Regioselective Arene and Heteroarene Functionalization: N-alkenoxypyridinium Salts as Electrophilic Alkylating Agents for the Synthesis of α-Aryl/α-Heteroaryl Ketones

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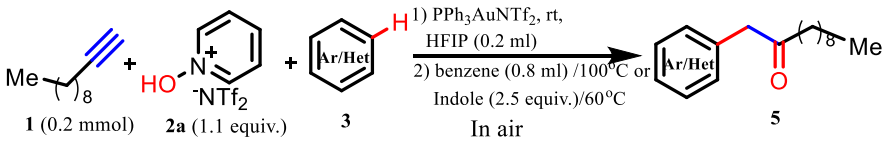
1. Screening of catalysts and conditions optimization

At the outset of our investigation, 1-undecyne was chosen as the model substrate and the reaction parameters include gold catalysts, acids, solvents and reaction temperatures all were thorough screened, results selected are shown in **Table 1**. With the initially optimized conditions, **5a** was formed with 66% overall Isolated yield (entry 1). The first step proceeded fast at room temperature in 2.5 h with >99% NMR yield in hexafluoroisopropanol (HFIP) or benzene, using commercial available PPh_3AuNTf_2 as the catalyst, while the second step required heating at 100 ˚C for 8 h with ArH as the cosolvent (totally 0.8 ml). For the formation of *N*-alkenoxypyridinium salts, besides $(CF_3)_2CHOH$, CF_3CH_2OH or DCM is also effective solvent (entries 2-3), but EtOH or THF is less effective (entries 4-5). Other commercial gold catalysts, such as Tri-p-tolylphosphineAuNTf$_2$, $Ph_3PAuOOCCF_3$ gave comparable yield, while JohnPhosAuNTf$_2$ and $Ph_3PAuSbF_6$ fared worse than PPh_3AuNTf_2 in terms of reaction rate and efficiency (entries 6-9). Protodeauration of the vinylgold intermediate and its decomposition into the corresponding gold carbene are competitive steps during the reaction. Strong acidity is favorable for the protodeauration of vinyl gold. MsOH and TFA which acidity are not as strong as Tf_2NH give moderate yield of the *N*-alkenoxypyridinium salts which may due to the chance for the formation of gold carbene increased (entries 10-11). Without gold catalyst or acid, the reaction could hardly happen (entry 12). Considering the polarity of the solvent may have influence on reaction rate and yield, different solvent such as DMF,THF, dioxane were also screened (Entry 13-16). Enhancing the reaction temperature to 110°C or 120 ^{o}C didn't benefit the yield (entry 17,18). Lowering the reaction temperature to 80 ^{o}C gave 33% yield with longer reaction time, but no reaction was found at room temperature (entries 19, 20). As such, the best reaction condition for the one-pot two steps process is by 2.5% PPh_3AuNTf_2 in HFIP or benzene(0.2 ml) at r.t. for the first step and benzene is used as not only nucleophile but also cosolvent for the second step (V_{HFIP}/V_{ArH} = 0.2 ml/0.8 ml or V_{ArH}/V_{ArH} = 0.2 ml/0.6 ml) (entry21 or 22) yields as determined by ^{1}H NMR. When heterocycle was used, the amount of the substrate can be lowered to 3 equiv. and the reaction temperature can be able to dropped to 60 ^{o}C (Entry 23-26).

Table S1 Initial reaction discovery and condition optimization.



Entry	Deviation from the initially optimized conditions	yield 1st step[a]	2st step[b]	over-all
1	HFIP or benzene as solvent 3h	>99%	67%	66%
2	CF_3CH_2OH as solvent 8h	94[b]	-	-
3	DCM as solvent, 12h	95	-	-
4[c]	EtOH as solvent, 24h	19	-	-
5	THF as solvent, 24h	80		
6	JohnPhosAuNTf$_2$ as catalyst, 8h	78%	-	-
7	Tri-p-tolylphosphineAuNTf$_2$ as catalyst, 8h	91%	-	-
8	$Ph_3PAuOOCCF_3$ as catalyst, 8h	95%	-	-
9	$Ph_3PAuSbF_6$ as catalyst, 8h	85%	-	-
10	MsOH as acid	70%	-	-
11	TFA as acid, 10 h	51%	-	-
12	Without PPh_3AuNTf_2 or without Tf_2NH	N.R.	-	-
13	for the 2nd, benzene (0.8 ml), DMF as solvent	-		N.R.
14	for the 2nd, benzene (0.8 ml), DCM as solvent	-		34%
15	for the 2nd, benzene (0.8 ml), Dioxane as solvent	-		24%
16	for the 2nd, benzene (0.8 ml), hexamethylene as solvent			35%

17	120°C for the 2nd, 2.5h	-	55%
18	110 °C for the 2nd, 5h	-	61%
19	80 °C for the 2nd, 24h		33%
20	25 °C for the 2nd, 24h	-	N. R.
21	Two steps in one pot, for the 2nd step, benzene (0.2 ml) /benzene (0.6 ml)	>99%	67%
22	Two steps in one pot, for the 2nd step, HFIP (0.2 ml) /benzene (0.8 ml)	>99%	66%
23	for the 2nd, Het-H(1.5 equiv.), HFIP(0.2 ml) as solvent, 4h		75%
24	for the 2nd, Het-H(3equiv.), HFIP (0.2 ml) as solvent, 4h		79%
25	for the 2nd, Het-H(5 equiv.), HFIP (0.2 ml) as solvent, 4h		80%
26	40°C for the 2nd, Het-H(3 equiv.)/HFIP (0.2 ml), 24h		25%
27	90°C for the 2nd, Het-H(3 equiv.)/HFIP (0.2 ml), 2h		73%

a Reactions run in vials; yields as determined by ^{1}H NMR. b Isolated yield. c 40% of methyl ketone formed. Conditions (entry 23~27) were applied to indole.

To our disappointment, when 5 equiv. of ArH was used, low reaction proceeded even heating to 100 °C for 24h. Increasing the amount of benzene should be helpful for the reaction. Indeed, when benzene was used not only as nucleophile but also as the cosolvent, the reaction could proceed smoothly and as the increase of a series of concentration reaction yield showed parabola relationship. When 0.8 ml benzene was used both as the sustrate and the solvent, the expected product could be obtained with the best yield **(**detail see **figure S1)**. The ratio of benzene/solvent affected the reaction heavily. Benzene can also used as the sole solvent with the same yield as HFIP of **5**, but further higher volumn of it results in diminished yields (detail see **Table S2**).

Table S2 The volume of benzene on reaction rate and reaction yield.

HFIP/ml	0.2	0.2	0.2	0.2	0.2	0.2	0.2
Benzene/equiv.	5	10	20	40	60	80	100
Yield/%	45	53	65	70	77	58	55

Reactions run in vials under the optimal conditions.

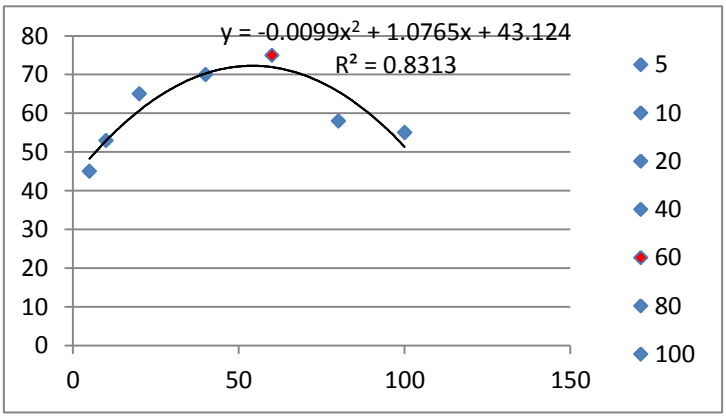


Fig. S1 The volume of benzene on reaction rate and reaction yield.

2. Determination of Rate Determining Step by Kinetic Isotopic Effect

To a vial, 4a (0.2 mmol, 89.2 mg) and 0.8 mL of benzene and 0.8 ml of C_6D_6 were added. Then the

reaction vial was sealed and heated to 100 °C. Aliquots of 0.1 mL of the reaction mixture were taken respectively 3 min, 6 min, 9 min, 12 min and 15 min after the reaction started. The reaction mixture was collected by the removal of organic solvent via rotary evaporation and then subjected to ^{1}H-NMR spectroscopy. The ratio between 5a and 5a-D was found to be 1:1.03 and was interpreted to represent the KIE for this reaction.

Scheme S1 Kinetic Isotopic Effect Studies.

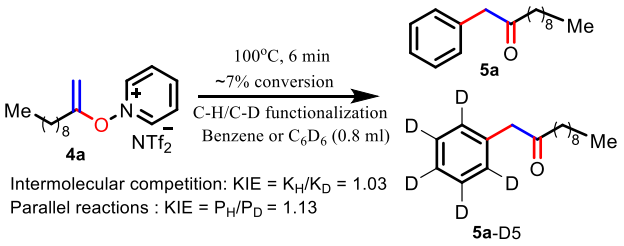


Table S3 Intermolecular competition for KIE measurement

Entry	**1**	**2**	**3**	**4**	**5**
Time/min	3	6	9	12	15
Conversion/%	1.58	4.39	7.27	9.63	13.5

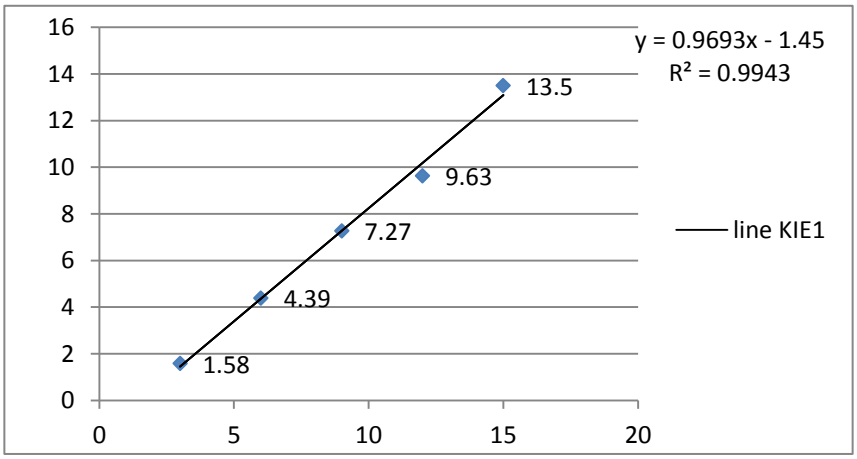


Fig. S2 Intermolecular competition for KIE measurement. **KIE = KH/KD = 1.03**

Table S4 Parallel test for KIE measurement

Entry	**1**	**2**	**3**	**4**	**5**
Time/min	3	6	9	12	15
Conversion/%	1.87	3.87	5.42	6.83	10.5

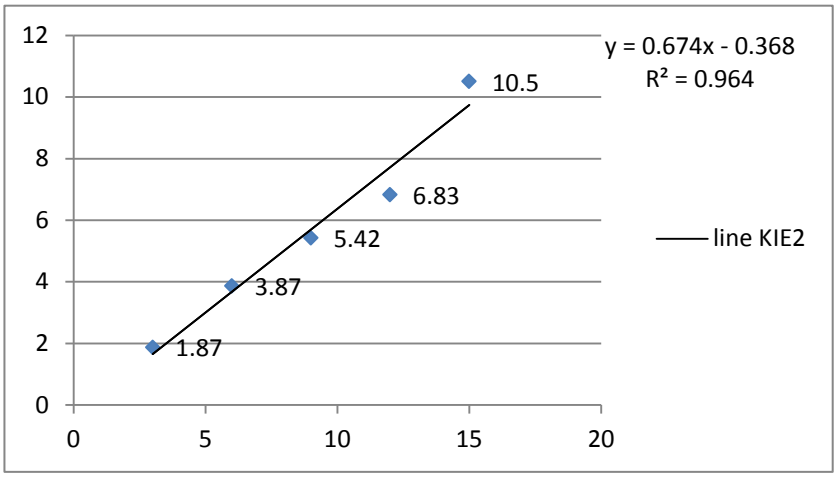


Fig. S3 Parallel reaction for KIE measurement. **KIE = PH/PD = 1.13**

3. Computational details

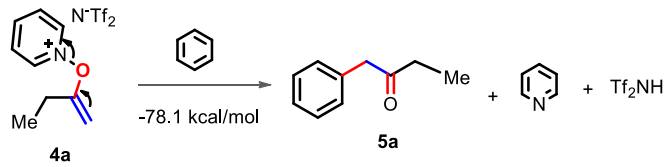
All calculations were carried out using the Gaussian 09 program package.[1] The structures were fully optimized by using the M06-2X[2] functional coupled with 6-31G(d,p) basis set. Frequency calculations were performed at the same level of theory to confirm all the stationary points as minima or transition states. Intrinsic reaction coordinate (IRC)[3] analysis were performed to ensure connectivity between the transition structures and the intermediates. For the identified stationary points, we performed additional single-point calculations using a more extended basis set 6-311++G(d,p) with M06-2X functional to obtain more accurate energies. The solvent effects (benzene) were considered by using the SMD[4] solvation model in both geometry optimization and single-point calculations. The energies discussed in the text are Gibbs free energies calculated at 373 K (experimental temperature) unless otherwise stated. To reduce the computational cost, the nonyl group in **4a** was substituted by ethyl group.

Results and Discussion

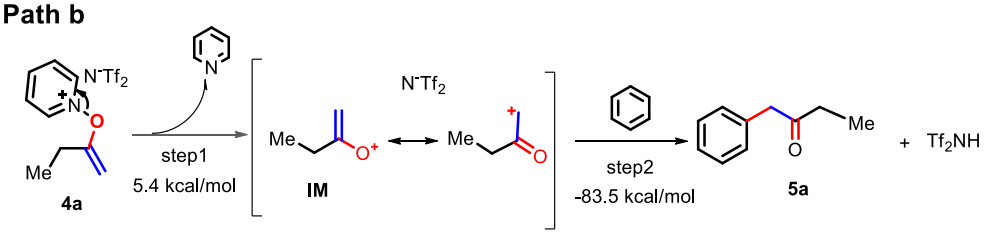
To get more insight into the experimental observations and the reaction mechanism, we conducted a DFT study on the mechanism of the reaction. We first check the thermodynamic possibility of the two pathways (Scheme S2). Our thermodynamic calculations reveal that the reaction of benzene with **4a** through path a is highly exergonic (ΔG= –78.1 kcal/mol), suggesting that this mechanism is thermodynamically favorable. For path b, the N–O bond cleavage step (step1 in path b) is slightly endergonic with free energy of 5.4 kcal/mol, whereas the reaction of benzene with carbocation **IM** (step 2) is highly exergonic with free energy of –83.5 kcal/mol. Thus, the overall reaction, i.e, the coupling reaction of step1 and step2, is an exergonic process, indicating that generation of the reactive species carbocation is likely.

Scheme S2 Two possible pathways for the reaction.

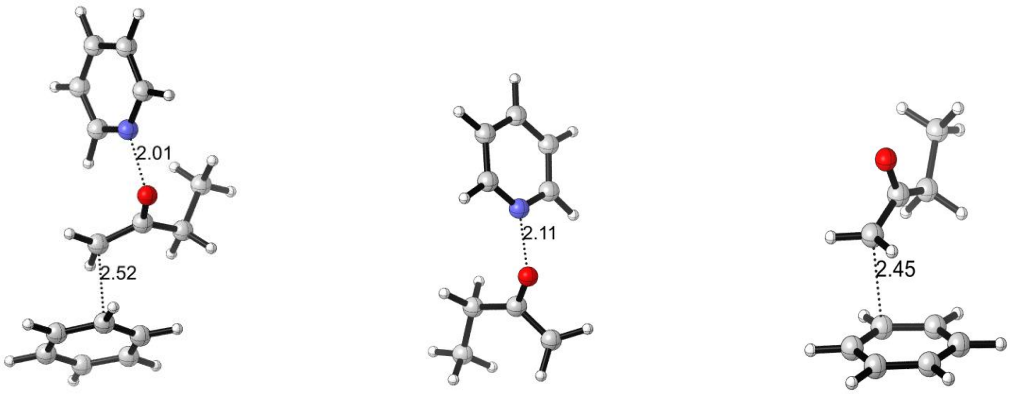
Path a



Path b



The optimized structures and the corresponding free energy barrier of the transition states involving in the two pathways were presented in Fig. S4. Our calculations reveal that the calculated barrier height in free energy of path a is quite high (43.4 kcal/mol), implying this pathway is kinetically unfavorable. The N-O bond cleavage step in path b needs to overcome a free energy barrier of 33.5 kcal/mol, whereas the barrier of the second step is only 14.8 kcal/mol, indicating that the first step is the rate-determining step in path b. It was noted that the barrier of the first step is much lower than 43.4 kcal/mol for path a. Therefore, path b is more facile than path a from the kinetic point of view. These results can account for the experimental observation.



TS1 (43.4) **TSN-O (33.5)** **TS2 (14.8)**

Fig. S4 The optimized structures and the corresponding free energy barrier (in kcal/mol) of the transition states involving in the two pathways.

References

1. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.;

Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, revision D.01*, Gaussian Inc., Wallingford, CT, 2013.

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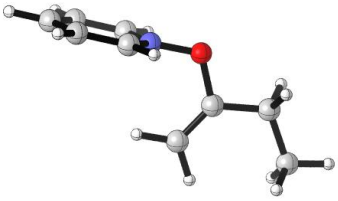
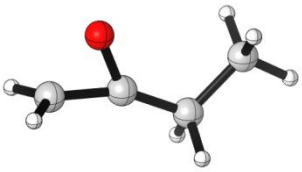
3. Gonzalez, C.; Schlegel, H. B. Reaction Path Following in Mass-Weighted Internal Coordinates. *J. Phys. Chem.* **1990**, 94, 5523-5527.
4. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Perspective on Foundations of Solvation Modeling: The Electrostatic Contribution to the Free Energy of Solvation. *J. Chem. Theory Comput*. **2008**, 4, 877-887.

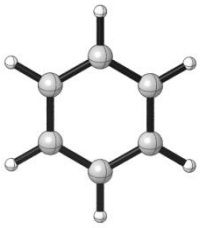
The optimized structures and cartesian coordinates of title compounds at the SMD-M062X-631G(d,p) level.



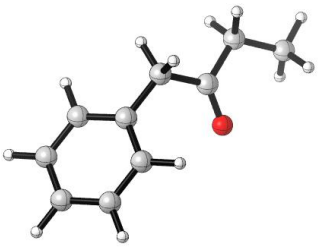
4a



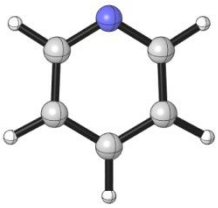
carbocation (IM)



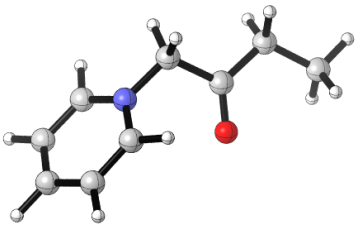
benzene



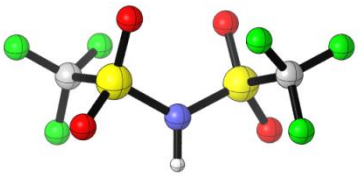
5a



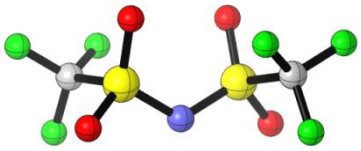
pyridine



5a’



$NHTf_2$



NTf_2-anion

NTf_2-anion

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$NHTf_2$

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4a

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5a

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pyridine

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5a’

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C	-3.02191800	-0.50001100	0.18153200
C	-0.55321800	-0.77902600	0.84691800
C	-4.03262700	0.40773500	-0.50246800
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H	-0.66585100	-1.85646100	0.71299200
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H	-3.82042100	0.48748700	-1.57033800
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C	2.83213000	-0.87829900	-0.67478200
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IM (carbocation)

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H	1.90686700	-1.02296900	-0.83638500
H	1.90804200	-0.94349900	0.93863500

TS1 (path a)

C	0.12200900	0.62438700	0.30936200
C	0.27885500	1.98126700	-0.33238100
C	0.85940400	-0.50762900	-0.10043000
C	-1.05187900	2.52729400	-0.85600700
H	1.02055200	1.92367500	-1.13449300
H	0.67303700	2.66503000	0.42822000
H	0.61174800	-1.46776800	0.34382500
H	1.54324300	-0.48286000	-0.94441400
H	-0.91106600	3.53372300	-1.25486000
H	-1.79155600	2.57940300	-0.05338800
H	-1.45600900	1.90173500	-1.65717200
C	3.29861900	0.78694500	0.67722400
C	2.96729800	-0.43911500	1.27983600
C	3.40995200	-1.64210100	0.70616000
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H	3.18553500	-2.58588200	1.19353800
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O	-0.70000200	0.44510500	1.25674000
C	-2.37426900	-0.71174100	-0.68554600
C	-3.60698900	0.06257900	1.12758000
C	-3.50807400	-1.21834600	-1.31532400
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C	-4.78795500	-0.41331400	0.56528400
H	-3.56365100	0.57293500	2.08485100
C	-4.73114000	-1.05808800	-0.66860300
H	-3.42851500	-1.71546200	-2.27479500
H	-5.72728800	-0.27625900	1.08851300
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N	-2.46830100	-0.10778100	0.47176700

$TS_{N\text{-}O}$ (path b)

C	-1.94464200	0.38312800	-0.22341500
C	-2.11902200	-0.98618700	0.30870400
C	-2.79722800	1.49738900	-0.33607800
N	0.85465400	0.19597500	-0.22434000
O	-1.02965100	0.78501100	-0.98081900
C	1.55547500	-0.61507500	-1.01073200

C	2.89808200	-0.87550500	-0.75763600
C	3.50143600	-0.25620200	0.33297500
C	2.75284400	0.60100000	1.13468700
C	1.41518300	0.80658500	0.81525500
C	-3.54090100	-1.26544400	0.78253400
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H	-1.77262100	-1.69517200	-0.44977200
H	-2.37998100	2.49604100	-0.27013400
H	-3.82052400	1.36717800	-0.68938300
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H	3.45123900	-1.54491400	-1.40632400
H	4.54840700	-0.43618100	0.55377200
H	3.19046100	1.10528000	1.98848500
H	0.78128200	1.46798900	1.40128500
H	-3.58394700	-2.23965700	1.27089600
H	-4.24430500	-1.27983500	-0.05356700
H	-3.87291800	-0.51551800	1.50645800

TS2 (path b)

C	1.67997800	-0.50566000	-0.14325700
C	2.39978400	0.68395000	0.32739800
C	0.38670400	-1.15816600	-0.07230100
O	2.02647000	-1.44383500	-0.85272600
C	3.88684100	0.63386400	-0.00264800
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C	-2.79210500	0.33730400	-0.99817200
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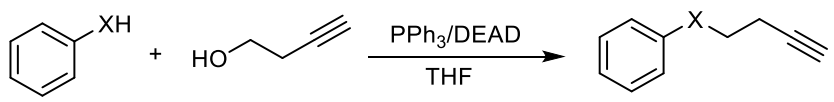
4. Preparation of Substrates

Alkynes expect for S1-S7 are commercial available. S1-S7 are known compounds and synthesized according to the literatures.[1-4]

Preparation of propargyl ether substrates:

General procedure A:



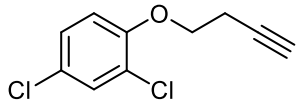
S1

X=O,S

These compounds were synthesized according to the literature. [1,2] To a mixture of S1 (10 mmol),

PPh_3 (2.62 g, 10 mmol) and but-3-yn-1-ol (0.84g, 12 mmol) in THF (25 mL) was added DEAD (10 mmol) at 0 ^{0}C. The mixture was stirred at reflux for 6 h and cooled to room temperature. After THF was removed under reduced pressure, the residue was chromatographed on silica gel to afford the desired alkynes.

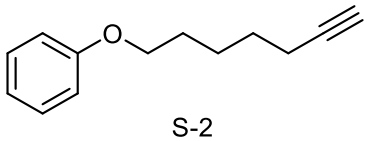
1-(but-3-yn-1-yloxy)-2,4-dichlorobenzene (S-1)



S-1

This compound was prepared in 78% yield according to the general procedure **A.** The spectra data were identical with the reported one. Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 2.3 Hz, 1H), 7.18 (dd, J = 8.7, 2.3 Hz, 1H), 6.86 (d, J = 8.7 Hz, 1H), 4.13 (t, J = 7.1 Hz, 2H), 2.73 (td, J = 7.1, 2.7 Hz, 2H), 2.07 (t, J = 2.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 130.1, 127.6 , 126.3, 124.1, 114.7, 79.7, 70.3, 67.6, 19.4.

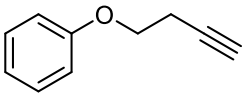
(hept-6-yn-1-yloxy)benzene (S-2)



S-2

Known compound which was prepared in 72% yield according to the general procedure **A**. Colorless liquid. The spectra data were identical with the reported one. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (t, J = 8.0 Hz, 2H), 6.96-6.89 (m, 3H), 3.97 (t, J = 6.4 Hz, 2H), 2.32-2.15 (m, 2H), 1.96 (t, J = 2.7 Hz, 1H), 1.89-1.74 (m, 2H), 1.71-1.50 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 129.3, 120.5, 114.4, 84.3, 68.3, 67.5, 28.7, 28.1, 25.2, 18.3.

(but-3-yn-1-yloxy)benzene (S-3)

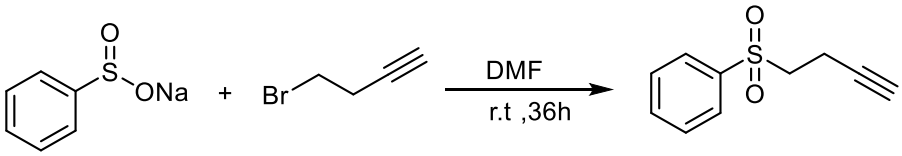


S-3

This compound was prepared in 88% yield according to the general procedure **A**. The spectra data were identical with the reported one. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, J = 8.0 Hz, 2H), 6.97 (t, J = 7.3 Hz, 1H), 6.92 (d, J = 8.2 Hz, 2H), 4.11 (t, J = 7.1 Hz, 2H), 2.69 (td, J = 7.0, 2.6 Hz, 2H), 2.05 (t, J = 2.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 129.4, 121.0, 114.6, 80.4, 69.8, 65.8, 19.5.

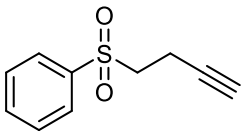
Preparation of sulfonyl-substituted substrates:

General procedure B:



These compounds were synthesized according to the literature.[2] To a solution of sodium benzenesulfinate (30 mmol, 4.92 g) in DMF (30 ml) was added homopropargyl bromide (30 mmol, 3.96g). The resulting mixture was stirred at room temperature for 36 h. The reaction was quenched with H_2O (300 mL) and extracted with Et_2O (2 x 300 mL). The combined organic layers were dried over Na_2SO_4, and the solution was concentrated in vacuo to directly afford (but-3-yn-1-ylsulfonyl)benzene (2.13 g, 78% yield) as a solid.

(but-3-yn-1-ylsulfonyl)benzene (S-4)



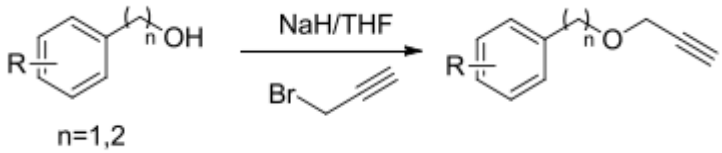
S-4

This compound was prepared in 77% yield according to the general procedure **B**. The spectra data were identical with the reported one.[1] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.93 (d, *J* = 7.8 Hz, 2H), 7.85-7.49 (m, 3H), 3.32 (t, *J* = 7.8 Hz, 2H), 2.85-2.48 (m, 2H), 1.96 (t, *J* = 2.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 138.7, 134.3, 129.7, 128.5, 79.5, 70.8, 54.8, 13.5.

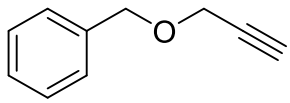
Preparation of propargyl ether substrates:

General procedure C:

These compounds were synthesized according to the literature.[4] To a solution of the alcohol (2 mmol) in anhydrous THF (10 ml) was added NaH (1.2 equiv.) in one portion at 0°C. The resulting mixture was stirred for 30 min. A solution of propargyl bromide (2 mmol, 80% in toluene) was then added dropwise. The reaction was monitored by TLC. Upon completion, the reaction was quenched with water and extracted with ethyl ether (10ml X3). The combined organic layers were dried over Na_2SO_4, filtered and concentrated. The residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired alkynes.



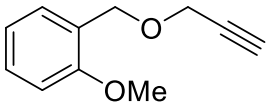
((Prop-2-yn-1-yloxy)methyl)benzene (S-5)



S-5

This compound was prepared in 59% yield according to the general procedure **C**. The spectra data were identical with those reported.[4] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.39–7.27 (m, 5H), 4.62 (s, 2H), 4.18 (d, *J* = 2.4 Hz, 2H), 2.47 (t, *J* = 2.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 137.1, 128.4, 128.0, 127.8, 79.6, 74.5, 71.4, 57.0.

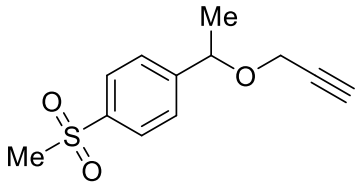
1-methoxy-2-((prop-2-yn-1-yloxy)methyl)benzene (S-6)



S-6

This compound was prepared in 63% yield according to the general procedure **C**. The spectra data were identical with those reported.[4] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (m, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 4.58 (s, 2H), 3.84(s, 3H), 4.16 (d, *J* = 2.4 Hz, 2H), 2.46 (t, *J* = 2.3 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 140.2, 129.3, 121.2, 114.6, 111.6, 79.7, 74.4, 71.3, 56.8, 55.3.

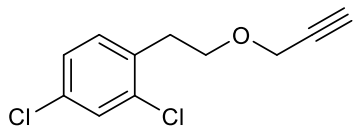
1-(methylsulfonyl)-4-(1-(prop-2-yn-1-yloxy)ethyl)benzene (S-7)



S-7

This compound was prepared in 59% yield according to the general procedure C. The spectra data were identical with those reported.[4] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, J = 7.6 Hz, 2H), 7.17 (d, J = 7.8 Hz, 2H), 4.50 (q, J = 6.4 Hz, 1H), 4.16 (d, J = 2.4 Hz, 2H), 2.46 (t, J = 2.3 Hz, 1H), 3.04 (s, 3H), 1.48 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.6, 134.1, 129.1, 128.2, 79.7, 74.4, 71.3, 56.8, 44.5, 21.1.

2,4-dichloro-1-(2-(prop-2-yn-1-yloxy)ethyl)benzene (S-8)



S-8

This compound was synthesized according to the general procedure **C.** The spectra data were identical with those reported.[4] Colorless liquid. ^{1}H NMR (400 MHz, $CDCl_3$) δ7.36 (d, J = 2.3 Hz, 1H), 7.33-7.26 (m, 2H), 4.17 (d, J = 1.8 Hz, 2H), 3.76 (td, J = 7.6, 2.3 Hz, 2H), 2.93 (t, J = 7.0 Hz, 2H), 2.46–2.37 (m, 1H); ^{13}C NMR(100 MHz, $CDCl_3$) δ 138.5, 128.8, 128.3, 126.2, 79.7, 74.3, 70.8, 58.1, 36.0.

5. References

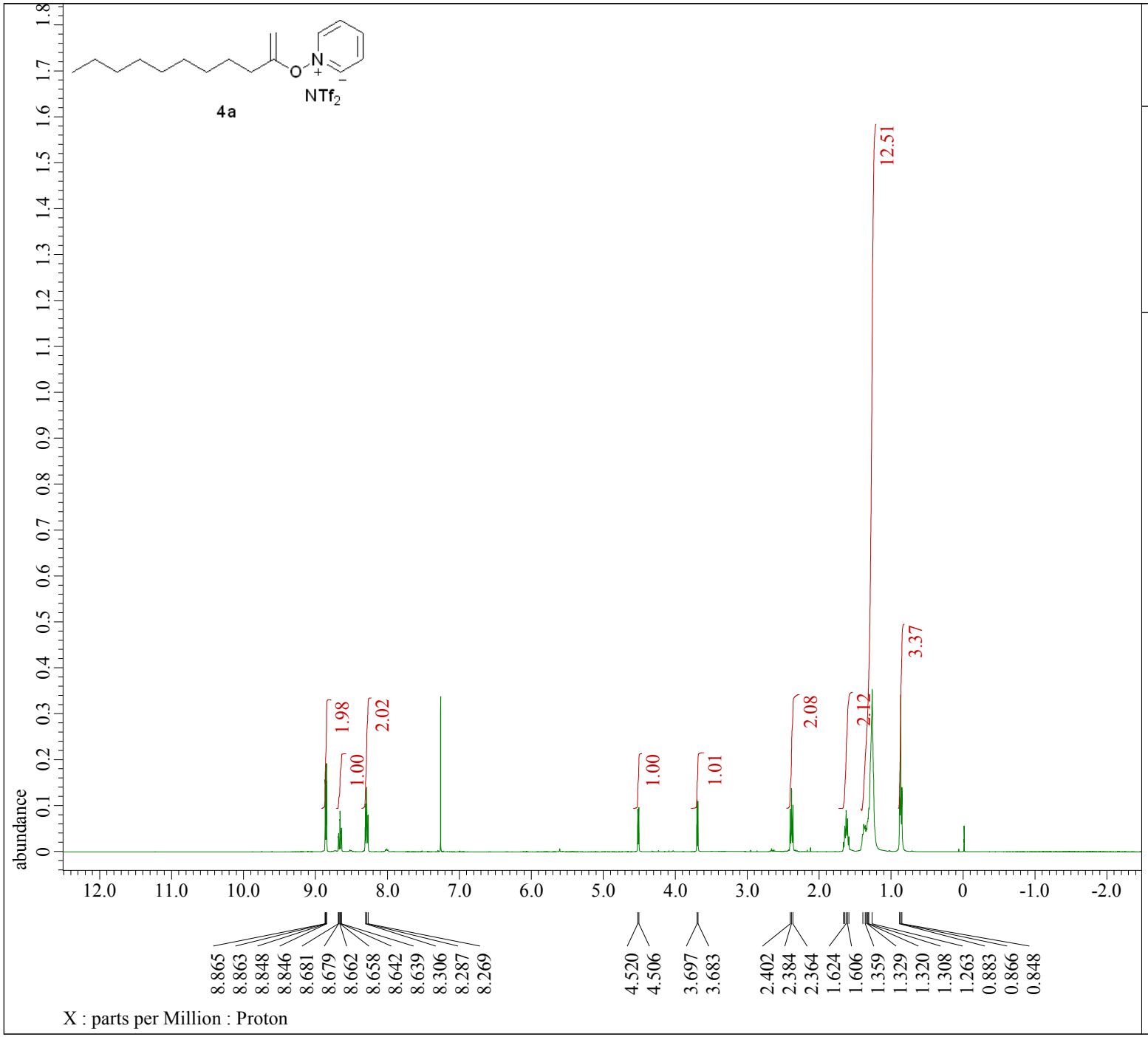
(1) Xu, Z.; Chen, H.; Wang, Z.; Ying, A.; Zhang, L. One-Pot Synthesis of Benzene-Fused Medium-Ring Ketones: Gold Catalysis-Enabled Enolate Umpolung Reactivity. *J. Am. Chem. Soc.* **2016**, *138*, 5515–5518.

(2) Murase, H.; Senda, K.; Senno, M.; Urabe, H. Rhodium-Catalyzed Intramolecular Hydroarylation of 1-Halo-1-Alkynes: Regioselective Synthesis of Semihydrogenated Aromatic Heterocycles. *Chem. Eur. J.* **2014**, 20, 317–322.

(3) Li, H.; Guillot, R.; Gandon, V. A Gallium-Catalyzed Cycloisomerization/Friedel−Crafts Tandem. *J. Org. Chem.* **2010**, *75*, 8435–8449.

(4) Xu, Z.; Zhai, R. L.; Liang, T.; Zhang, L. Efficient One-Pot Multifunctionalization of Alkynes en Route to α-Alkoxyketones, α-Thioketones, and α-Thio Thioketals by Using an Umpolung Strategy. *Chem. Eur. J.* **2017**, 23, 14133–14137.

6. Copies of ^{1}H NMR and ^{13}C NMR spectra of the products

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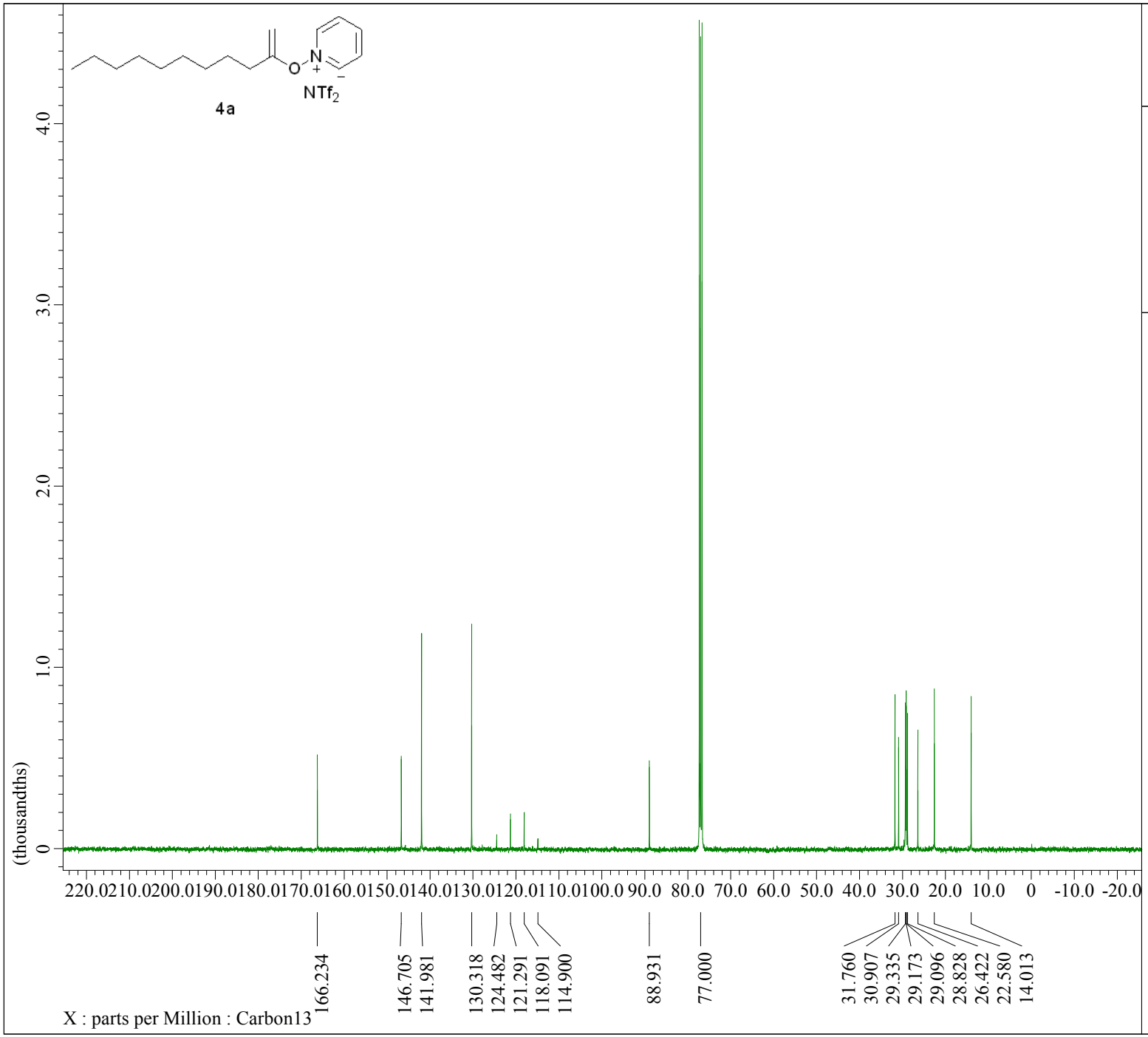


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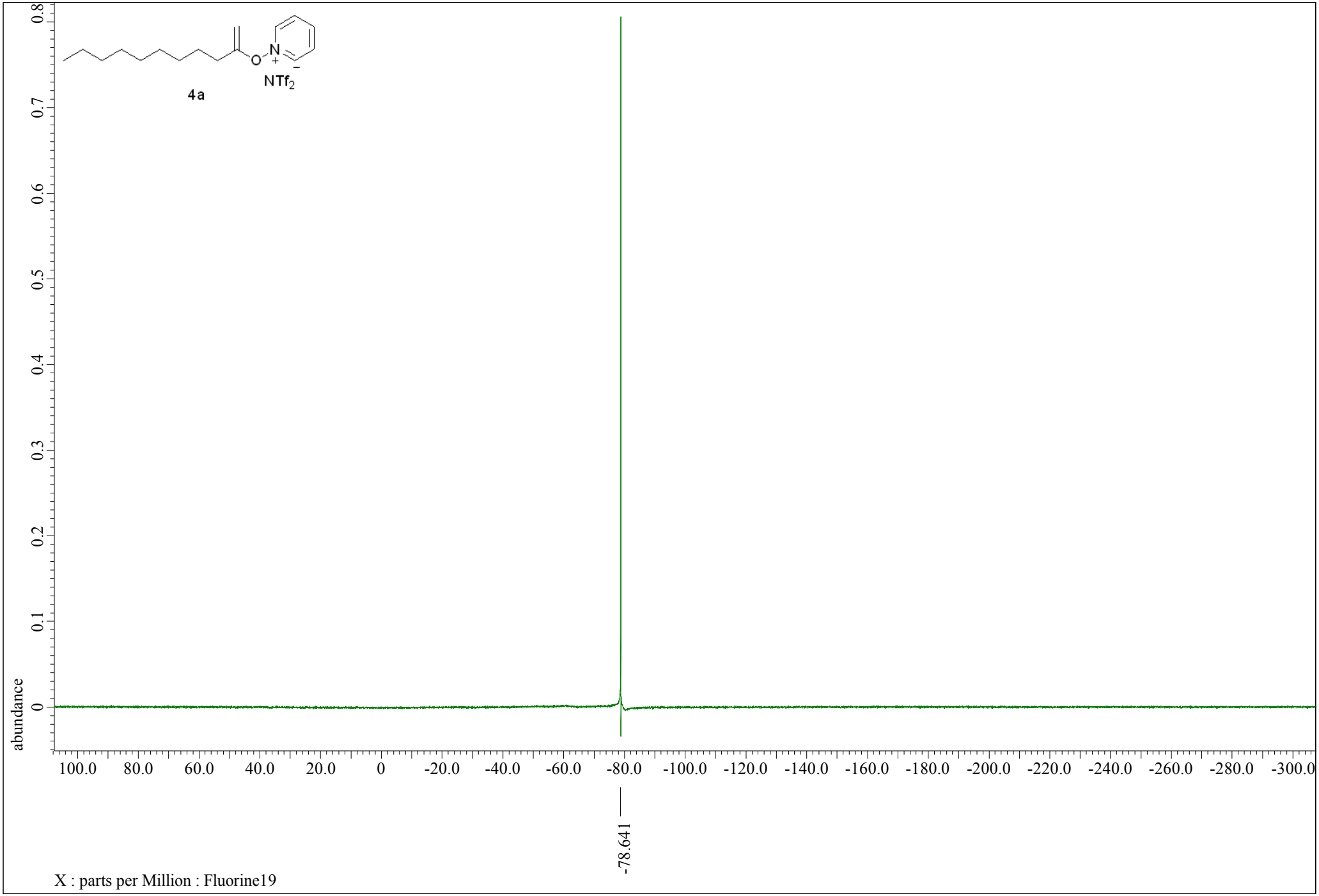
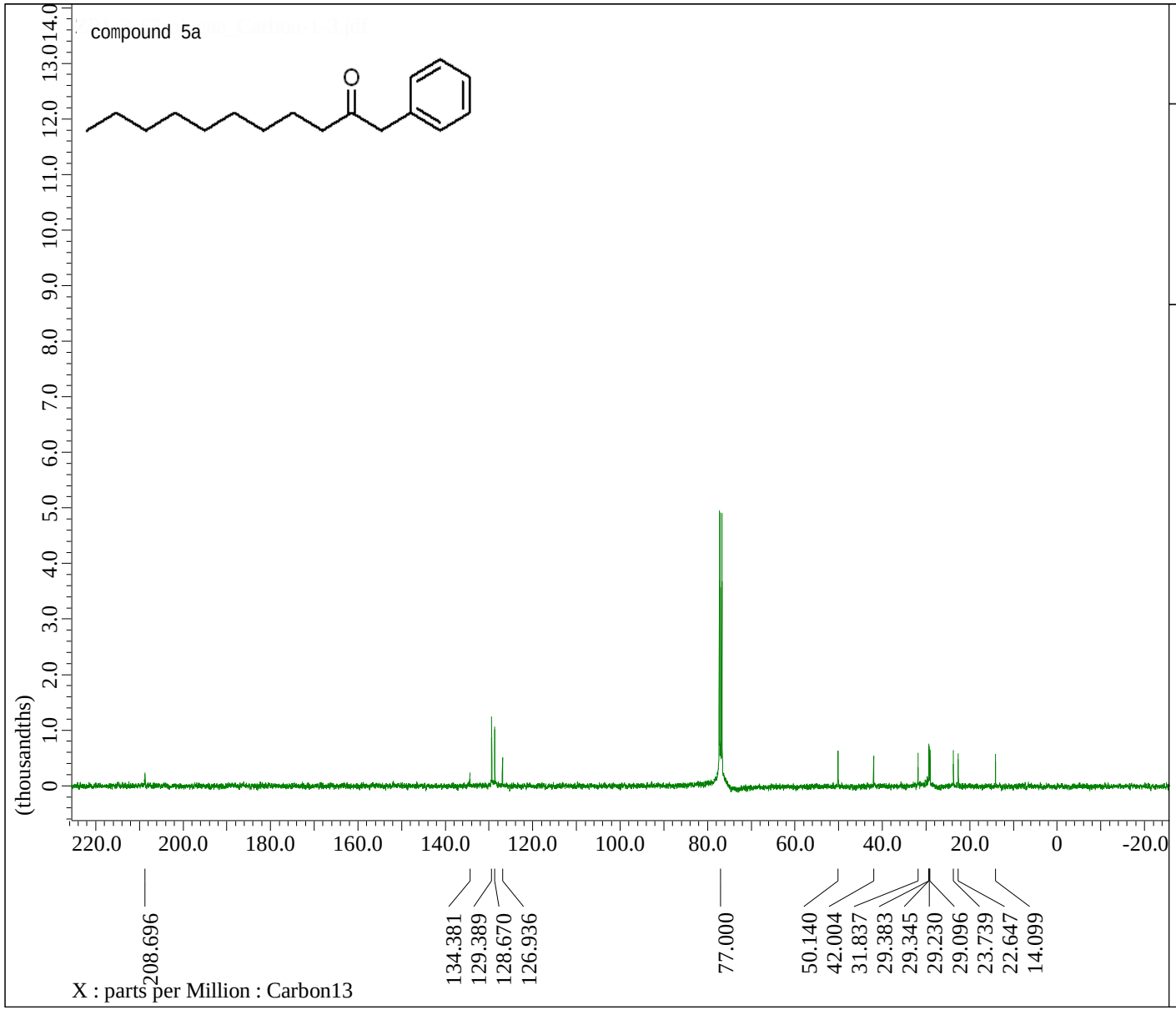
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (400[M
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MHz]
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz]
X_Sweep_Clipped           = 25.25252525[kHz]
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MHz]
Irr_Offset                = 5[ppm]
Clipped                   = TRUE
Scans                     = 25139
Total_Scans               = 25139

