Supporting Information

Photocatalytic 1,3-Difluoroalkylcarboxylation of Alkenes by Triple Kinetic-Controlled Radical Self-Ordering

Hong Fu, Zuo-Shuai Wang, Si-Jia Li, Lin-Yuan Zhu, Xiao-Jian Wang, Hong-Chen Wang, and Bing Han*

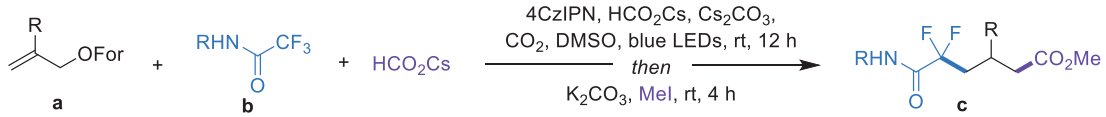
State Key Laboratory of Applied Organic Chemistry (SKLAOC), College of Chemistry and Chemical Engineering, Lanzhou University, 222 South Tianshui Road, Lanzhou, 730000, People's Republic of China，*Email：hanb@lzu.edu.cn

Contents

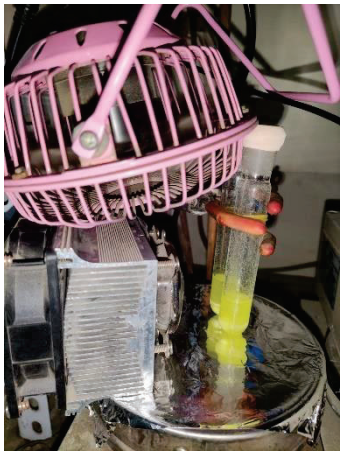
1 General information

All reagents were purchased from commercial suppliers and used without further purification. Flash chromatography was carried out with silica gel (200-300 mesh). Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. ^{1}H, ^{13}C, and ^{19}F NMR spectra were detected in $CDCl_3$ or CD_3OD on a Bruker AM 400 MHz spectrometer. Chemical shifts in ^{1}H NMR spectra were reported in parts per million (ppm) on the δ scale from an internal standard of residual TMS (0 ppm) or CD_3OD (3.31 ppm). Data for ^{1}H NMR were reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br s = broad single), coupling constant in Herts (Hz) and integration. Data for ^{13}C NMR spectra were reported in terms of chemical shift in ppm from the central peak of $CDCl_3$ (77.0 ppm). Data for ^{19}F NMR were reported in terms of chemical shift in ppm. The high-resolution mass spectra (HRMS) were measured on a Thermo QExactive by ESI. Photochemical reactions were carried with 30 W blue LEDs obtained from Wuhan Jiushang Technology Co., Ltd.

2 General procedure for unsymmetrical 1,3-difunctionalization of the olefin

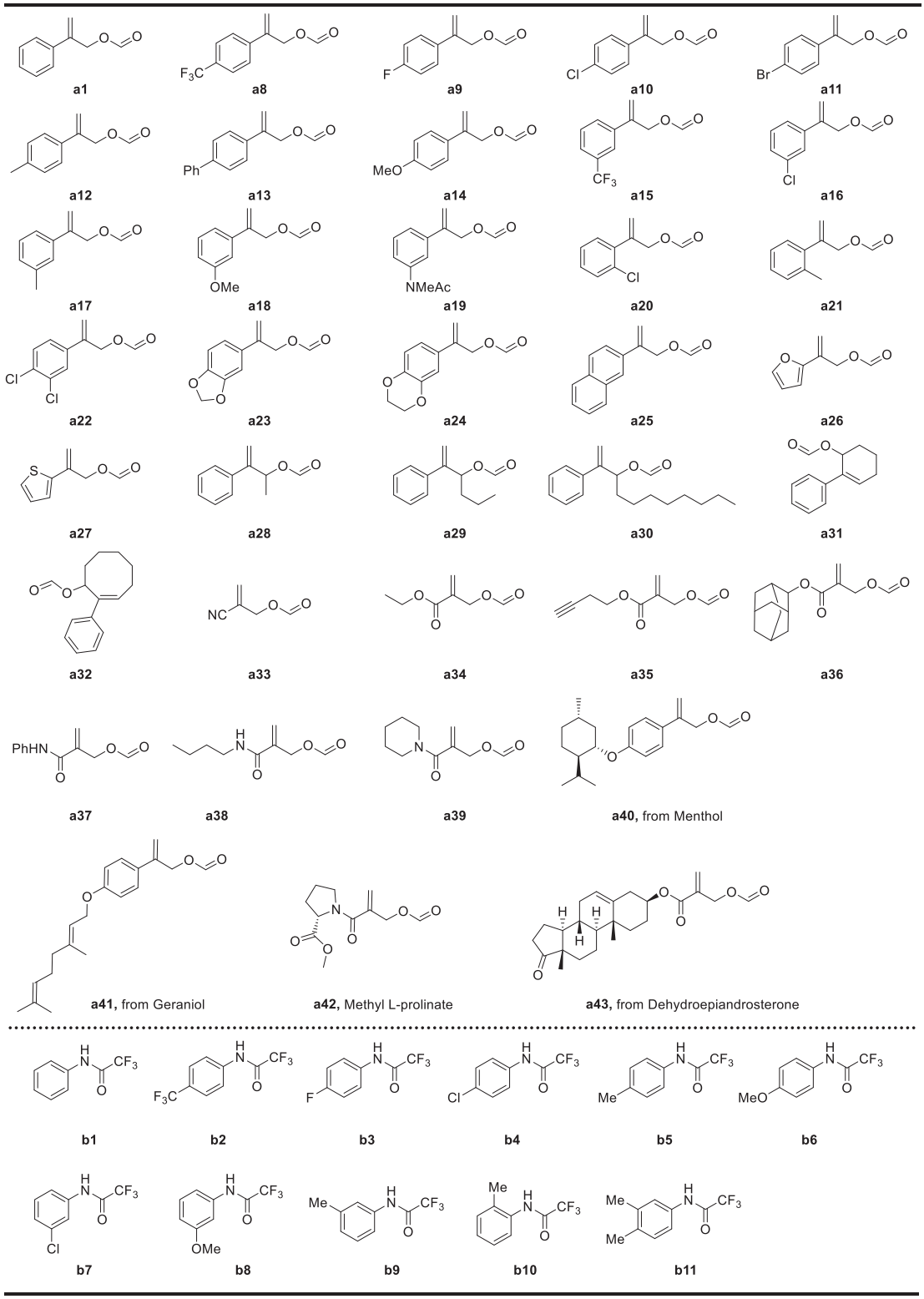


An oven-dried tube (15 mL) containing a stirring bar was charged with **a** (0.2 mmol), **b** (4 eq, 0.8 mmol), HCOOCs (2 eq, 0.4 mmol, 71.2 mg), 4CzIPN (2%, 3.2 mg), Cs_2CO_3 (0.5 eq, 0.1 mmol, 32.6 mg) and anhydrous DMSO (3 mL). The tube was evacuated and back-filled with CO_2 for 3 times. The reaction mixture was stirred and irradiated with blue LEDs (λ= 425 nm, 2 cm - 4cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30 °C) for 12 h. Then the reaction was added K_2CO_3 (1 mmol, 138.2 mg), MeI (0.3 mL), and further stirred at room temperature for 4h. The reaction was quenched by H_2O (10 mL) and extracted by EtOAc (30 mL × 4). The organic phase was dried and concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel to afford products **c**.



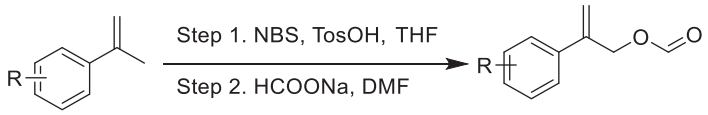
3 Synthesis of starting materials

3.1 The scope of various alkenes and 2, 2, 2-trifluoro-N-phenylacetamide



3.2 Preparation of substrates

Method A

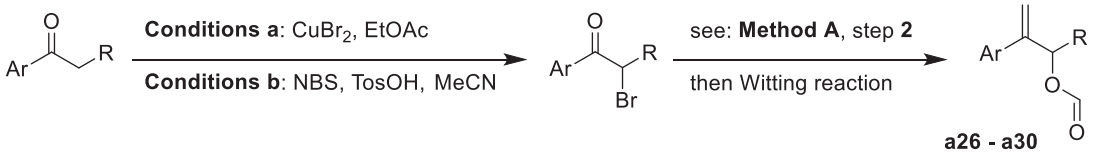


a1, **a8 - a25**, **a31**, **a32**, **a40**, **a41**

Step 1**:** In an oven dried flask olefins (1.0 eq. The raw materials are purchased or prepared by a simple Witting reaction of aryl ketones.) was taken and to this dry THF (1 M) was added. To the resulting solution N-Bromosuccinimide (1.05 eq) and TsOH (0.1 eq) was added and the solution was refluxed at 100°C for 4 h. Reaction mixture was cooled to rt and the reaction mixture was taken in EtOAc, washed with H_2O (15 mL × 3). Organic phase was dried over with Na_2SO_4, concentrated under reduced pressure to obtain a colroless oil. Purification by column chromatography afforded allyl bromide derivatives (65% - 85%).[1]

Step 2**:** To a solution of allyl bromide derivatives (10 mmol, 1 eq) in DMF (10 mL) was added sodium formate (3 eq) and the resulting mixture was stirred at 70°C for 3 - 6 h. The reaction was quenched with H_2O, and the product was extracted with AcOEt (20 mL × 3). The combined organic layer was washed with brine, dried over Na_2SO_4 and evaporated. The residue was purified by silica-gel column chromatography to provide **a** (90% - 100%).

Method B:

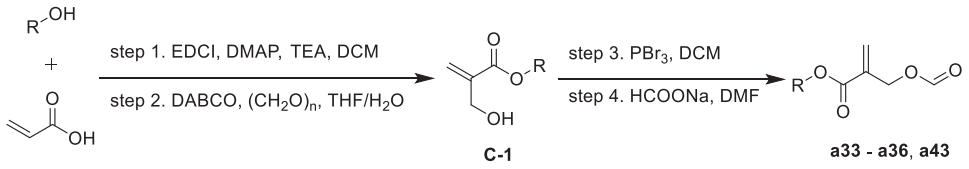


a26 - a30

Conditions a (for **a26**、**a27**): A solution of 2-acetylfuran (or 2-acetylthiophene) (20 mmol, 1.0 eq) in ethyl acetate (0.5 M) was added to a reaction flask equipped with a magnetic stir bar, followed by the addition of copper(II) bromide (1.7 eq). The reaction mixture was then stirred vigorously and heated to reflux. When the reaction reached completion, as judged by TLC, the reaction mixture was allowed to cool to room temperature, filtered, and evaporated under reduced pressure. The crude product was purified using silica gel column chromatography to afford the desired product (65%).[2] Then next step see **Method A,** step 2, and then Witting reaction.

Conditions b (for **a28 - a30**): N-bromosuccinimide (24 mol, 1.2 eq) was added to the stirred solution of acetophenone derivatives (20 mmol, 1eq) in acetonitrile (40 mL). The resulting reaction mixture was stirred for 10-15 min. After that p-TsOH (2 mmol, 0.1 eq) was added to the reaction mixture and refluxed for 2 - 4 h and monitored by TLC. After completion of reaction, the mixture was concentrated under reduced pressure. The obtained residues were purified by column chromatography afforded the desired product (90%).[3] Then next step see **Method A**, step 2, and then Witting reaction.

Method C:

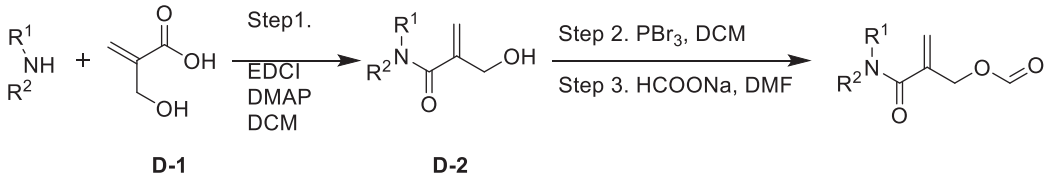


Step1: To a solution of acrylic acid (20 mmol, 1.0 eq), hydroxyl substrate (15 mmol, 1.5 eq), DMAP (2 mmol, 0.1 eq), 1-ethyl-3-(3-(dimethylamino)propyl)carbodiimide hydrochloride (EDCI, 15 mmol, 1.5 eq) and Et_3N (30 mmol, 3.0 eq) in CH_2Cl_2 (40.0 mL). The reaction mixture was stirred at room temperature overnight. Then the reaction was quenched with H_2O (10.0 mL) and extracted with DCM. The organic layer was dried over Na_2SO_4, concentrated and purified by flash chromatography to afford the desired product acrylic ester. [4]

Step 2: A solution of paraformaldehyde (1.3 eq) and acrylic ester (10mol, 1eq) in 1, 4-dioxane-water (10 mL) (1:1, v/v) was stirred at room temperature for 3-5 day in the presence of DABCO (1eq). The reaction was added with H_2O. The organic layer was separated and the aqueous phase was extracted with ethyl acetate (15 mL × 3), washed with brine, The combined organic phase dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography to afford the desired product **C-1**. [5]

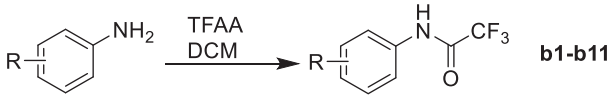
Step 3: To a solution of **C-1** (6 mmol) was added phosphorus (III) bromide (3 mmol) in DCM (10 mL) at -10 °C. The temperature was allowed to rise to 20 °C and stirring was continued for 2 h. Water (10 mL) was then added and the mixture was extracted with DCM (3 x 10 mL). The organic phase was washed with saturated sodium chloride solution (20 mL), dried with Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography to afford the desired product allyl bromide derivatives.[5] Then next step see **Method A**, step 2.

Method D:



Step 1: The EDCI (1.3 eq) was dissolved into the mixture of **D-1**[6] (1 eq, 10 mmol) and amines (1.3 eq) in 15 mL of DMF. The resulting mixture was stirred at room temperature overnight, and then 50 mL of water was added into the mixture. The resulting mixture was extracted with EtOAc. The organic layer was washed with water for three times and dried with Na_2SO_4. The solvent was removed under vacuum. The crude product was purified by flash column to give the product **D-2**.[6] Then next step see **Method C**, step 3 and **Method A**, step 2.

Method D:



Trifluoroacetic anhydride (1.2 eq) was added dropwise to a solution of aniline (3 mmol, 1 eq)

and NEt_3 (1.5 eq) in CH_2Cl_2 (15 ml) at 0 °C. The reaction mixture was then stirred at room temperature until TLC indicated the disappearance of aniline, the solvent was evaporated under reduced pressure. The crude residue was purified by flash column chromatography to give the desired product **b1-b11** (90% - 100%). [7]

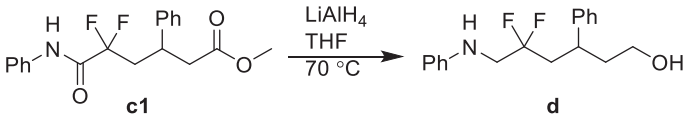
4 Gram-scale synthesis and follow-up transformations of c1

4.1 Gram-scale synthesis of c1

An oven-dried 200mL flask was charged with **1a** (6 mmol, 973.2 mg), **1b** (24 mmol, 4.54 g), HCOOCs (12 mmol, 2.2 g), 4CzIPN (0.12 mmol, 94.7 mg), Cs_2CO_3 (3 mmol, 977.4 mg) and anhydrous DMSO (90 mL). The flask was evacuated and back-filled with CO_2 for 3 times. The reaction mixture was stirred and irradiated with blue LEDs (λ = 425 nm) for 24 h. The reaction was added K_2CO_3 (20 mmol, 2.76 g), MeI (6 mL), and further stirred at room temperature for 8h. The reaction was quenched by H_2O (90 mL) and extracted by EtOAc (150 mL × 3). The organic phase was dried and concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel to afford products **c1** (1.19 g) in 57% yield.

4.2 Follow-up transformations of c1

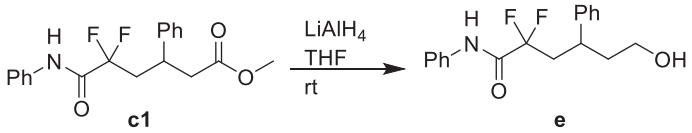
Procedure A:



c1 **d**

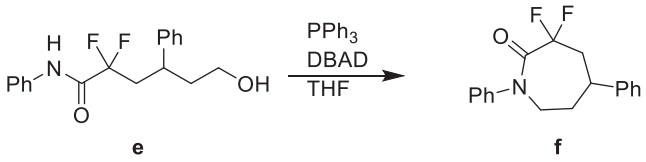
To a solution of **c1** (0.2 mmol, 69.5 mg) in anhydrous THF (2 mL), a solution of $LiAlH_4$ (4 eq, 30.4 mg) in anhydrous THF (2 mL) was added in an ice bath, the mixture was stirred at 70°C for 6 h before being quenched by MeOH (1 mL). The mixture concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel to afford products **d** in 56% yield. [8]

Procedure B:



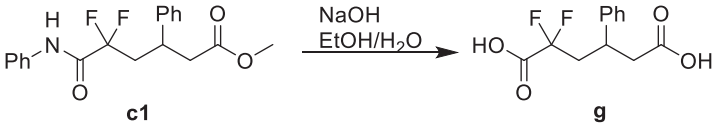
To a solution of **c1** (0.2 mmol, 69.5 mg) in anhydrous THF (2 mL), a solution of $LiAlH_4$ (1.5 eq, 11.4 mg) in anhydrous THF (2 mL) was added in an ice bath, the mixture was stirred at room temperature for 6 h before being quenched by MeOH (1 mL). The mixture concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel to afford products **e** in 70% yield. [9]

Procedure C:



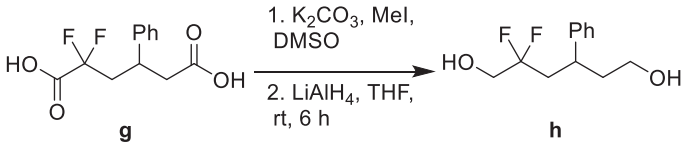
To a solution of triphenylphosphine (1.5 eq), di-tertbutyl azodicarboxylate (1.5 eq) in THF (2 mL) was allowed to premix for 10 min and a solution of **e** (0.2 mmol, 1 eq) in THF (1 mL) was added. Then, the reaction mixture was stirred for 5 h at 60 °C on a heating block. Then, the mixture was concentrated and purified via column chromatography to afford products **f** in 54% yield. [9]

Procedure D:



To a solution of **c1** (1 mmol, 0.35 g) in EtOH / H_2O (4 ml / 2 mL) was added NaOH (10 mmol, 0.4 g), the mixture stirred at 100 ºC for 12 h. Then, the reaction was allowed to cool to room temperature, diluted with 20 mL EtOAc and quenched by 5 mL HCl (aq., 2 N), then stirred for 10 min. The reaction mixture was extracted with EtOAc for over 10 times and the combined organic phases were concentrated under reduced pressure. The residue was purified by a silica gel flash column chromatography (1% AcOH in petroleum ether/EtOAc 10/1, then 2% AcOH in petroleum ether/EtOAc 3/1~1/1) to give the pure desired product **g** in 70% yield. [10]

Procedure E:



In a 20 ml round-bottom flask equipped with a magnetic stirring bar, **g** (1 mmol, 1 equiv.), K_2CO_3 (3.0 mmol, 3 equiv.) and DMSO (10 mL) were added. Then, methyl iodide (4 mmol, 4 equiv.) was added and the reaction mixture was stirred at room temperature for 5 h. Upon completion, the reaction crude was diluted with H_2O (30 mL) and EtOAc (30 mL). The organic phase was washed with H_2O (3 x 20 mL), saturated K_2CO_3 (3 x 20 mL),

brine (30 mL), dried over $MgSO_4$, and evaporated to dryness to afford the desired methyl ester derivative without further purification. To a solution of methyl ester derivative in anhydrous THF (4 mL), a solution of $LiAlH_4$ (1.5 eq, 11.4 mg) in anhydrous THF (2 mL) was added in an ice bath, the mixture was stirred at room temperature for 6 h before being quenched by MeOH (1 mL). The mixture concentrated under reduced pressure. The crude product was purified by column chromatography over silica gel to afford products **h** in 61% yield.

5 Rationaliztion of the stereoselectivity for c22-c26

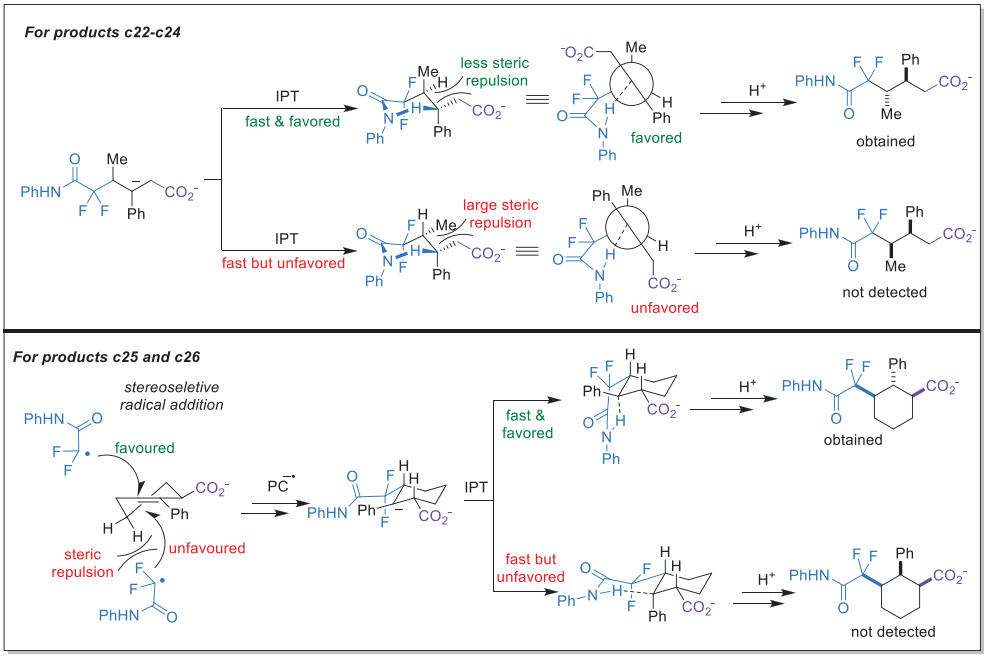


Figure S1. Rationaliztion of the stereoselectivity

For linear products **c22-c24**, the excellent diastereoselectivity is obtained by the fast intramolecular proton transfer (IPT) by a hydrogen bond-participated six-membered ring via a more stable configuration **A**, in which the lager steric repulsion is avoided between the phenyl group and methyl group. By contrast, for cyclic products **c25** and **c26** with three stereocenters, the excellent diastereoselectivity is controlled by two factors. One is the stereoselective radical addition of fluoroalkyl radical onto but-3-enoate which controls the product with 1,3-cis configuration, and the other is the subsequent IPT process in which a more stable cis-fused configuration **C** rather than trans-fused configuration **D** is involved, as the former have all 3 substituents on equatorial bonds.

6 Mchanistic investigations

6.1 Stern-Volmer quenching experiments

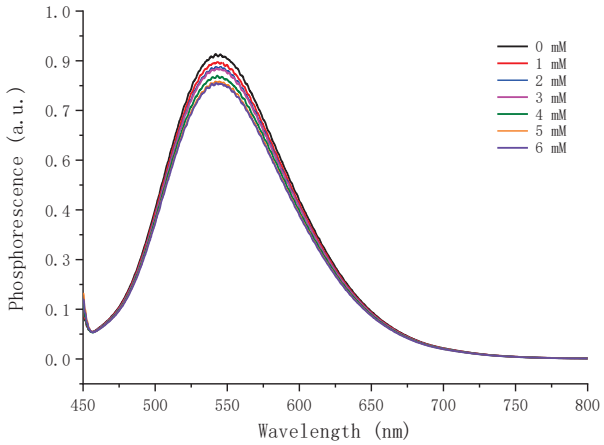


Figure S2. Fluorescence emission spectra of **PC1** (0.05 mM in DMSO) with different concentration of cesium formate

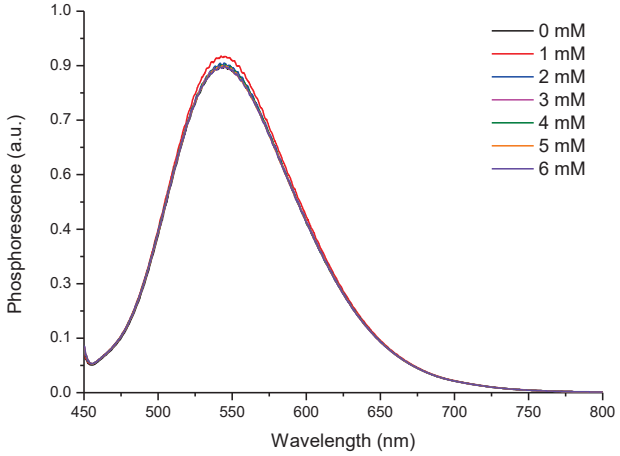


Figure S3. Fluorescence emission spectra of **PC1** (0.05 mM in DMSO) with different concentration of **b1**

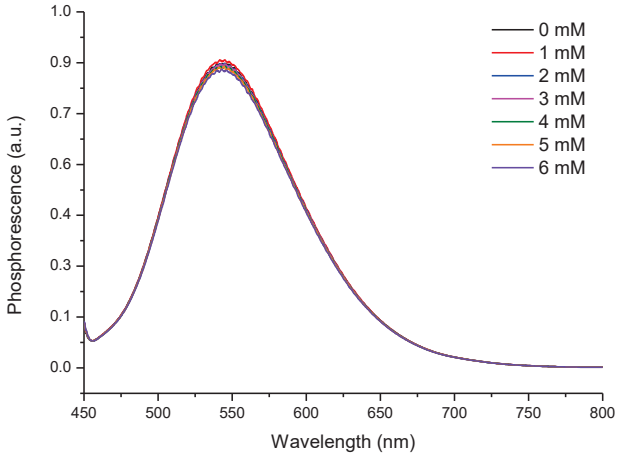


Figure S4. Fluorescence emission spectra of **PC1** (0.05 mM in DMSO) with different concentration of **a1**

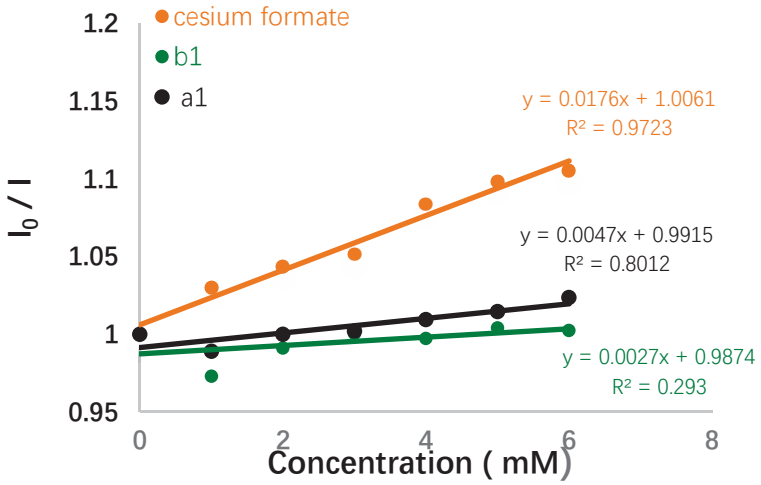
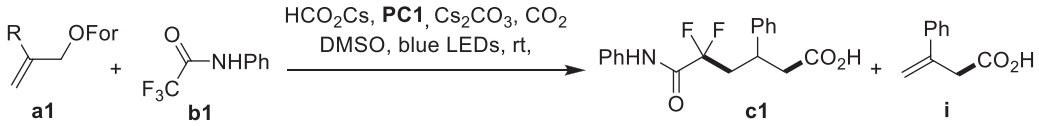


Figure S5. Stern-Volmer plot for the fluorescence quenching of **PC1** (0.05 mM in DMSO) by cesium formate, **a1**, **b1**

Stern-Volmer luminescence quenching analysis was conducted using a Jasco FP-8300 spectrofluorometer. The following parameters were employed: Excitation bandwidth = 10nm, data interval = 0.2 nm, scan speed = 12000 nm/min. The solution of **PC1** (0.05 mM in DMSO) were excited at λ_{ex} = 440 nm and the emission was collected at 542 nm. The substrates cesium formate, **a1**, **b1** were dissolved in DMSO (500 mM), respectively. For each quenching experiment, 25 µL of the stock solution were titrated to a solution (3 mL) of **PC1**. The addition of 25 µL stock solution refers to an increase of the quencher concentration of 5 mM. I_0 is the luminescence intensity without the quencher, I is the intensity in the presence of the quencher.

6.2 Reaction Kinetic Profile



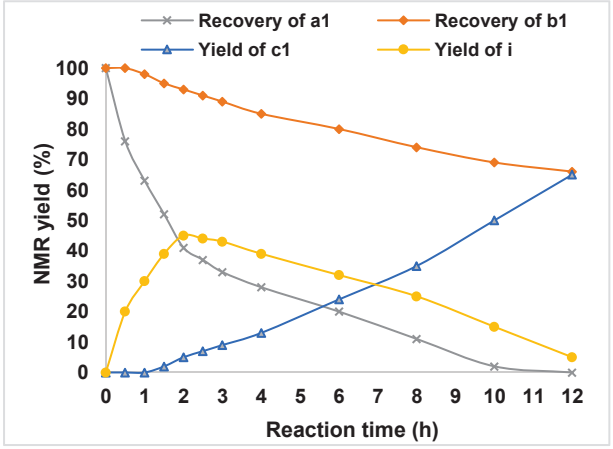


Figure S6. Reaction time-scale monitoring

An oven-dried 15mL tube was charged with **a1** (0.2 mmol), **b1** (4 eq, 0.8 mmol), HCOOCs (2 eq, 0.4 mmol), 4CzIPN (2%, 3.2 mg), Cs_2CO_3 (0.5 eq, 0.1 mmol). The tube was evacuated and back-filled with CO_2 for 3 times, then DMSO (3 mL) was added. The reaction mixture was stirred and irradiated with blue LEDs (λ = 425 nm, 2 cm - 4 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25~30°C). The tube was removed after 0.5 h, 1 h, 1.5 h, 2 h, 2.5 h, 3 h, 4 h, 6 h, 8 h, 10 h and 12 h respectively. The yield of each component in the reaction mixture was determined by NMR using diphenylmethane and benzotrifluoride as an internal standard.[12]

6.3 Cyclic voltammetry test

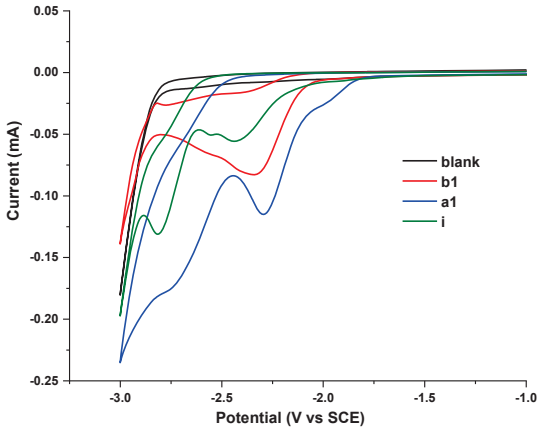
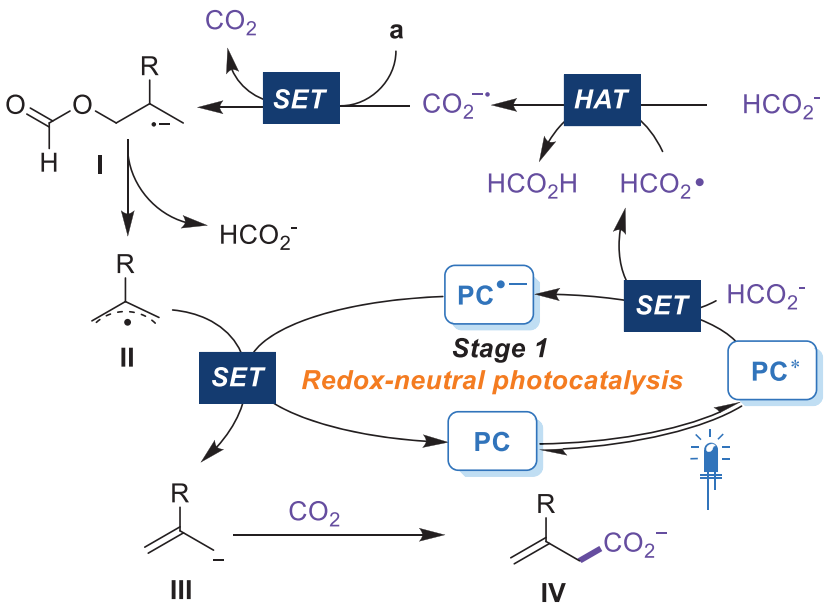


Figure S7. Figure S1. Cyclic voltammograms: (a) **a1** (10.0 mM); (b) **b1** (10.0 mM); (c) **i** (20.0 mM); (d) blank

Cyclic voltammetry (CV) experiments were conducted in a 10 mL glass vial fitted with a glassy carbon working electrode (3 mm in diameter), a $Ag/AgNO_3$ reference electrode, and a platinum wire counter electrode. The electrolyte of nBu_4NBF_4 (0.1 M) in DMSO (10 mL) was sparged with argon for 3-5 minutes before data collection. The scan rate is 100 mV/s.

6.4 Another proposed mechanism for producing but-3-enoate

The reaction is initiated by a photooxidation of formate by the excited **PC1*** to produce $PC^{-\bullet}$ and formoxyl radical by a single-electron transfer (SET) process. A hydrogen atom transfer (HAT) between formoxyl radical and formate would form formic acid and $CO_2^{-\bullet}$. $CO_2^{-\bullet}$ reduces the alkene substrate **a** to give anion radical **I** and releases CO_2. Then intermediate **I** eliminates formate by C-O bond cleavage to yield the allyl radical intermediate **II**. **II** would be further reduced by $PC^{-\bullet}$ to the allylic carbanion intermediate **III**, which is add to CO_2 to form the key intermediate but-3-enoate **IV**.



6.5 DFT calculations

Computational details and energy profiles

All the Density functional theory (DFT) calculations were performed with the GAUSSIAN 09 series of programs[13]. DFT method B3LYP[14] with a standard 6-31+G(d, p)[15] was used for geometry optimizations. The vibrational frequencies at the same level were computed to characterize all optimized structure as minima or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. IRC calculations were used to confirm that the transition states found from the optimization calculations connect the related reactants and products. The energies given in this work are Gibbs free energies in gas phase (Δ*G*).

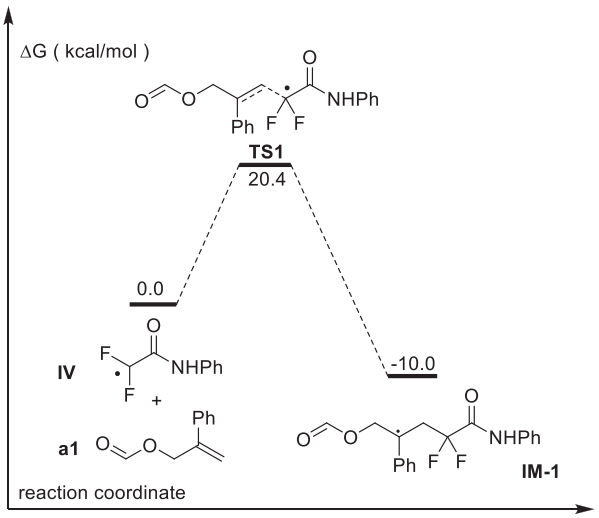


Figure S8. Calculated energy profiles of **IM-1**

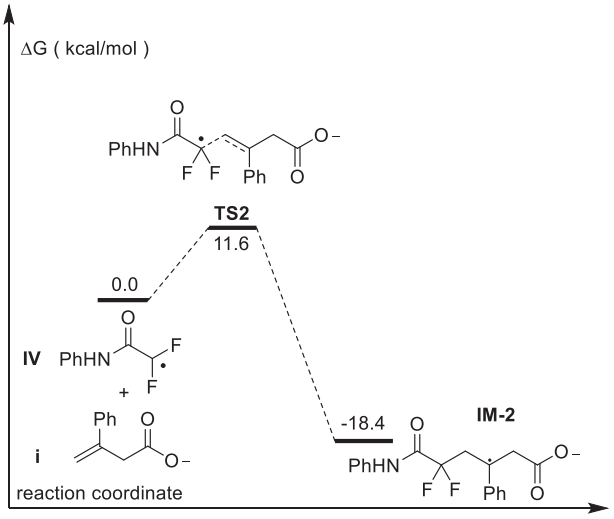


Figure S9. Calculated energy profiles of **IM-2**

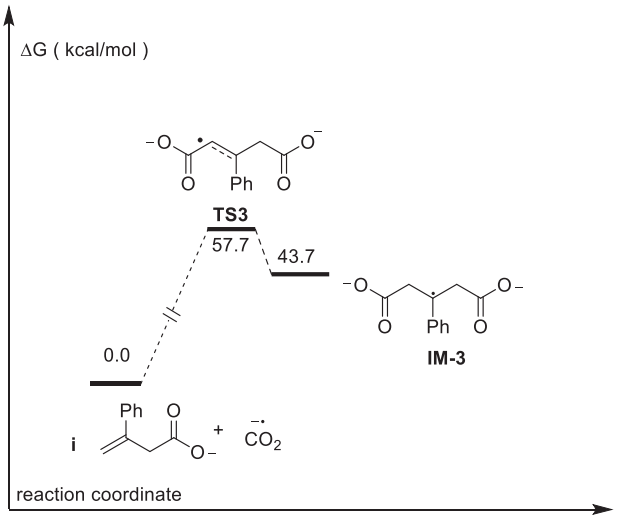


Figure S10. Calculated energy profiles of **IM-3**

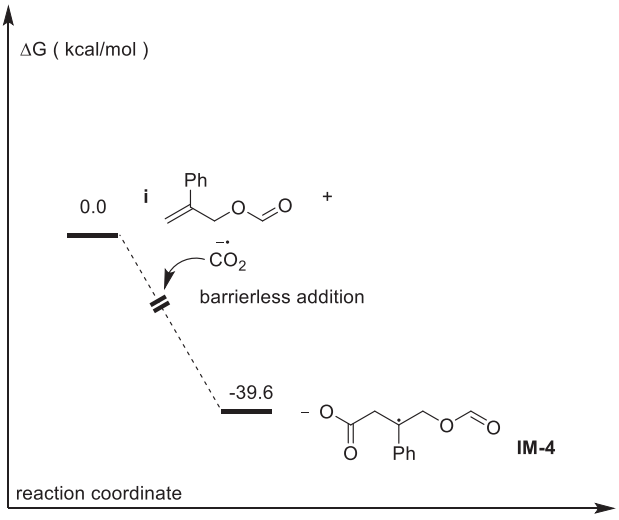


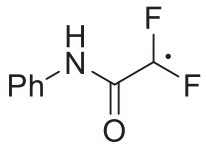
Figure S11. Calculated energy profiles of **IM-4**

Coordinates of all stationary points

Table S1. Coordinates of All Stationary Points

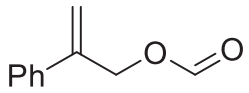
	E_{zero}	E	H	G	IF
IV	-637.985749	-637.975392	-637.974447	-638.023789	
a1	-537.366853	-537.366853	-537.355038	-537.405313	
IM-1	-1175.388938	-1175.388938	-1175.366129	-1175.444935	
TS1	-1175.340139	-1175.317914	-1175.316970	-1175.396561	-319.49
i2	-536.858824	-536.848450	-536.847506	-536.896045	
IM-2	-1174.895786	-1174.895786	-1174.895786	-1174.949222	
TS2	-1174.949222	-1174.823038	-1174.822094	-1174.822094	-112.60
$CO_2^{\bullet-}$	-188.572133	-188.569161	-188.568217	-188.595449	
IM-3	-725.378537	-725.365066	-725.365066	-725.421914	
TS3	-725.354671	-725.340697	-725.340697	-725.399455	-132.45
IM-4	-725.990353	-725.976556	-725.975612	-726.033828	

Sum of electronic and thermal free energies (G, in a.u.), sum of electronic and thermal enthalpies (H, in a.u.), sum of electronic and thermal Energies (E, in a.u.), sum of electronic and zero-point energies (E_{zero}, in a.u.), and imaginary frequencies for the transition states (IF).



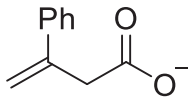
IV

C	-1.43289800	0.45237000	-0.06098100
O	-1.33186400	1.67357100	-0.00399500
N	-0.40184100	-0.45570900	-0.07726400
H	-0.66847800	-1.43163400	-0.09172000
C	-2.76400600	-0.18103700	-0.20402800
F	-3.83712800	0.50999900	0.12797300
F	-2.91089300	-1.48777600	0.07846000
C	0.98773700	-0.20775400	-0.03092800
C	1.83463700	-1.32930900	-0.00917100
C	1.54002300	1.08306800	-0.01201100
C	3.21699200	-1.16553700	0.02813200
H	1.40819500	-2.32985500	-0.02261300
C	2.92883400	1.22834900	0.02544900
H	0.89017400	1.94670700	-0.02270700
C	3.77400600	0.11695000	0.04560300
H	3.85772400	-2.04212900	0.04399600
H	3.34902600	2.22971100	0.03995700
H	4.85139500	0.24598700	0.07559900



a1

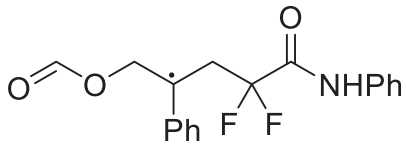
C	-0.35914700	1.13125400	0.15938100
C	0.91848900	0.37449000	0.05669800
C	0.94599200	-1.03019700	0.14190100
C	2.13971100	1.05389300	-0.11390900
C	2.15148200	-1.72762700	0.03765700
H	0.02042900	-1.58232000	0.26188800
C	3.34223800	0.35568800	-0.21760600
H	2.14991800	2.13926700	-0.13794100
C	3.35346200	-1.04047600	-0.14469700
H	2.14717300	-2.81229200	0.09479300
H	4.27225800	0.90307400	-0.34194100
H	4.28989500	-1.58511800	-0.22204100
C	-1.45724200	0.57250100	1.04142900
H	-1.05964100	0.19802800	1.98734600
H	-2.20271800	1.34583100	1.25495700
C	-0.56884900	2.29791600	-0.47446800
H	0.16761400	2.73198200	-1.14280200
H	-1.49584200	2.85060000	-0.35098100
O	-2.11599300	-0.57495600	0.43949300
C	-3.27443500	-0.36770100	-0.22009600
H	-3.63248400	0.67677400	-0.16659900
O	-3.85985700	-1.24807800	-0.79379500



i

C	0.58920600	1.06483700	-0.18291000
C	-0.75020900	0.41462400	-0.07966400
C	-0.86528000	-0.98859400	-0.00890400
C	-1.93357000	1.17862300	-0.06701200
C	-2.12130300	-1.59122000	0.09806900
H	0.04705000	-1.58722300	-0.01353200
C	-3.18718900	0.57195100	0.03786200
H	-1.86801100	2.25880500	-0.16292600
C	-3.28839000	-0.82034700	0.12438600
H	-2.18546900	-2.67506900	0.16405600
H	-4.08505300	1.18651900	0.03889300
H	-4.26310600	-1.29674200	0.20261000
C	1.68884000	0.33476400	-0.92014100
H	1.26219100	-0.26886100	-1.72853500
H	2.37347300	1.07132400	-1.34966800
C	0.81433600	2.26440000	0.39247400

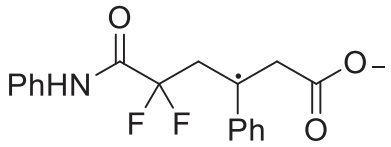
H	0.06401000	2.76387000	0.99988300
H	1.78900000	2.73727300	0.31991300
C	2.56510400	-0.61879100	0.01022100
O	3.56696900	-0.07325500	0.52822300
O	2.15761100	-1.80816800	0.10965500



IM-1

C	3.04047400	3.14814200	0.31319900
C	2.33785400	2.12779200	-0.31405800
C	2.74447900	0.76516800	-0.20316000
C	3.89331000	0.50516500	0.60389200
C	4.58882900	1.53296400	1.22647900
C	4.17455700	2.86396200	1.08523300
H	2.70073700	4.17419400	0.20492300
H	1.45634700	2.38538100	-0.88849900
H	4.22216800	-0.51530500	0.75924800
H	5.45671900	1.29634400	1.83521000
H	4.72029000	3.66453700	1.57517900
C	2.05226300	-0.29763400	-0.86795600
C	0.85716300	-0.06180400	-1.75748700
H	0.86625000	0.93558300	-2.20377200
H	0.85143400	-0.76231400	-2.59764700
C	2.54668900	-1.71357100	-0.75516400
H	2.01097100	-2.36482800	-1.45278100
H	3.61652400	-1.78452900	-0.97911100
C	-0.49381000	-0.22490600	-1.06071700
O	2.40435800	-2.24604500	0.59484200
C	1.59015900	-3.30342700	0.78740800
H	1.10659500	-3.66367500	-0.13799200
O	1.42313200	-3.80286300	1.86973200
C	-1.69532100	-0.09281400	-2.03606000
O	-1.49850900	-0.25201600	-3.23641500
N	-2.93056600	0.20995800	-1.54500400
H	-3.60361500	0.33195800	-2.29480800
C	-3.43403200	0.35294200	-0.21044400
C	-4.10143700	1.53767000	0.12189700
C	-3.33664500	-0.68381200	0.72314500
C	-4.66278000	1.68790200	1.39094100
H	-4.16823100	2.33784400	-0.60966300
C	-3.88159600	-0.51723500	1.99798800
H	-2.83650100	-1.60729200	0.45634600
C	-4.54785900	0.66363200	2.33493100

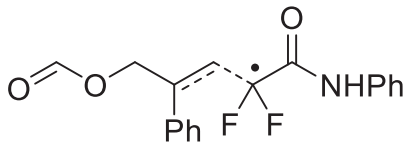
H	-5.17906500	2.60915300	1.64373300
H	-3.79265200	-1.31985600	2.72373400
H	-4.97653300	0.78408100	3.32515500
F	-0.56811200	-1.48847900	-0.48377200
F	-0.61001100	0.67687900	-0.03288400



IM-2

C	4.80340900	-1.55762100	0.01986500
C	3.44727800	-1.26229500	-0.06387100
C	2.95125200	0.05594300	0.17069200
C	3.92695100	1.05298000	0.47978800
C	5.28026700	0.74637300	0.55419600
C	5.73906000	-0.56061700	0.33080700
H	5.13563800	-2.57907400	-0.15252900
H	2.74982900	-2.06500900	-0.27594000
H	3.60835800	2.08096100	0.61132300
H	5.99108800	1.53937800	0.77583600
H	6.79852100	-0.79477200	0.39241600
C	1.55429400	0.37200300	0.09592900
C	0.59297500	-0.52184600	-0.64898100
H	-0.04554600	0.14881500	-1.24131900
H	1.09953800	-1.19261600	-1.34945600
C	0.99871400	1.67494300	0.55928400
H	0.04233800	1.50560100	1.06695500
H	1.66839800	2.18191400	1.25392000
C	-0.31752200	-1.42097900	0.18670800
C	-1.37907400	-2.13550900	-0.68710000
O	-1.04650600	-3.13186800	-1.32153200
N	-2.65603300	-1.64667400	-0.77738300
H	-3.21678600	-2.25486400	-1.36406400
C	-3.35338300	-0.52663900	-0.21598600
C	-4.56720300	-0.78773000	0.43558100
C	-2.91150000	0.79140500	-0.37599300
C	-5.33803400	0.26457400	0.93320400
H	-4.89503900	-1.81676100	0.55941700
C	-3.67949700	1.83495200	0.14778600
H	-1.98127500	1.04485700	-0.88217700
C	-4.89186100	1.58234900	0.79542200
H	-6.27715500	0.05147400	1.43715700
H	-3.31513300	2.85060000	0.02623200
H	-5.48443300	2.40388100	1.18896300
F	0.41476300	-2.41482500	0.80492800

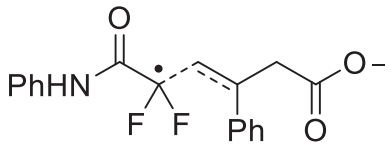
F	-0.93344300	-0.74077600	1.21762800
C	0.66357300	2.68158700	-0.64460500
O	1.37758100	3.70234600	-0.70328900
O	-0.29809800	2.31946000	-1.38073100



TS1

C	-3.06267600	-3.19640600	0.42841500
C	-2.27230800	-2.18226100	-0.10432100
C	-2.83906700	-0.96158200	-0.53365400
C	-4.23226900	-0.79781200	-0.37998300
C	-5.02323700	-1.81720300	0.14897300
C	-4.44545700	-3.02259100	0.55356500
H	-2.59772900	-4.12159300	0.75641000
H	-1.20026500	-2.33498200	-0.16749500
H	-4.70463800	0.13505900	-0.66328100
H	-6.09322400	-1.66324000	0.25279100
H	-5.06119400	-3.81306400	0.97229700
C	-2.00998800	0.09689400	-1.13675100
C	-0.73568700	-0.11720400	-1.59309100
H	-0.33173800	-1.11730100	-1.70396300
H	-0.22637500	0.66723500	-2.14209200
C	-2.58626400	1.48809700	-1.30471800
H	-1.81519500	2.16614300	-1.68248100
H	-3.41152700	1.48156300	-2.02420200
C	0.71024000	0.24054700	0.26724900
O	-3.16230600	2.02701500	-0.09417000
C	-2.37449800	2.80850300	0.68930400
H	-1.35245700	2.94768600	0.30052700
O	-2.79016500	3.29160200	1.71052700
C	1.50865800	1.40206800	-0.20001500
O	0.94820700	2.49742500	-0.29452300
N	2.76980400	1.19024300	-0.70643600
H	3.10303800	2.00518300	-1.21178500
C	3.76983000	0.26341000	-0.27686700
C	4.57819700	-0.34735400	-1.24260700
C	3.98859800	0.00748900	1.08207100
C	5.59863500	-1.21478000	-0.84891100
H	4.39750900	-0.14714900	-2.29472400
C	4.99402500	-0.88073500	1.46724000
H	3.38223800	0.50718200	1.83140000
C	5.80439000	-1.49065200	0.50578800
H	6.22409400	-1.68366700	-1.60262900

H	5.15376000	-1.08127000	2.52235500
H	6.59311900	-2.17175800	0.81014400
F	-0.13400800	0.48335200	1.26958600
F	1.28504500	-0.96186800	0.42896800

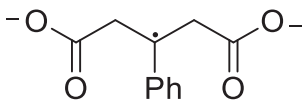


TS2

C	-4.67368900	-1.68111100	-0.53434600
C	-3.34723200	-1.36990400	-0.22838200
C	-2.93364200	-0.03156500	-0.08710800
C	-3.89012300	0.98910000	-0.26547500
C	-5.21711700	0.67183700	-0.55943300
C	-5.61714200	-0.66198500	-0.69912500
H	-4.96781900	-2.72145800	-0.65184400
H	-2.61709600	-2.16674900	-0.12231500
H	-3.58229700	2.02447300	-0.13035200
H	-5.94370800	1.47237400	-0.67616700
H	-6.65013600	-0.90418400	-0.93688200
C	-1.53543600	0.32341400	0.26115400
C	-0.82564600	-0.43153900	1.14698400
H	0.11012600	-0.05291200	1.53842900
H	-1.27123700	-1.27432300	1.66602900
C	-0.94291700	1.56759700	-0.34025000
H	0.07716700	1.35660800	-0.67052900
H	-1.52772500	1.89368500	-1.20317400
C	0.78625100	-1.95925100	-0.16818300
C	1.82281500	-2.24264100	0.84570200
O	1.69006500	-3.20781300	1.60565500
N	2.87026300	-1.36076400	0.99900900
H	3.46569000	-1.63792100	1.77041800
C	3.29848400	-0.22866700	0.22110500
C	4.36735700	-0.38858000	-0.67177200
C	2.71618300	1.03048500	0.39892300
C	4.84852700	0.70713600	-1.39125600
H	4.80701600	-1.37377300	-0.80126800
C	3.19283400	2.12052000	-0.33620900
H	1.88656300	1.20125400	1.08052800
C	4.25805700	1.96501000	-1.22616000
H	5.67594800	0.57605200	-2.08387600
H	2.70999500	3.08233800	-0.19272100
H	4.62637900	2.81726800	-1.79131700
F	0.00533800	-2.99957200	-0.49653900
F	1.12441800	-1.28404800	-1.28280900

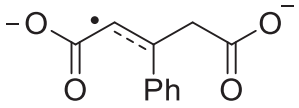
C	-0.86051000	2.76645200	0.70817200
O	-1.85561900	3.52746300	0.72863000
O	0.19794800	2.79376800	1.38822300

C	0.00000000	0.00000000	0.32874700
O	0.00000000	-1.15398500	-0.12328000
O	0.00000000	1.15398500	-0.12328000



IM-3

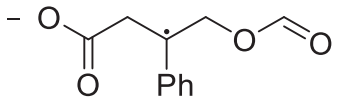
C	3.00729300	-1.13415000	0.41238600
C	1.61672400	-1.14360900	0.41914300
C	0.86320100	0.00047800	-0.00021000
C	1.61586400	1.14519000	-0.41938700
C	3.00644100	1.13682500	-0.41226200
C	3.72781300	0.00163400	0.00016200
H	3.54319900	-2.03190200	0.72070200
H	1.08235200	-2.05040600	0.69087900
H	1.08086500	2.05161300	-0.69115300
H	3.54170400	2.03502400	-0.72038700
H	4.81679600	0.00207800	0.00027000
C	-0.56904700	-0.00021000	-0.00030000
C	-1.33749500	-1.08121400	0.70079200
H	-0.83586100	-1.36925600	1.63170400
H	-2.32918000	-0.68818800	0.94514500
C	-1.33845000	1.08015000	-0.70114000
H	-0.83696400	1.36930500	-1.63176200
H	-2.32972800	0.68631500	-0.94589400
C	-1.56338200	2.42339900	0.13749600
O	-2.44481100	2.37430700	1.03207000
O	-0.84214100	3.40264000	-0.20588900
C	-1.56082400	-2.42485700	-0.13731400
O	-0.83878600	-3.40335200	0.20659400
O	-2.44201300	-2.37689400	-1.03223800



TS3

C	0.50164700	3.17872500	-0.39645200
C	-0.14295400	1.94405200	-0.43074200
C	0.53000900	0.73772300	-0.08216700
C	1.88825100	0.86368200	0.32470500

C	2.52348000	2.10379600	0.35584800
C	1.84655100	3.28113800	-0.00677300
H	-0.05709200	4.07662100	-0.66148300
H	-1.19489000	1.90371500	-0.69555400
H	2.44493100	-0.03904700	0.57012800
H	3.56961000	2.15216400	0.65812500
H	2.34872300	4.24708800	0.01890300
C	-0.13984800	-0.56077400	-0.12199600
C	-1.33056600	-0.72766500	-0.80236600
H	-1.67838400	-0.00751500	-1.53391800
H	-1.75232000	-1.72322700	-0.88862300
C	0.45425200	-1.72451100	0.65516300
H	0.83729700	-1.36859900	1.62044700
H	-0.35288700	-2.43795800	0.85241500
C	1.61642300	-2.53891600	-0.04551700
O	1.25736300	-3.41832100	-0.87279700
O	2.79666800	-2.25120700	0.31715600
C	-3.50101300	-0.09935200	0.26116700
O	-4.21186000	0.19180700	-0.69635600
O	-3.54746800	-0.21610700	1.47629000

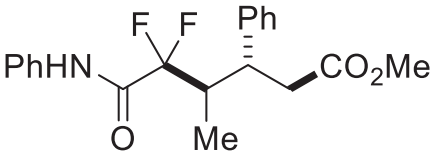


IM-4

C	3.03660600	-1.22958400	-0.65943500
C	1.72412300	-1.29853700	-0.20753800
C	1.08732600	-0.17550300	0.40208400
C	1.85693800	1.02317600	0.48996000
C	3.17220600	1.07624900	0.04172800
C	3.78185800	-0.04779100	-0.53329000
H	3.48267200	-2.10421000	-1.12749100
H	1.15921200	-2.21328900	-0.35147800
H	1.40480500	1.91742900	0.90334100
H	3.72701300	2.00757000	0.13152900
H	4.80742900	0.00061700	-0.88967100
C	-0.25212300	-0.26044400	0.90741500
C	-0.97835200	-1.55039600	1.03612000
H	-0.30252100	-2.40075300	1.13304600
H	-1.62780000	-1.52785100	1.92205300
C	-0.98933700	0.96244800	1.37905500
H	-2.02479000	0.69385200	1.60043300
H	-0.53589300	1.38989400	2.28398400
C	-1.98366300	-1.84356700	-0.19361500
O	-1.75496900	-2.90017600	-0.81436100

O	-2.87568900	-0.97116400	-0.35127400
O	-0.99360500	2.10370400	0.46109000
C	-1.77405100	2.00043900	-0.64138300
H	-2.29405400	1.03067800	-0.73656200
O	-1.86139400	2.92602600	-1.41992600

7 X-Ray single-crystal diffraction study for compound c22 and c25



c22

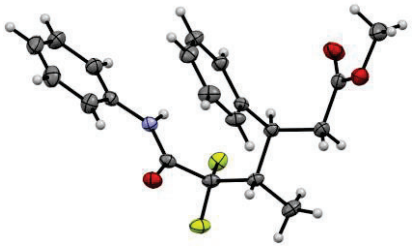
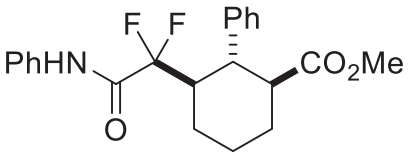


Table S2. The crystal data and refinement results of compound **C22**.

Compound number	**C22**
Formula	$C_{20}H_{21}F_2NO_3$
Formula weight	361.38
Temperature/K	280(1)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.45569(15)
b/Å	18.57018(19)
c/Å	10.44754(14)
α/°	90
β/°	115.8088(17)
γ/°	90
Volume/Å^3	1826.19(5)
Z	4
ρ_{calc}g/cm^3	1.314
μ/mm^{-1}	0.853
F(000)	760.0
Crystal size/mm^3	0.18 × 0.15 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.396 to 152.638
Index ranges	-11 ≤ h ≤ 13, -23 ≤ k ≤ 23, -13 ≤ l ≤ 11
CCDC number	2381321



c25

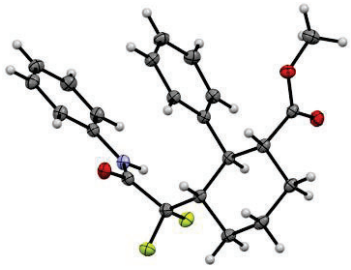


Table S3. The crystal data and refinement results of compound **C25**.

Compound number	**C25**
Empirical formula	C22H23F2NO3
Formula weight	387.41
Temperature/K	149.99(10)
Crystal system	triclinic
Space group	P-1
a/Å	9.9380(7)
b/Å	10.9753(9)
c/Å	11.0840(7)
α/°	108.444(6)
β/°	102.977(6)
γ/°	113.996(7)
Volume/Å3	956.77(13)
Z	2
ρcalcg/cm3	1.345
μ/mm-1	0.852
F(000)	408.0
Crystal size/mm3	0.09 × 0.08 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.21 to 151.824
Index ranges	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -9 ≤ l ≤ 13
CCDC number	2381323

8 References

[1] Tripathi C. B.; Mukherjee S., *Angew. Chem. Int. Ed.* **2013**, *52*, 8450.

[2] Lapointe D.; Markiewicz T.; Whipp C. J.; Toderian A.; Fagnou K., *J. Org. Chem.* **2011**, *76*, 749.

[3] Zhou W.; Zhang M.; Li H.; Chen W.; *Org. Lett.* **2017,** *19*, 2548.

[4] Du, X.; Zhen, J.-S.; Xu, X.-H.; Yuan, H.; Li, Y.-H.; Zheng, Y.; Xue, C.; Luo, Y. *Org. Lett.* **2022**, *24*, 3944.

[5] Li Y.; Zhang J.; Li D.; Chen Y.; *Org. Lett.* **2018**, 20, 3296.

[6] Wang L.; Liu M.; Lu M.; Wang B.; Han Q.; Jin J.; Yu S.; Wu Y.; Guo H. *Org. Chem. Front.*, **2023**, *10*, 813.

[7] (a) Ye J. H.; Bellotti P.; Heusel C., Glorius F. *Angew. Chem. Int. Ed.* **2022**, *61*, e202115456. (b) Liu C.; Shen N.; Shang R. *Nat. Commun.* **2022**, *13*, 354. (c) Zhu L.; Le L.; Yan M.; Au C.-T.; Qiu R.; Kambe N. *J. Org. Chem.* **2019**, *84*, 5635. (d). Monzón G.; Tirotta I.; Knochel P. *Angew. Chem. Int. Ed.* **2012**, *51*, 10624. (e) Shojae H.; Bossi M. L.; Belov V.N.; Hell S.W. *J. Org. Chem.* **2022**, *87*, 1, 56.

[8] Shen S.; Picci C.; Ustinova K.; Benoy V.; Kutil Z.; Zhang G.; Tavares M. T.; Pavlíček J.; Zimprich C. A.; Robers M. B.; Bosch L. V. D.; Bařinka C.; Langley B.; Kozikowski A. P. *J. Med. Chem.* **2021**, *64*, 4810.

[9] Lee K.; Cho S.; Lim S.; Lee Y. *Org. Chem. Front.* **2024**, *11*, 1366.

[10] Hall C. J. J.; Goundry W. R. F.; Donohoe T. J. *Angew. Chem. Int. Ed.* **2021**, 60, 6981.

[11] Lv H.; Xiao L.-J.; Zhao D.; Zhou Q.-L. *Chem. Sci.* **2018**, *9*, 6839

[12] Li W.; Meng H.; Ming J.; Chen S. *Org. Lett.* **2024**, *26*, 1364.

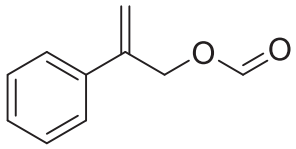
[13] Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, 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, Inc., Wallingford CT, **2009**.

[14] (a) Becke, A.-D. *Chem. Phys*. **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R.-G. *Phys. Rev.B.* **1988**, *37*, 785.

[15] (a) Clark, T.; Chandrasekhar, J.; Spitznagel, G.-W.; Schleyer, P.-V. *J. Comput. Chem.* **1983**, *4*, 294-301. (b) Krishnan, R.; Binkley, J.-S.; Seeger, R.; Pople, J.- A. *J. Chem. Phys.* **1980**, *72*, 650.

9 Analytical data for substrates and products

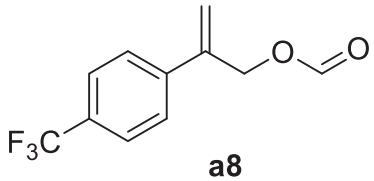
2-phenylallyl formate



a1

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.077 (s, 1H), 7.431 – 7.408 (m, 2H), 7.368 – 7.282 (m, 3H), 5.568 (s, 1H), 5.390 (d, J = 1 Hz, 2H), 5.064(s, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.53, 141.90, 137.68, 128.48, 128.14, 125.91, 115.92, 65.03.

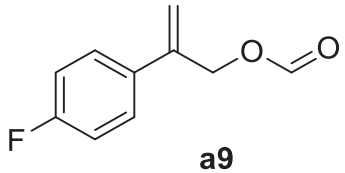
2-(4-(trifluoromethyl)phenyl)allyl formate



a8

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.102 (s, 1H), 7.623 (d, J = 8.3 Hz, 2H), 7.541 (d, J = 8.3 Hz, 2H), 5.666 (s, 1H), 5.530 (s, 1H), 5.092 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 160.48 (s), 141.22 (s), 140.93 (s), 130.12 (q, *J* =33.3 Hz), 126.34 (s), 125.50 (q, *J* = 4.0 Hz), 121.29 (9, *J* = 272.7 Hz), 118.28 (s), 64.78 (s).

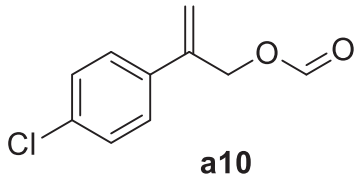
2-(4-fluorophenyl)allyl formate



a9

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.093 (s, 1H), 7.416-7.381 (m, 2H), 7.063-7.020 (m, 2H), 5.524 (s, 1H), 5.388 (s, 1H), 5.042 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 162.59 (d, *J* = 247.5 Hz), 160.51 (s), 140.89 (s), 133.72 (d, *J* = 3.3 Hz), 127.65 (d, *J* = 8.1 Hz), 116.04 (s), 115.39 (d, *J* = 21.5 Hz), 65.02 (s).

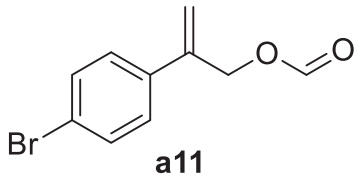
2-(4-chlorophenyl)allyl formate



a10

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.094 (s, 1H), 7.373 – 7.312 (m, 4H), 5.572 (s, 1H), 5.425 (s, 1H), 5.044 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 160.50, 140.83, 136.07, 134.04, 128.68, 127.27, 116.70, 64.89.

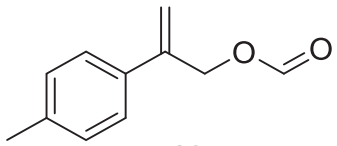
2-(4-bromophenyl)allyl formate



a11

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.100 (s, 1H), 7.488 (d, J = 8.5 Hz, 2H), 7.300 (d, J = 8.6 Hz, 2H), 5.585 (s, 2H), 5.435 (s, 1H), 5.047 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.45, 140.98, 136.60, 131.65, 127.61, 122.25, 116.74, 64.83.

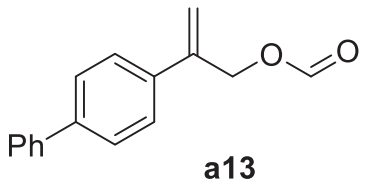
2-(p-tolyl)allyl formate



a12

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.084 (s, 1H), 7.321 (d, J = 8 Hz, 2H), 7.160 (d, J = 8 Hz, 2H), 5.540 (s, 1H), 5.345 (s, 1H), 5.054 (s, 2H), 2.346 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.62, 141.65, 138.06, 134.74, 129.21, 125.78, 115.17, 65.16, 21.08.

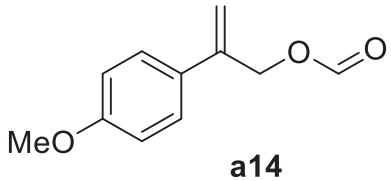
2-([1,1'-biphenyl]-4-yl)allyl formate



a13

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.079 (s, 1H), 7.582 – 7.561 (m, 4H), 7.484 (d, J = 8.4 Hz, 2H), 7.418 (t, J = 7.6 Hz, 2H), 7.329 (t, J = 7.6 Hz, 1H) 5.623 (s, 1H), 5.407 (s, 1H), 5.085 (s, 2H)^{13}C NMR (101 MHz, $CDCl_3$) δ 160.58, 141.25, 140.88, 140.27, 136.38, 128.73 (s), 127.39, 127.13, 126.88, 126.25, 116.00, 64.98.

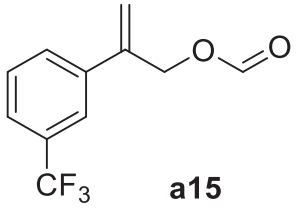
2-(4-methoxyphenyl)allyl formate



a14

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.089 (s, 1H), 7.366 (d, J = 9 Hz, 2H), 6.880 (d, J = 9 Hz, 2H), 5.492 (s, 1H), 5.302 (d, J = 0.4 Hz 1H), 5.041 (s, 2H), 3.799 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.60, 159.53, 141.13, 130.02, 127.04, 114.31, 113.82, 65.16, 55.17.

