Supporting Information For

Palladium-Catalyzed Enantioselective Redox-Relay Heck Arylation of 1,1-Disubstituted Homoallylic Alcohols

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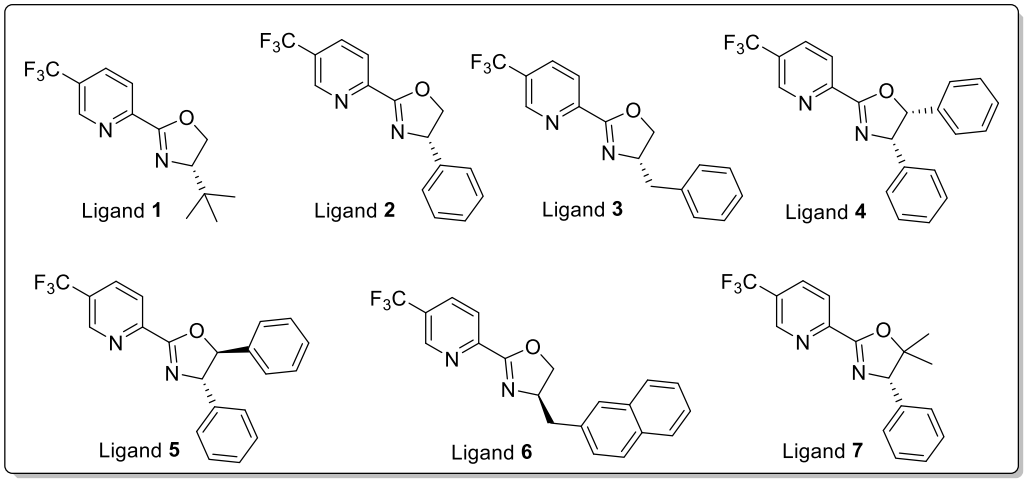
General information:

MeOH was dried by distilling from CaH_2; DCM, Et_2O, THF, and CH_3CN were dried by passing through a column of activated alumina. Powdered 4 Å molecular sieves were activated by flowing N_2 through a glass tube of sieves maintained at 200 °C. Boronic acids were purchased from Aldrich, Alfa or Combi-Blocks. $Pd(CH_3CN)_2(OTs)_2$ and $Pd(CH_3CN)_4(OTf)_2$ were synthesized according to literature procedures.[1,2] Thin-layer chromatography was performed with EMD silica gel 60 F_{254} plates eluting with solvents indicated, visualized by a 254 nm UV lamp and stained with phosphomolybdic acid (PMA). Flash chromatography was performed using EM reagent silica 60 (230-400 mesh). ^{1}H-NMR spectra were obtained at 300 MHz or 500 MHz. Chemical shifts are reported in ppm and referenced to $CDCl_3$ (δ = 7.26 ppm). ^{13}C-NMR spectra were obtained at 75 MHz, or 125 MHz, and referenced to $CDCl_3$ (δ = 77.00 ppm). IR spectra were recorded using a Thermo Nicolet FT-IR. High resolution mass spectrometry (HRMS) data were obtained on a Waters LCP Premier XE instrument by ESI/TOF. SFC (supercritical fluid chromatography) analysis was performed at 40 ºC, using a Thar instrument fitted with OZ-H, OJ-H, AY-H, AD-H, and AS-H columns. Optical rotations were measured (Na D line) on a Perkin Elmer Model 343 Polarimeter fitted with a micro cell with a 1 dm path length; concentrations are reported in g/100 mL.

Experimental details for substrates and products

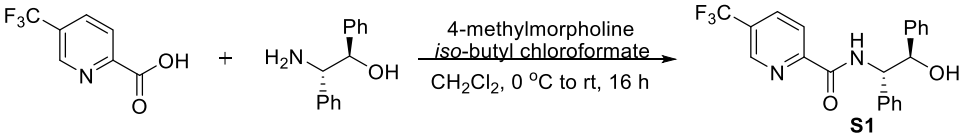
1.1 Procedures for the synthesis of PyrOx ligands according to the literature procedure.[3]

Figure S1. Ligands screened in this report

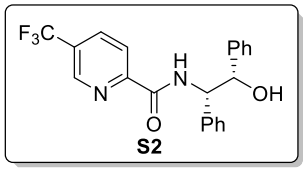


L1, **L2**, **L3**, and **L6** are known compounds and the analytical data (^{1}H-NMR and ^{13}C-NMR) matches with the literature.[3]

Synthesis of *N*-((*1S,2R*)-2-hydroxy-1,2-diphenylethyl)-5-(trifluoromethyl)picolinamide (**S1**):

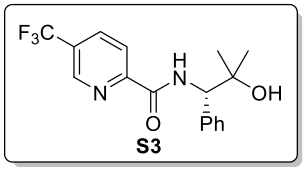


To a dry 250 mL round-bottom flask containing a stir bar was added 5-(trifluoromethyl)picolinic acid (1.91 g, 10.0 mmol, 1.0 equiv). Under an N_2 atmosphere, DCM (100 mL) and 4-methylmorpholine (1.27 mL, 11.5 mmol, 1.15 equiv) were added. Then, the reaction mixture was cooled to 0 °C, *iso*-butylchloroformate was added (1.57 mL, 12 mmol, 1.20 equiv) via syringe. The reaction mixture was stirred for another 30 min, then (1*R*,2*S*)-2-amino-1,2-diphenylethanol (2.35 g, 11 mmol, 1.1 equiv) was added. The mixture was allowed to slowly warm to room temperature and stirred for 16 h. The reaction was quenched *via* addition of water (10 mL). The aqueous layer was extracted with DCM (2 x 10 mL), and the combined organic layers were washed with brine (1 x 30 mL). The combined organic layers were dried over Na_2SO_4, and concentrated in vacuo and the residue was purified by flash column chromatography (1:5 EtOAc:hexanes) to give **S1** as a white solid (3.01 g, 78% yield), R_f = 0.30 (1:2 EtOAc:hexanes).



N-((1*S*,2*S*)-2-hydroxy-1,2-diphenylethyl)-5-(trifluoromethyl)picolinamide

The same procedure as used for the synthesis of **S1** (above) was followed using 5-(trifluoromethyl)picolinic acid (191 mg, 1.0 mmol, 1.0 equiv) in dichloromethane (10 mL), 4-methylmorpholine (0.13 mL, 1.15 mmol, 1.15 equiv), *iso*-butylchloroformate (0.16 mL, 1.2 mmol, 1.2 equiv), and (1*S*,2*S*)-2-amino-1,2-diphenylethanol (235 mg, 1.1 mmol, 1.1 equiv). Purification by silica gel flash chromatography (1:5 EtOAc:hexanes) to give **S2** as a white solid (320 mg, 83% yield), R_f = 0.30 (1:2 EtOAc:hexanes).

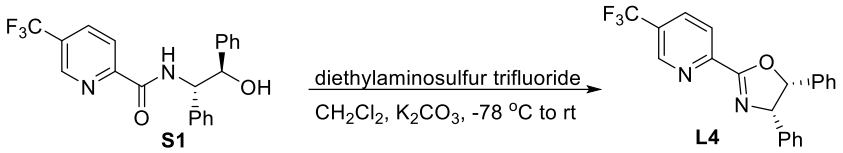


(*S*)-*N*-(2-hydroxy-2-methyl-1-phenylpropyl)-5-(trifluoromethyl)picolinamide

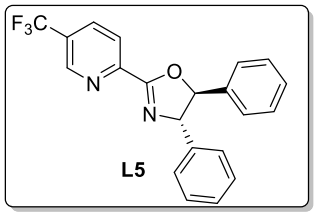
The same procedure as used for the synthesis of **S1** (above) was followed using 5-(trifluoromethyl)picolinic acid (300 mg, 1.57 mmol, 1.00 equiv) in dichloromethane (25 mL), 4-methylmorpholine (0.20 mL, 1.81 mmol, 1.15 equiv), *iso*-butylchloroformate (0.23 mL, 1.88 mmol,

1.20 equiv), and (S)-1-amino-2-methyl-1-phenylpropan-2-ol (285 mg, 1.73 mmol, 1.10 equiv). Purification by silica gel flash chromatography (1:6 EtOAc:hexanes) to give **S3** as a colorless oil (472 mg, 89% yield), R_f = 0.50 (1:2 EtOAc:hexanes).

Synthesis of (*4S,5R*)-4,5-diphenyl-2-(5-(trifluoromethyl)pyridin-2-yl)-4,5-dihydrooxazole (**L4**):

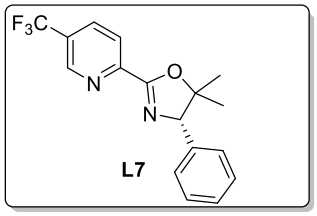


To a dry 100 mL round-bottom flask containing a stir bar was added *N*-((*1S,2R*)-2-hydroxy-1,2-diphenylethyl)-5-(trifluoromethyl)picolinamide **S1** (1.72 g, 4.4 mmol). Under an N_2 atmosphere, DCM (35 mL) was added and then the reaction mixture was cooled to -78 ^oC, the diethylaminosulfur trifluoride (0.83 mL, 6.2 mmol, 1.4 equiv) was added dropwise. The reaction mixture was stirred for 1 h. Then, potassium carbonate (1.23 g, 8.8 mmol, 2.0 equiv) was added. The mixture was allowed to warm to room temperature. The reaction was quenched *via* addition of water (5.0 mL). The aqueous layer was extracted with DCM (2 x 10 mL), and the combined organic layers were washed with brine (1 x 20 mL). The combined organic layers were dried over Na_2SO_4 and concentrated *in vacuo* and the residue was purified by flash column chromatography (1:12 EtOAc:hexanes) to give **L4** as a colorless oil (1.33 g, 82% yield), R_f = 0.40 (1:4 EtOAc:hexanes).



(4*S*,5*S*)-4,5-diphenyl-2-(5-(trifluoromethyl)pyridin-2-yl)-4,5-dihydrooxazole

The same procedure as used for the synthesis of **L4** was followed using 320 mg of **S2** (320 mg, 0.83 mmol, 1.0 equiv) in dichloromethane (10 mL), diethylaminosulfur trifluoride (0.16 mL, 1.16 mmol, 1.4 equiv), and potassium carbonate (232 mg, 1.66 mmol, 2.0 equiv). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **L5** as a colorless oil (61 mg, 20% yield), R_f = 0.40 (1:4 EtOAc:hexanes).

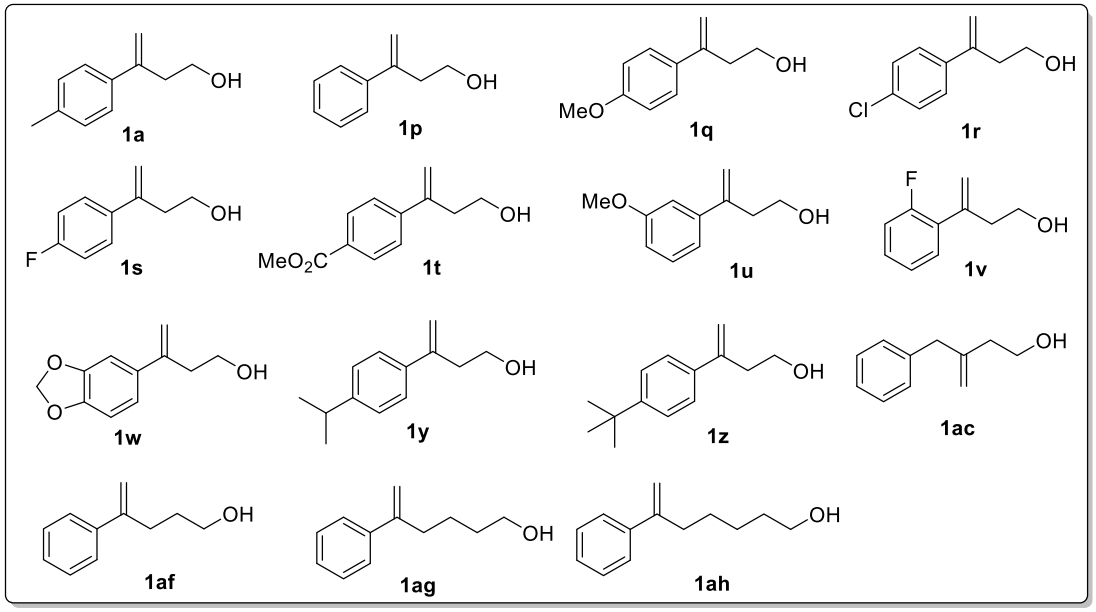


(*S*)-5,5-dimethyl-4-phenyl-2-(5-(trifluoromethyl)pyridin-2-yl)-4,5-dihydrooxazole

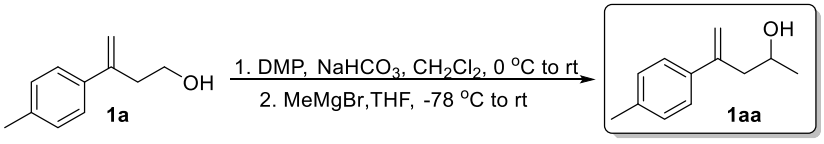
To a solution of **S3** (450 mg, 1.33 mmol, 1.00 equiv) in CH_2Cl_2 (15 mL) was added methanesulfonic acid (0.26 mL, 3.99 mmol, 3.00 equiv). The resulting reaction mixture was heated at reflux until consumption of starting material was observed by TLC analysis. After this time, the reaction was cooled to room temperature and saturated aq. $NaHCO_3$ (15 mL) was added. The layers were separated and the aqueous layer was extracted with CH_2Cl_2 (20 mL). The combined organic layers were washed with H_2O (10 mL) and brine (10 mL). The combined organic layers were dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the residue by silica gel flash chromatography (1:8 EtOAc:hexanes + 1% Et_3N) afforded **L7** as a colorless solid (120 mg, 28%), R_f = 0.40 (1:5 EtOAc:hexanes).

1.2 The substrates below are known compounds and were prepared according to the corresponding literature.[4] Analytical data (^{1}H-NMR and ^{13}C-NMR) matches with the literature.

Figure S2. 1,1-disubstituted alkenols examined in this report



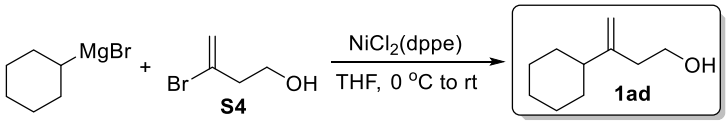
1.3 Procedure for the preparation of the substrate **1aa**:



$NaHCO_3$ (400 mg, 4.0 mmol) and Dess-Martin periodinane (1.27 g, 3.0 mmol) were successively added to a solution of alkenyl alcohol **1a** (324 mg, 2.0 mmol) in dry CH_2Cl_2 (10 mL) under N_2 at 0 ^oC. The reaction mixture was allowed to slowly warm to room temperature and stirred for 12 h. Then, saturated aqueous solution of $NaHCO_3$ (5 mL) and $Na_2S_2O_3$ (5 mL) was added to the reaction. The mixture was stirred for another 30 min and then the aqueous phase was extracted with CH_2Cl_2 (3 x 10 mL). The combined organic layers were dried over Na_2SO_4 and concentrated *in vacuo* and the residue was purified by flash column chromatography (1:10 EtOAc:hexanes) to provide the aldehyde intermediate as a colorless oil, which was directly used in the next step.

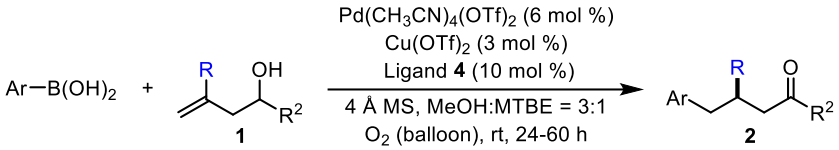
To a dry THF (10 mL) solution of the above aldehyde under N_2 at –78 ^oC was added methyl magnesium bromide (0.74 mL, 3 M solution in Et_2O, 2.2 mmol, 1.1 equiv) followed by warming of the reaction system to room temperature. The reaction was monitored by TLC until the aldehyde disappeared completely. Then, the reaction was quenched *via* addition of saturated aqueous NH_4Cl (5 mL), and diluted with Et_2O (5 mL). The organic layer was separated and aqueous layer was extracted with Et_2O (2 x 10 mL). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4 and concentrated *in vacuo*. Purification of this material by chromatography on silica gel (1:10 → 1:5 EtOAc:hexanes) gave the compound **1aa** as a light yellow oil (306 mg, 87% overall yield from **1a**), R_f = 0.30 (1:2 EtOAc:hexanes).

1.4 Procedure for the preparation of the substrate **1ad**:



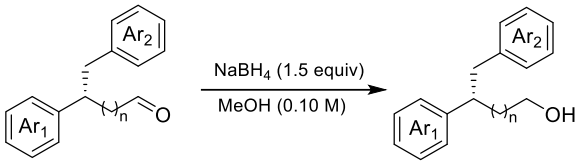
To a solution of alcohol **S4** (378 mg, 2.50 mmol, 1.0 equiv) and $NiCl_2$(dppe) (66 mg, 125 μmol, 0.05 equiv) in 10 mL dry THF at 0 °C was added cyclohexyl magnesium bromide (6.25 mL, 1M in THF, 6.25 mmol, 2.5 equiv) dropwise. The reaction mixture was allowed to slowly warm to room temperature and stirred for 36 h. The resulting mixture was quenched with saturated aqueous NH_4Cl (3 mL) and extracted with Et_2O (2 x 10 mL). The organic layers were combined and dried over Na_2SO_4 and concentrated. The crude residue was purified by flash column chromatography on silica gel (1:10 → 1:5 EtOAc:hexanes) to afford **1ad** as a colorless oil (254 mg, 66% yield) , R_f = 0.25 (1:2 EtOAc:hexanes).

1.5 General procedure for the enantioselective redox-relay Heck reaction of 1,1-disubstituted alkenols (**procedure A**):



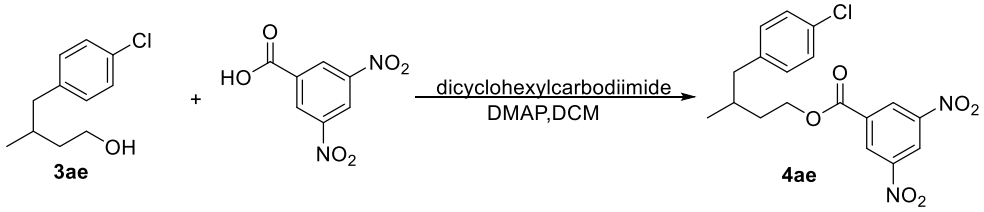
To a dry 10 mL Schlenk flask equipped with a stir bar was added $Pd(CH_3CN)_4(OTf)_2$ (10.3 mg, 0.018 mmol, 0.06 equiv), $Cu(OTf)_2$ (3.3 mg, 0.009 mmol, 0.03 equiv), ligand **4** (11.0 mg, 0.03 mmol, 0.1 equiv), 4Å M.S. (75.0 mg), and MeOH/MTBE (3:1, 2.0 mL). To this flask, a three-way adapter fitted with a balloon of O_2 was added, and the flask was evacuated *via* house vacuum and refilled with O_2 three times while stirring. The resulting mixture was stirred for 10-15 min. Then, the corresponding alkenyl alcohol (0.3 mmol, 1.0 equiv) and corresponding aryl boronic acid (0.9 mmol, 3.0 equiv) in the 1.0 mL of MeOH/MTBE (3:1) were added. The resulting mixture was stirred for another 24 h to 60 h at room temperature. The reaction was monitored by TLC until the alcohol disappeared completely. The solvent was concentrated under reduced pressure, and the resulting residue was purified by flash column chromatography on silica gel (1:16→1:6 EtOAc:hexanes) to give the corresponding aldehyde.

1.6 General procedure of reduction (**procedure B** for chiral separation)**:**



The aldehyde (1.0 equiv) was dissolved in MeOH in a 10 mL scintillation vial equipped with a stir bar. Sodium borohydride (1.5 equiv) was added, and the resulting mixture was stirred for 30 min. The solvent was removed under reduced pressure, and the resulting residue was transferred to a separatory funnel using Et_2O (10 mL) and H_2O (5 mL). The aqueous layer was extracted with Et_2O (2 x 10 mL), and the combined organic layers were washed with brine (10 mL). The organic layer was then dried over Na_2SO_4, and concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica gel (1:8→1:2 EtOAc:hexanes) to give the corresponding alcohol.

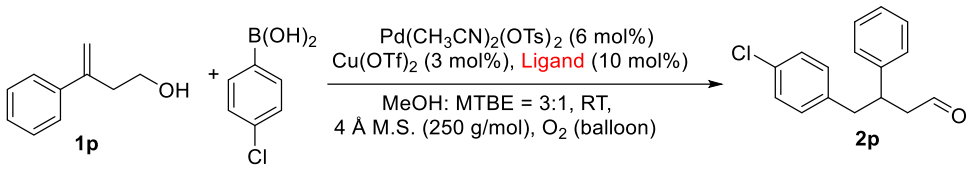
1.7 Procedure for the preparation of the ester **4ae** (for chiral separation)**:**



To a mixture of alcohol **3ae** (39.6 mg, 0.20 mmol, 1.0 equiv), DMAP (12.2 mg, 0.05 mmol, 0.25

equiv), and 3,5-dinitrobenzoic acid (50.9 mg, 0.24 mmol, 1.2 equiv) in DCM (5 mL) was added dicyclohexylcarbodiimide (49.5 mg, 0.24 mmol, 1.2 equiv) at room temperature. The resulting mixture was stirred 16 h. The resulting mixture was concentrated under reduced pressure. The crude residue was purified by flash column chromatography on silica gel (1:15→1:12 EtOAc:hexanes) to give the ester **4ae** (66 mg, 82% yield), R_f = 0.40 (1:4 EtOAc:hexanes).

1.8 Procedure for the modeling of ligands

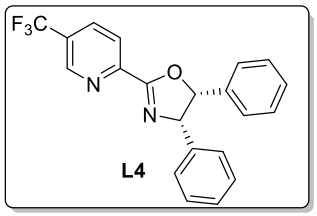


To a dry 10 mL Schlenk flask equipped with a stir bar was added $Pd(CH_3CN)_4(OTs)_2$ (9.5 mg, 0.018 mmol, 0.06 equiv), $Cu(OTf)_2$ (3.3 mg, 0.009 mmol, 0.03 equiv), ligand (0.03 mmol, 0.1 equiv), 4Å M.S. (75.0 mg), and MeOH/MTBE (3:1, 2.0 mL). To this flask, a three-way adapter fitted with a balloon of O_2 was added, and the flask was evacuated via house vacuum and refilled with O_2 three times while stirring. The resulting mixture was stirred for 10-15 min. Then, the alkenyl alcohol **1p** (44.4 mg, 0.3 mmol, 1.0 equiv) and 4-chlorophenylboronic acid (140.4 mg, 0.9 mmol, 3.0 equiv) in MeOH/MTBE (3:1, 1.0 mL) were added. The resulting mixture was stirred for another 24 h at room temperature. The reaction was monitored by TLC until the alcohol disappeared completely. The solvent was concentrated under reduced pressure, and the resulting residue was purified by flash column chromatography on silica gel (1:15 EtOAc:hexanes) to give aldehyde **2p** as a colorless oil.

Table S1. Ligand Screen Data

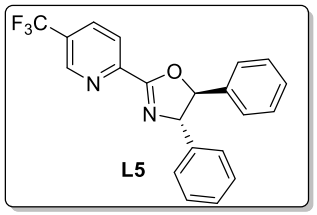
Ligand	**L1**	**L2**	**L3**	**L4**	**L5**	**L6**	**L7**
Isolated yield (%)	31	44	56	50	52	43	51
Er	39:61	16:84	58:42	6:94	7.5:92.5	44:56	9.5:90.5

Analytical data for the substrates and products:



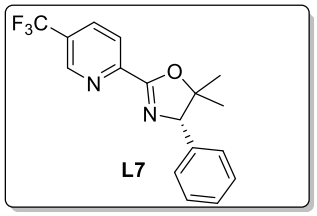
(4*S*,5*R*)-4,5-diphenyl-2-(5-(trifluoromethyl)pyridin-2-yl)-4,5-dihydrooxazole

^{1}H NMR (300 MHz, $CDCl_3$): δ 9.04 (s, 1H), 8.34 (d, *J* = 4.5 Hz, 1H), 8.05 (dd, *J* = 3.0, 1.5 Hz, 1H), 7.39-7.29 (m, 10H), 5.56 (d, *J* = 4.5 Hz, 1H), 5.36 (d, *J* = 4.5 Hz, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 162.0, 149.6, 146.7 (d, J_F = 1.5 Hz), 140.8, 139.4, 134.0 (d, J_F = 1.5 Hz), 128.9, 128.8, 127.9, 126.7, 126.6 (q, J_F = 272.2 Hz), 125.9, 124.0, 89.9, 78.9; **^{19}F NMR** (282 MHz, $CDCl_3$): δ –62.9; **IR** (neat): 1642, 1604, 1323, 1127, 1097, 697 cm^{-1}; $[\alpha]_D^{20}$ = –21.4 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{21}H_{15}F_3ON_2Na$ $(M+Na)^+$: 391.1034, found 391.1041.



(4*S*,5*S*)-4,5-diphenyl-2-(5-(trifluoromethyl)pyridin-2-yl)-4,5-dihydrooxazole

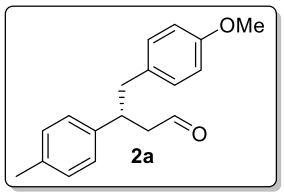
^{1}H NMR (500 MHz, $CDCl_3$): δ 8.95 (s, 1H), 8.28 (d, *J* = 5.0 Hz, 1H), 8.01 (d, J_2 = 2.5 Hz, 1H), 7.33-7.18 (m, 10H), 5.48 (d, *J* = 5.0 Hz, 1H), 5.28 (d, *J* = 5.0 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$,): δ 162.1, 149.7, 146.9, 140.9, 139.4, 134.1, 129.0, 128.8, 128.0, 126.8, 126.7 (q, J_F = 272.2 Hz), 126.0, 124.1, 90.0, 79.0; **^{19}F NMR** (282 MHz, $CDCl_3$): δ –63.0; **IR** (neat) ν = 1604, 1325, 1129, 1099, 698 cm^{-1}; $[\alpha]_D^{20}$ = -20.0 (c = 0.5, EtOH); **HRMS** m/z (ESI) calcd. for $C_{21}H_{15}F_3ON_2Na$ $(M+Na)^+$: 391.1034, found 391.1040.



(*S*)-5,5-dimethyl-4-phenyl-2-(5-(trifluoromethyl)pyridin-2-yl)-4,5-dihydrooxazole

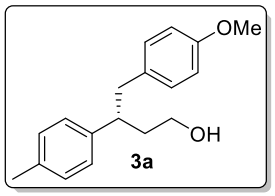
^{1}H NMR (500 MHz, $CDCl_3$): δ 9.00 (s, 1H), 8.36 (d, *J* = 5.0 Hz, 1H), 8.06 (d, *J* = 5.0 Hz, 1H), 7.37-7.24 (m, 5H), 5.14 (s, 1H), 1.73 (s, 3H), 1.01 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 161.9, 150.3, 146.6, 140.8, 138.0, 133.9, 128.4, 127.8, 127.2, 125.3 (q, J_F = 271.2 Hz), 123.9, 89.2, 78.7, 29.1, 23.8; **^{19}F NMR** (282 MHz, $CDCl_3$): δ -63.0; **IR** (neat) ν = 1637, 1603, 1324, 1127, 1092, 1015,

743, 701 cm^{-1}; $[\alpha]_D^{20}$ = +24.4 (c = 0.43, EtOH); **HRMS** m/z (ESI) calcd. for $C_{17}H_{15}F_3ON_2Na$ $(M+Na)^+$: 343.1034, found 343.1040.



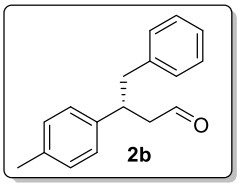
(*R*)-4-(4-methoxyphenyl)-3-(*p*-tolyl)butanal

General procedure A was followed using 4-methoxyphenylboronic acid (137 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:12 EtOAc:hexanes) to afford product **2a** as a colorless oil (35 mg, 43% yield, 7.5:92.5 er), R_f = 0.30 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.57 (t, *J* = 5.0 Hz, 1H), 7.09 (d, *J* = 5.0 Hz, 2H), 7.04 (d, *J* = 5.0 Hz, 2H), 6.97 (d, *J* = 5.0 Hz, 2H), 6.78-6.76 (m, 2H), 3.77 (s, 3H), 3.43-3.38 (m, 1H), 2.89 (dd, *J* = 7.5, 2.5, 1H), 2.79 (dd, *J* = 7.5, 2.5 Hz, 1H), 2.81-2.69 (m, 2H), 2.31 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.8, 158.1, 140.3, 136.2, 131.4, 130.2, 129.3, 127.4, 113.7, 55.2, 49.0, 42.5, 41.8, 21.0; **IR** (neat): 2920, 1722, 1512, 1246, 1035, 828 cm^{-1}; $[\alpha]_D^{20}$ = +51.8 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{20}O_2Na$ $(M+Na)^+$: 291.1361, found 291.1365.



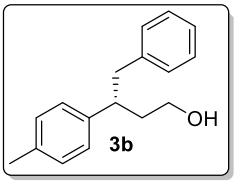
(*R*)-4-(4-methoxyphenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2a** (27 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:4 EtOAc:hexanes) to afford product **3a** as a colorless oil (25 mg, 92% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.10-7.02 (m, 4H), 6.96 (d, *J* = 4.5 Hz, 2H), 6.77-6.74 (m, 2H), 3.76 (s, 3H), 3.52-3.43 (m, 2H), 2.90-2.75 (m, 3H), 2.31 (s, 3H), 1.97-1.75 (m, 2H), 1.05 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 157.7, 141.3, 135.7, 132.5, 130.0, 129.1, 127.5, 113.5, 61.2, 55.2, 44.2, 43.0, 38.1, 21.0; **IR** (neat): 3351, 2931, 1512, 1246, 1037, 815 cm^{-1}; $[\alpha]_D^{20}$ = +64.5 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{22}O_2Na$ $(M+Na)^+$: 293.1517, found 293.1524.



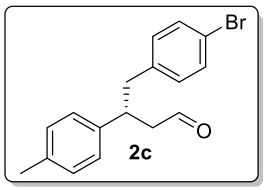
(*R*)-4-phenyl-3-(*p*-tolyl)butanal

General procedure A was followed using phenylboronic acid (110 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford product **2b** as a colorless oil (37 mg, 52% yield, 6:94 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.57 (t, *J* = 5.0 Hz, 1H), 7.25-7.22 (m, 2H), 7.19-7.16 (m, 1H), 7.10-7.05 (m, 6H), 3.49-3.43 (m, 1H), 2.96 (dd, *J* = 7.5, 2.5 Hz, 1H), 2.86 (dd, *J* = 7.5, 2.5 Hz, 1H), 2.76-2.67 (m, 2H), 2.30 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.8, 140.2, 139.4, 136.2, 129.3, 129.2, 128.3, 127.3, 126.3, 49.0, 43.4, 41.6, 21.0; **IR** (neat): 2922, 2360, 1723, 1514, 815, 701 cm^{-1}; $[\alpha]_D^{20}$ = +56.6 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{18}ONa$ $(M+Na)^+$: 261.1255, found 261.1266.



(*R*)-4-phenyl-3-(*p*-tolyl)butan-1-ol

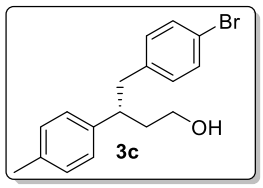
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2b** (24 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:5 EtOAc:hexanes) to afford **3b** as a colorless oil (23 mg, 95% yield), R_f = 0.30 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.28-7.16(m, 3H), 7.12-7.05 (m, 6H), 3.52-3.45 (m, 2H), 2.96-2.86 (m, 3H), 2.33 (s, 3H), 1.98-1.81 (m, 2H), 1.06(brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 141.2, 140.4, 135.8, 129.1, 128.1, 127.5, 125.9, 61.2, 44.1, 43.9, 38.2, 21.0; **IR** (neat): 3316, 2926, 1520, 1040, 815, 699 cm^{-1}; $[\alpha]_D^{20}$ = +53.0 (c = 0.2, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{20}ONa$ $(M+Na)^+$: 263.1412, found 263.1418.



(*R*)-4-(4-bromophenyl)-3-(*p*-tolyl)butanal

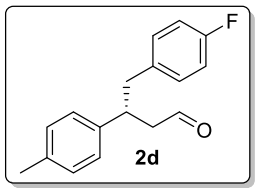
General procedure A was followed using 4-bromophenylboronic acid (181 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash

chromatography (1:15 EtOAc:hexanes) to afford **2c** as a colorless oil (52 mg, 55% yield, 5.5:94.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.62 (t, *J* = 5.0 Hz, 1H), 7.34-7.32 (m, 2H), 7.08 (d, *J* = 5.0 Hz, 2H), 7.01-7.00 (m, 2H), 6.91-6.88 (m, 2H), 3.44-3.38 (m, 1H), 2.86 (d, *J* = 2.5 Hz, 2H), 2.78-2.68 (m, 2H), 2.31 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.4, 139.6, 138.3, 136.4, 131.3, 130.9, 129.3, 127.3, 120.1, 49.1, 42.6, 41.4, 21.0; **IR** (neat): 2923, 2360, 1723, 1488, 1011, 816 cm^{-1}; $[\alpha]_D^{20}$ = +67.2 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}ONaBr$ $(M+Na)^+$: 339.0360, found 339.0344.



(*R*)-4-(4-bromophenyl)-3-(*p*-tolyl)butan-1-ol

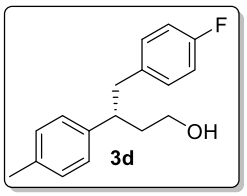
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2c** (32 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:5 EtOAc:hexanes) to afford **3c** as a colorless oil (29 mg, 93% yield), R_f = 0.30 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.32-7.30 (m, 2H), 7.07 (d, *J* = 5.0 Hz, 2H), 7.00 (d, *J* = 5.0 Hz, 2H), 6.89 (d, *J* = 5.0 Hz, 2H), 3.53-3.42 (m, 2H), 2.97-2.91 (m, 1H), 3.84 (m, 2H), 2.31 (s, 3H), 1.97-1.90 (m, 1H), 1.87-1.80 (m, 1H), 1.11 (brs, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 140.6, 139.3, 135.9, 131.1, 130.8, 129.2, 127.5, 119.6, 61.0, 43.9, 43.2, 38.3, 21.0; **IR** (neat): 3338, 2925, 1487, 1011, 1072, 815 cm^{-1}; $[\alpha]_D^{20}$ = +79.7 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}ONaBr$ $(M+Na)^+$: 341.0517, found 341.0513.



(*R*)-4-(4-fluorophenyl)-3-(*p*-tolyl)butanal

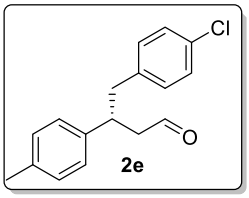
General procedure A was followed using 4-fluorophenylboronic acid (126 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2d** as a colorless oil (45 mg, 59% yield, 4.5:95.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.62-9.60 (m, 1H), 7.08 (d, *J* = 5.0 Hz, 2H), 7.02-6.97 (m, 4H), 6.92-6.88 (m, 2H), 3.41 (m, 1H), 2.88 (d, *J* = 2.5 Hz, 2H), 2.78-2.68 (m, 2H), 2.31 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.5, 161.5 (d, *J* = 121.2 Hz), 139.8, 136.3, 135.0 (d, *J* = 1.9 Hz), 130.6 (d, *J* = 3.8 Hz), 129.3, 127.4, 115.0 (d, *J* = 10.6 Hz), 49.1, 42.4, 41.7 (d, *J* = 0.6 Hz), 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –119.5; **IR** (neat): 2925, 2361, 1724, 1488, 1011,

816 cm^{-1}; $[\alpha]_D^{20}$ = +50.4 (c = 0.31, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}ONaF(M+Na)^+$: 279.1161, found 279.1157.



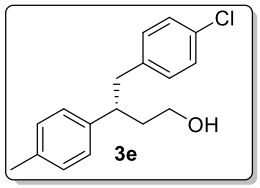
(*R*)-4-(4-fluorophenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2d** (26 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:5 EtOAc:hexanes) to afford **3d** as a colorless oil (24 mg, 93% yield), R_f = 0.30 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.10-7.07 (m, 2H), 7.02-6.95 (m, 4H), 6.92-6.85 (m, 2H), 3.53-3.41 (m, 2H), 2.98-2.84 (m, 3H), 2.32 (s, 3H), 2.00-1.77 (m, 2H), 1.23 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 161.2 (d, *J* = 121.2 Hz), 140.8, 136.0 (d, *J* = 1.5 Hz), 135.8, 130.4 (d, *J* = 4.1 Hz), 129.1, 127.5, 115.0 (d, *J* = 10.5 Hz), 61.0, 44.1, 43.0, 38.2, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –118.0; **IR** (neat): 3335, 2926, 1509, 1220, 1042, 815 cm^{-1}; $[\alpha]_D^{20}$ = +66.5 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}ONaF$ $(M+Na)^+$: 281.1318, found 281.1316.



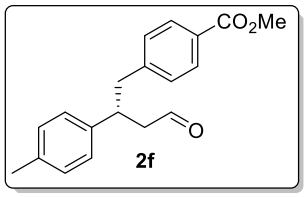
(*R*)-4-(4-chlorophenyl)-3-(*p*-tolyl)butanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2e** as a colorless oil (52 mg, 63% yield, 4.5:95.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.62 (t, *J* = 5.0 Hz, 1H), 7.20-7.17 (m, 2H), 7.08 (d, *J* = 5.0 Hz, 2H), 7.02-7.00 (m, 2H), 6.97-6.95 (m, 2H), 3.41 (m, 1H), 2.88 (d, *J* = 2.5 Hz, 2H), 2.79-2.68 (m, 2H), 2.31 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.4, 139.6, 137.8, 136.4, 132.0, 130.5, 129.3, 128.4, 127.3, 49.1, 42.5, 41.4, 21.0; **IR** (neat): 2924, 1722, 1492, 1092, 1015, 701 cm^{-1}; $[\alpha]_D^{20}$ = +75.4 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}ONaCl$ $(M+Na)^+$: 295.0866, found 295.0866.



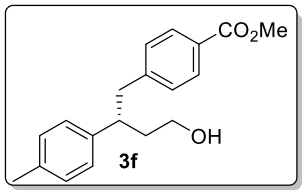
(*R*)-4-(4-chlorophenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2e** (27 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:5 EtOAc:hexanes) to afford **3e** as a colorless oil (25 mg, 96% yield). R_f = 0.30 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.17-7.15 (m, 2H), 7.08-7.07 (m, 2H), 7.01-6.99 (m, 2H), 6.96-6.94 (m, 2H), 3.55-3.40 (m, 2H), 2.92-2.84 (m, 3H), 2.31 (s, 3H), 1.93-1.82 (m 2H), 1.13 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 140.6, 138.8, 135.9, 131.6, 130.4, 129.2, 128.2, 127.5, 61.0, 44.0, 43.1, 38.3, 21.0; **IR** (neat): 3327, 2925, 1491, 1092, 1042, 816 cm^{-1}; $[\alpha]_D^{20}$ = +81.0 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}ONaCl$ $(M+Na)^+$: 297.1022, found 297.1024.



methyl (*R*)-4-(4-oxo-2-(*p*-tolyl)butyl)benzoate

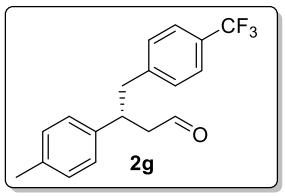
General procedure A was followed using 4-methoxycarbonylphenylboronic acid (162 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:8 EtOAc:hexanes) to afford **2f** as a colorless oil (49 mg, 55% yield, 4.5:95.5 er), R_f = 0.30 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.62 (m, 1H), 7.89-7.87 (m, 2H), 7.10-7.06 (m, 4H), 7.00-6.99 (m, 2H), 3.88 (s, 3H), 3.47 (m, 1H), 2.96-2.94 (m, 2H), 2.77-2.73 (m, 2H), 2.29 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.3, 167.0, 144.8, 139.4, 136.4, 129.6, 129.3, 129.2, 128.2, 127.3, 52.0, 49.2, 43.2, 41.3, 21.0; **IR** (neat): 1720, 1435, 1280, 1111, 1020 cm^{-1}; $[\alpha]_D^{20}$ = +96.4 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{19}H_{20}O_3Na$ $(M+Na)^+$: 319.1310, found 319.1316.



methyl (*R*)-4-(4-hydroxy-2-(*p*-tolyl)butyl)benzoate

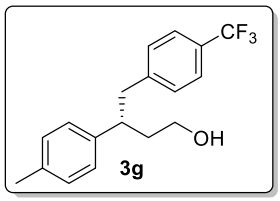
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2f** (30 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3

EtOAc:hexanes) to afford **3f** as a colorless oil (28 mg, 92% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.87-7.85 (m, 2H), 7.09-7.05 (m, 4H), 7.00-6.98 (m, 2H), 3.87 (s, 3H), 3.54-3.51 (m, 1H), 3.44-3.43 (m, 1H), 3.00-2.91 (m, 3H), 2.30 (s, 3H), 1.95-1.92 (m, 1H), 1.88-1.85 (m, 1H), 1.17 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 167.1, 145.9, 140.4, 136.0, 129.4, 129.2, 127.8, 127.4, 60.9, 51.9, 43.8, 38.4, 21.0; **IR** (neat): 3413, 2931, 1719, 1435, 1279, 1110 cm^{-1}; $[\alpha]_D^{20}$ = +99.3 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{19}H_{22}O_3Na$ $(M+Na)^+$: 321.1467, found 321.1469.



(*R*)-3-(*p*-tolyl)-4-(4-(trifluoromethyl)phenyl)butanal

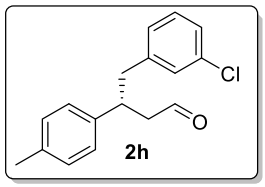
General procedure A was followed using 4-(trifluoromethyl)phenylboronic acid (171 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:14 EtOAc:hexanes) to afford **2g** as a colorless oil (59 mg, 64% yield, 4:96 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.64 (t, *J* = 5.0 Hz, 1H), 7.46 (d, *J* = 2.5 Hz, 2H), 7.13 (d, *J* = 5.0 Hz, 2H), 7.08 (d, *J* = 5.0 Hz, 2H), 7.02-7.00 (m, 2H), 3.46 (m, 1H), 2.97-2.95 (m, 2H), 2.78-2.74 (m, 2H), 2.31 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.1, 143.5, 139.4, 136.5, 129.5, 129.4, 128.6 (d, *J* = 16.1 Hz), 127.3, 126.4 (q, *J* = 270.0 Hz), 125.2 (q, *J* = 3.8 Hz) 49.2, 42.9, 41.2, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –62.8; **IR** (neat): 2360, 1725, 1325, 1123, 1067 cm^{-1}; $[\alpha]_D^{20}$ = +41.7 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{17}OF_3Na$ $(M+Na)^+$: 329.1129. found 329.1135.



(*R*)-3-(*p*-tolyl)-4-(4-(trifluoromethyl)phenyl)butan-1-ol

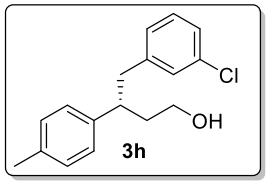
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2g** (31 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3g** as a colorless oil (28 mg, 90% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.46 (d, *J* = 4.5 Hz, 2H), 7.15-7.07 (m, 4H), 7.02-7.00 (m, 2H), 3.52-3.42 (m, 2H), 3.02-2.93 (m, 3H), 2.32 (s, 3H), 1.96-1.86 (m, 2H), 1.20 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 144.5, 140.4, 136.0, 129.4 129.2, 128.2 (d, *J* = 16.1 Hz), 127.9 (q, *J* = 270.0 Hz),

127.5, 125.0 (q, J = 3.8 Hz), 60.9, 43.8, 43.5, 38.3, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –62.7; **IR** (neat): 3339, 2931, 1325, 1163, 1123, 1067 cm^{-1}; $[\alpha]_D^{20}$ = +69.5 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{19}OF_3Na$ $(M+Na)^+$: 331.1286, found 331.1297.



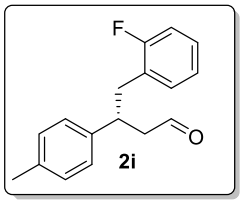
(*R*)-4-(3-chlorophenyl)-3-(*p*-tolyl)butanal

General procedure A was followed using 3-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:14 EtOAc:hexanes) to afford **2h** as a colorless oil (45 mg, 55% yield, 3.5:96.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.61 (t, J = 5.0 Hz, 1H), 7.16-7.14 (m, 2H), 7.10-7.06 (m, 3H), 7.03-7.02 (m, 2H), 6.92-6.90 (m, 1H), 3.44 (m, 1H), 2.92-2.84 (m, 2H), 2.79-2.68 (m, 2H), 2.31 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.3, 141.4, 139.6, 136.4, 134.0, 129.5, 129.3, 129.2, 127.4, 127.3, 126.5, 49.0, 42.9, 41.3, 21.0; **IR** (neat): 2924, 2359, 1723, 1515, 1080, 815 cm^{-1}; $[\alpha]_D^{20}$ = +53.0 (c = 0.24, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{74}H_{17}ONaCl$ $(M+Na)^+$: 295.0866, found 295.0868.



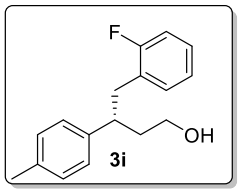
(*R*)-4-(3-chlorophenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2h** (27 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3h** as a colorless oil (26 mg, 94% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.13-7.00 (m, 7H), 6.92-6.89 (m, 1H), 3.51-3.41 (m, 2H), 2.96-2.84 (m, 3H), 2.31 (s, 3H), 1.95-1.83 (m, 2H), 1.16 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 142.4, 140.6, 136.0, 133.8, 129.3, 129.2, 127.4, 127.3, 126.1, 61.0, 43.8, 43.5, 38.1, 21.0; **IR** (neat): 3329, 2932, 1597, 1476, 1042, 814 cm^{-1}; $[\alpha]_D^{20}$ = +76.9 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}ONaCl$ $(M+Na)^+$: 297.1022, found 297.1020.



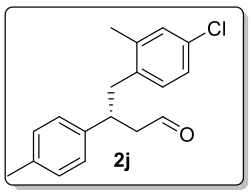
(*R*)-4-(2-fluorophenyl)-3-(*p*-tolyl)butanal

General procedure A was followed using 2-fluorophenylboronic acid (126 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:14 EtOAc:hexanes) to afford **2i** as a colorless oil (48 mg, 63% yield, 6:94 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.58 (t, *J* = 5.0 Hz, 1H), 7.18-7.14 (m, 1H), 7.09-7.05 (m, 4H), 7.01-6.98 (m, 3H), 3.57-3.47 (m, 1H), 2.94 (d, *J* = 5.0 Hz, 2H), 2.76-2.70 (m, 2H), 2.30 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.6, 161.2 (d, *J* = 121.5 Hz), 139.9, 136.3, 131.5 (d, *J* = 2.6 Hz), 129.3, 128.1 (d, *J* = 4.1 Hz), 127.2, 126.3 (d, *J* = 7.5 Hz), 123.8 (d, *J* = 1.5 Hz), 115.2 (d, *J* = 11.2 Hz), 48.8, 40.4, 36.4, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –118.4; **IR** (neat): 2925, 2361, 1724, 1491, 1229, 757 cm^{-1}; $[\alpha]_D^{20}$ = +55.0 (c = 0.3, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}ONaF$ $(M+Na)^+$: 279.1161, found 279.1149.



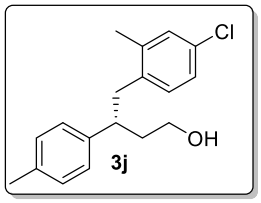
(*R*)-4-(2-fluorophenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2i** (26 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3i** as a colorless oil (24 mg, 93% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.17-6.94 (m, 8H), 3.56-3.39 (m, 2H), 3.02-2.88 (m, 3H), 2.32 (s, 3H), 1.95-1.88 (m, 2H), 1.22 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 161.2 (d, *J* = 121.5 Hz), 140.9, 135.8, 131.4 (d, *J* = 2.6 Hz), 129.1, 127.7, 127.6, 127.4, 123.6 (d, *J* = 1.9 Hz), 115.1 (d, *J* = 10.9 Hz), 61.1, 42.8, 38.0, 36.8 (d, *J* = 0.4 Hz), 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –118.6; **IR** (neat): 3329, 2926, 1491, 1229, 1043, 755 cm^{-1}; $[\alpha]_D^{20}$ = +65.1 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}ONaF$ $(M+Na)^+$: 281.1318, found 281.1320.



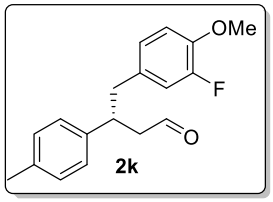
(*R*)-4-(4-chloro-2-methylphenyl)-3-(*p*-tolyl)butanal

General procedure A was followed using 4-chloro-2-methylphenylboronic acid (153 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:14 EtOAc:hexanes) to afford **2j** as a colorless oil (47 mg, 55% yield, 6.5:93.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.60 (m, 1H), 7.10-7.07 (m, 3H), 7.02-6.99 (m, 3H), 6.86-6.82 (m, 1H), 3.40-3.34 (m, 1H), 2.85-2.83 (m, 2H), 2.78-2.76 (m, 2H), 2.31 (s, 3H), 2.21 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.3, 139.9, 138.2, 136.4, 136.2, 131.8, 131.3, 130.1, 129.3, 127.2, 125.7, 49.1, 40.3, 40.1, 21.0, 19.3; **IR** (neat): 2929, 1723, 1518, 1275, 1126, 817 cm^{-1}; $[\alpha]_D^{20}$ = +84.3 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{19}ONaCl$ $(M+Na)^+$: 309.1022, found 309.1024.



(*R*)-4-(4-chloro-2-methylphenyl)-3-(*p*-tolyl)butan-1-ol

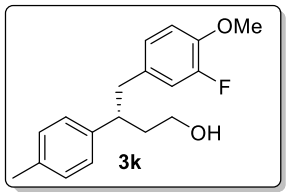
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2j** (29 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3j** as a colorless oil (28 mg, 96% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.10-7.07 (m, 3H), 7.02-6.98 (m, 3H), 6.86 (d, *J* = 3.0 Hz, 1H), 3.51-3.41 (m, 2H), 2.90-2.80 (m, 3H), 2.32 (s, 3H), 2.20 (s, 3H), 1.97-1.87 (m, 2H), 1.13 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 140.9, 138.1, 137.1, 136.0, 131.3, 131.2, 129.9, 129.2, 127.4, 125.5, 61.1, 42.8, 40.6, 38.0, 21.0, 19.4; **IR** (neat): 3320, 2926, 1484, 1040, 881 cm^{-1}; $[\alpha]_D^{20}$ = +90.3 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{21}ONaCl$ $(M+Na)^+$: 311.1179, found 311.1181.



(*R*)-4-(3-fluoro-4-methoxyphenyl)-3-(*p*-tolyl)butanal

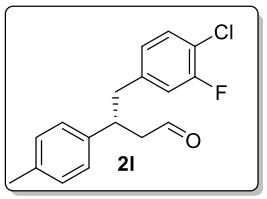
General procedure A was followed using 3-fluoro-4-methoxyphenylboronic acid (153 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:10 EtOAc:hexanes) to afford **2k** as a colorless oil (43 mg, 50% yield, 5:95 er), R_f = 0.30 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.60 (m, 1H), 7.08 (d, *J* = 5.0 Hz, 2H), 7.02 (d, *J* = 5.0 Hz, 2H), 6.83-6.73 (m, 3H), 3.84 (s, 3H), 3.43-3.37 (m, 1H), 2.84-2.83 (m, 2H), 2.71-2.69 (m, 2H), 2.31 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.5, 152.1 (d, *J* = 121.8 Hz), 146.0

(d, *J* = 5.2 Hz), 139.8, 136.4, 132.5 (d, *J* = 3.4 Hz), 129.3, 127.3, 124.7 (d, *J* = 1.5 Hz), 116.7 (d, *J* = 2.6 Hz), 113.2, 56.2, 49.0, 42.3, 41.5, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –136.0; **IR** (neat): 2960, 1723, 1492, 1093, 1016, 831 cm^{-1}; $[\alpha]_D^{20}$ = +63.8 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{19}O_2NaF$ $(M+Na)^+$: 309.1267, found 309.1273.



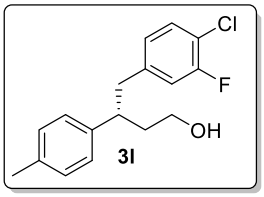
(*R*)-4-(3-fluoro-4-methoxyphenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2k** (29 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3k** as a colorless oil (27 mg, 94% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.08 (d, *J* = 3.0 Hz, 2H), 7.02-6.99 (m, 2H), 6.82-6.71 (m, 3H), 3.83 (s, 3H), 3.50-3.44 (m, 2H), 2.97-2.87 (m, 2H), 2.82-2.79 (m, 1H), 2.31 (s, 3H), 1.95-1.82 (m, 2H), 1.13 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 152.0 (d, *J* = 121.5 Hz), 145.6 (d, *J* = 5.2 Hz), 140.8, 135.9, 133.5 (d, *J* = 3.0 Hz), 129.2, 127.5, 124.6 (d, *J* = 1.5 Hz), 116.7 (d, *J* = 9.0 Hz), 113.1 (d, *J* = 1.1 Hz), 61.0, 56.2, 44.0, 42.8, 38.2, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –136.4; **IR** (neat): 3338, 2929, 1516, 1273, 1124, 1029, 815 cm^{-1}; $[\alpha]_D^{20}$ = +69.6 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{21}O_2FNa$ $(M+Na)^+$: 311.1423, found 311.1423.



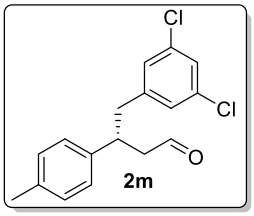
(*R*)-4-(4-chloro-3-fluorophenyl)-3-(*p*-tolyl)butanal

General procedure A was followed using 4-chloro-3fluorophenylboronic acid (157 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:12 EtOAc:hexanes) to afford **2l** as a colorless oil (54 mg, 62% yield, 4:96 er), R_f = 0.30 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.64 (m, 1H), 7.24-7.19 (m, 1H), 7.09-7.07 (m, 2H), 7.00-6.97 (m, 2H), 6.81-6.72 (m, 2H), 3.43-3.36 (m, 1H), 2.87-2.73 (m, 4H), 2.30 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.2, 157.8 (d, *J* = 123.4 Hz), 140.4 (d, *J* = 3.0 Hz), 139.2, 136.6, 130.2, 129.4, 127.3, 125.6, 118.5, 117.2 (d, *J* = 10.5 Hz), 49.2, 42.4, 41.2, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –116.4; **IR** (neat): 2924, 1723, 1491, 1156, 1063, 817 cm^{-1}; $[\alpha]_D^{20}$ = +74.6 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{16}ONaClF$ $(M+Na)^+$: 313.0771, found 313.0787.



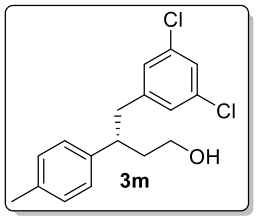
(*R*)-4-(4-chloro-3-fluorophenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2l** (29 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3l** as a colorless oil (28 mg, 97% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.22-7.16 (m, 1H), 7.08 (d, *J* = 4.5 Hz, 2H), 7.00 (d, *J* = 4.5 Hz, 2H), 6.81-6.72 (m, 2H), 3.53-3.42 (m, 2H), 2.96-2.90 (m, 1H), 2.86-2.83 (m, 2H), 2.31 (s, 3H), 1.95-1.82 (m, 2H), 1.22 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 157.6 (d, *J* = 123.4 Hz), 141.4 (d, *J* = 3.4 Hz), 140.1, 136.1, 130.0, 129.2, 127.4, 125.5 (d, *J* = 1.5 Hz), 118.1 (d, *J* = 8.6 Hz), 117.1 (d, *J* = 10.1 Hz), 60.8, 43.7, 43.0, 38.3, 21.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –116.7; **IR** (neat): 3328, 2930, 1580, 1423, 1060, 816 cm^{-1}; $[\alpha]_D^{20}$ = +137.7 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{18}ONaClF$ $(M+Na)^+$: 315.0928, found 315.0931.



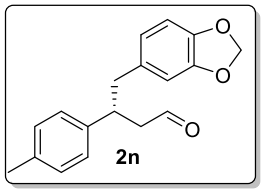
(*R*)-4-(3,5-dichlorophenyl)-3-(*p*-tolyl)butanal

General procedure A was followed using 3,5-dichlorophenylboronic acid (172 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:14 EtOAc:hexanes) to afford **2m** as a colorless oil (37 mg, 40% yield, 2:98 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.64 (m, 1H), 7.17 (s, 1H), 7.10 (d, *J* = 5.0 Hz, 2H), 7.01 (d, *J* = 2.5 Hz, 2H), 6.91 (s, 2H), 3.44-3.39 (m, 1H), 2.88-2.69 (m, 4H), 2.31 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.1, 142.8, 139.0, 136.7, 134.6, 129.4, 127.6, 127.3, 126.6, 49.0, 42.5, 41.0, 21.0; **IR** (neat): 2929, 1723, 1567, 1430, 797 cm^{-1}; $[\alpha]_D^{20}$ = +51.9 (c = 0.32, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{16}ONaCl_2$ $(M+Na)^+$: 329.0476, found 329.0464.



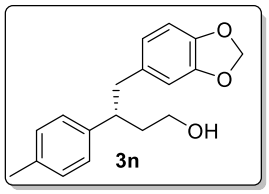
(*R*)-4-(3,5-dichlorophenyl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2m** (31 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3m** as a colorless oil (28 mg, 90% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.14 (s, 1H), 7.09 (d, *J* = 5.0 Hz, 2H), 7.00 (d, *J* = 5.0 Hz, 2H), 6.91 (m, 2H), 3.54-3.52 (m, 1H), 3.45-3.43 (m, 1H), 2.95-2.92 (m, 1H), 2.83 (d, *J* = 5.0 Hz, 2H), 2.31 (s, 3H), 1.94-1.91 (m, 1H), 1.87-1.81 (m, 1H), 1.11 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 143.7, 140.0, 136.2, 134.4, 129.3, 127.6, 127.4, 126.2, 60.8, 43.6, 43.2, 38.1, 21.0; **IR** (neat): 3322, 2925, 1589, 1430, 1043, 796 cm^{-1}; $[\alpha]_D^{20}$ = +69.2 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{18}ONaCl_2$ $(M+Na)^+$: 331.0632, found 331.0640.



(*R*)-4-(benzo[*d*][1,3]dioxol-5-yl)-3-(*p*-tolyl)butanal

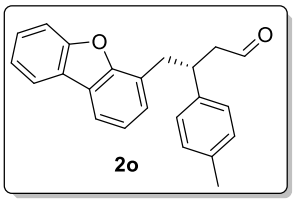
General procedure A was followed using 3,4-(methylenedioxy)phenylboronic acid (149 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:10 EtOAc:hexanes) to afford **2n** as a colorless oil (35 mg, 41% yield, 7.5:92.5 er), R_f = 0.25 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.58 (m, 1H), 7.10-7.03 (m, 4H), 6.69-6.66 (m, 1H), 6.57-6.52 (m, 2H), 5.90 (s, 2H), 3.43-3.36 (m, 1H), 2.85-2.68 (m, 4H), 2.31 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.7, 147.5, 146.0, 140.1, 136.3, 133.2, 129.3, 127.3, 122.2, 109.5, 108.0, 100.8, 49.0, 43.1, 41.8, 21.0; **IR** (neat): 2920, 1721, 1489, 1249, 1038 cm^{-1}; $[\alpha]_D^{20}$ = +57.8 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{18}O_3Na$ $(M+Na)^+$: 305.1154, found 305.1160.



(*R*)-4-(benzo[*d*][1,3]dioxol-5-yl)-3-(*p*-tolyl)butan-1-ol

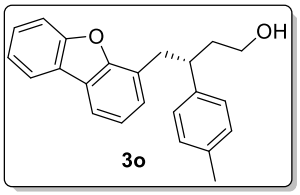
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2n** (28 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3n** as a colorless oil (26 mg, 91% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.11-7.02 (m, 4H), 6.66 (d, *J* = 4.5 Hz, 1H), 6.57-6.56 (m, 1H), 6.50 (d, *J* = 4.5 Hz,, 1H), 5.90 (s, 2H), 3.54-3.42 (m, 2H), 2.90-2.74 (m, 3H), 2.32 (s, 3H), 1.98-1.77 (m,

2H), 1.07 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 147.3, 145.6, 141.2, 135.8, 134.3, 129.2, 127.5, 122.0, 109.5, 107.9, 100.7, 61.2, 44.2, 43.6, 38.2, 21.0; **IR** (neat): 3333, 2923, 1488, 1430, 1245, 1039, 814 cm^{-1}; $[\alpha]_D^{20}$ = +71.1 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{20}O_3Na$ $(M+Na)^+$: 307.1310, found 307.1314.



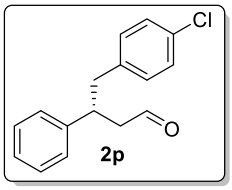
(*R*)-4-(dibenzo[*b*,*d*]furan-4-yl)-3-(*p*-tolyl)butanal

General procedure A was followed using dibenzo[*b*,*d*]furan-4-ylboronic acid (191 mg, 0.90 mmol) and 3-(*p*-tolyl)but-3-en-1-ol (**1a**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:8 EtOAc:hexanes) to afford **2o** as a colorless oil (51 mg, 52% yield, 7:93 er), R_f = 0.25 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.60 (m, 1H), 7.98-7.95 (m, 1H), 7.84-7.80 (m, 1H), 7.64-7.61 (m, 1H), 7.53-7.46 (m, 1H), 7.40-7.34 (m, 1H), 7.28-7.10 (m, 6H), 3.85-3.76 (m, 1H), 3.32-3.30 (m, 2H), 2.91-2.72 (m, 2H), 2.33 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.8, 156.0, 154.9, 140.2, 136.3, 129.3, 128.2, 127.3, 127.0, 123.4, 122.7, 120.7, 118.9, 111.7, 48.9, 40.2, 37.5, 21.0; **IR** (neat): 1722, 1451, 1184, 754 cm^{-1}; $[\alpha]_D^{20}$ = +69.0 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{23}H_{20}O_2Na$ $(M+Na)^+$: 351.1361, found 351.1363.



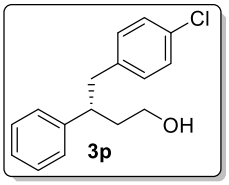
(*R*)-4-(dibenzo[*b*,*d*]furan-4-yl)-3-(*p*-tolyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and the aldehyde **2o** (33 mg, 0.1 mmol). The crude mixture was purified by silica gel flash chromatography with hexane/EtOAc = 3:1 as eluent to afford **3o** (30 mg, 90% yield) as a colorless oil. R_f = 0.2 (1:2 EtOAc:hexanes); **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 7.95-7.92 (m, 1H), 7.78-7.76 (m, 1H), 7.61-7.58 (m, 1H), 7.49-7.43 (m, 1H), 7.36-7.31 (m, 1H), 7.21-7.07 (m, 6H), 3.56-3.46 (m, 2H), 3.33-3.17 (m, 3H), 2.30 (s, 3H), 2.05-1.93 (m, 2H), 1.11 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 156.0, 154.9, 141.2, 135.8, 129.1, 128.1, 127.4, 126.9, 124.5, 122.5, 120.6, 118.4, 111.7, 61.2, 42.5, 38.2, 37.7, 21.0; **IR** (neat) 3340, 2925, 1450, 1422, 1180, 1044 cm^{-1}; $[\alpha]_D^{20}$ = +69.6 (c = 0.5, EtOH); **HRMS** (ESI) Calcd. for $C_{23}H_{22}O_2Na$ $(M+Na)^+$: 353.1527. Found 353.1524.



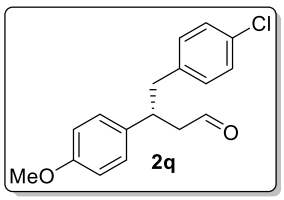
(*R*)-4-(4-chlorophenyl)-3-phenylbutanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-phenylbut-3-en-1-ol (**1p**, 44 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2p** as a colorless oil (48 mg, 62% yield, 4.5:95.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.64 (t, *J* = 3.0 Hz, 1H), 7.31-7.11 (m, 7H), 6.97-6.93 (m, 2H), 3.51-3.41 (m, 1H), 2.90 (d, *J* = 3.0 Hz, 2H), 2.80-2.76 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.3, 142.6, 137.7, 132.0, 130.5, 128.6, 128.4, 127.5, 126.8, 49.0, 42.5, 41.8; **IR** (neat): 2926, 1723, 1492, 1093, 1015, 701 cm^{-1}; $[\alpha]_D^{20}$ = +65.3 (c = 0.34, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{15}ONaCl$ $(M+Na)^+$: 281.0709, found 281.0709.



(*R*)-4-(4-chlorophenyl)-3-phenylbutan-1-ol

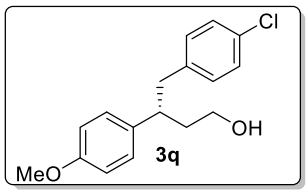
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2p** (26 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3p** as a colorless oil (25 mg, 97% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.29-7.09 (m, 7H), 6.96-6.92 (m, 2H), 3.56-3.37 (m, 2H), 2.97-2.85 (m, 3H), 1.97-1.86 (m, 2H), 1.27 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 143.7, 138.6, 131.6, 130.4, 128.4, 128.1, 127.6, 126.4, 60.8, 44.3, 43.0, 38.2; **IR** (neat): 3326, 2931, 1491, 1092, 1015, 700 cm^{-1}; $[\alpha]_D^{20}$ = +23.8 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{17}ONaCl$ $(M+Na)^+$: 283.0866, found 283.0869.



(*R*)-4-(4-chlorophenyl)-3-(4-methoxyphenyl)butanal

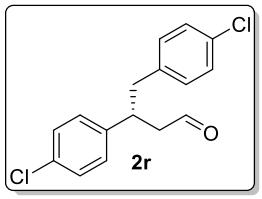
General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(4-methoxyphenyl)but-3-en-1-ol (**1q**, 53 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:8 EtOAc:hexanes) to afford **2q** as a colorless oil (50 mg, 58% yield,

3.5:96.5 er), R_f = 0.30 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.62 (s, 1H), 7.19-7.16 (m, 2H), 7.03-7.01 (m, 2H), 6.94-6.92 (m, 2H), 6.82-6.79 (m, 2H), 3.77 (s, 3H), 3.42-3.38 (m, 1H), 2.89-2.81 (m, 2H), 2.77-2.68 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.4, 158.4, 137.8, 134.6, 132.0, 130.5, 128.4, 128.3, 114.0, 55.2, 49.2, 42.7, 41.1; **IR** (neat): 1721, 1610, 1512, 1247, 829 cm^{-1}; $[\alpha]_D^{20}$ = +48.6 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}O_2NaCl$ $(M+Na)^+$: 311.0815, found 311.0816.



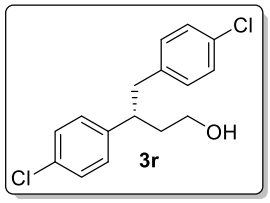
(*R*)-4-(4-chlorophenyl)-3-(4-methoxyphenyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2q** (29 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3q** as a colorless oil (28 mg, 96% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.16-7.14 (m, 2H), 7.02-7.00 (m, 2H), 6.92 (d, *J* = 5.0 Hz, 2H), 6.82-6.79 (m, 2H), 3.78 (s, 3H), 3.55-3.51 (m, 1H), 3.47-3.41 (m, 1H), 2.92-2.82 (m, 3H), 1.95-1.93 (m, 1H), 1.85-182 (m, 1H), 1.06 (t, *J* = 5.0 Hz, 1H) ; **^{13}C NMR** (125 MHz, $CDCl_3$): δ 158.1, 138.8, 135.6, 131.6, 130.5, 128.5, 128.2, 113.8, 61.0, 55.2, 43.6, 43.3, 38.4; **IR** (neat): 3339, 2932, 1512, 1247, 1035, 829 cm^{-1}; $[\alpha]_D^{20}$ = +89.4 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}O_2NaCl$ $(M+Na)^+$:313.0971, found 313.0971.



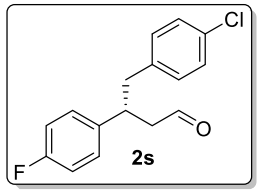
(*R*)-3,4-bis(4-chlorophenyl)butanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(4-chlorophenyl)but-3-en-1-ol (**1r**, 55 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2r** as a colorless oil (49 mg, 56% yield, 8.5:91.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.63 (m, 1H), 7.25-7.16 (m, 4H), 7.05-7.01 (m, 2H), 6.94-6.90 (m, 2H), 3.49-3.39 (m, 1H), 2.93-2.74 (m, 4H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 200.6, 141.2, 137.3, 132.6, 132.3, 130.5, 128.9, 128.8, 128.5, 49.0, 42.3, 41.1; **IR** (neat): 2925, 1723, 1492, 1408, 1093, 1014, 828 cm^{-1}; $[\alpha]_D^{20}$ = +35.7 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{14}ONaCl_2(M+Na)^+$: 315.0319, found 315.0324.



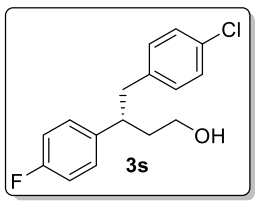
(*R*)-3,4-bis(4-chlorophenyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2r** (29 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3r** as a colorless oil (27 mg, 93% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.23-7.20 (m, 2H), 7.16-7.14 (m, 2H), 7.03-7.00 (m, 2H), 6.92-6.89 (m, 2H), 3.56-3.53 (m, 1H), 3.43-3.40 (m, 1H), 2.98-2.94 (m, 1H), 2.91-2.87 (m, 1H), 2.82-2.79 (m, 1H), 1.97-1.94 (m, 1H), 1.84-1.82 (m, 1H), 1.13 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 142.1, 138.2, 132.1, 131.9, 130.4, 129.0, 128.6, 128.3, 60.6, 43.7, 42.9, 38.2; **IR** (neat): 3335, 2933, 1491, 1408, 1093, 1014, 826 cm^{-1}; $[\alpha]_D^{20}$ = +82.0 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{16}ONaCl_2$ $(M+Na)^+$: 317.0476, found 317.0491.



(*R*)-4-(4-chlorophenyl)-3-(4-fluorophenyl)butanal

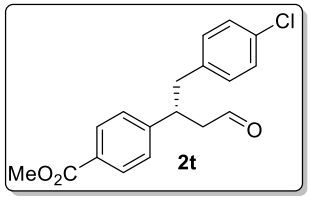
General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(4-fluorophenyl)but-3-en-1-ol (**1s**, 50 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2s** as a colorless oil (52 mg, 63% yield, 90:10 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.64 (m, 1H), 7.19-7.17 (m, 2H), 7.07-7.04 (m, 2H), 6.97-6.91 (m, 4H), 3.48-3.42 (m, 1H), 2.92-2.88 (m, 1H), 2.84-2.80 (m, 1H), 2.77-2.75 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 200.8, 161.6 (d, *J* = 120.0 Hz), 138.3, 137.4, 132.2, 130.5, 129.0 (d, *J* = 3.8 Hz), 128.4, 115.4 (d, *J* = 11.2 Hz), 49.2, 42.5, 41.0; **^{19}F NMR** (282 MHz, $CDCl_3$): –116.3; **IR** (neat): 2925, 1723, 1510, 1224, 1095, 834 cm^{-1}; $[\alpha]_D^{20}$ = +40.8 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{14}ONaClF$ $(M+Na)^+$: 299.0615, found 299.0614.



(*R*)-4-(4-chlorophenyl)-3-(4-fluorophenyl)butan-1-ol

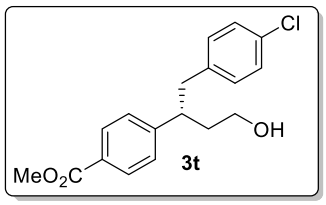
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2s**

(28 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3s** as a colorless oil (26 mg, 92% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.16-7.14 (m, 2H), 7.05-7.02 (m, 2H), 6.96-6.89 (m, 4H), 3.55-3.52 (m, 1H), 3.42-3.40 (m, 1H), 2.99-2.97 (m, 1H), 2.90-2.86 (m, 1H), 2.82-2.77 (m, 1H), 1.98-1.94 (m, 1H), 1.85-1.81 (m, 1H), 1.19 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 161.4 (d, *J* = 121.5 Hz), 139.2 (d, *J* = 1.5 Hz), 138.4, 131.7, 130.4, 129.0 (d, *J* = 3.8 Hz), 128.2, 115.2 (d, *J* = 10.5 Hz), 60.7, 43.6, 43.2, 38.3; **^{19}F NMR** (282 MHz, $CDCl_3$): –117.0; **IR** (neat): 3359, 2935, 1509, 1223, 1094, 833 cm^{-1}; $[\alpha]_D^{20}$ = +65.9 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{16}ONaClF$ $(M+Na)^+$: 301.0771, found 301.0767.



methyl (*R*)-4-(1-(4-chlorophenyl)-4-oxobutan-2-yl)benzoate

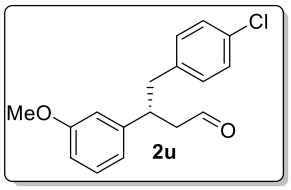
General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and methyl 4-(4-hydroxybut-1-en-2-yl)benzoate (**1t**, 62 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:8 EtOAc:hexanes) to afford **2t** as a colorless oil (41 mg, 43% yield, 6.5:93.5 er), R_f = 0.30 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.65 (m, 1H), 7.94-7.92 (m, 2H), 7.18-7.16 (m, 4H), 6.92-6.90 (m, 2H), 3.89 (s, 3H), 3.53-3.49 (m, 1H), 2.95-2.91 (m, 1H), 2.87-2.80 (m, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 200.4, 166.8, 148.0, 137.2, 132.3, 130.4, 129.9, 128.8, 128.5, 127.6, 52.1, 48.9, 42.1, 41.6; **IR** (neat): 2949, 1720, 1282, 1116, 710 cm^{-1}; $[\alpha]_D^{20}$ = +88.6 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{17}O_3NaCl$ $(M+Na)^+$: 339.0764, found 339.0761.



methyl (*R*)-4-(1-(4-chlorophenyl)-4-hydroxybutan-2-yl)benzoate

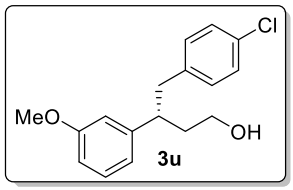
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2t** (32 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3t** as a colorless oil (29 mg, 91% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.92 (d, *J* = 5.0 Hz, 2H), 7.17-7.13 (m, 4H), 6.90 (d, *J* = 5.0 Hz, 2H), 3.89 (s, 3H), 3.55-3.52 (m, 1H), 3.44-3.40 (m, 1H), 3.20-3.15 (m, 1H), 2.95-2.91 (m, 1H), 2.86-2.80

(m, 1H), 2.01-1.98 (m, 1H), 1.91-1.89 (m, 1H), 1.19 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 167.0, 149.2, 138.1, 131.8, 130.4, 129.8, 128.5, 128.3, 127.8, 60.6, 52.0, 44.3, 42.7, 38.1; **IR** (neat): 3400, 2935, 1719, 1492, 1282, 709 cm^{-1}; $[\alpha]_D^{20}$ = +90.3 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{19}O_3NaCl$ $(M+Na)^+$: 341.0920, found 341.0921.



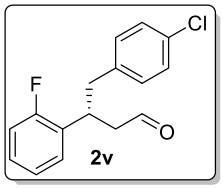
(*R*)-4-(4-chlorophenyl)-3-(3-methoxyphenyl)butanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(3-methoxyphenyl)but-3-en-1-ol (**1u**, 53 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:12 EtOAc:hexanes) to afford **2u** as a colorless oil (44 mg, 51% yield, 4:96 er), R_f = 0.35 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.63 (m, 1H), 7.21-7.18 (m, 3H), 6.97-6.95 (m, 2H), 6.75-6.70 (m, 2H), 6.65 (s, 1H), 3.77 (s, 3H), 3.43-3.40 (m, 1H), 2.88 (d, *J* = 5.0 Hz, 2H), 2.80-2.69 (m, 2H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.2, 159.8, 144.4, 137.7, 132.1, 130.5, 129.6, 128.4, 119.8, 113.6, 111.9, 55.2, 49.0, 42.4, 41.8; **IR** (neat): 2925, 1722, 1600, 1491, 1262, 1093, 701 cm^{-1}; $[\alpha]_D^{20}$ = +47.8 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}O_2NaCl$ $(M+Na)^+$: 311.0815, found 311.0821.



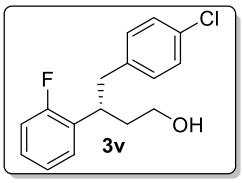
(*R*)-4-(4-chlorophenyl)-3-(3-methoxyphenyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2u** (29 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3u** as a colorless oil (29 mg, 98% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.21-7.14 (m, 3H), 6.96-6.94 (m, 2H), 6.72-6.69 (m, 2H), 6.65 (s, 1H), 3.76 (s, 3H), 3.54-3.51 (m, 1H), 3.46-3.44 (m, 1H), 2.95-2.90 (m, 1H), 2.87-2.84 (m, 2H), 1.95-1.85 (m, 2H), 1.12 (brs, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 159.6, 145.5, 138.7, 131.6, 130.4, 129.4, 128.2, 120.1, 113.7, 111.4, 60.9, 55.1, 44.4, 43.0, 38.2; **IR** (neat): 3340, 2931, 1608, 1490, 1259, 1042, 702 cm^{-1}; $[\alpha]_D^{20}$ = +70.4 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}O_2NaCl$ $(M+Na)^+$: 313.0971, found 313.0972.



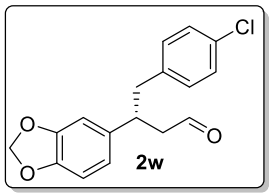
(*R*)-4-(4-chlorophenyl)-3-(2-fluorophenyl)butanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(2-fluorophenyl)but-3-en-1-ol (**1v**, 50 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2v** as a colorless oil (15 mg, 18% yield, 20:80 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.65 (m, 1H), 7.22-7.15 (m, 3H), 7.10-6.97 (m, 5H), 3.79-3.69 (m, 1H), 2.94 (d, *J* = 4.5 Hz, 2H), 2.83 (d, *J* = 3.0 Hz, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 200.8, 160.8 (d, *J* = 121.9 Hz), 137.5, 132.1, 130.4, 129.4, 129.1 (d, *J* = 2.6 Hz), 128.4 (d, *J* = 4.5 Hz), 128.3, 124.2 (d, *J* = 1.9 Hz), 115.7 (d, *J* = 11.2 Hz), 47.8, 40.6, 35.8; **^{19}F NMR** (282 MHz, $CDCl_3$): –117.8; **IR** (neat): 1724, 1491, 1228, 1095, 757 cm^{-1}; $[\alpha]_D^{20}$ = +33.0 (c = 0.16, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{14}ONaClF$ $(M+Na)^+$: 299.0615, found 299.0611.



(*R*)-4-(4-chlorophenyl)-3-(2-fluorophenyl)butan-1-ol

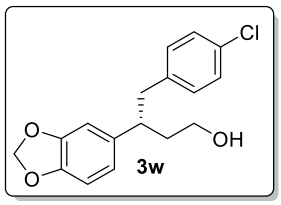
General procedure B was followed using sodium borohydride (3 mg, 0.075 mmol) and aldehyde **2v** (14 mg, 0.05 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3v** as a colorless oil (13 mg, 90% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.18-7.07 (m, 5H), 7.05-6.94 (m, 3H), 3.56-3.31 (m, 3H), 2.93 (d, *J* = 3.0 Hz, 2H), 2.04-1.89 (m, 2H), 1.21 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 161.1 (d, *J* = 121.5 Hz), 133.4, 131.8, 130.3, 130.1, 129.0 (d, *J* = 2.6 Hz), 128.2, 127.9 (d, *J* = 4.5 Hz), 124.1 (d, *J* = 1.9 Hz), 115.5 (d, *J* = 11.2 Hz), 60.9, 41.4, 37.6, 37.2; **^{19}F NMR** (282 MHz, $CDCl_3$): –118.4; **IR** (neat) 3336, 2933, 1491, 1225, 1094, 757 cm^{-1}; $[\alpha]_D^{20}$ = +43.0 (c = 0.22, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{16}ONaClF$ $(M+Na)^+$: 301.0771, found 301.0778.



(*R*)-3-(benzo[*d*][1,3]dioxol-5-yl)-4-(4-chlorophenyl)butanal

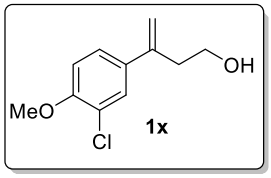
General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and

3-(benzo[*d*][1,3]dioxol-5-yl)but-3-en-1-ol (**1w**, 58 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:14 EtOAc:hexanes) to afford **2w** as a colorless oil (33 mg, 36% yield, 8.5:91.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.62 (m, 1H), 7.20-7.17 (m, 2H), 6.97-6.94 (m, 2H), 6.69-6.68 (m, 1H), 6.63-6.62 (m, 1H), 6.54-6.50 (m, 1H), 5.92 (m, 2H), 3.40-3.34 (m, 1H), 2.88-2.80 (m, 2H), 2.75-2.66 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.2, 147.8, 146.3, 137.7, 136.5, 132.1, 130.5, 128.4, 120.7, 108.3, 107.6, 101.0, 49.3, 42.6, 41.6; **IR** (neat): 1719, 1490, 1246, 1039, 668 cm^{-1}; $[\alpha]_D^{20}$ = +72.3 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{15}O_3NaCl$ $(M+Na)^+$: 325.0607, found 325.0603.



(*R*)-3-(benzo[*d*][1,3]dioxol-5-yl)-4-(4-chlorophenyl)butan-1-ol

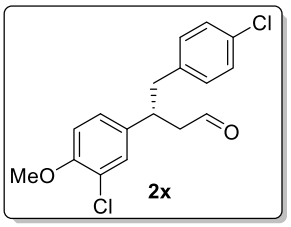
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2w** (30 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3w** as a colorless oil (28 mg, 93% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.18-7.15 (m, 2H), 6.96-6.92 (m, 2H), 6.66-6.63 (m, 2H), 6.53-6.49 (m, 1H), 5.93-5.91 (m, 2H), 3.55-3.51 (m, 1H), 3.48-3.43 (m, 1H), 2.91-2.79 (m, 3H), 1.93-1.87 (m, 1H), 1.84-1.74 (m, 1H), 1.12 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 147.8, 146.0, 138.6, 137.6, 131.6, 130.4, 128.2, 120.9, 108.2, 107.6, 100.8, 60.9, 44.2, 43.2, 38.5; **IR** (neat): 3361, 2922, 1488, 1245, 1040 cm^{-1}; $[\alpha]_D^{20}$ = +94.9 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}O_3NaCl$ $(M+Na)^+$: 327.0764, found 327.0757.



3-(3-chloro-4-methoxyphenyl)but-3-en-1-ol

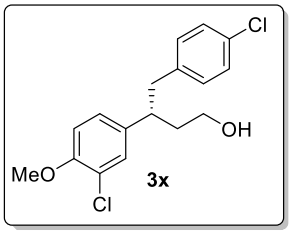
Prepared according to literature procedure[4b] using alcohol **S4** (378 mg, 2.50 mmol, 1.0 equiv) and (3-chloro-4-methoxyphenyl)boronic acid (930 mg, 5.0 mmol, 2.0 equiv). The crude mixture was purified by silica gel flash chromatography (1:4 EtOAc:hexanes) to afford **1x** as a colorless oil (414 mg, 78% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.44 (s, 1H), 7.29-7.7.27 (m, 1H), 6.88 (d, *J* = 2.5 Hz, 1H), 5.35 (s, 1H), 5.11 (s, 1H), 3.90 (s, 3H), 3.74-3.70 (m, 2H), 2.75-2.72 (m, 2H), 1.43 (t, *J* = 5.0 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 154.5, 143.1, 133.8,

128.0, 125.4, 122.4, 114.0, 111.8, 60.9, 56.2, 38.4; **IR** (neat): 3340, 2929, 1502, 1289, 1064 cm^{-1}; **HRMS** (ESI) *m/z* calcd. for $C_{11}H_{13}O_2NaCl$ $(M+Na)^+$: 235.0502, found 235.0508.



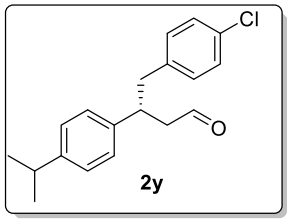
(*R*)-3-(3-chloro-4-methoxyphenyl)-4-(4-chlorophenyl)butanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(3-chloro-4-methoxyphenyl)but-3-en-1-ol (**1x**, 64 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:8 EtOAc:hexanes) to afford **2x** as a colorless oil (46 mg, 48% yield, 96:4 er), R_f = 0.20 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.62 (s, 1H), 7.19-7.15 (m, 3H), 6.94-6.90 (m, 3H), 6.79 (d, *J* = 5.0 Hz, 1H), 3.85 (s, 3H), 3.40-3.35 (m, 1H), 2.88-2.78 (m, 2H), 2.72 (d, *J* = 2.5 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 200.7, 153.7, 137.4, 135.8, 132.2, 130.4, 128.9, 128.4, 127.0, 122.5, 112.0, 56.1, 49.1, 42.4, 40.7; **IR** (neat): 2929, 1719, 1493, 1256, 1063, 813 cm^{-1}; $[\alpha]_D^{20}$ = +78.0 (c = 0.3, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{16}O_2NaCl_2$ $(M+Na)^+$: 345.0425, found 345.0434.



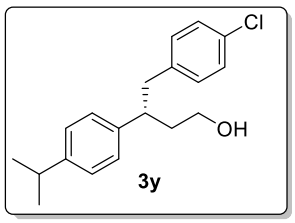
(*R*)-3-(3-chloro-4-methoxyphenyl)-4-(4-chlorophenyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2x** (32 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3x** as a colorless oil (31 mg, 95% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.17-7.13 (m, 3H), 6.93-6.88 (m, 3H), 6.81-6.78 (m, 1H), 3.87 (s, 3H), 3.56-3.53 (m, 1H), 3.44-3.40 (m, 1H), 2.92-2.88 (m, 1H), 2.85-2.83 (m, 1H), 2.81-2.79 (m, 1H), 1.95-1.92 (m, 1H), 1.82-1.79 (m, 1H), 1.12 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 153.4, 138.4, 136.8, 131.7, 130.4, 129.0, 128.2, 127.1, 122.3, 111.9, 60.7, 56.1, 43.3, 43.0, 38.2; **IR** (neat): 3357, 2926, 1493, 1258, 1064 cm^{-1}; $[\alpha]_D^{20}$ = +77.0 (c = 0.21, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{18}O_2NaCl_2$ $(M+Na)^+$: 347.0582, found 347.0594.



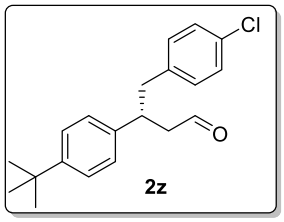
(*R*)-4-(4-chlorophenyl)-3-(4-isopropylphenyl)butanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(4-isopropylphenyl)but-3-en-1-ol (**1y**, 57 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2y** as a colorless oil (47 mg, 52% yield, 5:95 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.61 (s, 1H), 7.19 (d, *J* = 5.0 Hz, 2H), 7.14 (d, *J* = 2.5 Hz, 2H), 7.05 (d, *J* = 5.0 Hz, 2H), 6.96 (d, *J* = 2.5 Hz, 2H), 3.45-3.39 (m, 1H), 2.90-2.86 (m, 3H), 2.75-2.71 (m, 2H), 1.23 (d, *J* = 5.0 Hz, 6H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.5, 147.4, 140.0, 137.9, 132.0, 130.5, 128.4, 127.3, 126.6, 49.0, 42.5, 41.4, 33.6, 24.0; **IR** (neat): 2960, 1723, 1492, 1093, 1016, 831 cm^{-1}; $[\alpha]_D^{20}$ = +74.2 (c = 0.9, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{19}H_{21}ONaCl$ $(M+Na)^+$: 323.1179, found 323.1179.



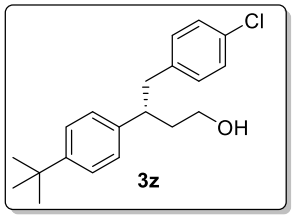
(*R*)-4-(4-chlorophenyl)-3-(4-isopropylphenyl)butan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2y** (30 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3y** as a colorless oil (29 mg, 96% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.10 (d, *J* = 5.0 Hz, 2H), 7.06 (d, *J* = 5.0 Hz, 2H), 6.97 (d, *J* = 5.0 Hz, 2H), 6.89 (d, *J* = 5.0 Hz, 2H), 3.45-3.39 (m, 1H), 3.37-3.34 (m, 1H), 2.87-2.76 (m, 4H), 1.86-1.83 (m, 1H), 1.78-1.75 (m, 1H), 1.16 (d, *J* = 5.0 Hz, 6H), 1.08 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 147.0, 141.0, 138.9, 131.6, 130.4, 128.1, 127.4, 126.5, 61.0, 43.9, 43.1, 38.1, 33.6, 24.0; **IR** (neat): 3317, 2958, 1491, 1092, 1015, 829 cm^{-1}; $[\alpha]_D^{20}$ = +79.2 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{19}H_{23}ONaCl$ $(M+Na)^+$: 325.1335, found 325.1338.



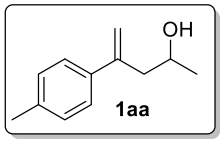
(*R*)-3-(4-(*tert*-butyl)phenyl)-4-(4-chlorophenyl)butanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-(4-(*tert*-butyl)phenyl)but-3-en-1-ol (**1z**, 61 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2z** as a colorless oil (38 mg, 40% yield, 5:95 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.60 (m, 1H), 7.30-7.27 (m, 2H), 7.20-7.17 (m, 2H), 7.07-7.04 (m, 2H), 6.98-6.95 (m, 2H), 3.46-3.40 (m, 1H), 2.91-2.83 (m, 2H), 2.74-2.70 (m, 2H), 1.30 (s, 9H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.5, 149.7, 139.6, 137.9, 132.0, 130.5, 128.4, 127.0, 125.5, 48.9, 42.5, 41.3, 34.4, 31.3; **IR** (neat): 2962, 1723, 1492, 1093, 1015, 831 cm^{-1}; $[\alpha]_D^{20}$ = +71.6 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{20}H_{23}ONaCl$ $(M+Na)^+$: 337.1335, found 337.1334.



(*R*)-3-(4-(*tert*-butyl)phenyl)-4-(4-chlorophenyl)butan-1-ol

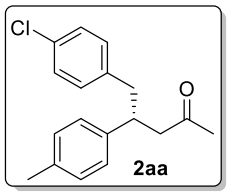
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2z** (32 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:3 EtOAc:hexanes) to afford **3z** as a colorless oil (30 mg, 93% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.30-7.26 (m, 2H), 7.18-7.16 (m, 2H), 7.06-7.04 (m, 2H), 6.98-6.96 (m, 2H), 3.54-3.49 (m, 1H), 3.44-3.39 (m, 1H), 2.94-2.83 (m, 3H), 1.93-1.90 (m, 1H), 1.84-1.82 (m, 1H), 1.31 (s, 9H), 1.13 (brs, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 149.2, 140.7, 138.9, 131.6, 130.5, 128.2, 127.2, 125.3, 61.0, 43.8, 43.1, 38.0, 34.4, 31.4; **IR** (neat): 3321, 2961, 1492, 1092, 1015, 834 cm^{-1}; $[\alpha]_D^{20}$ = +72.3 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{20}H_{25}ONaCl$ $(M+Na)^+$: 339.1492, found 339.1487.



4-(*p*-tolyl)pent-4-en-2-ol

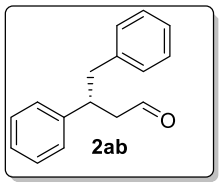
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.32 (d, *J* = 3.0 Hz, 2H), 7.16 (d, *J* = 4.5 Hz, 2H), 5.38 (d, *J* = 1.5 Hz,

1H), 5.12 (d, *J* = 1.5 Hz, 1H), 3.88-3.84 (m, 1H), 2.76-2.69 (m, 1H), 2.61-2.54 (m, 1H), 2.36 (s, 3H), 1.76 (brs, 1H), 1.23-1.20 (m, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 145.2, 137.5, 129.1, 126.0, 114.4, 65.7, 45.5, 22.8, 21.0; **IR** (neat): 3365, 2967, 2926, 1513, 1121, 1078, 824 cm^{-1}; **HRMS** (ESI) *m/z* calcd. for $C_{12}H_{16}ONa$ $(M+Na)^+$: 199.1099, found 199.1103.



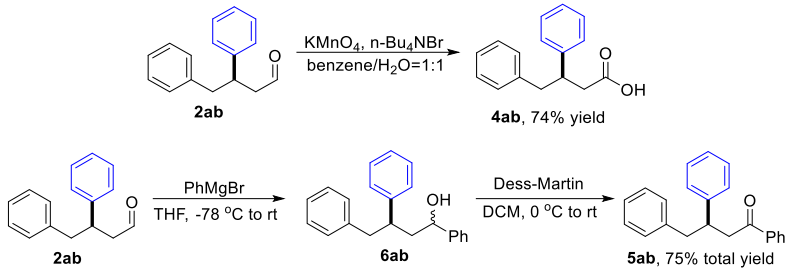
(*R*)-5-(4-chlorophenyl)-4-(*p*-tolyl)pentan-2-one

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 4-(*p*-tolyl)pent-4-en-2-ol (**1aa**, 53 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2aa** as a colorless oil (35 mg, 41% yield, 95.5:4.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.16 (d, *J* = 5.0 Hz, 2H), 7.05 (d, *J* = 5.0 Hz, 2H), 6.98 (d, *J* = 5.0 Hz, 2H), 6.94 (d, *J* = 5.0 Hz, 2H), 3.40-3.34 (m, 1H), 2.85-2.71 (m, 4H), 2.29 (s, 3H), 2.00 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 207.5, 140.2, 138.2, 136.0, 131.8, 130.5, 129.1, 128.2, 127.4, 49.3, 42.4, 42.3, 30.6, 21.0; **IR** (neat): 2922, 1713, 1491, 1356, 1092, 1015, 819 cm^{-1}; $[\alpha]_D^{20}$ = +88.5 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{19}ONaCl$ $(M+Na)^+$: 309.1022, found 309.1027.

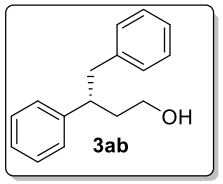


(*R*)-3,4-diphenylbutanal

General procedure A was followed using phenylboronic acid (110 mg, 0.90 mmol) and 3-phenylbut-3-en-1-ol (**1p**, 44 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2ab** as a colorless oil (34 mg, 51% yield, 5:95 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.59 (t, *J* = 3.0 Hz, 1H), 7.32-7.16 (m, 8H), 7.07 (d, *J* = 3.0 Hz, 2H), 3.55-3.45 (m, 1H), 3.01-2.83 (m, 2H), 2.78-2.69 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.6, 143.2, 139.2, 129.2, 128.6, 128.3, 127.5, 126.7, 126.3, 48.9, 43.3, 41.2; **IR** (neat): 2923, 1722, 1495, 1453, 761, 699 cm^{-1}; $[\alpha]_D^{20}$ = +57.4 (c = 0.5, EtOH) or $[\alpha]_D^{20}$ = +49.6 (c = 0.5, $CHCl_3$); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{16}ONa$ $(M+Na)^+$: 247.1099, found 247.1104.

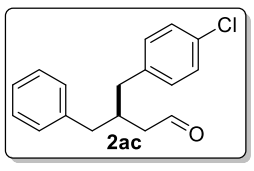


According to the literature,[5a] aldehyde **2ab** was converted into the reported 3,4-diphenyl butanoic acid **4ab**. The measured optical rotation: $[\alpha]_D^{20}$ = +51.4 (c = 0.7, benzene) was compared to the reported optical rotation value for (*R*)-3,4-diphenyl butanoic acid: $[\alpha]_D^{22}$ = +41.4 (c = 2.62, benzene, 65% ee).[5b] Aldehyde **2ab** was assigned with the absolute configuration of (*R*). In addition, we also converted aldehyde **2ab** to known 1,3,4-triphenyl-1-butanone **5ab** and measured its optical rotation: $[\alpha]_D^{20}$ = +30.5 (c = 0.5, $CHCl_3$, 90% ee). Compared to the known optical rotation value for (*S*)-1,3,4-triphenyl-1-butanone: $[\alpha]_D^{20}$ = –41.9 (c = 0.5, $CHCl_3$, 98% ee),[5c] configuration of aldehyde **2ab** was confirmed as (*R*).



(*R*)-3,4-diphenylbutan-1-ol

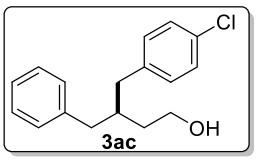
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2ab** (22 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:4 EtOAc:hexanes) to afford **3ab** as a colorless oil (22 mg, 97% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.28-7.25 (m, 3H), 7.22-7.13 (m, 5H), 7.04 (d, *J* = 1.5 Hz, 2H), 3.55-3.50 (m, 1H), 3.46-3.40 (m, 1H), 3.01-2.99 (m, 1H), 2.92-2.89 (m, 2H), 2.00-1.96 (m, 1H), 1.89-1.86 (m, 1H), 1.04 (t, *J* = 5.0 Hz, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 144.3, 140.3, 129.1, 128.4, 128.1, 127.7, 126.3, 125.9, 61.1, 44.5, 43.8, 38.2; **IR** (neat): 2923, 1722, 1495, 1453, 761, 699 cm^{-1}; $[\alpha]_D^{20}$ = +60.0 (c = 0.21, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{18}ONa$ $(M+Na)^+$: 249.1255, found 249.1261.



(*S*)-3-benzyl-4-(4-chlorophenyl)butanal

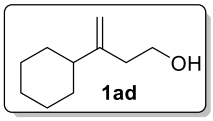
General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-benzylbut-3-en-1-ol (**1ac**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash

chromatography (1:15 EtOAc:hexanes) to afford **2ac** as a colorless oil (20 mg, 24% yield, 30.5:69.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.59 (t, *J* = 3.0 Hz, 1H), 7.32-7.07 (m, 9H), 2.71-2.55 (m, 5H), 2.32 (d, *J* = 1.5 Hz, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 201.9, 139.5, 138.3, 132.1, 130.5, 129.2, 128.6, 128.5, 126.4, 47.0, 40.3, 39.7, 37.2; **IR** (neat): 2922, 2361, 1721, 1492, 1088, 702 cm^{-1}; $[\alpha]_D^{20}$ = –8.3 (c = 0.31, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}ONaCl$ $(M+Na)^+$: 295.0866, found 295.0852.



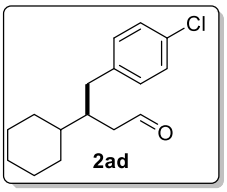
(*S*)-3-benzyl-4-(4-chlorophenyl)butan-1-ol

General procedure B was followed using sodium borohydride (3 mg, 0.075 mmol) and aldehyde **2ac** (14 mg, 0.05 mmol). The crude mixture was purified by silica gel flash chromatography (1:4 EtOAc:hexanes) to afford **3ac** as a colorless oil (13 mg, 92% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.30-7.19 (m, 5H), 7.15-7.06 (m, 4H), 3.67-3.60 (m, 2H), 2.59-2.54 (m, 4H), 2.13-2.09 (m, 1H), 1.57-1.51 (m, 2H), 1.02 (t, *J* = 3.0 Hz, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 140.8, 139.5, 131.9, 130.7, 129.4, 128.6, 128.6, 126.2, 61.1, 40.7, 40.1, 38.9, 36.4; **IR** (neat): 3362, 2925, 1089, 742, 700 cm^{-1}; $[\alpha]_D^{20}$ = –5.0 (c = 0.1, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}ONaCl$ $(M+Na)^+$: 297.1022, found 297.1021.



3-cyclohexylbut-3-en-1-ol

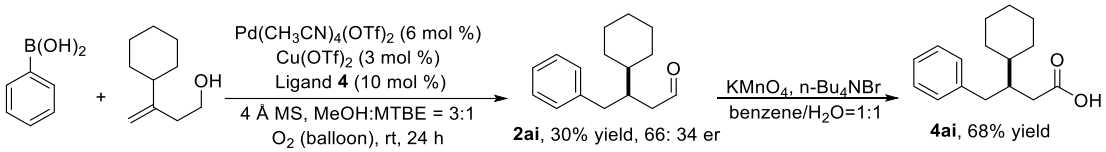
^{1}H NMR (300 MHz, $CDCl_3$): δ 4.84 (s, 1H), 4.75 (s, 1H), 3.71-3.65 (m, 2H), 2.31-2.27 (m, 2H), 1.77-1.65 (m, 7H), 1.32-1.06 (m, 5H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 151.4, 109.4, 60.8, 44.0, 38.0, 32.4, 26.7, 26.3; **IR** (neat): 3318, 2922, 1639, 1448, 1044, 887 cm^{-1}; **HRMS** (ESI) *m/z* calcd. for $C_{10}H_{19}O$ $(M+H)^+$:155.1436, found 155.1441.



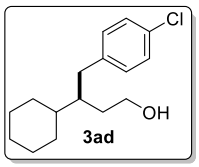
(*S*)-4-(4-chlorophenyl)-3-cyclohexylbutanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 3-cyclohexylbut-3-en-1-ol (**1ad**, 46 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2ad** as a colorless oil (27 mg, 34% yield,

32.5:67.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.59 (t, *J* = 3.0 Hz, 1H), 7.24 (d, *J* = 2.5 Hz, 2H), 7.08 (d, *J* = 2.5 Hz, 2H), 2.74-2.71 (m, 1H), 2.42-2.38 (m, 2H), 2.28-2.20 (m, 2H), 1.75-1.55 (m, 5H), 1.34-1.03 (m, 6H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 202.8, 139.3, 132.1, 130.7, 128.8, 45.4, 40.8, 40.6, 37.4, 30.5, 29.6, 26.8; **IR** (neat): 2924, 2852, 1730, 1092, 1015, 807 cm^{-1}; $[\alpha]_D^{20}$ = –2.7 (c = 0.5, EtOH) or $[\alpha]_D^{20}$ = +1.3 (c = 1.0, $CHCl_3$); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{21}ONaCl$ $(M+Na)^+$: 287.1179, found 287.1177.

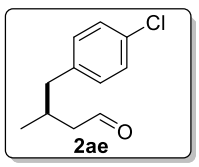


The absolute configuration of aldehydes **2ad** and **2ae** were defined by synthesizing 3-cyclohexyl-4-phenylbutyric acid **4ai**, which has been previously prepared. The measured optical rotation value: $[\alpha]_D^{20}$ = +1.7 (c = 0.5, $CHCl_3$, 32% ee) was compared to the reported optical rotation value for (*R*)-3-cyclohexyl-4-phenylbutyric acid: $[\alpha]_D^{25}$ = –8.0 (c = 2.3, $CHCl_3$).[5d] The aldehyde **2ai** was assigned the absolute configuration of (*S*). Thus, aldehyde **2ad** and **2ae** were assigned by analogy as (*S*).



(*S*)-4-(4-chlorophenyl)-3-cyclohexylbutan-1-ol

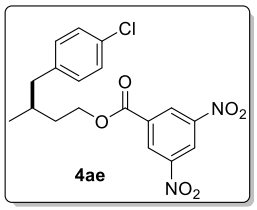
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2ad** (26 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:4 EtOAc:hexanes) to afford **3ad** as a colorless oil (25 mg, 92% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.24 (d, *J* = 4.5 Hz, 2H), 7.08 (d, *J* = 4.5 Hz, 2H), 3.56-3.55 (m, 2H), 2.66 (q, *J* = 6.0 Hz, 1H), 2.38 (q, *J* = 6.0 Hz, 1H), 1.74-1.53 (m, 7H), 1.45-1.07 (m, 8H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 140.3, 131.4, 130.4, 128.3, 61.6, 42.2, 39.9, 37.0, 33.5, 29.5, 29.4, 26.8; **IR** (neat): 3310, 2924, 2851, 1491, 1448, 1093, 1015 cm^{-1}; $[\alpha]_D^{20}$ = -3.0 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{16}H_{23}ONaCl$ $(M+Na)^+$: 289.1335, found 289.1326.



(*S*)-4-(4-chlorophenyl)-3-methylbutanal

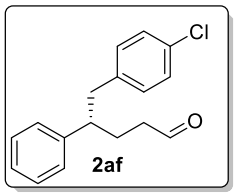
General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and

3-methylbut-3-en-1-ol (**1ae**, 30 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2ae** as a colorless oil (31 mg, 52% yield, 51.5:48.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.72 (t, *J* = 3.0 Hz, 1H), 7.27-7.24 (m, 2H), 7.10-7.07 (m, 2H), 2.62-2.22 (m, 5H), 0.96 (d, *J* = 4.5 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 202.2, 138.4, 132.0, 130.5, 128.5, 50.2, 42.4, 30.1, 19.8; **IR** (neat): 2959, 2927, 1724, 1492, 1089, 801 cm^{-1}; $[\alpha]_D^{20}$ = -1.0 (c = 0.2, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{11}H_{13}ONaCl$ $(M+Na)^+$: 219.0553, found 219.0542.



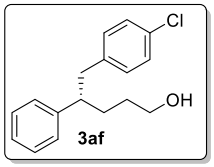
(*S*)-4-(4-chlorophenyl)-3-methylbutyl 3,5-dinitrobenzoate

^{1}H NMR (500 MHz, $CDCl_3$): δ 9.21 (s, 1H), 9.12-9.11 (m, 2H), 7.25-7.23 (m, 2H), 7.11-7.08 (m, 2H), 4.55-4.43 (m, 2H), 2.64 (q, *J* = 5.0 Hz, 1H), 2.52 (q, *J* = 5.0 Hz, 1H), 1.93-1.89 (m, 2H), 1.66-1.64 (m, 1H), 0.99 (d, *J* = 2.5 Hz, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 162.4, 148.6, 138.8, 133.9, 131.8, 130.4, 129.3, 128.4, 122.3, 65.3, 42.8, 34.8, 32.1, 19.4; **IR** (neat): 2923, 1730, 1544, 1344, 1278, 721 cm^{-1}; $[\alpha]_D^{20}$ = -2.0 (c = 0.2, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{17}N_2O_6Cl_2(M+Cl)^-$: 427.0464, found 427.0481.



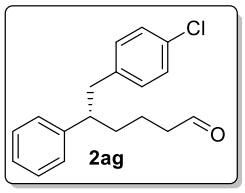
(*S*)-5-(4-chlorophenyl)-4-phenylpentanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 4-phenylpent-4-en-1-ol (**1af**, 49 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2af** as a colorless oil (42 mg, 51% yield, 88.5:11.5 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 9.62 (m, 1H), 7.28-7.24 (m, 2H), 7.21-7.13 (m, 3H), 7.07-7.04 (m, 2H), 6.94-6.90 (m, 2H), 2.89-2.85 (m, 1H), 2.82-2.77 (m, 2H), 2.28-2.24 (m, 2H), 2.06-2.03 (m, 1H), 1.91-1.87 (m, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$): δ 201.9, 143.1, 138.5, 131.8, 130.4, 128.6, 128.2, 127.7, 126.7, 47.2, 43.1, 42.0, 27.7; **IR** (neat): 2926, 2360, 1722, 1492, 1092, 1015, 702 cm^{-1}; $[\alpha]_D^{20}$ = +54.0 (c = 0.2, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{17}ONaCl$ $(M+Na)^+$: 295.0866, found 295.0868.



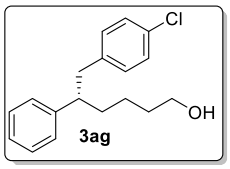
(*S*)-5-(4-chlorophenyl)-4-phenylpentan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2af** (27 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:4 EtOAc:hexanes) to afford **3af** as a colorless oil (26 mg, 95% yield), R_f = 0.20 (1:4 EtOAc:hexanes). **^{1}H NMR** (500 MHz, $CDCl_3$): δ 7.26-7.23 (m, 2H), 7.19-7.13 (m, 3H), 7.08-7.06 (m, 2H), 6.93-6.90 (m, 2H), 3.56-3.53 (m, 2H), 2.90-2.74 (m, 3H), 1.80-1.73 (m, 1H), 1.71-1.63 (m, 1H), 1.46-1.38 (m, 2H), 1.13 (t, *J* = 5.0 Hz, 1H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 144.2, 138.9, 131.5, 130.4, 128.3, 128.1, 127.7, 126.3, 62.9, 47.9, 43.2, 31.7, 30.8; **IR** (neat): 3334, 2935, 1491, 1092, 1091, 1015, 700 cm^{-1}; $[\alpha]_D^{20}$ = +65.2 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{17}H_{19}ONaCl$ $(M+Na)^+$: 297.1022, found 297.1021.



(*S*)-6-(4-chlorophenyl)-5-phenylhexanal

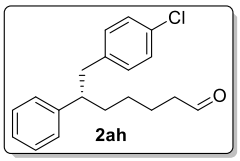
General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 5-phenylhex-5-en-1-ol (**1ag**, 53 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2ag** as a colorless oil (40 mg, 46% yield, 81:19 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.66 (m, 1H), 7.29-7.24 (m, 2H), 7.21-7.13 (m, 3H), 7.07 (d, *J* = 4.5 Hz, 2H), 6.92 (d, *J* = 4.5 Hz, 2H), 2.88-2.72 (m, 3H), 2.34-2.32 (m, 2H), 1.72-1.63 (m, 2H), 1.53-1.42 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 202.4, 143.8, 138.7, 131.5, 130.4, 128.4, 128.1, 127.6, 126.4, 47.9, 43.7, 43.0, 34.9, 20.1; **IR** (neat) 2927, 1723, 1491, 1092, 1015, 701 cm^{-1}; $[\alpha]_D^{20}$ = +41.6 (c = 0.5, EtOH); **HRMS** (ESI) Calcd. for $C_{18}H_{19}ONaCl$ $(M+Na)^+$: 309.1022. Found 309.1025.



(*S*)-6-(4-chlorophenyl)-5-phenylhexan-1-ol

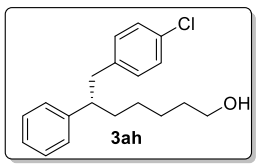
General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2ag** (29 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:4

EtOAc:hexanes) to afford **3ag** as a colorless oil (26 mg, 90% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.28-7.25 (m, 2H), 7.23-7.14 (m, 3H), 7.07 (d, *J* = 4.5 Hz, 2H), 6.92 (d, *J* = 4.5 Hz, 2H), 3.55-3.53 (m, 2H), 2.91-2.73 (m, 3H), 1.71-1.63 (m, 2H), 1.58-1.41 (m, 2H), 1.26-1.16 (m, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 144.4, 139.0, 131.5, 130.4, 128.3, 128.1, 127.7, 126.2, 62.8, 48.0, 43.1, 35.4, 32.7, 23.7; **IR** (neat): 3352, 2931, 1491, 1092, 1091, 1015, 700 cm^{-1}; $[\alpha]_D^{20}$ = +34.5 (c = 1.0, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{18}H_{21}ONaCl$ $(M+Na)^+$: 311.1179, found 311.1183.



(*S*)-7-(4-chlorophenyl)-6-phenylheptanal

General procedure A was followed using 4-chlorophenylboronic acid (140 mg, 0.90 mmol) and 6-phenylhept-6-en-1-ol (**1ah**, 57 mg, 0.30 mmol). The crude mixture was purified by silica gel flash chromatography (1:15 EtOAc:hexanes) to afford **2ah** as a colorless oil (38 mg, 42% yield, 22:78 er), R_f = 0.40 (1:4 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 9.69 (m, 1H), 7.28-7.23 (m, 2H), 7.20-7.14 (m, 3H), 7.06 (d, *J* = 3.0 Hz, 2H), 6.91 (d, *J* = 3.0 Hz, 2H), 2.90-2.70 (m, 3H), 2.35-2.30 (m, 2H), 1.66-1.54 (m, 4H), 1.22-1.13 (m, 2H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 202.5, 144.2, 138.9, 131.5, 130.4, 128.3, 128.1, 127.6, 126.2, 47.8, 43.7, 43.1, 35.3, 27.0, 22.0; **IR** (neat): 2929, 1723, 1492, 1093, 1015, 701 cm^{-1}; $[\alpha]_D^{20}$ = +39.9 (c = 0.5, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{19}H_{21}ONaCl$ $(M+Na)^+$: 323.1179, found 323.1180.



(*S*)-7-(4-chlorophenyl)-6-phenylheptan-1-ol

General procedure B was followed using sodium borohydride (6 mg, 0.15 mmol) and aldehyde **2ah** (30 mg, 0.10 mmol). The crude mixture was purified by silica gel flash chromatography (1:4 EtOAc:hexanes) to afford **3ah** as a colorless oil (28 mg, 94% yield), R_f = 0.20 (1:2 EtOAc:hexanes). **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.29-7.23 (m, 2H), 7.21-7.14 (m, 3H), 7.09-7.06 (m, 2H), 6.93-6.90 (m, 2H), 3.59-3.55 (m, 2H), 2.88-2.73 (m, 3H), 1.67-1.63 (m, 2H), 1.50-1.43 (m, 2H), 1.33-1.15 (m, 5H); **^{13}C NMR** (75 MHz, $CDCl_3$): δ 144.5, 139.1, 131.4, 130.4, 128.2, 128.1, 127.7, 126.1, 62.9, 48.0, 43.2, 35.5, 32.6, 27.3, 25.7; **IR** (neat): 3356, 2930, 1491, 1093, 1091, 1015, 700 cm^{-1}; $[\alpha]_D^{20}$ = +39.0 (c = 0.2, EtOH); **HRMS** (ESI) *m/z* calcd. for $C_{19}H_{23}ONaCl$ $(M+Na)^+$: 325.1335, found 325.1349.

Methods for Modeling Strategy

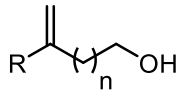
DFT Calculations

DFT calculations were performed using Gaussian 09 software.[6] The geometries of the substrates and PyrOx ligands were optimized using M06-2x/def2tzvp level of theory[7] with an ultrafine integration grid. IR frequencies and intensities as well as the polarizabilities of the entire molecule were obtained for the geometry optimized structure with the lowest-lying energy. Subsequently, Sterimol values of the alkene substituents and oxazoline substituents of the PyrOx ligands were calculated using Molecular Modeling Pro®.[8] NBO charges were calculated using version 6.0.[9]

Model Development

First, molecular descriptors or parameters that represent the steric and electronic perturbations induced by the substituents on the alkenyl alcohol substrates and the PyrOx ligands were identified. Parameters that were considered for the substrates include IR frequency and intensity of the alkene C=C stretch, IR frequencies and intensities of the alkenyl CH_2 symmetric, asymmetric, and wagging stretches, IR frequencies and intensities of the allylic CH_2 scissoring stretch, NBO charges at the allylic position, and Sterimol values of the variable alkene substituent (Table S2 and Figure S3). Parameters that were considered for the PyrOx ligands include IR frequency and intensity of the oxazoline C=N stretch, IR frequencies and intensities of the pyridine ring stretches, Sterimol values of the oxazoline substituent, and the polarizabilities of the ligand (Table S3 and Figure S4). Next, using MATLAB® R2014a software[10], a multiple linear regression model was developed to utilize these parameters in predicting the difference in transition state energies ($\Delta\Delta G^{\ddagger}$). These predicted $\Delta\Delta G^{\ddagger}$ values were then compared to the measured $\Delta\Delta G^{\ddagger}$ values calculated based on Curtin-Hammett principle using the formula, measured $\Delta\Delta G^{\ddagger}$= -RTln(er), where R is the gas constant, T is temperature, and er is the enantiomeric ratio. The measured $\Delta\Delta G^{\ddagger}$ was obtained from an average enantiomeric ratio of two experimental results and the temperature is set at 298K. A good correlation between the two indicates that the predicted $\Delta\Delta G^{\ddagger}$ approximates the measured $\Delta\Delta G^{\ddagger}$ adequately. Leave-K-Out plots were also generated using MATLAB. Linear regression plots were generated using OriginPro 9.0.

Table S2. Raw parameter values for alkenol substrates (n=1 unless otherwise noted).