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 21.8[dC]
X_90_Width                = 1[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 0.33333333[us]
Irr_Atn_Dec               = 23.66[dB]
Irr_Atn_Dec_Calc          = 23.66[dB]
Irr_Atn_Dec_Default_Calc  = 23.66[dB]
Irr_Atn_Noe               = 23.66[dB]
Irr_Dec_Bandwidth_Hz      = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm     = 11.96303566[ppm]
Irr_Dec_Freq              = 399.78219838[MHz]
```


4a
NTf2
abundance
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
100.0
80.0
60.0
40.0
20.0
0
-20.0
-40.0
-60.0
-80.0
-100.0
-120.0
-140.0
-160.0
-180.0
-200.0
-220.0
-240.0
-260.0
-280.0
-300.0
-78.641
X : parts per Million : Fluorine19




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

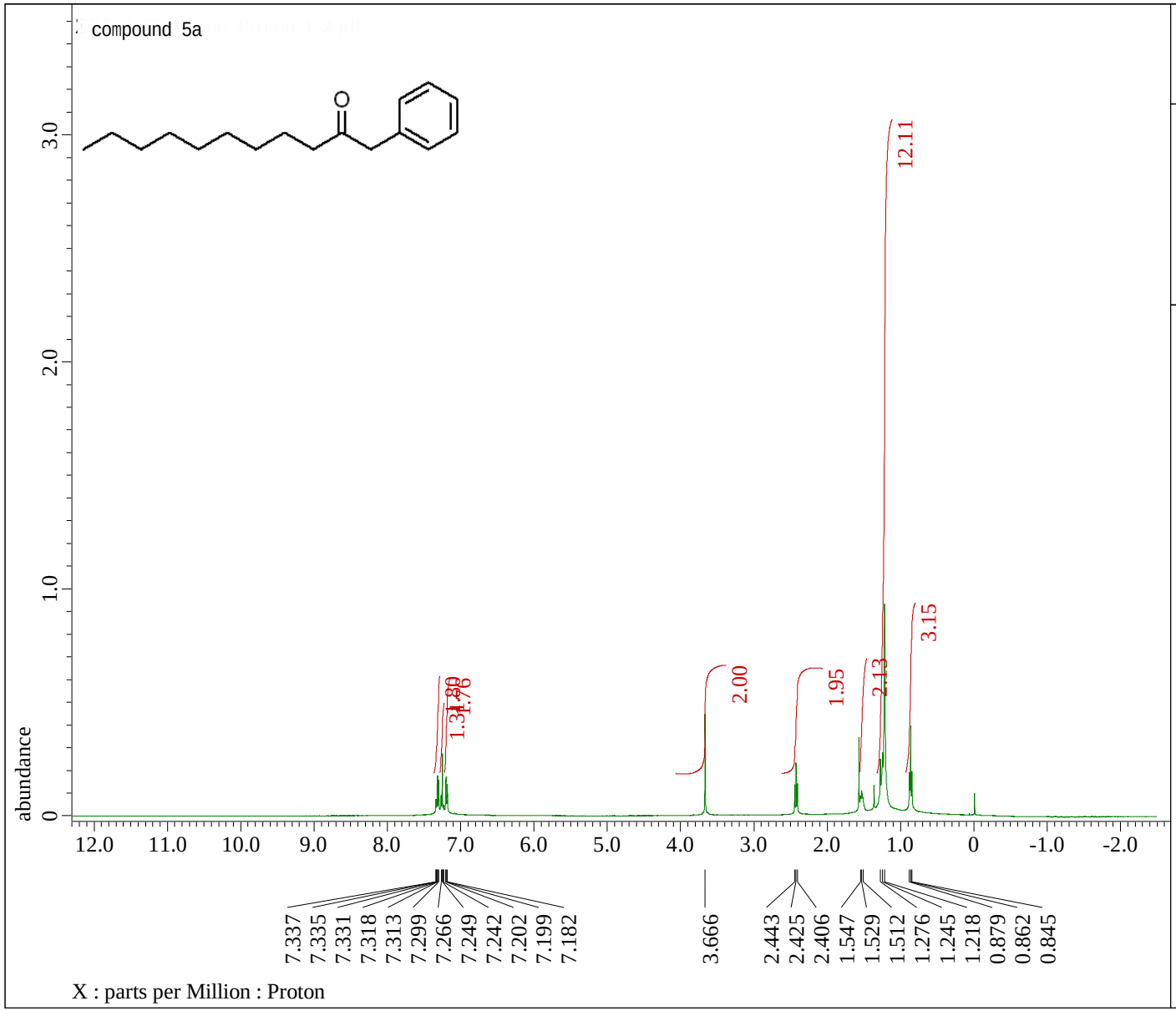
Derived from: ZRL-3-62toluene_Carbon-1-1.j
```

```
Filename                  = ZRL-3-62toluene
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-3-62toluene
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 15-JUL-2017 15:
Revision_Time             =  6-DEC-2017 13:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 21.7[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



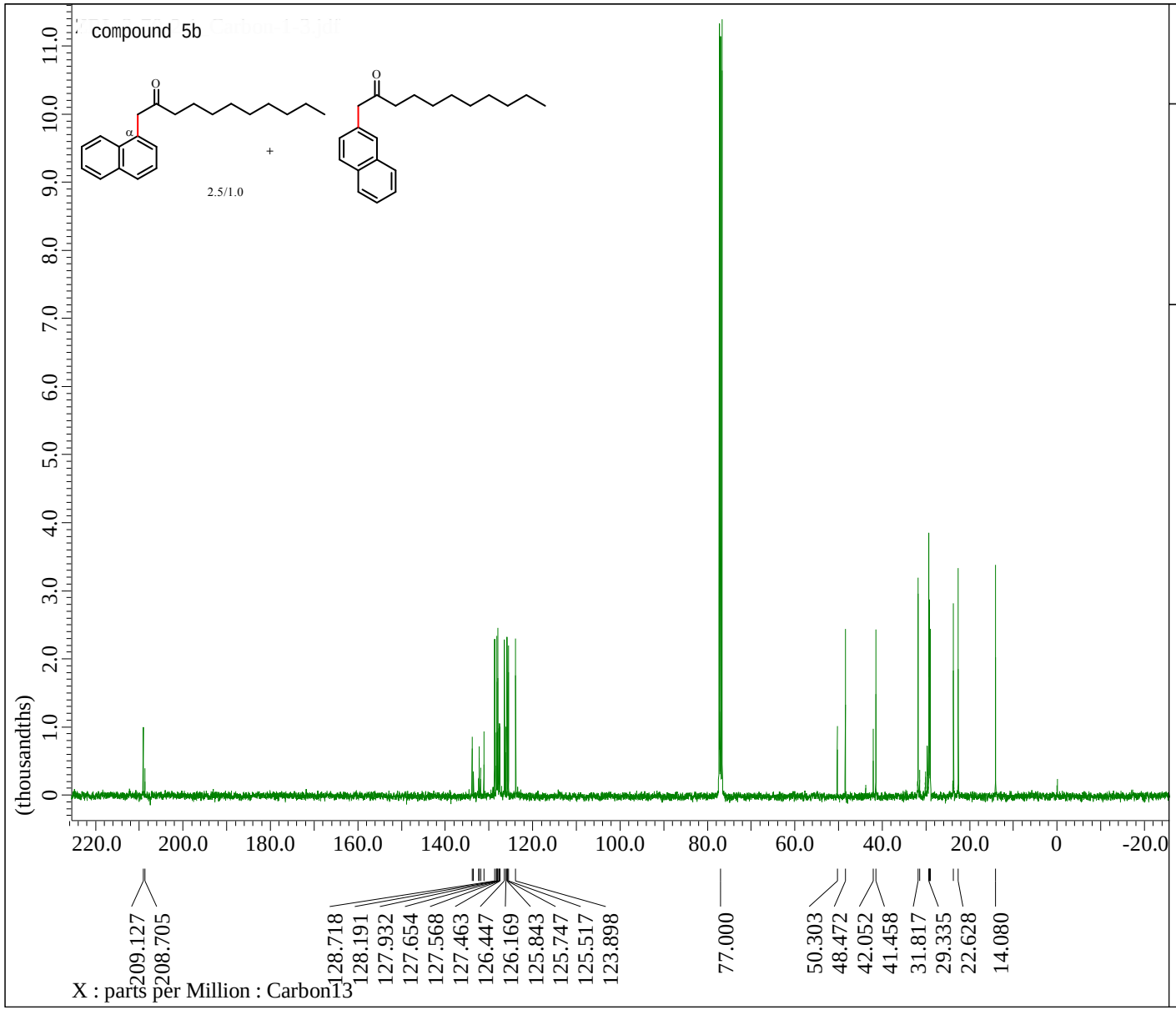

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-3-62toluene_Pr
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-62toluene
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 15-JUL-2017 15:14:
Revision_Time         = 21-FEB-2018 11:59:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 21.5[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

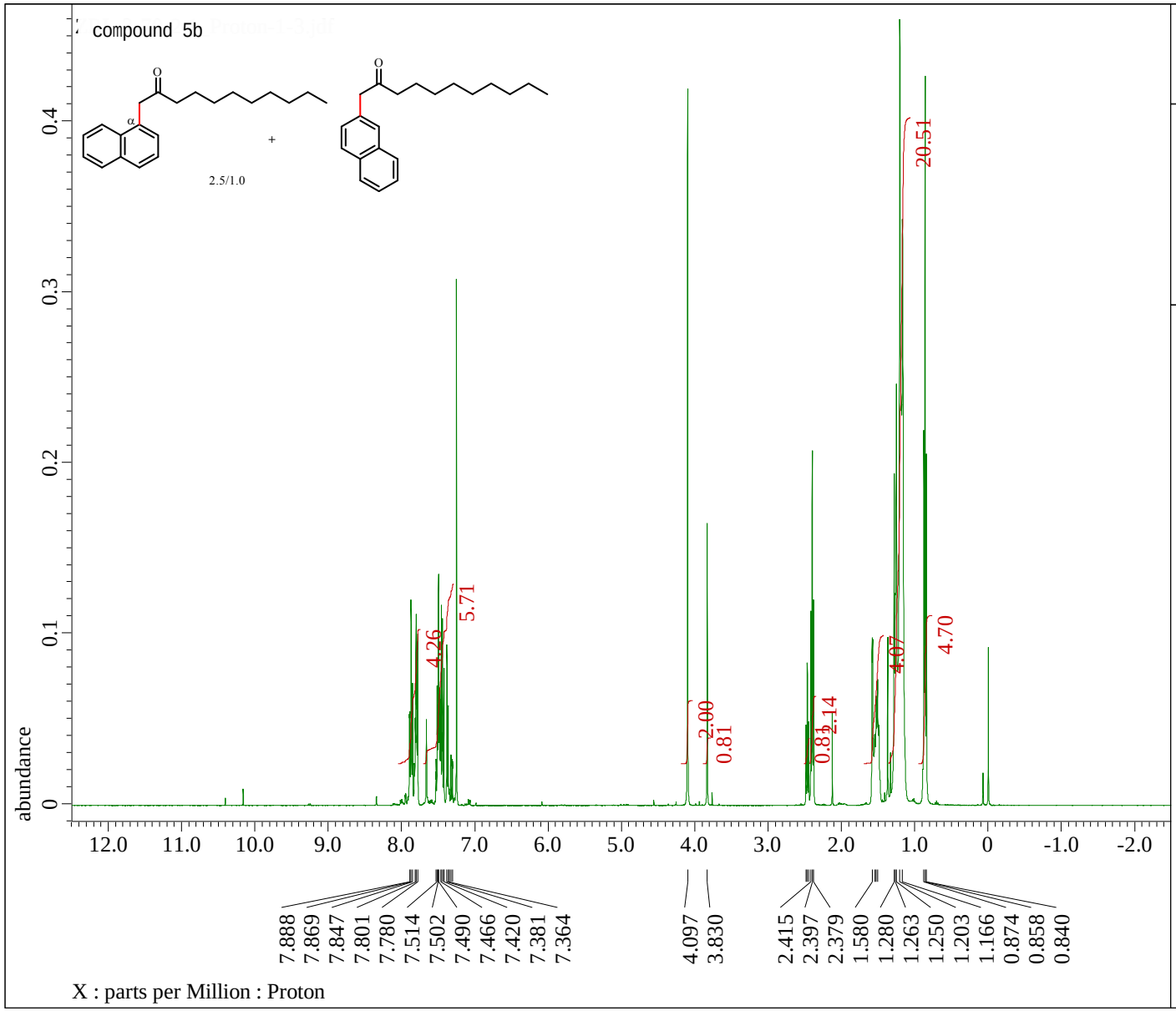
Derived from: ZRL-3-70-2 1_Carbon-1-1.jdf
```

```
Filename                  = ZRL-3-70-2 1_Ca
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-3-70-2 1
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 25-JUL-2017 21:
Revision_Time             =  6-FEB-2018 10:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 21.1[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

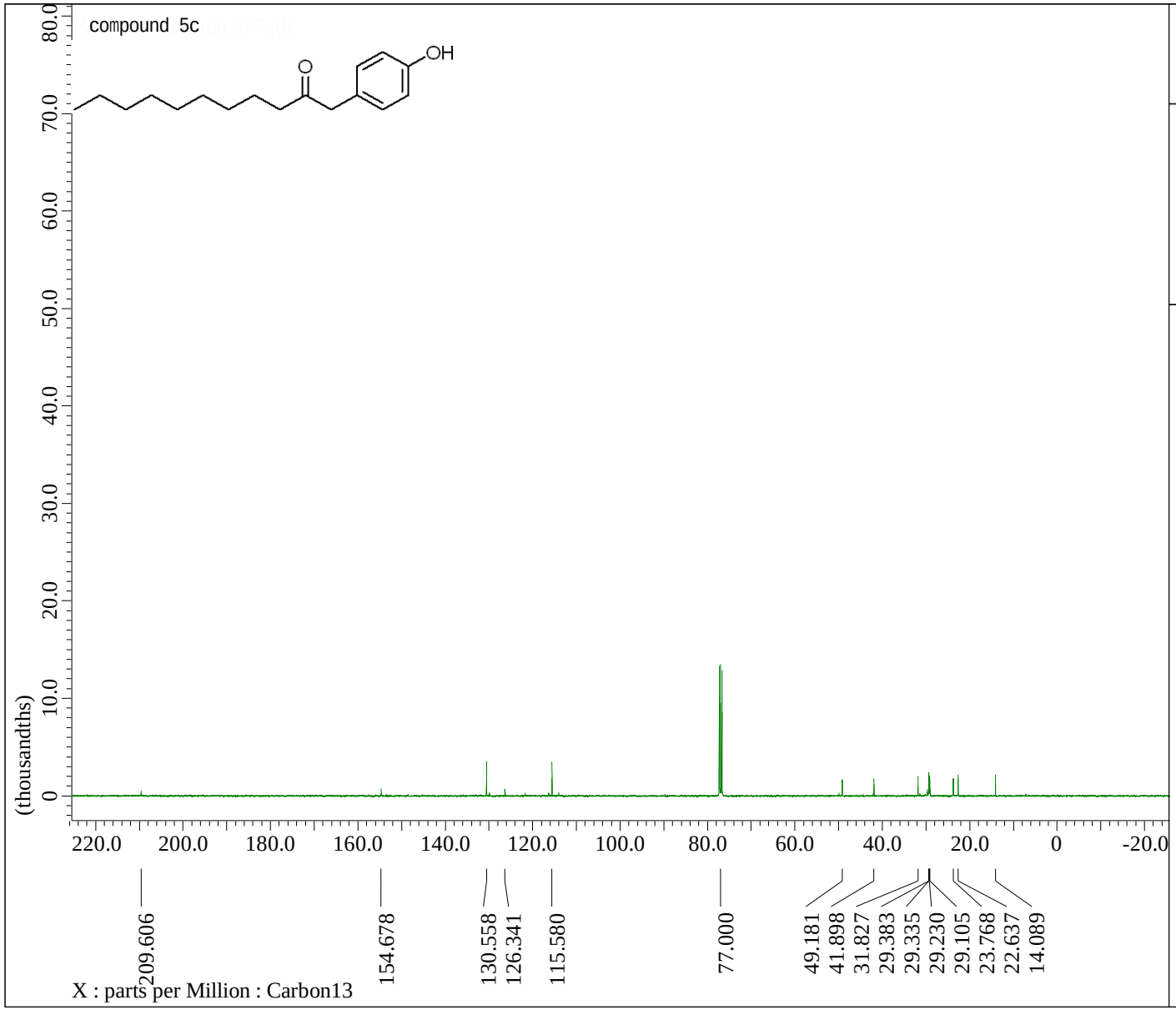
Derived from: ZRL-3-70-2 1_Proton-1-1.jdf
```

```
Filename              = ZRL-3-70-2 1_Proto
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-70-2 1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-JUL-2017 21:52:
Revision_Time         =  6-FEB-2018 10:46:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 21.2[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

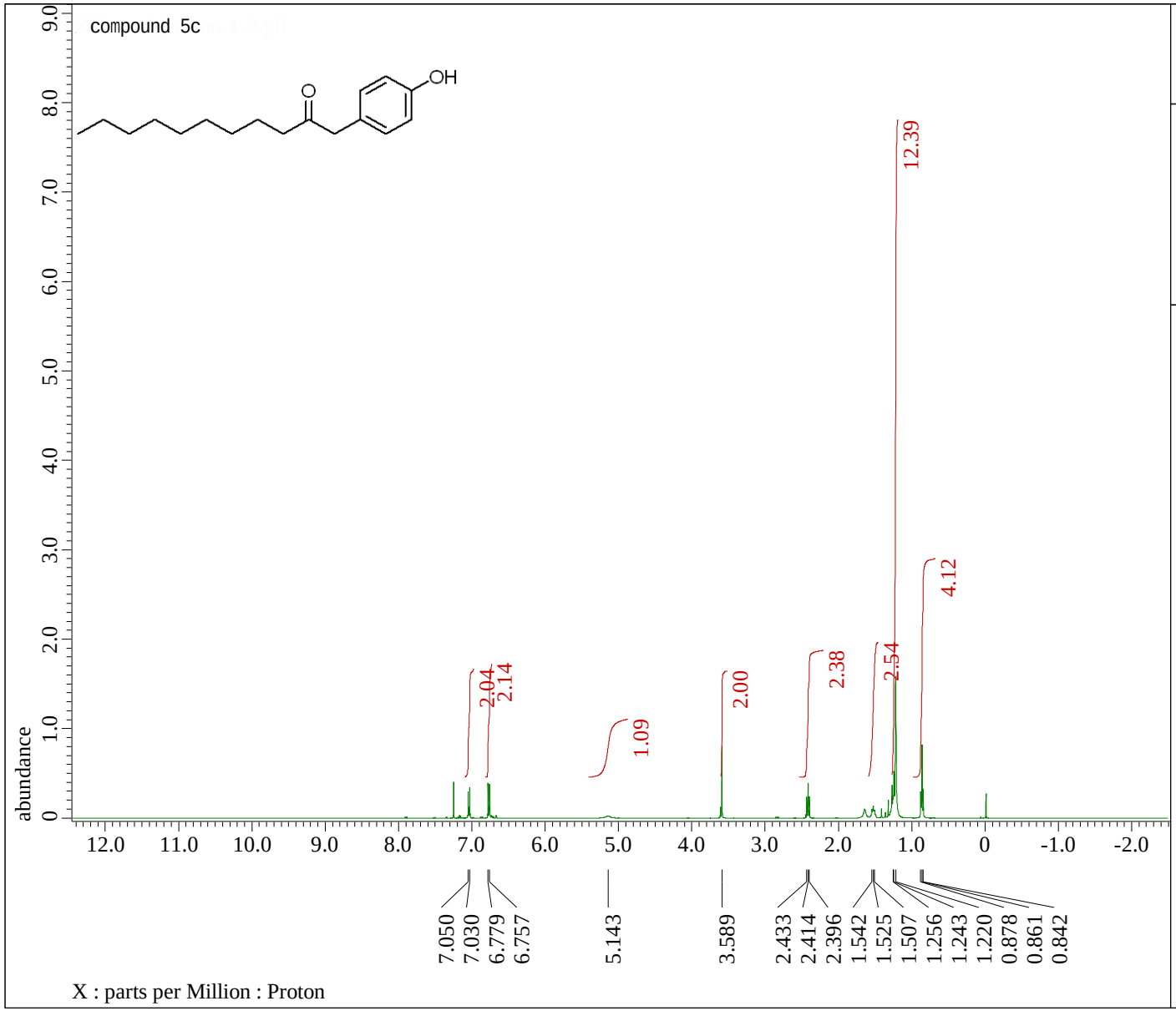
Derived from: ZRL-4-4_Carbon-1-1.jdf
```

```
Filename                = ZRL-4-4_Carbon-
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-4
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 20-SEP-2017 10:
Revision_Time           = 21-FEB-2018 17:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 520
Total_Scans             = 520

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 20.5[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



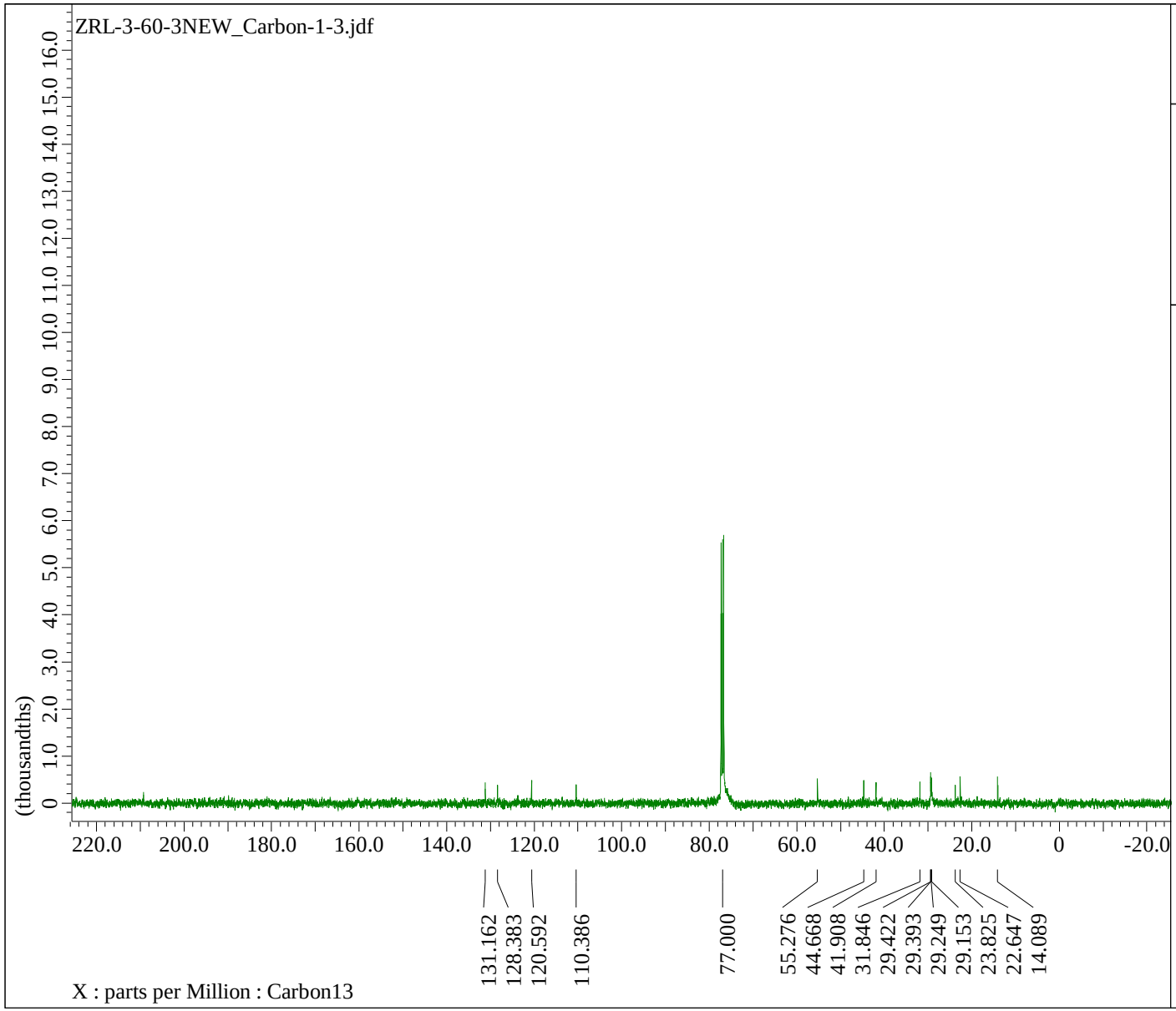

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-4_Proton-1-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-4
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 19-SEP-2017 21:49:
Revision_Time         = 21-FEB-2018 12:34:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 24.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

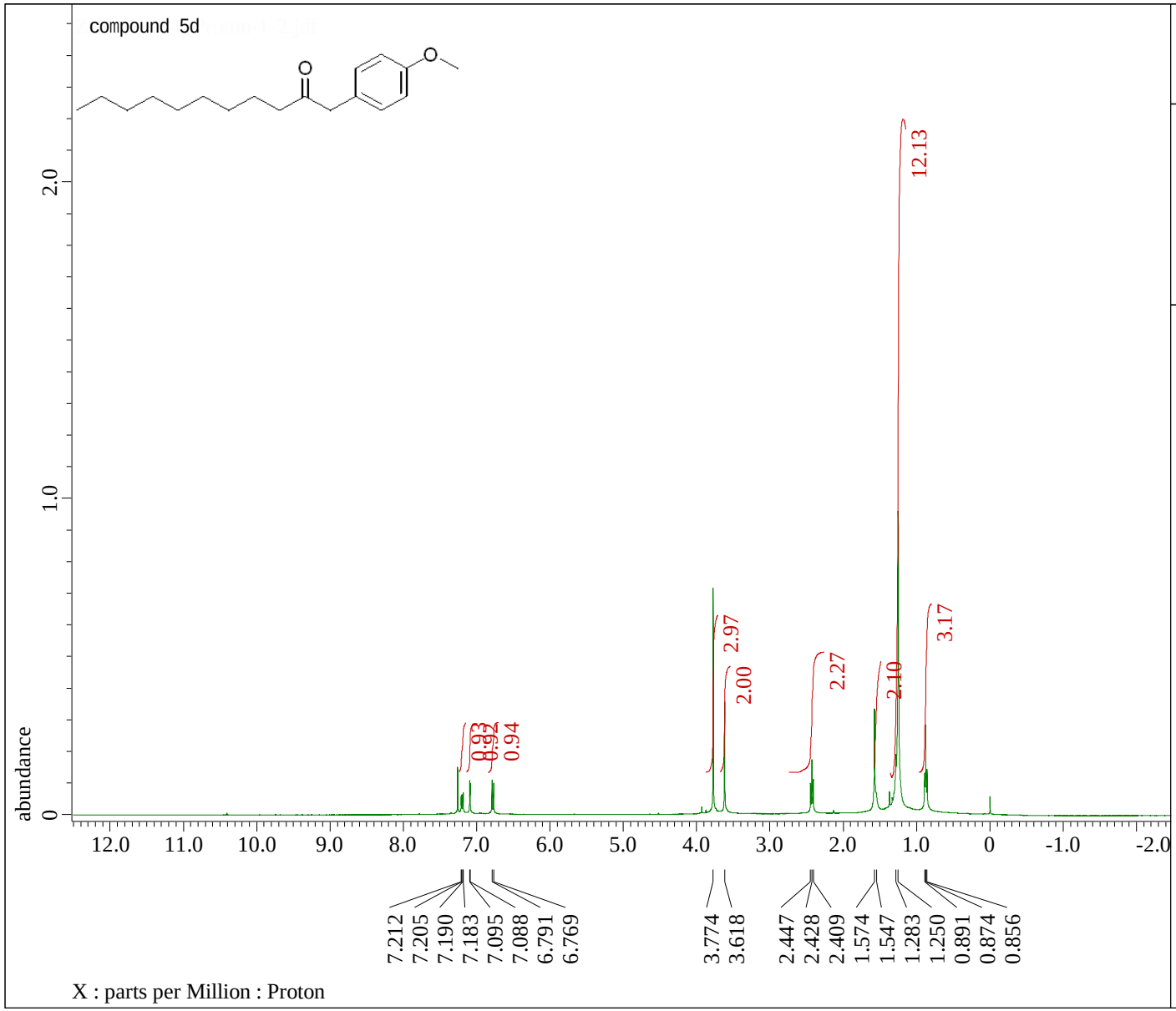
Derived from: ZRL-3-60-3NEW_Carbon-1-1.jdf
```

```
Filename                = ZRL-3-60-3NEW_C
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-3-60-3
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 15-JUL-2017 14:
Revision_Time           = 21-FEB-2018 17:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 317
Total_Scans             = 317

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 20.8[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



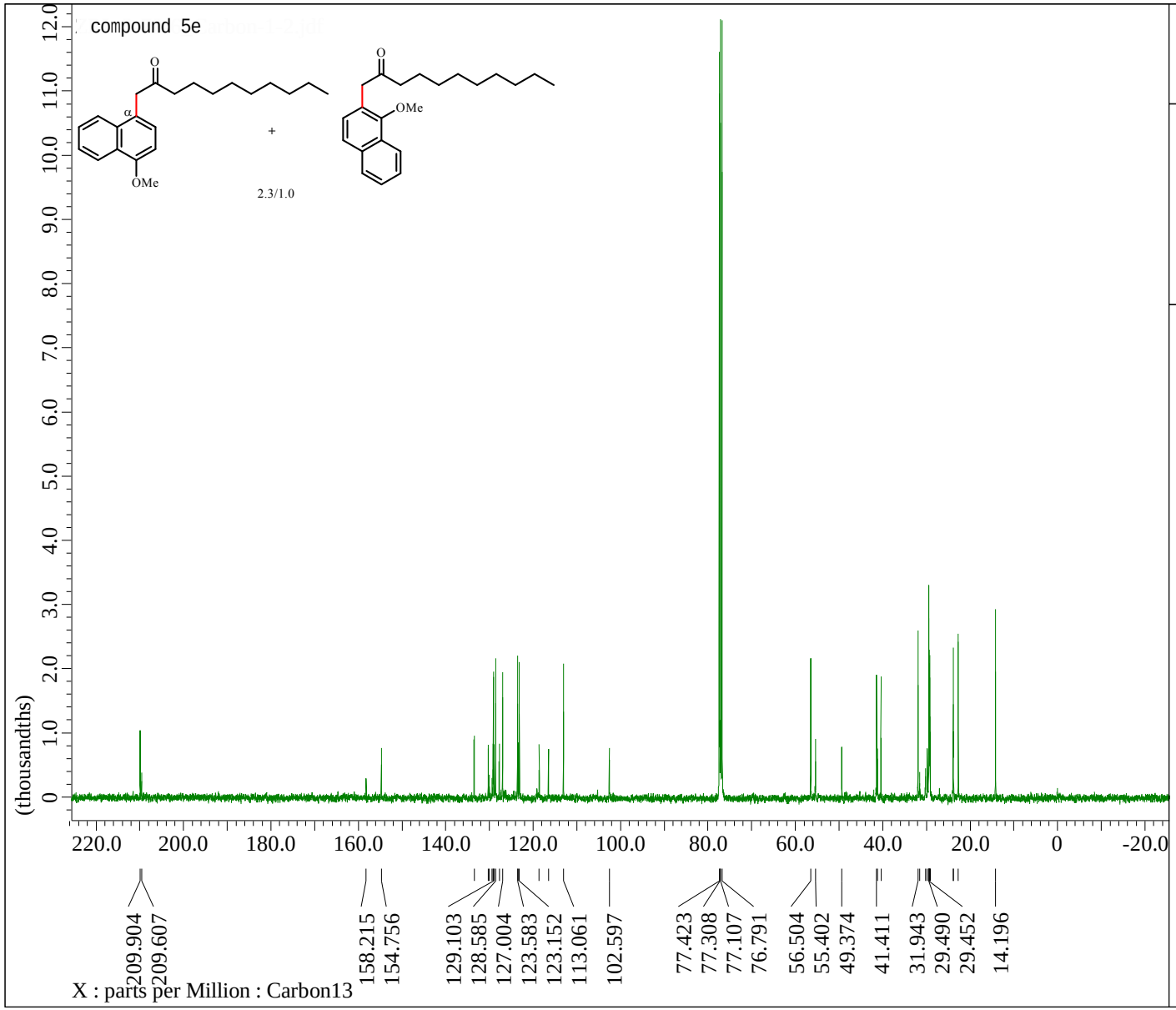

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-3-60-4_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-60-4
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 16-JUL-2017 15:09:
Revision_Time         = 21-FEB-2018 12:08:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 21.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

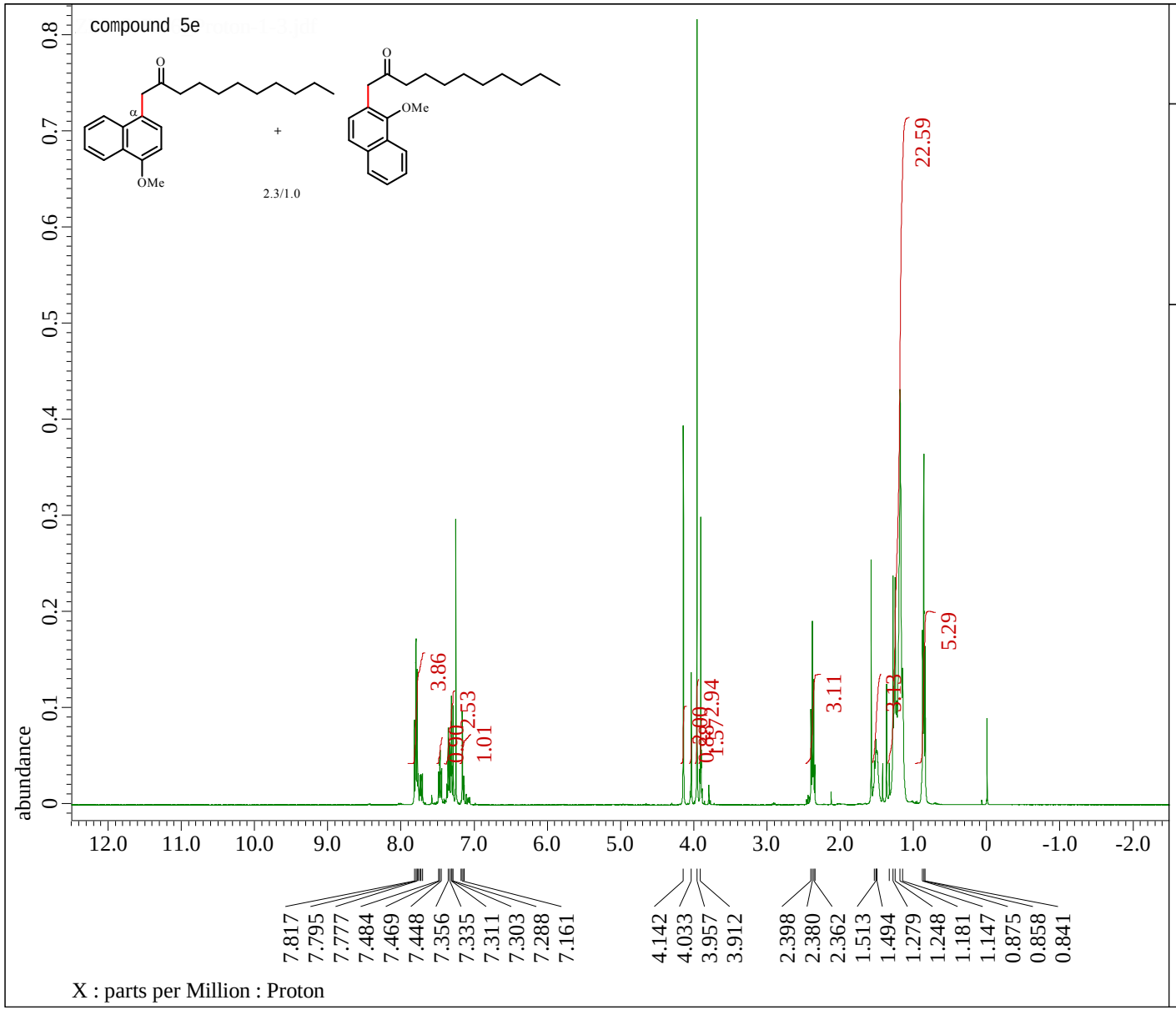
Derived from: ZRL-3-70-6_Carbon-1-1.jdf
```

```
Filename                  = ZRL-3-70-6_Carb
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-3-70-6
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 25-JUL-2017 20:
Revision_Time             =  6-FEB-2018 10:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 21.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

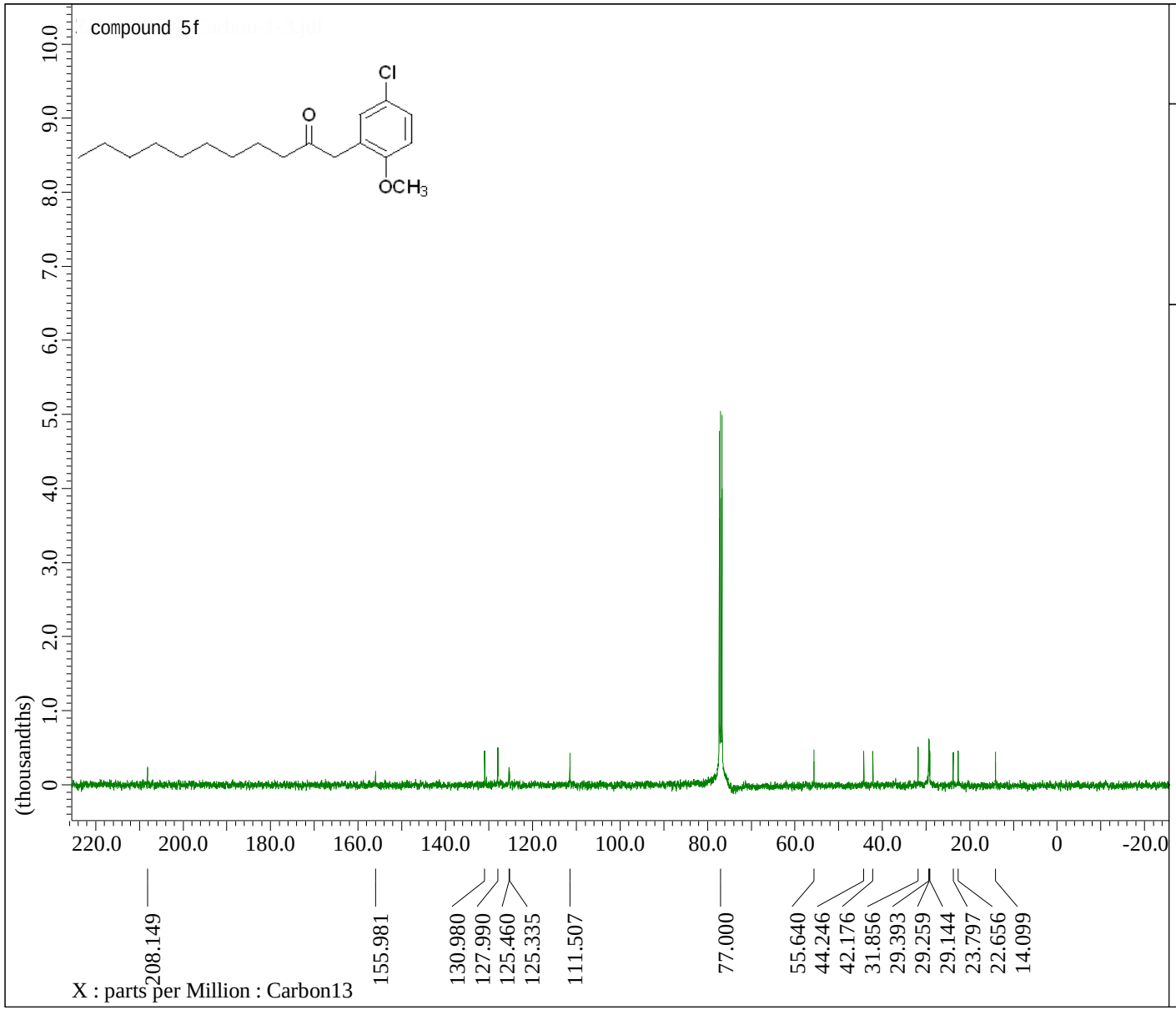
Derived from: ZRL-3-70-6_Proton-1-1.jdf
```

```
Filename              = ZRL-3-70-6_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-70-6
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-JUL-2017 20:53:
Revision_Time         =  6-FEB-2018 11:01:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 21.1[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

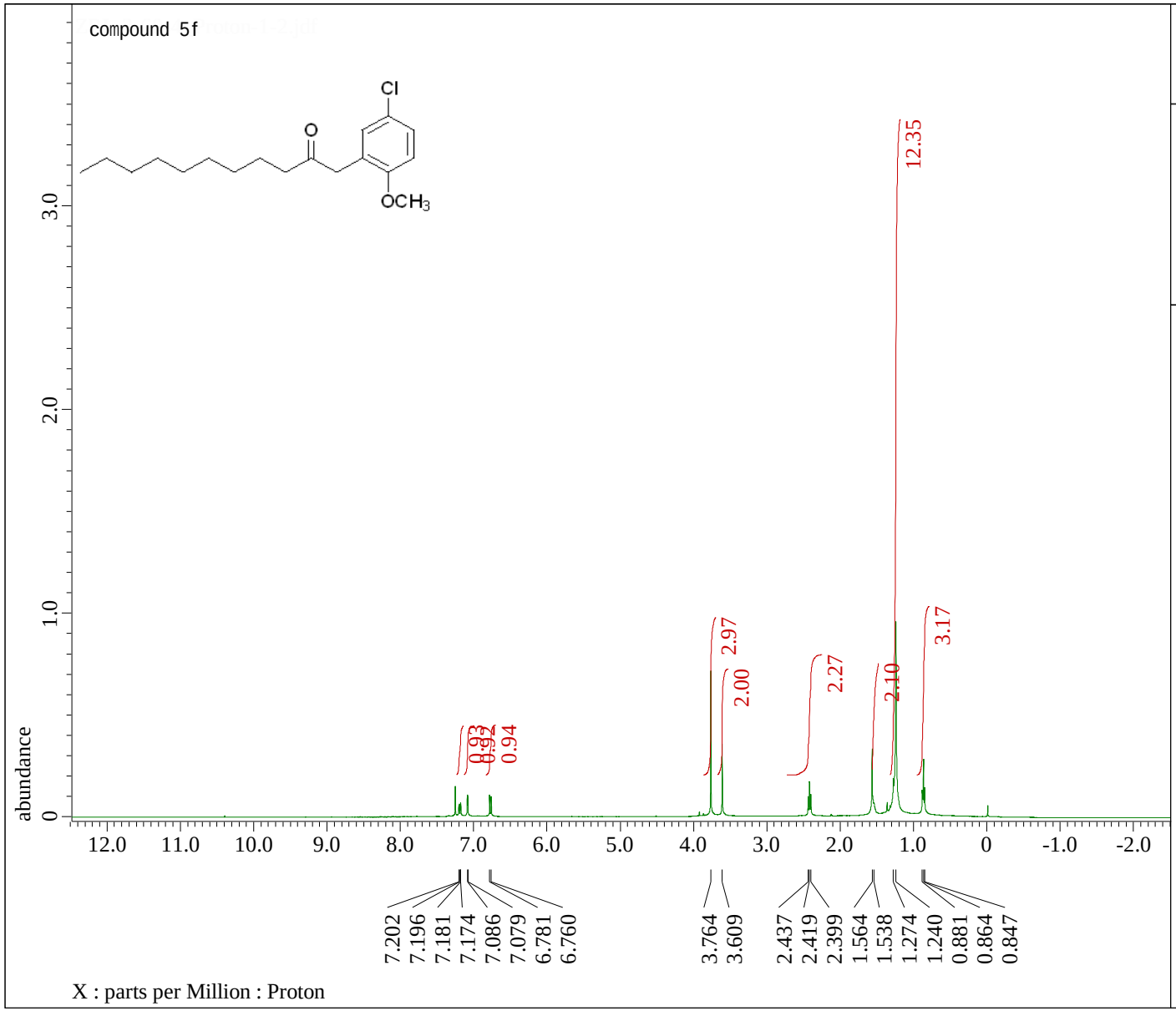
Derived from: ZRL-3-60-4_Carbon-1-1.jdf
```

```
Filename                 = ZRL-3-60-4_Carb
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-3-60-4
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 16-JUL-2017 15:
Revision_Time            =  6-DEC-2017 21:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 21.8[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



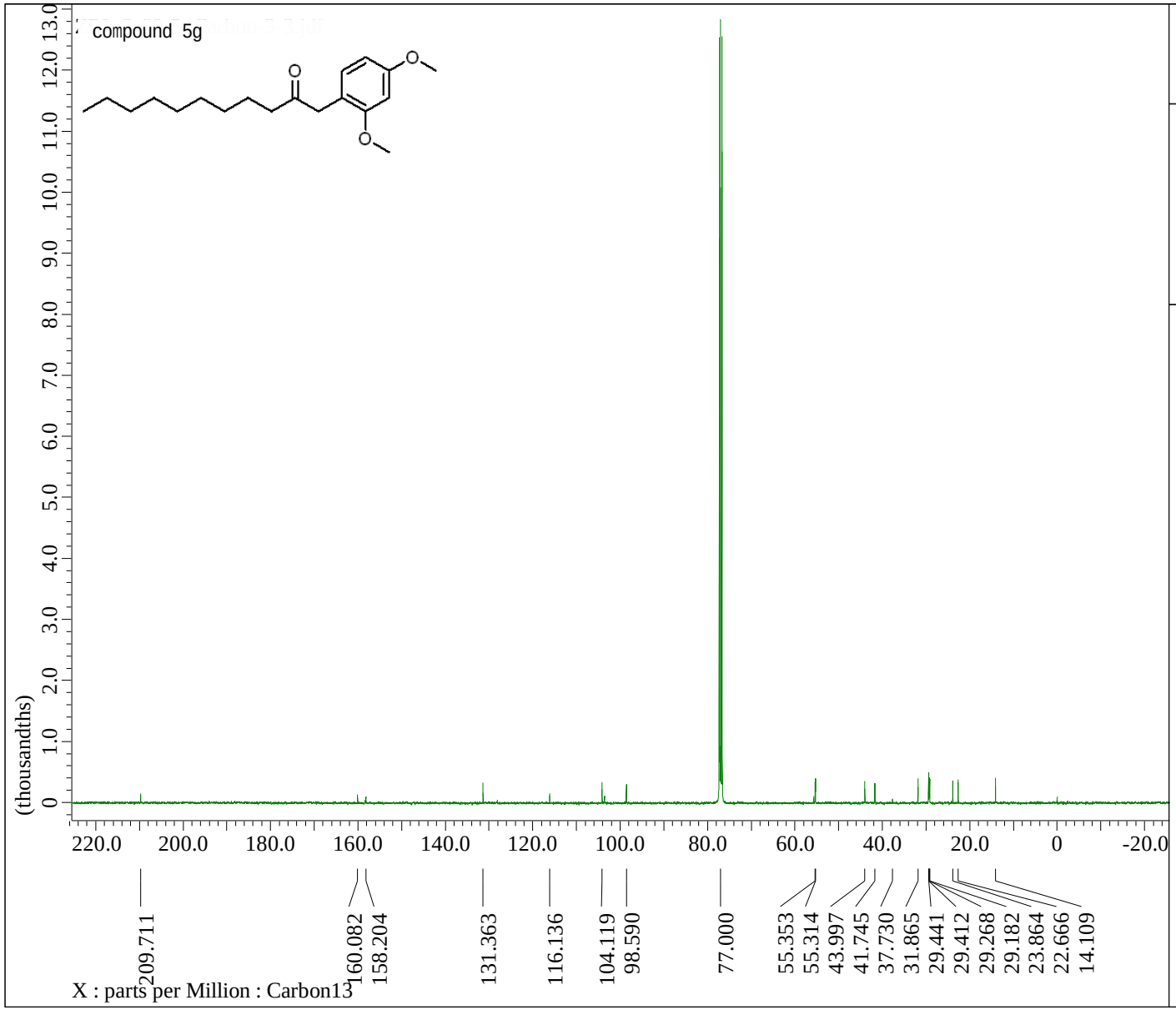

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

Filename              = ZRL-3-60-4_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-60-4
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 16-JUL-2017 15:09:
Revision_Time         = 21-FEB-2018 12:38:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 21.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

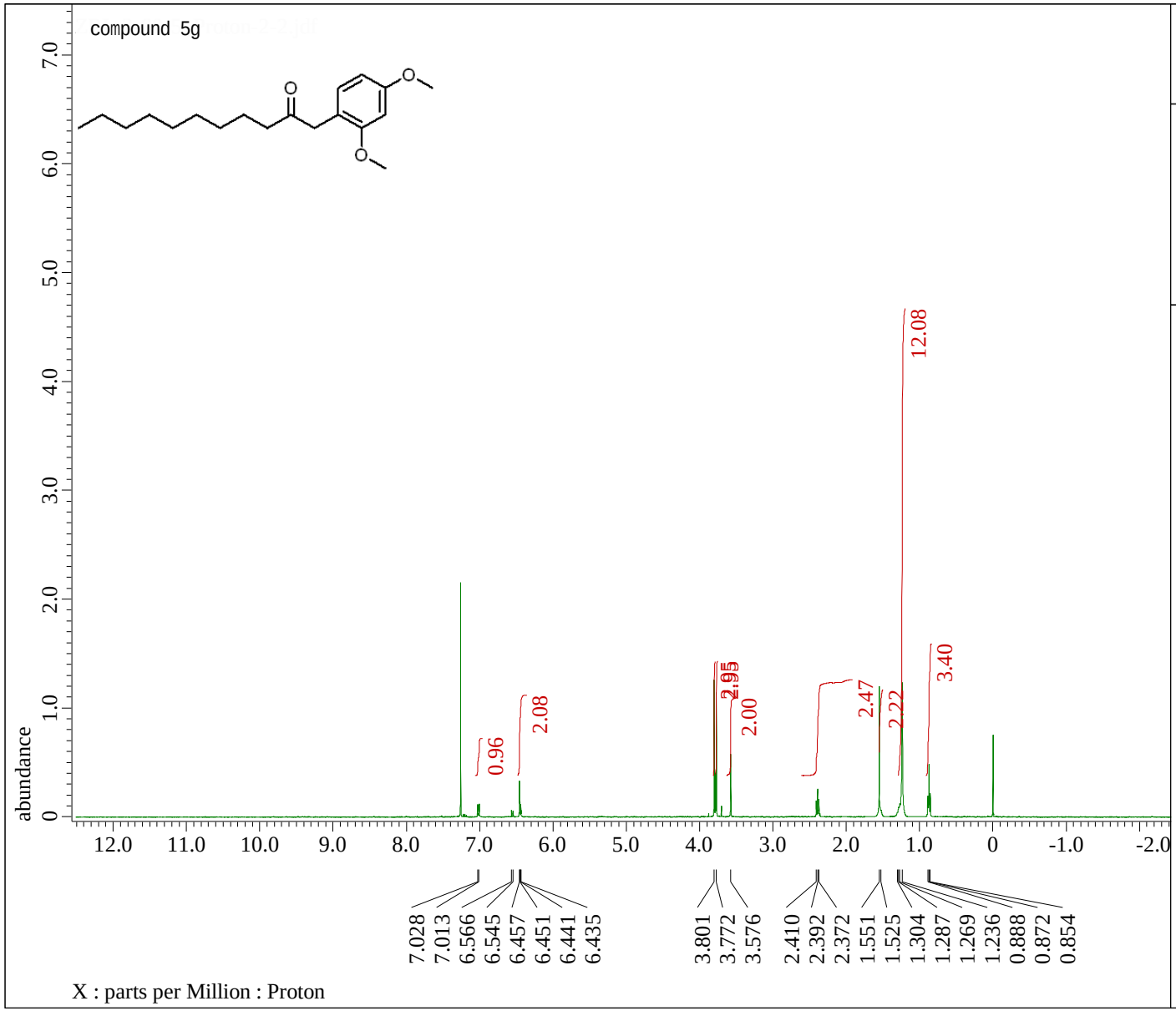
Derived from: ZRL-3-60-5_Carbon-3-1.jdf
```

```
Filename                  = ZRL-3-60-5_Carb
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-3-60-5
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 27-OCT-2017 22:
Revision_Time             =  6-DEC-2017 21:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 10240
Total_Scans               = 10240

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 19.8[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



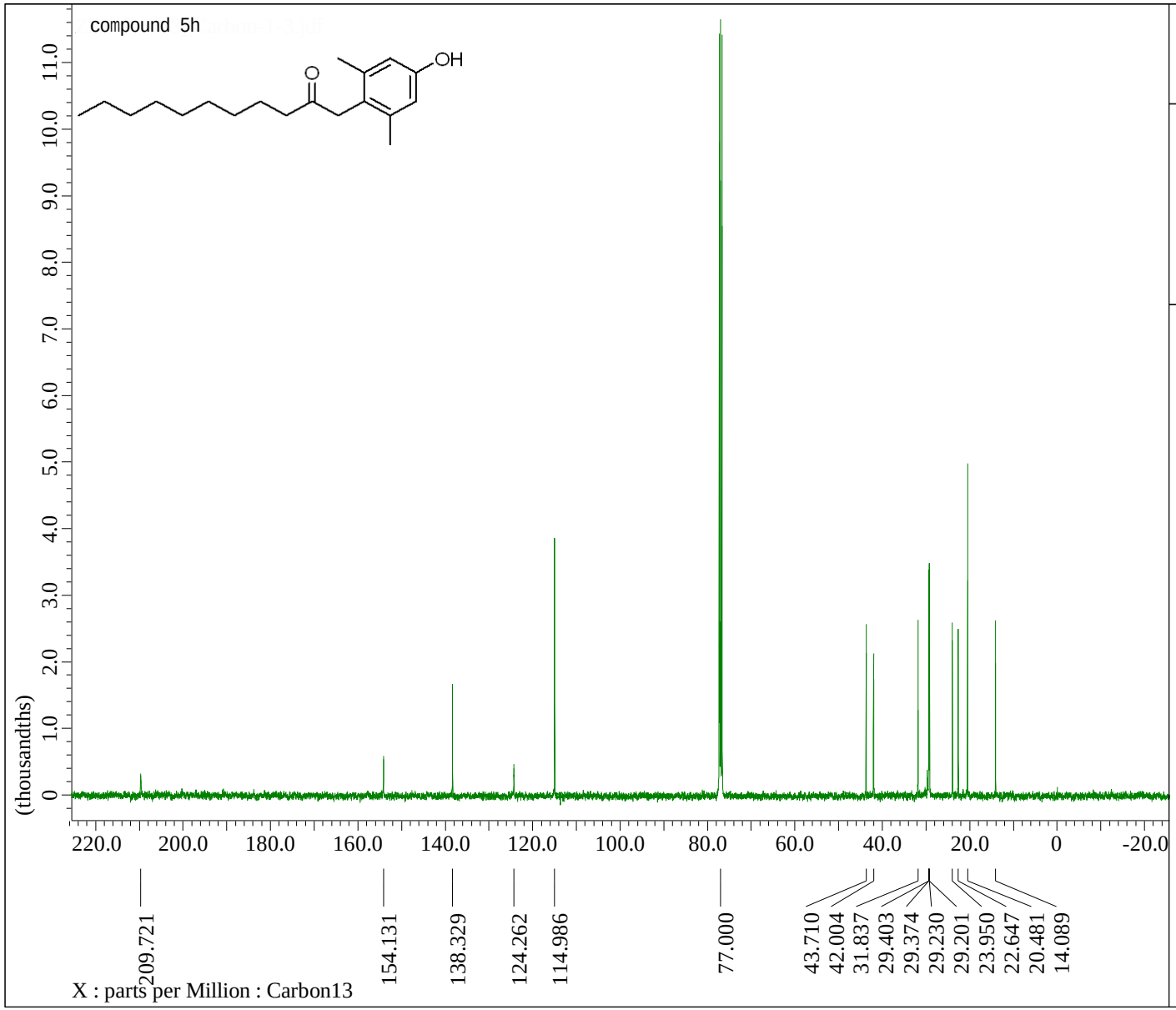

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-3-60-5_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-60-5
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 27-OCT-2017 21:37:
Revision_Time         = 21-FEB-2018 12:13:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 20.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

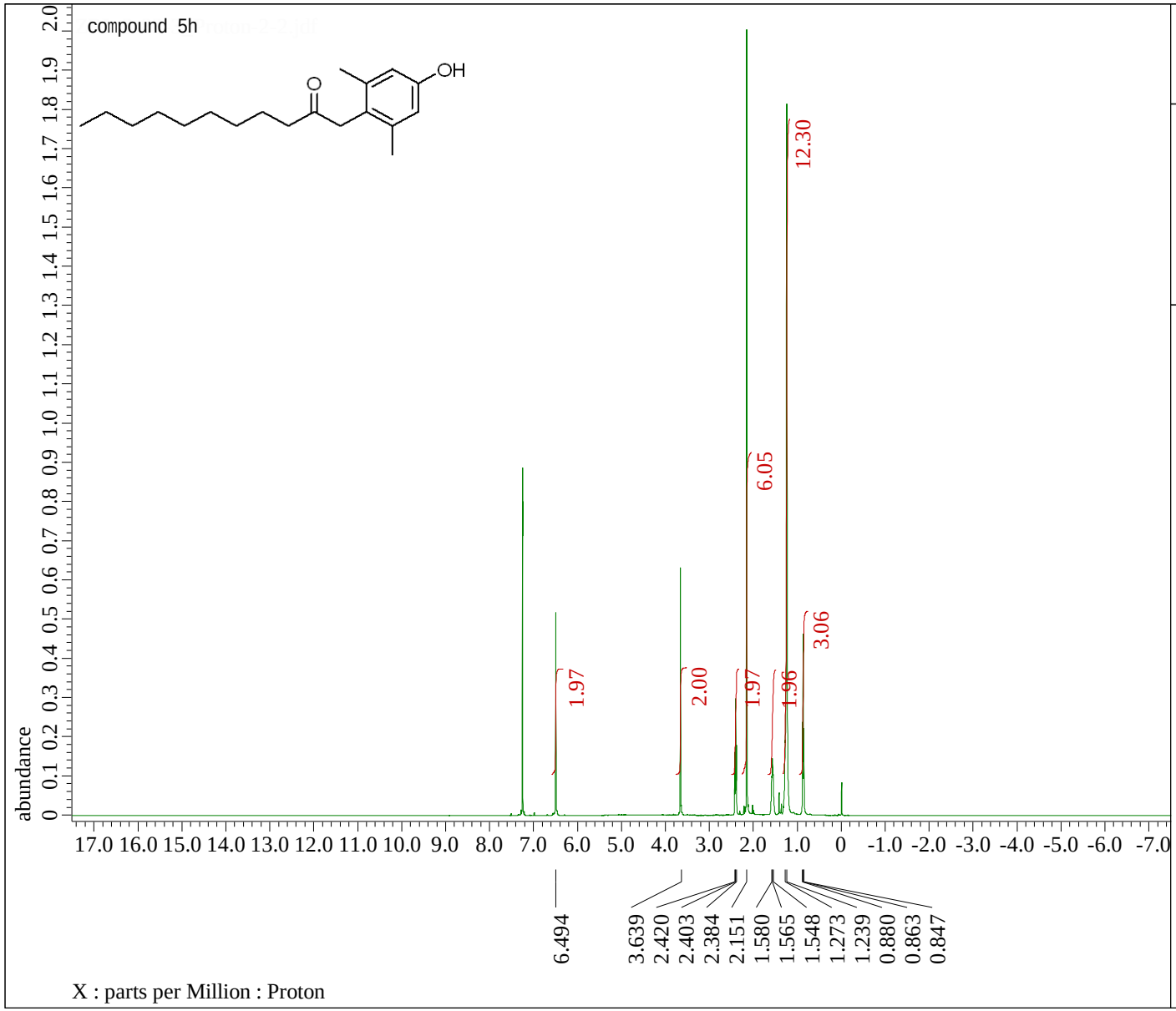
Derived from: ZRL-3-83-3_Carbon-1-1.jdf
```

```
Filename                  = ZRL-3-83-3_Carb
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-3-83-3
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 17-AUG-2017 16:
Revision_Time             =  6-DEC-2017 21:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 22.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



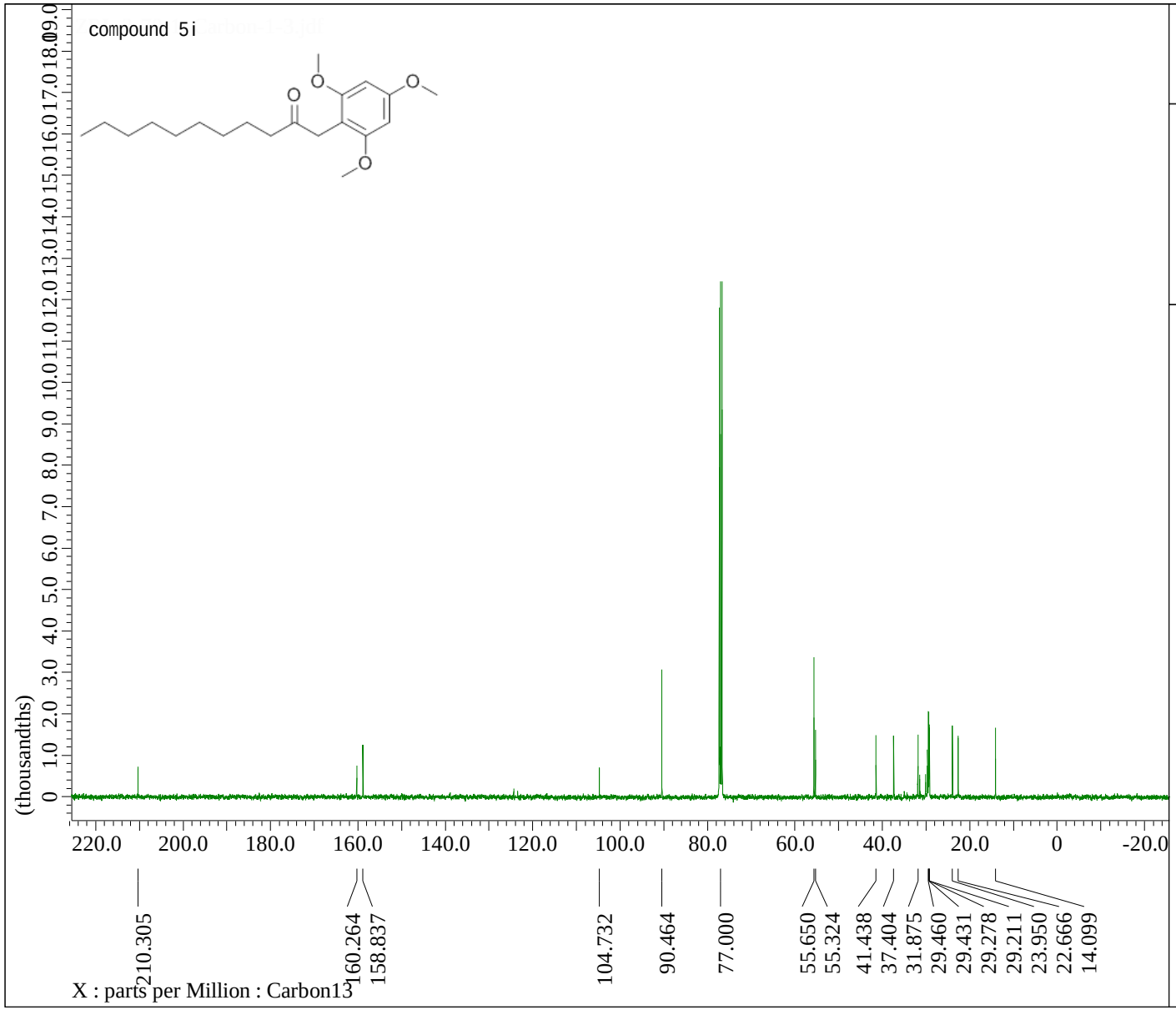

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-3-83-3_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-83-3
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 17-AUG-2017 16:16:
Revision_Time         = 21-FEB-2018 12:21:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 1.31072[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.76293945[Hz]
X_Sweep               = 12.5[kHz]
X_Sweep_Clipped       = 10[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 21.3[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 1.31072[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