2-(3-(trifluoromethyl)phenyl)allyl formate

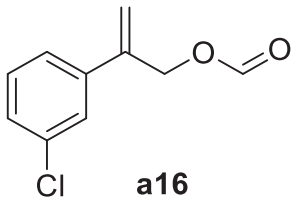


a15

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.082 (t, J = 0.8 Hz, 1H), 7.691 (s, 1H), 7.611 –

7.556 (m, 2H), 7.485 – 7.446 (m, 1H), 5.635 (s, 1H), 5.501 (s, 1H), 5.079 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.36 (s), 140.88 (s), 138.53 (s), 130.87 (q, J = 32.2 Hz), 129.20 (d, J = 1.1 Hz), 128.97 (s), 124.74 (q, J = 3.8 Hz), 123.96 (q, J = 272.4 Hz), 122.78 (q, J = 3.8 Hz), 117.62 (s), 64.63 (s).

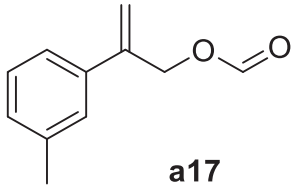
2-(3-chlorophenyl)allyl formate



a16

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.099 (s, 1H), 7.420 – 7.412(m, 1H), 7.300 – 7.290(m, 3H), 5.592 (s, 1H), 5.451 (s, 1H), 5.037 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.45, 140.87, 139.60, 134.53, 129.76, 128.21, 126.26, 124.12, 117.32, 64.84.

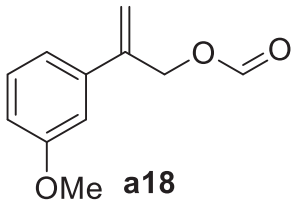
2-(m-tolyl)allyl formate



a17

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.069 (s, 1H), 7.234 – 7.202 (m, 3H), 7.126 – 7.109 (m, 1H), 5.547 (s, 1H), 5.364 (s, 1H), 5.046 (s, 2H), 2.349(s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.56, 141.89, 138.03, 137.58, 128.88, 128.35, 126.59, 122.96, 115.65, 65.03, 21.35.

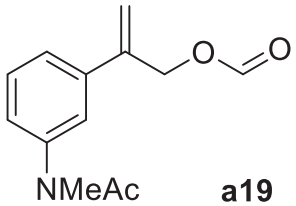
2-(3-methoxyphenyl)allyl formate



a18

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.083 (s, 1H), 7.284 – 7.244(m, 1H), 7.014 – 6.957 (m, 2H), 6.870 – 6.844 (m, 1H), 5.573 (s, 1H), 5.392 (s, 1H), 5.046 (s, 2H), 3.802 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.53, 159.60, 141.76, 139.11, 129.45, 118.32, 116.15, 113.38, 111.84, 65.00, 55.11.

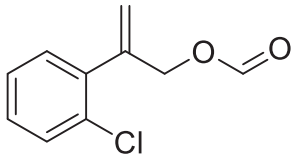
2-(3-(N-methylacetamido)phenyl)allyl formate



a19

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.126 (s, 1H), 7.454 – 7.419 (m, 2H), 7.285 (s, 1H), 7.181 – 7.160 (m, 1H), 5.64 (s, 1H), 5.498 (s, 1H), 5.087 (s, 2H), 3.282 (s, 3H), 1.898 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.32, 160.38, 144.71, 140.76, 139.36, 129.82, 126.63, 125.16, 124.57, 117.27, 64.73, 37.04, 22.34.

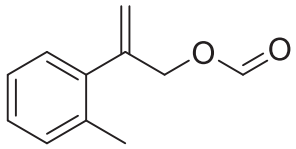
2-(2-chlorophenyl)allyl formate



a20

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.057 (s, 1H), 7.390 – 7.368 (m, 1H), 7.264 – 7.224 (m, 3H), 5.564 (s, 1H), 5.271 (s, 1H), 4.989 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 160.40, 142.07, 137.97, 132.28, 130.83, 129.57, 129.14, 126.73, 118.82, 65.40.

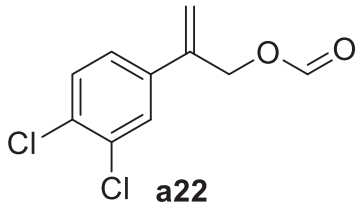
2-(o-tolyl)allyl formate



a21

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.041 (s, 1H), 7.184 – 7.106 (m, 4H), 5.472 (d, *J* = 0.8 Hz ,1H), 5.111 (s, 1H), 4.839 (s, 2H), 2.308 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) *δ* 160.38, 143.21, 138.62, 135.36, 130.15, 128.59, 127.64, 125.52, 116.42, 65.98, 19.61.

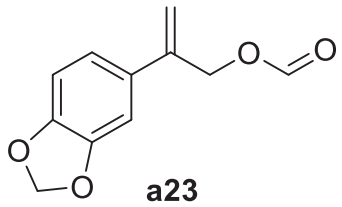
2-(3,4-dichlorophenyl)allyl formate



a22

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.102 (s, 1H), 7.52 (m, 1H), 7.43 (m, 1H), 7.26 (m, 1H), 5.604 (s, 1H), 5.479 (s, 1H), 5.025 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.42, 139.94, 137.69, 132.72, 132.18, 130.43, 128.00, 125.27, 117.90, 64.68.

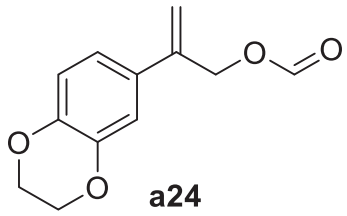
2-(benzo[d][1,3]dioxol-5-yl)allyl formate



a23

Colorless oil; Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.098 (s, 1H), 6.935 – 6.886 (m, 2H), 6.796 – 6.776 (m, 1H), 5.959 (s, 2H), 5.472 (s, 1H), 5.315 (s, 1H), 5.008 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.57, 147.86, 147.55, 141.30, 131.82, 119.55, 115.07, 108.15, 106.44, 101.13, 65.21.

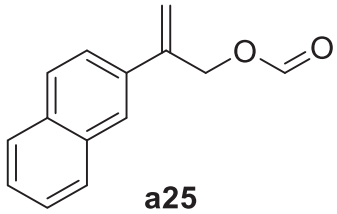
2-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)allyl formate



a24

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.096 (s, 1H), 6.960 – 6.910 (m, 2H), 6.848 – 6.827 (m, 1H), 5.487 (s, 1H), 5.304 (s, 1H), 5.007 (s, 2H), 4.251 (s, 4H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.59, 143.66, 143.36, 141.01, 131.14, 119.07, 117.22, 114.87, 65.16, 64.37, 64.28.

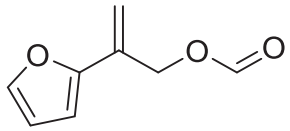
2-(naphthalen-2-yl)allyl formate



a25

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.106 (s, 1H), 7.829 -7.793 (m, 4H), 7.587-7.561 (m, 1H), 7.489 – 7.436 (m, 2H), 5.715 (s, 1H), 5.489 (s, 1H), 5.178 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.65, 141.61, 134.79, 133.15, 132.98, 128.20, 128.17, 127.51, 126.34, 126.23, 124.81, 123.92, 116.46, 65.10.

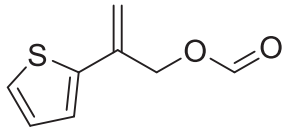
2-(furan-2-yl)allyl formate



a26

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.129 (s, 1H), 7.400 (d, J = 1.5 Hz, 1H), 6.409 (dd, J = 3.3, 1.8 Hz, 1H), 6.373 (d, J = 3.4 Hz, 1H), 5.748 (s, 1H), 5.312 (s, 1H), 4.955 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.55, 151.70, 142.46, 131.67, 113.32, 111.26, 106.99, 63.59.

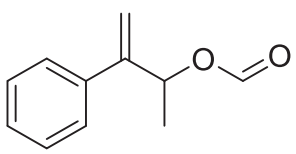
2-(thiophen-2-yl)allyl formate



a27

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.146 (s, 1H), 7.239 –7.224 (m, 1H), 7.080 – 7.069 (m, 1H), 7.018 – 6.997 (m, 1H), 5.620 (s, 1H), 5.306 (s, 1H), 5.031 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.54, 141.41, 135.57, 127.52, 124.99, 124.13, 114.61, 64.91.

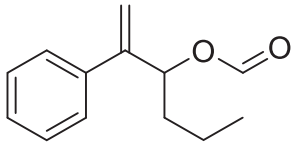
3-phenylbut-3-en-2-yl formate



a28

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.091 (s, 1H), 7.412 – 7.388 (m, 2H), 7.359 – 7.307 (m, 3H), 5.95 (q, J = 6.5 Hz, 1H), 5.360 (s, 1H), 5.337 (s, 1H), 1.398 (d, J = 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.25 (s), 148.61 (s), 138.99 (s), 128.39 (s), 127.88 (s), 126.80 (s), 113.71 (s), 71.18 (s), 19.90 (s).

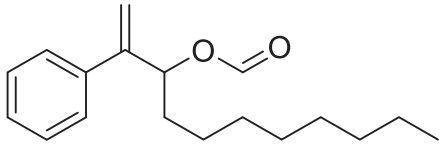
2-phenylhex-1-en-3-yl formate



a29

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.164 (s, 1H), 7.439 – 7.409 (m, 2H), 7.366 – 7.284 (m, 3H), 5.834 – 5.802 (m, 1H), 5.324 (s, 1H), 5.319 (d, J = 0.8 Hz, 1H), 1.683 – 1.622 (m, 2H), 1.407 – 1.256 (m, 2H), 0.863 (t, J = 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.35, 147.87, 139.21, 128.34, 127.81, 126.91, 114.26, 75.06, 35.84, 18.54, 13.57.

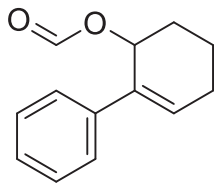
2-phenylundec-1-en-3-yl formate



a30

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.161 (s, 1H), 7.423 (dd, J = 8.0, 1.5 Hz, 2H), 7.362 – 7.298 (m, 3H), 5.80 (t, J = 6.4 Hz, 1H), 5.318 (d, J = 3.2, 2H), 1.685 – 1.631 (m, 2H), 1.375 – 1.208 (m, 12H), 0.861 (t, J = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.45 (s), 147.89 (s), 139.26 (s), 128.39 (s), 127.86 (s), 126.98 (s), 114.40 (s), 75.42 (s), 33.76 (s), 31.78 (s), 29.33 (s), 29.14 (s), 29.12 (s), 25.27 (s), 22.60 (s), 14.06 (s).

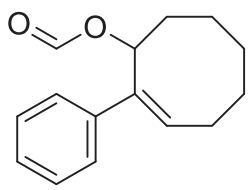
2,3,4,5-tetrahydro-[1,1'-biphenyl]-2-yl formate



a31

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.978 (s, 1H), 7.344 – 7.290 (m, 4H), 7.258 – 7.221 (m, 1H), 6.359 – 6.339 (m, 1H), 6.086 (s, 1H),, 2.375 – 2.294 (m, 1H), 2.245 – 2.167 (m, 1H), 2.087 –2.021 (m, 1H), 1.949 – 1.772 (m, 1H), 1.740 – 1.702 (m, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 160.77, 139.27, 134.91, 131.78, 128.41, 127.22, 125.57, 67.12, 28.94, 25.74, 17.30.

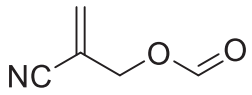
2-phenylcyclooct-2-en-1-yl formate



a32

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.916 (d, J = 0.8 Hz, 1H), 7.378 – 7.227 (m, 5H), 6.141 (dd, J = 11.1, 5.4 Hz, 1H), 5.921 – 5.877 (m, 1H), 2.410 – 2.358 (m, 2H), 2.130 – 1.972 (m, 2H), 1.873 – 1.722 (m, 3H), 1.627 – 1.544 (m, 1H), 1.503 – 1.431 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.34 (s), 139.85 (s), 139.21 (s), 131.50 (s), 127.87 (s), 127.78 (s), 126.92 (s), 72.49 (s), 35.26 (s), 29.75 (s), 26.98 (s), 26.95 (s), 23.71 (s).

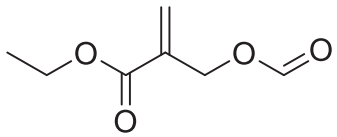
2-cyanoallyl formate



a33

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.126 (s, 1H), 6.160 (s, 1H), 6.108 (s, 1H), 4.780 (s, 2H).^{13}C NMR (101 MHz, $CDCl_3$) δ 159.57, 133.88, 117.64, 116.16, 62.27.

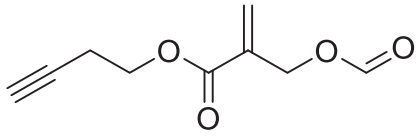
ethyl 2-((formyloxy)methyl)acrylate



a34

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.129 (s, 1H), 6.410 (s, 1H), 5.899 (s, 1H), 4.917 (s, 2H), 4.257 (q, J = 7.1 Hz, 2H), 1.322 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.95 (s), 160.30 (s), 134.76 (s), 127.90 (s), 61.87 (s), 61.07 (s), 14.08 (s).

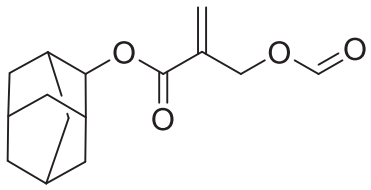
but-3-yn-1-yl 2-((formyloxy)methyl)acrylate



a35

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.120 (s, 1H), 6.448 (d, J = 0.4 Hz, 1H), 5.935 (s, 1H), 4.919 (s, 2H), 4.324 – 4.288 (m, 2H), 2.612 – 2.572 (m, 2H), 2.023 (t, J = 2.8 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 164.62, 160.21, 134.43, 128.62, 79.66, 70.04, 62.61, 61.74, 18.86.

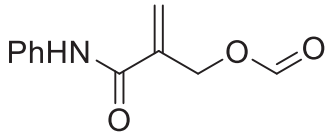
adamantan-2-yl 2-((formyloxy)methyl)acrylate



a36

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.130 (s, 1H), 6.443 (d, J = 0.8 Hz, 1H), 5.887 (d, J = 1.2 Hz, 1H), 5.050 (d, J = 3.2 Hz, 1H), 4.946 (s, 2H), 2.055 – 2.000 (m, 4H), 1.899 – 1.754 (m, 8H), 1.617 – 1.583 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.25, 160.33, 135.41, 127.70, 77.86, 62.03, 37.28, 36.25, 31.89, 31.86, 27.16, 26.90.

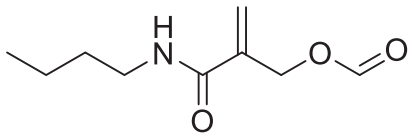
2-(phenylcarbamoyl)allyl formate



a37

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.155 – 8.079 (m, 2H), 7.564 (d, J = 8.4 Hz, 2H), 7.343 – 7.266 (m, 2H), 7.148 – 7.111 (m, 1H), 6.063 (d, J = 2 Hz, 1H), 5.762 (d, J = 4 Hz, 1H), 4.993 (d, J = 2.8 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.20, 160.52, 139.33, 137.37, 128.94, 124.66, 123.28, 120.18, 62.71.

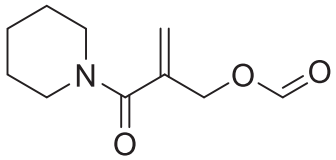
2-(butylcarbamoyl)allyl formate



a38

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.111 (s, 1H), 6.256 (s, 1H), 5.903 (s, 1H), 5.638 (s, 1H), 4.930 (s, 2H), 3.348 – 3.298 (m, 2H), 1.574 – 1.500 (m, 2H), 1.415 – 1.322 (m, 2H), 0.938 (t, J = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.95, 160.35, 139.08, 121.82, 62.85, 39.36, 31.42, 19.98, 13.62.

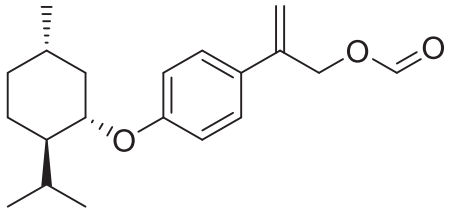
2-(piperidine-1-carbonyl)allyl formate



a39

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.099 (s, 1H), 5.490 (s, 1H), 5.292 (s, 1H), 4.877 (s, 2H), 3.589 –3.528 (m, 4H), 1.712 – 1.578 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.64, 160.20, 138.74, 117.33, 64.42, 48.06, 42.53, 26.50, 25.41, 24.42.

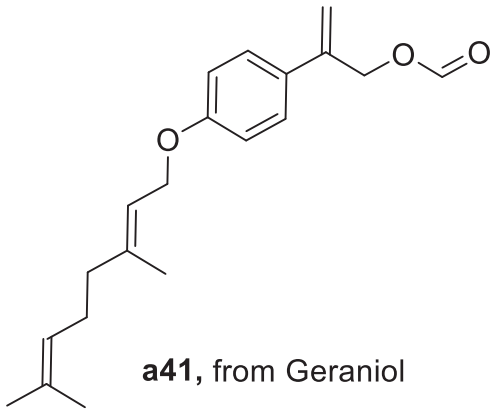
2-(4-(((1S,2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)phenyl)allyl formate



a40, from Menthol

Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.118 (s, 1H), 7.352 (d, J = 5.6 Hz, 2H), 6.877 (d, J = 5.6 Hz, 2H), 5.497 (s, 1H), 5.292 (s, 1H), 5.053 (s, 2H), 4.639 (d, J = 1.2 Hz, 1H), 2.105 – 2.078 (m, 1H), 1.786 – 1.732 (m, 2H), 1.690 – 1.646 (m, 2H), 1.588 – 1.556 (m, 1H), 1.073 – 1.033 (m, 1H), 1.014 – 0.944 (m, 2H), 0.924 (d, J = 4.4 Hz, 3H), 0.855 (d, J = 4.4 Hz, 3H), 0.811 (d, J = 4.4 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.73, 158.34, 141.18, 129.35, 127.08, 115.40, 114.09, 73.15, 65.30, 47.69, 37.54, 34.92, 29.24, 26.14, 24.79, 22.26, 21.03, 20.81.

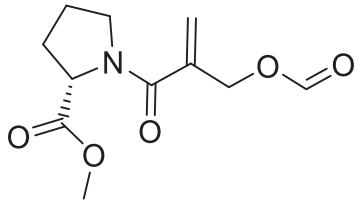
(E)-2-(4-((3,7-dimethylocta-2,6-dien-1-yl)oxy)phenyl)allyl formate



a41, from Geraniol

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.110 (s, 1H), 7.381 – 7.344 (m, 2H), 6.914 – 6.880 (m, 2H), 5.497 – 5.467 (m, 2H), 5.306 (d, J = 0.8 Hz, 1H), 5.106 – 5.052 (m, 3H), 4.549 (d, J = 6 Hz, 2H), 2.138 – 2.086 (m, 4H), 1.738(s, 3H), 1.678 (s, 3H), 1.606 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.72, 158.91, 141.43, 141.16, 131.84, 129.93, 127.05, 123.73, 119.23, 114.63, 114.38, 65.30, 64.84, 39.52, 26.24, 25.68, 17.70, 16.66.

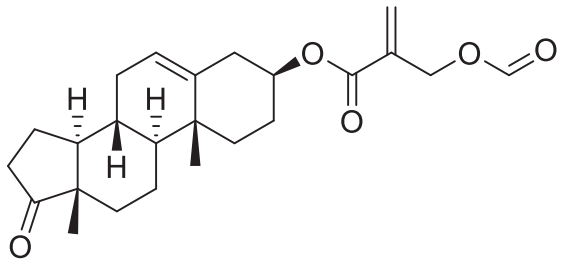
(E)-2-(4-((3,7-dimethylocta-2,6-dien-1-yl)oxy)phenyl)allyl formate



a42, Methyl L-prolinate

Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.103 (s, 1H), 5.663 (s, 1H), 5.579 (s, 1H), 4.957-4.802 (m, 2H), 4.568-4.535 (m, 1H), 3.747 (s, 3H), 3.703 -3.625 (m, 2H), 2.321 – 2.254 (m, 1H), 2.079 – 1.890 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.37, 167.30, 160.35, 139.14, 119.77, 63.85, 58.69, 52.2, 49.32, 29.23, 25.13.

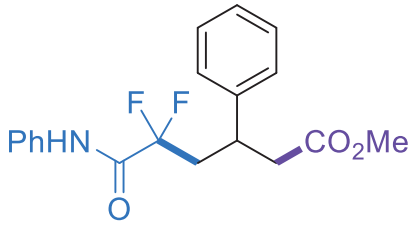
(3S,8R,9S,10R,13S,14S)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl 2-((formyloxy)methyl)acrylate



a43, from Dehydroepiandrosterone

White solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.126 (s, 1H), 6.394 (s, 1H), 5.881 (s, 1H), 5.430 (d, J = 4.8 Hz, 1H), 4.911 (s, 2H), 4.765 – 4.686 (m, 1H), 2.503 – 2.344 (m, 3H), 2.144 – 2.051 (m, 2H), 1.993 – 1.841 (m, 4H), 1.701 – 1.657 (m, 4H), 1.616 – 1.446 (m, 2H), 1.335 – 1.270 (m, 2H), 1.225 – 1.146 (m, 1H), 1.070 – 1.015 (m, 4H), 0.894 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.85, 164.28, 160.23, 139.59, 135.05, 127.67, 122.04, 74.51, 61.85, 51.60, 50.03, 47.42, 37.90, 36.78, 36.65, 35.73, 31.37, 31.31, 30.69, 27.56, 21.78, 20.24, 19.26, 13.45.

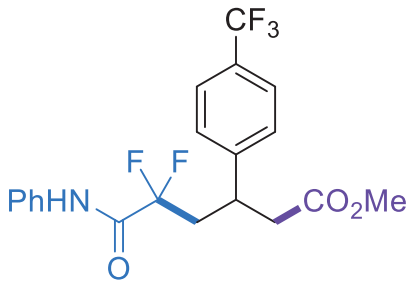
methyl 5,5-difluoro-6-oxo-3-phenyl-6-(phenylamino)hexanoate



c1

White solid; mp 81-84 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.804 (br s, 1H), 7.438 (d, *J* = 7.6 Hz, 2H), 7.339 – 7.300 (m, 2H), 7.266 – 7.127 (m, 6H), 3.567 (s, 3H), 3.538 – 3.485 (m, 1H), 2.789 – 2.567 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.74, 161.54 (t, *J* = 27 Hz), 141.89, 135.83, 129.01, 128.59, 127.38, 127.14, 125.46, 120.16, 117.52 (t, *J* = 256 Hz), 51.63, 41.49, 39.26 (t, *J* = 22 Hz), 36.10 (t, *J* = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.447 (d, *J* = 256 Hz, 1F), -105.126 (d, *J* = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{19}H_{19}F_2NO_3$ $[M+H]^+$ 348.1406, found 348.1401.

methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(4-(trifluoromethyl)phenyl)hexanoate

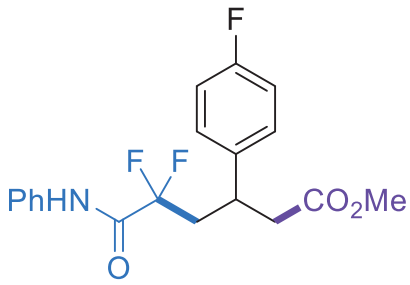


c2

White solid; mp 103-106 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.863 (br s, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.397 – 7.337 (m, 2H), 7.329 – 7.298 (m, 4H), 7.191 – 7.149 (m, 1H), 3.629 – 3.577 (m, 4H), 2.813 – 2.576 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.33, 161.24 (t, *J* = 28 Hz), 145.86, 135.57, 129.37 (q, *J* = 32 Hz),

129.09, 127.90, 125.64, 125.53 (q, *J* = 3 Hz), 123.76 (q, *J* = 272 Hz),120.06, 119.79, 117.26 (t, *J* = 257 Hz), 51.79, 41.08, 38.96 (t, *J* = 23 Hz), 35.87 (t, *J* = 4 Hz).^{19}F NMR (376 MHz, $CDCl_3$) *δ* -62.557 (s, 3F), -101.287 (d, J = 257 Hz, 1F), -105.559 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{18}F_5NO_3$ $[M+H]^+$ 416.1280, found 416.1266.

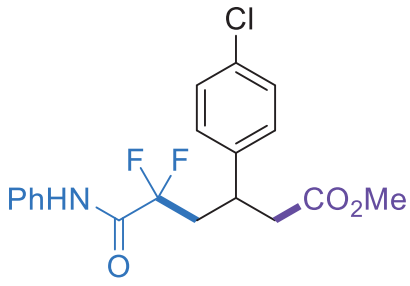
methyl 5,5-difluoro-3-(4-fluorophenyl)-6-oxo-6-(phenylamino)hexanoate



c3

White solid; mp 96-99 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.796 (br s, 1H), 7.435 – 7.413 (m, 2H), 7.356 – 7.316(m, 2H), 7.195 – 7.160 (m, 3H), 6.949 – 6.906 (m, 2H), 3.571 (s, 3H), 3.545 – 3.487(m, 1H), 2.777 – 2.545 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 171.57, 161.76 (d, *J* = 246 Hz), 161.41 (t, *J* = 28 Hz), 137.47 (d, *J* = 4 Hz), 135.71, 129.10, 128.98 (d, *J* = 8 Hz), 125.59, 120.05, 117.41 (t, *J* = 256 Hz), 115.45 (d, *J* = 21 Hz), 51.71, 41.53, 39.29 (t, *J* = 22 Hz), 35.42 (t, *J* = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -101.361 (d, *J* = 257 Hz, 1F), -105.455 (d, *J* = 257 Hz, 1F), -115.337 (s, 1F). ESI-HRMS: Calcd for $C_{19}H_{18}F_3NO_3$ $[M+H]^+$ 366.1312, found 366.1303.

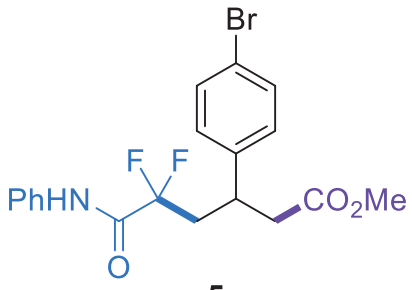
methyl 3-(4-chlorophenyl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c4

White solid; mp 90-94 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.816 (br s, 1H), 7.408 (d, *J* = 7.6 Hz, 2H), 7.359 – 7.319(m, 2H), 7.220 – 7.135 (m, 5H), 3.574 (s, 3H), 3.532 – 3.474 (m, 1H), 2.773 – 2.542 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 171.46, 161.35 (t, *J* = 28 Hz), 140.20, 135.64, 132.96, 129.11, 128.84, 128.73, 125.59, 120.08, 117.35 (t, *J* = 257 Hz), 51.74, 41.29, 39.11 (t, *J* = 22 Hz), 35.52 (t, *J* = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -101.263 (d, *J* = 257 Hz, 1F), -105.474 (d, *J* = 257.0 Hz, 1F). ESI-HRMS: Calcd for $C_{19}H_{18}ClF_2NO_3$ $[M+H]^+$ 382.1016, found 382.1008.

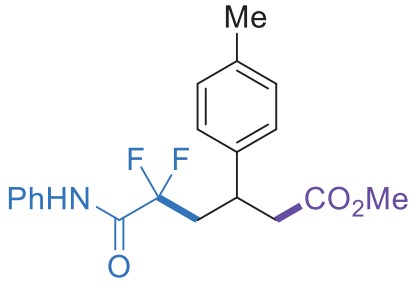
methyl 3-(4-bromophenyl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c5

White solid; mp 100-102 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.849 (br s, 1H), 7.409 – 7.316(m, 6H), 7.192 – 7.155 (m, 1H), 7.085(d, J = 9 Hz, 2H), 3.571 (s, 3H), 3.531 – 3.457 (m, 1H), 2.765 – 2.532 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.43, 161.33 (t, J = 28 Hz), 140.70, 135.61, 131.65, 129.19, 129.09, 125.57, 121.07, 120.10, 117.31 (t, J = 256 Hz), 51.74, 41.19, 39.03 (t, J = 23 Hz), 35.56 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.172 (d, J = 257 Hz, 1F), -105.548 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{19}H_{18}BrF_2NO_3$ $[M+H]^+$ 426.0511, found 426.0498.

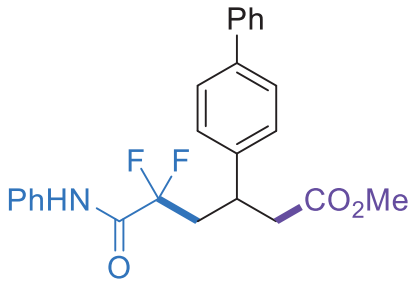
methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(p-tolyl)hexanoate



c6

White solid; mp 66-69 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.750 (br s, 1H), 7.376(d, J = 8 Hz, 2H), 7.325 – 7.285(m, 2H), 7.161 – 7.124(m, 1H), 7.091 – 7.003(m, 2H), 3.570 (s, 3H), 3.507 – 3.433 (m, 1H), 2.754 – 2.528 (m, 5H), 2.161 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.81, 161.53 (t, J = 28 Hz), 138.38, 136.86, 135.83, 129.23, 128.92, 127.29, 125.31, 120.00, 117.47 (t, J = 255 Hz), 51.63, 41.49, 39.26 (t, J = 23 Hz), 35.76 (t, J = 4 Hz), 20.85. ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.208 (d, J = 256 Hz, 1F), -106.331 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_3$ $[M+H]^+$ 362.1562, found 362.1552.

methyl 3-([1,1'-biphenyl]-4-yl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate

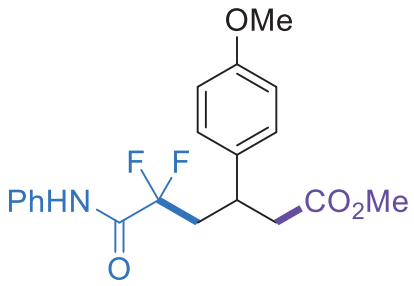


c7

White solid; mp 71-73 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.802 (br s, 1H), 7.458 – 7.359 (m, 8H), 7.328 – 7.301 (m, 1H), 7.281 – 7.236 (m, 4H),7.128 – 7.091 (m, 1H), 3.588 – 3.528 (m, 4H), 2.810 – 2.581 (m, 4H). ^{13}C NMR (101 MHz,

$CDCl_3$) δ 171.74, 161.48 (t, J = 22 Hz), 140.59, 140.46, 140.07, 135.75, 129.02, 128.59, 127.89, 127.24, 127.18, 126.95, 125.40, 120.07, 117.49 (t, J = 258 Hz), 51.71, 41.42, 39.20 (t, J = 22 Hz), 35.81 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.209 (d, J = 256 Hz, 1F), -106.107 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{25}H_{23}F_2NO_3$ $[M+H]^+$ 424.1719, found 424.1708.

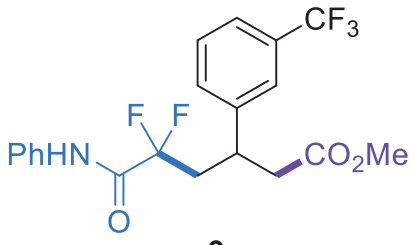
methyl 5,5-difluoro-3-(4-methoxyphenyl)-6-oxo-6-(phenylamino)hexanoate



c8

White solid; mp 75-78 °C; R_f = 0.3 (7:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.765 (br s, 1H), 7.386 (d, J = 8 Hz, 2H), 7.324 – 7.285(m, 2H), 7.167 – 7.097 (m, 3H), 6.729 (d, J = 9 Hz, 2H), 3.625 (s, 3H), 3.567 (s, 3H), 3.498 – 3.423 (m, 1H), 2.744 – 2.517 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.80, 161.53 (t, J = 28 Hz), 158.45, 135.84, 133.29, 128.91, 128.48, 125.31, 120.00, 117.46 (t, J = 255 Hz), 113.85, 54.97, 51.63, 41.61, 39.33 (t, J = 22 Hz), 35.41 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.081 (d, J = 256 Hz, 1F), -106.529 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_4$ $[M+H]^+$ 378.1511, found 378.1504.

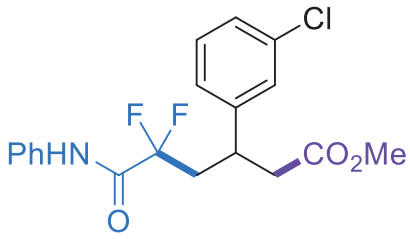
methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(3-(trifluoromethyl)phenyl)hexanoate



c9

White solid; mp 82-85 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.829 (br s, 1H), 7.469 (s, 1H), 7.439 – 7.396 (m, 5H), 7.378 – 7.306 (m, 2H), 7.190 – 7.154 (m, 1H), 3.653 – 3.596 (m, 1H), 3.578 (s, 3H), 2.828 – 2.597(m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.32, 161.28 (t, J = 28 Hz), 142.90, 135.65, 130.87, 130.86 (q, J = 32 Hz), 129.11, 129.09, 125.61, 124.30 (q, J = 4 Hz), 124.09 (q, J = 3 Hz), 123.90 (q, J = 274 Hz), 120.01 (s), 117.29 (t, J = 255 Hz), 51.78, 41.19, 38.95 (t, J = 23 Hz), 35.90 (t, J = 4 Hz). ^{9}F NMR (376 MHz, $CDCl_3$) δ -62.571(s, 3F), -101.725 (d, J = 257 Hz, 1F), -105.199 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{18}F_5NO_3$ $[M+H]^+$ 416.1280, found 416.1266.

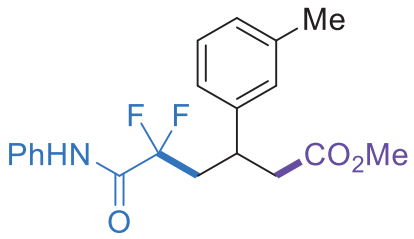
methyl 3-(3-chlorophenyl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c10

White solid; mp 79-82 ºC; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.855 (br s, 1H), 7.451 (d, J = 8 Hz, 2H), 7.355 – 7.316 (m, 2H), 7.207 – 7.162 (m, 3H), 7.125 – 7.094 (m, 2H), 3.587 (s, 3H), 3.546 – 3.473 (m, 1H), 2.784 – 2.551 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.42, 161.35 (t, J = 28 Hz), 143.94, 135.70, 134.31, 129.89, 129.06, 127.67, 127.37, 125.62, 125.57, 120.07, 117.30 (t, J = 256 Hz), 51.78, 41.15, 39.04 (t, J = 22 Hz), 35.76 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.717 (d, J = 256 Hz, 1F), -105.249 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{19}H_{18}ClF_2NO_3$ $[M+H]^+$ 382.1005, found 382.1005.

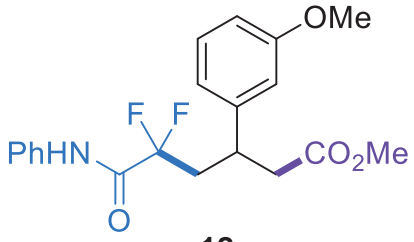
methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(m-tolyl)hexanoate



c11

White solid; mp 79-81 ºC; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.823 (br s, 1H), 7.417 (d, J = 8 Hz, 2H), 7.335 – 7.296 (m, 2H), 7.178 – 7.110 (m, 2H), 6.999 (d, J = 6 Hz, 2H), 6.932 (d, J = 8 Hz, 1H), 3.578 (s, 3H), 3.509 – 3.435 (m, 1H), 2.770 – 2.543 (m, 4H), 2.228 (s, 3H). ^{13}C NMR (101 MHz, DMSO) δ 171.84, 161.54 (t, J = 28 Hz), 141.72, 138.16, 135.85, 128.96, 128.43, 128.13, 127.91, 125.40, 124.33, 120.00, 117.49 (t, J = 256 Hz), 51.65, 41.48, 39.26 (t, J = 24 Hz), 35.99 (t, J = 4 Hz), 21.30. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.082 (d, J = 255 Hz, 1F), -105.633 (d, J = 255 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_3$ $[M+H]^+$ 362.1562, found 362.1553.

methyl 5,5-difluoro-3-(3-methoxyphenyl)-6-oxo-6-(phenylamino)hexanoate

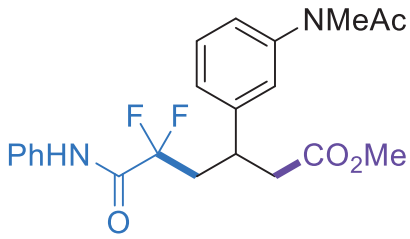


c12

Pale yellow oil; R_f = 0.3 (7:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.811 (br s, 1H), 7.429 (d, J = 28 Hz, 2H), 7.340 – 7.300 (m, 2H), 7.180 – 7.141 (m, 2H), 6.797(d, J = 28 Hz,1H), 6.745 – 6.745 (m, 1H), 6.665 – 6.640(m, 1H), 3.698 (s, 3H), 3.588 (s, 3H), 3.526 – 3.453 (m, 1H), 2.772 – 2.548 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.74, 161.52 (t, J = 28 Hz), 159.55, 143.37, 135.82, 129.60, 128.98, 125.41, 120.03, 119.61, 117.43

(t, *J* = 255 Hz), 113.48, 112.11, 55.02, 51.70, 41.36, 39.18 (t, *J* = 23 Hz), 36.10 (t, *J* = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -101.011 (d, *J* = 256 Hz, 1F), -105.705 (d, *J* = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_4$ $[M+H]^+$ 378.1511, found 378.1501.

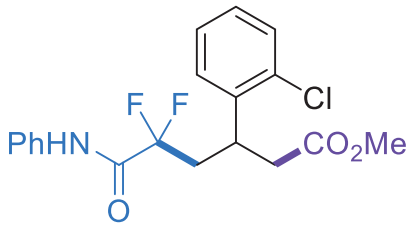
methyl 5,5-difluoro-3-(3-(N-methylacetamido)phenyl)-6-oxo-6-(phenylamino)hexanoate



c13

Colorless oil; R_f = 0.3 (1:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 8.136 (br s, 1H), 7.461 (d, *J* = 8 Hz, 2H), 7.346 – 7.277 (m, 3H), 7.218 – 7.151 (m, 2H), 7.066 (s, 1H), 6.989 (d, *J* = 8 Hz, 1H), 3.610 – 3.537 (m, 4H), 3.159 (s, 3H), 2.826 – 2.562 (m, 4H), 1.796 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 171.37, 170.52, 161.32 (t, *J* = 28 Hz), 144.60, 143.76, 135.78, 129.85, 129.02, 126.77, 126.31, 125.70, 125.54, 120.10, 117.29 (t, *J* = 256 Hz), 51.71, 41.28, 39.04 (t, *J* = 23 Hz), 36.94, 35.82 (t, *J* = 4 Hz), 22.26. ^{9}F NMR (376 MHz, $CDCl_3$) *δ* -101.324 (d, *J* = 257 Hz, 1F), -105.486 (d, *J* = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{22}H_{24}F_2N_2O_4$ $[M+H]^+$ 419.1777, found 419.1762.

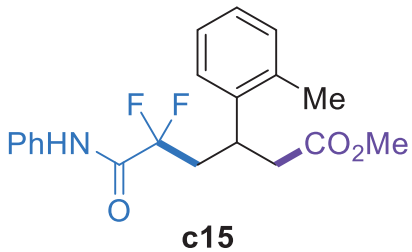
methyl 3-(2-chlorophenyl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c14

White solid; mp 85-87 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.939 (br s, 1H), 7.442 – 7.421 (m, 2H), 7.332 – 7.136(m, 7H), 7.080 – 7.038(m, 1H), 4.137 – 4.067 (m, 1H), 3.594 (s, 3H), 2.820 – 2.603 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 171.49, 161.33 (t, *J* = 28 Hz), 139.05, 135.84, 133.42, 129.89, 128.99, 128.46, 128.20, 127.15, 125.44, 120.10, 117.41 (t, *J* = 257 Hz), 51.72, 40.09, 38.25 (t, *J* = 23 Hz), 32.13 (t, *J* = 5 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -101.958 (d, *J* = 256 Hz, 1F), -105.307 (d, *J* = 256 Hz, 1F). ESI-HRMS: Calcd for C19H18ClF2NO3 $[M+H]^+$ 382.1016, found 382.1010.

methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(o-tolyl)hexanoate

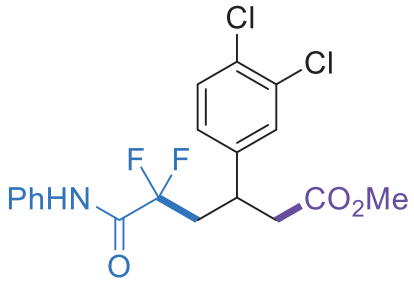


c15

White solid; mp 95-98 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz,

$CDCl_3$) δ 7.813 (br s, 1H), 7.439 (d, J = 8 Hz, 2H,), 7.352 – 7.313 (m, 2H), 7.188 – 7.123 (m, 3H), 7.092 – 7.024 (m, 2H), 3.905 – 3.833(m, 1H), 3.576 (s, 3H), 2.807 – 2.545 (m, 4H), 2.374 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.99, 161.59 (t, J = 28 Hz), 140.49, 135.87, 135.57, 130.61, 129.05, 126.73, 126.37, 125.96, 125.49, 120.16, 117.63 (d, J = 257 Hz), 51.63, 41.06, 39.26 (t, J = 23 Hz), 30.55 (t, J = 4 Hz), 19.46. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.645 (d, J = 256 Hz, 1F), -105.709 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_3$ $[M+H]^+$ 362.1562, found 362.1553.

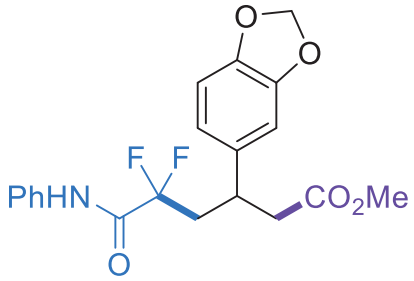
methyl 3-(3,4-dichlorophenyl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c16

White solid; mp 91-95 °C; R_f = 0.2 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.868 (br s, 1H), 7.443 – 7.419(m, 2H), 7.361 – 7.262 (m, 4H), 7.201 – 7.161(m, 1H), 7.077 – 7.051(m, 1H), 3.592 (s, 3H), 3.536 – 3.462(m, 1H), 2.771 – 2.534 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.20, 161.22 (t, J = 28 Hz), 142.04, 135.59, 132.51, 131.25, 130.53, 129.58, 129.13, 126.89, 125.65, 120.01, 117.18 (t, J = 256 Hz), 51.83, 40.99, 38.94 (t, J = 23 Hz), 35.30 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.512 (d, J = 257 Hz, 1F), -105.684 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{19}H_{17}Cl_2F_2NO_3$ $[M+H]^+$ 416.0626, found 416.0615.

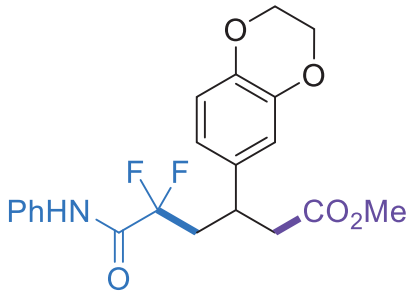
methyl 3-(benzo[d][1,3]dioxol-5-yl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c17

White solid; mp 96-98 °C; R_f = 0.3 (7:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.729 (br s, 1H), 7.446 – 7.424(m, 2H), 7.345 – 7.261 (m, 2H), 7.180 – 7.143 (m, 1H), 6.674 – 6.625 (m, 3H), 5.781 – 5.736 (m, 1H), 3.593 (s, 3H), 3.477 – 3.403 (m, 1H), 2.727 – 2.504 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.67, 161.52 (t, J = 28 Hz), 147.70, 146.58, 135.89, 135.20, 129.01, 125.38, 120.80, 119.91, 117.45 (t, J = 258 Hz), 108.24, 107.70, 100.94, 51.69, 41.59, 39.43 (t, J = 23 Hz), 36.02 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.049 (d, J = 256 Hz, 1F), -106.804 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{19}F_2NO_5$ $[M+H]^+$ 392.1304, found 392.1293.

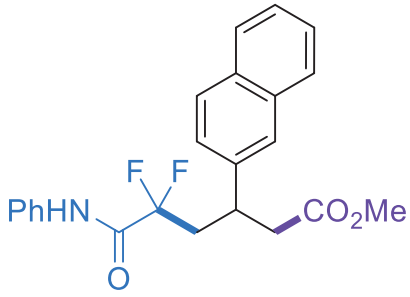
methyl 3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c18

Pale yellow oil; R_f = 0.4 (5:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.718 (br s, 1H), 7.425 (d, J = 8 Hz, 2H), 7.342 – 7.303 (m, 2H), 7.173 – 7.136 (m, 1H), 6.723 – 6.660 (m, 3H), 4.063 – 4.028 (m, 4H), 3.599 (s, 3H), 3.435 – 3.361 (m, 1H), 2.717 – 2.492 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.77, 161.54 (t, J = 28 Hz), 143.30, 142.52, 135.93, 134.57, 128.98, 125.29, 120.45, 119.96, 117.47 (t, J = 258 Hz), 117.27, 116.20, 64.10, 64.04, 51.68, 41.49, 39.33 (t, J = 23 Hz), 35.58 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -99.565 (d, J = 256 Hz, 1F), -107.120 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{21}H_{21}F_2NO_5$ $[M+H]^+$ 406.1461, found 406.1448.

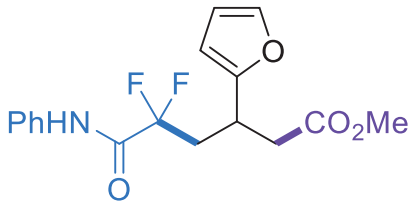
methyl 5,5-difluoro-3-(naphthalen-2-yl)-6-oxo-6-(phenylamino)hexanoate



c19

Colorless oil; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.752 – 7.704 (m, 3H), 7.650 (s, 1H), 7.443 – 7.377 (m, 2H), 7.352 – 7.326 (m, 1H), 7.258 – 7.192 (m, 4H), 7.114 – 7.072 (m, 1H), 3.733 – 3.660 (m, 1H), 3.550 (s, 3H), 2.865 – 2.605 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.71, 161.47 (t, J = 28 Hz), 139.05, 135.58, 133.26, 132.58, 128.92, 128.47, 127.60, 127.58, 126.42, 126.13, 125.78, 125.35, 125.16, 120.04, 117.51 (t, J = 257 Hz), 51.72, 41.42, 39.21 (t, J = 23 Hz), 36.30 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.040 (d, J = 256 Hz, 1F), -105.279 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{23}H_{21}F_2NO_3$ $[M+H]^+$ 398.1562, found 398.1548.

methyl 5,5-difluoro-3-(furan-2-yl)-6-oxo-6-(phenylamino)hexanoate

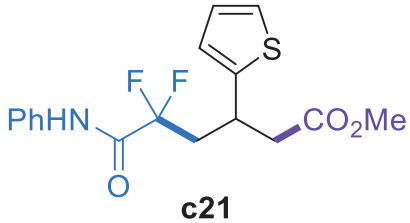


c20

Pale yellow solid; mp 78-80 ^{o}C; R_f = 0.36(10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400

MHz, $CDCl_3$) δ 7.989 (br s, 1H), 7.521 – 7.512 (d, J = 8 Hz, 2H), 7.368 – 7.329(m, 2H), 7.286 – 7.282 (m, 1H), 7.198 – 7.161(m, 1H), 6.210 (dd, J = 3, 2 Hz, 1H), 6.07 (d, J = 3 Hz, 1H), 3.695 – 3.623 (m, 4H), 2.805 – 2.682 (m, 3H), 2.608 – 2.473 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.60, 161.31 (t, J = 28 Hz), 154.29, 141.74, 135.89, 129.08, 125.48, 120.15, 117.33 (t, J = 256 Hz), 110.12, 106.02, 51.81, 38.77, 37.09 (t, J = 23 Hz), 29.61 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.883 (d, J = 257 Hz, 1F), -105.682 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{17}H_{17}F_2NO_4$ $[M+H]^+$ 338.1198, found 338.1193.

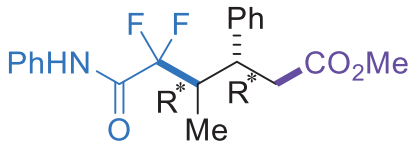
methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(thiophen-2-yl)hexanoate



c21

White solid; mp 79-82 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.920 (br s, 1H), 7.474 (d, J = 8 Hz, 2H), 7.358 – 7.318 (m, 2H), 7.194 – 7.157 (m, 1H), 7.109 (d, J = 5 Hz, 1H), 6.877 – 6.837 (m, 2H), 3.912 – 3.841 (m, 1H), 3.620 (s, 3H), 2.838 – 2.616 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.40, 161.41 (t, J = 28 Hz), 145.28, 135.80, 129.06, 126.69, 125.53, 124.70, 123.94, 120.19, 117.25 (t, J = 256 Hz), 51.79, 42.28, 40.21 (t, J = 23 Hz), 31.44 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.973 (d, J = 256 Hz, 1F), -105.409 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{17}H_{17}F_2NO_3S$ $[M+H]^+$ 354.0970., found 354.0977.

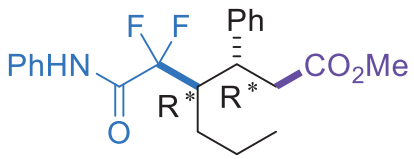
methyl (3R,4R)-5,5-difluoro-4-methyl-6-oxo-3-phenyl-6-(phenylamino)hexanoate



c22

White solid; mp 91-93 °C; R_f = 0.15 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.984 (br s, 1H), 7.513 (d, J = 8 Hz, 2H), 7.345 (t, J =8 Hz, 2H), 7.273 – 7.126 (m, 6H), 3.675 – 3.627 (m, 1H), 3.526 (s, 3H), 2.904 – 2.765 (m, 3H), 1.096 (d, J = 7 Hz, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 172.46 (s), 161.82 (t, J = 28.5 Hz), 141.64 (s), 135.95 (s), 129.07 (s), 128.44 (s), 127.86 (s), 126.98 (s), 125.51 (s), 120.26 (s), 119.32 (t, J = 258.3 Hz), 51.66 (s), 42.02 (t, J = 20.8 Hz), 39.92 (t, J = 3 Hz), 35.06 (s), 8.40 (t, J = 4.7 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -107.67 (d, J = 254.7 Hz, 1F), -111.54 (d, J = 254.7 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_3$ $[M+H]^+$ 362.1562, found 362.1551.

methyl (3R,4R)-4-(1,1-difluoro-2-oxo-2-(phenylamino)ethyl)-3-phenylheptanoate

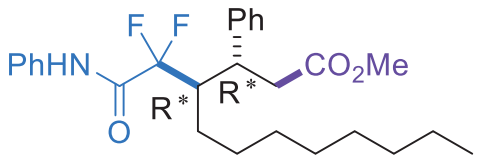


c23

Colorless oil; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ

7.869 (br s, 1H), 7.493 – 7.469 (m, 2H), 7.356 – 7.316 (m, 2H), 7.242 – 7.237 (d, *J* = 4 Hz, 4H), 7.186 – 7.149 (m, 1H), 7.131 – 7.088 (m, 1H), 3.658 – 3.608 (m, 1H), 3.534 (s, 3H), 2.925 – 2.761 (m, 3H), 1.619 – 1.570 (m, 1H), 1.528 – 1.480 (m, 1H), 1.433 – 1.343 (m, 1H), 1.285 – 1.242 (m, 1H), 0.787 (t, *J* = 6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 172.54, 162.06 (t, *J* = 28 Hz), 141.11, 136.00, 129.04, 128.32, 128.19, 127.00, 125.44, 120.20, 119.88 (t, *J* = 261 Hz), 51.67, 46.22 (t, *J* = 20 Hz), 39.71, 35.84, 26.89 (t, *J* = 4 Hz), 21.28, 14.05. ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -104.947 (d, *J* = 257 Hz, 1F), -109.484 (d, *J* = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{22}H_{25}F_2NO_3$ $[M+H]^+$ 390.1875, found 390.1865.

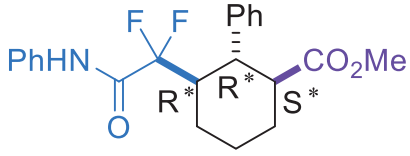
methyl (3R,4R)-4-(1,1-difluoro-2-oxo-2-(phenylamino)ethyl)-3-phenyldodecanoate



c24

White oil; R_f = 0.4 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.953 (br s, 1H), 7.477 (d, *J* = 8 Hz, 2H), 7.32 (t, *J* = 8 Hz, 2H), 7.246 – 7.202 (m, 4H), 7.173 – 7.082 (m, 2H), 3.665 – 3.616 (m, 1H), 3.520 (s, 3H), 2.920 – 2.730 (m, 3H), 1.651 – 1.468 (m, 2H), 1.346 – 1.156 (m, 12H), 0.85 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 172.53 (s), 162.08 (t, *J* = 28.4 Hz), 141.09 (s), 136.00 (s), 128.97 (s), 128.28 (s), 128.14 (s), 126.95 (s), 125.39 (s), 120.22 (s), 119.83 (t, *J* = 260 Hz), 51.62 (s), 46.40 (t, *J* = 19.9 Hz), 39.65 (d, *J* = 2.6 Hz), 35.74 (s), 31.73 (s), 29.48 (s), 29.07 (s), 27.94 (s), 24.58 (d, *J* = 3.3 Hz), 22.55 (s), 14.02 (s). ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -105.21 (d, *J* = 256.8 Hz, 1F), -109.30 (d, *J* = 256.8 Hz, 1F). ESI-HRMS: Calcd for $C_{27}H_{35}F_2NO_3$ $[M+H]^+$ 460.2658, found 460.2642.

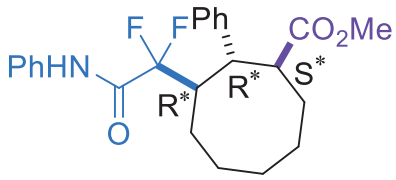
2,2-difluoro-2-((1R,2R,3S)-3-((methylperoxy)-l2-methyl)-2-phenylcyclohexyl)-N-phenylacetamide



c25

White solid; mp 75-77 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.313 (br s, 1H), 7.267 – 7.209 (m, 4H), 7.169 (d, *J* = 7 Hz, 2H), 7.125 – 7.087 (m, 3H), 6.928 – 6.892 (m, 1H), 3.299 (s, 3H), 2.975 – 2.822 (m, 2H), 2.677 – 2.612 (m, 1H), 2.213 – 2.193 (d, *J* = 8 Hz, 1H), 2.037 – 2.002 (m, 2H), 1.678 – 1.486 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) *δ* 174.47, 161.80 (t, *J* = 28 Hz), 139.49, 135.80, 128.73, 128.70, 128.10, 127.30, 125.14, 118.00, 117.94 (t, *J* = 257 Hz), 51.57, 51.29, 46.44 (t, *J* = 3 Hz), 44.55 (t, *J* = 21 Hz), 29.63, 24.73 (dd, *J* = 8, 2 Hz), 24.36. ^{19}F NMR (376 MHz, $CDCl_3$) *δ* -103.373 (d, *J* = 257 Hz, 1F), -113.616 (d, *J* = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{22}H_{23}F_2NO_3$ $[M+H]^+$ 388.1719, found 388.1706.

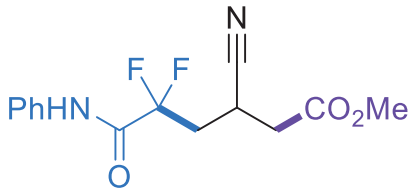
2,2-difluoro-2-((1R,2R,3S)-3-((methylperoxy)-l2-methyl)-2-phenylcyclooctyl)-N-phenylacetamide



c26

White oil; R_f = 0.4 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.668 (s, 1H), 7.310 – 7.255 (m, 4H), 7.184 – 7.054 (m, 6H), 3.594 (dd, J = 12.1, 3.0 Hz, 1H), 3.541 (s, 3H), 3.308 – 3.198 (m, 2H), 2.125 (d, J = 15.6 Hz, 1H), 1.985 – 1.850 (m, 3H), 1.807 – 1.730 (m, 1H), 1.664 – 1.493 (m, 4H) 1.425 – 1.325 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.94 (s), 161.70 (t, J = 28.6 Hz), 138.44 (s), 135.84 (s), 128.87 (s), 128.74 (s), 127.95 (s), 126.97 (s), 125.27 (s), 119.97, 119.37 (t, J = 261 Hz), 51.54 (s), 46.18 (t, J = 2 Hz), 44.85 (t, J = 20 Hz), 44.53 (s), 30.18 (s), 26.08 (s), 25.95 (t, J = 4 Hz), 25.58 (s), 24.81 (s). ^{19}F NMR (376 MHz, $CDCl_3$) δ -106.645 (d, J = 253.5 Hz, 1F), -108.276 (d, J = 253.6 Hz, 1F). ESI-HRMS: Calcd for $C_{24}H_{27}F_2NO_3$ $[M+H]^+$ 416.2032, found 416.2018.

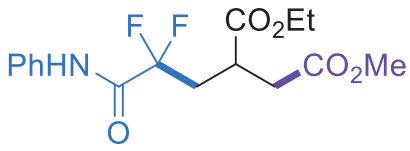
methyl 3-cyano-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c27

White solid; mp 88-91 °C; R_f = 0.3 (4:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.081 (br s, 1H), 7.569 (d, J = 7.6 Hz, 2H), 7.406 – 7.366 (m, 2H), 7.240 – 7.203 (m, 1H), 3.766 (s, 3H), 3.461 – 3.392 (m, 1H), 2.870 – 2.564 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.37, 160.53 (t, J = 28 Hz), 135.54, 129.29, 125.99, 120.41, 119.48, 116.16 (t, J = 258 Hz), 52.49, 36.30, 35.29 (t, J = 23 Hz), 21.27 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.905 (d, J = 262 Hz, 1F), -105.074 (d, J = 262 Hz, 1F). ESI-HRMS: Calcd for $C_{14}H_{14}F_2N_2O_3$ $[M+H]^+$ 297.1045, found 297.1037.

1-ethyl 4-methyl 2-(2,2-difluoro-3-oxo-3-(phenylamino)propyl)succinate

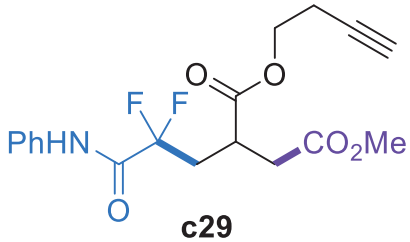


c28

Colorless oil; R_f = 0.4 (5:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.030 (br s, 1H), 7.580 (d, J = 8 Hz, 2H), 7.405 – 7.365 (m, 2H), 7.229 – 7.192 (m, 1H), 4.209 – 4.150 (m, 2H), 3.694 (s, 3H), 3.216 – 3.149 (m, 1H), 2.863 – 2.649 (m, 3H), 2.538 – 2.395 (m, 1H), 1.259 (t, J = 7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.01, 171.52, 161.27 (t, J = 28 Hz), 135.87, 129.19, 125.66, 120.22, 117.18 (t, J = 257 Hz), 61.38, 51.92, 35.83, 35.47 (t, J = 3 Hz), 35.02 (t, J = 23 Hz), 13.98. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.717 (d, J = 257 Hz, 1F), -104.494 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{16}H_{19}F_2NO_5$ $[M+H]^+$ 344.1304,

found 344.1295.

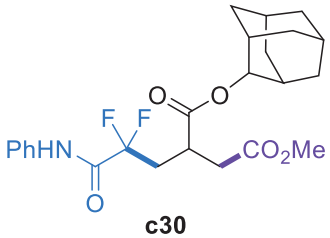
1-(but-3-yn-1-yl) 4-methyl 2-(2,2-difluoro-3-oxo-3-(phenylamino)propyl)succinate



c29

White solid; mp 92-96 °C; R_f = 0.2 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.079 (br s, 1H), 7.579 (d, J = 8 Hz, 2H), 7.399 – 7.360 (m, 2H), 7.225 – 7.189(m, 1H), 4.270 – 4.203 (m, 2H), 3.689 (s, 3H), 3.226 – 3.161 (m, 1H), 2.877 – 2.814 (m, 1H), 2.767 – 2.655 (m, 2H), 2.558 – 2.493 (m, 2H), 2.466 –2.414 (m, 1H), 1.996 (t, J = 2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.84, 171.38, 161.25 (t, J = 28 Hz), 135.84, 129.24, 125.75, 120.34, 117.17 (t, J = 257 Hz), 80.00, 70.04, 62.91, 51.98, 35.88, 35.49 (t, J = 4 Hz), 35.16 (t, J = 23 Hz), 18.78. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.466 (d, J = 257 Hz, 1F), -104.519 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{18}H_{19}F_2NO_5$ $[M+H]^+$ 368.1304, found 368.1297.

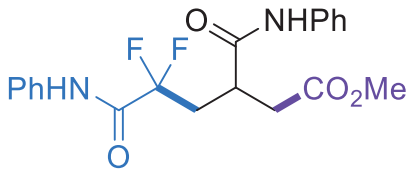
1-(adamantan-2-yl) 4-methyl 2-(2,2-difluoro-3-oxo-3-(phenylamino)propyl)succinate



c30

Colorless oil; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.066 (br s, 1H), 7.573 (d, J = 8 Hz, 2H), 7.390 – 7.351 (m, 2H), 7.216 – 7.179 (m, 1H), 4.969 (s, 1H), 3.679 (s, 3H), 3.255 – 3.188 (m, 1H), 2.875 – 2.681 (m, 3H), 2.578 – 2.434 (m, 1H), 1.989 – 1.982 (m, 4H), 1.832 (s, 4H), 1.762 – 1.730 (m, 4H), 1.577 – 1.551 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.25, 171.50, 161.34 (t, J = 28 Hz), 135.90, 129.18, 125.65, 120.26, 117.30 (t, J = 257 Hz), 78.14, 51.87, 37.27, 36.25, 36.24, 35.92, 35.87, 35.08 (t, J = 23 Hz), 31.71, 31.69, 29.67 (t, J = 4 Hz), 27.10, 26.89. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.641 (d, J = 257 Hz, 1F), -104.398 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{24}H_{29}F_2NO_5$ $[M+H]^+$ 450.2087, found 450.2074.

methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(phenylcarbamoyl)hexanoate

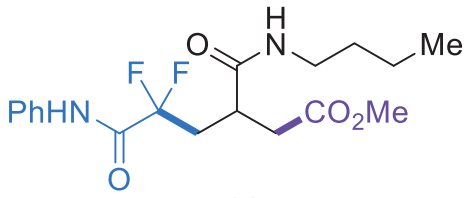


c31

White solid; mp 156-158 °C; R_f = 0.3 (3:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.280 (br s, 1H), 8.170 (br s, 1H), 7.550 (d, J = 8 Hz, 2H), 7.505 (d, J = 8 Hz, 2H), 7.377 – 7.337 (m, 2H), 7.307 – 7.268 (m, 2H), 7.221 – 7.184 (m, 1H), 7.112 – 7.075(m, 1H), 3.675 (s, 3H), 3.264 – 3.196 (m, 1H), 2.943 – 2.802 (m, 1H), 2.787 – 2.715 (m, 1H), 2.610 –

2.556(m, 1H), 2.416 – 2.279 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.38, 171.03, 161.66 (t, J = 28 Hz), 137.71, 135.64, 129.21, 128.89, 125.85, 124.40, 120.41, 119.95, 117.09 (t, J = 256 Hz), 52.13, 37.22 (t, J = 4 Hz), 36.86, 36.26 (t, J = 24 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -102.451 (d, J = 258 Hz, 1F), -104.463 (d, J = 258 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{20}F_2N_2O_4$ $[M+H]^+$ 391.1464, found 391.1454.

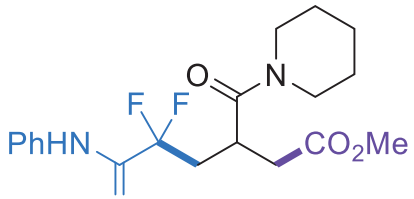
methyl 3-(butylcarbamoyl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c32

Colorless oil; R_f = 0.3 (2:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.032 (br s, 1H), 7.563 (d, J = 8 Hz, 2H), 7.400 – 7.360 (m, 2H), 7.227 – 7.190 (m, 1H), 6.047 (br s, 1H), 3.677 (s, 3H), 3.263 – 3.213 (m, 2H), 3.046 – 2.979 (m, 1H), 2.848 – 2.637 (m, 2H), 2.553 – 2.498 (m, 1H), 2.330 – 2.228 (m, 1H), 1.497 – 1.440 (m, 2H), 1.364 – 1.308 (m, 2H), 0.914 (t, J = 7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.59, 172.21, 161.60 (t, J = 28 Hz), 135.84, 129.22, 125.75, 120.33, 117.17 (t, J = 256 Hz), 51.92, 39.47, 37.03, 36.50 (t, J = 3 Hz), 36.25 (t, J = 23 Hz), 31.40, 19.95, 13.69. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.166 (d, J = 257 Hz, 1F), -104.734 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{18}H_{24}F_2N_2O_4$ $[M+H]^+$ 371.1777, found 371.1766.

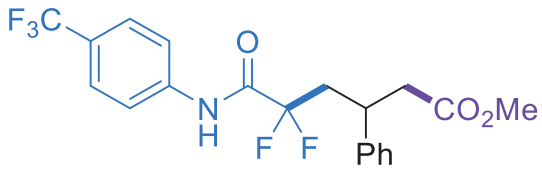
methyl 5,5-difluoro-6-oxo-6-(phenylamino)-3-(piperidine-1-carbonyl)hexanoate



c33

White solid; mp 69-73 °C; R_f = 0.3 (2:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.093 (br s, 1H), 7.572 – 7.551 (m, 2H), 7.388 – 7.349 (m, 2H), 7.214 – 7.177 (m, 1H), 3.665 (s, 3H), 3.647 – 3.621 (m, 1H), 3.606 – 3.553 (m, 4H), 2.913 – 2.849 (m, 1H), 2.731 – 2.600 (m, 1H), 2.582 – 2.500 (m, 1H), 2.409 – 2.268 (m, 1H), 1.655 (br, 4H), 1.541 (br s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.96, 171.28, 161.53 (t, J = 28 Hz), 136.02, 129.02, 125.47, 120.34, 117.13 (t, J = 255Hz), 51.72, 46.97, 43.33, 37.04, 36.23 (t, J = 23 Hz), 30.66 (t, J = 3 Hz), 26.08, 25.40, 24.46. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.455 (d, J = 255 Hz, 1F), -105.390 (d, J = 255 Hz, 1F). ESI-HRMS: Calcd for $C_{19}H_{24}F_2N_2O_4$ $[M+H]^+$ 383.1777, found 383.1765.

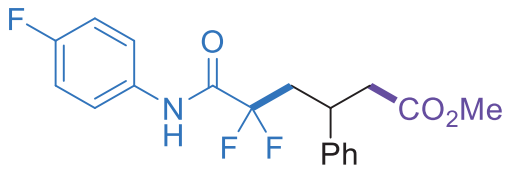
methyl 5,5-difluoro-6-oxo-3-phenyl-6-((4-(trifluoromethyl)phenyl)amino)hexanoate



c34

White solid; mp 88-91 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.920 (br s, 1H), 7.579 (d, J = 9 Hz, 2H), 7.529 (d, J = 9 Hz, 2H), 7.263 – 7.187 (m, 4H), 7.140 – 7.097 (m, 1H), 3.590 (s, 3H), 3.545 – 3.471 (m, 1H), 2.786 – 2.572 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.82, 161.83 (t, J = 28 Hz), 141.48, 138.82, 128.64, 127.42, 127.30, 127.24 (q, J = 30 Hz), 126.26 (q, J = 4 Hz), 119.83, 117.36 (t, J = 257 Hz), 51.76, 41.48, 39.16 (t, J = 23 Hz), 36.10 (t, J = 4Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.557 (s, 3F), -101.287 (d, J = 257 Hz, 1F), -105.560 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{18}F_5NO_3$ $[M+H]^+$ 416.1280, found 416.1267.

