

Auxiliary-assisted palladium-catalyzed halogenation of C(sp³)-H bonds at room temperature

SUPPORTING INFORMATION

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I. Materials and Methods

All commercial materials (Alfa Aesar, Aladdin, J&K Chemical LTD.) were used without further purification. All solvents were analytical grade. The ^1H -NMR and ^{13}C -NMR spectra were recorded on a Bruker 400 MHz spectrometer in CD_3OD , DMSO-d_6 or CDCl_3 using TMS or solvent peak as a standard. All ^{13}C -NMR spectra were recorded with complete proton decoupling. Low-resolution mass spectral analyses were performed with a Waters AQUITY UPLCTM/MS. All reactions were carried out in oven-dried sealed tube. Analytical TLC was performed on Yantai Chemical Industry Research Institute silica gel 60 F254 plates and flash column chromatography was performed on Qingdao Haiyang Chemical Co. Ltd silica gel 60 (200-300 mesh). The rotavapor was BUCHI's Rotavapor R-3.

II. Density functional theory (DFT) calculation

1,computational details:

All the calculations were carried out with the Gaussian 09 package.¹ Geometry optimizations were performed with B3LYP². LANL2DZ+f (1.472 for Pd) basis set³ with effective core potential (ECP) was used for metal centers, and the 6-31G (d) basis set⁴ was used for other atoms. Frequency was calculated at the same level of theory to obtain zero-point energy (ZPE) corrections and to verify the stationary points to be minima. Because the M06⁵ functional includes noncovalent interactions and gives refined energies for organo transition metal systems, single-point energies were conducted by using M06/SDD⁶-6-311++G(d,p)⁷. Solvation effects were evaluated with SMD solvation model.⁸ Acetic acid was chosen as the solvent. The relative energies with ZPE corrections and free energies (at 298.15K) are in kcal/mol.

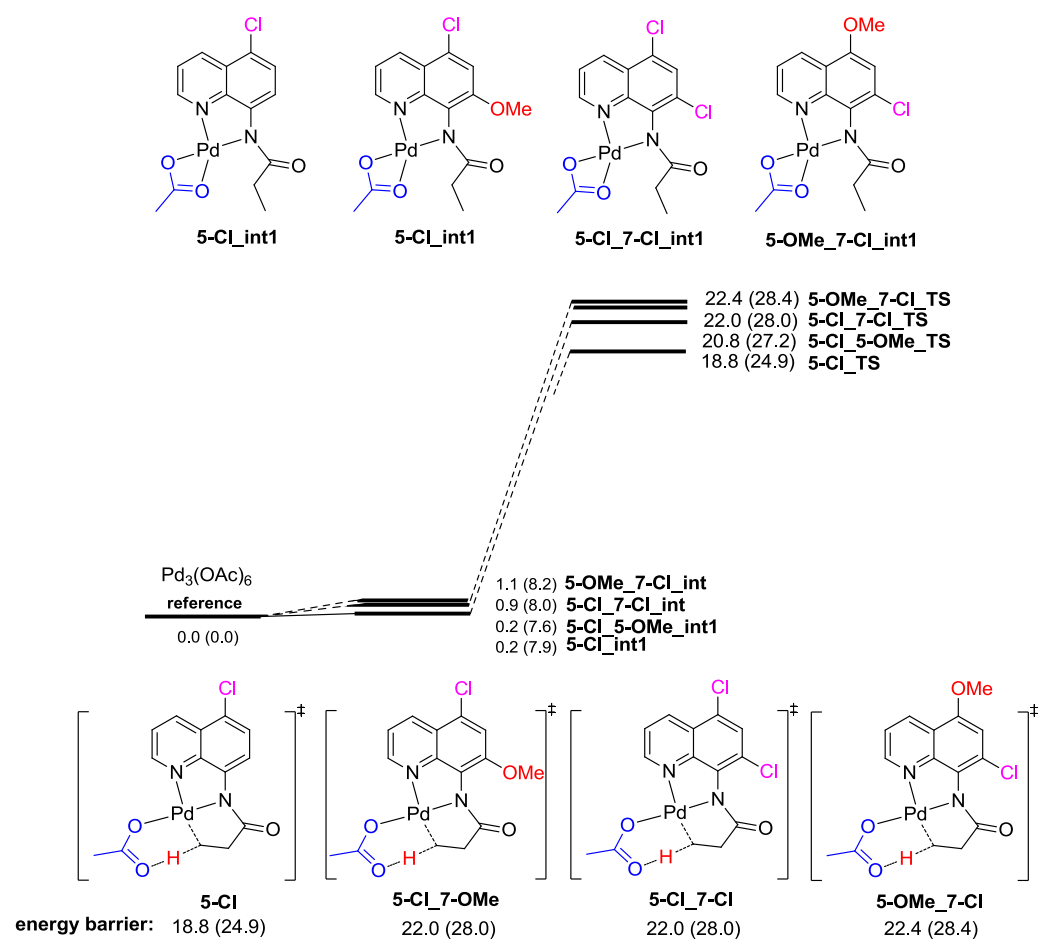


Figure S1. Potential energy surface (free energies and electronic energies in parentheses) and energy barriers for the Pd catalyzed C-H activation with different kinds of bidentate directing groups (in kcal/mol).

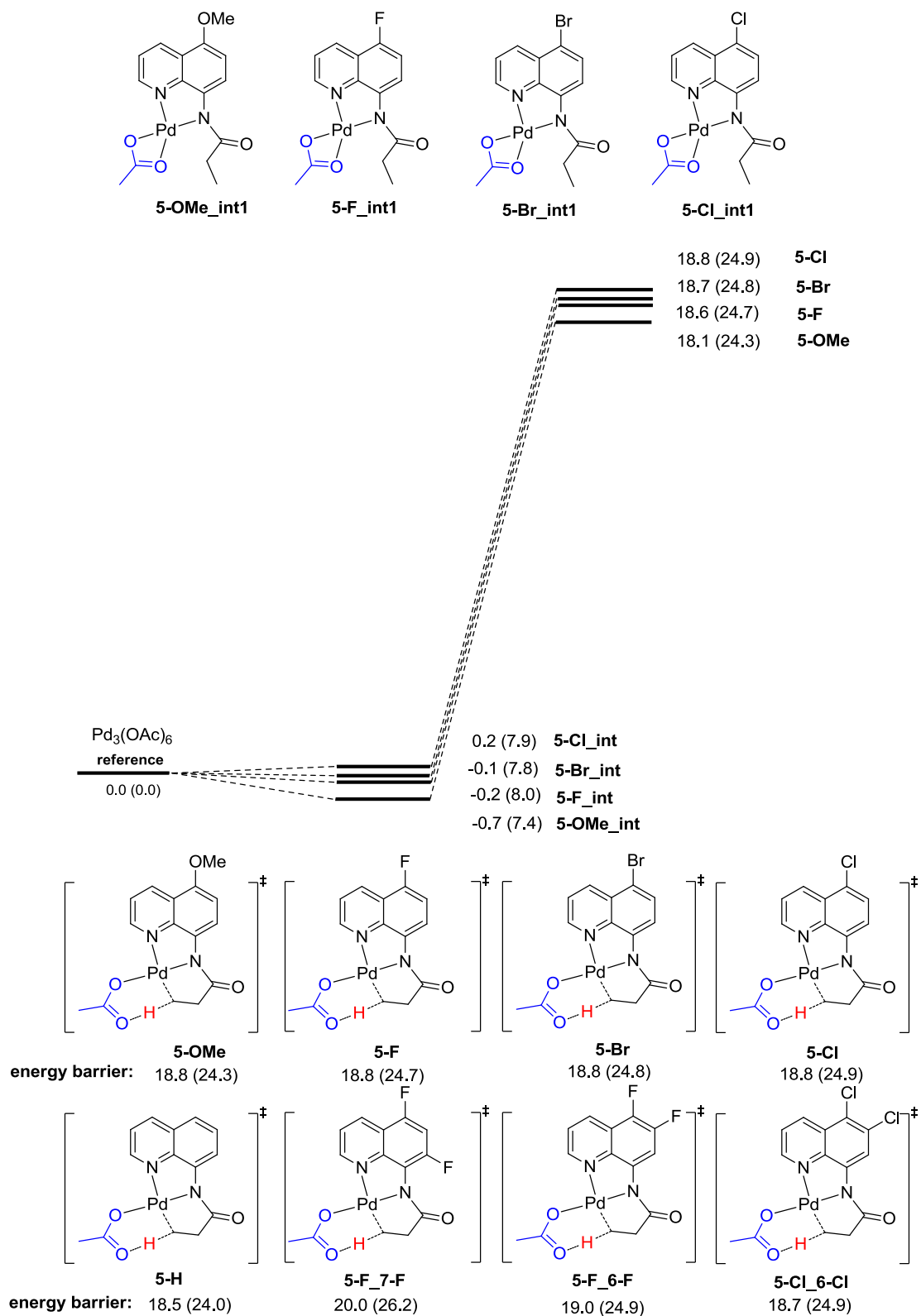
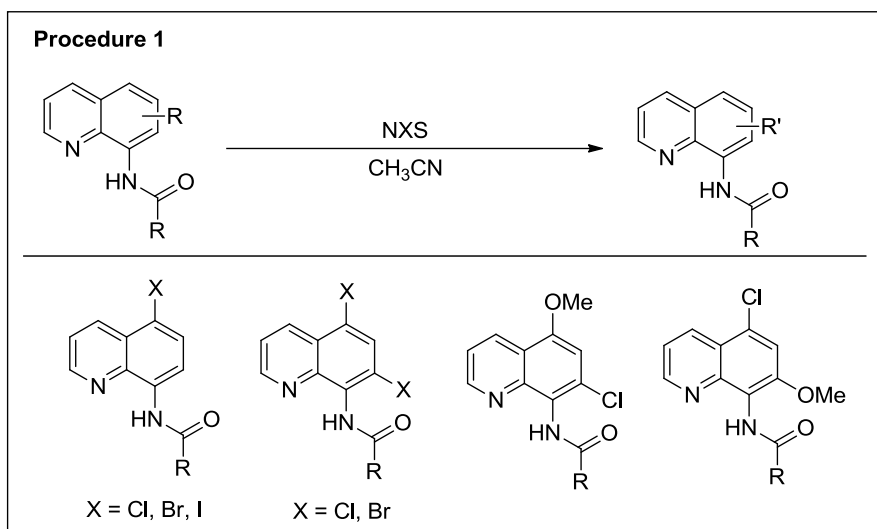


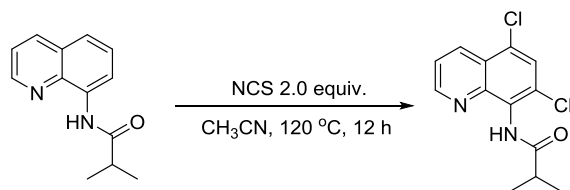
Figure S2. Potential energy surface (free energies and electronic energies in parentheses) and energy barriers for the Pd catalyzed C(sp³)-H activation with different substituent pattern directing groups (in kcal/mol).

II. Directing groups synthesis and screening

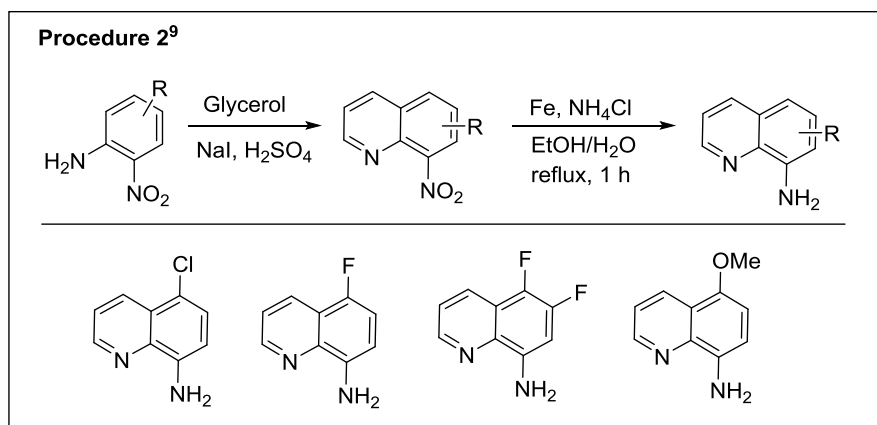
a) Different directing groups were synthesized by following procedures.

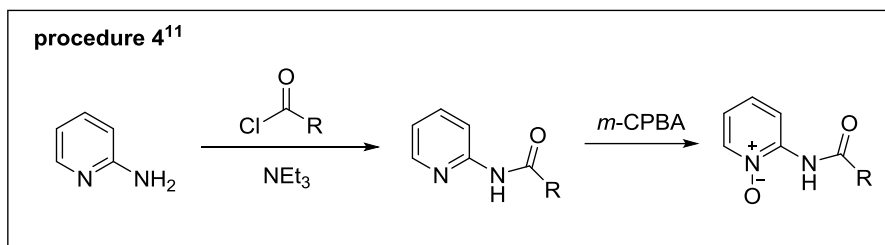
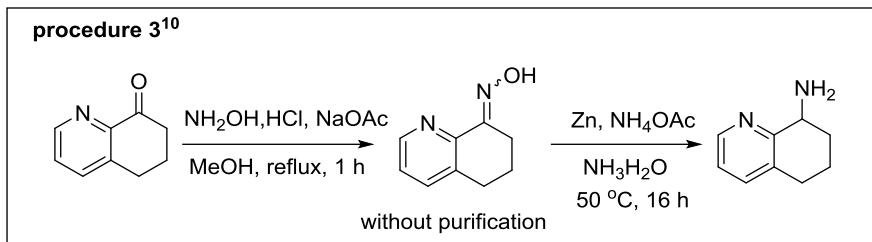


Example



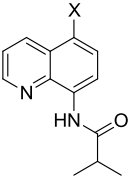
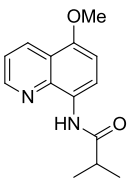
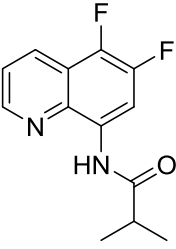
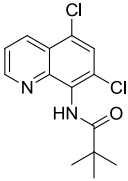
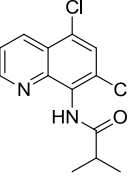
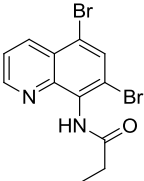
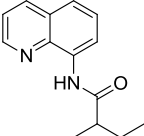
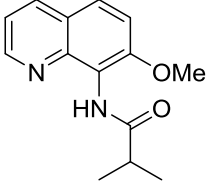
To a 10 mL sealed tube were added N-(quinolin-8-yl)isobutyramide (214 mg, 1.0 mmol), NCS (267 mg, 2.0 mmol) and CH_3CN (4 mL). The tube was sealed and heated at 120 °C for 12 h. The reaction mixture was cooled to RT, H_2O was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography (Petroleum ether:Ethylacetate = 2:1) to give the desired product.

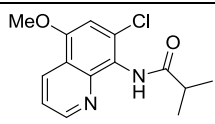
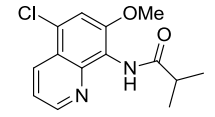




b) Halogenation reactivity of different directing groups

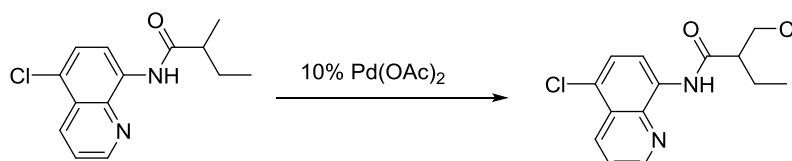
substrates	Conditions ^a Pd(OAc) ₂ 10%	Halogenated Products (NMR yield)
	NCS 2.0 eq, AcOH, 80 °C, 3.5 h	Cl trace
	NCS 2.0 eq, AcOH, rt, 12 h, 50 °C, 1 h	NR
	NBS 2.0 eq, AcOH, 80 °C, 6 h	NR
	NBS 2.0 eq, AcOH, 80 °C, 12 h	Br 20%
	NCS 2.0 eq, CH ₃ CN, 80 °C, 12 h	Mono-Cl 15%; di-Cl 11%
	NCS 1.5 eq, AcOH (2.5eq), DCE, 80 °C, 12 h	Mono-Cl 24%
	Cl-1 1.5 eq, AcOH (2.5 eq), DCE, 80 °C, 12 h	Mono-Cl 20%
	NCS 2.0 eq, AcOH, 80 °C, 12 h	Mono-Cl 40%; di-Cl 20%
	NCS 2.0 eq, AcOH, 120 °C, 2 h	Cl 28%

 <p>X = Cl, Br, I</p>	NIS (2.0 eq), AcOH, 25 °C, 48 h	I 60%
	NCS 1.1 eq, AcOH, 25 °C, 24 h	Mono-Cl 32%; di-Cl 25%
	NIS 1.1 eq, AcOH, 25 °C, 24 h	I trace
	NCS 2.0eq, AcOH, 50 °C, 2.5 h	Cl, Conversion ratio: Mono-Cl 20%; di-Cl 70%
	NCS 2.0 eq, AcOH, 80 °C, 3 h	Tri-Cl 36%; Di-Cl 16%; Mono-Cl 15%
	NBS 3.0 eq, AcOH, 80 °C, 10 h	Br 10%
	NCS 2.0 eq, AcOH, 80 °C, 15 h	Cl Mono 14%
	NCS 3.0 eq, AcOH, 80 °C, 12 h	Cl trace
	NBS 3.0 eq, AcOH, 80 °C, 12 h	Br trace
	NBS 2.0 eq, AcOH, rt, 24 h	Br 50%
	NCS 2.0 eq, AcOH, 25 °C, 14 h	Trace

	NBS 2.0 eq, AcOH, 25 °C, 12 h	trace
	NCS (2.0eq), AcOH, rt, 24 h	trace

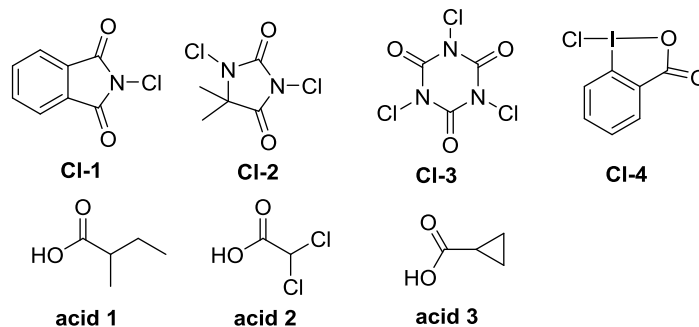
- a. Reaction was carried out following General procedure for Pd-catalyzed C(sp³)-H halogenation reaction

II. Optimization of reaction conditions



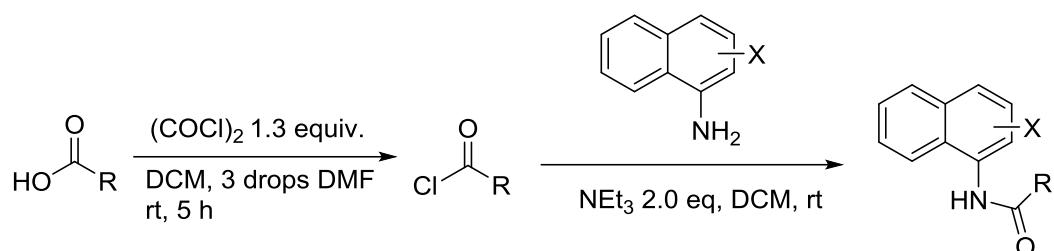
Entry	conditions	NMR yield(%) ^a
1	NCS 1.5 eq, TFA , 50 °C, 3.5 h	7
2	NCS 1.5 eq, CH ₃ CN , 50 °C, 3.5 h	9
3	NCS 1.5 eq, AcOH/Ac ₂ O, 50 °C, 3.5 h	55
4	NCS 1.5 eq, AcOH/CH ₃ CN, 50 °C, 3.5 h	55
5	NCS 1.5 eq, propanoic acid, 35 °C, 8 h	65
6	NCS 1.5 eq, AcOH/DCE, 50 °C, 3.5 h	17
7	Cl-1 2.0 eq, AcOH, 50 °C, 3.5 h	38
8	Cl-2 2.0 eq, AcOH, 50 °C, 3.5 h	28
9	Cl-3 2.0 eq, AcOH, 50 °C, 3.5 h	NR ^b
10	Cl-4 2.0 eq, AcOH, 50 °C, 3.5 h	NR ^b
11	NCS 1.5 eq, AcOH, 50 °C, 3.5 h	67
12	NCS 2.0 eq, AcOH, 50 °C, 5 h	57(54 ^c)
13	NCS 2.0 eq, AcOH, RT, 35 h	71(70 ^c)(77 ^{c,d})
14	NCS 1.5 eq, AcOH, RT, 35 h	75
15	NCS 1.5 eq, acid 1, 35 °C, 8 h	62
16	NCS 1.5 eq, acid 2, 35 °C, 8 h	18
17	NCS 1.5 eq, acid 3, 35 °C, 8 h	68

a. 0.1mmol scale, less than 10% methylene C-H chlorination was observed by H-NMR b, chlorination happens at sp² position c. isolated yield d. 0.5mmol scale



IV. Substrates preparation

General procedure 1

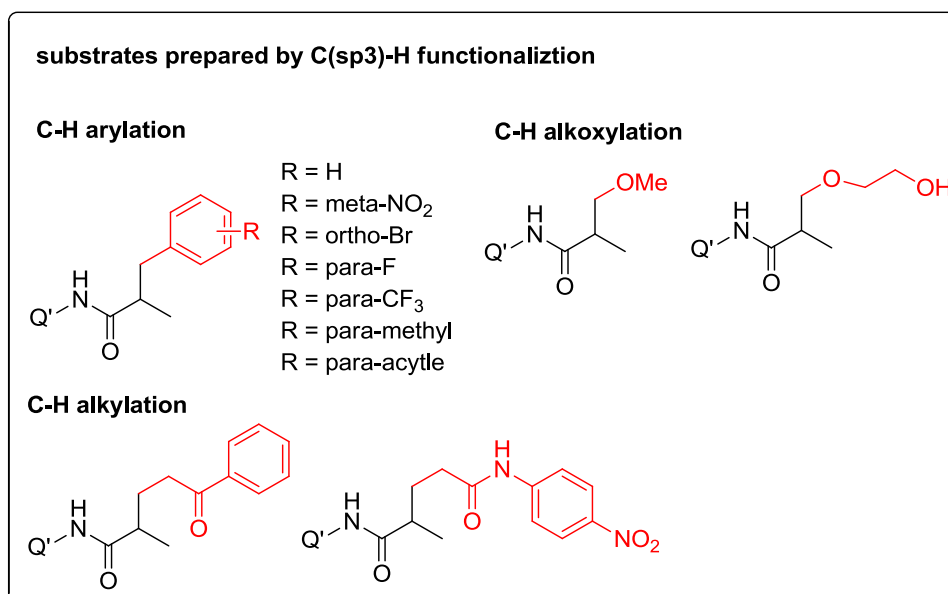


To a solution of the acid in DCM, 1.3 equiv. of oxalyl chloride and 1-2 drops of DMF were added. The mixture was allowed to stir at rt for 5 h. Then the mixture was concentrated to remove the solvent and excess oxalyl chloride to afford the crude acyl chloride, which was subsequently dissolved in DCM followed by addition of 1.0 equiv of directing group and 2.0 equiv of Et_3N in ice-water bath. The mixture was stirred for 5 h (monitored by TLC). Then water was added to quench the reaction. The reaction mixture was extracted with DCM for 3 times. The combined organic layer was dried over Na_2SO_4 . After filtration and concentration, the residue was purified by column chromatography to afford the pure compound, which was confirmed by NMR and LC-MS analysis.

General procedure 2



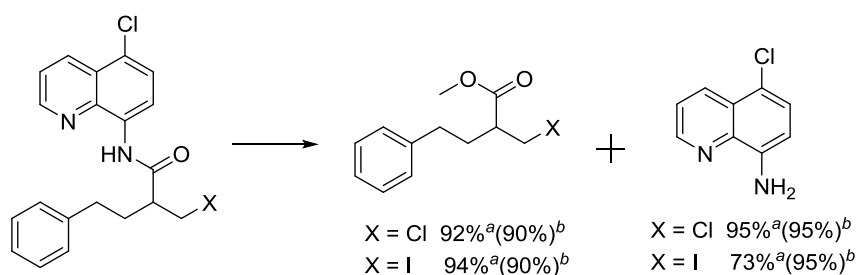
Referring to recent published papers¹², Pd-catalyzed $\text{C}(\text{sp}^3)\text{-H}$ functionalization methods were applied with isobutyric acid derivative as substrate.



V. General procedure for Pd-catalyzed C(sp³)-H halogenation reaction

To a 10ml round bottom flask were added amide (1.0 equiv.), Pd(OAc)₂ (0.1 equiv.), NXS (1.0-4.0 equiv.) and AcOH. The reaction was stirred at rt for 12-48 h or 50 °C for 1-4 h and monitored by TLC. Water was added to dilute the reaction mixture and NaHCO₃ was added to neutralize the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography to give the desired product.

VI. General procedure for Directing Group Removing

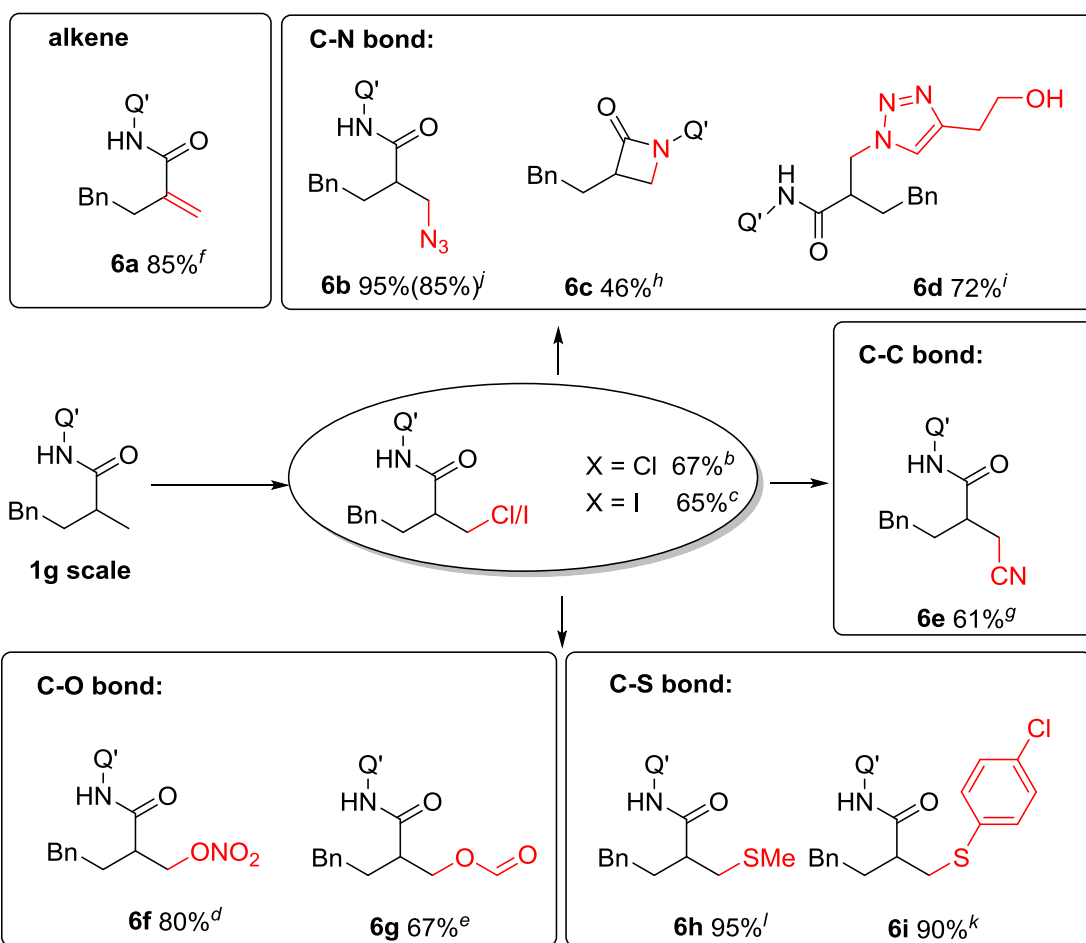


condition a: BF₃.Et₂O 5 equiv., MeOH, 100 °C, 24 h

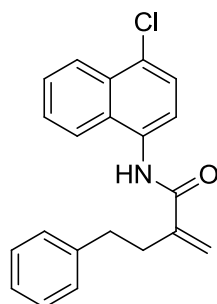
condition b: con.H₂SO₄ 5 equiv., MeOH, 100 °C, 20 h

To a 10 mL sealed tube were added halogenated product (1.0 equiv.), BF₃.Et₂O (5.0 equiv.) or concentrated H₂SO₄ (5.0 equiv.) and MeOH (2 mL) were added. The tube was sealed and heated at 100 °C for 20-24 h. The reaction mixture was cooled to RT, H₂O was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography to give the desired product.

VII. Product transformation

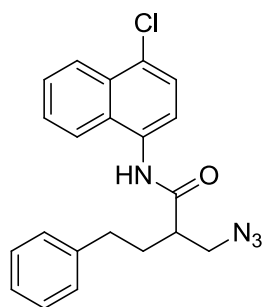


a) isolated yield. b) 10% mol Pd(OAc)₂, 2.0equiv NCS, AcOH, rt, 48h c) 10% mol Pd(OAc)₂, 2.0equiv NCS, AcOH, rt, 22h d) 2.0equiv AgNO₃, 2.0equiv Cu(OAc)₂, EtOH, rt, 0.5h e) 4.0equiv AgSCF₃, DMF, 100°C, 1.5h f) 5.0equiv NaN₃, DMF, rt, 1h g) 2.0equiv CuCN, 2.0equiv Cu(OAc)₂, DMF, 100°C, 1.5h h) 2.0equiv NaSMe, DMF, rt, 0.5h i) 2.0equiv NaN₃, 2.0equiv Cu(OAc)₂, DMF, rt, 0.5h then 20% mol CuI, 40% mol L-ascorbate, 1.5 equiv K₂CO₃, 1.5equiv. but-3-yn-1-ol, MeOH/H₂O, rt, 3h j) 2.0equiv NaN₃, 2.0equiv Cu(OAc)₂, DMF, rt, 0.5h k) 5.0 equiv 4-chlorobenzenethiol, DMF, 100 °C, 5 h l) 2.0equiv NaSMe, EtOH, rt, 0.5h



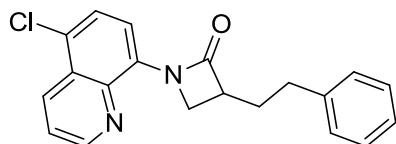
To a 10 ml round bottom flask were added I-substrate (0.1 mmol, 46.3 mg), NaN₃ (0.5 mmol, 32.5 mg), and DMF(0.5 mL). The reaction was stirred at rt for 1 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 15:1).

Finally, compound **6a** (28 mg, white solid) was isolated in 85% yield.

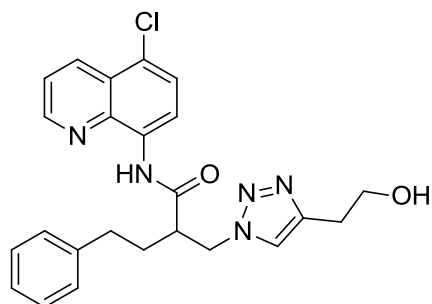


To a 10 ml round bottom flask were added iodinated substrate (0.1 mmol, 46.3 mg), NaN_3 (0.2 mmol, 13 mg), $\text{Cu}(\text{OAc})_2$ (0.2 mmol, 36 mg) and DMF(0.5 mL). The reaction was stirred at rt for 1 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 15:1). Finally, compound **6b** (36 mg, colorless oil) was isolated in 95% yield.

To a 10 ml round bottom flask were added chlorinated substrate (0.1 mmol, 37 mg), NaN_3 (0.2 mmol, 13 mg), $\text{Cu}(\text{OAc})_2$ (0.2 mmol, 36 mg) and DMF(0.5 mL). The reaction was stirred at 80 °C for 2.5 h. The reaction mixture was cooled to room temperature and water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 15:1). Finally, compound **6b** (32 mg, colorless oil) was isolated in 85% yield.

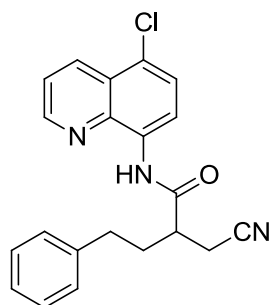


To a 10 ml round bottom flask were added iodinated substrate (0.1 mmol, 46.3 mg), NaSMe (15 wt% in H_2O) (0.1 mmol, 48 mg), and DMF (1 mL). The reaction was stirred at rt for 0.5 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 25:1). Finally, compound **6c** (15 mg,) was isolated in 46% yield.



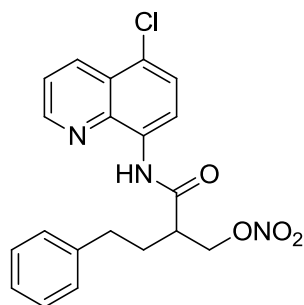
To a 10 ml round bottom flask were added iodinated substrate (0.1 mmol, 46.3 mg), NaN_3 (0.2 mmol, 13 mg), $\text{Cu}(\text{OAc})_2$ (0.2 mmol, 36 mg) and DMF(0.5 mL). The reaction was stirred at rt for 1 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM

for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. To the residue was added CuI (0.02 mmol, 3.8 mg), L-ascorbate (0.04 mmol, 7.9 mg), K_2CO_3 (0.15 mmol, 21 mg), but-3-yn-1-ol (0.15 mmol, 11.4 μL) and $\text{MeOH}/\text{H}_2\text{O}$ (0.5 ml / 0.5 ml). The reaction was stirred at rt for 3 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue purified by silical gel column chromatography (DCM:MeOH = 20:1). Finally, compound **6d** (32 mg, yellow oil) was isolated in 72% yield.

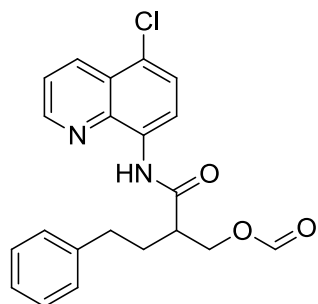


To a 10 ml round bottom flask were added iodinated substrate (0.05 mmol, 23 mg), CuCN (0.2 mmol, 13 mg), $\text{Cu}(\text{OAc})_2$ (0.2 mmol, 36 mg) and DMF (0.5 mL). The reaction was stirred at rt for 1 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 15:1). Finally, compound **6e** (10.6 mg, yellow oil) was isolated in 56% yield.

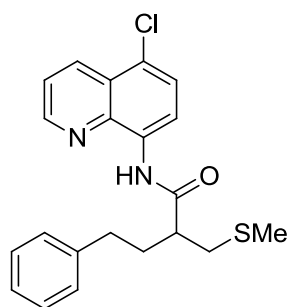
To a 10 ml round bottom flask were added chlorinated substrate (0.1 mmol, 37 mg), NaN_3 (0.2 mmol, 13 mg), $\text{Cu}(\text{OAc})_2$ (0.2 mmol, 36 mg) and DMF (0.5 mL). The reaction was stirred at 80 $^\circ\text{C}$ for 2.5 h. The reaction mixture was cooled to room temperature and water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 5:1). Finally, compound **6e** (11 mg, yellow oil) was isolated in 61% yield.



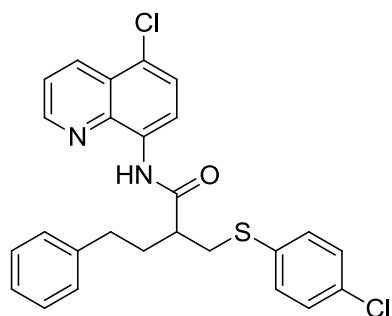
To a 10 ml round bottom flask were added iodinated substrate (0.05 mmol, 23 mg), AgNO_3 (0.1 mmol, 17 mg), $\text{Cu}(\text{OAc})_2$ (0.1 mmol, 18 mg) and EtOH (0.5 mL). The reaction was stirred at rt for 0.5 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 10:1). Finally, compound **6f** (16 mg) was isolated in 80% yield.



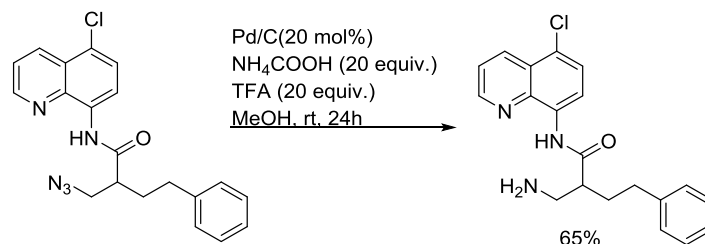
To a 10 ml round bottom flask were added iodinated substrate (0.05 mmol, 23 mg), AgSCF_3 (0.2 mmol, 42 mg), and DMF (1 mL). The reaction was stirred at 100 °C for 1.5 h. The reaction mixture was cooled to room temperature and water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 10:1). Finally, compound **6g** (13 mg, colorless oil) was isolated in 67% yield.



To a 10ml round bottom flask were added iodinated substrate (0.05 mmol, 23 mg), NaSMe (15 wt% in H_2O) (0.1 mmol, 48 mg), and EtOH (2 mL).. The reaction was stirred at rt for 0.5 h. Water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 10:1). Finally, compound **6h** (18 mg,) was isolated in 95% yield.



To a 10 ml round bottom flask were added iodinated substrate (0.05 mmol, 23 mg), 4-chlorobenzenethiol (0.25 mmol, 36 mg), and DMF (1 mL). The reaction was stirred at 100 °C for 5 h. The reaction mixture was cooled to room temperature and water was added to dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 20:1). Finally, compound **6i** (22 mg, colorless oil) was isolated in 90% yield.



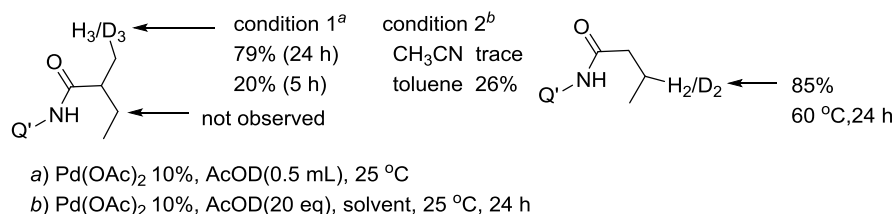
To a 10ml round bottom flask were added 6b (0.05 mmol, 19 mg), Pd/C (20%, 3.8 mg), NH₄COOH (1.0 mmol, 63 mg) and MeOH (1 mL). The reaction was stirred at rt for 24 h. The reaction mixture was filtrated and the filter liquor was concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (DCM:MeOH = 20:1). Finally, compound **6i** (11 mg, colorless oil) was isolated in 65% yield.

To a 10 ml round bottom flask were added 6b (0.05 mmol, 19 mg), Pd/C (20%, 3.8 mg), NH₄COOH (1.0 mmol, 63 mg) and MeOH (1 mL). The reaction was stirred at rt for 24 h. The reaction mixture was filtrated and the filter liquor was concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (DCM:MeOH = 20:1). Finally, compound **6i** (11 mg, colorless oil) was isolated in 65% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.17 (s, 1H), 8.86-8.85 (m, 1H), 8.73 (d, *J* = 8.4 Hz, 1H), 8.56 (d, *J* = 8.4 Hz, H), 7.61-7.56 (m, 2H), 7.28-7.18 (m, 5H), 3.16-3.14 (m, 1H), 3.03-3.01 (m, 1H), 2.78-2.65 (m, 3H), 2.51 (br, 2H), 2.20-2.19 (m, 1H), 1.91-1.90 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 173.7, 148.9, 141.5, 139.3, 133.9, 133.5, 128.6, 127.3, 126.2, 126.1, 122.5, 117.0, 50.8, 44.5, 33.7, 32.1; LRMS (ESI) calcd for C₂₀H₂₀ClN₃O [M+H]⁺: 354.13, found 354.07

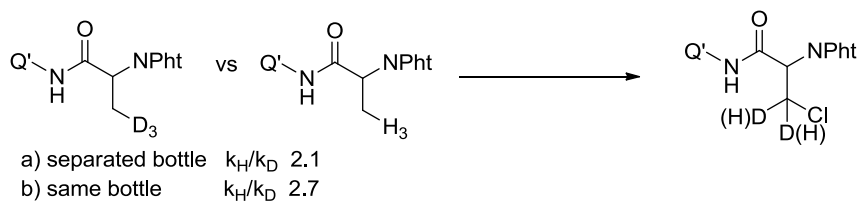
VIII. Mechanism study

a) General procedure for substrate deuteration studies at room temperature



To a 10 ml round bottom flask were added amide (1.0 equiv.), Pd(OAc)₂ (10%) and solvent system (0.5 mL). The reaction was stirred at 25-60 °C for 5-24 h. Water was added to dilute the reaction mixture and NaHCO₃ was added to neutralize the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography to give the desired product. Deuteration ratio was analyzed by ¹H-NMR.

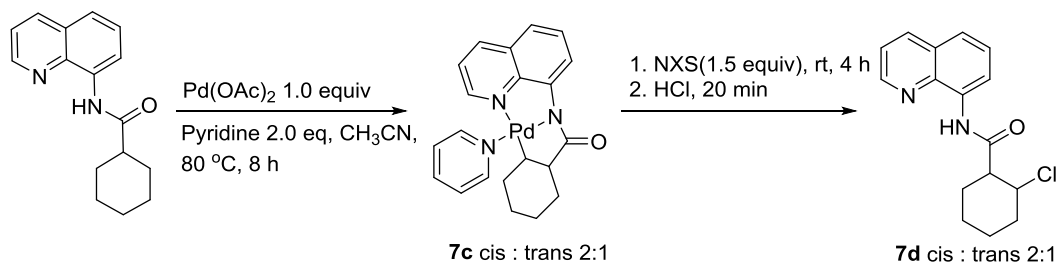
b) KIE study



N-(5-chloroquinolin-8-yl)-2-(1,3-dioxisoindolin-2-yl)propanamide and its deuterated analogue (0.05 mmol) were added to two 10 ml round bottom flasks separately followed by NCS (13.3 mg, 0.1 mmol), Pd(OAc)₂ (1.1 mg, 0.005 mmol) and AcOH (0.5 ml). The reaction mixture was stirred for 3 h. Water was added to dilute the reaction mixture and NaHCO₃ was added to neutralize the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography. 3-chloro-N-(5-chloroquinolin-8-yl)-2-(1,3-dioxisoindolin-2-yl)propanamide and deuterated analogue was obtained in 45% and 21% NMR yield with p-nitrobenzaldehyde as internal standard. ¹H-NMR shows $k_H/k_D = 2.1:1$.

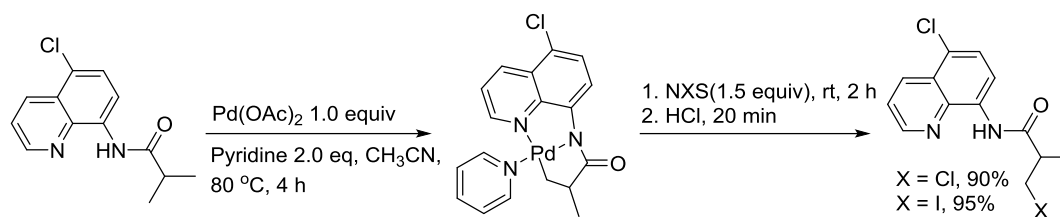
N-(5-chloroquinolin-8-yl)-2-(1,3-dioxisoindolin-2-yl)propanamide and its deuterated analogue (0.05 mmol) were added to 10ml round bottom flask followed by NCS (13.3 mg, 0.1 mmol), Pd(OAc)₂ (1.1 mg, 0.005 mmol) and AcOH (0.5 ml). The reaction mixture was stirred for 3h. Water was added to dilute the reaction mixture and NaHCO₃ was added to neutralize the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography. ¹H-NMR shows $k_H/k_D = 2.77:1$

c) Synthesis and reactivity of cyclopalladium



To a 15 ml sealed-tube were added N-(quinolin-8-yl)cyclohexanecarboxamide (127 mg, 0.50 mmol), Pd(OAc)₂(112 mg, 0.5 mmol), pyridine (80 ul, 1.0 mmol) and CH₃CN(4 mL). The reaction mixture was stirred at 60 °C for 12 h. The reaction mixture was cooled to RT and filtrated to get yellow solid, filtrate was concentrated on rotavapor under reduced pressure and purified by silica gel column chromatography (Petroleum ether: Ethyl acetate = 1:2), two portions were combined affording 192 mg (88%,yellow solid) of **7c**.

To a 5 ml round bottom flask were added palladium complex (44 mg, 0.1 mmol), NCS (16 mg, 0.12 mmol) and CH₃CN (1 mL). The mixture was stirred at rt for 4 h. Concentrated HCl (0.5 mL) was added and the mixture was stirred for another 20 min to remove the palladium. Dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to wash the reaction mixture. Then the organic layer was dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. The residue was purified by silical gel column chromatography (Petroleum ether:Ethylacetate = 15:1). Finally, compound **7d(cis)** (17 mg, colourless oil) and **7d(cis)** (8 mg, colourless oil) was isolated in 90% yield.



To a 15 ml sealed-tube were added N-(5-chloroquinolin-8-yl)isobutyramide (124 mg, 0.5 mmol), Pd(OAc)₂ (112 mg, 0.5 mmol), pyridine (80 μ L, 1.0 mmol) and CH₃CN (5 ml). The tube was sealed and heated at 80 °C for 4 h. The reaction mixture was cooled to RT and concentrated on rotavapor under reduced pressure. Then the palladium complexes were purified by silica gel column chromatography (Ethylacetate). Finally, complex (**7e**) (18 mg, yellow solid) was isolated in 95% yield.

To a 5 ml round bottom flask were added palladium complex (22 mg, 0.05 mmol), NCS (10 mg, 0.075 mmol) and CH₃CN (1 mL). The mixture was stirred at rt for 2 h. Concentrated HCl (0.5 mL) was added and the mixture was stirred for another 20 min to remove the palladium. Dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to wash the reaction mixture. Then the organic layer was dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. The residue was purified by silica gel column chromatography (Petroleum ether:Ethylacetate = 15:1). Finally, compound (**3c1**) (13 mg, white solid) was isolated in 90% yield.

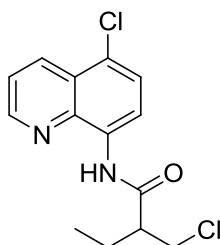
To a 5 ml round bottom flask were added palladium complex (22 mg, 0.05 mmol), NIS (17 mg, 0.075 mmol) and CH₃CN (1 mL). The mixture was stirred at rt for 2 h. Concentrated HCl (0.5 mL) was added and the mixture was stirred for another 20 min to remove the palladium. Dichloromethane was added to dilute the reaction mixture and saturated aqueous NaHCO₃ was added to wash the reaction mixture. Then the organic layer was dried over anhydrous Na₂SO₄ and concentrated on rotavapor under reduced pressure. The residue was purified by silica gel column chromatography (Petroleum ether:Ethylacetate = 15:1). Finally, compound (**7f**) (18 mg, white solid) was isolated in 95% yield.

IX Reference

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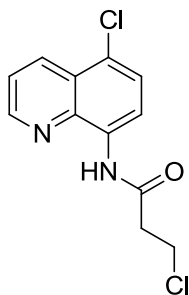
XI. Date of products



2-(chloromethyl)-N-(5-chloroquinolin-8-yl)butanamide (**2**)

Following the general procedure, substrate (132 mg, 0.50 mmol), NCS (133 mg, 1.0 mmol), Pd(OAc)₂ (11 mg, 0.05 mmol) and 5 ml AcOH were used. The reaction mixture was stirred at rt for 35 h. After completion of the reaction, the residue was purified by silical gel column chromatography (petroleum ether: ethyl acetate = 15:1). Finally, compound (**2**) (111 mg, white solid) was isolated in 75% yield.

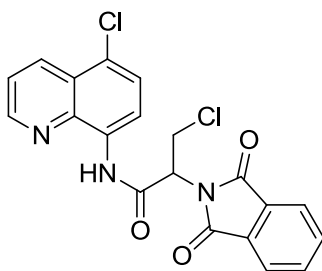
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.91 (s, 1H), 8.83 (d, *J* = 4.2 Hz, 1H), 8.75 (d, *J* = 8.4 Hz, 1H), 8.52 (d, *J* = 8.5 Hz, 1H), 7.59-7.52 (m, 2H), 3.90 (t, *J* = 10.5 Hz, 1H), 3.70-3.67 (m, 1H), 2.84-2.77 (m, 1H), 1.93-1.71 (m, 2H), 1.05 (t, *J* = 7.5 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.45, 148.85, 139.01, 133.44, 127.23, 125.97, 124.73, 122.47, 116.71, 53.19, 44.99, 24.35, 11.76; LRMS (ESI) calcd for C₁₄H₁₄Cl₂N₂O [M+H]⁺: 297.05, found 297.38



3-Chloro-N-(5-chloroquinolin-8-yl)propanamide (**3a**)

Following the general procedure, substrate (23.4 mg, 0.10 mmol), NCS (33 mg, 0.25 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate=15: 1). Finally, compound (**3a**) (14 mg, white solid) was isolated in 52% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.84 (s, 1H), 8.84 (t, *J* = 1.2 Hz, 1H), 8.71 (d, *J* = 8.4 Hz, 1H), 8.55 (d, *J* = 8.5 Hz, 1H), 7.60-7.55 (m, 2H), 3.95 (t, *J* = 6.6 Hz, 2H), 3.03 (t, *J* = 6.5 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 168.06, 148.84, 138.92, 133.55, 133.47, 127.30, 126.03, 124.79, 122.53, 116.72, 40.98, 39.76; LRMS (ESI) calcd for C₁₂H₁₀Cl₂N₂O [M+H]⁺: 269.02, found 269.49



3-Chloro-N-(5-chloroquinolin-8-yl)-2-(1,3-dioxoisindolin-2-yl)propanamide (**3b**)

Following the general procedure, substrate (38 mg, 0.10 mmol), NCS (27 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 36 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 3: 1). Finally, compound (**3b**) (35 mg, white solid) was isolated in 85% yield.

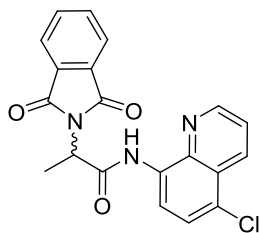
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.28 (s, 1H), 8.64-8.60 (m, 2H), 8.51 (dd, *J* = 8.5 Hz, *J* = 1.4 Hz, 1H), 7.95 (dd, *J* = 5.4 Hz, *J* = 3.1 Hz, 2H), 7.81 (dd, *J* = 5.4 Hz, *J* = 3.1 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.51-7.48 (m, 1H), 5.41-5.38 (m, 1H), 4.56-4.45 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 167.68, 164.44, 149.08, 139.02, 134.77, 133.51, 132.76, 131.67, 127.15, 125.99, 125.42, 124.11, 122.57, 116.94, 56.24, 41.16; LRMS (ESI) calcd for C₂₀H₁₃Cl₂N₃O₃ [M+H]⁺: 414.03, found 413.92

Chiral HPLC Data

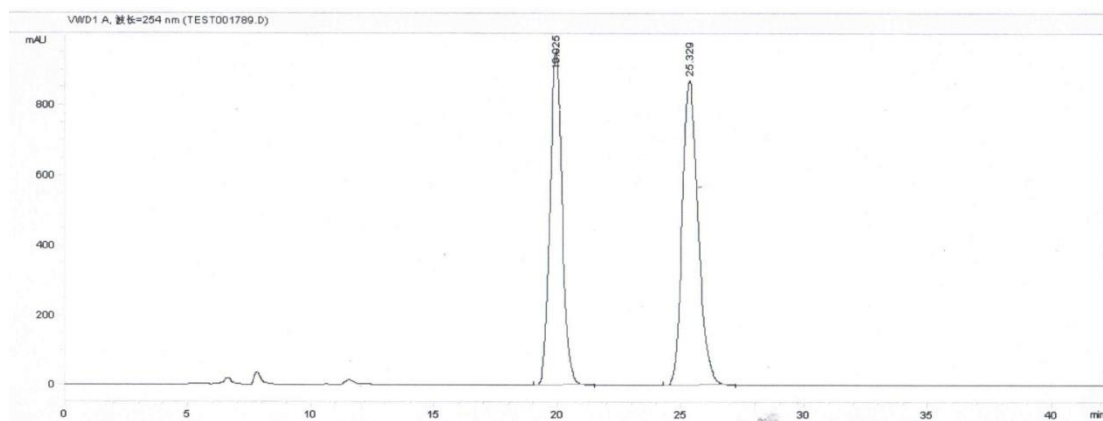
HPLC Conditions:

Chiral stationary phase: CHIRALPAK[®] AD-H, *n*-hexane/isopropanol = 50:50, 0.60 mL/min

Signal: VWD1 A, Wavelength = 254 nm

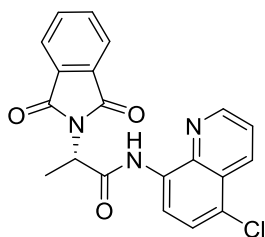


DL-Starting material

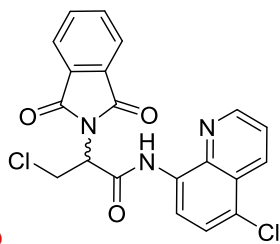
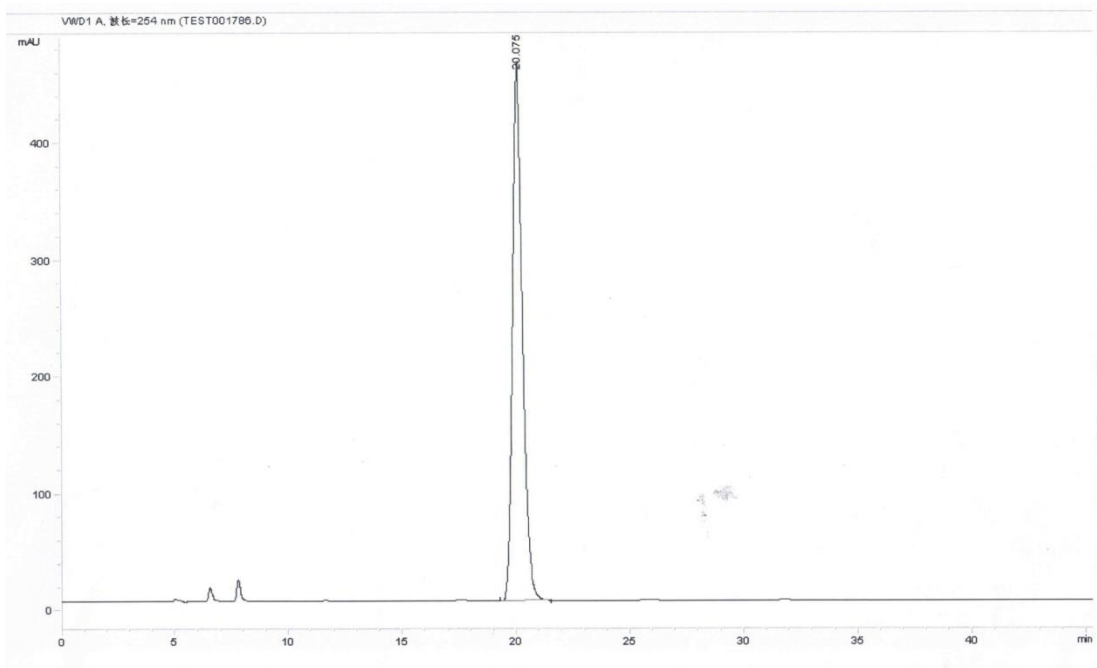


Area% report for DL- Starting material:

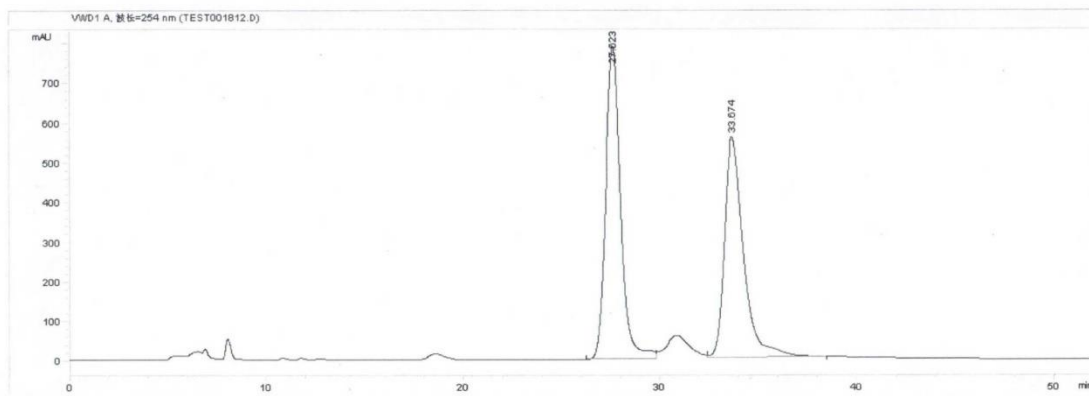
Retention Time (min)	Area	Area %	Height	Symmetry Factor
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25.329	39240.3	54.406	869.2	0.769



L- Starting material

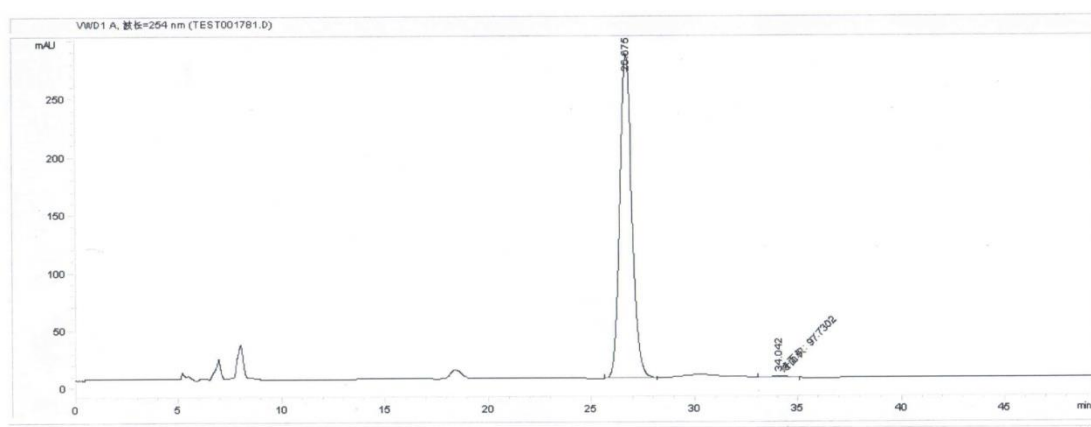
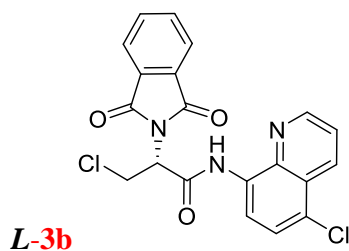


DL-3b



Area% report for DL-3b:

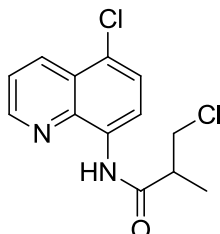
Retention Time (min)	Area	Area %	Height	Symmetry Factor
27.623	41356.2	52.533	786.5	0.913
33.674	37367.7	47.467	557.5	0.640



Area% report for L-3b:

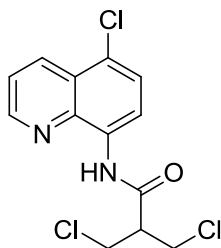
Retention Time (min)	Area	Area %	Height	Symmetry Factor
26.675	11598.3	99.164	279.7	0.925
34.042	97.7	0.836	1.7	0.992

3-Chloro-N-(5-chloroquinolin-8-yl)-2-methylpropanamide (3c1)



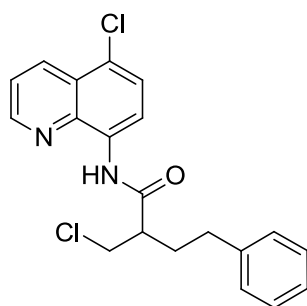
Following the general procedure, substrate (50 mg, 0.2 mmol), NCS (80 mg, 0.6 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 25 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate =20: 1). Finally, compound (**3c1**) (14 mg, white solid) and compound (**3c2**) (32mg, white solid)was isolated in 25% yield and 50% yield respectively.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.95 (s, 1H), 8.86 (dd, *J* = 4.2 Hz, *J* = 1.5 Hz, 1H), 8.74 (d, *J* = 8.4 Hz, 1H), 8.58 (dd, *J* = 8.5 Hz, *J* = 1.5 Hz, 1H), 7.62-7.57 (m, 2H), 3.94-3.89 (m, 1H), 3.70-3.65 (m, 1H), 3.03-3.00 (m, 1H), 1.45 (d, *J* = 7.0 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.91, 148.91, 139.14, 133.61, 127.35, 126.10, 124.82, 122.55, 116.79, 46.49, 45.65, 16.35; LRMS (ESI) calcd for C₁₃H₁₂Cl₂N₂O [M+H]⁺: 283.03, found 283.52



3-Chloro-2-(chloromethyl)-N-(5-chloroquinolin-8-yl)propanamide (3c2)

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 10.06 (s, 1H), 8.87 (dd, $J = 4.2$ Hz, $J = 1.4$ Hz, 1H), 8.72 (d, $J = 8.4$ Hz, 1H), 8.58 (dd, $J = 8.5$ Hz, $J = 1.4$ Hz, 1H), 7.62-7.58 (m, 2H), 4.00-3.95 (m, 2H), 3.90-3.86 (m, 2H), 3.30-3.23 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 168.14, 149.06, 139.08, 133.64, 133.14, 127.26, 126.11, 125.34, 122.67, 117.01, 53.31, 42.77; LRMS (ESI) calcd for $\text{C}_{13}\text{H}_{11}\text{Cl}_3\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 316.99, found 316.94



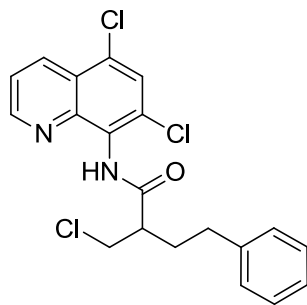
2-(chloromethyl)-N-(5-chloroquinolin-8-yl)-4-phenylbutanamide (3d1)

Following the general procedure, substrate (135.2 mg, 0.4 mmol), NCS (80 mg, 0.6 mmol), $\text{Pd}(\text{OAc})_2$ (9 mg, 0.04 mmol) and 4 ml AcOH were used. The reaction mixture was stirred at rt for 24h. After completion of the reaction, the residue was purified by silical gel column chromatography (toluene: petroleum ether = 3:1-5:1). Finally, compound (**3d1**) (100 mg, yellow solid) was isolated in 68% yield.

3.0mmol scale

Following the general procedure, substrate (1014 mg, 3.0 mmol), NCS (801 mg, 6.0 mmol), $\text{Pd}(\text{OAc})_2$ (67 mg, 0.3 mmol) and 10 ml AcOH were used. The reaction mixture was stirred at rt for 48h. After completion of the reaction, the residue was purified by silical gel column chromatography (toluene: petroleum ether = 3:1-5:1). Finally, compound (**3d1**) (446 mg, white solid) and compound (**3d2**) (330mg, white solid) were isolated in 40% and 27% yield.

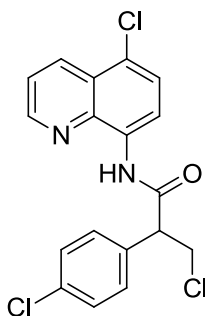
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.92 (s, 1H), 8.87 (d, $J = 3.9$ Hz, 1H), 8.78 (d, $J = 8.4$ Hz, 1H), 8.58 (d, $J = 8.5$ Hz, 1H), 7.63-7.58 (m, 2H), 7.30-7.20 (m, 5H), 3.91 (t, $J = 10.1$ Hz, 1H), 3.69-3.65 (m, 1H), 2.89-2.78 (m, 2H), 2.73-2.65 (m, 1H), 2.24-2.17 (m, 1H), 2.06-2.00 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 171.22, 148.91, 140.77, 139.11, 133.56, 133.42, 128.71, 128.60, 127.32, 126.39, 126.09, 124.92, 122.57, 116.87, 50.91, 45.38, 33.32, 32.63; LRMS (ESI) calcd for $\text{C}_{20}\text{H}_{19}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 373.08, found 372.93



2-(chloromethyl)-N-(5,7-dichloroquinolin-8-yl)-4-phenylbutanamide (3d2)

0.1mmol scale

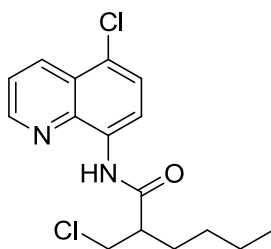
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 8.88-8.87 (m, 1H), 8.49-8.46 (m, 1H), 8.41 (s, 1H), 7.67 (s, 1H), 7.52-7.49 (m, 1H), 7.34-7.31 (m, 4H), 7.26-7.21 (m, 1H), 3.95-3.90 (m, 1H), 3.69-3.65 (m, 1H), 2.97-2.93 (m, 2H), 2.86-2.81 (m, 1H), 2.24-2.19 (m, 1H), 2.09-2.03 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 171.01, 150.96, 143.74, 141.30, 133.26, 130.83, 130.55, 129.33, 128.67, 128.63, 128.29, 126.29, 125.21, 122.42, 49.81, 45.29, 33.06, 32.66, 29.81; LRMS (ESI) calcd for $\text{C}_{20}\text{H}_{18}\text{Cl}_3\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 409.04, found 408.90



3-Chloro-2-(4-chlorophenyl)-N-(5-chloroquinolin-8-yl)propanamide (3e)

Following the general procedure, substrate (33 mg, 0.10 mmol), NCS (16 mg, 0.12 mmol), $\text{Pd}(\text{OAc})_2$ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 30 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 3: 1). Finally, compound (3e) (20 mg, yellow solid) was isolated in 55% yield.

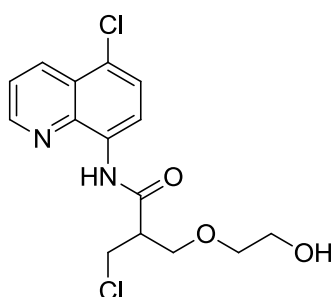
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.87 (s, 1H), 8.80 (t, $J = 2.4$ Hz, 1H), 8.70 (d, $J = 8.5$ Hz, 1H), 8.54 (d, $J = 8.5$ Hz, 1H), 7.59-7.57 (m, 2H), 7.44 (d, $J = 7.0$ Hz, 2H), 7.37 (d, $J = 7.0$ Hz, 2H), 4.31 (t, $J = 10.5$ Hz, 1H), 4.07 (t, $J = 6.7$ Hz, 1H), 3.80 (dd, $J = 10.8$ Hz, $J = 6.4$ Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 168.75, 148.94, 138.98, 134.99, 134.56, 133.58, 133.34, 129.54, 129.52, 127.23, 126.04, 125.08, 122.57, 116.73, 56.49, 45.07; LRMS (ESI) calcd for $\text{C}_{18}\text{H}_{13}\text{Cl}_3\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 379.01, found 378.93



2-(Chloromethyl)-N-(5-chloroquinolin-8-yl)hexanamide (**3f**)

Following the general procedure, substrate (35 mg, 0.12 mmol), NCS (32 mg, 0.24 mmol), Pd(OAc)₂ (2.7 mg, 0.012 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 27 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1 - 5: 1). Finally, compound (**3f**) (35 mg, colorless oil) was isolated in 90% yield.

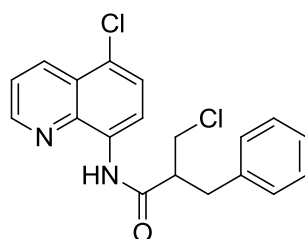
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.91 (s, 1H), 8.85 (d, *J* = 3.9 Hz, 1H), 8.75 (d, *J* = 8.4 Hz, 1H), 8.54 (d, *J* = 8.5 Hz, 1H), 7.60-7.54 (m, 2H), 3.92-3.87 (m, 1H), 3.68 (dd, *J* = 10.8 Hz, *J* = 5.0 Hz, 1H), 2.88-2.83 (m, 1H), 1.87-1.80 (m, 1H), 1.72-1.67 (m, 1H), 1.39-1.25 (m, 4H), 0.88 (t, *J* = 7.1 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.63, 148.87, 139.04, 133.46, 127.26, 126.00, 124.74, 122.48, 116.74, 51.81, 45.34, 30.92, 29.41, 22.74, 13.94; LRMS (ESI) calcd for C₁₆H₁₉Cl₂N₂O [M+H]⁺: 325.08, found 325.47



3-Chloro-N-(5-chloroquinolin-8-yl)-2-((2-hydroxyethoxy)methyl)propanamide (**3g**)

Following the general procedure, substrate (31 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 2: 1). Finally, compound (**3g**) (19 mg) was isolated in 56% yield.

¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.90-8.88 (m, 1H), 8.65 (d, *J* = 8.4 Hz, 1H), 8.60-8.58 (m, 1H), 7.64-7.55 (m, 2H), 3.93-3.90 (m, 4H), 3.82-3.80 (m, 2H), 3.71-3.68 (m, 2H), 3.25-3.19 (m, 1H); ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 169.97, 148.73, 138.79, 133.09, 132.87, 126.39, 125.59, 124.55, 122.11, 116.67, 72.49, 68.96, 60.52, 49.77, 41.38; LRMS (ESI) calcd for C₁₅H₁₆Cl₂N₂O₃ [M+H]⁺: 343.05, found 343.35.

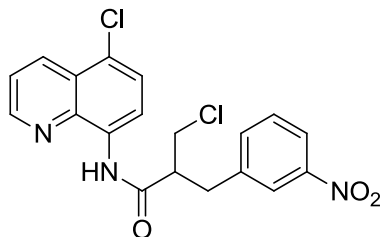


2-Benzyl-3-chloro-N-(5-chloroquinolin-8-yl)propanamide (**3h**)

Following the general procedure, substrate (32,4 mg, 0.10 mmol), NCS (16 mg, 1.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2ml ACOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1). Finally, compound (**3h**) (18 mg, yellow oil) was isolated in 50% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.73 (s, 1H), 8.77 (t, *J* = 1.3 Hz, 1H), 8.72 (d, *J* = 8.4 Hz, 1H),

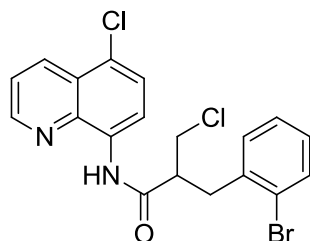
8.53 (dd, $J = 8.5$ Hz, $J = 1.3$ Hz, 1H), 7.58 (d, $J = 8.4$ Hz, 1H), 7.54-7.51 (m, 1H), 7.25-7.24 (m, 4H), 7.17-7.15 (m, 1H), 3.94-3.89 (m, 1H), 3.71 (dd, $J = 10.9$ Hz, $J = 4.5$ Hz, 1H), 3.17-3.04 (m, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 170.71, 148.77, 139.00, 137.89, 133.44, 133.35, 129.06, 128.87, 127.26, 126.97, 125.97, 124.82, 122.47, 116.75, 53.38, 44.75, 37.07; LRMS (ESI) calcd for $\text{C}_{19}\text{H}_{17}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 359.06, found 358.95



3-Chloro-N-(5-chloroquinolin-8-yl)-2-(3-nitrobenzyl)propanamide (**3i**)

Following the general procedure, substrate (37 mg, 0.10 mmol), NCS (20 mg, 0.15 mmol), $\text{Pd}(\text{OAc})_2$ (2.2 mg, 0.01 mmol) and 2ml ACOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 10: 1). Finally, compound (**3i**) (27 mg, white solid) was isolated in 67% yield.

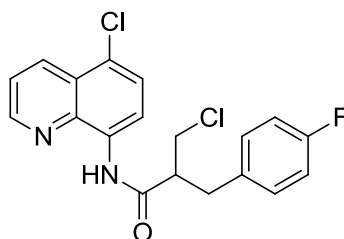
^1H -NMR (400 MHz, $(\text{CD}_3)_2\text{SO}$) δ (ppm) 10.38 (s, 1H), 8.96 (d, $J = 3.4$ Hz, 1H), 8.57 (t, $J = 8.4$ Hz, 1H), 8.25 (s, 1H), 8.09 (d, $J = 8.1$ Hz, 1H), 7.79-7.73 (m, 3H), 7.52 (t, $J = 7.9$ Hz, 1H), 3.92-3.88 (m, 1H), 3.83-3.80 (m, 1H), 3.74-3.70 (m, 1H), 3.16-3.05 (m, 2H); ^{13}C -NMR (100 MHz, $(\text{CD}_3)_2\text{SO}$) δ (ppm) 170.81, 149.57, 147.77, 140.52, 138.93, 135.98, 133.77, 132.77, 129.67, 126.93, 125.27, 123.72, 123.56, 123.23, 121.45, 117.51, 49.86, 45.02, 35.74; LRMS (ESI) calcd for $\text{C}_{19}\text{H}_{15}\text{Cl}_2\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 404.05, found 403.88



2-(2-Bromobenzyl)-3-chloro-N-(5-chloroquinolin-8-yl)propanamide (**3j**)

Following the general procedure, substrate (41 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), $\text{Pd}(\text{OAc})_2$ (3.4 mg, 0.015 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 10: 1). Finally, compound (**3j**) (26.5 mg) was isolated in 61% yield.

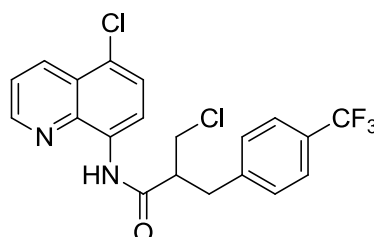
^1H -NMR (400 MHz, CDCl_3) δ (ppm) 9.80 (s, 1H), 8.80-8.79 (m, 1H), 8.72 (d, $J = 8.2$ Hz, 1H), 8.55-8.53 (m, 1H), 7.60-7.54 (m, 3H), 7.26-7.25 (m, 1H), 7.16-7.12 (m, 1H), 7.05-7.01 (m, 1H), 3.99-3.94 (m, 1H), 3.73-3.71 (m, 1H), 3.32-3.14 (m, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 170.43, 148.85, 139.08, 137.43, 133.45, 133.32, 131.66, 128.84, 127.81, 127.27, 126.02, 124.87, 124.70, 122.48, 116.80, 51.14, 44.46, 37.70; LRMS (ESI) calcd for $\text{C}_{19}\text{H}_{15}\text{BrCl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 436.97, found 437.65



3-Chloro-N-(5-chloroquinolin-8-yl)-2-(4-fluorobenzyl)propanamide (**3k**)

Following the general procedure, substrate (34 mg, 0.10 mmol), NCS (27 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 40 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 10: 1). Finally, compound (**3k**) (23 mg, white solid) was isolated in 62% yield.

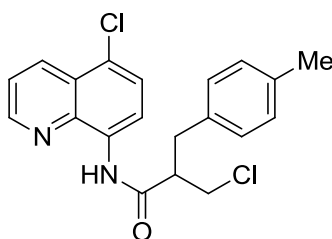
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.68 (s, 1H), 8.78-8.76 (m, 1H), 8.69 (d, *J* = 8.4 Hz, 1H), 8.54 (dd, *J* = 8.5 Hz, *J* = 1.4 Hz, 1H), 7.60-7.53 (m, 2H), 7.22-7.19 (m, 2H), 6.91 (t, *J* = 8.6 Hz, 2H), 3.94-3.89 (m, 1H), 3.72-3.69 (m, 1H), 3.12-3.04 (m, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.45, 161.97 (d, *J*_{C-F} = 244 Hz), 148.82, 139.01, 133.68, 133.57 (d, *J*_{C-F} = 14 Hz), 133.27, 130.57 (d, *J*_{C-F} = 8 Hz), 127.26, 126.04, 124.96, 122.52, 116.80, 115.82, 115.61, 53.57, 44.70, 36.25; LRMS (ESI) calcd for C₁₉H₁₅Cl₂FN₂O [M+H]⁺: 377.05, found 376.93



3-Chloro-N-(5-chloroquinolin-8-yl)-2-(4-(trifluoromethyl)benzyl)propanamide (**3l**)

Following the general procedure, substrate (40 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), Pd(OAc)₂ (3.4 mg, 0.015 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 6: 1). Finally, compound (**3l**) (36 mg) was isolated in 85% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.64 (s, 1H), 8.72-8.66 (m, 2H), 8.51 (d, *J* = 8.4 Hz, 1H), 7.58-7.46 (m, 4H), 7.36 (d, *J* = 7.9 Hz, 2H), 3.96-3.92 (m, 1H), 3.75-3.71 (m, 1H), 3.22-3.13 (m, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.04, 148.80, 142.14, 138.85, 133.42, 133.04, 129.42, 129.28 (q, *J*_{C-F} = 32 Hz), 127.15, 125.94, 125.77 (q, *J*_{C-F} = 4 Hz), 125.04, 124.17 (q, *J*_{C-F} = 271 Hz), 122.50, 116.75, 53.16, 44.67, 36.75; LRMS (ESI) calcd for C₂₀H₁₅Cl₂F₃N₂O [M+H]⁺: 427.05, found 427.03.

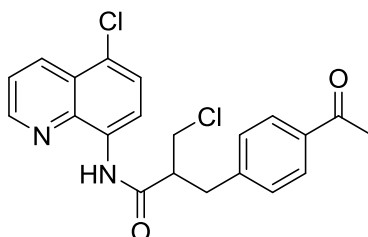


3-Chloro-N-(5-chloroquinolin-8-yl)-2-(4-methylbenzyl)propanamide (**3m**)

Following the general procedure, substrate (34 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), Pd(OAc)₂ (3.4 mg, 0.015 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 36 h.

After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 6: 1). Finally, compound (**3m**) (19 mg) was isolated in 51% yield.

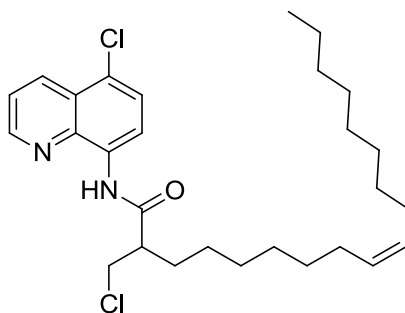
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.74 (s, 1H), 8.79-8.78 (m, 1H), 8.72 (d, *J* = 8.3 Hz, 1H), 8.56-8.54 (m, 1H), 7.61-7.54 (m, 2H), 7.13 (d, *J* = 7.6 Hz, 2H), 7.05 (d, *J* = 7.6 Hz, 2H), 3.93-3.88 (m, 1H), 3.71-3.68 (m, 1H), 3.15-3.11 (m, 2H), 3.04-2.97 (m, 1H), 2.24 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.82, 148.71, 139.02, 136.49, 134.73, 133.43, 133.41, 129.52, 128.91, 127.27, 125.97, 124.76, 122.42, 116.75, 53.43, 44.72, 36.65, 21.11; LRMS (ESI) calcd for C₂₀H₁₈Cl₂N₂O [M+H]⁺: 373.08, found 373.03.



2-(4-acetylbenzyl)-3-chloro-N-(5-chloroquinolin-8-yl)propanamide (**3n**)

Following the general procedure, substrate (37 mg, 0.10 mmol), NCS (54 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: ethyl acetate= 10: 1). Finally, compound (**3n**) (20 mg, yellow oil) was isolated in 50% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.74 (s, 1H), 8.79-8.78 (m, 1H), 8.72 (d, *J* = 8.4 Hz, 1H), 8.55-8.53 (m, 1H), 7.60-7.53 (m, 2H), 7.13 (d, *J* = 7.9 Hz, 2H), 7.05 (d, *J* = 7.9 Hz, 2H), 3.93-3.88 (m, 1H), 3.72-3.68 (m, 1H), 3.16-3.08 (m, 2H), 3.04-2.97 (m, 1H), 2.24 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 197.8, 170.5, 148.9, 143.7, 139.0, 136.0, 133.6, 133.1, 129.4, 129.0, 127.3, 126.1, 125.1, 122.6, 116.9, 53.7, 40.0, 26.7, 5.0; LRMS (ESI) calcd for C₂₁H₁₈Cl₂N₂O₂ [M+H]⁺: 401.07, found 401.13.

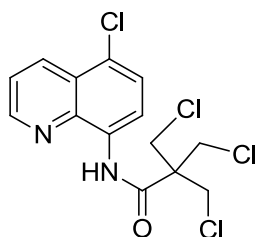


(Z)-2-(chloromethyl)-N-(5-chloroquinolin-8-yl)octadec-9-enamide (**3o**)

Following the general procedure, substrate (30 mg, 0.067 mmol), NCS (18 mg, 0.134 mmol), Pd(OAc)₂ (1.5 mg, 0.007 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 24 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1). Finally, compound (**3o**) (15 mg, colorless oil) was isolated in 46% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.92 (s, 1H), 8.87-8.85 (m, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.57 (dd, *J* = 8.5 Hz, *J* = 1.5 Hz, 1H), 7.62-7.56 (m, 2H), 5.34-5.27 (m, 2H), 3.90 (dd, *J* = 10.8 Hz, *J* = 8.9 Hz, 1H), 3.67 (dd, *J* = 10.8 Hz, *J* = 5.1 Hz, 1H), 2.89-2.82 (m, 1H), 2.03-1.95 (m, 3H), 1.89-1.80 (m, 1H),

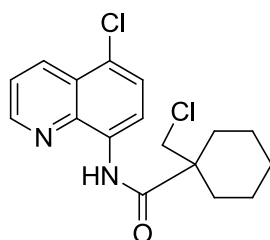
1.74-1.65 (m, 1H), 1.45-1.21 (m, 21H), 0.89 (t, $J = 6.9$ Hz, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 171.63, 148.89, 139.11, 133.54, 133.49, 130.18, 129.73, 127.32, 126.07, 124.79, 122.51, 116.79, 51.83, 45.34, 32.02, 31.22, 29.87, 29.76, 29.64, 29.56, 29.44, 29.12, 27.33, 27.29, 27.23, 22.81, 14.25; LRMS (ESI) calcd for $\text{C}_{28}\text{H}_{41}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 491.25, found 491.14



3-Chloro-2,2-bis(chloromethyl)-*N*-(5-chloroquinolin-8-yl)propanamide (3p)

Following the general procedure, substrate (26 mg, 0.1 mmol), NCS (54 mg, 0.4 mmol), $\text{Pd}(\text{OAc})_2$ (4.5 mg, 0.02 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 10: 1). Finally, compound (3p) (25.5 mg) was isolated in 70% yield.

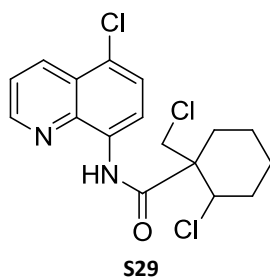
^1H -NMR (400 MHz, CDCl_3) δ (ppm) 10.37 (s, 1H), 8.90 (d, $J = 4.1$ Hz, 1H), 8.70 (d, $J = 8.4$ Hz, 1H), 8.59 (d, $J = 8.5$ Hz, 1H), 7.61 (t, $J = 7.7$ Hz, 2H), 4.10 (s, 6H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 166.93, 149.25, 139.35, 133.67, 132.86, 127.25, 126.13, 125.62, 122.73, 117.16, 55.81, 44.60; LRMS (ESI) calcd for $\text{C}_{14}\text{H}_{12}\text{Cl}_4\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 364.97, found 364.94.



1-(Chloromethyl)-*N*-(5-chloroquinolin-8-yl)cyclohexanecarboxamide (3q1)

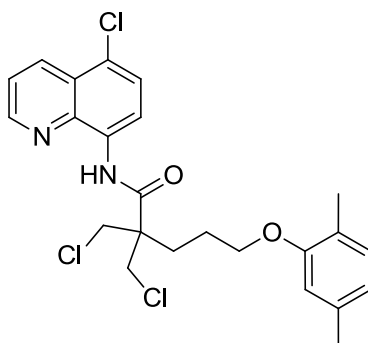
Following the general procedure, substrate (30 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), $\text{Pd}(\text{OAc})_2$ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 36 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 40: 1). Finally, compound (3q1) (8 mg, colorless oil) and compound (3q2) (15 mg,) were isolated in 25% yield and 40% respectively.

