   0.00 Hz
GB                       0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               200.000 ppm
F1              25156.08 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            8.77193 ppm/cm
HZCM          1103.33691 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME          EJT-IV-284
EXPNO                 20
PROCNO                 1

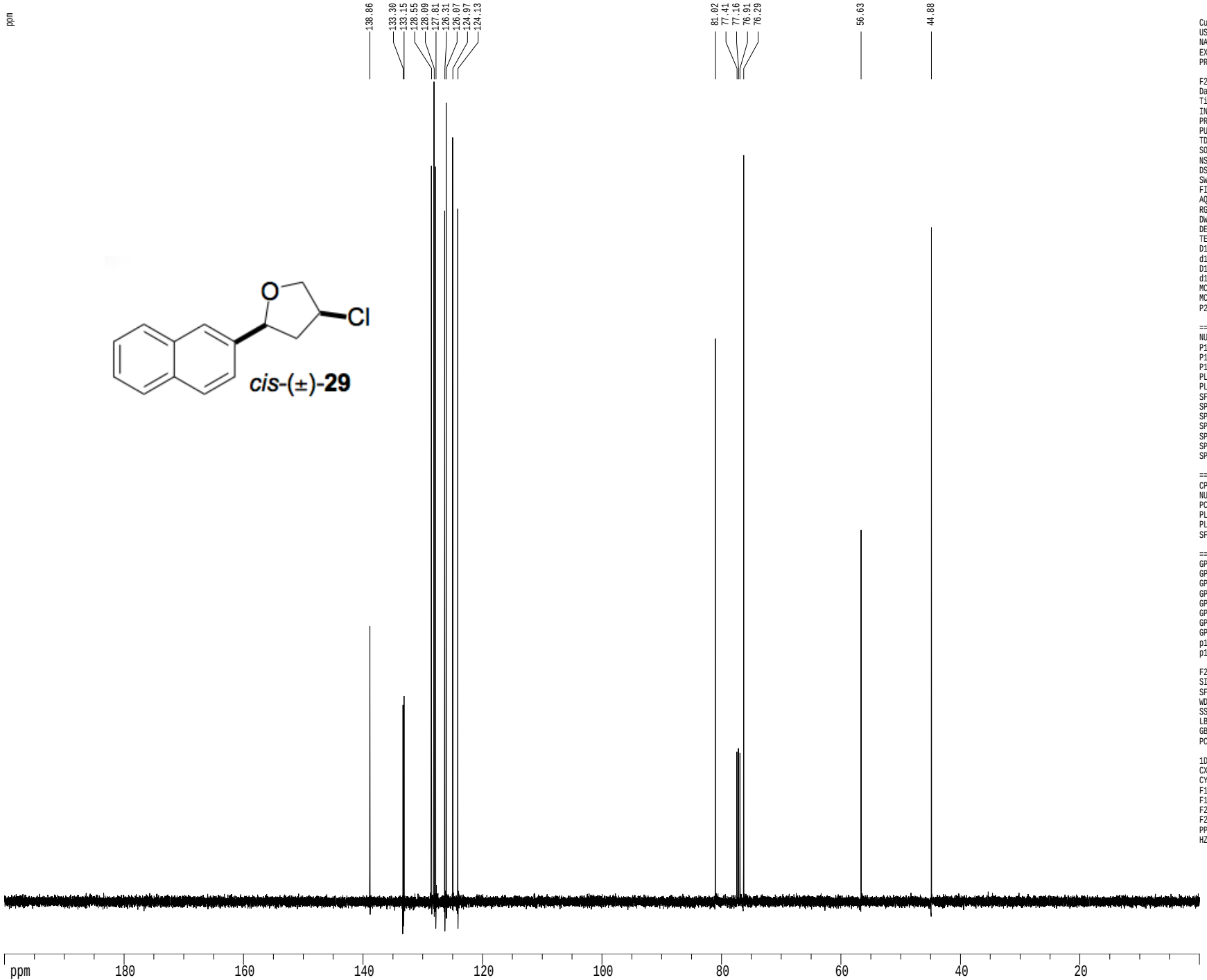
F2 - Acquisition Parameters
Date_           20150406
Time              21.11
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 Hz
AQ              5.0998774 sec
RG                   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           500.2200513 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 4.00

1D NMR plot parameters
CX                22.80 cm
CY                15.00 cm
F1P               9.000 ppm
F1              4501.98 Hz
F2P              -0.500 ppm
F2              -250.11 Hz
PPMCM           0.41667 ppm/cm
HZCM          208.42503 Hz/cm
```

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




```
Current Data Parameters
USER                emilyt
NAME            EJT-IV-284
EXPNO                   21
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150406
Time                 21.14
INSTRUM            cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                      75
DS                      16
SWH              30303.031 Hz
FIDRES            0.462388 Hz
AQ                1.0813940 sec
RG                   13004
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                   16.55 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1           125.7942548 MHz
SP1                   2.70 dB
SP2                   2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

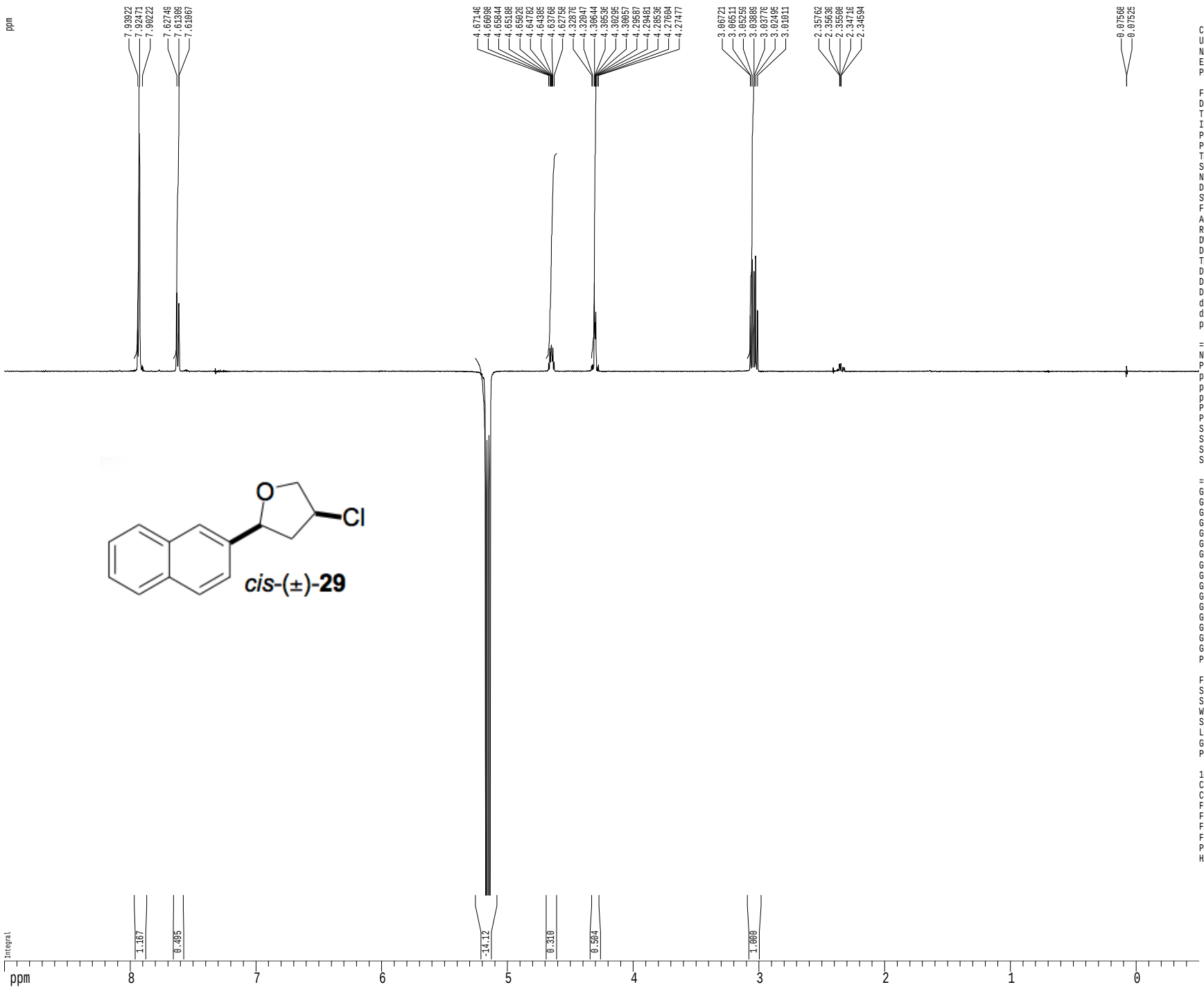
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               100.00 usec
PL2                   1.60 dB
PL12                 24.50 dB
SFO2           500.2225011 MHz

====== 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             125.7804173 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     2.00