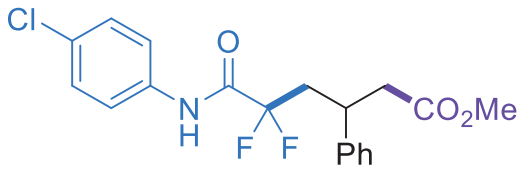
methyl 5,5-difluoro-6-((4-fluorophenyl)amino)-6-oxo-3-phenylhexanoate



c35

White solid; mp 76-79 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.820 (br s, 1H), 7.381 – 7.347 (m, 2H), 7.263 – 7.191 (m, 4H), 7.166 – 7.124 (m, 1H), 7.029 – 6.986 (m, 2H), 3.577 (s, 3H), 3.545 – 3.472 (m, 1H), 2.784 – 2.555 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.80, 161.52 (t, J = 28 Hz), 159.92 (d, J = 246 Hz), 141.67, 131.77 (d, J = 3 Hz), 128.59, 127.40, 127.19, 121.99 (d, J = 8 Hz), 117.46 (t, J = 255 Hz), 115.73 (d, J = 22.7 Hz), 51.70, 41.49, 39.17 (t, J = 23 Hz), 36.08 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.804 (d, J = 257 Hz, 1F), -105.807 (d, J = 257 Hz, 1F), -116.136 (s, 1F). ESI-HRMS: Calcd for $C_{19}H_{18}F_3NO_3$ $[M+H]^+$ 366.1312, found 366.1300.

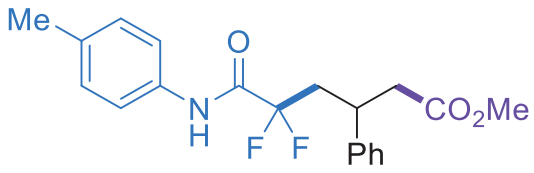
methyl 6-((4-chlorophenyl)amino)-5,5-difluoro-6-oxo-3-phenylhexanoate



c36

White solid; mp 93-96 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.831 (br s, 1H), 7.351 (d, J = 9 Hz, 2H), 7.285 – 7.181 (m, 6H), 7.153 – 7.117(m, 1H), 3.576 (s, 3H), 3.537 – 3.464 (m, 1H), 2.778 – 2.551 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.79, 161.55 (t, J = 28 Hz), 141.58, 134.35, 130.53, 129.03, 128.60, 127.39, 127.23, 121.36, 117.39 (t, J = 256 Hz), 51.71, 41.46, 39.16 (t, J = 23 Hz), 36.07 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.611 (d, J = 257 Hz, 1F), -105.888 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{19}H_{18}ClF_2NO_3$ $[M+H]^+$ 382.1016, found 382.1006.

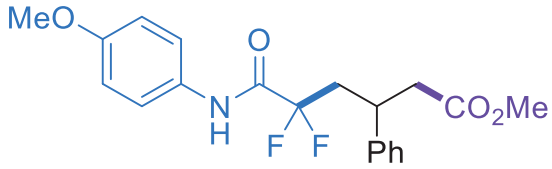
methyl 5,5-difluoro-6-oxo-3-phenyl-6-(p-tolylamino)hexanoate



c37

White solid; mp 105-107 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.741 (br s, 1H), 7.298 (d, J = 9 Hz, 2H), 7.266 (d, J = 7 Hz, 2H), 7.238 – 7.159(m, 1H), 7.123 (d, J = 8 Hz, 2H), 3.568 (s, 3H), 3.535 – 3.481 (m, 1H), 2.792 – 2.562 (m, 4H), 2.321 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.76, 161.39 (t, J = 28 Hz), 141.90, 135.24, 133.21, 129.52, 128.59, 127.38, 127.15, 120.14, 117.55 (t, J = 256 Hz), 51.67, 41.48, 39.25 (t, J = 23 Hz), 36.08 (t, J = 4 Hz), 20.91. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.586 (d, J = 256 Hz, 1F), -105.106 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_3$ $[M+H]^+$ 362.1562, found 362.1553.

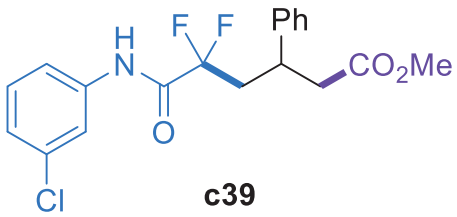
methyl 5,5-difluoro-6-((4-methoxyphenyl)amino)-6-oxo-3-phenylhexanoate



c38

White solid; mp 101-103 °C; R_f = 0.3 (6:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.758 (br s, 1H), 7.337 – 7.306(m, 2H), 7.298 – 7.145 (m, 5H), 6.856 – 6.833 (m, 2H), 3.791 (s, 3H), 3.568 (s, 3H), 3.533 – 3.480 (m, 1H), 2.790 – 2.555 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.77, 161.31 (t, J = 28 Hz), 157.07, 141.84, 128.75, 128.56, 127.38, 127.12, 121.87, 117.56 （t, J = 256 Hz）, 114.06, 55.39, 51.67, 41.47, 39.22 (t, J = 23 Hz), 36.06 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.396 (d, J = 255 Hz, 1F), -105.342 (d, J = 255 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_4$ $[M+H]^+$ 378.1511, found 378.1501.

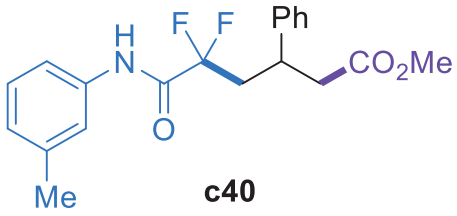
methyl 6-((3-chlorophenyl)amino)-5,5-difluoro-6-oxo-3-phenylhexanoate



c39

White solid; mp 73-76 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.849 (br s, 1H), 7.497 (s, 1H), 7.260 – 7.183 (m, 6H), 7.156 – 7.121 (m, 2H), 3.579 (s, 3H), 3.536 – 3.463 (m, 1H), 2.779 – 2.551 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.80, 161.63 (t, J = 28 Hz), 141.53, 136.86, 134.60, 129.95, 128.61, 127.39, 127.24, 125.52, 120.31, 118.13, 117.34 (t, J = 256 Hz), 51.72, 41.48, 39.15 (t, J = 23 Hz), 36.08 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.560 (d, J = 257 Hz, 1F), -105.938 (d, J = 257 Hz) , 1F. ESI-HRMS: Calcd for $C_{19}H_{18}ClF_2NO_3$ $[M+H]^+$ 382.1016., found 382.1006.

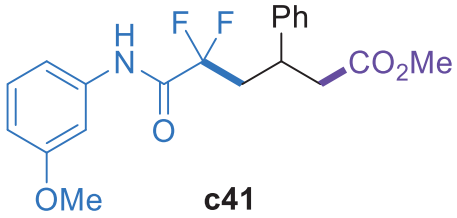
methyl 5,5-difluoro-6-oxo-3-phenyl-6-(m-tolylamino)hexanoate



c40

Colorless oil; R_f = 0.4 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.764 (br s, 1H), 7.275 – 7.238 (m, 3H), 7.215 – 7.177 (m, 4H), 7.159 – 7.141 (m, 1H), 6.989 – 6.971 (m, 1H), 3.568 (s, 3H), 3.535 – 3.482 (m, 1H), 2.792 – 2.562 (m, 4H), 2.333 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.74, 161.46 (t, J = 28 Hz), 141.88, 139.01, 135.66, 128.82, 128.58, 127.37, 127.12, 126.27, 120.78, 117.52 (t, J = 257 Hz), 117.24, 51.65, 41.48, 39.23 (t, J = 23 Hz), 36.07 (t, J = 4 Hz), 21.39. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.599 (d, J = 256 Hz), -105.072 (d, J = 256 Hz). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_3$ $[M+H]^+$ 362.1562, found 362.1553.

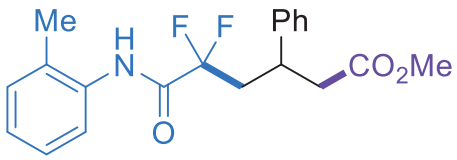
methyl 5,5-difluoro-6-((3-methoxyphenyl)amino)-6-oxo-3-phenylhexanoate



c41

White solid; mp 61-65 °C; R_f = 0.3 (6:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.828 (br s, 1H), 7.268 – 7.188 (m, 5H), 7.170 – 7.135 (m, 5H), 6.915 – 6.892 (m, 1H), 6.725 – 6.699 (m, 1H), 3.784 (s, 3H), 3.566 (s, 3H), 3.531 – 3.477(m, 1H), 2.785 – 2.558 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.75, 161.52 (t, J = 28 Hz), 160.01, 141.82, 136.97, 129.69, 128.57, 127.36, 127.14, 117.46 （t, J = 256 Hz）, 112.26, 111.35, 105.77, 55.27, 51.65, 41.45, 39.22 (t, J = 23 Hz), 36.04 (t, J = 4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.553 (d, J = 256 Hz, 1F), -105.205 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_4$ $[M+H]^+$ 378.1511., found 378.1508.

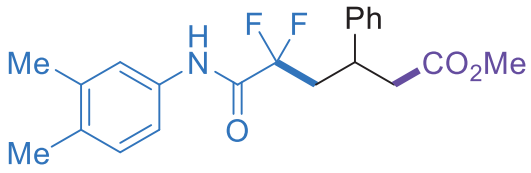
methyl 5,5-difluoro-6-oxo-3-phenyl-6-(o-tolylamino)hexanoate



c42

Colorless oil; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.711 (br s, 1H), 7.692 – 7.173 (m, 7H), 7.135 – 7.098(m, 1H), 3.572 – 3.511 (m, 4H), 2.808 – 2.592 (m, 4H), 2.212 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.71, 161.58 (t, J = 28 Hz), 141.96, 133.67, 130.55, 128.94, 128.61, 127.38, 127.13, 126.85, 126.04, 122.43, 117.77 (t, J = 256 Hz), 51.66, 41.53, 39.13 (t, J = 23 Hz), 36.09 (t, J = 4 Hz), 17.35. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.347 (d, J = 257 Hz, 1F), -104.809 (d, J = 257 Hz, 1F). ESI-HRMS: Calcd for $C_{20}H_{21}F_2NO_3$ $[M+H]^+$ 362.1562, found 362.1553.

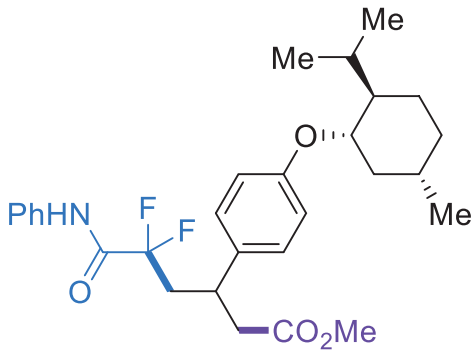
methyl 6-((3,4-dimethylphenyl)amino)-5,5-difluoro-6-oxo-3-phenylhexanoate



c43

White Solid; mp 63-65 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.756 (br s, 1H), 7.269 – 7.210 (m, 2H), 7.205 – 7.123 (m, 5H), 7.056 (d, *J* = 8 Hz, 1H), 3.553 (s, 3H), 3.534 – 3.477 (m, 1H), 2.782 – 2.550 (m, 4H), 2.224 (s, 3H), 2.215 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.70, 161.39 (t, *J* = 28 Hz), 142.03, 137.30, 133.91, 133.48, 129.94, 128.55, 127.36, 127.07, 121.52, 120.10, 117.57 (t, *J* = 256 Hz), 51.56, 41.46, 39.28 (t, *J* = 23 Hz), 36.08 (t, *J* = 4 Hz), 19.75, 19.17. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.784 (d, *J* = 256 Hz, 1F), -104.818 (d, *J* = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{21}H_{23}F_2NO_3$ $[M+H]^+$ 376.1719, found 376.1707.

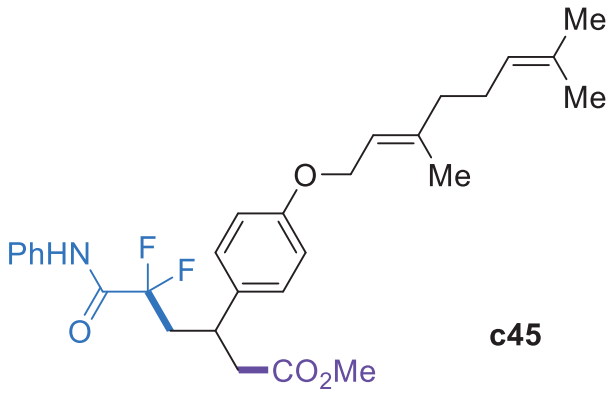
methyl 5,5-difluoro-3-(4-(((1S,2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)phenyl)-6-oxo-6-(phenylamino)hexanoate



c44

White Solid; mp 90-94 °C; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); a mixture of diastereoisomers, dr = 1:1 (the ratio was determined by ^{19}F NMR analysis);^{1}H NMR (400 MHz, $CDCl_3$) δ 7.854 (br s, 1H), 7.436 (d, *J* = 8 Hz, 2H), 7.342 – 7.303 (m, 2H), 7.177 – 7.140 (m, 1H), 7.080 (d, *J* = 8 Hz, 2H), 6.769 (d, *J* = 8 Hz, 2H), 4.515 (s, 1H), 3.572 (s, 3H), 3.497 – 3.424 (m, 1H), 2.762 – 2.531 (m, 4H), 1.987 (d, *J* = 14 Hz, 1H), 1.771 – 1.473 (m, 5H), 1.026 – 0.893 (m, 6H), 0.822 – 0.789 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.99, 161.60 (t, *J* = 28 Hz), 157.27, 135.81, 133.35, 129.05, 128.30, 125.45, 117.59 (t, *J* = 256 Hz), 115.06, 73.38, 73.36, 51.61, 47.74, 41.71, 39.41 (t, *J* = 23 Hz), 37.61, 35.28 (t, *J* = 4 Hz), 34.93, 29.12, 26.08, 24.70, 22.29, 20.99, 20.88. ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.375 (dd, *J* = 255, 3 Hz, 1F), -105.246 (dd, *J* = 255, 16 Hz, 1F). ESI-HRMS: Calcd for $C_{29}H_{37}F_2NO_4$ $[M+H]^+$ 502.2763, found 502.2752.

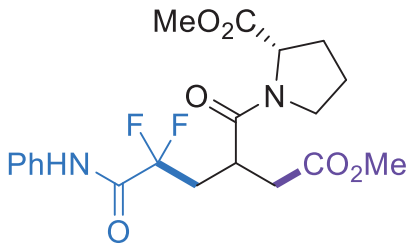
methyl (E)-3-(4-((3,7-dimethylocta-2,6-dien-1-yl)oxy)phenyl)-5,5-difluoro-6-oxo-6-(phenylamino)hexanoate



c45

Colorless oil; R_f = 0.3 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.681 (br s, 1H), 7.396 (d, J = 8 Hz, 2H), 7.337 – 7.297 (m, 2H), 7.171 – 7.095 (m, 3H), 6.756 (d, J = 9 Hz, 2H), 5.412 (t, J = 6 Hz, 1H), 5.097 (t, J = 6 Hz, 1H), 4.370 – 4.290 (m, 2H), 3.579 (s, 3H), 3.498 – 3.424 (m, 1H), 2.749 – 2.529 (m, 4H), 2.131 – 2.067 (m, 4H), 1.691 (d, J = 2 Hz, 6H), 1.611 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.84, 161.55 (t, J = 28 Hz), 157.91, 141.09, 135.84, 133.23, 131.80, 128.99, 128.47, 125.36, 123.76, 119.99, 119.32, 117.54 (t, J = 258 Hz), 114.58, 64.64, 51.68, 41.67, 39.58, 39.36 (t, J = 18 Hz), 35.46 (t, J = 4 Hz), 26.25, 25.69, 17.69, 16.60. ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.108 (d, J = 256 Hz, 1F), -106.424 (d, J = 256 Hz, 1F). ESI-HRMS: Calcd for $C_{29}H_{35}F_2NO_4$ $[M+H]^+$ 500.2606, found 500.2598.

methyl (4,4-difluoro-2-(2-methoxy-2-oxoethyl)-5-oxo-5-(phenylamino)pentanoyl)-L-prolinate

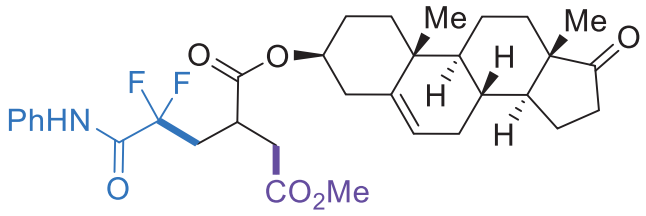


c46

Colorless oil; R_f = 0.3 (1:1 petroleum ether / ethyl acetate); a mixture of diastereoisomers (dr 1:0.24, the ratio was determined by ^{1}H NMR analysis), ^{1}H NMR (400 MHz, CDCl3) δ 8.479 (br s, 0.24H), 8.352 (br s, 1H), 7.627 – 7.605 (m, 0.47H), 7.580 – 7.558 (m, 2H), 7.371 – 7.325 (m, 2.56H), 7.199 – 7.148 (m, 1.24H), 4.95 (dd, J = 8.6, 2.1 Hz, 1H), 4.968 – 4.941(m, 0.24H), 4.452 – 4.420(m, 1H), 3.887 – 3.812(m, 1.19H), 3.727 (s, 0.82H), 3.706 (s, 3.19H), 3.672 (s, 3.11H), 3.642 (s, 0.80H), 3.519 – 3.455 (m, 1.31H), 2.981 – 2.780 (m, 1.39H), 2.752 – 2.626 (m, 1.49H), 2.535 – 2.477 (m, 1.12H), 2.392 – 2.255 (m, 1.54H), 2.190 – 2.124 (m, 1.33H), 2.075 – 1.963 (m, 3.86H), 1.907 – 1.859 (m, 0.66H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.11 (s), 172.23 (s), 172.20 (s), 171.90 (s), 171.48 (s), 161.51 (t, J = 28.5 Hz), 136.29 (s), 136.03 (s), 129.05 (s), 128.99 (s), 125.50 (s), 125.32 (s), 120.32 (s), 120.19 (s), 116.96 (t, J = 256 Hz), 59.42 (s), 58.90 (s), 52.57 (s), 52.02 (s), 51.93 (s), 51.82 (s), 47.03 (s), 46.70 (s), 36.97 (s), 36.78 (s), 35.98 (t, J = 23.4 Hz), 33.66 (t, J = 2.0 Hz), 33.39 (t, J = 3.0 Hz), 31.26 (s), 29.08 (s), 24.61 (s), 22.45 (s).^{19}F NMR (376 MHz, $CDCl_3$) δ -101.924 (d, J = 254.0 Hz, 0.24F), -103.861 (d, J = 253.3 Hz, , 1F), -106.049 (d, J = 254.0 Hz, 0.2F), -106.110 (d, J = 253.3 Hz, 1.04F). ESI-HRMS: Calcd for $C_{20}H_{24}F_2N_2O_6$ $[M+H]^+$ 427.1675, found

427.1661.

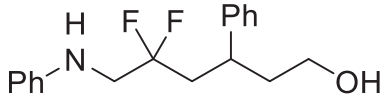
1-((3S,8R,9S,10R,13S,14S)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl) 4-methyl 2-(2,2-difluoro-3-oxo-3-(phenylamino)propyl)succinate



c47

Colorless oil; R_f = 0.3 (4:1 petroleum ether / ethyl acetate); a mixture of diastereoisomers (dr 1:1, the ratio was determined by ^{13}C NMR analysis),^1H NMR (400 MHz, $CDCl_3$) δ 8.123 (br s, 1H), 7.582 (d, *J* = 8 Hz, 2H), 7.393 – 7.354(m, 2H), 7.200 (t, *J* = 7 Hz, 1H), 5.390 – 5.376 (m, 1H), 4.656 – 4.614 (m, 1H), 3.689 (s, 3H), 3.176 – 3.126 (m, 1H), 2.841 – 2.640 (m, 3H), 2.495 – 2.319 (m, 4H), 2.137 – 2.044 (m, 2H), 1.983 – 1.938 (m, 1H), 1.885 – 1.832 (m, 2H), 1.679 – 1.427 (m, 6H), 1.324 – 1.256 (m, 3H), 1.160 – 1.099(m, 1H), 1.033 – 0.961 (m, 4H), 0.884 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 221.03, 172.41, 172.39, 171.48, 161.31 (t, *J* = 28 Hz), 139.64, 139.63, 135.93, 129.18, 125.64, 122.03, 122.02, 120.26, 117.19 (t, *J* = 256 Hz), 74.75, 51.89, 51.65, 50.08, 47.48, 37.73, 36.80, 36.67, 35.93, 35.80, 35.70 (t, *J* = 3 Hz), 35.07 (t, *J* = 23 Hz), 31.41, 31.36, 30.73, 27.43, 27.41, 21.83, 20.28, 19.29, 13.50. ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.958 (d, *J* = 8 Hz, 2F). ESI-HRMS: Calcd for $C_{33}H_{41}F_2NO_6$ $[M+H]^+$ 586.2975, found 586.2972.

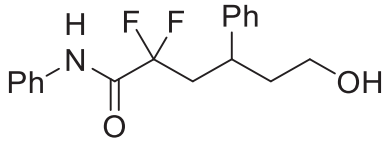
5,5-difluoro-3-phenyl-6-(phenylamino)hexan-1-ol



d

Brown oil; R_f = 0.3 (2:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, $CDCl_3$) δ 7.304 (t, *J* = 7.3 Hz, 2H), 7.241 – 7.190 (m, 3H), 7.150 –7.111 (m, 2H), 6.713 (t, *J* = 7.3 Hz, 1H), 6.493 (d, *J* = 7.8 Hz, 2H), 3.626 (s, 1H), 3.484 – 3.428 (m, 1H), 3.386 – 3.087 (m, 4H), 2.438 – 2.202 (m, 2H), 2.016 – 1.933 (m, 1H), 1.845 – 1.757 (m, 1H), 1.536 (br s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.09, 143.76, 129.16, 128.70, 127.49, 126.75, 123.70 (t, *J* = 243.6 Hz), 118.20, 113.02, 60.30, 48.57 (dd, *J* = 30.5, 28.3 Hz), 41.02 (t, *J* = 23.6 Hz), 39.85, 36.37 (dd, *J* = 4.8, 3.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -97.554 (d, *J* = 247.6 Hz, 1F), -102.354 (d, *J* = 247.6 Hz, 1F). ESI-HRMS: Calcd for $C_{18}H_{21}F_2NO$ $[M+H]^+$ 306.1664, found 306.1656.

2,2-difluoro-6-hydroxy-N,4-diphenylhexanamide

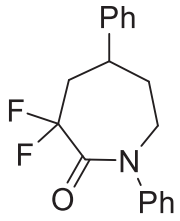


e

Colorless oil ; R_f = 0.25 (2:1 petroleum ether / ethyl acetate); ^1H NMR (400 MHz, $CDCl_3$) δ

7.982 (s, 1H), 7.408 – 7.388 (m, 2H), 7.316 – 7.277 (m, 2H), 7.252 – 7.215 (m, 2H), 7.164 – 7.116 (m, 4H), 3.502 – 3.446 (m, 1H), 3.379 – 3.318 (m, 1H), 3.149 – 3.075 (m, 1H), 2.628 – 2.515 (m, 2H), 2.005 – 1.923 (m, 2H), 1.857 – 1.770 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.96 (t, J = 28.4 Hz), 142.60, 135.76, 128.94, 128.52, 127.53, 126.79, 125.43, 120.23, 117.77 (t, J = 254.5 Hz), 59.96, 39.90 (t, J = 22.3 Hz), 39.58, 36.18 (t, J = 3.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -101.53 (d, J = 254.9 Hz, 1F), -103.78 (d, J = 254.9 Hz, 1F). ESI-HRMS: Calcd for $C_{18}H_{19}F_2NO_2$ $[M+H]^+$ 320.1457, found 320.1451.

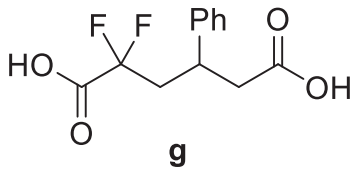
3,3-difluoro-1,5-diphenylazepan-2-one



f

White solid; 142-144 ^{o}C; R_f = 0.4 (10:1 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.434 – 7.396 (m, 2H), 7.369 – 7.126 (m, 8H), 4.265 – 4.199 (m, 1H), 3.78 – 3.60 (m, 1H), 3.721 – 3.652 (m, 1H), 3.271 (t, J = 12.4 Hz, 1H) 2.614 –2.519 (m, 1H), 2.437 – 2.286 (m, 1H), 2.180 – 2.122 (m, 1H), 2.056 – 1.961 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.17 (dd, J = 31.0, 28.0 Hz), 143.82, 143.81, 143.43, 129.40, 128.91, 127.37, 127.18, 126.66, 125.90, 116.55 (dd, J = 250.9, 247.0 Hz), 51.22, 51.16, 41.21, 41.11, 40.18 (dd, J = 25.3, 23.4 Hz), 36.33. ^{19}F NMR (376 MHz, $CDCl_3$) δ -92.194 (d, J = 259.8 Hz, 1F), -105.502 (d, J = 260.0 Hz, 1F). ESI-HRMS: Calcd for $C_{18}H_{17}F_2NO$ $[M+H]^+$ 302.1351, found 302.1341.

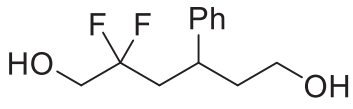
2,2-difluoro-4-phenylhexanedioic acid



g

Colorless oil; R_f = 0.1 (2% AcOH in 1:1 petroleum ether / ethyl acetate,); ^{1}H NMR (400 MHz, CDOD) δ 7.186 – 7.135 (m, 4H), 7.103 – 7.060 (M, 1H), 3.360 – 3.288 (m, 1H), 2.675(dd, J = 6, 15.6 Hz, 1H), 2.516 (dd, J = 8.8, 15.6 Hz, 1H), 2.428 – 2.328 (m, 2H). ^{13}C NMR (101 MHz, CDOD) δ 178.52, 171.35 (t, J = 25.3 Hz), 145.96, 129.27, 128.45, 127.26, 119.44 (t, J = 251.5 Hz), 44.15 (t, J = 4 Hz), 41.85 (t, J = 22.2 Hz), 37.82.^{19}F NMR (376 MHz, CDOD) δ -103.359 (d, J = 242.1 Hz, 1F), -104.269 (d, J = 242.9 Hz, 1F). ESI-HRMS: Calcd for $C_{12}H_{12}F_2O_4$ $[M+H]^+$ 259.0776, found 259.0779.

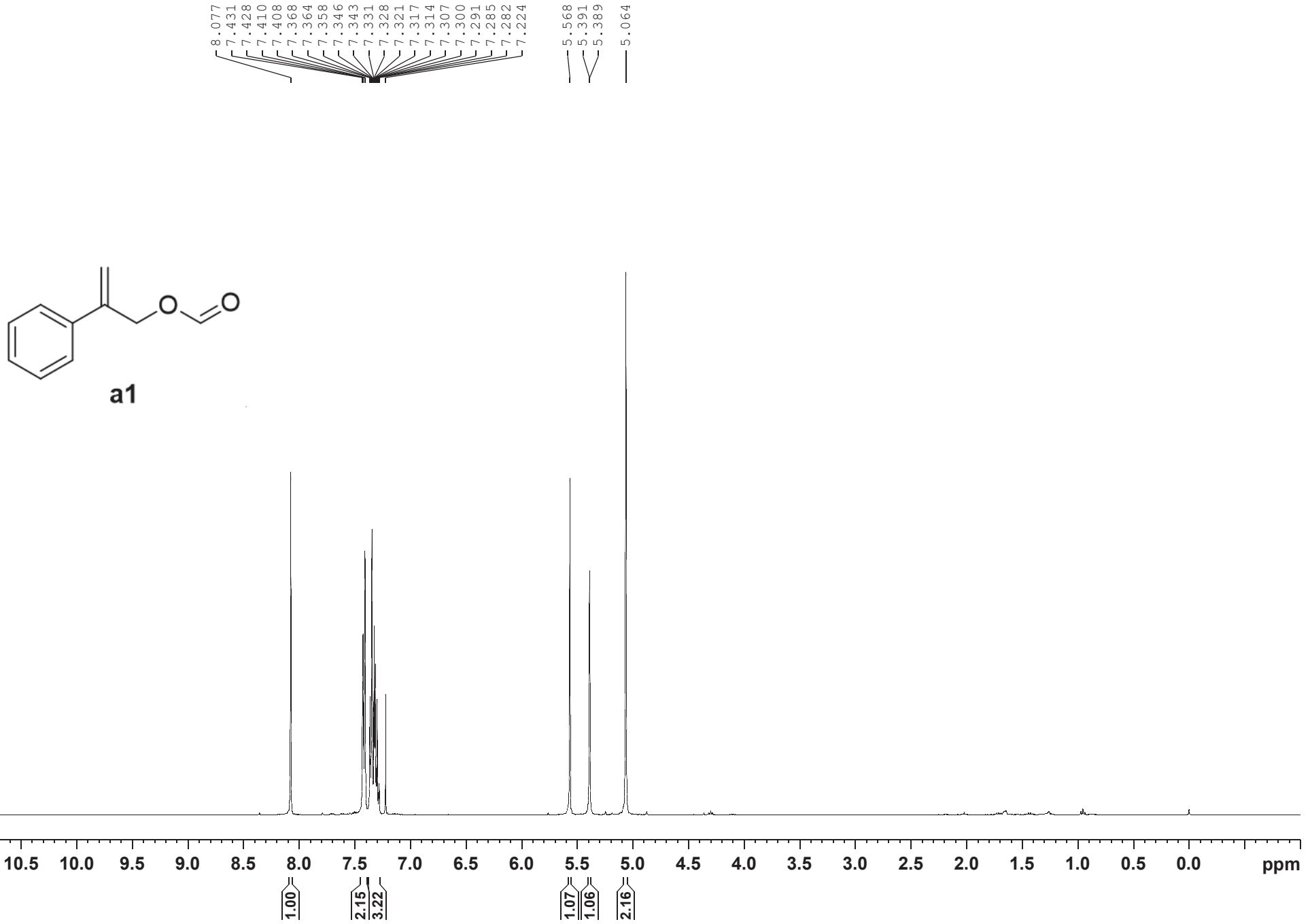
2,2-difluoro-4-phenylhexane-1,6-diol

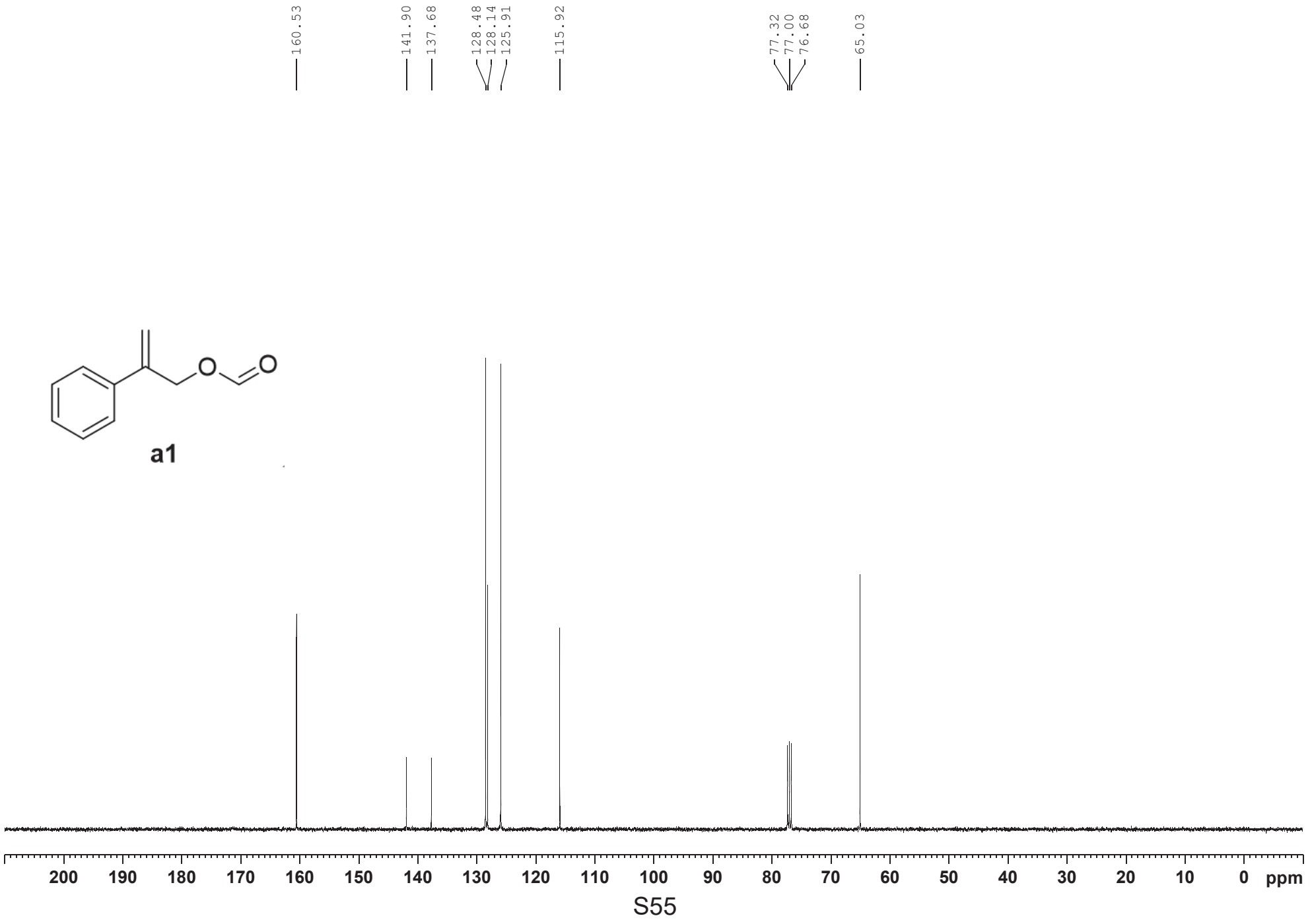


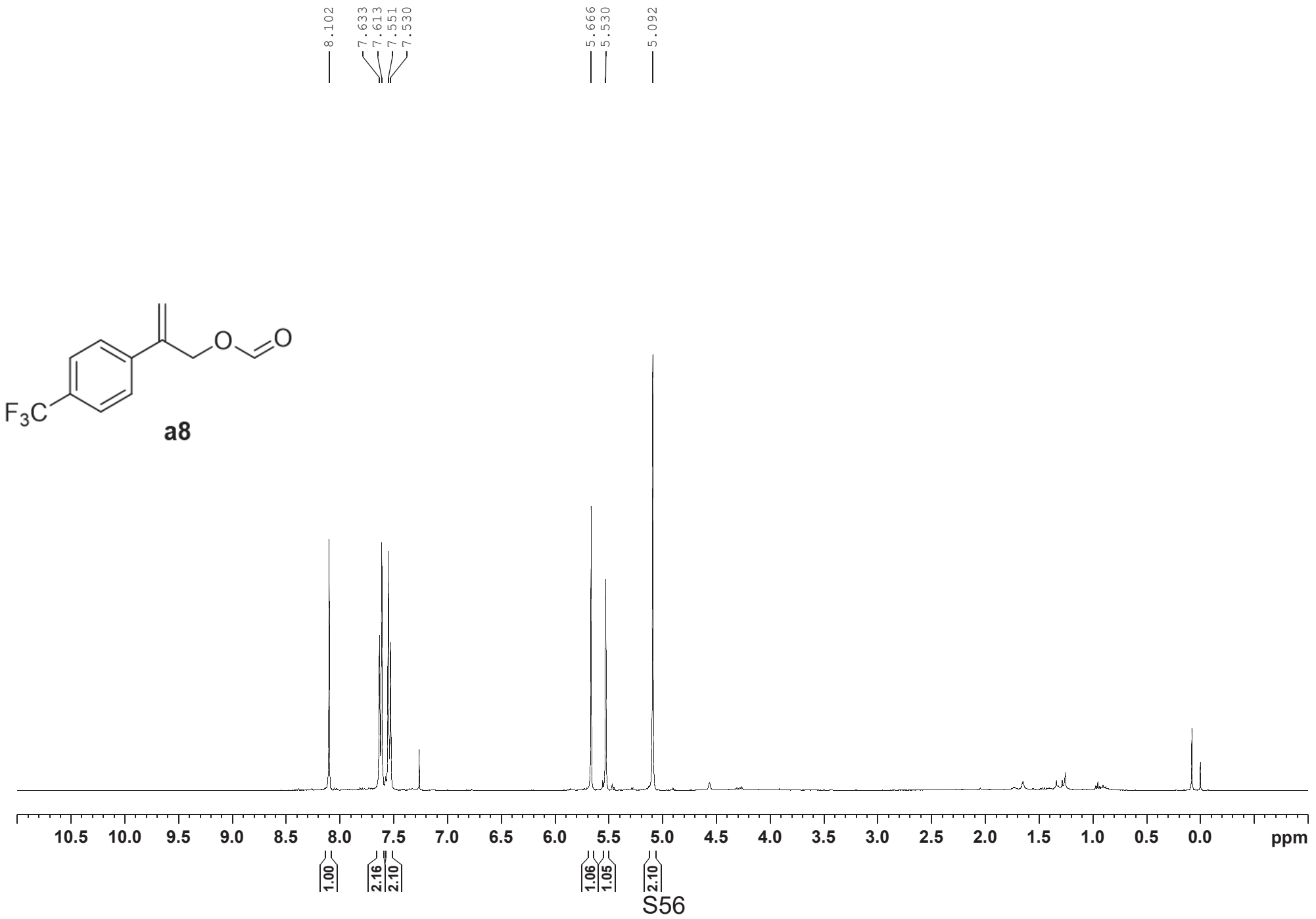
h

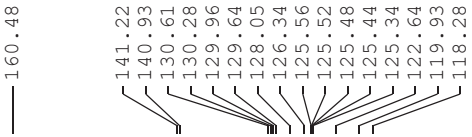
Colorless oil; R_f = 0.2 (1:2 petroleum ether / ethyl acetate); ^{1}H NMR (400 MHz, CDCl3) δ 7.303 (t, J = 7.3 Hz, 2H), 7.234 – 7.189 (m, 3H), 3.625 – 3.359 (m, 4H), 3.144 – 3.072 (m, 1H), 2.775 (br s, 1H), 2.359 – 2.248 (m, 2H), 2.037 – 1.956 (m, 2H), 1.863 – 1.776 (m, 1H).^{13}C NMR (101 MHz, CDCl3) δ 143.89, 128.67, 127.41, 126.72, 123.09 (t, J = 242.9 Hz), 63.89 (t, J = 31.9 Hz), 60.33, 39.71, 39.69 (t, J = 23.2 Hz), 36.17 (t, J = 4.0 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ -103.515 (d, J = 251.2 Hz, 1F), -106.217 (d, J = 251.2 Hz, 1F). ESI-HRMS: Calcd for $C_{12}H_{16}F_2O_2$ $[M+H]^+$ 231.1191, found 231.1193.

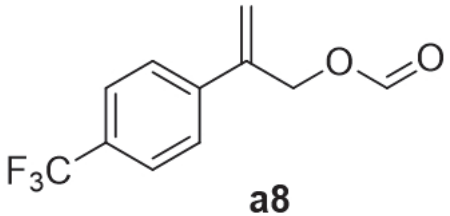
10 Copies of ^{1}H, ^{19}F and ^{13}C NMR spectra



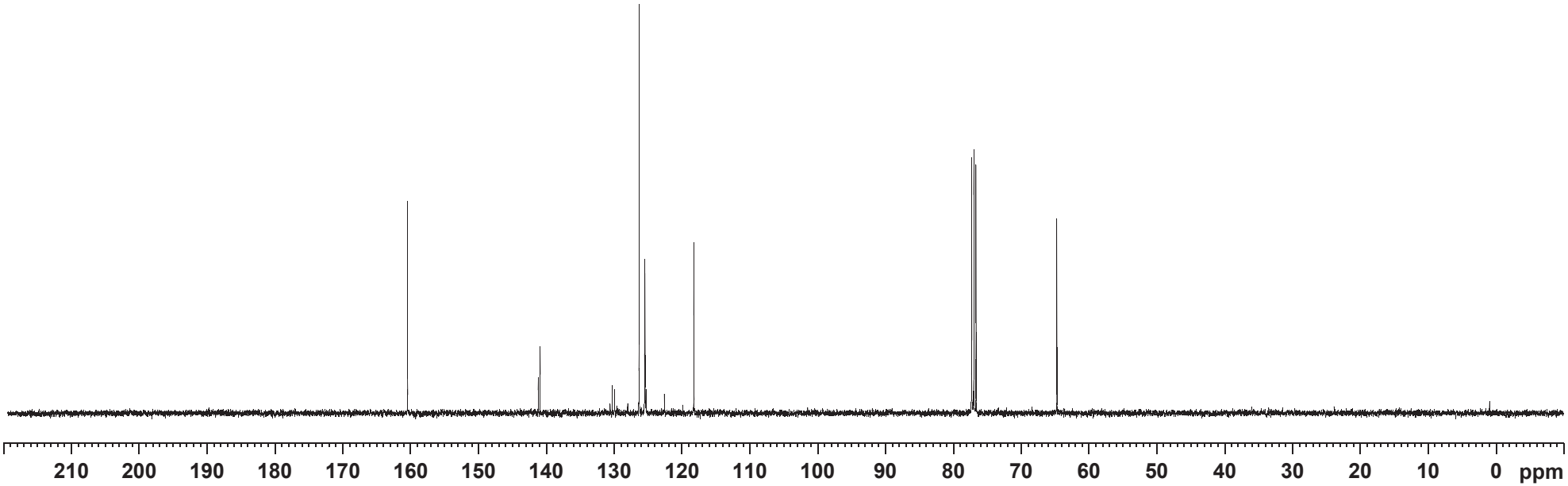

160.53
141.90
137.68
128.48
128.14
125.91
115.92
77.32
77.00
76.68
65.03
O
O
a1
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

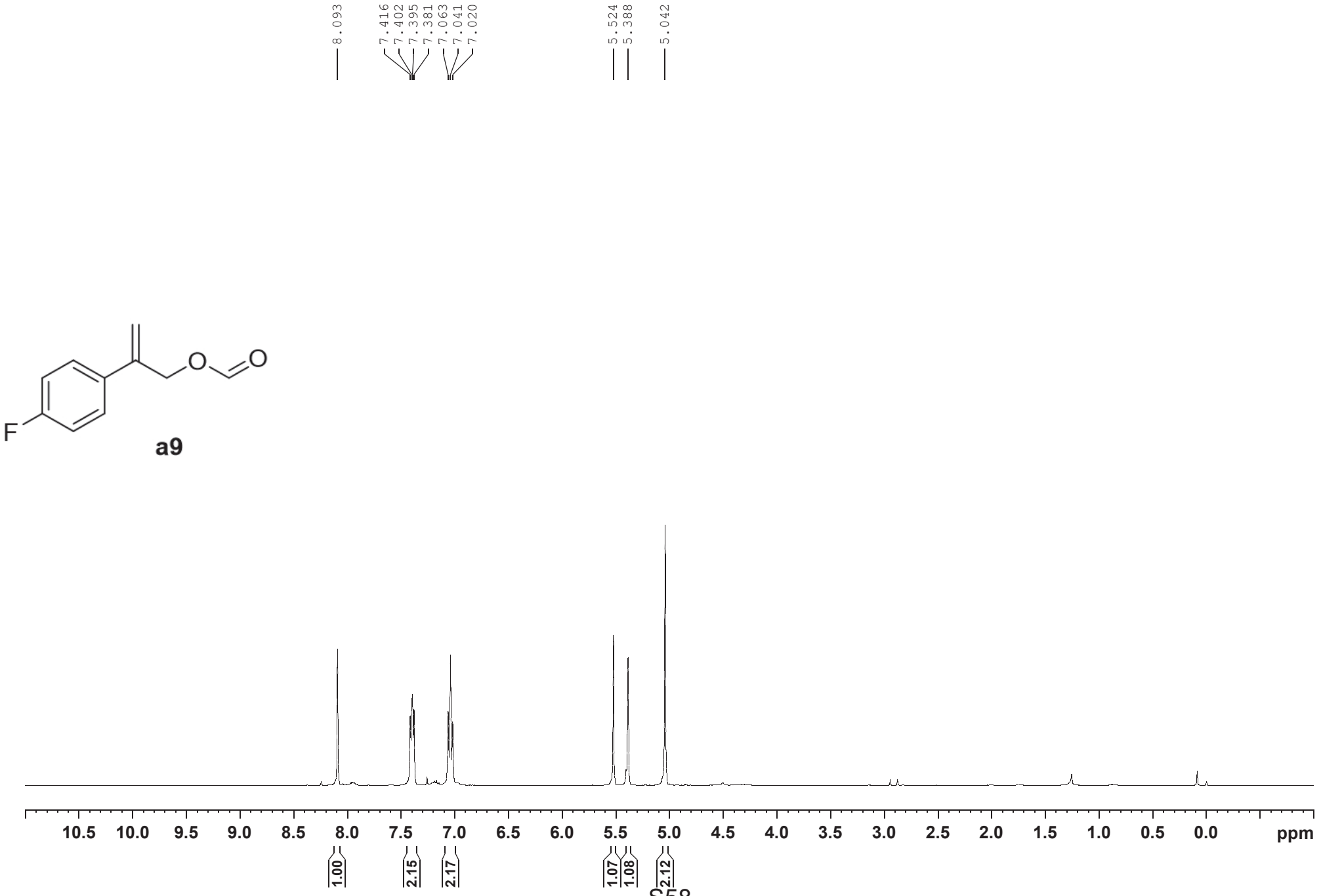

8.102
7.633
7.613
7.551
7.530
5.666
5.530
5.092
O
O
F3C
a8
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.16
2.10
1.06
1.05
2.10

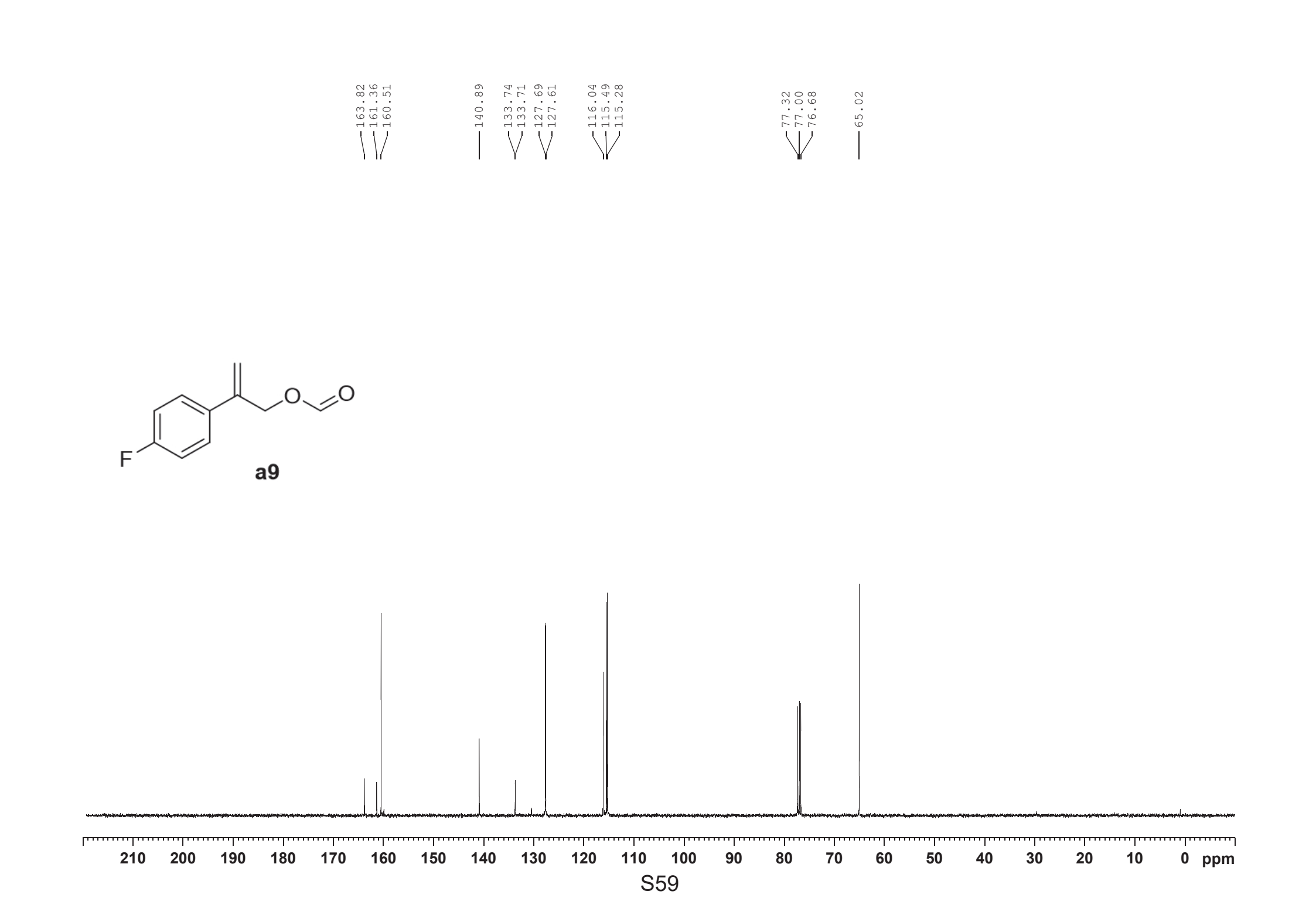

160.48
141.22
140.93
130.61
130.28
129.96
129.64
128.05
126.34
125.56
125.52
125.48
125.44
125.34
122.64
119.93
118.28
77.32
77.00
76.68
64.78

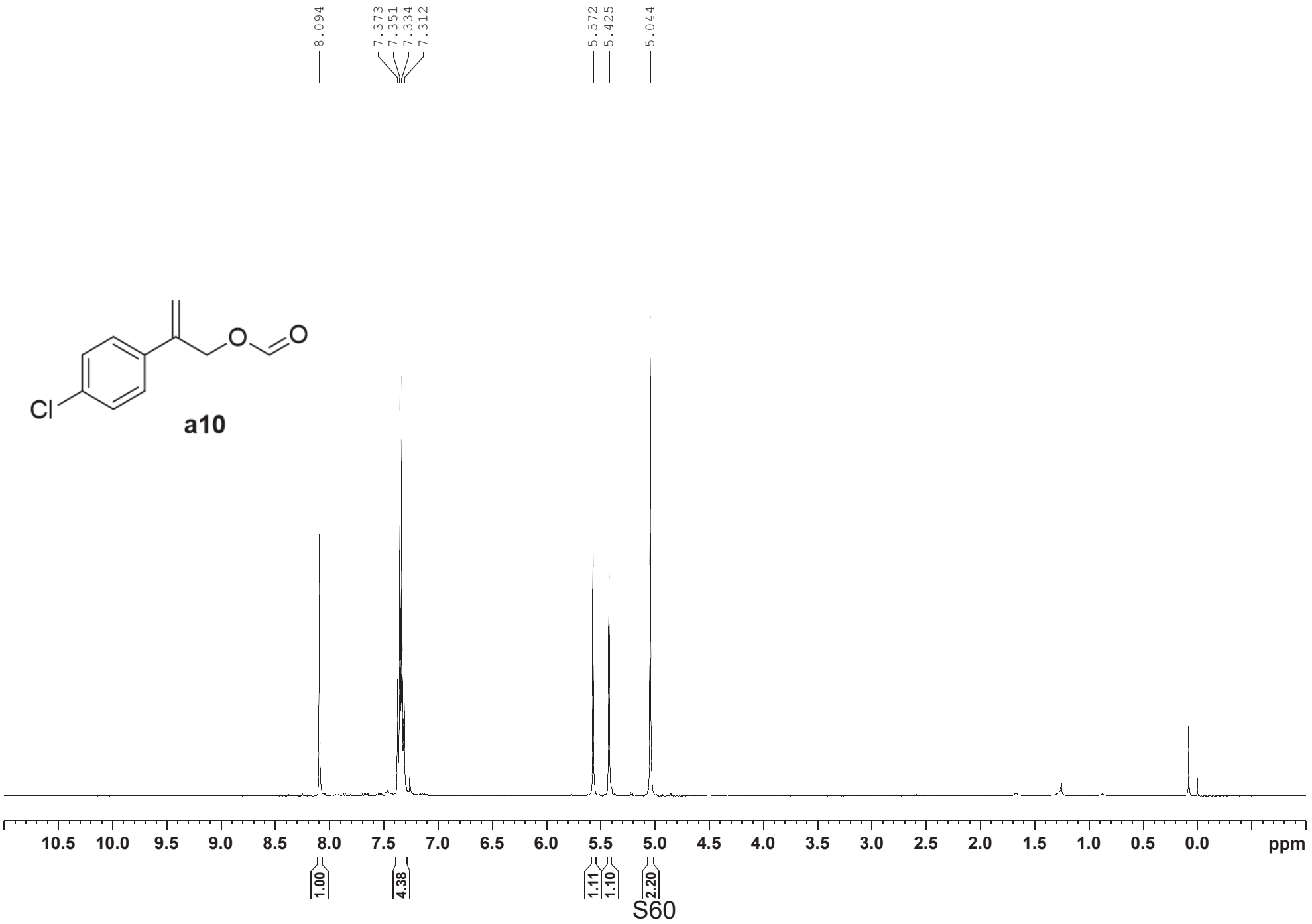

O
O
F3C

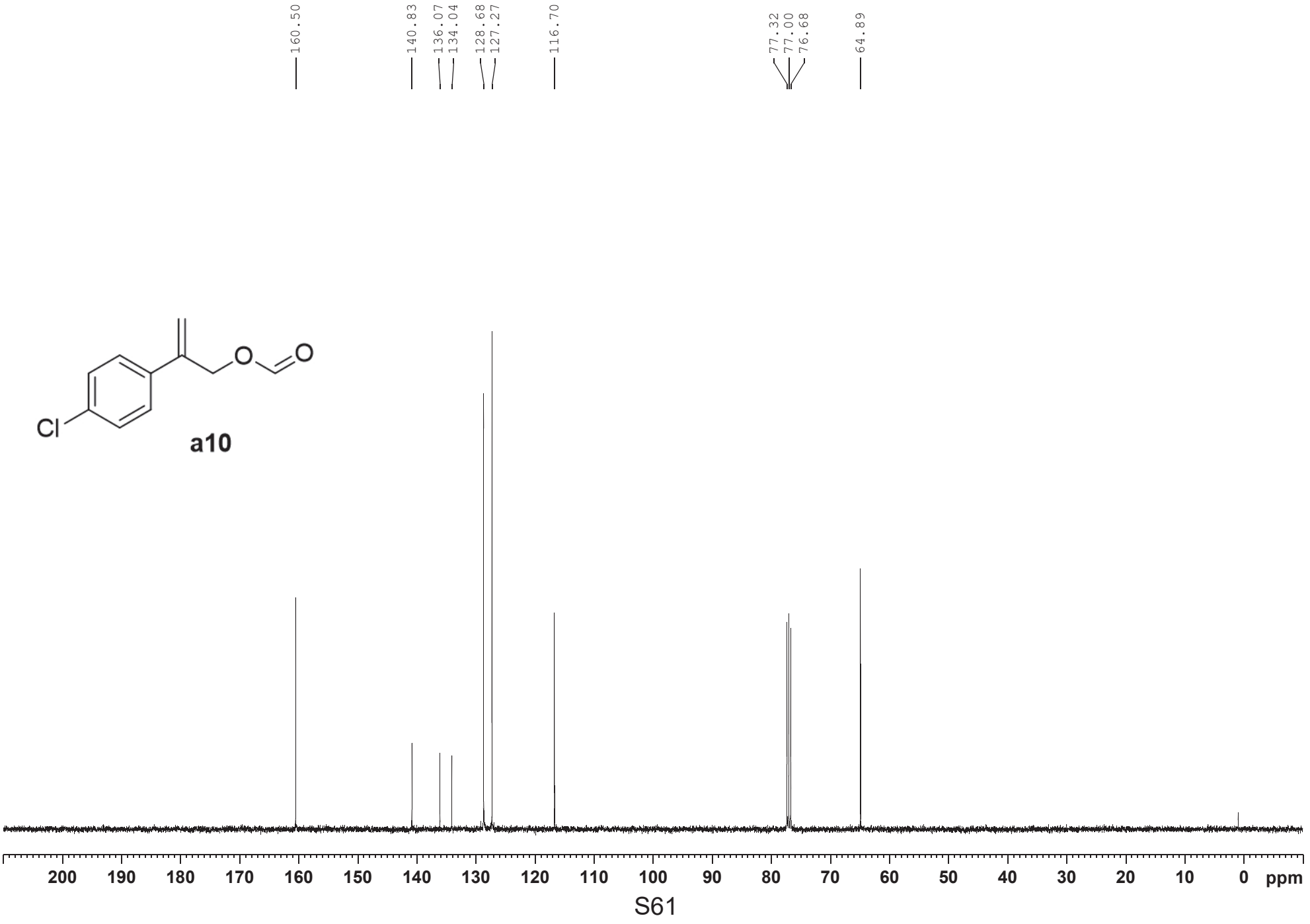
a8

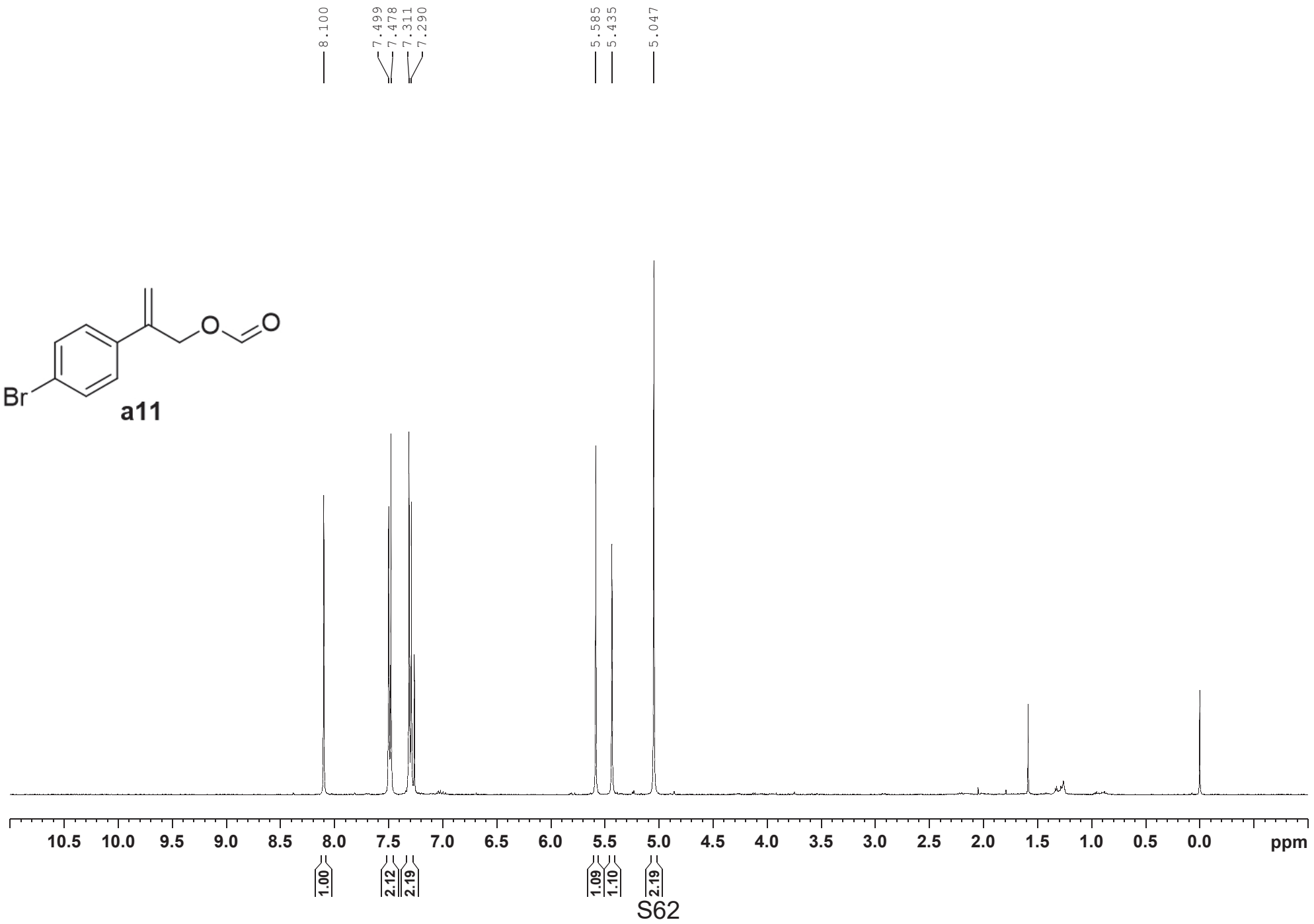

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

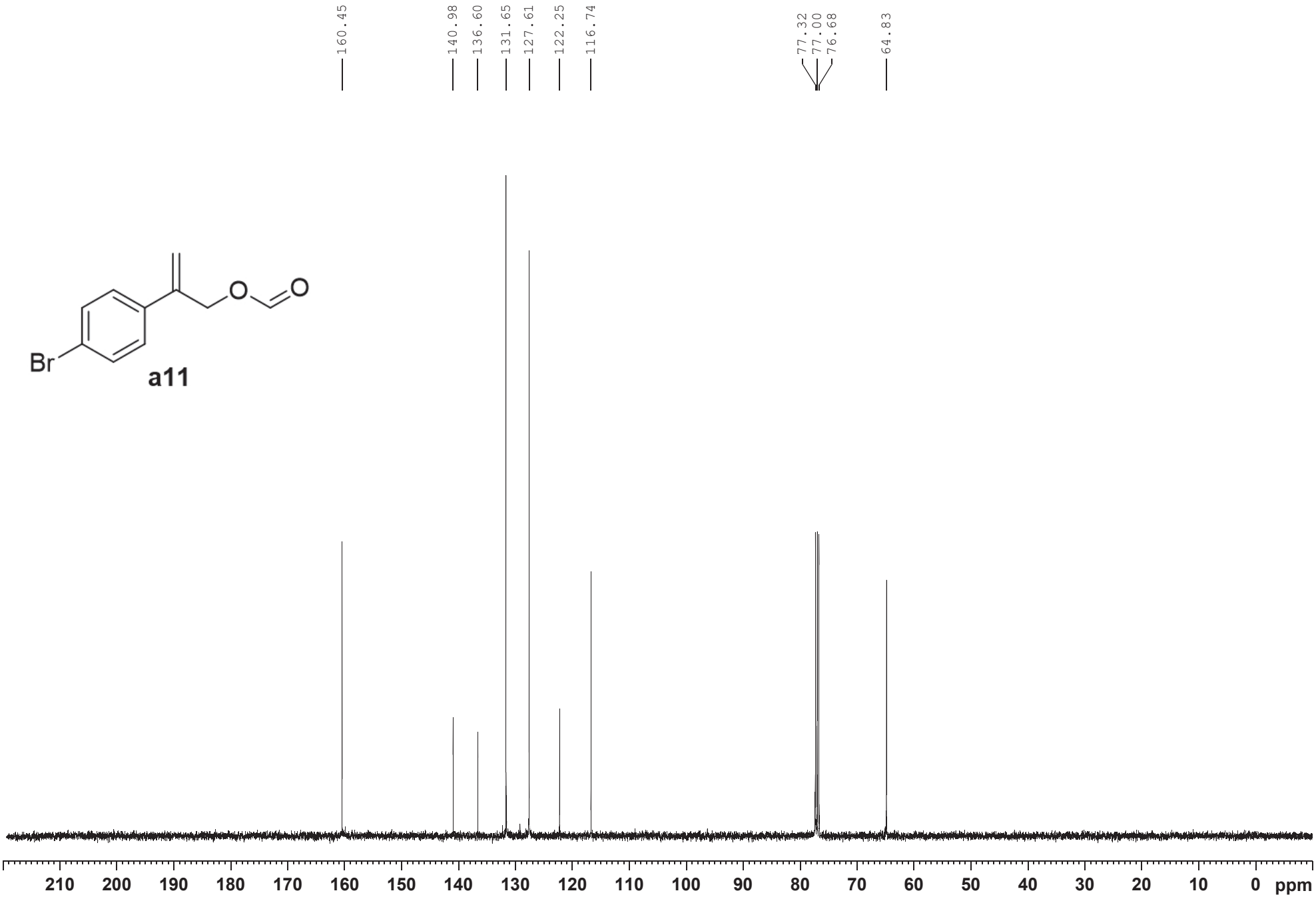

8.093
7.416
7.402
7.395
7.381
7.063
7.041
7.020
5.524
5.388
5.042
O
O
F
a9
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.15
2.17
1.07
1.08
2.12

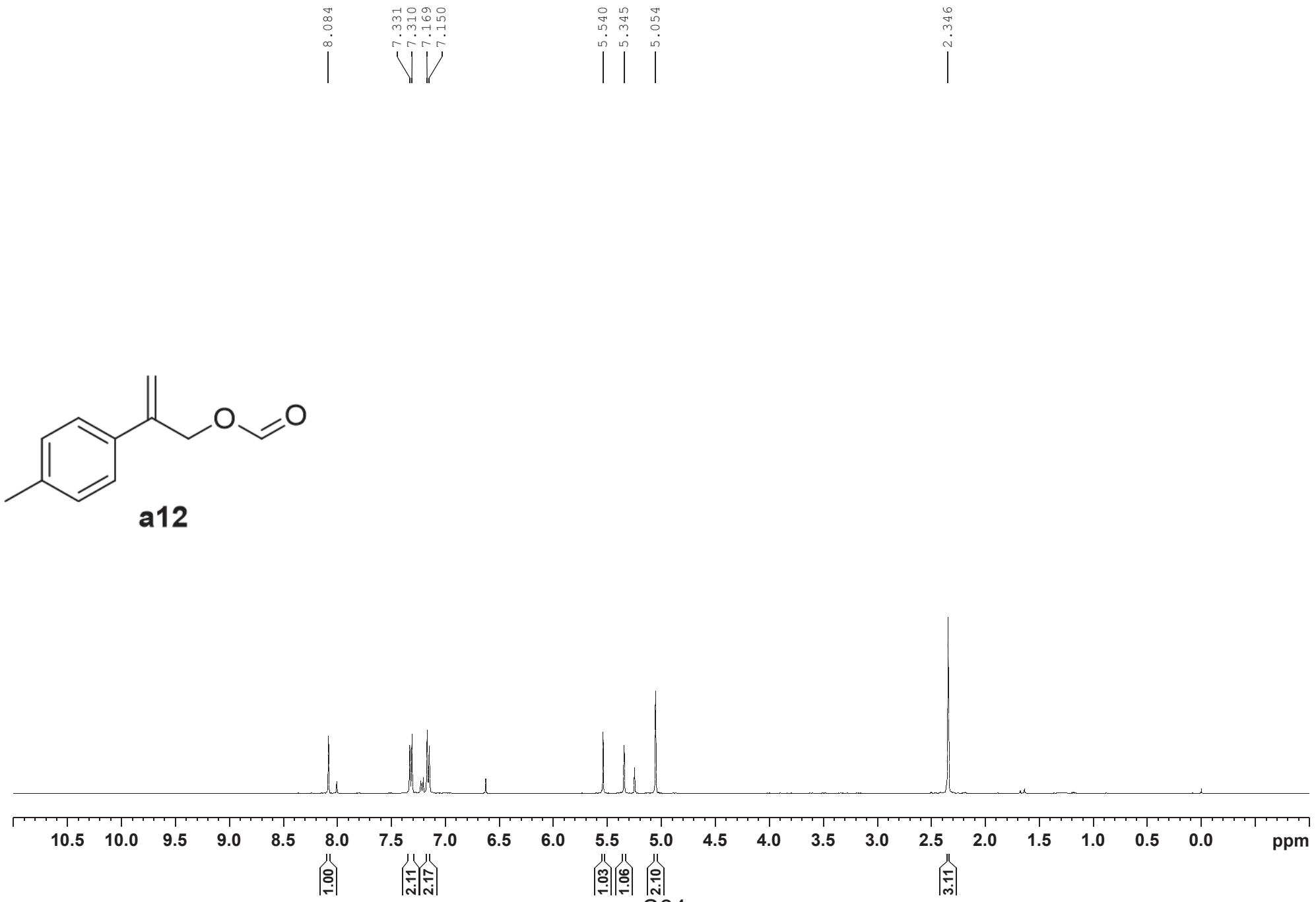

163.82
161.36
160.51
140.89
133.74
133.71
127.69
127.61
116.04
115.49
115.28
77.32
77.00
76.68
65.02
O
O
F
a9
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

