

Supporting Information

Oxazolidine Synthesis by Complementary Stereospecific and Stereoconvergent Strategies

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I. General Procedures.

All reactions were carried out under an atmosphere of N₂. All glassware was either oven or flame-dried prior to use. Tetrahydrofuran (THF), diethyl ether (Et₂O), dichloromethane (CH₂Cl₂), and acetonitrile (MeCN), 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 h) to remove H₂O. ¹H NMR spectra were recorded on Bruker GN-500 (500 MHz ¹H, 125.7 MHz ¹³C), CRYO-500 (500 MHz ¹H, 125.7 MHz ¹³C), DRX-400 (400 MHz ¹H, 100 MHz ¹³C, 161.9 MHz ³¹P, 376.5 MHz ¹⁹F), or Avance-600 (600 MHz ¹H, 150 MHz ¹³C).

spectrometers. Proton chemical shifts are reported in ppm (δ) relative to internal tetramethylsilane (TMS, δ 0.00). Data are reported as follows: chemical shift (multiplicity [singlet (s), broad singlet (br s), doublet (d), doublet of doublets (dd), triplet (t), doublet of triplets (dt), doublet of doublet of triplets (ddt), triplet of triplets (tt), quartet (q), multiplet (m), apparent doublet (ad), broad doublet (br d) and broad multiplet (br m)], coupling constants [Hz], integration). The apparent multiplet (am) designation is given to resonances of the minor diastereomer which are overlapping with resonances of the major diastereomer and coupling constants could not precisely be extracted. Carbon chemical shifts are reported in ppm (δ) relative to TMS with the respective solvent resonance as the internal standard (CDCl_3 , δ 77.23 ppm; d_6 -DMSO, δ 39.51 ppm; CD_2Cl_2 , δ 54.00 ppm; CD_3OD , δ 49.15 ppm). Unless otherwise indicated, NMR data were collected at 25 °C. Infrared spectra were obtained on a Perkin-Elmer *Spectrum RX I* spectrometer. Analytical thinlayer chromatography (TLC) was performed using Silica Gel 60 F254 precoated plates (0.25 mm thickness). Visualization was accomplished by irradiation with a UV lamp and/or staining with KMnO_4 , ceric ammonium molybdate (CAM), or *p*-anisaldehyde (PAA) solutions. Flash chromatography was performed using Silica Gel 60A (170-400 mesh) from Fisher Scientific. Melting points (m.p.) were obtained using a Mel-Temp melting point apparatus and are uncorrected. High resolution mass spectrometry was performed by the University of California, Irvine Mass Spectrometry Center.

$\text{Rh}(\text{cod})\text{OTf}$ was obtained as a gift by Heraeus Chemical Co. and was stored indefinitely in an inert air glovebox.

$\text{Ni}(\text{cod})_2$ was purchased from Strem Chemical Co. and used as received within an inert atmosphere glovebox.

$\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ was used as received from Strem Chemical Co.

(*R,R*)-Dipamp = (*R,R*)-Ethylenebis[(2-methoxyphenyl)phenylphosphine], and (*S,S*)-Dipamp were purchased from Sigma-Aldrich Co. Josiphos, Walphos, and MeO-Biphep chiral-bidentate ligands were received as a gift from Solvias Chemical Co. These ligands were stored indefinitely in an inert air glovebox. All phosphine ligands were utilized as received and stored and used in an inert atmosphere glovebox.

Butadiene monoxide was purchased from Alfa Aesar, 98% and used as received in the nickel-catalyzed reaction. Distillation of commercial material over MgSO_4 at atmospheric pressure was performed for use in the palladium-catalyzed stereoselective reactions.

Enantiopure butadiene monoxide for use in Table 1 and Table 4 was prepared through the Jacobsen hydrolytic kinetic resolution of epoxides.¹

¹ Schaus, S. E.; Brandes, B. D.; Larrow, J. F.; Tokunaga, M.; Hansen, K. B.; Gould, A. E.; Furrow, M. E.; Jacobsen, E. N. *J. Am. Chem. Soc.* **2002**, *124*, 1307.

TBAT (tetrabutylammonium difluorotriphenylsilicate) was purchased from Sigma-Aldrich Co. as a crystalline white solid, kept in an inert atmosphere glovebox, and used as received.

Titanium(IV) isopropoxide was distilled at a pressure of less than 1 Torr, at approximately 90 °C (external temp.).

Diglyme was distilled fresh over CaH₂ and stored over 4 Å molecular sieves for no longer than three days.

4 Å Molecular sieves were dried and stored in an oven at 170 °C.

All other chemicals were purchased commercially and used as received.

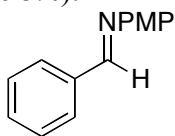
II. Procedures for Rhodium-Catalyzed Stereospecific Synthesis of Oxazolidines (Tables 1).

A. Synthesis and Characterization of Imines:

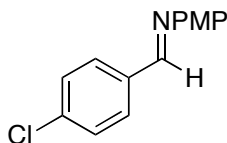
General Procedure for Imine Synthesis:

All imines were synthesized according to the modified procedure of Anderson and co-workers as described below.² Spectral data for imines **1b** and **1c** was consistent with the literature values.³

In a round-bottom flask *p*-anisidine (0.615 g, 5.00 mmol, 1 equiv) was taken up in CH₂Cl₂ (25 mL), 2.0 g anhydrous magnesium sulfate was added, followed by addition of benzaldehyde (0.505 mL, 5.00 mmol, 1 equiv). The reaction was allowed to stir overnight and was then filtered and the solvent removed *in vacuo*. The off-white solid obtained was then washed with pentanes and brought to dryness under vacuum (1.04 g, 98%).



(E)-N-benzylidene-4-methoxybenzenamine (1a) ¹H NMR (CDCl₃, 500 MHz) δ 8.47 (s, 1H), 7.91–7.85 (m, 2H), 7.48–7.43 (m, 3H), 7.23 (ad, *J* = 8.9 Hz, 2H), 6.93 (ad, *J* = 8.4 Hz, 2H), 3.82 (s, 3H). Analytical data is consistent with reported literature values.⁴

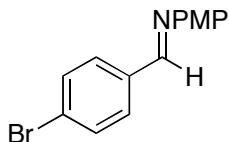


² Anderson, J. C.; Howell, G. P.; Lawrence, R. M.; Wilson, C. S. *J. Org. Chem.* **2005**, *70*, 5665.

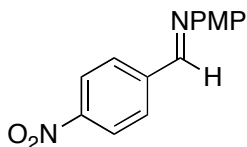
³ (a) Cabiddu, S.; Caldoni, E.; Ianni, A.; Gelli, G.; Melis, S.; Bernard, A. M.; Cabiddu, M. G.; De Montis, S.; Fattuoni, C. *Eur. J. Org. Chem.* **2002**, 3393. (b) Wang, J.; Fu, Y.; Zhang, B.; Cui, X.; Lei, L.; Guo, Q. *Tetrahedron Lett.* **2006**, *47*, 8293.

⁴ Nakajima, T.; Inada, T.; Igarashi, T.; Sekioka, T.; Shimizu, I. *Bull. Chem. Soc. Jpn.* **2006**, *79*, 1941.

(*E*)-*N*-(4-chlorobenzylidene)-4-methoxybenzenamine (1d) was prepared in quantitative yield from 4-chlorobenzaldehyde (0.703 g, 5.00 mmol) and *p*-anisidine (0.615 g, 5.00 mmol) according to the general procedure. ¹H NMR (CDCl₃, 400 MHz) δ 8.44 (s, 1H), 7.82 (ad, *J* = 8.4 Hz, 2H), 7.43 (ad, *J* = 8.4 Hz, 2H), 7.23 (ad, *J* = 9.0 Hz, 2H), 6.93 (ad, *J* = 9.0 Hz, 2H), 3.83 (s, 3H). Analytical data is consistent with reported literature values.²



(*E*)-*N*-(4-bromobenzylidene)-4-methoxybenzenamine (1e) was prepared in quantitative yield from 4-bromobenzaldehyde (0.925 g, 5.00 mmol) and *p*-anisidine (0.615 g, 5.00 mmol) according to the general procedure. ¹H NMR (CDCl₃, 500 MHz) δ 8.43 (s, 1H), 7.76 (ad, *J* = 10.5 Hz, 2H), 7.59 (ad, *J* = 10.5 Hz, 2H), 7.24 (ad, *J* = 11.0 Hz, 2H), 6.93 (ad, *J* = 11.2 Hz, 2H), 3.84 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 158.7, 157.0, 144.7, 135.6, 132.2, 130.1, 125.7, 122.5, 114.6, 55.7; IR (film, cm⁻¹) 3055, 2962, 2933, 1512, 1265; HRMS-ESI (*m/z*): [M+H]⁺ calcd for C₁₄H₁₂NOBr requires 290.0180, found 290.0180; mp 146 °C; TLC R_f = 0.5 (5% Et₂O/pentanes).



(*E*)-*N*-(4-nitrobenzylidene)-4-methoxybenzenamine (1f) was prepared in quantitative yield from 4-nitrobenzaldehyde (0.756 g, 5 mmol) and *p*-anisidine (0.615 g, 5 mmol) according to the general procedure. ¹H NMR (CDCl₃, 400 MHz) δ 8.58 (s, 1H), 8.31 (ad, *J* = 8.7 Hz, 2H), 8.06 (ad, *J* = 8.8 Hz, 2H), 7.31 (ad, *J* = 9.0 Hz, 2H), 6.96 (ad, *J* = 8.5 Hz, 2H), 3.85 (s, 3H). Analytical data is consistent with reported literature values.⁵

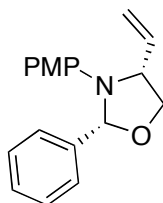
B. Procedure for the Rhodium Catalyzed Stereospecific Synthesis of 1,3-Oxazolidines and Characterization of Products:

Procedure with Racemic Vinyl Epoxide:

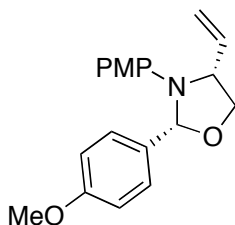
In an inert atmosphere glovebox, rhodiumbis(cyclooctadiene)trifluoromethanesulfonate (5 mg, 0.01 mmol) was weighed into a round bottom flask. The flask was sealed with a rubber septum and removed from the glovebox. Outside of the glovebox the septum was removed briefly to add imine (0.2 mmol, 1 equiv) and 4 Å molecular sieves (40 mg). The septum was replaced and CH₂Cl₂ (1.0 mL) and butadienemonoxide (24 µL, 0.30 mmol, 1.5 equiv) were then added. The reaction was stirred under a N₂ atmosphere at room temperature and monitored by thin layer chromatography. When the reaction was complete the mixture was diluted with 10 mL of CH₂Cl₂, 10 mL of brine was then added and the layers separated. The aqueous layer was washed 3 times with 10 mL of CH₂Cl₂

⁵ Del Buttero, P.; Baldoli, C.; Molteni, G.; Pilati, T. *Tetrahedron: Asymmetry* **2000**, *11*, 1927.

and the combined organic layers were then dried over sodium sulfate and concentrated *in vacuo*. The crude material was purified by flash chromatography using Davisil® to yield an inseparable mixture of diastereomers.

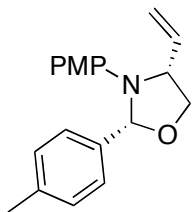


(±)-3-(4-methoxyphenyl)-2-phenyl-4-vinyloxazolidine (3c) Following the general procedure above imine **1c** (0.2 mmol, 42 mg) was reacted with butadienemmonoxide (24 μ L, 0.3 mmol, 1.5 equiv) for 4 hours. Purification by column chromatography using Davisil® eluting with 5% Et₂O/pentanes afforded **3c** (47 mg, 86% yield). ¹H NMR (CDCl₃, 400 MHz) δ 7.60 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.47–7.32 (m, 3H), 6.79 (d, *J* = 9.0 Hz, 2H), 6.60 (d, *J* = 9.1 Hz, 2H), 6.10–5.98 (m, 1H), 5.86 (s, 1H), 5.39 (d, *J* = 17.3 Hz, 1H), 5.34 (d, *J* = 10.3 Hz, 1H), 4.36–4.30 (m, 1H), 4.23 (dd, *J* = 8.3, 7.6 Hz, 1H), 3.87 (dd, *J* = 8.5, 6.1 Hz, 1H), 3.74 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 152.6, 140.9, 140.0, 138.2, 129.0, 128.7, 127.4, 117.3, 114.9, 114.6, 94.7, 70.8, 63.5, 55.8; IR (film, cm⁻¹) 3064, 2983, 2933, 2868, 1641, 1618, 1512, 1454, 1242; HRMS-ESI (*m/z*): [M+H]⁺ calcd for C₁₈H₁₉NO₂ requires 282.1494, found 282.1486; TLC R_f = 0.4 (5% Et₂O/pentanes).

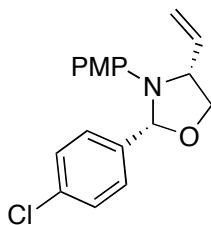


(±)-2,3-bis(4-methoxyphenyl)-4-vinyloxazolidine (3d) Following the general procedure above imine **1d** (0.2 mmol, 48 mg) was reacted with butadienemmonoxide (32 μ L, 0.4 mmol, 2 equiv) for 15 hours. Purification by column chromatography using Davisil® eluting with 10% Et₂O/pentanes afforded **3d** (60% yield as determined by ¹H NMR spectroscopy; product is inseparable from *p*-methoxybenzaldehyde). ¹H NMR (CDCl₃, 400 MHz) δ 7.51 (d, *J* = 8.6 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.78 (d, *J* = 9.0 Hz, 2H), 6.59 (d, *J* = 9.3 Hz, 2H), 6.09–5.98 (m, 1H), 5.80 (s, 1H), 5.53 (d, *J* = 17.7 Hz, 1H), 5.33 (d, *J* = 10.2 Hz, 1H), 4.32–4.24 (m, 1H), 4.20 (dd, *J* = 8.3, 7.0 Hz, 1H), 3.87 (dd, *J* = 8.5, 6.2 Hz, 1H), 3.83 (s, 3H), 3.74 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 160.1, 152.6, 140.9, 138.4, 132.1, 128.6, 117.2, 114.9, 114.6, 114.0, 94.4, 70.7, 63.5, 55.8, 55.4; IR (film, cm⁻¹) 3068, 2999, 2935, 2835, 1695, 1610, 1512, 1244; HRMS-ESI (*m/z*): [M+H]⁺ calcd for C₁₉H₂₁NO₃ requires 312.1600, found 312.1593; TLC R_f = 0.4 (10% Et₂O/pentanes).

Et₂O/pentanes).



(±)-3-(4-methoxyphenyl)-2-*p*-tolyl-4-vinyloxazolidine (3e) Following the general procedure above imine **1e** (0.2 mmol, 45 mg) was reacted with butadienemonoxide (32 μ L, 0.4 mmol, 2 equiv) for 4 hours. Purification by column chromatography using Davisil® eluting with 5% Et₂O/pentanes afforded **3e** (51 mg, 86% yield). ¹H NMR (CDCl₃, 500 MHz) δ 7.45 (d, J = 8.0 Hz, 2H), 7.30–7.11 (m, 3H), 6.75 (d, J = 8.9 Hz, 2H), 6.56 (d, J = 9.2 Hz, 2H), 6.04–5.93 (m, 1H), 5.79 (s, 1H), 5.50 (d, J = 17.6 Hz, 1H), 5.30 (d, J = 10.1 Hz, 1H), 4.31–4.23 (m, 1H), 4.22–4.13 (m, 1H), 3.83 (dd, J = 8.6, 6.1 Hz, 1H), 3.71 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 152.6, 140.9, 138.8, 138.3, 137.1, 129.4, 127.3, 117.2, 114.8, 114.6, 94.6, 70.8, 63.4, 55.8; IR (film, cm⁻¹) 2981, 2931, 2866, 1614, 1464, 1512, 1244, 1041; HRMS-ESI (m/z): [M+H]⁺ calcd for C₁₉H₂₁NO₂ requires 296.1650, found 296.1645; TLC R_f = 0.4 (5% Et₂O/pentanes).

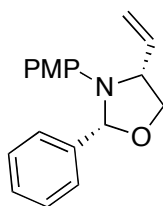


(±)-2-(4-chlorophenyl)-3-(4-methoxyphenyl)-4-vinyloxazolidine (3f) Following the general procedure above imine **1f** (0.2 mmol, 49 mg) was reacted with butadienemonoxide (32 μ L, 0.4 mmol, 2 equiv) for 15 hours. Purification by column chromatography using Davisil® eluting with 5% Et₂O/pentanes afforded **3f** (55 mg, 88% yield). ¹H NMR (CDCl₃, 500 MHz) δ 7.50 (d, J = 8.3 Hz, 2H), 7.36 (d, J = 8.7 Hz, 2H), 6.76 (d, J = 9.0 Hz, 2H), 6.55 (d, J = 9.0 Hz, 2H), 6.03–5.91 (m, 1H), 5.79 (s, 1H), 5.49 (d, J = 16.8 Hz, 1H), 5.31 (d, J = 10.3 Hz, 1H), 4.32–4.25 (m, 1H), 4.20 (dd, J = 8.4, 7.0 Hz, 1H), 3.80 (dd, J = 8.5, 6.0 Hz, 1H), 3.72 (s, 3H); ¹³C NMR (CDCl₃, 125 MHz) δ 152.8, 140.6, 138.7, 138.0, 134.7, 128.9, 128.8, 117.5, 115.0, 114.7, 94.0, 70.8, 63.5, 55.8; IR (film, cm⁻¹) 3068, 2985, 2935, 2870, 2835, 1597, 1511, 1244, 1090; HRMS-ESI (m/z): [M+H]⁺ calcd for C₁₈H₁₈ClNO₂ requires 316.1104, found 316.1095; TLC R_f = 0.4 (5% Et₂O/pentanes).

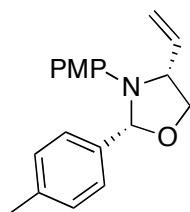
Procedure with Enantioenriched Vinyl Epoxide:

In an inert atmosphere glovebox, rhodiumbis(cyclooctadiene)trifluoromethanesulfonate (5 mg, 0.01 mmol) was weighed into a round bottom flask. The flask was sealed with a rubber septum and removed from the glovebox. Outside of the glovebox the septum was

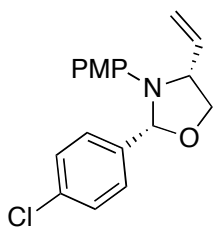
removed briefly to add imine (0.2 mmol, 1 equiv) and 4 Å molecular sieves (40 mg). The septum was replaced and CH₂Cl₂ (1.0 mL) and butadienemonoxide (32 µL, 0.40 mmol, 2 equiv) were then added. The reaction was stirred under a N₂ atmosphere and monitored by thin layer chromatography. When the reaction was complete the mixture was diluted with 10 mL of CH₂Cl₂ and decanted away from the molecular sieves, 10 mL of brine was then added and the layers separated. The aqueous layer was washed 3 times with 10 mL of CH₂Cl₂ and the combined organic layers were then dried over sodium sulfate and concentrated *in vacuo*. The crude material was purified by flash chromatography using Davisil® to yield an inseparable mixture of diastereomers. NMR data is reported for the major diastereomer only.



(2R,4R)-3-(4-methoxyphenyl)-2-phenyl-4-vinyloxazolidine (3c) Following the general procedure above imine **1c** (42 mg, 0.2 mmol) was reacted with butadienemonoxide (32 µL, 0.4 mmol, 2 equiv) for 6 hours. Purification by column chromatography using Davisil® eluting with 10% Et₂O/pentanes afforded **3c** (46 mg, 82% yield). Analytical data reported above for racemic compound. $[\alpha]^{24}_{\text{D}}$ -31.2, $[\alpha]^{24}_{577}$ -33.6, $[\alpha]^{24}_{546}$ -35.3, $[\alpha]^{24}_{435}$ -44.6; SFC analysis (CHIRALPAK AD-H, 5.0% *i*-PA, 1.5 mL/min, 215 nm) indicated 99% ee for major diastereomer: t_{R} (major) = 3.53 min, t_{R} (minor) = 4.19 min.



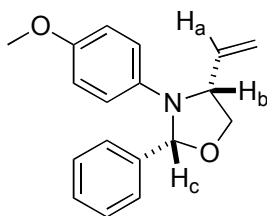
(2R,4R)-3-(4-methoxyphenyl)-2-*p*-tolyl-4-vinyloxazolidine (3e) Following the general procedure above imine **1e** (45 mg, 0.2 mmol) was reacted with butadienemonoxide (32 µL, 0.4 mmol, 2 equiv) for 10 hours. Purification by column chromatography using Davisil® eluting with 5-1% Et₂O/pentanes afforded **3e** (48 mg, 82% yield). Analytical data reported above for racemic compound. $[\alpha]^{24}_{\text{D}}$ -49.5, $[\alpha]^{24}_{577}$ -45.8, $[\alpha]^{24}_{546}$ -55.5, $[\alpha]^{24}_{435}$ -69.5; SFC analysis (CHIRALPAK AD-H, 5.0% *i*-PA, 1.5 mL/min, 215 nm) indicated 99% ee for major diastereomer: t_{R} (major) = 4.27 min, t_{R} (minor) = 4.92 min.



(2*R*,4*R*)-2-(4-chlorophenyl)-3-(4-methoxyphenyl)-4-vinyloxazolidine (3f) Following the general procedure above imine **1f** (49 mg, 0.2 mmol) was reacted with butadienemonoxide (32 μ L, 0.4 mmol, 2 equiv) for 12 hours. Purification by column chromatography using Davisil® eluting with 5-1% Et₂O/pentanes afforded **3f** (52 mg, 83% yield). Analytical data reported above for racemic compound. $[\alpha]^{24}_{\text{D}}$ -40.5, $[\alpha]^{24}_{577}$ -43.6, $[\alpha]^{24}_{546}$ -47.2, $[\alpha]^{24}_{435}$ -71.3. **SFC** analysis (CHIRALPAK AD-H, 5.0% *i*-PA, 1.5 mL/min, 215 nm) indicated 99% ee for major diastereomer: t_{R} (major) = 4.90 min, t_{R} (minor) = 6.68 min.

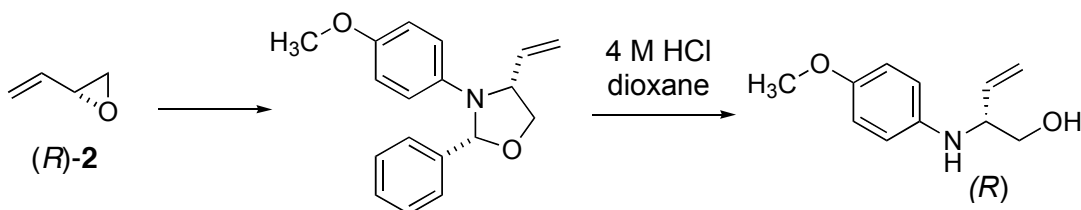
C. Determination of Relative and Absolute Stereochemistry

1. Determination of relative stereochemistry of 1,3-oxazolidine:



To determine the relative stereochemistry of H_b and H_c NOE experiments were performed. When H_a was irradiated interaction with the phenyl ring was observed, but not with H_c and when H_b was irradiated interaction with H_c was observed but not with the phenyl ring. This supports a relative *syn* stereochemistry.

2. Determination of absolute stereochemistry:



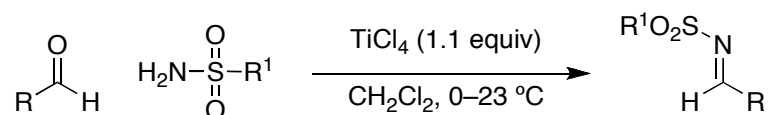
After determination of the relative stereochemistry, the absolute stereochemistry of the product was determined by hydrolysis of the oxazolidine to the aminoalcohol with 4 M

HCl in dioxane. The optical rotation of the amino alcohol was then taken and compared to literature values.⁶ $[\alpha]_D^{24} +13.3$ ($c=1.0$, CH_2Cl_2).

III. Procedures for the Nickel and Palladium Catalyzed Stereoselective Synthesis of 1,3-Oxazolidines

A. Synthesis and Characterization of Imines: Methanesulfonyl imines **4a-4e** were prepared according to a modified procedure reported by Jennings and Lovely, as described below.⁷ While Lovely and Jennings report catalytic use of titanium(IV) chloride, using 1.0-1.1 equiv of reagent provided consistently higher yields in our hands. Flame-dried glassware in each manipulation and anhydrous solvents were utilized to minimize hydrolysis of the imines. Toluenesulfonyl imine **1a** and (*E*)-*N*-benzylidene-4-methylbenzenesulfonamide **4a** are known and spectra were consistent with literature values.^{8,9}

1. General procedure for the synthesis of sulfonyl imines.



To a 500 mL round bottom flask with magnetic stir bar was added methane- or toluenesulfonamide (20.0 mmol, 1.00 equiv) followed by CH_2Cl_2 (150 mL), aryl aldehyde (21.0 mmol, 1.05 equiv), and Et_3N (9.8 mL, 70.0 mmol, 3.50 equiv). After the stirring solution became homogeneous, the flask was placed in an ice bath and cooled to 0 °C. Once at 0 °C, a freshly prepared 1 M solution of TiCl_4 in CH_2Cl_2 (20 mL, 1.0 equiv) was added slowly over 10 minutes. A color change over the time of addition of the titanium reagent was observed. After addition of the titanium reagent, the solution was allowed to warm to room temperature slowly over 2 h and then continued to stir.

After approximately 12–16 h, the crude reaction mixture was filtered through a pad of celite, washing with further CH_2Cl_2 (100 mL), then the filtrate was concentrated in vacuo at 40 °C to achieve a thorough removal of the solvent. Next, anhydrous toluene (200 mL) was added and the crude solution was stirred for 4 h at room temperature. At this time the solution was again filtered through a pad of Celite, washing further with anhydrous toluene (100 mL), and the solvent was removed in vacuo at 50 °C. This procedure furnished material which was $\geq 95\%$ pure after further drying at low pressure (~ 0.5 torr) and ambient temperature. A drying tube fitted with a P_2O_5 sidearm could be utilized to obtain rigorously dry compound.

⁶ Gnam, C.; Franck, G.; Miller, N.; Stork, T.; Brödner, K.; Helmchen, G. *Synthesis* **2008**, 3331-3350.

⁷ Prepared according to: Jennings, W. B.; Lovely, C. J. *Tetrahedron* **1991**, 47, 5561.

⁸ Alonso, I.; Esquivias, J.; Gomez-Arrayas, R.; Carretero, J. C. *J. Org. Chem.* **2008**, 73, 6401.

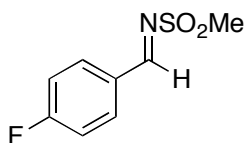
⁹ Chen, D.; Chen, T.; Kong, L.; Zhen, R.; Zhen, S.; Wen, Y.; Zhu, G. *Tetrahedron Lett.* **2010**, 51, 5131.



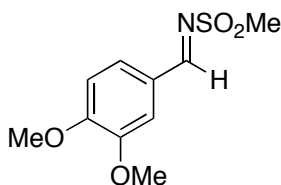
(E)-N-benzylidenemethanesulfonamide (4a) was prepared from benzaldehyde (831 μ L, 869 mg, 8.19 mmol) according to the general procedure and isolated as an amorphous yellow solid (66%, 1.00 g). $^1\text{H NMR}$ δ (CDCl_3 , 500 MHz) δ 9.05 (s, 1H), 7.91 (d, J = 8.1 Hz, 2H), 7.40 (d, J = 8.1 Hz, 2H), 3.19 (s, 3H), 2.52 (s, 3H); $^{13}\text{C NMR}$ δ (CDCl_3 , 125 MHz) δ 171.6, 146.9, 131.6, 130.3, 129.8, 40.6, 22.3; **IR** (film CDCl_3 , cm^{-1}) 2929, 2883, 1493, 1460, 1451, 1345, 1208, 1157, 1103; **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_9\text{H}_{11}\text{NO}_2\text{S}$ requires 220.0408; found 220.0404; **Mp** = 88-89 $^\circ\text{C}$; **TLC** R_f = 0.6 (50% EtOAc/Hexanes, visualized under UV).



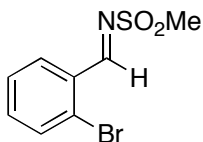
(E)-N-(4-methylbenzylidene)methanesulfonamide (4b) was prepared from *p*-tolylaldehyde (0.94 mL, 8.0 mmol) according to the general procedure and isolated as an amorphous yellow solid. $^1\text{H NMR}$ δ (CDCl_3 , 500 MHz) δ 8.99 (s, 1H), 7.86 (d, J = 8.1 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 3.13 (s, 3H), 2.46 (s, 3H); $^{13}\text{C NMR}$ δ (CDCl_3 , 125 MHz) δ 171.6, 146.0, 131.6, 130.3, 129.7, 40.6, 22.3; **IR** (film CH_2Cl_2 , cm^{-1}) 3054, 2983, 1599, 1569, 1421, 1316, 1264, 1144; **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_9\text{H}_{11}\text{NO}_2\text{S}$ requires 220.0408; found 220.0404; **Mp** = 76-77 $^\circ\text{C}$; **TLC** R_f = 0.4 (25% EtOAc/Hexanes, visualized under UV).



(E)-N-(4-fluorobenzylidene)methanesulfonamide (4c) was prepared from *p*-fluorobenzaldehyde (550 μ L, 5.00 mmol) according to the general procedure and isolated as an amorphous yellow solid (64%, 642 mg). $^1\text{H NMR}$ δ (CDCl_3 , 500 MHz) δ 9.01 (s, 1H), 8.02–7.98 (m, 2H), 7.23 (t, J = 8.5 Hz, 2H), 3.14 (s, 3H); $^{13}\text{C NMR}$ δ (CDCl_3 , 125 MHz) δ 170.4, 167.3 (d, J = 25.8 Hz), 134.2 (d, J = 9.7 Hz), 128.9 (d, J = 2.8 Hz), 117.2 (d, J = 22.2 Hz), 40.7; **IR** (film CH_2Cl_2 , cm^{-1}) 3049, 2983, 1599, 1583, 1508, 1418, 1319, 1264, 1144; **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_8\text{H}_8\text{FNO}_2\text{S}$ requires 224.0157; found 224.0149; **Mp** = 109-111 $^\circ\text{C}$; **TLC** R_f = 0.3 (25% EtOAc/Hexanes, visualized under UV).



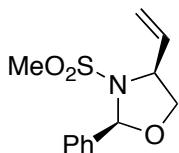
***N*-(3,4-dimethoxybenzylidene)methanesulfonamide (4d)** was prepared from 3,4-dimethoxybenzaldehyde (835 μ L, 5.00 mmol) according to the general procedure and isolated as an amorphous yellow solid (81%, 989 mg). ^1H NMR (CDCl_3 , 500 MHz) δ 8.91 (s, 1H), 7.57 (d, J = 1.59 Hz), 7.47 (dd, J = 8.2, 1.8 Hz, 1H), 6.98 (d, J = 8.2 Hz, 1H), 3.99 (s, 3H), 3.96 (s, 3H), 3.13 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 171.0, 155.7, 150.0, 129.6, 125.4, 110.9, 110.2, 56.5, 56.3, 40.7; **IR** (film CH_2Cl_2 , cm^{-1}) 3032, 3015, 2967, 2935, 2840, 1875, 1598, 1515, 1440, 1295, 1140; **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{10}\text{H}_{13}\text{NO}_4\text{S}$ requires 266.0463; found 266.0456; **Mp** = 133-134 $^\circ\text{C}$; **TLC** R_f = 0.1 (25% EtOAc/Hexanes, visualized under UV).



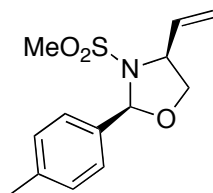
***N*-(2-bromobenzylidene)methanesulfonamide (4e)** was prepared according to the general procedure from *o*-bromobenzaldehyde (590 μ L, 5.00 mmol) and isolated as an amorphous white solid (65%, 850 mg). ^1H NMR (CDCl_3 , 500 MHz) δ 9.48 (s, 1H), 8.21 (dd, J = 7.7, 1.7 Hz, 1H), 7.71 (d, J = 7.8 Hz, 1H), 7.43–7.52 (m, 2H), 3.16 (s, 3H); ^{13}C NMR (CDCl_3 , 125 MHz) δ 171.1, 136.2, 134.2, 131.1, 130.7, 129.4, 128.3, 40.5; **IR** (film CH_2Cl_2 , cm^{-1}) 3024, 3008, 2928, 1602, 1582, 1559, 1462, 1429, 1307, 1271, 1141; **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_8\text{H}_8\text{BrNO}_2\text{S}$ requires 283.9357; found 283.9352; **Mp** = 119-120 $^\circ\text{C}$; **TLC** R_f = 0.3 (25% EtOAc/Hexanes, visualized under UV).

B. General Procedure for the Palladium-Catalyzed Stereoselective Synthesis of 1,3-Oxazolidines and Characterization of Products: To an 8 mL screw top vial, in an inert atmosphere glove box, was added $\text{Pd}_2(\text{dba})_3\text{CHCl}_3$ (2.6 mg, 0.0025 mmol, 2.5 mol %), Josiphos-SL-J006-1 ligand (5.2 mg, 0.006 mmol, 6 mol %) and a magnetic stir bar. The vial was closed with a cap fitted with a Teflon septum and removed from the glovebox. A nitrogen line was affixed to the vial and diglyme (500 μ L) was added at room temperature. The vial was then stirred at room temperature for fifteen minutes. Next, the vial was opened briefly under a high nitrogen flow and imine (0.10 mmol, 1.0 equiv) was added. The solution was stirred another 5 minutes at room temperature followed by the addition of butadiene monoxide via syringe (10 μ L, 0.12 mmol, 1.2 equiv). The reaction was stirred at room temperature for approximately twenty-four hours. The crude reaction mixture was then diluted with CH_2Cl_2 (5 mL) and SiO_2 gel was added. After adsorption of the crude compound onto SiO_2 by concentration of the solvent in vacuo, this material was loaded onto a SiO_2 column for flash chromatography. An inseparable mixture of diastereomers was eluted utilizing a solvent gradient of EtOAc/Hexanes. Visualization of the 1,3-oxazolidine products on TLC was accomplished via staining with PAA solution

(dark violet spot).

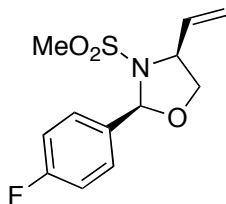


(2S,4S)-3-(methylsulfonyl)-2-phenyl-4-vinyloxazolidine (5a): Following the general procedure above imine **4a** (18 mg, 0.10 mmol) was reacted with butadienemonoxide (10 μ L, 0.12 mmol, 1.2 equiv) for 22 hours. Purification by column chromatography with a gradient from 5-15% EtOAc/Hexanes afforded **5a** (2:1 dr) as a yellow oil (24 mg, 96% yield). **¹H NMR** (CDCl₃, 500 MHz) *Major Diastereomer*: δ 7.55 (dd, J = 8.1, 1.3 Hz, 2H) 7.43–7.35 (m, 3H), 6.22 (s, 1H), 5.78 (ddd, J = 17.4, 9.8, 7.3 Hz, 1H), 5.36 (d, J = 17.1 Hz, 1H), 5.23 (d, J = 10.2 Hz, 1H), 4.55–4.49, (m, 1H), 4.28 (dd, J = 8.9, 7.2 Hz, 1H), 3.83 (dd, J = 9.1, 5.6 Hz, 1H), 2.81 (s, 3H); *Minor Diastereomer*: δ 7.51 (dd, J = 7.8, 1.7 Hz, 2H), 7.35–7.43 (am, 3H), 6.12 (s, 1H), 6.07 (ddd, J = 17.1, 8.1, 7.2 Hz, 1H), 5.46 (d, J = 17.1 Hz, 1H), 5.37 (d, J = 9.9 Hz, 1H), 4.46–4.55 (am, 1H), 4.23–4.31 (am, 1H), 3.89 (dd, J = 8.7, 3.6 Hz, 1H), 2.71 (s, 3H); **¹³C NMR** (CDCl₃, 125.7 MHz) *Major Diastereomer*: δ 137.6, 135.9, 129.4, 128.7, 127.6, 119.1, 92.0, 71.2, 61.9, 39.4; *Minor Diastereomer*: δ 138.1, 134.6, 129.6, 128.7, 127.6, 120.1, 91.4, 71.1, 62.1, 41.5; **HRMS-ESI** (m/z): [M+Na]⁺ calcd for C₁₃H₁₇NO₃S requires 290.0827; found 290.0833; **TLC** R_f = 0.4 (25% EtOAc/Hexanes, visualized under UV, PAA stains blue); [α]_D¹⁷ –28.6 (c 0.9, CHCl₃); **SFC** analysis (AD-H, 10.0% MeOH, 1.5 mL/min, 215 nm) indicated 91% ee for major diastereomer: t_R (minor) = 3.27 min, t_R (major) = 4.35 min.