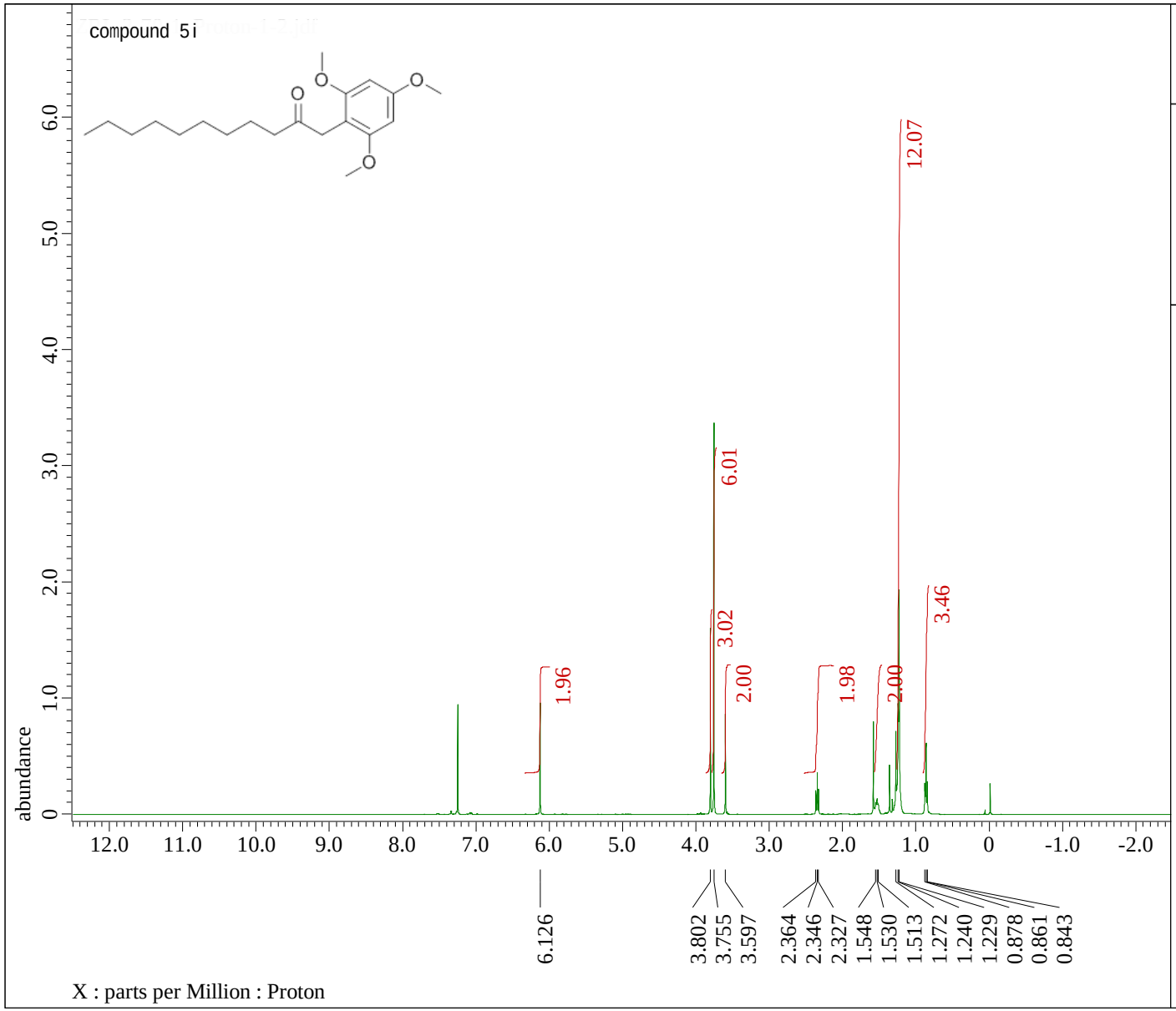
Derived from: ZRL-3-70-1_Carbon-1-1.jdf
```

```
Filename                  = ZRL-3-70-1_Carb
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-3-70-1
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 25-JUL-2017 19:
Revision_Time             =  6-DEC-2017 21:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 21.7[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



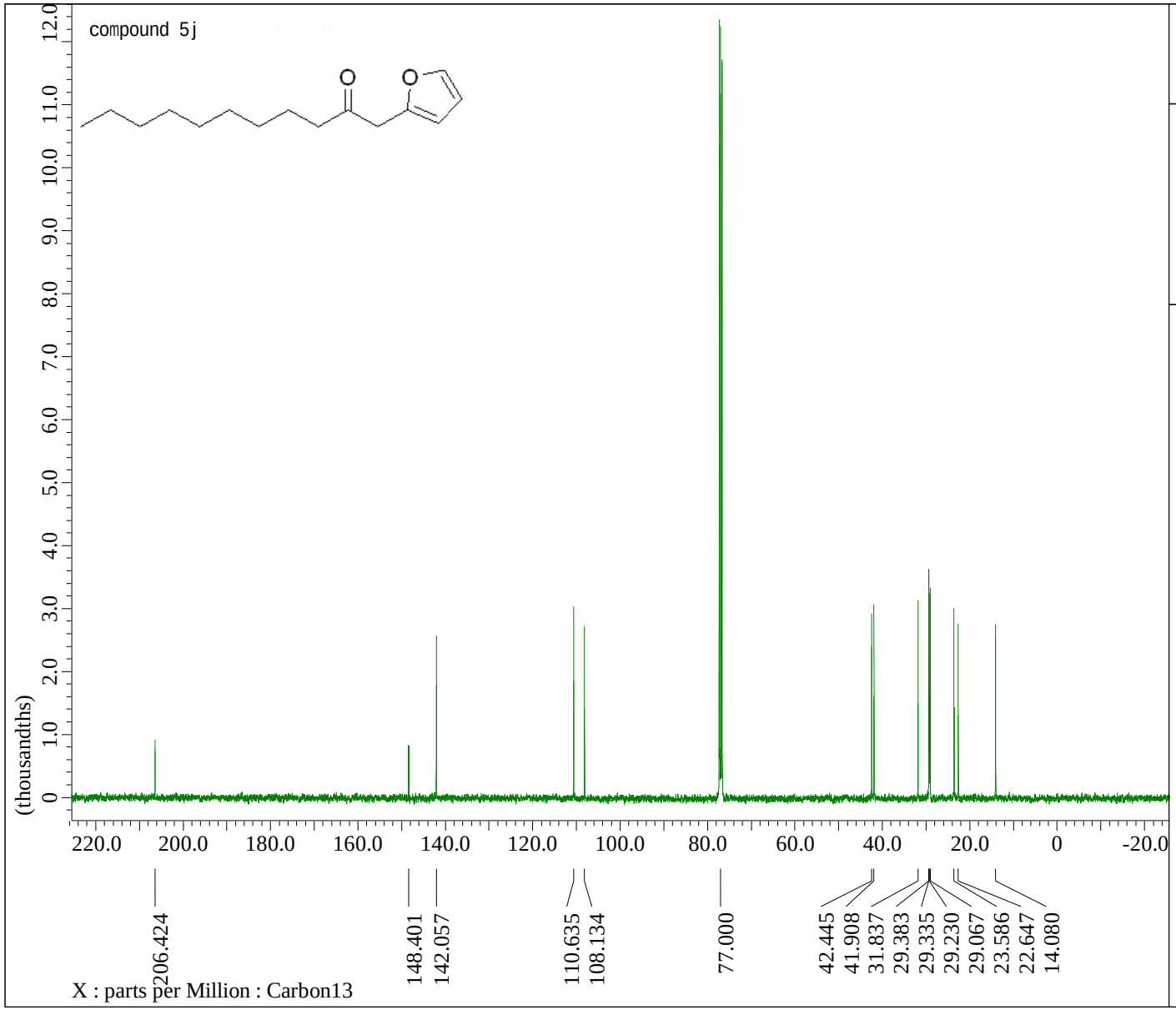

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-3-70-1_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-3-70-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-JUL-2017 19:54:
Revision_Time         = 21-FEB-2018 12:17:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 21.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

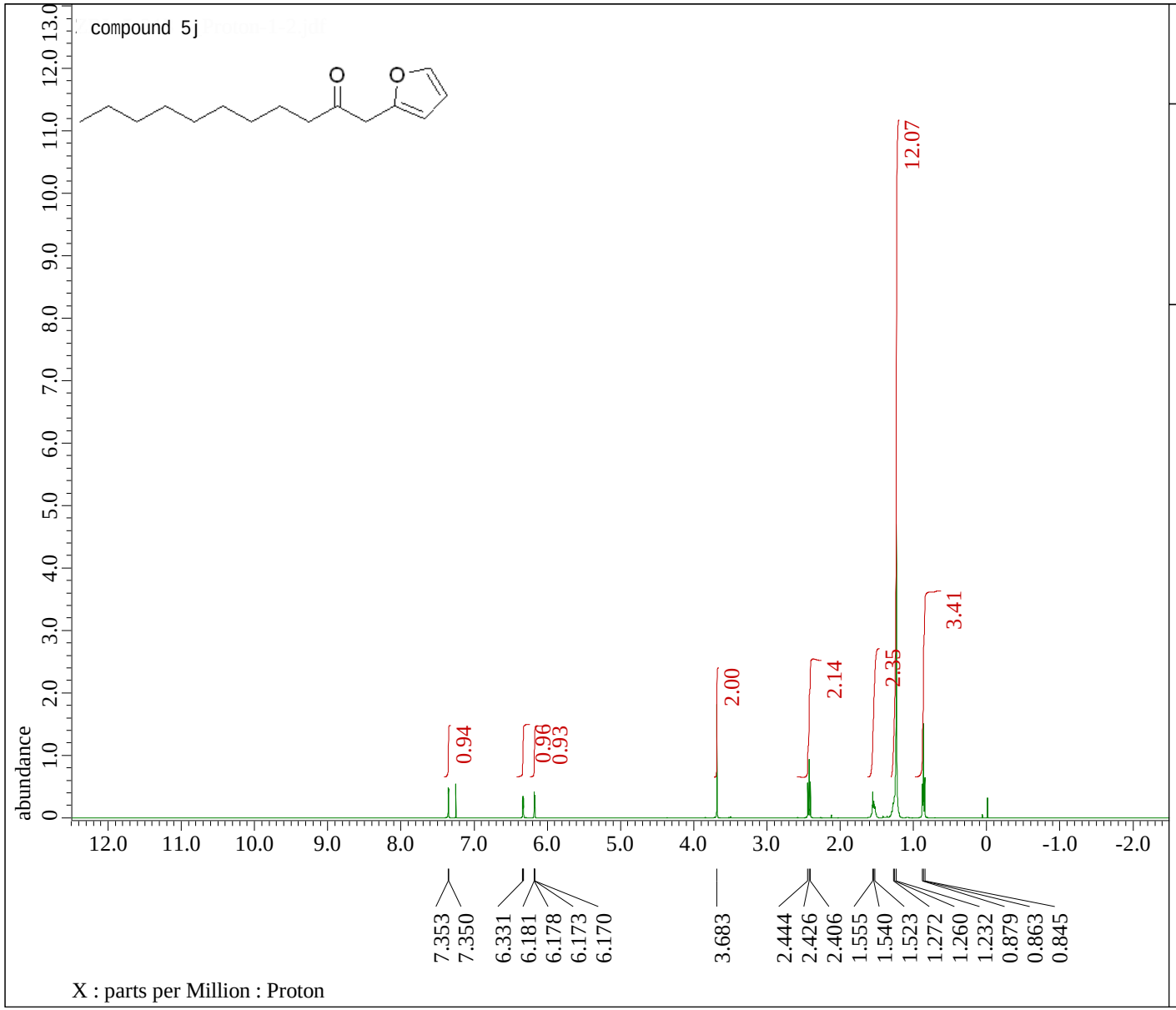
Derived from: ZRL-5-213 1_Carbon-1-1.jdf
```

```
Filename                  = ZRL-5-213 1_Car
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-213 1
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 26-NOV-2017 17:
Revision_Time             =  6-DEC-2017 13:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 22.9[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



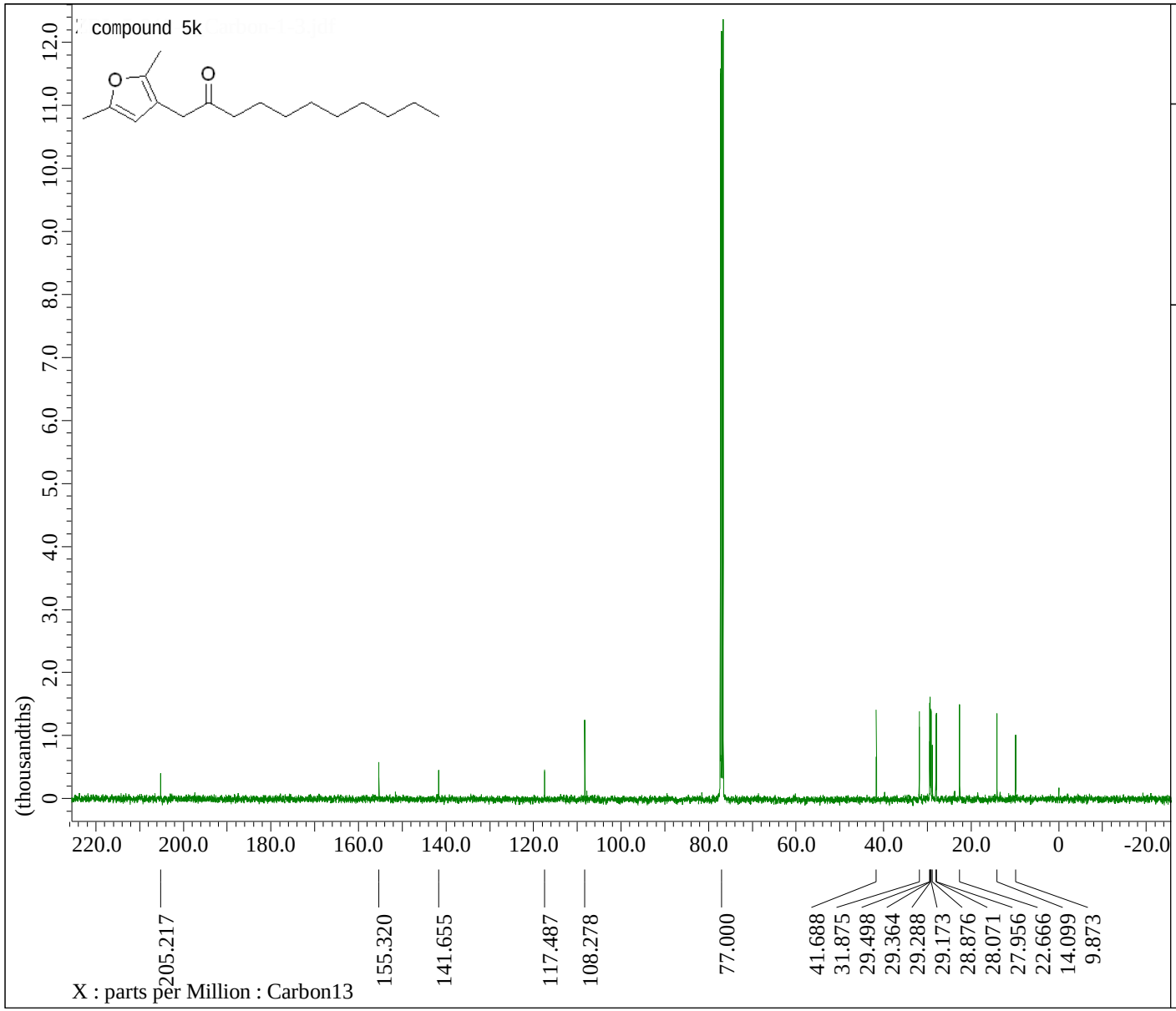

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-213 1_Proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-213 1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 26-NOV-2017 17:15:
Revision_Time         = 21-FEB-2018 13:12:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

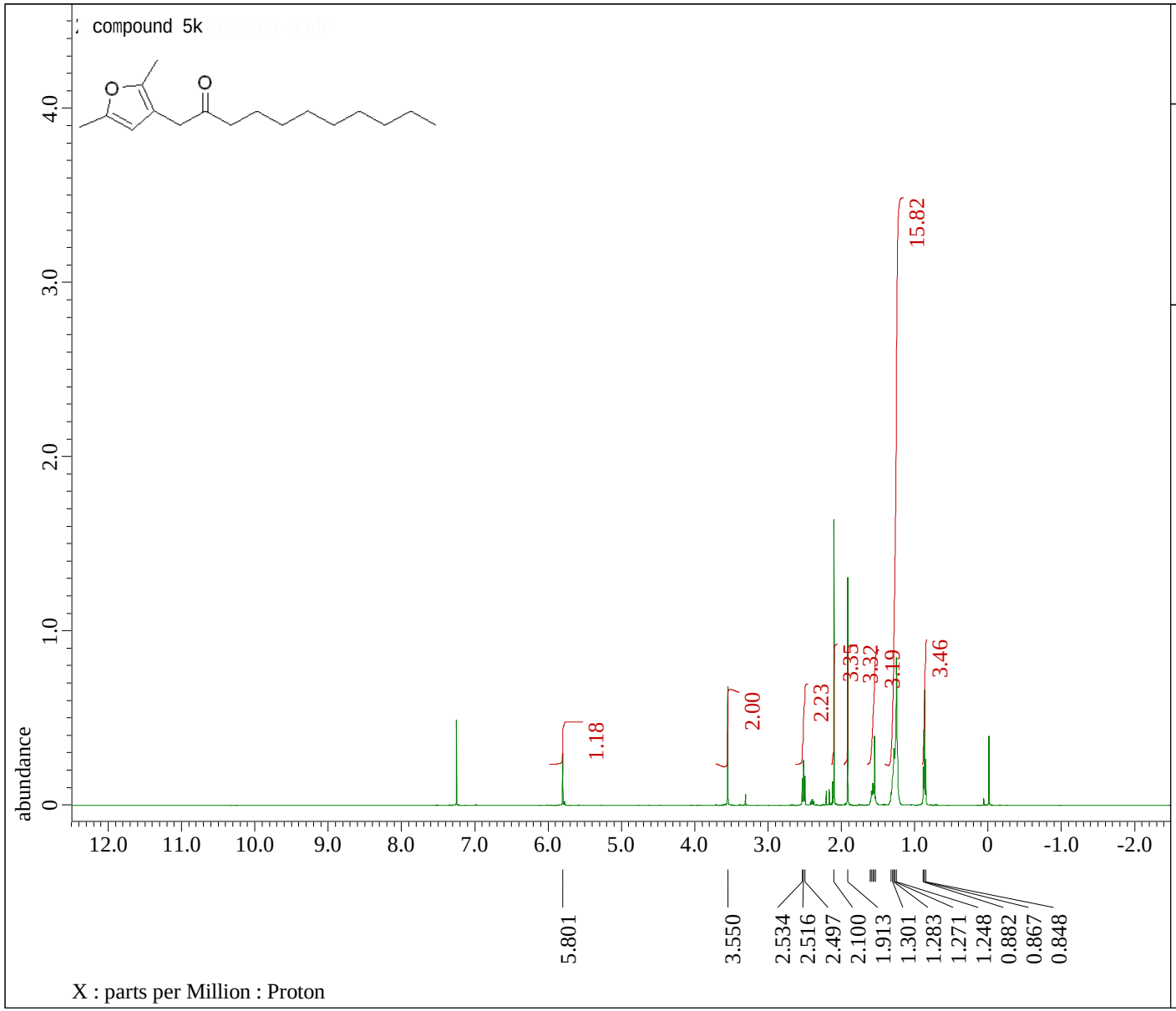
Derived from: ZRL-5-212-1_Carbon-1-1.jdf
```

```
Filename                 = ZRL-5-212-1_Car
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-5-212-1
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 25-NOV-2017 17:
Revision_Time            =  7-DEC-2017 17:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 22.4[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

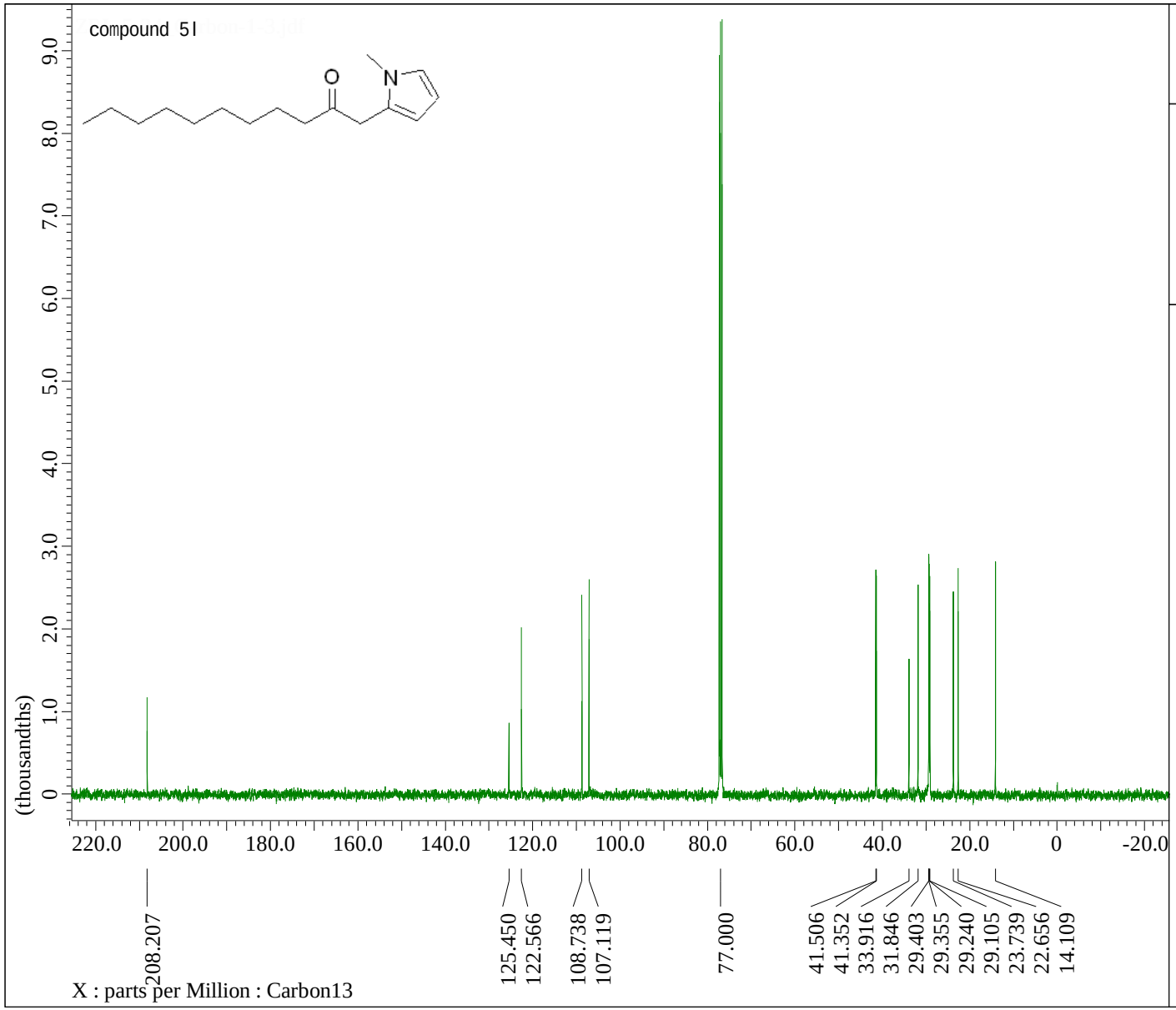
Derived from: ZRL-5-212-1_Proton-1-1.jdf
```

```
Filename              = ZRL-5-212-1_Proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-212-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-NOV-2017 16:59:
Revision_Time         =  5-DEC-2017 22:31:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

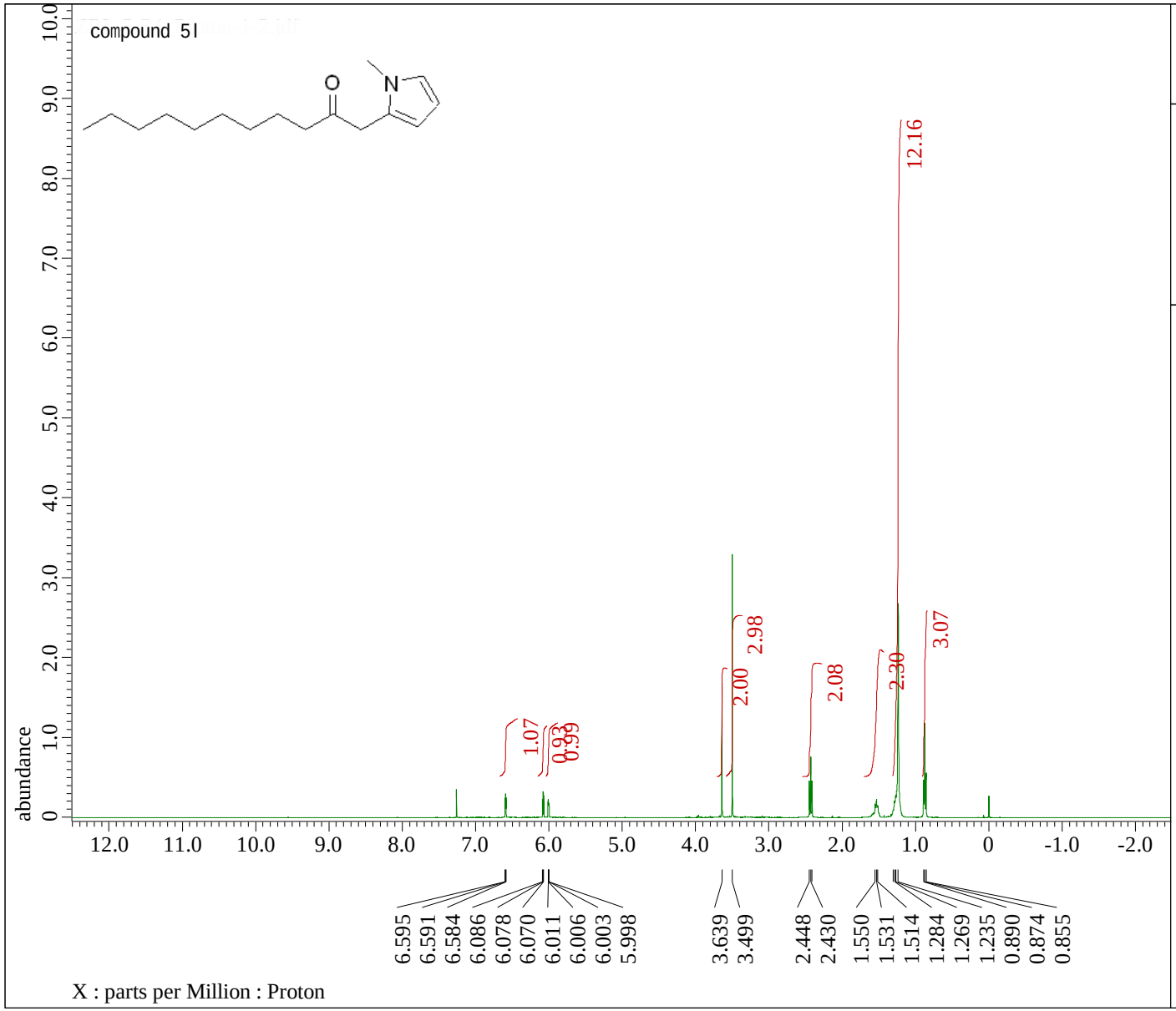
Derived from: ZRL-5-34_Carbon-1-1.jdf
```

```
Filename                  = ZRL-5-34_Carbon
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-34
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 23-NOV-2017 08:
Revision_Time             =  5-DEC-2017 20:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 17.9[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



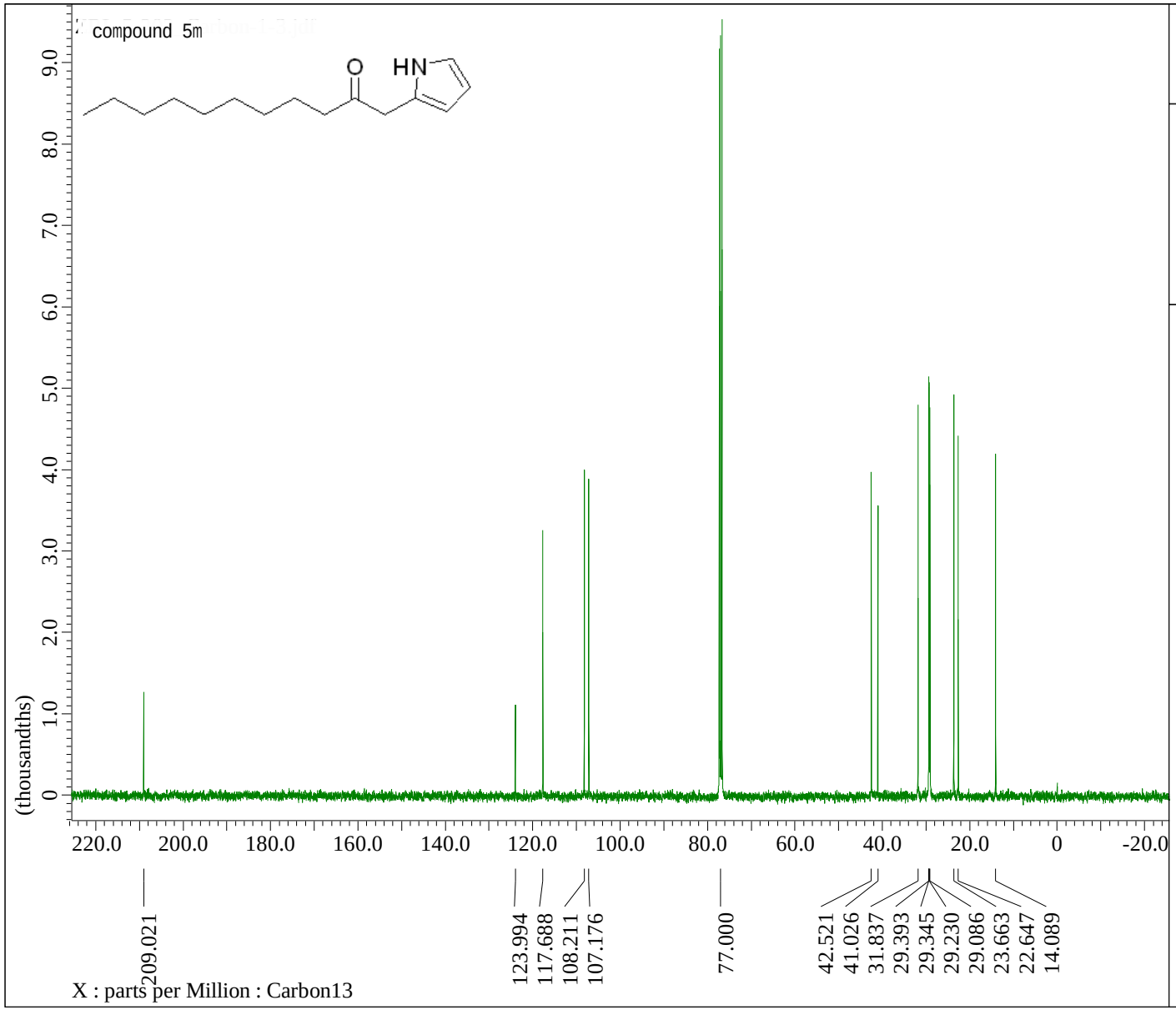

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-34_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-34
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 23-NOV-2017 08:05:
Revision_Time         = 21-FEB-2018 12:52:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 17.5[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

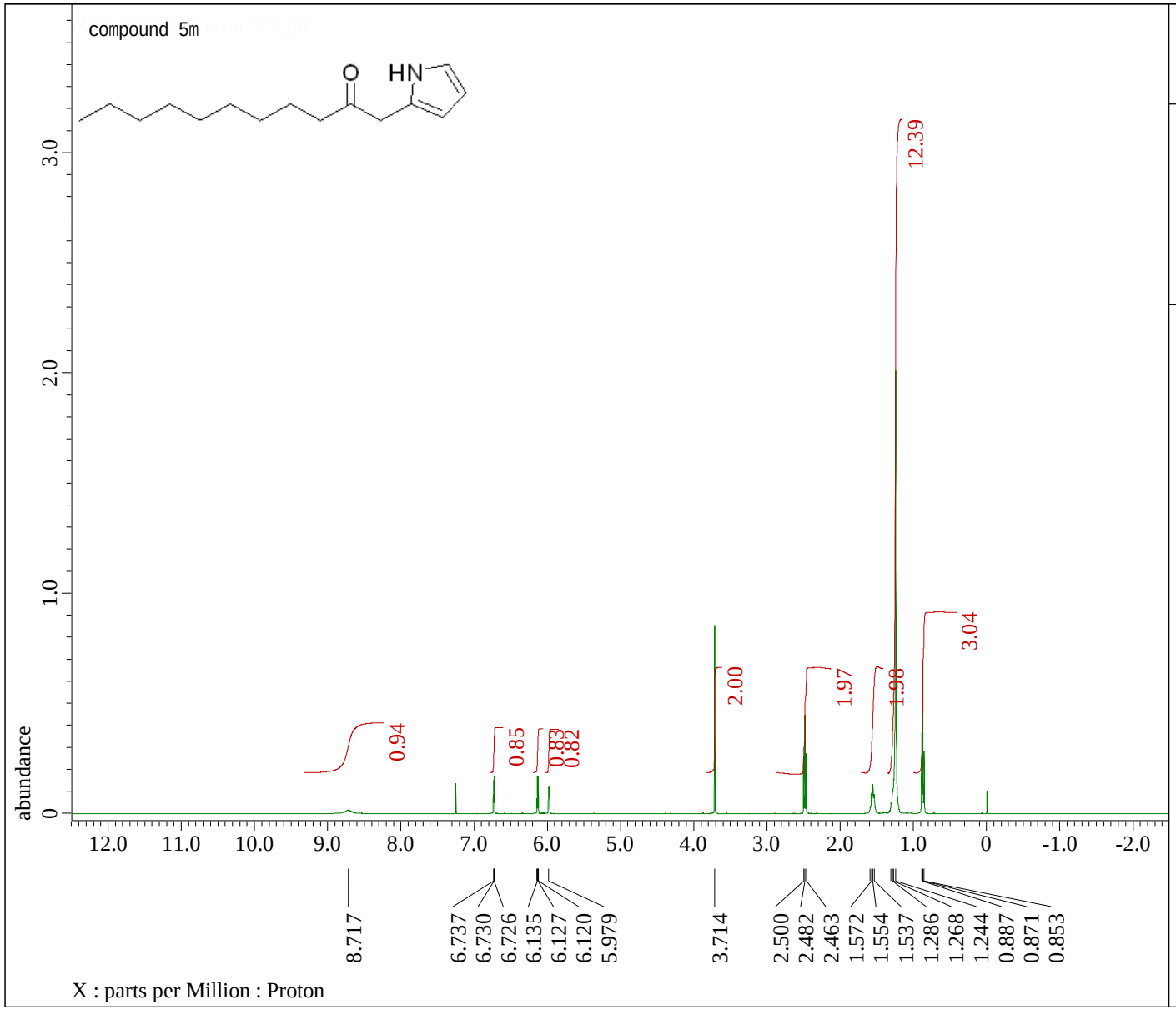
Derived from: ZRL-5-202_Carbon-1-1.jdf
```

```
Filename                  = ZRL-5-202_Carbo
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-202
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 25-NOV-2017 15:
Revision_Time             =  5-DEC-2017 22:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 23.8[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



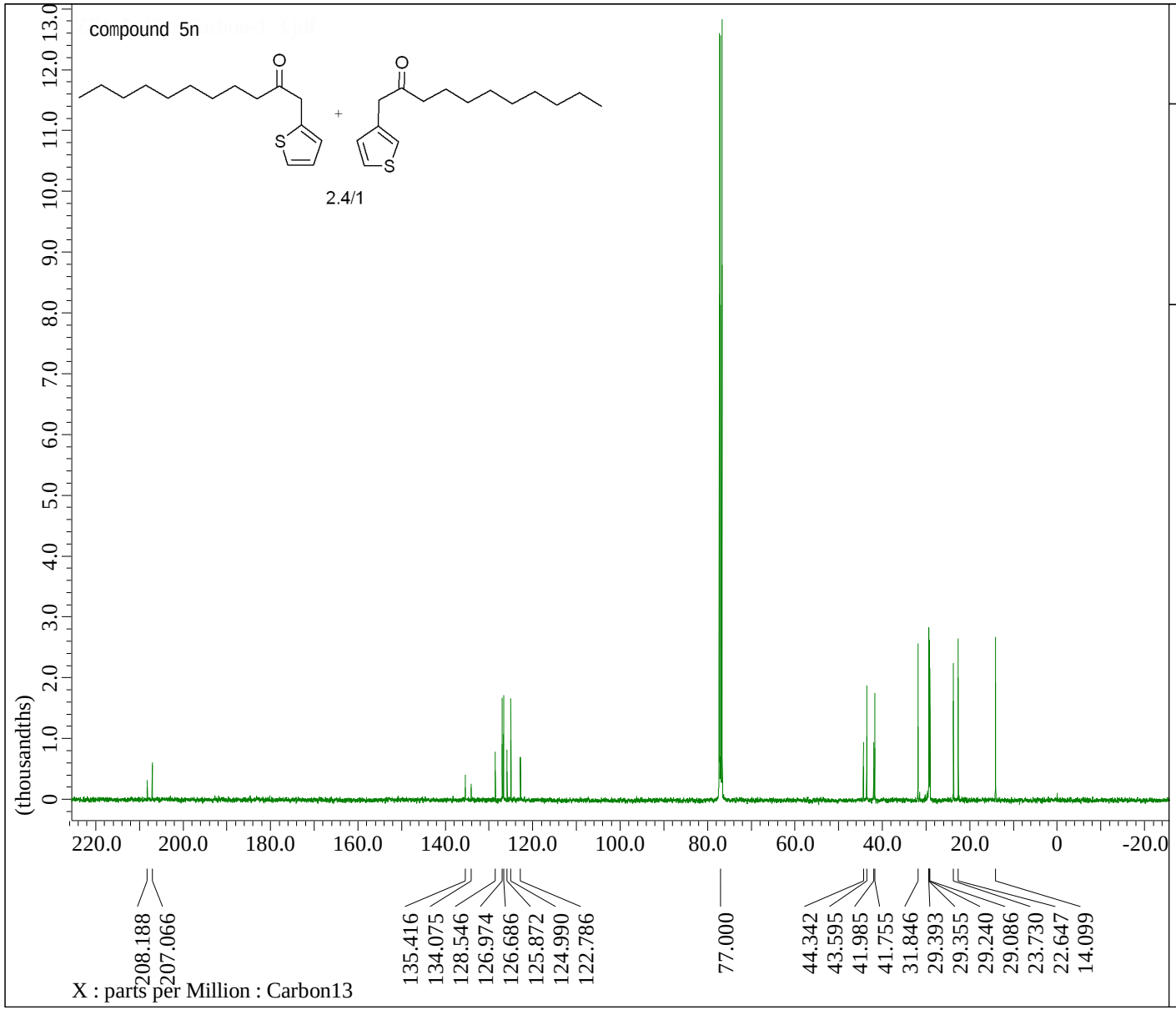

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-202_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-202
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-NOV-2017 14:58:
Revision_Time         = 21-FEB-2018 13:08:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 22.7[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



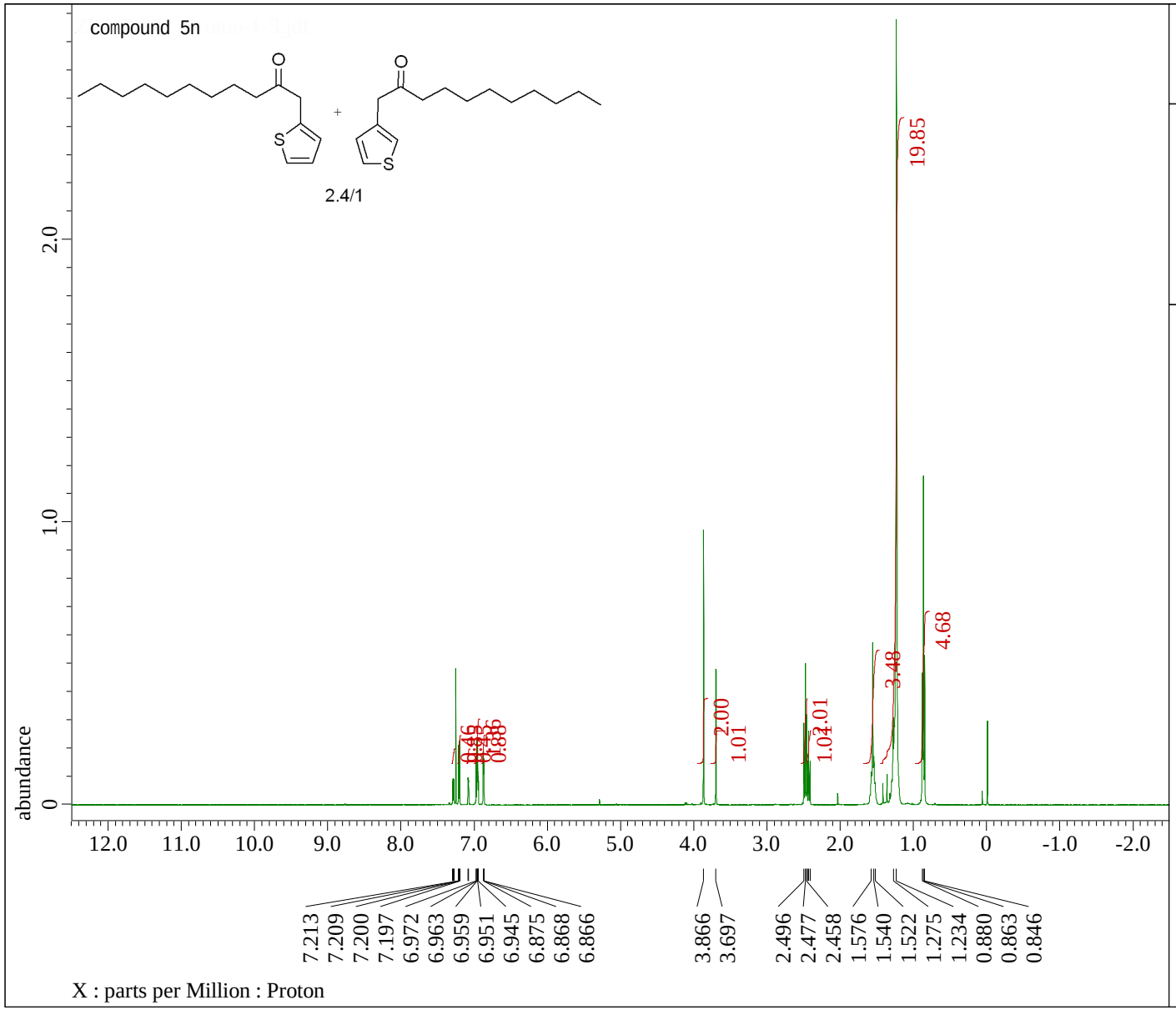

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-5-221_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-5-221
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 26-NOV-2017 00:
Revision_Time           =  6-FEB-2018 11:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 2400
Total_Scans             = 2400

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 22[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



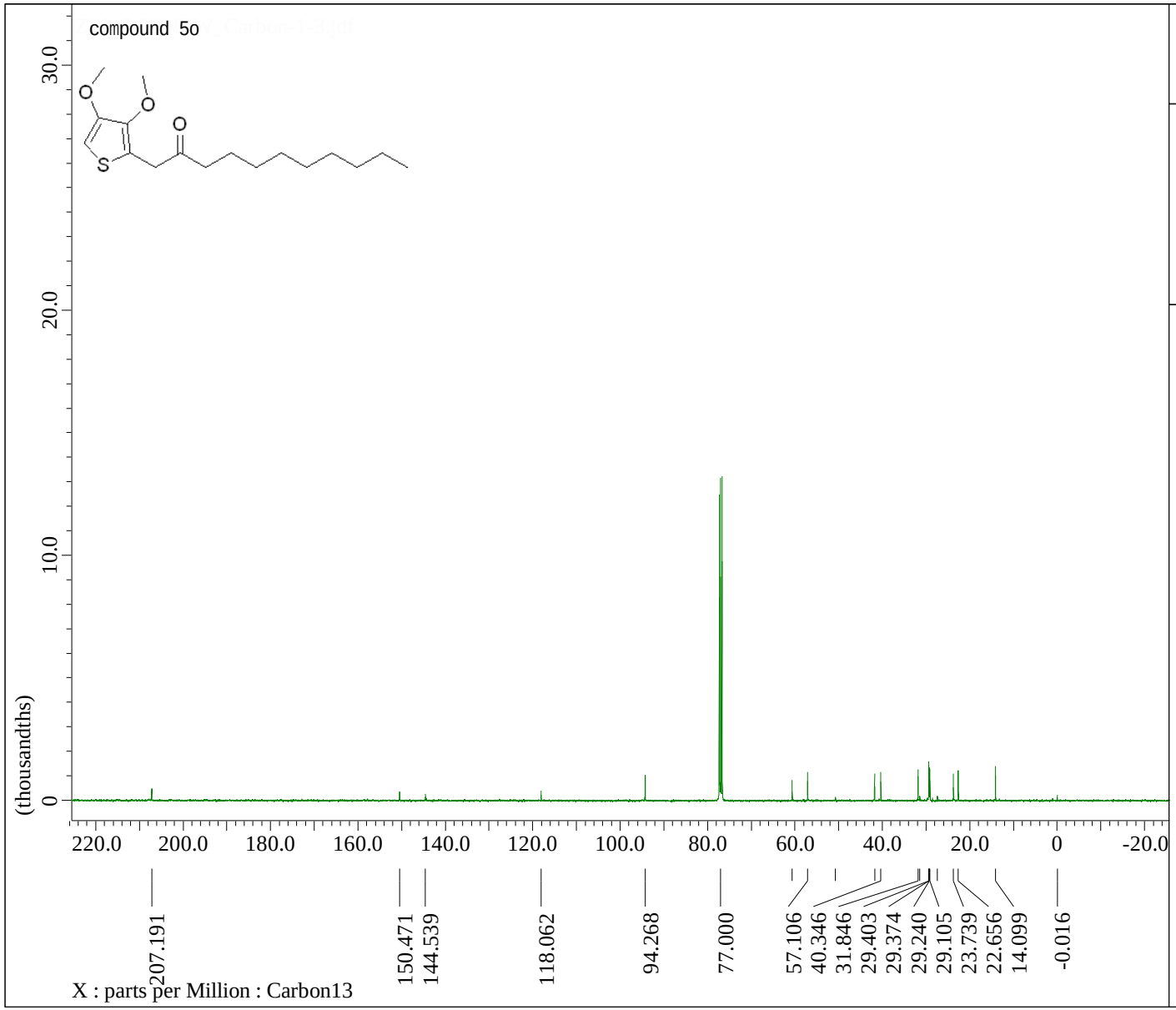

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-221_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-221
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 26-NOV-2017 00:26:
Revision_Time         =  6-FEB-2018 11:13:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 21.3[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



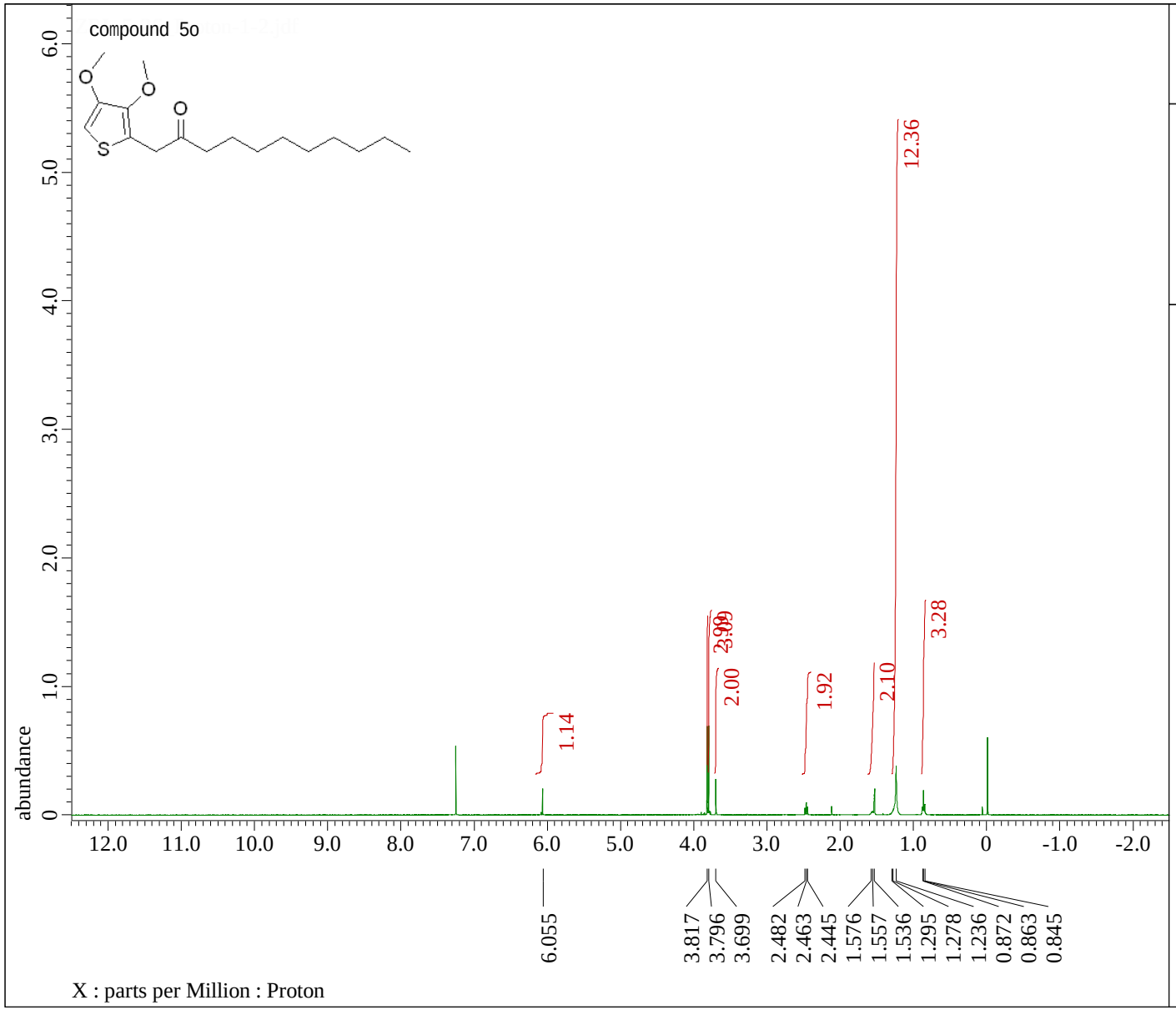

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-5-36NEW_Car
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-5-36NEW
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 25-NOV-2017 22:
Revision_Time           = 22-FEB-2018 21:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 2400
Total_Scans             = 2400

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 21.2[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



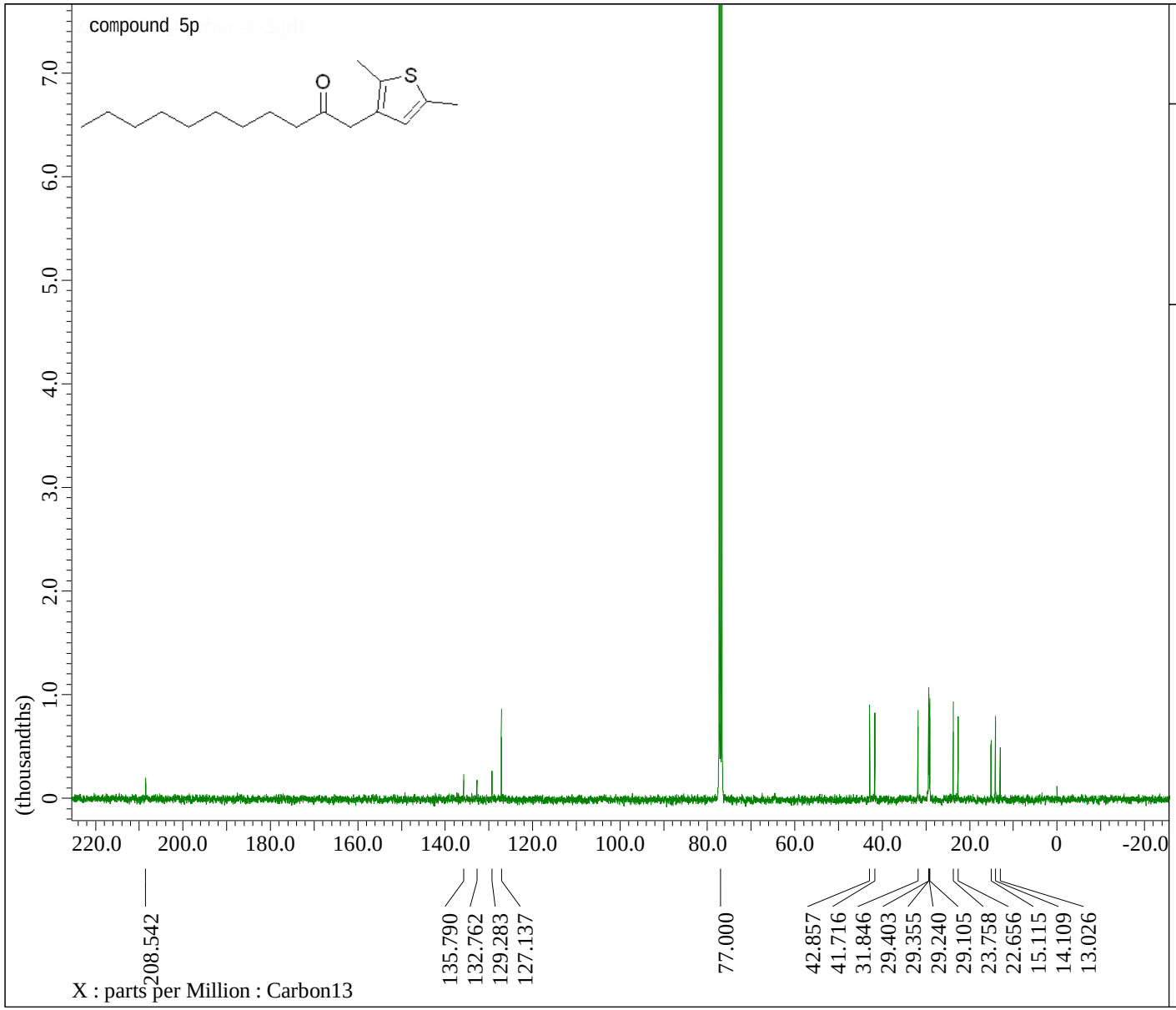

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-36_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-36
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-NOV-2017 20:04:
Revision_Time         = 21-FEB-2018 13:11:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

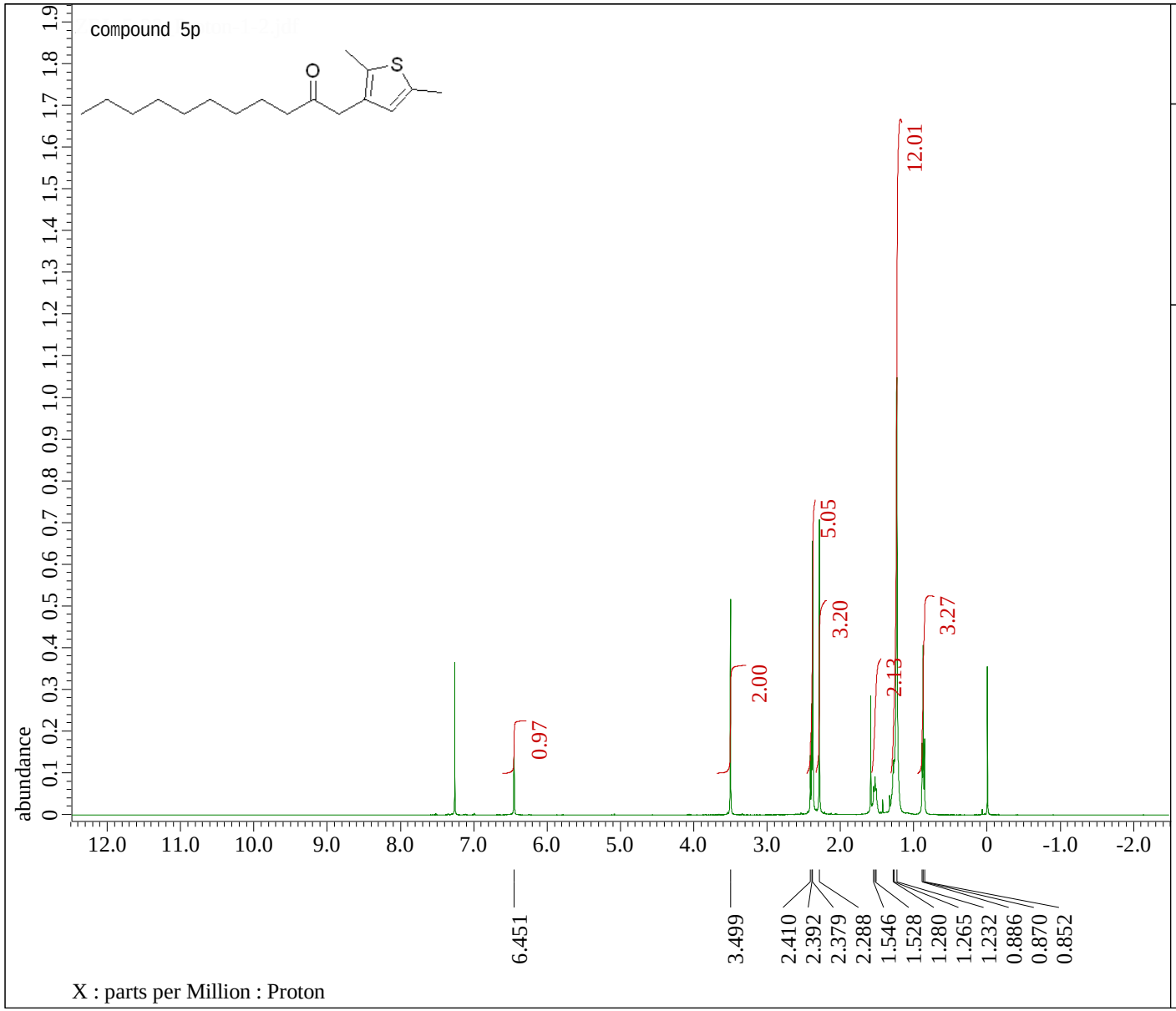
Derived from: ZRL-5-22_Carbon-1-1.jdf
```

```
Filename                  = ZRL-5-22_Carbon
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-22
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 20-NOV-2017 11:
Revision_Time             =  5-DEC-2017 20:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 2400
Total_Scans               = 2400

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 19[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



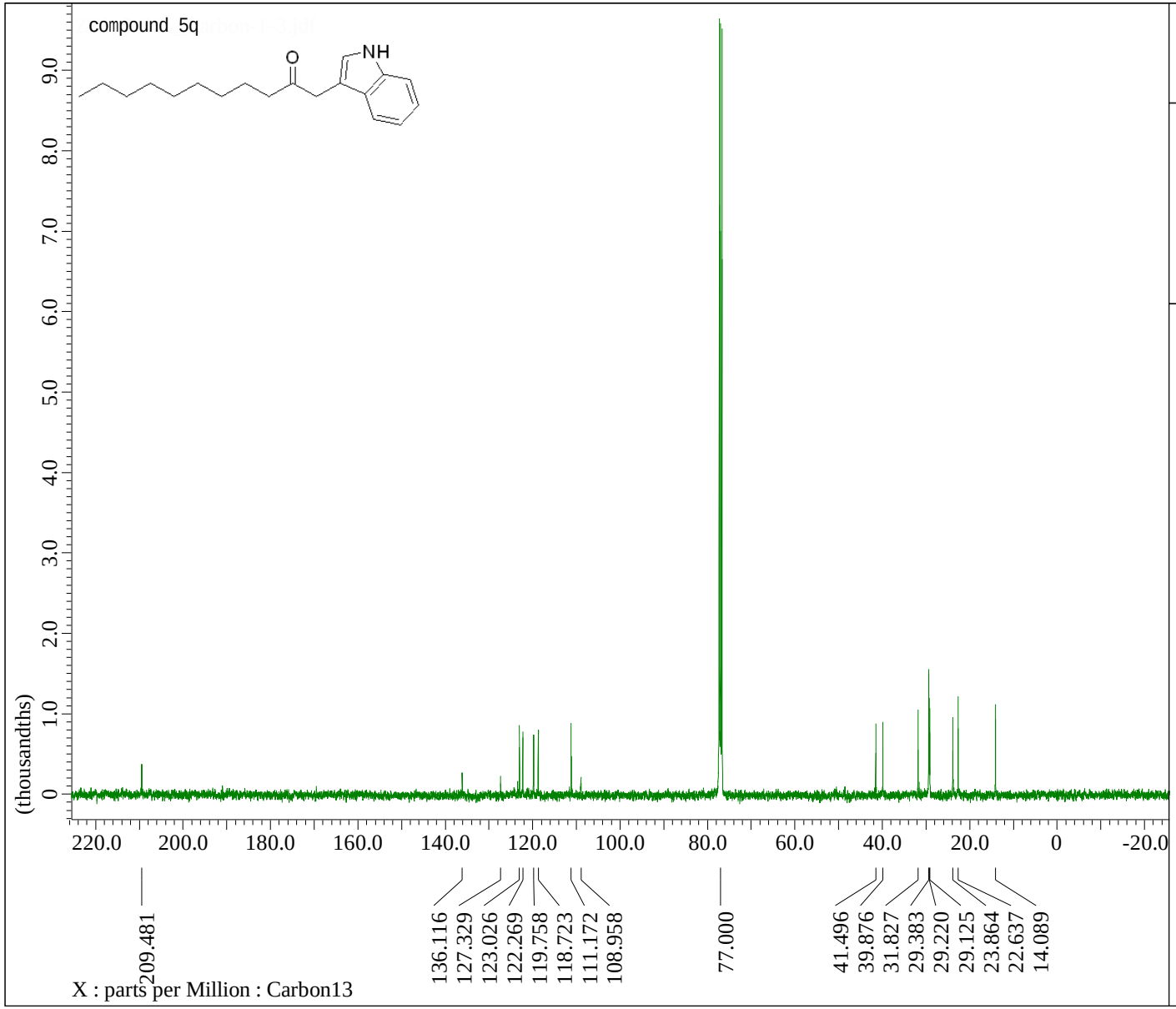

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-22_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-22
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 20-NOV-2017 10:51:
Revision_Time         = 21-FEB-2018 12:47:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 12.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

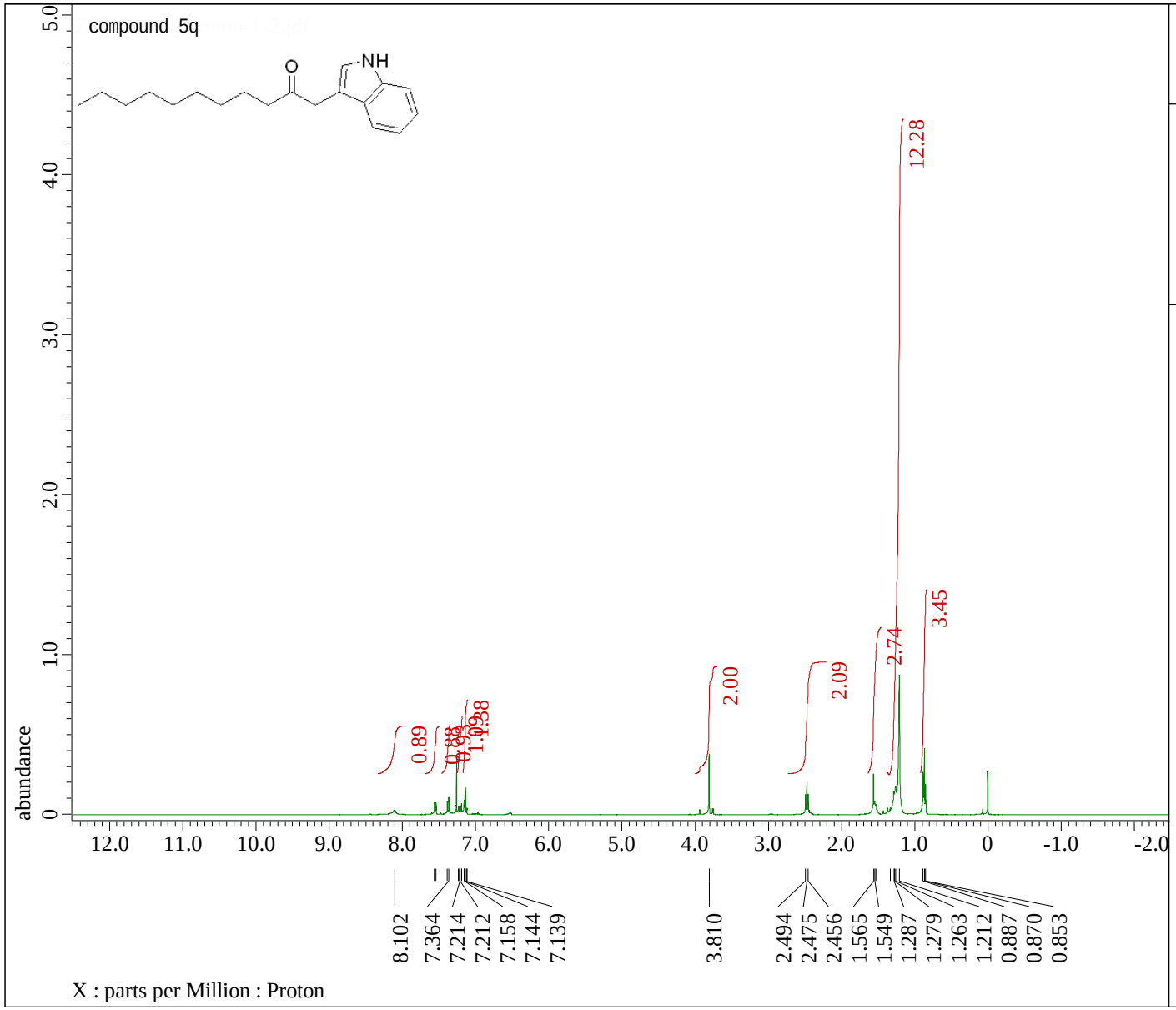
Derived from: ZRL-5-201_Carbon-1-1.jdf
```

```
Filename                 = ZRL-5-201_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-5-201
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 25-NOV-2017 21:
Revision_Time            =  5-DEC-2017 22:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 21.6[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



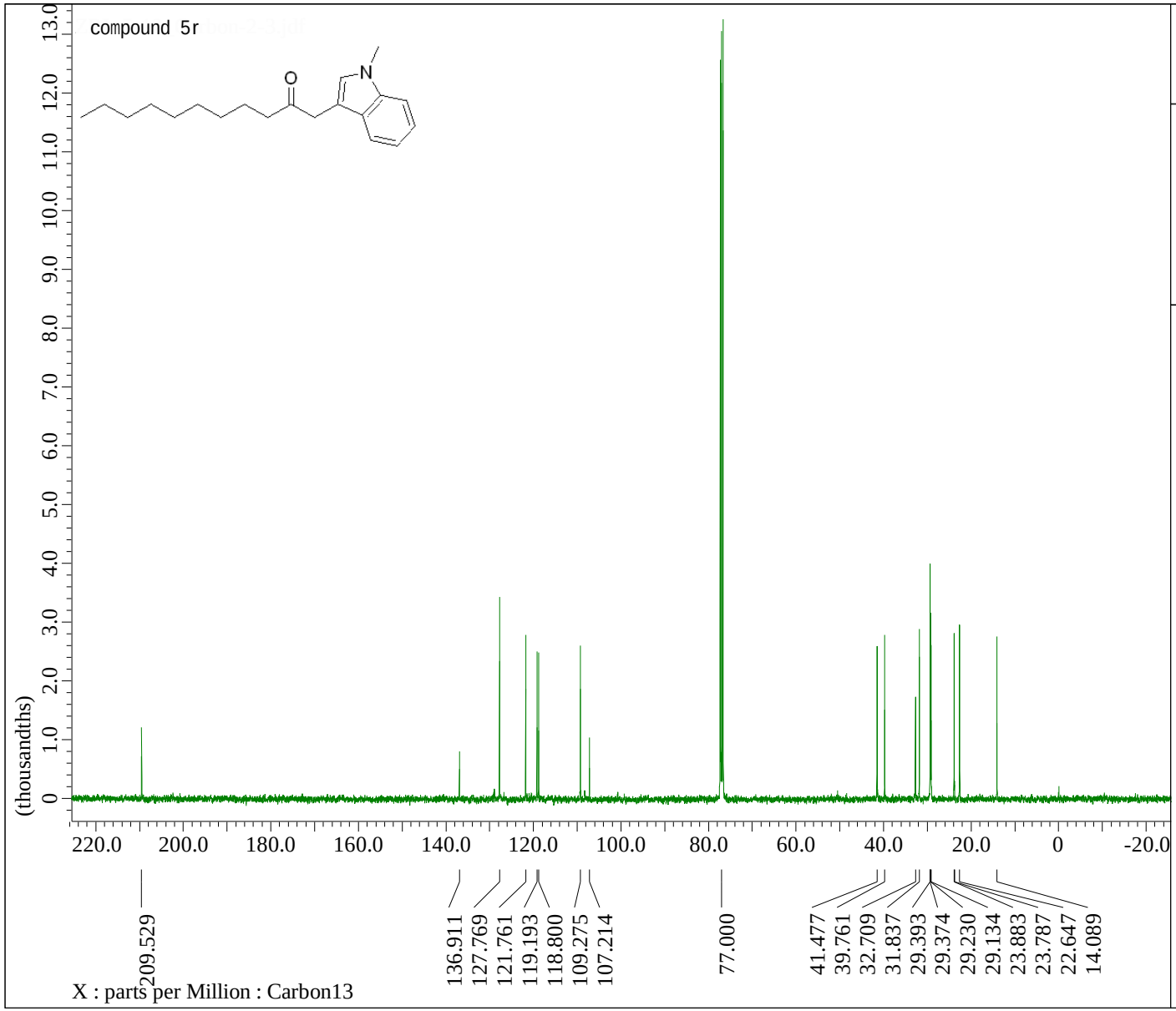

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-201_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-201
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-NOV-2017 21:20:
Revision_Time         = 21-FEB-2018 13:06:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

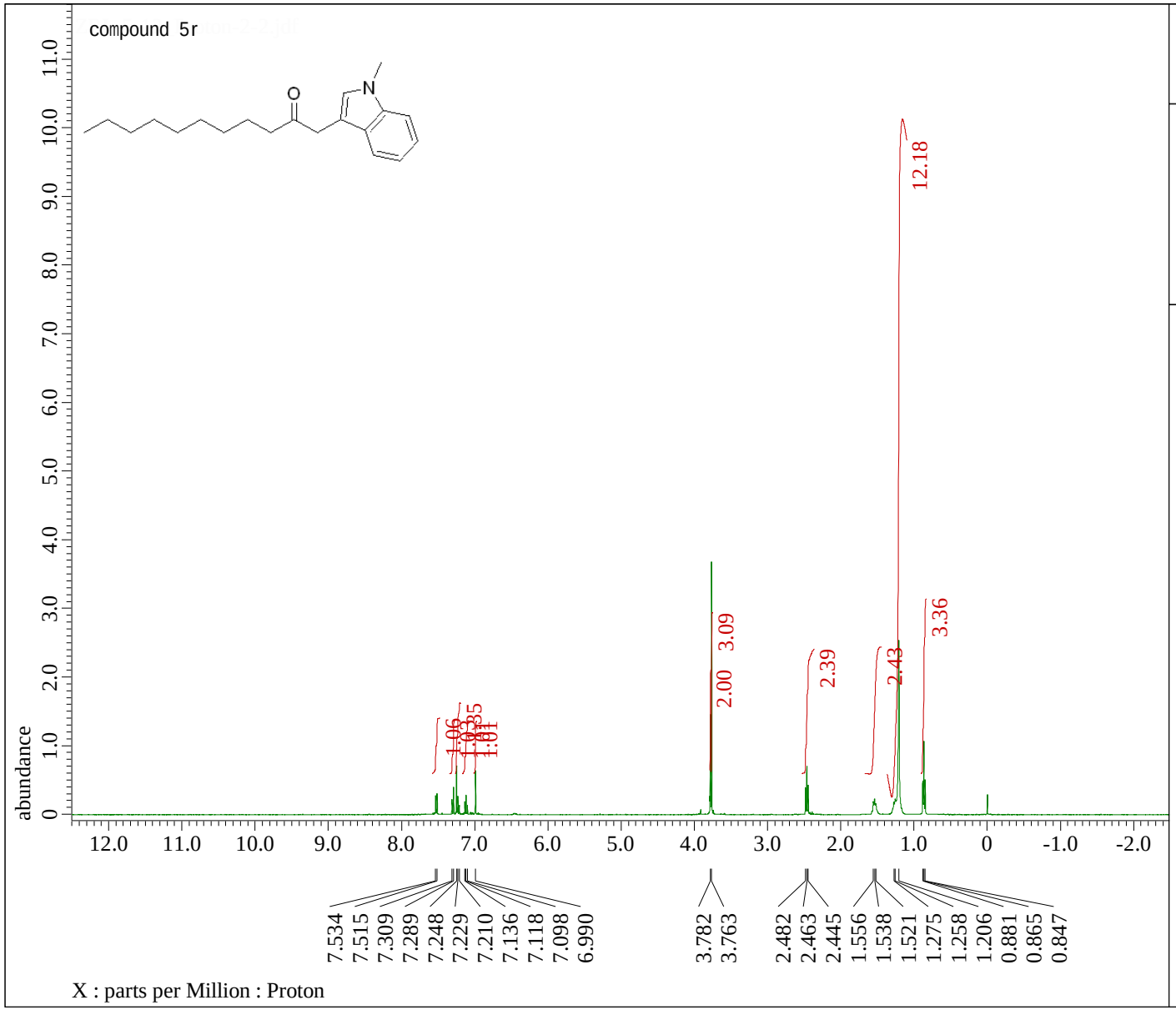
Derived from: ZRL-5-12_Carbon-2-1.jdf
```

```
Filename                  = ZRL-5-12_Carbon
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-12
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 24-NOV-2017 15:
Revision_Time             =  5-DEC-2017 21:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 21.9[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



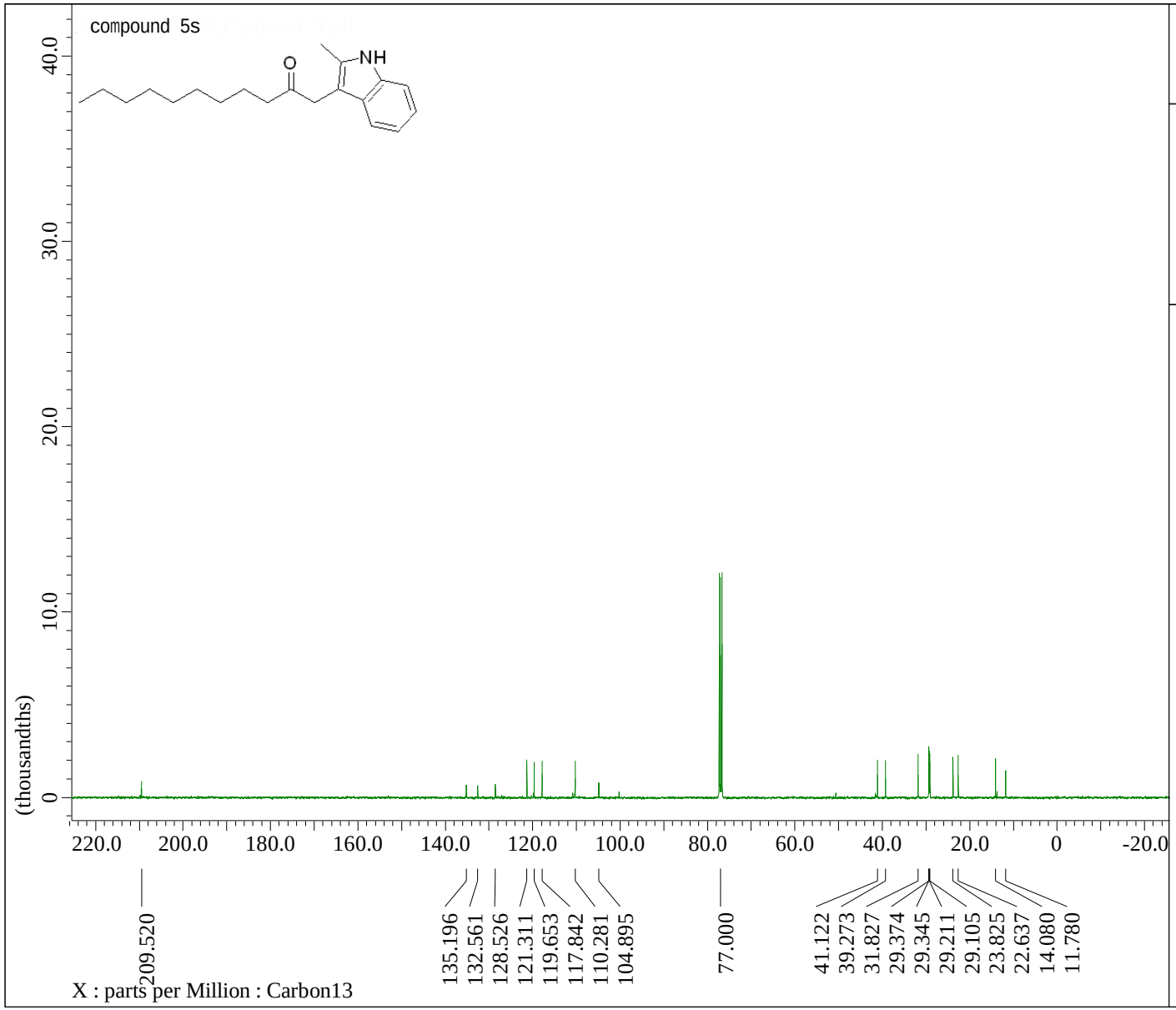

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-12_Proton-2-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-12