R	ν C=C	*I* C=C	ν =CH_2 asym	*I* =CH_2 asym	ν =CH_2 sym	*I* C=CH_2 sym	ν =CH_2 wag	*I* =CH_2 wag	ν allyl CH_2 scissor	*I* allyl CH_2 scissor	NBO allyl-C	L	B_1	B_5
(4-OMe)Ph	1721.84	26.9206	3264.74	9.3446	3185.10	1.5627	1449.34	1.0489	1483.32	15.9334	-0.44549	8.54	1.89	3.25
(3-OMe)Ph	1723.88	17.6910	3265.04	8.5775	3184.63	1.5627	1452.72	2.3763	1482.30	8.9254	-0.44573	7.15	1.88	4.75
(4-Cl)Ph	1722.97	20.9431	3266.47	7.7882	3186.64	1.1884	1458.20	6.1235	1483.89	11.3034	-0.44545	7.74	1.77	3.23
(2-F)Ph	1728.69	21.9004	3279.47	3.8839	3196.31	2.7816	1455.92	5.4583	1484.57	10.2745	-0.44343	6.35	1.77	3.83
(4-Me)Ph	1722.26	23.1808	3265.27	8.7888	3186.10	2.1979	1457.68	3.1886	1483.74	9.3298	-0.44539	7.40	1.83	3.32
(4-*t*Bu)Ph	1722.87	24.1886	3264.85	8.9807	3185.25	1.5172	1458.19	7.0080	1484.79	9.8060	-0.44519	8.73	2.86	3.43
Ph	1723.80	20.2544	3265.37	8.3275	3185.98	1.4631	1452.42	2.4599	1483.25	9.1329	-0.44546	6.34	1.77	3.23
(4-CO_2Me)Ph	1722.05	17.7991	3267.96	7.3247	3187.94	1.1798	1471.23	7.5554	1483.25	17.1525	-0.44552	9.30	1.98	3.22
(4-F)Ph	1724.05	23.4591	3265.57	8.0327	3186.24	1.3007	1447.88	1.2607	1483.42	10.6687	-0.44554	7.03	1.77	3.23
(4-*i*Pr)Ph	1723.09	23.782	3266.90	8.9181	3187.87	1.9005	1449.52	5.1413	1484.78	9.9313	-0.44502	8.76	2.15	3.45
(4-OMe,3-Cl) Ph	1721.38	24.5167	3265.64	8.4454	3185.51	1.4333	1457.61	7.6325	1483.19	18.8190	-0.44677	8.61	1.91	4.00
3,4-(CH_2dioxy)Ph	1723.45	21.2797	3266.05	9.0432	3185.99	1.4806	1450.46	7.942	1482.28	13.3234	-0.44536	7.63	1.78	3.71
CH_2Ph	1740.40	26.4429	3250.88	10.7353	3170.33	3.8496	1455.18	4.6221	1478.86	7.9633	-0.46176	4.96	1.71	6.00
Me	1746.94	24.969	3252.52	11.7705	3172.65	3.8720	1453.10	1.641	1480.14	5.4506	-0.62681	3.07	1.70	2.19
Cy	1735.11	28.6708	3262.60	10.6694	3187.77	4.0618	1455.91	6.1847	1479.33	5.3164	-0.45225	6.49	2.13	3.64
Ph, n=2	1724.81	17.6791	3268.57	6.2069	3185.88	1.7399	1453.63	7.2528	1478.47	7.7103	-0.42348	6.34	1.77	3.23
Ph, n=3	1723.10	19.036	3267.92	7.7403	3185.54	1.8688	1452.32	4.8331	1475.23	7.1978	-0.41847	6.34	1.77	3.23
Ph, n=4	1723.11	18.7924	3268.49	7.4459	3186.28	1.8843	1452.25	5.4012	1474.8	7.0049	-0.41971	6.34	1.77	3.23

Figure S3. Depictions of the parameters evaluated to describe substrate effects.

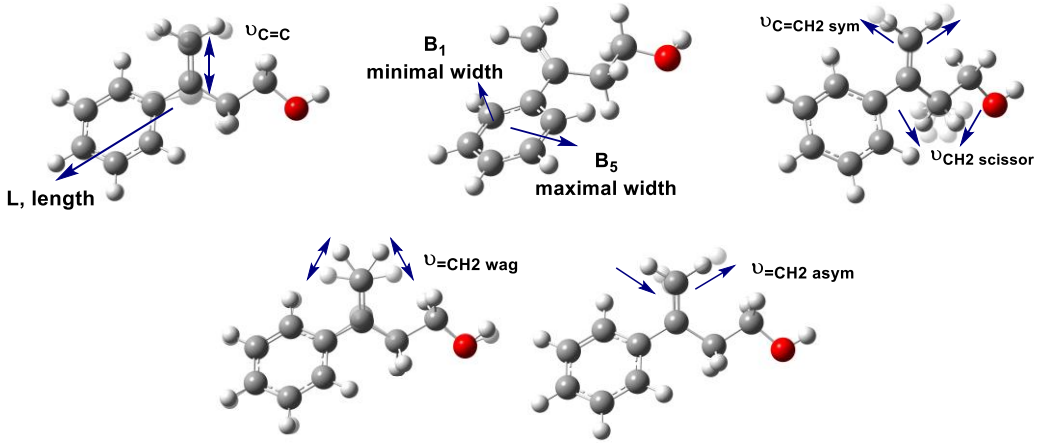
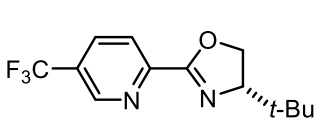
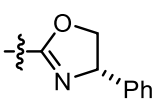


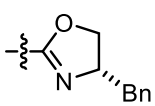
Table S3. Raw parameter values for PyrOx ligands.



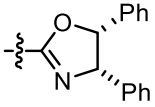
Ligand **1**



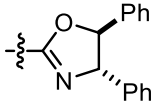
Ligand **2**



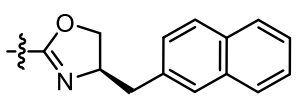
Ligand **3**



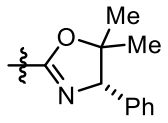
Ligand **4**



Ligand **5**



Ligand **6**



Ligand **7**

Ligand	ν C=N ox	I C=N ox	ν py ring 1	*I* py ring 1	ν py ring 2	*I* py ring 2	ν py ring 3	*I* py ring 3	Dihedral Angle	B_1 ox	B_5 ox	L ox	polar
1	1775.85	108.7417	1686.88	78.1699	1649.49	58.8413	1550.99	5.2579	61.2	2.92	3.35	4.35	230.496
2	1772.37	130.421	1688.16	70.3881	1650.40	65.6686	1551.09	3.9118	12.2	1.77	3.21	6.38	269.027
3	1773.42	135.4201	1686.21	81.3039	1647.93	52.7276	1552.36	8.2620	70.4	1.72	5.97	4.65	271.035
4	1766.49	102.4718	1687.67	72.2049	1650.39	61.4205	1550.62	3.7490	20.6	1.77	3.21	6.38	329.547
5	1768.68	119.4807	1686.81	75.1524	1649.37	61.1527	1550.14	4.0311	20.4	1.77	3.21	6.38	335.135
6	1773.57	146.0401	1685.87	79.6678	1648.20	57.7636	1552.56	9.0713	70.1	1.72	8.14	5.13	312.415
7	1762.8	119.3274	1687.34	76.5438	1649.08	65.1753	1550.83	3.3047	21.8	1.77	3.21	6.38	291.705

Figure S4. Depictions of the parameters evaluated to describe PyrOx ligands.

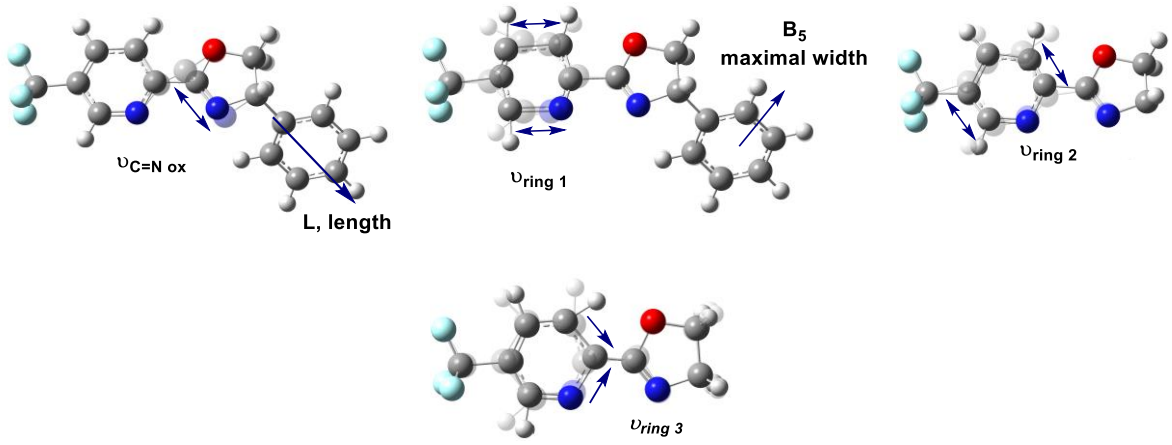


Table S4. Measured and predicted enantioselectivity values for substrates.

Substrate	% ee	Measured ΔΔG‡ (kcal/mol)	Predicted ΔΔG‡ (kcal/mol)	Predicted ΔΔG‡ (LKO) (kcal/mol, K=6)
(4-OMe)Ph	93	1.963951	1.849753	1.841188
(3-OMe)Ph	92	1.881808	1.674524	1.684881
(4-Cl)Ph	83	1.407053	1.638762	1.671659
(2-F)Ph	60	0.820861	0.486502	0.624547
(4-Me)Ph	91	1.808974	1.731657	1.717441
(4-^{t}Bu)Ph	90	1.743479	1.680311	1.817261
Ph	91	1.808974	1.676364	1.684116
(4-CO_2Me)Ph	87	1.578702	1.689607	1.670306
(4-F)Ph	80	1.301034	1.430107	1.459981
(4-*i*Pr)Ph	90	1.743479	1.817584	1.712121
(4-OMe,3-Cl) Ph	92	1.881808	1.965595	1.869275
3,4-(CH_2dioxy)Ph	83	1.407053	1.547234	1.578588
CH_2Ph	-39	-0.487675	--	--
Me	-3	-0.035538	-0.050959	0.187645
Cy	-35	-0.432777	-0.184883	0.170290
Ph, n=2	77	1.208325	0.862826	0.782118
Ph, n=3	62	0.858589	1.012742	1.093515
Ph, n=4	56	0.749434	0.867480	0.884033

Figure S5. Leave-K-Out Plot for Substrate Model (K = 6).

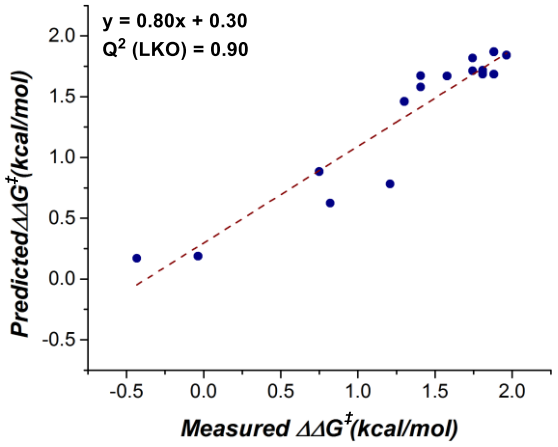


Figure S6. Chain length trend, relating $NBO_{allyl\text{-}C}$ with measured $\Delta\Delta G^{\ddagger}$ (R^2 = 0.92).

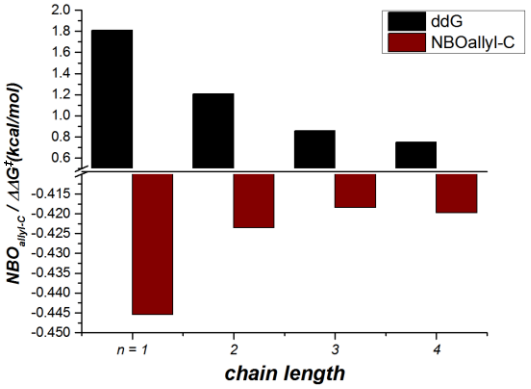
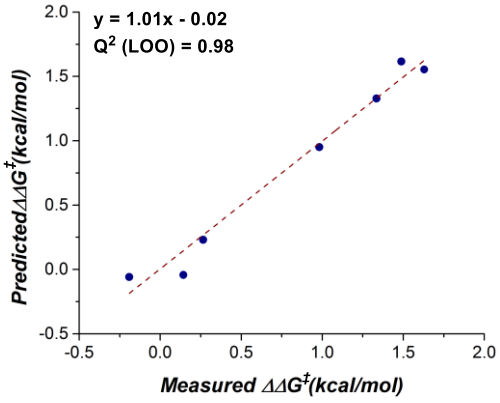


Table S5. Measured and predicted enantioselectivity values for ligands.

Ligand	Measured $\Delta\Delta G^{\ddagger}$ (kcal/mol)	Predicted $\Delta\Delta G^{\ddagger}$ (kcal/mol)	Predicted $\Delta\Delta G^{\ddagger}$ (LOO) (kcal/mol)
1	0.264865	0.250927	0.230741
2	0.981890	0.959520	0.950686
3	-0.191122	-0.115250	-0.059500
4	1.629255	1.581703	1.553647
5	1.487601	1.564424	1.616056
6	0.142798	0.078634	-0.043010
7	1.334686	1.330004	1.328236

Figure S8. Leave-One-Out Plot for Ligand Model (LOO).



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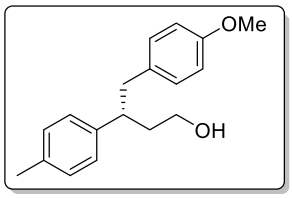
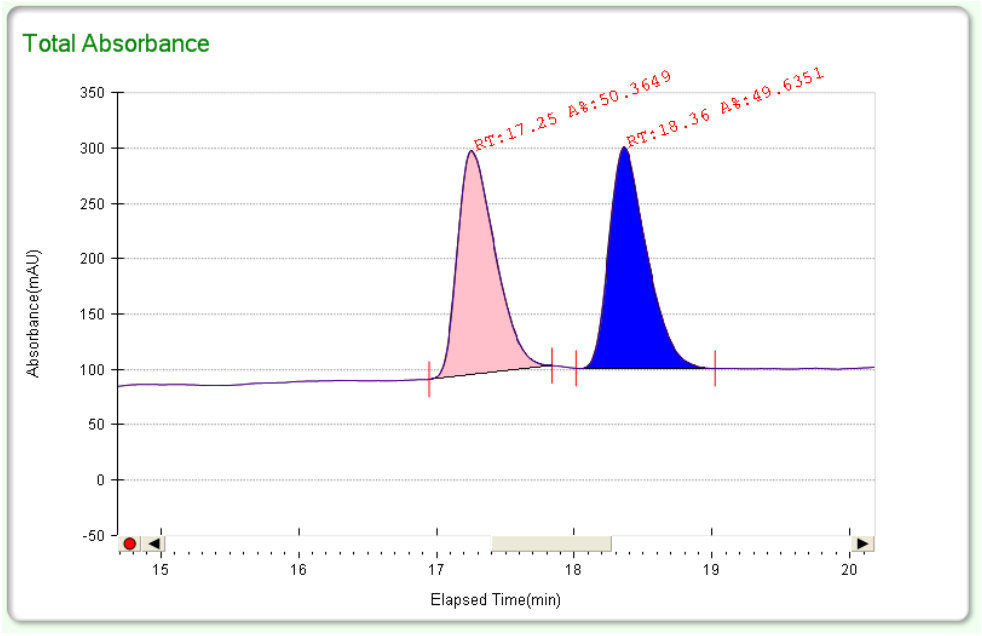
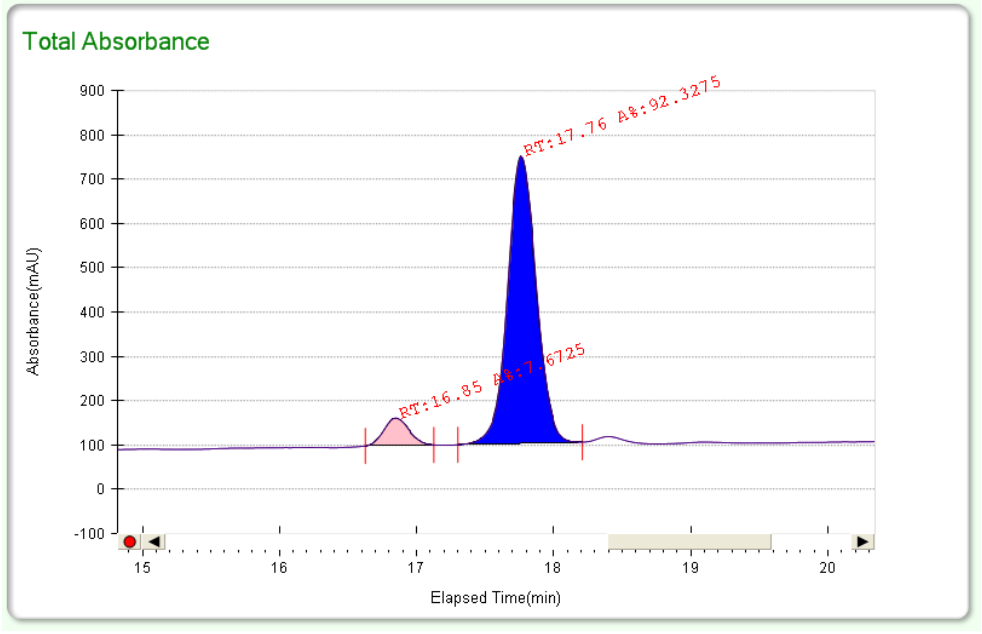
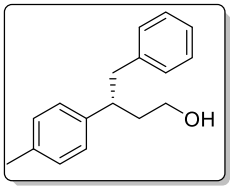


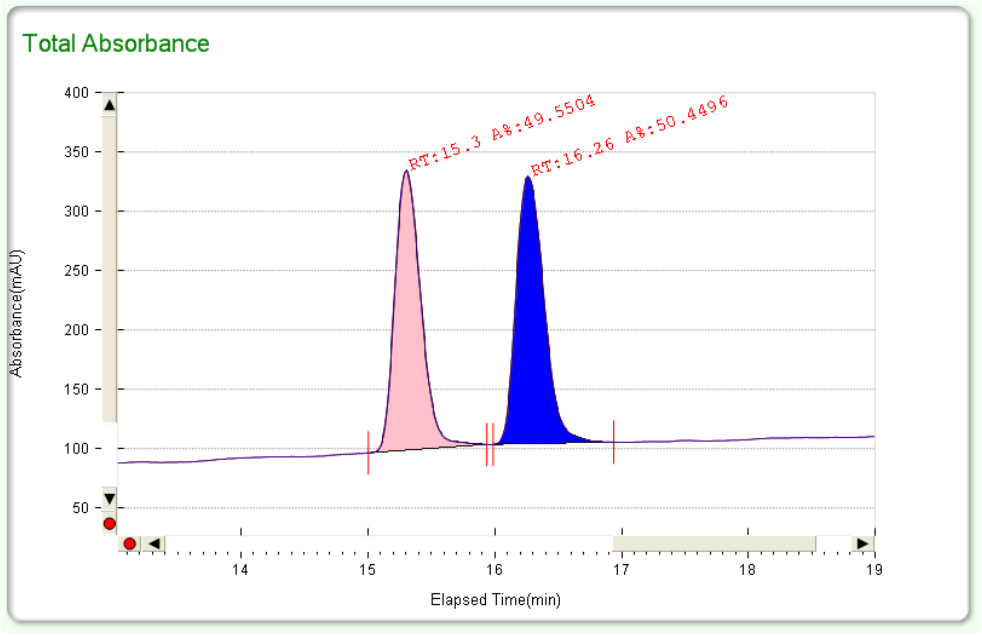
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 16.8, t_2 = 17.8; er = 7.5:92.5.

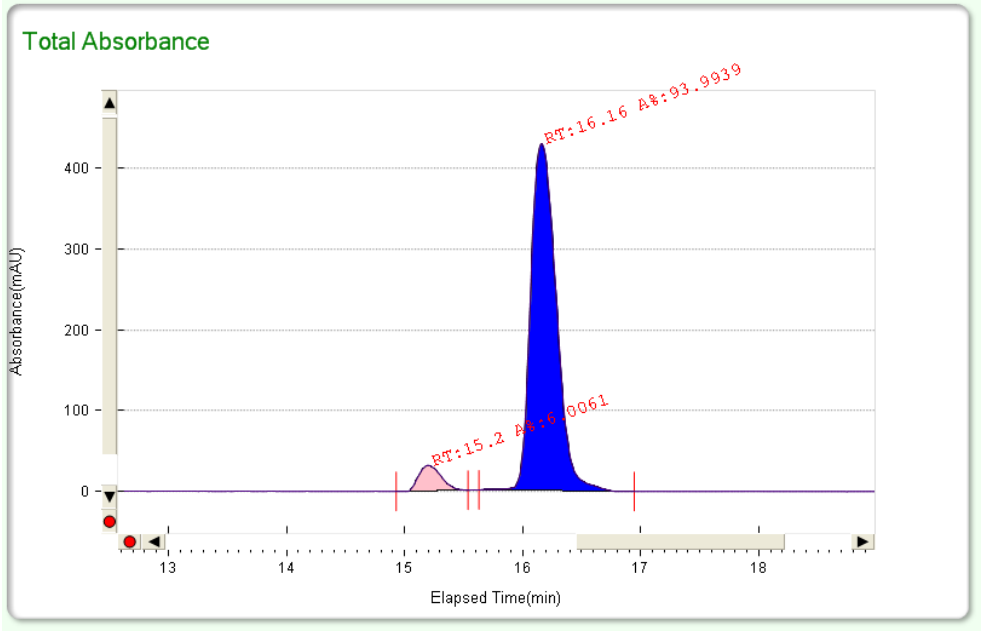


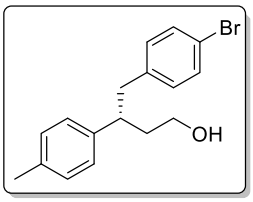




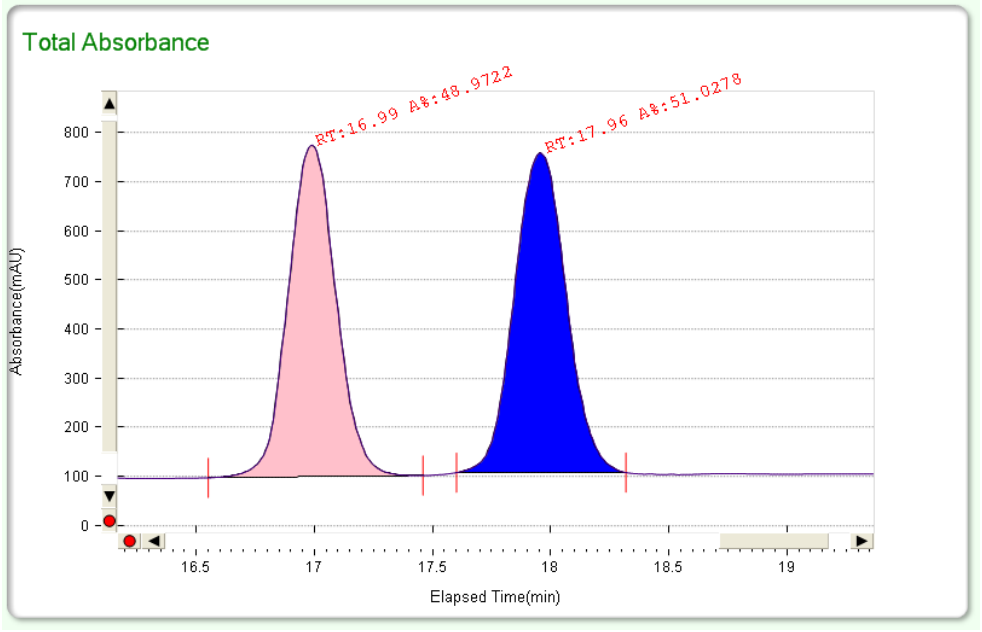
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 15.2, t_2 = 16.2; er = 6:94.

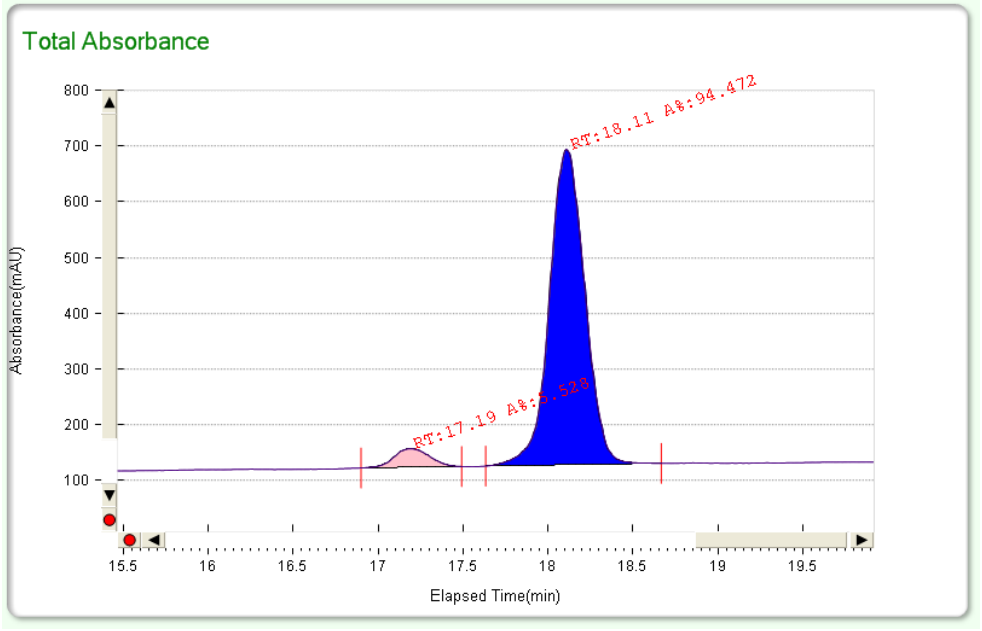


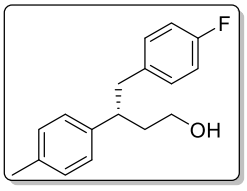




Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 17.2, t_2 = 18.1; er = 5.5:94.5.







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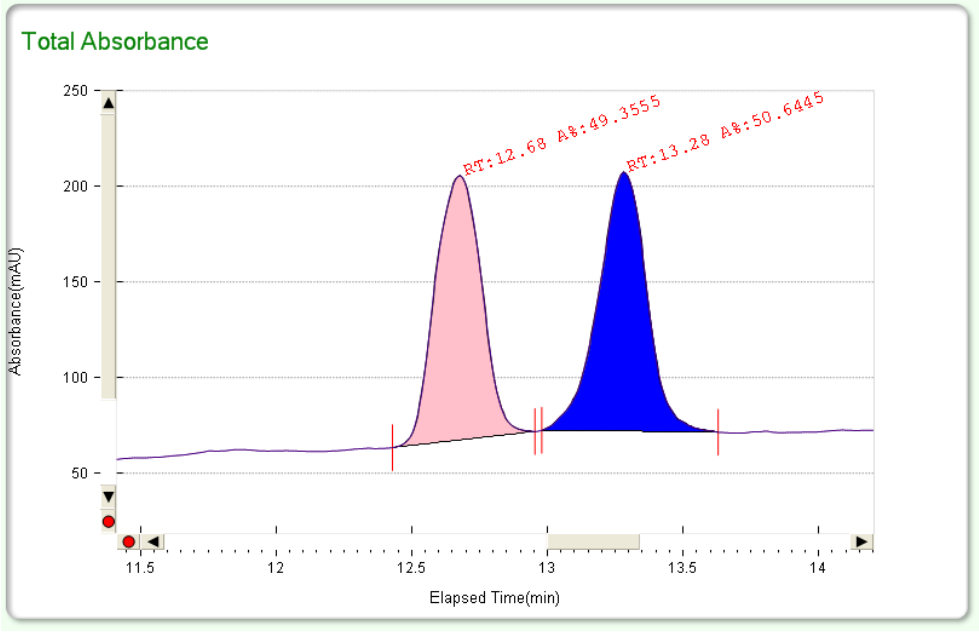

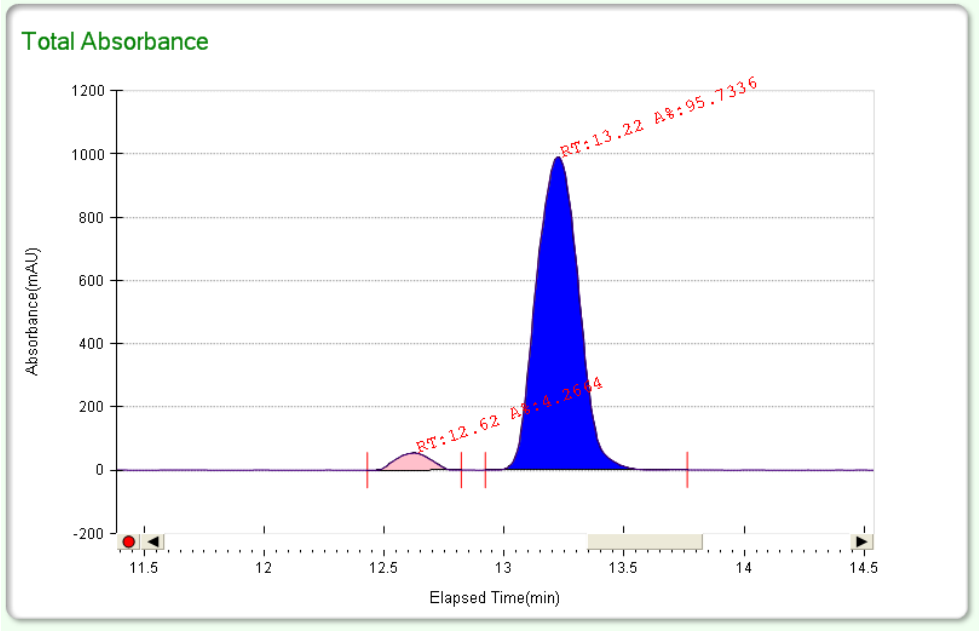

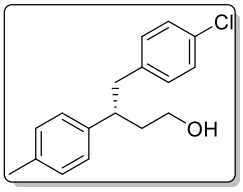

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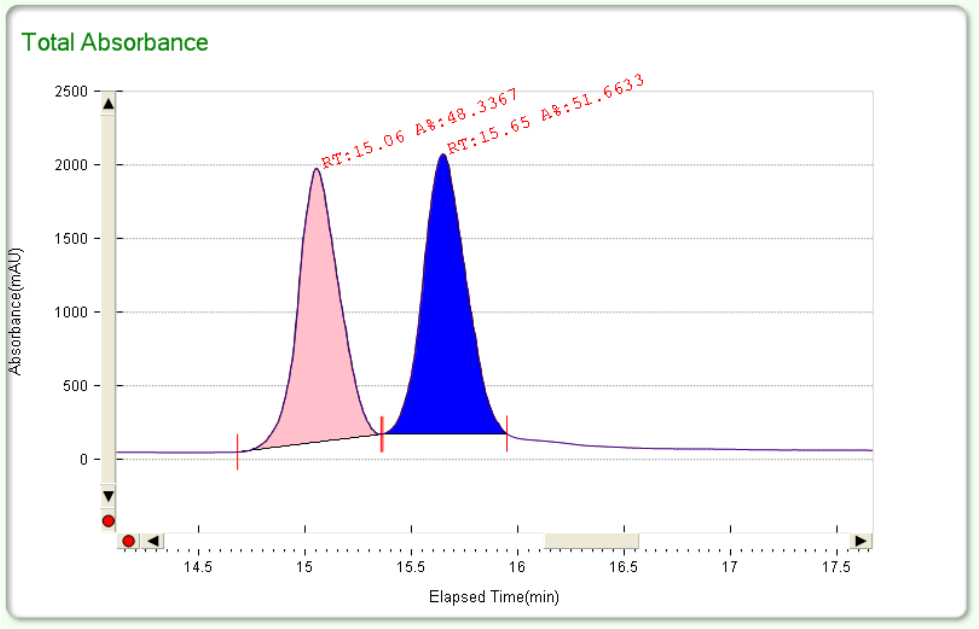

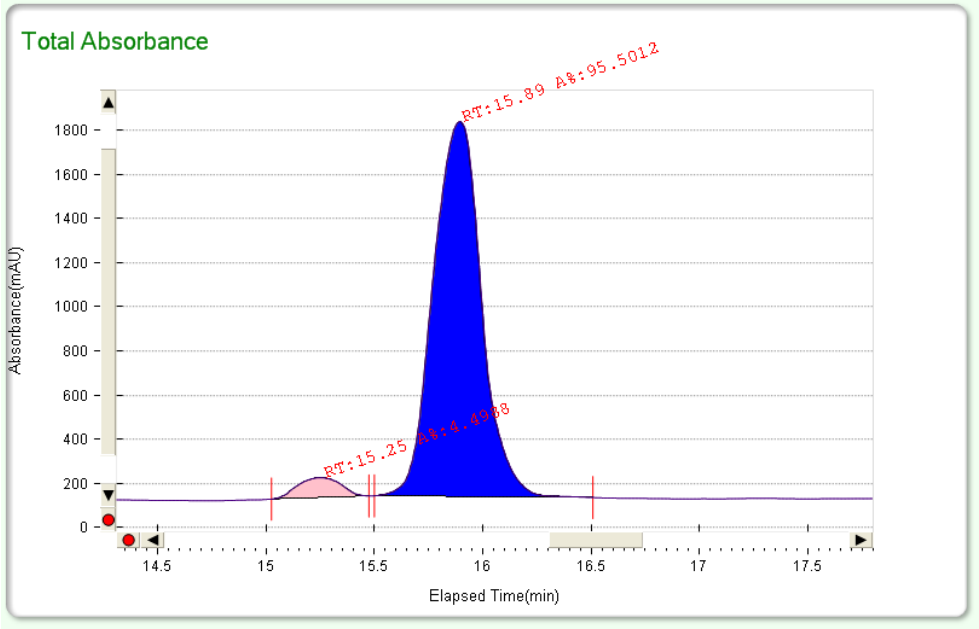

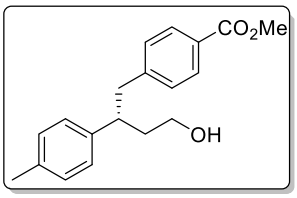

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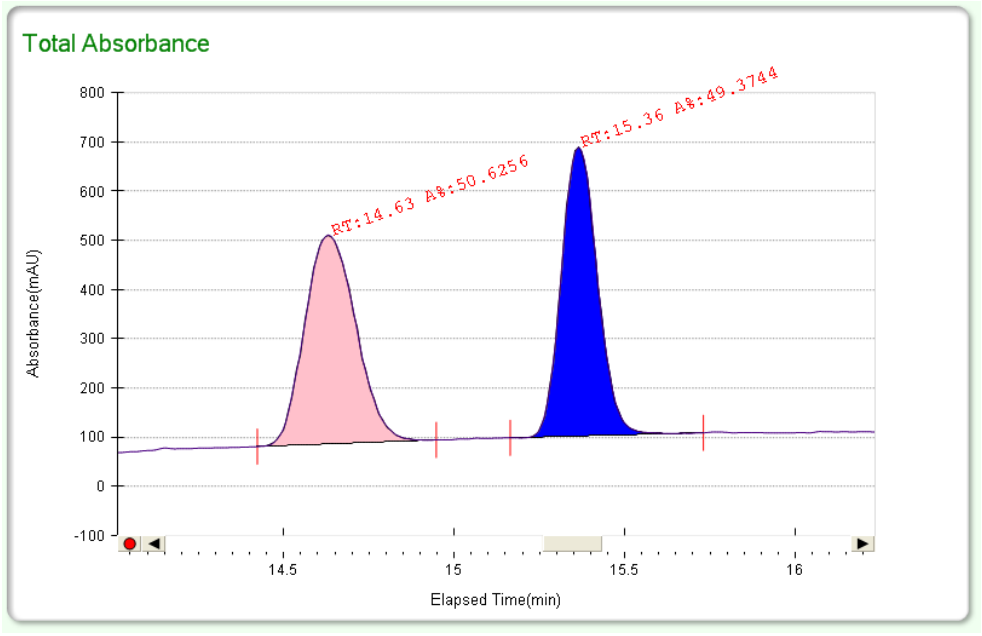

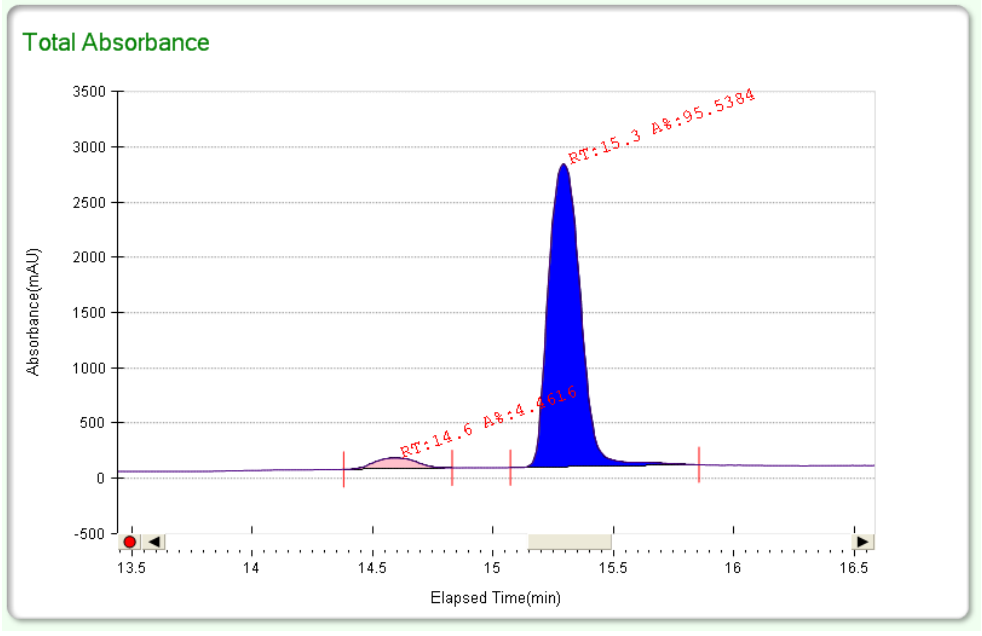

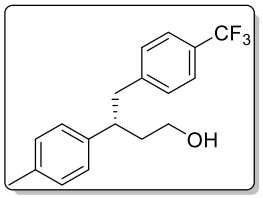

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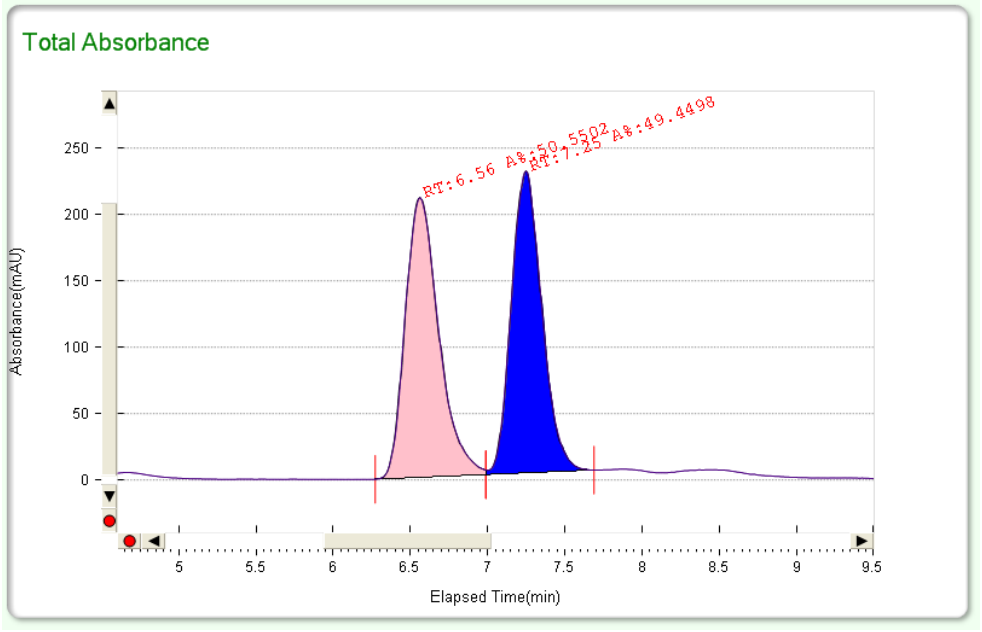

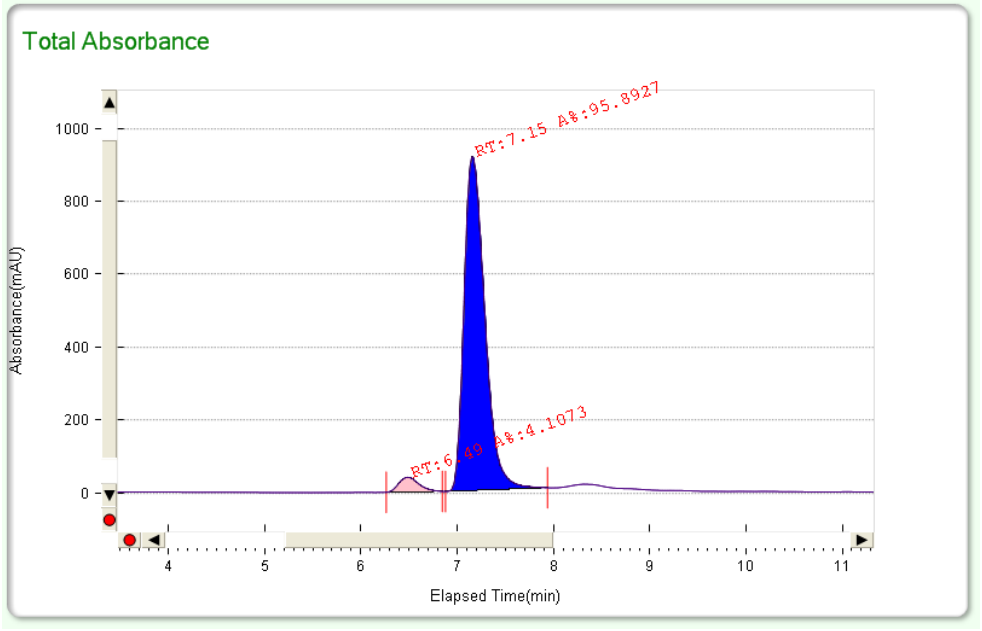

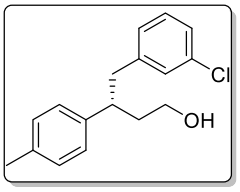

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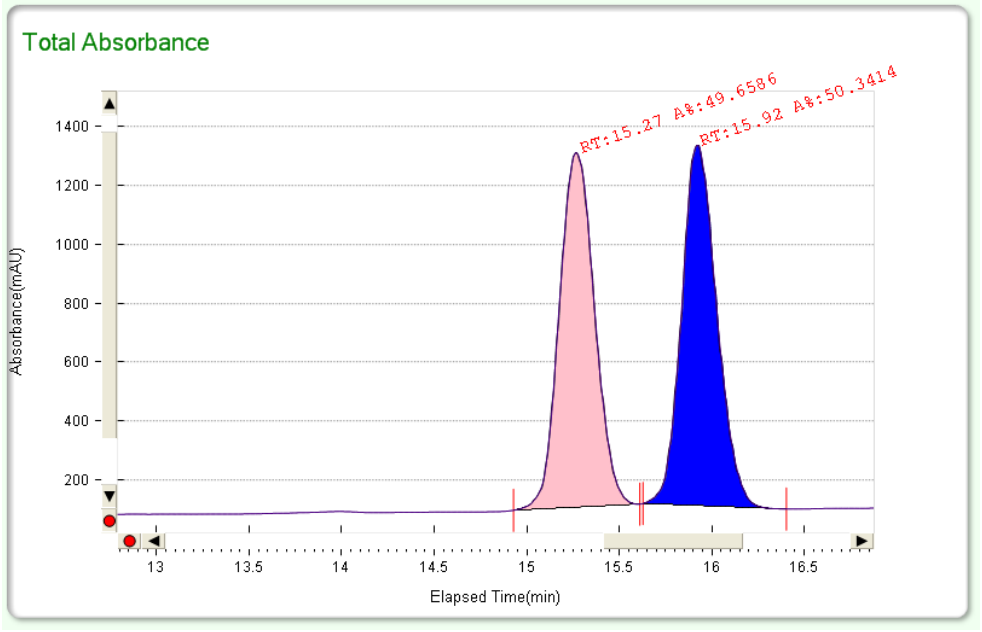

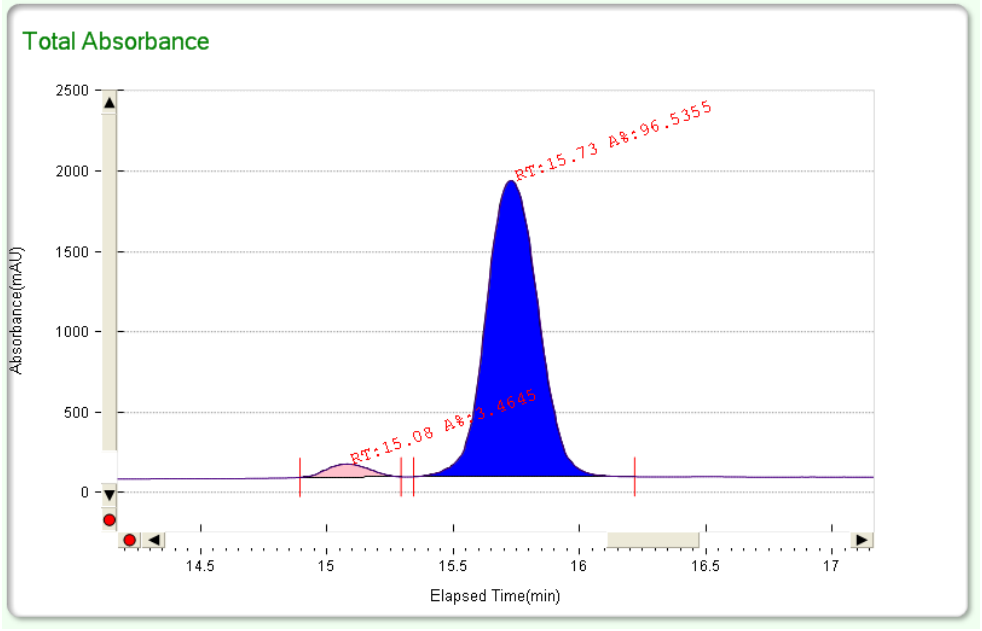

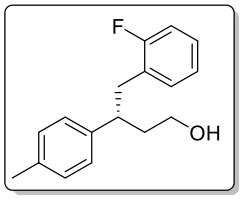

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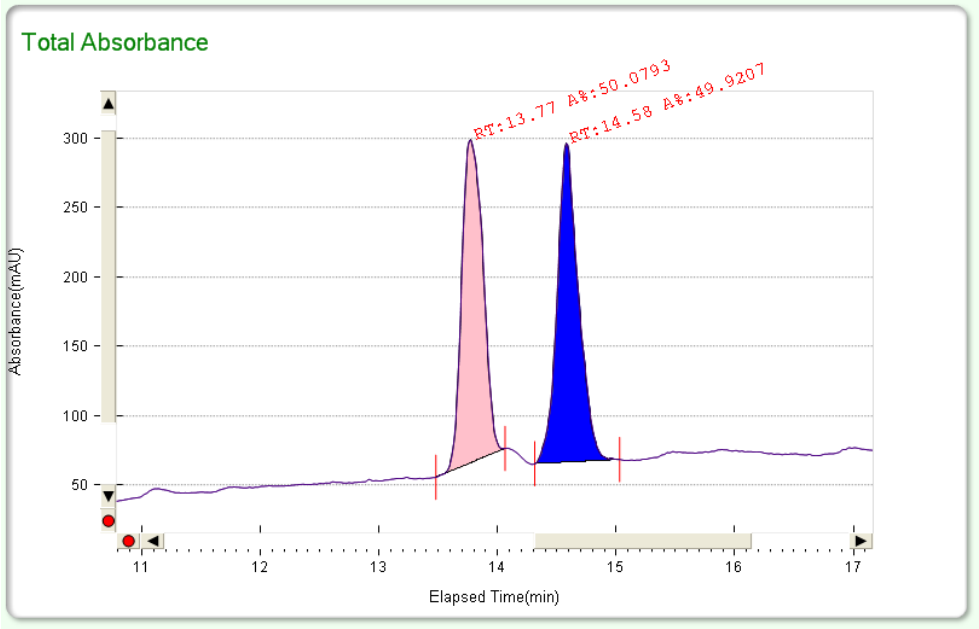

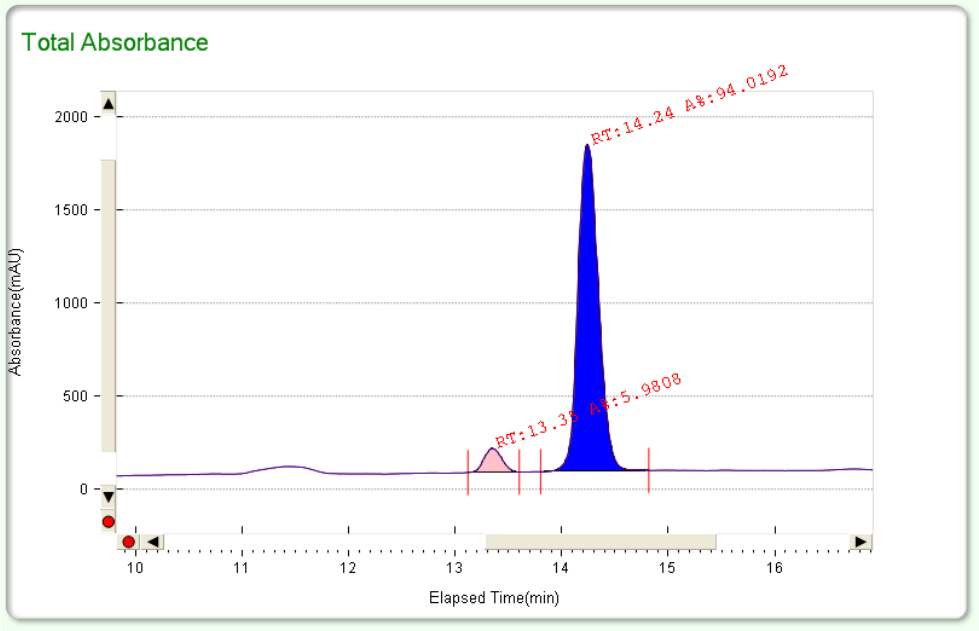

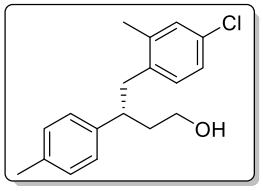

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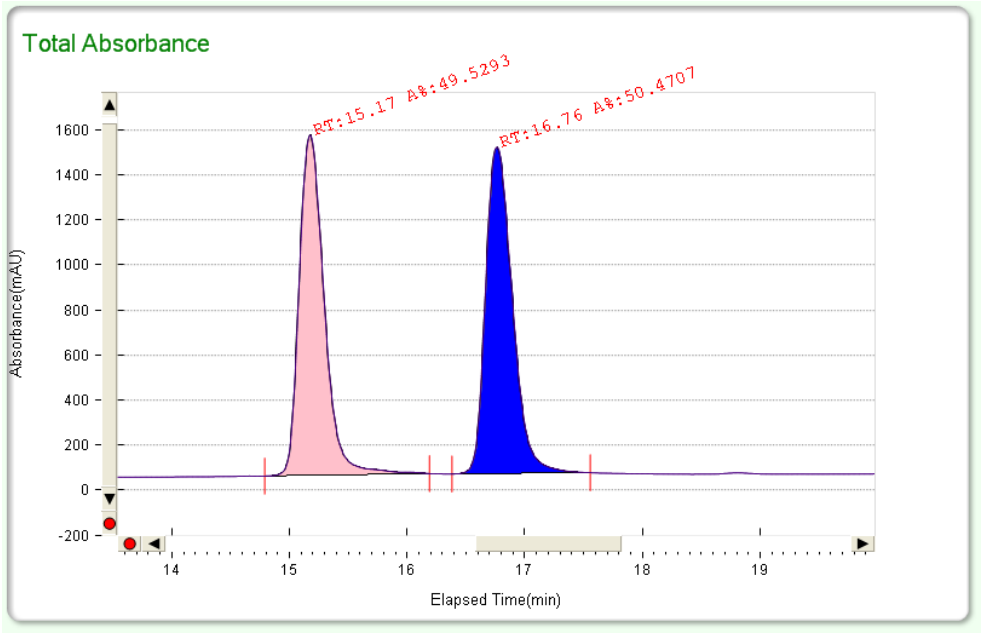
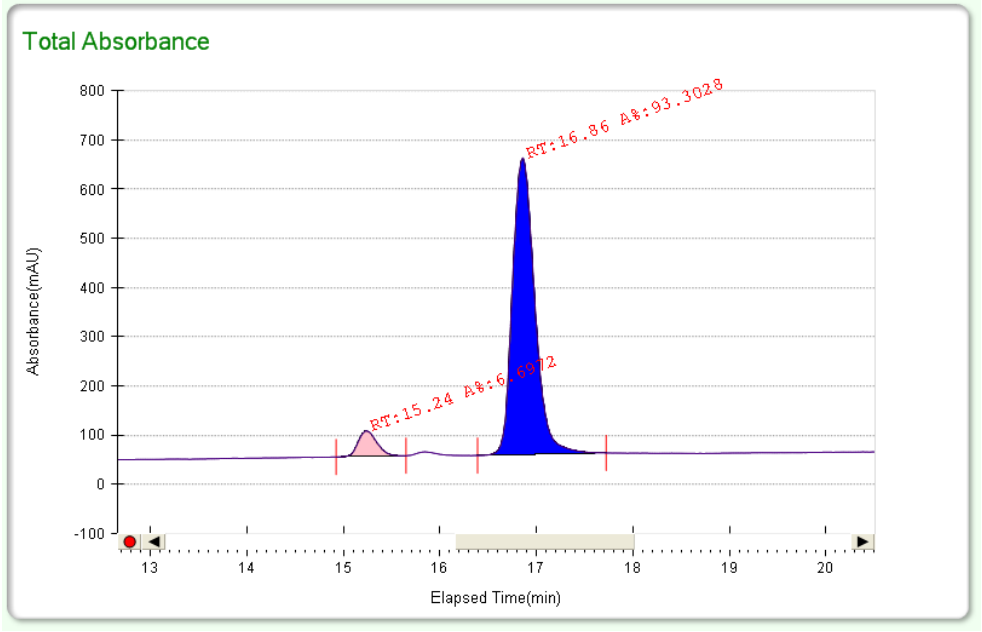
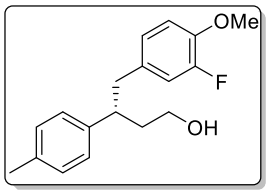
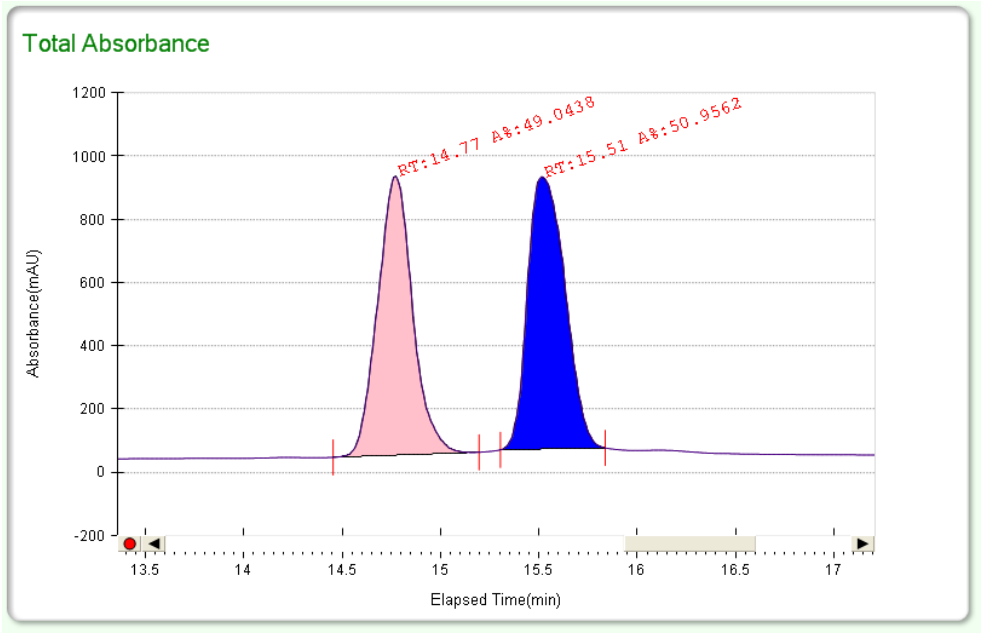
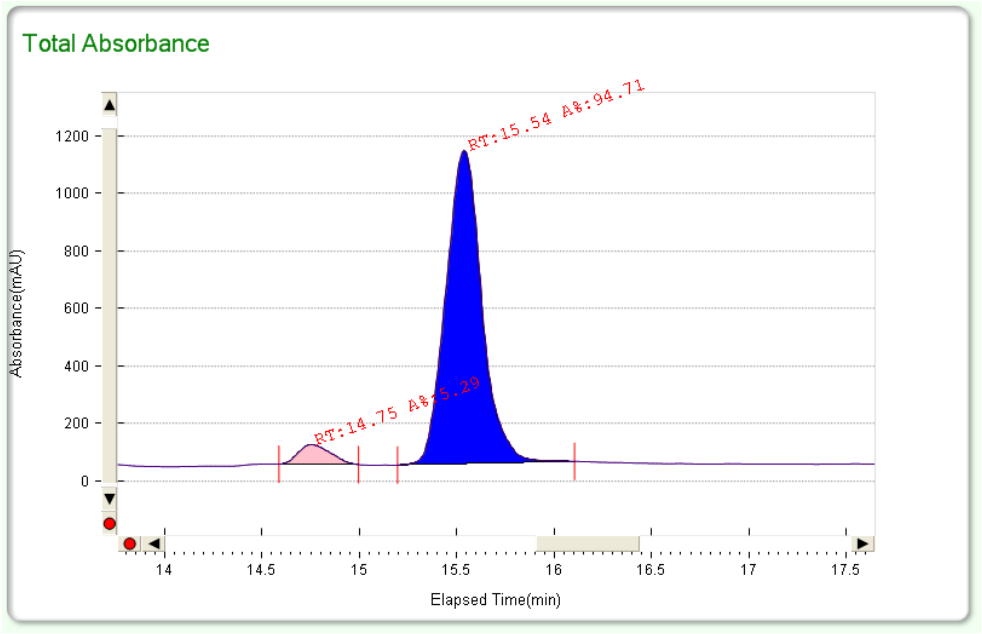


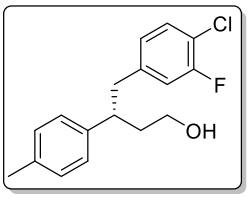




Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 14.8, t_2 = 15.5; er = 5:95.







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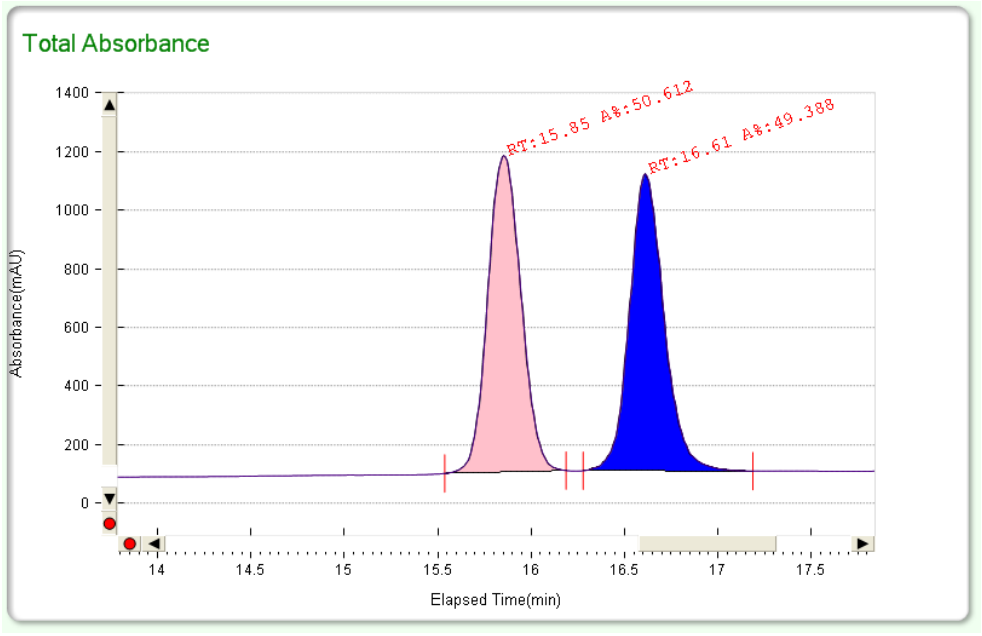

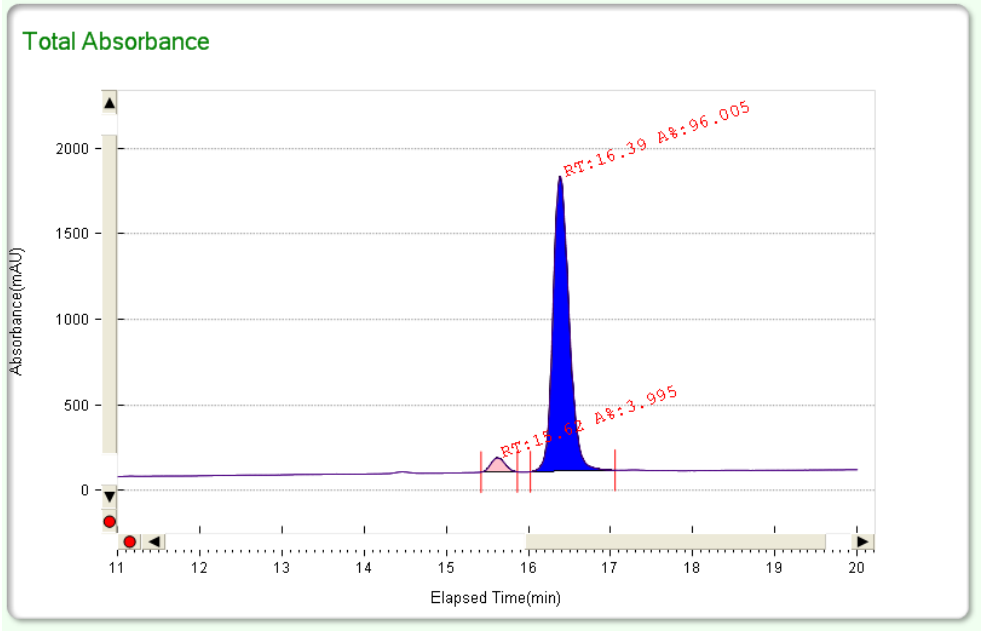

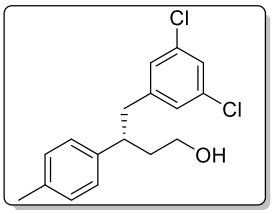

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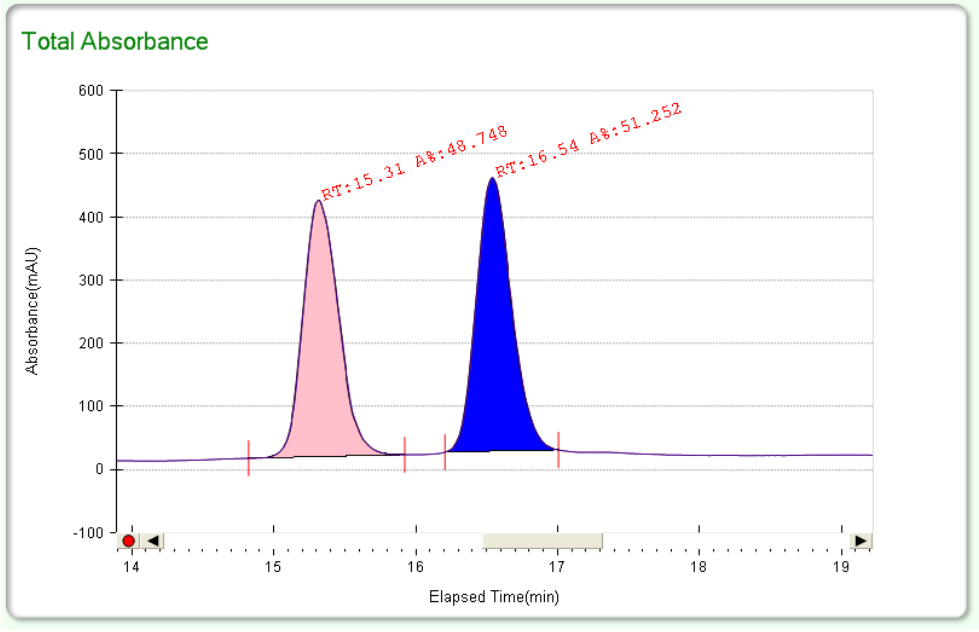
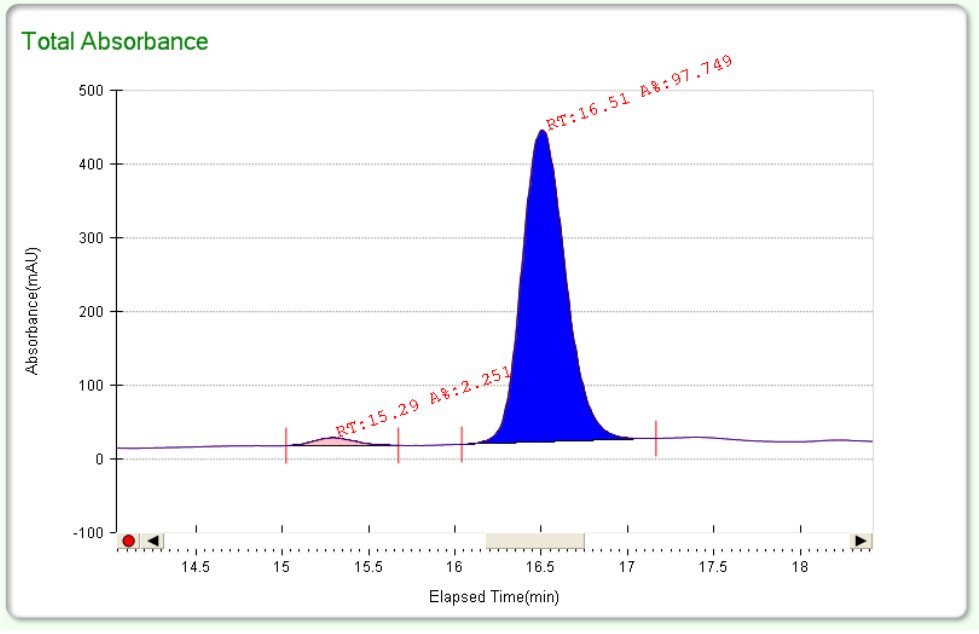
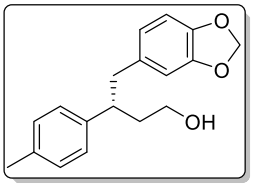
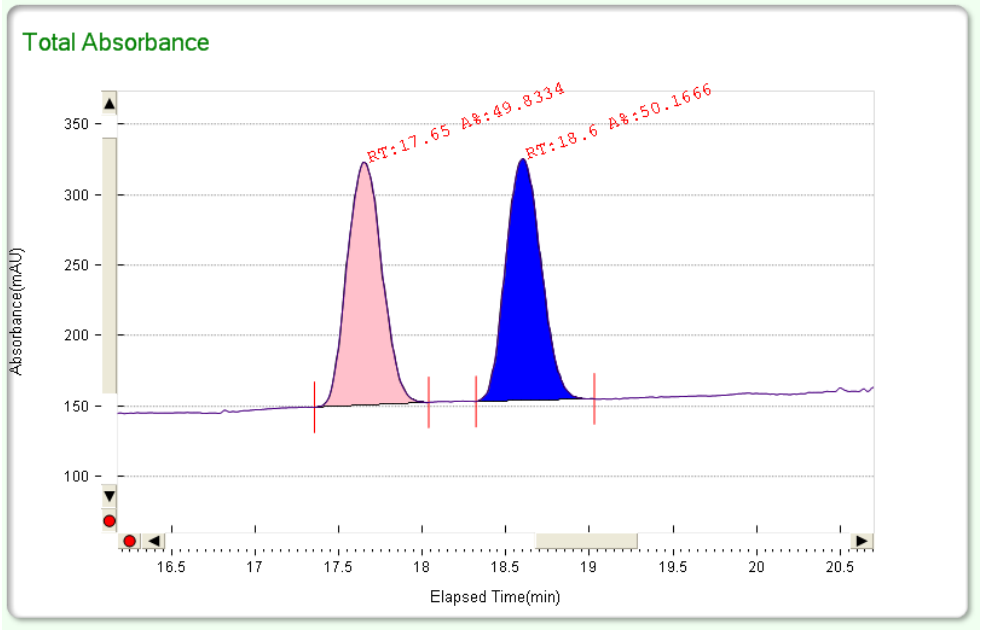
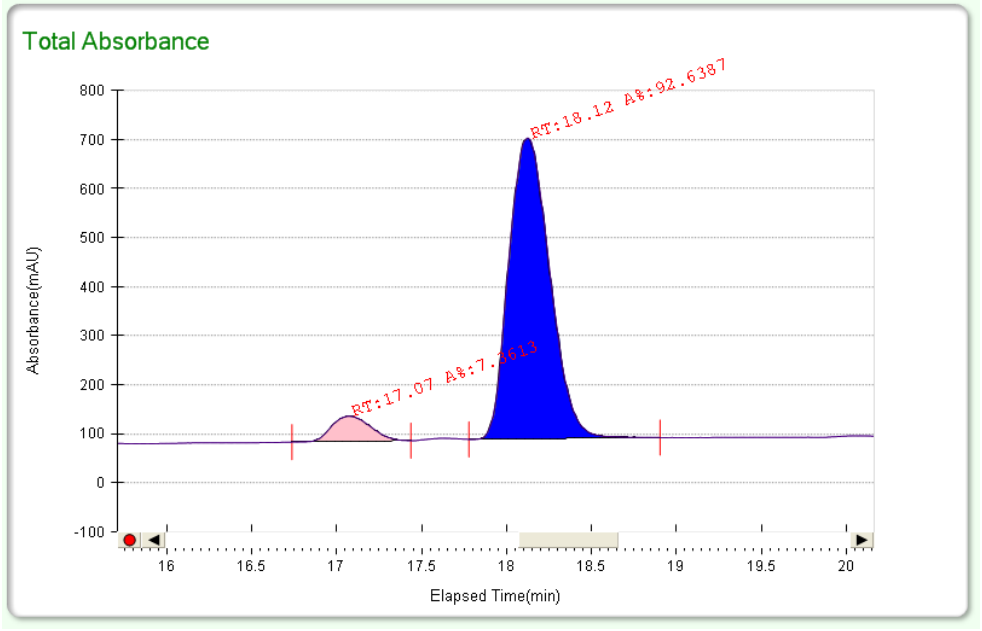


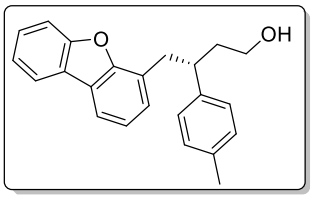




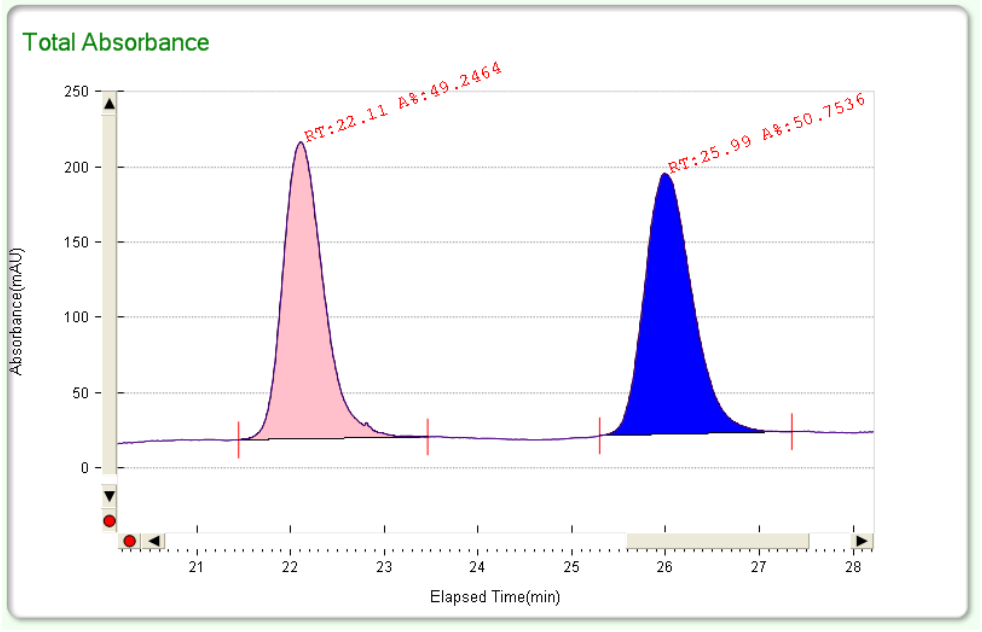
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 17.1, t_2 = 18.1; er = 7.5:92.5.

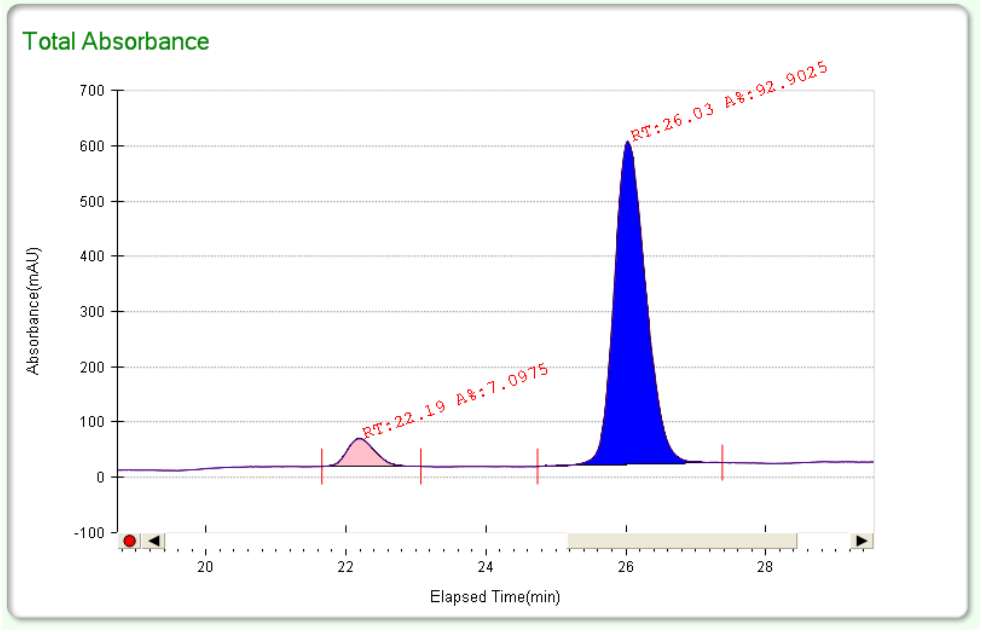


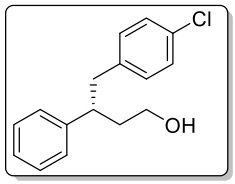




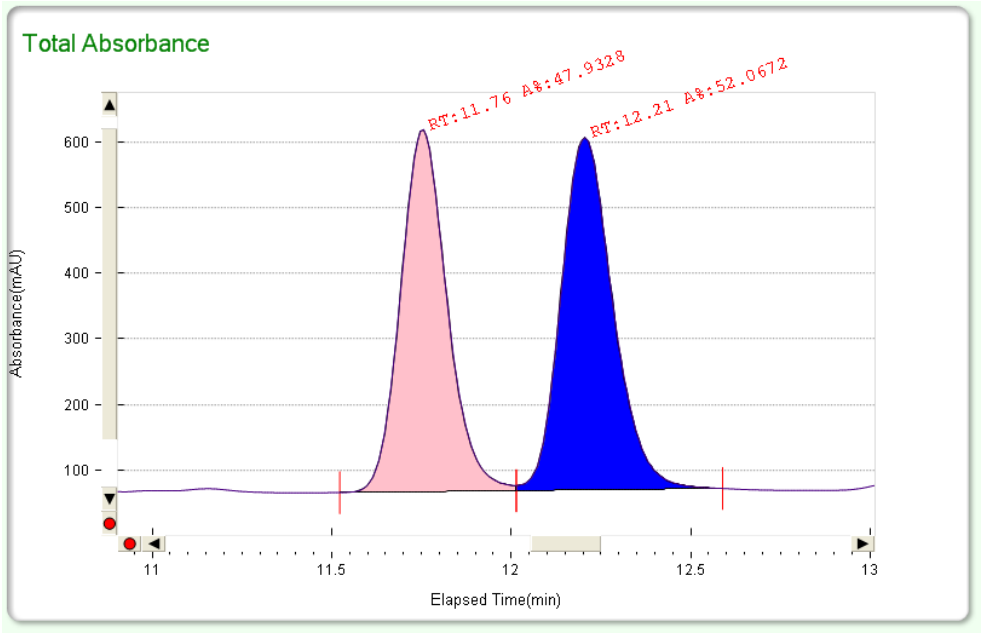
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-15:85-20:80-50:50 (50 min), 2mL/min, 160bar, t_1 = 22.2, t_2 = 26.0; er = 7:93.

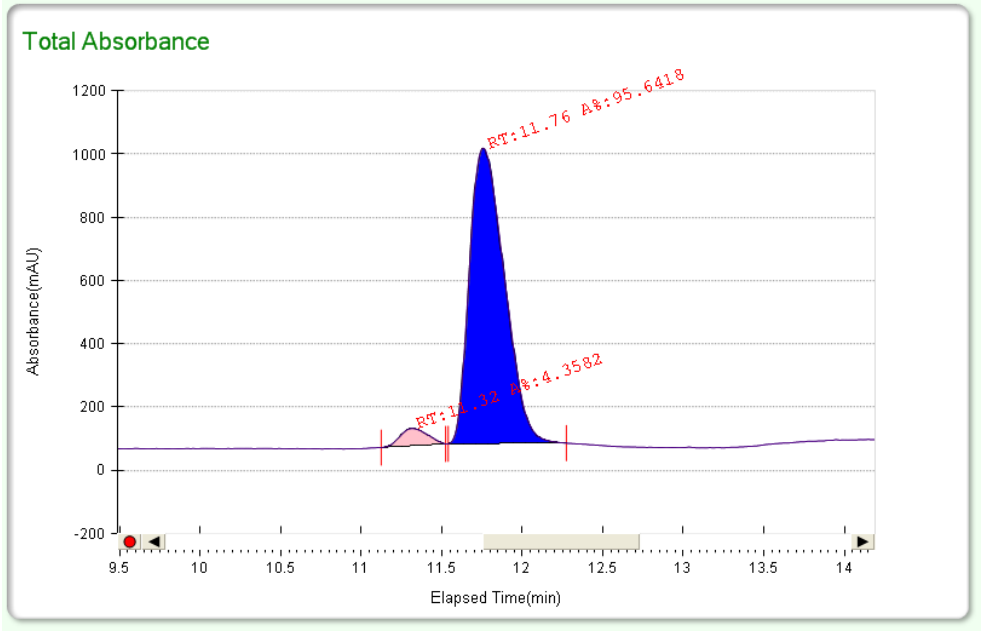


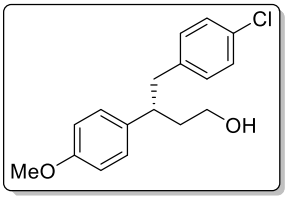




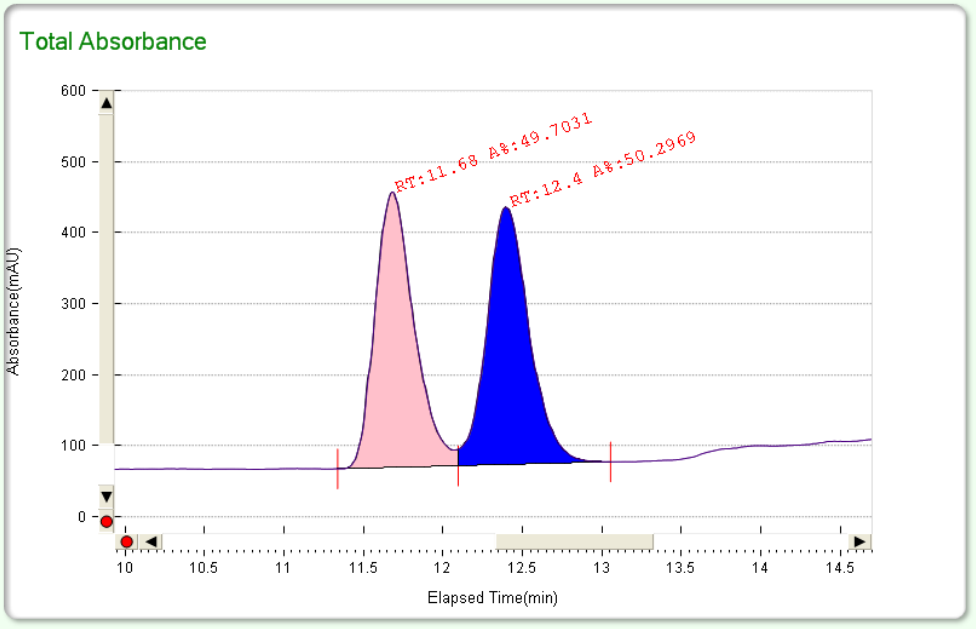
Separation of enantiomers by SFC. Chiralcel® Column AD-H, 40 °C, $^{i-}$PrOH: CO_2 = 5:95-15:85-50:50 (30 min), 2mL/min, 160bar, t_1 = 11.3, t_2 = 11.8; er = 4.5:95.5.

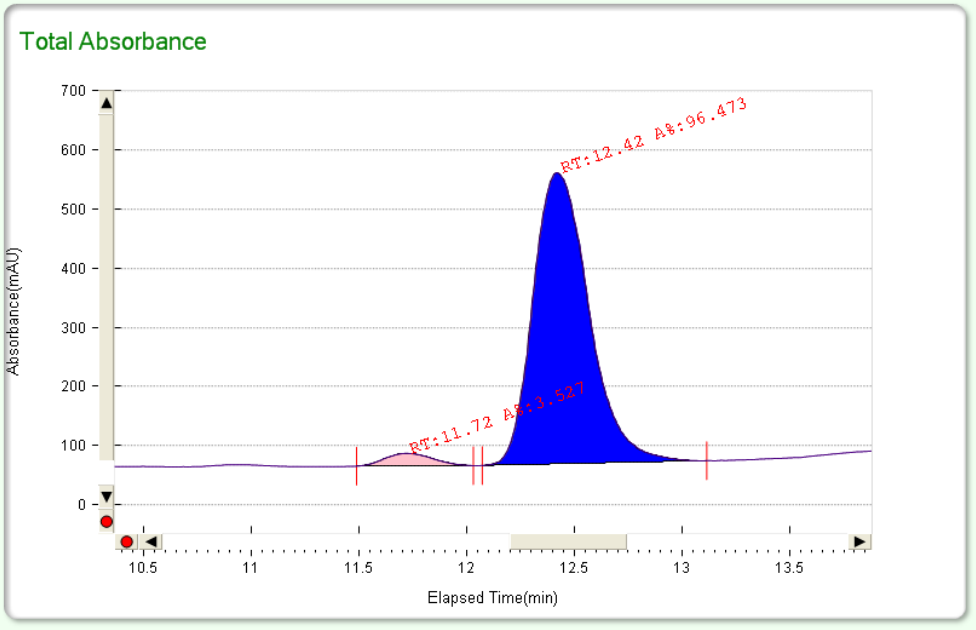


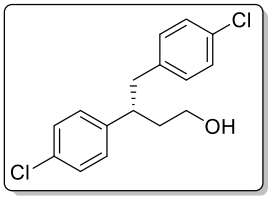




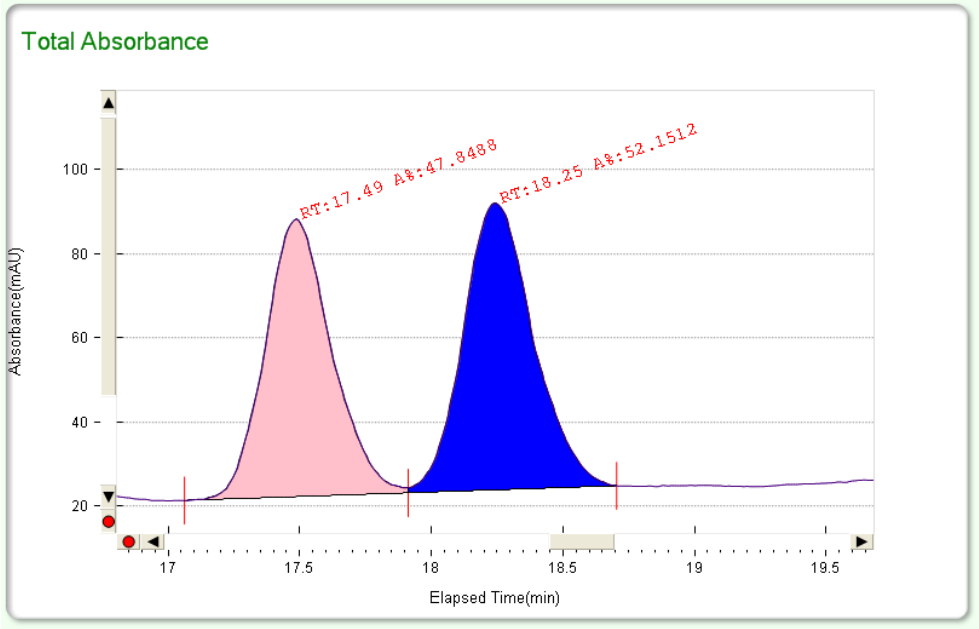
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-15:85-50:50 (30 min), 2mL/min, 160bar, t_1 = 11.7, t_2 = 12.4; er = 3.5:96.5.

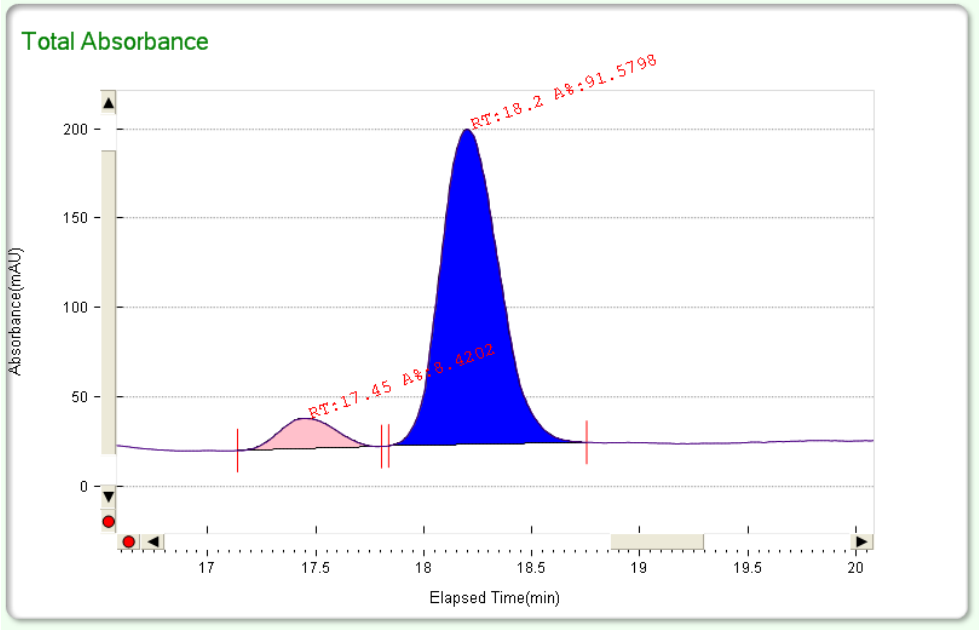


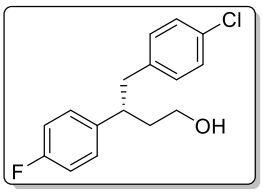




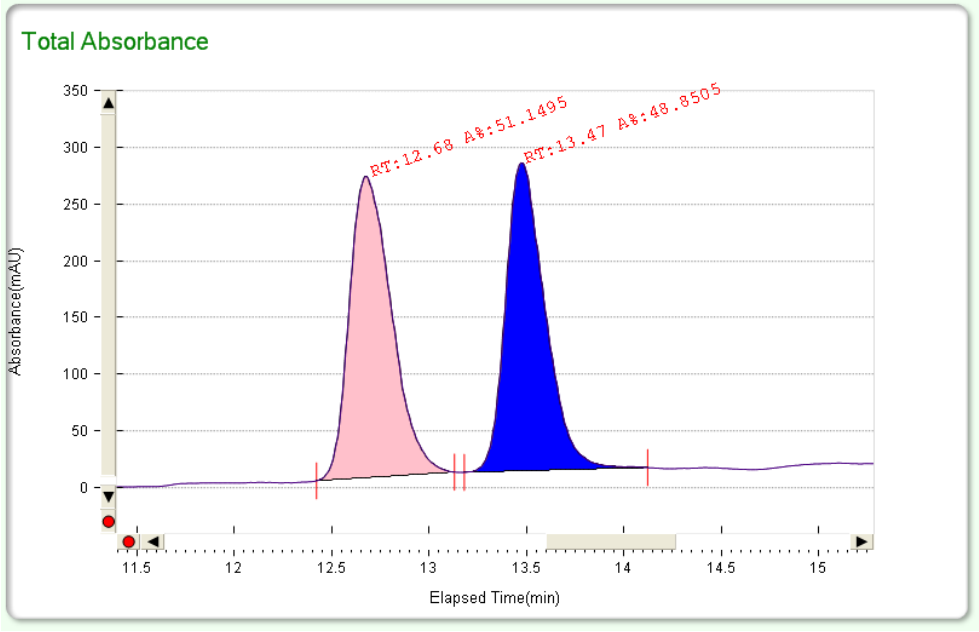
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-15:85 (20 min), 2mL/min, 160bar, t_1 = 17.4, t_2 = 18.2; er = 8.5:91.5.

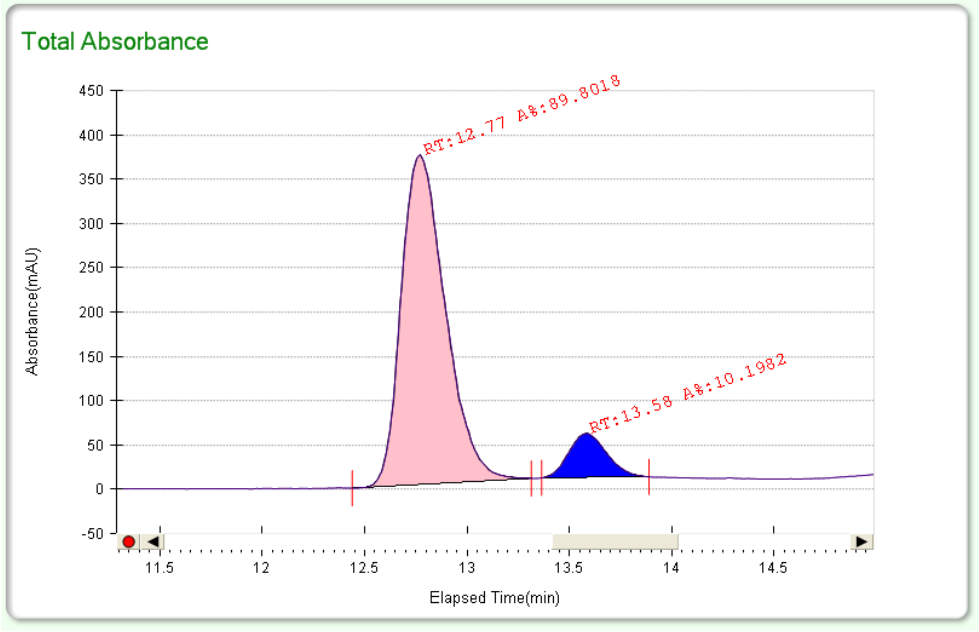


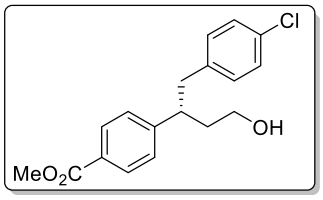




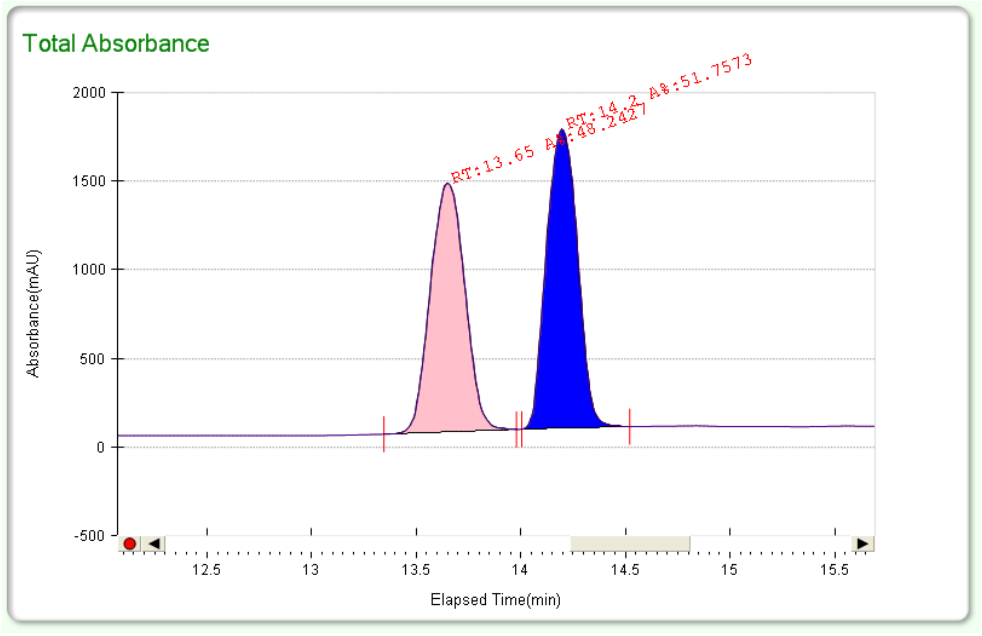
Separation of enantiomers by SFC. Chiralcel® Column AY-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-15:85 (20 min), 2mL/min, 160bar, t_1 = 12.8, t_2 = 13.6; er = 90:10.

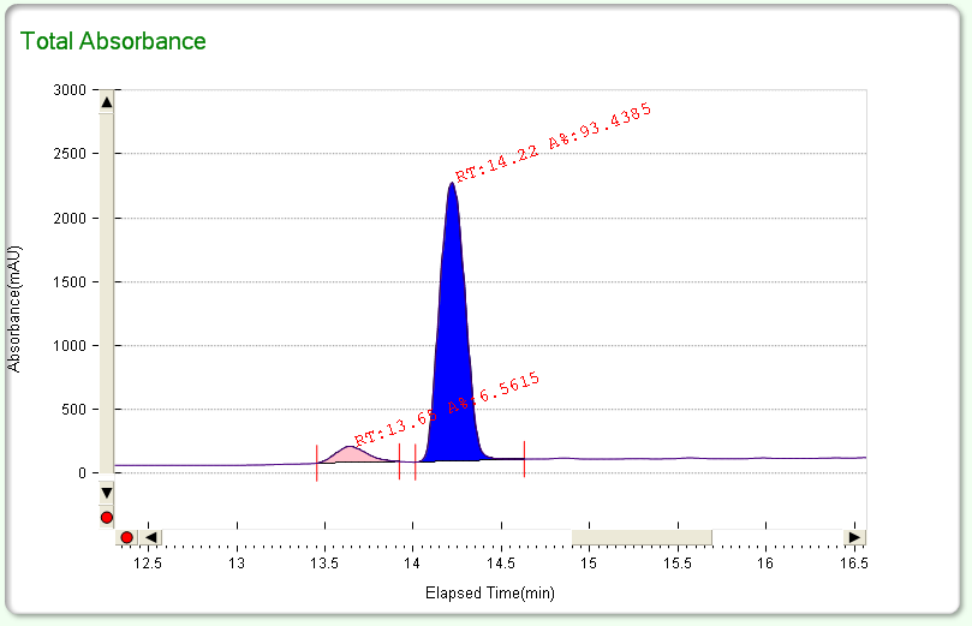


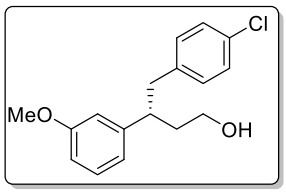




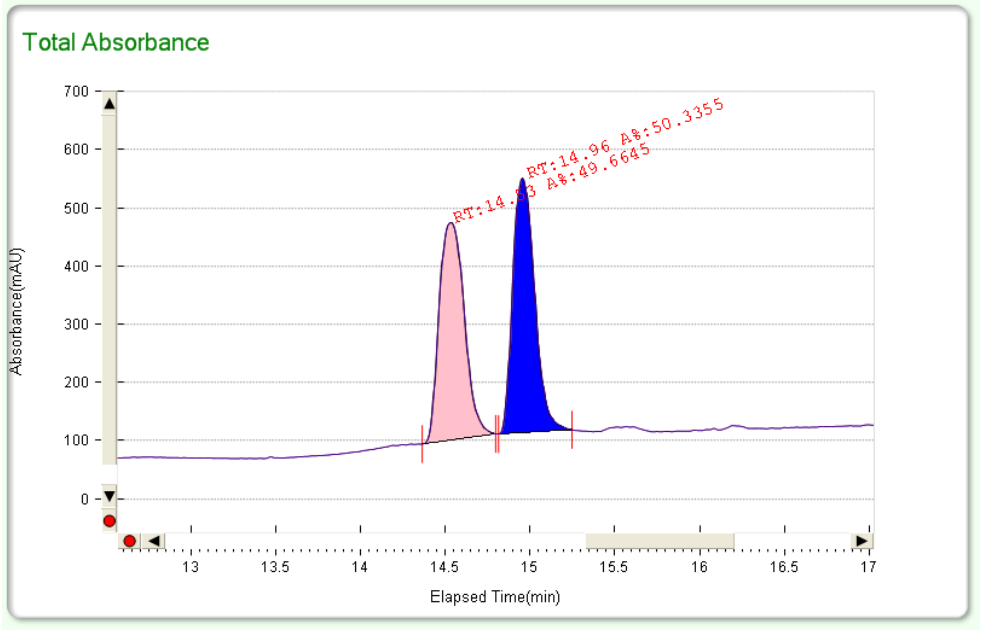
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-15:85-50:50 (30 min), 2mL/min, 160bar, t_1 = 13.6, t_2 = 14.2; er = 6.5:93.5.

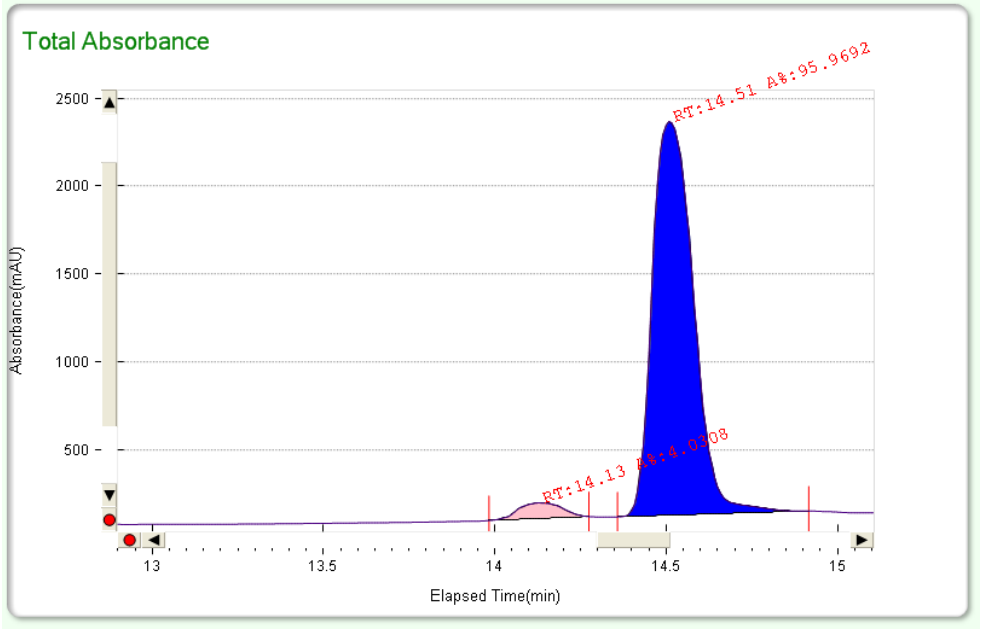


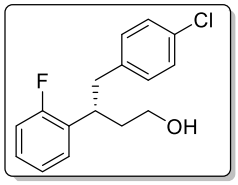




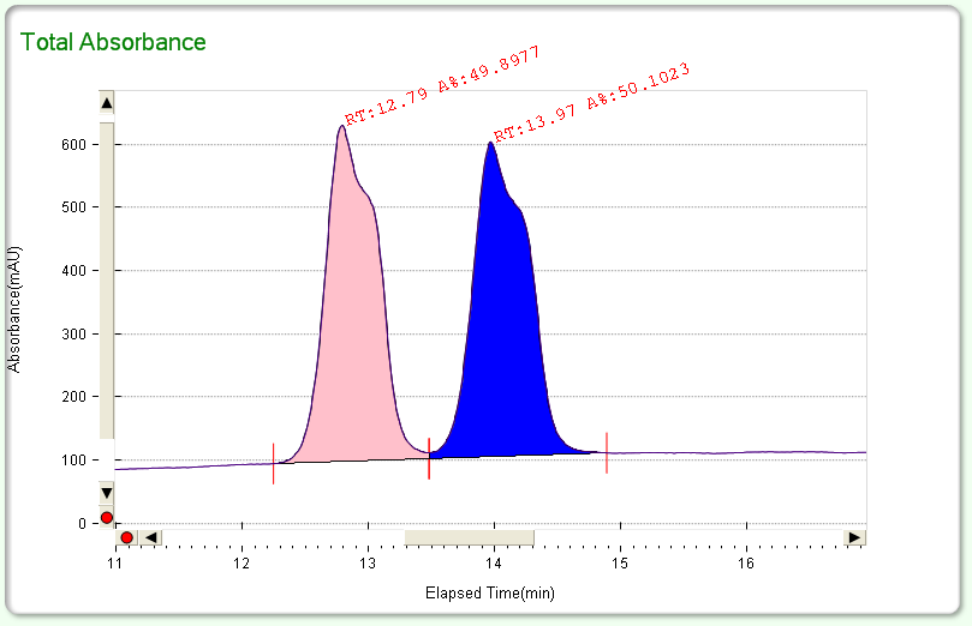
Separation of enantiomers by SFC. Chiralcel® Column AD-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-15:85-50:50 (30 min), 2mL/min, 160bar, t_1 = 14.1, t_2 = 14.5; er = 4:96.

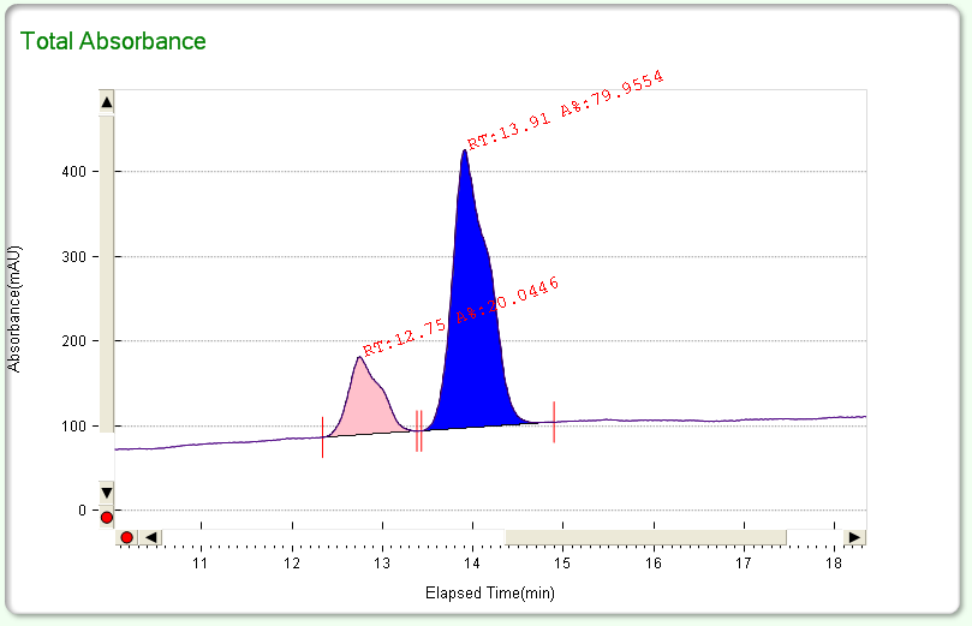


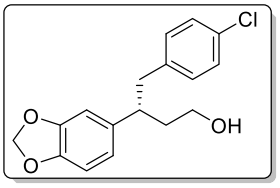




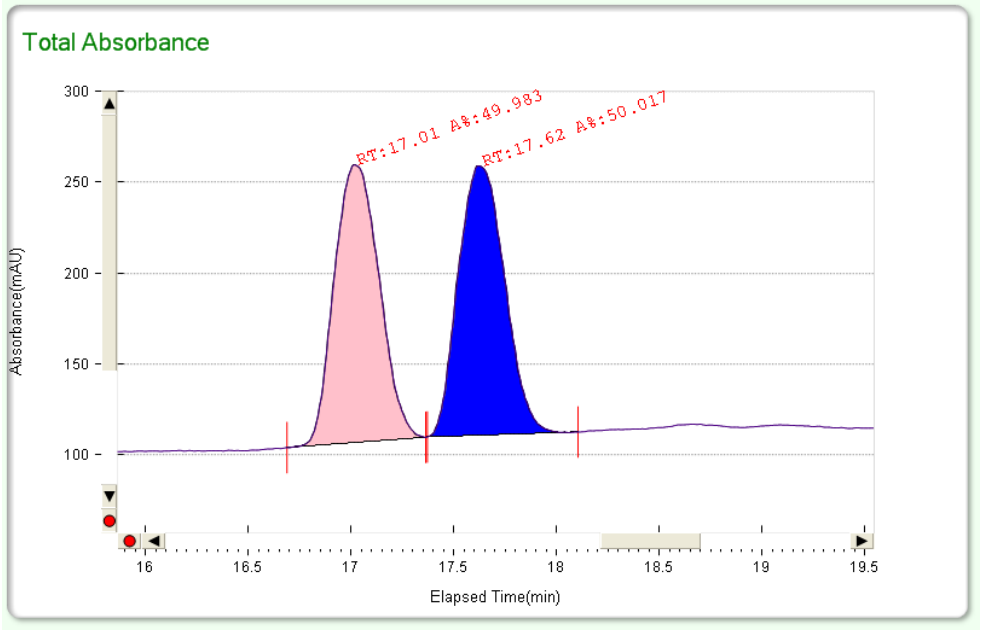
Separation of enantiomers by SFC. Chiralcel® Column OJ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 12.8, t_2 = 13.9; er = 20:80.

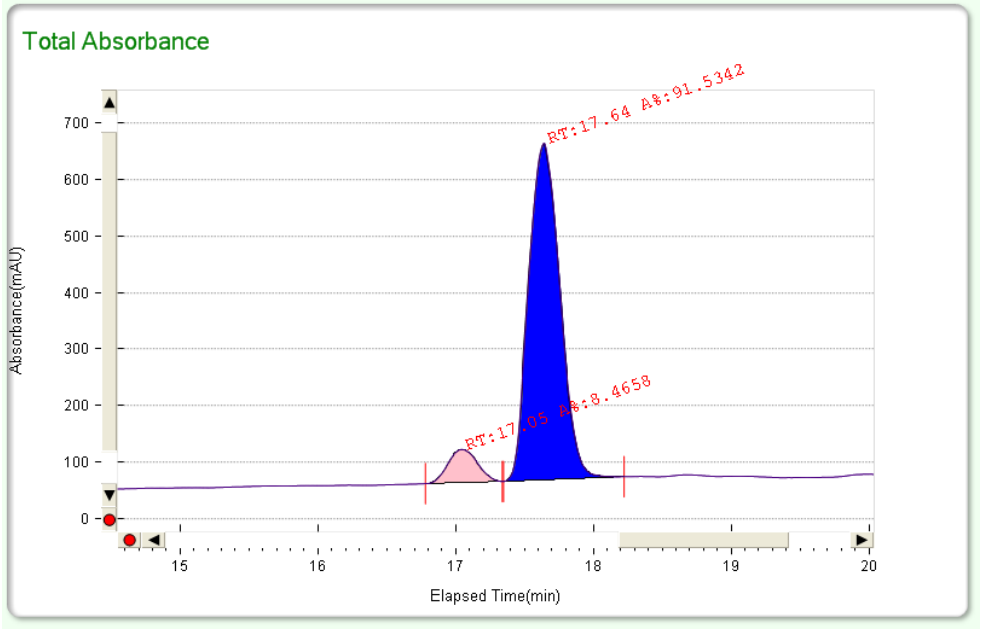


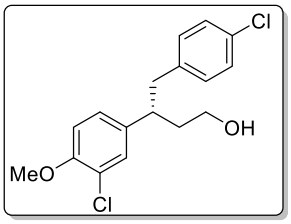




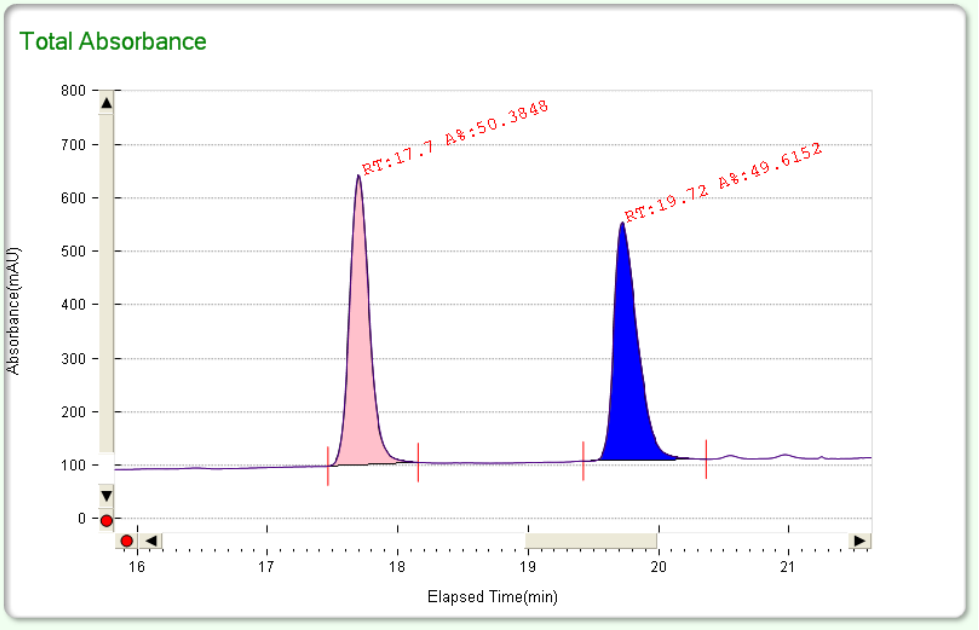
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 17.0, t_2 = 17.6; er = 8.5:91.5.

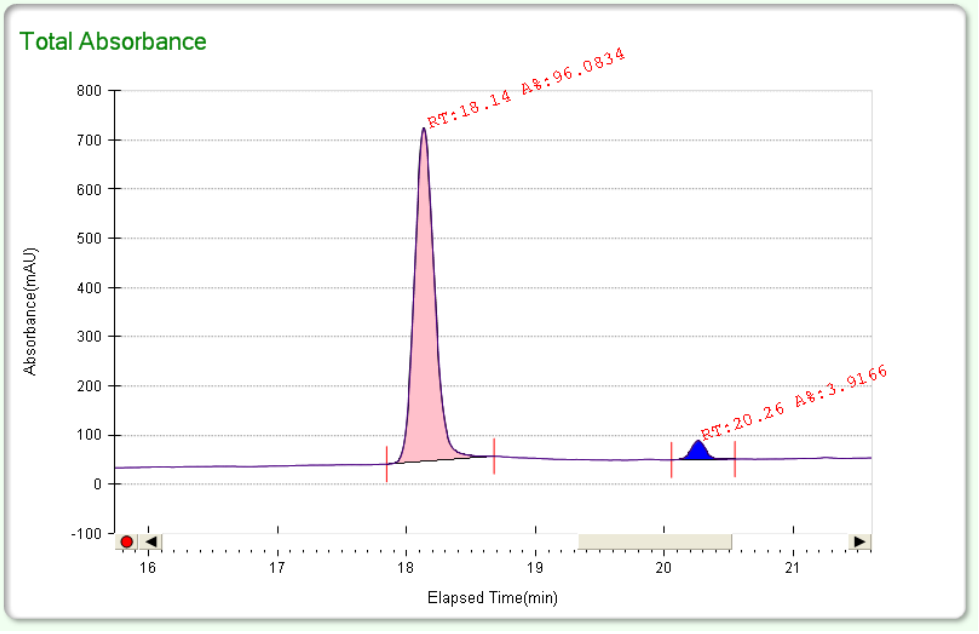


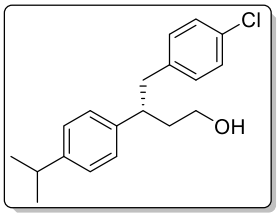




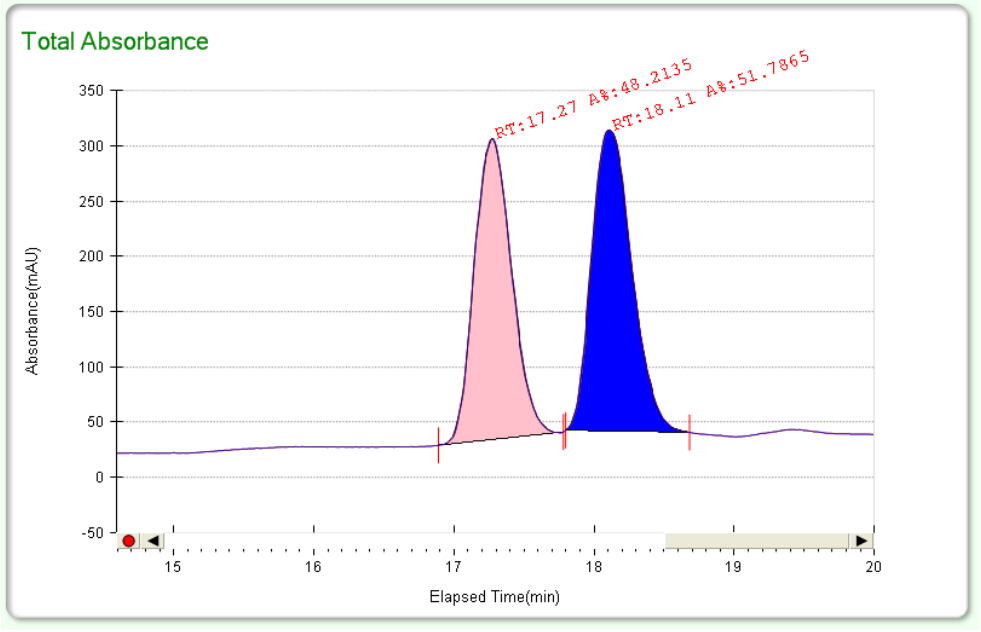
Separation of enantiomers by SFC. Chiralcel® Column AY-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-15:85-50:50 (30 min), 2mL/min, 160bar, t_1 = 18.1, t_2 = 20.3; er = 96:4.