1D NMR plot parameters
CX                    22.80 cm
CY                    15.65 cm
F1P                 200.000 ppm
F1                25156.08 Hz
F2P                   0.000 ppm
F2                    0.00 Hz
PPMCM              8.77193 ppm/cm
HZCM            1103.33704 Hz/cm
```

gnoe



Current Data Parameters
USER emilyt
NAME EJT-IV-284 noe
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150206
Time 22.57
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG gnoe1cc.wu
TD 65536
SOLVENT CDCl3
NS 256
DS 8
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 40.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
D8 5.00000000 sec
D16 0.00020000 sec
d21 3.34876490 sec
d22 1.64899695 sec
p2 15.00 usec

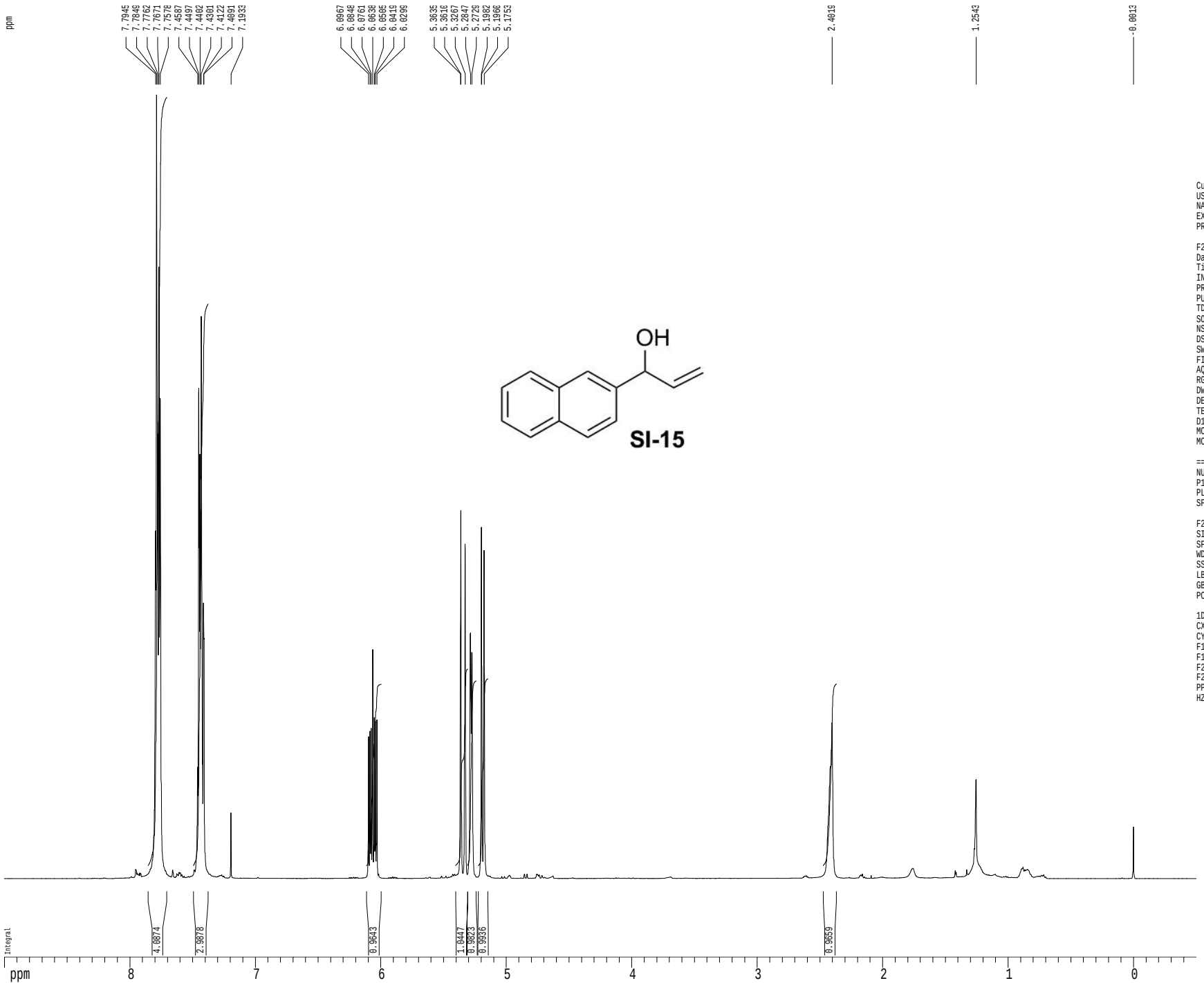
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
p3 22.50 usec
p4 30.00 usec
p5 20.00 usec
P12 40000.00 usec
PL1 1.60 dB
SFO1 500.2225782 MHz
SP1 61.60 dB
SPNAM1 gauss1.512
SPOFF1 0.00 Hz

====== GRADIENT CHANNEL =====
GPNAM1 sine.100
GPNAM2 sine.100
GPNAM3 sine.100
GPNAM4 sine.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPX4 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPY4 0.00 %
GPZ1 7.00 %
GPZ2 3.00 %
GPZ3 2.30 %
GPZ4 -2.30 %
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.80 cm
CY 50.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42500 Hz/cm

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-252-cryo4
EXPNO                    1
PROCNO                   1

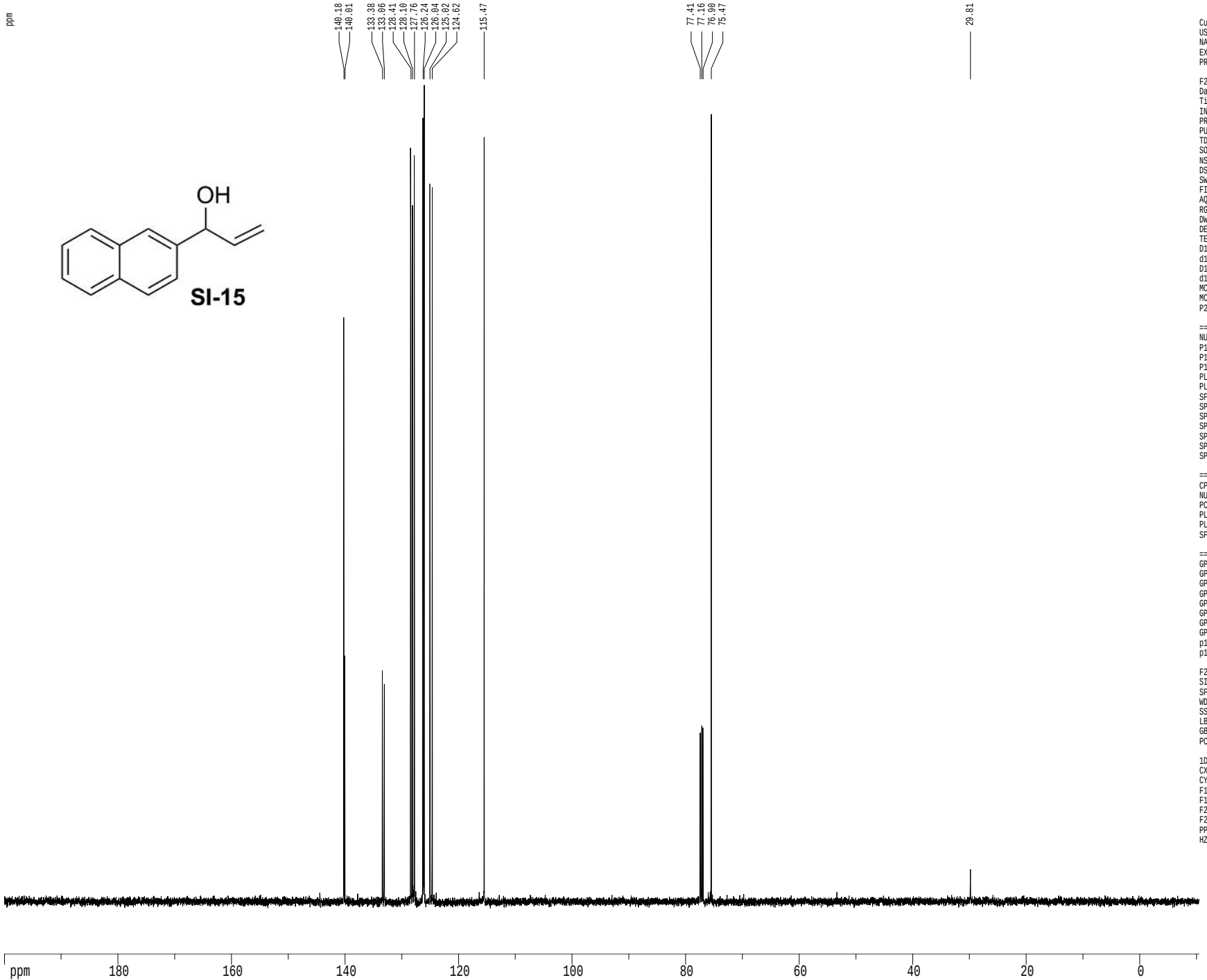
F2 - Acquisition Parameters
Date_            20150324
Time                17.47
INSTRUM          cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG              zg30
TD                  48074
SOLVENT             CDCl3
NS                      8
DS                      2
SWH              8012.820 Hz
FIDRES           0.166677 Hz
AQ               2.9998677 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            500.2200639 MHz
WDW                    EM
SSB                     0
LB                  0.30 Hz
GB                      0
PC                   4.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.00 cm
F1P                 9.000 ppm
F1                4501.98 Hz
F2P                -0.500 ppm
F2                -250.11 Hz
PPMCM            0.41667 ppm/cm
HZCM           208.42503 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-252-cryo4
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150324
Time                17.48
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                     39
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                33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

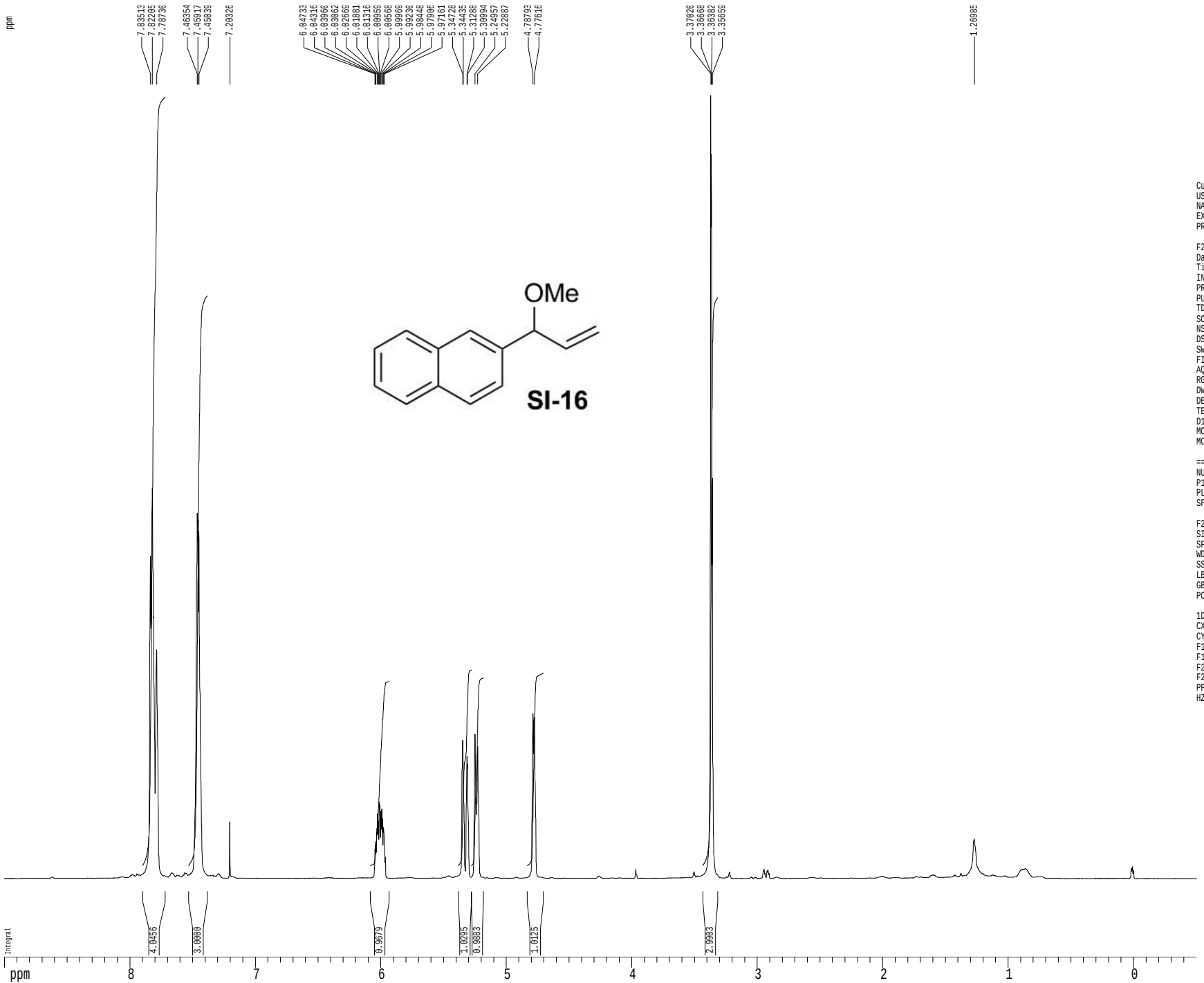
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== 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           125.7804228 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               200.000 ppm
F1              25156.09 Hz
F2P               -10.490 ppm
F2              -1319.48 Hz
PPMCM             9.23203 ppm/cm
HZCM           1161.20923 Hz/cm
```

1H spectrum



Current Data Parameters
USER lucase
NAME LWE-II-253-cryo8
EXPNO 1
PROCNO 1

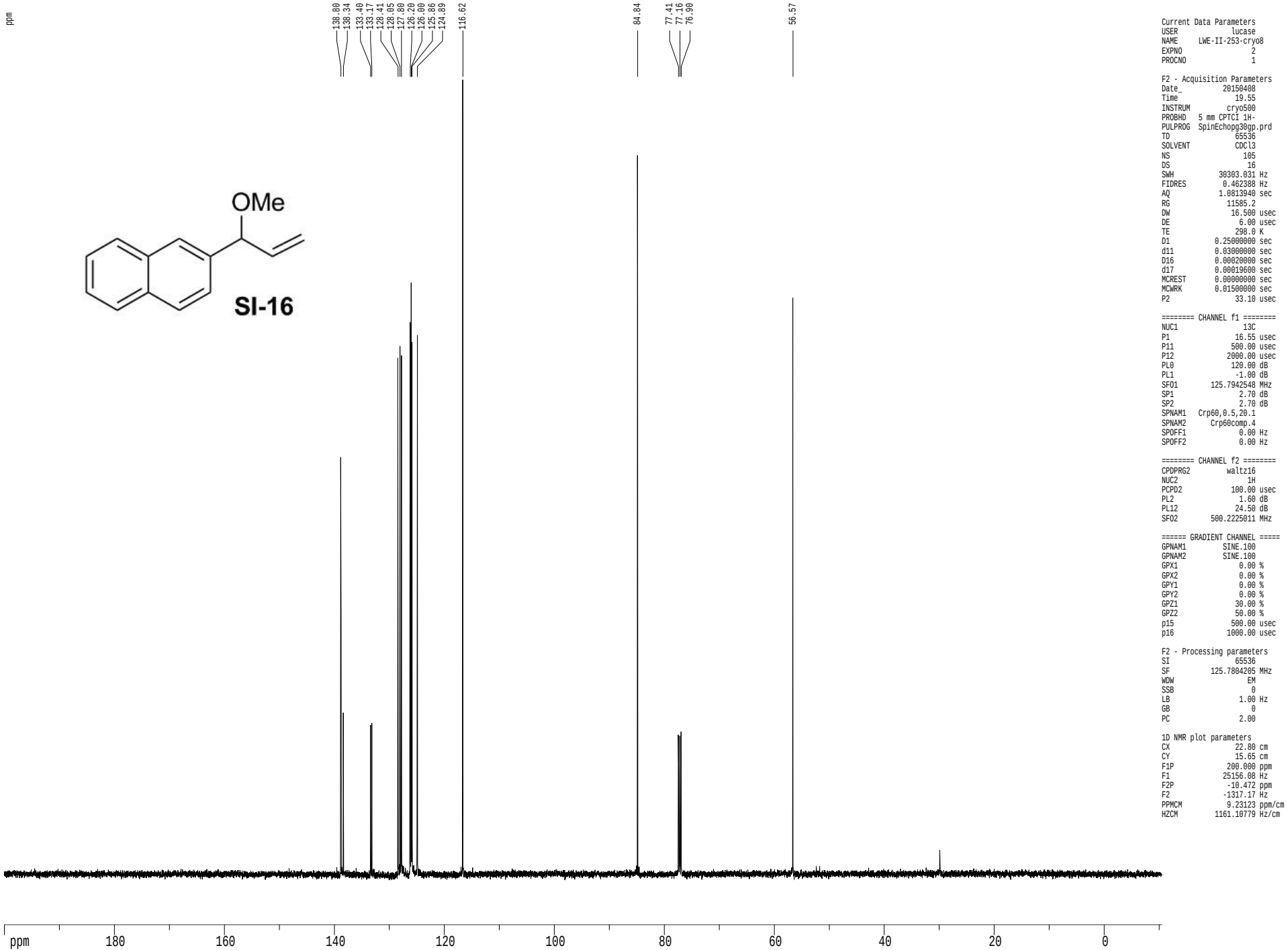
F2 - Acquisition Parameters
Date_ 20150408
Time 19.51
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 4.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200589 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42503 Hz/cm

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-253-cryo8
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150408
Time                19.55
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    105
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                11585.2
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                33.10 usec