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 24-NOV-2017 15:39:
Revision_Time         = 21-FEB-2018 13:03:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.1[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

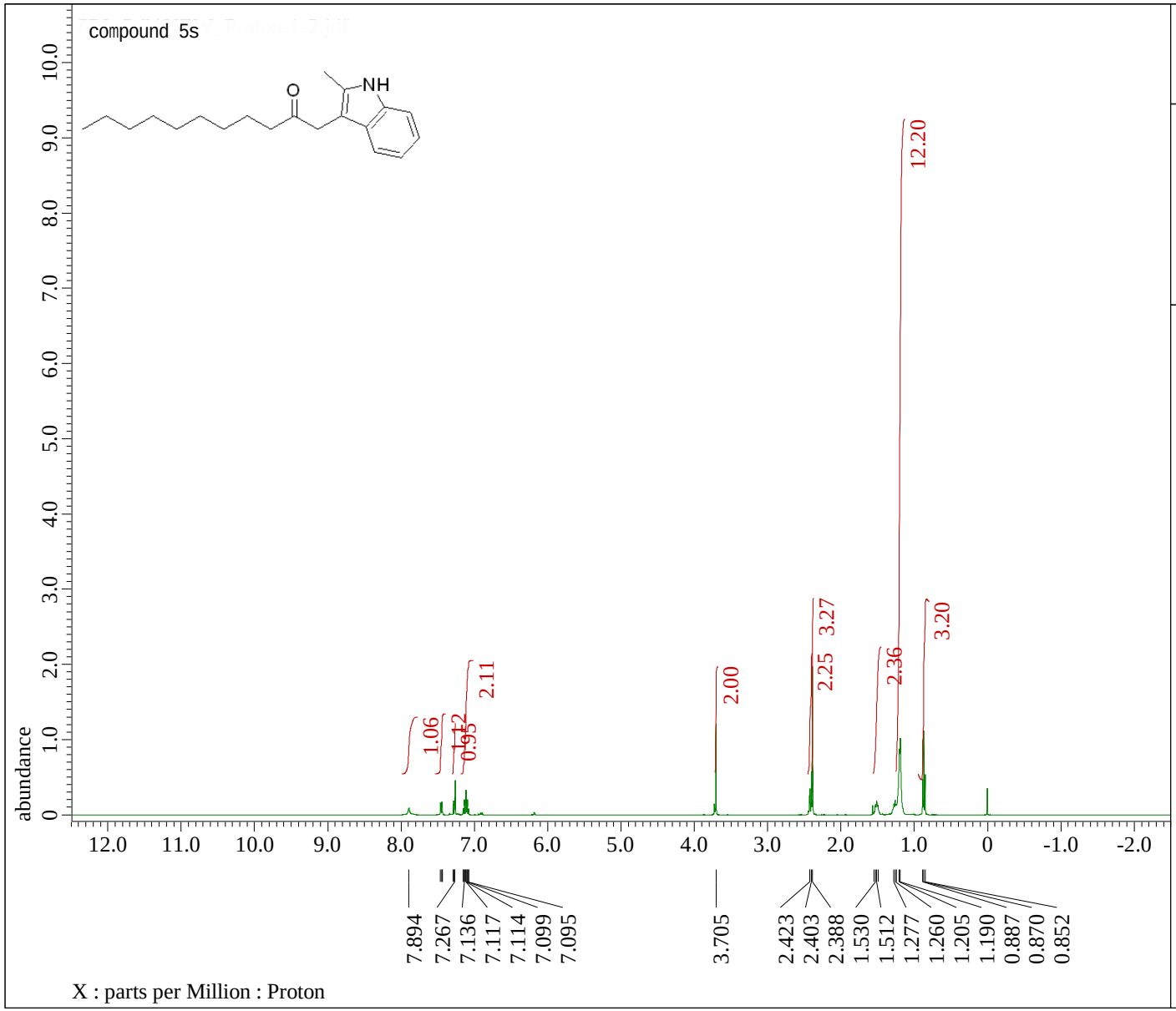
Derived from: ZRL-5-31NEW_Carbon-1-1.jdf
```

```
Filename                  = ZRL-5-31NEW_Car
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-31NEW
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 23-NOV-2017 16:
Revision_Time             =  7-DEC-2017 17:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1016
Total_Scans               = 1016

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 22.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



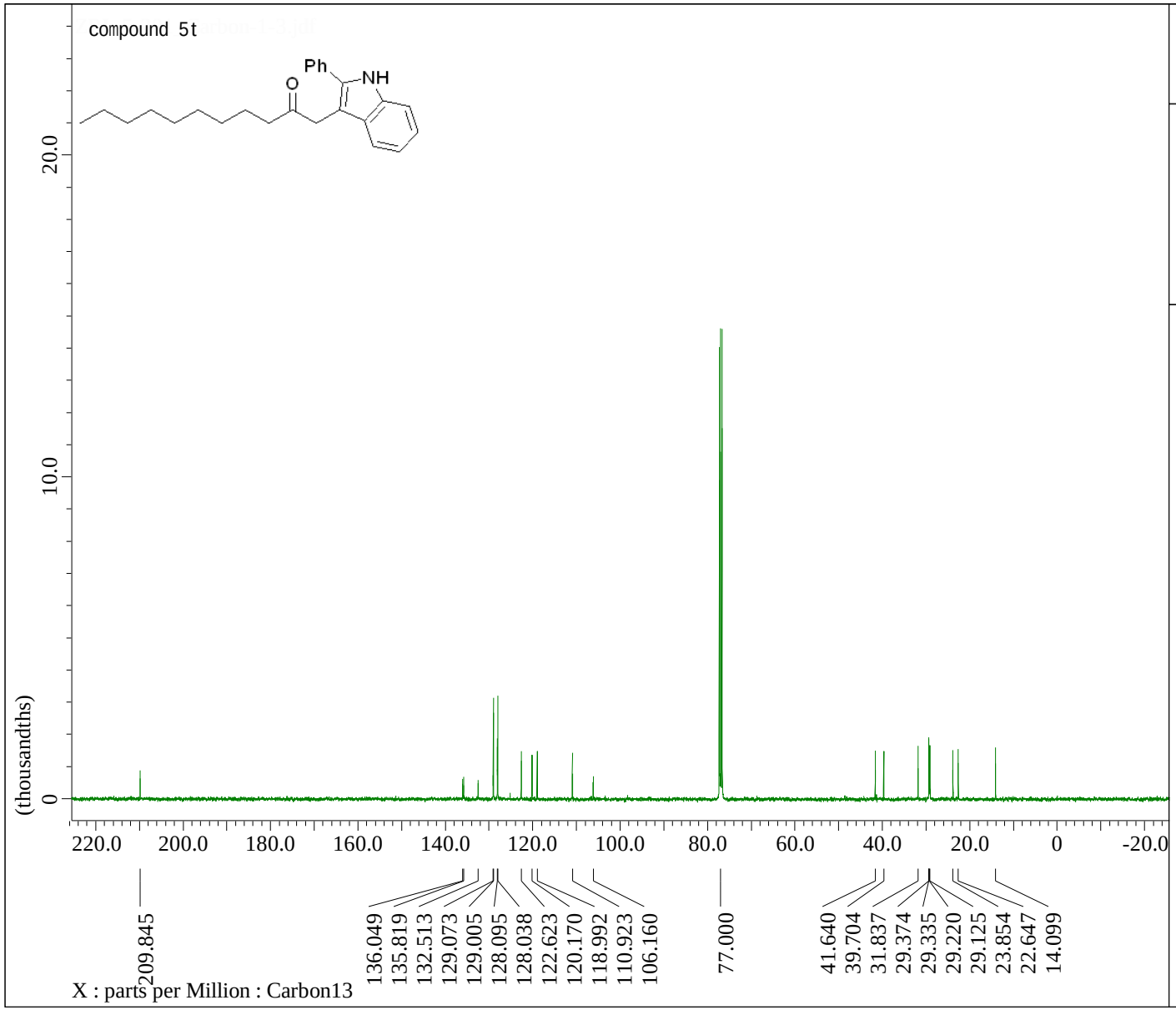

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-31NEW_Proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-31NEW
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 23-NOV-2017 16:18:
Revision_Time         = 21-FEB-2018 13:01:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

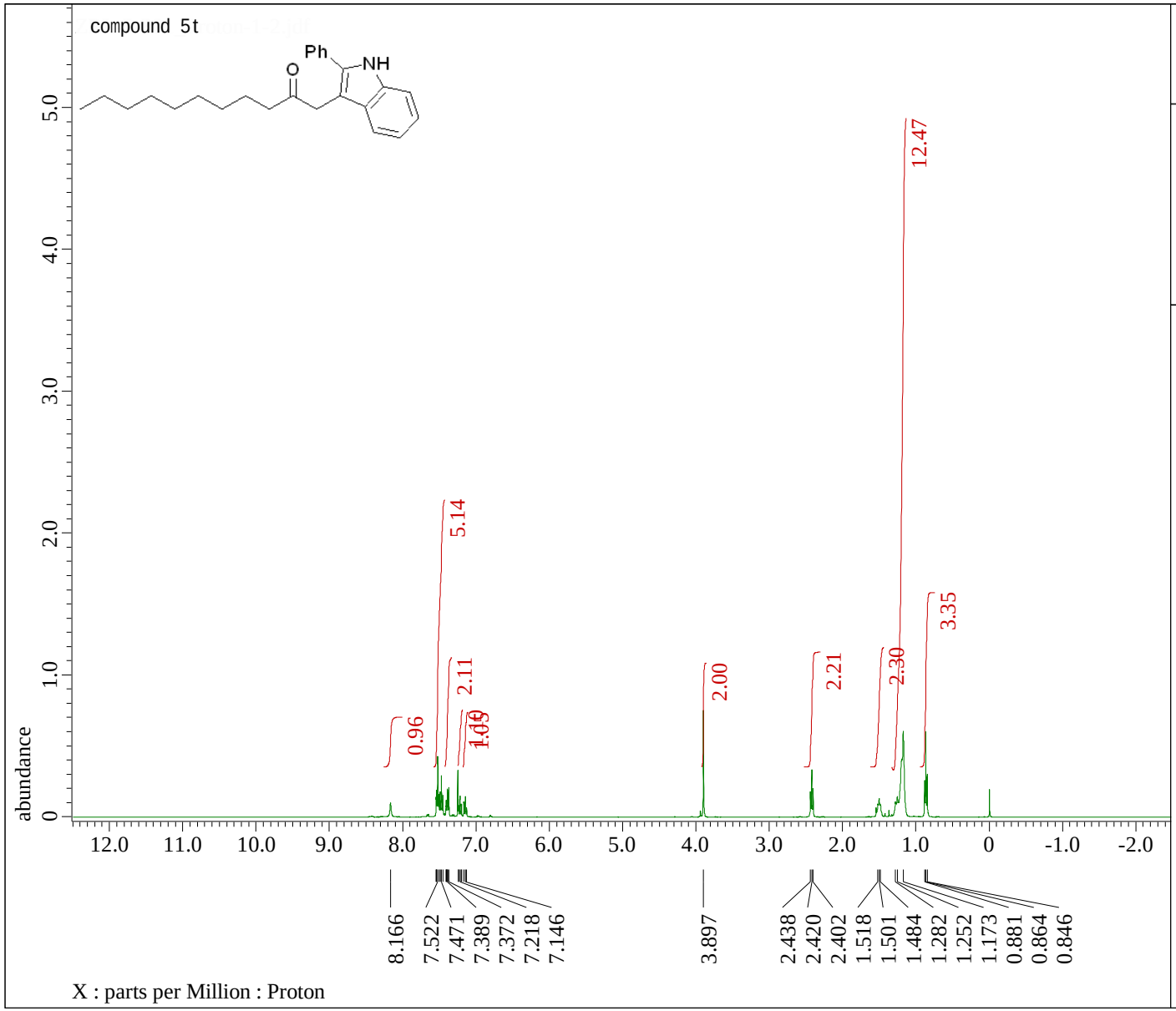
Derived from: ZRL-5-301_Carbon-1-1.jdf
```

```
Filename                 = ZRL-5-301_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-5-301
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 29-NOV-2017 19:
Revision_Time            =  6-DEC-2017 12:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 22.9[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



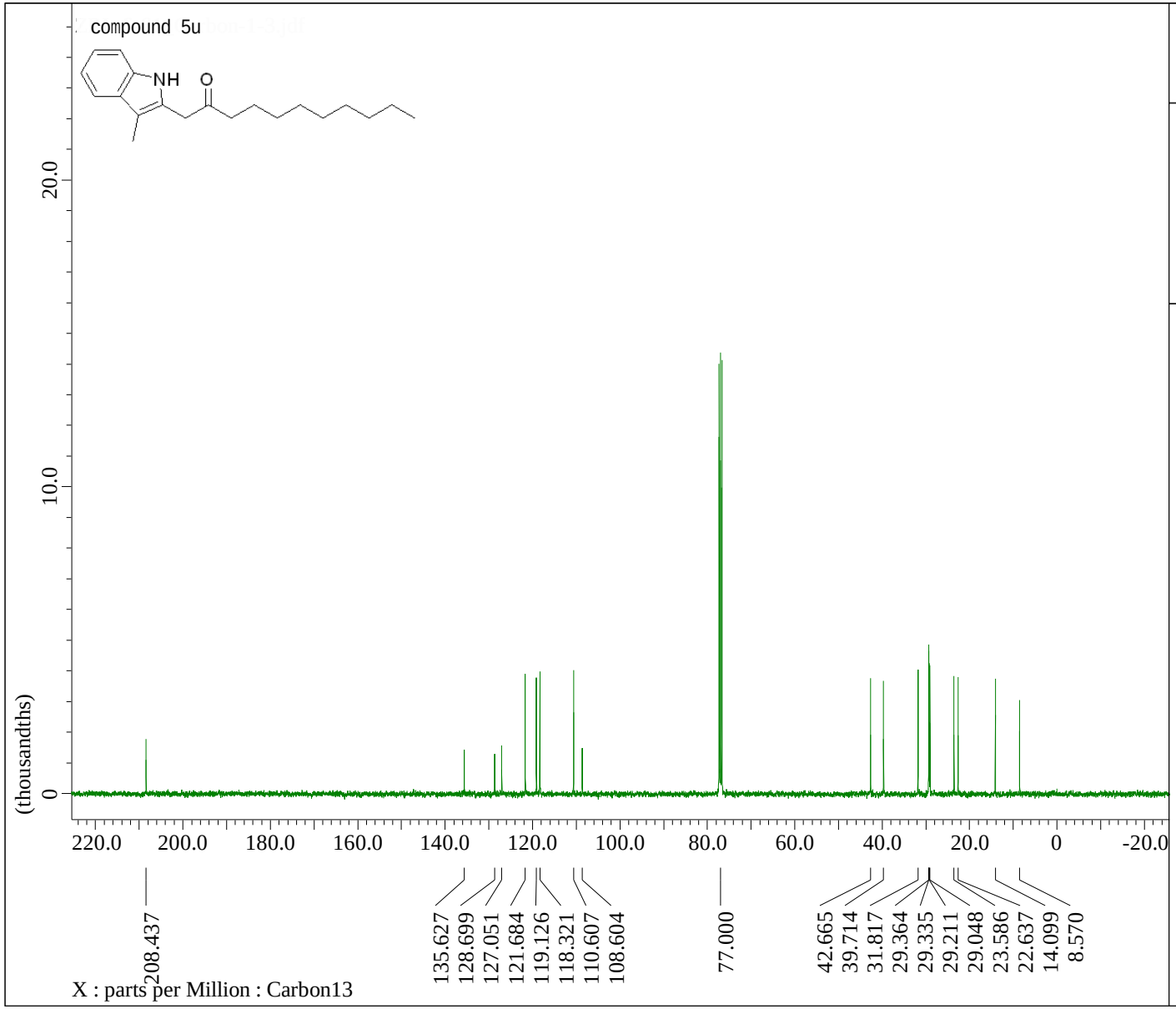

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-301_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-301
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 29-NOV-2017 19:01:
Revision_Time         = 21-FEB-2018 13:16:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.9[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

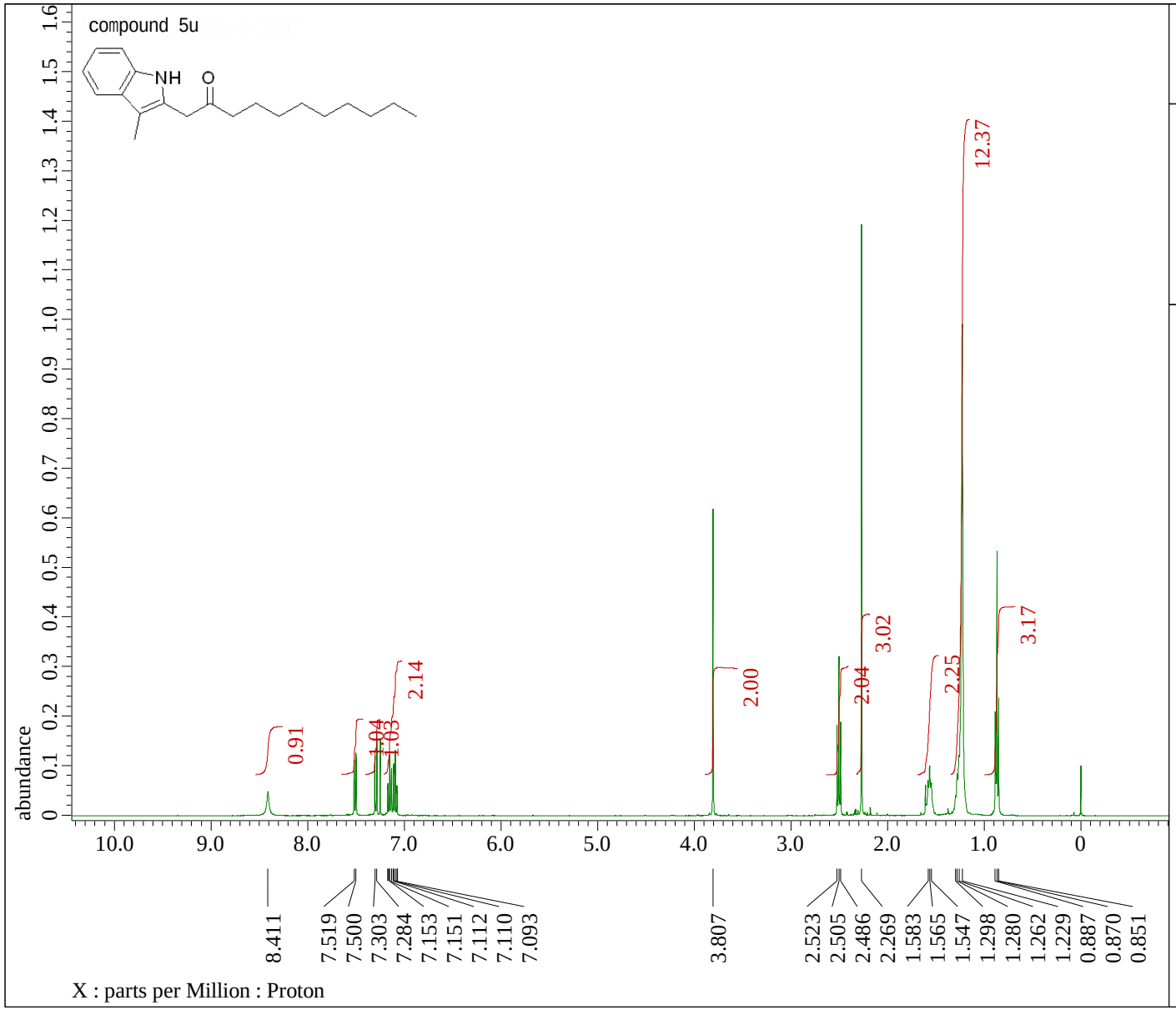
Derived from: ZRL-6-61_Carbon-1-1.jdf
```

```
Filename                 = ZRL-6-61_Carbon
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-6-61
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 25-JAN-2018 17:
Revision_Time            = 29-JAN-2018 10:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 461
Total_Scans              = 461

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 17.1[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



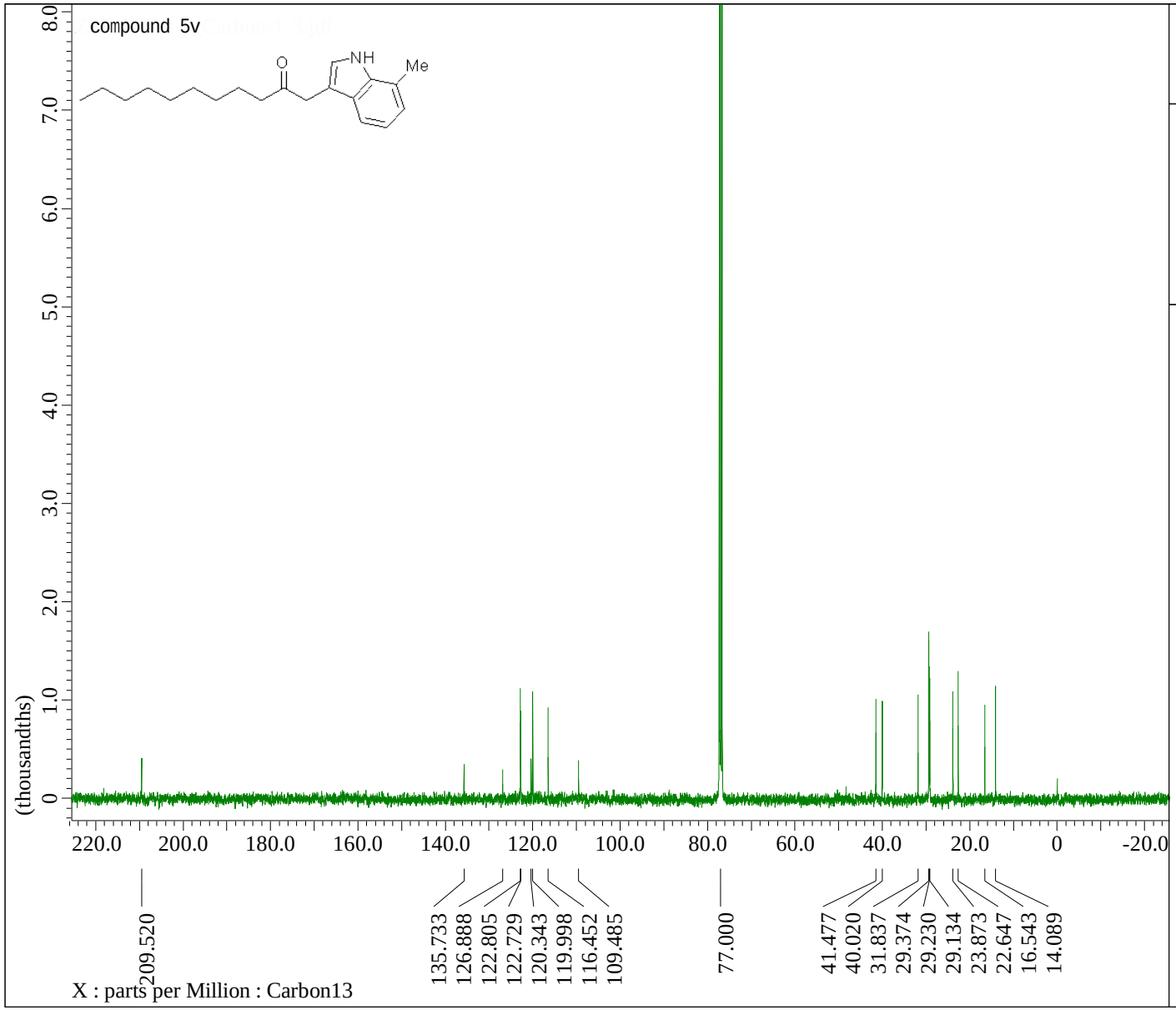

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-6-61_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-6-61
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-JAN-2018 17:01:
Revision_Time         = 29-JAN-2018 10:28:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 46
Temp_Get              = 16.3[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

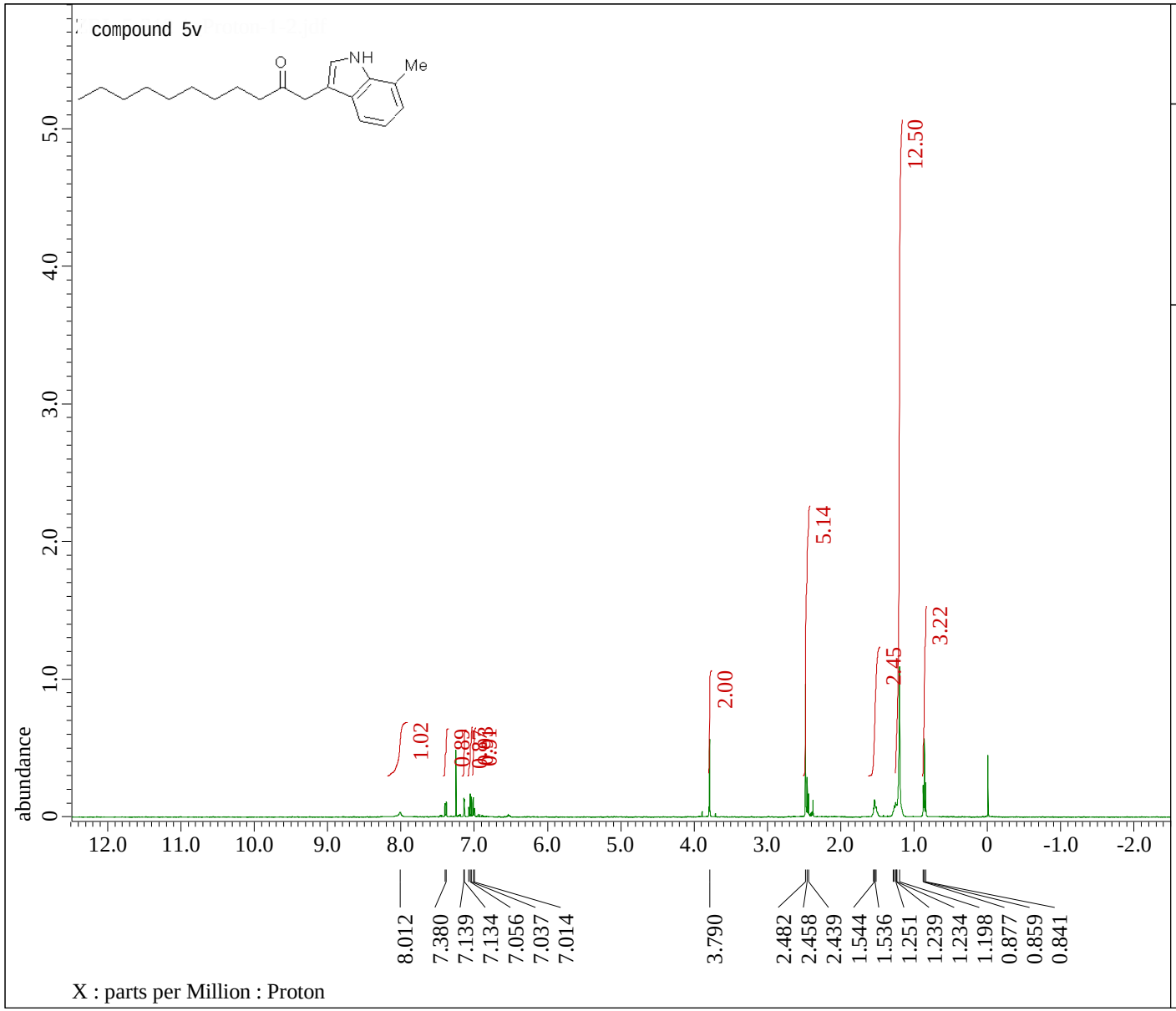
Derived from: ZRL-5-312 1_Carbon-1-1.jdf
```

```
Filename                = ZRL-5-312 1_Car
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-5-312 1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 29-NOV-2017 18:
Revision_Time           =  5-DEC-2017 21:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 23.1[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



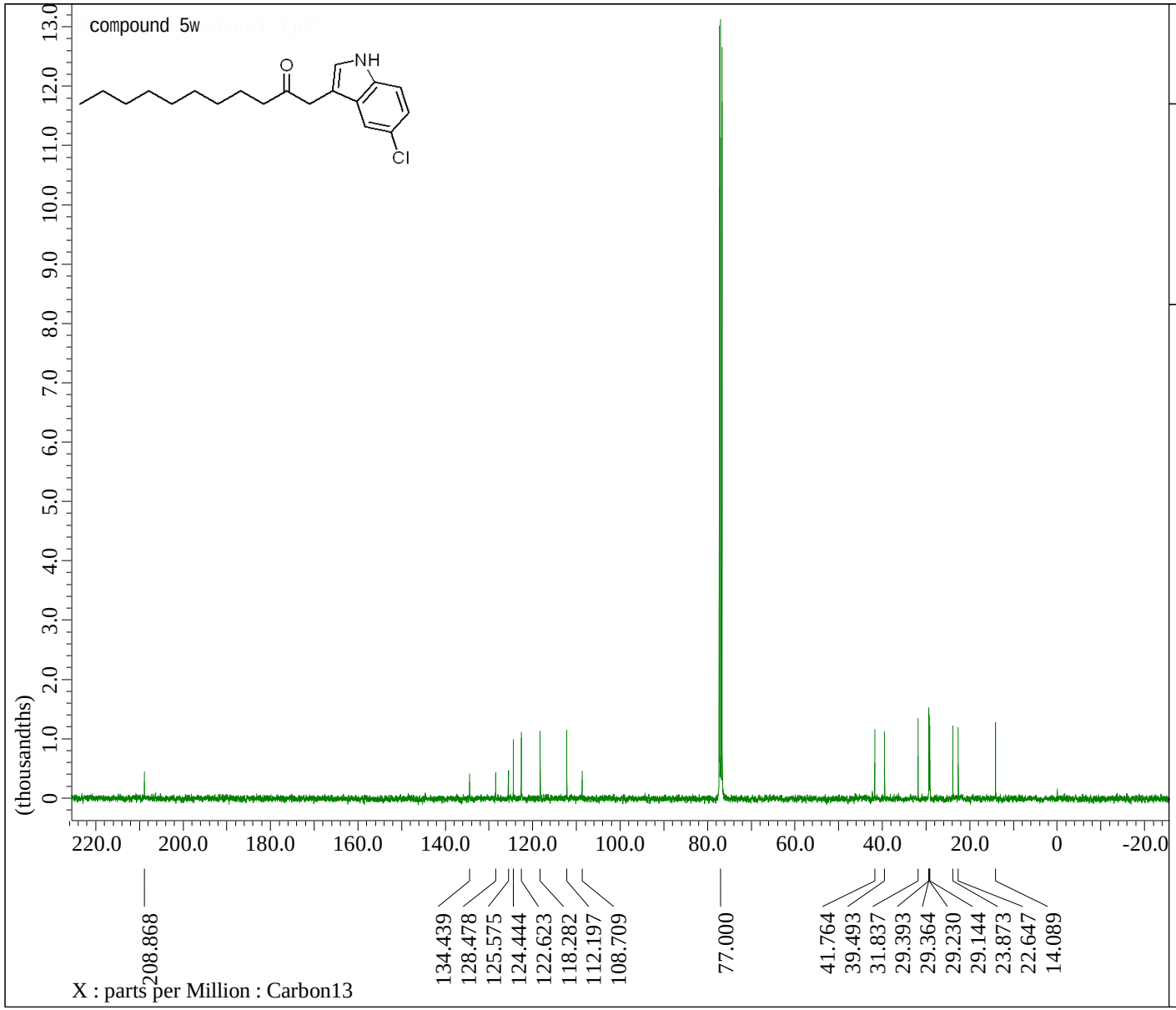

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-312 1_Proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-312 1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 29-NOV-2017 17:58:
Revision_Time         = 21-FEB-2018 13:18:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

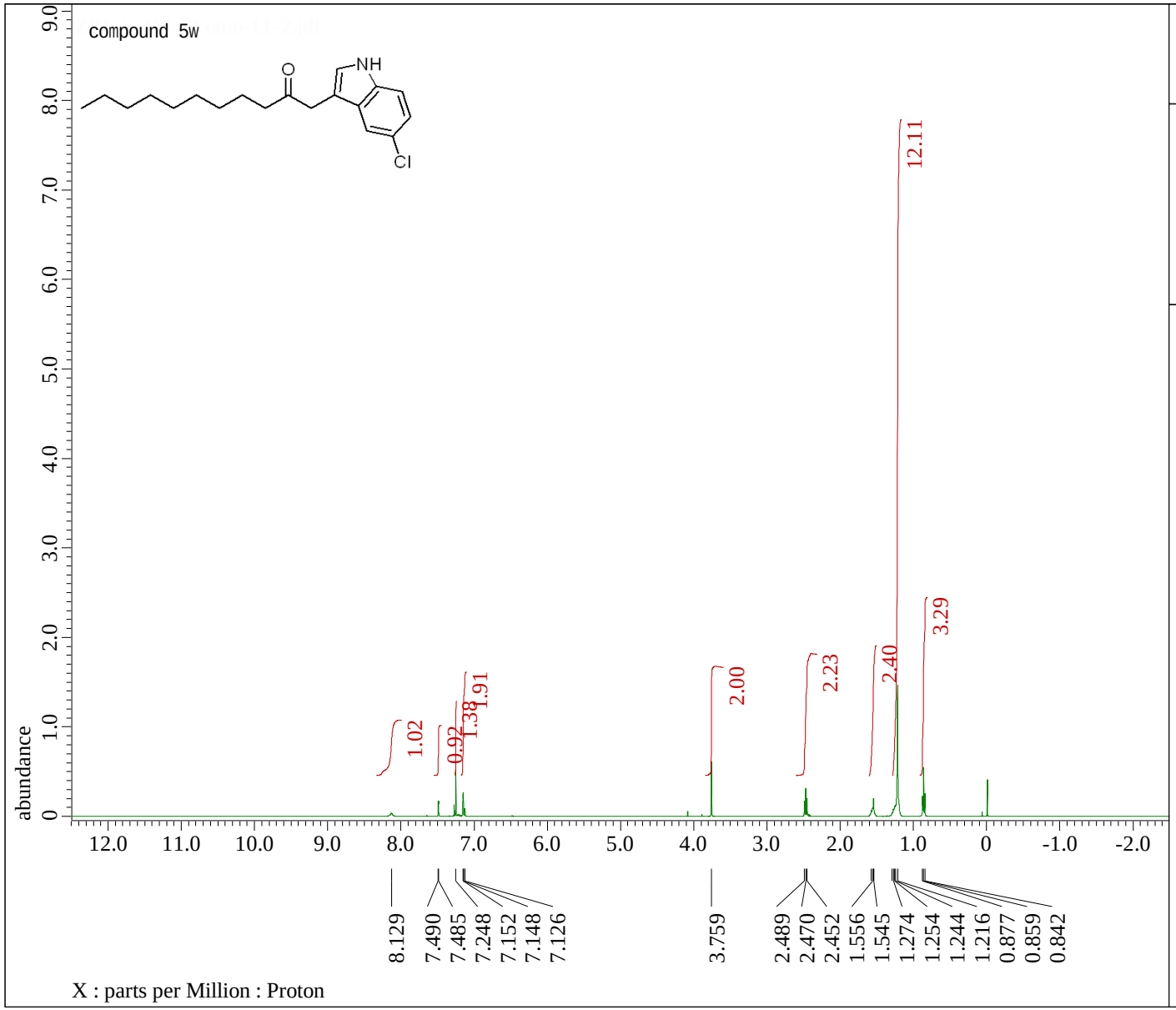
Derived from: ZRL-5-311_Carbon-1-1.jdf
```

```
Filename                 = ZRL-5-311_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-5-311
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 30-NOV-2017 23:
Revision_Time            =  6-DEC-2017 08:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 23.4[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



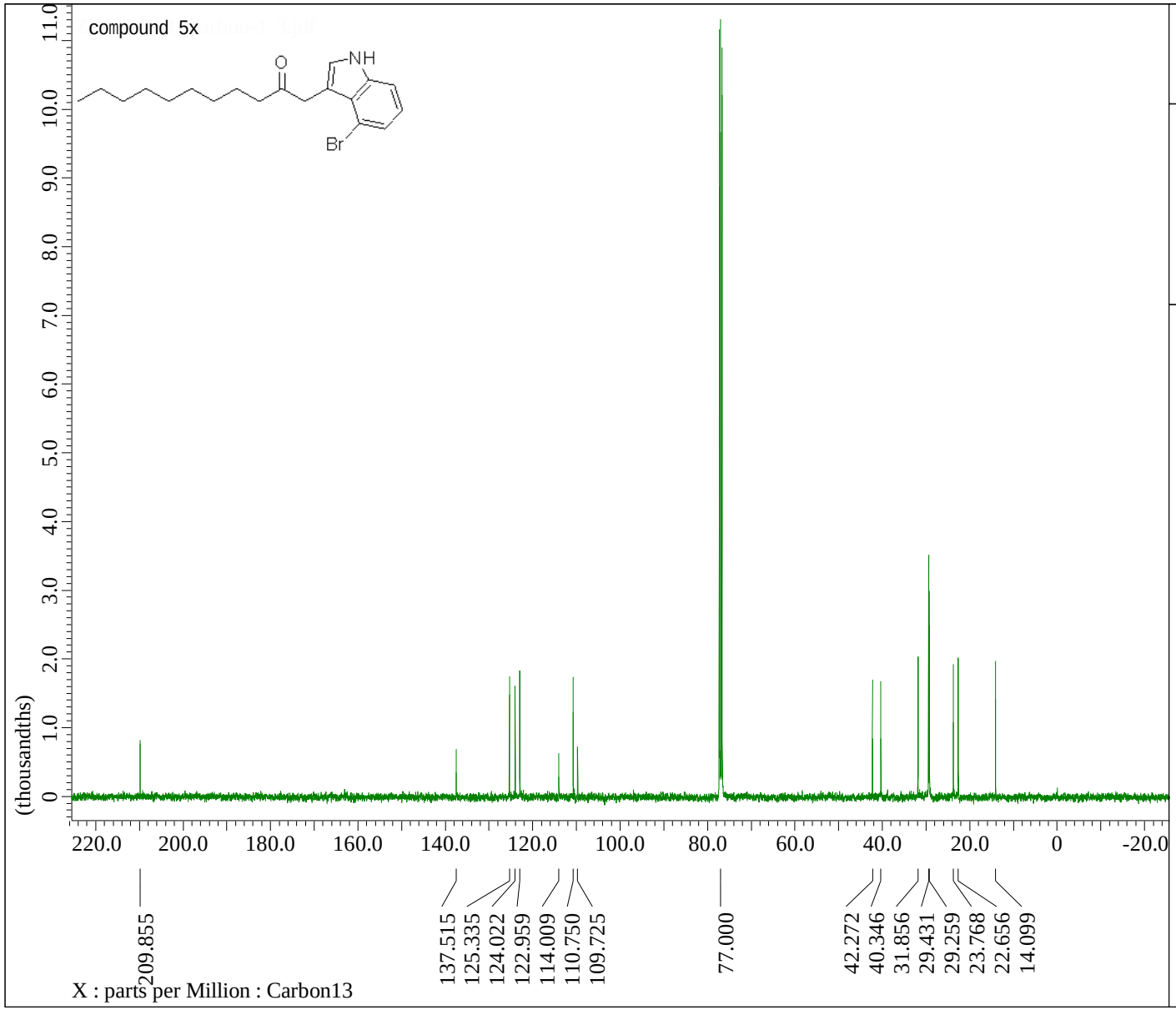

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-311_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-311
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 30-NOV-2017 23:17:
Revision_Time         = 21-FEB-2018 13:21:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.8[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

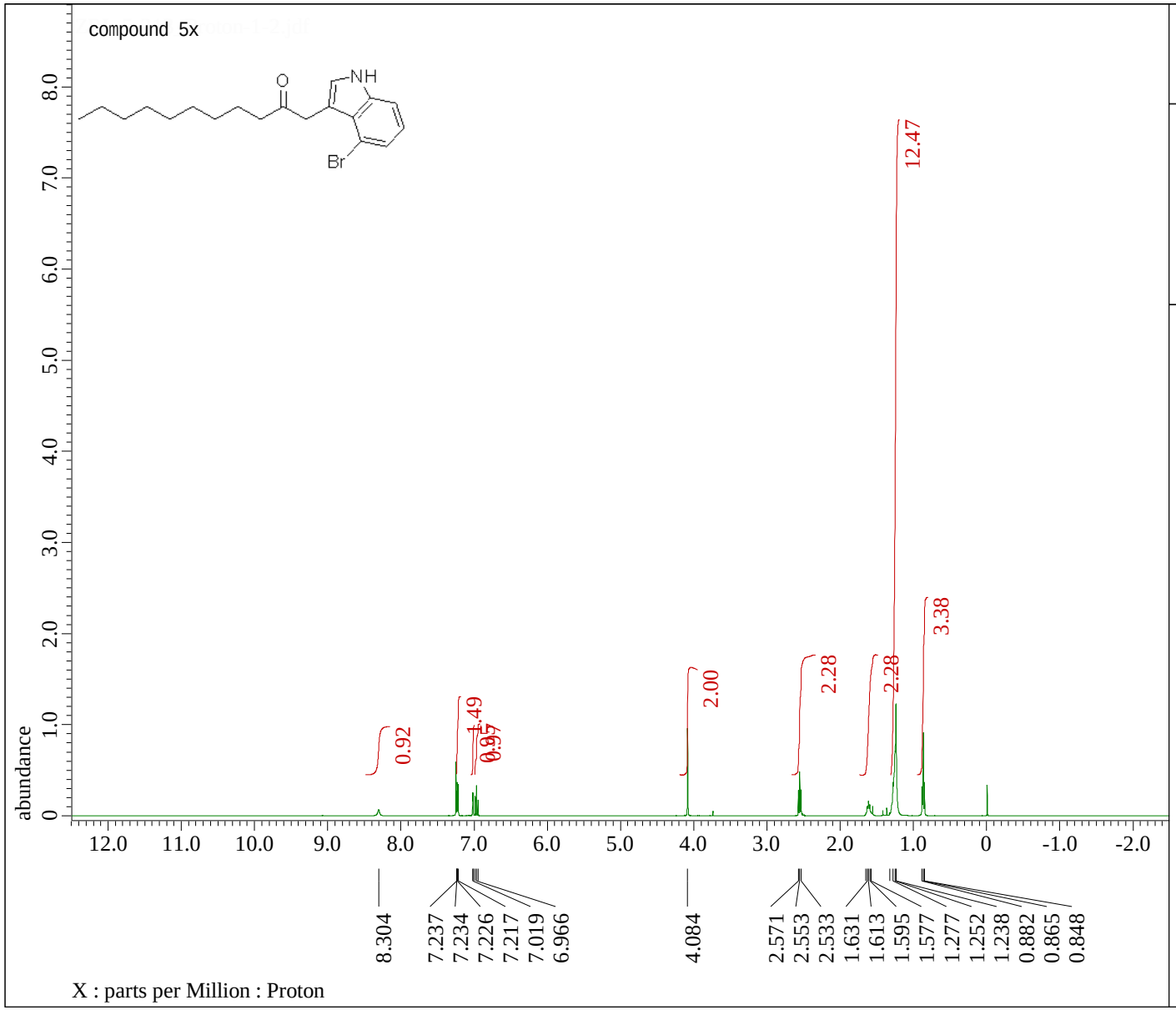
Derived from: ZRL-5-313_Carbon-1-1.jdf
```

```
Filename                  = ZRL-5-313_Carbo
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-313
Solvent                   = CHLOROFORM-D
Actual_Start_Time         =  1-DEC-2017 00:
Revision_Time             =  6-DEC-2017 08:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 23.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



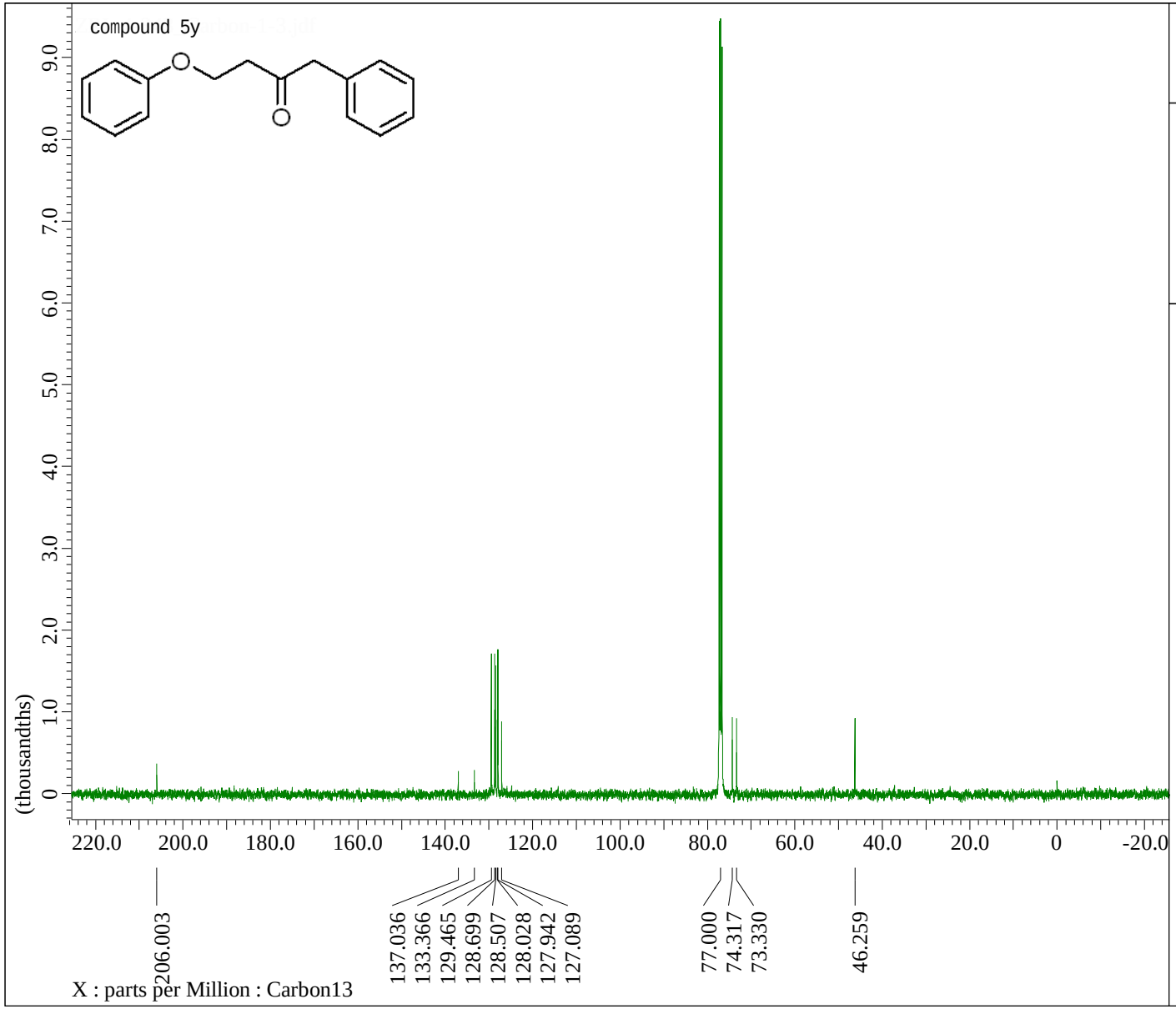

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-313_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-313
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  1-DEC-2017 00:15:
Revision_Time         = 21-FEB-2018 13:22:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.9[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



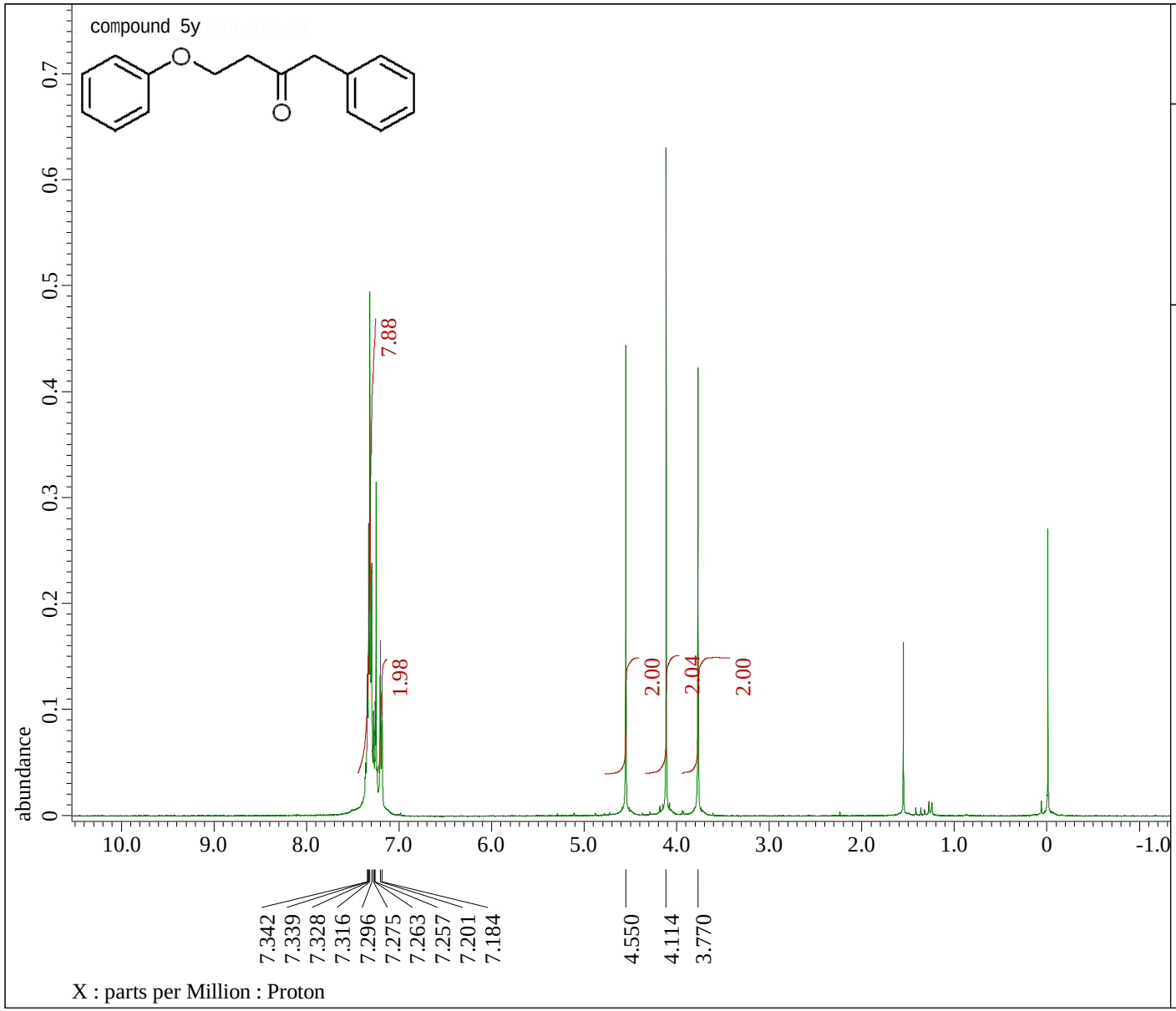

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                 = ZRL-4-343_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-4-343
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 10-NOV-2017 14:
Revision_Time            = 14-NOV-2017 22:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 18.4[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



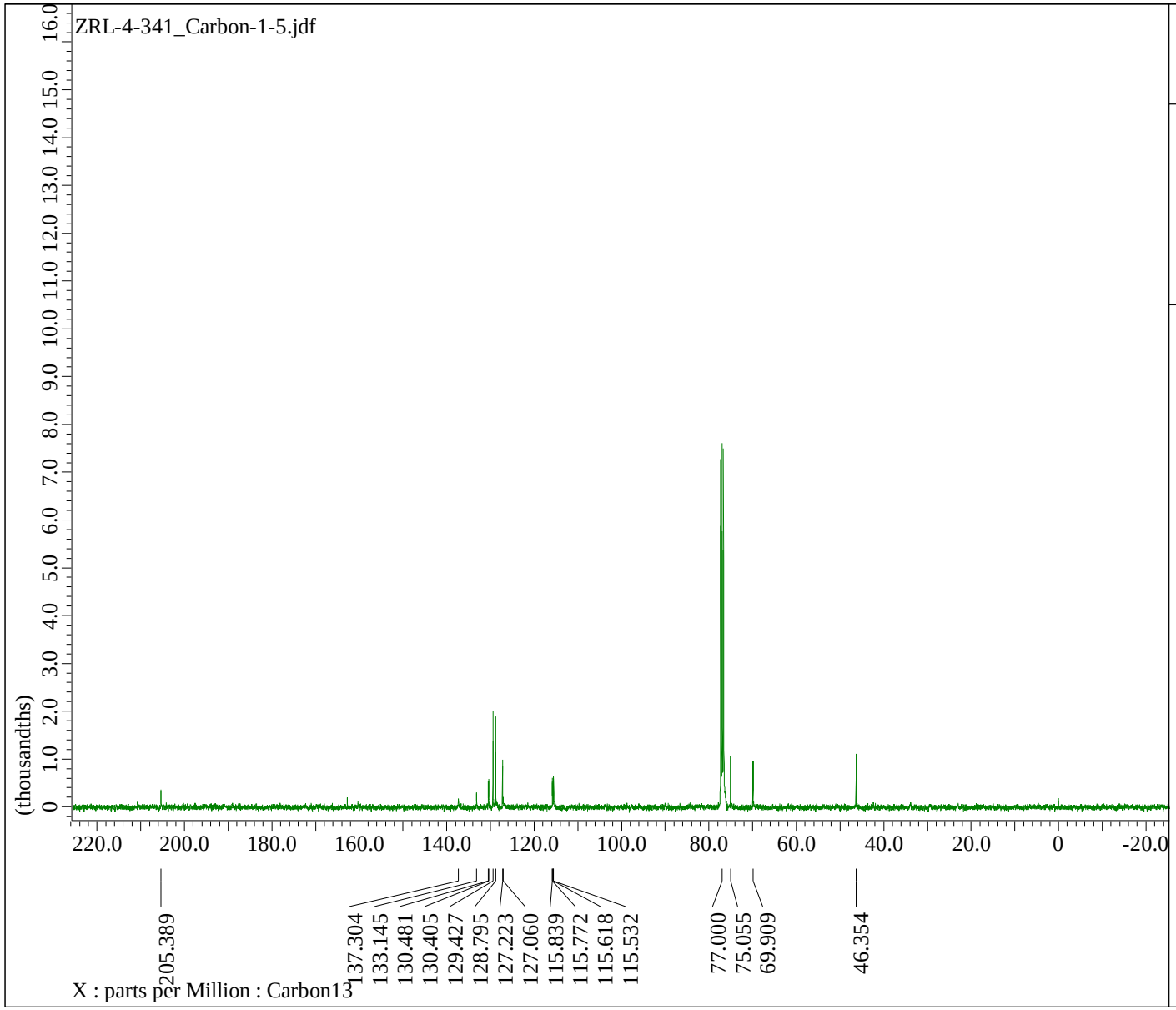

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-343_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-343
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 10-NOV-2017 14:50:
Revision_Time         = 14-NOV-2017 22:25:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 17.8[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

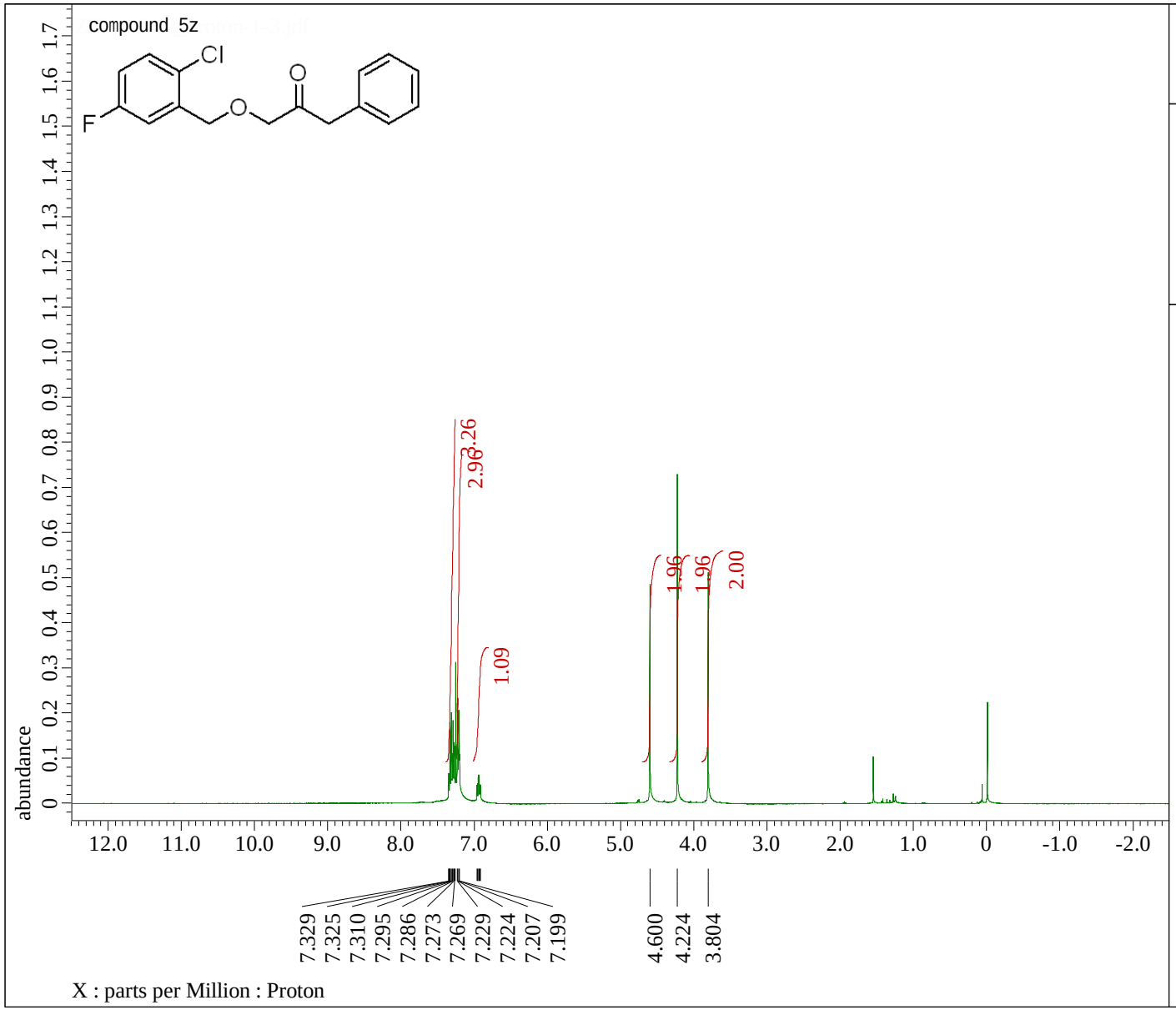
Derived from: ZRL-4-341_Carbon-1-1.jdf
```

```
Filename                = ZRL-4-341_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-341
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  9-NOV-2017 16:
Revision_Time           = 21-FEB-2018 17:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 19.5[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



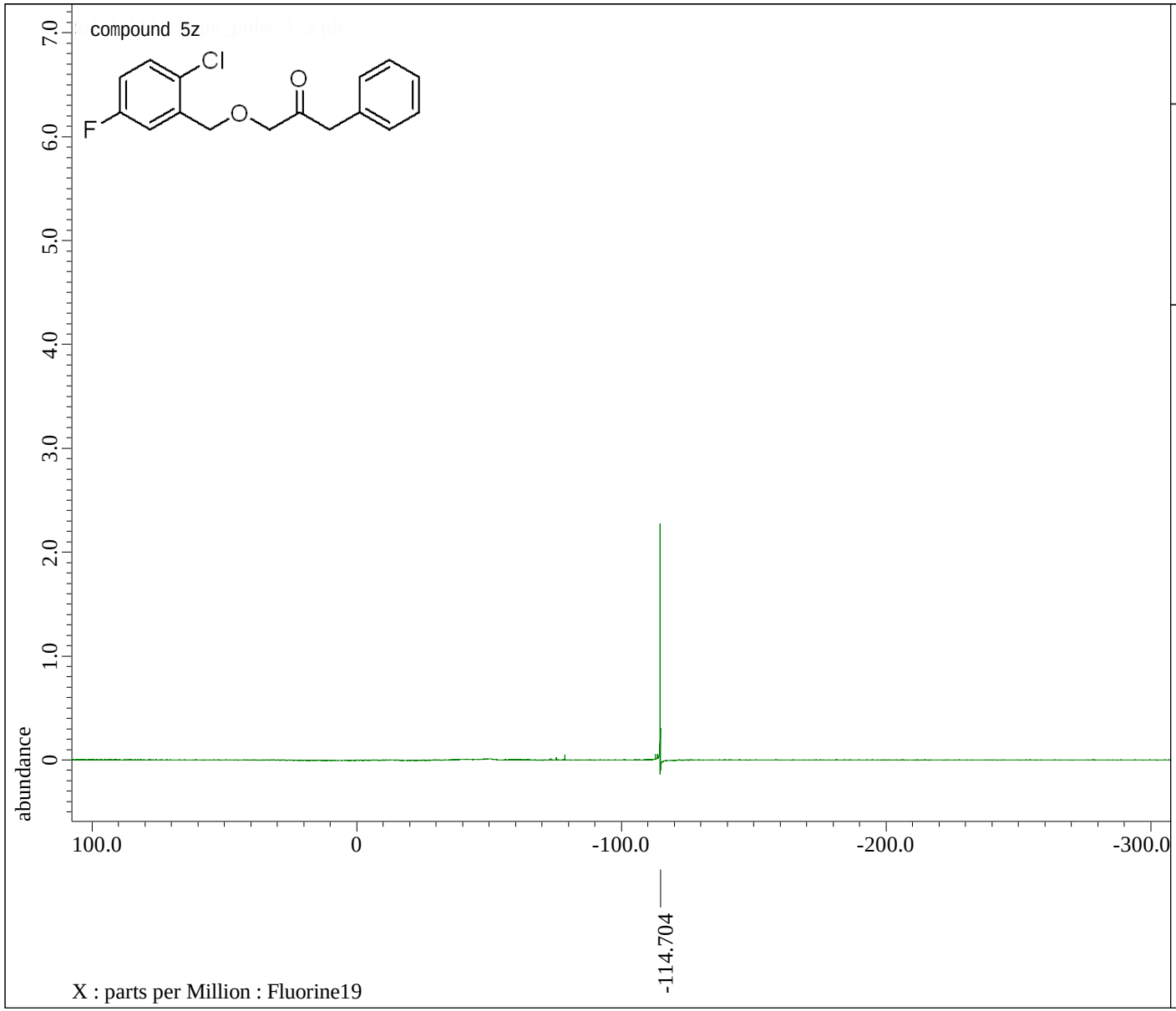

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-341_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-341
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  9-NOV-2017 16:25:
Revision_Time         = 14-NOV-2017 22:14:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 19.1[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

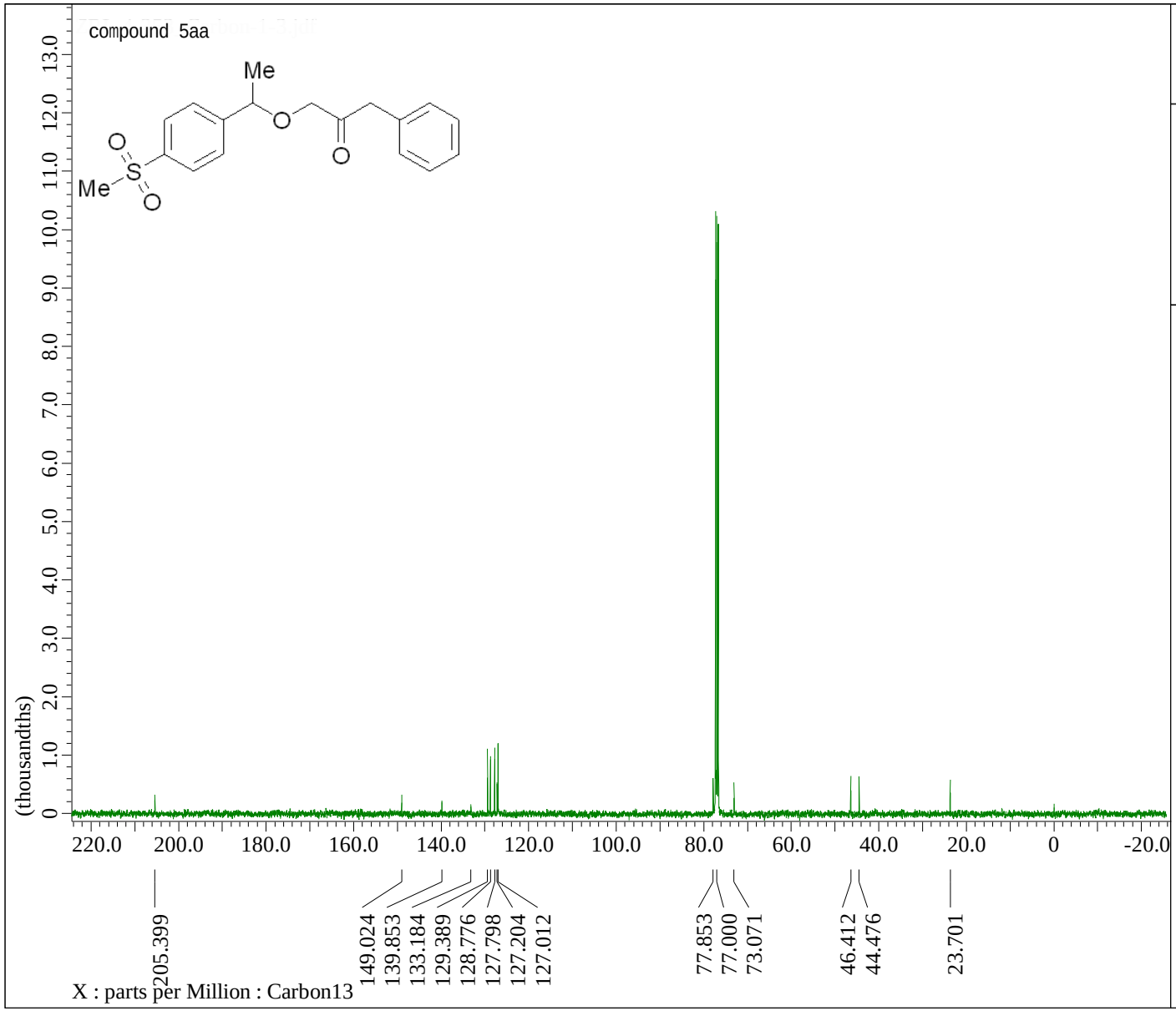
Derived from: zrl-4-341_single_pulse-1-1.j
```

```
Filename              = zrl-4-341_single_p
Author                = delta
Experiment            = single_pulse.jxp
Sample_Id             = zrl-4-341
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  7-DEC-2017 17:33:
Revision_Time         =  6-FEB-2018 14:53:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Fluorine19
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 83.88608[ms]
X_Domain              = 19F
X_Freq                = 376.17105393[MHz]
X_Offset              = -100[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 11.92092896[Hz]
X_Sweep               = 195.3125[kHz]
X_Sweep_Clipped       = 156.25[kHz]
Irr_Domain            = Fluorine19
Irr_Freq              = 376.17105393[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Fluorine19
Tri_Freq              = 376.17105393[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 50
Temp_Get              = 24.3[dC]
X_90_Width            = 10[us]
X_Acq_Time            = 83.88608[ms]
```