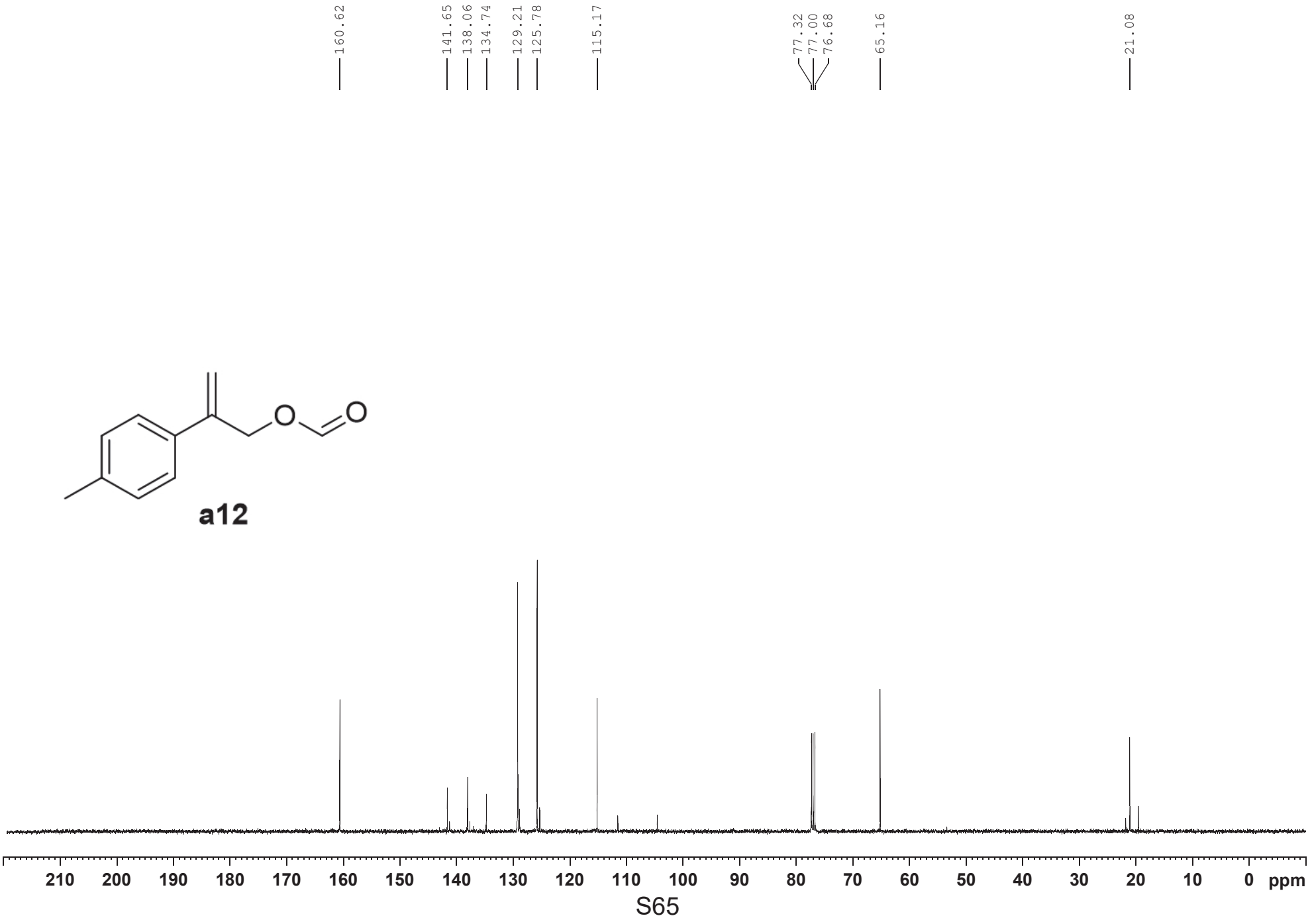

8.094
7.373
7.351
7.334
7.312
5.572
5.425
5.044
Cl
O
O
a10
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.38
1.11
1.10
2.20

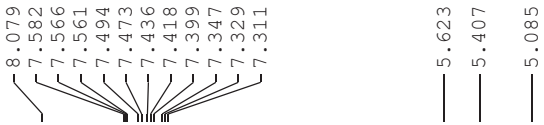

160.50
140.83
136.07
134.04
128.68
127.27
116.70
77.32
77.00
76.68
64.89
Cl
O
O
a10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

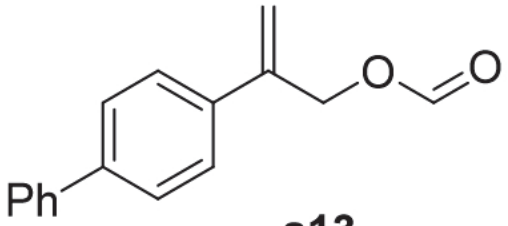

8.100
7.499
7.478
7.311
7.290
5.585
5.435
5.047
Br
O
O
a11
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.12
2.19
1.09
1.10
2.19


160.45
140.98
136.60
131.65
127.61
122.25
116.74
77.32
77.00
76.68
64.83
Br
O
O
a11
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

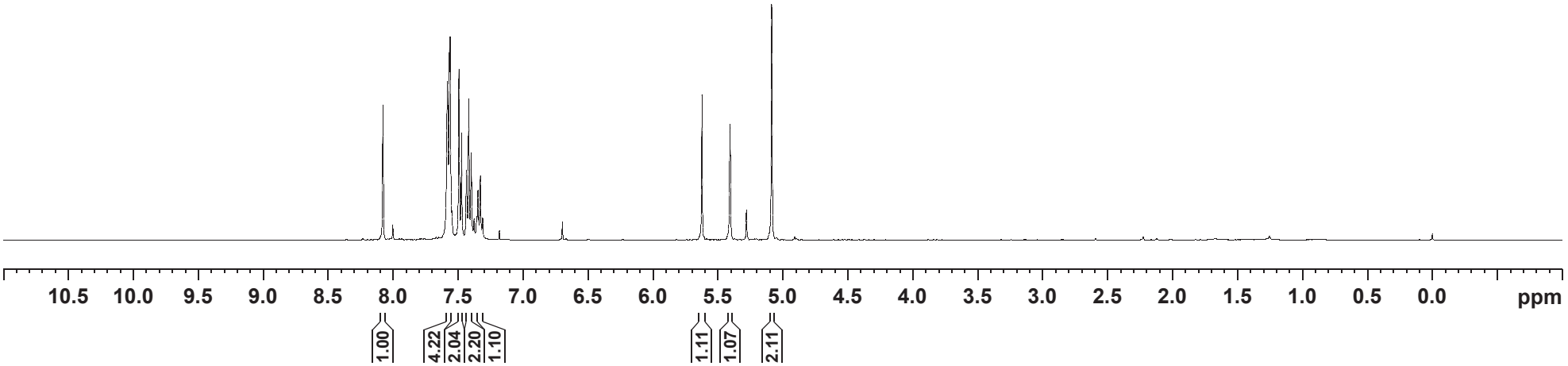

8.084
7.331
7.310
7.169
7.150
5.540
5.345
5.054
2.346
O
O
a12
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.11
2.17
1.03
1.06
2.10
3.11

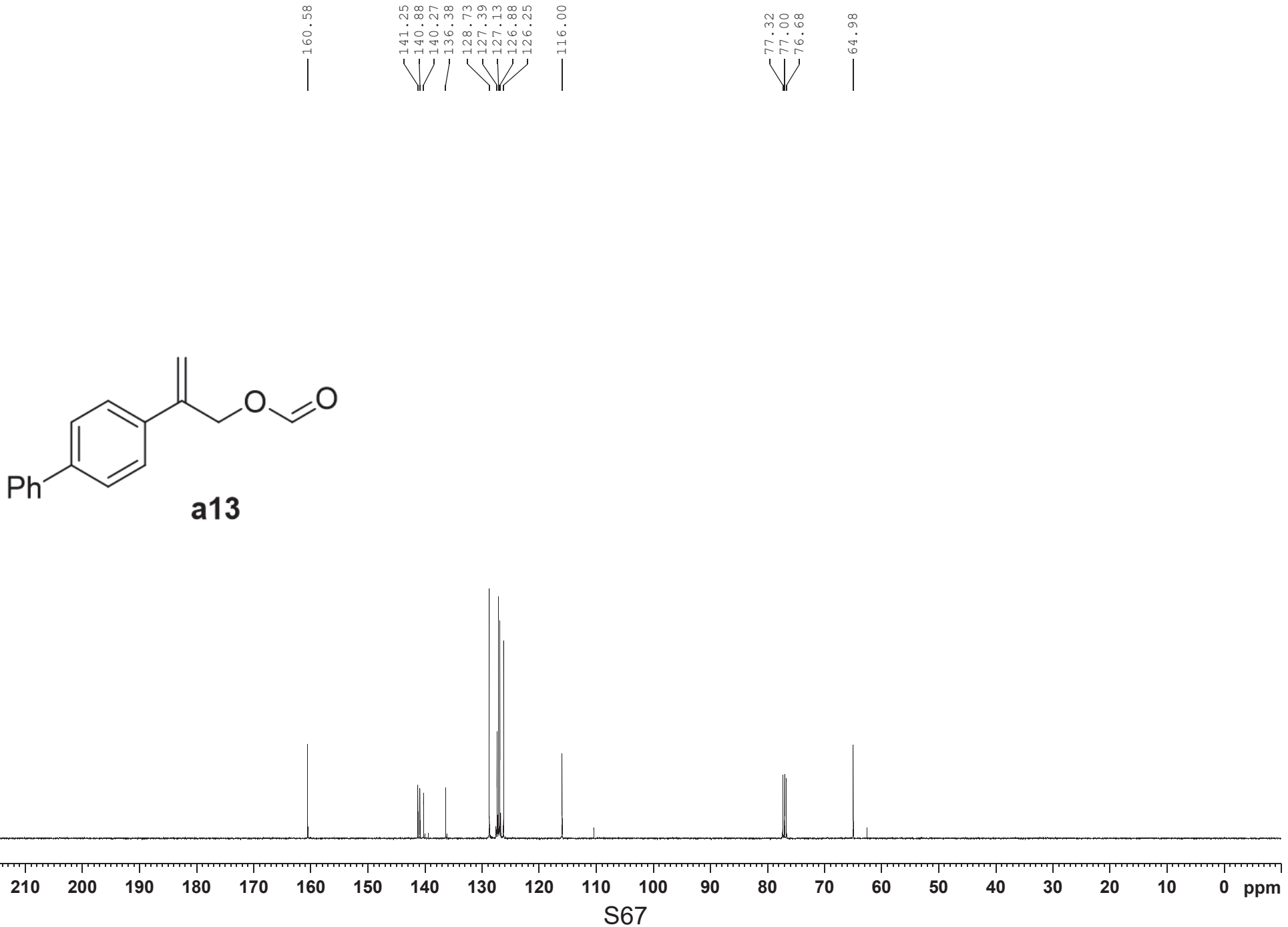

160.62
141.65
138.06
134.74
129.21
125.78
115.17
77.32
77.00
76.68
65.16
21.08
O
O
a12
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

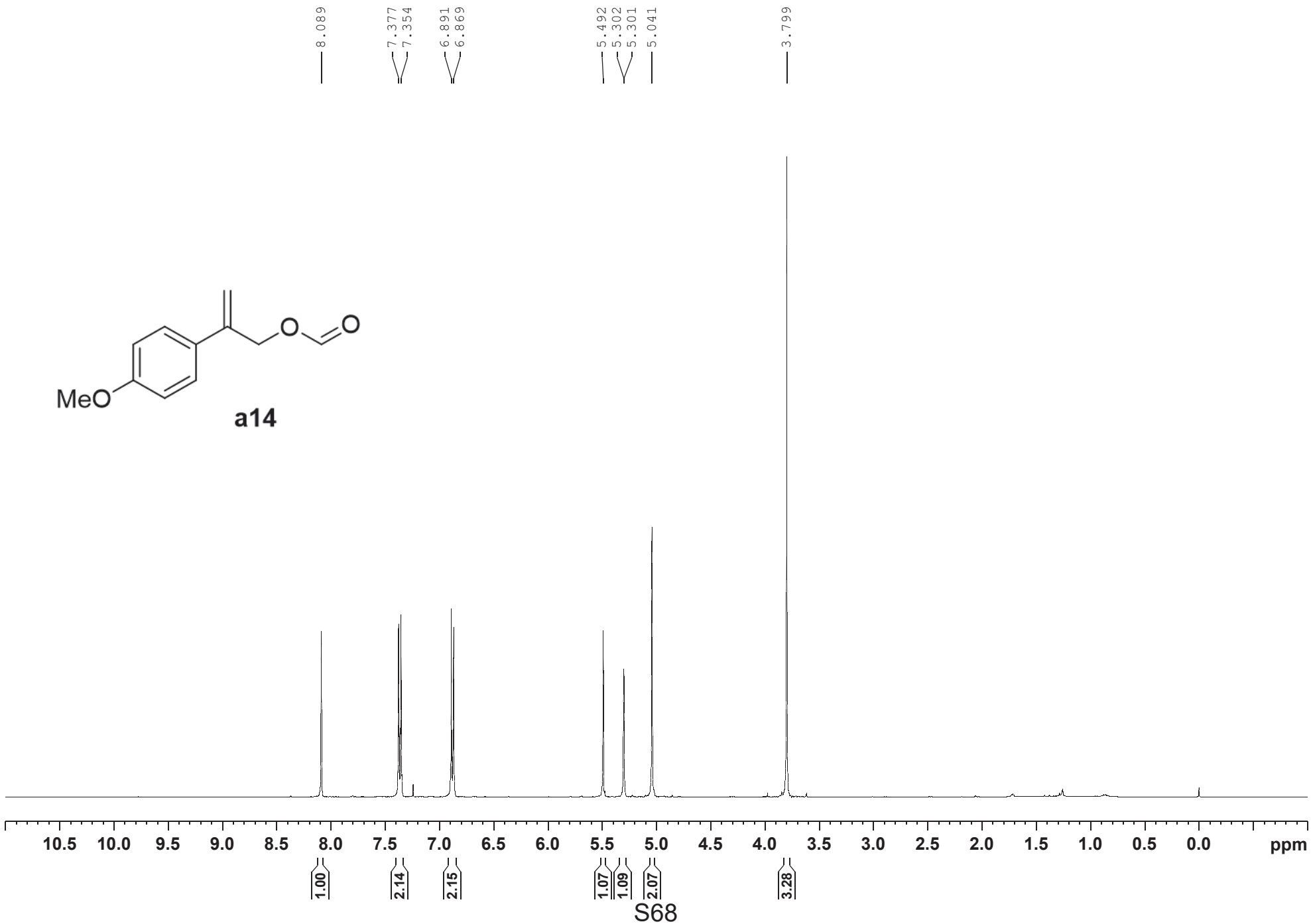

8.079
7.582
7.566
7.561
7.494
7.473
7.436
7.418
7.399
7.347
7.329
7.311
5.623
5.407
5.085

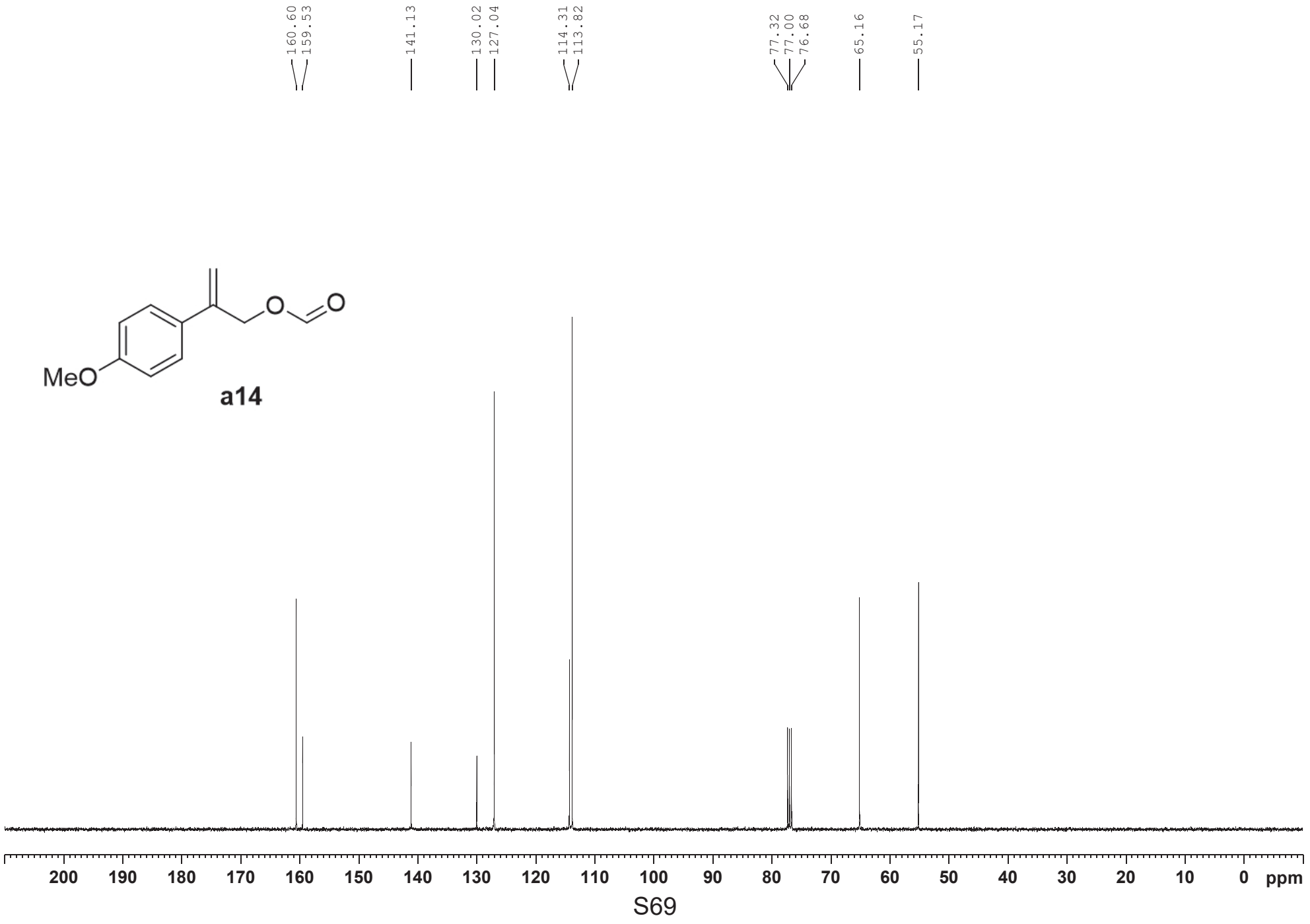

O
O
Ph

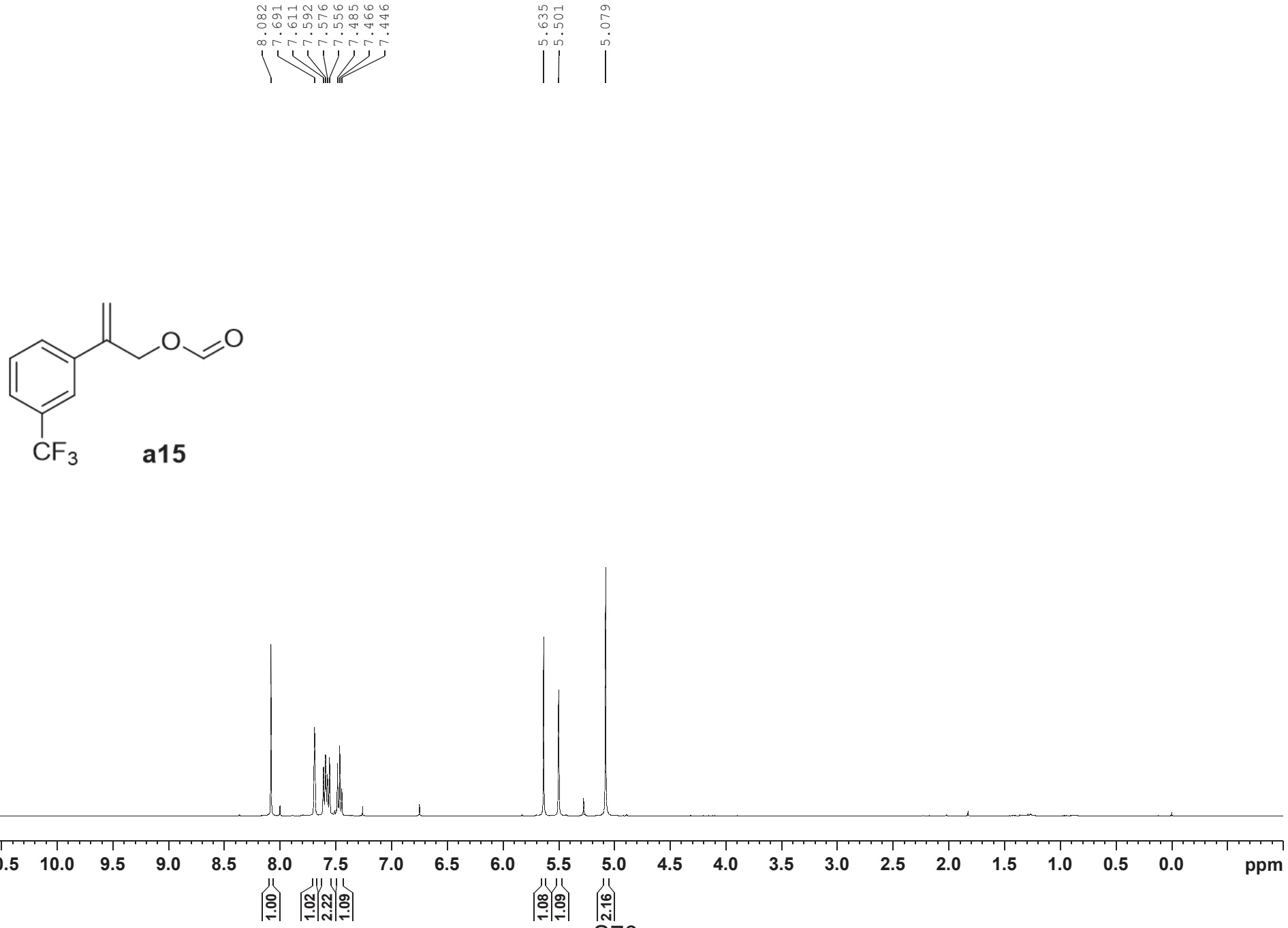
a13

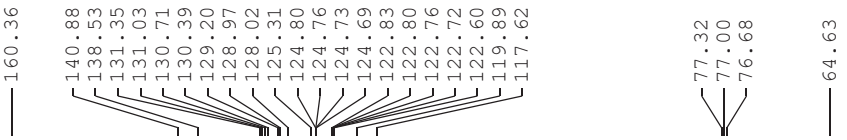

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.22
2.04
2.20
1.10
1.11
1.07
2.11

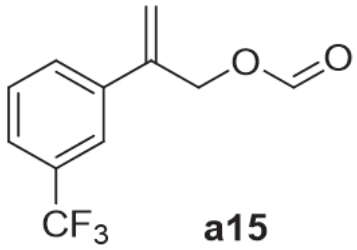

160.58
141.25
140.88
140.27
136.38
128.73
127.39
127.13
126.88
126.25
116.00
77.32
77.00
76.68
64.98
O
O
Ph
a13
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.089
7.377
7.354
6.891
6.869
5.492
5.302
5.301
5.041
3.799
MeO
O
O
a14
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.14
2.15
1.07
1.09
2.07
3.28

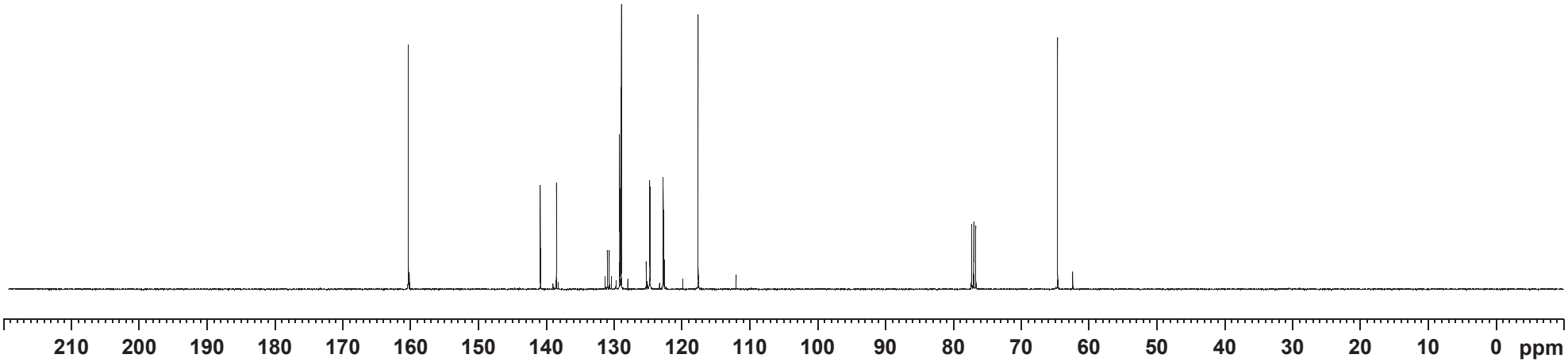

160.60
159.53
141.13
130.02
127.04
114.31
113.82
77.32
77.00
76.68
65.16
55.17
MeO
O
O
a14
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

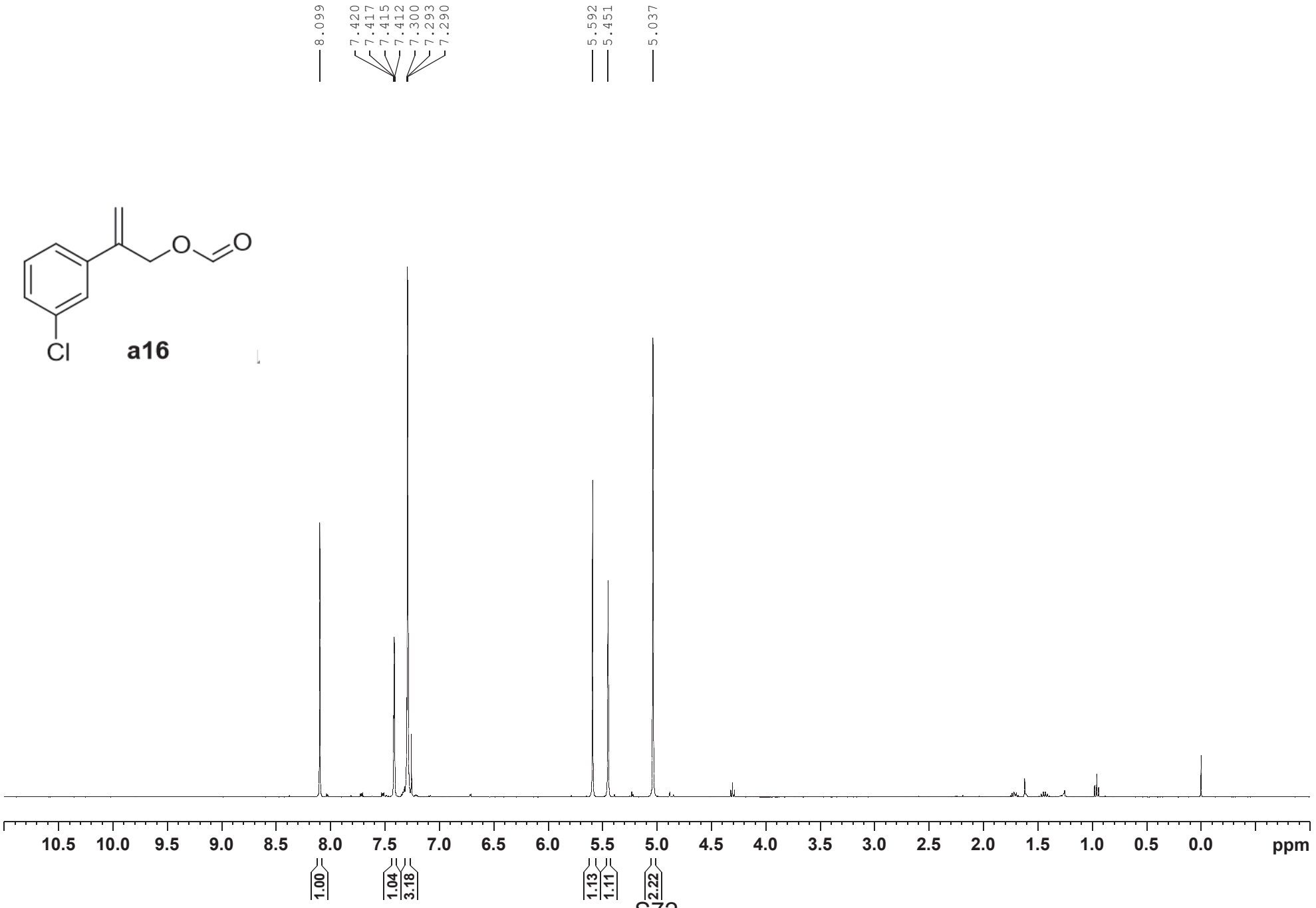

8.082
7.691
7.611
7.592
7.576
7.556
7.485
7.466
7.446
5.635
5.501
5.079
O
O
CF3
a15
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.02
2.22
1.09
1.08
1.09
2.16

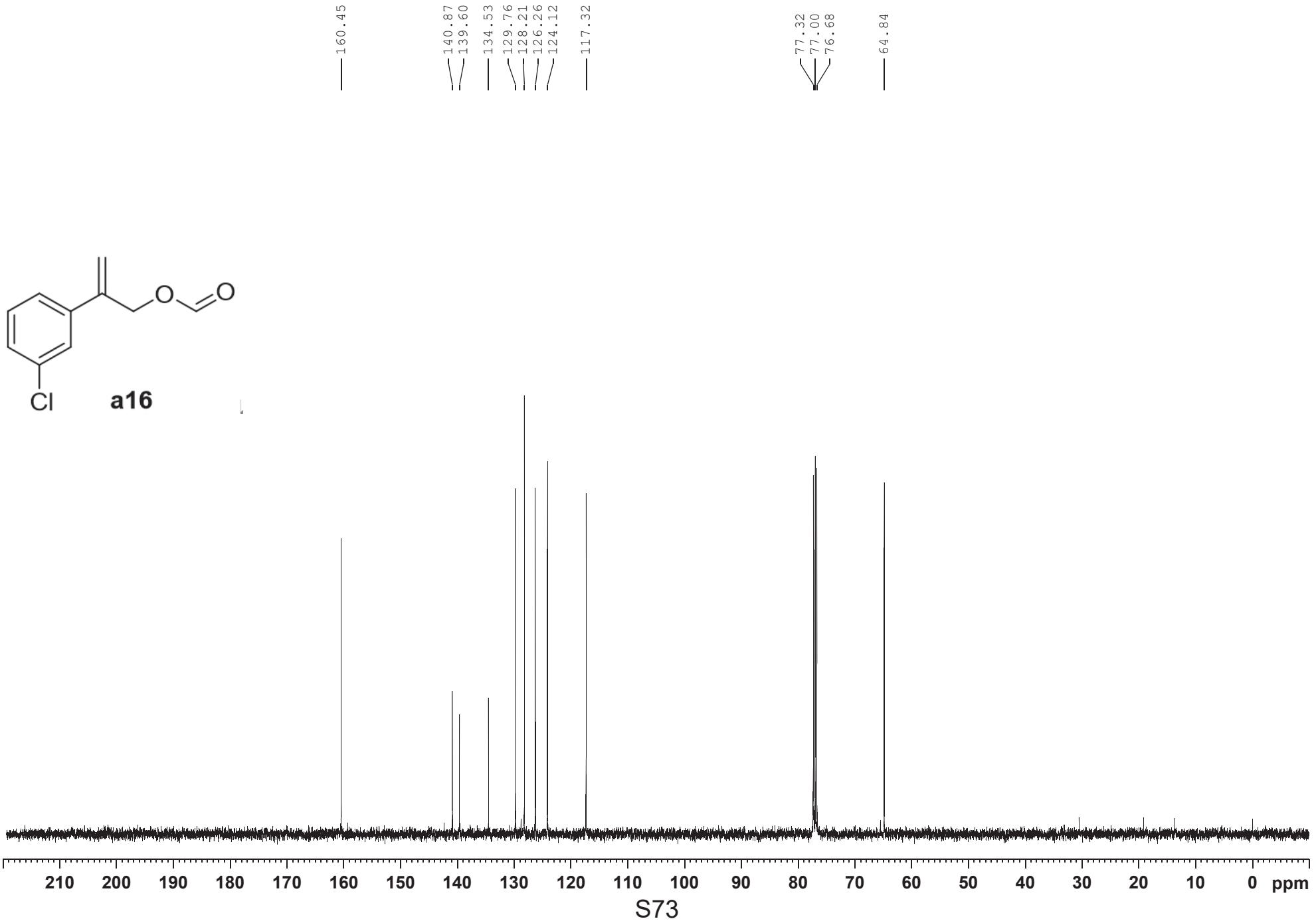

160.36
140.88
138.53
131.35
131.03
130.71
130.39
129.20
128.97
128.02
125.31
124.80
124.76
124.73
124.69
122.83
122.80
122.76
122.72
122.60
119.89
117.62
77.32
77.00
76.68
64.63

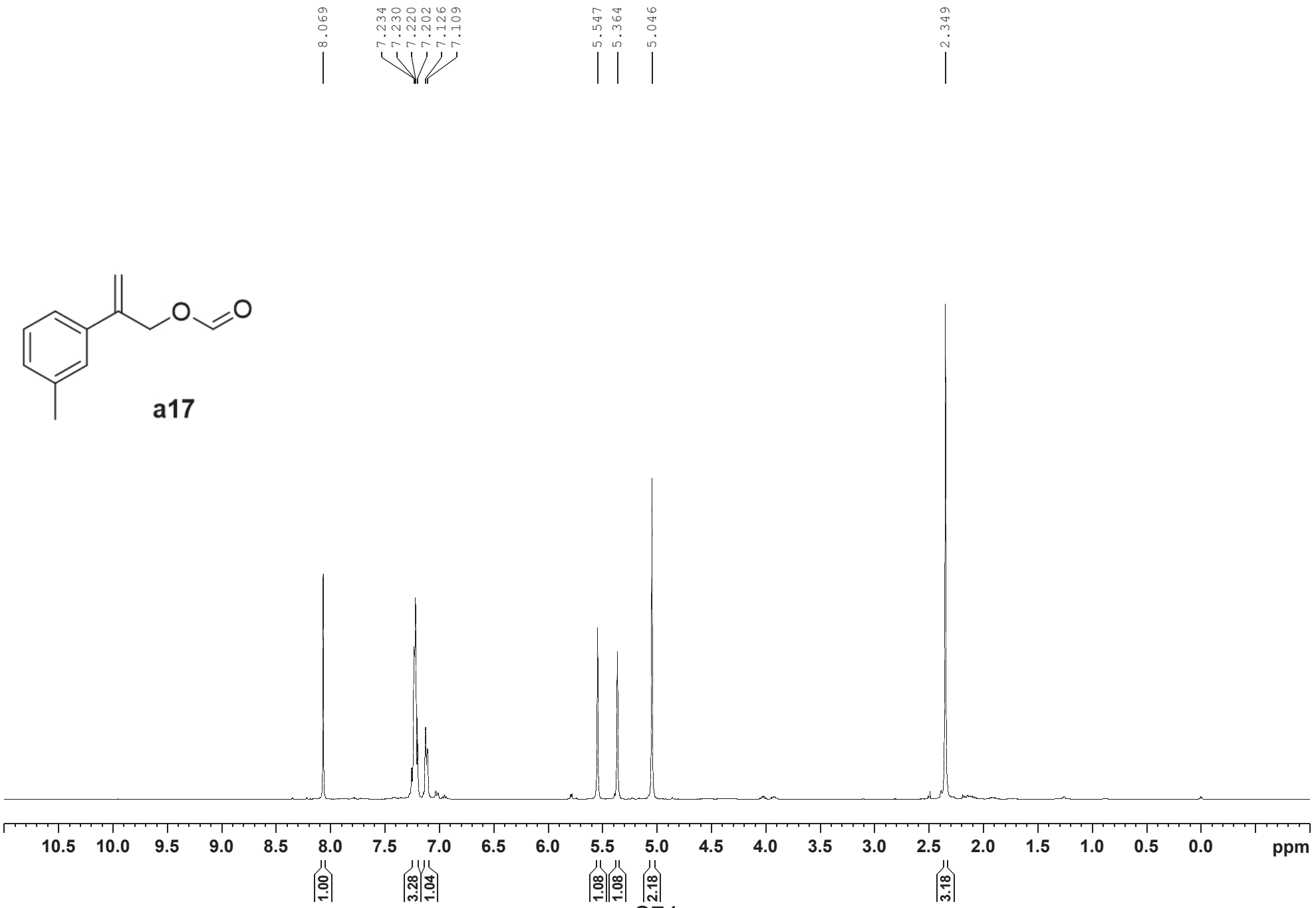

O
O
CF3

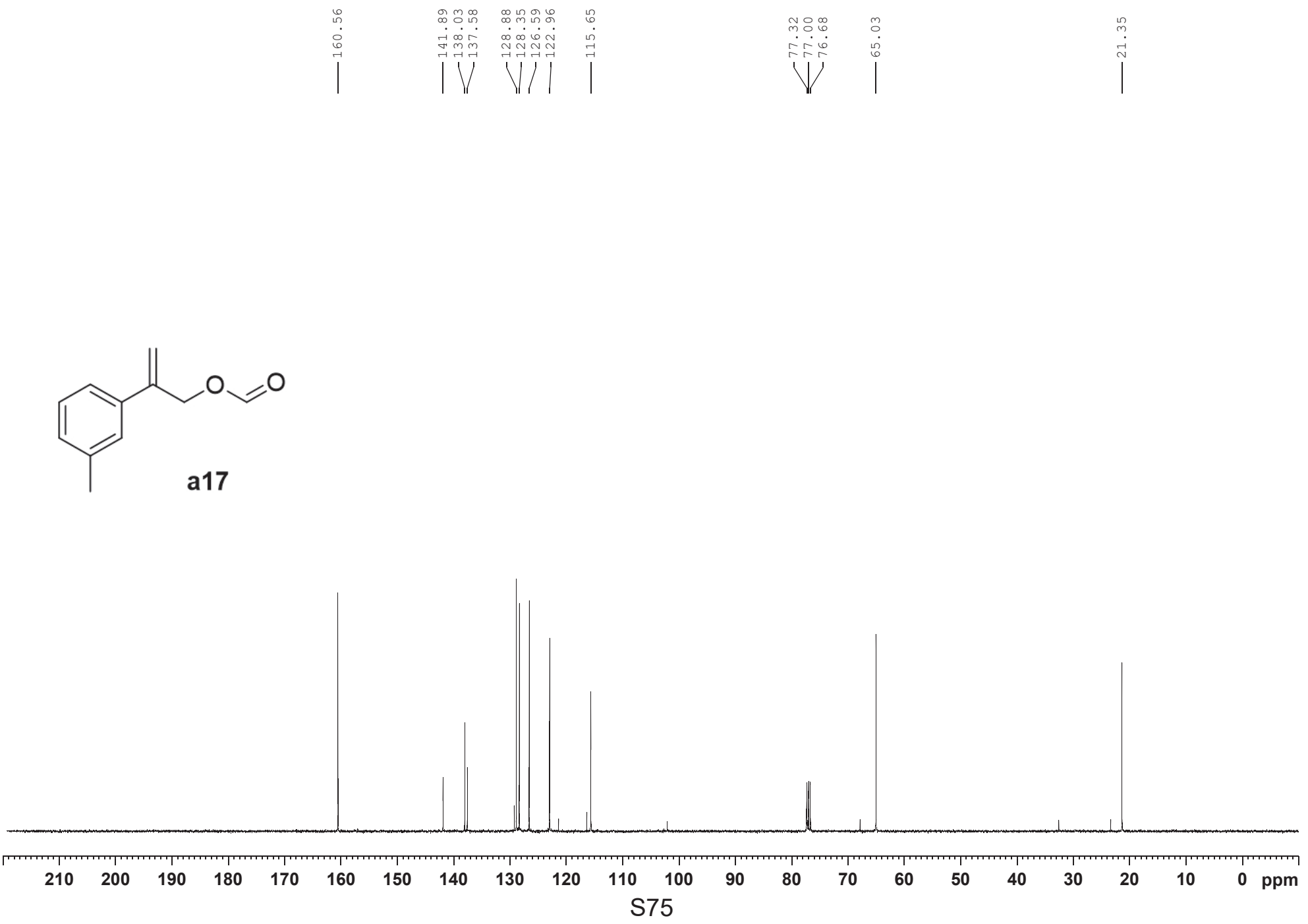
a15

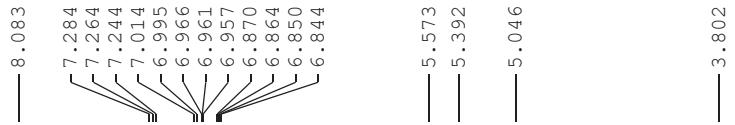

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

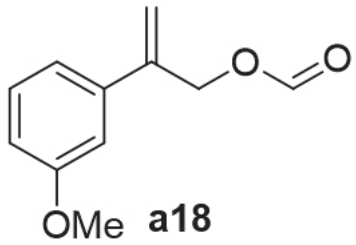

8.099
7.420
7.417
7.415
7.412
7.300
7.293
7.290
5.592
5.451
5.037
Cl
a16
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.04
3.18
1.13
1.11
2.22


160.45
140.87
139.60
134.53
129.76
128.21
126.26
124.12
117.32
77.32
77.00
76.68
64.84
O
O
Cl
a16
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

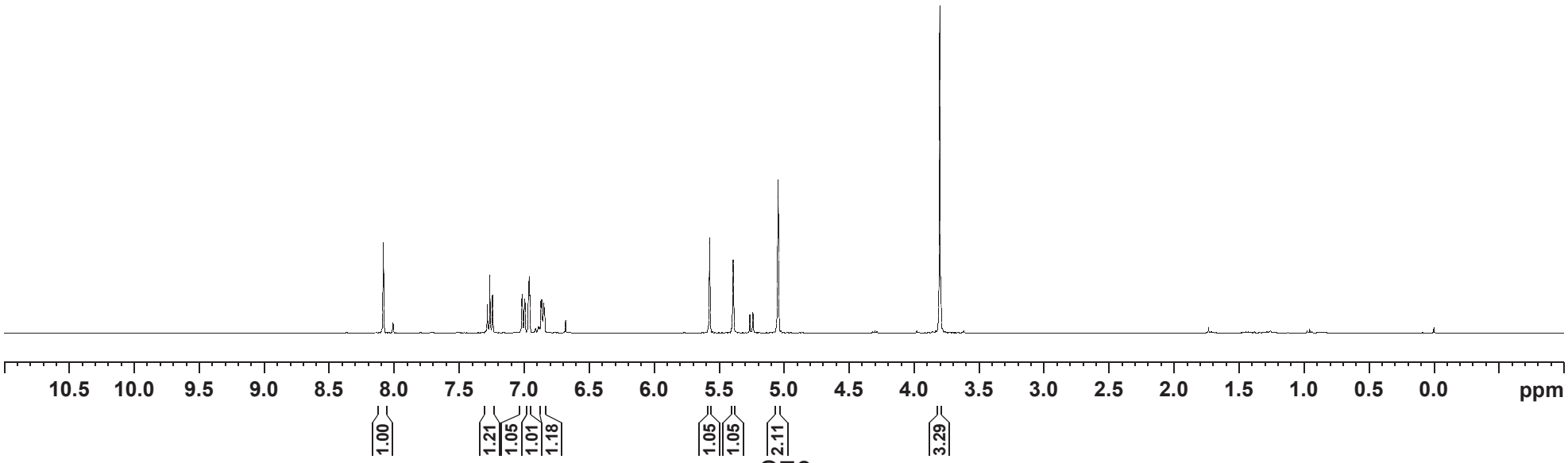

8.069
7.234
7.230
7.220
7.202
7.126
7.109
5.547
5.364
5.046
2.349
a17
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
3.28
1.04
1.08
1.08
2.18
3.18

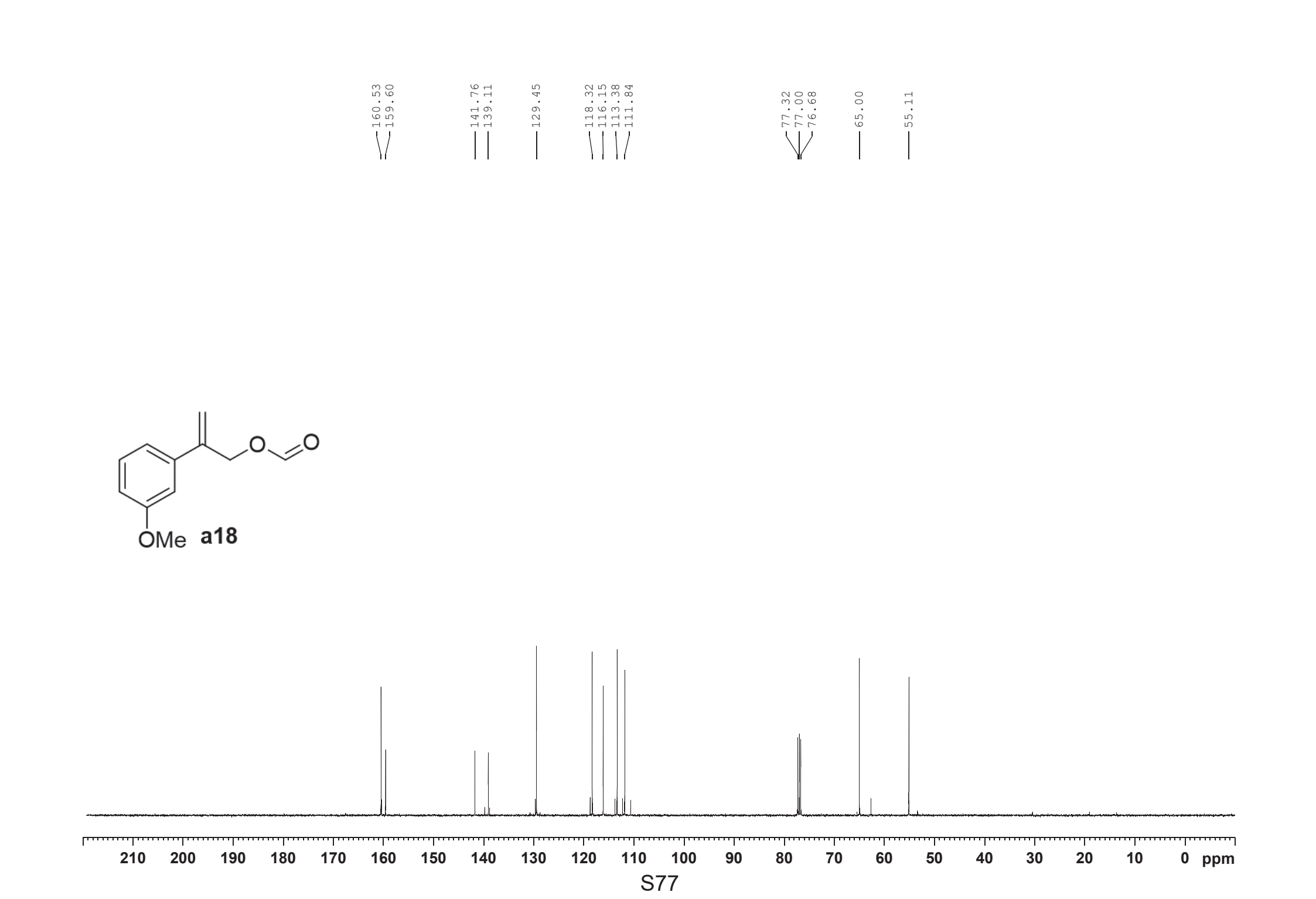

160.56
141.89
138.03
137.58
128.88
128.35
126.59
122.96
115.65
77.32
77.00
76.68
65.03
21.35
O
O
a17
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.083
7.284
7.264
7.244
7.014
6.995
6.966
6.961
6.957
6.870
6.864
6.850
6.844
5.573
5.392
5.046
3.802

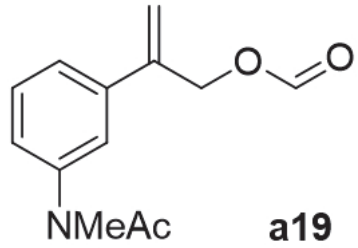

O
O
OMe

a18

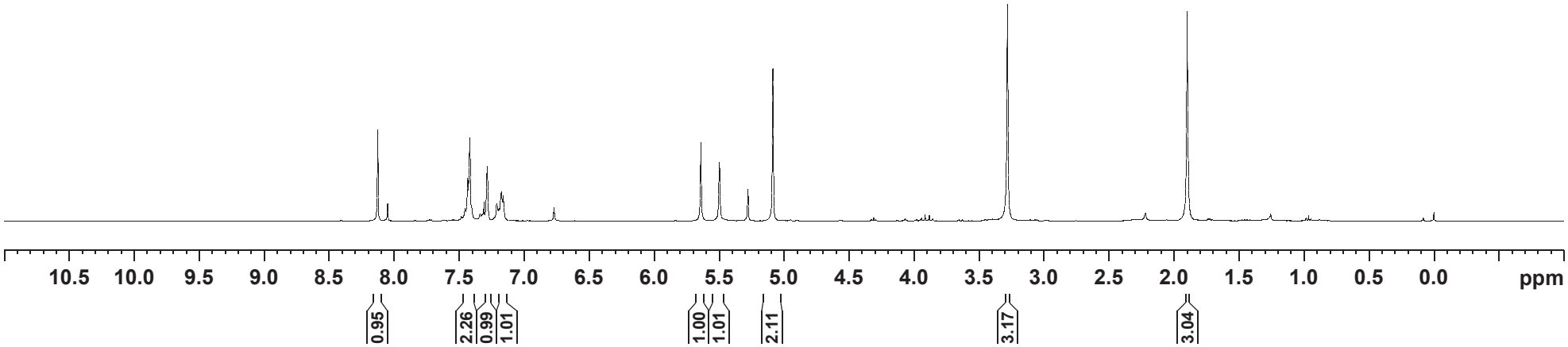

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.21
1.05
1.01
1.18
1.05
1.05
2.11
3.29

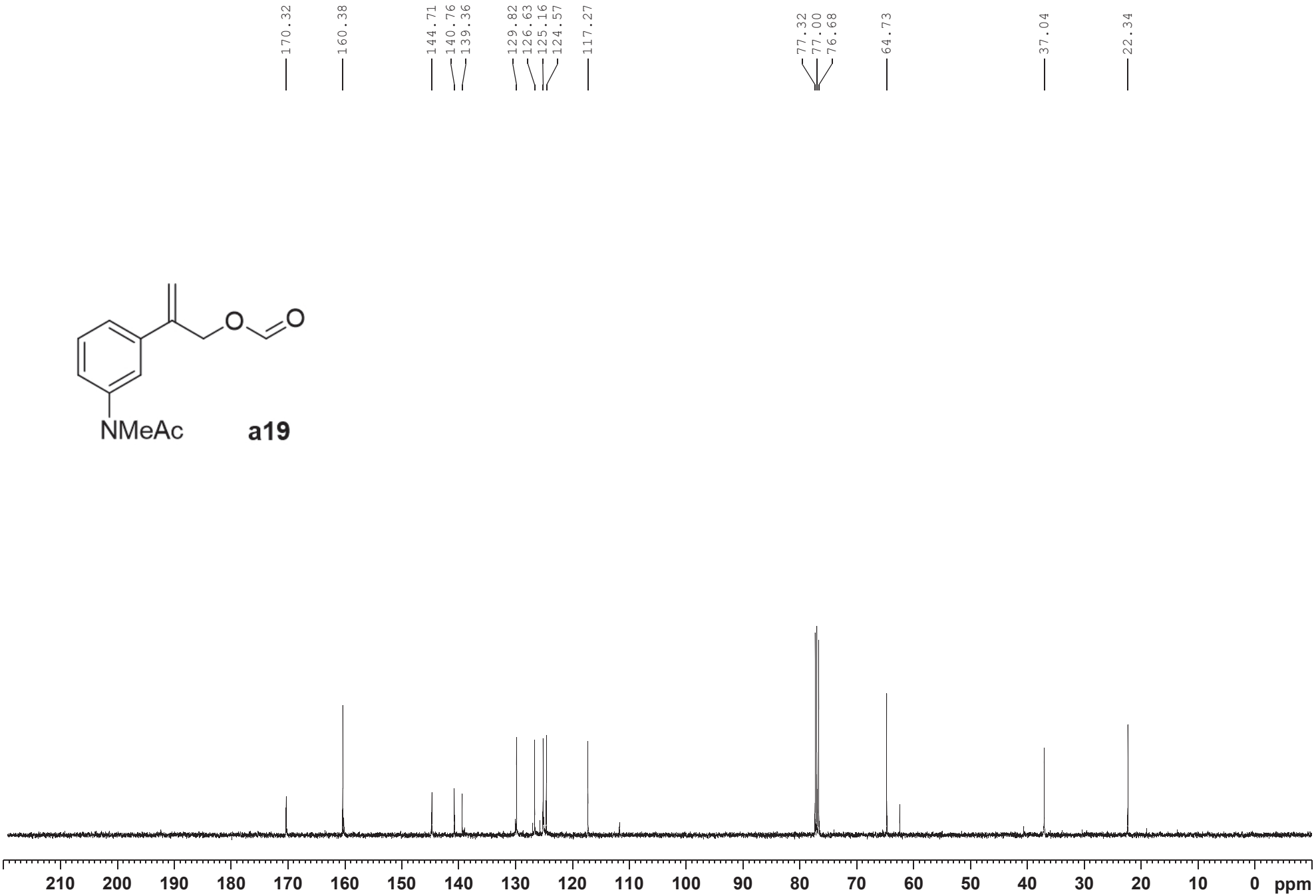

160.53
159.60
141.76
139.11
129.45
118.32
116.15
113.38
111.84
77.32
77.00
76.68
65.00
55.11
OMe
a18
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

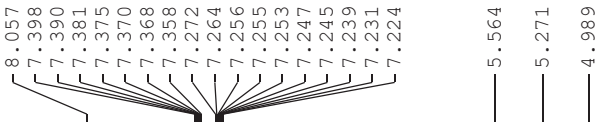

8.126
7.454
7.435
7.419
7.285
7.181
7.176
7.166
7.160
5.640
5.498
5.087
3.282
1.898

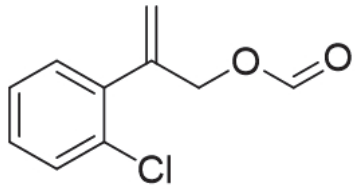

O
O
NMeAc

a19

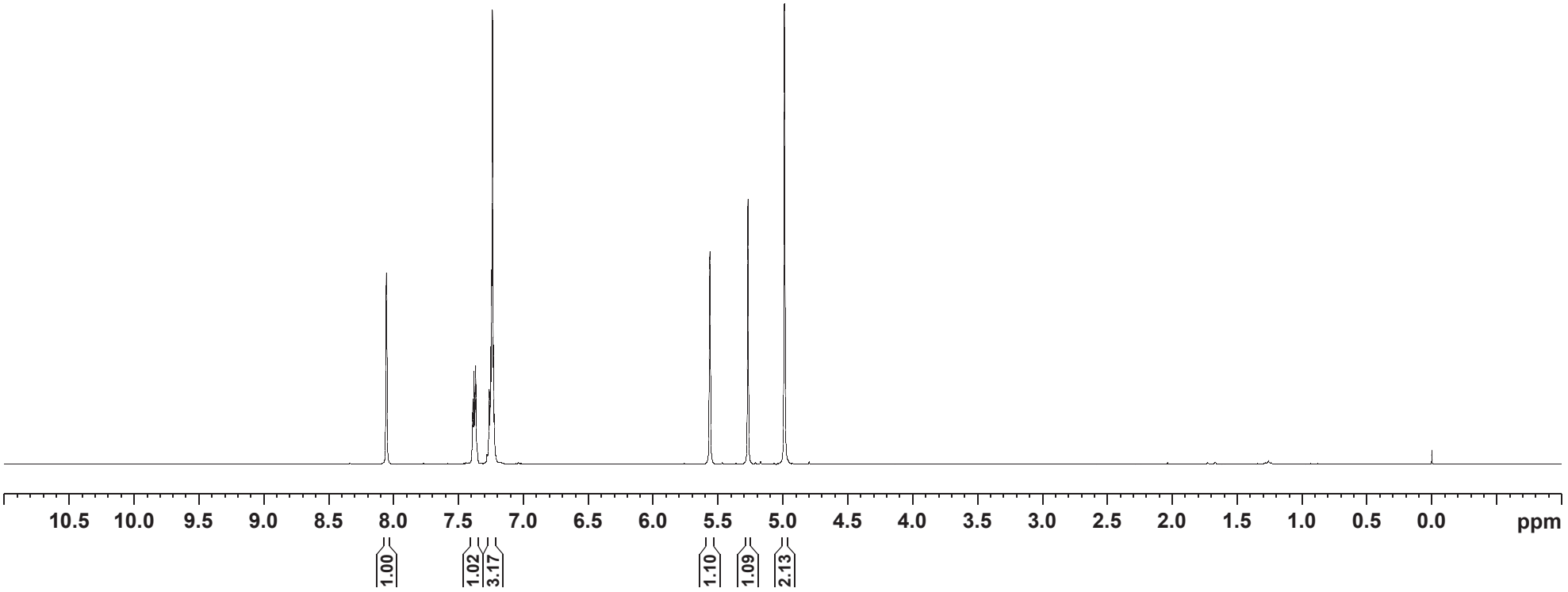

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.95
2.26
0.99
1.01
1.00
1.01
2.11
3.17
3.04

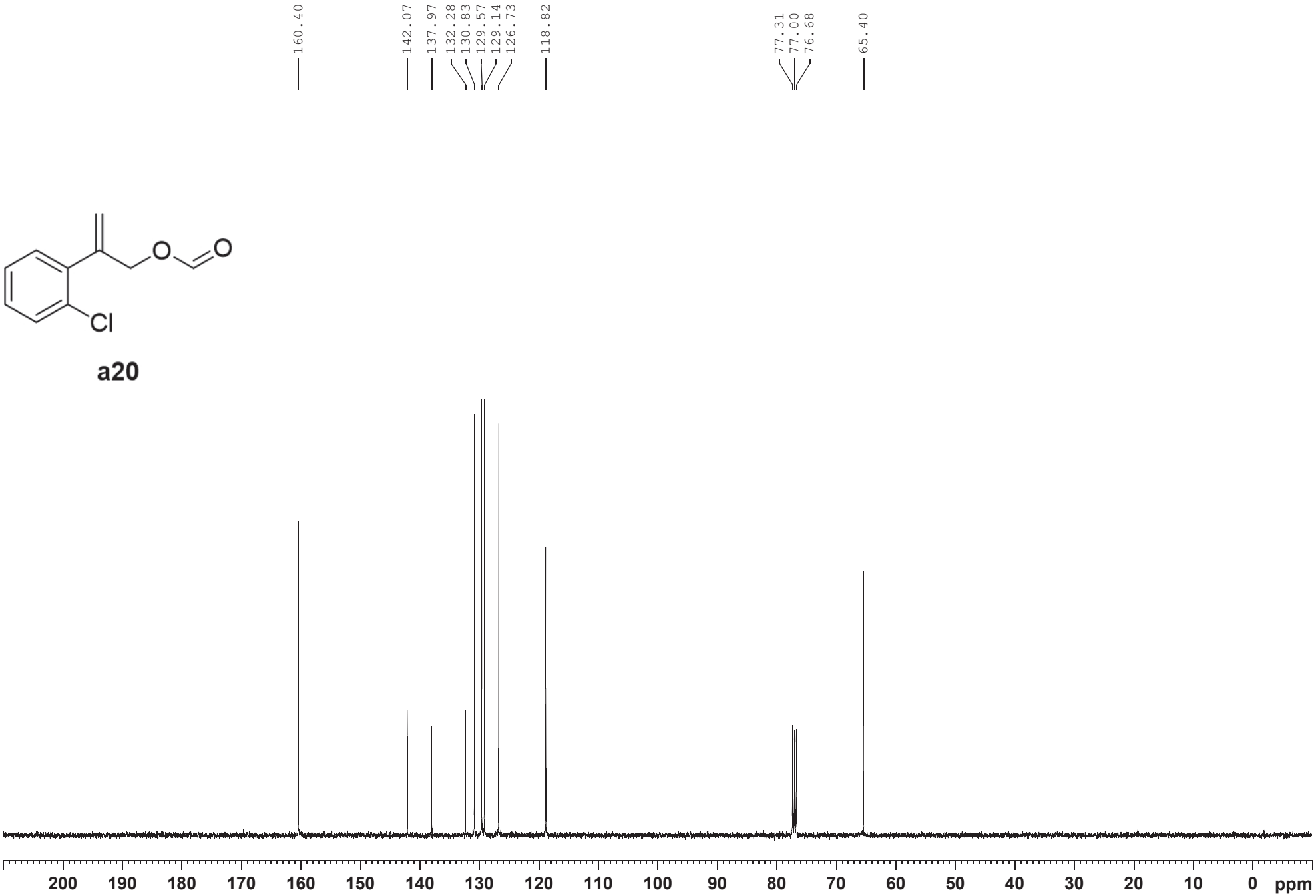

170.32
160.38
144.71
140.76
139.36
129.82
126.63
125.16
124.57
117.27
77.32
77.00
76.68
64.73
37.04
22.34
O
O
NMeAc
a19
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

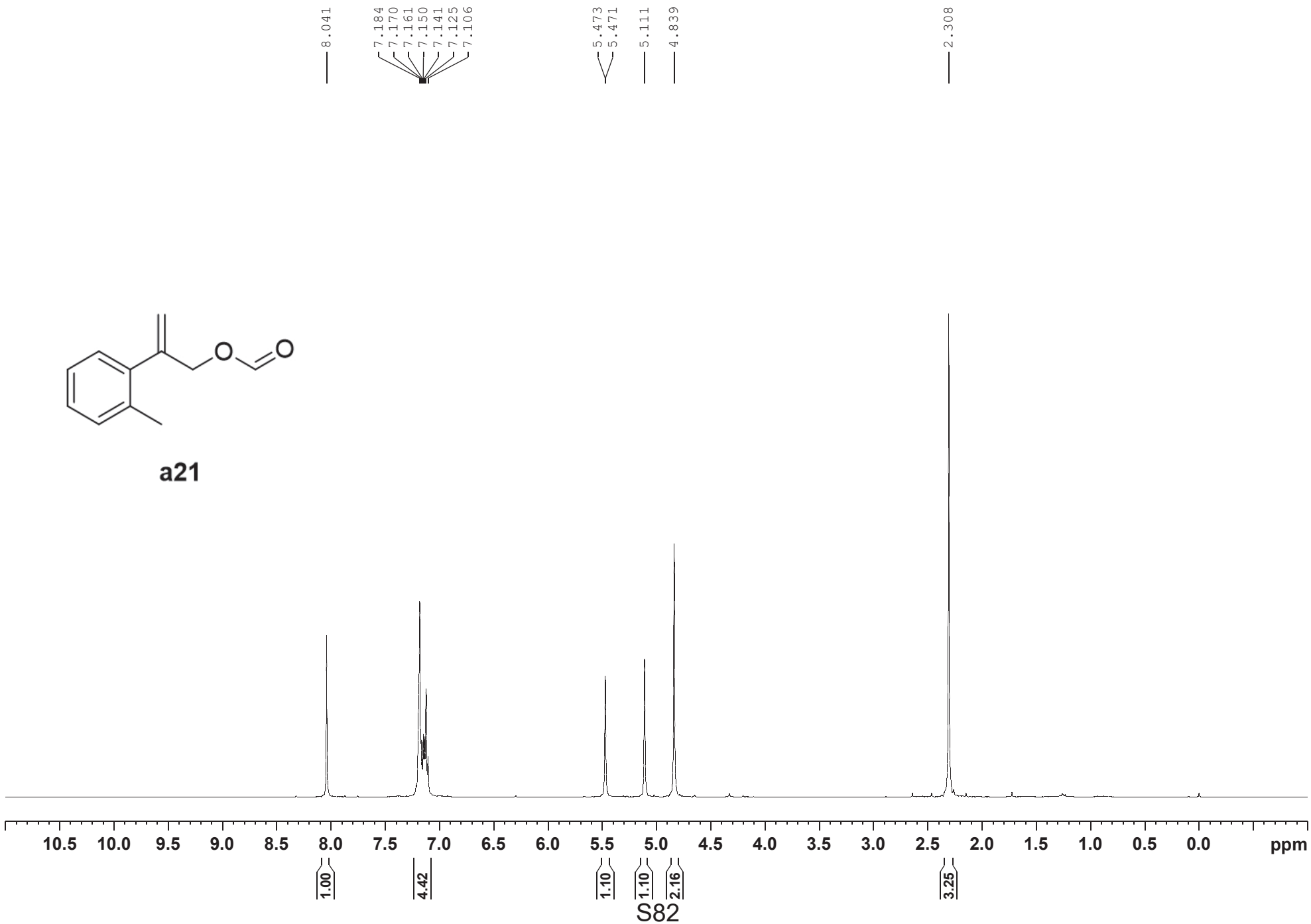

8.057
7.398
7.390
7.381
7.375
7.370
7.368
7.358
7.272
7.264
7.256
7.255
7.253
7.247
7.245
7.239
7.231
7.224
5.564
5.271
4.989