======== CHANNEL f1 ========
NUC1                  13C
P1                 16.55 usec
P11               500.00 usec
P12              2000.00 usec
PL0               120.00 dB
PL1                -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

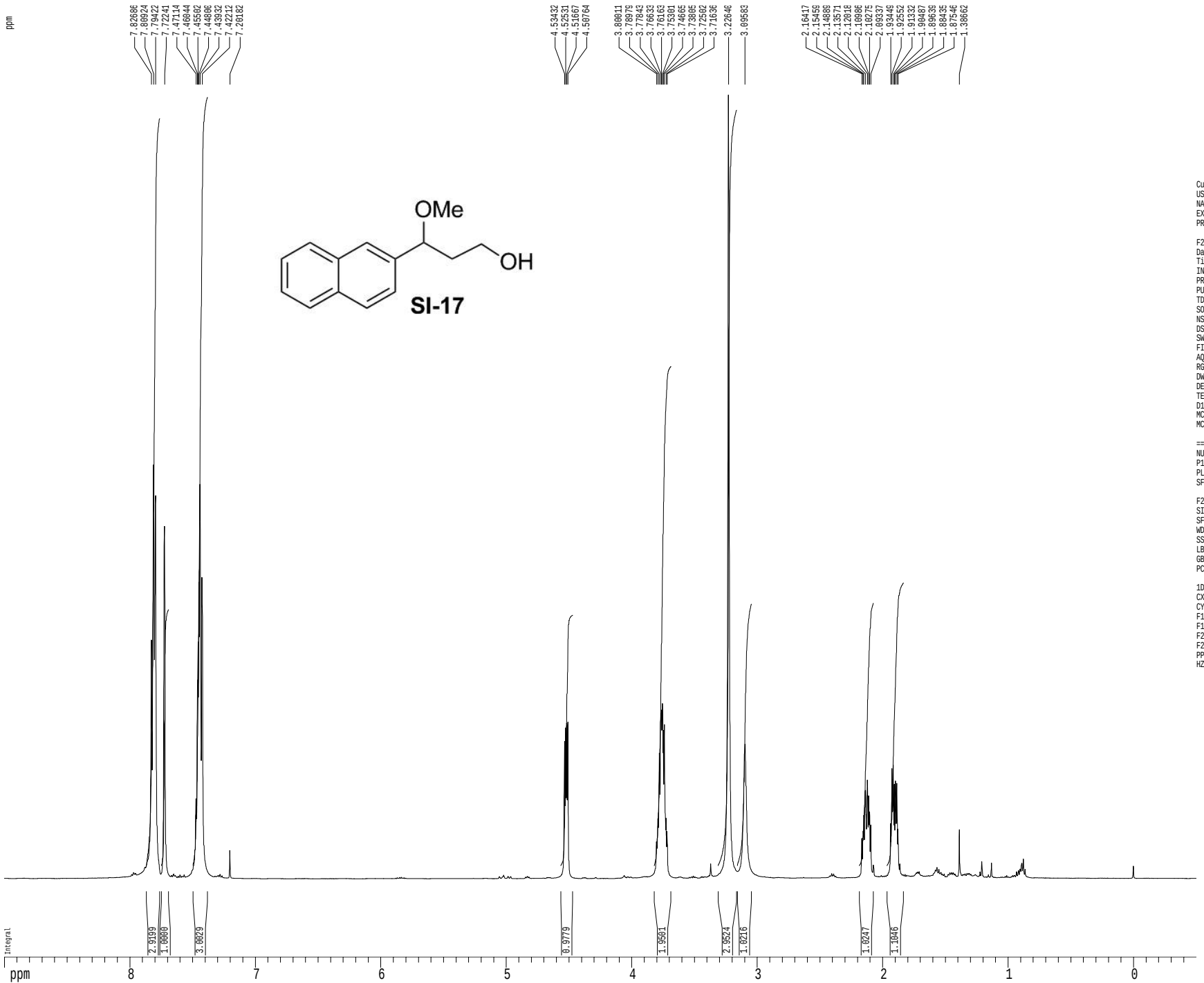
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             100.00 usec
PL2                1.60 dB
PL12               24.50 dB
SFO2         500.2225011 MHz

====== 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           125.7804205 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               200.000 ppm
F1              25156.08 Hz
F2P               -10.472 ppm
F2              -1317.17 Hz
PPMCM            9.23123 ppm/cm
HZCM          1161.10779 Hz/cm
```

1H spectrum



Current Data Parameters
USER lucase
NAME LWE-II-275-cryolast
EXPNO 1
PROCNO 1

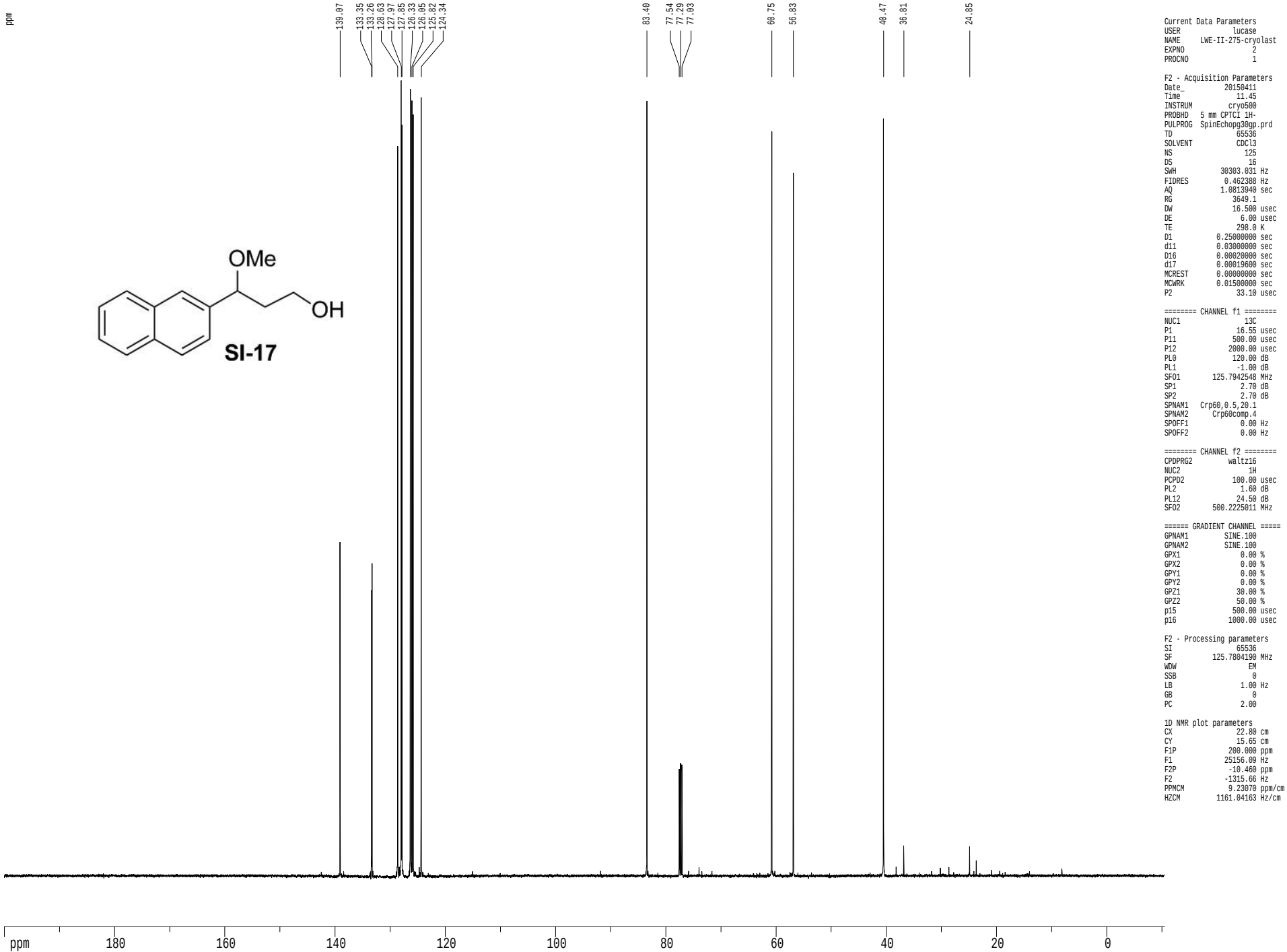
F2 - Acquisition Parameters
Date_ 20150411
Time 11.41
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 2.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200588 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 9.000 ppm
F1 4501.98 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.41667 ppm/cm
HZCM 208.42503 Hz/cm

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-275-cryolast
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20150411
Time                  11.45
INSTRUM            cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG   SpinEchopg30gp.prd
TD                    65536
SOLVENT               CDCl3
NS                      125
DS                       16
SWH              30303.031 Hz
FIDRES            0.462388 Hz
AQ                1.0813940 sec
RG                   3649.1
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                   16.55 usec
P11                 500.00 usec
P12                2000.00 usec
PL0                 120.00 dB
PL1                  -1.00 dB
SFO1           125.7942548 MHz
SP1                   2.70 dB
SP2                   2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1                0.00 Hz
SPOFF2                0.00 Hz

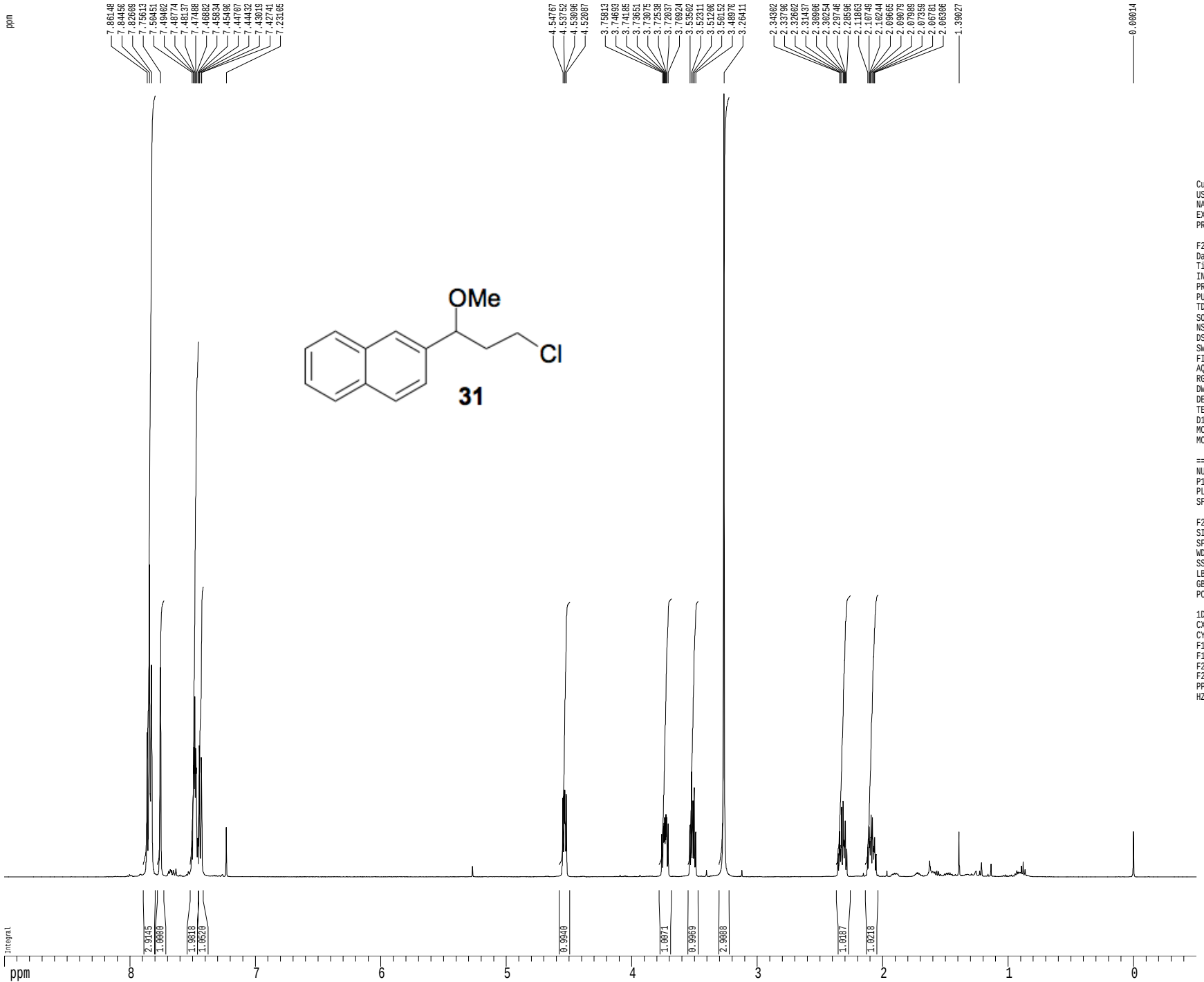
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               100.00 usec
PL2                   1.60 dB
PL12                 24.50 dB
SFO2           500.2225011 MHz

====== 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             125.7804190 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     2.00

1D NMR plot parameters
CX                    22.80 cm
CY                    15.65 cm
F1P                 200.000 ppm
F1                25156.09 Hz
F2P                -10.460 ppm
F2                -1315.66 Hz
PPMCM              9.23070 ppm/cm
HZCM            1161.04163 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER                lucase
NAME      LWE-II-276-cryo
EXPNO                    1
PROCNO                   1

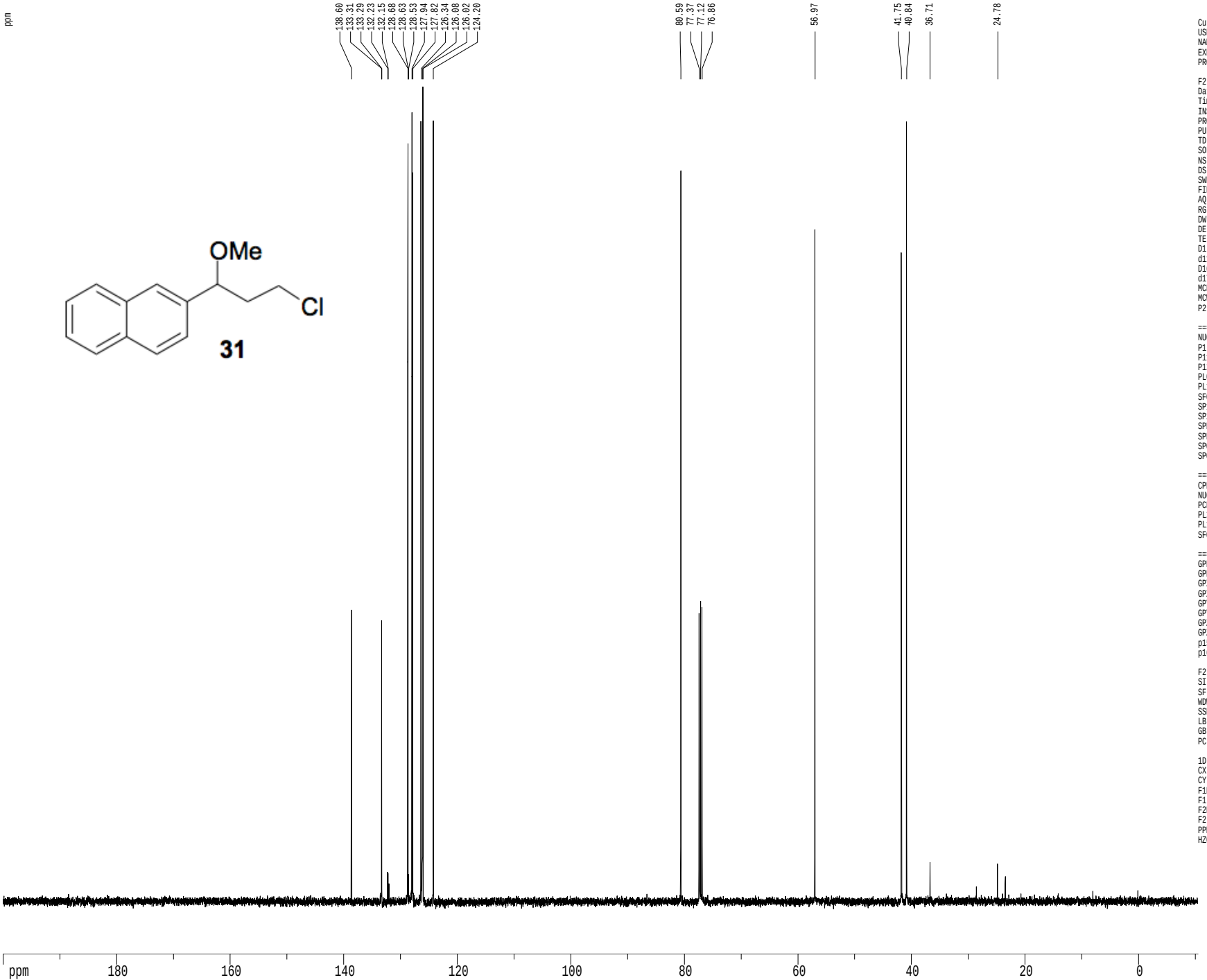
F2 - Acquisition Parameters
Date_             20150411
Time                 17.44
INSTRUM            cryo500
PROBHD    5 mm CPTCI 1H-
PULPROG                zg30
TD                    81728
SOLVENT               CDCl3
NS                        8
DS                        2
SWH                8012.820 Hz
FIDRES                0.098043 Hz
AQ                 5.0998774 sec
RG                      3.2
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                500.2200451 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                     4.00

1D NMR plot parameters
CX                     22.80 cm
CY                     15.00 cm
F1P                     9.000 ppm
F1                   4501.98 Hz
F2P                    -0.500 ppm
F2                   -250.11 Hz
PPMCM                0.41667 ppm/cm
HZCM               208.42502 Hz/cm
```