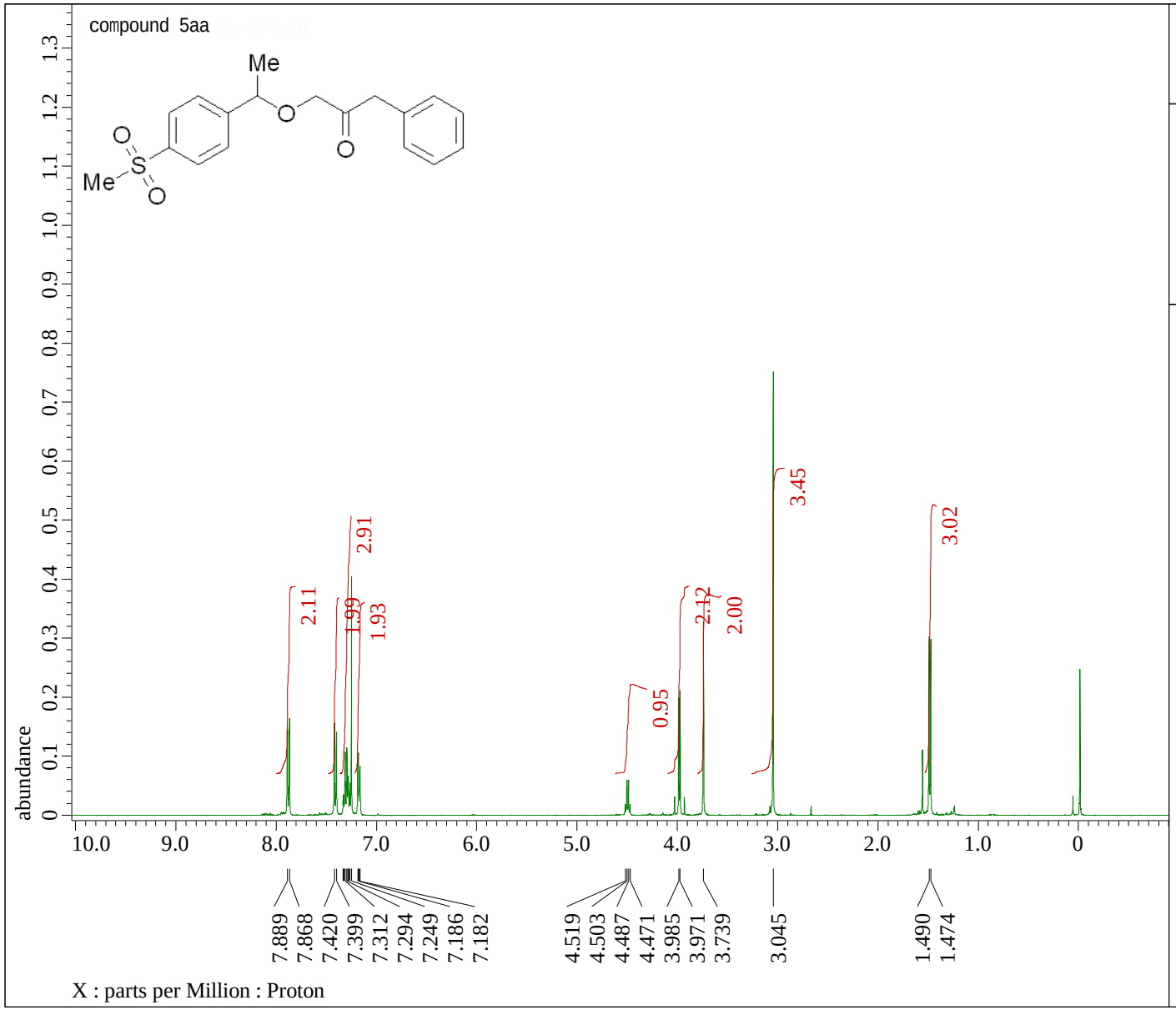

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-353_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-353
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 13-NOV-2017 11:
Revision_Time           = 22-FEB-2018 21:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 16.6[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



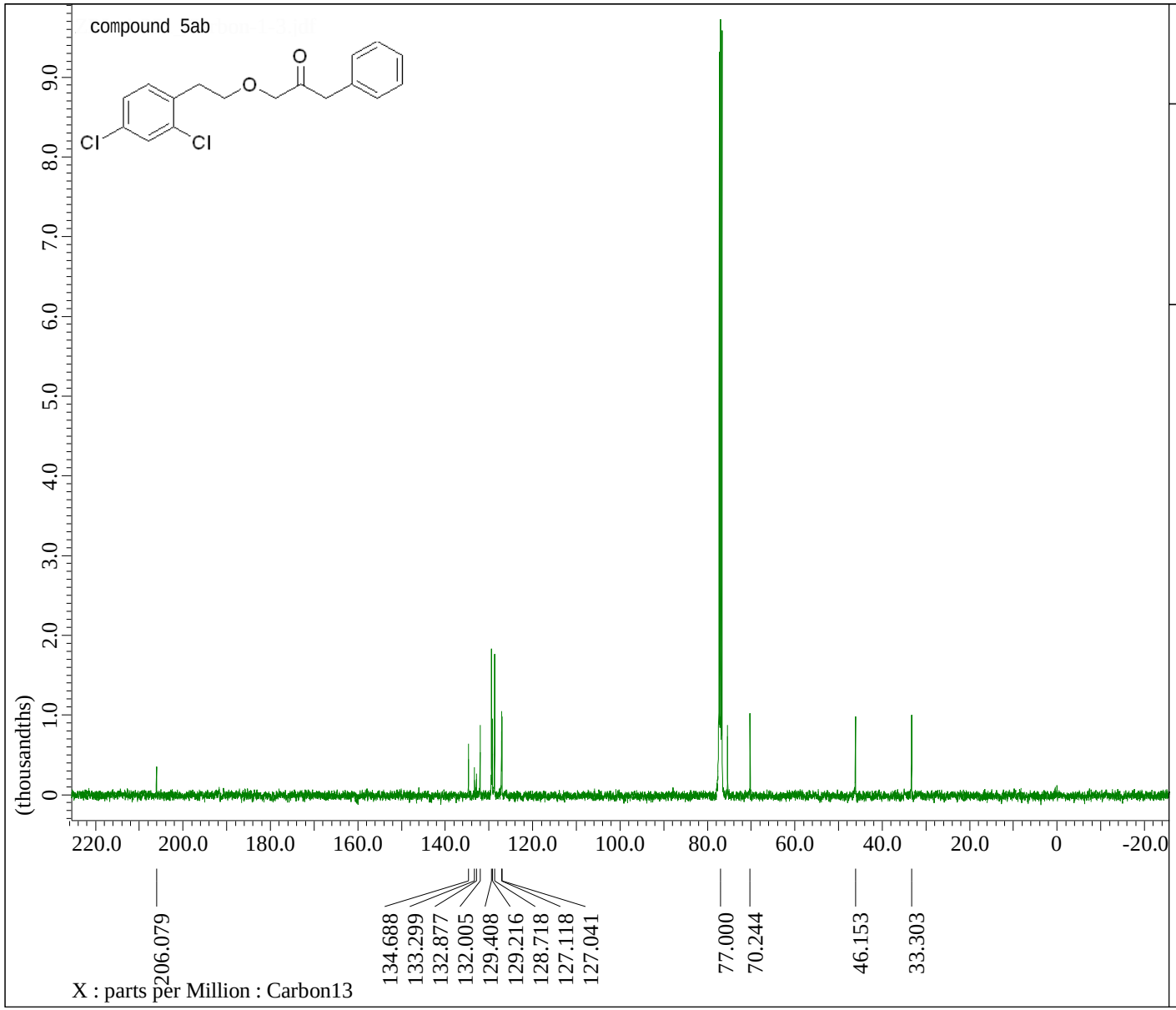

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-353_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-353
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 13-NOV-2017 11:22:
Revision_Time         =  5-DEC-2017 20:04:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 16.1[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



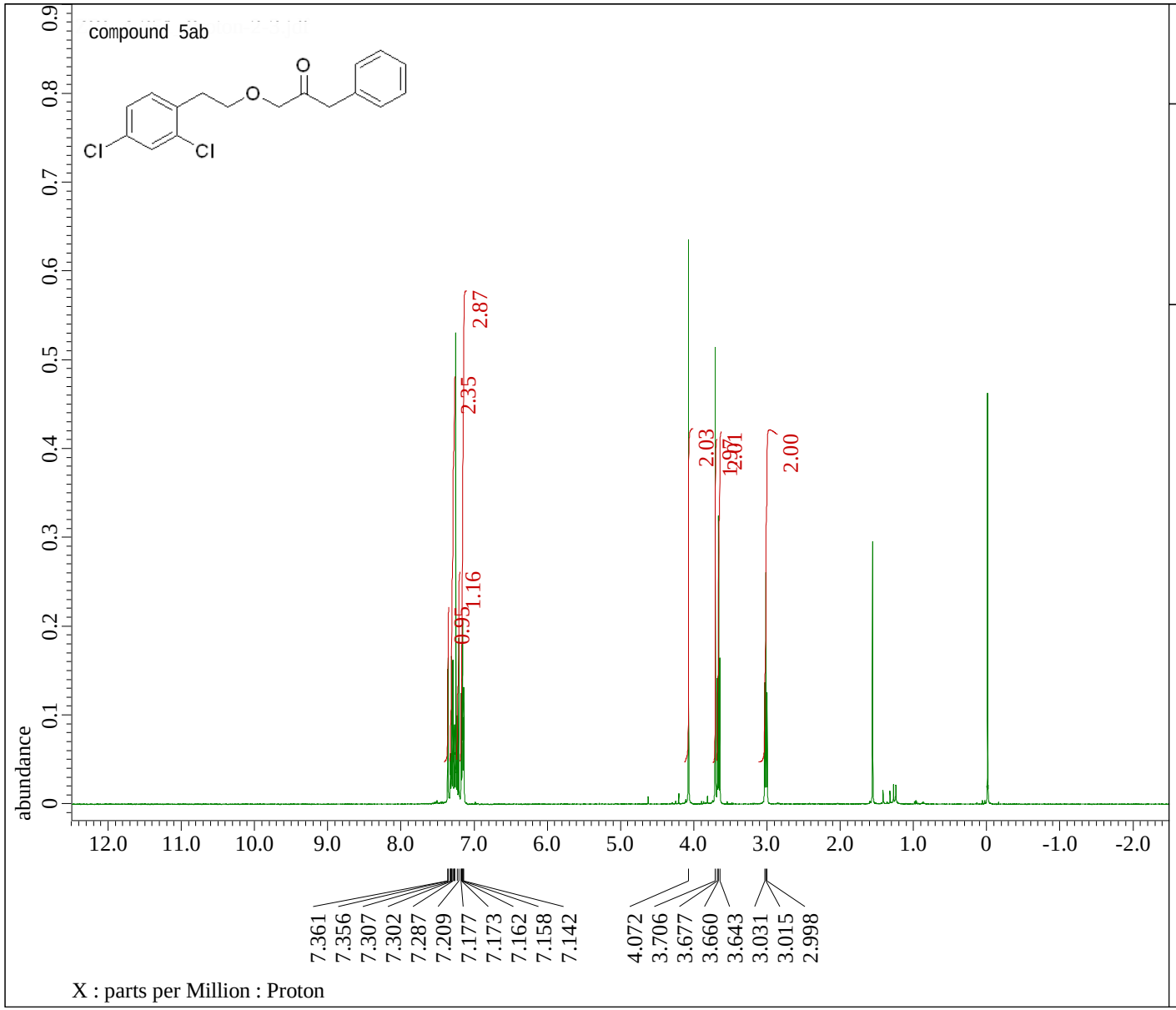

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-351_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-351
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 11-NOV-2017 21:
Revision_Time           = 14-NOV-2017 22:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 17.3[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

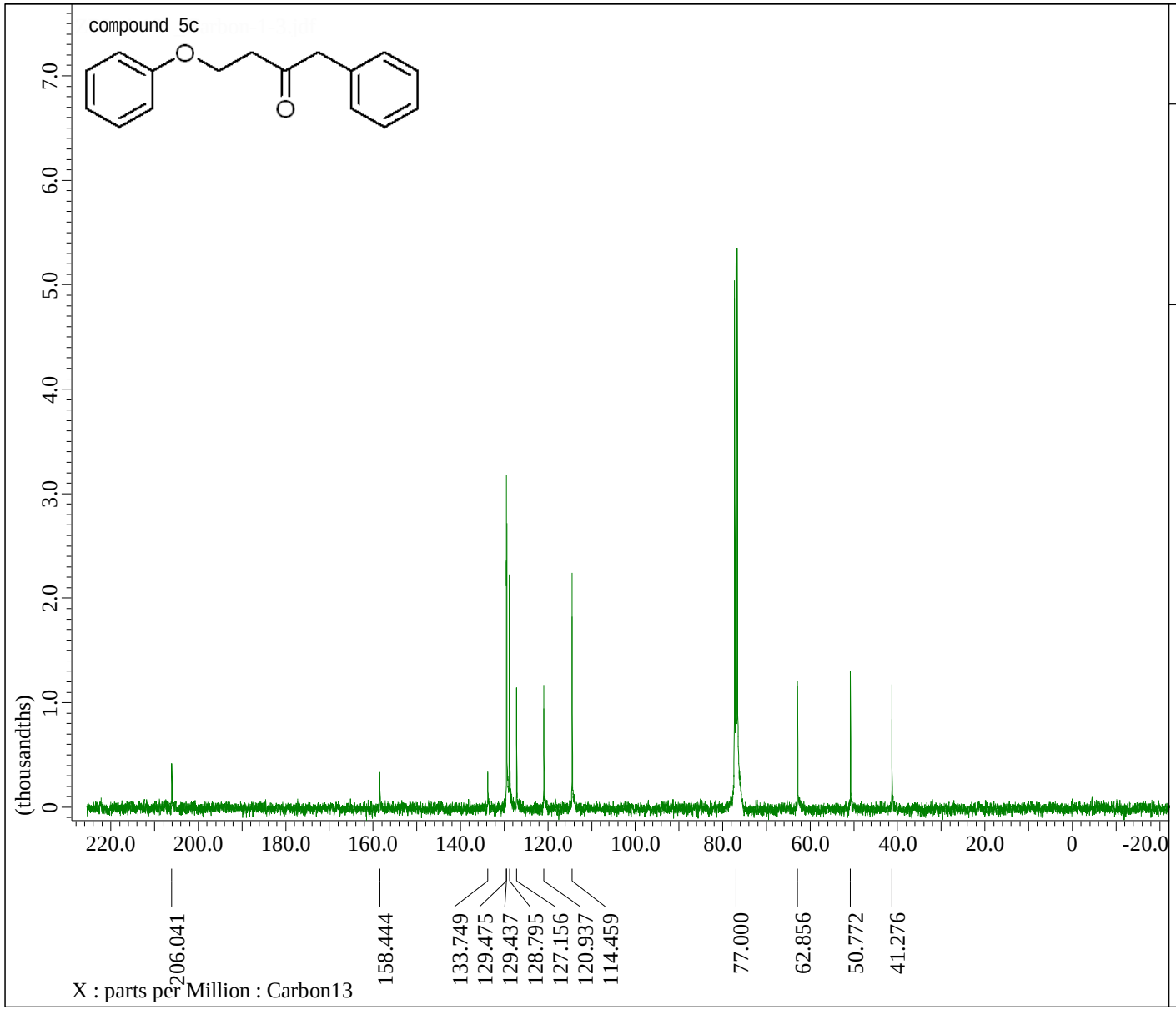
Derived from: ZRL-4-351_Proton-2-1.jdf
```

```
Filename              = ZRL-4-351_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-351
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 13-NOV-2017 09:55:
Revision_Time         = 14-NOV-2017 22:45:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 15.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



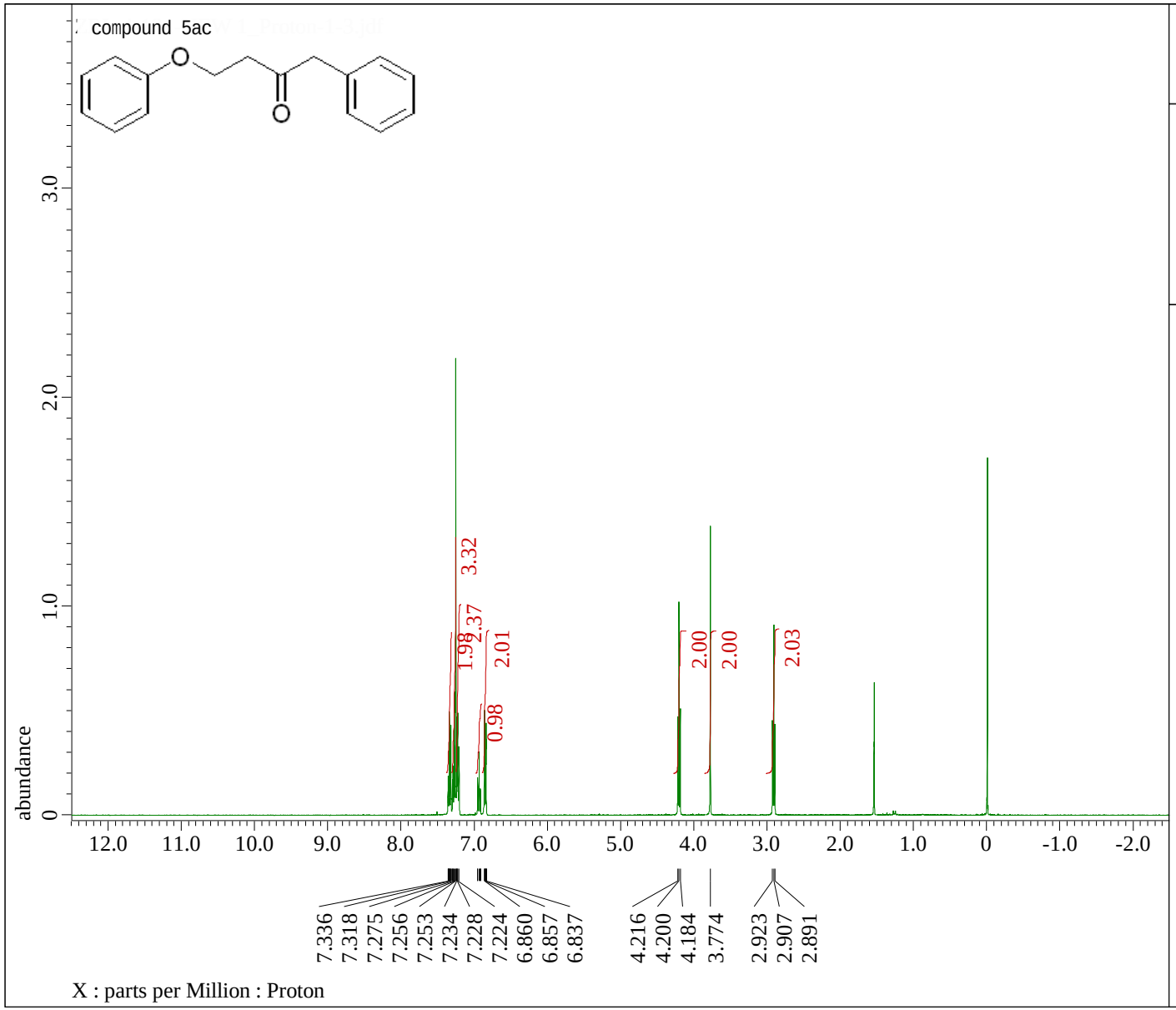

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-191_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-191
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 21-OCT-2017 15:
Revision_Time           =  5-NOV-2017 17:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 21.1[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



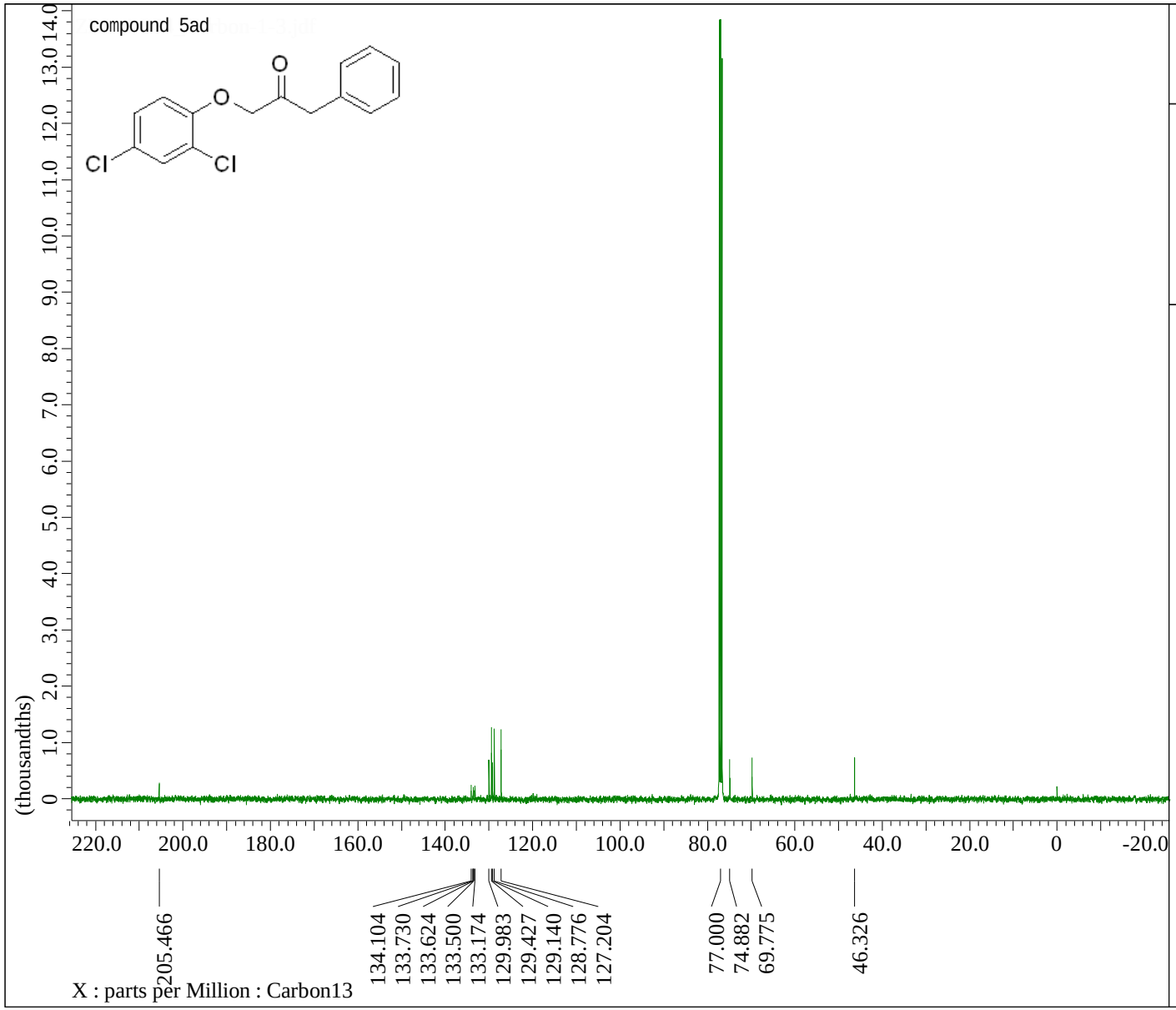

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-191-NEW 1_Pr
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-191-NEW 1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 21-OCT-2017 16:33:
Revision_Time         =  5-NOV-2017 17:35:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 20.8[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

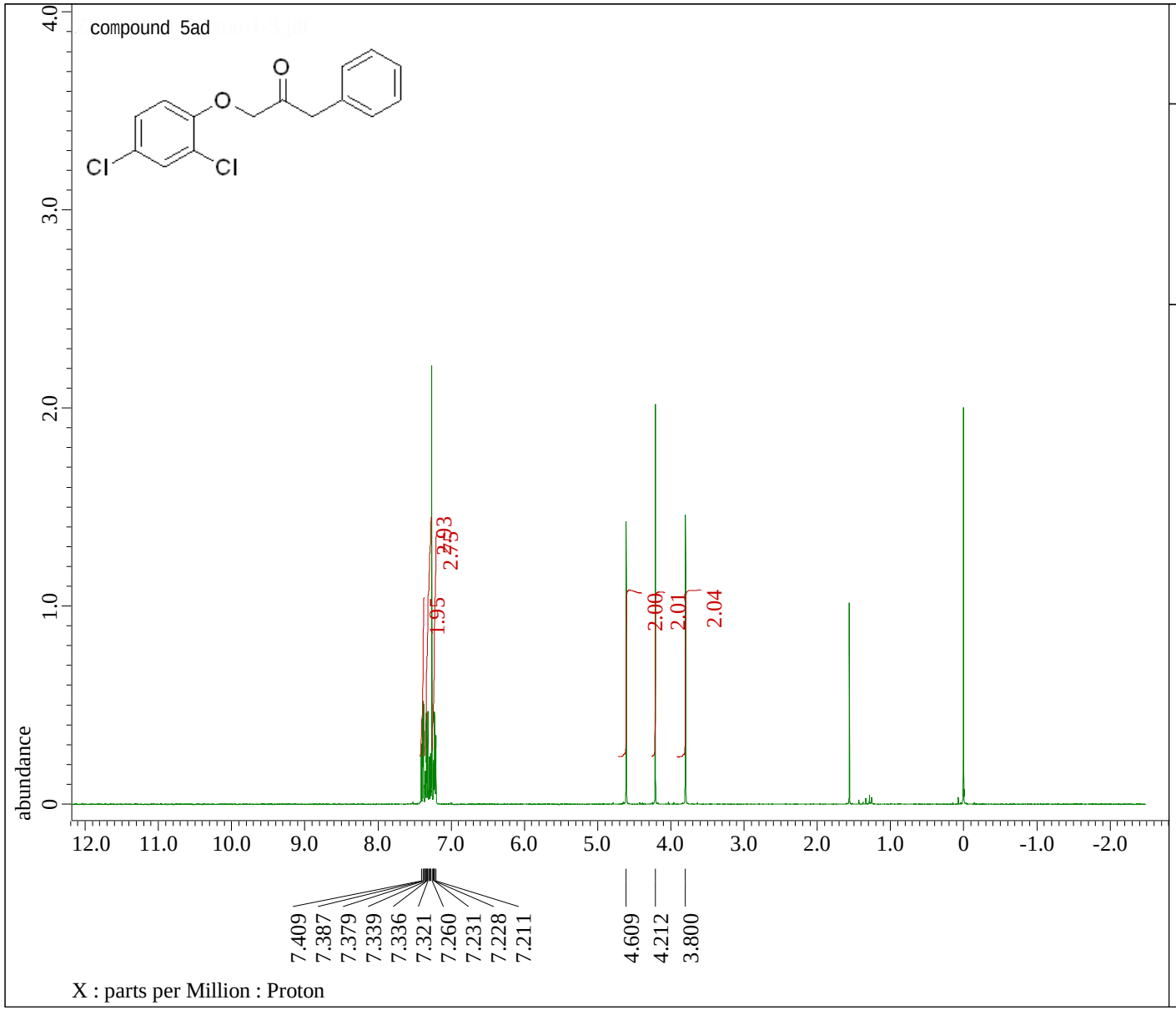
Derived from: ZRL-4-354_Carbon-1-1.jdf

Filename                  = ZRL-4-354_Carbo
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-4-354
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 11-NOV-2017 22:
Revision_Time             =  5-DEC-2017 19:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 17.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



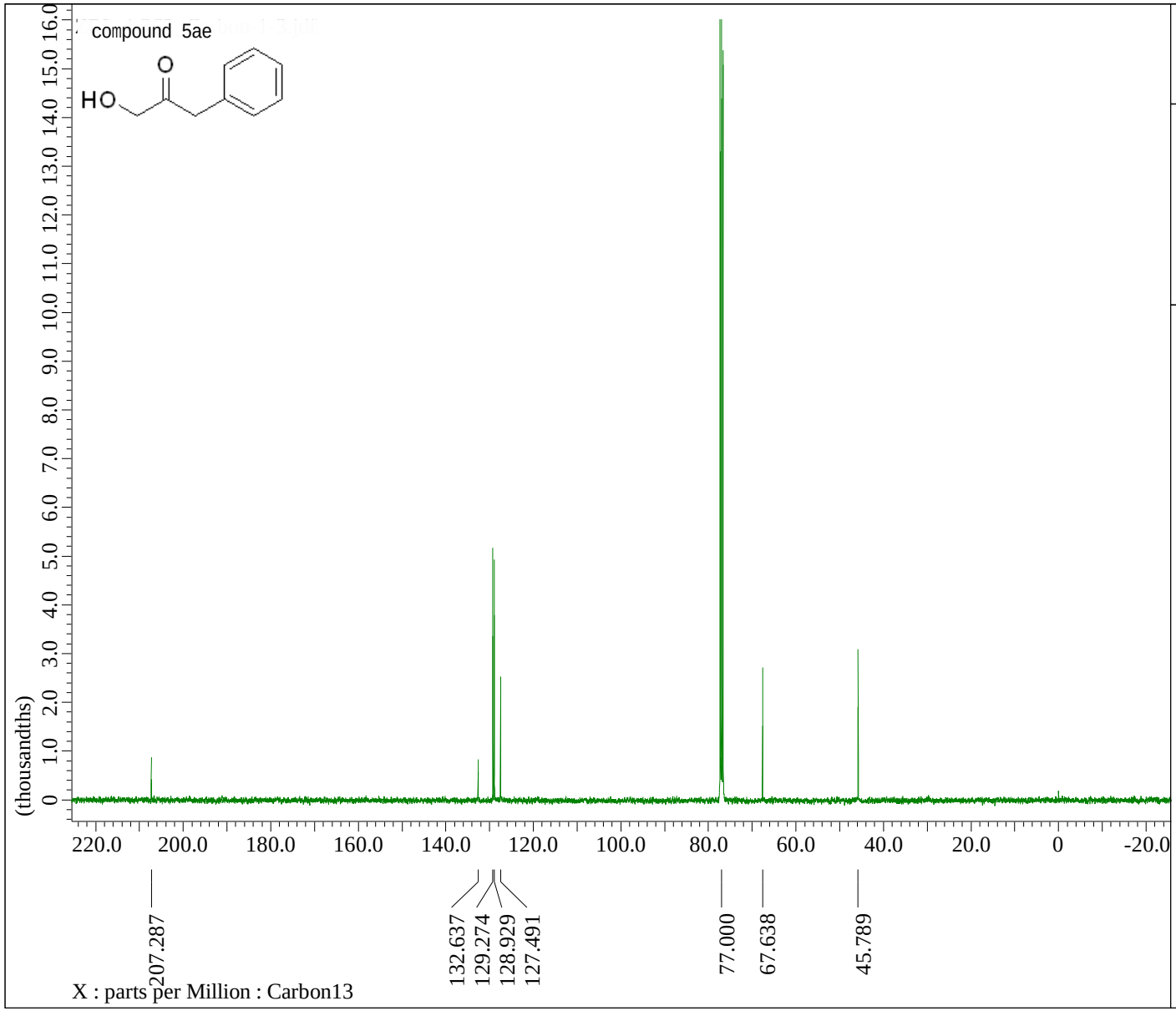

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-354_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-354
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 11-NOV-2017 22:13:
Revision_Time         =  5-DEC-2017 19:32:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 17.1[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



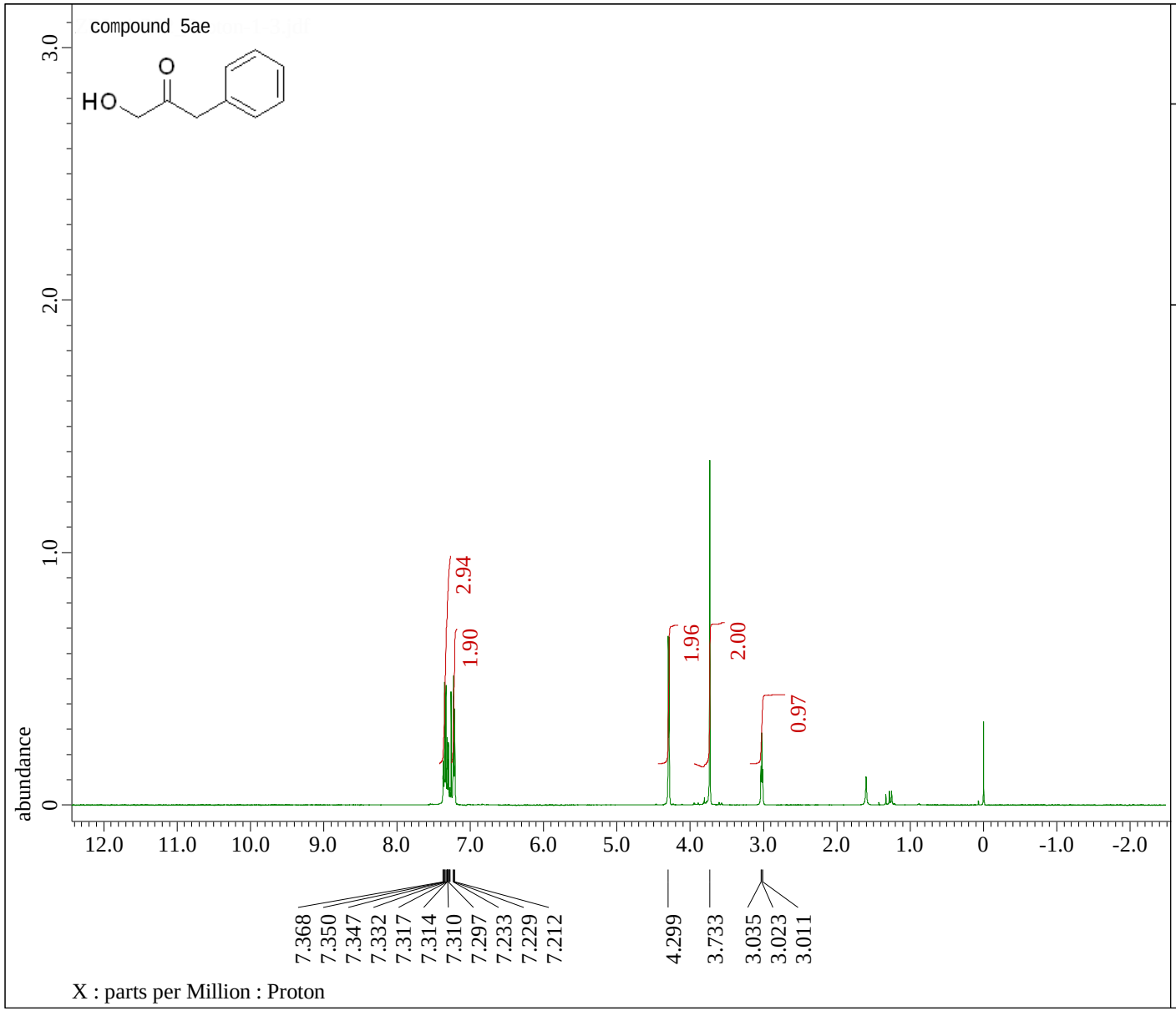

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                  = ZRL-4-362_Carbo
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-4-362
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 11-NOV-2017 23:
Revision_Time             =  5-DEC-2017 19:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 1024
Total_Scans               = 1024

