

Supporting Information

***N*-Heterocyclic Carbene-Catalysed Intramolecular Hydroacylation to Form Basic**

Nitrogen-Containing Heterocycles

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General Experimental Details

All air-sensitive procedures were conducted under inert atmosphere in a nitrogen-filled dry box or by standard Schlenk techniques. All reactions were performed under an atmosphere of nitrogen unless otherwise stated. All glassware for moisture sensitive

reactions was dried at 140 °C in an oven. Tetrahydrofuran, methylene chloride and *N,N*-dimethylformamide were degassed by purging with argon for 45 minutes and dried with a solvent purification system by passing through a one-meter column of activated alumina. Anhydrous 1,4-dioxane was purchased from Aldrich. Flash column chromatography was performed on SiliFlash® P60 silica gel (40-63 μm, 60Å) or using a Teledyne Isco Combiflash® Rf system with RediSep Gold™ columns using hexanes/ethyl acetate or dichloromethane/methanol mixtures as eluents. Reaction products were visualized on TLC by UV light or by staining with KMnO₄.

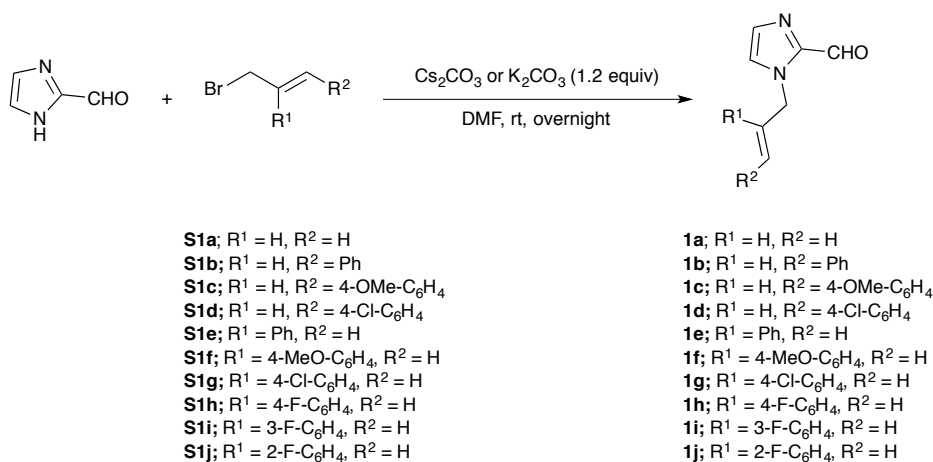
HRMS (ESI) analysis was performed at the Iowa State University Chemical Instrumentation Facility on an Agilent 6540 QTOF spectrometer. NMR spectra were acquired on Varian MR-400 and Bruker Avance III 600 spectrometers at the Iowa State University Chemical Instrumentation Facility. Chemical shifts are reported in ppm relative to a residual solvent peak (CDCl₃ = 7.26 ppm for ¹H and 77.16 ppm for ¹³C, DMSO-*d*₆ = 2.50 for ¹H and 39.52 for ¹³C). ¹⁹F NMR shifts are reported in ppm relative to trifluoroacetic acid as an external standard (F₃CCO₂H = -76.55 ppm). Coupling constants are reporting in hertz

Materials

(*E*)-1-(3-Bromoprop-1-en-1-yl)-4-methoxybenzene (**S1c**), (*E*)-1-(3-Bromoprop-1-en-2-yl)-4-chlorobenzene (**S1d**) were synthesized according to reported literature procedures.¹ 1-(3-Bromoprop-1-en-2-yl)-4-fluorobenzene (**S1h**), 1-(3-bromoprop-1-en-2-yl)-4-chlorobenzene (**S1g**), 1-(3-bromoprop-1-en-2-yl)-4-methoxybenzene (**S1f**), 1-(3-bromoprop-1-en-2-yl)-3-fluorobenzene (**S1i**), 1(3-bromoprop-1-en-2-yl)-2-fluorobenzene (**S1j**), and (3-bromoprop-1-en-2-yl)benzene (**S1e**) were synthesized according to a literature procedure.² (1*H*-Benzo[*d*]imidazol-2-yl)methanol and (5,6-dimethyl-1*H*-

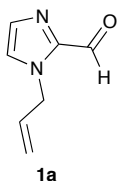
benzo[*d*]imidazol-2-yl)methanol were synthesized according to a literature procedure.³ Cinnamyl bromide (**S1b**), allyl bromide (**S1a**), activated manganese dioxide, anhydrous 1,4-dioxane, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) were purchased from Aldrich and used without further purification. Imidazole-2-carboxaldehyde was purchased from AK Scientific and used without further purification. Triazolium chloride **2** was synthesized according to a literature procedure.⁴ Triazolium tetrafluoroborate **7** was synthesized according to a literature procedure.⁵

General Procedure A: Synthesis of *N*-allylimidazole-2-carboxaldehydes (**1a-j**):

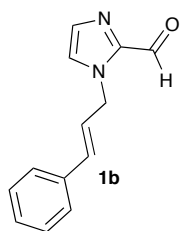


N-Allylimidazole-2-carboxaldehydes (**1a-j**) were prepared according to a modified literature procedure from the appropriate allyl bromides (**S1a-j**) and imidazole-2-carboxaldehyde.⁶ To the appropriate *N*-allylimidazole-carboxaldehyde (1.0 equiv) and Cs₂CO₃ or K₂CO₃ (1.2 equiv) was added DMF (0.27 M). The resulting mixture was stirred at room temperature for 0.5 h. The appropriate allyl bromide (1.2 equiv) was added dropwise. The mixture was stirred at room temperature until the reaction was judged to be complete by thin-layer chromatography. Water was added to the reaction mixture and the resulting solution was extracted with EtOAc (3x). The combined organic layers were

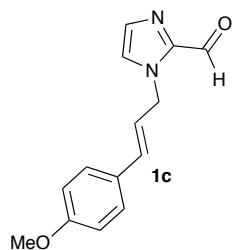
washed with water and brine, dried over Na₂SO₄, and concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (hexane:EtOAc) to give the appropriate *N*-allylimidazole-2-carboxaldehyde (**1a-j**).



1-allyl-1*H*-imidazole-2-carboxaldehyde (1a): Prepared according to general procedure A from imidazole-2-carboxaldehyde (0.500 g, 5.20 mmol) and allyl bromide **S1a** (0.674 mL, 7.80 mmol). The crude reaction mixture was purified by flash column chromatography (90:10 hexane:EtOAc) to give **1a** as a brown oil in 49% yield (350 mg, 2.54 mmol) ¹H NMR (400 MHz, CDCl₃) δ 4.96 (d, *J* = 6.0 Hz, 2H), 5.02 (dd, *J* = 16.0, 0.8 Hz, 1H), 5.17 (dd, *J* = 10.4, 0.8 Hz, 1H), 5.89 (ddt, *J* = 16.0, 10.4, 6.0 Hz, 1H), 7.11 (app s, 1H), 7.21 (app s, 1H), 9.72 (s, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 49.7, 118.5, 126.0, 131.6, 132.4, 143.1, 181.9. HRMS (ESI): Calcd. for C₇H₉N₂O⁺ ([M+H]⁺): 137.0709, Found: 137.0718.



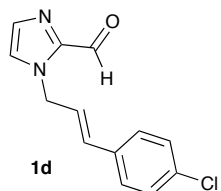
1-cinnamyl-1*H*-imidazole-2-carboxaldehyde (1b): Prepared according to general procedure A from imidazole-2-carboxaldehyde (1.44 g, 15.0 mmol) and cinnamyl bromide **S1b** (3.31 mL, 22.5 mmol). The crude reaction mixture was purified by flash column chromatography (70:30 hexanes:EtOAc) to give **1b** as a light yellow solid in 51% yield (1.63 g, 7.68 mmol). ¹H NMR (400 MHz, CDCl₃) δ 5.12 (dd, *J* = 6.4, 1.2 Hz, 2H), 6.22 (dt, *J* = 15.6, 6.4 Hz, 1H), 6.47 (d, *J* = 15.6 Hz, 1H), 7.16 (app s, 1H), 7.18-7.30 (m, 6H), 9.77 (s, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 49.5, 123.3, 126.0, 126.7, 128.4, 128.8, 131.9, 134.4, 135.8, 143.3, 182.3. HRMS (ESI): Calcd. for C₁₃H₁₃N₂O⁺ ([M+H]⁺): 213.1022, Found: 213.1026.



(E)-1-(3-(4-methoxyphenyl)allyl)-1H-imidazole-2-carboxaldehyde

(1c): Prepared according to general procedure A from imidazole-2-carboxaldehyde (62.0 mg, 0.640 mmol), and *trans-p*-methoxycinnamyl bromide **S1c** (0.219 g, 0.970 mmol). The crude reaction mixture was

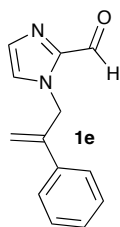
purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **1c** as a brown oil in 39% yield (0.060 g, 0.25 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 3.73 (s, 3H), 5.09 (d, *J* = 6.0 Hz, 2H), 6.09 (dt, *J* = 15.6, 6.0 Hz, 1H), 6.44 (d, *J* = 15.6 Hz, 1H), 6.78 (d, *J* = 8.0 Hz, 2H), 7.14-7.30 (m, 4H), 9.77 (s, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 49.7, 55.4, 114.2, 120.9, 125.9, 128.0, 128.5, 131.9, 134.0, 143.3, 159.9, 182.3. **HRMS** (ESI): Calcd. for C₁₄H₁₅N₂O₂⁺ ([M+H]⁺): 243.1128, Found: 243.1135.



(E)-1-(3-(4-chlorophenyl)allyl)-1H-imidazole-2-carboxaldehyde

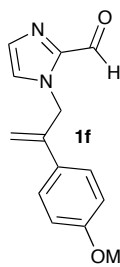
(1d): Prepared according to general procedure A from imidazole-2-carboxaldehyde (0.140 g, 1.44 mmol) and *trans-p*-chlorocinnamyl bromide **S1d** (0.500 g, 2.16 mmol). The crude reaction mixture was purified by flash

column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **1d** as an off-white solid in 23% yield (0.082 g, 0.33 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 5.11 (d, *J* = 8.0 Hz, 2H), 6.18 (dt, *J* = 16.0, 8.0 Hz, 1H), 6.38 (d, *J* = 16.0 Hz, 1H), 7.15 (app s, 1H), 7.17-7.22 (m, 4H), 7.25 (app s, 1H), 9.77 (s, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 49.4, 124.1, 126.0, 127.9, 129.0, 132.0, 132.9, 134.1, 134.3, 143.3, 182.3. **HRMS** (ESI): Calcd. for C₁₃H₁₂ClN₂O⁺ ([M+H]⁺): 247.0633, Found: 247.0642.



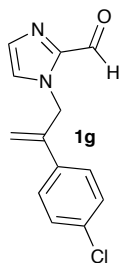
1-(2-phenylallyl)-1H-imidazole-2-carboxaldehyde (1e): Prepared according to general procedure A from imidazole-2-carboxaldehyde (0.200 g, 2.08 mmol) and 2-phenylallyl bromide **S1e** (0.615 g, 3.12 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to

90:10 hexanes:EtOAc) to give **1e** as a brown oil in 65% yield (0.286 g, 1.35 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 4.81 (s, 1H), 5.38 (app s, 3H), 7.05 (app s, 1H), 7.16 (app s, 1H), 7.18-7.28 (m, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.31 (dd, *J* = 8.0, 1.2 Hz, 2H), 9.74 (s, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 50.8, 115.2, 126.2, 126.3, 128.5, 128.7, 131.8, 137.8, 143.3, 143.6, 182.2. **HRMS** (ESI): Calcd. for C₁₃H₁₃N₂O⁺ ([M+H]⁺): 213.1022, Found: 213.1020



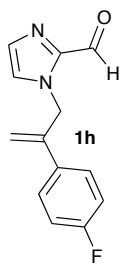
1-(2-(4-methoxyphenyl)allyl)-1H-imidazole-2-carboxaldehyde (1f):

Prepared according to general procedure A from imidazole-2-carbaldehyde (0.455 g, 4.74 mmol) and 1-(3-bromoprop-1-en-2-yl)-4-methoxybenzene **S1f** (1.29g, 5.68 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **1f** as a light-brown solid in 12% yield (0.138 g, 0.570 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 3.79 (s, 3H), 4.85 (s, 1H), 5.41 (s, 1H), 5.44 (s, 2H), 6.84 (d, *J* = 8.4 Hz, 2H), 7.13 (app s, 1H), 7.24 (app s, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 9.83 (s, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 51.0, 55.4, 114.0, 114.1, 126.3, 127.4, 130.2, 131.8, 142.9, 143.4, 159.9, 182.3. **HRMS** (ESI): Calcd. for C₁₄H₁₅N₂O₂⁺ ([M+H]⁺): 243.1128, Found:243.1127



1-(2-(4-chlorophenyl)allyl)-1H-imidazole-2-carboxaldehyde (1g):

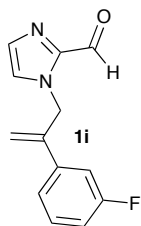
Prepared according to general procedure A from imidazole-2-carboxaldehyde (0.390 g, 4.11 mmol) and 1-(3-bromoprop-1-en-2-yl)-4-chlorobenzene **S1g** (1.14 g, 4.93 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **1g** as a off-white solid in 30% yield (0.300 g, 1.23 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 4.94 (s, 1H), 5.45 (s, 2H), 5.47 (s, 1H), 7.14 (app s, 1H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.27 (app s, 1H), 7.46 (d, *J* = 8.4 Hz, 2H), 9.82 (s, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 50.7, 115.9, 122.7, 126.3, 127.9, 131.9, 132.0, 136.8, 142.8, 143.3, 182.3. **HRMS** (ESI): Calcd. for C₁₃H₁₂ClN₂O⁺ ([M+H]⁺): 247.0633, Found: 247.0624



1-(2-(4-fluorophenyl)allyl)-1H-imidazole-2-carboxaldehyde (1h):

Prepared according to general procedure A from imidazole-2-carboxaldehyde (0.306 g, 3.19 mmol) and 1-(3-bromoprop-1-en-2-yl)-4-fluorobenzene **S1h** (0.823 g, 3.83 mmol). The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **1h** as a brown amorphous solid in 23% yield (0.168 g, 0.730 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 4.88 (s, 1H), 5.40 (s, 1H), 5.43 (s, 2H), 7.00 (dd, *J* = 8.8, 8.8 Hz, 2H), 7.13 (app s, 1H), 7.25 (d, *J* = 0.8 Hz, 1H), 7.35 (dd, *J* = 8.8, 5.2 Hz, 2H), 9.81 (d, *J* = 1.2 Hz, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 50.9, 115.3 (d, *J* = 1.2 Hz, 2C), 115.7 (d, *J* = 21.8 Hz, 2C), 126.3, 128.0 (d, *J* = 8 Hz, 1C), 131.9, 133.9 (d, *J* = 3.4 Hz, 1C), 142.8, 143.3, 162.9 (d, *J* = 249.5 Hz, 1C), 182.3. **¹⁹F NMR** (CDCl₃, 376 MHz): δ -113.48 (m, 1F). **HRMS** (ESI): Calcd. for C₁₃H₁₂FN₂O⁺ ([M+H]⁺): 231.0928, Found: 231.0922

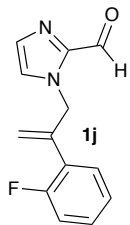
1-(2-(3-fluorophenyl)allyl)-1H-imidazole-2-carboxaldehyde (1i):



Prepared according to general procedure A from imidazole-2-carboxaldehyde (0.291 g, 3.03 mmol) and 1-(3-bromoprop-1-en-2-yl)-3-fluorobenzene **S1i** (0.784 g, 3.64 mmol). The crude reaction mixture was purified by flash column

chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **1i** as a brown oil in 28% yield (0.195 g, 0.846 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 4.94 (s, 1H), 5.46 (s, 2H), 5.50 (s, 1H), 7.00 (m, 1H), 7.10 (app dt, *J* = 15.6, 2.4 Hz, 1H), 7.15 (app s, 1H), 7.18(ddd, *J* = 7.6, 1.6, 0.8 Hz, 1H), 7.28 (d, *J* = 0.8 Hz, 1H), 7.28-7.34 (m, 1H), 9.83 (d, *J* = 0.8 Hz, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 50.6, 113.4 (d, *J* = 22.2 Hz, 1C), 115.4 (d, *J* = 21.2 Hz, 1C), 116.1, 121.9 (d, *J* = 3.0 Hz, 1C), 126.3, 130.3 (d, *J* = 8.4 Hz, 1C), 131.9, 140.1 (d, *J* = 7.6 Hz, 1C), 142.7 (d, *J* = 2.2 Hz, 1C), 143.3, 162.9 (d, *J* = 247.6 Hz, 1C), 182.2. **¹⁹F NMR** (CDCl₃ 376 MHz): δ -112.71 (m, 1F). **HRMS** (ESI): Calcd. for C₁₃H₁₂FN₂O⁺ ([M+H]⁺): 231.0928, Found: 231.0922

1(2-(2-fluorophenyl)allyl)-1H-imidazole-2-carbaldehyde (1j):

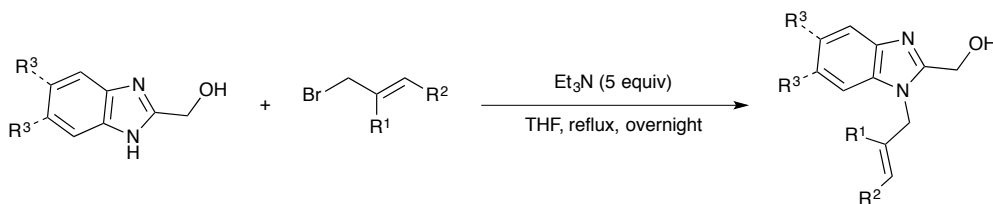


Prepared according to general procedure A from imidazole-2-carbaldehyde (0.570 g, 5.88 mmol) and 1-(3-bromoprop-1-en-2-yl)-2-fluorobenzene **S1j** (1.52 g, 7.01 mmol). The crude reaction mixture was purified by flash column

chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **1j** as a brown oil in 15% yield (0.200 g, 0.866 mmol). **¹H NMR** (400 MHz, CDCl₃) δ 5.12 (s, 1H), 5.38 (s, 1H), 5.42 (s, 2H), 7.02-7.12 (m, 2H), 7.14 (s, 1H), 7.20-7.32 (m, 3H), 9.80 (d, *J* = 0.8 Hz, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 51.4, 115.9 (d, *J* = 22.4 Hz, 1C), 118.6 (d, *J* = 2.2 Hz, 1C), 124.5 (d, *J* = 3.4 Hz, 1C), 126.2 (d, *J* = 14.4 Hz, 1C), 126.6, 130.1 (d, *J* = 8.4 Hz, 1C), 130.2 (d, *J* = 3.8 Hz,

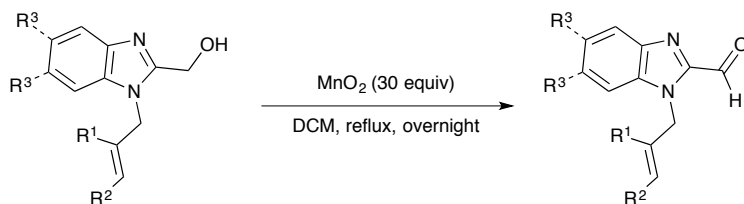
1C), 131.7, 140.0, 143.4, 159.9 (d, $J = 248.6$ Hz, 1C), 181.9. ^{19}F NMR (CDCl_3 , 376 MHz): δ -115.31 (m, 1F). HRMS (ESI): Calcd. for $\text{C}_{13}\text{H}_{12}\text{FN}_2\text{O}^+$ ($[\text{M}+\text{H}]^+$): 231.0928, Found: 231.0926.

General Procedure B: Synthesis of *N*-allylbenzimidazole-2-carboxaldehyde (**5a-f**)



S1a; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{H}$
S1b; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{Ph}$
S1c; $\text{R}^1 = \text{H}$, $\text{R}^2 = 4\text{-Cl-C}_6\text{H}_4$
S1d; $\text{R}^1 = \text{Ph}$, $\text{R}^2 = \text{H}$

S2a; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{H}$
S2b; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{Ph}$, $\text{R}^3 = \text{H}$
S2c; $\text{R}^1 = \text{H}$, $\text{R}^2 = 4\text{-Cl-C}_6\text{H}_4$, $\text{R}^3 = \text{H}$
S2d; $\text{R}^1 = \text{Ph}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{H}$
S2e; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{CH}_3$
S2f; $\text{R}^1 = \text{H}$, $\text{R}^2 = 4\text{-Cl-C}_6\text{H}_4$, $\text{R}^3 = \text{CH}_3$

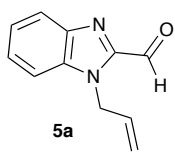


S2a; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{H}$
S2b; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{Ph}$, $\text{R}^3 = \text{H}$
S2c; $\text{R}^1 = \text{H}$, $\text{R}^2 = 4\text{-Cl-C}_6\text{H}_4$, $\text{R}^3 = \text{H}$
S2d; $\text{R}^1 = \text{Ph}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{H}$
S2e; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{CH}_3$
S2f; $\text{R}^1 = \text{H}$, $\text{R}^2 = 4\text{-Cl-C}_6\text{H}_4$, $\text{R}^3 = \text{CH}_3$

5a; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{H}$
5b; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{Ph}$, $\text{R}^3 = \text{H}$
5c; $\text{R}^1 = \text{H}$, $\text{R}^2 = 4\text{-Cl-C}_6\text{H}_4$, $\text{R}^3 = \text{H}$
5d; $\text{R}^1 = \text{Ph}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{H}$
5e; $\text{R}^1 = \text{H}$, $\text{R}^2 = \text{H}$, $\text{R}^3 = \text{CH}_3$
5f; $\text{R}^1 = \text{H}$, $\text{R}^2 = 4\text{-Cl-C}_6\text{H}_4$, $\text{R}^3 = \text{CH}_3$

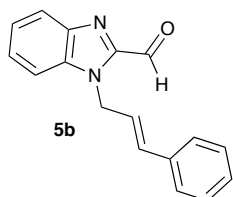
N-allylbenzimidazole-2-carboxaldehydes (**5a-f**) were prepared according to a modified literature procedure from (1*H*-benzo[*d*]imidazol-2-yl)methanol or (5,6-dimethyl-1*H*-benzo[*d*]imidazol-2-yl)methanol.⁷ To a solution of (1*H*-benzo[*d*]imidazol-2-yl)methanol or (5,6-dimethyl-1*H*-benzo[*d*]imidazol-2-yl)methanol in THF (0.3M) was added Et_3N (5 equiv). The solution was refluxed for 1 h. The appropriate allyl bromide (1.2-5.0 equiv)(**S1a-d**) was added, and the mixture refluxed overnight. Water was added to the cooled reaction mixture. The resulting mixture was extracted with Et_2O (3x). The organic layer was dried (Na_2SO_4) and concentrated under reduced pressure to afford the

appropriate crude *N*-allylbenzimidazol-2-methanol (**S2a-f**). To a solution of the crude *N*-allylbenzimidazol-2-methanol (1.00 equiv) in DCM (4 mM) was added activated MnO₂ (30.0 equiv). The resulting mixture was refluxed overnight. The cooled reaction mixture was filtered through a plug of celite. The combined organic layers were concentrated under reduced pressure. The crude product was purified by flash column chromatography on silica gel (DCM:EtOAc or hexanes:EtOAc) to give the appropriate *N*-allylbenzimidazole-2-carboxaldehyde (**5a-f**).



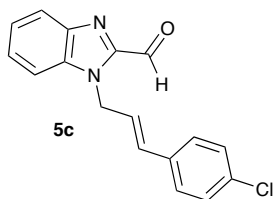
1-allyl-1H-benzo[d]imidazole-2-carboxaldehyde (5a): Prepared according to general procedure B from (1*H*-benzo[d]imidazol-2-yl)methanol (0.500 g, 3.37 mmol) and allyl bromide **S1a** (291 μ L, 3.37

mmol) to give the crude product **S2a** (0.201 g, 1.06 mmol). Oxidation with MnO₂ (0.929 mg, 10.69 mmol) generated crude **5a**. The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes EtOAc) to give **5a** as an orange solid in 20% yield over two-steps (0.128 g, 0.687 mmol). ¹H NMR (600 MHz, CDCl₃) δ 5.03 (dd, *J* = 16.8, 0.6 Hz, 1H), 5.19 (dd, *J* = 10.2, 0.6 Hz, 1H), 5.25 (app dt, *J* = 5.4, 1.2 Hz, 2H), 5.98 (ddt, *J* = 16.8, 10.2, 5.4 Hz, 1H), 7.37-7.40 (m, 1H), 7.45-7.46 (m, 2H), 7.93 (d, *J* = 8.4 Hz, 1H), 10.10 (s, 1H). ¹³C NMR (151 MHz, CDCl₃) δ 46.9, 111.2, 117.8, 122.5, 124.3, 127.0, 132.1, 136.4, 143.0, 145.8, 184.9 HRMS (ESI): Calcd. for C₁₁H₁₁N₂O⁺ ([M+H]⁺): 187.0866, Found: 187.0872



1-cinnamyl-1H-benzo[d]imidazole-2-carboxaldehyde (5b): Prepared according to general procedure B from (1*H*-benzo[d]imidazol-2-yl)methanol (0.801 g, 5.41 mmol) and **S1b** (4.00 mL, 27.0 mmol) to

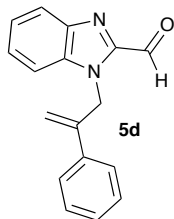
give the crude product **S2b** (0.258 g, 0.980 mmol). Oxidation with MnO₂ (2.55 g, 29.3 mmol) generated crude **5b**. The crude reaction mixture was purified by flash column chromatography (100:0 DCM:EtOAc to 95:5 DCM:EtOAc) to give **5b** as a light-orange solid in 9% yield over two-steps (0.132 g, 0.500 mmol). **¹H NMR** (600 MHz, CDCl₃) δ 5.43 (dd, *J* = 6.0, 1.2, Hz, 2H), 6.34 (dt, *J* = 16.2, 6.0 Hz, 1H), 6.56 (d, *J* = 16.2 Hz, 1H), 7.25 (t, *J* = 7.2 Hz, 1H), 7.30 (t, *J* = 7.2 Hz, 2H), 7.33 (d, *J* = 7.2 Hz, 2H), 7.44 (ddd, *J* = 15.6, 8.4, 1.2 Hz, 1H), 7.50 (ddd, *J* = 15.6, 8.4, 1.2 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 10.17 (s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 46.7, 111.2, 122.5, 123.2, 124.3, 126.6, 127.1, 128.2, 128.6, 133.4, 135.8, 136.3, 143.0, 145.8, 184.9. **HRMS** (ESI): Calcd. for C₁₇H₁₅N₂O⁺ ([M+H]⁺): 263.1179, Found: 263.1181.



(E)-1-(3-(4-chlorophenyl)allyl)-1H-benzo[d]imidazole-2-carboxaldehyde (5c): Prepared according to general procedure B from (1H-benzo[d]imidazol-2-yl)methanol (0.452 g, 3.05 mmol) and

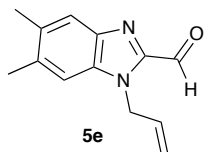
S1c (3.53 g, 15.2 mmol) to give the crude product **S2c** (0.227 g, 0.765 mmol). Oxidation with MnO₂ (1.98 g, 22.8 mmol) generated crude **5c**. The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 85:15 hexanes:EtOAc) to give **5c** as a white solid in 7% yield over two-steps (0.059 g, 0.20 mmol). **¹H NMR** (600 MHz, CDCl₃) δ 5.40 (dd, *J* = 6.0, 1.2 Hz, 2H), 6.29 (dt, *J* = 15.6, 6.0 Hz, 1H), 6.46 (d, *J* = 15.6 Hz, 1H), 7.20-7.24 (m, 4H), 7.41 (ddd, *J* = 15.0, 8.4, 1.2 Hz, 1H), 7.48, (ddd, *J* = 15.0, 8.4, 1.2 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.4 Hz, 1H), 10.13 (s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 46.5, 111.1, 122.7, 123.9, 124.4, 127.2, 127.9, 128.9, 132.1, 133.9, 134.4, 136.4,

143.0, 145.8, 185.1. **HRMS** (ESI): Calcd. for $C_{17}H_{14}ClN_2O^+$ ($[M+H]^+$): 297.0789, Found: 297.0789.



1-(2-phenylallyl)-1H-benzo[d]imidazole-2-carboxaldehyde (5d):

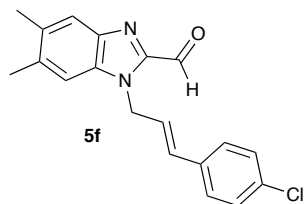
Prepared according to general procedure B from (1H-benzo[d]imidazol-2-yl)methanol (0.725 g, 4.89 mmol) and **S1d** (4.82 g, 24.5 mmol) to give the crude product **S2d** (0.437 g, 1.65 mmol), Oxidation with MnO_2 (4.31 g, 49.6 mmol) generate crude **5d**. The crude reaction mixture was purified by flash column chromatography (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to give **5d** as an orange solid in 16% yield over two-steps (0.210 g, 0.801 mmol). **1H NMR** (600 MHz, $CDCl_3$) δ 4.51 (s, 1H), 5.33 (s, 1H), 5.67 (s, 2H), 7.30-7.38 (m, 3H), 7.38-7.42 (m, 1H), 7.43-7.48 (m, 4H), 7.94 (d, $J = 8.4$ Hz, 1H), 10.11 (s, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 48.2, 111.6, 113.1, 122.5, 124.4, 126.4, 127.2, 128.5, 128.7, 136.7, 138.5, 142.9, 143.3, 146.0, 184.9. **HRMS** (ESI): Calcd. for $C_{17}H_{15}N_2O^+$ ($[M+H]^+$): 263.1179, Found: 263.1184.



1-allyl-5,6-dimethyl-1H-benzo[d]imidazole-2-carboxaldehyde (5e):

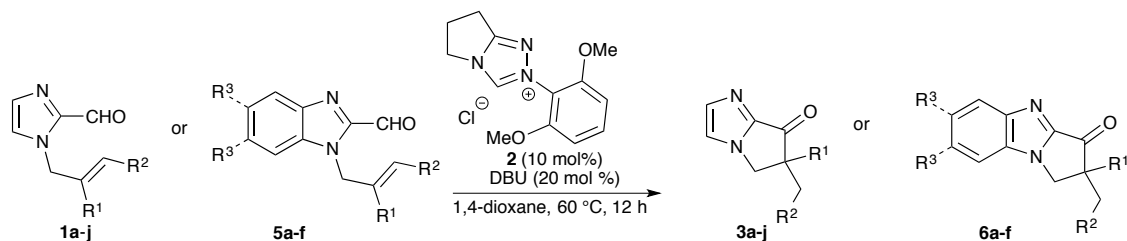
Prepared according to general procedure B from (5,6-dimethyl-1H-benzo[d]imidazol-2-yl)methanol (1.00 g, 5.67 mmol) and **S1a** (0.589 ml, 6.81 mmol) to give the crude product **S2e** (0.289 g, 1.35 mmol). Oxidation with MnO_2 (3.55 g, 41.9 mmol) generated crude **5e**. The crude reaction mixture was purified by flash column chromatography (100:0 DCM:EtOAc to 90:10 DCM:EtOAc) to give **5e** as a white solid in 4% yield over two-steps (0.047 g, 0.22 mmol). **1H NMR** (400 MHz, $CDCl_3$) δ 2.39 (s, 3H), 2.42 (s, 3H), 5.00 (dd, $J = 17.2, 0.8$ Hz, 1H), 5.18 (dd, $J = 10.4, 0.8$ Hz, 1H), 5.21 (m, 2H), 5.93-6.02 (m, 1H), 7.20 (s, 1H), 7.66 (s, 1H), 10.05 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 20.6, 21.2,

46.9, 110.9, 117.5, 121.9, 132.3, 134.0, 135.2, 137.5, 141.9, 145.4, 184.7. **HRMS** (ESI): Calcd. for $C_{13}H_{15}N_2O^+$ ($[M+H]^+$): 215.1179, Found: 215.1184.



(E)-1-(3-(4-chlorophenyl)allyl)-5,6-dimethyl-1H-benzo[d]imidazole-2-carboxaldehyde (5f): Prepared according to general procedure B from (5,6-dimethyl-1H-benzo[d]imidazol-2-yl)methanol (1.00 g, 5.74 mmol) and **S1c** (1.58 g, 6.81 mmol) to give the crude product **S2f** (0.330 g, 1.01 mmol). Oxidation with MnO_2 (2.65 g, 30.5 mmol) generated crude **5f**. The crude reaction mixture was purified by flash column chromatography (100:0 DCM:EtOAc to 90:10 DCM:EtOAc) to give **5f** as a yellow oil in 3% yield over two-steps (0.050 g, 0.15 mmol). **1H NMR** (400 MHz, $CDCl_3$) δ 2.40 (s, 3H), 2.42 (s, 3H), 5.34 (d, $J = 5.6$ Hz, 2H), 6.28 (dt, $J = 16.0, 5.6$ Hz, 1H), 6.41 (d, $J = 16$ Hz, 1H), 7.18-7.23 (m, 4H), 7.25 (s, 1H), 7.68 (s, 1H), 10.07 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 20.6, 21.3, 46.3, 110.7, 122.0, 124.2, 127.8, 128.8, 131.7, 133.8, 134.1, 134.5, 135.1, 137.6, 141.9, 145.3, 184.7. **HRMS** (ESI): Calcd. for $C_{19}H_{18}ClN_2O^+$ ($[M+H]^+$): 325.1102, Found: 325.1093

General Procedure C: Synthesis of dihydropyrroloimidazolones (3a-j), dihydrobenzopyrroloimidazolones (6a-f)



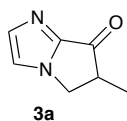
1a; R¹ = H, R² = H
1b; R¹ = H, R² = Ph
1c; R¹ = H, R² = 4-OMe-C₆H₄
1d; R¹ = H, R² = 4-Cl-C₆H₄
1e; R¹ = Ph, R² = H
1f; R¹ = 4-MeO-C₆H₄, R² = H
1g; R¹ = 4-Cl-C₆H₄, R² = H
1h; R¹ = 4-F-C₆H₄, R² = H
1i; R¹ = 3-F-C₆H₄, R² = H
1j; R¹ = 2-F-C₆H₄, R² = H

5a; R¹ = H, R² = H, R³ = H
5b; R¹ = H, R² = Ph, R³ = H
5c; R¹ = H, R² = 4-Cl-C₆H₄, R³ = H
5d; R¹ = Ph, R² = H, R³ = H
5e; R¹ = H, R² = H, R³ = CH₃
5f; R¹ = H, R² = 4-Cl-C₆H₄, R³ = CH₃

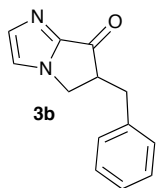
3a; R¹ = H, R² = H
3b; R¹ = H, R² = Ph
3c; R¹ = H, R² = 4-OMe-C₆H₄
3d; R¹ = H, R² = 4-Cl-C₆H₄
3e; R¹ = Ph, R² = H
3f; R¹ = 4-MeO-C₆H₄, R² = H
3g; R¹ = 4-Cl-C₆H₄, R² = H
3h; R¹ = 4-F-C₆H₄, R² = H
3i; R¹ = 3-F-C₆H₄, R² = H
3j; R¹ = 2-F-C₆H₄, R² = H

6a; R¹ = H, R² = H, R³ = H
6b; R¹ = H, R² = Ph, R³ = H
6c; R¹ = H, R² = 4-Cl-C₆H₄, R³ = H
6d; R¹ = Ph, R² = H, R³ = H
6e; R¹ = H, R² = H, R³ = CH₃
6f; R¹ = H, R² = 4-Cl-C₆H₄, R³ = CH₃

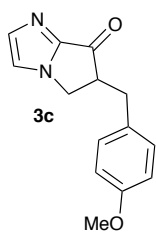
Dihydropyrroloimidazolones (**3a-j**) and dihydrobenzopyrroloimidazolones (**6a-f**) were prepared according to a modified literature procedure from the appropriate carboxaldehyde (**1a-j**) or (**5a-f**).⁴ In a nitrogen-filled glovebox, to a 1-dram vial was added triazolium **2** (0.020 mmol, 0.10 equiv), the appropriate carboxaldehyde **1a-j** or **5a-f** (0.20 mmol, 1.0 equiv), DBU (6 μ L, 0.04 mmol, 0.2 equiv), and 1,4-dioxane (0.4 mL, 0.5 M). The vial was sealed with a teflon-lined septum cap. The reaction vessel was removed from the glovebox and the reaction mixture was stirred at 60 °C for 12 h. The reaction was cooled to room temperature and filtered through a plug of silica gel with EtOAc as eluent. The filtrate was concentrated under reduced pressure. The crude product was purified by flash column silica gel chromatography (hexane:EtOAc) to give the appropriate dihydropyrroloimidazolones (**3a-j**) and dihydrobenzopyrroloimidazolones (**6a-f**).



6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3a): Prepared according to general procedure C from 1-allyl-1H-imidazole-2-carbaldehyde **1a** (0.041 g, 0.30 mmol), DBU (9 μ L, 0.06 mmol) and triazolium **2** (9.0 mg, 0.030 mmol). The crude reaction mixture was purified by column chromatography (100:0 hexane:EtOAc to 90:10 hexane:EtOAc) to afford **3a** in 96% yield (0.039 g, 0.29 mmol) as a yellow oil. **¹H NMR** (600 MHz, CDCl₃) δ 1.40 (d, J = 7.8 Hz, 3H), 3.19-3.24 (m, 1H), 3.92 (dd, J = 12.0, 3.6 Hz, 1H), 4.58 (dd, J = 12.0, 7.8 Hz, 1H), 7.23 (app s, 1H), 7.57 (app s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 15.4, 44.9, 48.7, 120.0, 139.4, 146.5, 190.3. **HRMS** (ESI): Calcd. for C₇H₉N₂O⁺ ([M+H]⁺): 137.0709, Found 137.0716.