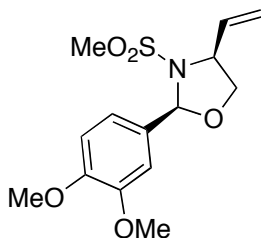


(2S,4S)-3-(methylsulfonyl)-2-p-tolyl-4-vinyloxazolidine (5b): Following the general procedure above imine **4b** (20 mg, 0.10 mmol) was reacted with butadienemonoxide (10 μ L, 0.12 mmol, 1.2 equiv) for 23 hours. Purification by column chromatography with a gradient from 5-15% EtOAc/Hexanes afforded **5b** (3:1 dr) as an orange-brown oil (27 mg, 99% yield). **¹H NMR** (CDCl₃, 500 MHz) *Major Diastereomer*: δ 7.43 (d, J = 8.1 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 6.17 (s, 1H), 5.80 (ddd, J = 17.6, 9.8, 7.5 Hz, 1H), 5.35 (d, J = 17.2 Hz, 1H), 5.23 (d, J = 10.3 Hz, 1H), 4.50 (aq, J = 6.8 Hz, 1H), 4.26 (dd, J = 9.0, 7.2 Hz, 1H), 3.83 (dd, J = 9.1, 5.4 Hz, 1H), 2.79 (s, 3H), 2.36 (s, 3H); *Minor Diastereomer*: δ 7.39 (d, J = 8.0 Hz, 2H), 7.17–7.22 (am, 2H), 6.08 (s, 1H), 6.00–6.10 (m, 1H), 5.45 (d, J = 17.0 Hz, 1H), 5.32–5.39 (am, 2H), 4.45–4.54 (am, 1H), 4.23–4.29 (am, 1H), 3.87 (dd, J = 8.7, 3.7 Hz, 1H), 2.69 (s, 3H), 2.36 (am, 3H); **¹³C NMR** (CDCl₃, 125.7 MHz) *Major Diastereomer*: δ 139.3, 136.0, 134.6, 129.4, 127.3, 119.0, 92.1, 71.2, 61.8, 39.5, 21.4; *Minor Diastereomer*: δ 139.6, 135.2, 134.7, 129.4, 127.5, 119.9, 91.4, 71.0, 62.1, 41.5, 21.5; **IR** (film CH₂Cl₂, cm⁻¹) 3049, 2983, 1421, 1347, 1264, 1155;

HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{13}H_{17}NO_3S$ requires 290.0827; found 290.0828; **TLC** R_f = 0.4 (25% EtOAc/Hexanes, visualized under UV, PAA stains blue); $[\alpha]^{24}_D$ –30.8 (c 2.6, $CHCl_3$); **SFC** analysis (OD-H, 2.50% MeOH, 2.5 mL/min, 215 nm) indicated 94% ee for the major diastereomer: t_R (major) = 7.15 min, t_R = 8.27 min.

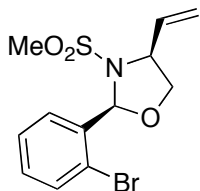


(2S,4S)-2-(4-fluorophenyl)-3-(methylsulfonyl)-4-vinyloxazolidine (5c): Following the general procedure above imine **4c** (20 mg, 0.10 mmol) was reacted with butadienemonoxide (10 μ L, 0.12 mmol, 1.2 equiv) for 25h. Purification by column chromatography with a gradient from 5-15% EtOAc/Hexanes afforded **5c** (2:1 dr) as a yellow oil (26 mg, 96% yield). **¹H NMR** (δ ($CDCl_3$, 500 MHz) *Major Diastereomer*: δ 7.55–7.51 (m, 2H), 7.11–7.06 (m, 2H), 6.23 (s, 1H), 5.76, (ddd, 17.5, 10.3, 7.8 Hz, 1H), 5.35, (dt, J = 17.2, 0.9 Hz, 1H), 5.24 (dt, J = 10.3, 0.9 Hz, 1H), 4.53–4.47 (m, 1H), 4.28 (dd, J = 9.1, 7.2 Hz, 1H), 3.82 (dd, J = 9.1, 5.4 Hz, 1H), 2.82 (s, 3H); *Minor Diastereomer*: δ 7.46–7.58 (am, 2H), 7.03–7.13 (am, 2H), 6.10 (s, 1H), 6.00–6.11 (am, 1H), 5.47 (d, J = 17.2 Hz, 1H), 5.39 (d, J = 10.0 Hz, 1H), 4.44–4.53 (am, 1H), 4.21 (dd, J = 8.7, 6.0 Hz, 1H), 3.88 (dd, J = 8.9, 3.6 Hz, 1H), 2.76 (s, 3H); **¹³C NMR** ($CDCl_3$, 125.7 MHz) *Major Diastereomer*: δ 164.4 (d, J = 7.9 Hz), 135.8, 133.6 (d, J = 2.8 Hz), 129.2 (d, J = 8.3 Hz), 119.2, 115.7 (d, J = 21.7 Hz), 91.4, 71.12, 61.8, 39.3; *Minor Diastereomer*: δ 162.4 (d, J = 7.4 Hz), 134.3, 134.2 (d, J = 3.2 Hz), 129.4 (d, J = 8.3 Hz), 120.4, 115.6 (d, J = 21.7 Hz), 90.7, 70.9, 62.1, 41.5; **IR** (film CH_2Cl_2 , cm^{-1}) 3054, 2983, 1604, 1423, 1347, 1264, 1226, 1155, 1091; **HRMS-ESI** (m/z): $[M+Na]^+$ calcd for $C_{12}H_{14}FNO_3S$ requires 294.0576; found 294.0580; **TLC** R_f = 0.3 (25% EtOAc/Hexanes, visualized under UV, PAA stains blue); $[\alpha]^{24}_D$ –10.8 (c 2.8, $CHCl_3$); **SFC** analysis (AD-H, 10.0% MeOH, 2.0 mL/min, 215 nm) indicated 91% ee for the major diastereomer: t_R (minor) = 3.56 min, t_R (major) = 4.02 min.

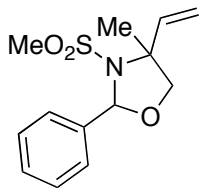


(2S,4S)-2-(3,4-dimethoxyphenyl)-3-(methylsulfonyl)-4-vinyloxazolidine (5d): Following the general procedure above imine **4d** (24 mg, 0.10 mmol) was reacted with butadienemonoxide (10 μ L, 0.12 mmol, 1.2 equiv) for 23 hours. Purification by column chromatography with a gradient from 10-25% EtOAc/Hexanes afforded **5d** (3:1 dr) as a tan oil (30 mg, 97% yield). **¹H NMR** (δ ($CDCl_3$, 500 MHz) *Major Diastereomer*: δ 7.11 (adt, J = 8.6, 1.7 Hz, 1H), 7.06 (ad, J = 1.5 Hz, 1H), 6.88 (d, J = 8.3 Hz, 1H), 6.16 (s,

1H), 5.81 (ddd, $J = 17.4, 10.2, 7.6$ Hz, 1H), 5.37 (ad, $J = 17.0$ Hz, 1H), 5.25 (d, $J = 10.2$ Hz, 1H), 4.52 (aq, $J = 6.4$ Hz, 1H), 4.27 (ad, 8.9 Hz, 1H), 3.90 (s, 6H), 3.83–3.88 (m, 1H), 2.80 (s, 3H); *Minor Diastereomer*: δ 7.08–7.14 (am, 1H), 7.00 (d, $J = 1.7$ Hz, 1H), 6.88 (d, $J = 8.2$ Hz, 1H), 6.06 (s, 1H), 6.02–6.10 (m, 1H), 5.45 (d, $J = 17.1$ Hz, 1H), 5.34–5.40 (am, 1H), 4.46–4.55 (am, 1H), 4.24–4.29 (am, 1H), 3.97 (dd, $J = 13.6, 6.5$ Hz, 1H), 3.91 (s, 3H), 2.71 (s, 3H); ^{13}C NMR δ (CDCl₃, 125.7 MHz) *Major Diastereomer*: δ 149.7, 149.2, 136.1, 129.9, 120.0, 118.9, 110.9, 110.1, 92.0, 71.1, 61.7, 56.1, 40.7; *Minor Diastereomer*: δ 151.0, 149.2, 134.6, 130.4, 120.2, 119.9, 110.8, 110.5, 91.3, 71.0, 62.1, 56.2, 40.7 (2C); IR (film CH₂Cl₂, cm⁻¹) 3015, 2967, 2935, 2840, 1598, 1515, 1440, 1378, 1295, 1140, 1020; HRMS-ESI (m/z): [M+Na]⁺ calcd for C₁₄H₁₉NO₅S requires 336.0882; found 336.0877; TLC R_f = 0.6 (50% EtOAc/Hexanes, visualized under UV, PAA stains blue); [α]_D²⁴ –56.6 (c 0.3, CHCl₃); SFC analysis (AD-H, 10.0% MeOH, 2.0 mL/min, 215 nm) indicated 89% ee for the major diastereomer: t_R (minor) = 5.82 min, t_R (major) = 6.23 min.



(2S,4S)-2-(2-bromophenyl)-3-(methylsulfonyl)-4-vinyloxazolidine (5e): Following the general procedure above imine **4e** (26 mg, 0.10 mmol) was reacted with butadienemonoxide (10 μ L, 0.12 mmol, 1.2 equiv) for 24 hours. Purification by column chromatography with a gradient from 5–15% EtOAc/Hexanes afforded **5e** (2:1 dr) as an orange-brown oil (22 mg, 67% yield). ^1H NMR (CDCl₃, 500 MHz) *Major Diastereomer*: δ 7.65 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.61 (ad, $J = 7.8$ Hz, 1H), 7.37 (t, $J = 7.7$ Hz, 1H), 7.23–7.27 (m, 1H), 6.48 (s, 1H), 6.00–6.08 (m, 1H), 5.47 (d, $J = 17.1$ Hz, 1H), 5.38 (d, $J = 10.4$ Hz, 1H), 4.52 (q, $J = 7.0$ Hz, 1H), 4.24 (dd, $J = 9.2, 6.9$ Hz, 1H), 3.80 (dd, $J = 9.2, 6.2$ Hz, 1H), 2.92 (s, 3H); *Minor Diastereomer*: 7.58–7.63 (am, 2H), 7.35–7.39 (am, 1H), 7.21–7.27 (am, 1H), 6.40 (s, 1H), 6.03 (am, 1H), 5.54 (d, $J = 17.0$ Hz, 1H), 5.43 (d, $J = 10.0$ Hz, 1H), (ddd, $J = 7.3, 5.8, 1.5$ Hz, 1H), 4.13 (dd, $J = 9.2, 5.8$ Hz, 1H), 3.87 (dd, $J = 9.2, 1.8$ Hz, 1H), 2.98 (s, 3H); ^{13}C NMR *Major Diastereomer*: δ (CDCl₃, 125.7 MHz) δ 136.4, 135.1, 133.8, 131.1, 129.1, 127.5, 124.1, 120.1, 91.8, 70.6, 62.4, 39.0; *Minor Diastereomer*: δ 136.7, 134.5, 133.6, 130.9, 129.1, 127.3, 123.5, 121.1, 94.4, 70.2, 62.5, 41.4; IR (film CH₂Cl₂, cm⁻¹) 3054, 2989, 2928, 2879, 1437, 1344, 1262, 1201, 1102, 1023; HRMS-ESI (m/z): [M+Na]⁺ calcd for C₁₂H₁₄BrNO₃S requires 353.9775; found 353.9764; TLC R_f = 0.3 (25% EtOAc/Hexanes, visualized under UV, PAA stains blue); SFC analysis (AD-H, 5.0% MeOH, 2.0 mL/min, 215 nm) indicated 86% ee for the major diastereomer: t_R (major) = 6.65 min, t_R (minor) = 7.25 min.

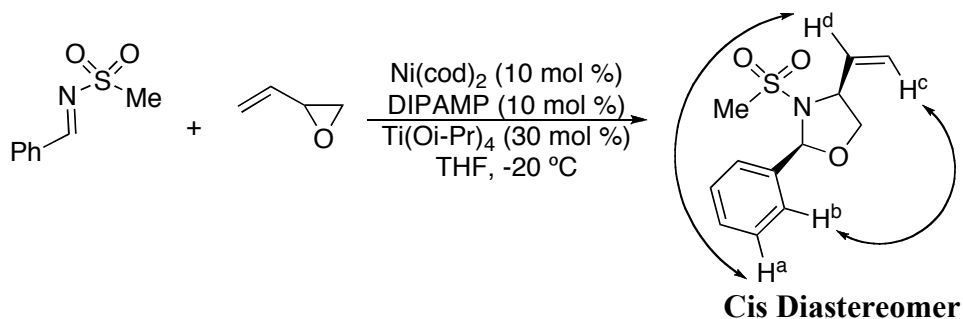


(2S,4S)-4-methyl-3-(methanesulfonyl)-2-phenyl-4-vinyloxazolidine (5f): Except for the following modifications, the general procedure above was followed. Imine **4a** (36 mg, 0.2 mmol) was reacted with isoprene monoxide (49 μ L, 0.50 mmol, 2.5 equiv) in diglyme (1 mL) for 48 hours. Purification by column chromatography with a gradient from 5–15% EtOAc/Hexanes afforded **5f** (3:1 dr) as a yellow oil (52 mg, 96% yield). $^1\text{H NMR}$ δ (CDCl_3 , 500 MHz) *Major Diastereomer*: δ 7.53–7.59 (m, 2H), 7.36–7.44 (m, 3H), 6.26 (d, J = 10.6 Hz, 1H), 6.22 (d, J = 10.8 Hz, 1H), 6.12 (s, 1H), 5.43 (d, J = 17.5 Hz, 1H), 5.35 (d, J = 10.5 Hz, 1H), 3.96 (d, J = 8.9 Hz, 1H), 3.83 (d, J = 8.9 Hz, 1H), 2.75 (s, 3H), 1.68 (s, 3H); *Minor Diastereomer*: δ 7.53–7.60 (am, 2H), 7.35–7.44 (am, 3H), 6.10–6.19 (am, 1H), 6.12 (am, 1H), 5.36–5.41 (am, 1H), 5.32 (d, J = 11.0 Hz, 1H), 4.06 (d, J = 8.7 Hz, 1H), 3.81–3.85 (am, 1H), 2.58 (s, 3H), 1.78 (s, 3H); $^{13}\text{C NMR}$ δ (CDCl_3 , 125 Hz) δ 139.2, 138.39, 129.43, 128.7, 127.7, 116.3, 92.38, 77.32, 66.26, 41.54, 22.05; **IR** (film CH_2Cl_2 , cm^{-1}) 3060, 2983, 2934, 2873, 1454, 1412, 1338, 1264, 1202, 1154, 1075, 1026; **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{13}\text{H}_{17}\text{NO}_3\text{S}$ requires 290.0827; found 290.0833; **TLC** R_f = 0.5 (50% EtOAc/Hexanes, visualized under UV, PAA stains blue); $[\alpha]_D^{24}$ +15.8 (c 3.9, CHCl_3); **SFC** analysis (CHIRALPAK AD-H, *Gradient*: (2.5% *i*-PA-18.5 min, 10.0% *i*PA-10 min), 215 nm) indicated 62% ee for the major diastereomer: t_R (minor) = 13.1 min, t_R (major) = 23.5 min.

C. Determination of Stereochemistry in the Nickel- and Palladium-Catalyzed Reaction:

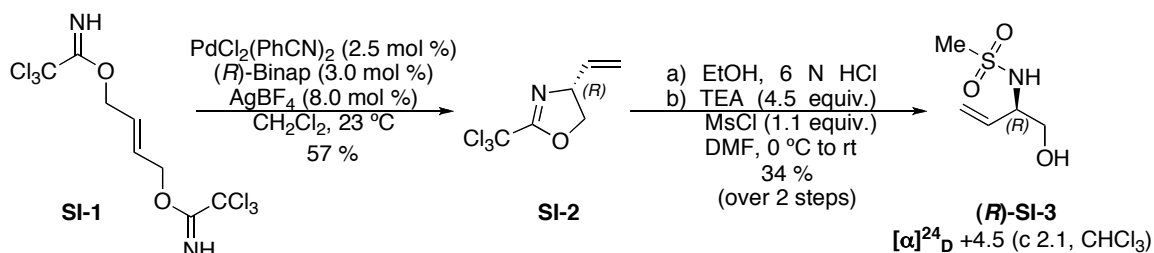
1. Determination of relative stereochemistry: Determined through NOESY correlation as is shown below. *Only cross peaks related to the cis-diastereomer were identified* when a purified sample of the major diastereomer in the nickel-catalyzed reaction was analyzed. NOESY analysis showed NOE cross-peaks between the aryl ring protons (H^a and H^b) and the vinyl protons (H^c and H^d) of the 1,3-oxazolidine ring. Note: the $^1\text{H NMR}$ chemical shifts of this diastereomer matched the chemical shifts of the major diastereomer in the palladium-catalyzed reaction employing the Josiphos ligand. This leads us to conclude that both nickel(DIPAMP) catalyst and palladium(Josiphos) catalyst reactions afford the *cis*-isomer as the major diastereomer.

NOESY: Observed Cross Peaks



2. Determination of absolute stereochemistry.

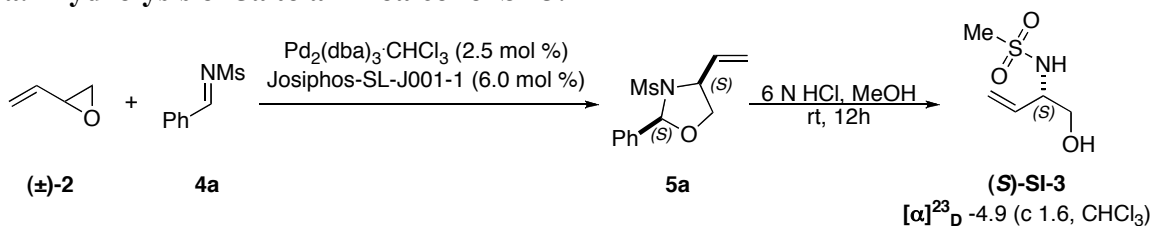
a. Preparation of authentic aminoalcohol (*R*)-SI-3: The following modified sequence was employed to produce (*R*)-SI-3 for comparison to material obtained from our catalytic reaction. Overman rearrangement of SI-1 to provide (*R*)-SI2 was accomplished according to the procedure of Jirgensons and co-workers, and (*R*)-SI2 had spectral and optical rotation that were in good agreement with the reported values.⁸ Hydrolysis and subsequent mesylation of SI-2 was then accomplished by a two step procedure described below to provide (*R*)-SI-3.



SI-2 (277 mg, 1.29 mmol, 1.00 equiv) was dissolved in EtOH (2.0 mL) and 6 N HCl (2.0 mL) was added at room temperature and stirred for 1 h. After stirring for 1 h, the crude reaction mixture was concentrated in vacuo to give the HCl salt of the amino alcohol. The product was then taken on directly by dissolving in DMF (2.5 mL), adding TEA (800 μL, 5.81 mmol) and stirring for 30 min. After 30 min, MsCl (110 μL, 1.42 mmol) was added via syringe to the stirring reaction mixture and the reaction was monitored by TLC for completion. After no starting material remained the crude reaction mixture was diluted with EtOAc (15 mL) and NH₄Cl (5 mL) and the organic layer was extracted (4x EtOAc). The combined organic layers were then dried over Na₂SO₄, decanted and concentrated in vacuo to give a crude oil. Purification was achieved by column chromatography eluting with a gradient from 20-40% EtOAc/Hexanes to produce (*R*)-SI-3, a clear oil (213 mg, 34%). ¹H NMR δ (500 MHz, CDCl₃) δ 5.82 (ddd, *J* = 17.0, 10.5, 6.60 Hz, 1H), 5.41 (d, *J* = 17.1 Hz, 1H), 5.33 (d, *J* = 10.4 Hz, 1H), 5.01 (bd, 7.34 Hz, 1H), 4.09 (add, *J* = 12.4, 10.2, 5.75 Hz, 1H), 3.79 (dd, *J* = 11.3, 4.16 Hz, 1H), 3.62 (dd, *J* = 11.0, 6.24 Hz, 1H), 3.01 (s, 3H), 2.11 (bs, 1H); ¹³C NMR δ (125 MHz, CDCl₃) δ 134.9, 118.6, 65.25, 58.17, 42.15; IR (film CH₂Cl₂, cm⁻¹) 3500, 3362, 3285, 3054, 2989, 2934, 1421, 1325, 1267, 1152, 1075, 984; HRMS-ESI (*m/z*): [M+Na]⁺ calcd for

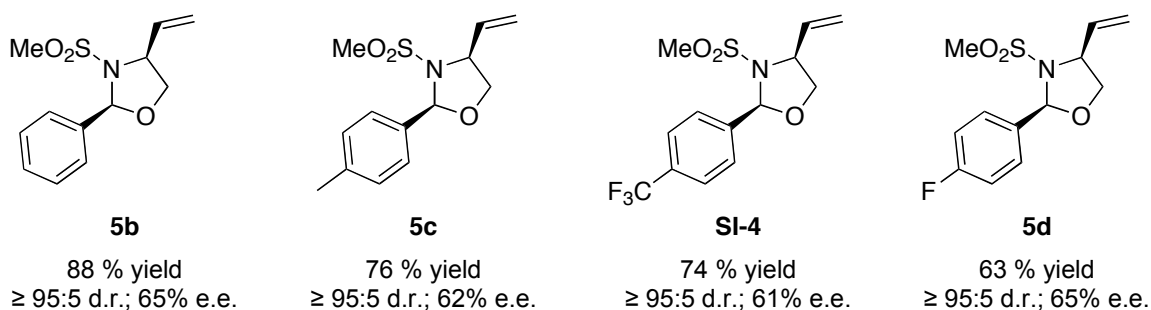
C₅H₁₁NO₃S requires 188.0357; found 188.0359; **TLC** **R_f** = .05 (50% EtOAc/Hexanes, PAA stain purple); [α]²⁴_D +4.85 (*c* 2.1, CHCl₃).

a. Hydrolysis of 5a to aminoalcohol SI-3:



(S)-N-(1-hydroxybut-3-en-2-yl)methanesulfonamide (S)-SI-3 Oxazolidine **5a** (72 mg, 0.28 mmol), which had been prepared according to the general asymmetric palladium-catalyzed method using Josiphos ligand SL-J001-1, was dissolved in MeOH (1 mL) followed by addition of 6 N HCl (260 μ L, 1.55 mmol) and stirring for 1 hour. After 1 hour the crude reaction solution was diluted with EtOAc (15 mL) and satd. NaCl solution (5 mL) and the organic layer was extracted (3x EtOAc). The combined organic layers were dried over Na₂SO₄, decanted and concentrated in vacuo. The crude oil was then purified by column chromatography to remove benzaldehyde. A small plug of silica eluting first with 20% EtOAc/Hexanes, followed by 75% EtOAc/hexanes produced clean **(S)-SI-3**. The optical rotation of the was then taken: [α]²⁴_D -4.95 (*c* 1.4, CHCl₃), and is consistent with the formation of the (*S,S*)-1,3-oxazolidine.

D. Nickel-Catalyzed Synthesis of 1,3-Oxazolidines: General Procedure, Substrate Scope and Mechanistic Reactions (Table 6):

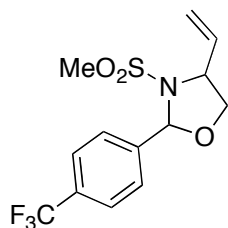


1. General procedure for the nickel-catalyzed synthesis of 1,3-oxazolidines: To an 8 mL screw-top vial with septum, in an inert-air glove box, was added Ni(cod)₂ (5.5 mg, 10 mol %) and (*S,S*)- or (*R,R*)- DIPAMP ligand (9.2 mg, 0.02 mmol, 10.0 mol %). TBAT (108 mg, 0.20 mmol) was then added, the vial was capped and subsequently removed from the glove box. An N₂ line was added, followed by the addition of 1 mL THF and the vial was placed in a bath at -20 °C to stir for 15 min. After the 15 min. pre-stir, the vial was briefly removed from the bath, opened under high flow of N₂ for addition of the solid aryl imine (0.20 mmol), then placed back in the -20 °C bath. After another 5 minutes of stirring, butadiene monoxide (\pm)-**2** (19 μ L, 0.24 mmol) was added

via syringe, followed immediately by addition of $\text{Ti}(\text{Oi-Pr})_4$ (18 μL , 0.30 mmol) via syringe. The reaction was then stirred for 16-24 h while monitoring conversion by TLC for disappearance of imine (UV). When the reaction was judged complete, it was filtered through a small pad of celite rinsing with CH_2Cl_2 (15 mL). The filtrate was then diluted with DI water (5 mL) and extracted with CH_2Cl_2 (x 3). The combined organic layers were dried with Na_2SO_4 , decanted and concentrated in vacuo. Purification was achieved through SiO_2 gel chromatography (15-25% Et_2O /pentanes) to provide analytically pure products. Characterization data for compounds **5a-5c** matched values for oxazolidine products produced using the palladium-catalyzed method (with the exception of optical rotation).

2. Nickel-catalyzed mechanistic experiments (Table 6): For reactions performed utilizing enantiopure (99% ee) butadiene monoxide [(*R*)-**2**], the general nickel-catalyzed procedure above was followed. The only deviations from the general nickel-catalyzed reaction procedure were the use of enantiopure vinyl epoxide (*R*)-**2** and the use of either dppe, (*R,R*)- or (*S,S*)-Dipamp as ligand.

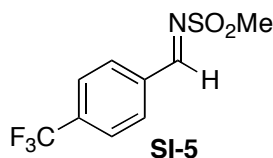
3. Characterization data for SI-4 and SI-5



3-(methylsulfonyl)-2-(4-(trifluoromethyl)phenyl)-4-vinyloxazolidine (SI-4):

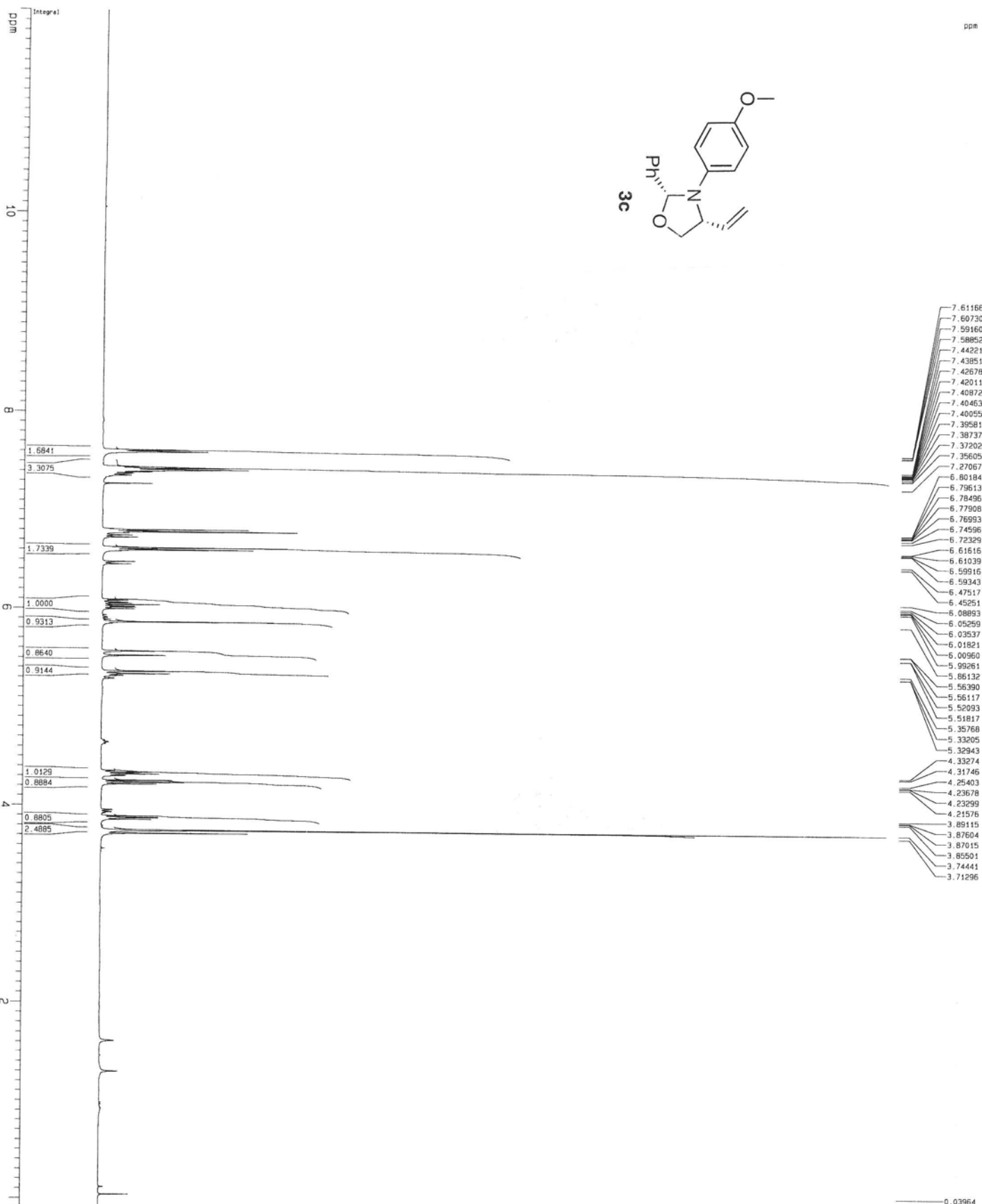
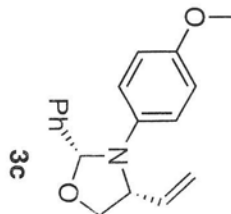
Following the general procedure above imine **SI-5** (50 mg, 0.20 mmol) was reacted with butadienemonoxide (19 μL , 0.24 mmol, 1.2 equiv) for 48 hours. Purification by column chromatography with a gradient from 15-25% Et_2O /pentanes afforded **SI-4** (19:1 dr) as a pale yellow oil (41 mg, 67% yield). ^1H NMR δ (CDCl_3 , 600 MHz) δ 7.69 (d, J = 8.2 Hz, 2H), 7.65 (d, J = 8.2 Hz, 2H), 6.27 (s, 1H), 5.71 (ddd, J = 17.5, 9.8, 7.2, 1H), 5.35 (d, J = 17.0 Hz, 1H), 5.23 (d, J = 10.1 Hz, 1H), 4.50 (aq, J = 6.8 Hz, 1H), 4.32 (dd, J = 9.1, 7.2, 1H), 3.79 (dd, J = 9.2, 6.2, 1H), 2.90 (s, 3H); ^{13}C NMR δ (CDCl_3 , 125 MHz) 141.9, 135.4, 131.5 (d, J = 32 Hz), 127.7, 125.75 (q, J = 3.9 Hz), 125.70 (d, J = 2.2 Hz), 119.4, 91.1, 71.3, 62.0, 38.3; HRMS-ESI (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{13}\text{H}_{14}\text{F}_3\text{NO}_3\text{S}$ requires 344.0544; found 344.0543; SFC analysis (AD-H, 10.0% MeOH, 1.5 mL/min, 215 nm) indicated 61% ee for the major diastereomer: t_R (major) = 4.04 min, t_R (minor) = 4.39 min.

(*E*)-*N*-(4-(trifluoromethyl)benzylidene)methanesulfonamide (SI-5)



SI-5 was prepared from 4-trifluoromethylbenzaldehyde (550 μ L, 5.00 mmol) according to the general procedure and isolated as an amorphous yellow solid (57%, 714 mg). ^1H **NMR** (CDCl_3 , 500 MHz) δ 9.10 (s, 1H), 8.10 (d, J = 8.0 Hz, 2H), 7.81 (d, J = 8.1 Hz, 2H), 3.18 (s, 3H); ^{13}C **NMR** (CDCl_3 , 125 MHz) δ 170.2, 136.1 (q, 32.8 Hz), 135.1, 131.4, 126.3 (q, 3.70 Hz), 123.4 (d, 273 Hz), 40.3; **IR**; **HRMS-ESI** (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_9\text{H}_8\text{F}_3\text{NO}_2\text{S}$ requires 274.0125; found 274.0127.