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




```
Current Data Parameters
USER                lucase
NAME      LWE-II-276-cryo
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20150411
Time                17.49
INSTRUM           cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     144
DS                      16
SWH              30303.031 Hz
FIDRES           0.462388 Hz
AQ               1.0813940 sec
RG                    6502
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                  33.10 usec

======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                  2.70 dB
SP2                  2.70 dB
SPNAM1    Crp60,0.5,20.1
SPNAM2       Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

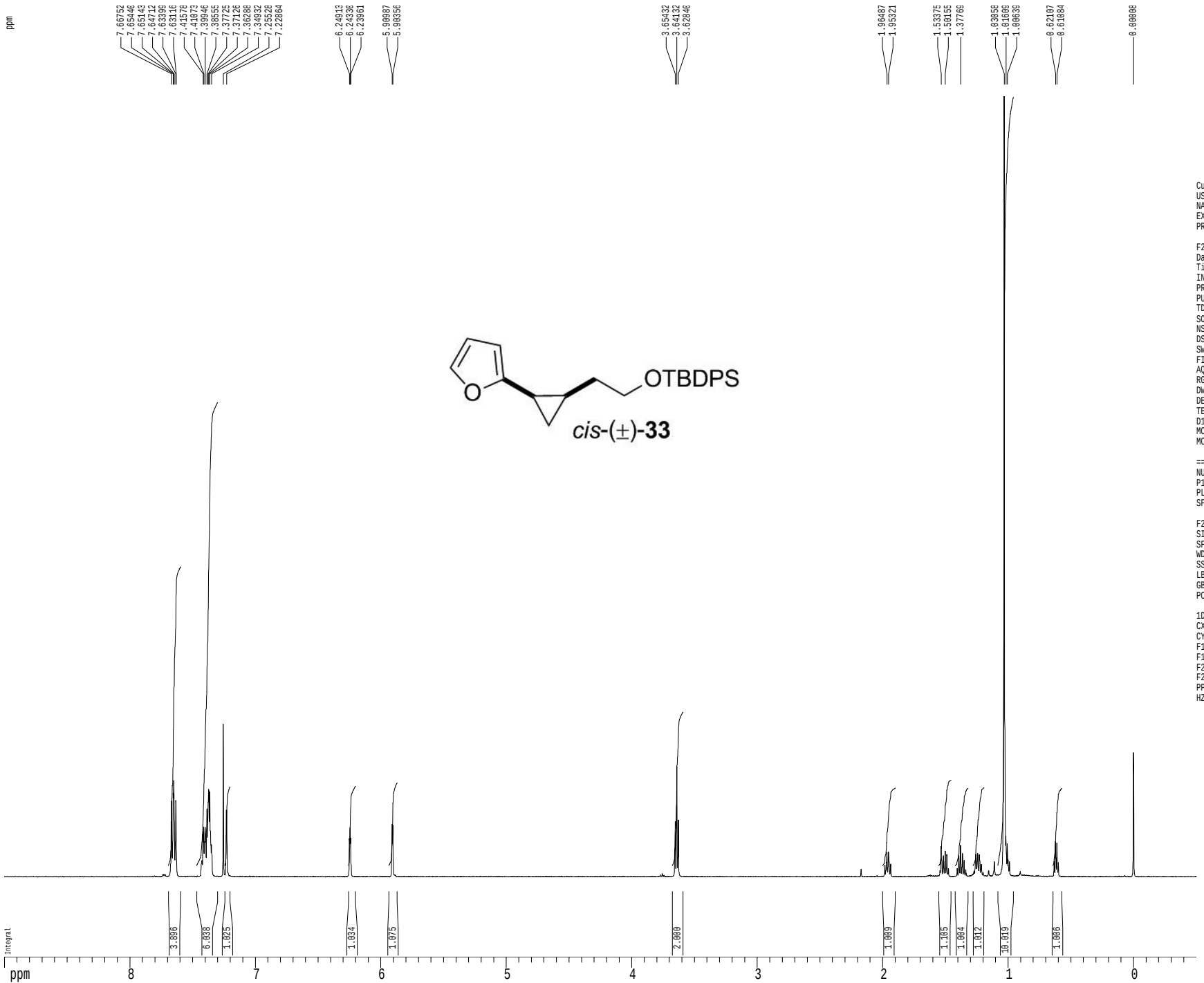
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                 1.60 dB
PL12                24.50 dB
SFO2          500.2225011 MHz

====== 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            125.7804190 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.80 cm
CY                   15.65 cm
F1P                200.000 ppm
F1               25156.09 Hz
F2P                -10.460 ppm
F2               -1315.66 Hz
PPMCM             9.23070 ppm/cm
HZCM           1161.04163 Hz/cm
```

1H spectrum




```
Current Data Parameters
USER              emilyt
NAME         EJT-V-056-A
EXPNO                10
PROCNO                1

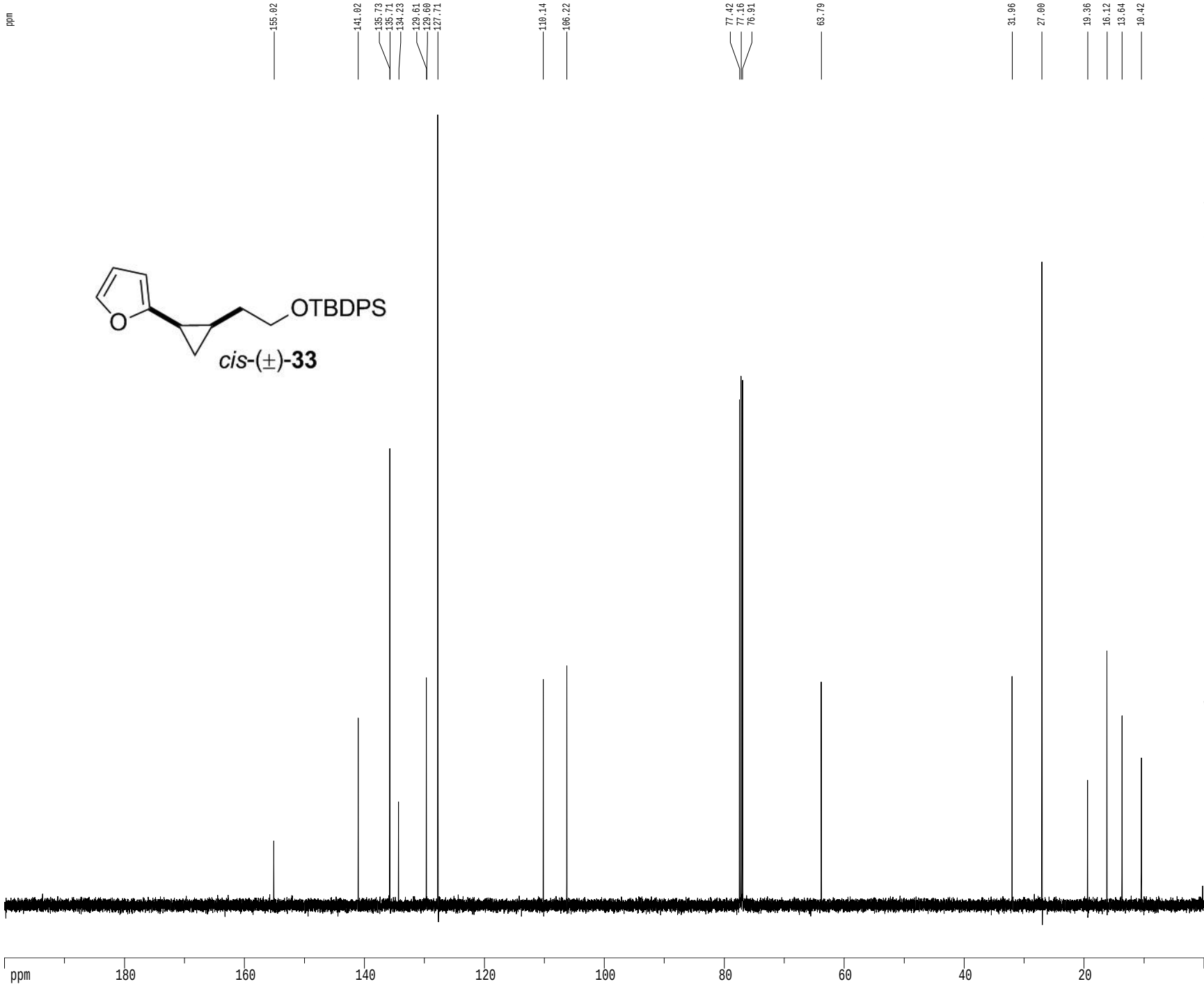
F2 - Acquisition Parameters
Date_          20150316
Time              20.34
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 81728
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.098043 Hz
AQ              5.0998774 sec
RG                   3.6
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           500.2200335 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  4.00

1D NMR plot parameters
CX                 22.80 cm
CY                 15.00 cm
F1P                9.000 ppm
F1               4501.98 Hz
F2P               -0.500 ppm
F2               -250.11 Hz
PPMCM           0.41667 ppm/cm
HZCM          208.42502 Hz/cm
```