^1H -NMR (400 MHz, CDCl_3) δ (ppm) 10.35 (s, 1H), 8.88-8.86 (m, 1H), 8.78 (d, $J = 8.4$ Hz, 1H), 8.56 (dd, $J = 8.5$ Hz, $J = 1.6$ Hz, 1H), 7.61-7.55 (m, 2H), 3.76 (s, 2H), 2.31-2.27 (m, 2H), 1.73-1.67 (m, 7H), 1.66-1.57 (m, 1H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 172.70, 149.00, 139.55, 133.66, 133.49, 127.35, 126.07, 124.57, 122.46, 116.58, 51.90, 49.75, 32.33, 27.05, 25.81, 22.69; LRMS (ESI) calcd for $\text{C}_{17}\text{H}_{19}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 337.08, found 337.02



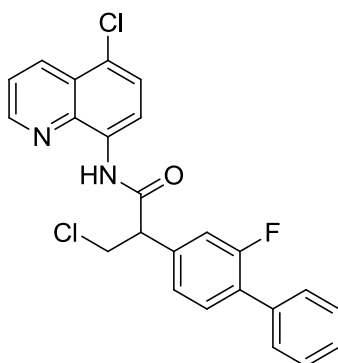
2-Chloro-1-(chloromethyl)-N-(5-chloroquinolin-8-yl)cyclohexanecarboxamide (3q2)

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.45 (s, 1H), 8.89-8.87 (m, 1H), 8.79 (d, *J* = 8.4 Hz, 1H), 8.55 (dd, *J* = 8.5 Hz, *J* = 1.6 Hz, 1H), 7.61-7.55 (m, 2H), 4.60 (t, *J* = 4.0 Hz, 1H), 4.00-3.92 (m, 2H), 2.46-2.39 (m, 1H), 2.28-2.24 (m, 1H), 2.13-1.99 (m, 2H), 1.90-1.82 (m, 2H), 1.64-1.59 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.83, 149.03, 139.59, 133.45, 133.37, 127.29, 126.06, 124.96, 122.49, 116.91, 62.07, 54.52, 47.46, 31.01, 27.04, 20.86; LRMS (ESI) calcd for C₁₇H₁₈Cl₃N₂O [M+H]⁺: 371.04, found 370.98

**2,2-Bis(chloromethyl)-N-(5-chloroquinolin-8-yl)-5-(2,5-dimethylphenoxy)pentanamide (3r)**

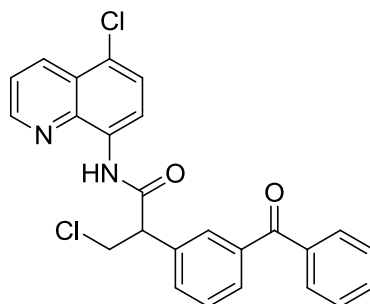
Following the general procedure, substrate (53 mg, 0.13 mmol), NCS (35 mg, 0.26 mmol), Pd(OAc)₂ (3 mg, 0.013 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 18 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1). Finally, compound (3r) (36 mg, colorless oil) was isolated in 58% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.32 (s, 1H), 8.85 (t, *J* = 1.3 Hz, 1H), 8.69 (d, *J* = 8.4 Hz, 1H), 8.58-8.56 (m, 1H), 7.61-7.57 (m, 2H), 6.90 (d, *J* = 7.4 Hz, 1H), 6.59 (d, *J* = 7.4 Hz, 1H), 6.52 (s, 1H), 4.07 (t, *J* = 12.4 Hz, 4H), 3.97 (t, *J* = 5.8 Hz, 2H), 2.24 (s, 3H), 2.19-2.15 (m, 2H), 2.07 (s, 3H), 1.93-1.89 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 169.65, 156.68, 149.06, 139.25, 136.51, 133.59, 133.08, 130.35, 127.22, 126.07, 125.10, 123.55, 122.60, 120.95, 116.74, 111.83, 66.92, 53.63, 45.86, 29.97, 24.33, 21.43, 15.78; HRMS (ESI) calcd for C₂₄H₂₆Cl₃N₂O₂ [M+H]⁺: 479.10599, found 479.10356

**3-Chloro-N-(5-chloroquinolin-8-yl)-2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanamide (3s)**

Following the general procedure, substrate (40 mg, 0.1 mmol), NCS (16 mg, 0.12 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 36 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 2: 1). Finally, compound (3s) (30 mg, white solid) was isolated in 69% yield.

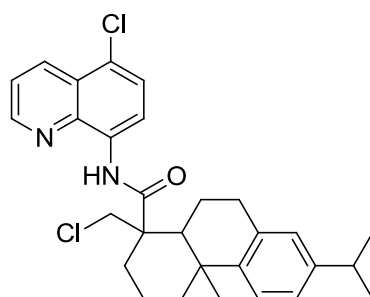
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.98 (s, 1H), 8.81-8.80 (m, 1H), 8.74 (d, $J = 8.4$ Hz, 1H), 8.55-8.53 (m, 1H), 7.61-7.33 (m, 10H), 4.39-4.34 (m, 1H), 4.15-4.11 (m, 1H), 3.90-3.86 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 168.56, 161.28, 158.80, 148.95, 139.03, 137.69, 137.62, 135.27, 133.57, 133.38, 131.59, 131.55, 129.39, 129.25, 129.09, 129.06, 128.65, 128.06, 127.26, 126.07, 125.11, 124.23, 124.20, 122.58, 116.80, 116.10, 115.86, 56.63, 45.00; LRMS (ESI) calcd for $\text{C}_{24}\text{H}_{17}\text{Cl}_2\text{FN}_2\text{O}$ $[\text{M}+\text{H}]^+$: 439.07, found 438.93



2-(3-Benzoylphenyl)-3-chloro-N-(5-chloroquinolin-8-yl)propanamide (3t)

Following the general procedure, substrate (41 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), $\text{Pd}(\text{OAc})_2$ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 60 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: ethyl acetate= 100: 1). Finally, compound (**3t**) (16 mg, yellow oil) was isolated in 35% yield.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.95 (s, 1H), 8.80-8.78 (m, 1H), 8.71 (d, $J = 8.4$ Hz, 1H), 8.56-8.54 (m, 1H), 7.94 (t, $J = 1.7$ Hz, 1H), 7.81-7.75 (m, 4H), 7.60-7.52 (m, 4H), 7.45 (t, $J = 7.9$ Hz, 2H), 4.39-4.34 (m, 1H), 4.20-4.16 (m, 1H), 3.91-3.86 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 196.28, 168.67, 148.97, 139.01, 138.54, 137.39, 136.91, 133.58, 133.34, 132.84, 131.82, 130.26, 130.07, 129.36, 128.52, 127.24, 126.05, 125.11, 122.61, 116.75, 56.91, 45.09; LRMS (ESI) calcd for $\text{C}_{25}\text{H}_{18}\text{Cl}_2\text{N}_2\text{O}_2$ $[\text{M}+\text{H}]^+$: 449.07, found 449.02

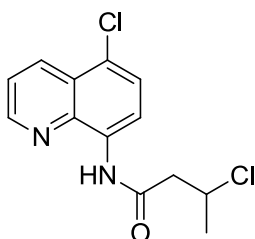


1-(Chloromethyl)-N-(5-chloroquinolin-8-yl)-7-isopropyl-4a-methyl-1,2,3,4,9,10,10a-octahydrophenanthrene-1-carboxamide (3u)

Following the general procedure, substrate (35 mg, 0.076 mmol), NCS (20 mg, 0.15 mmol), $\text{Pd}(\text{OAc})_2$ (1.5 mg, 0.007 mmol) and 2ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1). Finally, compound (**3u**) (21 mg, white solid) was isolated in 56% yield.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 10.46 (s, 1H), 8.86-8.81 (m, 2H), 8.56 (d, $J = 8.5$ Hz, 1H), 7.62-7.56 (m, 2H), 7.22 (d, $J = 8.2$ Hz, 1H), 7.04 (d, $J = 8.0$ Hz, 1H), 6.86 (s, 1H), 4.35 (d, $J = 11.6$ Hz, 1H), 4.22 (d, $J = 11.6$ Hz, 1H), 2.88-2.80 (m, 3H), 2.57-2.47 (m, 2H), 2.37 (d, $J = 12.7$ Hz, 1H),

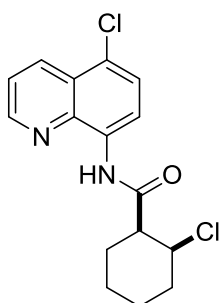
2.00-1.73 (m, 6H), 1.34 (s, 3H), 1.21 (d, $J = 6.9$ Hz, 6H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 172.80, 148.94, 146.50, 146.30, 139.51, 134.47, 133.94, 133.48, 127.34, 127.04, 126.04, 124.49, 124.31, 124.26, 122.44, 116.73, 54.16, 47.70, 44.62, 38.31, 37.87, 33.59, 32.24, 30.24, 26.29, 24.09, 24.06, 20.51, 18.72; LRMS (ESI) calcd for $\text{C}_{29}\text{H}_{32}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 495.19, found 495.04



3-Chloro-*N*-(5-chloroquinolin-8-yl)butanamide (**3v**)

Following the general procedure, substrate (25 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), $\text{Pd}(\text{OAc})_2$ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at 55 °C for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 20: 1). Finally, compound (**3v**) (8 mg, white solid) were isolated in 28% yield.

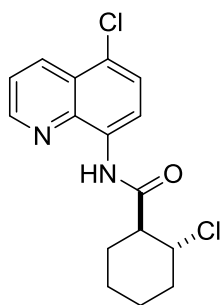
^1H -NMR (400 MHz, CDCl_3) δ (ppm) 9.85 (s, 1H), 8.85-8.84 (m, 1H), 8.72 (d, $J = 8.4$ Hz, 1H), 8.57 (dd, $J = 8.5$ Hz, $J = 1.2$ Hz, 1H), 7.61-7.56 (m, 2H), 4.68-4.60 (m, 1H), 3.04-2.92 (m, 2H), 1.68 (d, $J = 6.6$ Hz, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 167.98, 148.88, 139.03, 133.58, 133.55, 127.32, 126.08, 124.81, 122.54, 116.75, 53.73, 48.83, 25.34; HRMS (ESI) calcd for $\text{C}_{13}\text{H}_{12}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 283.04049, found 283.03949



(2S)-2-chloro-*N*-(5-chloroquinolin-8-yl)cyclohexanecarboxamide (**3w1**)

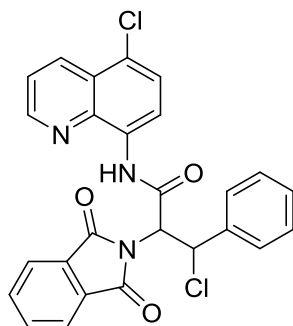
Following the general procedure, substrate (57.6 mg, 0.20 mmol), NCS (53 mg, 0.4 mmol), $\text{Pd}(\text{OAc})_2$ (4.5 mg, 0.02 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at 55 °C for 2 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 30: 1). Finally, compound (**3w1**) (13 mg, colorless oil) and compound (8 mg, colorless oil) was isolated in 20% yield and 12% yield.

^1H -NMR (400 MHz, CDCl_3) δ (ppm) 10.09 (s, 1H), 8.87 (d, $J = 3.7$ Hz, 1H), 8.77 (d, $J = 8.4$ Hz, 1H), 8.57 (d, $J = 8.4$ Hz, 1H), 7.61-7.56 (m, 2H), 4.94 (s, 1H), 2.85 (d, $J = 11.8$ Hz, 1H), 2.22-2.15 (m, 2H), 2.08-1.85 (m, 4H), 1.64-1.57 (m, 1H), 1.46-1.38 (m, 1H); ^{13}C -NMR (100 MHz, CDCl_3) δ (ppm) 170.74, 148.93, 139.43, 133.62, 133.56, 127.40, 126.11, 124.64, 122.49, 116.75, 60.70, 50.94, 34.31, 24.87, 22.81, 19.92; LRMS (ESI) calcd for $\text{C}_{16}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 323.06, found 322.98



(2R)-2-chloro-N-(5-chloroquinolin-8-yl)cyclohexanecarboxamide (3w2)

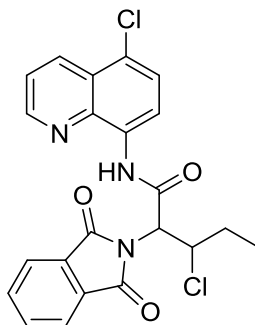
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.85 (s, 1H), 8.87-8.86 (m, 1H), 8.78 (d, $J = 8.4$ Hz, 1H), 8.57 (dd, $J = 8.5$ Hz, $J = 1.3$ Hz, 1H), 7.62-7.56 (m, 2H), 4.29-4.23 (m, 1H), 2.71-2.65 (m, 1H), 2.39-2.35 (m, 1H), 2.15-2.11 (m, 1H), 1.88-1.69 (m, 4H), 1.56-1.44 (m, 2H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 171.91, 148.79, 139.12, 133.69, 133.56, 127.36, 126.07, 124.63, 122.47, 116.80, 60.16, 56.41, 36.56, 30.79, 25.96, 24.58; LRMS (ESI) calcd for $\text{C}_{16}\text{H}_{16}\text{Cl}_2\text{N}_2\text{O}$ $[\text{M}+\text{H}]^+$: 323.06, found 322.98



3-chloro-N-(5-chloroquinolin-8-yl)-2-(1,3-dioxisoindolin-2-yl)-3-phenylpropanamide (3x)

Following the general procedure, substrate (36 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), $\text{Pd}(\text{OAc})_2$ (2.2 mg, 0.01 mmol) and 2 ml propanoic acid were used. The reaction mixture was stirred at 55°C for 8 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: ethyl acetate= 50: 1). Finally, compound (3x) (17 mg, white solid) were isolated in 45% yield.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 10.65 (s, 1H), 8.93 (d, $J = 2.8$ Hz, 1H), 8.76 (d, $J = 8.8$ Hz, 1H), 8.57 (d, $J = 8.8$ Hz, 1H), 7.723-7.717 (m, 2H), 7.64-7.46 (m, 4H), 7.48-7.46 (m, 2H), 7.28-7.20 (m, 3H), 6.27 (d, $J = 10.8$ Hz, 1H), 5.65 (d, $J = 10.8$ Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 167.1, 164.3, 149.3, 139.3, 137.2, 134.5, 133.5, 131.2, 129.3, 128.9, 128.0, 127.2, 126.1, 125.4, 123.8, 122.6, 117.3, 60.6, 57.9; LRMS (ESI) calcd for $\text{C}_{26}\text{H}_{17}\text{Cl}_2\text{N}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 390.06, found 390.07

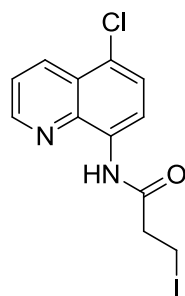


3-chloro-N-(5-chloroquinolin-8-yl)-2-(1,3-dioxisoindolin-2-yl)pentanamide (3y)

Following the general procedure, substrate (41 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), $\text{Pd}(\text{OAc})_2$

(4.4 mg, 0.02 mmol) and 2 ml propanoic acid were used. The reaction mixture was stirred at 55°C for 12 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: ethyl acetate= 50: 1). Finally, compound (**3y**) (18 mg, white solid) were isolated in 42% yield.

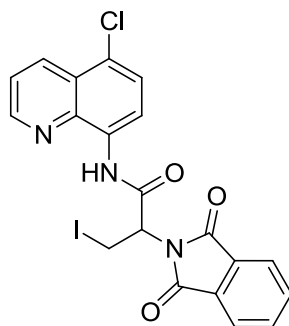
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.54 (s, 1H), 8.89 (d, *J* = 2.4 Hz, 1H), 8.69 (d, *J* = 8.8 Hz, 1H), 8.55 (d, *J* = 8.4 Hz, 1H), 7.90-7.89 (m, 2H), 7.77-7.76 (m, 2H), 7.57-7.55 (m, 2H), 5.30-5.21 (m, 2H), 2.00-1.94 (m, 1H), 1.74-1.67 (m, 1H), 1.21 (t, *J* = 7.2 Hz, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 167.7 164.8, 149.2, 139.3, 134.7, 133.4, 131.6, 127.2, 126.1, 125.3, 124.1, 122.6, 117.2, 60.3, 59.5, 27.8, 10.0; LRMS (ESI) calcd for C₂₂H₁₇Cl₂N₃O₃ [M+H]⁺: 442.06, found 442.15



***N*-(5-chloroquinolin-8-yl)-3-iodopropanamide (**4a**)**

Following the general procedure, substrate (21 mg, 0.1 mmol), NIS (45 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 24 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 30: 1). Finally, compound (**4a**) (16 mg, white solid) were isolated in 45% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.80 (s, 1H), 8.85 (d, *J* = 2.9 Hz, 1H), 8.72 (d, *J* = 8.4 Hz, 1H), 8.59-8.57 (m, 1H), 7.62-7.57 (m, 2H), 3.52 (t, *J* = 7.1 Hz, 2H), 3.22 (t, *J* = 7.0 Hz, 2H); LRMS (ESI) calcd for C₁₂H₁₀ClN₂O [M+H]⁺: 360.95, found 360.85



***N*-(5-chloroquinolin-8-yl)-2-(1,3-dioxisoindolin-2-yl)-3-iodopropanamide (**4b**)**

Following the general procedure, substrate (19 mg, 0.05 mmol), NIS (22 mg, 0.1 mmol), Pd(OAc)₂ (1.1 mg, 0.005 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at 50 °C for 22 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 3: 1). Finally, compound (**4b**) (26 mg, white solid) were isolated in 52% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.27 (s, 1H), 8.66 (d, *J* = 2.5 Hz, 1H), 8.60 (d, *J* = 8.4 Hz, 1H), 8.51 (d, *J* = 8.1 Hz, 1H), 7.95 (d, *J* = 2.8 Hz, 2H), 7.81 (d, *J* = 2.8 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.52-7.48 (m, 1H), 5.36-5.29 (m, 1H), 4.29 (t, *J* = 11.0 Hz, 1H), 4.15-4.11 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 167.53, 164.26, 149.08, 139.05, 134.73, 133.52, 132.89, 131.72, 127.17,

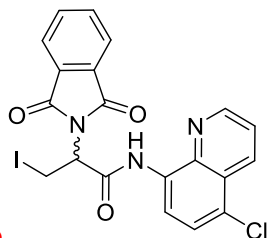
126.01, 125.42, 124.11, 122.57, 116.94, 57.30, 0.62; LRMS (ESI) calcd for C₂₀H₁₃ClIN₃O₃ [M+H]⁺: 505.97, found 505.86

Chiral HPLC Data

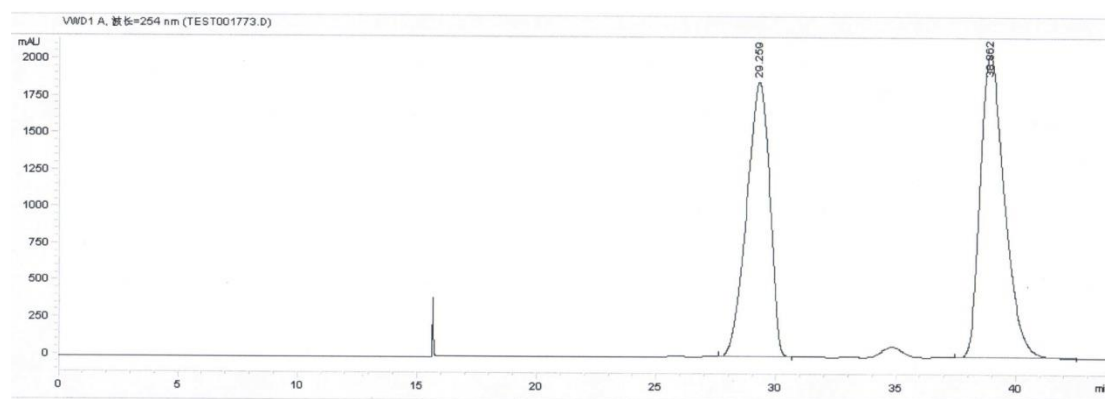
HPLC Conditions:

Chiral stationary phase: CHIRALPAK[®] AD-H, *n*-hexane/isopropanol = 50:50, 0.60 mL/min

Signal: VWD1 A, Wavelength = 254 nm

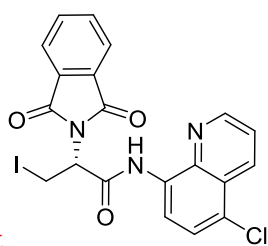


DL-4b

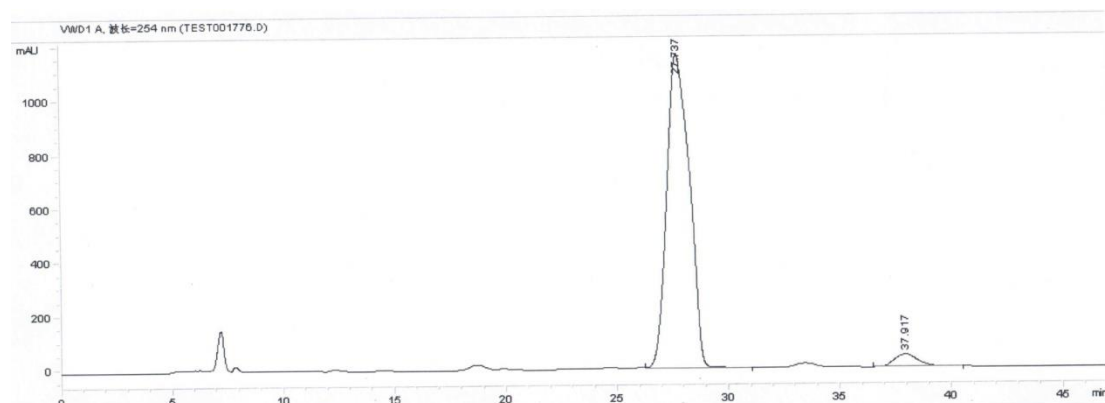


Area% report for DL-1a:

Retention Time (min)	Area	Area %	Height	Symmetry Factor
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38.862	146707.1	53.678	2048.6	0.616

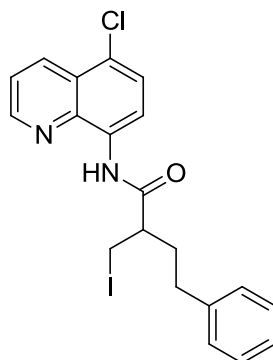


L-4b-product



Area% report for DL-1a:

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37.917	3355.1	3.921	45.9	0.815

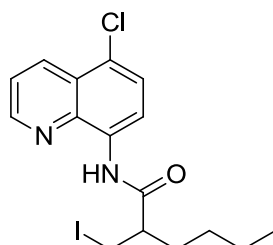
**N-(5-chloroquinolin-8-yl)-2-(iodomethyl)-4-phenylbutanamide (4c)****0.1mmol scale**

Following the general procedure, substrate (35 mg, 0.12 mmol), NIS (54 mg, 0.24 mmol), Pd(OAc)₂ (2.7 mg, 0.012 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 36 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1 – 5: 1). Finally, compound (**4c**) (32 mg, yellow solid) was isolated in 65% yield.

3.0mmol scale

Following the general procedure, substrate (1014 mg, 3.0 mmol), NIS (1.35 g, 6.0 mmol), Pd(OAc)₂ (67 mg, 0.3 mmol) and 10 ml AcOH were used. The reaction mixture was stirred at rt for 22 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1 - 5: 1). Finally, compound (**4c**) (890 mg, yellow solid) was isolated in 64% yield.

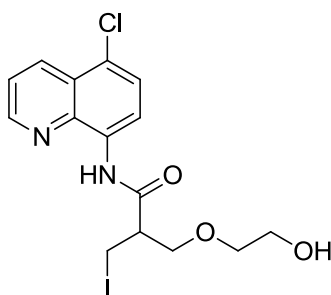
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.87 (s, 1H), 8.88 (t, *J* = 2.3 Hz, 1H), 8.78 (d, *J* = 8.3 Hz, 1H), 8.58 (d, *J* = 8.4 Hz, 1H), 7.64-7.58 (m, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.21 (d, *J* = 6.9 Hz, 3H), 3.56 (t, *J* = 9.3 Hz, 1H), 3.34-3.31 (m, 1H), 2.87-2.77 (m, 2H), 2.73-2.67 (m, 1H), 2.25-2.20 (m, 1H), 2.07-2.03 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.50, 148.90, 140.75, 139.11, 133.56, 133.31, 128.69, 128.58, 127.32, 126.37, 126.09, 124.93, 122.57, 116.88, 51.21, 35.58, 33.46, 5.73; HRMS (ESI) calcd for C₂₀H₁₉ClIN₂O [M+H]⁺: 465.02306, found 465.02154

**N-(5-chloroquinolin-8-yl)-2-(iodomethyl)hexanamide (4d)**

Following the general procedure, substrate (35 mg, 0.12 mmol), NIS (54 mg, 0.24 mmol), Pd(OAc)₂ (2.7 mg, 0.012 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 36 h. After completion of the reaction, the residue was purified by silica gel column

chromatography (toluene: petroleum ether= 3: 1 - 5: 1). Finally, compound (**4d**) (32 mg, colorless oil) was isolated in 64% yield.

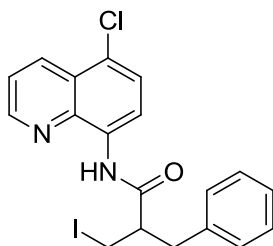
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.86 (s, 1H), 8.87-8.86 (m, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.58-8.55 (m, 1H), 7.61-7.56 (m, 2H), 3.54 (t, *J* = 9.4 Hz, 1H), 3.35-3.31 (m, 1H), 2.88-2.84 (m, 1H), 1.88-1.81 (m, 1H), 1.75-1.65 (m, 1H), 1.44-1.25 (m, 4H), 0.89 (t, *J* = 7.0 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.89, 148.90, 139.14, 133.53, 133.43, 127.32, 126.08, 124.79, 122.50, 116.81, 52.19, 33.91, 29.54, 22.71, 13.94, 5.87; LRMS (ESI) calcd for C₁₆H₁₈ClIN₂O [M+H]⁺: 417.02, found 416.94



***N*-(5-chloroquinolin-8-yl)-3-(2-hydroxyethoxy)-2-(iodomethyl)propanamide (**4e**)**

Following the general procedure, substrate (31 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate = 2: 1). Finally, compound (**4e**) (24 mg) was isolated in 56% yield.

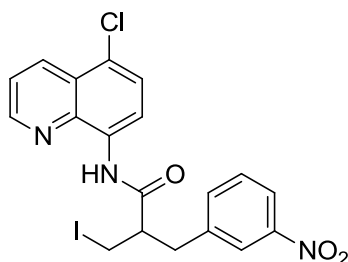
¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.95-8.94 (m, 1H), 8.66-8.59 (m, 2H), 7.70-7.67 (m, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 3.90-3.82 (m, 2H), 3.78 (t, *J* = 4.8 Hz, 2H), 3.68 (t, *J* = 5.0 Hz, 2H), 3.54 (d, *J* = 7.1 Hz, 2H), 3.28-3.21 (m, 1H) ; ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 172.21, 150.61, 140.62, 135.08, 134.21, 128.01, 127.20, 125.96, 123.94, 118.30, 74.10, 73.02, 62.16, 51.69, 1.45; LRMS (ESI) calcd for C₁₅H₁₆ClIN₂O₃ [M+H]⁺: 434.99, found 435.37.



2-Benzyl-*N*-(5-chloroquinolin-8-yl)-3-iodopropanamide (**4f)**

Following the general procedure, substrate (32.4 mg, 0.10 mmol), NIS (54 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 4: 1). Finally, compound (**4f**) (25 mg, yellow oil) was isolated in 56% yield.

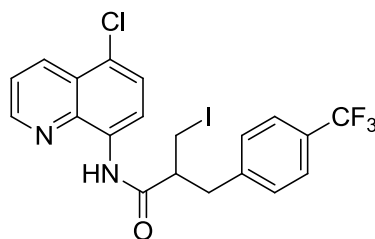
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.66 (s, 1H), 8.78-8.71 (m, 2H), 8.54-8.52 (m, 1H), 7.60-7.52 (m, 2H), 7.26-7.21 (m, 4H), 7.17-7.14 (m, 1H), 3.58-3.54 (m, 1H), 3.37-3.33 (m, 1H), 3.18-3.02 (m, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.02, 148.75, 139.01, 137.94, 133.43, 133.26, 129.03, 128.84, 127.27, 126.96, 125.98, 124.81, 122.45, 116.76, 53.83, 39.93, 5.29; LRMS (ESI) calcd for C₁₉H₁₇ClIN₂O [M+H]⁺: 451.00, found 450.92



***N*-(5-chloroquinolin-8-yl)-3-iodo-2-(3-nitrobenzyl)propanamide (**4g**)**

Following the general procedure, substrate (37 mg, 0.10 mmol), NIS (54 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 10: 1). Finally, compound (**4g**) (25 mg, white solid) was isolated in 50% yield.

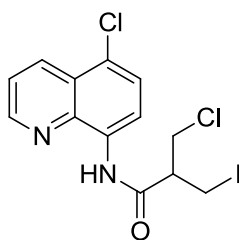
¹H-NMR (400 MHz, (CD₃)₂SO) δ (ppm) 10.36 (s, 1H), 8.97 (d, *J* = 4.1 Hz, 1H), 8.59-8.56 (m, 2H), 8.24 (s, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.80-7.73 (m, 3H), 7.52 (t, *J* = 7.9 Hz, 1H), 3.81-3.77 (m, 1H), 3.45 (t, *J* = 9.6 Hz, 1H), 3.30-3.28 (m, 1H), 3.15-3.02 (m, 2H); ¹³C-NMR (100 MHz, (CD₃)₂SO) δ (ppm) 171.39, 149.62, 147.79, 140.58, 138.99, 136.05, 133.82, 132.83, 129.70, 127.00, 125.32, 123.77, 123.56, 123.30, 121.49, 117.55, 50.05, 38.55, 6.33; LRMS (ESI) calcd for C₁₉H₁₅ClIN₃O₃ [M+H]⁺: 495.98, found 495.77



***N*-(5-chloroquinolin-8-yl)-3-iodo-2-(4-(trifluoromethyl)benzyl)propanamide (**4h**)**

Following the general procedure, substrate (40 mg, 0.1 mmol), NIS (45 mg, 0.2 mmol), Pd(OAc)₂ (3.4 mg, 0.015 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate = 6: 1). Finally, compound (**4h**) (37 mg) was isolated in 71% yield.

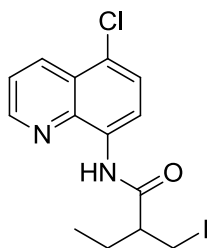
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.55 (s, 1H), 8.73-8.66 (m, 2H), 8.54-8.51 (m, 1H), 7.59-7.51 (m, 2H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 3.61-3.57 (m, 1H), 3.37-3.34 (m, 1H), 3.21-3.09 (m, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.35, 148.82, 142.20, 138.92, 133.48, 133.00, 129.40, 129.32 (q, *J*_{C-F} = 32 Hz), 127.21, 126.00, 125.78 (q, *J*_{C-F} = 4 Hz), 125.09, 124.19 (q, *J*_{C-F} = 290 Hz), 122.53, 116.81, 53.68, 39.69, 4.87; LRMS (ESI) calcd for C₂₀H₁₅ClF₃IN₂O [M+H]⁺: 518.99, found 518.88.



3-Chloro-N-(5-chloroquinolin-8-yl)-2-(iodomethyl)propanamide (4i)

Following the general procedure, substrate (29 mg, 0.1 mmol), NIS (57 mg, 0.25 mmol), Pd(OAc)₂ (2.3 mg, 0.01 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 4: 1). Finally, compound (**4i**) (26 mg) was isolated in 64% yield.

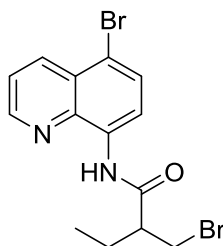
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.01 (s, 1H), 8.87 (s, 1H), 8.72 (d, *J* = 8.2 Hz, 1H), 8.57 (d, *J* = 8.4 Hz, 1H), 7.62-7.57 (m, 2H), 3.96-3.92 (m, 1H), 3.85-3.81 (m, 1H), 3.60-3.56 (m, 1H), 3.49-3.45 (m, 1H), 3.23-3.20 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 168.48, 149.04, 139.06, 133.61, 133.06, 127.25, 126.08, 125.32, 122.65, 117.00, 53.58, 45.10, 1.37; LRMS (ESI) calcd for C₁₃H₁₁Cl₂IN₂O [M+H]⁺: 408.93, found 408.85.



N-(5-chloroquinolin-8-yl)-2-(iodomethyl)butanamide (4j)

Following the general procedure, substrate (26.2 mg, 0.1 mmol), NIS (45 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 35 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 3: 1). Finally, compound (**4j**) (23 mg, white solid) were isolated in 60% yield.

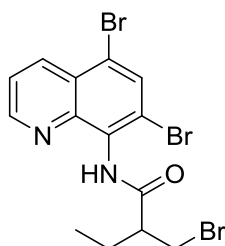
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.87 (s, 1H), 8.87 (d, *J* = 4.1 Hz, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.57 (d, *J* = 8.5 Hz, 1H), 7.62-7.56 (m, 2H), 3.54 (t, *J* = 9.1 Hz, 1H), 3.36-3.32 (m, 1H), 2.83-2.79 (m, 1H), 1.92-1.76 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.77, 148.91, 139.12, 133.57, 133.41, 127.33, 126.08, 124.81, 122.53, 116.80, 53.61, 27.33, 11.91, 5.50; LRMS (ESI) calcd for C₁₄H₁₄ClIN₂O [M+H]⁺: 388.98, found 388.87



2-(bromomethyl)-N-(5-bromoquinolin-8-yl)butanamide (4k1)

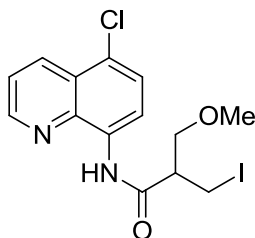
Following the general procedure, substrate (61 mg, 0.2 mmol), NBS (53 mg, 0.3 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol) and 2ml AcOH were used. The reaction mixture was stirred at rt for 48h. After completion of the reaction, the residue was purified by silical gel column chromatography (petroleum ether: ethyl acetate = 20:1 then toluene: petroleum ether = 3:1). Finally, compound (**4k1**) (16 mg, white solid) and compound (**4k2**) (23mg, white solid) were isolated in 22% yield and 23% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.93 (s, 1H), 8.85 (dd, *J* = 4.2 Hz, *J* = 1.6 Hz, 1H), 8.72 (d, *J* = 8.4 Hz, 1H), 8.54 (dd, *J* = 8.5 Hz, *J* = 1.6 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.60-7.57 (m, 1H), 3.78-3.73 (m, 1H), 3.55-3.53 (m, 1H), 2.88-2.84 (m, 1H), 1.93-1.76 (m, 2H), 1.05 (t, *J* = 7.5 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.62, 148.95, 139.3, 136.2, 134.1, 131.0, 127.4, 122.9, 117.4, 114.8, 53.3, 32.9, 25.6, 11.9; LRMS (ESI) calcd for C₁₄H₁₄Br₂N₂O [M+H]⁺: 386.95, found 386.82



2-(bromomethyl)-N-(5,7-dibromoquinolin-8-yl)butanamide (4k2)

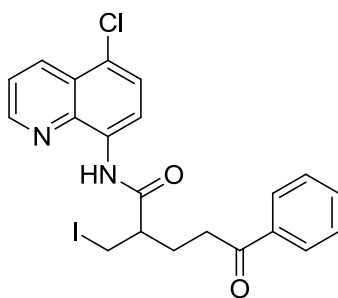
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 8.88-8.87 (m, 1H), 8.49-8.47 (m, 1H), 8.38 (s, 1H), 8.06 (s, 1H), 7.57-7.54 (m, 1H), 3.80-3.76 (m, 1H), 3.56-3.52 (m, 1H), 2.91-2.87 (m, 1H), 1.97-1.82 (m, 2H), 1.16 (t, *J* = 7.5 Hz, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.1, 150.9, 144.0, 136.0, 134.4, 133.6, 127.0, 122.9, 120.4, 119.4, 32.9, 31.1, 25.6, 11.9; LRMS (ESI) calcd for C₁₄H₁₃Br₃N₂O [M+H]⁺: 466.85, found 466.72



N-(5-chloroquinolin-8-yl)-3-iodo-2-(methoxymethyl)propanamide (4l)

Following the general procedure, substrate (28 mg, 0.1 mmol), NCS (27 mg, 0.2 mmol), Pd(OAc)₂ (4.5 mg, 0.02 mmol) and 1 ml AcOH were used. The reaction mixture was stirred at 50 °C for 8 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: petroleum ether= 2: 1). Finally, compound (**4l**) (21.5 mg) was isolated in 53% yield.

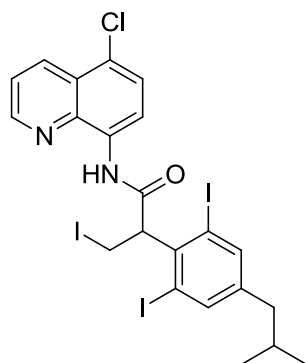
¹H-NMR (400 MHz, CD₃OD) δ (ppm) 8.71-8.70 (m, 1H), 8.49 (d, *J* = 8.4 Hz, 1H), 8.40-8.37 (m, 1H), 7.44-7.40 (m, 2H), 3.66-3.57 (m, 2H), 3.38-3.28 (m, 5H), 2.95-2.88 (m, 1H) ; ¹³C-NMR (100 MHz, CD₃OD) δ (ppm) 170.03, 148.83, 139.02, 133.26, 133.13, 126.80, 125.81, 124.77, 122.31, 116.70, 72.96, 58.96, 50.34, 0.77; LRMS (ESI) calcd for C₁₄H₁₄ClIN₂O₂ [M+H]⁺: 404.98, found 405.34.



***N*-(5-chloroquinolin-8-yl)-2-(iodomethyl)-5-oxo-5-phenylpentanamide (4m)**

Following the general procedure, substrate (47 mg, 0.13 mmol), NIS (58 mg, 0.26 mmol), Pd(OAc)₂ (3 mg, 0.013 mmol) and 2ml AcOH were used. The reaction mixture was stirred at rt for 60 h. After completion of the reaction, the residue was purified by silica gel column chromatography (toluene: ethyl acetate= 60: 1). Finally, compound (4m) (35 mg, white solid) was isolated in 55% yield.

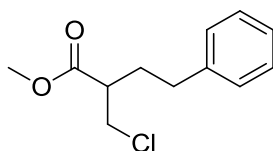
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.91 (s, 1H), 8.78-8.72 (m, 2H), 8.55-8.53 (m, 1H), 7.90 (d, *J* = 7.4 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.56-7.47 (m, 2H), 7.37 (t, *J* = 7.8 Hz, 2H), 3.58 (t, *J* = 9.4 Hz, 1H), 3.39-3.36 (m, 1H), 3.19-3.06 (m, 3H), 2.28-2.22 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 199.03, 171.31, 148.93, 139.08, 136.68, 133.46, 133.32, 133.27, 128.67, 128.13, 127.22, 126.03, 124.99, 122.52, 116.90, 50.69, 35.49, 28.31, 5.06; LRMS (ESI) calcd for C₂₁H₁₈ClIN₂O₂ [M+H]⁺: 493.01, found 492.90



***N*-(5-chloroquinolin-8-yl)-2-(2,6-diiodo-4-isobutylphenyl)-3-iodopropanamide (4n)**

Following the general procedure, substrate (37 mg, 0.1 mmol), NIS (45 mg, 0.2 mmol), Pd(OAc)₂ (2.2 mg, 0.01 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 20: 1). Finally, compound (4n) (30 mg, white solid) was isolated in 40% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.66 (s, 1H), 8.67 (d, *J* = 8.4 Hz, 1H), 8.54-8.48 (m, 2H), 7.92 (s, 1H), 7.73 (s, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.48-7.45 (m, 1H), 5.12-5.08 (m, 1H), 4.24-4.20 (m, 1H), 4.06 (t, *J* = 9.5 Hz, 1H), 2.42(d, *J* = 7.3 Hz, 2H), 1.97-1.87 (m, 1H), 0.97-0.95 (m, 6H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 167.66, 148.76, 145.69, 143.44, 141.39, 139.17, 138.82, 133.70, 133.33, 127.29, 126.02, 124.70, 122.38, 116.36, 106.32, 94.87, 62.62, 43.68, 30.15, 22.38, 22.33, 2.30; HRMS (ESI) calcd for C₂₂H₂₀ClI₃N₂O [M+H]⁺: 744.84765, found 744.84489

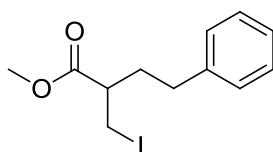


Methyl 2-(chloromethyl)-4-phenylbutanoate (**5a**)

Following the general procedure, substrate (37 mg, 0.1 mmol), $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (63 μL , 0.5 mmol) and 1 ml MeOH were used. The reaction mixture was stirred at 100 °C for 24 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 50: 1 - 10: 1). Finally, ester (**5a**) (21 mg, colorless oil) and amine (17 mg, yellow solid) was isolated in 92% yield and 95% yield respectively.

Following the general procedure, substrate (37 mg, 0.1 mmol), H_2SO_4 (27 μL , 0.5 mmol) and 1 ml MeOH were used. The reaction mixture was stirred at 100 °C for 24 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 50: 1 - 10: 1). Finally, ester (**5a**) (20 mg, colorless oil) and amine (17 mg, yellow solid) was isolated in 90% yield and 95% yield respectively.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 7.32-7.26 (m, 2H), 7.23-7.17 (m, 3H), 3.77-3.72 (m, 4H), 3.67-3.63 (m, 1H), 2.84-2.77 (m, 1H), 2.70-2.61 (m, 2H), 2.12-2.02 (m, 1H), 1.97-1.88 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 173.44, 140.88, 128.64, 128.52, 126.35, 52.16, 47.48, 44.55, 33.15, 31.60

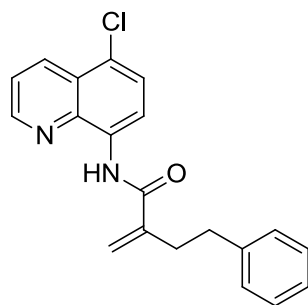


Methyl 2-(iodomethyl)-4-phenylbutanoate (**5b**)

Following the general procedure, substrate (46 mg, 0.1 mmol), $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (63 μL , 0.5 mmol) and 1 ml MeOH were used. The reaction mixture was stirred at 100 °C for 24 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 50: 1 - 10: 1). Finally, ester (**5b**) (30 mg, colorless oil) and amine (13 mg, yellow solid) was isolated in 94% yield and 73% yield respectively.

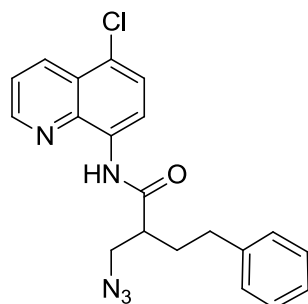
Following the general procedure, substrate (37 mg, 0.1 mmol), H_2SO_4 (27 μL , 0.5 mmol) and 1 ml MeOH were used. The reaction mixture was stirred at 100 °C for 24 h. After completion of the reaction, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate= 50: 1 - 10: 1). Finally, ester (**5b**) (29 mg, colorless oil) and amine (17 mg, yellow solid) was isolated in 90% yield and 95% yield respectively.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 7.31-7.26 (m, 2H), 7.22-7.17 (m, 3H), 3.74 (s, 3H), 3.39-3.28 (m, 2H), 2.78-2.71 (m, 1H), 2.67-2.62 (m, 2H), 2.12-2.02 (m, 1H), 1.94-1.85 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 173.55, 140.87, 128.66, 128.54, 126.36, 52.20, 47.51, 34.68, 33.17, 4.94



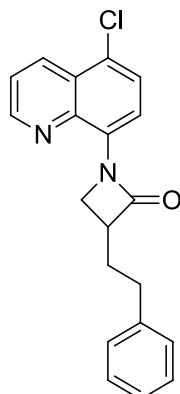
***N*-(5-chloroquinolin-8-yl)-2-methylene-4-phenylbutanamide (6a)**

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.28 (s, 1H), 8.83 (d, *J* = 3.5 Hz, 1H), 8.76 (d, *J* = 8.4 Hz, 1H), 8.54 (d, *J* = 8.4 Hz, 1H), 7.61-7.53 (m, 2H), 7.31-7.27 (m, 4H), 7.20 (d, *J* = 6.5 Hz, 1H), 5.98 (s, 1H), 5.50 (s, 1H), 2.91 (t, *J* = 6.8 Hz, 2H), 2.81 (t, *J* = 6.8 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 166.53, 148.80, 145.06, 141.36, 139.27, 133.84, 133.52, 128.65, 128.51, 127.36, 126.15, 126.05, 124.51, 122.46, 119.94, 116.51, 35.01, 34.55; LRMS (ESI) calcd for C₂₀H₁₇ClN₂O [M+H]⁺: 337.10, found 337.16



2-(Azidomethyl)-*N*-(4-chloronaphthalen-1-yl)-4-phenylbutanamide (6b)

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.93 (s, 1H), 8.88-8.87 (m, 1H), 8.77 (d, *J* = 8.4 Hz, 1H), 8.59-8.57 (m, 1H), 7.63-7.57 (m, 2H), 7.30-7.20 (m, 5H), 3.81-3.76 (m, 1H), 3.54-3.50 (m, 1H), 2.84-2.65 (m, 3H), 2.24-2.14 (m, 1H), 1.98-1.90 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.61, 148.91, 140.86, 139.12, 133.55, 133.48, 128.70, 128.58, 127.32, 126.37, 126.08, 124.88, 122.55, 116.87, 53.45, 48.02, 33.32, 31.99; LRMS (ESI) calcd for C₂₀H₁₉ClN₅O [M+H]⁺: 380.12, found 379.95

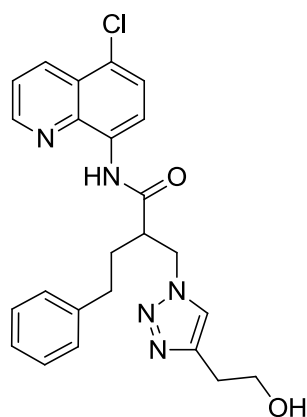


1-(5-Chloroquinolin-8-yl)-3-phenethylazetidin-2-one (6c)

To a 10 mL sealed tube were added *N*-(5-chloroquinolin-8-yl)-2-(iodomethyl)-4-phenylbutanamide (93 mg, 0.2 mmol), NaSMe (267mg, 0.4 mmol) and DMF (0.5 mL). The tube was sealed at rt for 1.5 h. H₂O was added to

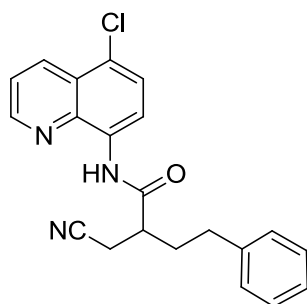
dilute the reaction mixture. Then reaction mixture was extracted by DCM for three times, the organic layer dried over anhydrous Na_2SO_4 and concentrated on rotavapor under reduced pressure. Finally, the residue was purified by silica gel column chromatography (petroleum ether: ethylacetate = 20: 1). Finally, compound (**6c**) (31 mg) was isolated in 46% yield.

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 8.86-8.84 (m, 1H), 8.55-8.52 (m, 1H), 8.42 (d, $J = 8.4$ Hz, 1H), 7.57-7.49 (m, 2H), 7.33-7.29 (m, 2H), 7.25-7.19 (m, 3H), 4.60-4.57 (m, 1H), 4.22-4.19 (m, 1H), 3.45-3.39 (m, 1H), 2.86 (t, $J = 7.1$ Hz, 2H), 2.34-2.24 (m, 1H), 2.14-2.05 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 170.21, 149.03, 141.32, 140.98, 134.42, 132.94, 128.67, 128.63, 126.89, 126.76, 126.26, 125.35, 122.10, 119.15, 52.10, 50.67, 33.58, 31.06; LRMS (ESI) calcd for $\text{C}_{20}\text{H}_{17}\text{ClN}_2\text{O}$ $[\text{M}+\text{H}]^+$: 337.10, found 337.41.



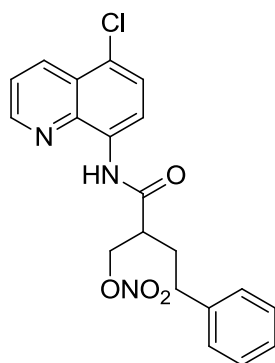
***N*-(5-chloroquinolin-8-yl)-2-((4-(2-hydroxyethyl)-2,3-dihydro-1H-1,2,3-triazol-1-yl)methyl)-4-phenylbutanamide (6c)**

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.72 (s, 1H), 8.83-8.82 (m, 1H), 8.67 (d, $J = 8.4$ Hz, 1H), 8.57-8.54 (m, 1H), 7.60-7.56 (m, 2H), 7.40 (s, 1H), 7.28-7.17 (m, 5H), 4.73-4.68 (m, 1H), 4.59-4.54 (m, 1H), 3.75 (s, 2H), 3.24-3.19 (m, 1H), 2.88-2.69 (m, 4H), 2.50 (s, 1H), 2.27-2.18 (m, 1H), 2.01-1.93 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 171.16, 149.04, 140.45, 138.92, 133.52, 133.08, 128.77, 128.55, 127.12, 126.50, 126.04, 125.24, 122.69, 116.73, 61.66, 51.84, 49.00, 33.19, 32.39, 28.59; LRMS (ESI) calcd for $\text{C}_{24}\text{H}_{25}\text{ClN}_5\text{O}_2$ $[\text{M}+\text{H}]^+$: 450.16, found 450.09



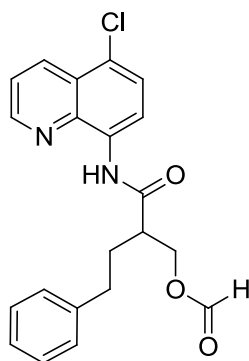
***N*-(5-chloroquinolin-8-yl)-2-(cyanomethyl)-4-phenylbutanamide (6e)**

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.92 (s, 1H), 8.87 (d, $J = 3.9$ Hz, 1H), 8.72 (d, $J = 8.4$ Hz, 1H), 8.60 (d, $J = 8.5$ Hz, 1H), 7.64-7.59 (m, 2H), 7.31-7.21 (m, 5H), 2.90-2.80 (m, 3H), 2.75-2.66 (m, 2H), 2.30-2.23 (m, 1H), 2.17-2.10 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 170.50, 149.00, 140.21, 139.08, 133.68, 133.13, 128.84, 128.59, 127.30, 126.59, 126.14, 125.30, 122.70, 118.03, 117.00, 44.07, 34.03, 33.00, 20.53; LRMS (ESI) calcd for $\text{C}_{21}\text{H}_{19}\text{ClN}_3\text{O}$ $[\text{M}+\text{H}]^+$: 364.11, found 363.96



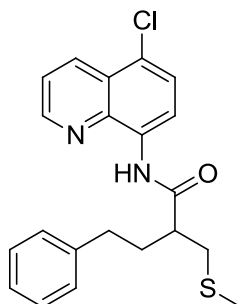
2-((5-Chloroquinolin-8-yl)carbamoyl)-4-phenylbutyl nitrate (6f)

$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.90 (s, 1H), 8.88-8.87 (m, 1H), 8.73 (d, $J = 8.4$ Hz, 1H), 8.60 (d, $J = 8.5$ Hz, 1H), 7.64-7.59 (m, 2H), 7.30-7.20 (m, 5H), 4.87-4.82 (m, 1H), 4.61-4.57 (m, 1H), 2.93-2.80 (m, 2H), 2.76-2.70 (m, 1H), 2.26-2.21 (m, 1H), 2.04-1.97 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 170.17, 148.98, 140.40, 139.06, 133.63, 133.25, 128.80, 128.58, 127.28, 126.55, 126.12, 125.18, 122.65, 116.94, 45.53, 33.12, 31.10; LRMS (ESI) calcd for $\text{C}_{20}\text{H}_{18}\text{ClN}_3\text{O}_4$ $[\text{M}+\text{H}]^+$: 400.10, found 400.03



2-((5-Chloroquinolin-8-yl)carbamoyl)-4-phenylbutyl formate (6g)

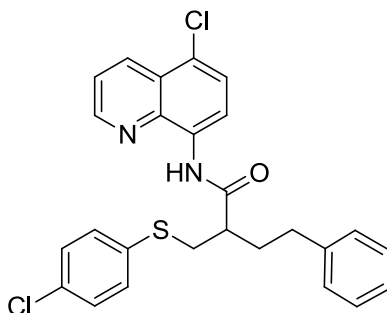
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.91 (s, 1H), 8.88-8.86 (m, 1H), 8.76 (d, $J = 8.4$ Hz, 1H), 8.61-8.58 (m, 1H), 8.03 (s, 1H), 7.64-7.58 (m, 2H), 7.30-7.20 (m, 5H), 4.49-4.40 (m, 2H), 2.91-2.78 (m, 2H), 2.75-2.69 (m, 1H), 2.24-2.16 (m, 1H), 1.99-1.91 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 171.27, 160.73, 148.91, 140.86, 139.13, 133.63, 133.53, 128.72, 128.61, 127.36, 126.40, 126.13, 124.91, 122.58, 116.87, 64.80, 47.19, 33.31, 30.93; LRMS (ESI) calcd for $\text{C}_{21}\text{H}_{19}\text{ClN}_3\text{O}_3$ $[\text{M}+\text{H}]^+$: 383.11, found 383.02



N-(5-chloroquinolin-8-yl)-2-((methylthio)methyl)-4-phenylbutanamide (6h)

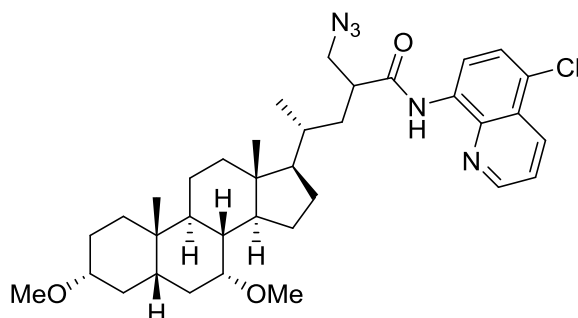
$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.91 (s, 1H), 8.88 (d, $J = 4.1$ Hz, 1H), 8.79 (d, $J = 8.4$ Hz, 1H), 8.58 (d, $J = 8.5$ Hz, 1H), 7.63-7.57 (m, 2H), 7.29-7.17 (m, 5H), 3.00-2.95 (m, 1H), 2.80-2.66 (m, 4H), 2.26-2.17 (m, 1H), 2.11 (s, 3H), 2.08-2.02 (m, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 172.91,

148.84, 141.24, 139.16, 133.65, 133.53, 128.60, 127.36, 126.20, 126.09, 124.65, 122.50, 116.76, 48.64, 37.28, 34.26, 33.57, 16.54; LRMS (ESI) calcd for C₂₁H₂₁ClN₂OS [M+H]⁺: 385.11, found 385.02



2-(((4-Chlorophenyl)thio)methyl)-N-(5-chloroquinolin-8-yl)-4-phenylbutanamide (6i)

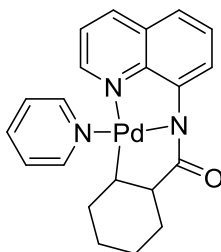
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.77 (s, 1H), 8.87-8.85 (m, 1H), 8.71 (d, *J* = 8.4 Hz, 1H), 8.60-8.58 (m, 1H), 7.62-7.58 (m, 2H), 7.28-7.14 (m, 10H), 3.36-3.31 (m, 1H), 3.12-3.07 (m, 1H), 2.80-2.73 (m, 1H), 2.69-2.60 (m, 2H), 2.28-2.19 (m, 1H), 2.05-1.98 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 172.29, 148.80, 141.04, 139.08, 134.00, 133.59, 133.43, 132.73, 131.87, 129.21, 128.64, 128.57, 127.35, 126.27, 126.08, 124.77, 122.54, 116.80, 48.20, 37.26, 34.24, 33.49; LRMS (ESI) calcd for C₂₆H₂₃Cl₂N₂OS [M+H]⁺: 481.08, found 480.85



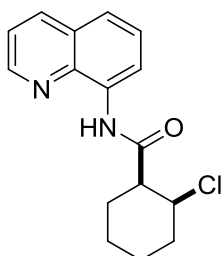
(4R)-2-(azidomethyl)-N-(4-chloronaphthalen-1-yl)-4-((3R,5S,7R,8R,9S,10S,13R,14S,17R)-3,7-dimethoxy-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-yl)pentanamide (6j)

Following the general procedure, substrate (40 mg, 0.67 mmol), NCS (18 mg, 0.14 mmol), Pd(OAc)₂ (1.5 mg, 0.07 mmol) and 2 ml AcOH were used. The reaction mixture was stirred at rt for 48 h. After completion of the reaction, NaN₃ (33mg, 0.5mmol), Cu(OAc)₂ (36mg, 0.2mmol) and 1mL DMF was added to the residue, the reaction mixture was stirred at 80°C for half an hour. After workup, the residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate=15: 1). Finally, compound (6j) (28 mg, colorless oil) was isolated in 65% yield.

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.92 (s, 1H), 8.88 (s, 1H), 8.3 (d, *J* = 8.4 Hz, 1H), 8.57 (d, *J* = 8.8 Hz, 1H), 7.61-7.59 (m, 2H), 3.74-3.69 (m, 1H), 3.46-3.41 (m, 1H), 3.33, (s, 3HHHHHhijhuip-), 3.23 (s, 3H), 3.14 (s, 1H), 2.99 (m 1H), 2.83 (s, 1H), 2.14-0.86 (m, 30H), 0.55 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 172.0, 149.0, 139.2, 133.6, 133.5, 127.3, 126.1, 124.7, 122.6, 116.9, 80.8, 56.5, 56.0, 55.5, 54.7, 50.3, 46.4, 42.6, 42.0, 39.7, 36.9, 35.43, 35.35, 34.8, 34.4, 33.8, 29.8, 28.4, 28.0, 26.9, 23.8, 23.1, 20.9, 18.9, 14.3, 11.9; HRMS (ESI) calcd for C₃₇H₅₁ClN₄O₃ [M+H]⁺: 636.36804, found 636.36680

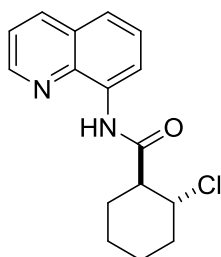


¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.14-9.10 (m, 1.42H), 8.95-8.94 (m, 2.93H), 8.14-8.12 (m, 1.45H), 7.92-7.88 (m, 1.41H), 7.77-7.67 (m, 1.55H), 7.53-7.45 (m, 4.31H), 7.23-7.17 (m, 2.94H), 2.94-2.82 (m, 1.43H), 2.63-2.51 (m, 1.46H), 2.14-2.11 (m, 1H), 1.96 (br, 0.49H), 1.76-1.09 (m, 11.35H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 185.76, 184.46, 152.60, 152.35, 147.21, 145.10, 144.91, 144.87, 137.84, 137.79, 137.44, 130.01, 129.94, 129.33, 125.72, 125.64, 120.51, 120.21, 120.17, 117.70, 117.66, 60.15, 56.01, 34.80, 34.66, 32.84, 32.77, 31.50, 28.96, 27.56, 27.19, 25.31; LRMS (ESI) calcd for C₂₁H₂₂N₃OPd [M+H]⁺: 438.07, found 437.90



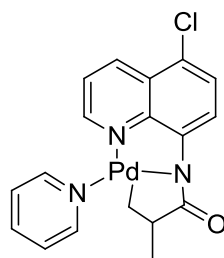
(1S,2S)-2-chloro-N-(quinolin-8-yl)cyclohexane-1-carboxamide

¹H-NMR (400 MHz, CDCl₃) δ (ppm) 10.14 (s, 1H), 8.83-8.81 (m, 2H), 8.16-8.14 (m, 1H), 7.56-7.43 (m, 3H), 4.96 (d, J = 1.4 Hz, 1H), 2.87-2.84 (m, 1H), 2.24-2.20 (m, 2H), 2.10-1.85 (m, 4H), 1.65-1.63 (m, 1H), 1.43-1.40 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 170.7, 148.4, 138.8, 136.4, 134.3, 128.1, 127.5, 121.8, 121.7, 116.8, 60.8, 50.9, 34.3, 24.9, 22.8, 19.9; LRMS (ESI) calcd for C₁₆H₁₇ClN₂O [M+H]⁺: 289.10, found 289.07



(1S,2R)-2-chloro-N-(quinolin-8-yl)cyclohexane-1-carboxamide

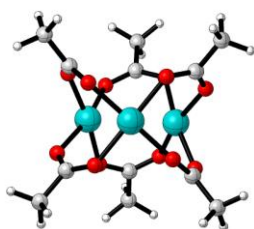
¹H-NMR (400 MHz, CDCl₃) δ (ppm) 9.91 (s, 1H), 8.84-8.81 (m, 2H), 8.17-8.15 (m, 1H), 7.56-7.44 (m, 3H), 4.28 (td, J = 10.7 Hz, J = 4.2 Hz, 1H), 2.70 (td, J = 11.8 Hz, J = 3.8 Hz, 1H), 2.39-2.34 (m, 1H), 2.15-2.12 (m, 1H), 2.19-1.72 (m, 4H), 1.47-1.40 (m, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ (ppm) 171.9, 148.3, 138.6, 136.5, 134.4, 128.1, 127.6, 121.84, 121.76, 116.9, 60.3, 56.4, 36.6, 30.9, 26.0, 24.6; LRMS (ESI) calcd for C₁₆H₁₇ClN₂O [M+H]⁺: 289.10, found 289.07



$^1\text{H-NMR}$ (400 MHz, CDCl_3) δ (ppm) 9.10 (d, $J = 8.6$ Hz, 1H), 8.82-8.81 (m, 2H), 8.56 (d, $J = 8.6$ Hz, 1H), 7.93-7.88 (m, 2H), 7.56-7.47 (m, 3H), 7.38-7.35 (m, 1H), 2.91-2.85 (m, 1H), 1.90 (t, $J = 8.2$ Hz, 1H), 1.57 (t, $J = 8.7$ Hz, 1H), 1.27-1.25 (m, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ (ppm) 187.90, 152.34, 146.47, 145.92, 145.39, 137.63, 134.89, 129.15, 127.51, 125.82, 121.26, 120.32, 120.21, 47.34, 21.34, 19.21; LRMS (ESI) calcd for $\text{C}_{18}\text{H}_{17}\text{ClN}_3\text{OPd}$ $[\text{M}+\text{H}]^+$:434.00, found 433.91

Cartesian coordinates (in Å) of related structures which calculated at the B3LYP/Lanl2dz + 6-31G(d) level of theory.

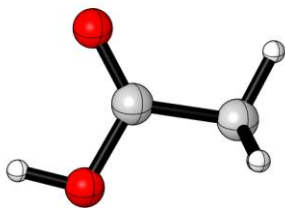
Pd3(OAc)6



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O	1.04306300	2.41870300	-1.28785500
O	-1.17047300	2.03750200	-1.63766000
C	-2.27679100	-1.26108000	1.89219700
O	-1.54781200	-2.11771700	1.31084200
O	-2.35771900	-0.01908700	1.65045800
C	-3.18399200	-1.78937100	2.98645000
H	-3.45042500	-0.98878100	3.67891400
H	-4.10289000	-2.16823500	2.52377000
H	-2.70064700	-2.61478800	3.51312400
C	-0.06696100	3.64838100	-2.97668900
H	0.89297200	3.65373300	-3.49714400
H	-0.88619600	3.46227800	-3.67360100
H	-0.21637400	4.63426600	-2.52102100
Pd	-0.00137800	-1.86134600	-0.00019000
C	-2.26830100	-1.34837800	-1.84767700
O	-2.65299300	-0.30004400	-1.24903300
O	-1.22867100	-2.03454400	-1.61581500
C	0.06542900	2.60373200	1.87744000

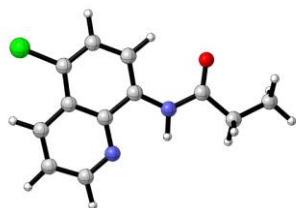
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O	-1.03965000	2.42052700	1.28788700
C	0.07253800	3.64762800	2.97728000
H	-0.88894700	3.65807400	3.49473400
H	0.88862700	3.45702500	3.67668800
H	0.22896100	4.63274300	2.52228300
C	-3.15645100	-1.82484800	-2.98071100
H	-3.11492800	-1.09396100	-3.79533600
H	-2.83124200	-2.80057800	-3.34375000
H	-4.19318200	-1.87436200	-2.63540100
Pd	-1.61369500	0.92869800	0.01071500
C	2.26616900	-1.35186200	1.84764700
O	2.65264100	-0.30415100	1.24904200
O	1.22555600	-2.03644500	1.61553300
C	3.15312800	-1.82951600	2.98111100
H	3.10978700	-1.09997000	3.79686100
H	2.82802700	-2.80599900	3.34223200
H	4.19039200	-1.87769400	2.63727400
C	2.27526300	-1.26390900	-1.89247000
O	2.35840500	-0.02211100	-1.65036800
O	1.54464200	-2.11937000	-1.31148500
C	3.18165900	-1.79352200	-2.98674800
H	4.09934900	-2.17515200	-2.52394700
H	2.69647400	-2.61728200	-3.51433700
H	3.45043300	-0.99303600	-3.67842000

AcOH



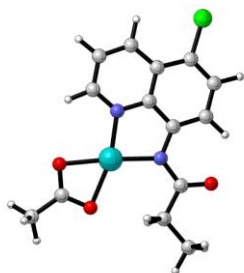
C	1.39644000	-0.09796500	0.00001100
H	1.68937000	-0.67787800	-0.88150700
H	1.68950700	-0.67615000	0.88262900
H	1.90754200	0.86497800	-0.00092100
C	-0.09571100	0.12412500	-0.00001900
O	-0.77154800	-1.05403300	0.00025200
H	-1.71869300	-0.81848700	0.00032100
O	-0.65840000	1.19566900	-0.00012800

5-Cl_sub



C	-4.39425400	-0.63601800	-1.16700100
C	-2.73490200	0.41062400	0.04407900
C	-3.32803100	1.69896900	-0.14686100
C	-4.52612400	1.74818500	-0.90350100
C	-5.05973900	0.58647100	-1.41301000
H	-4.79810600	-1.56769800	-1.56030700
C	-1.52017500	0.27701300	0.80130300
C	-2.68065300	2.82589200	0.43039300
H	-5.00845400	2.70506200	-1.07159500
H	-5.97574100	0.59776400	-1.99530500
C	-1.51841100	2.67744600	1.15074600
C	-0.93057900	1.40758000	1.34163400
H	-1.04030900	3.55038900	1.58241700
H	-0.01707400	1.30981600	1.91086500
N	-3.27908500	-0.72640100	-0.46892300
N	-1.03262700	-1.02418600	0.92445500
H	-1.62158100	-1.70401700	0.45117200
C	0.08334600	-1.46299200	1.60515700
O	0.85030700	-0.71834900	2.20055500
C	0.26488200	-2.98120400	1.56641600
H	-0.51247800	-3.42697600	2.20409700
H	0.06671300	-3.34582900	0.54949800
C	1.65131000	-3.41482400	2.04043400
H	1.84994600	-3.03786700	3.04700300
H	1.72769200	-4.50705100	2.05173900
H	2.43257000	-3.02119300	1.38263600
Cl	-3.36815700	4.43460200	0.22568100

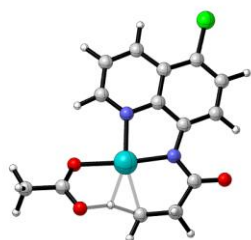
5-Cl_int



C	-4.46259300	3.75733500	0.57581000
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C	-2.10924300	3.26120000	0.85338000
C	-2.40067200	1.93501100	0.40890800
C	-3.70889400	1.49341800	0.04253100
C	-4.73107000	2.44421700	0.13977000
H	-0.51325100	4.55500800	1.52484600
H	-5.28503500	4.46282700	0.63625200
C	-0.76370200	3.55625800	1.18391200
H	-5.73784000	2.16323100	-0.12436900
C	-0.14350200	1.30083000	0.62895200
C	0.21126800	2.58714200	1.07372400
H	0.57883600	0.49823800	0.52204800
H	1.24547300	2.79738800	1.32325200
N	-1.39944200	1.00929800	0.31565700
C	-4.99841200	-0.40863100	-0.75595500
O	-6.06028100	0.21155200	-0.76627700
C	-4.95068700	-1.87135900	-1.17932300
H	-4.22674900	-1.98461000	-1.99468800
H	-4.54496600	-2.46849000	-0.35398500
N	-3.79301200	0.16173200	-0.36677000
Pd	-1.98923600	-0.79077100	-0.32362200
C	-0.83778700	-2.93914500	-0.75201200
C	-0.10558100	-4.21900900	-1.03173800
H	0.18014600	-4.24534800	-2.09009500
H	0.80207500	-4.27652500	-0.42671400
H	-0.75560300	-5.07481500	-0.83415000
O	-2.09215700	-2.83620000	-0.94594300
O	-0.21295000	-1.90283900	-0.33021500
Cl	-2.92655700	5.82295500	1.46149700
C	-6.32280100	-2.39825300	-1.60073300
H	-7.04524600	-2.31772600	-0.78321300
H	-6.72263900	-1.82842600	-2.44473500
H	-6.24707800	-3.45048500	-1.89616400

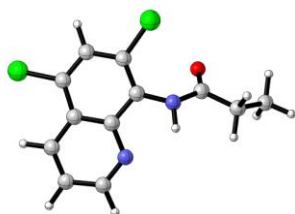
5-Cl



C	-4.53671400	3.77240700	0.65391600
C	-3.28016100	4.23393700	0.98558200

C	-2.15209100	3.37613100	0.89455900
C	-2.38275500	2.03837000	0.45274800
C	-3.68599500	1.55646200	0.10914000
C	-4.75218200	2.44927600	0.21858700
H	-0.60799100	4.74477200	1.54474800
H	-5.38542900	4.44427400	0.73032400
C	-0.81655000	3.73603600	1.20481800
H	-5.74592300	2.11315000	-0.04020400
C	-0.10090700	1.51184000	0.62982700
C	0.19971000	2.81409600	1.07448700
H	0.65887500	0.74697800	0.50759600
H	1.22672400	3.07385400	1.30766600
N	-1.34147600	1.15209800	0.33557100
C	-4.84908700	-0.41513000	-0.78661700
O	-5.97136400	0.07851200	-0.85012500
C	-4.54220200	-1.82534100	-1.28047600
H	-5.43344900	-2.43769700	-1.09972500
H	-4.43290000	-1.76143400	-2.37218900
C	-3.29112700	-2.46953900	-0.66685200
H	-3.39921400	-2.63028200	0.41283700
N	-3.73028000	0.23316900	-0.30849300
Pd	-1.98001900	-0.70780100	-0.28065500
C	0.09019000	-2.49536000	-1.08666800
C	1.47177500	-3.07339800	-1.28251700
H	2.21550000	-2.51218200	-0.71540900
H	1.47314100	-4.12003900	-0.96088800
H	1.72325800	-3.06016700	-2.34757300
O	-0.87511100	-3.01472400	-1.72767000
O	-0.05341200	-1.51957800	-0.28451400
H	-1.99184300	-2.48689000	-1.25187200
H	-3.19599700	-3.48536000	-1.07685200
Cl	-3.07771800	5.89570900	1.52516600

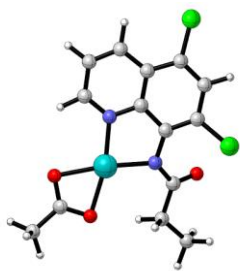
5-Cl_7-Cl_sub



C	-3.89076800	-0.94431700	-0.65232500
C	-2.26317500	0.54432100	0.01485500
C	-3.21162700	1.60831100	0.12991000

C	-4.55903000	1.31546500	-0.19422200
C	-4.90126500	0.04162100	-0.58723200
H	-4.13993300	-1.96178900	-0.94991700
C	-0.87424300	0.75148900	0.32327300
C	-2.73397700	2.87724400	0.56012000
H	-5.30556700	2.09913000	-0.12331200
H	-5.92565000	-0.21264000	-0.83997700
C	-1.41651200	3.06185000	0.89752700
C	-0.49206700	1.99285000	0.80731900
H	-1.07092300	4.02447400	1.25443800
N	-2.62392900	-0.71086200	-0.36909700
N	-0.02180800	-0.34950900	0.17447900
H	-0.54221800	-1.22221100	0.16022800
C	1.14545000	-0.34372800	-0.59681500
O	1.61392000	0.66430200	-1.08951500
C	1.79272100	-1.72198500	-0.71638900
H	2.23522000	-1.96168900	0.26084300
H	1.01618100	-2.48055100	-0.88716800
C	2.85583200	-1.77318700	-1.81266800
H	3.61989500	-1.01002000	-1.64343400
H	3.33812000	-2.75603300	-1.83360200
H	2.41583900	-1.58441100	-2.79710600
Cl	1.11293000	2.29310500	1.41654700
Cl	-3.84110000	4.23532300	0.69354400

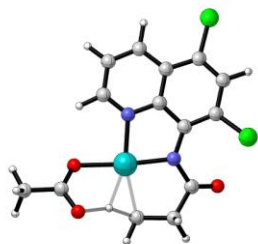
5-Cl_7-Cl_int



C	-4.53528900	3.56010300	0.39266200
C	-3.43354900	4.16500800	0.95248000
C	-2.18522000	3.48959900	0.98864400
C	-2.16476100	2.15990200	0.47597700
C	-3.31324300	1.47337300	-0.01883400
C	-4.47811100	2.24226300	-0.11828700
H	-0.95349400	5.03125800	1.87101600
H	-5.47184400	4.10080400	0.32323500
C	-0.96572200	4.02489400	1.46665800
C	0.14887500	1.98492400	0.84945800
C	0.19209400	3.27663700	1.40496600

H	1.03489000	1.36707100	0.74494600
H	1.13710000	3.67115800	1.76148900
N	-0.98823400	1.46209900	0.40948700
C	-4.04766300	-0.82102300	-0.03881000
O	-4.98632700	-0.57016700	0.70419400
C	-3.82274300	-2.21245500	-0.61706600
H	-3.53363500	-2.11899400	-1.66935100
H	-2.95523500	-2.66315300	-0.11753600
N	-3.11507800	0.15499400	-0.41916100
Pd	-1.13697000	-0.29902000	-0.55620000
C	0.40888400	-1.99006800	-1.46518100
C	1.35474300	-2.99286900	-2.05740500
H	2.28554300	-3.01833200	-1.48606700
H	0.88950100	-3.98110400	-2.08191400
H	1.58920000	-2.69902500	-3.08752500
O	-0.85425800	-2.11399500	-1.59969200
O	0.84211500	-0.96613300	-0.83057300
C	-5.04981200	-3.11081400	-0.45235100
H	-5.32998000	-3.20259500	0.60053400
H	-5.91338100	-2.69993900	-0.98527400
H	-4.84372600	-4.11078600	-0.84936500
Cl	-5.89168200	1.68072300	-0.96144500
Cl	-3.56832600	5.79868400	1.57680500

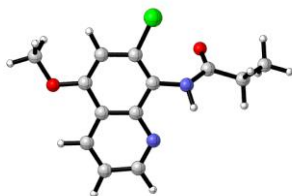
5-Cl_7-Cl



C	-4.47557000	3.87740700	0.34761200
C	-3.27169000	4.26148800	0.88907700
C	-2.17657000	3.35770200	0.91717600
C	-2.41623900	2.03662300	0.43688400
C	-3.69465700	1.58236000	-0.03404700
C	-4.68152200	2.57013800	-0.15085100
H	-0.66259600	4.66400200	1.73735400
H	-5.28852000	4.59027500	0.27523400
C	-0.86805300	3.66853100	1.35883700
C	-0.16788100	1.44418400	0.77889600
C	0.13008800	2.71958500	1.29336400
H	0.57983000	0.66367300	0.68396300

H	1.13993800	2.94151000	1.62075000
N	-1.38986600	1.12784700	0.37412800
C	-4.85814700	-0.57872400	-0.30550800
O	-5.88757900	-0.29054800	0.28104700
C	-4.61494100	-1.91268100	-1.00175600
H	-5.41066300	-2.60069600	-0.69823000
H	-4.72799100	-1.74025700	-2.08078400
C	-3.23198400	-2.52093900	-0.71910600
H	-3.13417500	-2.83479500	0.32740200
N	-3.74799400	0.25694600	-0.42922900
Pd	-1.99309900	-0.69542100	-0.36233400
C	0.09577600	-2.42865800	-1.20526100
C	1.48242900	-2.99310800	-1.40504200
H	2.20414500	-2.50128800	-0.75166300
H	1.46750400	-4.06843000	-1.20017700
H	1.77743500	-2.86547400	-2.45138000
O	-0.85035300	-2.88983000	-1.91480400
O	-0.07037000	-1.51870900	-0.33139100
H	-1.98762000	-2.40548300	-1.40859200
H	-3.15772100	-3.45342300	-1.29644700
Cl	-6.16909100	2.31104100	-1.01652900
Cl	-3.08257100	5.89736200	1.49599800

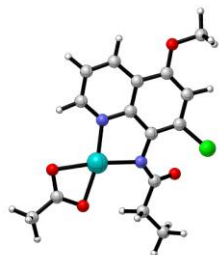
5-OMe_7-Cl_sub



C	-3.90355500	-0.98889700	-0.73920400
C	-2.28835400	0.41887600	0.10681800
C	-3.24390200	1.45327400	0.32835800
C	-4.58573500	1.20198800	-0.03804200
C	-4.92028100	-0.02205800	-0.57609000
H	-4.14573700	-1.96786600	-1.15122200
C	-0.90807000	0.60490400	0.45953500
C	-2.80838600	2.68667200	0.90681800
H	-5.32992100	1.97581700	0.11565800
H	-5.94051700	-0.25143200	-0.86719400
C	-1.49170800	2.83832200	1.28268000
C	-0.55841500	1.78831900	1.08266000
H	-1.13718700	3.74661500	1.75151300

N	-2.63834000	-0.78777000	-0.41892000
N	-0.02995200	-0.46263700	0.20347700
H	-0.52788200	-1.34417400	0.12185600
C	1.11459700	-0.35680400	-0.58693100
O	1.56450600	0.70489900	-0.97663500
C	1.77401400	-1.70590800	-0.87437800
H	2.14140900	-2.10882700	0.07970700
H	1.01024100	-2.41467100	-1.22473400
C	2.91345800	-1.59334200	-1.88569900
H	3.67073800	-0.88639800	-1.53637100
H	3.38741000	-2.56849800	-2.04051700
H	2.54768500	-1.22945200	-2.85084500
Cl	1.04304400	2.03947200	1.73262500
O	-3.77586400	3.63247900	1.05808200
C	-3.41089200	4.87863900	1.63447700
H	-2.64624100	5.38648600	1.03310900
H	-4.32158900	5.47946800	1.64915200
H	-3.04082100	4.75028300	2.65974600

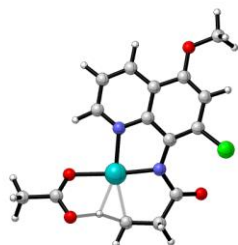
5-OMe_7-Cl_int



C	-4.52731300	3.59370000	0.13778800
C	-3.44377800	4.21086200	0.72796700
C	-2.20895500	3.50104800	0.82544500
C	-2.18168500	2.15911500	0.35708500
C	-3.31401200	1.47393900	-0.16346400
C	-4.45661100	2.25508800	-0.32897500
H	-1.01855500	5.07131200	1.70215200
H	-5.46346200	4.11942600	0.00195700
C	-1.01278600	4.05147300	1.33309300
C	0.11428700	1.98855800	0.82545900
C	0.14488500	3.29589100	1.34230300
H	1.00127300	1.36515200	0.77353400
H	1.07841100	3.69616600	1.72204100
N	-1.00668600	1.45389300	0.35594000
C	-4.04525700	-0.81771200	-0.09087700
O	-5.01251000	-0.52558700	0.60180400
C	-3.79380200	-2.24818600	-0.55678900

H	-3.44877600	-2.23259800	-1.59563500
H	-2.95666400	-2.66118200	0.02191000
N	-3.11495300	0.13308500	-0.51886100
Pd	-1.13530200	-0.32454900	-0.58456400
C	0.42541100	-2.03733800	-1.43312500
C	1.37803300	-3.05472700	-1.99130800
H	2.29546800	-3.07926000	-1.39867100
H	0.90667600	-4.04015500	-2.01379300
H	1.63784200	-2.77611100	-3.01957000
O	-0.83422900	-2.15502400	-1.59974000
O	0.85247500	-1.01140000	-0.79904500
C	-5.03068100	-3.13344500	-0.39308400
H	-5.36964100	-3.14415900	0.64635400
H	-5.86183800	-2.76483600	-1.00319600
H	-4.80682500	-4.16083400	-0.70101700
Cl	-5.84791900	1.67504800	-1.20110600
O	-3.42530100	5.48360300	1.21107000
C	-4.62007700	6.24905500	1.12547300
H	-5.43911800	5.77005900	1.67660700
H	-4.38967900	7.21381200	1.57989600
H	-4.92256700	6.39937500	0.08129200

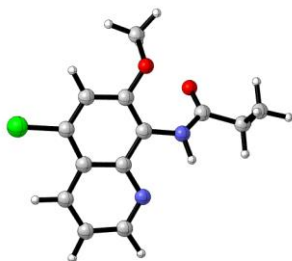
5-OMe_7-Cl



C	-4.58173700	3.78692600	0.46533900
C	-3.38705600	4.18592100	1.02477800
C	-2.28298900	3.28089700	1.02031500
C	-2.49328300	1.97190500	0.50548700
C	-3.75767800	1.50889100	0.01775900
C	-4.75361800	2.48362300	-0.06988700
H	-0.81941300	4.61224300	1.87652700
H	-5.42151700	4.46603700	0.39579500
C	-0.98955500	3.61976500	1.47371900
C	-0.23075100	1.43105700	0.83739300
C	0.03538100	2.69800900	1.38712400
H	0.53751800	0.67320700	0.72284400
H	1.03917900	2.93538200	1.72238300
N	-1.44324500	1.09148300	0.41927100

C	-4.86704700	-0.67268300	-0.29699700
O	-5.90240300	-0.41764100	0.29819500
C	-4.60188600	-1.99191900	-1.01540400
H	-5.37319300	-2.70519800	-0.70650000
H	-4.74147800	-1.80832100	-2.08944500
C	-3.19844000	-2.56845600	-0.76988600
H	-3.07885400	-2.91224400	0.26505200
N	-3.78356600	0.18907200	-0.42731800
Pd	-2.00618700	-0.72140400	-0.37325100
C	0.12431700	-2.38601900	-1.25639500
C	1.52168300	-2.91818100	-1.47238600
H	2.23438200	-2.42931400	-0.80689400
H	1.52842300	-3.99856800	-1.29535500
H	1.81309500	-2.75775400	-2.51523700
O	-0.81203200	-2.84703400	-1.98067600
O	-0.06000100	-1.50574200	-0.35808400
H	-1.95512400	-2.40195700	-1.46517600
H	-3.10485600	-3.47938600	-1.37808800
Cl	-6.23929300	2.21877300	-0.94217900
O	-3.13676800	5.41187500	1.56429600
C	-4.19153500	6.36389200	1.57601500
H	-3.78602500	7.25347600	2.06048100
H	-4.51214100	6.61639900	0.55714400
H	-5.05310000	5.99583500	2.14746000

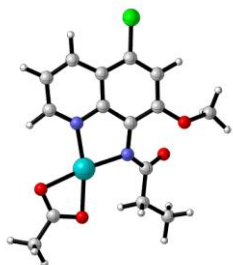
5-Cl_7-OMe_sub



C	-1.33712000	3.21664200	-0.10190900
C	-0.68138500	1.00903900	-0.20513700
C	-2.01773300	0.55029000	0.03028000
C	-3.01964400	1.53369000	0.21390800
C	-2.68349100	2.86711300	0.14976600
H	-1.05014400	4.26546900	-0.16625000
C	0.39159000	0.08010300	-0.38836400
C	-2.23355500	-0.85430800	0.05933200
H	-4.04238800	1.22273800	0.39861500
H	-3.43060500	3.64283900	0.28415700

C	-1.20869200	-1.73839600	-0.17068500
C	0.11039300	-1.28123000	-0.42826700
H	-1.41225100	-2.80229900	-0.19593800
N	-0.37115500	2.33478500	-0.26985700
N	1.67308400	0.61368000	-0.58962200
H	1.64089800	1.59053200	-0.86433800
C	2.82420800	0.19697300	0.06256600
O	2.87008300	-0.76473000	0.81247200
C	4.05522700	1.03521300	-0.28282000
H	4.41096400	0.69730800	-1.26664100
H	3.76947900	2.08777400	-0.41219600
C	5.16606700	0.89487800	0.75771600
H	5.42825400	-0.15703900	0.89665300
H	6.06021500	1.44339600	0.44335500
H	4.84780200	1.28612700	1.72972200
Cl	-3.84894200	-1.48815600	0.36044400
O	1.08371400	-2.14938900	-0.81236800
C	1.33501700	-3.27722000	0.03019300
H	2.16969300	-3.80864600	-0.43012100
H	1.62097300	-2.94204600	1.03043800
H	0.46995600	-3.95053600	0.08103900

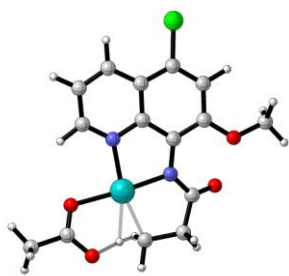
5-Cl_7-OMe_int



C	3.39869400	0.80592100	-0.43441600
C	3.60966100	-0.51352900	-0.10137700
C	2.51462400	-1.38149500	0.14281300
C	1.21545500	-0.79146600	0.07826700
C	0.98062900	0.58432200	-0.16511800
C	2.09604400	1.36181900	-0.51248500
H	3.56362700	-3.23938800	0.48580400
H	4.24929600	1.43150000	-0.67833000
C	2.59006000	-2.76462900	0.42527900
C	0.18678200	-2.86161100	0.50469900
C	1.43626100	-3.50027700	0.61060400
H	-0.75026900	-3.39816700	0.61420300
H	1.47410400	-4.56297100	0.82269800
N	0.09485900	-1.56341200	0.24986200

C	-0.64949000	2.22434200	0.49467100
O	0.20022400	2.91761800	1.04614200
C	-2.11071900	2.65578600	0.43330500
H	-2.49769900	2.46434900	-0.57324400
H	-2.69675300	2.00570200	1.09598200
N	-0.34944900	1.00757900	-0.11338300
Pd	-1.62929700	-0.56977800	-0.07231200
C	-4.01165800	-1.14637200	-0.34922300
C	-5.45333500	-1.50586500	-0.56269000
H	-5.69948100	-2.42116600	-0.01952200
H	-6.09802200	-0.68308100	-0.24448700
H	-5.62470000	-1.68057900	-1.63157800
O	-3.61269400	0.06198100	-0.44650500
O	-3.13834300	-2.04485700	-0.09012700
C	-2.30064000	4.12027000	0.83133100
H	-1.91675800	4.30620100	1.83819700
H	-1.76351400	4.78720700	0.14894500
H	-3.36321600	4.38601200	0.80625400
Cl	5.25273400	-1.13340900	-0.03013100
O	1.89786400	2.60384100	-1.01308200
C	2.69093900	3.67539300	-0.49749800
H	2.58455300	3.73072100	0.58886200
H	3.74674400	3.57523900	-0.77993500
H	2.28916100	4.58268500	-0.95104100

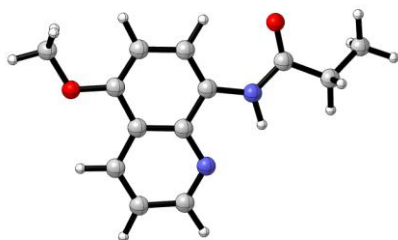
5-Cl_7-OMe



C	-4.34322600	3.99799700	0.30103000
C	-3.13571000	4.34398800	0.86961700
C	-2.06142600	3.42179900	0.91134400
C	-2.32680800	2.11006400	0.40627700
C	-3.59492000	1.70239700	-0.08986700
C	-4.57064300	2.70694100	-0.23532000
H	-0.53147100	4.67374900	1.78396300
H	-5.12351800	4.74604600	0.23566800
C	-0.75710100	3.68852000	1.38976300
C	-0.10907800	1.44566200	0.81218600
C	0.21393000	2.71009900	1.34278000