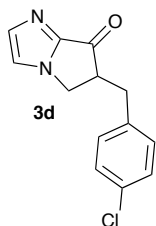
6-benzyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3b): Prepared according to general procedure C from 1-cinnamyl-1H-imidazole-2-carbaldehyde **1b** (0.064 g, 0.30 mmol), DBU (8.97 μ L, 0.0600 mmol) and triazolium **2** (9.0 mg, 0.030 mmol). The crude reaction mixture was purified by flash column chromatography (90:10 hexanes:EtOAc) to afford **3b** in 96% yield (0.061 mg, 0.29 mmol) as an off-white solid. **¹H NMR** (400 MHz, CDCl₃) δ 2.82 (dd, J = 14.0, 10.4 Hz, 1H), 3.35 (dd, J = 14.0, 4.4 Hz, 1H), 3.45 (dddd, J = 10.4, 7.6, 4.4, 4.0 Hz, 1H), 3.98 (dd, J = 12.0, 4.0 Hz, 1H), 4.28 (dd, J = 12.0, 7.6 Hz, 1H), 7.11 (app s, 1H), 7.12-7.27 (m, 5H), 7.52 (app s, 1H). **¹³C NMR** (101 MHz, CDCl₃) δ 36.1, 46.1, 51.5, 120.2, 127.1, 128.9, 129.0, 137.7, 139.5, 146.7, 188.8. **HRMS** (ESI): Calcd. for C₁₃H₁₃N₂O⁺ ([M+H]⁺): 213.1022, Found: 213.1019.



6-(4-methoxybenzyl)-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one

(3c): Prepared according to general procedure C from (*E*)-1-(3-(4-methoxyphenyl)allyl)-1*H*-imidazole-2-carbaldehyde **1c** (0.048 g, 0.20 mmol), DBU (6 μ L, 0.04 mmol) and triazolium **2** (6 mg, 0.02 mmol). The crude

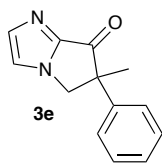
reaction mixture was purified by column chromatography (90:10 hexanes:EtOAc) to afford **3c** in 85% yield (0.041 g, 0.17 mmol) as an off-white solid. **¹H NMR** (600 MHz, CDCl₃) δ 2.87 (dd, $J = 14.4, 9.6$ Hz, 1H), 3.32 (dd, $J = 14.4, 4.8$ Hz, 1H), 3.43-3.49 (m, 1H), 3.77 (s, 3H), 4.03 (dd, $J = 12.0, 3.6$ Hz, 1H), 4.33 (dd, $J = 12.0, 7.8$ Hz, 1H), 6.82 (d, $J = 7.8$ Hz, 2H), 7.11 (d, $J = 7.8$ Hz, 2H), 7.16 (app s, 1H), 7.57 (app s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 35.2, 46.0, 51.7, 55.4, 114.4, 120.1, 129.5, 129.9, 139.5, 146.8, 158.7, 188.9. **HRMS** (ESI): Calcd. for C₁₄H₁₅N₂O₂⁺ ([M+H]⁺): 243.1128, Found 243.1121.



6-(4-chlorobenzyl)-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3d):

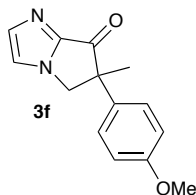
Prepared according to general procedure C from (*E*)-1-(3-(4-chlorophenyl)allyl)-1*H*-imidazole-2-carbaldehyde **1d** (0.049 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol). The crude

reaction mixture was purified by flash column chromatography with (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to afford **3d** in 99% yield (0.049 g, 0.20 mmol) as an off-white solid. **¹H NMR** (600 MHz, CDCl₃) δ 2.88 (dd, $J = 14.4, 10.2$ Hz, 1H), 3.32 (dd, $J = 14.4, 4.2$ Hz, 1H), 3.43-3.49 (m, 1H), 4.00 (dd, $J = 12.0, 4.2$ Hz, 1H), 4.36 (dd, $J = 12.0, 7.8$ Hz, 1H), 7.13 (d, $J = 7.8$ Hz, 2H), 7.17 (app s, 1H), 7.24 (d, $J = 7.8$ Hz, 2H), 7.54 (app s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 35.3, 46.0, 51.2, 120.3, 129.1, 130.2, 132.9, 136.1, 139.5, 146.5, 188.4. **HRMS** (ESI): Calcd. for C₁₃H₁₂ClN₂O⁺ ([M+H]⁺): 247.0633, Found 247.0632.



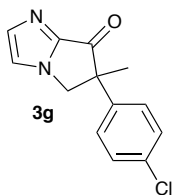
6-methyl-6-phenyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3e):

Prepared according to general procedure C from 1-(2-phenylallyl)-1H-imidazole-2-carbaldehyde **1e** (0.042 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3e** in 99% yield (0.042 g, 0.20 mmol) as an off white solid. **¹H NMR** (600 MHz, CDCl₃) δ 1.78 (s, 3H), 4.42 (d, J = 12.0 Hz, 1H), 4.66 (d, J = 12.0 Hz, 1H), 7.25-7.37 (m, 6H), 7.69 (app s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 23.7, 56.7, 57.2, 120.2, 125.9, 127.7, 129.1, 139.9, 141.3, 145.9, 190.3. **HRMS** (ESI): Calcd. for C₁₃H₁₃N₂O⁺ ([M+H]⁺): 213.1022, Found: 213.1029.



6-(4-methoxyphenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3f): Prepared according to general procedure C from

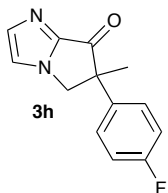
1-(2-(4-methoxyphenyl)allyl)-1H-imidazole-2-carbaldehyde **1f** (0.048 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol), and DBU (6 μ L, 0.04 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3f** in 99% yield (0.048 g, 0.20 mmol) as an off white solid. **¹H NMR** (600 MHz, CDCl₃) δ 1.73 (s, 3H), 3.76 (s, 3H), 4.37 (d, J = 12.0 Hz, 1H), 4.61 (d, J = 12.0 Hz, 1H), 6.84 (d, J = 9.0 Hz, 2H), 7.19 (d, J = 9.0 Hz, 2H), 7.27 (d, J = 0.6 Hz, 1H), 7.65 (d, J = 0.6 Hz, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 23.8, 55.4, 56.1, 57.2, 114.5, 120.1, 127.1, 133.3, 139.8, 146.0, 159.1, 190.6. **HRMS** (ESI): Calcd. for C₁₄H₁₅N₂O₂⁺ ([M+H]⁺): 243.1128, Found: 243.1123.



6-(4-chlorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-

7-one (3g): Prepared according to general procedure C from 1-(2-(4-chlorophenyl)allyl)-1H-imidazole-2-carbaldehyde **1g** (0.049 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol). The crude

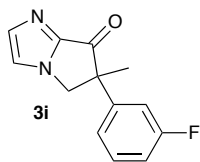
reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3g** 95% yield (0.047 g, 0.19 mmol) as an off white solid. **¹H NMR** (600 MHz, CDCl₃) δ 1.73 (s, 3H), 4.41 (d, J = 12.0 Hz, 1H), 4.60 (d, J = 12.0 Hz, 1H), 7.16 (d, J = 8.4 Hz, 2H), 7.30 (app s, 1H), 7.44 (d, J = 8.4 Hz, 2H), 7.67 (app s, 1H). **¹³C NMR** (151 MHz, CDCl₃) 23.8, 56.3, 56.8, 120.4, 121.8, 127.8, 132.2, 140.2, 140.3, 145.6, 189.7. **HRMS** (ESI): Calcd. for C₁₃H₁₂ClN₂O⁺ ([M+H]⁺): 247.0633, Found: 247.0638.



6-(4-fluorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-

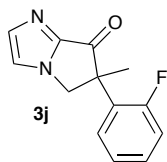
7-one (3h): Prepared according to general procedure C from 1-(2-(4-fluorophenyl)allyl)-1H-imidazole-2-carbaldehyde **1h** (0.046 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol). The crude reaction mixture

was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3h** in 99% yield (0.046 g, 0.20 mmol) as an orange oil. **¹H NMR** (600 MHz, CDCl₃) δ 1.77 (s, 3H), 4.45 (d, J = 12.0 Hz, 1H), 4.64 (d, J = 12.0 Hz, 1H), 7.03 (dd, J = 9.0, 9.0 Hz, 2H), 7.28 (dd, J = 9.0, 5.4 Hz, 2H), 7.33 (app s, 1H), 7.69 (app s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 23.7, 56.1, 57.1, 115.9 (d, J = 21.4 Hz, 2C), 120.3, 127.7 (d, J = 8.2 Hz, 2C), 137.0 (d, J = 3.2 Hz, 1C), 140.1, 145.7, 162.1 (d, J = 247.2 Hz, 1C), 190.1. **¹⁹F NMR** (CDCl₃, 565 MHz): δ -115.08 (s, 1F) **HRMS** (ESI): Calcd. for C₁₃H₁₂FN₂O⁺ ([M+H]⁺): 231.0928, Found: 231.0923.



6-(3-fluorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3i):

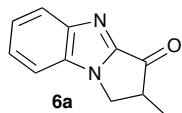
Prepared according to general procedure C from 1-(2-(3-fluorophenyl)allyl)-1H-imidazole-2-carbaldehyde **1i** (0.046 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3i** in 99% yield (0.046 g, 0.20 mmol) as an orange oil. **¹H NMR** (600 MHz, CDCl₃) δ 1.78 (s, 3H), 4.45 (d, J = 12.0 Hz, 1H), 4.66 (d, J = 12.0 Hz, 1H), 6.95-7.01 (m, 1H), 7.03-7.07 (m, 2H), 7.32 (ddd, 12, 10.2, 3.6 Hz, 1H), 7.35 (app s, 1H), 7.71 (app s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 23.7, 56.4 (d, J = 1.66 Hz, 1C), 56.9, 113.4 (d, J = 22.6 Hz, 1C), 114.7 (d, J = 19.6 Hz, 1C), 120.4, 121.6 (d, J = 3.0 Hz, 1C), 130.7 (d, J = 8.2 Hz, 1C), 140.2, 143.7 (d, J = 6.0 Hz, 1C), 145.7, 163.1 (d, J = 247.0 Hz, 1C), 189.6. **¹⁹F NMR** (CDCl₃, 565 MHz): δ -111.98 (s, 1F). **HRMS** (ESI): Calcd. for C₁₃H₁₂FN₂O⁺ ([M+H]⁺): 231.0928, Found: 231.0929.



6-(2-fluorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3j):

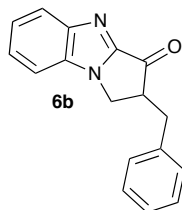
Prepared according to general procedure C from 1-(2-(2-fluorophenyl)allyl)-1H-imidazole-2-carbaldehyde **1j** (0.046 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3j** in 99% yield (0.046 g, 0.20 mmol) as an off-white solid. **¹H NMR** (600 MHz, CDCl₃) δ 1.74 (s, 3H), 4.39 (d, J = 12.0 Hz, 1H), 4.53 (d, J = 12.0 Hz, 1H), 7.03 (dd, J = 12.0, 7.8 Hz, 1H), 7.15 (t, J = 7.8 Hz, 1H), 7.25 (app s, 1H), 7.29 (m, 1H), 7.48 (t, J = 7.8 Hz, 1H), 7.64 (s, 1H). **¹³C NMR** (151 MHz, CDCl₃) δ 23.2, 54.1, 56.2 (d, J = 4.6 Hz, 1C), 116.2 (d, J = 21.6 Hz, 1C), 119.9, 124.5 (d, J = 3.2 Hz, 1C), 128.1 (d, J = 12.8 Hz, 1C), 128.2 (d, J = 4.0 Hz, 1C), 129.9 (d, J = 8.8 Hz, 1C),

139.6, 145.5, 160.7 (d, $J = 246.8$ Hz, 1C), 189.9. ^{19}F NMR (CDCl_3 , 565 MHz): δ -113.05 (s, 1F). **HRMS** (ESI): Calcd. for $\text{C}_{13}\text{H}_{12}\text{FN}_2\text{O}^+$ ($[\text{M}+\text{H}]^+$): 231.0928, Found: 231.0928.



2-methyl-1,2-dihydro-3H-benzo[d]pyrrolo[1,2-a]imidazol-3-one (6a):

Prepared according to general procedure C from 1-allyl-1H-benzo[d]imidazole-2-carbaldehyde **5a** (0.037 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μL , 0.04 mmol). The crude reaction mixture was purified by flash column chromatography (90:10 hexanes:EtOAc) to afford **6a** in 97% yield (0.036 g, 0.19 mmol) as a white solid. ^1H NMR (600 MHz, CDCl_3) δ 1.47 (d, $J = 7.2$ Hz, 3H), 3.33 (m, 1H), 4.03 (dd, $J = 11.4, 4.2$ Hz, 1H), 4.71 (dd, $J = 11.4, 7.8$ Hz, 1H), 7.38 (ddd, $J = 7.8, 7.2, 1.2$ Hz, 1H), 7.41 (ddd, $J = 7.8, 7.2, 1.2$ Hz, 1H), 7.48 (d, $J = 7.8$ Hz, 1H), 7.92 (d, $J = 7.8$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 15.4, 45.0, 47.0, 111.0, 123.21, 124.8, 125.6, 132.8, 149.1, 149.4, 193.7. **HRMS** (ESI): Calcd. for $\text{C}_{11}\text{H}_{11}\text{N}_2\text{O}^+$ ($[\text{M}+\text{H}]^+$): 187.0866, Found: 187.0866.

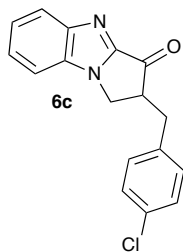


2-benzyl-1,2-dihydro-3H-benzo[d]pyrrolo[1,2-a]imidazol-3-one (6b):

Prepared according to general procedure C from 1-cinnamyl-1H-benzo[d]imidazole-2-carbaldehyde **5b** (0.052 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μL , 0.04 mmol). The crude reaction mixture was purified by flash column chromatography with (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to afford **6b** in 87% yield (0.045 g, 0.17 mmol) as a white solid. ^1H NMR (400 MHz, CDCl_3) δ 2.96 (dd, $J = 14.0, 10.0$ Hz, 1H), 3.51 (dd, $J = 14.0, 4.4$ Hz, 1H), 3.61-3.70 (m, 1H), 4.18 (dd, $J = 11.6, 4.0$ Hz, 1H), 4.51 (dd, $J = 11.6, 7.6$ Hz, 1H), 7.24-7.30 (m, 3H), 7.31-7.37 (m, 2H), 7.38-7.49 (m, 3H), 7.94 (dd, $J = 6.8, 2.8$ Hz, 1H). ^{13}C NMR (101 MHz, CDCl_3) δ 36.1, 44.6,

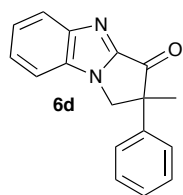
51.6, 111.1, 123.4, 125.0, 125.8, 127.3, 128.9, 129.1, 132.9, 137.6, 149.2, 149.5, 192.2.

HRMS (ESI): Calcd. for $C_{17}H_{15}N_2O^+$ ($[M+H]^+$): 263.1179, Found: 263.1177.



2-(4-chlorobenzyl)-1,2-dihydro-3H-benzo[d]pyrrolo[1,2-a]imidazol-3-one (6c): Prepared according to general procedure C from (*E*)-1-(3-(4-chlorophenyl)allyl)-1*H*-benzo[d]imidazole-2-carbaldehyde **5c** (0.059 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol).

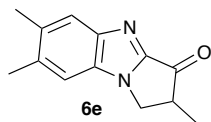
The crude reaction mixture was purified by flash column chromatography with (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) as eluent to afford **6c** in 84% yield (0.050 g, 0.17 mmol). **1H NMR** (600 MHz, d_6 -DMSO) δ 3.00 (dd, J = 14.4, 10.8 Hz, 1H), 3.28 (dd, J = 14.4, 4.8 Hz, 1H), 3.75-3.82 (m, 1H), 4.21 (dd, J = 11.4, 4.2 Hz, 1H), 4.56 (dd, J = 11.4, 7.8 Hz, 1H), 7.35-7.41 (m, 5H), 7.42-7.45 (m, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H). **^{13}C NMR** (101 MHz, d_6 -DMSO) δ 34.1, 44.6, 50.8, 112.3, 122.0, 124.3, 124.9, 128.5, 130.8, 131.3, 132.7, 137.6, 148.5, 149.6, 193.5. **HRMS** (ESI): Calcd. for $C_{17}H_{14}ClN_2O^+$ ($[M+H]^+$): 297.0789, Found: 297.0789.



2-methyl-2-phenyl-1,2-dihydro-3H-benzo[d]pyrrolo[1,2-a]imidazol-3-one (6d): Prepared according to general procedure C from 1-(2-phenylallyl)-1*H*-benzo[d]imidazole-2-carbaldehyde **5d** (0.052 g, 0.20 mmol), triazolium **2** (6 mg, 0.02 mmol) and DBU (6 μ L, 0.04 mmol). The crude reaction

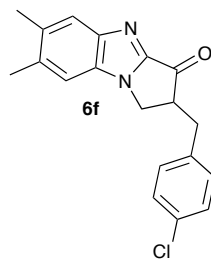
mixture was purified by flash column chromatography with (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) as eluent to afford **6d** in 93% yield (0.048 g, 0.19 mmol) as a white solid. **1H NMR** (600 MHz, $CDCl_3$) δ 1.86 (s, 3H), 4.57 (d, J = 11.4 Hz, 1H), 4.84 (d, J = 11.4 Hz, 1H), 7.25-7.36 (m, 5H), 7.45 (ddd, J = 8.4, 7.8, 1.2 Hz, 1H), 7.48 (ddd, J = 8.4, 7.8, 1.2 Hz, 1H), 7.57

(dd, $J = 7.8, 1.2$ Hz, 1H), 8.01 (dd, $J = 7.8, 1.2$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 23.8, 55.5, 56.7, 111.2, 123.4, 125.0, 125.9, 125.93, 127.9, 129.2, 132.8, 140.9, 148.6, 149.8, 193.8. HRMS (ESI): Calcd. for $\text{C}_{17}\text{H}_{15}\text{N}_2\text{O}^+$ ($[\text{M}+\text{H}]^+$): 263.1179, Found: 263.1181.



2,6,7-trimethyl-1,2-dihydro-3H-benzo[d]pyrrolo[1,2-a]imidazol-3-one (6e): Prepared according to general procedure C from 1-allyl-5,6-

dimethyl-1H-benzo[d]imidazole-2-carbaldehyde **5e** (0.021 g, 0.10 mmol), triazolium **2** (3 mg, 0.01 mmol) and DBU (2.9 μL , 0.020 mmol). The crude reaction mixture was purified by flash column chromatography with (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to afford **6e** in 66% yield (0.014 g, 0.066 mmol) as a white solid. ^1H NMR (600 MHz, CDCl_3) δ 1.48 (d, $J = 7.2$ Hz, 3H), 2.39 (s, 3H), 2.41 (s, 3H), 3.29-3.35 (m, 1H), 3.99 (dd, $J = 11.4, 4.2$ Hz, 1 H), 4.67 (dd, $J = 11.4, 7.8$ Hz, 1H), 7.26 (s, 1H), 7.68 (s, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 1.1, 15.5, 20.7, 20.9, 45.0, 47.0, 110.7, 122.6, 131.6, 134.6, 135.9, 148.5, 193.4. HRMS (ESI): Calcd. for $\text{C}_{13}\text{H}_{15}\text{N}_2\text{O}^+$ ($[\text{M}+\text{H}]^+$): 215.1179, Found: 215.1178.

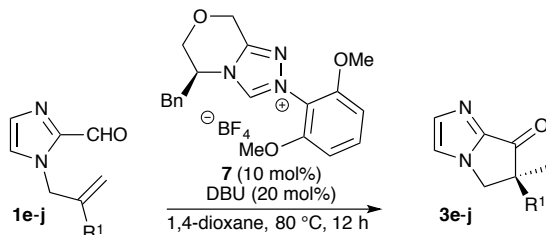


2-(4-chlorobenzyl)-6,7-dimethyl-1,2-dihydro-3H-benzo[d]pyrrolo[1,2-a]imidazol-3-one (6f): Prepared according to general procedure C (*E*)-1-(3-(4-chlorophenyl)allyl)-5,6-dimethyl-1H-benzo[d]imidazole-2-carbaldehyde **5f** (0.032 g, 0.10 mmol), triazolium **2**

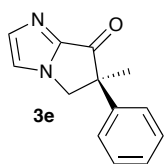
(3 mg, 0.01 mmol) and DBU (3 μL , 0.02 mmol). The crude reaction mixture was purified by column chromatography with (100:0 hexanes:EtOAc to 90:10 hexanes:EtOAc) to afford **6f** in 88% yield (0.028 g, 0.088 mmol) as a white solid. ^1H NMR (600 MHz, CDCl_3) δ 2.38 (app s, 6H), 2.95 (dd, $J = 14.4, 10.2$ Hz, 1H), 3.41 (dd, $J = 14.4, 4.2$ Hz, 1H), 3.54-3.60 (m, 1H), 4.05 (dd, $J = 11.4, 3.6$ Hz, 1H), 4.44 (dd, $J = 11.4, 7.2$ Hz, 1H), 7.18 (d, $J = 7.8$ Hz, 2H), 7.20 (s, 1H),

7.28 (d, $J = 7.8$ Hz, 2H), 7.66 (s, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 20.8, 21.0, 35.5, 44.3, 51.4, 110.7, 122.7, 129.2, 130.3, 130.8, 131.6, 133.1, 134.9, 136.2, 148.3, 148.4, 191.5. HRMS (ESI): Calcd. for $\text{C}_{19}\text{H}_{18}\text{ClN}_2\text{O}^+$ ($[\text{M}+\text{H}]^+$): 325.1102, Found: 325.1103.

General Procedure D: Enantioselective synthesis of **3e-j**



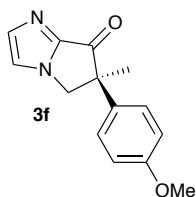
In a nitrogen-filled glovebox, to a 1-dram vial was added triazolium **7** (0.010 mmol, 0.10 equiv), the appropriate *N*-allylimidazole-2-carboxaldehyde **1e-j** (0.10 mmol, 1.0 equiv), DBU (3 μL , 0.02 mmol, 0.2 equiv), and 1,4-dioxane (0.2 mL, 0.5 M). The vial was sealed with a teflon-lined septum cap. The reaction vessel was removed from the glovebox and the reaction mixture was stirred at 80 $^\circ\text{C}$ for 12 h. The reaction was cooled to room temperature and filtered through a plug of silica gel with EtOAc as eluent. The filtrate was concentrated under reduced pressure. The crude product was purified by flash column silica gel chromatography (hexane:EtOAc) to give the appropriate dihydropyrroloimidazolones (**3e-j**).



(*S*)-6-methyl-6-phenyl-5,6-dihydro-7*H*-pyrrolo[1,2-*a*]imidazole-7-one

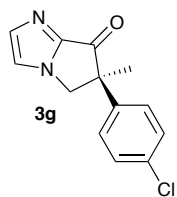
(3e): Prepared according to general procedure D from 1-(2-phenylallyl)-1*H*-imidazole-2-carbaldehyde **1e** (0.021 g, 0.10 mmol), triazolium **7** (4 mg, 0.01 mmol) and DBU (3 μL , 0.02 mmol). The crude reaction mixture was purified by flash

column chromatography with (90:10 hexanes:EtOAc) to afford **3e** in 90% yield (0.019 g, 0.090 mmol) as an off white solid. The enantiomeric excess was determined by HPLC analysis (254 nm, 25 °C) t_R 27.1 min (major); t_R 32.4 min (minor) [Chiracel AD-H (0.46 cm x 25 cm)(from Daicel Chemical Ind., hexane/*i*-PrOH, 90:10, 1.0 mL/min] to be 71% ee. $[\alpha]_D^{24} = -188.8^\circ$ (c 0.63, CHCl₃). NMR spectra is consistent with racemic spectra above.



(S)-6-(4-methoxyphenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3f): Prepared according to general procedure D from

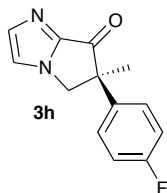
1-(2-(4-methoxyphenyl)allyl)-1*H*-imidazole-2-carbaldehyde **1f** (0.024 g, 0.10 mmol), triazolium **7** (4 mg, 0.01 mmol), and DBU (3 μ L, 0.02 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3f** in 98% yield (0.024 g, 0.097 mmol) as an off white solid. The enantiomeric excess was determined by HPLC analysis (254 nm, 25 °C) t_R 44.3 min (major); 56.9 min (minor) [Chiracel AD-H (0.46 cm x 25 cm)(from Daicel Chemical Ind., Ltd.) hexane/*i*-PrOH, 90:10, 1.0 mL/min] to be 79% ee. $[\alpha]_D^{23} = -84.9^\circ$ (c 1.06, CHCl₃). NMR spectra is consistent with racemic spectra above.



(S)-6-(4-chlorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3g): Prepared according to general procedure D from

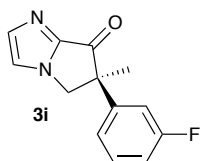
1-(2-(4-chlorophenyl)allyl)-1*H*-imidazole-2-carbaldehyde **1g** (0.025 g, 0.10 mmol), triazolium **7** (4 mg, 0.01 mmol) and DBU (3 μ L, 0.02 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3g** 96% yield (0.024 g, 0.096 mmol) as an off white solid. The enantiomeric excess was determined by HPLC analysis (254 nm, 25 °C) t_R 36.1 min (major); 45.7 min (minor)

[Chiracel AD-H (0.46 cm x 25 cm)(from Daicel Chemical Ind., Ltd.) hexane/*i*-PrOH, 90:10, 1.0 mL/min] to be 67% ee. $[\alpha]_D^{22} = -156.9^\circ$ (c 1.02, CHCl₃). NMR spectra is consistent with racemic spectra above.



(S)-6-(4-fluorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3h): Prepared according to general procedure D from

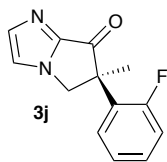
1-(2-(4-fluorophenyl)allyl)-1*H*-imidazole-2-carbaldehyde **1h** (0.023 g, 0.10 mmol), triazolium **7** (4 mg, 0.01 mmol) and DBU (3 μ L, 0.02 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3h** in 81% yield (0.019 g, 0.083 mmol) as an orange oil. The enantiomeric excess was determined by HPLC analysis (254 nm, 25 $^\circ$ C) t_R 33.3 min (major); t_R 39.8 min (minor) [Chiracel AD-H (0.46 cm x 25 cm)(from Daicel Chemical Ind., Ltd.) hexane/*i*-PrOH, 90:10, 1.0 mL/min] to be 75% ee. $[\alpha]_D^{23} = -40.5^\circ$ (c 0.84, CHCl₃). NMR spectra is consistent with racemic spectra above.



(S)-6-(3-fluorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3i): Prepared according to general procedure D from

1-(2-(3-fluorophenyl)allyl)-1*H*-imidazole-2-carbaldehyde **1i** (0.023 g, 0.10 mmol), triazolium **7** (4 mg, 0.01 mmol) and DBU (3 μ L, 0.02 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3i** in 93% yield (0.021 g, 0.093 mmol) as an orange oil. The enantiomeric excess was determined by HPLC analysis (254 nm, 25 $^\circ$ C) t_R 29.2 min (major); t_R 33.5 min (minor) [Chiracel AD-H (0.46 cm x 25 cm)(from Daicel Chemical Ind., Ltd.) hexane/*i*-PrOH, 90:10,

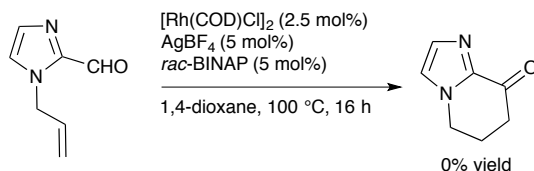
1.0 mL/min] to be 67% ee. $[\alpha]_D^{23} = -51.2^\circ$ (c 1.01, CHCl_3). NMR spectra is consistent with racemic spectra above.



(S)-6-(2-fluorophenyl)-6-methyl-5,6-dihydro-7H-pyrrolo[1,2-a]imidazole-7-one (3j): Prepared according to general procedure D from 1-(2-(2-fluorophenyl)allyl)-1H-imidazole-2-carbaldehyde **1j** (0.023 g, 0.10

mmol), triazolium **7** (4 mg, 0.01 mmol) and DBU (3 μL , 0.02 mmol). The crude reaction mixture was purified by flash column chromatography with (90:10 hexanes:EtOAc) to afford **3j** in 39% yield (0.089 g, 0.038 mmol) as an off-white solid. The enantiomeric excess was determined by HPLC analysis (254 nm, 25 $^\circ\text{C}$) t_R 29.0 min (major); t_R 35.4 min (minor) [Chiracel AD-H (0.46 cm x 25 cm)(from Daicel Chemical Ind., Ltd.) hexanes/*i*-PrOH, 90:10, 1.0 mL/min] to be 56% ee. $[\alpha]_D^{23} = +28.6^\circ$ (c 0.35, CHCl_3). NMR spectra is consistent with racemic spectra above.

Representative Procedure for Rhodium-Catalysed Hydroacylation of 1a



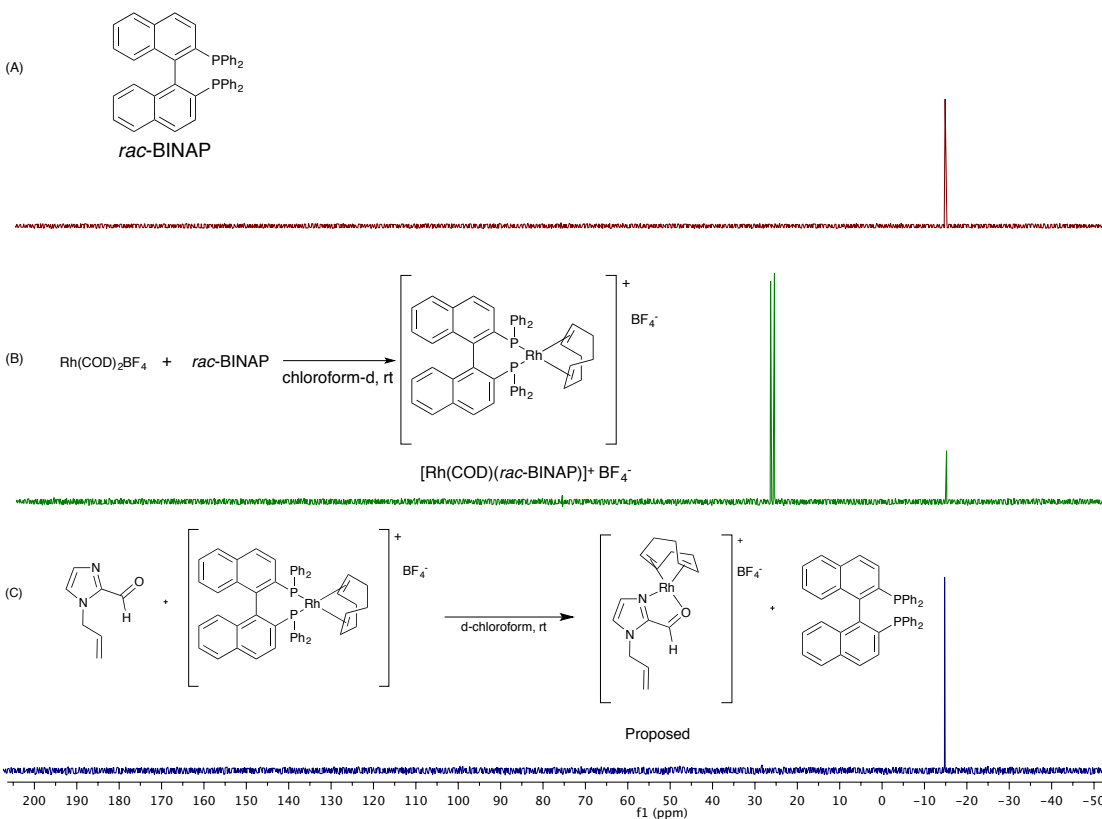
In a nitrogen-filled glovebox, 1-allyl-1H-imidazole-2-carboxaldehyde (13.6 mg, 0.100 mmol, 1.00 equiv), $[\text{Rh}(\text{COD})\text{Cl}]_2$ (1.2 mg, 0.0025 mmol, 0.025 equiv), racemic-BINAP (3.1 mg, 0.0050 mmol, 0.050 equiv), AgBF_4 (1.0 mg, 0.0050 mmol, 0.050 equiv) and 1,4-dioxane (0.25 mL, 0.40M) were added to 1-dram vial. The vial was sealed with a Teflon-lined septum cap and removed from the glovebox. The reaction mixture was stirred at 100 $^\circ\text{C}$ in an oil bath for 16 h. The vial was removed from the oil bath and allowed to cool to room

temperature. The reaction mixture was filtered through a short plug of silica gel with 100% EtOAc as eluent. The crude reaction mixture was concentrated under reduced pressure. The crude residue was analyzed by ^1H NMR spectroscopy with dibromomethane as the internal standard. Only unreacted starting material was observed by ^1H NMR spectroscopy.

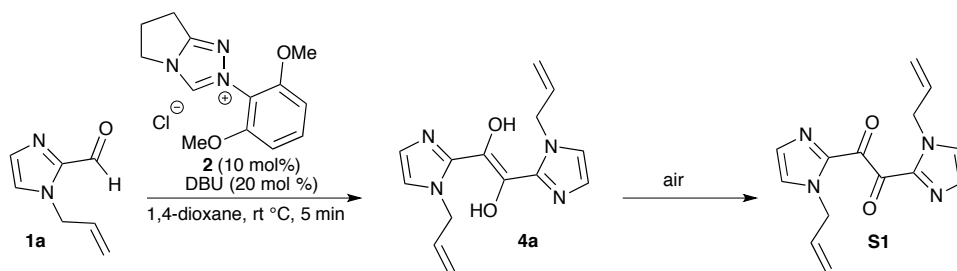
Evaluation of Rhodium-Catalysed Hydroacylation of **1a by ^{31}P NMR Spectroscopy**

In a nitrogen-filled glovebox, *rac*-BINAP (6.2 mg, 0.010 mmol, 0.050 equiv) and CDCl_3 (0.5 mL) was added to 1-dram vial and stirred until *rac*-BINAP fully dissolved. The reaction mixture was then transferred to an NMR tube and sealed. A ^{31}P spectrum was obtained to give spectrum A in Figure S1. The sealed NMR tube was returned to the glovebox. To a 1-dram vial was added $\text{Rh}(\text{COD})_2\text{BF}_4$ (4.1 mg, 0.010 mmol, 0.050 equiv) and the solution containing *rac*-BINAP in CDCl_3 , and the resulting solution was stirred for 15 minutes at room temperature. After stirring, the solution was returned to the NMR tube, sealed, and spectrum B in Figure S1 was obtained, showing that the formation of $[\text{Rh}(\text{COD})(\textit{rac}\text{-BINAP})]^+\text{BF}_4^-$. The NMR tube was returned to the nitrogen-filled glovebox. To a 1-dram vial containing 1-allyl-1*H*-imidazole-2-carboxaldehyde **1a** (27.2 mg, 0.200 mmol, 1.00 equiv) was added the solution containing $[\text{Rh}(\text{COD})(\textit{rac}\text{-BINAP})]^+\text{BF}_4^-$, and the resulting solution was stirred for 15 minutes. After stirring, the solution was returned to the NMR tube, sealed, and spectrum C in Figure S1 was obtained, showing the displacement of *rac*-BINAP from the rhodium.

Figure S1



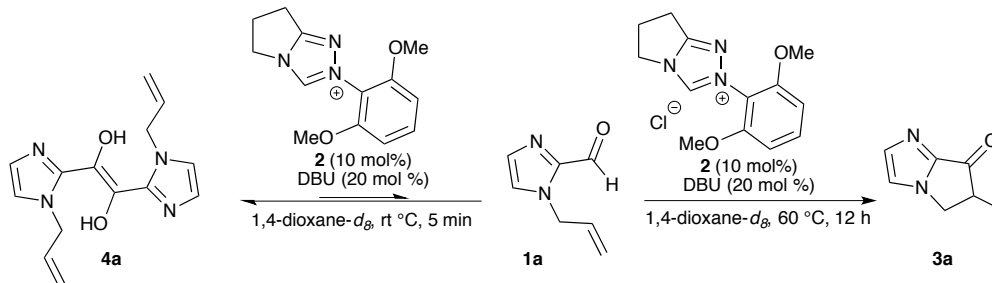
Synthesis of Diketone S1



1,2-Bis(1-allyl-1*H*-imidazol-2-yl)ethane-1,2-dione was prepared according to the following procedure from carboxaldehyde **1a**. In a nitrogen-filled glovebox, to a 1-dram vial was added triazolium **2** (9.0 mg, 0.030 mmol, 0.10 equiv), 1-allyl-1*H*-imidazole-2-carboxaldehyde **1a** (0.041 g, 0.30 mmol, 1.0 equiv), DBU (9 μL , 0.06 mmol, 0.2 equiv), and

1,4-dioxane (0.6 mL, 0.5 M). The vial was sealed with a teflon-lined septum cap. The reaction vessel was removed from the glovebox, and the reaction mixture was stirred at rt for 5 minutes. The reaction was cooled to room temperature, exposed to air, and filtered through a plug of silica gel with EtOAc as eluent. The filtrate was concentrated under reduced pressure. The reaction mixture was purified by column chromatography (100% DCM) to afford diketone **S1** in 90% yield (0.037 g, 0.13 mmol) as an off-white solid. **¹H NMR** (400 MHz, CDCl₃) δ 5.08 (d, *J* = 6.0 Hz, 4H), 5.17 (dd, *J* = 17.2, 1.2 Hz, 2H), 5.24 (dd, *J* = 10.4, 1.2 Hz, 2H), 5.93-6.04 (m, 2H), 7.14 (d, *J* = 0.8 Hz, 2H), 7.20 (d, *J* = 0.8 Hz, 2H). **¹³C NMR** (101 MHz, CDCl₃) δ 50.7, 119.5, 126.3, 132.1, 132.2, 140.3, 183.2. **HRMS** (ESI): Calcd. for C₁₄H₁₅N₄O₂⁺ ([M+H]⁺): 271.1190, Found: 271.1194.