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 17.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



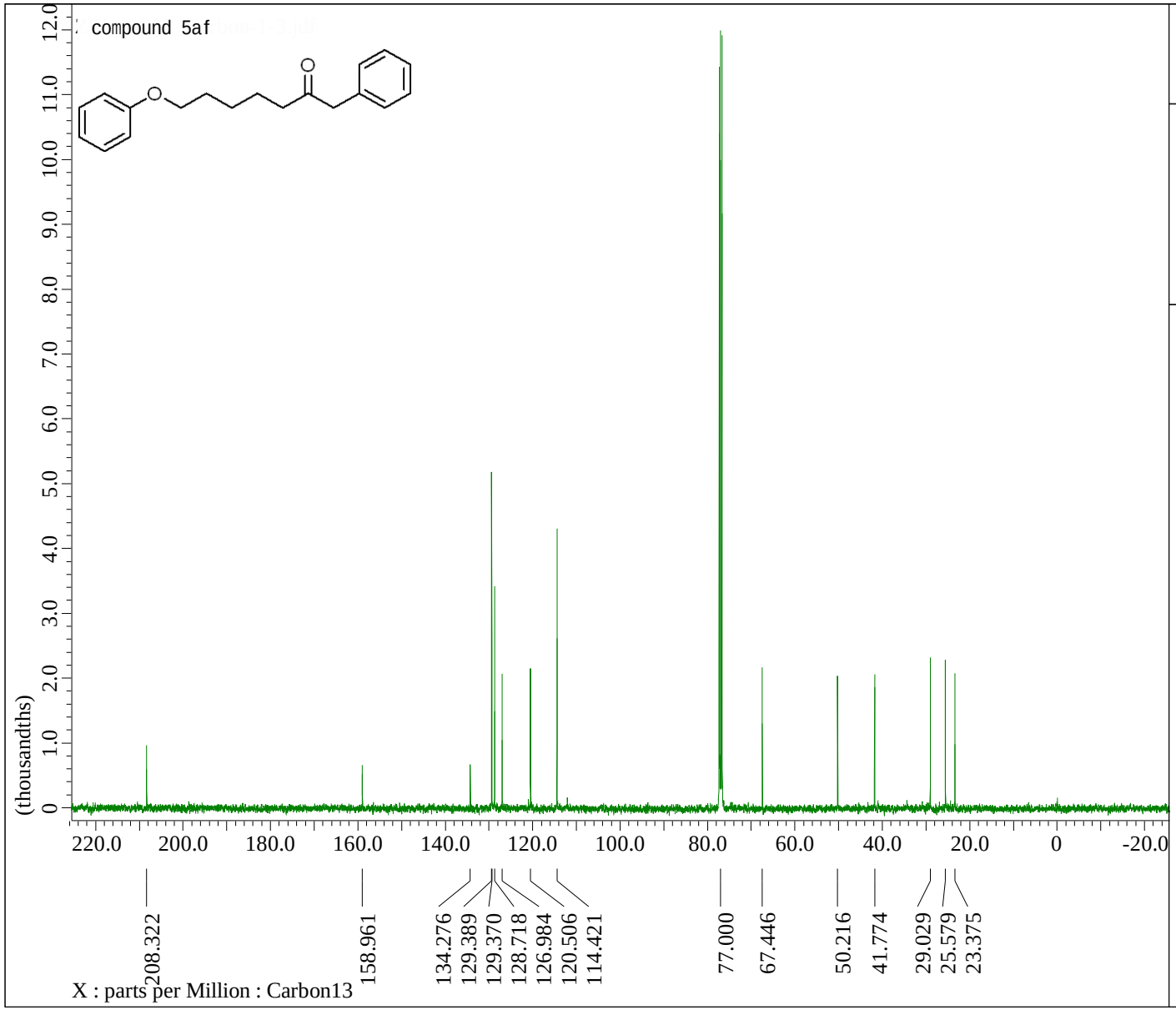

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-362_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-362
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 11-NOV-2017 23:11:
Revision_Time         =  5-DEC-2017 19:45:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 17.2[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



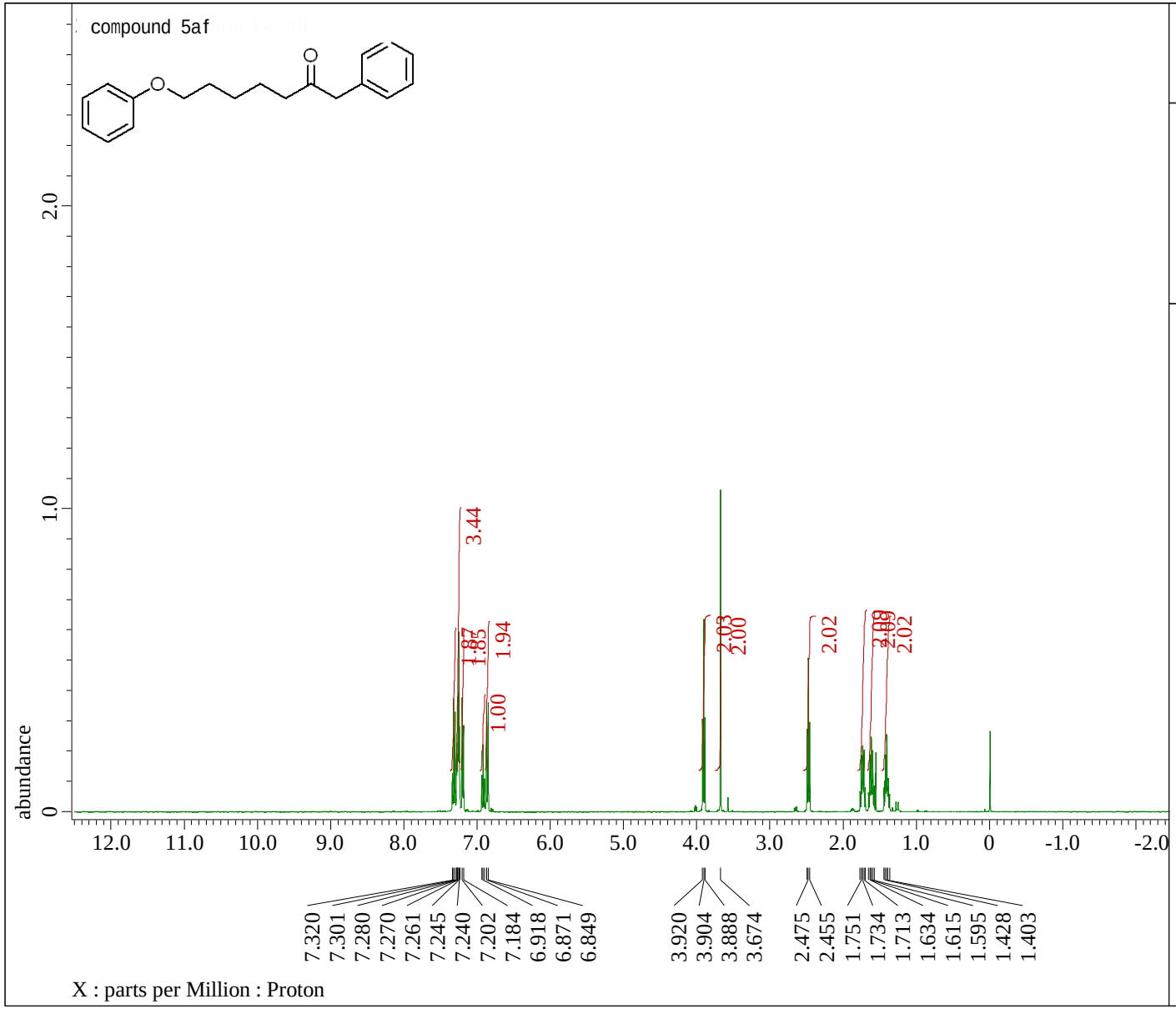

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-252_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-252
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 20-OCT-2017 20:
Revision_Time           =  5-NOV-2017 17:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 20.8[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



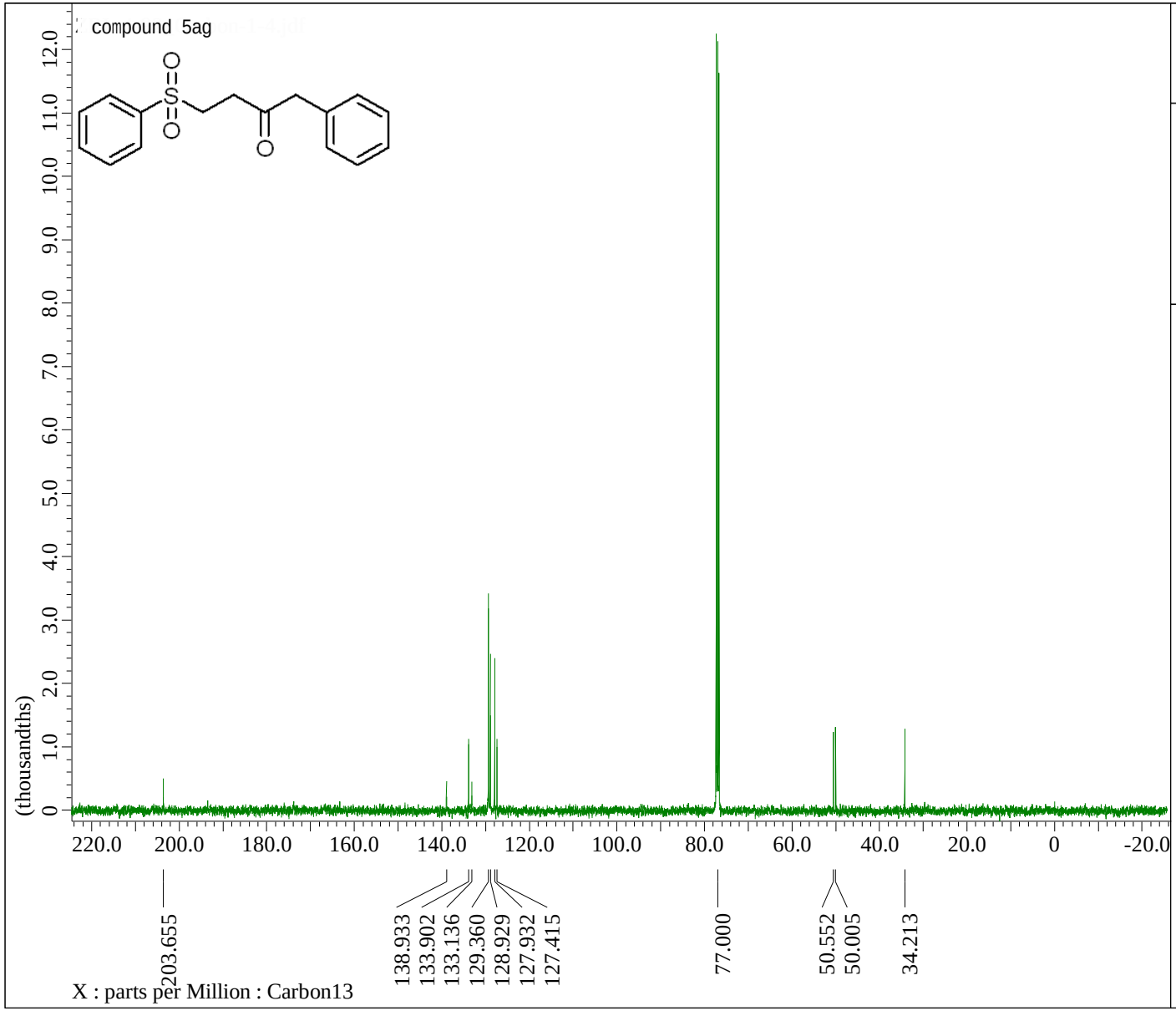

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-252_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-252
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 20-OCT-2017 20:00:
Revision_Time         =  5-NOV-2017 17:47:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 20.5[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



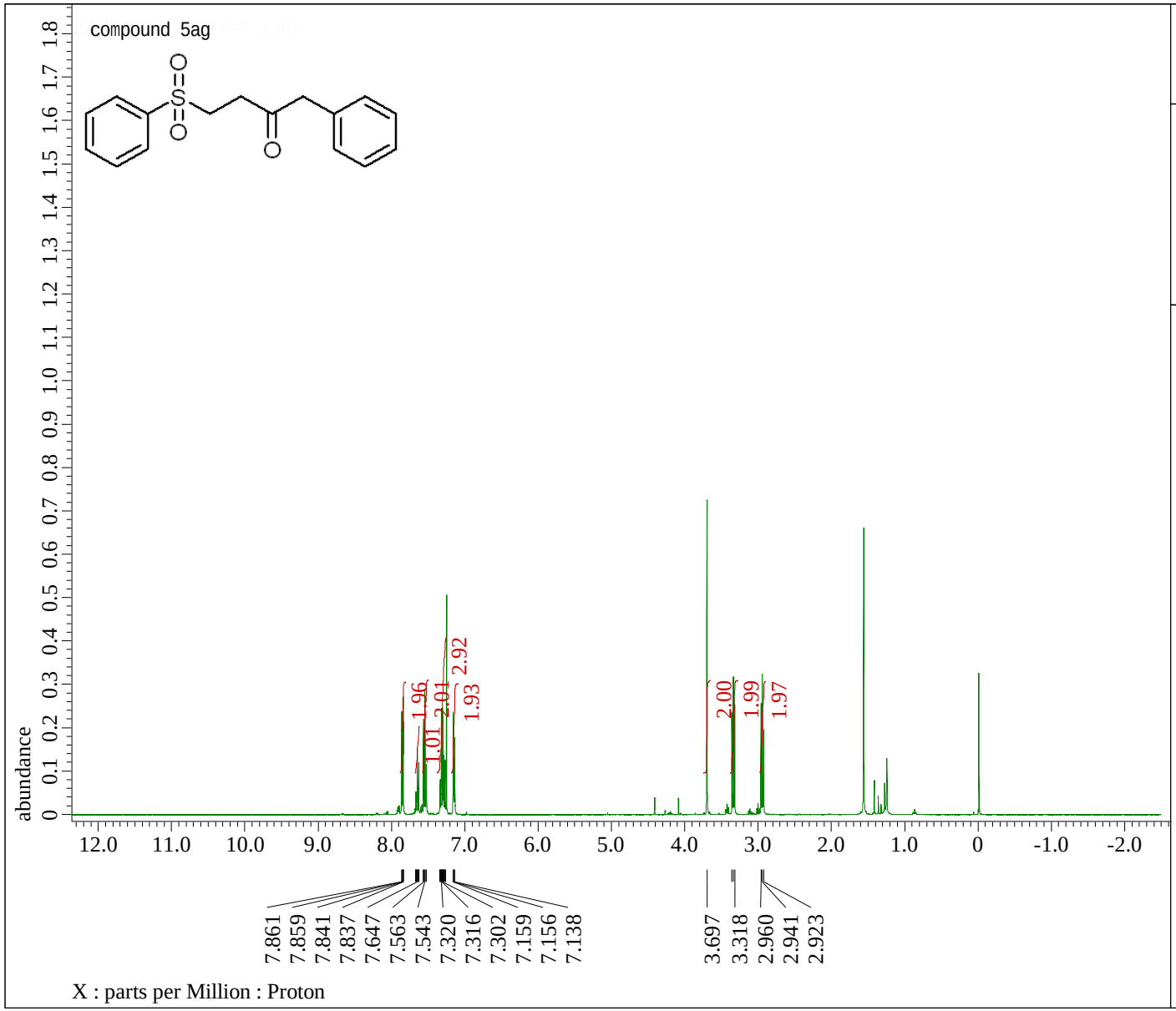

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                 = ZRL-4-92_Carbon
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-4-92
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 22-SEP-2017 17:
Revision_Time            =  5-NOV-2017 16:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 582
Total_Scans              = 582

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 24.7[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



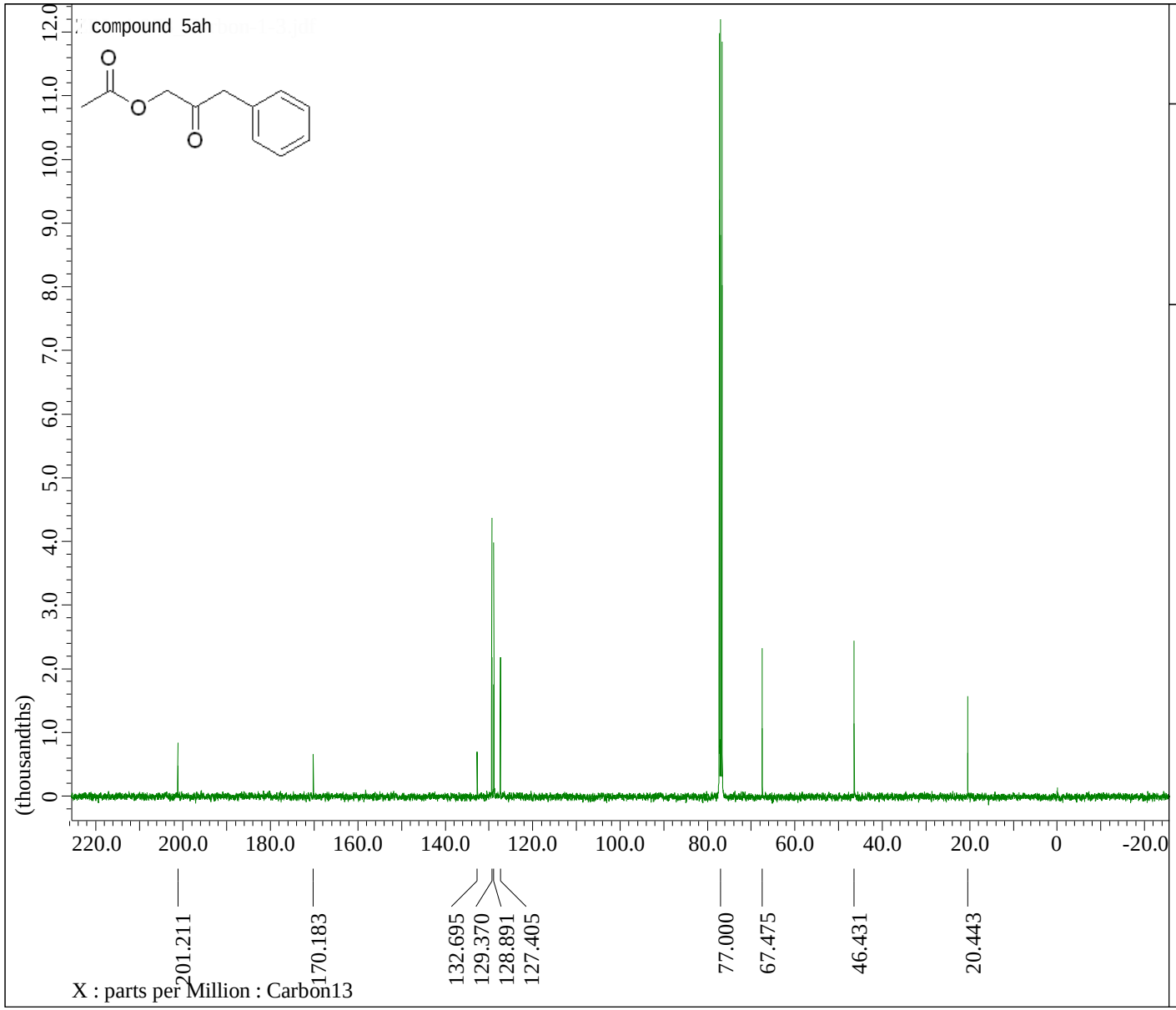

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-92_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-92
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 22-SEP-2017 15:50:
Revision_Time         =  5-NOV-2017 16:58:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 24.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



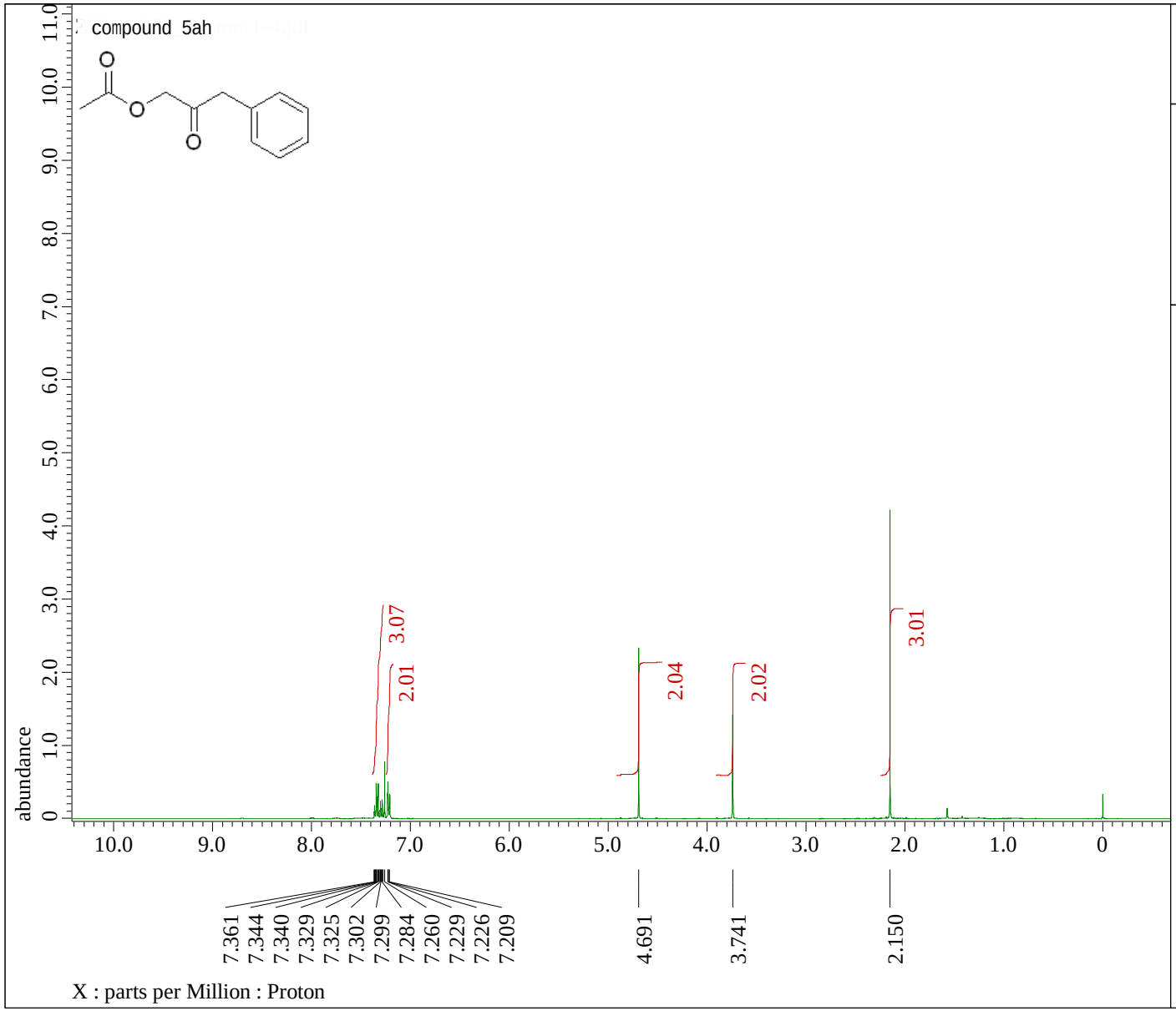

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-273_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-273
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 28-OCT-2017 17:
Revision_Time           = 28-OCT-2017 20:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 20.5[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



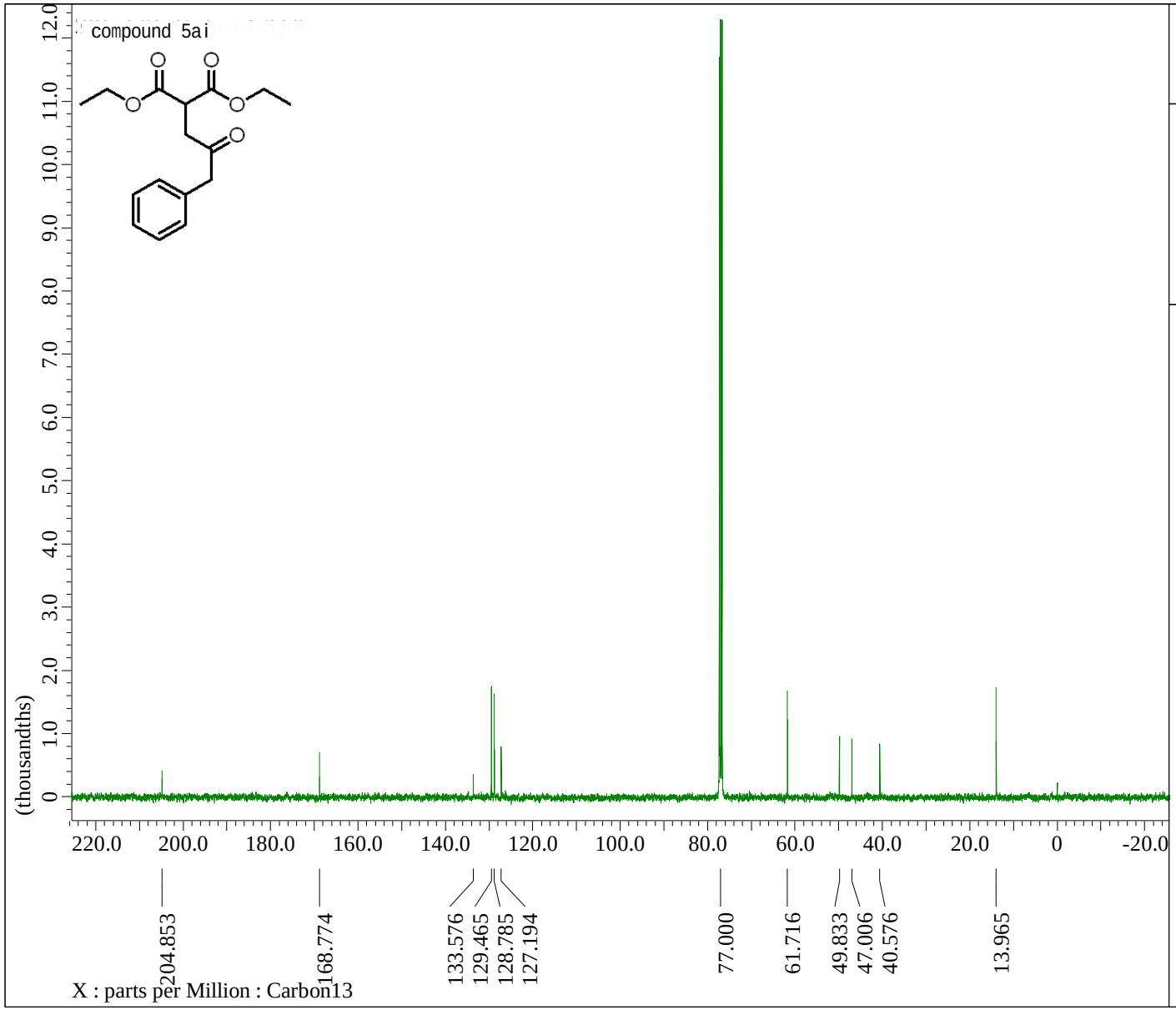

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-273_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-273
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 28-OCT-2017 17:54:
Revision_Time         = 28-OCT-2017 20:44:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 20.3[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



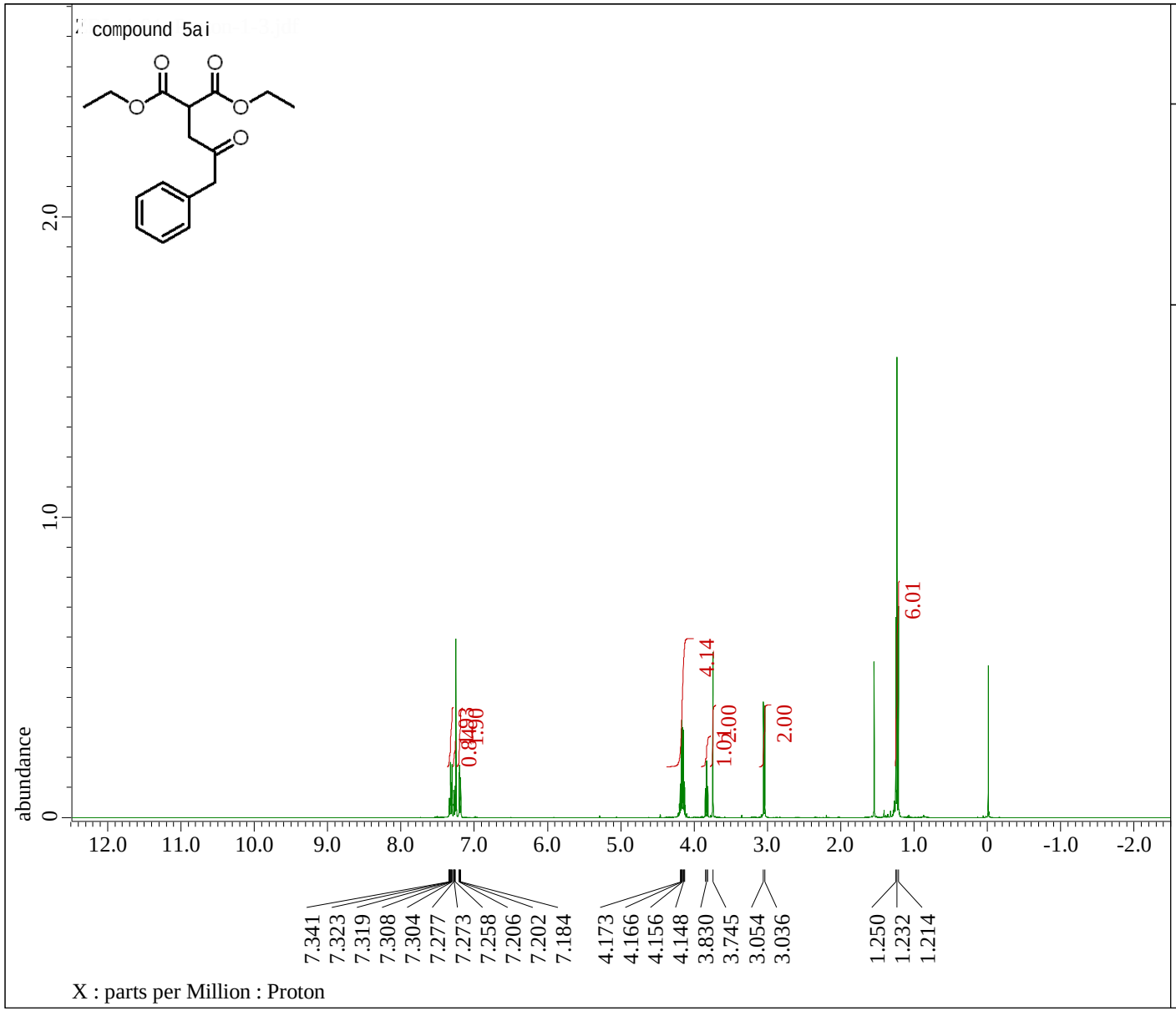

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                 = ZRL-4-91_Carbon
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-4-91
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 25-SEP-2017 17:
Revision_Time            = 28-OCT-2017 20:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 24[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



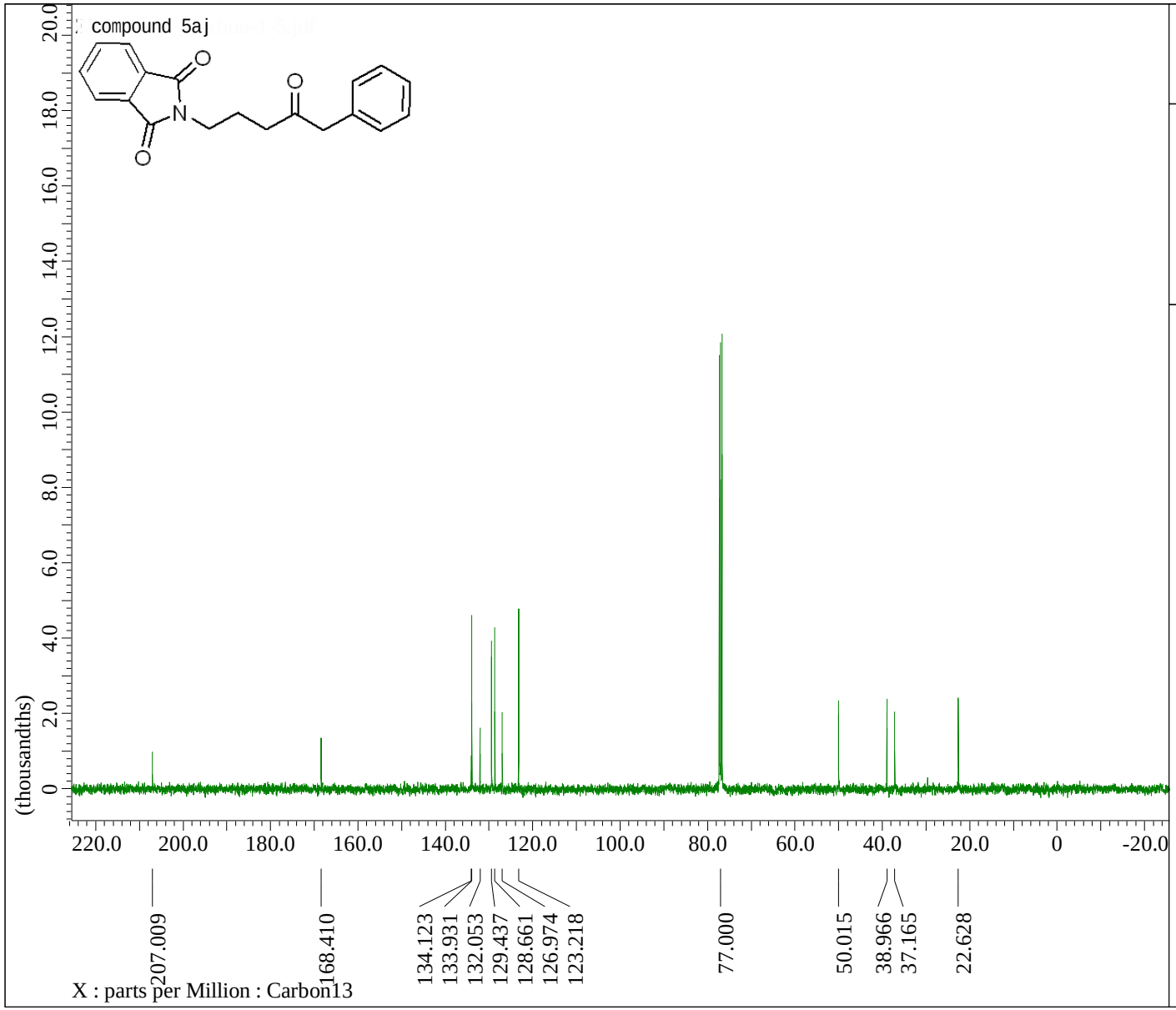

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-91_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-91
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 25-SEP-2017 17:54:
Revision_Time         = 28-OCT-2017 21:08:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 23.3[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



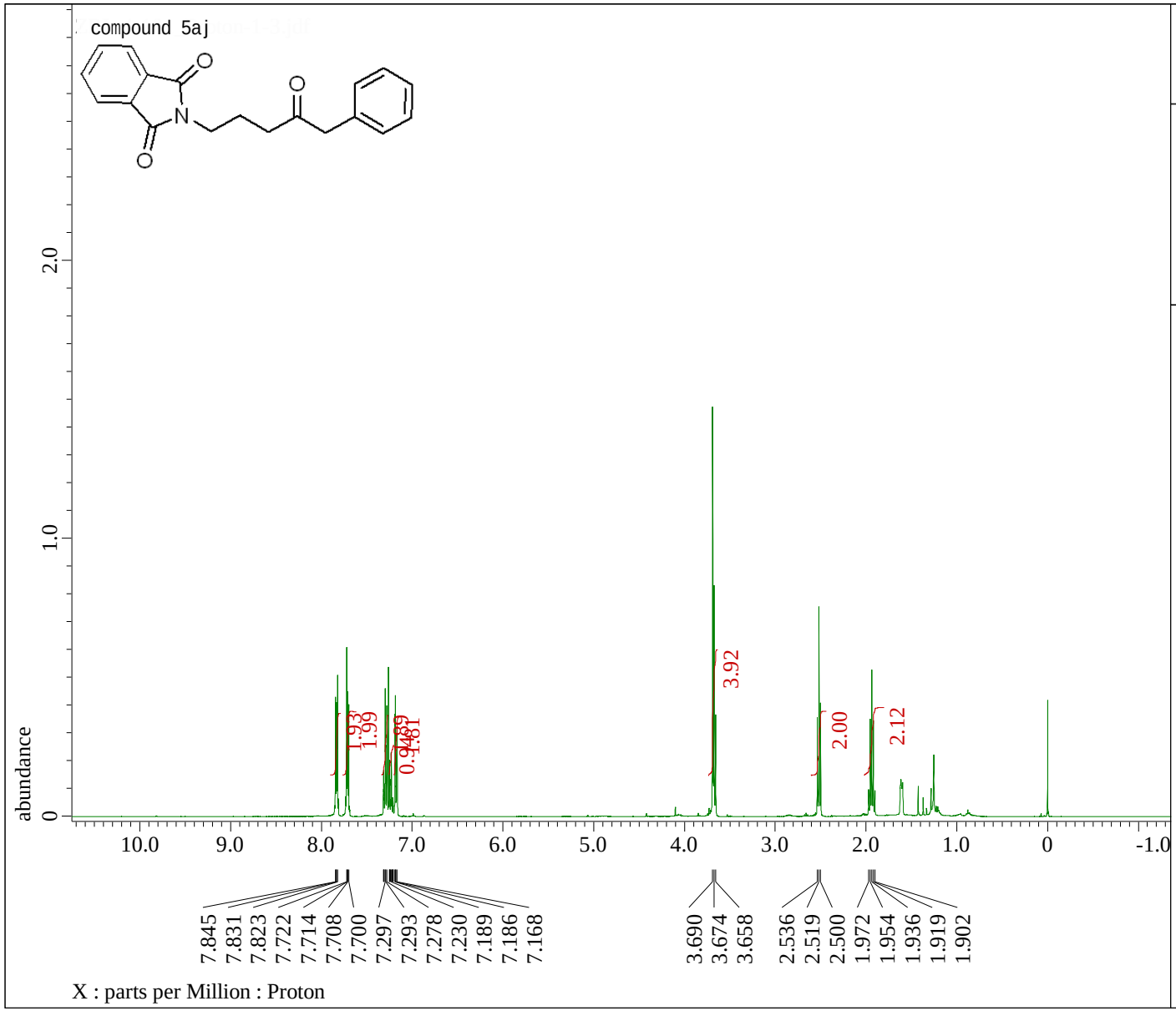

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-101_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-101
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 22-SEP-2017 17:
Revision_Time           =  5-NOV-2017 16:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 207.0
Total_Scans             = 207.0

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 24.7[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



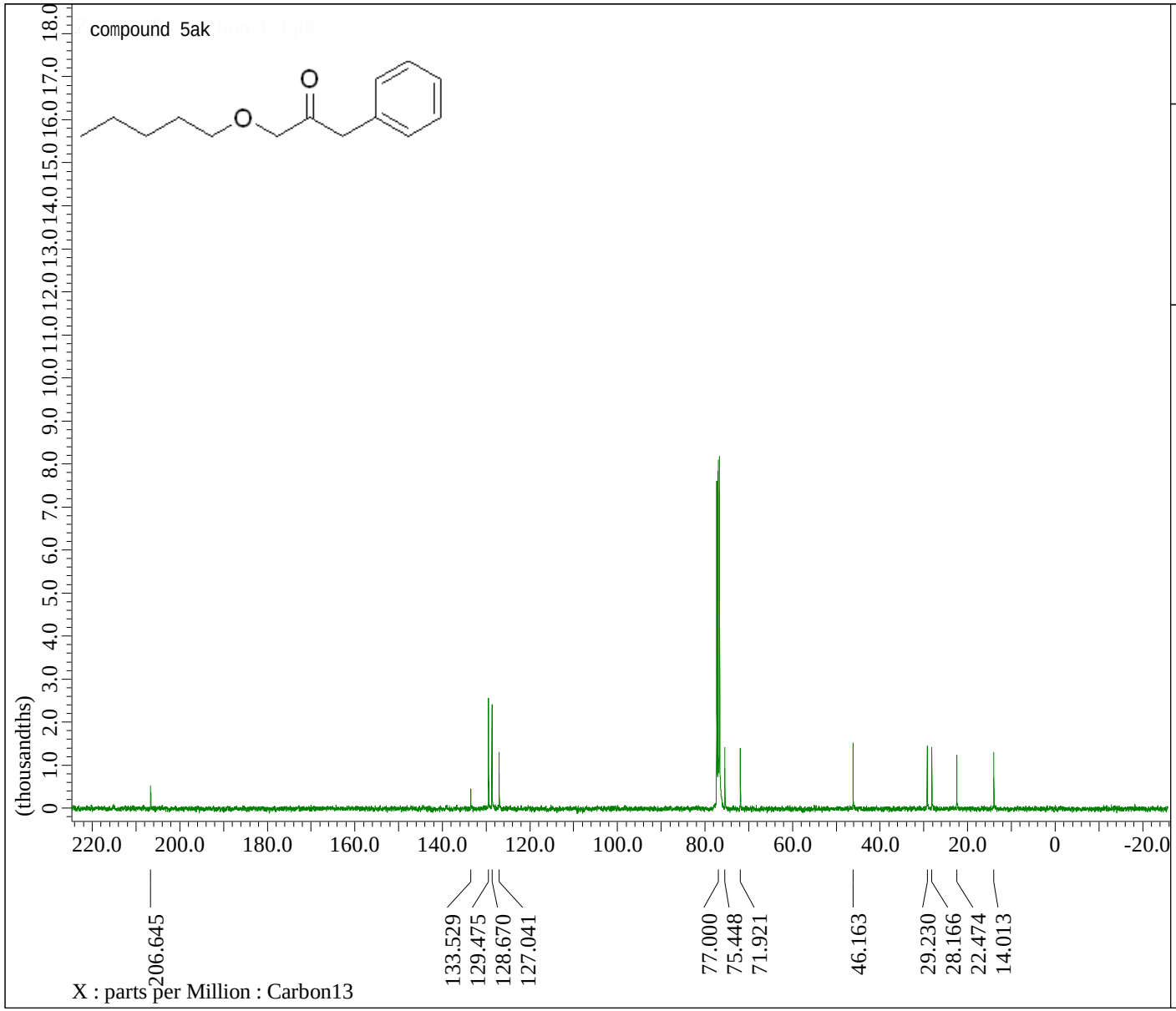

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-101_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-101
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 22-SEP-2017 15:55:
Revision_Time         =  5-NOV-2017 16:29:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 24.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



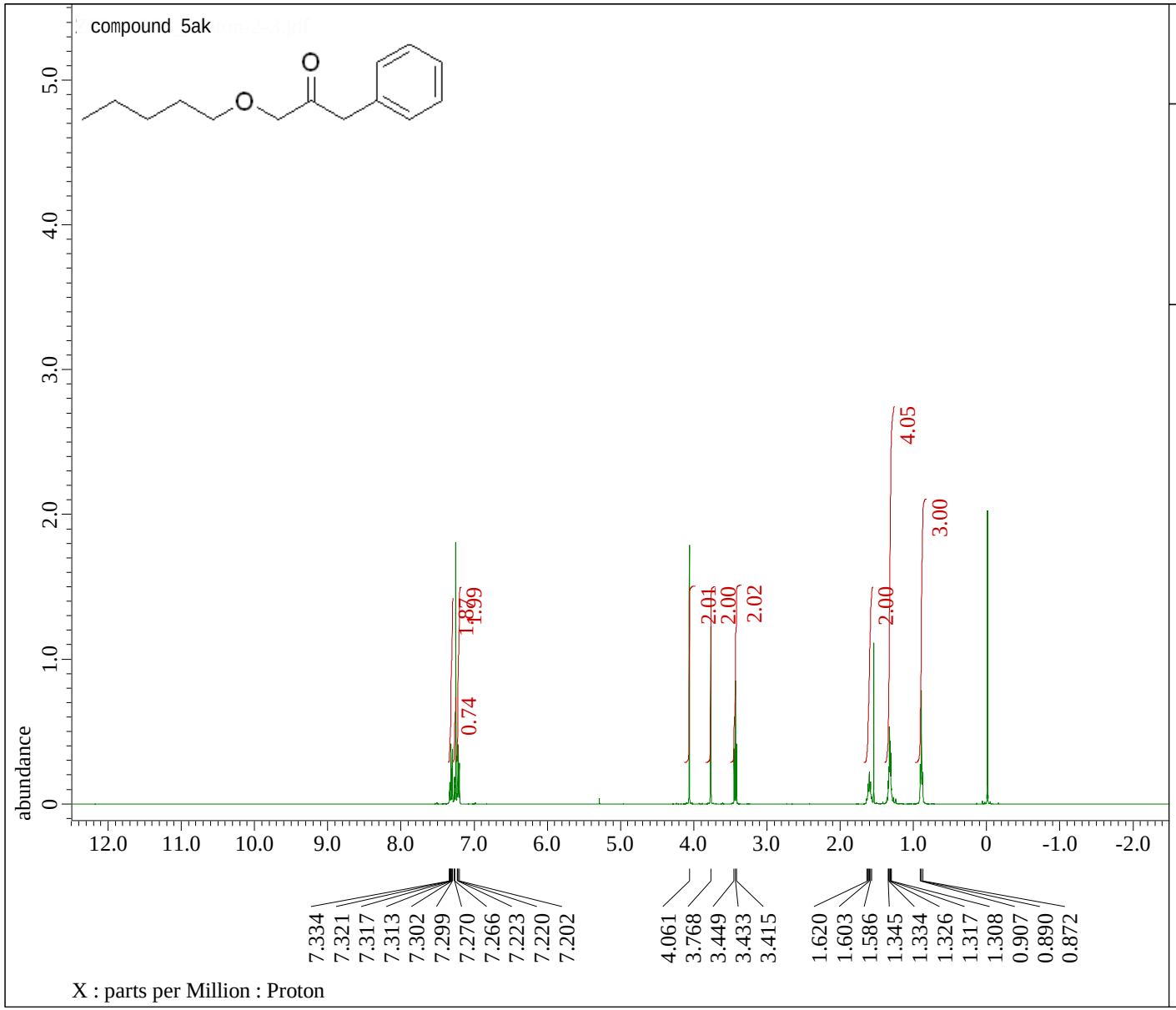

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-333_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-333
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  9-NOV-2017 15:
Revision_Time           = 22-FEB-2018 21:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 19.3[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



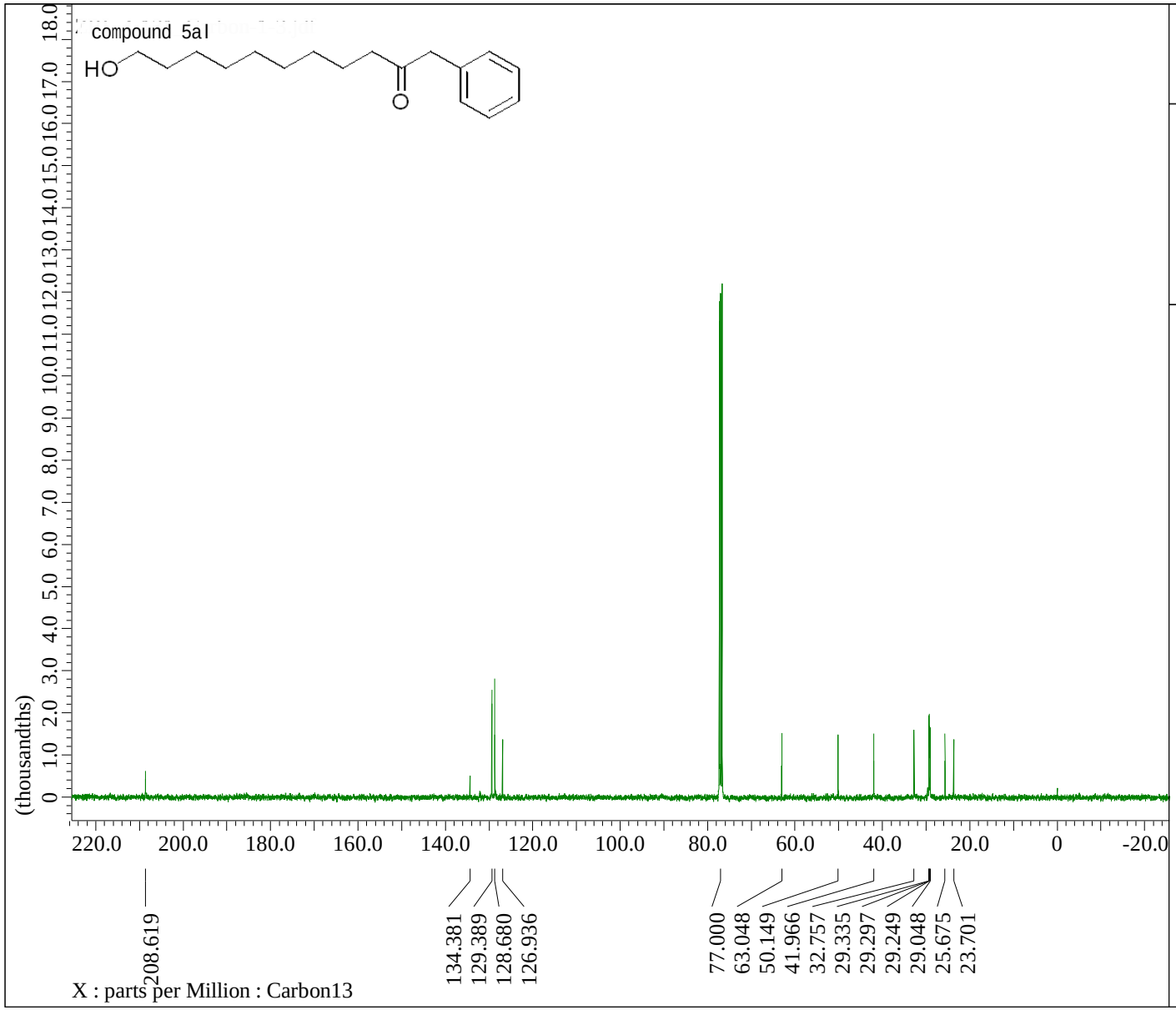

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-333_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-333
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  9-NOV-2017 18:54:
Revision_Time         = 14-NOV-2017 22:02:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 19.7[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



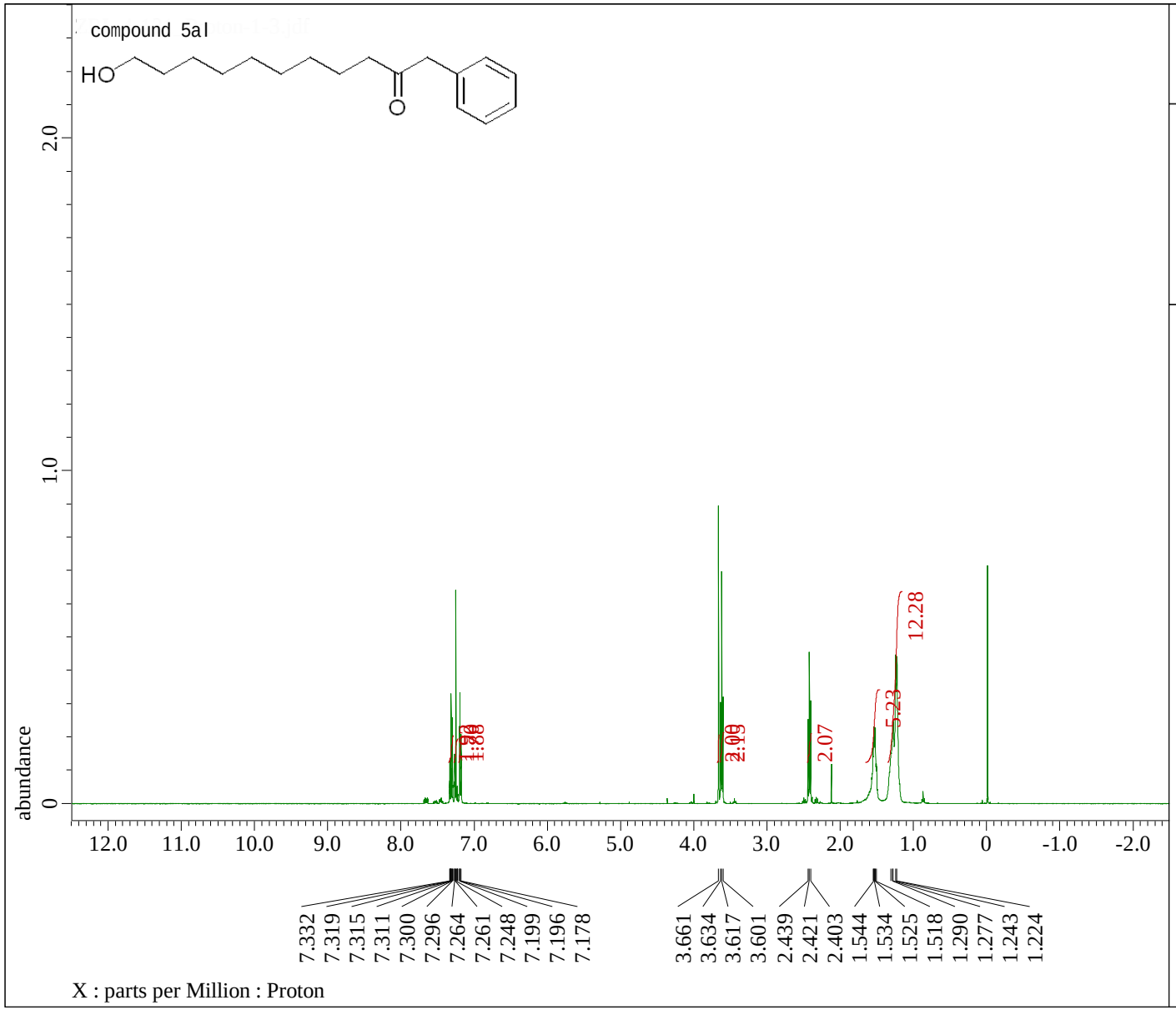

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                 = ZRL-4-131_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-4-131
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 26-SEP-2017 15:
Revision_Time            =  5-NOV-2017 16:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 707
Total_Scans              = 707

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 24.8[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



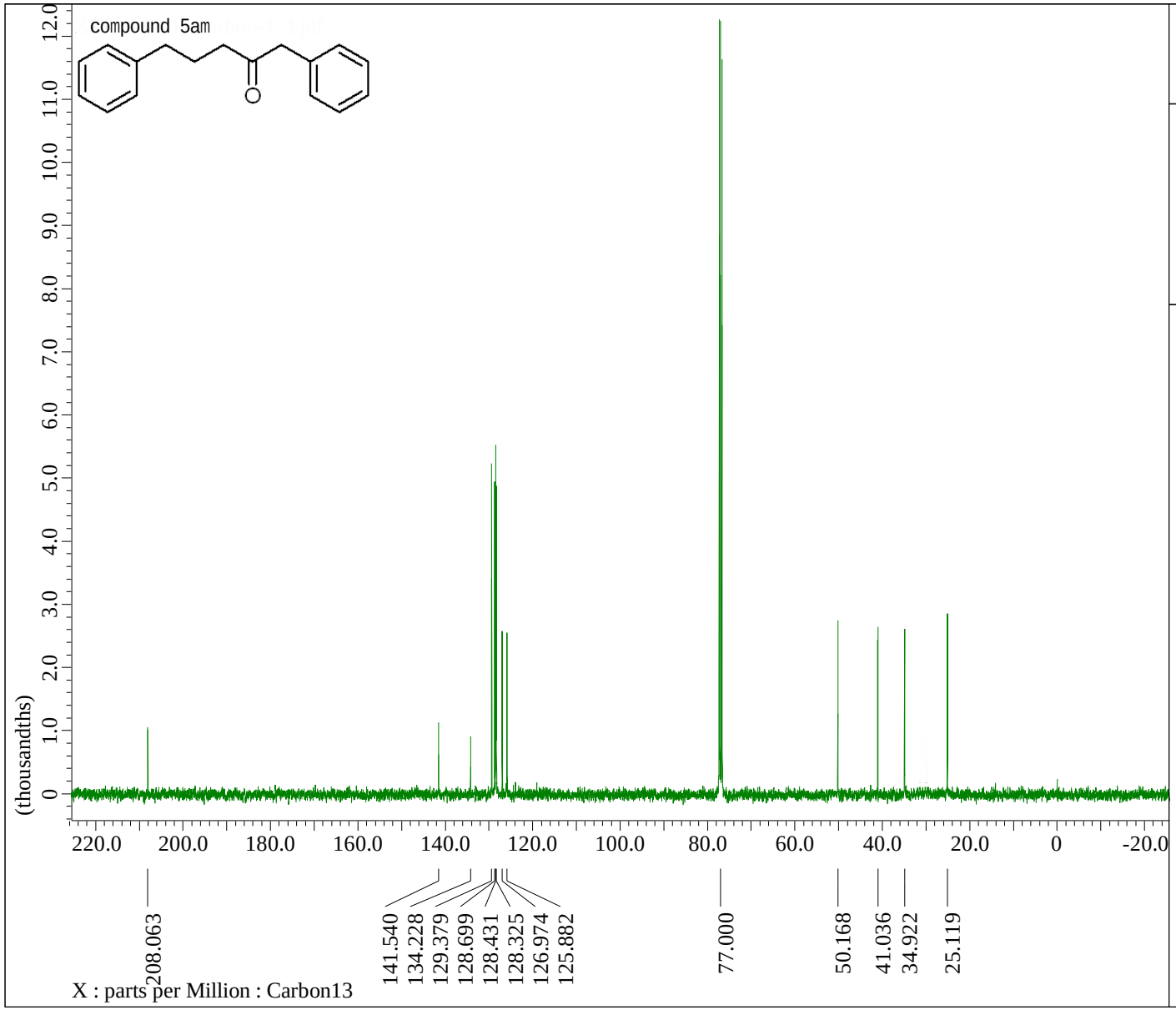

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-131_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-131
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 26-SEP-2017 15:09:
Revision_Time         =  5-NOV-2017 16:48:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 24.7[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