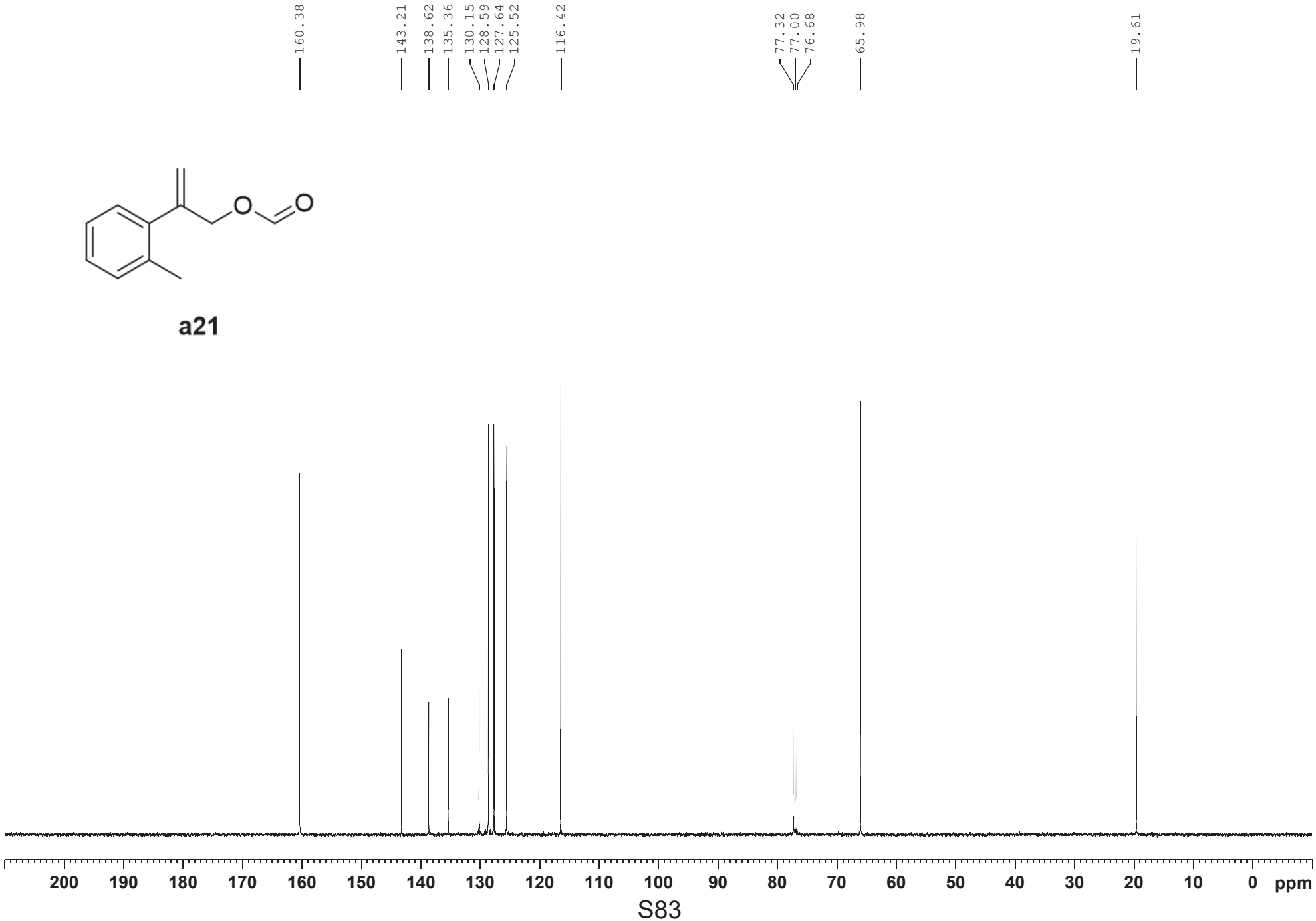

O
O
Cl

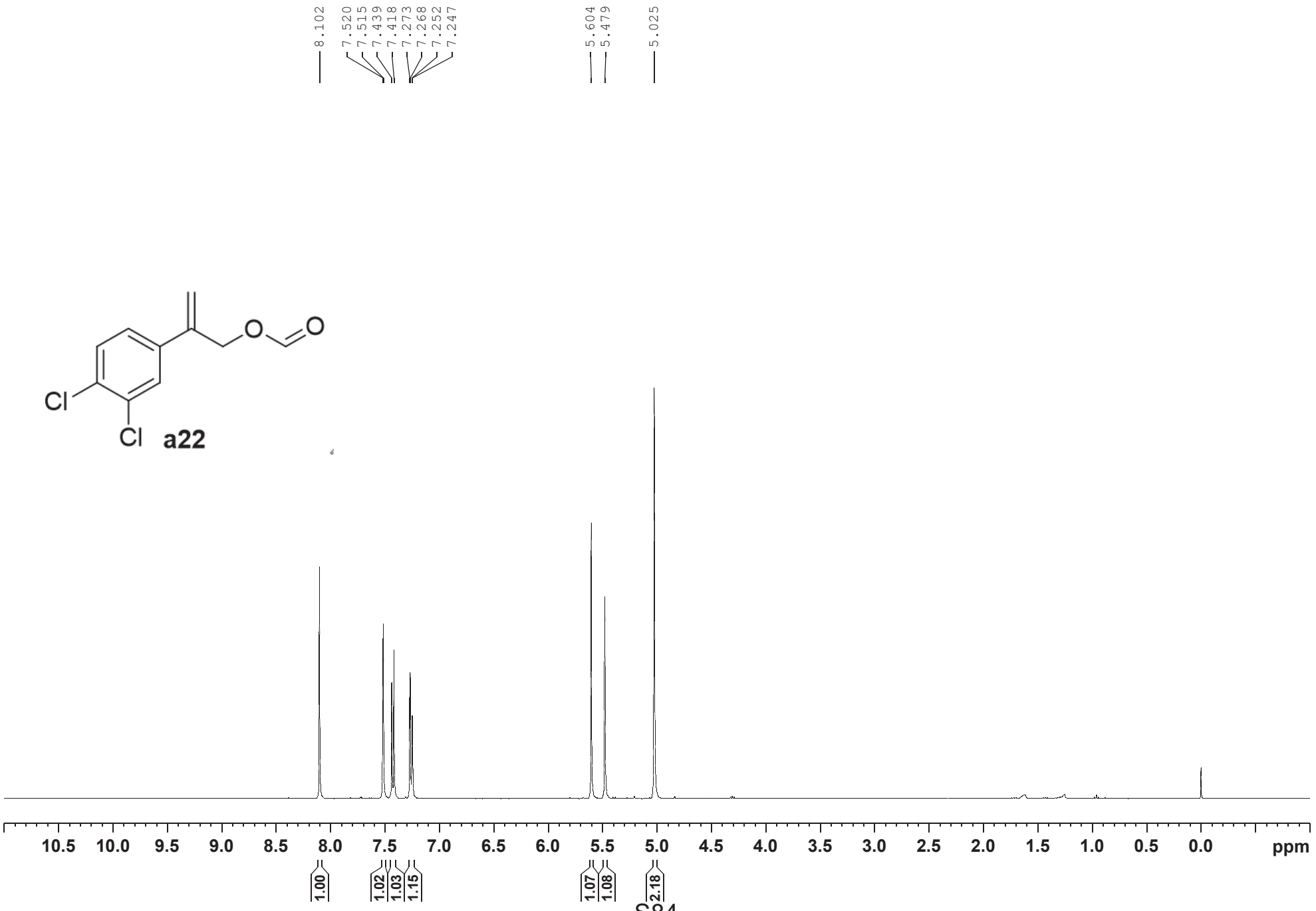
a20

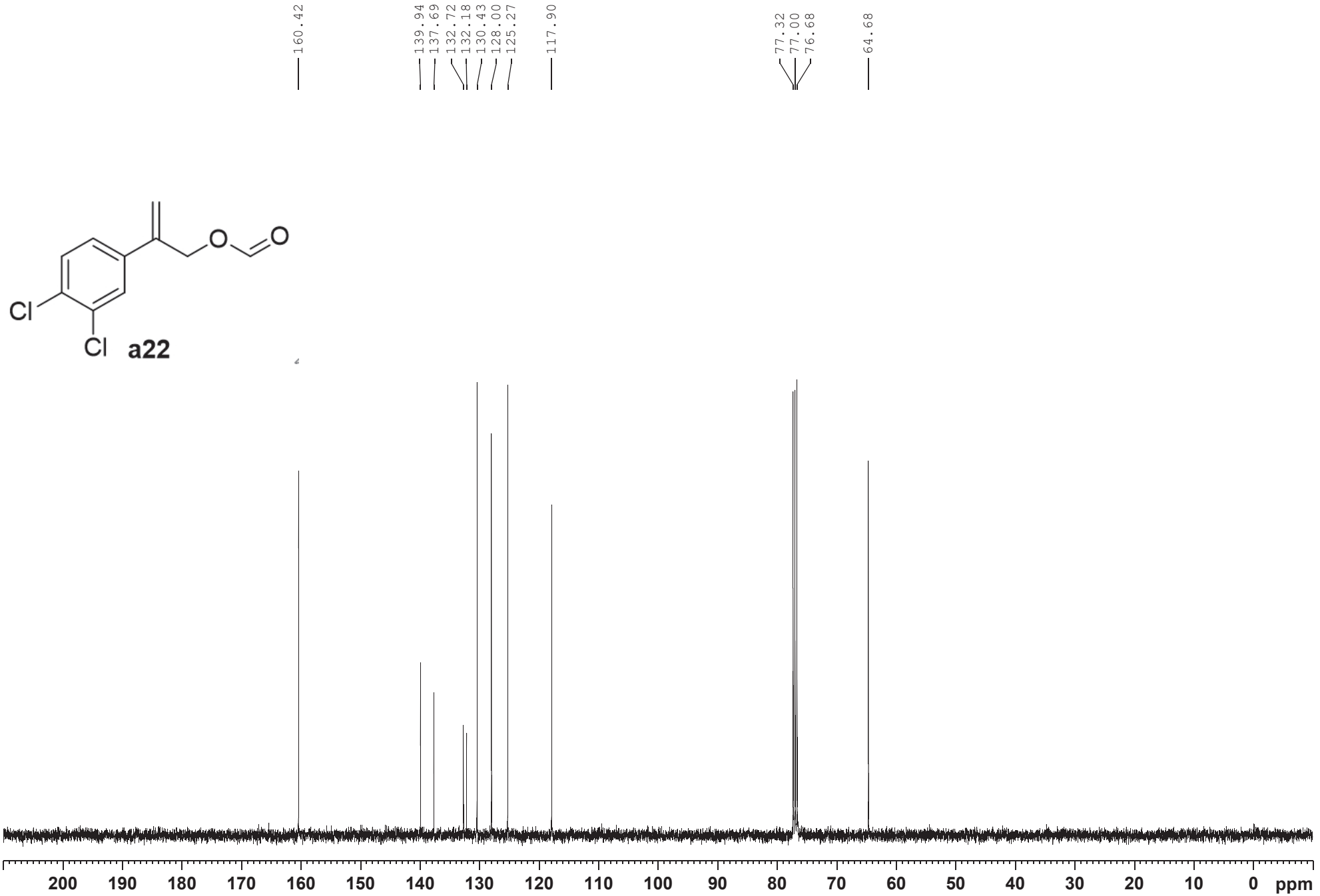

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.02
3.17
1.10
1.09
2.13

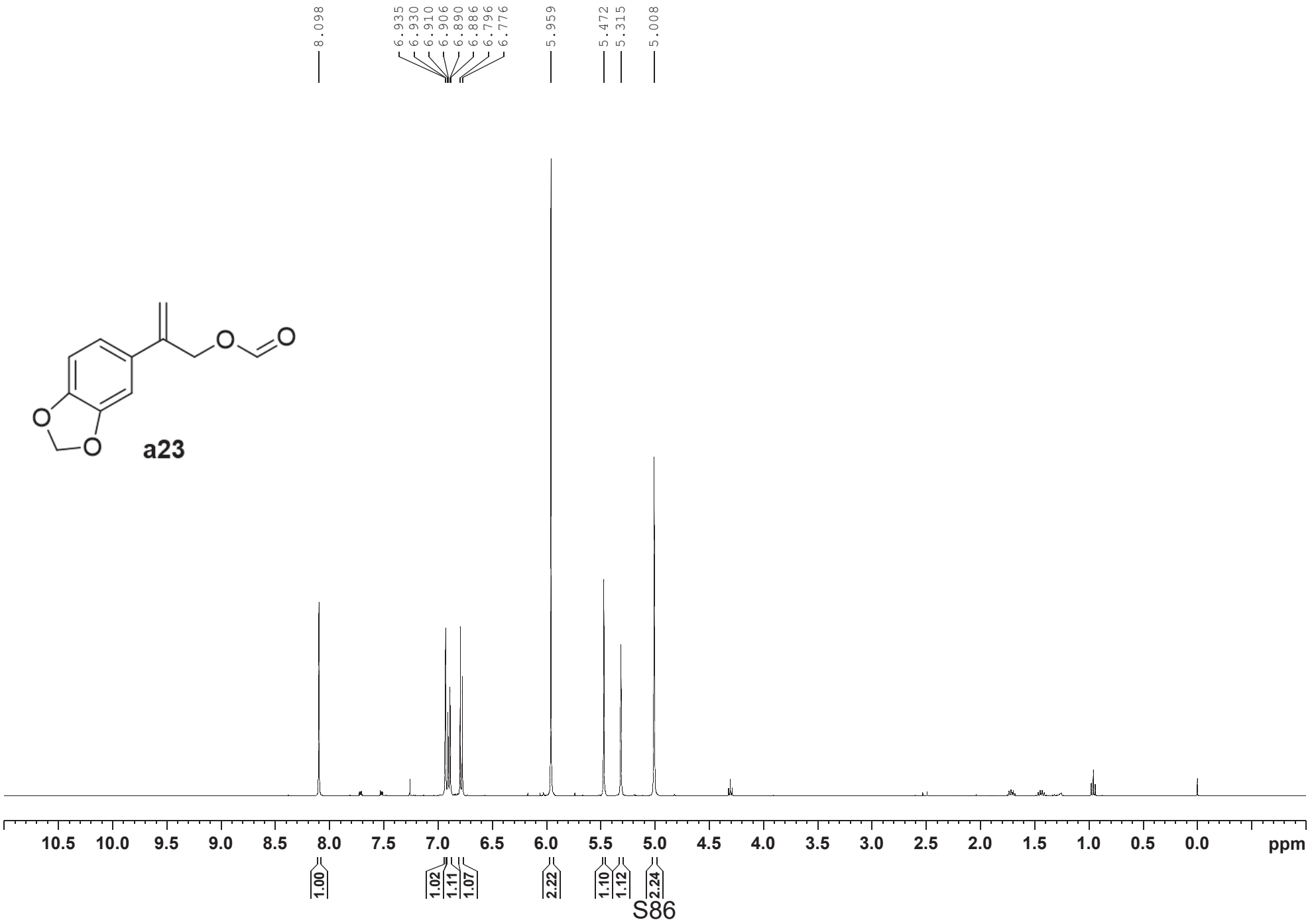

160.40
142.07
137.97
132.28
130.83
129.57
129.14
126.73
118.82
77.31
77.00
76.68
65.40
O
O
Cl
a20
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

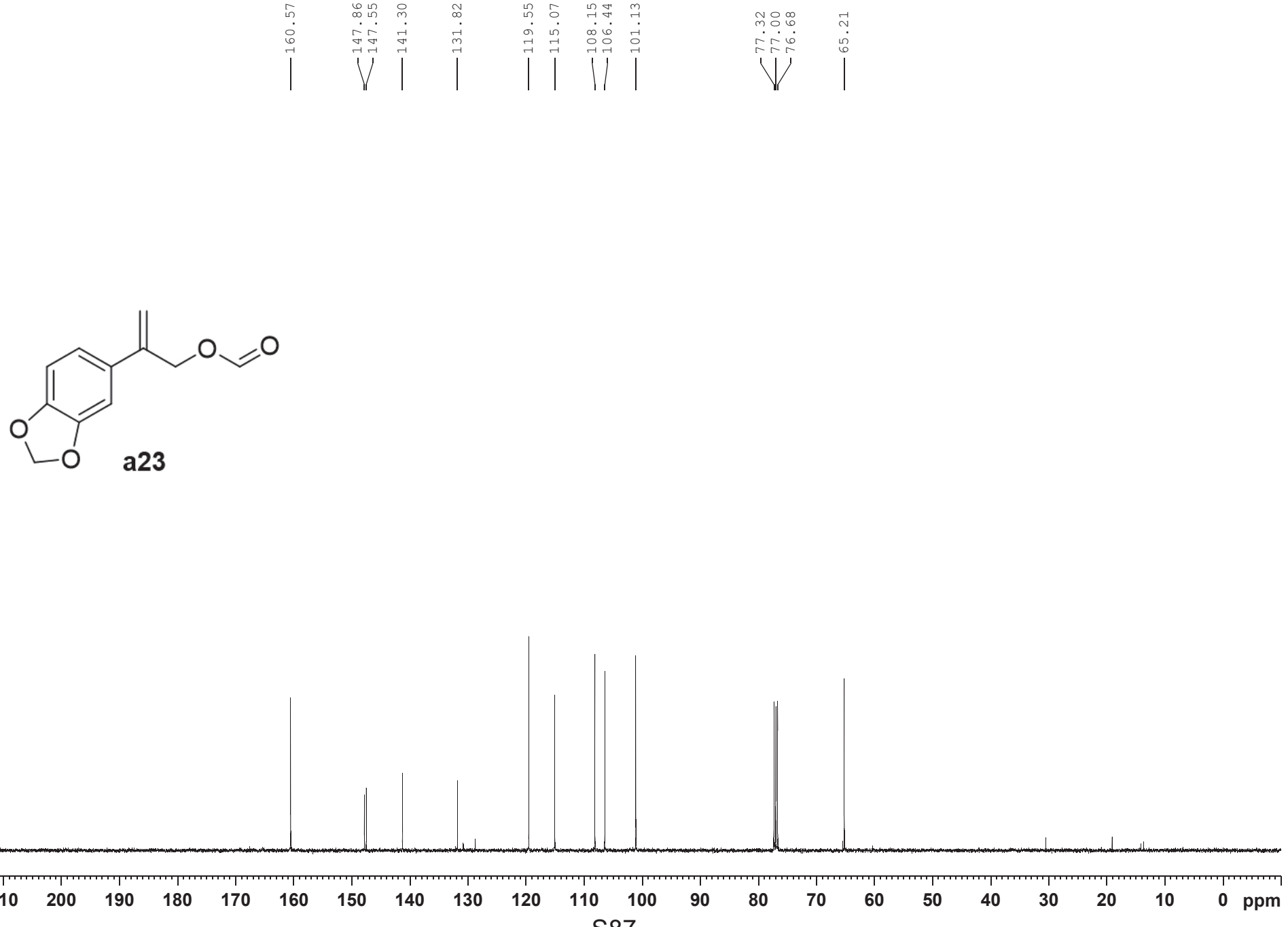

8.041
7.184
7.170
7.161
7.150
7.141
7.125
7.106
5.473
5.471
5.111
4.839
2.308
a21
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.42
1.10
1.10
2.16
3.25

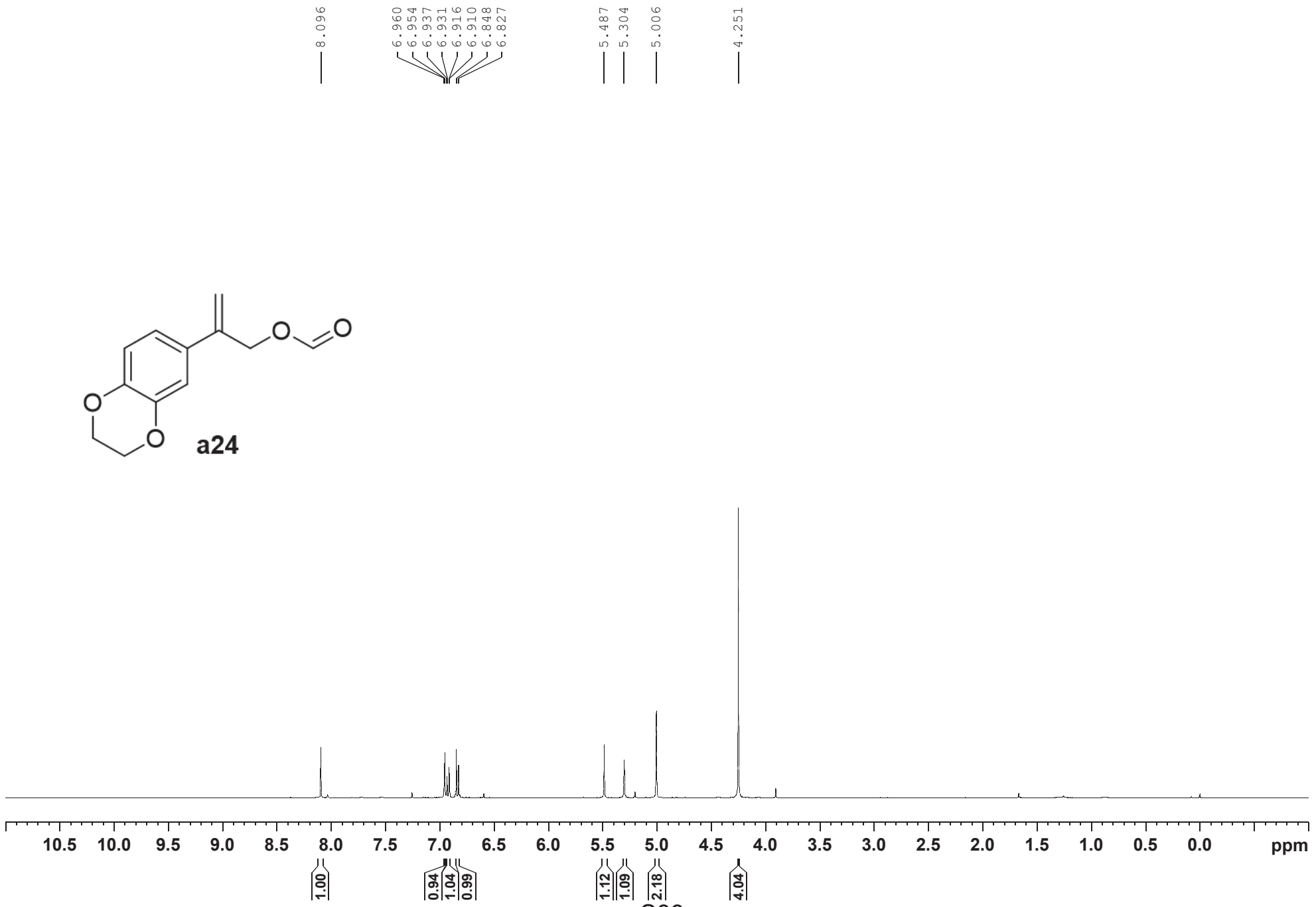

160.38
143.21
138.62
135.36
130.15
128.59
127.64
125.52
116.42
77.32
77.00
76.68
65.98
19.61
O
O
a21
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

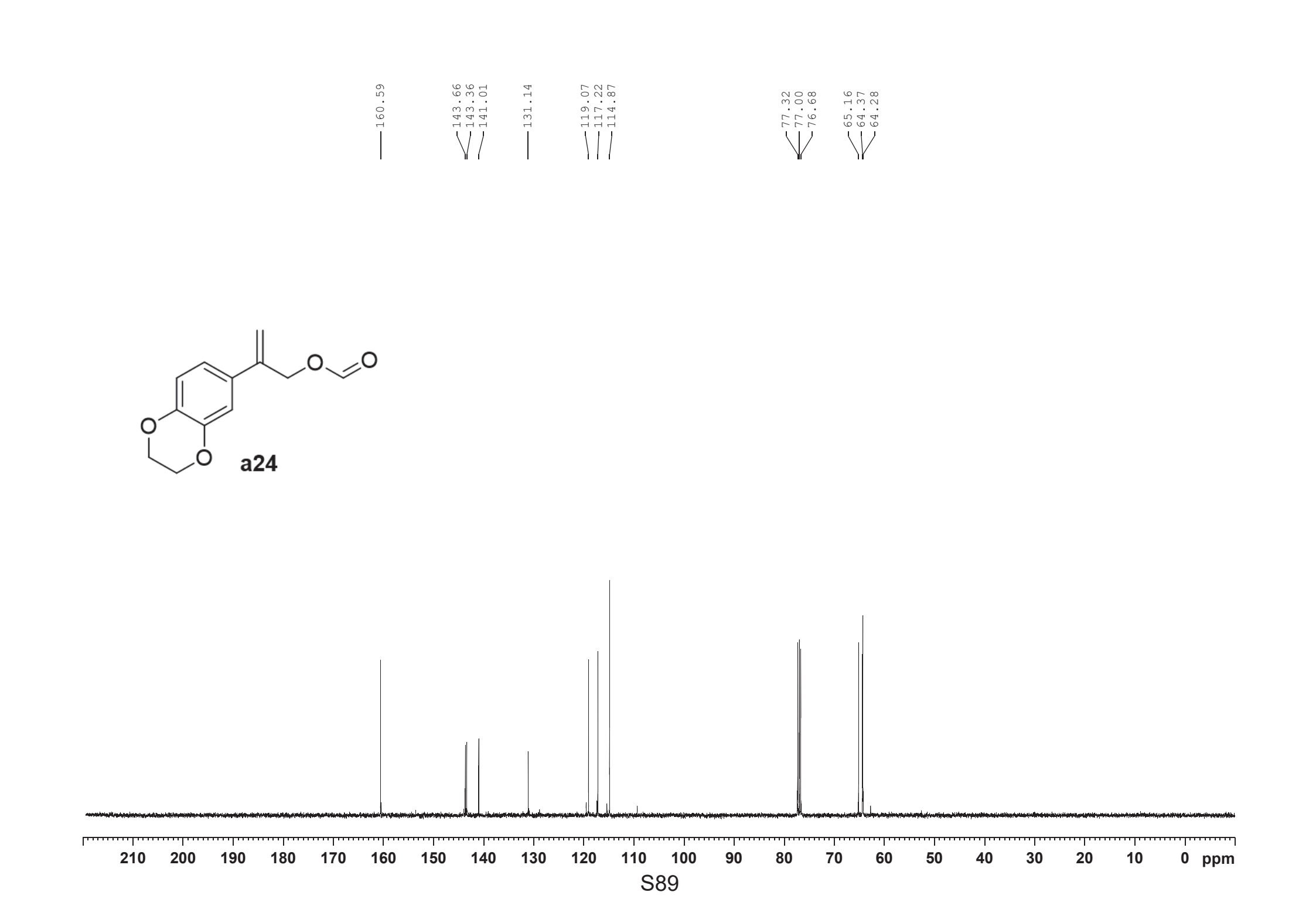

8.102
7.520
7.515
7.439
7.418
7.273
7.268
7.252
7.247
5.604
5.479
5.025
Cl
Cl
O
O
a22
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.02
1.03
1.15
1.07
1.08
2.18

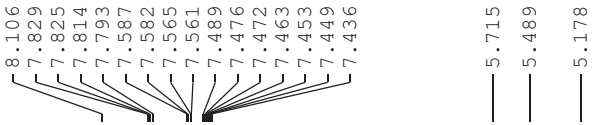

160.42
139.94
137.69
132.72
132.18
130.43
128.00
125.27
117.90
77.32
77.00
76.68
64.68
Cl
Cl
O
O
a22
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

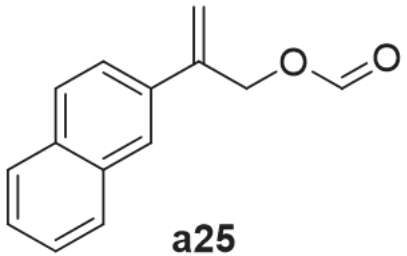

8.098
6.935
6.930
6.910
6.906
6.890
6.886
6.796
6.776
5.959
5.472
5.315
5.008
a23
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.02
1.11
1.07
2.22
1.10
1.12
2.24


160.57
147.86
147.55
141.30
131.82
119.55
115.07
108.15
106.44
101.13
77.32
77.00
76.68
65.21
a23
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

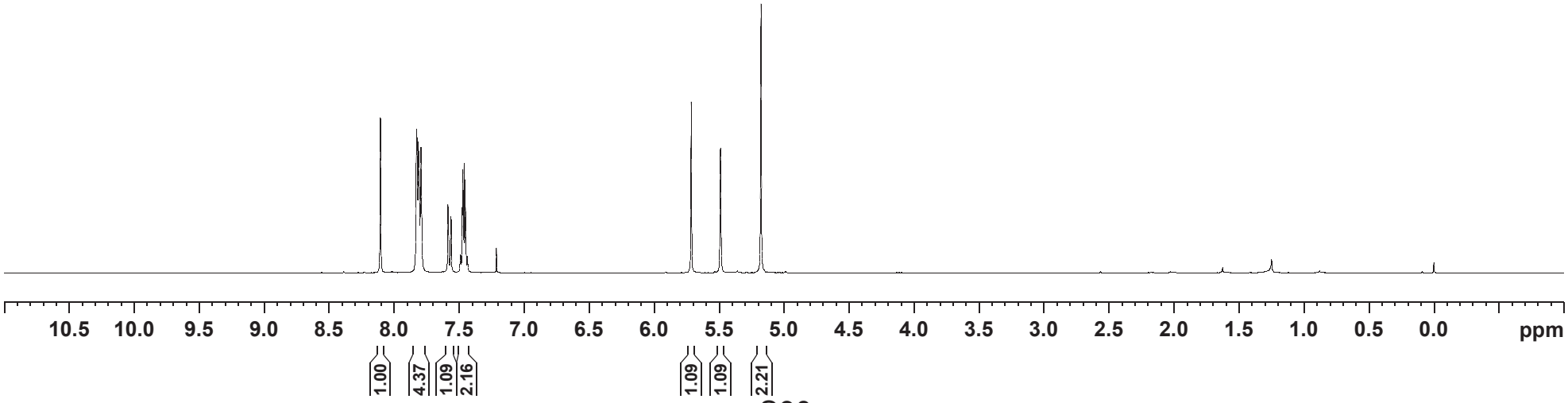

8.096
6.960
6.954
6.937
6.931
6.916
6.910
6.848
6.827
5.487
5.304
5.006
4.251
a24
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
0.94
1.04
0.99
1.12
1.09
2.18
4.04

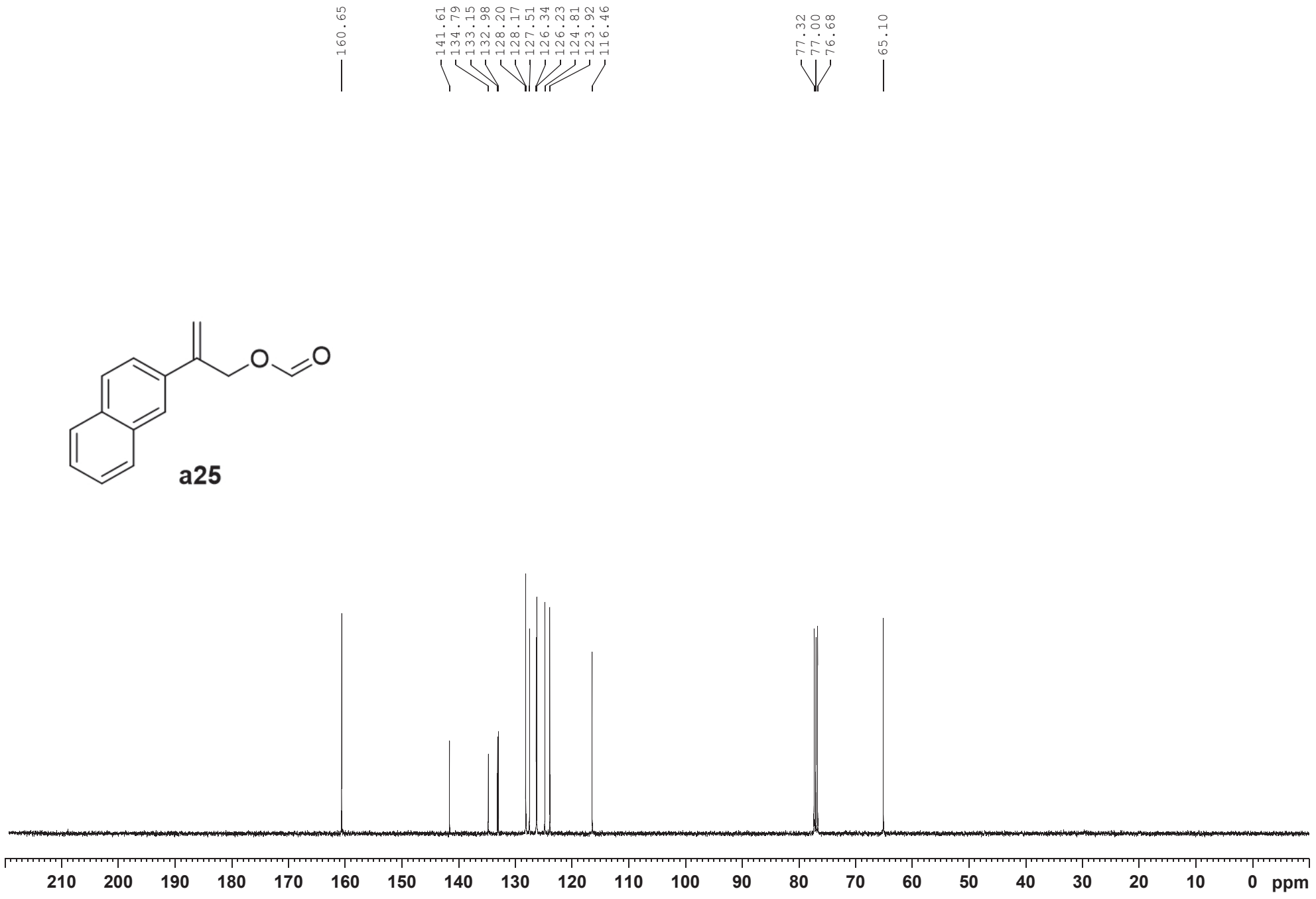

160.59
143.66
143.36
141.01
131.14
119.07
117.22
114.87
77.32
77.00
76.68
65.16
64.37
64.28
a24
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

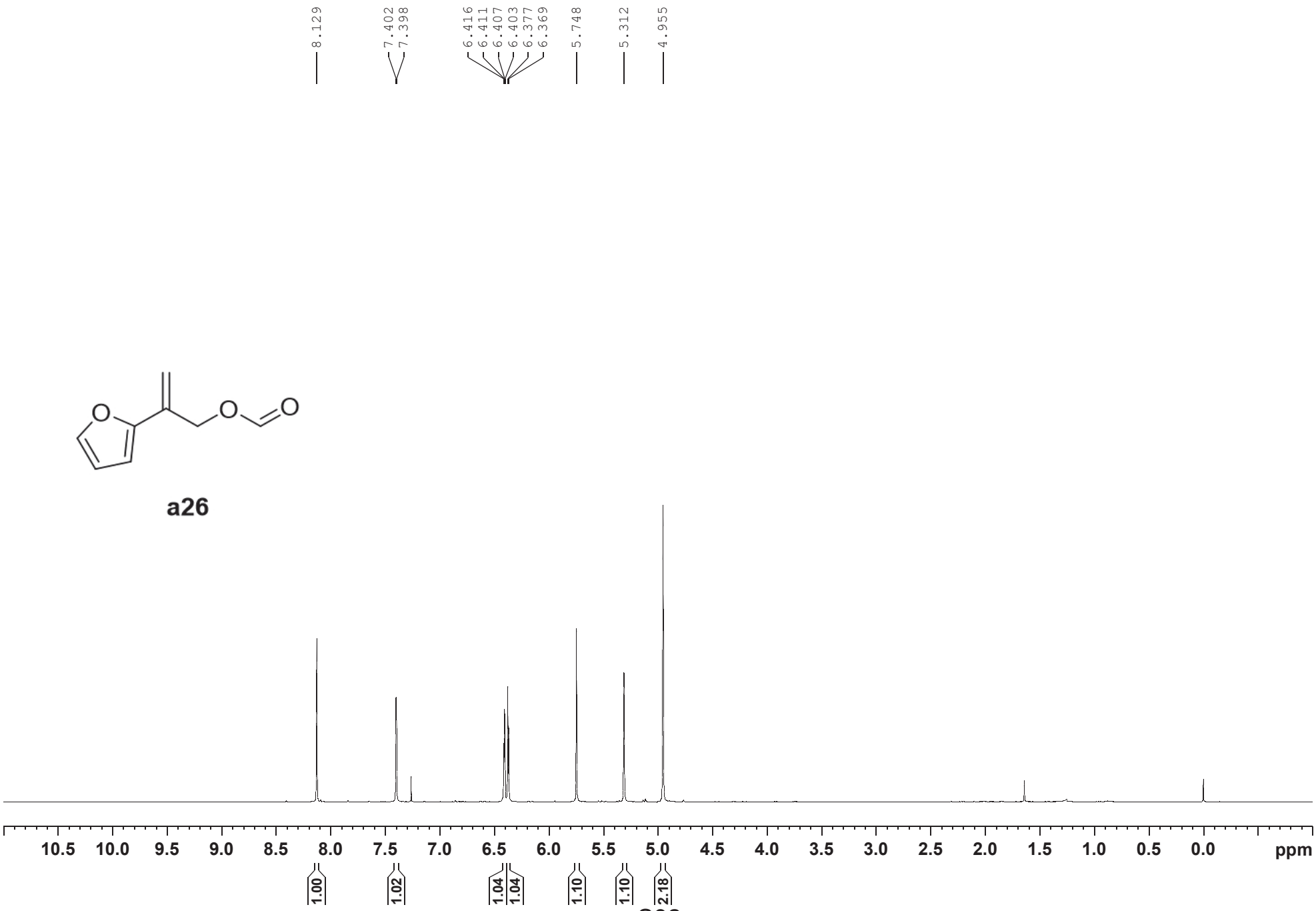

8.106
7.829
7.825
7.814
7.793
7.587
7.582
7.565
7.561
7.489
7.476
7.472
7.463
7.453
7.449
7.436
5.715
5.489
5.178

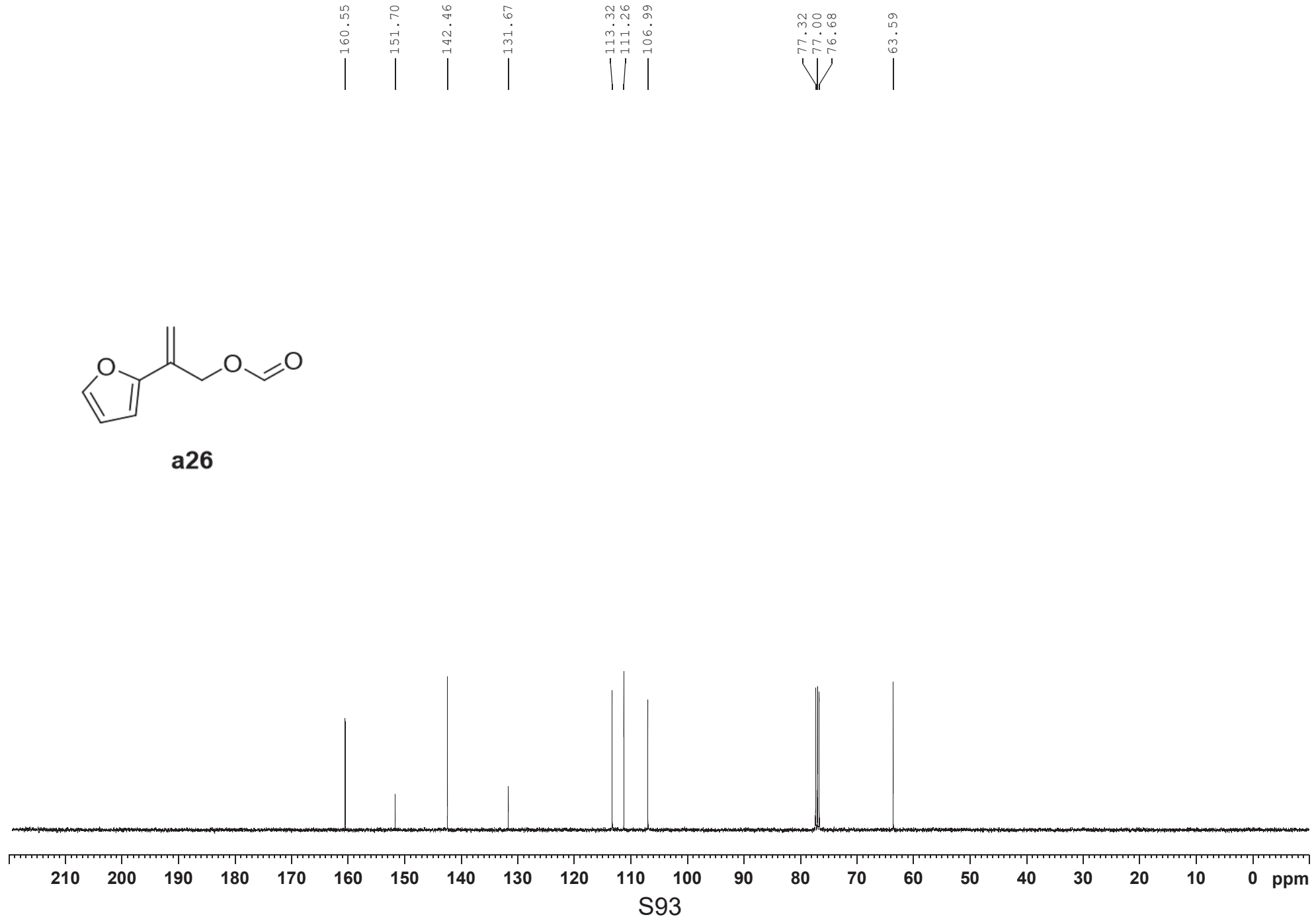


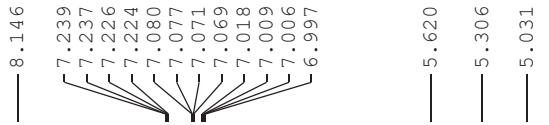
a25

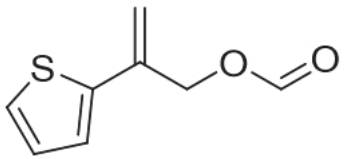

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.37
1.09
2.16
1.09
1.09
2.21


160.65
141.61
134.79
133.15
132.98
128.20
128.17
127.51
126.34
126.23
124.81
123.92
116.46
77.32
77.00
76.68
65.10
O
O
a25
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

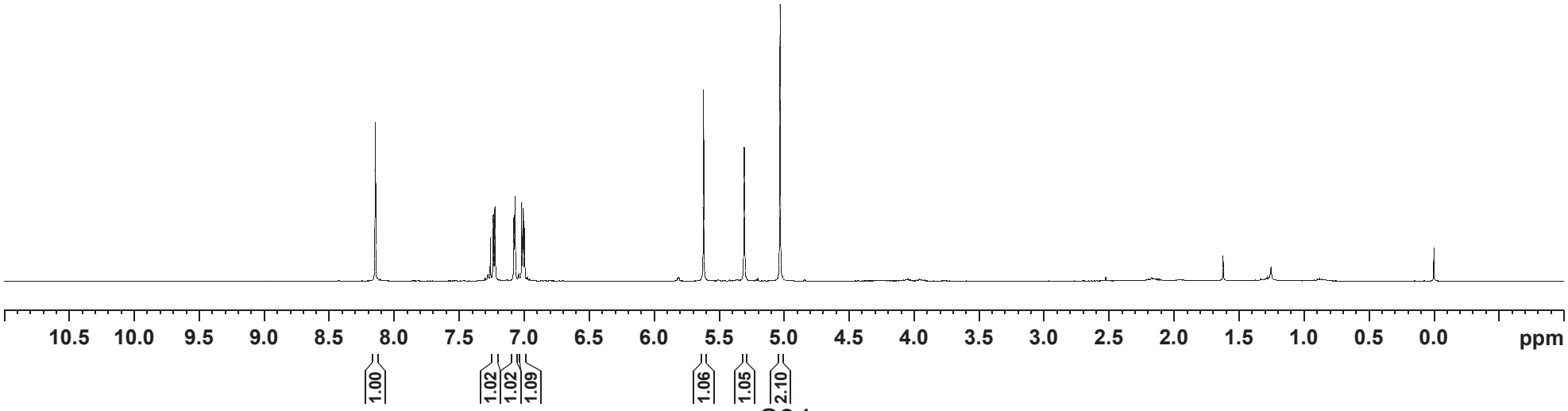

8.129
7.402
7.398
6.416
6.411
6.407
6.403
6.377
6.369
5.748
5.312
4.955
a26
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.02
1.04
1.04
1.10
1.10
2.18

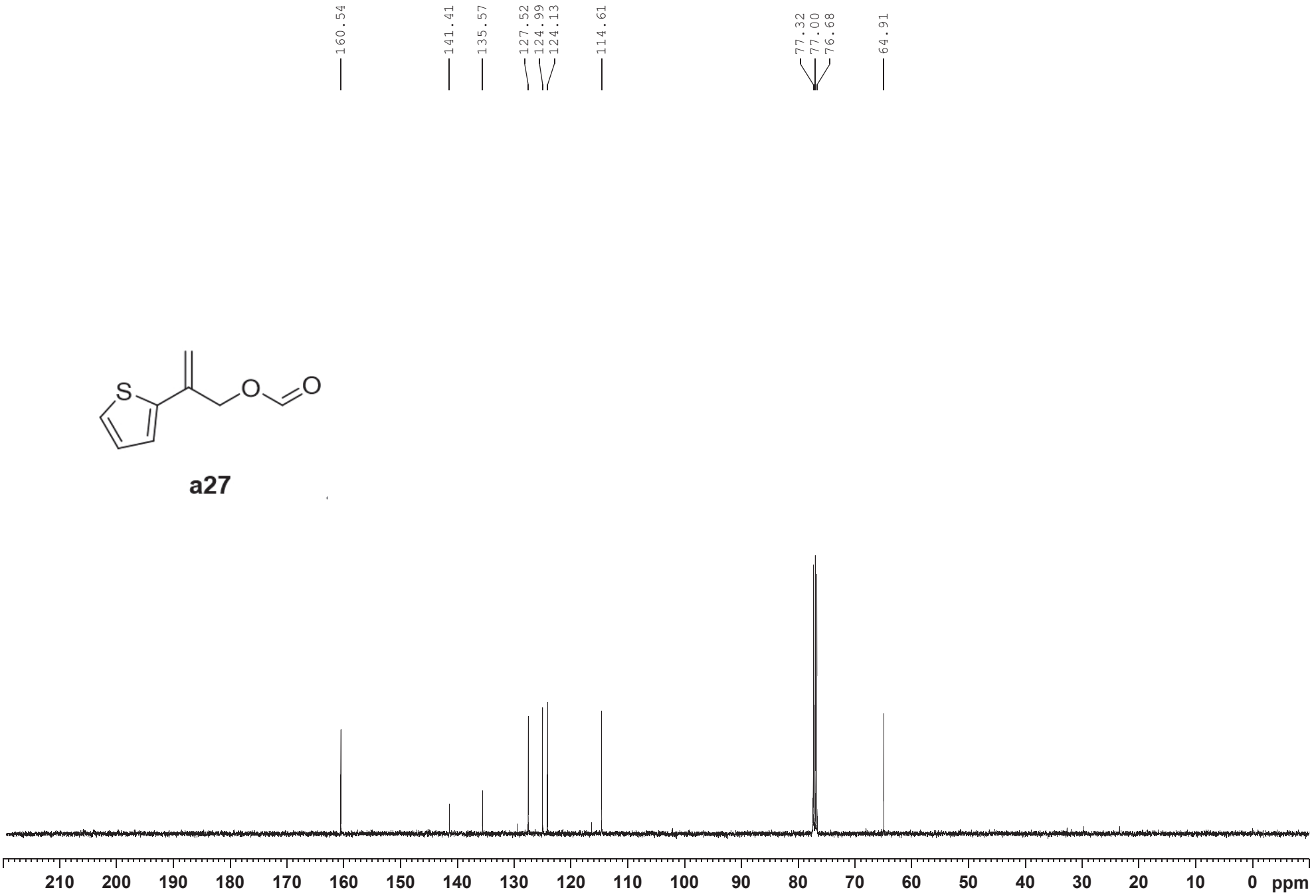

160.55
151.70
142.46
131.67
113.32
111.26
106.99
77.32
77.00
76.68
63.59
O
O
O
a26
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

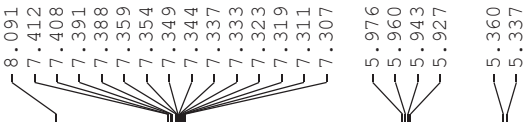

8.146
7.239
7.237
7.226
7.224
7.080
7.077
7.071
7.069
7.018
7.009
7.006
6.997
5.620
5.306
5.031

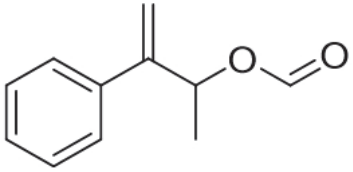

S
O
O

a27

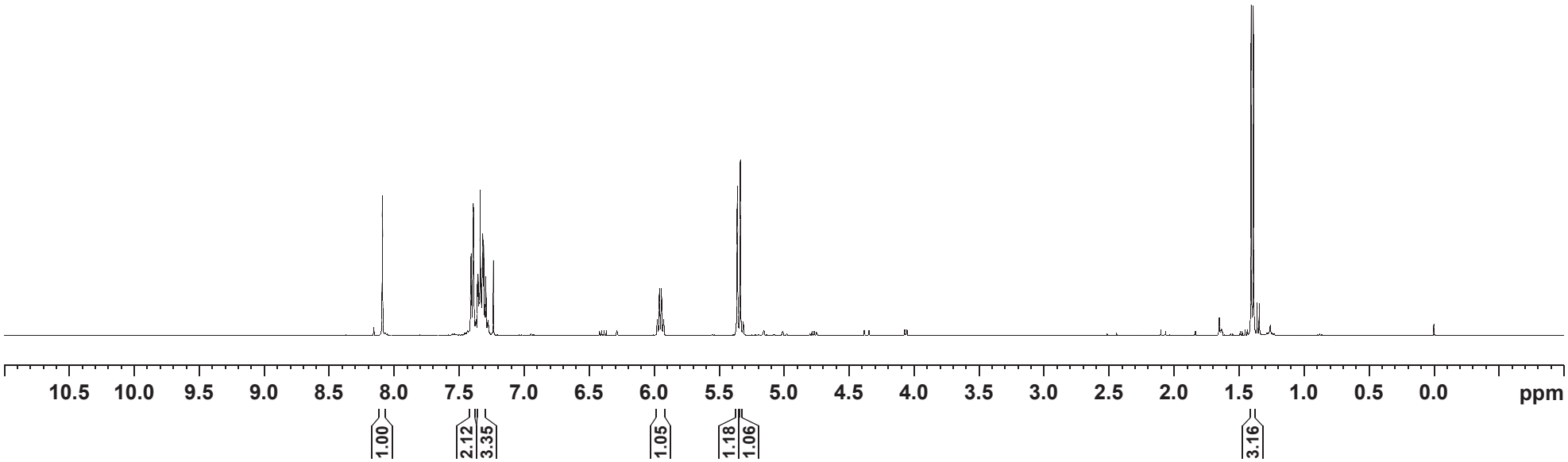

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.02
1.02
1.09
1.06
1.05
2.10


160.54
141.41
135.57
127.52
124.99
124.13
114.61
77.32
77.00
76.68
64.91
S
O
O
a27
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

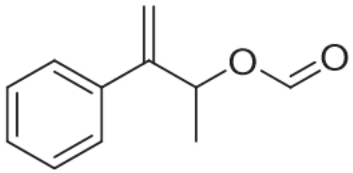

8.091
7.412
7.408
7.391
7.388
7.359
7.354
7.349
7.344
7.337
7.333
7.323
7.319
7.311
7.307
5.976
5.960
5.943
5.927
5.360
5.337
1.406
1.390


O
O

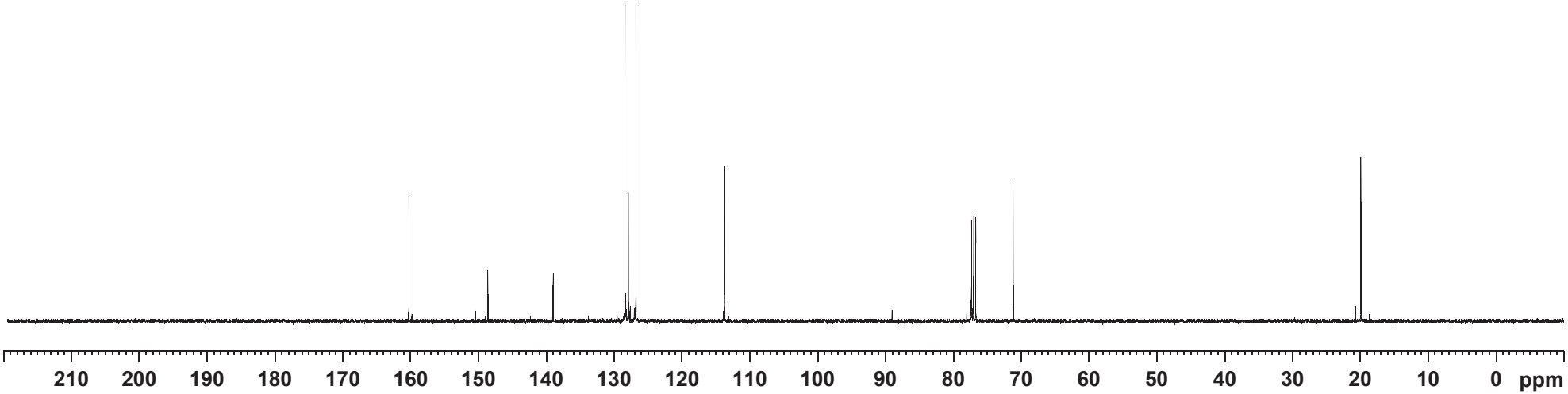
a28

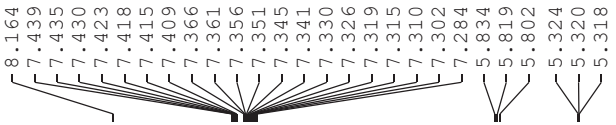

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.12
3.35
1.05
1.18
1.06
3.16

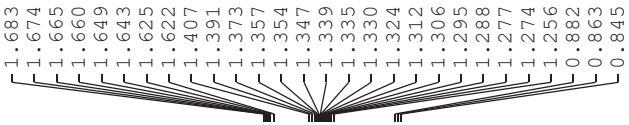

160.25
148.61
138.99
128.39
127.88
126.80
113.71
77.32
77.00
76.68
71.18
19.90

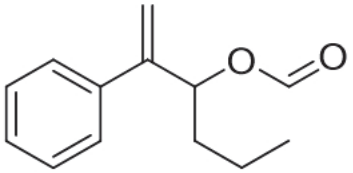

O
O

a28

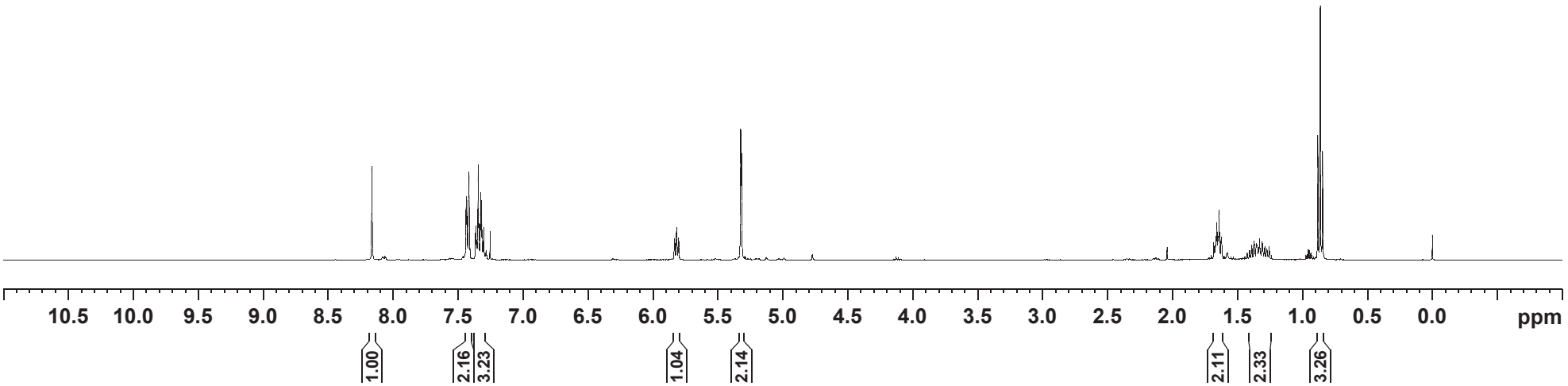

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

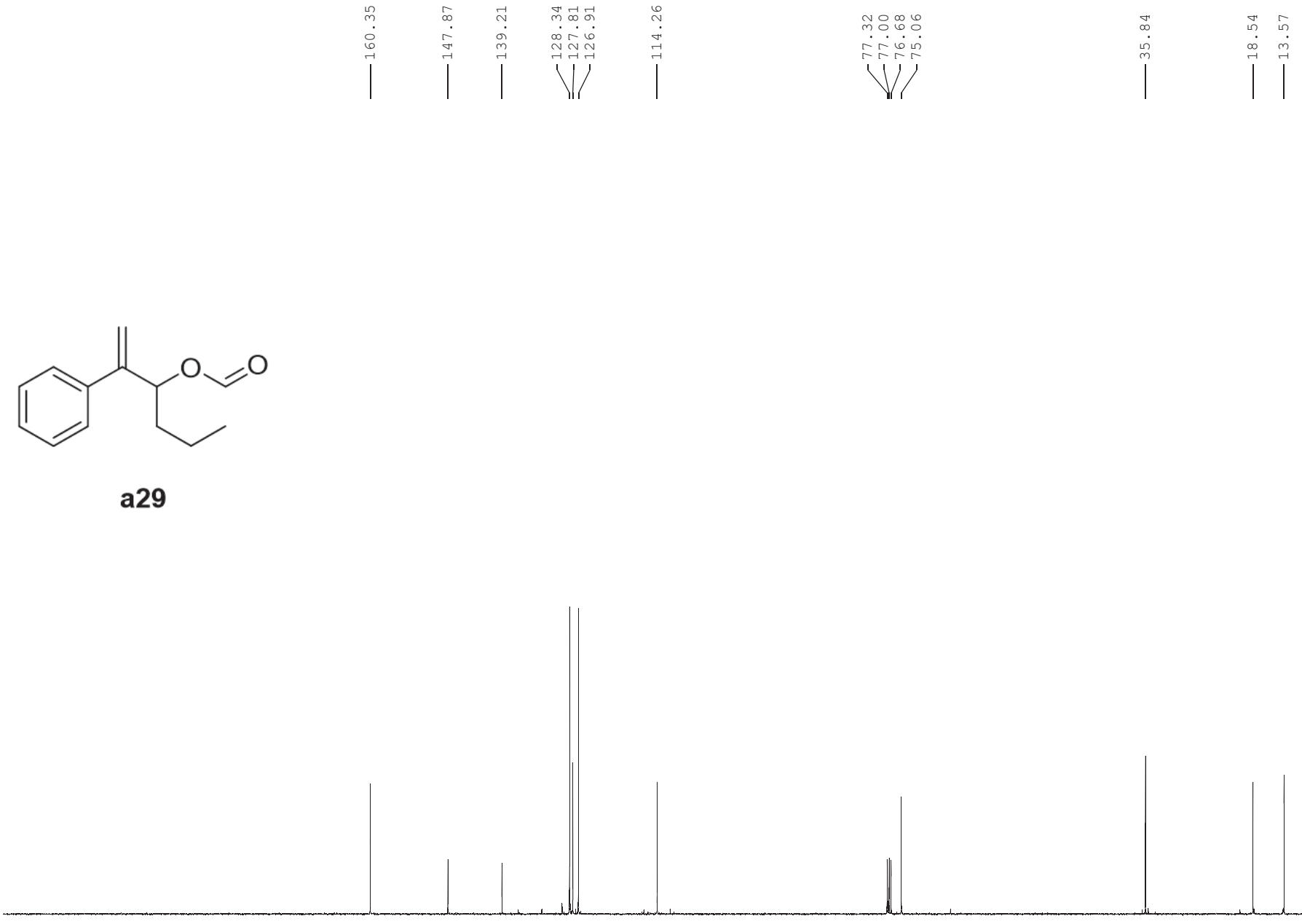

8.164
7.439
7.435
7.430
7.423
7.418
7.415
7.409
7.366
7.361
7.356
7.351
7.345
7.341
7.330
7.326
7.319
7.315
7.310
7.302
7.284
5.834
5.819
5.802
5.324
5.320
5.318

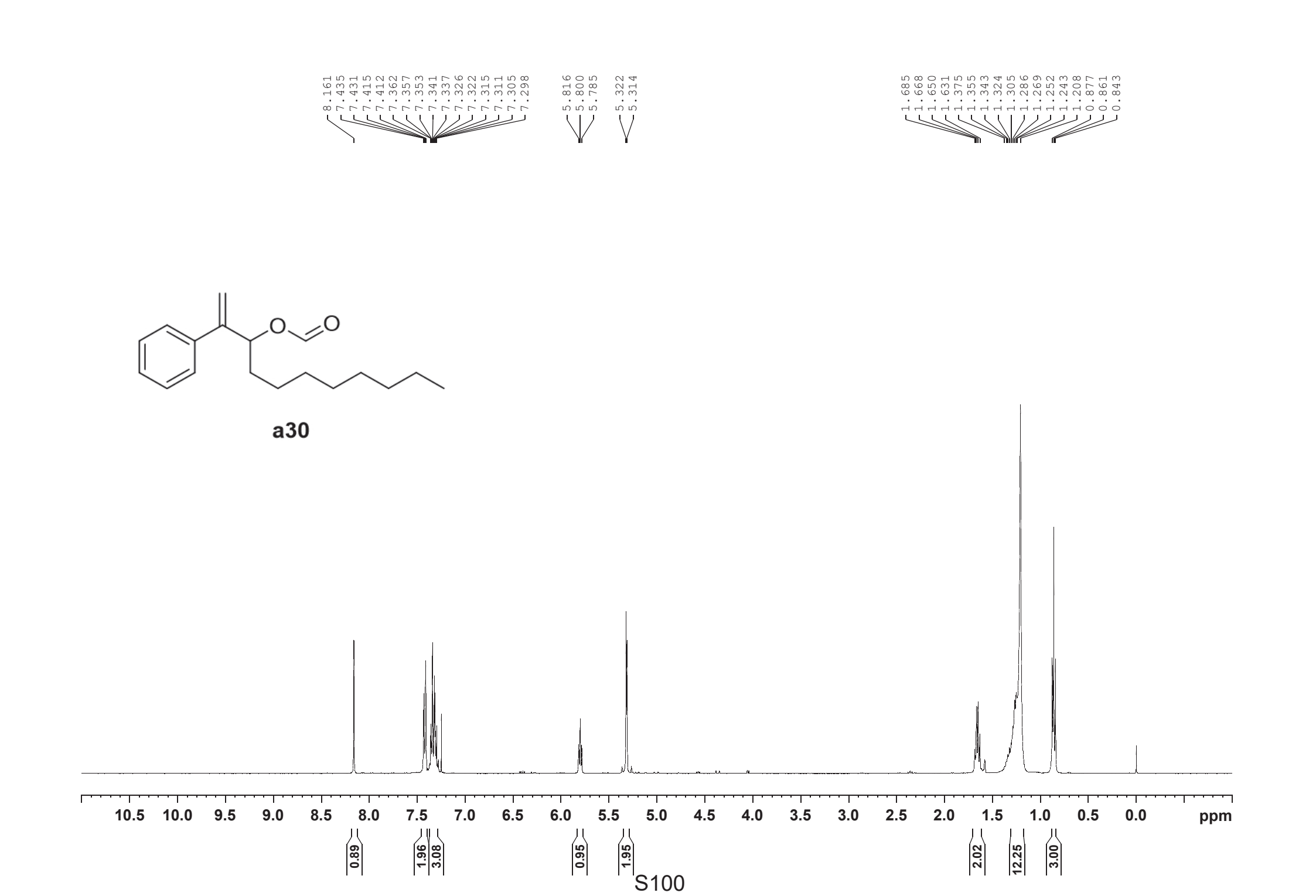

1.683
1.674
1.665
1.660
1.649
1.643
1.625
1.622
1.407
1.391
1.373
1.357
1.354
1.347
1.339
1.335
1.330
1.324
1.312
1.306
1.295
1.288
1.277
1.274
1.256
0.882
0.863
0.845

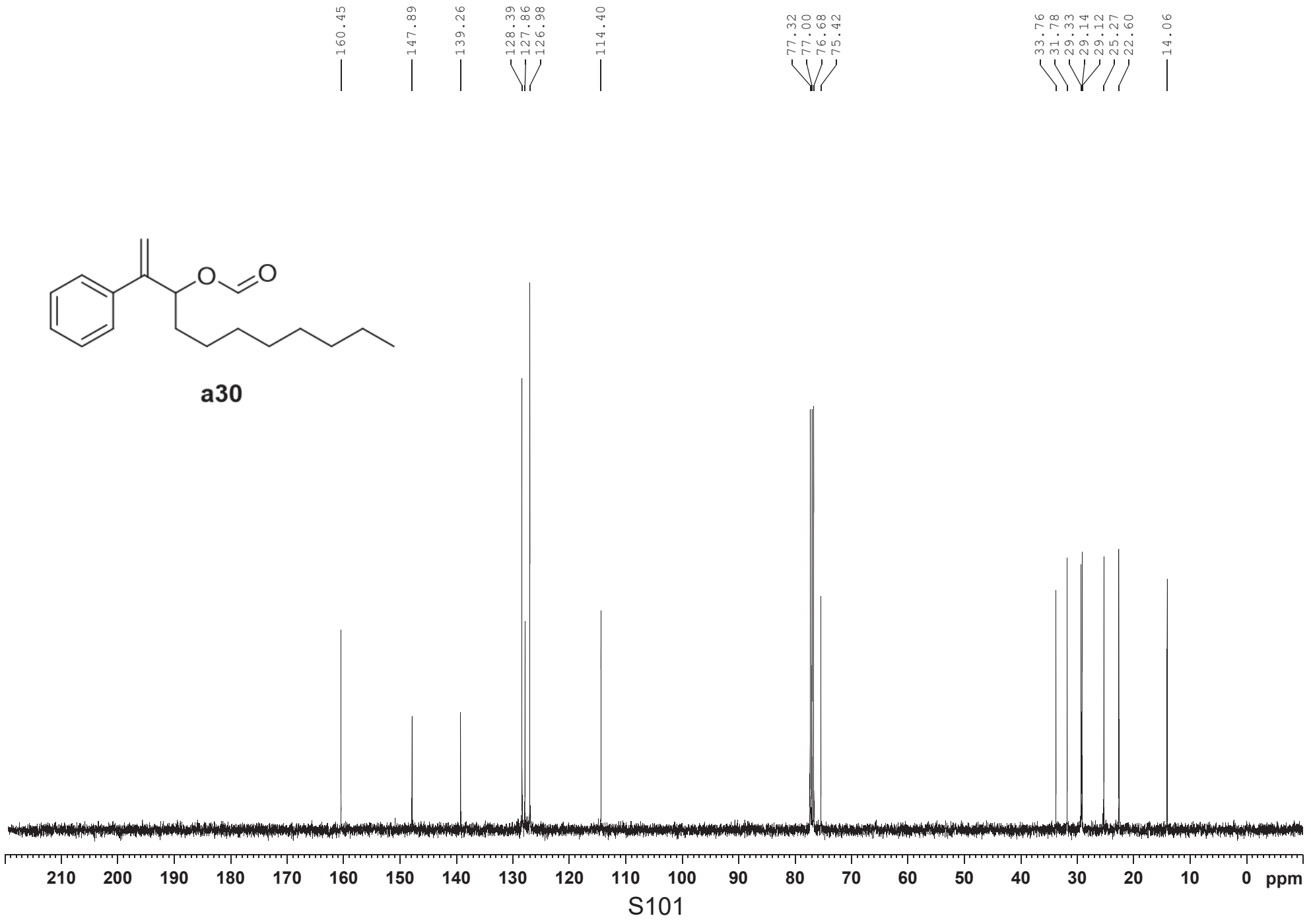

O
O

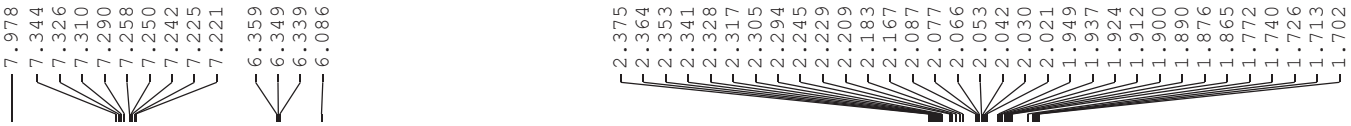
a29

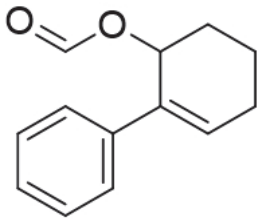

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.16
3.23
1.04
2.14
2.11
2.33
3.26


160.35
147.87
139.21
128.34
127.81
126.91
114.26
77.32
77.00
76.68
75.06
35.84
18.54
13.57
O
O
a29
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

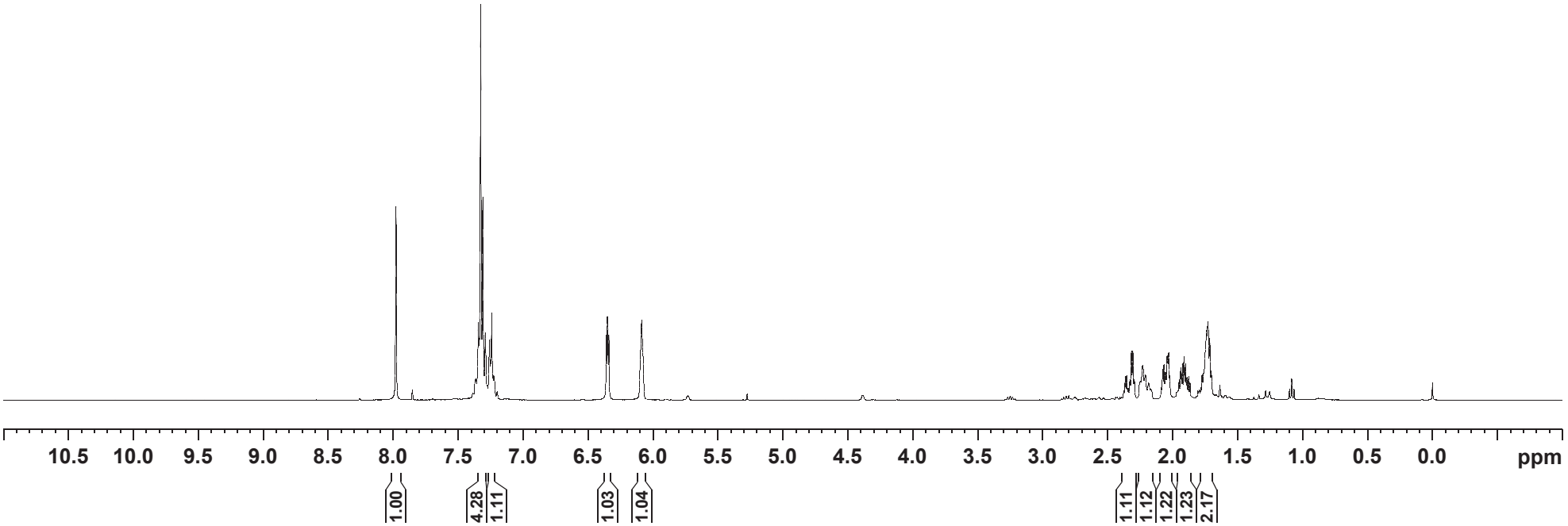

8.161
7.435
7.431
7.415
7.412
7.362
7.357
7.353
7.341
7.337
7.326
7.322
7.315
7.311
7.305
7.298
5.816
5.800
5.785
5.322
5.314
1.685
1.668
1.650
1.631
1.375
1.355
1.343
1.324
1.305
1.286
1.269
1.252
1.243
1.208
0.877
0.861
0.843
O
O
a30
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.89
1.96
3.08
0.95
1.95
2.02
12.25
3.00