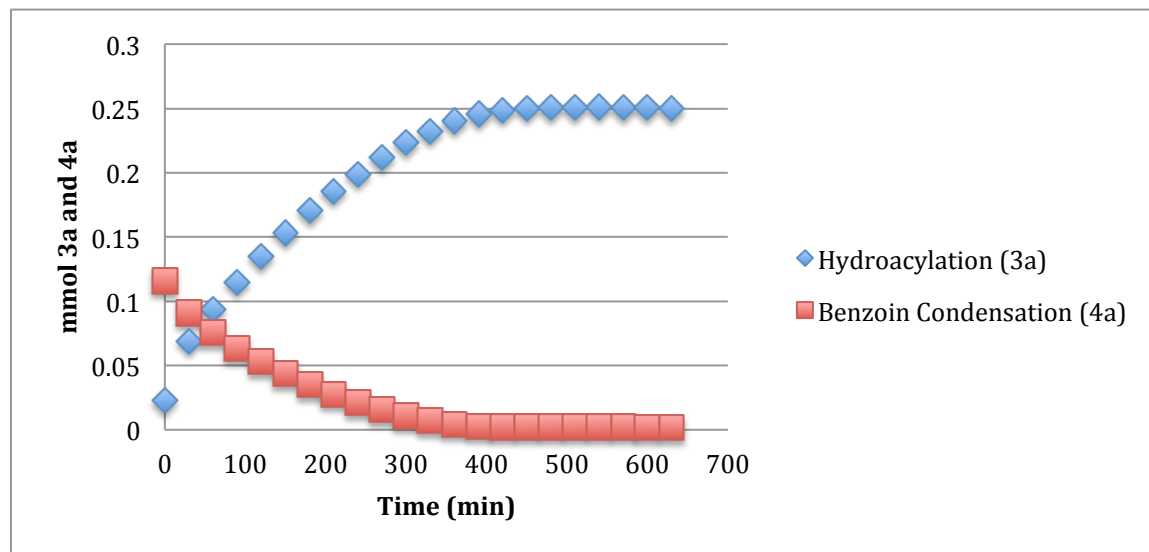
Evaluation of NHC-Catalysed Hydroacylation of **1a** by ¹H NMR Spectroscopy



In a nitrogen-filled glovebox, to a 1-dram vial was added triazolium **2** (7.1 mg, 0.025 mmol, 0.10 equiv), 1-allyl-1H-imidazole-2-carboxaldehyde **1a** (34.0 mg, 0.250 mmol, 1.0 equiv), 1,4-dioxane-*d*₈ (0.5 mL, 0.5 M), and finally DBU (7.5 μL, 0.050 mmol, 0.20 equiv). The reaction mixture was immediately added to a NMR tube and sealed with a teflon-lined septum cap. The reaction vessel was removed from the glovebox and immediately inserted into the Bruker Avance III 600 that was preheated to 60 °C. Spectra were collected every 10 seconds for the first 42 minutes, every 27 seconds for the following 112 minutes, every 57

seconds for the next 237 minutes, and every 117 seconds for the remainder of the reaction time. Within the time taken to prepare the sample, **1a** is converted to **4a** at room temperature. Upon heating the mixture containing **4a** at 60 °C in the NMR spectrometer, **4a** is converted to hydroacylation product **3a** over the course of the experiment as shown in Figure S2. Upon completion of the NMR experiment, the reaction was cooled to room temperature and filtered through a plug of silica gel with EtOAc as eluent. The filtrate was concentrated under reduced pressure. The crude product was purified by flash column silica gel chromatography (90:10 hexane:EtOAc) to give **3a** in 96% yield (32 mg, 0.24 mmol).

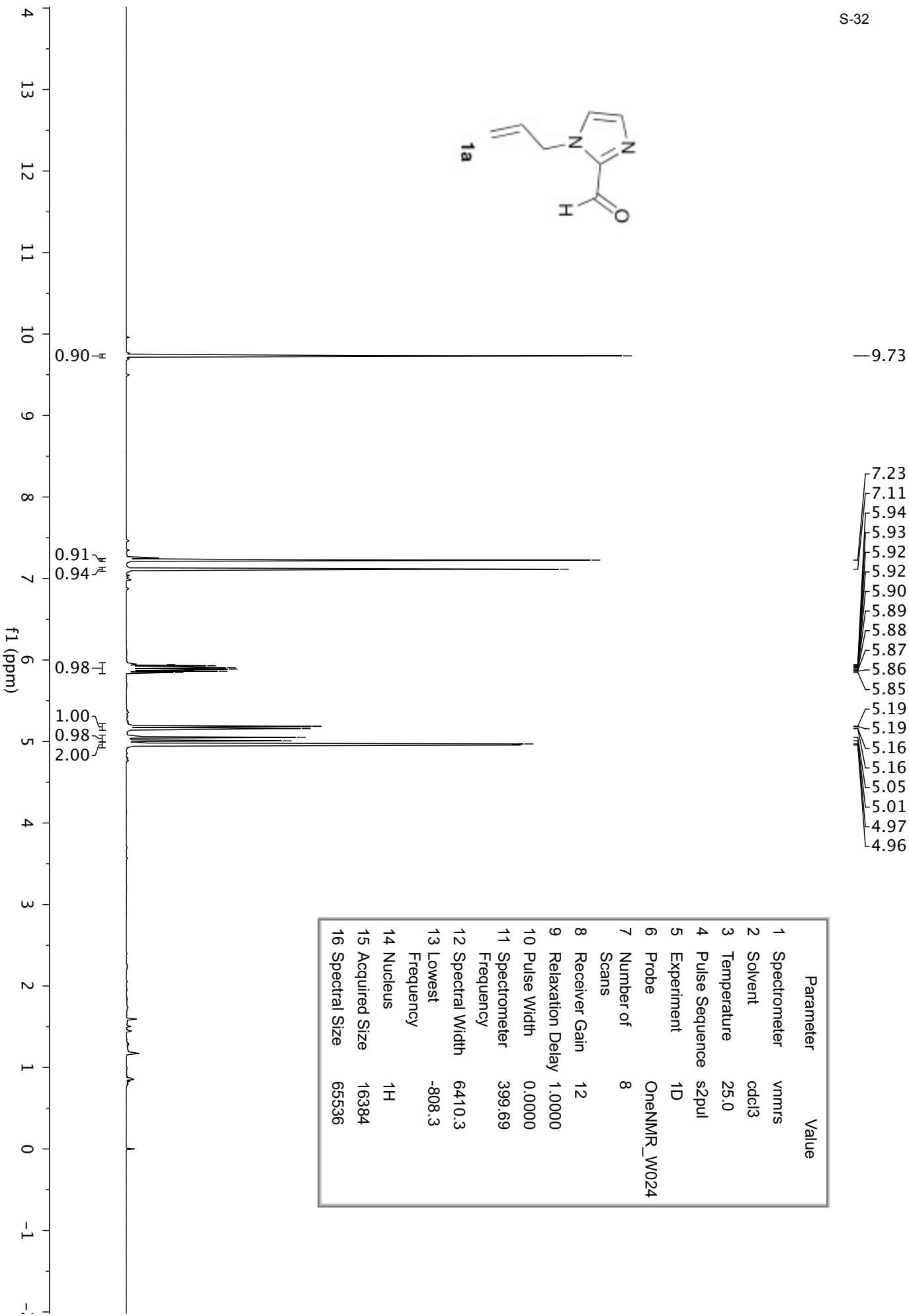
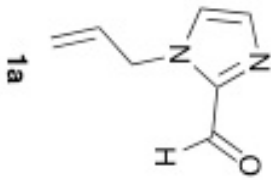
Figure S2

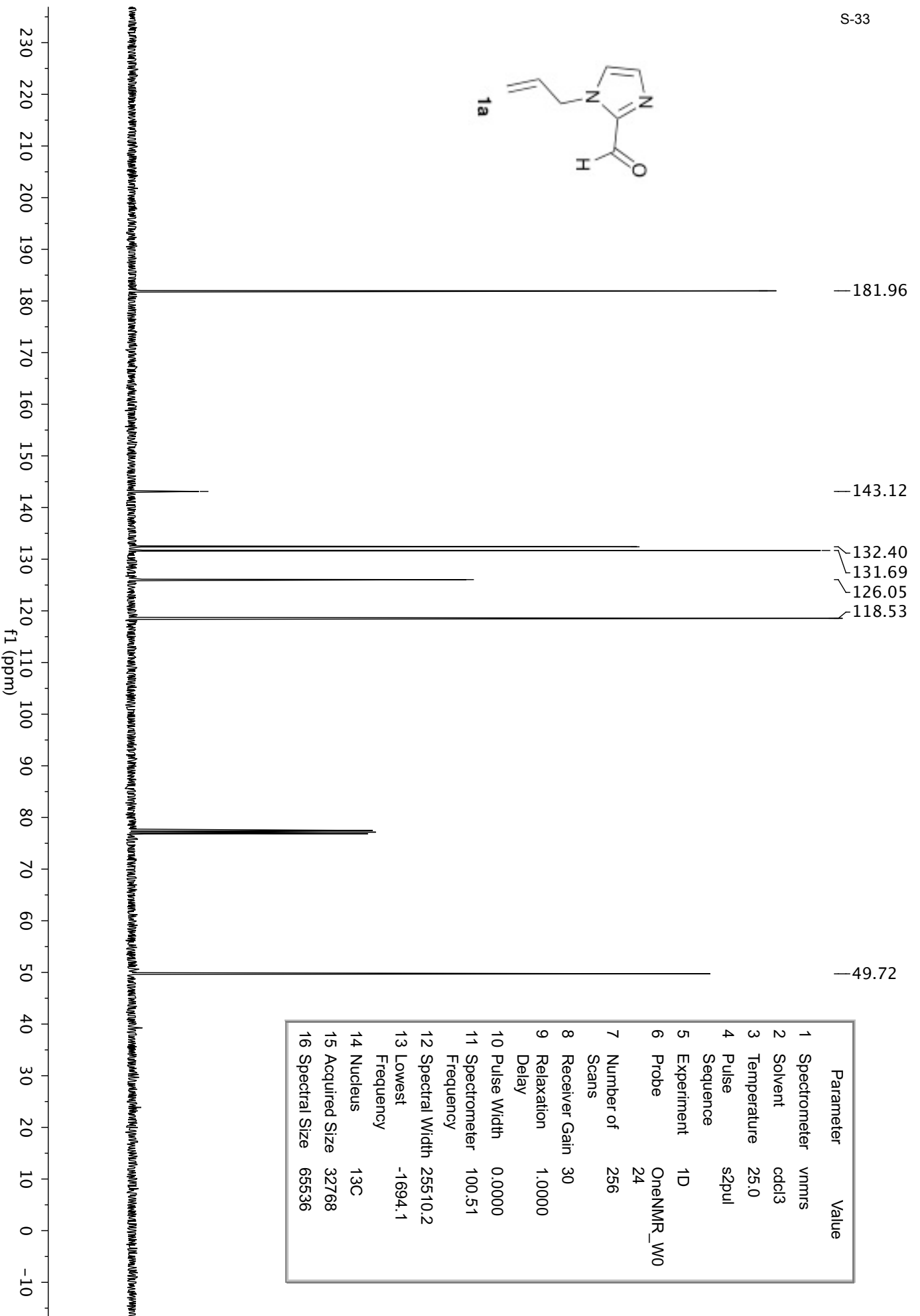
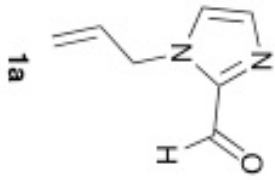


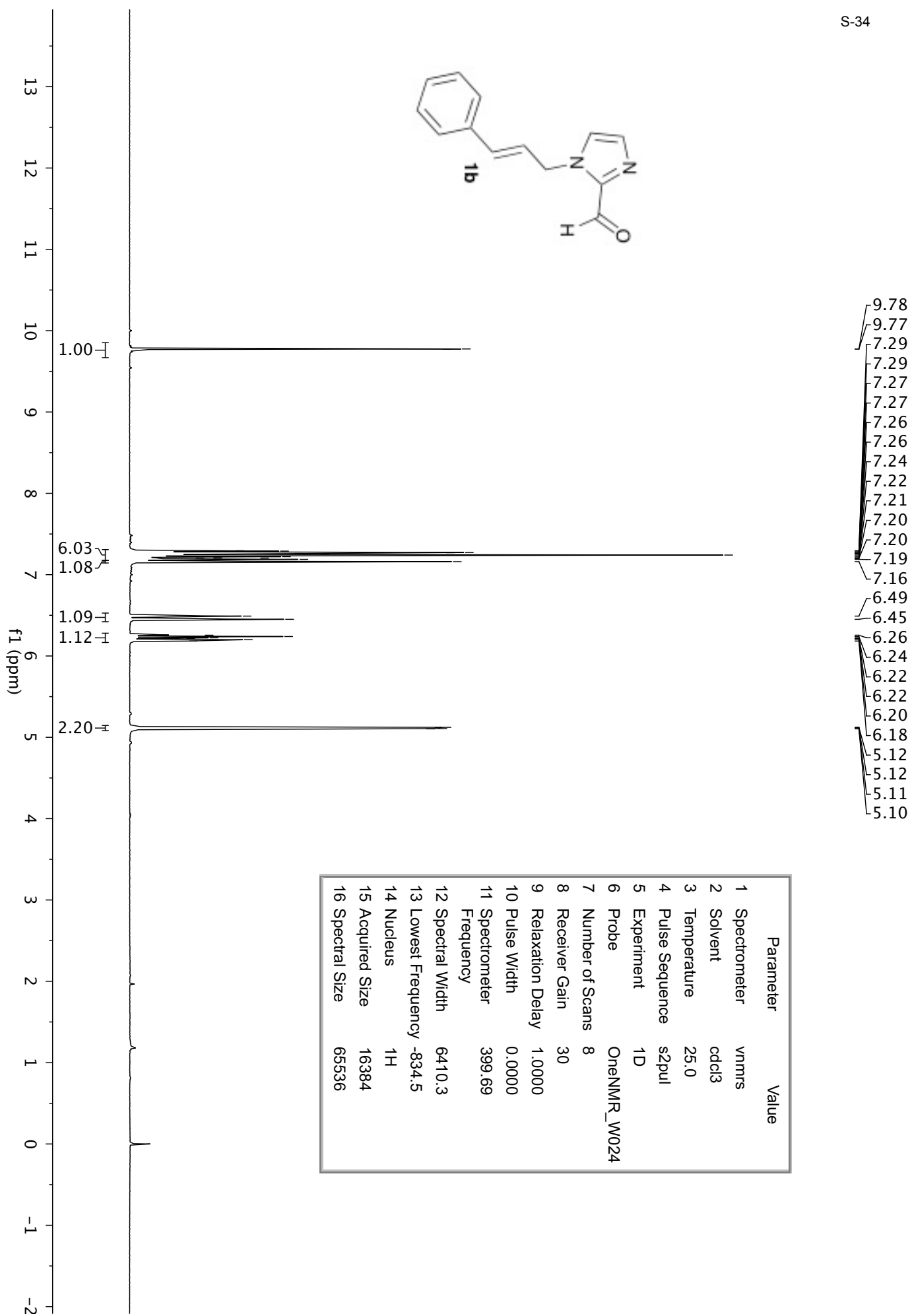
References

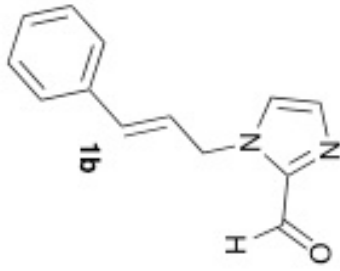
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3. A. F. Alasmary, M. A. Snelling, E. M. Zain, M. A. Alafeefy, S. A. Awaad and N. Karodia, *Molecules*, 2015, **20**.

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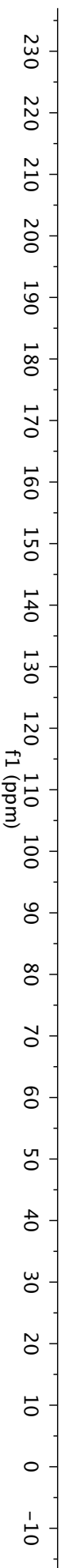


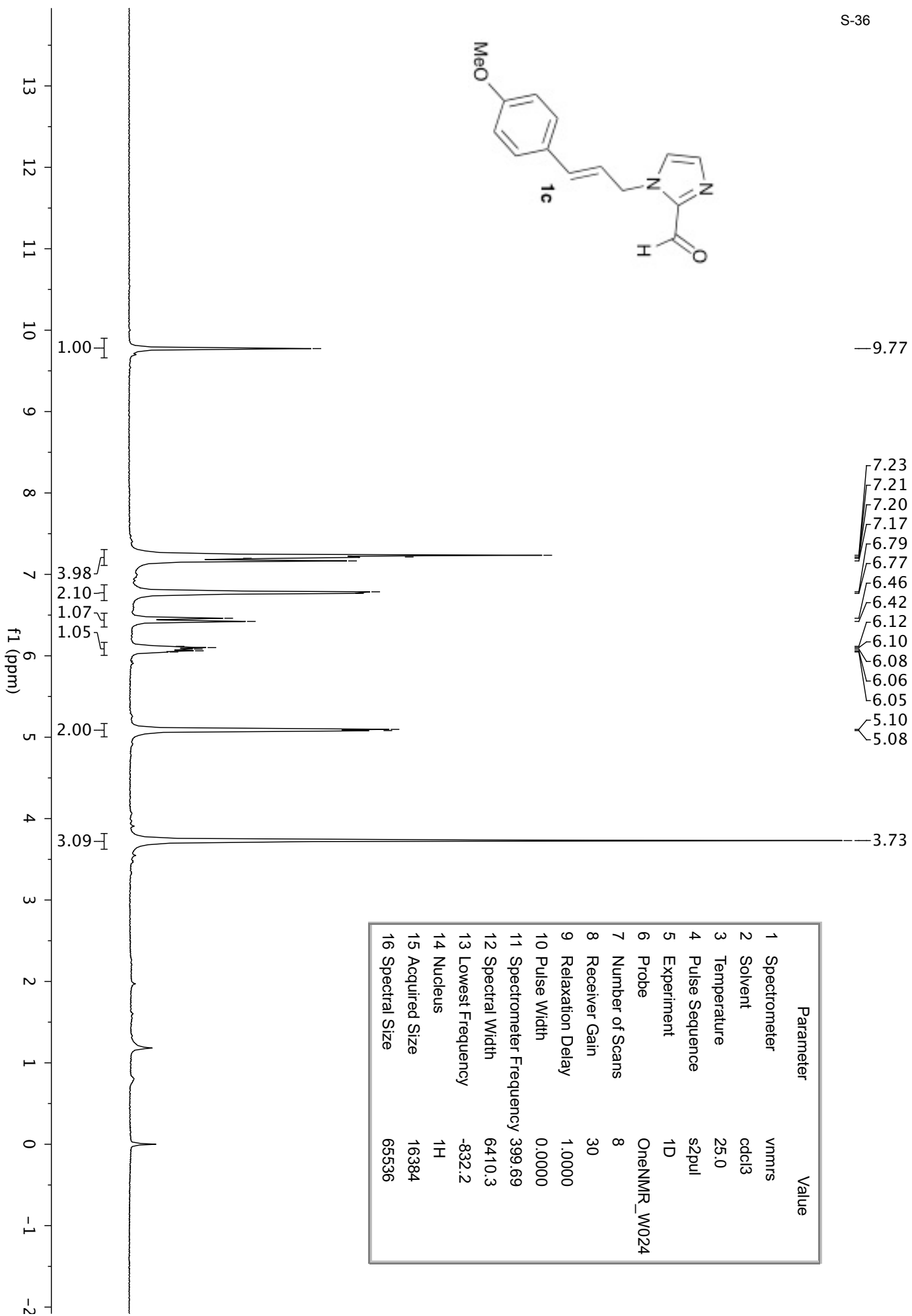
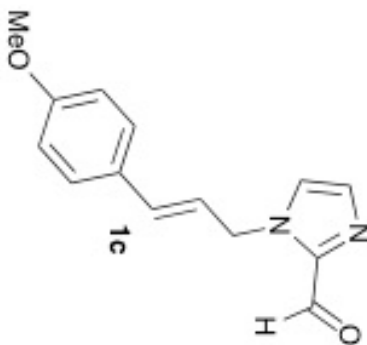
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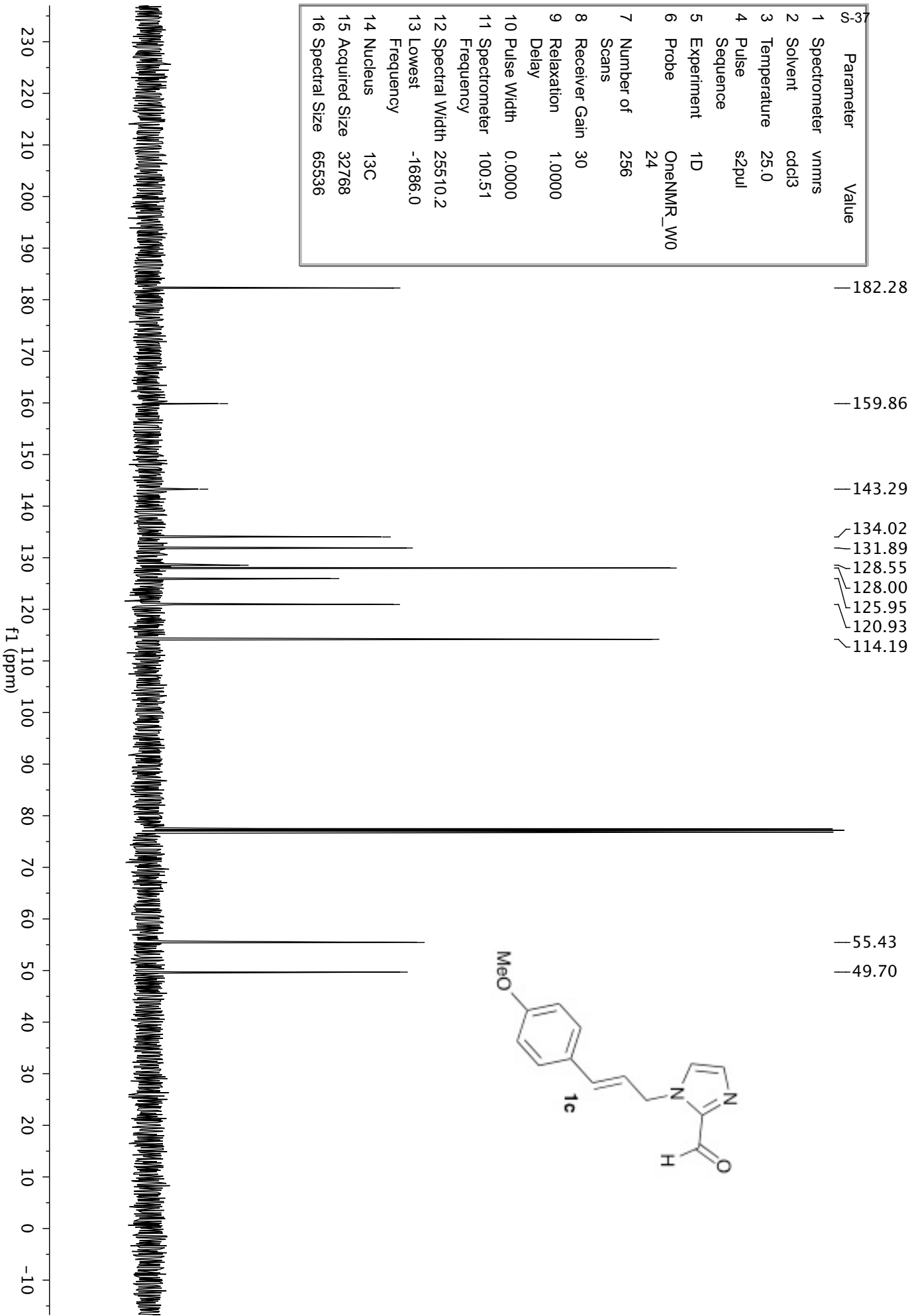
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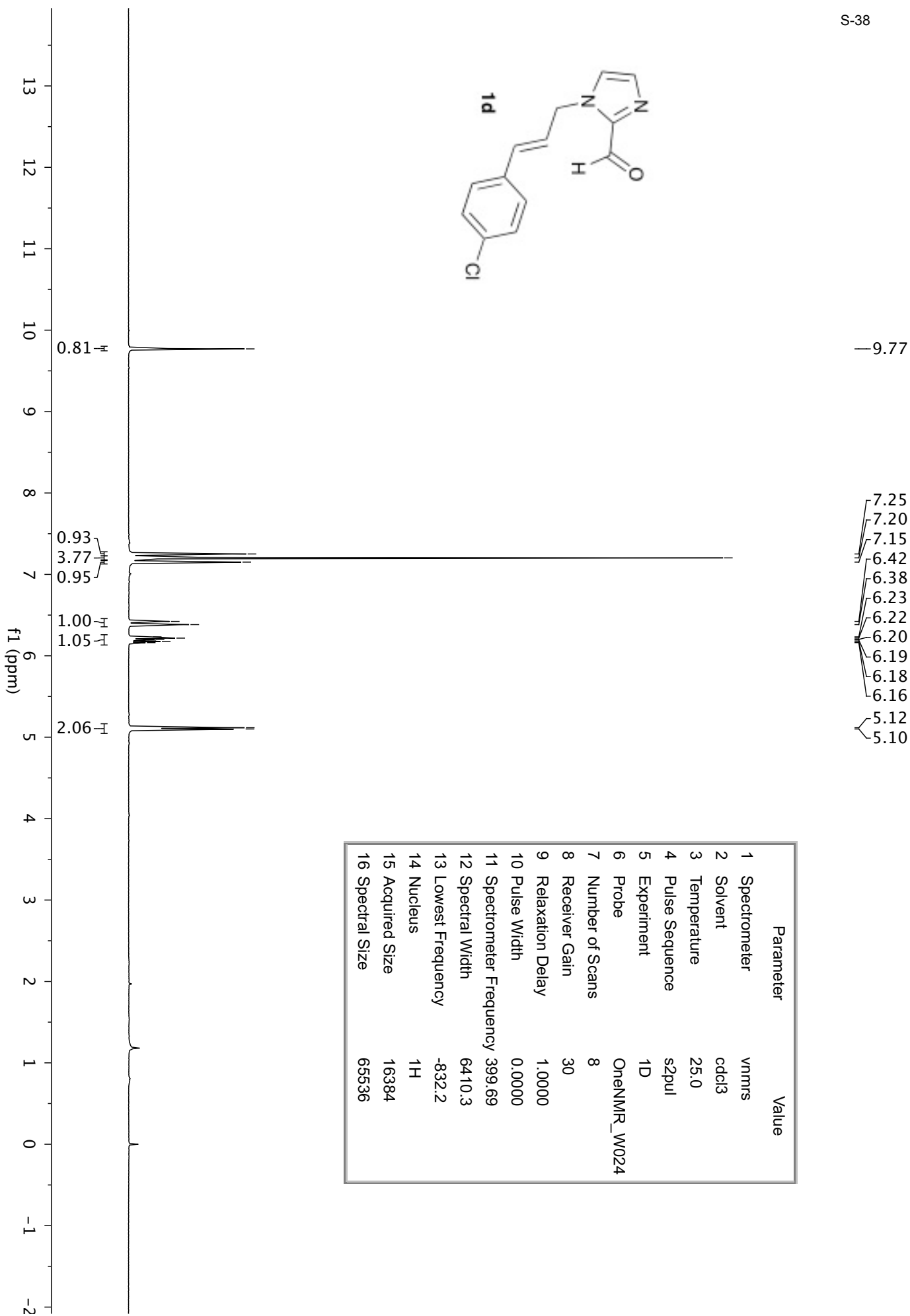
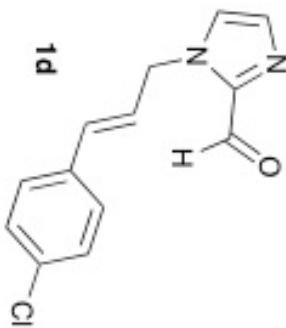
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5 Experiment	1D
6 Probe	OneNMR_w024
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8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	100.51
12 Spectral Width	25510.2
13 Lowest Frequency	-1687.7
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536

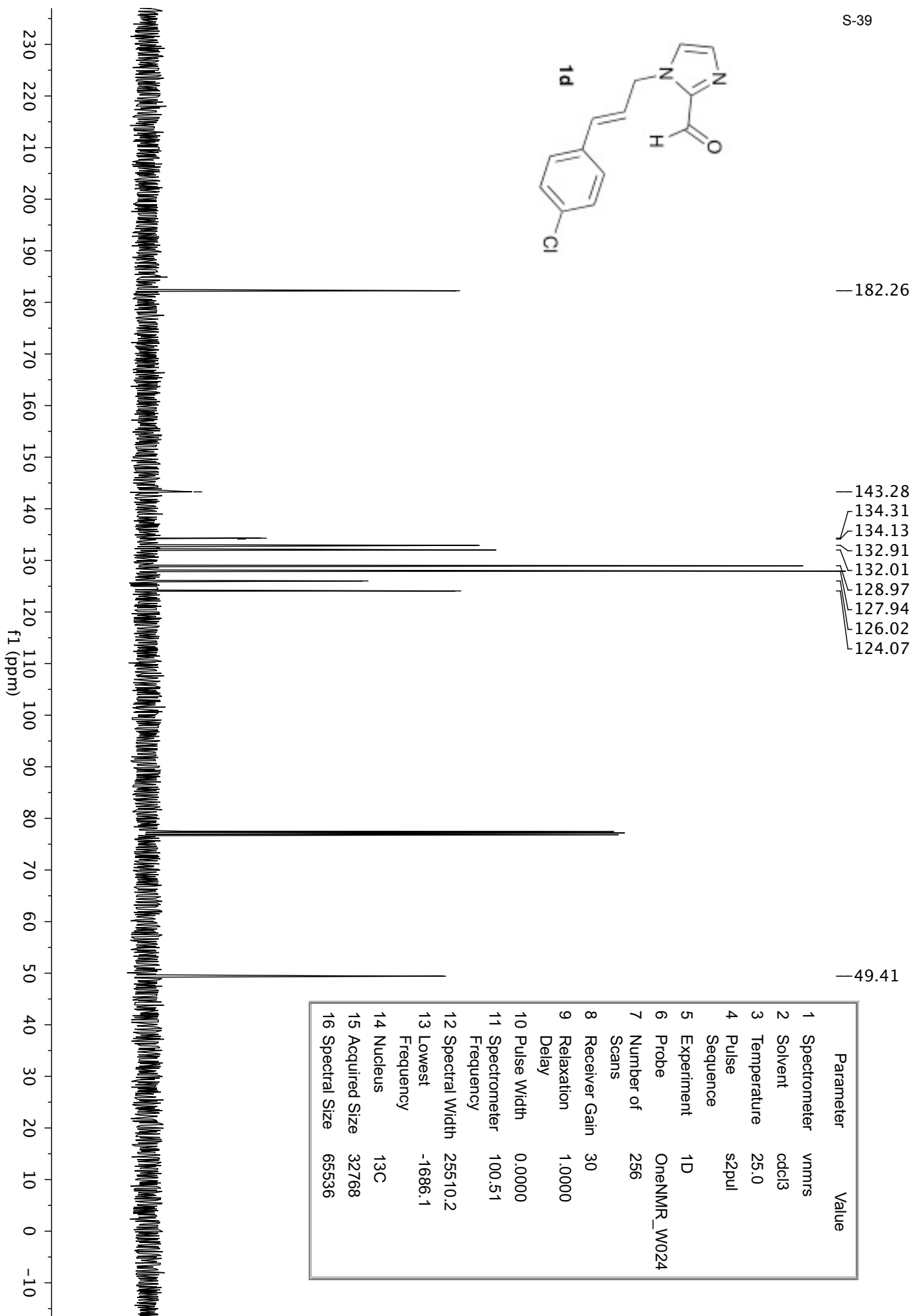
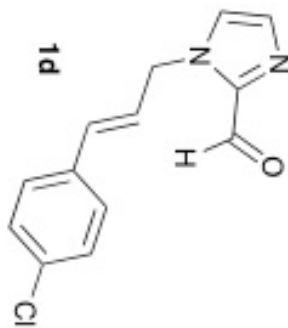


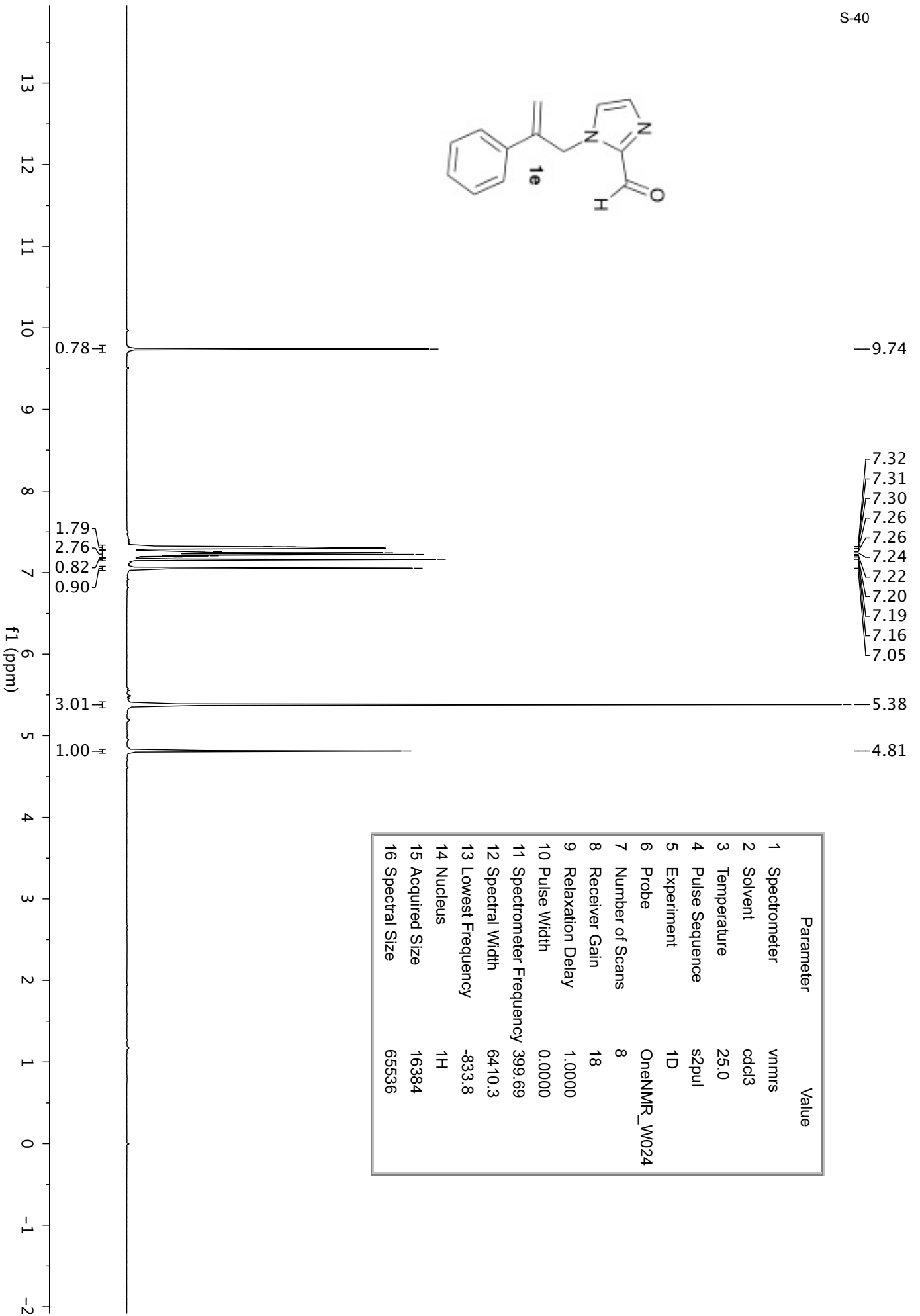
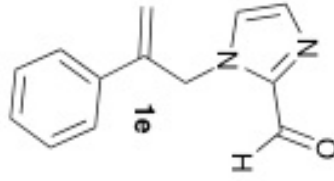