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




```
Current Data Parameters
USER              emilyt
NAME          EJT-V-056-A
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150316
Time                20.40
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                  65536
SOLVENT             CDCl3
NS                    475
DS                     16
SWH             30303.031 Hz
FIDRES          0.462388 Hz
AQ              1.0813940 sec
RG                   3251
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                 33.10 usec

======== CHANNEL f1 ========
NUC1                13C
P1                16.55 usec
P11              500.00 usec
P12             2000.00 usec
PL0              120.00 dB
PL1               -1.00 dB
SFO1         125.7942548 MHz
SP1                2.70 dB
SP2                2.70 dB
SPNAM1   Crp60,0.5,20.1
SPNAM2      Crp60comp.4
SPOFF1               0.00 Hz
SPOFF2               0.00 Hz

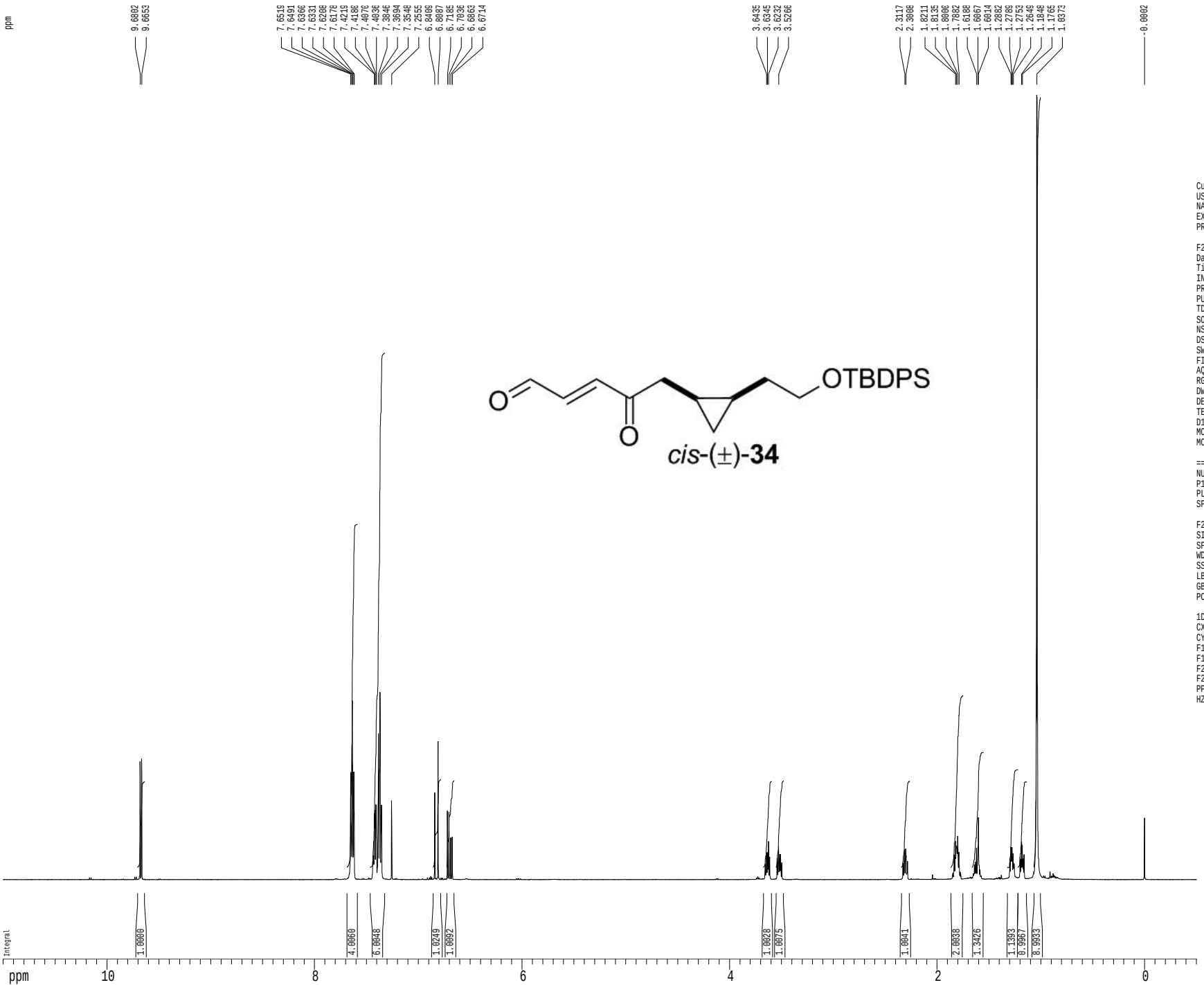
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2            100.00 usec
PL2                1.60 dB
PL12              24.50 dB
SFO2         500.2225011 MHz

====== 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           125.7804076 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P              200.000 ppm
F1              25156.08 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           8.77193 ppm/cm
HZCM          1103.33691 Hz/cm
```

1H spectrum



Current Data Parameters
USER emilyt
NAME EJT-V-057
EXPNO 10
PROCNO 1

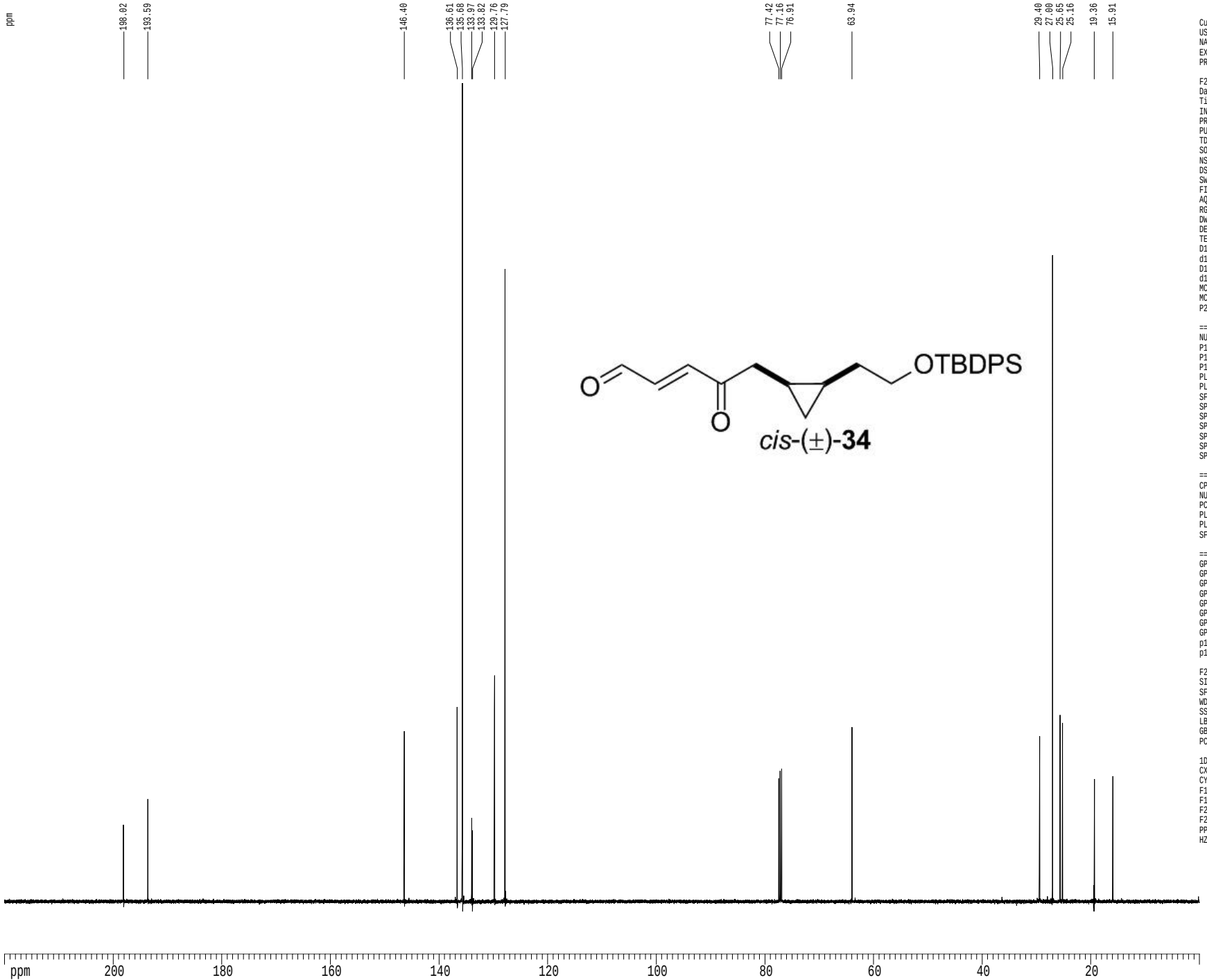
F2 - Acquisition Parameters
Date_ 20150318
Time 22.02
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 3.2
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

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

F2 - Processing parameters
SI 65536
SF 500.2200332 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 11.000 ppm
F1 5502.42 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.50439 ppm/cm
HZCM 252.30397 Hz/cm

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




```
Current Data Parameters
USER                emilyt
NAME             EJT-V-057
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150318
Time                 22.08
INSTRUM            cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG  SpinEchopg30gp.prd
TD                   65536
SOLVENT              CDCl3
NS                     569
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                  33.10 usec

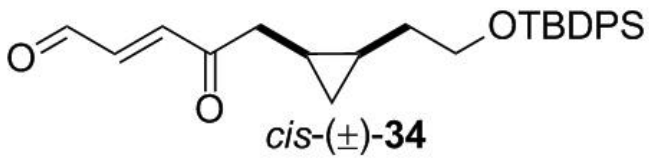
======== CHANNEL f1 ========
NUC1                   13C
P1                  16.55 usec
P11                500.00 usec
P12               2000.00 usec
PL0                120.00 dB
PL1                 -1.00 dB
SFO1          125.7942548 MHz
SP1                  2.70 dB
SP2                  2.70 dB
SPNAM1    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            125.7804103 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.80 cm
CY                  15.65 cm
F1P               220.000 ppm
F1              27671.69 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            9.64912 ppm/cm
HZCM          1213.67065 Hz/cm
```