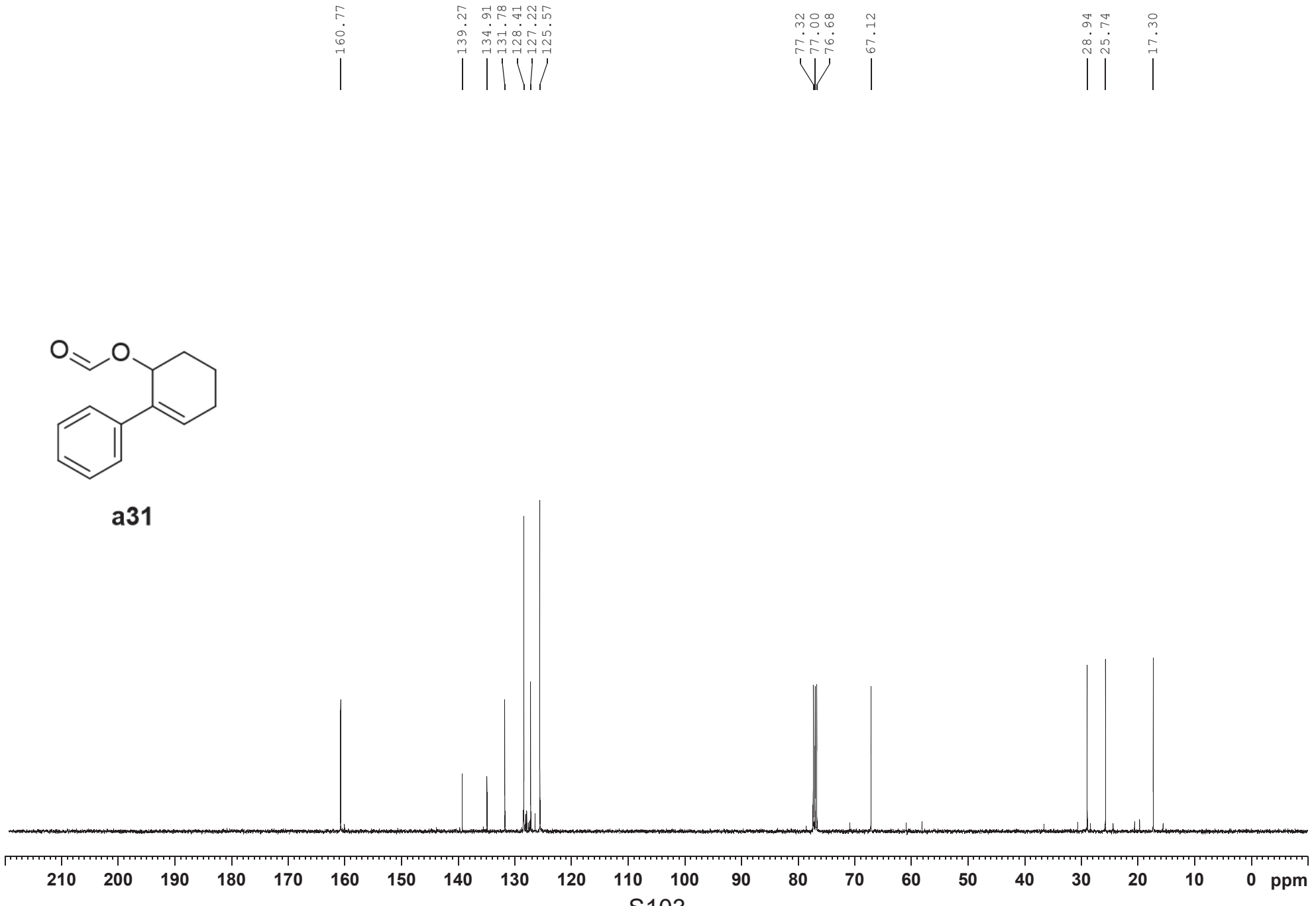

160.45
147.89
139.26
128.39
127.86
126.98
114.40
77.32
77.00
76.68
75.42
33.76
31.78
29.33
29.14
29.12
25.27
22.60
14.06
O
O
a30
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

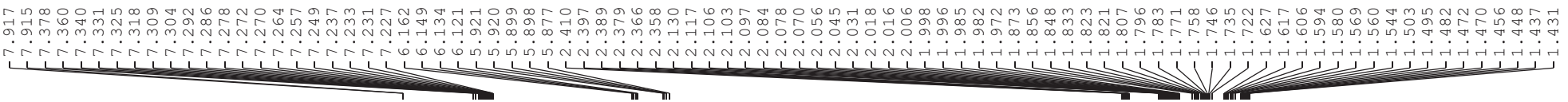

7.978
7.344
7.326
7.310
7.290
7.258
7.250
7.242
7.225
7.221
6.359
6.349
6.339
6.086
2.375
2.364
2.353
2.341
2.328
2.317
2.305
2.294
2.245
2.229
2.209
2.183
2.167
2.087
2.077
2.066
2.053
2.042
2.030
2.021
1.949
1.937
1.924
1.912
1.900
1.890
1.876
1.865
1.772
1.740
1.726
1.713
1.702

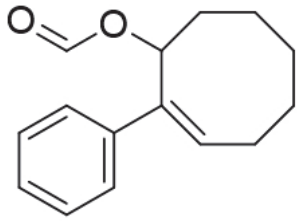


a31

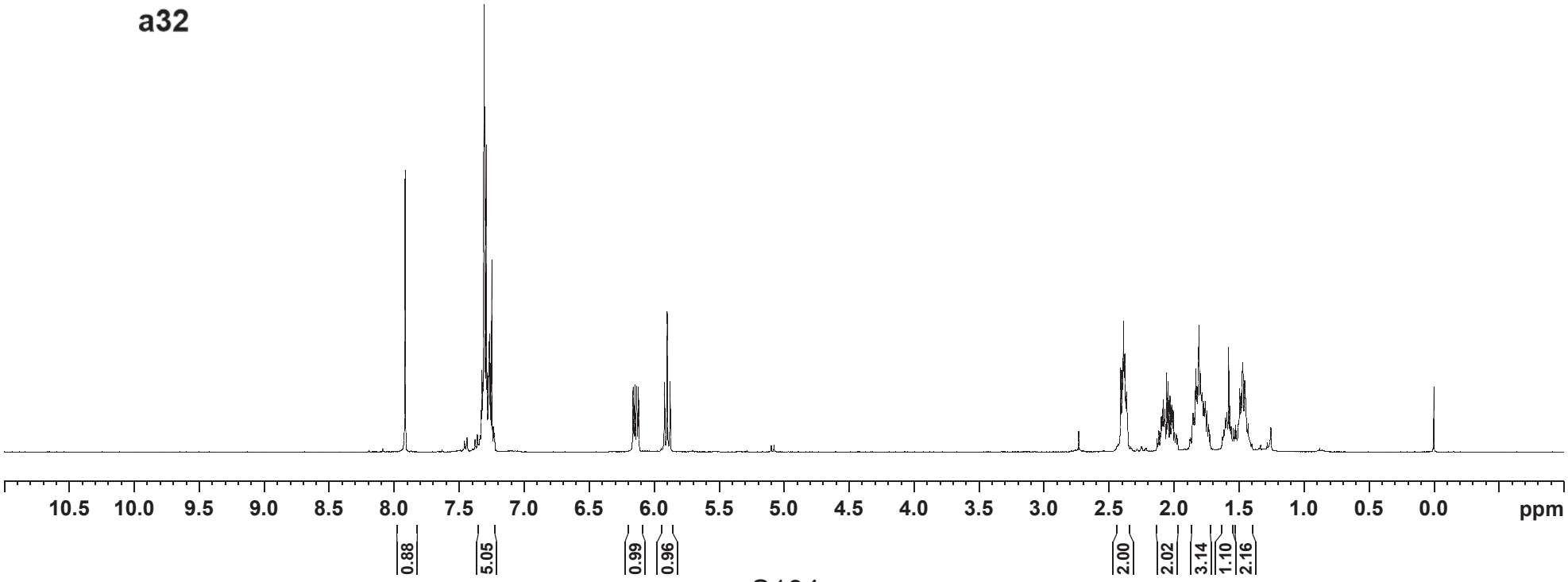

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.28
1.11
1.03
1.04
1.11
1.12
1.22
1.23
2.17

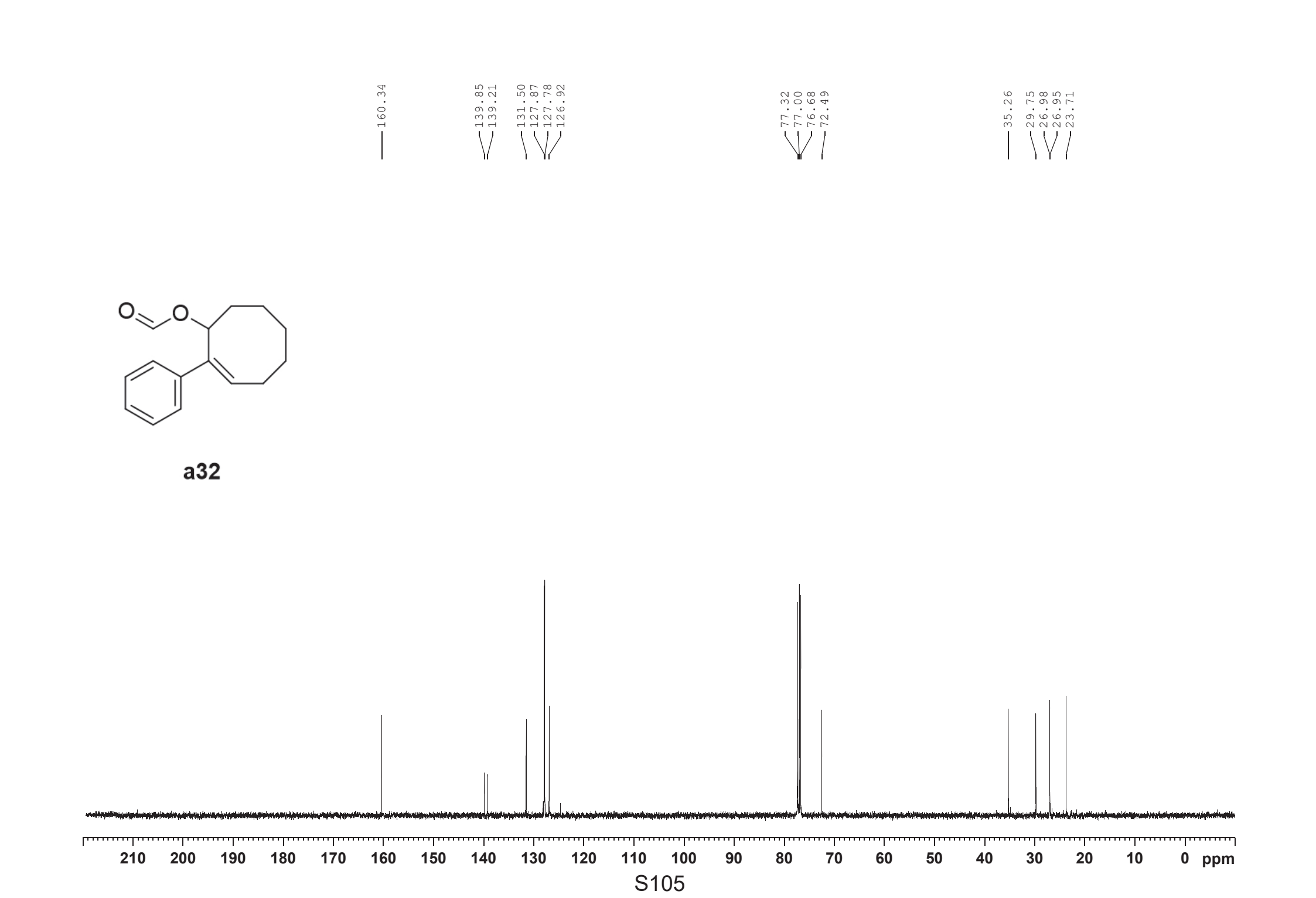

160.77
139.27
134.91
131.78
128.41
127.22
125.57
77.32
77.00
76.68
67.12
28.94
25.74
17.30
a31
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

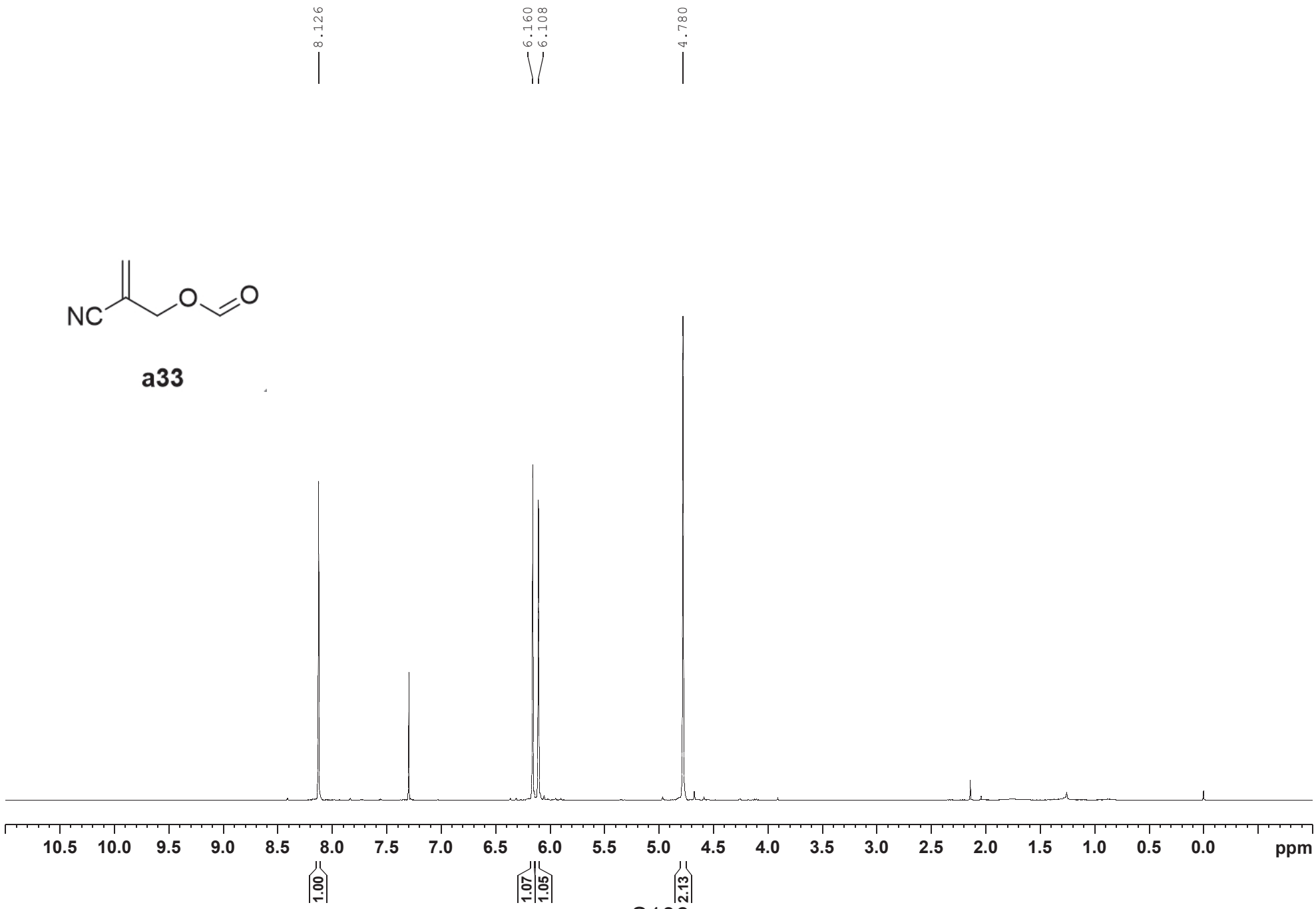

7.917
7.915
7.378
7.360
7.340
7.331
7.325
7.318
7.309
7.304
7.292
7.286
7.278
7.272
7.270
7.264
7.257
7.249
7.237
7.233
7.231
7.227
6.162
6.149
6.134
6.121
5.921
5.920
5.899
5.898
5.877
2.410
2.397
2.389
2.379
2.366
2.358
2.130
2.117
2.106
2.103
2.097
2.084
2.078
2.070
2.056
2.045
2.031
2.018
2.016
2.006
1.998
1.996
1.985
1.982
1.972
1.873
1.856
1.848
1.833
1.823
1.821
1.807
1.796
1.783
1.771
1.758
1.746
1.735
1.722
1.627
1.617
1.606
1.594
1.580
1.569
1.560
1.544
1.503
1.495
1.482
1.472
1.470
1.456
1.448
1.437
1.431

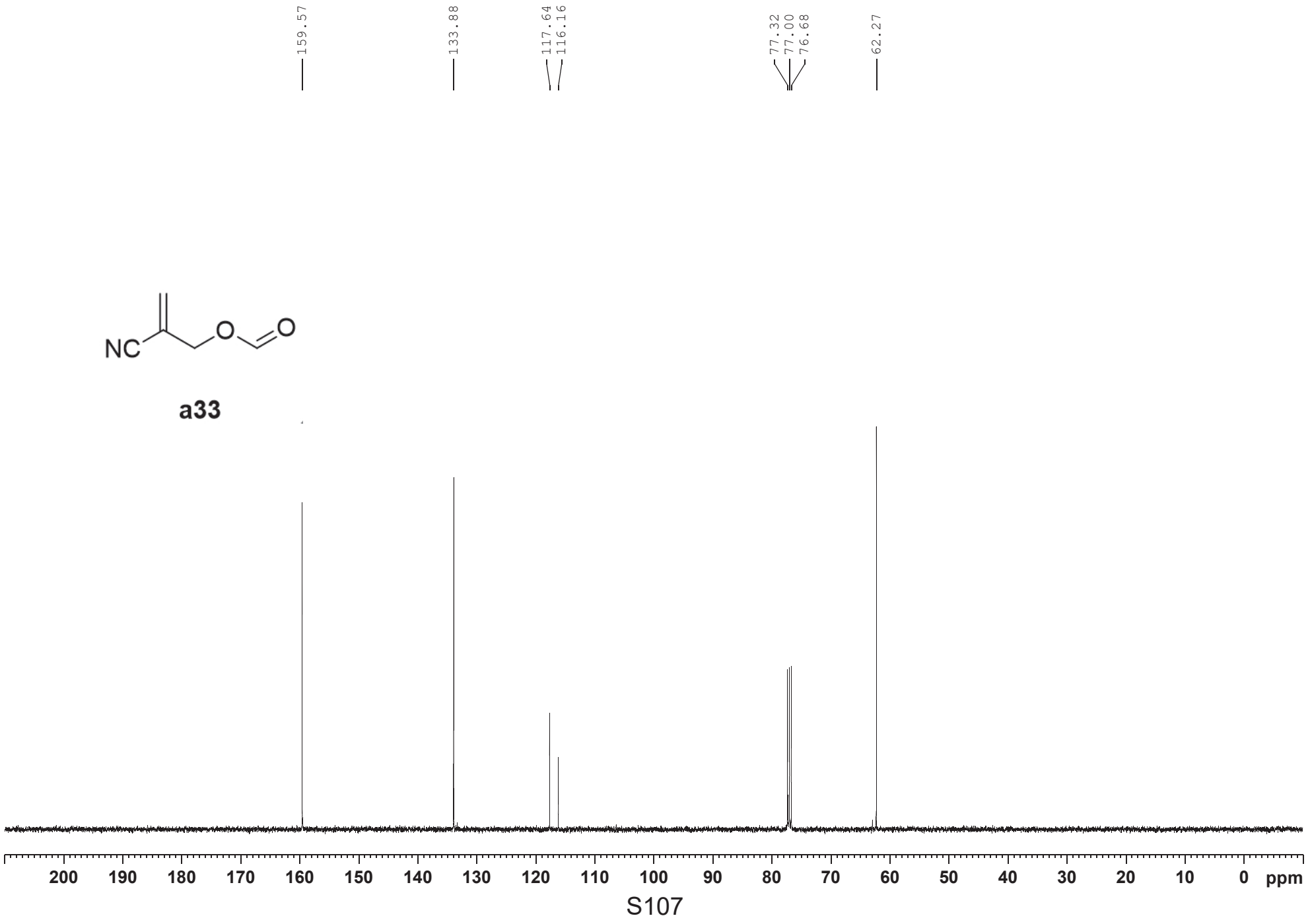


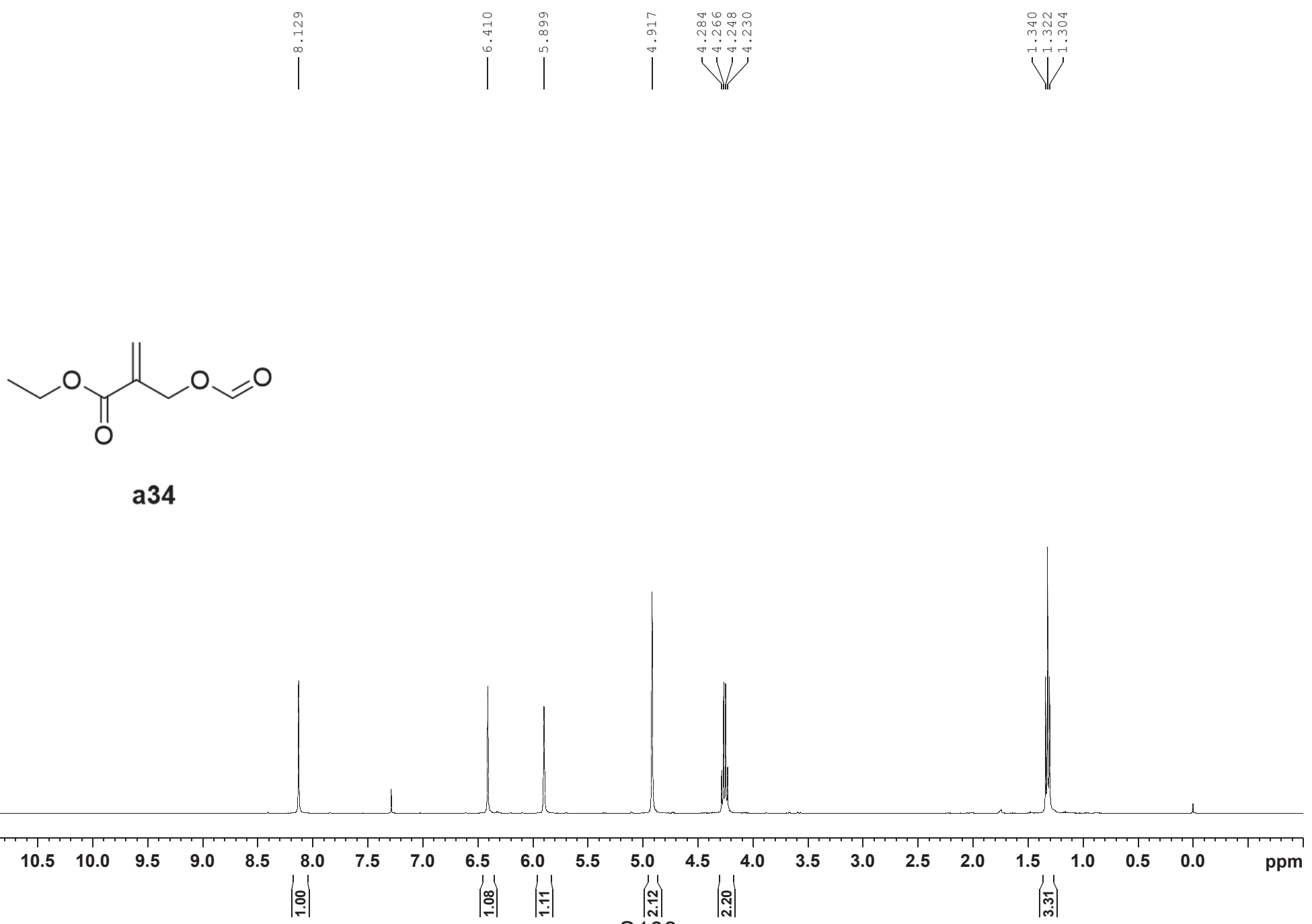
a32

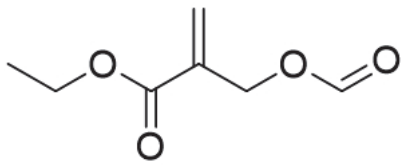

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.88
5.05
0.99
0.96
2.00
2.02
3.14
1.10
2.16


160.34
139.85
139.21
131.50
127.87
127.78
126.92
77.32
77.00
76.68
72.49
35.26
29.75
26.98
26.95
23.71
O
O
a32
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.126
6.160
6.108
4.780
NC
O
O
a33
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.07
1.05
2.13

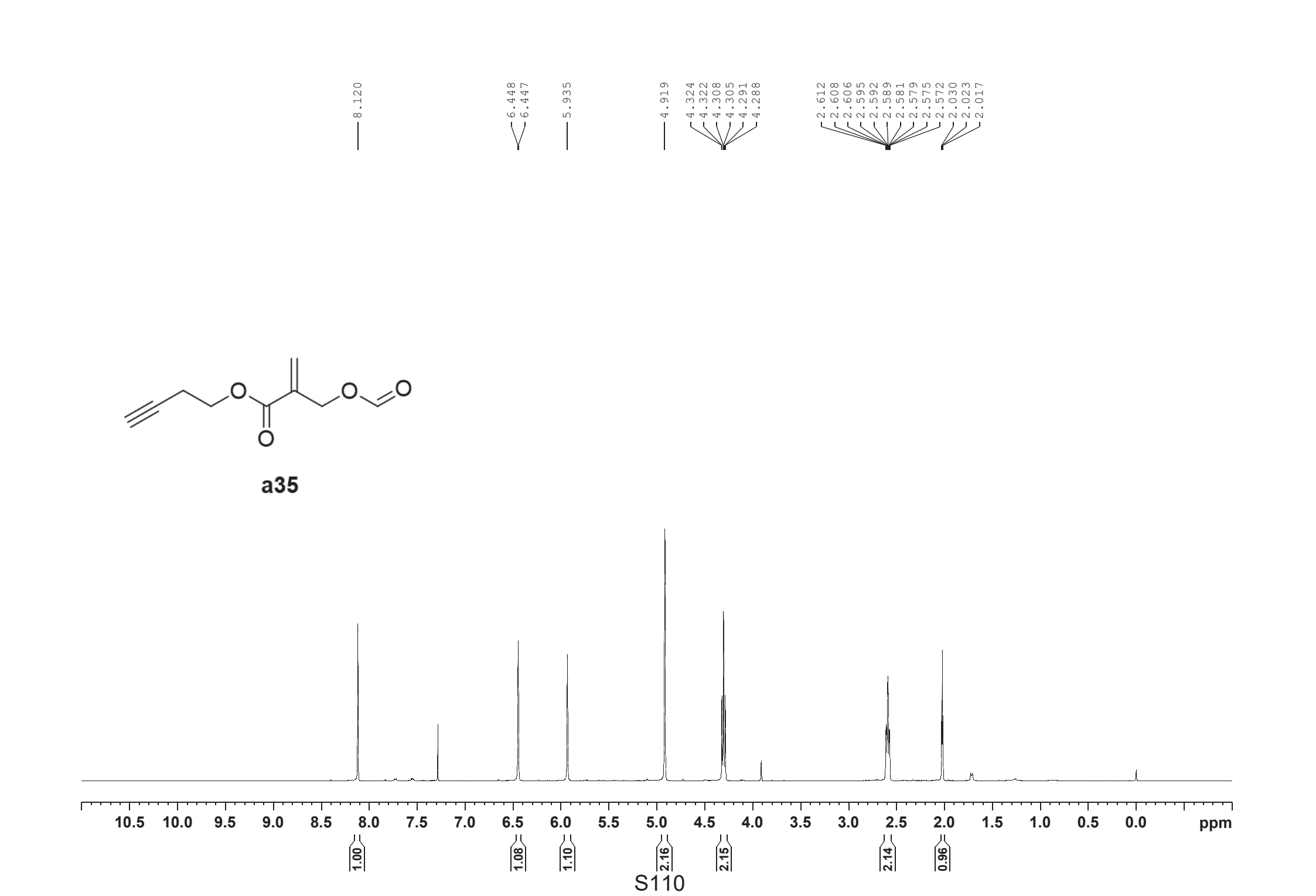

159.57
133.88
117.64
116.16
77.32
77.00
76.68
62.27
NC
O
O
a33
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

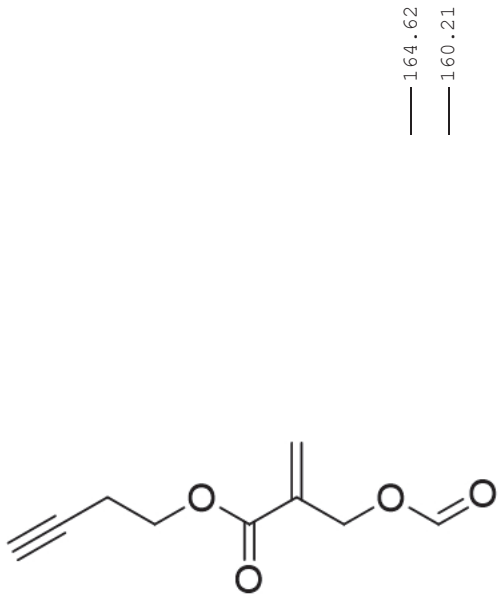

8.129
6.410
5.899
4.917
4.284
4.266
4.248
4.230
1.340
1.322
1.304
a34
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.08
1.11
2.12
2.20
3.31



a34

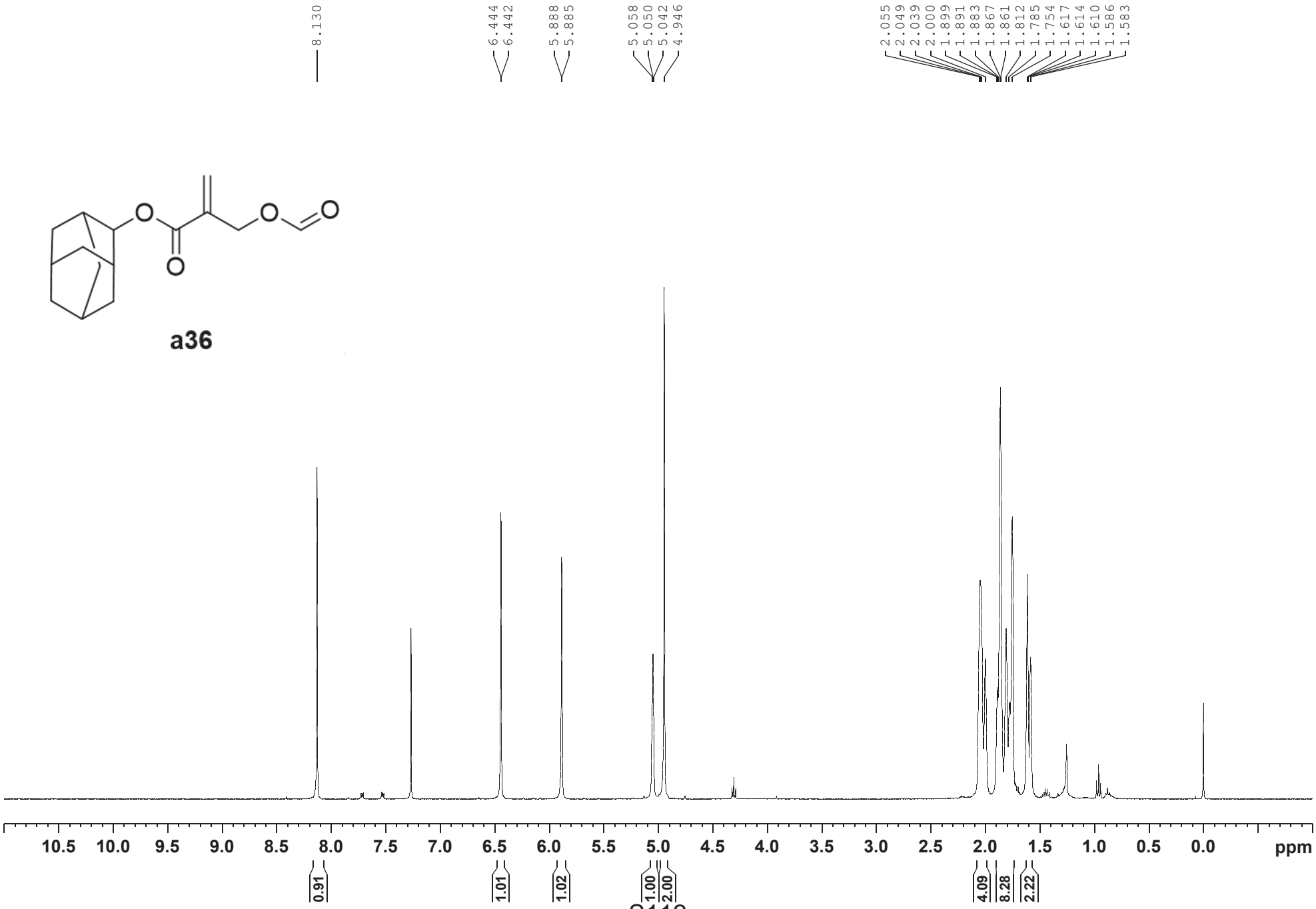
164.95
160.30
134.76
127.90
77.32
77.00
76.68
61.87
61.07
14.08
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

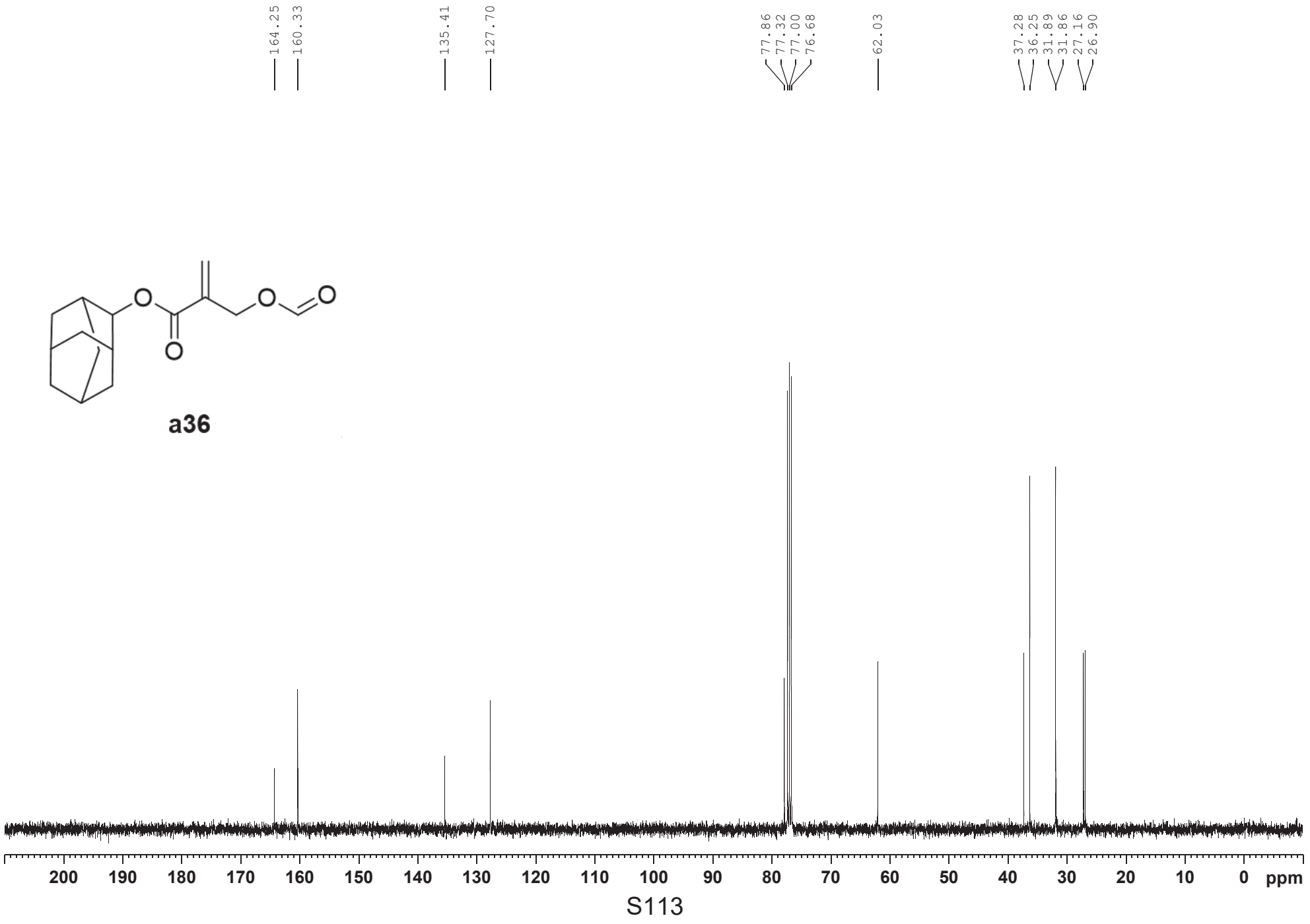

8.120
6.448
6.447
5.935
4.919
4.324
4.322
4.308
4.305
4.291
4.288
2.612
2.608
2.606
2.595
2.592
2.589
2.581
2.579
2.575
2.572
2.030
2.023
2.017
O
O
O
O
a35
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.08
1.10
2.16
2.15
2.14
0.96

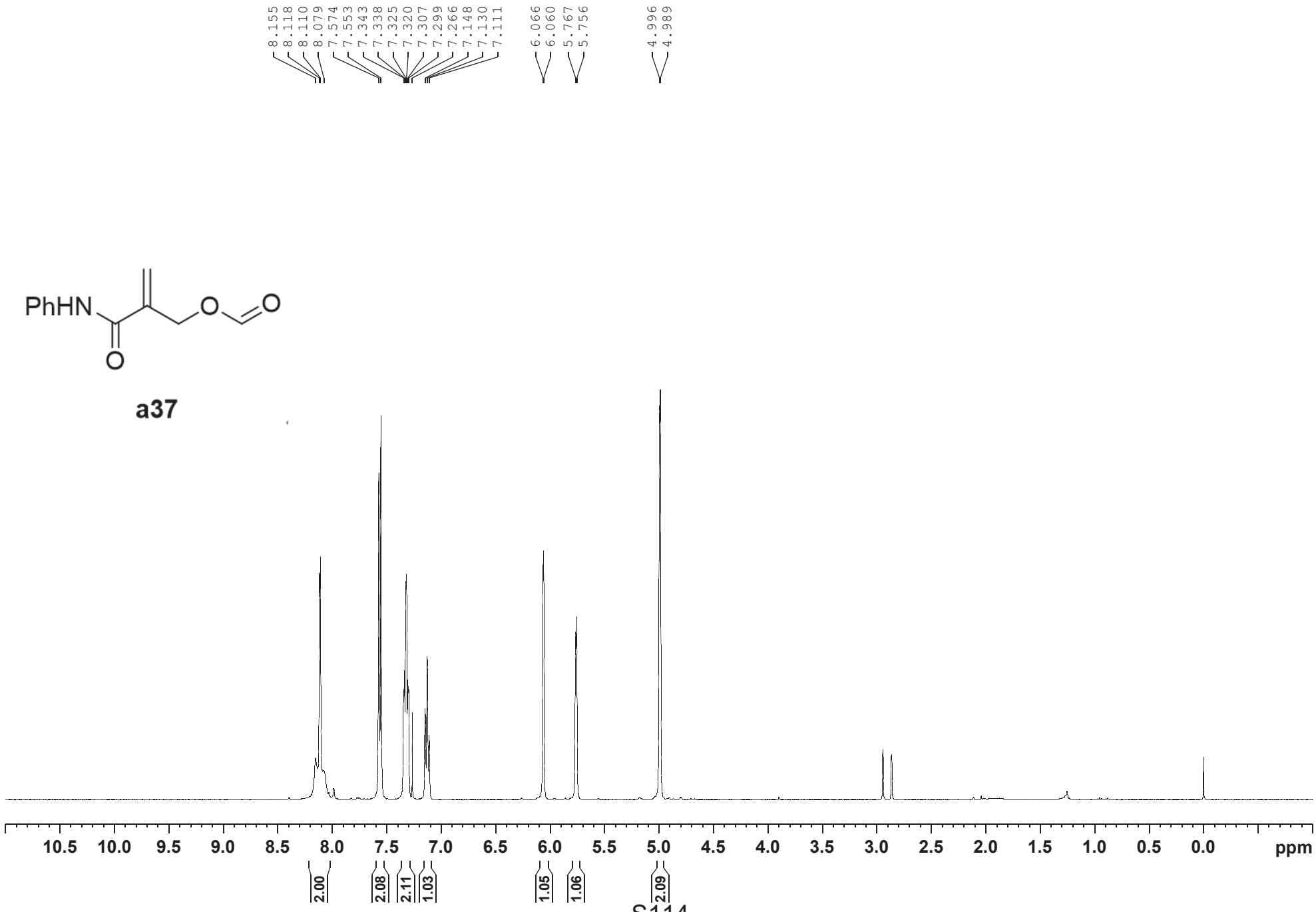


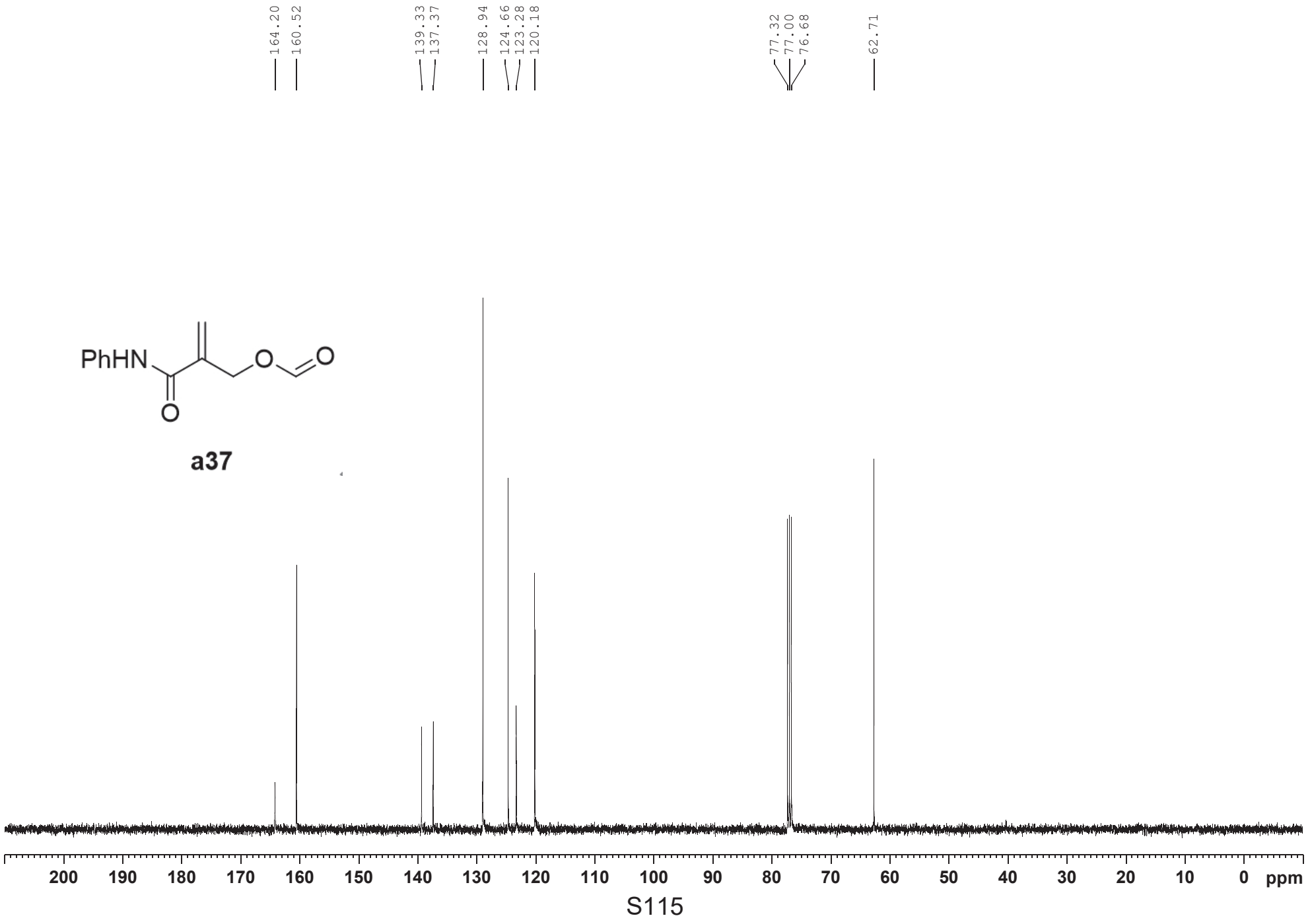
a35

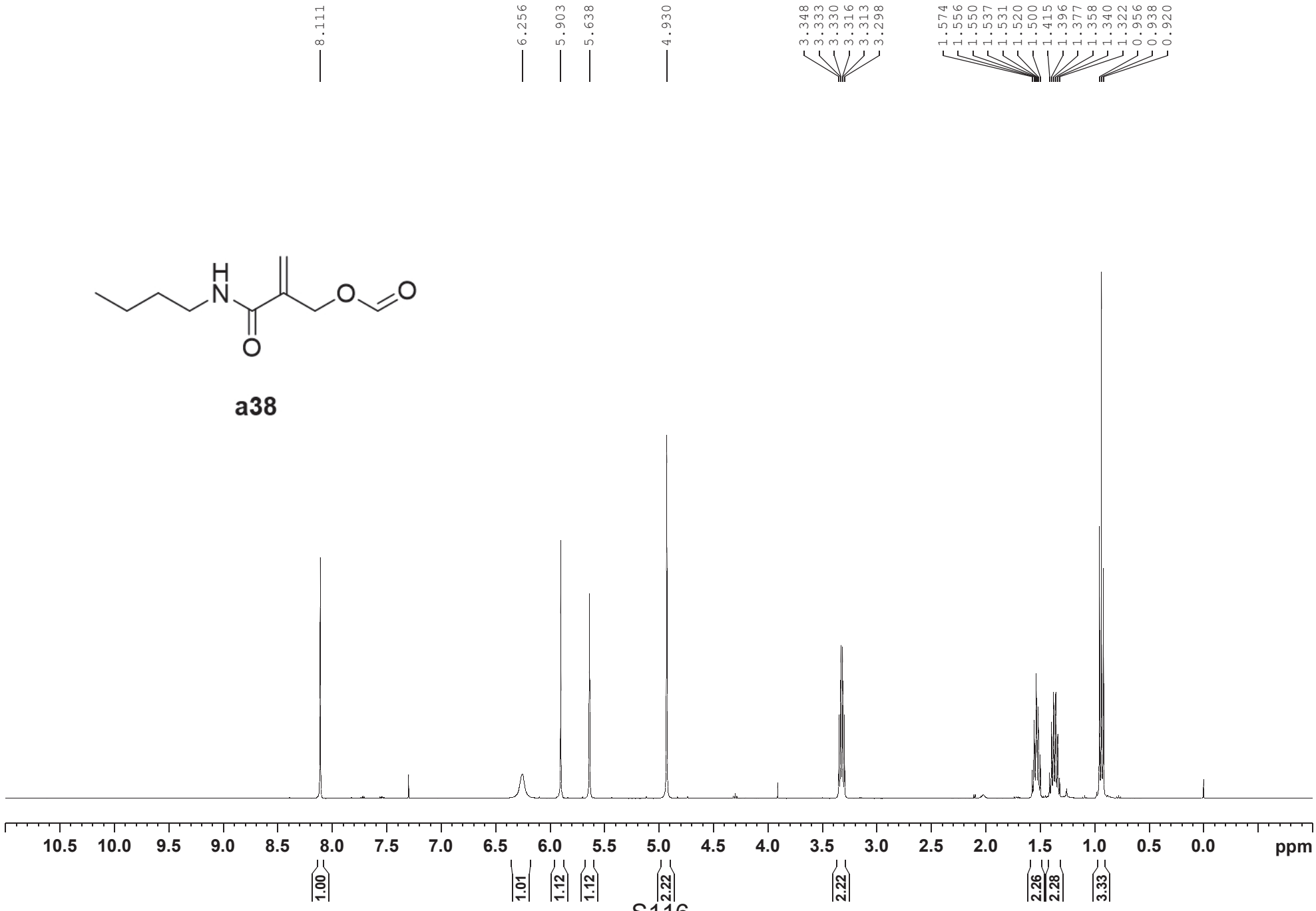
164.62
160.21
134.43
128.62
79.66
77.32
77.00
76.68
70.04
62.61
61.74
18.86
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

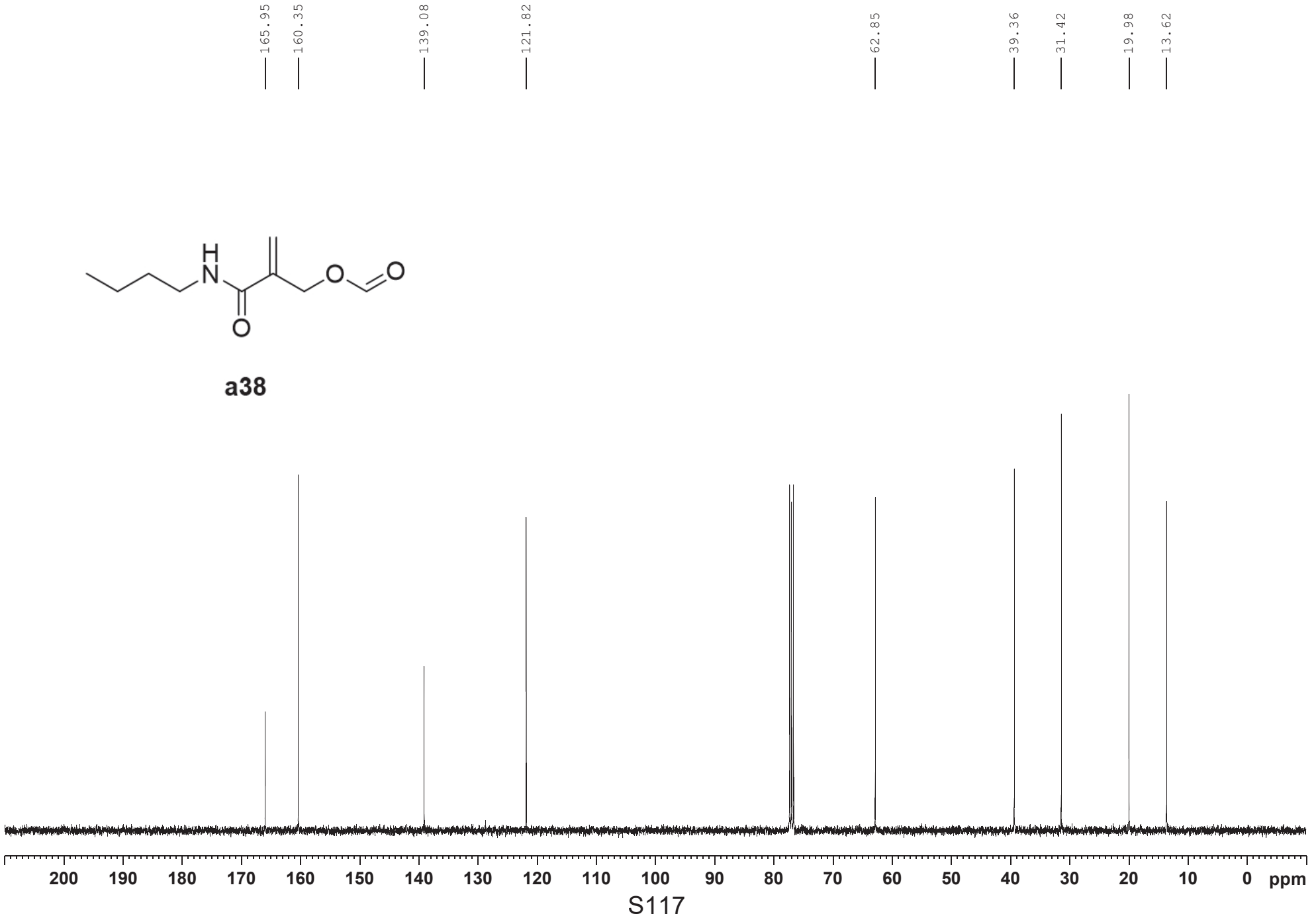

8.130
6.444
6.442
5.888
5.885
5.058
5.050
5.042
4.946
2.055
2.049
2.039
2.000
1.899
1.891
1.883
1.867
1.861
1.812
1.785
1.754
1.617
1.614
1.610
1.586
1.583
a36
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.91
1.01
1.02
1.00
2.00
4.09
8.28
2.22

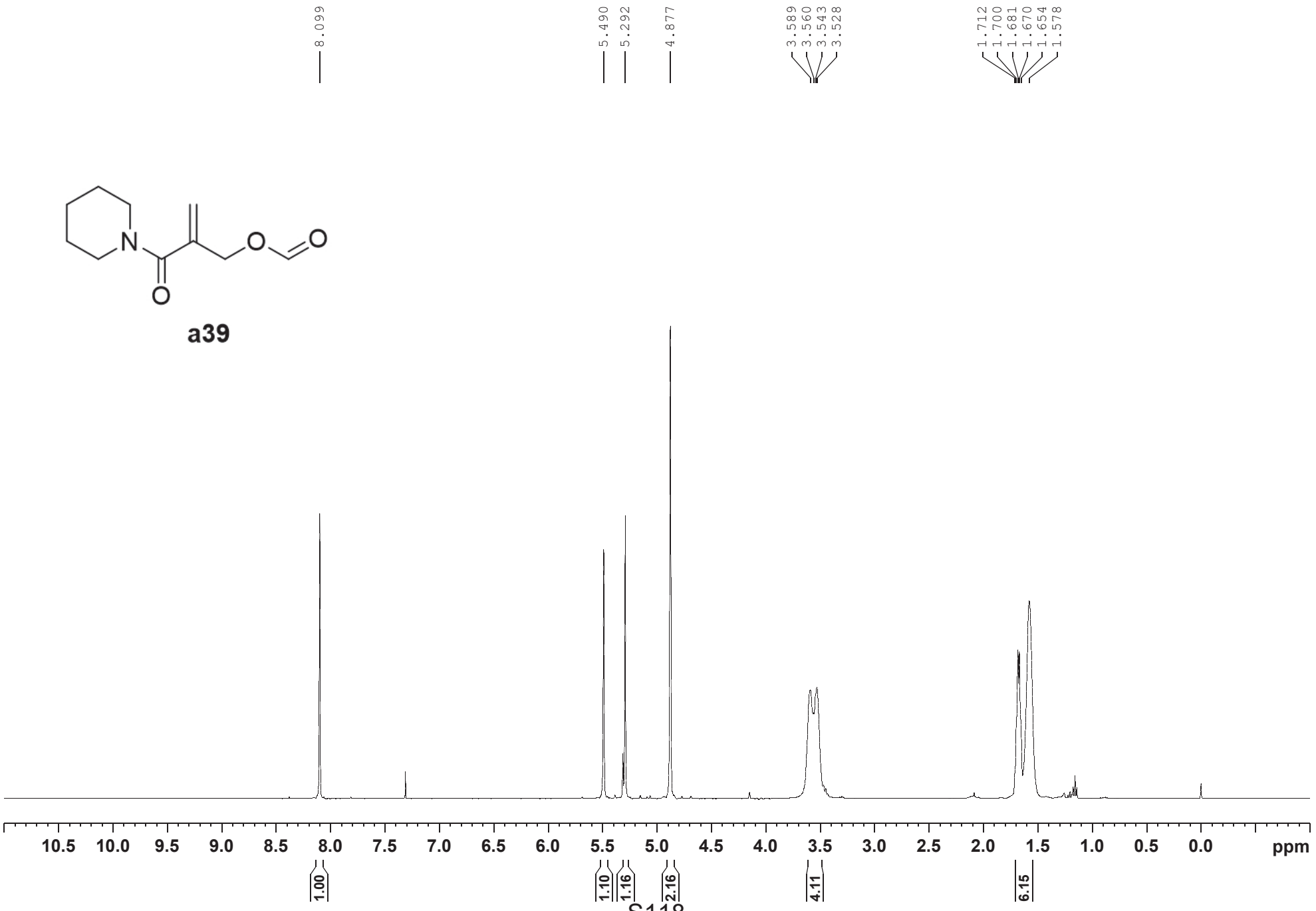

164.25
160.33
135.41
127.70
77.86
77.32
77.00
76.68
62.03
37.28
36.25
31.89
31.86
27.16
26.90
a36
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

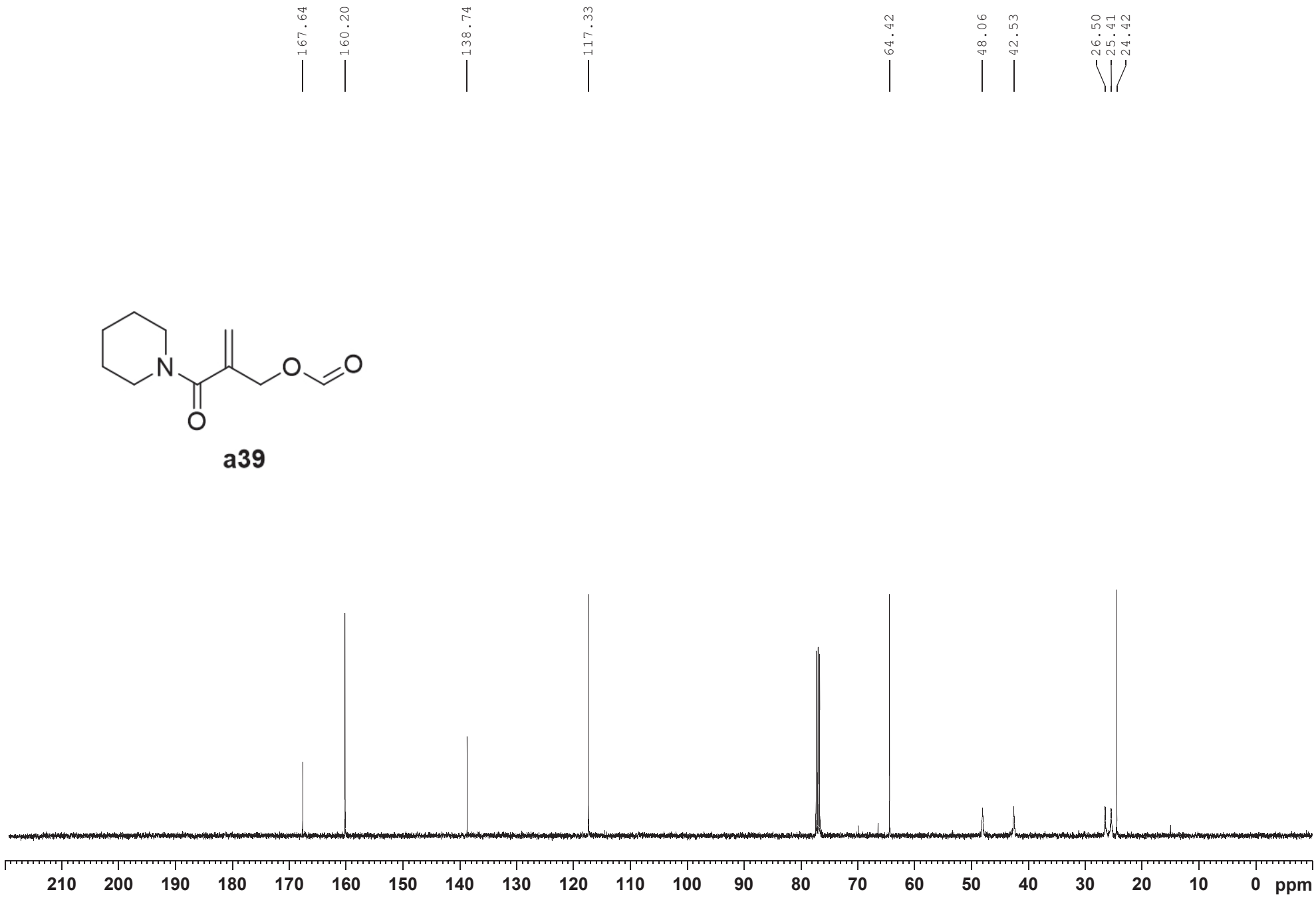

8.155
8.118
8.110
8.079
7.574
7.553
7.343
7.338
7.325
7.320
7.307
7.299
7.266
7.148
7.130
7.111
6.066
6.060
5.767
5.756
4.996
4.989
PhHN
O
O
O
a37
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
2.08
2.11
1.03
1.05
1.06
2.09

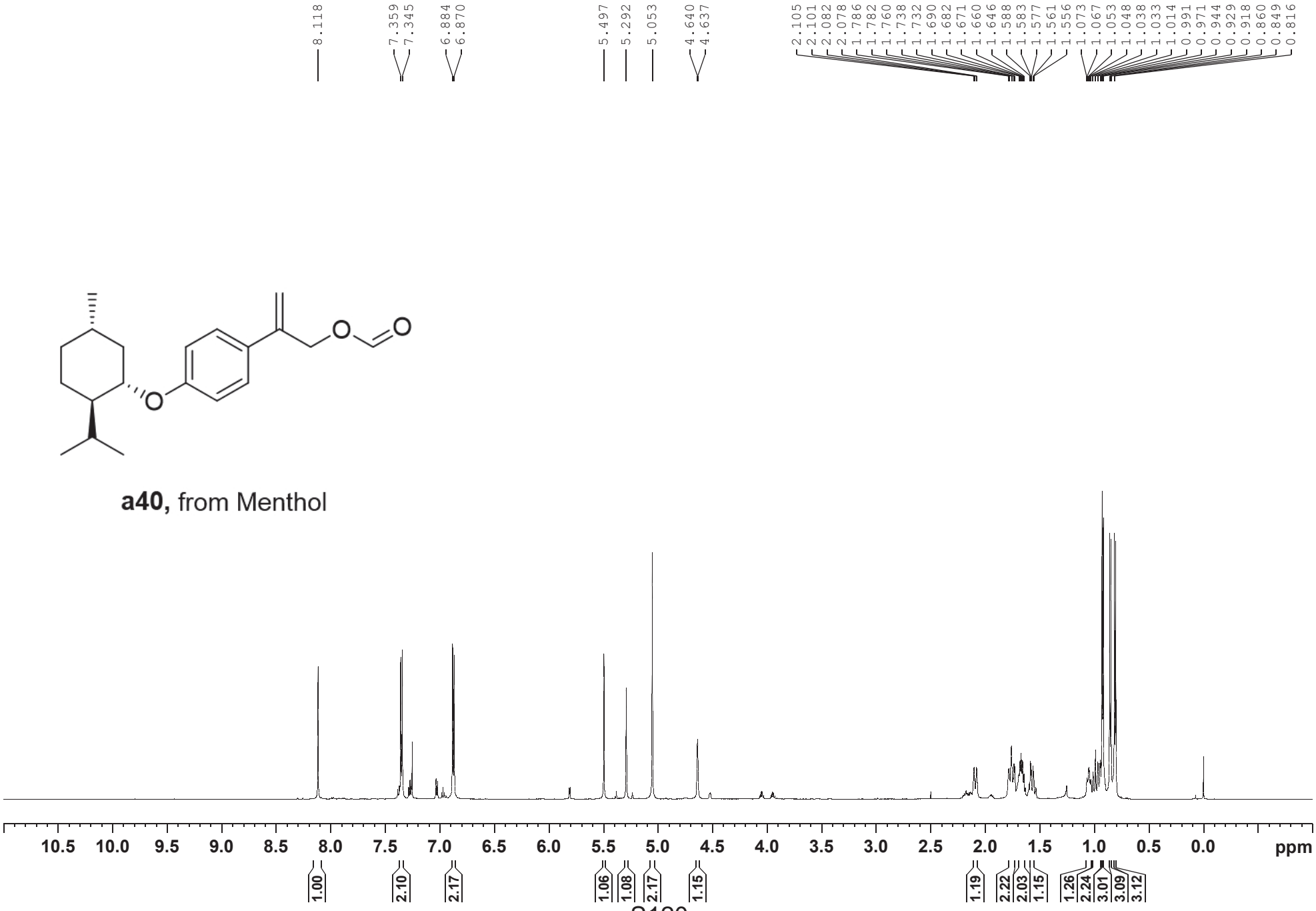

164.20
160.52
139.33
137.37
128.94
124.66
123.28
120.18
77.32
77.00
76.68
62.71
PhHN
O
O
O
a37
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

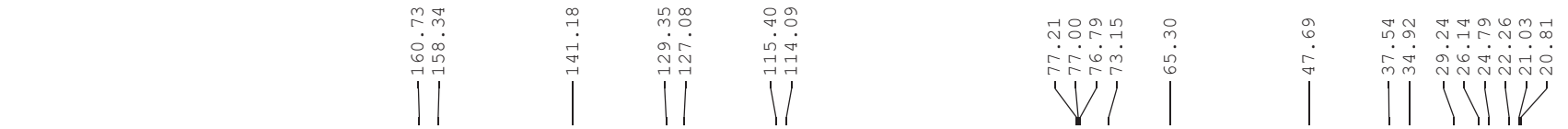

8.111
6.256
5.903
5.638
4.930
3.348
3.333
3.330
3.316
3.313
3.298
1.574
1.556
1.550
1.537
1.531
1.520
1.500
1.415
1.396
1.377
1.358
1.340
1.322
0.956
0.938
0.920
H
N
O
O
O
a38
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.01
1.12
1.12
2.22
2.22
2.26
2.28
3.33

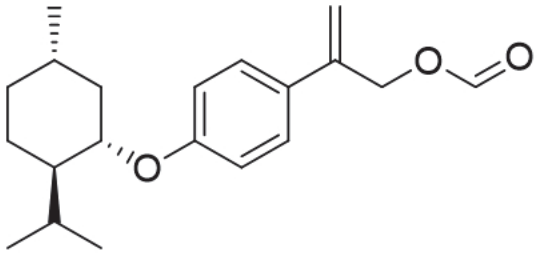

165.95
160.35
139.08
121.82
62.85
39.36
31.42
19.98
13.62
H
N
O
O
O
a38
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.099
5.490
5.292
4.877
3.589
3.560
3.543
3.528
1.712
1.700
1.681
1.670
1.654
1.578
N
O
O
O
a39
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.10
1.16
2.16
4.11
6.15

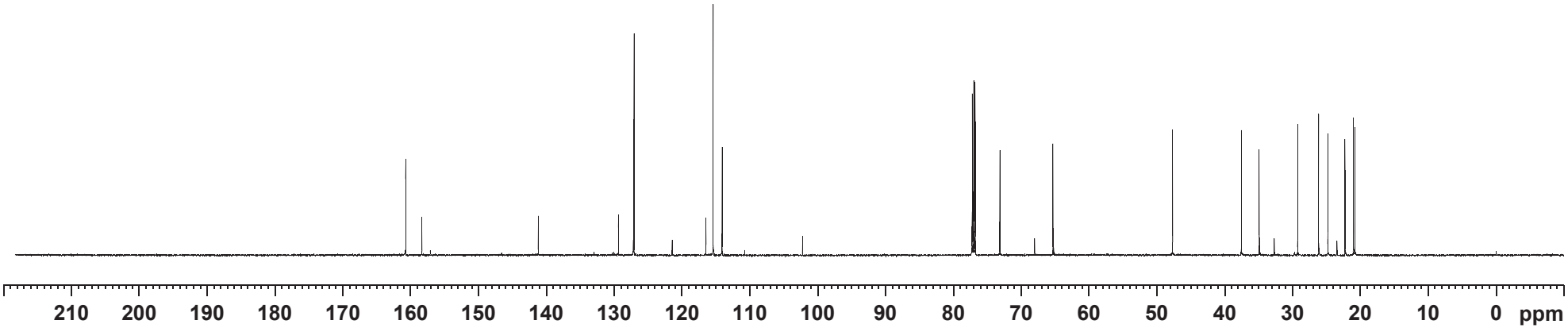

167.64
160.20
138.74
117.33
64.42
48.06
42.53
26.50
25.41
24.42
N
O
O
O
a39
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