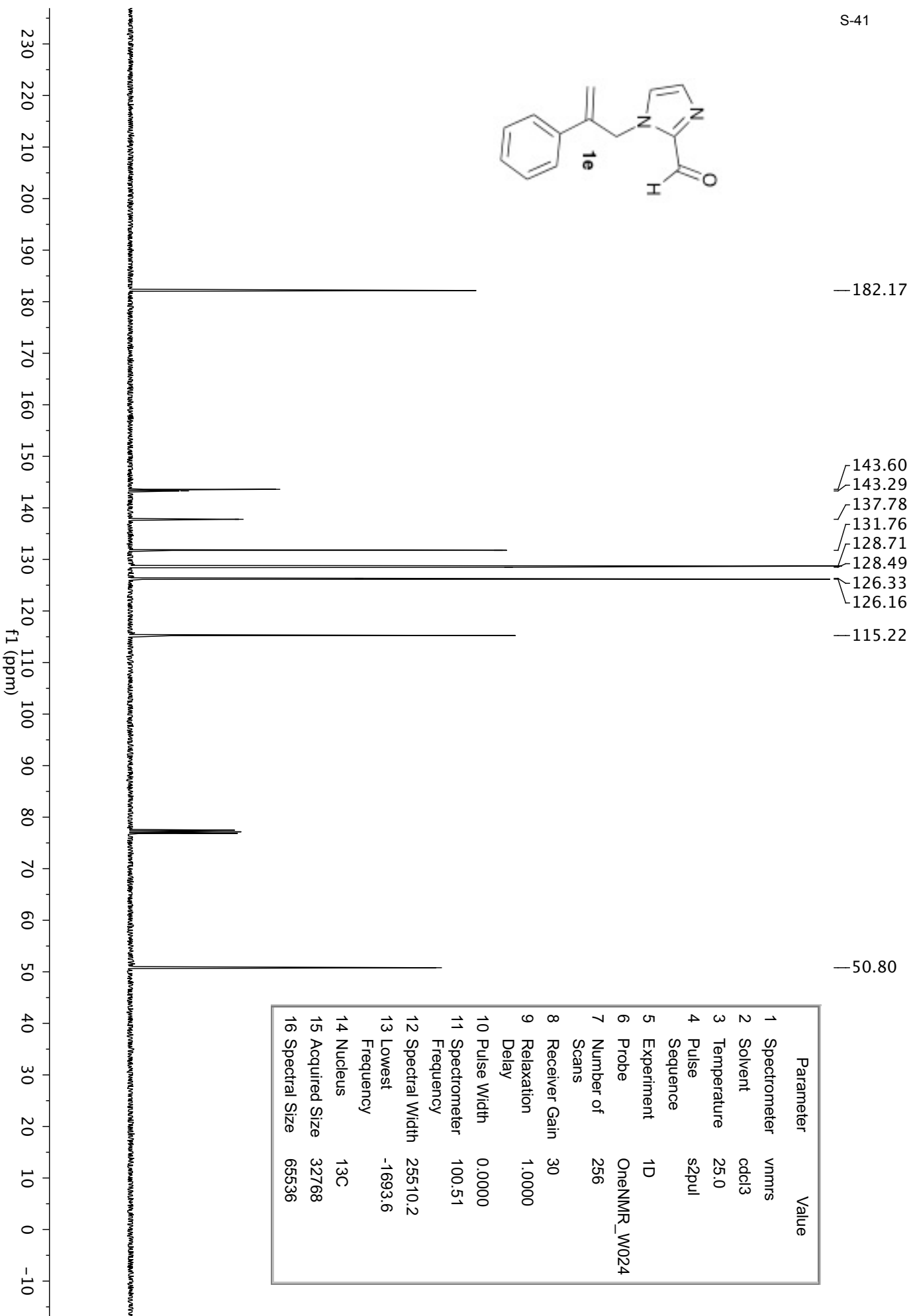
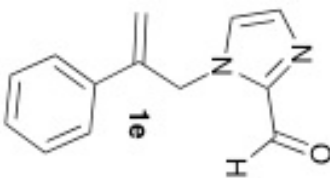
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7 Number of Scans	256
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
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12 Spectral Width	25510.2
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14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536

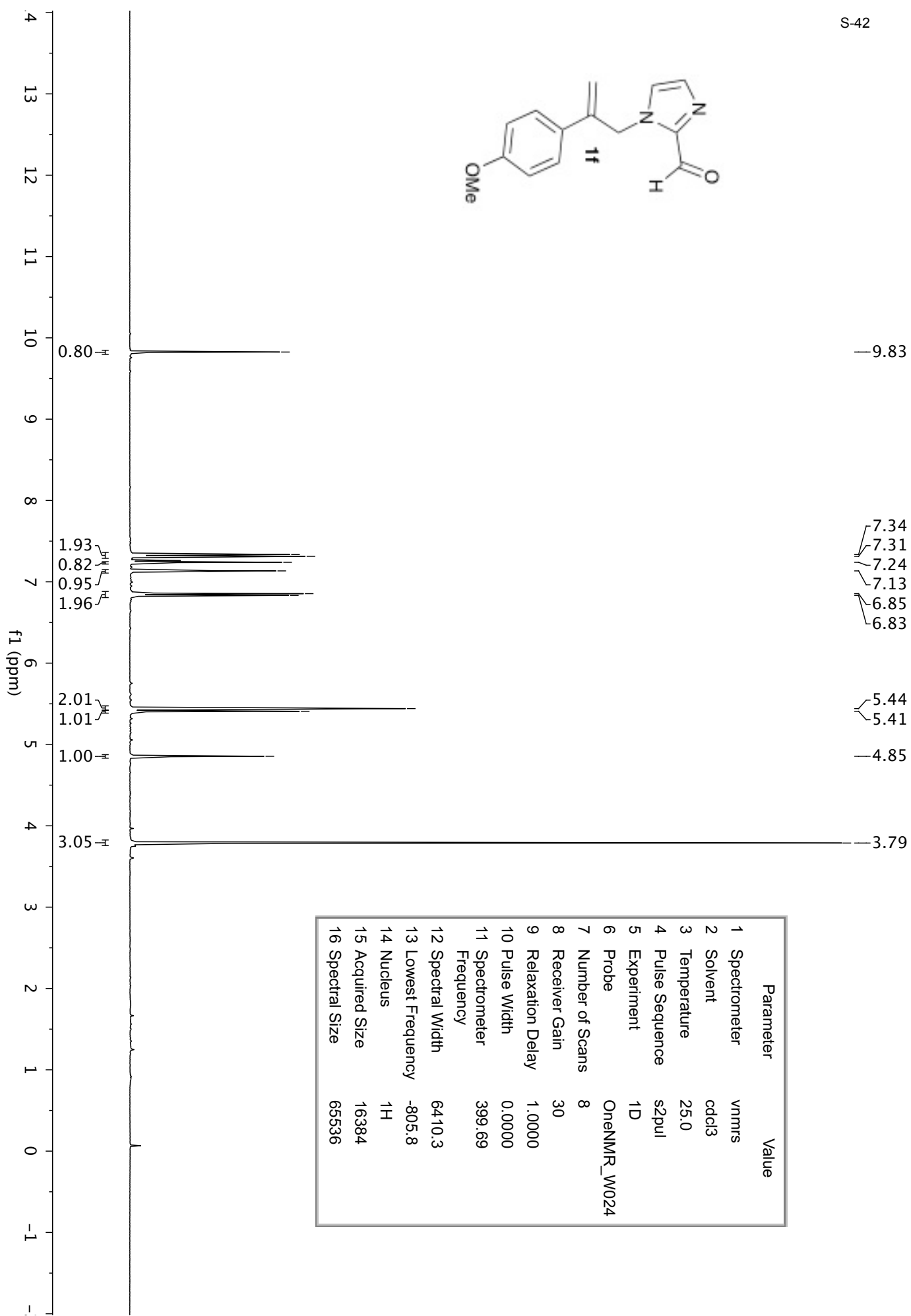
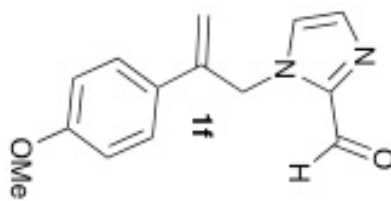


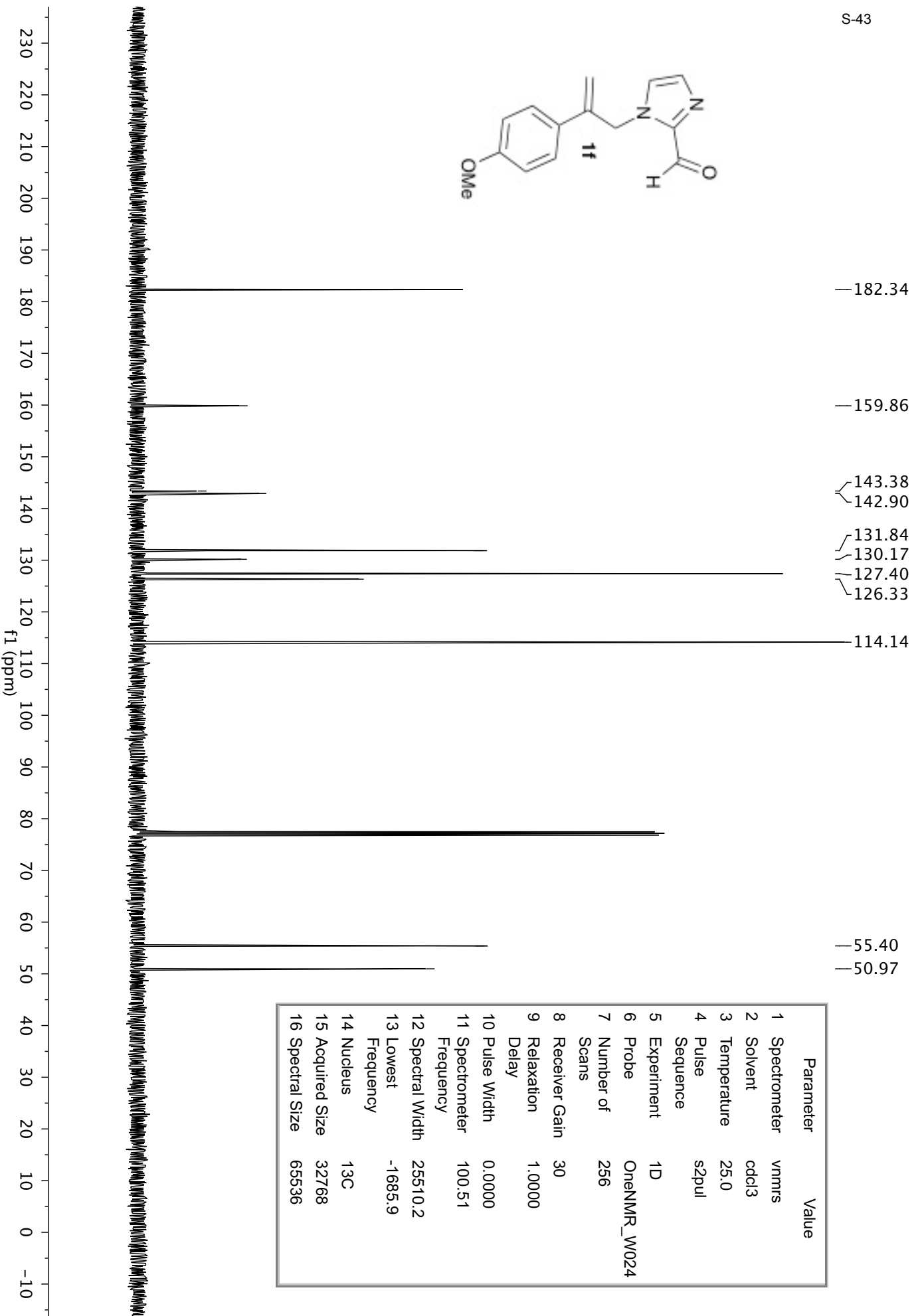
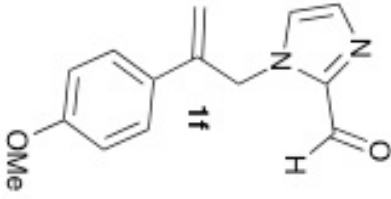


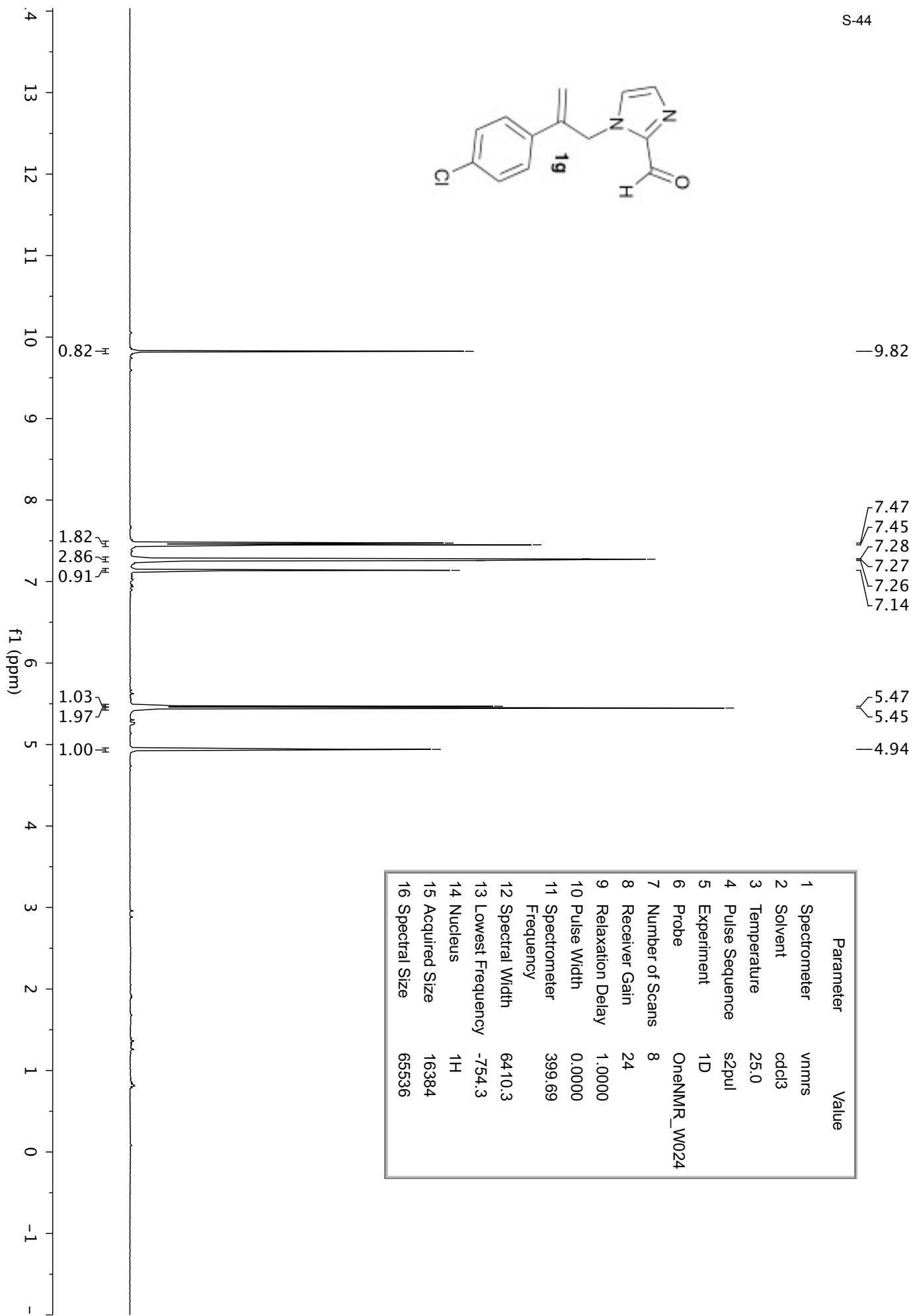
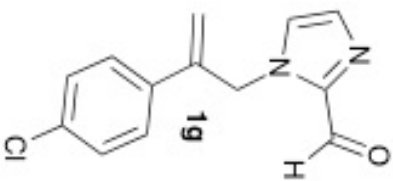




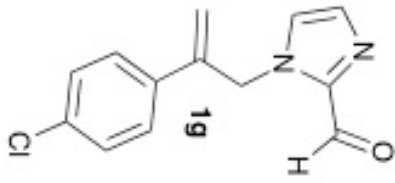








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10 Pulse Width	0.0000
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14 Nucleus	¹ H
15 Acquired Size	16384
16 Spectral Size	65536

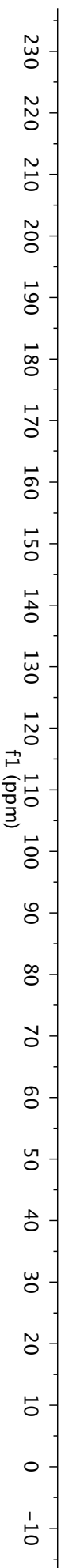


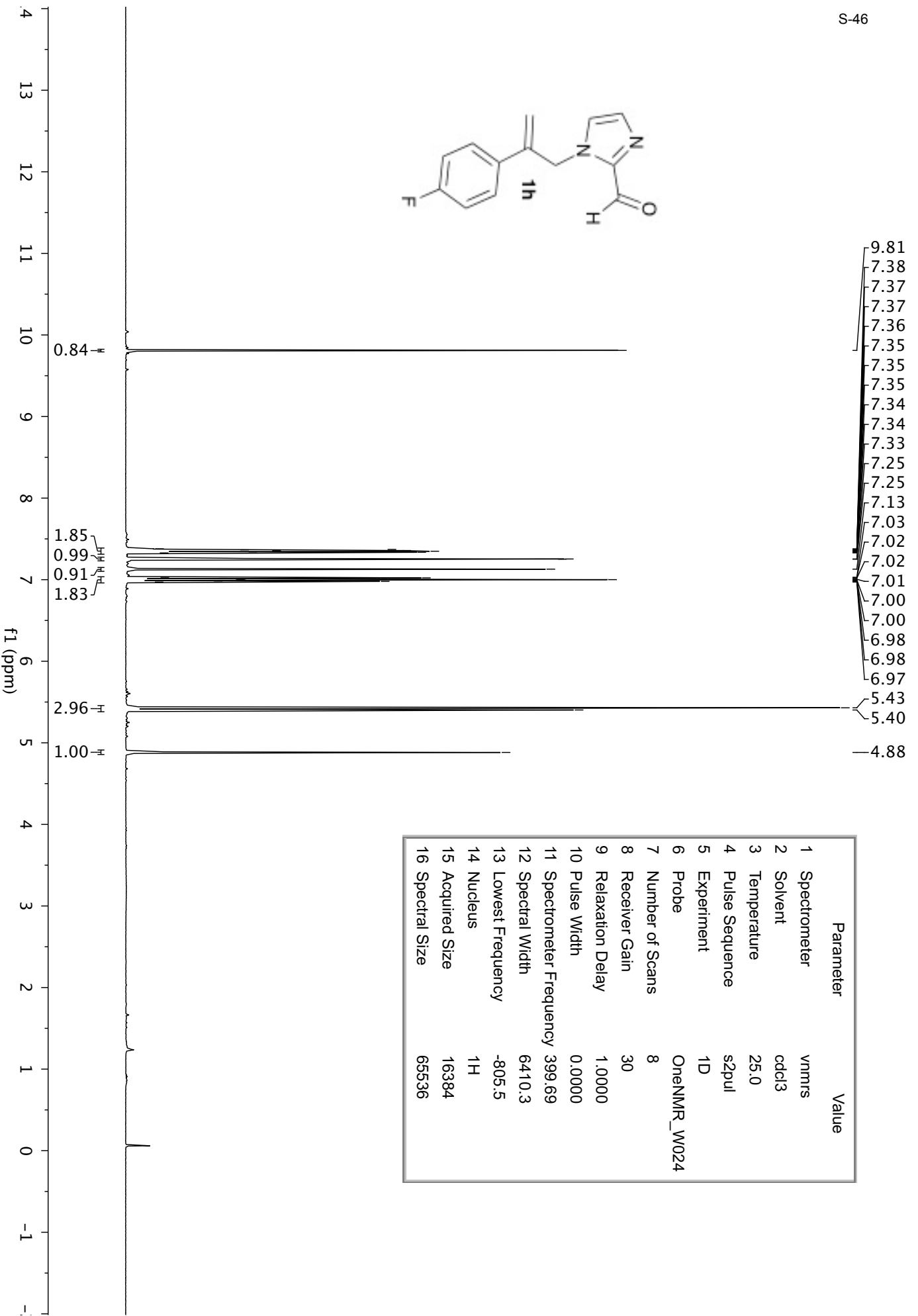
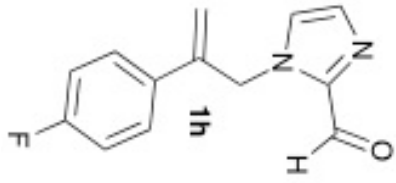
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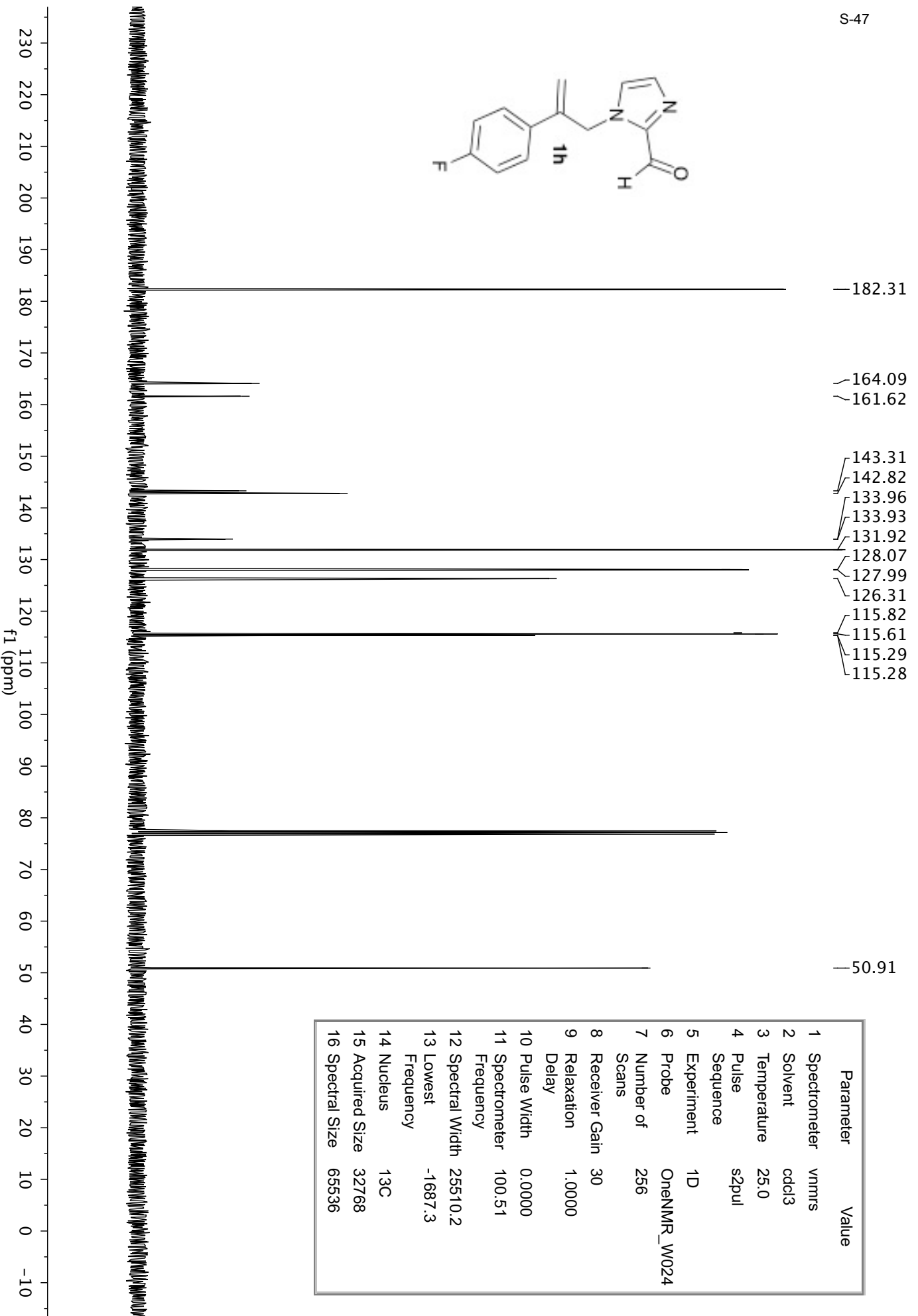
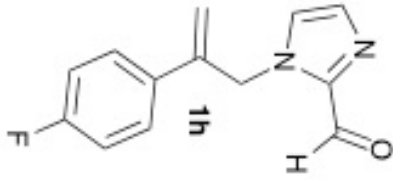
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—50.67

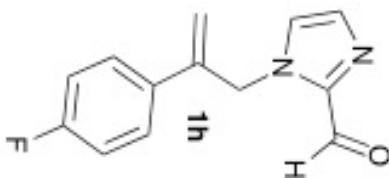
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14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



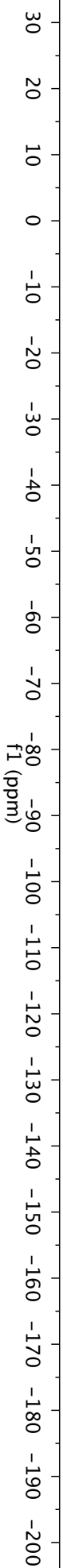


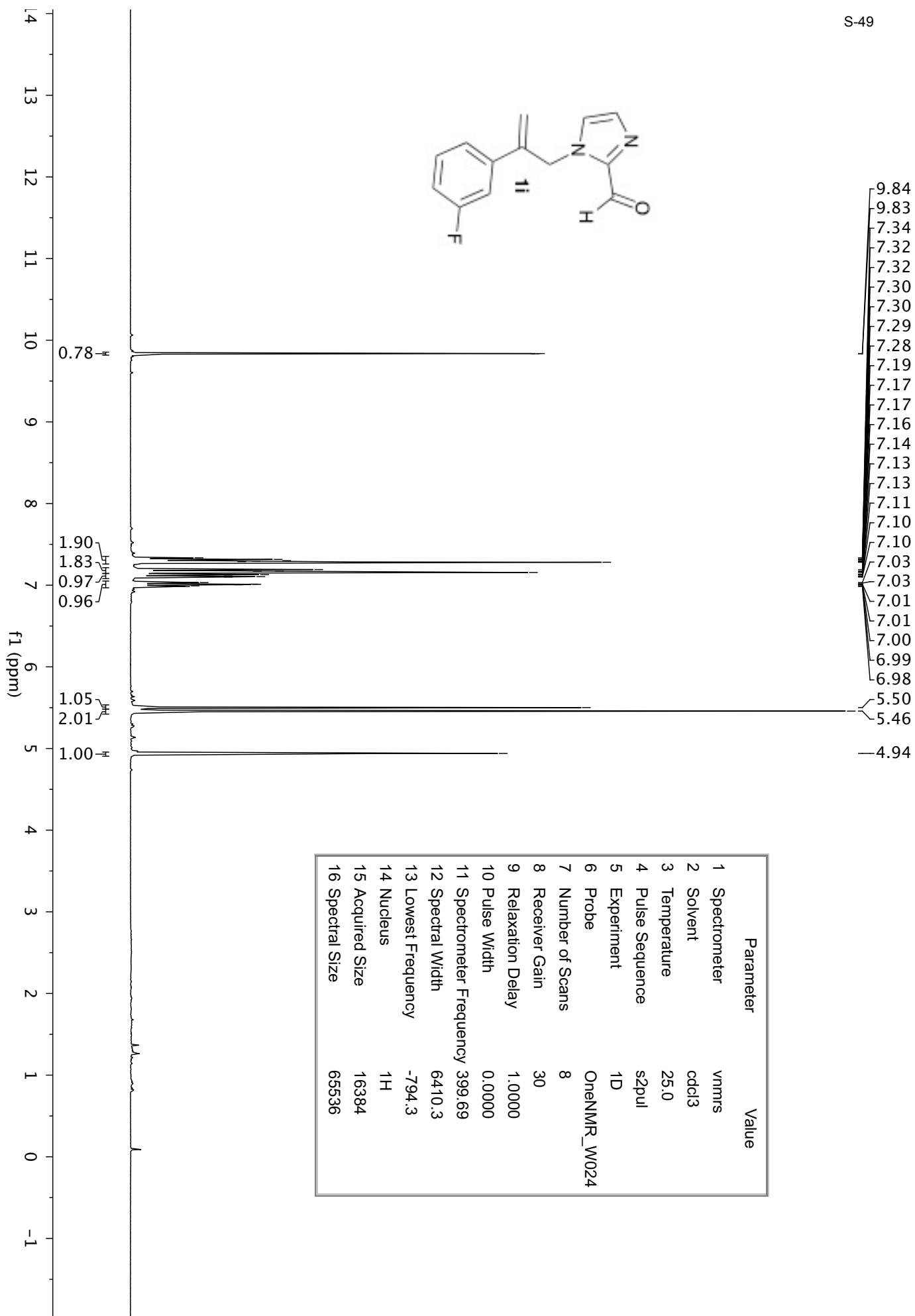
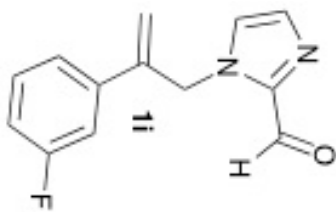


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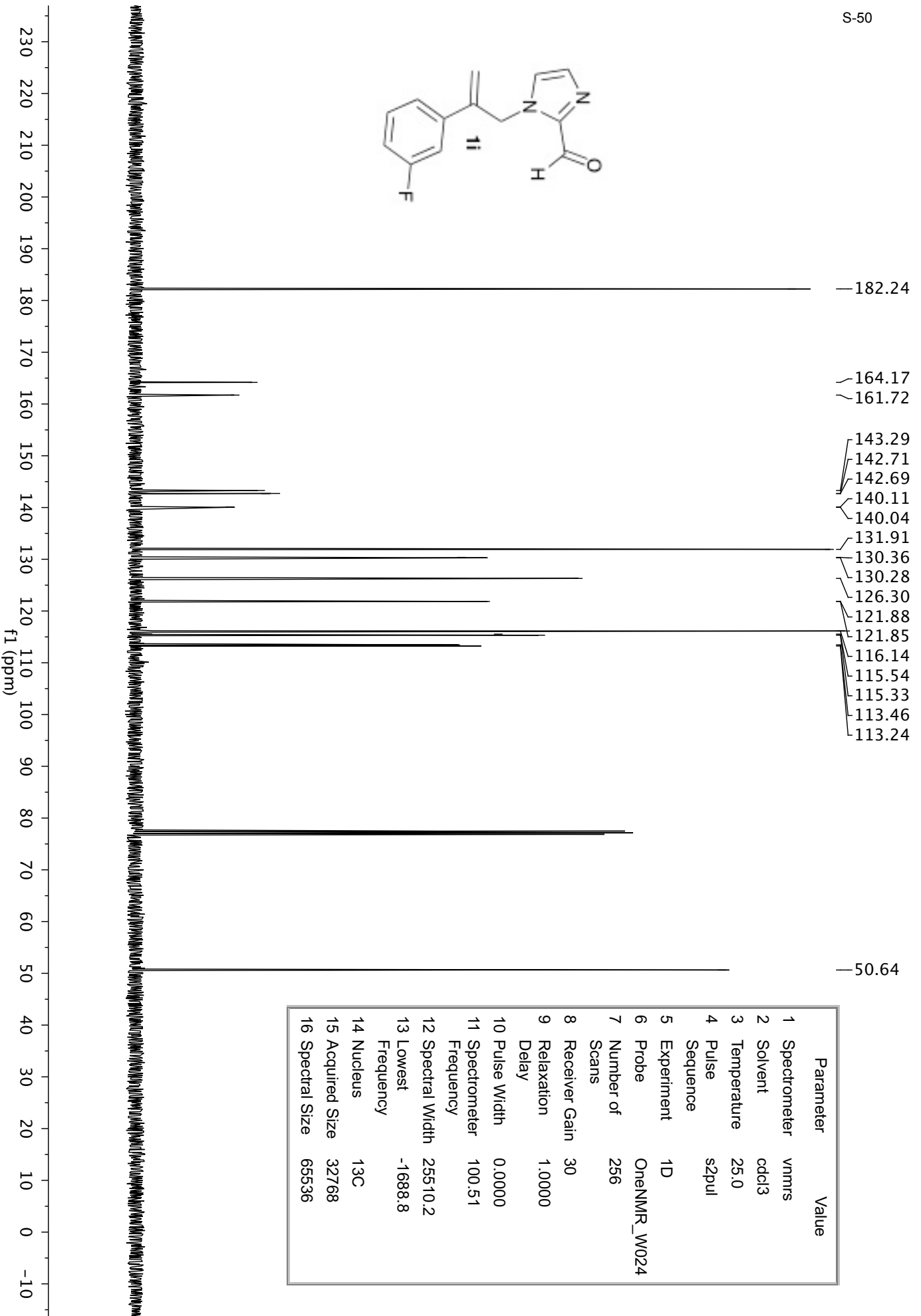
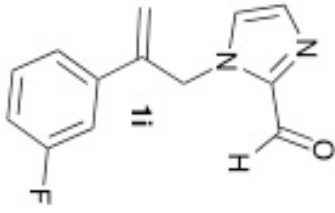


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15 Acquired Size	65536
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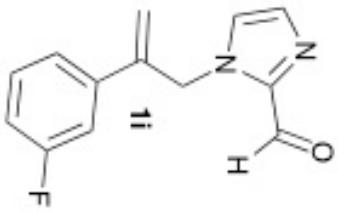




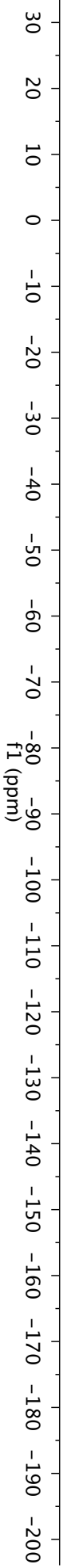
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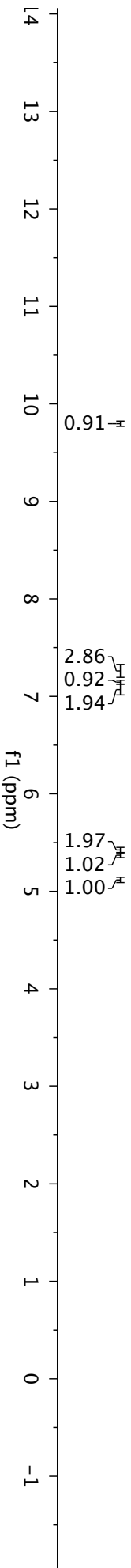
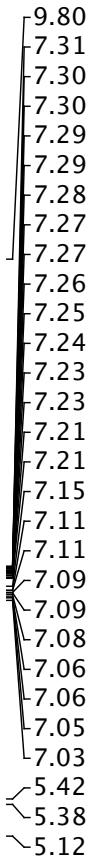
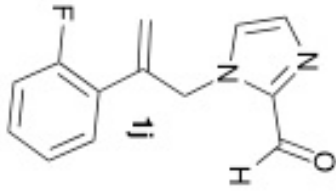


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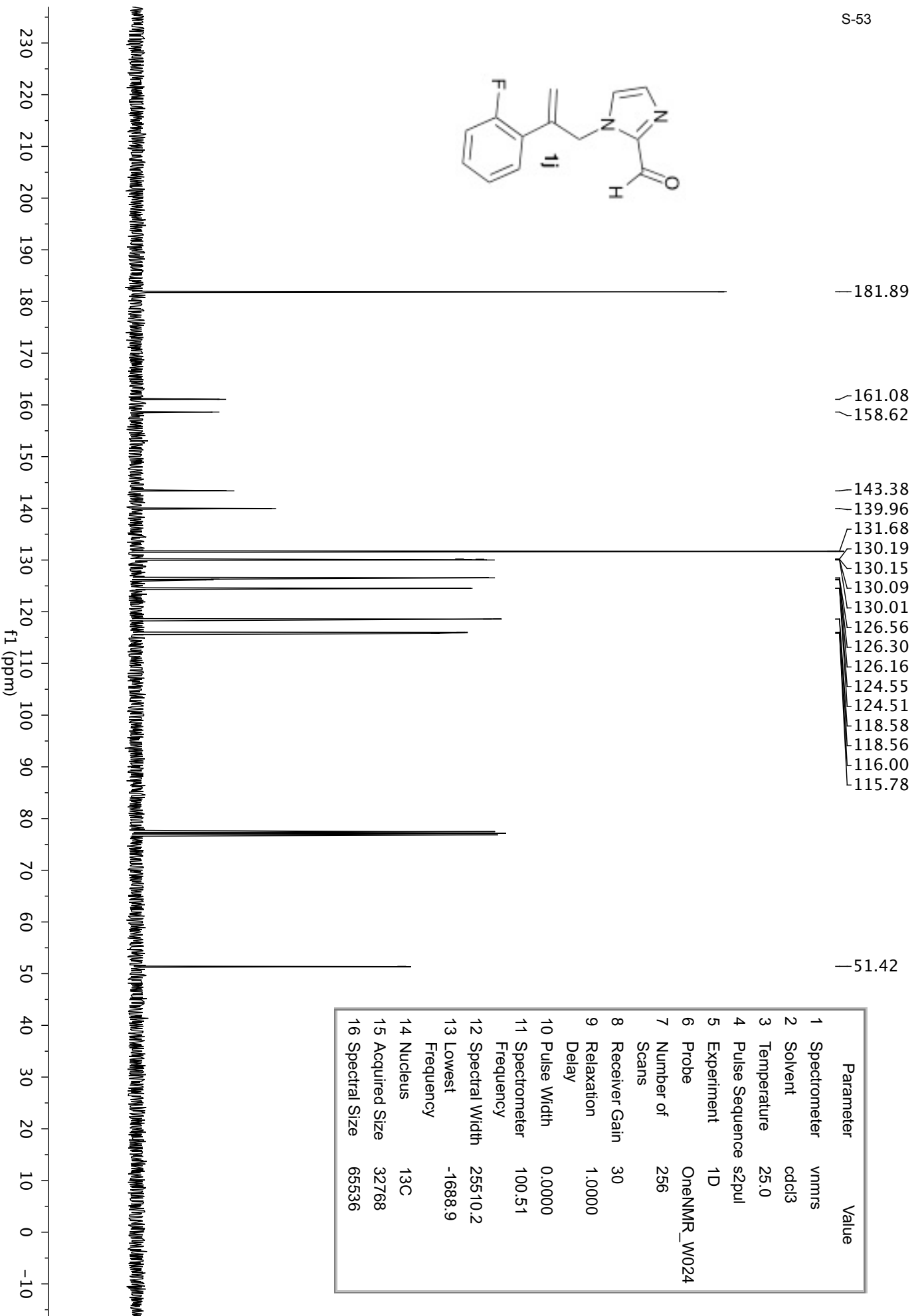
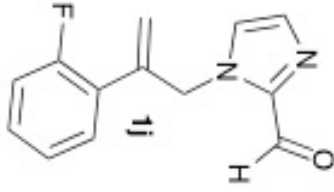