H	0.61812000	0.64366500	0.73683100
H	1.22094800	2.89881000	1.69834600
N	-1.32530300	1.16710400	0.36877300
C	-4.84963700	-0.39290200	-0.44875600
O	-5.90390200	-0.05743200	0.06960700
C	-4.63086100	-1.73971500	-1.13202900
H	-5.46757200	-2.39367100	-0.86464200
H	-4.68718800	-1.56760000	-2.21564300
C	-3.28841800	-2.40403100	-0.78665000
H	-3.25015800	-2.71502100	0.26467500
N	-3.69585500	0.38025000	-0.50435100
Pd	-1.98299900	-0.63353400	-0.38589800
C	0.06061100	-2.45693500	-1.15543000
C	1.42589700	-3.08536100	-1.30859000
H	2.15464600	-2.60291900	-0.65592100
H	1.36121700	-4.15149400	-1.06746000
H	1.74677700	-3.00676600	-2.35199700
O	-0.88260300	-2.88333000	-1.89197800
O	-0.09239100	-1.53543900	-0.29347400
H	-2.00871000	-2.34832900	-1.42820200
H	-3.22915700	-3.34314900	-1.35509600
Cl	-2.92842600	5.96900800	1.50858700
O	-5.67238300	2.40490900	-0.95214700
C	-6.85273700	3.17840000	-0.78845900
H	-7.12608700	3.26245200	0.26991000
H	-6.74657200	4.18037500	-1.22536500
H	-7.63439000	2.63546600	-1.32100000

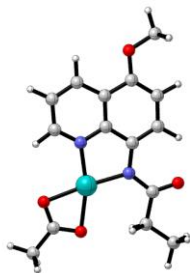
5- OMe_sub



C	-4.33957100	-0.59536600	-1.20399800
C	-2.69809900	0.40812000	0.06555200
C	-3.25506100	1.70399300	-0.14798400
C	-4.42176100	1.79016700	-0.94390700
C	-4.96742300	0.64122600	-1.47418800
H	-4.75255400	-1.51702500	-1.61230100
C	-1.51482200	0.25845800	0.86494200
C	-2.62308200	2.84336800	0.44036100

H	-4.86729300	2.76263400	-1.12316000
H	-5.86167800	0.67278600	-2.08891500
C	-1.48691100	2.66956700	1.20375300
C	-0.93224500	1.38341500	1.41668500
H	-0.99042100	3.51842500	1.65949600
H	-0.04054900	1.27258600	2.01778200
N	-3.25127900	-0.71686300	-0.46686300
N	-1.05087900	-1.05570700	1.01121200
H	-1.63531200	-1.72661100	0.52168400
C	0.03051400	-1.50630700	1.72655900
O	0.79578500	-0.77192800	2.34222000
C	0.19100700	-3.02791000	1.72176700
H	-0.35953300	-3.41321300	2.59213800
H	-0.28893800	-3.46277800	0.83585500
C	1.65886700	-3.45098000	1.81196200
H	2.13590400	-2.97353400	2.67160900
H	1.74324600	-4.53766500	1.91740700
H	2.21175000	-3.15068200	0.91516200
O	-3.22748100	4.04048000	0.17927900
C	-2.65000000	5.21168900	0.73273900
H	-3.27872600	6.04126300	0.40420300
H	-2.64022400	5.17382500	1.83001400
H	-1.62546000	5.36403000	0.36853100

5- OMe_int



C	-4.56258300	3.68219100	0.42083600
C	-3.34732000	4.18737800	0.84166400
C	-2.21064200	3.32725600	0.83461100
C	-2.38684900	1.98366500	0.39320500
C	-3.63593400	1.45781000	-0.04216200
C	-4.71360800	2.34456000	-0.01490900
H	-0.76747000	4.74568200	1.57861200
H	-5.44519800	4.31188900	0.41474700
C	-0.91760900	3.72627000	1.24019800
H	-5.68305000	1.99700000	-0.33493000
C	-0.10869000	1.51457500	0.75915700
C	0.13062400	2.82703700	1.20312400

H	0.67304100	0.76339800	0.71003600
H	1.13146400	3.11096900	1.50942700
N	-1.31963600	1.12822100	0.37537000
C	-4.74095100	-0.53198400	-0.90420100
O	-5.83946800	0.01950600	-0.99139900
C	-4.57545400	-1.99122300	-1.31509900
H	-3.79072300	-2.06277700	-2.07723900
H	-4.19459700	-2.56242200	-0.46042600
N	-3.60833500	0.11192400	-0.44138700
Pd	-1.75663800	-0.71928400	-0.25285300
C	-0.46034700	-2.81097500	-0.52951900
C	0.34336200	-4.07021400	-0.68404100
H	1.39366300	-3.88518200	-0.45129200
H	-0.05338500	-4.84047400	-0.01394400
H	0.24638400	-4.44446700	-1.70822600
O	-1.70213300	-2.78572900	-0.81238300
O	0.07941400	-1.73042800	-0.10484500
C	-5.88040200	-2.60031200	-1.82934800
H	-6.66220700	-2.56257100	-1.06498000
H	-6.25367900	-2.05553700	-2.70164800
H	-5.72171400	-3.64652000	-2.11392600
O	-3.11359700	5.46061500	1.27659500
C	-4.21043500	6.36092900	1.31167800
H	-3.81185600	7.30518600	1.68667200
H	-4.63368500	6.51514400	0.31059100
H	-4.99939000	6.00378400	1.98628400

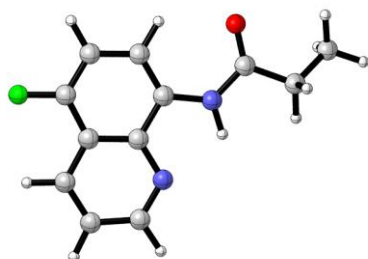
5- OMe



C	-4.62895300	3.73463600	0.52574800
C	-3.38254700	4.23154400	0.85890500
C	-2.24892600	3.36665500	0.78758500
C	-2.45161000	2.01898000	0.37506300
C	-3.74061900	1.51114400	0.03362500
C	-4.81389100	2.39263600	0.11768100
H	-0.75626600	4.79100400	1.42004900
H	-5.50398200	4.37301200	0.57138600
C	-0.93066200	3.76863300	1.10268000

H	-5.80040400	2.03574500	-0.14222000
C	-0.16070400	1.54882300	0.58634200
C	0.10956900	2.86613700	1.00355900
H	0.61707100	0.79831300	0.48893500
H	1.12895500	3.15189700	1.24003800
N	-1.39010900	1.15204800	0.28810900
C	-4.85872000	-0.50110700	-0.83334300
O	-5.98948400	-0.02566400	-0.92482100
C	-4.52698400	-1.91938800	-1.28895500
H	-5.40813000	-2.54233700	-1.09385100
H	-4.41550300	-1.88431000	-2.38177200
C	-3.26713300	-2.52524100	-0.65424800
H	-3.38135200	-2.66717300	0.42750800
N	-3.76032900	0.17104100	-0.35716100
Pd	-1.99243900	-0.73151500	-0.29362000
C	0.11977700	-2.49699000	-1.04629900
C	1.51171600	-3.05693400	-1.22319900
H	2.24279000	-2.47260800	-0.66290200
H	1.52826300	-4.09696600	-0.88110400
H	1.76970800	-3.06034800	-2.28681600
O	-0.83226600	-3.04651100	-1.68414000
O	-0.04543600	-1.50926600	-0.26550800
H	-1.95651300	-2.53138000	-1.23085400
H	-3.14733800	-3.54663200	-1.04365300
O	-3.11383600	5.50829000	1.26346500
C	-4.19925300	6.41777900	1.35637900
H	-3.77046100	7.36385400	1.69141600
H	-4.68522000	6.56171600	0.38256200
H	-4.94577400	6.07663000	2.08543600

5- F_sub



C	-4.35452600	-0.62300000	-1.22082600
C	-2.72405200	0.39478500	0.04831800
C	-3.30660500	1.68215900	-0.15599800
C	-4.47908300	1.76119300	-0.94598100
C	-5.00519300	0.60702000	-1.48019600
H	-4.75568900	-1.54702000	-1.63480900

C	-1.53426600	0.26633900	0.84320500
C	-2.68041000	2.80112200	0.44095500
H	-4.94110500	2.72824000	-1.11607800
H	-5.90222100	0.62569500	-2.09111500
C	-1.54569700	2.67272600	1.19735200
C	-0.96435600	1.39892700	1.40262600
H	-1.09488200	3.55579100	1.63792900
H	-0.06853500	1.29815600	1.99874900
N	-3.26152500	-0.73441300	-0.48983500
N	-1.04606000	-1.03715900	0.98094600
H	-1.61852400	-1.71845700	0.49136700
C	0.04903800	-1.47147100	1.69175000
O	0.80098100	-0.72390900	2.30512200
C	0.23384600	-2.98967800	1.67968300
H	-0.36135700	-3.39447400	2.51112000
H	-0.18966500	-3.41782300	0.76211900
C	1.69975400	-3.39391500	1.84669000
H	2.12137000	-2.92760100	2.74064200
H	1.79241500	-4.48118500	1.93671100
H	2.29849700	-3.06924700	0.98892500
F	-3.23882600	4.01799600	0.24183200

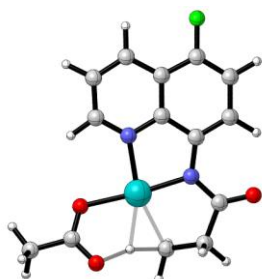
5- F_int



C	-4.52955700	3.73914000	0.59103000
C	-3.29116700	4.21647100	0.93979700
C	-2.15229500	3.38608700	0.88397300
C	-2.35168000	2.04192700	0.45231800
C	-3.62552100	1.51784200	0.08392200
C	-4.70717200	2.40368600	0.16542000
H	-0.67572100	4.81368100	1.55463000
H	-5.38599500	4.40375300	0.64485200
C	-0.84128100	3.79344300	1.22436700
H	-5.69082400	2.05341200	-0.10311800
C	-0.05848700	1.58002100	0.70009300
C	0.20157000	2.89506700	1.13293500
H	0.72271000	0.83218900	0.61029300
H	1.21692300	3.17853600	1.38732700

N	-1.28568300	1.18976700	0.37863800
C	-4.77844700	-0.47445900	-0.70500200
O	-5.87903800	0.07599500	-0.72953800
C	-4.63406700	-1.93501900	-1.11521300
H	-3.90556500	-2.00702200	-1.93136600
H	-4.18824400	-2.49660400	-0.28597200
N	-3.61840800	0.17521600	-0.31272600
Pd	-1.75462100	-0.65478200	-0.23740200
C	-0.47297400	-2.73630500	-0.61867500
C	0.33519000	-3.97383800	-0.87980000
H	0.62383500	-3.99700600	-1.93746000
H	1.24365400	-3.96924400	-0.27323400
H	-0.26297600	-4.86428600	-0.67176000
O	-1.73022100	-2.71185000	-0.82157900
O	0.08613600	-1.65890500	-0.20873600
C	-5.96825900	-2.55642000	-1.52955000
H	-6.69312900	-2.51856500	-0.71099000
H	-6.40747700	-2.02147900	-2.37680400
H	-5.82241200	-3.60356800	-1.81697400
F	-3.12490800	5.49578000	1.34696400

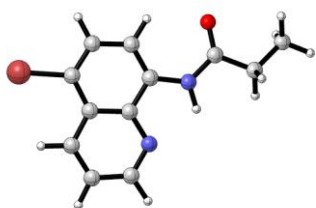
5- F



C	-4.53629000	3.77678600	0.66217400
C	-3.27683300	4.21559000	0.98830300
C	-2.15443900	3.36268200	0.89732300
C	-2.38475500	2.02828600	0.45503900
C	-3.68849000	1.55390200	0.11277200
C	-4.75218300	2.45083200	0.22449700
H	-0.63512800	4.75508800	1.55200800
H	-5.37267600	4.46344200	0.74485000
C	-0.82797900	3.74258400	1.21268100
H	-5.74563400	2.11483900	-0.03567900
C	-0.10178400	1.52016500	0.63771100
C	0.19340200	2.82547800	1.08376900
H	0.66449900	0.76132000	0.51742700
H	1.21964100	3.08747600	1.31778600
N	-1.33838700	1.14809900	0.33984100

C	-4.84965100	-0.41712800	-0.78927800
O	-5.97168700	0.07894800	-0.85696400
C	-4.54413500	-1.82832800	-1.28227800
H	-5.43471400	-2.44093400	-1.09864300
H	-4.43700600	-1.76656000	-2.37430100
C	-3.29192900	-2.47129700	-0.66964900
H	-3.39988500	-2.63338300	0.40986300
N	-3.73359100	0.22726700	-0.30747200
Pd	-1.98058600	-0.71080100	-0.27983500
C	0.09013900	-2.49560300	-1.09106600
C	1.47123900	-3.07410800	-1.29000800
H	2.21573500	-2.51536800	-0.72142900
H	1.47219700	-4.12188600	-0.97208400
H	1.72209200	-3.05727200	-2.35517400
O	-0.87577300	-3.01276500	-1.73341600
O	-0.05227600	-1.52257100	-0.28594200
H	-1.99164100	-2.48665100	-1.25609100
H	-3.19453800	-3.48651700	-1.08067700
F	-3.07288700	5.48532900	1.40934400

5- Br_sub



C	-4.38772900	-0.63786500	-1.17492400
C	-2.73353800	0.41176800	0.04102400
C	-3.33091800	1.69941200	-0.14485400
C	-4.52838600	1.74420800	-0.90250900
C	-5.05757300	0.58281800	-1.41683200
H	-4.78728200	-1.56995800	-1.57161800
C	-1.51850400	0.27845400	0.79807000
C	-2.68758200	2.82543800	0.43750400
H	-5.01262200	2.70085200	-1.06651500
H	-5.97320100	0.59325300	-1.99973000
C	-1.52539100	2.67682200	1.15732200
C	-0.93269400	1.40843600	1.34341800
H	-1.04827000	3.54736900	1.59404500
H	-0.01897900	1.31183200	1.91260300
N	-3.27270800	-0.72556300	-0.47641800
N	-1.02730300	-1.02150700	0.91552300

H	-1.61444400	-1.70080100	0.43910000
C	0.09045800	-1.46027700	1.59375900
O	0.85541700	-0.71615700	2.19217800
C	0.27615200	-2.97772400	1.54732300
H	-0.50277800	-3.42923000	2.17902900
H	0.08303200	-3.33678900	0.52743600
C	1.66172100	-3.41071100	2.02428200
H	1.85528000	-3.04002600	3.03417100
H	1.74087600	-4.50278900	2.02862700
H	2.44462000	-3.01065400	1.37236900
Br	-3.43113500	4.57789300	0.22963100

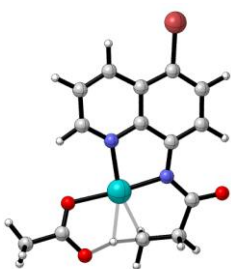
5- Br_int



C	-4.48307300	3.74188600	0.58728900
C	-3.22662100	4.19985300	0.92072500
C	-2.10919900	3.32836900	0.84791100
C	-2.35405200	1.98793900	0.41978300
C	-3.65342700	1.50605600	0.07335500
C	-4.70903500	2.41534800	0.16797600
H	-0.55601400	4.68278800	1.49455500
H	-5.32907900	4.41810700	0.64777800
C	-0.77208700	3.67203400	1.16554000
H	-5.70609700	2.08839400	-0.08612100
C	-0.07425400	1.43301300	0.62709000
C	0.23407900	2.73654500	1.05833000
H	0.67014600	0.65215800	0.52136500
H	1.26161400	2.98600000	1.29948200
N	-1.31971400	1.09321400	0.32562400
C	-4.90489000	-0.42487800	-0.68389400
O	-5.98498400	0.16504500	-0.68581800
C	-4.82958100	-1.88868900	-1.11492600
H	-4.10864800	-1.95395300	-1.93816600
H	-4.38969600	-2.46452000	-0.29067300
N	-3.71224300	0.17222800	-0.32098100
Pd	-1.89105700	-0.73203100	-0.29320000
C	-0.55376000	-2.65394700	-0.59656400
C	0.37873200	-3.82351300	-0.83384300

H	1.07874800	-3.57212600	-1.63770700
H	0.96730700	-4.01306000	0.06900400
H	-0.18400500	-4.71909500	-1.10712800
O	-1.78554100	-2.71589000	-0.78448400
O	-0.01913700	-1.53525300	-0.20726700
C	-6.16066400	-2.50095900	-1.52998900
H	-6.84175100	-2.66734300	-0.67267800
H	-6.65700200	-1.92937000	-2.31944400
H	-6.00146900	-3.51866600	-1.91242900
Br	-3.00475100	6.01346300	1.48067100

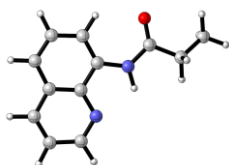
5- Br



C	-4.53521100	3.77278100	0.65125600
C	-3.27946600	4.23580300	0.98272100
C	-2.15150100	3.37832700	0.89273700
C	-2.38178900	2.03981900	0.45156100
C	-3.68506800	1.55708900	0.10798200
C	-4.75138400	2.44960800	0.21675700
H	-0.60781000	4.74440800	1.54215100
H	-5.38567100	4.44196700	0.72624000
C	-0.81509000	3.73522400	1.20250200
H	-5.74534100	2.11367200	-0.04156200
C	-0.10020600	1.51109200	0.62873000
C	0.20090000	2.81313900	1.07286600
H	0.65878000	0.74540900	0.50671600
H	1.22787400	3.07285500	1.30627900
N	-1.34118600	1.15265400	0.33472400
C	-4.84871500	-0.41474400	-0.78605100
O	-5.97094600	0.07880800	-0.84915300
C	-4.54198700	-1.82509300	-1.27949500
H	-5.43339400	-2.43720000	-1.09871900
H	-4.43256600	-1.76138300	-2.37121500
C	-3.29104700	-2.46934200	-0.66566500
H	-3.39911200	-2.62954100	0.41410800
N	-3.72945700	0.23395700	-0.30872000
Pd	-1.97962600	-0.70751100	-0.28048500
C	0.09007600	-2.49602800	-1.08569200

C	1.47151800	-3.07446000	-1.28132300
H	2.21533700	-2.51339100	-0.71419900
H	1.47255000	-4.12107800	-0.95962500
H	1.72310700	-3.06137700	-2.34635800
O	-0.87535100	-3.01548100	-1.72644600
O	-0.05331400	-1.51984300	-0.28399100
H	-1.99182700	-2.48723800	-1.25081000
H	-3.19633100	-3.48538600	-1.07519800
Br	-3.07366000	6.04468600	1.56597000

5- H_sub



C	2.25797200	-2.26589200	-0.00020800
C	1.17539100	-0.23313500	-0.00555800
C	2.40546500	0.49146900	0.03117500
C	3.59890600	-0.27456300	0.05174300
C	3.53107500	-1.64923900	0.03633400
H	2.17967600	-3.35220700	-0.01306300
C	-0.06970000	0.48514400	-0.02834000
C	2.38118800	1.91008600	0.04498500
H	4.55766700	0.23802900	0.07981500
H	4.42816600	-2.26056200	0.05161000
C	1.17187100	2.56822600	0.02321700
C	-0.05844800	1.87081200	-0.01292300
H	1.14797700	3.65455400	0.03417300
H	-0.99763400	2.40567000	-0.02866900
N	1.12261400	-1.59418700	-0.02056400
N	-1.21547000	-0.31388700	-0.06450700
H	-0.99255000	-1.30524900	-0.07338400
C	-2.53514200	0.07464100	-0.11477700
O	-2.90220500	1.24275200	-0.09997700
C	-3.51845900	-1.09211100	-0.22514600
H	-3.60533100	-1.34302800	-1.29241600
H	-3.10641500	-1.98301000	0.26605700
C	-4.89590900	-0.74278400	0.34033700
H	-5.27783600	0.16821600	-0.12723000
H	-5.60486100	-1.55762200	0.16040600
H	-4.84528800	-0.56506100	1.41988100
H	3.31881400	2.45885500	0.07308800

5- H_int



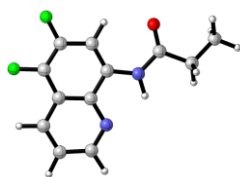
C	-3.92390500	1.63397500	0.00781400
C	-4.33231700	0.31597000	0.00821700
C	-3.34766100	-0.70004100	0.00450300
C	-1.97473700	-0.31287200	0.00078200
C	-1.55012000	1.05046300	0.00044600
C	-2.56407500	2.01554000	0.00381000
H	-4.66499400	-2.41618300	0.00690300
H	-4.67075600	2.42365700	0.01052100
C	-3.62838500	-2.08879200	0.00419200
H	-2.29301800	3.05900600	0.00350700
C	-1.27122900	-2.55836000	-0.00289500
C	-2.60354500	-3.01252300	0.00033000
H	-0.42321800	-3.23530400	-0.00575500
H	-2.80076600	-4.07904600	-0.00027700
N	-0.99036200	-1.26099800	-0.00243200
C	0.40398200	2.50274600	-0.00179300
O	-0.26089800	3.53776200	0.00281400
C	1.92703600	2.56244400	-0.00752700
H	2.31105500	2.00288600	0.85331100
H	2.30225400	2.02466300	-0.88631500
N	-0.16446100	1.23676000	-0.00320000
Pd	0.86679000	-0.52496400	-0.00626800
C	3.12924400	-1.53334400	-0.00790300
C	4.48685200	-2.17341800	0.03057800
H	4.81440900	-2.25742900	1.07371300
H	4.44623700	-3.17610500	-0.40097300
H	5.21042200	-1.55279600	-0.50350100
O	2.99495600	-0.26726600	-0.01145000
O	2.06585200	-2.24776500	-0.01127700
C	2.45096800	3.99882400	0.00770500
H	2.09796900	4.55748300	-0.86413700
H	2.10756200	4.53511700	0.89733500
H	3.54660200	4.00003100	0.00199900
H	-5.38423800	0.04650200	0.01116600

5- H



C	-4.30295000	0.71811000	0.16445200
C	-4.31827200	-0.66199300	0.13999300
C	-3.09037700	-1.36457100	0.06120000
C	-1.87913300	-0.61557000	0.00734100
C	-1.87334500	0.81507000	0.03188600
C	-3.10553500	1.46527500	0.11186100
H	-3.88183400	-3.37978200	0.07102900
H	-5.24227100	1.26145000	0.22544200
C	-2.97750900	-2.77749000	0.03232800
H	-3.12381800	2.54533800	0.13754200
C	-0.58417000	-2.57002400	-0.09032300
C	-1.73847100	-3.37785300	-0.04290200
H	0.41576100	-2.98719000	-0.14860400
H	-1.63332400	-4.45737800	-0.06573500
N	-0.66283400	-1.24724100	-0.06606100
C	-0.34269600	2.74014700	0.09666700
O	-1.19403000	3.61897100	0.20247400
C	1.15290900	3.04088900	0.12467200
H	1.29890900	4.02268400	-0.34111600
H	1.43188500	3.16055700	1.18099400
C	2.04108900	1.97518200	-0.53246600
H	1.85089800	1.89000000	-1.60948900
N	-0.60972000	1.39375200	-0.01974400
Pd	0.89162900	0.09896300	-0.17241300
C	3.48823900	-1.01910100	0.21105400
C	4.58799500	-2.04511300	0.35129900
H	4.23127900	-3.04054500	0.08363100
H	5.42625900	-1.76573000	-0.29537700
H	4.95737500	-2.04323800	1.38153000
O	3.74306600	0.18184100	0.53809200
O	2.35867200	-1.39359400	-0.23362500
H	2.72033600	0.91845700	0.14936500
H	3.08398100	2.31902600	-0.47494700
H	-5.25079500	-1.21698800	0.17948100

5-F_6-F_sub



C	-1.49099200	2.98946300	0.00564700
C	-0.74596100	0.81074600	-0.00133100
C	-2.08079300	0.30250400	0.01003600
C	-3.14276900	1.24125500	0.01898600
C	-2.84777300	2.58505800	0.01672300
H	-1.23873400	4.04863400	0.00372500
C	0.36495400	-0.10180300	-0.01232500
C	-2.28010000	-1.09520700	0.01112100
H	-4.16749900	0.88451300	0.02740200
H	-3.63422600	3.33318600	0.02322000
C	-1.19786900	-1.94208900	0.00075200
C	0.12650100	-1.46615600	-0.01074000
N	-0.47797700	2.14398800	-0.00301400
N	1.62799300	0.48968300	-0.02345500
H	1.58041600	1.50471100	-0.02383500
C	2.86108500	-0.12656500	-0.06142500
O	3.00826000	-1.34127800	-0.06051100
C	4.03413900	0.85166500	-0.12958100
H	4.05419600	1.27649400	-1.14388300
H	3.84699700	1.69545800	0.54797300
C	5.37025200	0.18162000	0.18895700
H	5.54265400	-0.66821300	-0.47633000
H	6.19329700	0.89411400	0.07169800
H	5.38554700	-0.19667200	1.21600200
F	-3.53644400	-1.58522100	0.02252300
F	-1.40236500	-3.26924900	0.00203900
H	0.94640400	-2.17041600	-0.01857900

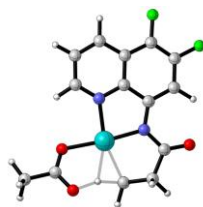
5-F_6-F_int



C	-3.64321400	1.08143000	0.00536100
C	-3.88316500	-0.27532100	0.00474300
C	-2.79317300	-1.16550800	0.00151300
C	-1.47990200	-0.60916700	-0.00115700

C	-1.22671000	0.79642700	-0.00094800
C	-2.34982600	1.62987700	0.00238600
H	-3.90926500	-3.01767200	0.00273700
C	-2.91804800	-2.57634500	0.00078100
C	-0.51720900	-2.75430600	-0.00464200
C	-1.78711500	-3.36481700	-0.00246100
H	0.40491000	-3.32599900	-0.00691600
H	-1.85435300	-4.44719500	-0.00335800
N	-0.39178500	-1.43296300	-0.00380200
C	0.52083700	2.48432500	-0.00305200
O	-0.27755100	3.41983100	0.00121100
C	2.02201700	2.74229000	-0.00855700
H	2.47464900	2.23760600	0.85299100
H	2.46367400	2.25655400	-0.88689400
N	0.12193900	1.15437000	-0.00404500
Pd	1.36235200	-0.46866000	-0.00615200
C	3.73060600	-1.17920400	-0.00559000
C	5.15832100	-1.63912200	0.03426700
H	5.49280800	-1.68029000	1.07777300
H	5.24706400	-2.63869600	-0.39721900
H	5.79648300	-0.93055400	-0.49922700
O	3.43283300	0.05930700	-0.00988600
O	2.76615500	-2.02305900	-0.00970100
C	2.35421200	4.23470800	0.00555800
H	1.93205500	4.74185300	-0.86696800
H	1.94382200	4.72237600	0.89473200
H	3.44026100	4.37828200	0.00013000
F	-5.14012400	-0.76173700	0.00723600
F	-4.69015300	1.92056400	0.00887900
H	-2.23619000	2.70257700	0.00290500

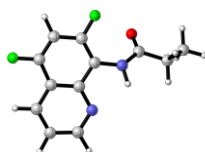
5-F_6-F_TS



C	-3.84478800	0.71606900	0.10463500
C	-3.85729000	-0.66221200	0.07893300
C	-2.64042300	-1.37015500	0.01310500
C	-1.43090600	-0.61791000	-0.02755100
C	-1.42579900	0.81287900	-0.00313200
C	-2.65666800	1.46509200	0.06475000
H	-3.45292200	-3.37589800	0.01488200

C	-2.54410800	-2.78385400	-0.01406900
C	-0.14530800	-2.57726200	-0.10977700
C	-1.30410800	-3.38172600	-0.07542800
H	0.85349400	-2.99832100	-0.15622800
H	-1.20128900	-4.46134800	-0.09701800
N	-0.21857400	-1.25425200	-0.08683200
C	0.09462600	2.73982800	0.07459800
O	-0.76541500	3.61100600	0.16821100
C	1.58833400	3.04495100	0.11852600
H	1.73844200	4.02390900	-0.35162200
H	1.85484000	3.17140300	1.17717600
C	2.48623200	1.97745000	-0.52314400
H	2.31009800	1.88658200	-1.60197800
N	-0.16505300	1.39180900	-0.04171500
Pd	1.33860600	0.09664600	-0.17460200
C	3.92948100	-1.01286500	0.24370400
C	5.02789600	-2.03820600	0.39657000
H	4.67491900	-3.03417800	0.12615100
H	5.87254900	-1.75873900	-0.24168400
H	5.38647300	-2.03470600	1.43055800
O	4.17700700	0.18772000	0.57402400
O	2.80531500	-1.38976500	-0.21596800
H	3.15274200	0.92669600	0.16894600
H	3.52790400	2.32250700	-0.45370800
F	-5.01953200	-1.34450200	0.11596300
F	-5.01430700	1.37057800	0.16879200
H	-2.70144900	2.54465300	0.09280300

5-F_7-F_sub



C	-1.74318900	2.77908000	-0.10498700
C	-0.90978700	0.63444700	-0.16012500
C	-2.20456000	0.08348100	0.09182600
C	-3.28879700	0.97694900	0.25917700
C	-3.05890600	2.33054800	0.16280100
H	-1.54386400	3.84615900	-0.19456200
C	0.22362300	-0.22215900	-0.33965500
C	-2.32516500	-1.32436900	0.15922400
H	-4.27965500	0.58042400	0.45571100
H	-3.86236100	3.05014600	0.28303900
C	-1.25459800	-2.15391300	-0.04200500

C	0.00853800	-1.58868500	-0.31756100
H	-1.36275900	-3.23165100	-0.01368600
N	-0.70613800	1.97774000	-0.25962600
N	1.46710600	0.37504400	-0.58839300
H	1.37555300	1.34476600	-0.87468600
C	2.65146800	0.02327400	0.05404400
O	2.74590700	-0.93358700	0.80094400
C	3.82847600	0.92912200	-0.30702400
H	4.11670400	0.69886800	-1.34250200
H	3.49845500	1.97727700	-0.31405800
C	5.01786800	0.73906200	0.63310600
H	5.33416600	-0.30716300	0.64547900
H	5.86241800	1.35917600	0.31468200
H	4.75605600	1.01435500	1.65974400
F	-3.54322200	-1.84628700	0.41499400
F	1.00338200	-2.43973300	-0.59538300

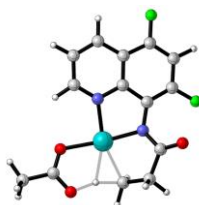
5-F_7-F_int



C	-3.68367800	1.15228900	-0.46575800
C	-3.96213600	-0.15255000	-0.14534400
C	-2.92904300	-1.08008300	0.11212300
C	-1.59537300	-0.57859500	0.06512700
C	-1.26638400	0.77689300	-0.19233700
C	-2.34680600	1.59845500	-0.51787200
H	-4.12824000	-2.84809900	0.43629200
H	-4.47913500	1.84962600	-0.70215900
C	-3.11893400	-2.45203800	0.39122000
C	-0.72826700	-2.71594300	0.50035800
C	-2.02252700	-3.26634100	0.59187700
H	0.16513300	-3.32047900	0.62054700
H	-2.13494000	-4.32361400	0.80447500
N	-0.53549400	-1.42783900	0.24795000
C	0.46913100	2.33386600	0.38345100
O	-0.34174900	3.09454800	0.89710100
C	1.95204400	2.67457100	0.29859200
H	2.50848300	1.99551200	0.95704500
H	2.31077900	2.45133100	-0.71246800
N	0.09040400	1.10862400	-0.17146000

Pd	1.25656000	-0.55423500	-0.06495800
C	3.60149100	-1.28762900	-0.27464000
C	5.02122000	-1.74186700	-0.44822500
H	5.70926600	-0.96711800	-0.10103400
H	5.18879600	-2.67660500	0.09147100
H	5.21416500	-1.91502000	-1.51366500
O	3.28132200	-0.05967000	-0.41240600
O	2.66749300	-2.12127100	-0.01035700
C	2.23423100	4.12882700	0.67891100
H	1.72199500	4.82020500	0.00224300
H	1.88241100	4.34483700	1.69151700
H	3.30980800	4.33164200	0.63085900
F	-5.23786800	-0.58863500	-0.09956900
F	-2.15779800	2.84853800	-0.94621600

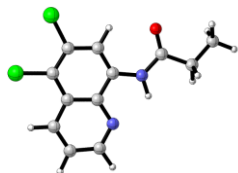
5-F_7-F_TS



C	-3.97874800	0.65824700	-0.09439100
C	-3.95416500	-0.70460000	0.05499100
C	-2.73606100	-1.41954300	0.09153600
C	-1.53539100	-0.65480400	0.01309700
C	-1.52094100	0.76906500	-0.07639900
C	-2.77020000	1.37897400	-0.19165300
H	-3.53950900	-3.41983000	0.24217100
H	-4.91768500	1.19531600	-0.16366000
C	-2.63298000	-2.82683300	0.17776800
C	-0.23922400	-2.60956600	0.06849200
C	-1.38836200	-3.42080500	0.16897700
H	0.76252100	-3.02621200	0.04220500
H	-1.27601500	-4.49780300	0.22894200
N	-0.31655300	-1.28866200	-0.00592300
C	0.03655500	2.59981000	0.42567900
O	-0.76570100	3.32432800	0.99432100
C	1.51747000	2.95343400	0.28312900
H	1.57097600	3.96835400	-0.13275800
H	1.92328300	3.02735100	1.30034200
C	2.34369900	1.96690400	-0.55300900
H	2.04037200	1.95998400	-1.60597100
N	-0.26404900	1.36522200	-0.12900200

Pd	1.23797300	0.05637000	-0.21997000
C	3.85363500	-1.04765900	0.12826500
C	4.95689800	-2.07049100	0.26436400
H	4.57340600	-3.08163200	0.12175200
H	5.73236600	-1.86249400	-0.48044400
H	5.42020100	-1.97844100	1.25132400
O	4.13222800	0.16952400	0.35815700
O	2.69727300	-1.44245800	-0.22012100
H	3.08520900	0.89182600	0.01486000
H	3.38516100	2.31901300	-0.57857400
F	-5.10569100	-1.40294400	0.13885200
F	-2.87945900	2.68424000	-0.45007500

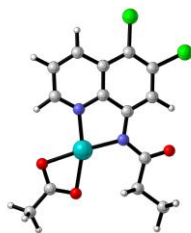
5-Cl_6-Cl_sub



C	-0.53822300	3.49279100	0.00457500
C	-0.21174600	1.21200700	-0.00148400
C	-1.61509900	0.94516000	0.00558200
C	-2.47661700	2.07247400	0.01184500
C	-1.94256400	3.34109600	0.01133000
H	-0.09301400	4.48628200	0.00410100
C	0.72644100	0.12265600	-0.00961400
C	-2.06475100	-0.40812500	0.00536700
H	-3.55010000	1.92114400	0.01706800
H	-2.58317200	4.21731500	0.01604700
C	-1.13401200	-1.43052500	-0.00203400
C	0.25727800	-1.17722300	-0.00931900
N	0.29745100	2.47205200	-0.00159000
N	2.07007100	0.48813600	-0.01697900
H	2.19614500	1.49677000	-0.01736500
C	3.18264800	-0.32960900	-0.04577400
O	3.12132500	-1.55074400	-0.04388400
C	4.50330900	0.43809200	-0.09990200
H	4.57494700	0.91238600	-1.08958100
H	4.47305700	1.26094500	0.62719600
C	5.71251900	-0.46285300	0.14644900
H	5.73478900	-1.28550900	-0.57299300
H	6.64077800	0.11034500	0.05419500
H	5.67664800	-0.90350300	1.14754200
H	0.95448000	-2.00230700	-0.01475200

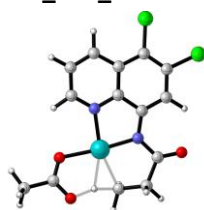
Cl	-3.78135800	-0.74355400	0.01457100
Cl	-1.62822500	-3.10496800	-0.00236700

5-Cl_6-Cl_int



C	-3.27732100	0.88295600	0.00377300
C	-3.46460000	-0.49069100	0.00295300
C	-2.31946700	-1.33216000	-0.00087600
C	-1.03290600	-0.71751000	-0.00306200
C	-0.84097100	0.69858600	-0.00248300
C	-1.99855900	1.47975300	0.00066700
H	-3.31878500	-3.25038300	-0.00181500
C	-2.35730100	-2.74958800	-0.00279700
C	0.04668300	-2.80843700	-0.00744900
C	-1.18786300	-3.48064500	-0.00623700
H	0.99877800	-3.32863100	-0.00967800
H	-1.20376500	-4.56497000	-0.00803000
N	0.09790300	-1.48216000	-0.00578200
C	0.82624300	2.46826400	-0.00449600
O	-0.01228000	3.36669200	-0.00049000
C	2.31409900	2.79205300	-0.00992400
H	2.78803100	2.30852100	0.85229900
H	2.77680700	2.32512700	-0.88761900
N	0.48686800	1.11927200	-0.00522100
Pd	1.80510000	-0.43971900	-0.00625900
C	4.20313700	-1.04171100	-0.00233400
C	5.64983500	-1.43676100	0.03953800
H	5.98415300	-1.46320100	1.08357800
H	5.78419800	-2.43116600	-0.39209100
H	6.25619300	-0.69993600	-0.49273900
O	3.84907800	0.18189400	-0.00717300
O	3.27725700	-1.92799500	-0.00764700
C	2.58019300	4.29766400	0.00269200
H	2.13672000	4.78478400	-0.87064800
H	2.14848500	4.76771700	0.89122400
H	3.65886700	4.48857300	-0.00244700
H	-1.91590700	2.55446700	0.00091200
Cl	-5.05850700	-1.20499000	0.00677700
Cl	-4.64628200	1.96622800	0.00879200

5-Cl_6-Cl_TS



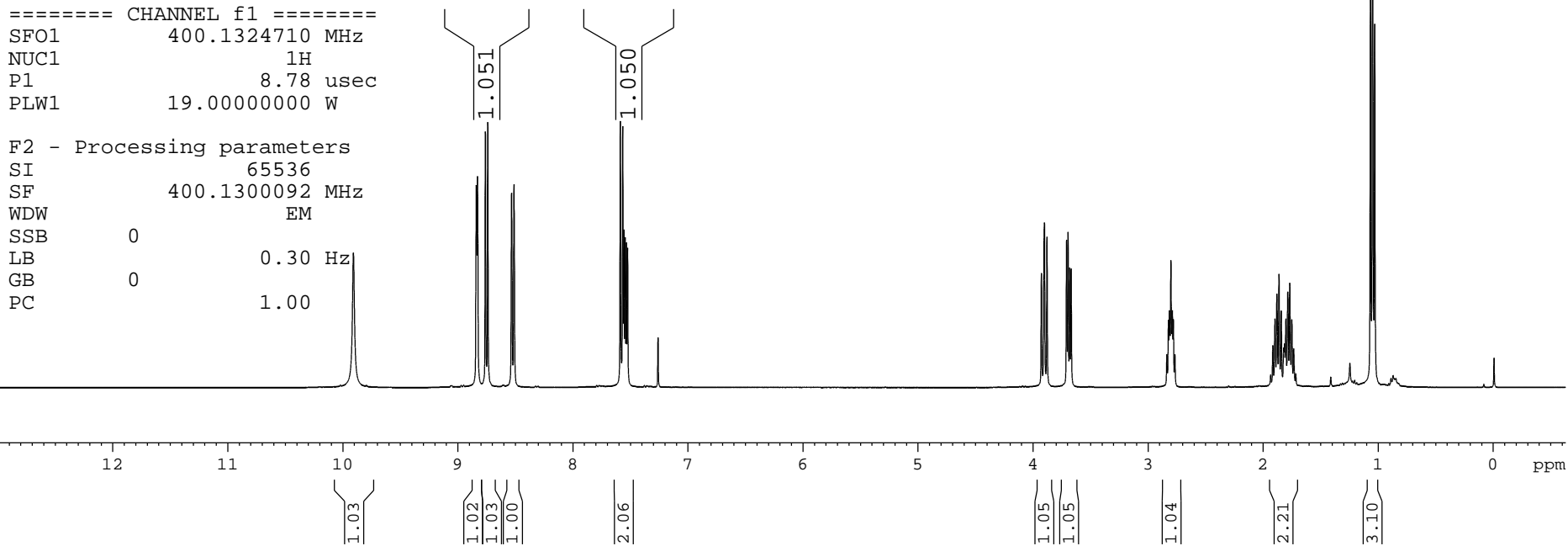
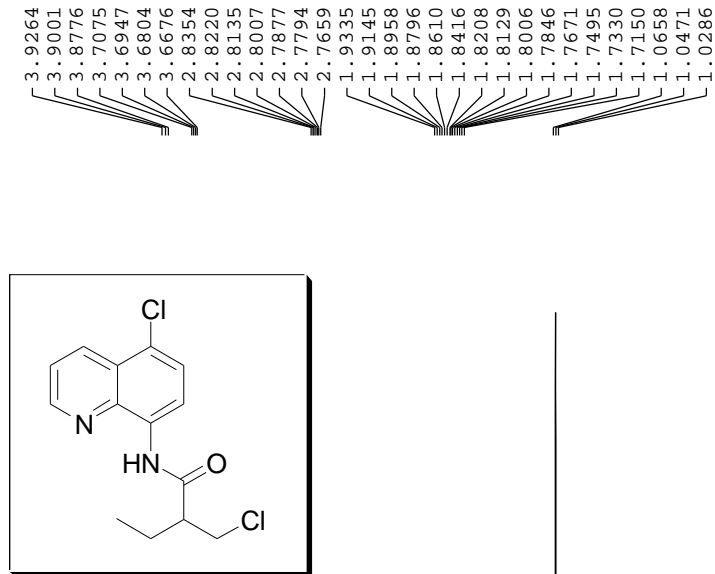
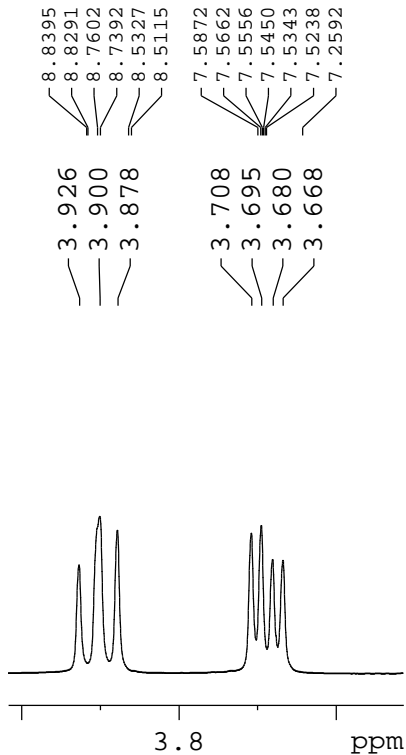
C	-3.43006100	0.70320600	0.06468400
C	-3.44676500	-0.68358700	0.04241600
C	-2.21123000	-1.38812500	-0.01293700
C	-1.00364700	-0.63272800	-0.04559000
C	-1.00020900	0.79881600	-0.02402800
C	-2.23108000	1.44677400	0.03220500
H	-2.98294700	-3.41069300	-0.01579800
C	-2.08655600	-2.80127300	-0.03775700
C	0.30865800	-2.57713400	-0.11509200
C	-0.84091800	-3.38927600	-0.08852700
H	1.31313600	-2.98521500	-0.15341600
H	-0.73218600	-4.46833700	-0.10763300
N	0.21648800	-1.25538300	-0.09445200
C	0.50973000	2.73499800	0.06097800
O	-0.35367200	3.60272100	0.14315000
C	2.00148100	3.04599900	0.11881900
H	2.15091000	4.02673900	-0.34762100
H	2.25733600	3.17120900	1.18025500
C	2.91044300	1.98423600	-0.51654300
H	2.74301800	1.89222200	-1.59664900
N	0.25567000	1.38330400	-0.05324100
Pd	1.76873200	0.09935300	-0.17342100
C	4.36210200	-0.99835500	0.26208500
C	5.46285900	-2.01983700	0.42258300
H	5.11437700	-3.01762900	0.15310700
H	6.30944200	-1.73924600	-0.21260800
H	5.81674400	-2.01243200	1.45814800
O	4.60327100	0.20356100	0.59114300
O	3.24133100	-1.37999900	-0.20298200
H	3.57737100	0.93818100	0.17906100
H	3.94925300	2.33614100	-0.43929200
H	-2.26279900	2.52619100	0.05593400
Cl	-4.94519600	-1.58194900	0.08032900
Cl	-4.91813900	1.61281000	0.13305200

Current Data Parameters
 NAME YXL-8-149-H-141104
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141104
 Time 13.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 14
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 32.58
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME YXL-8-149-C-141104
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141104
Time 13.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 123
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

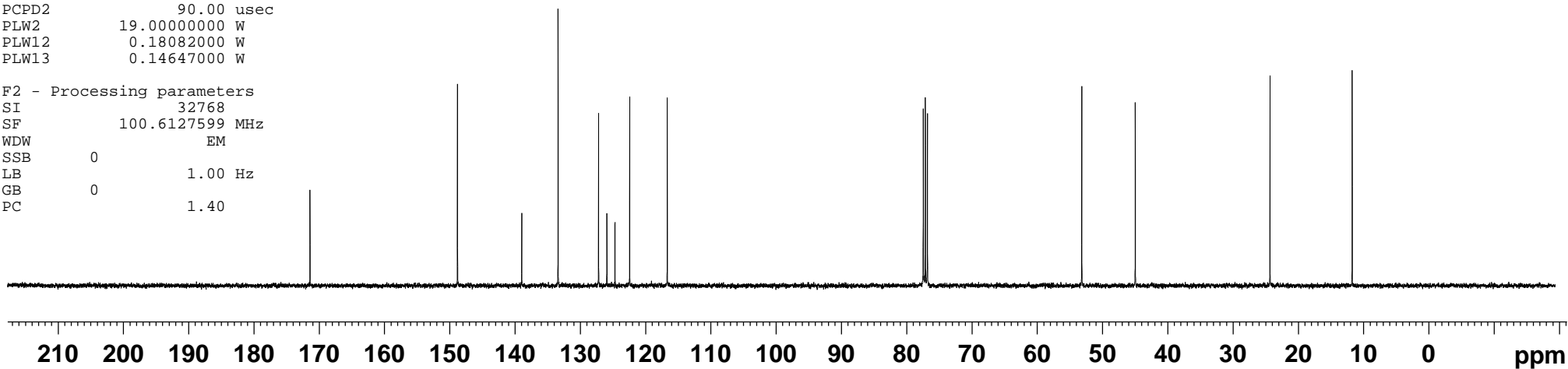
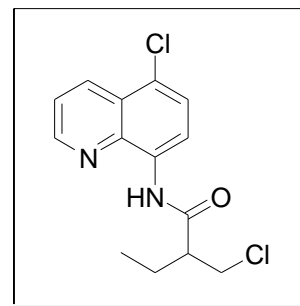
==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127599 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

— 171.45
— 148.85
— 139.01
— 133.44
— 127.23
— 125.97
— 124.73
— 122.47
— 116.71

77.48
77.16
76.84
— 53.19
— 44.99
— 24.35
— 11.76



Current Data Parameters
NAME YXL-9-4-H-20150101
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150101
Time 22.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 130.81
DW 60.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

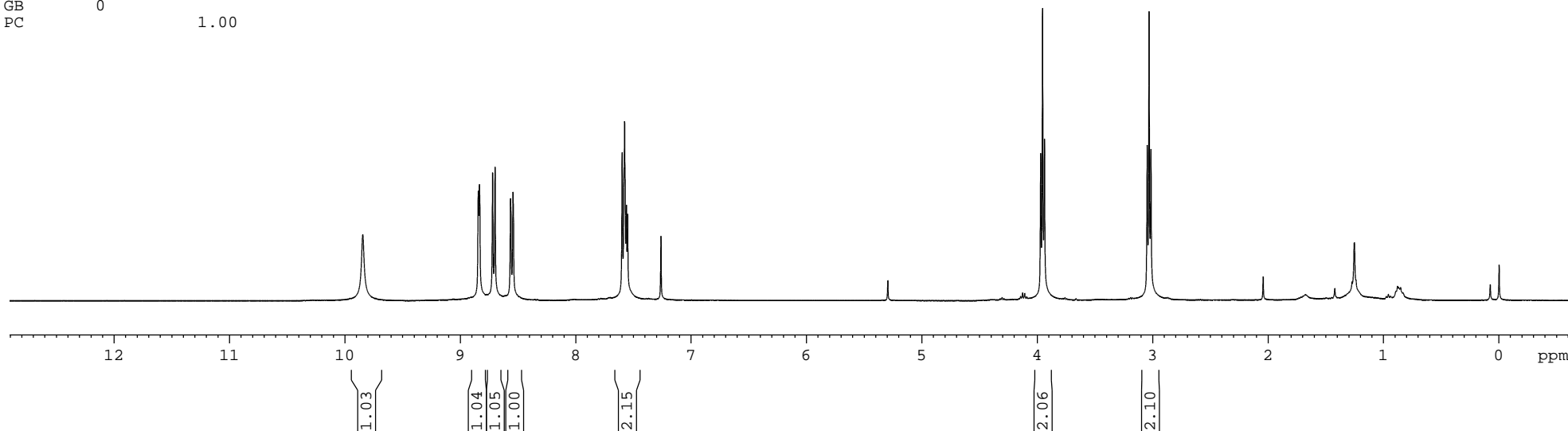
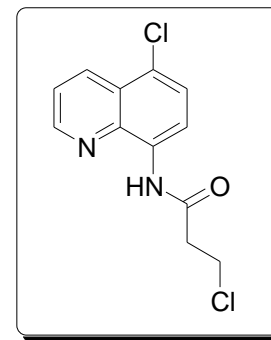
9.8446

8.8436
8.8405
8.8334
8.7189
8.6980
8.5638
8.5425

7.5962
7.5798
7.5751
7.5594
7.5488
7.2599

3.9690
3.9526
3.9364

3.0461
3.0298
3.0135



Current Data Parameters
NAME YXL-9-4-C-20150102
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150103
Time 0.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 490
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 63.51
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

168.06

148.84

138.92

133.55

133.47

127.30

126.03

124.79

122.53

116.72

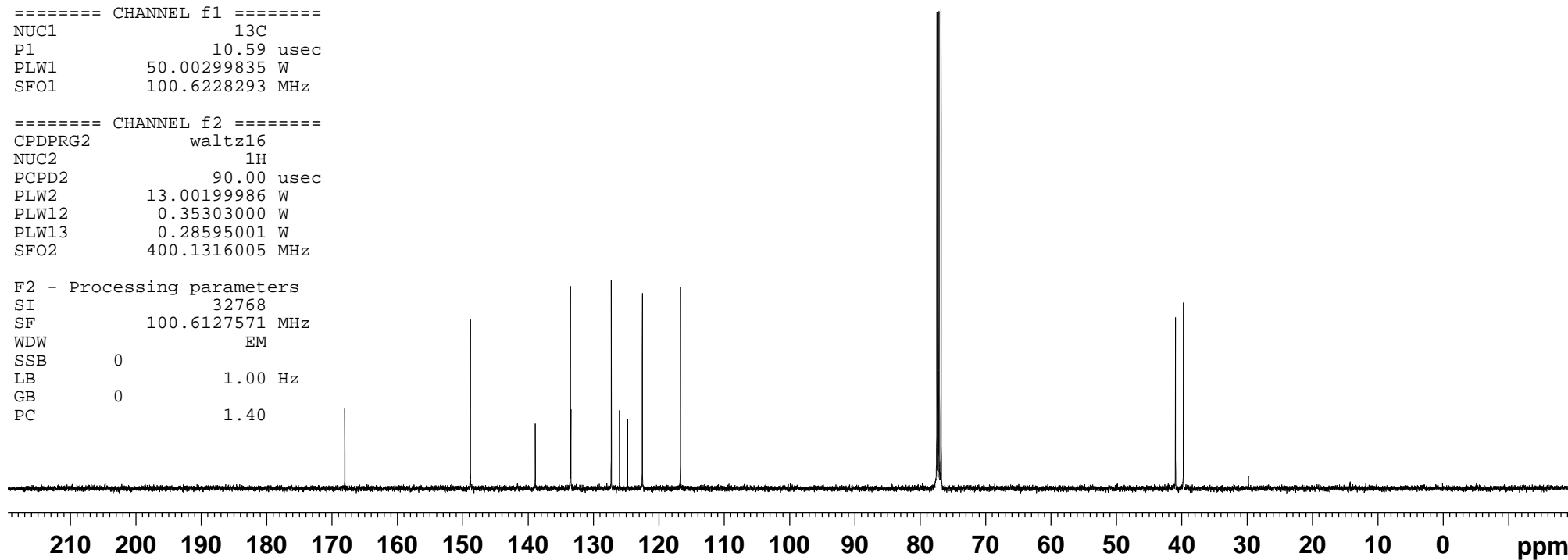
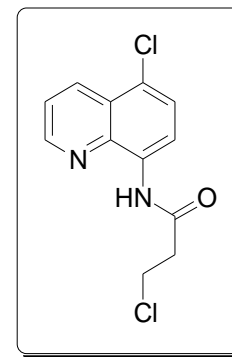
77.47

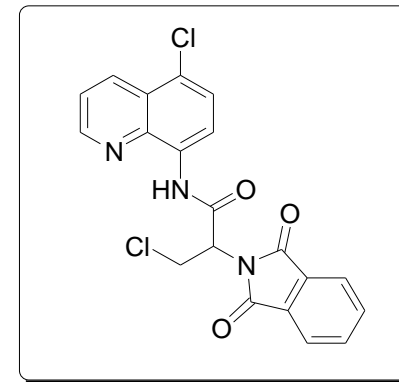
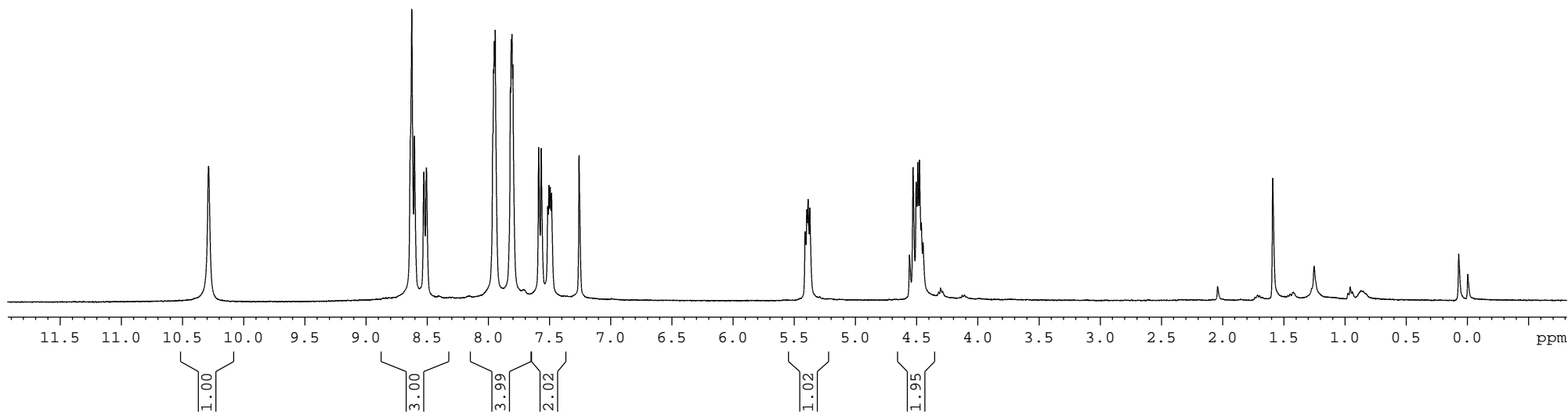
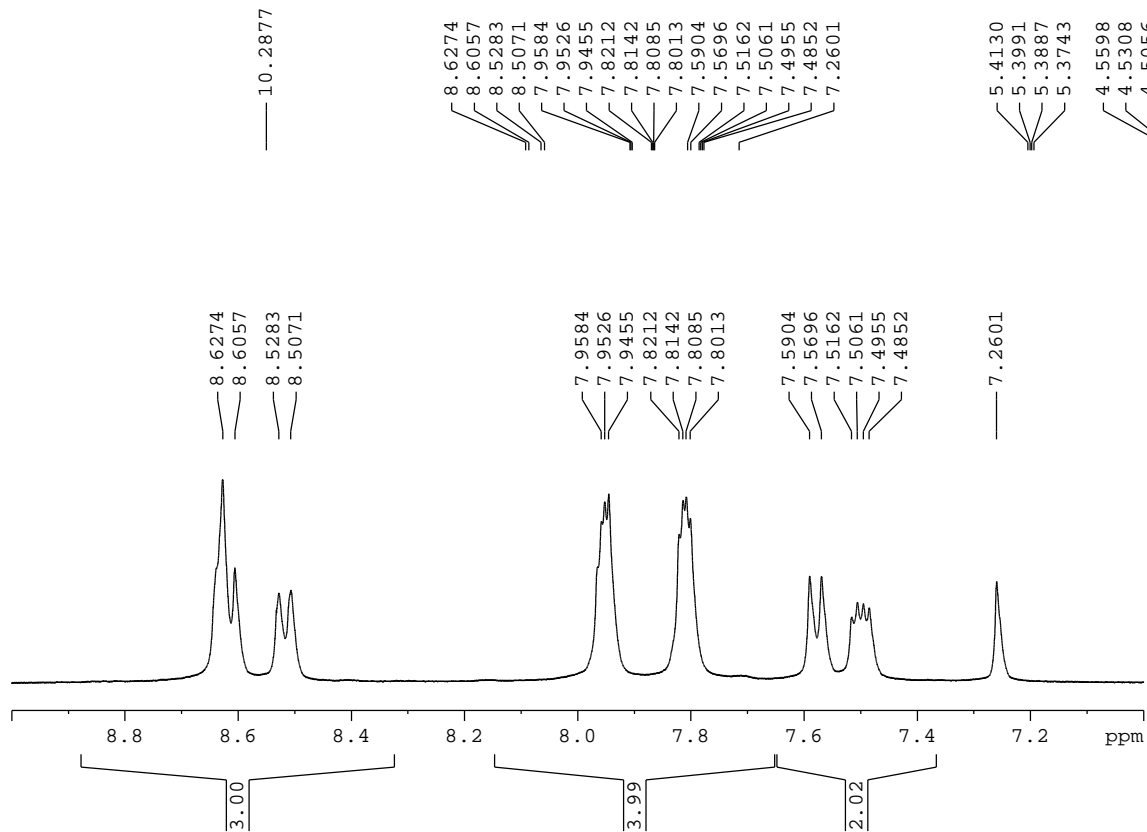
77.16

76.84

40.98

39.76





Current Data Parameters
 NAME syh-9-229-1-p
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160304
 Time 22.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 165.63
 DW 60.800 usec
 DE 6.50 usec
 TE 298.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.80 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME zx-1-138-c-141023-
EXPNO 10
PROCNO 1

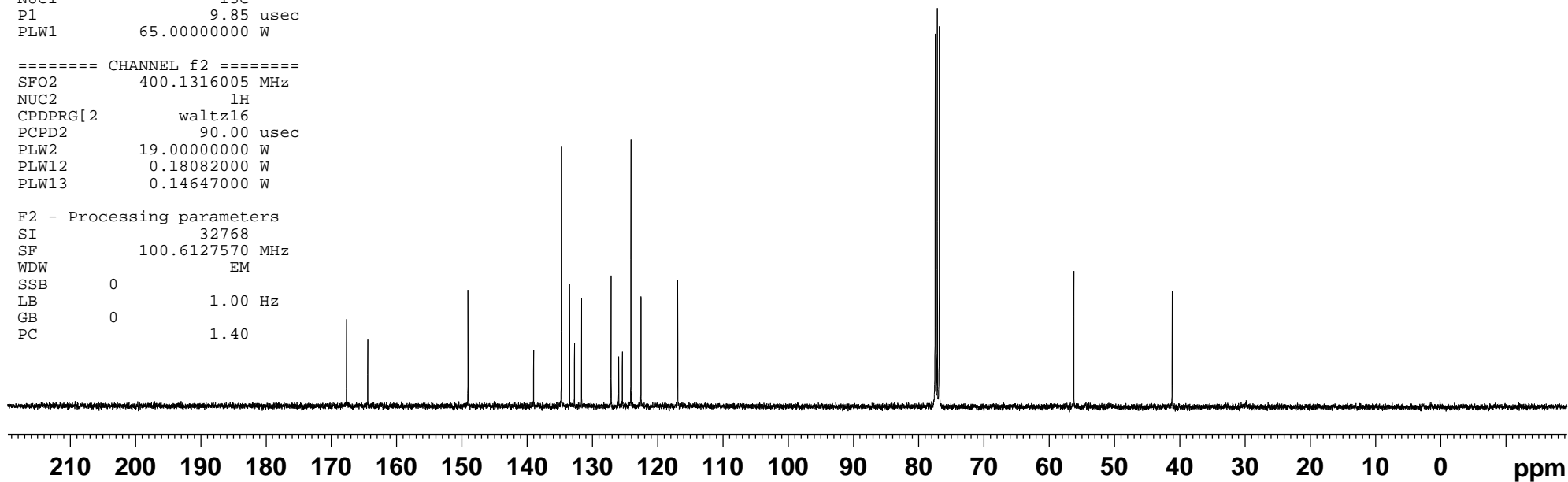
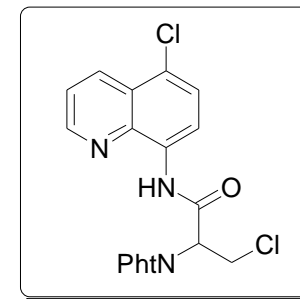
F2 - Acquisition Parameters
Date_ 20141024
Time 7.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 480
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

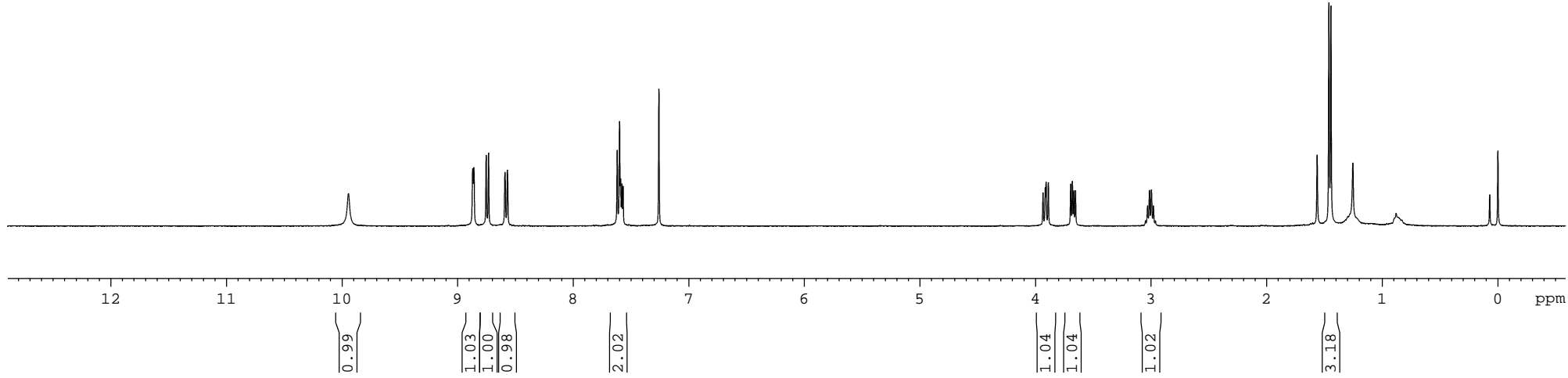
==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

167.68
164.44
149.08
139.02
134.77
133.51
132.76
131.67
127.15
125.99
125.42
124.11
122.57
116.94
77.48
77.16
76.84
56.24
41.16





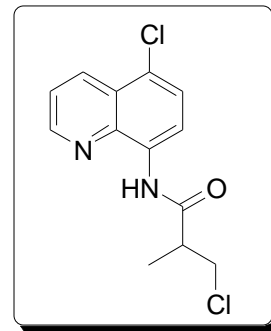
— 9.9467

8.8717
8.8615
8.7548
8.7337
8.5924
8.5712

7.6205
7.6004
7.5914
7.5803
7.5699
7.2597

3.9359
3.9163
3.9090
3.8895
3.6960
3.6817
3.6690
3.6547
3.0145
2.9977

1.4616
1.4443



— 171.91
 — 148.91
 — 139.14
 — 133.61
 — 127.35
 — 126.10
 — 124.82
 — 122.55
 — 116.79

Current Data Parameters
 NAME zx-1-196-2-c-20141204-
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141204
 Time 23.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 470
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

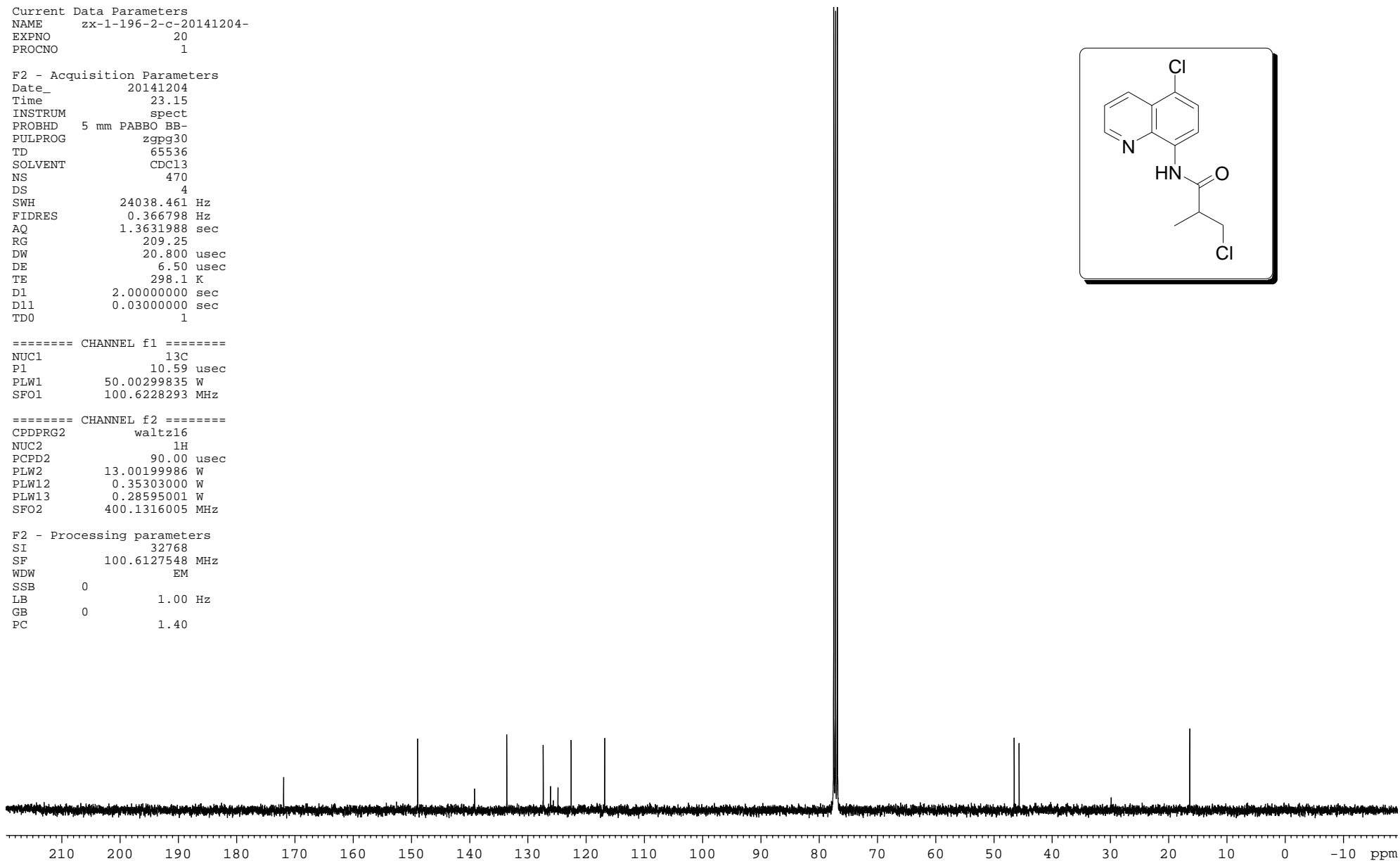
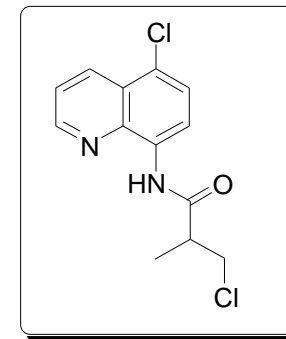
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127548 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

— 46.49
 — 45.65

— 16.35



210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

Current Data Parameters
 NAME zx-1-196-1-h-20141204-
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141204
 Time 20.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 184.16
 DW 60.800 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300100 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10.0619

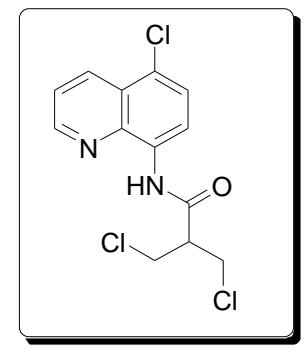
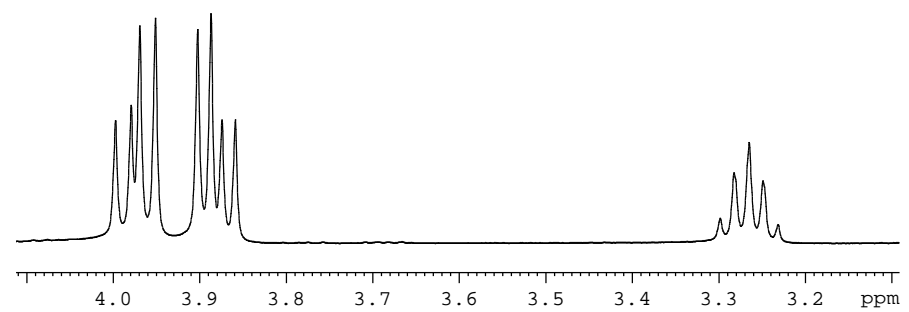
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8.8714
8.8679
8.7266
8.7056
8.5946
8.5910
8.5733
8.5698
7.6235
7.6113
7.6022
7.5901
7.5795
7.2600

3.997
3.979
3.969
3.951
3.902
3.887
3.874
3.858

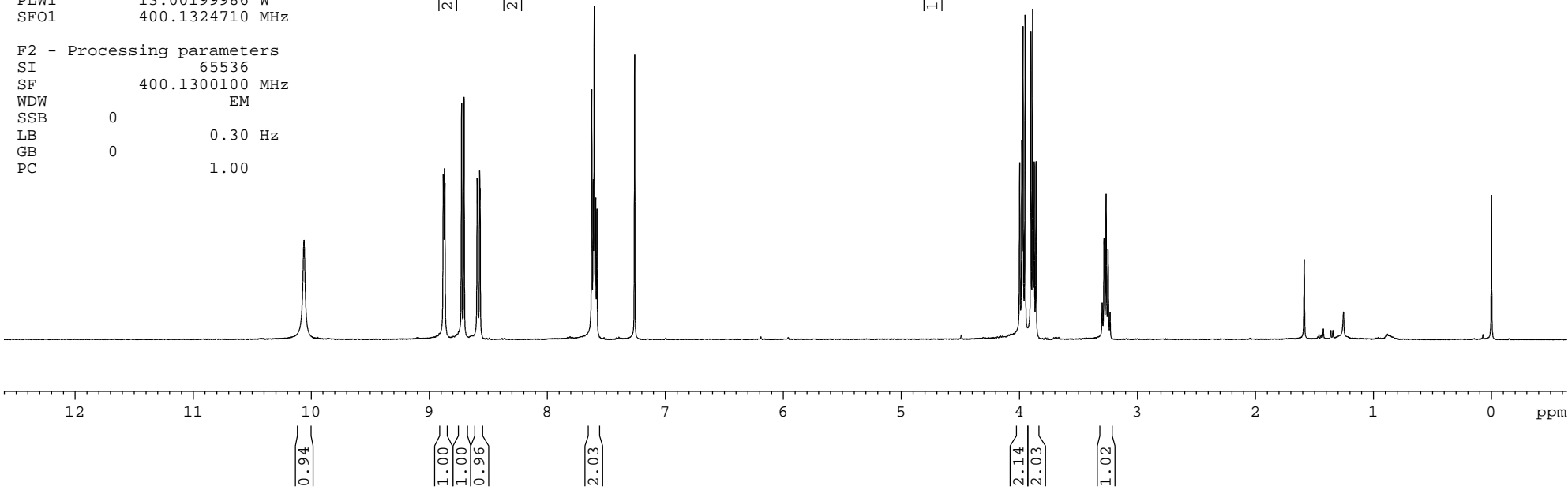
3.298
3.282
3.265
3.249
3.231

3.9971
3.9790
3.9690
3.9509
3.9021
3.8866
3.8740
3.8585
3.2980
3.2821
3.2646
3.2487
3.2311

1.5864
1.2536



2.136
2.032
1.016



Current Data Parameters
NAME zx-1-196-1-c-20141204-
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141204
Time 22.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 440
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

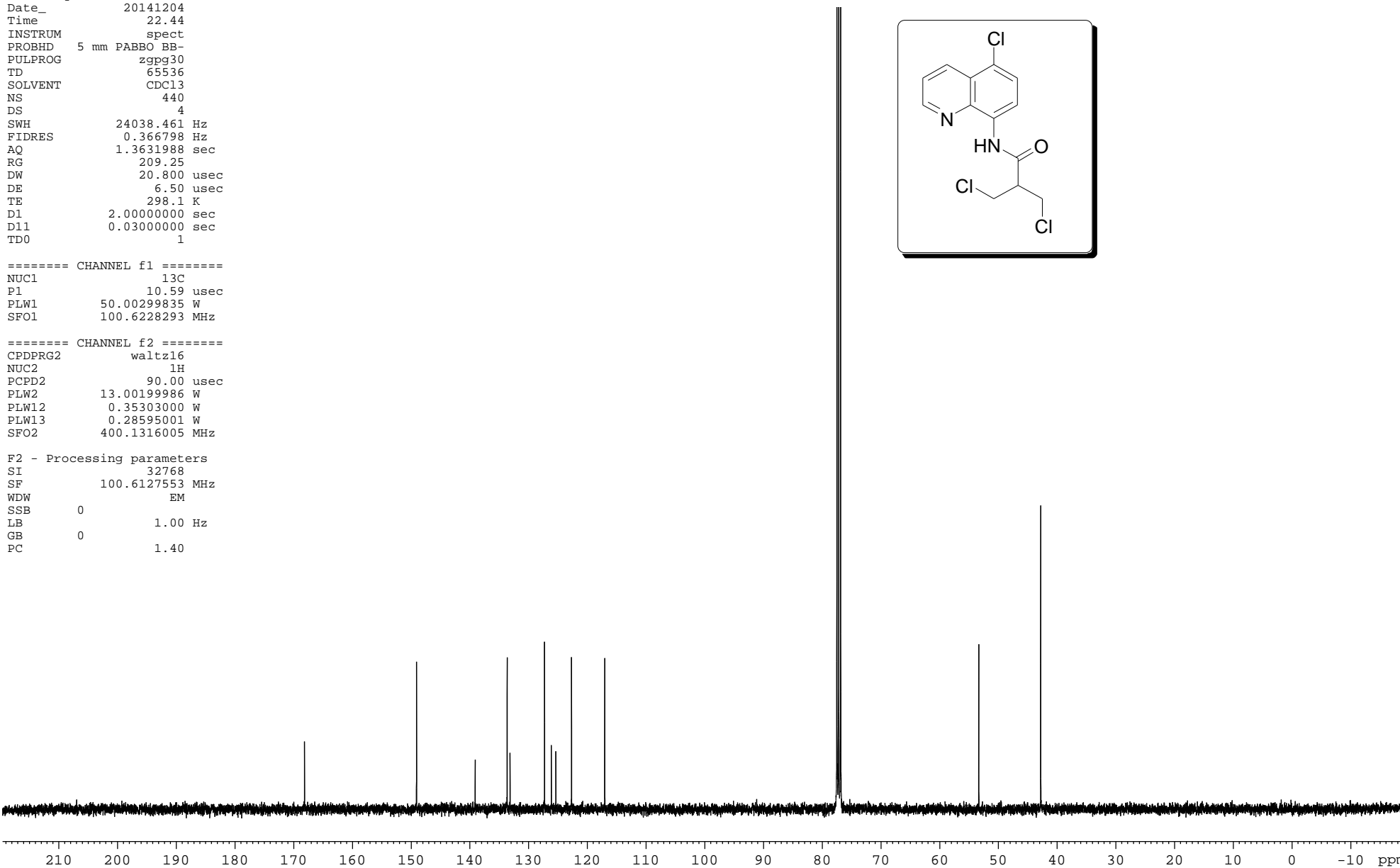
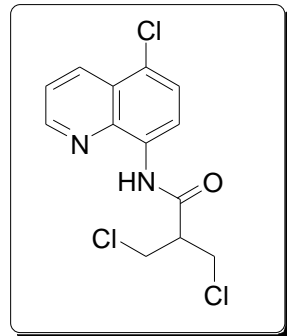
==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127553 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

168.14
149.06
139.08
133.64
133.14
127.26
126.11
125.34
122.67
117.01

53.31
42.77

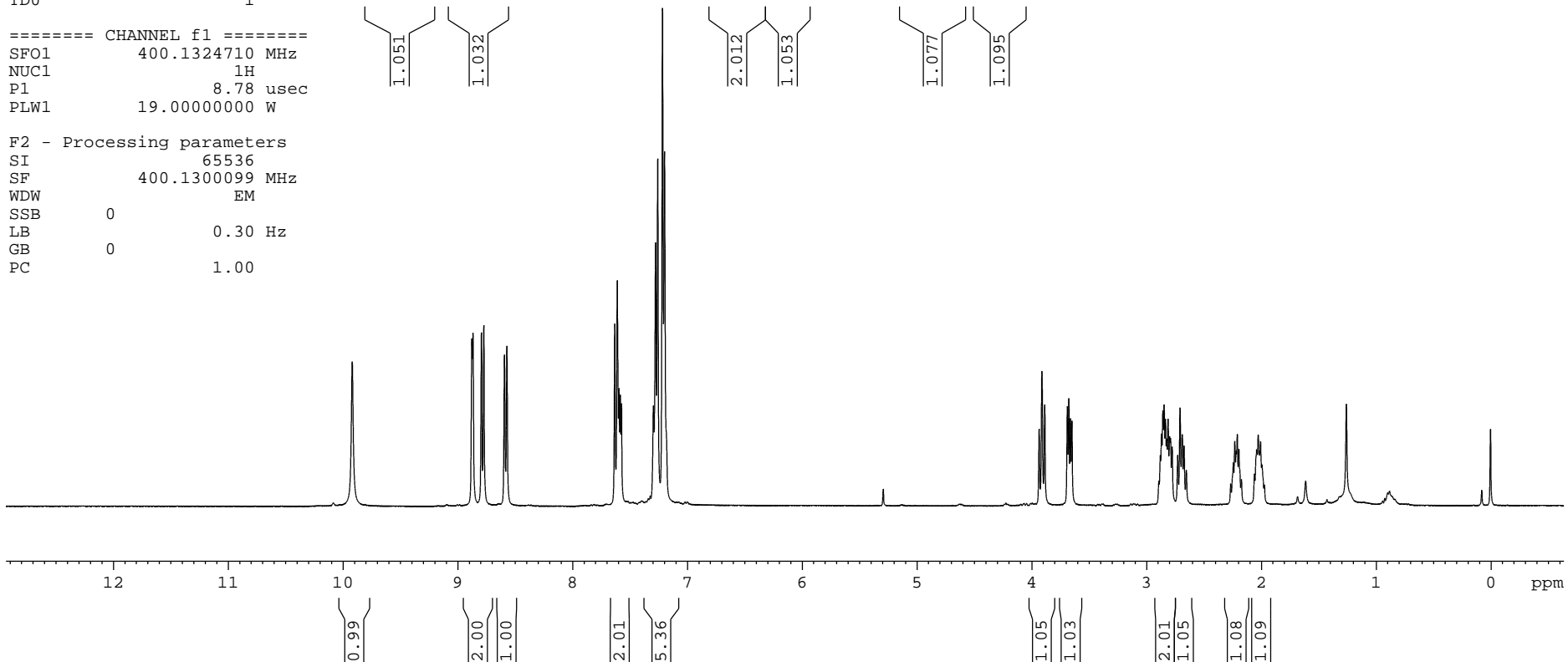
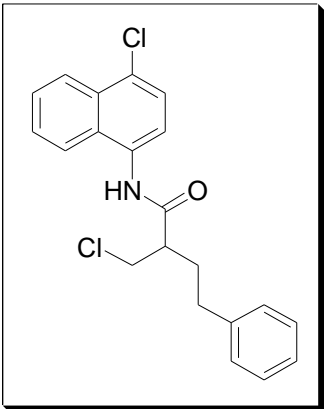
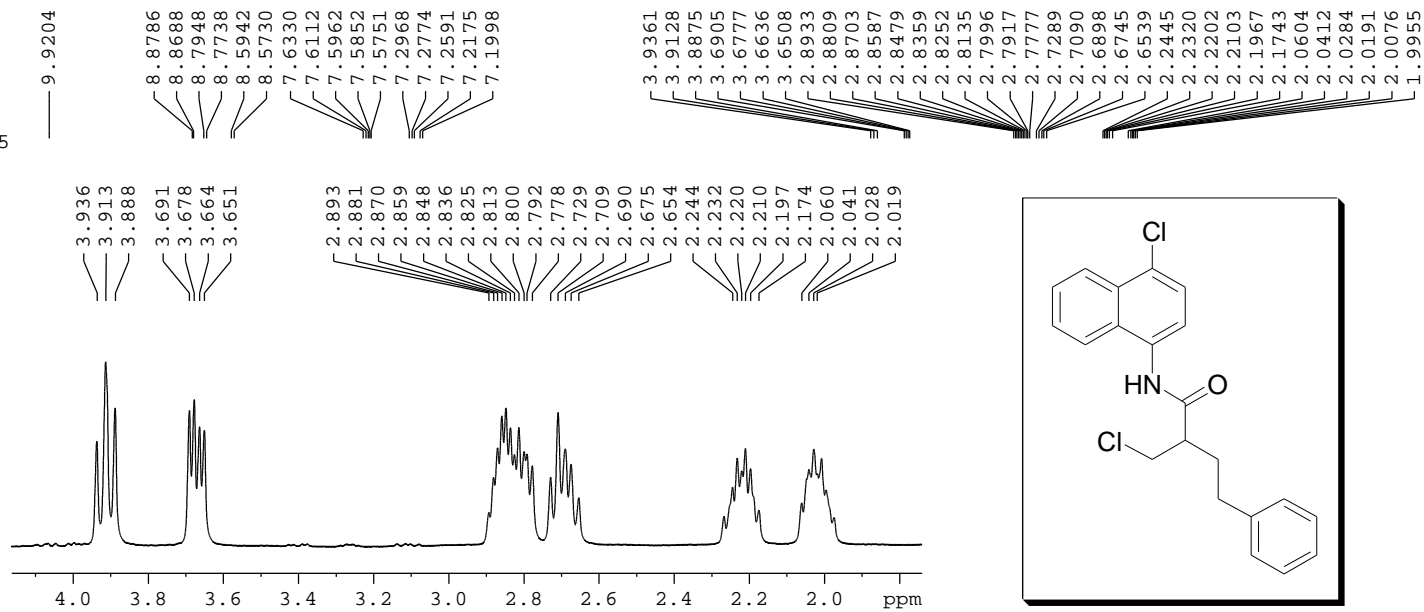


Current Data Parameters
 NAME YXL-8-140-1-H-141105
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141105
 Time 13.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 73.55
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME YXL-8-140-1-C-141105
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141106
Time 1.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 470
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

=====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

=====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

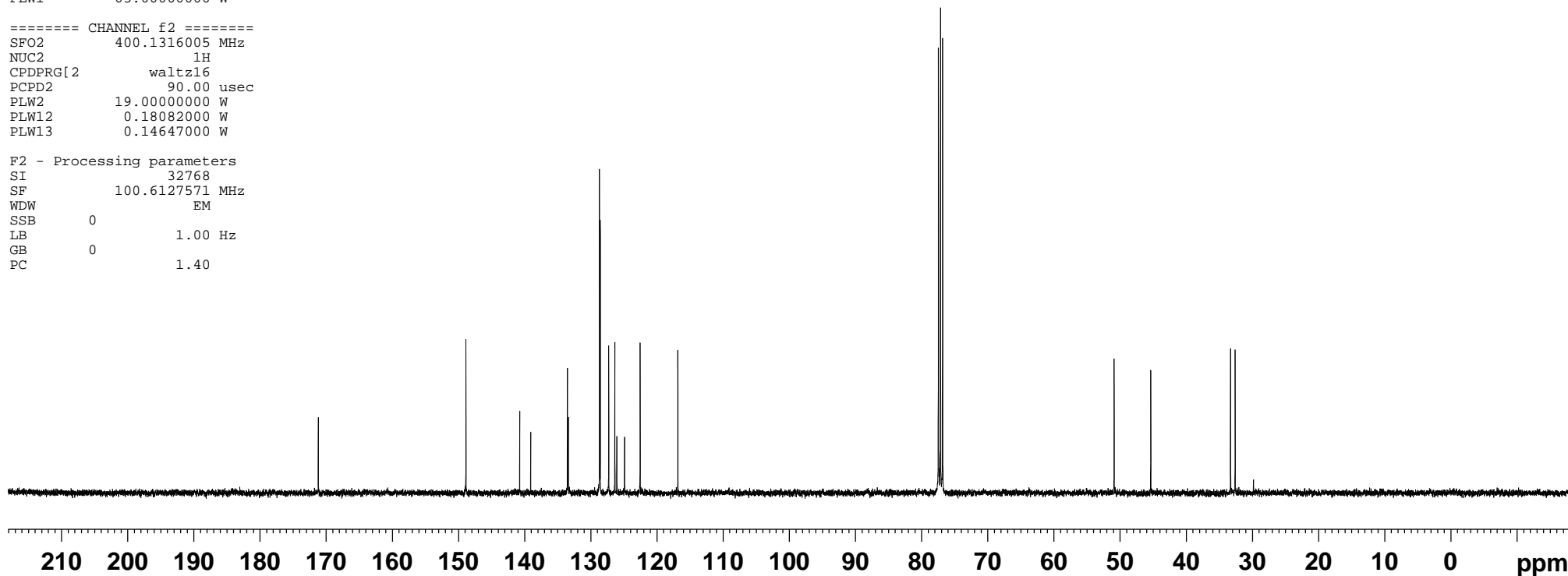
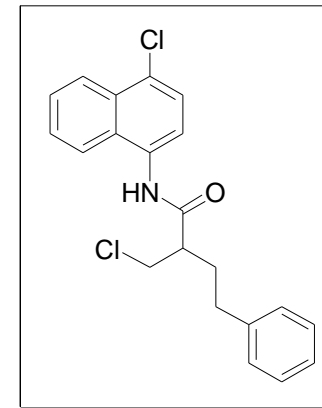
171.22