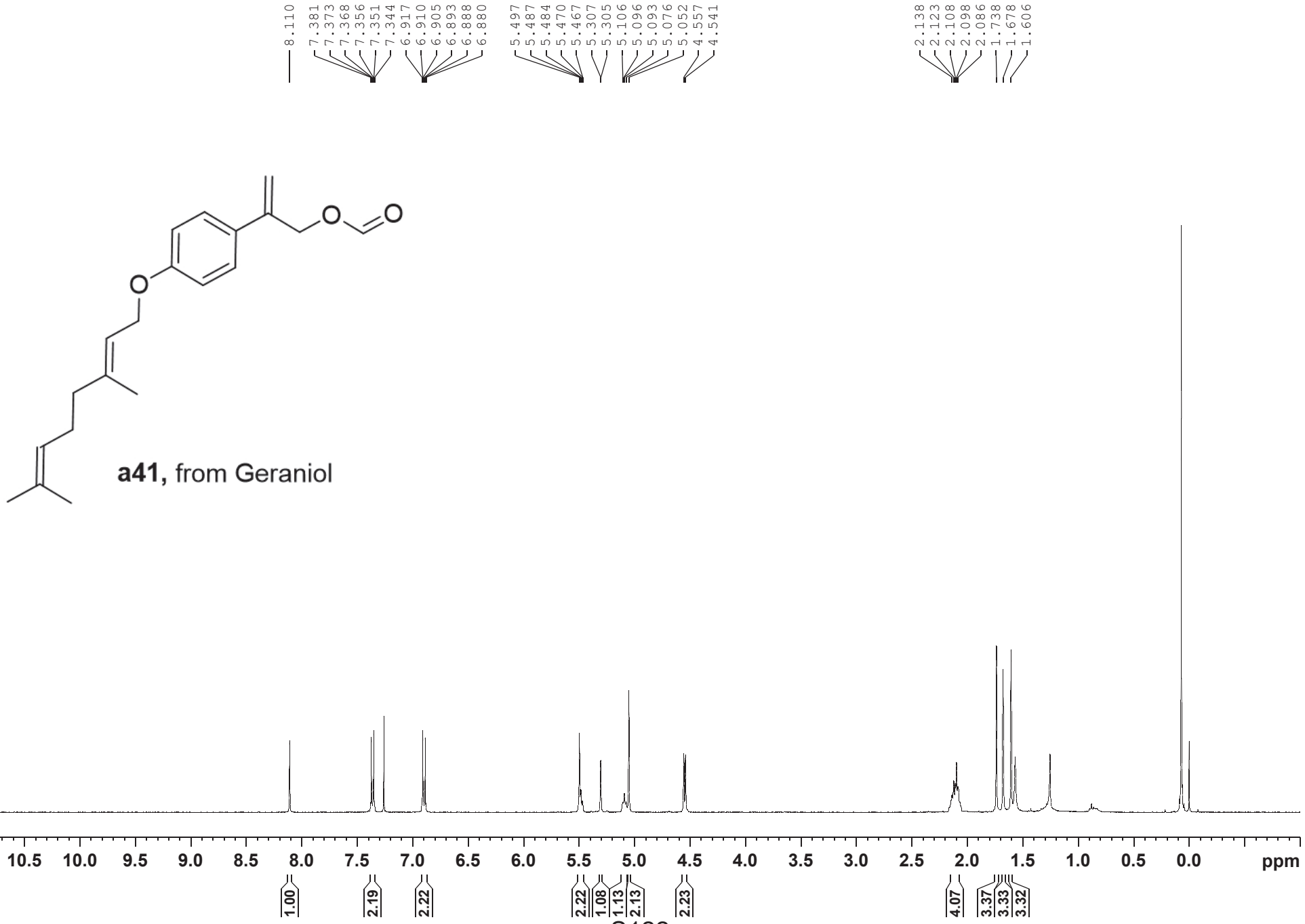

8.118
7.359
7.345
6.884
6.870
5.497
5.292
5.053
4.640
4.637
2.105
2.101
2.082
2.078
1.786
1.782
1.760
1.738
1.732
1.690
1.682
1.671
1.660
1.646
1.588
1.583
1.577
1.561
1.556
1.073
1.067
1.053
1.048
1.038
1.033
1.014
0.991
0.971
0.944
0.929
0.918
0.860
0.849
0.816
O
O
O
a40, from Menthol
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
2.10
2.17
1.06
1.08
2.17
1.15
1.19
2.22
2.03
1.15
1.26
2.24
3.01
3.09
3.12

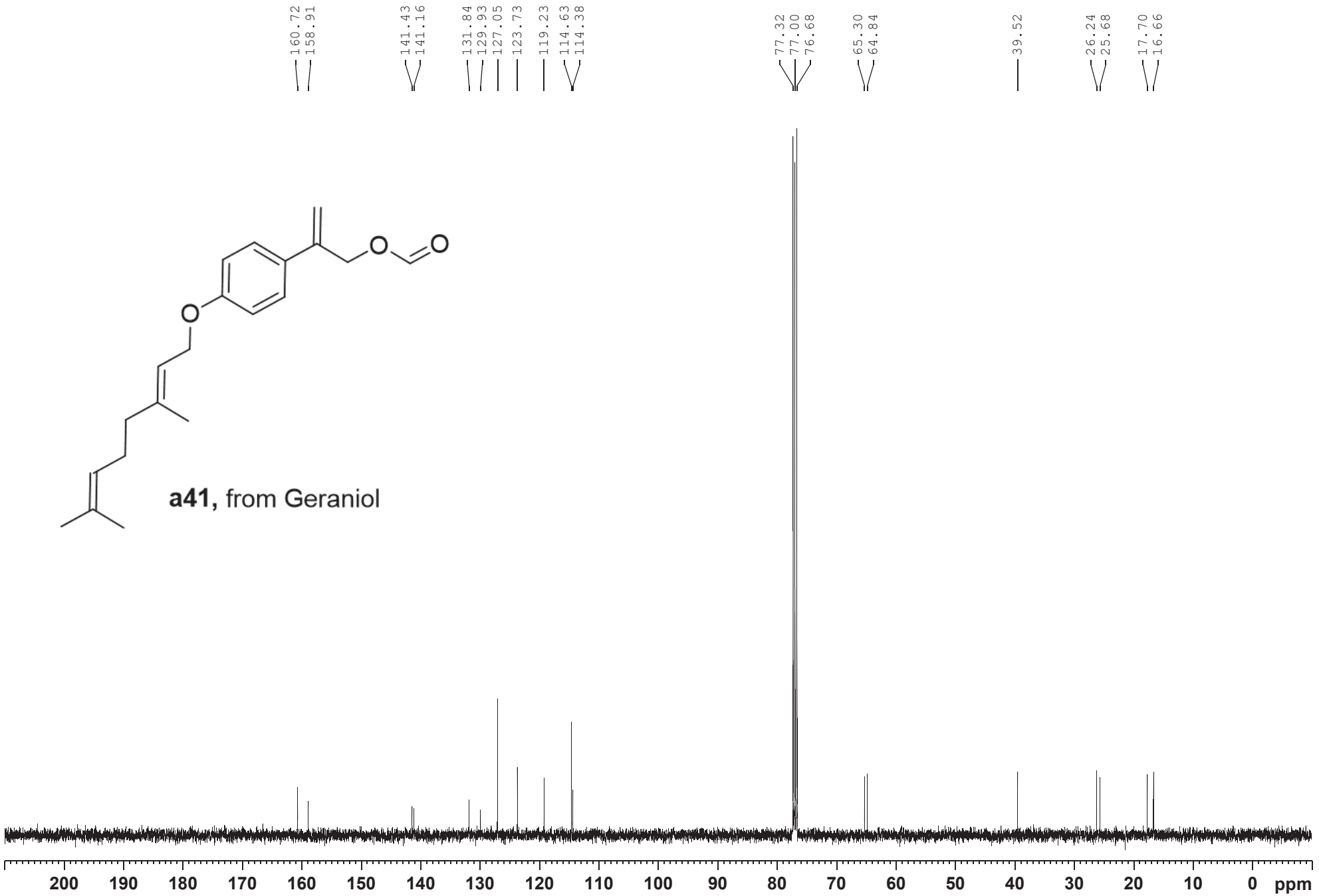


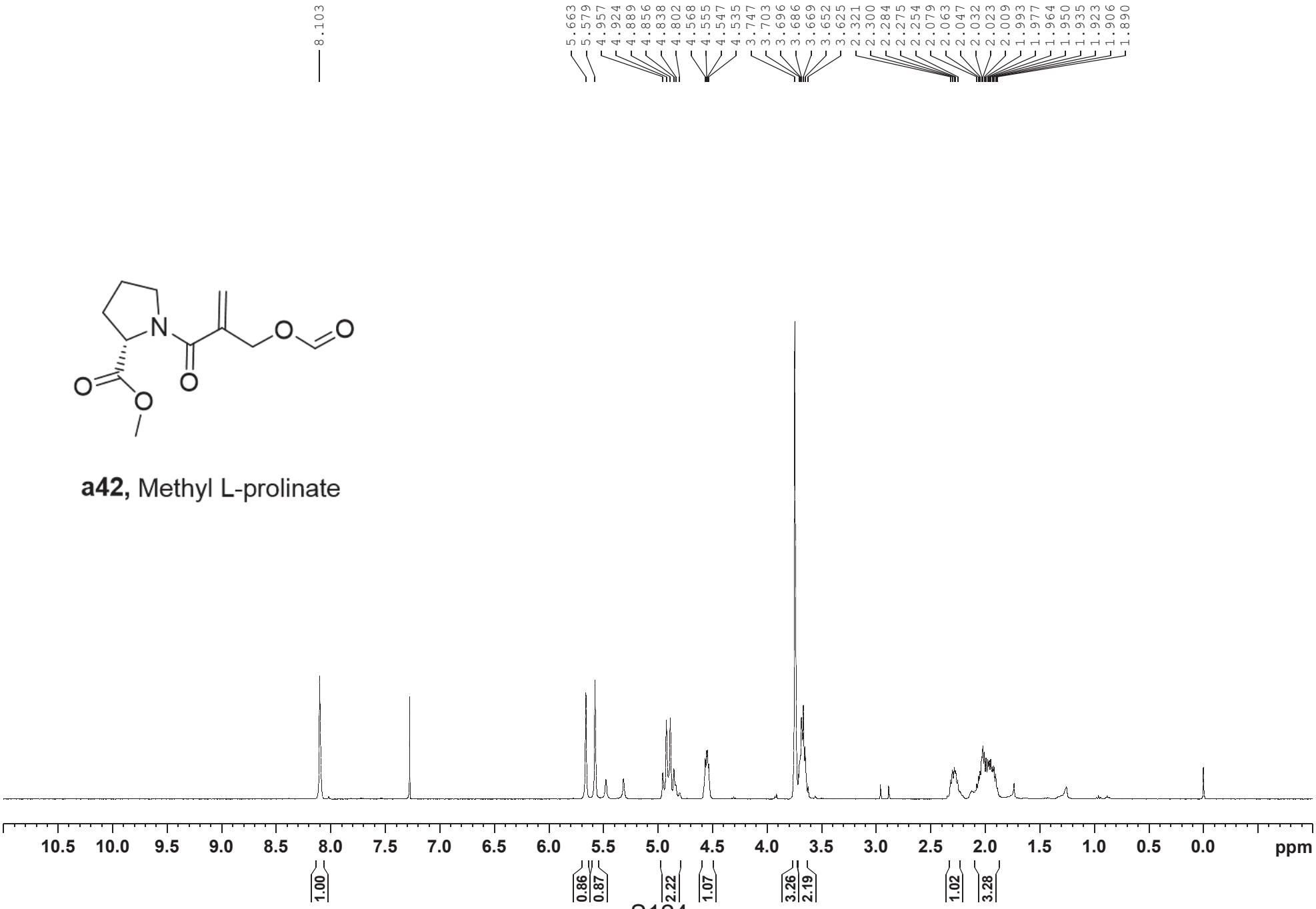


a40, from Menthol

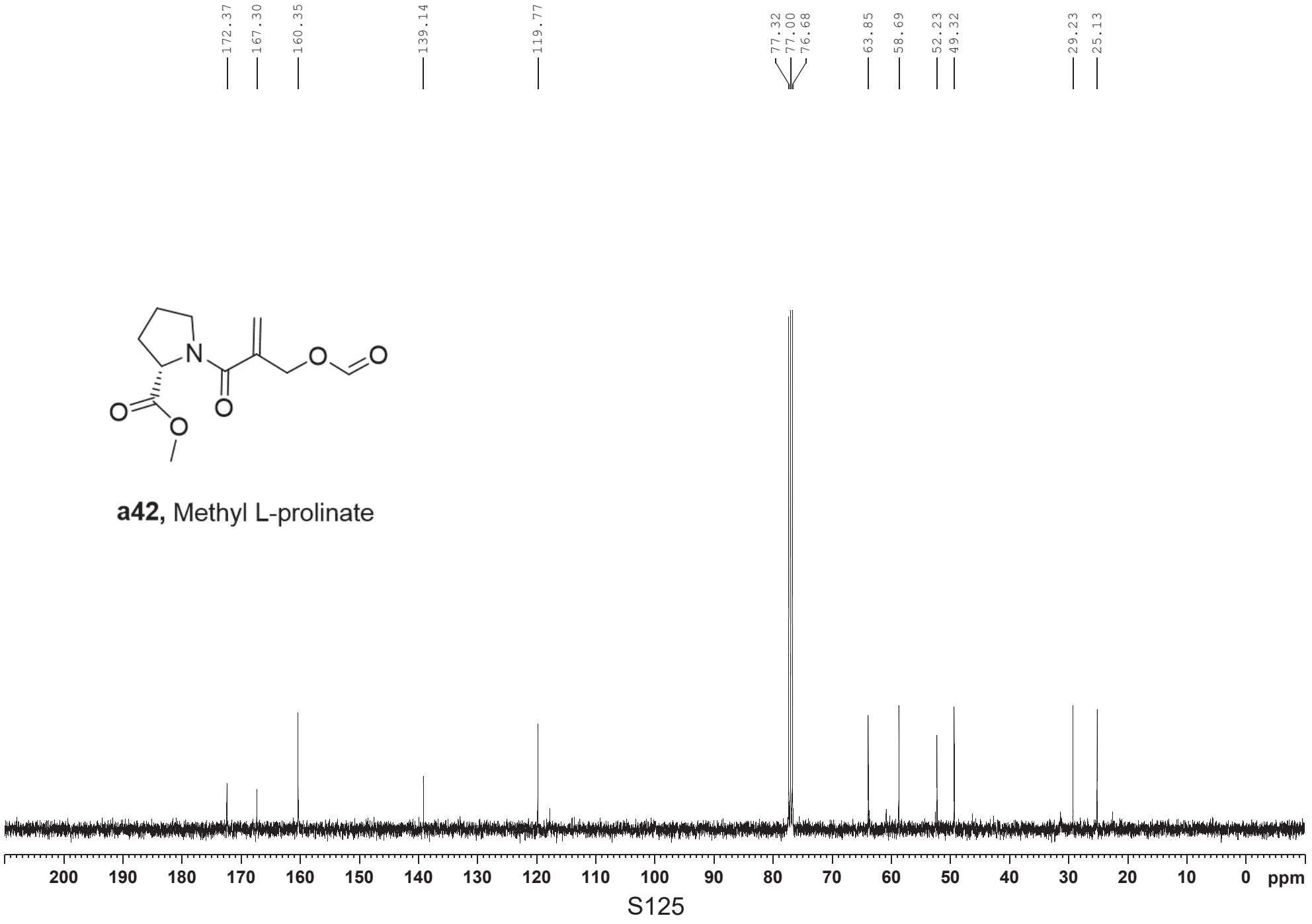



8.110
7.381
7.373
7.368
7.356
7.351
7.344
6.917
6.910
6.905
6.893
6.888
6.880
5.497
5.487
5.484
5.470
5.467
5.307
5.305
5.106
5.096
5.093
5.076
5.052
4.557
4.541
2.138
2.123
2.108
2.098
2.086
1.738
1.678
1.606
O
O
O
a41, from Geraniol
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.19
2.22
2.22
1.08
1.13
2.13
2.23
4.07
3.37
3.33
3.32

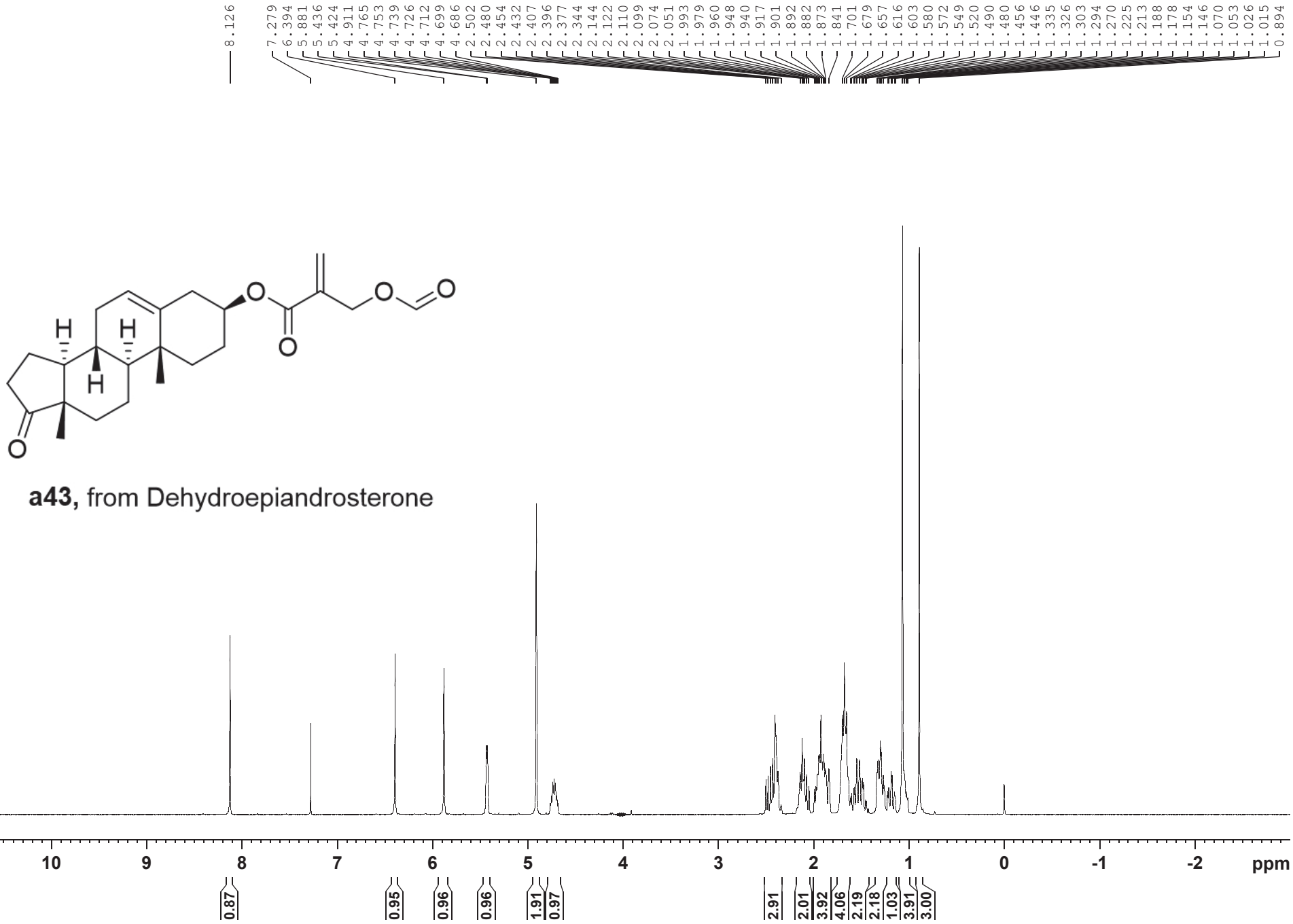

160.72
158.91
141.43
141.16
131.84
129.93
127.05
123.73
119.23
114.63
114.38
77.32
77.00
76.68
65.30
64.84
39.52
26.24
25.68
17.70
16.66
a41, from Geraniol
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

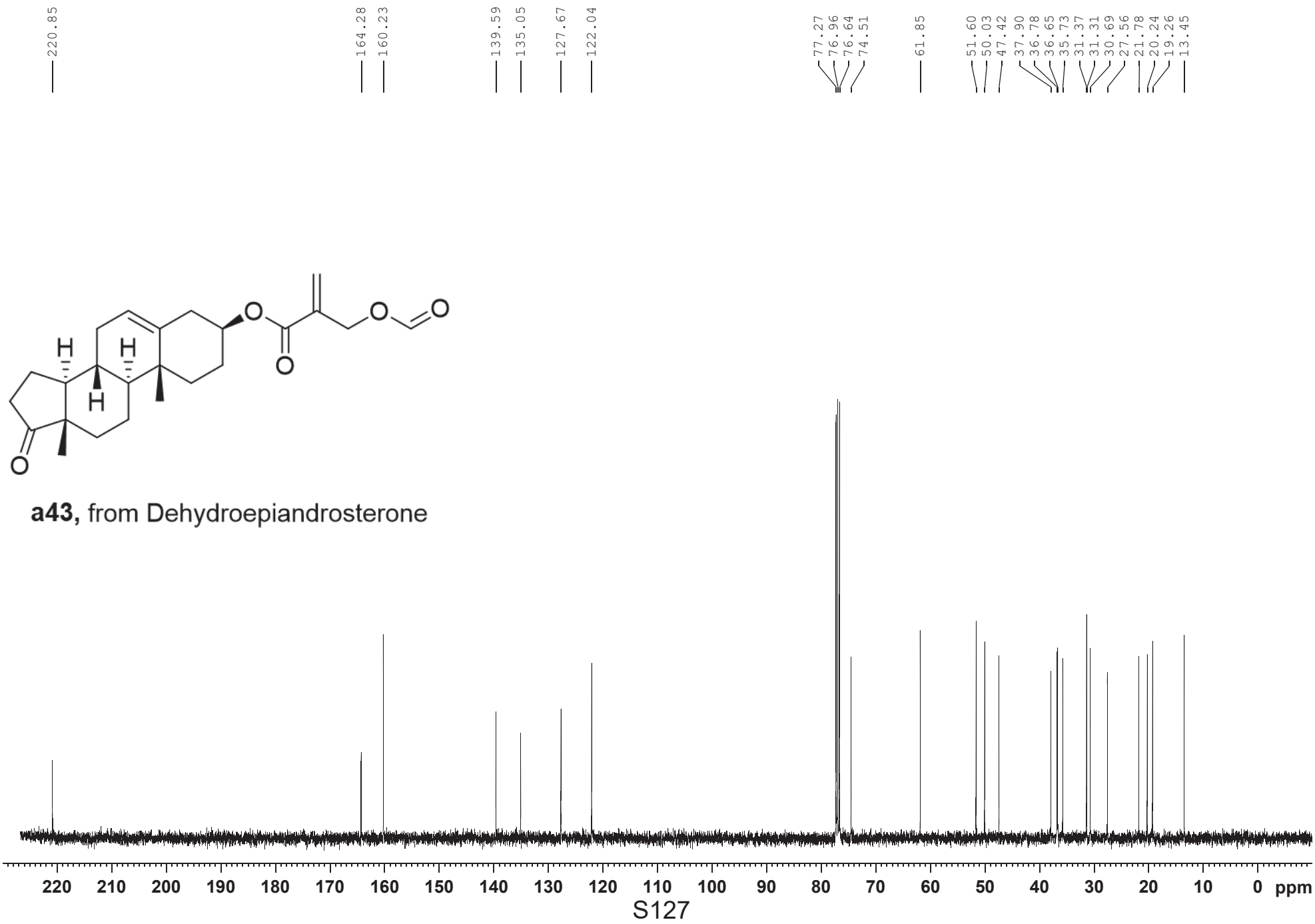


a42, Methyl L-prolinate

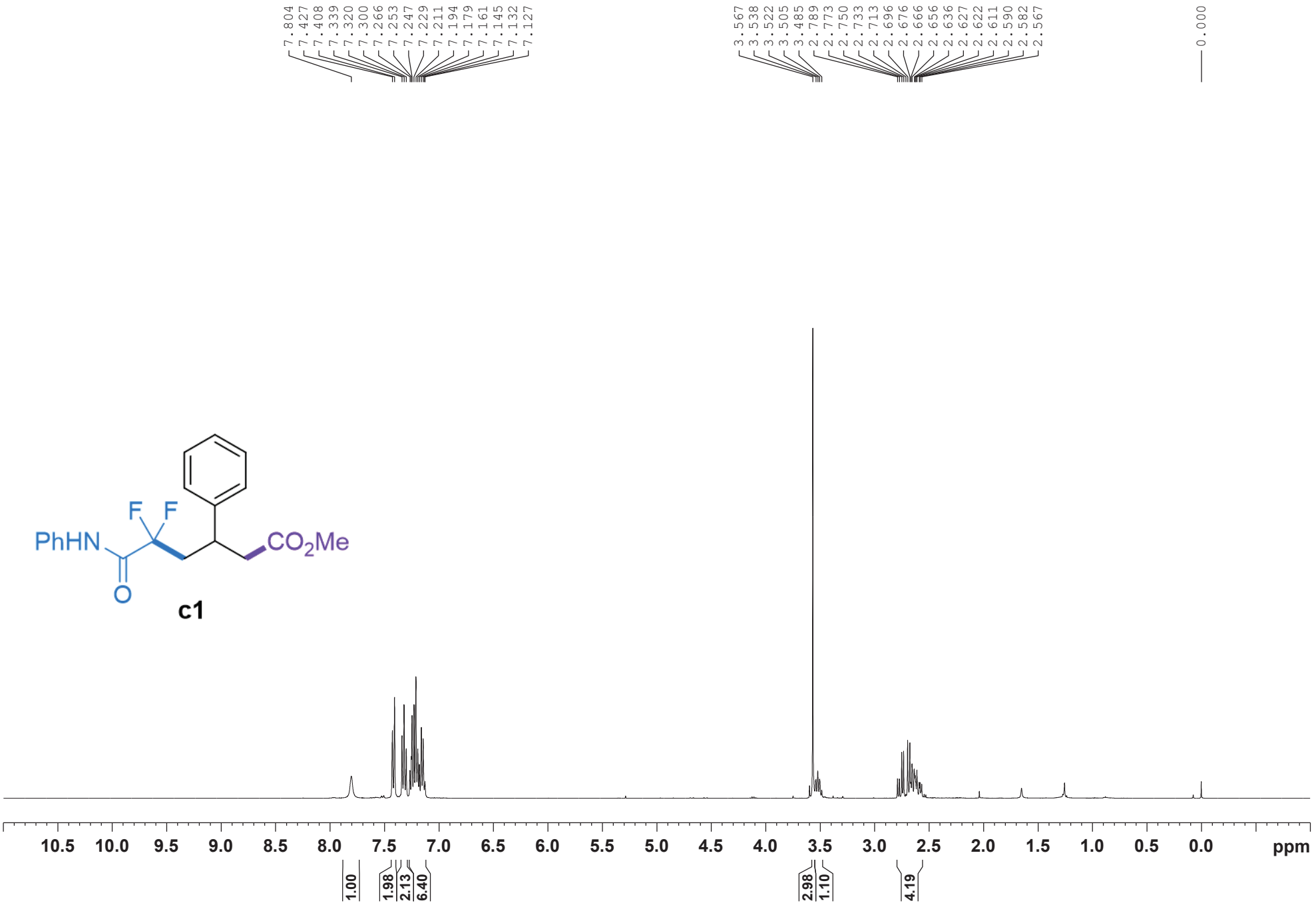


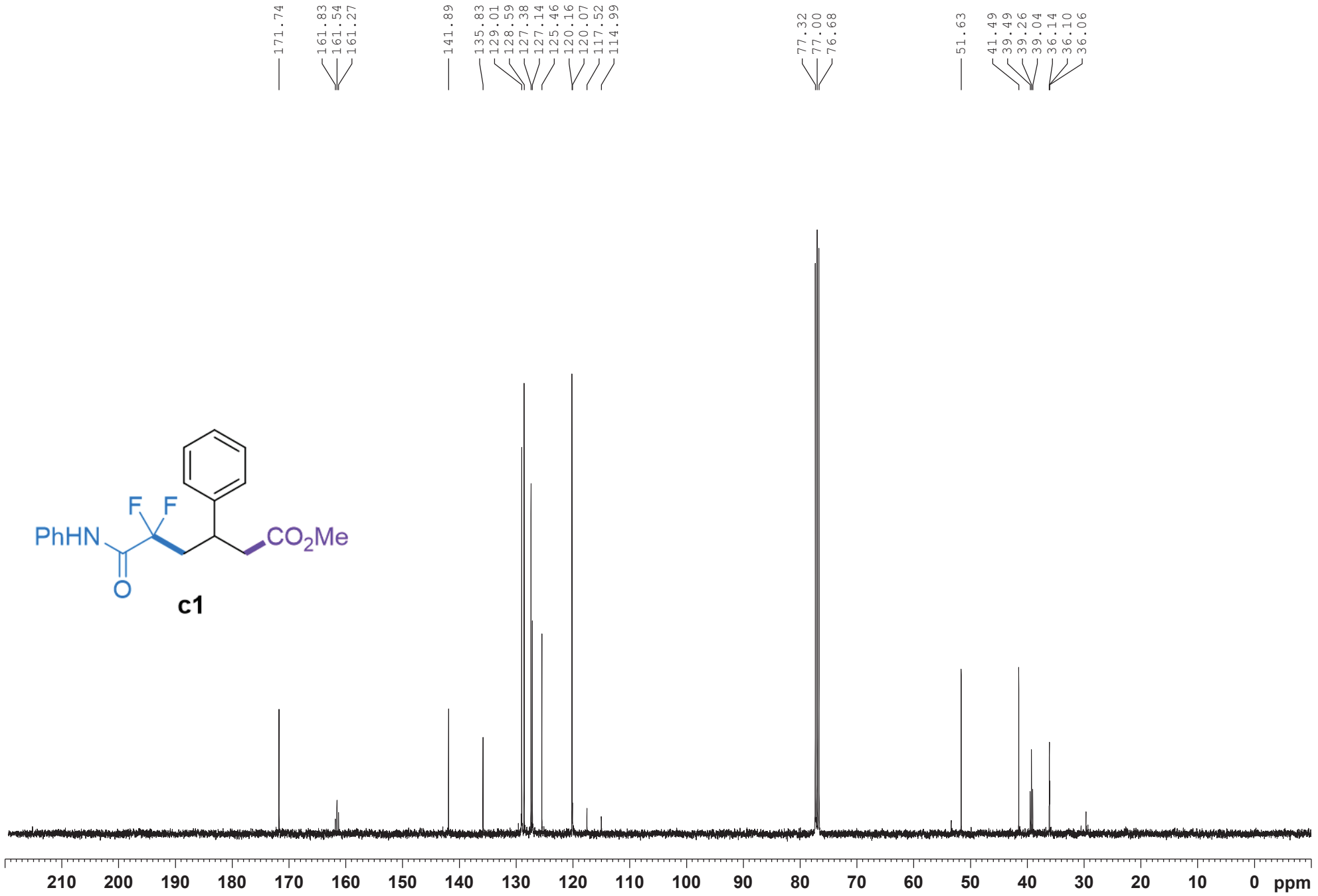
a42, Methyl L-prolinate

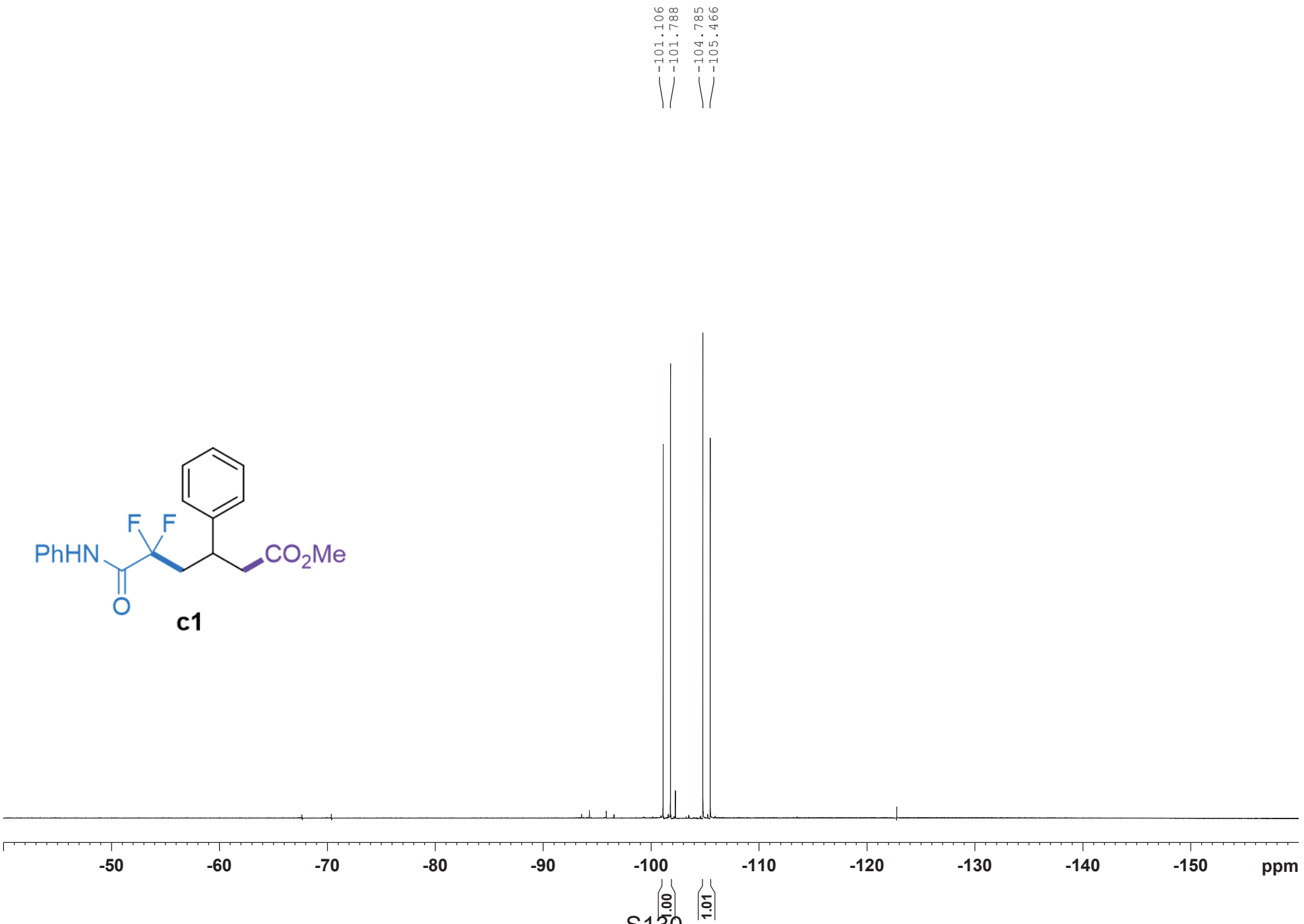

8.126
7.279
6.394
5.881
5.436
5.424
4.911
4.765
4.753
4.739
4.726
4.712
4.699
4.686
2.502
2.480
2.454
2.432
2.407
2.396
2.377
2.344
2.144
2.122
2.110
2.099
2.074
2.051
1.993
1.979
1.960
1.948
1.940
1.917
1.901
1.892
1.882
1.873
1.841
1.701
1.679
1.657
1.616
1.603
1.580
1.572
1.549
1.520
1.490
1.480
1.456
1.446
1.335
1.326
1.303
1.294
1.270
1.225
1.213
1.188
1.178
1.154
1.146
1.070
1.053
1.026
1.015
0.894
O
O
O
O
H
H
H
O
a43, from Dehydroepiandrosterone
10
9
8
7
6
5
4
3
2
1
0
-1
-2
ppm
0.87
0.95
0.96
0.96
1.91
0.97
2.91
2.01
3.92
4.06
2.19
2.18
1.03
3.91
3.00

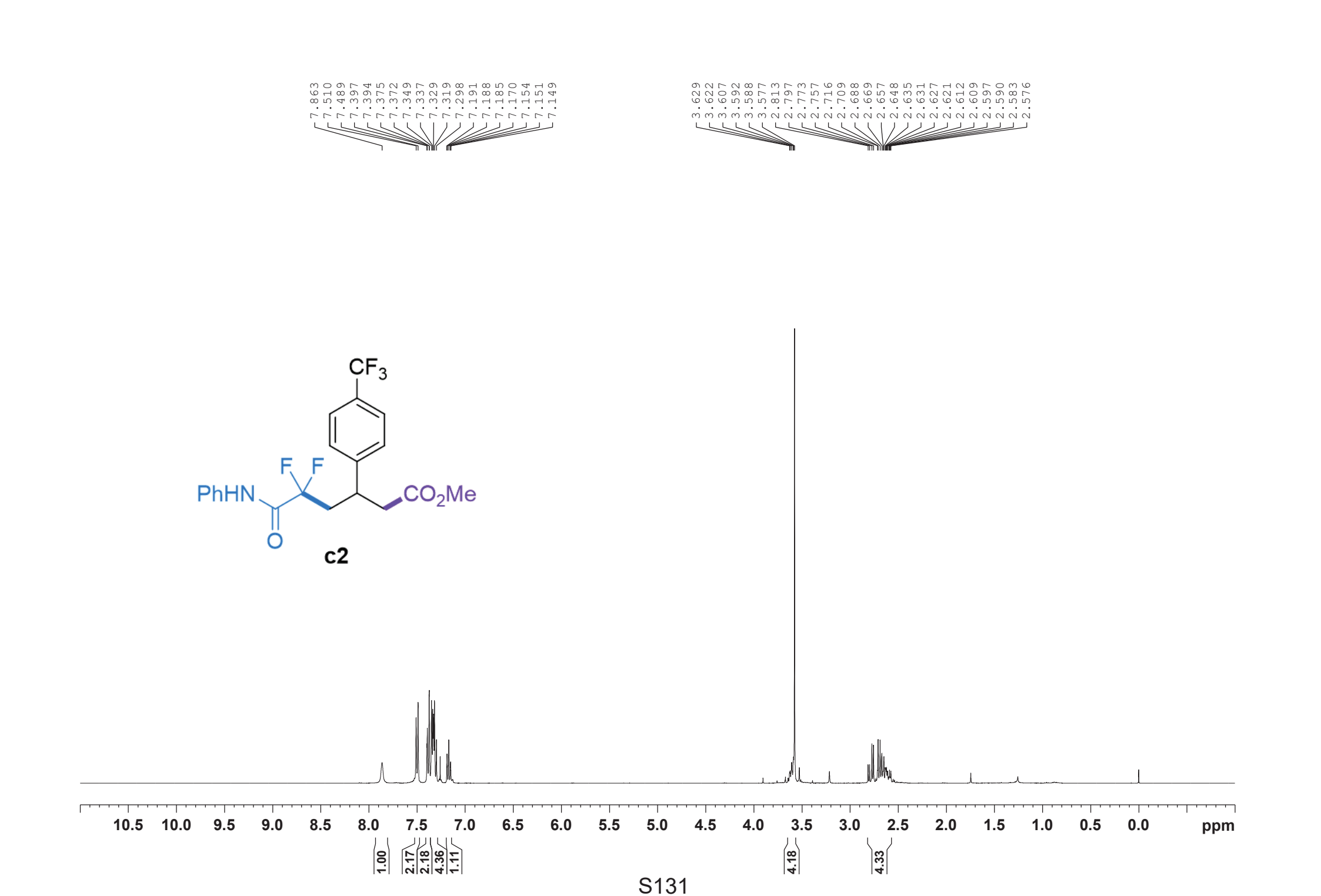


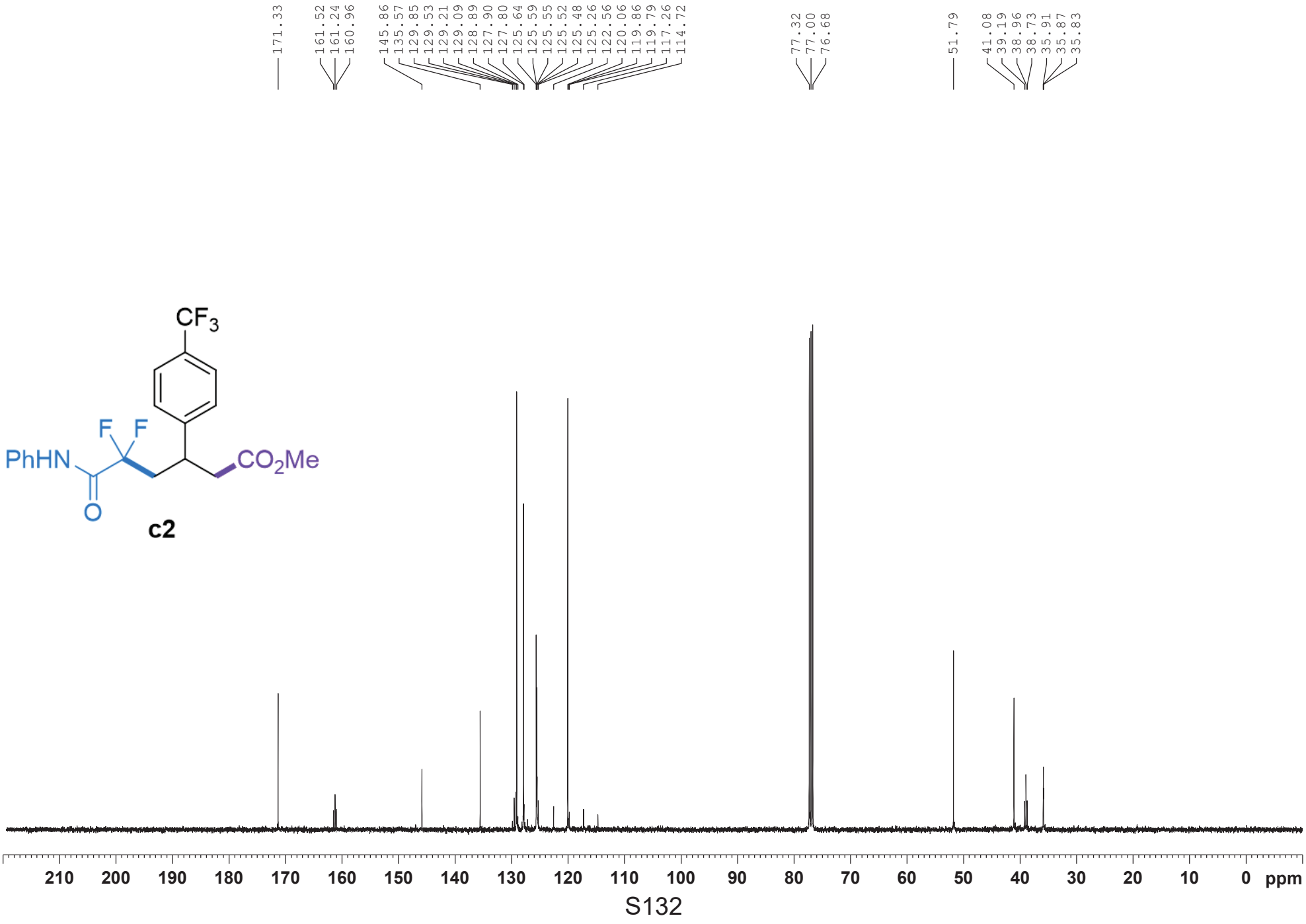
a43, from Dehydroepiandrosterone

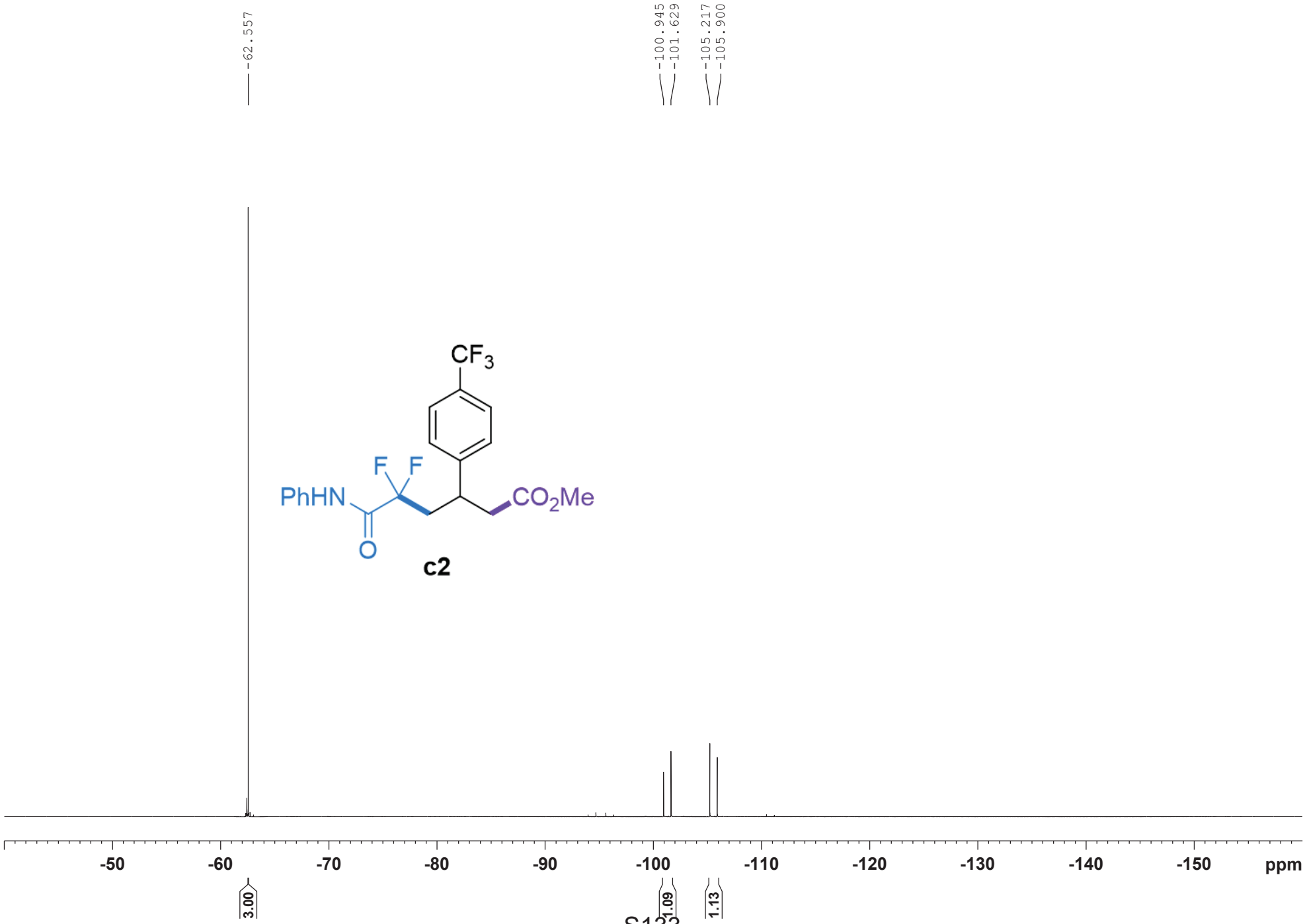

7.804
7.427
7.408
7.339
7.320
7.300
7.266
7.253
7.247
7.229
7.211
7.194
7.179
7.161
7.145
7.132
7.127
3.567
3.538
3.522
3.505
3.485
2.789
2.773
2.750
2.733
2.713
2.696
2.676
2.666
2.656
2.636
2.627
2.622
2.611
2.590
2.582
2.567
0.000
F
F
PhHN
O
CO2Me
c1
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.98
2.13
6.40
2.98
1.10
4.19

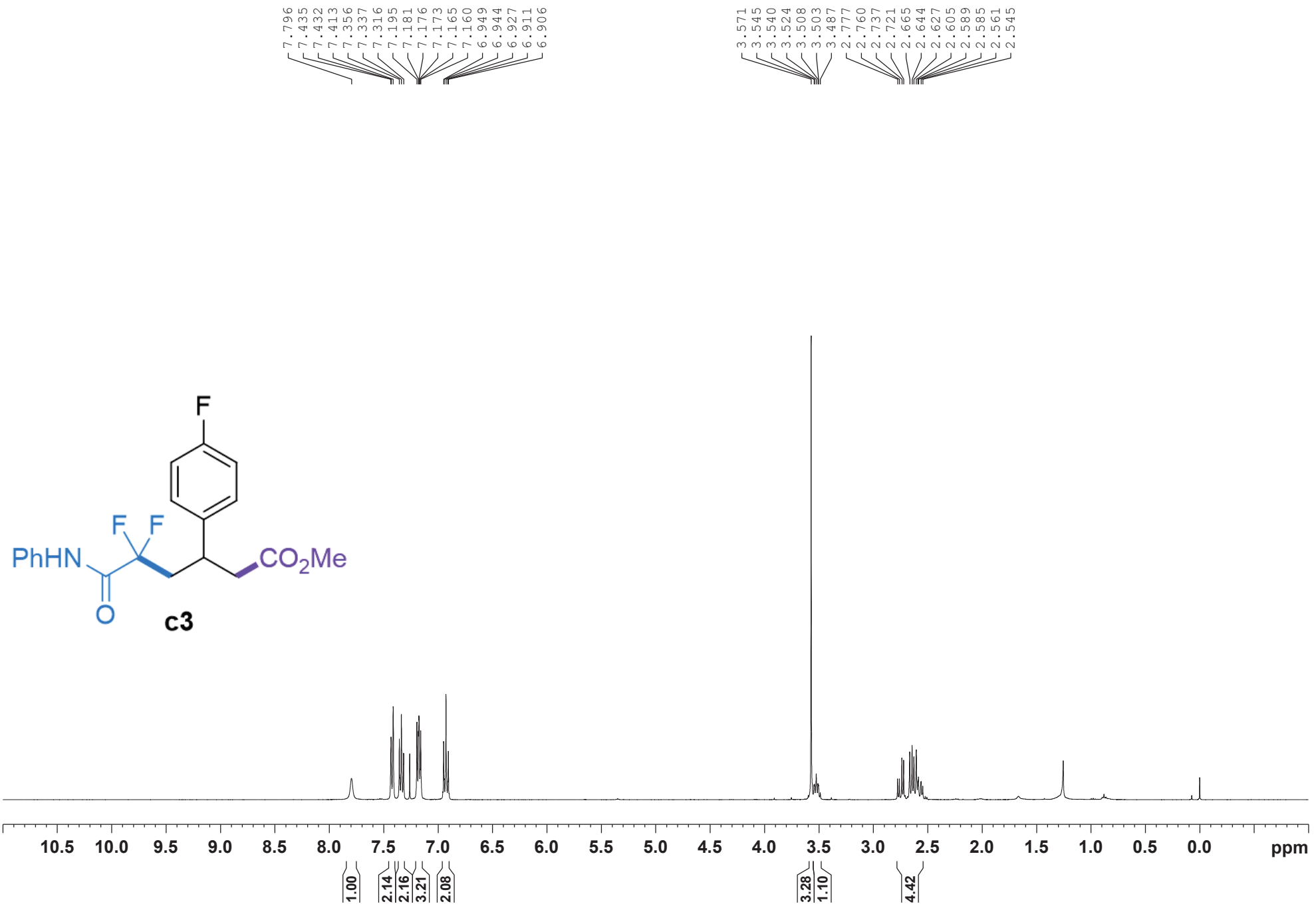

171.74
161.83
161.54
161.27
141.89
135.83
129.01
128.59
127.38
127.14
125.46
120.16
120.07
117.52
114.99
77.32
77.00
76.68
51.63
41.49
39.49
39.26
39.04
36.14
36.10
36.06
F
F
PhHN
O
CO2Me
c1
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

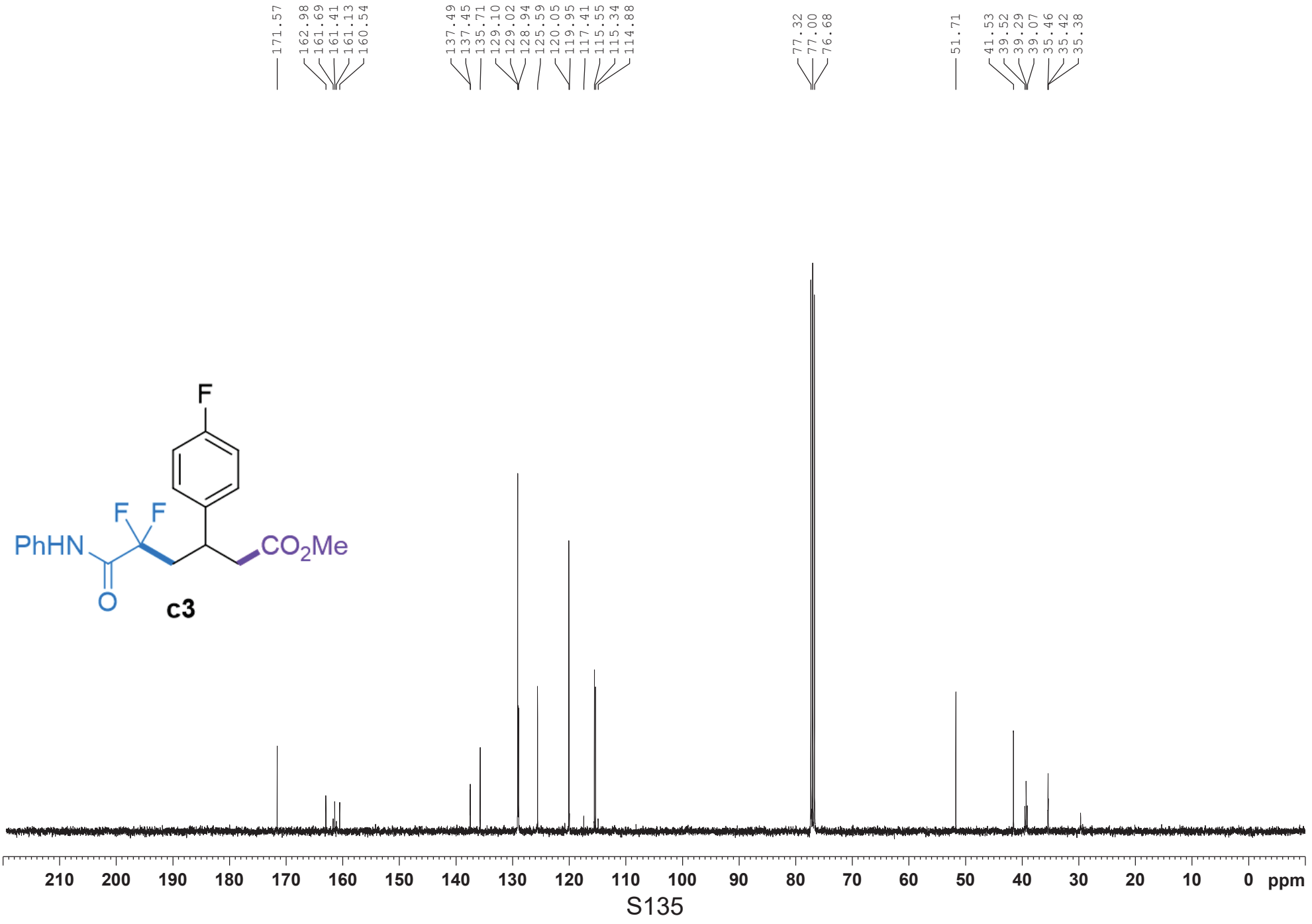

-101.106
-101.788
-104.785
-105.466
PhHN
F
F
O
CO2Me
c1
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

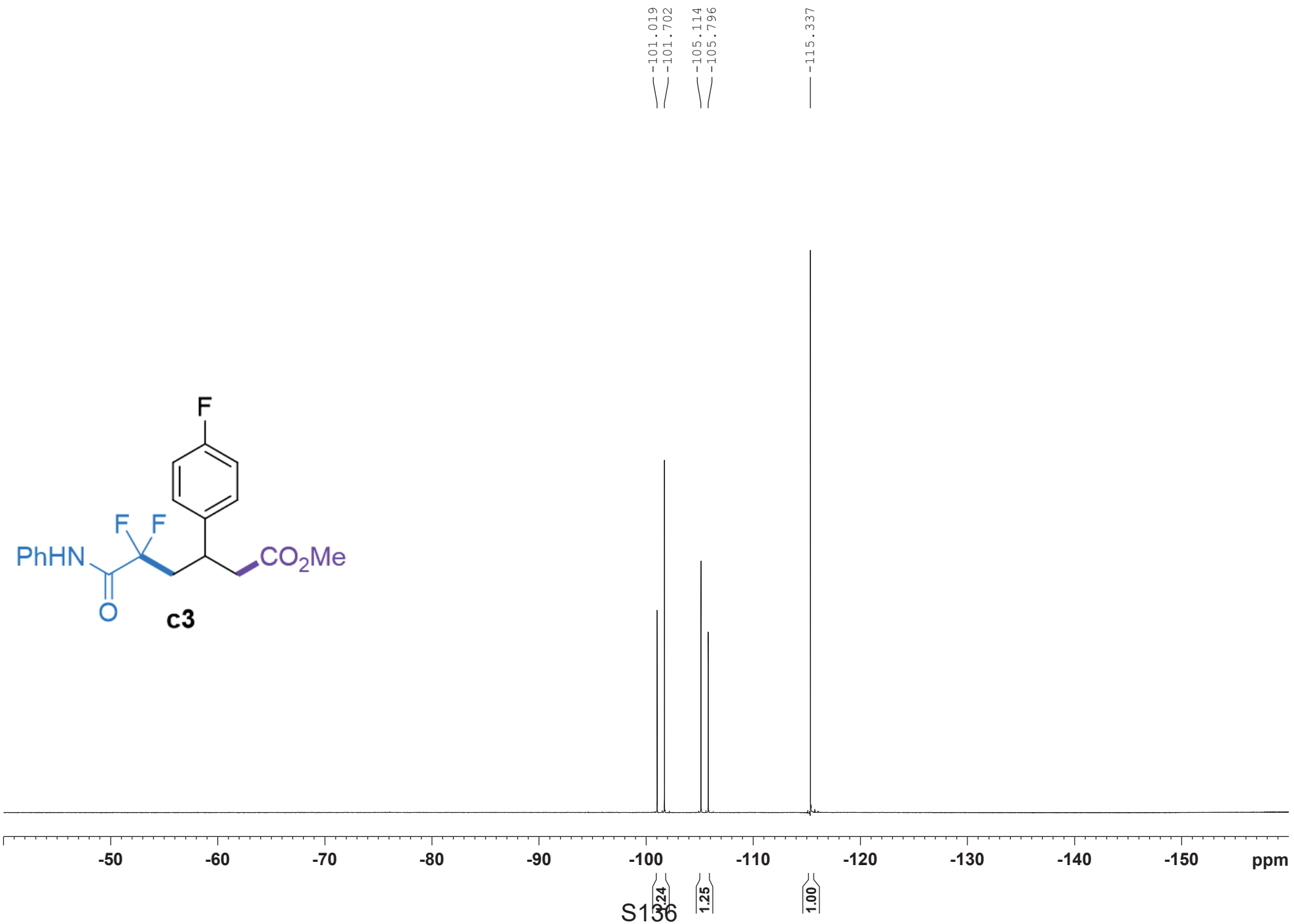

7.863
7.510
7.489
7.397
7.394
7.375
7.372
7.349
7.337
7.329
7.319
7.298
7.191
7.188
7.185
7.170
7.154
7.151
7.149
3.629
3.622
3.607
3.592
3.588
3.577
2.813
2.797
2.773
2.757
2.716
2.709
2.688
2.669
2.657
2.648
2.635
2.631
2.627
2.621
2.612
2.609
2.597
2.590
2.583
2.576
CF3
F F
PhHN
CO2Me
O
c2
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
2.17
2.18
4.36
1.11
4.18
4.33

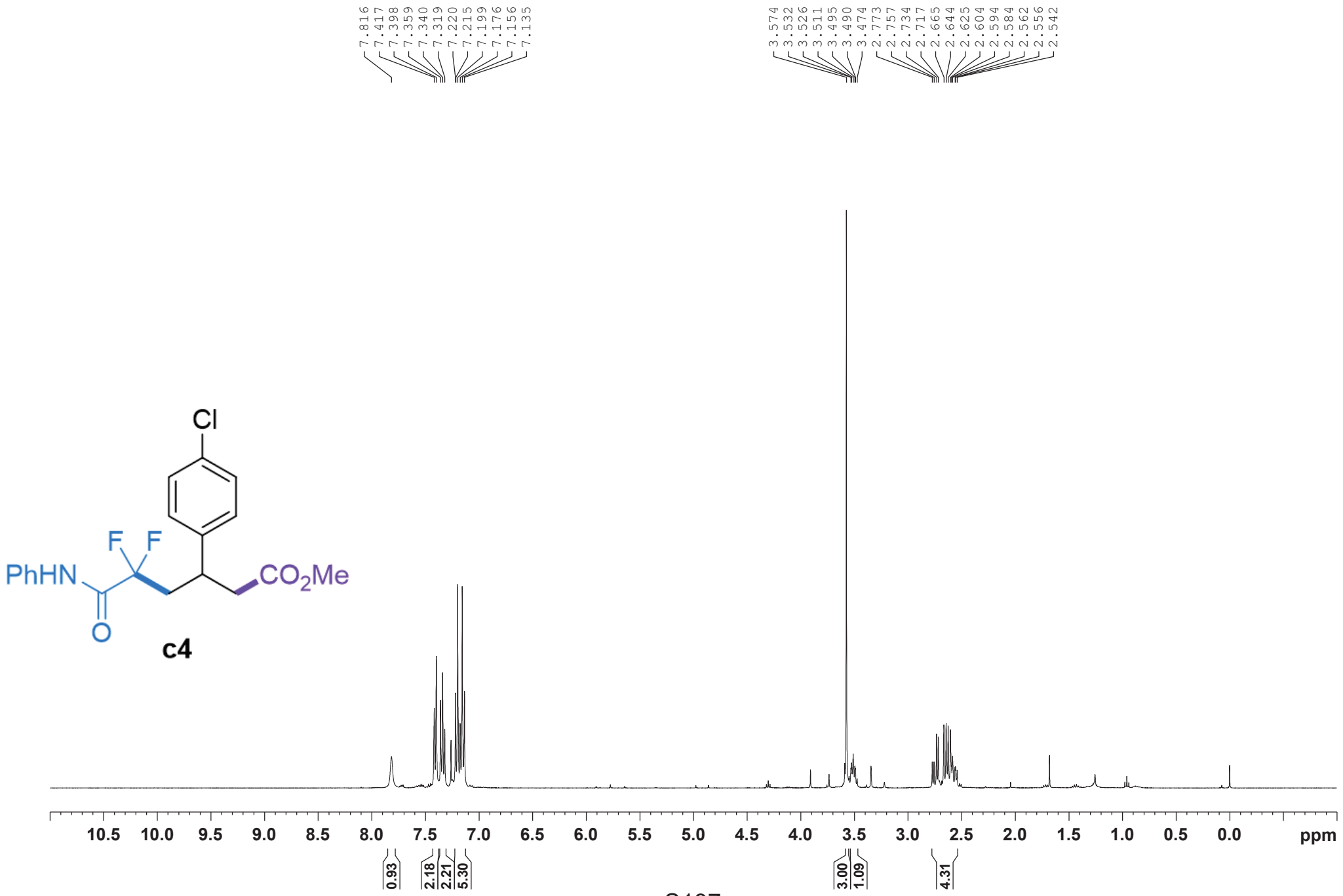

171.33
161.52
161.24
160.96
145.86
135.57
129.85
129.53
129.21
129.09
128.89
127.90
127.80
125.64
125.59
125.55
125.52
125.48
125.26
122.56
120.06
119.86
119.79
117.26
114.72
77.32
77.00
76.68
51.79
41.08
39.19
38.96
38.73
35.91
35.87
35.83
CF3
F
F
PhHN
CO2Me
O
c2
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

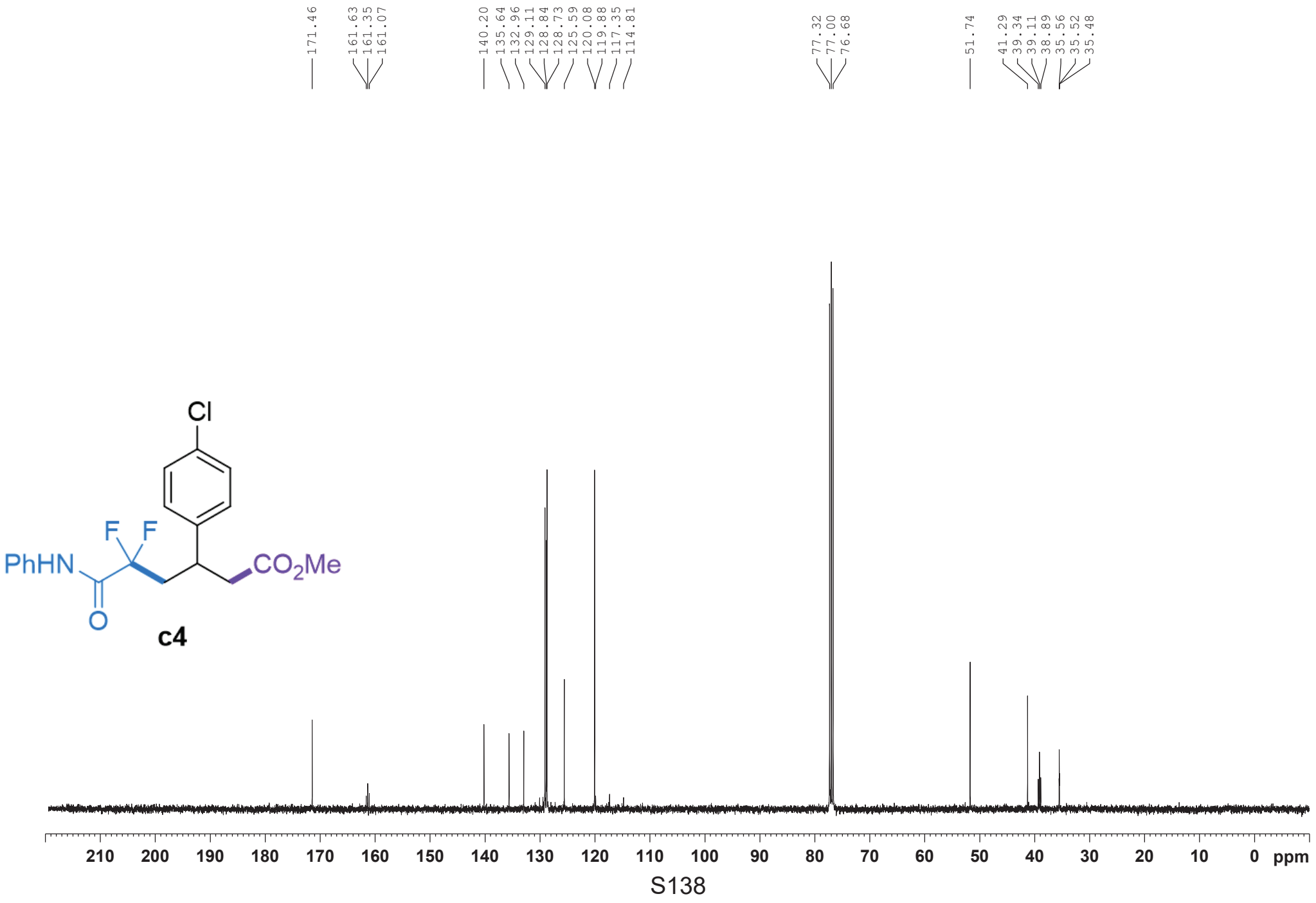

-62.557
-100.945
-101.629
-105.217
-105.900
CF3
F F
PhHN
CO2Me
O
c2
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
3.00
1.09
1.13