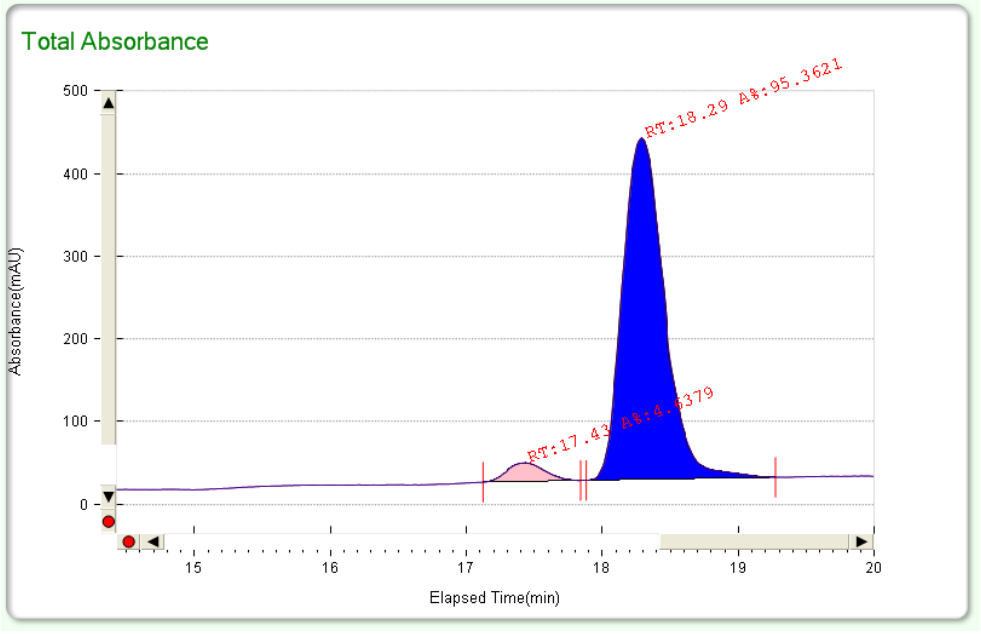


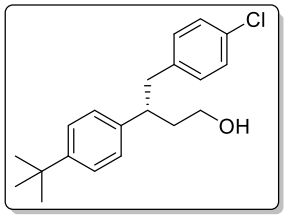




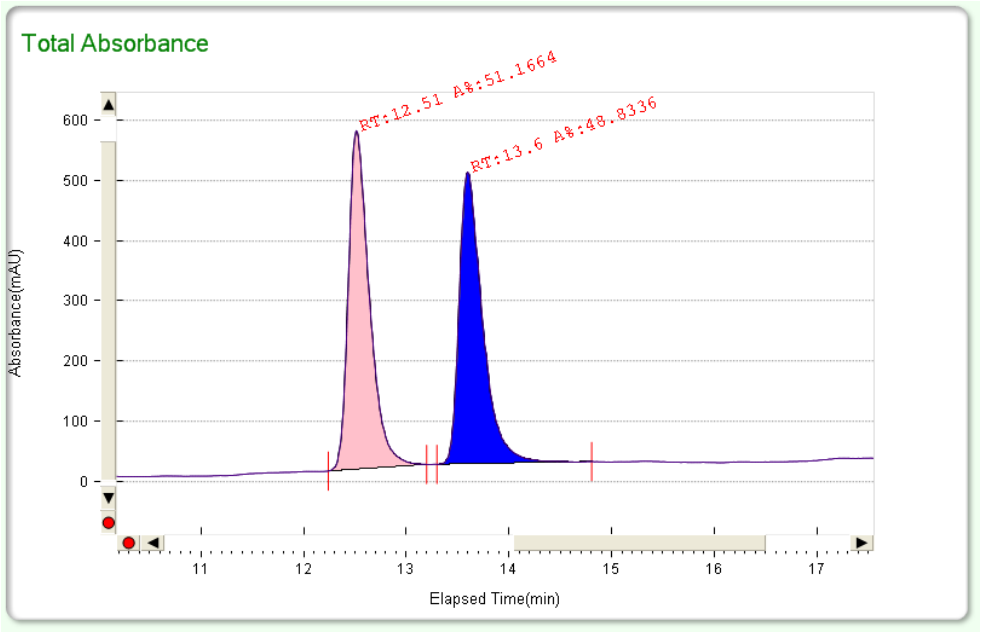
Separation of enantiomers by SFC. Chiralcel® Column OZ-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-15:85 (20 min), 2mL/min, 160bar, t_1 = 17.4, t_2 = 18.3; er = 5:95.

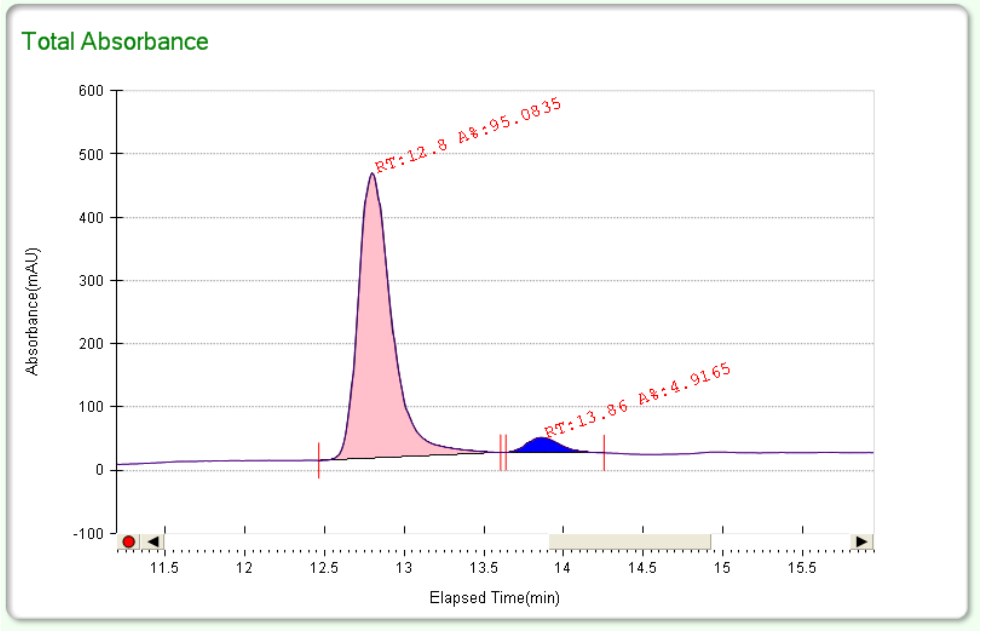


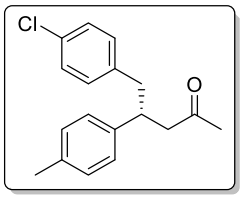




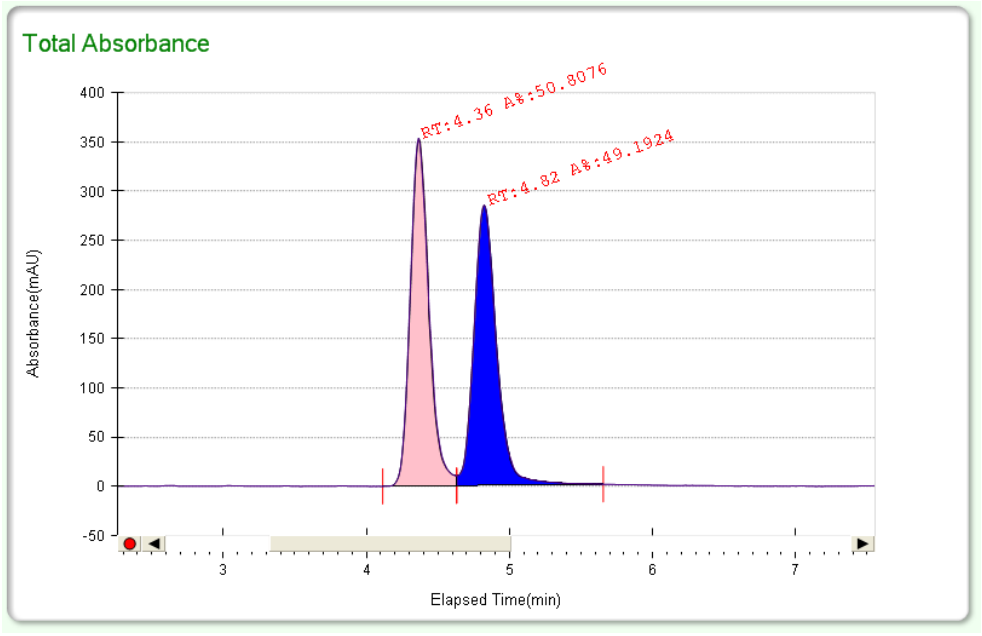
Separation of enantiomers by SFC. Chiralcel® Column AY-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-15:85 (20 min), 2mL/min, 160bar, t_1 = 12.8, t_2 = 13.9; er = 95:5.

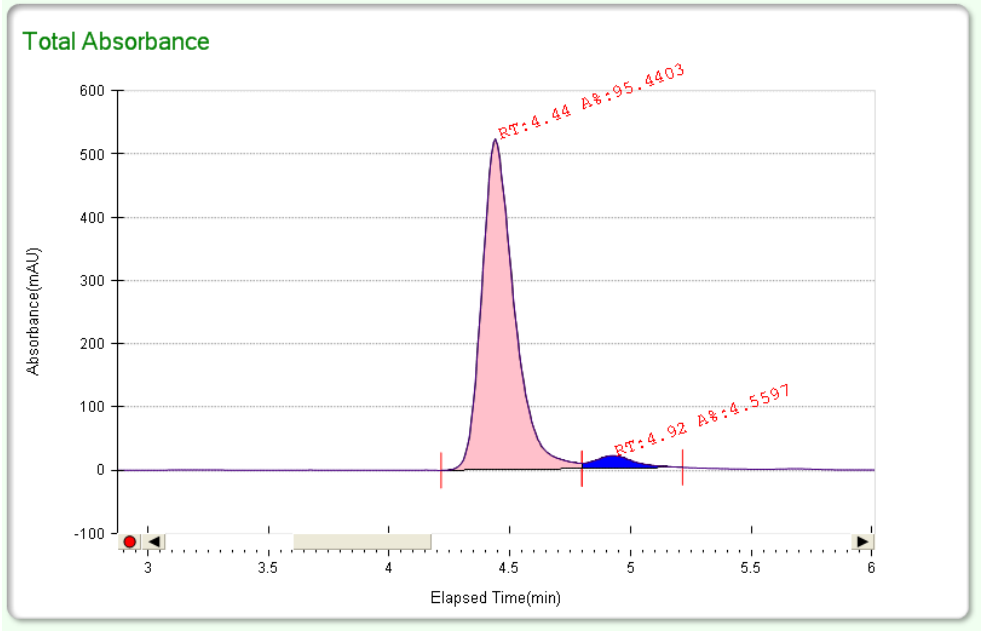


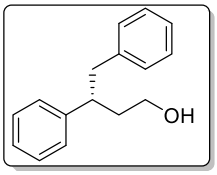




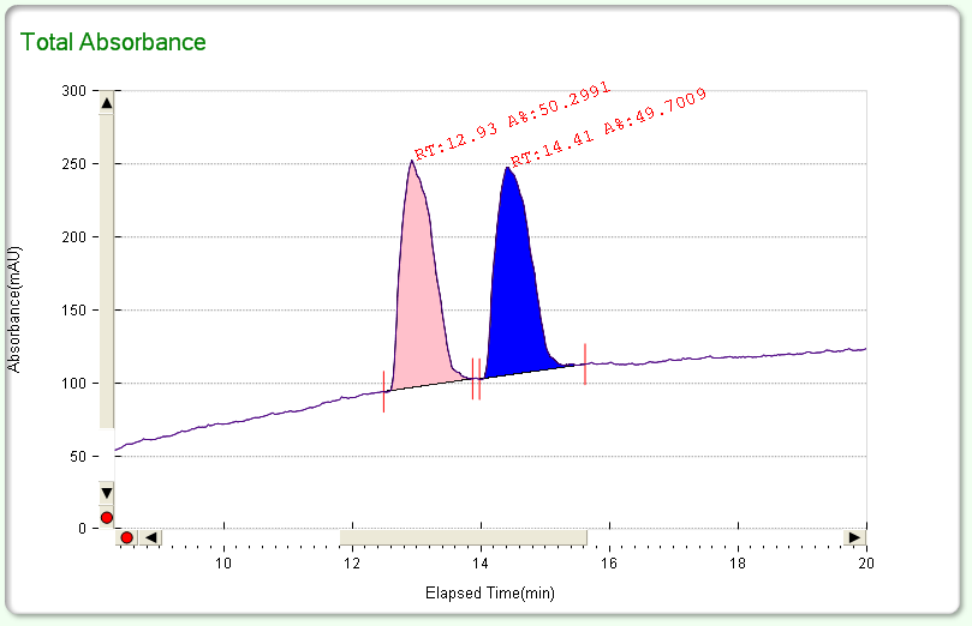
Separation of enantiomers by SFC. Chiralcel® Column AY-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95 (30 min), 3mL/min, 180bar, t_1 = 4.4, t_2 = 4.9; er = 95.5:4.5.

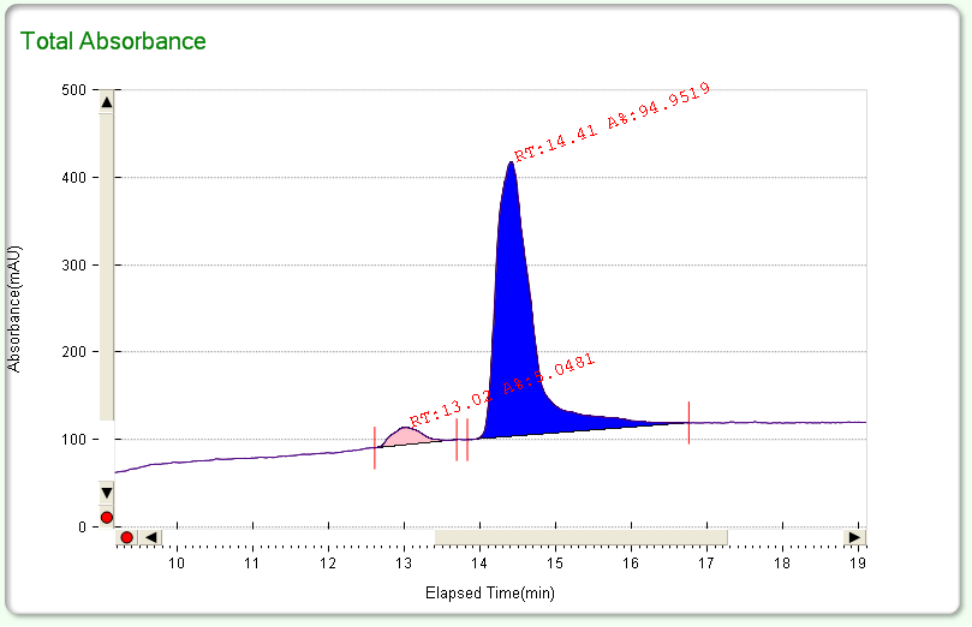


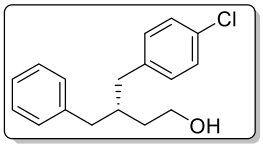




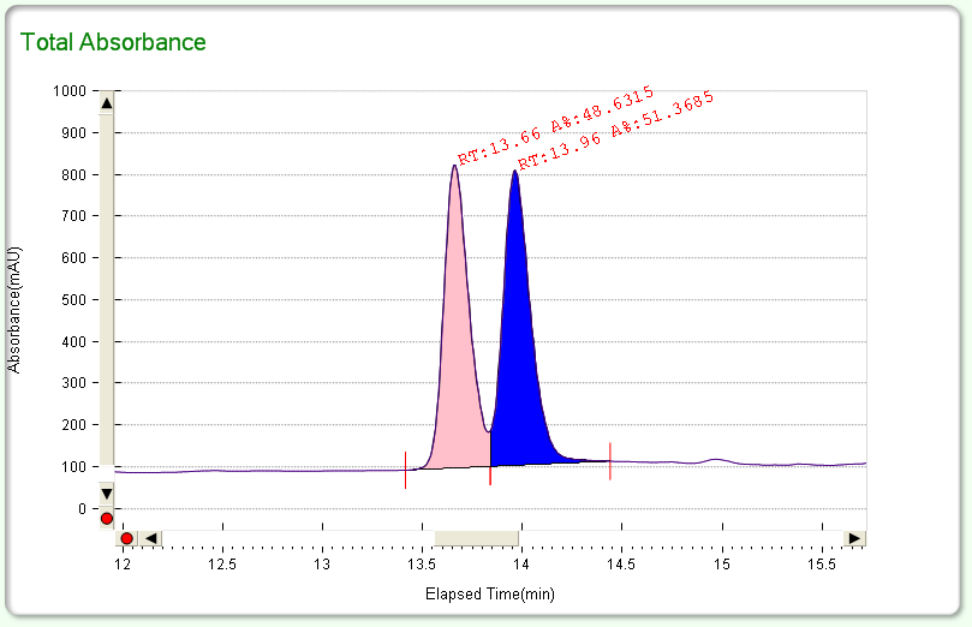
Separation of enantiomers by SFC. Chiralcel® Column OJ-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 13.0, t_2 = 14.4; er = 5:95.

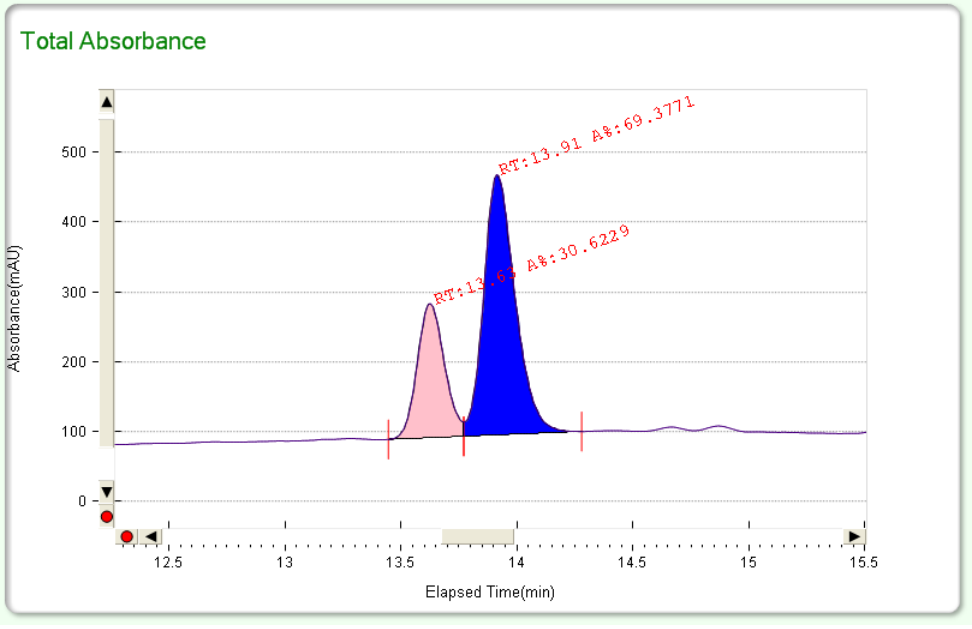


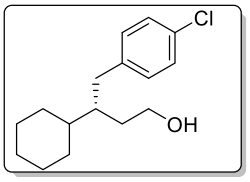




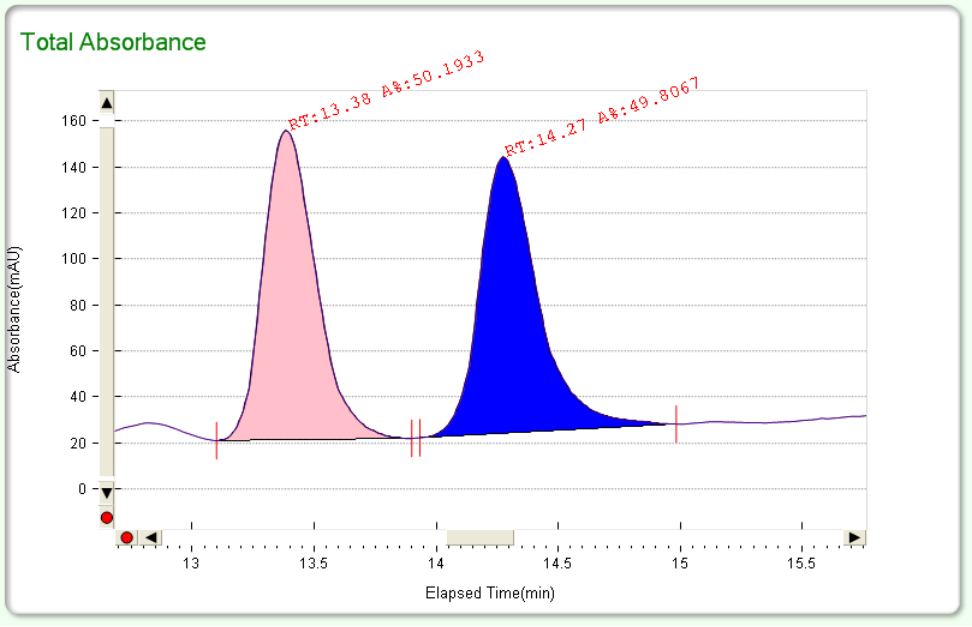
Separation of enantiomers by SFC. Chiralcel® Column AY-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 13.6, t_2 = 13.9; er = 30.5:69.5.

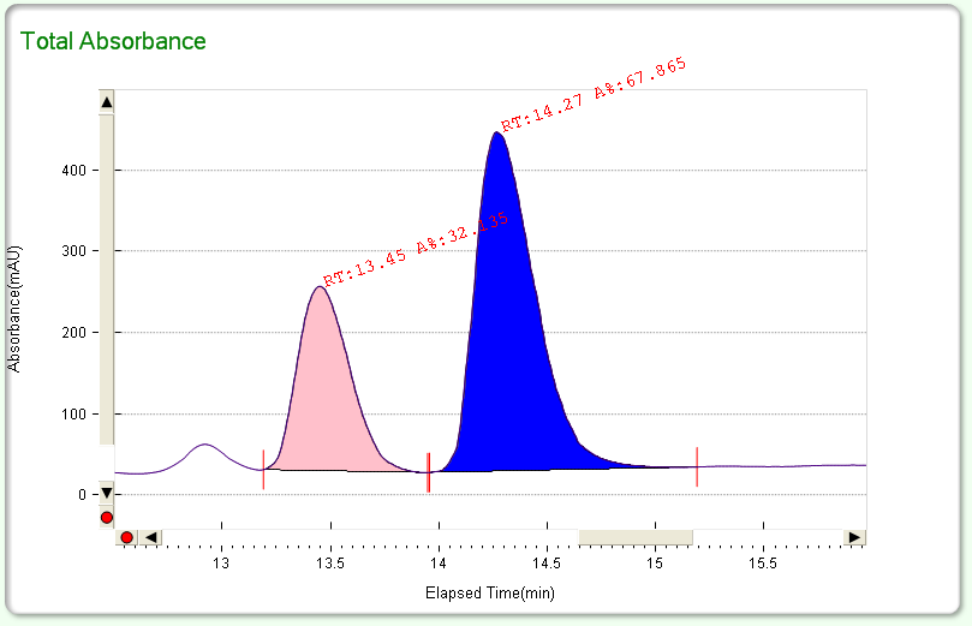


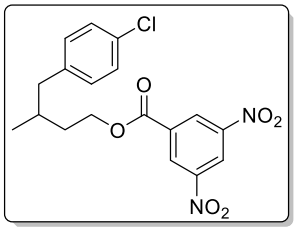




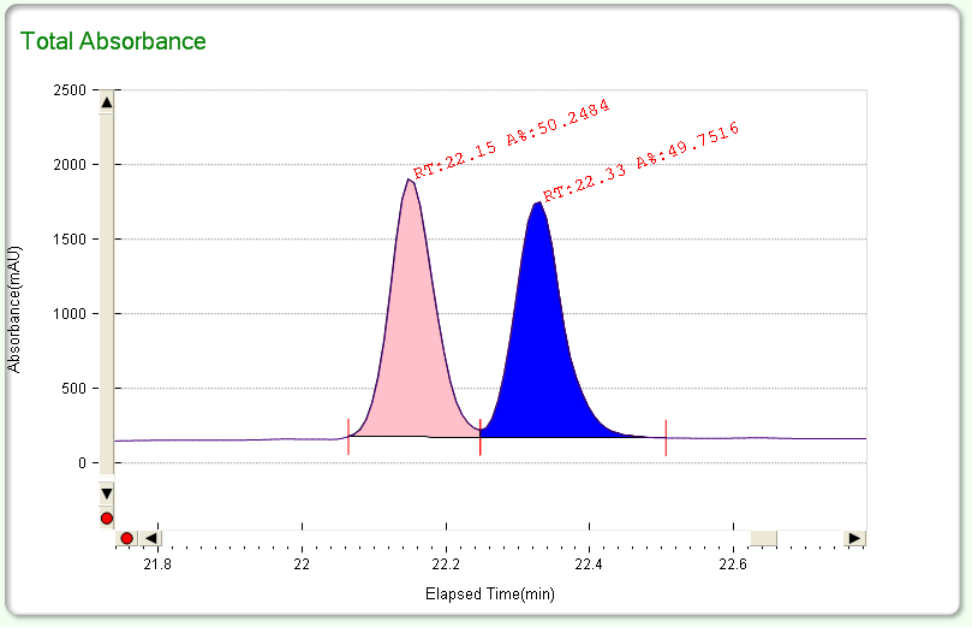
Separation of enantiomers by SFC. Chiralcel® Column AS-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-15:85 (20 min), 2mL/min, 160bar, t_1 = 13.4, t_2 = 14.3; er = 32.5:67.5.

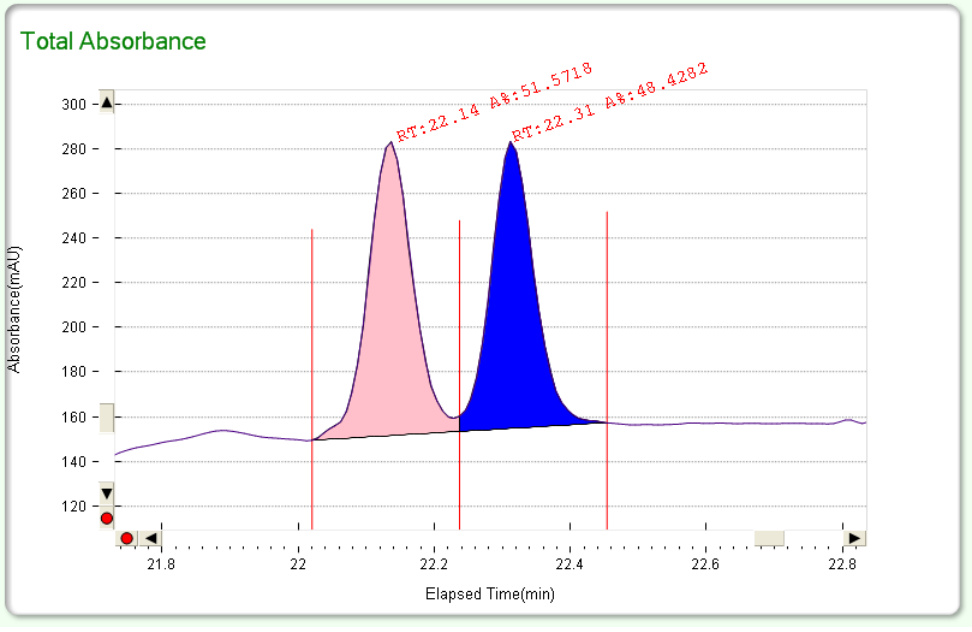


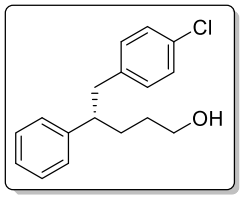




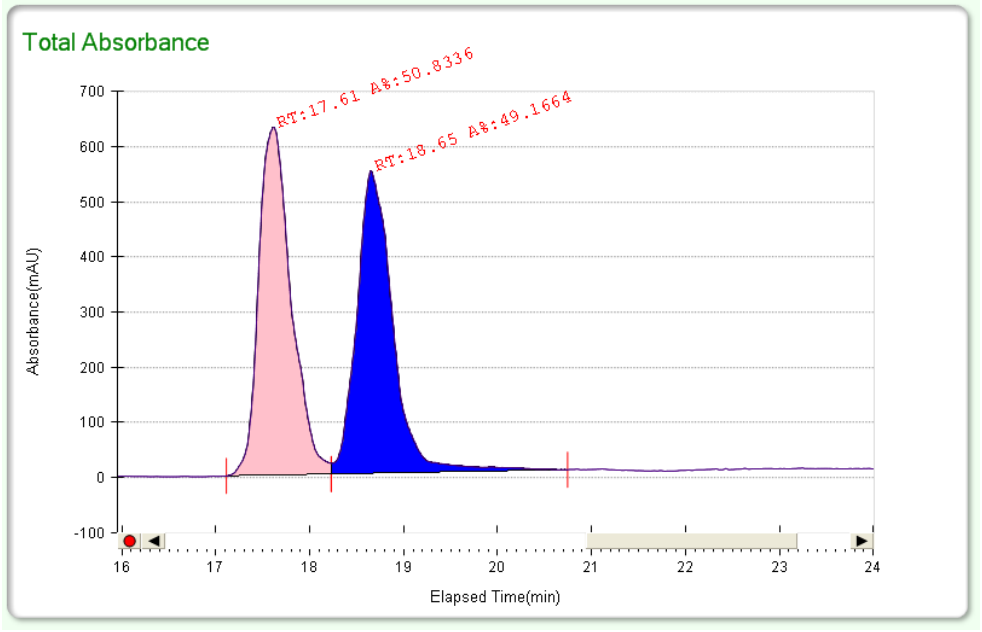
Separation of enantiomers by SFC. Chiralcel® Column AY-H, 40 °C, ^{i}-PrOH: CO_2 = 2:98-20:80 (20 min), 2mL/min, 160bar, t_1 = 22.1, t_2 = 22.3; er = 51.5:48.5.

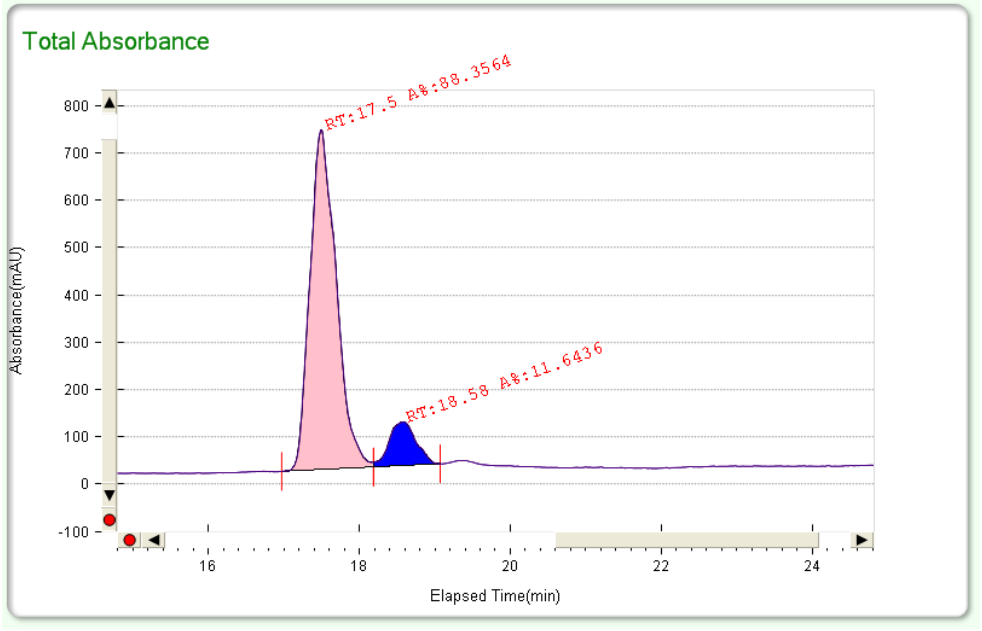


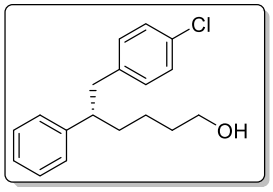




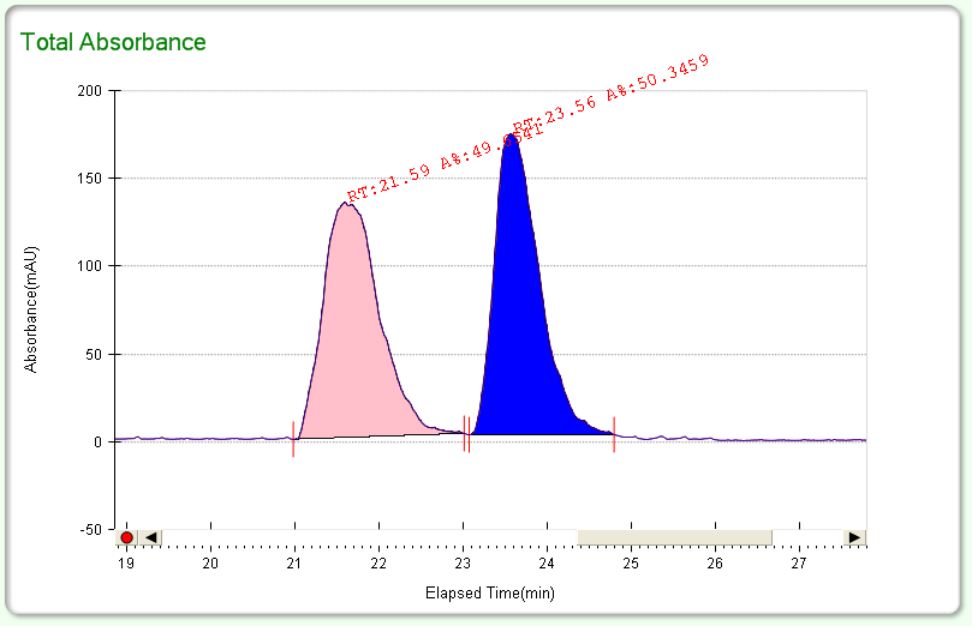
Separation of enantiomers by SFC. Chiralcel® Column AY-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-20:80-50:50 (50 min), 2mL/min, 160bar, t_1 = 17.5, t_2 = 18.6; er = 88.5:11.5.

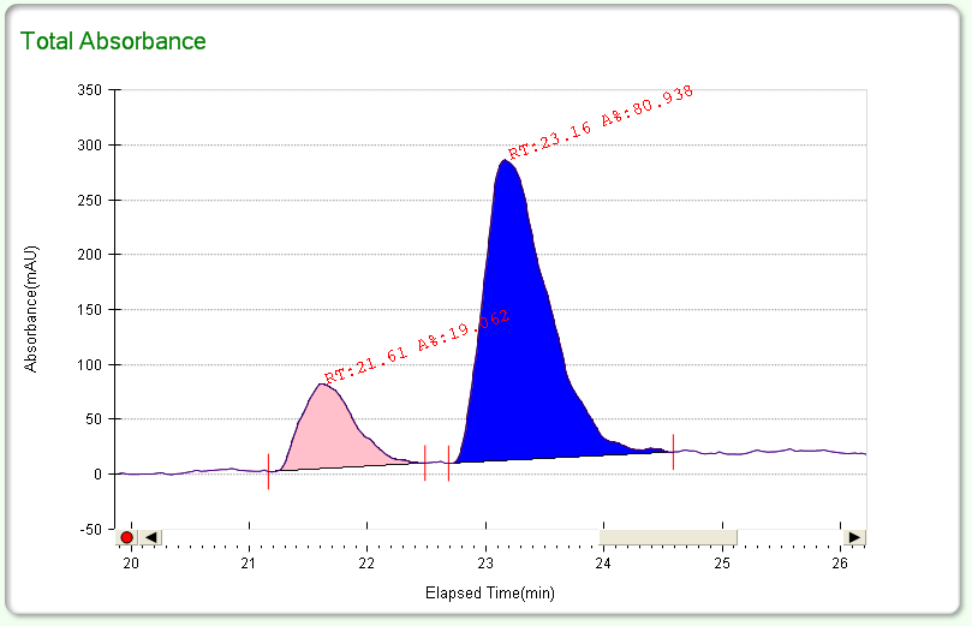


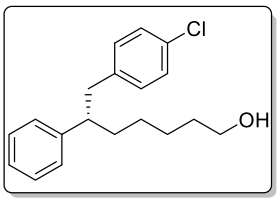




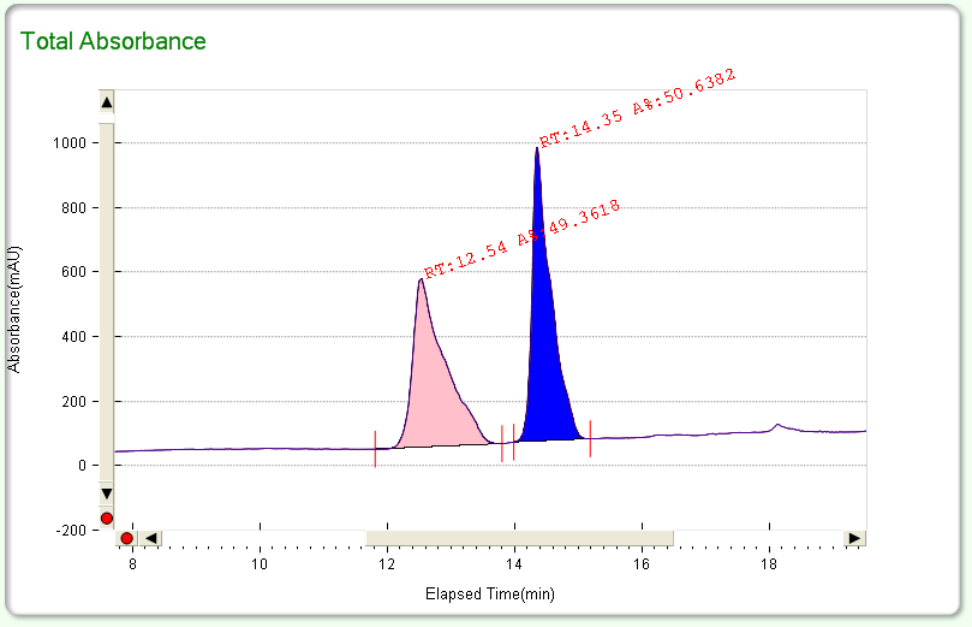
Separation of enantiomers by SFC. Chiralcel® Column OJ-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-10:90-15:85 (20 min), 2mL/min, 160bar, t_1 = 21.6, t_2 = 23.6; er = 19:81.

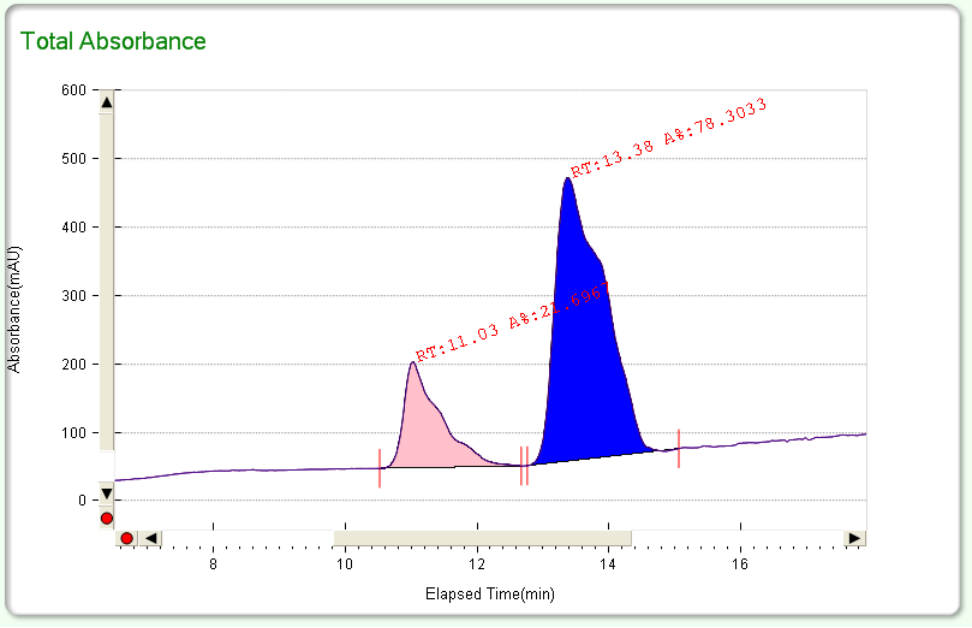


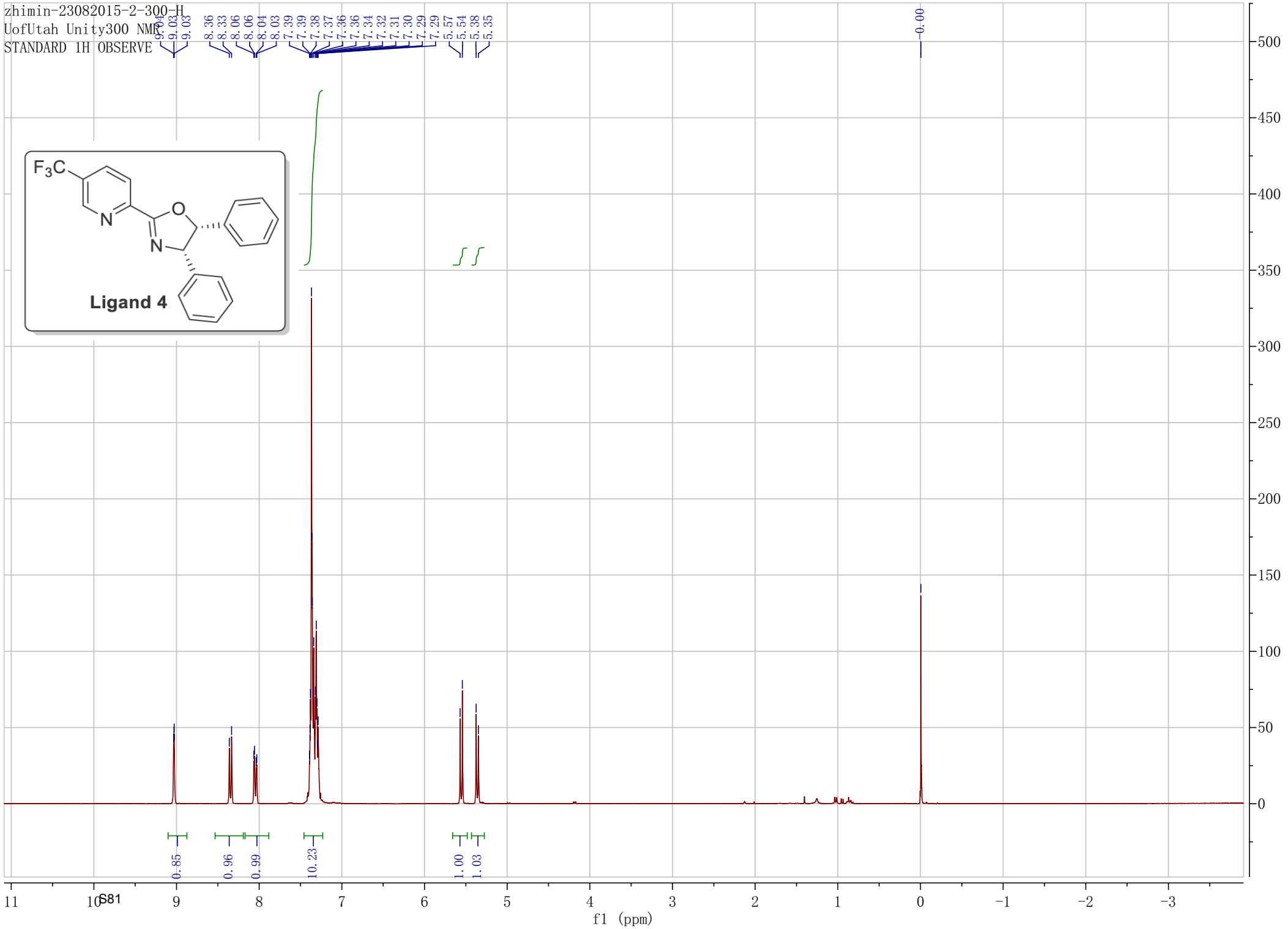


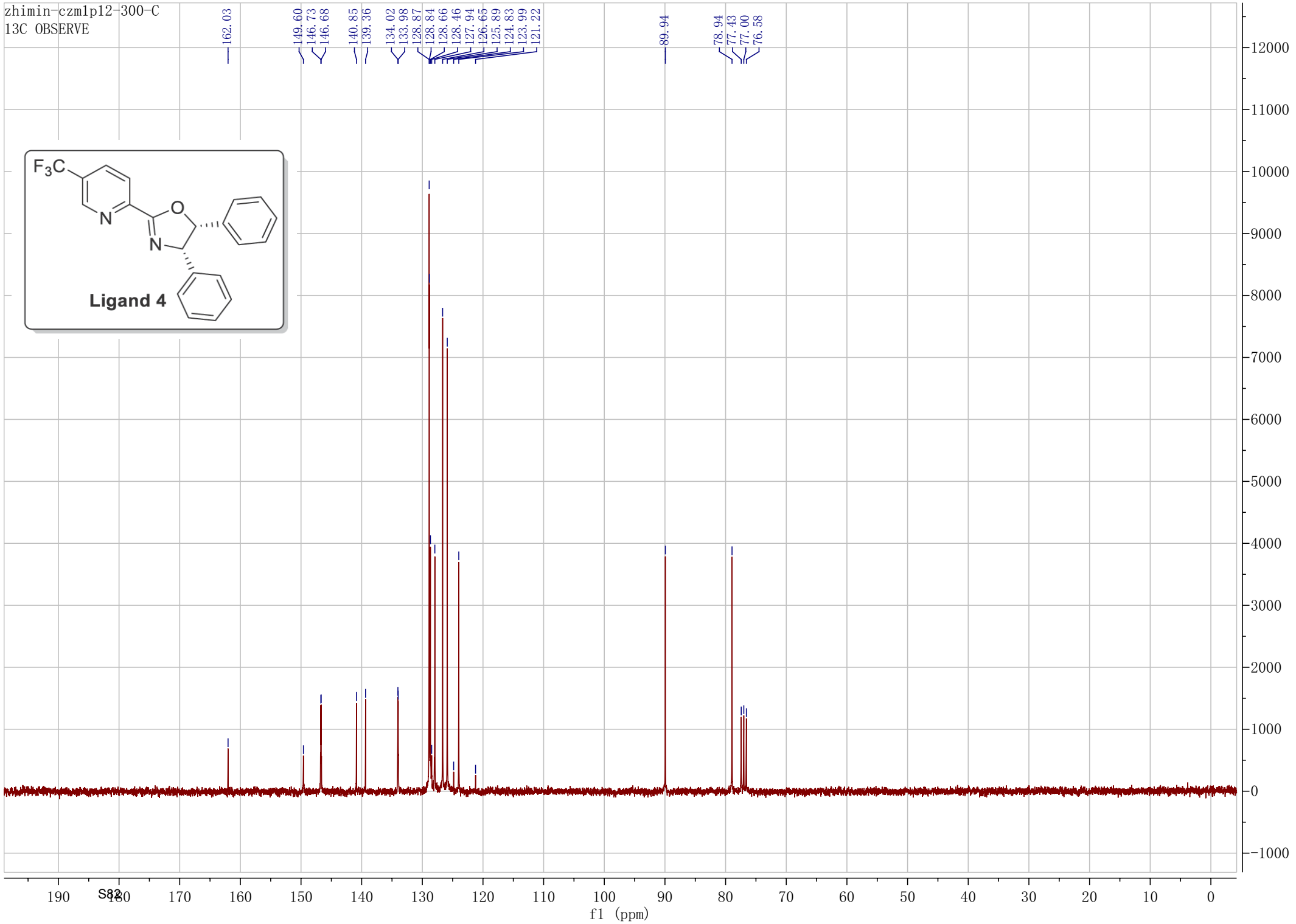


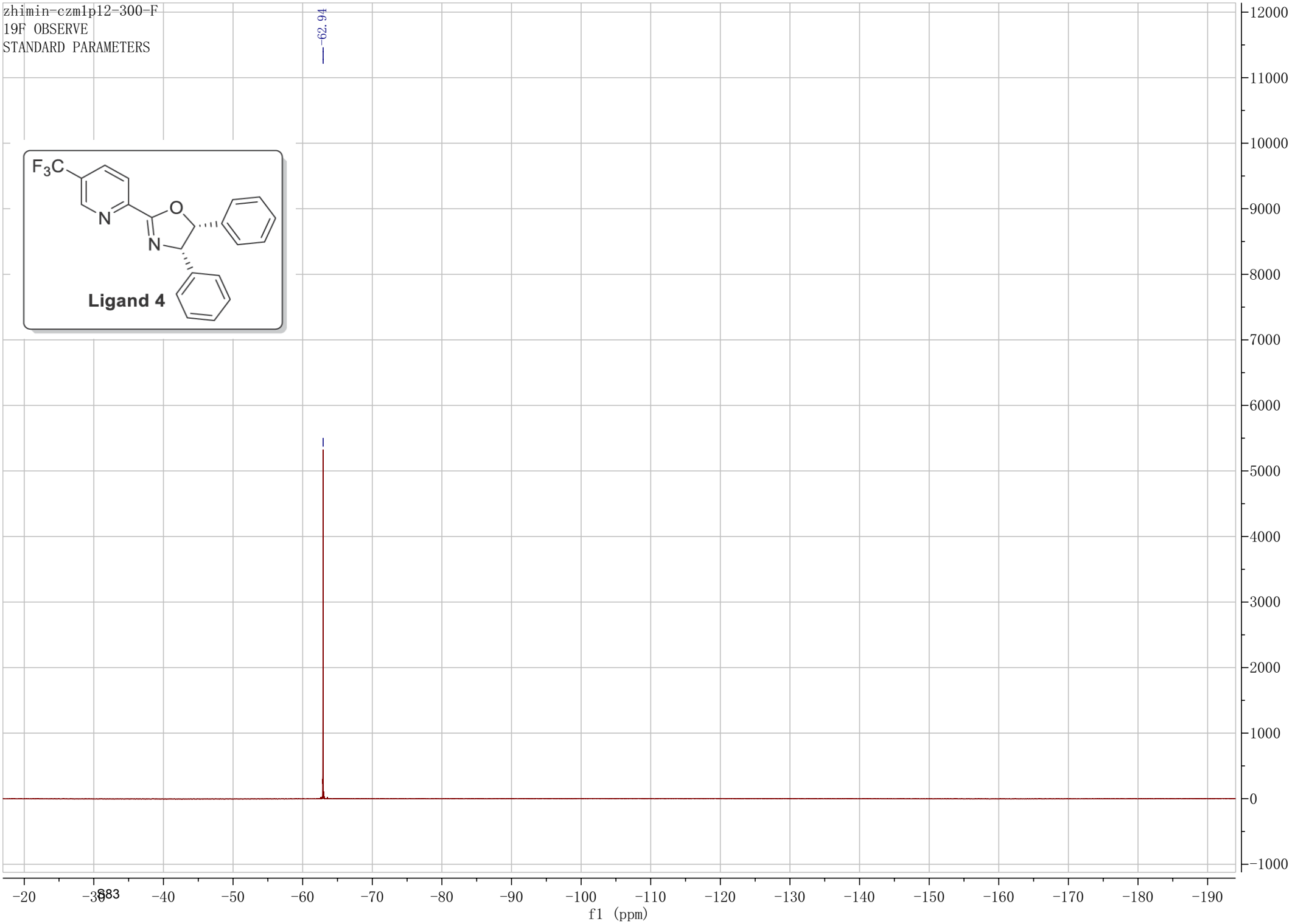
Separation of enantiomers by SFC. Chiralcel® Column OJ-H, 40 °C, ^{i}-PrOH: CO_2 = 5:95-15:85-50:50 (30 min), 2mL/min, 160bar, t_1 = 11.0, t_2 = 13.4; er = 22:78.

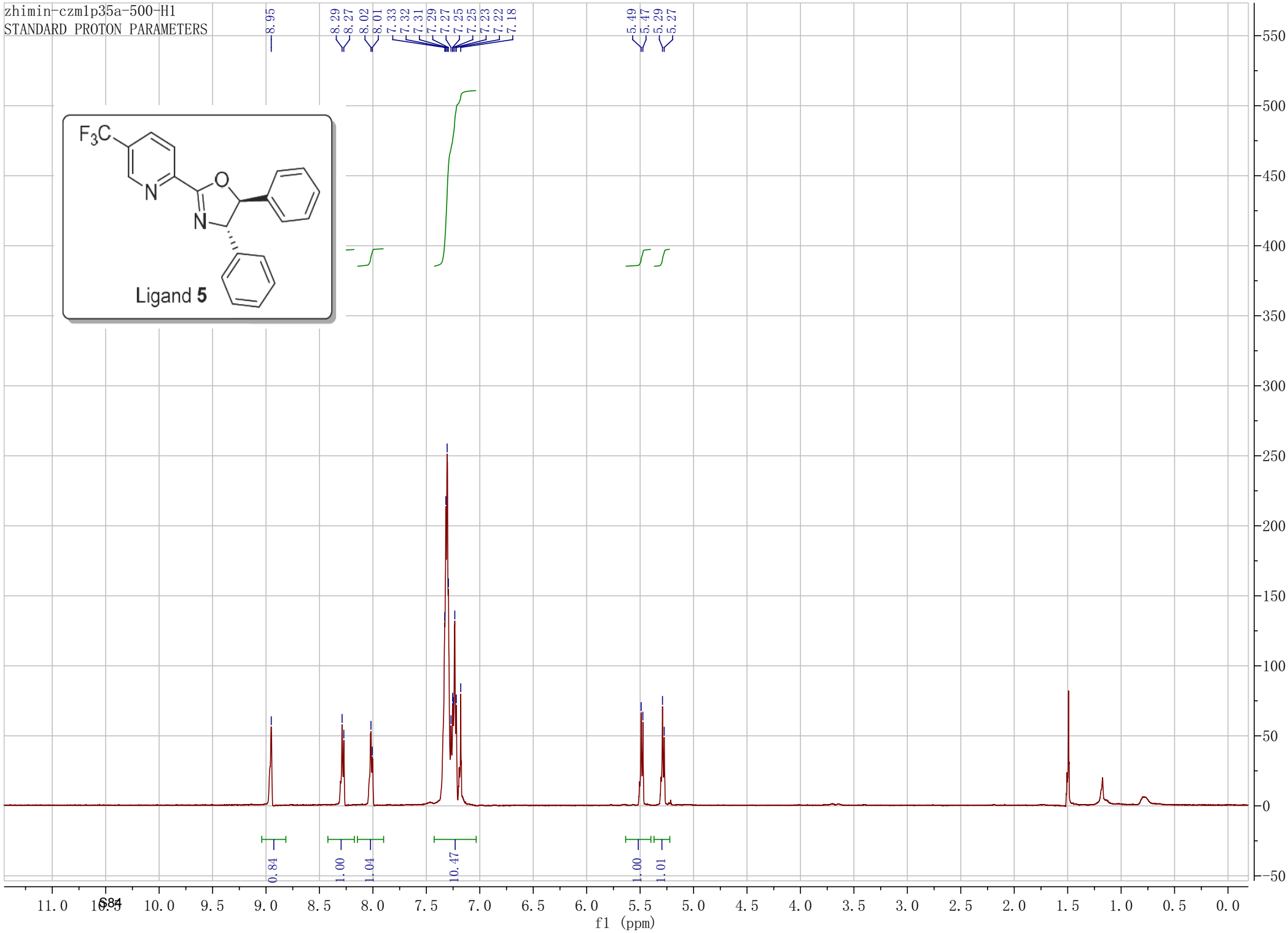


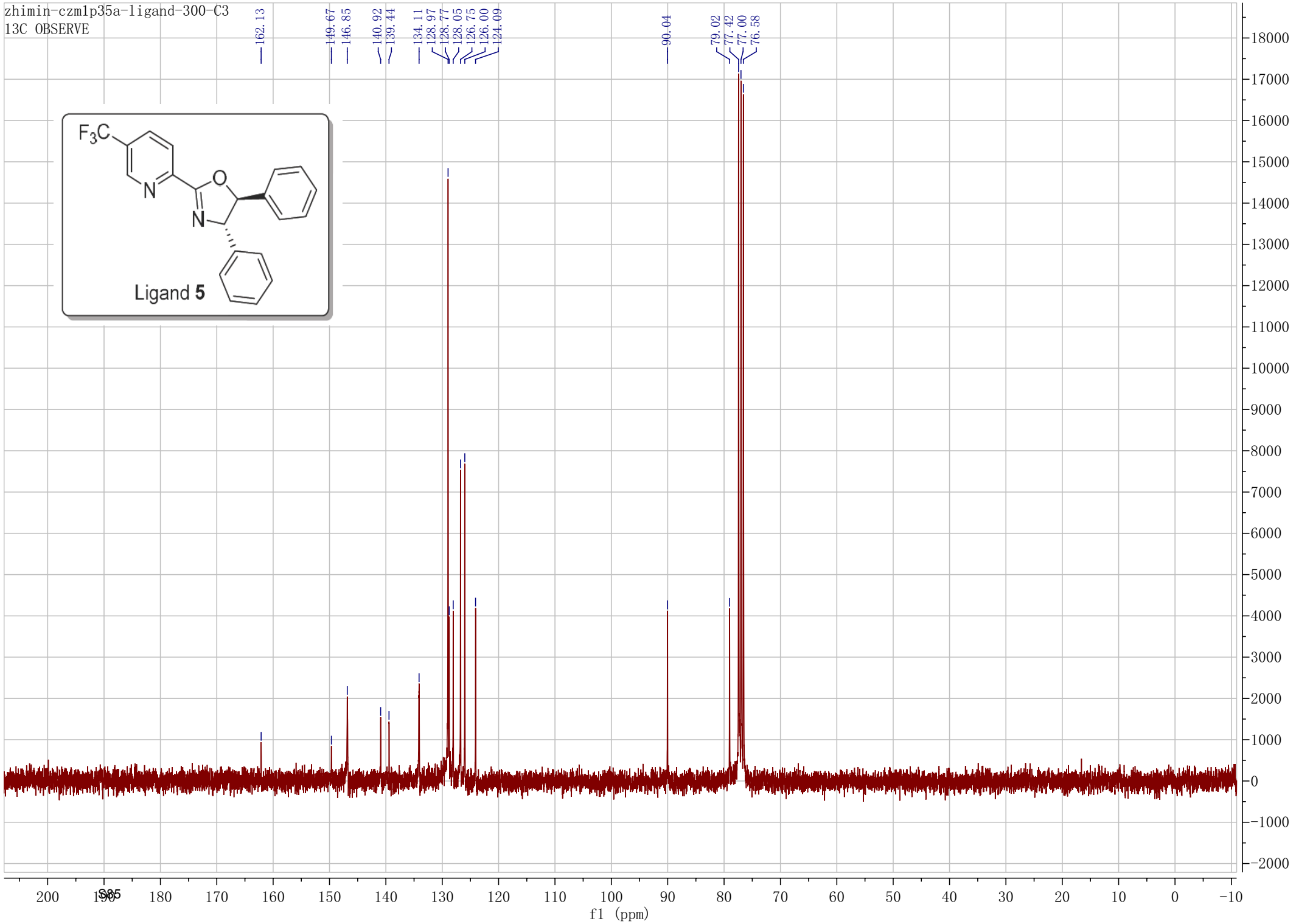


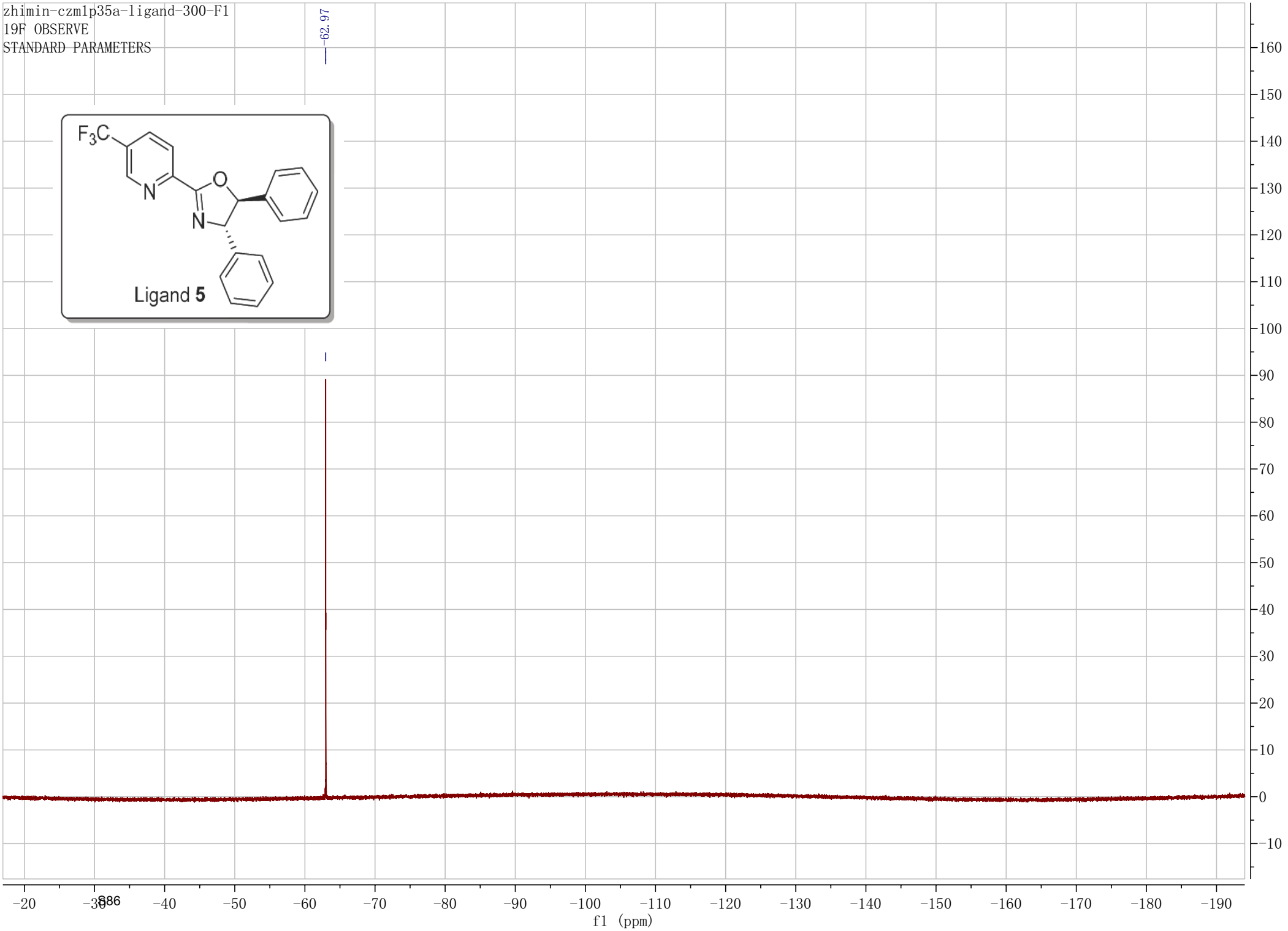

zhimin-23082015-2-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
9.04
9.03
9.03
8.36
8.33
8.06
8.06
8.04
8.03
7.39
7.39
7.38
7.37
7.36
7.36
7.34
7.32
7.31
7.30
7.29
7.29
5.57
5.54
5.38
5.35
0.00
F3C
N
O
N
Ligand 4
0.85
0.96
0.99
10.23
1.00
1.03
f1 (ppm)

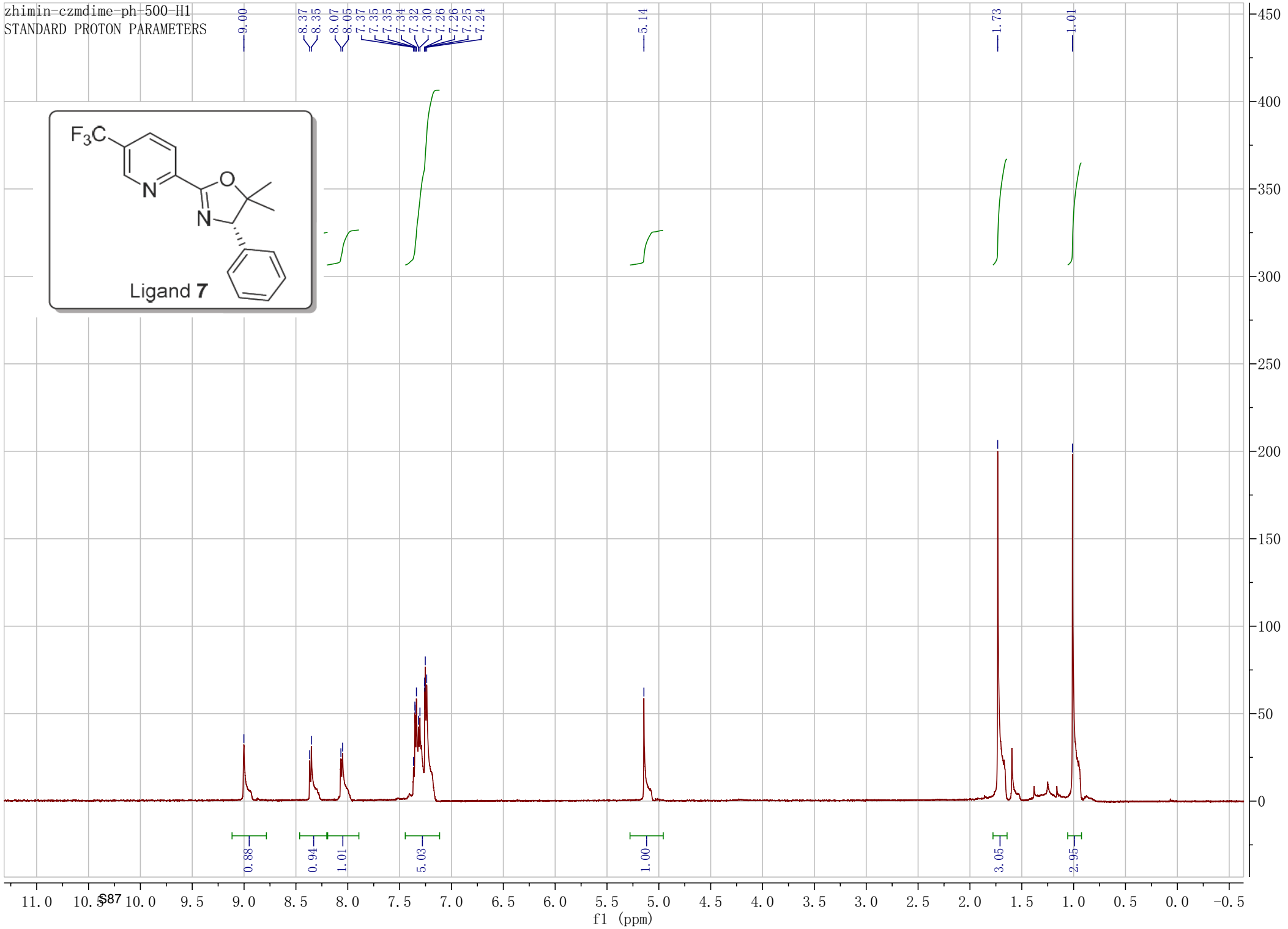

zhimin-czm1p12-300-C
13C OBSERVE
162.03
149.60
146.73
146.68
140.85
139.36
134.02
133.98
128.87
128.84
128.66
128.46
127.94
126.65
125.89
124.83
123.99
121.22
89.94
78.94
77.43
77.00
76.58
F3C
N
O
N
Ligand 4
f1 (ppm)

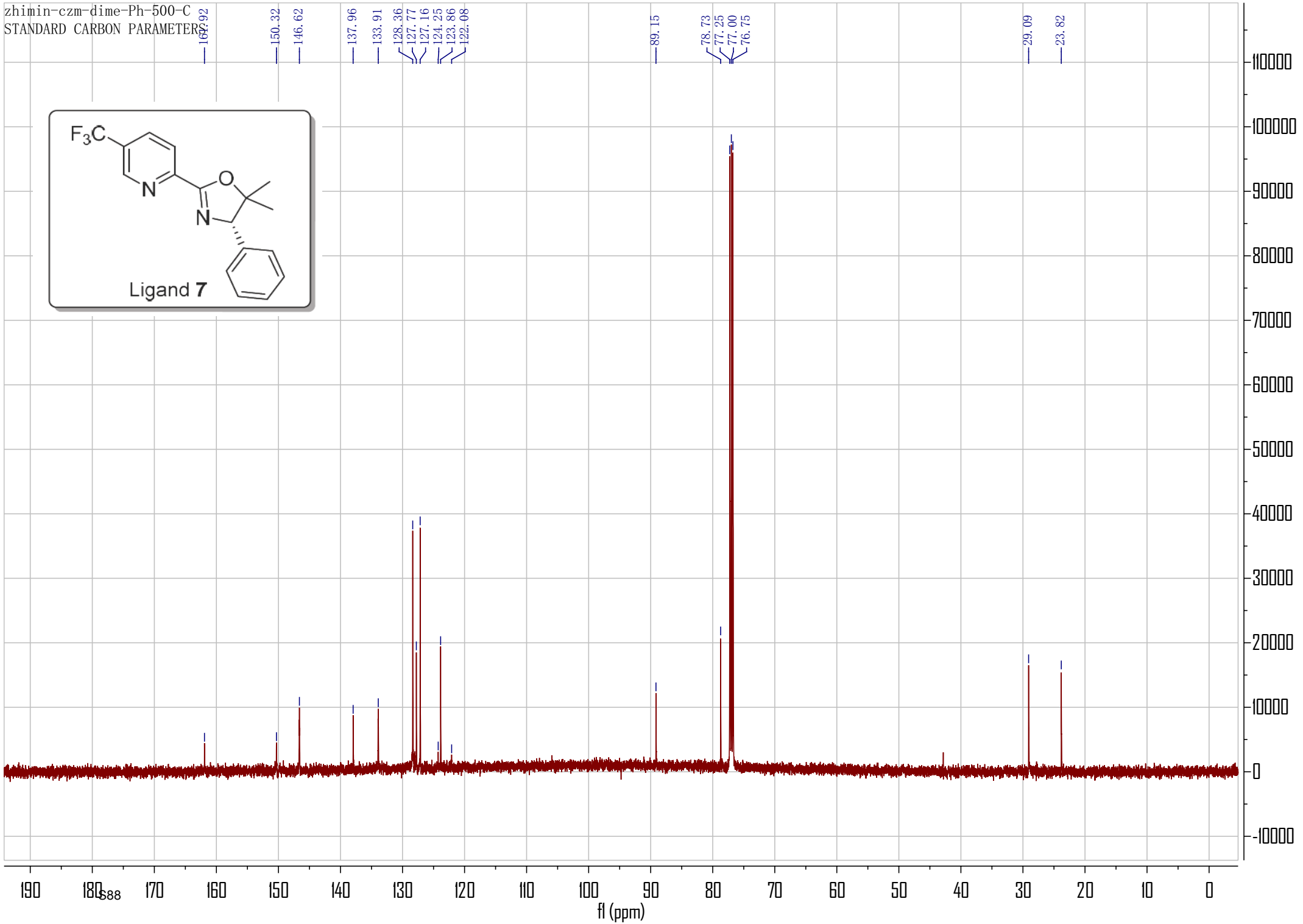

zhimin-czm1p12-300-F
19F OBSERVE
STANDARD PARAMETERS
-62.94
F3C
N
O
N
Ligand 4
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

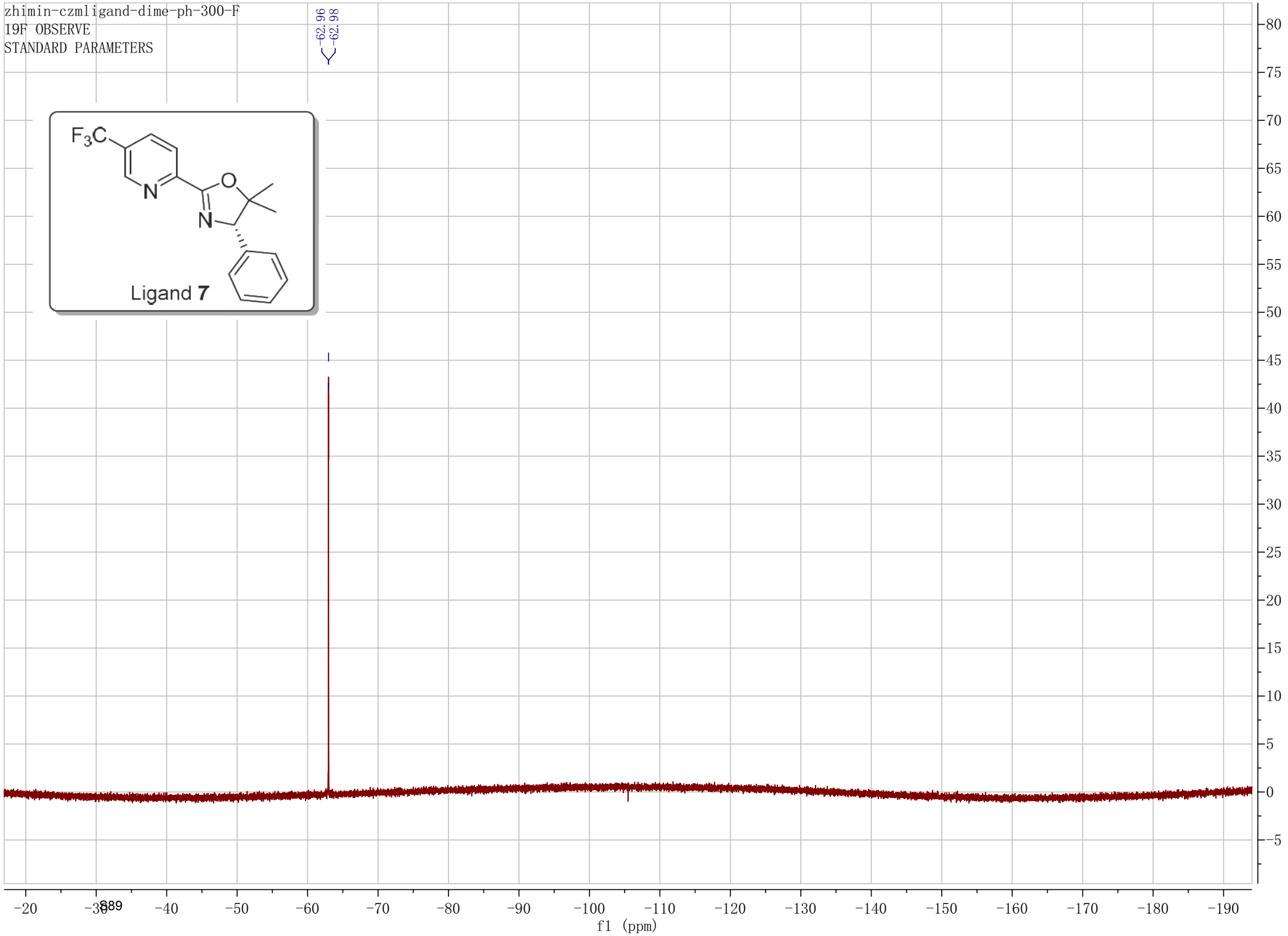

zhimin-czm1p35a-500-H1
STANDARD PROTON PARAMETERS
8.95
8.29
8.27
8.02
8.01
7.33
7.32
7.31
7.29
7.27
7.25
7.25
7.23
7.22
7.18
5.49
5.47
5.29
5.27
F3C
N
O
N
Ligand 5
0.84
1.00
1.04
10.47
1.00
1.01
f1 (ppm)


zhimin-czm1p35a-ligand-300-C3
13C OBSERVE
162.13
149.67
146.85
140.92
139.44
134.11
128.97
128.77
128.05
126.75
126.00
124.09
90.04
79.02
77.42
77.00
76.58
F3C
N
O
N
Ligand 5
f1 (ppm)

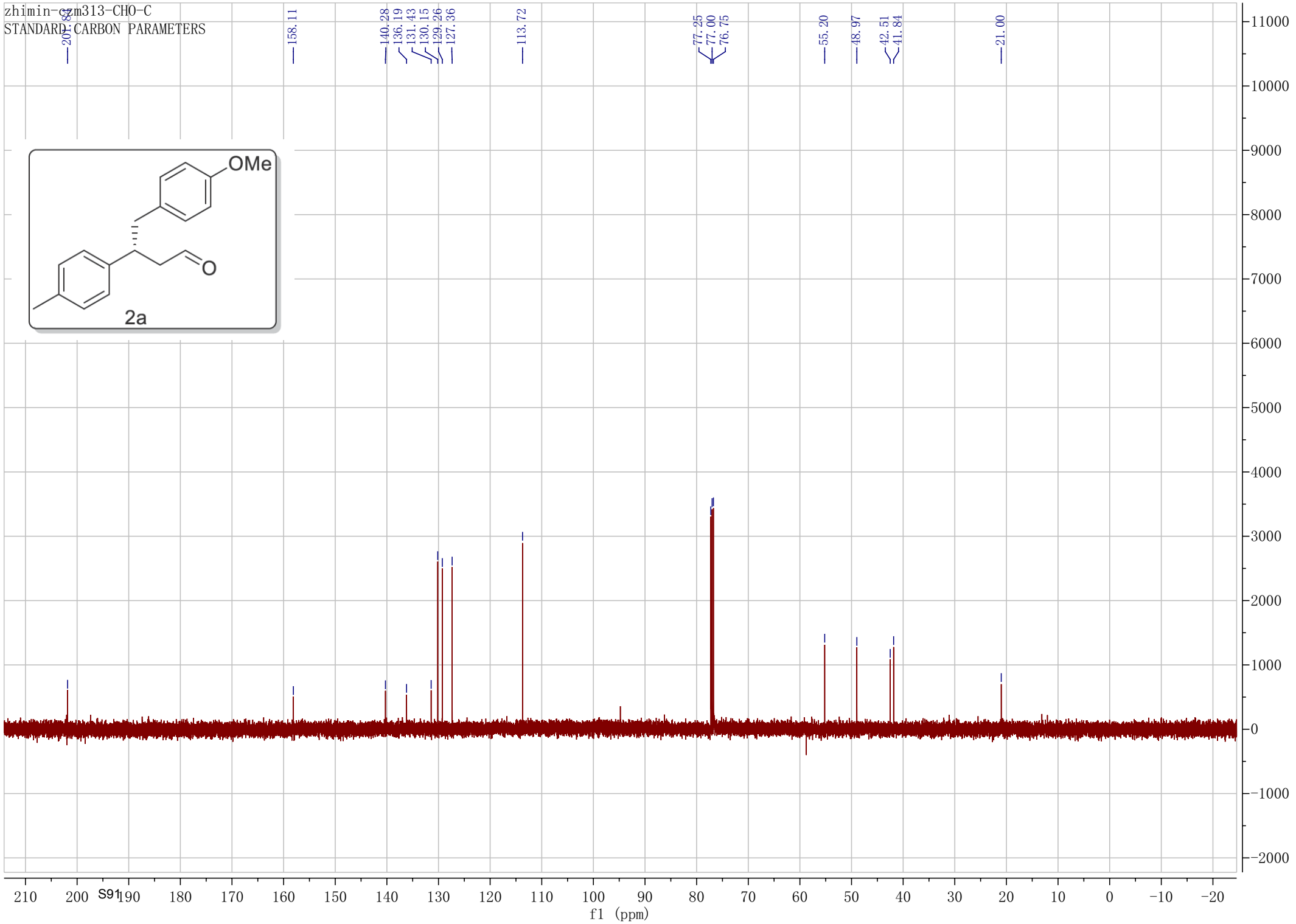

zhimin-czm1p35a-ligand-300-F1
19F OBSERVE
STANDARD PARAMETERS
-62.97
F3C
N
O
N
Ligand 5
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

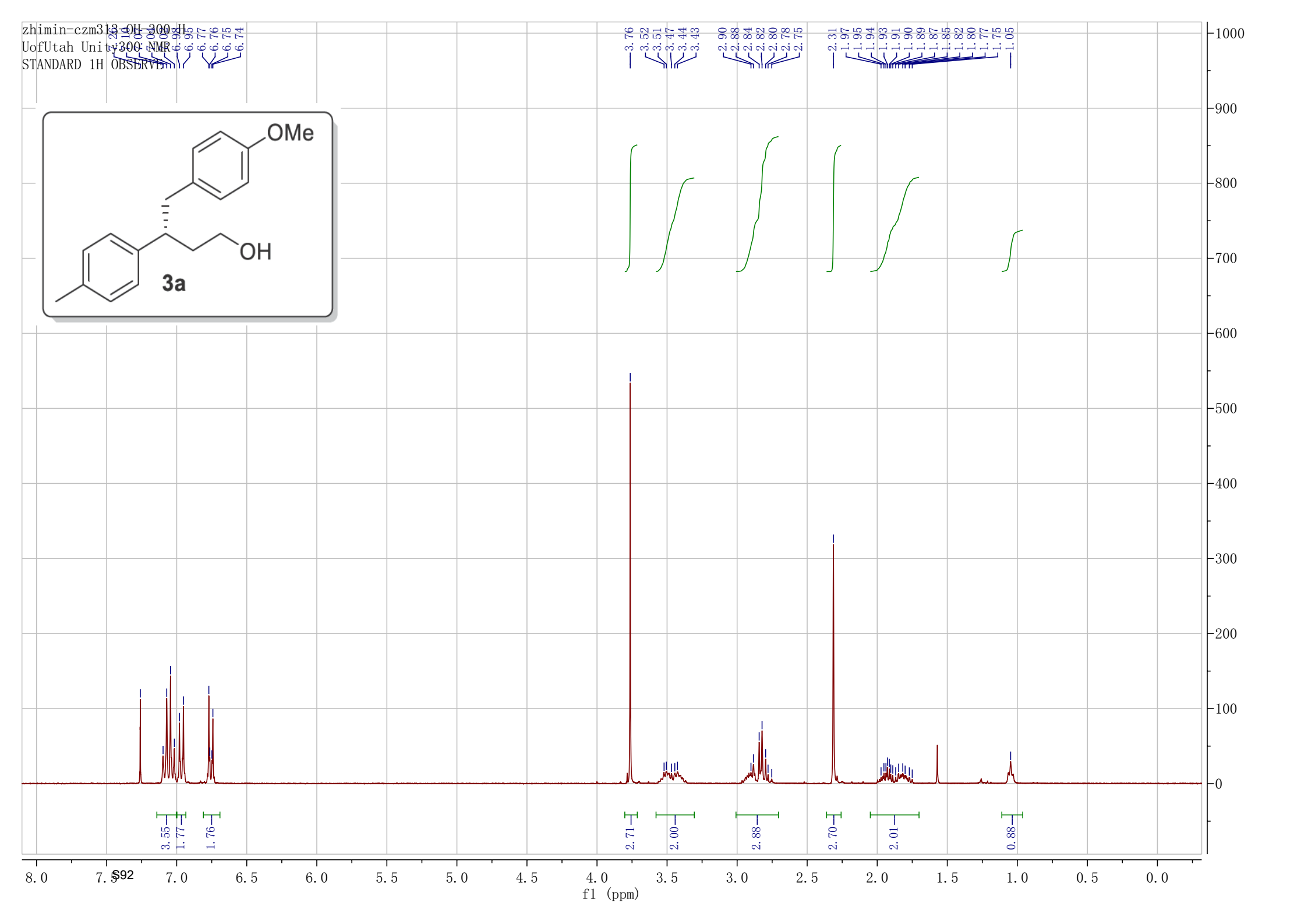

zhimin-czmdime-ph-500-H1
STANDARD PROTON PARAMETERS
9.00
8.37
8.35
8.07
8.05
7.37
7.35
7.35
7.34
7.32
7.30
7.26
7.26
7.25
7.24
5.14
1.73
1.01
F3C
N
O
N
Ligand 7
0.88
0.94
1.01
5.03
1.00
3.05
2.95
f1 (ppm)

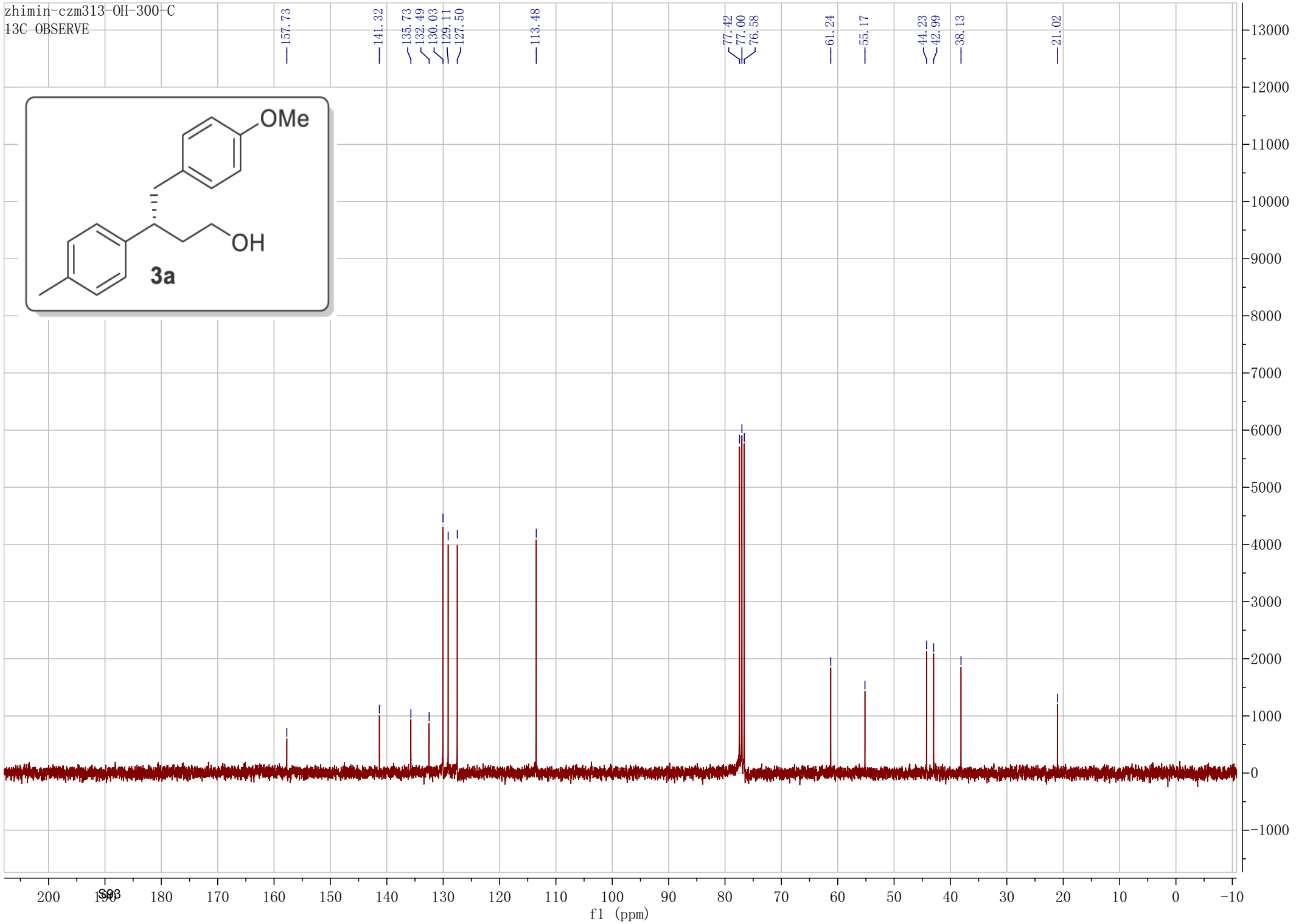

zhimin-czm-dime-Ph-500-C
STANDARD CARBON PARAMETERS
167.92
150.32
146.62
137.96
133.91
128.36
127.77
127.16
124.25
123.86
122.08
89.15
78.73
77.25
77.00
76.75
29.09
23.82
F3C
N
O
N
Ligand 7
f1 (ppm)

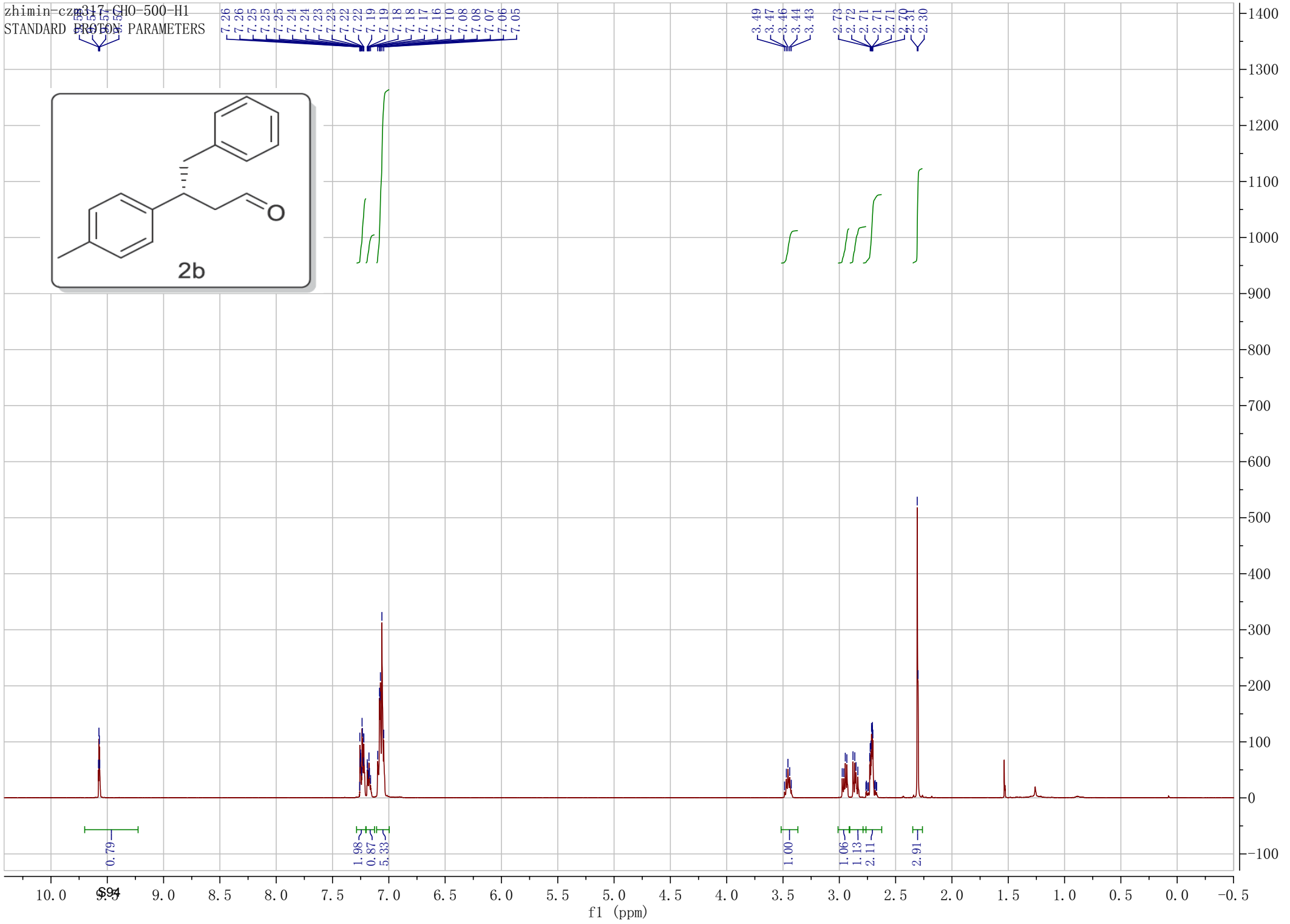

zhimin-czmligand-dime-ph-300-F
19F OBSERVE
STANDARD PARAMETERS
-62.96
-62.98
F3C
N
O
N
Ligand 7
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

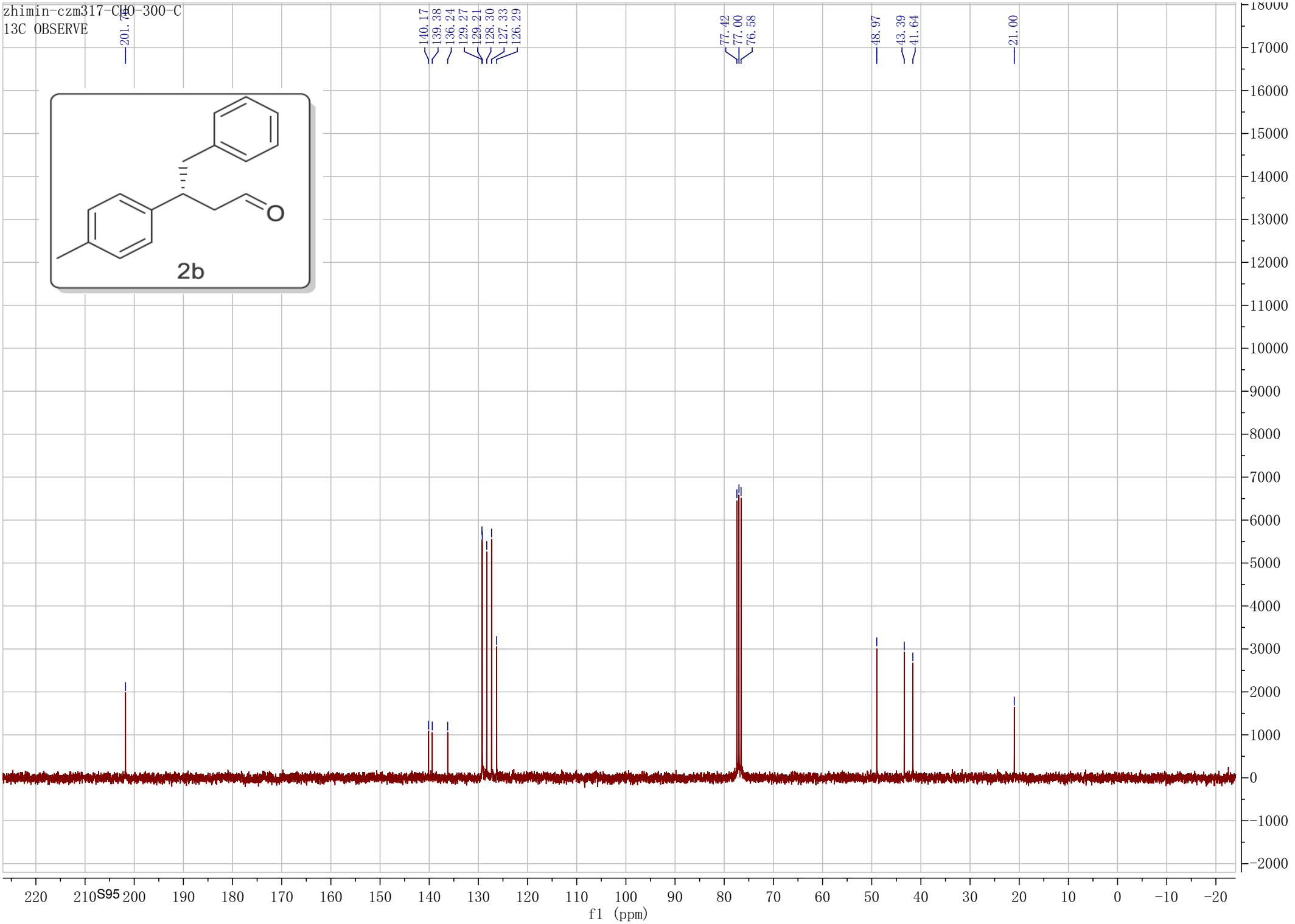

zhimin-czm313-CHO-H
STANDARD PROTON PARAMETERS
7.26
7.25
7.09
7.08
7.05
7.03
6.98
6.96
6.95
6.78
6.77
6.77
6.76
3.77
3.77
3.42
3.40
3.39
3.37
2.81
2.71
2.70
2.69
2.69
2.31
OMe
O
2a
0.75
1.69
1.85
1.77
1.64
2.86
1.00
1.05
1.06
1.99
2.79
f1 (ppm)

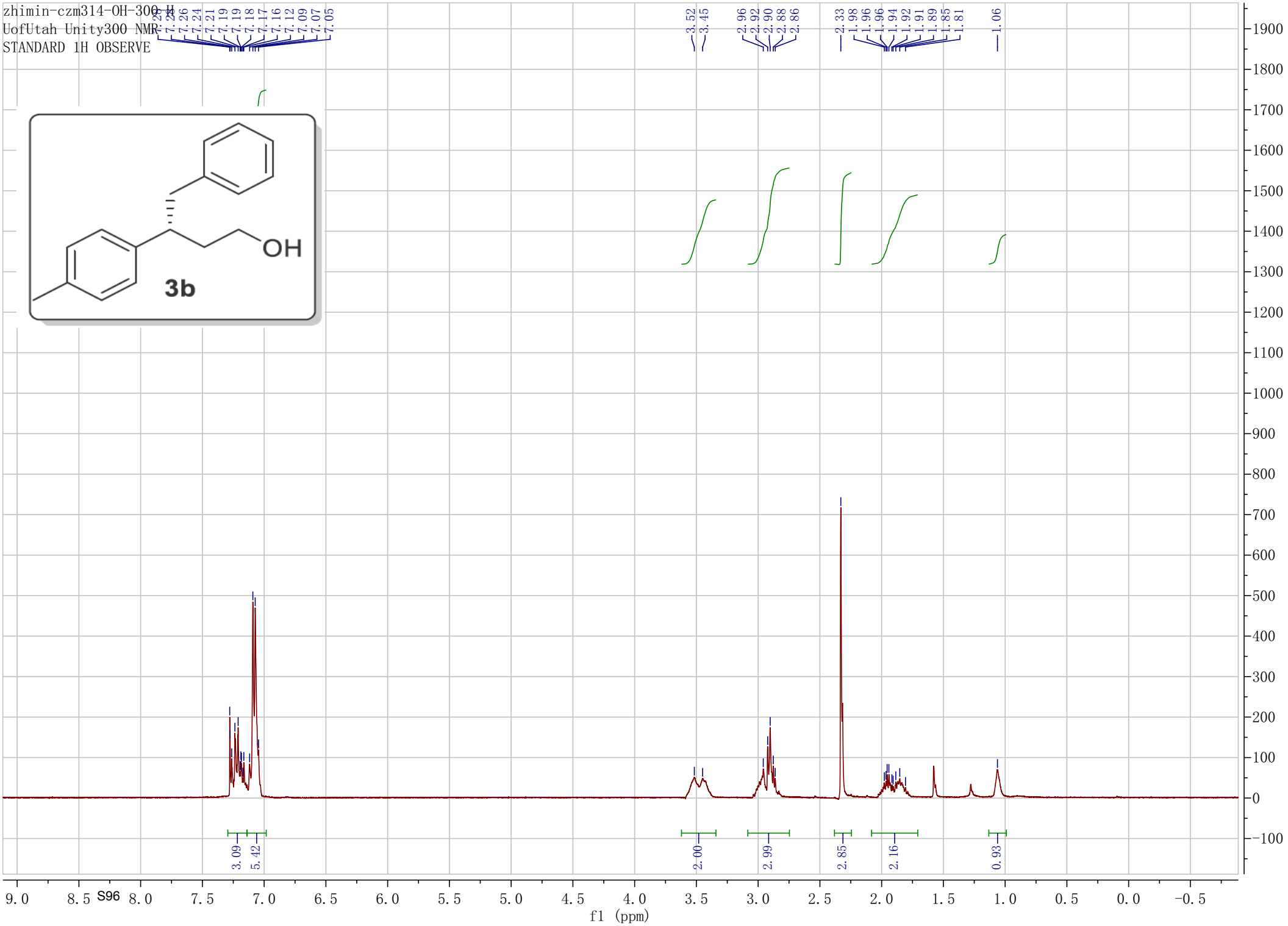

zhimin-czm313-CHO-C
STANDARD CARBON PARAMETERS
OMe
O
2a
158.11
140.28
136.19
131.43
130.15
129.26
127.36
113.72
77.25
77.00
76.75
55.20
48.97
42.51
41.84
21.00
f1 (ppm)

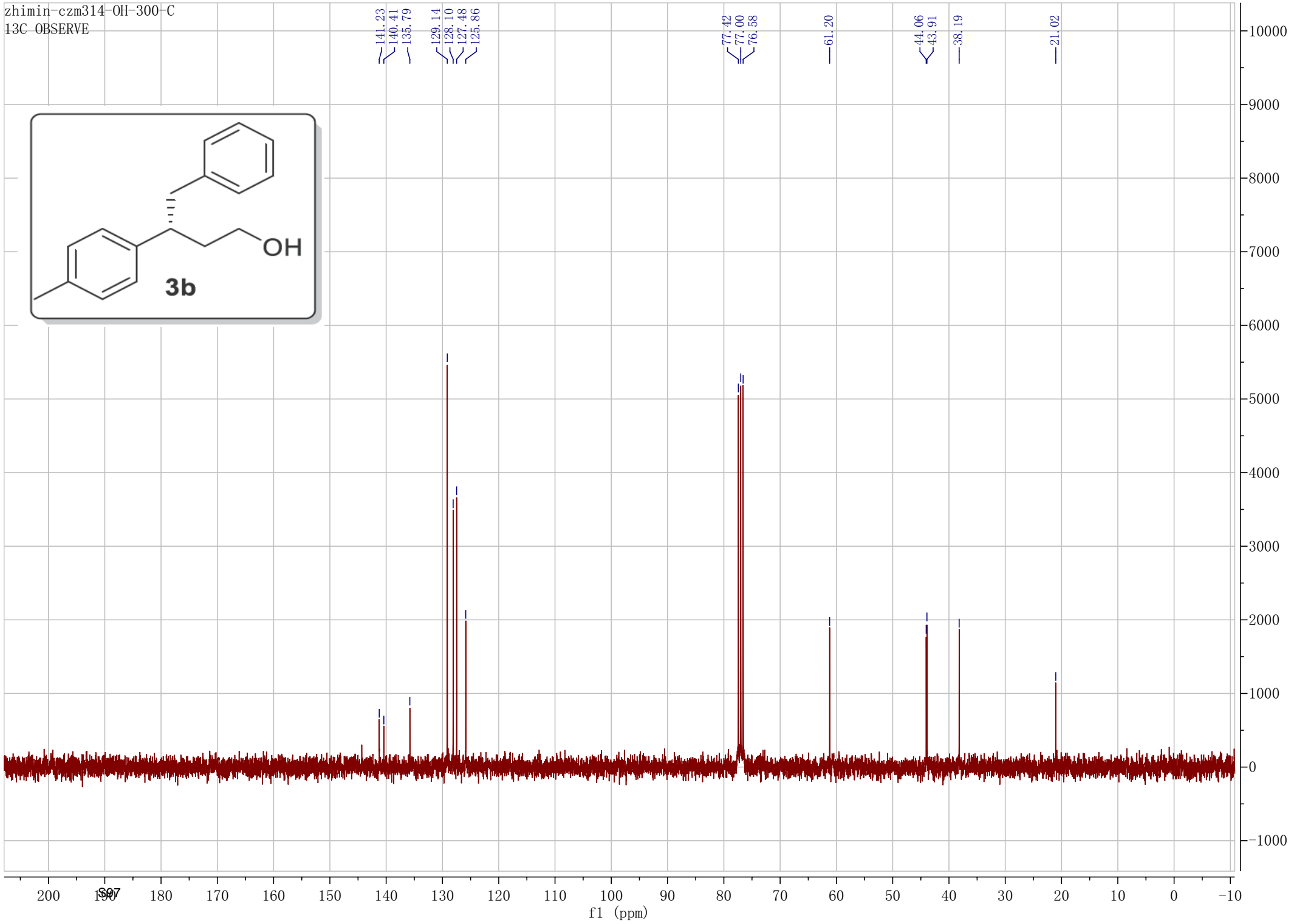

zhimin-czm313-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
OMe
OH
3a
f1 (ppm)

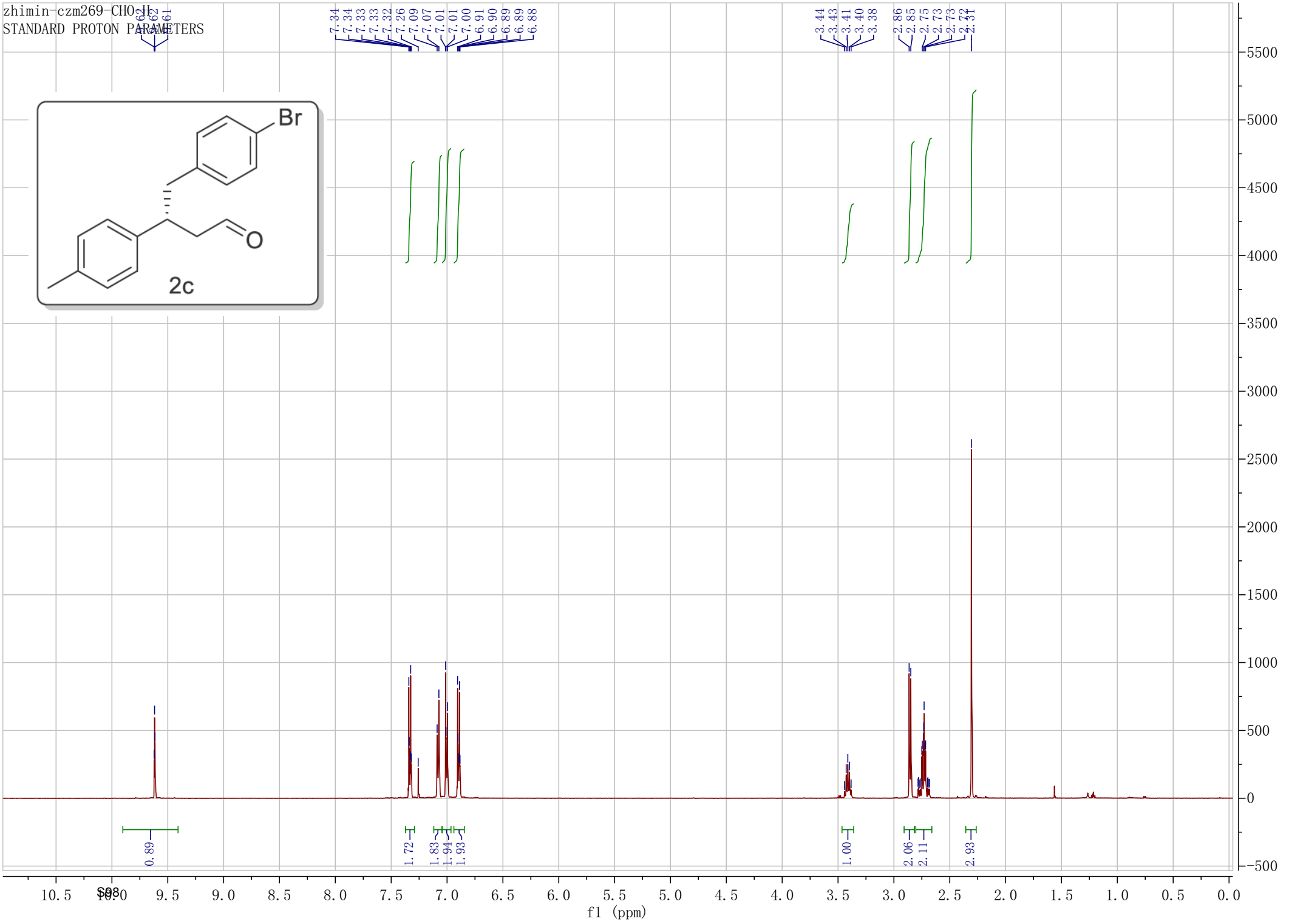

zhimin-czm313-OH-300-C
13C OBSERVE
157.73
141.32
135.73
132.49
130.03
129.11
127.50
113.48
77.42
77.00
76.58
61.24
55.17
44.23
42.99
38.13
21.02
OMe
OH
3a
f1 (ppm)

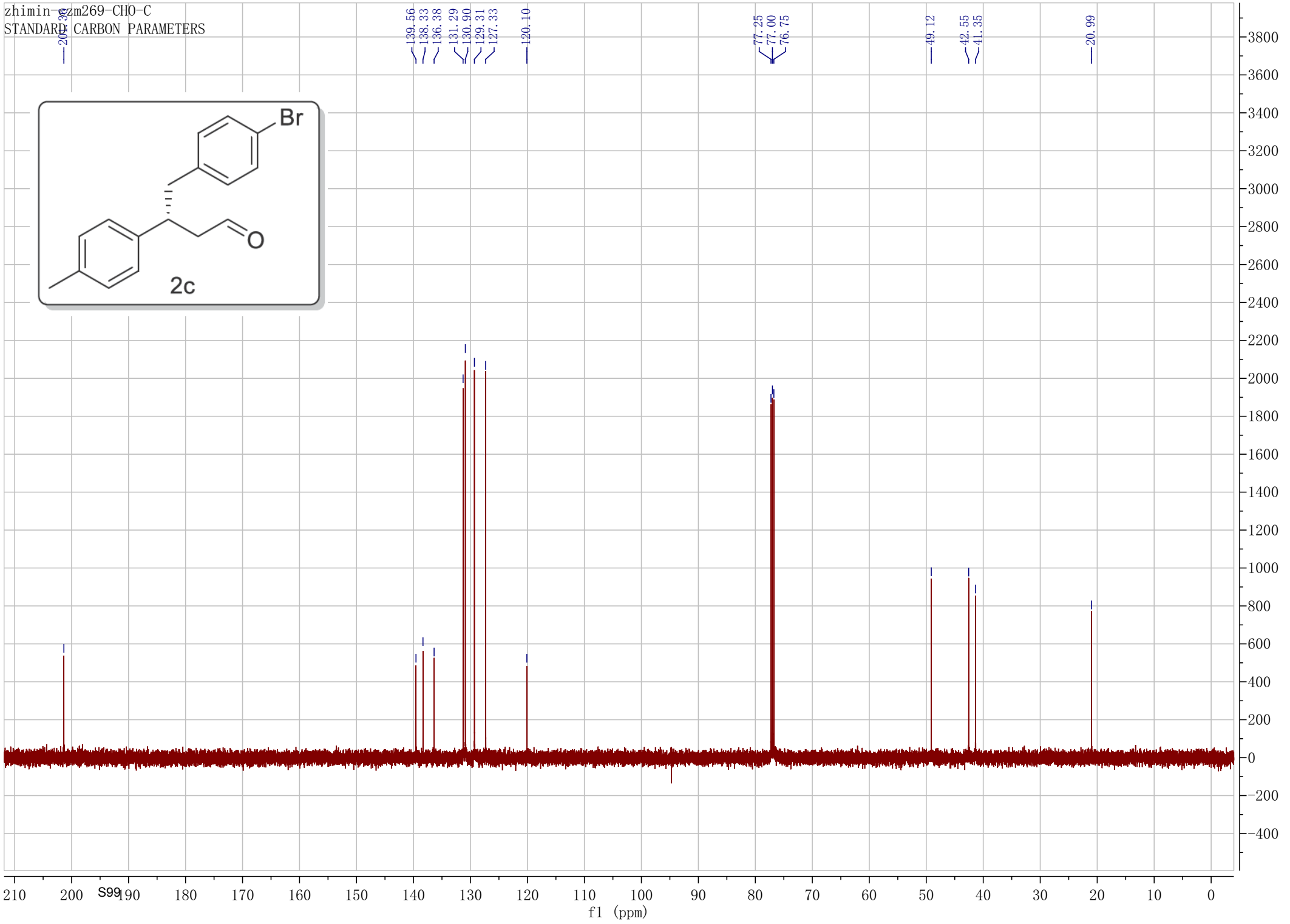

zhimin-czm317-CHO-500-H1
STANDARD PROTON PARAMETERS
2b
O
7.26
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.22
7.19
7.19
7.18
7.18
7.17
7.16
7.10
7.08
7.08
7.07
7.06
7.05
3.49
3.47
3.46
3.44
3.43
2.73
2.72
2.71
2.71
2.71
2.70
2.31
2.30
0.79
1.98
0.87
5.33
1.00
1.06
1.13
2.11
2.91
f1 (ppm)

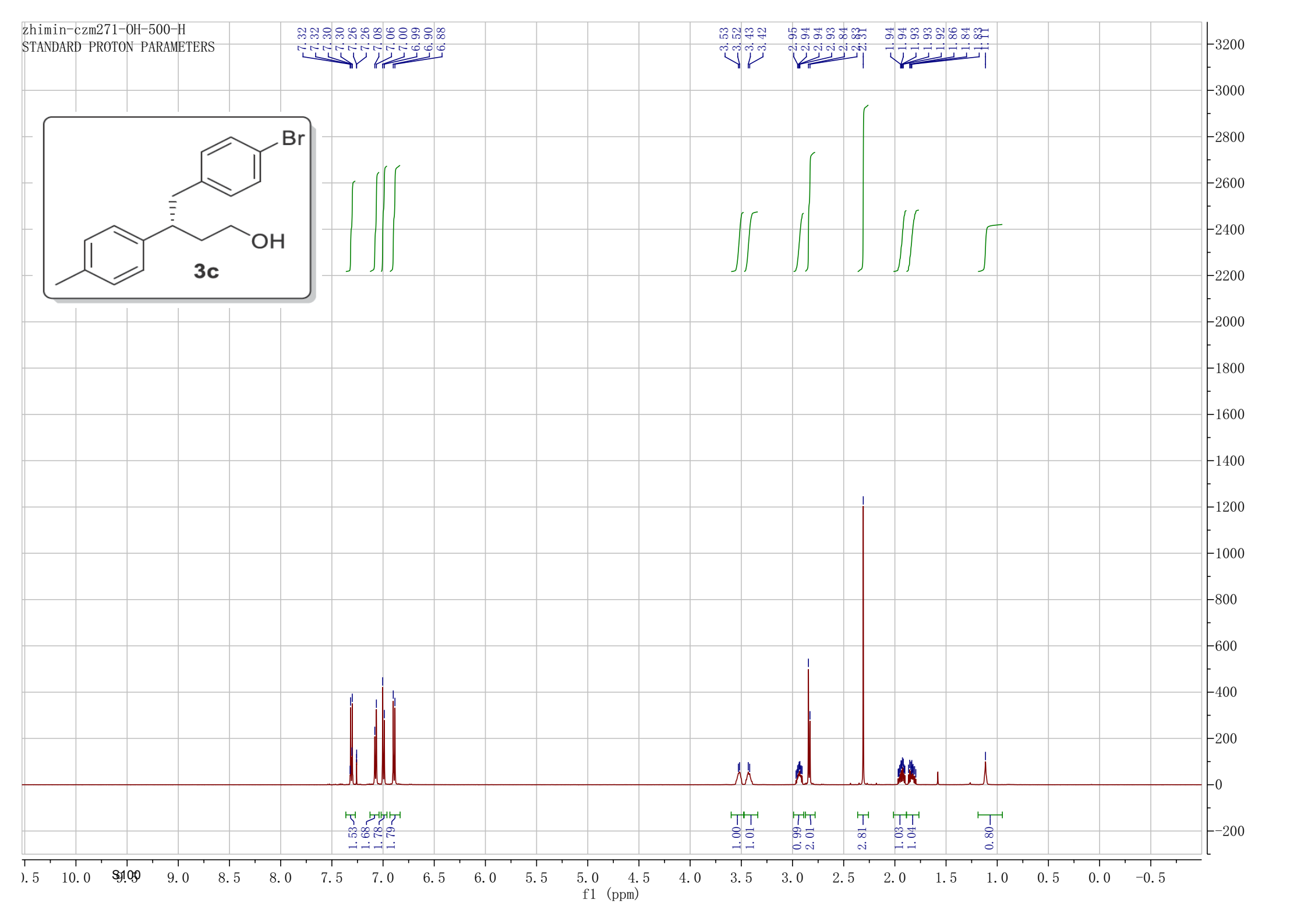

zhimin-czm317-CHO-300-C
13C OBSERVE
201.74
140.17
139.38
136.24
129.27
129.21
128.30
127.33
126.29
77.42
77.00
76.58
48.97
43.39
41.64
21.00
O
2b
f1 (ppm)

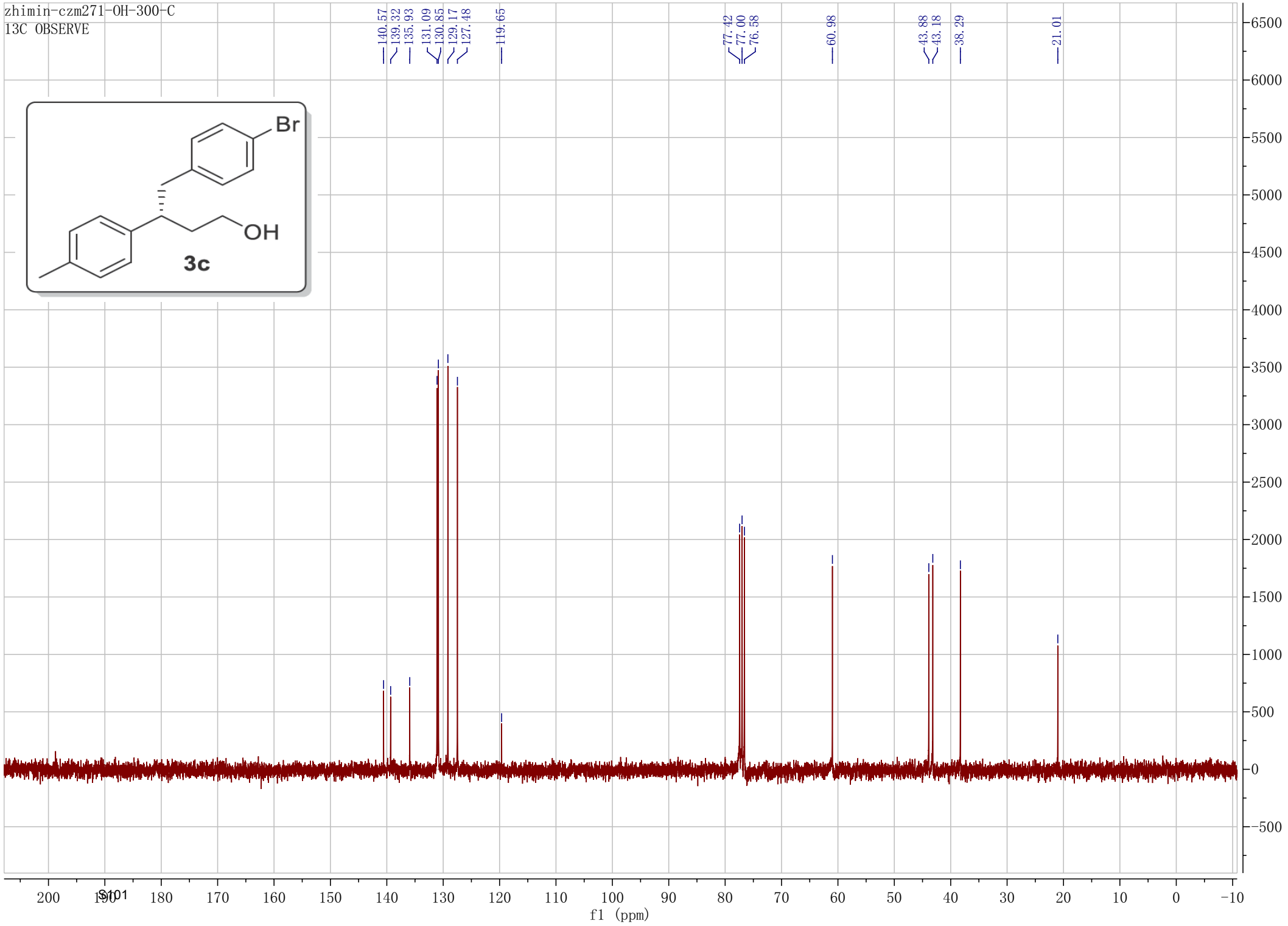

zhimin-czm314-OH-300 H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.28
7.26
7.24
7.21
7.19
7.19
7.18
7.17
7.16
7.12
7.09
7.07
7.05
3.52
3.45
2.96
2.92
2.90
2.88
2.86
2.33
1.98
1.96
1.96
1.94
1.92
1.91
1.89
1.85
1.81
1.06
OH
3b
3.09
5.42
2.00
2.99
2.85
2.16
0.93
f1 (ppm)