148.91
140.77
139.11
133.56
133.42
128.71
128.60
127.32
126.39
126.09
124.92
122.57
116.87

77.48
77.16
76.84

50.91
45.38

33.32
32.63



Current Data Parameters
 NAME YXL-8-115-H-141031
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141031
 Time 9.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 89.81
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

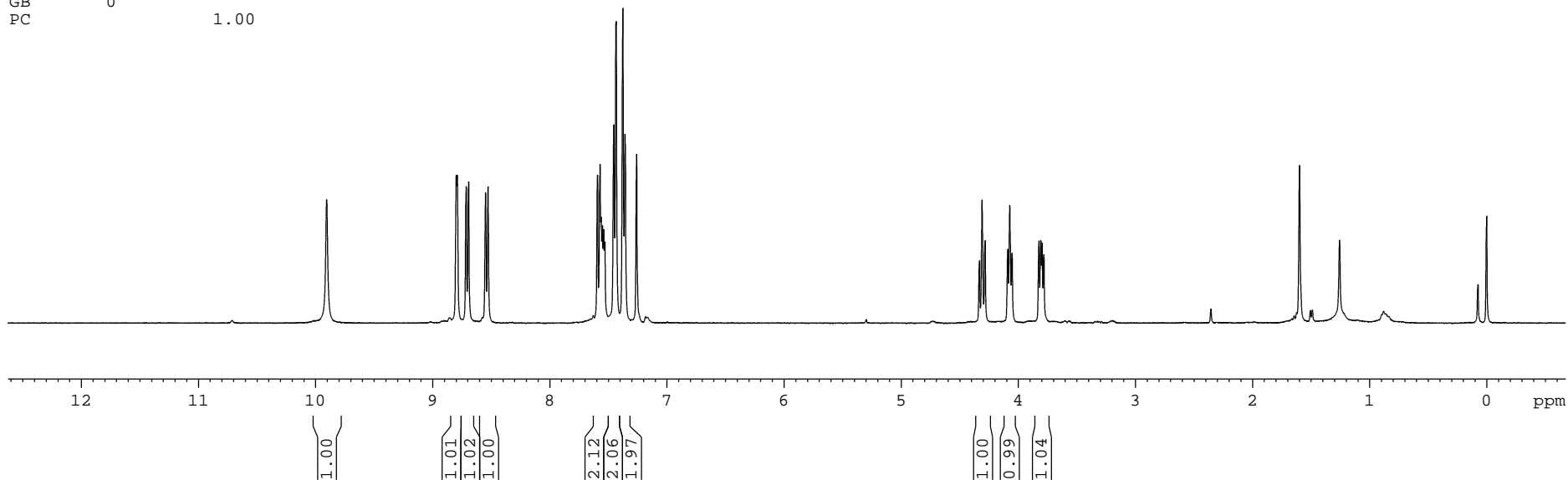
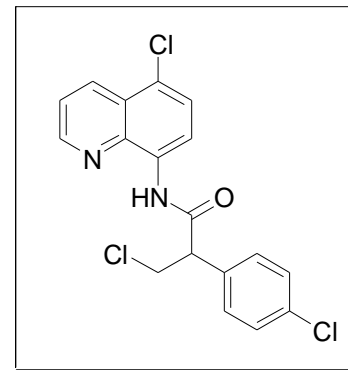
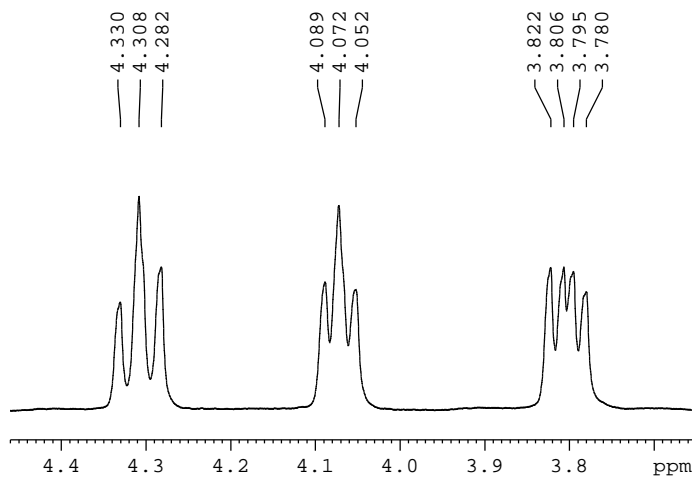
==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300089 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.7992
8.7953
8.7891
8.7133
8.6923
8.5485
8.5272
7.5917
7.5704
7.4533
7.4353
7.4326
7.3754
7.3579
7.2578

4.3303
4.3082
4.2819
4.0886
4.0723
4.0522
3.8221
3.8064
3.7952
3.7800

1.5974
1.2561



Current Data Parameters
 NAME YXL-9-166-CL-H-20150307
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150307
 Time 21.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 12
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 63.51
 DW 60.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

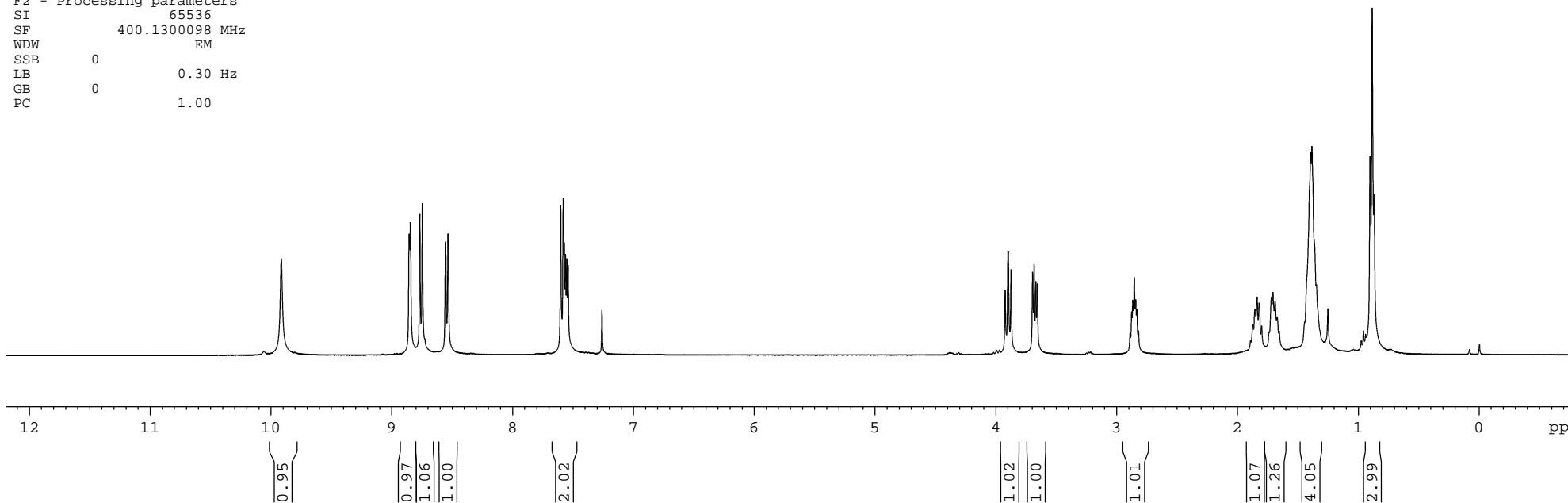
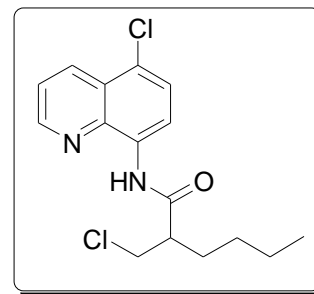
F2 - Processing parameters
 SI 65536
 SF 400.1300098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.9121

8.8561
 8.8464
 8.7675
 8.7466
 8.5554
 8.5342

7.6014
 7.5803
 7.5723
 7.5615
 7.5507
 7.5403
 7.2594

3.9227
 3.8990
 3.8965
 3.8737
 3.6956
 3.6831
 3.6687
 3.6561
 2.8753
 2.8659
 2.8536
 2.8415
 2.8320
 1.8727
 1.8548
 1.8371
 1.8202
 1.7995
 1.7191
 1.7063
 1.6880
 1.6705
 1.3933
 1.3834
 1.3464
 1.2505
 0.9025
 0.8848
 0.8660



— 171.59

— 148.85

— 139.06

— 133.46

— 127.25

— 126.01

— 124.73

— 122.46

— 116.74

— 77.45

— 77.13

— 76.81

— 51.79

— 45.32

— 30.89

— 29.39

— 22.71

— 13.90

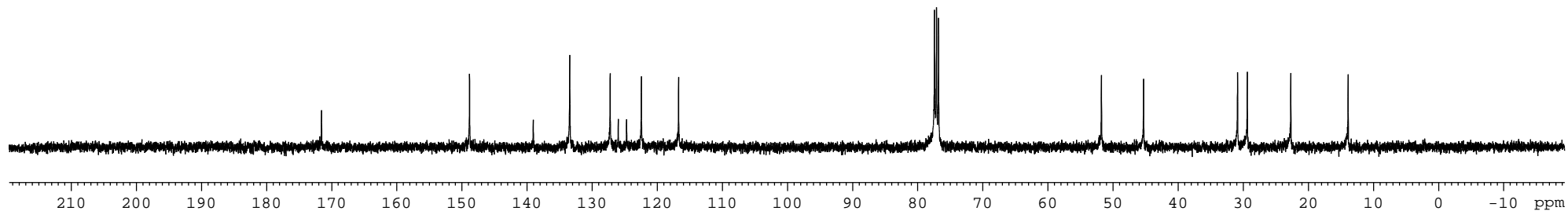
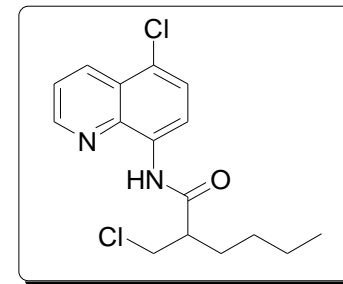
Current Data Parameters
NAME YXL-9-166-CL-C-20150307
EXPNO 32
PROCNO 1

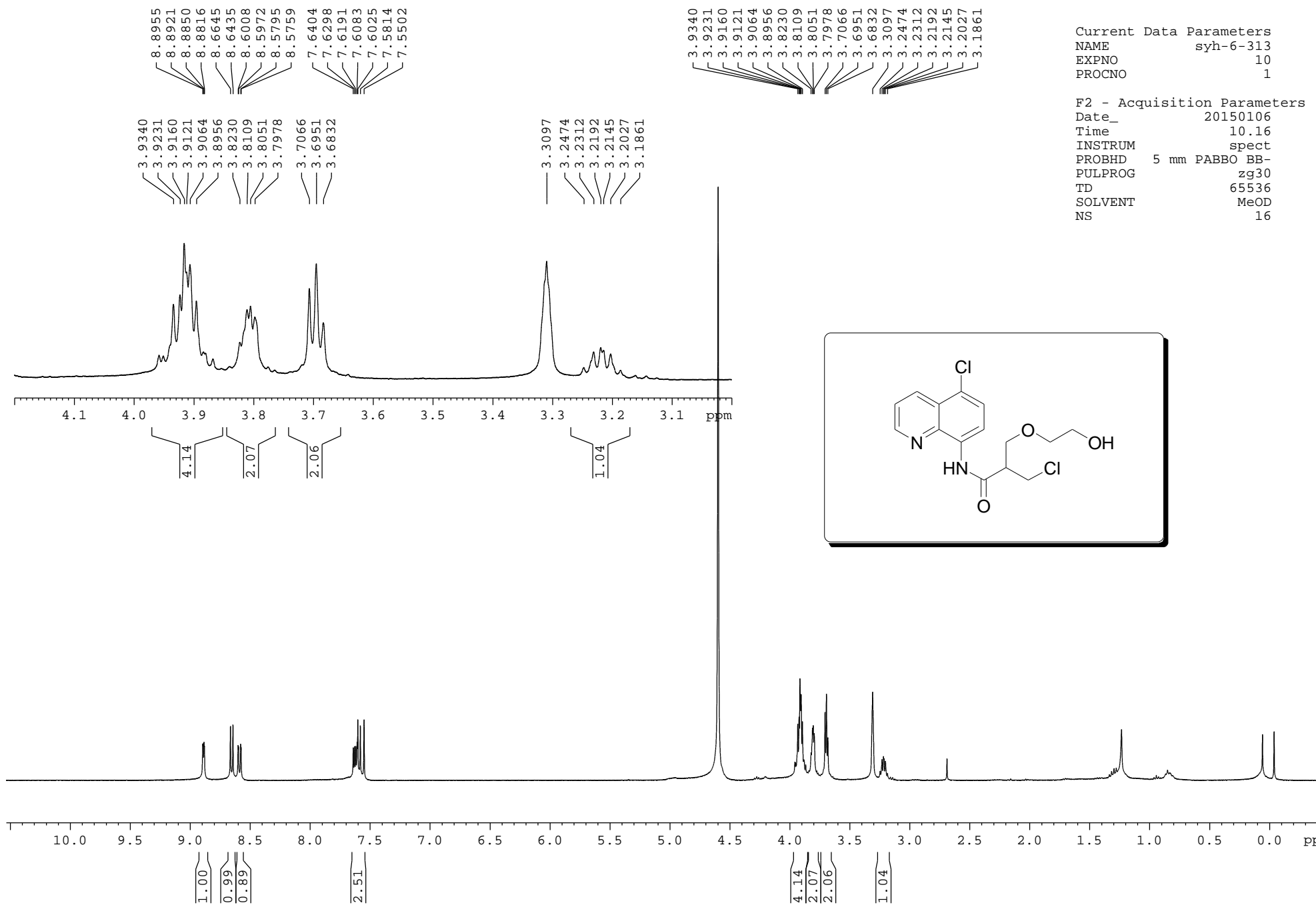
F2 - Acquisition Parameters
Date_ 20150308
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

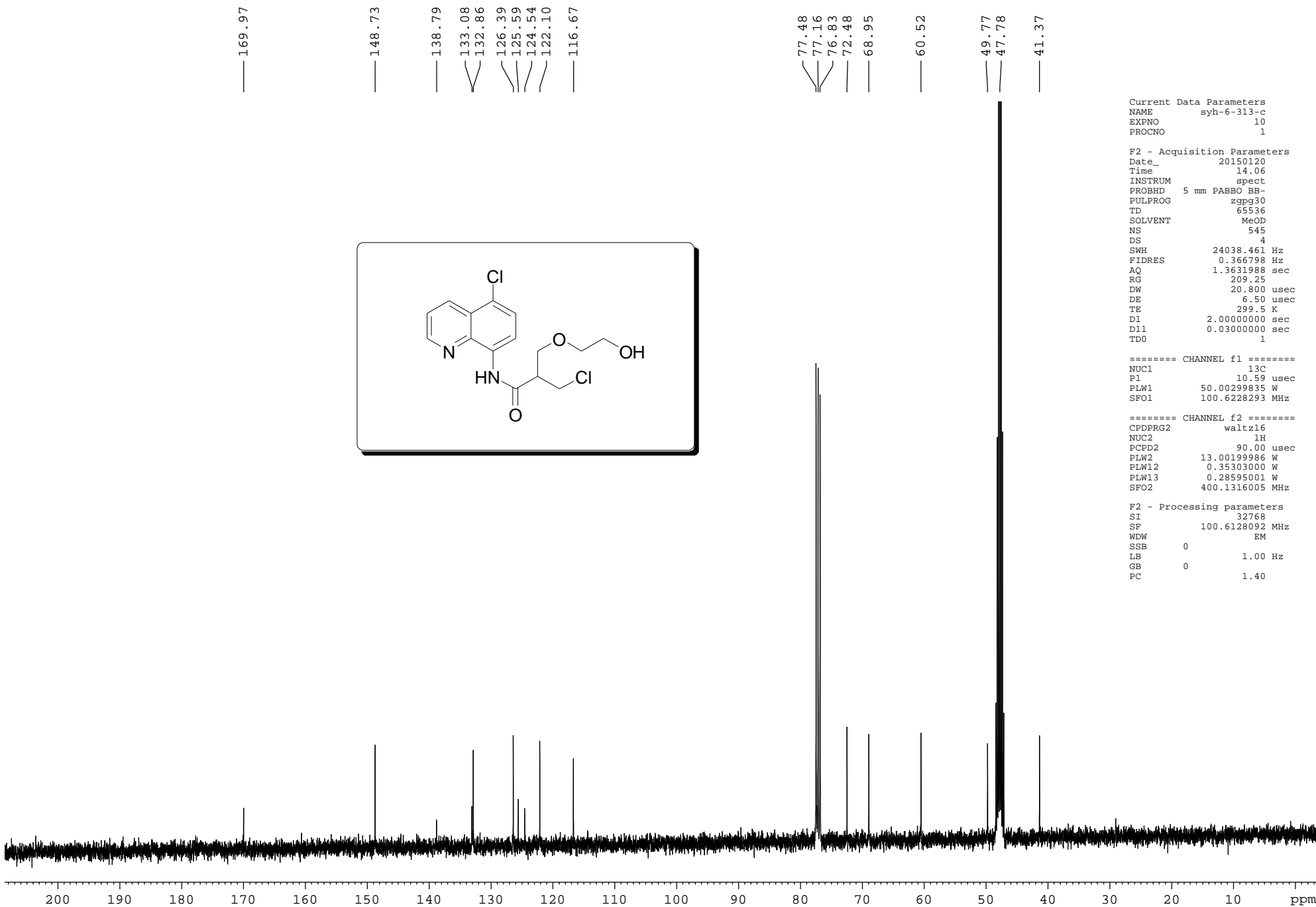
F2 - Processing parameters
SI 32768
SF 100.6127597 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





Current Data Parameters
 NAME syh-6-313
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150106
 Time 10.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16



Current Data Parameters
 NAME syh-6-313-c
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150120
 Time 14.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 545
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 299.5 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SPO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6128092 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME 20150421-zx-2-a-h
 EXPNO 10
 PROCNO 1

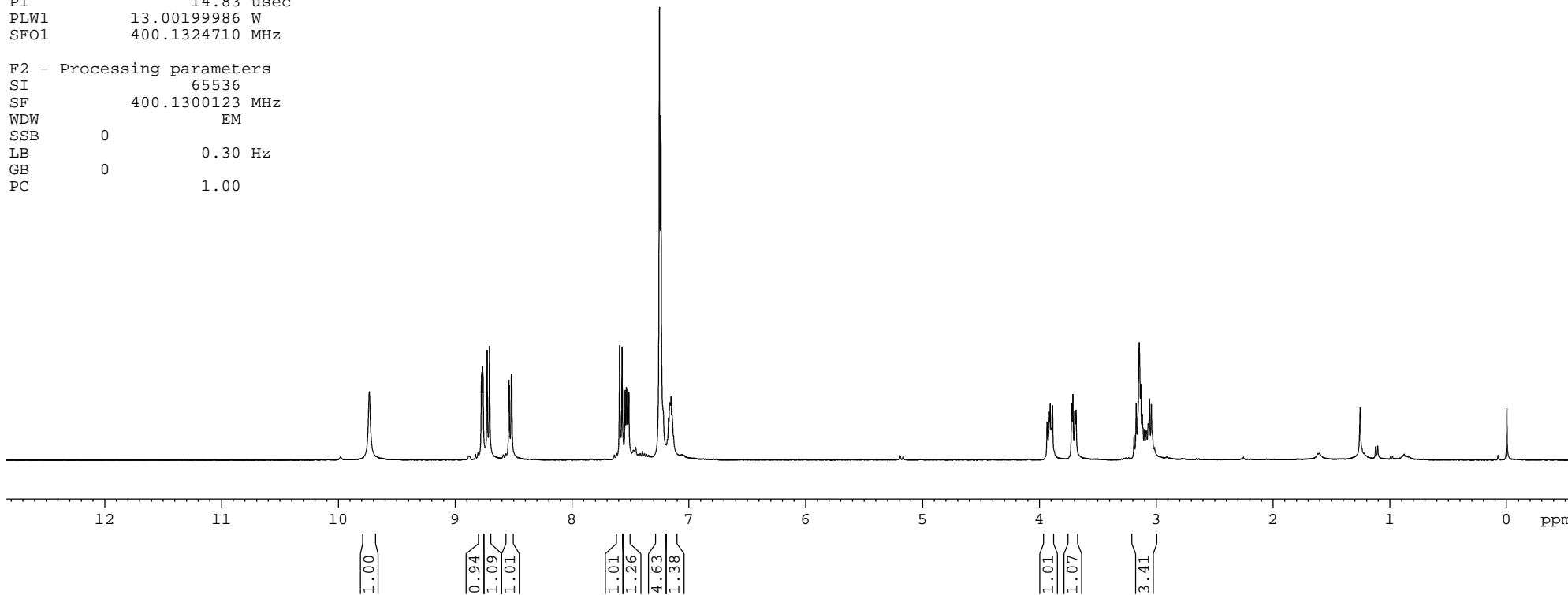
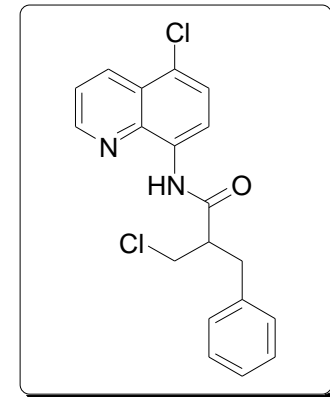
F2 - Acquisition Parameters
 Date_ 20150421
 Time 17.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 130.81
 DW 60.800 usec
 DE 6.50 usec
 TE 301.3 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.0019986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300123 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.7343
 8.7741
 8.7708
 8.7638
 8.7259
 8.7049
 8.5392
 8.5359
 8.5180
 8.5147
 7.5914
 7.5704
 7.5443
 7.5338
 7.5231
 7.5126
 7.2506
 7.2409
 7.1727
 7.1643
 7.1604
 7.1513
 7.1452

3.9354
 3.9158
 3.9082
 3.8999
 3.8886
 3.7258
 3.7145
 3.6986
 3.6872
 3.1721
 3.1465
 3.1332
 3.1209
 3.1146
 3.0702
 3.0585
 3.0430



Current Data Parameters
NAME 3h-c
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150422
Time 7.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1020
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W

170.71

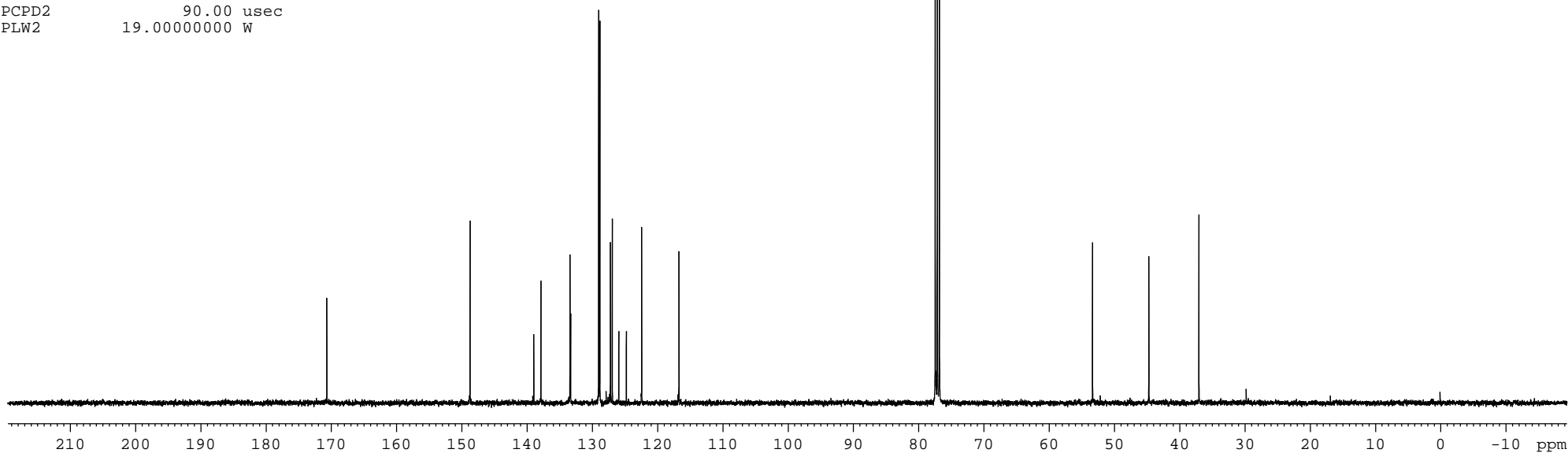
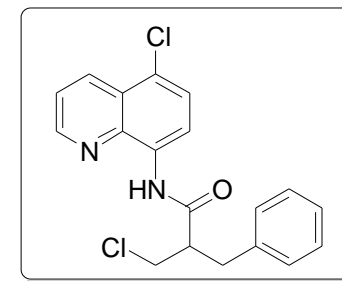
148.76
138.99
137.89
133.44
133.35
129.05
128.86
127.26
126.96
125.97
124.81
122.46
116.75

77.47
77.16
76.84

53.37

44.74

37.06



— 10.3845

8.9643
8.9558
8.5879
8.5658
8.5425
8.2459
8.0077
7.9875
7.7875
7.7771
7.7660
7.7532
7.7318
7.5405
7.5208
7.5010

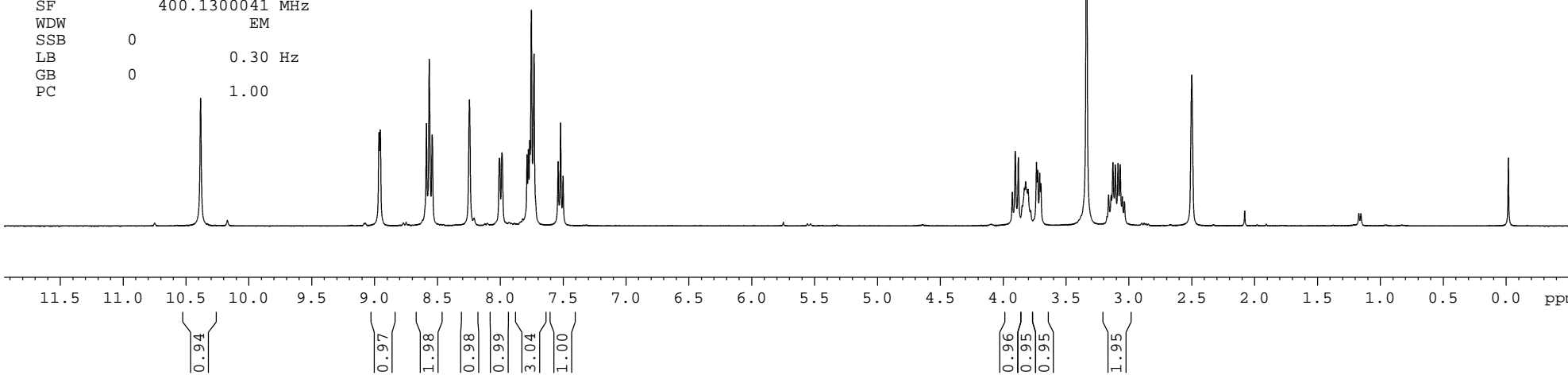
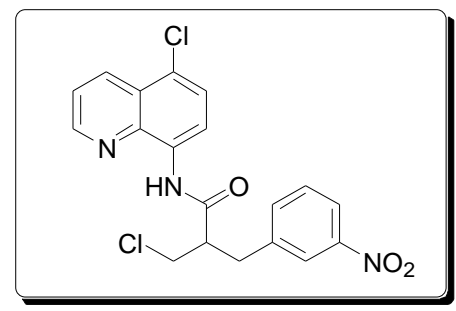
3.9271
3.9038
3.8794
3.8314
3.8212
3.8020
3.7351
3.7254
3.7095
3.7000
3.3365
3.1613
3.1414
3.1271
3.1079
3.0862
3.0692
3.0522

Current Data Parameters
NAME YXL-8-216-H-20141129
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141129
Time 22.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 130.81
DW 60.800 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300041 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME YXL-8-216-C-20141129
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141130
Time 10.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 490
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

=====
CHANNEL f1
=====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

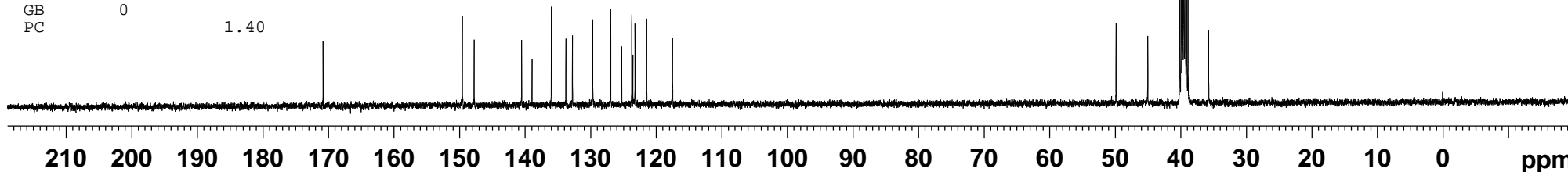
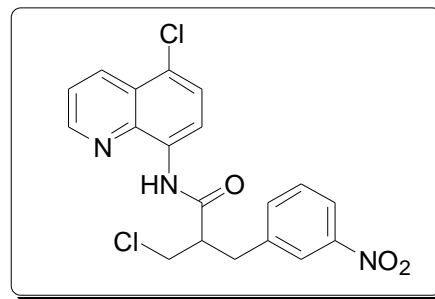
=====
CHANNEL f2
=====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

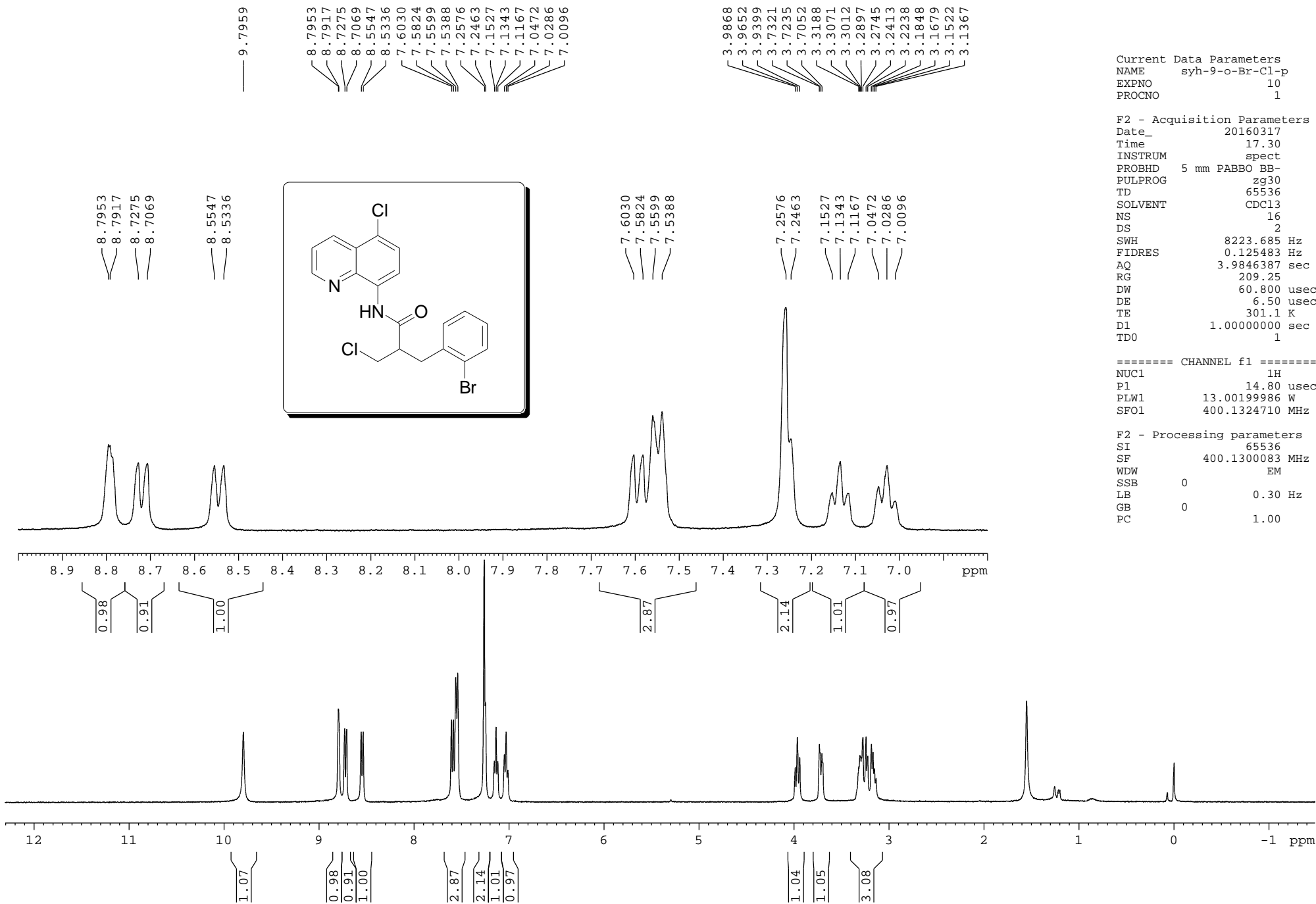
F2 - Processing parameters
SI 32768
SF 100.6128190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170.81

149.57
147.77
140.52
138.93
135.98
133.77
132.77
129.67
126.93
125.27
123.72
123.56
123.23
121.45
117.51

49.86
45.02
40.14
39.93
39.72
39.52
39.31
39.10
38.89
35.74



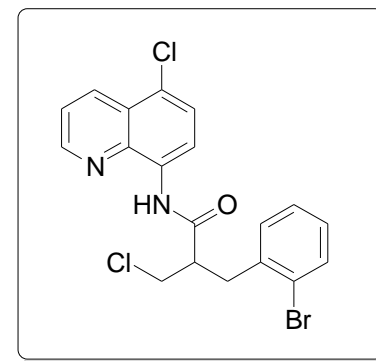
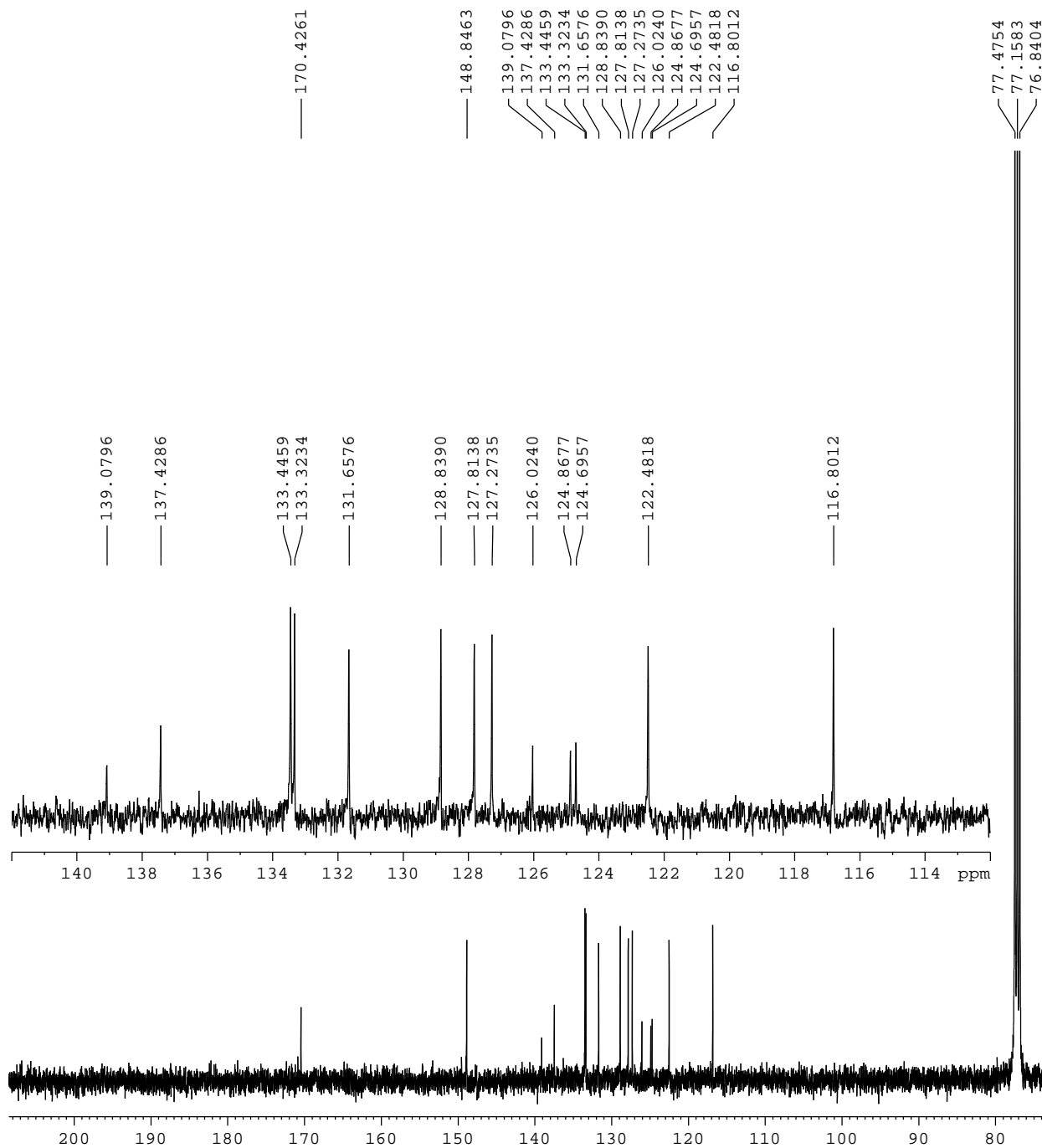


Current Data Parameters
 NAME syh-9-o-Br-Cl-p
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160317
 Time 17.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 209.25
 DW 60.800 usec
 DE 6.50 usec
 TE 301.1 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.80 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300083 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME syh-9-o-Br-Cl-p-c
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160318
 Time 0.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1536
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 302.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.90 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.38069001 W
 PLW13 0.30836001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127528 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

9.6760
8.7758
8.7724
8.7655
8.7620
8.7025
8.6815
8.5543
8.5508
8.5331
8.5296
7.5964
7.5755
7.5622
7.5516
7.5409
7.5303
7.2594
7.2232
7.2096
7.2021
7.1886
6.9362
6.9146
6.8930

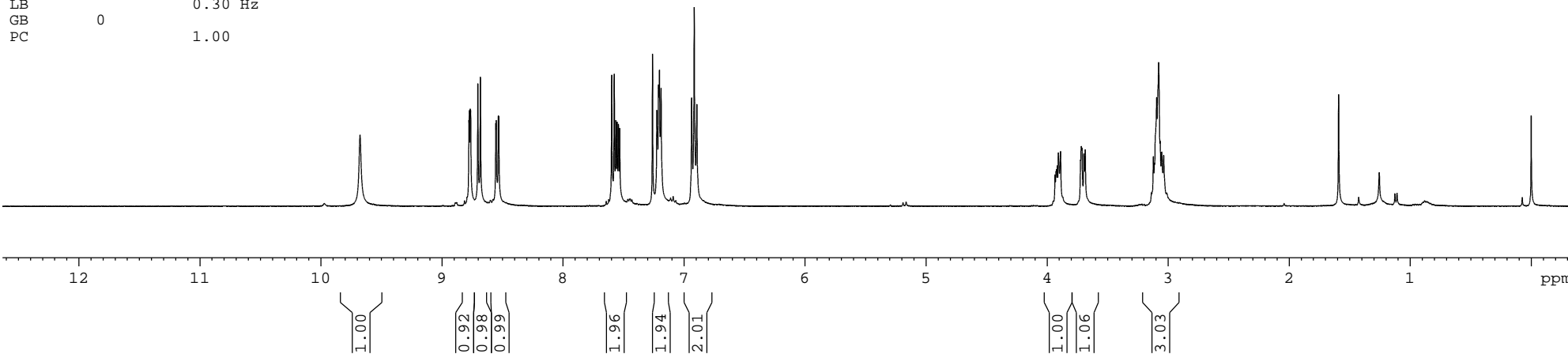
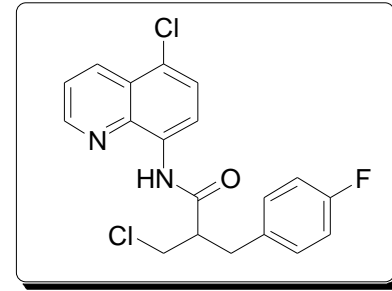
3.9355
3.9279
3.9239
3.9165
3.9079
3.8898
3.7249
3.7179
3.7131
3.6971
3.6860
3.1229
3.1141
3.0956
3.0791
3.0670
3.0548
3.0379

Current Data Parameters
NAME 20150418-zx-2-h
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150418
Time 10.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 165.63
DW 60.800 usec
DE 6.50 usec
TE 300.8 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SF01 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



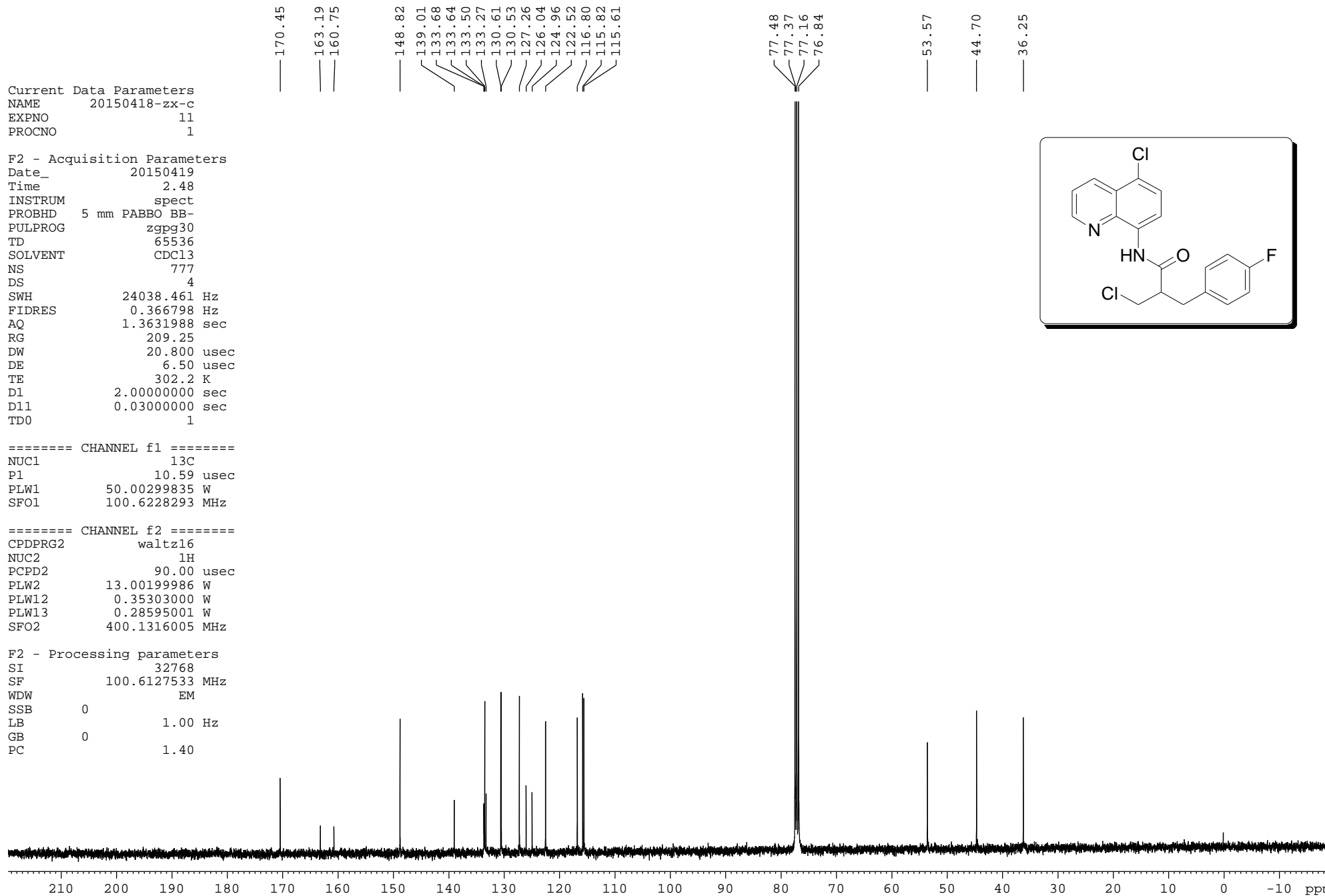
Current Data Parameters
NAME 20150418-zx-c
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150419
Time 2.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 777
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 302.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

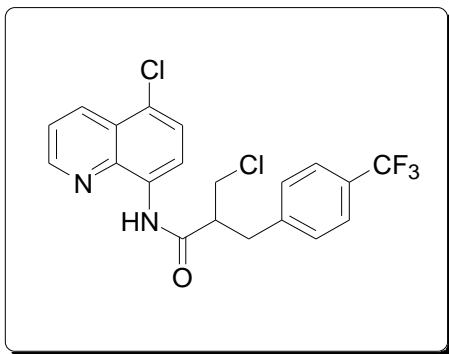
F2 - Processing parameters
SI 32768
SF 100.6127533 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



9.639

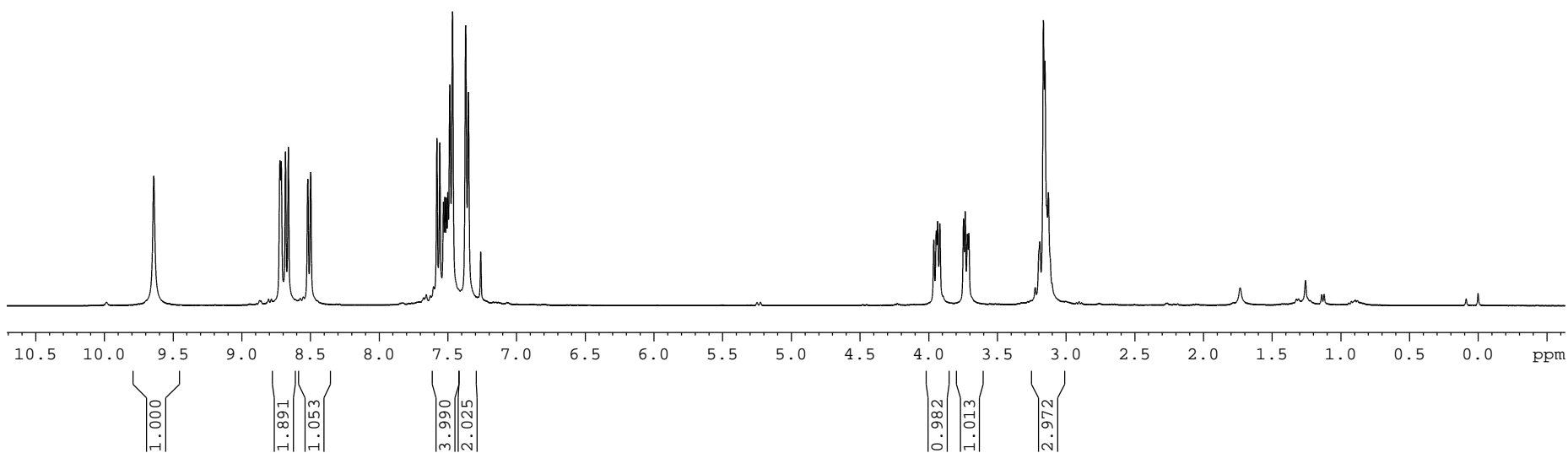
8.721
8.712
8.681
8.660
8.518
8.497
7.579
7.558
7.531
7.521
7.510
7.499
7.485
7.465
7.369
7.349
7.260

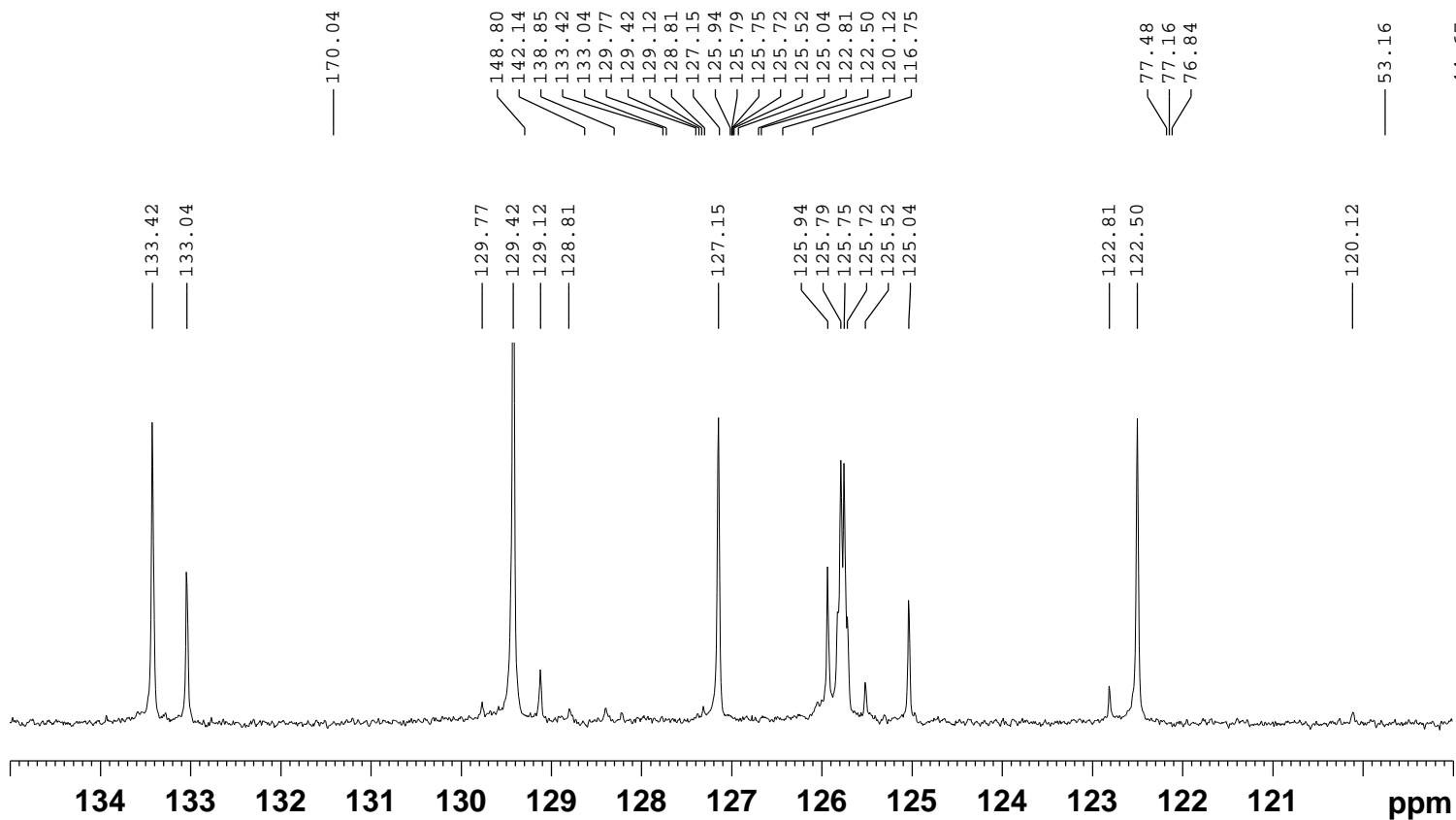
3.962
3.944
3.934
3.917
3.745
3.733
3.717
3.707
3.224
3.190
3.164
3.153
3.139
3.128



Current Data Parameters
NAME syh-7-233-1
EXPNO 10
PROCNO 1

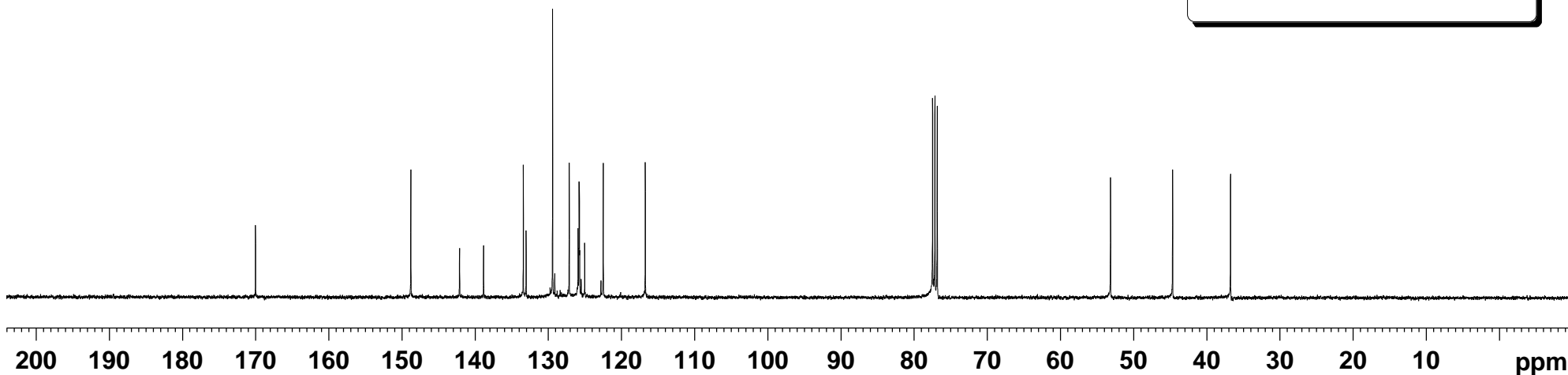
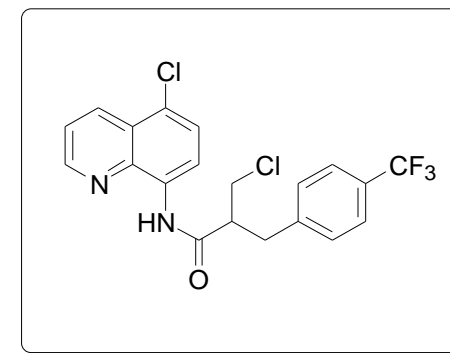
F2 - Acquisition Parameters
Date_ 20150425
Time 21.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13

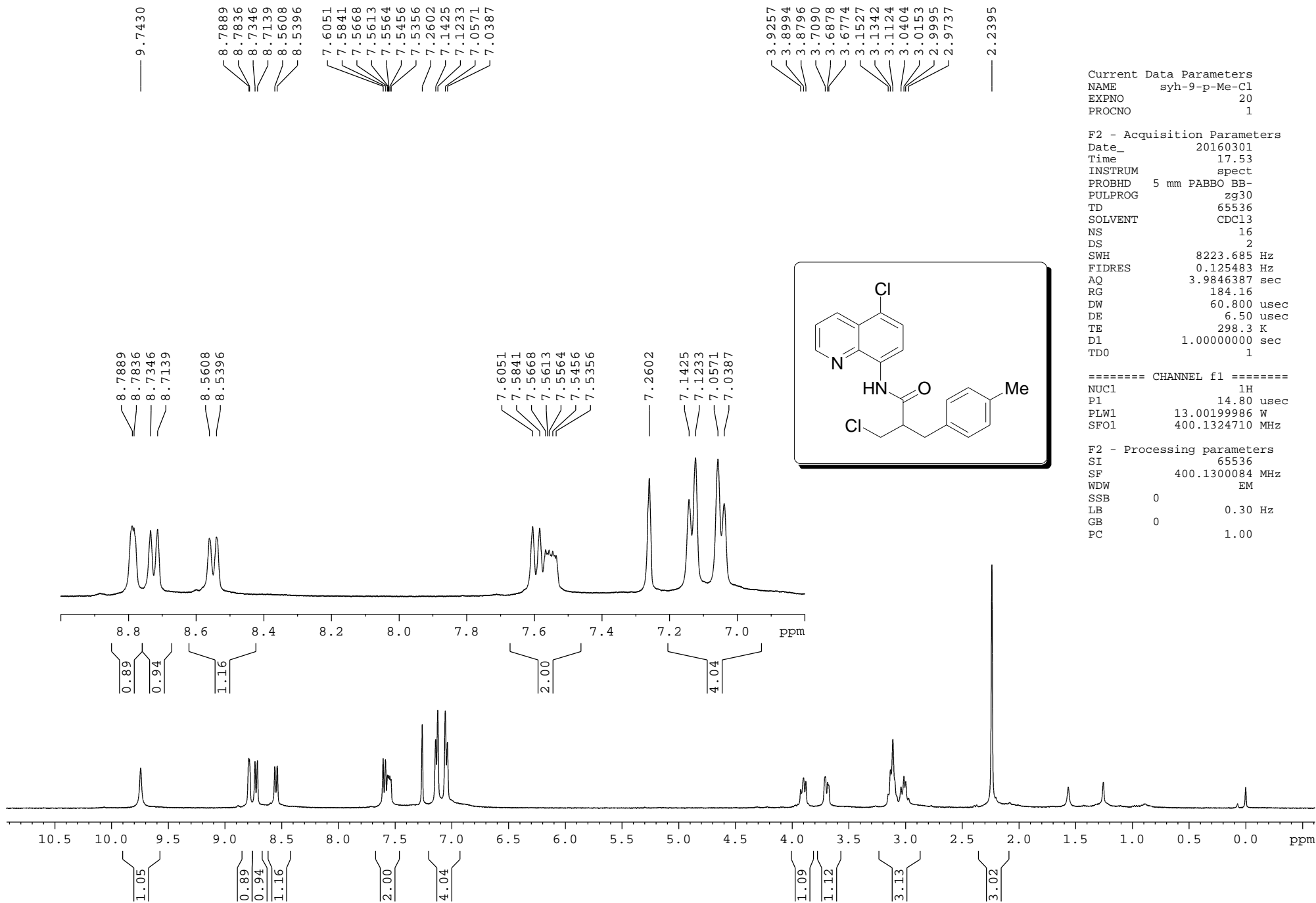




Current Data Parameters
 NAME syh-7-233-1-c
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150426
 Time 8.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13



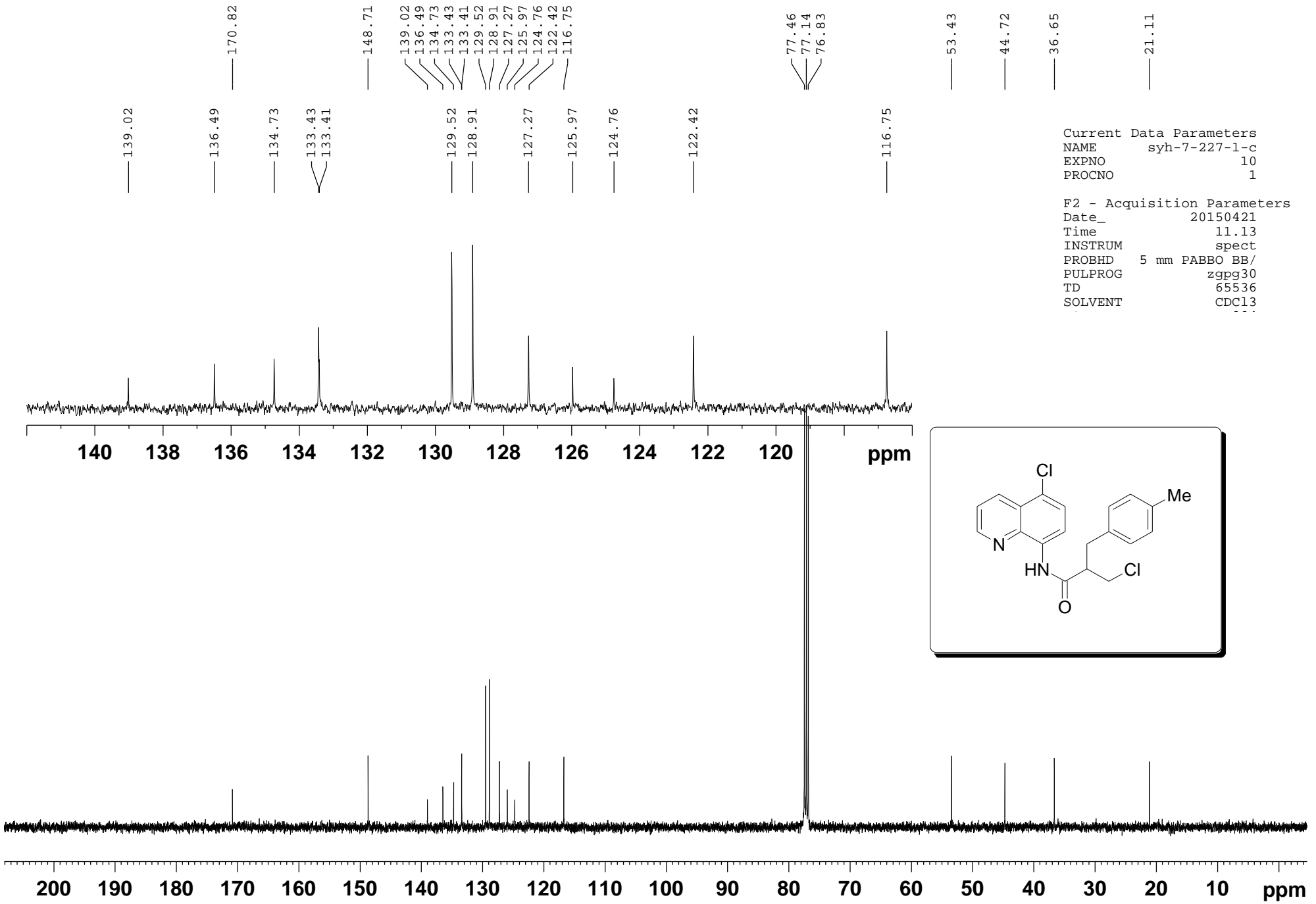


Current Data Parameters
 NAME syh-9-p-Me-Cl
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160301
 Time 17.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 184.16
 DW 60.800 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.80 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300084 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME syh-7-227-1-c
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150421
 Time 11.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13

9.5874
 8.7315
 8.7239
 8.6844
 8.6634
 8.5404
 8.5192
 7.8129
 7.7930
 7.5935
 7.5726
 7.5452
 7.5348
 7.5241
 7.5139
 7.3417
 7.3219
 7.2590

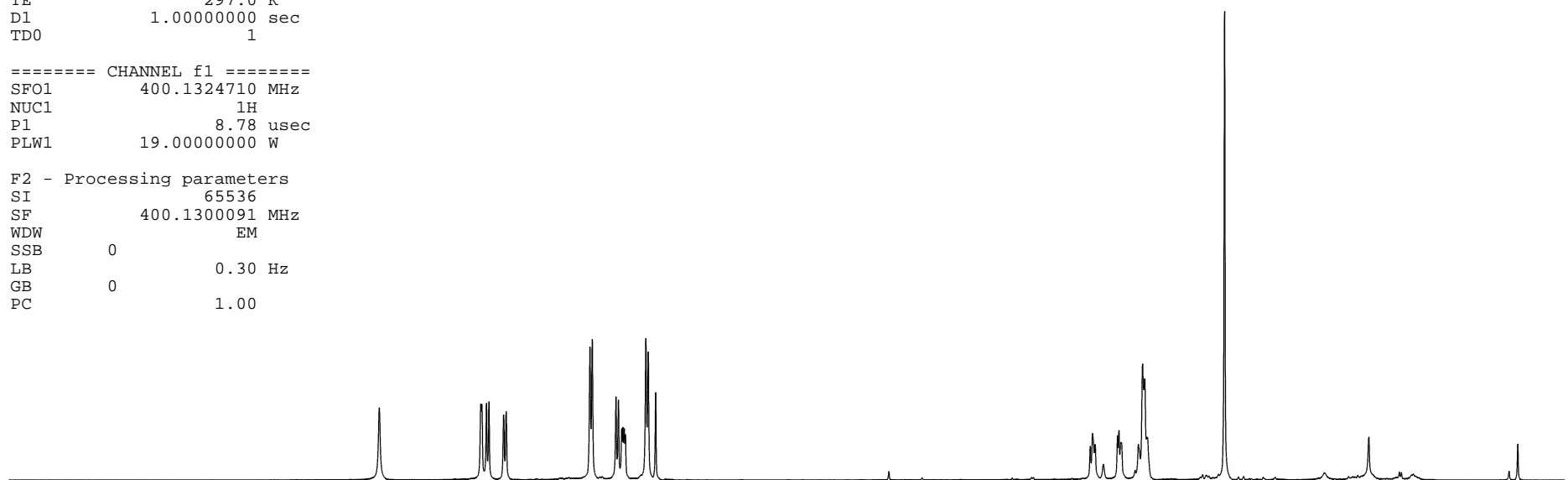
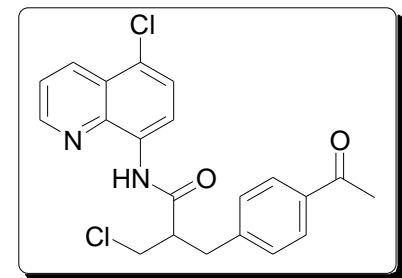
3.5980
 3.5793
 3.5576
 3.3683
 3.3565
 3.3400
 3.1930
 3.1576
 3.1396
 3.1218
 3.1150
 2.4664

Current Data Parameters
 NAME YXL-8-263-2-H-141213
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141213
 Time 15.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 89.81
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

1.07
 2.06
 1.00
 2.08
 2.19
 2.09
 1.07
 1.09
 3.07
 2.99

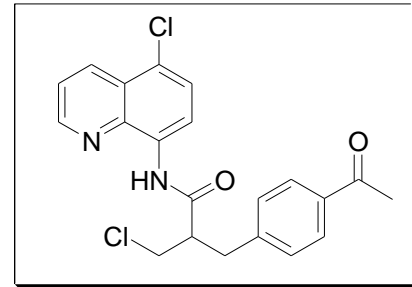
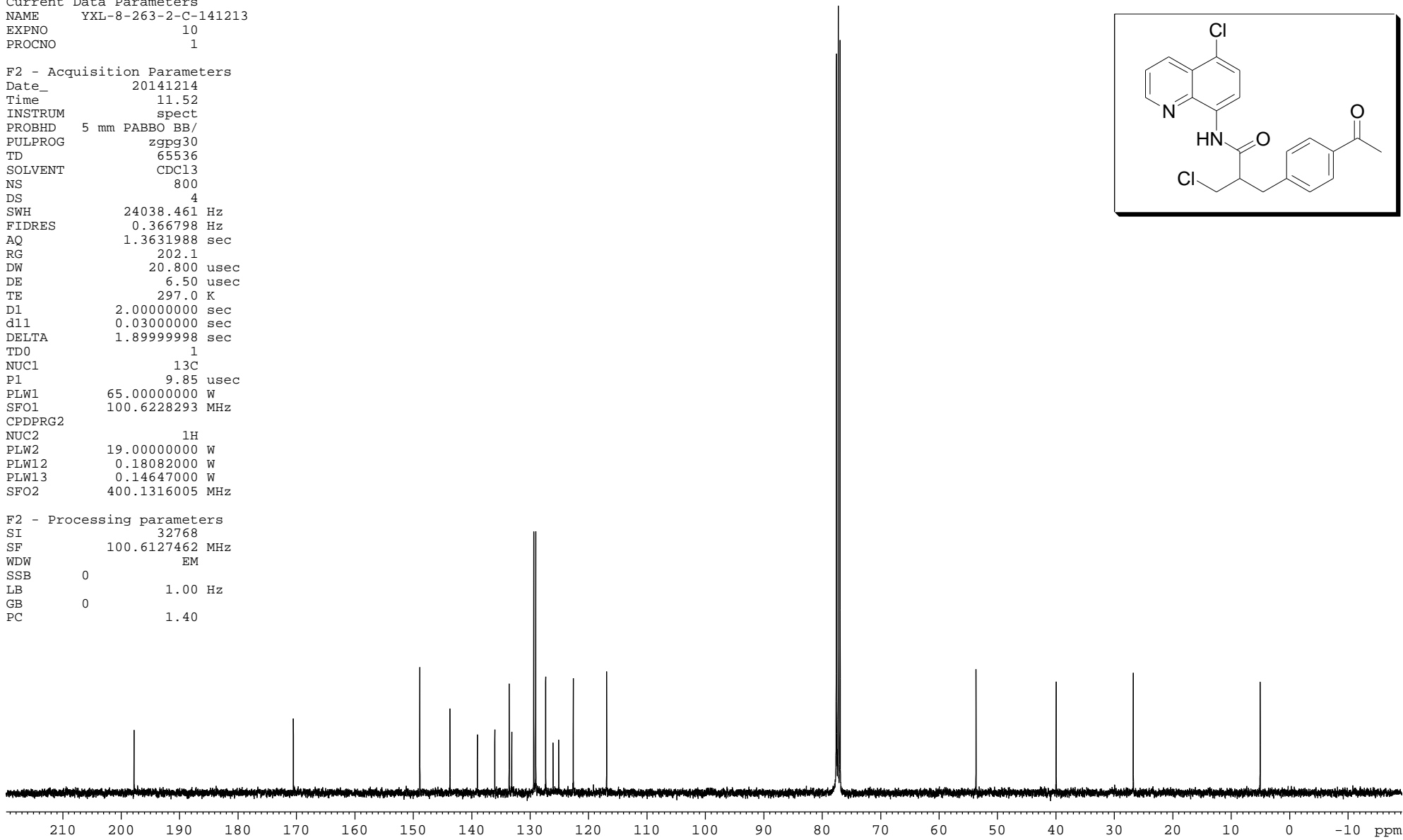
— 197.80
 — 170.53
 — 148.88
 — 143.73
 — 139.03
 — 136.04
 — 133.59
 — 133.14
 — 129.37
 — 129.03
 — 127.34
 — 126.08
 — 125.12
 — 122.62
 — 116.90

— 77.58
 — 77.26
 — 76.94
 — 53.67
 — 39.95
 — 26.74
 — 5.02

Current Data Parameters
 NAME YXL-8-263-2-C-141213
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141214
 Time 11.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 800
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 202.1
 DW 20.800 usec
 DE 6.50 usec
 TE 297.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1
 NUC1 13C
 P1 9.85 usec
 PLW1 65.00000000 W
 SFO1 100.6228293 MHz
 CPDPRG2
 NUC2 1H
 PLW2 19.00000000 W
 PLW12 0.18082000 W
 PLW13 0.14647000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127462 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME YXL-9-235-H-20150330
 EXPNO 20
 PROCNO 1

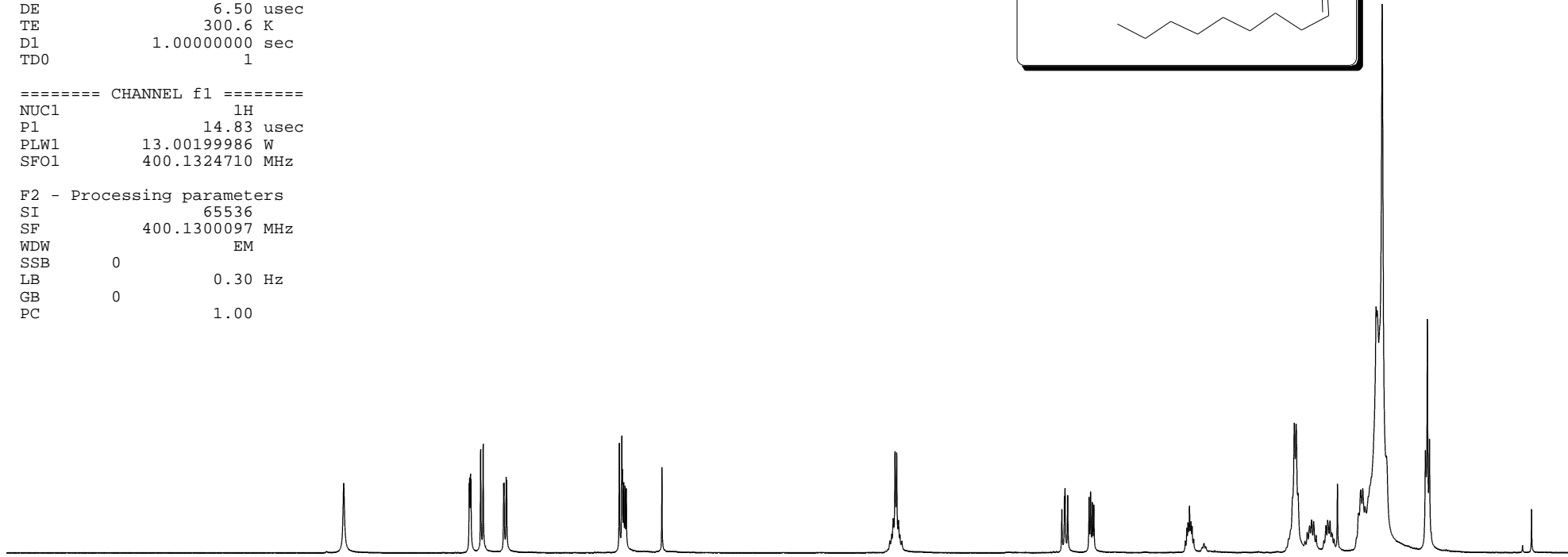
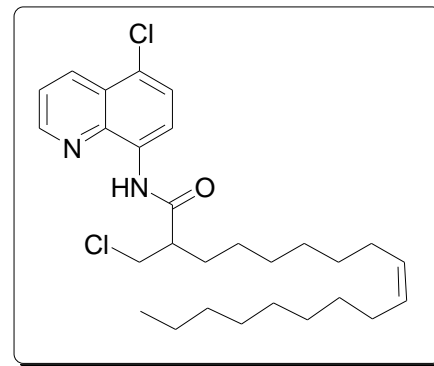
F2 - Acquisition Parameters
 Date_ 20150330
 Time 14.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 63.51
 DW 60.800 usec
 DE 6.50 usec
 TE 300.6 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.9166
 8.8686
 8.8648
 8.8581
 8.8544
 8.7732
 8.7522
 8.5814
 8.5777
 8.5601
 8.5564
 7.6154
 7.5943
 7.5892
 7.5785
 7.5678
 7.5572
 7.2598

5.3409
 5.3287
 5.3133
 5.2995
 5.2847
 5.2725
 3.9207
 3.8984
 3.8938
 3.8717
 3.6933
 3.6806
 3.6662
 3.6536
 2.8918
 2.8787
 2.8697
 2.8569
 2.8441
 2.8351
 2.8221
 2.0301
 1.9814
 1.9664
 1.9508
 1.8931
 1.8743
 1.8542
 1.8381
 1.8211
 1.7996
 1.7358
 1.7176
 1.7034
 1.6836
 1.6690
 1.6500
 1.4460
 1.4277
 1.4101
 1.3914
 1.2992
 1.2903
 1.2485



0.97
 0.95
 1.05
 1.00
 2.06
 1.97
 1.00
 1.03
 0.99
 3.76
 1.12
 1.13
 21.44
 3.12

Current Data Parameters
 NAME 30-C
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150331
 Time 1.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.1
 DW 20.800 usec
 DE 6.50 usec
 TE 297.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 100.6228293 MHz
 NUC1 13C
 P1 9.85 usec
 PLW1 65.00000000 W

==== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 19.00000000 W
 PLW12 0.18082000 W
 PLW13 0.14647000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127567 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0

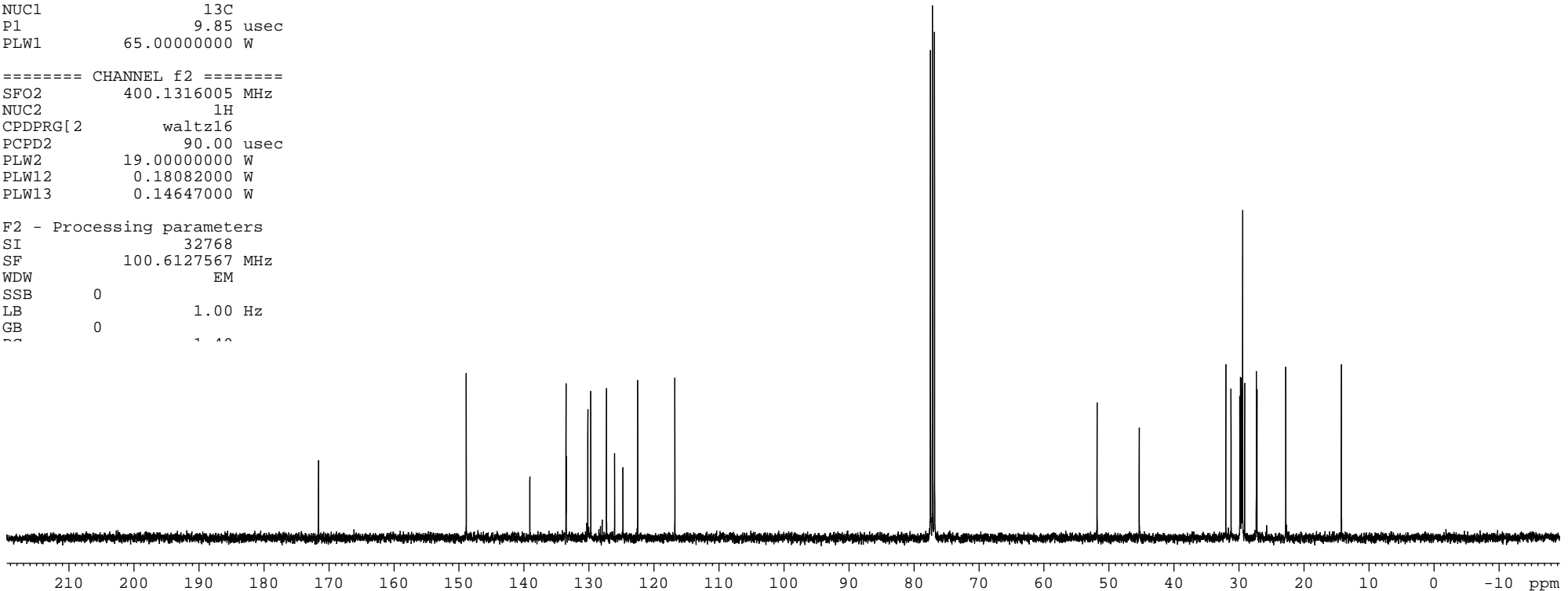
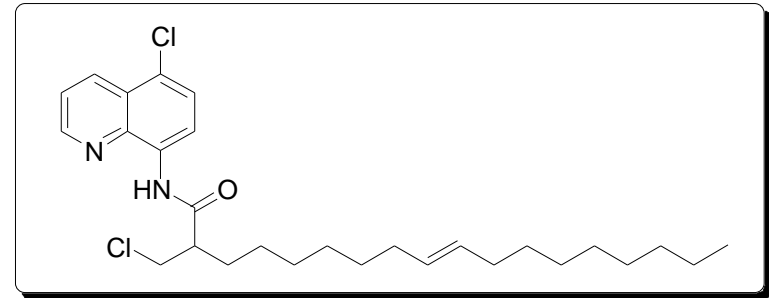
171.63

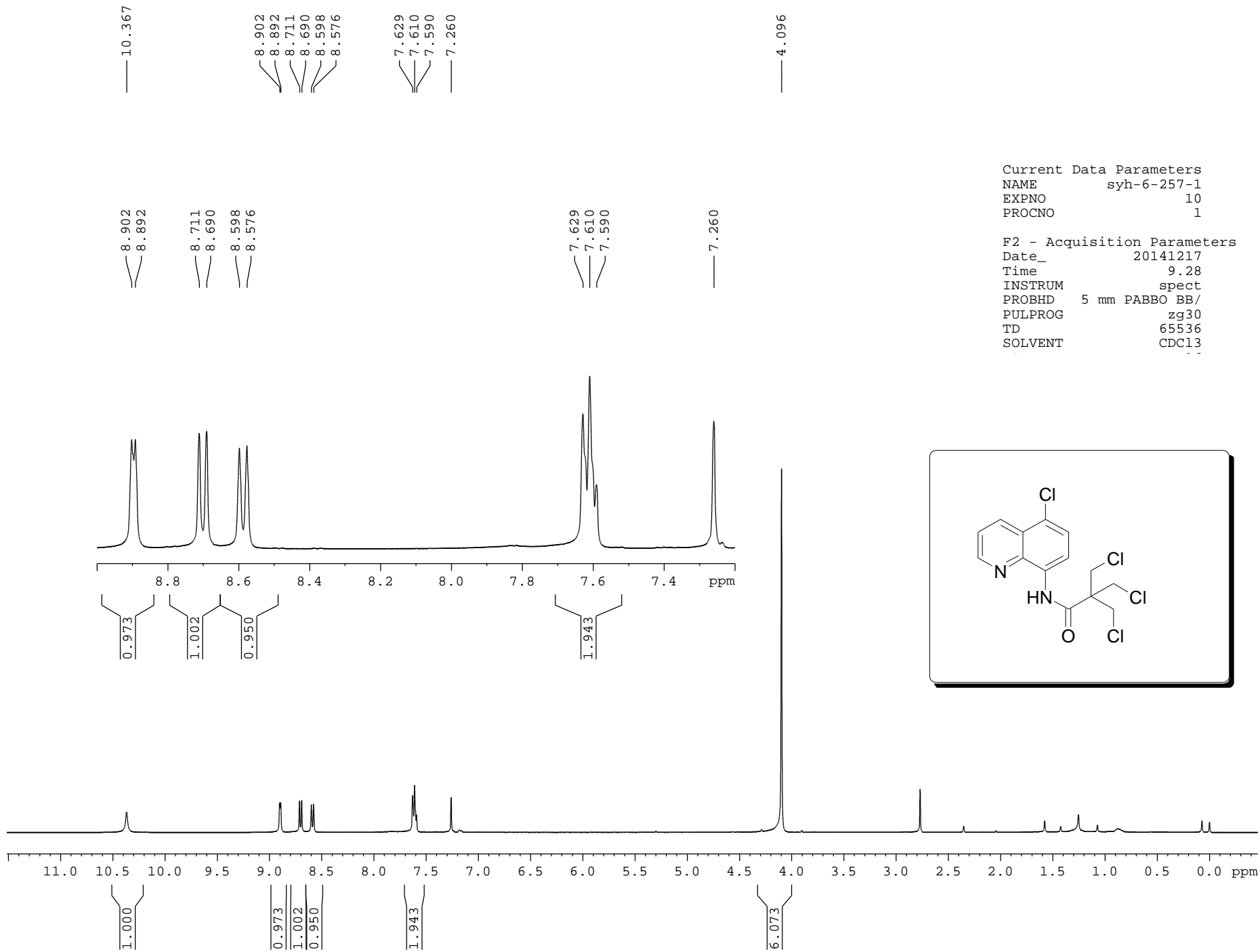
148.89

139.11
 133.54
 133.49
 130.18
 129.73
 127.32
 126.07
 124.79
 122.51
 116.79

77.47
 77.16
 76.84

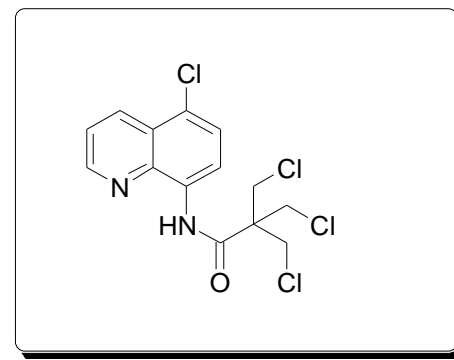
51.82
 45.34
 32.02
 31.21
 29.87
 29.75
 29.63
 29.56
 29.43
 29.12
 27.33
 27.29
 27.23
 22.81
 14.25

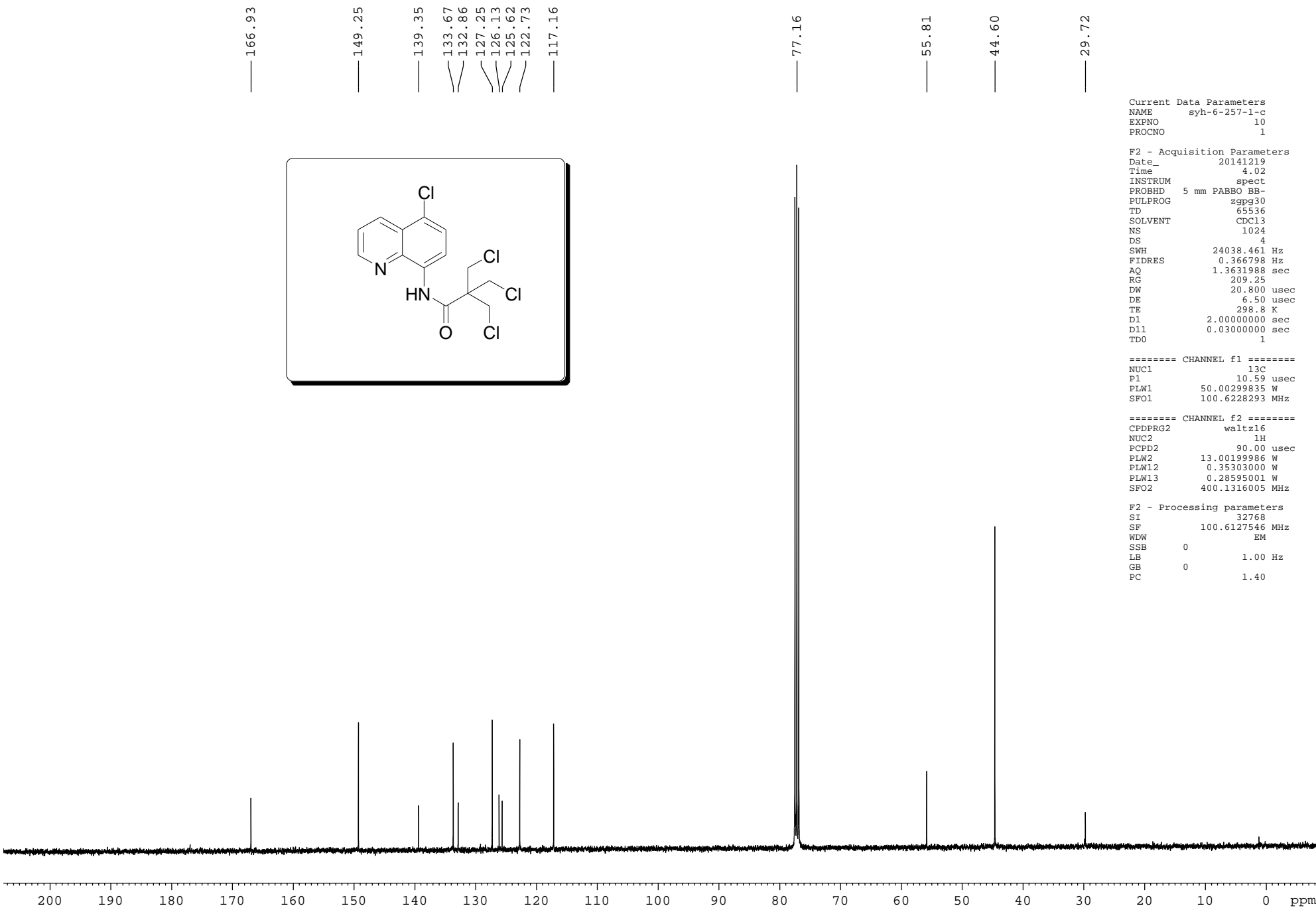




Current Data Parameters
 NAME syh-6-257-1
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141217
 Time 9.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3