Parameter	Value
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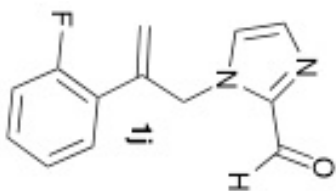




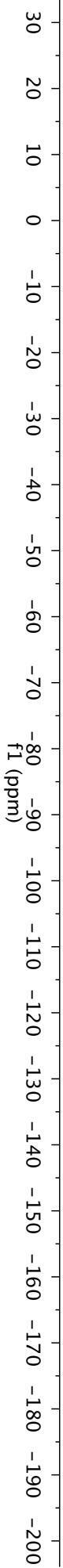
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7 Number of Scans	8
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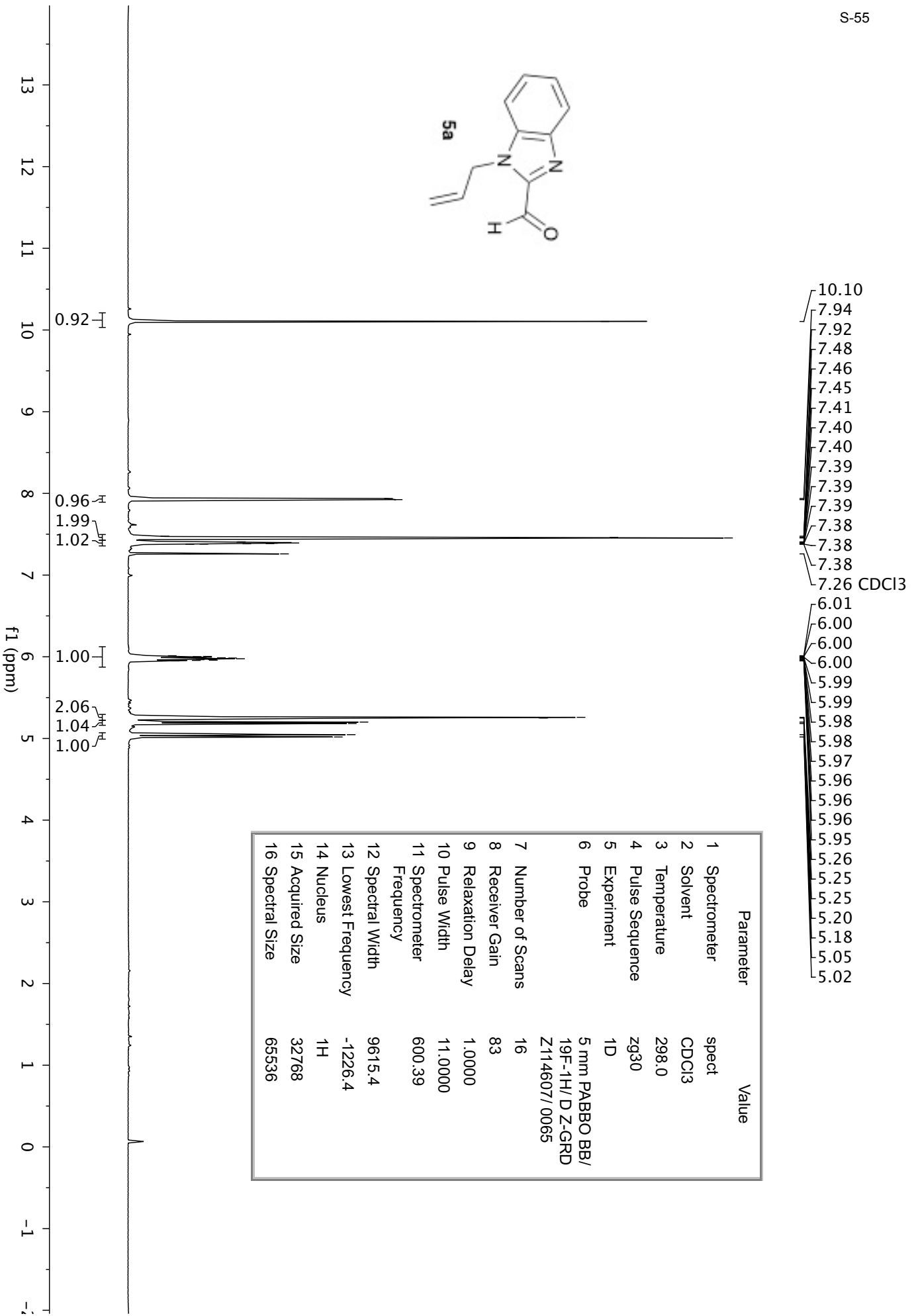
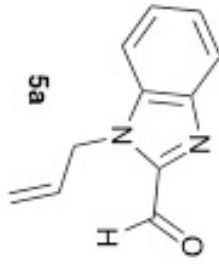


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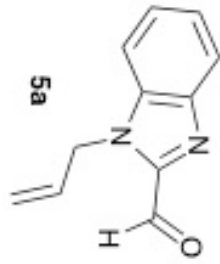


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10 Pulse Width	0.0000
11 Spectrometer Frequency	376.05
12 Spectral Width	89285.7
13 Lowest Frequency	-76610.2
14 Nucleus	19F
15 Acquired Size	65536
16 Spectral Size	131072





— 184.89



145.85

142.98

136.43

132.11

127.04

124.27

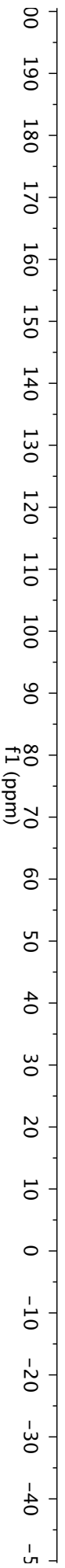
122.55

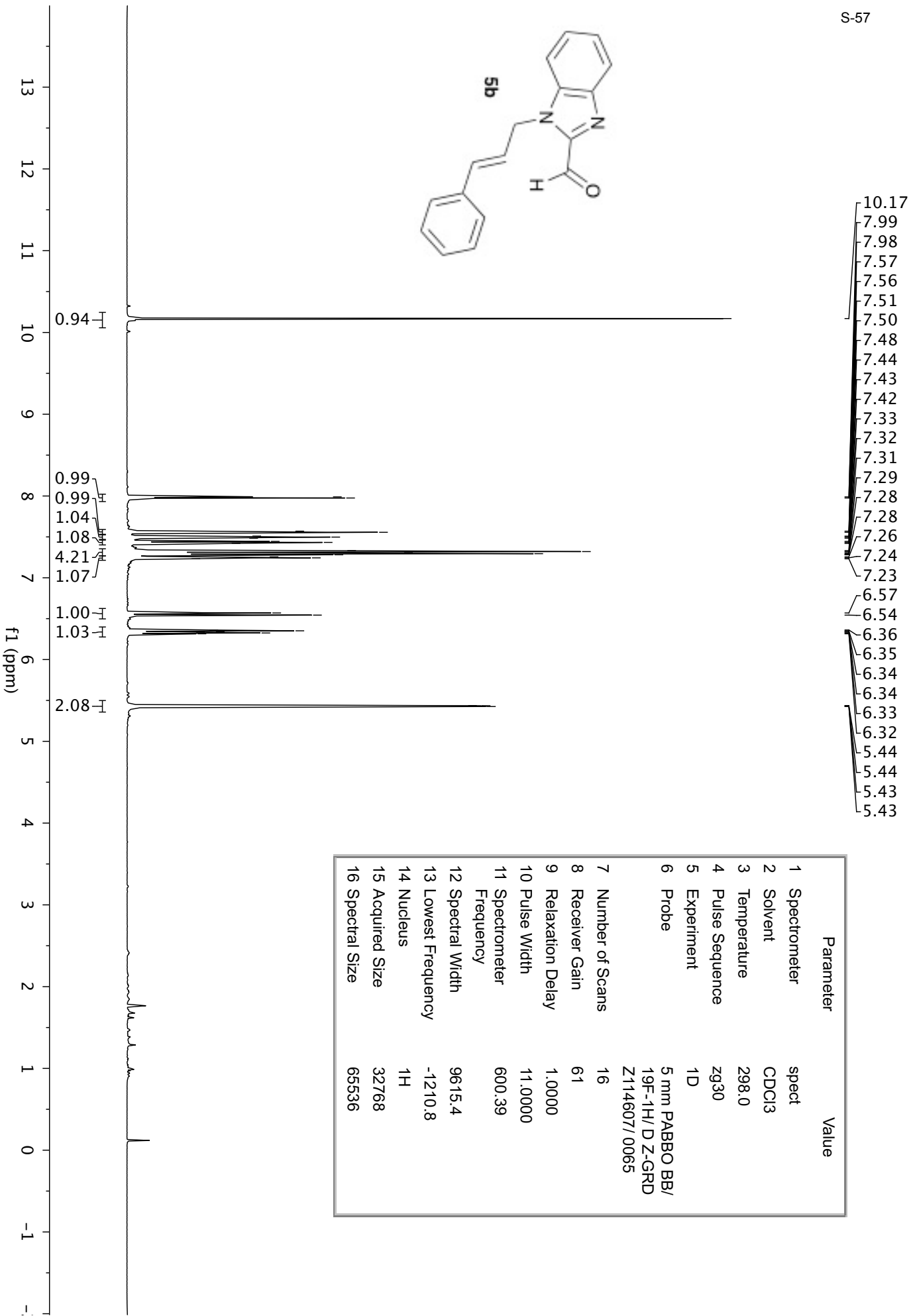
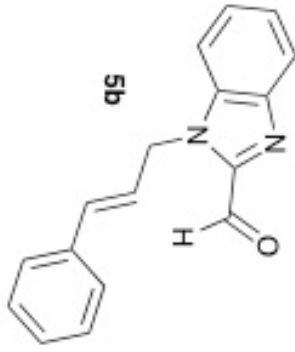
117.83

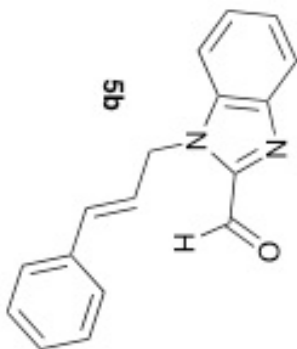
111.25

— 46.94

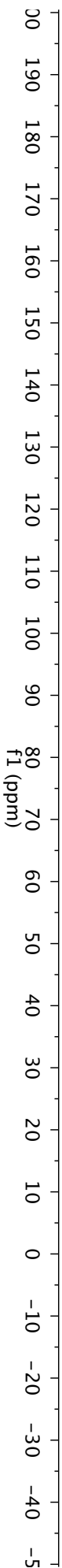
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	232
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7601.2
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536





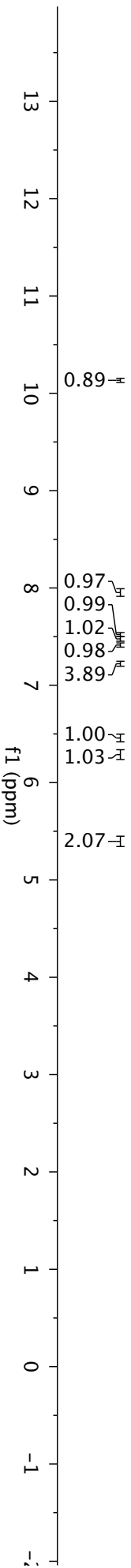
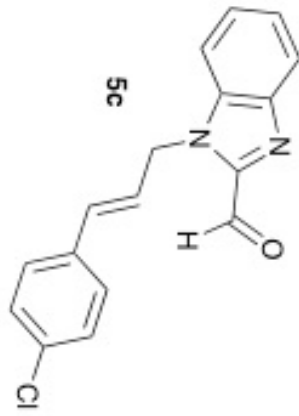


- 184.92
- 145.77
- 142.98
- 136.34
- 135.84
- 133.36
- 128.65
- 128.19
- 127.06
- 126.60
- 124.27
- 123.18
- 122.54
- 111.24



— 46.57

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zpgp30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D-Z-GRD Z114607/ 0065
7 Number of Scans	225
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7612.7
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536



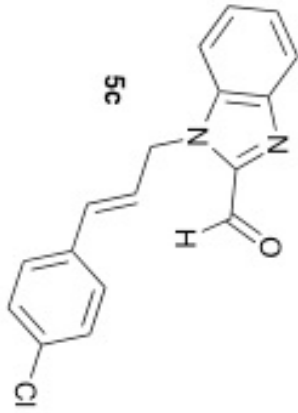
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7.96
7.95
7.53
7.51
7.49
7.49
7.48
7.47
7.46
7.42
7.42
7.41
7.41
7.40
7.40
7.24
7.23
7.22
7.21
6.47
6.45
6.31
6.30
6.29
6.29
6.28
6.27
5.40
5.40
5.39
5.39

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/ 0065
7 Number of Scans	16
8 Receiver Gain	68
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1225.8
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536

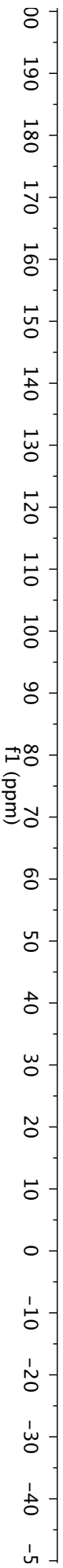
— 185.01

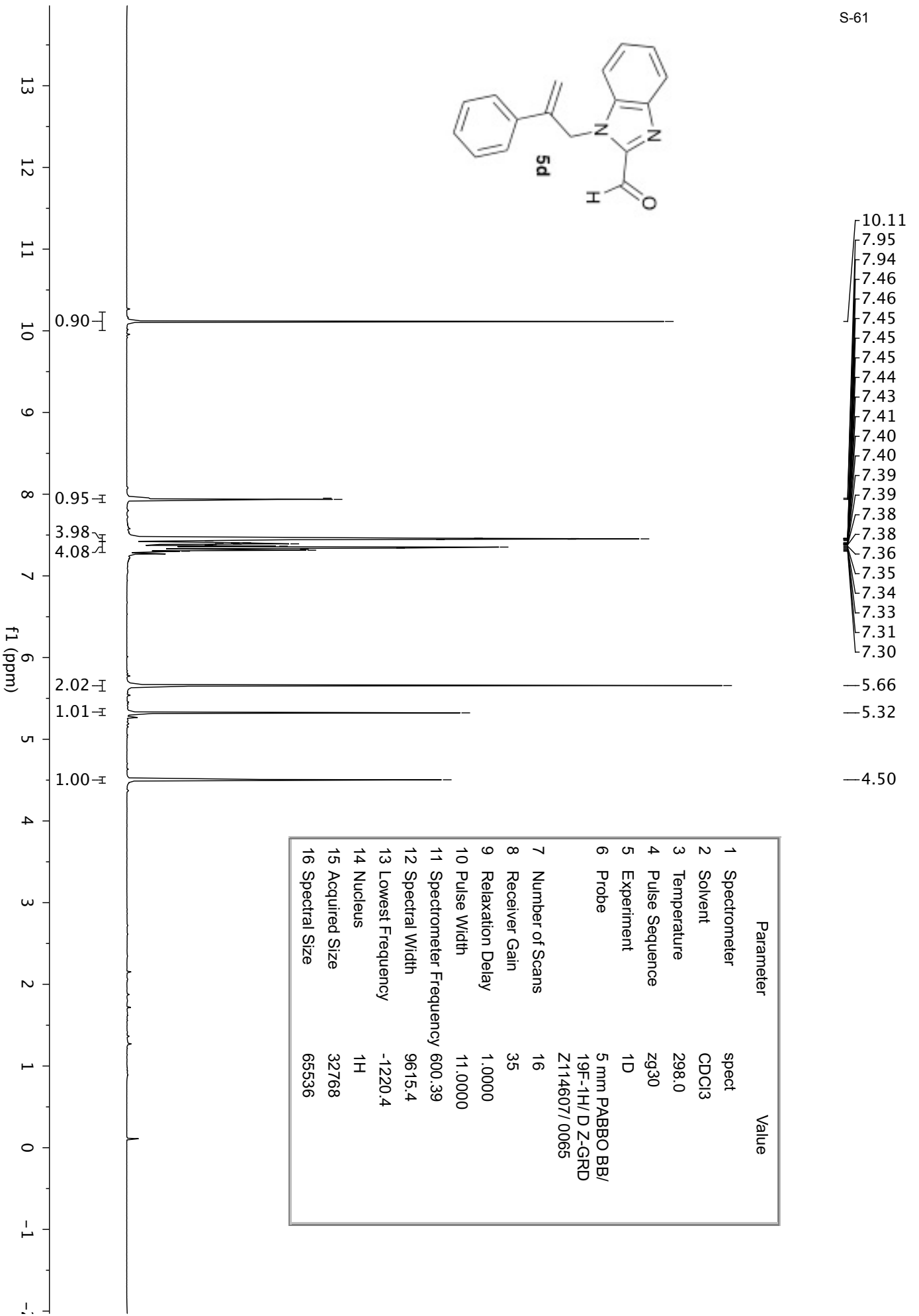
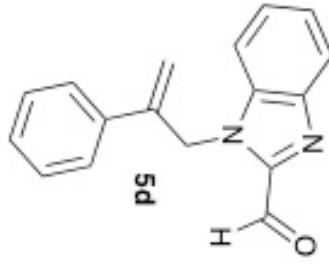
145.81
 143.04
 136.35
 134.39
 133.94
 132.12
 128.87
 127.86
 127.20
 124.39
 123.94
 122.68
 — 111.14

— 46.49



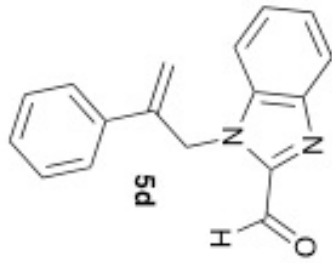
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.1
4 Pulse Sequence	zpgp30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/ 0065
7 Number of Scans	288
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7602.6
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536





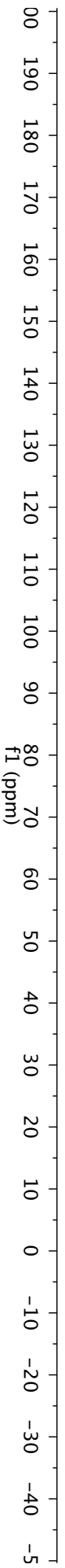
— 184.89

146.06
 143.31
 142.93
 138.53
 136.74
 128.73
 128.50
 127.18
 126.36
 124.35
 122.56
 113.11
 111.55



— 48.22

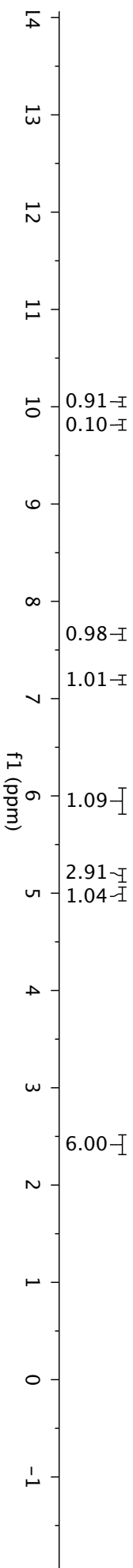
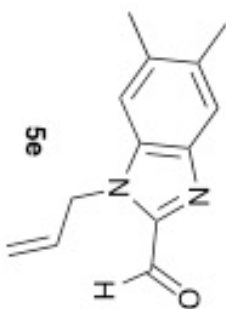
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	361
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7601.8
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



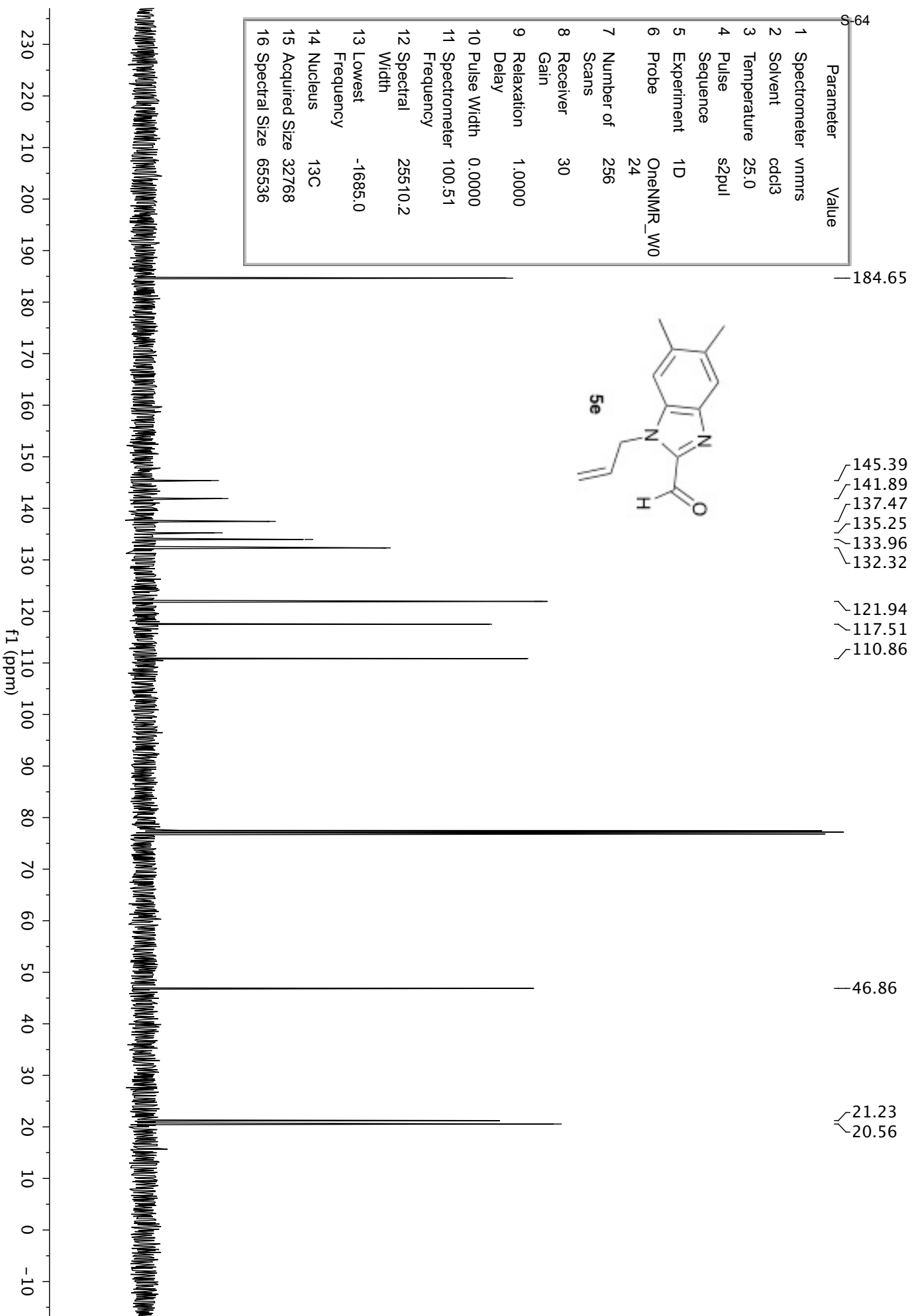
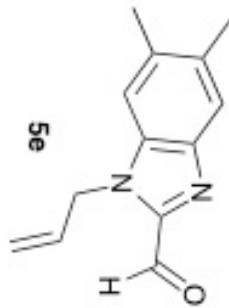
Parameter	Value
1 Spectrometer	vmnrs
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	szpul
5 Experiment	1D
6 Probe	OneNMNMR_W024
7 Number of Scans	8
8 Receiver Gain	18
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	399.69
12 Spectral Width	6410.3
13 Lowest Frequency	-786.7
14 Nucleus	1H
15 Acquired Size	16384
16 Spectral Size	65536

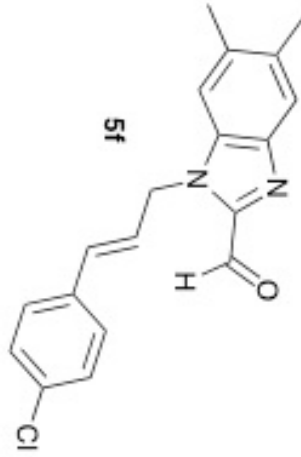
10.05

- 7.66
- 7.19
- 6.02
- 6.01
- 6.00
- 5.99
- 5.98
- 5.97
- 5.97
- 5.96
- 5.94
- 5.93
- 5.21
- 5.20
- 5.20
- 5.19
- 5.19
- 5.18
- 5.17
- 5.17
- 5.16
- 5.02
- 5.02
- 5.02
- 4.98
- 4.98
- 4.97
- 2.42
- 2.39



Parameter	Value
1 Spectrometer	nmrns
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	szpul
5 Experiment	1D
6 Probe	OneNMNMR_w0 24
7 Number of Scans	256
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	100.51
12 Spectral Width	25510.2
13 Lowest Frequency	-1685.0
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536

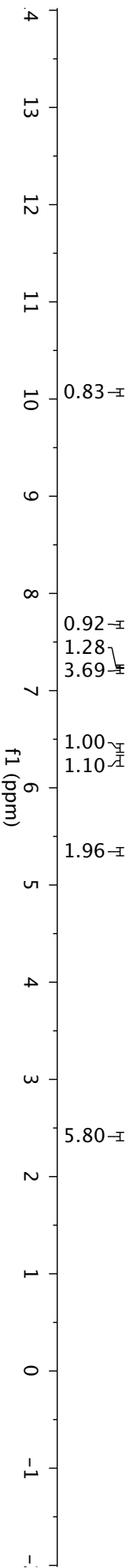




— 10.07

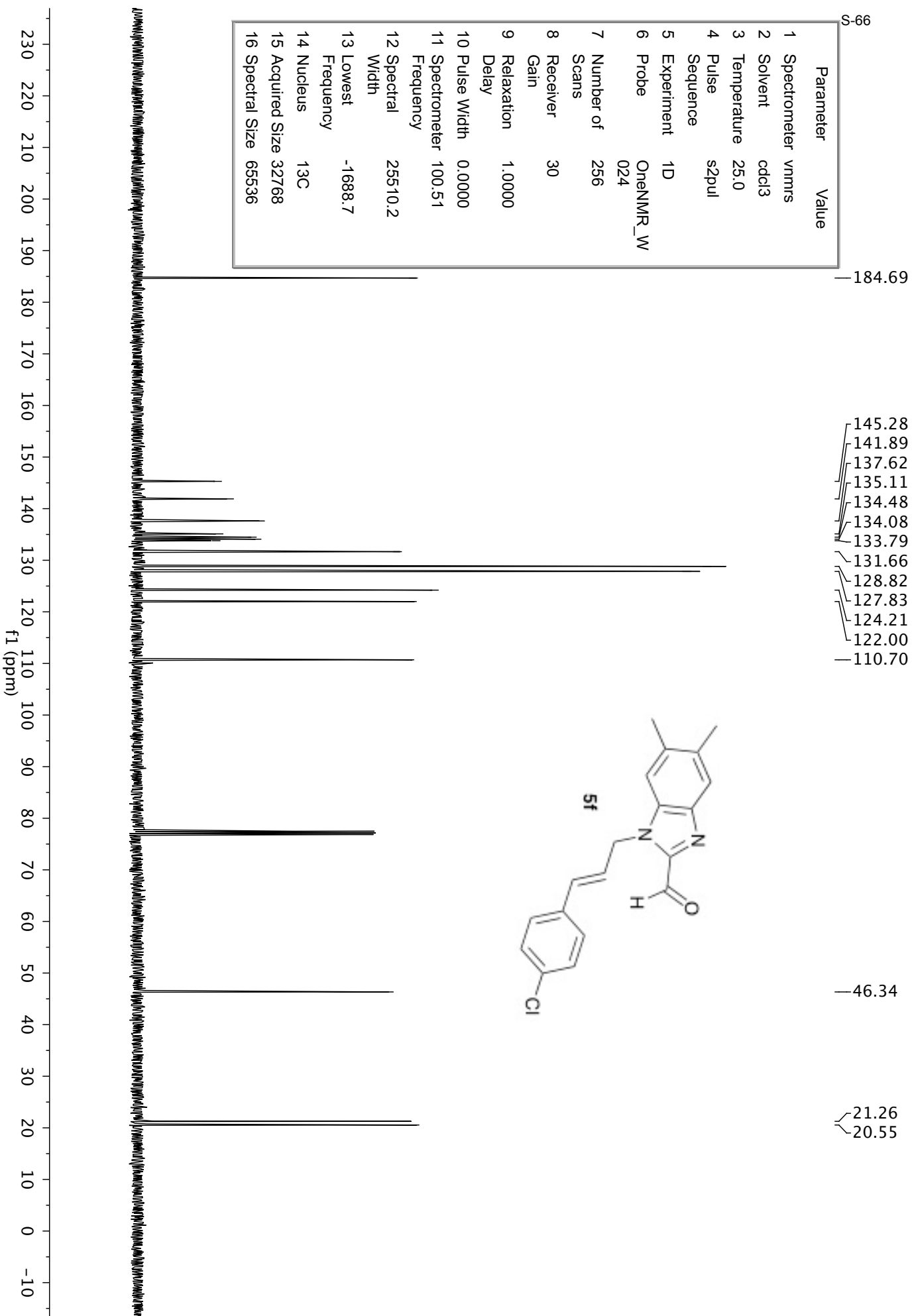
7.68
7.25
7.22
6.43
6.39
6.31
6.30
6.29
6.27
6.26
6.25
5.35
5.33

2.42
2.40

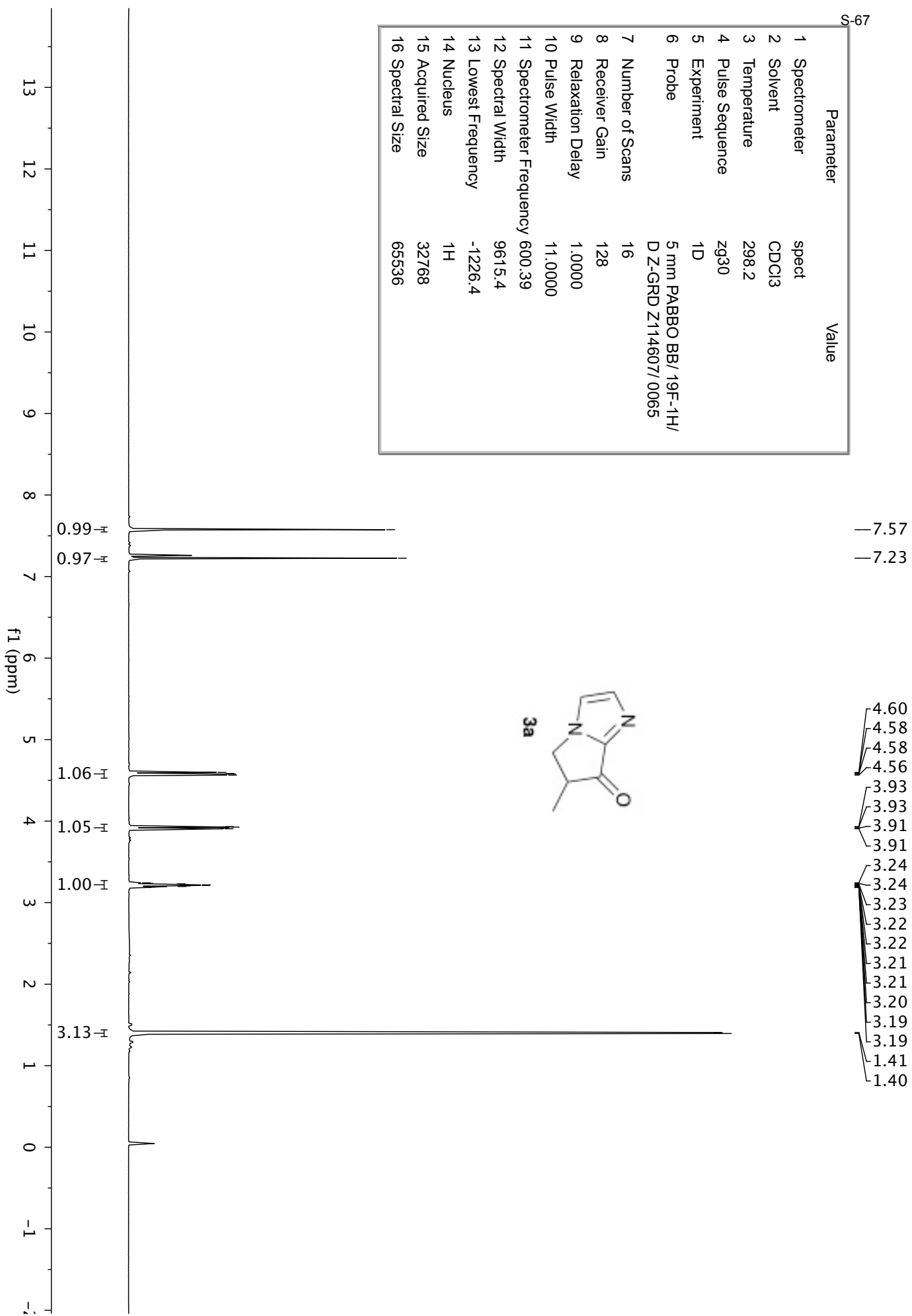


Parameter	Value
1 Spectrometer	vmrms
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	s2pul
5 Experiment	1D
6 Probe	OneNMR_W024
7 Number of Scans	8
8 Receiver Gain	18
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	399.69
12 Spectral Width	6410.3
13 Lowest Frequency	-805.7
14 Nucleus	¹ H
15 Acquired Size	16384
16 Spectral Size	65536

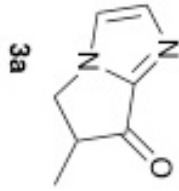
Parameter	Value
1 Spectrometer	vmrms
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	s2pul
5 Experiment	1D
6 Probe	OneNMW_024
7 Number of Scans	256
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	100.51
12 Spectral Width	25510.2
13 Lowest Frequency	-1688.7
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.2
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/ 0065
7 Number of Scans	16
8 Receiver Gain	128
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1226.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



S-68
— 190.27



— 146.53

— 139.35

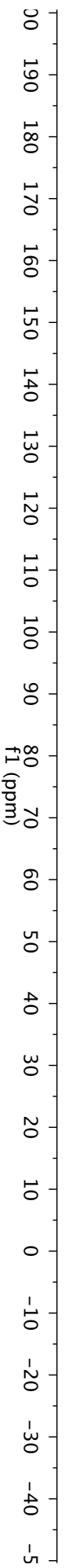
— 119.97

— 48.65

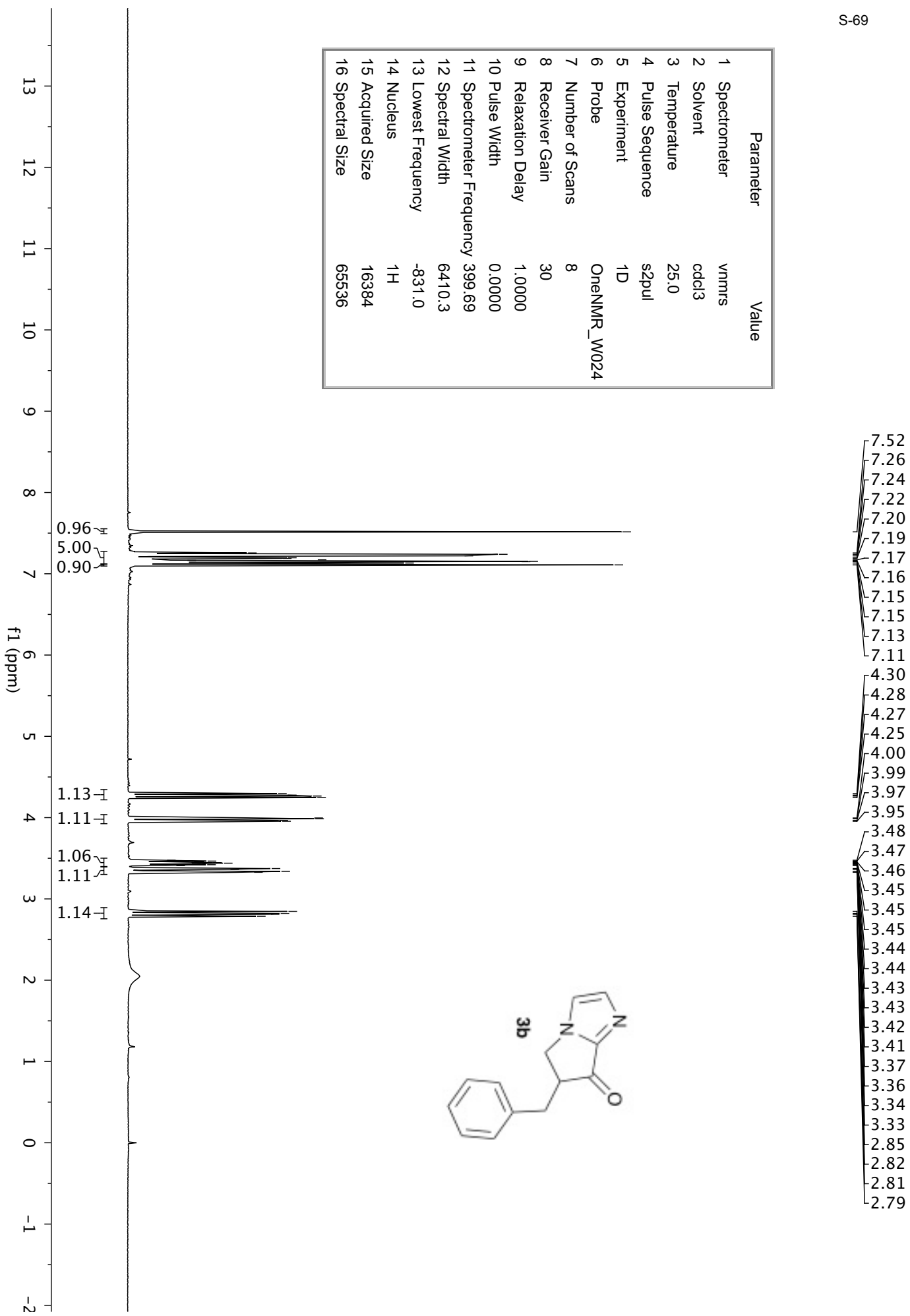
— 44.92

— 15.40

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.2
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ DZ- GRD Z114607/ 0065
7 Number of Scans	158
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7604.2
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536