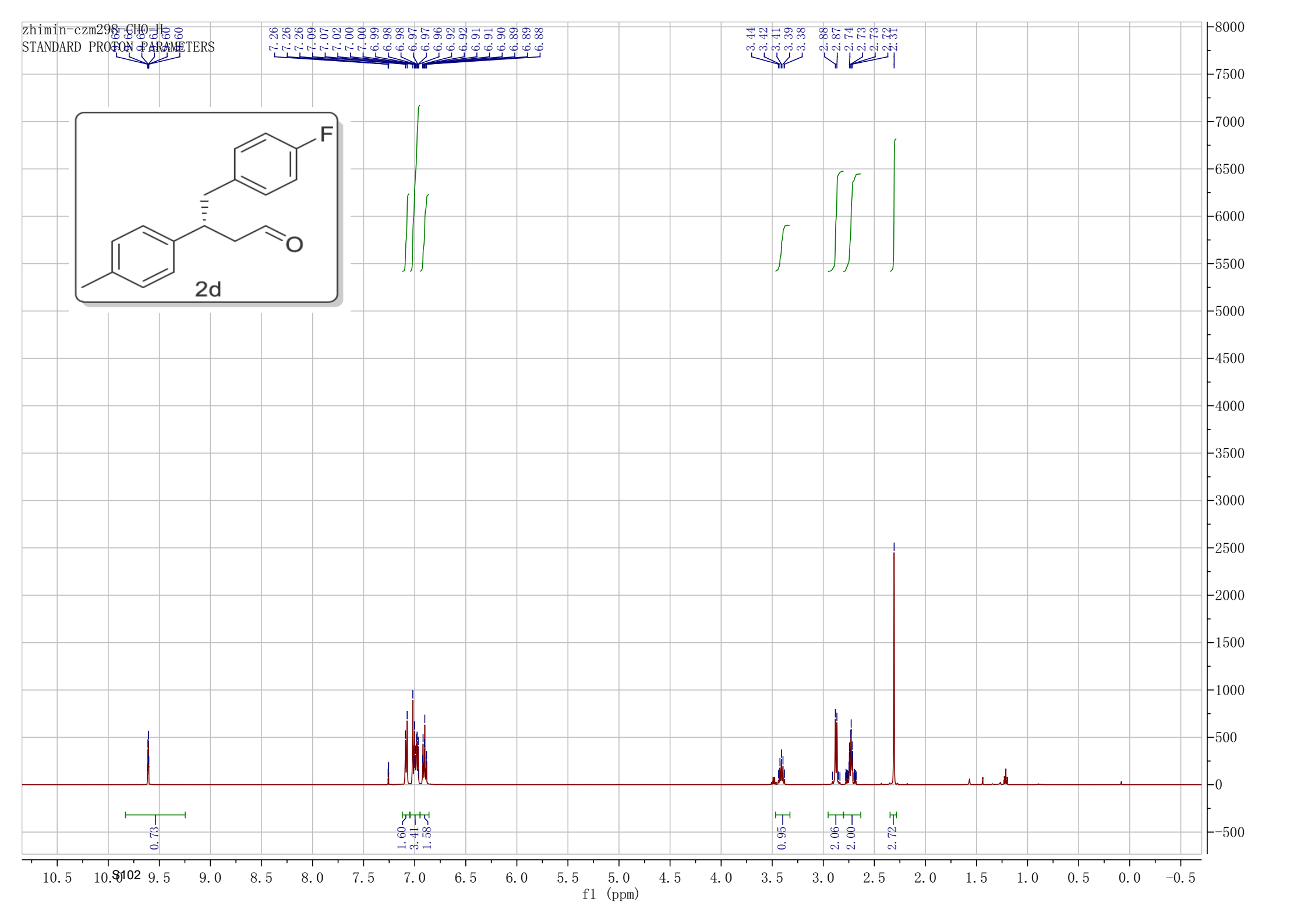

zhimin-czm314-OH-300-C
13C OBSERVE
141.23
140.41
135.79
129.14
128.10
127.48
125.86
77.42
77.00
76.58
61.20
44.06
43.91
38.19
21.02
OH
3b
f1 (ppm)

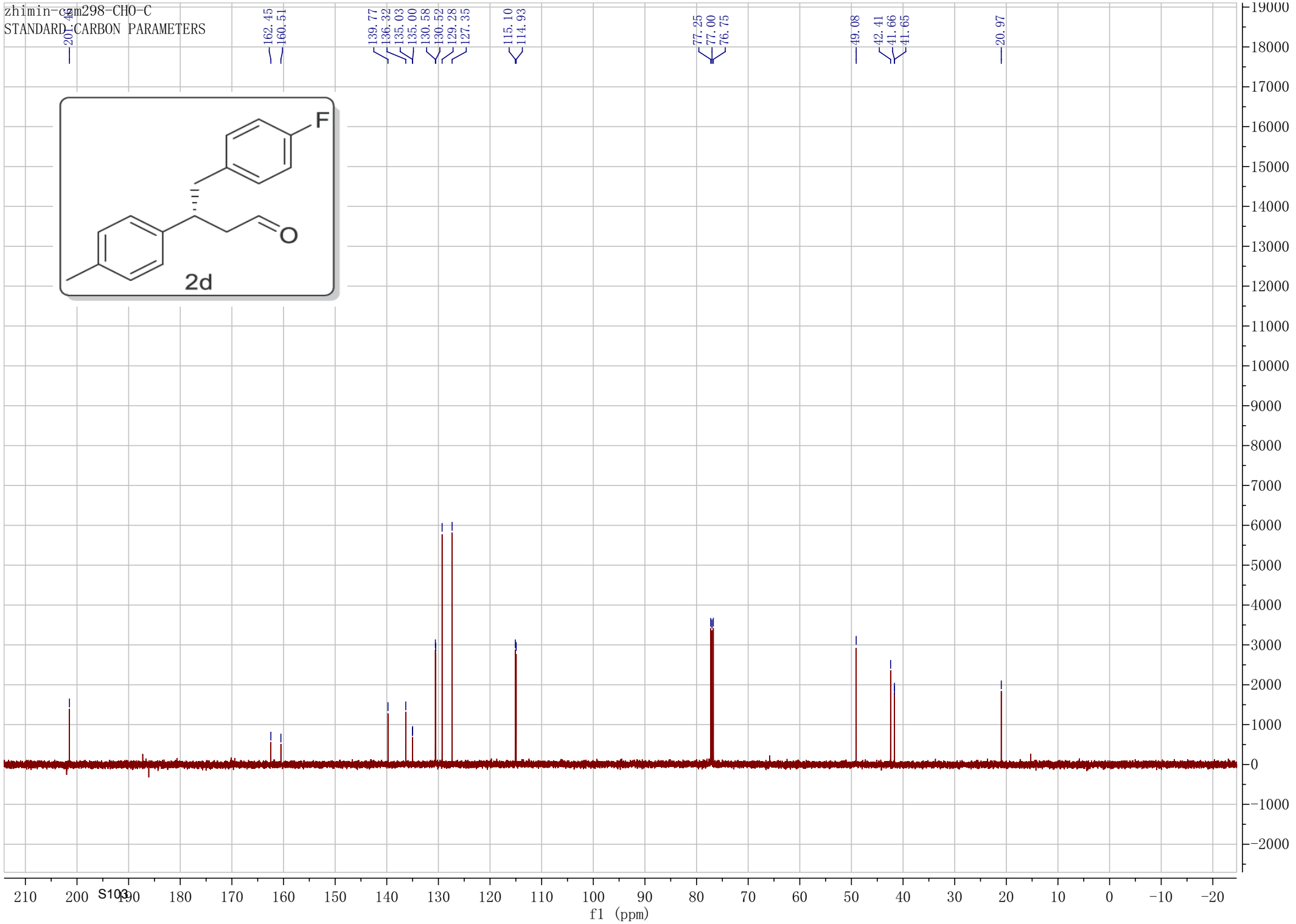

zhimin-czm269-CHO-H
STANDARD PROTON PARAMETERS
9.62
9.61
7.34
7.34
7.33
7.33
7.32
7.26
7.09
7.07
7.01
7.01
7.00
6.91
6.90
6.89
6.89
6.88
3.44
3.43
3.41
3.40
3.38
2.86
2.85
2.75
2.73
2.72
2.31
Br
O
2c
0.89
1.72
1.83
1.94
1.93
1.00
2.06
2.11
2.93
f1 (ppm)

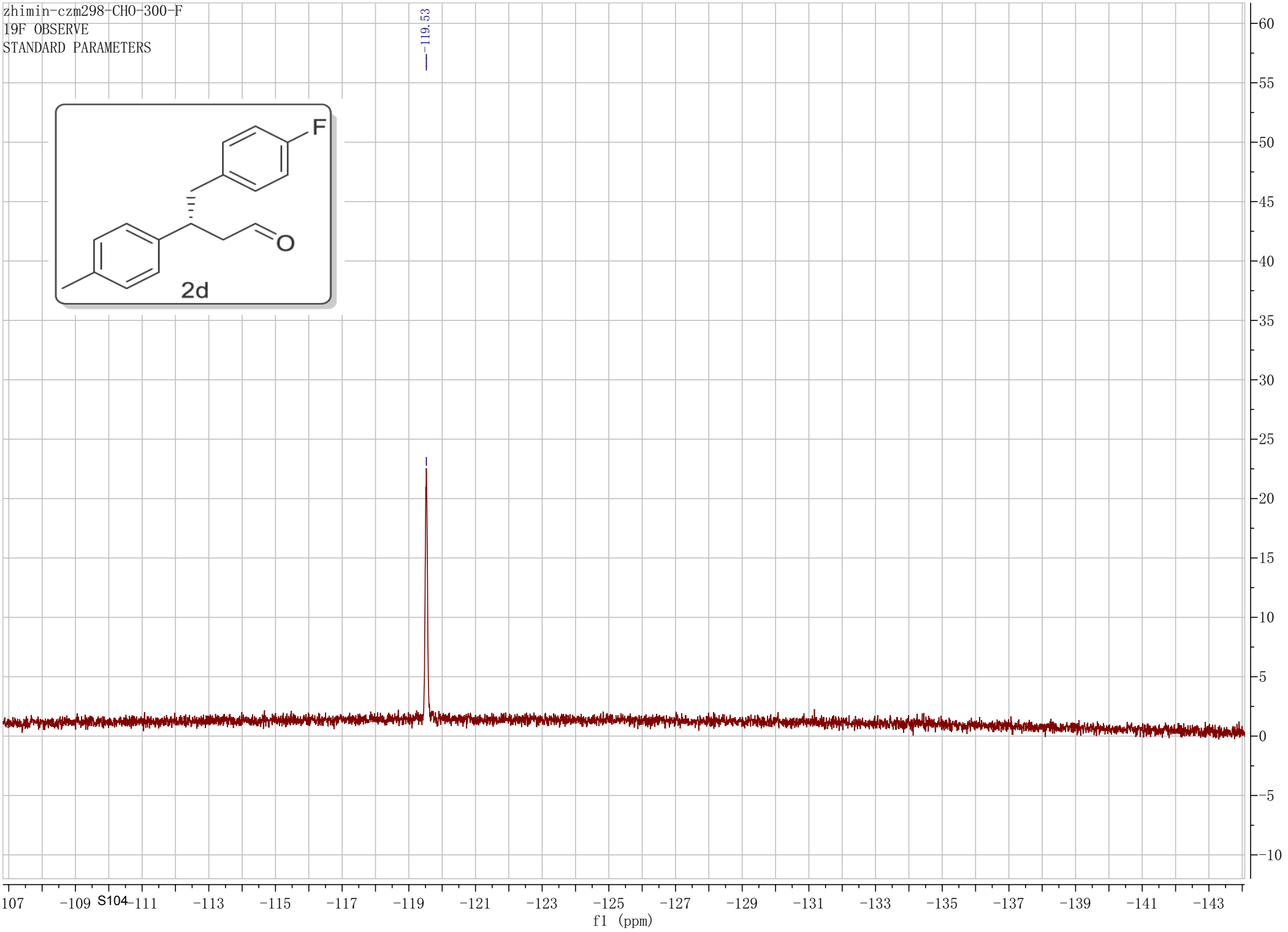

zhimin-czm269-CHO-C
STANDARD CARBON PARAMETERS
200.30
139.56
138.33
136.38
131.29
130.90
129.31
127.33
120.10
77.25
77.00
76.75
49.12
42.55
41.35
20.99
Br
O
2c
f1 (ppm)

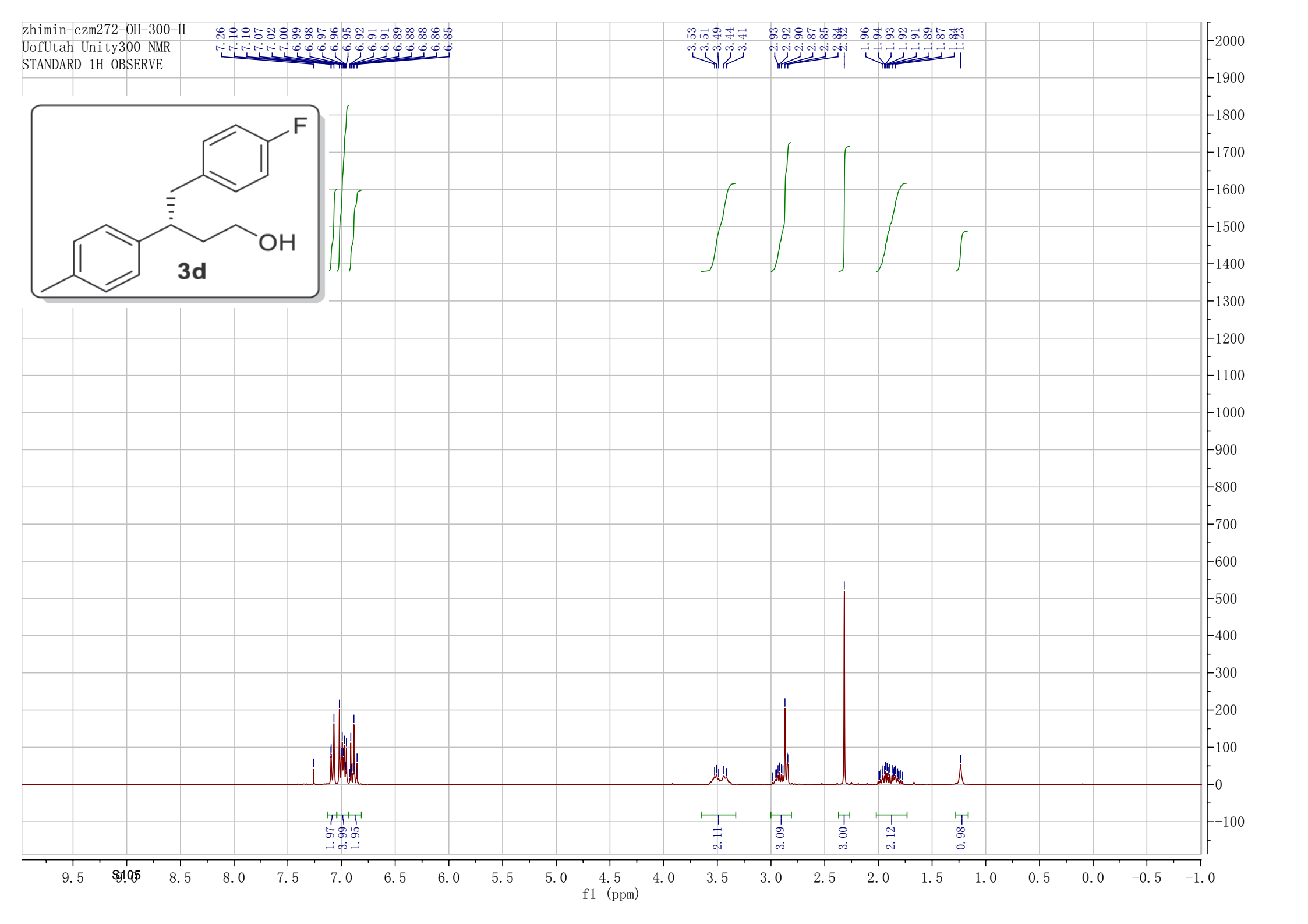

zhimin-czm271-OH-500-H
STANDARD PROTON PARAMETERS
7.32
7.32
7.30
7.30
7.26
7.26
7.08
7.06
7.00
6.99
6.90
6.88
3.53
3.52
3.43
3.42
2.95
2.94
2.94
2.93
2.84
2.83
2.81
1.94
1.94
1.93
1.93
1.92
1.86
1.84
1.83
1.81
Br
OH
3c
1.53
1.68
1.78
1.79
1.00
1.01
0.99
2.01
2.81
1.03
1.04
0.80
f1 (ppm)

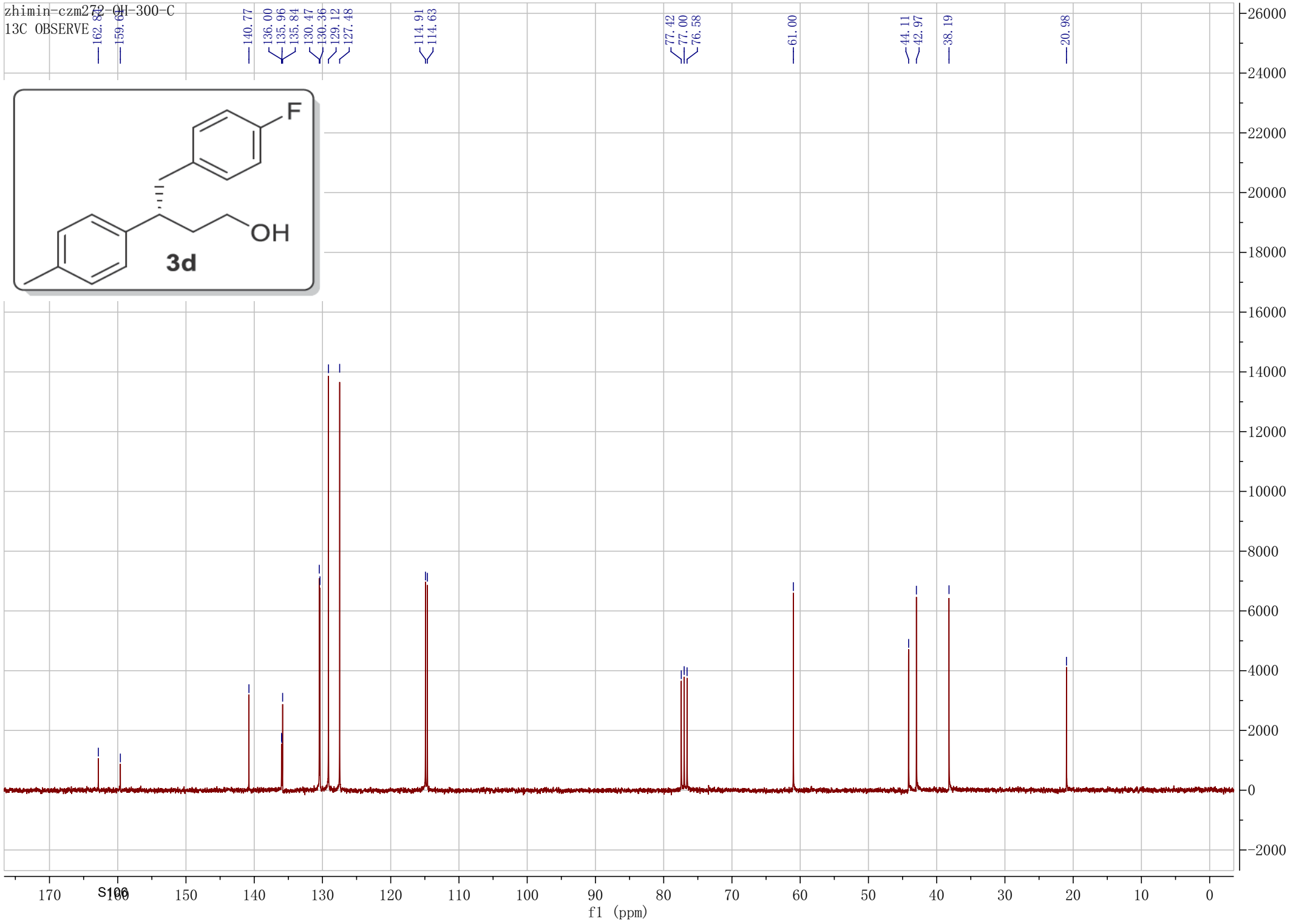

zhimin-czm271-OH-300-C
13C OBSERVE
140.57
139.32
135.93
131.09
130.85
129.17
127.48
119.65
77.42
77.00
76.58
60.98
43.88
43.18
38.29
21.01
Br
OH
3c
f1 (ppm)


zhimin-czm298-CHO-H
STANDARD PROTON PARAMETERS
F
O
2d
f1 (ppm)

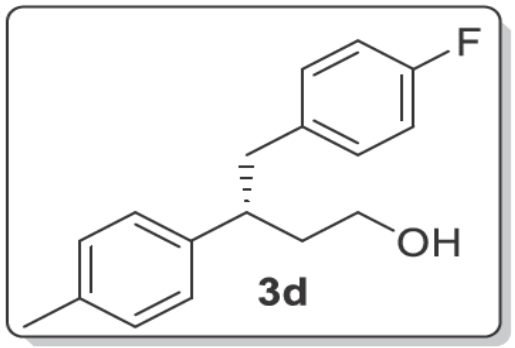

zhimin-cxm298-CHO-C
STANDARD-CARBON PARAMETERS
20.44
162.45
160.51
139.77
136.32
135.03
135.00
130.58
130.52
129.28
127.35
115.10
114.93
77.25
77.00
76.75
49.08
42.41
41.66
41.65
20.97
F
O
2d
f1 (ppm)


zhimin-czm298-CHO-300-F
19F OBSERVE
STANDARD PARAMETERS
-119.53
F
O
2d
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
107
-109
-111
-113
-115
-117
-119
-121
-123
-125
-127
-129
-131
-133
-135
-137
-139
-141
-143
f1 (ppm)

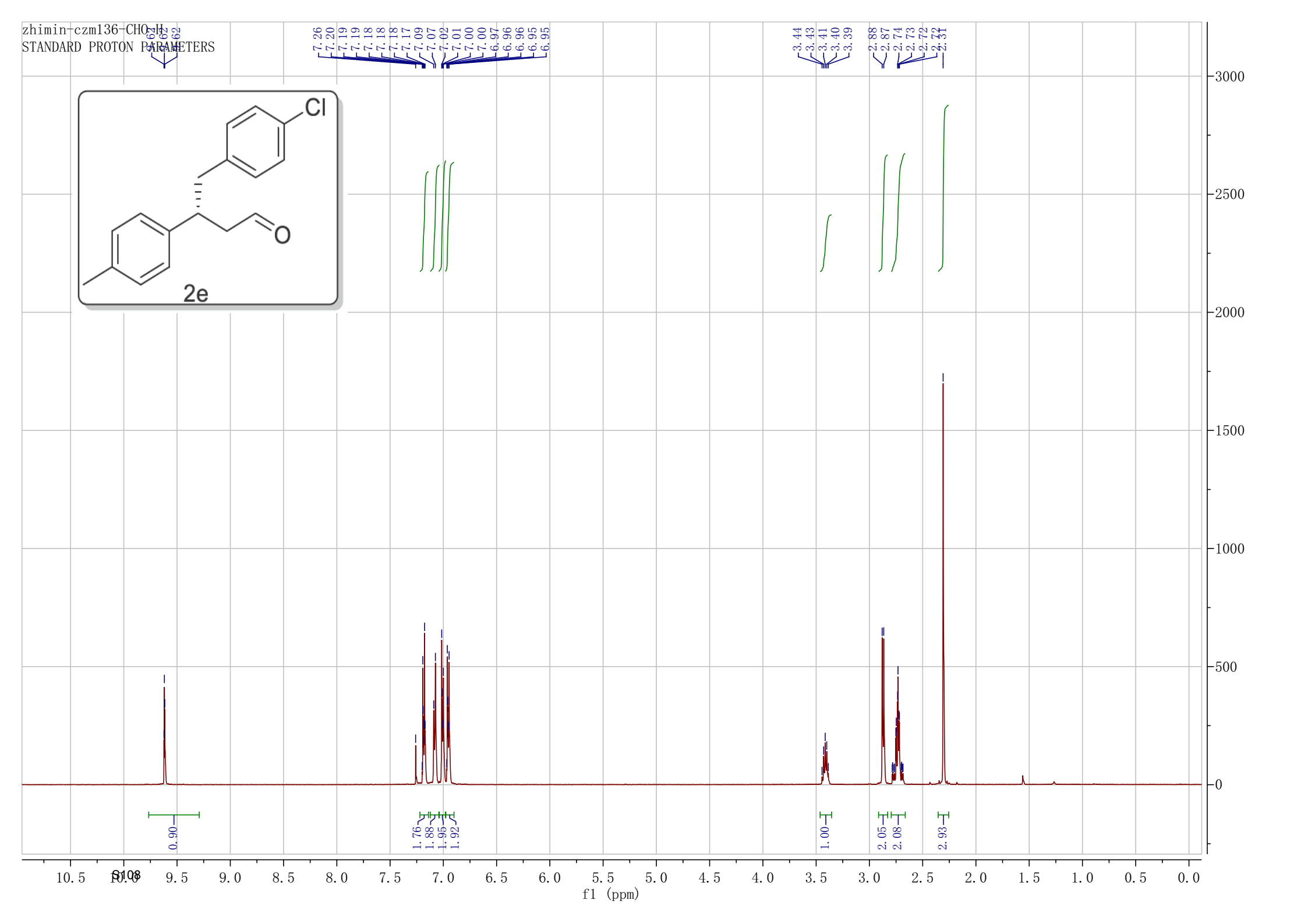

zhimin-czm272-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
F
OH
3d
f1 (ppm)

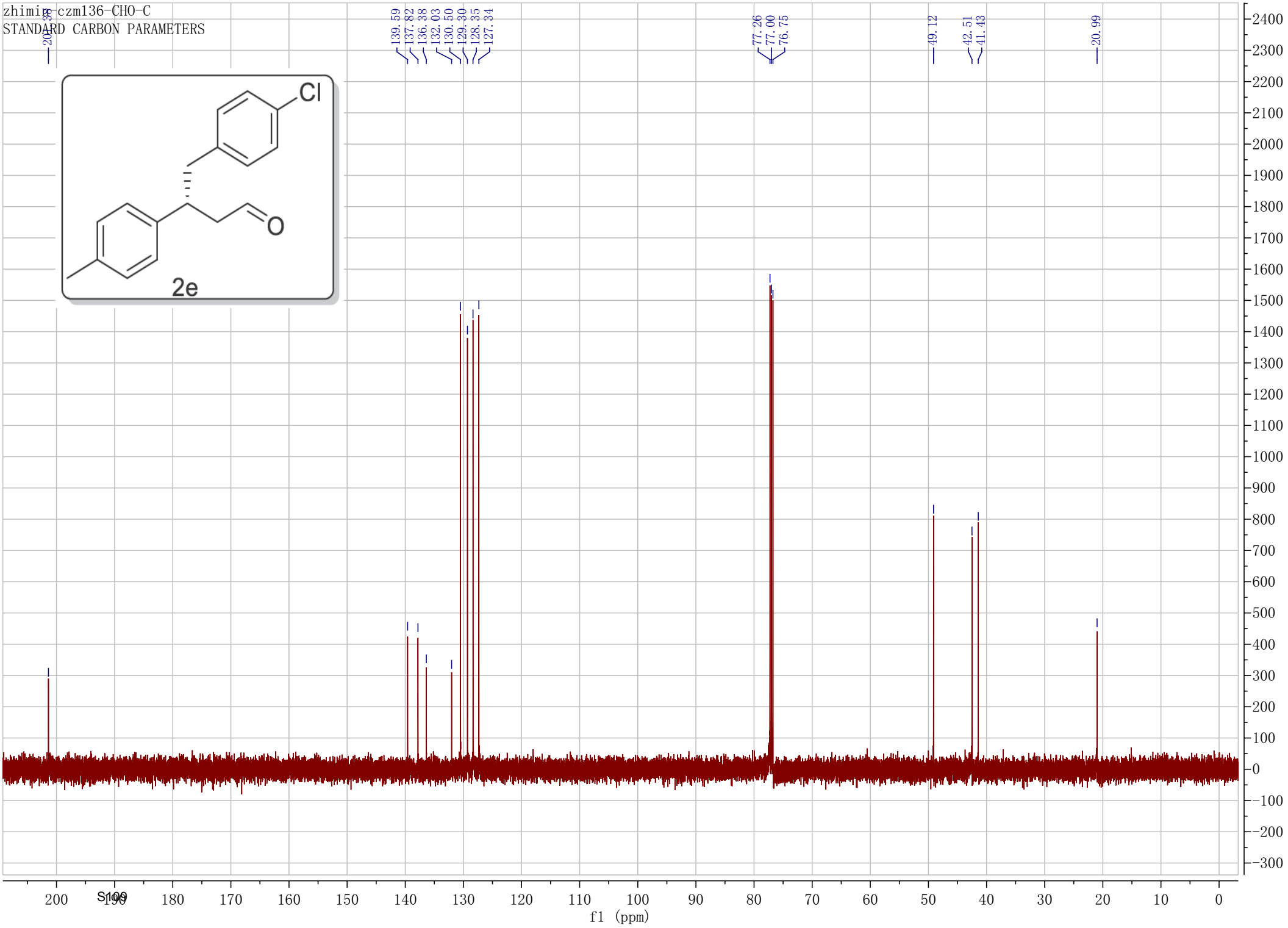

zhimin-czm272-OH-300-C
13C OBSERVE
162.82
159.69
140.77
136.00
135.96
135.84
130.47
130.36
129.12
127.48
114.91
114.63
77.42
77.00
76.58
61.00
44.11
42.97
38.19
20.98
F
OH
3d
f1 (ppm)

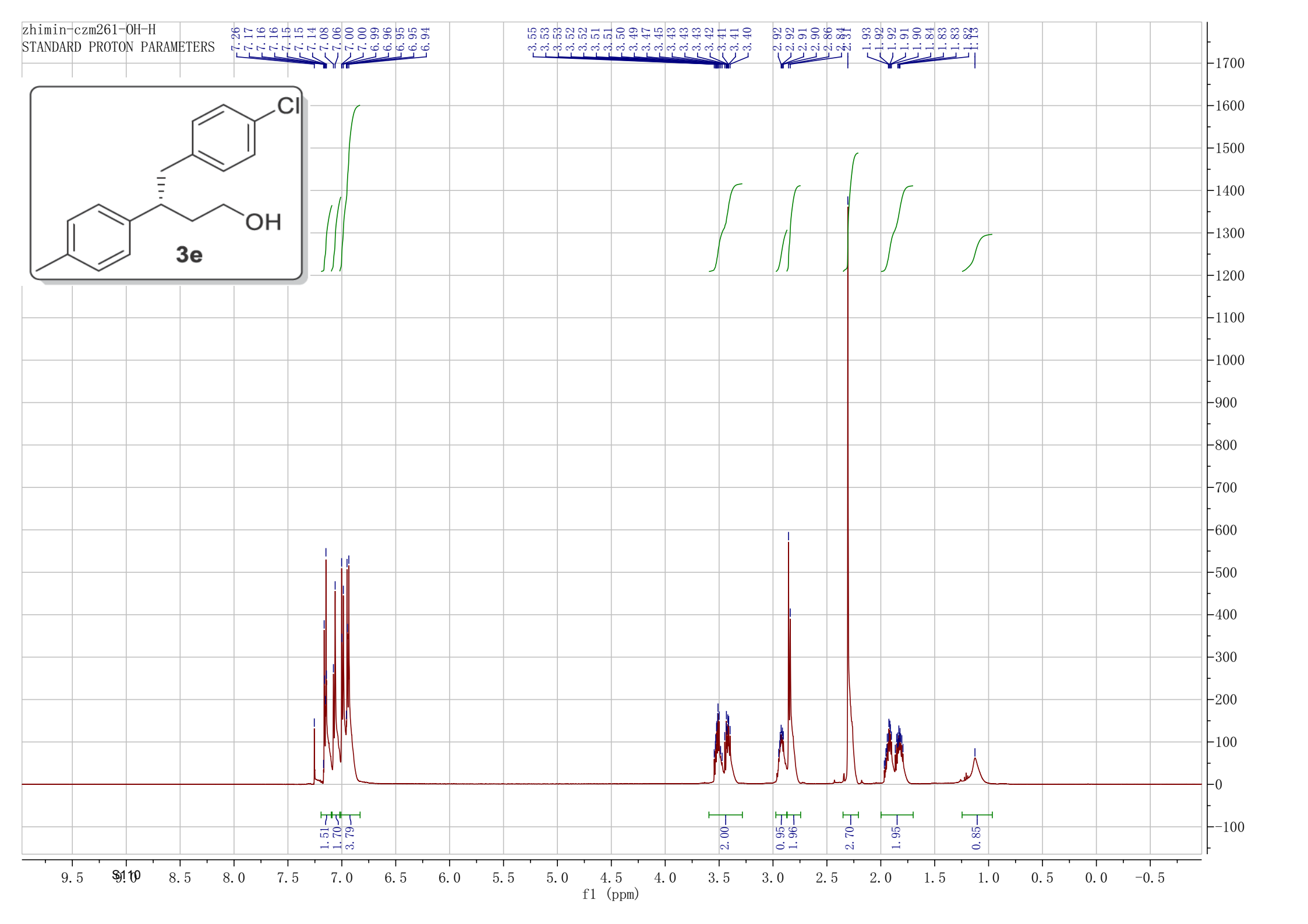
zhimin-czm272-OH-300-F
19F OBSERVE
STANDARD PARAMETERS

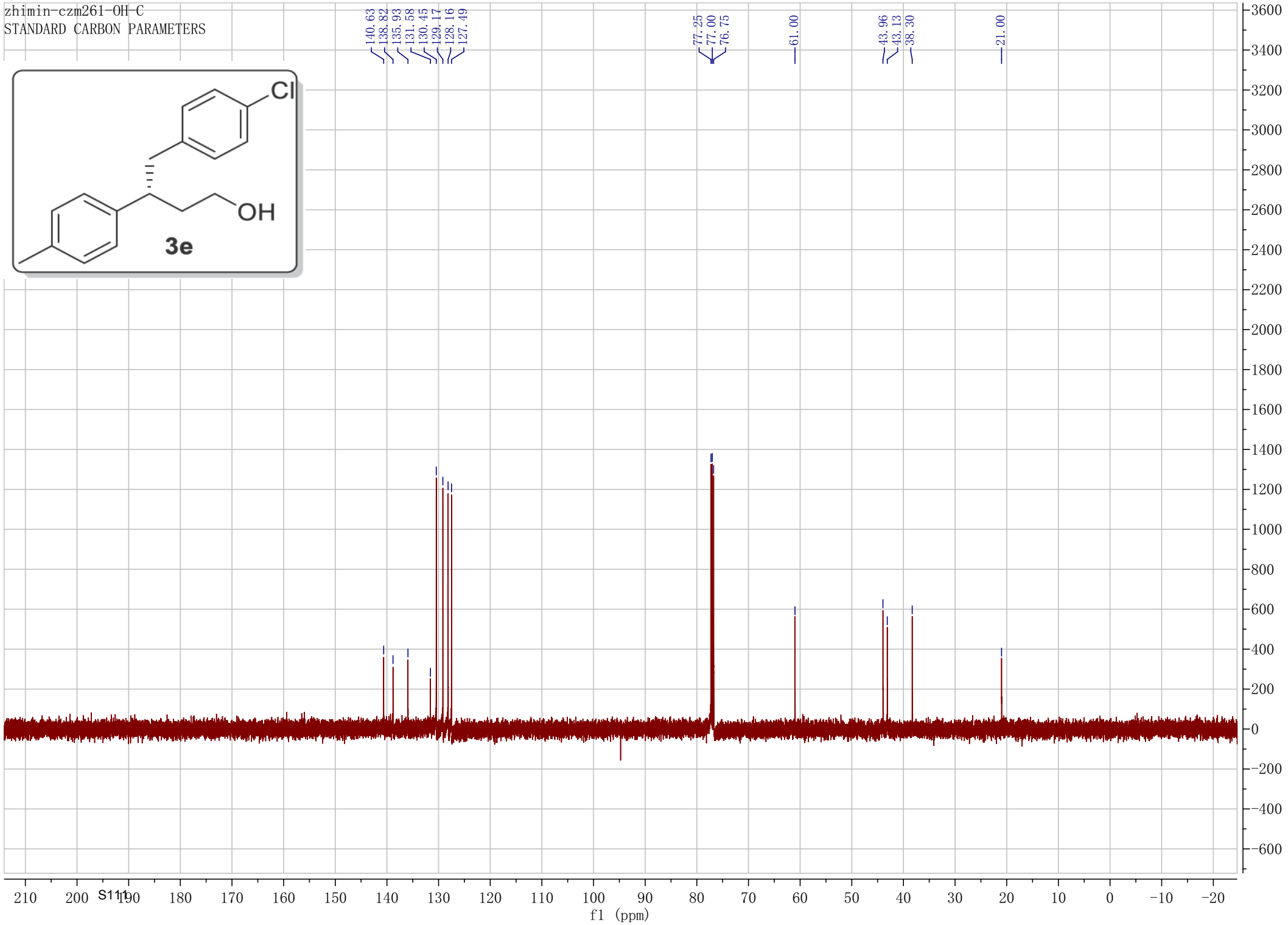


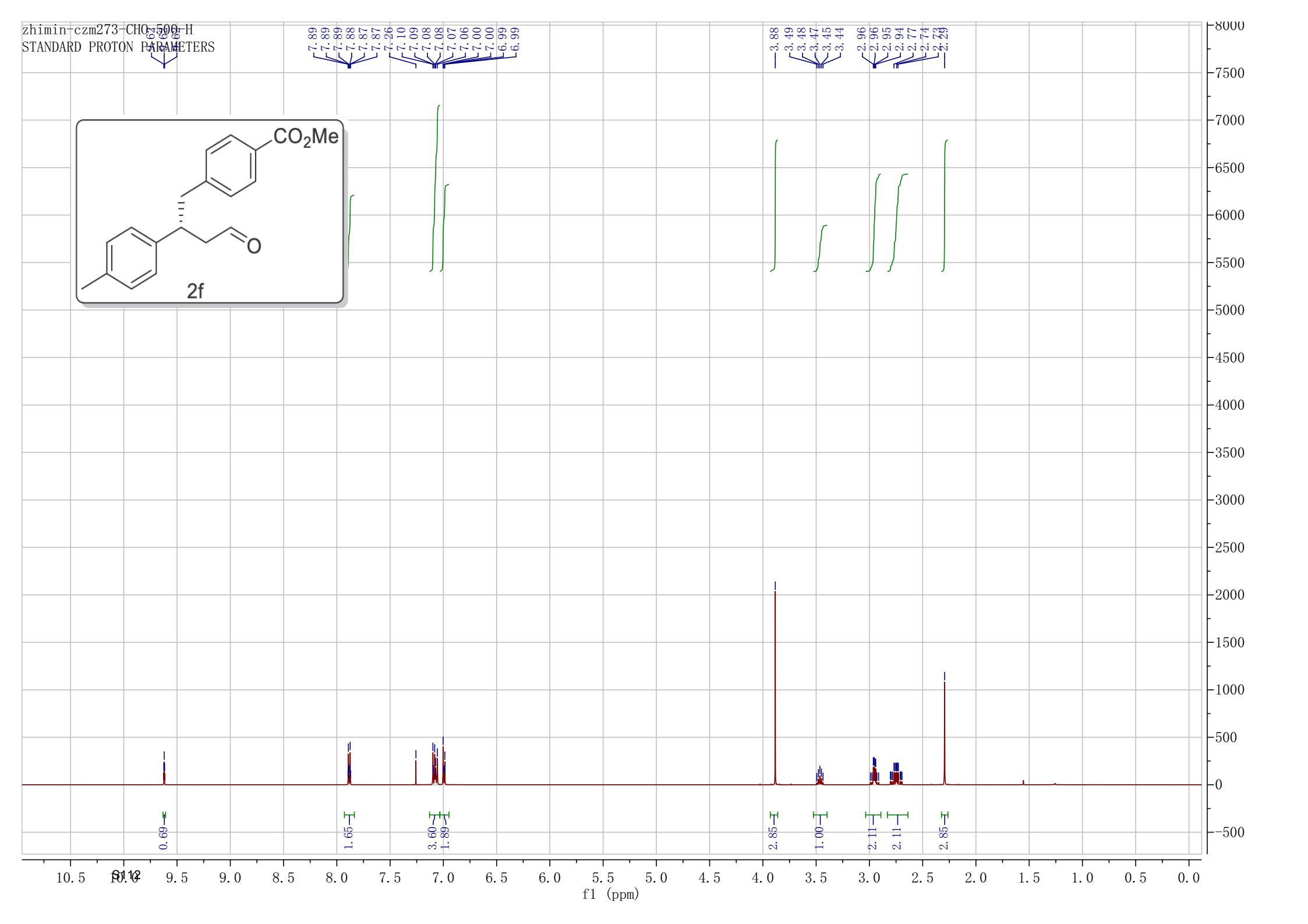
-117.96
-117.98
-117.99
-118.01
-118.02
-118.04
-118.06

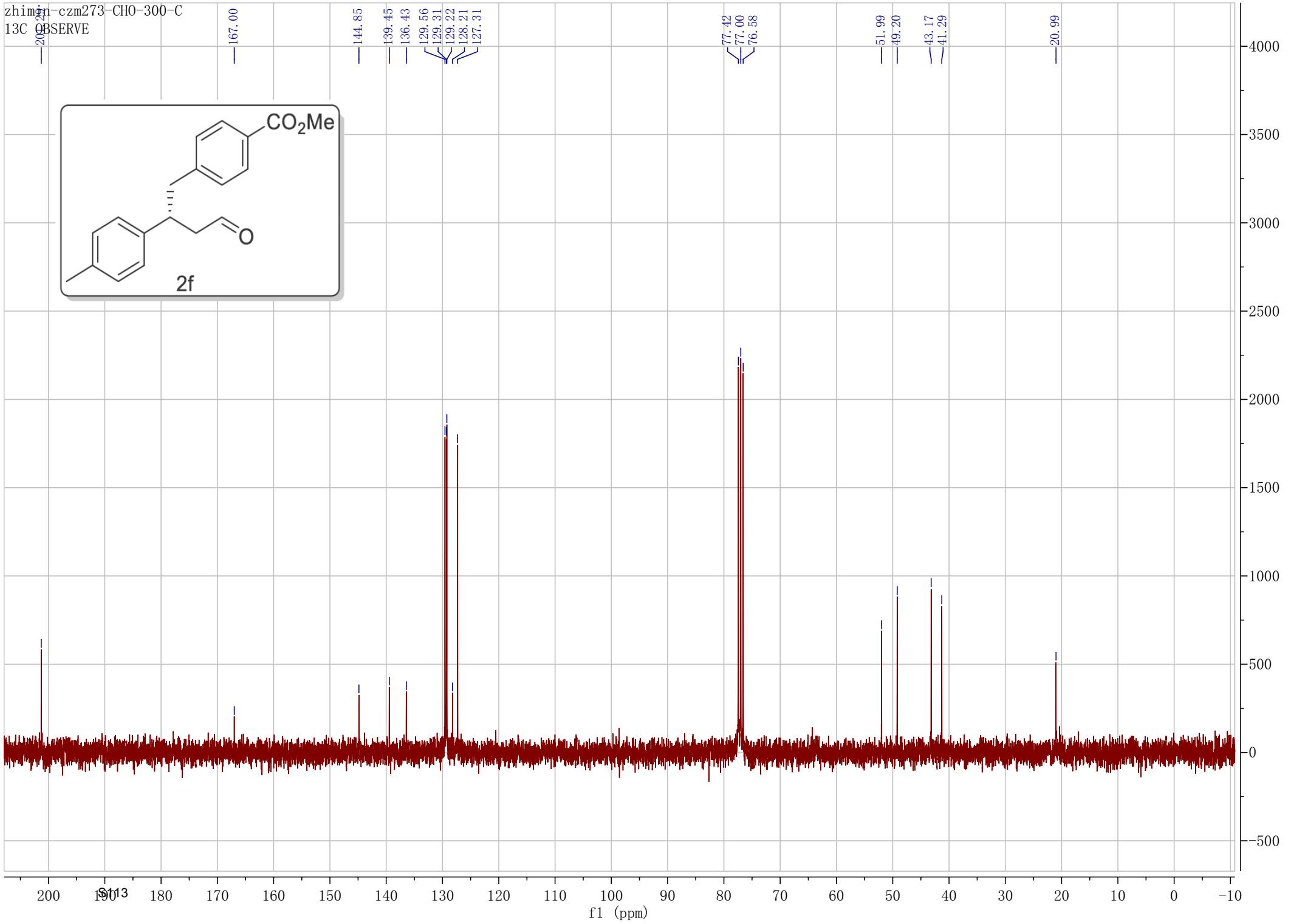

zhimin-czm136-CHO-1H
STANDARD PROTON PARAMETERS
9.62
7.26
7.20
7.19
7.19
7.18
7.18
7.17
7.09
7.07
7.02
7.01
7.00
7.00
6.97
6.96
6.96
6.95
6.95
3.44
3.43
3.41
3.40
3.39
2.88
2.87
2.74
2.73
2.72
2.31
Cl
O
2e
0.90
1.76
1.88
1.95
1.92
1.00
2.05
2.08
2.93
3000
2500
2000
1500
1000
500
0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

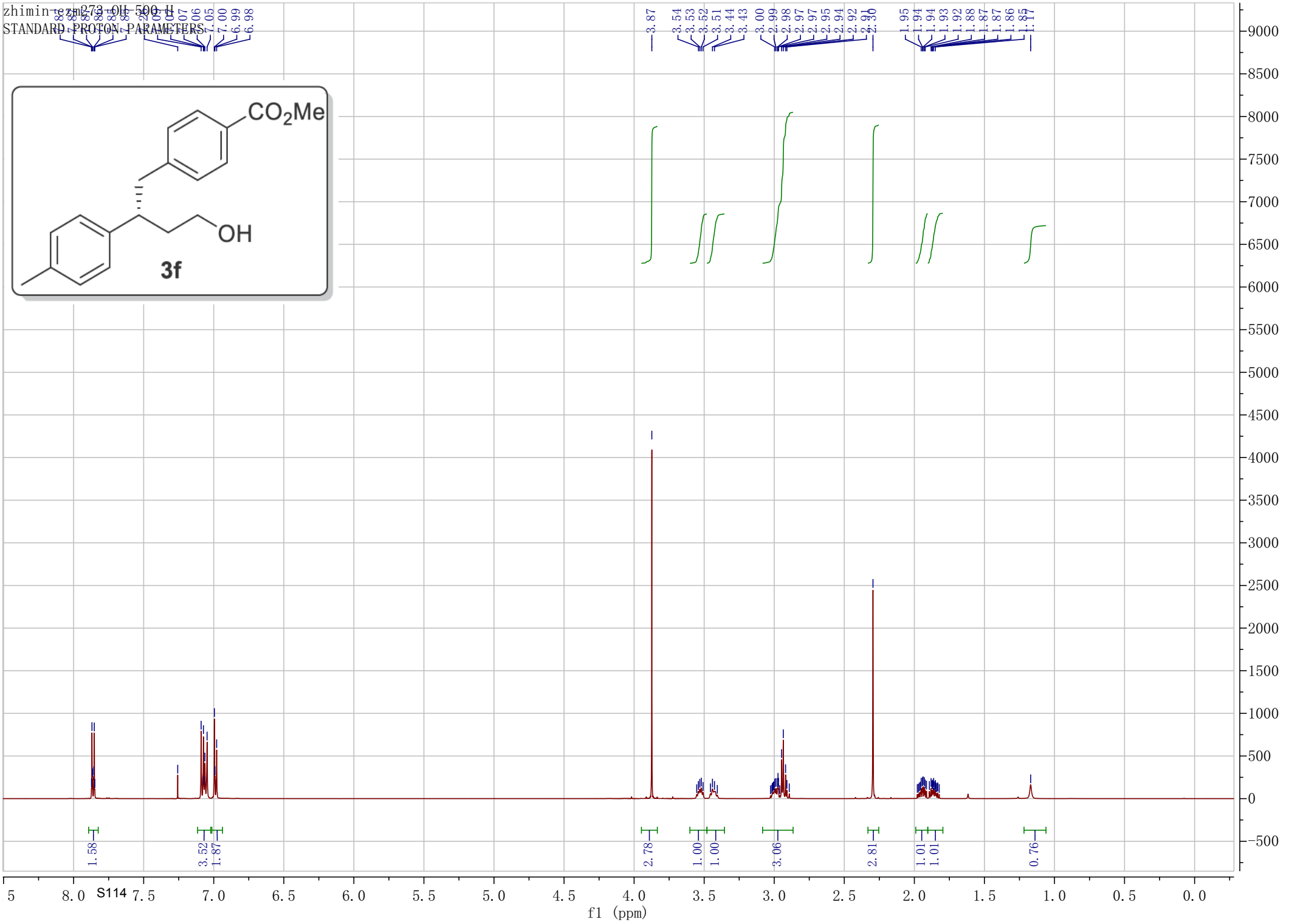

zhimin-czm136-CHO-C
STANDARD CARBON PARAMETERS
139.59
137.82
136.38
132.03
130.50
129.30
128.35
127.34
77.26
77.00
76.75
49.12
42.51
41.43
20.99
Cl
O
2e
f1 (ppm)

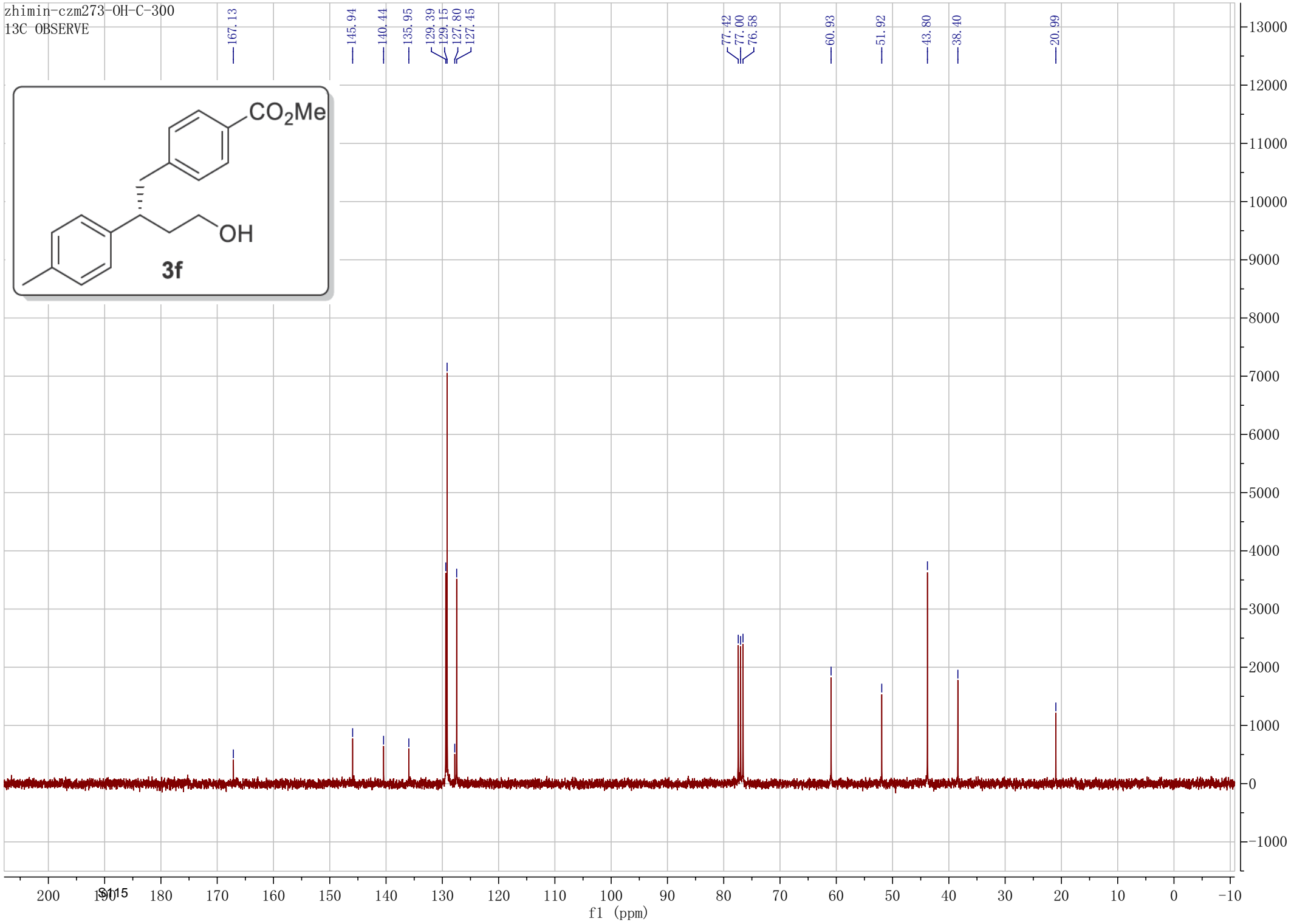

zhimin-czm261-OH-H
STANDARD PROTON PARAMETERS
7.26 7.17 7.16 7.16 7.15 7.15 7.14 7.08 7.06 7.00 7.00 6.99 6.96 6.95 6.95 6.94
3.55 3.53 3.53 3.52 3.52 3.51 3.51 3.50 3.49 3.47 3.45 3.43 3.43 3.43 3.42 3.41 3.41 3.40
2.92 2.92 2.91 2.90 2.86 2.84 2.81
1.93 1.92 1.92 1.91 1.90 1.84 1.83 1.83 1.82 1.81
Cl
OH
3e
1.51 1.70 3.79 2.00 0.95 1.96 2.70 1.95 0.85
f1 (ppm)

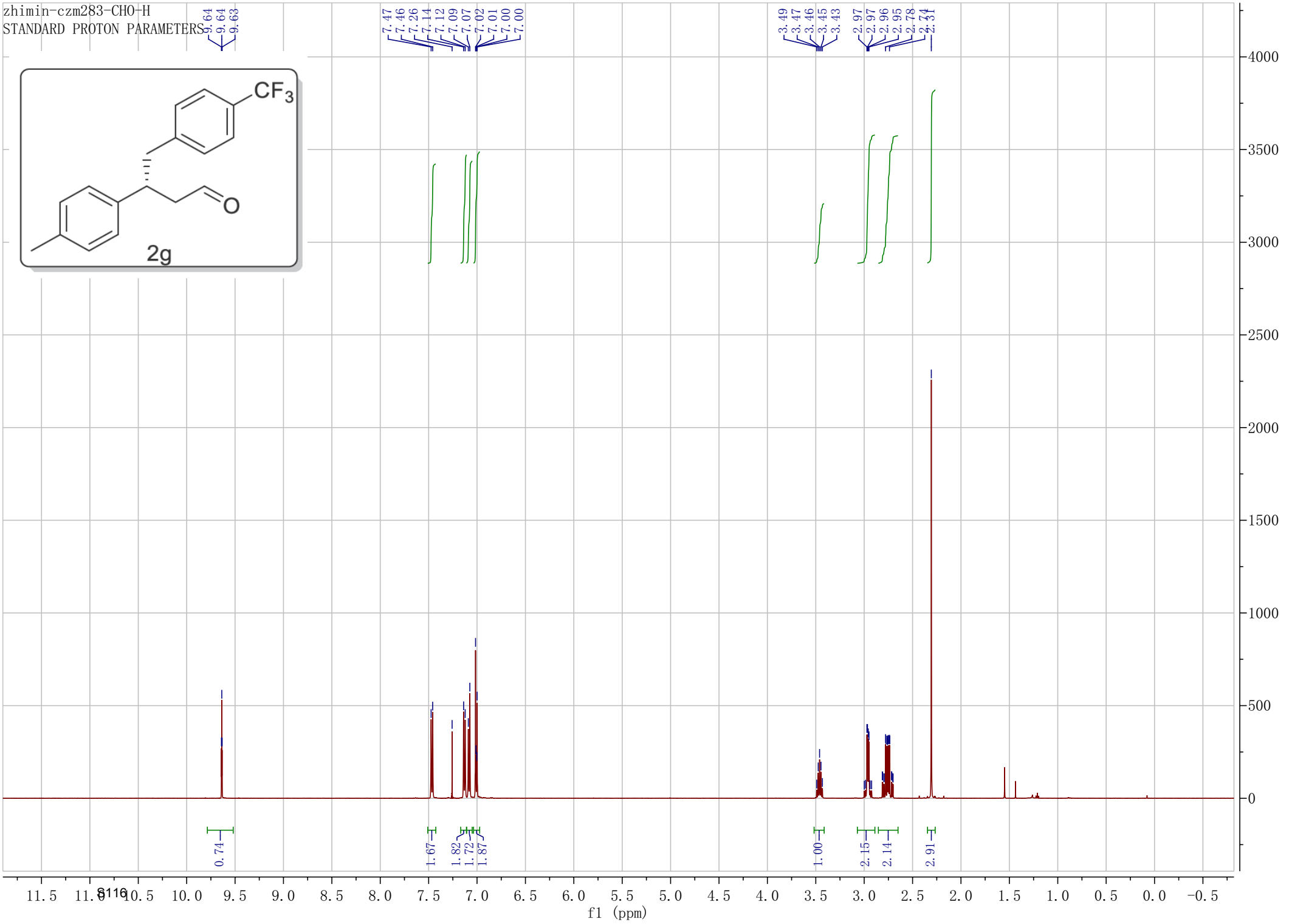

zhimin-czm261-OH-C
STANDARD CARBON PARAMETERS
140.63
138.82
135.93
131.58
130.45
129.17
128.16
127.49
77.25
77.00
76.75
61.00
43.96
43.13
38.30
21.00
Cl
OH
3e
f1 (ppm)

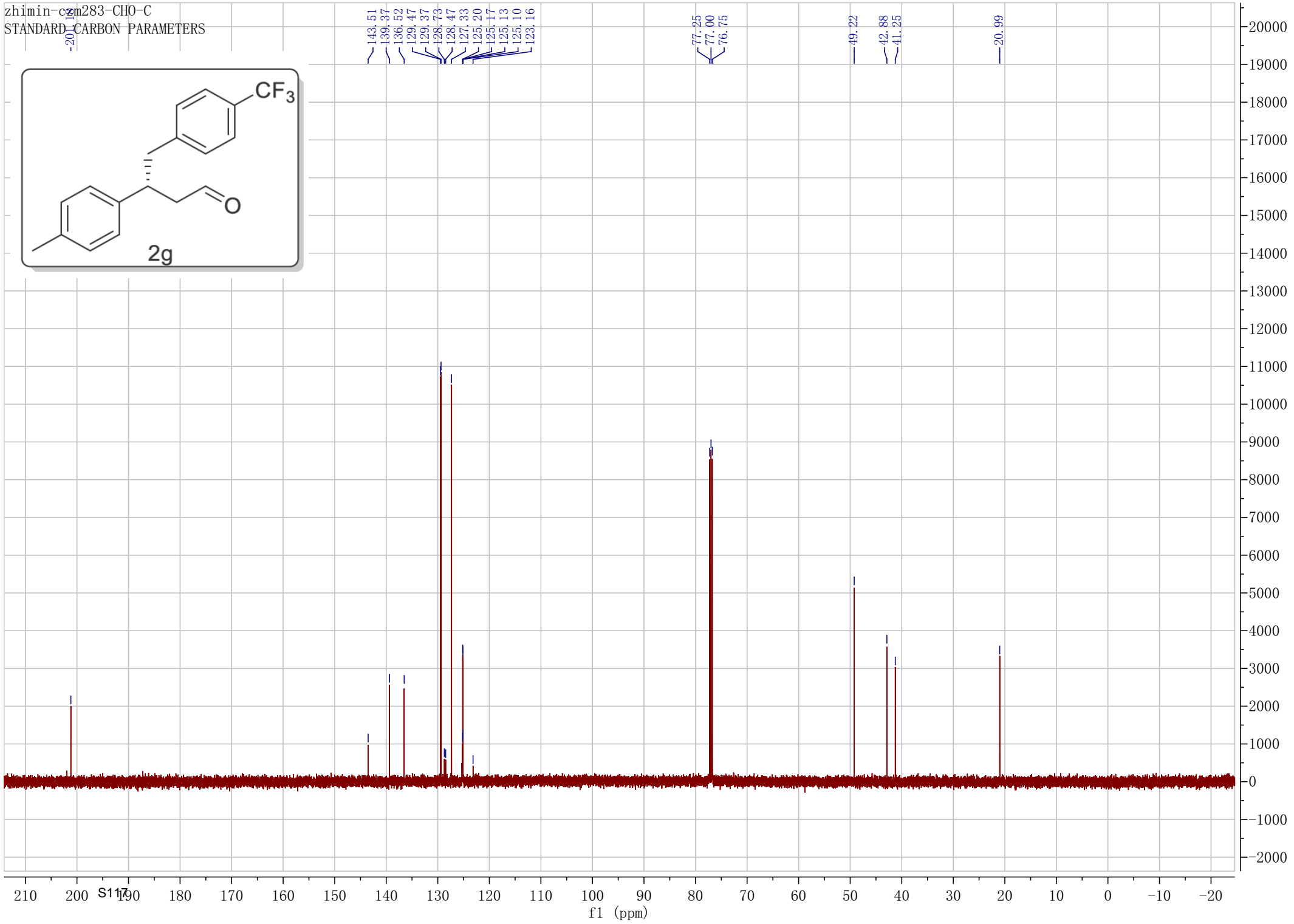

zhimin-czm273-CHO-500-H
STANDARD PROTON PARAMETERS
CO2Me
O
2f
f1 (ppm)

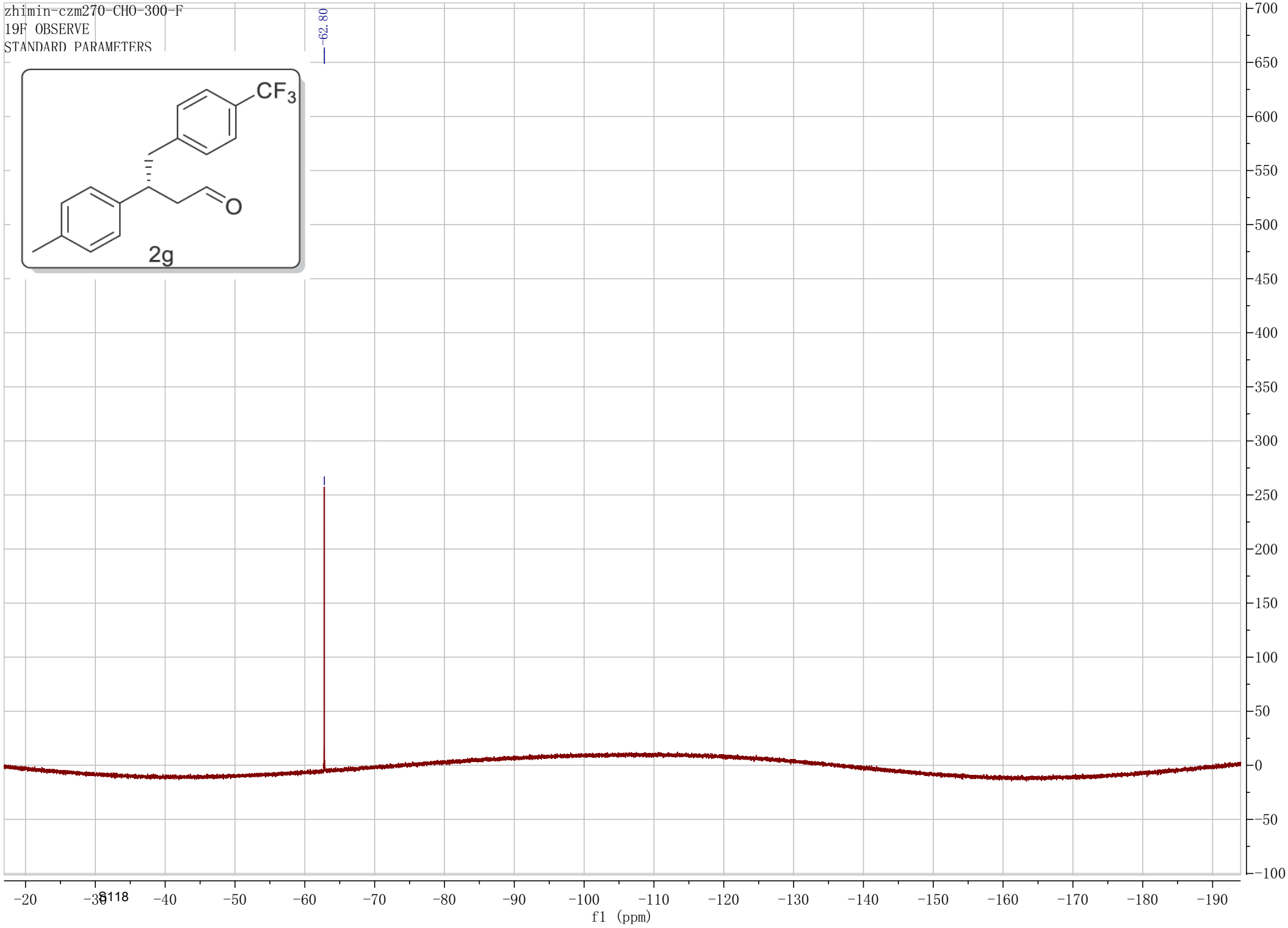

zhimm-czm273-CHO-300-C
13C OBSERVE
200.22
167.00
144.85
139.45
136.43
129.56
129.31
129.22
128.21
127.31
77.42
77.00
76.58
51.99
49.20
43.17
41.29
20.99
CO2Me
O
2f
f1 (ppm)

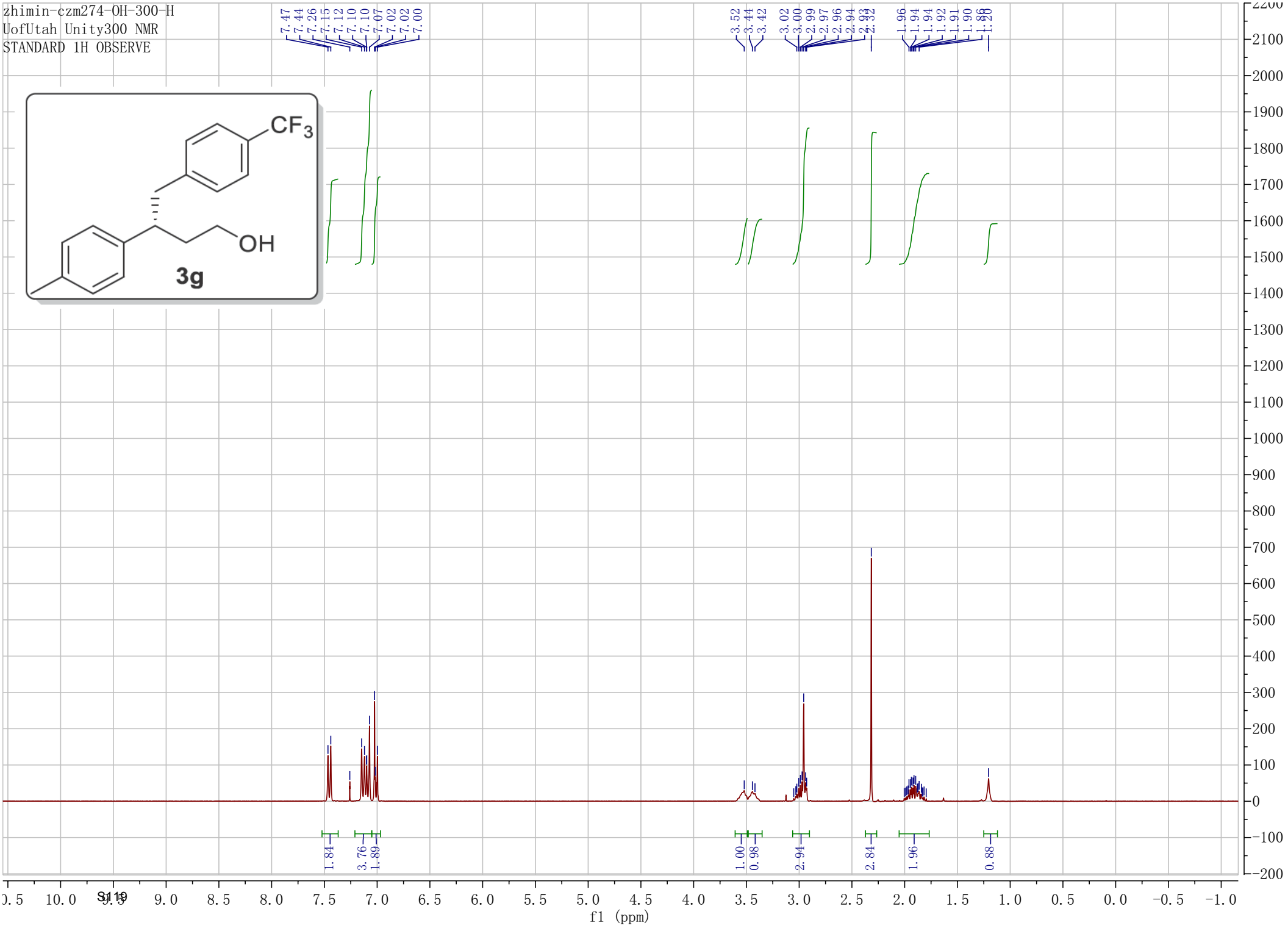

zhimin-ezm273-OH-500 H
STANDARD PROTON PARAMETERS
CO2Me
OH
3f
f1 (ppm)

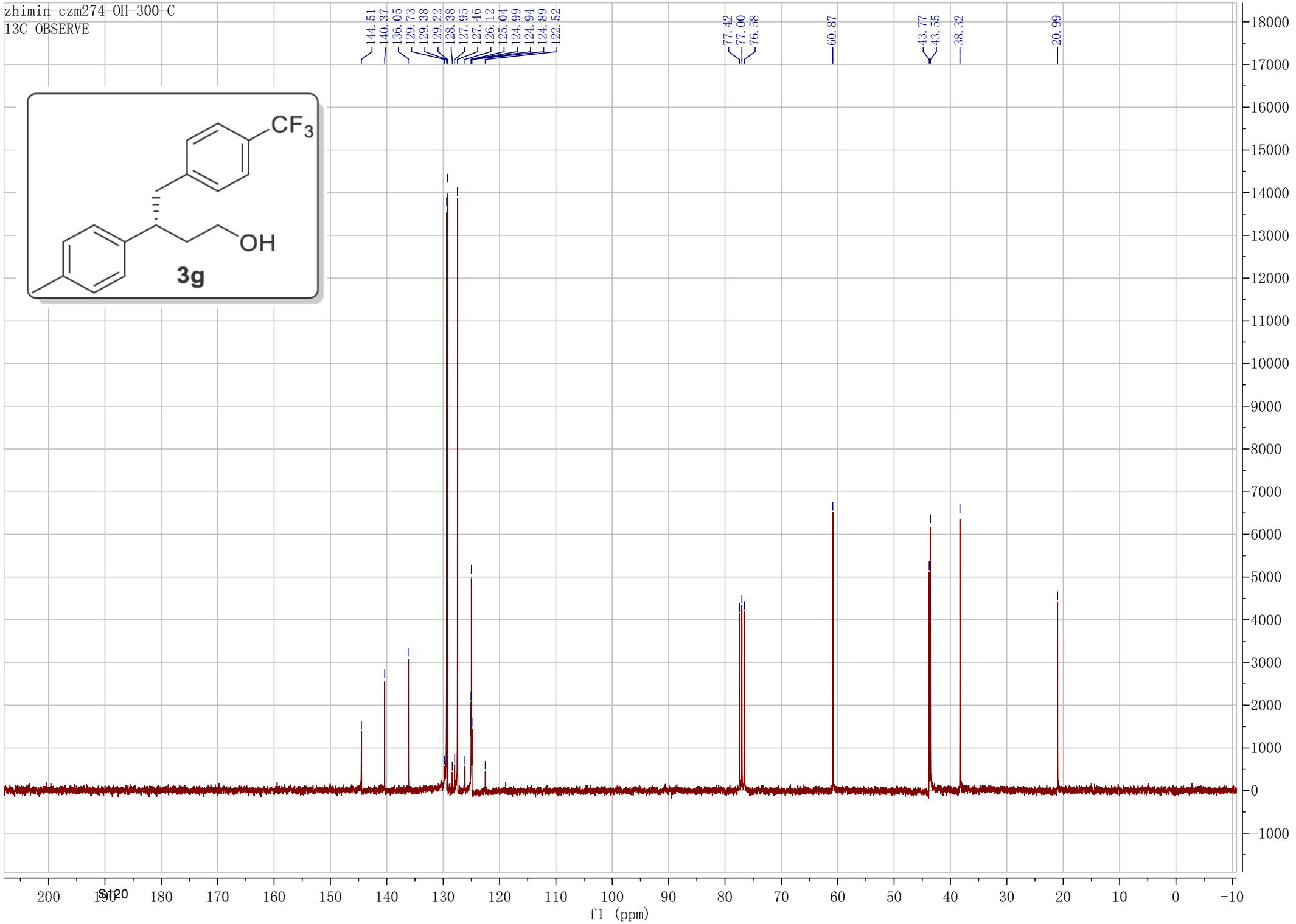

zhimin-czm273-OH-C-300
13C OBSERVE
167.13
145.94
140.44
135.95
129.39
129.15
127.80
127.45
77.42
77.00
76.58
60.93
51.92
43.80
38.40
20.99
CO2Me
OH
3f
f1 (ppm)


zhimin-czm283-CHO-H
STANDARD PROTON PARAMETERS
9.64
9.64
9.63
7.47
7.46
7.26
7.14
7.12
7.09
7.07
7.02
7.01
7.00
7.00
3.49
3.47
3.46
3.45
3.43
2.97
2.97
2.96
2.95
2.78
2.74
2.31
CF3
O
2g
0.74
1.67
1.82
1.72
1.87
1.00
2.15
2.14
2.91
4000
3500
3000
2500
2000
1500
1000
500
0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


zhimin-czm283-CHO-C
STANDARD CARBON PARAMETERS
-20.
143.51
139.37
136.52
129.47
129.37
128.73
128.47
127.33
125.20
125.17
125.13
125.10
123.16
77.25
77.00
76.75
49.22
42.88
41.25
20.99
CF3
O
2g
f1 (ppm)

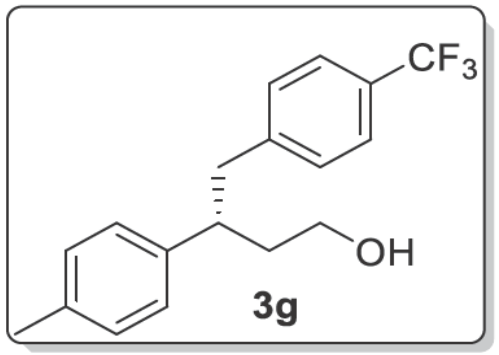

zhimin-czm270-CHO-300-F
19F OBSERVE
STANDARD PARAMETERS
-62.80
CF3
O
2g
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
-100
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


zhimin-czm274-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.47
7.44
7.26
7.15
7.12
7.10
7.10
7.07
7.02
7.02
7.00
3.52
3.44
3.42
3.02
3.00
2.99
2.97
2.96
2.94
2.93
2.32
1.96
1.94
1.94
1.92
1.91
1.90
1.86
1.20
CF3
OH
3g
1.84
3.76
1.89
1.00
0.98
2.94
2.84
1.96
0.88
f1 (ppm)

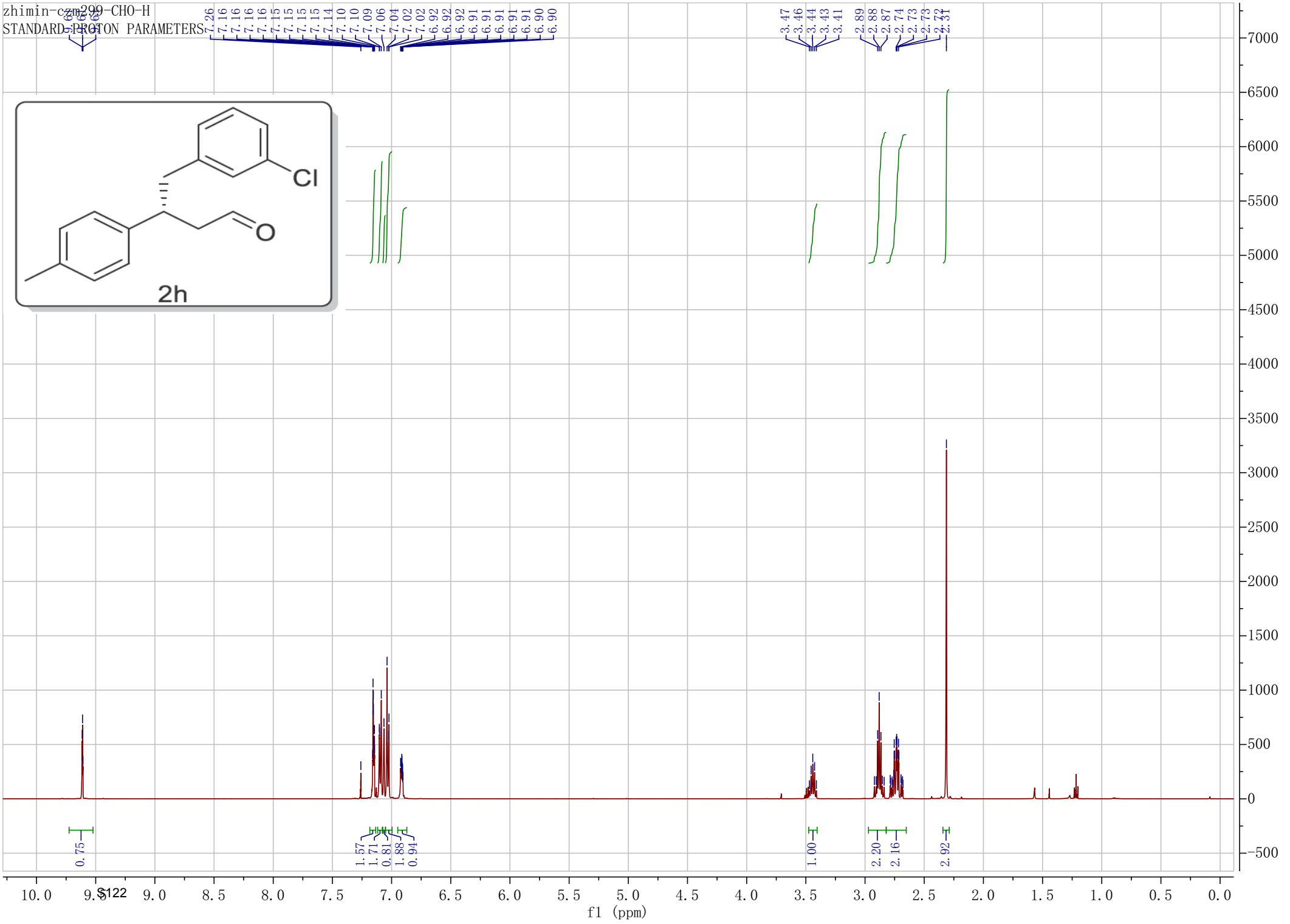

zhimin-czm274-OH-300-C
13C OBSERVE
144.51
140.37
136.05
129.73
129.38
129.22
128.38
127.95
127.46
126.12
125.04
124.99
124.94
124.89
122.52
77.42
77.00
76.58
60.87
43.77
43.55
38.32
20.99
CF3
OH
3g
f1 (ppm)

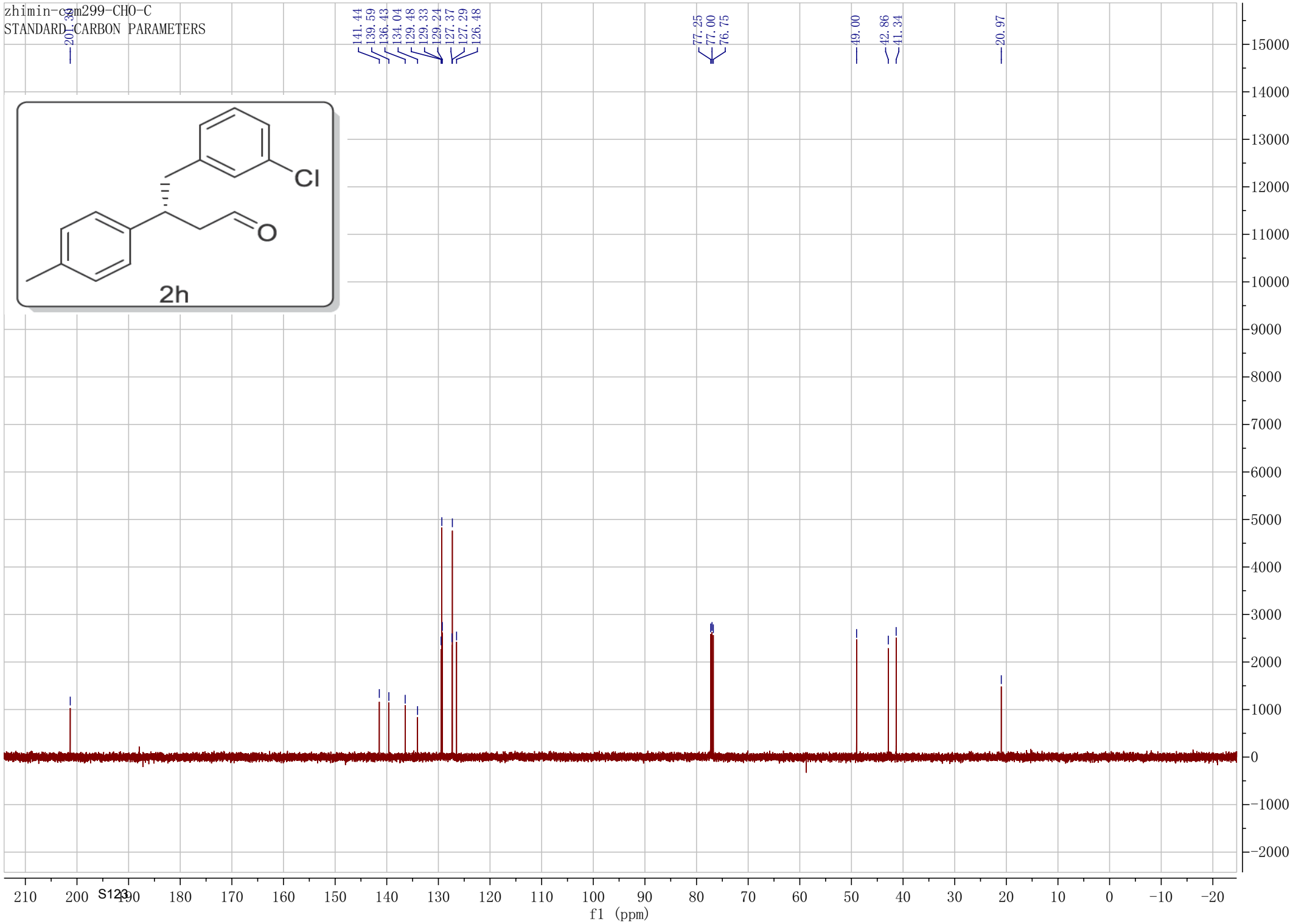
zhimin-czm274-OH-300-F
19F OBSERVE
STANDARD PARAMETERS

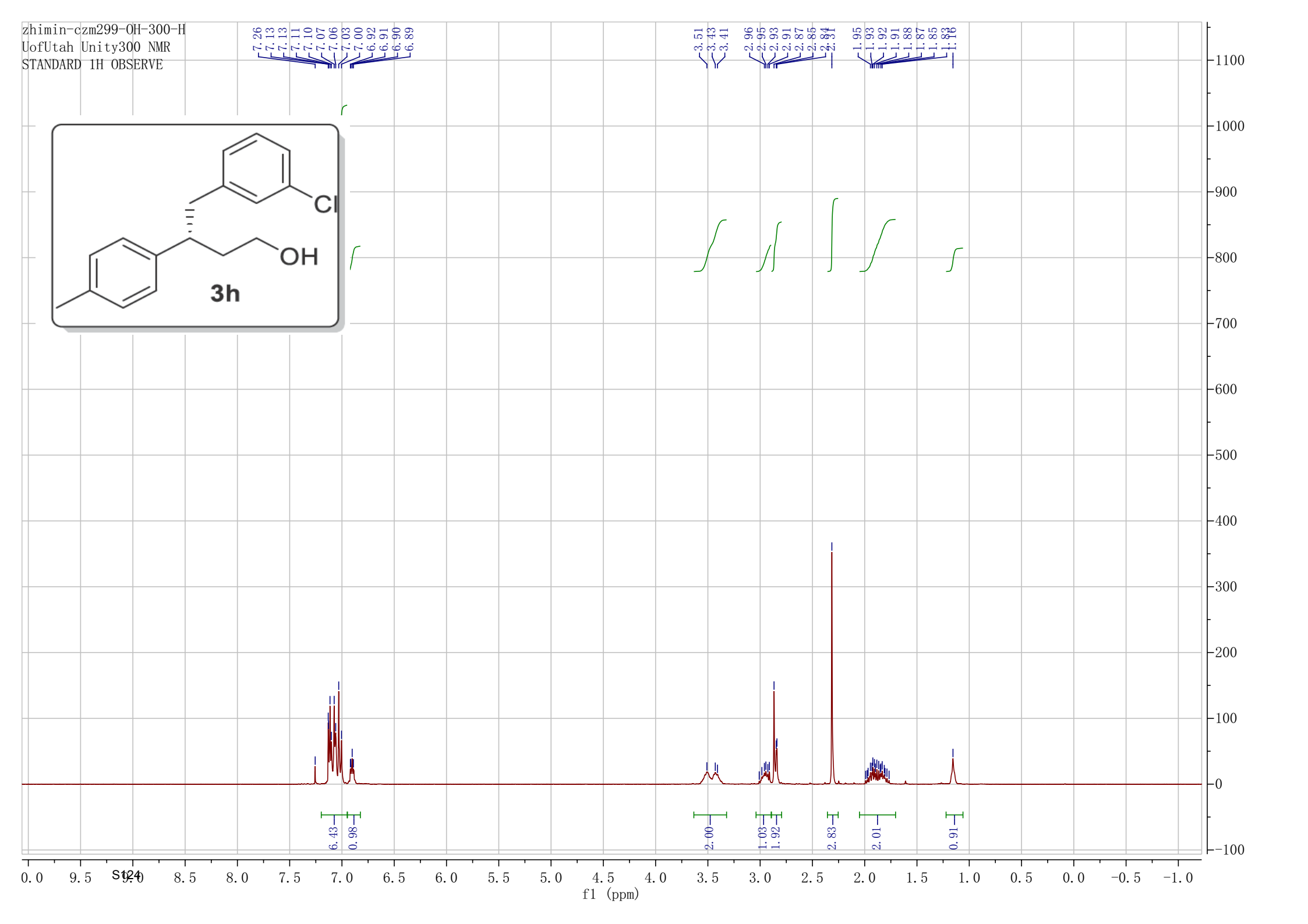
-62.70

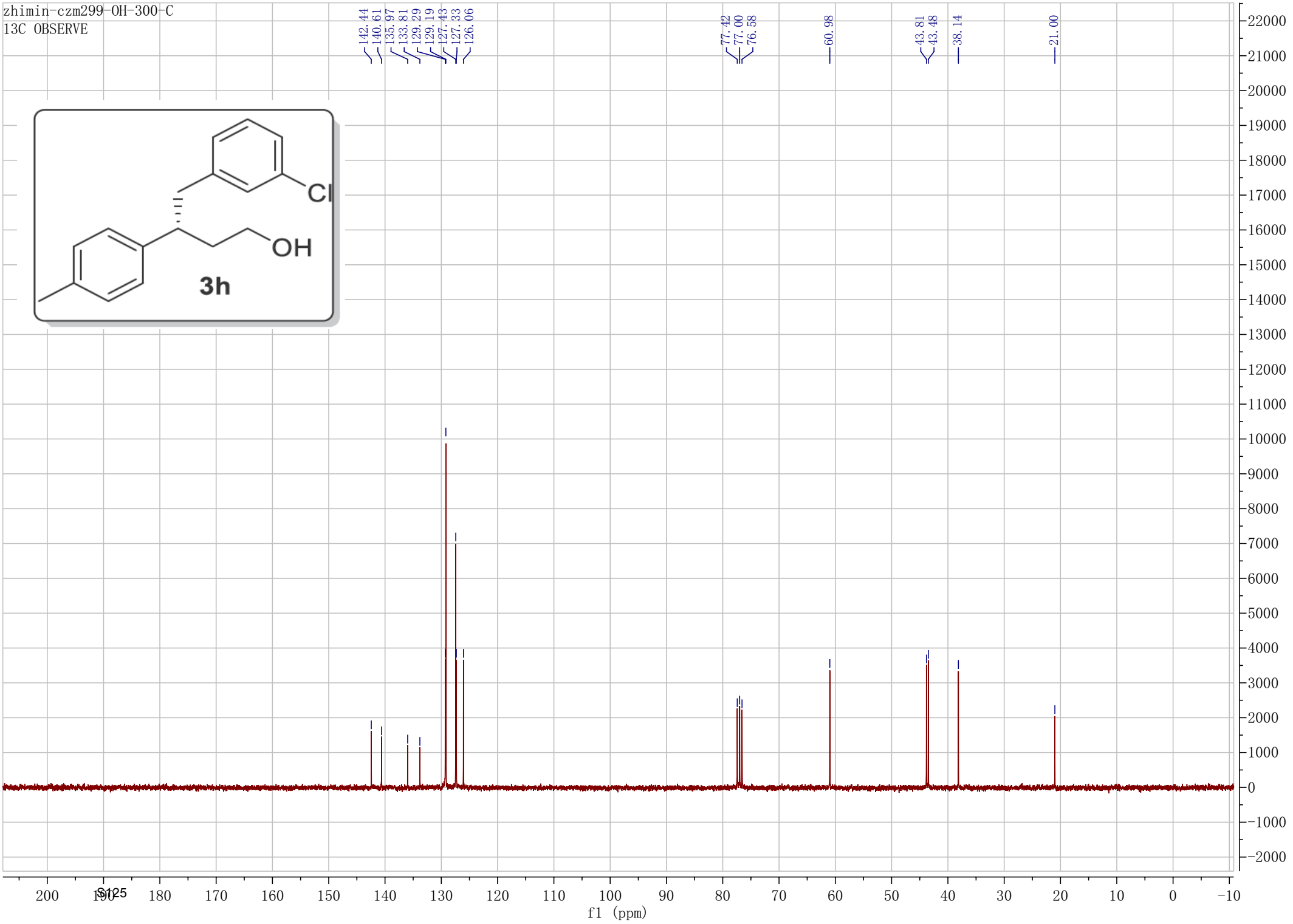


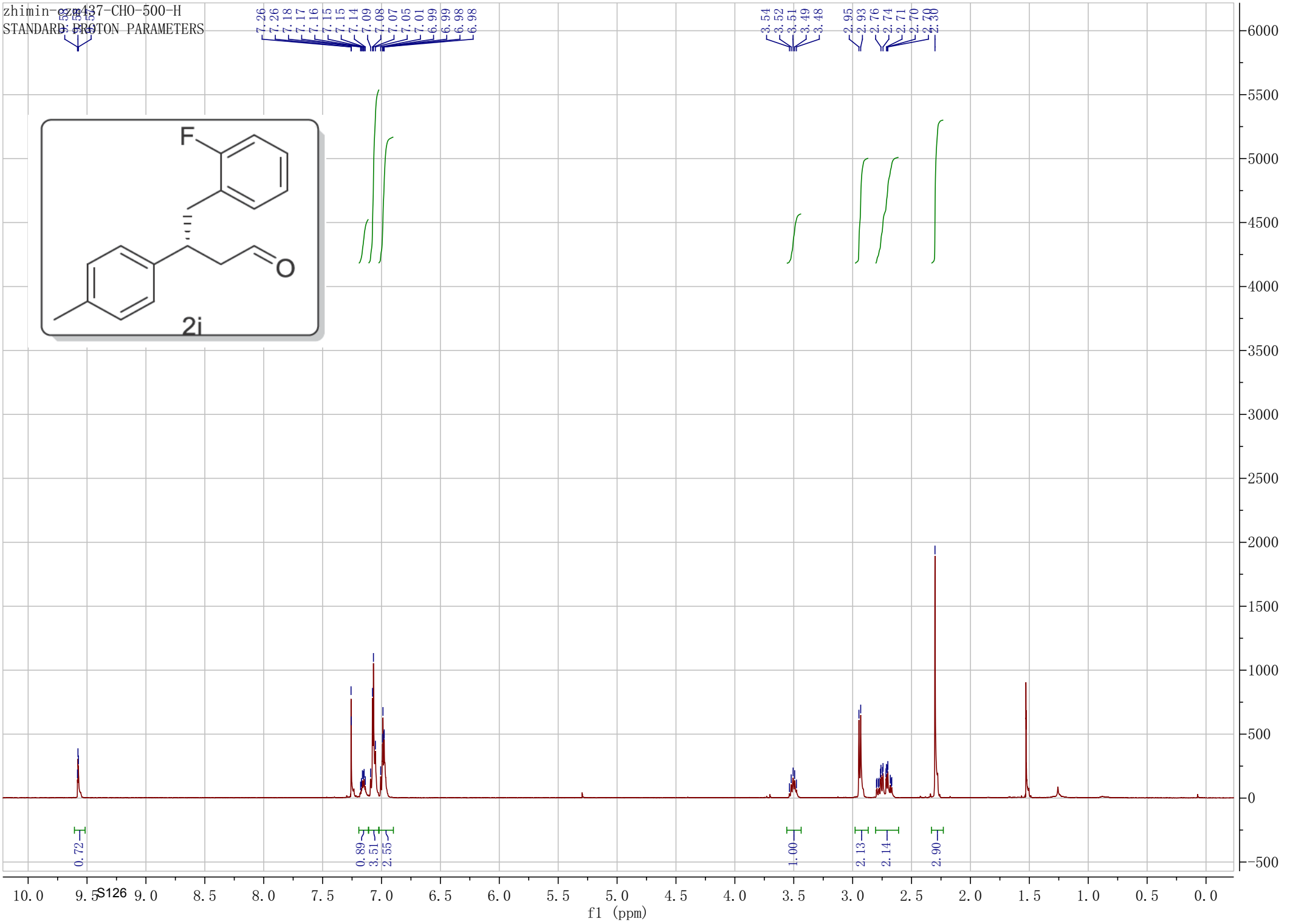
f1 (ppm)

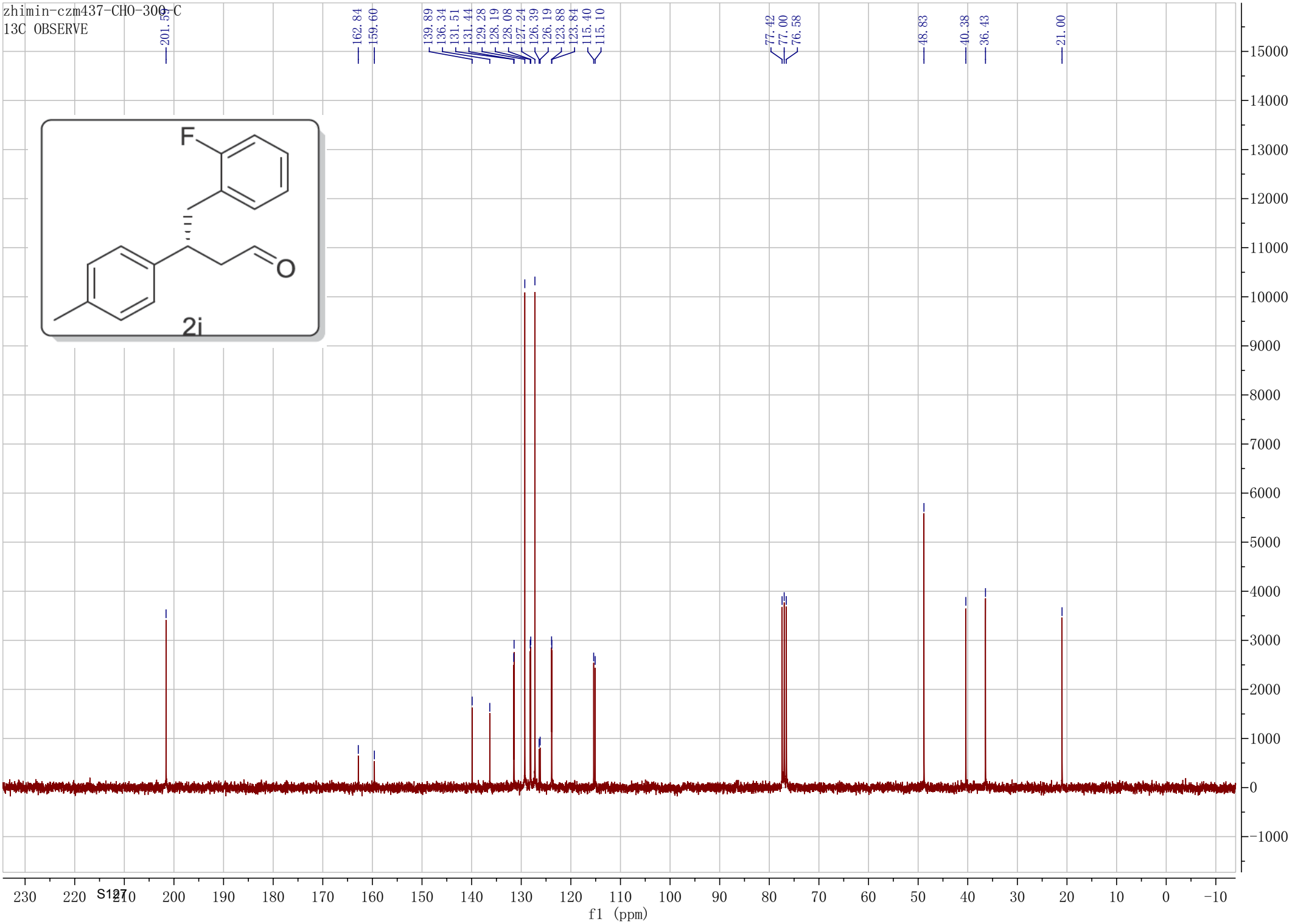

zhimin-czm299-CHO-H
STANDARD PROTON PARAMETERS
Cl
O
2h
f1 (ppm)

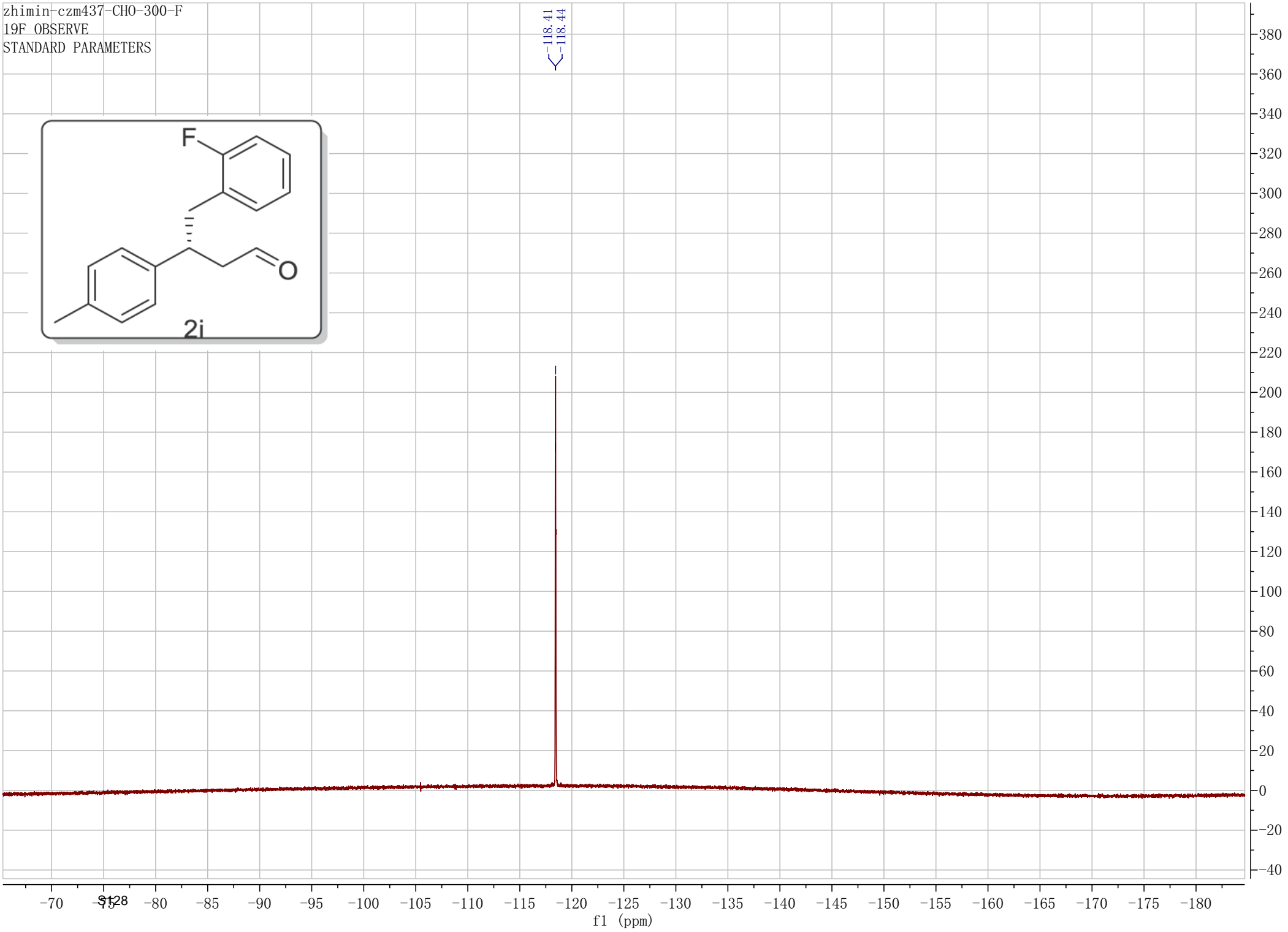

zhimin-cxm299-CHO-C
STANDARD-CARBON PARAMETERS
20.38
141.44
139.59
136.43
134.04
129.48
129.33
129.24
127.37
127.29
126.48
77.25
77.00
76.75
49.00
42.86
41.34
20.97
Cl
O
2h
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

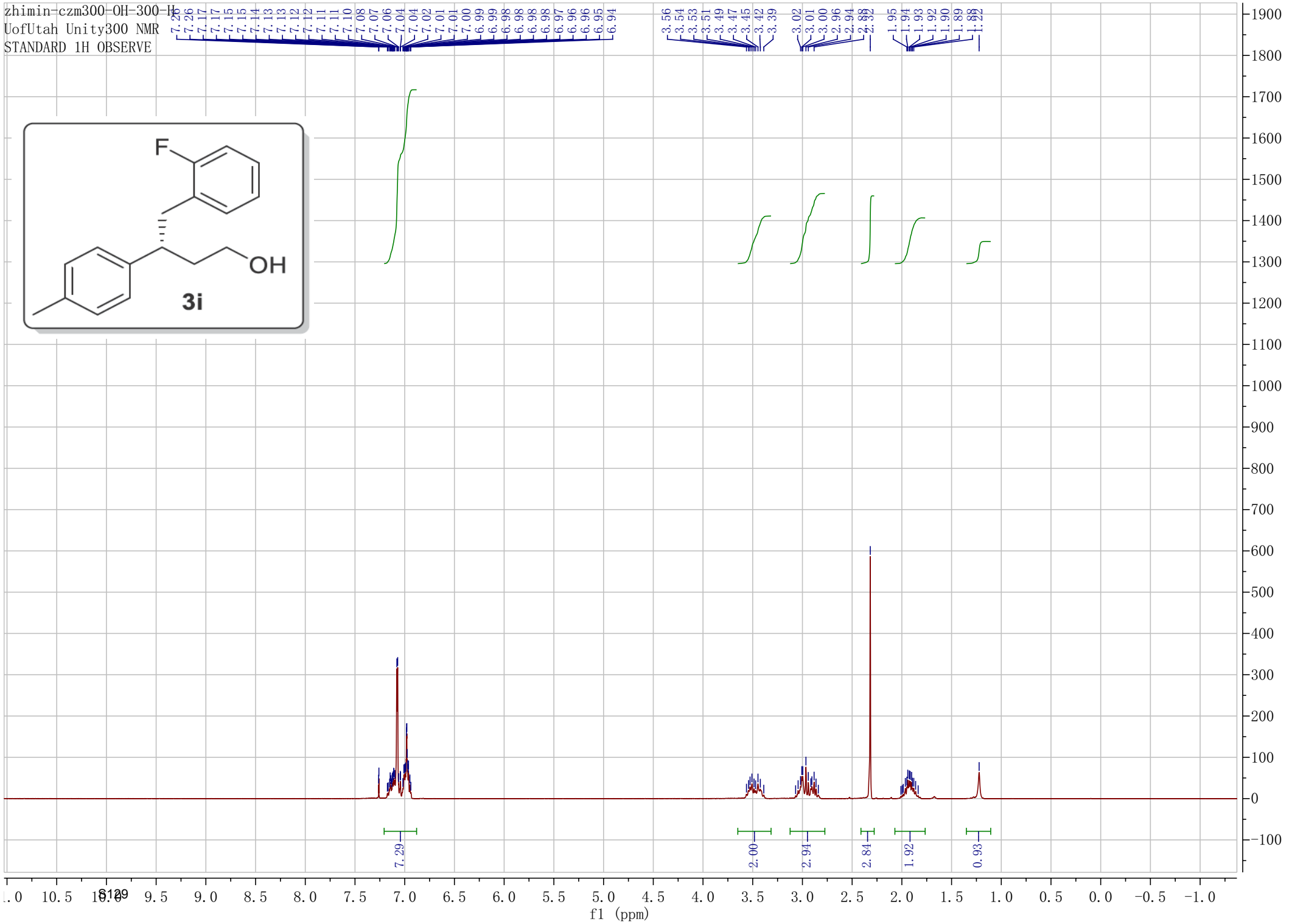

zhimin-czm299-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.26
7.13
7.13
7.11
7.10
7.07
7.06
7.03
7.00
6.92
6.91
6.90
6.89
3.51
3.43
3.41
2.96
2.95
2.93
2.91
2.87
2.85
2.84
2.81
1.95
1.93
1.92
1.91
1.88
1.87
1.85
1.83
1.16
Cl
OH
3h
6.43
0.98
2.00
1.03
1.92
2.83
2.01
0.91
f1 (ppm)

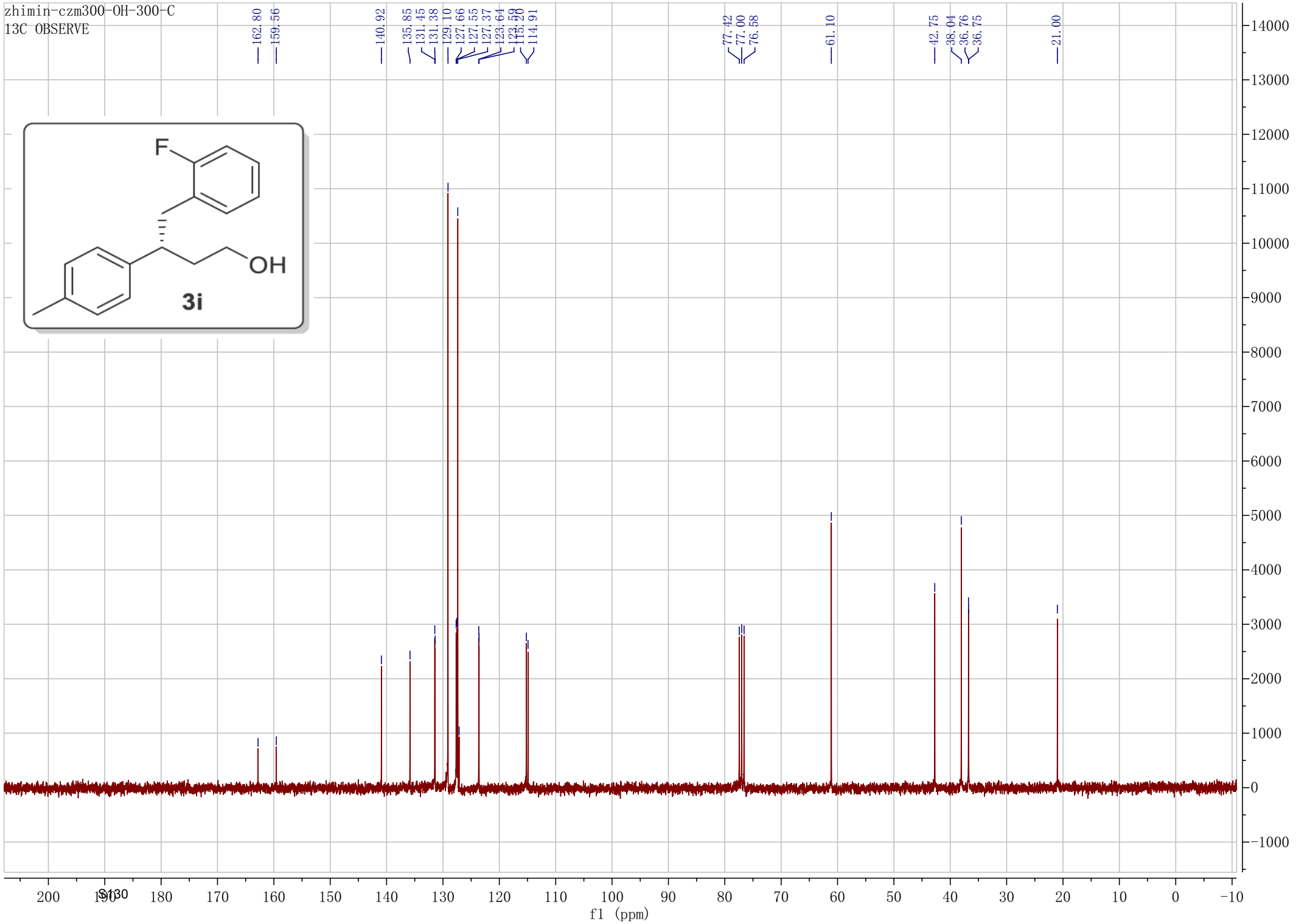

zhimin-czm299-OH-300-C
13C OBSERVE
142.44
140.61
135.97
133.81
129.29
129.19
127.43
127.33
126.06
77.42
77.00
76.58
60.98
43.81
43.48
38.14
21.00
Cl
OH
3h
f1 (ppm)


zhimin-czm437-CHO-500-H
STANDARD PROTON PARAMETERS
7.26
7.26
7.18
7.17
7.16
7.15
7.15
7.14
7.09
7.08
7.07
7.05
7.01
6.99
6.99
6.98
6.98
3.54
3.52
3.51
3.49
3.48
2.95
2.93
2.76
2.74
2.71
2.70
2.30
F
O
2i
0.72
0.89
3.51
2.55
1.00
2.13
2.14
2.90
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