cis-(±)-**34**

gcosy60


```
        Current Data Parameters
USER              emilyt
NAME           EJT-V-057
EXPNO                 12
PROCNO                 1

      F2 - Acquisition Parameters
Date_           20150318
Time               22.18
INSTRUM          cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG    cosygp60.prd
TD                  2048
SOLVENT            CDCl3
NS                     2
DS                    16
SWH             5733.945 Hz
FIDRES          2.799778 Hz
AQ              0.1786356 sec
RG                  35.9
DW                87.200 usec
DE                 6.00 usec
TE                298.0 K
d0            0.00000300 sec
D1            1.00000000 sec
d13           0.00000300 sec
D16           0.00020000 sec
IN0           0.00017440 sec

     ======== CHANNEL f1 ========
NUC1                  1H
P1                  7.50 usec
PL1                 1.60 dB
SFO1         500.2226544 MHz

     ====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPX1                0.00 %
GPX2                0.00 %
GPY1                0.00 %
GPY2                0.00 %
GPZ1               17.00 %
GPZ2               17.00 %
P16              1000.00 usec

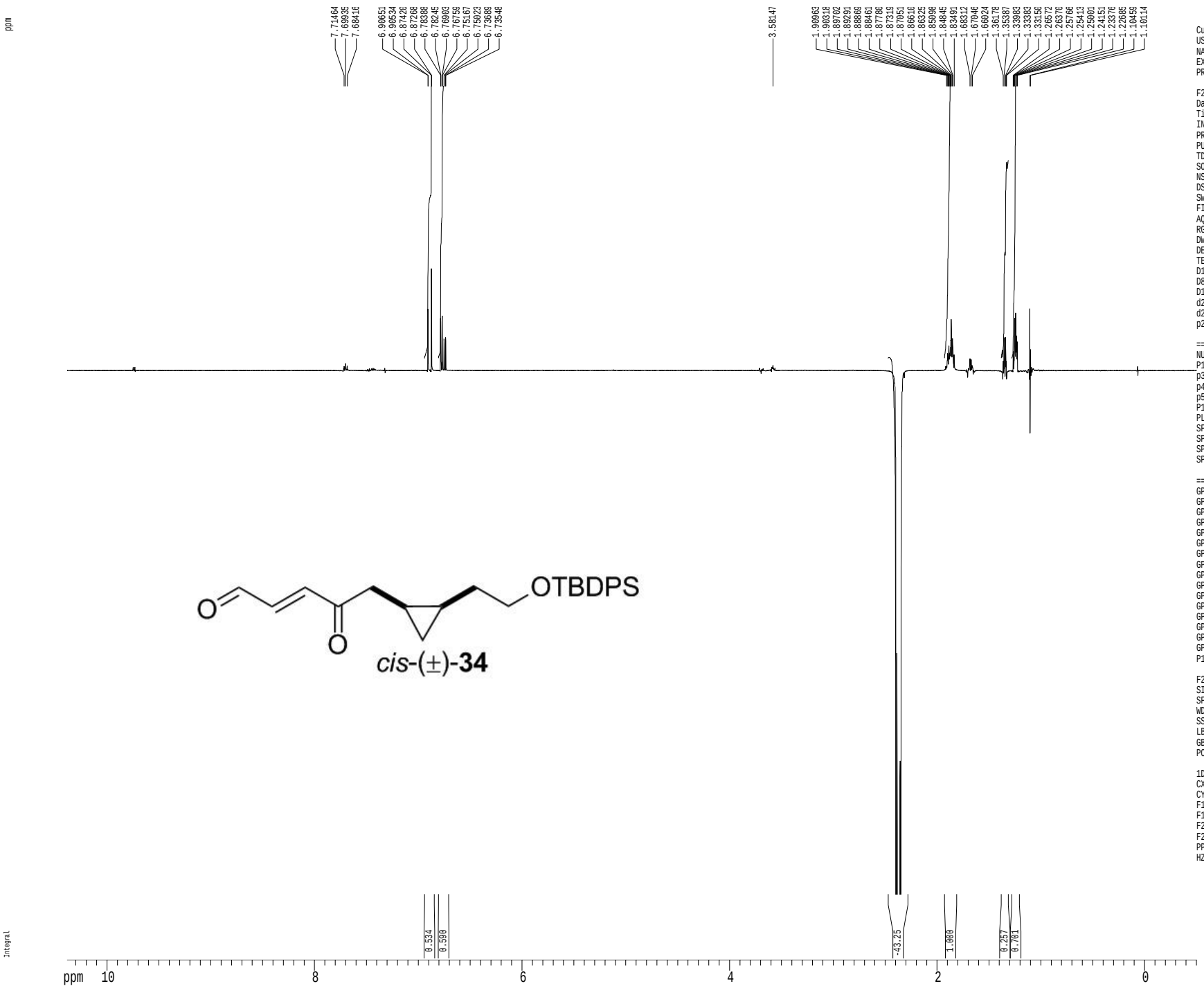
      F1 - Acquisition parameters
ND0                    1
TD                   128
SFO1           500.2227 MHz
FIDRES         44.796444 Hz
SW                11.463 ppm
FnMODE         undefined

      F2 - Processing parameters
SI                  1024
SF           500.2200332 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  4.00

      F1 - Processing parameters
SI                  1024
MC2                   QF
SF           500.2200332 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0

        2D NMR plot parameters
CX2                15.00 cm
CX1                15.00 cm
F2PLO             10.971 ppm
F2LO             5488.13 Hz
F2PHI             -0.491 ppm
F2HI             -245.82 Hz
F1PLO             10.971 ppm
F1LO             5488.13 Hz
F1PHI             -0.491 ppm
F1HI             -245.82 Hz
F2PPMCM          0.76419 ppm/cm
F2HZCM         382.26297 Hz/cm
F1PPMCM          0.76419 ppm/cm
F1HZCM         382.26297 Hz/cm
```

gnoe




```
Current Data Parameters
USER              emilyt
NAME           EJT-V-057
EXPNO                 13
PROCNO                 1

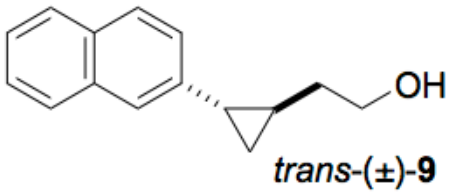
F2 - Acquisition Parameters
Date_           20150318
Time              22.51
INSTRUM         cryo500
PROBHD   5 mm CPTCI 1H-
PULPROG       gnoe1cc.wu
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     8
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894966 sec
RG                   128
DW                62.400 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
D8             0.50000000 sec
D16            0.00020000 sec
d21            0.33376500 sec
d22            0.16399699 sec
p2                15.00 usec

======== CHANNEL f1 ========
NUC1                 1H
P1                 7.50 usec
p3                22.50 usec
p4                30.00 usec
p5                20.00 usec
P12            40000.00 usec
PL1                1.60 dB
SFO1         500.2211869 MHz
SP1                61.60 dB
SPNAM1        gauss1.512
SPOFF1             0.00 Hz

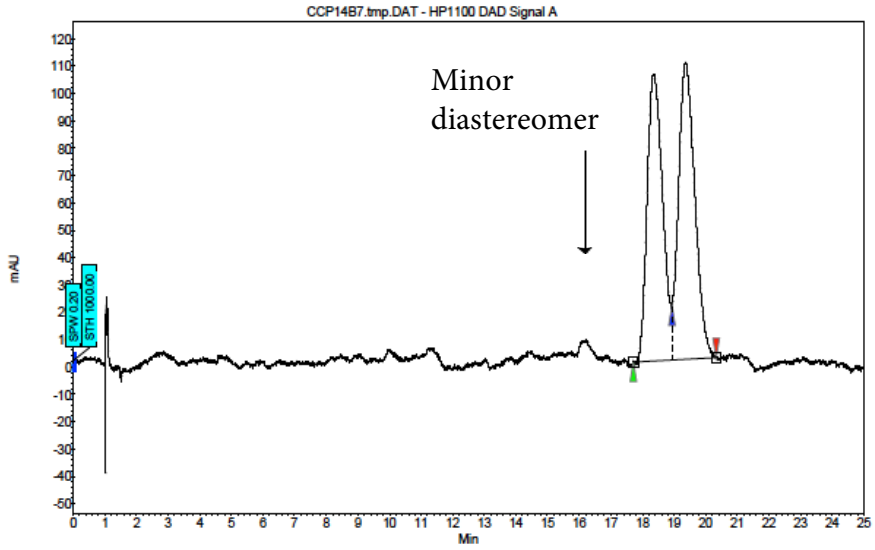
====== GRADIENT CHANNEL =====
GPNAM1          sine.100
GPNAM2          sine.100
GPNAM3          sine.100
GPNAM4          sine.100
GPX1               0.00 %
GPX2               0.00 %
GPX3               0.00 %
GPX4               0.00 %
GPY1               0.00 %
GPY2               0.00 %
GPY3               0.00 %
GPY4               0.00 %
GPZ1               7.00 %
GPZ2               3.00 %
GPZ3               2.30 %
GPZ4              -2.30 %
P16             1000.00 usec

F2 - Processing parameters
SI                 65536
SF          500.2200000 MHz
WDW                   no
SSB                    0
LB                 0.00 Hz
GB                     0
PC                 1.00

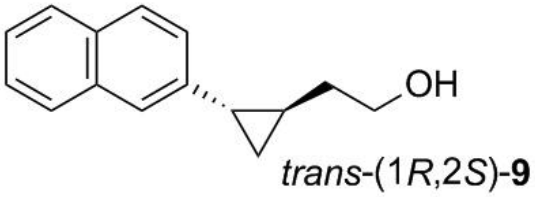
1D NMR plot parameters
CX                22.80 cm
CY                50.00 cm
F1P              11.000 ppm
F1             5502.42 Hz
F2P              -0.500 ppm
F2             -250.11 Hz
PPMCM          0.50439 ppm/cm
HZCM         252.30396 Hz/cm
```



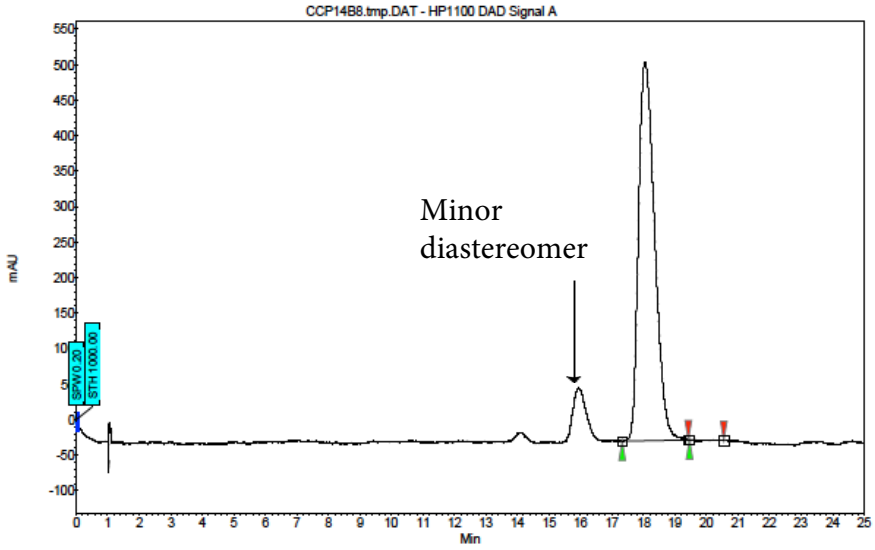
trans-(±)-**9**



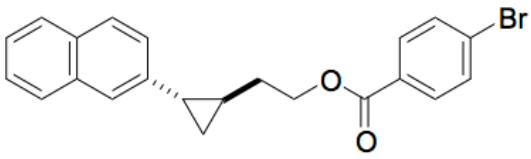
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	17.71	18.35	18.93	0.00	47.68	105.1	59.5	47.685
2	UNKNOWN	18.93	19.36	20.33	0.00	52.32	108.7	65.3	52.315
Total						100.00	213.8	124.7	100.000



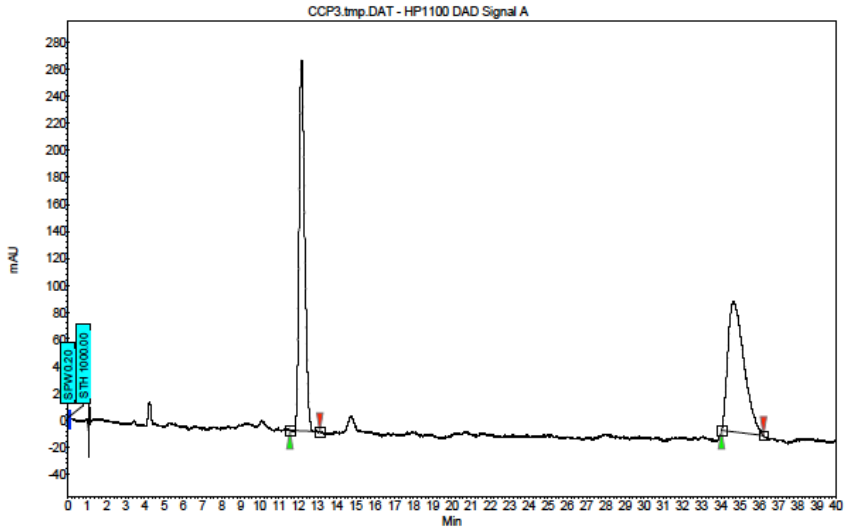
trans-(1*R*,2*S*)-**9**



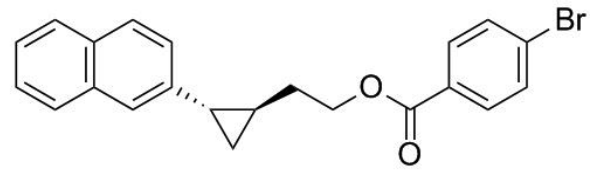
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	17.33	18.05	19.42	0.00	99.92	533.7	315.0	99.920
2	UNKNOWN	19.46	19.67	20.54	0.00	0.08	1.7	0.3	0.080
Total						100.00	535.4	315.3	100.000



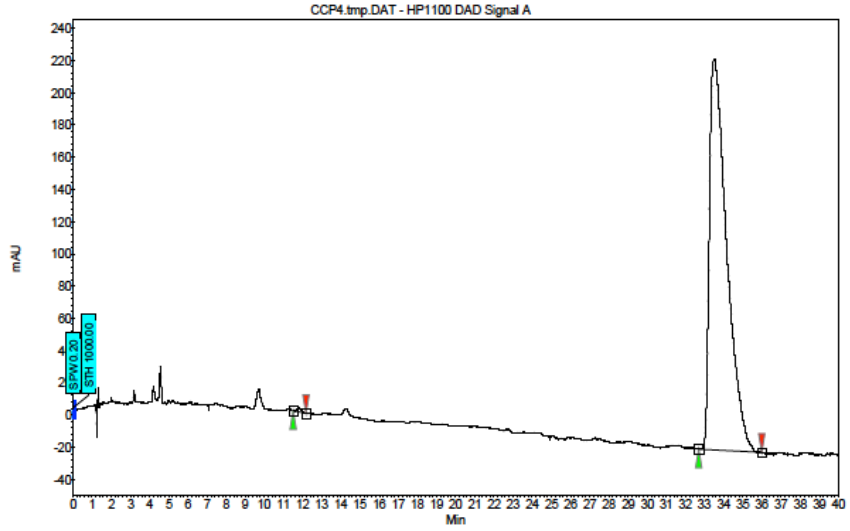
trans-(±)-**SI-2**



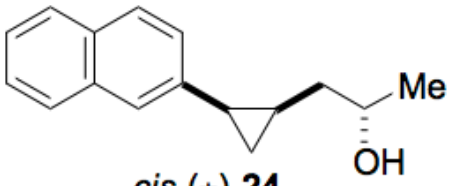
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	11.55	12.16	13.11	0.00	49.87	274.7	93.3	49.870
2	UNKNOWN	34.03	34.64	36.21	0.00	50.13	96.9	93.7	50.130
Total						100.00	371.7	187.0	100.000