Parameter	Value
1 Spectrometer	vmrms
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	s2pul
5 Experiment	1D
6 Probe	OneNMR_W024
7 Number of Scans	8
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	399.69
12 Spectral Width	6410.3
13 Lowest Frequency	-831.0
14 Nucleus	¹ H
15 Acquired Size	16384
16 Spectral Size	65536



— 188.77

~ 146.68

~ 139.51

~ 137.70

~ 129.01

~ 128.85

~ 127.12

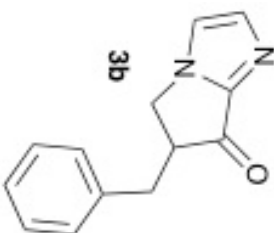
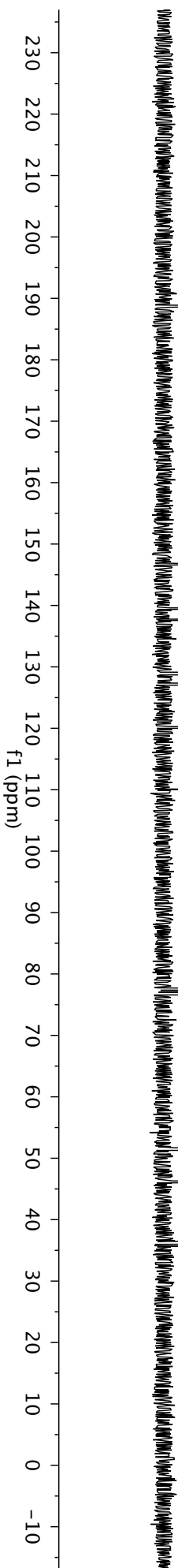
~ 120.17

— 51.51

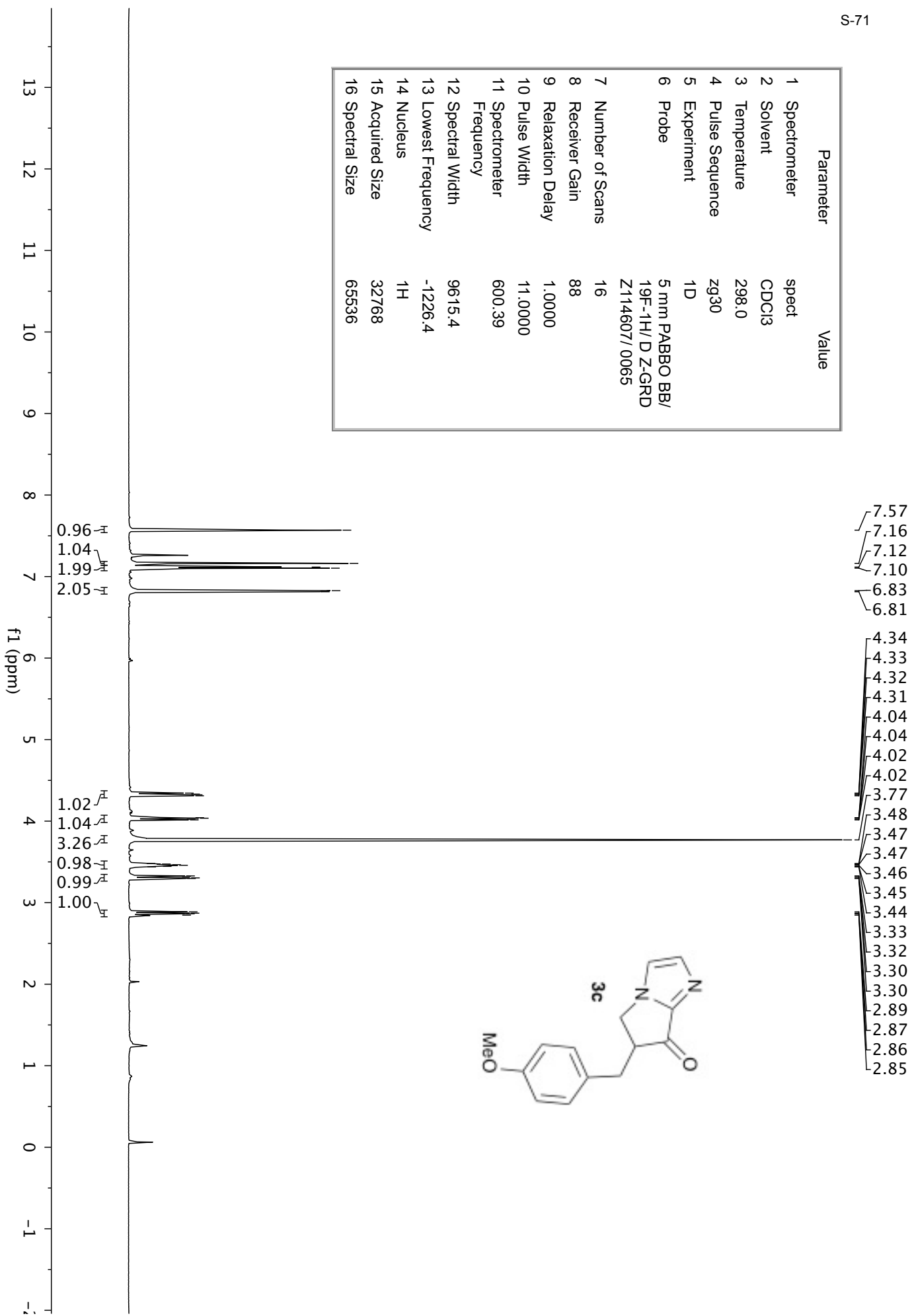
— 46.14

— 36.12

Parameter	Value
1 Spectrometer	vmrms
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	szpul
5 Experiment	1D
6 Probe	OneNMR_W024
7 Number of Scans	256
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	100.51
12 Spectral Width	25510.2
13 Lowest Frequency	-1688.4
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	88
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1226.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



S-72

— 188.91

— 158.70

— 146.81

— 139.46

— 129.92

— 129.53

— 120.13

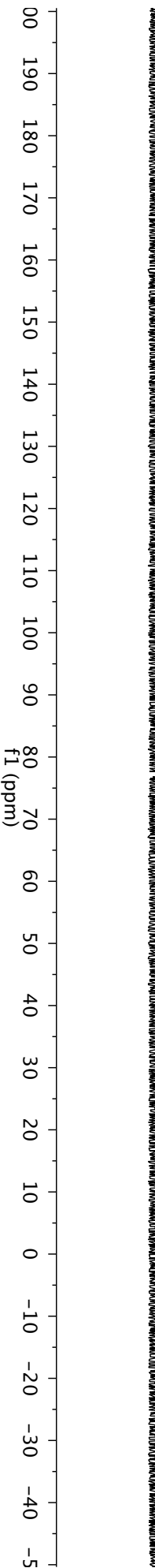
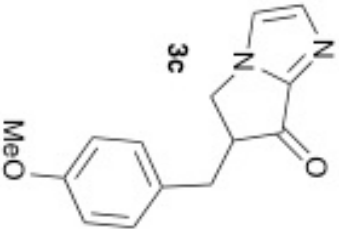
— 114.38

— 55.38

— 51.69

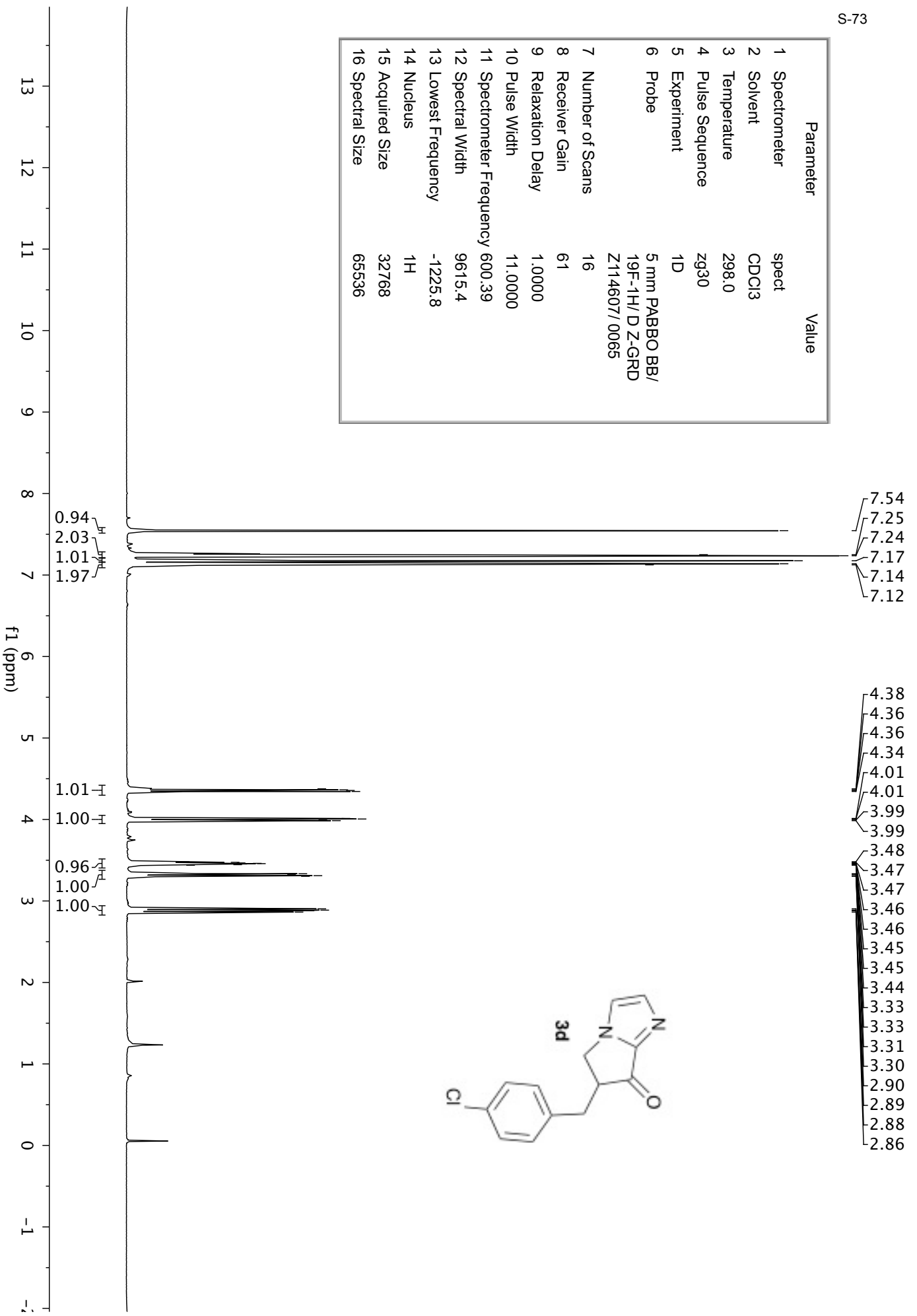
— 46.01

— 35.23

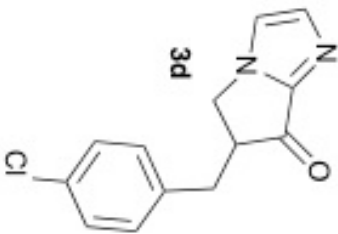


Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCI3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D-Z- GRD Z114607/ 0065
7 Number of Scans	708
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7602.0
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	61
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1225.8
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



S-74



— 188.40

~ 146.54
 ~ 139.52
 ~ 136.12
 ~ 132.94
 ~ 130.24
 ~ 129.08

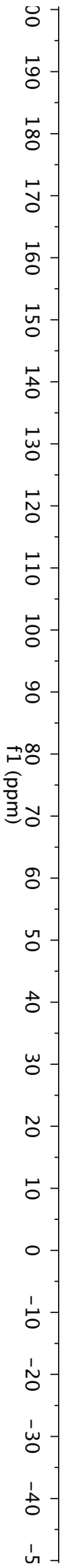
— 120.27

— 51.21

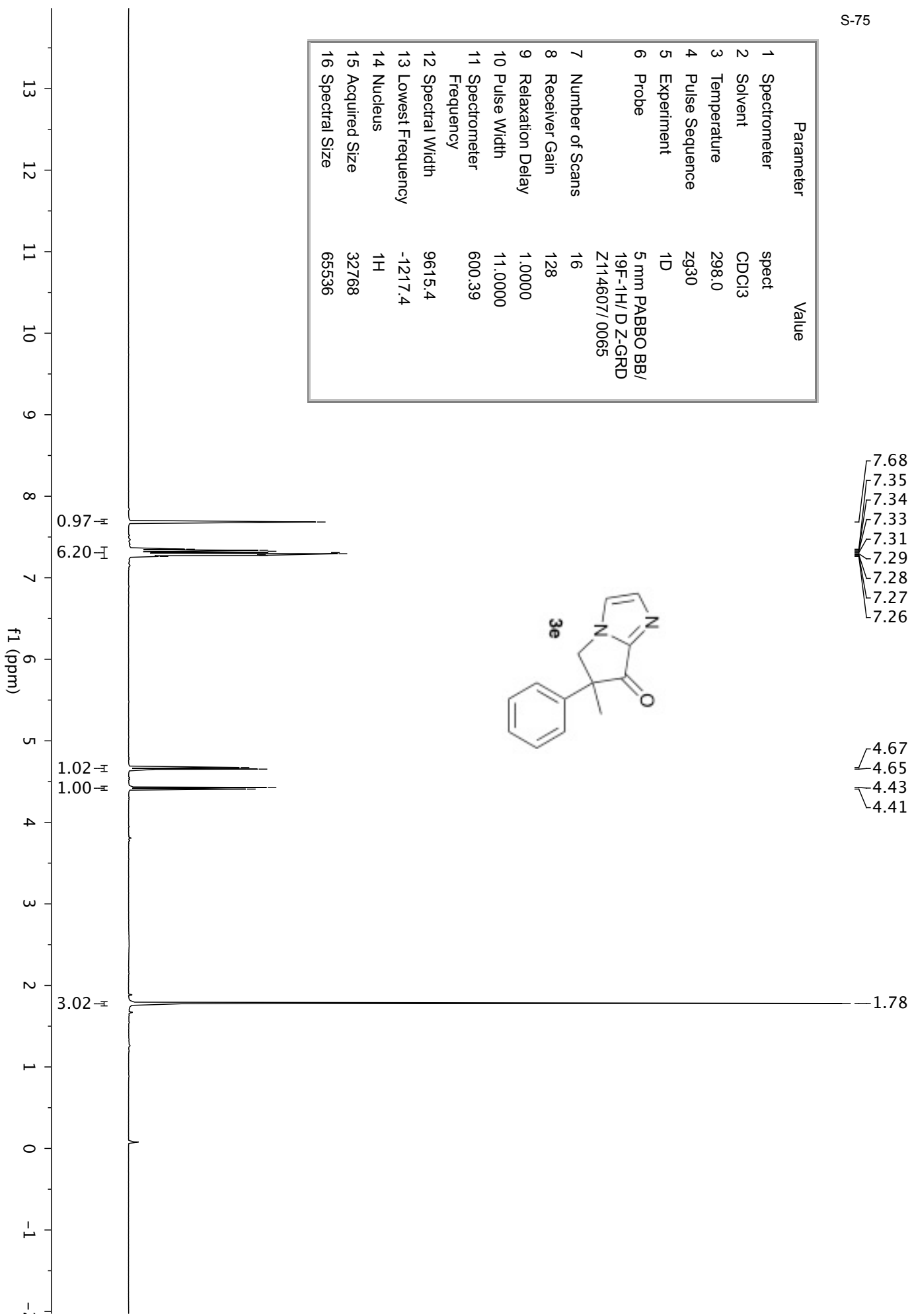
— 45.96

— 35.31

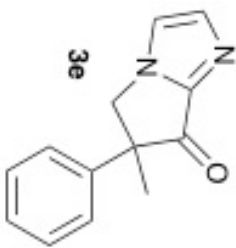
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/ DZ-GRD Z114607/ 0065
7 Number of Scans	266
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7608.2
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/D-Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	128
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1217.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



— 190.35

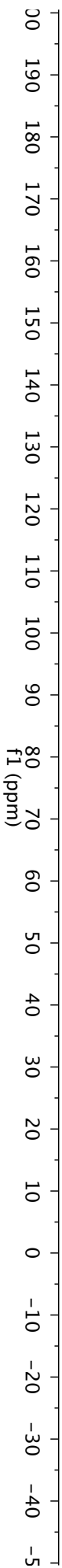


145.95
141.27
139.93

129.10
127.73
125.92
120.21

57.19
56.66

— 23.66



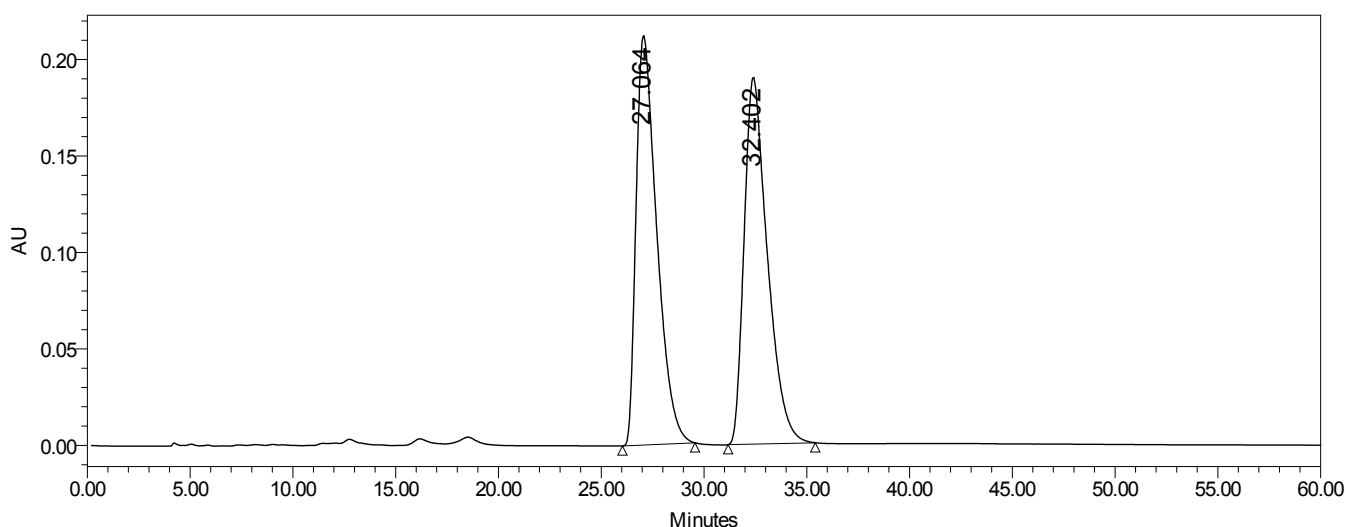
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	200
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7604.6
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



Injection Summary Report

SAMPLE INFORMATION

Sample Name:	JWN_1a_ADH90_10_1mpm	Acquired By:	System
Sample Type:	Unknown	Sample Set Name	James_ChemComm_racemic
Vial:	63	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #:	1	Processing Method	
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired:	7/27/2016 6:48:54 PM CDT		
Date Processed:	8/15/2016 11:13:54 PM CDT		



Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21667; Processing Method: jwn4_1a_ADH_90_10_1_mpm_254nm

Processed Channel Descr.: W2489 ChA 254nm

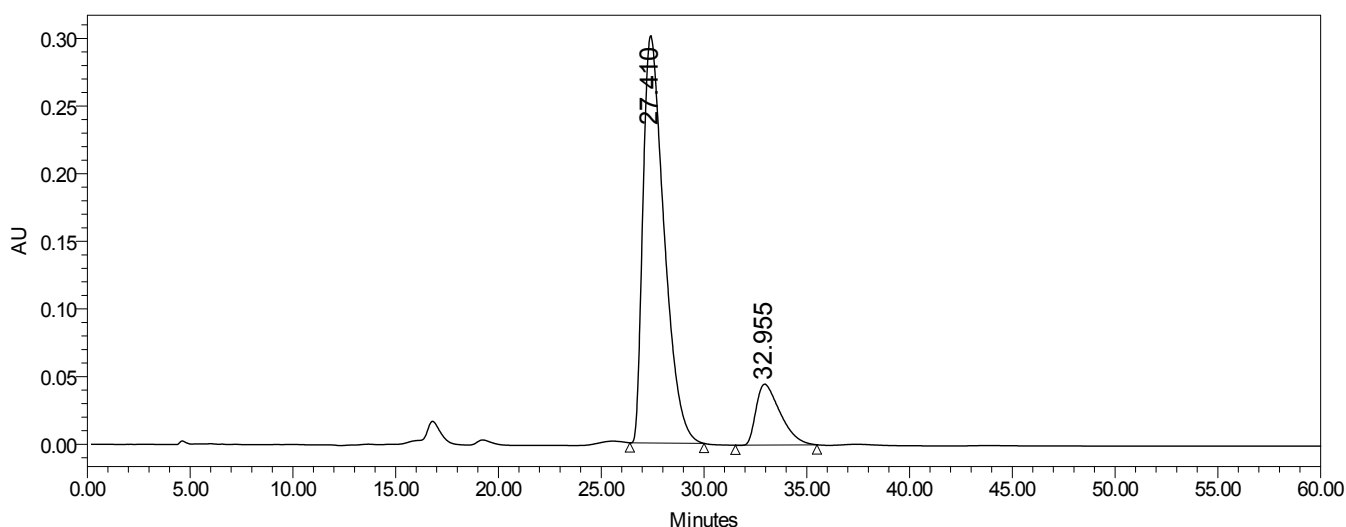
	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	27.064	14821276	49.87	212100
2	W2489 ChA 254nm	32.402	14899260	50.13	190013



Injection Summary Report

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	jwn4_75_asymmetric
Vial: 3	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1A_254nm
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/8/2016 8:48:15 PM CDT		
Date Processed: 8/15/2016 11:15:43 PM CDT		

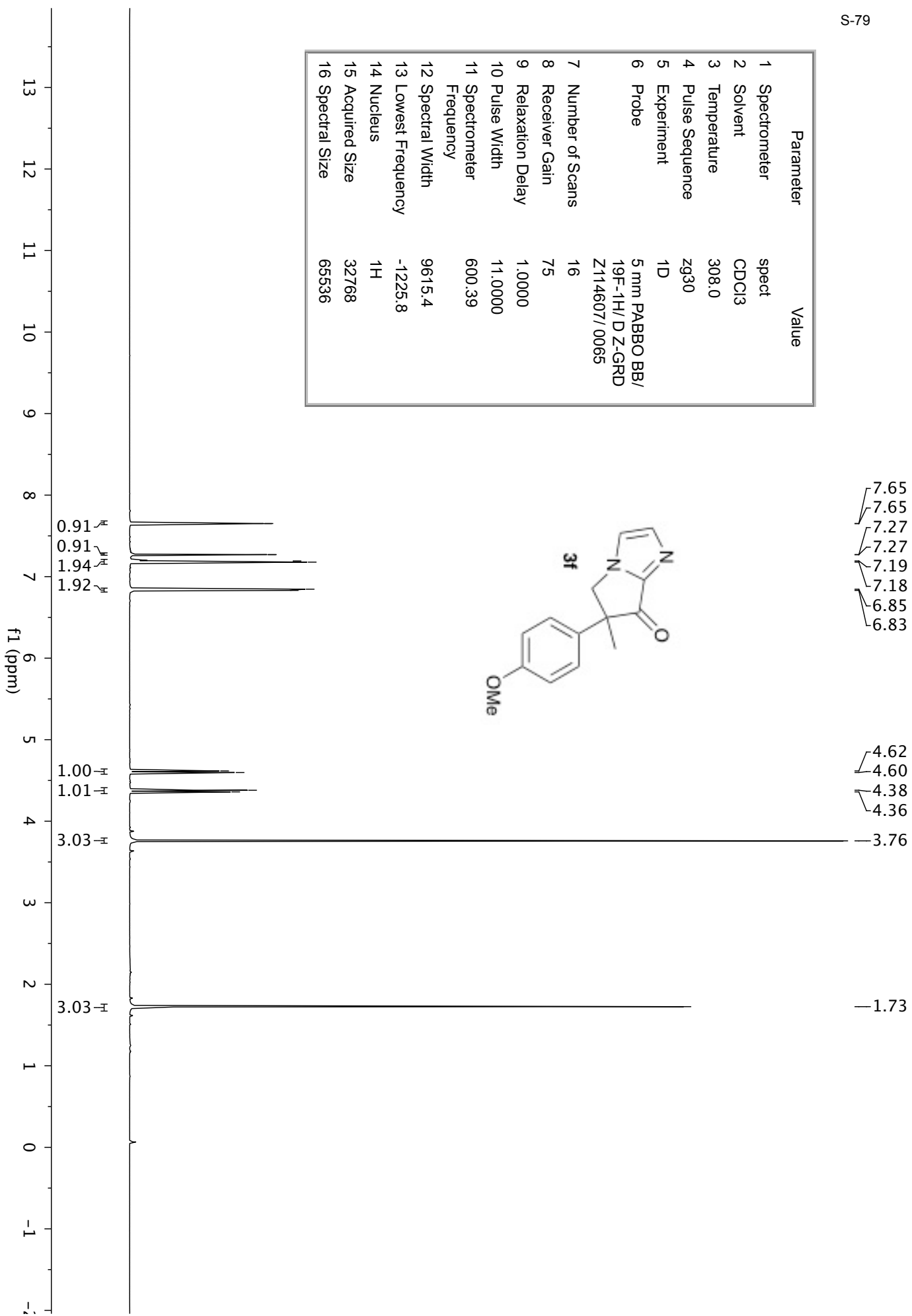


Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21669; Processing Method: jwn4_1A_254nm

Processed Channel Descr.: W2489 ChA 254nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	27.410	21458893	85.39	301014
2	W2489 ChA 254nm	32.955	3672257	14.61	45039

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl ₃
3 Temperature	308.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/D-Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	75
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1225.8
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



S-80

— 190.60

— 159.06

146.03

139.84

133.33

127.09

120.09

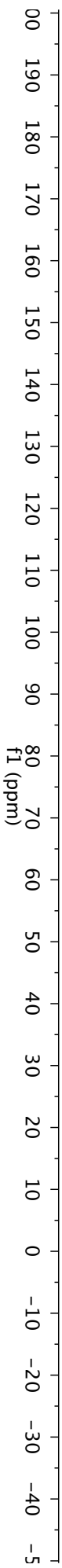
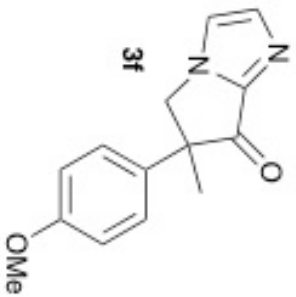
114.48

57.20

56.12

55.42

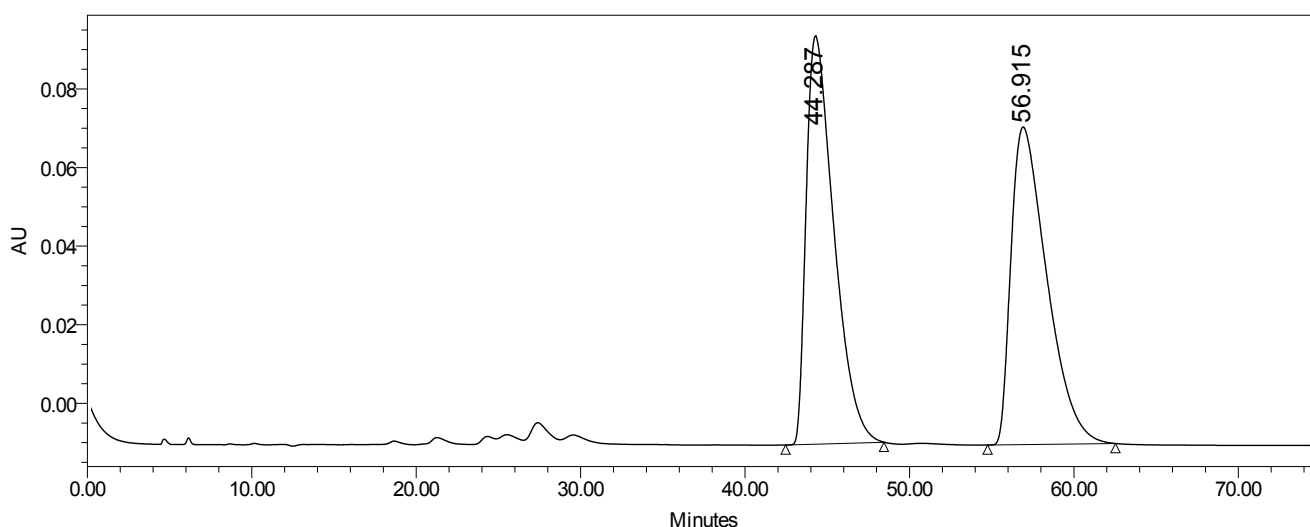
— 23.82



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	308.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	64
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7600.3
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

SAMPLE INFORMATION

Sample Name:		Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	jwn4_78_racemic_samples
Vial:	7	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #:	1	Processing Method:	jwn4_1F_racemic
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	75.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/9/2016 8:36:08 PM CDT			
Date Processed: 8/15/2016 11:32:50 PM CDT			



Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21687; Processing Method: jwn4_1F_racemic

Processed Channel Descr.: W2489 ChA 254nm

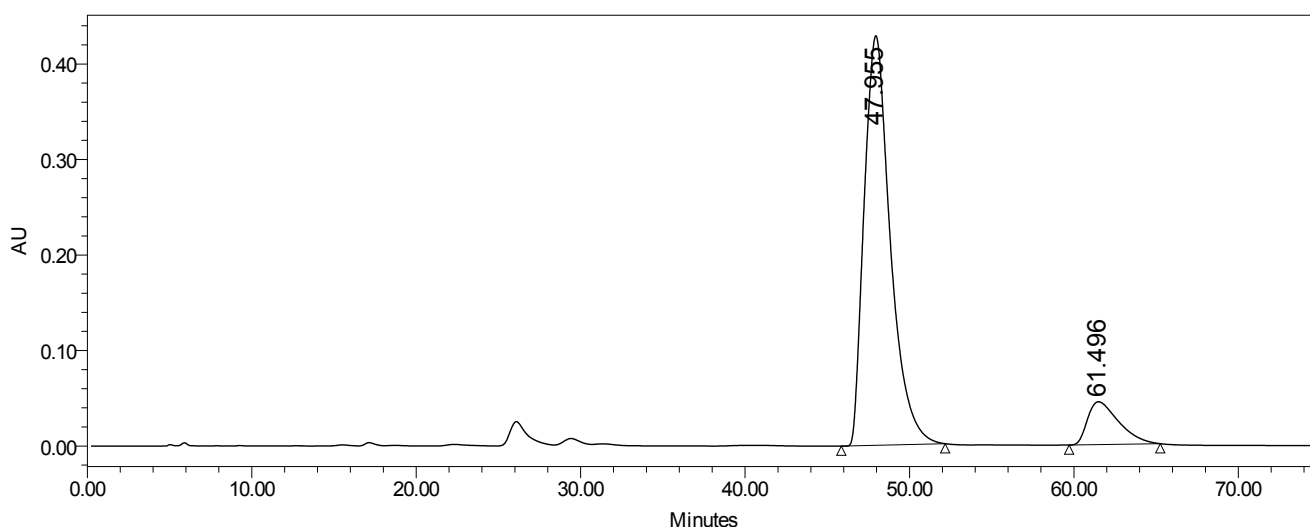
	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	44.287	12150312	49.86	103862
2	W2489 ChA 254nm	56.915	12220951	50.14	80801



Injection Summary Report

SAMPLE INFORMATION

<p>Sample Name: Sample Type: Unknown Vial: 11 Injection #: 1 Injection Volume: 10.00 ul Run Time: 75.0 Minutes</p>	<p>Acquired By: System Sample Set Name: jwn4_OBC_79_82 Acq. Method Set: 1_ADH 90_10 1mpm Processing Method: jwn4_1f_asymmetric Channel Name: W2489 ChA Proc. Chnl. Descr.: W2489 ChA 254nm</p>
<p>Date Acquired: 8/11/2016 3:17:47 PM CDT Date Processed: 8/15/2016 11:33:51 PM CDT</p>	

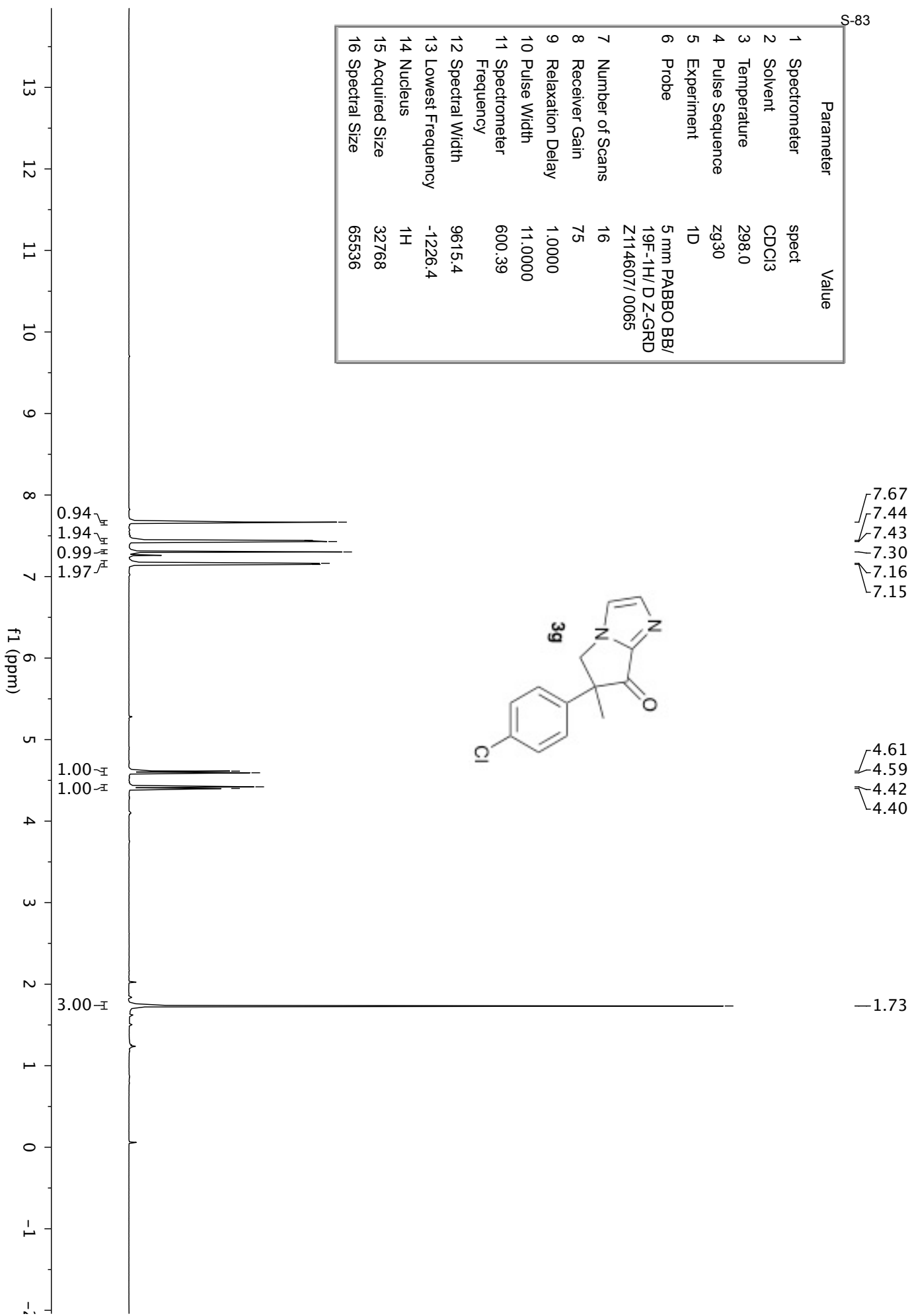


Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21689; Processing Method: jwn4_1f_asymmetric

Processed Channel Descr.: W2489 ChA 254nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	47.955	47353053	88.90	428726
2	W2489 ChA 254nm	61.496	5912714	11.10	44868

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl ₃
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	75
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1226.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