¹H spectrum



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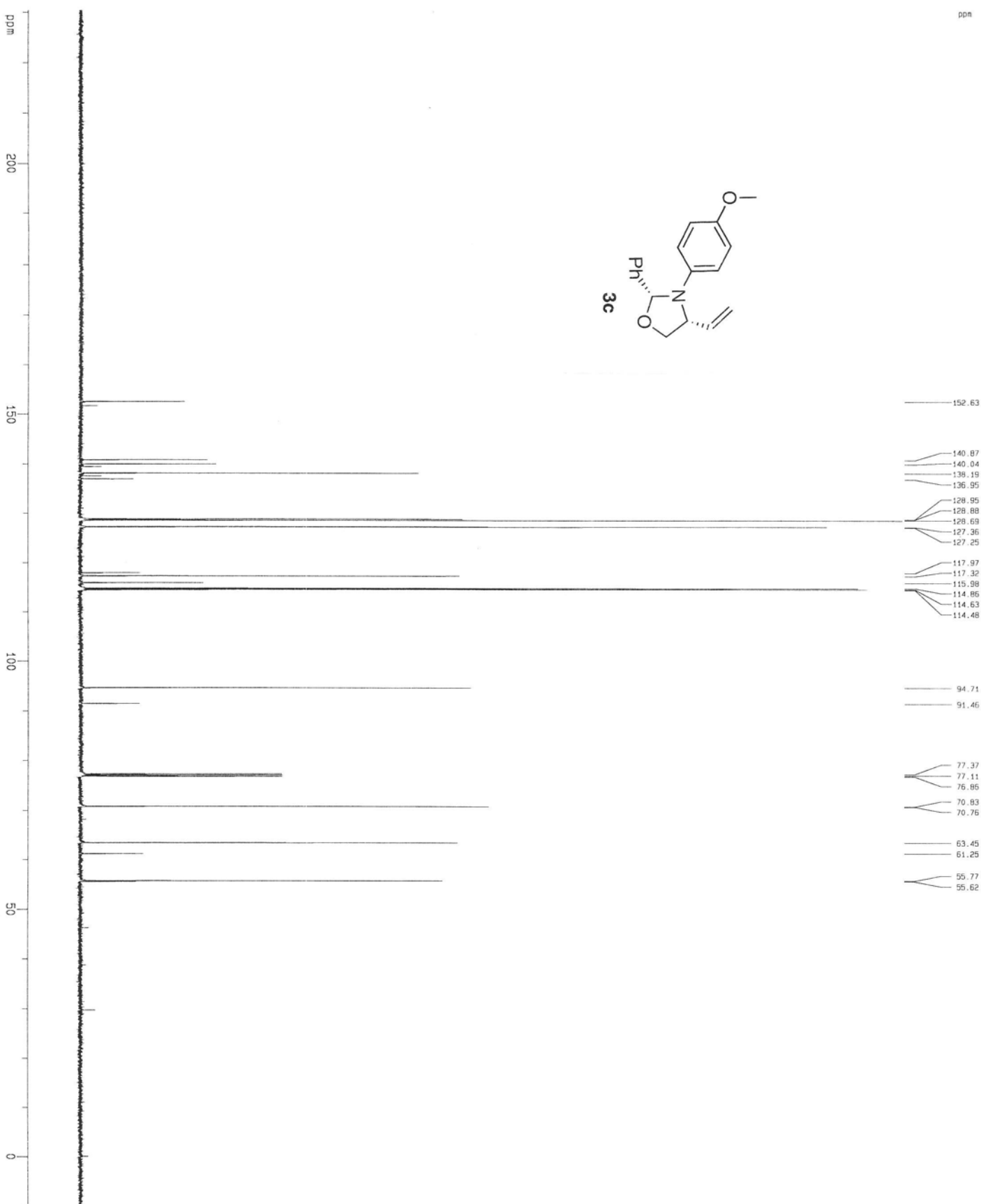
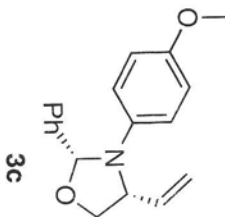
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1D NMR plot parameters
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Z-restored spin-echo 13C spectrum with 1H decoupling



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 SFO90: 500.136456 MHz
 SFO91: 500.136456 MHz
 SFO92: 500.136456 MHz
 SFO93: 500.136456 MHz
 SFO94: 500.136456 MHz
 SFO95: 500.136456 MHz
 SFO96: 500.136456 MHz
 SFO97: 500.136456 MHz
 SFO98: 500.136456 MHz
 SFO99: 500.136456 MHz
 SFO100: 500.136456 MHz

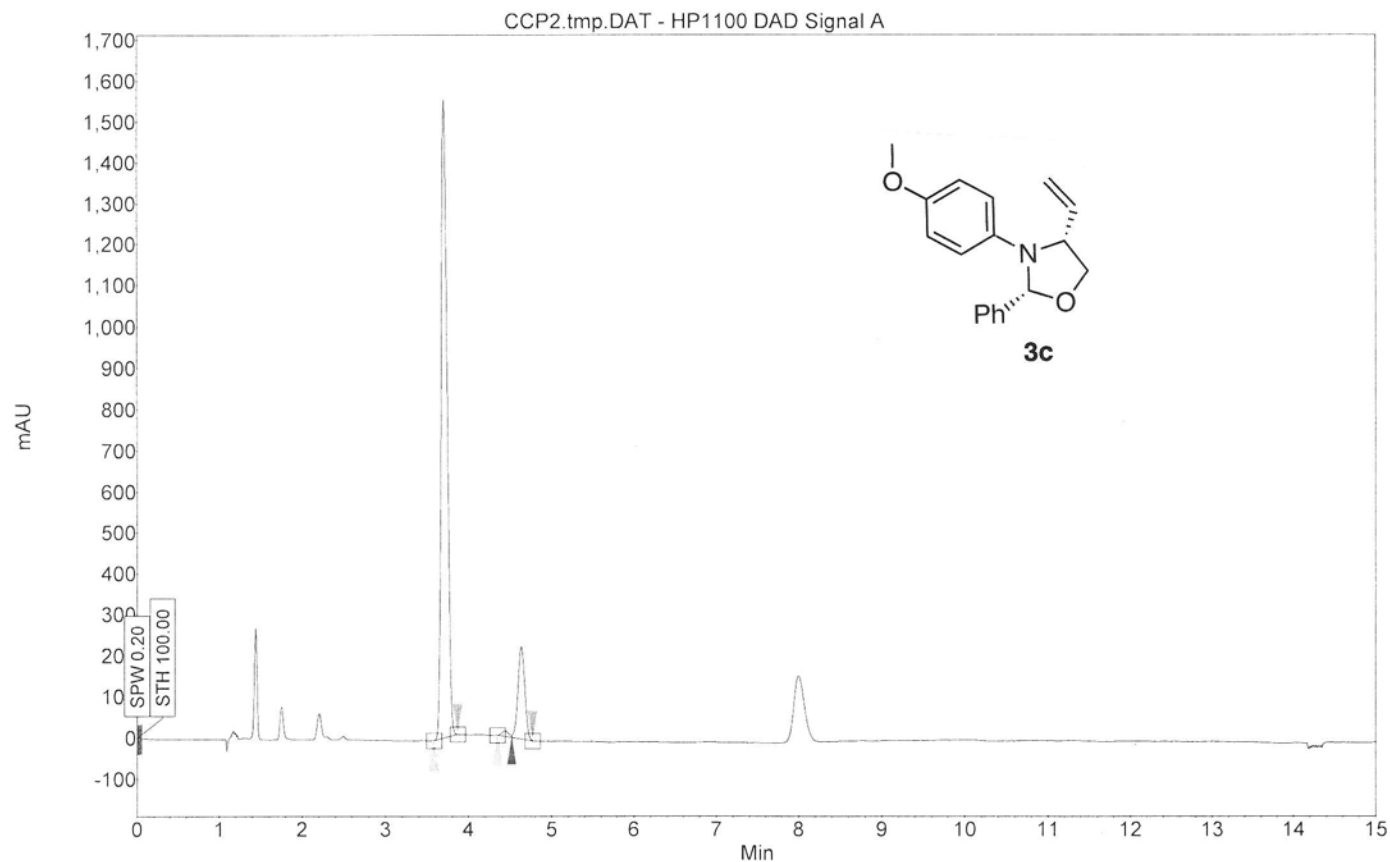
***** GRADIENT CHANNEL *****
 GRAD1: SINE 100
 GRAD2: SINE 100
 GRAD3: SINE 100
 GRAD4: SINE 100
 GRAD5: SINE 100
 GRAD6: SINE 100
 GRAD7: SINE 100
 GRAD8: SINE 100
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 GRAD10: SINE 100
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 GRAD14: SINE 100
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 GRAD93: SINE 100
 GRAD94: SINE 100
 GRAD95: SINE 100
 GRAD96: SINE 100
 GRAD97: SINE 100
 GRAD98: SINE 100
 GRAD99: SINE 100
 GRAD100: SINE 100

F2 - Processing parameters
 SI: 32768
 SF: 125.760450 MHz
 K0: 0
 L0: 1.00 Hz
 L8: 1.00 Hz
 L9: 0
 G0: 2.00
 G8: 0
 G9: 0

10 NMR plot parameters
 CY: 22.80 cm
 CX: 15.65 cm
 F1P: 230.637 ppm
 F1: 29009.66 Hz
 F2P: -10.287 ppm
 F2: -1293.96 Hz
 PPM0K: 10.0688 ppm/cm
 HZ0K: 1329.10708 Hz/cm

Method Name:REG-ADH-5IPA-15mlmin
Run Name:REG_IV_874

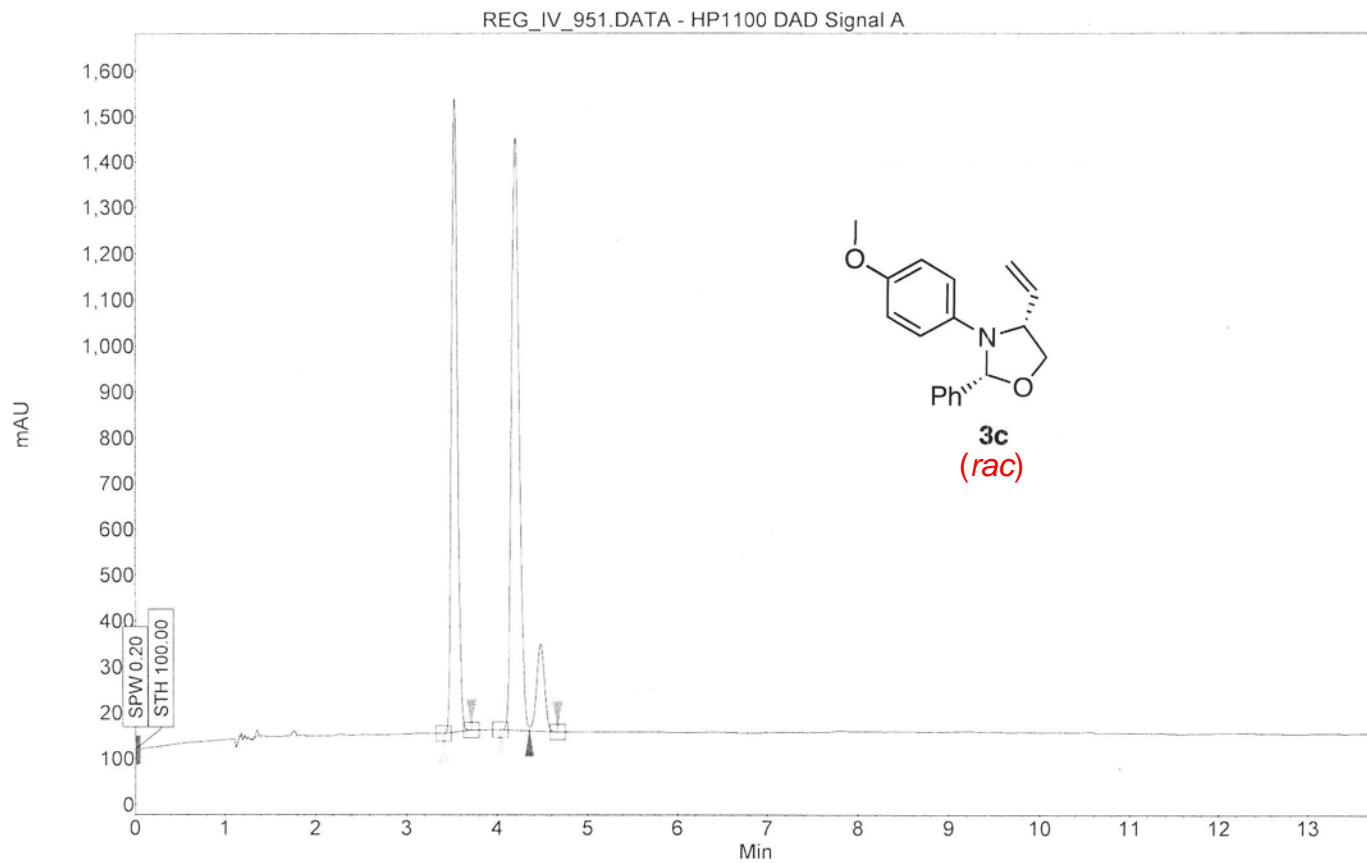
Date:5/18/2011
Time:5:30:33 PM



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
3	UNKNOWN	3.58	3.70	3.87	0.00	84.81	1553.8	127.6	84.806
1	UNKNOWN	4.35	4.44	4.52	0.00	0.90	13.8	1.4	0.902
2	UNKNOWN	4.52	4.63	4.77	0.00	14.29	223.7	21.5	14.292
Total						100.00	1791.3	150.4	100.000

Method Name:REG-ADH-5IPA-15ml/min
Run Name:REG_IV_951

Date:5/16/2011
Time:1:09:51 PM



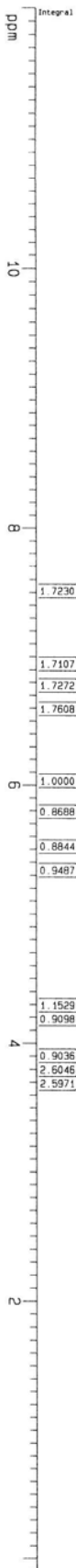
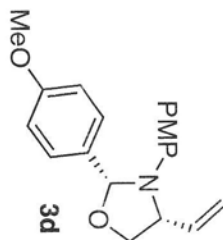
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	3.40	3.53	3.71	0.00	41.44	1380.9	104.2	41.445
2	UNKNOWN	4.03	4.19	4.35	0.00	50.96	1290.3	128.2	50.960
3	UNKNOWN	4.35	4.47	4.66	0.00	7.60	189.0	19.1	7.595
Total						100.00	2860.3	251.5	100.000

ppm

7.52554
7.52072
7.50863
7.50390
7.33054
7.27037
6.95317
6.94815
6.93634
6.93138
6.89769
6.87594
6.78983
6.78410
6.77289
6.76708
6.73829
6.71562
6.60742
6.60161
6.59036
6.58471
6.46759
6.44494
6.05189
6.04228
6.03479
6.01767
6.00894
5.99209
5.80071
5.54845
5.50549
5.34666
5.32110
5.30502
4.29748
4.28273
4.26581
4.22506
4.20769
4.20408
4.18685
3.90912
3.89119
3.87685
3.87022
3.85587
3.83420
3.80289
3.73651
3.70851

1.62654

0.03244



Current Data Parameters
USER: fprote
NAME: REG_IV_91_1
EXPNO: 1
PROCNO: 1

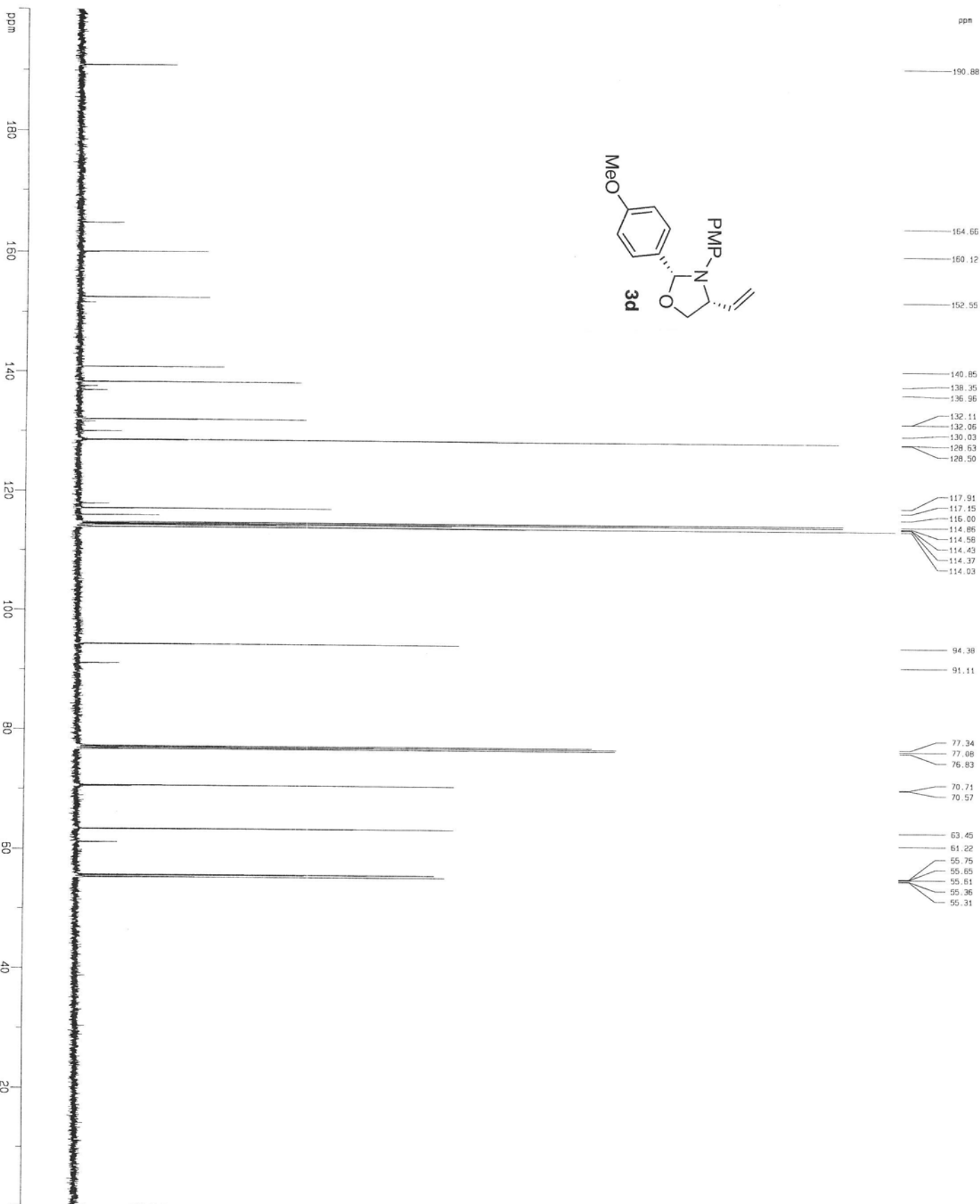
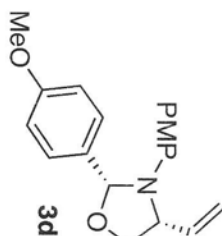
F2 - Acquisition Parameters
Date_: 20091022
Time: 13.55
INSTRUM: zgpg30
PROBHD: 5 mm QNP 1H/13
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 2
DS: 2
SWH: 6410.256 Hz
FIDRES: 0.097813 Hz
AQ: 5.116979 sec
RG: 90.5
DM: 78.000 usec
DE: 645.00 usec
TE: 297.2 K
D1: 0.1000000 sec
d11: 297.2 K
MCOREST: 0.0000000 sec
MCOREX: 0.0150000 sec

***** CHANNEL f1 *****
NUC1: 1H
P1: 12.00 usec
PL1: 0.00 dB
SFO1: 400.126009 MHz

F2 - Processing parameters
SI: 65536
SF: 400.150073 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: 12.000 ppm
F2P: 4801.56 Hz
F3P: -0.100 ppm
PCHN: 0.59075556/cm
H2CH: 212.34972 Hz/cm

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



Current Data Parameters

NAME	VALUE
USER	REG JV 91.2C
INSTRUM	CRYM500
PROBHD	5 mm CPTC 1H-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	564
DS	16
SWH	30303.031 Hz
FIDRES	0.4622889 Hz
AQ	1.0914105 sec
RG	3248
RM	16.500 usec
DE	15.00 usec
TE	298.0 K
O1	0.25000000 sec
O11	0.03000000 sec
O16	0.00020000 sec
O17	0.00019600 sec
MCOREST	0.00000000 sec
MCORCK	0.01500000 sec
P2	31.00 usec

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

NAME	VALUE
NUC1	¹³ C
P1	15.50 usec
P11	500.00 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	-1.00 dB
PL2	125.734248 MHz
SP1	3.20 dB
SP2	3.20 dB
SPNAM1	CP60.0.5.20.1
SPNAM2	CP600cap.4
SPOFF1	0.00 Hz
SPOFF2	0.00 Hz

===== CHANNEL f2 =====

NAME	VALUE
CPROG2	zgpg30
NUC2	¹ H
P2	100.00 usec
PL2	1.60 dB
PL12	24.60 dB
SP2	500.2222011 MHz

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

NAME	VALUE
GRAD1	100.00 usec
GRAD2	100.00 usec
GRAD3	100.00 usec
GRAD4	100.00 usec
GRAD5	100.00 usec
GRAD6	100.00 usec
GRAD7	100.00 usec
GRAD8	100.00 usec
GRAD9	100.00 usec
GRAD10	100.00 usec
GRAD11	100.00 usec
GRAD12	100.00 usec
GRAD13	100.00 usec
GRAD14	100.00 usec
GRAD15	100.00 usec
GRAD16	100.00 usec
GRAD17	100.00 usec
GRAD18	100.00 usec
GRAD19	100.00 usec
GRAD20	100.00 usec
GRAD21	100.00 usec
GRAD22	100.00 usec
GRAD23	100.00 usec
GRAD24	100.00 usec
GRAD25	100.00 usec
GRAD26	100.00 usec
GRAD27	100.00 usec
GRAD28	100.00 usec
GRAD29	100.00 usec
GRAD30	100.00 usec
GRAD31	100.00 usec
GRAD32	100.00 usec
GRAD33	100.00 usec
GRAD34	100.00 usec
GRAD35	100.00 usec
GRAD36	100.00 usec
GRAD37	100.00 usec
GRAD38	100.00 usec
GRAD39	100.00 usec
GRAD40	100.00 usec
GRAD41	100.00 usec
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GRAD75	100.00 usec
GRAD76	100.00 usec
GRAD77	100.00 usec
GRAD78	100.00 usec
GRAD79	100.00 usec
GRAD80	100.00 usec
GRAD81	100.00 usec
GRAD82	100.00 usec
GRAD83	100.00 usec
GRAD84	100.00 usec
GRAD85	100.00 usec
GRAD86	100.00 usec
GRAD87	100.00 usec
GRAD88	100.00 usec
GRAD89	100.00 usec
GRAD90	100.00 usec
GRAD91	100.00 usec
GRAD92	100.00 usec
GRAD93	100.00 usec
GRAD94	100.00 usec
GRAD95	100.00 usec
GRAD96	100.00 usec
GRAD97	100.00 usec
GRAD98	100.00 usec
GRAD99	100.00 usec
GRAD100	100.00 usec

10 NMR Plot Parameters

NAME	VALUE
CX	22.80 cm
CV	15.65 cm
F1P	200.000 ppm
F1	25156.08 Hz
F2P	0.000 ppm
F2	0.00 Hz
NUC1	¹³ C
NUC2	¹ H
NUC3	¹ H
NUC4	¹ H
NUC5	¹ H
NUC6	¹ H
NUC7	¹ H
NUC8	¹ H
NUC9	¹ H
NUC10	¹ H
NUC11	¹ H
NUC12	¹ H
NUC13	¹ H
NUC14	¹ H
NUC15	¹ H
NUC16	¹ H
NUC17	¹ H
NUC18	¹ H
NUC19	¹ H
NUC20	¹ H
NUC21	¹ H
NUC22	¹ H
NUC23	¹ H
NUC24	¹ H
NUC25	¹ H
NUC26	¹ H
NUC27	¹ H
NUC28	¹ H
NUC29	¹ H
NUC30	¹ H
NUC31	¹ H
NUC32	¹ H
NUC33	¹ H
NUC34	¹ H
NUC35	¹ H
NUC36	¹ H
NUC37	¹ H
NUC38	¹ H
NUC39	¹ H
NUC40	¹ H
NUC41	¹ H
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NUC64	¹ H
NUC65	¹ H
NUC66	¹ H
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NUC68	¹ H
NUC69	¹ H
NUC70	¹ H
NUC71	¹ H
NUC72	¹ H
NUC73	¹ H
NUC74	¹ H
NUC75	¹ H
NUC76	¹ H
NUC77	¹ H
NUC78	¹ H
NUC79	¹ H
NUC80	¹ H
NUC81	¹ H
NUC82	¹ H
NUC83	¹ H
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NUC85	¹ H
NUC86	¹ H
NUC87	¹ H
NUC88	¹ H
NUC89	¹ H
NUC90	¹ H
NUC91	¹ H
NUC92	¹ H
NUC93	¹ H
NUC94	¹ H
NUC95	¹ H
NUC96	¹ H
NUC97	¹ H
NUC98	¹ H
NUC99	¹ H
NUC100	¹ H

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

NAME	VALUE
CPROG1	zgpg30
NUC1	¹³ C
P1	15.50 usec
P11	500.00 usec
P12	2000.00 usec
PL0	120.00 dB
PL1	-1.00 dB
PL2	125.734248 MHz
SP1	3.20 dB
SP2	3.20 dB
SPNAM1	CP60.0.5.20.1
SPNAM2	CP600cap.4
SPOFF1	0.00 Hz
SPOFF2	0.00 Hz

===== CHANNEL f2 =====

NAME	VALUE
CPROG2	zgpg30
NUC2	¹ H
P2	100.00 usec
PL2	1.60 dB
PL12	24.60 dB
SP2	500.2222011 MHz

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

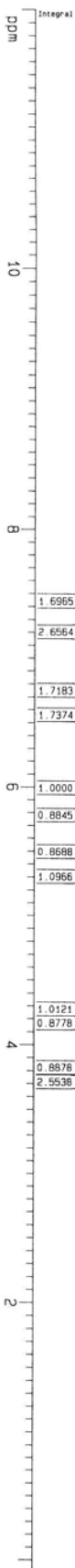
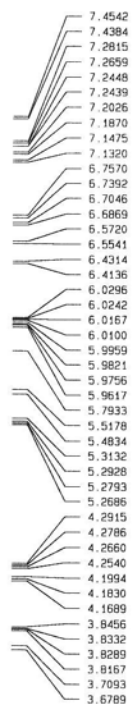
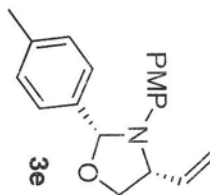
NAME	VALUE
GRAD1	100.00 usec
GRAD2	100.00 usec
GRAD3	100.00 usec
GRAD4	100.00 usec
GRAD5	100.00 usec
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GRAD7	100.00 usec
GRAD8	100.00 usec
GRAD9	100.00 usec
GRAD10	100.00 usec
GRAD11	100.00 usec
GRAD12	100.00 usec
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GRAD27	100.00 usec
GRAD28	100.00 usec
GRAD29	100.00 usec
GRAD30	100.00 usec
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GRAD33	100.00 usec
GRAD34	100.00 usec
GRAD35	100.00 usec
GRAD36	100.00 usec
GRAD37	100.00 usec
GRAD38	100.00 usec
GRAD39	100.00 usec
GRAD40	100.00 usec
GRAD41	100.00 usec
GRAD42	100.00 usec
GRAD43	100.00 usec
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GRAD82	100.00 usec
GRAD83	100.00 usec
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GRAD91	100.00 usec
GRAD92	100.00 usec
GRAD93	100.00 usec
GRAD94	100.00 usec
GRAD95	100.00 usec
GRAD96	100.00 usec
GRAD97	100.00 usec
GRAD98	100.00 usec
GRAD99	100.00 usec
GRAD100	100.00 usec

10 NMR Plot Parameters

NAME	VALUE
CX	22.80 cm
CV	15.65 cm
F1P	200.000 ppm
F1	25156.08 Hz
F2P	0.000 ppm
F2	0.00 Hz
NUC1	¹³

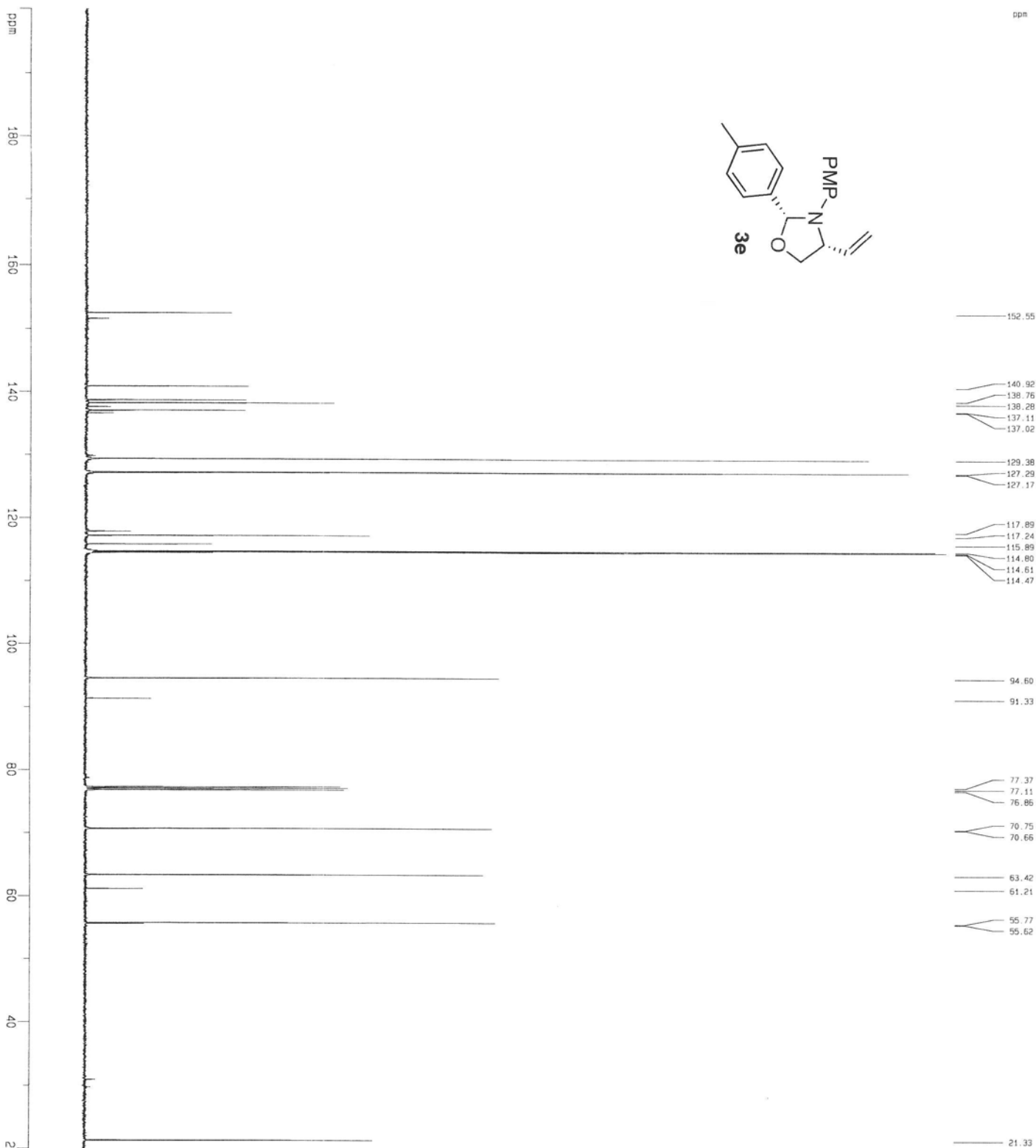
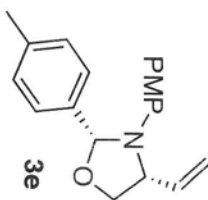
¹H spectrum

ppm



Current Data Parameters
 USER: reg_iv_b3_x
 NAME: REG_IV_B3_X
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20091204
 Time: 15:04
 INSTRUM: spect
 CHANNEL: 5 mm CP131-
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 6012.820 Hz
 FIDRES: 0.098043 Hz
 AQ: 5.0998774 sec
 RG: 4
 DM: 62.400 uspc
 DE: 6.00 uspc
 TE: 300.2 K
 D1: 0.1000000 sec
 MCOREST: 0.0000000 sec
 MCORR: 0.0150000 sec
 ***** CHANNEL f1 *****
 NUC1: ¹H
 P1: 7.50 usec
 PL1: 1.50 dB
 SF01: 500.225015 MHz
 F2 - Processing parameters
 SI: 65536
 SF: 500.225015 MHz
 KW: 65536
 SSF: 0
 LB: 0.30 Hz
 GB: 0
 PC: 4.00
 1D NMR plot parameters
 CX: 22.80 cm
 CY: 15.00 cm
 F1P: 12.000 ppm
 F1: 8002.84 Hz
 F2P: -0.100 ppm
 F2: -50.102 Hz
 PPM0K: 0.00000000
 HZ0K: 285.46705 Hz/cm

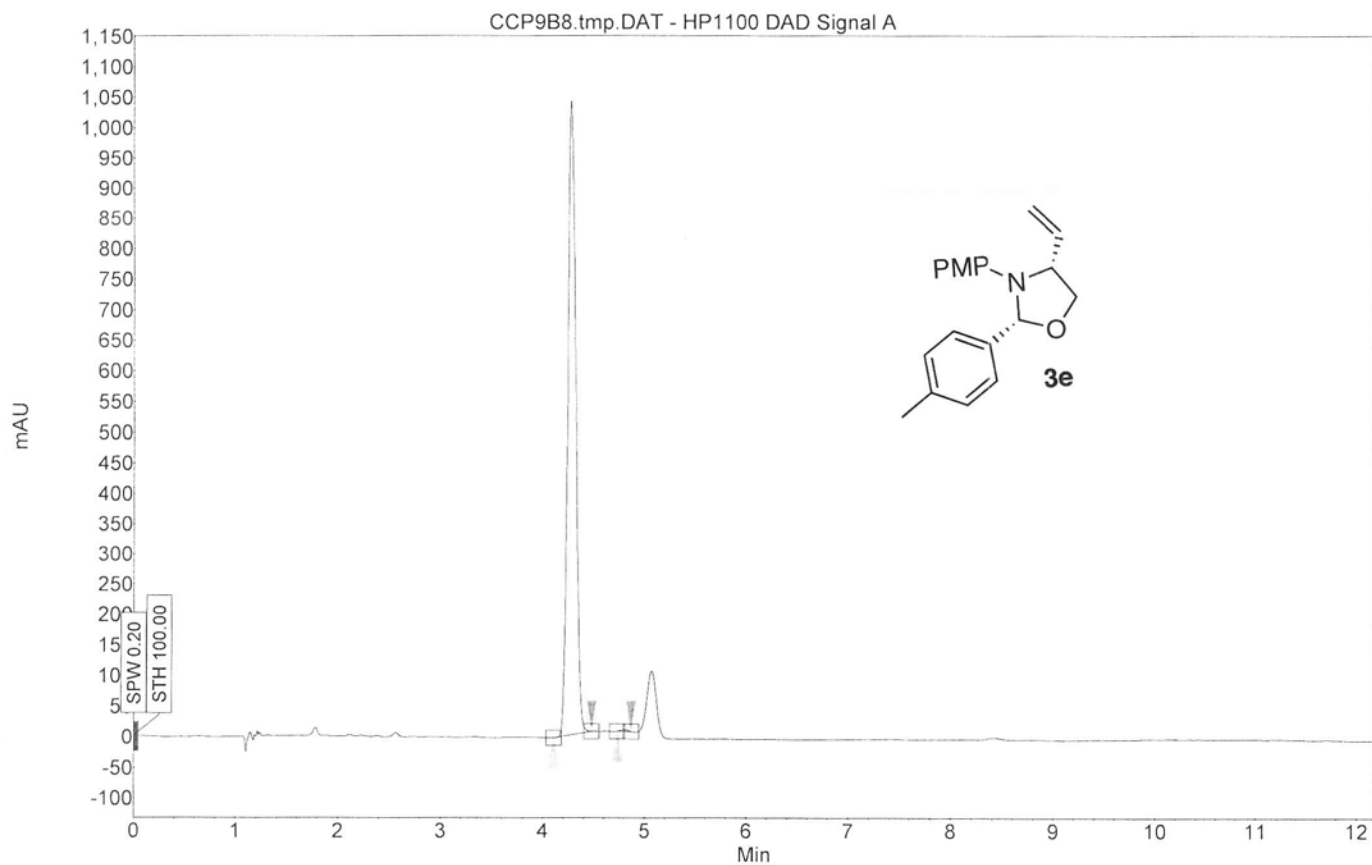
Z-restored spin-echo 13C spectrum with 1H decoupling