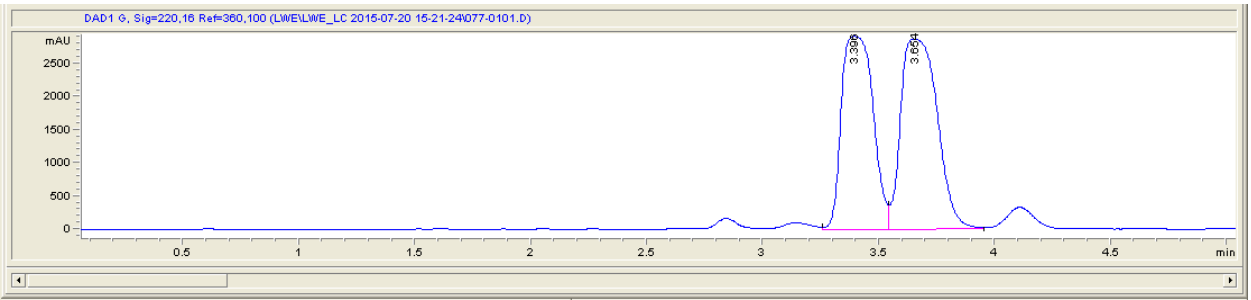
trans-(1*R*,2*S*)-**SI-2**



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	11.49	11.81	12.16	0.00	0.23	2.5	0.6	0.229
1	UNKNOWN	32.69	33.51	35.98	0.00	99.77	242.8	253.8	99.771
Total						100.00	245.3	254.4	100.000

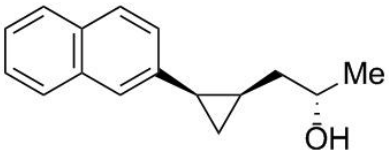


cis-(±)-**24**

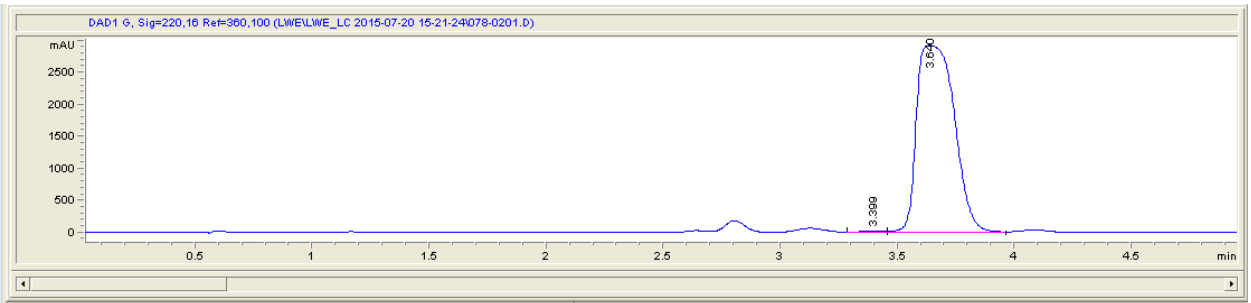


File Information	
LC-File	077-0101.D
File Path	C:\CHEM32\1\DATA\LWE\LWE_LC 2015-07-20 15-21-24\
Date	20-Jul-15, 15:22:00
Sample	LWE-III-027
Sample Info	
Barcode	
Operator	LWE
Method	LWE_ODH.M
Analysis Time	29.997 min
Sampling Rate	0.0033 min (0.198 sec), 9000 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	3.396	27713.5	2916.2	0.1539	46.801	0.705
2	3.654	31501.7	2877.3	0.1767	53.199	0.595

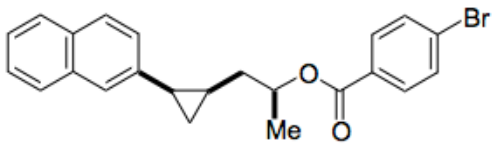


(1*S*)-(*cis*-(1*R*,2*R*)-**24**

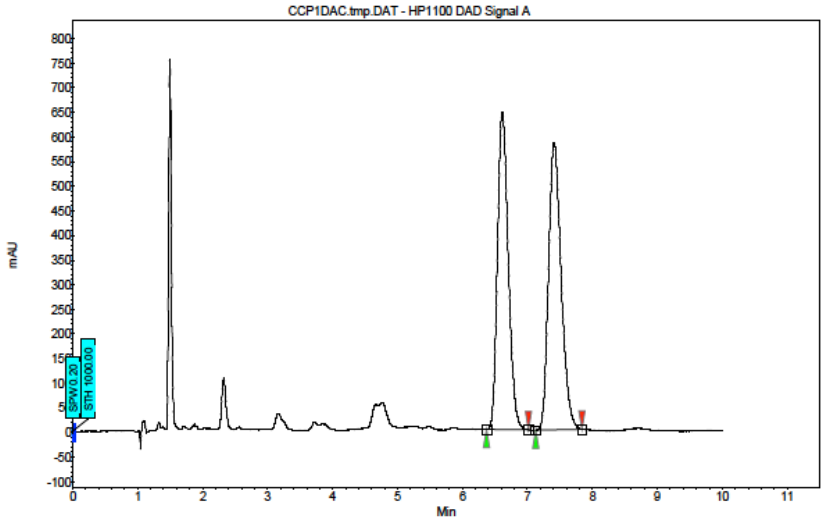


File Information	
LC-File	078-0201.D
File Path	C:\CHEM32\1\DATA\LWE\LWE_LC 2015-07-20 15-21-24\
Date	20-Jul-15, 15:53:39
Sample	LWE-II-285
Sample Info	
Barcode	
Operator	LWE
Method	LWE_ODH.M
Analysis Time	29.997 min
Sampling Rate	0.0033 min (0.198 sec), 9000 datapoints

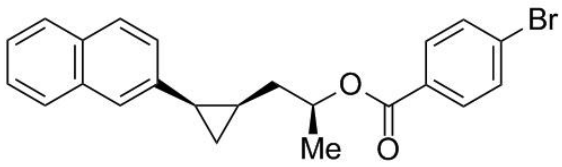
#	Time	Area	Height	Width	Area%	Symmetry
1	3.399	212.1	30.7	0.1026	0.643	1.259
2	3.64	32783.9	2926.5	0.1827	99.357	0.549



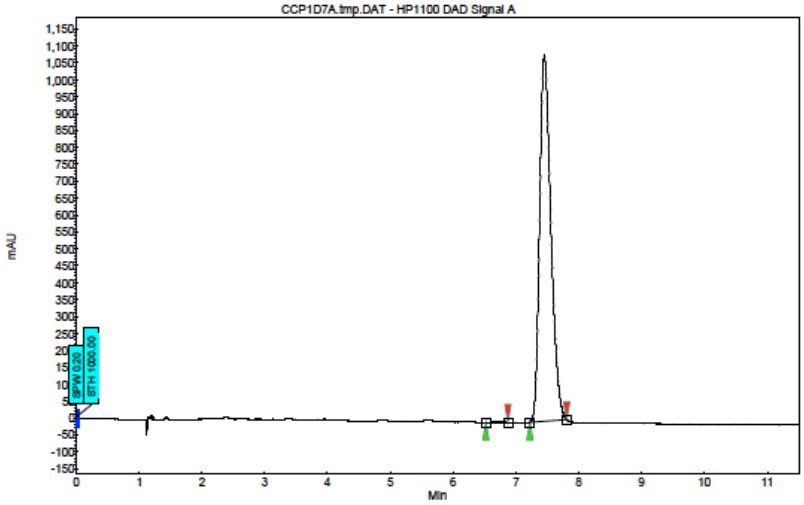
cis-(±)-**SI-3**



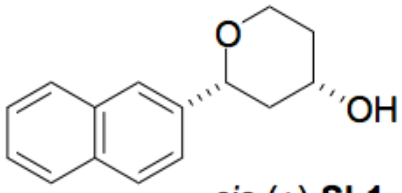
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.37	6.62	7.02	0.00	48.54	643.3	123.5	48.544
2	UNKNOWN	7.13	7.41	7.84	0.00	51.46	583.2	130.9	51.456
Total						100.00	1226.5	254.4	100.000



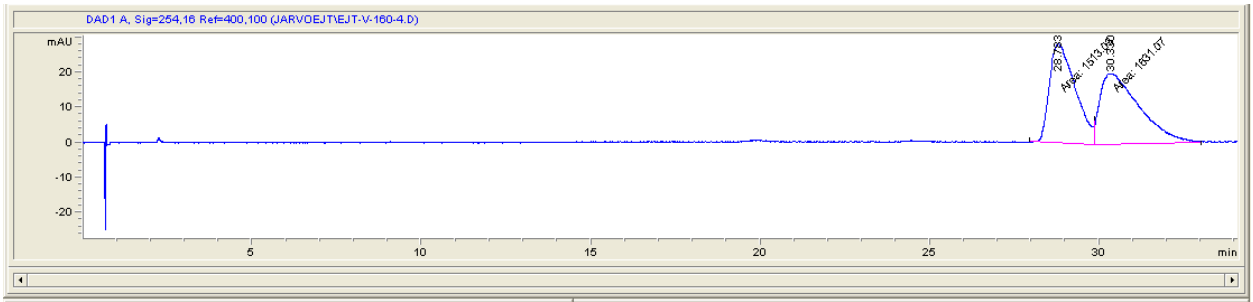
(1*S*)-(*cis*-(1*R*,2*R*))-**SI-3**



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	6.53	6.70	6.88	0.00	0.21	3.1	0.5	0.210
1	UNKNOWN	7.23	7.46	7.81	0.00	99.79	1081.5	223.3	99.790
Total						100.00	1084.6	223.8	100.000

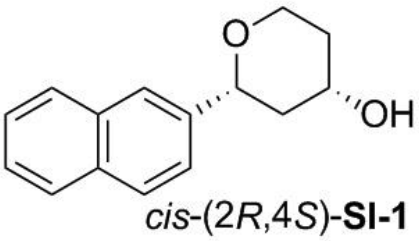


cis-(±)-**SI-1**

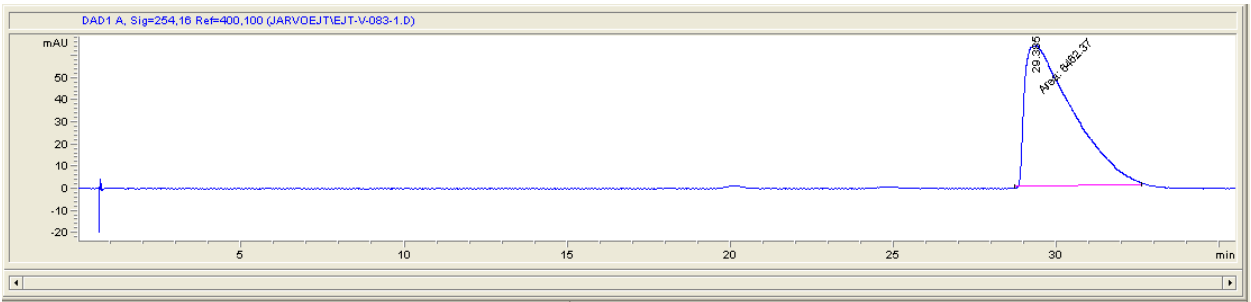


File Information	
LC-File	EJT-V-160-4.D
File Path	C:\CHEM32\1\DATA\JARVOEJT\
Date	27-Jun-15, 20:43:25
Sample	EJT-V-160-4
Sample Info	ODH, 5% IPA, 2.5 mL/min, 44C, 10uL
Barcode	
Operator	EJT
Method	MRH-OD-H.M
Analysis Time	34.1 min
Sampling Rate	0.0033 min (0.198 sec), 10231 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	28.783	1513	28.1	0.8983	48.123	0.479
2	30.33	1631.1	20.2	1.3476	51.877	0.334

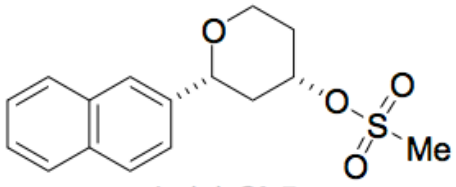


cis-(2*R*,4*S*)-**SI-1**

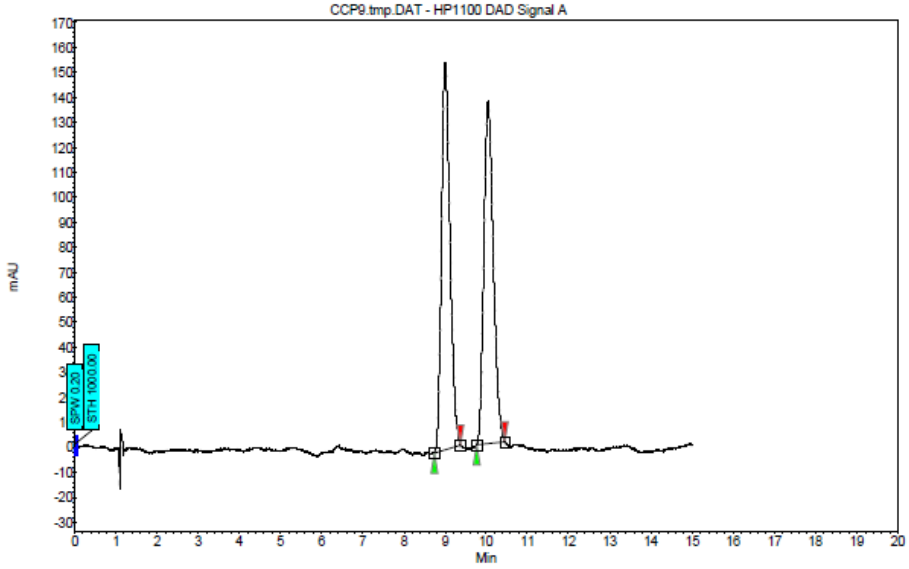


File Information	
LC-File	EJT-V-083-1.D
File Path	C:\CHEM32\1\DATA\JARVOEJT\
Date	27-Jun-15, 18:44:58
Sample	EJT-V-083-1
Sample Info	ODH, 5% IPA, 2.5 mL/min, 44C, 10uL
Barcode	
Operator	EJT
Method	MRH-OD-H.M
Analysis Time	35.507 min
Sampling Rate	0.0033 min (0.198 sec), 10653 datapoints