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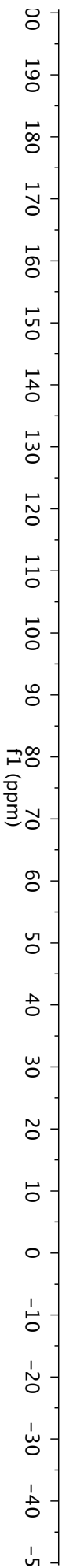
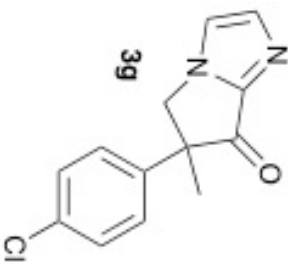
— 189.74

145.65
140.26
140.16

132.16
127.77
121.84
120.38

56.84
56.28

— 23.81



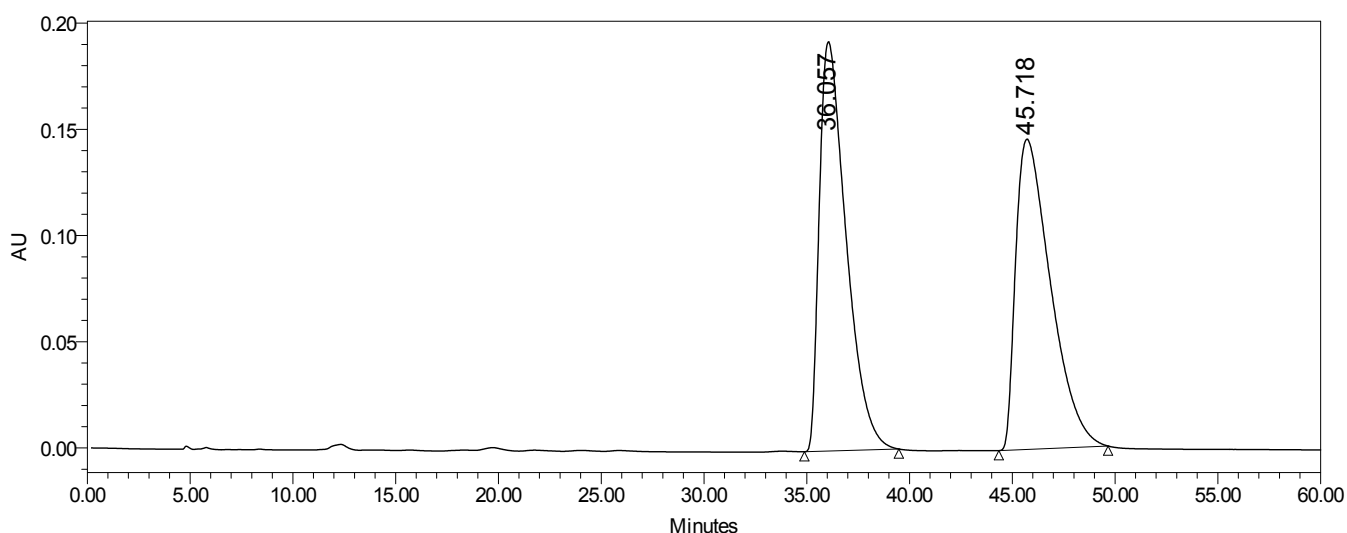
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	51
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7605.8
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536



Injection Summary Report

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	JWN4_1B
Vial: 12	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1B_racemic
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/4/2016 12:00:57 PM CDT		
Date Processed: 8/15/2016 11:18:36 PM CDT		



Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21671; Processing Method: jwn4_1B_racemic

Processed Channel Descr.: W2489 ChA 254nm

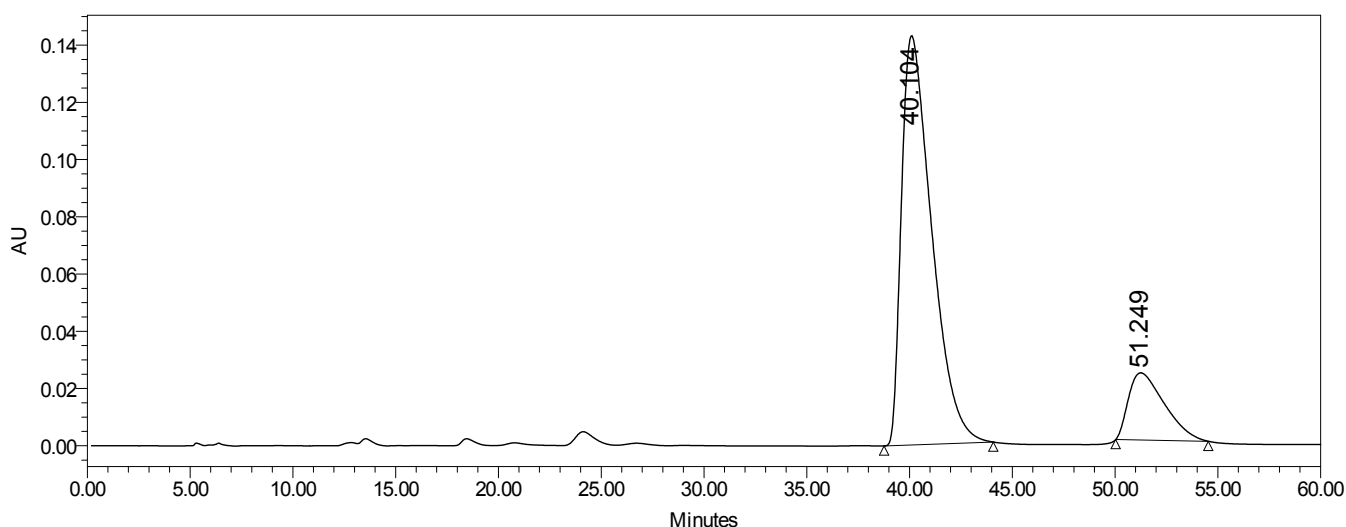
	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	36.057	17467416	50.34	192696
2	W2489 ChA 254nm	45.718	17228521	49.66	146064



Injection Summary Report

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	JWN4_72
Vial: 1	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1B_asymmetric
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/5/2016 7:15:02 PM CDT		
Date Processed: 8/15/2016 11:19:52 PM CDT		

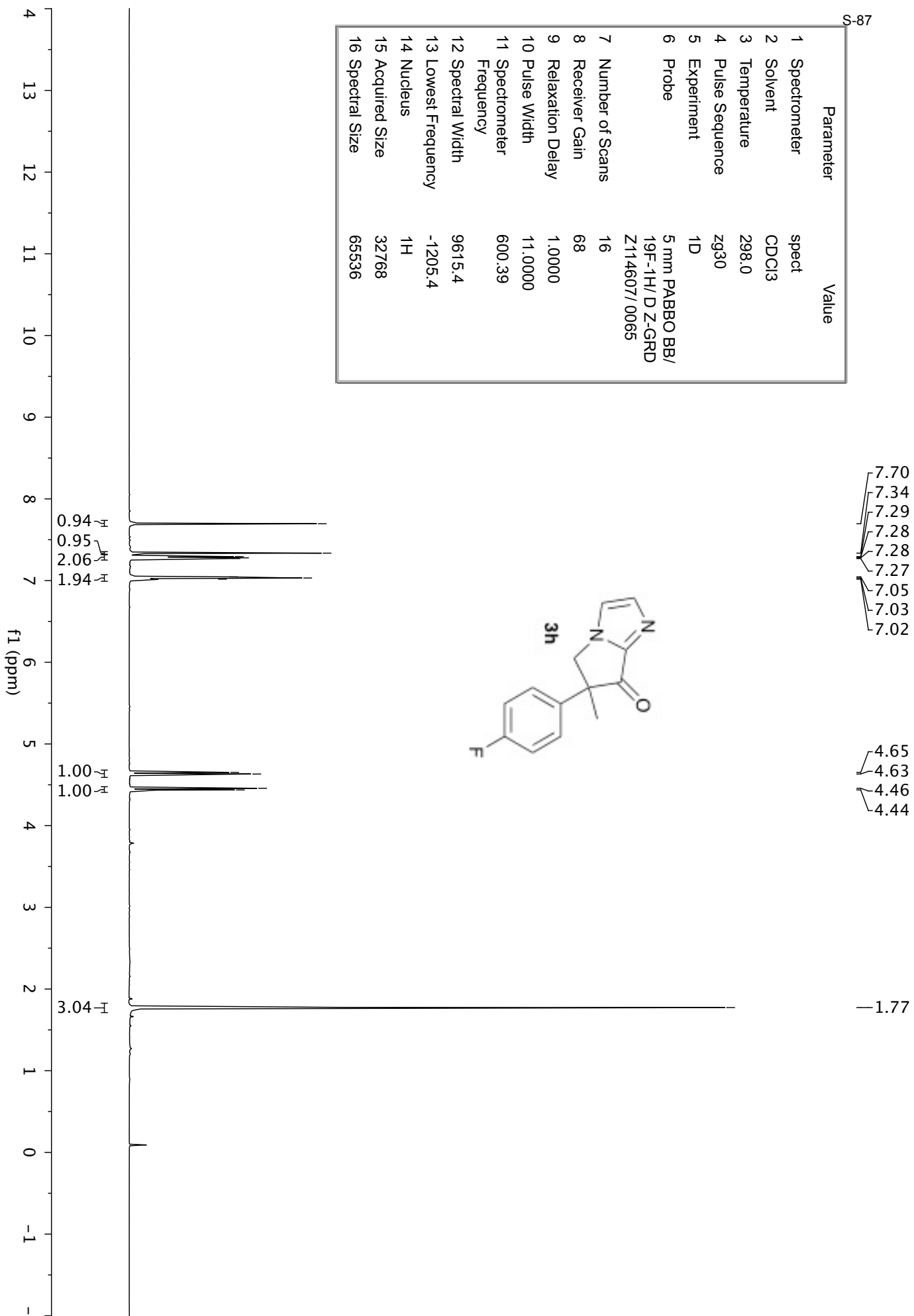


Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21673; Processing Method: jwn4_1B_asymmetric

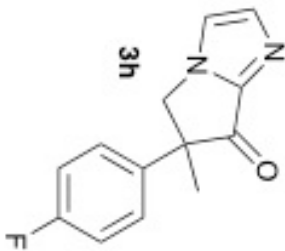
Processed Channel Descr.: W2489 ChA 254nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	40.104	14617661	83.68	142945
2	W2489 ChA 254nm	51.249	2851736	16.32	23466

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	68
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1205.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536

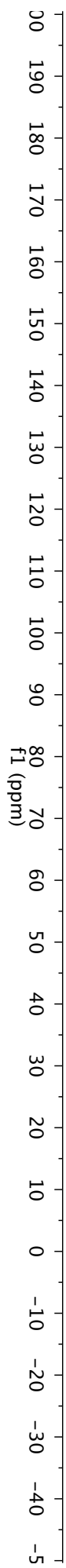


S-88
 — 190.15
 162.90
 161.27
 145.71
 140.08
 137.04
 137.02
 127.77
 127.71
 120.34
 116.00
 115.85

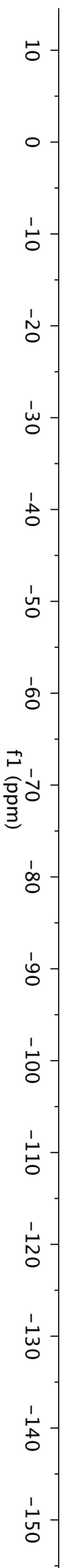
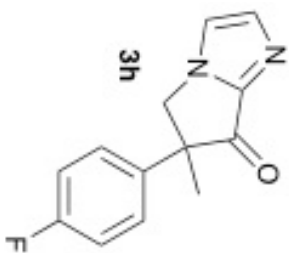


57.09
 56.12
 — 23.96

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/DZ-GRD Z114607/0065
7 Number of Scans	105
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7606.1
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536



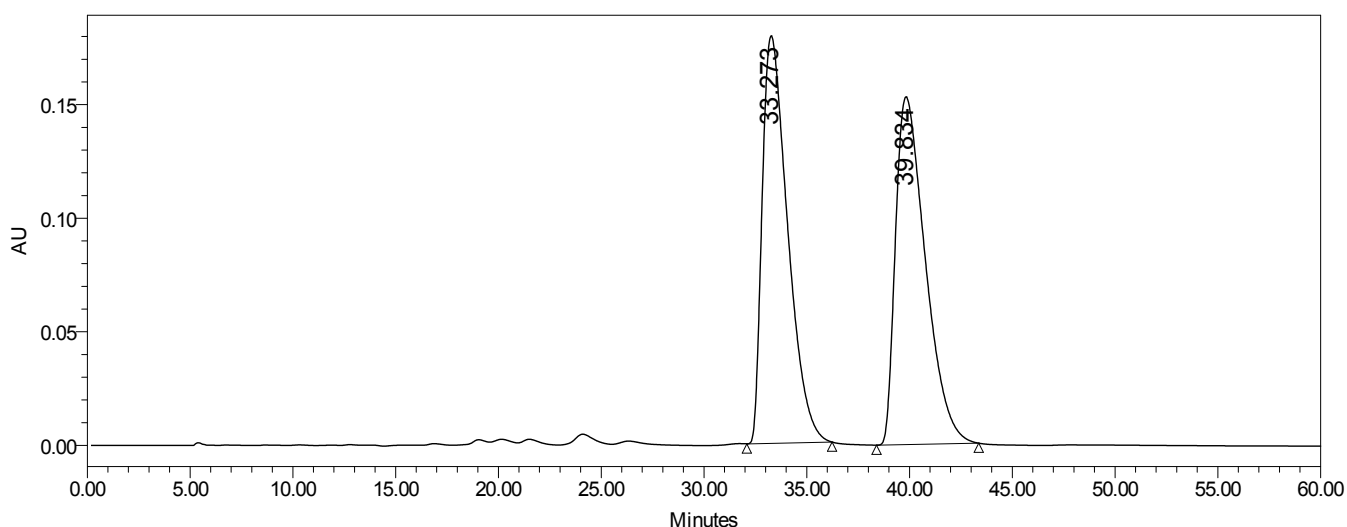
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCI3
3 Temperature	298.0
4 Pulse Sequence	zgfhigqn
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/D Z-GRD Z114607/ 0065
7 Number of Scans	1
8 Receiver Gain	177
9 Relaxation Delay	5.0000
10 Pulse Width	14.0000
11 Spectrometer Frequency	564.89
12 Spectral Width	96153.8
13 Lowest Frequency	-87622.1
14 Nucleus	19F
15 Acquired Size	32768
16 Spectral Size	65536



--115.08

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	jwn4_78_racemic_samples
Vial: 4	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1C_racemic
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/9/2016 4:33:30 PM CDT		
Date Processed: 8/15/2016 11:22:42 PM CDT		



Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21675; Processing Method: jwn4_1C_racemic

Processed Channel Descr.: W2489 ChA 254nm

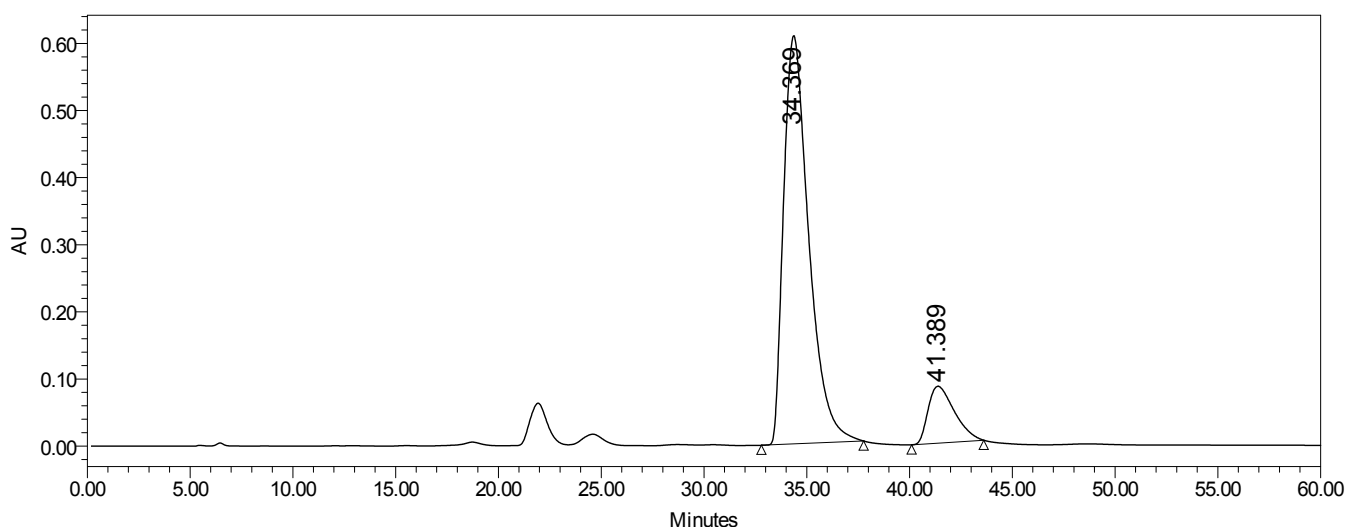
	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	33.273	15454949	50.01	179410
2	W2489 ChA 254nm	39.834	15451491	49.99	153077



Injection Summary Report

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	jwn4_OBC_79_82
Vial: 8	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1C_asymmetric
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/11/2016 12:15:51 PM CDT		
Date Processed: 8/15/2016 11:23:55 PM CDT		

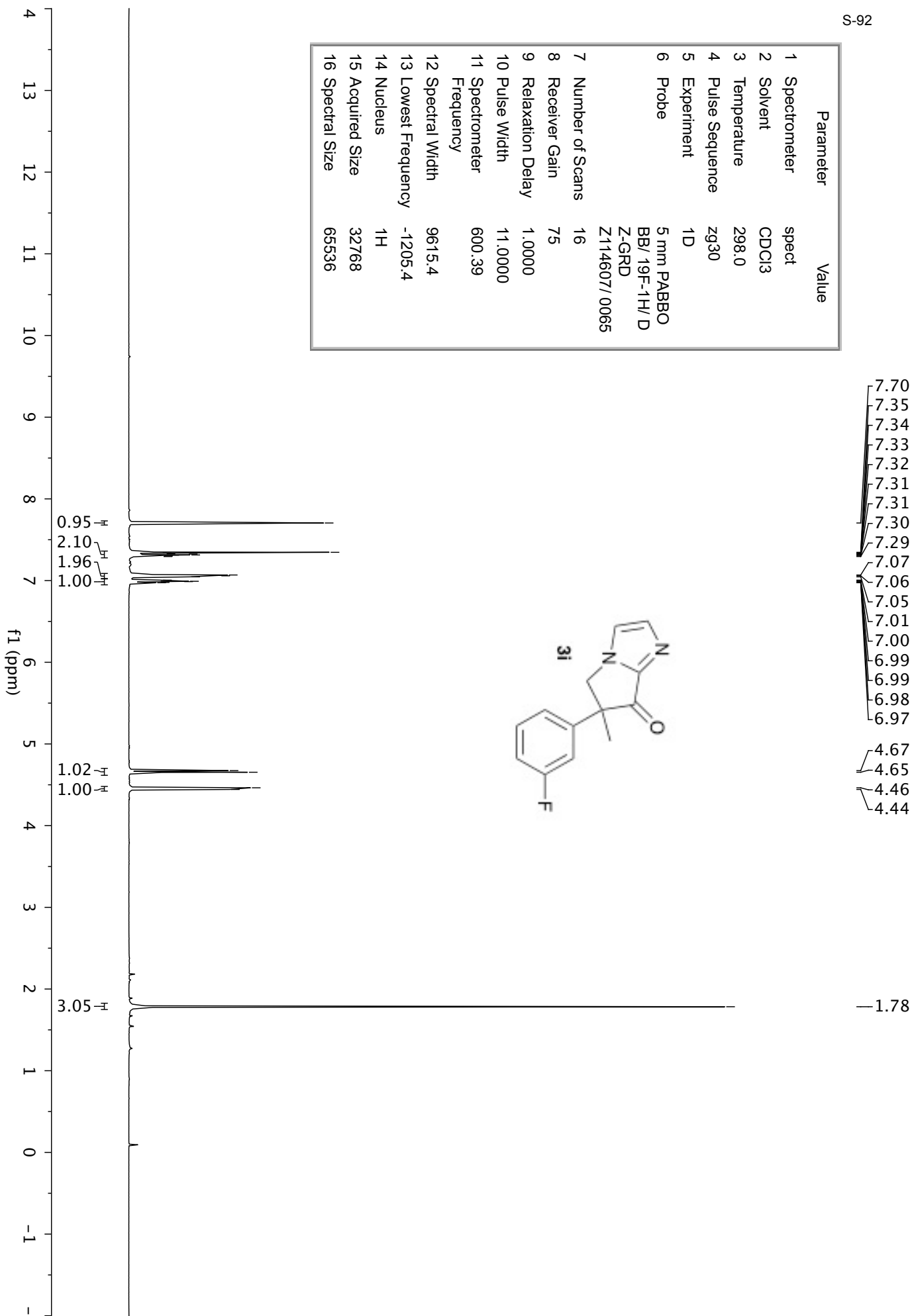


Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21677; Processing Method: jwn4_1C_asymmetric

Processed Channel Descr.: W2489 ChA 254nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	34.369	51704082	87.29	607983
2	W2489 ChA 254nm	41.389	7530643	12.71	84727

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	75
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1205.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



S-93

— 189.59

163.90
162.26

145.65
143.71
143.67
140.19

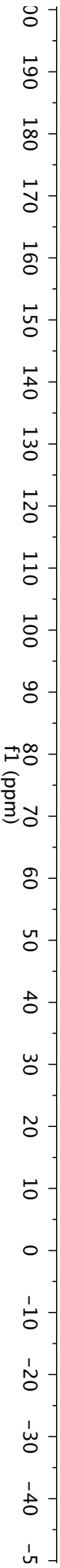
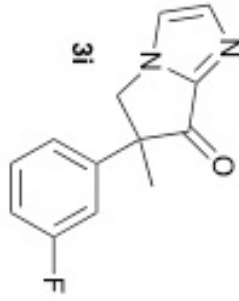
130.70
130.64

121.65
121.63
120.40

114.79
114.66
113.48
113.33

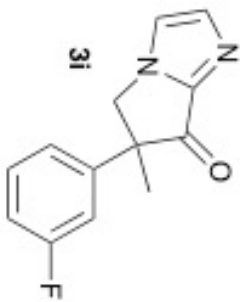
56.91
56.41
56.40

— 23.73

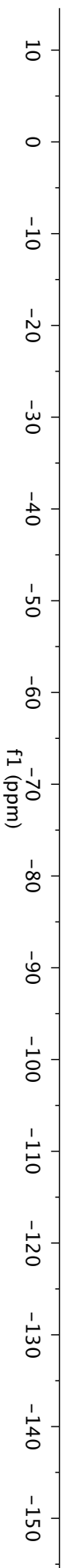


Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCI3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	149
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7604.9
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgffhigqn
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/ 0065
7 Number of Scans	1
8 Receiver Gain	177
9 Relaxation Delay	5.0000
10 Pulse Width	14.0000
11 Spectrometer Frequency	564.89
12 Spectral Width	96153.8
13 Lowest Frequency	-87622.1
14 Nucleus	19F
15 Acquired Size	32768
16 Spectral Size	65536



--111.98

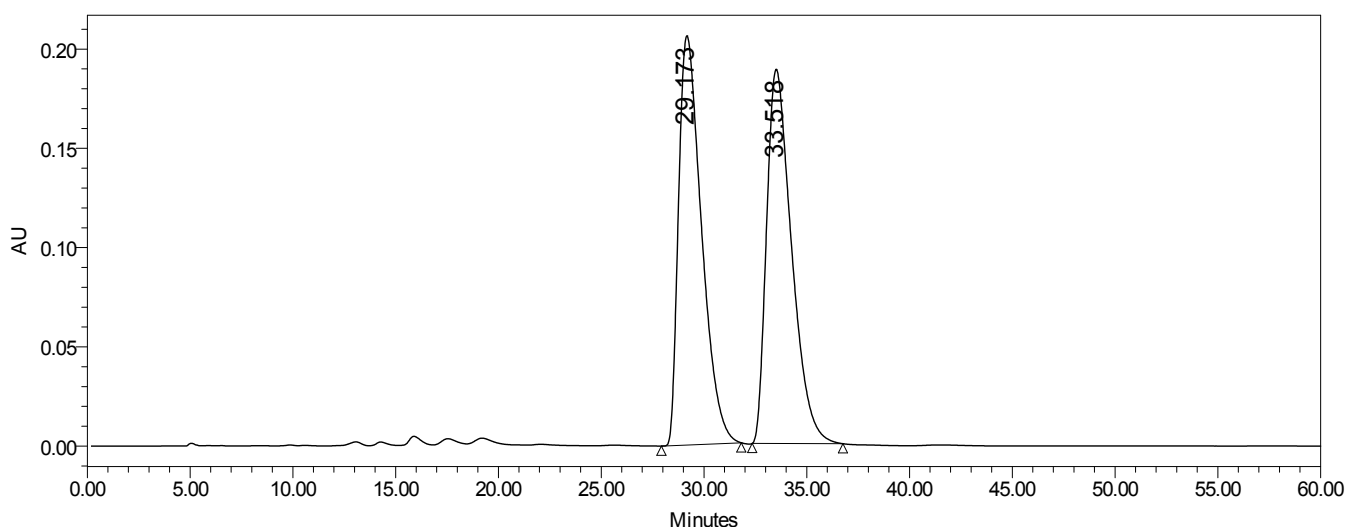




Injection Summary Report

SAMPLE INFORMATION

Sample Name: Sample Type: Unknown Vial: 5 Injection #: 1 Injection Volume: 10.00 ul Run Time: 60.0 Minutes Date Acquired: 8/9/2016 5:34:12 PM CDT Date Processed: 8/15/2016 11:25:26 PM CDT	Acquired By: System Sample Set Name: jwn4_78_racemic_samples Acq. Method Set: 1_ADH 90_10 1mpm Processing Method: jwn4_1D_racemic Channel Name: W2489 ChA Proc. Chnl. Descr.: W2489 ChA 254nm
--	--



Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21679; Processing Method: jwn4_1D_racemic

Processed Channel Descr.: W2489 ChA 254nm

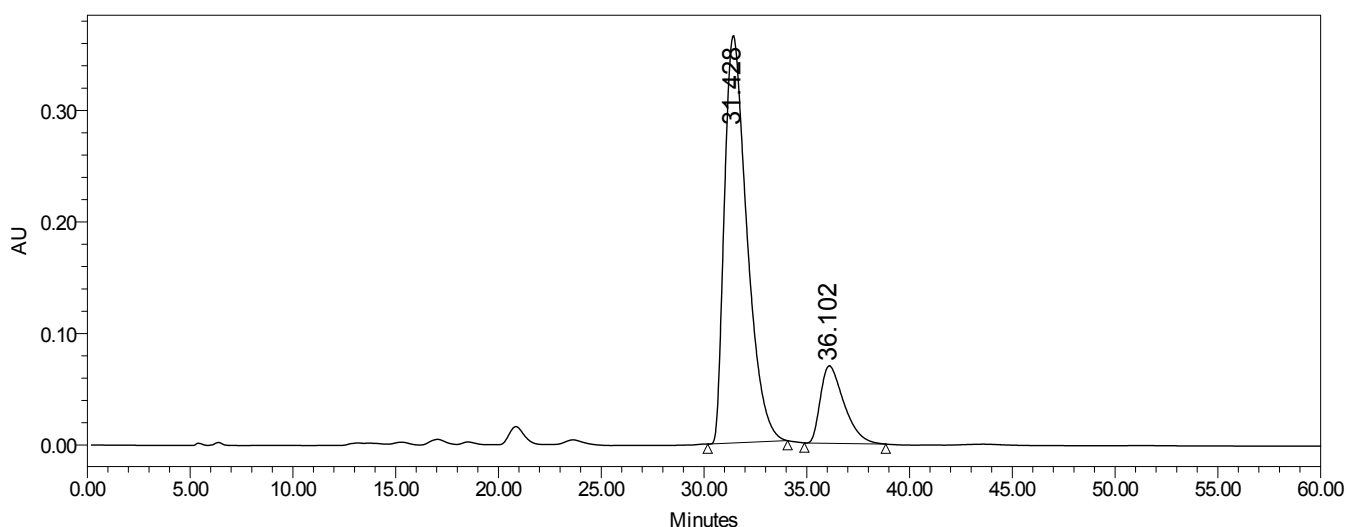
	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	29.173	15992960	50.11	206110
2	W2489 ChA 254nm	33.518	15924692	49.89	188484



Injection Summary Report

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	jwn4_OBC_79_82
Vial: 9	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1d_asymmetric
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/11/2016 1:16:30 PM CDT		
Date Processed: 8/15/2016 11:26:29 PM CDT		

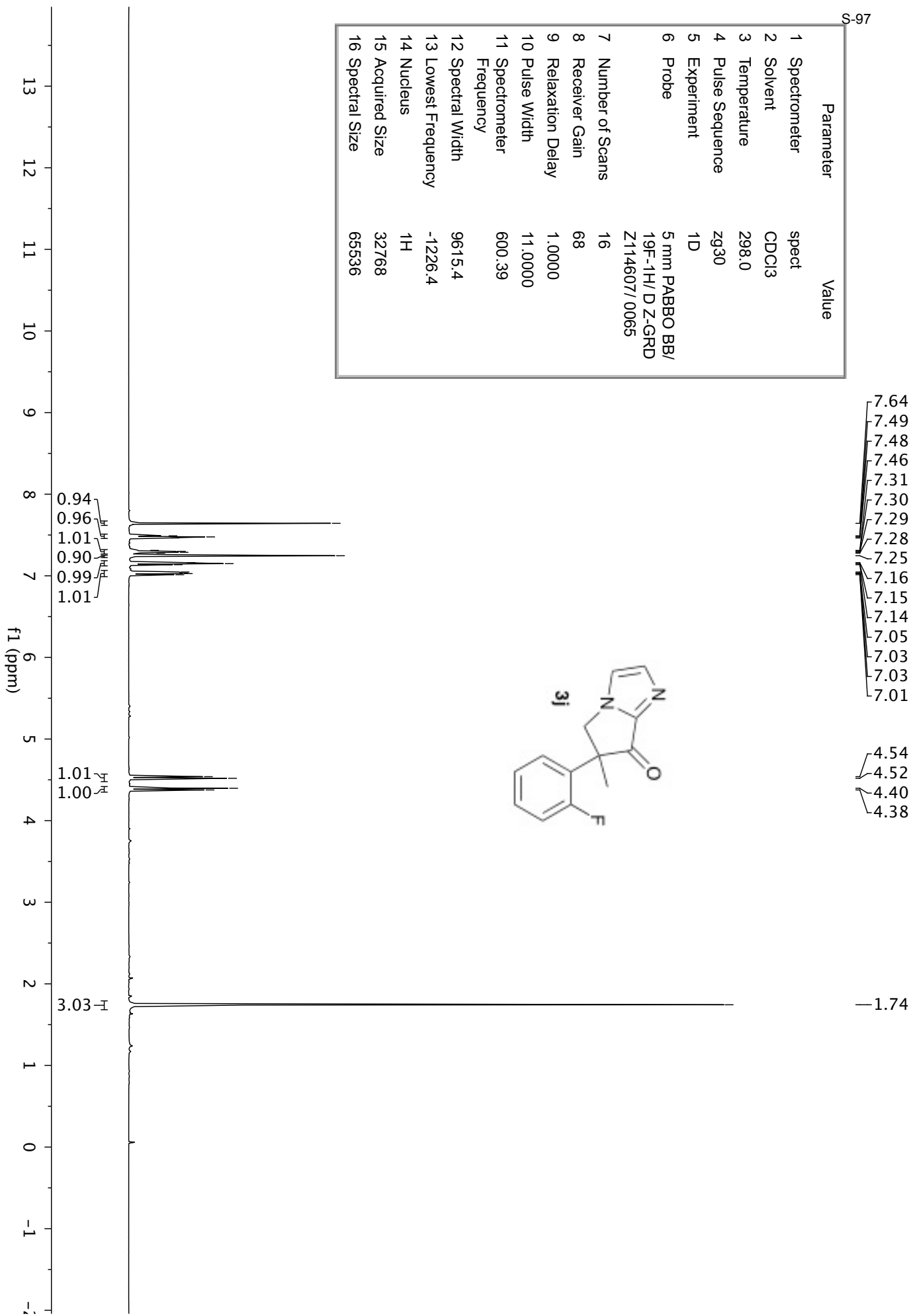


Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21681; Processing Method: jwn4_1d_asymmetric

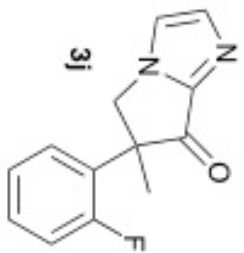
Processed Channel Descr.: W2489 ChA 254nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	31.428	27787054	83.39	364987
2	W2489 ChA 254nm	36.102	5533299	16.61	69388

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	68
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1226.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536

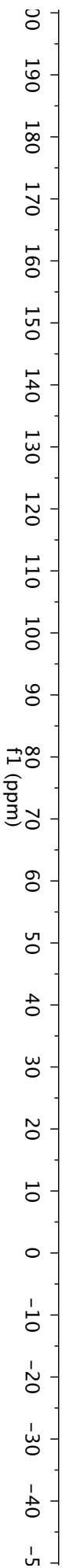


S-98
 — 189.90
 ~ 161.54
 ~ 159.91
 — 145.51
 — 139.59
 — 129.95
 — 129.89
 — 128.22
 — 128.19
 — 128.11
 — 128.02
 — 124.55
 — 124.52
 — 119.87
 — 116.22
 — 116.08



56.21
 56.18
 54.09
 — 23.20

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zpgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/ D-Z-GRD Z114607/ 0065
7 Number of Scans	109
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7605.2
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

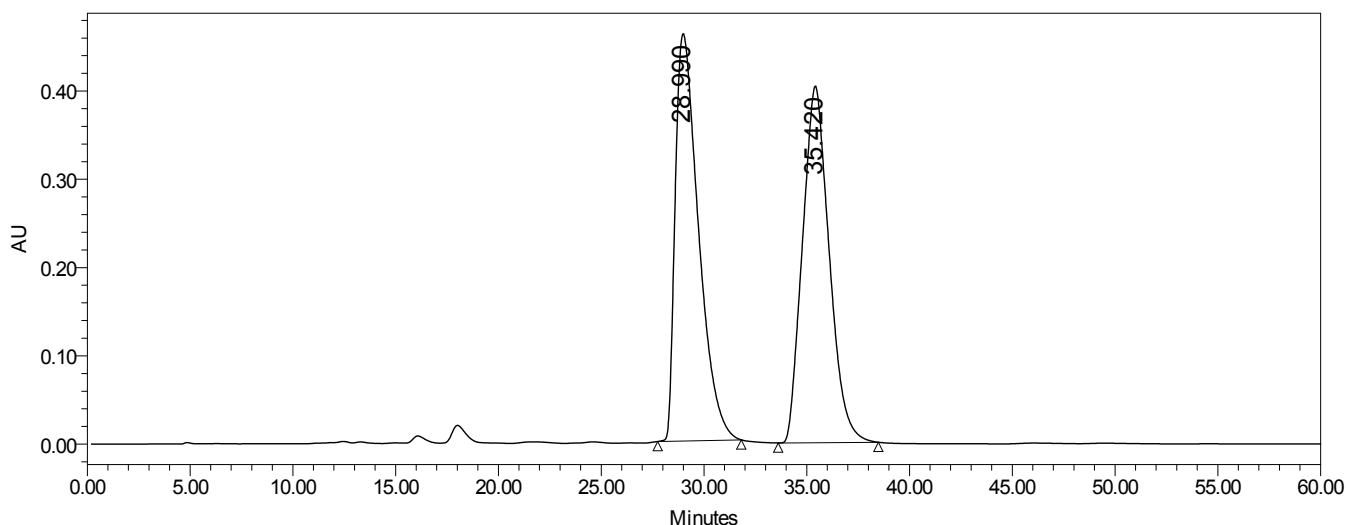




Injection Summary Report

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	jwn4_78_racemic_samples
Vial: 6	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1e_racemic
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm
Date Acquired: 8/9/2016 6:34:49 PM CDT		
Date Processed: 8/15/2016 11:30:04 PM CDT		



Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21683; Processing Method: jwn4_1e_racemic

Processed Channel Descr.: W2489 ChA 254nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	28.990	36251472	49.90	461213
2	W2489 ChA 254nm	35.420	36393626	50.10	403818

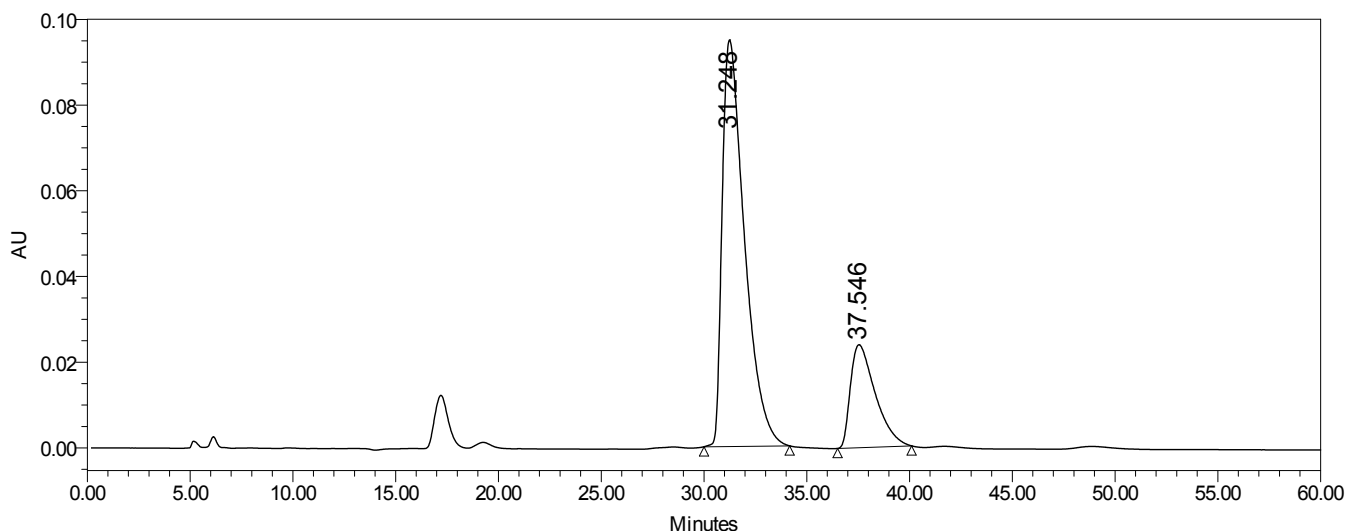


Injection Summary Report

SAMPLE INFORMATION

Sample Name:	Acquired By:	System
Sample Type: Unknown	Sample Set Name:	jwn4_OBC_79_82
Vial: 10	Acq. Method Set:	1_ADH 90_10 1mpm
Injection #: 1	Processing Method:	jwn4_1e_asymmetric
Injection Volume: 10.00 ul	Channel Name:	W2489 ChA
Run Time: 60.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 254nm