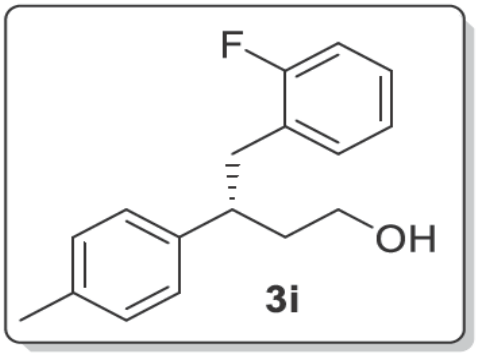

zhimin-czm437-CHO-300-C
13C OBSERVE
201.53
162.84
159.60
139.89
136.34
131.51
131.44
129.28
128.19
128.08
127.24
126.39
126.19
123.88
123.84
115.40
115.10
77.42
77.00
76.58
48.83
40.38
36.43
21.00
F
O
2i
S127
f1 (ppm)


zhimin-czm437-CHO-300-F
19F OBSERVE
STANDARD PARAMETERS
-118.41
-118.44
F
O
2i
f1 (ppm)


zhimin-czm300-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
F
OH
3i
7.29
2.00
2.94
2.84
1.92
0.93
f1 (ppm)


zhimin-czm300-OH-300-C
13C OBSERVE
162.80
159.56
140.92
135.85
131.45
131.38
129.10
127.66
127.55
127.37
123.64
123.59
115.20
114.91
77.42
77.00
76.58
61.10
42.75
38.04
36.76
36.75
21.00
F
OH
3i
f1 (ppm)

zhimin-czm300-OH-300-F
19F OBSERVE
STANDARD PARAMETERS

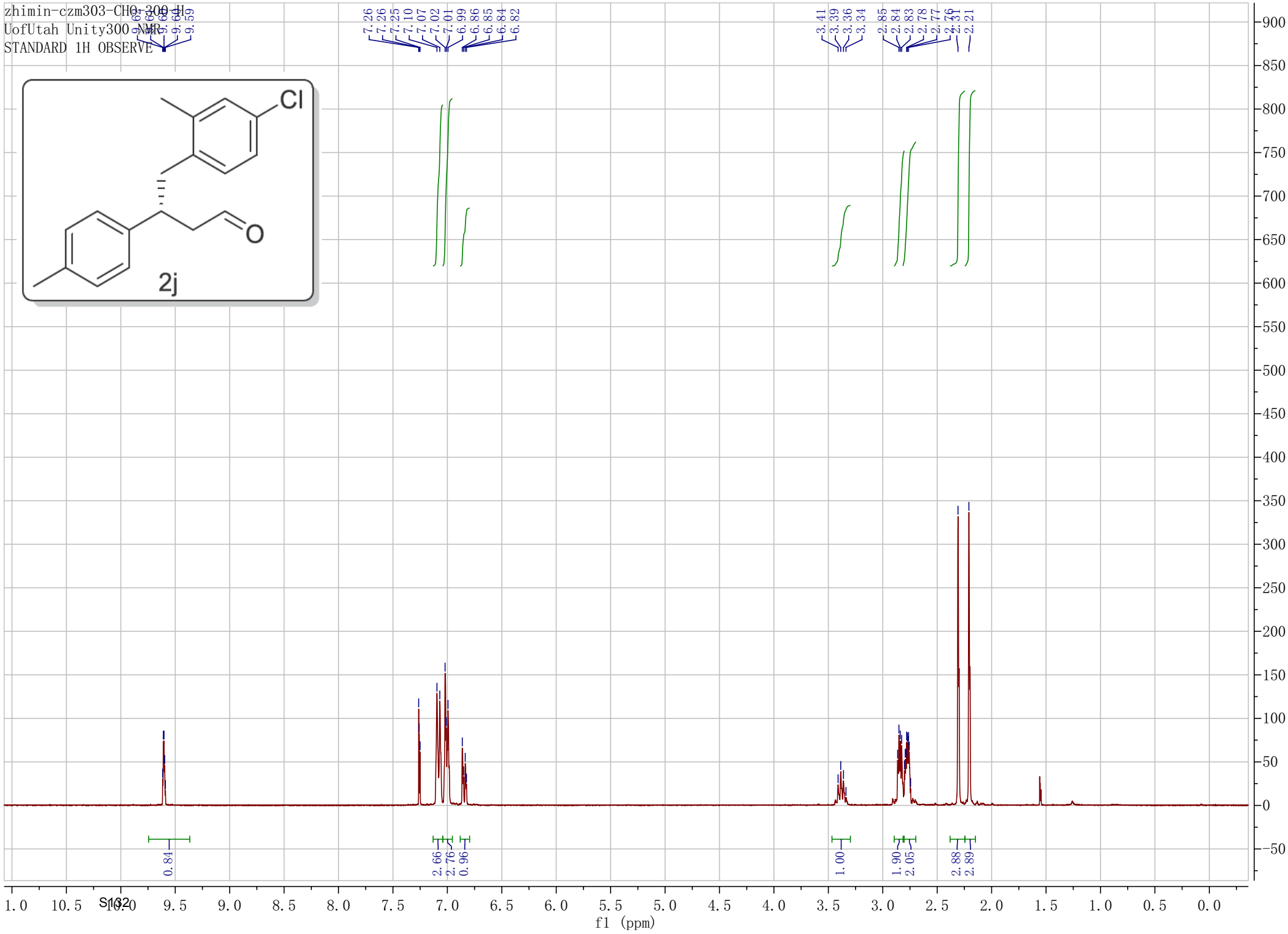


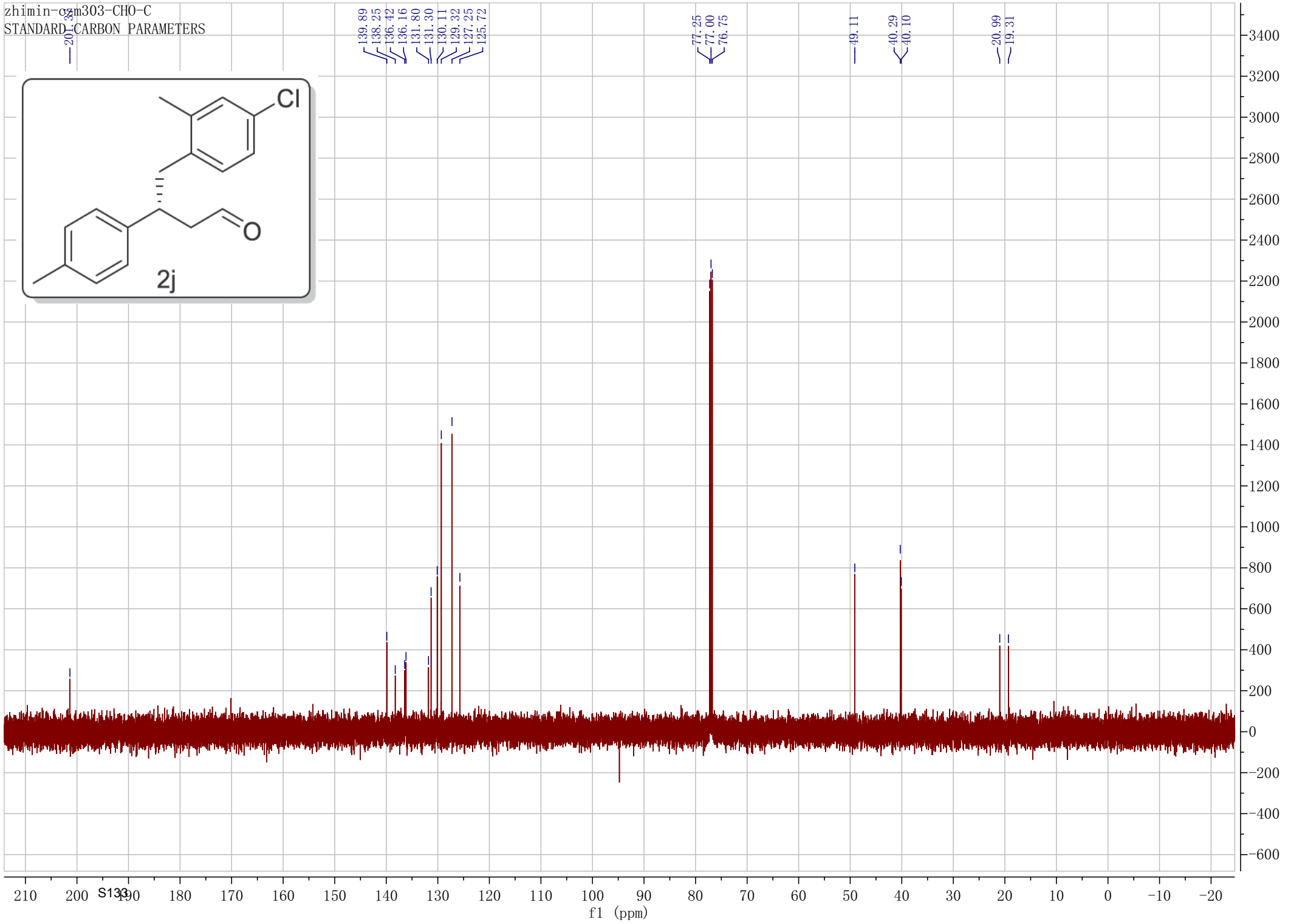
-118.56
-118.58
-118.60
-118.61
-118.64

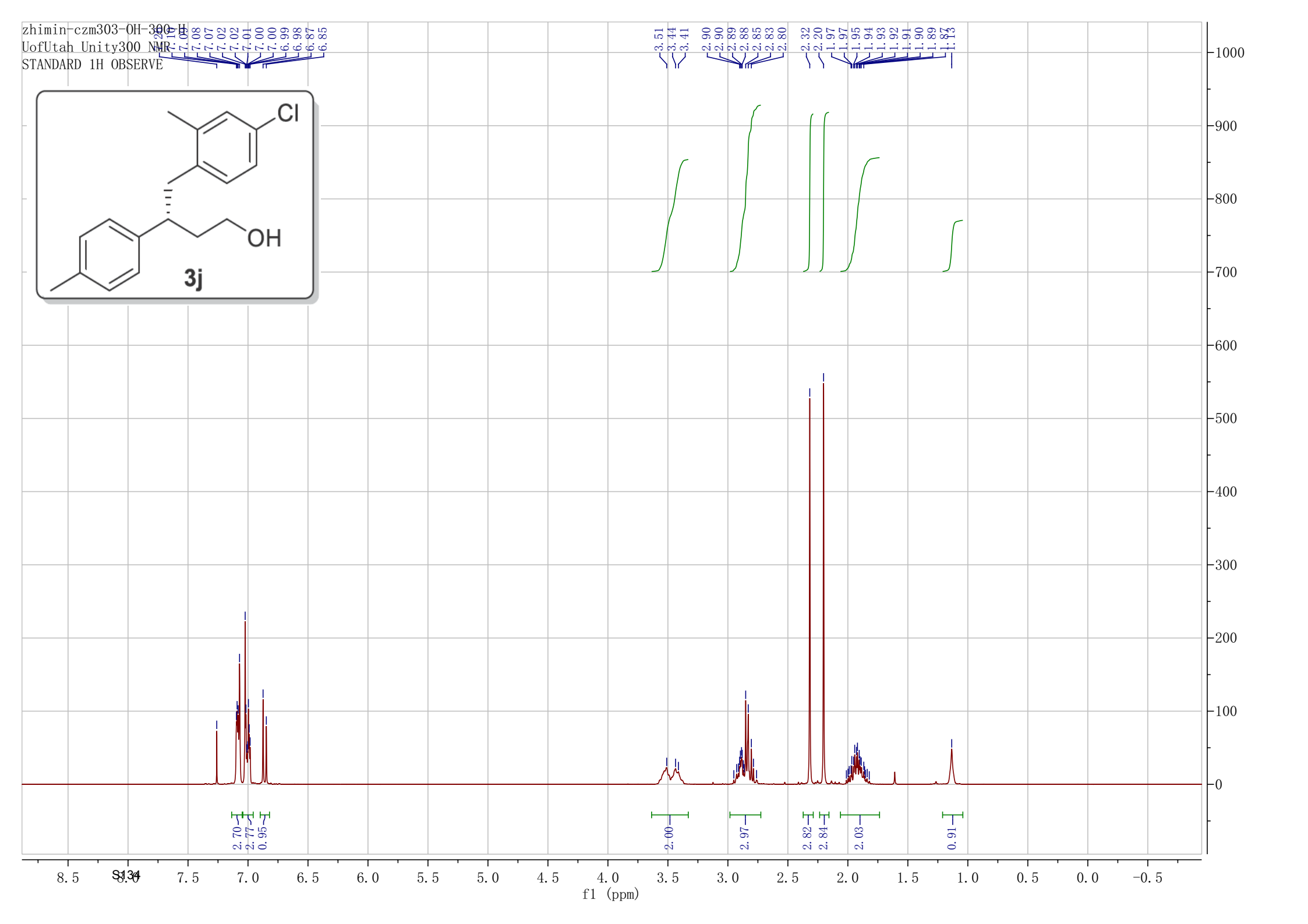
1100
1000
900
800
700
600
500
400
300
200
100
0
-100

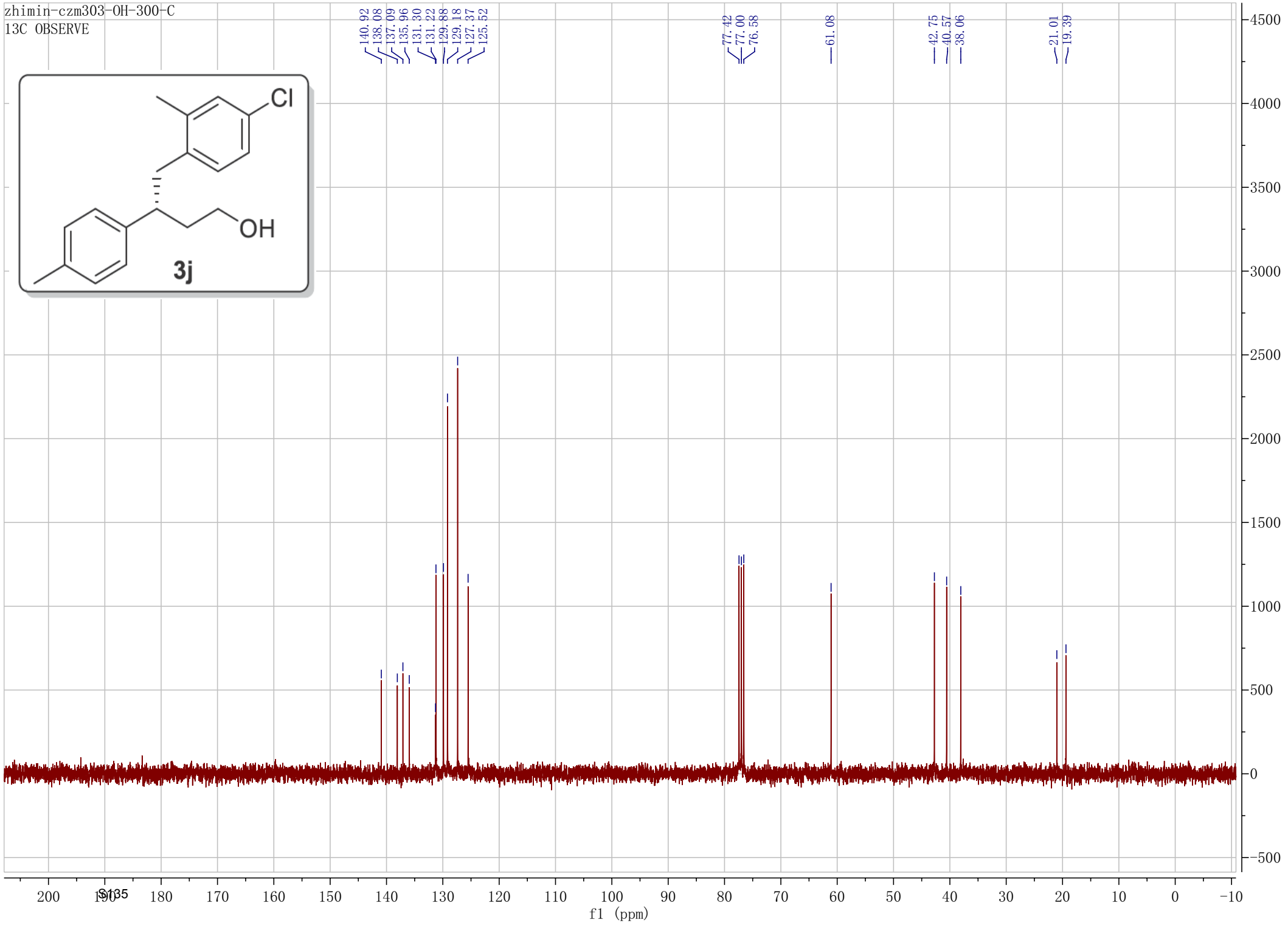
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190

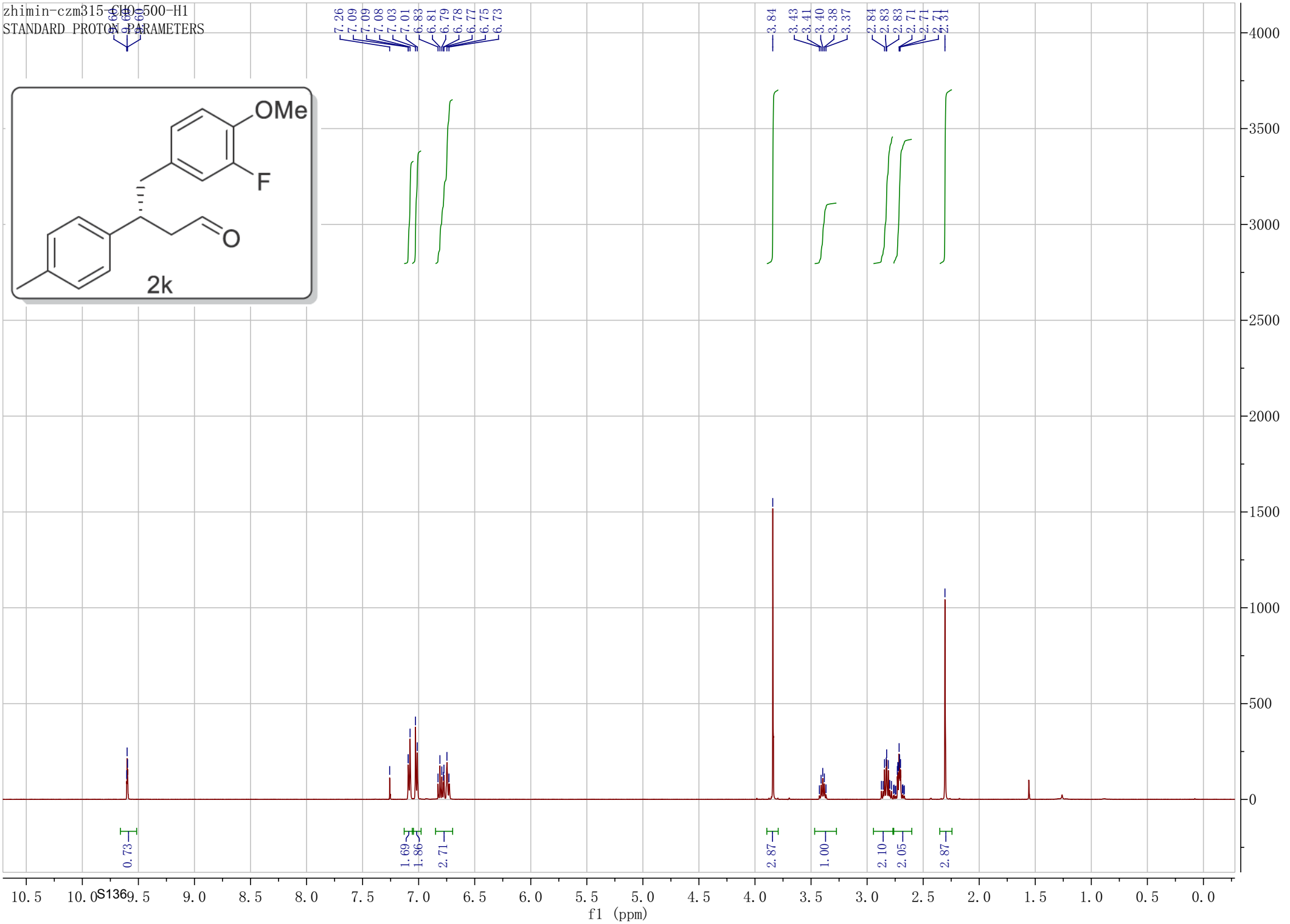
f1 (ppm)

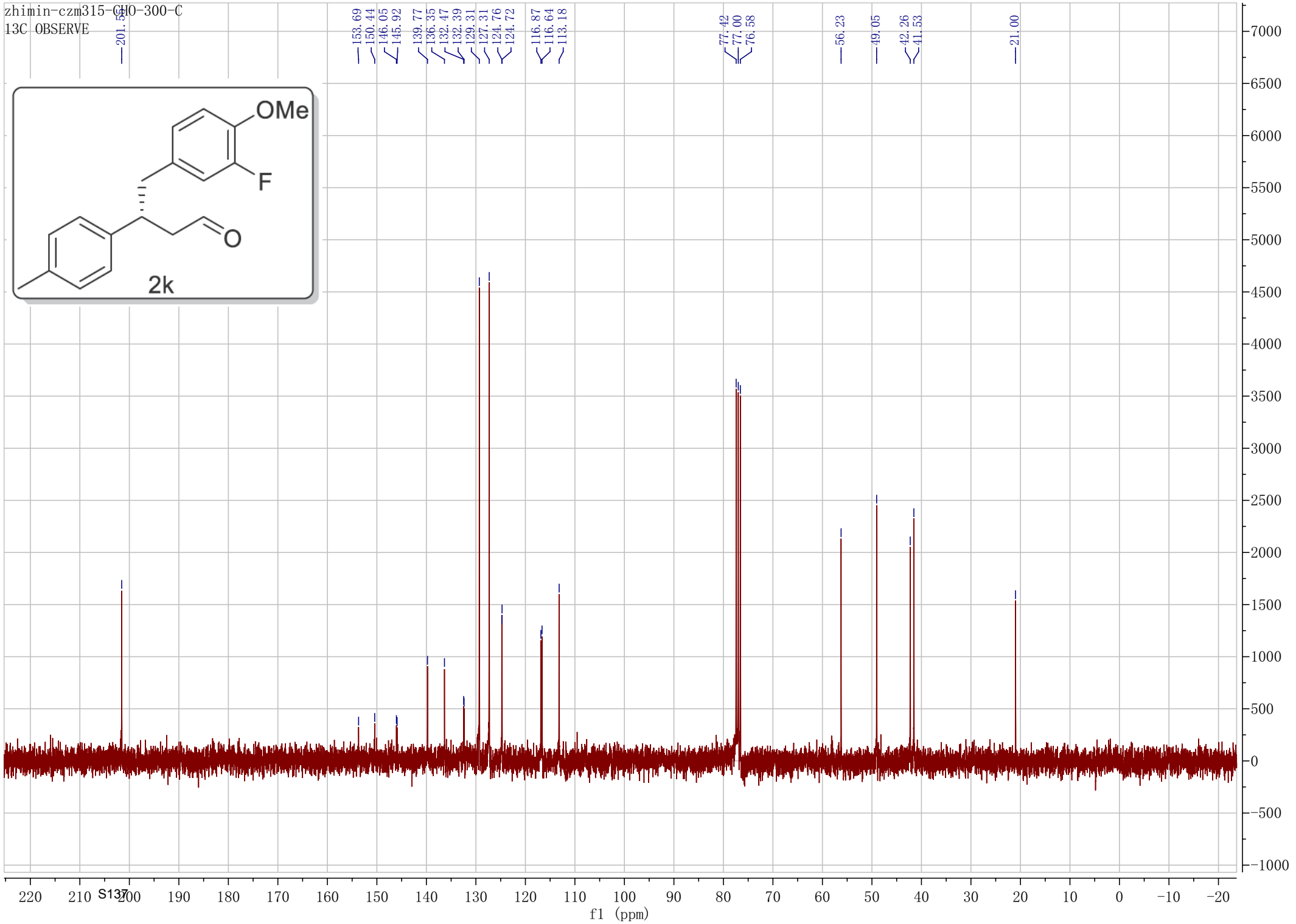

zhimin-czm303-CHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
9.65
9.64
9.59
7.26
7.25
7.10
7.07
7.02
7.01
6.99
6.86
6.85
6.84
6.82
3.41
3.39
3.36
3.34
2.85
2.84
2.83
2.78
2.77
2.76
2.31
2.21
Cl
O
2j
0.84
2.66
2.76
0.96
1.00
1.90
2.05
2.88
2.89
f1 (ppm)

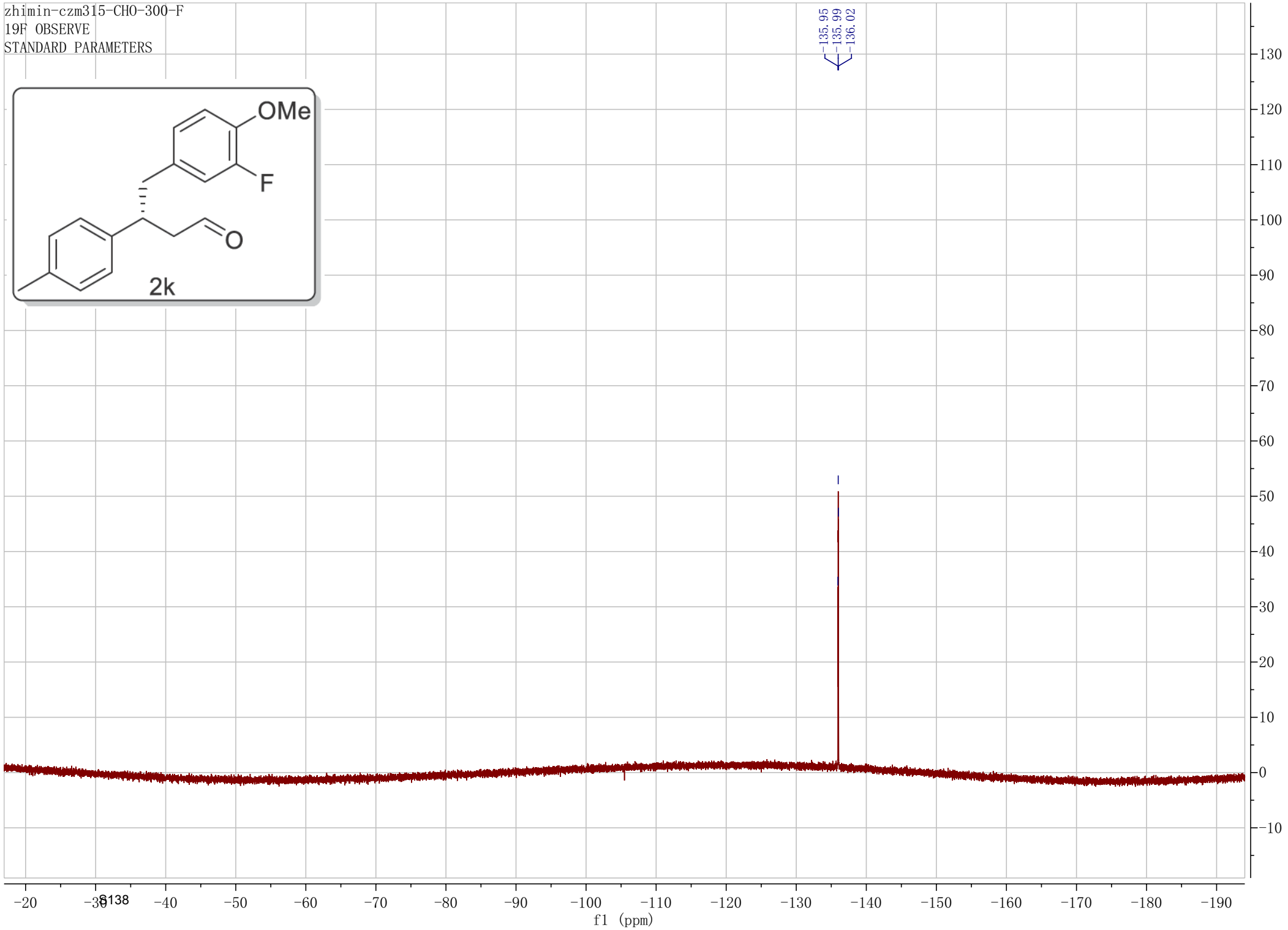

zhimin-ozm303-CHO-C
STANDARD-CARBON PARAMETERS
139.89
138.25
136.42
136.16
131.80
131.30
130.11
129.32
127.25
125.72
77.25
77.00
76.75
49.11
40.29
40.10
20.99
19.31
Cl
O
2j
f1 (ppm)

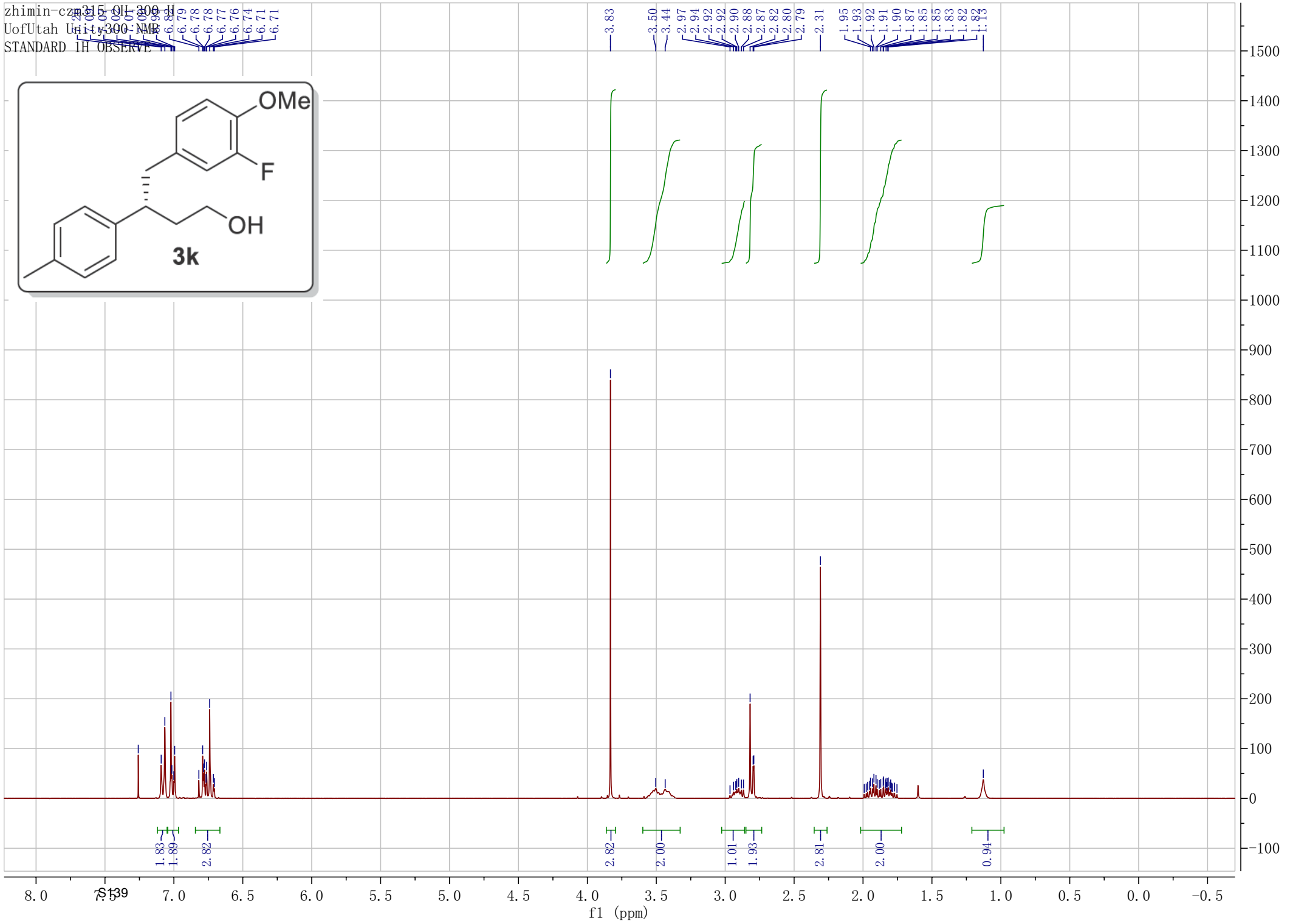

zhimin-czm303-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
OH
3j
f1 (ppm)

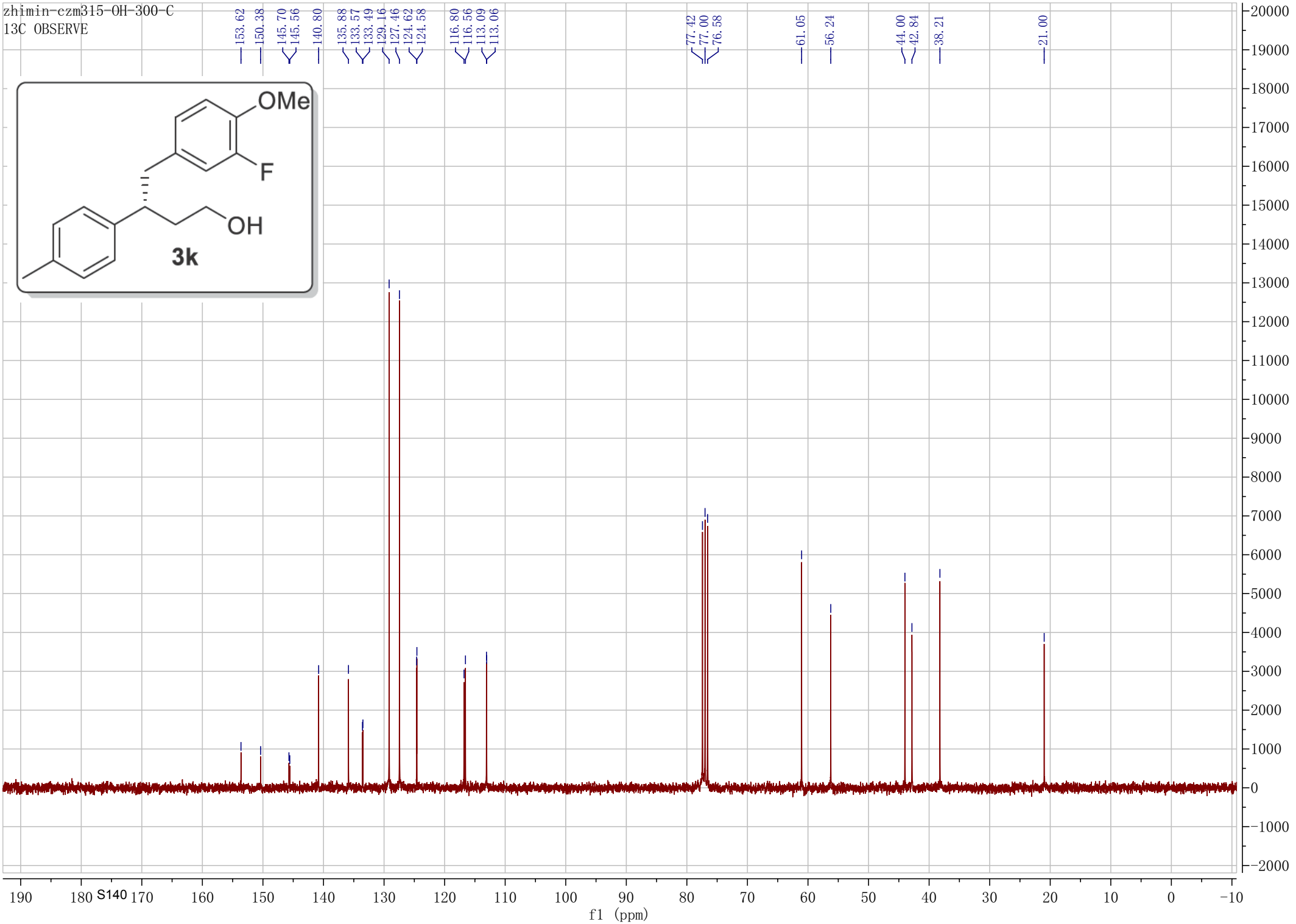

zhimin-czm303-OH-300-C
13C OBSERVE
140.92
138.08
137.09
135.96
131.30
131.22
129.88
129.18
127.37
125.52
77.42
77.00
76.58
61.08
42.75
40.57
38.06
21.01
19.39
Cl
OH
3j
f1 (ppm)

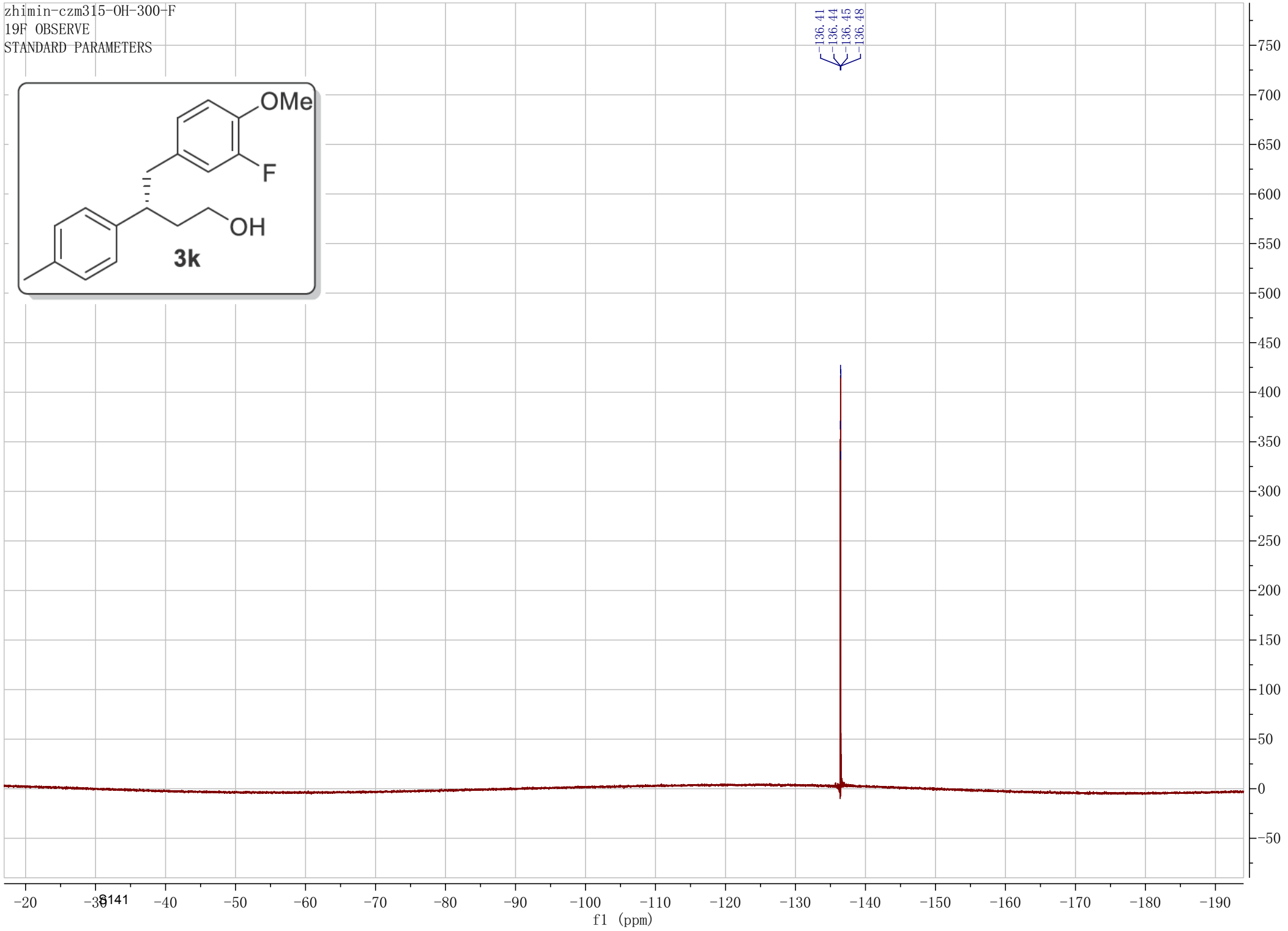

zhimin-czm315-CHO-500-H1
STANDARD PROTON PARAMETERS
OMe
F
O
2k
7.26
7.09
7.09
7.08
7.03
7.01
6.83
6.81
6.79
6.78
6.77
6.75
6.73
3.84
3.43
3.41
3.40
3.38
3.37
2.84
2.83
2.83
2.71
2.71
2.31
0.73
1.69
1.86
2.71
2.87
1.00
2.10
2.05
2.87
S136
f1 (ppm)


zhimin-czm315-CHO-300-C
13C OBSERVE
201.58
153.69
150.44
146.05
145.92
139.77
136.35
132.47
132.39
129.31
127.31
124.76
124.72
116.87
116.64
113.18
77.42
77.00
76.58
56.23
49.05
42.26
41.53
21.00
OMe
F
O
2k
S137
f1 (ppm)

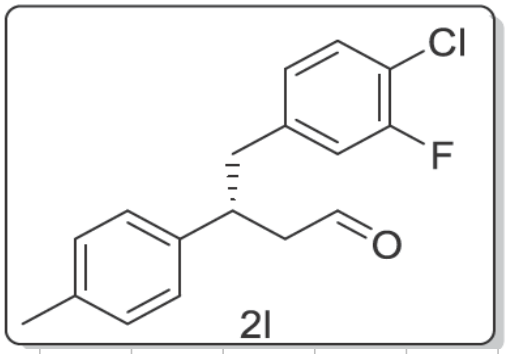

zhimin-czm315-CHO-300-F
19F OBSERVE
STANDARD PARAMETERS
-135.95
-135.99
-136.02
OMe
F
O
2k
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


zhimin-czm315-OH-300-H
UofUtah Unity300-NMR
STANDARD 1H OBSERVE
OMe
F
OH
3k
f1 (ppm)


zhimin-czm315-OH-300-C
13C OBSERVE
153.62
150.38
145.70
145.56
140.80
135.88
133.57
133.49
129.16
127.46
124.62
124.58
116.80
116.56
113.09
113.06
77.42
77.00
76.58
61.05
56.24
44.00
42.84
38.21
21.00
OMe
F
OH
3k
f1 (ppm)


zhimin-czm315-OH-300-F
19F OBSERVE
STANDARD PARAMETERS
136.41
136.44
136.45
136.48
OMe
F
OH
3k
f1 (ppm)

zhimin-czm304-CHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE

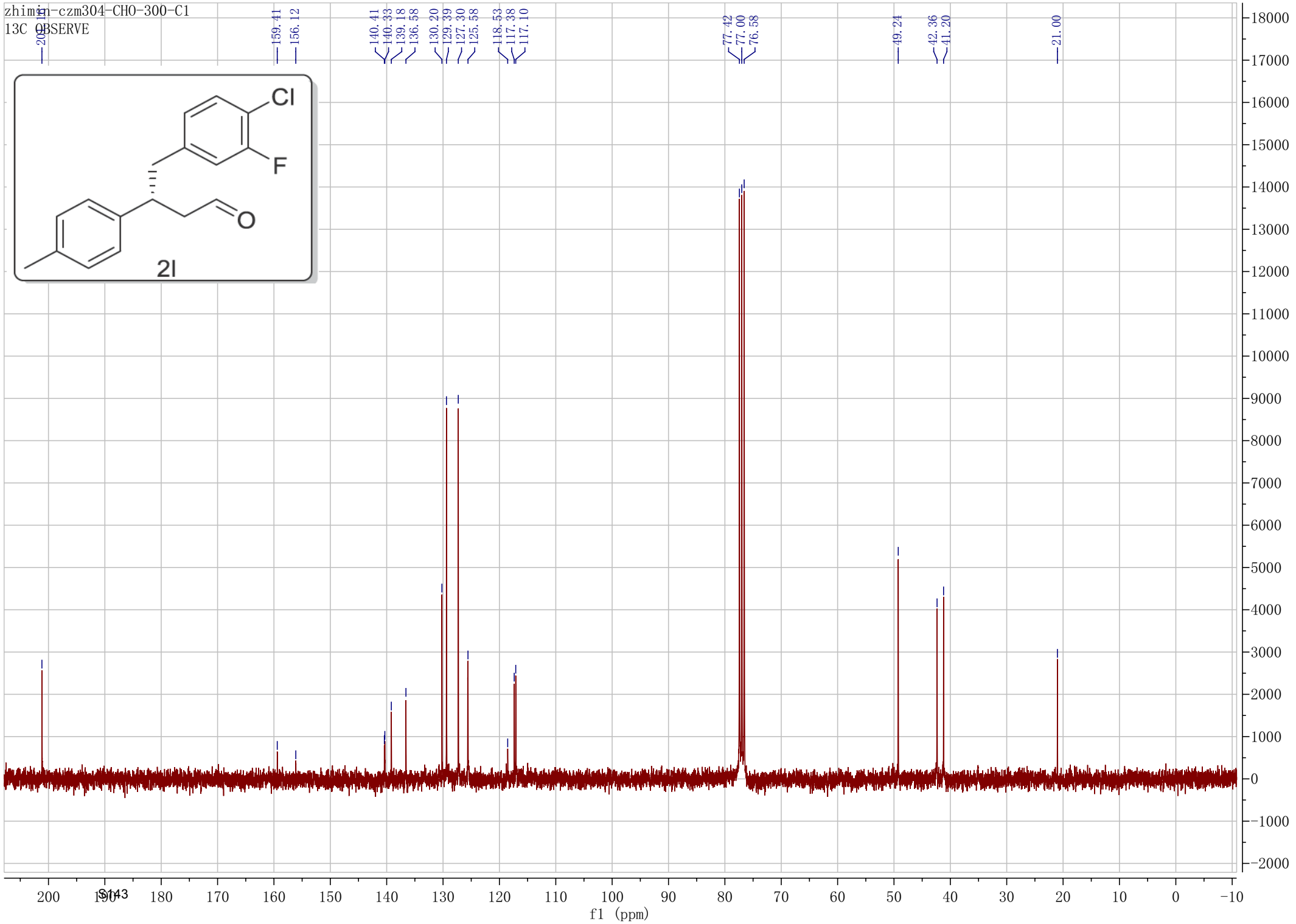


7.26 7.24 7.21 7.19 7.09 7.07 7.00 6.97 6.81 6.77 6.75 6.72

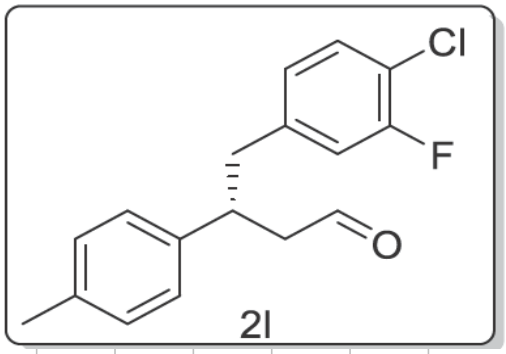
3.43 3.41 3.39 3.36 2.87 2.76 2.75 2.74 2.74 2.73 2.30

0.78 1.25 1.89 1.71 1.68 1.00 2.08 1.82 2.70

f1 (ppm)


zhimin-czm304-CHO-300-C1
13C OBSERVE
159.41
156.12
140.41
140.33
139.18
136.58
130.20
129.39
127.30
125.58
118.53
117.38
117.10
77.42
77.00
76.58
49.24
42.36
41.20
21.00
Cl
F
O
2l
f1 (ppm)

zhimin-czm304-CHO-300-F
19F OBSERVE
STANDARD PARAMETERS



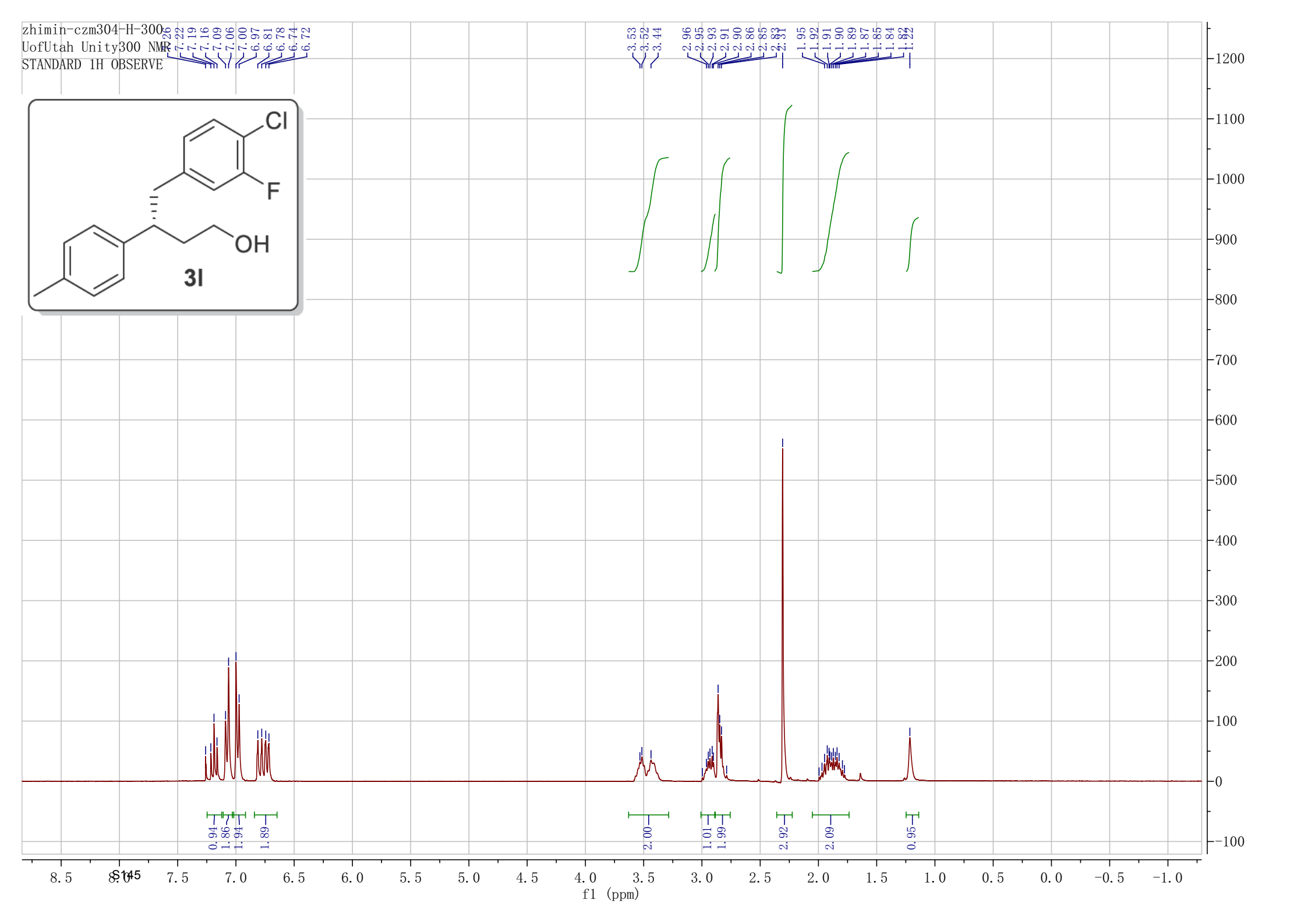
2l

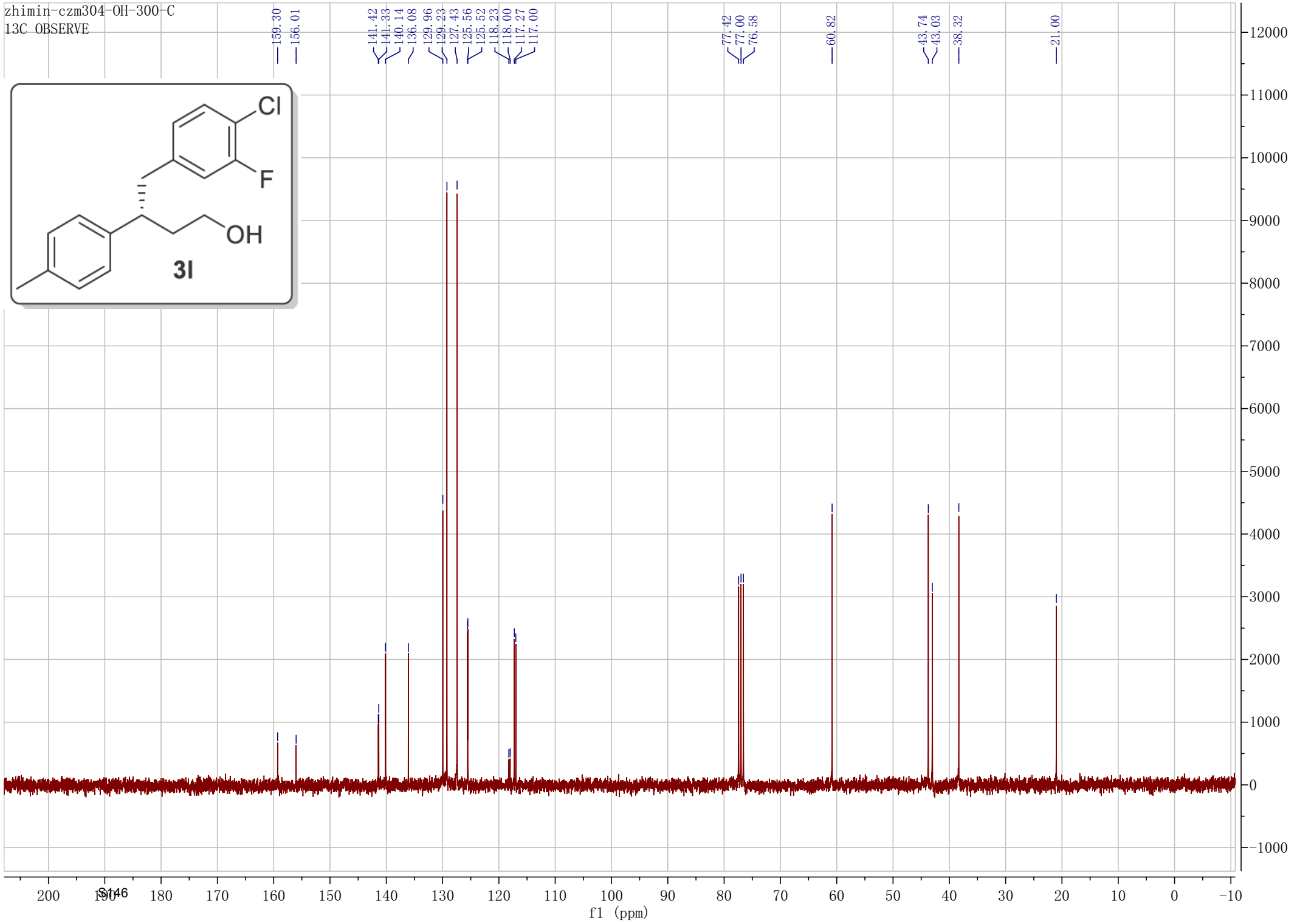
−116.32
−116.36
−116.38

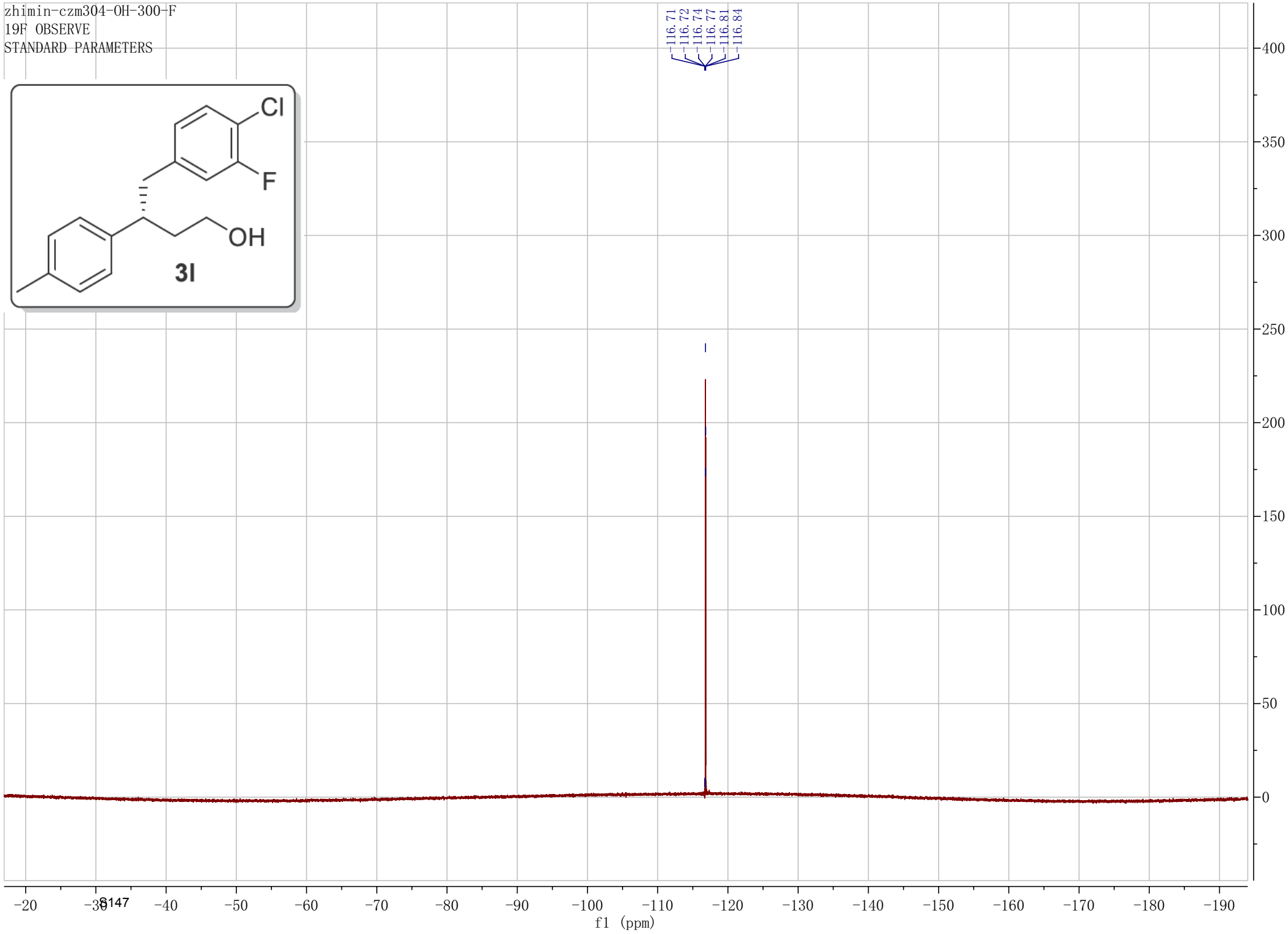
700
650
600
550
500
450
400
350
300
250
200
150
100
50
0
−50

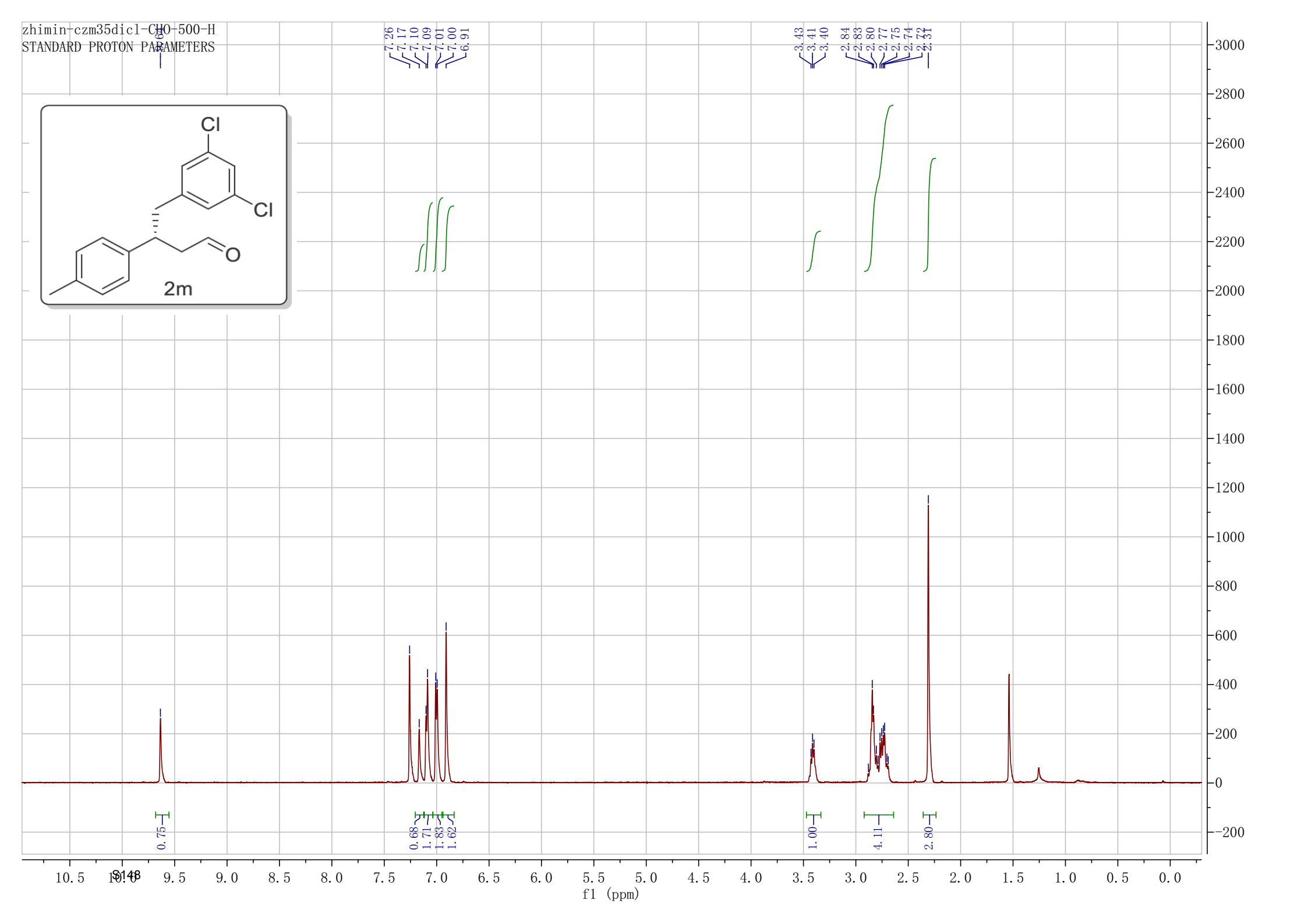
−114.0 −114.4 −114.8 −115.2 −115.6 −116.0 −116.4 −116.8 −117.2 −117.6 −118.0 −118.4 −118.8

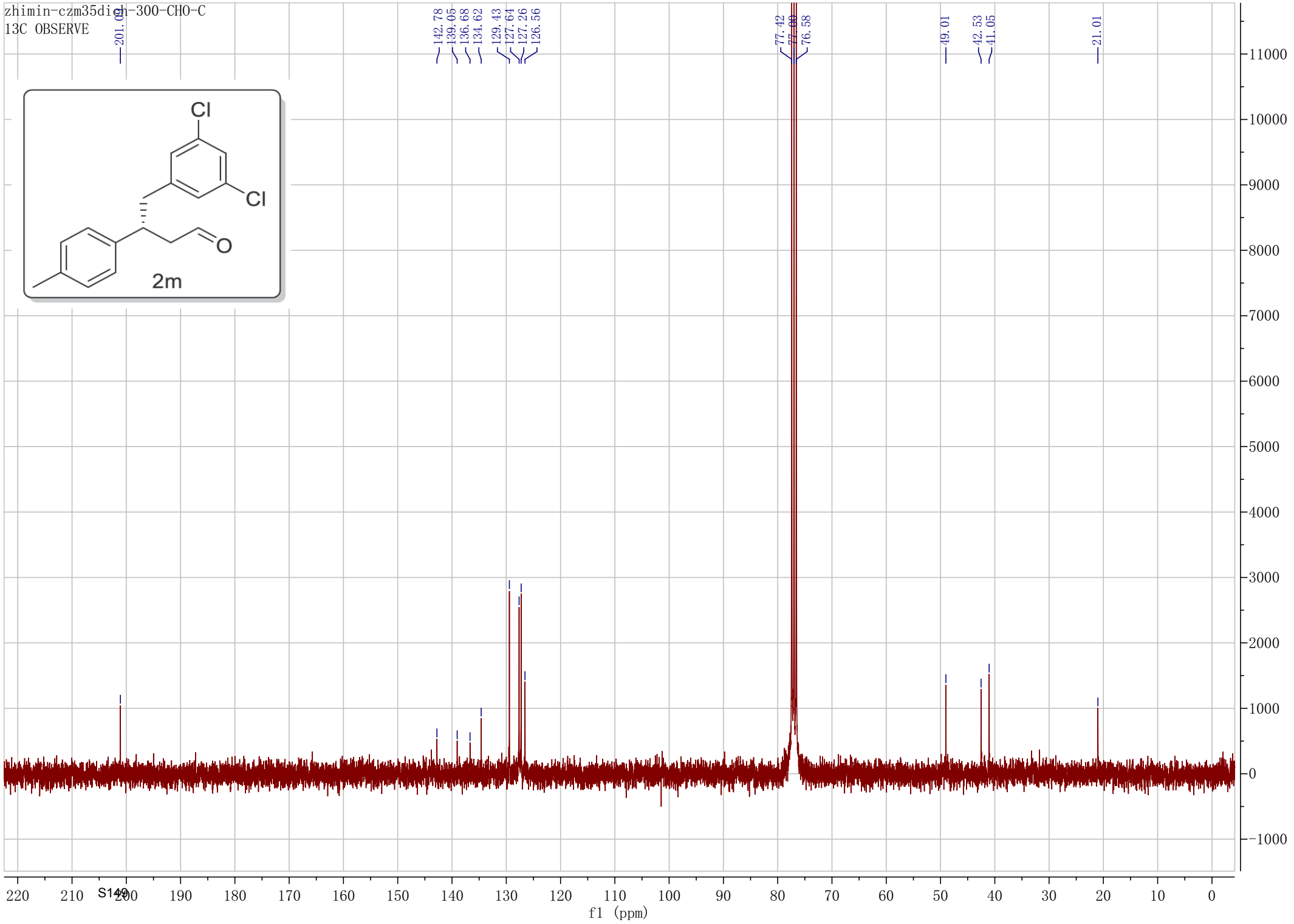
f1 (ppm)

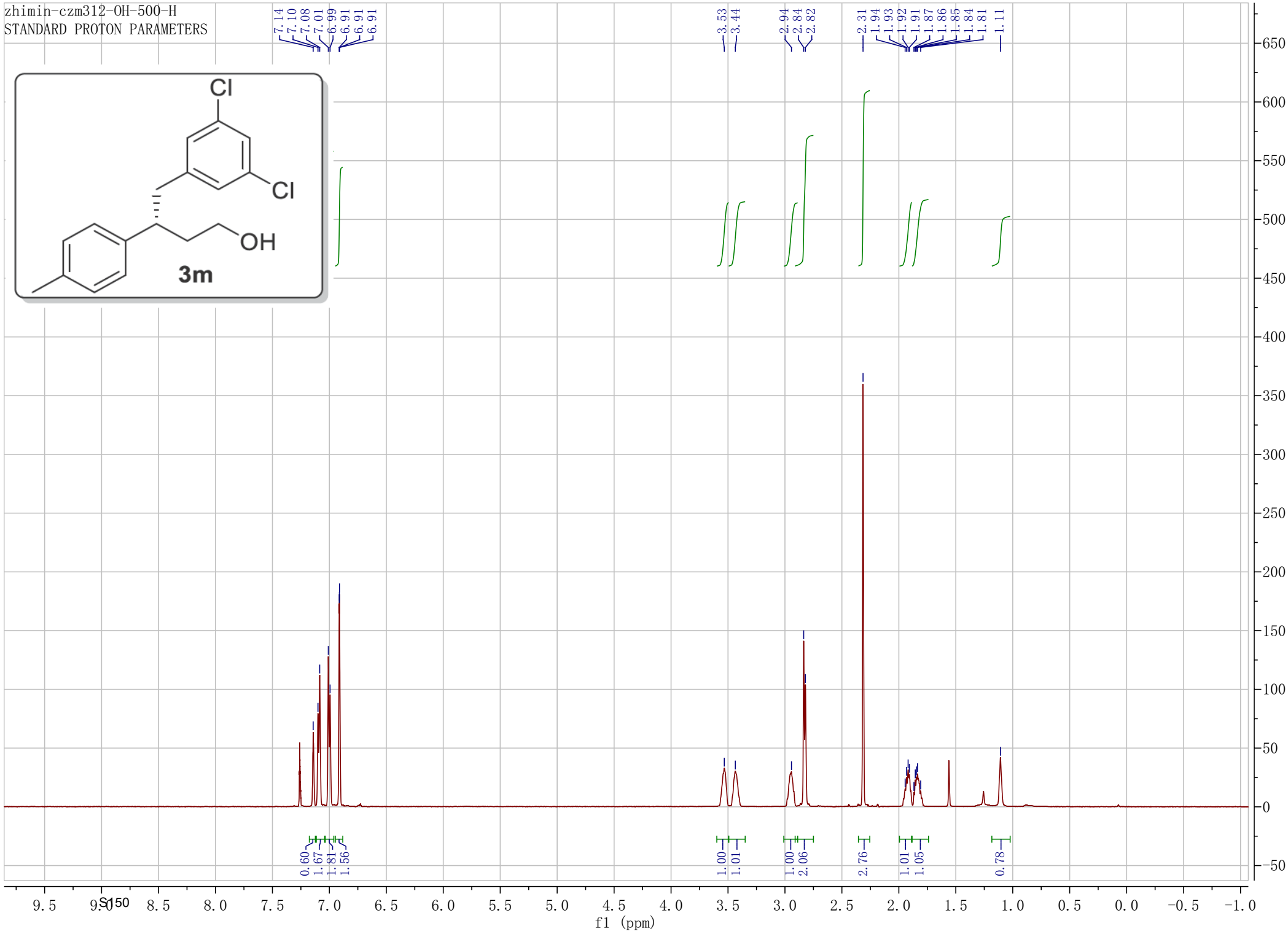

zhimin-czm304-H-300
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
F
OH
3l
f1 (ppm)

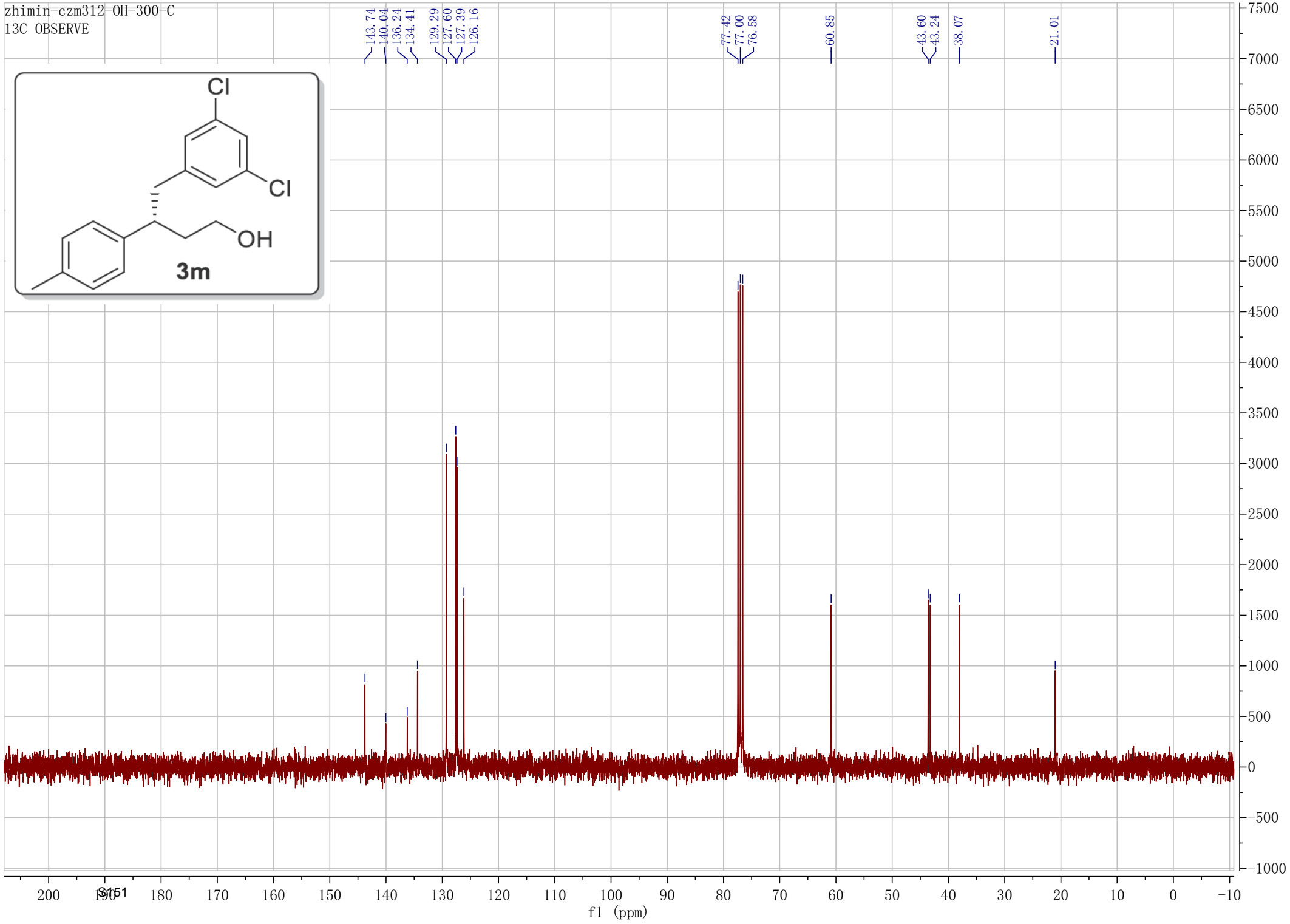

zhimin-czm304-OH-300-C
13C OBSERVE
159.30
156.01
141.42
141.33
140.14
136.08
129.96
129.23
127.43
125.56
125.52
118.23
118.00
117.27
117.00
77.42
77.00
76.58
60.82
43.74
43.03
38.32
21.00
Cl
F
OH
3l
f1 (ppm)

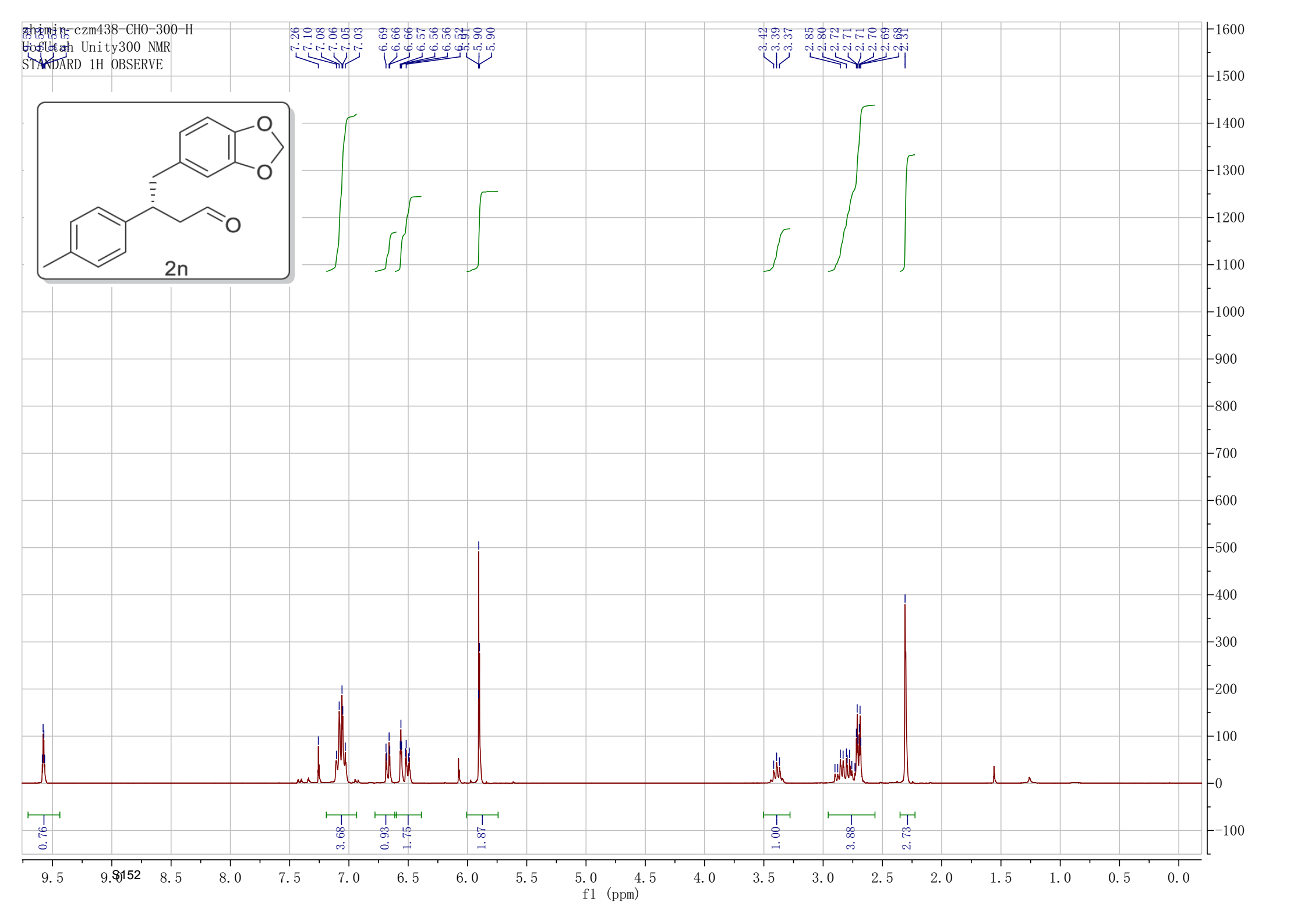

zhimin-czm304-OH-300-F
19F OBSERVE
STANDARD PARAMETERS
116.71
116.72
116.74
116.77
116.81
116.84
Cl
F
OH
3l
400
350
300
250
200
150
100
50
0
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

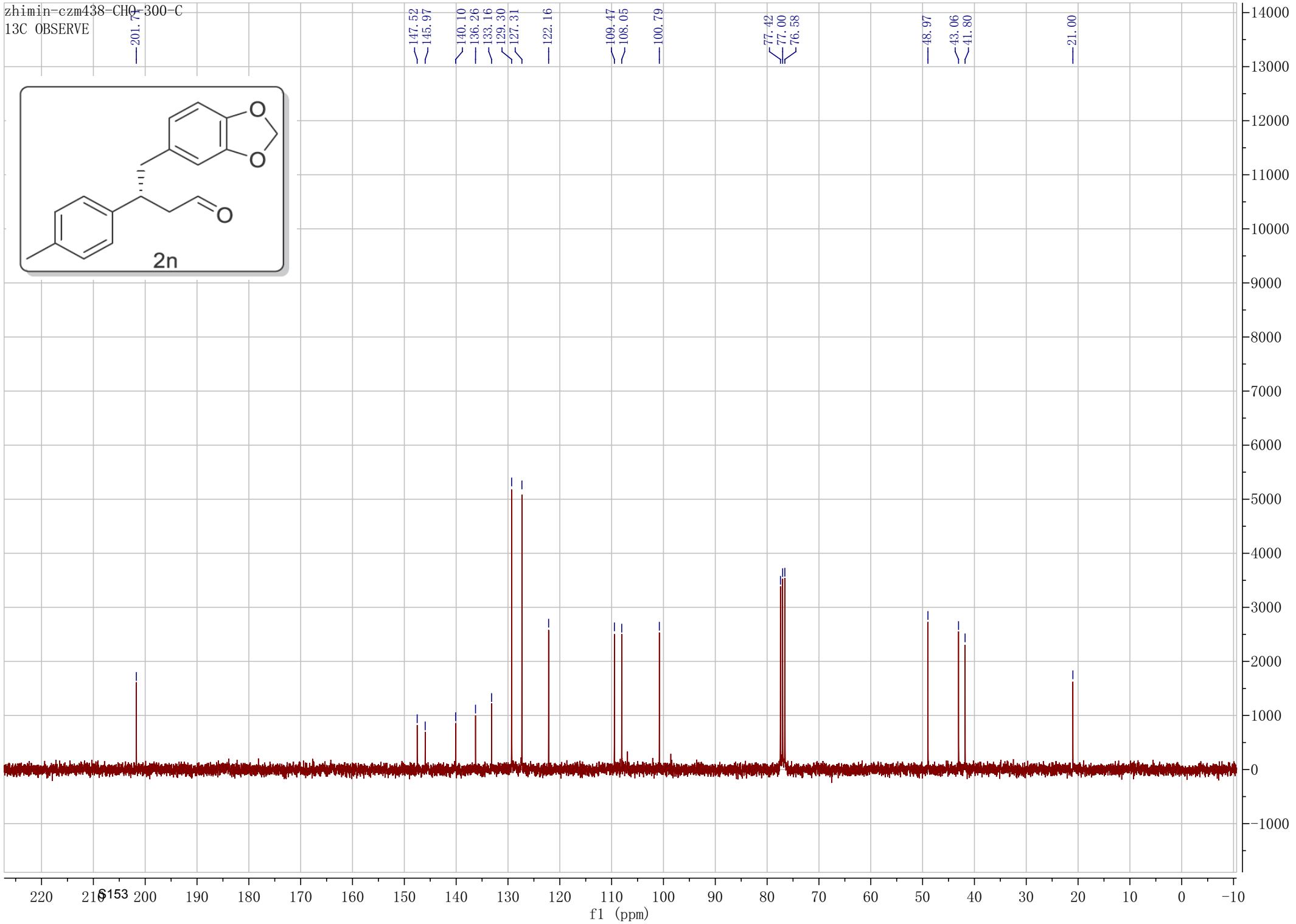

zhimin-czm35dicl-CHO-500-H
STANDARD PROTON PARAMETERS
9.68
7.26
7.17
7.10
7.09
7.01
7.00
6.91
3.43
3.41
3.40
2.84
2.83
2.80
2.77
2.75
2.74
2.72
2.31
Cl
Cl
O
2m
0.75
0.68
1.71
1.83
1.62
1.00
4.11
2.80
f1 (ppm)

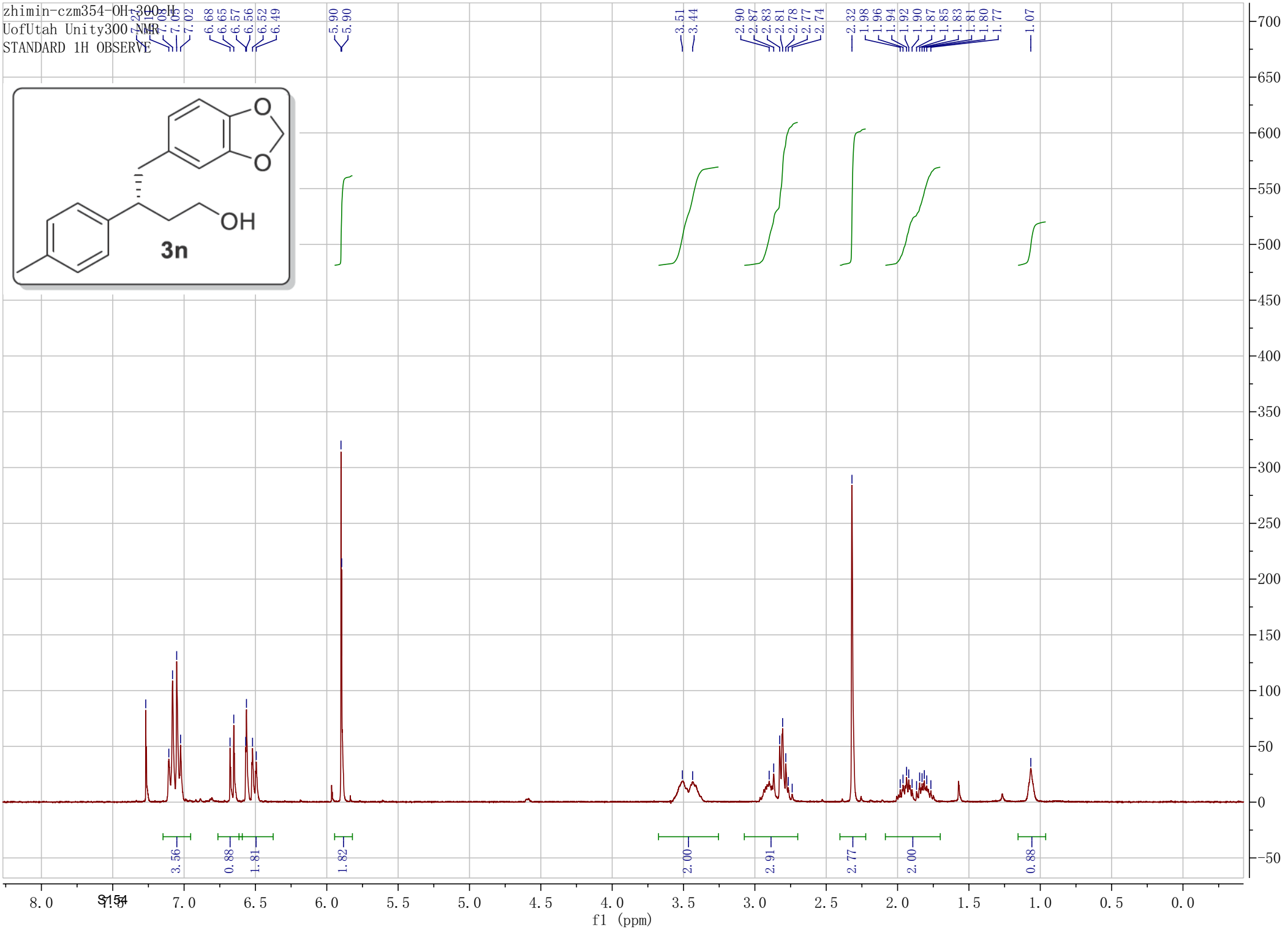

zhimin-czm35dich-300-CHO-C
13C OBSERVE
201.02
142.78
139.05
136.68
134.62
129.43
127.64
127.26
126.56
77.42
77.00
76.58
49.01
42.53
41.05
21.01
Cl
Cl
O
2m
f1 (ppm)

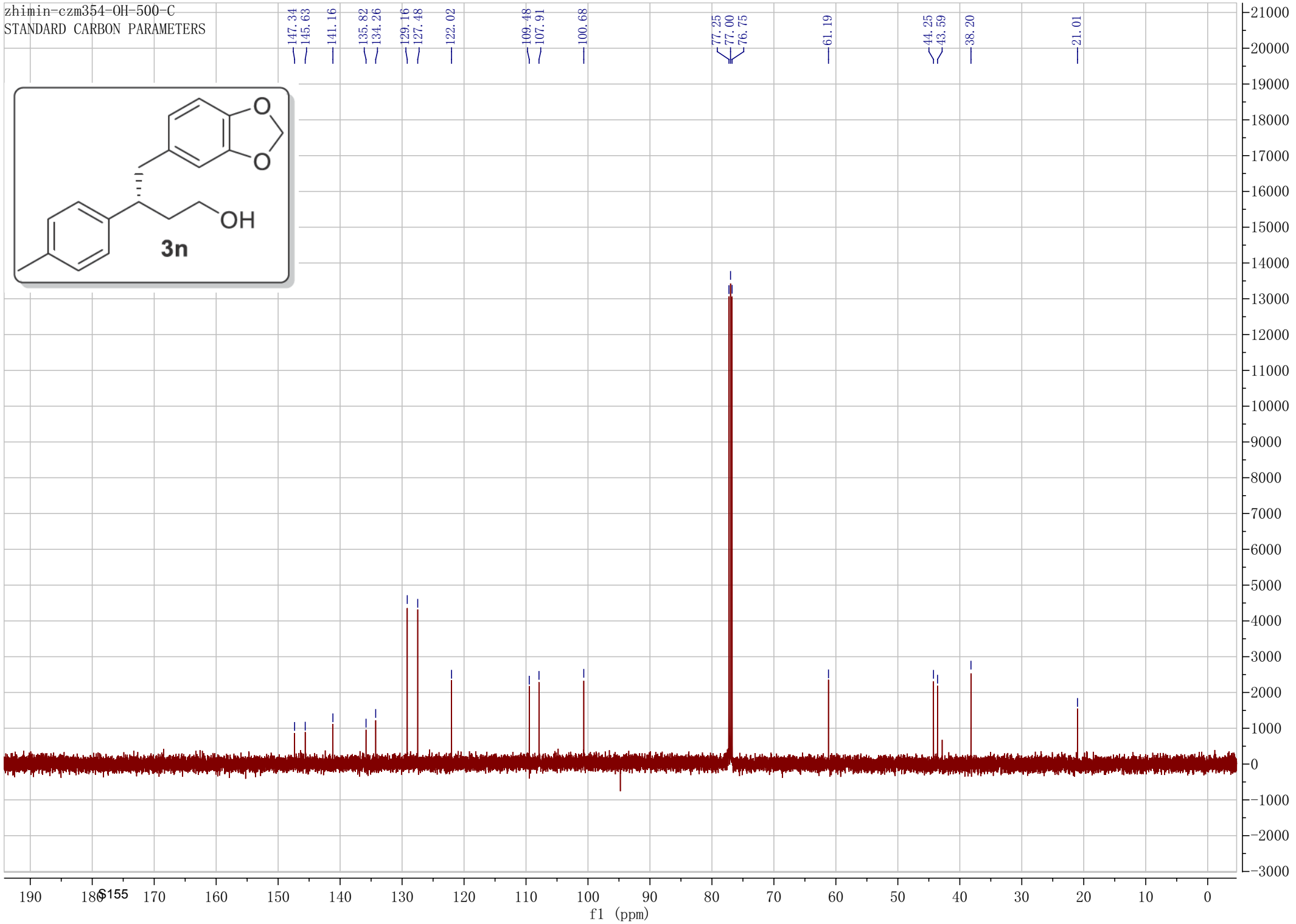

zhimin-czm312-OH-500-H
STANDARD PROTON PARAMETERS
7.14
7.10
7.08
7.01
6.99
6.91
6.91
6.91
3.53
3.44
2.94
2.84
2.82
2.31
1.94
1.93
1.92
1.91
1.87
1.86
1.85
1.84
1.81
1.11
Cl
Cl
OH
3m
0.60
1.67
1.81
1.56
1.00
1.01
1.00
2.06
2.76
1.01
1.05
0.78
650
600
550
500
450
400
350
300
250
200
150
100
50
0
-50
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

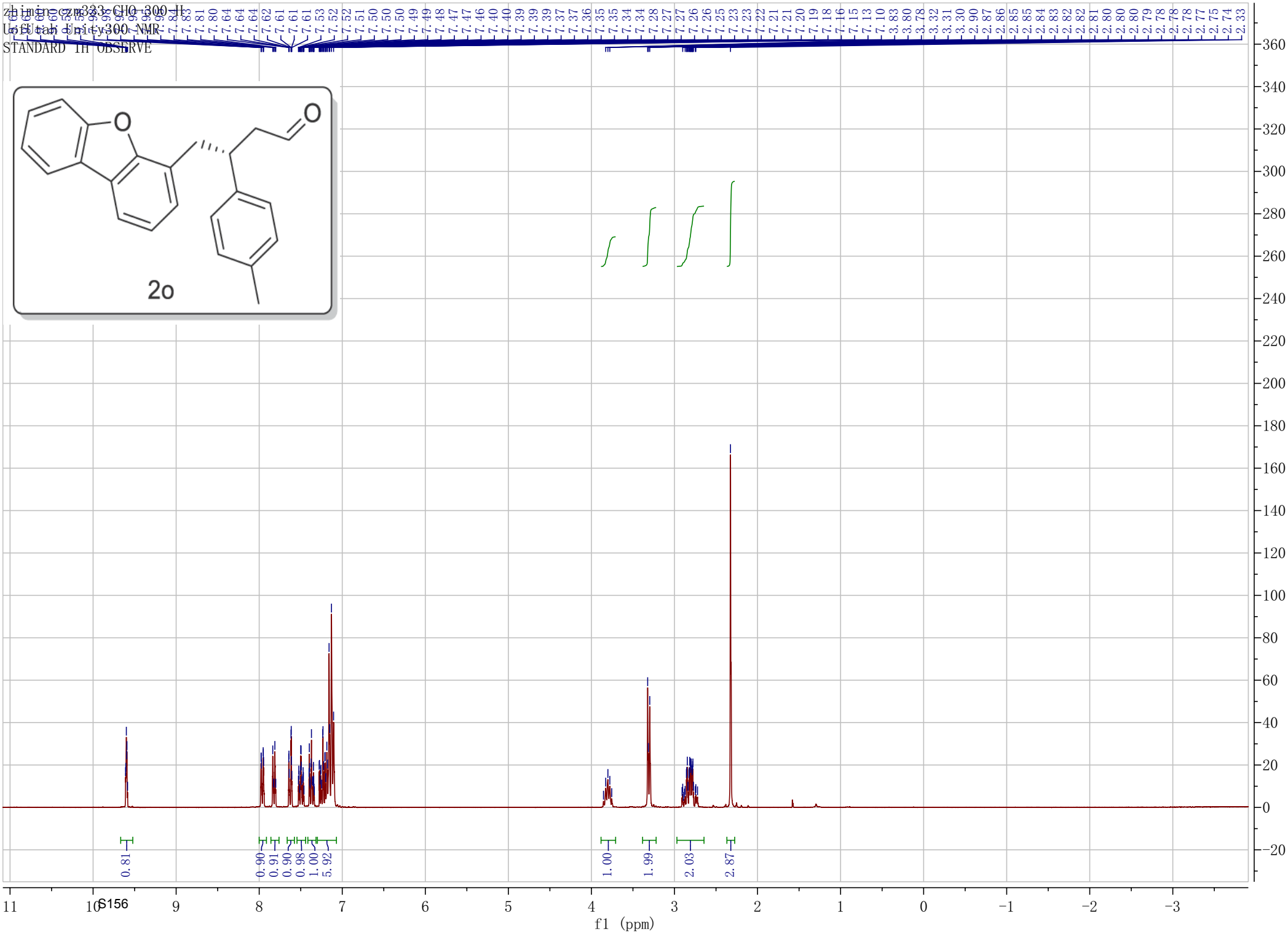

zhimin-czm312-OH-300-C
13C OBSERVE
143.74
140.04
136.24
134.41
129.29
127.60
127.39
126.16
77.42
77.00
76.58
60.85
43.60
43.24
38.07
21.01
Cl
Cl
OH
3m
f1 (ppm)

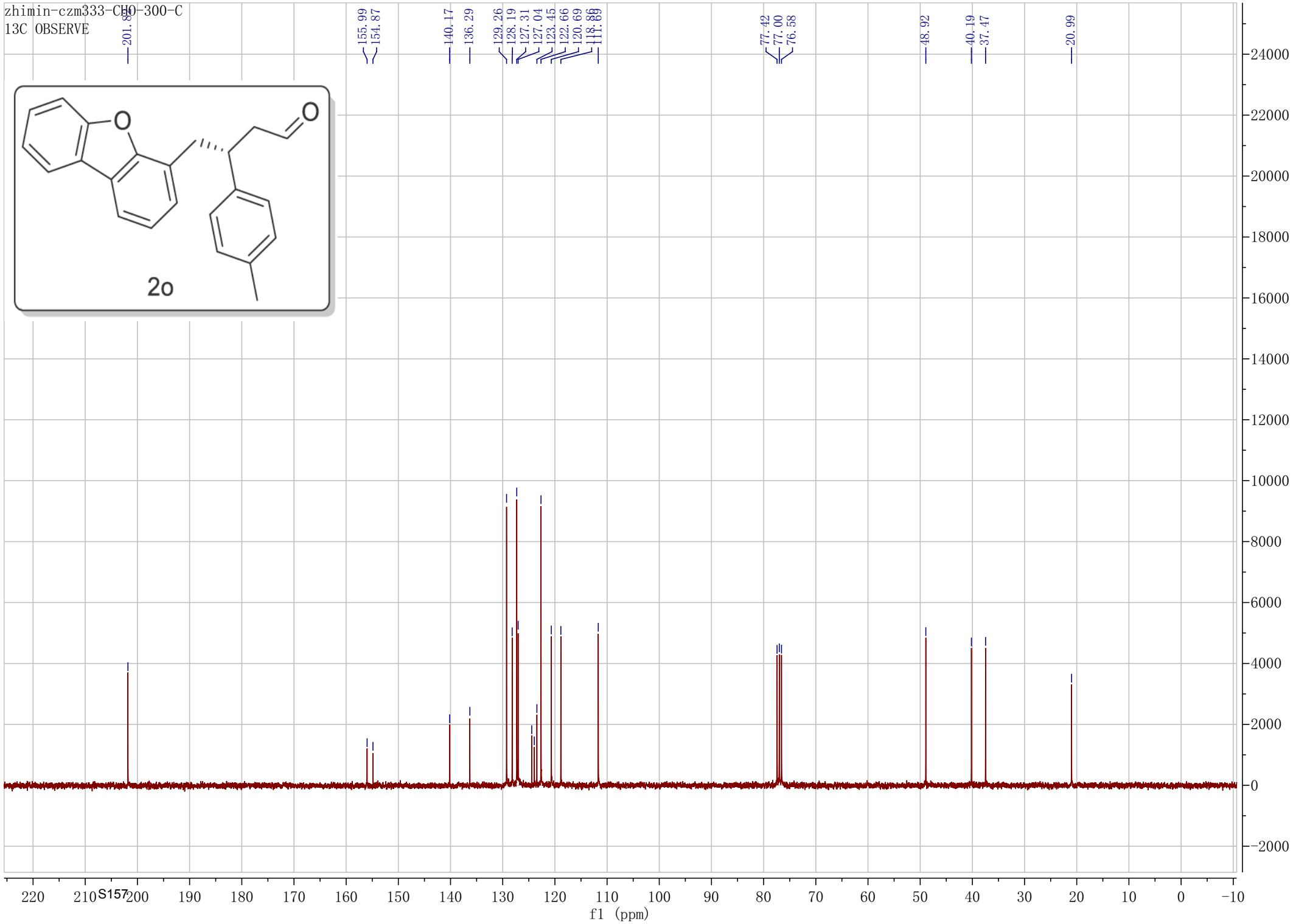

zhimin-czm438-CHO-300-H
Varian Unity300 NMR
STANDARD 1H OBSERVE
7.26
7.10
7.08
7.06
7.05
7.03
6.69
6.66
6.66
6.57
6.56
6.56
5.91
5.90
5.90
3.42
3.39
3.37
2.85
2.80
2.72
2.71
2.71
2.70
2.69
2.68
2.31
2n
0.76
3.68
0.93
1.75
1.87
1.00
3.88
2.73
f1 (ppm)

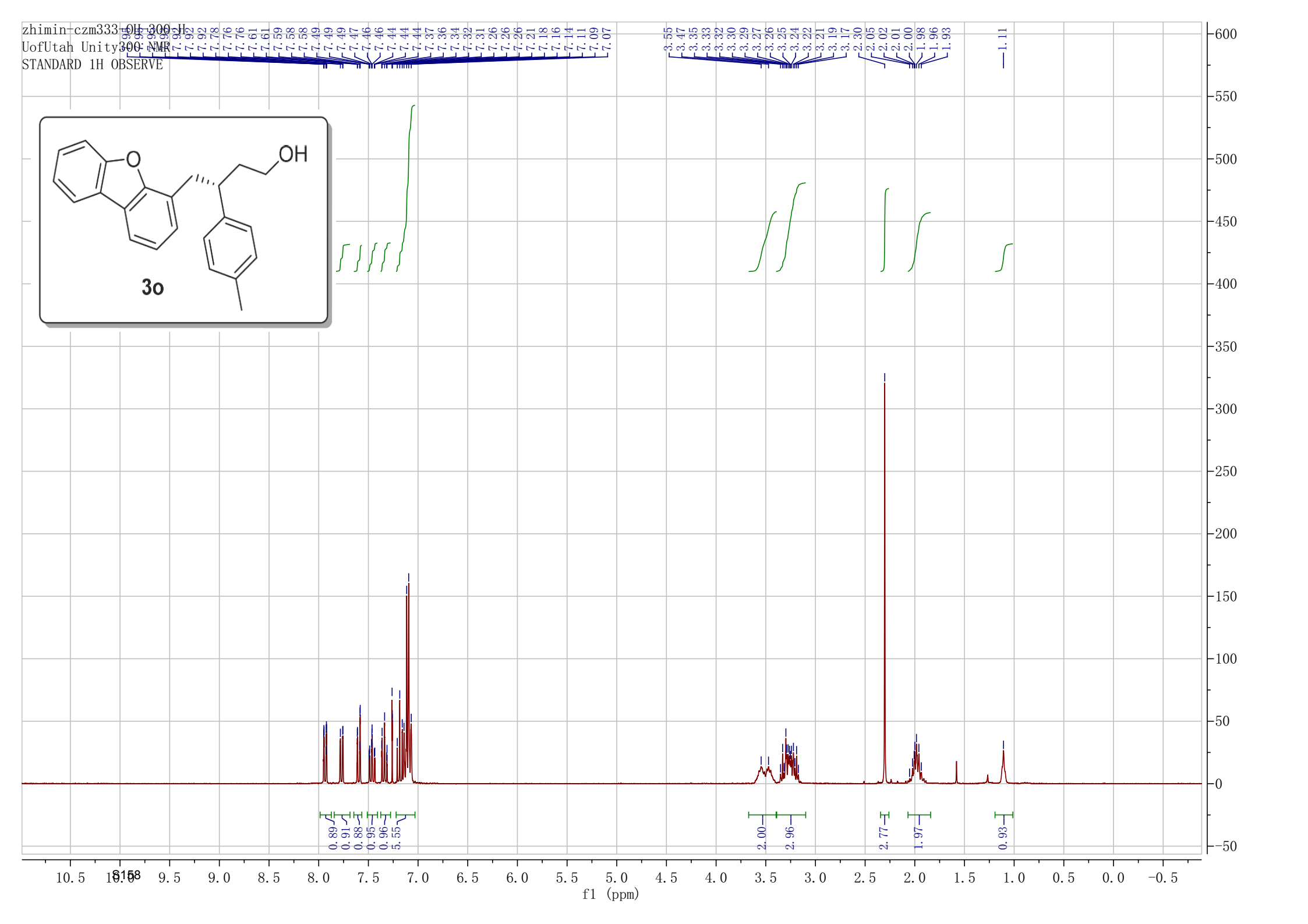

zhimin-czm438-CHO-300-C
13C OBSERVE
201.77
147.52
145.97
140.10
136.26
133.16
129.30
127.31
122.16
109.47
108.05
100.79
77.42
77.00
76.58
48.97
43.06
41.80
21.00
2n
f1 (ppm)

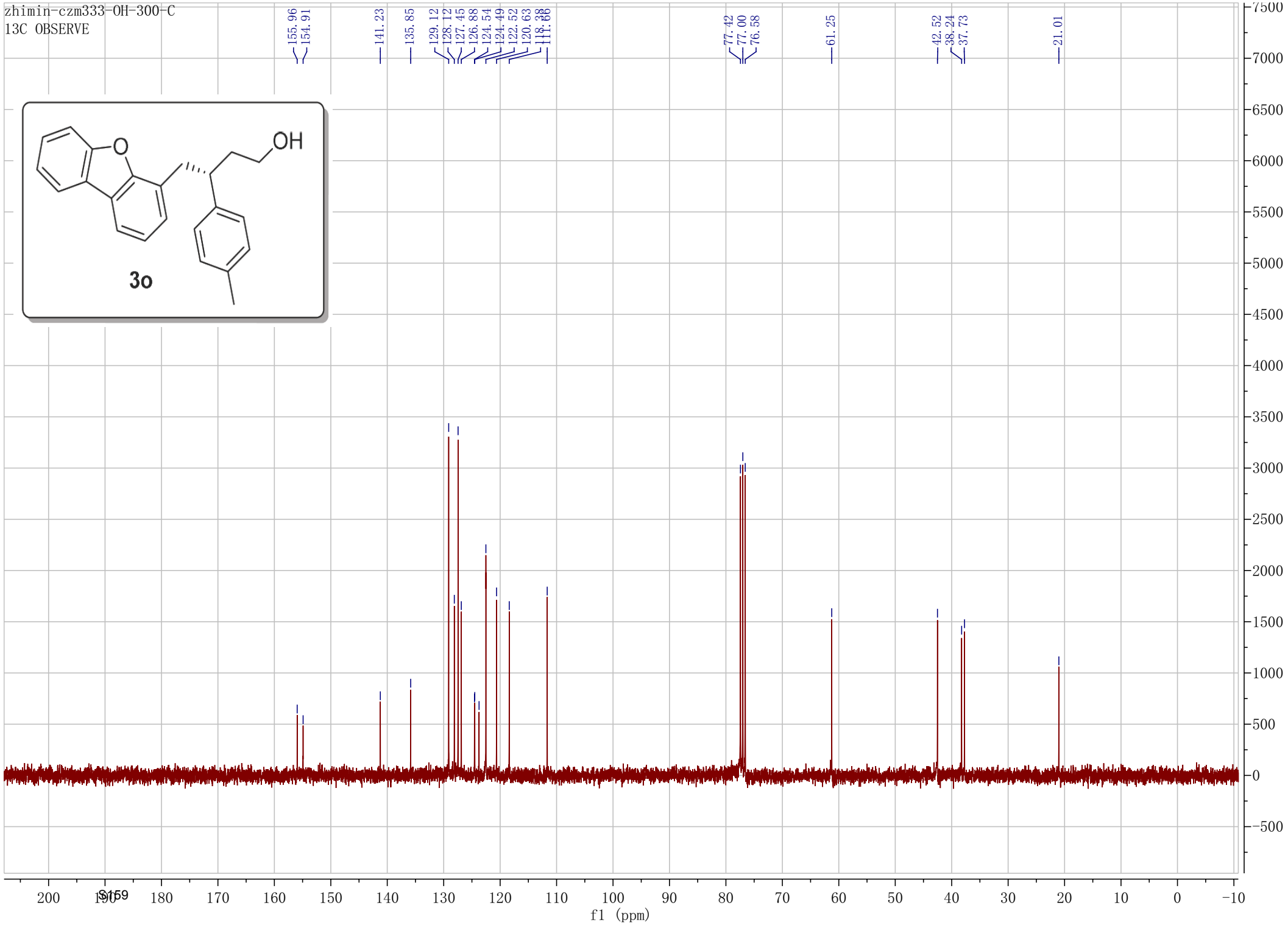

zhimin-czm354-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.08
7.05
7.02
6.68
6.65
6.57
6.56
6.52
6.49
5.90
5.90
3.51
3.44
2.90
2.87
2.83
2.81
2.78
2.77
2.74
2.32
1.98
1.96
1.94
1.92
1.90
1.87
1.85
1.83
1.81
1.80
1.77
1.07
OH
3n
3.56
0.88
1.81
1.82
2.00
2.91
2.77
2.00
0.88
f1 (ppm)

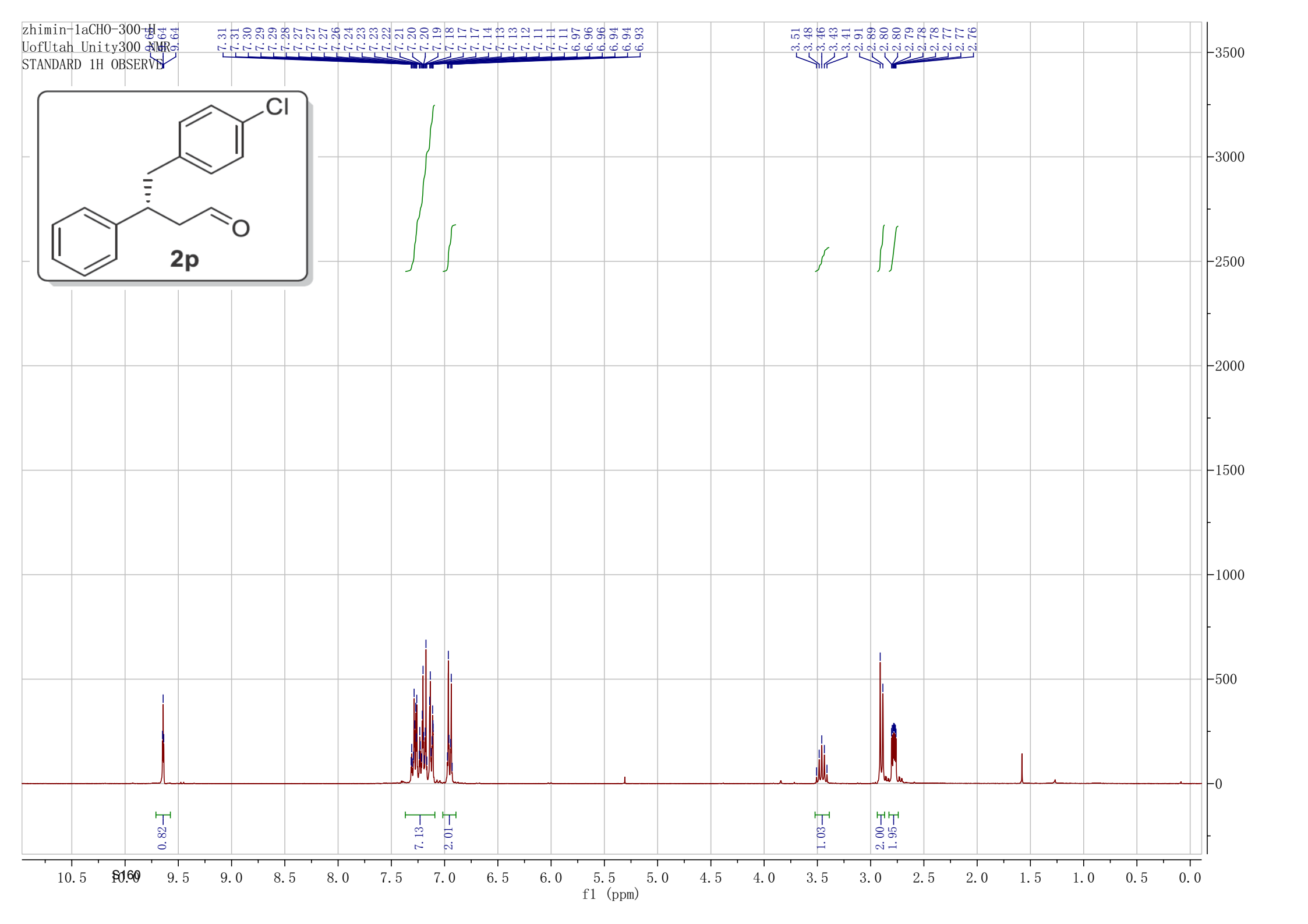

zhimin-czm354-OH-500-C
STANDARD CARBON PARAMETERS
147.34
145.63
141.16
135.82
134.26
129.16
127.48
122.02
109.48
107.91
100.68
77.25
77.00
76.75
61.19
44.25
43.59
38.20
21.01
OH
3n
f1 (ppm)

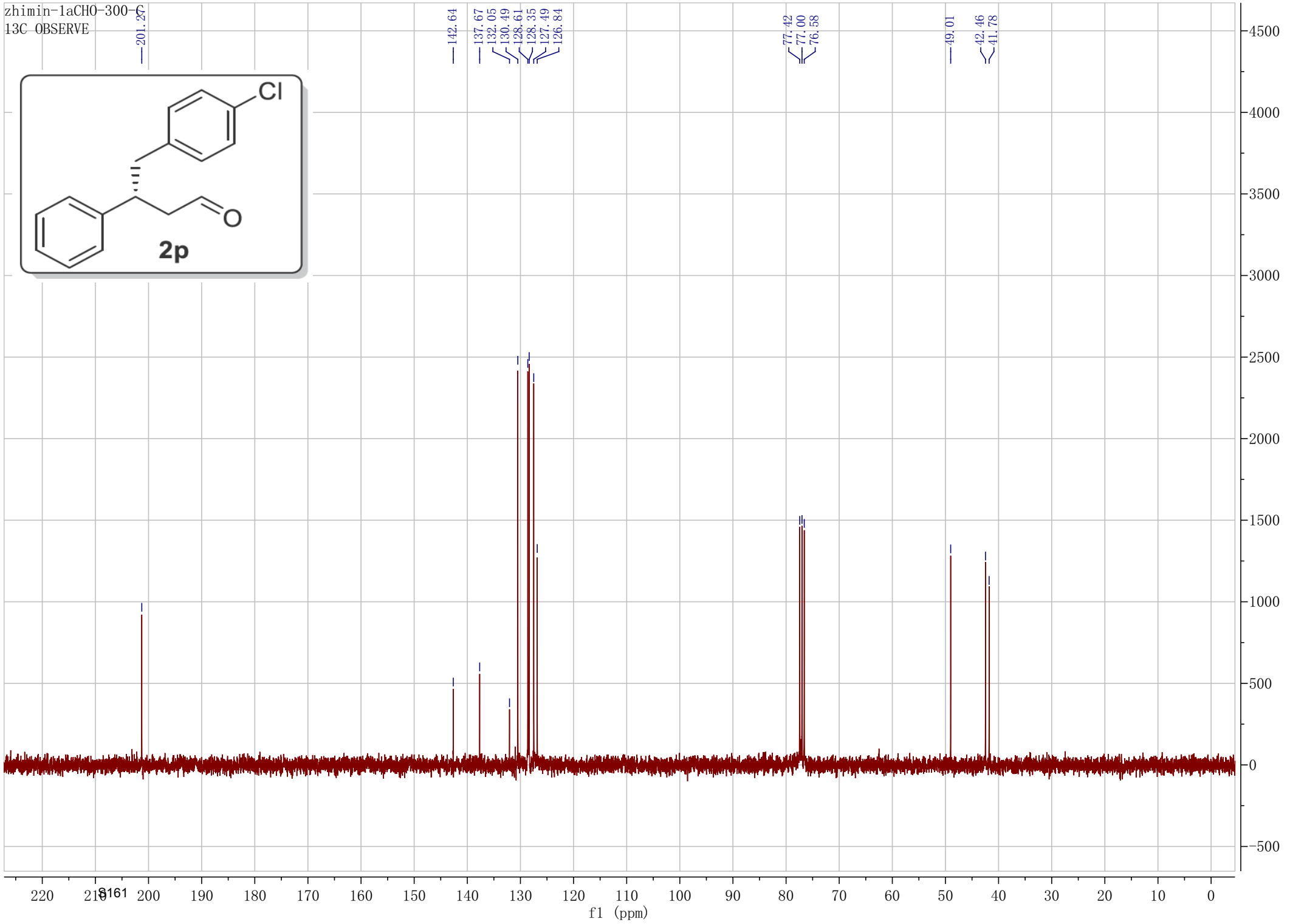

zhimin_czm333_CH0-300-H
UserTab_univ300 NMR
STANDARD 1H OBSERVE
2o
0.81
0.90
0.91
0.90
0.98
1.00
5.92
1.00
1.99
2.03
2.87
f1 (ppm)

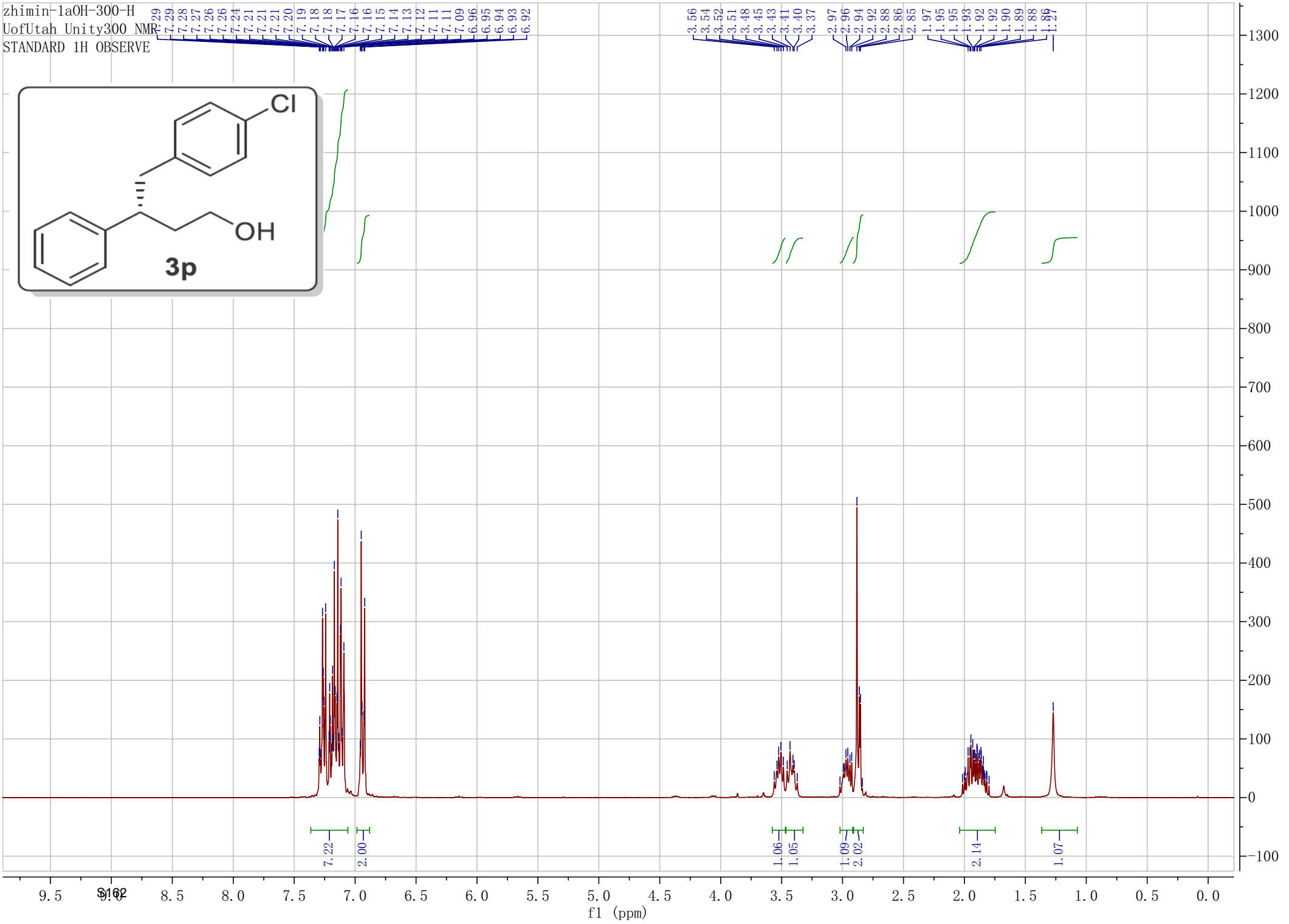

zhimin-czm333-CHO-300-C
13C OBSERVE
201.88
155.99
154.87
140.17
136.29
129.26
128.19
127.31
127.04
123.45
122.66
120.69
118.86
111.69
77.42
77.00
76.58
48.92
40.19
37.47
20.99
2o
f1 (ppm)

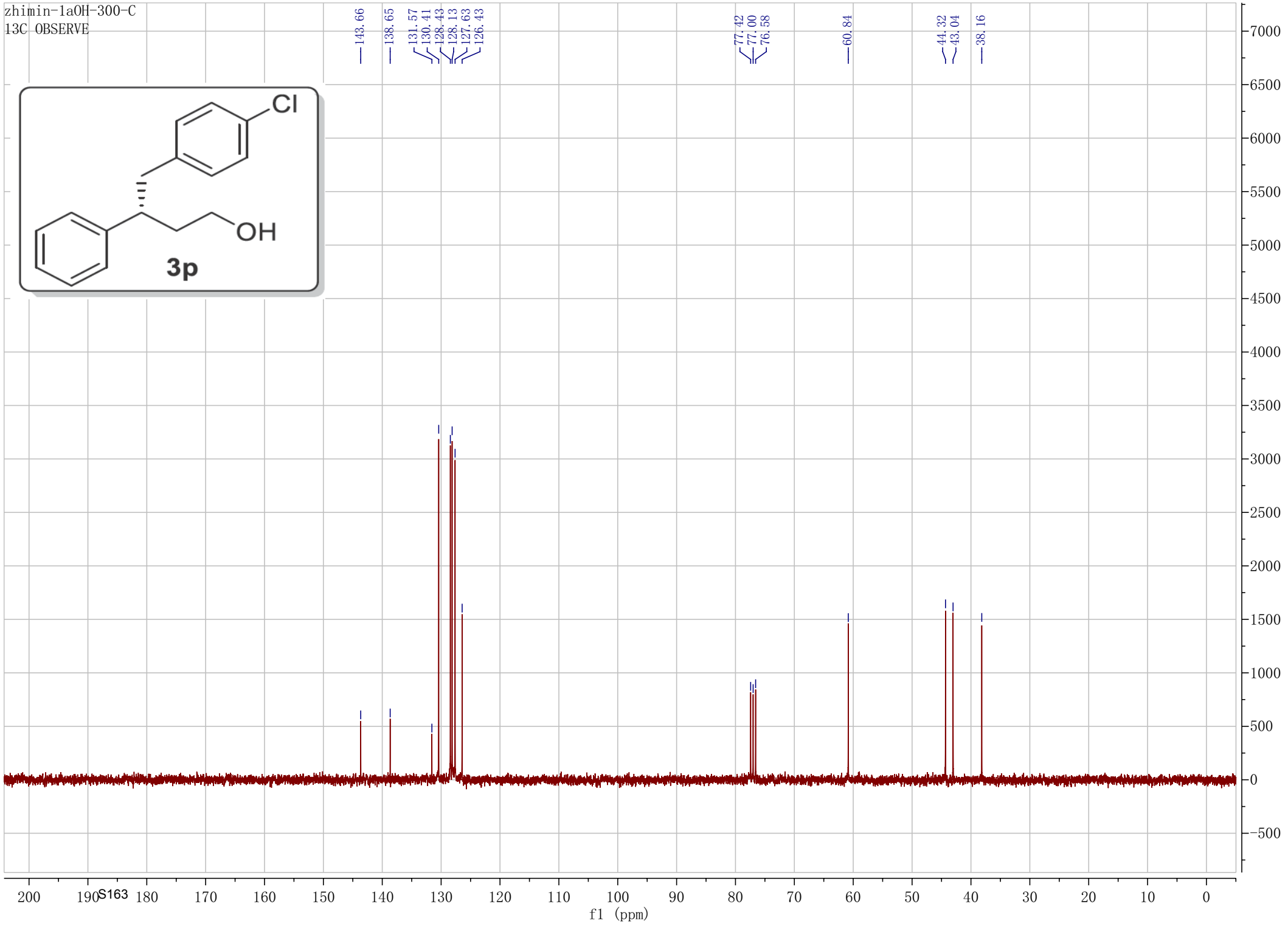

zhimin-czm333-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
OH
3o
f1 (ppm)