Current Data Parameters
 NAME syh-6-257-1-c
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141219
 Time 4.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 298.8 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127546 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
NAME 3Q1-H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150422
Time 16.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 60.76
DW 62.400 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 8.78 usec
PLW1 19.00000000 W

F2 - Processing parameters

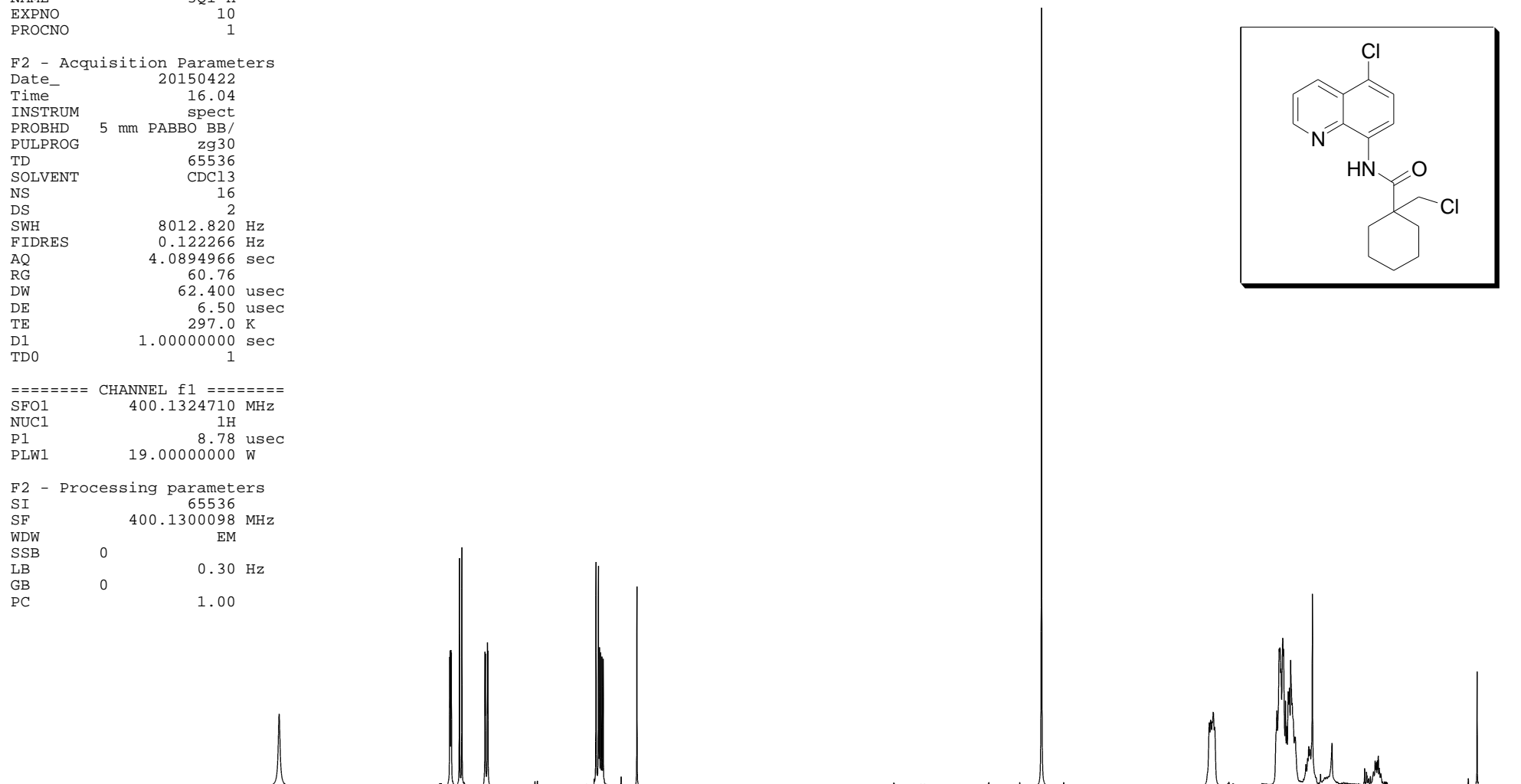
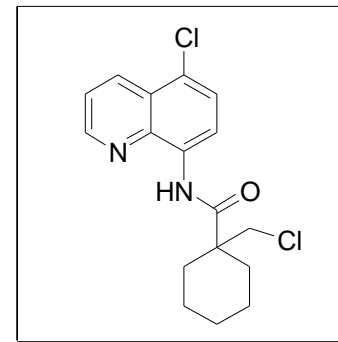
SI 65536
SF 400.130098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10.353

8.879
8.874
8.868
8.864
8.794
8.773
8.573
8.569
8.552
8.548
7.614
7.593
7.583
7.573
7.562
7.552
7.260

3.765

2.313
2.301
2.288
2.280
2.268
1.729
1.710
1.702
1.694
1.679
1.673
1.655
1.645
1.632
1.621
1.610
1.597
1.576
1.569
1.478
1.464
1.454
1.443
1.423



12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

0.95
1.00
1.00
2.06
1.99
2.04
7.42
1.35

— 172.70

— 149.00

— 139.55

— 133.66

— 133.49

— 127.35

— 126.07

— 124.57

— 122.46

— 116.58

— 51.90

— 49.75

— 32.33

— 25.81

— 22.69

Current Data Parameters

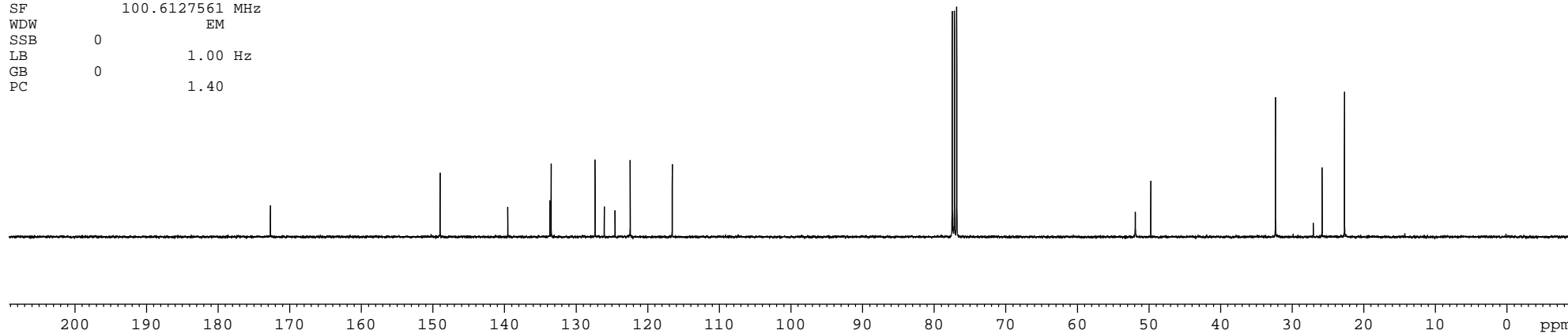
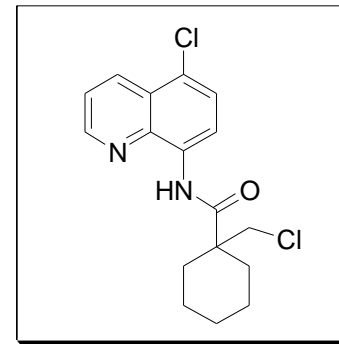
NAME 3Q1-C
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150422
Time 18.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 518
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W
SFO1 100.6228293 MHz
CPDPRG2
NUC2 1H
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6127561 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME 3Q2-H
 EXPNO 10
 PROCNO 1

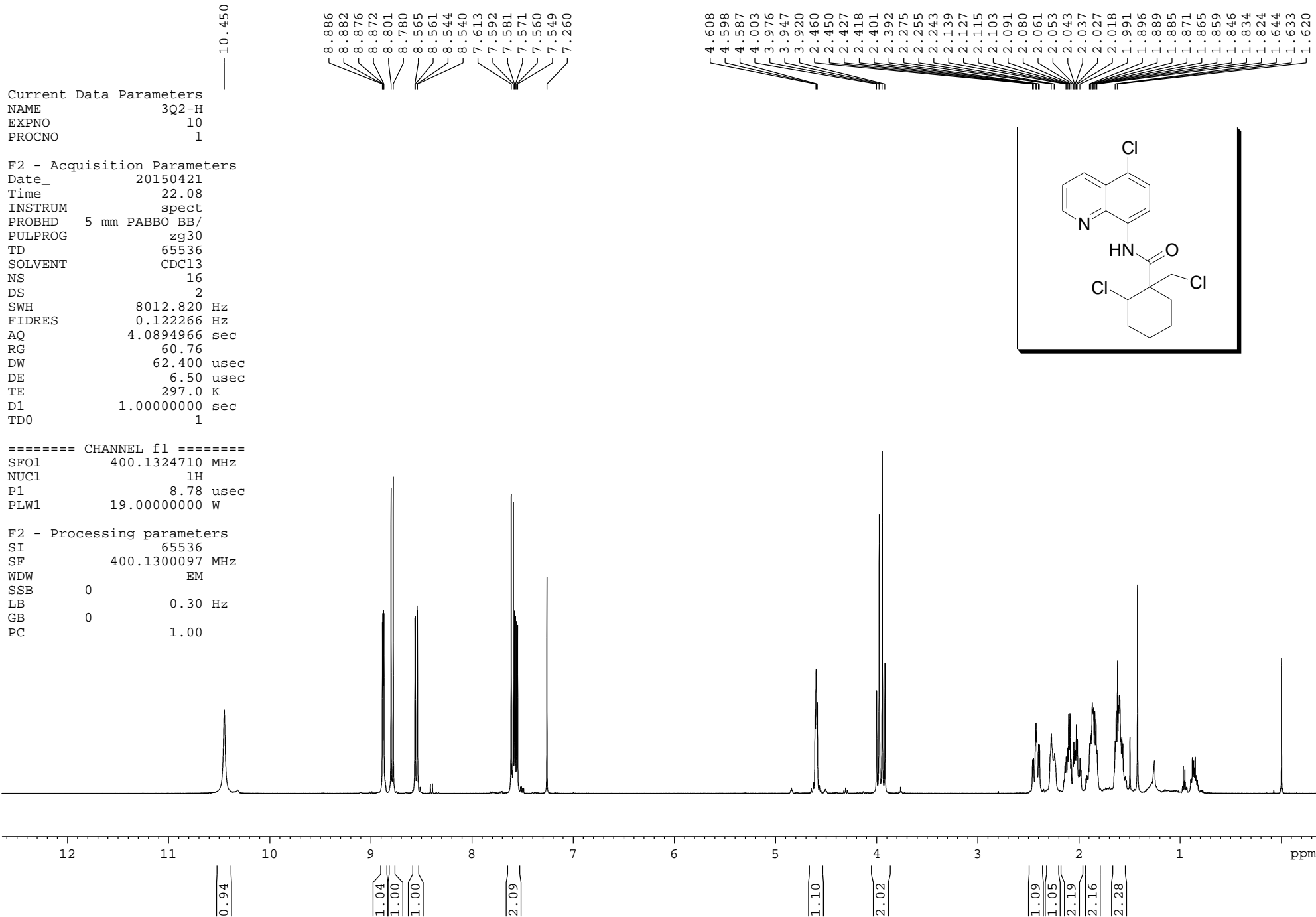
F2 - Acquisition Parameters

Date_ 20150421
 Time 22.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 60.76
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters

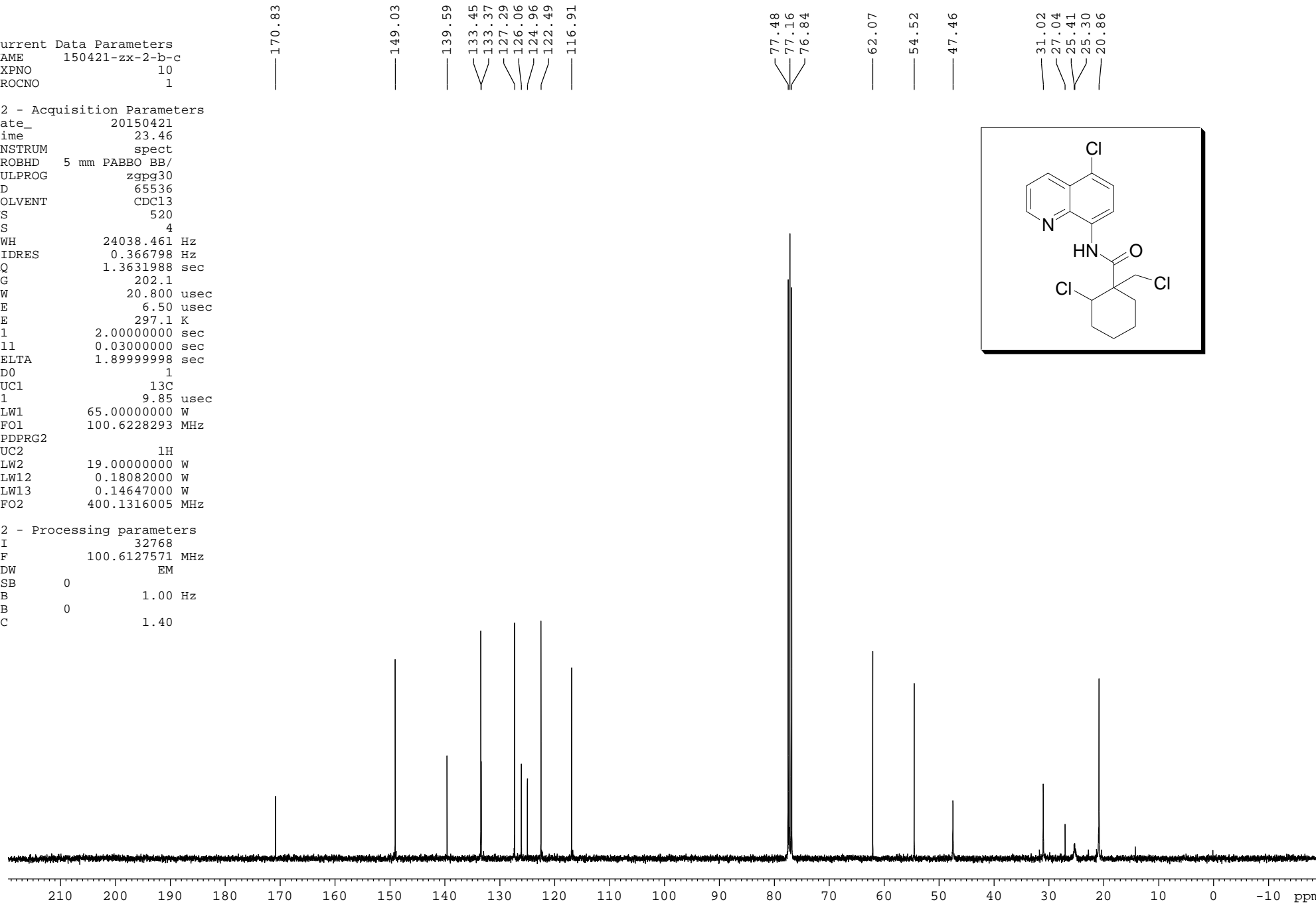
SI 65536
 SF 400.1300097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME 150421-zx-2-b-c
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150421
Time 23.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 520
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W
SFO1 100.6228293 MHz
CPDPRG2
NUC2 1H
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



— 170.83

— 149.03

— 139.59

— 133.45

— 133.37

— 127.29

— 126.06

— 124.96

— 122.49

— 116.91

— 77.48

— 77.16

— 76.84

— 62.07

— 54.52

— 47.46

— 31.02

— 27.04

— 25.41

— 25.30

— 20.86

10.3191

8.8573
8.8501
8.8469
8.6956
8.6747
8.5816
8.5784
8.5604
8.5572
7.6127
7.5997
7.5912
7.5785
7.5679
7.2595
6.9066
6.8880
6.6035
6.5849
6.5201

4.1050
4.0739
4.0437
3.9840
3.9693
3.9547

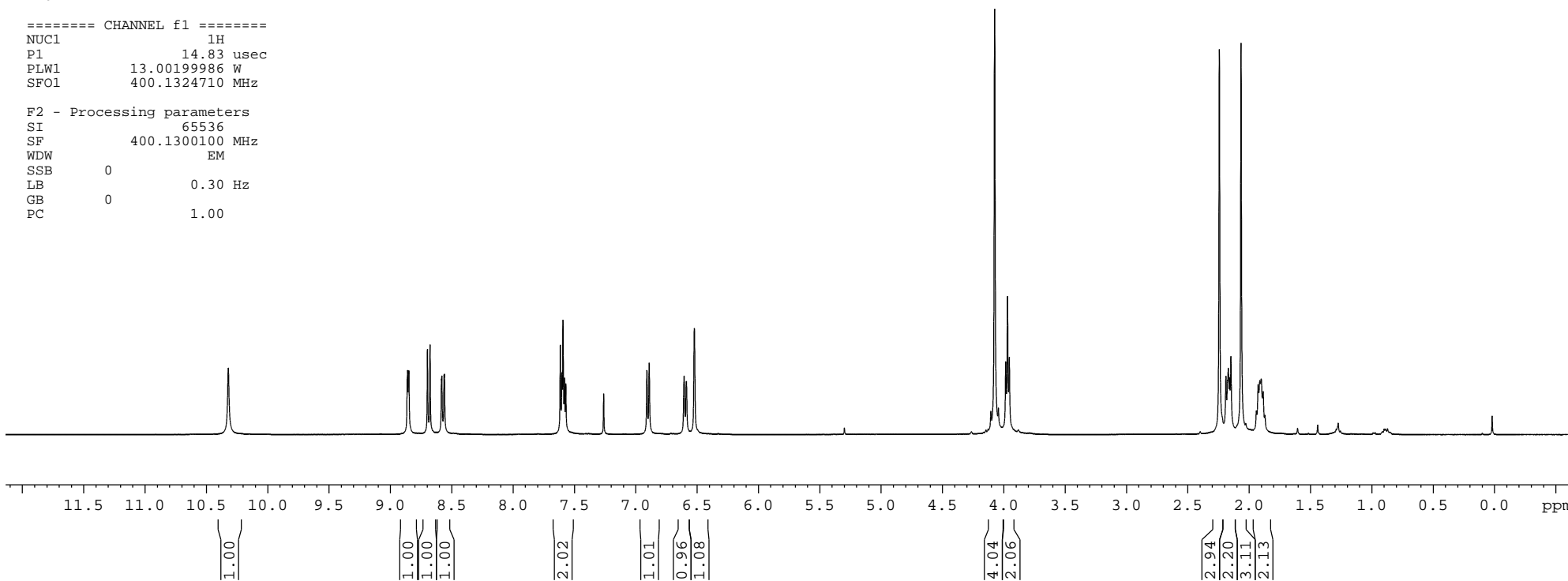
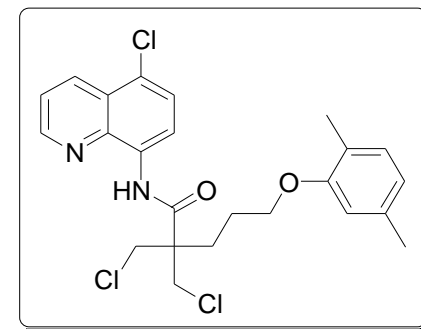
2.2425
2.1891
2.1763
2.1694
2.1591
2.1482
2.0657
1.9262
1.9126
1.9010
1.8855

Current Data Parameters
NAME YXL-9-171-C-H-20150309
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150309
Time 21.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 63.51
DW 60.800 usec
DE 6.50 usec
TE 0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME YXL-9-171-C-C-20150309
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150310
Time 4.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127578 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

— 169.65
— 156.68
— 149.06
— 139.25
— 136.51
— 133.59
— 133.08
— 130.35
— 127.22
— 126.07
— 125.10
— 123.55
— 122.60
— 120.95
— 116.74
— 111.83

— 77.48
— 77.16
— 76.84

— 66.92

— 53.63

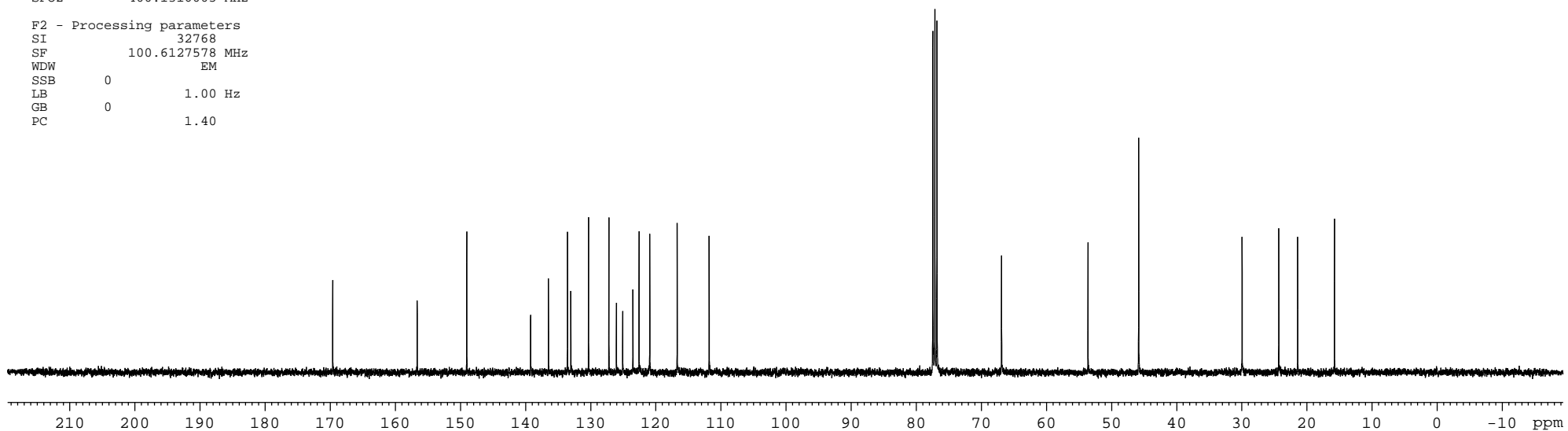
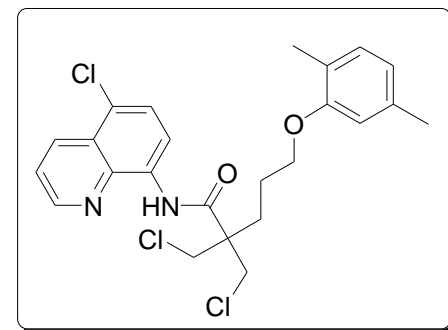
— 45.86

— 29.97

— 24.33

— 21.43

— 15.78



9.9782
8.8144
8.8107
8.8039
8.8003
8.7511
8.7301
8.5548
8.5511
8.5335
8.5298
7.6078
7.5868
7.5605
7.5499
7.5373
7.5328
7.5288
7.5161
7.4929
7.4721
7.4528
7.4352
7.4160
7.3850
7.3666
7.3597
7.3551
7.3498
7.3310
7.3274
7.2601

4.3891
4.3676
4.3622
4.3406
4.1504
4.1350
4.1294
4.1139
3.9037
3.8885
3.8767
3.8614

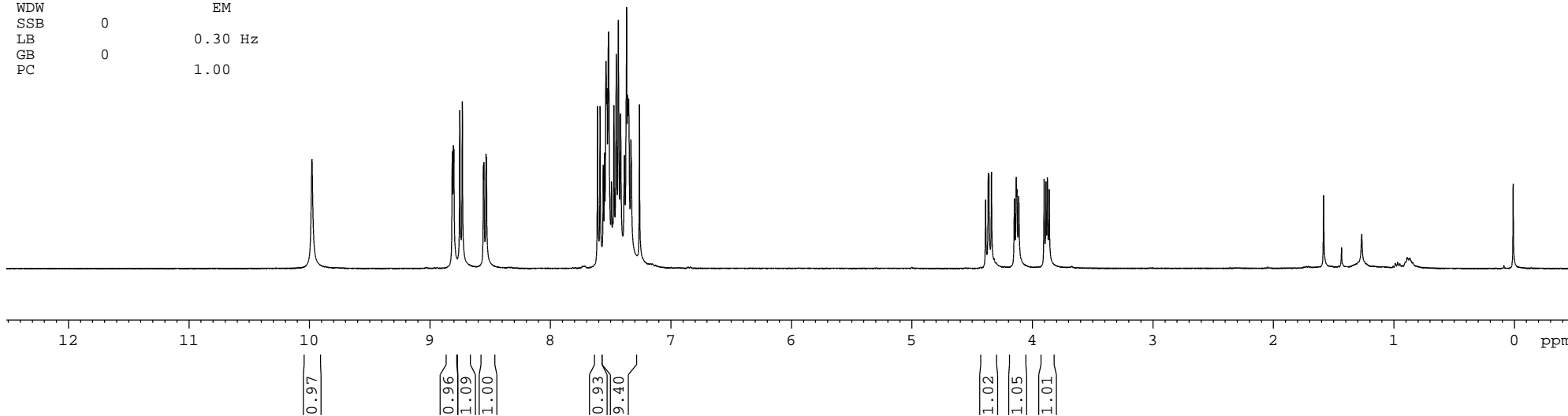
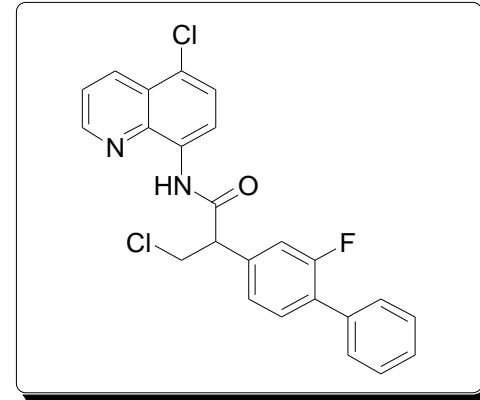
1.5842

Current Data Parameters
NAME 20150412-zx-2-77
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144.49
DW 60.800 usec
DE 6.50 usec
TE 304.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.130096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



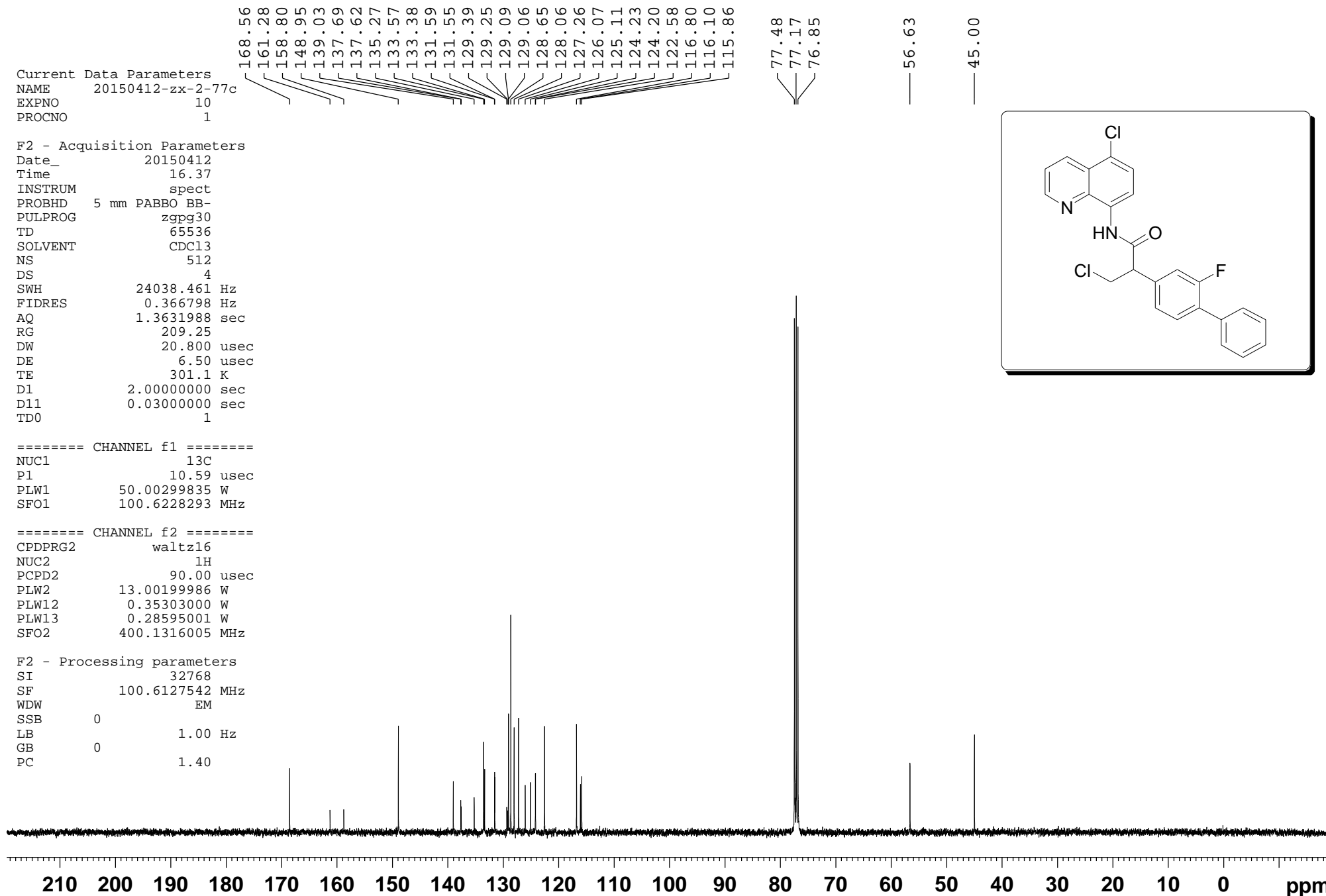
Current Data Parameters
 NAME 20150412-zx-2-77c
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150412
 Time_ 16.37
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 301.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

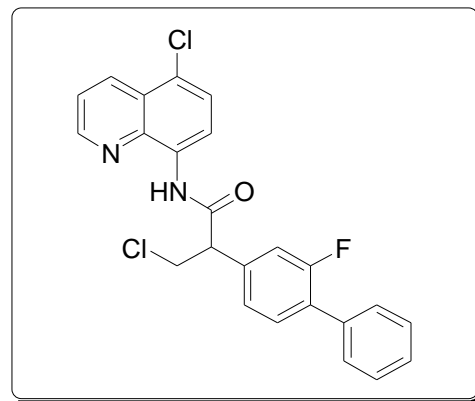
F2 - Processing parameters
 SI 32768
 SF 100.6127542 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



77.48
 77.17
 76.85

56.63

45.00



9.9538
 8.7978
 8.7938
 8.7872
 8.7832
 8.7232
 8.7021
 8.5616
 8.5576
 8.5403
 8.5363
 8.794
 8.787
 8.783
 8.723
 8.702
 8.8077
 8.7901
 8.7867
 8.7765
 8.7722
 8.7573
 8.7531
 8.6037
 8.5922
 8.5827
 8.5736
 8.5691
 8.5584
 8.5477
 8.5433
 8.5371
 8.5239
 8.4685
 8.4487
 8.4300
 8.2600

 4.3866
 4.3656
 4.3596
 4.3386
 4.1984
 4.1826
 4.1775
 4.1617
 3.9072
 3.8915
 3.8801
 3.8644

Current Data Parameters
 NAME YXL-9-299-CL-H-150416
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters

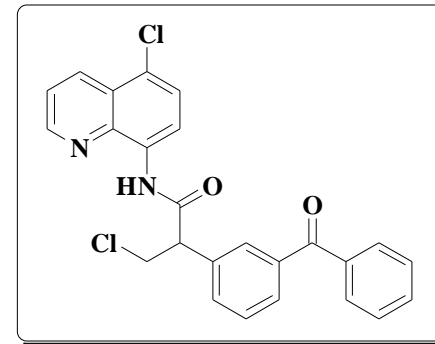
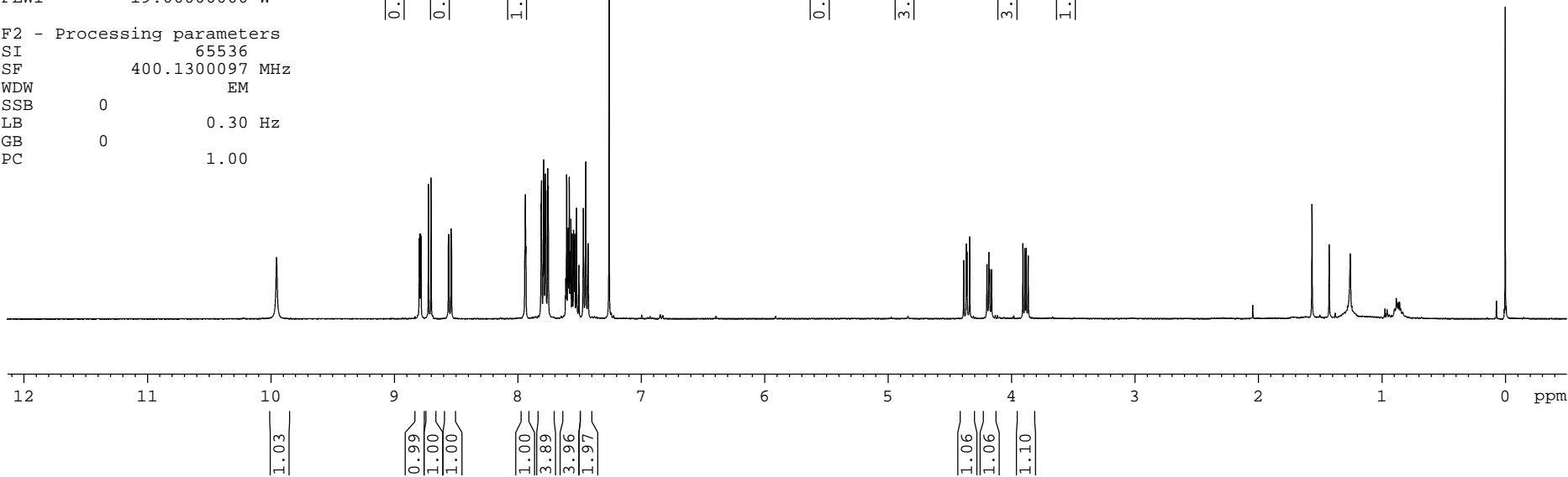
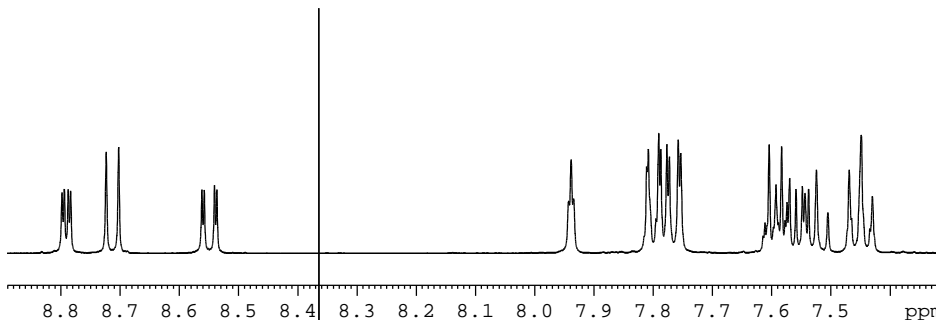
Date_ 20150416
 Time 20.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 128.61
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.798
 8.794
 8.787
 8.783
 8.723
 8.702
 8.562
 8.558
 8.540
 8.536

 7.942
 7.938
 7.934
 7.811
 7.808
 7.790
 7.787
 7.777
 7.772
 7.757
 7.753
 7.604
 7.592
 7.583
 7.574
 7.569
 7.558
 7.548
 7.543
 7.537



196.28
 168.67
 Current Data Parameters
 NAME YXL-9-299-CL-C-150416
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150417
 Time 8.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1300
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 202.1
 DW 20.800 usec
 DE 6.50 usec
 TE 297.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

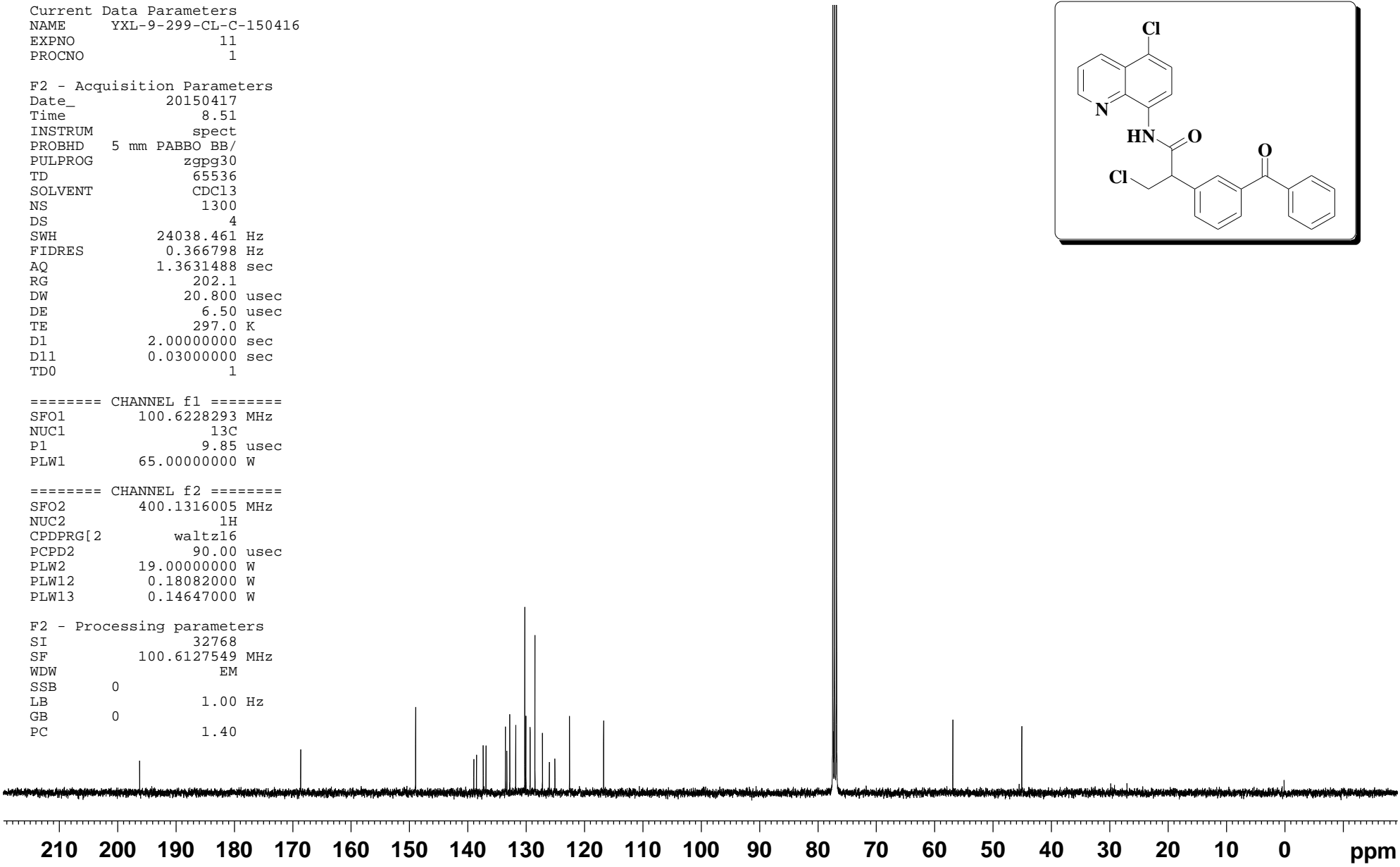
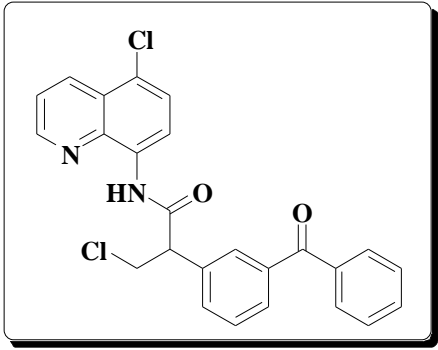
===== CHANNEL f1 =====
 SFO1 100.6228293 MHz
 NUC1 13C
 P1 9.85 usec
 PLW1 65.0000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 19.0000000 W
 PLW12 0.18082000 W
 PLW13 0.14647000 W

F2 - Processing parameters
 SI 32768
 SF 100.6127549 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

148.97
 139.01
 138.54
 137.39
 136.91
 133.58
 133.34
 132.84
 131.82
 130.26
 130.07
 129.36
 128.52
 127.24
 126.05
 125.11
 122.61
 116.75

77.48
 77.16
 76.84
 56.91
 45.09



Current Data Parameters
 NAME YXL-9-219-C-H-20150324
 EXPNO 10
 PROCNO 1

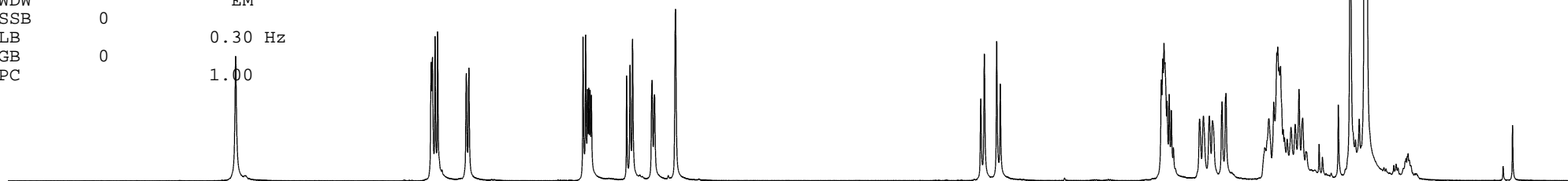
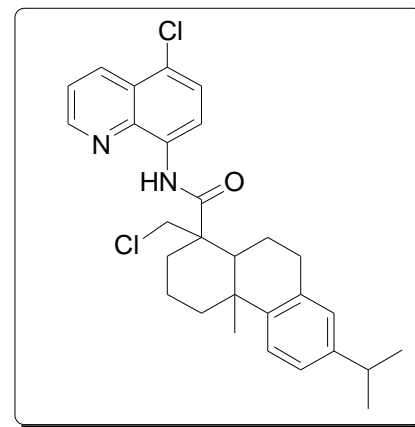
F2 - Acquisition Parameters
 Date_ 20150324
 Time 10.58
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 70.24
 DW 60.800 usec
 DE 6.50 usec
 TE 298.5 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300100 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.8582
8.8479
8.8268
8.8057
8.5710
8.5498
7.6162
7.5952
7.5797
7.5692
7.5585
7.5480
7.2597
7.2313
7.2107
7.0513
7.0312
6.8596

4.3616
4.3325
4.2314
4.2023
2.8843
2.8727
2.8626
2.8549
2.8374
2.8198
2.8026
2.5716
2.5397
2.4918
2.4656
2.3871
2.3554
2.0040
1.9645
1.9394
1.9320
1.9208
1.9091
1.8871
1.8766
1.8236
1.7891
1.7579
1.7280
1.4363
1.3389
1.2670
1.2240
1.2068



12.0 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 ppm

1.01 2.04 1.03 2.06 1.06 1.01 1.00 0.97 1.09 3.07 2.01 1.10 6.56 3.20 6.37

172.80

148.94
146.50
146.30
139.51
134.47
133.94
133.48
127.34
127.04
126.04
124.49
124.31
124.26
122.44
116.73

77.48
77.16
76.84

54.16
47.70
44.62
38.31
37.87
33.59
32.24
30.24
26.29
24.09
24.06
20.51
18.72

Current Data Parameters
NAME YXL-9-219-C-C-20150324
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150324
Time 14.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 460
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====

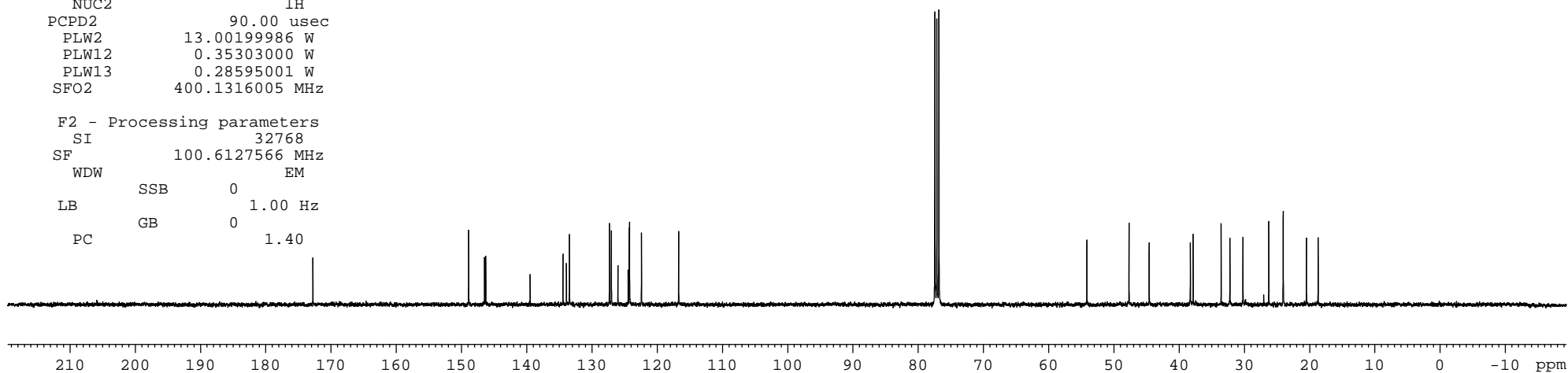
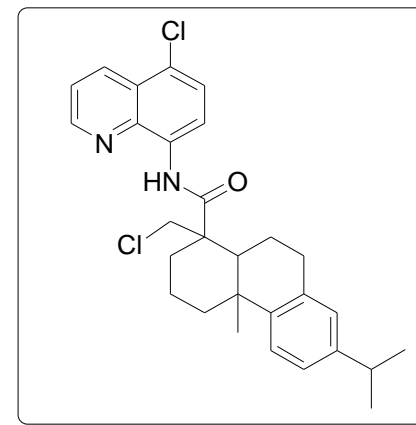
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6127566 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME YXL-9-255-H-20150401
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150401
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 165.63
DW 60.800 usec
DE 6.50 usec
TE 300.6 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

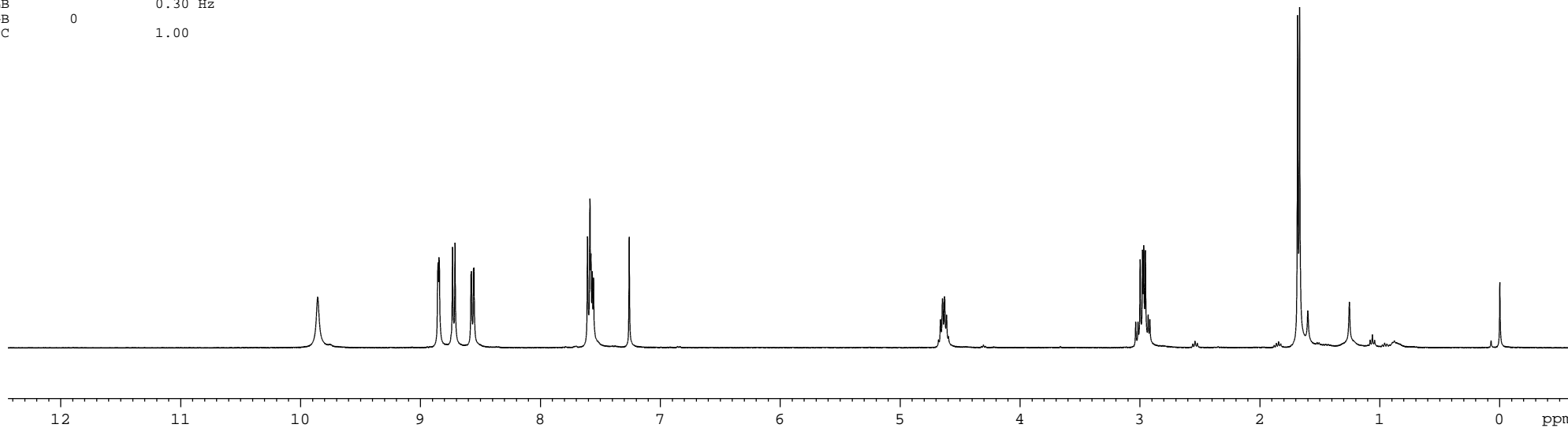
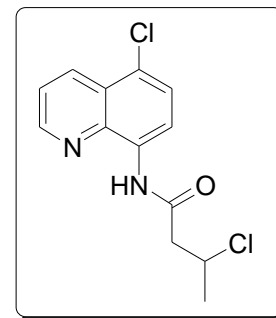
9.8548

8.8527
8.8455
8.8426
8.7323
8.7114
8.5781
8.5750
8.5568
8.5538
7.6066
7.5861
7.5779
7.5670
7.5564
7.2588

4.6791
4.6628
4.6462
4.6289
4.6124
4.5961

3.0351
3.0153
2.9978
2.9780
2.9681
2.9540
2.9307
2.9166

1.6847
1.6683



1.04

0.99

1.03

1.00

2.14

0.99

2.06

2.94

— 167.98
 — 148.88
 — 139.03
 133.58
 133.55
 127.32
 126.08
 124.81
 122.54
 — 116.75
 77.48
 77.16
 76.84
 — 53.73
 — 48.83
 — 25.34

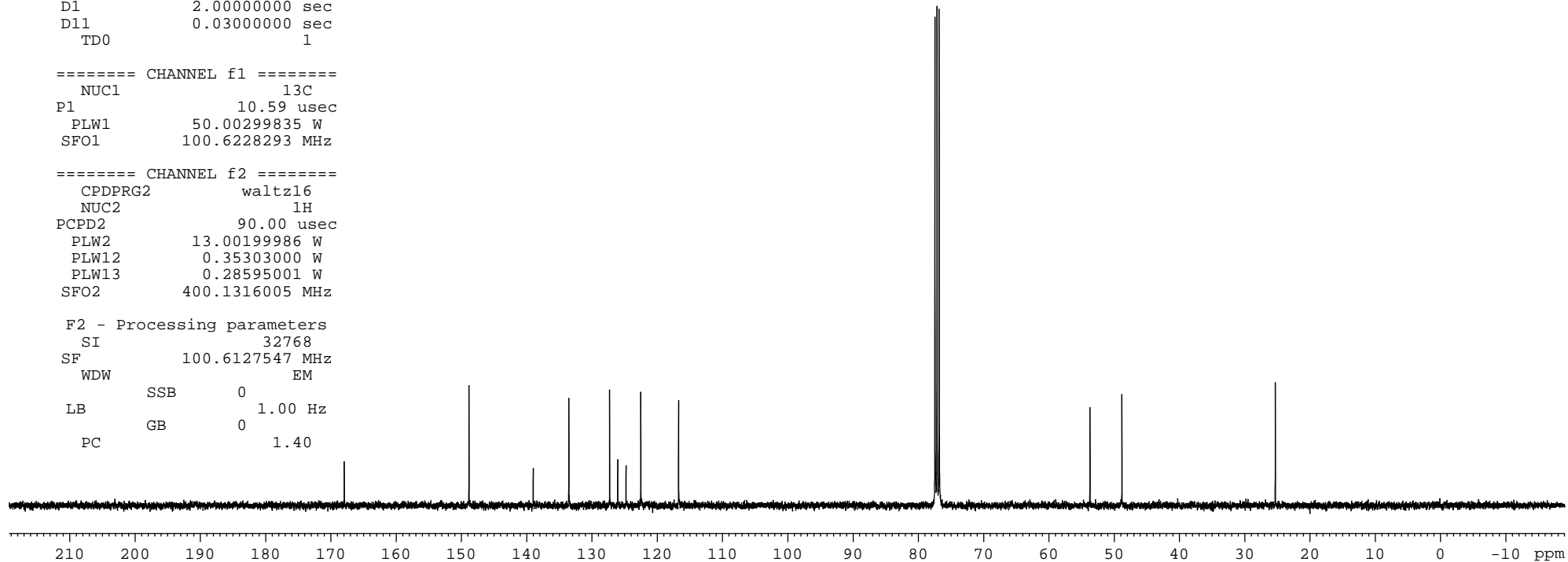
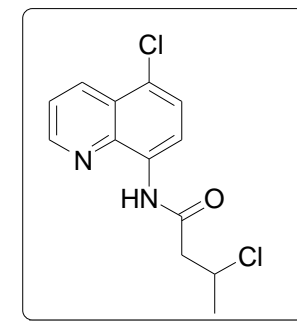
Current Data Parameters
 NAME YXL-9-255-C-20150401
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150402
 Time 8.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 450
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127547 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters

NAME 20150407-zx-2-76-2-p-h
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

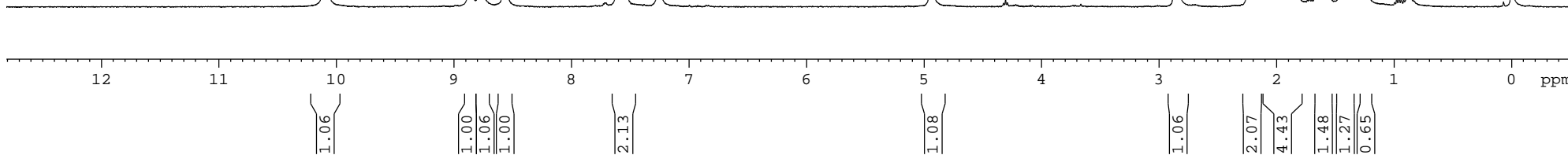
Date_ 20150407
Time 9.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 209.25
DW 60.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 =====

NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters

SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



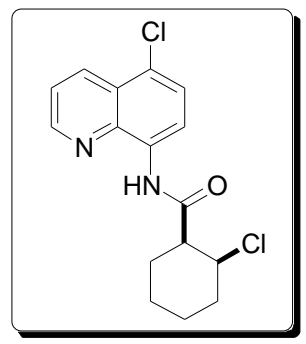
10.0938

8.8706
8.8613
8.7799
8.7590
8.5780
8.5570

7.6110
7.5897
7.5791
7.5681
7.5576
7.2598

4.9372

2.8669
2.8375
2.2231
2.2133
2.1936
2.1843
2.1624
2.1538
2.0804
2.0495
2.0150
1.9821
1.9590
1.9512
1.9196
1.8857
1.8510
1.6387
1.6098
1.5711
1.4628
1.4318
1.4011
1.3793
1.2533
-0.0013



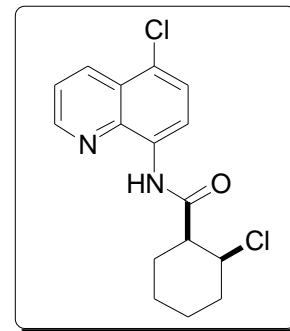
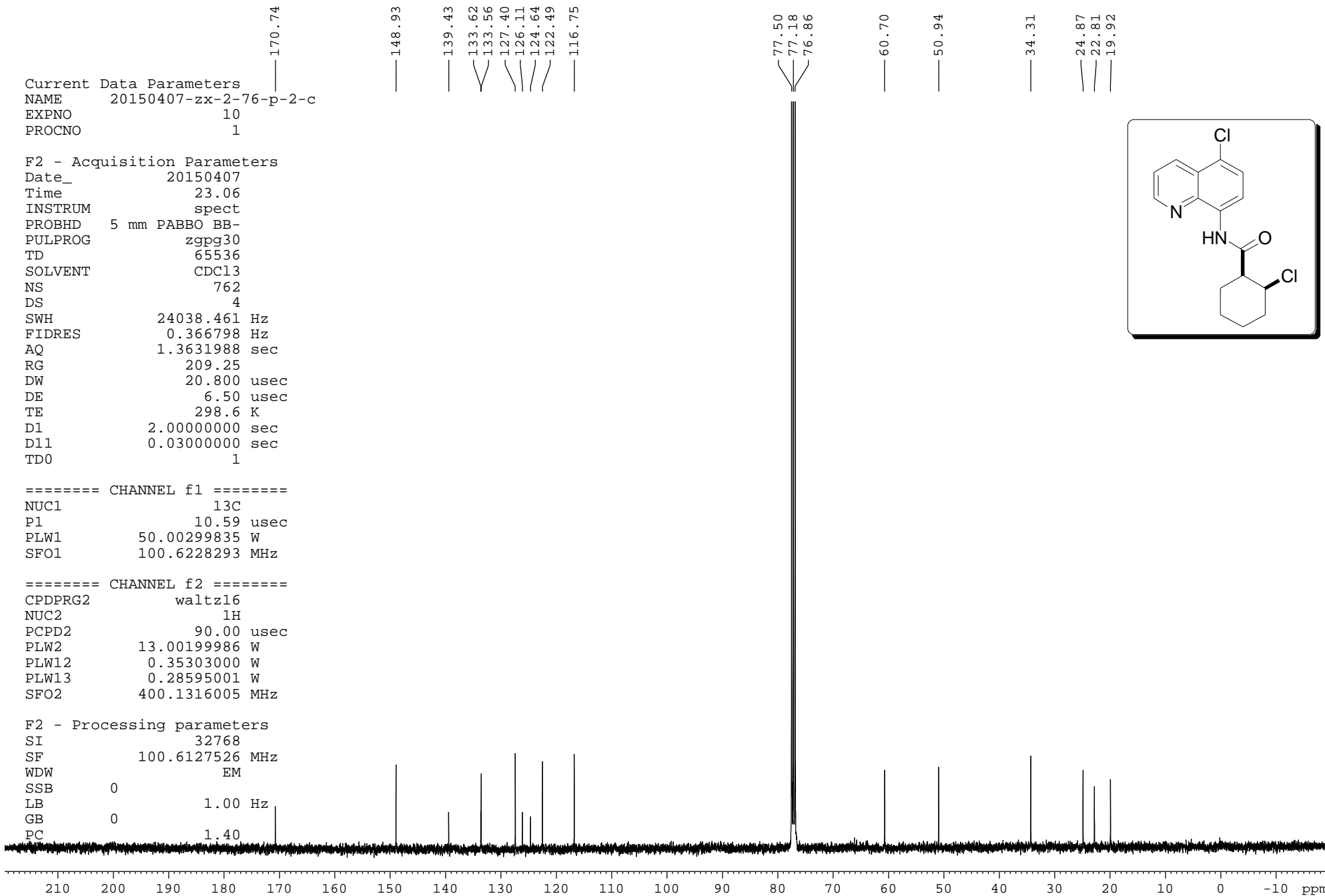
Current Data Parameters
 NAME 20150407-zx-2-76-p-2-c
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150407
 Time 23.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 762
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 298.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127526 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME zx-2-76-pl-h-20150405-
 EXPNO 11
 PROCNO 1

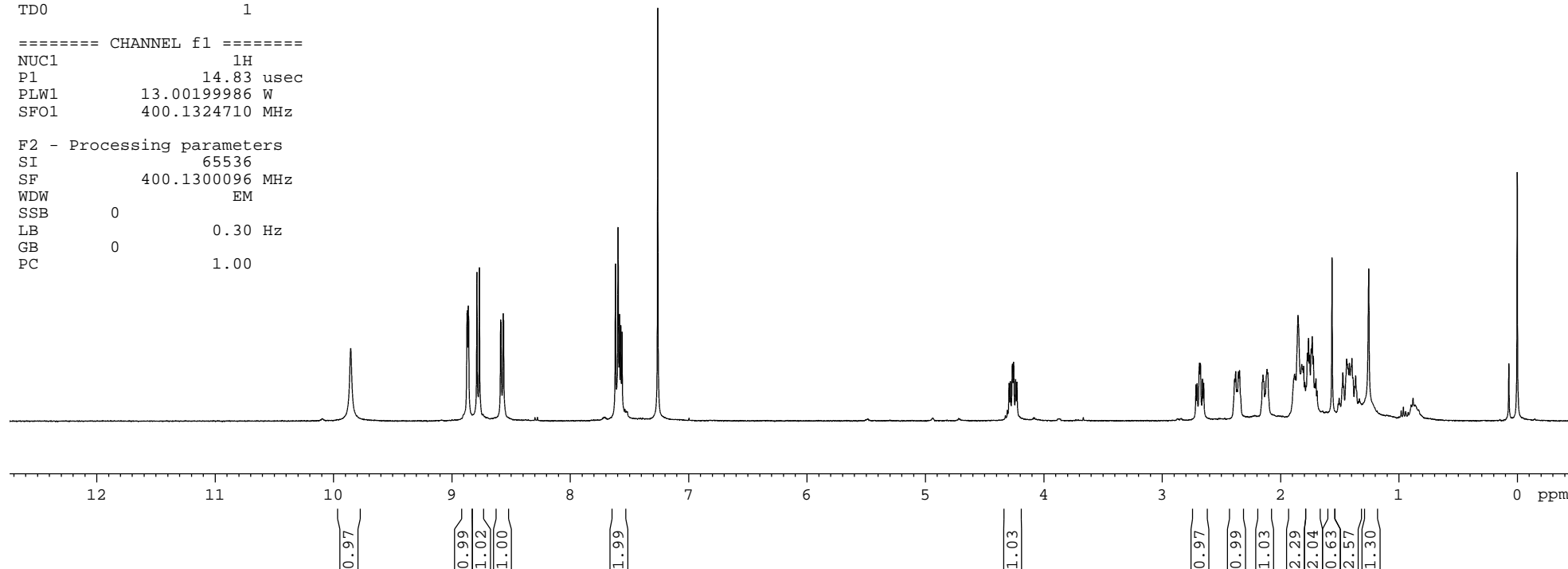
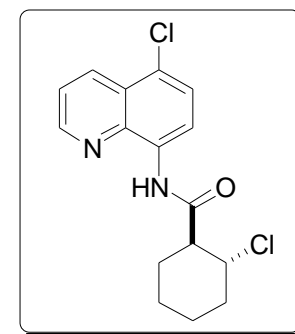
F2 - Acquisition Parameters
 Date_ 20150405
 Time 20.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 209.25
 DW 60.800 usec
 DE 6.50 usec
 TE 299.1 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.8544
 8.8715
 8.8682
 8.8612
 8.8580
 8.7880
 8.7670
 8.5871
 8.5838
 8.5659
 8.5626
 7.6175
 7.5960
 7.5831
 7.5723
 7.5618
 7.2601

4.2923
 4.2815
 4.2639
 4.2548
 4.2370
 4.2262
 2.7136
 2.7039
 2.6840
 2.6768
 2.6578
 2.6485
 2.3782
 2.3666
 2.3543
 2.3458
 2.1470
 2.1136
 2.1066
 1.8808
 1.8724
 1.8515
 1.8200
 1.8040
 1.7939
 1.7835
 1.7731
 1.7632
 1.7533
 1.7401
 1.7318
 1.7225
 1.7089
 1.7002
 1.6905
 1.5643
 1.5044
 1.4728
 1.4650
 1.4404



— 171.91
 — 148.79
 — 139.12
 133.69
 133.56
 127.36
 126.07
 124.63
 122.47
 — 116.80

Current Data Parameters
 NAME 20150405-zx-2-76-p2-h
 EXPNO 10
 PROCNO 1

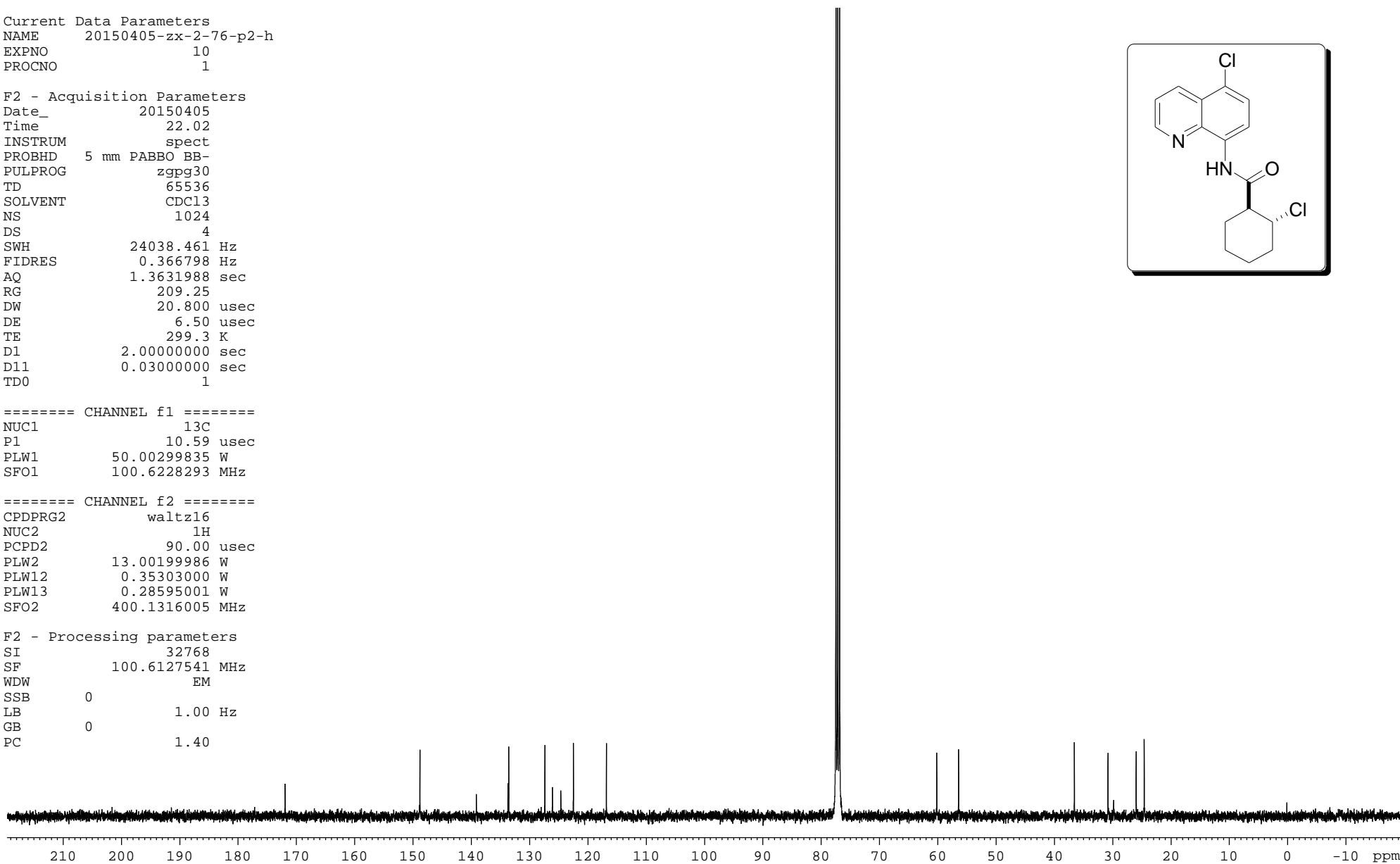
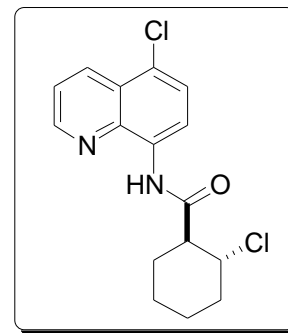
F2 - Acquisition Parameters
 Date_ 20150405
 Time 22.02
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 299.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

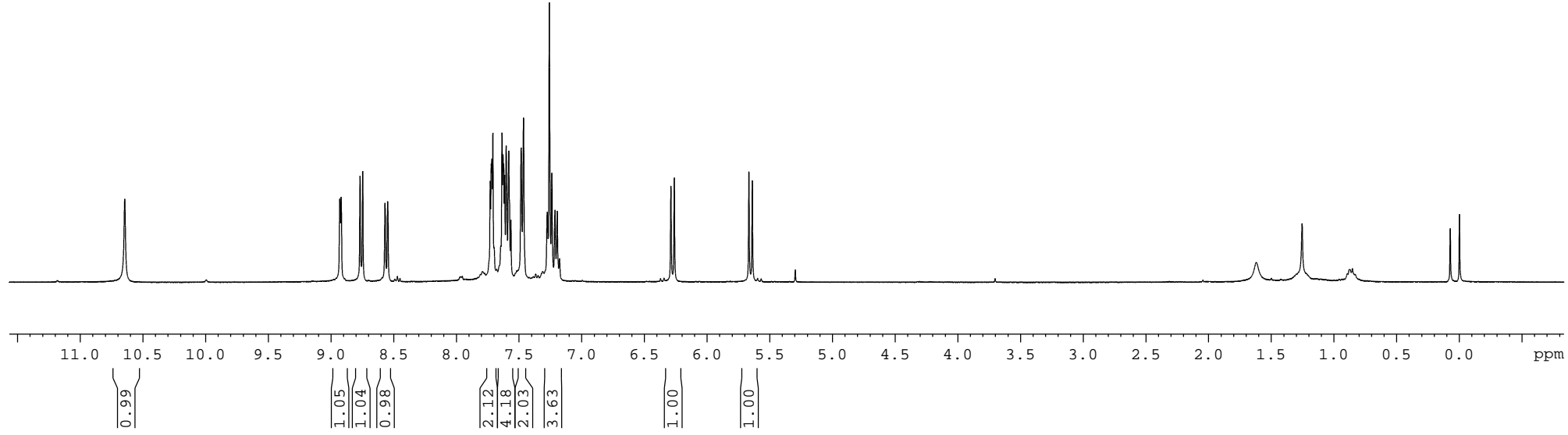
===== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127541 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

77.45
 77.13
 76.82
 — 60.16
 — 56.41
 — 36.56
 — 30.79
 25.96
 24.58

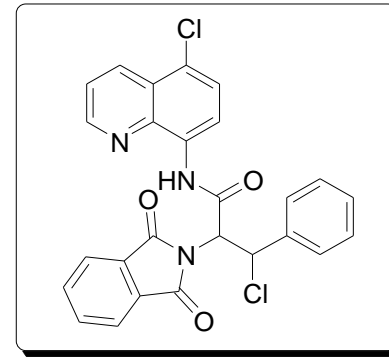


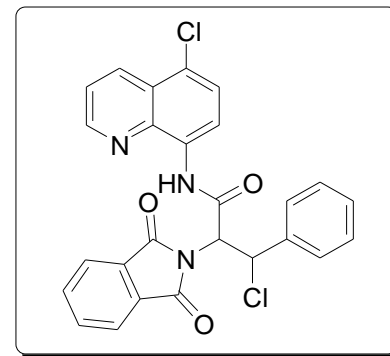
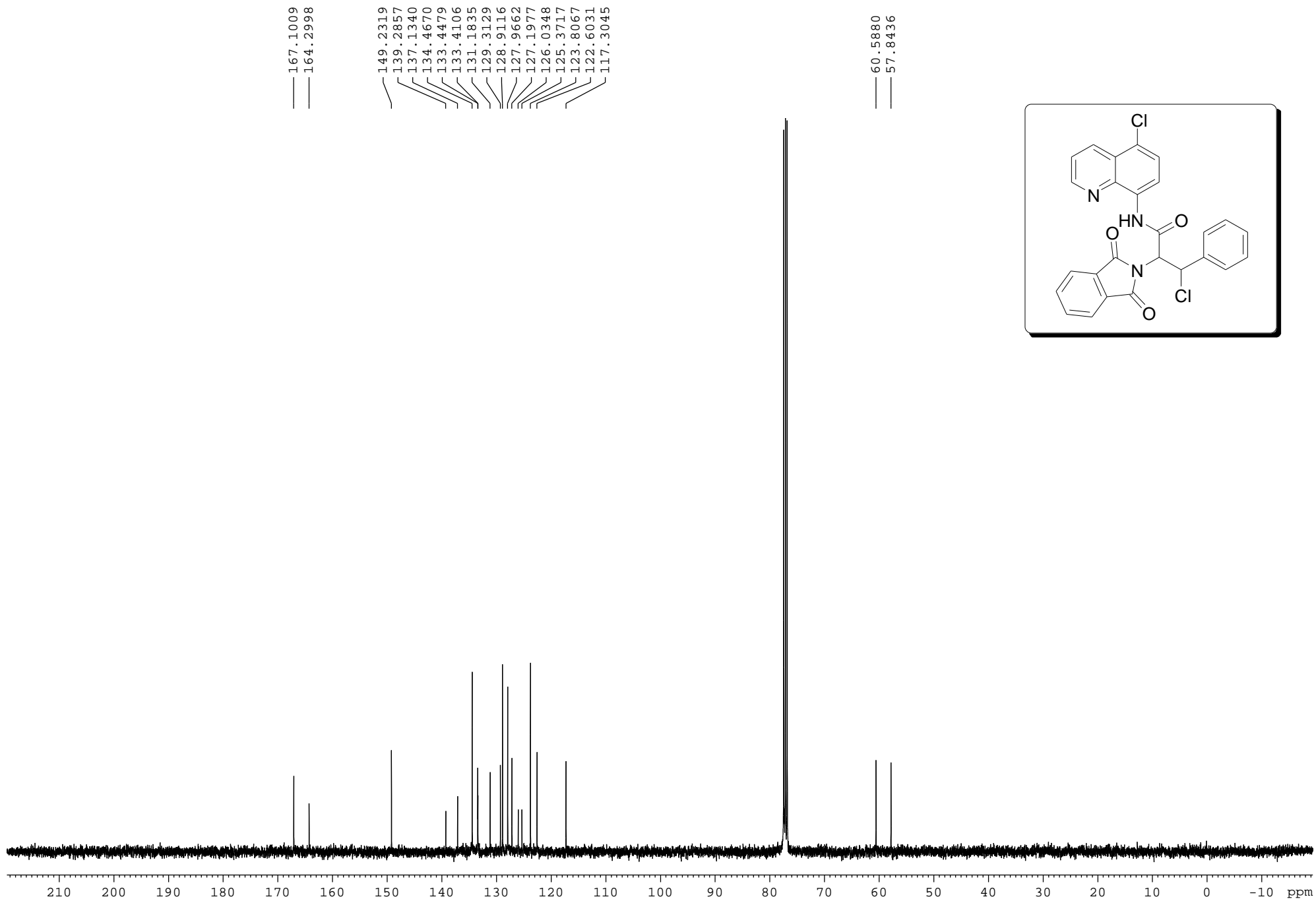


— 10.6453

8.9316
8.9214
8.7698
8.7488
8.5709
8.5497
7.7314
7.7234
7.7180
7.7103
7.6372
7.6296
7.6238
7.6160
7.6041
7.5833
7.5667
7.4843
7.4658
7.2763
7.2601
7.2398
7.2146
7.1969
6.2900
6.2630

5.6676
5.6406





Current Data Parameters
 NAME YXL-10-81-H-20150916
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150916
 Time 20.51
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 209.25
 DW 60.800 usec
 DE 6.50 usec
 TE 297.1 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.80 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

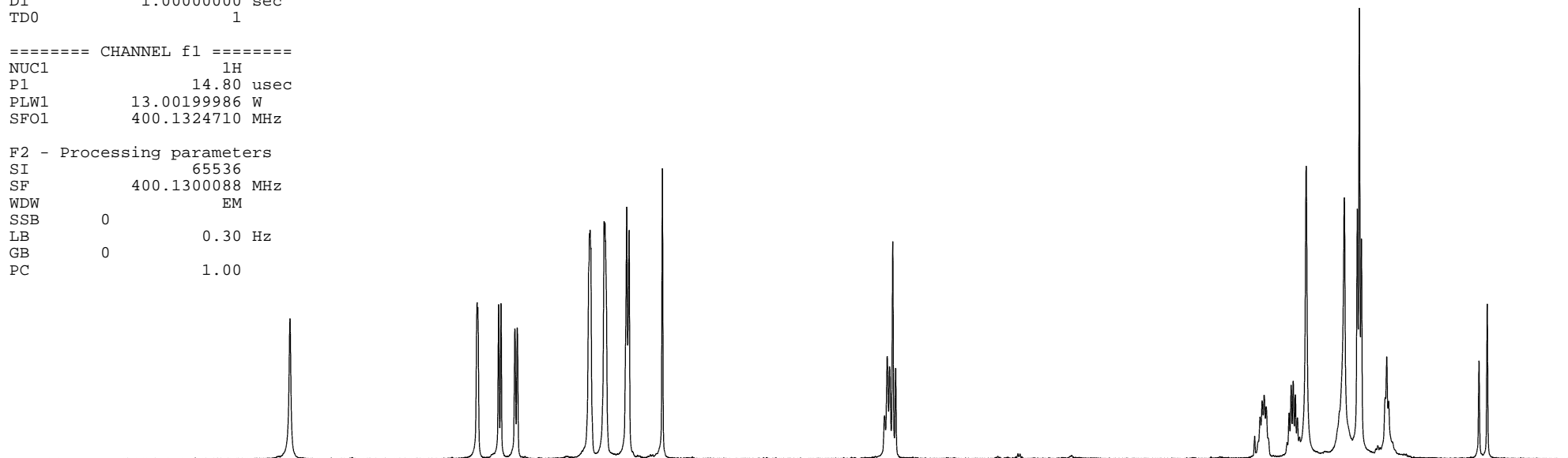
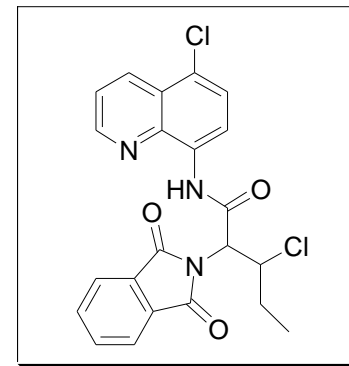
F2 - Processing parameters
 SI 65536
 SF 400.1300088 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10.541

8.892
8.886
8.703
8.681
8.560
8.539
7.903
7.897
7.890
7.774
7.766
7.761
7.574
7.553
7.260

5.304
5.280
5.259
5.231
5.205

2.044
1.996
1.978
1.960
1.942
1.759
1.741
1.722
1.704
1.685
1.667
1.139
1.121
1.103



1.02

1.02
1.02
1.00

2.09
2.12
2.09

2.10

1.18
1.27

3.25

ppm

Current Data Parameters
NAME YXL-10-81-C-20150916
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150917
Time_ 2.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 450
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

=====
CHANNEL f1
NUC1 13C
P1 10.90 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.38069001 W
PLW13 0.30836001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127567 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

167.68
164.79

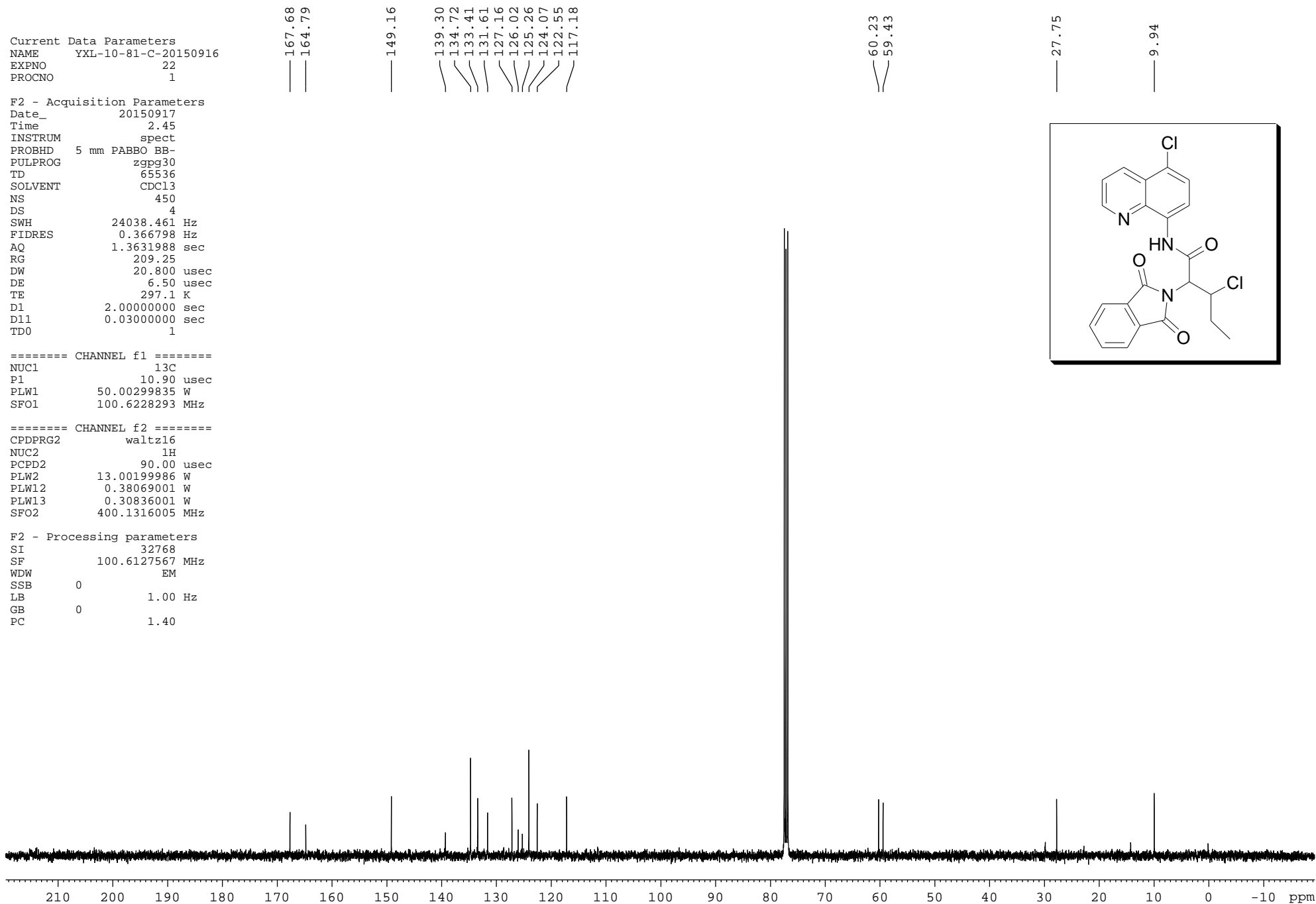
149.16

139.30
134.72
133.41
131.61
127.16
126.02
125.26
124.07
122.55
117.18

60.23
59.43

27.75

9.94



Current Data Parameters
NAME YXL-8-299-I-H-20141229
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141229
Time 22.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 209.25
DW 60.800 usec
DE 6.50 usec
TE 297.7 K
D1 1.00000000 sec
TD0 1

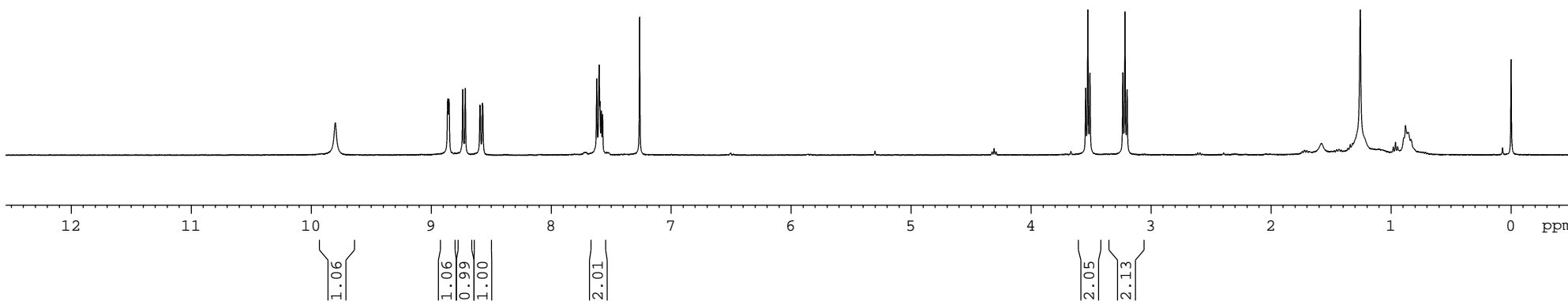
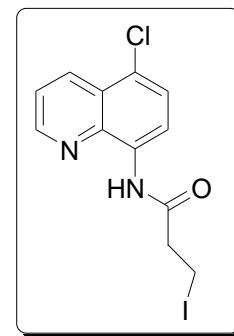
==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9.7968

8.8581
8.8508
8.7346
8.7136
8.5916
8.5887
8.5704
8.5675
7.6182
7.5975
7.5906
7.5797
7.5691
7.2602