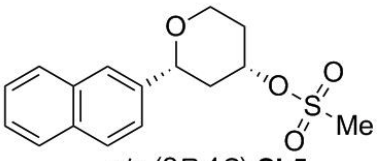
#	Time	Area	Height	Width	Area%	Symmetry
1	29.385	6462.4	63.4	1.6989	100.000	0.294



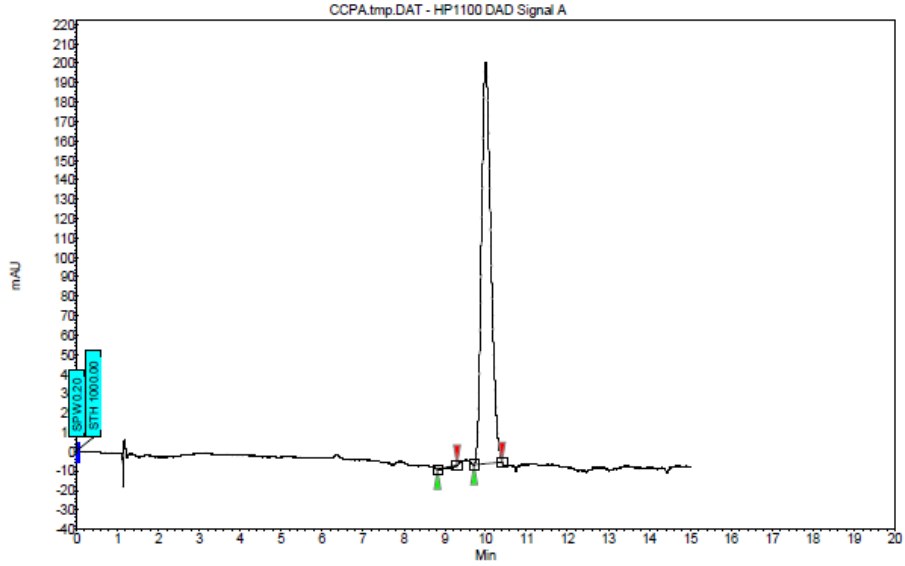
cis-(±)-**SI-5**



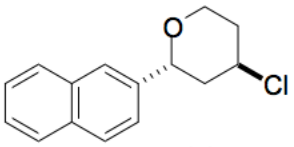
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	8.73	9.00	9.37	0.00	50.45	155.1	37.0	50.452
2	UNKNOWN	9.77	10.05	10.45	0.00	49.55	136.9	36.4	49.548
Total						100.00	291.9	73.4	100.000



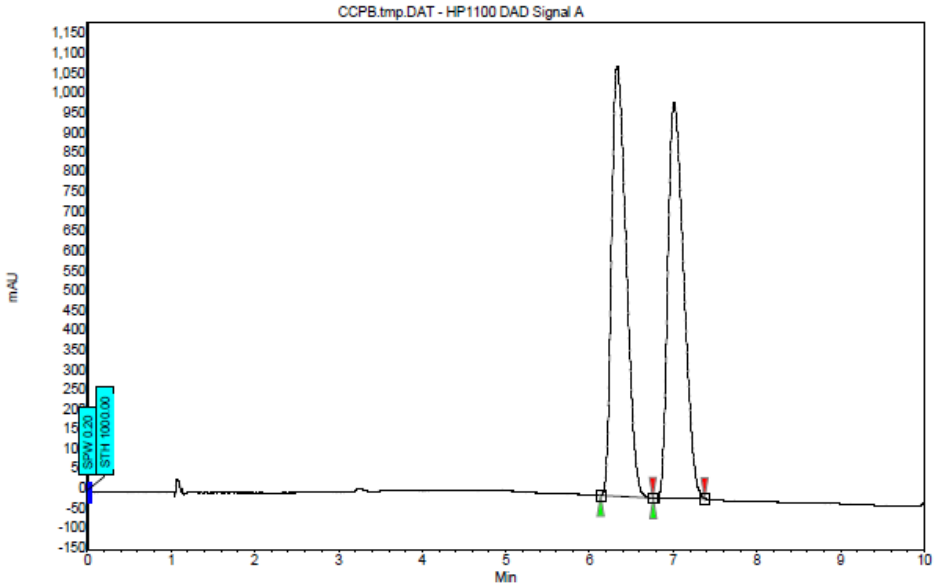
cis-(2*R*,4*S*)-**SI-5**



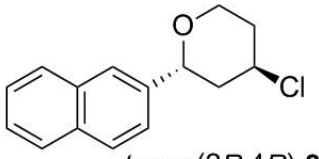
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	8.82	9.18	9.30	0.00	0.30	0.9	0.2	0.298
1	UNKNOWN	9.72	10.00	10.40	0.00	99.70	206.9	54.8	99.702
Total						100.00	207.8	54.9	100.000



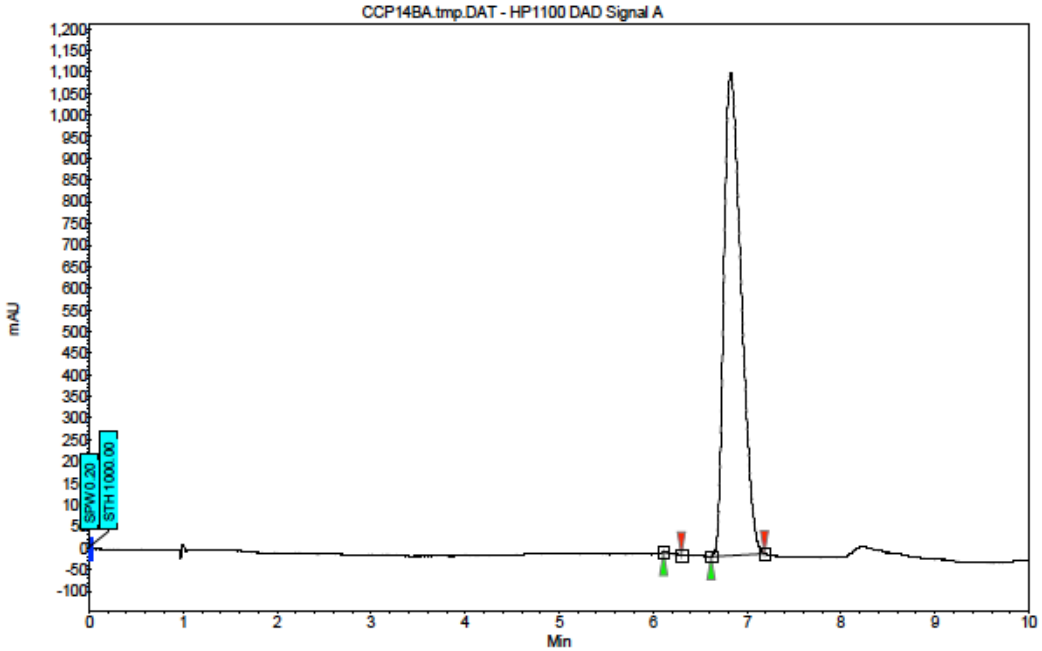
trans-(±)-**8**



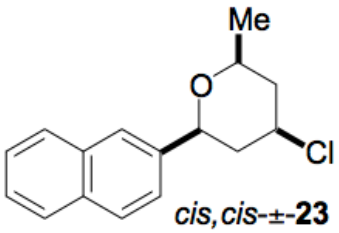
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
1	UNKNOWN	6.14	6.33	6.76	0.00	50.09	1087.7	220.0	50.091
2	UNKNOWN	6.76	7.01	7.37	0.00	49.91	1001.3	219.2	49.909
Total						100.00	2088.9	439.2	100.000



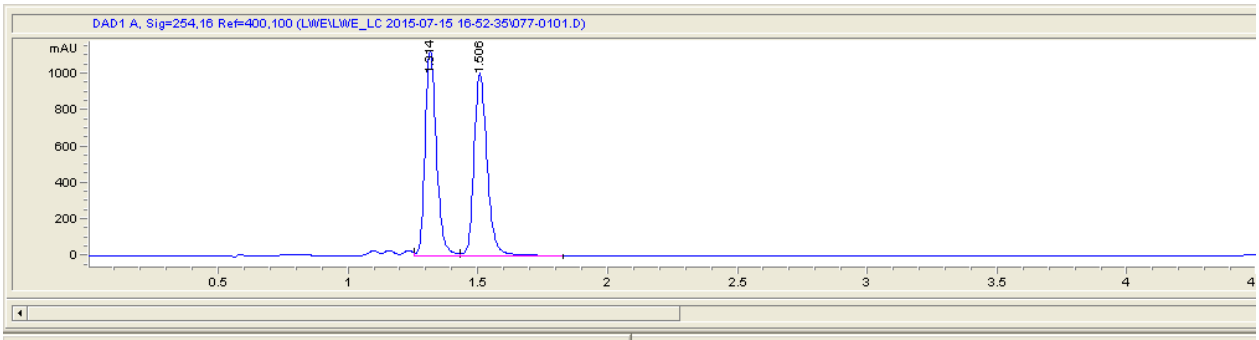
trans-(2*R*,4*R*)-**8**



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[µV]	[µV.Min]	[%]
2	UNKNOWN	6.11	6.18	6.30	0.00	0.07	1.7	0.2	0.073
1	UNKNOWN	6.62	6.83	7.19	0.00	99.93	1116.3	236.7	99.927
Total						100.00	1118.0	236.9	100.000

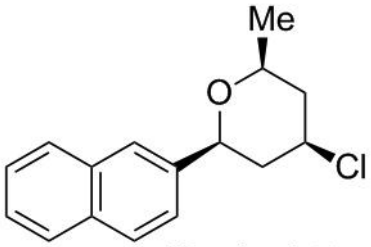


cis,cis-±-**23**

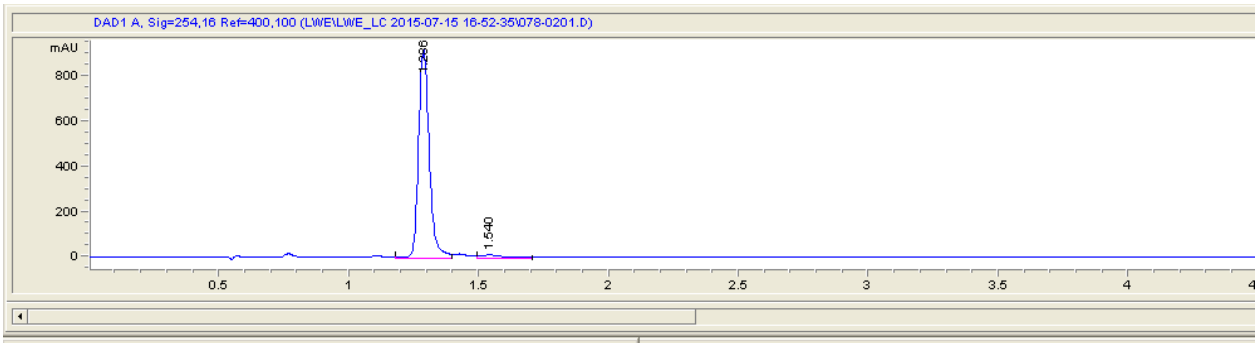


File Information	
LC-File	077-0101.D
File Path	C:\CHEM32\1\DATA\LWE\LWE_LC 2015-07-15 16-52-35\
Date	15-Jul-15, 16:53:10
Sample	LWE-II-228
Sample Info	
Barcode	
Operator	LWE
Method	LWE_ODH.M
Analysis Time	9.997 min
Sampling Rate	0.0033 min (0.198 sec), 3000 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	1.314	3481.2	1131.3	0.0469	48.966	0.754
2	1.506	3628.2	1010.8	0.0549	51.034	0.715



cis,cis-(2*R*,4*R*,6*S*)-**23**



File Information	
LC-File	078-0201.D
File Path	C:\CHEM32\1\DATA\LWE\LWE_LC 2015-07-15 16-52-35\
Date	15-Jul-15, 17:04:50
Sample	LWE-II-277
Sample Info	
Barcode	
Operator	LWE
Method	LWE_ODH.M
Analysis Time	9.997 min
Sampling Rate	0.0033 min (0.198 sec), 3000 datapoints

#	Time	Area	Height	Width	Area%	Symmetry
1	1.286	2717.7	925.6	0.0453	94.614	0.778
2	1.54	154.7	18.1	0.1117	5.386	0.313