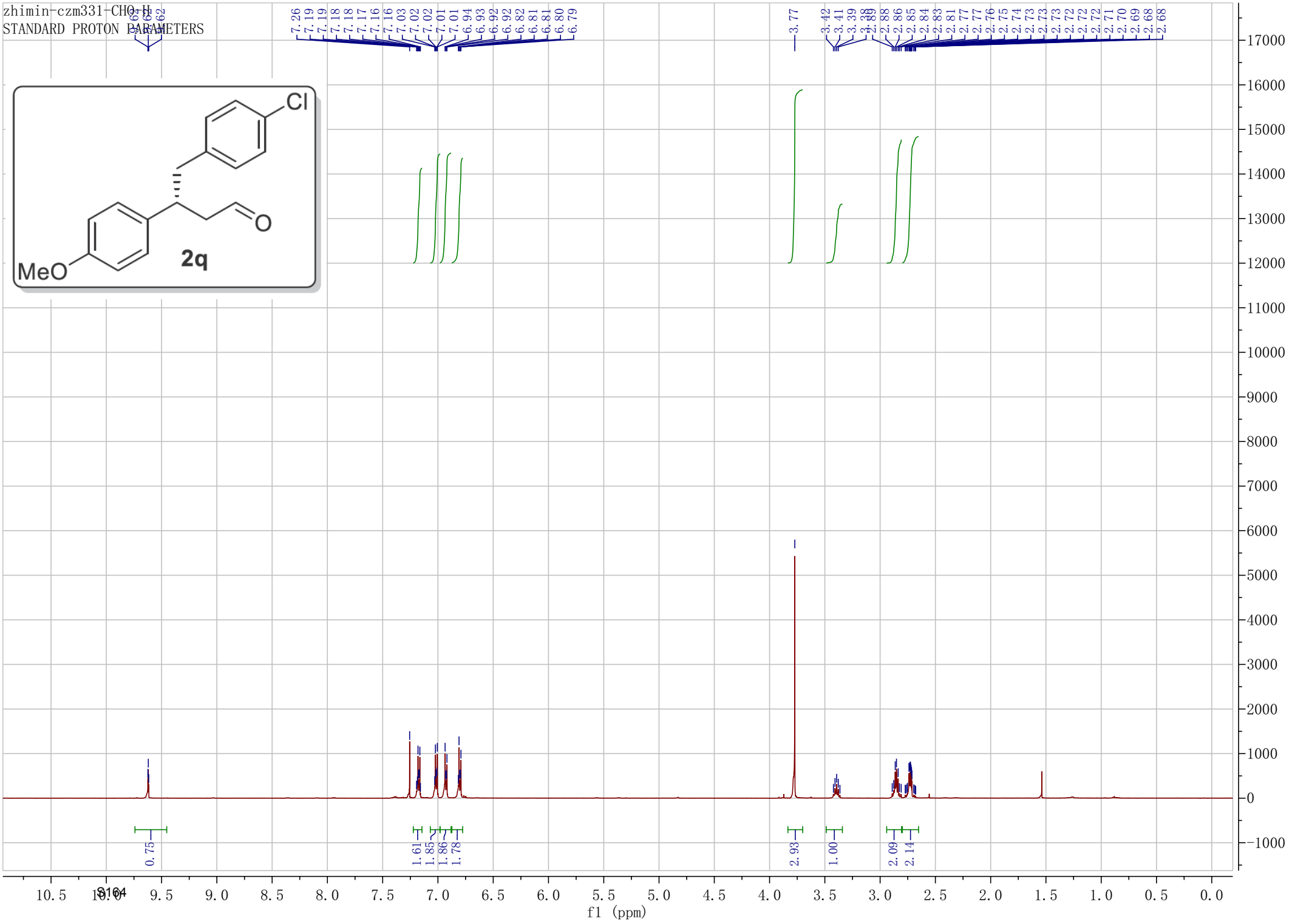

zhimin-czm333-OH-300-C
13C OBSERVE
155.96
154.91
141.23
135.85
129.12
128.12
127.45
126.88
124.54
124.49
122.52
120.63
118.38
111.66
77.42
77.00
76.58
61.25
42.52
38.24
37.73
21.01
OH
O
3o
f1 (ppm)

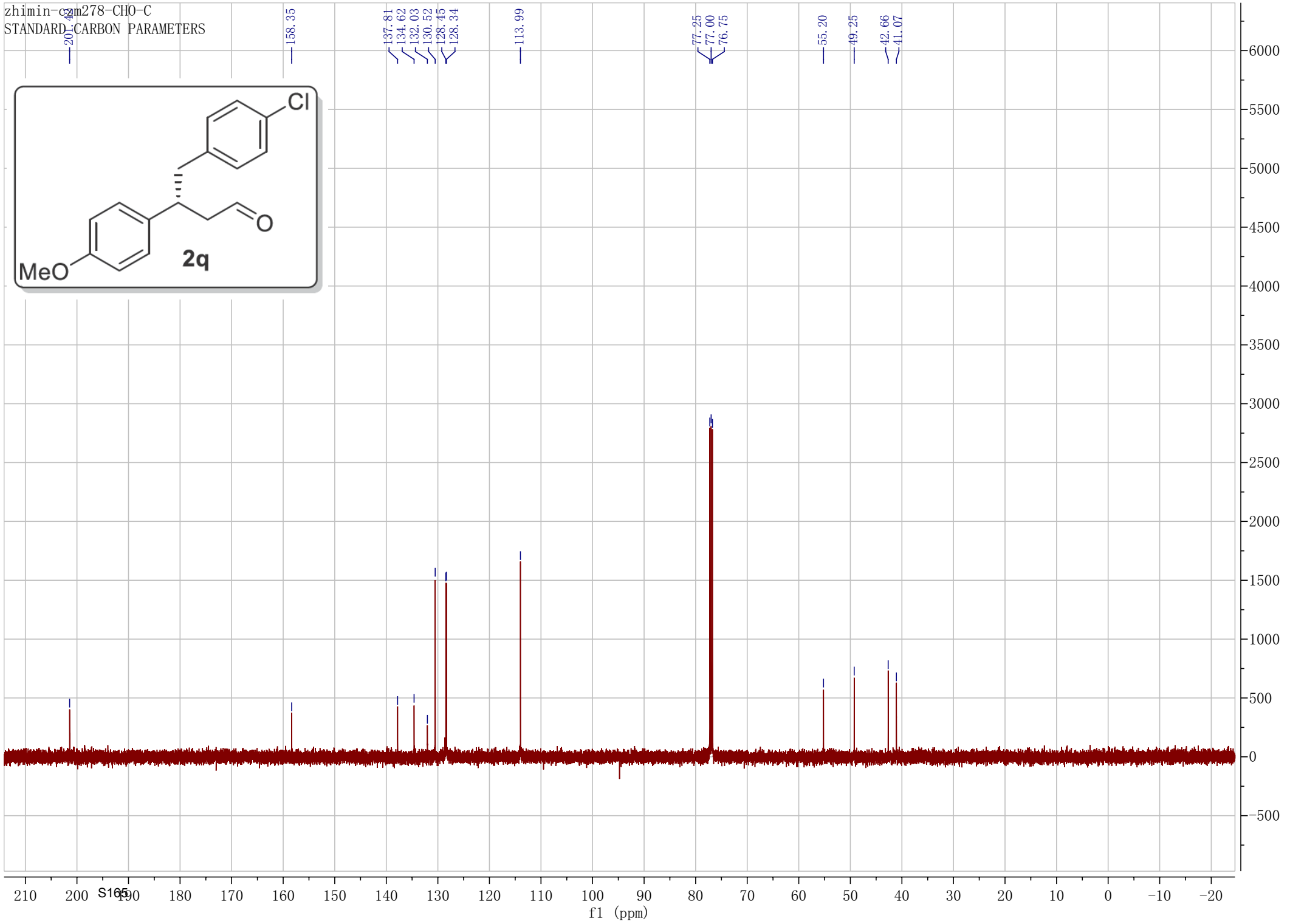

zhimin-1aCHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
9.64
7.31 7.30 7.29 7.28 7.27 7.26 7.24 7.23 7.22 7.21 7.20 7.19 7.18 7.17 7.14 7.13 7.12 7.11 6.97 6.96 6.94 6.93
3.51 3.48 3.46 3.43 3.41 2.91 2.89 2.80 2.79 2.78 2.77 2.76
Cl
O
2p
0.82
7.13
2.01
1.03
2.00
1.95
f1 (ppm)

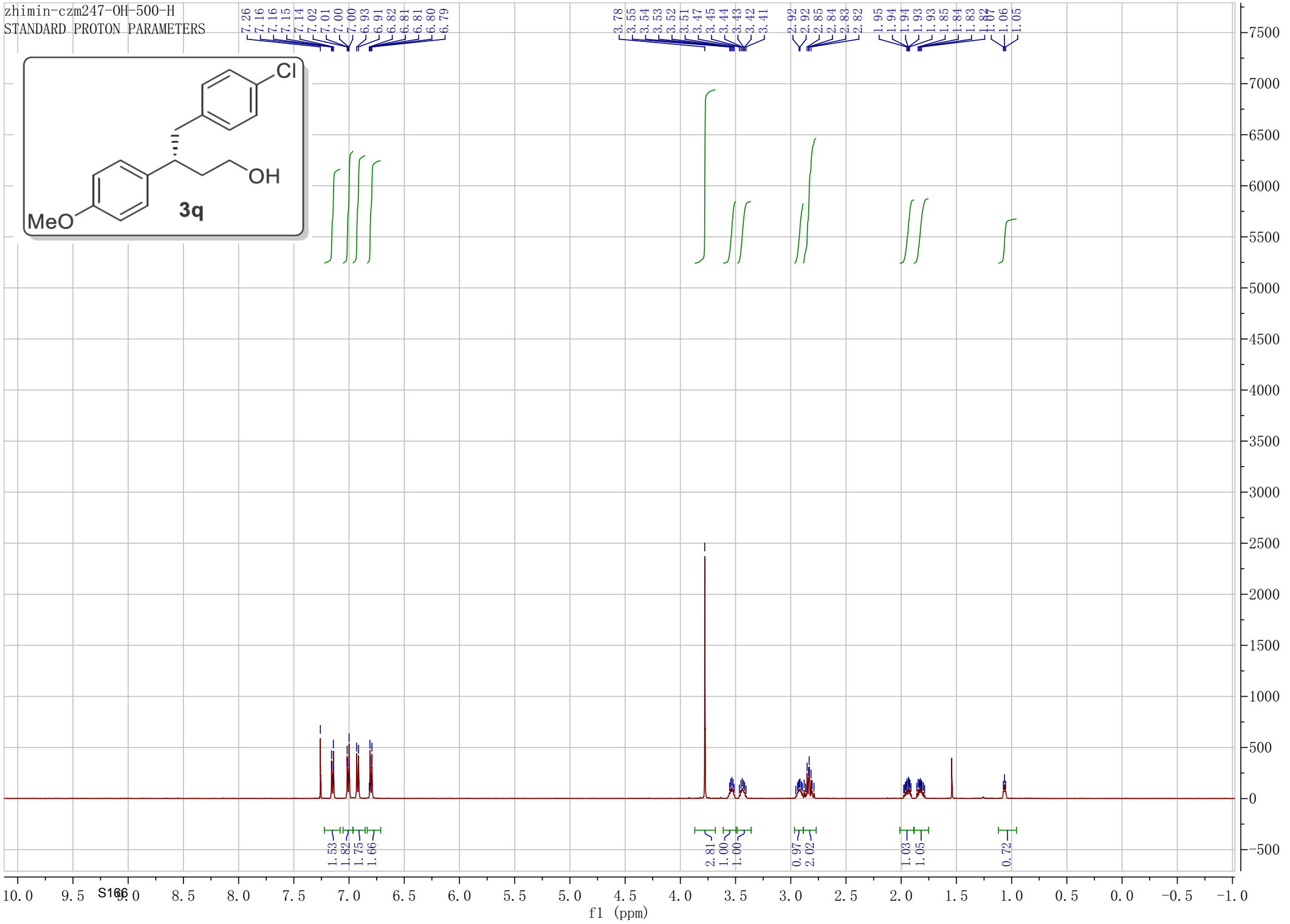

zhimin-1aCHO-300-C
13C OBSERVE
201.27
142.64
137.67
132.05
130.49
128.61
128.35
127.49
126.84
77.42
77.00
76.58
49.01
42.46
41.78
Cl
O
2p
S161
f1 (ppm)

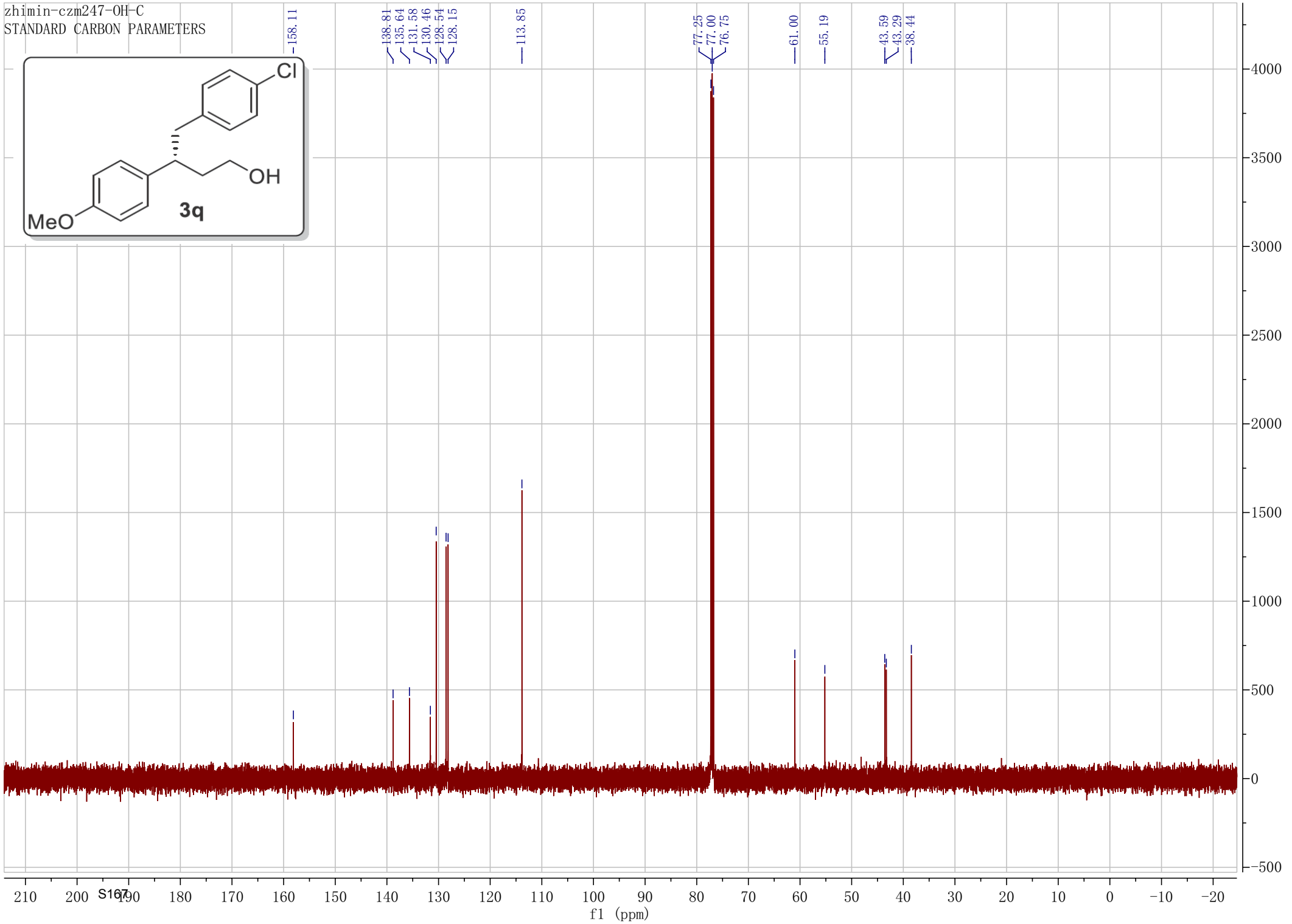

zhimin-1aOH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
OH
3p
7.22
2.00
1.06
1.05
1.09
2.02
2.14
1.07
f1 (ppm)

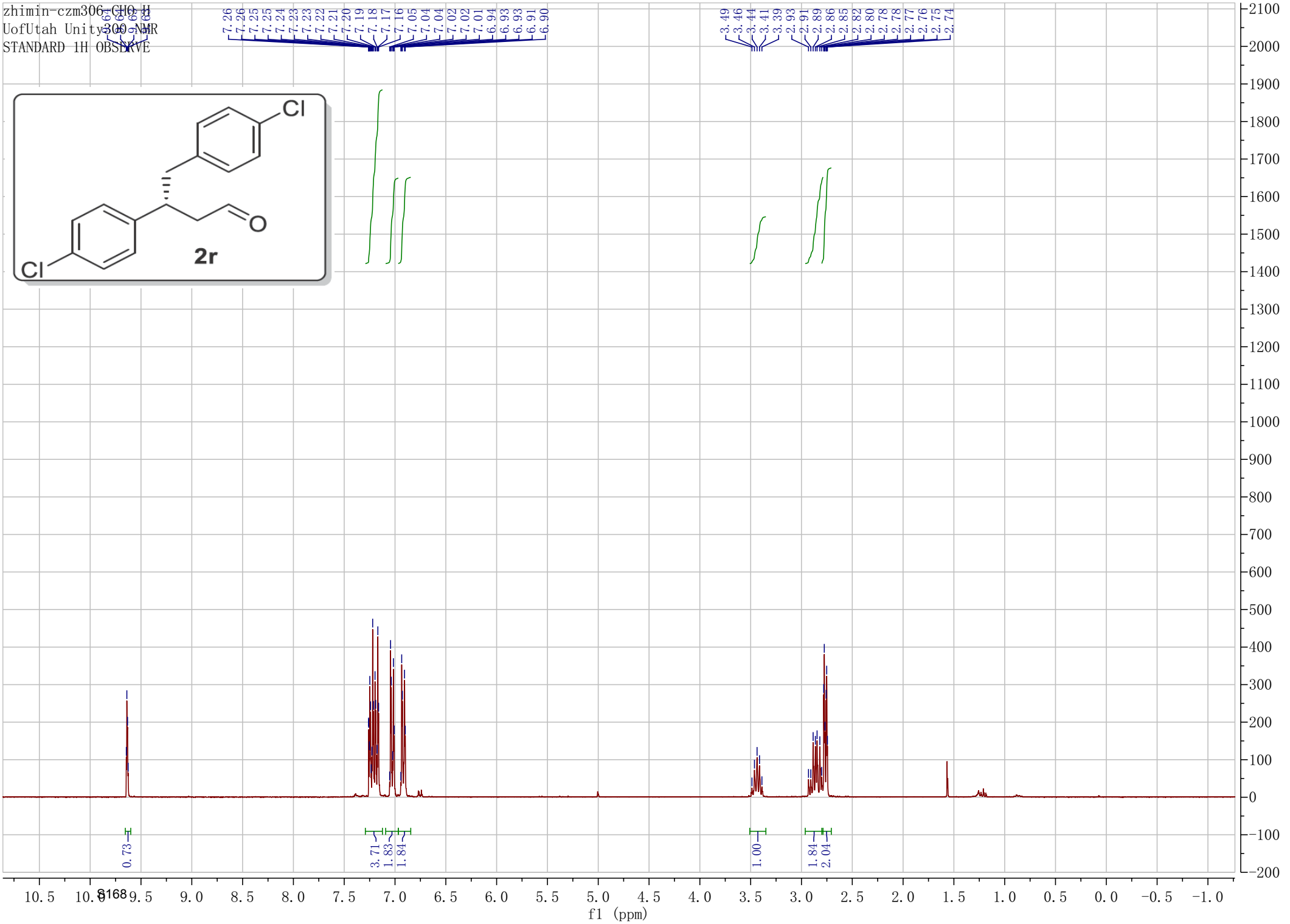

zhimin-1aOH-300-C
13C OBSERVE
143.66
138.65
131.57
130.41
128.43
128.13
127.63
126.43
77.42
77.00
76.58
60.84
44.32
43.04
38.16
Cl
OH
3p
f1 (ppm)

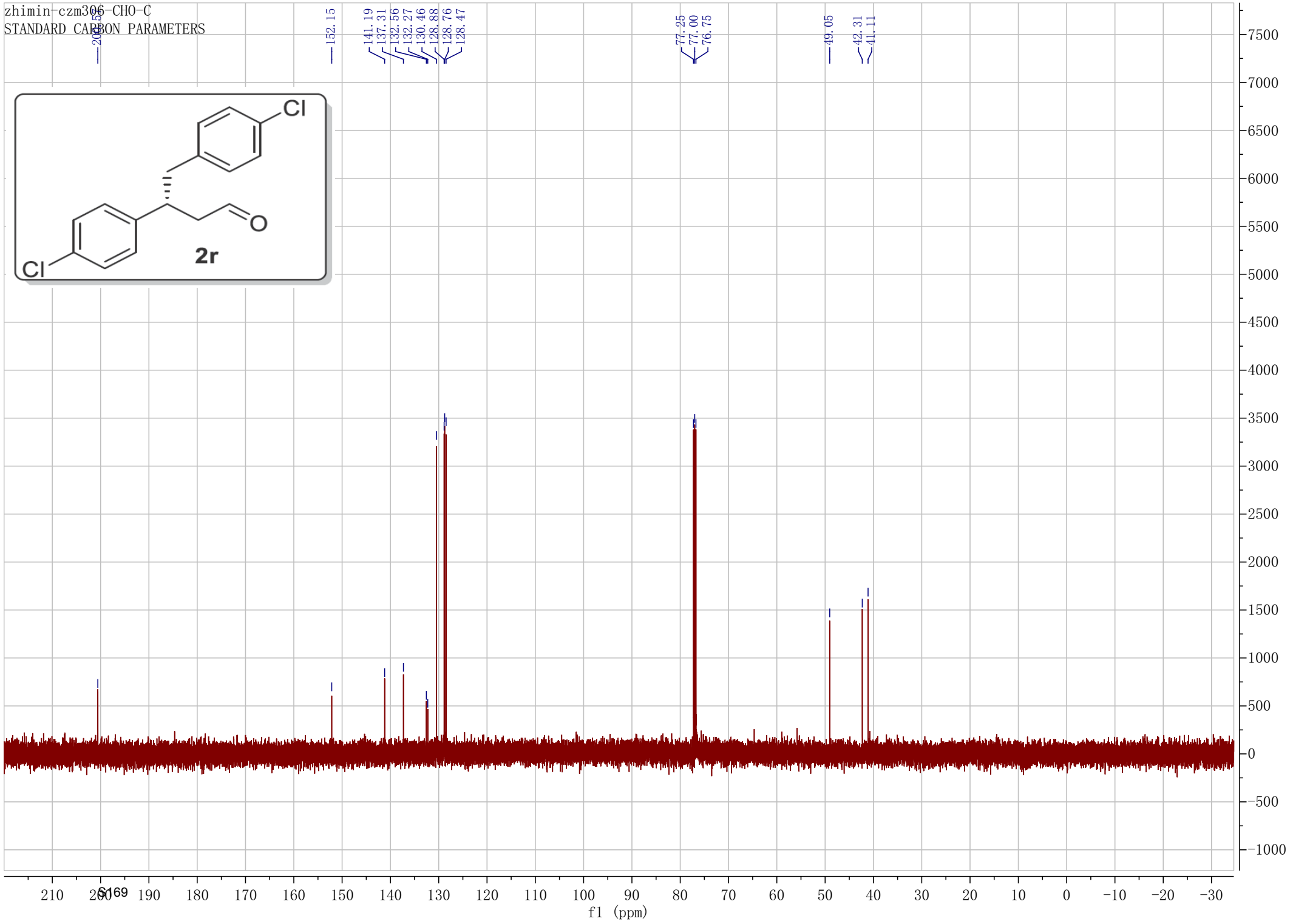

zhimin-czm331-CHO-H
STANDARD PROTON PARAMETERS
Cl
O
MeO
2q
f1 (ppm)

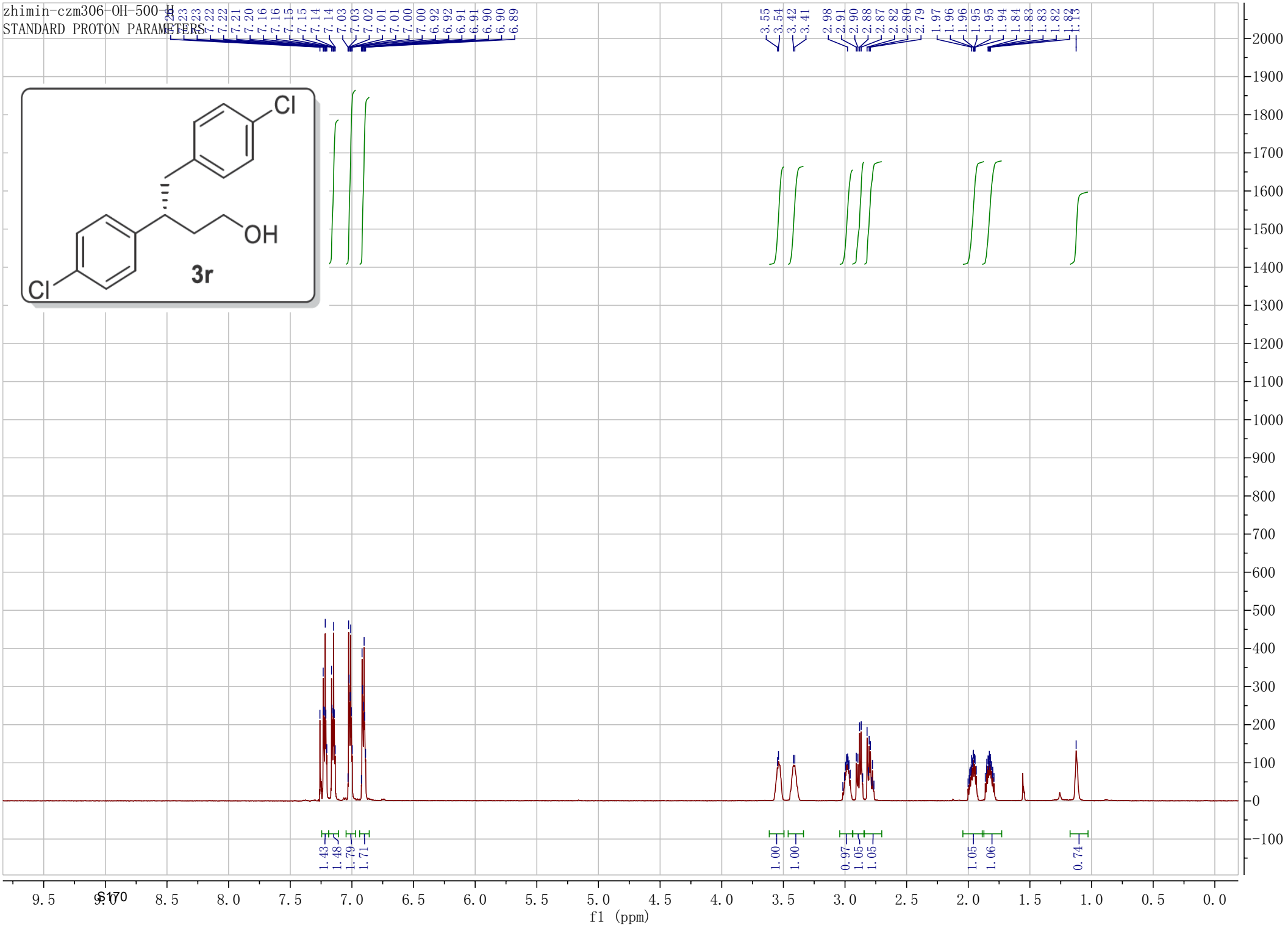

zhimin-cam278-CHO-C
STANDARD-CARBON PARAMETERS
201.44
158.35
137.81
134.62
132.03
130.52
128.45
128.34
113.99
77.25
77.00
76.75
55.20
49.25
42.66
41.07
Cl
O
MeO
2q
f1 (ppm)

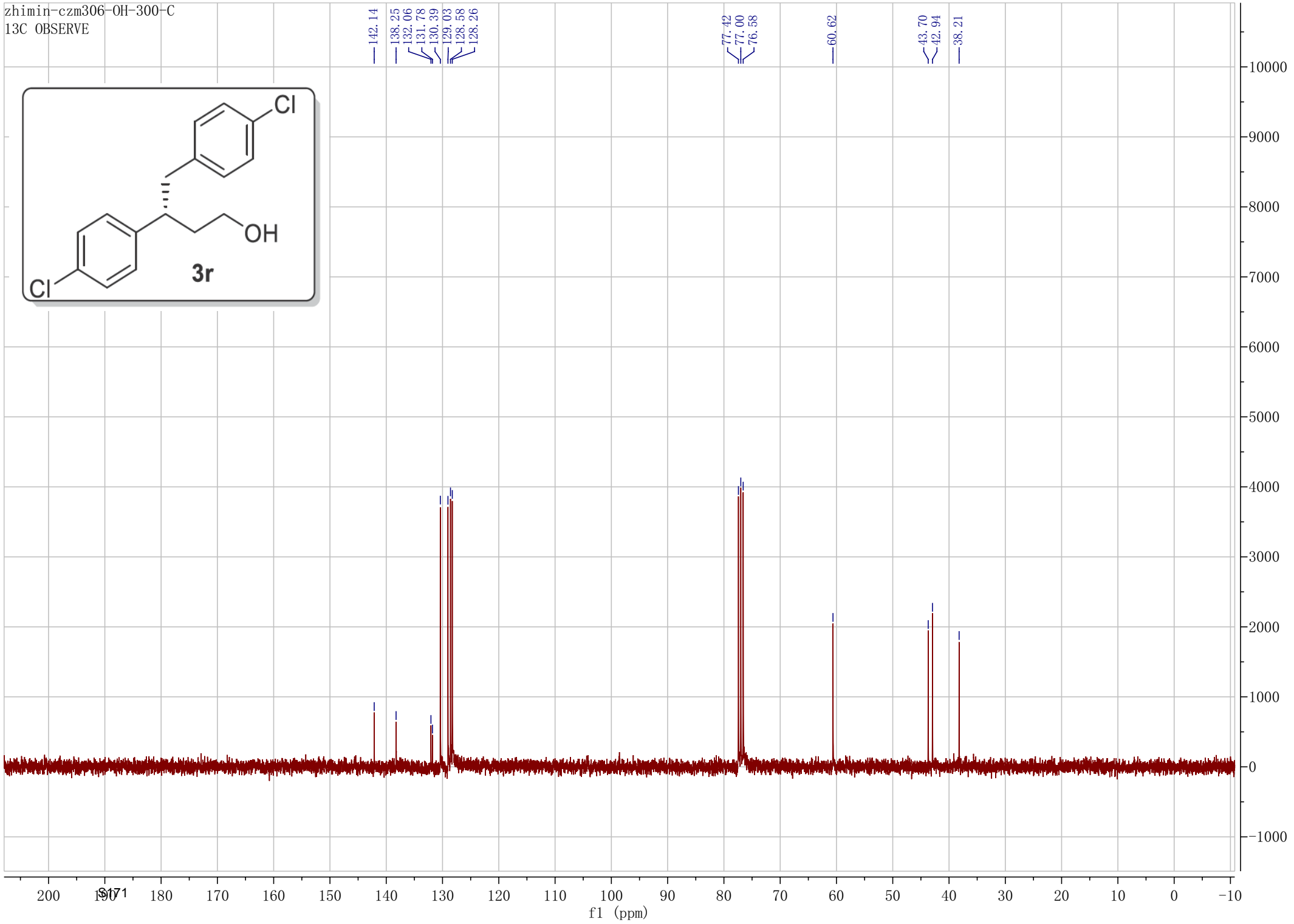

zhimin-czm247-OH-500-H
STANDARD PROTON PARAMETERS
7.26 7.16 7.16 7.15 7.14 7.02 7.01 7.00 7.00 6.93 6.91 6.82 6.81 6.81 6.80 6.79
3.78 3.55 3.54 3.53 3.52 3.51 3.47 3.45 3.44 3.43 3.42 3.41
2.92 2.92 2.85 2.84 2.83 2.82
1.95 1.94 1.94 1.93 1.93 1.85 1.84 1.83 1.82 1.07 1.06 1.05
Cl
OH
MeO
3q
1.53 1.82 1.75 1.66
2.81 1.00 1.00
0.97 2.02
1.03 1.05
0.72
f1 (ppm)

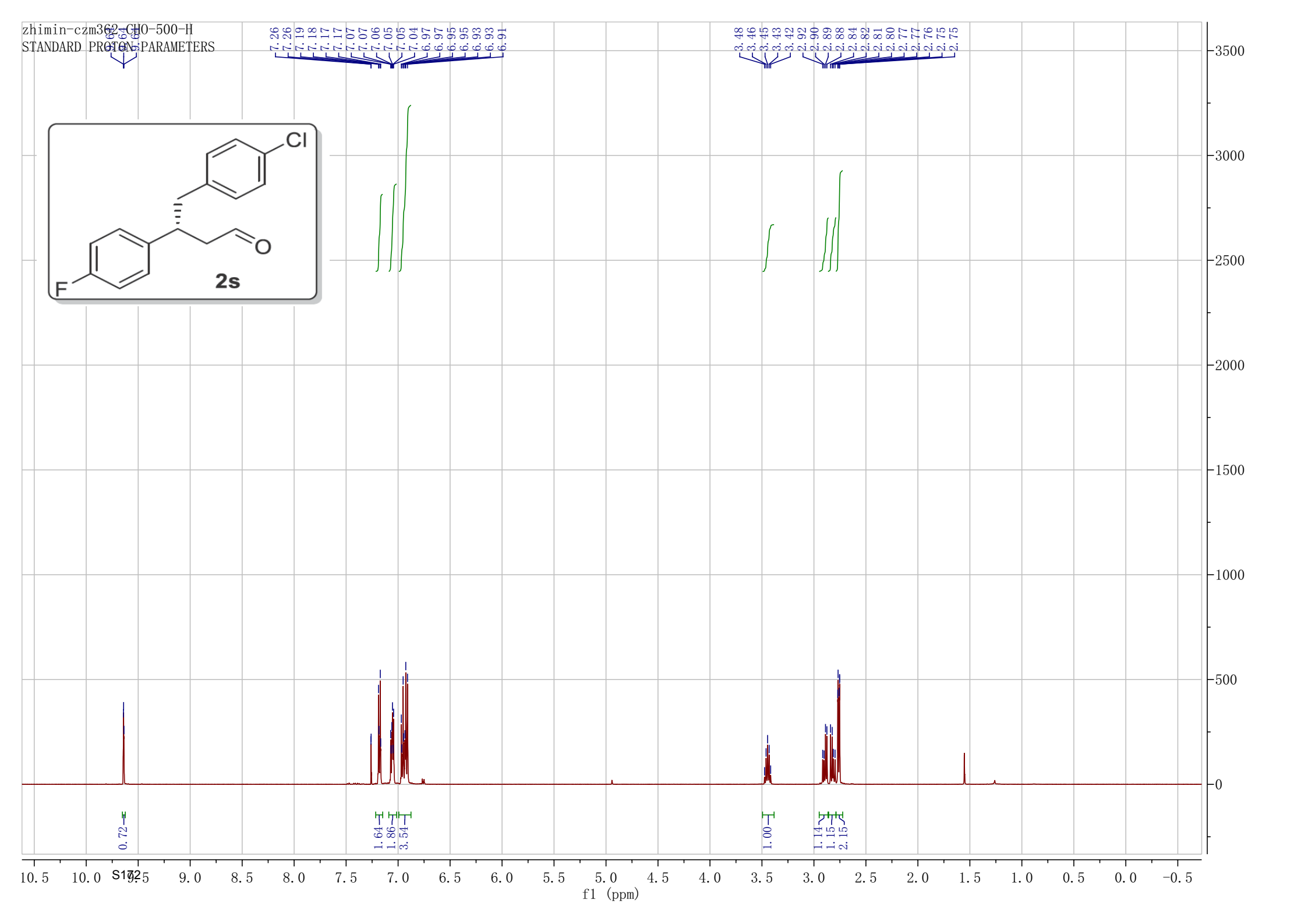

zhimin-czm247-OH-C
STANDARD CARBON PARAMETERS
158.11
138.81
135.64
131.58
130.46
128.54
128.15
113.85
77.25
77.00
76.75
61.00
55.19
43.59
43.29
38.44
Cl
OH
MeO
3q
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

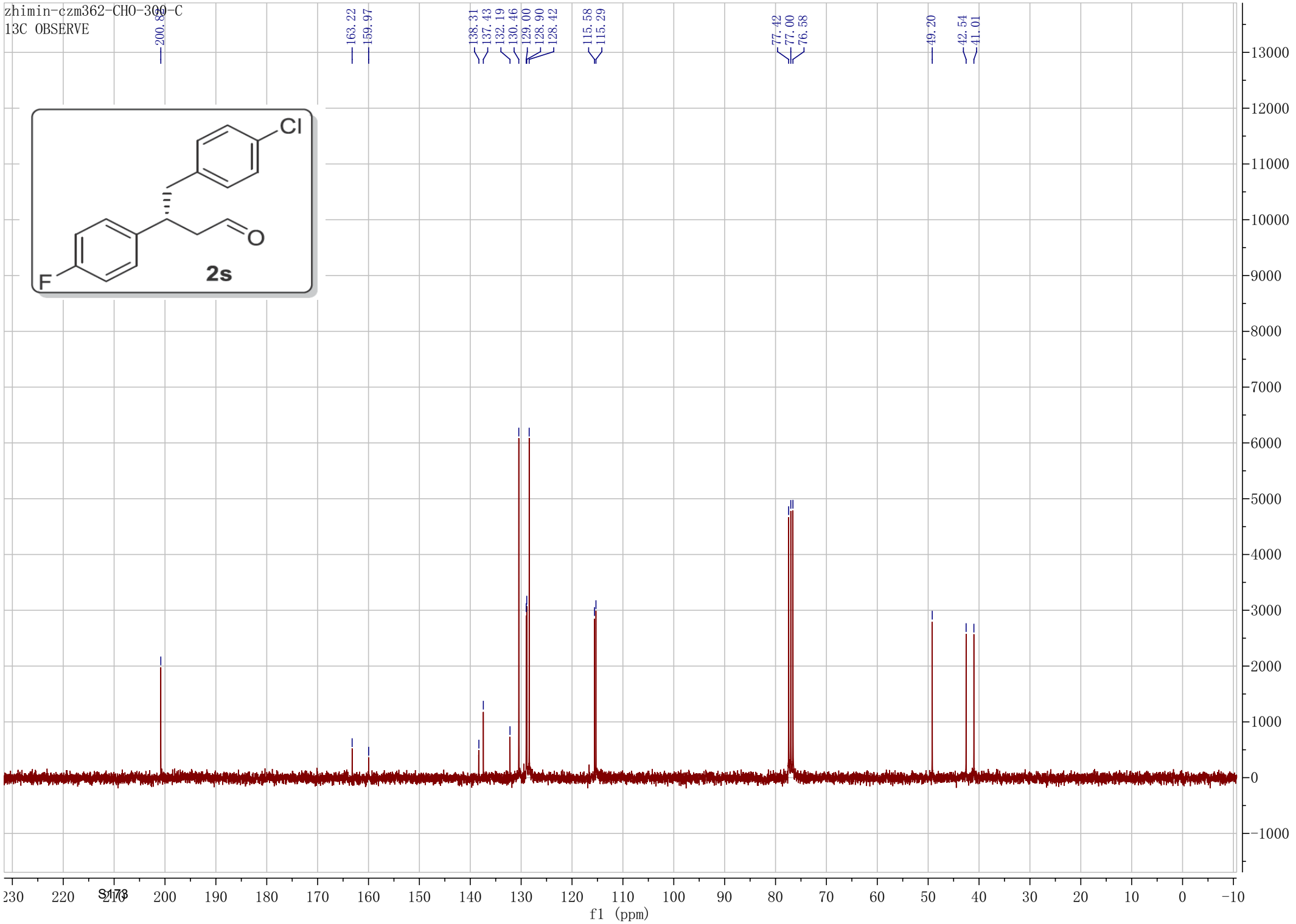

zhimin-czm306-CH0-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
O
Cl
2r
f1 (ppm)

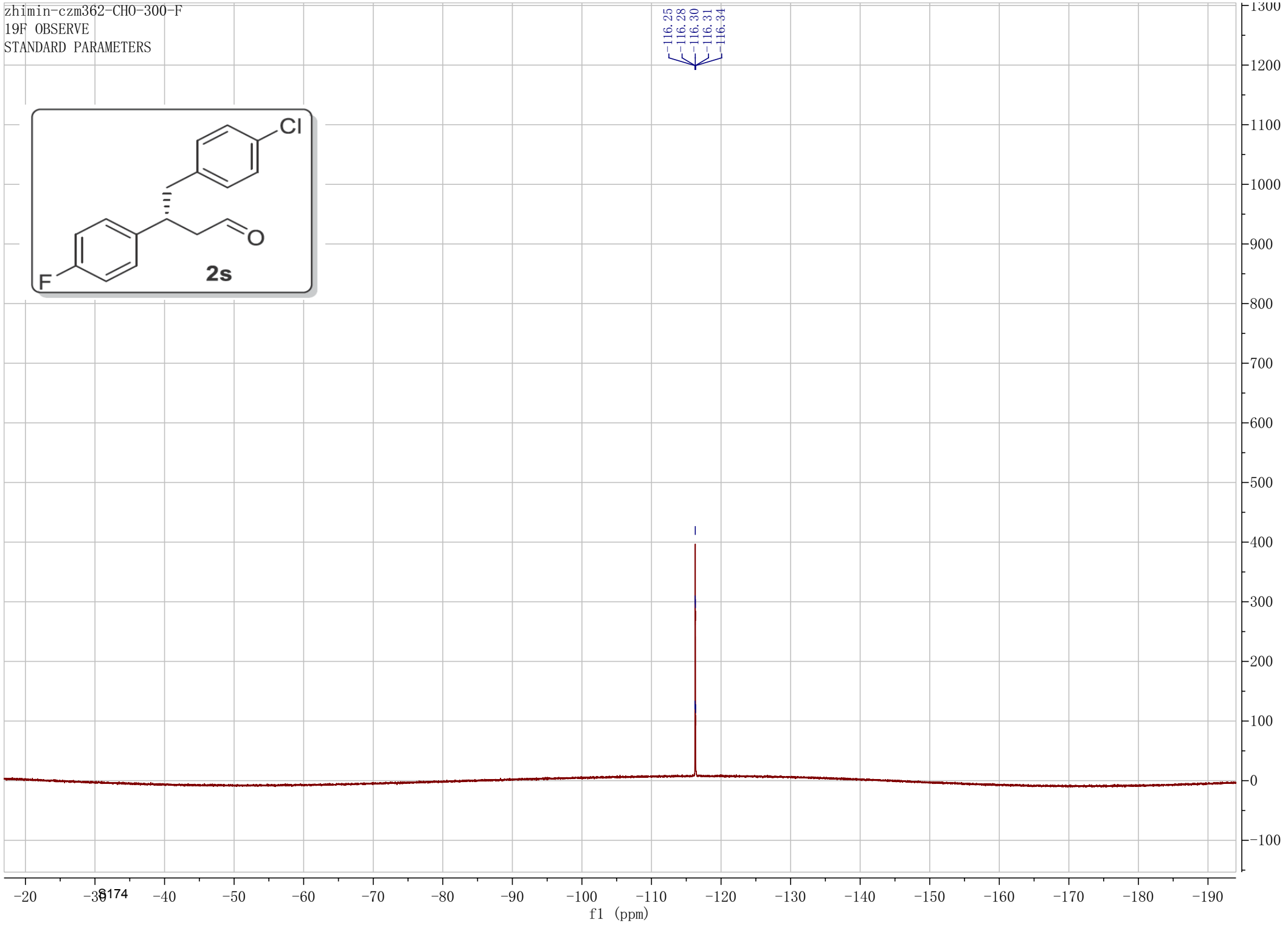

zhimin-czm306-CHO-C
STANDARD CARBON PARAMETERS
206.55
152.15
141.19
137.31
132.56
132.27
130.46
128.88
128.76
128.47
77.25
77.00
76.75
49.05
42.31
41.11
Cl
O
Cl
2r
f1 (ppm)

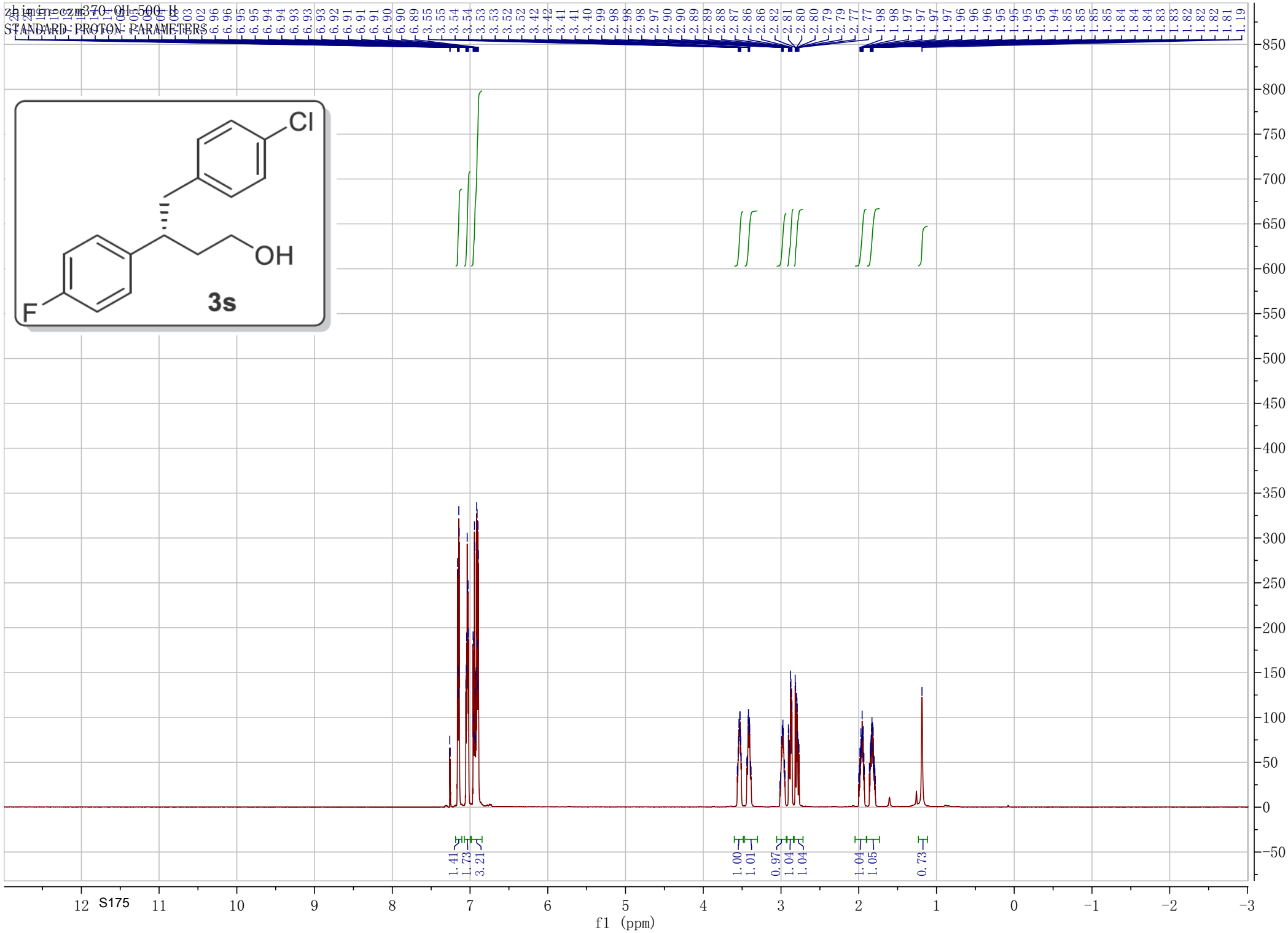

zhimin-czm306-OH-500-H
STANDARD PROTON PARAMETERS
Cl
OH
Cl
3r
f1 (ppm)

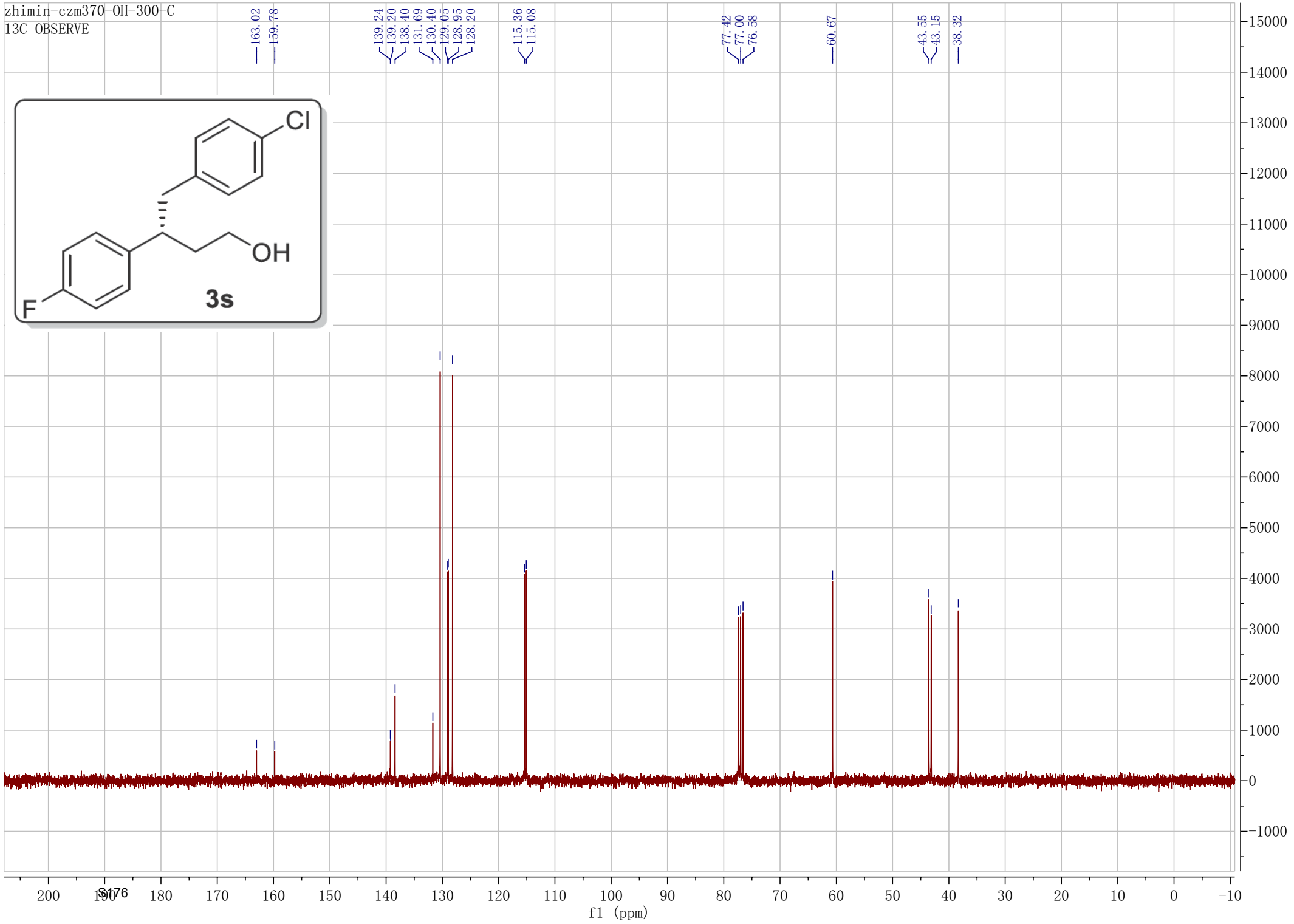

zhimin-czm306-OH-300-C
13C OBSERVE
142.14
138.25
132.06
131.78
130.39
129.03
128.58
128.26
77.42
77.00
76.58
60.62
43.70
42.94
38.21
Cl
OH
Cl
3r
f1 (ppm)

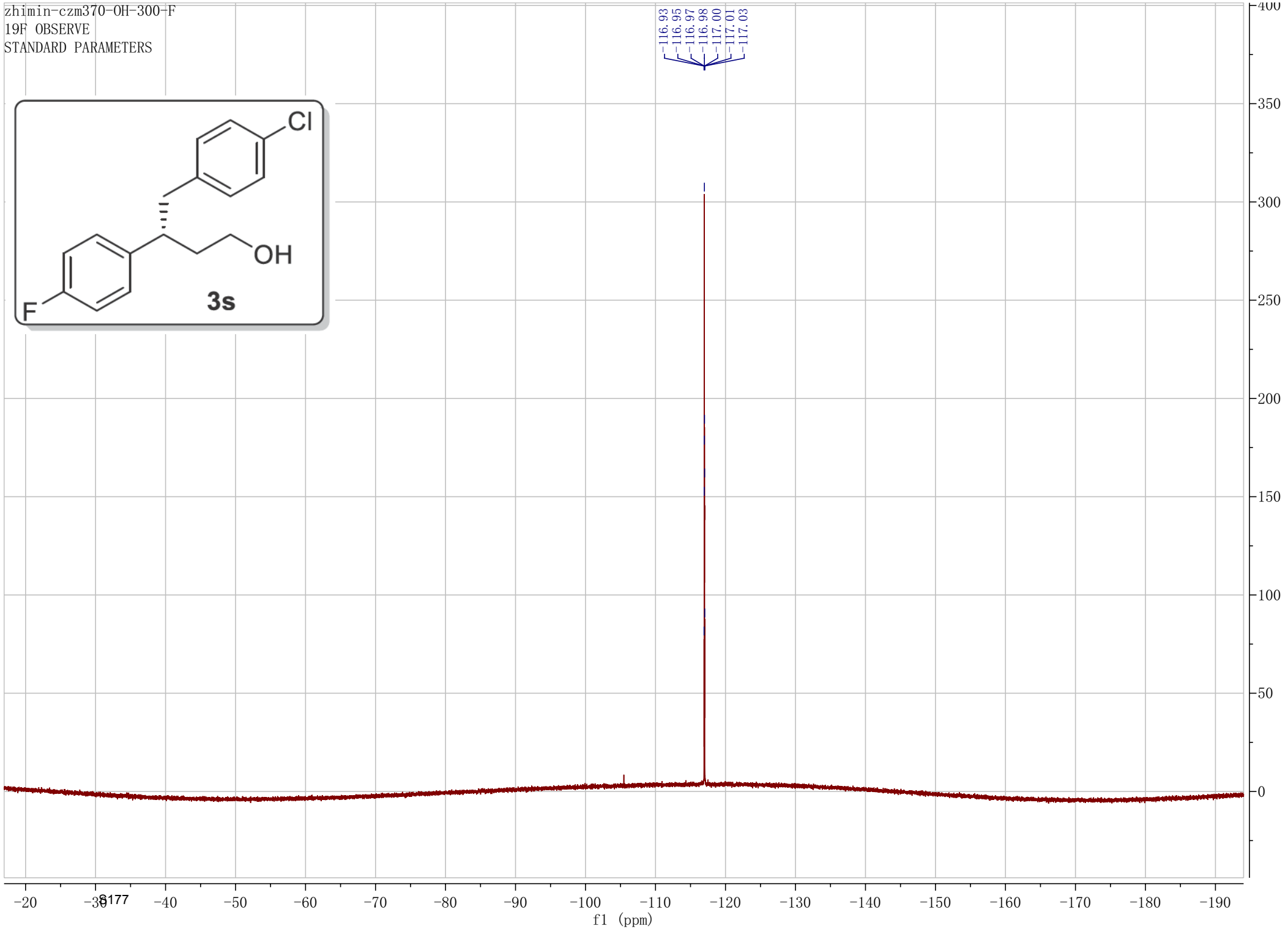

zhimin-czm362-CHO-500-H
STANDARD PROTON PARAMETERS
Cl
O
F
2s
f1 (ppm)

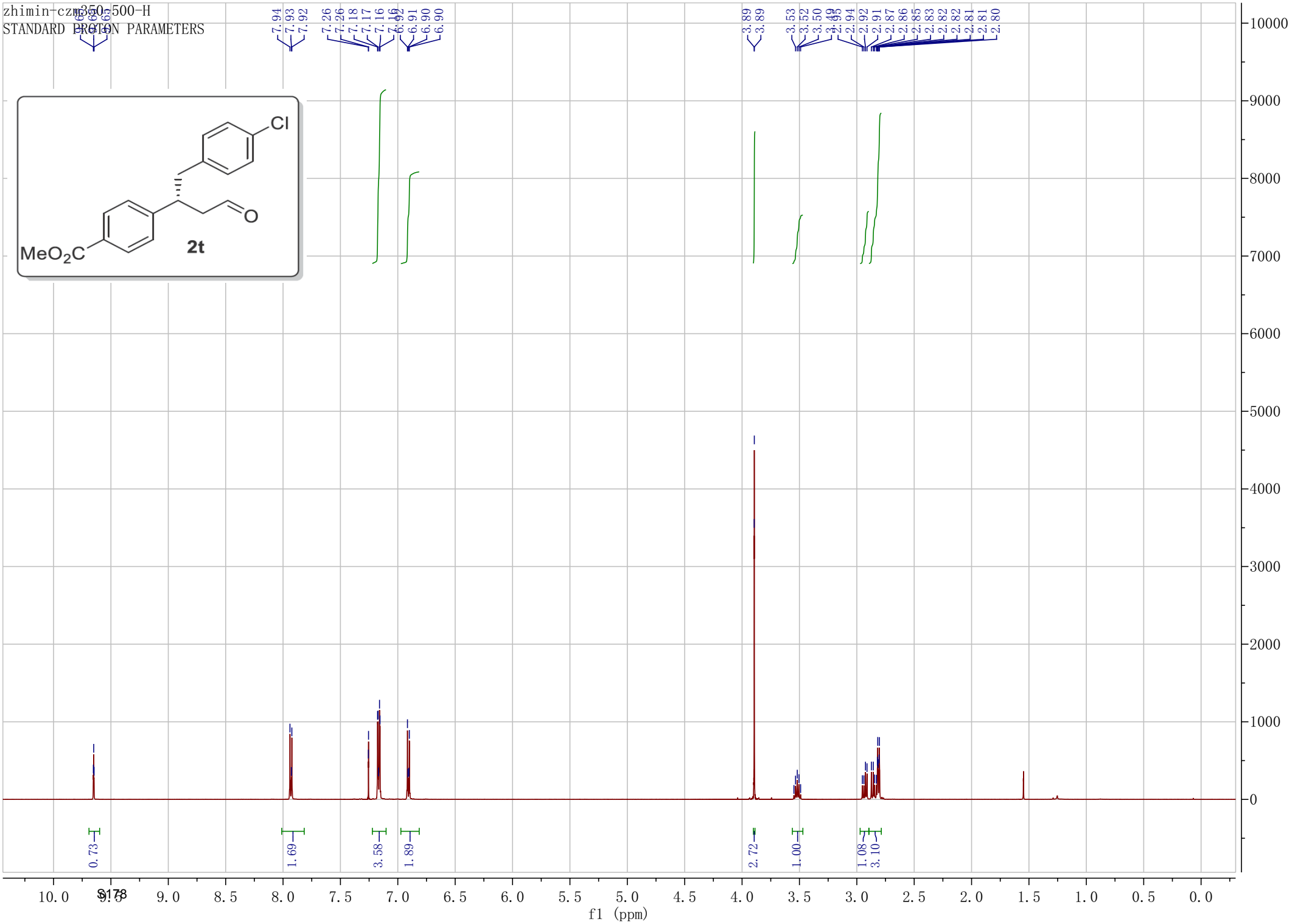

zhimin-czm362-CHO-300-C
13C OBSERVE
200.80
163.22
159.97
138.31
137.43
132.19
130.46
129.00
128.90
128.42
115.58
115.29
77.42
77.00
76.58
49.20
42.54
41.01
Cl
O
F
2s
f1 (ppm)

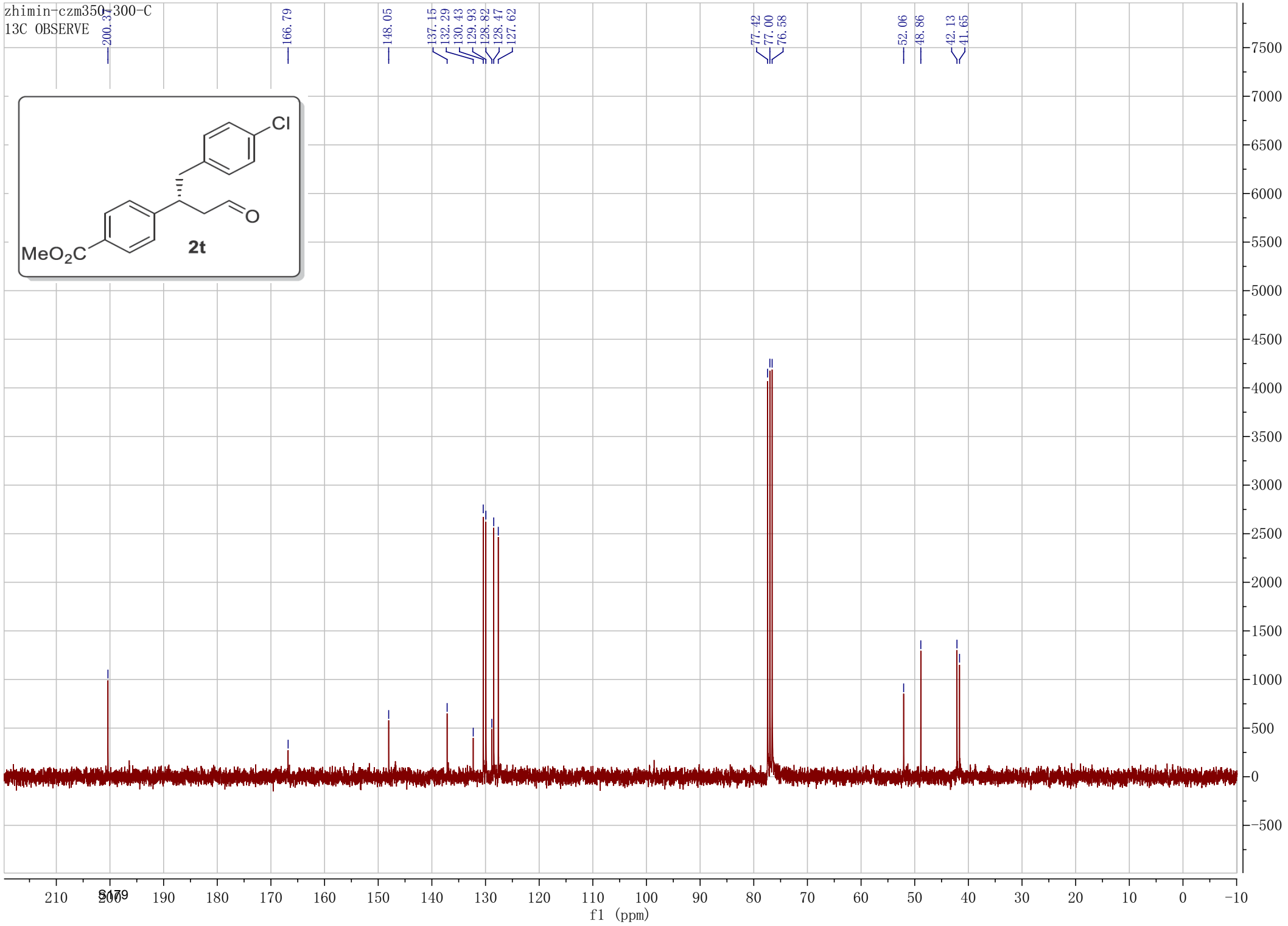

zhimin-czm362-CHO-300-F
19F OBSERVE
STANDARD PARAMETERS
-116.25
-116.28
-116.30
-116.31
-116.34
Cl
O
F
2s
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

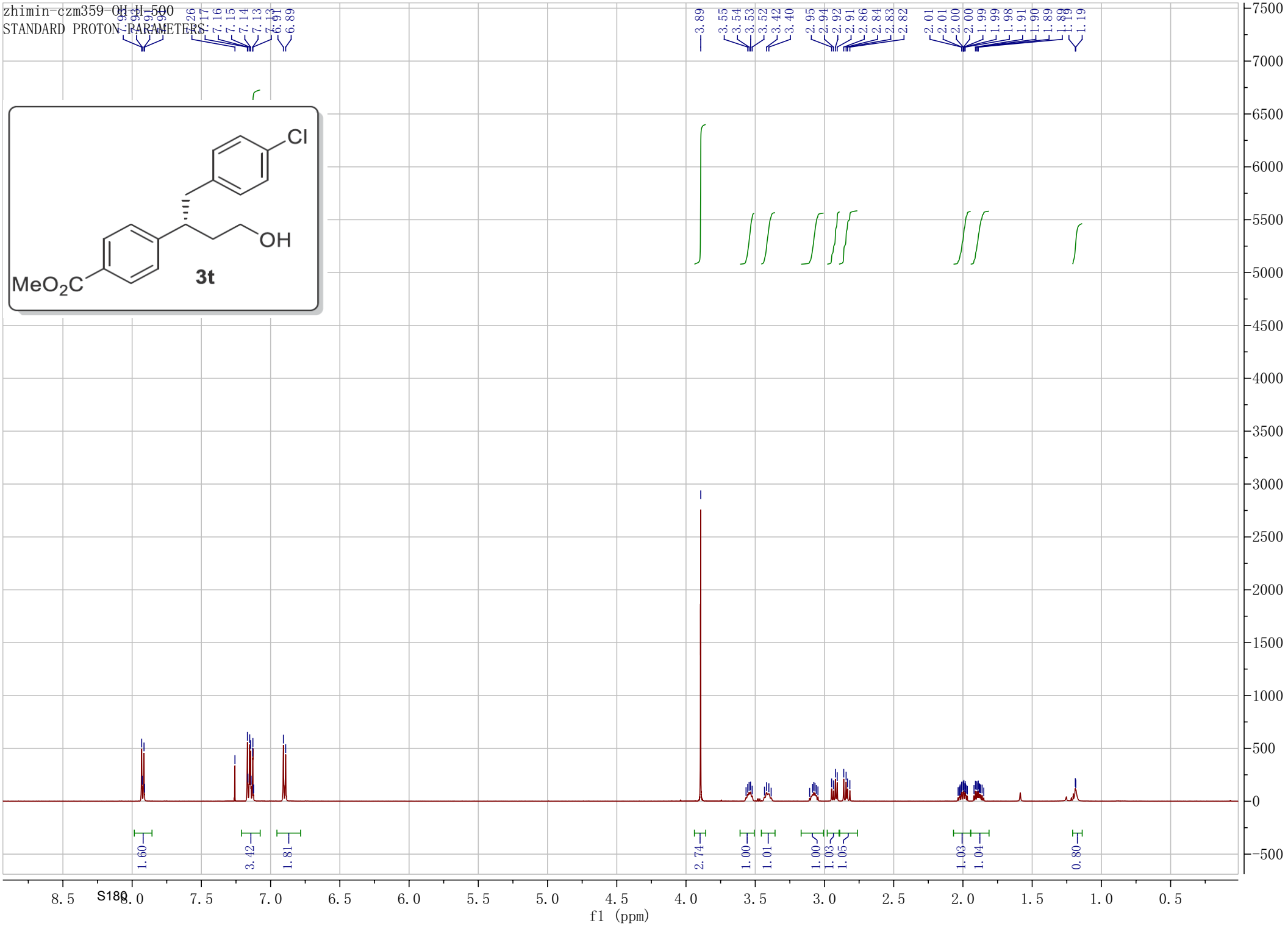

zhiqing-czm-370-OH-500-H
STANDARD PROTON PARAMETERS
Cl
OH
F
3s
1.41
1.73
3.21
1.00
1.01
0.97
1.04
1.04
1.04
1.05
0.73
S175
f1 (ppm)

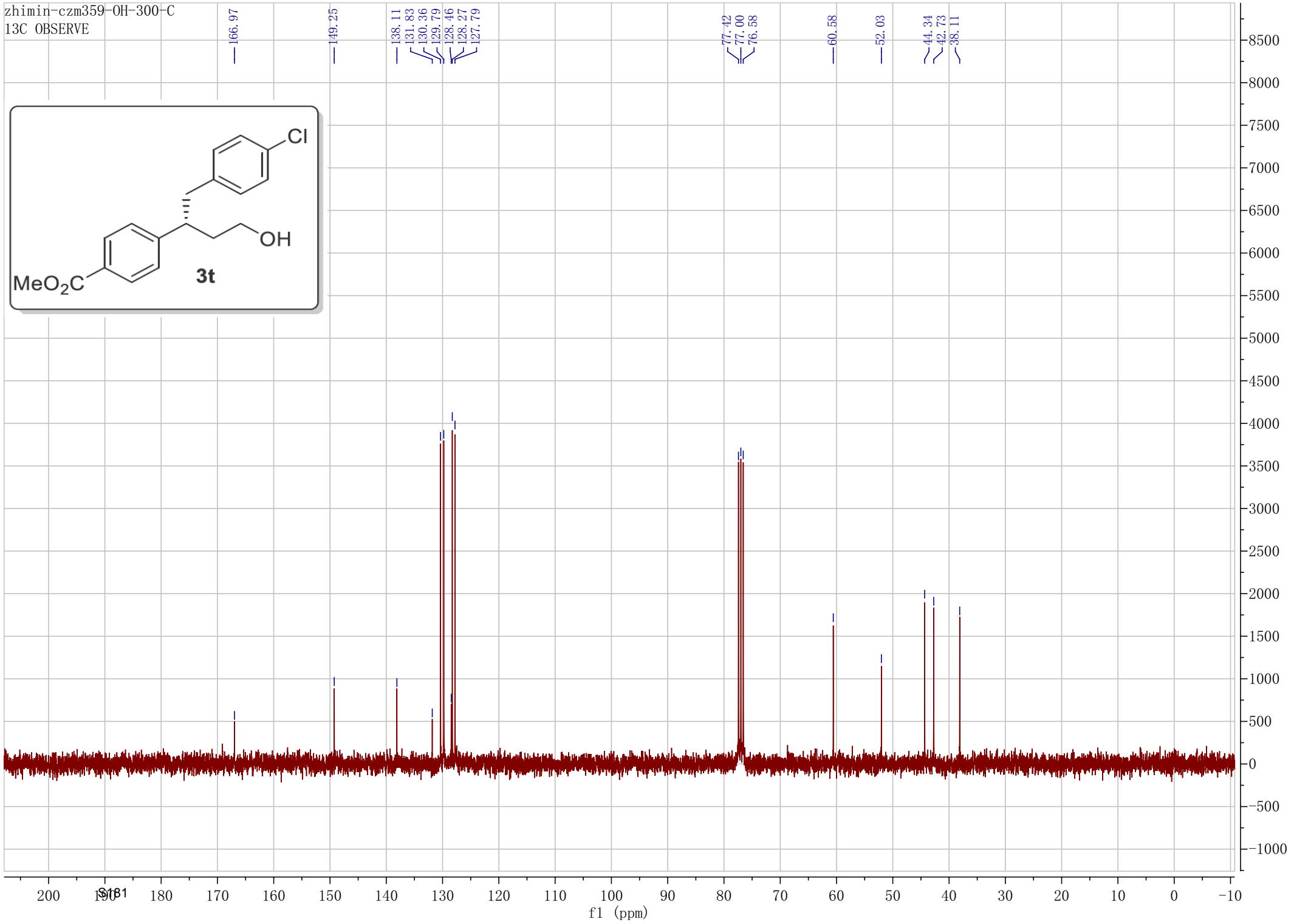

zhimin-czm370-OH-300-C
13C OBSERVE
163.02
159.78
139.24
139.20
138.40
131.69
130.40
129.05
128.95
128.20
115.36
115.08
77.42
77.00
76.58
60.67
43.55
43.15
38.32
Cl
OH
F
3s
f1 (ppm)

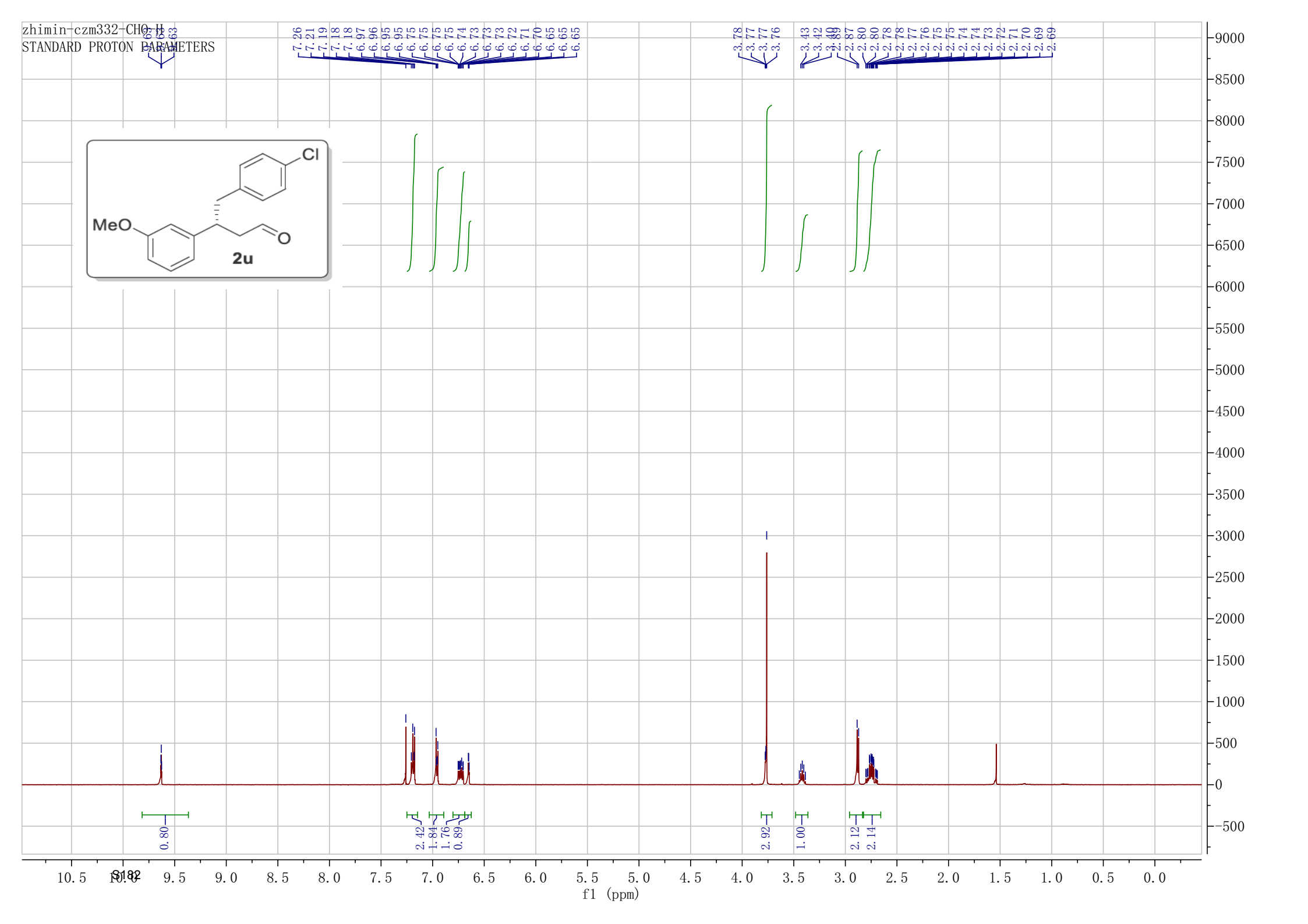

zhimin-czm370-OH-300-F
19F OBSERVE
STANDARD PARAMETERS
-116.93
-116.95
-116.97
-116.98
-117.00
-117.01
-117.03
Cl
OH
F
3s
400
350
300
250
200
150
100
50
0
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)

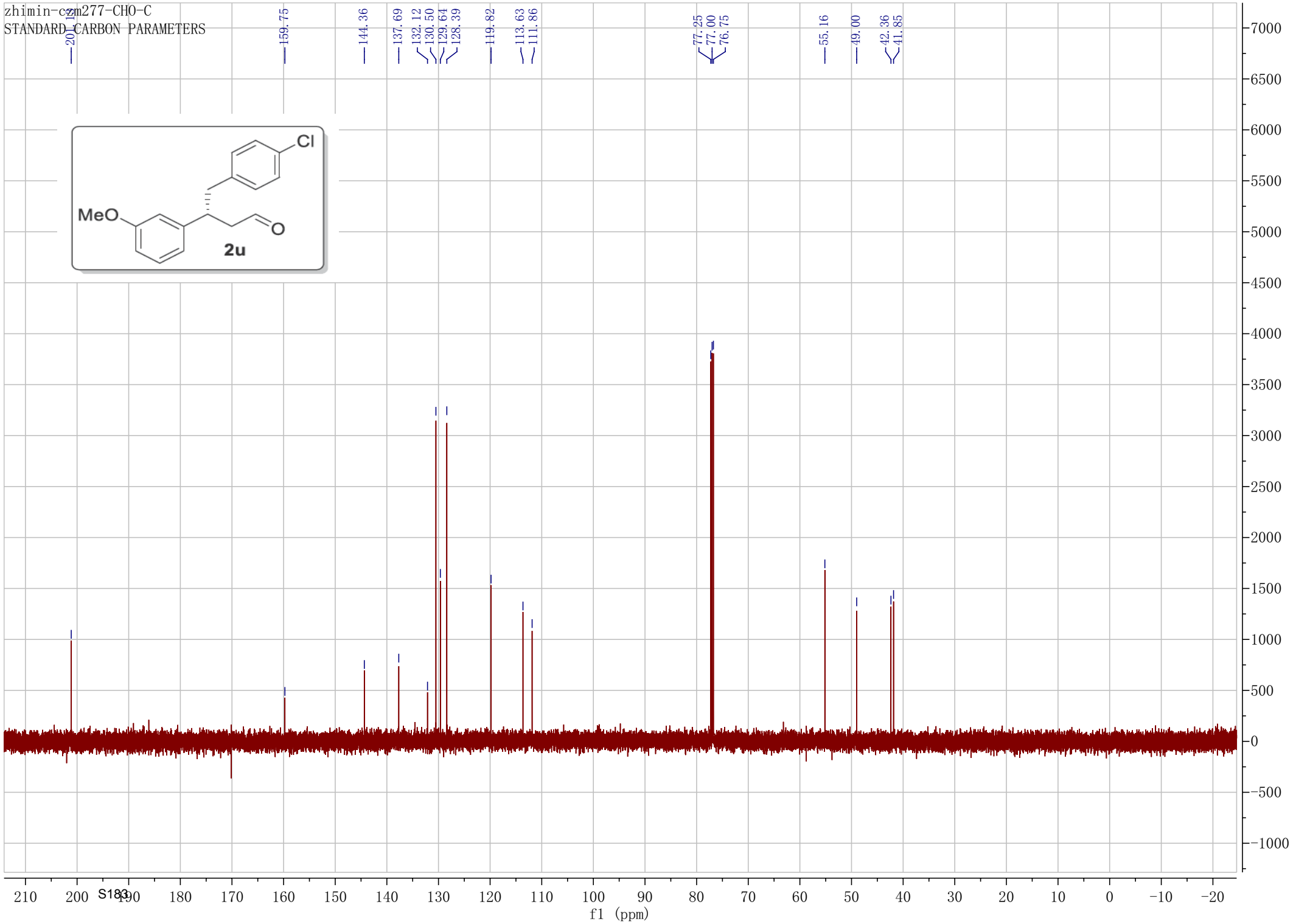

zhimin-czm-350-500-H
STANDARD PROTON PARAMETERS
Cl
O
MeO2C
2t
f1 (ppm)

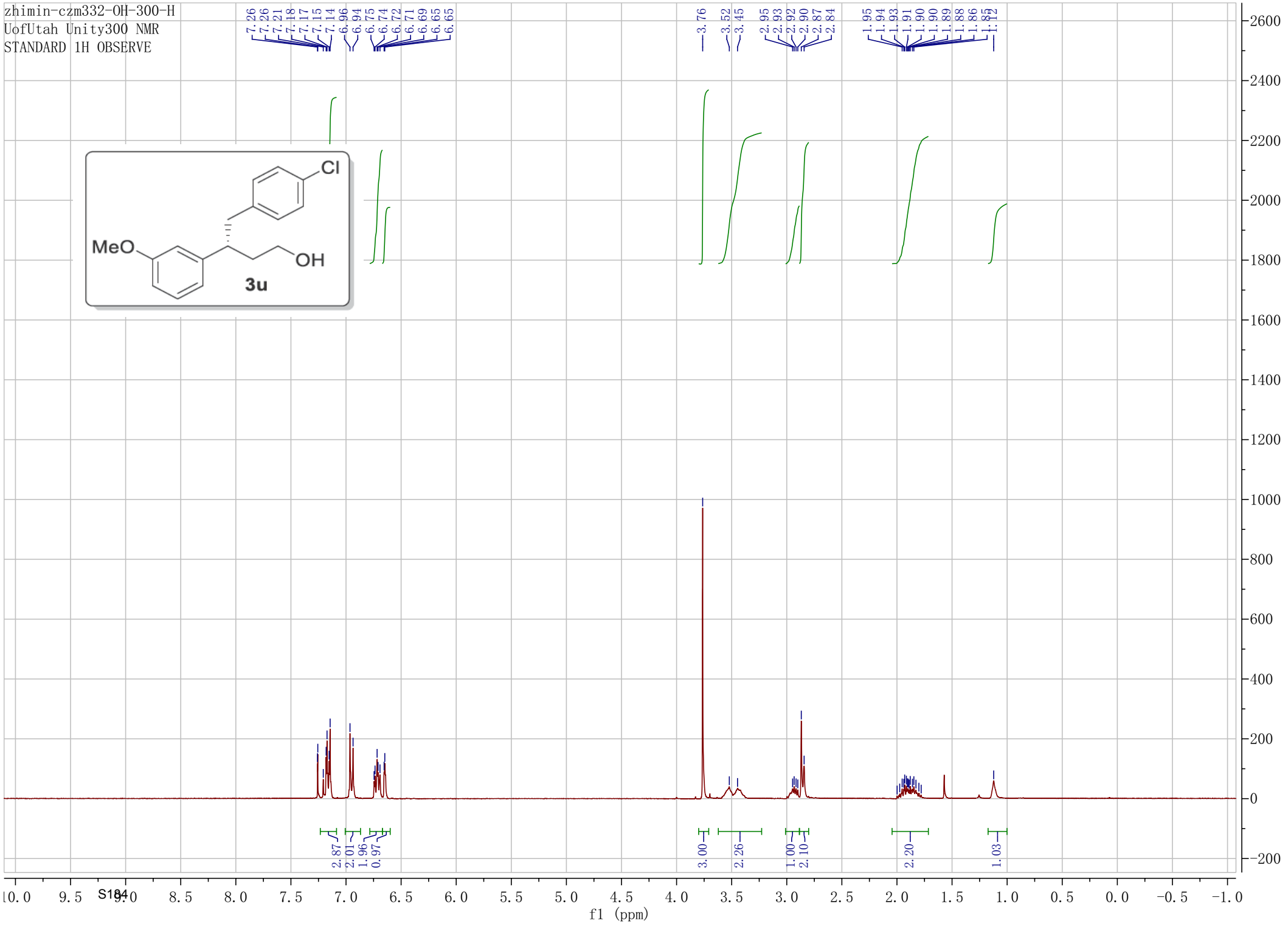

zhimin-czm350-300-C
13C OBSERVE
200.33
166.79
148.05
137.15
132.29
130.43
129.93
128.82
128.47
127.62
77.42
77.00
76.58
52.06
48.86
42.13
41.65
Cl
O
MeO2C
2t
f1 (ppm)

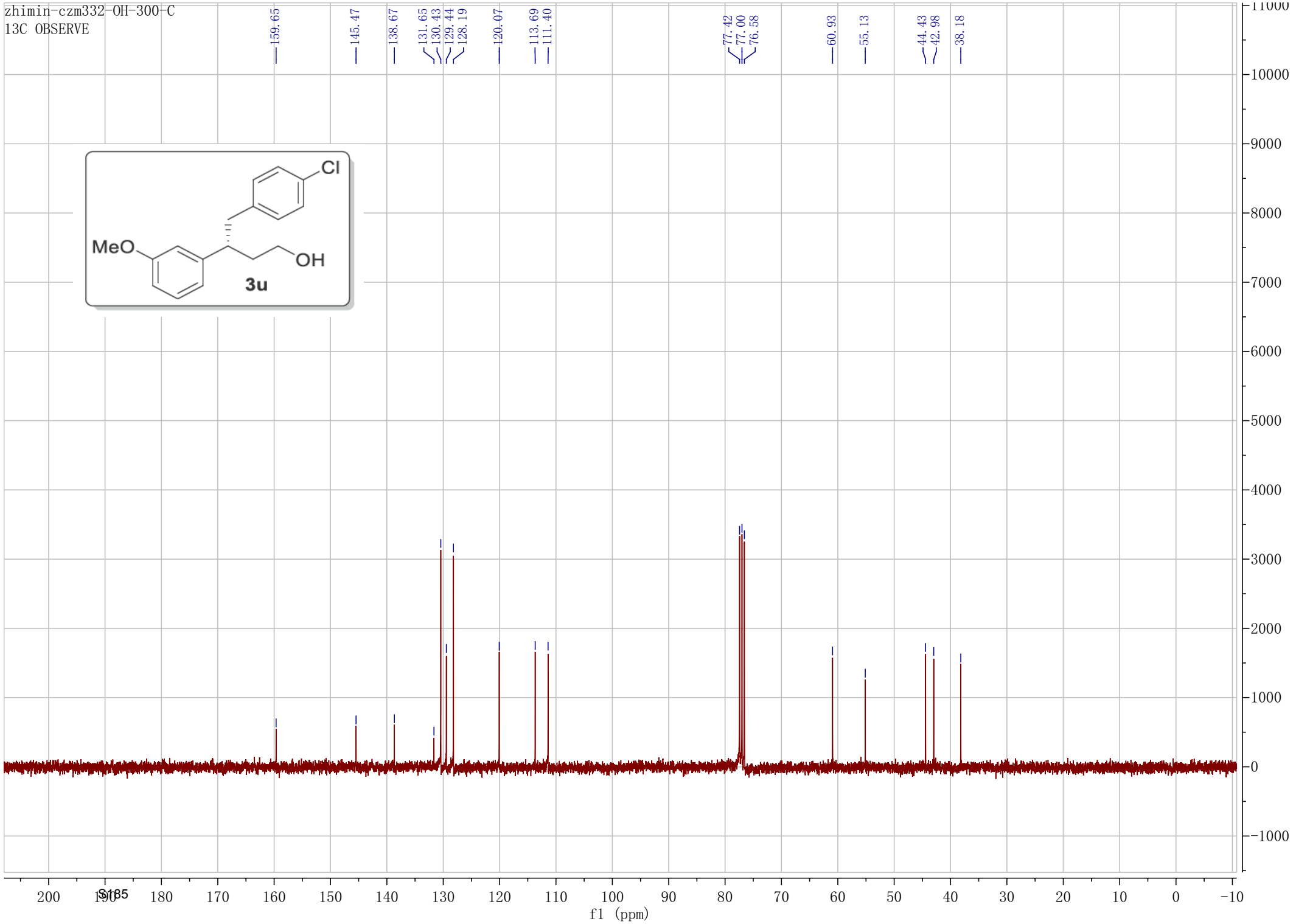

zhimin-czm359-OH-H-500
STANDARD PROTON PARAMETERS
Cl
OH
MeO2C
3t
f1 (ppm)

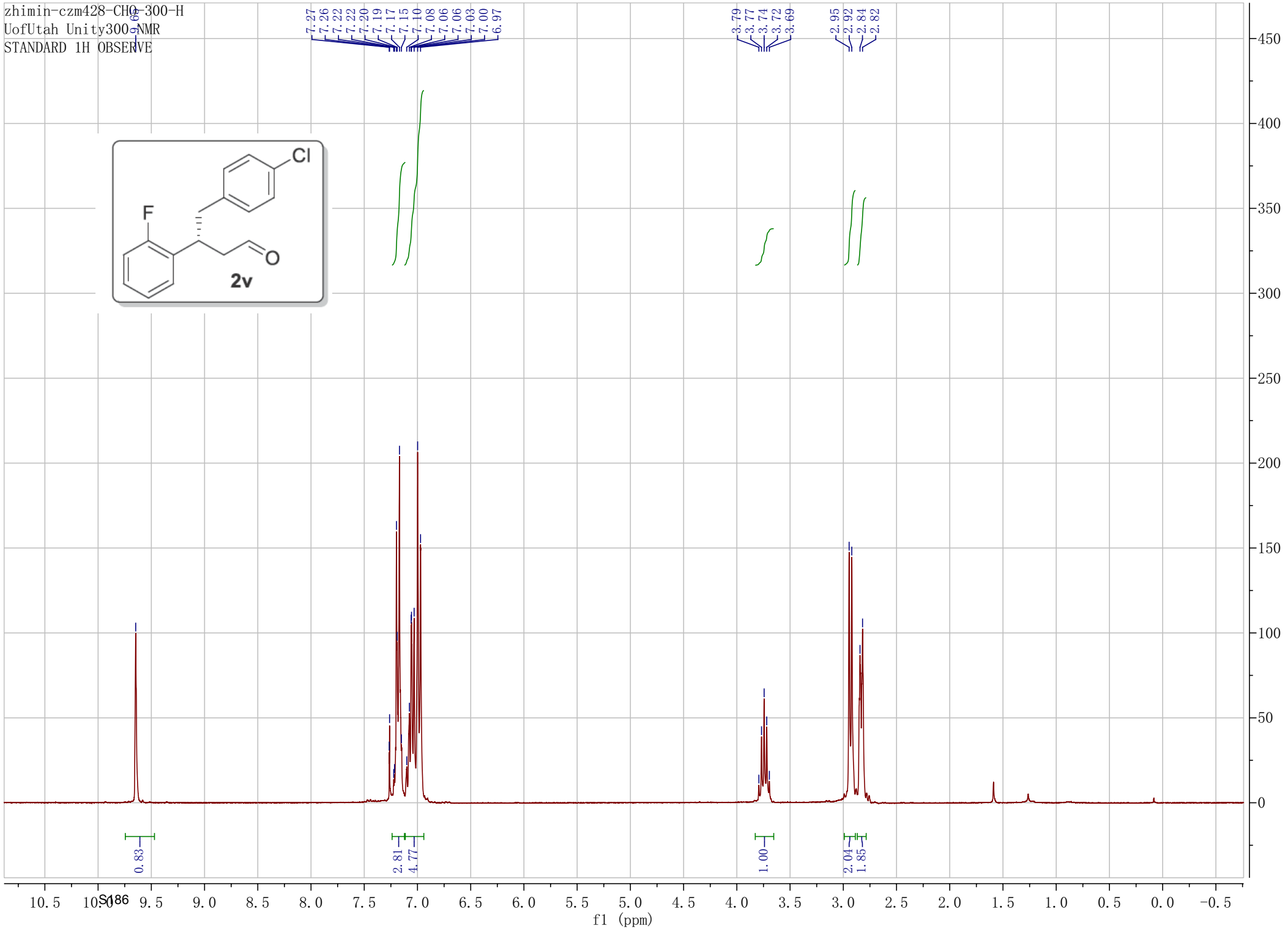

zhimin-czm359-OH-300-C
13C OBSERVE
166.97
149.25
138.11
131.83
130.36
129.79
128.46
128.27
127.79
77.42
77.00
76.58
60.58
52.03
44.34
42.73
38.11
Cl
OH
MeO2C
3t
f1 (ppm)

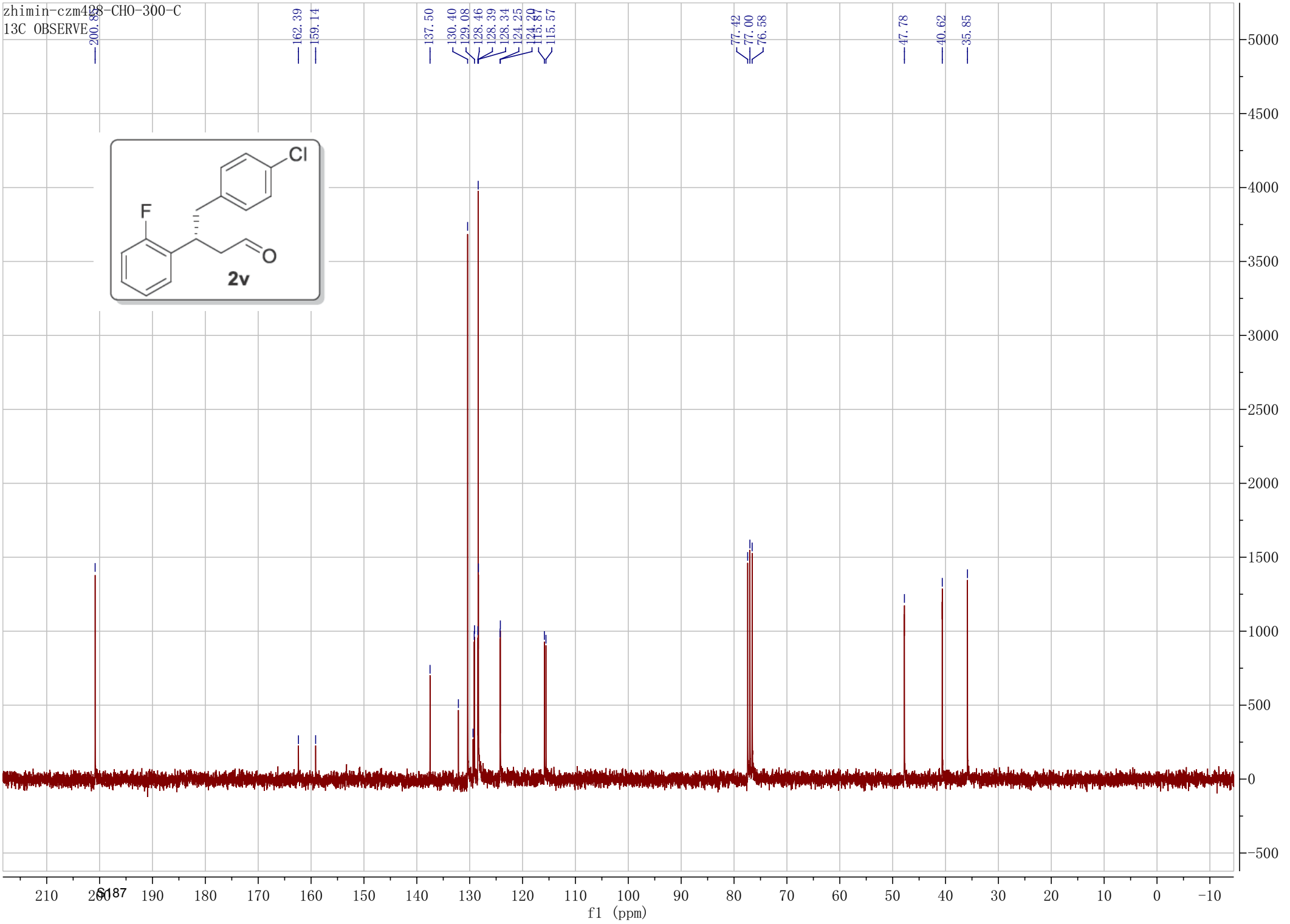

zhimin-czm332-CHO-H
STANDARD PROTON PARAMETERS
Cl
MeO
O
2u
f1 (ppm)


zhimin-czm277-CHO-C
STANDARD_CARBON PARAMETERS
201.15
159.75
144.36
137.69
132.12
130.50
129.64
128.39
119.82
113.63
111.86
77.25
77.00
76.75
55.16
49.00
42.36
41.85
Cl
MeO
O
2u
f1 (ppm)

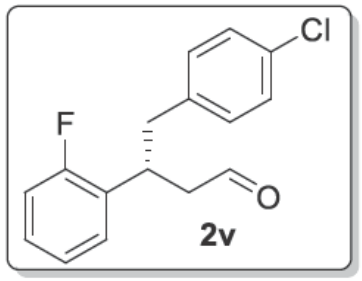

zhimin-czm332-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.26
7.26
7.21
7.18
7.17
7.15
7.14
6.96
6.94
6.75
6.74
6.72
6.71
6.69
6.65
6.65
3.76
3.52
3.45
2.95
2.93
2.92
2.90
2.87
2.84
1.95
1.94
1.93
1.91
1.90
1.90
1.89
1.88
1.86
1.85
1.12
Cl
MeO
OH
3u
2.87
2.01
1.96
0.97
3.00
2.26
1.00
2.10
2.20
1.03
f1 (ppm)


zhimin-czm332-OH-300-C
13C OBSERVE
159.65
145.47
138.67
131.65
130.43
129.44
128.19
120.07
113.69
111.40
77.42
77.00
76.58
60.93
55.13
44.43
42.98
38.18
Cl
MeO
OH
3u
f1 (ppm)


zhimin-czm428-CHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
9.69
7.27
7.26
7.22
7.22
7.20
7.19
7.17
7.15
7.10
7.08
7.06
7.06
7.03
7.00
6.97
3.79
3.77
3.74
3.72
3.69
2.95
2.92
2.84
2.82
Cl
F
O
2v
0.83
2.81
4.77
1.00
2.04
1.85
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)
450
400
350
300
250
200
150
100
50
0


zhimin-czm428-CHO-300-C
13C OBSERVE
200.88
162.39
159.14
137.50
130.40
129.08
128.46
128.39
128.34
124.25
124.20
115.87
115.57
77.42
77.00
76.58
47.78
40.62
35.85
Cl
F
O
2v
f1 (ppm)

zhimin-czm428-CHO-300-F
19F OBSERVE
STANDARD PARAMETERS



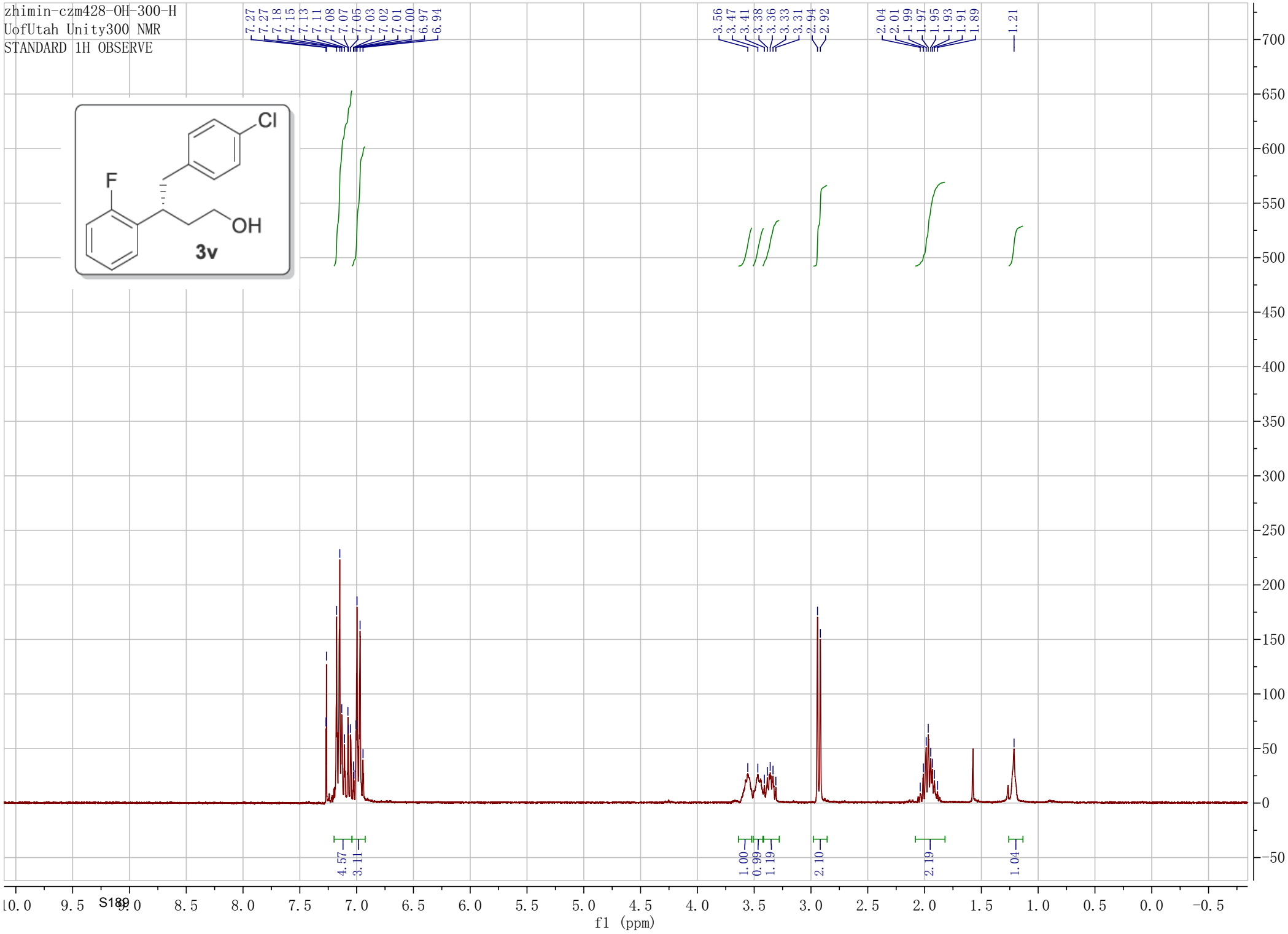
-117.80
-117.82
-117.84
-117.85
-117.88

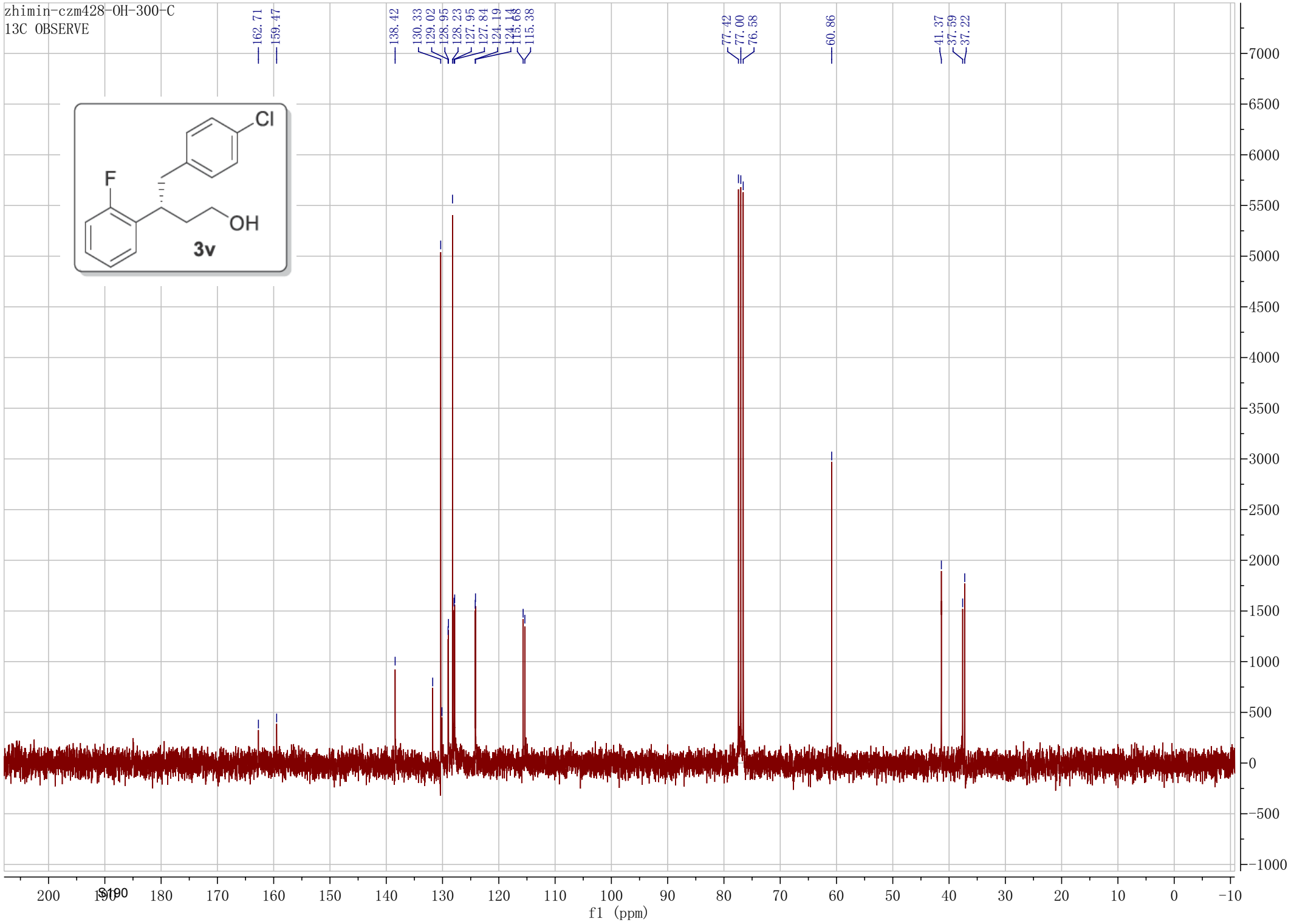
450
400
350
300
250
200
150
100
50
0

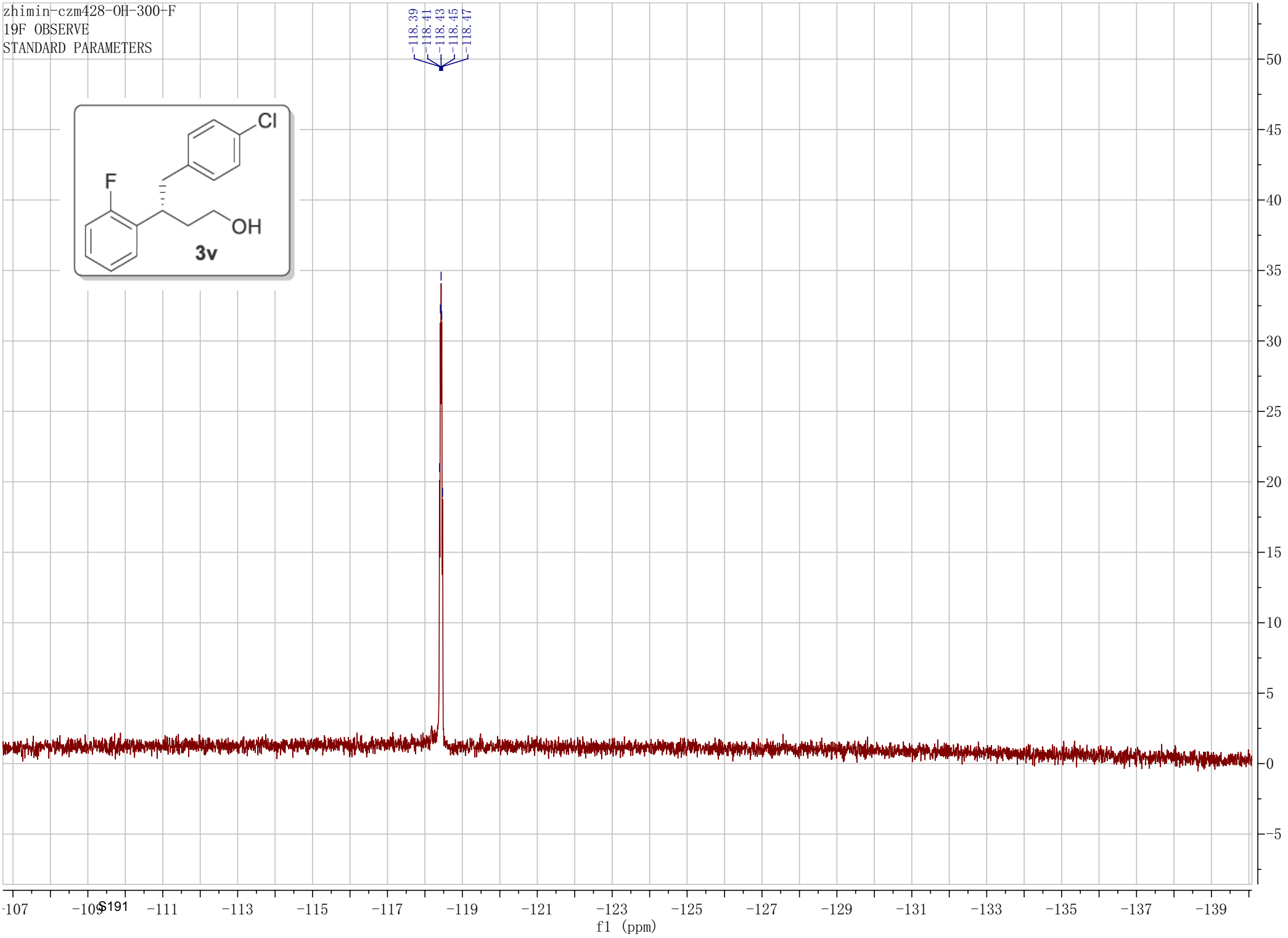
-20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190

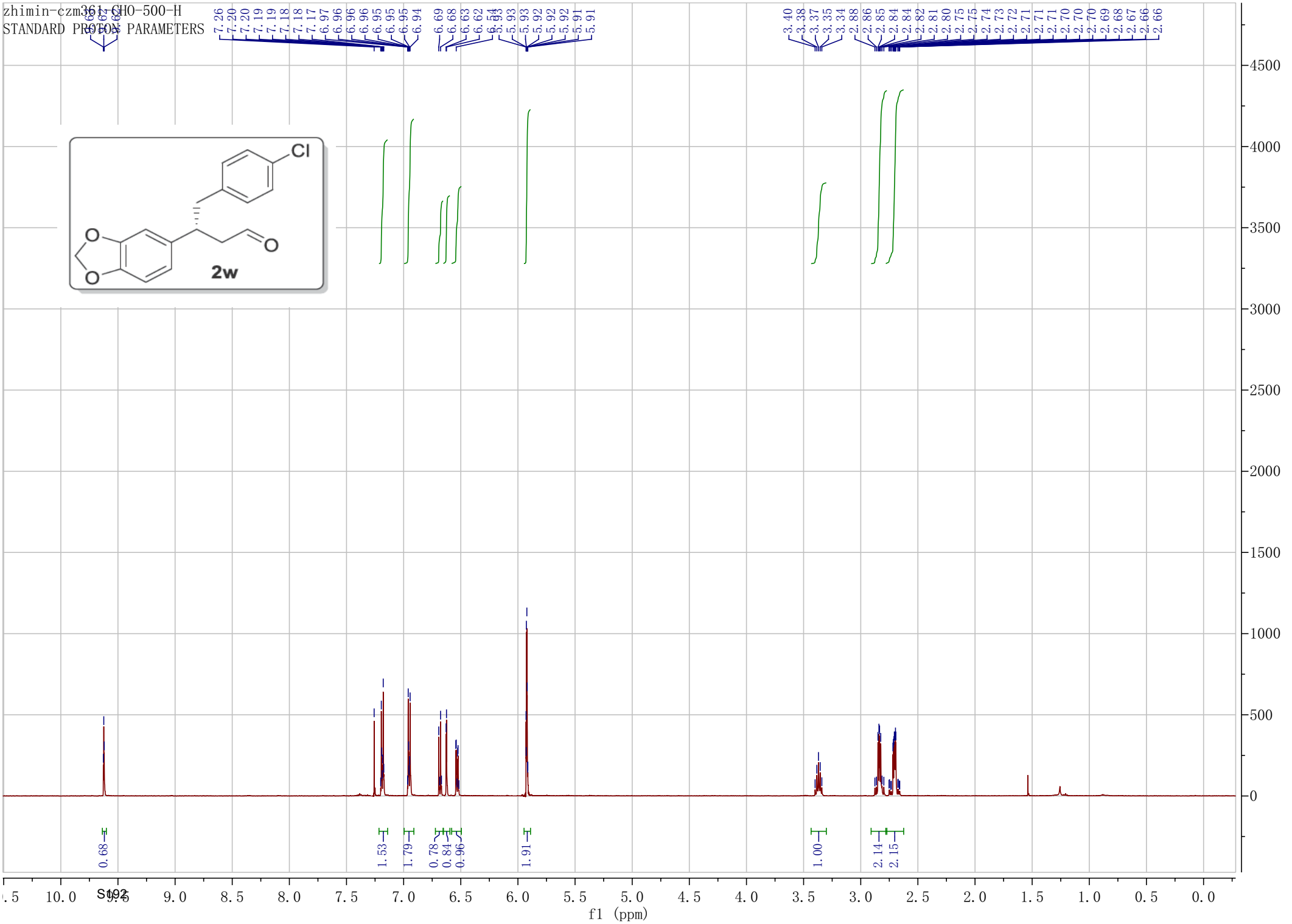
S188

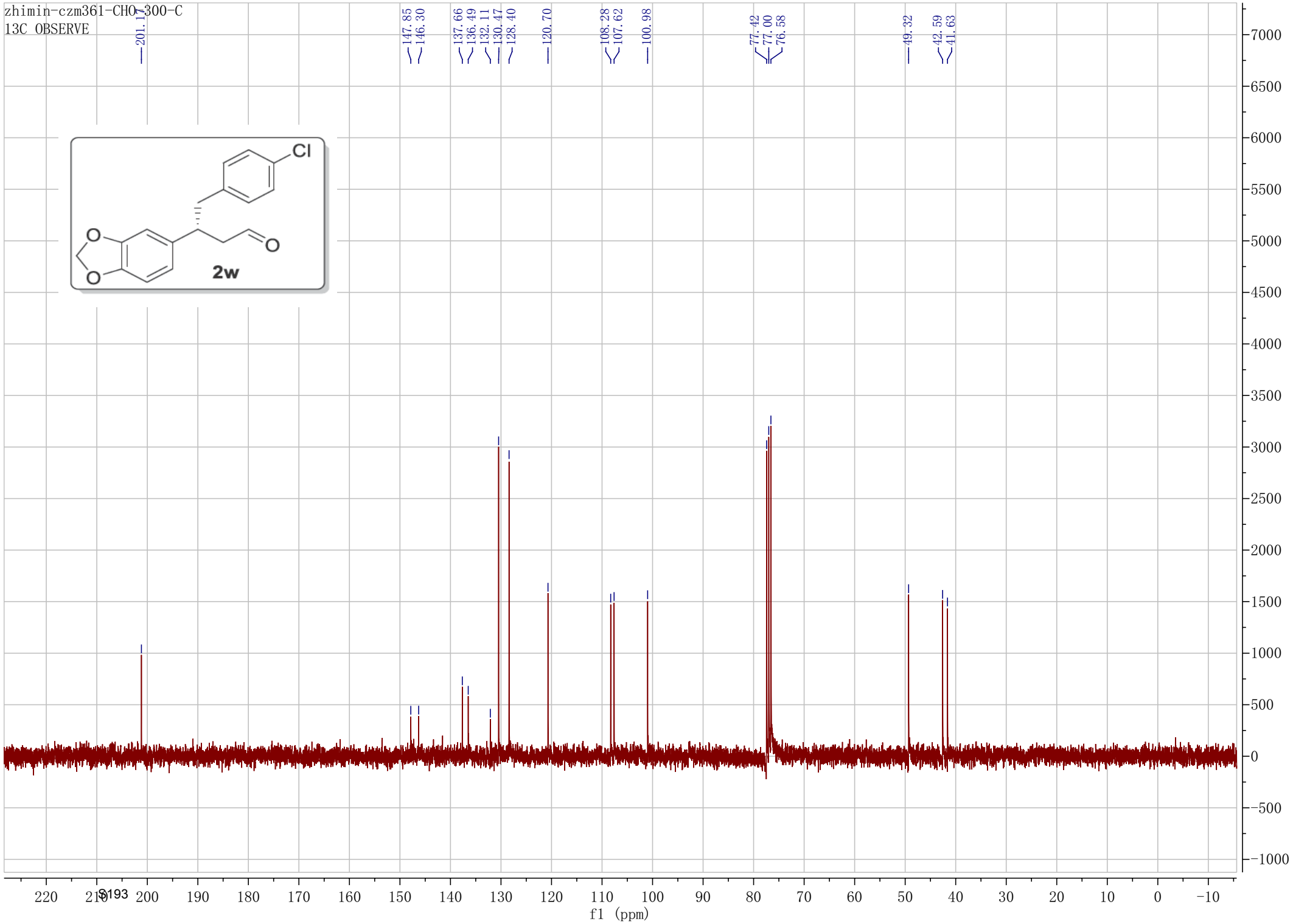
f1 (ppm)

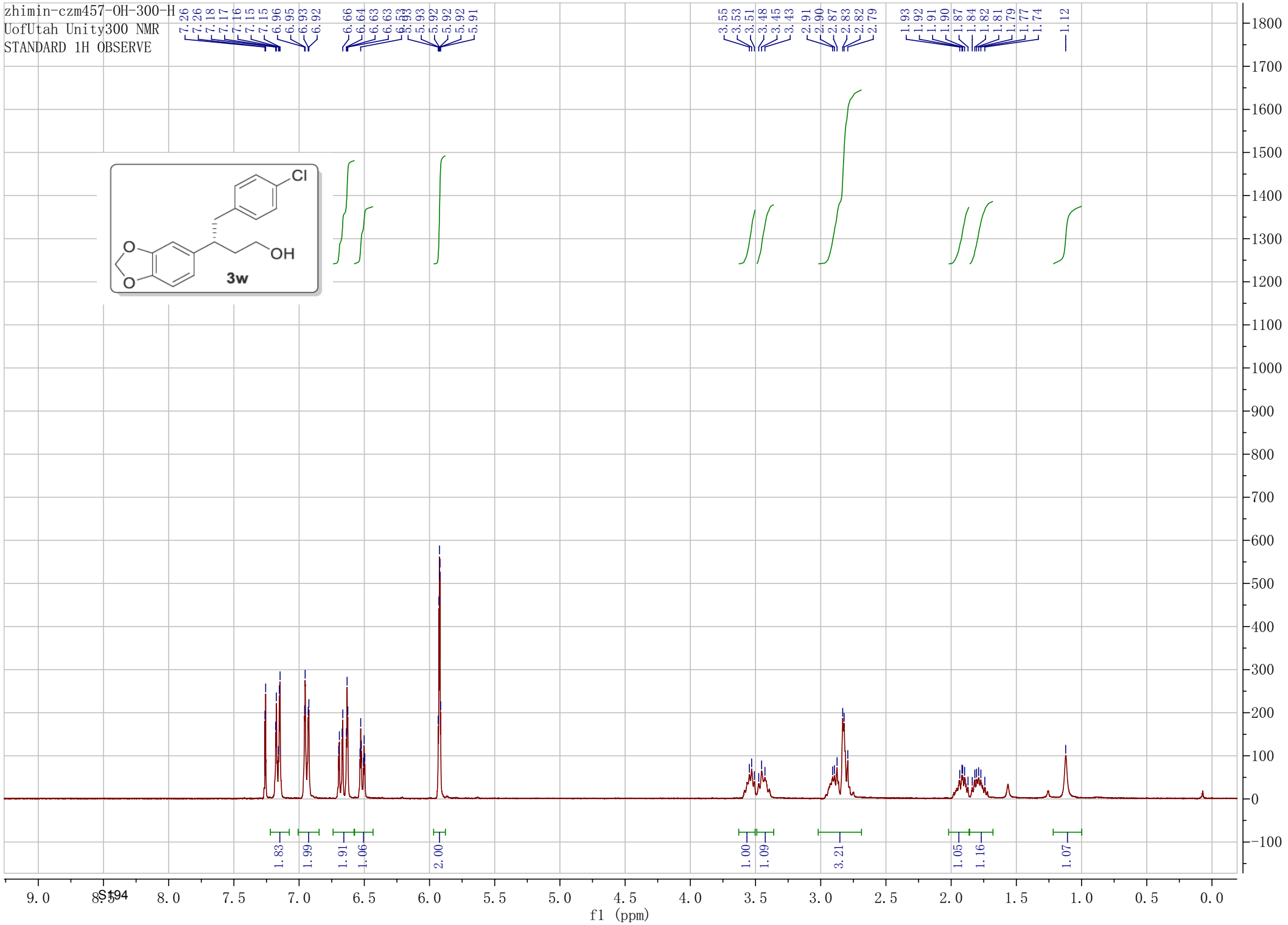

zhimin-czm428-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.27
7.27
7.18
7.15
7.13
7.11
7.08
7.07
7.05
7.03
7.02
7.01
7.00
6.97
6.94
3.56
3.47
3.41
3.38
3.36
3.33
3.31
2.94
2.92
2.04
2.01
1.99
1.97
1.95
1.93
1.91
1.89
1.21
Cl
F
OH
3v
4.57
3.11
1.00
0.99
1.19
2.10
2.19
1.04
f1 (ppm)