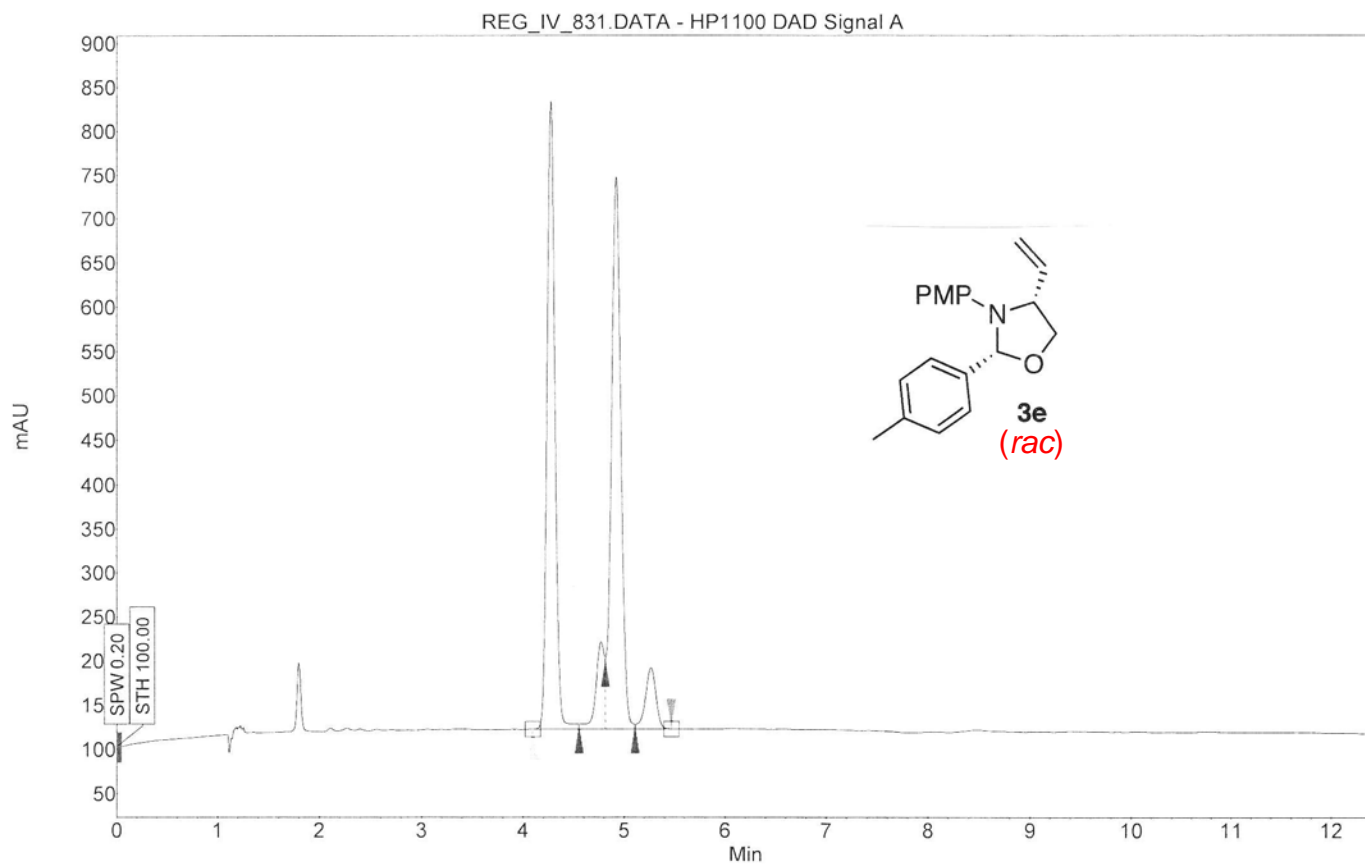
Current Data Parameters
 USER: REG_LV_B3_C
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20080114
 Time: 20.48
 INSTRUM: cryo500
 PROBO: 5 mm CP1CI 1H-
 PULPROG: zgpg30
 TO: 65536
 SOLVENT: DMSO-d6
 NS: 659
 DS: 4
 SWH: 30393.013 Hz
 FIDRES: 0.462386 Hz
 AQ: 1.084105 sec
 RG: 7298.2
 DM: 16.500 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 0.2500000 sec
 d11: 0.0300000 sec
 O16: 0.0000000 sec
 d17: 0.0000000 sec
 MCOREST: 0.0000000 sec
 MCHRG: 0.0150000 sec
 P2: 31.00 usec
 ***** CHANNEL f1 *****
 NUC1: 13C
 P1: 14.50 usec
 PL1: 50.00 dB
 P12: 500.00 usec
 PL2: 2000.00 usec
 PL0: 120.00 dB
 PL1: -1.00 dB
 SF01: 125.794248 MHz
 SP1: 3.20 dB
 SFO1: 125.794248 MHz
 SFO2: 500.136049 MHz
 SFOFF1: 0.00 Hz
 SFOFF2: 0.00 Hz
 ***** CHANNEL f2 *****
 NUC2: 1H
 P2: 100.00 usec
 PL2: 19.00 dB
 PL12: 24.80 dB
 SF02: 500.225011 MHz
 ***** GRADIENT CHANNEL *****
 GPMAG1 SINE: 100
 GPMAG2 SINE: 100
 GPR1: 0.00 x
 GPR2: 0.00 x
 GPR3: 0.00 x
 GPR4: 0.00 x
 GPR5: 0.00 x
 GPR6: 0.00 x
 GPR7: 0.00 x
 GPR8: 0.00 x
 GPR9: 0.00 x
 GPR10: 0.00 x
 GPR11: 0.00 x
 GPR12: 0.00 x
 GPR13: 0.00 x
 GPR14: 0.00 x
 GPR15: 0.00 x
 GPR16: 0.00 x
 GPR17: 0.00 x
 GPR18: 0.00 x
 GPR19: 0.00 x
 GPR20: 0.00 x
 GPR21: 0.00 x
 GPR22: 0.00 x
 GPR23: 0.00 x
 GPR24: 0.00 x
 GPR25: 0.00 x
 GPR26: 0.00 x
 GPR27: 0.00 x
 GPR28: 0.00 x
 GPR29: 0.00 x
 GPR30: 0.00 x
 GPR31: 0.00 x
 GPR32: 0.00 x
 GPR33: 0.00 x
 GPR34: 0.00 x
 GPR35: 0.00 x
 GPR36: 0.00 x
 GPR37: 0.00 x
 GPR38: 0.00 x
 GPR39: 0.00 x
 GPR40: 0.00 x
 GPR41: 0.00 x
 GPR42: 0.00 x
 GPR43: 0.00 x
 GPR44: 0.00 x
 GPR45: 0.00 x
 GPR46: 0.00 x
 GPR47: 0.00 x
 GPR48: 0.00 x
 GPR49: 0.00 x
 GPR50: 0.00 x
 GPR51: 0.00 x
 GPR52: 0.00 x
 GPR53: 0.00 x
 GPR54: 0.00 x
 GPR55: 0.00 x
 GPR56: 0.00 x
 GPR57: 0.00 x
 GPR58: 0.00 x
 GPR59: 0.00 x
 GPR60: 0.00 x
 GPR61: 0.00 x
 GPR62: 0.00 x
 GPR63: 0.00 x
 GPR64: 0.00 x
 GPR65: 0.00 x
 GPR66: 0.00 x
 GPR67: 0.00 x
 GPR68: 0.00 x
 GPR69: 0.00 x
 GPR70: 0.00 x
 GPR71: 0.00 x
 GPR72: 0.00 x
 GPR73: 0.00 x
 GPR74: 0.00 x
 GPR75: 0.00 x
 GPR76: 0.00 x
 GPR77: 0.00 x
 GPR78: 0.00 x
 GPR79: 0.00 x
 GPR80: 0.00 x
 GPR81: 0.00 x
 GPR82: 0.00 x
 GPR83: 0.00 x
 GPR84: 0.00 x
 GPR85: 0.00 x
 GPR86: 0.00 x
 GPR87: 0.00 x
 GPR88: 0.00 x
 GPR89: 0.00 x
 GPR90: 0.00 x
 GPR91: 0.00 x
 GPR92: 0.00 x
 GPR93: 0.00 x
 GPR94: 0.00 x
 GPR95: 0.00 x
 GPR96: 0.00 x
 GPR97: 0.00 x
 GPR98: 0.00 x
 GPR99: 0.00 x
 GPR100: 0.00 x
 F2 - Processing Parameters
 SI: 65536
 SF: 125.780418 MHz
 KHZ: 125.780418
 MD: 0
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 2.00
 10 NMR plot parameters
 CX: 22.00 cm
 CY: 14.00 cm
 CZ: 14.00 cm
 F1: 200.000 ppm
 F2: 25156.08 Hz
 F3: 0.000 ppm
 F4: 0.00 Hz
 F5: 8.77193 DMSO/cm
 F6: 1103.3704 Hz/cm
 F7: 0.00 Hz
 F8: 0.00 Hz
 F9: 0.00 Hz
 F10: 0.00 Hz
 F11: 0.00 Hz
 F12: 0.00 Hz
 F13: 0.00 Hz
 F14: 0.00 Hz
 F15: 0.00 Hz
 F16: 0.00 Hz
 F17: 0.00 Hz
 F18: 0.00 Hz
 F19: 0.00 Hz
 F20: 0.00 Hz
 F21: 0.00 Hz
 F22: 0.00 Hz
 F23: 0.00 Hz
 F24: 0.00 Hz
 F25: 0.00 Hz
 F26: 0.00 Hz
 F27: 0.00 Hz
 F28: 0.00 Hz
 F29: 0.00 Hz
 F30: 0.00 Hz
 F31: 0.00 Hz
 F32: 0.00 Hz
 F33: 0.00 Hz
 F34: 0.00 Hz
 F35: 0.00 Hz
 F36: 0.00 Hz
 F37: 0.00 Hz
 F38: 0.00 Hz
 F39: 0.00 Hz
 F40: 0.00 Hz
 F41: 0.00 Hz
 F42: 0.00 Hz
 F43: 0.00 Hz
 F44: 0.00 Hz
 F45: 0.00 Hz
 F46: 0.00 Hz
 F47: 0.00 Hz
 F48: 0.00 Hz
 F49: 0.00 Hz
 F50: 0.00 Hz
 F51: 0.00 Hz
 F52: 0.00 Hz
 F53: 0.00 Hz
 F54: 0.00 Hz
 F55: 0.00 Hz
 F56: 0.00 Hz
 F57: 0.00 Hz
 F58: 0.00 Hz
 F59: 0.00 Hz
 F60: 0.00 Hz
 F61: 0.00 Hz
 F62: 0.00 Hz
 F63: 0.00 Hz
 F64: 0.00 Hz
 F65: 0.00 Hz
 F66: 0.00 Hz
 F67: 0.00 Hz
 F68: 0.00 Hz
 F69: 0.00 Hz
 F70: 0.00 Hz
 F71: 0.00 Hz
 F72: 0.00 Hz
 F73: 0.00 Hz
 F74: 0.00 Hz
 F75: 0.00 Hz
 F76: 0.00 Hz
 F77: 0.00 Hz
 F78: 0.00 Hz
 F79: 0.00 Hz
 F80: 0.00 Hz
 F81: 0.00 Hz
 F82: 0.00 Hz
 F83: 0.00 Hz
 F84: 0.00 Hz
 F85: 0.00 Hz
 F86: 0.00 Hz
 F87: 0.00 Hz
 F88: 0.00 Hz
 F89: 0.00 Hz
 F90: 0.00 Hz
 F91: 0.00 Hz
 F92: 0.00 Hz
 F93: 0.00 Hz
 F94: 0.00 Hz
 F95: 0.00 Hz
 F96: 0.00 Hz
 F97: 0.00 Hz
 F98: 0.00 Hz
 F99: 0.00 Hz
 F100: 0.00 Hz

Method Name:REG-ADH-5IPA-15ml/min
Run Name:REG_IV_891

Date:5/16/2011
Time:12:54:10 PM



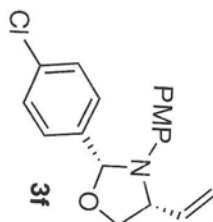
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	4.11	4.27	4.48	0.00	99.75	1040.4	94.7	99.746
2	UNKNOWN	4.73	4.80	4.87	0.00	0.25	3.3	0.2	0.254
Total						100.00	1043.7	95.0	100.000



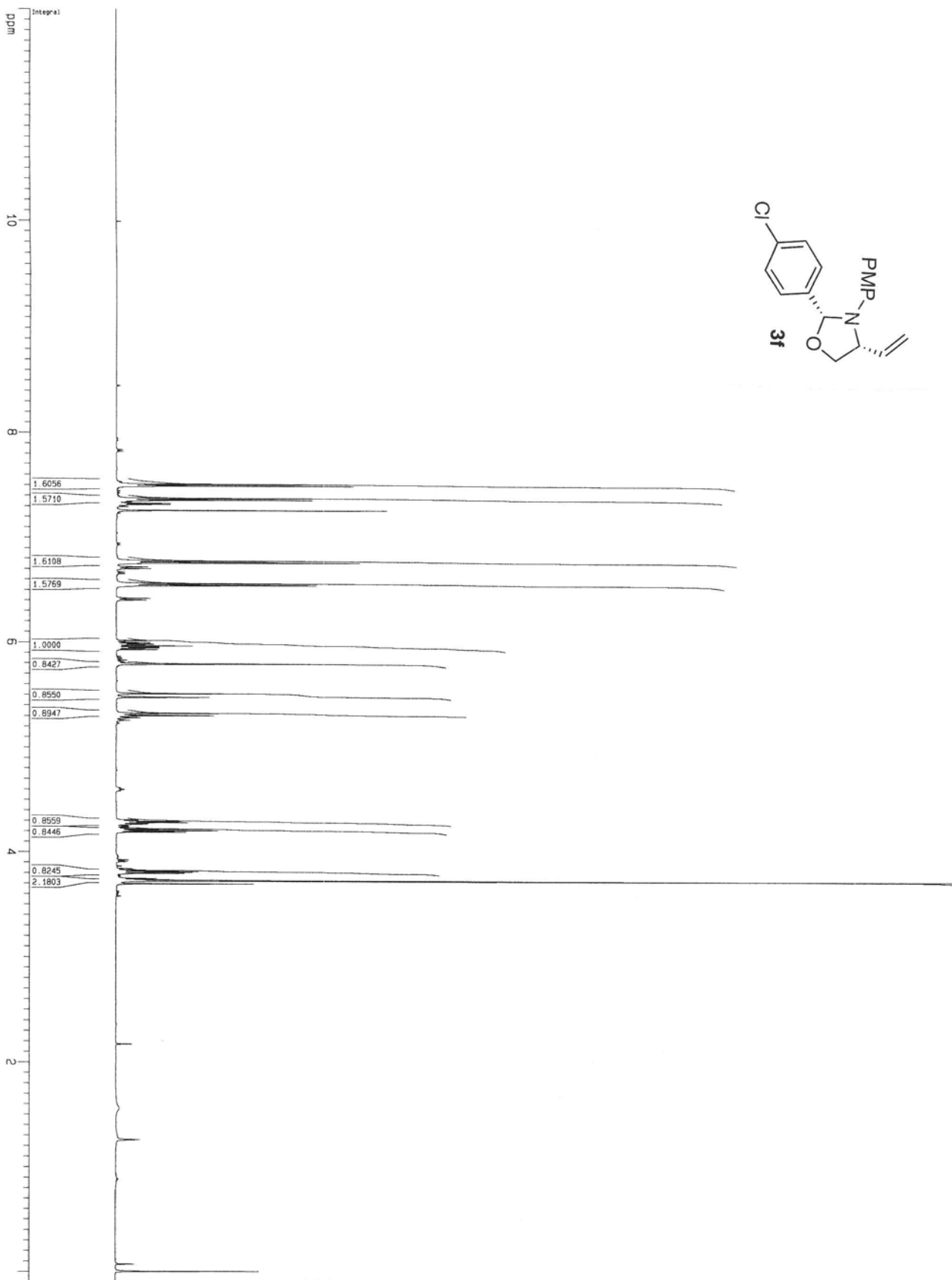
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	4.09	4.27	4.55	0.00	42.61	712.2	64.3	42.613
2	UNKNOWN	4.55	4.77	4.81	0.00	6.62	98.3	10.0	6.619
3	UNKNOWN	4.81	4.92	5.11	0.00	45.20	625.1	68.2	45.202
4	UNKNOWN	5.11	5.26	5.47	0.00	5.57	69.2	8.4	5.566
Total						100.00	1504.8	150.9	100.000

¹H spectrum

ppm



7.50354
7.48669
7.36840
7.35153
7.32257
7.31160
7.25491
6.77151
6.76713
6.75789
6.75346
6.71700
6.69894
6.55571
6.55121
6.54188
6.53798
6.41737
6.39932
6.01236
5.93633
5.98271
5.97586
5.96209
5.94833
5.94148
5.92786
5.78682
5.50633
5.47196
5.32086
5.30037
4.29072
4.27772
4.26428
4.21733
4.20337
4.20039
4.18659
3.81931
3.80692
3.80236
3.79001
3.74382
3.72145
3.69263



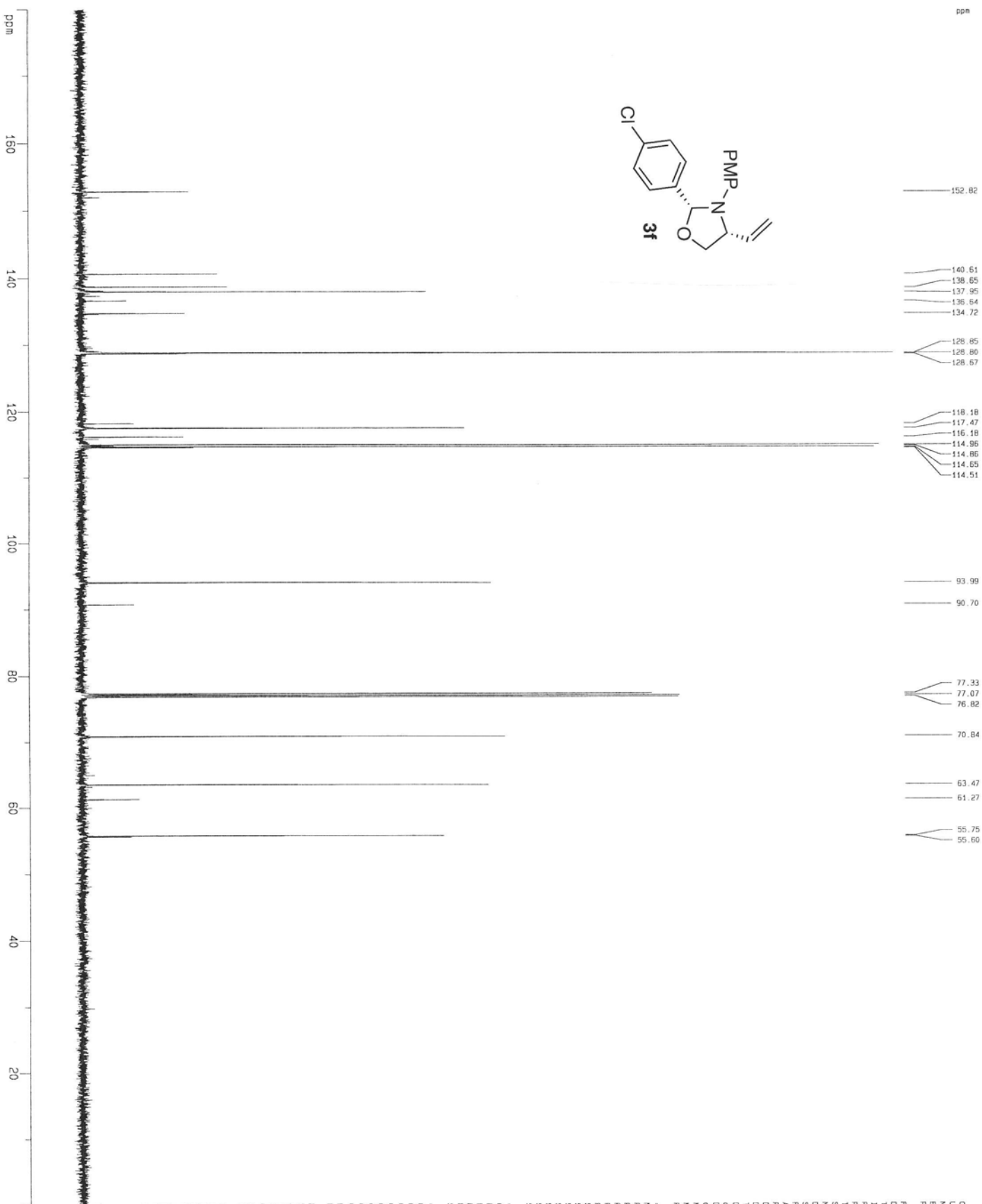
Current Data Parameters
USER rgrote
NAME REG_LV_79_X
EXPNO 1
PROCNO 1

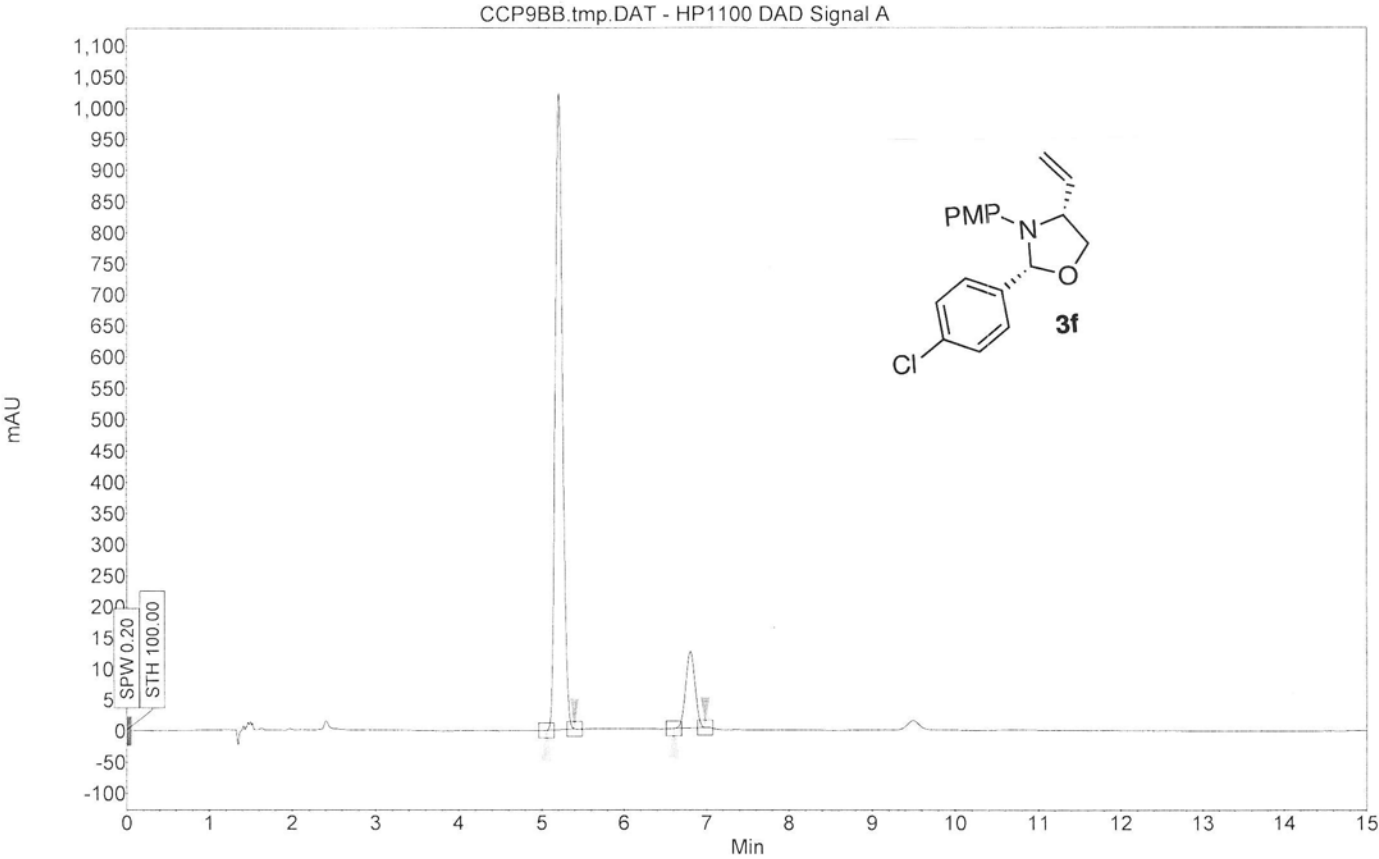
F2 - Acquisition Parameters
Date_ 20091204
Time 16.06
INSTRUM cryp500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TO 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098943 Hz
AQ 5.0589774 sec
RG 62.460
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
WDECT 0.00000000 sec
MCORC 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.265015 MHz

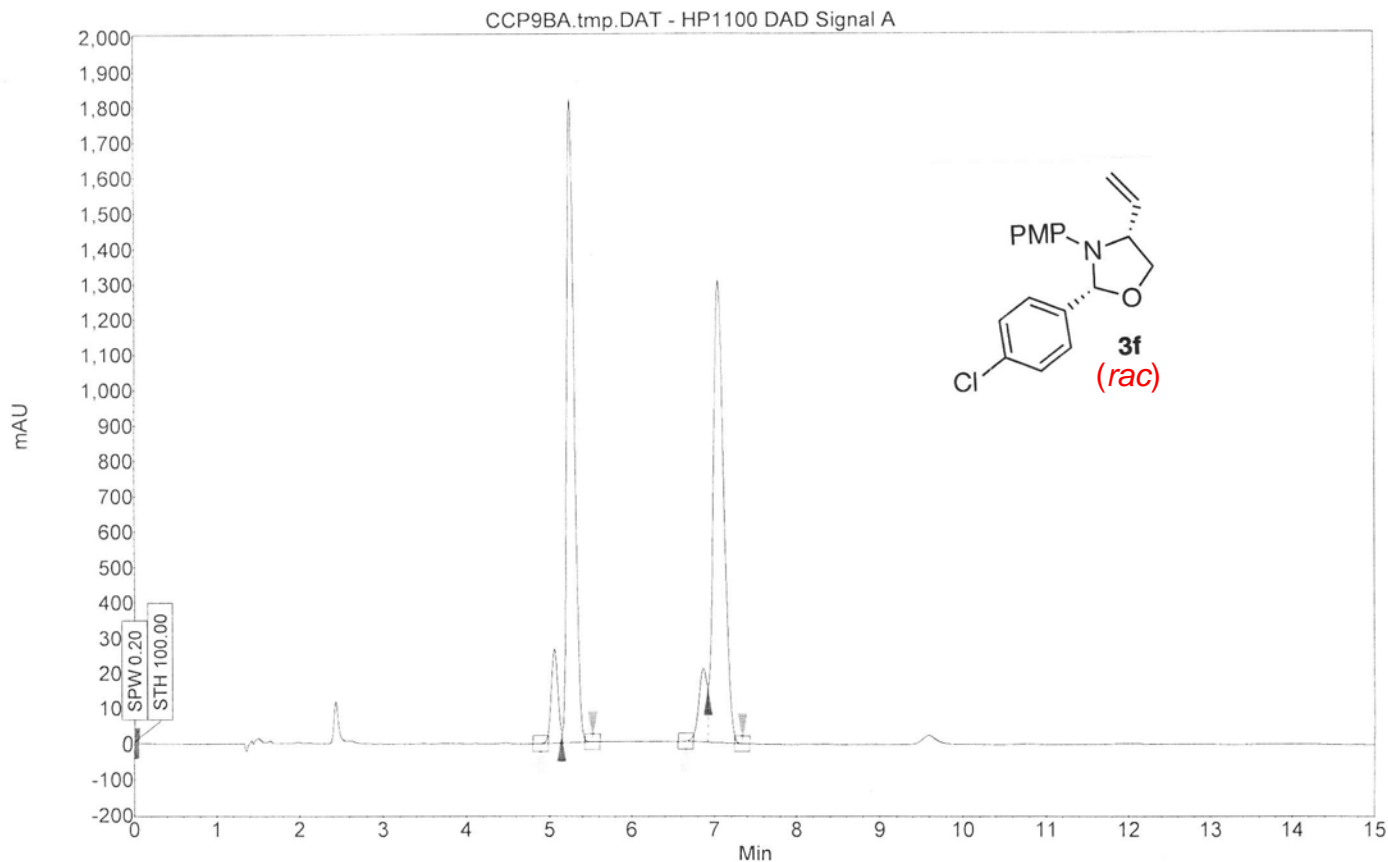
F2 - Processing parameters
SI 32768
SF 500.265015 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

10 NMR plot parameters
CX 22.60 cm
CY 15.00 cm
F1P 12.000 ppm
F1 8002.64 Hz
F2P -50.00 ppm
F2 -50.00 Hz
PRCKH 0.53570 ppm/cH
HZCM 265.46765 Hz/cH

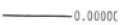
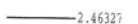
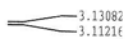
C#CC1OCC(N1C2=CC=CC=C2Cl)C3=CC=CC=C3[illegible]



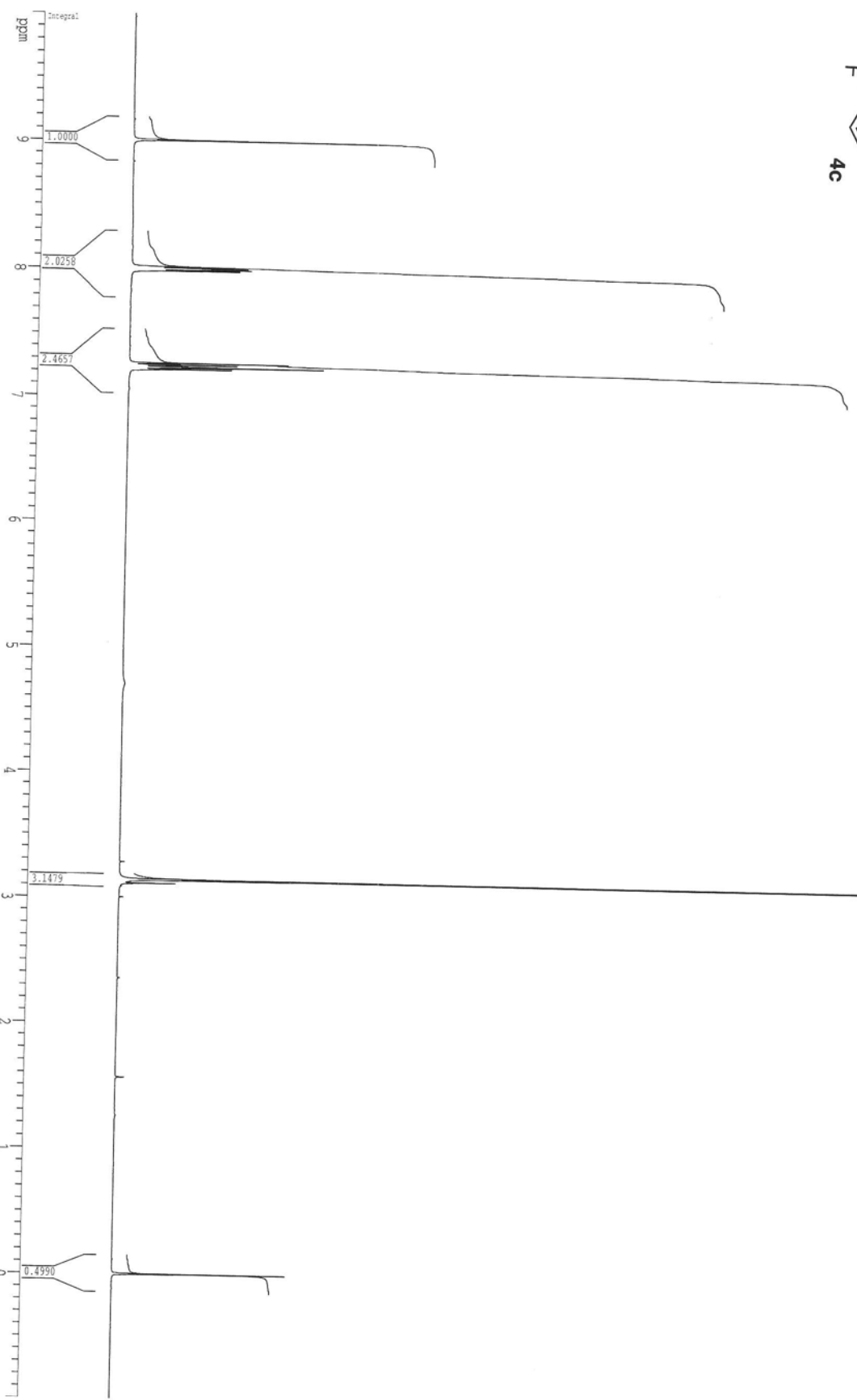
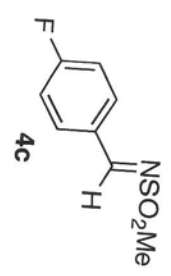
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	5.06	5.21	5.40	0.00	86.58	1021.8	105.2	86.583
2	UNKNOWN	6.60	6.81	6.98	0.00	13.42	123.4	16.3	13.417
Total						100.00	1145.2	121.6	100.000



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	4.89	5.06	5.15	0.00	5.77	266.9	25.1	5.774
2	UNKNOWN	5.15	5.26	5.52	0.00	43.95	1817.3	191.1	43.949
3	UNKNOWN	6.65	6.87	6.92	0.00	5.57	208.8	24.2	5.566
4	UNKNOWN	6.92	7.05	7.34	0.00	44.71	1304.3	194.4	44.712
Total						100.00	3597.3	434.8	100.000



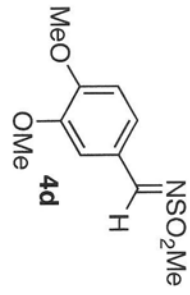
Current Data Parameters	
USER	mscanna
NAME	mscanna
EXNO	4
PRODMO	1
Data - Acquisition Parameters	
Date	20091111
Time	8:54
File	crf050
PROB	1 m CTR1
PRGMO	CTR1
PRGMO	8178
PRGMO	3010
PRGMO	COG3
PRGMO	2
PRGMO	2
PRGMO	8012.310 Hz
PRGMO	5.098717 sec
PRGMO	5.098717 sec
PRGMO	62.40 J/sec
PRGMO	218.1 Hz
PRGMO	0.1000000 sec
PRGMO	0.0000000 sec
PRGMO	0.0100000 sec
Parameters CONTROL: 11 parameters	
P1	0.0000000 sec
P2	1.66 dB
P3	500.2253819 Hz
P4	0
P5	0
P6	0.36 Hz
P7	4.00
13 NMR pulse parameters	
P1	1.76 sec
P2	1.76 sec
P3	10.000 ppm
P4	500.00 Hz
P5	500.00 Hz
P6	-500.00 Hz
P7	0.46164 sec/cm
P8	261.33333 Hz/cm



Current Data Parameters
USER: shapla
NAME: NS-CHXK-4-F-Aldehyde
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20091116
Time: 23.29
INSTRUM: spect
PROBHD: 5 mm broad
PULPROG: zgpg30
TD: 65536
FIDRES: 0.1728
SOLVENT: CDCl3
NS: 8
DS: 2
SWH: 8012.823 Hz
FIDRES: 0.09864 Hz
AQ: 5.0998774 sec
RG: 1448.2
RW: 62.400 Hz
TE: 300.2 K
DE: 0.10000000 sec
O1: 0.00000000 sec
WCWST: 0.01500000 sec
MCWST: 0.01500000 sec
----- CHANNEL f1 -----
NUC1: 1H
P1: 12.00 usec
PL1: -1.00 dB
SFO1: 499.8234973 MHz
F2 - Processing parameters
SI: 499.8234973 MHz
SF: 499.8234973 MHz
WDW: EM
SSB: 0
ZG: 0.30 Hz
PC: 1.00
ID NMR plot parameters
CX: 22.80 cm
CY: 15.00 cm
ETP: 13.00000000
F1: 4996.20 Hz
F2: -1.000 Hz
FREQ: 0.48246 Hz/cm
NUC1: 241.04815 Hz/cm

ppm

8.91325
7.57026
7.56713
7.47690
7.47355
7.46042
7.45711
7.26385
6.98546
6.96894



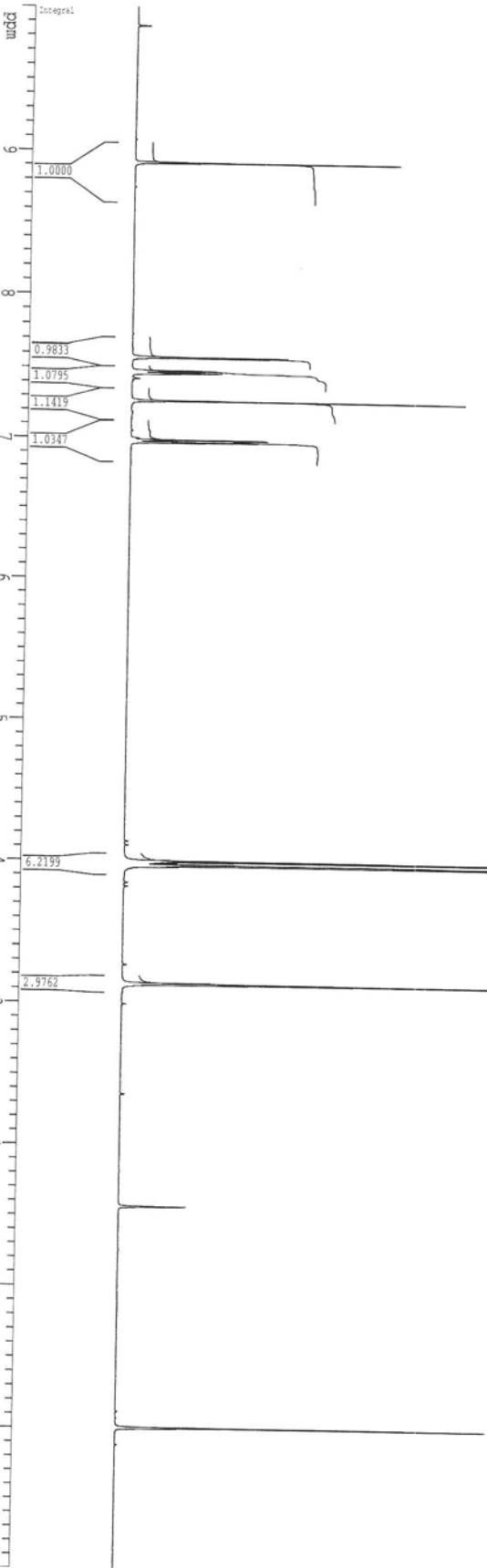
3.99187
3.97895
3.96443
3.95430

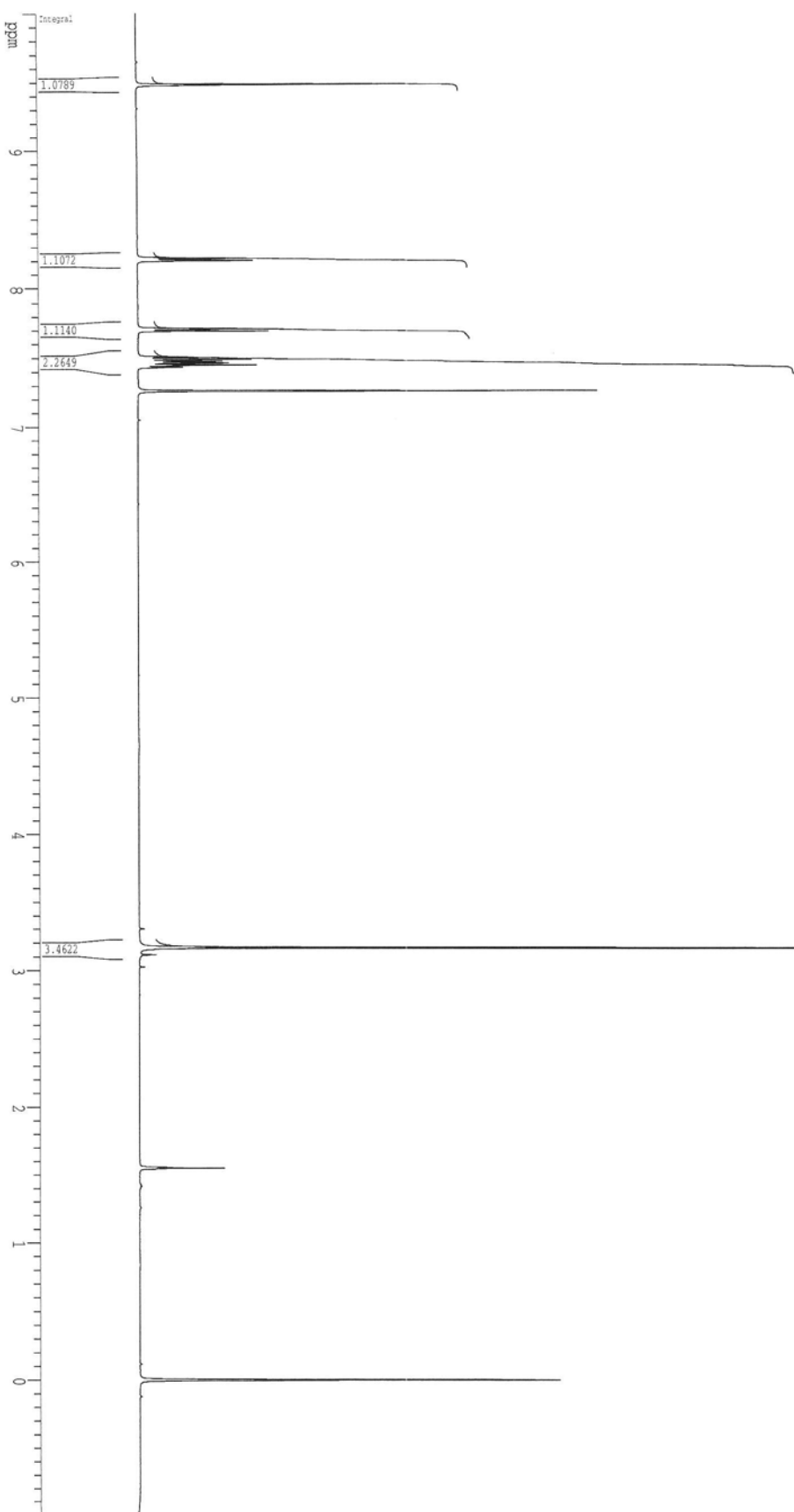
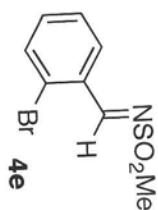
3.13012