3.5424
3.5247
3.5072
3.2327
3.2152
3.1975

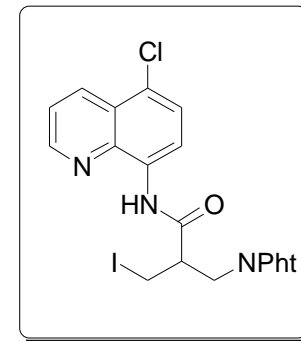
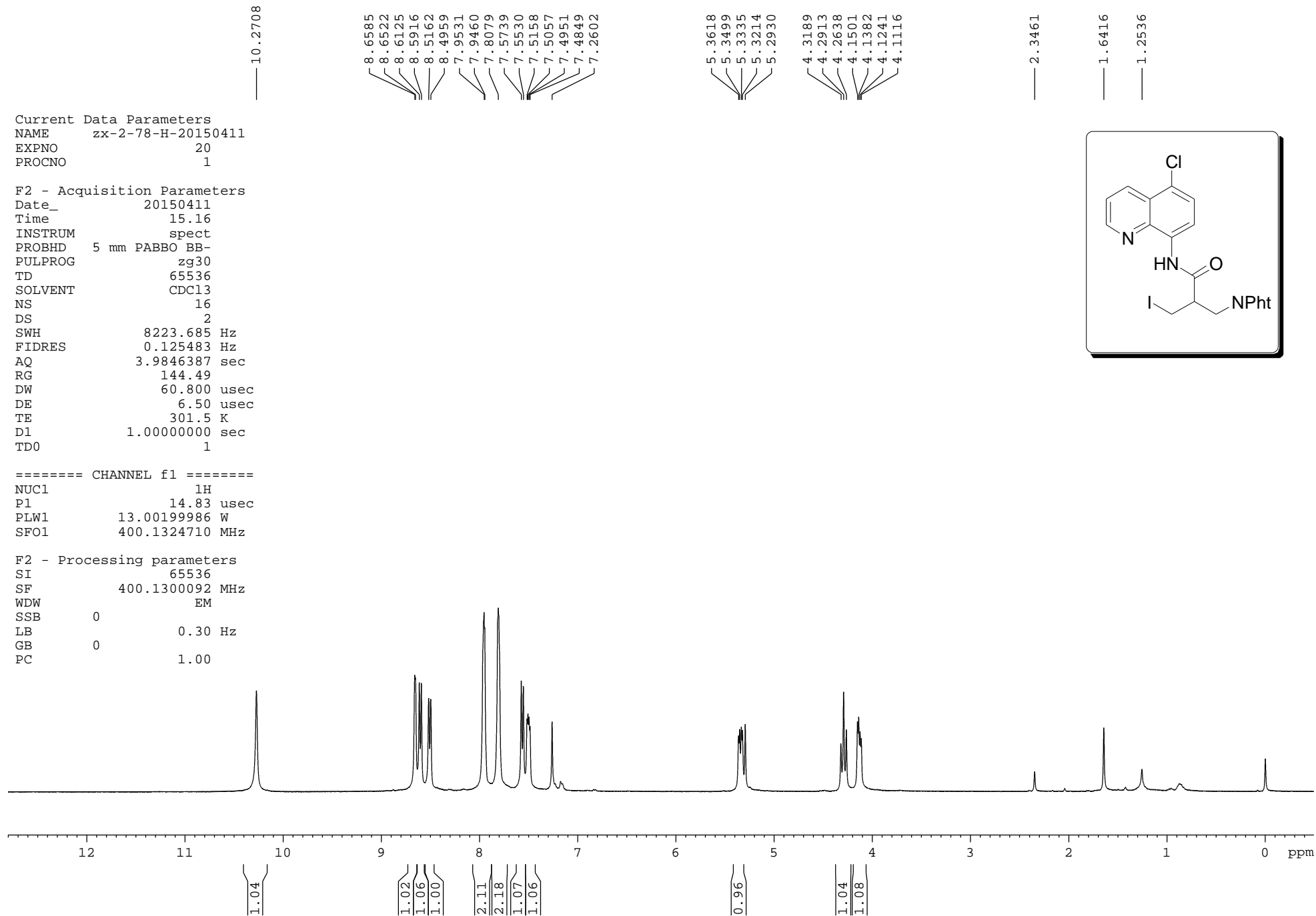


Current Data Parameters
NAME zx-2-78-H-20150411
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150411
Time 15.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144.49
DW 60.800 usec
DE 6.50 usec
TE 301.5 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 20150412-zx-2-78c
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 15.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 302.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

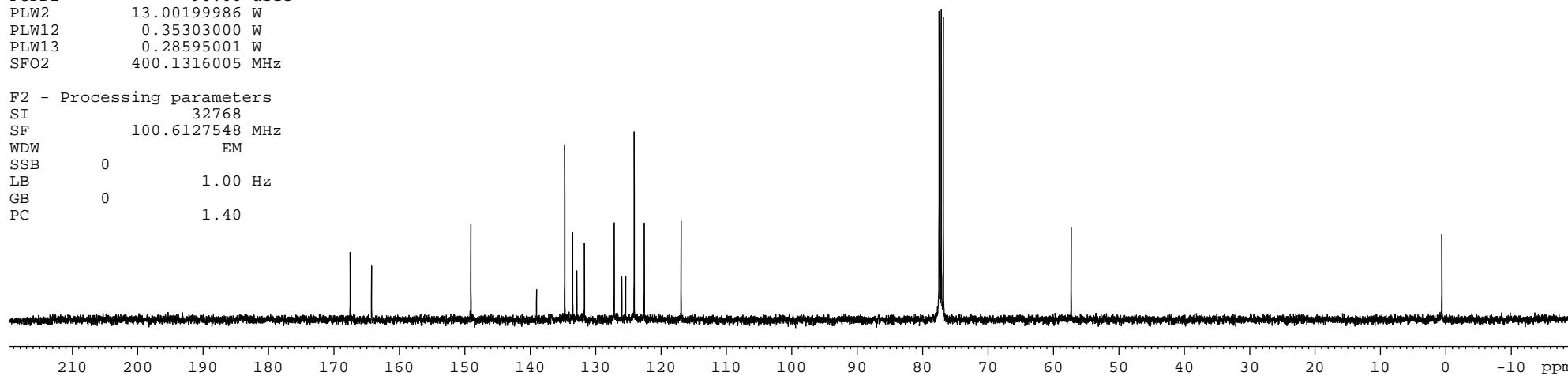
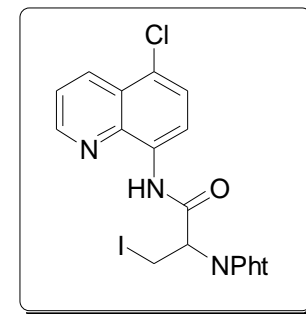
F2 - Processing parameters
SI 32768
SF 100.6127548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

167.53
164.26
149.08
139.05
134.73
133.52
132.89
131.72
127.17
126.01
125.42
124.11
122.57
116.94

77.49
77.17
76.85

57.30

0.62

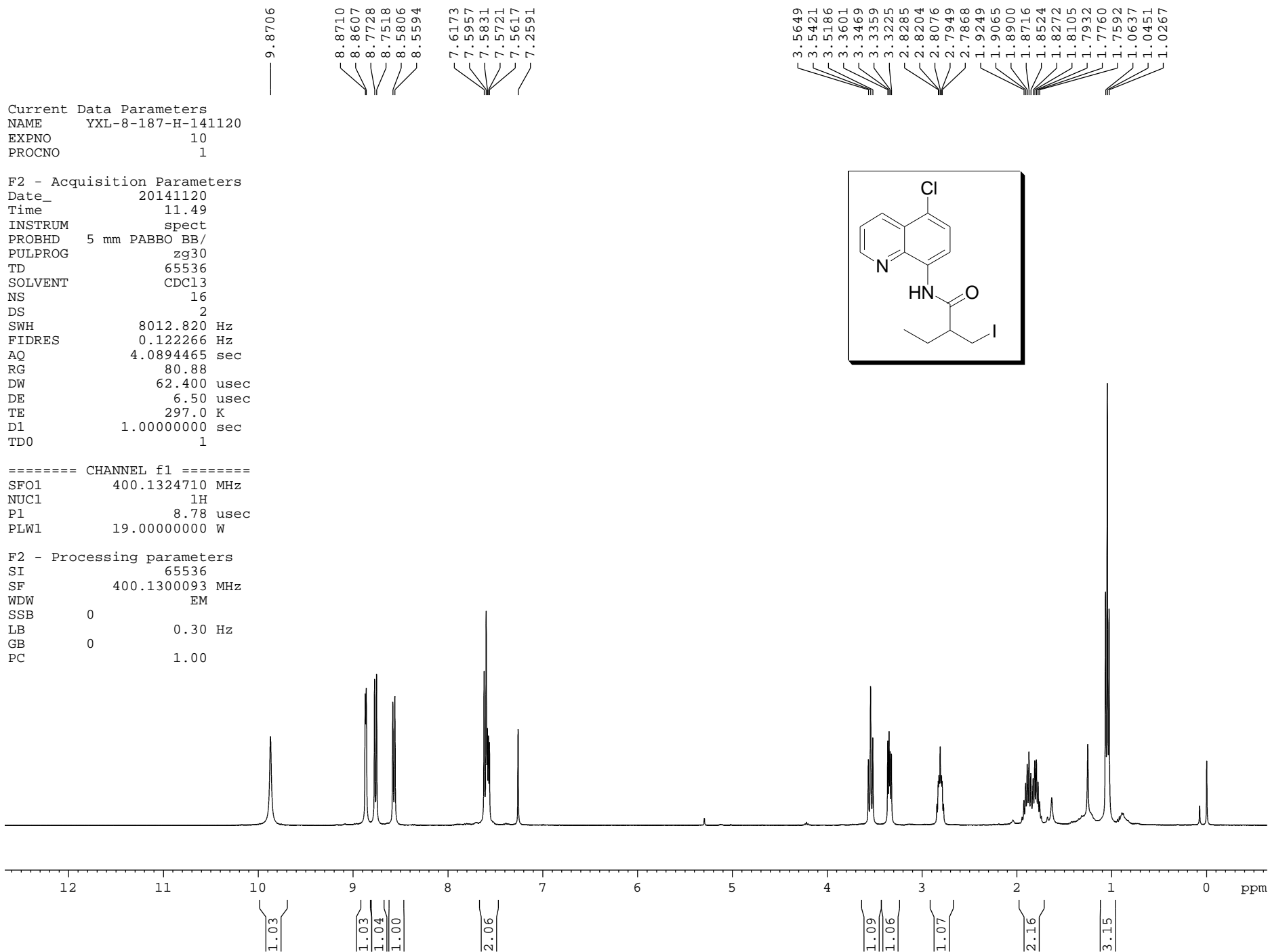


Current Data Parameters
 NAME YXL-8-187-H-141120
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141120
 Time 11.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 80.88
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300093 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME YXL-8-187-C-141120
EXPNO 10
PROCNO 1

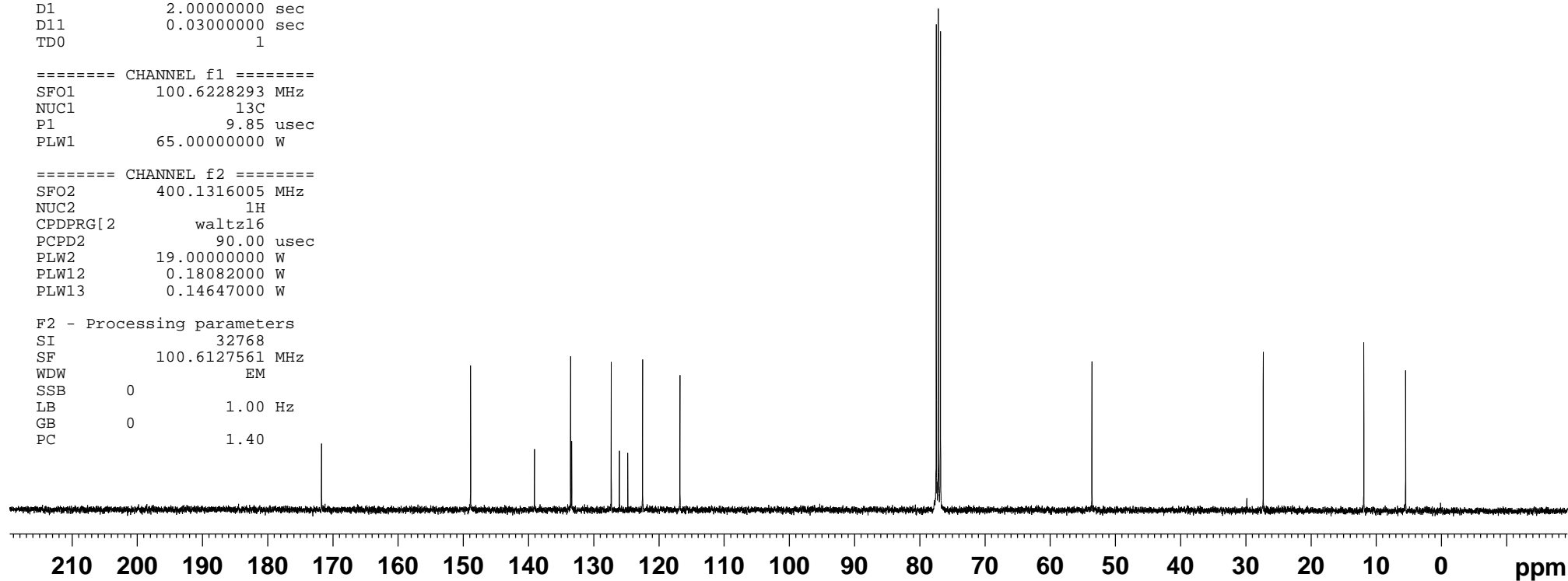
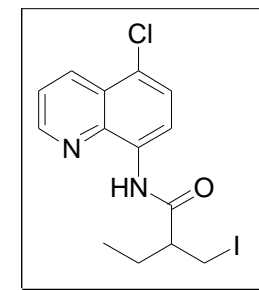
F2 - Acquisition Parameters
Date_ 20141121
Time 1.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 480
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127561 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

171.77
148.91
139.12
133.57
133.41
127.33
126.08
124.81
122.53
116.80
77.48
77.16
76.85
53.61
27.33
11.91
5.50

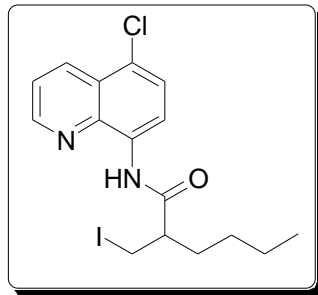
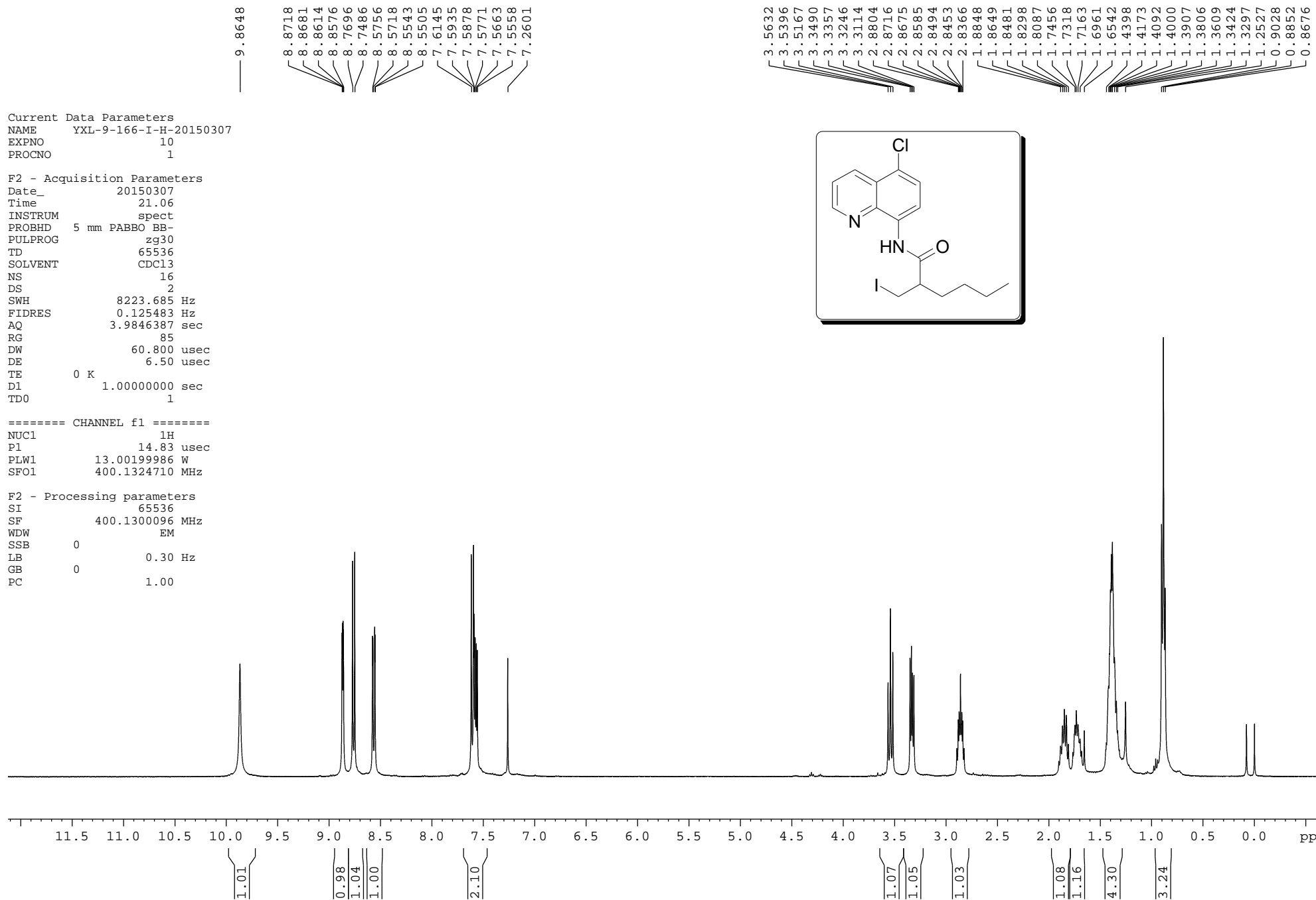


Current Data Parameters
 NAME YXL-9-166-I-H-20150307
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150307
 Time 21.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 85
 DW 60.800 usec
 DE 6.50 usec
 TE 0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME YXL-9-166-I-C-20150307
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150308
Time 10.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SF01 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127566 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

— 171.89

— 148.90

— 139.14

— 133.53

— 133.43

— 127.32

— 126.08

— 124.79

— 122.50

— 116.81

— 77.47

— 77.16

— 76.84

— 52.19

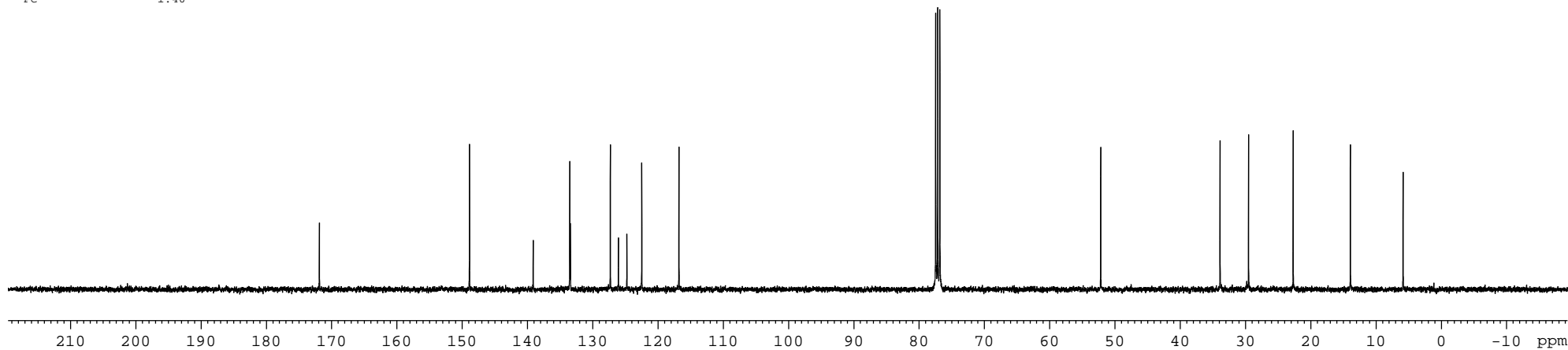
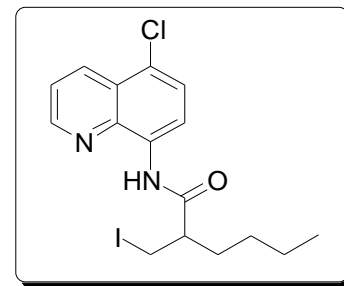
— 33.91

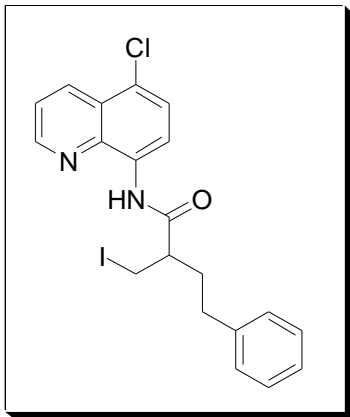
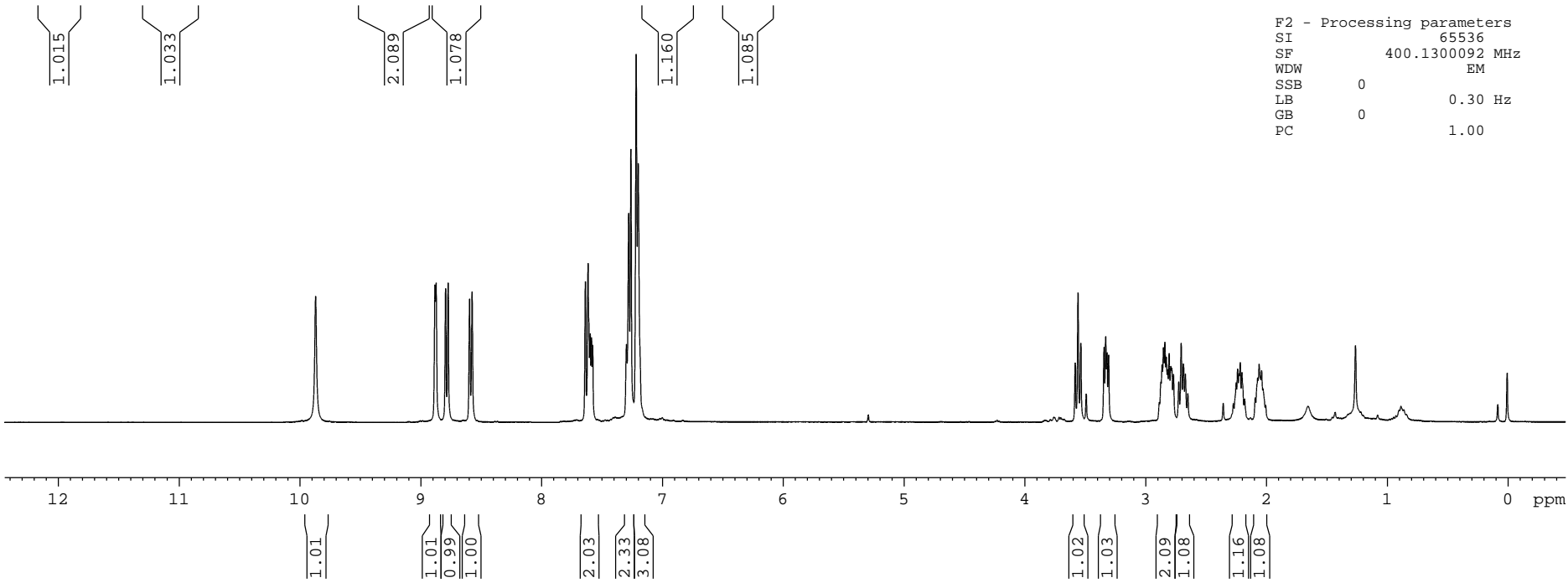
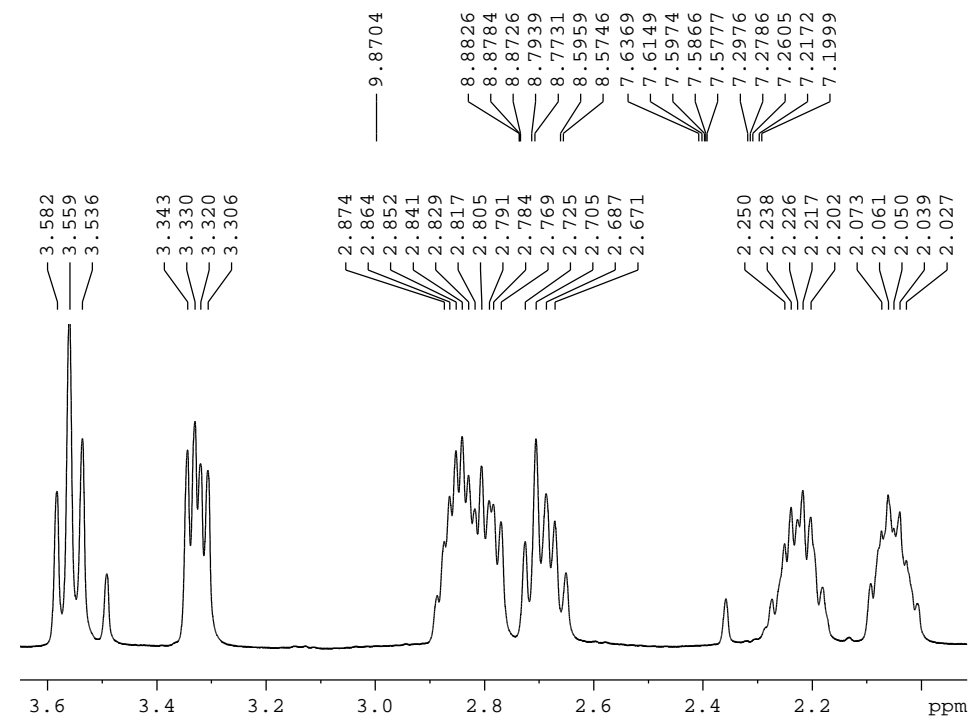
— 29.54

— 22.71

— 13.94

— 5.87





Current Data Parameters
 NAME YXL-8-139-3-H-141030
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141030
 Time 20.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 57.28
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Current Data Parameters
NAME YXL-8-139-3-C-141030
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

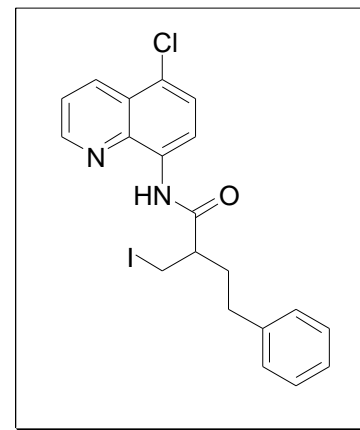
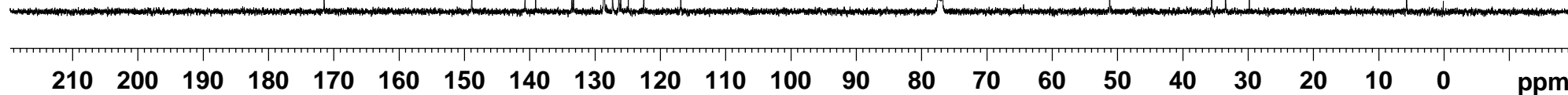
Date_ 20141031
Time 1.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 480
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters

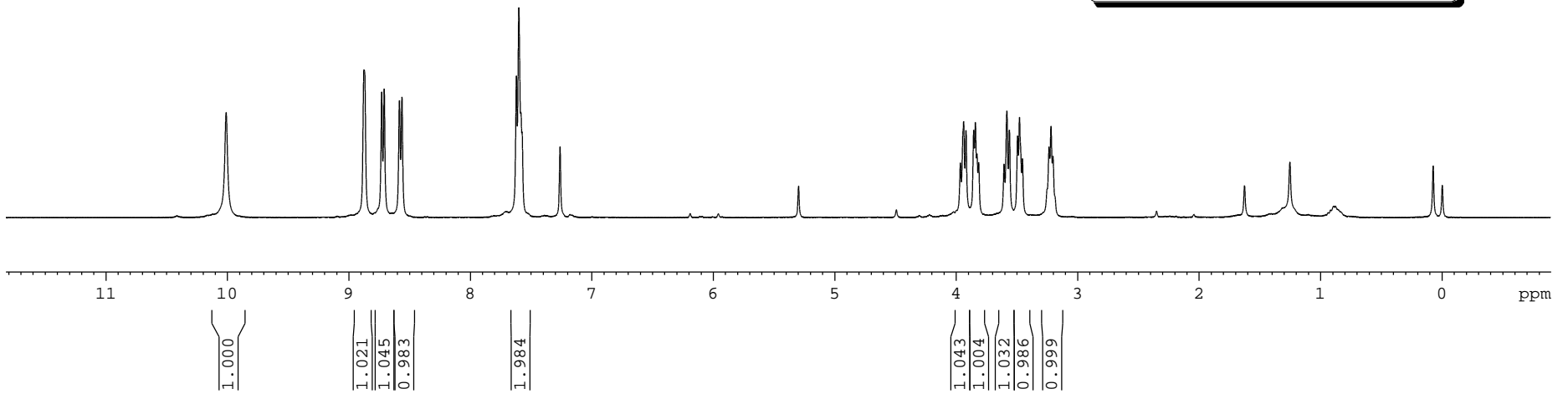
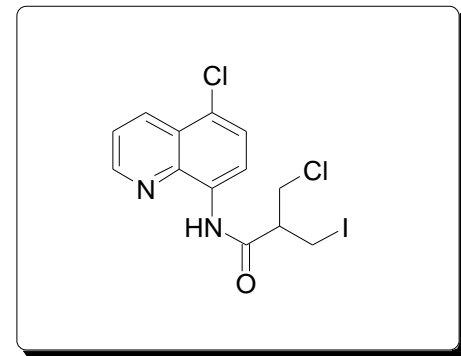
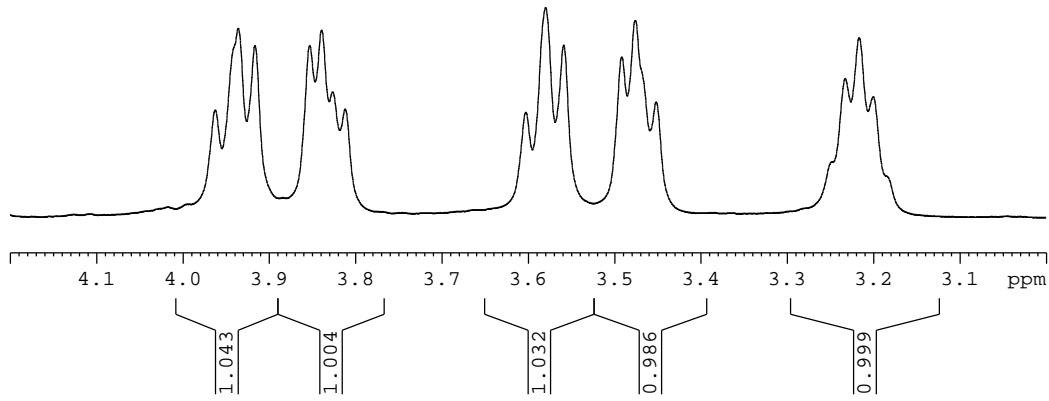
SI 32768
SF 100.6127586 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



10.007
 3.962
 3.936
 3.916
 3.853
 3.839
 3.826
 3.812
 8.873
 8.727
 8.706
 8.581
 8.560
 7.618
 7.598
 7.581
 7.571
 7.258
 3.602
 3.579
 3.559
 3.491
 3.476
 3.451
 3.232
 3.216
 3.200
 3.962
 3.936
 3.916
 3.853
 3.839
 3.826
 3.812
 3.602
 3.579
 3.559
 3.491
 3.476
 3.451
 3.232
 3.216
 3.200

Current Data Parameters
 NAME syh-6-241
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141212
 Time 10.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3



— 168.48
— 149.04
— 139.06
— 133.61
— 133.06
— 127.25
— 126.08
— 125.32
— 122.65
— 117.00

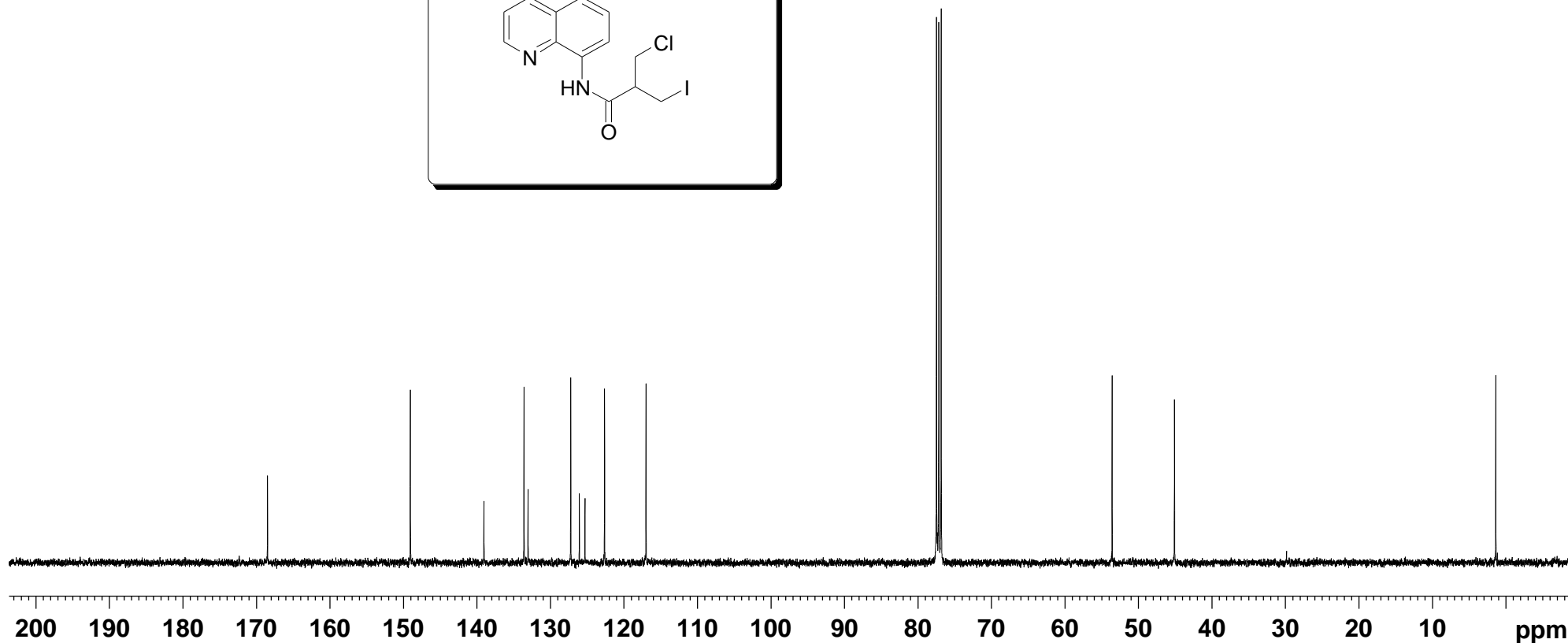
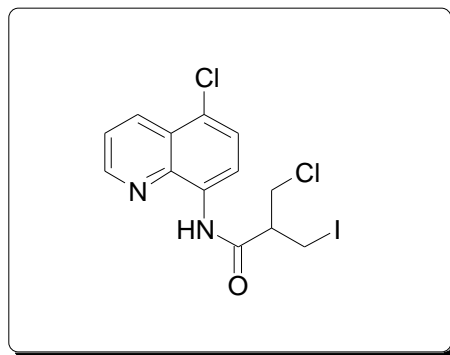
77.48
77.16
76.84

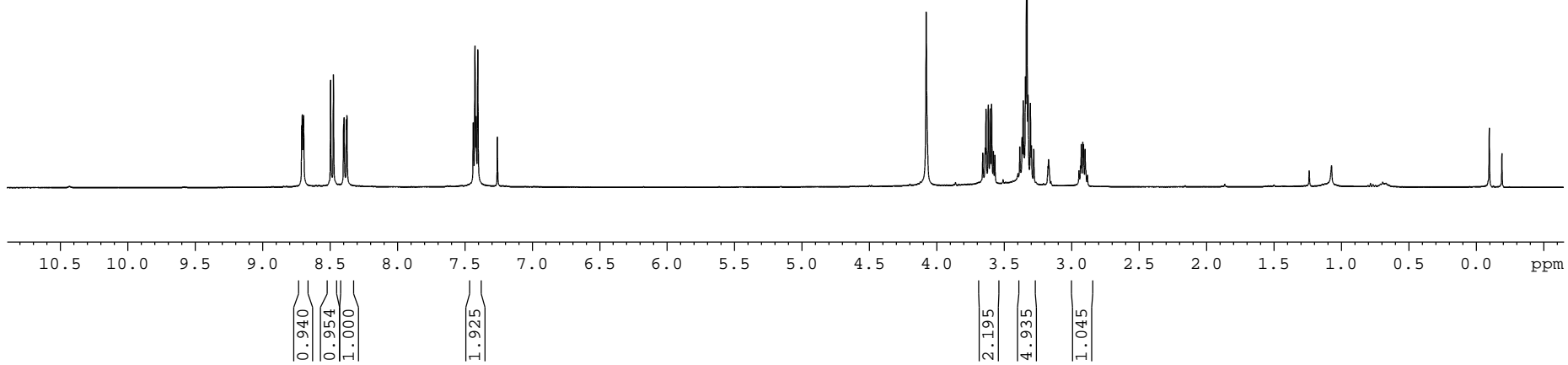
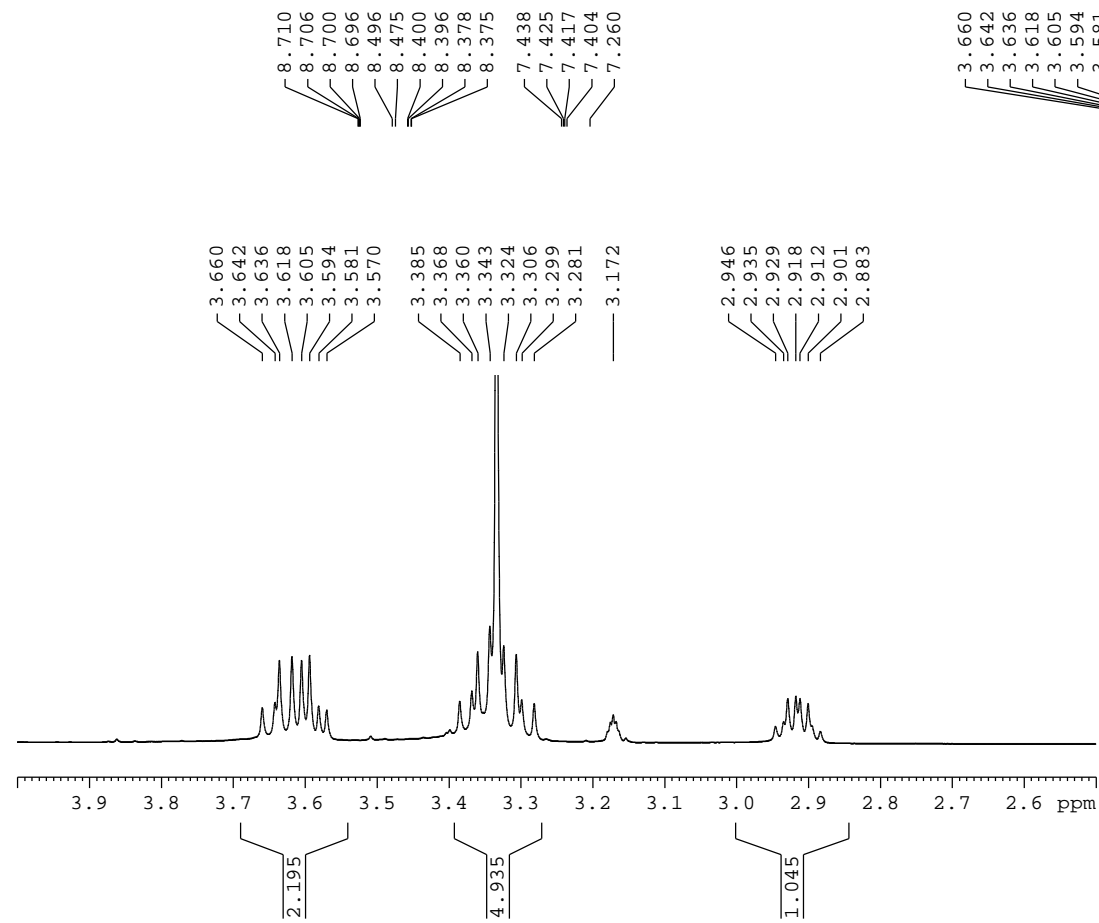
— 53.58
— 45.10

— 1.37

Current Data Parameters
NAME syh-6-241-c
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141212
Time 13.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13

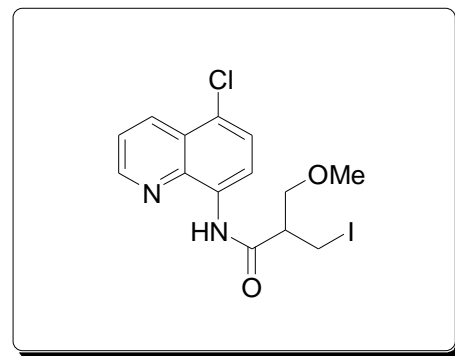


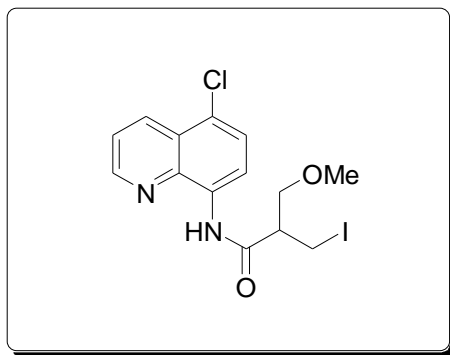


3.660
3.642
3.636
3.618
3.605
3.594
3.581
3.570
3.385
3.368
3.360
3.343
3.324
3.306
3.299
3.281
3.172
2.946
2.935
2.929
2.918
2.912
2.901
2.883

Current Data Parameters
 NAME syh-6-285-2
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141226
 Time 15.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT MeOD





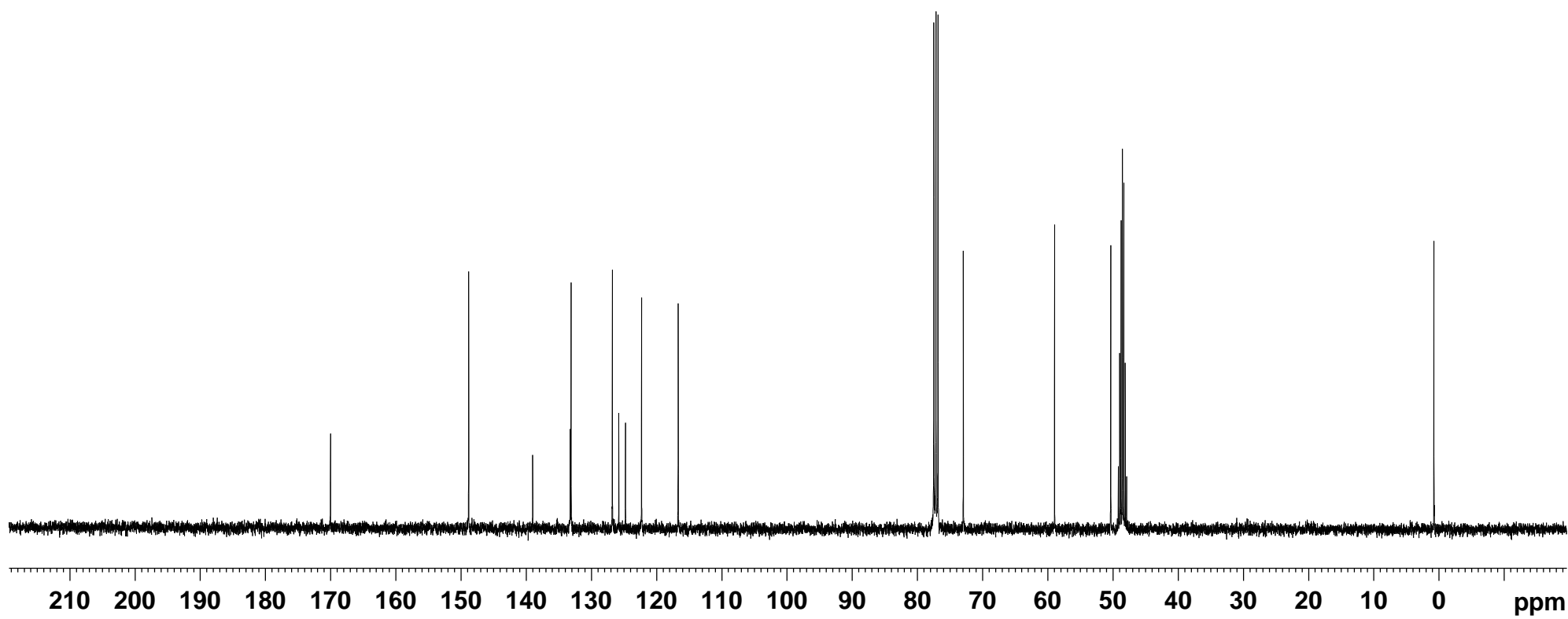
— 170.03
 — 148.83
 — 139.02
 — 133.26
 — 133.13
 — 126.80
 — 125.81
 — 124.77
 — 122.31
 — 116.70

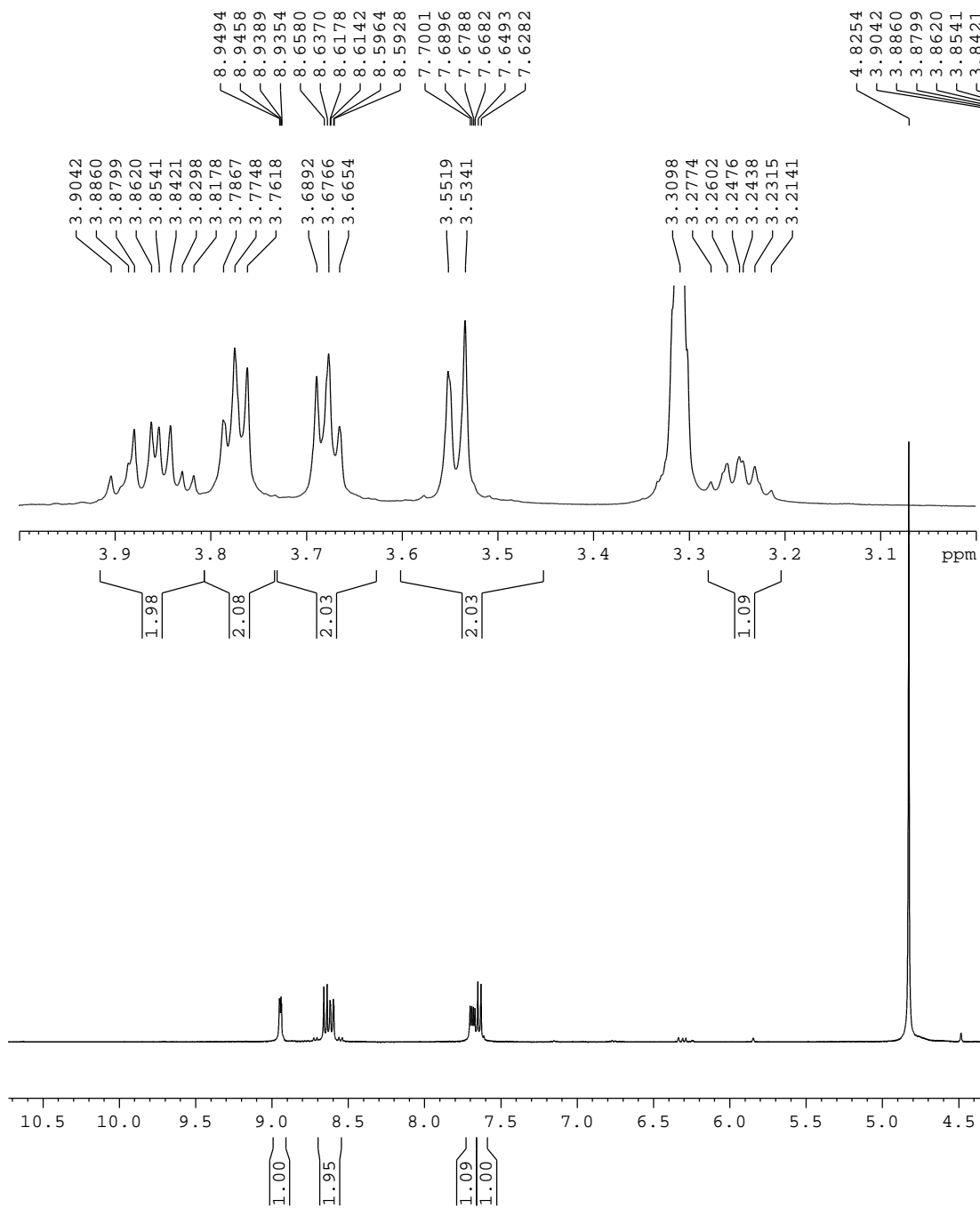
— 77.48
 — 77.16
 — 76.84
 — 72.96
 — 58.96
 — 50.34
 — 48.55

— 0.77

Current Data Parameters
 NAME syh-6-285-2-c
 EXPNO 30
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141227
 Time 1.28
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD

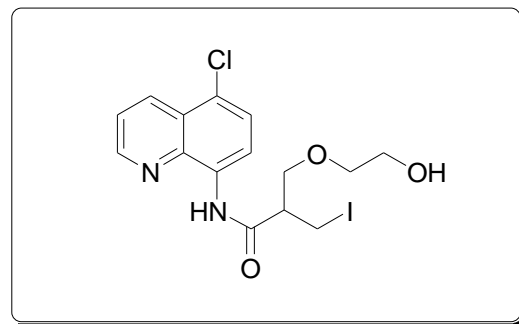


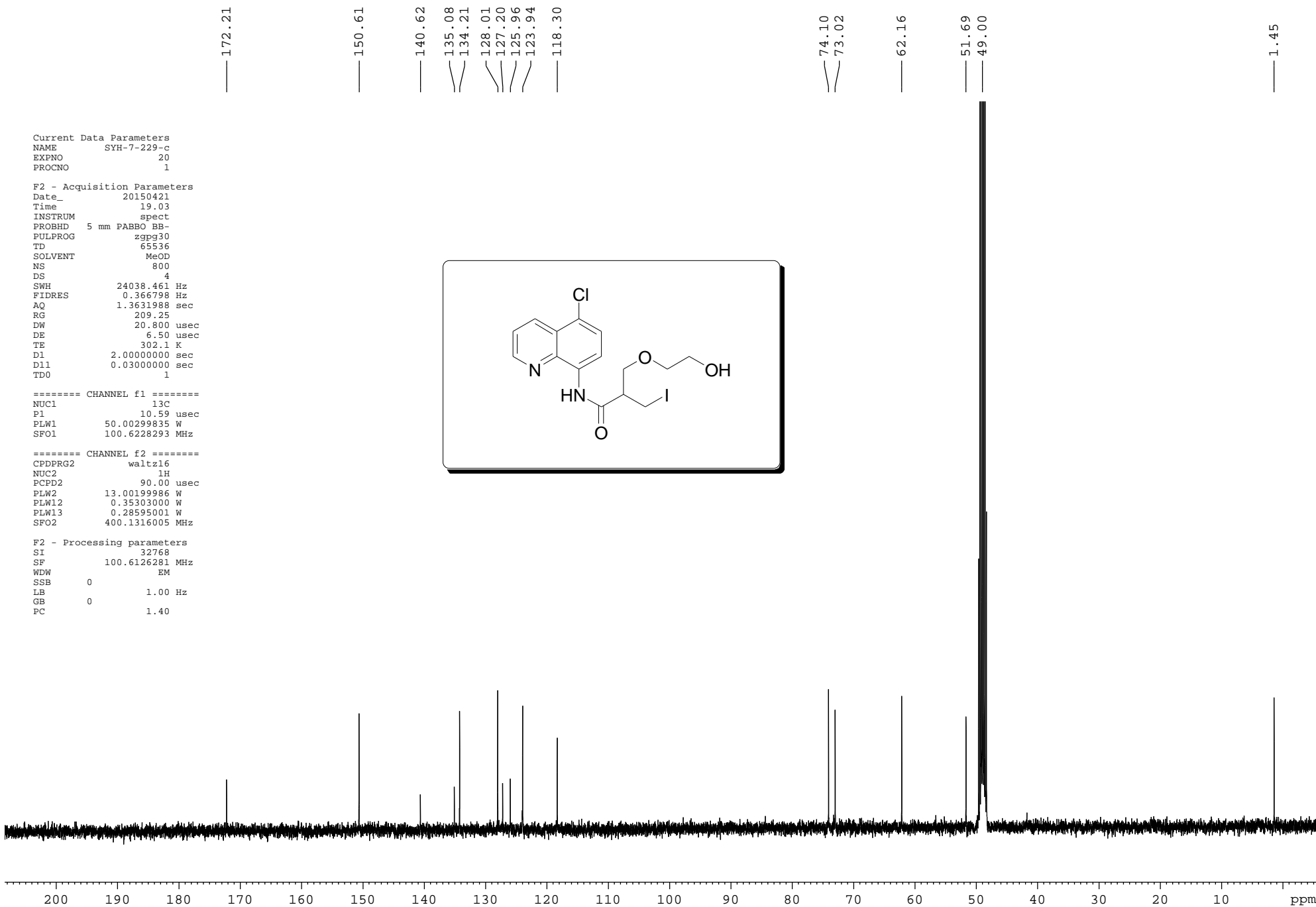


4.8254
 3.9042
 3.8860
 3.8799
 3.8620
 3.8541
 3.8421
 3.8298
 3.8178
 3.7867
 3.7748
 3.7618
 3.6892
 3.6766
 3.6654
 3.5519
 3.5341
 3.3098
 3.2774
 3.2602
 3.2476
 3.2438
 3.2315
 3.2141

Current Data Parameters
 NAME SYH-7-229
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150421
 Time 17.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16





Current Data Parameters
 NAME SYH-7-229-c
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150421
 Time 19.03
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 800
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 302.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 FCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6126281 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Current Data Parameters
 NAME YXL-9-95-2-H-150124
 EXPNO 10
 PROCNO 1

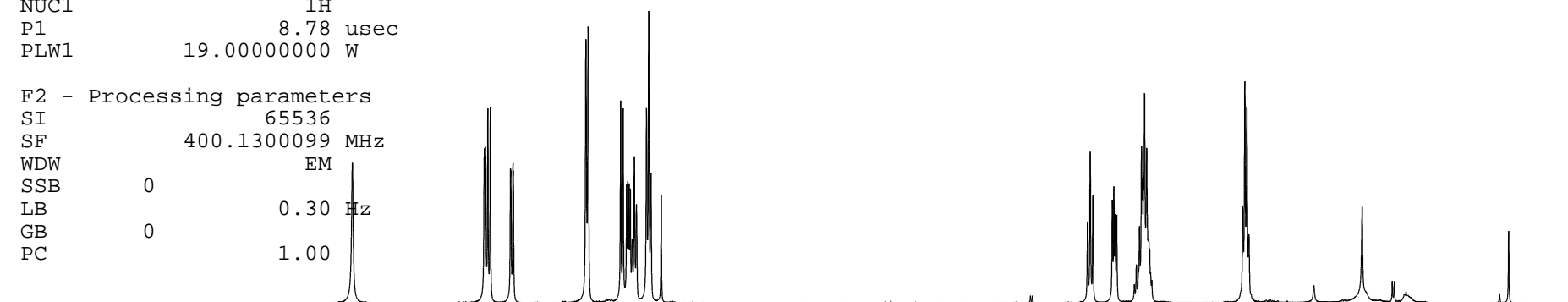
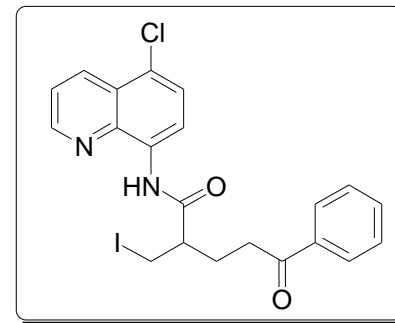
F2 - Acquisition Parameters
 Date_ 20150124
 Time 16.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 73.55
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.9057
 8.7765
 8.7733
 8.7663
 8.7631
 8.7449
 8.7240
 8.5509
 8.5477
 8.5297
 8.5265
 7.9044
 7.8859
 7.6070
 7.5860
 7.5557
 7.5451
 7.5344
 7.5239
 7.5082
 7.4898
 7.4713
 7.3855
 7.3661
 7.3472
 7.2592

3.6067
 3.5833
 3.5602
 3.3942
 3.3808
 3.3696
 3.3562
 3.1880
 3.1704
 3.1611
 3.1440
 3.1359
 3.1266
 3.1175
 3.0996
 3.0866
 3.0808
 3.0739
 3.0660
 3.0556
 2.2762
 2.2585
 2.2413
 2.2237



1.01
 2.02
 1.00
 2.02
 1.03
 2.11
 2.05
 1.04
 1.05
 3.14
 2.09

199.03

171.31

148.93

139.08
136.68
133.46
133.32
133.27
128.67
128.13
127.22
126.03
124.99
122.52
116.90

77.48
77.16
76.84

50.69

35.49

28.31

5.06

Current Data Parameters
NAME YXL-9-95-2-c-150124
EXPNO 10
PROCNO 1

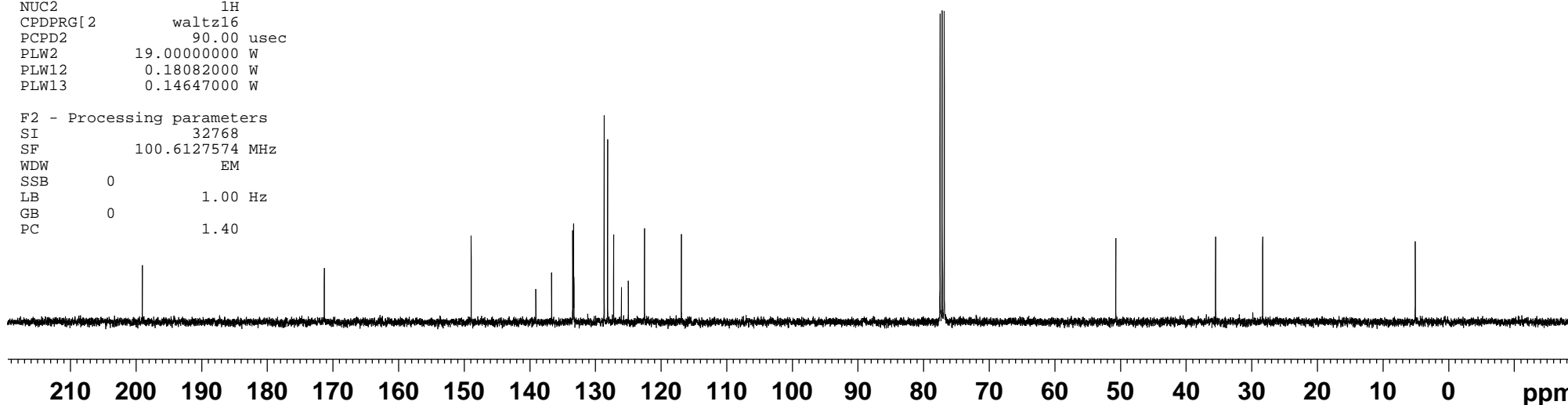
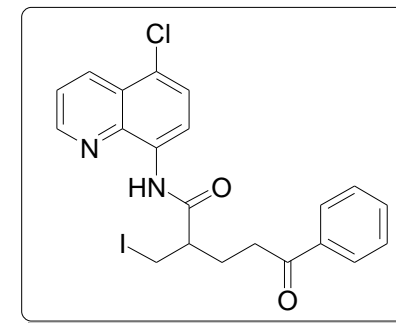
F2 - Acquisition Parameters

Date_ 20150124
Time_ 16.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 95
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127574 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME YXL-8-137-2-H-20141031
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20141031
 Time 22.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 115.38
 DW 60.800 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.00000000 sec
 TD0 1

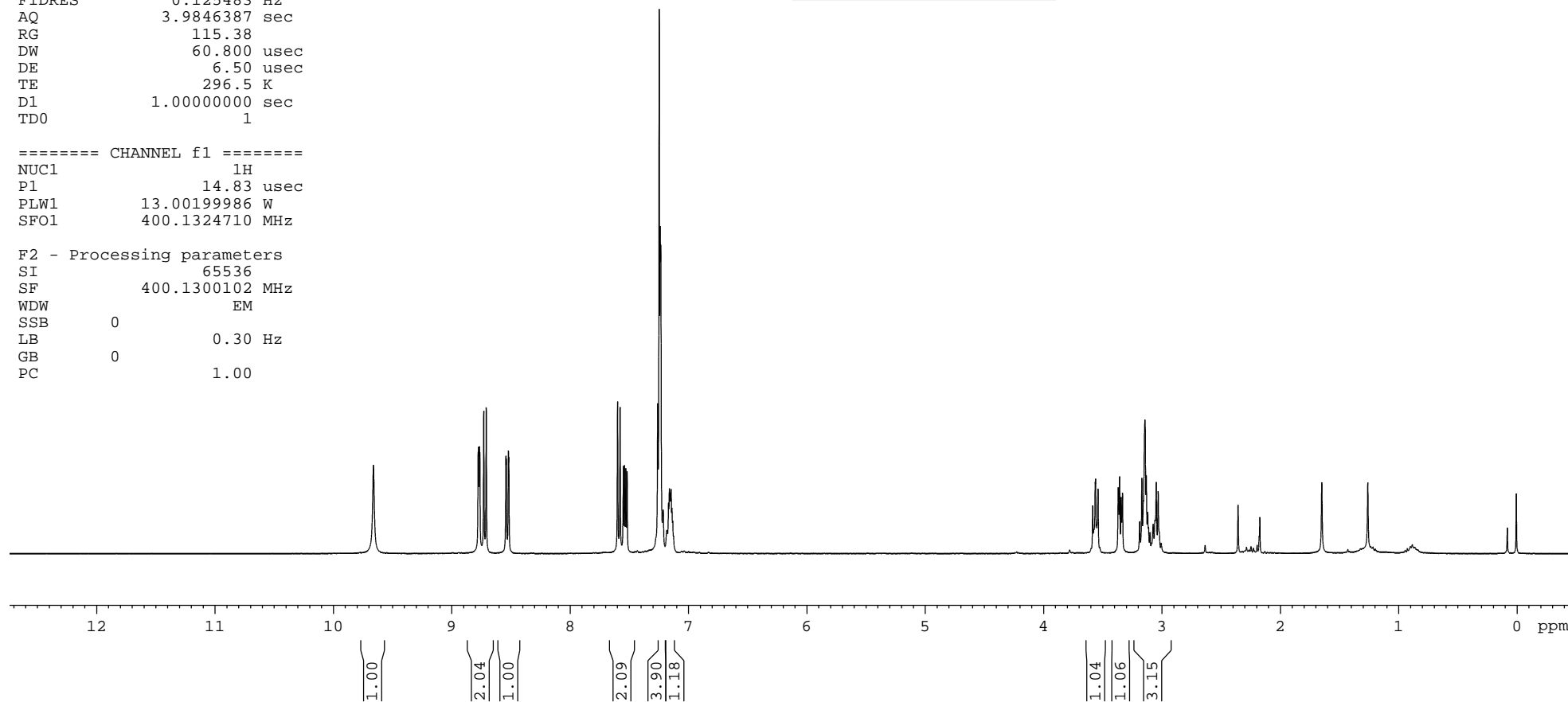
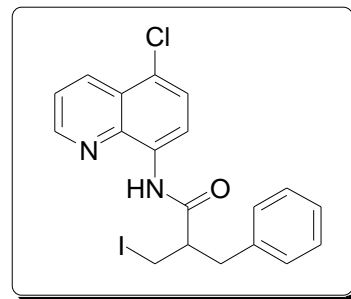
==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters

SI 65536
 SF 400.1300102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.6610
 8.7761
 8.7727
 8.7657
 8.7624
 8.7289
 8.7079
 8.5417
 8.5383
 8.5205
 8.5170
 7.5983
 7.5773
 7.5498
 7.5393
 7.5285
 7.5180
 7.2597
 7.2463
 7.2383
 7.2336
 7.2130
 7.1677
 7.1607
 7.1526
 7.1463
 7.1393

3.5837
 3.5751
 3.5626
 3.5594
 3.5518
 3.5386
 3.3683
 3.3565
 3.3436
 3.3320
 3.1872
 3.1684
 3.1560
 3.1432
 3.1312
 3.1194
 3.1123
 3.0732
 3.0568
 3.0471
 3.0308
 3.0218
 2.3559
 2.1776
 2.1716
 1.6482
 1.2595



Current Data Parameters
 NAME YXL-8-137-2-C-20141031
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141101
 Time 9.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 480
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 298.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127569 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

171.02

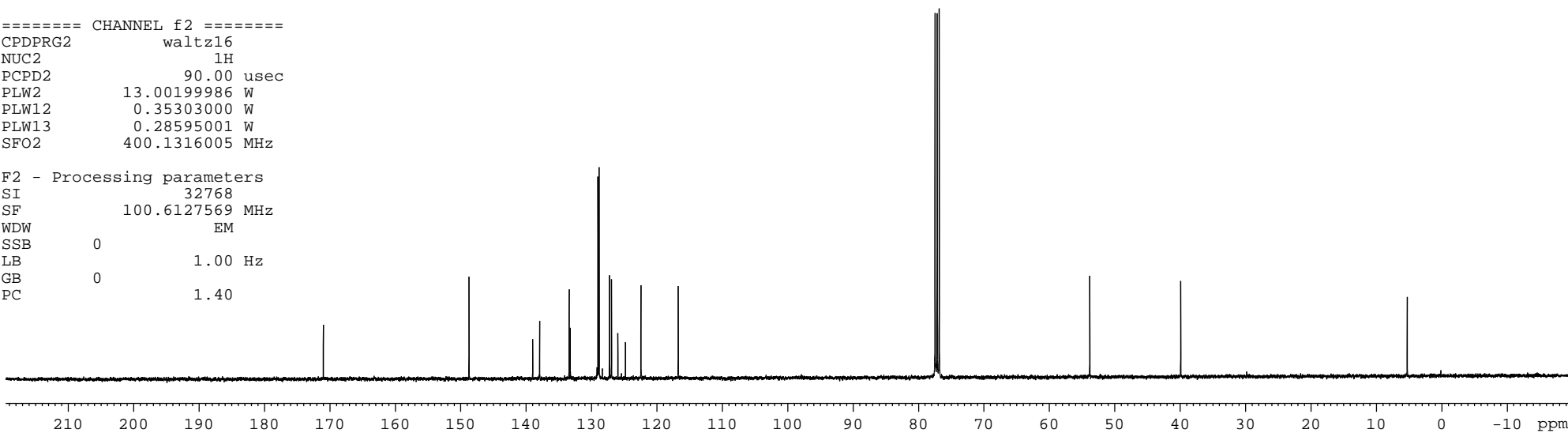
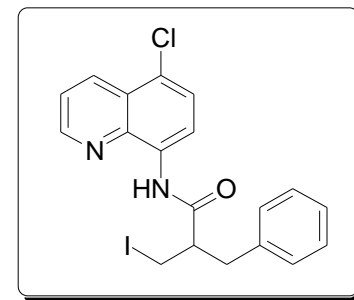
148.75
 139.01
 137.94
 133.43
 133.26
 129.03
 128.84
 127.27
 126.96
 125.98
 124.81
 122.45
 116.76

77.48
 77.17
 76.85

53.83

39.93

5.29

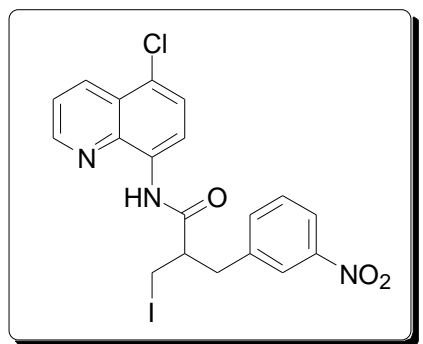
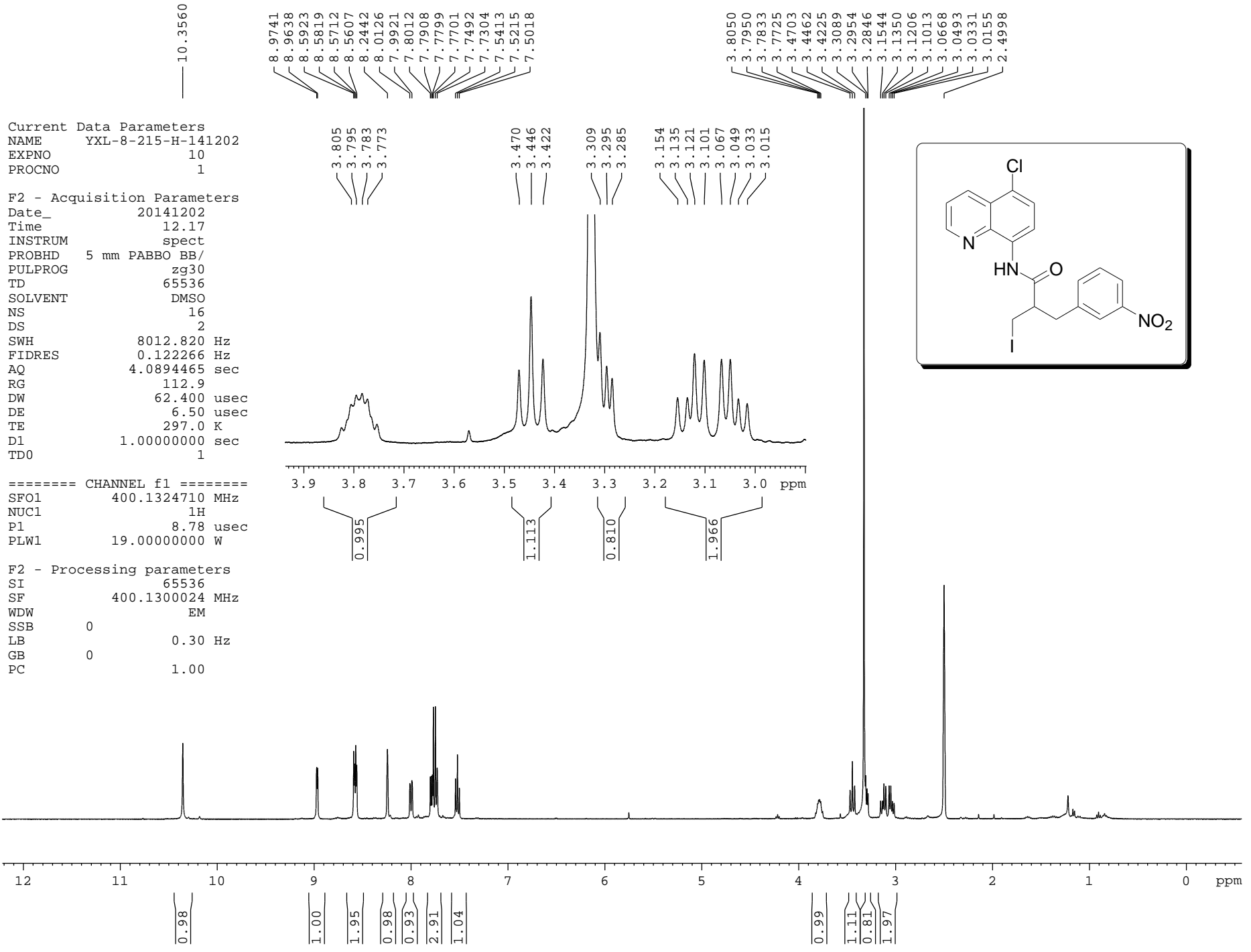


Current Data Parameters
 NAME YXL-8-215-H-141202
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141202
 Time 12.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 112.9
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SF01 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300024 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME YXL-8-215-C-141202
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141203
Time 4.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1000
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6128156 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

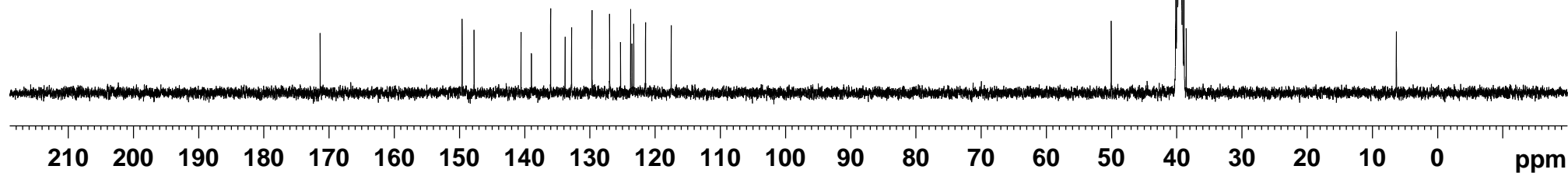
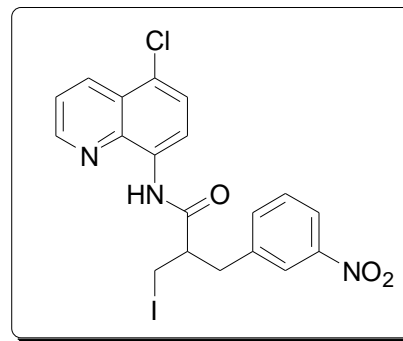
171.39

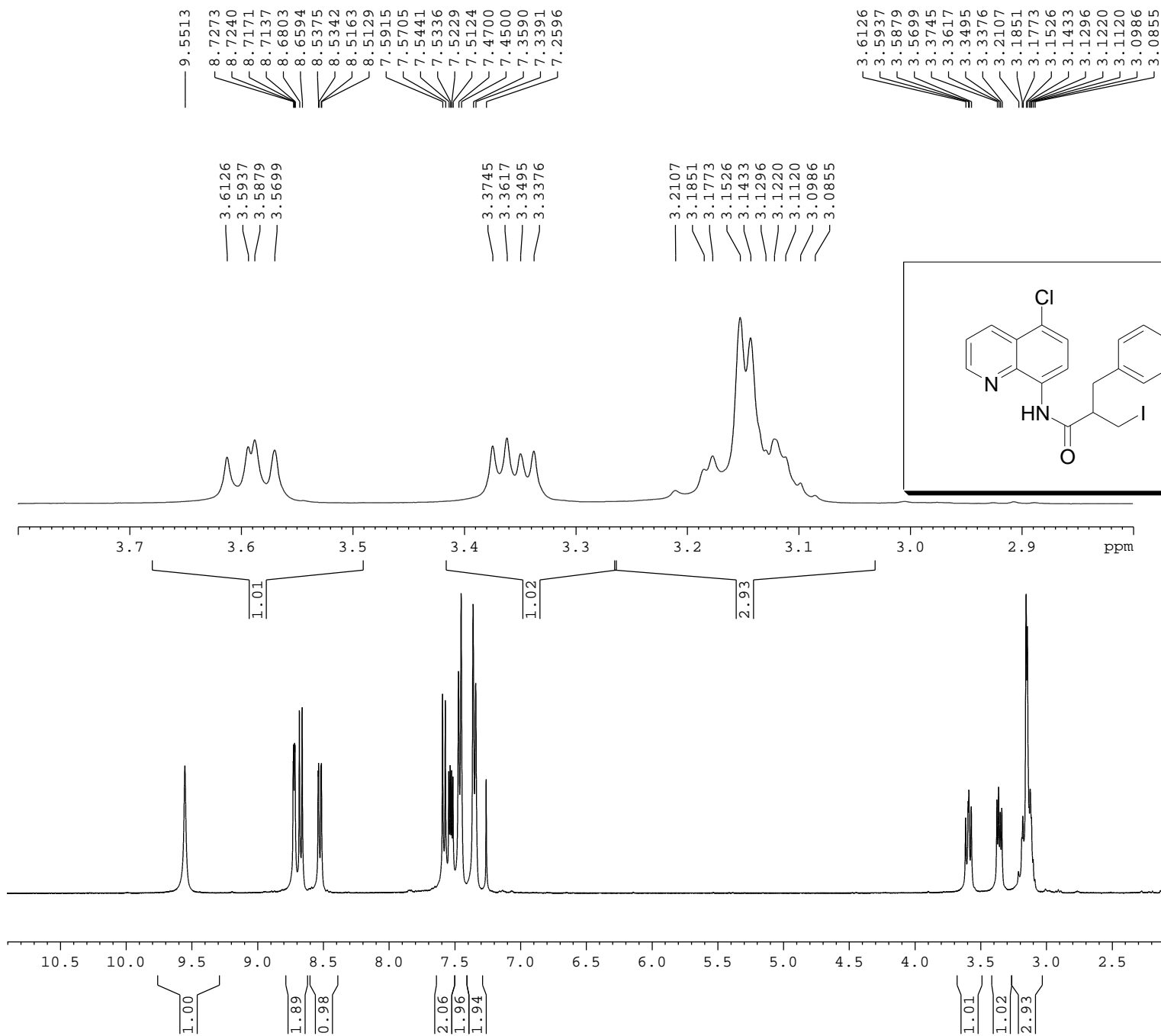
149.62
147.79
140.58
138.99
136.05
133.82
132.83
129.70
127.00
125.32
123.77
123.56
123.30
121.49
117.55

50.05

38.55

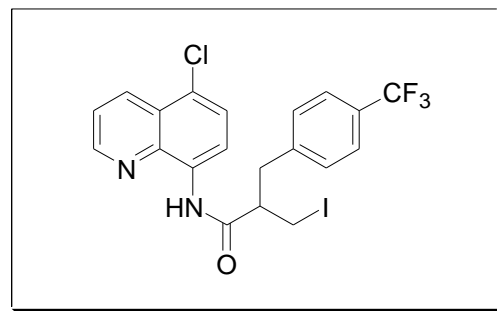
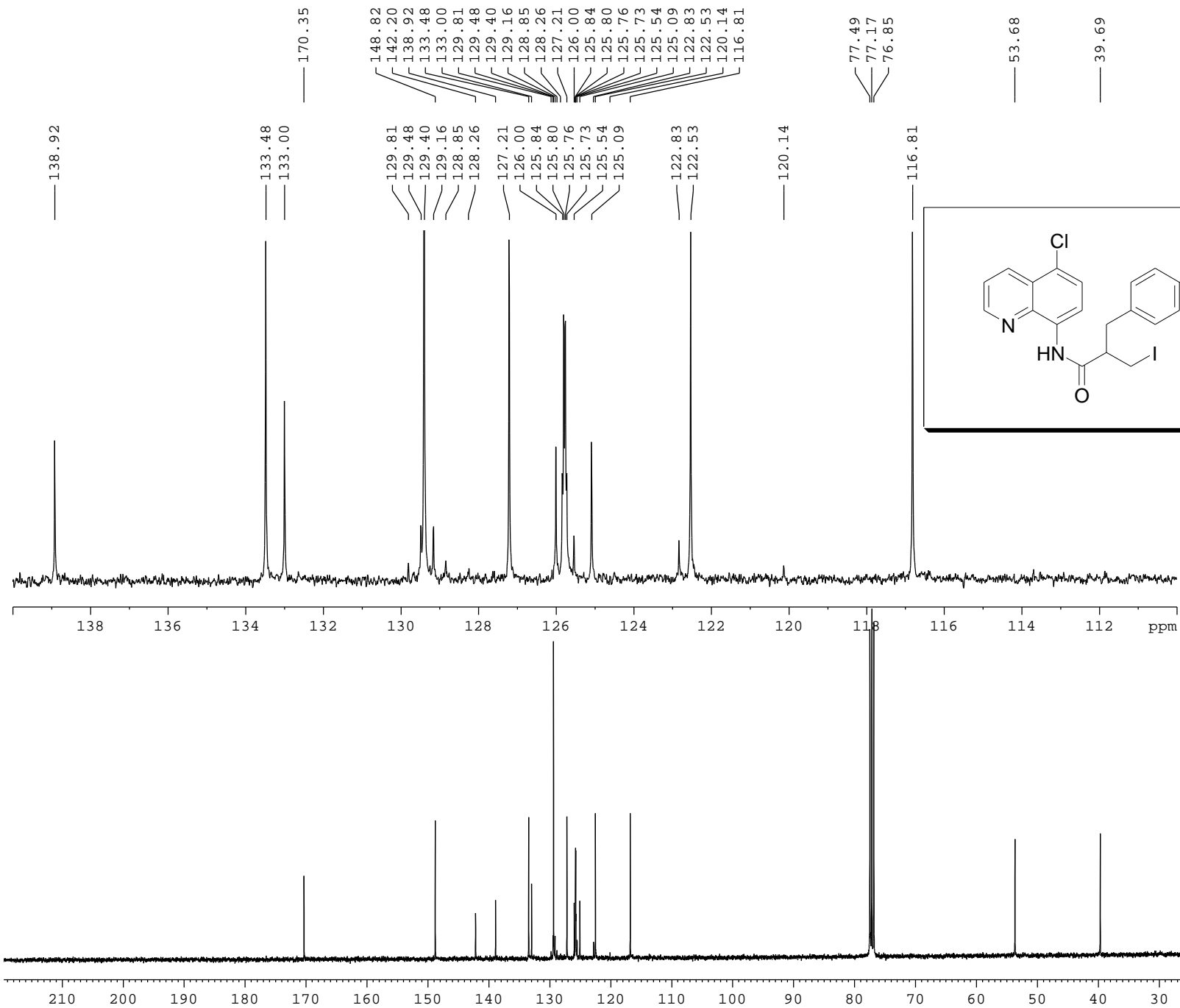
6.33