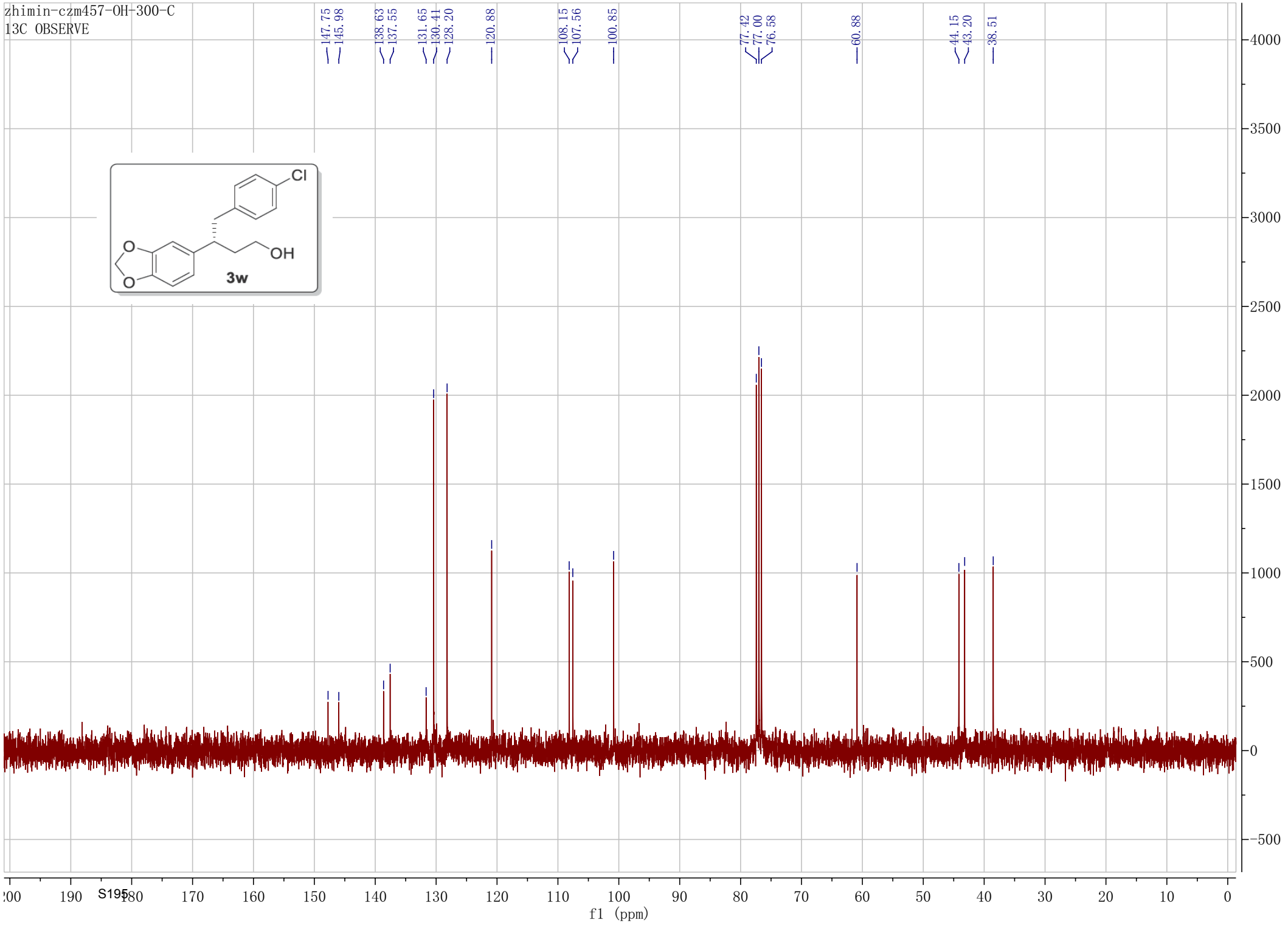

zhimin-czm428-OH-300-C
13C OBSERVE
162.71
159.47
138.42
130.33
129.02
128.95
128.23
127.95
127.84
124.19
124.14
115.68
115.38
77.42
77.00
76.58
60.86
41.37
37.59
37.22
Cl
F
OH
3v
f1 (ppm)

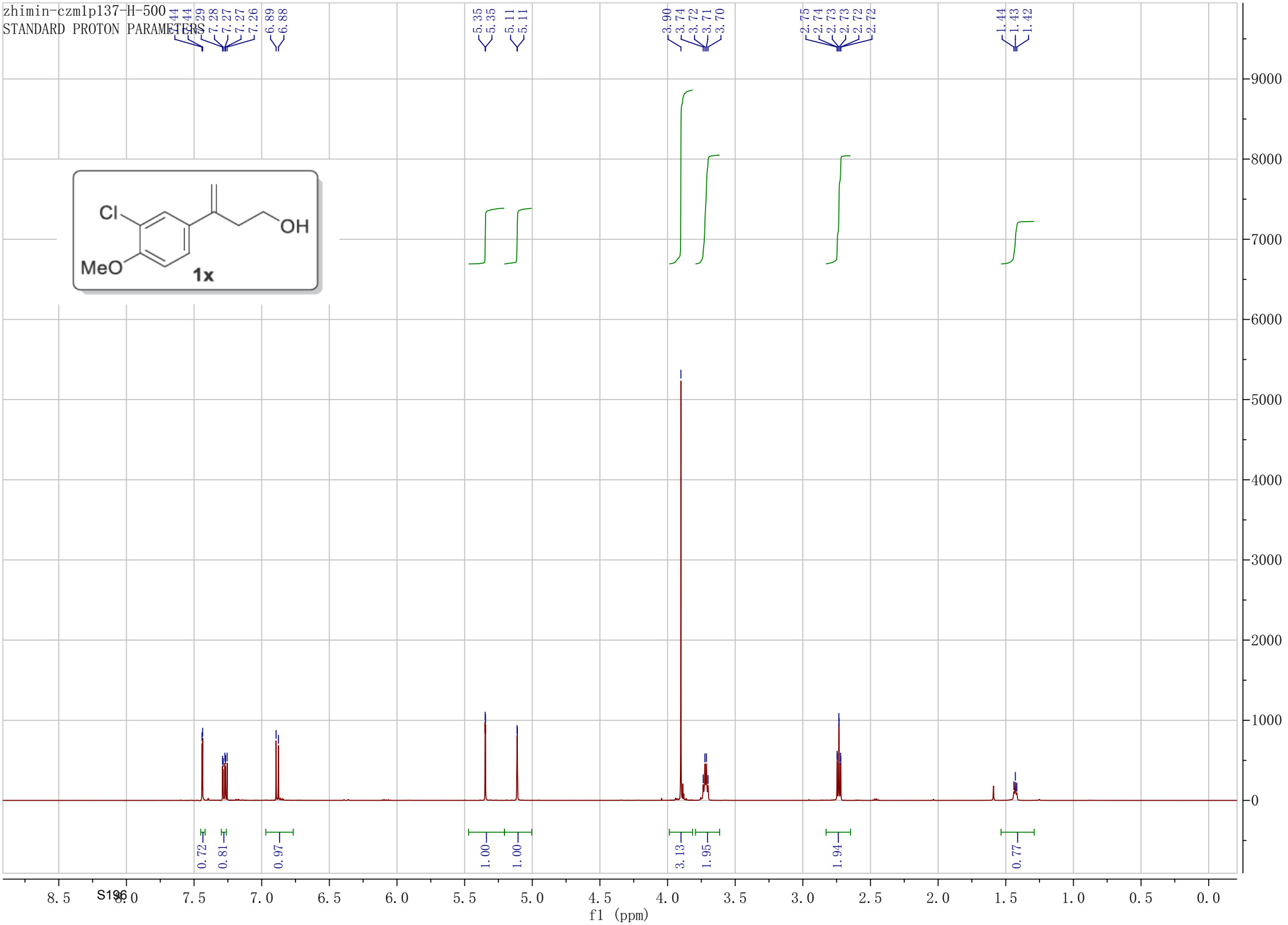

zhimin-czm428-OH-300-F
19F OBSERVE
STANDARD PARAMETERS
-118.39
-118.41
-118.43
-118.45
-118.47
Cl
F
OH
3v
50
45
40
35
30
25
20
15
10
5
0
-5
-107
-109
-111
-113
-115
-117
-119
-121
-123
-125
-127
-129
-131
-133
-135
-137
-139
f1 (ppm)

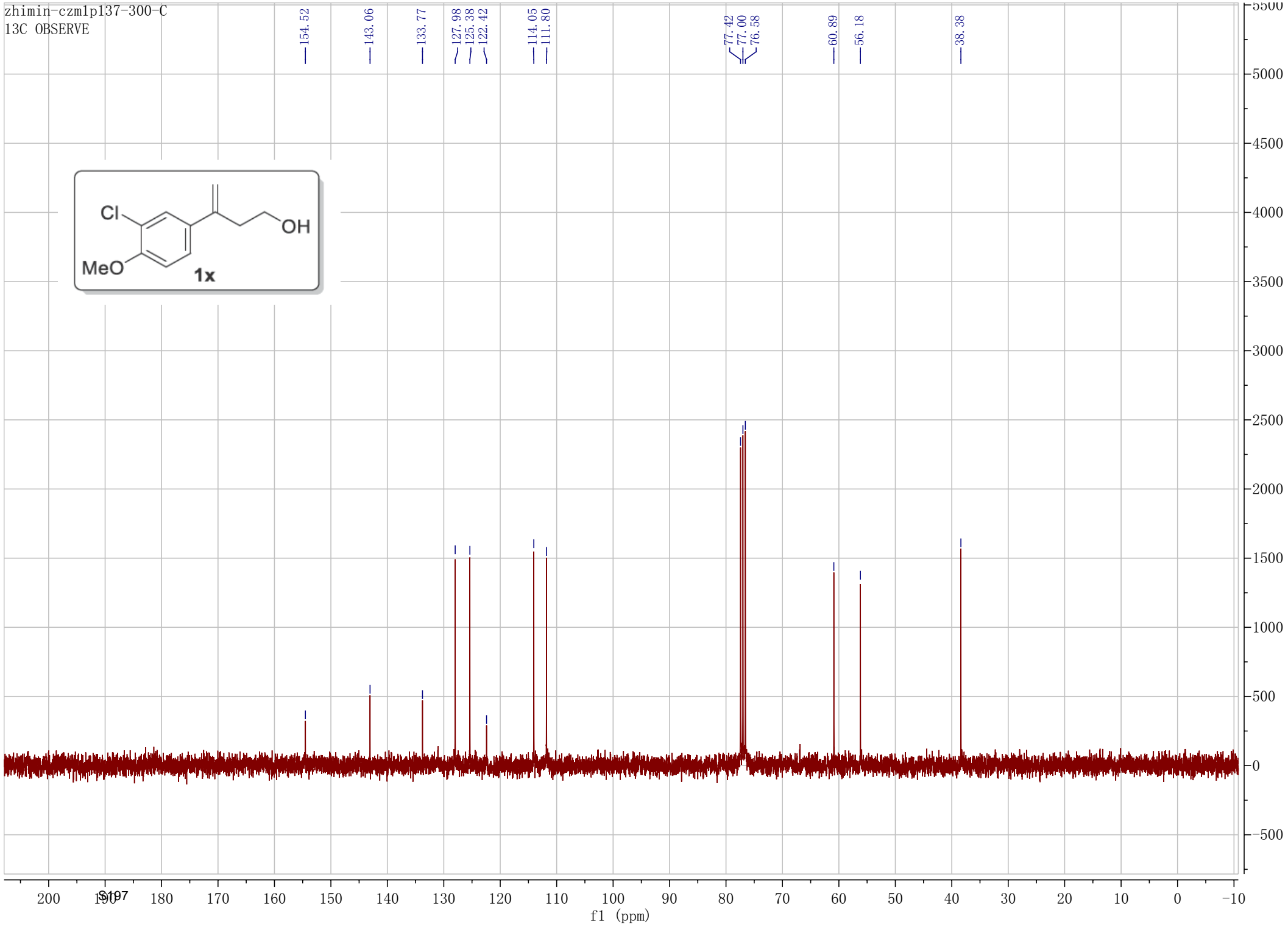

zhimin-czm361-CHO-500-H
STANDARD PROTON PARAMETERS
Cl
O
O
O
2w
f1 (ppm)

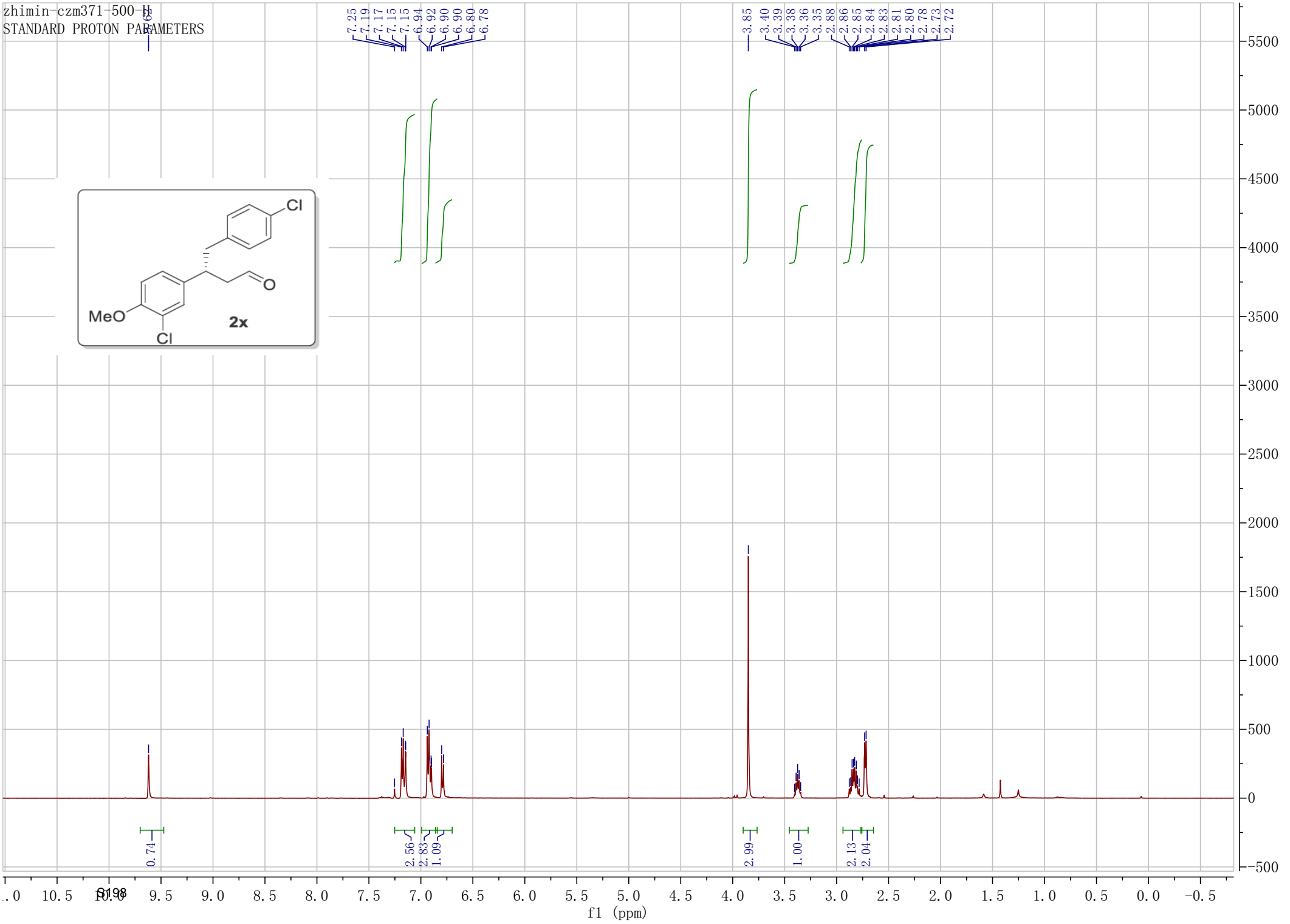

zhimin-czm361-CHO-300-C
13C OBSERVE
201.17
147.85
146.30
137.66
136.49
132.11
130.47
128.40
120.70
108.28
107.62
100.98
77.42
77.00
76.58
49.32
42.59
41.63
Cl
O
O
O
2w
f1 (ppm)

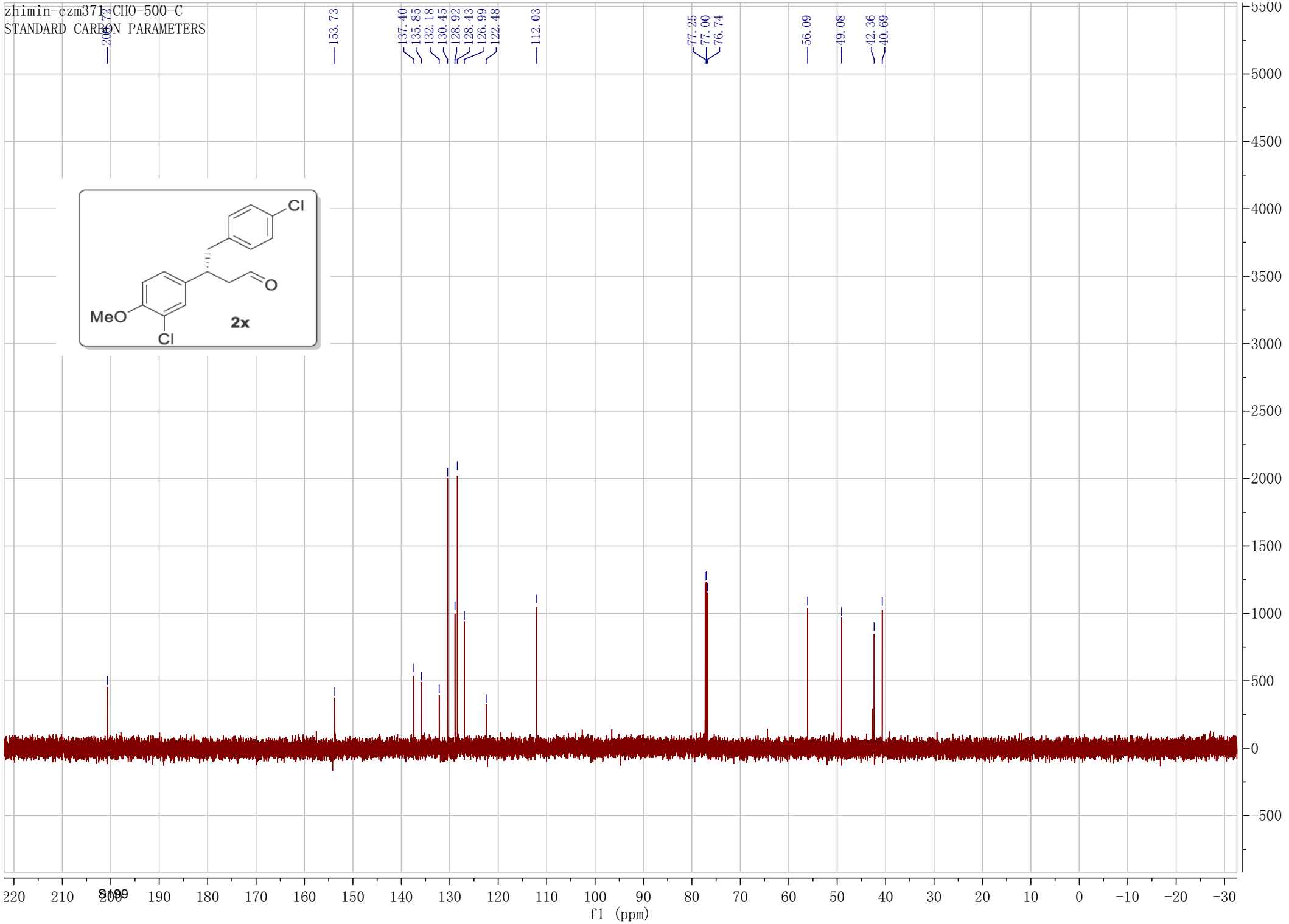

zhimin-czm457-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.26 7.26 7.18 7.17 7.16 7.15 7.15 6.96 6.95 6.93 6.92
6.66 6.64 6.63 6.63 6.53 5.93 5.92 5.92 5.91
3.55 3.53 3.51 3.48 3.45 3.43
2.91 2.90 2.87 2.83 2.82 2.79
1.93 1.92 1.91 1.90 1.87 1.84 1.82 1.81 1.79 1.77 1.74
1.12
Cl
OH
O
O
3w
1.83 1.99 1.91 1.06 2.00 1.00 1.09 3.21 1.05 1.16 1.07
f1 (ppm)


zhimin-czm457-OH-300-C
13C OBSERVE
147.75
145.98
138.63
137.55
131.65
130.41
128.20
120.88
108.15
107.56
100.85
77.42
77.00
76.58
60.88
44.15
43.20
38.51
Cl
O
O
OH
3w
f1 (ppm)

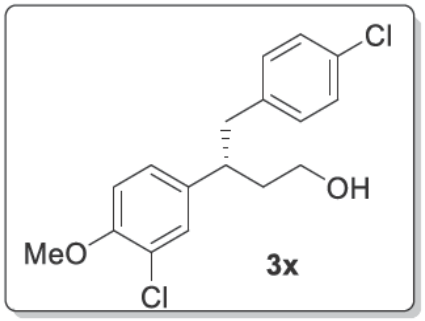

zhimin-czm1p137-H-500
STANDARD PROTON PARAMETERS
7.44
7.44
7.29
7.28
7.27
7.27
7.26
6.89
6.88
5.35
5.35
5.11
5.11
3.90
3.74
3.72
3.71
3.70
2.75
2.74
2.73
2.73
2.72
2.72
1.44
1.43
1.42
Cl
OH
MeO
1x
0.72
0.81
0.97
1.00
1.00
3.13
1.95
1.94
0.77
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


zhimin-czmlp137-300-C
13C OBSERVE
154.52
143.06
133.77
127.98
125.38
122.42
114.05
111.80
77.42
77.00
76.58
60.89
56.18
38.38
Cl
OH
MeO
1x
f1 (ppm)

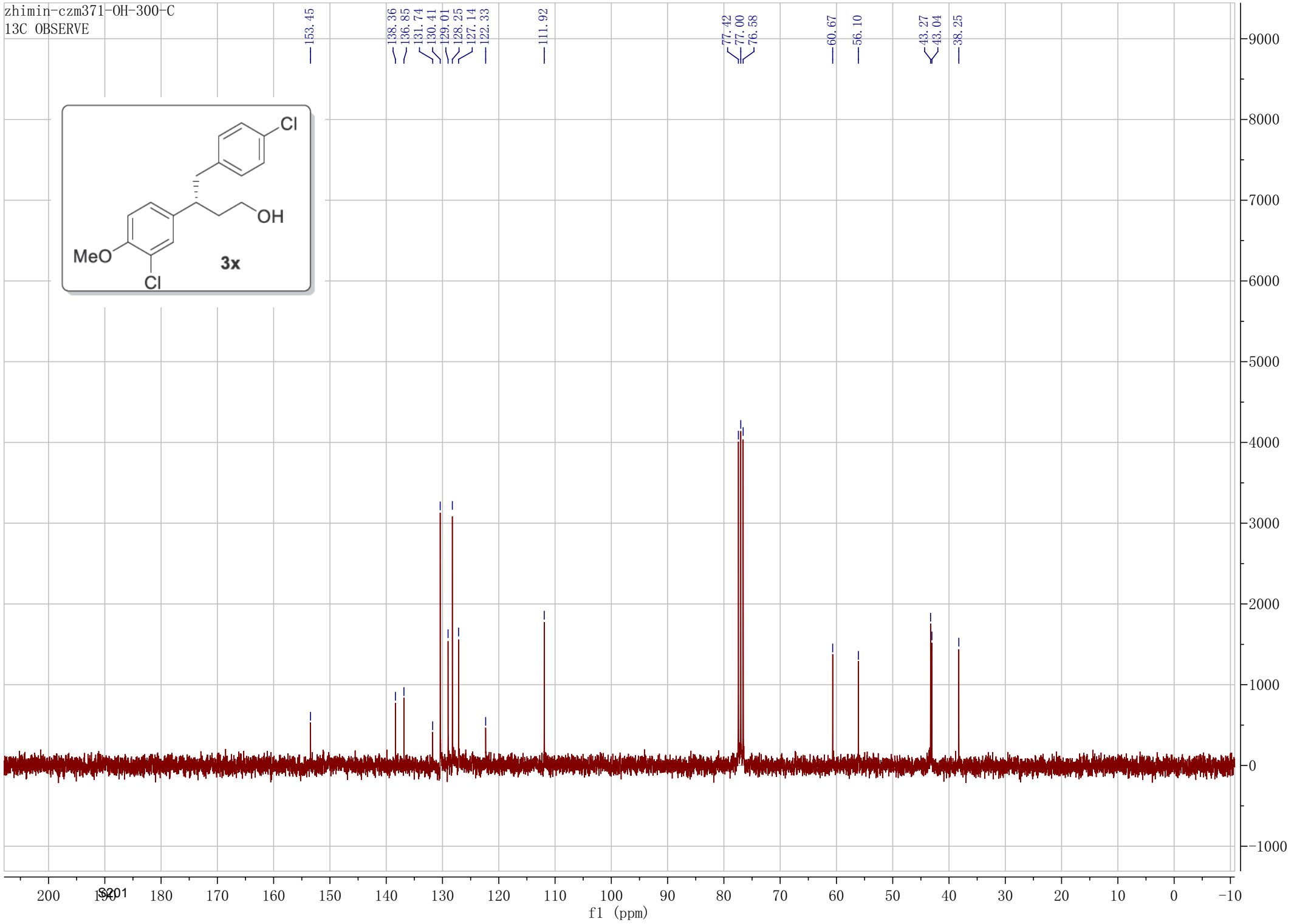

zhimin-czm371-500-H
STANDARD PROTON PARAMETERS
7.25
7.19
7.17
7.15
7.15
6.94
6.92
6.90
6.90
6.80
6.78
3.85
3.40
3.39
3.38
3.36
3.35
2.88
2.86
2.85
2.84
2.83
2.81
2.80
2.78
2.73
2.72
Cl
O
MeO
Cl
2x
0.74
2.56
2.83
1.09
2.99
1.00
2.13
2.04
f1 (ppm)

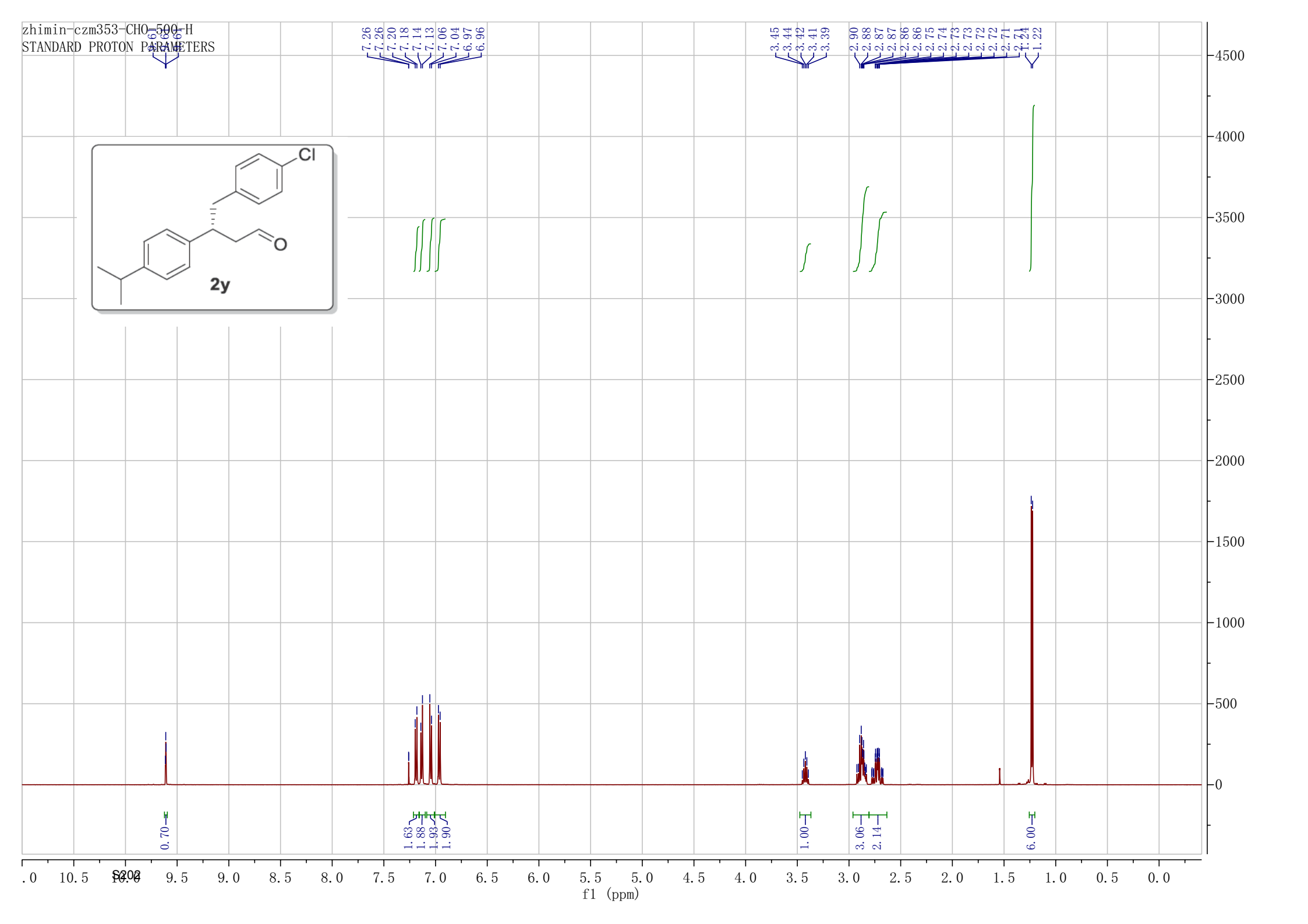

zhimin-czm371-CHO-500-C
STANDARD CARBON PARAMETERS
153.73
137.40
135.85
132.18
130.45
128.92
128.43
126.99
122.48
112.03
77.25
77.00
76.74
56.09
49.08
42.36
40.69
Cl
O
MeO
Cl
2x
f1 (ppm)

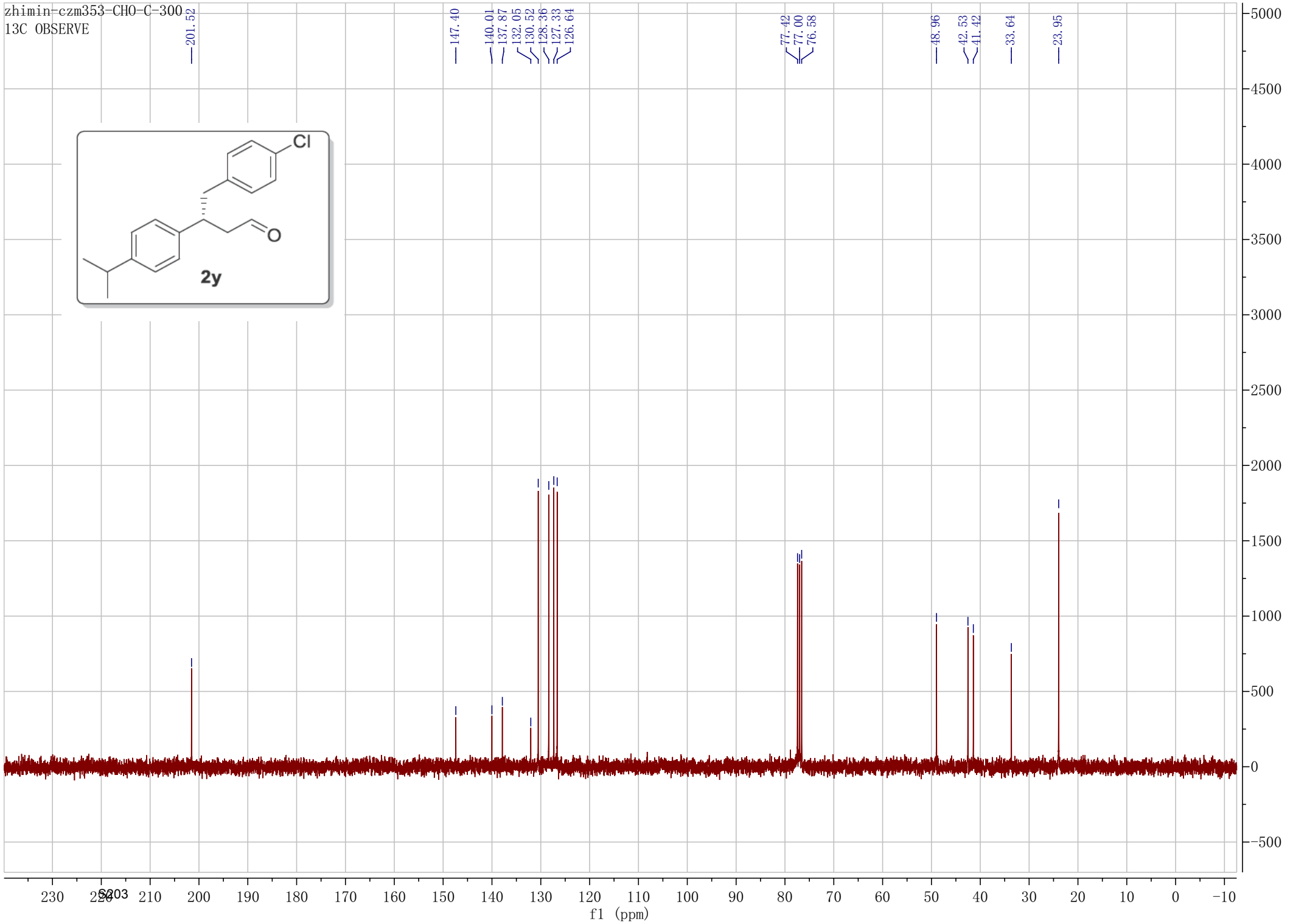
zhimin-czm371-OH-500-H
STANDARD PROTON PARAMETERS

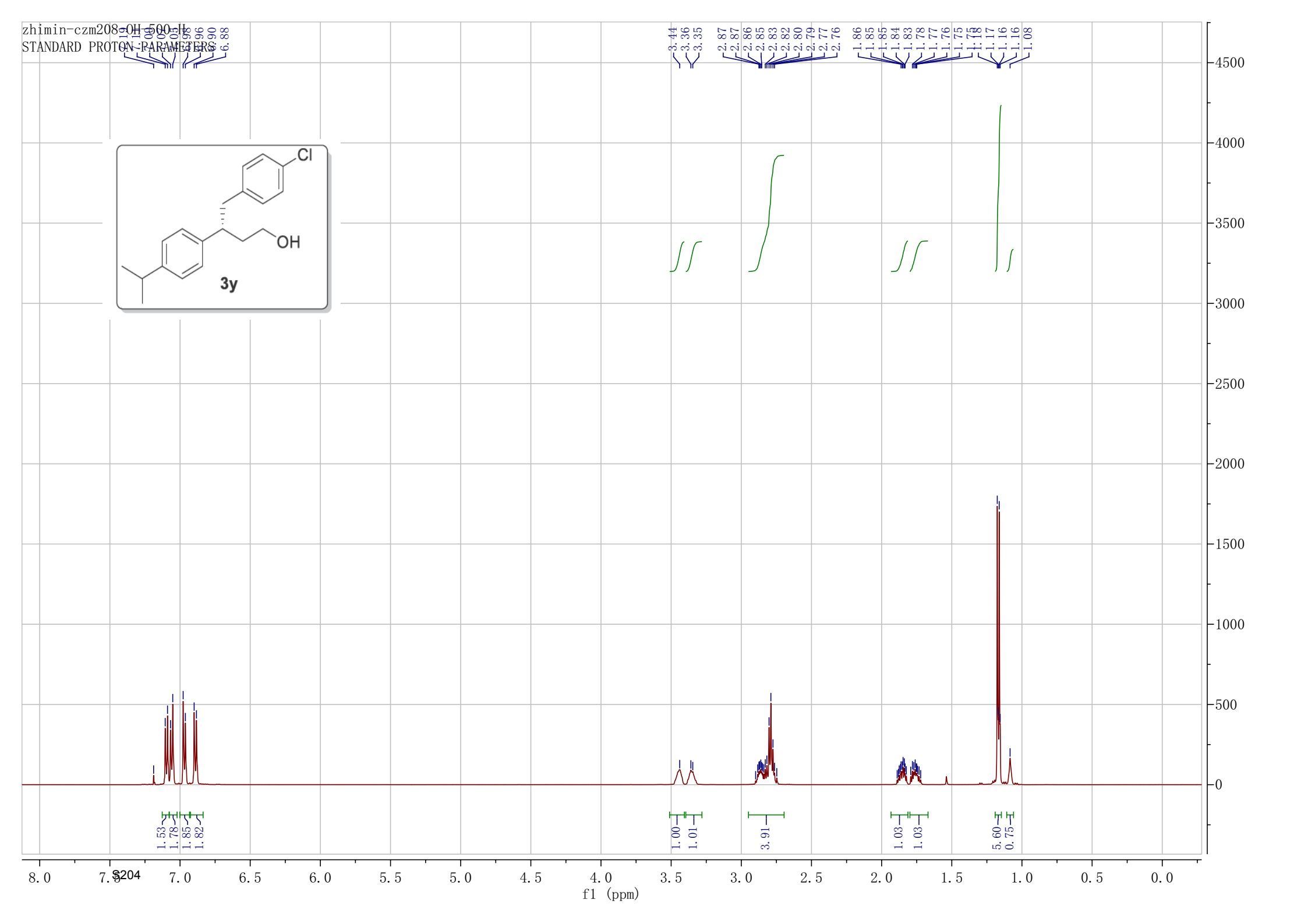


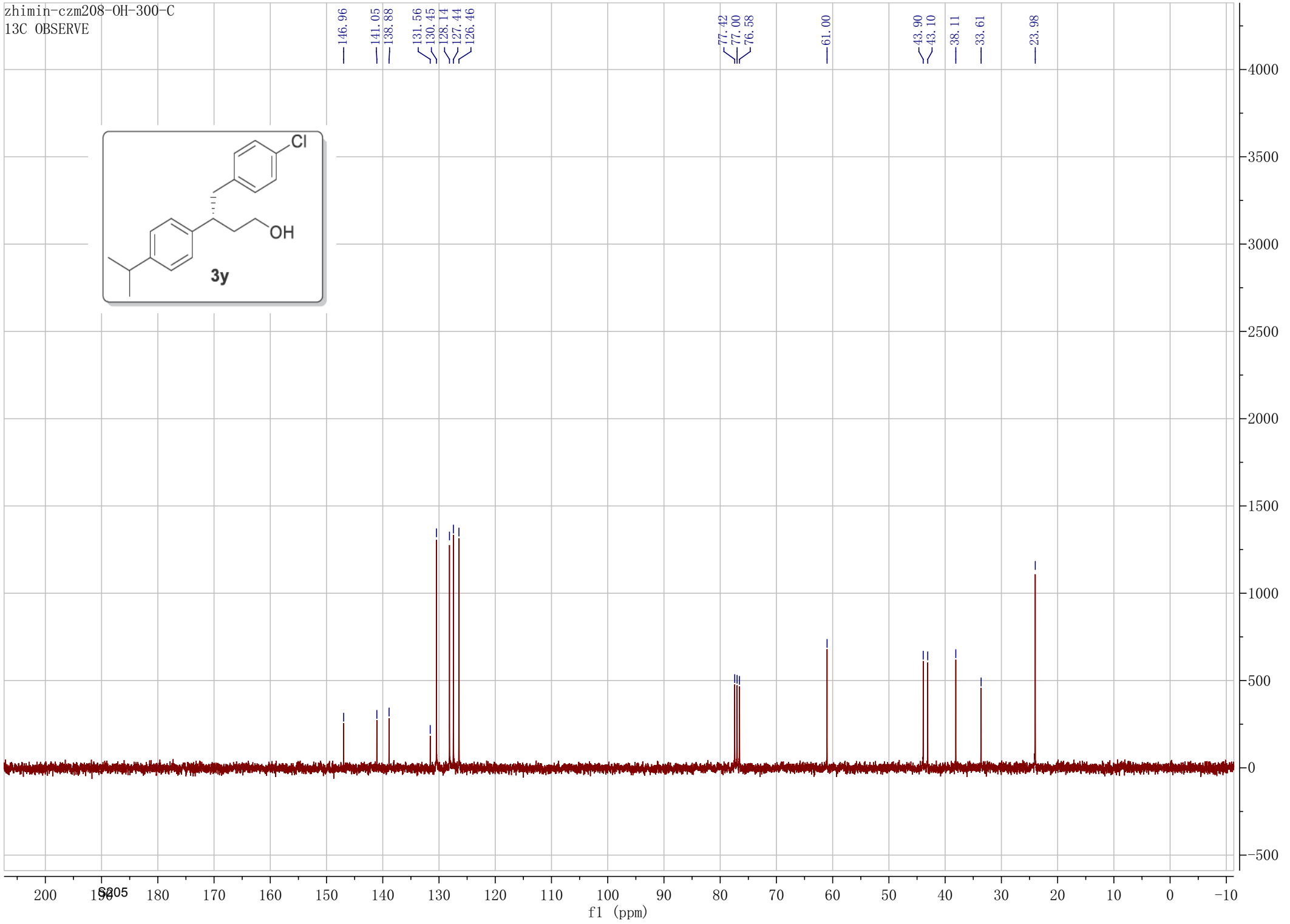
f1 (ppm)

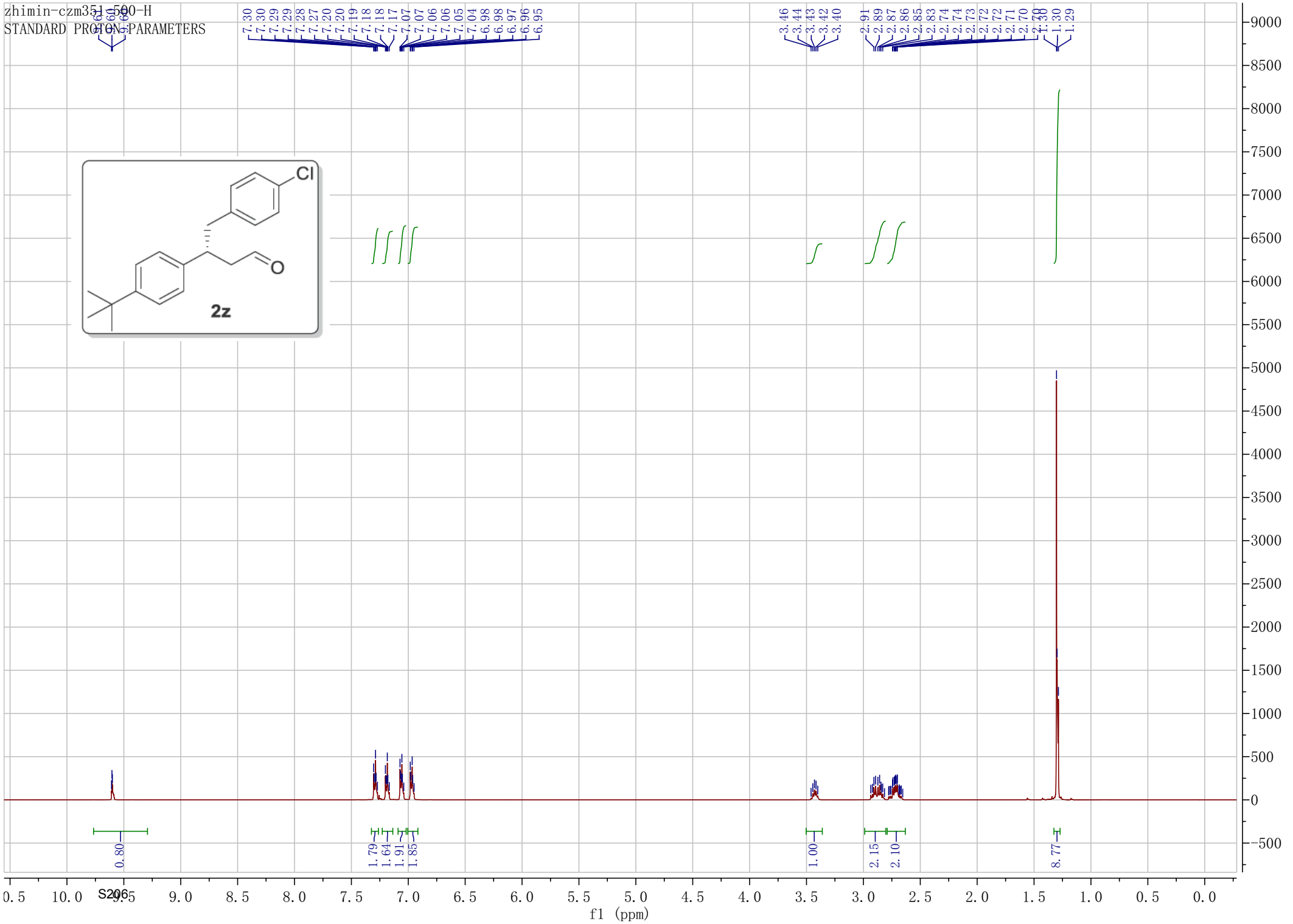

zhimin-czm371-OH-300-C
13C OBSERVE
153.45
138.36
136.85
131.74
130.41
129.01
128.25
127.14
122.33
111.92
77.42
77.00
76.58
60.67
56.10
43.27
43.04
38.25
Cl
OH
MeO
Cl
3x
f1 (ppm)

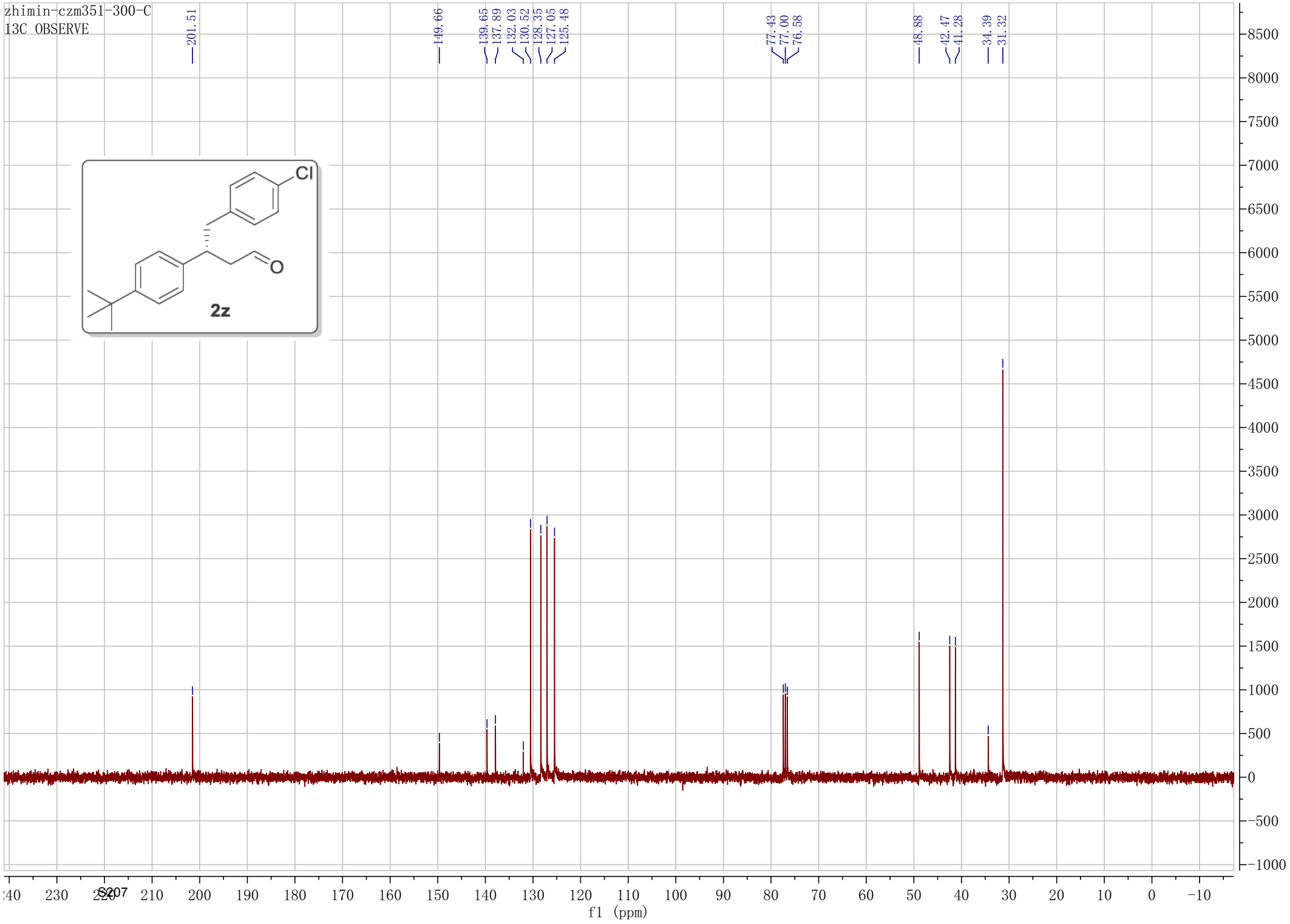

zhimin-czm353-CHO-500-H
STANDARD PROTON PARAMETERS
Cl
O
2y
f1 (ppm)

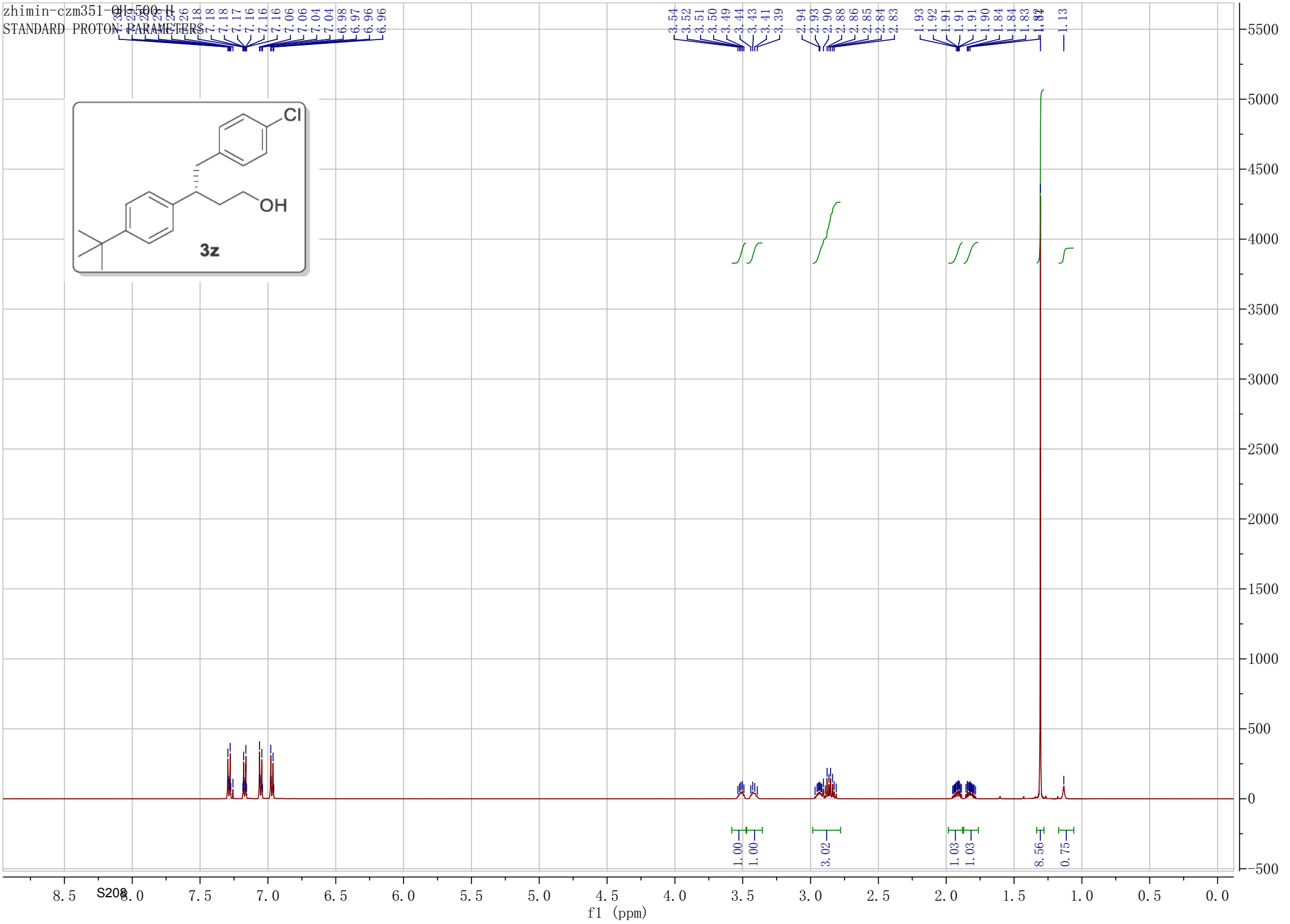

zhimin-czm353-CHO-C-300
13C OBSERVE
201.52
147.40
140.01
137.87
132.05
130.52
128.36
127.33
126.64
77.42
77.00
76.58
48.96
42.53
41.42
33.64
23.95
Cl
O
2y
f1 (ppm)

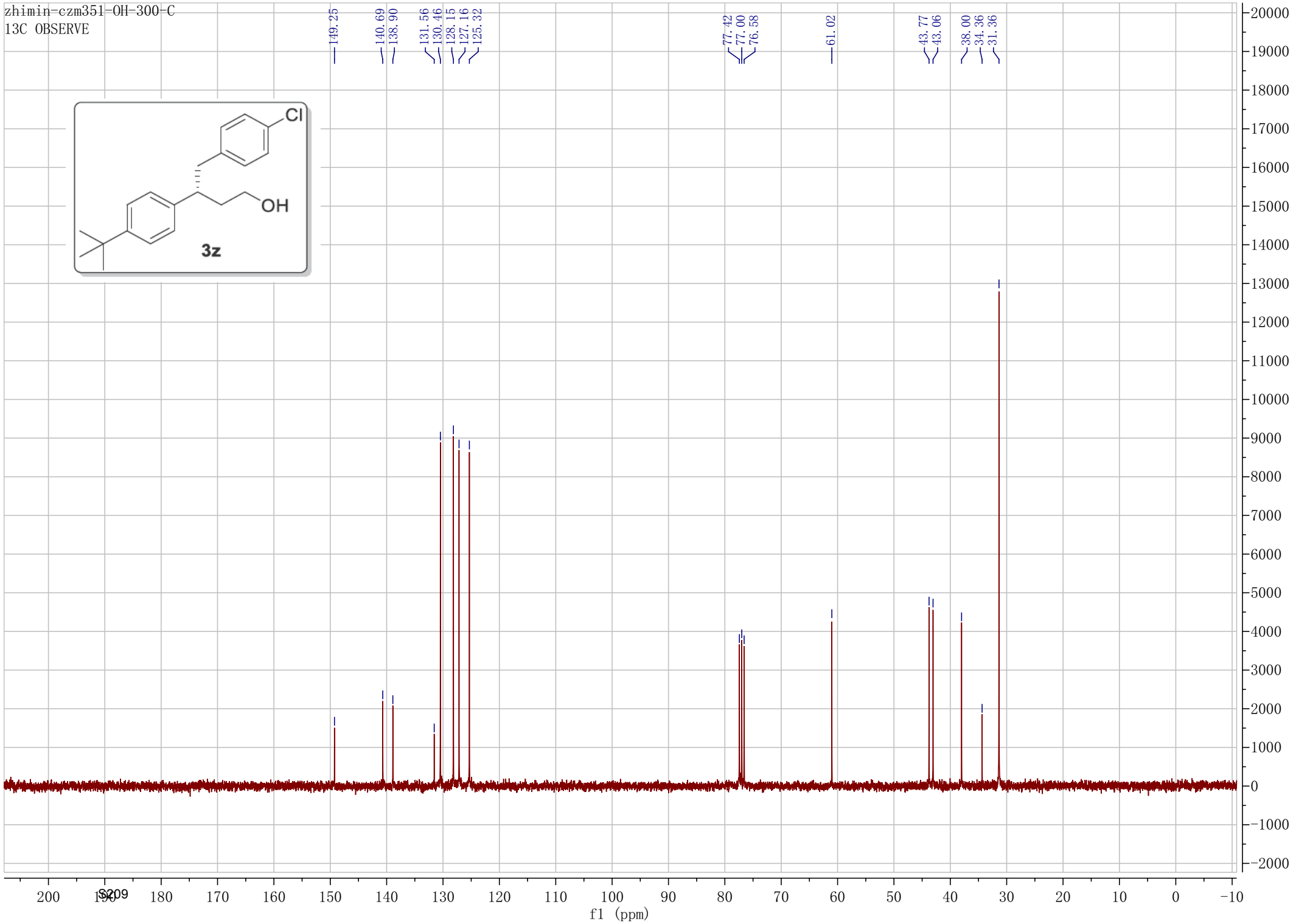

zhimin-czm208-OH-500-H
STANDARD PROTON PARAMETERS
Cl
OH
3y
S204
f1 (ppm)

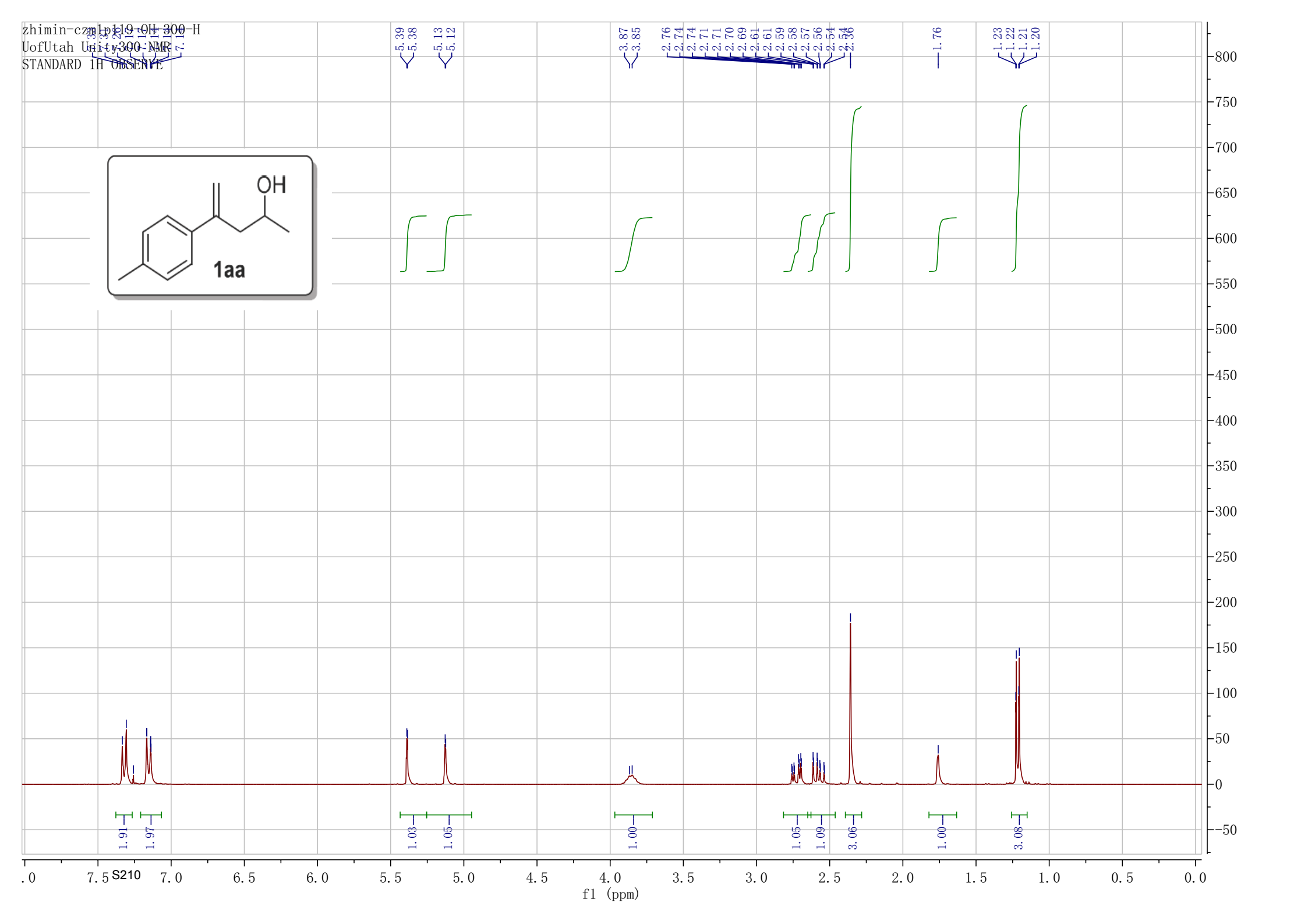

zhimin-czm208-OH-300-C
13C OBSERVE
146.96
141.05
138.88
131.56
130.45
128.14
127.44
126.46
77.42
77.00
76.58
61.00
43.90
43.10
38.11
33.61
23.98
Cl
OH
3y
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

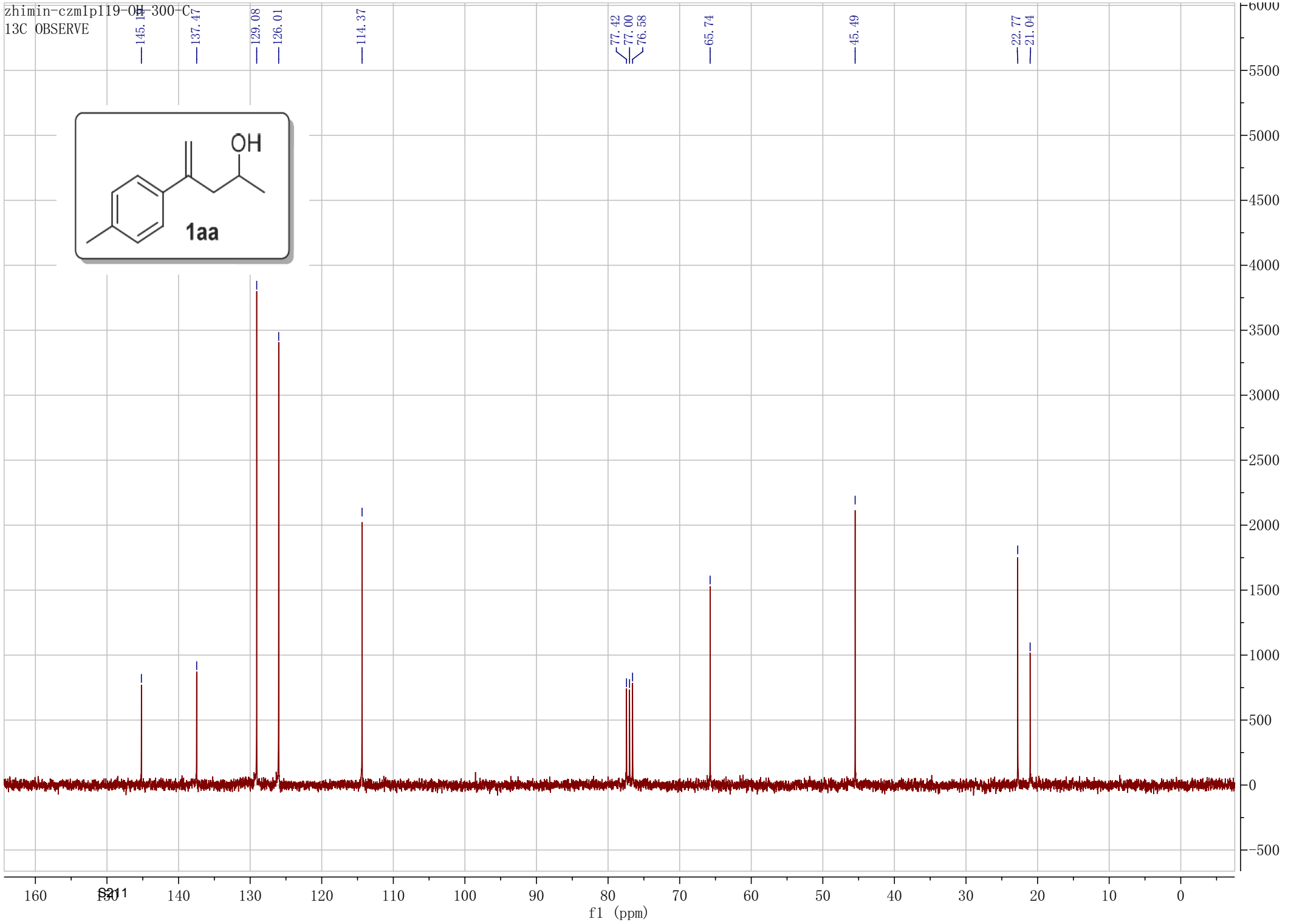

zhimin-czm351-500-H
STANDARD PROTON PARAMETERS
Cl
O
2z
f1 (ppm)

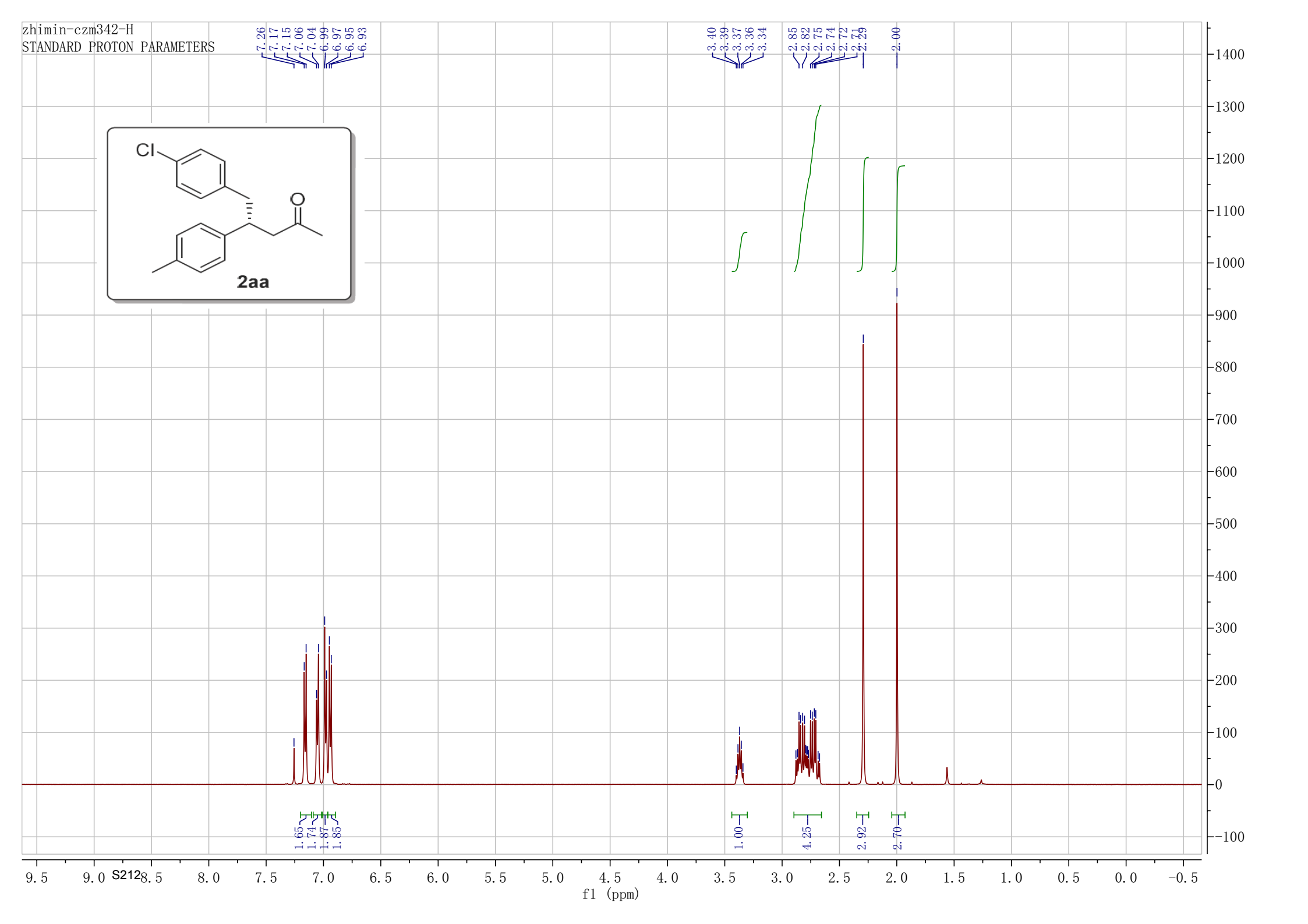

zhimin-czm351-300-C
13C OBSERVE
201.51
149.66
139.65
137.89
132.03
130.52
128.35
127.05
125.48
77.43
77.00
76.58
48.88
42.47
41.28
34.39
31.32
Cl
O
2z
f1 (ppm)

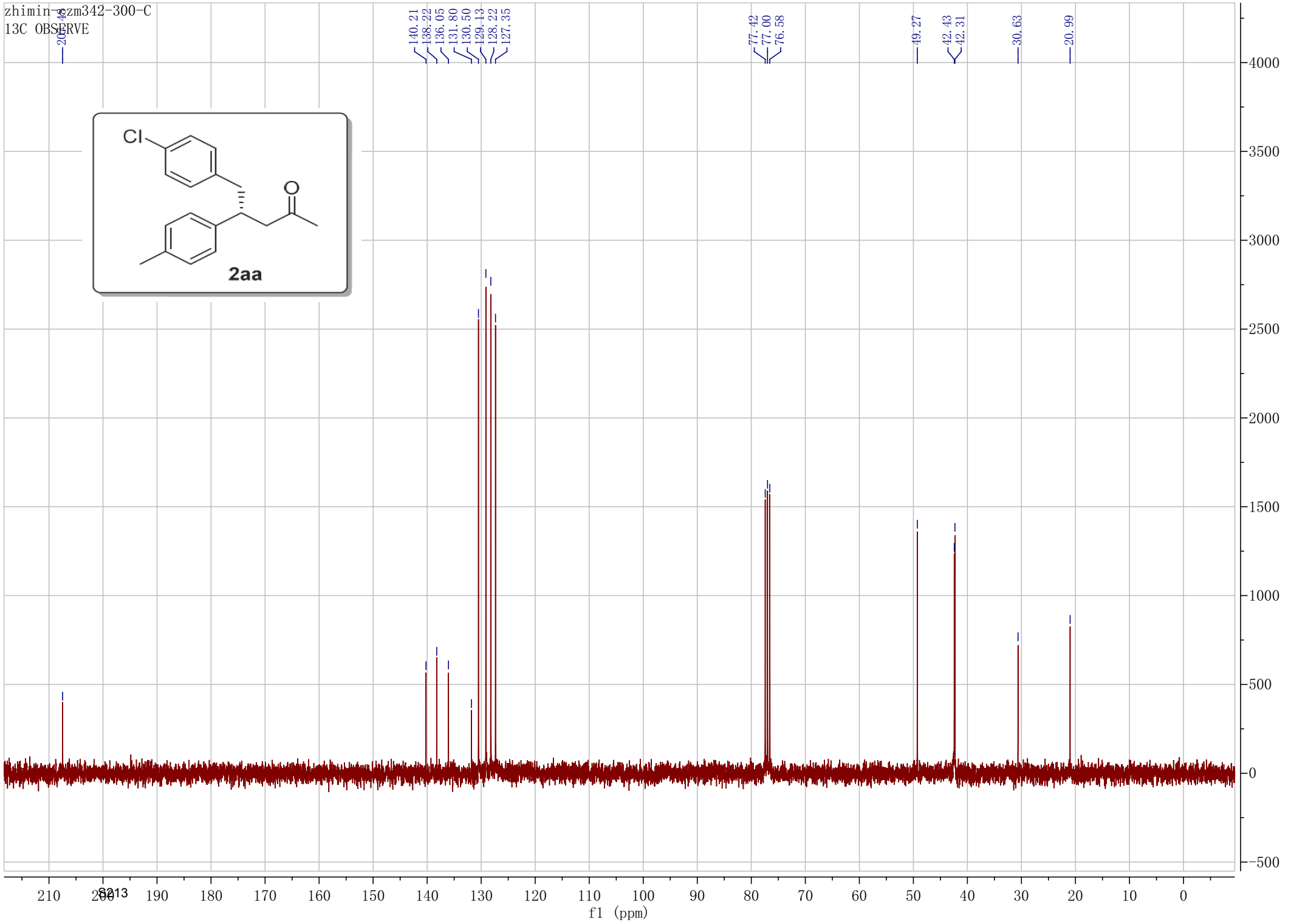

zhimin-czm351-OH-500-H
STANDARD PROTON PARAMETERS
Cl
OH
3z
f1 (ppm)

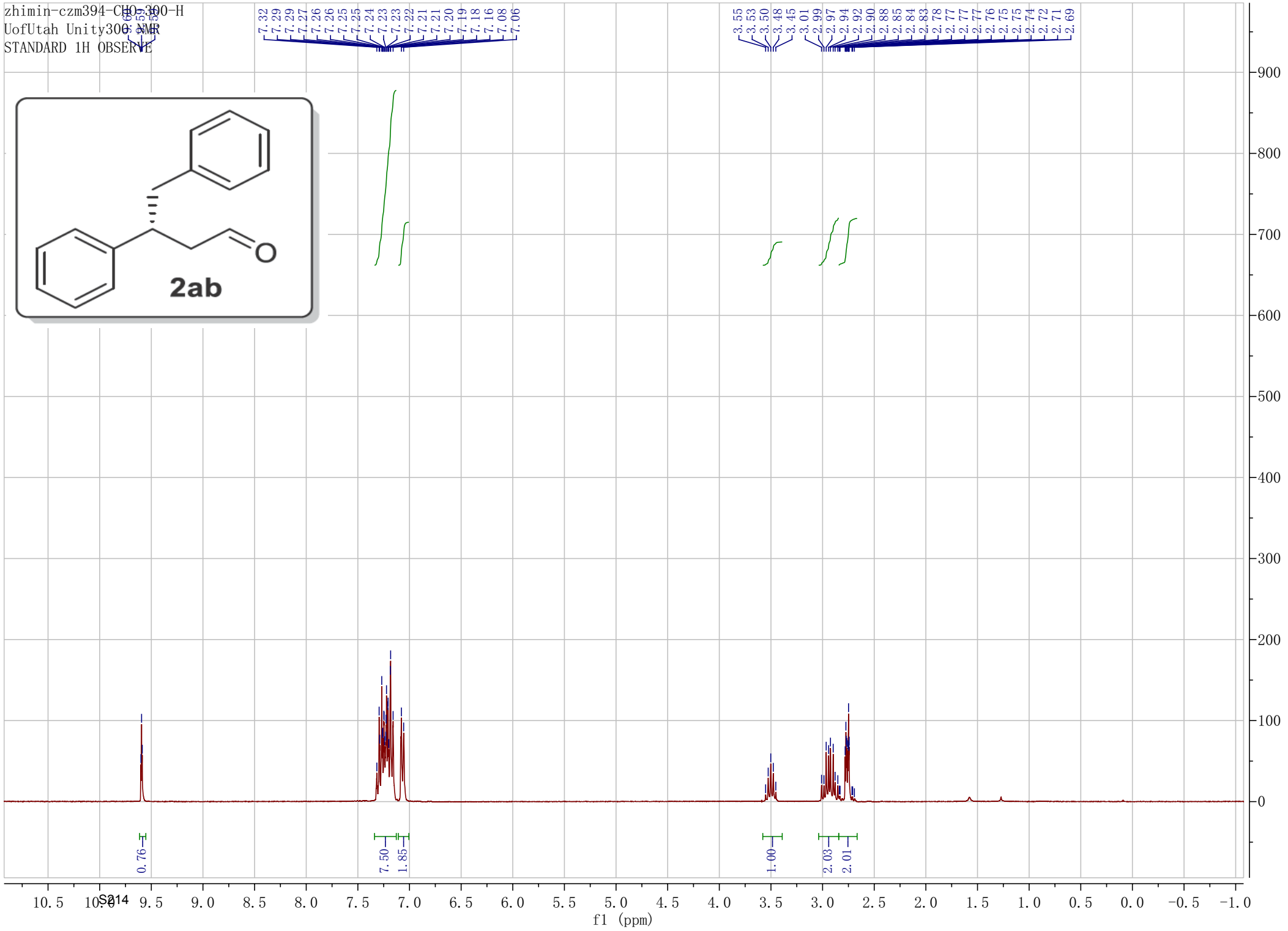

zhimin-czm351-OH-300-C
13C OBSERVE
149.25
140.69
138.90
131.56
130.46
128.15
127.16
125.32
77.42
77.00
76.58
61.02
43.77
43.06
38.00
34.36
31.36
Cl
OH
3z
f1 (ppm)

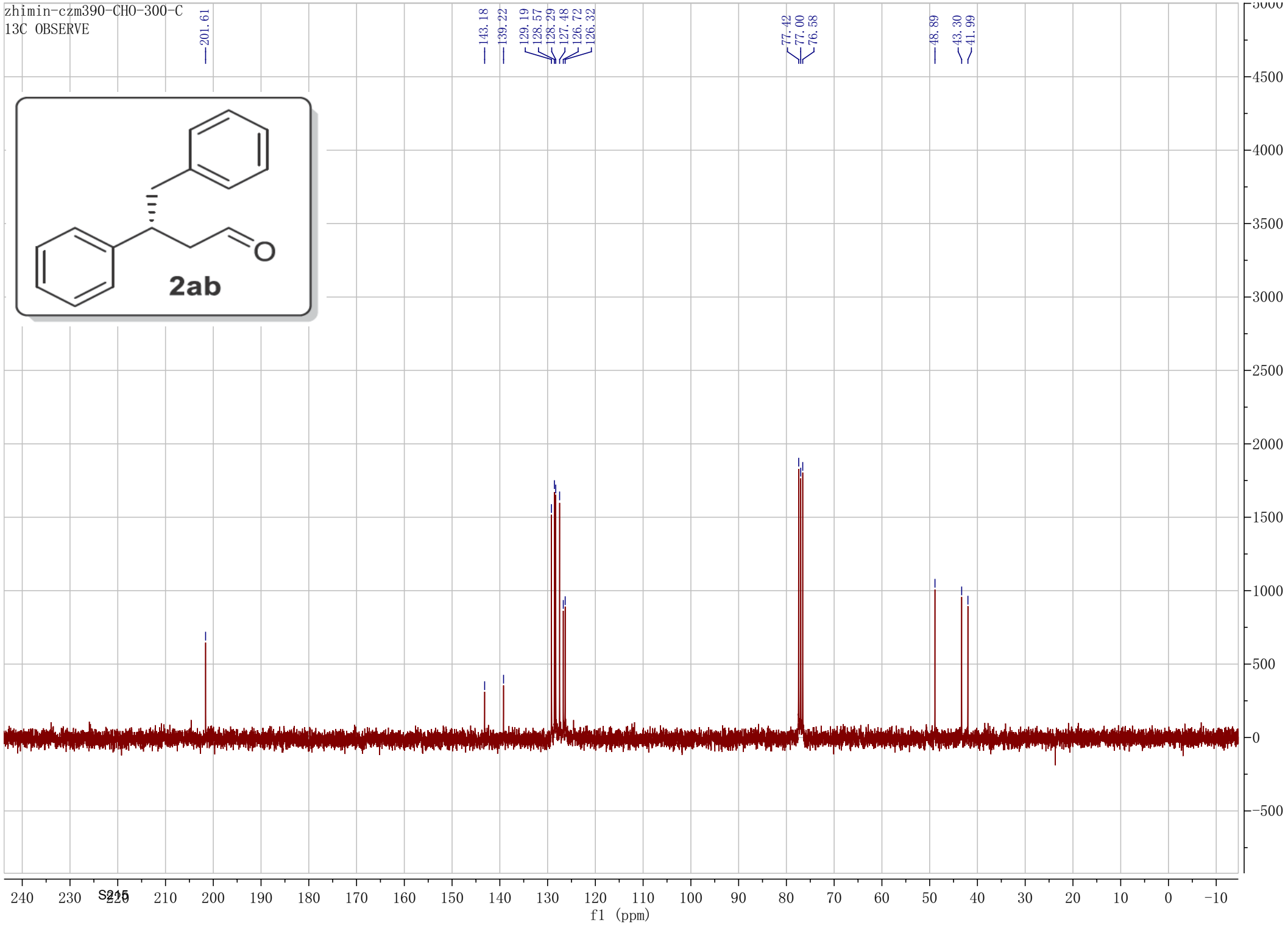

zhimin-czmlpe119-OH-300-H
UofUtah Unity300-NMR
STANDARD 1H OBSERVE
OH
1aa
5.39
5.38
5.13
5.12
3.87
3.85
2.76
2.74
2.74
2.71
2.71
2.70
2.69
2.61
2.61
2.59
2.58
2.57
2.56
2.54
2.36
1.76
1.23
1.22
1.21
1.20
1.91
1.97
1.03
1.05
1.00
1.05
1.09
3.06
1.00
3.08
f1 (ppm)

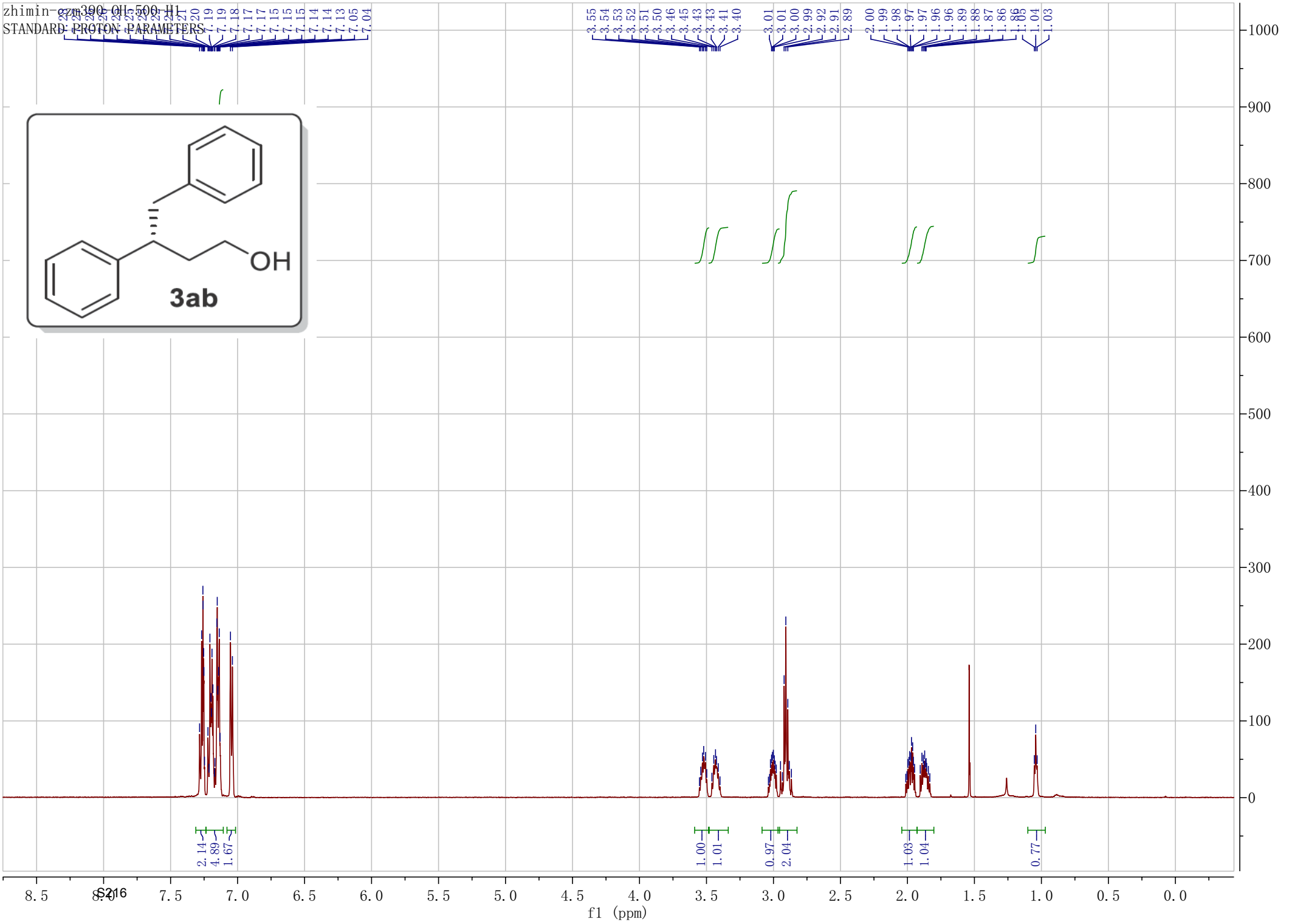

zhimin-czmlp119-OH-300-C
13C OBSERVE
145.14
137.47
129.08
126.01
114.37
77.42
77.00
76.58
65.74
45.49
22.77
21.04
OH
1aa
f1 (ppm)

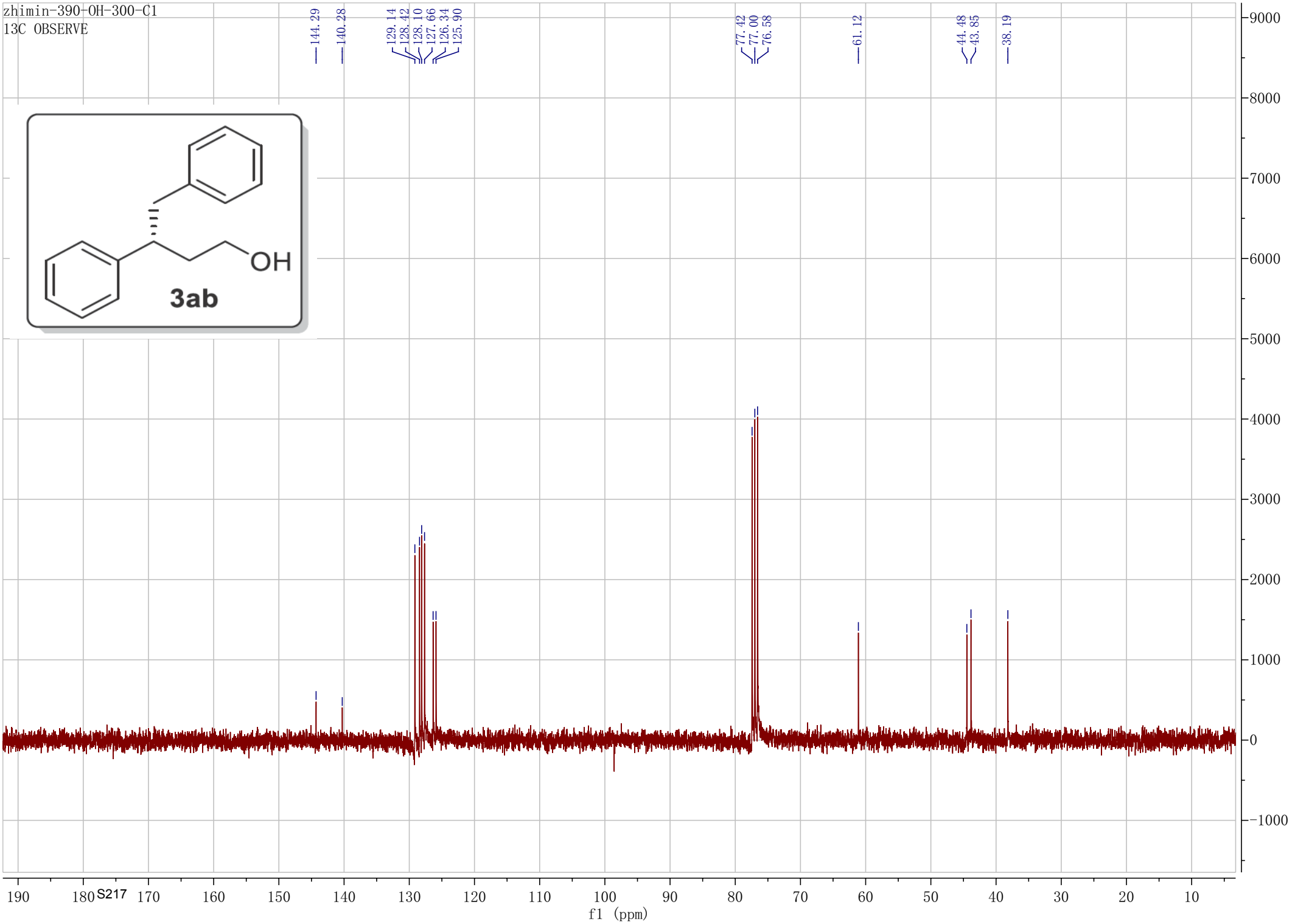

zhimin-czm342-H
STANDARD PROTON PARAMETERS
7.26
7.17
7.15
7.06
7.04
6.99
6.97
6.95
6.93
3.40
3.39
3.37
3.36
3.34
2.85
2.82
2.75
2.74
2.72
2.71
2.29
2.00
Cl
O
2aa
1.65
1.74
1.87
1.85
1.00
4.25
2.92
2.70
f1 (ppm)

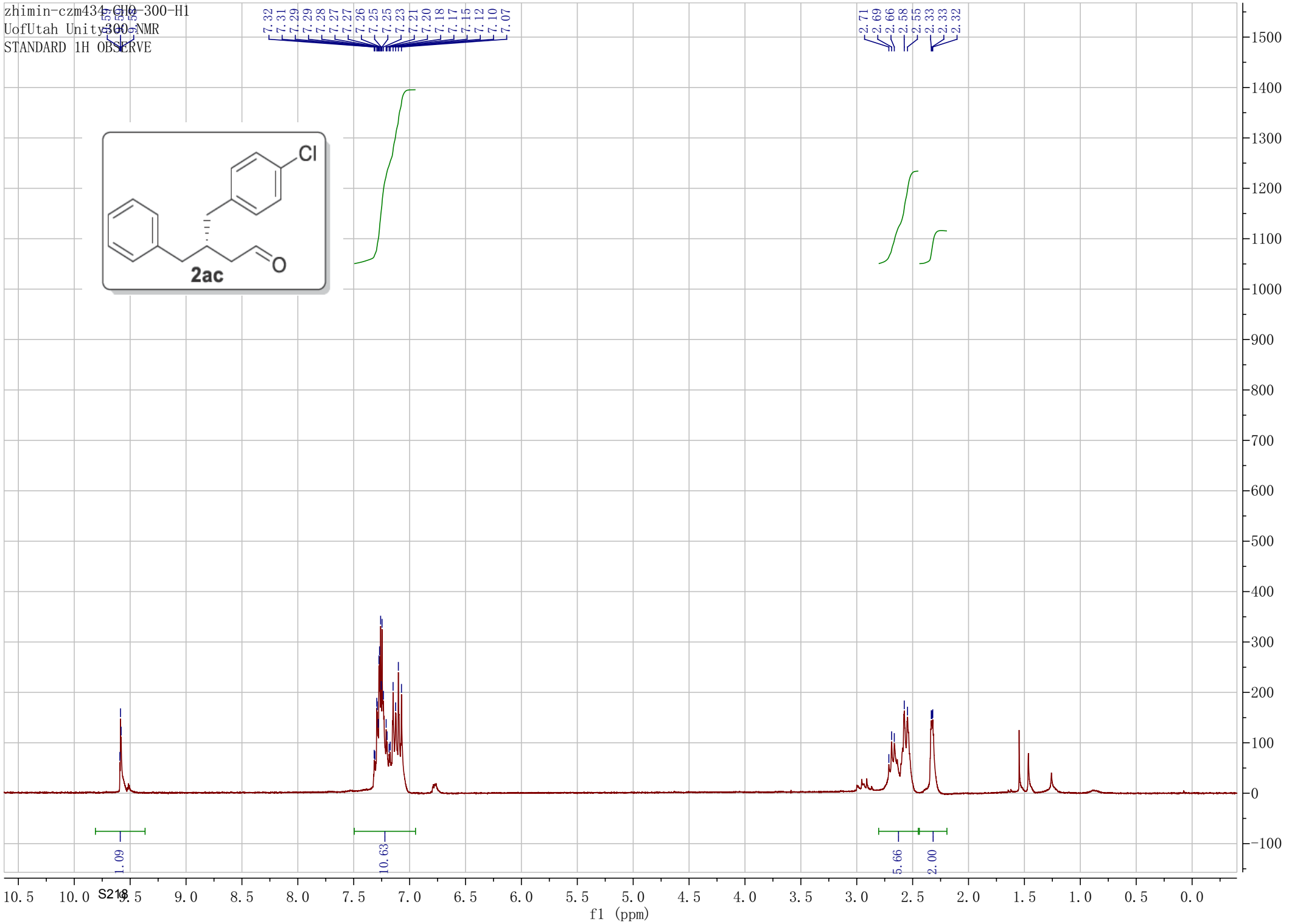

zhimin-czm342-300-C
13C OBSERVE
206.46
140.21
138.22
136.05
131.80
130.50
129.13
128.22
127.35
77.42
77.00
76.58
49.27
42.43
42.31
30.63
20.99
Cl
O
2aa
4000
3500
3000
2500
2000
1500
1000
500
0
-500
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

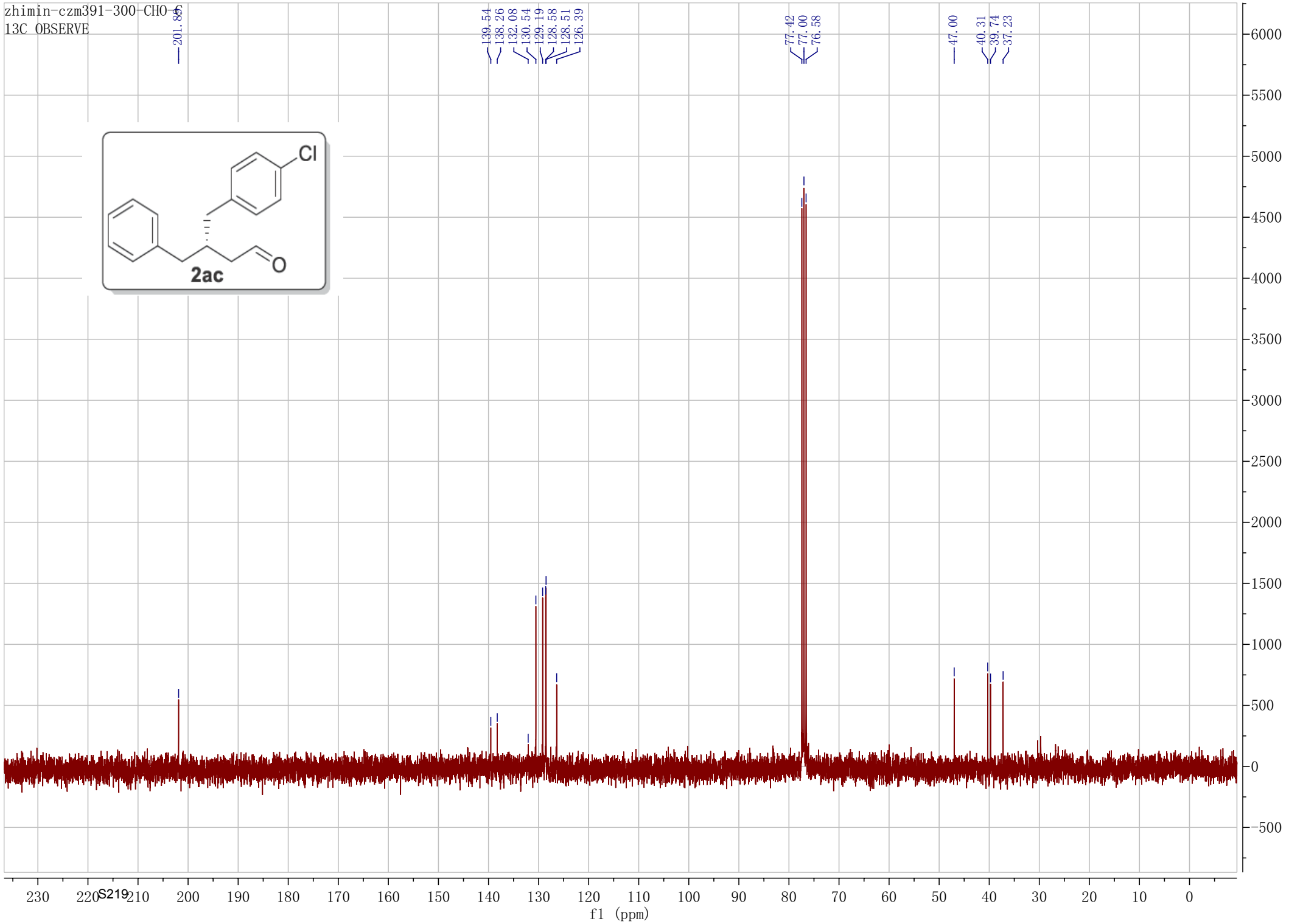

zhimin-czm394-CHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
2ab
O
7.32 7.29 7.29 7.27 7.26 7.26 7.25 7.25 7.24 7.23 7.23 7.22 7.21 7.21 7.20 7.19 7.18 7.16 7.08 7.06
3.55 3.53 3.50 3.48 3.45 3.01 2.99 2.97 2.94 2.92 2.90 2.88 2.85 2.84 2.83 2.78 2.77 2.77 2.77 2.76 2.75 2.75 2.74 2.72 2.71 2.69
0.76
7.50
1.85
1.00
2.03
2.01
f1 (ppm)

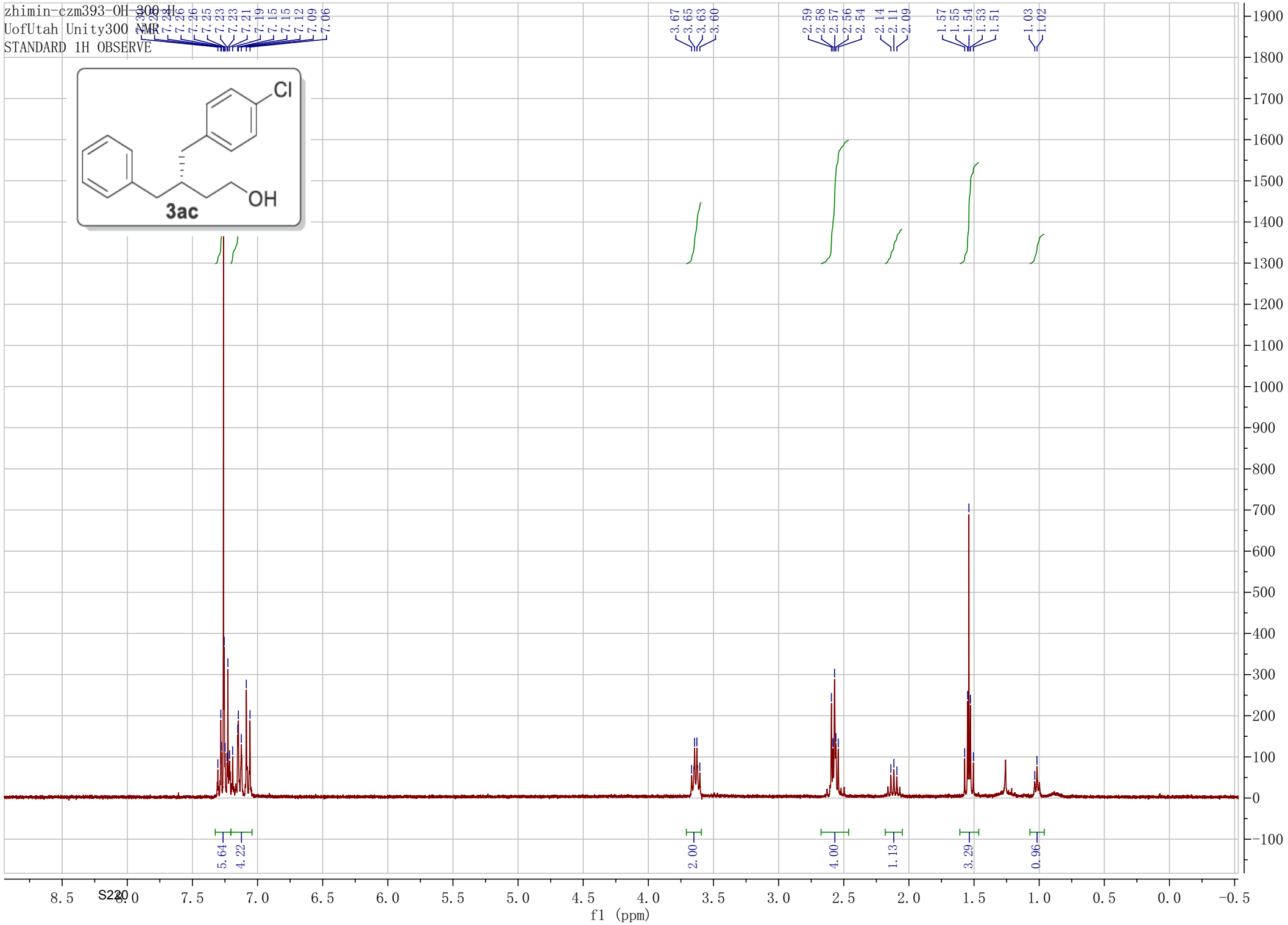

zhimin-czm390-CHO-300-C
13C OBSERVE
201.61
143.18
139.22
129.19
128.57
128.29
127.48
126.72
126.32
77.42
77.00
76.58
48.89
43.30
41.99
O
2ab
f1 (ppm)

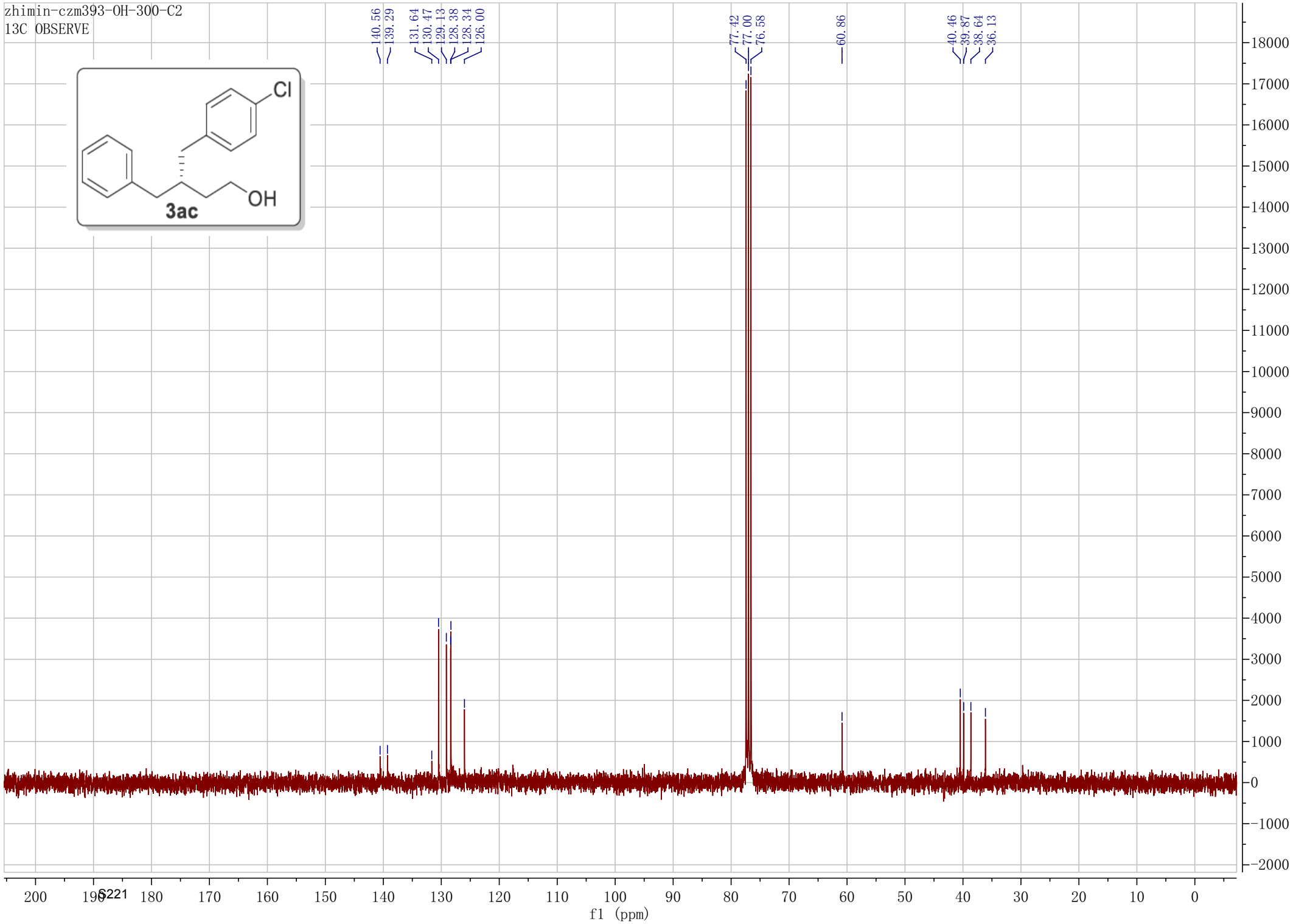

zhimin-czm390-OH-500-H1
STANDARD PROTON PARAMETERS
OH
3ab
f1 (ppm)

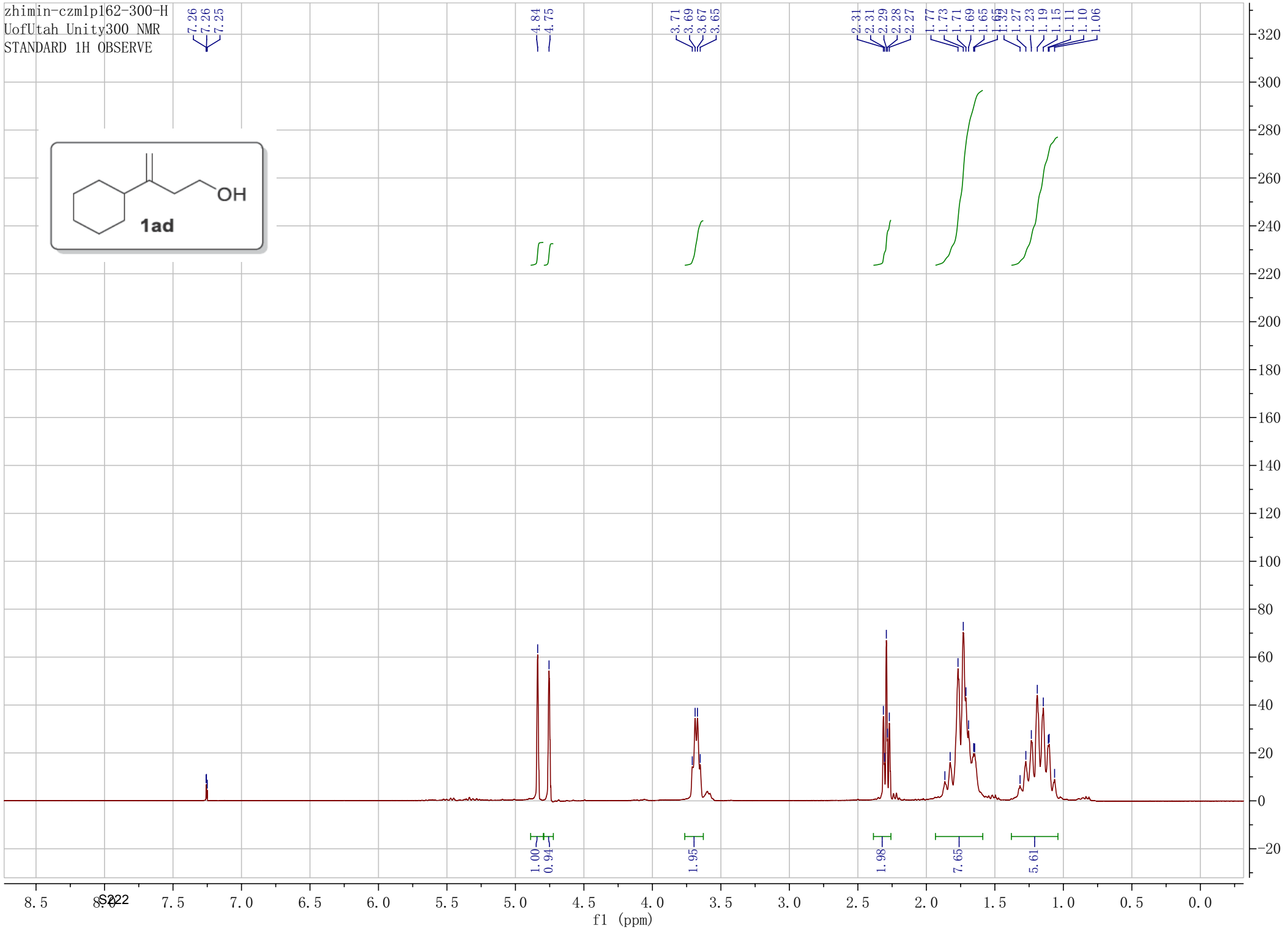

zhimin-390-OH-300-C1
13C OBSERVE
144.29
140.28
129.14
128.42
128.10
127.66
126.34
125.90
77.42
77.00
76.58
61.12
44.48
43.85
38.19
OH
3ab
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

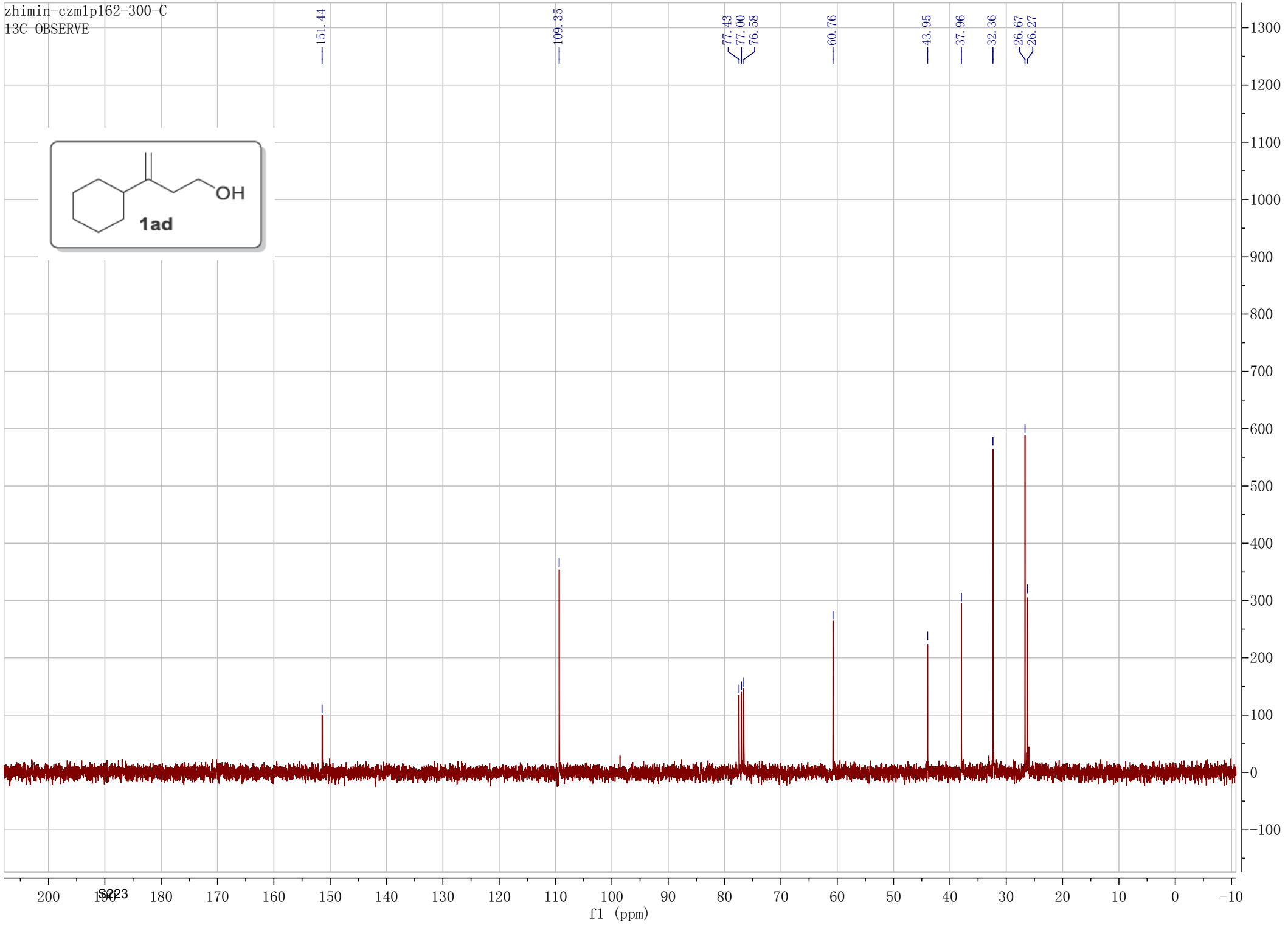

zhimin-czm434-CH0-300-H1
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.32
7.31
7.29
7.28
7.27
7.27
7.26
7.25
7.25
7.23
7.21
7.20
7.18
7.17
7.15
7.12
7.10
7.07
2.71
2.69
2.66
2.58
2.55
2.33
2.33
2.32
Cl
O
2ac
1.09
10.63
5.66
2.00
f1 (ppm)

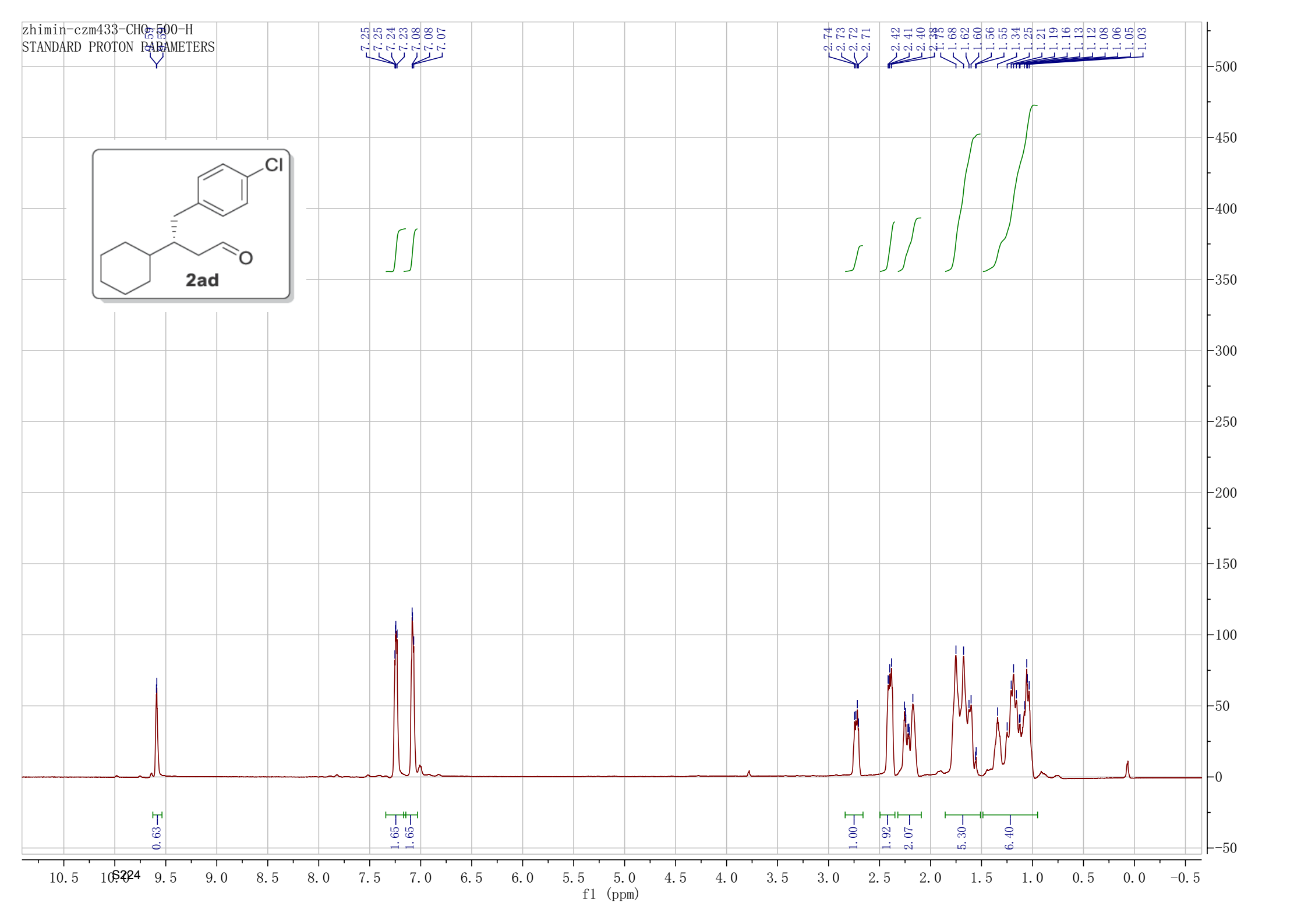

zhimin-czm391-300-CHO-C
13C OBSERVE
201.85
139.54
138.26
132.08
130.54
129.19
128.58
128.51
126.39
77.42
77.00
76.58
47.00
40.31
39.74
37.23
Cl
O
2ac
f1 (ppm)