1.55772

0.00000

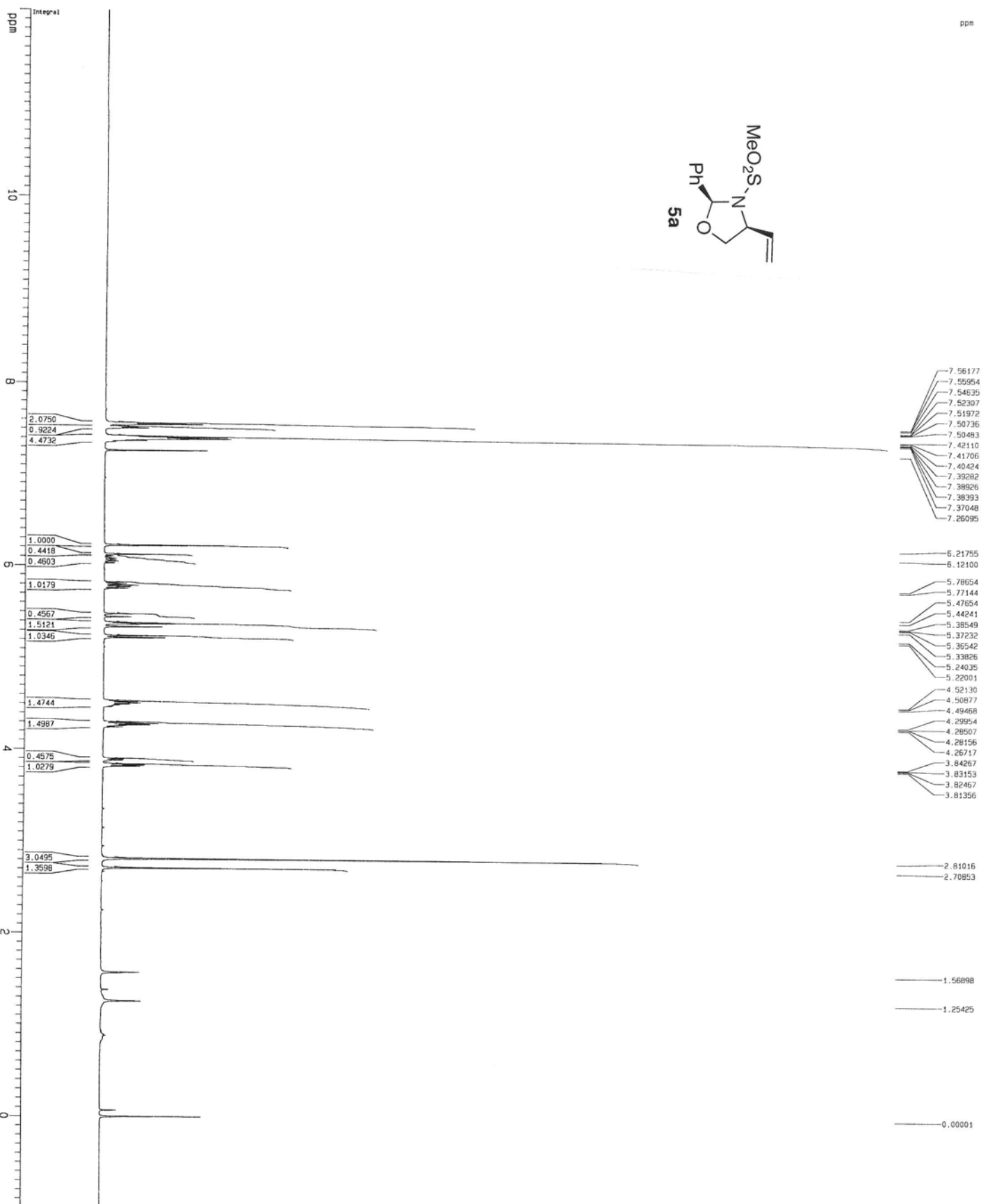
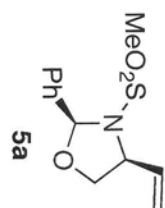
Current Data Parameters
NAME: Me-5-[3-(4-MeO)-H-COMe]
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20100220
Time: 22.41
INSTRUM: spect
PROBHD: 5 mm CPXI-1H-
PULPROG: zgpg30
TD: 65536
FIDRES: 0.1773
AQ: 0.000000
RG: 327.5
SD: 0.000000
DE: 0.000000
TE: 300.2 K
NUC1: 1H
NUC2: 13C
PC: 1.60 dB
SFO1: 500.225015 MHz
F2 - Processing parameters
SI: 65536
SF: 500.2200107 MHz
DS: 4
AS: 0
LA: 0.10 Hz
GB: 0
PC: 4.00
1D NMR plot parameters
CX: 21.80 cm
CY: 1.00 cm
FID: 1.16 dB
F1: 5001.20 Hz
F2: 1.000 ppm
FREQM: 500.136129 MHz
GPROG: 2d13c1h2
HDCO: 2d13c1h2 Hz/cm



¹H spectrum[illegible]

¹H spectrum

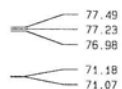
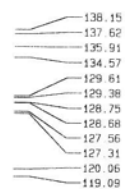
ppm



Current Data Parameters
 USER: shupia
 NAME: MS-5-23B-A-1H-CHALC
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20110420
 Time: 23.53
 INSTRUM: crys500
 PULPROG: zgpg30
 PRGNAME: 5 mm OPTCI 1H-
 F4: 400.146363
 F2: 101.254850
 SOLVENT: CDCl3
 NS: 8
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.096043 Hz
 AQ: 0.0395398 sec
 RG: 327.5
 DE: 62.400 uS
 TE: 298.0 K
 D1: 0.10000000 sec
 DELTA: 0.00000000 sec
 ACQRES: 0.01500000 sec
 ***** CHANNEL f1 *****
 NUC1: 1H
 P1: 7.50 uS
 PL1: 1.60 dB
 SFO1: 500.2620015 MHz
 F2 - Processing parameters
 SI: 65536
 SF: 500.2600119 MHz
 KW: EM
 LB: 0.3 Hz
 GB: 0
 PC: 4.00
 1D NMR D101 Parameters
 C1: 22.80 cm
 C2: 8.80 cm
 F1P: 12.000 cm
 F1: 6002.64 Hz
 F2P: -1.000 ppm
 F2: -500.22 Hz
 PPMCH: 0.57018 ppm/cm
 NUCN: 285.8180 MHz/cm

C=C[C@H]1O[C@@H](C(=O)OC(=O)S1)c2ccccc2

5a



```
Current Data Parameters
USER          shagna
NAME          MS-5-238-A-13C-CHAPAC
EXPNO         1
PROCNO        1
```

```
F2 - Acquisition Parameters
Date_ 20110421
Time 0.18
```

INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
QNP 1500 501Echard3000 444

TO	65536
SOLVENT	CDCl ₃

OS	15
SWH	30303.031 Hz

RG	1.0914105 sec	7299.2
AG		
RG		

OM	16.500 USE
OE	6.00 USE
TE	298.0 K

01	0.25000000 sec
011	0.03000000 sec
015	0.00200000 sec

d17	0.00019500	sec
MCPEST	0.00000000	sec
MCPEX	0.01500000	sec

P2	31.00 use
----	-----------

MLCT	13C
P1	15.50 use

P14	500.00	USE
P12	2000.00	USE
PL0	120.00	GB

```
PL1 -1.00 dB
SF01 125.7942548 MHz
SP1 3.20 dB
```

SP2	3.20 d8
SPNAM1	Cp60, 0.5, 20.1
SPNAM2	Conform 4

Sp0ff1	0.00 Hz
Sp0ff2	0.00 Hz

```
***** CHANNEL f2 *****
CP0PRG2      woltz16
```

PCP02	100.00	USE
PL2	1.60	08

PLATE 500.2225011 MHz

```
***** CHANNEL *****
GPNUM1 SINE.100
GPNUM2 SINE.100
```

GPX1	GPX2	GPX3
0.00	0.00	0.00
0.00	0.00	0.00
0.00	0.00	0.00

GPY2	0.00 X
GPZ1	30.00 X
GPZ2	60.00 X

p15	500.00 usec
p16	1000.00 usec

F2 - Processing parameters
51 65536

SEC	ACC./1000000 PWT
MDK	EM
SSB	0

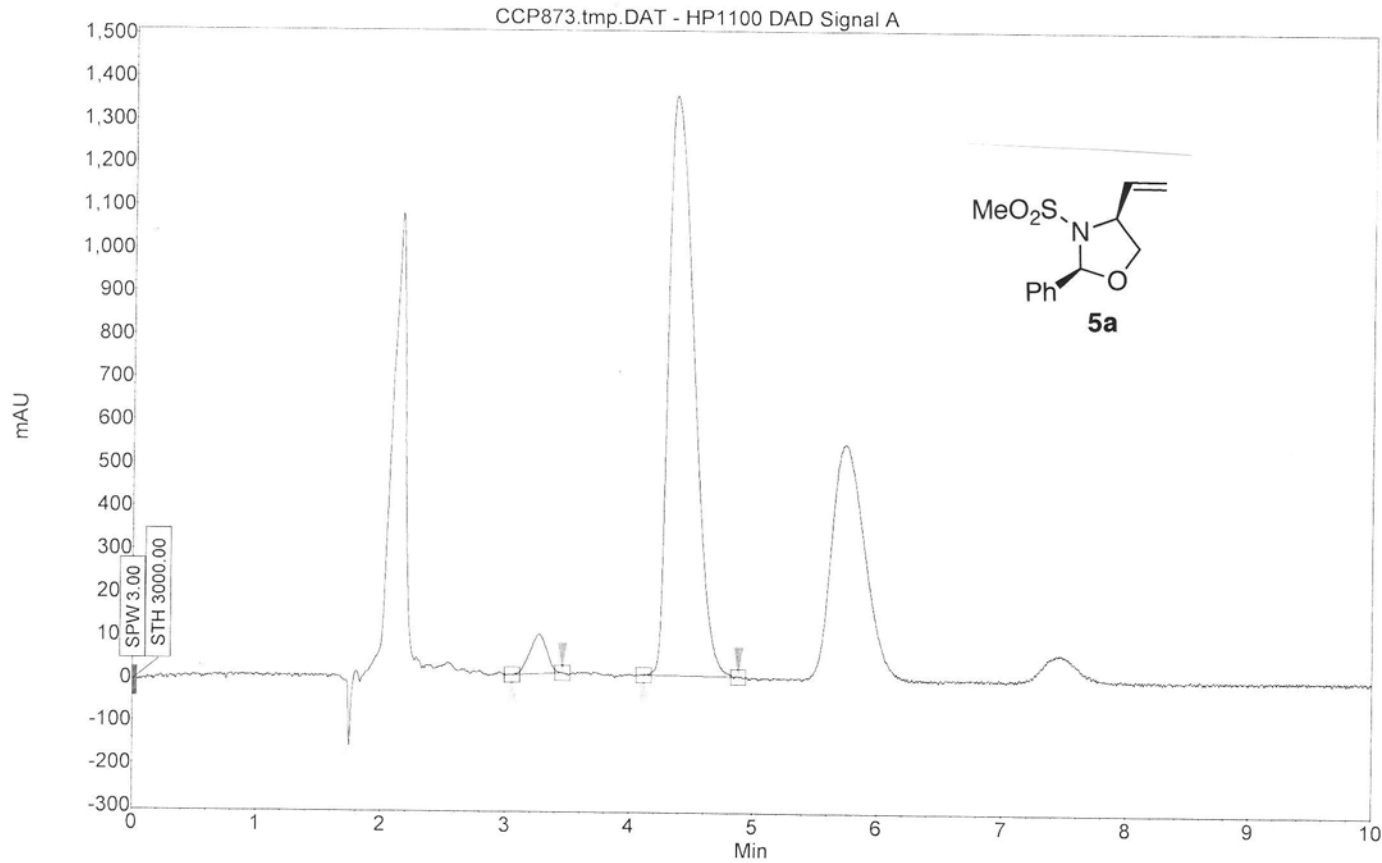
LB	1.00 Hz
GB	0
PC	2.00

10 Mm plot parameters
CV 22.80 cm

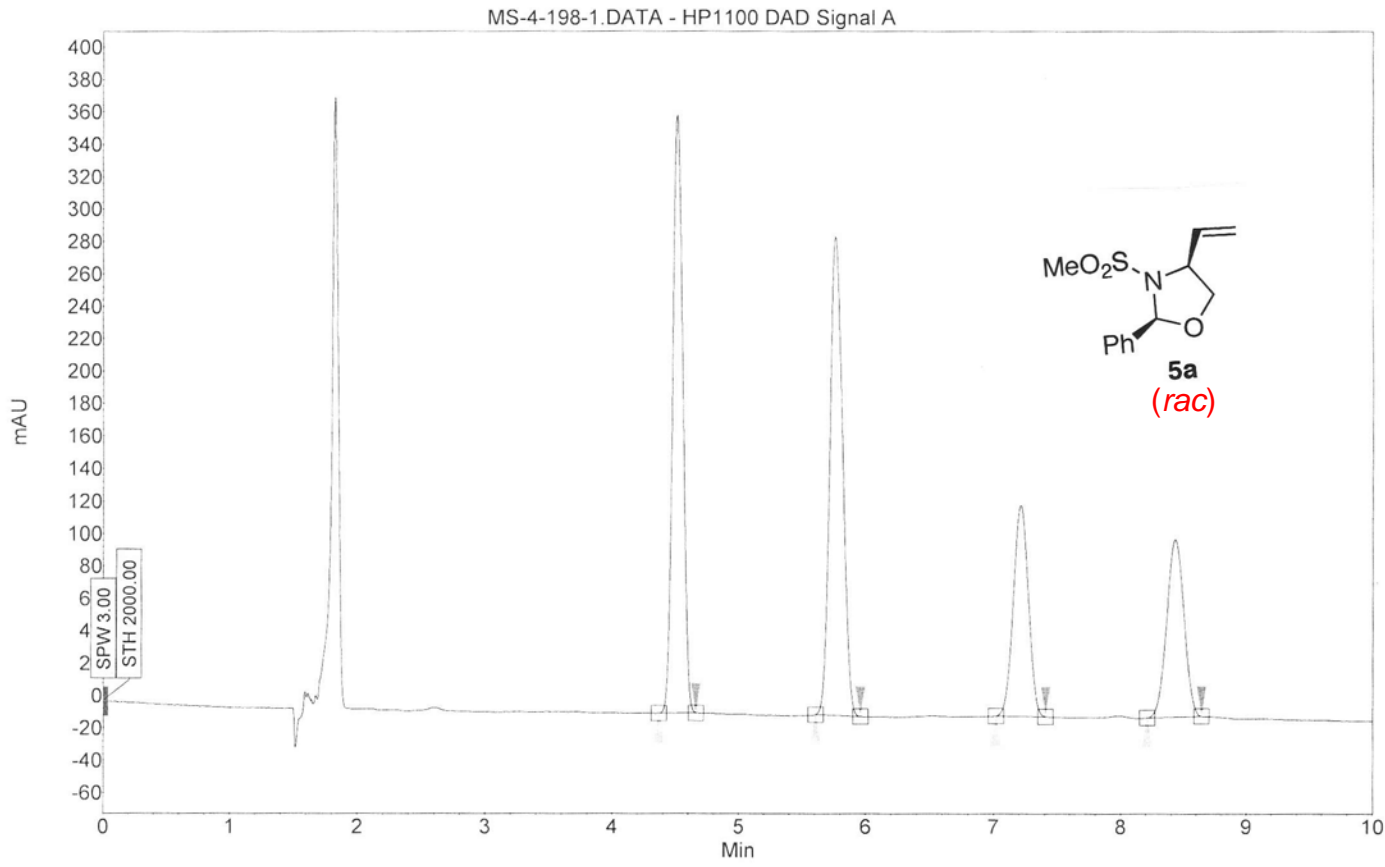
CY	15.65 cm
F1P	210.000 ppm
CA	9643.00 Hz

F ₂ P	-10,000 ppm
F ₂	-1257.80 Hz

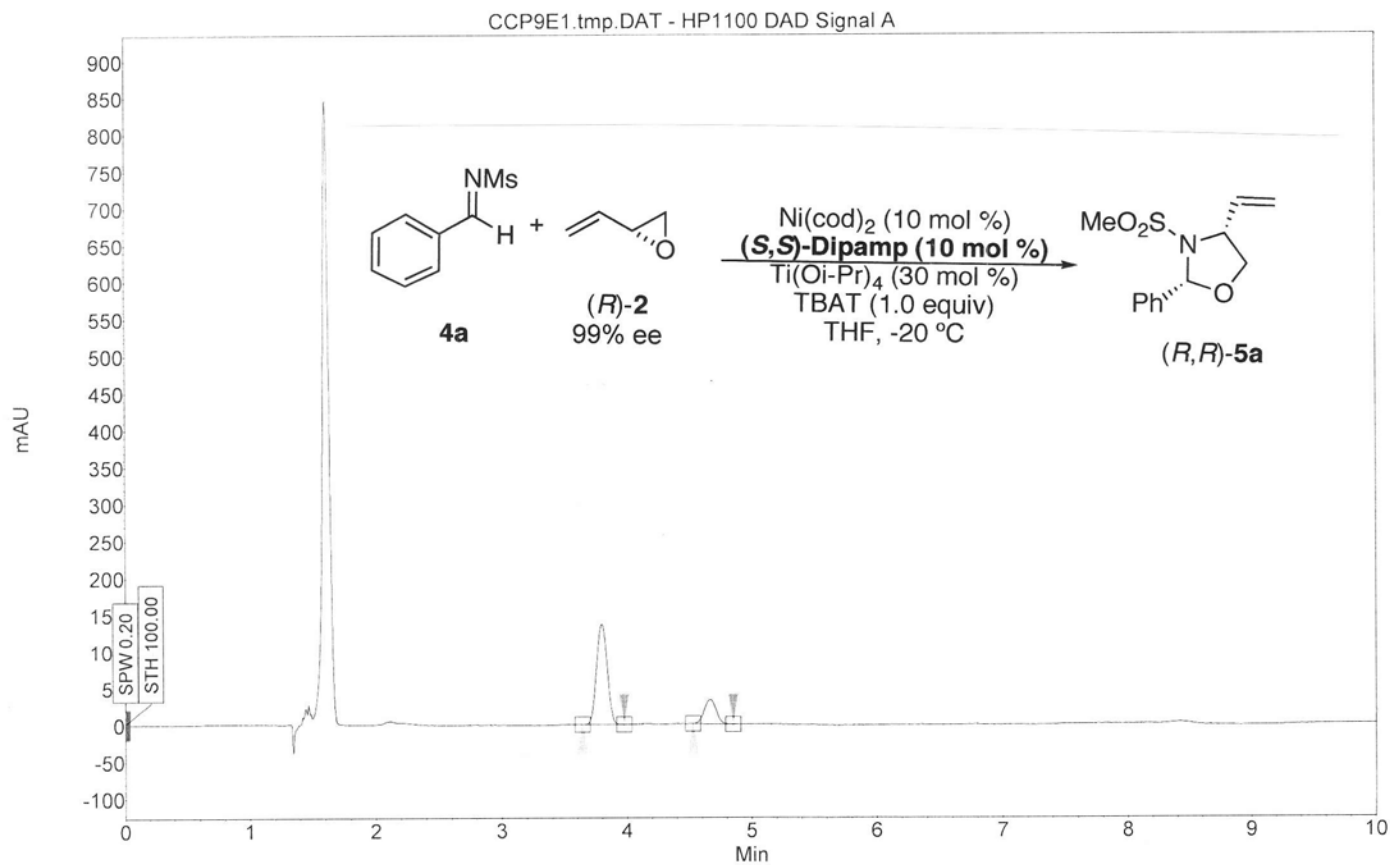
HZCM 1213.67065 Hz/c



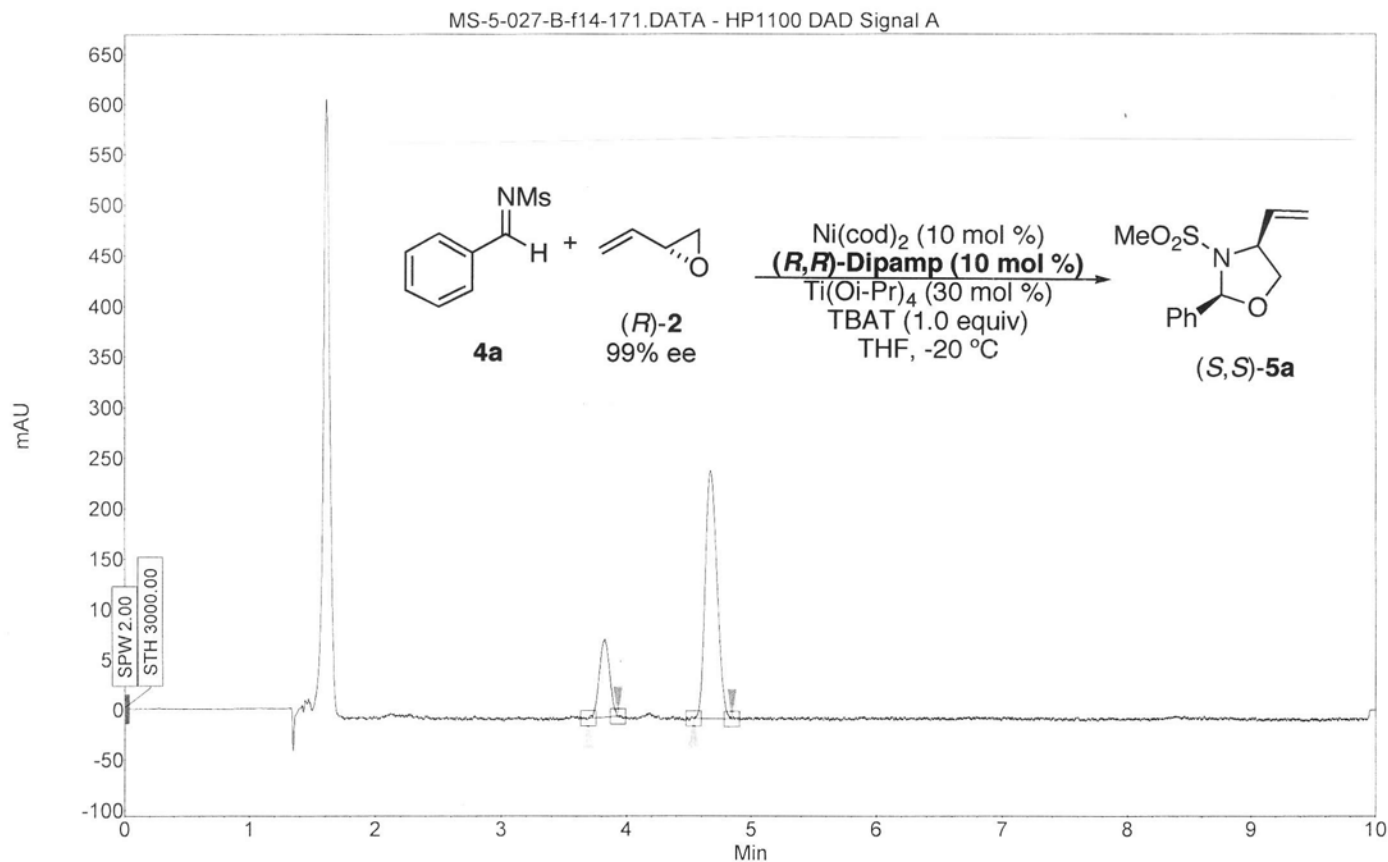
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
2	UNKNOWN	3.05	3.27	3.46	0.00	4.38	93.3	14.7	4.383
1	UNKNOWN	4.12	4.35	4.88	0.00	95.62	1346.9	321.5	95.617
Total						100.00	1440.3	336.2	100.000



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
3	UNKNOWN	4.37	4.51	4.66	0.00	32.95	369.0	34.3	32.949
4	UNKNOWN	5.61	5.76	5.96	0.00	32.99	295.2	34.3	32.987
1	UNKNOWN	7.02	7.21	7.41	0.00	17.18	130.3	17.9	17.176
2	UNKNOWN	8.21	8.43	8.64	0.00	16.89	109.7	17.6	16.888
Total						100.00	904.1	104.0	100.000

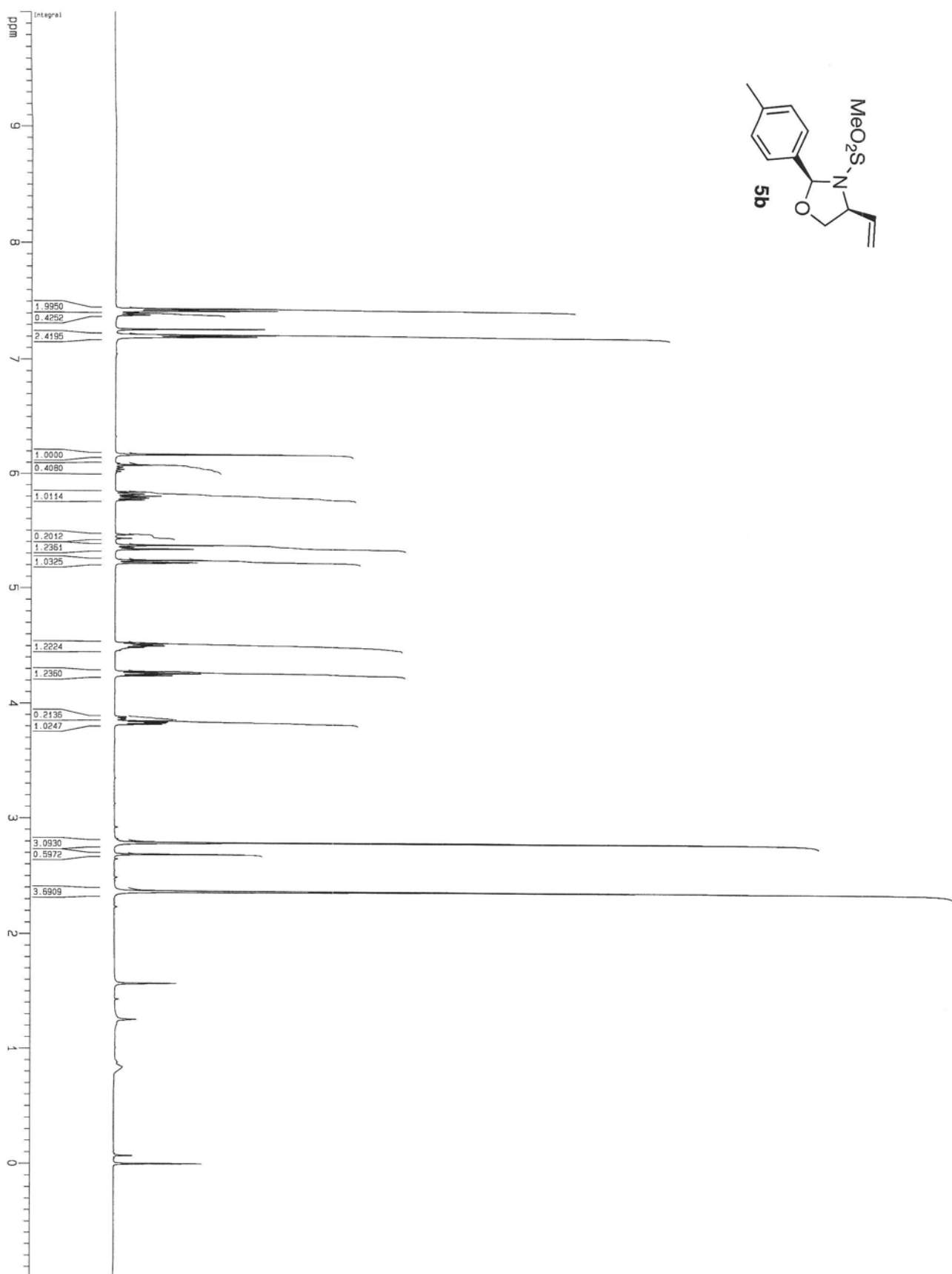
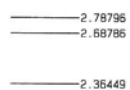
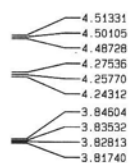
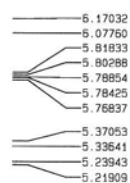
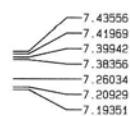
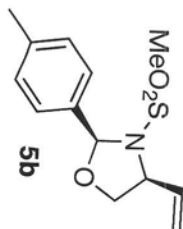


Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	3.64	3.80	3.98	0.00	78.95	136.8	13.8	78.953
2	UNKNOWN	4.53	4.67	4.85	0.00	21.05	32.8	3.7	21.047
Total						100.00	169.6	17.4	100.000

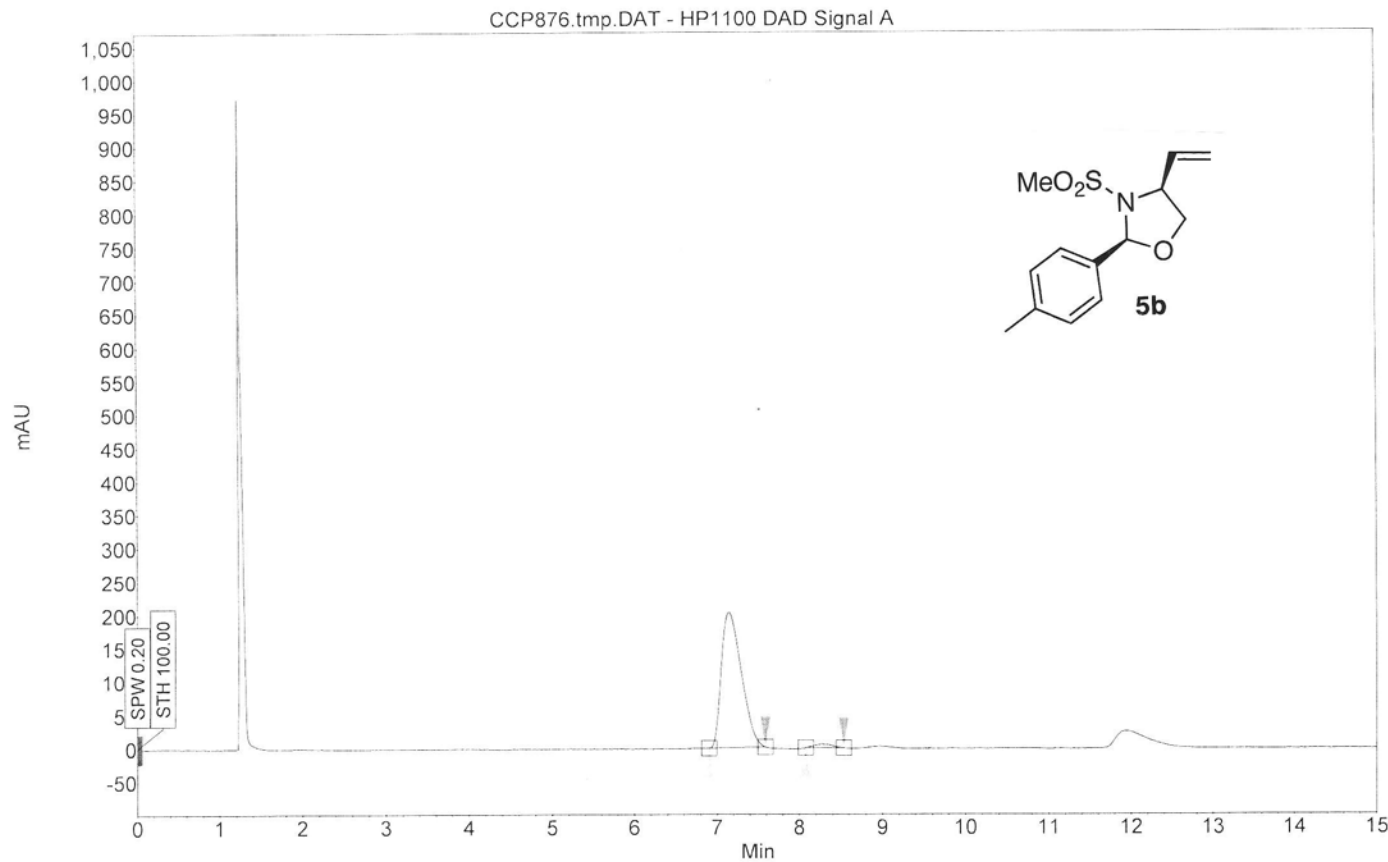


Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μ V]	[μ V.Min]	[%]
1	UNKNOWN	3.69	3.83	3.93	0.00	21.81	77.5	7.5	21.811
2	UNKNOWN	4.54	4.68	4.85	0.00	78.19	245.2	27.1	78.189
Total						100.00	322.8	34.6	100.000

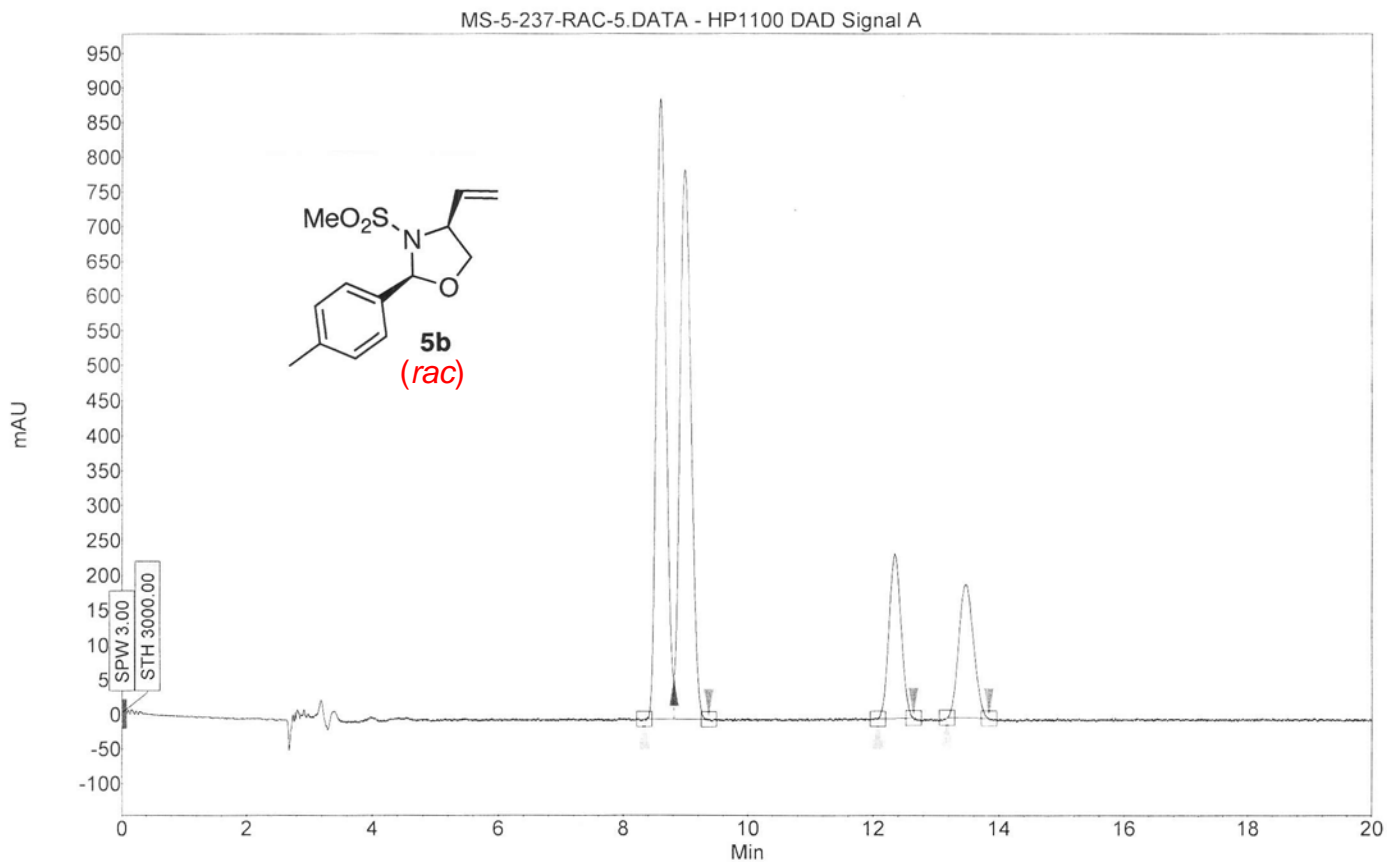
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Current Data Parameters		User		Name	
USER	msghs	MS-211-4-H-CHAND			
EXPNO					
PROCNO	1				
F2 - Acquisition Parameters					
Date_	20110601				
Time	07:00:00				
INSTRUM	CRYDOMO				
PROBHD	5 mm CPMG 1H-				
PULPROG	zg30				
TD	81789				
DO	0.00137				
NS	2				
DS	4				
SWH	8012.820 Hz				
F2 - F1	0.0090423 Hz				
F1	5.0958743 Hz				
AD	0.0000000 sec				
DE	6.00 usec				
TE	298.1 K				
1	0.1000000 sec				
DELTA	0.1000000 sec				
NUC1	1H				
NUC2	13C				
NUC3	13C				
NUC4	13C				
NUC5	13C				
NUC6	13C				
NUC7	13C				
NUC8	13C				
NUC9	13C				
NUC10	13C				
NUC11	13C				
NUC12	13C				
NUC13	13C				
NUC14	13C				
NUC15	13C				
NUC16	13C				
NUC17	13C				
NUC18	13C				
NUC19	13C				
NUC20	13C				
NUC21	13C				
NUC22	13C				
NUC23	13C				
NUC24	13C				
NUC25	13C				
NUC26	13C				
NUC27	13C				
NUC28	13C				
NUC29	13C				
NUC30	13C				
NUC31	13C				
NUC32	13C				
NUC33	13C				
NUC34	13C				
NUC35	13C				
NUC36	13C				
NUC37	13C				
NUC38	13C				
NUC39	13C				
NUC40	13C				
NUC41	13C				
NUC42	13C				
NUC43	13C				
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NUC45	13C				
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NUC47	13C				
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NUC57	13C				
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NUC59	13C				
NUC60	13C				
NUC61	13C				
NUC62	13C				
NUC63	13C				
NUC64	13C				
NUC65	13C				
NUC66	13C				
NUC67	13C				