Date Acquired: 8/11/2016 2:17:07 PM CDT
 Date Processed: 8/15/2016 11:31:22 PM CDT

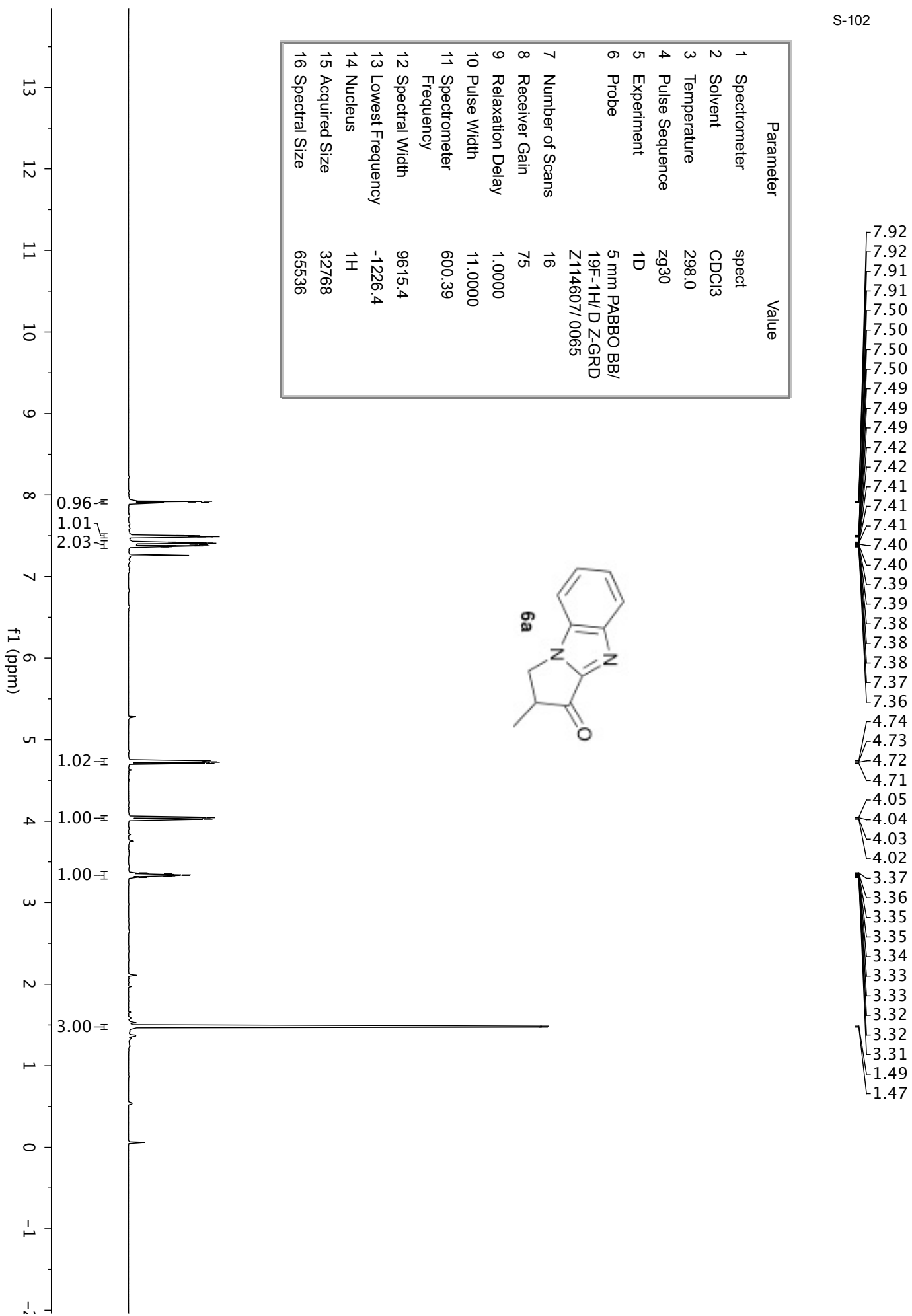
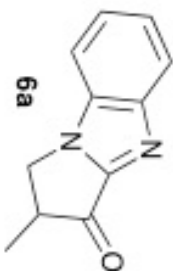


Channel: W2489 ChA; Processed Channel: W2489 ChA 254nm; Result Id: 21685; Processing Method: jwn4_1e_asymmetric

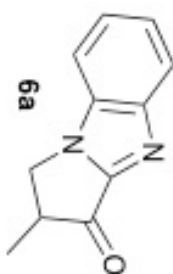
Processed Channel Descr.: W2489 ChA 254nm

	Processed Channel Descr.	RT	Area	% Area	Height
1	W2489 ChA 254nm	31.248	7147758	78.00	94883
2	W2489 ChA 254nm	37.546	2016177	22.00	24023

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	75
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1226.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



S-103
— 193.66



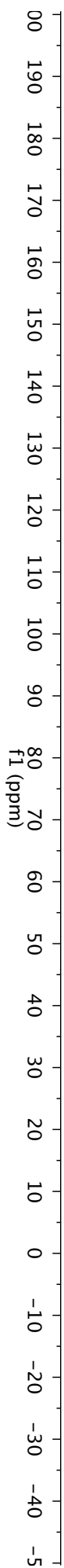
149.44
149.13

132.76
125.64
124.85
123.22

— 111.05

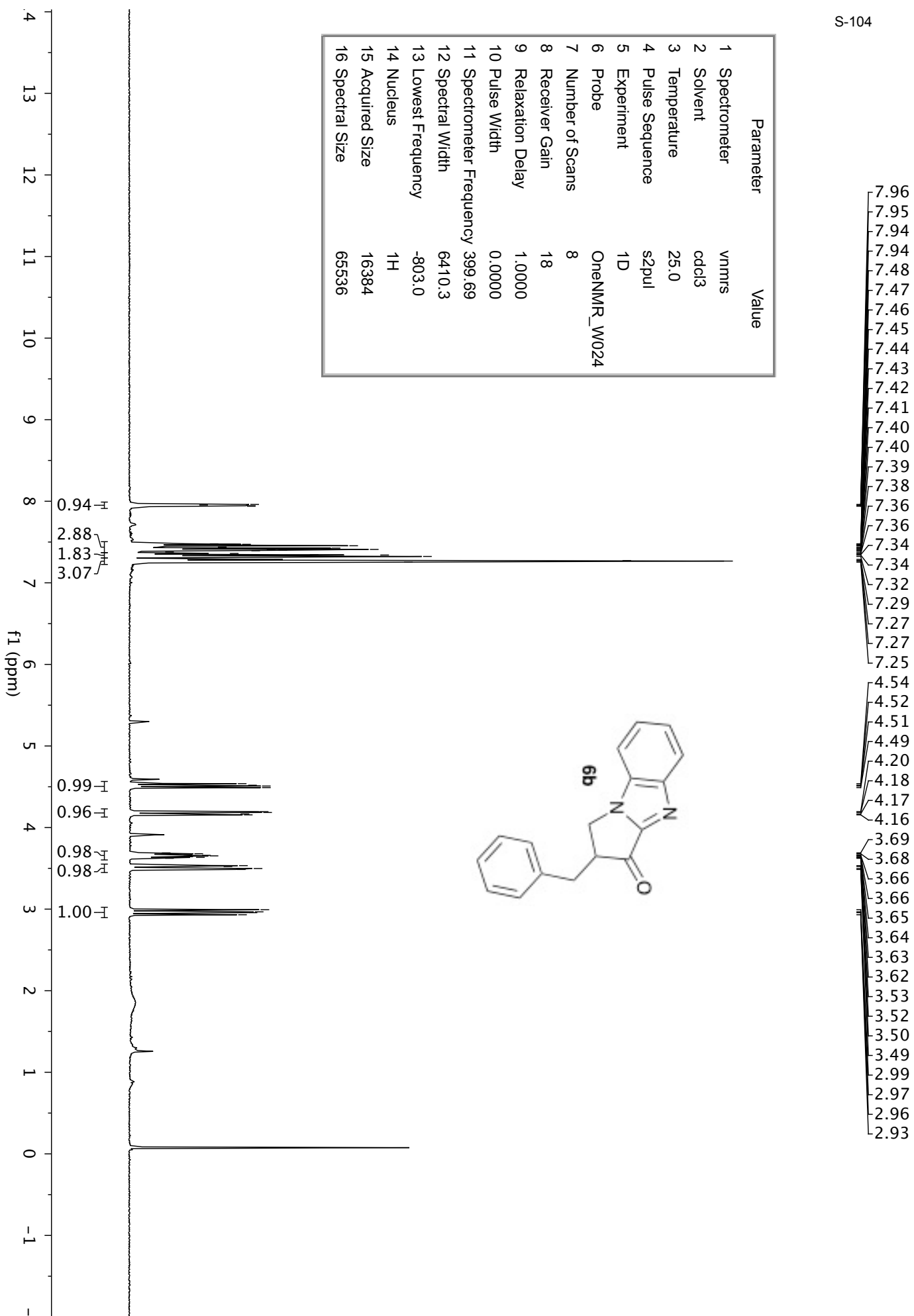
47.02
45.03

— 15.37



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zpgp30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/D-Z- GRD Z114607/ 0065
7 Number of Scans	127
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7603.6
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

Parameter	Value
1 Spectrometer	nmrs
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	s2pul
5 Experiment	1D
6 Probe	OneNMR_W024
7 Number of Scans	8
8 Receiver Gain	18
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	399.69
12 Spectral Width	6410.3
13 Lowest Frequency	-803.0
14 Nucleus	¹ H
15 Acquired Size	16384
16 Spectral Size	65536



— 192.23

149.48
 149.23
 137.59
 132.85
 129.12
 128.88
 127.27
 125.78
 124.98
 123.36

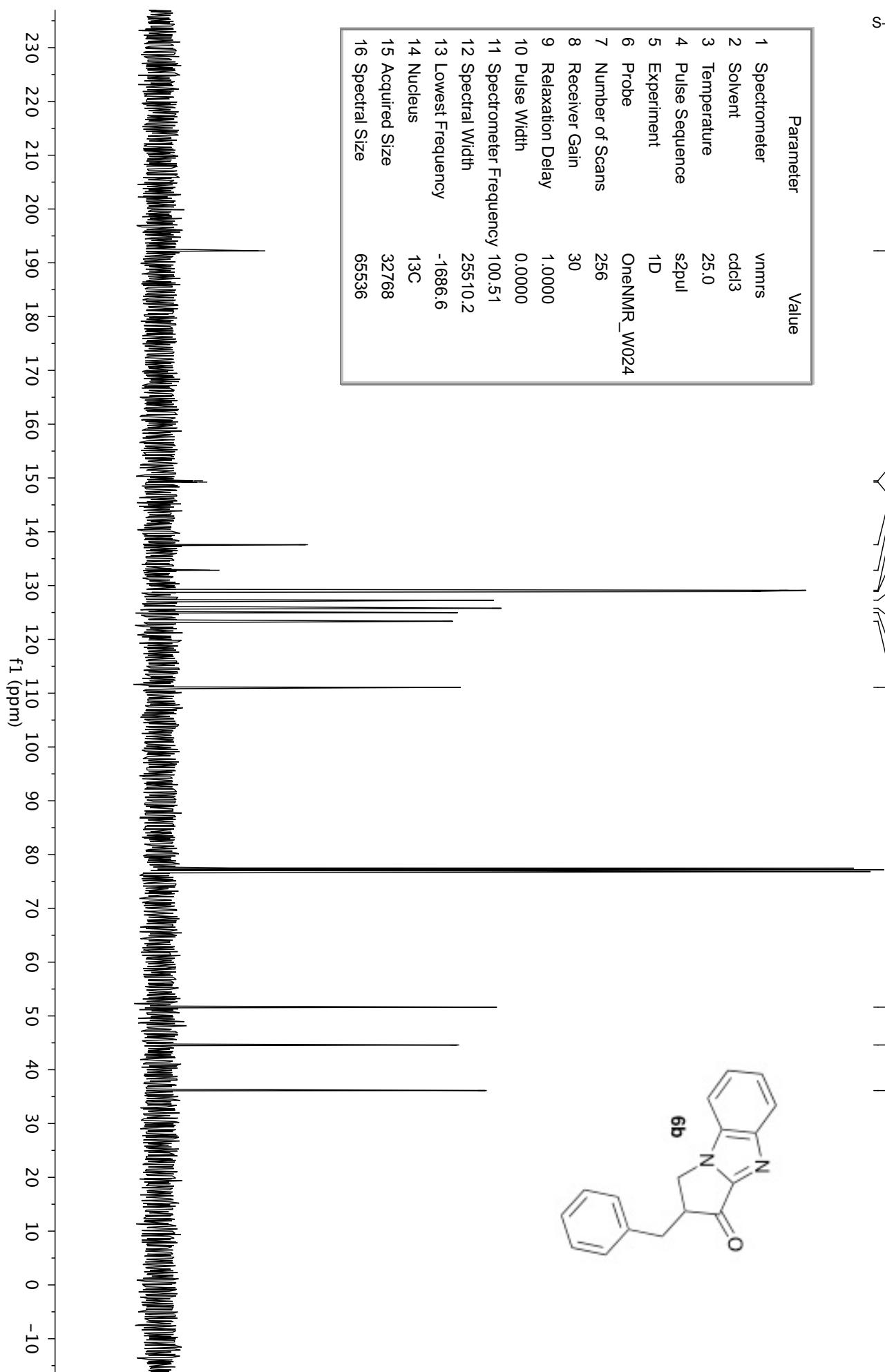
— 111.07

— 51.63

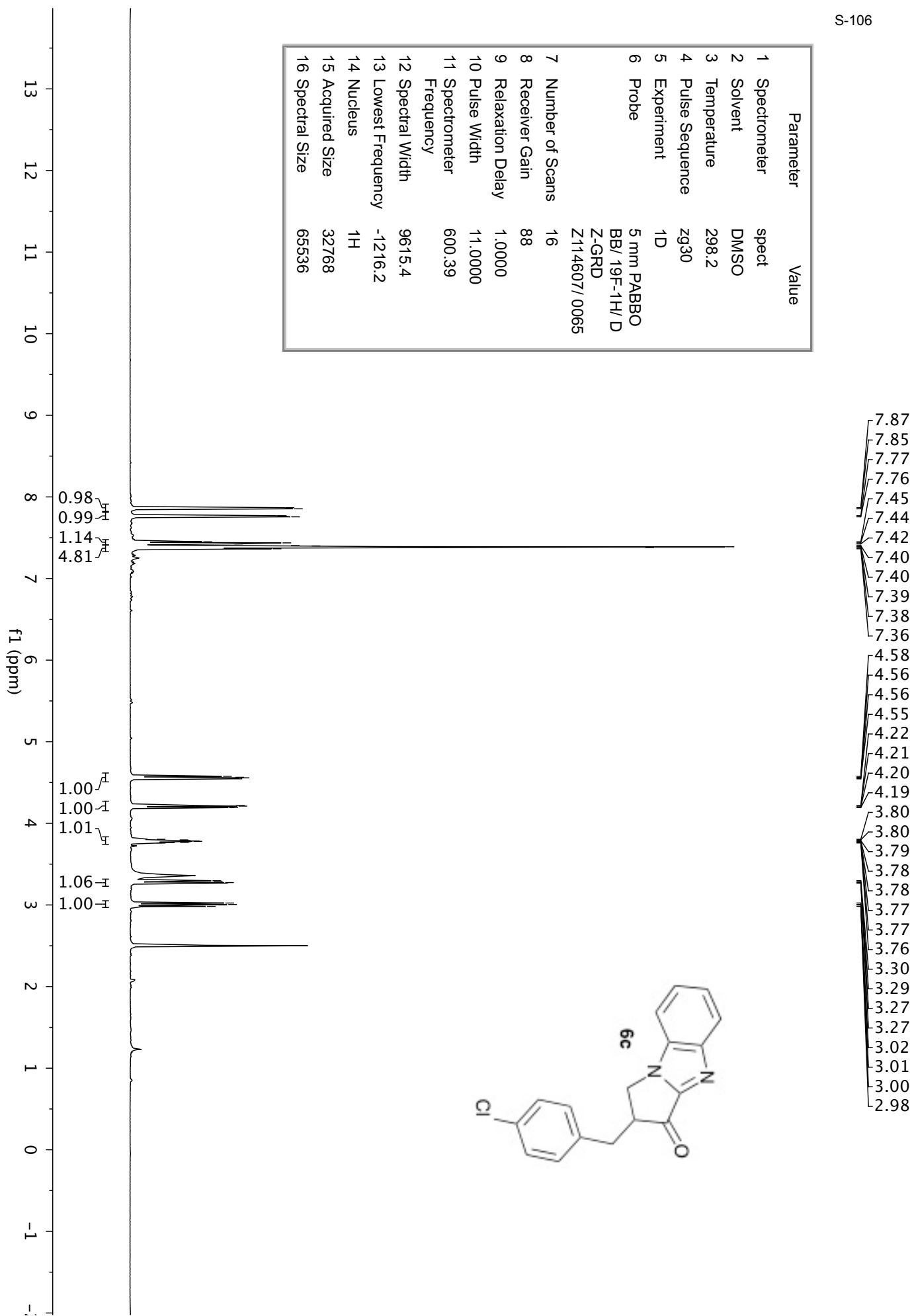
— 44.60

— 36.13

Parameter	Value
1 Spectrometer	vmrns
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	s2pul
5 Experiment	1D
6 Probe	OneNMW024
7 Number of Scans	256
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	100.51
12 Spectral Width	25510.2
13 Lowest Frequency	-1686.6
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



Parameter	Value
1 Spectrometer	spect
2 Solvent	DMSO
3 Temperature	298.2
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	88
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1216.2
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



— 193.54

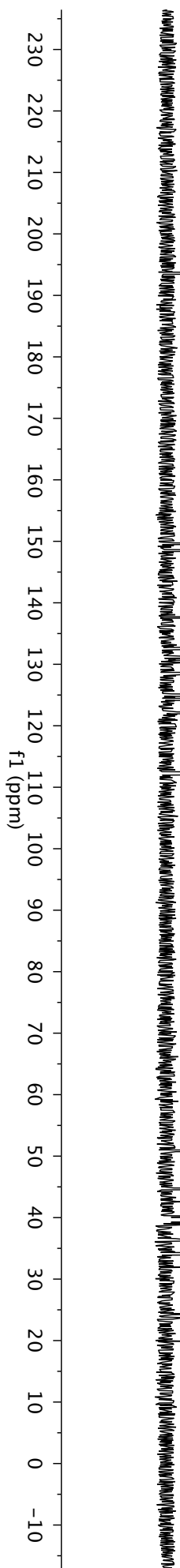
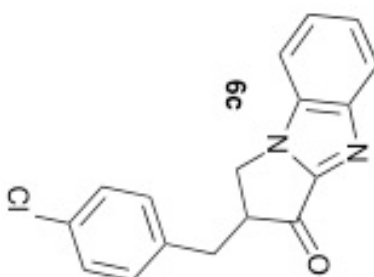
149.61
 148.48
 137.61
 132.65
 131.26
 130.77
 128.51
 124.91
 124.30
 122.04
 — 112.29

Parameter	Value
1 Spectrometer	vmrs
2 Solvent	dmso
3 Temperature	25.0
4 Pulse Sequence	s2pul
5 Experiment	1D
6 Probe	OneNMR_W024
7 Number of Scans	256
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	100.51
12 Spectral Width	25510.2
13 Lowest Frequency	-1741.7
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536

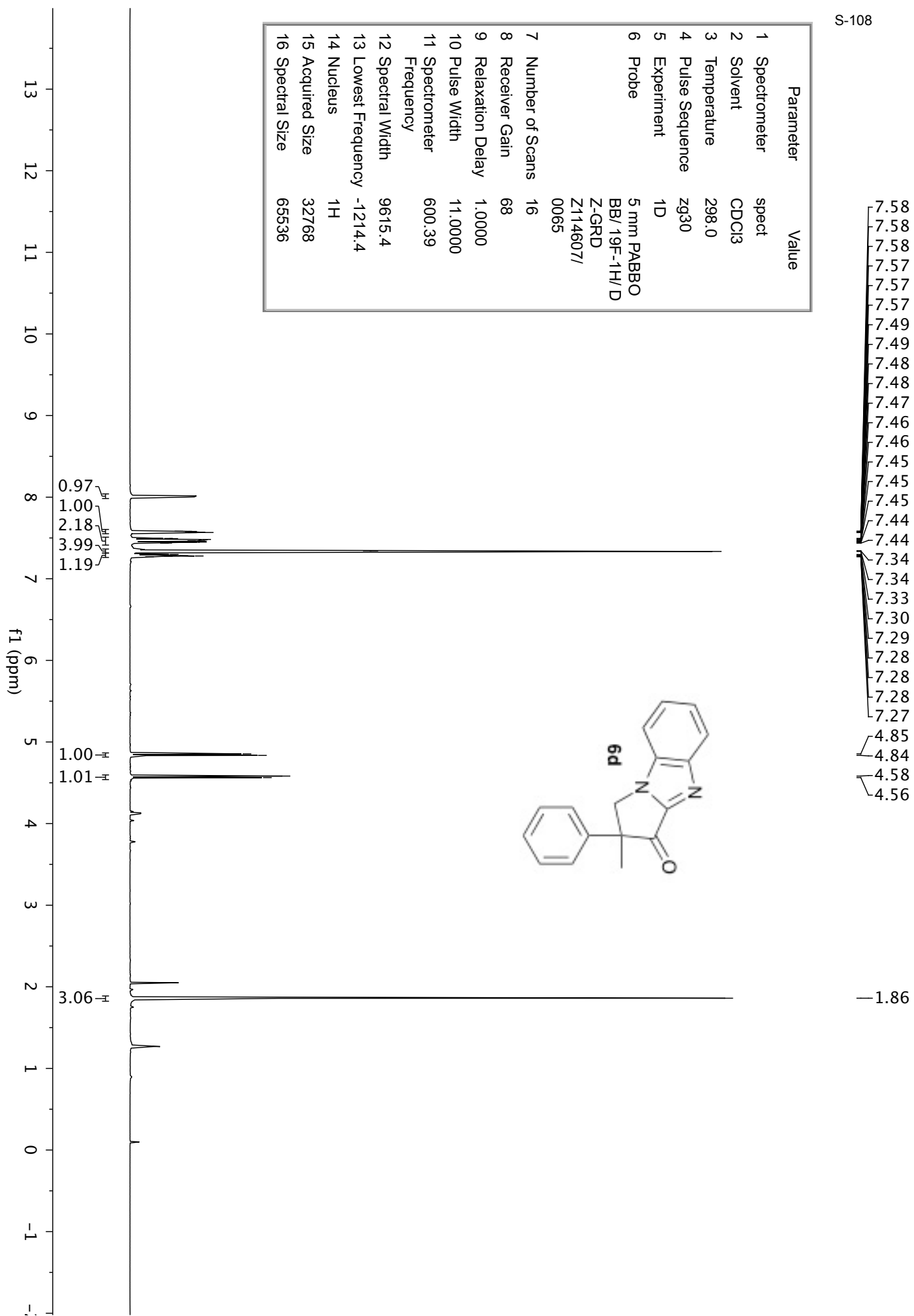
— 50.81

— 44.62

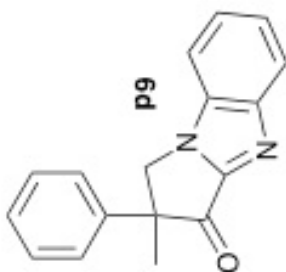
— 34.06



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl ₃
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/ 0065
7 Number of Scans	16
8 Receiver Gain	68
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1214.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



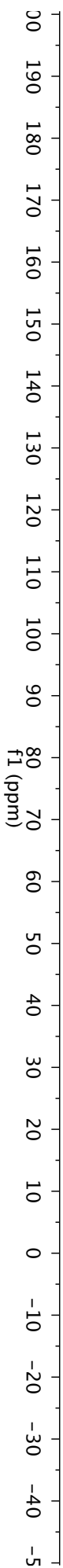
S-109
— 193.80



149.77
148.62
— 140.92
132.84
129.18
127.86
125.93
125.90
125.02
123.38
111.19

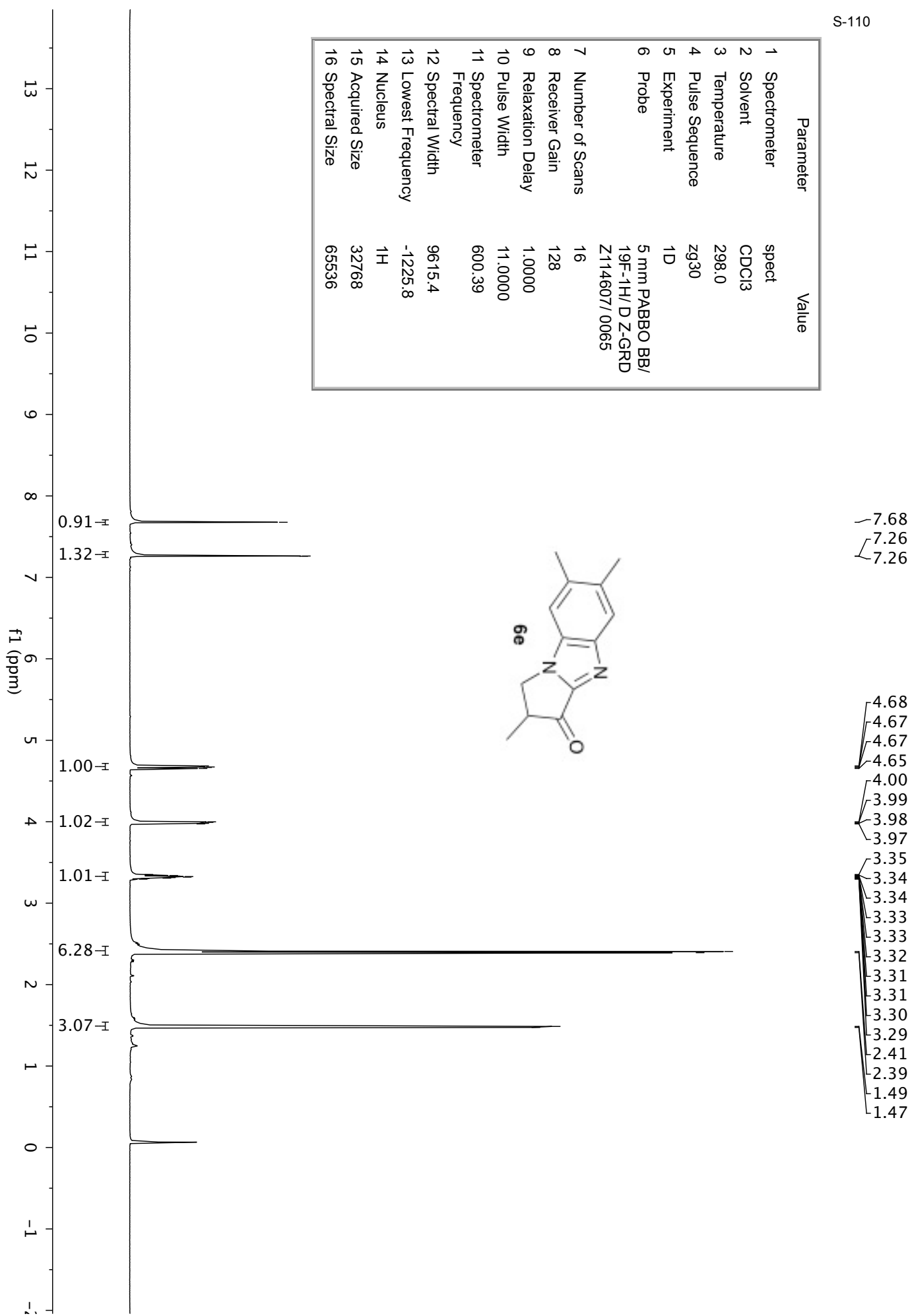
56.71
55.50

— 23.78



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	278
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7607.9
14 Nucleus	13C
15 Acquired Size	32768
16 Spectral Size	65536

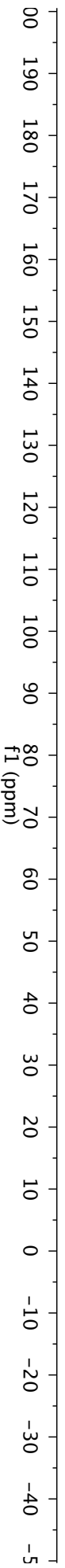
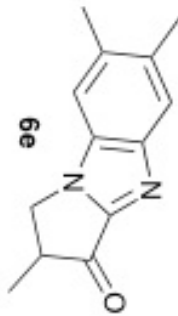
Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	128
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1225.8
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



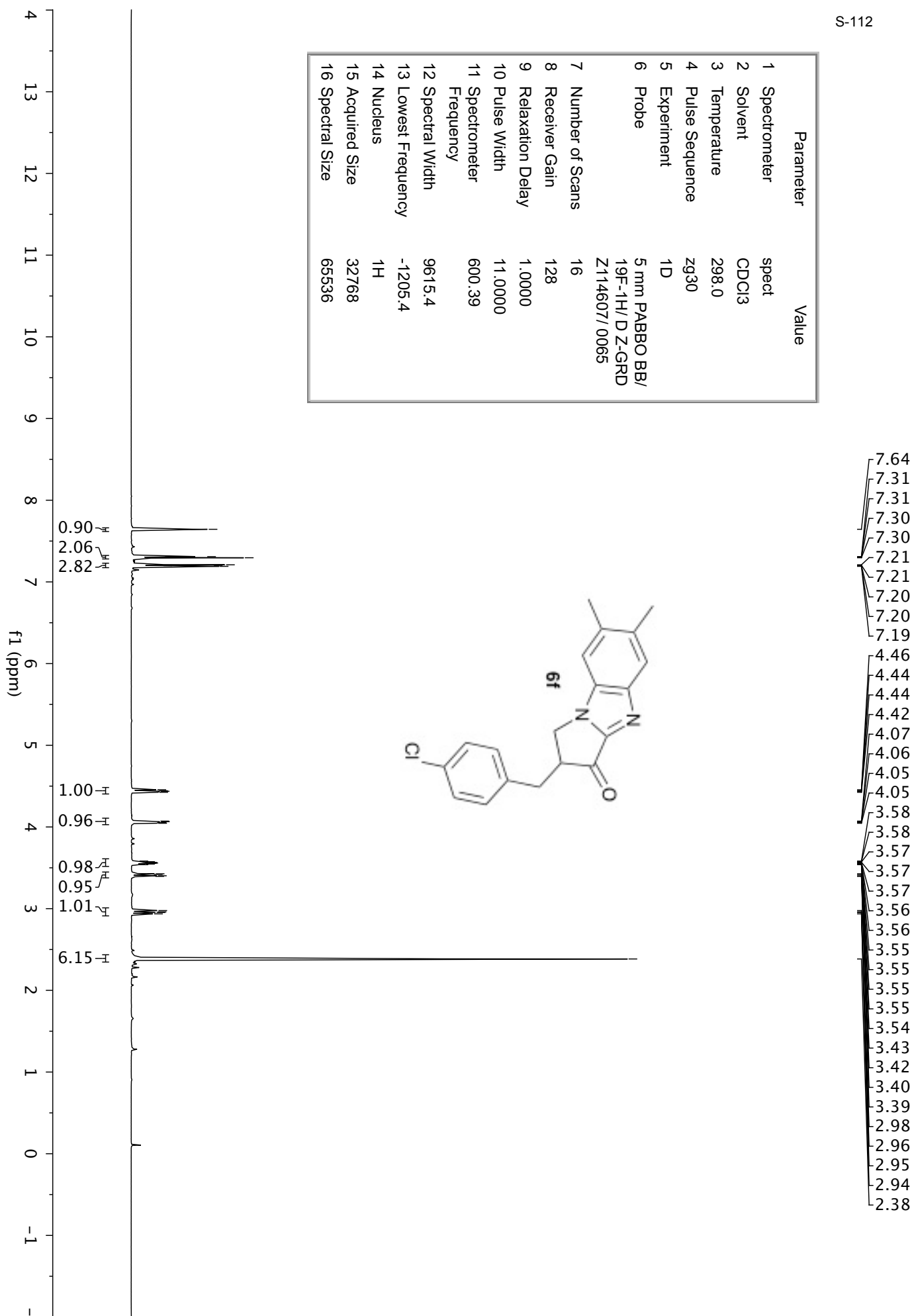
S-111
 — 193.36
 — 148.47
 — 135.88
 — 134.60
 — 131.56
 — 122.65
 — 110.70

Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z114607/0065
7 Number of Scans	1053
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7599.6
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536

— 46.96
 — 45.05
 — 20.95
 — 20.75
 — 15.50
 — 1.15



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCl3
3 Temperature	298.0
4 Pulse Sequence	zg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/ 19F-1H/DZ-GRD Z114607/0065
7 Number of Scans	16
8 Receiver Gain	128
9 Relaxation Delay	1.0000
10 Pulse Width	11.0000
11 Spectrometer Frequency	600.39
12 Spectral Width	9615.4
13 Lowest Frequency	-1205.4
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



— 191.55

 148.31
 148.29

 136.21
 136.06

134.77

133.02

131.51

130.26

129.15

122.50

— 110.70

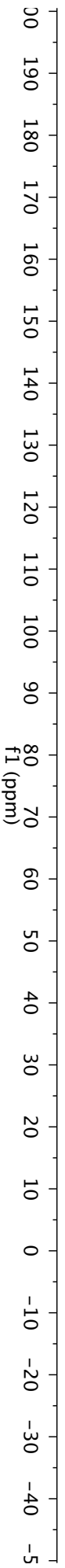
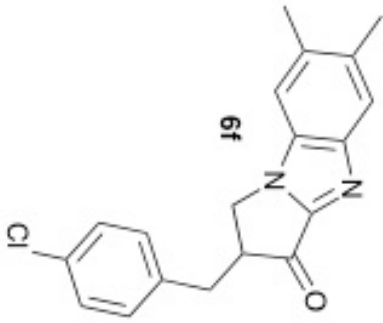
— 51.32

— 44.31

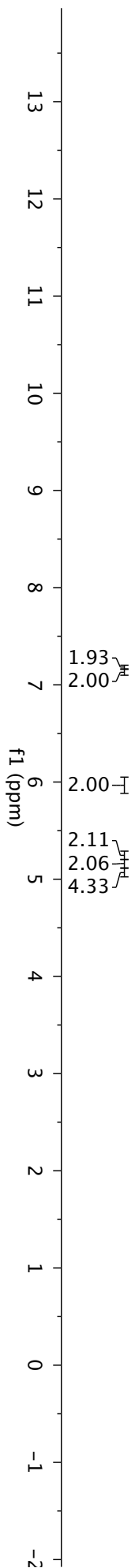
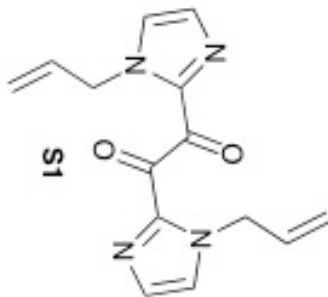
— 35.38

20.90

20.69



Parameter	Value
1 Spectrometer	spect
2 Solvent	CDCI3
3 Temperature	298.0
4 Pulse Sequence	zpgpg30
5 Experiment	1D
6 Probe	5 mm PABBO BB/19F-1H/D Z-GRD Z114607/0065
7 Number of Scans	147
8 Receiver Gain	177
9 Relaxation Delay	3.0000
10 Pulse Width	11.6000
11 Spectrometer Frequency	150.98
12 Spectral Width	37878.8
13 Lowest Frequency	-7604.6
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536



Parameter	Value
1 Spectrometer	vnmr5
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	sZpul
5 Experiment	1D
6 Probe	OneNMR_W024
7 Number of Scans	8
8 Receiver Gain	18
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	399.69
12 Spectral Width	6410.3
13 Lowest Frequency	-829.5
14 Nucleus	¹ H
15 Acquired Size	16384
16 Spectral Size	65536

— 183.21

— 140.29

— 132.18

— 132.13

— 126.32

— 119.50

— 50.66

Parameter	Value
1 Spectrometer	nmrs
2 Solvent	cdcl3
3 Temperature	25.0
4 Pulse Sequence	s2pul
5 Experiment	1D
6 Probe	OneNMR_W024
7 Number of Scans	256
8 Receiver Gain	30
9 Relaxation Delay	1.0000
10 Pulse Width	0.0000
11 Spectrometer Frequency	100.51
12 Spectral Width	25510.2
13 Lowest Frequency	-1686.6
14 Nucleus	¹³ C
15 Acquired Size	32768
16 Spectral Size	65536