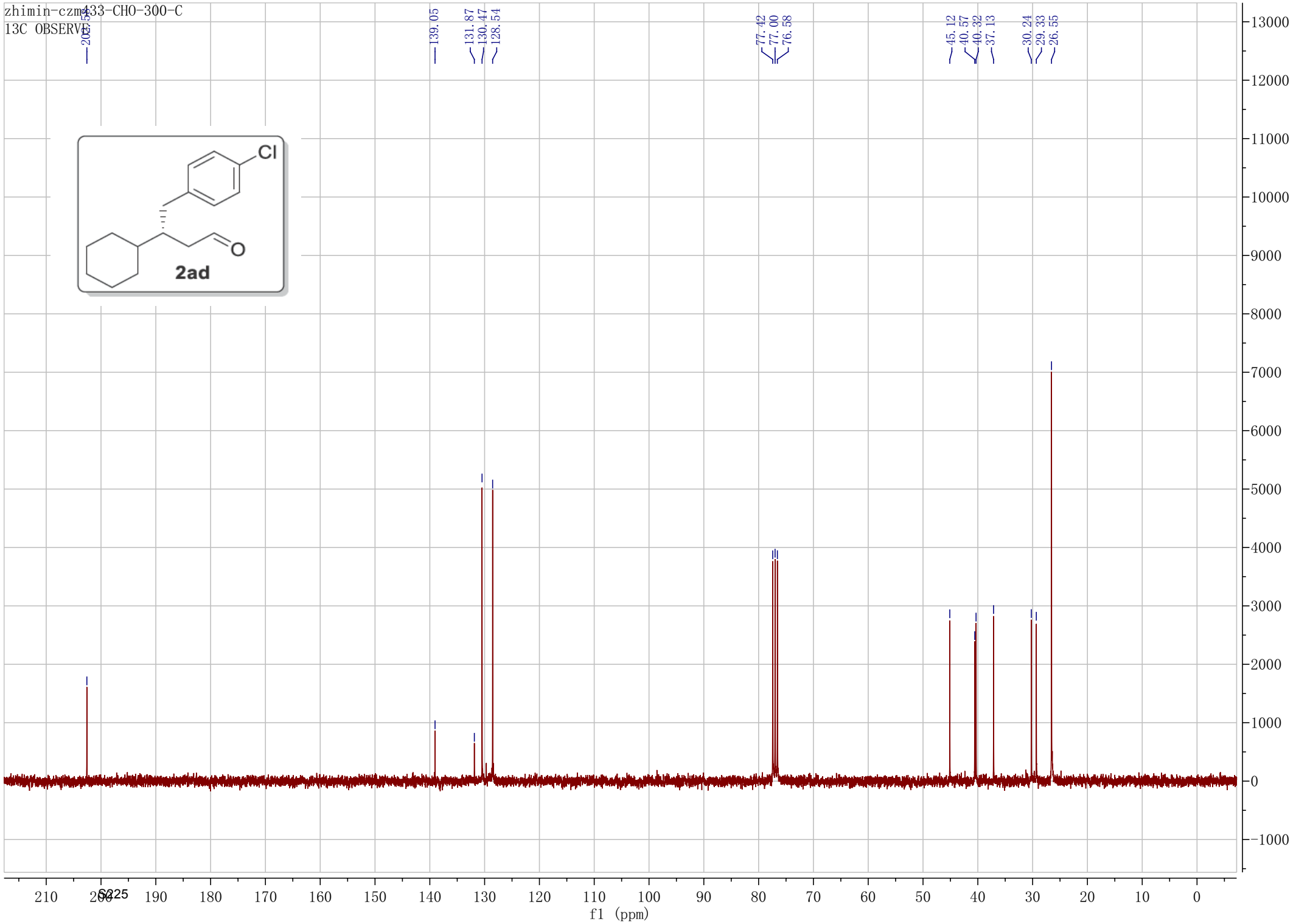

zhimin-czm393-OH-300 H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
OH
3ac
f1 (ppm)

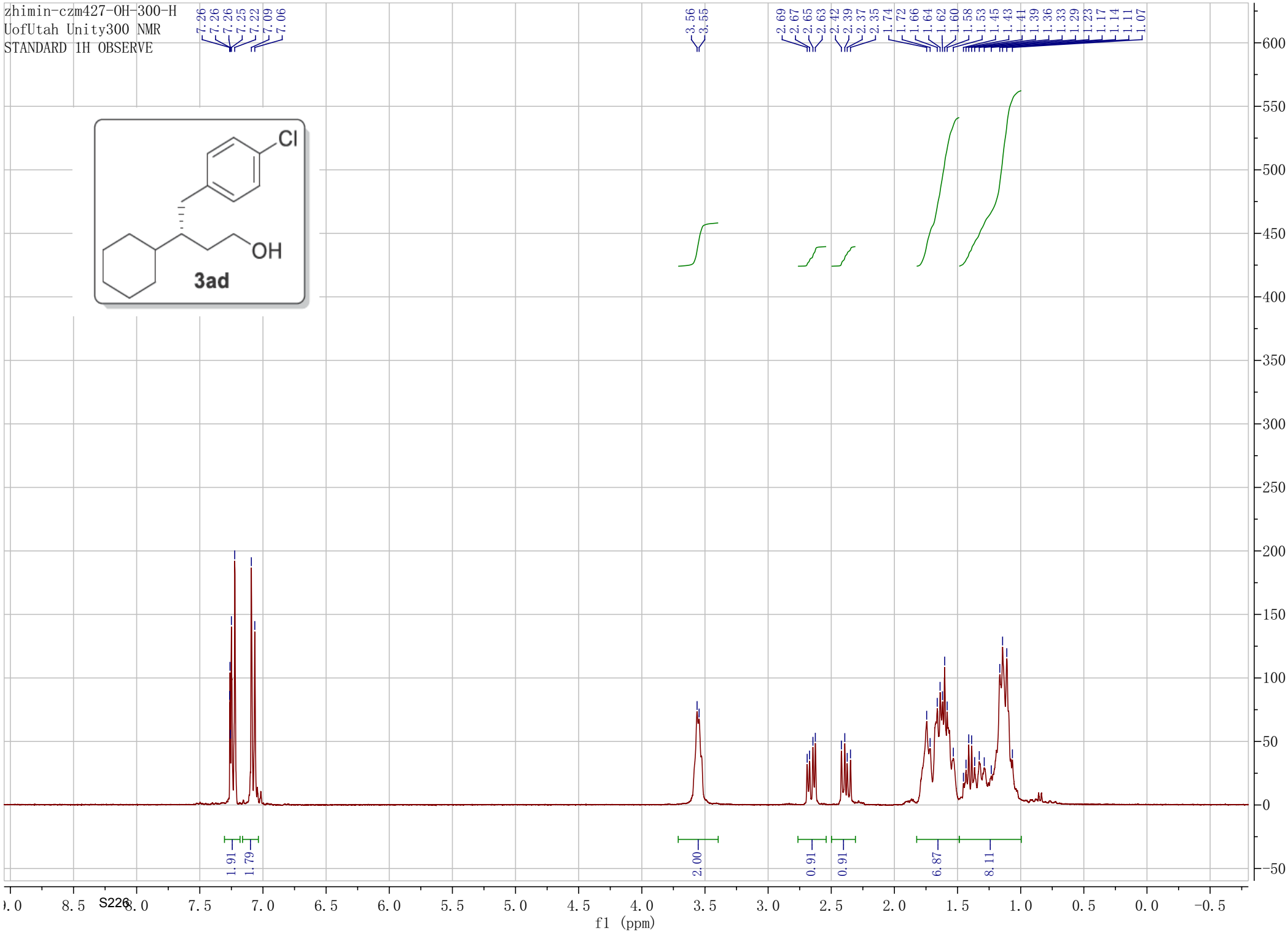

zhimin-czm393-OH-300-C2
13C OBSERVE
140.56
139.29
131.64
130.47
129.13
128.38
128.34
126.00
77.42
77.00
76.58
60.86
40.46
39.87
38.64
36.13
Cl
OH
3ac
f1 (ppm)

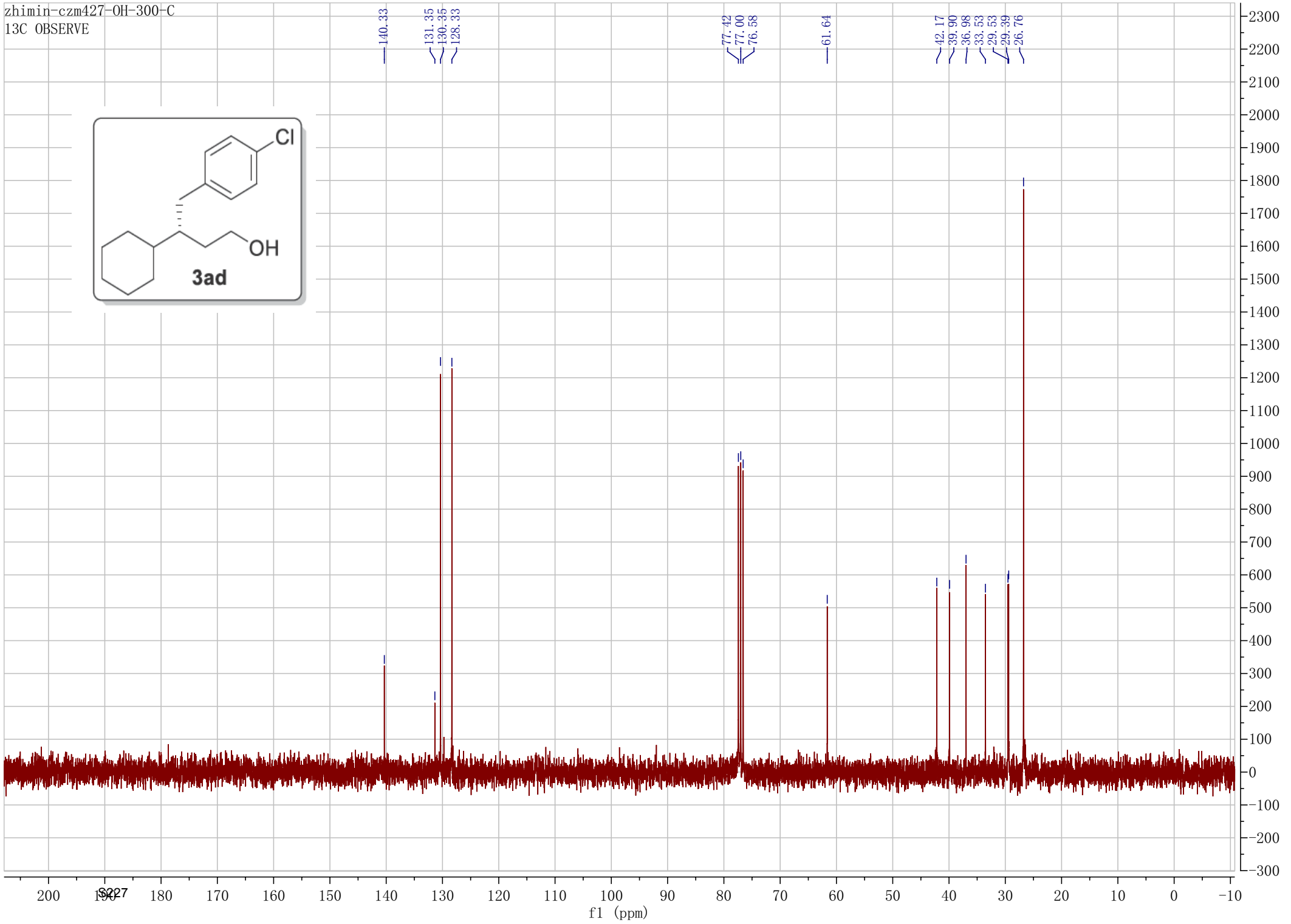

zhimin-czm1p162-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.26
7.26
7.25
4.84
4.75
3.71
3.69
3.67
3.65
2.31
2.31
2.29
2.28
2.27
1.77
1.73
1.71
1.69
1.65
1.32
1.27
1.23
1.19
1.15
1.11
1.10
1.06
OH
1ad
1.00
0.94
1.95
1.98
7.65
5.61
f1 (ppm)

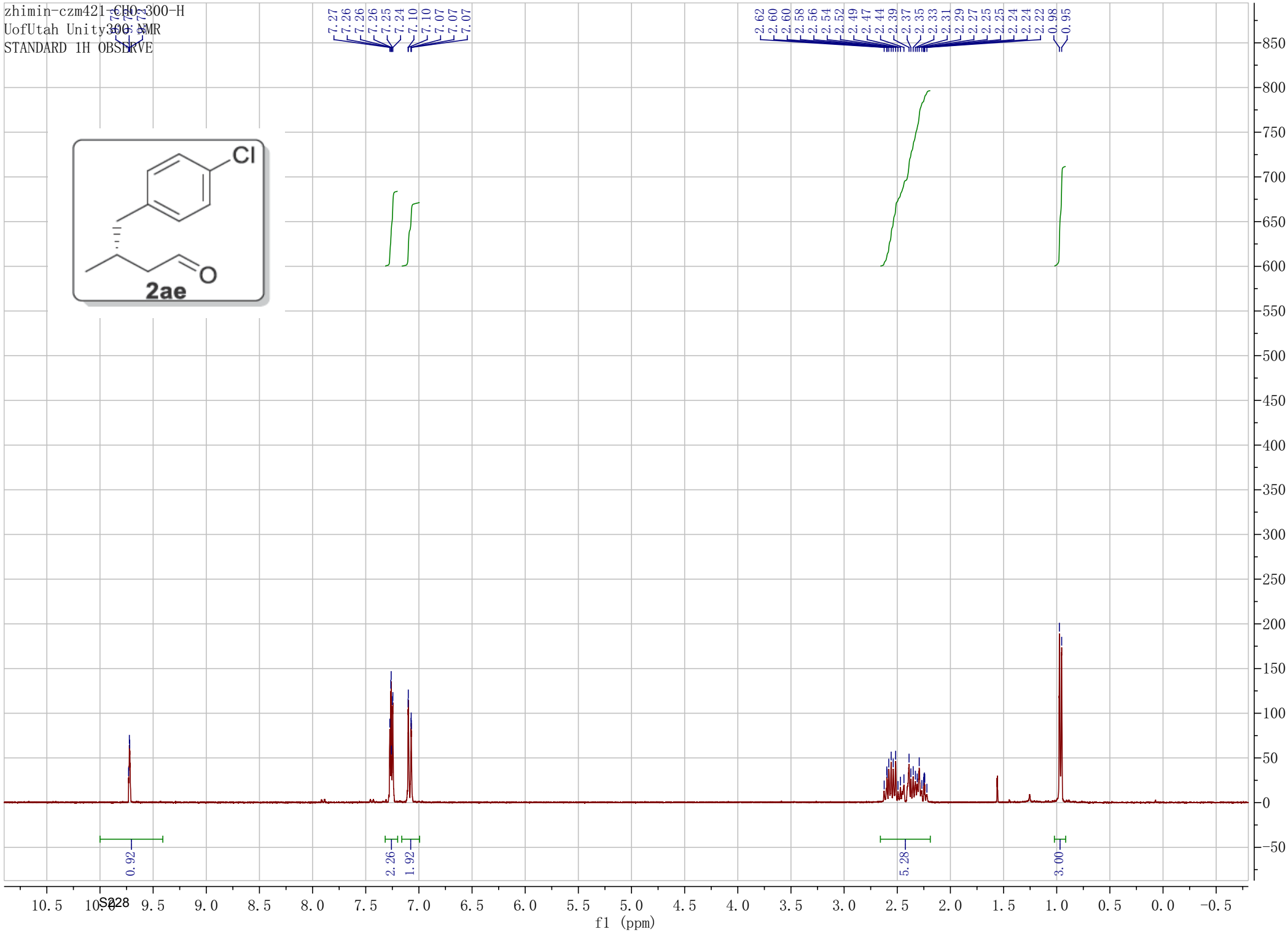

zhimin-czm1p162-300-C
13C OBSERVE
151.44
109.35
77.43
77.00
76.58
60.76
43.95
37.96
32.36
26.67
26.27
OH
1ad
f1 (ppm)

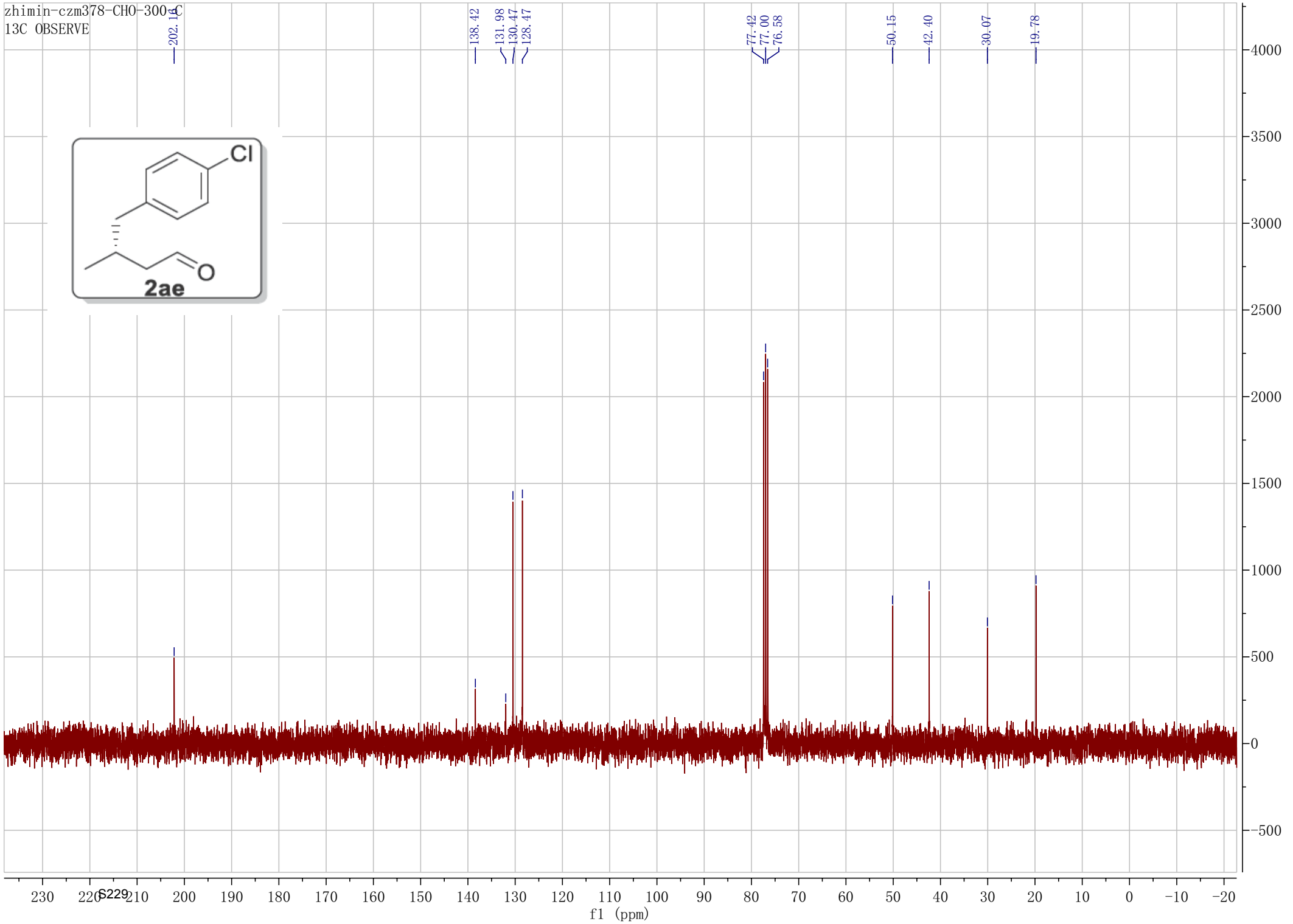

zhimin-czm433-CHO-500-H
STANDARD PROTON PARAMETERS
7.25
7.25
7.24
7.23
7.08
7.08
7.07
2.74
2.73
2.72
2.71
2.42
2.41
2.40
2.38
1.75
1.68
1.62
1.60
1.56
1.55
1.34
1.25
1.21
1.19
1.16
1.13
1.12
1.08
1.06
1.05
1.03
Cl
O
2ad
0.63
1.65
1.65
1.00
1.92
2.07
5.30
6.40
C224
f1 (ppm)

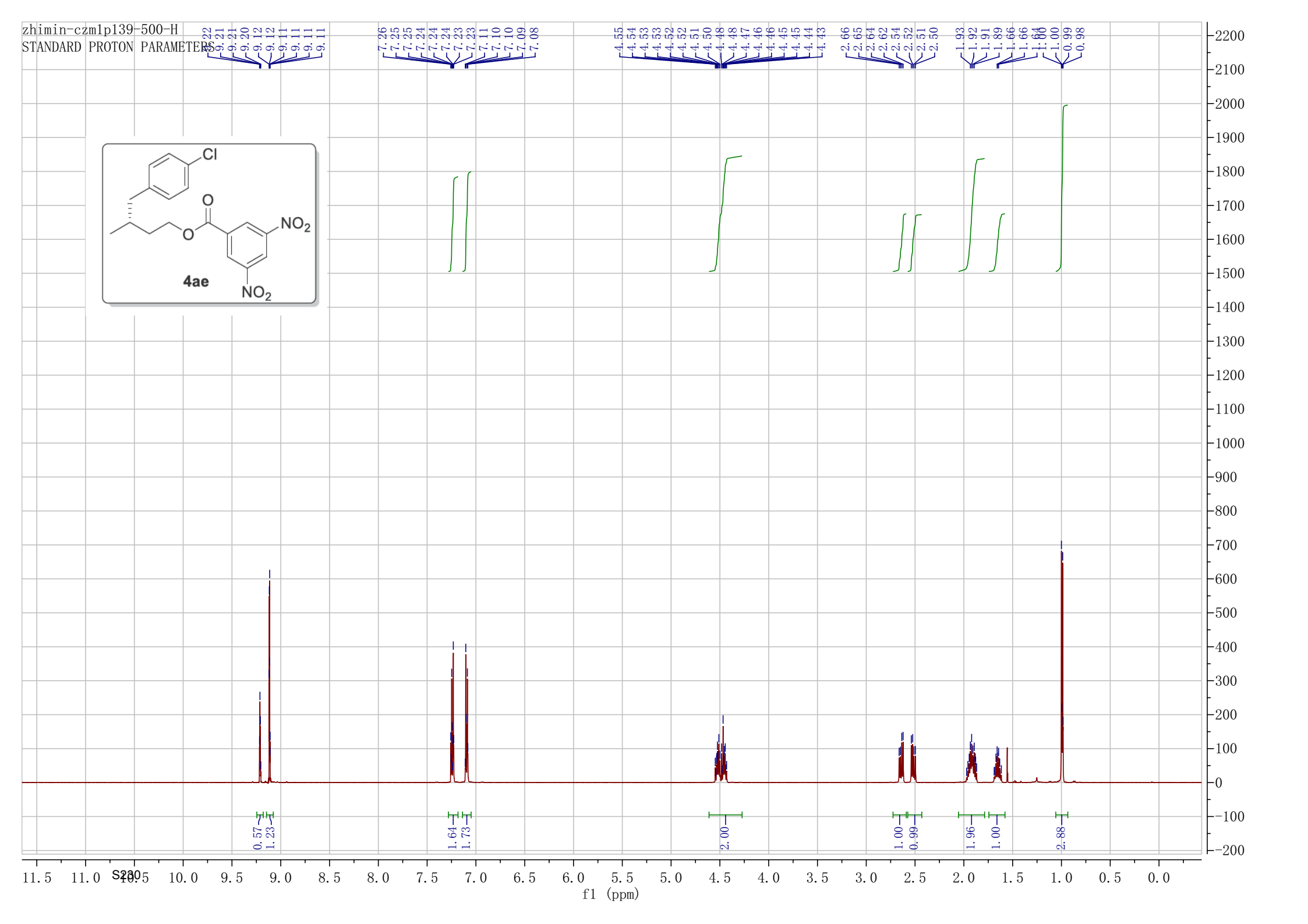

zhimin-czm433-CHO-300-C
13C OBSERVE
202.58
139.05
131.87
130.47
128.54
77.42
77.00
76.58
45.12
40.57
40.32
37.13
30.24
29.33
26.55
Cl
O
2ad
f1 (ppm)

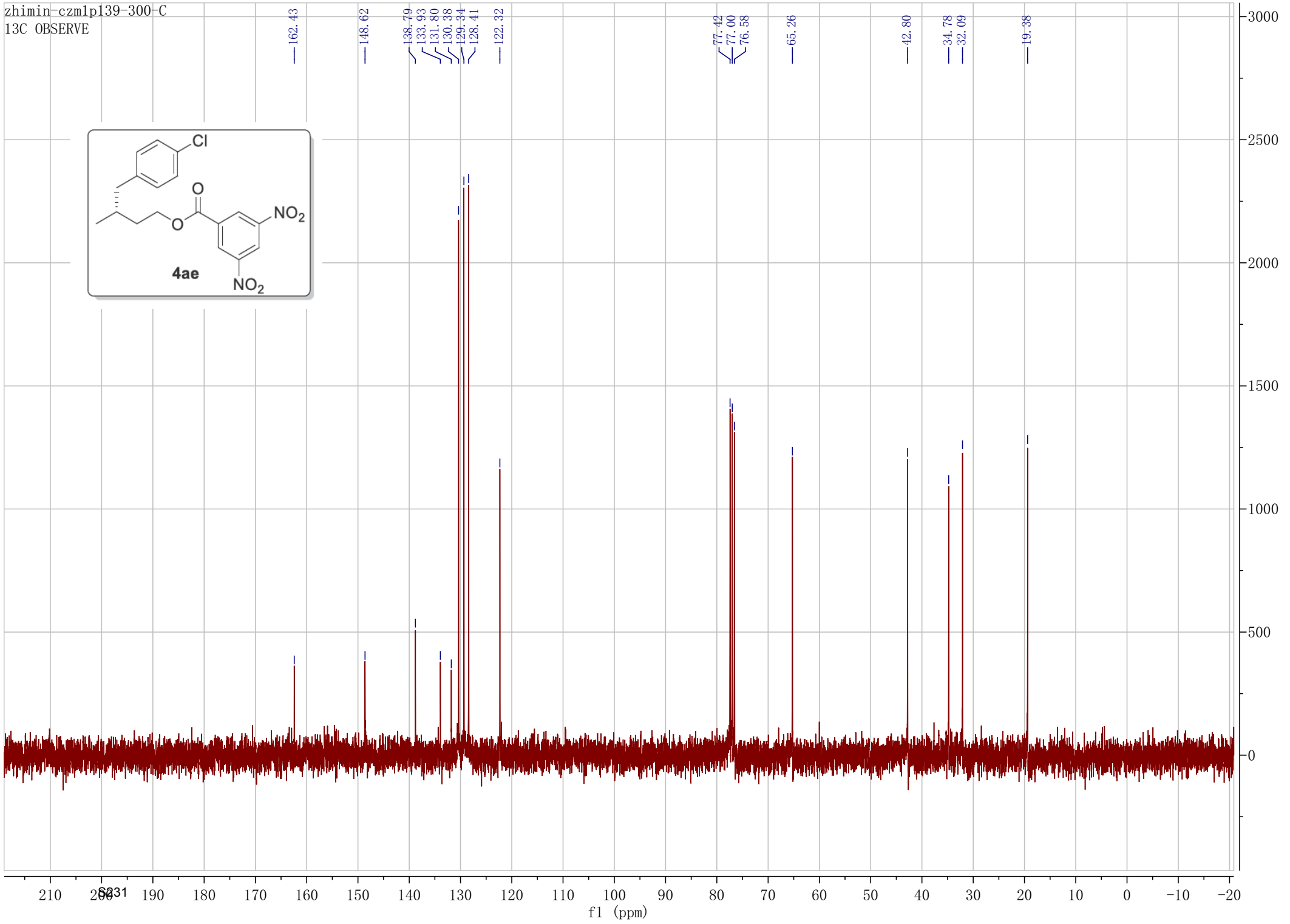

zhimin-czm427-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.26
7.26
7.26
7.25
7.22
7.09
7.06
3.56
3.55
2.69
2.67
2.65
2.63
2.42
2.39
2.37
2.35
1.74
1.72
1.66
1.64
1.62
1.60
1.58
1.53
1.45
1.43
1.41
1.39
1.36
1.33
1.29
1.23
1.17
1.14
1.11
1.07
Cl
OH
3ad
1.91
1.79
2.00
0.91
0.91
6.87
8.11
f1 (ppm)

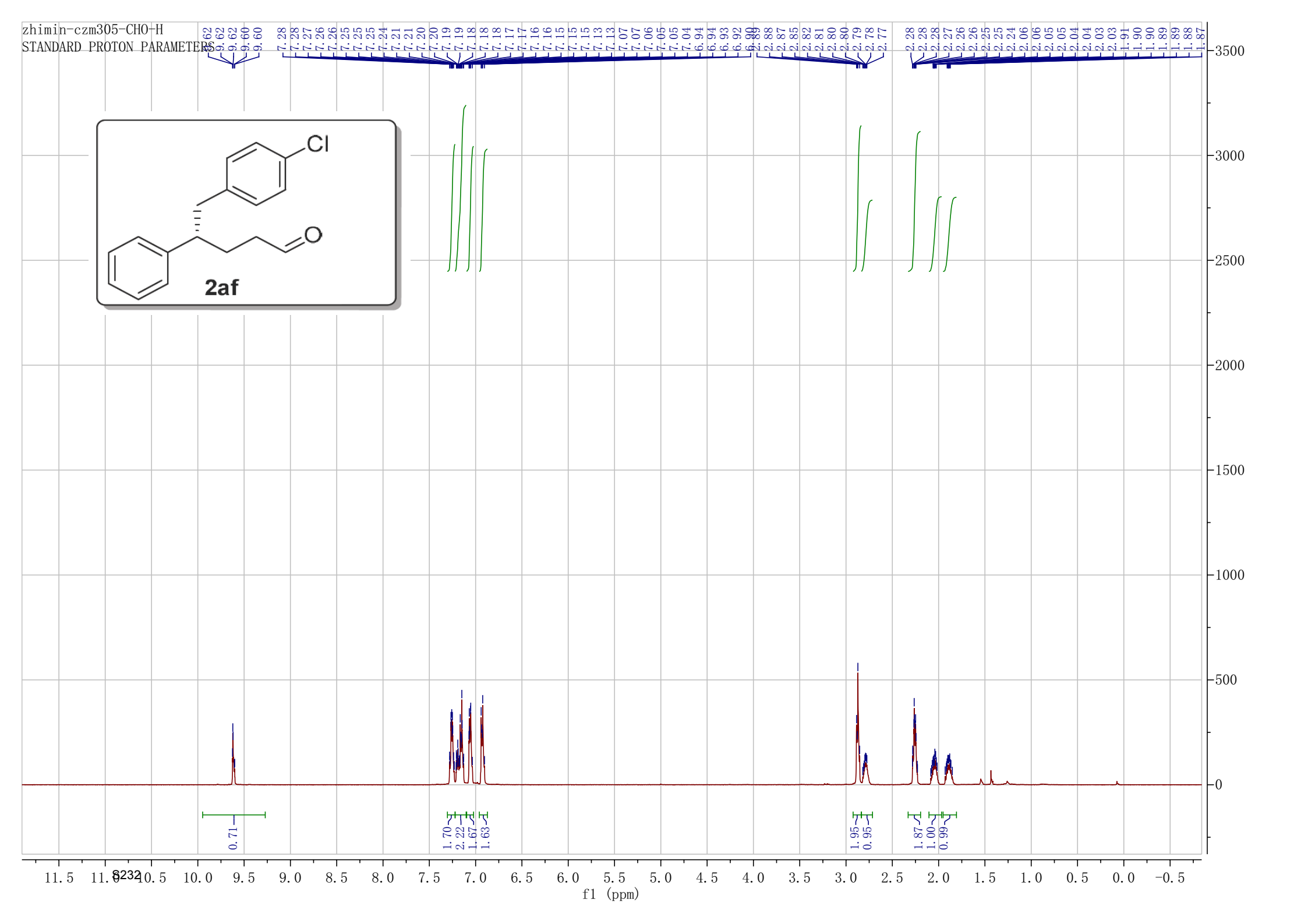

zhimin-czm427-OH-300-C
13C OBSERVE
140.33
131.35
130.35
128.33
77.42
77.00
76.58
61.64
42.17
39.90
36.98
33.53
29.53
29.39
26.76
Cl
OH
3ad
f1 (ppm)

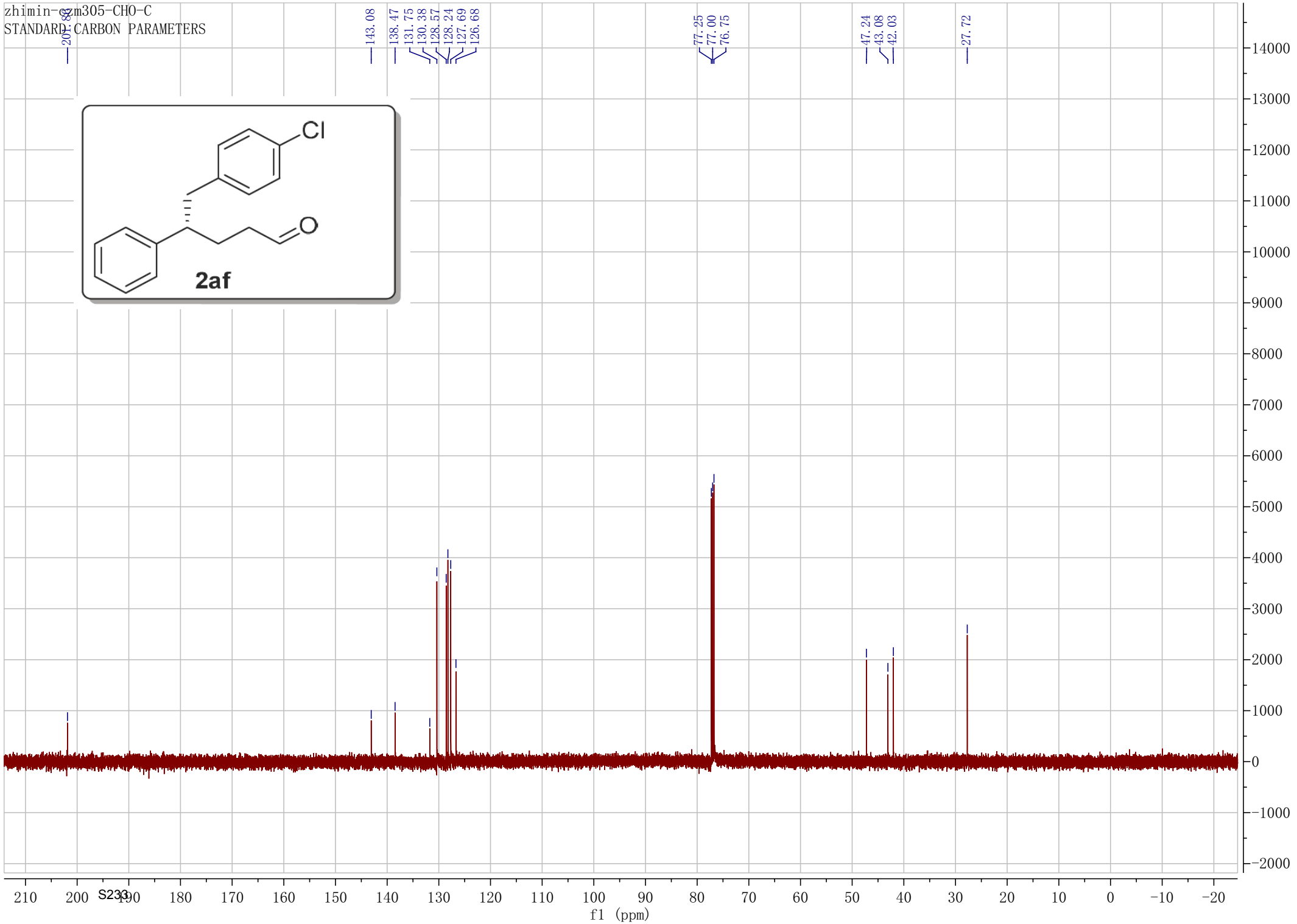

zhimin-czm421-CHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
7.27
7.26
7.26
7.25
7.24
7.10
7.07
7.07
7.07
2.62
2.60
2.60
2.58
2.56
2.54
2.52
2.49
2.47
2.44
2.39
2.37
2.35
2.33
2.31
2.29
2.27
2.25
2.25
2.24
2.24
2.22
0.98
0.95
Cl
O
2ae
0.92
2.26
1.92
5.28
3.00
f1 (ppm)

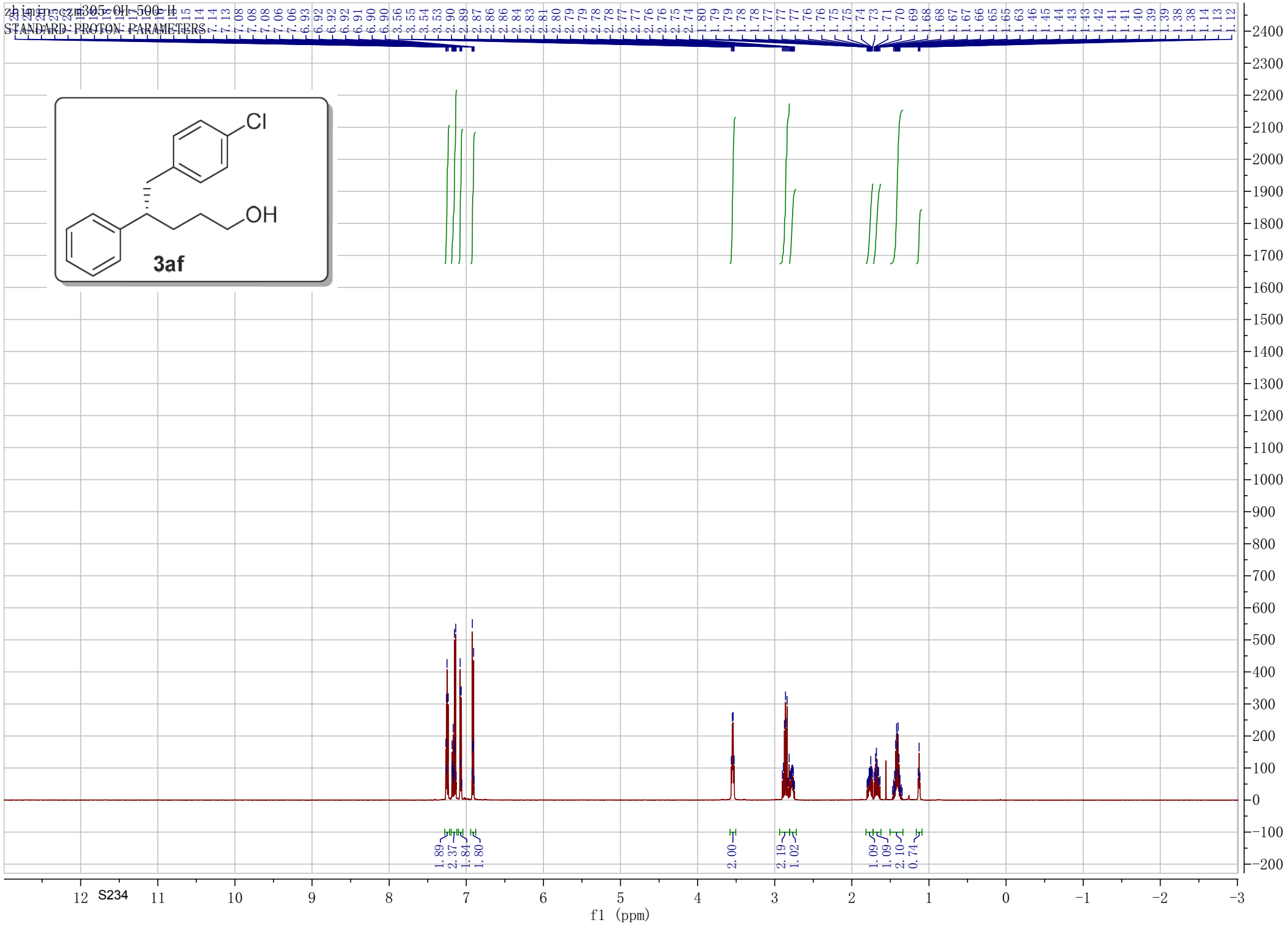

zhimin-czm378-CHO-300-C
13C OBSERVE
202.18
138.42
131.98
130.47
128.47
77.42
77.00
76.58
50.15
42.40
30.07
19.78
Cl
O
2ae
f1 (ppm)

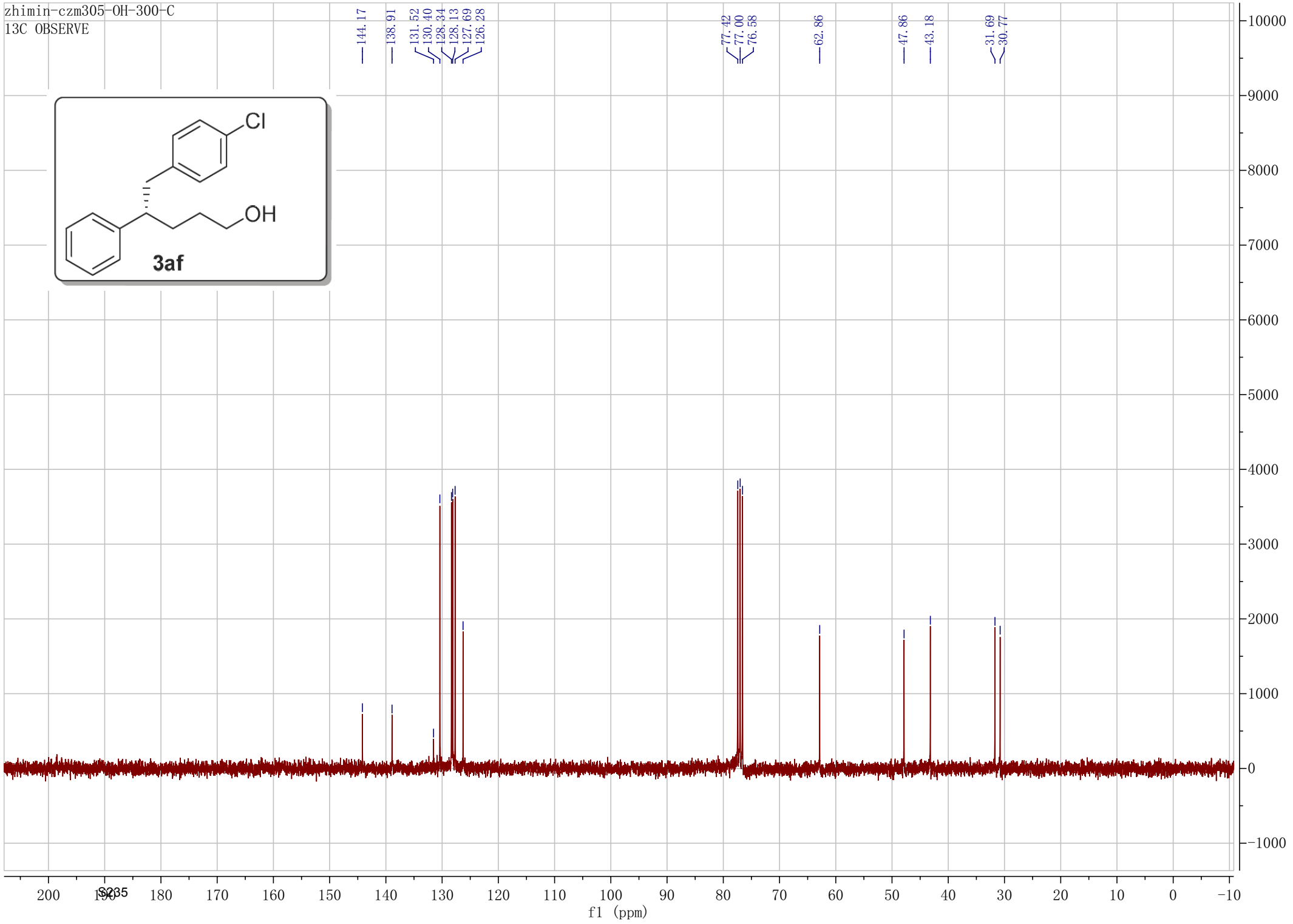

zhimin-czm1p139-500-H
STANDARD PROTON PARAMETERS
Cl
O
O
NO2
NO2
4ae
f1 (ppm)

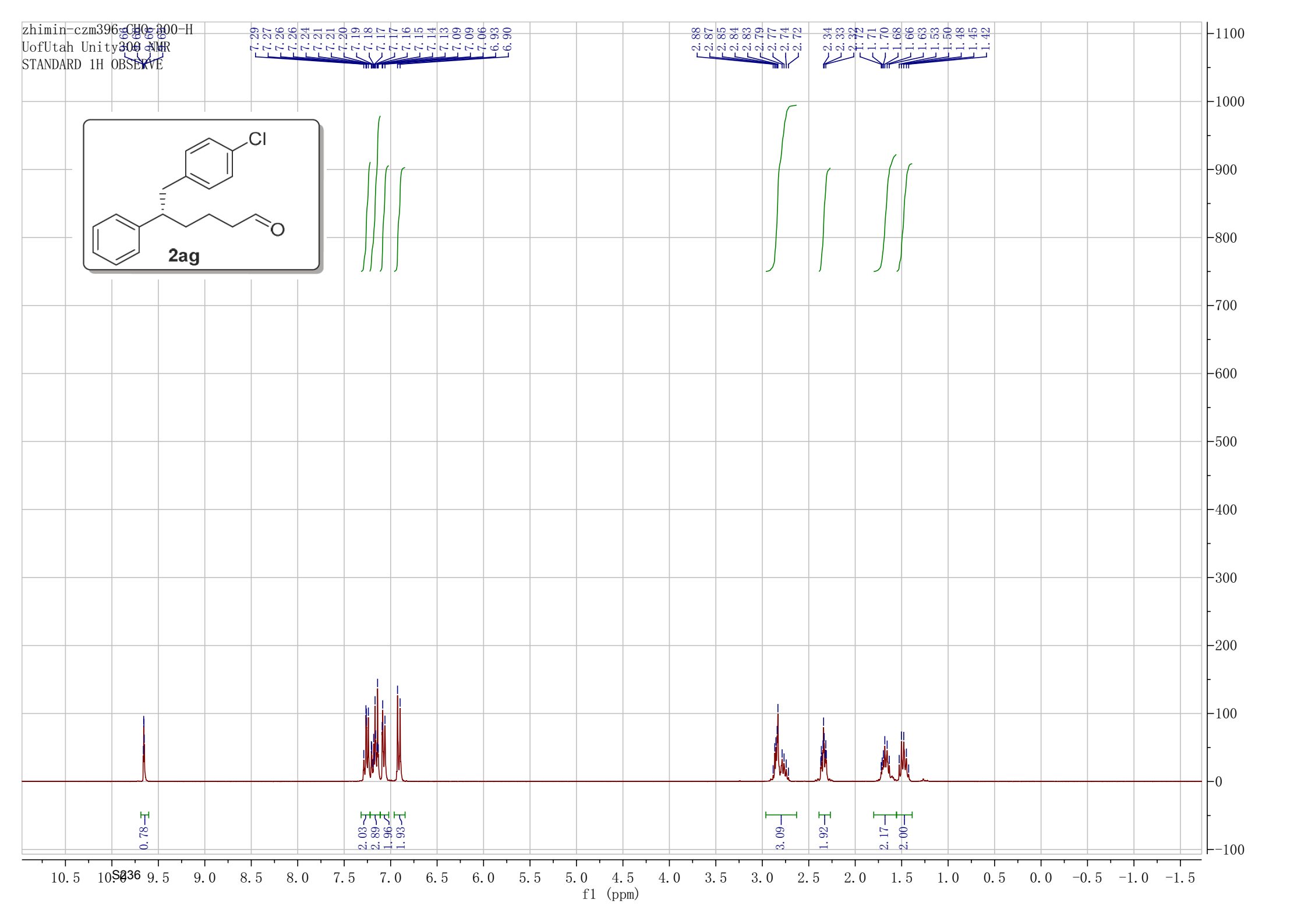

zhimin-czm1p139-300-C
13C OBSERVE
162.43
148.62
138.79
133.93
131.80
130.38
129.34
128.41
122.32
77.42
77.00
76.58
65.26
42.80
34.78
32.09
19.38
Cl
O
O
NO2
NO2
4ae
3000
2500
2000
1500
1000
500
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

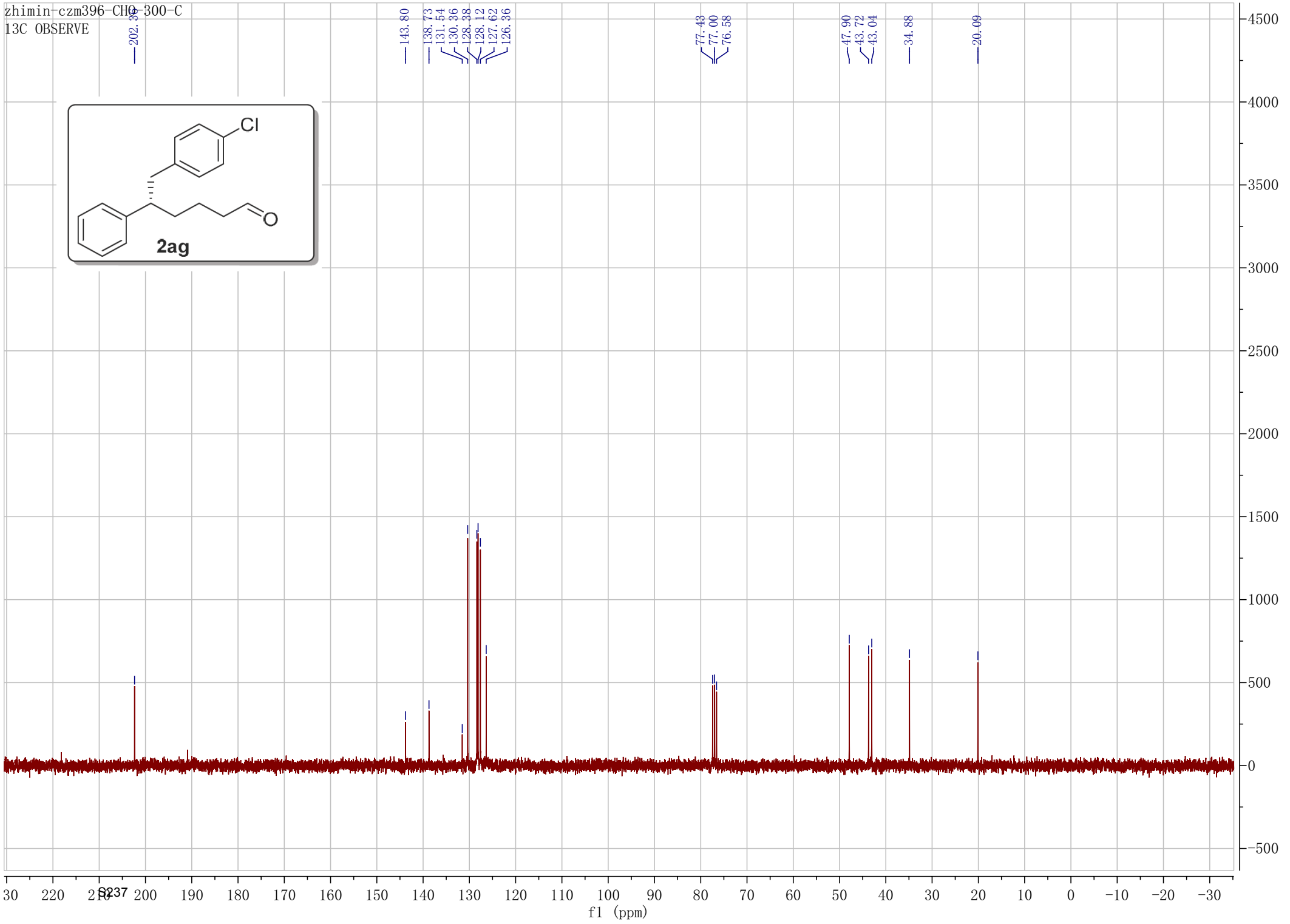

zhimin-czm305-CHO-H
STANDARD PROTON PARAMETERS
Cl
O
2af
f1 (ppm)

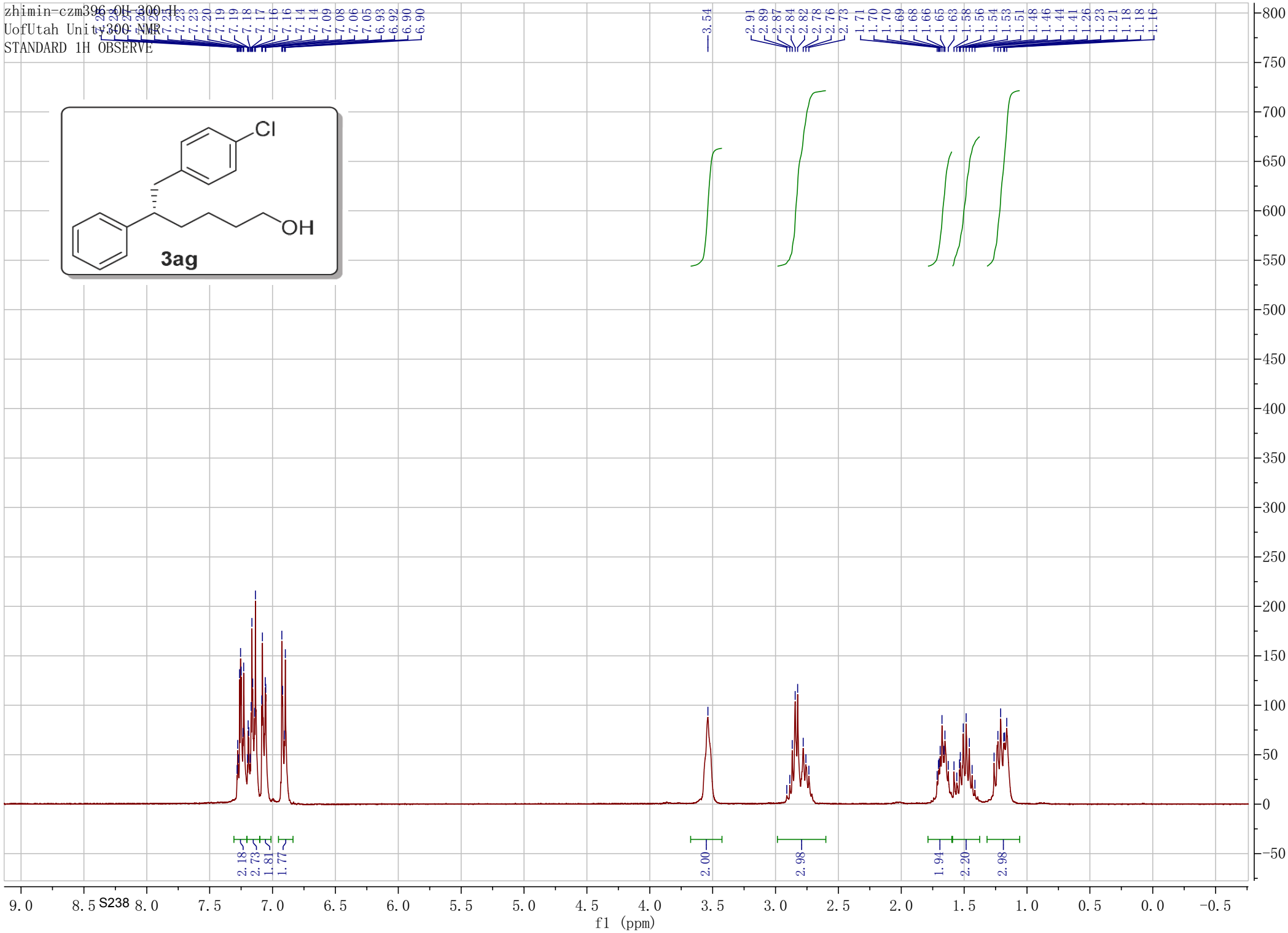

zhimin-czm305-CHO-C
STANDARD CARBON PARAMETERS
201.88
143.08
138.47
131.75
130.38
128.57
128.24
127.69
126.68
77.25
77.00
76.75
47.24
43.08
42.03
27.72
Cl
O
2af
f1 (ppm)

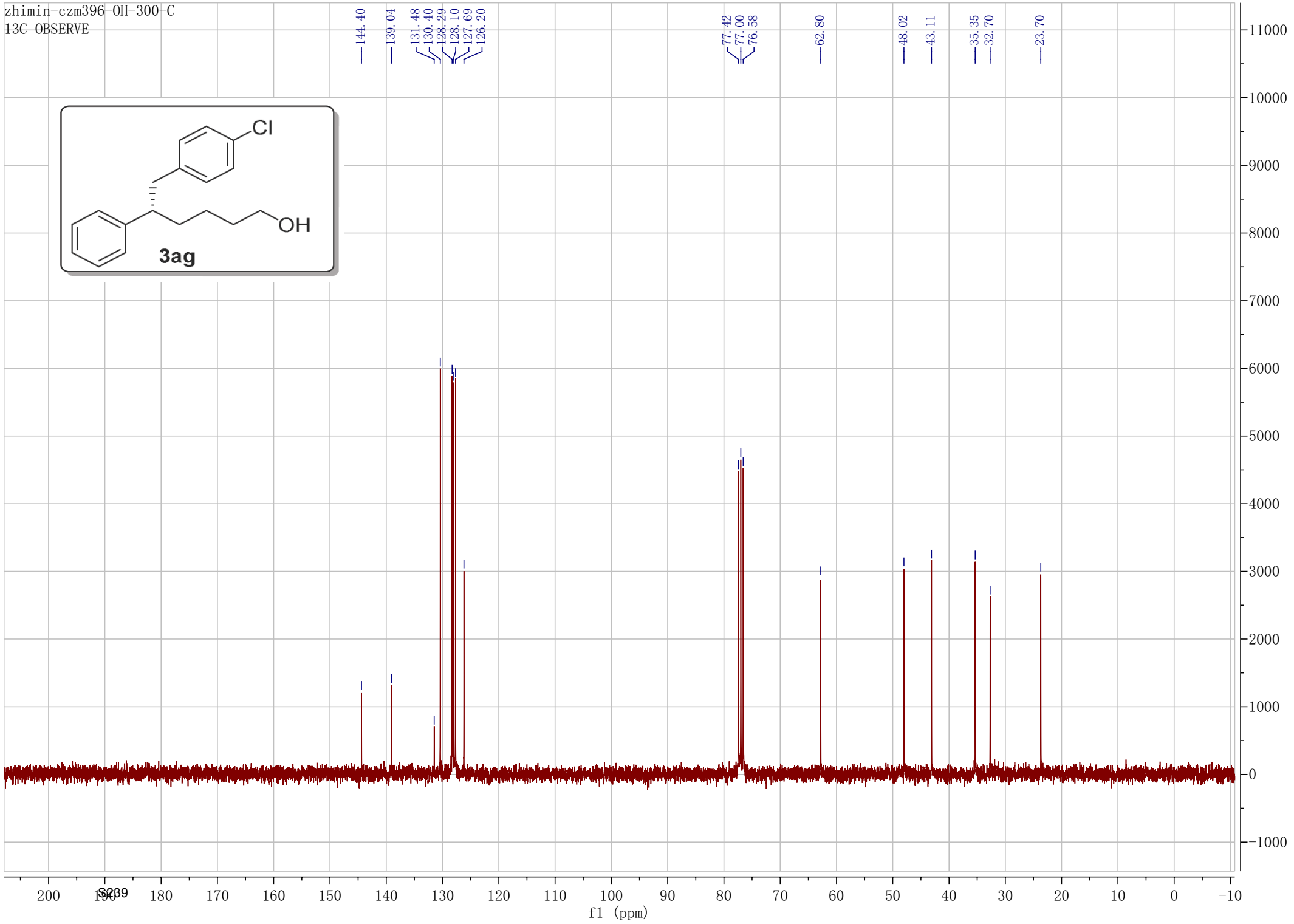

zhimin-czm305-OH-500-H
STANDARD PROTON PARAMETERS
Cl
OH
3af
1.89
2.37
1.84
1.80
2.00
2.19
1.02
1.09
1.09
2.10
0.74
f1 (ppm)

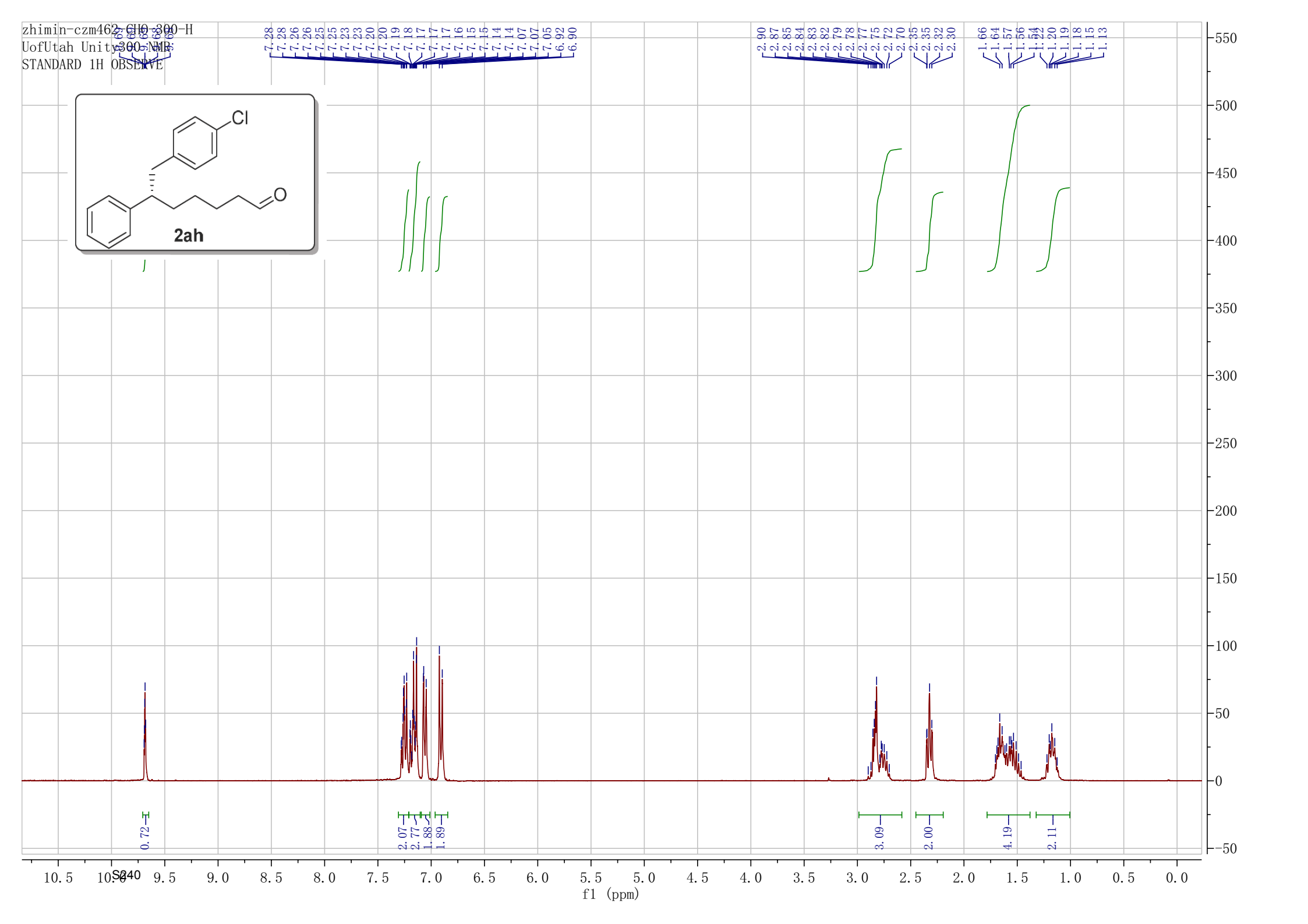

zhimin-czm305-OH-300-C
13C OBSERVE
144.17
138.91
131.52
130.40
128.34
128.13
127.69
126.28
77.42
77.00
76.58
62.86
47.86
43.18
31.69
30.77
Cl
OH
3af
f1 (ppm)

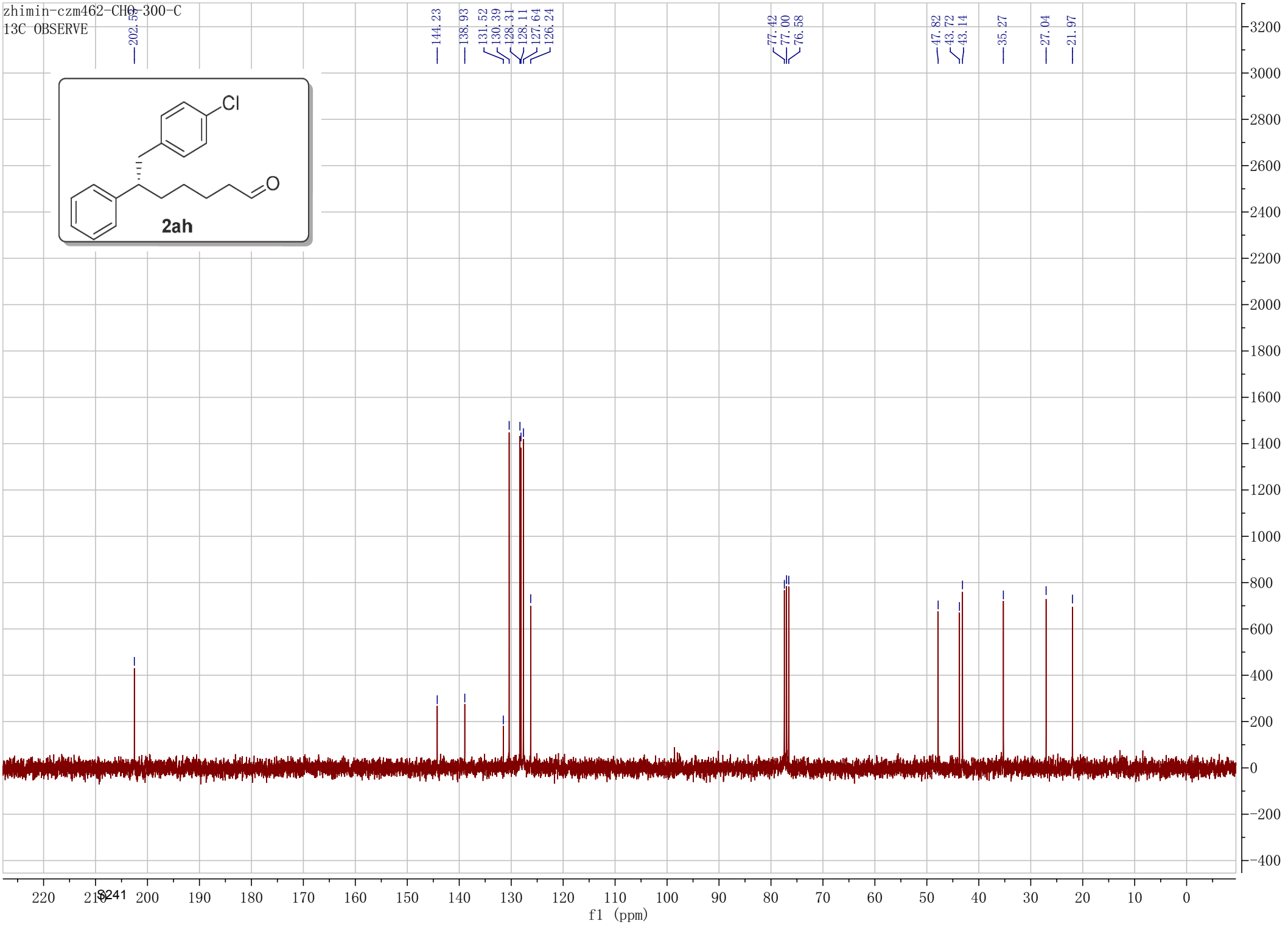

zhimin-czm396-CHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
O
2ag
7.29
7.27
7.26
7.26
7.24
7.21
7.21
7.20
7.19
7.18
7.17
7.17
7.16
7.15
7.14
7.13
7.09
7.09
7.06
6.93
6.90
2.88
2.87
2.85
2.84
2.83
2.79
2.77
2.74
2.72
2.34
2.33
2.32
1.71
1.70
1.68
1.66
1.63
1.53
1.50
1.48
1.45
1.42
0.78
2.03
2.89
1.96
1.93
3.09
1.92
2.17
2.00
f1 (ppm)

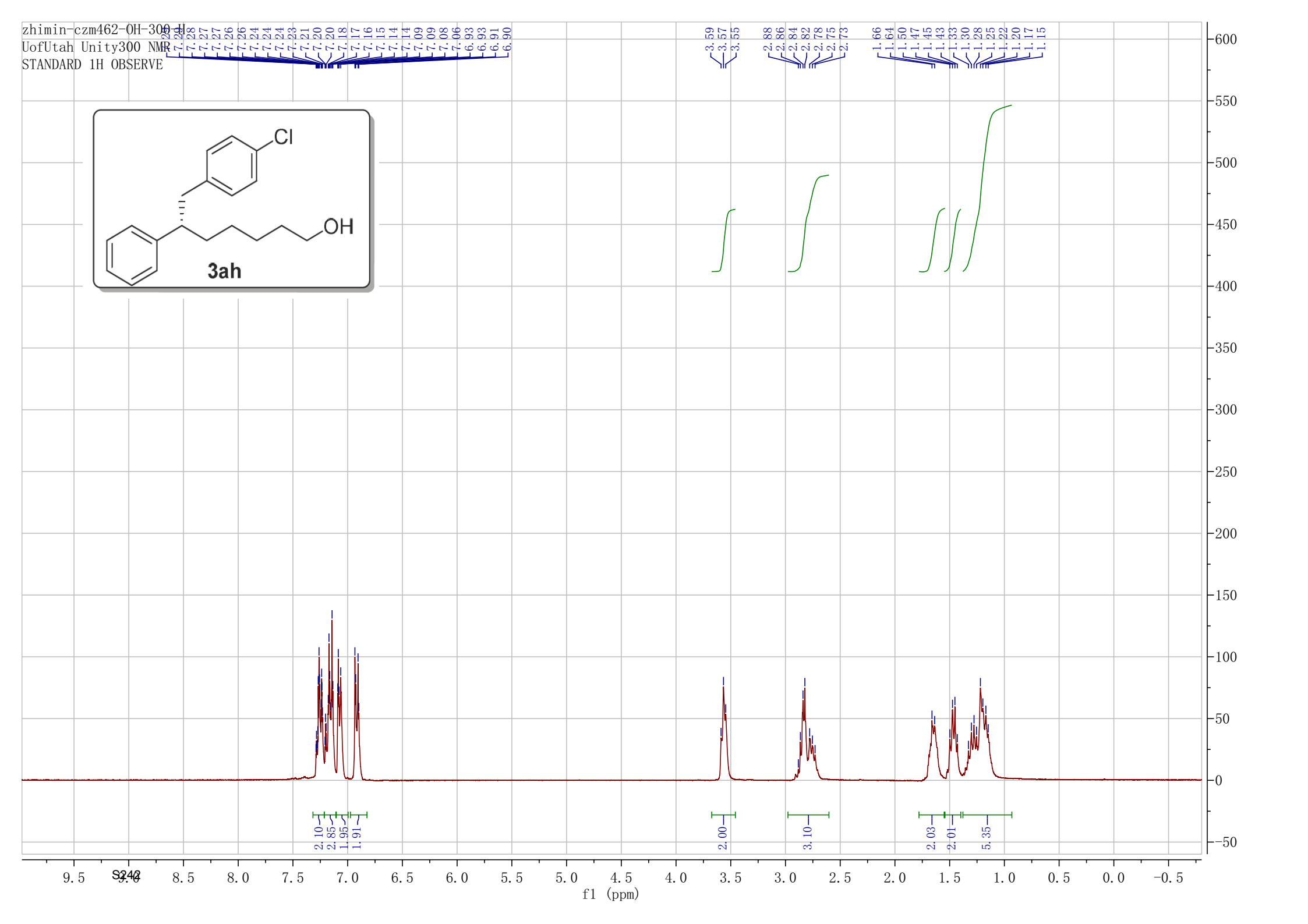

zhimin-czm396-CHO-300-C
13C OBSERVE
202.39
143.80
138.73
131.54
130.36
128.38
128.12
127.62
126.36
77.43
77.00
76.58
47.90
43.72
43.04
34.88
20.09
Cl
O
2ag
f1 (ppm)

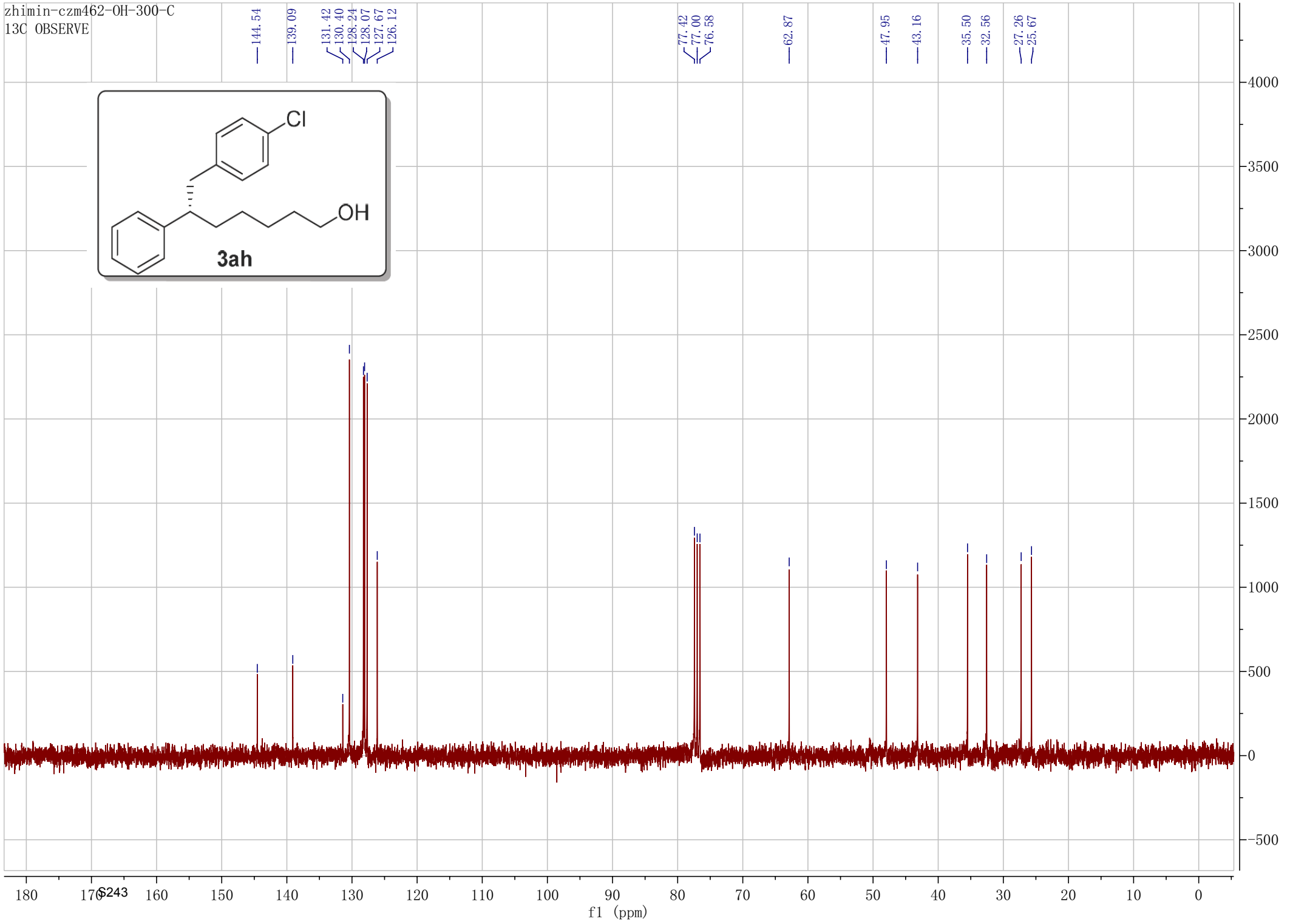

zhimin-czm396-OH-300-1H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
OH
3ag
2.18
2.73
1.81
1.77
2.00
2.98
1.94
2.20
2.98
f1 (ppm)


zhimin-czm396-OH-300-C
13C OBSERVE
144.40
139.04
131.48
130.40
128.29
128.10
127.69
126.20
77.42
77.00
76.58
62.80
48.02
43.11
35.35
32.70
23.70
Cl
OH
3ag
f1 (ppm)


zhimin-czm462-CHO-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
O
2ah
f1 (ppm)


zhimin-czm462-CHO-300-C
13C OBSERVE
202.59
144.23
138.93
131.52
130.39
128.31
128.11
127.64
126.24
77.42
77.00
76.58
47.82
43.72
43.14
35.27
27.04
21.97
Cl
O
2ah
f1 (ppm)


zhimin-czm462-OH-300-H
UofUtah Unity300 NMR
STANDARD 1H OBSERVE
Cl
OH
3ah
f1 (ppm)


zhimin-czm462-OH-300-C
13C OBSERVE
144.54
139.09
131.42
130.40
128.24
128.07
127.67
126.12
77.42
77.00
76.58
62.87
47.95
43.16
35.50
32.56
27.26
25.67
Cl
OH
3ah
f1 (ppm)

Cartesian coordinates for optimized structures:

Substrates

1a

C	2.07779900	-1.24607500	-0.34540300
C	0.72515200	-0.94310900	-0.42311400
C	0.25325700	0.32926600	-0.10712300
C	1.18707700	1.27697200	0.32125200
C	2.53287300	0.97006200	0.40156400
C	3.00596000	-0.29706900	0.06329400
H	2.41506500	-2.24237600	-0.60642200
H	0.03599800	-1.71194500	-0.74649700
H	0.84623000	2.25935700	0.62215800
H	3.23242000	1.72334500	0.74635100
C	-1.19052900	0.66702100	-0.20709300
C	-1.58573800	1.90363000	-0.50606900
H	-0.87020200	2.68594100	-0.72163800
H	-2.63036200	2.17666100	-0.56513700
C	-2.16073400	-0.45970600	0.03939900
H	-2.06285100	-1.20981600	-0.75068600
H	-1.89371600	-0.96903600	0.96968300
C	-3.61753600	-0.05773200	0.11285900
H	-3.93674400	0.38453600	-0.83721500
H	-3.76076000	0.68944100	0.90165300
O	-4.35727400	-1.23421800	0.38917500
H	-5.29081900	-1.01423000	0.43304600
C	4.47315200	-0.61405100	0.14284300
H	5.03052200	-0.06545000	-0.61914900
H	4.88303200	-0.33082200	1.11335100
H	4.65597900	-1.67712300	-0.00735100

1p

C	-2.46121200	-1.48034700	0.29316200
C	-1.13352200	-1.09137900	0.39818500
C	-0.74057900	0.21147300	0.08864300
C	-1.71749200	1.10342500	-0.35934300
C	-3.04300000	0.71576200	-0.46844000
C	-3.42240800	-0.57839300	-0.13779800
H	-2.74357300	-2.49353400	0.54881800
H	-0.40049400	-1.81065000	0.73828300
H	-1.42668600	2.10476700	-0.64977800
H	-3.78102100	1.42321400	-0.82423900
H	-4.45703900	-0.88318000	-0.22540300
C	0.67753600	0.63929600	0.21927200
C	0.98346300	1.88976900	0.56090800
H	0.21262500	2.61411000	0.78848100
H	2.00614600	2.23106600	0.64456300
C	1.72266200	-0.41283200	-0.04879000
H	1.66427100	-1.19424200	0.71428400
H	1.50190500	-0.90665600	-0.99936500
C	3.15034600	0.08679100	-0.08649700
H	3.42627600	0.51723800	0.88241200
H	3.25392200	0.86789500	-0.84820700
O	3.97016400	-1.02819100	-0.38930000
H	4.88759500	-0.74589500	-0.41126500

1q

C	-1.60849100	-1.32842800	0.43121100
C	-0.27088500	-0.99221300	0.47705600
C	0.17009500	0.29677200	0.15691200
C	-0.79154800	1.21996600	-0.24189200
C	-2.14144600	0.89900700	-0.29849000
C	-2.55690800	-0.38293500	0.04595600
H	-1.94701600	-2.32289400	0.68974300
H	0.44147000	-1.74742400	0.78166600
H	-0.48015100	2.21212900	-0.54284200
H	-2.84952800	1.64740100	-0.62330700
C	1.60708900	0.66491100	0.22674900
C	1.98520500	1.90385900	0.53893100
H	1.25967000	2.66493800	0.79399300
H	3.02483700	2.19959200	0.56867600
C	2.59352700	-0.43530500	-0.07104700
H	2.53033300	-1.20613000	0.70254400
H	2.31365900	-0.92768200	-1.00671300
C	4.03992600	-0.00241800	-0.16950700
H	4.37240800	0.42568900	0.78249100
H	4.14968100	0.76435200	-0.94473700
O	4.79628500	-1.15731500	-0.48895900
H	5.72417900	-0.91773800	-0.54738100
O	-3.84613900	-0.80270600	0.02548200
C	-4.83260000	0.12706500	-0.35887500
H	-4.67167900	0.47468400	-1.38302100
H	-5.78323300	-0.39607900	-0.30083500
H	-4.84958900	0.98764000	0.31551700

1r

C	-1.71720800	-1.13802900	0.39492800
C	-0.35851100	-0.86989100	0.45888700
C	0.15149700	0.38413900	0.12132600
C	-0.74923500	1.35793300	-0.31510600
C	-2.10801200	1.10480000	-0.38793400
C	-2.58540200	-0.14537800	-0.02611000
H	-2.10319400	-2.11028300	0.66838700
H	0.30711800	-1.65506700	0.79094400
H	-0.37753500	2.32451400	-0.62904300
H	-2.79605900	1.86357500	-0.73432300
C	1.60646300	0.67377000	0.20945100
C	2.04162600	1.89817900	0.50157000
H	1.35307100	2.70350800	0.72041100
H	3.09470600	2.13796300	0.55282200
C	2.53618500	-0.48548400	-0.04065300
H	2.42278000	-1.22813400	0.75448500
H	2.24393000	-0.99048000	-0.96576300
C	4.00460600	-0.13111600	-0.13081300
H	4.34770000	0.30426900	0.81411600
H	4.16348300	0.60784700	-0.92434000
O	4.70061700	-1.33252500	-0.40942000
H	5.64087300	-1.14568800	-0.46365900
Cl	-4.28434500	-0.47325600	-0.11893900

1s

C	-2.10310300	-1.28048300	0.35412100
C	-0.75656500	-0.95781200	0.43269600
C	-0.29432100	0.31855800	0.10859900

C	-1.22735100	1.26055600	-0.33093100
C	-2.57538100	0.95671500	-0.41940400
C	-2.99129000	-0.31299200	-0.06835800
H	-2.46789900	-2.26483200	0.61345100
H	-0.06183000	-1.71680700	0.76575400
H	-0.88789600	2.24232200	-0.63377400
H	-3.30068600	1.67969600	-0.76675100
C	1.14701200	0.66623600	0.21511400
C	1.53029300	1.90284000	0.52790100
H	0.80788100	2.67624000	0.75290700
H	2.57234300	2.18461300	0.58969800
C	2.12566900	-0.45017100	-0.04345400
H	2.03442400	-1.20991300	0.73831700
H	1.86338000	-0.95122900	-0.97960500
C	3.57950600	-0.03592800	-0.11161100
H	3.89437400	0.39901100	0.84327300
H	3.71721400	0.72036800	-0.89264800
O	4.32684900	-1.20414100	-0.39929700
H	5.25917200	-0.97835100	-0.44060300
F	-4.29467600	-0.61701200	-0.15374200

1t

C	1.08160400	-0.87318000	-0.33514400
C	-0.29501100	-0.74069700	-0.41533400
C	-0.91764000	0.47998000	-0.14791300
C	-0.11652400	1.56033600	0.23429100
C	1.25653100	1.43303600	0.31935400
C	1.86451900	0.21534800	0.03019600
H	1.55210300	-1.82113100	-0.55538300
H	-0.88733400	-1.59855600	-0.70285500
H	-0.58293800	2.50187400	0.49236900
H	1.87806900	2.26594600	0.62048600
C	-2.39278200	0.62717500	-0.25331700
C	-2.93345900	1.78471000	-0.62969800
H	-2.31742800	2.63205800	-0.89982900
H	-4.00334000	1.92372800	-0.70245700
C	-3.21499800	-0.59215900	0.07524700
H	-3.03199100	-1.37311200	-0.66832200
H	-2.88212100	-1.00550400	1.03156300
C	-4.70950100	-0.36490800	0.14459100
H	-5.08649800	-0.02823400	-0.82741800
H	-4.93663700	0.41017600	0.88535200
O	-5.29665900	-1.60135600	0.50737300
H	-6.25026300	-1.49667000	0.54768900
C	3.34569000	0.12920800	0.13854600
O	4.05687400	1.04458500	0.45775400
O	3.81597200	-1.08951100	-0.16097400
C	5.23146900	-1.22924000	-0.07501800
H	5.44587700	-2.25915400	-0.34342700
H	5.72178100	-0.54215300	-0.76318300
H	5.57182700	-1.01666600	0.93738200

1u

C	1.38662200	1.97990300	0.36137500
C	0.11599300	1.44028600	0.43050300
C	-0.07293100	0.06491500	0.25296300
C	1.03338700	-0.72893600	-0.01866000
C	2.31145900	-0.18103300	-0.09061900
C	2.49679400	1.18359300	0.10289300
H	1.52562300	3.04301800	0.51076800

H	-0.72594300	2.08567700	0.63730000
H	0.92351500	-1.78873900	-0.20659500
H	3.47779700	1.63165300	0.04731800
C	-1.42828400	-0.54166800	0.34382600
C	-1.59395500	-1.76623100	0.83978900
H	-0.75540800	-2.33459500	1.22001500
H	-2.56548500	-2.23730100	0.90088000
C	-2.57342700	0.30575300	-0.14698900
H	-2.68030900	1.18753200	0.49097000
H	-2.33807600	0.68652600	-1.14490600
C	-3.91616400	-0.38936200	-0.20049700
H	-4.21291000	-0.71584100	0.80233600
H	-3.85457800	-1.27521200	-0.84275700
O	-4.84615800	0.54660600	-0.71675100
H	-5.71474200	0.13889200	-0.75076800
O	3.31245000	-1.05565300	-0.36574500
C	4.62160400	-0.54438400	-0.46285200
H	5.26350100	-1.39189800	-0.68772100
H	4.70022800	0.19373500	-1.26577000
H	4.93987000	-0.08809400	0.47851700

1v

C	-2.20574100	-1.86618200	0.24081800
C	-0.91605400	-1.38110100	0.38560700
C	-0.60109200	-0.03425200	0.18303900
C	-1.66029500	0.78748500	-0.19940900
C	-2.95292100	0.32881700	-0.36126400
C	-3.23036100	-1.00921400	-0.13306400
H	-2.40818500	-2.91377100	0.41803900
H	-0.12878400	-2.06382800	0.67469700
H	-3.71727900	1.02964900	-0.66837000
H	-4.24018800	-1.37798800	-0.25327900
C	0.79004100	0.46294500	0.34533500
C	1.04601800	1.67465000	0.83345800
H	0.25413300	2.34444400	1.13440000
H	2.05852800	2.03501300	0.95483200
C	1.87866600	-0.49822000	-0.06331800
H	1.88619900	-1.36374600	0.60506000
H	1.65642400	-0.89096400	-1.05956800
C	3.27750200	0.07914200	-0.07903400
H	3.56400900	0.40706700	0.92614600
H	3.31628700	0.94814800	-0.74538600
O	4.14057100	-0.94833200	-0.53303900
H	5.04158300	-0.61691400	-0.54804700
F	-1.44020800	2.08723700	-0.45413600

1w

C	-1.74479900	-0.61588400	0.21746400
C	-0.38380800	-0.59256200	0.36921100
C	0.28093100	0.61916800	0.10037600
C	-0.45398200	1.72288400	-0.32583800
C	-1.84321300	1.68479500	-0.47616700
C	-2.46360900	0.49518400	-0.19379700
H	0.14405400	-1.47475400	0.70142100
H	0.07250500	2.63384500	-0.57600400
H	-2.40304400	2.54705500	-0.80948900
C	1.75626300	0.71326600	0.25706000
C	2.32688300	1.83524900	0.69262100
H	1.73063700	2.68920800	0.98578100
H	3.39923000	1.93751800	0.78754000

C	2.54571400	-0.51889600	-0.10351400
H	2.29871100	-1.33145100	0.58589200
H	2.23967000	-0.86547600	-1.09473300
C	4.04943500	-0.35176500	-0.09434500
H	4.39252400	-0.07433500	0.90840600
H	4.34211200	0.44520400	-0.78724300
O	4.60547900	-1.59406300	-0.48753300
H	5.56309600	-1.52499400	-0.48108400
O	-3.79534800	0.18859900	-0.22368400
O	-2.61003600	-1.64698200	0.46154500
C	-3.85629000	-1.22378500	-0.07381500
H	-4.00577600	-1.68614900	-1.05564800
H	-4.65563700	-1.48202300	0.61699800

1x

C	-1.40381300	0.77717200	-0.14124400
C	-0.03799500	0.61521800	-0.25522200
C	0.55098700	-0.64700900	-0.15368400
C	-0.28667600	-1.72902600	0.09816900
C	-1.65952700	-1.57431900	0.21844600
C	-2.24249600	-0.31705000	0.09492000
H	0.56177100	1.49562600	-0.43940500
H	0.14098900	-2.71408700	0.23032200
H	-2.27281600	-2.43964100	0.42336500
C	2.01903800	-0.82195200	-0.29724000
C	2.52683000	-1.94289300	-0.80718100
H	1.88696800	-2.73615800	-1.17039300
H	3.59223700	-2.10347000	-0.89756800
C	2.87790200	0.32906000	0.15921500
H	2.70093300	1.19816100	-0.48117400
H	2.57255700	0.63170200	1.16490800
C	4.36749700	0.06293700	0.16878100
H	4.71717600	-0.16600100	-0.84388100
H	4.59019200	-0.79811500	0.80915600
O	4.99203800	1.23513500	0.66051000
H	5.94356700	1.10687000	0.66227400
O	-3.56372100	-0.07055500	0.19790900
C	-4.42144800	-1.16497300	0.43449800
H	-4.18933500	-1.64972800	1.38630300
H	-5.42691600	-0.75568000	0.47223700
H	-4.35617900	-1.89894900	-0.37285900
Cl	-2.09585100	2.35234300	-0.28984600

1y

C	-1.38815300	-0.94379900	0.31714400
C	-0.01917900	-0.73621700	0.42172500
C	0.56470900	0.46028400	0.01025900
C	-0.27501000	1.43112800	-0.54132300
C	-1.63746800	1.21936700	-0.64684800
C	-2.22449900	0.03040100	-0.21546500
H	-1.79956700	-1.88686500	0.65374200
H	0.59530600	-1.52175600	0.84136200
H	0.15265500	2.35067600	-0.92001800
H	-2.26352800	1.98698500	-1.08918100
C	2.02695200	0.69338100	0.13645400
C	2.50974300	1.91826000	0.33976000
H	1.85198800	2.76932100	0.45631600
H	3.57033200	2.11495500	0.41549800
C	2.91128100	-0.52234300	0.02910000
H	2.72481600	-1.18958500	0.87552400

H	2.63742900	-1.09001100	-0.86472500
C	4.39744400	-0.24214300	-0.01589600
H	4.71630100	0.25772200	0.90533000
H	4.62910000	0.41799600	-0.85944200
O	5.04959400	-1.49213000	-0.15712100
H	5.99893900	-1.34986000	-0.17519500
C	-3.72631900	-0.13771400	-0.30354100
H	-4.05454700	0.40691300	-1.19408600
C	-4.17433300	-1.58881600	-0.44819600
H	-5.24693900	-1.63196000	-0.64107900
H	-3.65690600	-2.08820000	-1.26815800
H	-3.98693800	-2.15338000	0.46727700
C	-4.39546600	0.50887400	0.91384500
H	-4.12402400	1.56136300	1.00111100
H	-5.48222900	0.43585300	0.84255500
H	-4.07715600	0.00289500	1.82803900

1z

C	1.03933700	-1.03214700	-0.41885900
C	-0.33138900	-0.80549900	-0.46719700
C	-0.87369600	0.43031100	-0.12909100
C	0.01399200	1.42479000	0.29133300
C	1.37512100	1.19461000	0.34212500
C	1.92543500	-0.03923200	-0.01694500
H	1.40612700	-2.00855900	-0.70329700
H	-0.97779900	-1.61144300	-0.78877500
H	-0.37384200	2.38439500	0.60861200
H	2.02324600	1.99350800	0.68192700
C	-2.33610100	0.68367400	-0.19918100
C	-2.80910400	1.90027000	-0.46562700
H	-2.14534900	2.72848000	-0.67515500
H	-3.86895900	2.11128700	-0.50330100
C	-3.23358000	-0.50363900	0.03812000
H	-3.10056200	-1.23231000	-0.76672000
H	-2.92450000	-1.01227100	0.95569900
C	-4.71087500	-0.19188800	0.13589000
H	-5.06802600	0.24713600	-0.80212500
H	-4.88908300	0.53097600	0.94005000
O	-5.37489100	-1.41570500	0.39882700
H	-6.31955300	-1.25360900	0.45502700
C	3.43613100	-0.24746100	0.05656800
C	3.84647500	-1.65364900	-0.37969900
H	4.93127900	-1.75170200	-0.31477600
H	3.40319300	-2.41802200	0.26104900
H	3.55365300	-1.85471200	-1.41180600
C	4.13368600	0.76588000	-0.86164000
H	3.91203400	1.79217900	-0.56741900
H	5.21631200	0.62874600	-0.81720700
H	3.81177600	0.63405900	-1.89607700
C	3.90964500	-0.03249400	1.50101200
H	4.98999700	-0.17869700	1.56694100
H	3.68439300	0.97541900	1.85075300
H	3.42432200	-0.74037000	2.17513000

1ac

C	-1.89539400	2.04075800	-0.37523500
H	-1.48958500	3.04508900	-0.37782100
H	-2.81252900	1.88633400	-0.92883800
C	-1.78604200	-0.35465200	0.33950000
H	-1.01040100	-1.02375400	-0.04634400

H	-1.92787900	-0.64080400	1.38749700
C	-3.07203700	-0.62270900	-0.40954200
H	-2.93933700	-0.39228400	-1.47267500
H	-3.87383600	0.01555900	-0.02100900
O	-3.38652300	-1.99194200	-0.22583600
H	-4.19288400	-2.19527300	-0.70567000
C	-1.28615500	1.06138600	0.28411200
C	-0.00214500	1.30972100	1.03976400
H	0.22379600	2.37777200	1.02209600
H	-0.13857800	1.02227300	2.08600900
C	1.16421500	0.53465600	0.46758500
C	1.81682600	-0.44406000	1.20780500
C	1.59292000	0.78527400	-0.83417300
C	2.87964500	-1.15598100	0.66503100
H	1.48922400	-0.65223100	2.21987700
C	2.65372700	0.07939200	-1.37919100
H	1.08032700	1.53833500	-1.42246500
C	3.30143600	-0.89538500	-0.62958700
H	3.37614800	-1.91539200	1.25540000
H	2.97685600	0.28786600	-2.39114700
H	4.12888300	-1.44836100	-1.05463100

1ad

C	1.07969500	-1.73064300	0.76697600
H	0.27643900	-2.39293900	1.05962200
H	2.07844100	-2.04298500	1.04246900
C	1.95708300	0.32187800	-0.33712100
H	1.93942200	0.39264900	-1.42978600
H	1.76197400	1.33515000	0.02581300
C	3.35487600	-0.06592800	0.09099200
H	3.61392000	-1.04992000	-0.31524400
H	3.40947700	-0.12429100	1.18393500
O	4.23464600	0.92864100	-0.40558600
H	5.13443800	0.70117800	-0.15983200
C	0.85126700	-0.60034000	0.10563700
C	-0.53935400	-0.12934700	-0.26261600
C	-1.59851600	-1.23065500	-0.29835200
C	-1.00914100	0.99760200	0.67376500
H	-0.47483900	0.29867400	-1.27274300
C	-2.94942100	-0.68233400	-0.75277300
H	-1.71432000	-1.65304700	0.70531800
H	-1.26973700	-2.04260200	-0.95079100
C	-2.36573800	1.55230900	0.24428800
H	-1.08060400	0.58828500	1.68746300
H	-0.27197500	1.80161000	0.70710600
C	-3.41679400	0.44886900	0.15964700
H	-3.69095700	-1.48339200	-0.77440300
H	-2.86031900	-0.30631100	-1.77766100
H	-2.68725100	2.33164300	0.93821900
H	-2.26239900	2.02634900	-0.73772500
H	-4.36697700	0.85529200	-0.19259500
H	-3.59564700	0.04706200	1.16286300

1ae

C	-1.28767100	1.40595300	0.00002000
H	-2.28836600	1.81989100	-0.00000600
H	-0.46952300	2.11439900	0.00005400
C	0.26495400	-0.55170000	0.00007200
H	0.34939900	-1.20879000	0.87202500
H	0.34938400	-1.20897300	-0.87174400

C	1.44286400	0.39661200	-0.00004200
H	1.40628400	1.03931500	0.88672100
H	1.40623500	1.03913300	-0.88692900
O	2.61831300	-0.39517900	0.00002000
H	3.38493900	0.18278600	-0.00022700
C	-1.09396100	0.09186700	0.00001600
C	-2.24171400	-0.87647800	-0.00004400
H	-2.19531000	-1.52617600	-0.87755800
H	-2.19542500	-1.52616100	0.87748900
H	-3.20094400	-0.36151100	-0.00011500

1af

C	1.62884700	-1.08425300	-0.44742500
C	1.27341000	0.22007100	-0.10021900
C	2.26570700	1.05397200	0.42000500
C	3.56994800	0.60933400	0.56505900
H	2.00120700	2.05492900	0.73607700
H	4.31994500	1.27268800	0.97648600
C	-0.12034200	0.71173700	-0.26527100
C	-0.35964200	1.97565000	-0.60681600
H	0.45073000	2.66324800	-0.81050400
H	-1.36438000	2.36061500	-0.71203700
C	-1.22103400	-0.29413100	-0.02737400
H	-1.14809700	-1.07839400	-0.78847200
H	-1.02215200	-0.79538000	0.92632400
H	0.88424000	-1.75873100	-0.84888500
C	2.93513200	-1.53024000	-0.30664500
H	3.18902100	-2.54265300	-0.59357200
C	3.91219000	-0.68532200	0.19823900
H	4.92989300	-1.03463300	0.31351400
C	-2.63549500	0.26325100	-0.03265200
H	-2.87421400	0.69650600	-1.00652900
H	-2.73477000	1.06003000	0.70813400
C	-3.65756600	-0.81110300	0.27327600
H	-3.46032200	-1.24020900	1.26319000
H	-3.57892000	-1.61981300	-0.46387800
O	-4.94188800	-0.21642200	0.23034000
H	-5.60400700	-0.88061600	0.43636100

1ag

C	2.09696300	-1.09423700	-0.48123300
C	1.82074300	0.21701900	-0.09101300
C	2.85367700	0.96267400	0.48145700
C	4.12219600	0.42702500	0.63527600
H	2.64873800	1.96637200	0.83130800
H	4.90476100	1.02284900	1.08737900
C	0.46629600	0.80602300	-0.26575100
C	0.32018800	2.09624200	-0.55942300
H	1.17867700	2.73606000	-0.71637200
H	-0.65378300	2.55197000	-0.67084700
C	-0.70324500	-0.13300900	-0.09435700
H	-0.66465100	-0.89098900	-0.88373700
H	-0.56559600	-0.68414100	0.84206800
H	1.31852400	-1.70243300	-0.92227900
C	3.36754300	-1.63118500	-0.33169000
H	3.56037300	-2.64698600	-0.65214000
C	4.38650900	-0.87281400	0.22508600
H	5.37610800	-1.29332500	0.34713500
C	-2.08269300	0.50821000	-0.10915200
H	-2.24514000	1.00790000	-1.06886500

H	-2.13259500	1.28425600	0.66080100
C	-3.18726300	-0.51525100	0.12165500
H	-3.04706100	-1.01279500	1.08488400
H	-3.14897400	-1.29335300	-0.64549500
C	-4.56445500	0.11193500	0.10075100
H	-4.73503200	0.59831200	-0.86756200
H	-4.63182100	0.88241500	0.87860800
O	-5.51786200	-0.91164100	0.32343600
H	-6.39839200	-0.52876700	0.31799000

1ah

C	2.64523700	-1.09980500	-0.48880500
C	2.38179800	0.21021800	-0.08574500
C	3.41610800	0.93285500	0.51309000
C	4.67394800	0.37640100	0.68040300
H	3.22011100	1.93500200	0.87240100
H	5.45764900	0.95463500	1.15292300
C	1.03924400	0.82171300	-0.27434400
C	0.91753800	2.11668600	-0.55781100
H	1.78836300	2.74409300	-0.69608000
H	-0.04750300	2.58866200	-0.67885200
C	-0.14758300	-0.10000800	-0.12835600
H	-0.10980700	-0.85029500	-0.92546100
H	-0.02977300	-0.66319800	0.80391800
H	1.86520100	-1.69004400	-0.95100400
C	3.90517200	-1.65755400	-0.32588600
H	4.08852600	-2.67168900	-0.65709200
C	4.92589100	-0.92181500	0.25745700
H	5.90710500	-1.35855600	0.38982200
C	-1.51620000	0.56315000	-0.15360800
H	-1.66345200	1.07285600	-1.11018500
H	-1.56627500	1.33351500	0.62163400
C	-2.64548100	-0.43880300	0.05634200
H	-2.50347200	-0.94680200	1.01609400
H	-2.58799300	-1.21526600	-0.71407500
C	-4.02210200	0.21143600	0.02230400
H	-4.18143600	0.70689600	-0.93913300
H	-4.09309800	0.98417900	0.79241100
C	-5.13785100	-0.78763700	0.23906700
H	-5.09617800	-1.56281200	-0.53594800
H	-5.01010000	-1.27967200	1.21103800
O	-6.37037300	-0.09130200	0.18688800
H	-7.08918300	-0.71211600	0.32784100

Ligands

L1

C	-0.34933100	0.35207300	0.24825700
C	-1.12560700	1.43621400	-0.14418300
C	-2.49451200	1.25797200	-0.26985700
C	-3.01944900	0.00986100	0.00228000
C	-2.15829400	-1.01542000	0.38820900
N	-0.85402500	-0.85395400	0.50932500
H	-3.13858000	2.07308100	-0.57055600
H	-0.66005100	2.38993100	-0.34270500
H	-2.55031100	-2.00351500	0.60695700
C	3.00760100	1.68800100	0.31620900
C	3.27048300	0.21891800	0.72189400

H	3.52829700	1.99736200	-0.58829800
H	3.22920100	2.39437400	1.11559300
H	3.71693300	0.16819500	1.71882900
O	1.59657100	1.73380700	0.05500300
N	1.92956300	-0.37051300	0.78879800
C	4.18570400	-0.58022700	-0.22998200
C	1.11769100	0.50766800	0.39434600
C	-4.48749800	-0.27867100	-0.12039400
F	-4.73607600	-1.14306400	-1.11221100
F	-5.19667500	0.82546000	-0.36894300
F	-4.97521600	-0.82563500	0.99900800
C	5.56596200	0.07767900	-0.25496700
H	6.24868100	-0.50799500	-0.87320300
H	5.53444200	1.08772100	-0.66884500
H	5.98964000	0.13407000	0.75070100
C	4.31738600	-2.00501000	0.30918900
H	4.75021000	-2.00193800	1.31237600
H	3.34316600	-2.48968200	0.36082900
H	4.97019600	-2.59384600	-0.33829000
C	3.59571600	-0.62413700	-1.63916400
H	2.62540700	-1.12247200	-1.63555200
H	3.46776400	0.37463900	-2.06290500
H	4.26027600	-1.17949100	-2.30350400

L2

C	-0.88879800	0.51252400	0.13334900
C	-1.73307100	1.40083400	-0.52175700
C	-3.08214600	1.09165500	-0.60275100
C	-3.51873200	-0.08619900	-0.02931700
C	-2.59315500	-0.91334800	0.60428400
N	-1.30807400	-0.62509600	0.68747900
H	-3.77786800	1.75340200	-1.10041500
H	-1.33489000	2.30727700	-0.95258300
H	-2.91555700	-1.84350600	1.06111000
C	2.38288800	1.97276300	-0.27883200
C	2.69494400	0.83992100	0.72830500
H	2.78670600	1.75422400	-1.26890600
H	2.70905000	2.95837500	0.04470000
H	2.92070200	1.25521400	1.71575100
O	0.94997600	1.96767300	-0.35990300
N	1.42573500	0.11734900	0.83690200
C	0.55861700	0.81286400	0.24248800
C	-4.95890900	-0.50801200	-0.07721300
F	-5.11557400	-1.63502400	-0.78239300
F	-5.73579100	0.42302500	-0.63650600
F	-5.43981500	-0.74915000	1.14779800
C	3.85379700	-0.02527300	0.30073400
C	5.14521600	0.49203100	0.36687000
C	3.66054100	-1.30809300	-0.19537000
C	6.22833500	-0.25760700	-0.06497300
H	5.30411100	1.48807900	0.76663500
C	4.74661100	-2.06125900	-0.62354900
H	2.65852100	-1.71509100	-0.22785500
C	6.03011800	-1.53916400	-0.56285300
H	7.22746200	0.15463800	-0.00739400
H	4.58728300	-3.06250900	-1.00282200
H	6.87413200	-2.12871800	-0.89626900

L3

C	-1.16580200	0.72755800	0.10915000

C	-2.23750400	1.61660500	0.05588100
C	-3.51757000	1.09734300	0.01639400
C	-3.67220300	-0.27935000	0.02934800
C	-2.54078800	-1.08378000	0.08109700
N	-1.31120500	-0.59353400	0.12109900
H	-4.38307400	1.74700400	-0.02278900
H	-2.05724500	2.68108000	0.04718500
H	-2.63488100	-2.16296300	0.09168000
C	1.73475700	2.87553400	0.01946300
C	2.39657000	1.50841200	0.29140600
H	1.96561200	3.25173500	-0.97992200
H	1.97284800	3.63730800	0.75866500
H	2.84614400	1.47097700	1.28759300
O	0.32737700	2.60227200	0.08256600
N	1.27487500	0.56460900	0.26790100
C	0.22203000	1.24742300	0.15819200
C	-5.05211500	-0.86729900	-0.02287600
F	-5.67201100	-0.55667100	-1.16906300
F	-5.82090900	-0.39753100	0.96785900
F	-5.03943700	-2.19738800	0.07587800
C	3.46444000	1.14165500	-0.74100900
H	4.15861300	1.98168100	-0.82791700
H	2.96835100	1.02759600	-1.70888100
C	4.23014400	-0.10607900	-0.38866800
C	3.64598200	-1.36456300	-0.52180900
C	5.52975200	-0.02070600	0.10131200
C	4.35036600	-2.50734600	-0.17489100
H	2.62781500	-1.43989500	-0.88147400
C	6.23698400	-1.16368600	0.45030800
H	5.99701500	0.95221500	0.20576900
C	5.64786900	-2.41126600	0.31179300
H	3.88337500	-3.47787600	-0.28298700
H	7.24844100	-1.07805700	0.82634900
H	6.19601900	-3.30493900	0.58059500

L4

C	-1.73917900	-0.09845800	-0.54311100
C	-2.26314500	-1.24659700	0.03859600
C	-3.61043800	-1.26469200	0.36583900
C	-4.36391400	-0.13932900	0.09663600
C	-3.74561700	0.96486700	-0.48751400
N	-2.46388300	0.99059400	-0.80031100
H	-4.06313000	-2.13557100	0.81997300
H	-1.62512400	-2.09756000	0.22531400
H	-4.31953700	1.85996400	-0.70498300
C	1.70270600	-0.97480300	-1.16131000
C	1.70381800	0.54439400	-1.55125800
H	1.66384500	-1.57004700	-2.07779400
H	2.08527000	0.65685900	-2.56649500
O	0.42820900	-1.12043600	-0.51292900
N	0.28167300	0.89119000	-1.51853900
C	-0.30309200	-0.04359800	-0.90648100
C	-5.82957700	-0.06771400	0.41483700
F	-6.09911400	0.93796300	1.25567700
F	-6.27575300	-1.19205200	0.98024000
F	-6.55982300	0.14381900	-0.68644100
C	2.51534500	1.42816300	-0.62980000
C	3.89613000	1.49339600	-0.79936500
C	1.93045900	2.12348700	0.42064700
C	4.68232900	2.22277800	0.07720700
H	4.35968500	0.95575000	-1.61900500

C	2.71719000	2.86003700	1.29801500
H	0.85524300	2.10125400	0.54297600
C	4.09292300	2.90694000	1.13327900
H	5.75481300	2.25953500	-0.06349300
H	2.24999000	3.40168400	2.11047600
H	4.70426200	3.47992800	1.81825100
C	2.82016300	-1.46103400	-0.29188400
C	3.91825000	-2.07776000	-0.87817100
C	2.81478100	-1.23872000	1.08158900
C	5.01008200	-2.45413300	-0.10736900
H	3.92085400	-2.26323600	-1.94662700
C	3.90037000	-1.62108100	1.85292800
H	1.95935000	-0.75975500	1.54015500
C	5.00295500	-2.22455800	1.26016400
H	5.86106400	-2.93245800	-0.57457400
H	3.88946600	-1.44307800	2.92035600
H	5.85071500	-2.51935200	1.86471200

L5

C	1.71058900	0.04608500	0.06198500
C	2.31509500	-0.96007800	-0.68188000
C	3.70001000	-0.99865000	-0.73703500
C	4.40901800	-0.03235100	-0.05137700
C	3.71054100	0.93796100	0.66523400
N	2.39303400	0.97996000	0.72488800
H	4.21531800	-1.76341700	-1.30198200
H	1.70910800	-1.68825600	-1.20010500
H	4.24891100	1.70709000	1.20980400
C	-1.81615400	-0.48874300	-0.49800400
C	-1.84736200	0.57209500	0.64104900
H	-2.06275300	-0.01199400	-1.45074900
H	-2.16519700	0.09748000	1.57585800
O	-0.42565100	-0.85374100	-0.54624600
N	-0.44499800	0.95863200	0.79456800
C	0.23241000	0.11577500	0.14613400
C	5.91001300	0.00538400	-0.05381500
F	6.36988800	1.15961800	-0.55110000
F	6.43535700	-0.98177000	-0.78365300
F	6.40447100	-0.10554500	1.18478300
C	-2.77927400	1.71397300	0.33705500
C	-4.14769800	1.54631100	0.53295100
C	-2.30715100	2.91064600	-0.18860600
C	-5.03451500	2.55874800	0.19722000
H	-4.51718900	0.61809500	0.95523800
C	-3.19494400	3.92596700	-0.51833000
H	-1.24096700	3.04654000	-0.31703100
C	-4.55888300	3.75185100	-0.33058000
H	-6.09616000	2.41992100	0.35606800
H	-2.81849800	4.85862600	-0.91850300
H	-5.24865000	4.54556100	-0.58641900
C	-2.69381100	-1.68182900	-0.27226900
C	-3.91972100	-1.77022100	-0.92095800
C	-2.32482900	-2.67486500	0.63061600
C	-4.77400300	-2.83489400	-0.66524100
H	-4.20664400	-0.99944600	-1.62704900
C	-3.17265200	-3.74301100	0.87795500
H	-1.36536200	-2.61213900	1.12944400
C	-4.40095100	-3.82363800	0.23294100
H	-5.72688800	-2.89489400	-1.17474500
H	-2.87576500	-4.51534400	1.57560600
H	-5.06211200	-4.65785800	0.42779500

L6

C	-2.12711700	0.94025900	0.09711000
C	-3.35968300	1.58669600	0.07121200
C	-4.50655000	0.81347300	0.03612300
C	-4.37153300	-0.56373900	0.02397400
C	-3.09510500	-1.11612600	0.04728400
N	-1.99450600	-0.38362300	0.08331500
H	-5.48741800	1.27020200	0.01145900
H	-3.40447400	2.66546900	0.07737200
H	-2.96385300	-2.19196500	0.03018900
C	0.26279800	3.64523300	0.02540500
C	1.19644400	2.44109100	0.26676700
H	0.39945100	4.07773100	-0.96855000
H	0.34581800	4.42749800	0.77680200
O	-1.05632900	3.08444800	0.09410400
N	0.29598000	1.28499100	0.23158000
C	-0.87699300	1.73595800	0.14363800
C	-5.58588300	-1.44632300	0.02627300
F	-5.33043500	-2.64858500	-0.49545600
F	-6.58852300	-0.90624400	-0.67530800
F	-6.04514500	-1.64586600	1.26872100
C	2.30499700	2.31637300	-0.78054500
H	1.83266300	2.11890900	-1.74619300
H	2.81556600	3.28008900	-0.85796200
H	1.65438800	2.48011300	1.25925000
C	3.30373200	1.24016900	-0.44886700
C	3.02926900	-0.08053000	-0.68559500
C	4.53635500	1.58673200	0.15751900
C	3.95198800	-1.09621400	-0.34225700
H	2.07966400	-0.36256700	-1.12543900
C	5.44920200	0.63067000	0.50041200
H	4.75458800	2.63238500	0.34387300
C	3.67896100	-2.46616900	-0.58056500
C	5.18493000	-0.73824600	0.25962200
H	6.39076200	0.90900900	0.95890100
C	4.58692200	-3.42807700	-0.24139100
H	2.73277900	-2.73488500	-1.03466100
C	6.10734200	-1.75793600	0.59940000
C	5.81721000	-3.06991500	0.35538000
H	4.36765400	-4.47157900	-0.42696300
H	7.04805000	-1.47729800	1.05835200
H	6.52790800	-3.84228000	0.61946000

L7

C	1.17700100	0.30047200	-0.20174100
C	1.98623900	1.30086700	0.32355900
C	3.34864200	1.06469800	0.42358600
C	3.83363400	-0.15603300	-0.00248000
C	2.94122900	-1.09635000	-0.51404700
N	1.64371100	-0.87807400	-0.61489500
H	4.01750900	1.81379800	0.82488900
H	1.55016900	2.23563900	0.64268600
H	3.30180400	-2.06203300	-0.85386400
C	-2.17389200	1.63435100	0.13926600
C	-2.41431100	0.40016100	-0.78369100
H	-2.59217500	0.75591300	-1.80577700
O	-0.72199800	1.73009900	0.10509600
N	-1.12663200	-0.29695300	-0.78712500
C	-0.28416600	0.52105100	-0.32379300
C	5.29251700	-0.50241100	0.07043800

F	5.50290600	-1.57624400	0.84133100
F	6.02152200	0.49787200	0.57209400
F	5.78887300	-0.79229800	-1.13814800
C	-3.57585400	-0.47035900	-0.38419800
C	-4.87010500	-0.08716000	-0.72494100
C	-3.38690300	-1.63104800	0.35659000
C	-5.96143600	-0.83778200	-0.31287800
H	-5.02415600	0.80111200	-1.32812700
C	-4.47772600	-2.38606500	0.76540600
H	-2.37808400	-1.94475900	0.59310000
C	-5.76678500	-1.98920300	0.43809600
H	-6.96245900	-0.52982200	-0.58617000
H	-4.31949000	-3.29111200	1.33775200
H	-6.61561500	-2.58021400	0.75643000
C	-2.75522800	2.91928300	-0.40643900
H	-3.84386400	2.84682500	-0.42867500
H	-2.48192400	3.76391600	0.22663200
H	-2.39368500	3.10516400	-1.41769300
C	-2.56780300	1.39705400	1.58667400
H	-2.20985500	2.22478400	2.19910300
H	-3.65107700	1.32364800	1.68270300
H	-2.13068900	0.46840700	1.95644400