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	6.90	7.15	7.59	0.00	97.68	202.6	56.9	97.675
2	UNKNOWN	8.08	8.27	8.54	0.00	2.32	5.5	1.4	2.325
Total						100.00	208.1	58.2	100.000



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	8.34	8.60	8.82	0.00	37.51	891.6	162.7	37.513
2	UNKNOWN	8.82	8.99	9.37	0.00	37.92	788.4	164.5	37.924
3	UNKNOWN	12.08	12.35	12.65	0.00	12.40	236.2	53.8	12.399
4	UNKNOWN	13.18	13.47	13.84	0.00	12.16	193.0	52.8	12.164
Total						100.00	2109.1	433.8	100.000

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

ppm

7.54964
7.53852
7.53332
7.52205
7.50402
7.49835
7.48730
7.26236
7.10253
7.08550
7.06844

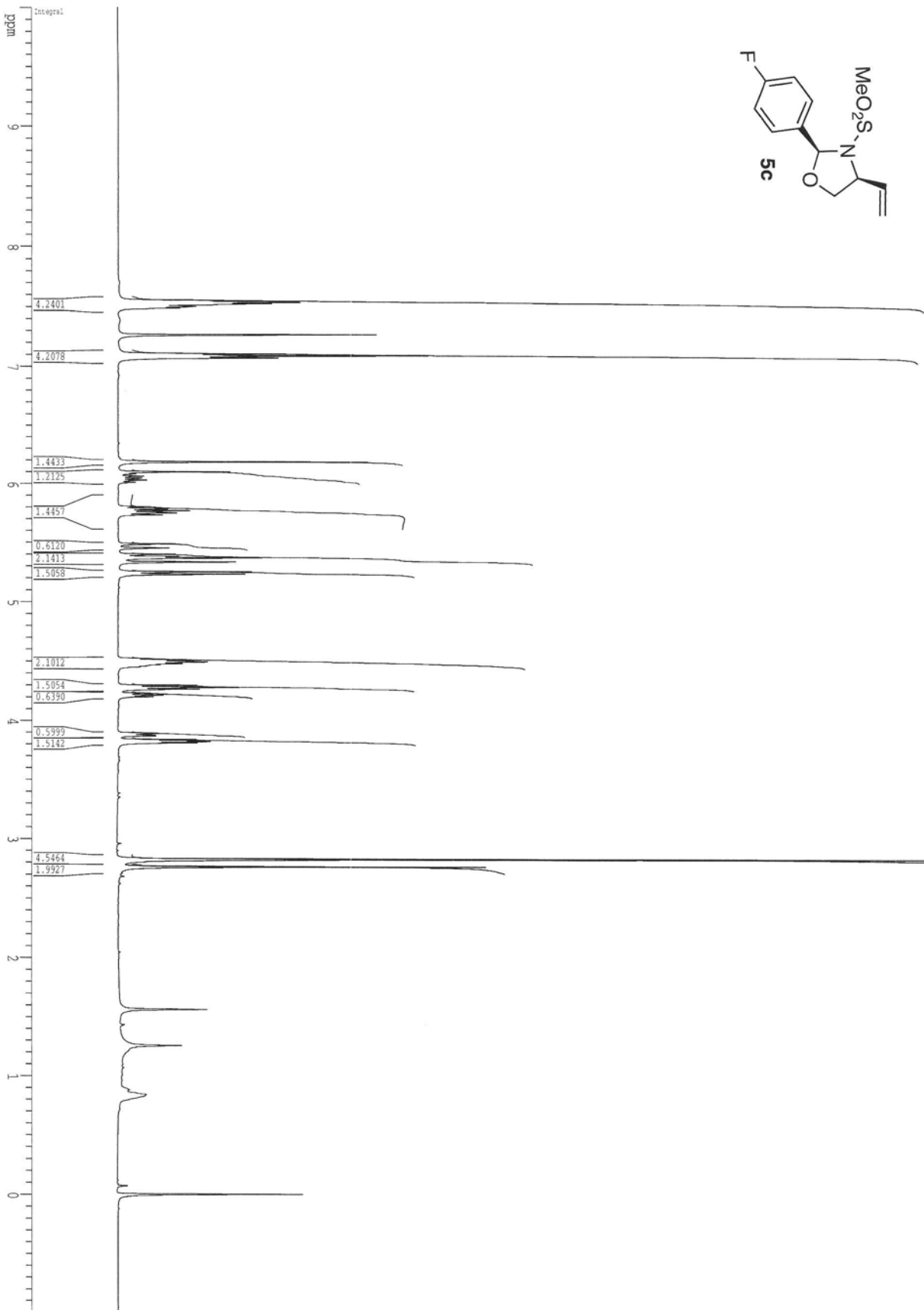
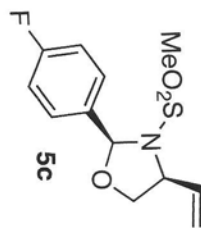
6.18451
6.09966
5.80324
5.78763
5.78325
5.76847
5.75362
5.74924
5.73361
5.48476
5.45065
5.39863
5.37824
5.36770
5.33357
5.24967
5.22934
4.51995
4.50596
4.49337
4.47997
4.46928
4.29524
4.27742
4.26291
4.23020
4.21821
4.21256
4.20086
3.89397
3.88741
3.87643
3.86983
3.83731
3.82643
3.81965
3.80850

2.82281
2.76130

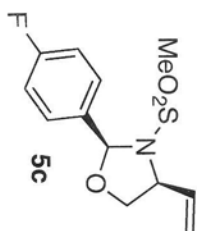
1.56302

1.25452

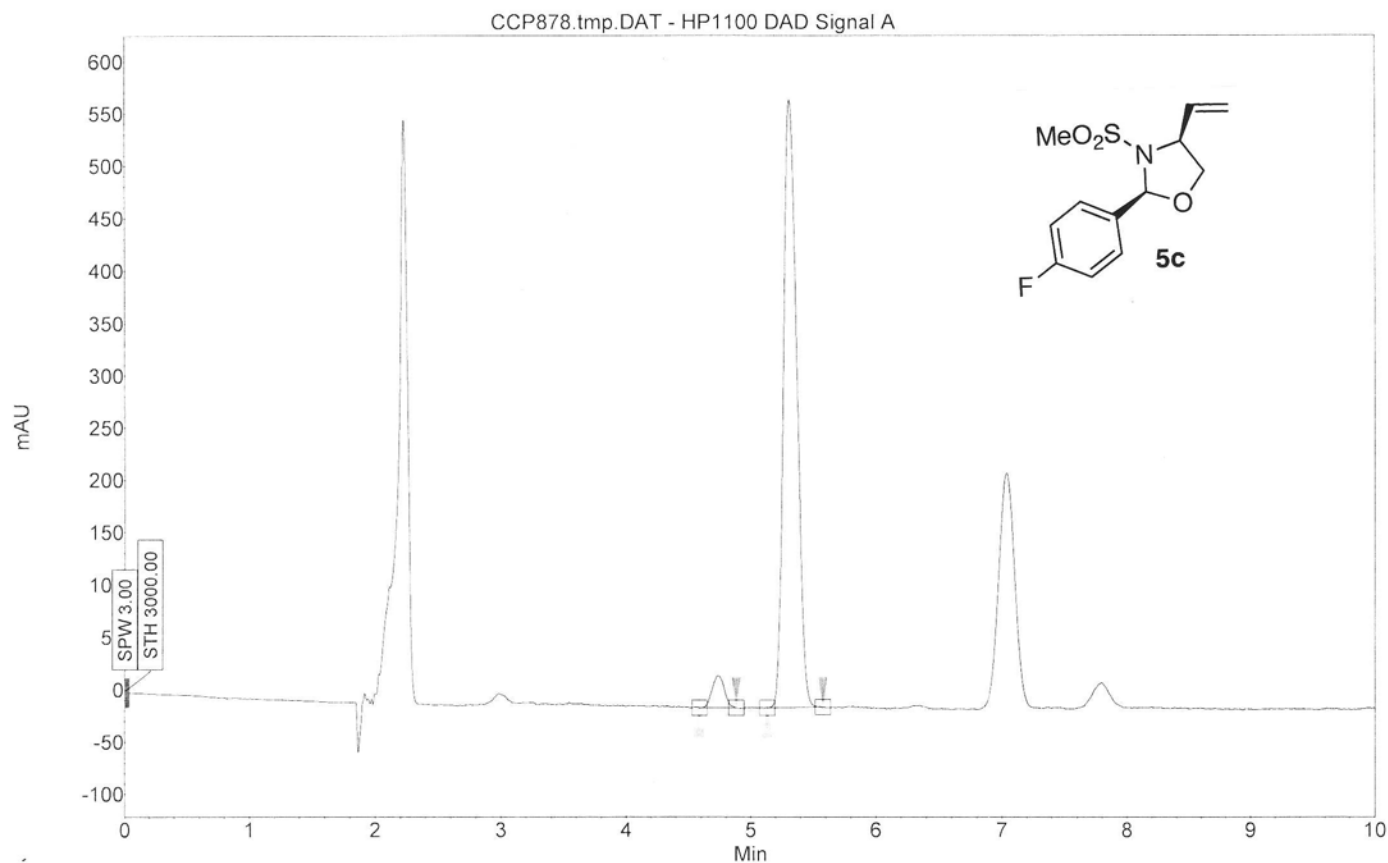
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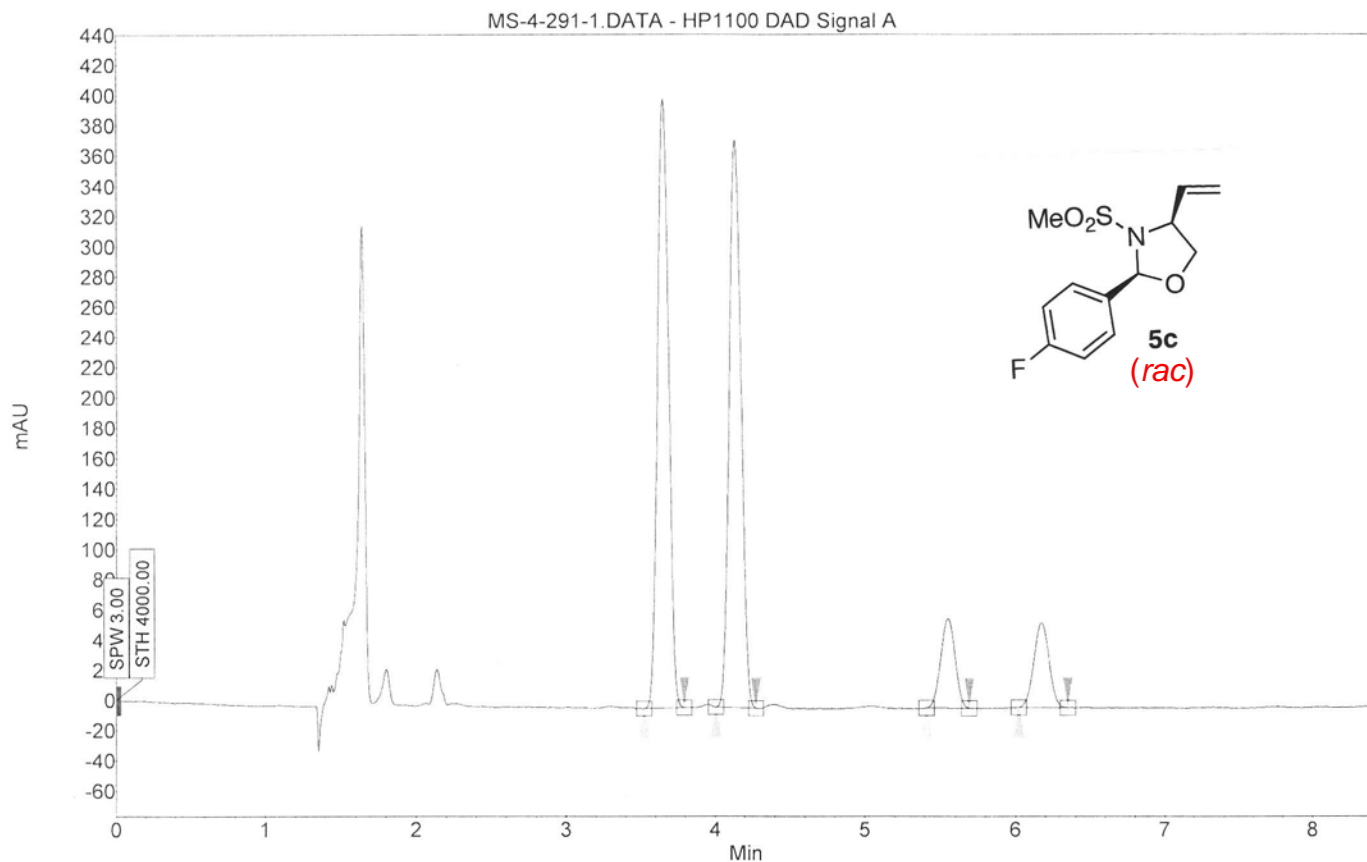
Current Data Parameters
 USER shahla
 NAME NS-5-211-B-1H-CHARAC
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110101
 Time 20.29
 INSTRUM cryo500
 PROBHD 5 mm CPXI 1H-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 801.2 KHz
 FIDRES 0.09644 Hz
 AQ 0.098174 sec
 SFO1 500.136199 MHz
 INE 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.1000000 sec
 DELTA 0.0000000 sec
 ACQRES 0.0130000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 1.60 dB
 SFO1 500.2235015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200114 MHz
 NW 8K
 SSF 0
 DSF 1.00 Hz
 GB 2.00
 PC 2.00
 ID NMR plot parameters
 CX 22.80 cm
 CZ 15.00 cm
 FID 10.00 usec
 FI 5002.20 Hz
 F2P -1.000 ppm
 F3P -500.22 Hz
 FWHM 0.48246 ppm/cm
 HZCM 2411.31423 Hz/cm



Current Data Parameters		shajaba	
OSZS	NAME	MS-5-211-b-13C-CH4-Pd	
NAME	EXPNO	1	
PROCNO	PROCNO	1	
F1 - Acquisition Parameters			
Date_	20110101		
Time	20.39		
INSTRUM	cryosol50		
PROBHD	5 mm cryoProbe		
PULPROG	zgpg30		
TD	Spiralchirp 128 pt		
SOLVENT	CDCl3		
NS	967		
DS	3		
SWH	30031.01 Hz		
F2 - Processing parameters	46.2318 MHz		
F1F2	0.462318 Hz		
RG	1.0813330 sec		
RG2	4095		
DE	16.500 uSAC		
DE2	6.50 uSAC		
DE3	0.2500000 sec		
DE4	0.0000000 sec		
DE5	0.0000000 sec		
DE6	0.0000000 sec		
DE7	0.0000000 sec		
DE8	0.0000000 sec		
DE9	0.0000000 sec		
DE10	0.0000000 sec		
DE11	0.0000000 sec		
DE12	0.0000000 sec		
DE13	0.0000000 sec		
DE14	0.0000000 sec		
DE15	0.0000000 sec		
DE16	0.0000000 sec		
DE17	0.0000000 sec		
DE18	0.0000000 sec		
DE19	0.0000000 sec		
DE20	0.0000000 sec		
DE21	0.0000000 sec		
DE22	0.0000000 sec		
DE23	0.0000000 sec		
DE24	0.0000000 sec		
DE25	0.0000000 sec		
DE26	0.0000000 sec		
DE27	0.0000000 sec		
DE28	0.0000000 sec		
DE29	0.0000000 sec		
DE30	0.0000000 sec		
DE31	0.0000000 sec		
DE32	0.0000000 sec		
DE33	0.0000000 sec		
DE34	0.0000000 sec		
DE35	0.0000000 sec		
DE36	0.0000000 sec		
DE37	0.0000000 sec		
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DE42	0.0000000 sec		
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DE44	0.0000000 sec		
DE45	0.0000000 sec		
DE46	0.0000000 sec		
DE47	0.0000000 sec		
DE48	0.0000000 sec		
DE49	0.0000000 sec		
DE50	0.0000000 sec		
DE51	0.0000000 sec		
DE52	0.0000000 sec		
DE53	0.0000000 sec		
DE54	0.0000000 sec		
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DE58	0.0000000 sec		
DE59	0.0000000 sec		
DE60	0.0000000 sec		
DE61	0.0000000 sec		
DE62	0.0000000 sec		
DE63	0.0000000 sec		
DE64	0.0000000 sec		
DE65	0.0000000 sec		
DE66	0.0000000 sec		
DE67	0.0000000 sec		
DE68	0.0000000 sec		
DE69	0.0000000 sec		
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DE80	0.0000000 sec		
DE81	0.0000000 sec		
DE82	0.0000000 sec		
DE83	0.0000000 sec		
DE84	0.0000000 sec		
DE85	0.0000000 sec		
DE86	0.0000000 sec		
DE87	0.0000000 sec		
DE88	0.0000000 sec		
DE89	0.0000000 sec		
DE90	0.0000000 sec		
DE91	0.0000000 sec		
DE92	0.0000000 sec		
DE93	0.0000000 sec		
DE94	0.0000000 sec		
DE95	0.0000000 sec		
DE96	0.0000000 sec		
DE97	0.0000000 sec		
DE98	0.0000000 sec		
DE99	0.0000000 sec		
DE100	0.0000000 sec		
DE101			

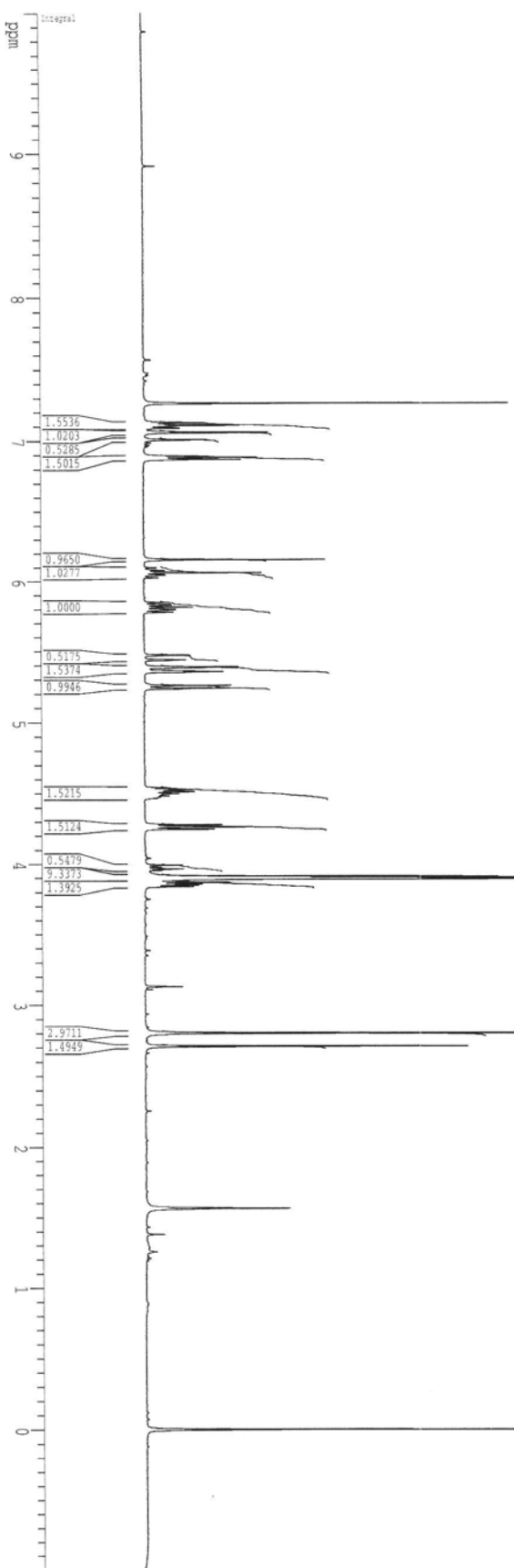
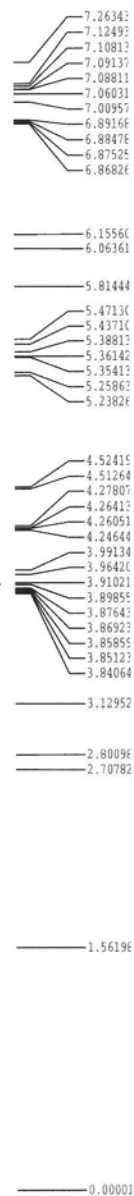
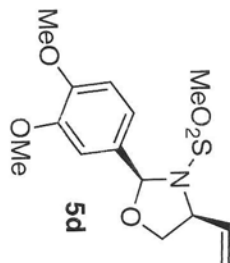


Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	4.59	4.74	4.88	0.00	4.69	30.8	3.5	4.691
2	UNKNOWN	5.13	5.31	5.58	0.00	95.31	579.6	71.3	95.309
Total						100.00	610.3	74.8	100.000



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	3.52	3.65	3.79	0.00	42.13	402.3	34.9	42.135
2	UNKNOWN	4.00	4.13	4.27	0.00	41.88	374.9	34.7	41.882
3	UNKNOWN	5.41	5.55	5.69	0.00	7.95	59.3	6.6	7.954
4	UNKNOWN	6.02	6.17	6.35	0.00	8.03	56.2	6.6	8.030
Total						100.00	892.6	82.8	100.000

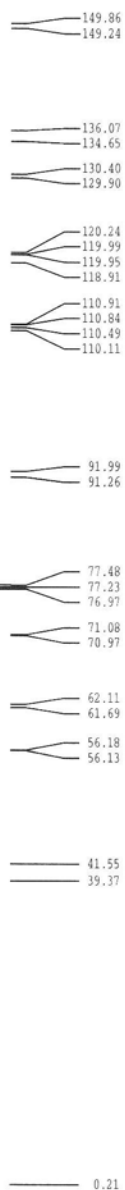
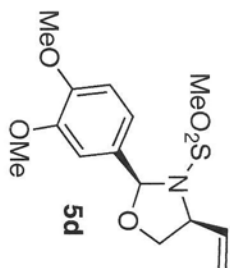
ppm



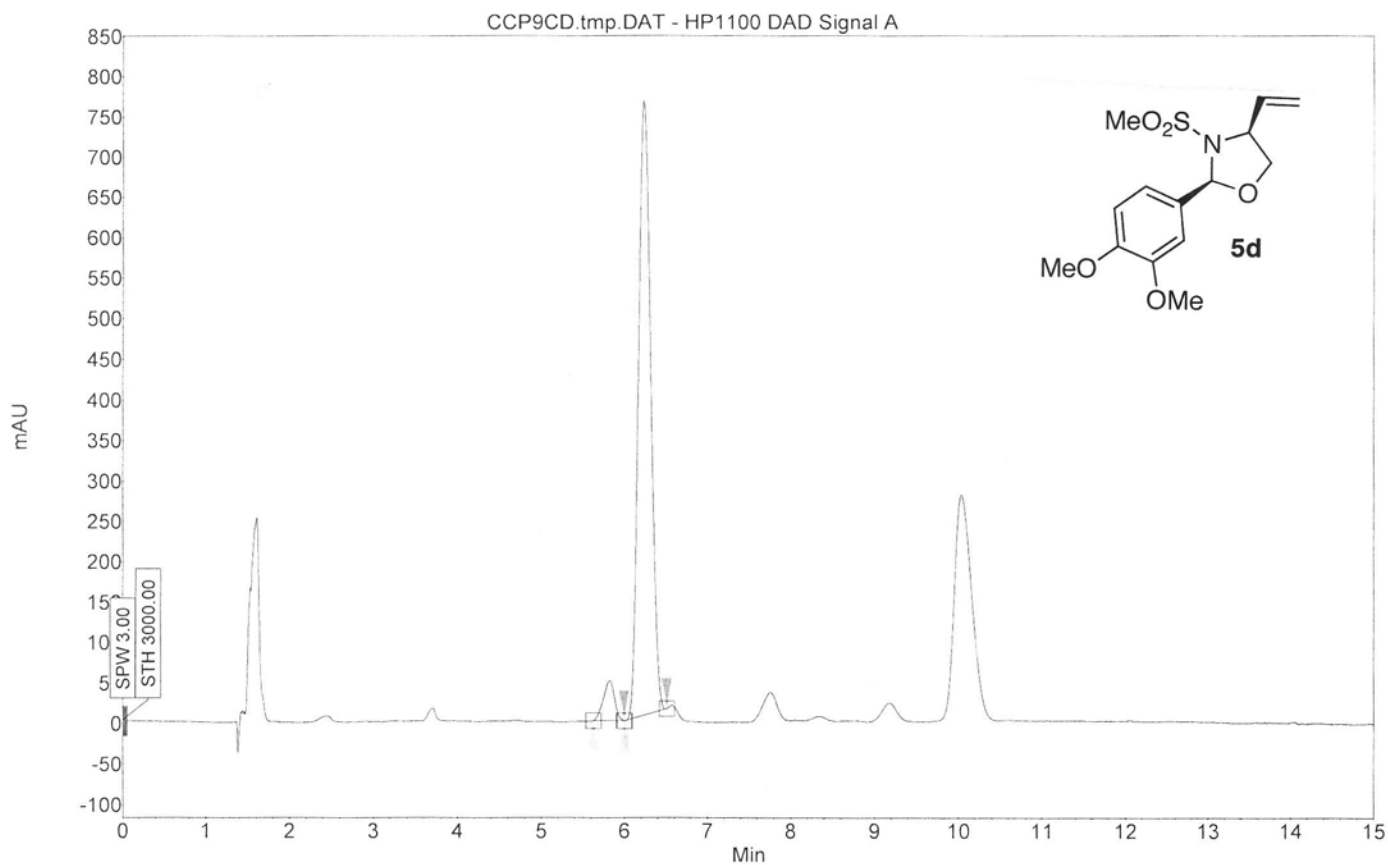
Current Data Parameters
 Name: MS-5-218-C-1H-CHLORAC
 EXPNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 2010020
 Time: 12:15
 INSTRUM: cryo500
 PROBRD: 5 mm CPXI 1H-
 PULPROG: zg30
 TP: 81728
 SOLVENT: CDCl3
 NS: 5
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.098643 Hz
 AQ: 5.0987714 sec
 RG: 5
 IN: 62.400 umsec
 DE: 1.0000000 sec
 TE: 298.0 K
 DI: 0.10000000 sec
 ACQRES: 0.01500000 sec
 F2 - Processing parameters
 SI: 500.135000 MHz
 SF: 500.135000 MHz
 KW: 0
 SSF: 0
 LB: 0.30 Hz
 GB: 0
 PC: 4.00
 ID: NMR plot parameters
 CX: 22.80 cm
 CY: 15.00 cm
 F1P: 10.000 ppm
 F2P: 5002.20 Hz
 F1: 10.000 ppm
 F2: -500.22 ppm
 FREQ1: 0.48246 ppm/cm
 FREQ2: 241.31423 Hz/cm