Current Data Parameters
 NAME syh-7-233-2
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150427
 Time 11.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16



```

Current Data Parameters
NAME      ayh-7-233-2-c
EXPNO    20
PROCNO    1

F2 - Acquisition Parameters
Date_     20150428
Time      2.24
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         1024
DS         4
SWH        24038.461 Hz
FIRRES     0.366798 Hz
AQ         1.3631988 sec
RG         209.25
DW         20.800 usec
DE         6.50 usec
TE         300.2 K
D1         2.0000000 sec
d11        0.0300000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         10.59 usec
PLM1       50.00299835 W
SFO1       100.6228293 MHz

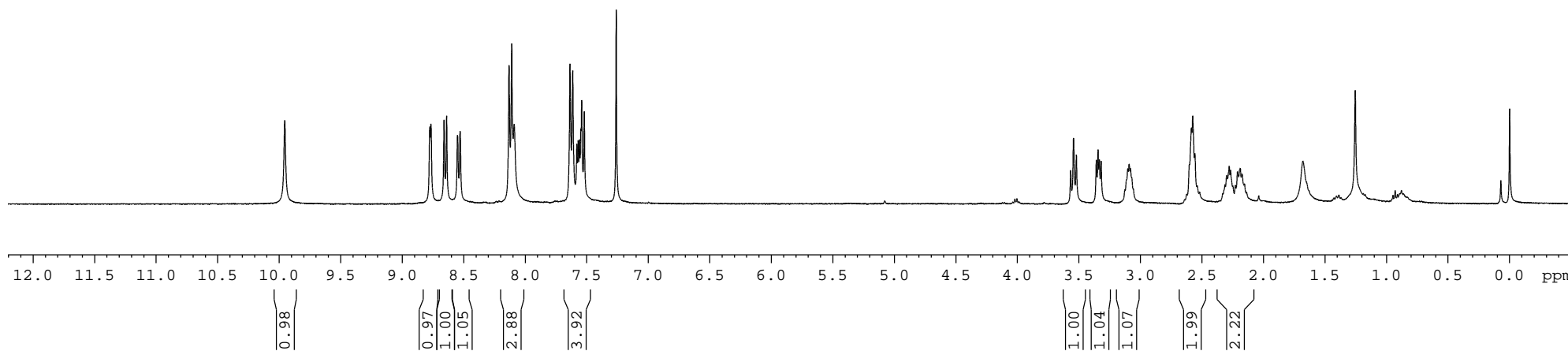
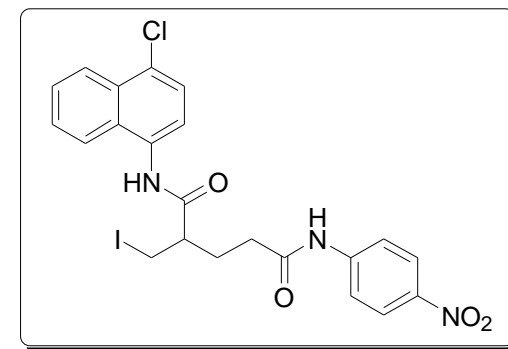
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2        1H
PCPD2       90.00 usec
PLW2        13.00199986 W
PLM2        0.35303000 W
PLM3        0.28595001 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI          32768
SF          100.6127545 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```

Current Data Parameters
NAME YXL-9-231-H-20150330
EXPNO 10
PROCNO 1

9.9521
8.7742
8.7665
8.6593
8.6384
8.5503
8.5294
8.1316
8.1091
8.0896
7.6359
7.6135
7.5800
7.5696
7.5589
7.5476
7.5408
7.5198
7.2601

3.5661
3.5430
3.5200
3.3579
3.3437
3.3332
3.3189
3.1022
3.0915
3.0810
2.6016
2.5849
2.5744
2.5568
2.5366
2.3118
2.2965
2.2779
2.2665
2.2486
2.2276
2.2110
2.1881
2.1722
2.1538



Current Data Parameters
NAME YXL-9-231-C-150330
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150331
Time 1.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

=====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

=====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127557 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

171.31
170.61

149.12
143.76
143.54
139.02
133.69
132.87
127.08
126.10
125.56
125.11
122.73
119.08
117.01

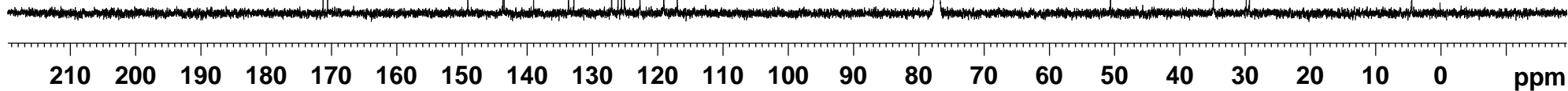
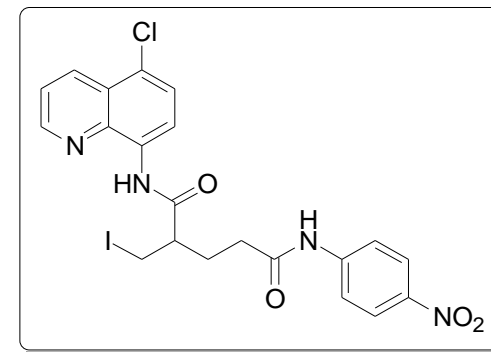
77.48
77.16
76.84

50.63

34.86

29.33

4.47

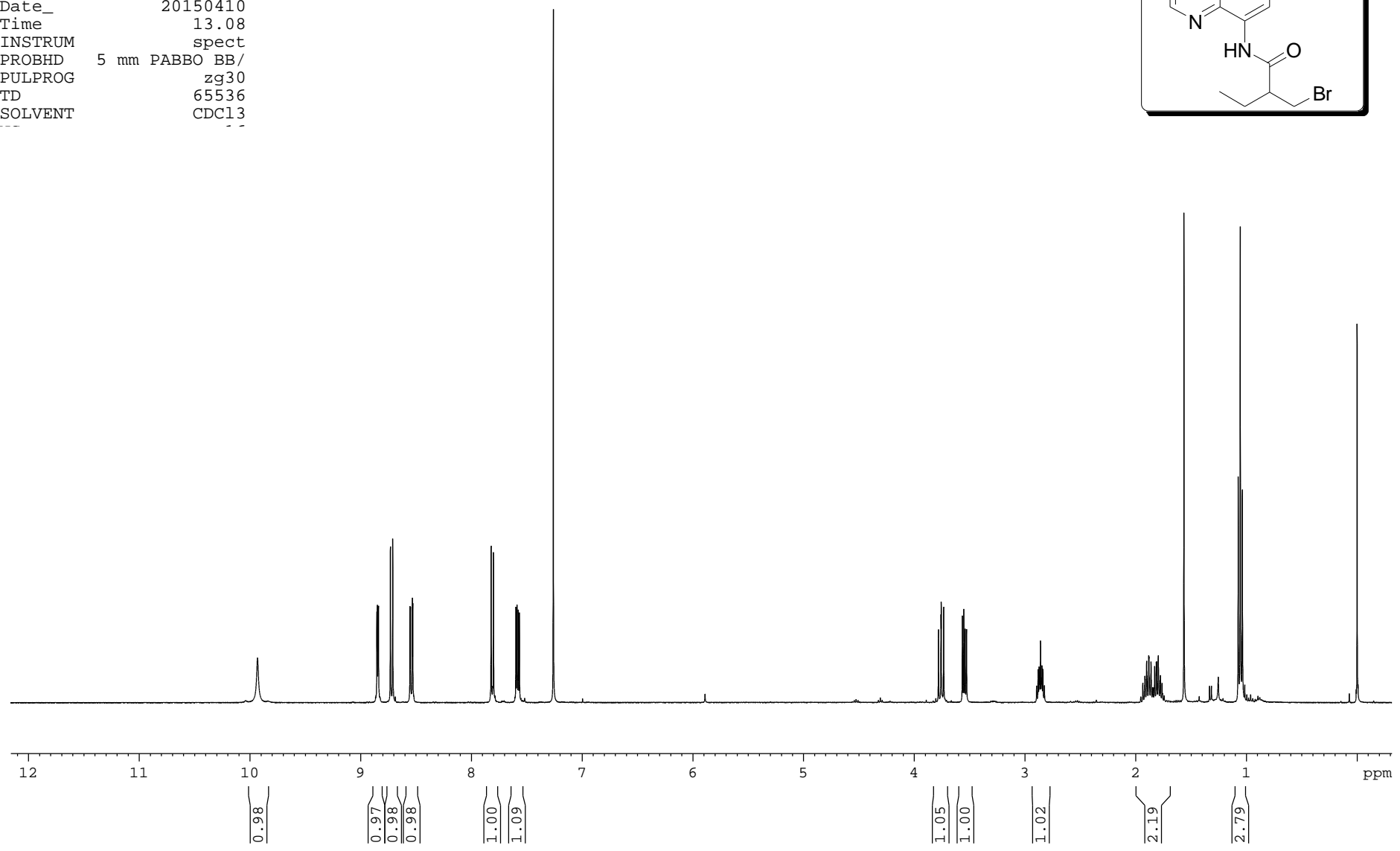
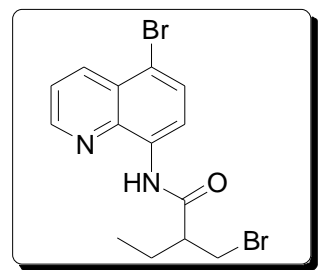


9.9320
 8.8537
 8.8498
 8.8431
 8.8392
 8.7317
 8.7107
 8.5546
 8.5506
 8.5333
 8.5293
 7.8214
 7.8004
 7.5980
 7.5897
 7.5874
 7.5766
 7.5661
 7.2599

3.7806
 3.7584
 3.7557
 3.7336
 3.5647
 3.5518
 3.5396
 3.5268
 2.8803
 2.8720
 2.8587
 2.8454
 2.8370
 1.9345
 1.9159
 1.9136
 1.9001
 1.8949
 1.8814
 1.8792
 1.8750
 1.8604
 1.8276
 1.8136
 1.8090
 1.7948
 1.7793
 1.7750
 1.7608
 1.0729
 1.0543
 1.0356

Current Data Parameters
 NAME YXL-9-287-1-H-150410
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150410
 Time 13.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13



— 171.62

— 148.95

— 139.27

— 136.17

— 134.11

— 131.03

— 127.37

— 122.88

— 117.39

— 114.78

— 53.29

— 32.93

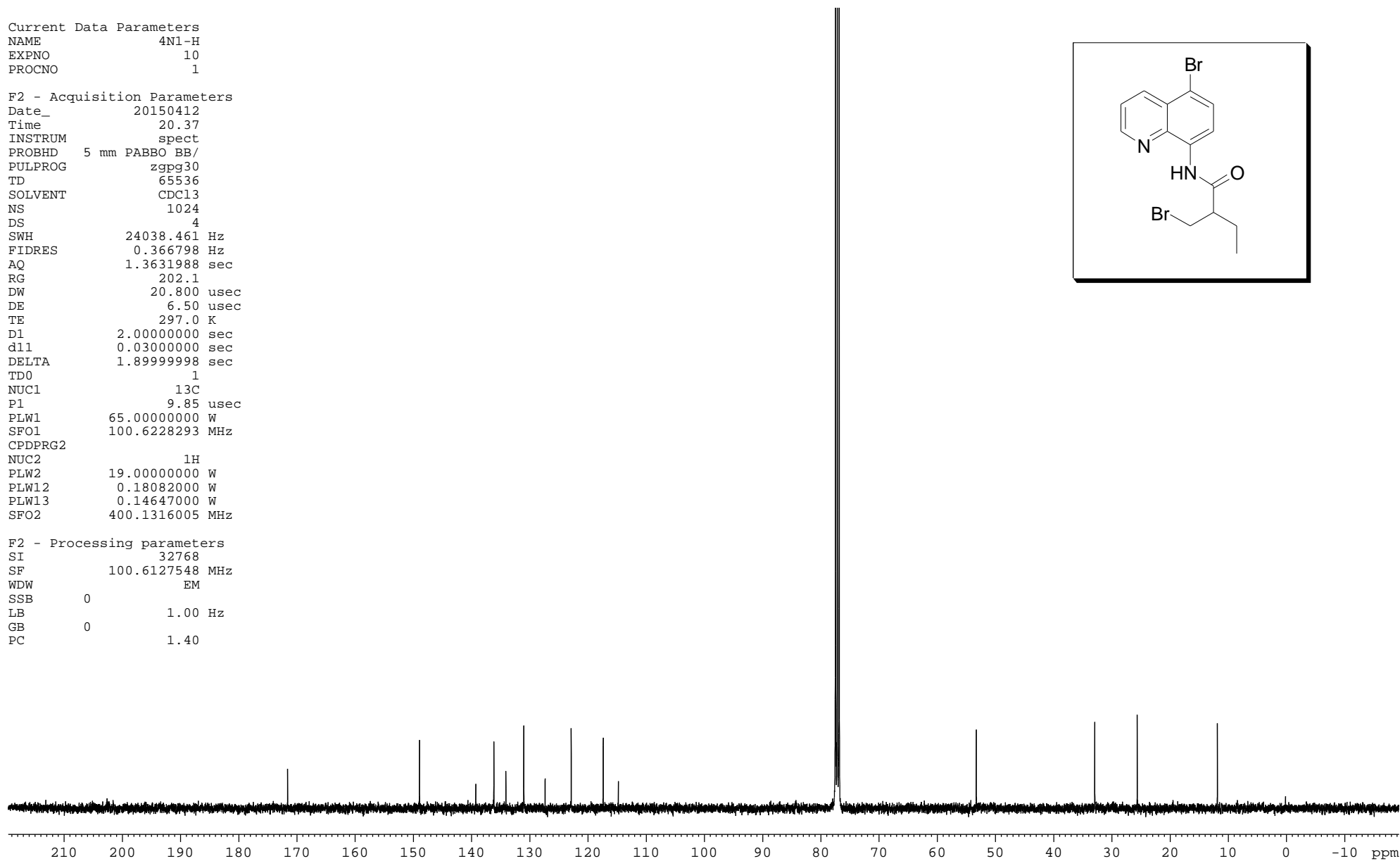
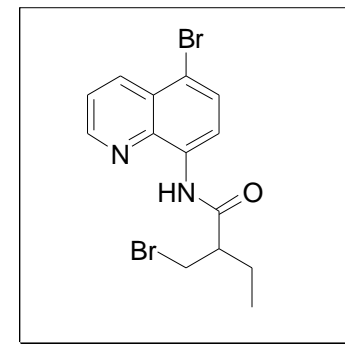
— 25.64

— 11.87

Current Data Parameters
NAME 4N1-H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150412
Time 20.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W
SFO1 100.6228293 MHz
CPDPRG2
NUC2 1H
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME YXL-9-287-2-H-20150411
 EXPNO 10
 PROCNO 1

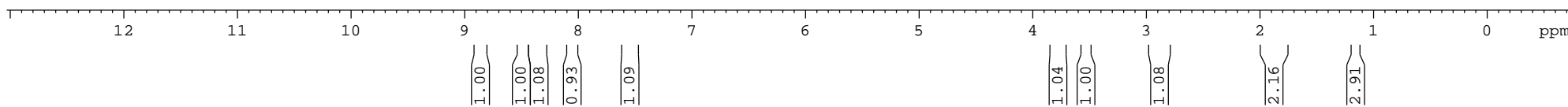
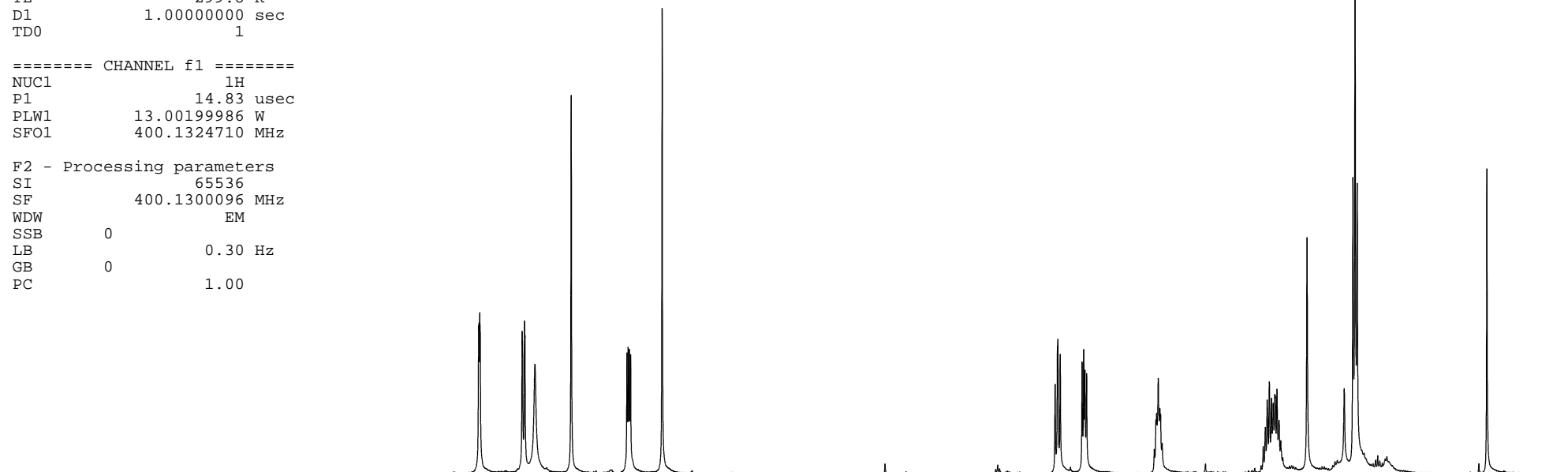
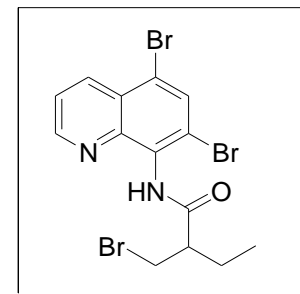
F2 - Acquisition Parameters
 Date_ 20150411
 Time 11.11
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 209.25
 DW 60.800 usec
 DE 6.50 usec
 TE 299.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.876
8.872
8.865
8.493
8.489
8.472
8.468
8.380
8.061
7.570
7.559
7.549
7.538
7.260

3.801
3.780
3.776
3.756
3.563
3.549
3.538
3.524
2.913
2.907
2.893
2.879
2.873
1.969
1.950
1.934
1.916
1.896
1.881
1.867
1.863
1.849
1.830
1.815
1.179
1.161
1.142

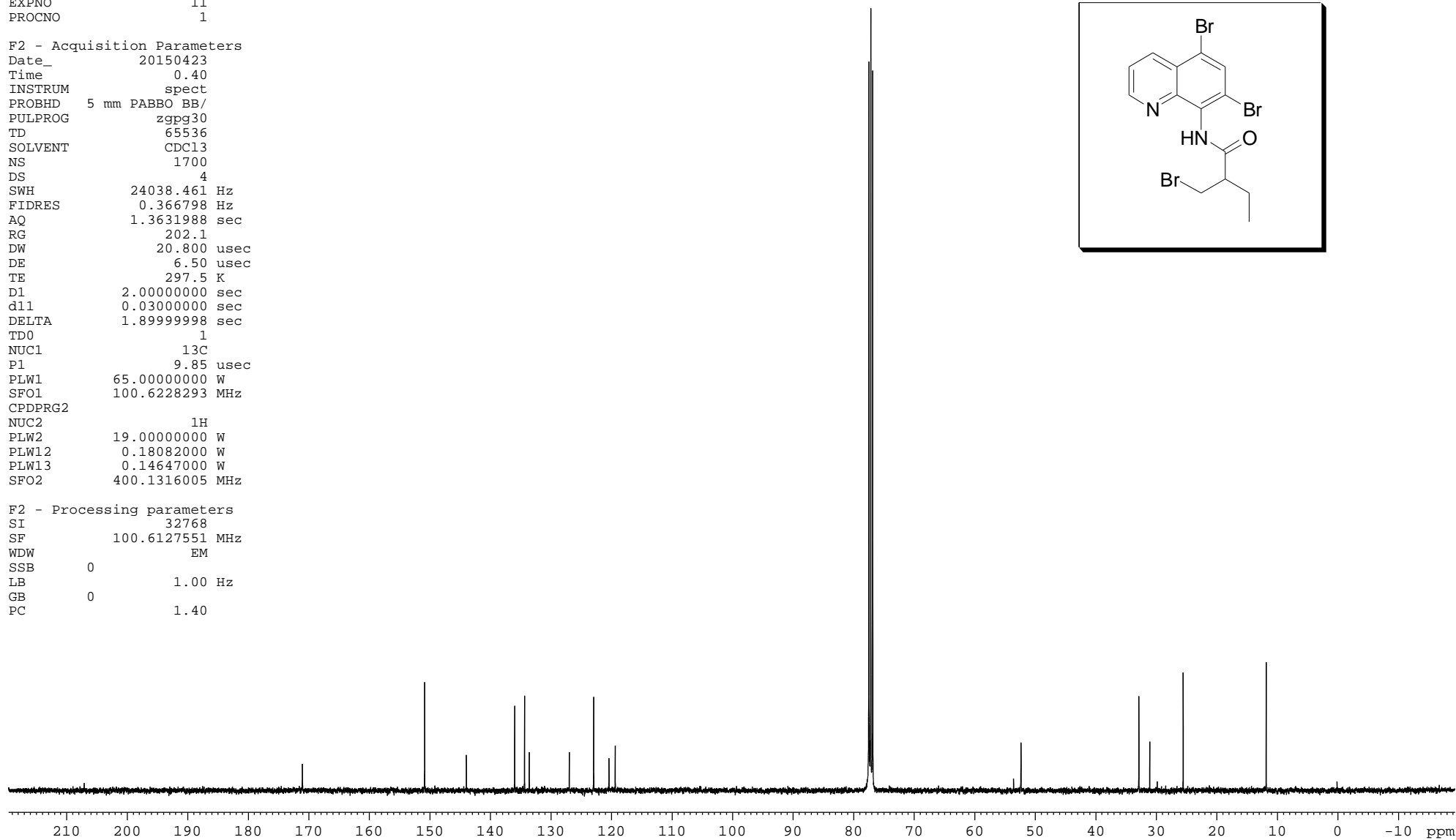
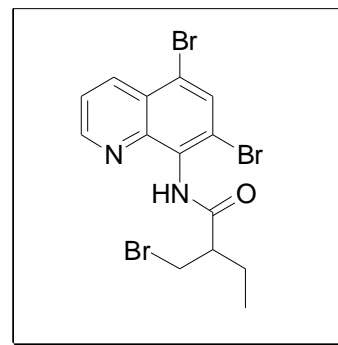


— 171.08
 — 150.88
 — 143.97
 136.00
 134.37
 133.59
 — 126.97
 — 122.94
 — 120.42
 — 119.39
 — 52.35
 — 32.87
 — 25.56
 — 11.84

Current Data Parameters
 NAME 4N2-H
 EXPNO 11
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150423
 Time 0.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 1700
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 202.1
 DW 20.800 usec
 DE 6.50 usec
 TE 297.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1
 NUC1 13C
 P1 9.85 usec
 PLW1 65.00000000 W
 SFO1 100.6228293 MHz
 CPDPRG2
 NUC2 1H
 PLW2 19.00000000 W
 PLW12 0.18082000 W
 PLW13 0.14647000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127551 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Current Data Parameters
 NAME YXL-9-294-1--H-20150418
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150418
 Time 19.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 130.81
 DW 60.800 usec
 DE 6.50 usec
 TE 301.3 K
 D1 1.00000000 sec
 TD0 1

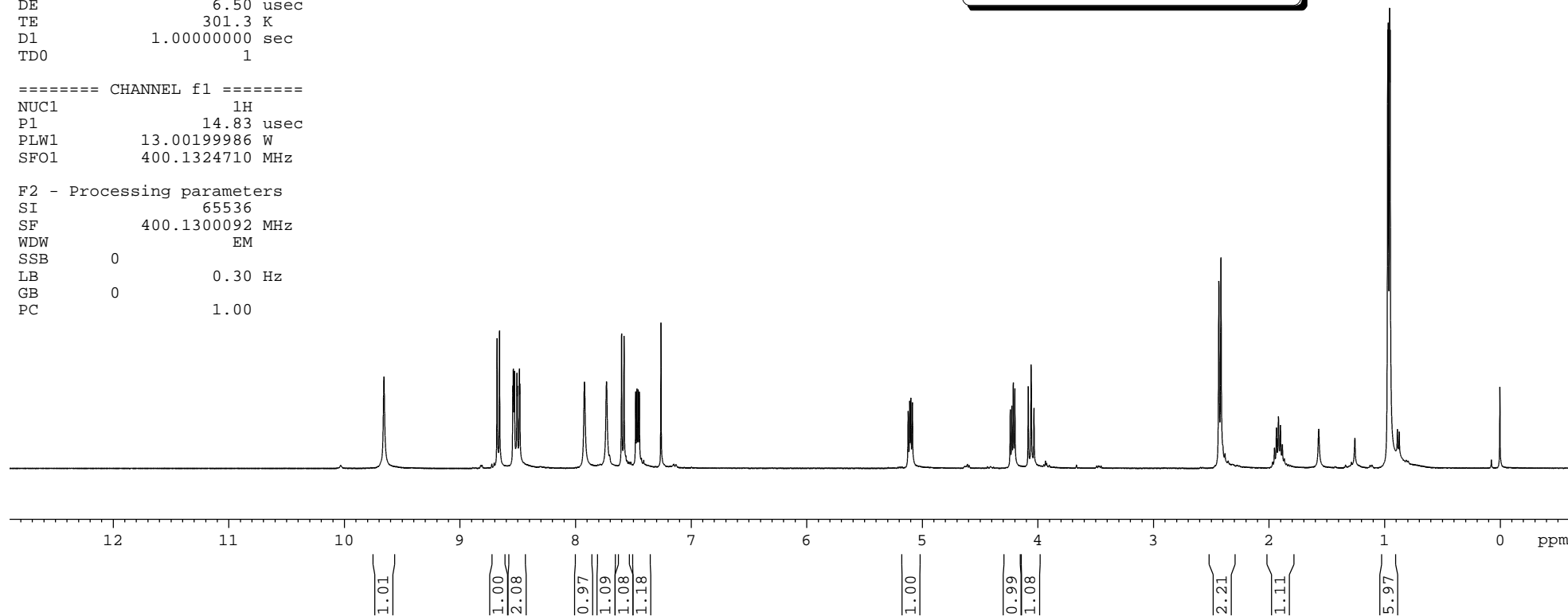
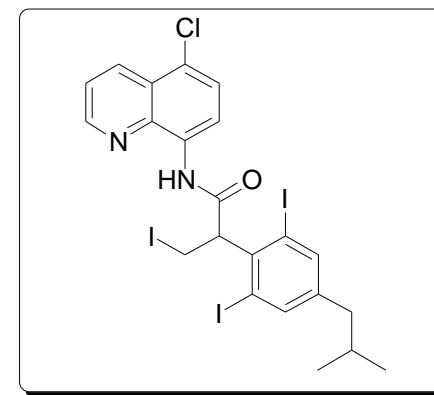
==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.6570
 8.6780
 8.6571
 8.5416
 8.5379
 8.5311
 8.5274
 8.5063
 8.5025
 8.4850
 8.4812
 7.9221
 7.7315
 7.6008
 7.5798
 7.4789
 7.4683
 7.4576
 7.4470
 7.2600

5.1216
 5.1081
 5.0982
 5.0847
 4.2379
 4.2244
 4.2118
 4.1983
 4.0820
 4.0582
 4.0324

2.4332
 2.4150
 1.9683
 1.9515
 1.9345
 1.9176
 1.9007
 1.8838
 1.8667
 0.9720
 0.9676
 0.9556
 0.9512



Current Data Parameters
 NAME YXL-9-294-1--c-20150418
 EXPNO 22
 PROCNO 1

F2 - Acquisition Parameters

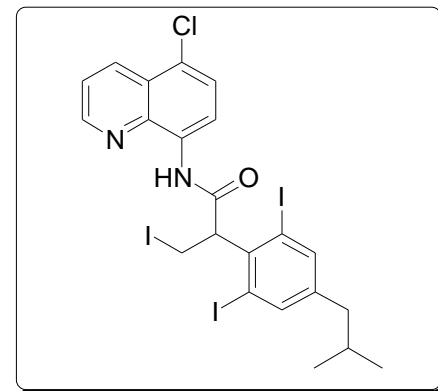
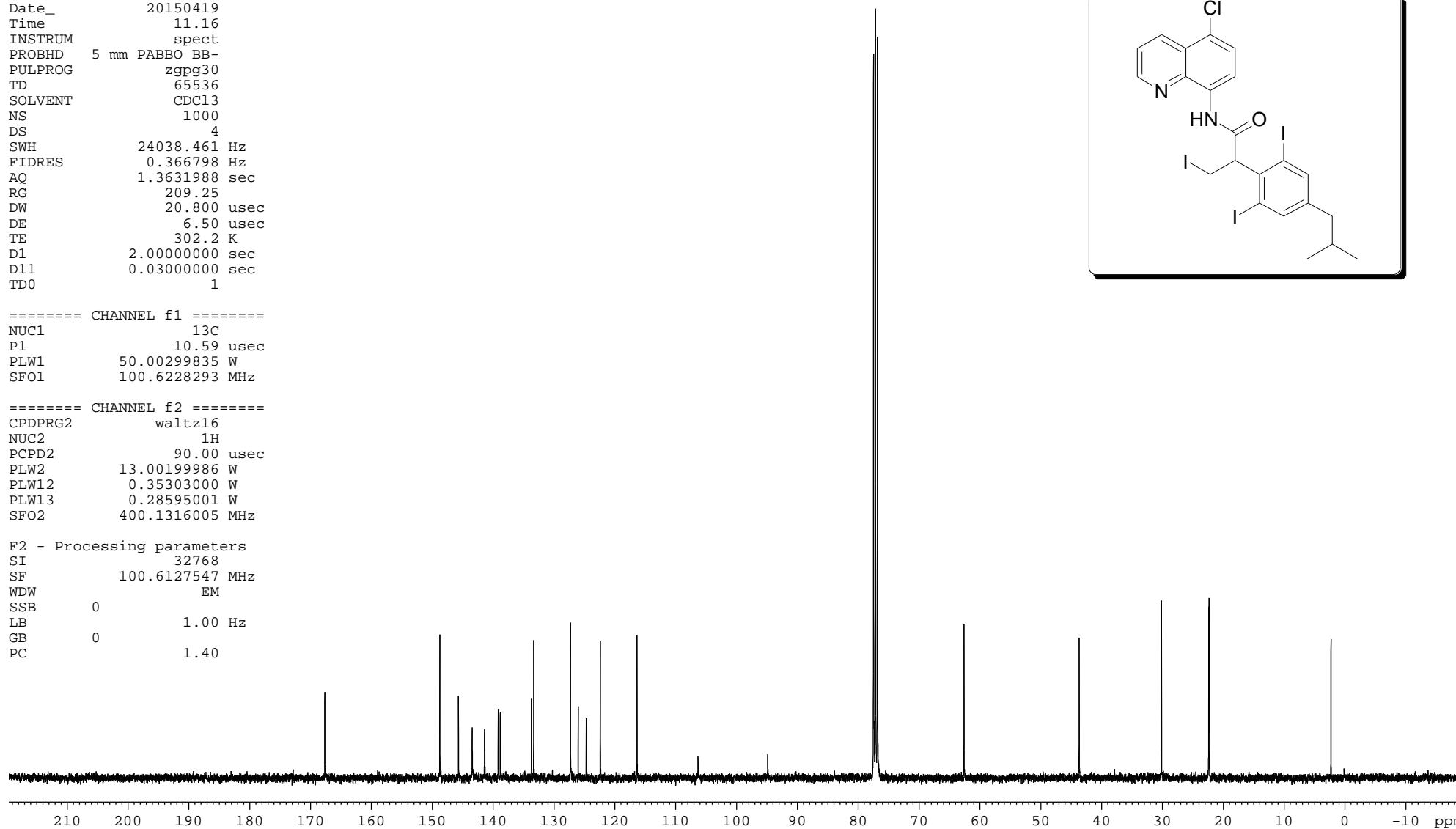
Date_ 20150419
 Time 11.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1000
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 302.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 10.59 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

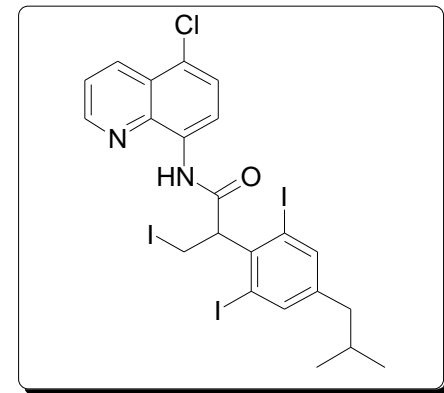
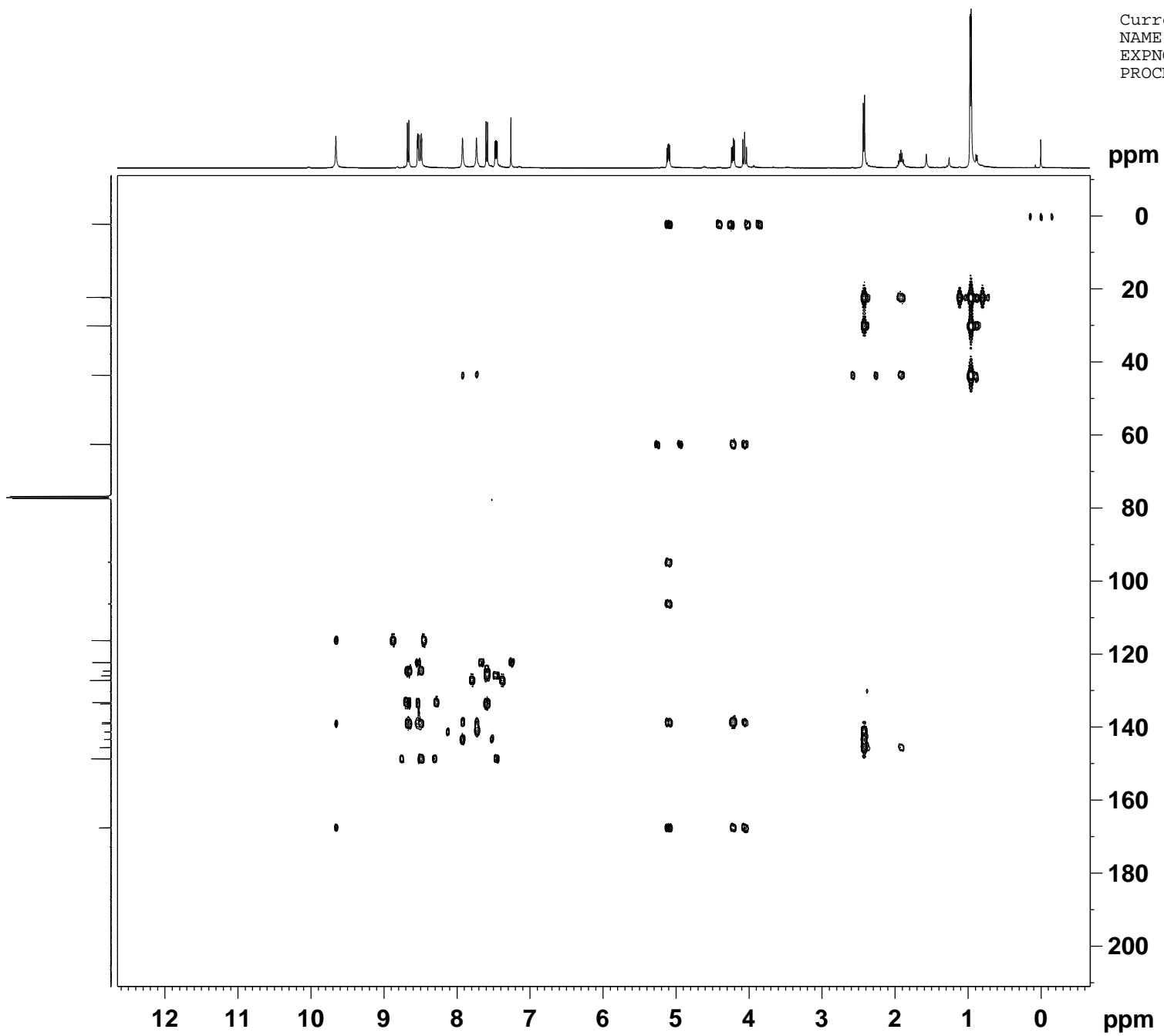
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.35303000 W
 PLW13 0.28595001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127547 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

167.66
 148.76
 145.69
 143.44
 141.39
 139.17
 138.82
 133.70
 133.33
 127.29
 126.02
 124.70
 122.38
 116.36
 106.32
 94.87
 77.48
 77.16
 76.84
 62.62
 43.68
 30.15
 22.38
 22.33
 2.30



Current Data Parameters
NAME YXL-9-294-1--HMBC-20150418
EXPNO 24
PROCNO 1



Current Data Parameters
 NAME YXL-9-139-2-1-H-20150210
 EXPNO 10
 PROCNO 1

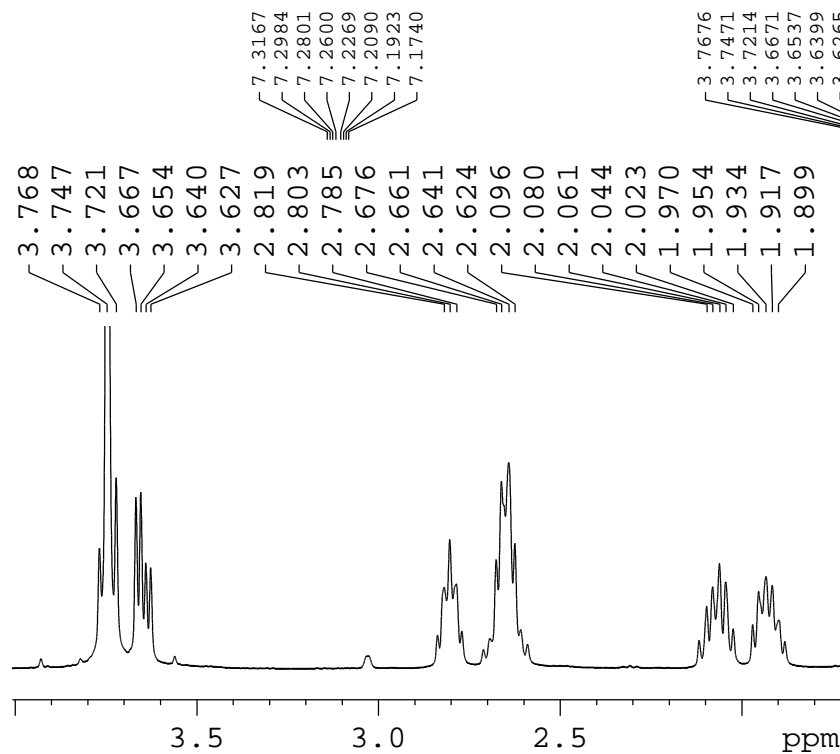
F2 - Acquisition Parameters

Date_ 20150210
 Time 11.54
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 85
 DW 60.800 usec
 DE 6.50 usec
 TE 294.2 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

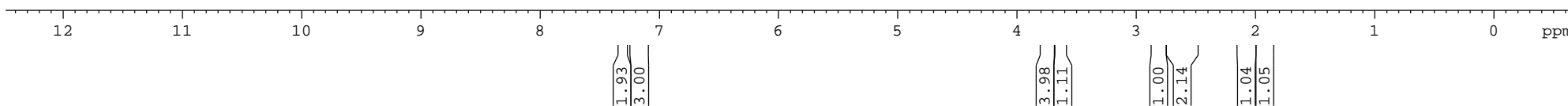
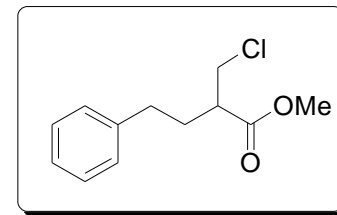
F2 - Processing parameters

SI 65536
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



7.3167
7.2984
7.2801
7.2600
7.2269
7.2090
7.1923
7.1740

3.7676
3.7471
3.7214
3.6671
3.6537
3.6399
3.6265
2.8370
2.8189
2.8033
2.7849
2.7701
2.6931
2.6755
2.6610
2.6408
2.6242
2.6078
2.1170
2.0962
2.0798
2.0611
2.0438
2.0233
1.9704
1.9539
1.9338
1.9166
1.8993



Current Data Parameters
NAME YXL-9-51-2-H-150115
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150115
Time 15.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters

SI 32768
SF 100.6127575 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

173.44

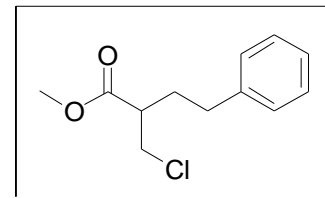
140.88

128.64
128.52
126.35

77.48
77.16
76.84

52.16
47.48
44.55

33.15
31.60



200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

Current Data Parameters
NAME YXL-9-51-1-1-1-H-20150114
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters

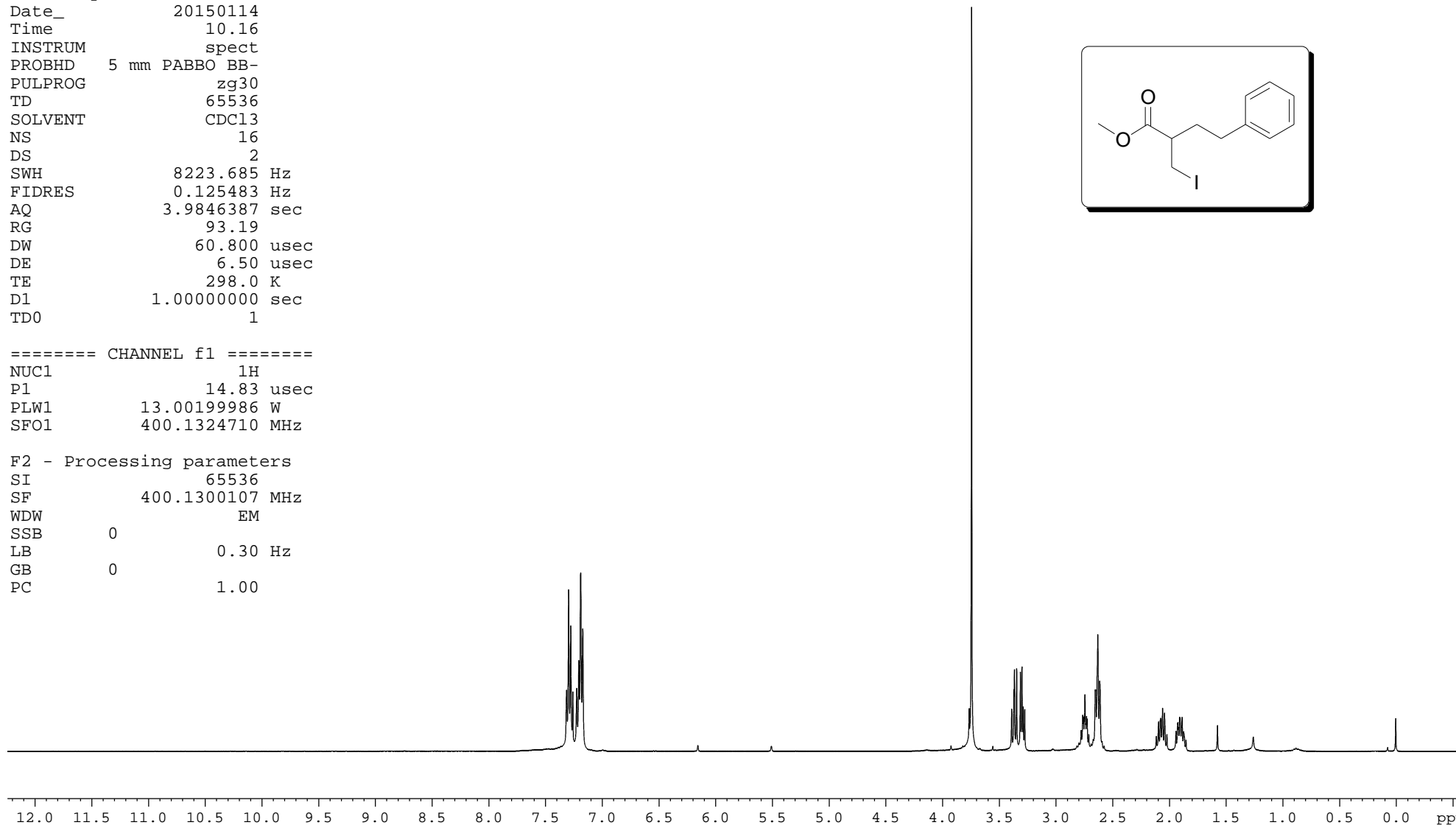
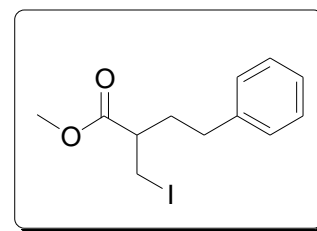
Date_ 20150114
Time 10.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 93.19
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

7.3131
7.2953
7.2765
7.2579
7.2236
7.2055
7.1996
7.1886
7.1705

3.7444
3.3917
3.3719
3.3670
3.3475
3.3146
3.3011
3.2898
3.2763
2.7795
2.7658
2.7597
2.7459
2.7397
2.7321
2.7260
2.7123
2.6729
2.6548
2.6511
2.6327
2.6154
2.1165
2.0960
2.0818
2.0780
2.0611
2.0440
1.9434
1.9290
1.9257
1.9207
1.9112
1.9087
1.8946
1.8897
1.8764
1.8732
1.8689
1.8547



2.19
2.90

2.98

1.91

1.12
1.96

1.00
0.96

— 173.54

— 140.87

128.65
128.54
126.36

— 52.19

— 47.50

34.68
33.17

— 4.94

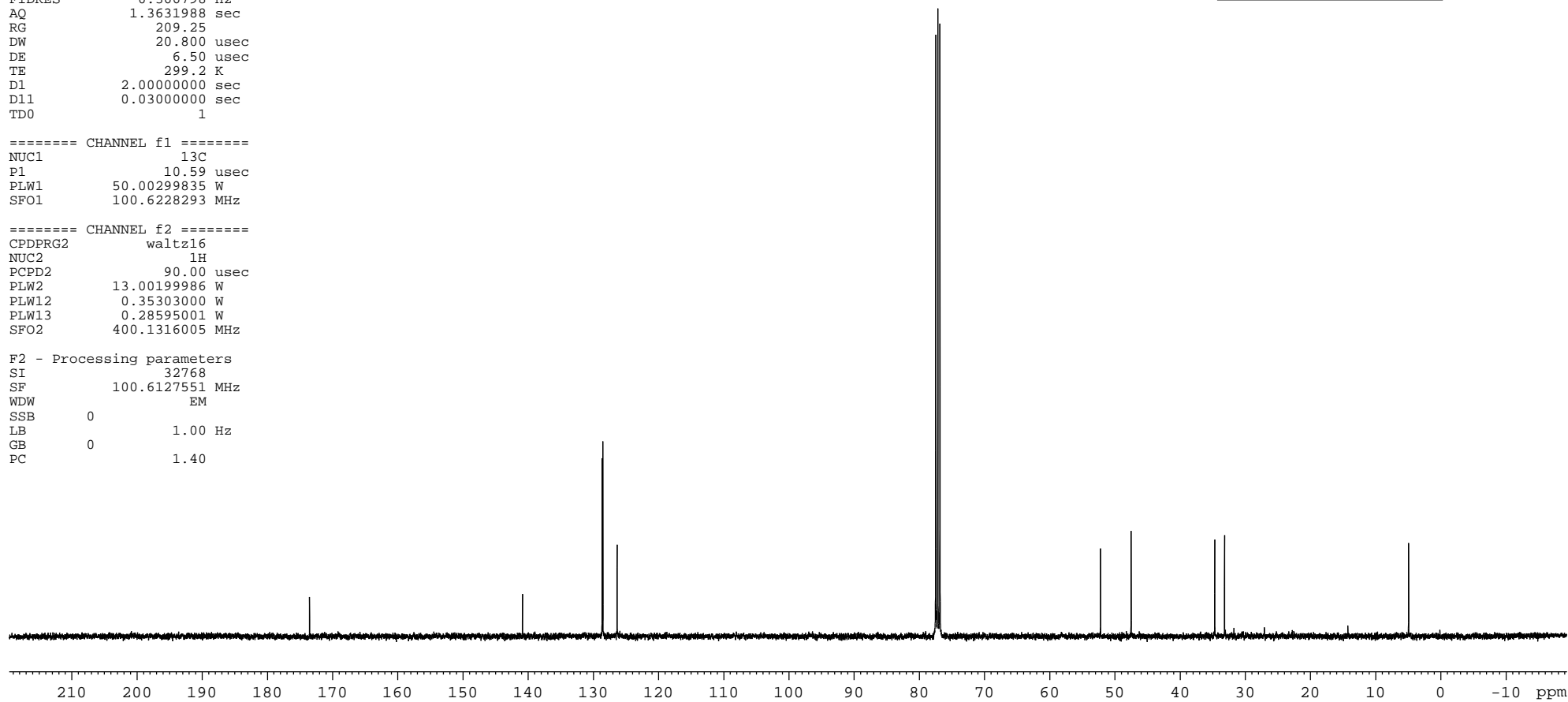
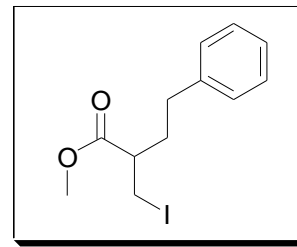
Current Data Parameters
NAME 5B-C
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141230
Time 2.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME YXL-9-139-1-2-H-20150213
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150213
 Time 21.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 165.63
 DW 60.800 usec
 DE 6.50 usec
 TE 295.4 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.7968
 8.7867
 8.4764
 8.4552
 7.4983
 7.4880
 7.4771
 7.4667
 7.3979
 7.3776
 7.2599
 6.8411
 6.8208

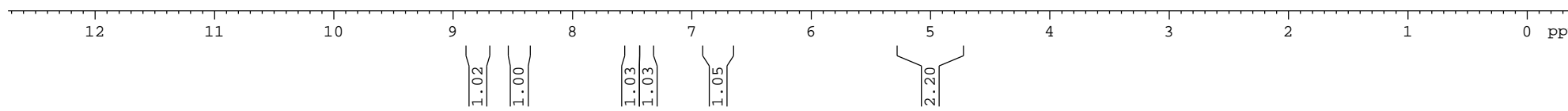
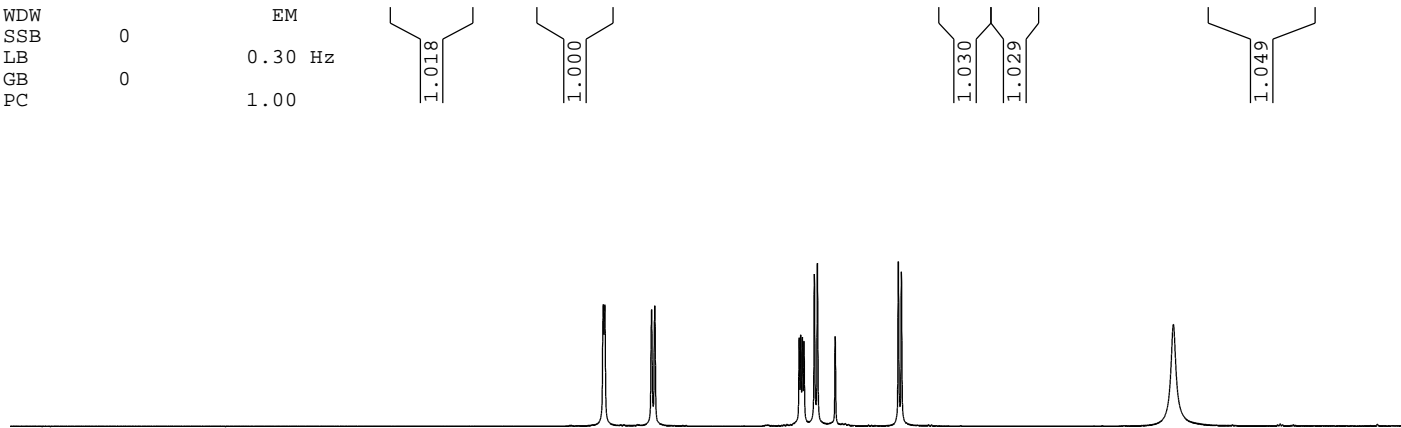
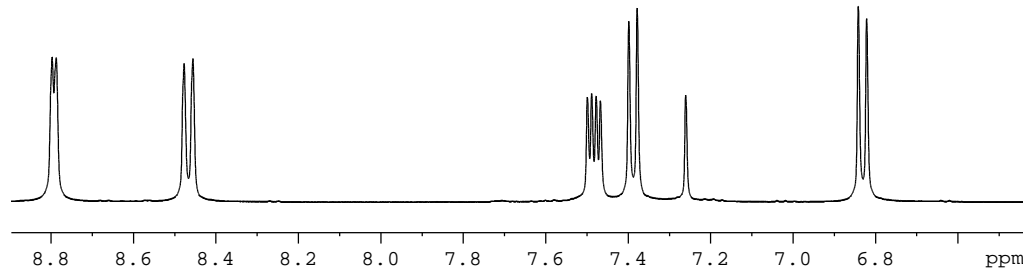
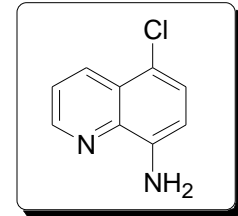
5.0176

8.797
 8.787

8.476
 8.455

7.498
 7.488
 7.477
 7.467
 7.398
 7.378
 7.260

6.841
 6.821

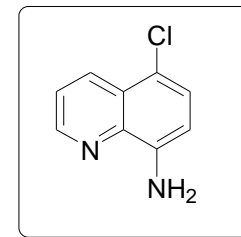


Current Data Parameters
NAME YXL-9-139-1-2-C-20150213
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150213
Time 22.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

— 147.91
— 143.43
— 138.90
— 133.02
— 127.36
— 126.66
— 122.21
— 118.17
— 109.59

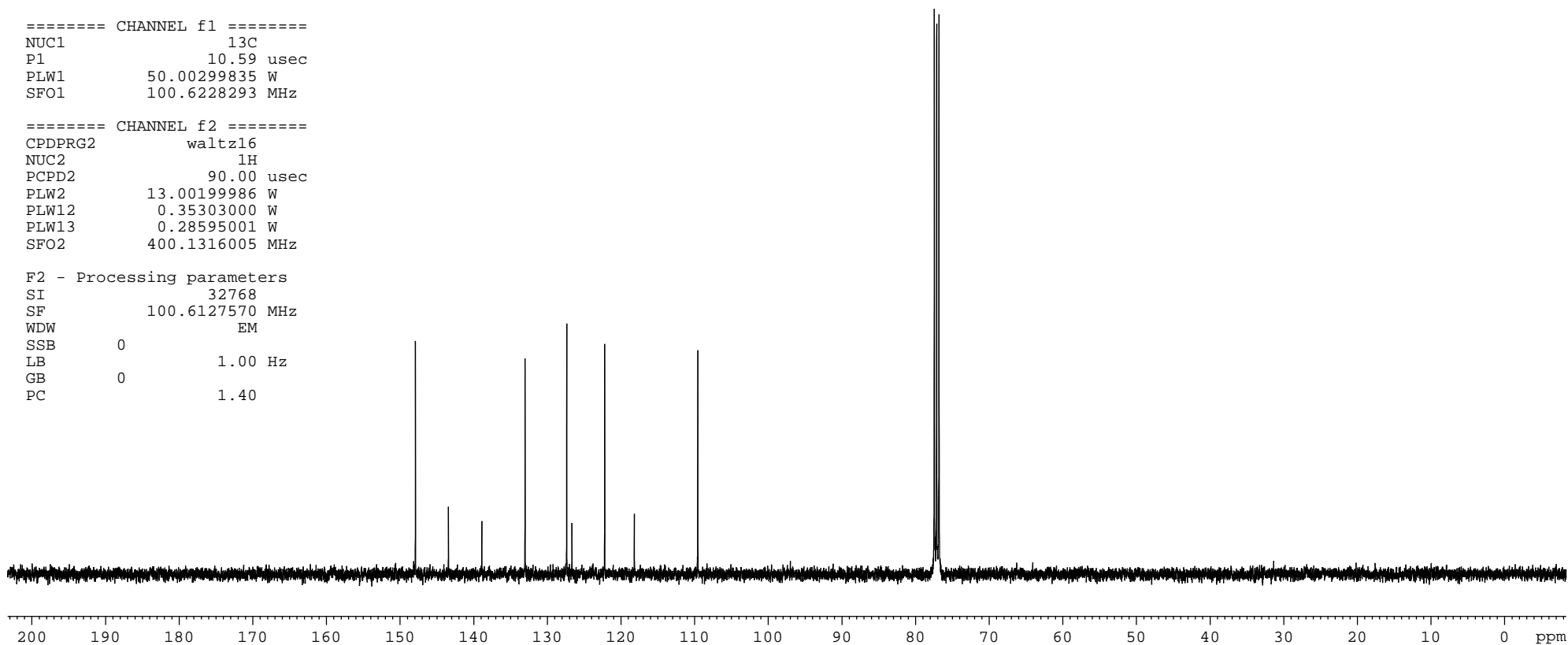
77.47
77.16
76.84



=====
CHANNEL f1
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



10.2827

8.8385
8.8298
8.7690
8.7481
8.5526
8.5316
7.6065
7.5856
7.5616
7.5515
7.5408
7.5306
7.3054
7.2868
7.2690
7.2039
7.1876

5.9842

5.4967

2.9316
2.9146
2.8945
2.8330
2.8132
2.7961

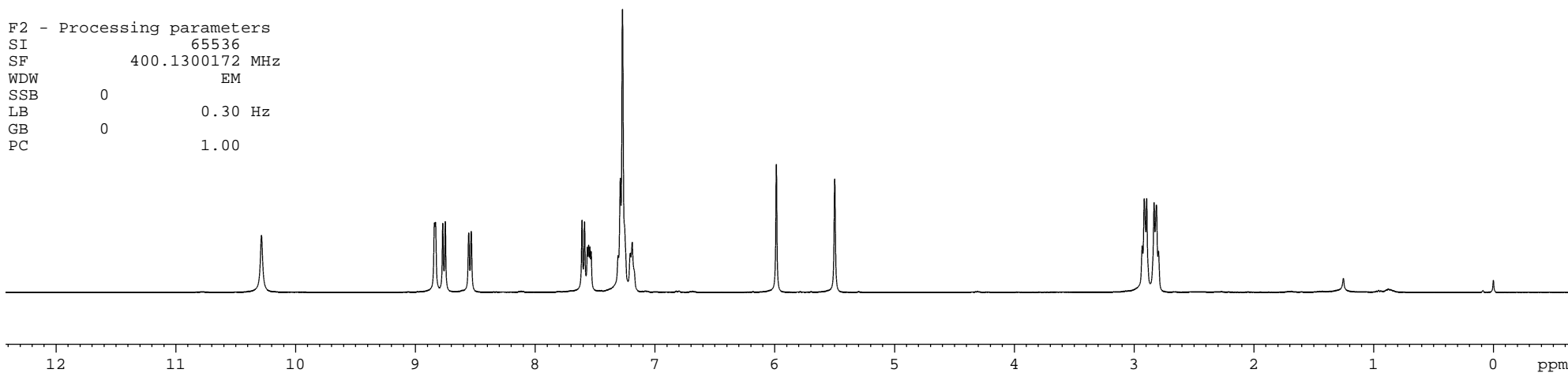
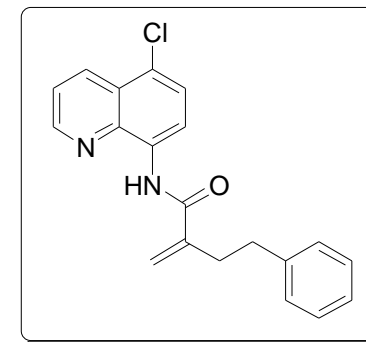
Current Data Parameters
NAME YXL-9-ELIMINATED-20150122
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20150122
Time 9.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 63.51
DW 60.800 usec
DE 6.50 usec
TE 299.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.0019986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300172 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



0.99

1.04
1.00
0.97

2.05
4.21
0.99

1.00

0.99

2.17
2.03

Current Data Parameters
NAME YXL-9-ELIMINATED-C-20150122
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150122
Time 9.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 63
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

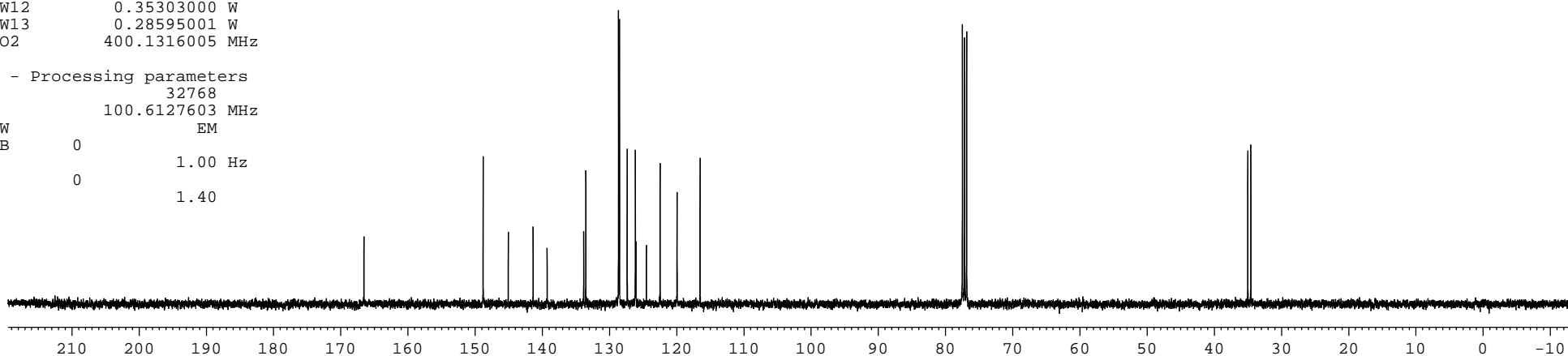
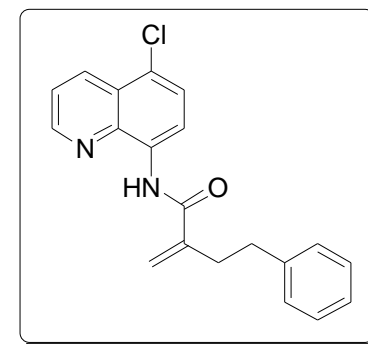
F2 - Processing parameters
SI 32768
SF 100.6127603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

166.53

148.80
145.06
141.36
139.27
133.84
133.52
128.65
128.51
127.36
126.15
126.05
124.51
122.46
119.94
116.51

77.48
77.16
76.84

35.01
34.55



Current Data Parameters
 NAME YXL-9-75-H-20150117
 EXPNO 20
 PROCNO 1

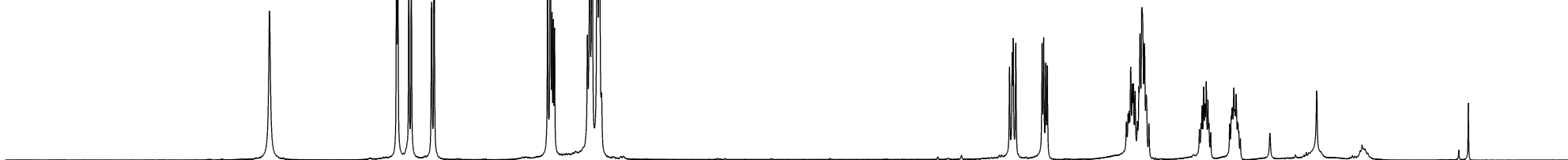
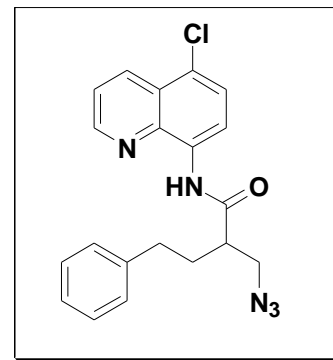
F2 - Acquisition Parameters
 Date_ 20150117
 Time 20.55
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 93.19
 DW 60.800 usec
 DE 6.50 usec
 TE 297.8 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300105 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.9344
 8.8843
 8.8809
 8.8740
 8.8706
 8.7812
 8.7602
 8.5942
 8.5907
 8.5729
 8.5695
 7.6315
 7.6104
 7.6062
 7.5952
 7.5844
 7.5739
 7.3017
 7.2815
 7.2647
 7.2596
 7.2205
 7.2025

3.8082
 3.7863
 3.7780
 3.7561
 3.5386
 3.5255
 3.5083
 3.4953
 2.8402
 2.8262
 2.8173
 2.8048
 2.7916
 2.7828
 2.7688
 2.7495
 2.7366
 2.7276
 2.7126
 2.6917
 2.6757
 2.6538
 2.2361
 2.2220
 2.2136
 2.2004
 2.1885
 2.1790
 2.1653
 2.1568
 2.1427
 1.9848
 1.9723
 1.9663
 1.9622
 1.9502
 1.9437
 1.9385
 1.9317
 1.9199
 1.9157
 1.9098
 1.8971



12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

0.99
 1.02
 1.04
 1.00
 2.10
 5.33
 1.03
 1.00
 3.14
 1.06
 1.02

Current Data Parameters
NAME YXL-9-75-C-20150117
EXPNO 22
PROCNO 1

171.61

148.91
140.86
139.12
133.55
133.48
128.70
128.58
127.32
126.37
126.08
124.88
122.55
116.87

77.48
77.16
76.84

53.45
48.02

33.32
31.99

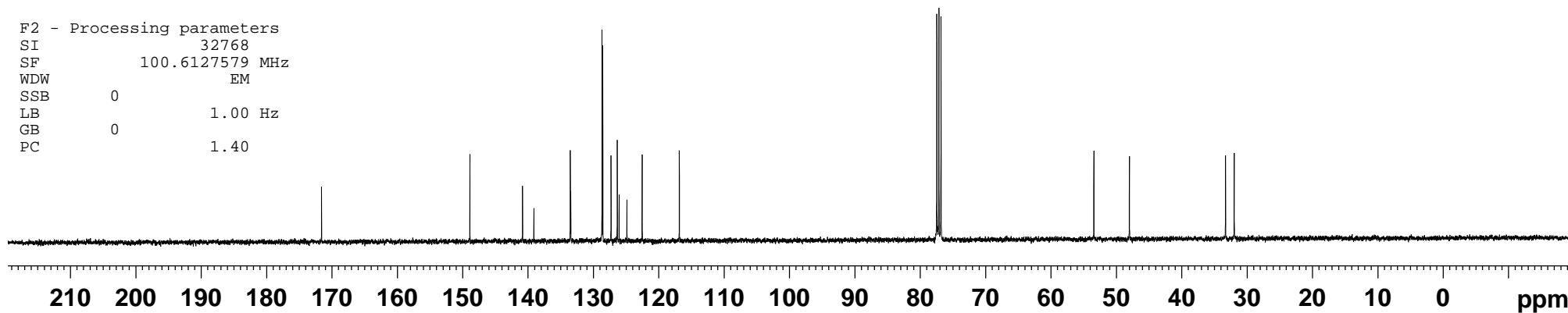
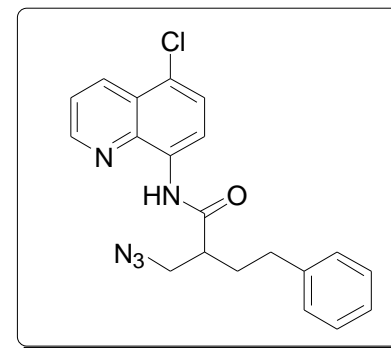
F2 - Acquisition Parameters

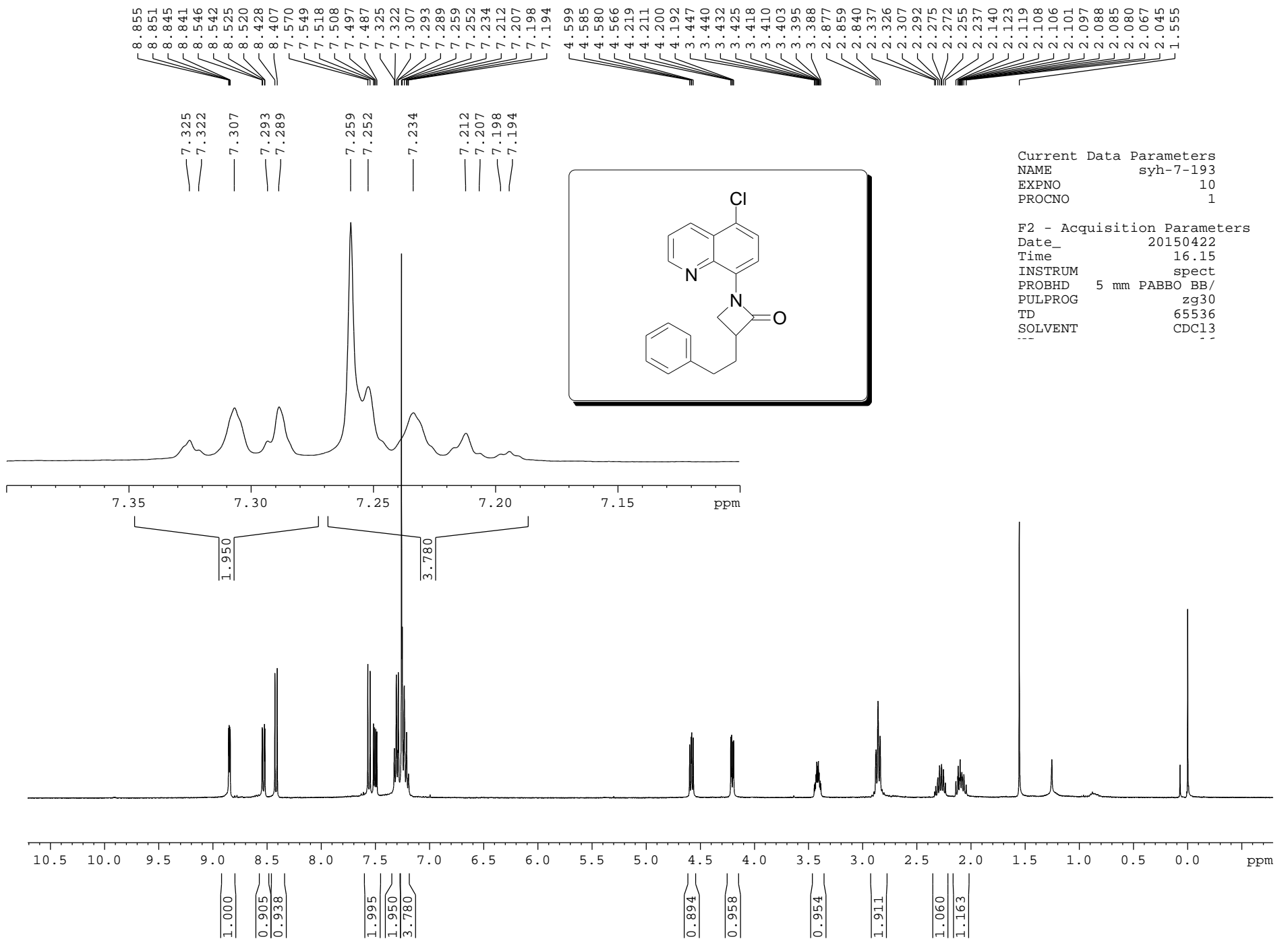
Date_ 20150118
Time 1.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

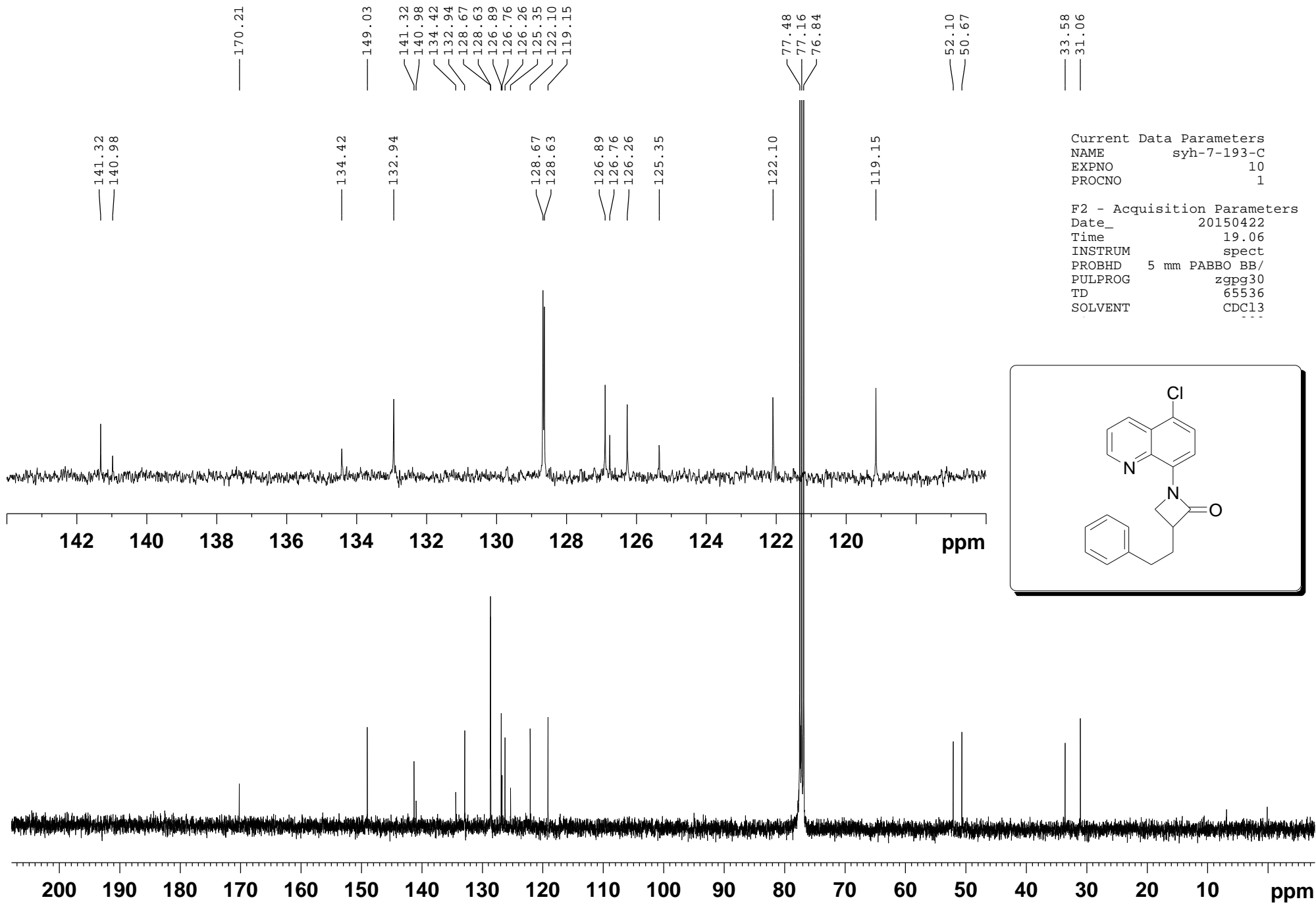
=====
CHANNEL f1
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127579 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

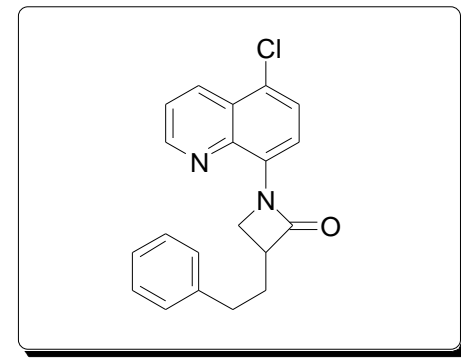






Current Data Parameters
 NAME syh-7-193-C
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150422
 Time 19.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13



Current Data Parameters

NAME 6D-H
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

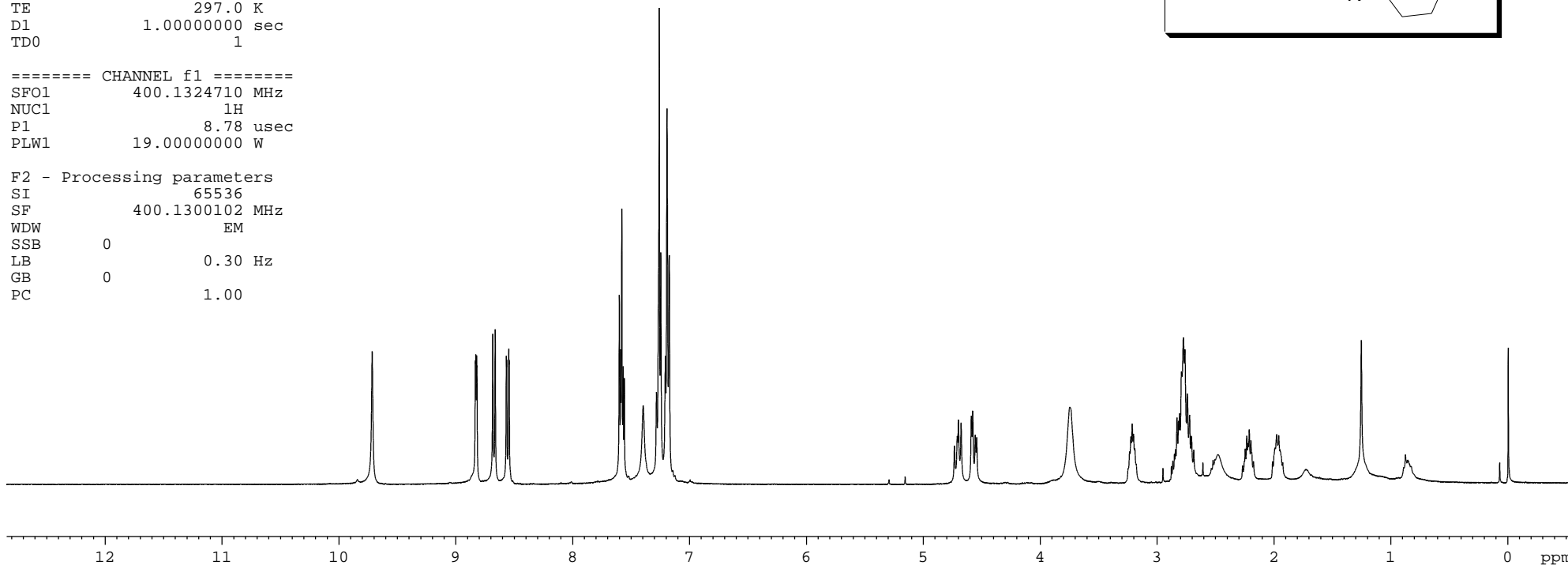
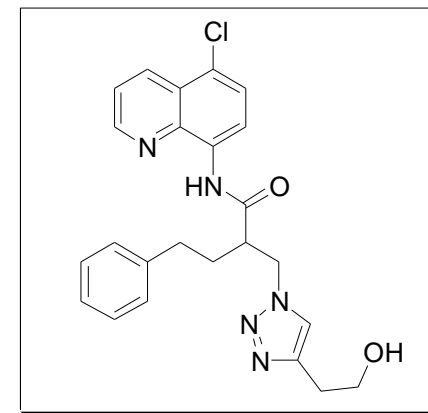
Date_ 20150519
Time 9.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 80.88
DW 62.400 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 8.78 usec
PLW1 19.00000000 W

F2 - Processing parameters

SI 65536
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9.715
8.832
8.829
8.822
8.818
8.683
8.662
8.567
8.564
8.546
8.543
7.600
7.589
7.579
7.568
7.557
7.396
7.282
7.259
7.245
7.205
7.192
7.173
4.733
4.709
4.699
4.676
4.589
4.577
4.555
4.543
3.747
3.235
3.224
3.212
3.201
3.190
2.864
2.850
2.841
2.829
2.816
2.807
2.791
2.774
2.761
2.741
2.721
2.707
2.686
2.607
2.520
2.504
2.480
2.268
2.253
2.245
2.232
2.220
2.211
2.197
2.189
2.175
2.011
1.993
1.988
1.977
1.958



— 171.16
 — 149.04
 140.45
 138.92
 133.52
 133.08
 128.76
 128.54
 127.11
 126.50
 126.04
 125.23
 122.69
 116.73

77.48
 77.16
 76.84

— 61.66

— 51.83
 — 48.99

33.18
 32.38
 — 28.59

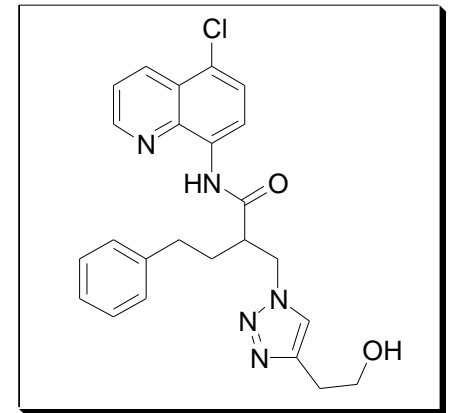
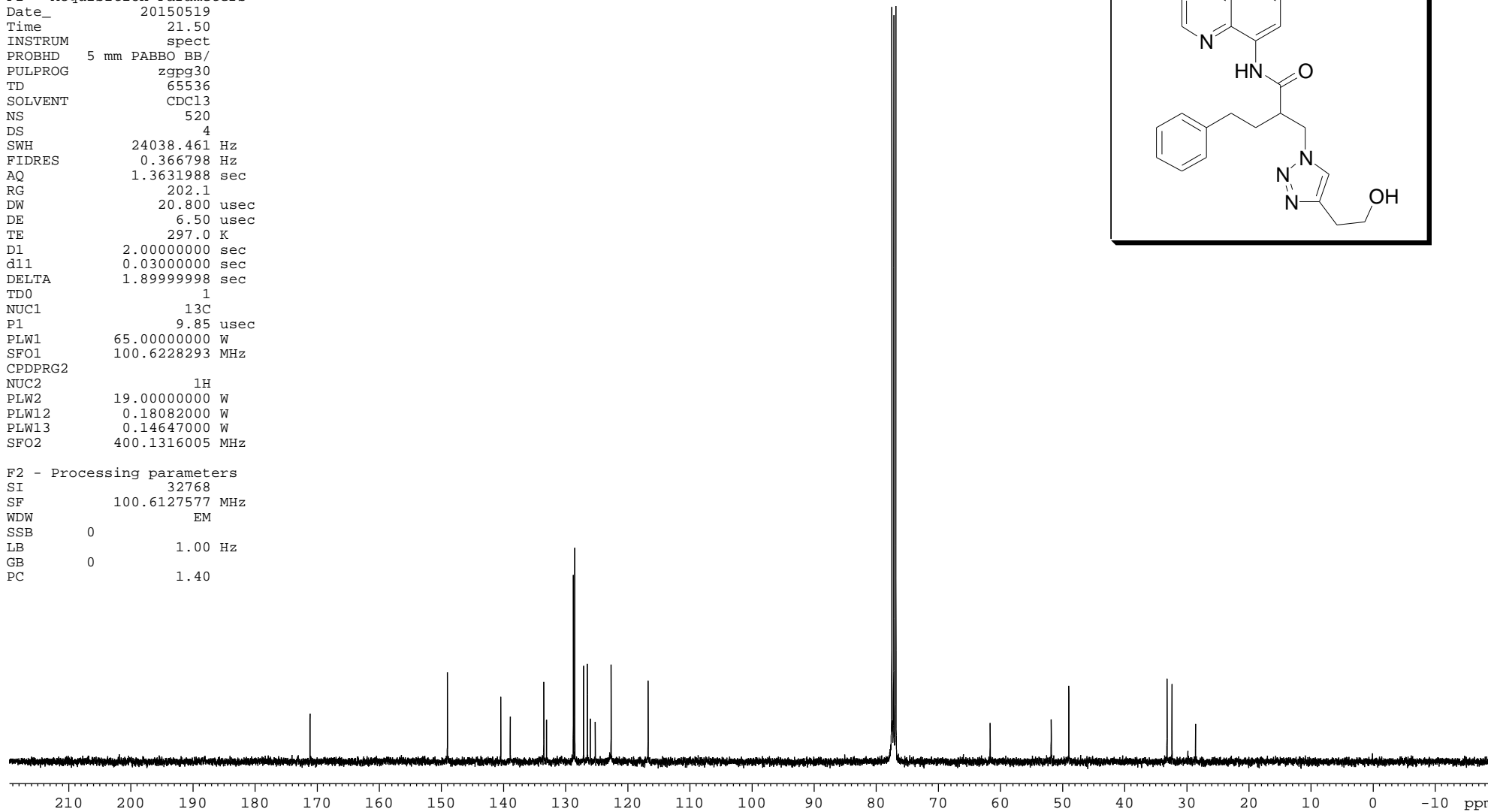
Current Data Parameters
 NAME 6D-C
 EXPNO 10
 PROCNO 1

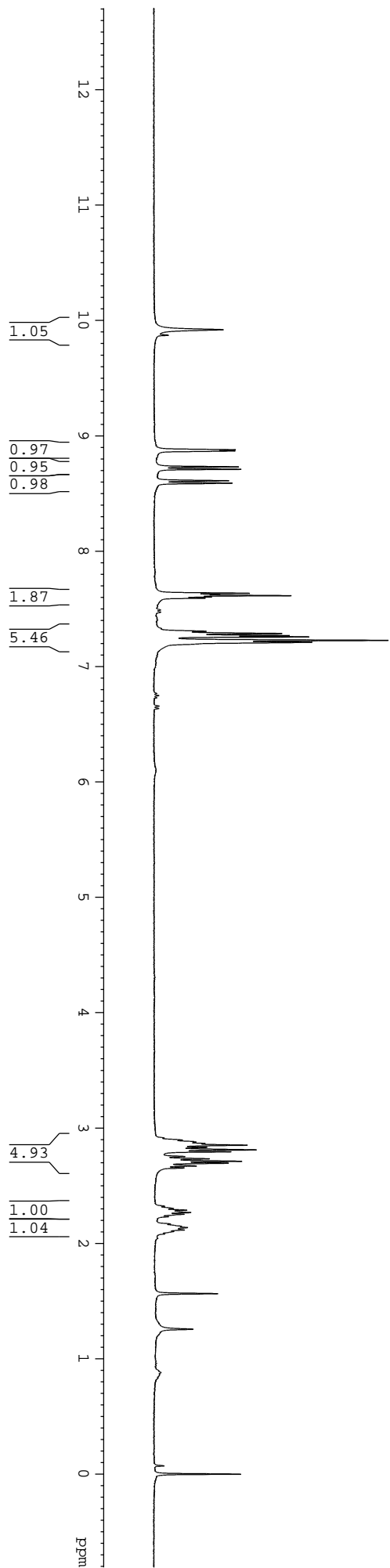
F2 - Acquisition Parameters

Date_ 20150519
 Time 21.50
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 520
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 202.1
 DW 20.800 usec
 DE 6.50 usec
 TE 297.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1
 NUC1 13C
 P1 9.85 usec
 PLW1 65.00000000 W
 SFO1 100.6228293 MHz
 CPDPRG2
 NUC2 1H
 PLW2 19.00000000 W
 PLW12 0.18082000 W
 PLW13 0.14647000 W
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
 SF 100.6127577 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

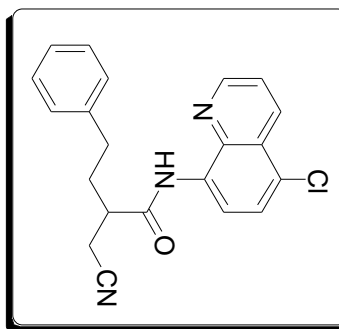




9.9215

8.8809
8.8772
8.8707
8.7324
8.7115
8.6125
8.5912
7.6366
7.6256
7.6157
7.6049
7.5946
7.3076
7.2880
7.2700
7.2581
7.2288
7.2114

2.9154
2.8976
2.8795
2.8674
2.8526
2.8337
2.8119
2.7956
2.7544
2.7347
2.7130
2.6969
2.6718
2.6557
2.3237
2.3036
2.2894
2.2684
2.2539
2.2328
2.1700
2.1503
2.1385
2.1286
2.1174
2.1045
2.0830



Current Data Parameters
NAME YXL-9-93-C-20150122
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150122
Time 19.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 250
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

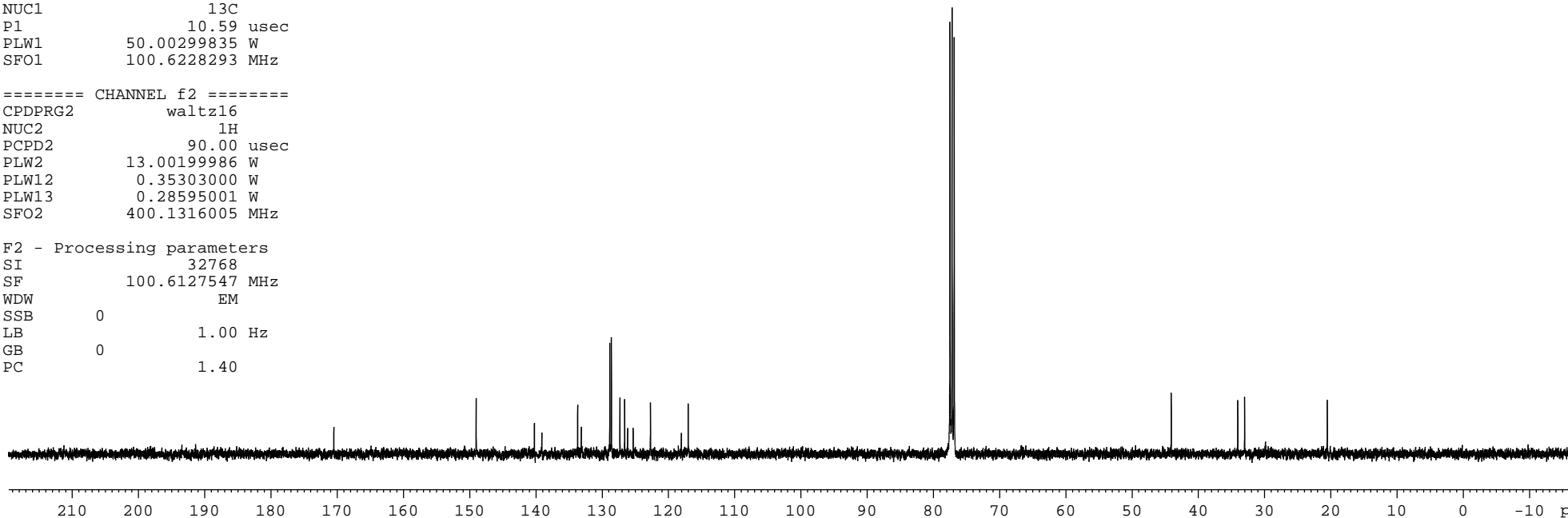
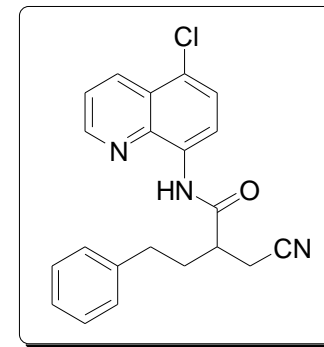
==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127547 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

170.50
149.00
140.21
139.08
133.68
133.13
128.84
128.59
127.30
126.59
126.14
125.30
122.70
118.03
117.00

44.07
34.03
33.00
20.53



Current Data Parameters
 NAME 6F-H