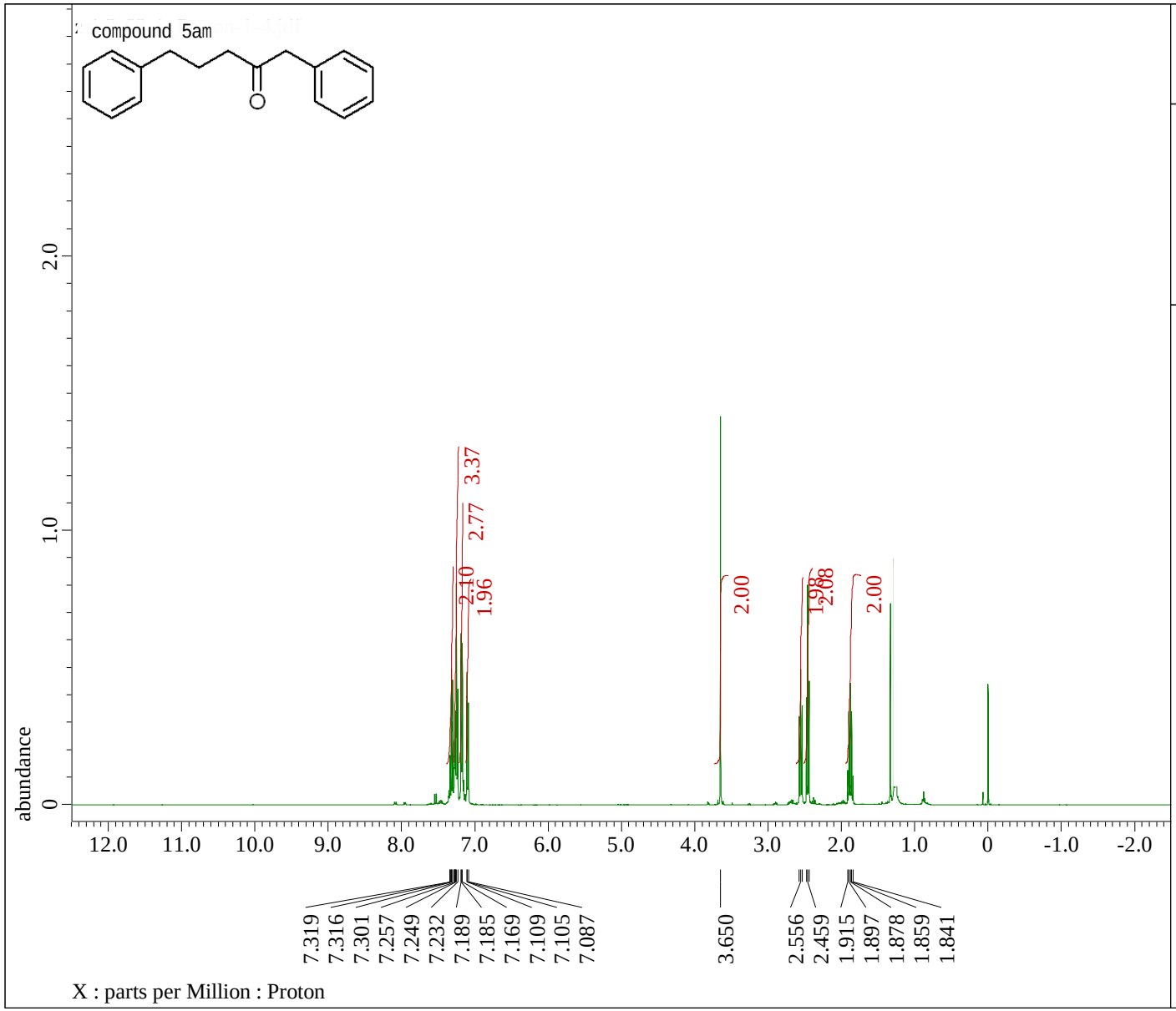
Derived from: ZRL-3-68-1_Carbon-1-1.jdf
```

```
Filename                  = ZRL-3-68-1_Carb
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-3-68-1
Solvent                   = CHLOROFORM-D
Actual_Start_Time         =  9-DEC-2017 20:
Revision_Time             = 29-JAN-2018 10:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 400
Total_Scans               = 400

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 25[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



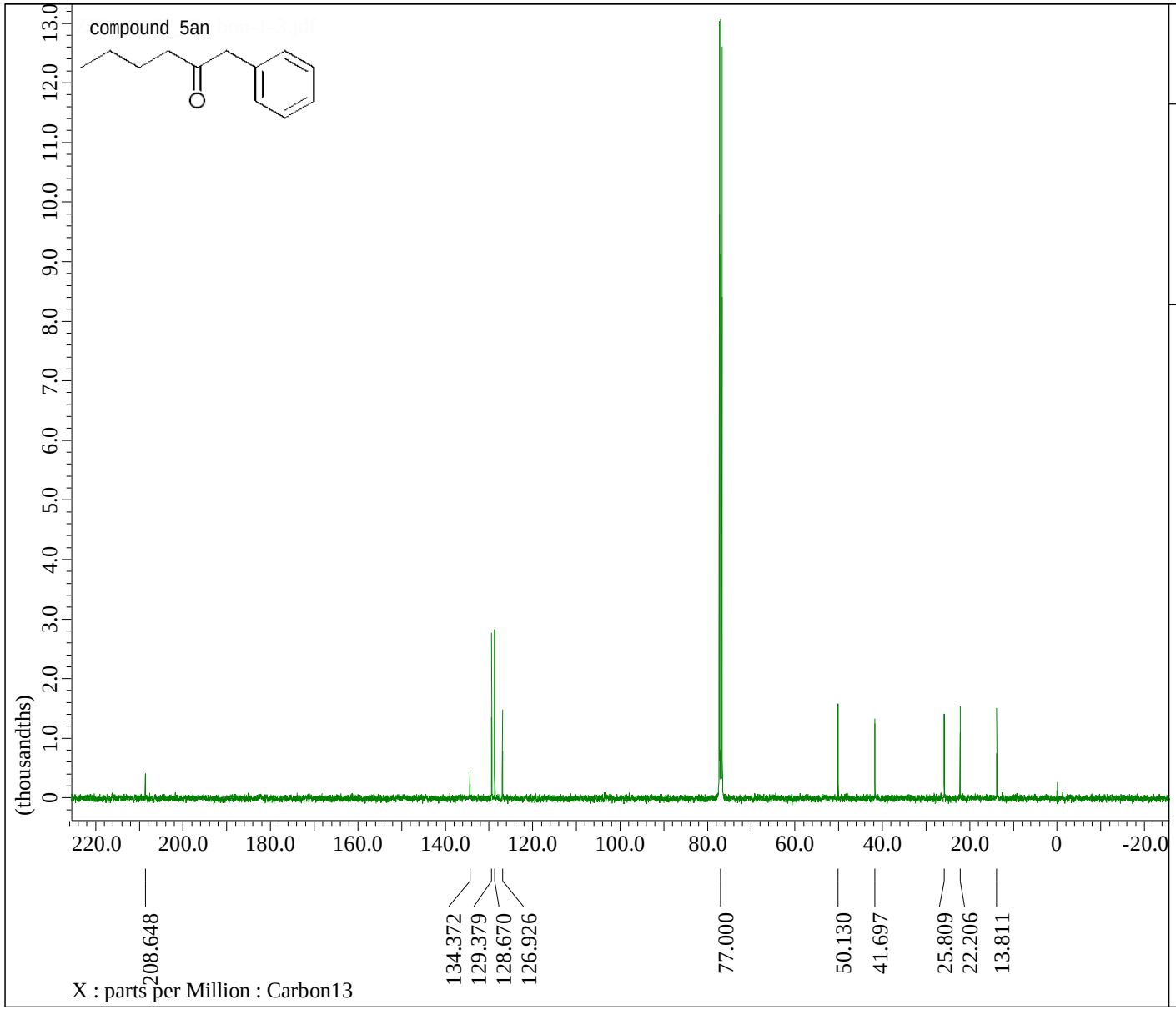

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = zrl-3-68-1_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = zrl-3-68-1
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  7-DEC-2017 17:38:
Revision_Time         = 29-JAN-2018 10:46:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 24.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



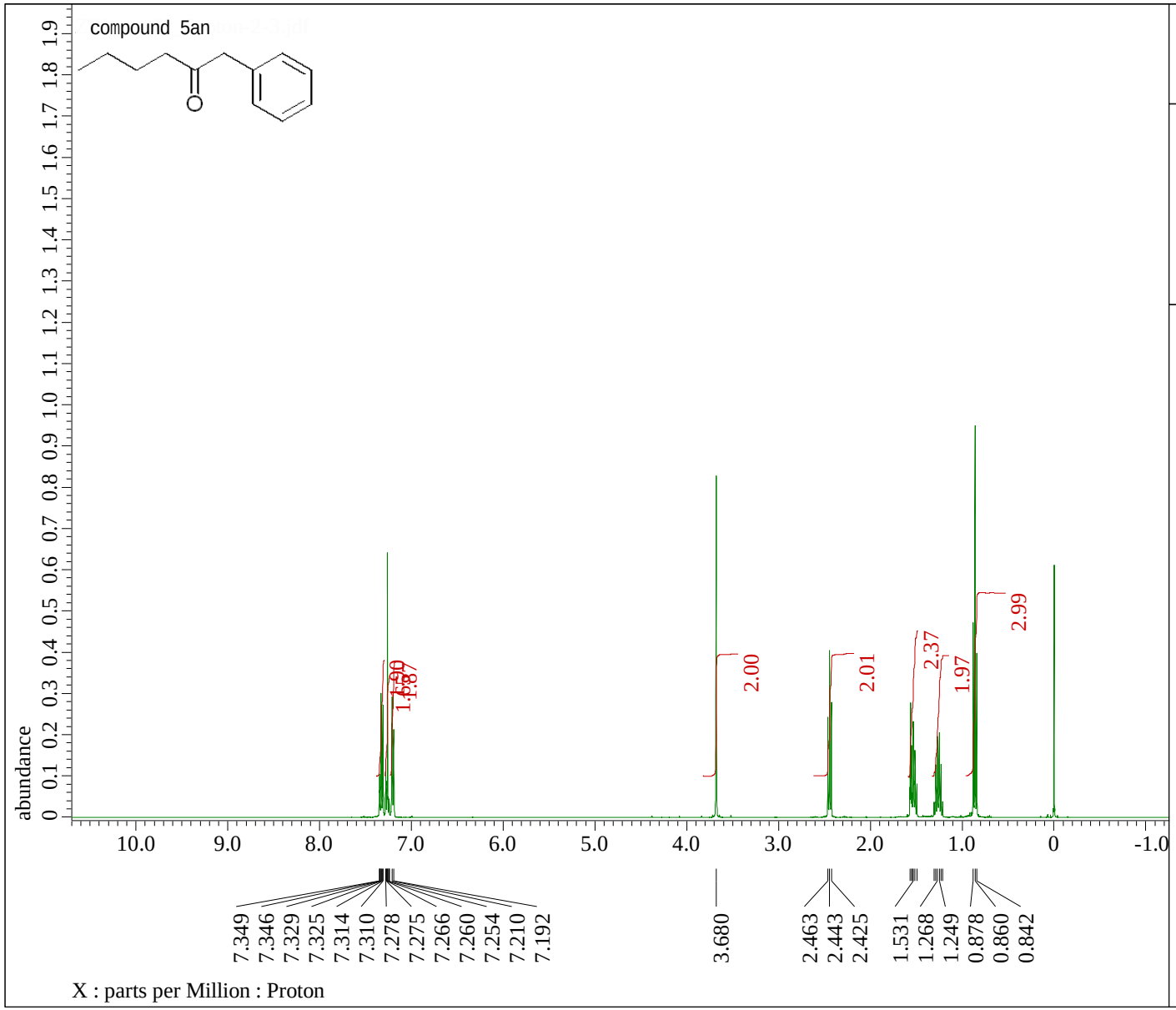

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                 = ZRL-4-162_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-4-162
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 16-OCT-2017 16:
Revision_Time            =  5-NOV-2017 16:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 20[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



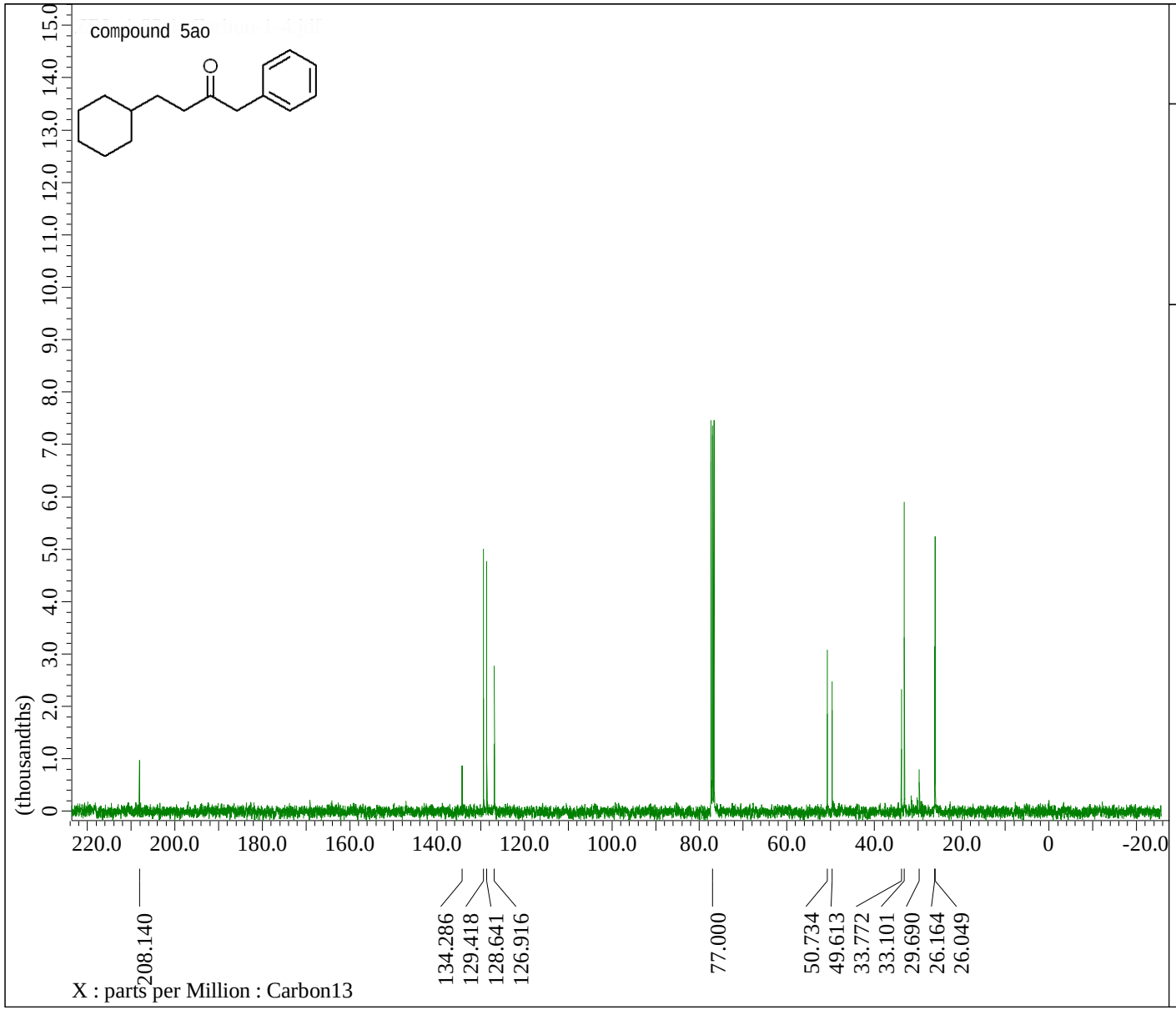

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-162_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-162
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 16-OCT-2017 16:19:
Revision_Time         =  5-NOV-2017 16:15:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 19.7[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



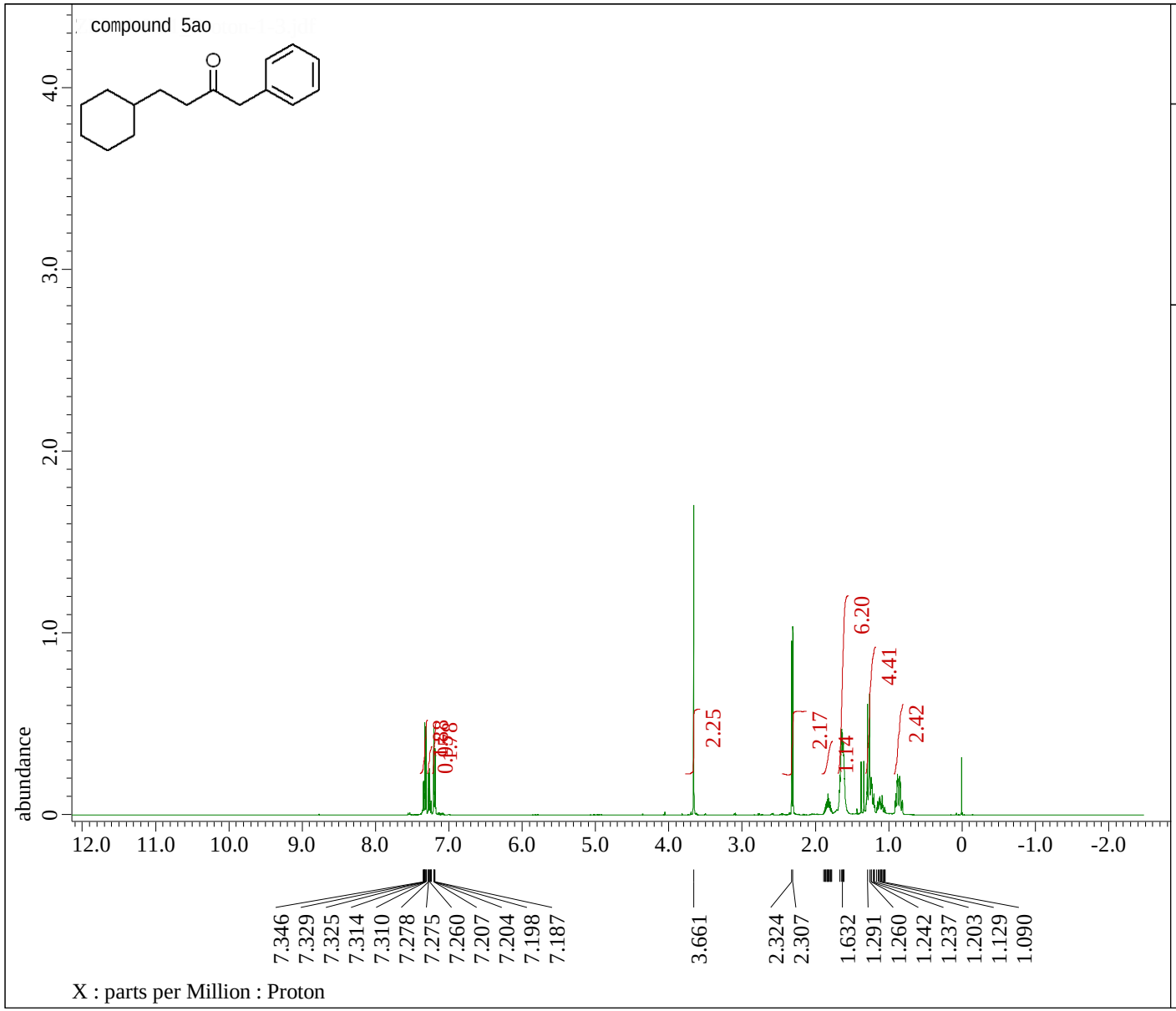

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-82 1_Carb
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-82 1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 22-SEP-2017 18:
Revision_Time           =  5-NOV-2017 17:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 235
Total_Scans             = 235

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 24.6[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



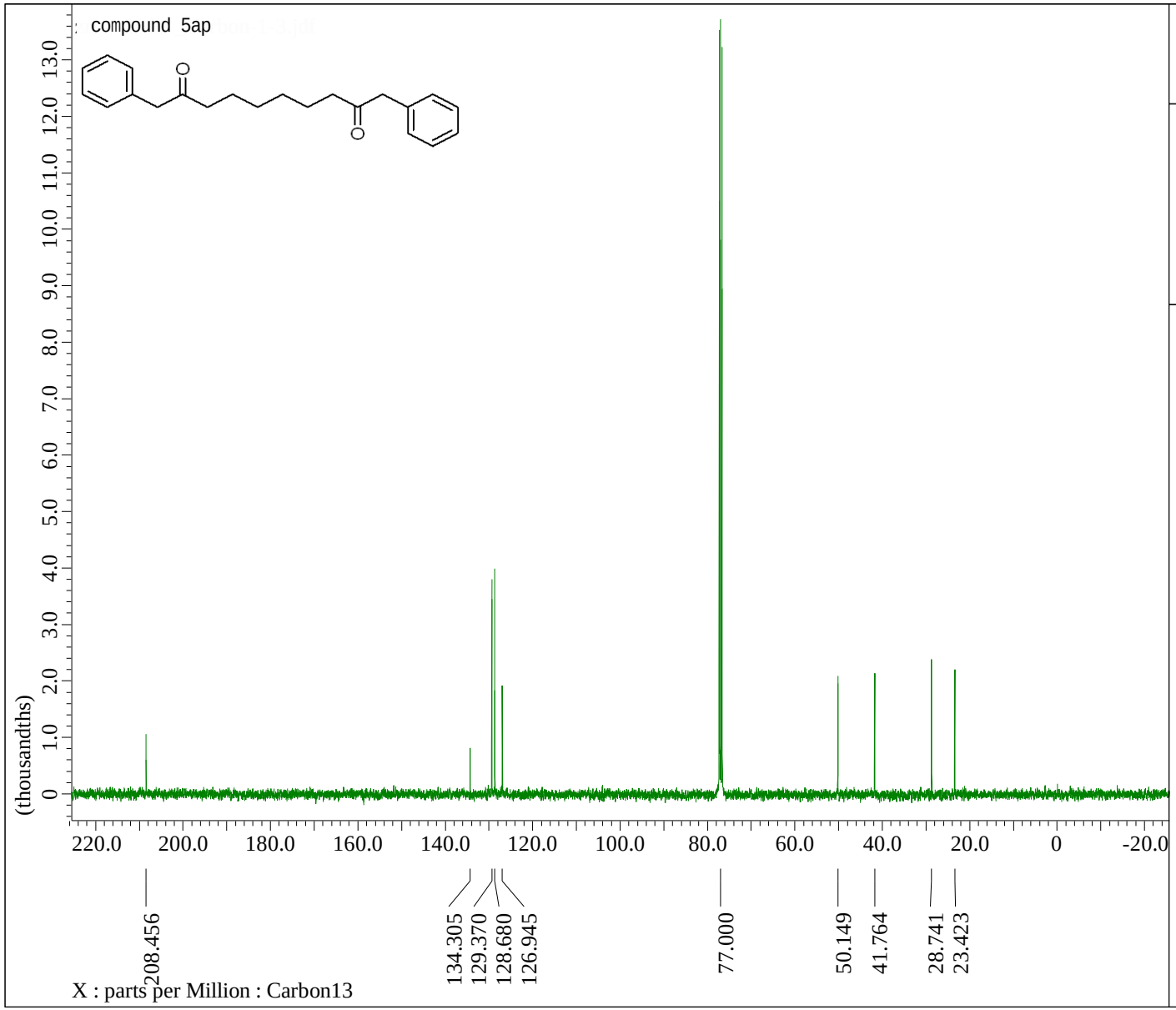

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-82 1_Proton-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-82 1
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 22-SEP-2017 18:01:
Revision_Time         =  5-NOV-2017 17:21:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 24.5[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

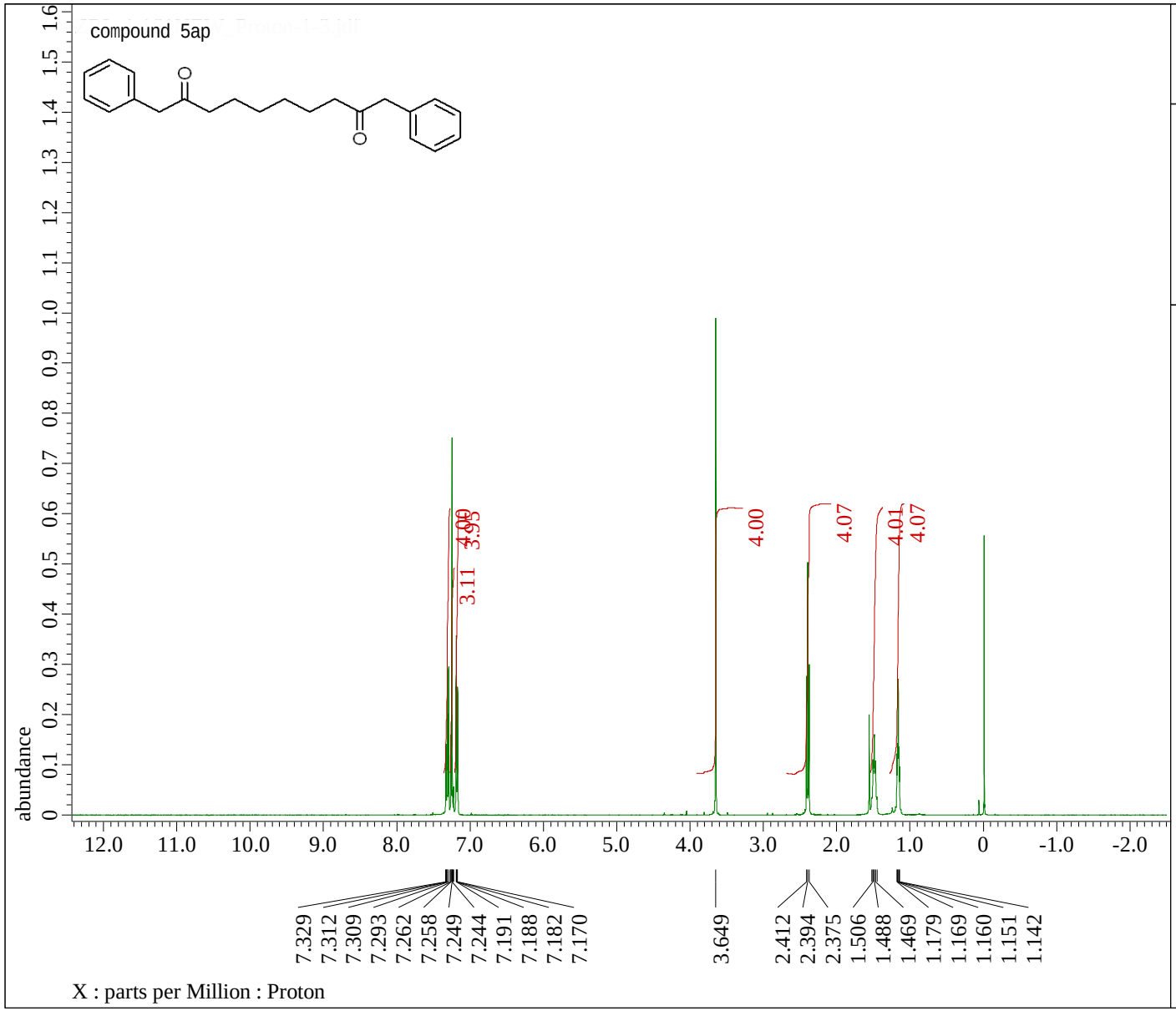
Derived from: zrl-4-161 1_Carbon-1-1.jdf
```

```
Filename                 = zrl-4-161 1_Car
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = zrl-4-161 1
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 17-OCT-2017 16:
Revision_Time            =  6-DEC-2017 22:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 423
Total_Scans              = 423

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 20.8[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



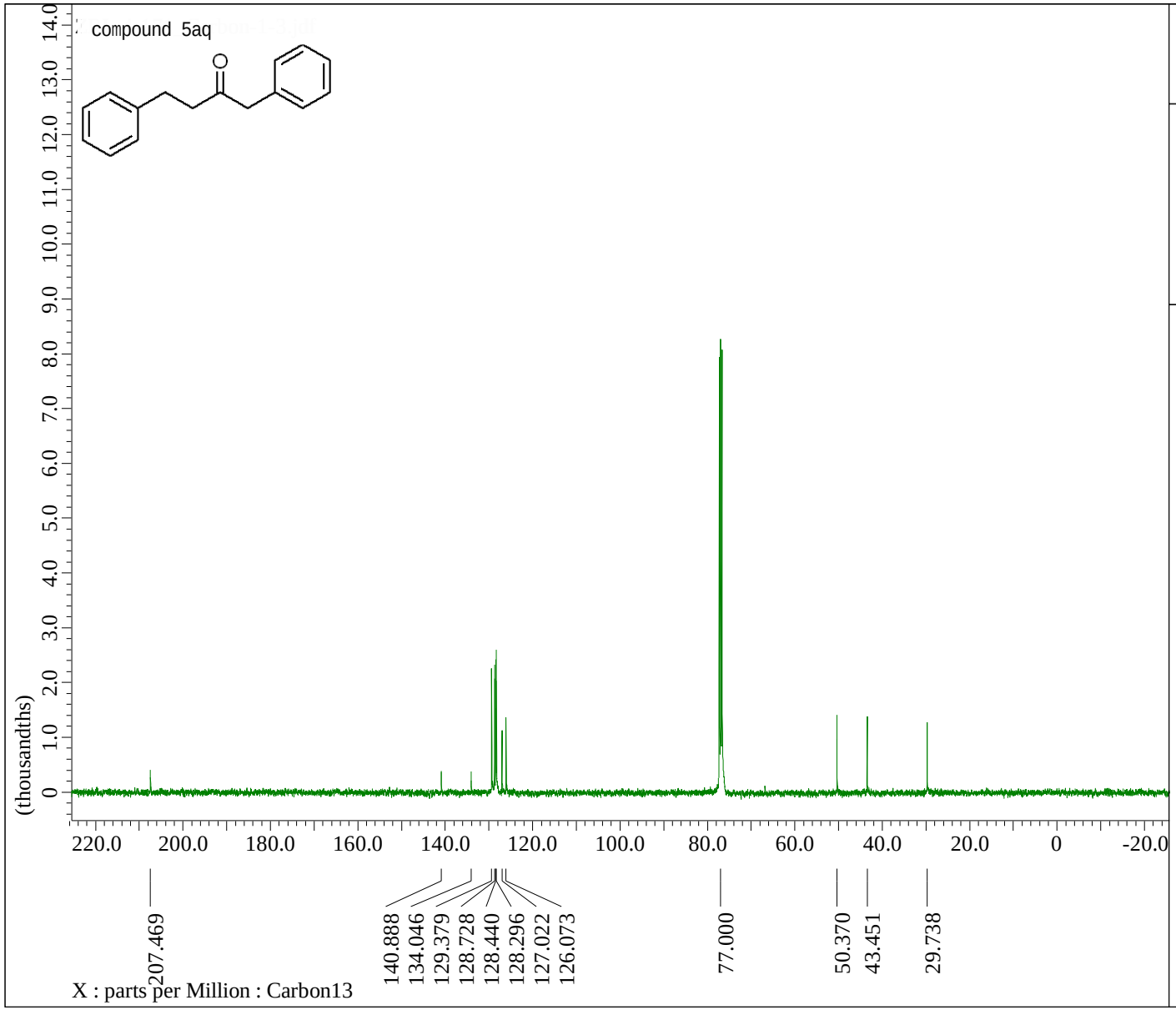

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-161NEW_Proto
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-161NEW
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 18-OCT-2017 10:05:
Revision_Time         =  6-DEC-2017 22:12:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 19.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



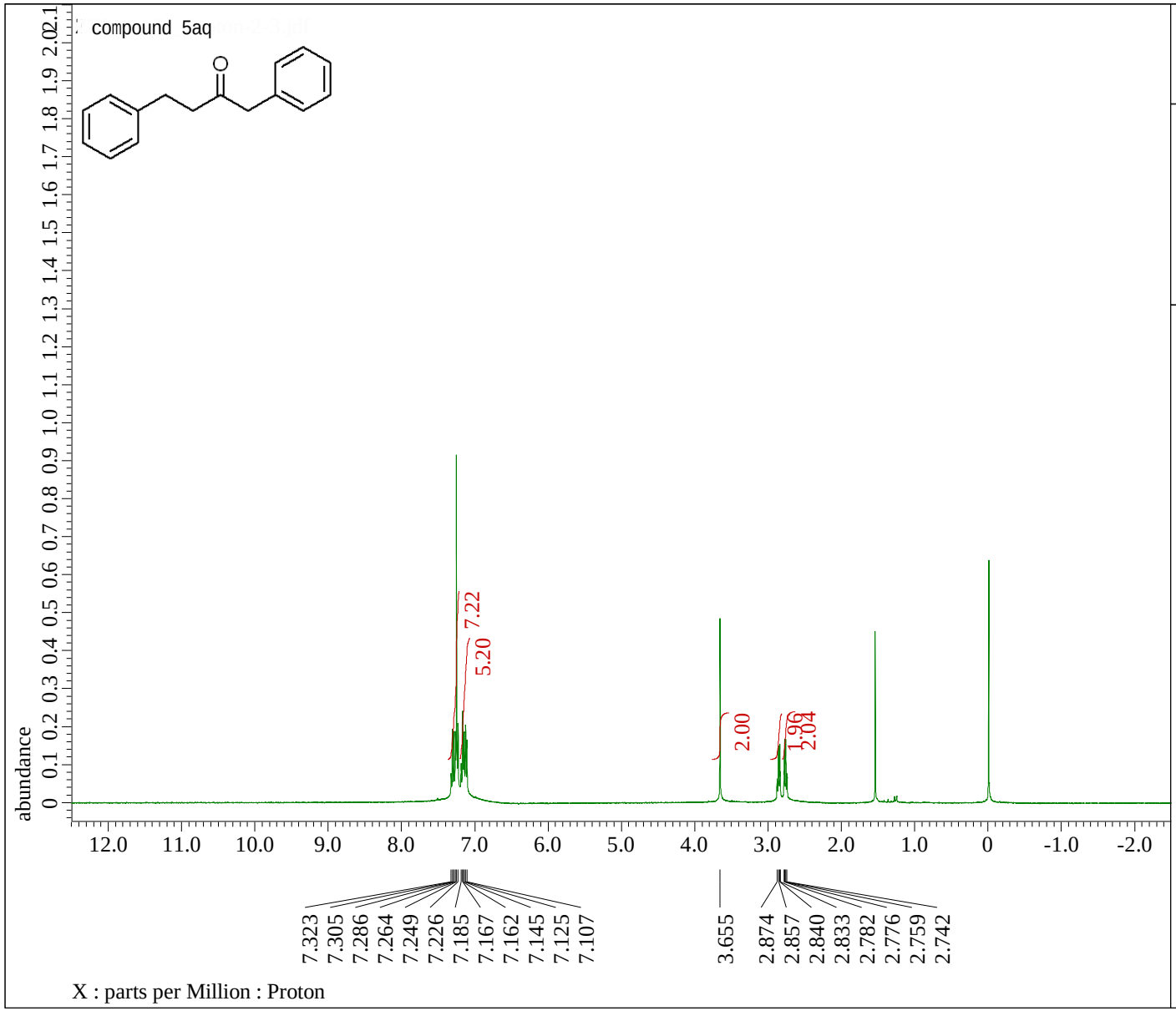

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                 = ZRL-4-171_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-4-171
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 18-OCT-2017 17:
Revision_Time            =  5-DEC-2017 19:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 19.8[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



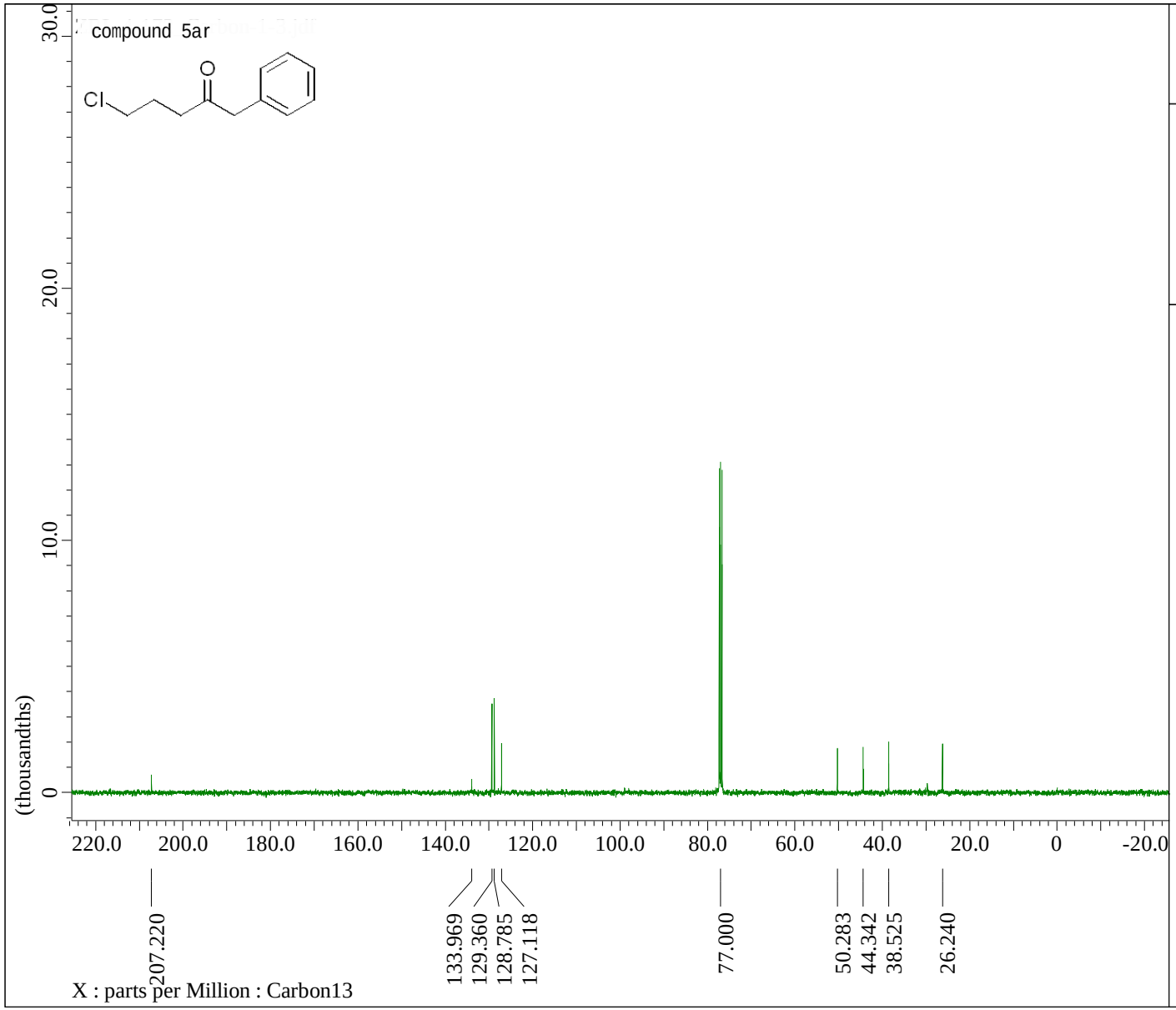

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-171_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-171
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 18-OCT-2017 19:29:
Revision_Time         =  5-DEC-2017 19:18:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 19.8[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



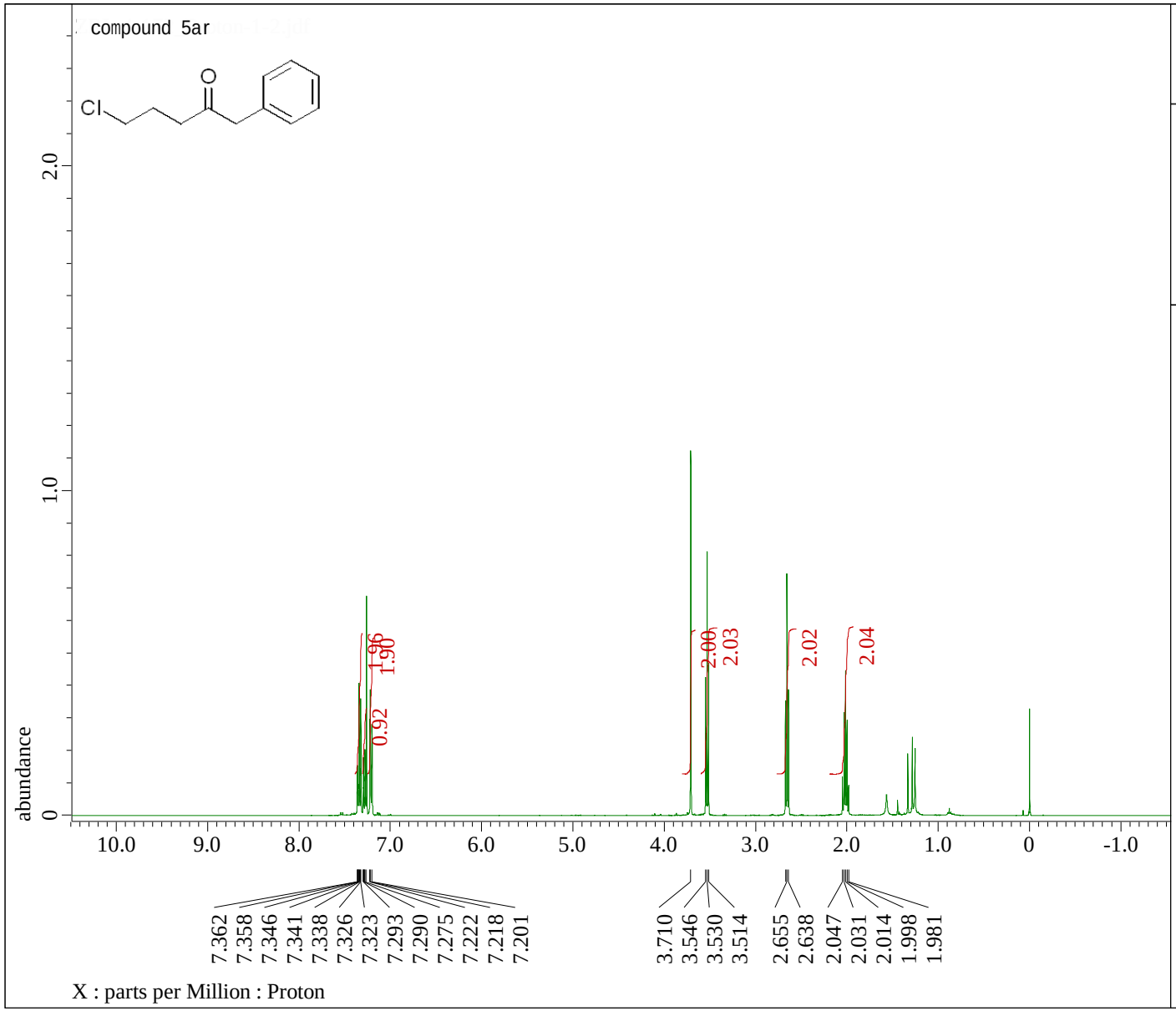

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-172_Carbo
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-172
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 16-OCT-2017 17:
Revision_Time           =  5-NOV-2017 15:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 351
Total_Scans             = 351

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 20[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



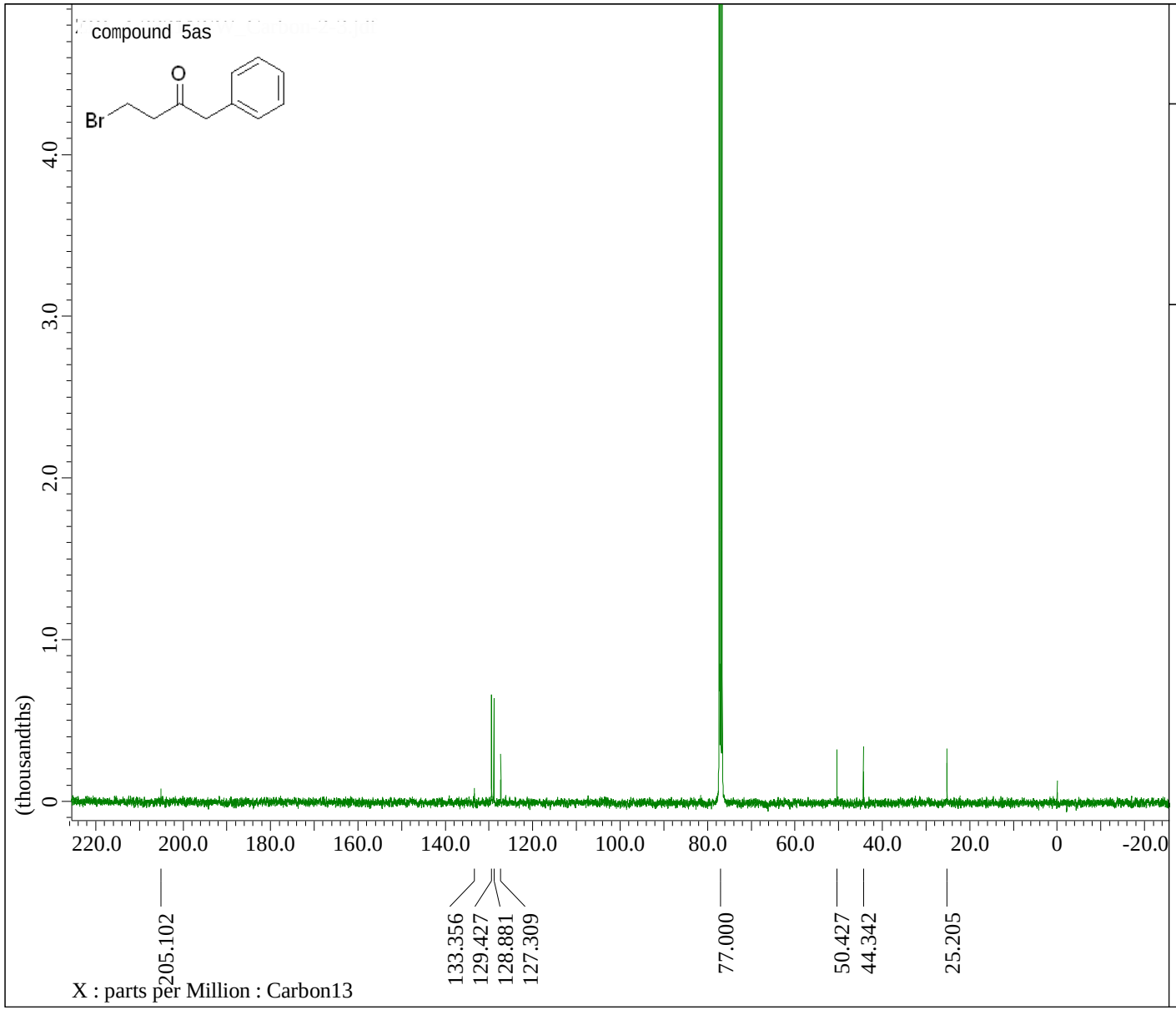

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-172_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-172
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 16-OCT-2017 16:04:
Revision_Time         =  5-NOV-2017 15:57:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 19.7[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



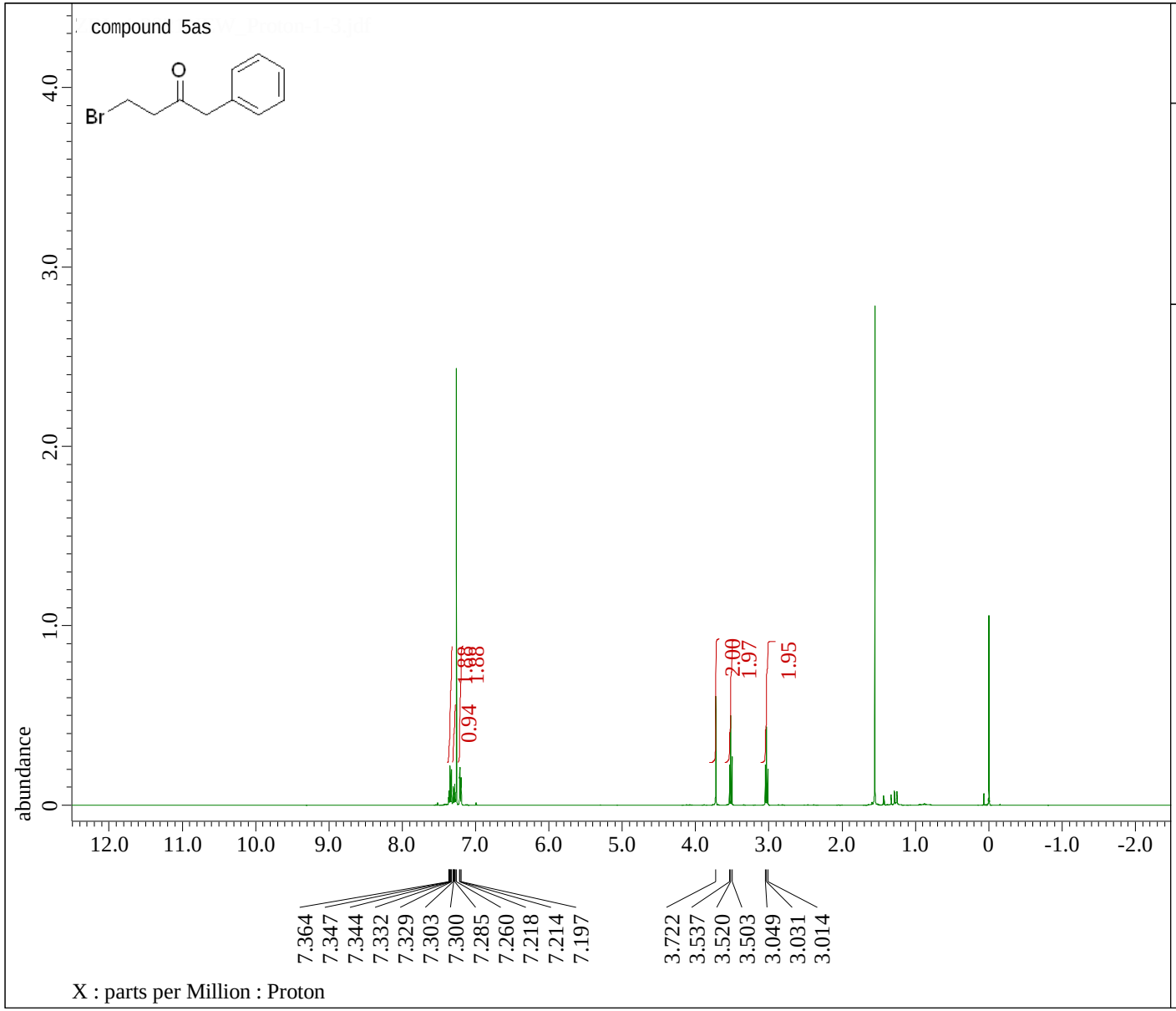

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                = ZRL-4-2321NEW_C
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-4-2321NEW
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 20-OCT-2017 21:
Revision_Time           = 28-OCT-2017 21:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 5000
Total_Scans             = 5000

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 20.6[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



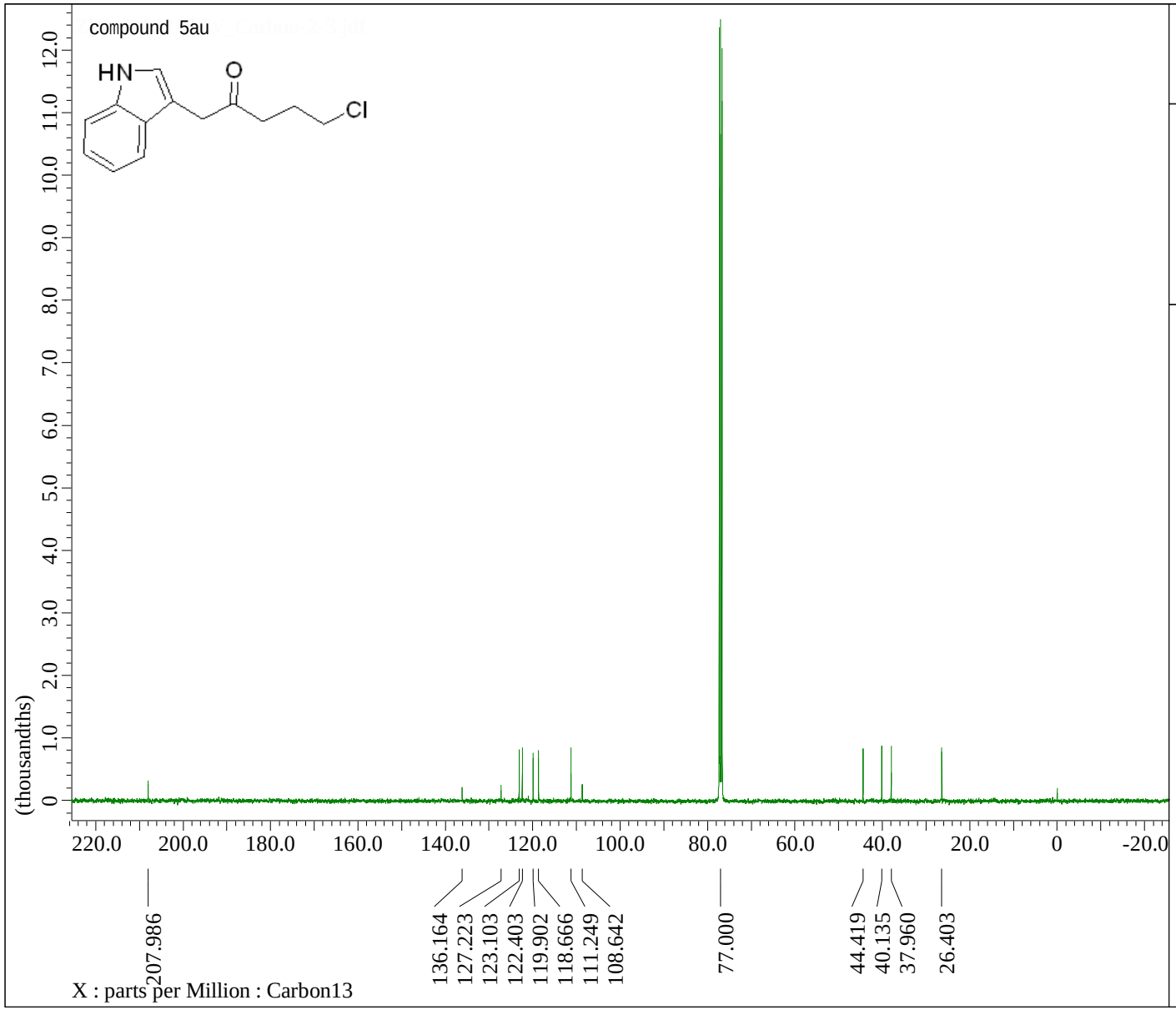

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-4-2321NEW_Prot
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-4-2321NEW
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 20-OCT-2017 21:04:
Revision_Time         = 28-OCT-2017 21:23:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 16
Total_Scans           = 16

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 20.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

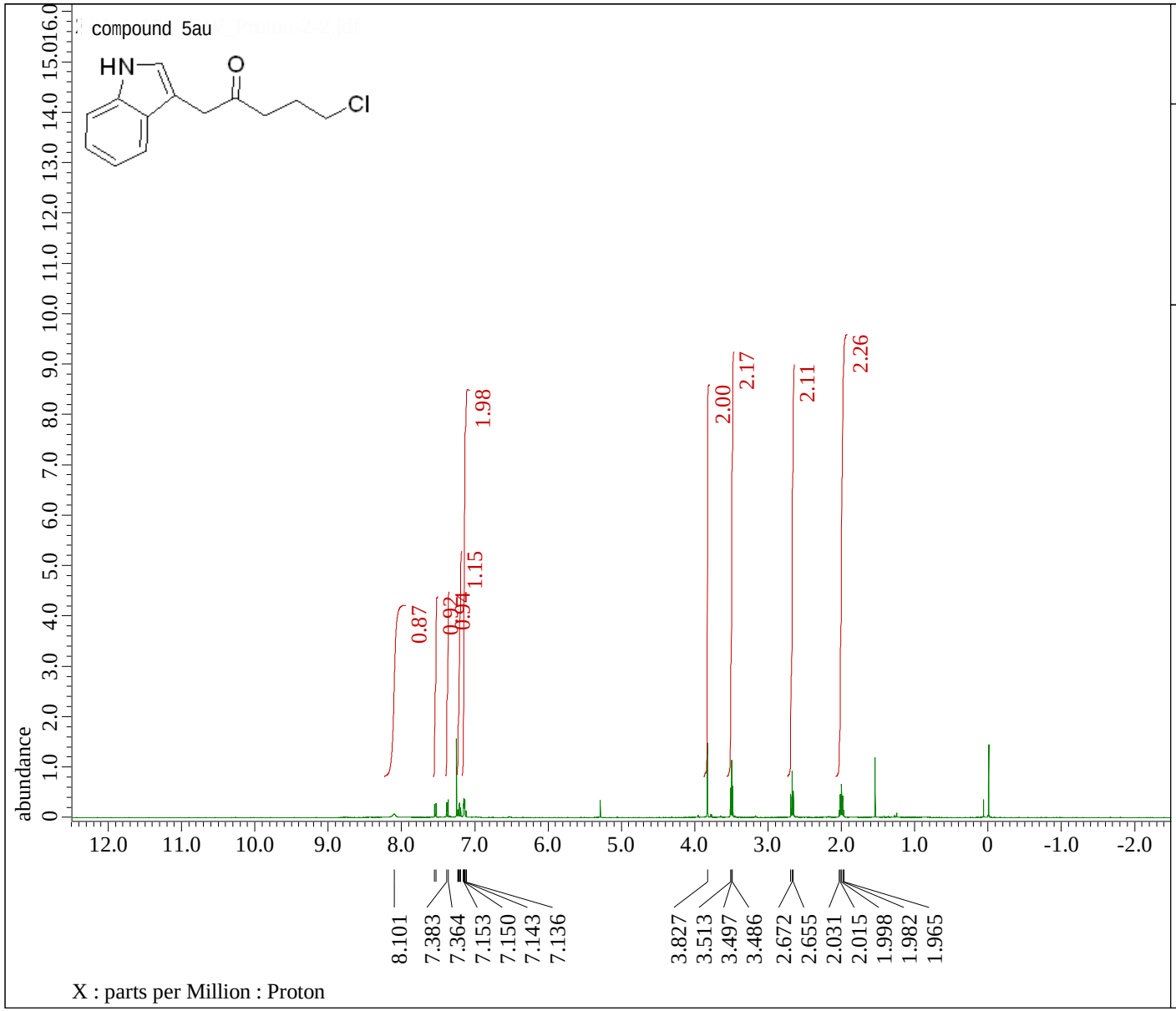
Derived from: ZRL-5-172NEW_Carbon-2-1.jdf
```