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

ppm



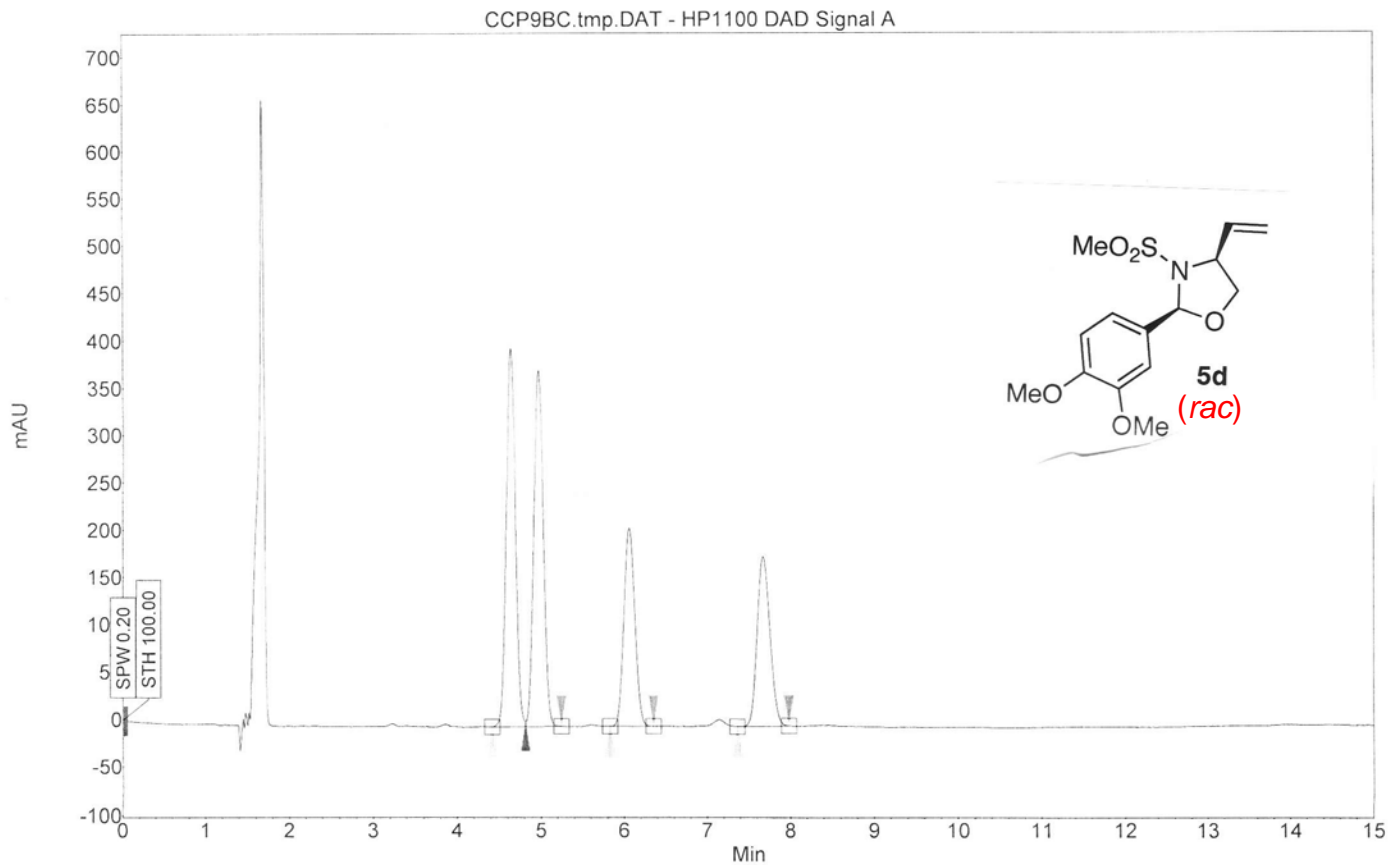
Current Data Parameters
 INSTR NS-5238-C-13C-CryoDAC
 NAME abnba
 EXPTNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20101010
 Time 22:08
 INSTRM cryos500
 PROBRD 5 mm CPXI 1H-
 PULPROG zgpg30
 F2PRG2 spinchase13pp.prf
 SOLVENT CDCl3
 NS 1024
 DS 16
 SFO 100.001 011 Hz
 SWH 0.462188 Hz
 FIDRES 1.72942
 RG 32768
 DE 16.500 uS
 TE 298.0 K
 DT 0.200000 sec
 D1 0.200000 sec
 D16 0.000000 sec
 d17 0.0001960 sec
 ACQRES 0.000000 sec
 MCXRES 0.0150000 sec
 F2 31.00 uS
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 15.50 uS
 PL1 500.00 uS
 PL2 200.00 uS
 PL3 20.00 dB
 PL4 -1.00 dB
 SFO1 125.7942548 MHz
 SFO2 500.2225011 MHz
 ===== CHANNEL f2 =====
 NUC2 1H
 P2 100.00 uS
 PL2 1.50 dB
 PL3 24.50 dB
 SFO2 500.2225011 MHz
 ===== CHANNEL f3 =====
 NUC3 1H
 P3 100.00 uS
 PL3 1.50 dB
 PL4 24.50 dB
 SFO3 500.2225011 MHz
 ===== CHANNEL f4 =====
 NUC4 1H
 P4 100.00 uS
 PL4 1.50 dB
 PL5 24.50 dB
 SFO4 500.2225011 MHz
 ===== CHANNEL f5 =====
 NUC5 1H
 P5 100.00 uS
 PL5 1.50 dB
 PL6 24.50 dB
 SFO5 500.2225011 MHz
 ===== CHANNEL f6 =====
 NUC6 1H
 P6 100.00 uS
 PL6 1.50 dB
 PL7 24.50 dB
 SFO6 500.2225011 MHz
 ===== CHANNEL f7 =====
 NUC7 1H
 P7 100.00 uS
 PL7 1.50 dB
 PL8 24.50 dB
 SFO7 500.2225011 MHz
 ===== CHANNEL f8 =====
 NUC8 1H
 P8 100.00 uS
 PL8 1.50 dB
 PL9 24.50 dB
 SFO8 500.2225011 MHz
 ===== CHANNEL f9 =====
 NUC9 1H
 P9 100.00 uS
 PL9 1.50 dB
 PL10 24.50 dB
 SFO9 500.2225011 MHz
 ===== CHANNEL f10 =====
 NUC10 1H
 P10 100.00 uS
 PL10 1.50 dB
 PL11 24.50 dB
 SFO10 500.2225011 MHz
 ===== CHANNEL f11 =====
 NUC11 1H
 P11 100.00 uS
 PL11 1.50 dB
 PL12 24.50 dB
 SFO11 500.2225011 MHz
 ===== CHANNEL f12 =====
 NUC12 1H
 P12 100.00 uS
 PL12 1.50 dB
 PL13 24.50 dB
 SFO12 500.2225011 MHz
 ===== CHANNEL f13 =====
 NUC13 1H
 P13 100.00 uS
 PL13 1.50 dB
 PL14 24.50 dB
 SFO13 500.2225011 MHz
 ===== CHANNEL f14 =====
 NUC14 1H
 P14 100.00 uS
 PL14 1.50 dB
 PL15 24.50 dB
 SFO14 500.2225011 MHz
 ===== CHANNEL f15 =====
 NUC15 1H
 P15 100.00 uS
 PL15 1.50 dB
 PL16 24.50 dB
 SFO15 500.2225011 MHz
 ===== CHANNEL f16 =====
 NUC16 1H
 P16 100.00 uS
 PL16 1.50 dB
 PL17 24.50 dB
 SFO16 500.2225011 MHz
 ===== CHANNEL f17 =====
 NUC17 1H
 P17 100.00 uS
 PL17 1.50 dB
 PL18 24.50 dB
 SFO17 500.2225011 MHz
 ===== CHANNEL f18 =====
 NUC18 1H
 P18 100.00 uS
 PL18 1.50 dB
 PL19 24.50 dB
 SFO18 500.2225011 MHz
 ===== CHANNEL f19 =====
 NUC19 1H
 P19 100.00 uS
 PL19 1.50 dB
 PL20 24.50 dB
 SFO19 500.2225011 MHz
 ===== CHANNEL f20 =====
 NUC20 1H
 P20 100.00 uS
 PL20 1.50 dB
 PL21 24.50 dB
 SFO20 500.2225011 MHz
 ===== CHANNEL f21 =====
 NUC21 1H
 P21 100.00 uS
 PL21 1.50 dB
 PL22 24.50 dB
 SFO21 500.2225011 MHz
 ===== CHANNEL f22 =====
 NUC22 1H
 P22 100.00 uS
 PL22 1.50 dB
 PL23 24.50 dB
 SFO22 500.2225011 MHz
 ===== CHANNEL f23 =====
 NUC23 1H
 P23 100.00 uS
 PL23 1.50 dB
 PL24 24.50 dB
 SFO23 500.2225011 MHz
 ===== CHANNEL f24 =====
 NUC24 1H
 P24 100.00 uS
 PL24 1.50 dB
 PL25 24.50 dB
 SFO24 500.2225011 MHz
 ===== CHANNEL f25 =====
 NUC25 1H
 P25 100.00 uS
 PL25 1.50 dB
 PL26 24.50 dB
 SFO25 500.2225011 MHz
 ===== CHANNEL f26 =====
 NUC26 1H
 P26 100.00 uS
 PL26 1.50 dB
 PL27 24.50 dB
 SFO26 500.2225011 MHz
 ===== CHANNEL f27 =====
 NUC27 1H
 P27 100.00 uS
 PL27 1.50 dB
 PL28 24.50 dB
 SFO27 500.2225011 MHz
 ===== CHANNEL f28 =====
 NUC28 1H
 P28 100.00 uS
 PL28 1.50 dB
 PL29 24.50 dB
 SFO28 500.2225011 MHz
 ===== CHANNEL f29 =====
 NUC29 1H
 P29 100.00 uS
 PL29 1.50 dB
 PL30 24.50 dB
 SFO29 500.2225011 MHz
 ===== CHANNEL f30 =====
 NUC30 1H
 P30 100.00 uS
 PL30 1.50 dB
 PL31 24.50 dB
 SFO30 500.2225011 MHz
 ===== CHANNEL f31 =====
 NUC31 1H
 P31 100.00 uS
 PL31 1.50 dB
 PL32 24.50 dB
 SFO31 500.2225011 MHz
 ===== CHANNEL f32 =====
 NUC32 1H
 P32 100.00 uS
 PL32 1.50 dB
 PL33 24.50 dB
 SFO32 500.2225011 MHz
 ===== CHANNEL f33 =====
 NUC33 1H
 P33 100.00 uS
 PL33 1.50 dB
 PL34 24.50 dB
 SFO33 500.2225011 MHz
 ===== CHANNEL f34 =====
 NUC34 1H
 P34 100.00 uS
 PL34 1.50 dB
 PL35 24.50 dB
 SFO34 500.2225011 MHz
 ===== CHANNEL f35 =====
 NUC35 1H
 P35 100.00 uS
 PL35 1.50 dB
 PL36 24.50 dB
 SFO35 500.2225011 MHz
 ===== CHANNEL f36 =====
 NUC36 1H
 P36 100.00 uS
 PL36 1.50 dB
 PL37 24.50 dB
 SFO36 500.2225011 MHz
 ===== CHANNEL f37 =====
 NUC37 1H
 P37 100.00 uS
 PL37 1.50 dB
 PL38 24.50 dB
 SFO37 500.2225011 MHz
 ===== CHANNEL f38 =====
 NUC38 1H
 P38 100.00 uS
 PL38 1.50 dB
 PL39 24.50 dB
 SFO38 500.2225011 MHz
 ===== CHANNEL f39 =====
 NUC39 1H
 P39 100.00 uS
 PL39 1.50 dB
 PL40 24.50 dB
 SFO39 500.2225011 MHz
 ===== CHANNEL f40 =====
 NUC40 1H
 P40 100.00 uS
 PL40 1.50 dB
 PL41 24.50 dB
 SFO40 500.2225011 MHz
 ===== CHANNEL f41 =====
 NUC41 1H
 P41 100.00 uS
 PL41 1.50 dB
 PL42 24.50 dB
 SFO41 500.2225011 MHz
 ===== CHANNEL f42 =====
 NUC42 1H
 P42 100.00 uS
 PL42 1.50 dB
 PL43 24.50 dB
 SFO42 500.2225011 MHz
 ===== CHANNEL f43 =====
 NUC43 1H
 P43 100.00 uS
 PL43 1.50 dB
 PL44 24.50 dB
 SFO43 500.2225011 MHz
 ===== CHANNEL f44 =====
 NUC44 1H
 P44 100.00 uS
 PL44 1.50 dB
 PL45 24.50 dB
 SFO44 500.2225011 MHz
 ===== CHANNEL f45 =====
 NUC45 1H
 P45 100.00 uS
 PL45 1.50 dB
 PL46 24.50 dB
 SFO45 500.2225011 MHz
 ===== CHANNEL f46 =====
 NUC46 1H
 P46 100.00 uS
 PL46 1.50 dB
 PL47 24.50 dB
 SFO46 500.2225011 MHz
 ===== CHANNEL f47 =====
 NUC47 1H
 P47 100.00 uS
 PL47 1.50 dB
 PL48 24.50 dB
 SFO47 500.2225011 MHz
 ===== CHANNEL f48 =====
 NUC48 1H
 P48 100.00 uS
 PL48 1.50 dB
 PL49 24.50 dB
 SFO48 500.2225011 MHz
 ===== CHANNEL f49 =====
 NUC49 1H
 P49 100.00 uS
 PL49 1.50 dB
 PL50 24.50 dB
 SFO49 500.2225011 MHz
 ===== CHANNEL f50 =====
 NUC50 1H
 P50 100.00 uS
 PL50 1.50 dB
 PL51 24.50 dB
 SFO50 500.2225011 MHz
 ===== CHANNEL f51 =====
 NUC51 1H
 P51 100.00 uS
 PL51 1.50 dB
 PL52 24.50 dB
 SFO51 500.2225011 MHz
 ===== CHANNEL f52 =====
 NUC52 1H
 P52 100.00 uS
 PL52 1.50 dB
 PL53 24.50 dB
 SFO52 500.2225011 MHz
 ===== CHANNEL f53 =====
 NUC53 1H
 P53 100.00 uS
 PL53 1.50 dB
 PL54 24.50 dB
 SFO53 500.2225011 MHz
 ===== CHANNEL f54 =====
 NUC54 1H
 P54 100.00 uS
 PL54 1.50 dB
 PL55 24.50 dB
 SFO54 500.2225011 MHz
 ===== CHANNEL f55 =====
 NUC55 1H
 P55 100.00 uS
 PL55 1.50 dB
 PL56 24.50 dB
 SFO55 500.2225011 MHz
 ===== CHANNEL f56 =====
 NUC56 1H
 P56 100.00 uS
 PL56 1.50 dB
 PL57 24.50 dB
 SFO56 500.2225011 MHz
 ===== CHANNEL f57 =====
 NUC57 1H
 P57 100.00 uS
 PL57 1.50 dB
 PL58 24.50 dB
 SFO57 500.2225011 MHz
 ===== CHANNEL f58 =====
 NUC58 1H
 P58 100.00 uS
 PL58 1.50 dB
 PL59 24.50 dB
 SFO58 500.2225011 MHz
 ===== CHANNEL f59 =====
 NUC59 1H
 P59 100.00 uS
 PL59 1.50 dB
 PL60 24.50 dB
 SFO59 500.2225011 MHz
 ===== CHANNEL f60 =====
 NUC60 1H
 P60 100.00 uS
 PL60 1.50 dB
 PL61 24.50 dB
 SFO60 500.2225011 MHz
 ===== CHANNEL f61 =====
 NUC61 1H
 P61 100.00 uS
 PL61 1.50 dB
 PL62 24.50 dB
 SFO61 500.2225011 MHz
 ===== CHANNEL f62 =====
 NUC62 1H
 P62 100.00 uS
 PL62 1.50 dB
 PL63 24.50 dB
 SFO62 500.2225011 MHz
 ===== CHANNEL f63 =====
 NUC63 1H
 P63 100.00 uS
 PL63 1.50 dB
 PL64 24.50 dB
 SFO63 500.2225011 MHz
 ===== CHANNEL f64 =====
 NUC64 1H
 P64 100.00 uS
 PL64 1.50 dB
 PL65 24.50 dB
 SFO64 500.2225011 MHz
 ===== CHANNEL f65 =====
 NUC65 1H
 P65 100.00 uS
 PL65 1.50 dB
 PL66 24.50 dB
 SFO65 500.2225011 MHz
 ===== CHANNEL f66 =====
 NUC66 1H
 P66 100.00 uS
 PL66 1.50 dB
 PL67 24.50 dB
 SFO66 500.2225011 MHz
 ===== CHANNEL f67 =====
 NUC67 1H
 P67 100.00 uS
 PL67 1.50 dB
 PL68 24.50 dB
 SFO67 500.2225011 MHz
 ===== CHANNEL f68 =====
 NUC68 1H
 P68 100.00 uS
 PL68 1.50 dB
 PL69 24.50 dB
 SFO68 500.2225011 MHz
 ===== CHANNEL f69 =====
 NUC69 1H
 P69 100.00 uS
 PL69 1.50 dB
 PL70 24.50 dB
 SFO69 500.2225011 MHz
 ===== CHANNEL f70 =====
 NUC70 1H
 P70 100.00 uS
 PL70 1.50 dB
 PL71 24.50 dB
 SFO70 500.2225011 MHz
 ===== CHANNEL f71 =====
 NUC71 1H
 P71 100.00 uS
 PL71 1.50 dB
 PL72 24.50 dB
 SFO71 500.2225011 MHz
 ===== CHANNEL f72 =====
 NUC72 1H
 P72 100.00 uS
 PL72 1.50 dB
 PL73 24.50 dB
 SFO72 500.2225011 MHz
 ===== CHANNEL f73 =====
 NUC73 1H
 P73 100.00 uS
 PL73 1.50 dB
 PL74 24.50 dB
 SFO73 500.2225011 MHz
 ===== CHANNEL f74 =====
 NUC74 1H
 P74 100.00 uS
 PL74 1.50 dB
 PL75 24.50 dB
 SFO74 500.2225011 MHz
 ===== CHANNEL f75 =====
 NUC75 1H
 P75 100.00 uS
 PL75 1.50 dB
 PL76 24.50 dB
 SFO75 500.2225011 MHz
 ===== CHANNEL f76 =====
 NUC76 1H
 P76 100.00 uS
 PL76 1.50 dB
 PL77 24.50 dB
 SFO76 500.2225011 MHz
 ===== CHANNEL f77 =====
 NUC77 1H
 P77 100.00 uS
 PL77 1.50 dB
 PL78 24.50 dB
 SFO77 500.2225011 MHz
 ===== CHANNEL f78 =====
 NUC78 1H
 P78 100.00 uS
 PL78 1.50 dB
 PL79 24.50 dB
 SFO78 500.2225011 MHz
 ===== CHANNEL f79 =====
 NUC79 1H
 P79 100.00 uS
 PL79 1.50 dB
 PL80 24.50 dB
 SFO79 500.2225011 MHz
 ===== CHANNEL f80 =====
 NUC80 1H
 P80 100.00 uS
 PL80 1.50 dB
 PL81 24.50 dB
 SFO80 500.2225011 MHz
 ===== CHANNEL f81 =====
 NUC81 1H
 P81 100.00 uS
 PL81 1.50 dB
 PL82 24.50 dB
 SFO81 500.2225011 MHz
 ===== CHANNEL f82 =====
 NUC82 1H
 P82 100.00 uS
 PL82 1.50 dB
 PL83 24.50 dB
 SFO82 500.2225011 MHz
 ===== CHANNEL f83 =====
 NUC83 1H
 P83 100.00 uS
 PL83 1.50 dB
 PL84 24.50 dB
 SFO83 500.2225011 MHz
 ===== CHANNEL f84 =====
 NUC84 1H
 P84 100.00 uS
 PL84 1.50 dB
 PL85 24.50 dB
 SFO84 500.2225011 MHz
 ===== CHANNEL f85 =====
 NUC85 1H
 P85 100.00 uS
 PL85 1.50 dB
 PL86 24.50 dB
 SFO85 500.2225011 MHz
 ===== CHANNEL f86 =====
 NUC86 1H
 P86 100.00 uS
 PL86 1.50 dB
 PL87 24.50 dB
 SFO86 500.2225011 MHz
 ===== CHANNEL f87 =====
 NUC87 1H
 P87 100.00 uS
 PL87 1.50 dB
 PL88 24.50 dB
 SFO87 500.2225011 MHz
 ===== CHANNEL f88 =====
 NUC88 1H
 P88 100.00 uS
 PL88 1.50 dB
 PL89 24.50 dB
 SFO88 500.2225011 MHz
 ===== CHANNEL f89 =====
 NUC89 1H
 P89 100.00 uS
 PL89 1.50 dB
 PL90 24.50 dB
 SFO89 500.2225011 MHz
 ===== CHANNEL f90 =====
 NUC90 1H
 P90 100.00 uS
 PL90 1.50 dB
 PL91 24.50 dB
 SFO90 500.2225011 MHz
 ===== CHANNEL f91 =====
 NUC91 1H
 P91 100.00 uS
 PL91 1.50 dB
 PL92 24.50 dB
 SFO91 500.2225011 MHz
 ===== CHANNEL f92 =====
 NUC92 1H
 P92 100.00 uS
 PL92 1.50 dB
 PL93 24.50 dB
 SFO92 500.2225011 MHz
 ===== CHANNEL f93 =====
 NUC93 1H
 P93 100.00 uS
 PL93 1.50 dB
 PL94 24.50 dB
 SFO93 500.2225011 MHz
 ===== CHANNEL f94 =====
 NUC94 1H
 P94 100.00 uS
 PL94 1.50 dB
 PL95 24.50 dB
 SFO94 500.2225011 MHz
 ===== CHANNEL f95 =====
 NUC95 1H
 P95 100.00 uS
 PL95 1.50 dB
 PL96 24.50 dB
 SFO95 500.2225011 MHz
 ===== CHANNEL f96 =====
 NUC96 1H
 P96 100.00 uS
 PL96 1.50 dB
 PL97 24.50 dB
 SFO96 500.2225011 MHz
 ===== CHANNEL f97 =====
 NUC97 1H
 P97 100.00 uS
 PL97 1.50 dB
 PL98 24.50 dB
 SFO97 500.2225011 MHz
 ===== CHANNEL f98 =====
 NUC98 1H
 P98 100.00 uS
 PL98 1.50 dB
 PL99 24.50 dB
 SFO98 500.2225011 MHz
 ===== CHANNEL f99 =====
 NUC99 1H
 P99 100.00 uS
 PL99 1.50 dB
 PL100 24.50 dB
 SFO99 500.2225011 MHz
 ===== CHANNEL f100 =====
 NUC100 1H
 P100 100.00 uS
 PL100 1.50 dB
 PL101 24.50 dB
 SFO100 500.2225011 MHz
 ===== CHANNEL f101 =====
 NUC101 1H
 P101 100.00 uS
 PL101 1.50 dB
 PL102 24.50 dB
 SFO101 500.2225011 MHz
 ===== CHANNEL f102 =====
 NUC102 1H
 P102 100.00 uS
 PL102 1.50 dB
 PL103 24.50 dB
 SFO102 500.2225011 MHz
 ===== CHANNEL f103 =====
 NUC103 1H
 P103 100.00 uS
 PL103 1.50 dB
 PL104 24.50 dB
 SFO103 500.2225011 MHz
 ===== CHANNEL f104 =====
 NUC104 1H
 P104 100.00 uS
 PL104 1.50 dB
 PL105 24.50 dB
 SFO104 500.2225011 MHz
 ===== CHANNEL f105 =====
 NUC105 1H
 P105 100.00 uS
 PL105 1.50 dB
 PL106 24.50 dB
 SFO105 500.2225011 MHz
 ===== CHANNEL f106 =====
 NUC106 1H
 P106 100.00 uS
 PL106 1.50 dB
 PL107 24.50 dB
 SFO106 500.2225011 MHz
 ===== CHANNEL f107 =====
 NUC107 1H
 P107 100.00 uS
 PL107 1.50 dB
 PL108 24.50 dB
 SFO107 500.2225011 MHz
 ===== CHANNEL f108 =====
 NUC108 1H
 P108 100.00 uS
 PL108 1.50 dB
 PL109 24.50 dB
 SFO108 500.2225011 MHz
 ===== CHANNEL f109 =====
 NUC109 1H
 P109 100.00 uS
 PL109 1.50 dB
 PL110 24.50 dB
 SFO109 500.2225011 MHz
 ===== CHANNEL f110 =====
 NUC110 1H
 P110 100.00 uS
 PL110 1.50 dB
 PL111 24.50 dB
 SFO110 500.2225011 MHz
 ===== CHANNEL f111 =====
 NUC111 1H
 P111 100.00 uS
 PL111 1.50 dB
 PL112 24.50 dB
 SFO111 500.2225011 MHz
 ===== CHANNEL f112 =====
 NUC112 1H
 P112 100.00 uS
 PL112 1.50 dB
 PL113 24.50 dB
 SFO112 500.2225011 MHz
 ===== CHANNEL f113 =====
 NUC113 1H
 P113 100.00 uS
 PL113 1.50 dB
 PL114 24.50 dB
 SFO113 500.2225011 MHz
 ===== CHANNEL f114 =====
 NUC114 1H
 P114 100.00 uS
 PL114 1.50 dB
 PL115 24.50 dB
 SFO114 500.2225011 MHz
 ===== CHANNEL f115 =====
 NUC115 1H
 P115 100.00 uS
 PL115 1.50 dB
 PL116 24.50 dB
 SFO115 500.2225011 MHz
 ===== CHANNEL f116 =====
 NUC116 1H
 P116 100.00 uS
 PL116 1.50 dB
 PL117 24.50 dB
 SFO116 500.2225011 MHz
 ===== CHANNEL f117 =====
 NUC117 1H
 P117 100.00 uS
 PL117 1.50 dB
 PL118 24.50 dB
 SFO117 500.2225011 MHz
 ===== CHANNEL f118 =====
 NUC118 1H
 P118 100.00 uS
 PL118 1.50 dB
 PL119 24.50 dB
 SFO118 500.2225011 MHz
 ===== CHANNEL f119 =====
 NUC119 1H
 P119 100.00 uS
 PL119 1.50 dB
 PL120 24.50 dB
 SFO119 500.2225011 MHz
 ===== CHANNEL f120 =====
 NUC120 1H
 P120 100.00 uS
 PL120 1.50 dB
 PL121 24.50 dB
 SFO120 500.2225011 MHz
 ===== CHANNEL f121 =====
 NUC121 1H
 P121 100.00 uS
 PL121 1.50 dB
 PL122 24.50 dB
 SFO121 500.2225011 MHz
 ===== CHANNEL f122 =====
 NUC122 1H
 P122 100.00 uS
 PL122 1.50 dB
 PL123 24.50 dB
 SFO122 500.2225011 MHz
 ===== CHANNEL f123 =====
 NUC123 1H
 P123 100.00 uS
 PL123 1.50 dB
 PL124 24.50 dB
 SFO123 500.2225011 MHz
 ===== CHANNEL f124 =====
 NUC124 1H
 P124 100.00 uS
 PL124 1.50 dB
 PL125 24.50 dB
 SFO124 500.2225011 MHz
 ===== CHANNEL f125 =====
 NUC125 1H
 P125 100.00 uS
 PL125 1.50 dB
 PL126 24.50 dB
 SFO125 500.2225011 MHz
 ===== CHANNEL f126 =====
 NUC126 1H
 P126 100.00 uS
 PL126 1.50 dB
 PL127 24.50 dB
 SFO126 500.2225011 MHz
 ===== CHANNEL f127 =====
 NUC127 1H
 P127 100.00 uS
 PL127 1.50 dB
 PL128 24.50 dB
 SFO127 500.2225011 MHz
 ===== CHANNEL f128 =====
 NUC128 1H
 P128 100.00 uS
 PL128 1.50 dB
 PL129 24.50 dB
 SFO128 500.2225011 MHz
 ===== CHANNEL f129 =====
 NUC129 1H
 P12



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	5.63	5.82	6.00	0.00	5.53	49.5	7.6	5.534
2	UNKNOWN	6.01	6.23	6.51	0.00	94.47	760.1	130.0	94.466
Total						100.00	809.6	137.6	100.000

Method Name:MS-ADH-10MeOH-2mlmin
Run Name:MS-5-181-B-RAC-2

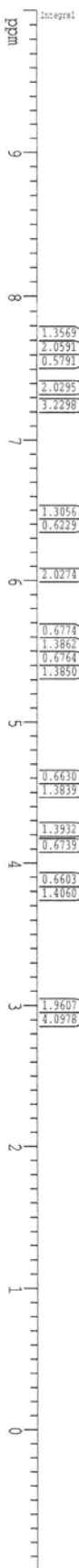
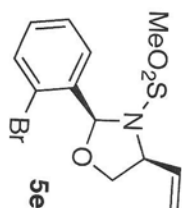
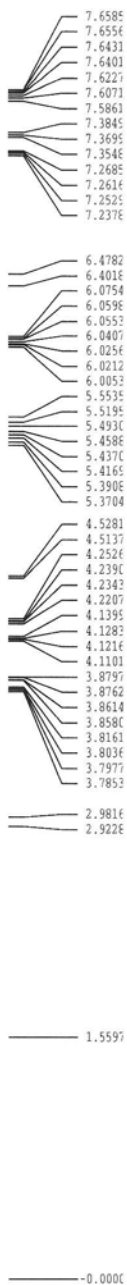
Date:5/16/2011
Time:3:40:01 PM



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	4.41	4.63	4.81	0.00	30.75	398.8	50.4	30.754
2	UNKNOWN	4.81	4.96	5.24	0.00	30.39	375.2	49.8	30.389
3	UNKNOWN	5.83	6.06	6.35	0.00	19.41	208.8	31.8	19.413
4	UNKNOWN	7.36	7.67	7.98	0.00	19.44	178.5	31.9	19.444
Total						100.00	1161.4	163.9	100.000

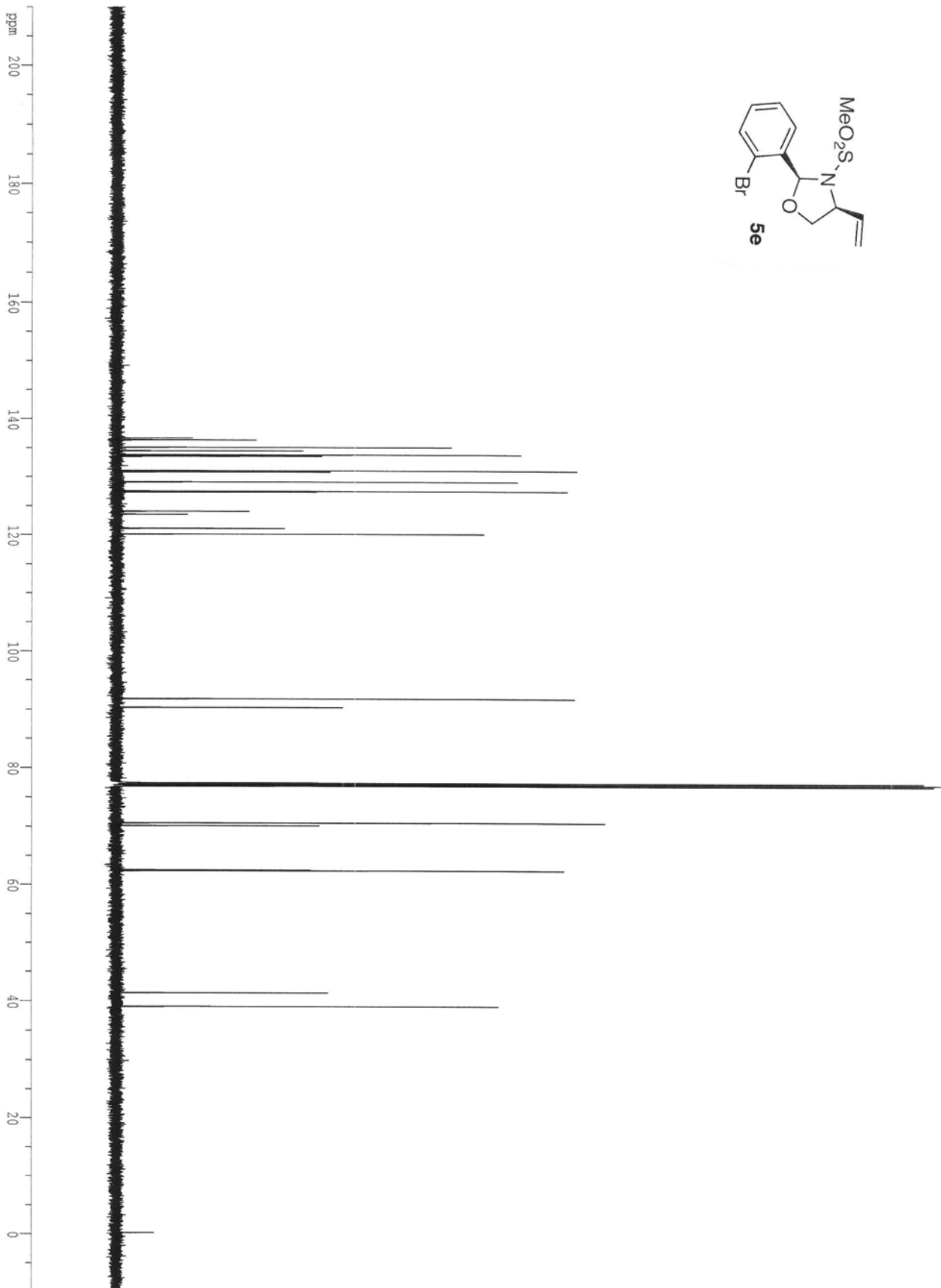
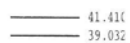
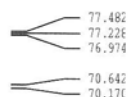
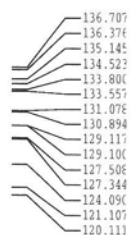
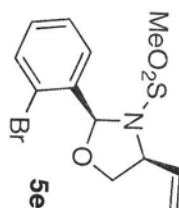
1H spectrum

ppm



Current Data Parameters
USER: shajin
NAME: MS-5-21-19-1H-CH-0406
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20110101
Time: 21.00
INSTRUM: spect
PROBHD: 5 mm CPD1
PULPROG: zgpg30
TO: 81728
SOLVENT: CDCl3
NS: 8
DS: 2
SWH: 8013.824 Hz
FIDRES: 0.09864 Hz
AQ: 0.09864 Hz
RG: 10.1
BW: 62.400 kHz
DE: 6.00 uS
TE: 300.2 K
NUC1: 1H
NUC2: 13C
INVERT: 0.0000000 sec
MIXER: 0.0150000 sec
===== CHANNEL f1 =====
NUC1: 1H
P1: 12.50 uS
PL1: 0.00 dB
SFO1: 500.225015 MHz
F2 - Processing parameters
SI: 65536
SF: 500.225015 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 4.00
ID: NMR plot parameters
CX: 22.80 cm
CY: 13.73 cm
FLP: 10.000 ppm
F1: 5002.20 Hz
F2: -1.000 ppm
F3: 0.4844561/cm
F4: 241.3422 Hz/cm

ppm



```
Current Data Parameters
USER          shagha
NAME          MS-5-217-B-11C-CHARAC
EXPNO        1
PROCNO       1
```

```
F2 - Acquisition Parameters
Date_      20110301
Time       21 11
```

INSTRUM	CRY0500
PROBHD	5 mm CPICI 1H-
DATA PROC	SolventChem3Dm and

TD	65536
SOLVENT	CDCl ₃
MS	941

DS	16
SMH	30303.031 Hz
FREQ	0.46328e Hz

AQ	1.0613940 sec
PC	7298.2
PC	15.600

DE	6.00 use
TE	298.0 K

dl1	0.0300000 sec
D16	0.0002000 sec
dl7	0.0000000 sec

MCREST	0.0000000	SEC
MCERR	0.0150000	SEC

```
===== CHANNEL f1 =====
```

PROCS	400
P1	15.50 use
P11	500.00 use

PL1	-1.00 dB
PL0	120.00 dB
PL2	4000.00 dB

SP4	3.20 dB
SP1	3.20 dB
SP2	3.20 dB

SPNRM1	Crp60,9.3,20.1
SPNRM2	Crp60comp.4
SPOFL1	0.00 Hz

```
SPORT 0.00 HZ
===== CHANNEL F2 =====
```

CPUtime	0.01216
NOU2	1H
PCPD2	100.00 usec

PL2	1.60 GB
PL12	24.60 DB
SFO2	500.2225011 MHz

```
===== GRADIENT CHANNEL =====
CPNAM1      SINE,100
```

GPMM2	SINE,100
GPX1	0.00
GPX2	0.00

GP11	0.00	g
GP12	0.00	g
GP21	30.00	g

GP22	50.00 \$
p15	500.00 usec
p16	1000.00 usec

F2 - Processing parameters
ST 65536

125.7804006 MHz
SF
WDM
CCR

Frequency (Hz)	Amplitude (V)
0.30	0.30
0.30	0.30
0.30	0.30

ID NMR plot parameters 33.80 cm

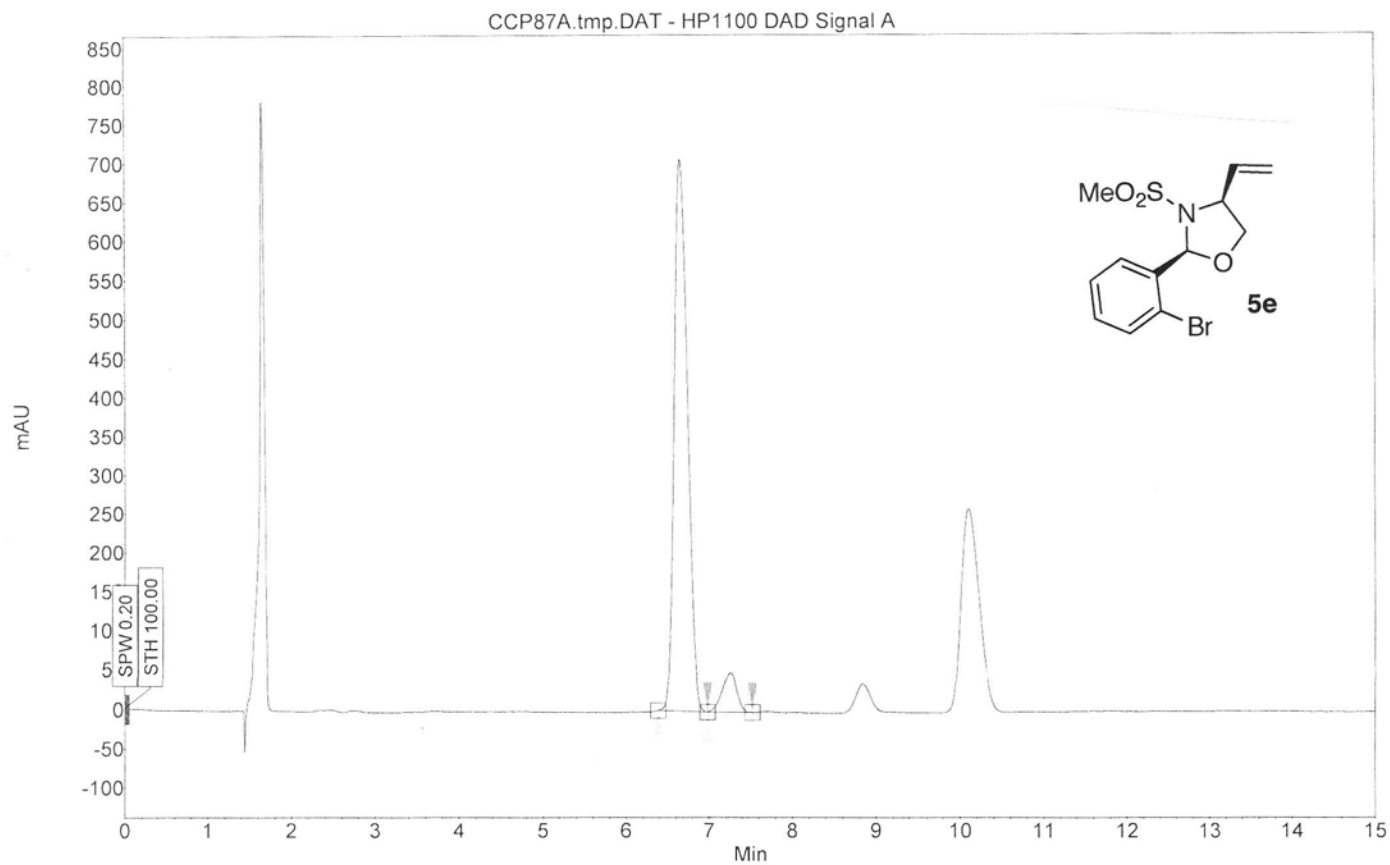
Cy	15.00	cm
ELP	210.000	pgm
EL	26413.88	Hz

F2P	-10.000 ppm
F2	-1257.80 Hz
Frequency	0.64013 MHz

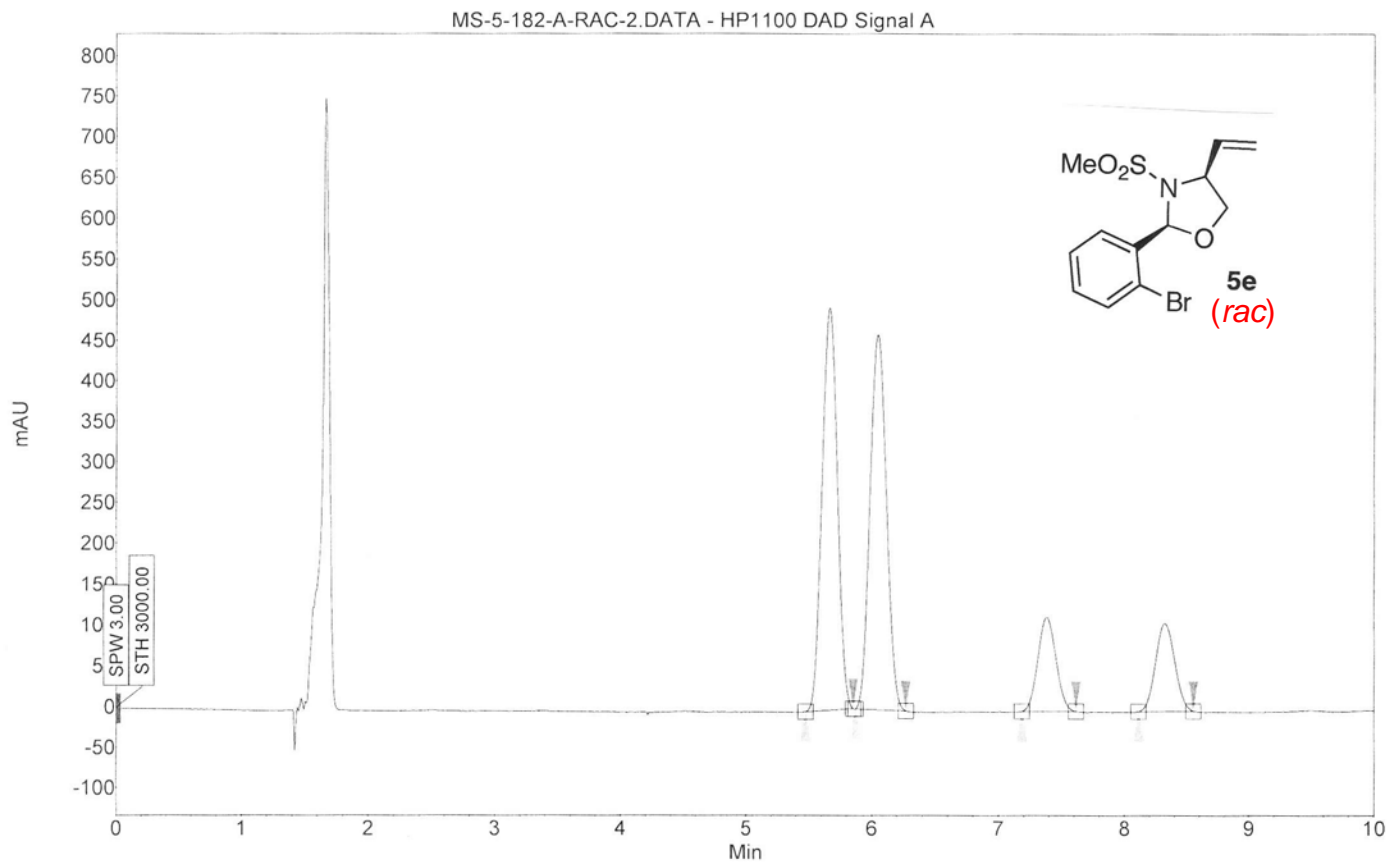
Hz/cm	1213.67053 Hz/cm
Hz/cm	1213.67053 Hz/cm