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20150119
 Time 21.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 112.9
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

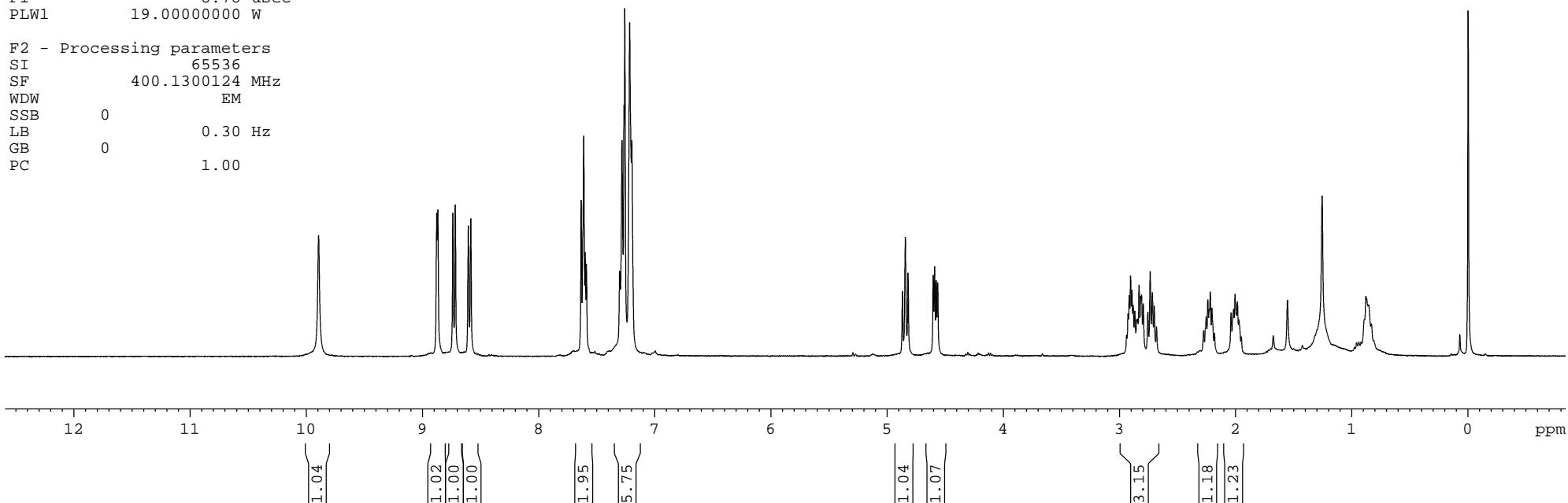
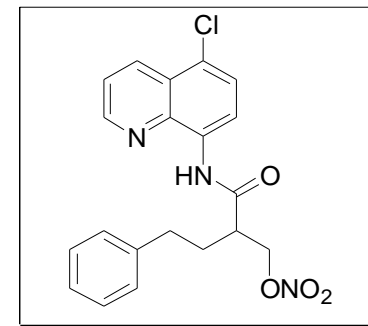
==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 8.78 usec
 PLW1 19.00000000 W

F2 - Processing parameters

SI 65536
 SF 400.1300124 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.894
 8.877
 8.870
 8.867
 8.738
 8.717
 8.604
 8.583
 7.634
 7.611
 7.599
 7.589
 7.302
 7.282
 7.264
 7.258
 7.215
 7.197

4.870
 4.845
 4.822
 4.605
 4.593
 4.579
 4.566
 2.940
 2.927
 2.917
 2.906
 2.894
 2.884
 2.869
 2.853
 2.845
 2.832
 2.818
 2.811
 2.796
 2.757
 2.737
 2.718
 2.702
 2.682
 2.277
 2.255
 2.241
 2.229
 2.219
 2.206
 2.183
 2.041
 2.019
 2.006
 1.985
 1.972
 1.953



Current Data Parameters
NAME YXL-8-81-3-C-150119
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 3.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 750
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

=====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

=====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127560 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

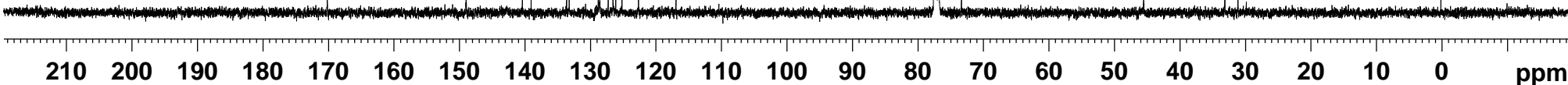
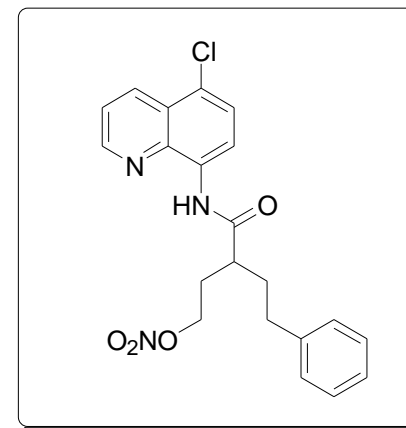
170.17

148.98
140.40
139.06
133.63
133.25
128.80
128.58
127.28
126.55
126.12
125.18
122.65
116.94

77.47
77.15
76.83
73.34

45.53

33.12
31.10



9.9068
 8.8766
 8.8731
 8.8662
 8.8626
 8.7748
 8.7538
 8.6079
 8.6043
 8.5866
 8.5830
 8.0340
 7.6354
 7.6148
 7.6059
 7.5951
 7.5845
 7.2952
 7.2752
 7.2589
 7.2159
 7.1975

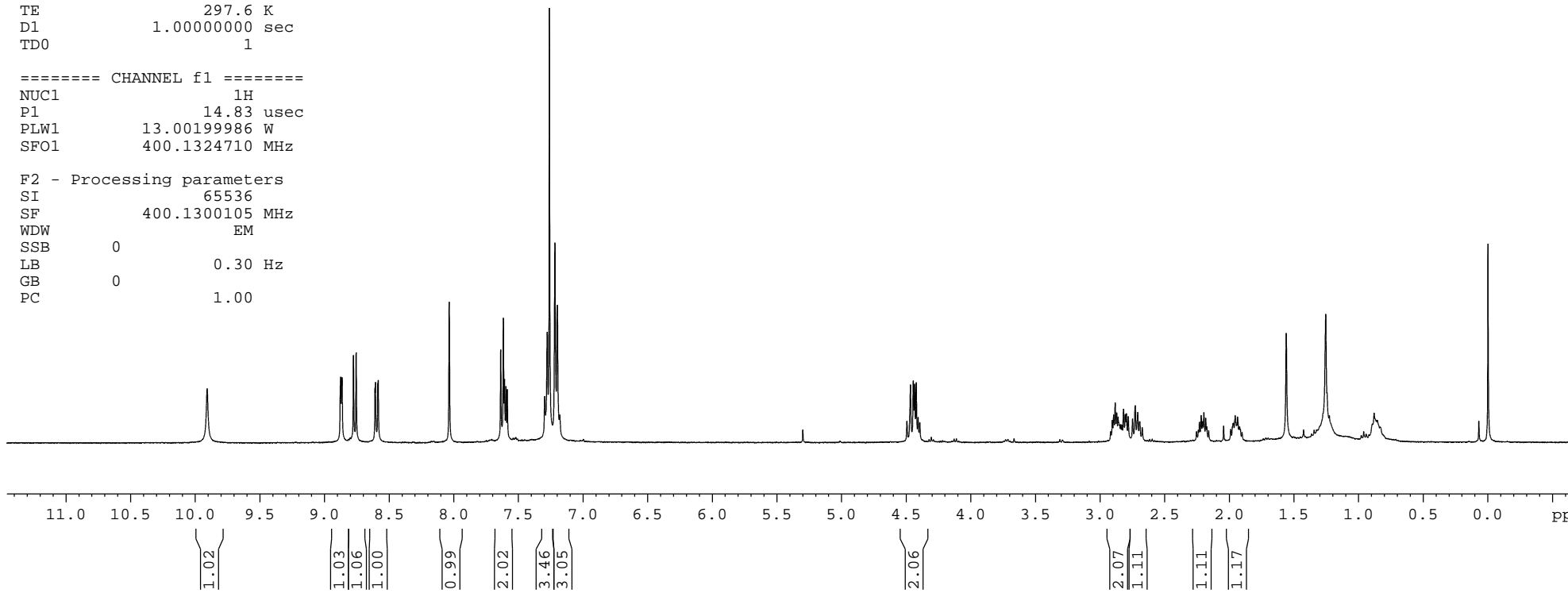
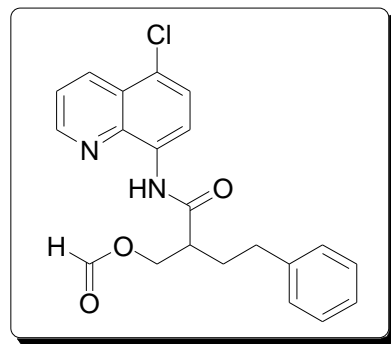
4.4944
 4.4673
 4.4454
 4.4354
 4.4225
 4.4080
 4.3954
 2.9060
 2.8949
 2.8834
 2.8715
 2.8610
 2.8488
 2.8405
 2.8317
 2.8186
 2.8056
 2.7969
 2.7826
 2.7489
 2.7279
 2.7090
 2.6933
 2.2400
 2.2317
 2.2180
 2.2063
 2.1972
 2.1833
 2.1749
 2.1604
 2.0446
 1.9896
 1.9770
 1.9717
 1.9669
 1.9550
 1.9490
 1.9432
 1.9367
 1.9249
 1.9202
 1.9148
 1.5601

Current Data Parameters
 NAME YXL-9-61-H-20150115
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150115
 Time 16.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 209.25
 DW 60.800 usec
 DE 6.50 usec
 TE 297.6 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300105 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
NAME YXL-9-99-1-C-20150123
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150123
Time 13.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 480
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 209.25
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127544 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

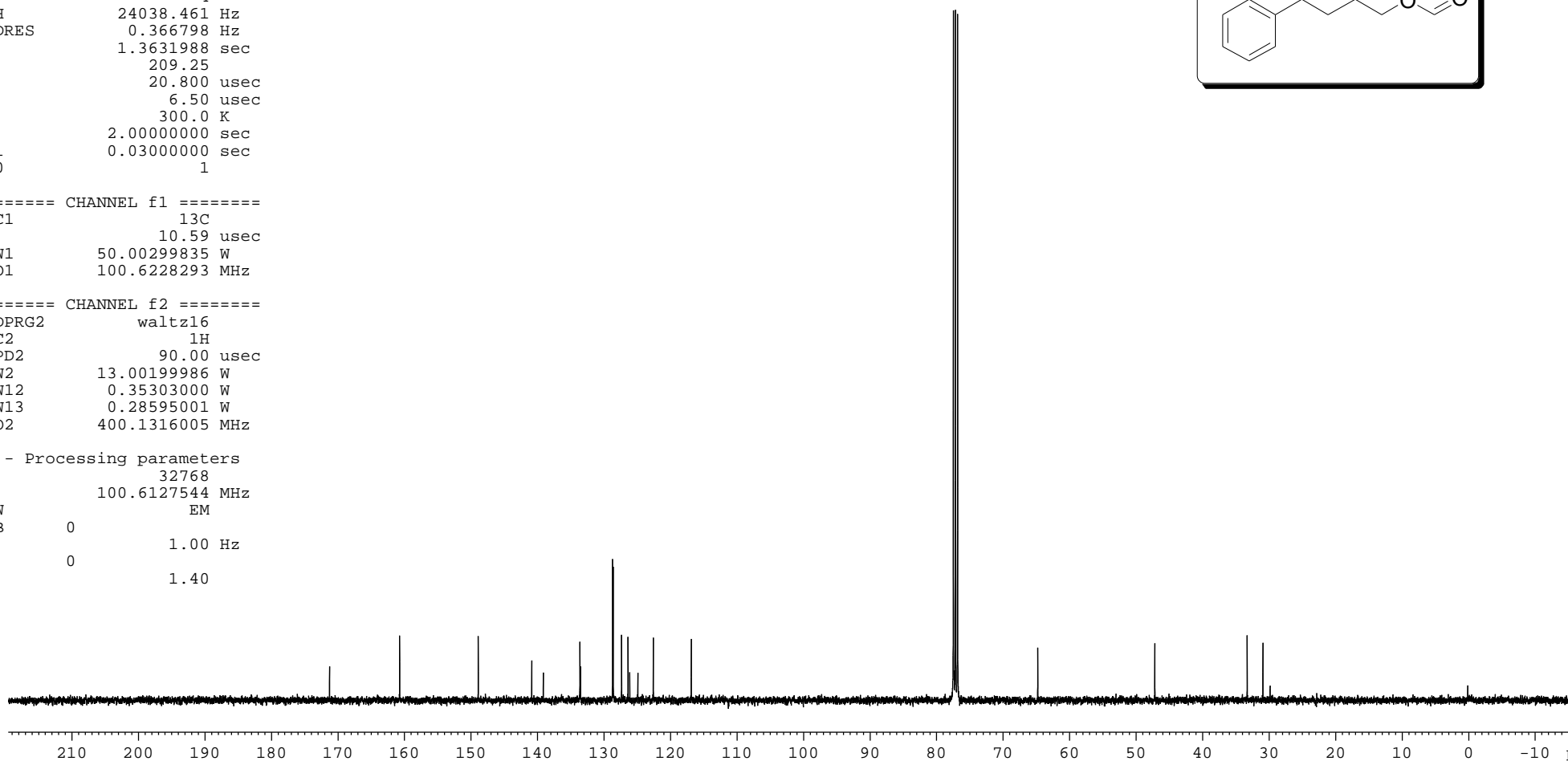
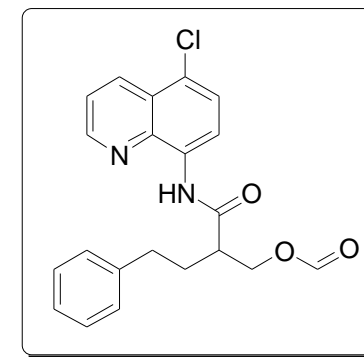
171.27
160.73
148.91
140.86
139.13
133.63
133.53
128.72
128.61
127.36
126.40
126.13
124.91
122.58
116.87

77.48
77.16
76.84

64.80

47.19

33.31
30.93



Current Data Parameters
NAME YXL-9-47-H-20150117
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150117
Time 20.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 115.38
DW 60.800 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1

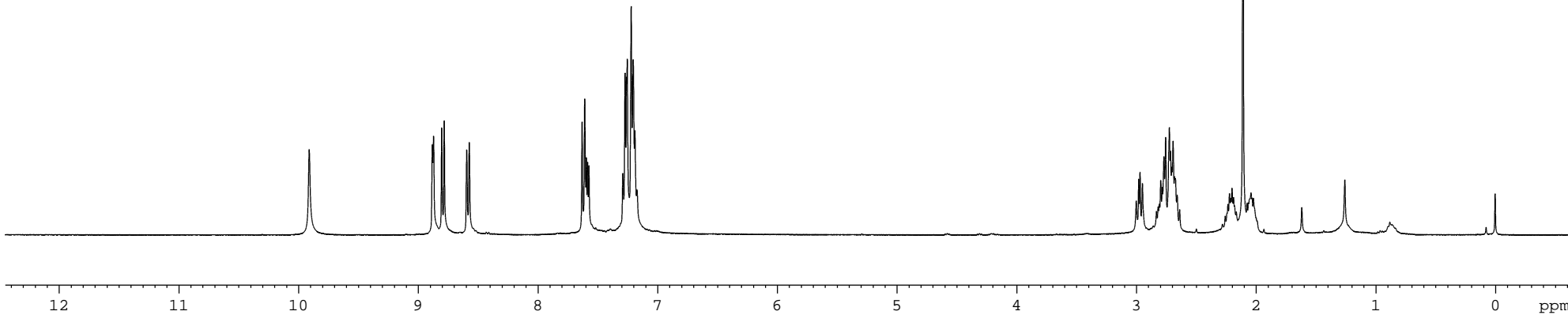
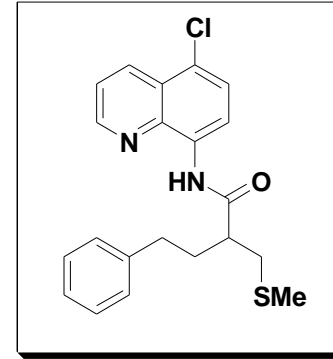
==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9.9100

8.8816
8.8714
8.8033
8.7824
8.5944
8.5732
7.6307
7.6085
7.5950
7.5842
7.5737
7.2901
7.2712
7.2583
7.2531
7.2204
7.2034
7.1888
7.1716

3.0029
2.9825
2.9714
2.9513
2.7984
2.7855
2.7716
2.7574
2.7263
2.7169
2.7061
2.6952
2.6826
2.6756
2.6611
2.2594
2.2371
2.2244
2.2131
2.2028
2.1898
2.1815
2.1671
2.1121
2.0772
2.0655
2.0437
2.0358
2.0243



0.97

2.06

1.03

2.03

5.69

1.09

4.18

1.31

2.82

1.15

ppm

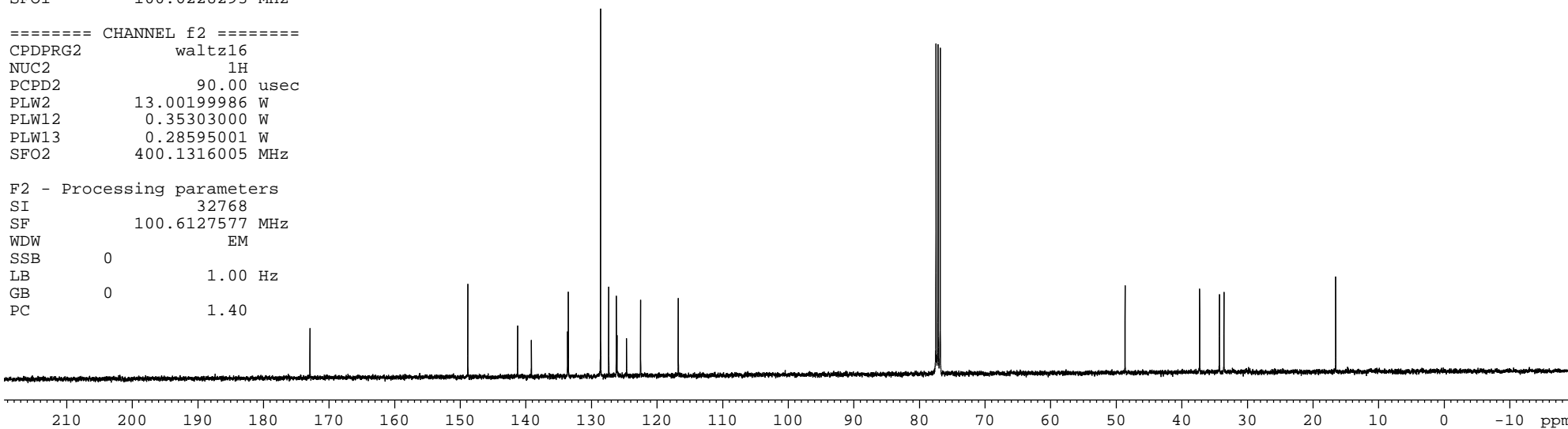
Current Data Parameters
NAME YXL-9-47-C-20150117
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150118
Time 1.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 450
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 184.16
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 10.59 usec
PLW1 50.00299835 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 13.00199986 W
PLW12 0.35303000 W
PLW13 0.28595001 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127577 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



172.91

148.84

141.24

139.16

133.65

133.53

128.60

127.36

126.20

126.09

124.65

122.50

116.76

77.47

77.35

77.15

76.83

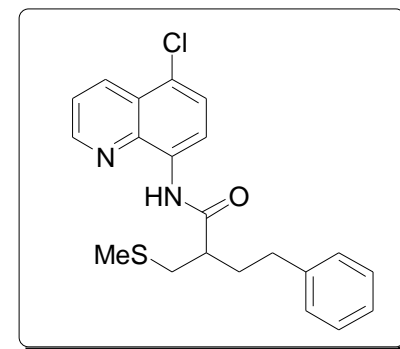
48.64

37.28

34.26

33.57

16.54

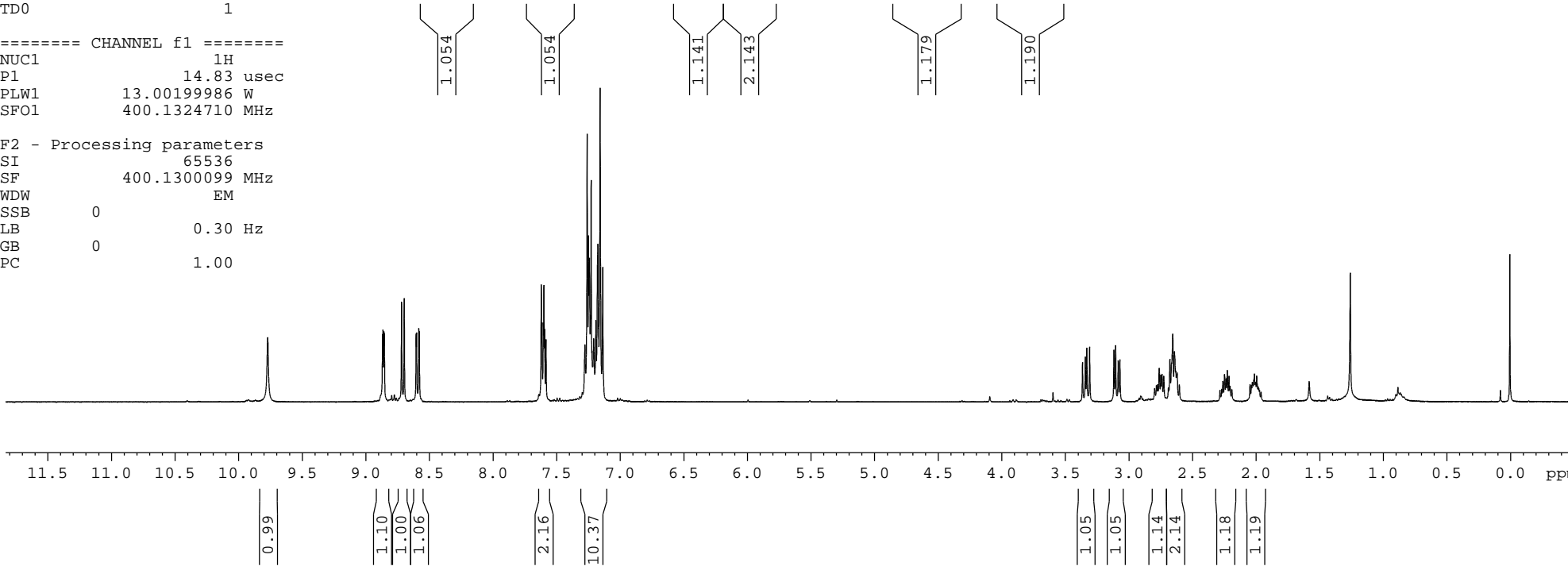
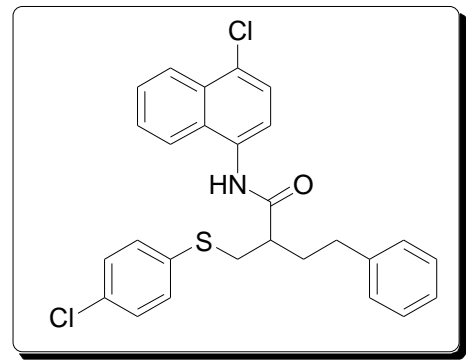
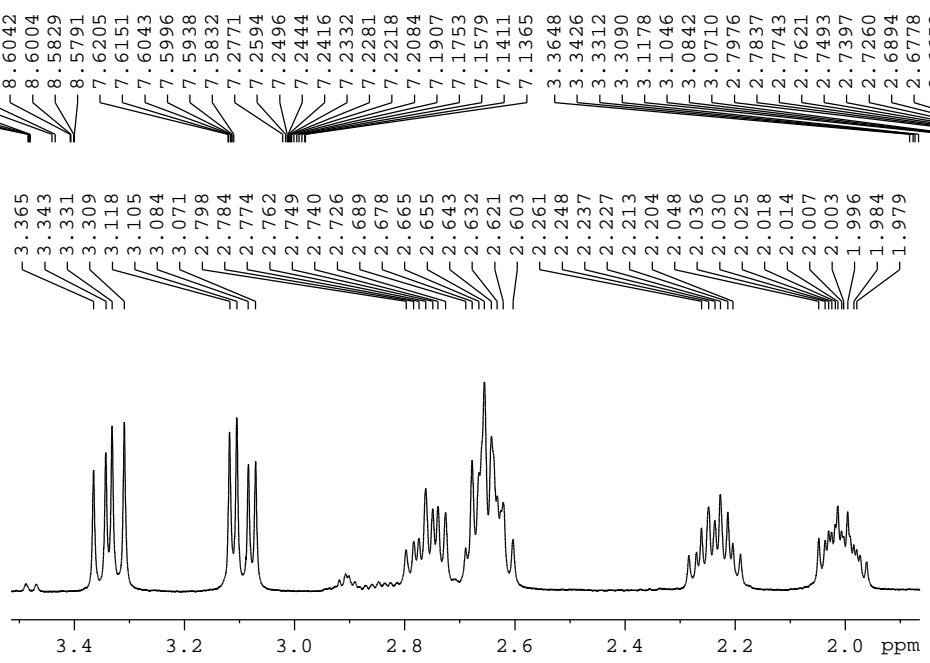


Current Data Parameters
 NAME YXL-9-78-H-20150121
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150121
 Time 9.41
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 130.81
 DW 60.800 usec
 DE 6.50 usec
 TE 299.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300099 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



9.7712
8.8681
8.8644
8.8577
8.8539
8.7186
8.6976
8.6042
8.6004
8.5829
8.5791
7.6205
7.6151
7.6043
7.5996
7.5938
7.5832
7.2771
7.2594
7.2496
7.2444
7.2416
7.2332
7.2281
7.2218
7.2084
7.1907
7.1753
7.1579
7.1411
7.1365
3.3648
3.3426
3.3312
3.3090
3.1178
3.1046
3.0842
3.0710
2.7976
2.7837
2.7743
2.7621
2.7493
2.7397
2.7260
2.6894
2.6778
2.6653
2.6554
2.6426
2.6322
2.6211
2.6035
2.2841
2.2701
2.2612
2.2481
2.2368
2.2269
2.2132
2.2042
2.1903
2.0480
2.0364
2.0301
2.0247
2.0182
2.0136
2.0067
1.9956
1.9845
1.9792

3.365
3.343
3.331
3.309
3.118
3.105
3.084
3.071
2.798
2.784
2.774
2.762
2.749
2.740
2.726
2.689
2.678
2.665
2.655
2.643
2.632
2.621
2.603
2.261
2.248
2.237
2.227
2.213
2.204
2.048
2.036
2.030
2.025
2.018
2.014
2.007
2.003
1.996
1.984
1.979

1.054
1.054
1.141
2.143
1.179
1.190

0.99
1.10
1.00
1.06
2.16
10.37
1.05
1.05
1.14
2.14
1.18
1.19

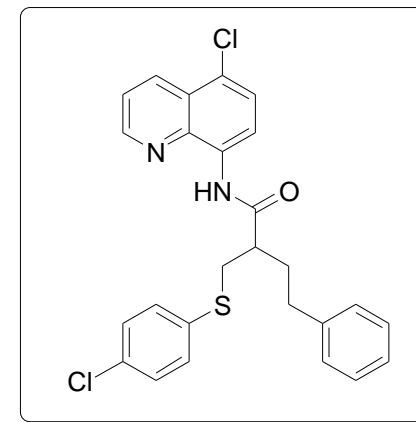
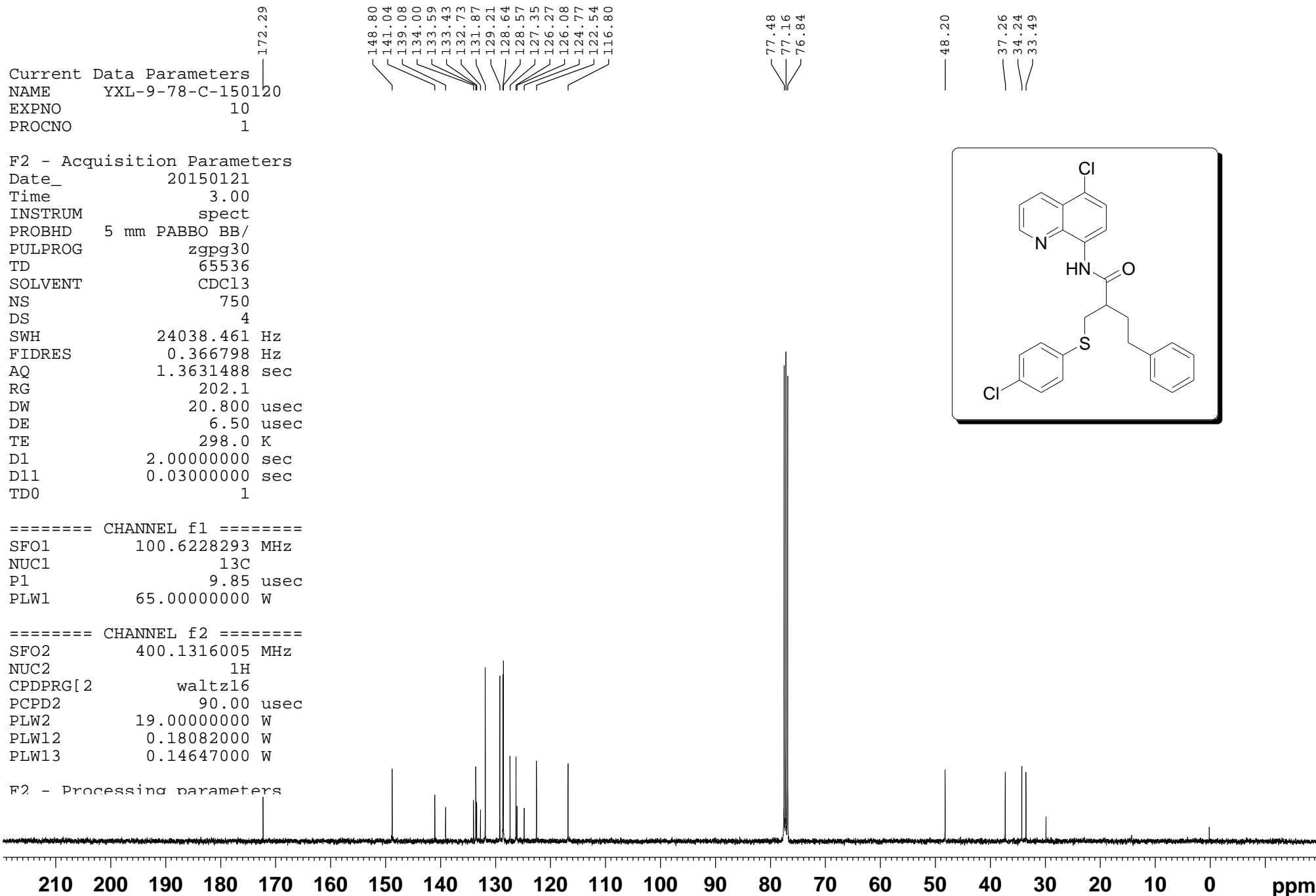
Current Data Parameters
NAME YXL-9-78-C-150120
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150121
Time 3.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 750
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters

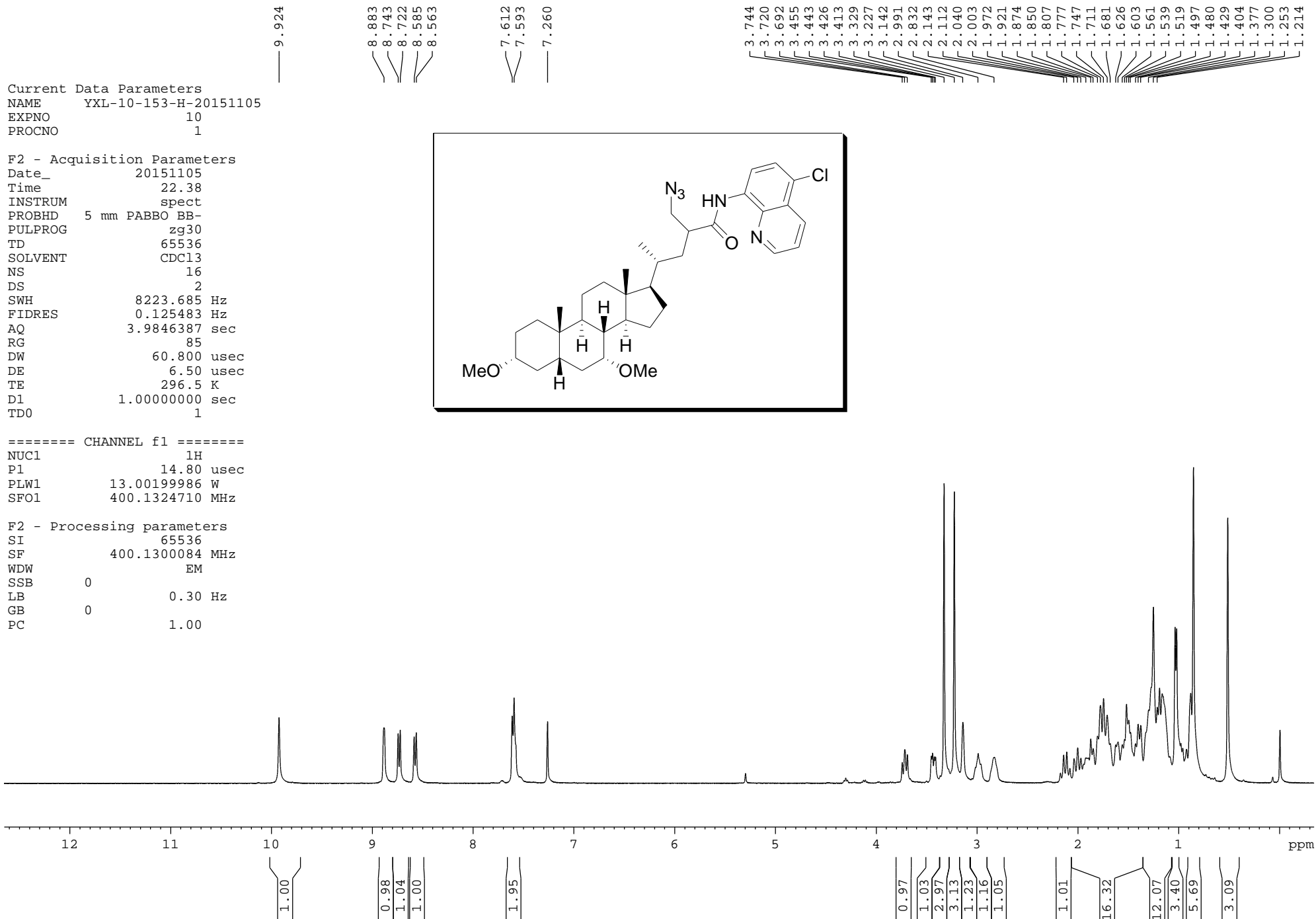
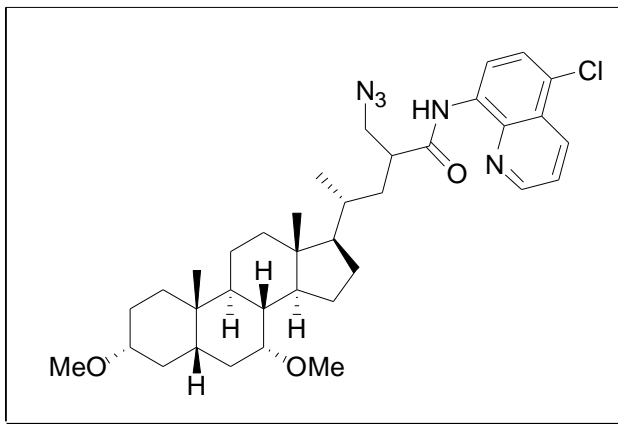


Current Data Parameters
 NAME YXL-10-153-H-20151105
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151105
 Time 22.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 85
 DW 60.800 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.80 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300084 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME YXL-10-153-C-20151105
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20151106
 Time 6.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 450
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 209.25
 DW 20.800 usec
 DE 6.50 usec
 TE 297.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

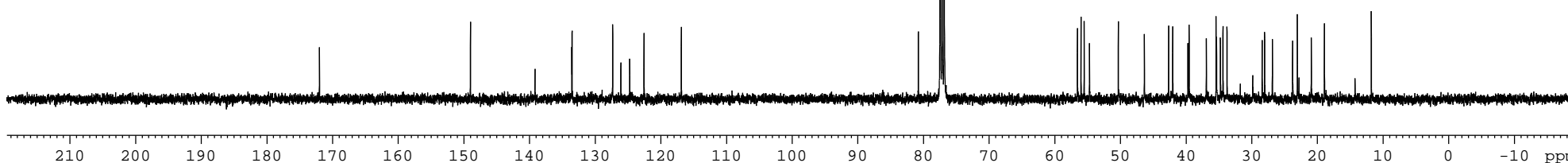
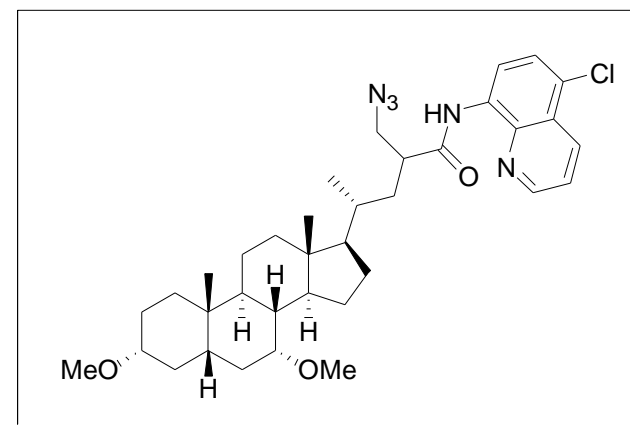
==== CHANNEL f1 =====
 NUC1 13C
 P1 10.90 usec
 PLW1 50.00299835 W
 SFO1 100.6228293 MHz

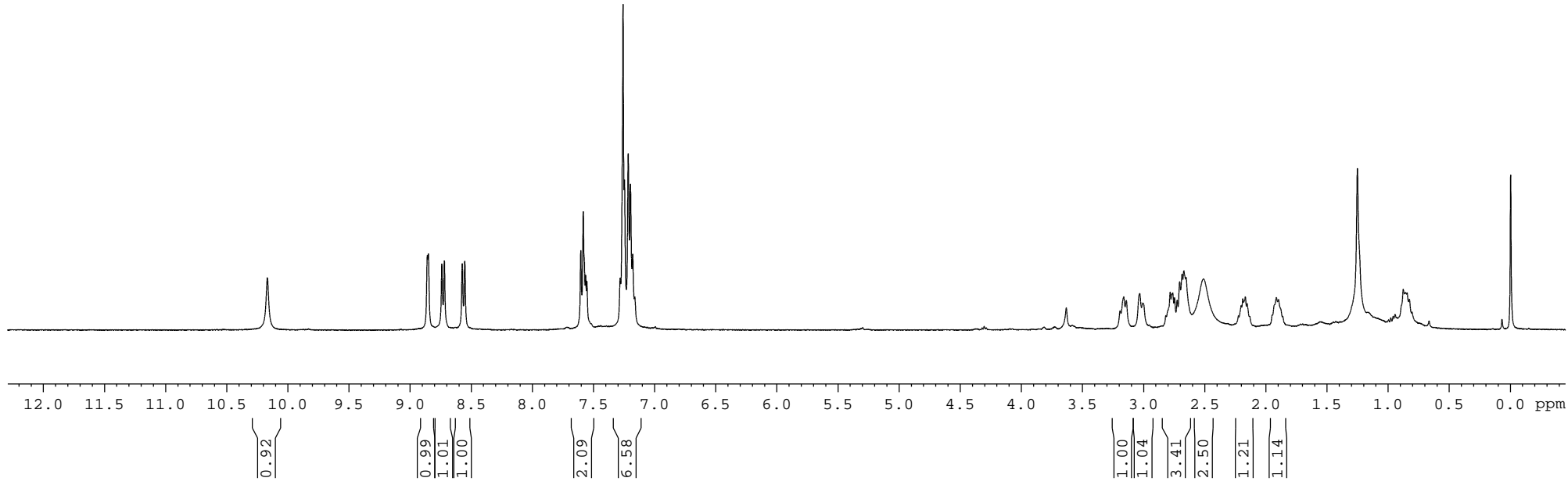
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PLW2 13.00199986 W
 PLW12 0.38069001 W
 PLW13 0.30836001 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127551 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

— 172.00
 — 149.00
 — 139.16
 — 133.56
 — 133.52
 — 127.33
 — 126.09
 — 124.74
 — 122.56
 — 116.88

80.78
 77.48
 77.42
 77.16
 76.84
 56.54
 56.00
 55.52
 54.71
 50.32
 46.35
 42.64
 42.03
 39.71
 39.53
 36.91
 35.43
 35.35
 34.76
 34.37
 33.76
 29.84
 28.40
 28.03
 26.85
 23.77
 23.05
 20.92
 18.92
 14.26
 11.78



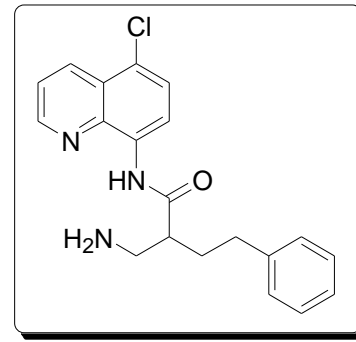


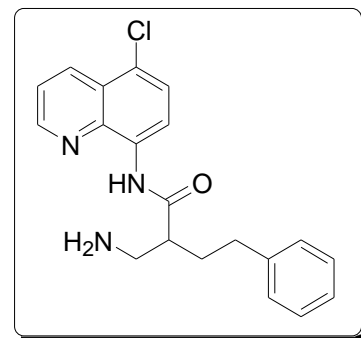
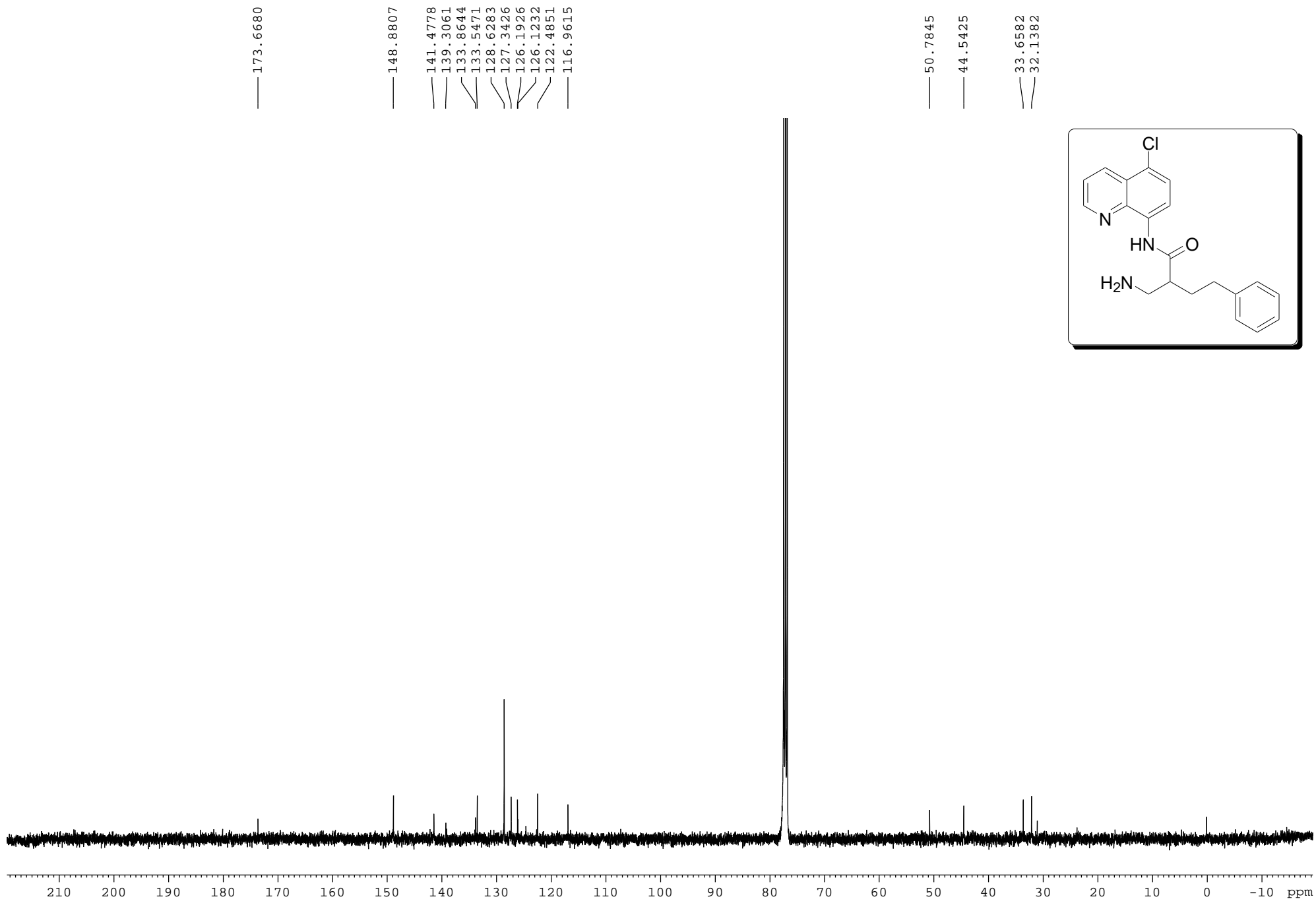
— 10.1699

8.8610
8.8526
8.7423
8.7214
8.5752
8.5543

7.6056
7.5853
7.5657
7.5554
7.2833
7.2596
7.2480
7.2171
7.1990
7.1808

3.1633
3.1419
3.0323
3.0082
2.7832
2.7695
2.7619
2.7480
2.7259
2.7062
2.6858
2.6719
2.6526
2.5088
2.2031
2.1892
2.1684
2.1534
1.9145
1.8970



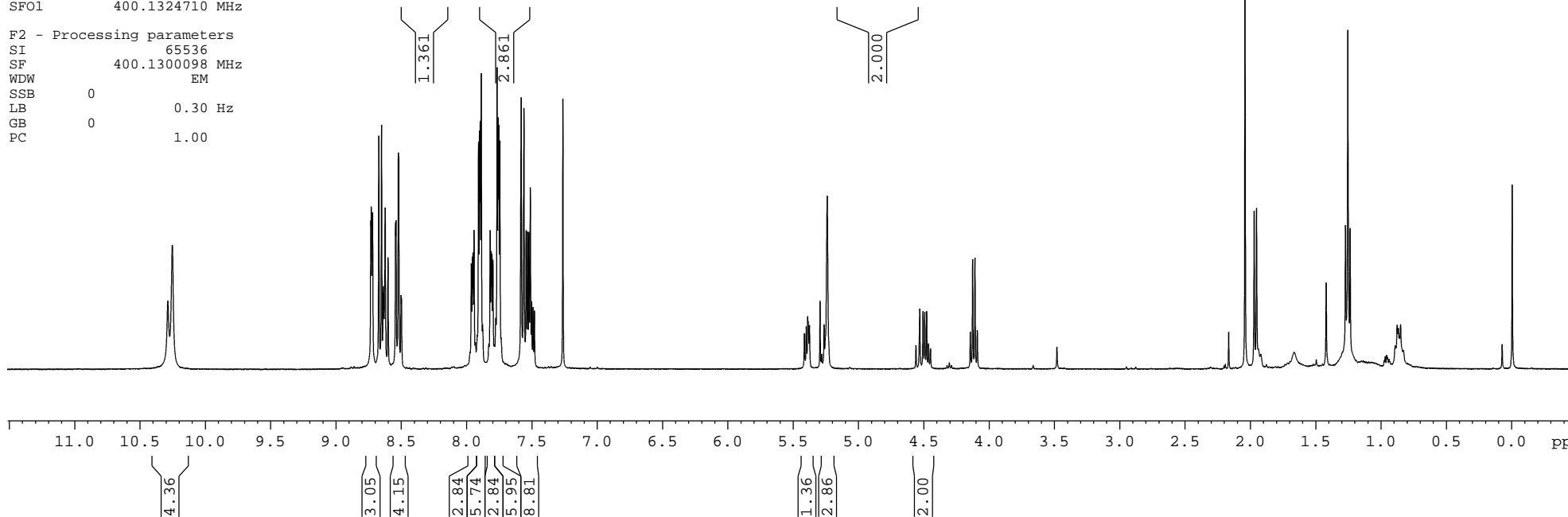
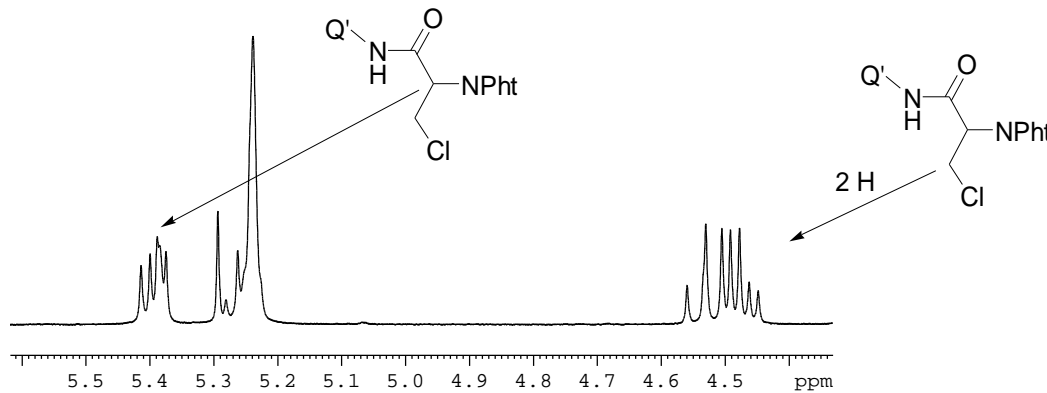
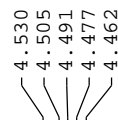
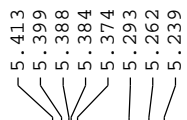
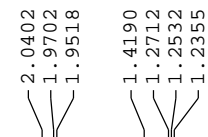
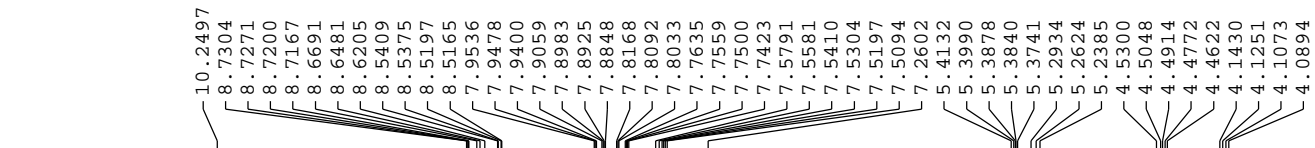


Current Data Parameters
 NAME YXL-8-293-H-20141222
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141222
 Time 21.10
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 144.49
 DW 60.800 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



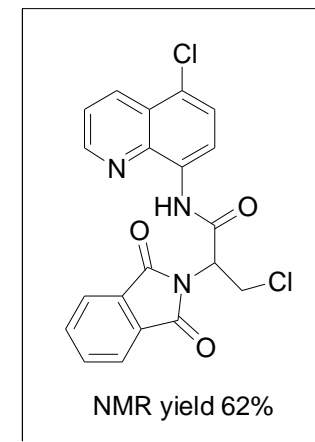
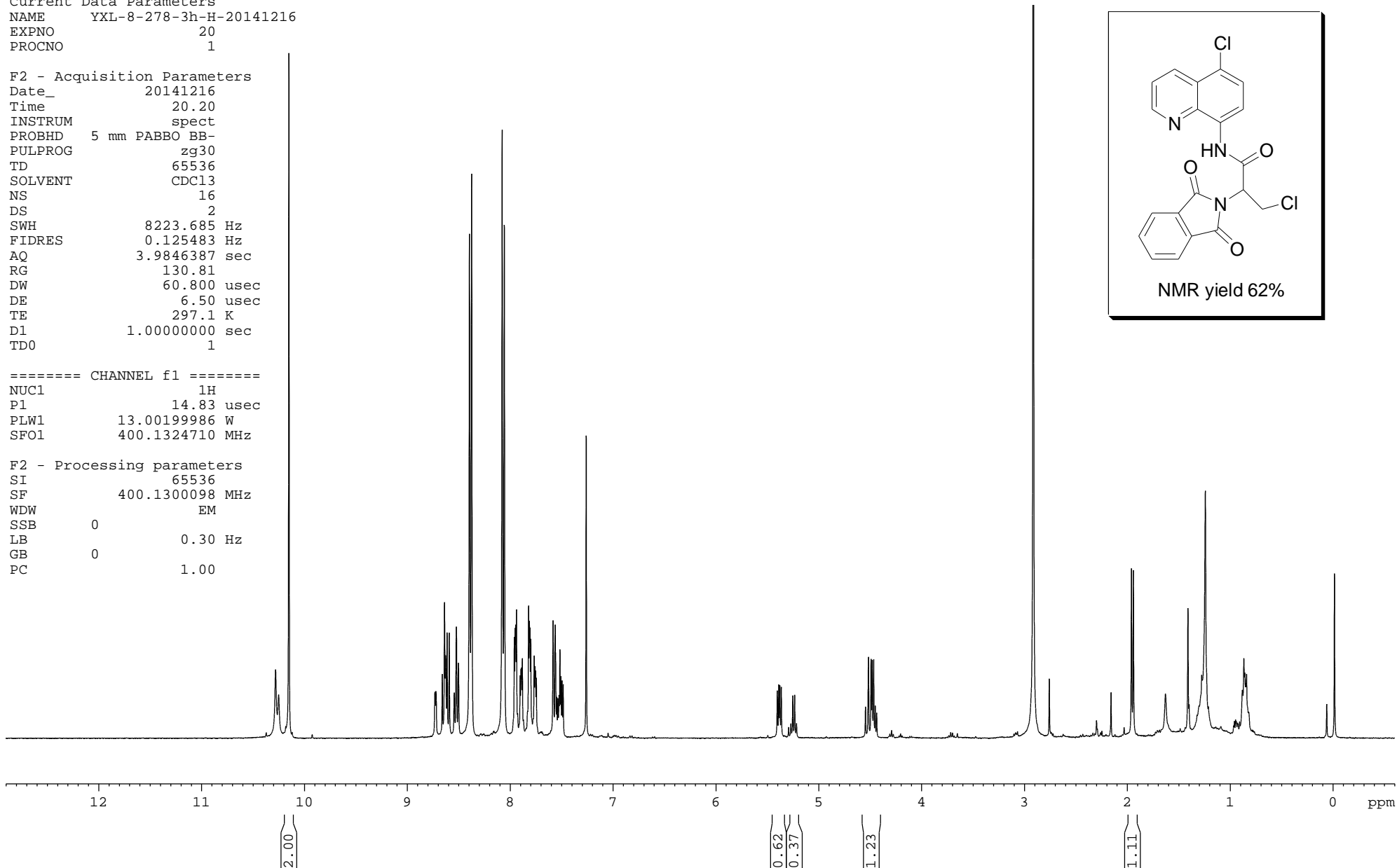
Current Data Parameters
NAME YXL-8-278-3h-H-20141216
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141216
Time 20.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 130.81
DW 60.800 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.83 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

10.281
10.151
8.660
8.638
8.628
8.613
8.592
8.523
8.504
8.396
8.375
8.078
8.057
7.959
7.951
7.946
7.938
7.902
7.895
7.889
7.881
7.821
7.813
7.807
7.800
7.766
7.759
7.753
7.745
7.583
7.562
7.516
7.506
7.495
7.484
7.260
5.403
5.389
5.378
5.364
5.292
5.270
5.252
5.234
5.216
4.547
4.518
4.493
4.482
4.468
4.453
4.439



10.250
 10.154
 8.732
 8.725
 8.667
 8.646
 8.550
 8.547
 8.528
 8.400
 8.378
 8.080
 8.059
 7.942
 7.907
 7.899
 7.893
 7.885
 7.822
 7.768
 7.761
 7.755
 7.747
 7.583
 7.562
 7.549
 7.538
 7.527
 7.517
 7.260

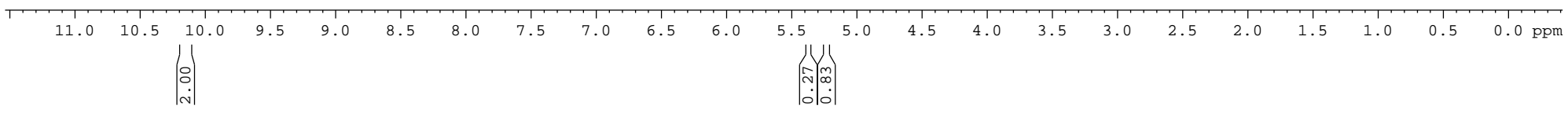
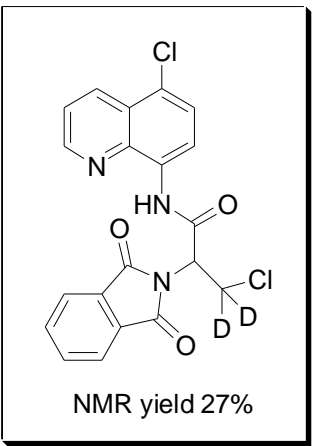
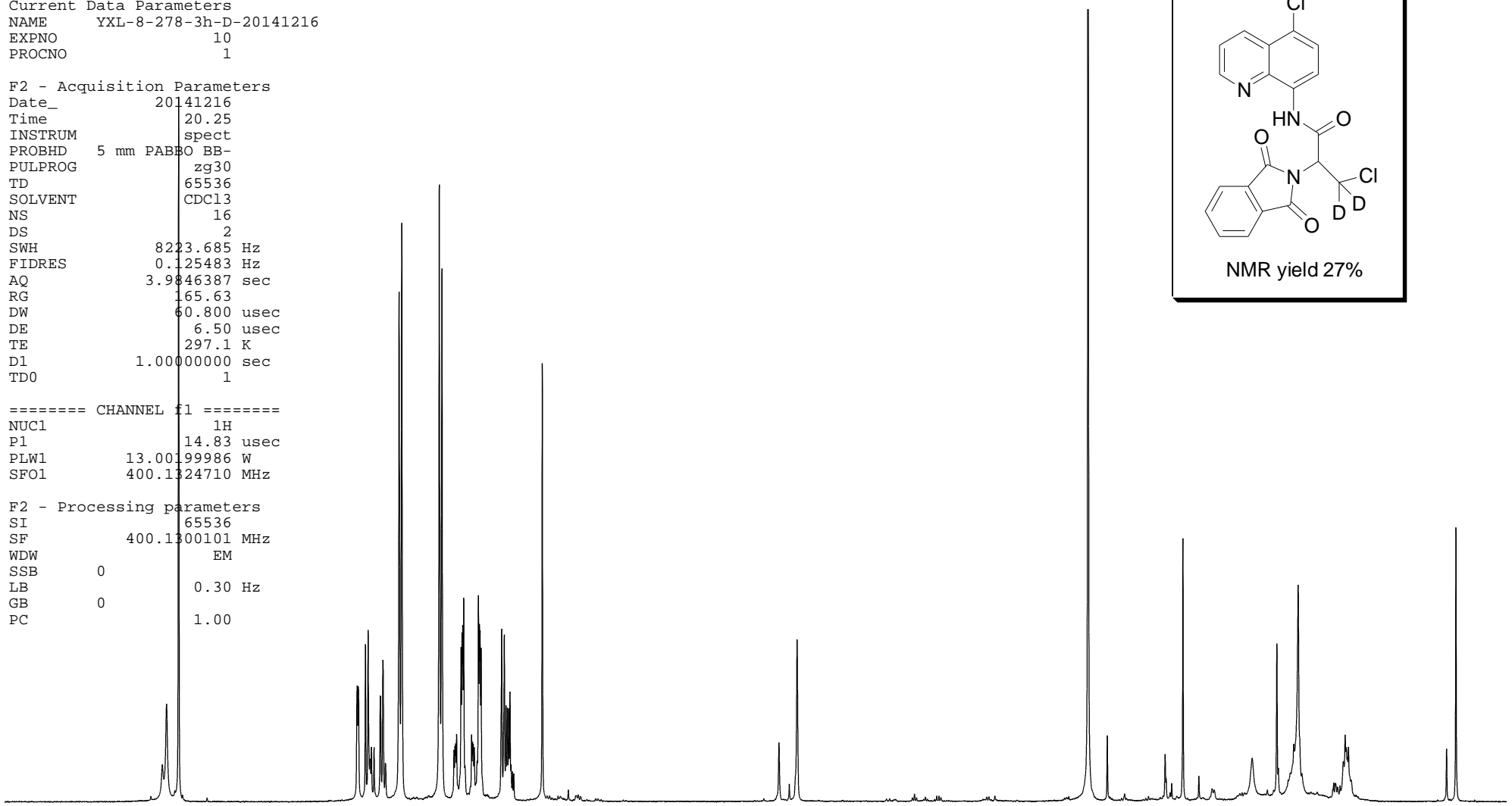
5.377
 5.232

Current Data Parameters
 NAME YXL-8-278-3h-D-20141216
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20141216
 Time 20.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 165.63
 DW 60.800 usec
 DE 6.50 usec
 TE 297.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300101 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Current Data Parameters
 NAME YXL-9-257-H-20150401
 EXPNO 10
 PROCNO 1

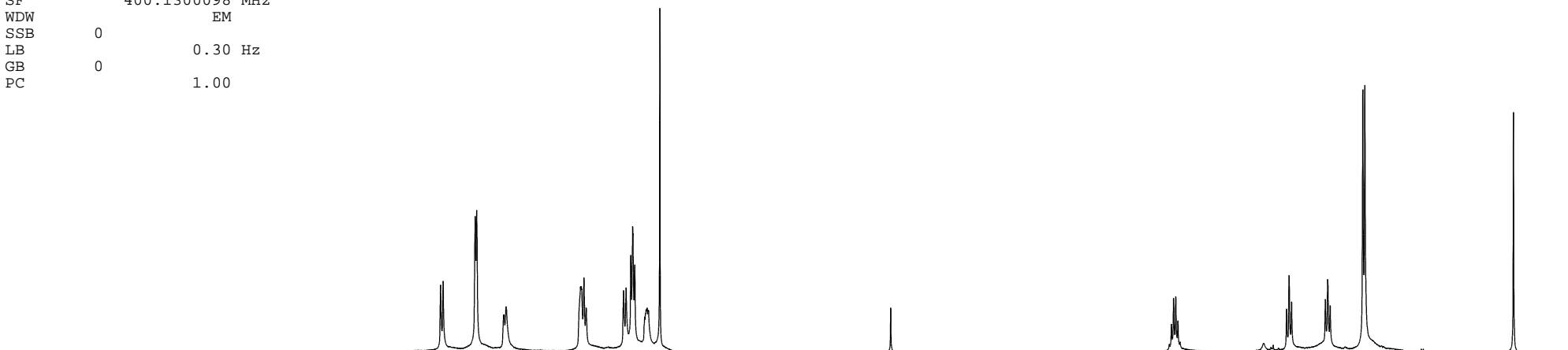
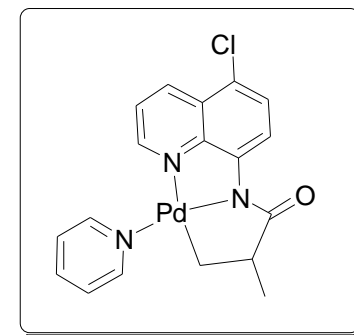
F2 - Acquisition Parameters
 Date_ 20150401
 Time 21.04
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 209.25
 DW 60.800 usec
 DE 6.50 usec
 TE 299.4 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.83 usec
 PLW1 13.00199986 W
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300098 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.1237
 9.1021
 8.8287
 8.8166
 8.5873
 8.5840
 8.5663
 7.9354
 7.9315
 7.9292
 7.9253
 7.9058
 7.8866
 7.5686
 7.5470
 7.5074
 7.4914
 7.4886
 7.4727
 7.3889
 7.3776
 7.3725
 7.3677
 7.3611
 7.3565
 7.2598

2.9070
 2.8885
 2.8699
 2.8513
 1.9266
 1.9059
 1.8842
 1.5969
 1.5776
 1.5557
 1.2784
 1.2607



12

11

10

1.00

2.14

1.04

2.00

2.91

1.14

1.02

1.01

1.18

3.10

0 ppm

— 187.90

— 152.34
— 146.47
— 145.92
— 145.39
— 137.63
— 134.89
— 129.15
— 127.51
— 125.82
— 121.26
— 120.32
— 120.21

— 77.48
— 77.16
— 76.84

— 47.34

— 21.34
— 19.21

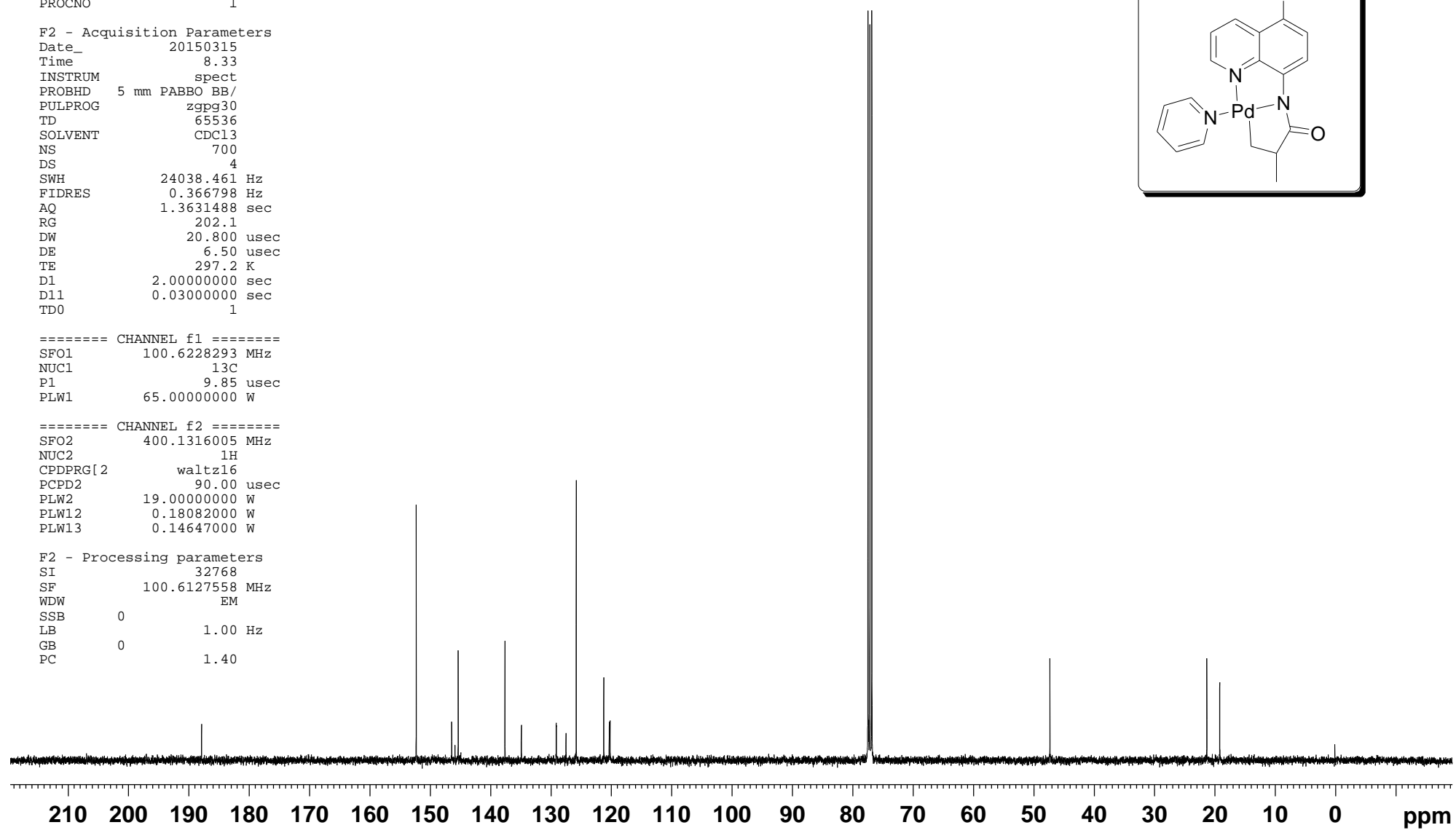
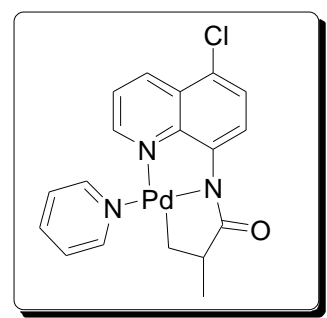
Current Data Parameters
NAME YXL-9-193-S-C-150315
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150315
Time 8.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 700
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 9.85 usec
PLW1 65.00000000 W

==== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 90.00 usec
PLW2 19.00000000 W
PLW12 0.18082000 W
PLW13 0.14647000 W

F2 - Processing parameters
SI 32768
SF 100.6127558 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



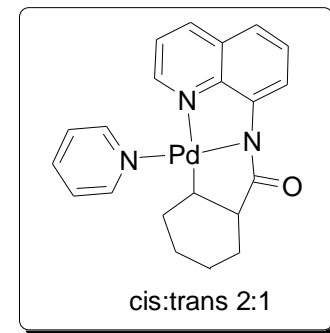
9.1419
9.1221
9.0956
8.9491
8.9369
8.1398
8.1310
8.1221
8.1192
7.9158
7.8966
7.8811
7.8775
7.7712
7.7680
7.7600
7.7568
7.6859
7.6778
7.6745
7.5275
7.5181
7.5075
7.4989
7.4871
7.4841
7.4809
7.4649
7.4492
7.2600
7.2278
7.2158
7.2071
7.1951
7.1840
7.1726
2.9420
2.9283
2.9146
2.9009
2.8587
2.8514
2.6253
2.6130
2.6031
2.5909
2.5783
2.5436
2.5363
2.1427
2.1261
2.1115
1.9621
1.7560
1.7467
1.7338
1.7231
1.7121
1.7008
1.6904
1.6789
1.6617
1.6218
1.6113
1.5973
1.5880
1.5775
1.5635
1.5544
1.5390
1.5103
1.4805
1.4391
1.4321
1.4167
1.3805
1.3638
1.3330
1.3088
1.2880
1.2801
1.2534
1.2355
1.2128
1.2062
1.1906
1.1161
1.0910

Current Data Parameters

NAME YXL-7-149-S-H-20140405
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140405
Time 21.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 184.16
DW 60.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

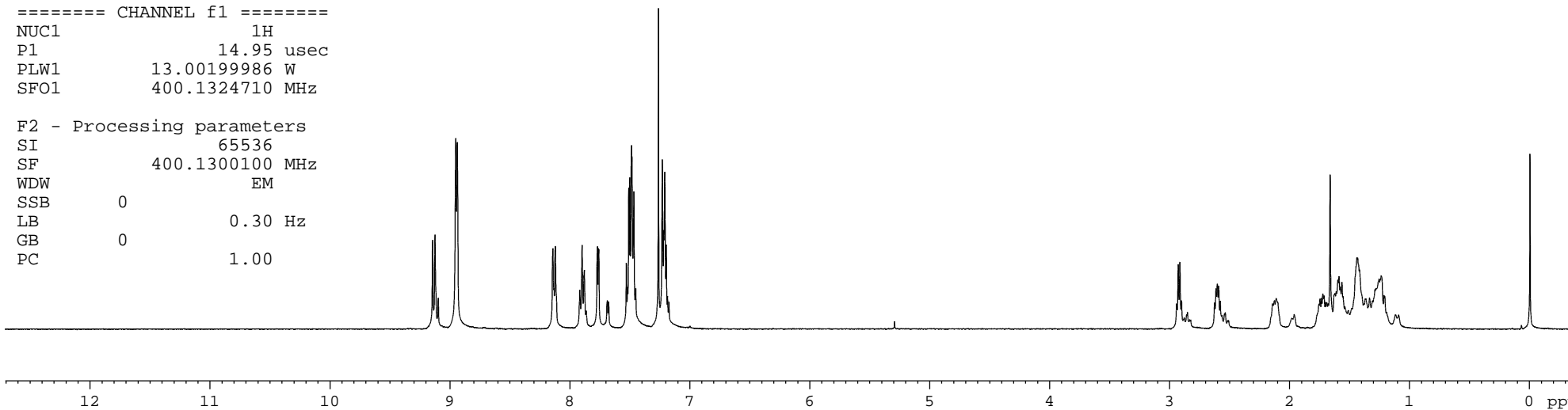


==== CHANNEL f1 =====

NUC1 1H
P1 14.95 usec
PLW1 13.00199986 W
SFO1 400.1324710 MHz

F2 - Processing parameters

SI 65536
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.42
2.93
1.45
1.41
1.08
0.47
4.31
2.94
1.00
0.43
1.03
0.44
1.09
0.49
11.35
0.94

185.76
184.46

152.60
152.35
147.21
145.10
144.91
144.87
137.84
137.79
137.44
130.01
129.94
129.33
125.72
125.64
120.51
120.21
120.17
117.70
117.66

60.15
56.01

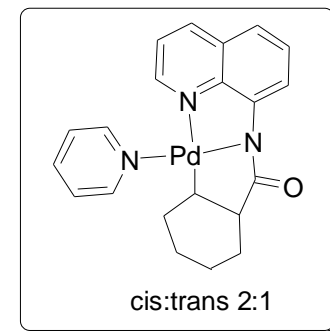
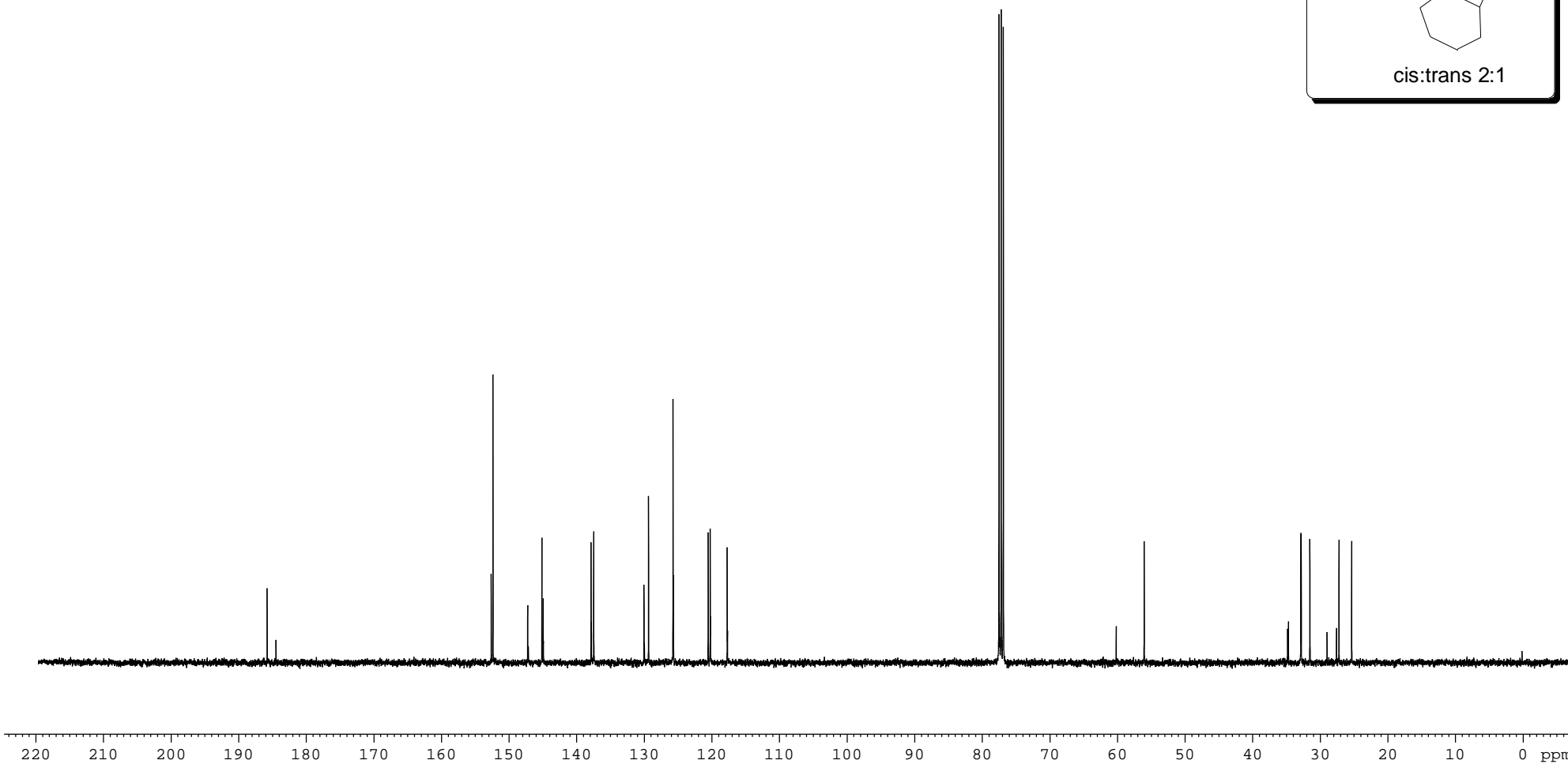
34.80
34.66
32.84
32.77
31.50
28.96
27.56
27.19
25.31

Current Data Parameters

NAME YXL-7-269-S-C-201405

EXPNO 10

PROCNO 1



Current Data Parameters
 NAME YXL-7-142-2-1-H-140401
 EXPNO 20
 PROCNO 1

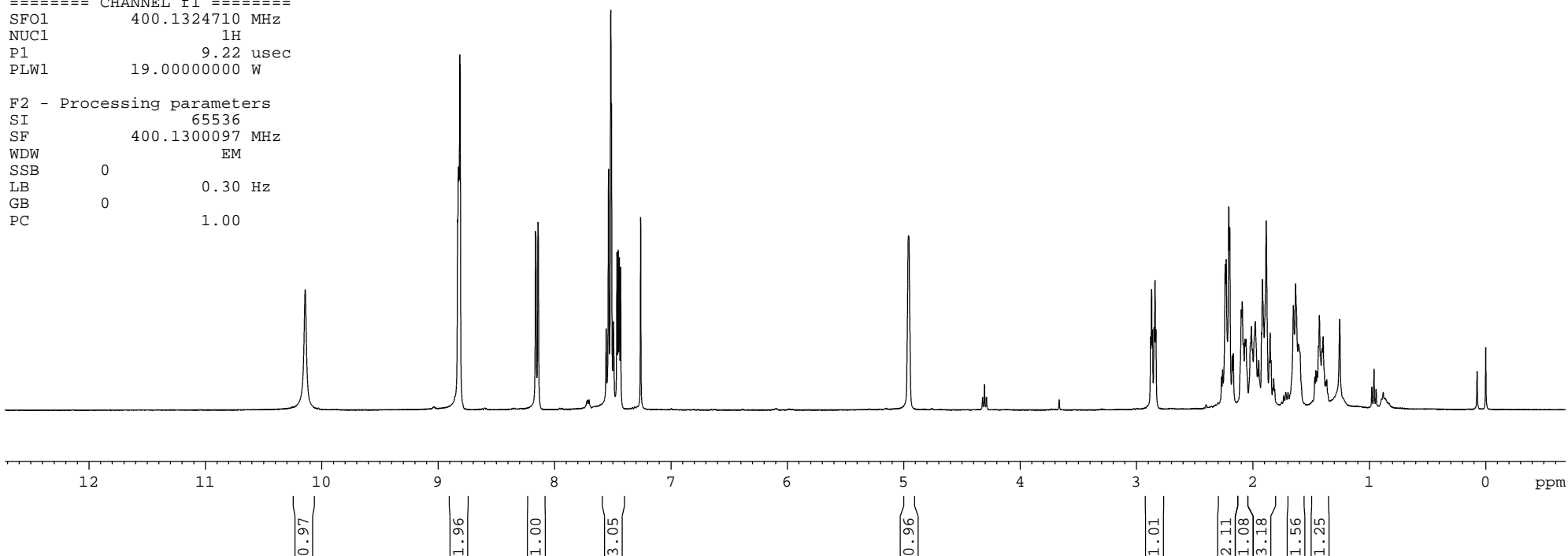
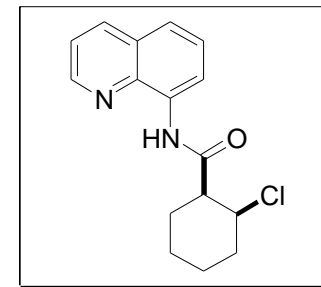
F2 - Acquisition Parameters
 Date_ 20140401
 Time 13.00
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 73.55
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 9.22 usec
 PLW1 19.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300097 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10.142
 8.832
 8.824
 8.820
 8.814
 8.811
 8.163
 8.160
 8.142
 7.536
 7.517
 7.511
 7.494
 7.463
 7.453
 7.443
 7.432
 7.260

4.956
 2.878
 2.870
 2.862
 2.849
 2.841
 2.833
 2.269
 2.260
 2.237
 2.229
 2.207
 2.199
 2.177
 2.168
 2.099
 2.091
 2.081
 2.068
 2.059
 2.020
 2.012
 2.003
 1.979
 1.957
 1.949
 1.925
 1.918
 1.886
 1.859
 1.852
 1.844
 1.829
 1.821
 1.812
 1.718
 1.698
 1.651
 1.633
 1.608
 1.468



— 171.91

— 148.33

— 138.56

— 136.52

— 134.44

— 128.08

— 127.56

— 121.84

— 121.76

— 116.88

— 77.48

— 77.37

— 77.16

— 76.85

— 60.25

— 56.42

— 36.59

— 30.86

— 26.00

— 24.63

Current Data Parameters

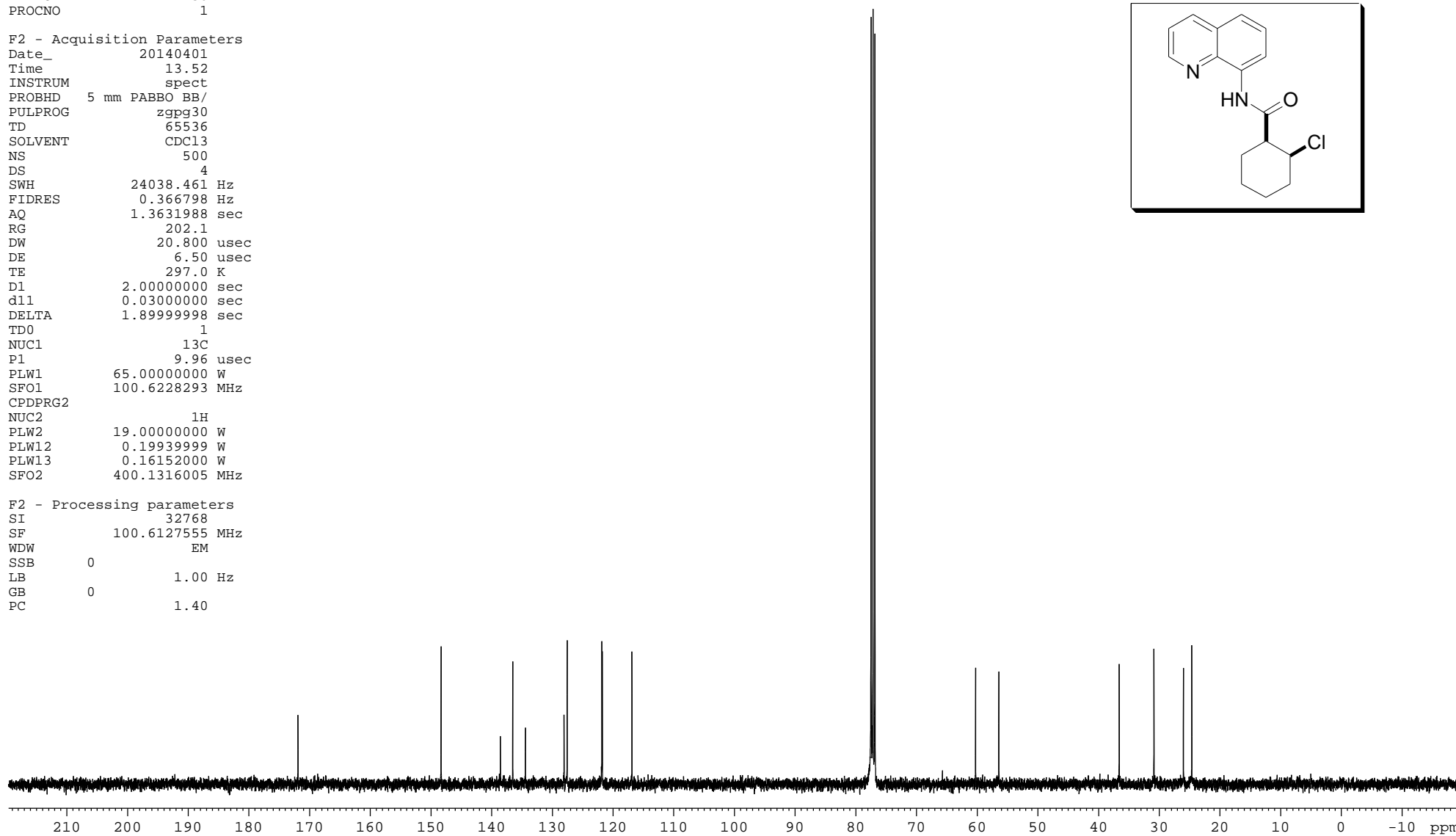
NAME YXL-7-142-2-1-c-140401
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters

Date_ 20140401
Time 13.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 202.1
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
NUC1 13C
P1 9.96 usec
PLW1 65.00000000 W
SFO1 100.6228293 MHz
CPDPRG2
NUC2 1H
PLW2 19.00000000 W
PLW12 0.19939999 W
PLW13 0.16152000 W
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
SF 100.6127555 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
 NAME YXL-7-142-2-1-H-140401
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20140401
 Time 12.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 89.81
 DW 62.400 usec
 DE 6.50 usec
 TE 297.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 9.22 usec
 PLW1 19.00000000 W

F2 - Processing parameters

SI 65536
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

9.905
 8.844
 8.839
 8.826
 8.822
 8.815
 8.812
 8.174
 8.170
 8.153
 8.150
 7.564
 7.544
 7.525
 7.519
 7.503
 7.473
 7.463
 7.452
 7.442
 7.260

4.312
 4.301
 4.285
 4.274
 4.256
 4.246
 2.728
 2.719
 2.699
 2.692
 2.673
 2.663
 2.385
 2.376
 2.364
 2.352
 2.344
 2.154
 2.147
 2.119
 1.876
 1.867
 1.846
 1.809
 1.795
 1.780
 1.764
 1.753
 1.734
 1.723
 1.701
 1.692
 1.622
 1.503
 1.471
 1.463
 1.439
 1.432
 1.425
 1.415
 1.401