```
Filename                  = ZRL-5-172NEW_Ca
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-172NEW
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 27-NOV-2017 01:
Revision_Time             =  6-DEC-2017 13:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 3000
Total_Scans               = 3000

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 22.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



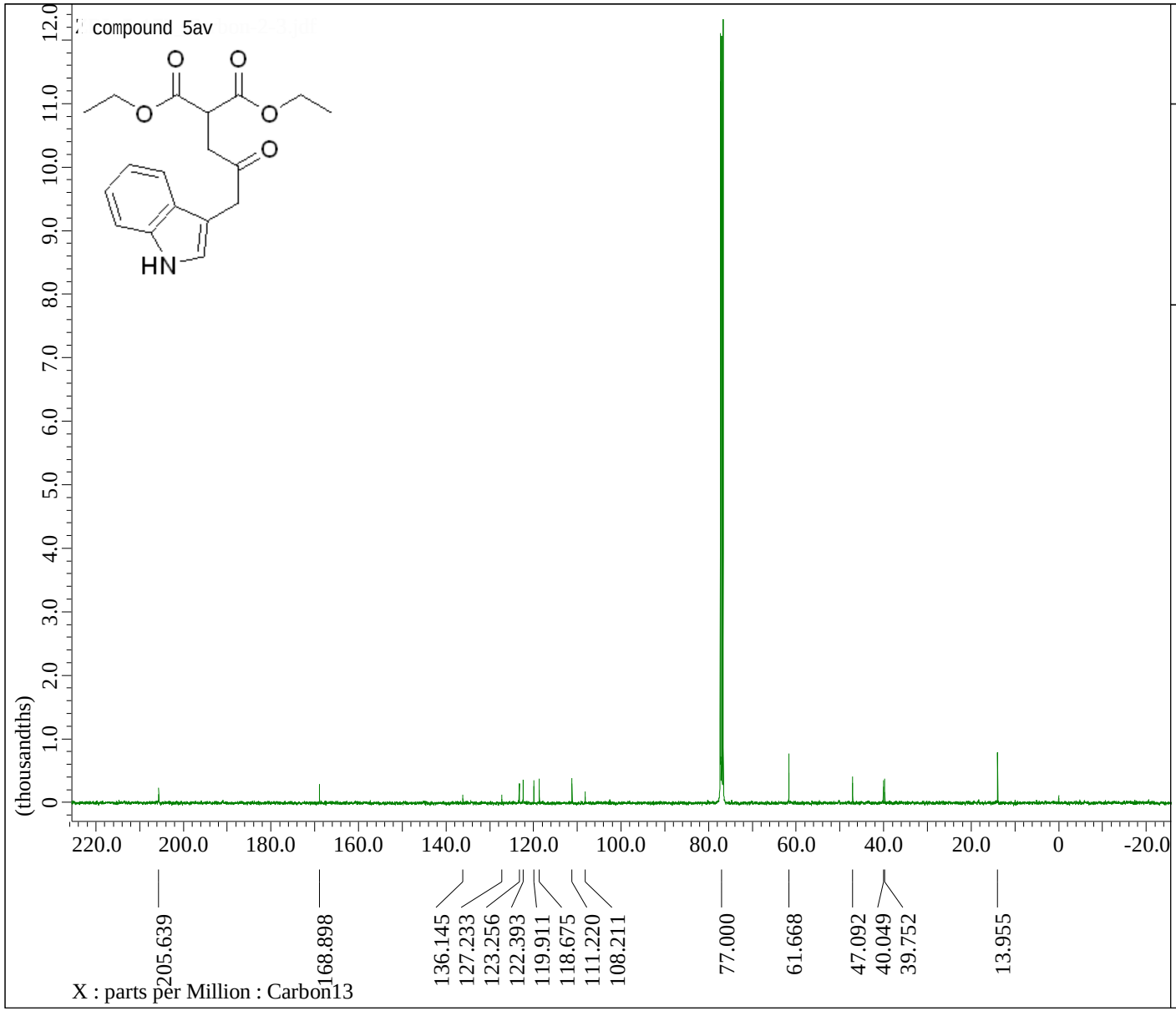

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-172NEW_Proto
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-172NEW
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 27-NOV-2017 01:41:
Revision_Time         = 21-FEB-2018 17:56:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 23.2[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



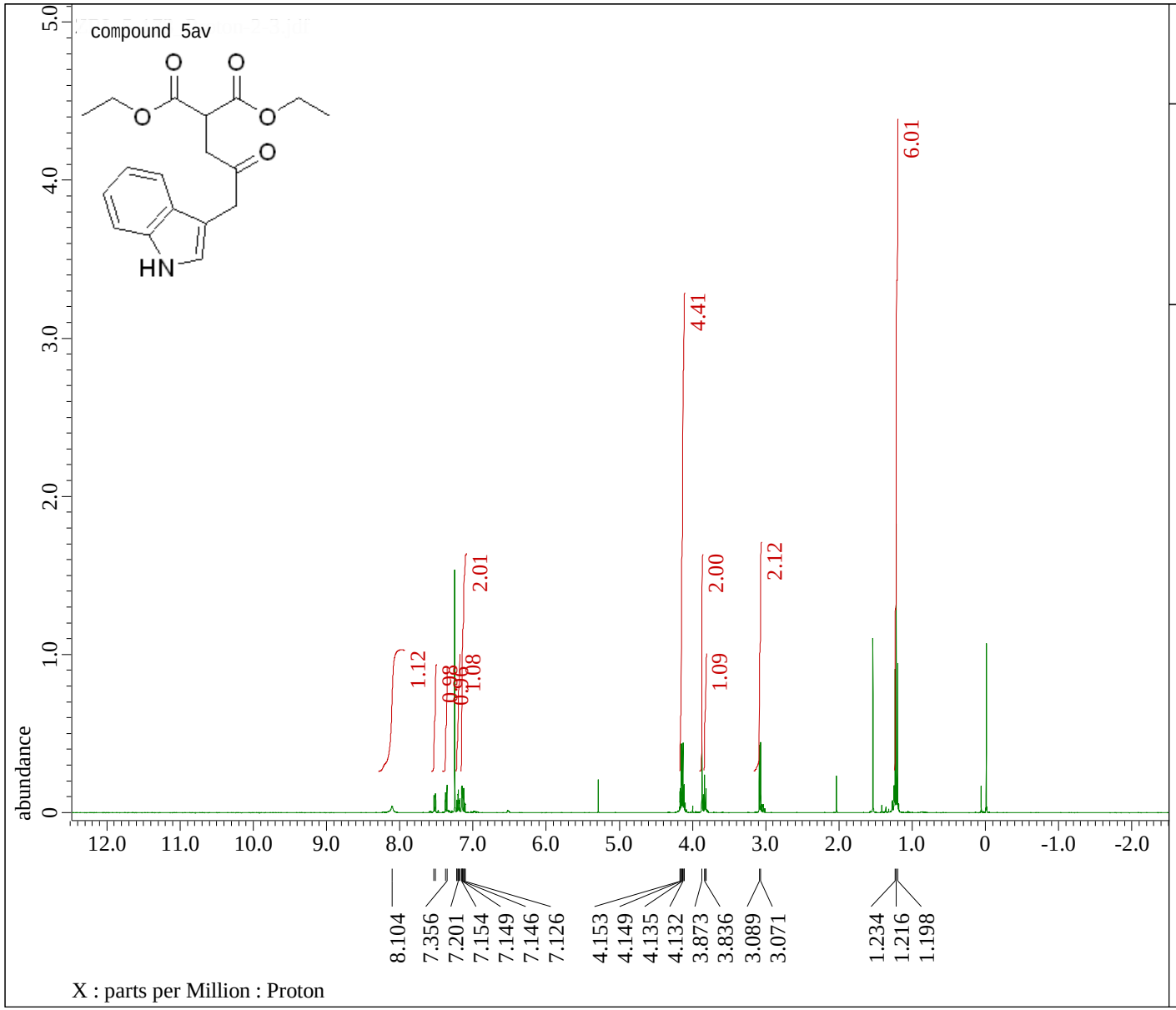

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename                  = ZRL-5-173_Carbo
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-173
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 28-NOV-2017 03:
Revision_Time             =  7-DEC-2017 17:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 5000
Total_Scans               = 5000

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 22.2[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



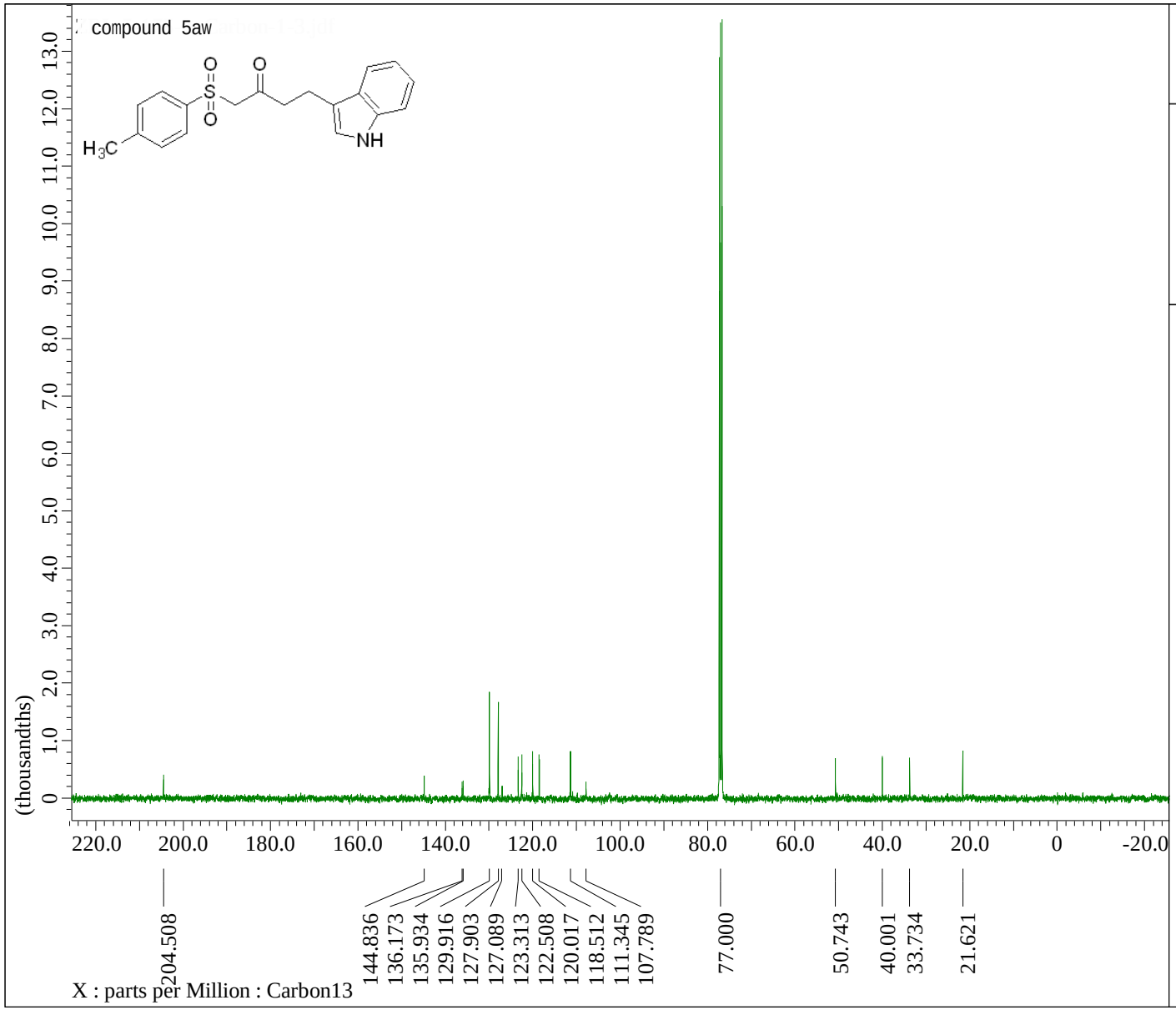

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-173_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-173
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 27-NOV-2017 18:04:
Revision_Time         =  6-DEC-2017 13:03:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 22.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

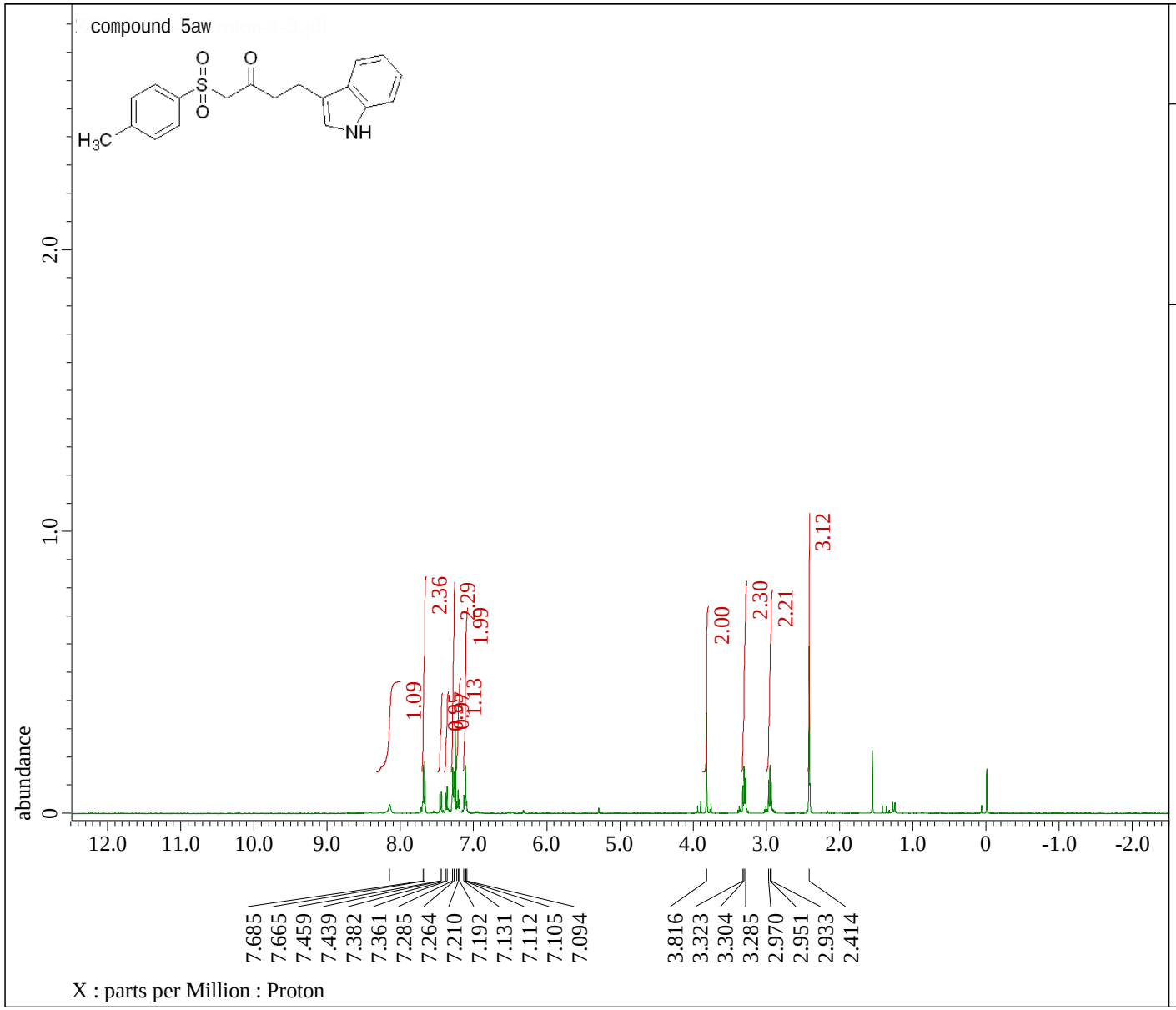
Derived from: ZRL-5-175-2_Carbon-1-1.jdf
```

```
Filename                = ZRL-5-175-2_Car
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = ZRL-5-175-2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 27-NOV-2017 12:
Revision_Time           =  6-DEC-2017 12:

Comment                 = single pulse de
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (40
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MH
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz
X_Sweep_Clipped         = 25.25252525[kHz
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MH
Irr_Offset              = 5[ppm]
Clipped                 = FALSE
Scans                   = 1024
Total_Scans             = 1024

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 22.9[dC]
X_90_Width              = 8.8[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 3.4[dB]
X_Pulse                 = 2.93333333[us]
```



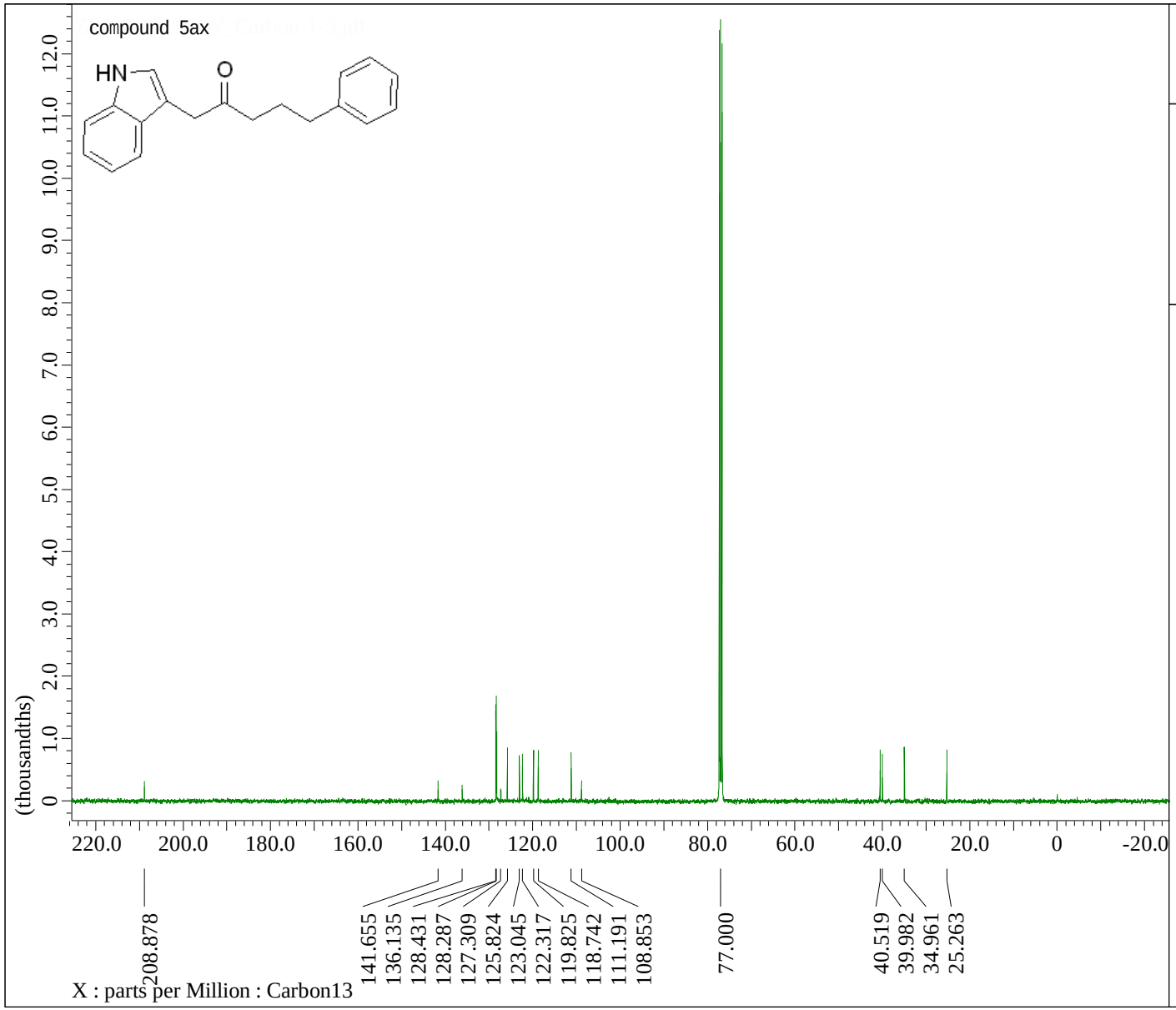

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-175-2_Proton
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-175-2
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 27-NOV-2017 12:16:
Revision_Time         =  6-DEC-2017 12:33:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.4[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

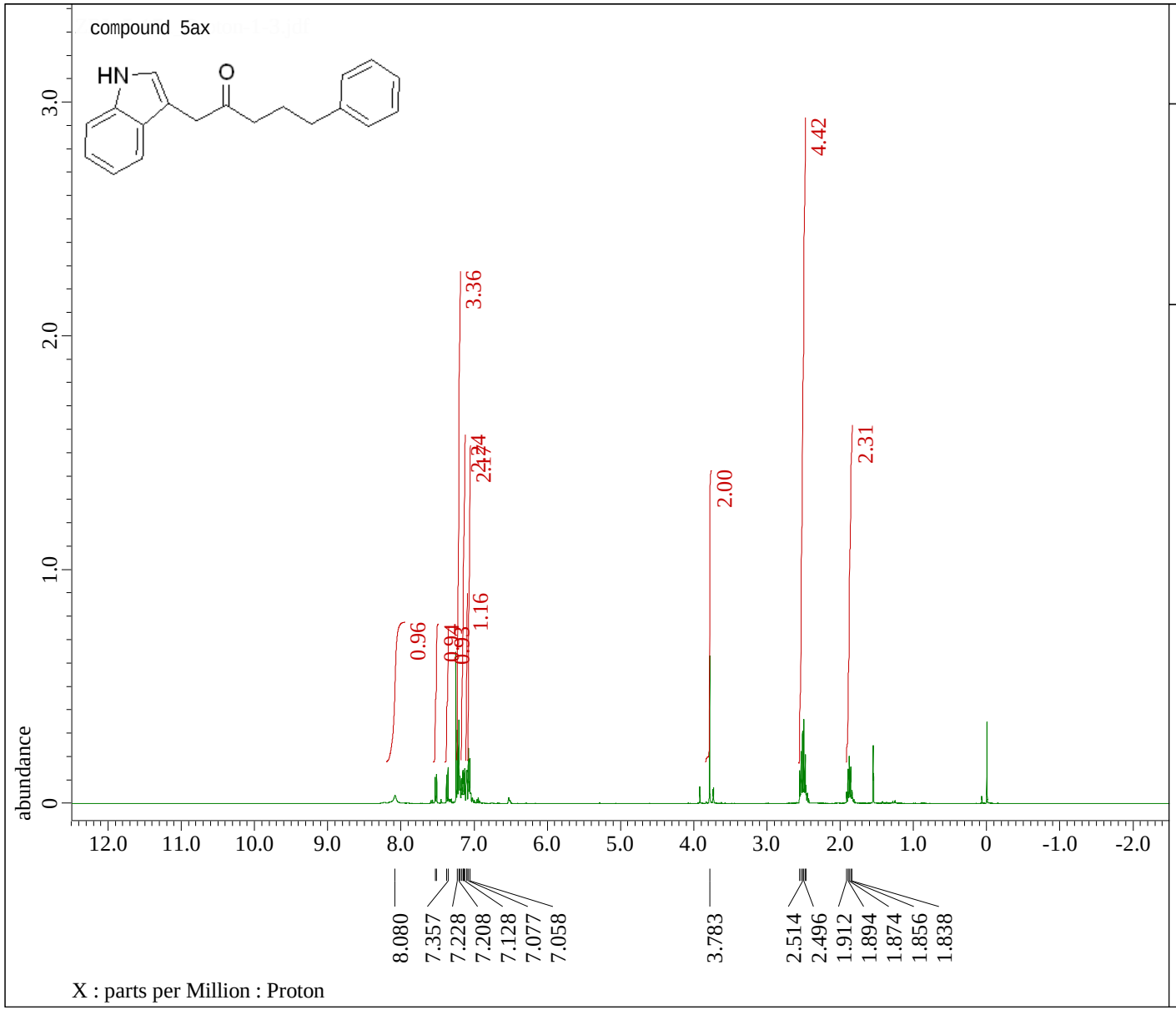
Derived from: ZRL-5-171NEW_Carbon-1-1.jdf
```

```
Filename                  = ZRL-5-171NEW_Ca
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-171NEW
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 26-NOV-2017 23:
Revision_Time             =  6-DEC-2017 13:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 3000
Total_Scans               = 3000

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 23.2[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



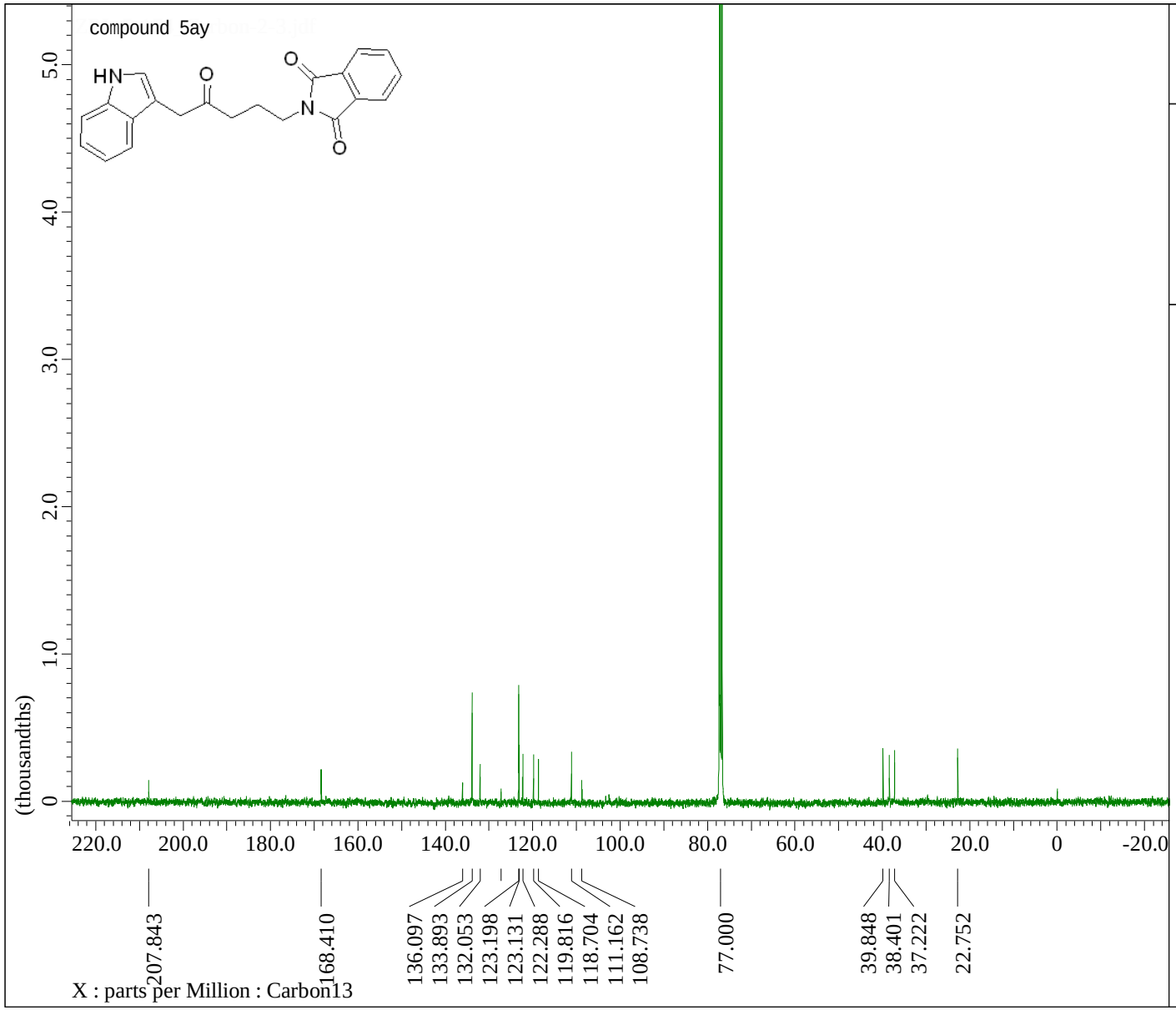

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-171_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-171
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 26-NOV-2017 19:56:
Revision_Time         =  6-DEC-2017 13:27:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 22.6[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```



JEOL

```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

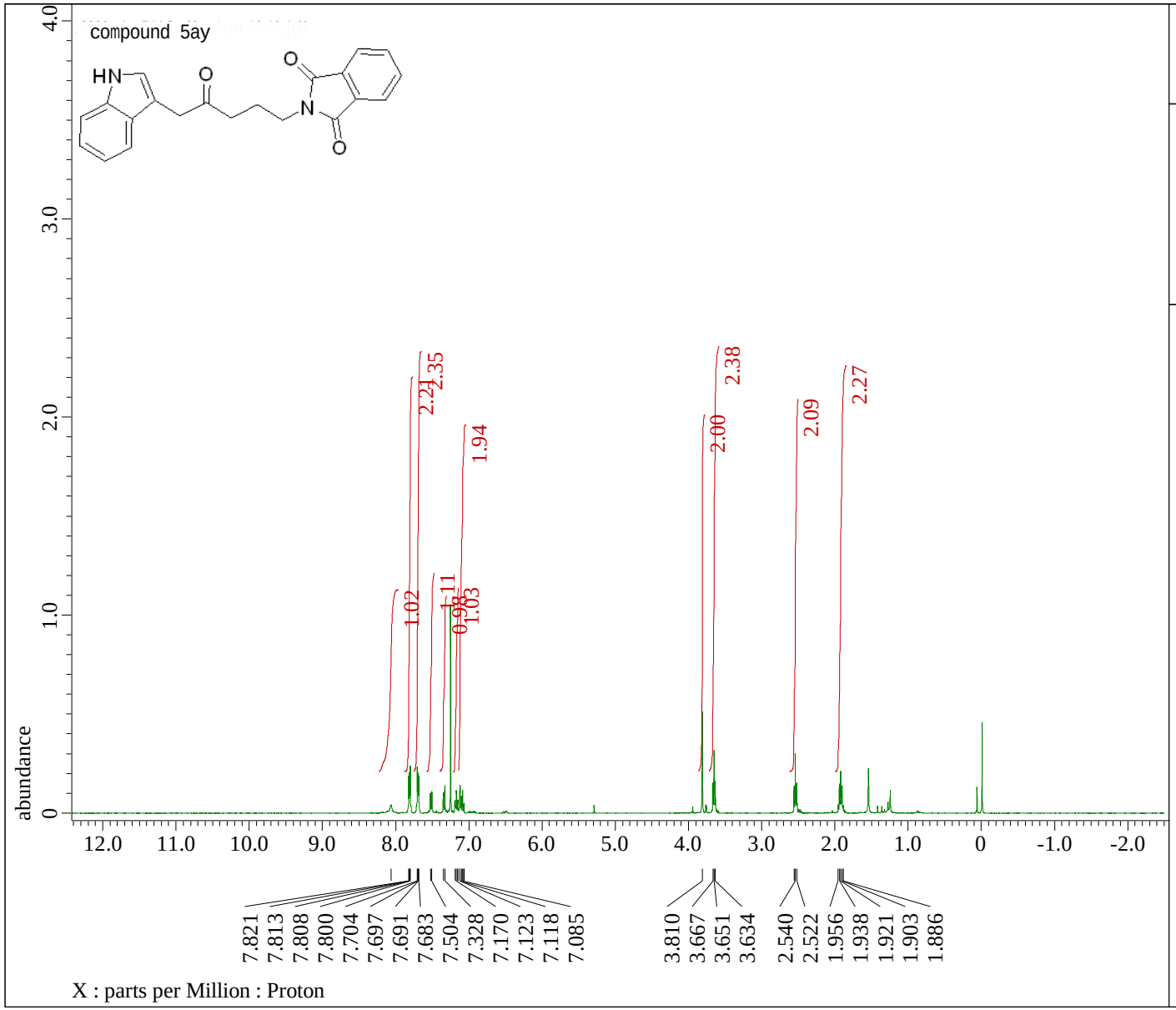
Derived from: ZRL-5-174_Carbon-2-1.jdf
```

```
Filename                  = ZRL-5-174_Carbo
Author                    = delta
Experiment                = carbon.jxp
Sample_Id                 = ZRL-5-174
Solvent                   = CHLOROFORM-D
Actual_Start_Time         = 27-NOV-2017 23:
Revision_Time             =  6-DEC-2017 12:

Comment                   = single pulse de
Data_Format               = 1D COMPLEX
Dim_Size                  = 26214
Dim_Title                 = Carbon13
Dim_Units                 = [ppm]
Dimensions                = X
Spectrometer              = JNM-ECZ400S/L1

Field_Strength            = 9.389766[T] (40
X_Acq_Duration            = 1.03809024[s]
X_Domain                  = 13C
X_Freq                    = 100.52530333[MH
X_Offset                  = 100[ppm]
X_Points                  = 32768
X_Prescans                = 4
X_Resolution              = 0.96330739[Hz]
X_Sweep                   = 31.56565657[kHz
X_Sweep_Clipped           = 25.25252525[kHz
Irr_Domain                = Proton
Irr_Freq                  = 399.78219838[MH
Irr_Offset                = 5[ppm]
Clipped                   = FALSE
Scans                     = 5000
Total_Scans               = 5000

Relaxation_Delay          = 2[s]
Recvr_Gain                = 50
Temp_Get                  = 22.4[dC]
X_90_Width                = 8.8[us]
X_Acq_Time                = 1.03809024[s]
X_Angle                   = 30[deg]
X_Atn                     = 3.4[dB]
X_Pulse                   = 2.93333333[us]
```



JEOL

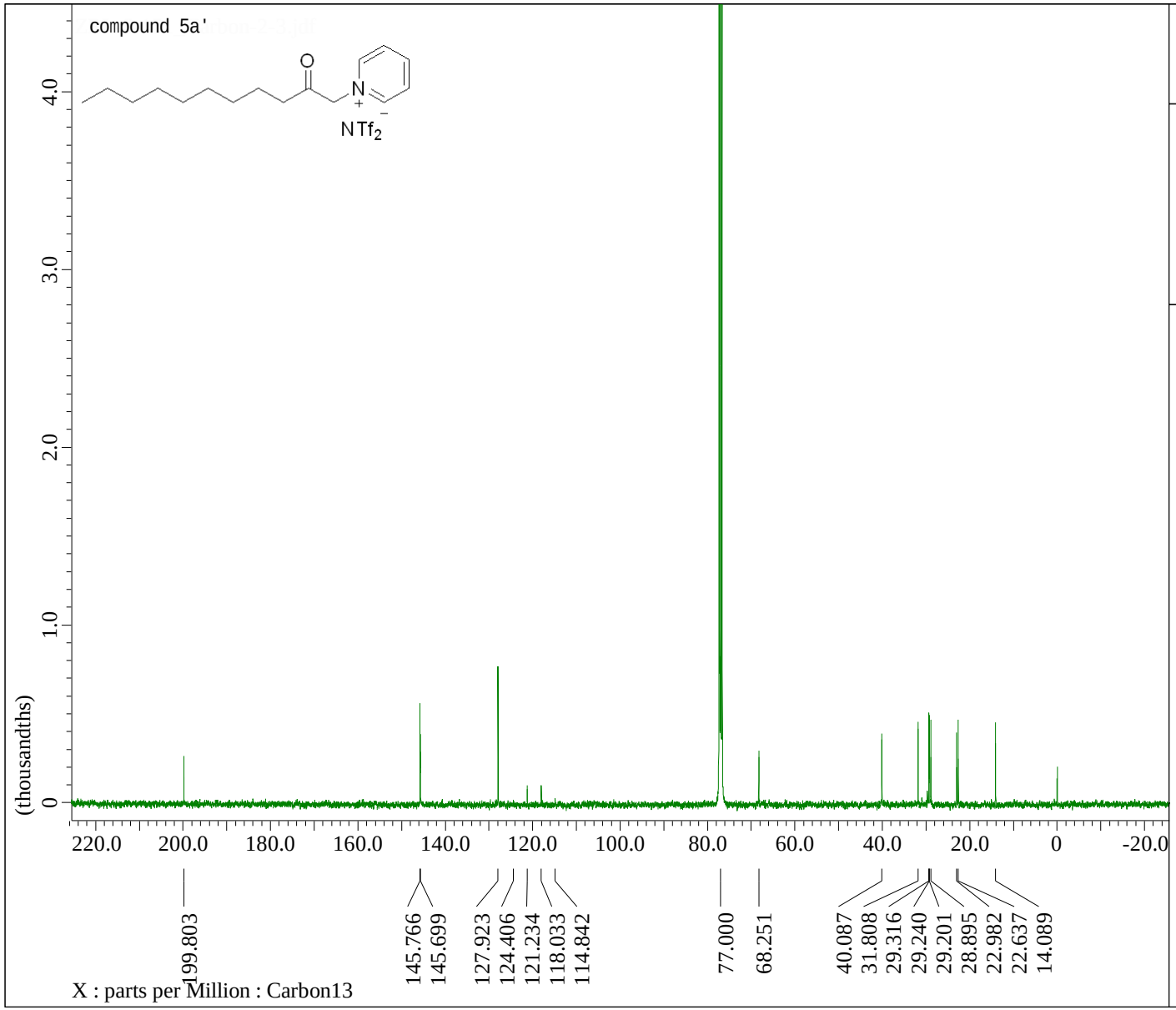
```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-174_Proton-2
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-174
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 27-NOV-2017 20:43:
Revision_Time         =  6-DEC-2017 12:50:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 23[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

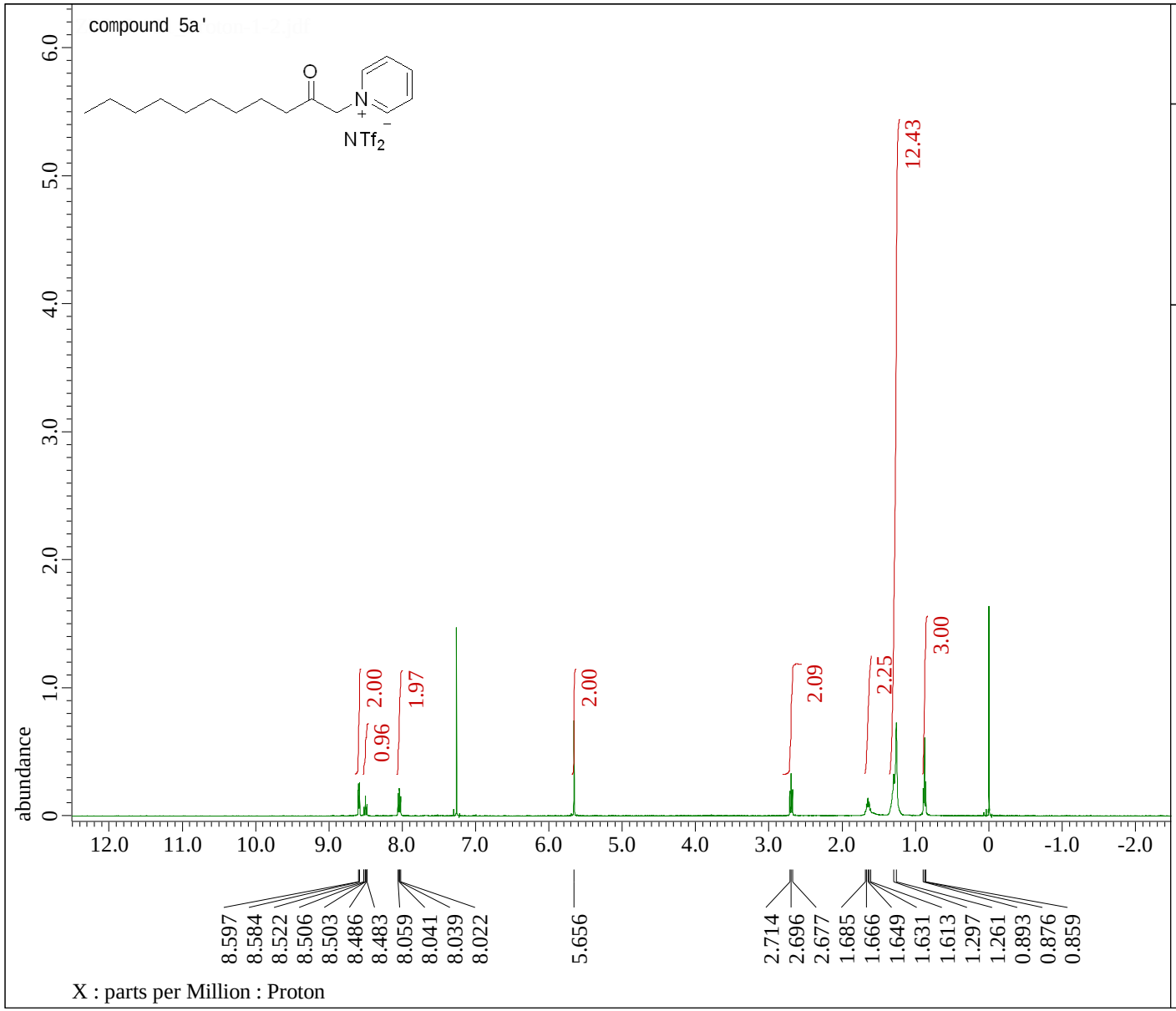
Derived from: ZRL-6-151_Carbon-2-1.jdf
```

```
Filename                 = ZRL-6-151_Carbo
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-6-151
Solvent                  = CHLOROFORM-D
Actual_Start_Time        =  2-FEB-2018 09:
Revision_Time            =  6-FEB-2018 11:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = TRUE
Scans                    = 10000
Total_Scans              = 10000

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 18.1[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```



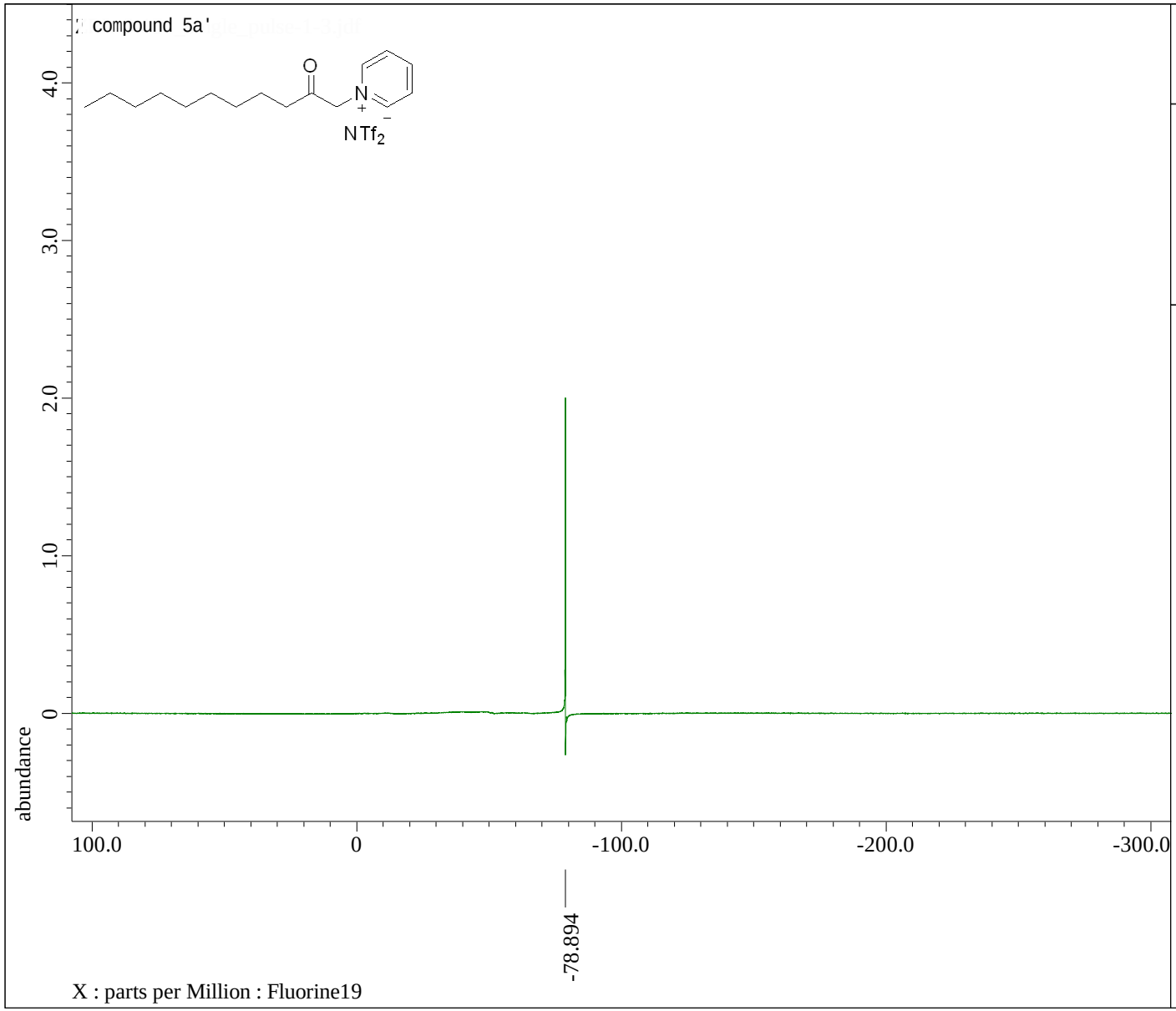

```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-6-151_Proton-1
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-6-151
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  1-FEB-2018 23:26:
Revision_Time         = 21-FEB-2018 13:24:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 66
Temp_Get              = 21.5[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

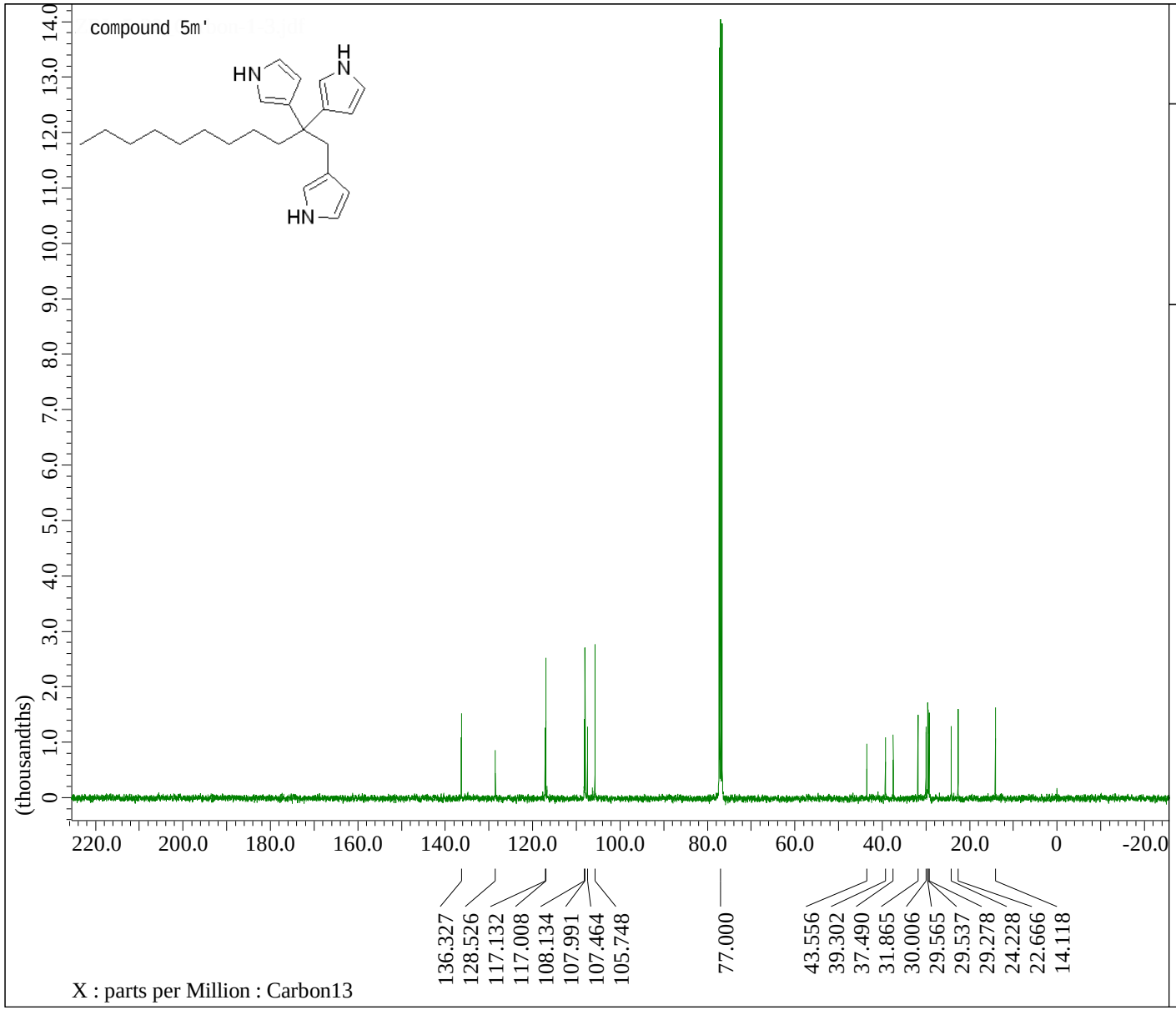
Derived from: ZRL-6-151_single_pulse-1-1.j
```

```
Filename              = ZRL-6-151_single_p
Author                = delta
Experiment            = single_pulse.jxp
Sample_Id             = ZRL-6-151
Solvent               = CHLOROFORM-D
Actual_Start_Time     =  3-FEB-2018 15:48:
Revision_Time         =  6-FEB-2018 17:18:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Fluorine19
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 83.88608[ms]
X_Domain              = 19F
X_Freq                = 376.17105393[MHz]
X_Offset              = -100[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 11.92092896[Hz]
X_Sweep               = 195.3125[kHz]
X_Sweep_Clipped       = 156.25[kHz]
Irr_Domain            = Fluorine19
Irr_Freq              = 376.17105393[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Fluorine19
Tri_Freq              = 376.17105393[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 50
Temp_Get              = 19.3[dC]
X_90_Width            = 10[us]
X_Acq_Time            = 83.88608[ms]
```




```
---- PROCESSING PARAMETERS ----
sexp( 2.0[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm

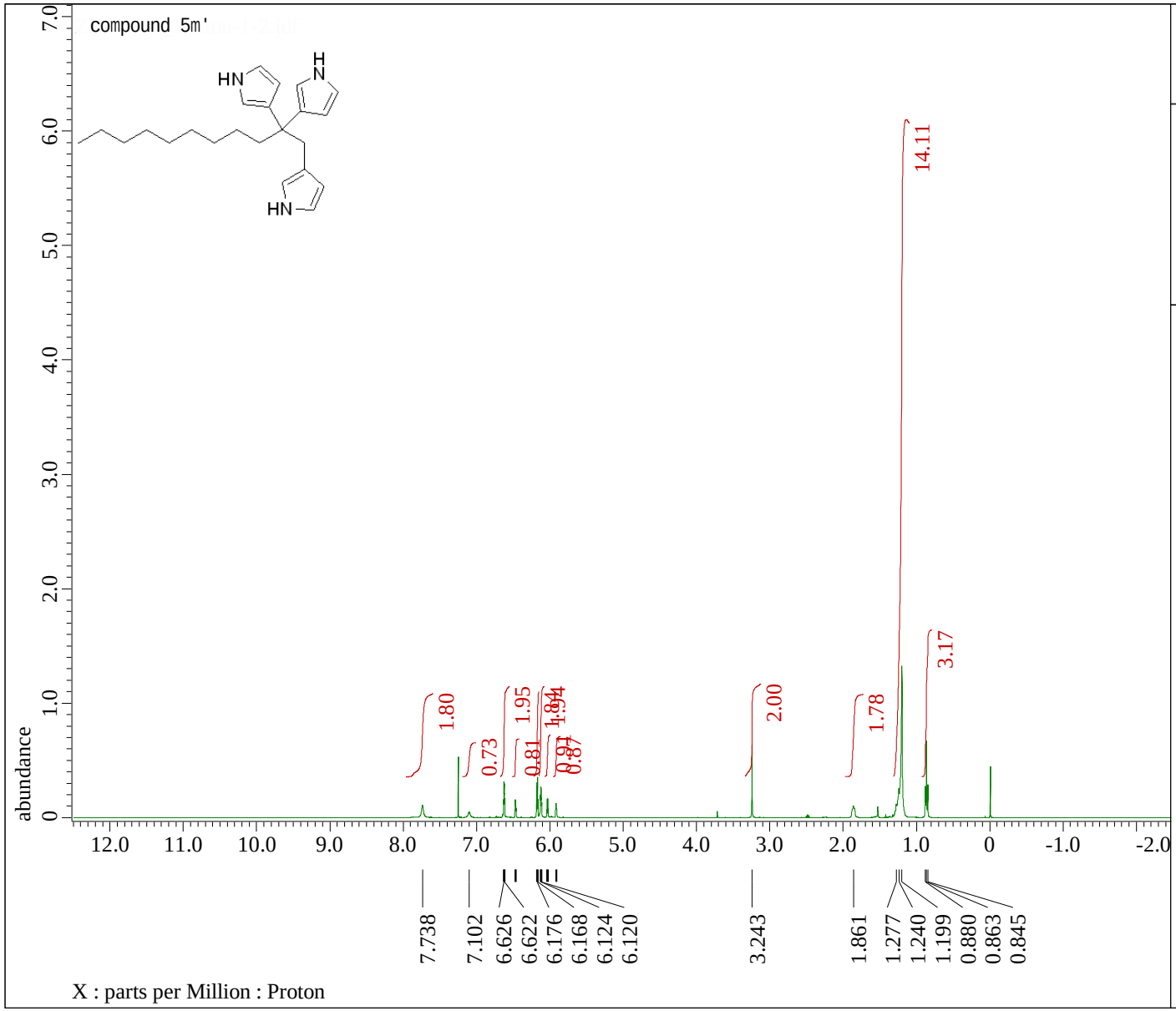
Derived from: ZRL-5-32_Carbon-1-1.jdf
```

```
Filename                 = ZRL-5-32_Carbon
Author                   = delta
Experiment               = carbon.jxp
Sample_Id                = ZRL-5-32
Solvent                  = CHLOROFORM-D
Actual_Start_Time        = 23-NOV-2017 07:
Revision_Time            =  5-DEC-2017 20:

Comment                  = single pulse de
Data_Format              = 1D COMPLEX
Dim_Size                 = 26214
Dim_Title                = Carbon13
Dim_Units                = [ppm]
Dimensions               = X
Spectrometer             = JNM-ECZ400S/L1

Field_Strength           = 9.389766[T] (40
X_Acq_Duration           = 1.03809024[s]
X_Domain                 = 13C
X_Freq                   = 100.52530333[MH
X_Offset                 = 100[ppm]
X_Points                 = 32768
X_Prescans               = 4
X_Resolution             = 0.96330739[Hz]
X_Sweep                  = 31.56565657[kHz
X_Sweep_Clipped          = 25.25252525[kHz
Irr_Domain               = Proton
Irr_Freq                 = 399.78219838[MH
Irr_Offset               = 5[ppm]
Clipped                  = FALSE
Scans                    = 1024
Total_Scans              = 1024

Relaxation_Delay         = 2[s]
Recvr_Gain               = 50
Temp_Get                 = 17.7[dC]
X_90_Width               = 8.8[us]
X_Acq_Time               = 1.03809024[s]
X_Angle                  = 30[deg]
X_Atn                    = 3.4[dB]
X_Pulse                  = 2.93333333[us]
```




```
---- PROCESSING PARAMETERS ----
sexp( 0.2[Hz], 0.0[s] )
trapezoid( 0[%], 0[%], 80[%], 100[%] )
zerofill( 1 )
fft( 1, TRUE, TRUE )
machinephase
ppm
```

```
Filename              = ZRL-5-32_Proton-1-
Author                = delta
Experiment            = proton.jxp
Sample_Id             = ZRL-5-32
Solvent               = CHLOROFORM-D
Actual_Start_Time     = 23-NOV-2017 07:07:
Revision_Time         = 21-FEB-2018 12:55:

Comment               = single_pulse
Data_Format           = 1D COMPLEX
Dim_Size              = 13107
Dim_Title             = Proton
Dim_Units             = [ppm]
Dimensions            = X
Spectrometer          = JNM-ECZ400S/L1

Field_Strength        = 9.389766[T] (400[M
X_Acq_Duration        = 2.18628096[s]
X_Domain              = 1H
X_Freq                = 399.78219838[MHz]
X_Offset              = 5[ppm]
X_Points              = 16384
X_Prescans            = 1
X_Resolution          = 0.45739775[Hz]
X_Sweep               = 7.4940048[kHz]
X_Sweep_Clipped       = 5.99520384[kHz]
Irr_Domain            = Proton
Irr_Freq              = 399.78219838[MHz]
Irr_Offset            = 5[ppm]
Tri_Domain            = Proton
Tri_Freq              = 399.78219838[MHz]
Tri_Offset            = 5[ppm]
Clipped               = FALSE
Scans                 = 8
Total_Scans           = 8

Relaxation_Delay      = 5[s]
Recvr_Gain            = 56
Temp_Get              = 17.1[dC]
X_90_Width            = 9.5[us]
X_Acq_Time            = 2.18628096[s]
```