Method Name:MS-ADH-5MeOH-2mlmin
Run Name:MS-5-217-B-2

Date:4/21/2011
Time:5:07:58 PM



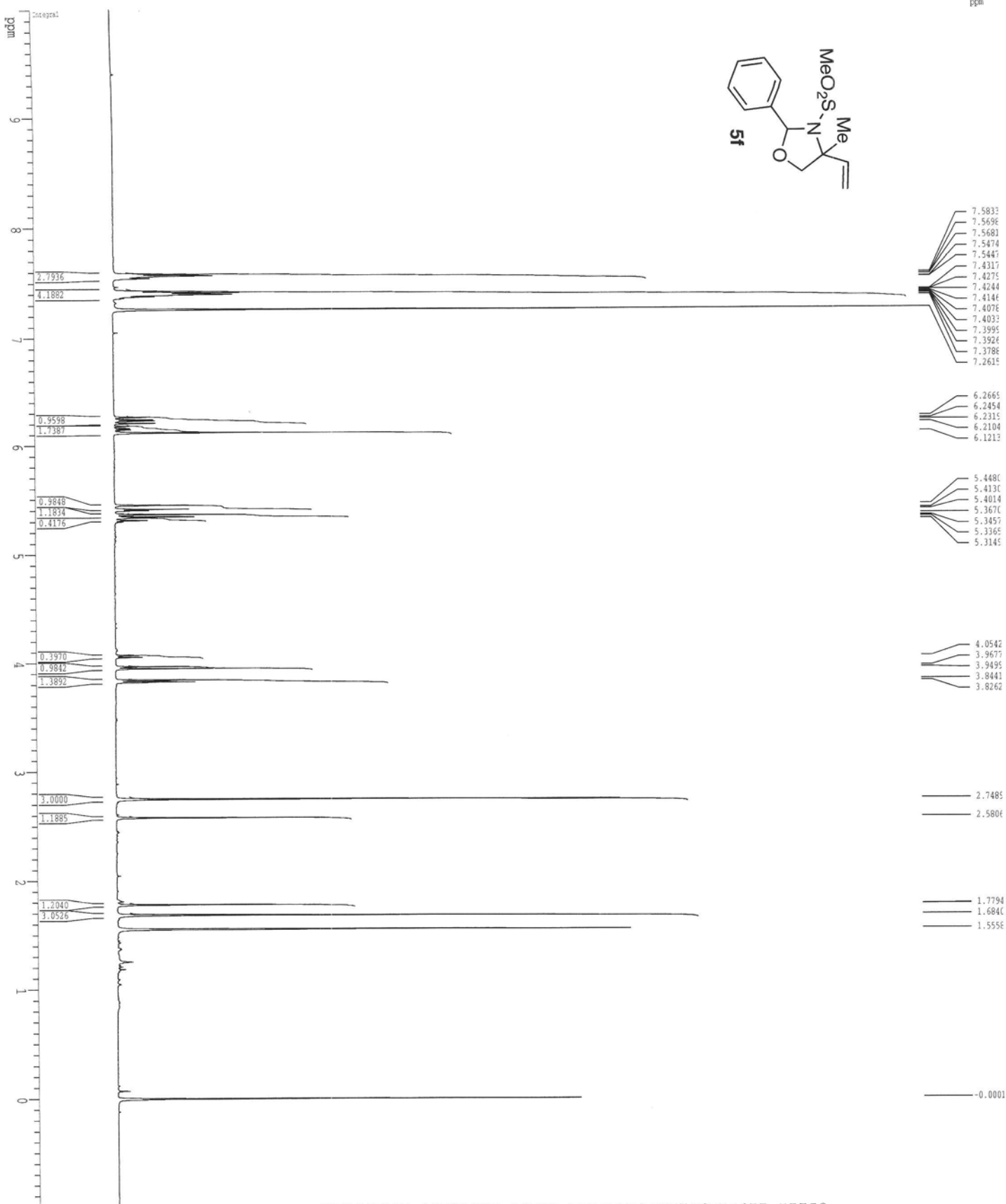
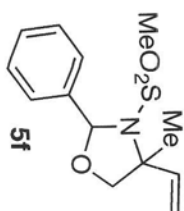
Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	6.39	6.65	6.98	0.00	92.78	705.8	130.9	92.776
2	UNKNOWN	6.98	7.25	7.52	0.00	7.22	50.0	10.2	7.224
Total						100.00	755.8	141.1	100.000



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	5.48	5.66	5.85	0.00	39.06	494.5	69.3	39.057
2	UNKNOWN	5.87	6.05	6.27	0.00	38.99	460.9	69.2	38.995
3	UNKNOWN	7.19	7.38	7.61	0.00	11.01	116.0	19.5	11.010
4	UNKNOWN	8.11	8.32	8.55	0.00	10.94	108.6	19.4	10.939
Total						100.00	1179.9	177.4	100.000

¹H spectrum

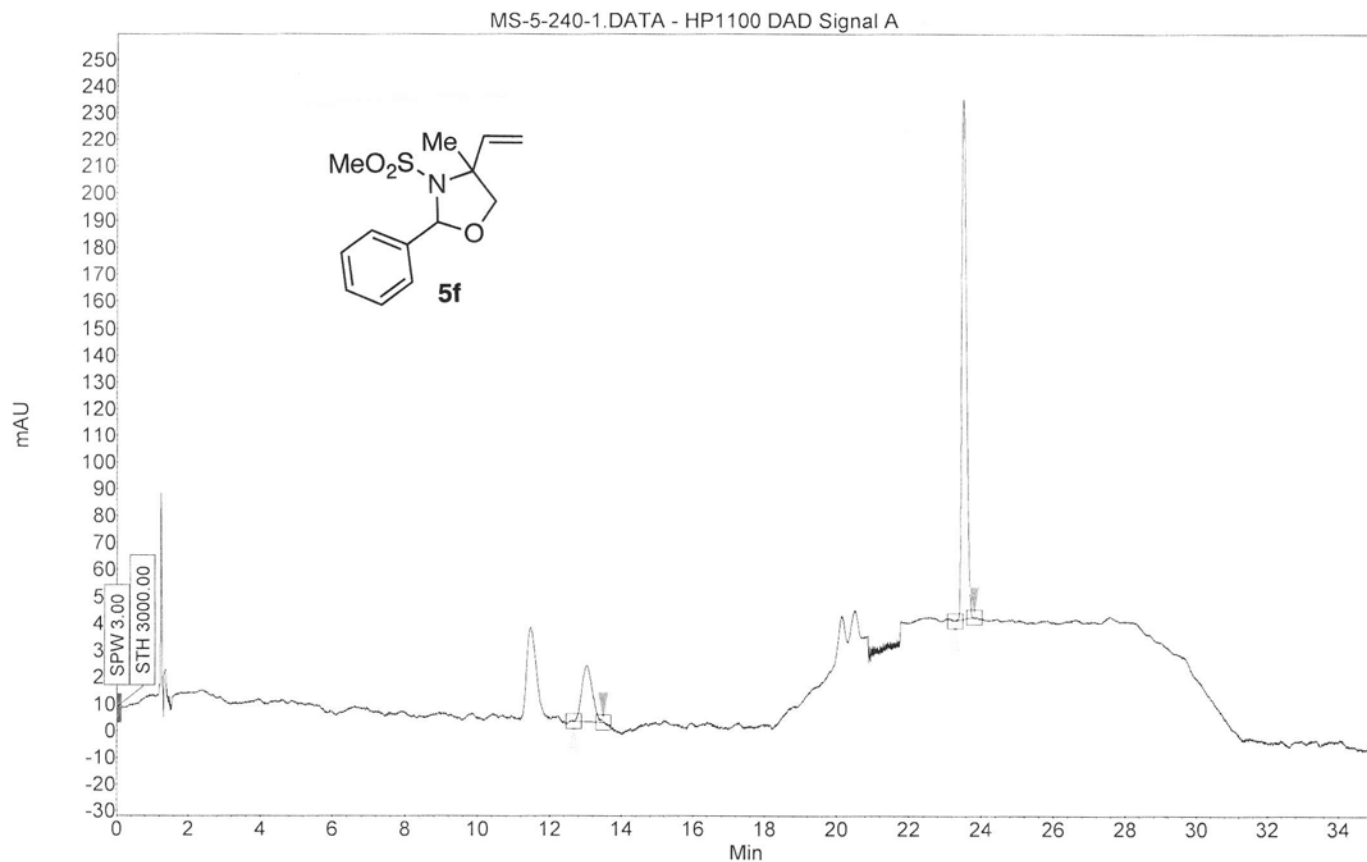
ppm



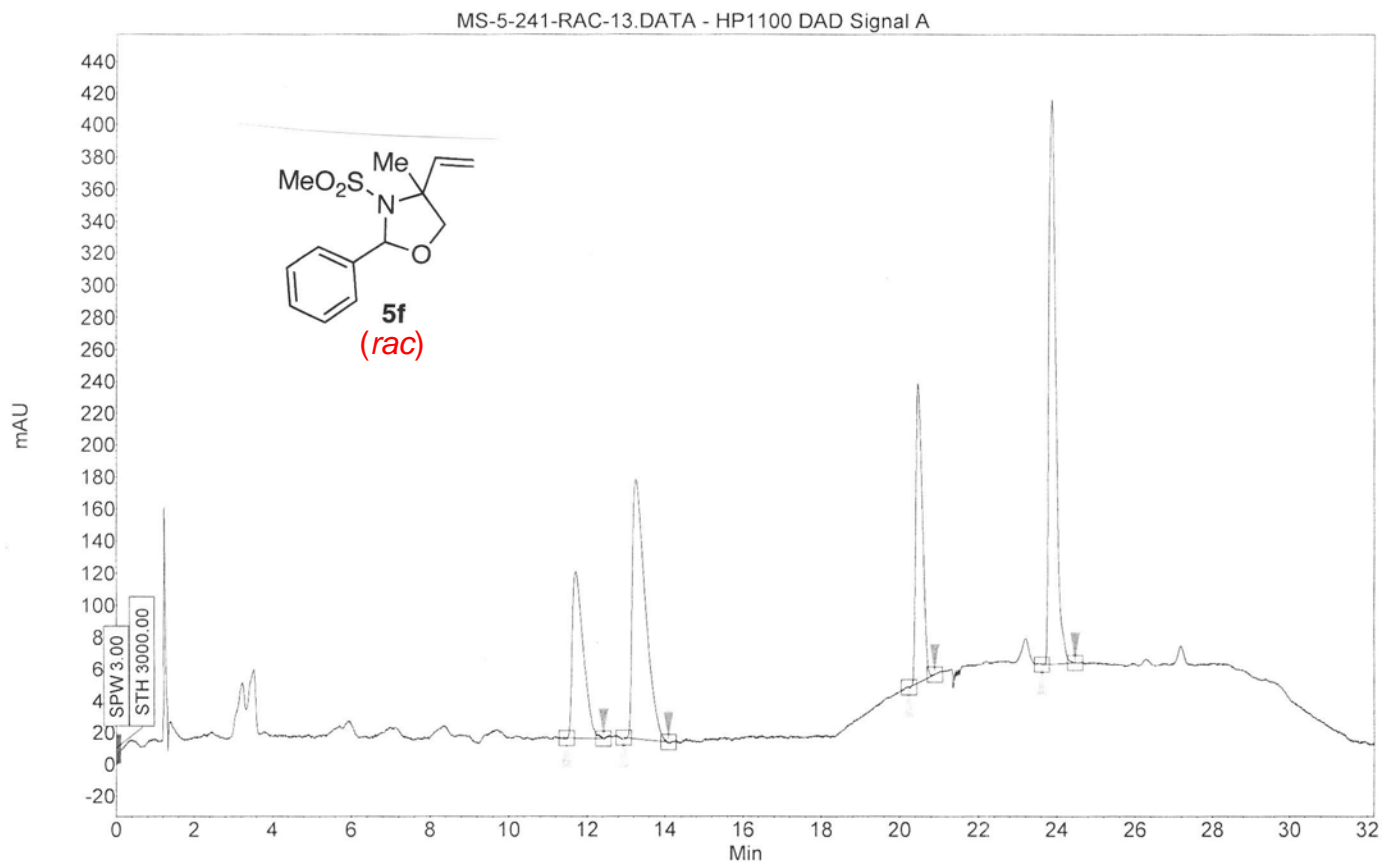
Current Data Parameters
 USER shapla
 NAME MS-5-216-1H-CDMSAC
 EXPTNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110402
 Time 12.28
 INSTRUM cryo500
 PROBHD 5 mm CPCL 1H-
 PULPROG zgpg30
 TD 32768
 SFO 500.136250
 SOLVENT CDCL3
 NS 8
 DS 2
 SWH 8012.820 Hz
 SFO 500.136250 Hz
 FIDRES 0.099043 Hz
 AQ 5.0998774 sec
 RG 14.3
 DW 62.400 usec
 DE 28.00 usec
 TE 300.2 K
 D1 0.10000000 sec
 D11 0.00000000 sec
 MCOREST 0.01500000 sec
 MCOREX 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 1.50 usec
 PL 0.00 dB
 SFO1 500.2235015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200100 MHz
 ACQ 64
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00
 ID MS6 plot parameters
 CX 22.80 cm
 CY 16.61 cm
 F1P 10.000 ppm
 F1 10.000 Hz
 F2P -1.000 ppm
 F2 -1.000 Hz
 FREQ1 0.48216 ppm/cm
 HZCM 241.3342 Hz/cm

Method Name:MS-ADH-2.5-10iPAGRAD-1.5mlmin-110mbar-2
Run Name:MS-5-240-1

Date:5/16/2011
Time:2:42:23 PM

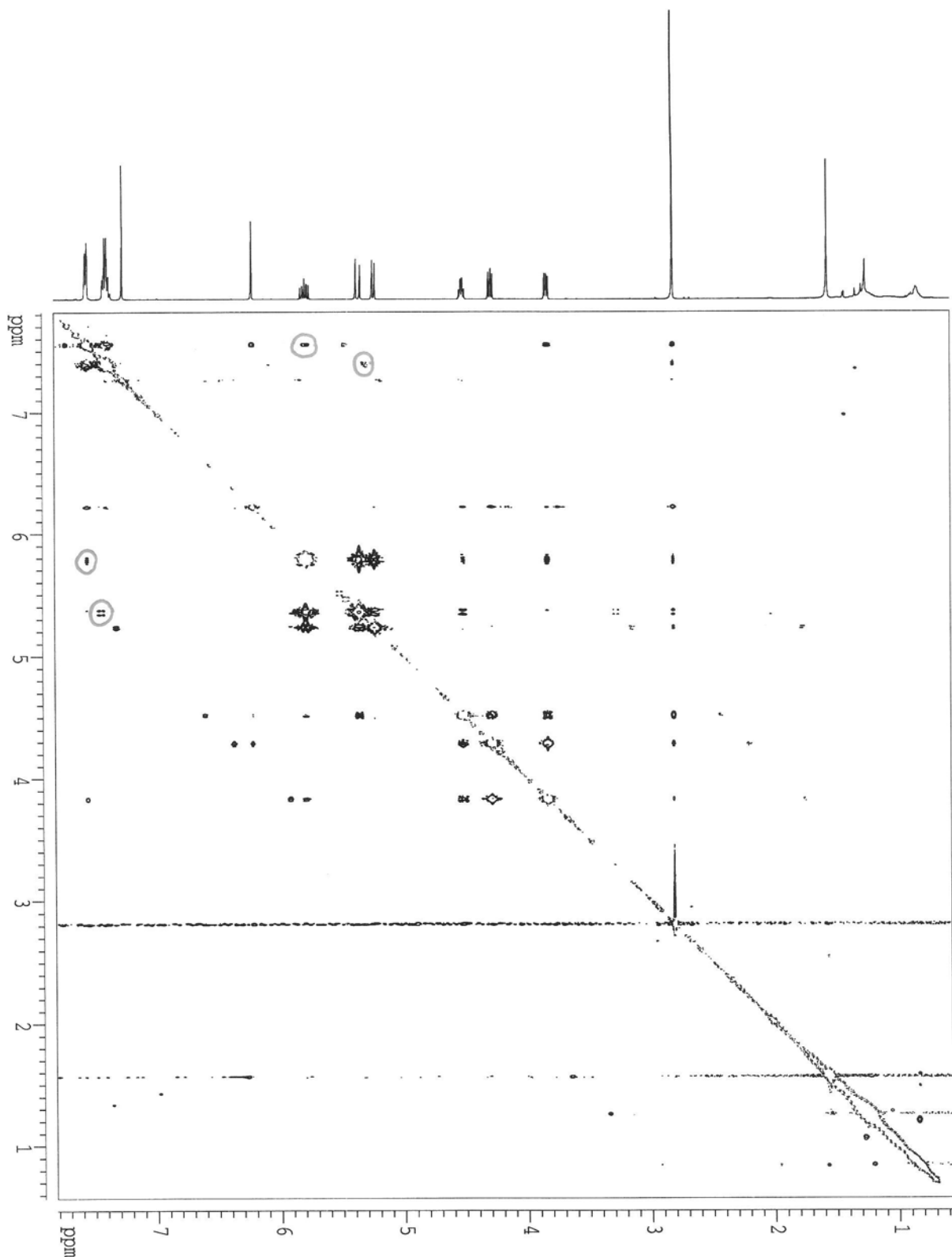
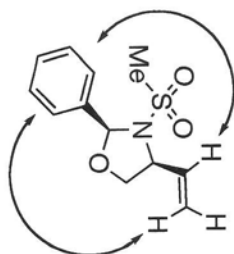


Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	12.67	13.05	13.50	0.00	19.41	21.0	7.1	19.412
2	UNKNOWN	23.28	23.50	23.80	0.00	80.59	193.8	29.7	80.588
Total						100.00	214.7	36.8	100.000



Index	Name	Start	Time	End	RT Offset	Quantity	Height	Area	Area
		[Min]	[Min]	[Min]	[Min]	[% Area]	[μV]	[μV.Min]	[%]
1	UNKNOWN	11.47	11.71	12.42	0.00	16.75	104.8	34.4	16.750
2	UNKNOWN	12.94	13.25	14.09	0.00	30.48	162.3	62.7	30.482
3	UNKNOWN	20.24	20.46	20.89	0.00	17.58	187.6	36.1	17.578
4	UNKNOWN	23.61	23.87	24.46	0.00	35.19	353.2	72.3	35.189
Total						100.00	807.9	205.6	100.000

gnoesy



Current Data Parameters
NAME MS-CHARAC-5-27-MOESY
EXNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20091117
Time 19.16
INSTRUM CQY500
PROBHD 5 mm CPYCI 1H-
PULPROG zgpg30
TD 2048
SOLVENT CDCl3
NS 2
DS 16
SWH 4166.667 Hz
FIDRES 2.034505 Hz
AQ 0.2458100 sec
RG 50.8
RG 50.8
IN 120.000 usec
DE 6.00 usec
TE 298.0 K
DO 0.00000300 sec
DL 2.00000000 sec
DB 0.80000001 sec
DI 6 0.0002000 sec
D16 0.3988002 sec
D20 0.0001200 sec
D30 0.0001200 sec

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

NUC1 1H
P1 7.50 usec
P2 15.00 usec
PL1 1.60 dB
SFO1 500.2222897 MHz

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

GNAM1 sine,100
GNAM2 sine,100
GPH1 0.00 %
GPH2 0.00 %
GPI1 0.00 %
GPI2 0.00 %
GPR1 40.00 %
GPR2 -40.00 %
PL6 1000.00 usec

F1 - Acquisition Parameters

ND0 2
TD 400
SFO1 500.2223 MHz
FIDRES 10.416667 Hz
SN 8.350 ppm
FMODE undefined

F2 - Processing parameters

SI 1024
SF 500.2200300 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0
PC 2.00

F1 - Processing parameters

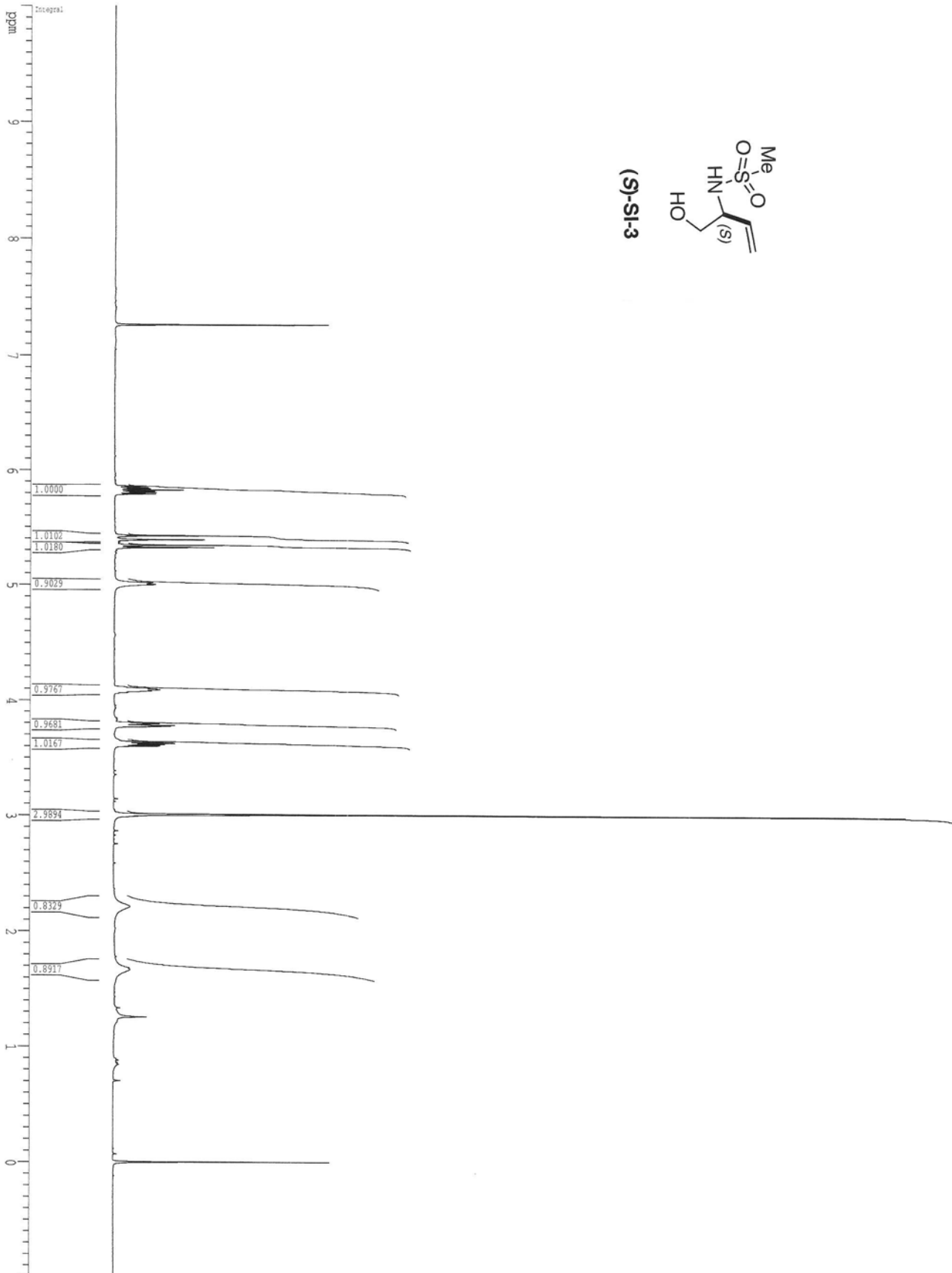
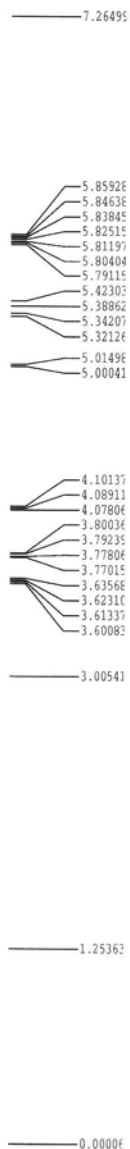
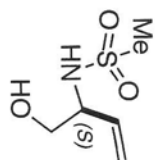
SI 1024
MC2 TPI
SF 500.2200300 MHz
WDW QSI
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters

CK2 15.00 cm
CX1 15.00 cm
F2P10 7.818 ppm
F2P10 3910.56 Hz
F2P10 0.570 ppm
F2P10 285.47 Hz
F1P10 7.818 ppm
F1P10 3910.56 Hz
F1P10 0.570 ppm
F1P10 285.47 Hz
F2P10 0.48316 ppm/cm
F2P10 241.68602 Hz/cm
F1P10 0.48316 ppm/cm
F1P10 241.68602 Hz/cm

¹H spectrum

ppm



Current Data Parameters
 USER: shupha
 NAME: NS-5-229-1H-CM04C
 EXPNO: 1
 PROCNO: 1

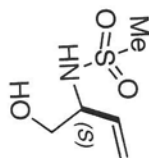
F2 - Acquisition Parameters
 Date_: 20110420
 Time: 22.35
 INSTRUM: cryo500
 PROBRD: 5 mm CPCL 1H-
 PULPROG: zgpg30
 TD: 65536
 SFO: 500.13627
 SOLVENT: CDCl3
 NS: 8
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.098043 Hz
 AQ: 5.098774 sec
 RG: 5.7
 TD: 62.400 usec
 DE: 1.1000000
 TE: 298.0 K
 D1: 0.10000000 sec
 ACQRES: 0.00000000 sec
 MCNEX: 0.01500000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.2235015 MHz

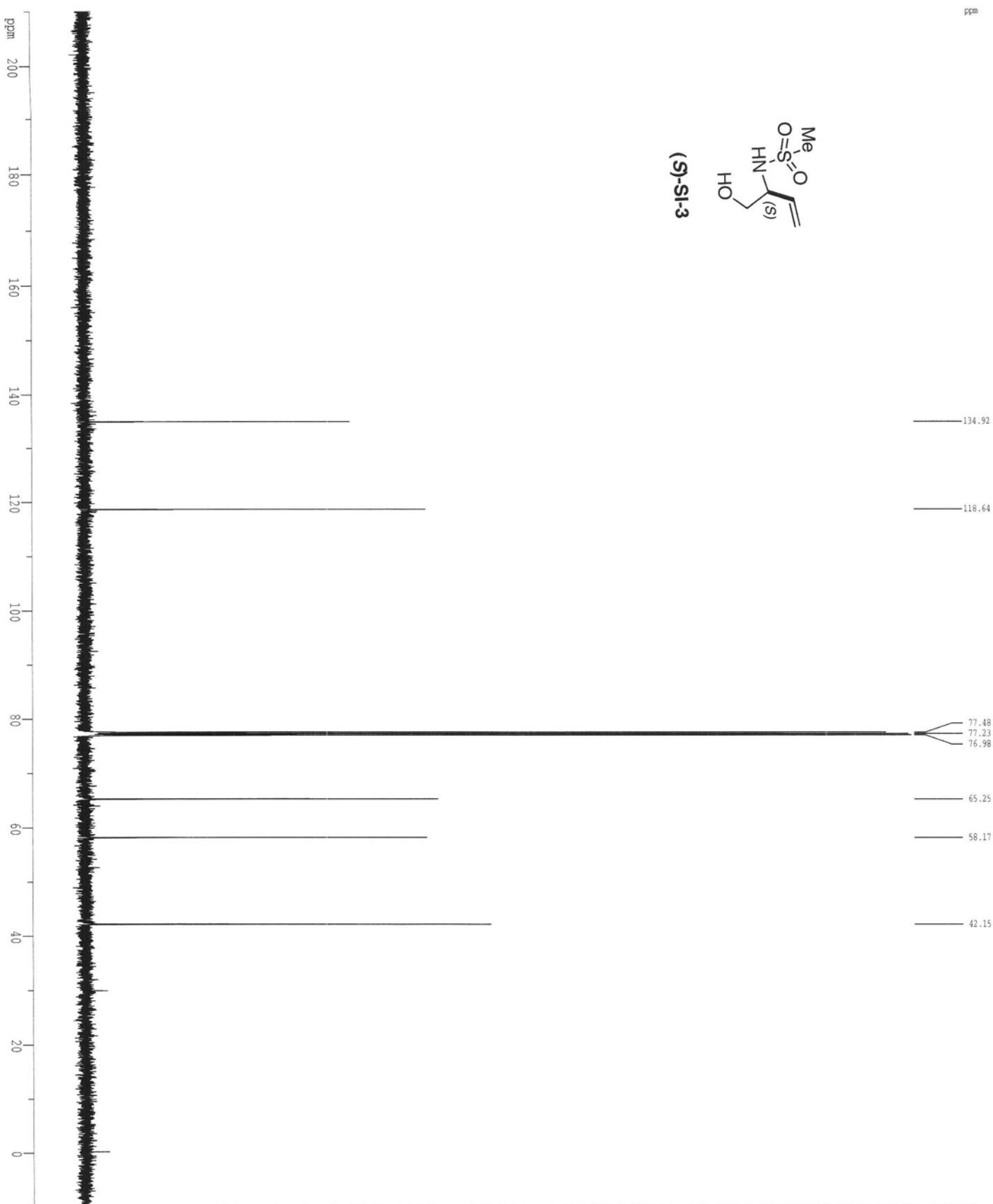
F2 - Processing parameters
 SI: 65536
 SF: 500.2200102 MHz
 KW: BM
 SSB: 0
 LB: 0.10 Hz
 GB: 0
 PC: 4.00

1D NMR plot parameters
 CX: 22.80 cm
 CY: 14.10 cm
 FIP: 10.000 ppm
 F2P: 5002.20 Hz
 F2R: -50.422 ppm
 FREQM: 0.48846 ppm/cm
 RECN: 241.31423 Hz/cm

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



(S)-SI-3



Current Data Parameters
NAME Shalpa
INSTRUM cryo500
PROBHD 5 mm CPY1 1H-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 501
DS 16
SH 3010.011 Hz
FIDRES 0.46288 Hz
AQ 1.061240 sec
RG 320
NU 16.500 usec
OR 6.00 usec
TE 298.0 K
D1 0.2500000 sec
d11 0.0100000 sec
d16 0.0002000 sec
d17 0.0002000 sec
DELTA 0.0000000 sec
NUC1 13C
NUC2 1H
MAGNET 0.0150000 sec
MCHX 0.0150000 sec
P2 11.00 usec

===== CHANNEL F1 =====
NUC1 13C
P1 12.50 usec
PL1 5.00 dB
P2 2000.00 usec
PL2 120.00 dB
P4 1.00 dB
P4L 1.00 dB
SP01 125.7942548 MHz
SP1 3.20 dB
SP2 3.20 dB
CTP6 0.5.12.1
STAND CT60000.1
SFOF1 0.00 Hz
SFOF2 0.00 Hz

===== CHANNEL F2 =====
NUC2 1H
P1 1.00 usec
PL1 1.60 dB
P2 24.60 dB
P4 24.60 dB
SP02 500.225011 MHz

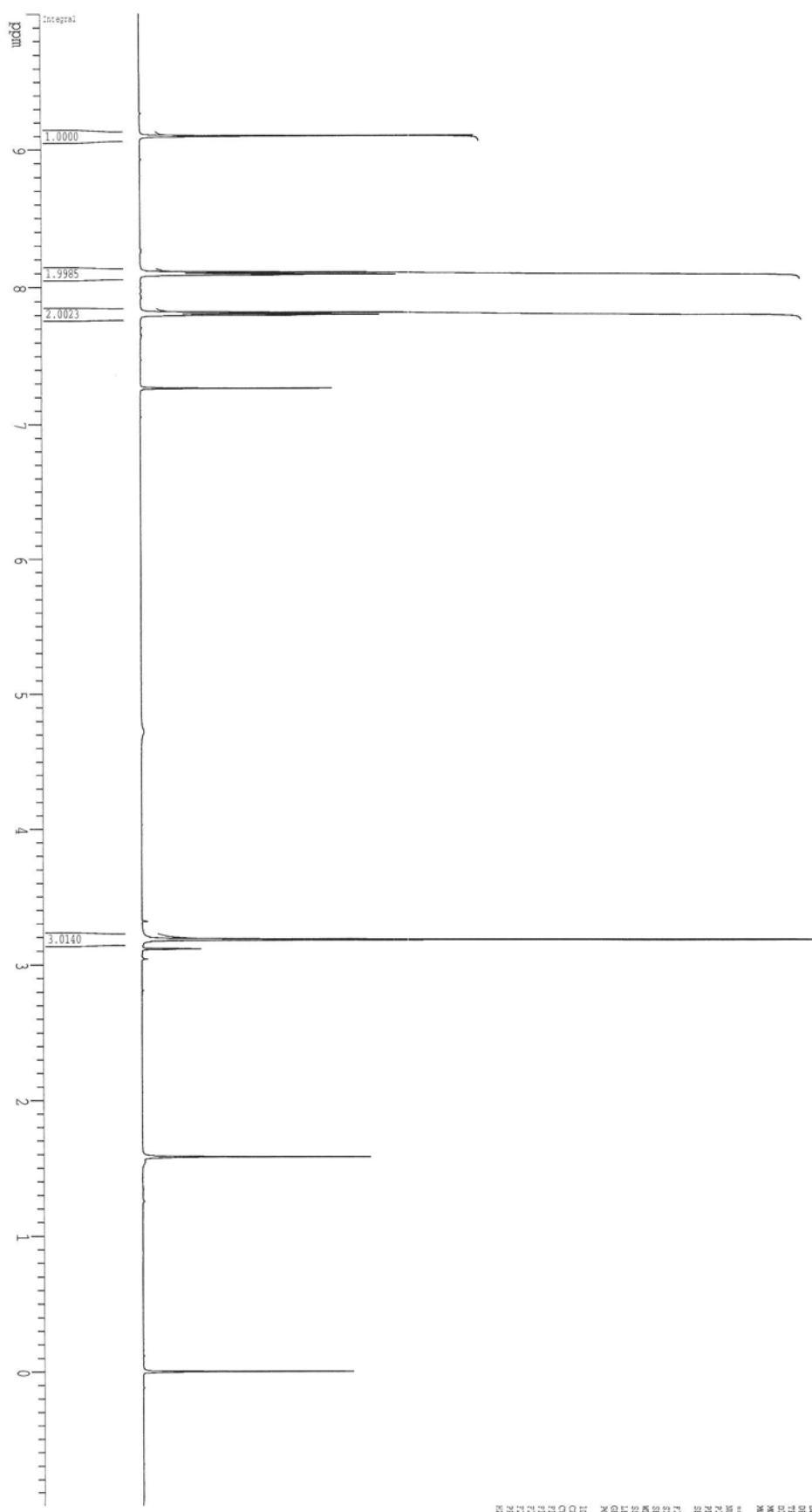
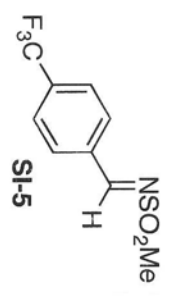
===== GRADIENT CHANNEL =====
GNAME SHINE-100
GPRG1 SHINE-100
GPR2 0.00 %
GPR3 0.00 %
GPR4 0.00 %
GPR5 0.00 %
GPR6 0.00 %
GPR7 0.00 %
GPR8 0.00 %
GPR9 0.00 %
GPR10 0.00 %
GPR11 0.00 %
GPR12 0.00 %
GPR13 0.00 %
GPR14 0.00 %
GPR15 0.00 %
GPR16 0.00 %
GPR17 0.00 %
GPR18 0.00 %
GPR19 0.00 %
GPR20 0.00 %
GPR21 0.00 %
GPR22 0.00 %
GPR23 0.00 %
GPR24 0.00 %
GPR25 0.00 %
GPR26 0.00 %
GPR27 0.00 %
GPR28 0.00 %
GPR29 0.00 %
GPR30 0.00 %
GPR31 0.00 %
GPR32 0.00 %
GPR33 0.00 %
GPR34 0.00 %
GPR35 0.00 %
GPR36 0.00 %
GPR37 0.00 %
GPR38 0.00 %
GPR39 0.00 %
GPR40 0.00 %
GPR41 0.00 %
GPR42 0.00 %
GPR43 0.00 %
GPR44 0.00 %
GPR45 0.00 %
GPR46 0.00 %
GPR47 0.00 %
GPR48 0.00 %
GPR49 0.00 %
GPR50 0.00 %
GPR51 0.00 %
GPR52 0.00 %
GPR53 0.00 %
GPR54 0.00 %
GPR55 0.00 %
GPR56 0.00 %
GPR57 0.00 %
GPR58 0.00 %
GPR59 0.00 %
GPR60 0.00 %
GPR61 0.00 %
GPR62 0.00 %
GPR63 0.00 %
GPR64 0.00 %
GPR65 0.00 %
GPR66 0.00 %
GPR67 0.00 %
GPR68 0.00 %
GPR69 0.00 %
GPR70 0.00 %
GPR71 0.00 %
GPR72 0.00 %
GPR73 0.00 %
GPR74 0.00 %
GPR75 0.00 %
GPR76 0.00 %
GPR77 0.00 %
GPR78 0.00 %
GPR79 0.00 %
GPR80 0.00 %
GPR81 0.00 %
GPR82 0.00 %
GPR83 0.00 %
GPR84 0.00 %
GPR85 0.00 %
GPR86 0.00 %
GPR87 0.00 %
GPR88 0.00 %
GPR89 0.00 %
GPR90 0.00 %
GPR91 0.00 %
GPR92 0.00 %
GPR93 0.00 %
GPR94 0.00 %
GPR95 0.00 %
GPR96 0.00 %
GPR97 0.00 %
GPR98 0.00 %
GPR99 0.00 %
GPR100 0.00 %

F2 - Processing parameters
SI 65536
SF 125.7803988 MHz
WDW EM
SSB 0
GB 0
CB 0
PC 2.00

ID NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 210.000 MHz
F1 261.518 MHz
F2P -10.000 MHz
F2 -1257.80 Hz
FREQM 9.64912 MHz/cm
HQM 1213.67053 Hz/cm

¹H spectrum

ppm



Current Data Parameters
NAME: 4-((4-fluorophenyl)diazenyl)benzoic acid
EXPNO: 3
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20091121
Time: 8:20
INSTRUM: spect
PROBHD: 5 mm QNP1H-1H
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 8
DS: 2
SWH: 801.420 MHz
FIDRES: 0.1000000 Hz
AQ: 5.0399714 sec
RG: 9
BW: 62.400 kHz
C4: 4.00
TE: 298.2 K
T2: 298.2 K
T2RHO: 0.1000000 sec
NUC1: 1H
NUC2: 1H
ACQ: 0.1000000 sec
===== CHANNEL f1 =====
NUC1: 1H
P1: 12.50 usec
PL1: 0.00 dB
FREQ: 500.136015 MHz
===== CHANNEL f2 =====
NUC2: 13C
P2: 12.50 usec
PL2: 0.00 dB
FREQ: 125.760150 MHz
===== Processing parameters =====
SI: 65536
SF: 500.136015 MHz
WDW: EM
SSB: 0
LB: 0.10 Hz
GB: 0
PC: 4.00
===== 1D NMR plot parameters =====
CX: 22.00 cm
CT: 15.00 cm
CT2: 10.00 cm
F1: 500.136015 MHz
F2: 125.760150 MHz
F2F: -1.000 MHz
F2F2: 125.760150 MHz
F2F2F: 125.760150 MHz
F2F2F2: 125.760150 MHz