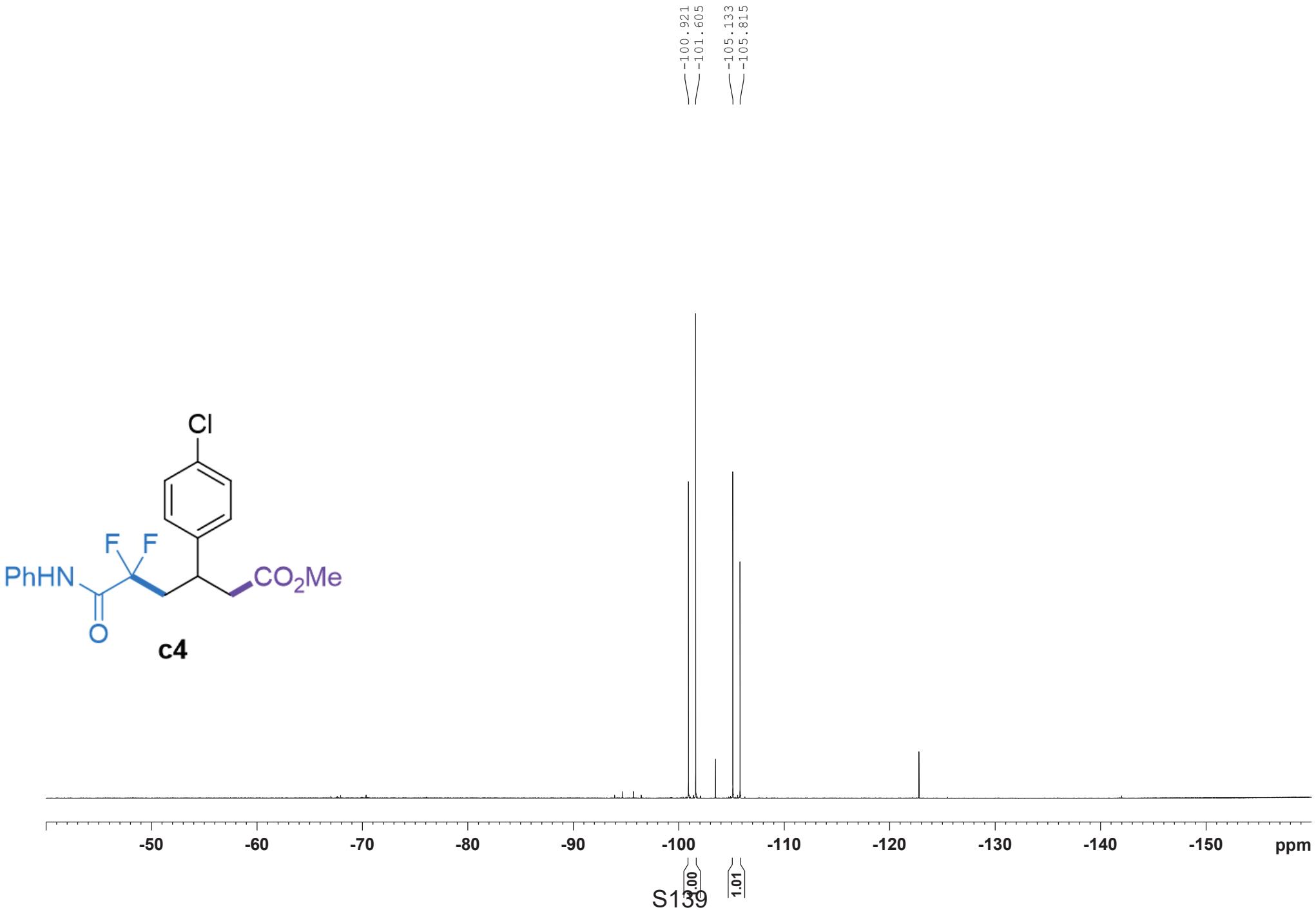

7.796
7.435
7.432
7.413
7.356
7.337
7.316
7.195
7.181
7.176
7.173
7.165
7.160
6.949
6.944
6.927
6.911
6.906
3.571
3.545
3.540
3.524
3.508
3.503
3.487
2.777
2.760
2.737
2.721
2.665
2.644
2.627
2.605
2.589
2.585
2.561
2.545
F
F
F
PhHN
CO2Me
O
c3
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.14
2.16
3.21
2.08
3.28
1.10
4.42

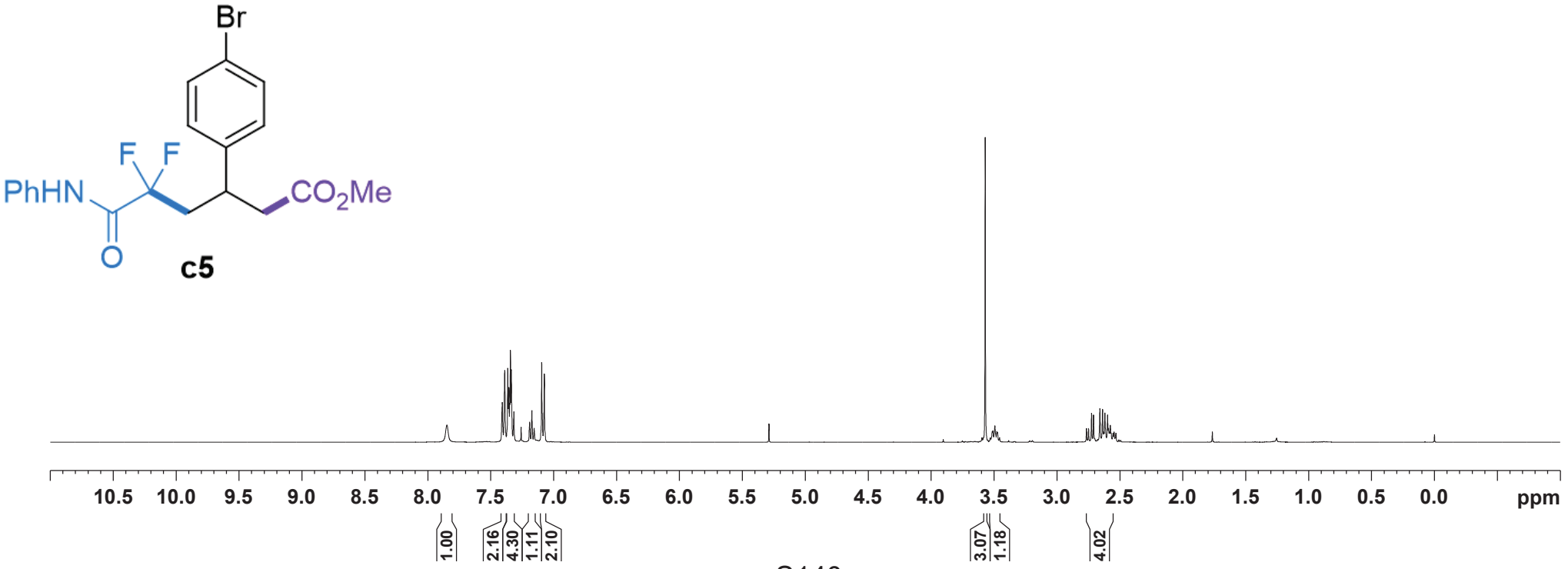

171.57
162.98
161.69
161.41
161.13
160.54
137.49
137.45
135.71
129.10
129.02
128.94
125.59
120.05
119.95
117.41
115.55
115.34
114.88
77.32
77.00
76.68
51.71
41.53
39.52
39.29
39.07
35.46
35.42
35.38
F
F
F
PhHN
O
CO2Me
c3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

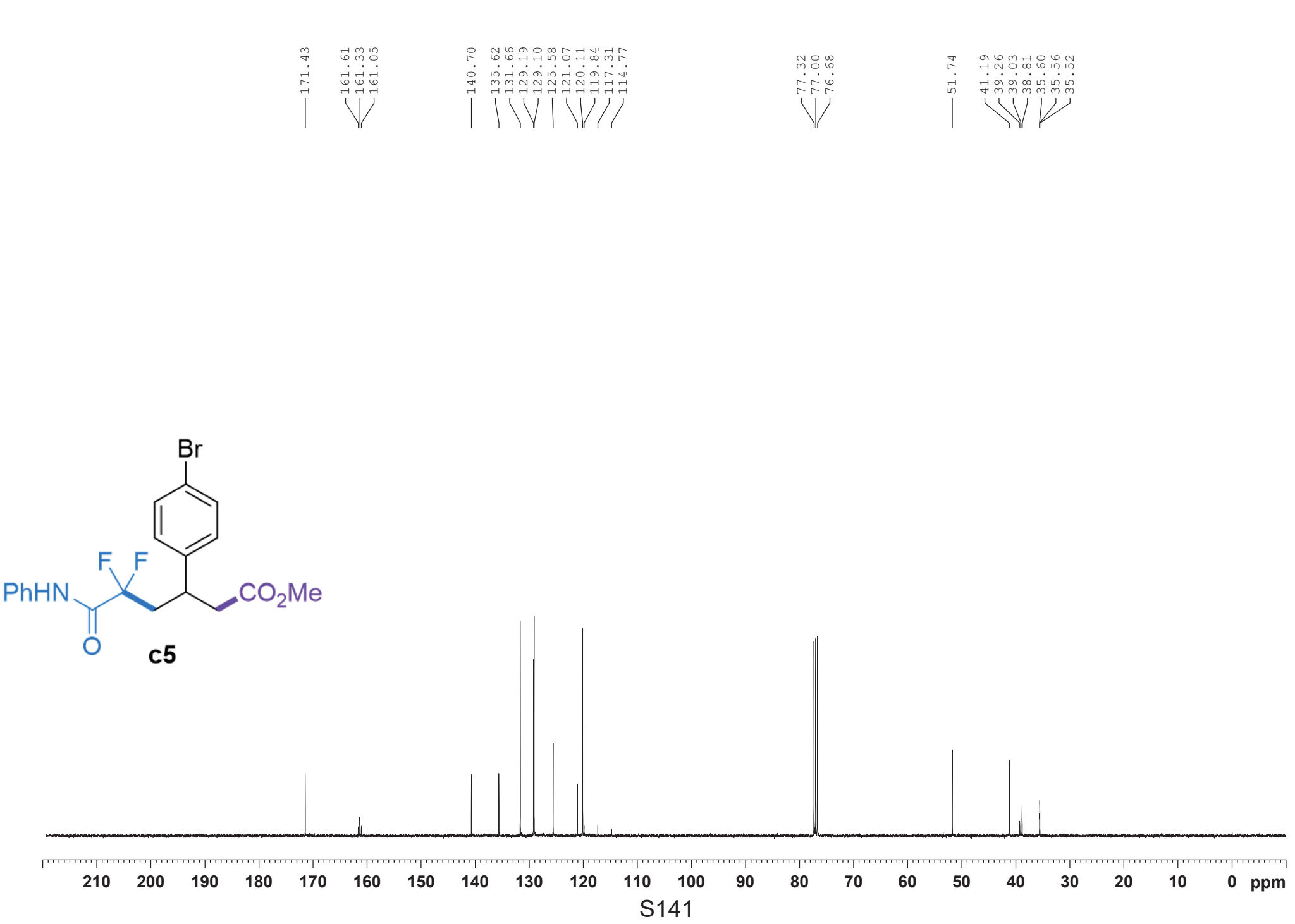

-101.019
-101.702
-105.114
-105.796
-115.337
F
F
F
PhHN
O
CO2Me
c3
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
3.24
1.25
1.00

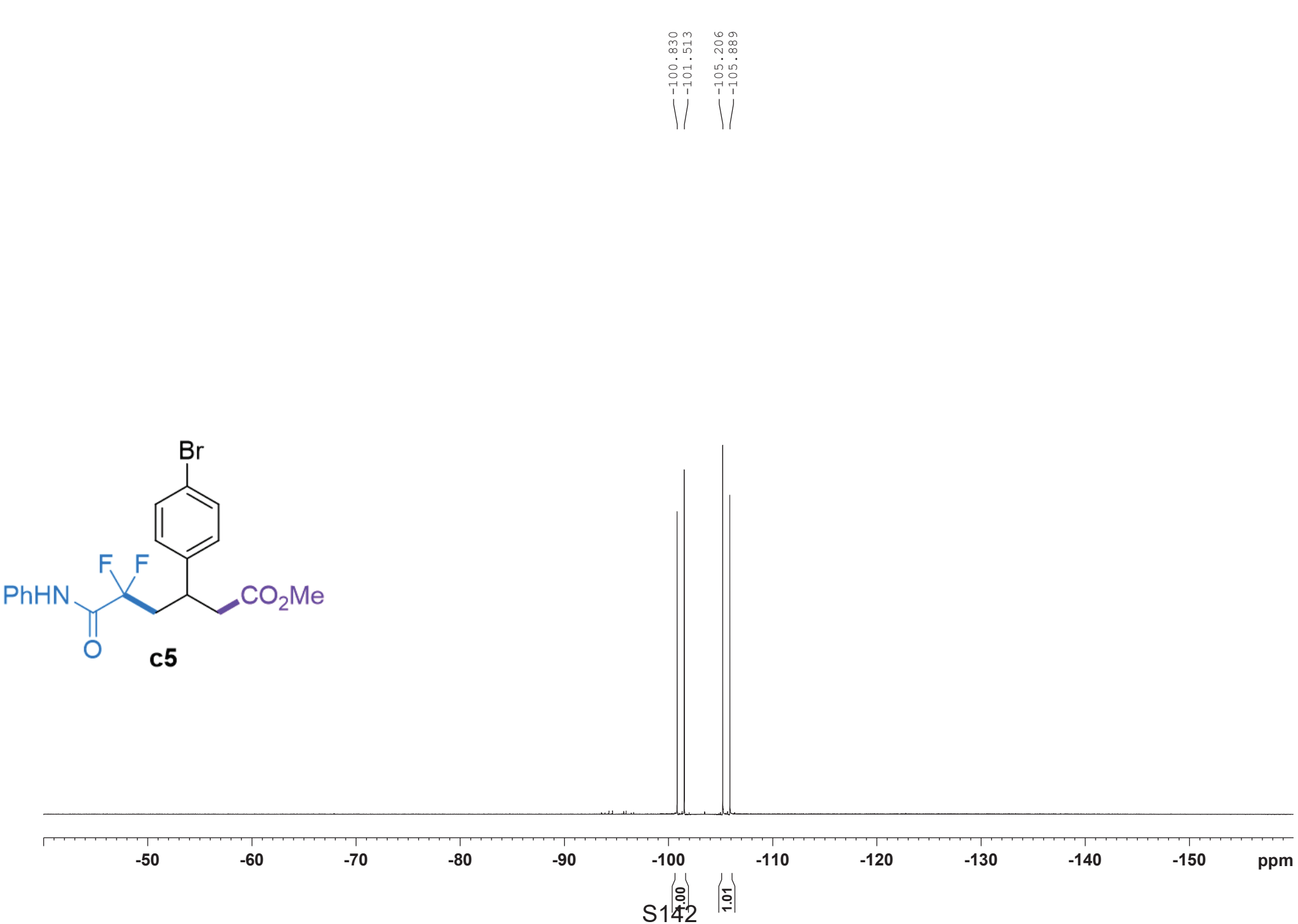

7.816
7.417
7.398
7.359
7.340
7.319
7.220
7.215
7.199
7.176
7.156
7.135
3.574
3.532
3.526
3.511
3.495
3.490
3.474
2.773
2.757
2.734
2.717
2.665
2.644
2.625
2.604
2.594
2.584
2.562
2.556
2.542
Cl
F
F
PhHN
CO2Me
O
c4
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.93
2.18
2.21
5.30
3.00
1.09
4.31

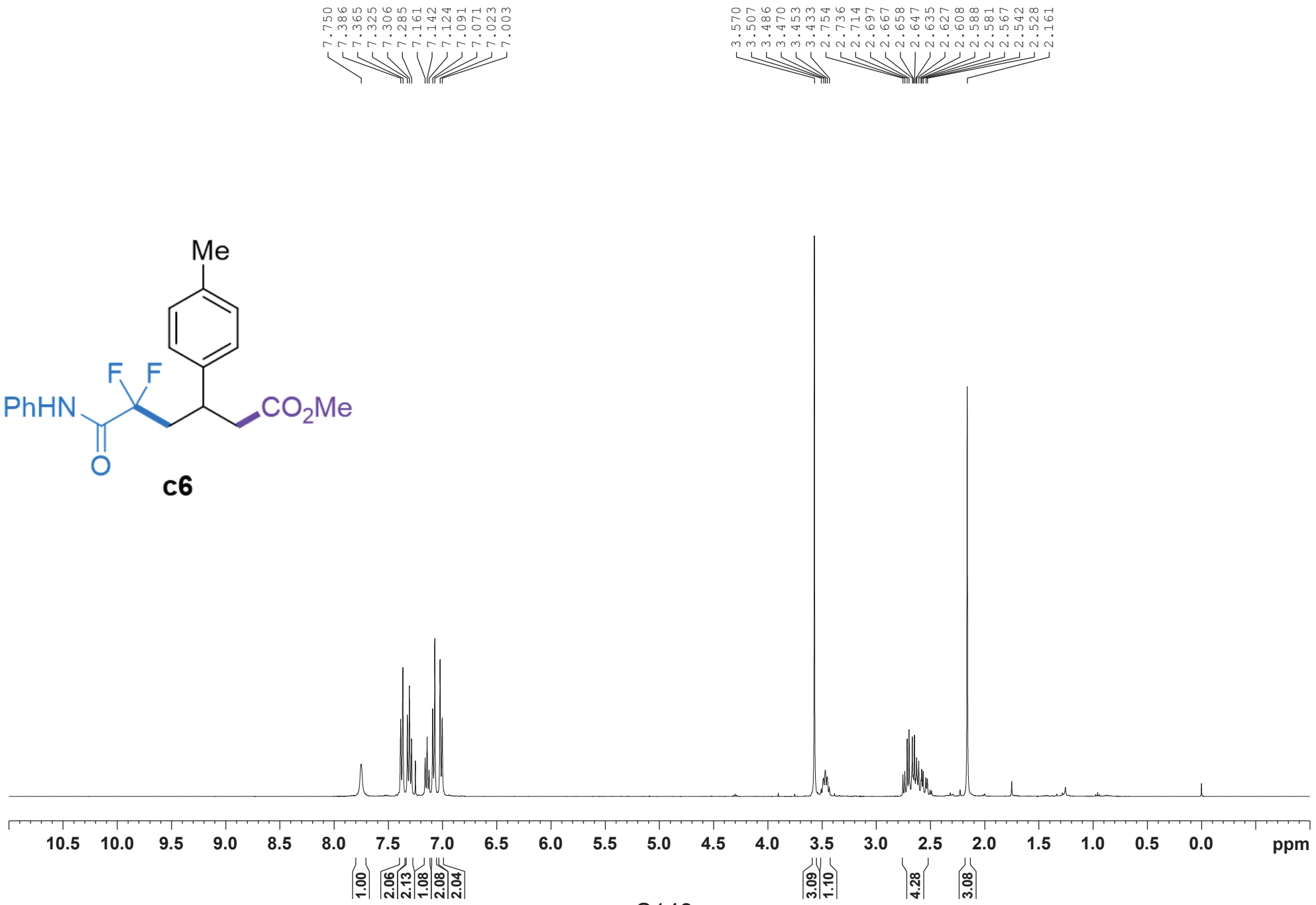

171.46
161.63
161.35
161.07
140.20
135.64
132.96
129.11
128.84
128.73
125.59
120.08
119.88
117.35
114.81
77.32
77.00
76.68
51.74
41.29
39.34
39.11
38.89
35.56
35.52
35.48
Cl
F
F
PhHN
O
CO2Me
c4
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

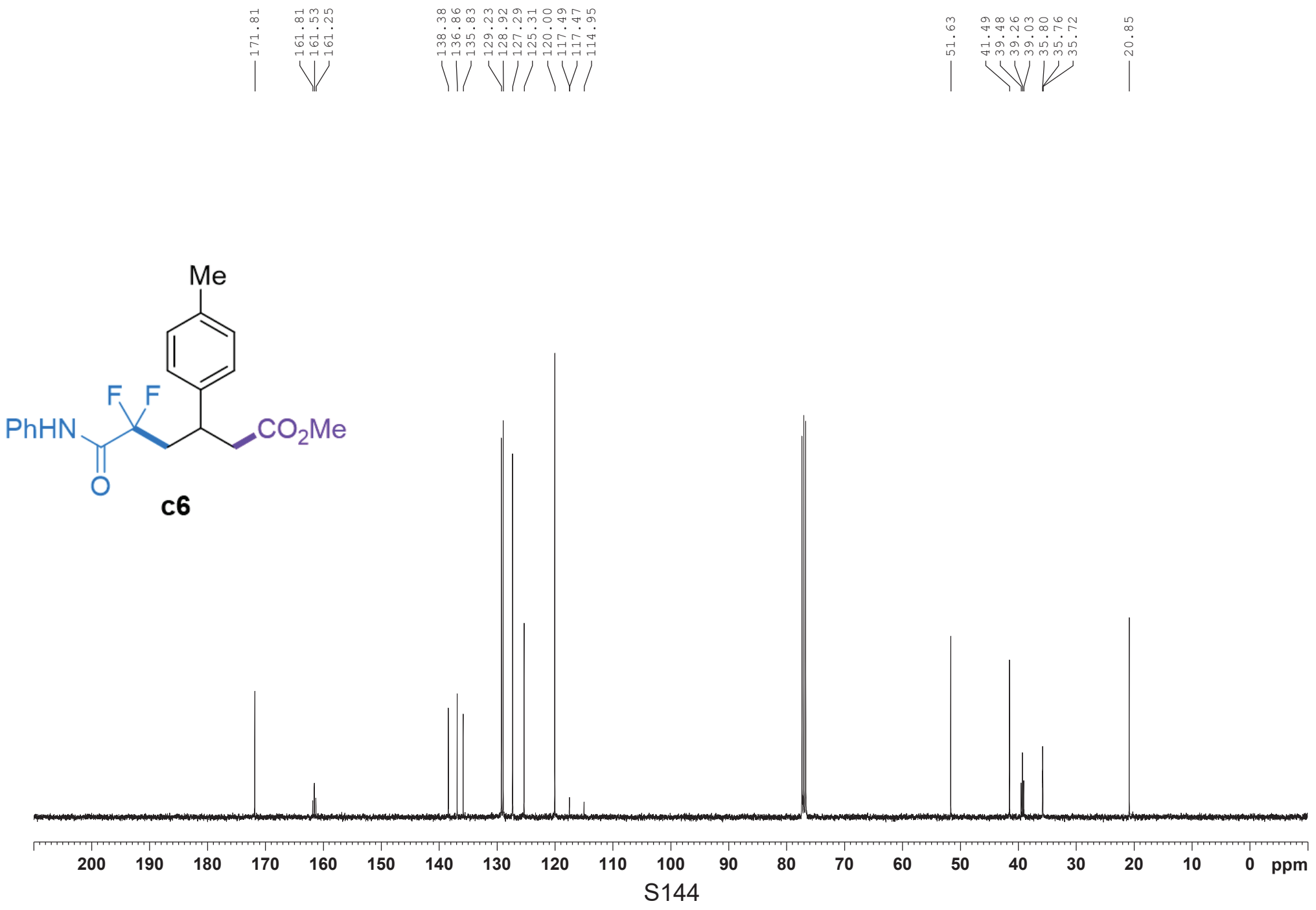

-100.921
-101.605
-105.133
-105.815
Cl
F
F
PhHN
O
CO2Me
c4
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
2.00
1.01

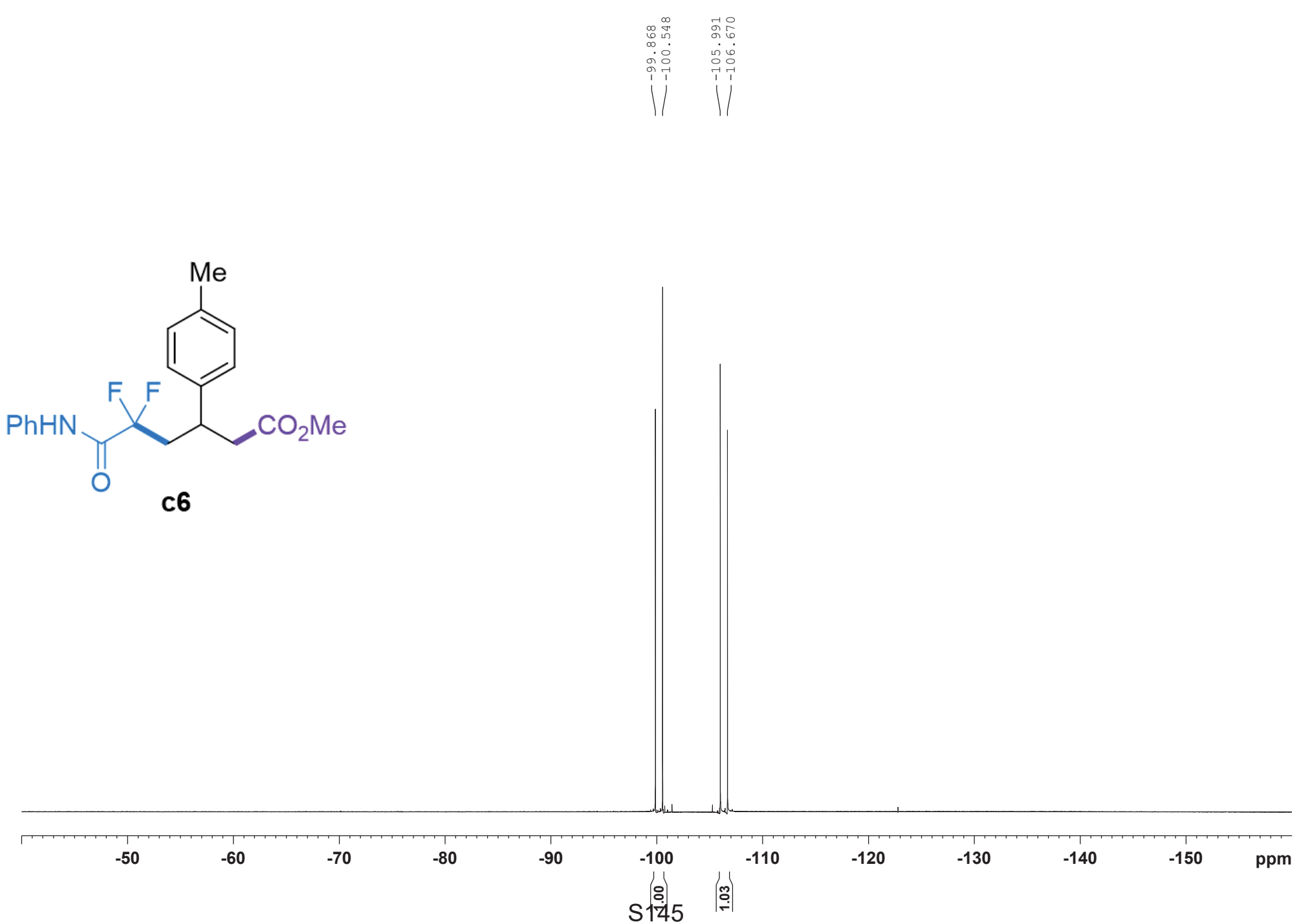

7.849
7.409
7.390
7.365
7.360
7.356
7.349
7.344
7.337
7.316
7.191
7.173
7.155
7.095
7.074
3.571
3.531
3.515
3.510
3.494
3.478
3.473
3.457
2.765
2.749
2.726
2.709
2.659
2.638
2.628
2.619
2.598
2.591
2.584
2.576
2.570
2.554
2.546
2.532
Br
F
F
PhHN
O
CO2Me
c5
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.16
4.30
1.11
2.10
3.07
1.18
4.02

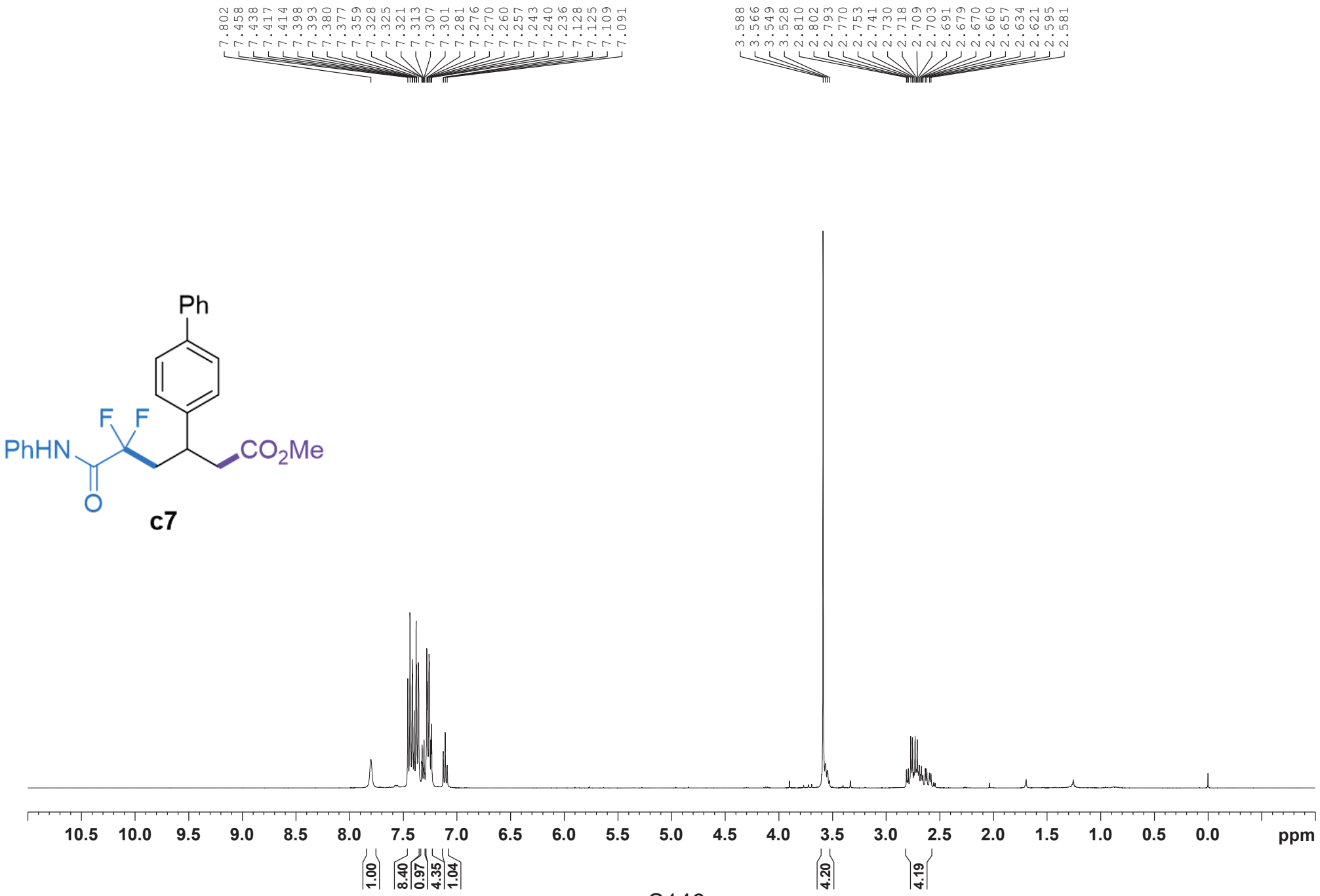

171.43
161.61
161.33
161.05
140.70
135.62
131.66
129.19
129.10
125.58
121.07
120.11
119.84
117.31
114.77
77.32
77.00
76.68
51.74
41.19
39.26
39.03
38.81
35.60
35.56
35.52
Br
F
F
PhHN
O
CO2Me
c5
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

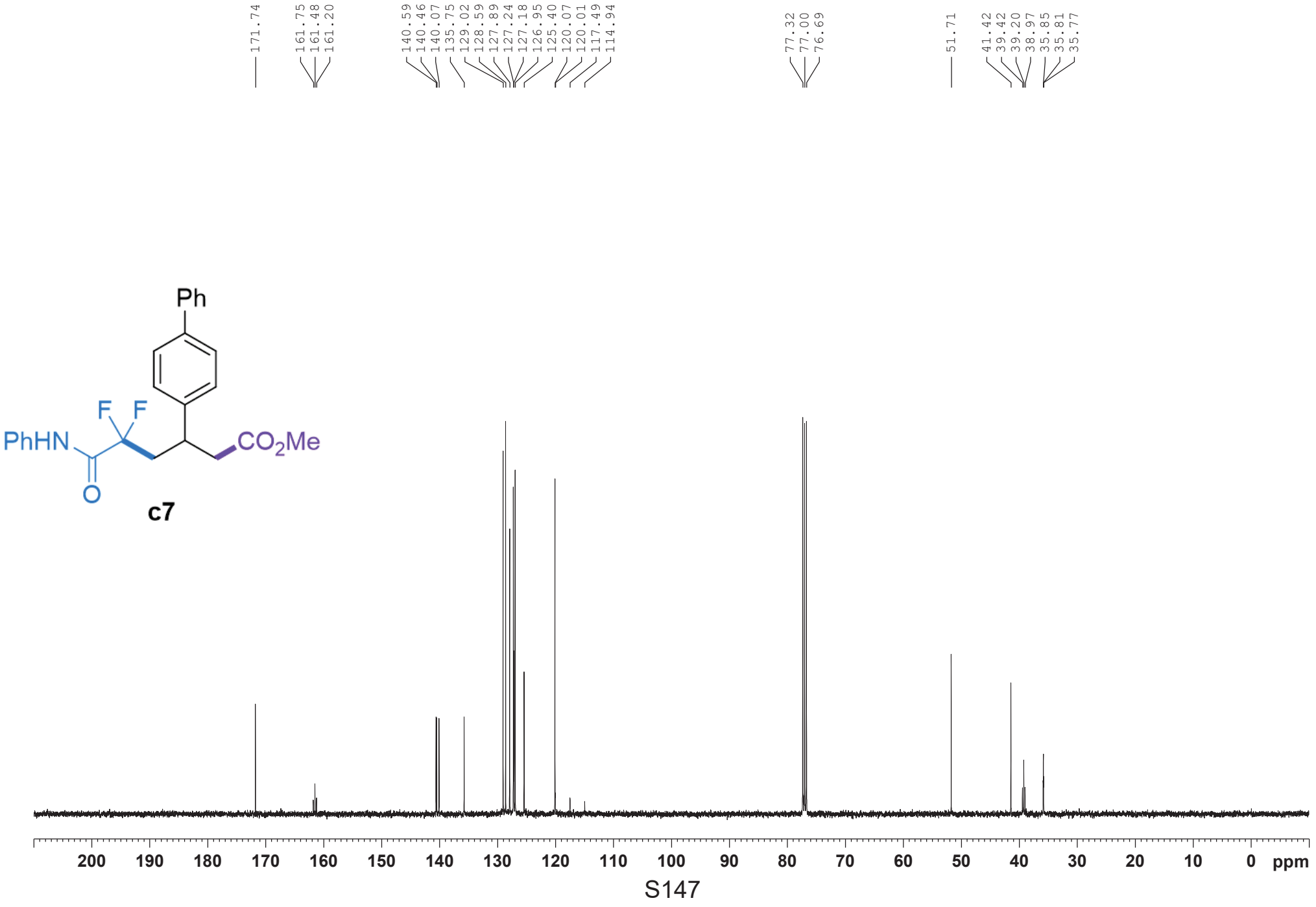

-100.830
-101.513
-105.206
-105.889
Br
F
F
PhHN
O
CO2Me
c5
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

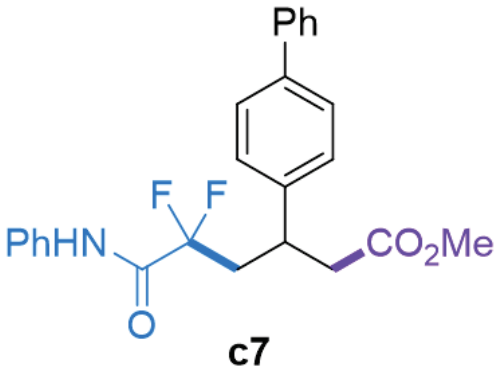

7.750
7.386
7.365
7.325
7.306
7.285
7.161
7.142
7.124
7.091
7.071
7.023
7.003
3.570
3.507
3.486
3.470
3.453
3.433
2.754
2.736
2.714
2.697
2.667
2.658
2.647
2.635
2.627
2.608
2.588
2.581
2.567
2.542
2.528
2.161
Me
F
F
PhHN
CO2Me
O
c6
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.06
2.13
1.08
2.08
2.04
3.09
1.10
4.28
3.08


171.81
161.81
161.53
161.25
138.38
136.86
135.83
129.23
128.92
127.29
125.31
120.00
117.49
117.47
114.95
51.63
41.49
39.48
39.26
39.03
35.80
35.76
35.72
20.85
Me
F
F
PhHN
O
CO2Me
c6
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-99.868
-100.548
-105.991
-106.670
Me
F
F
PhHN
O
CO2Me
c6
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.03

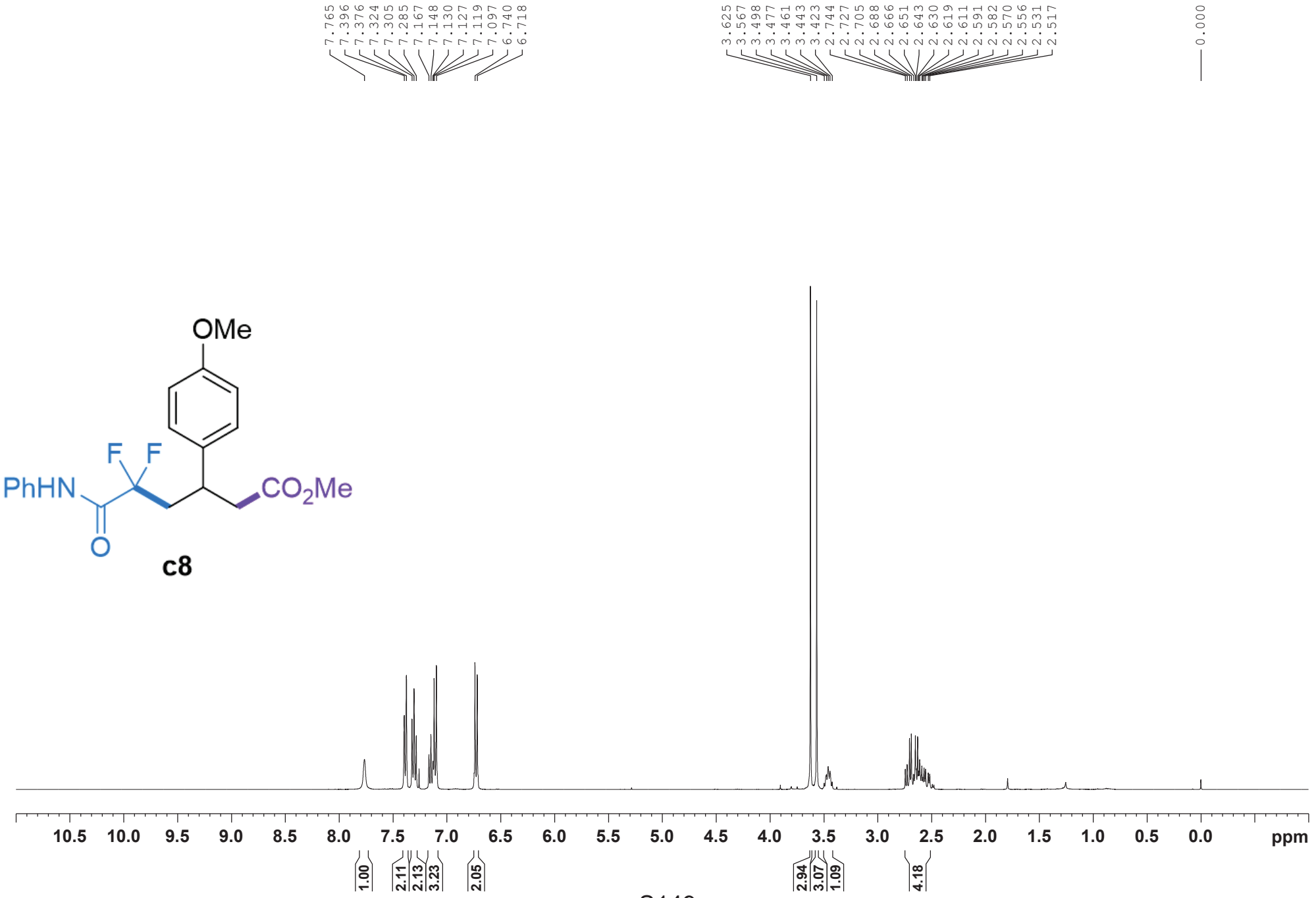

7.802
7.458
7.438
7.417
7.414
7.398
7.393
7.380
7.377
7.359
7.328
7.325
7.321
7.313
7.307
7.301
7.281
7.276
7.270
7.260
7.257
7.243
7.240
7.236
7.128
7.125
7.109
7.091
3.588
3.566
3.549
3.528
2.810
2.802
2.793
2.770
2.753
2.741
2.730
2.718
2.709
2.703
2.691
2.679
2.670
2.660
2.657
2.634
2.621
2.595
2.581
Ph
F
F
PhHN
O
CO2Me
c7
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
8.40
0.97
4.35
1.04
4.20
4.19

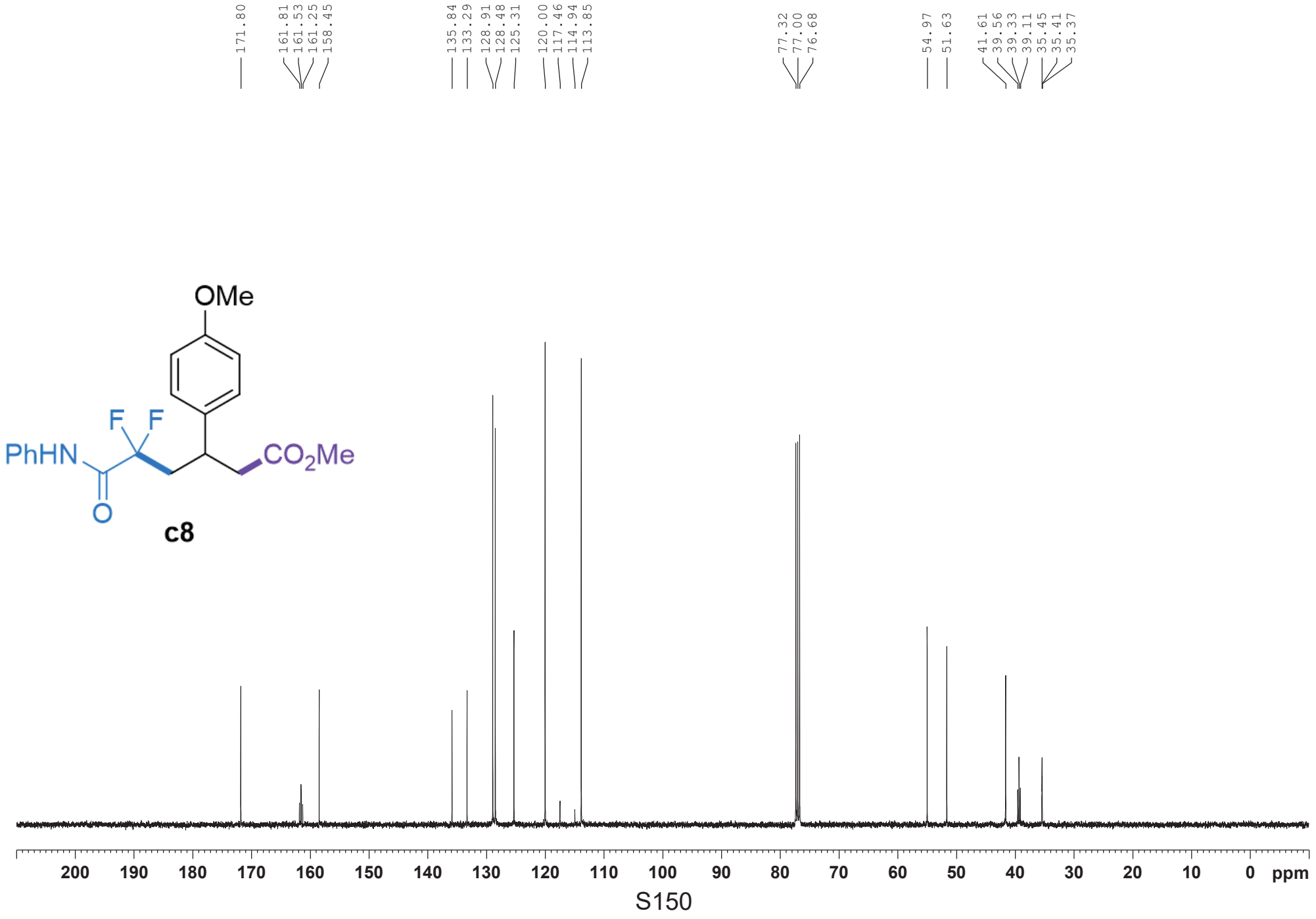

171.74
161.75
161.48
161.20
140.59
140.46
140.07
135.75
129.02
128.59
127.89
127.24
127.18
126.95
125.40
120.07
120.01
117.49
114.94
77.32
77.00
76.69
51.71
41.42
39.42
39.20
38.97
35.85
35.81
35.77
Ph
F
F
PhHN
O
CO2Me
c7
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

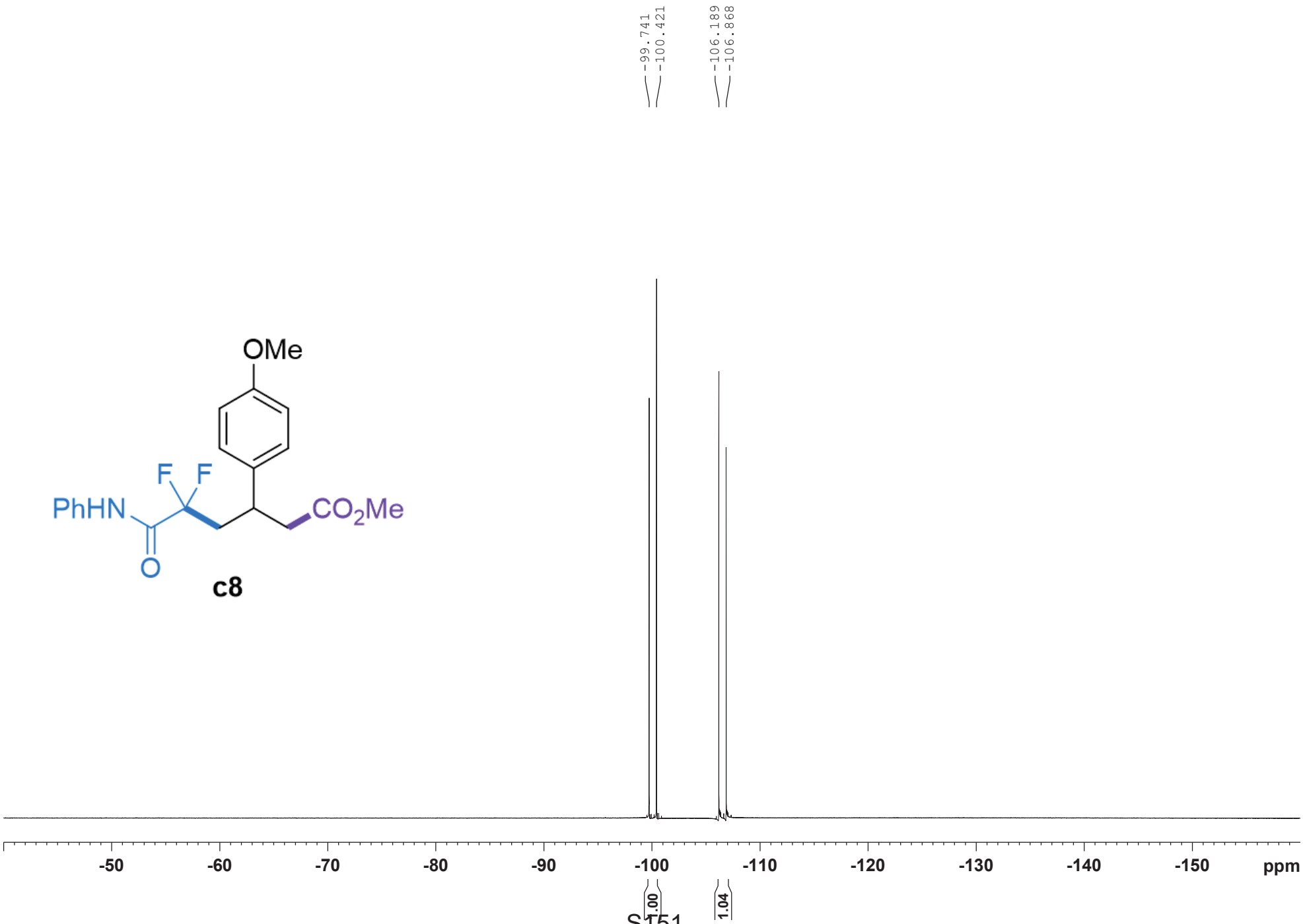

Ph
F
F
PhHN
CO2Me
O

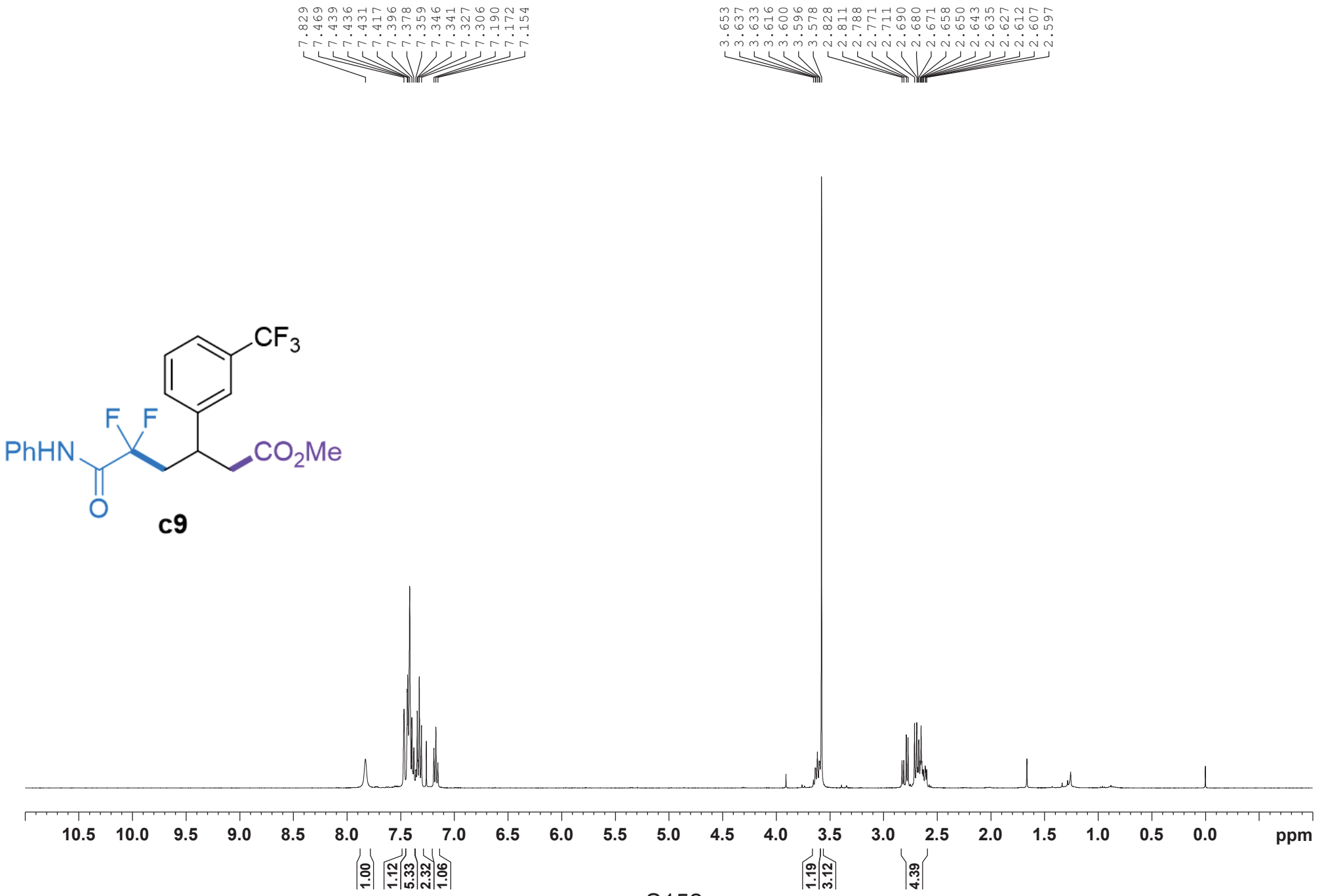
c7

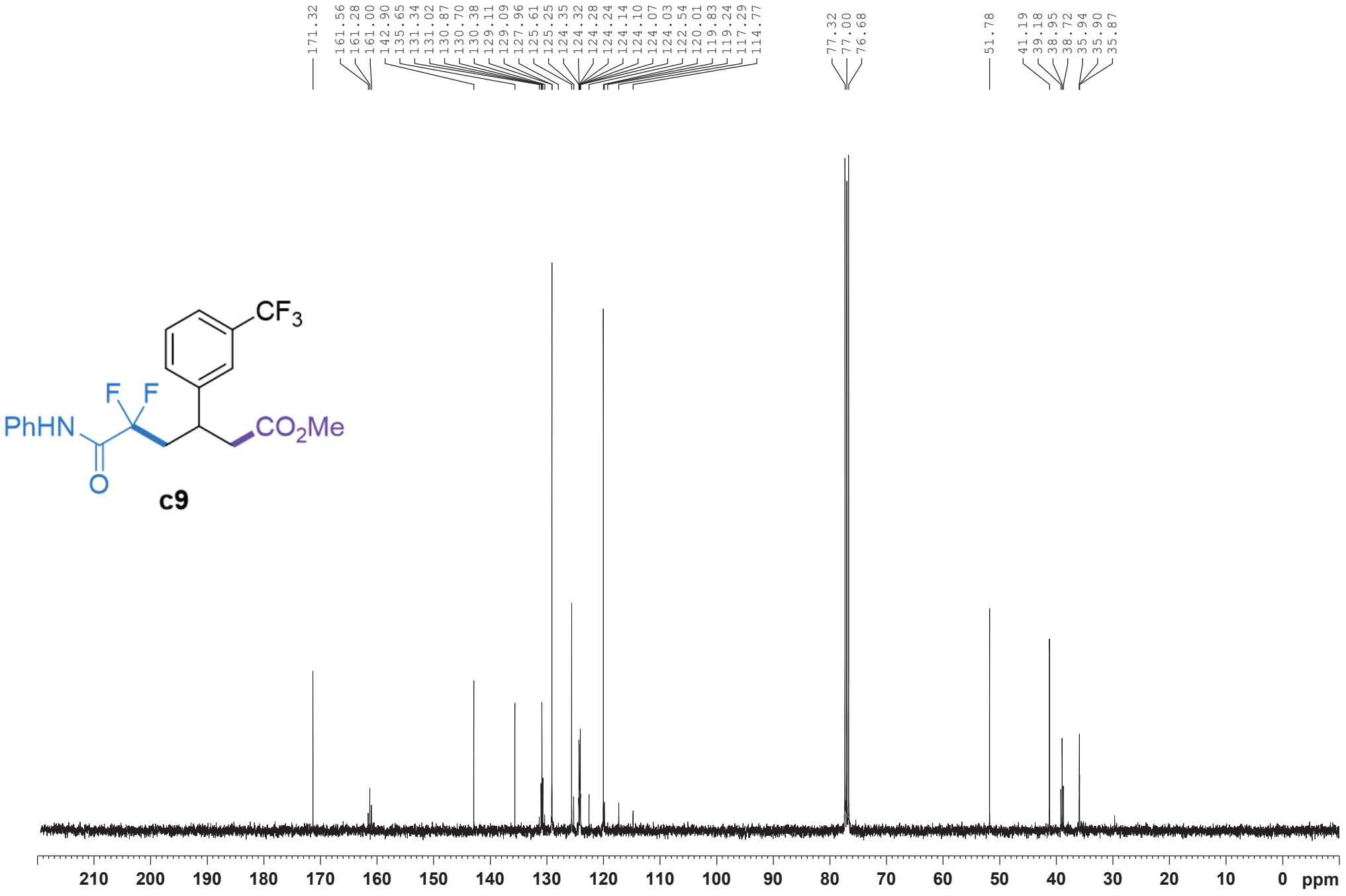
-99.868
-100.549
-105.766
-106.448
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

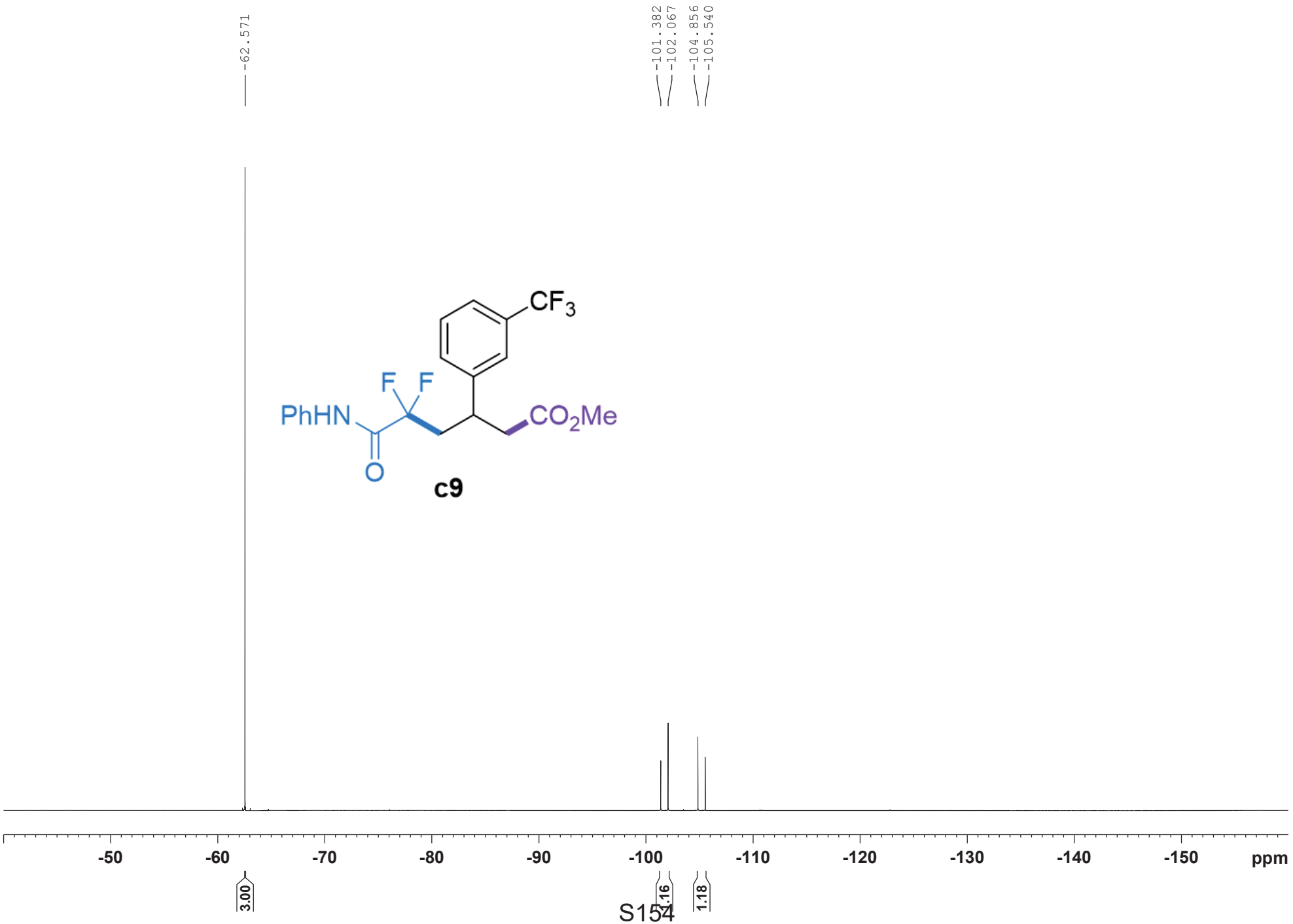

7.765
7.396
7.376
7.324
7.305
7.285
7.167
7.148
7.130
7.127
7.119
7.097
6.740
6.718
3.625
3.567
3.498
3.477
3.461
3.443
3.423
2.744
2.727
2.705
2.688
2.666
2.651
2.643
2.630
2.619
2.611
2.591
2.582
2.570
2.556
2.531
2.517
0.000
OMe
F
F
PhHN
CO2Me
O
c8
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.11
2.13
3.23
2.05
2.94
3.07
1.09
4.18

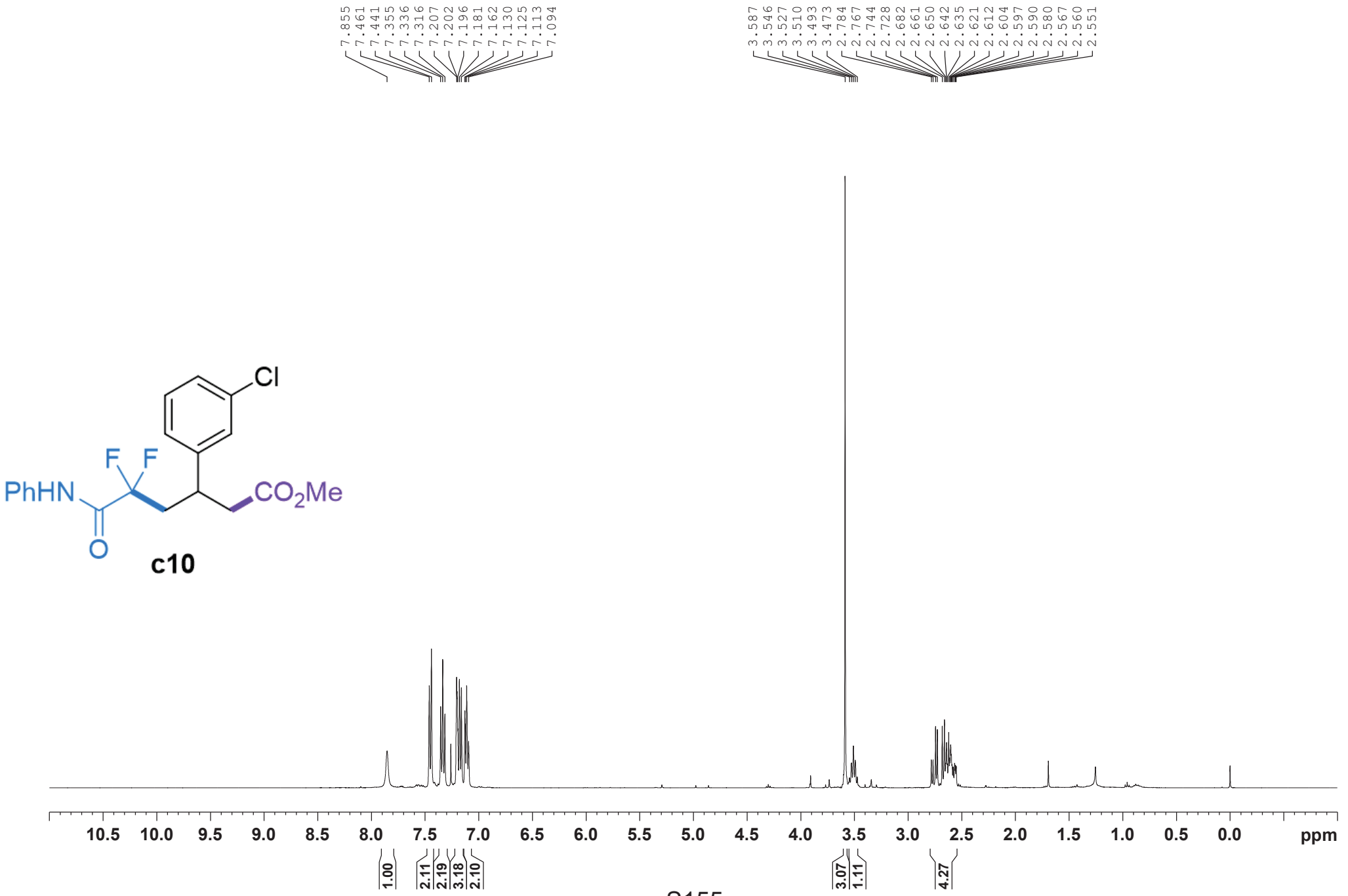

171.80
161.81
161.53
161.25
158.45
135.84
133.29
128.91
128.48
125.31
120.00
117.46
114.94
113.85
77.32
77.00
76.68
54.97
51.63
41.61
39.56
39.33
39.11
35.45
35.41
35.37
OMe
F
F
PhHN
CO2Me
O
c8
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

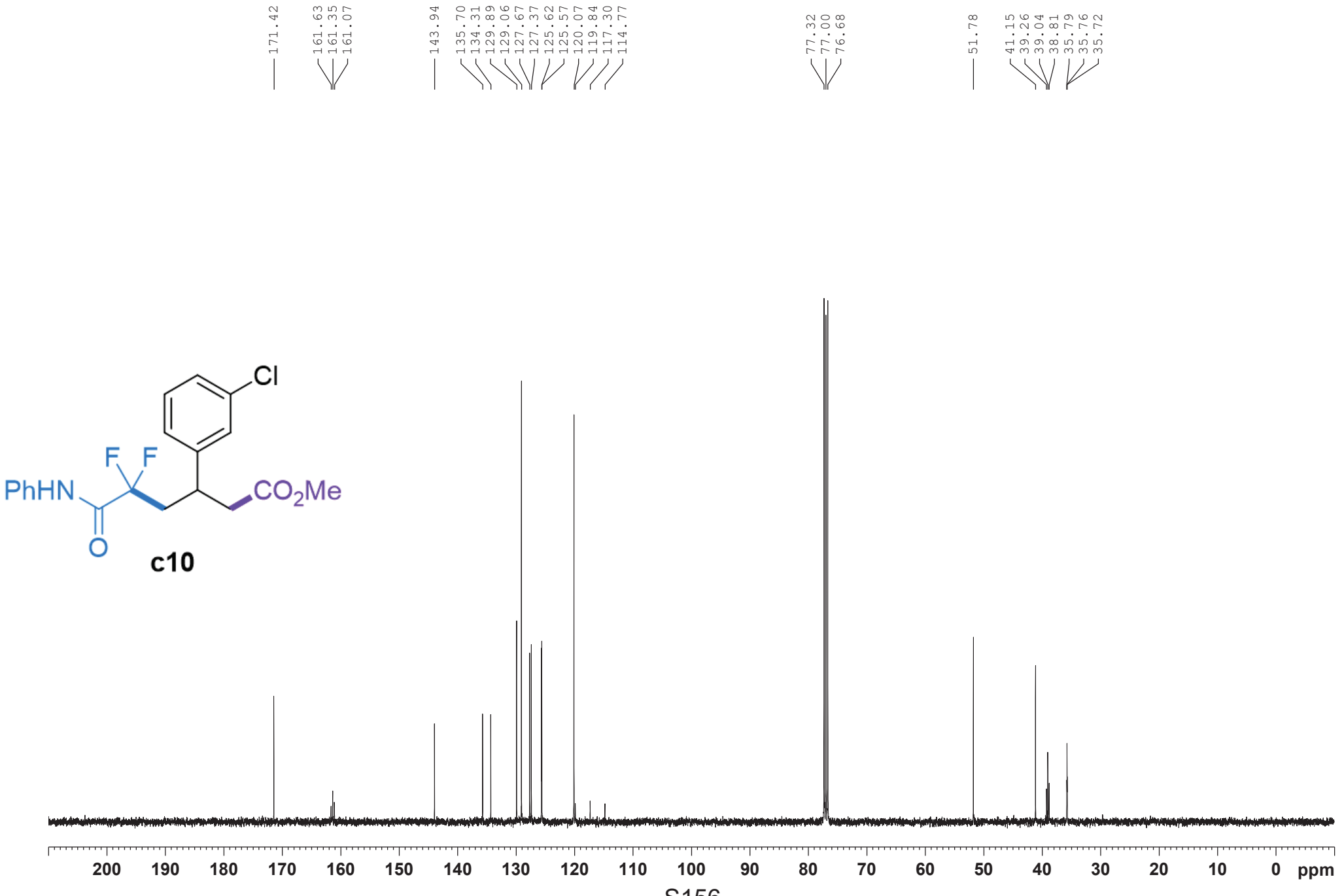

-99.741
-100.421
-106.189
-106.868
OMe
F
F
PhHN
O
CO2Me
c8
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.04

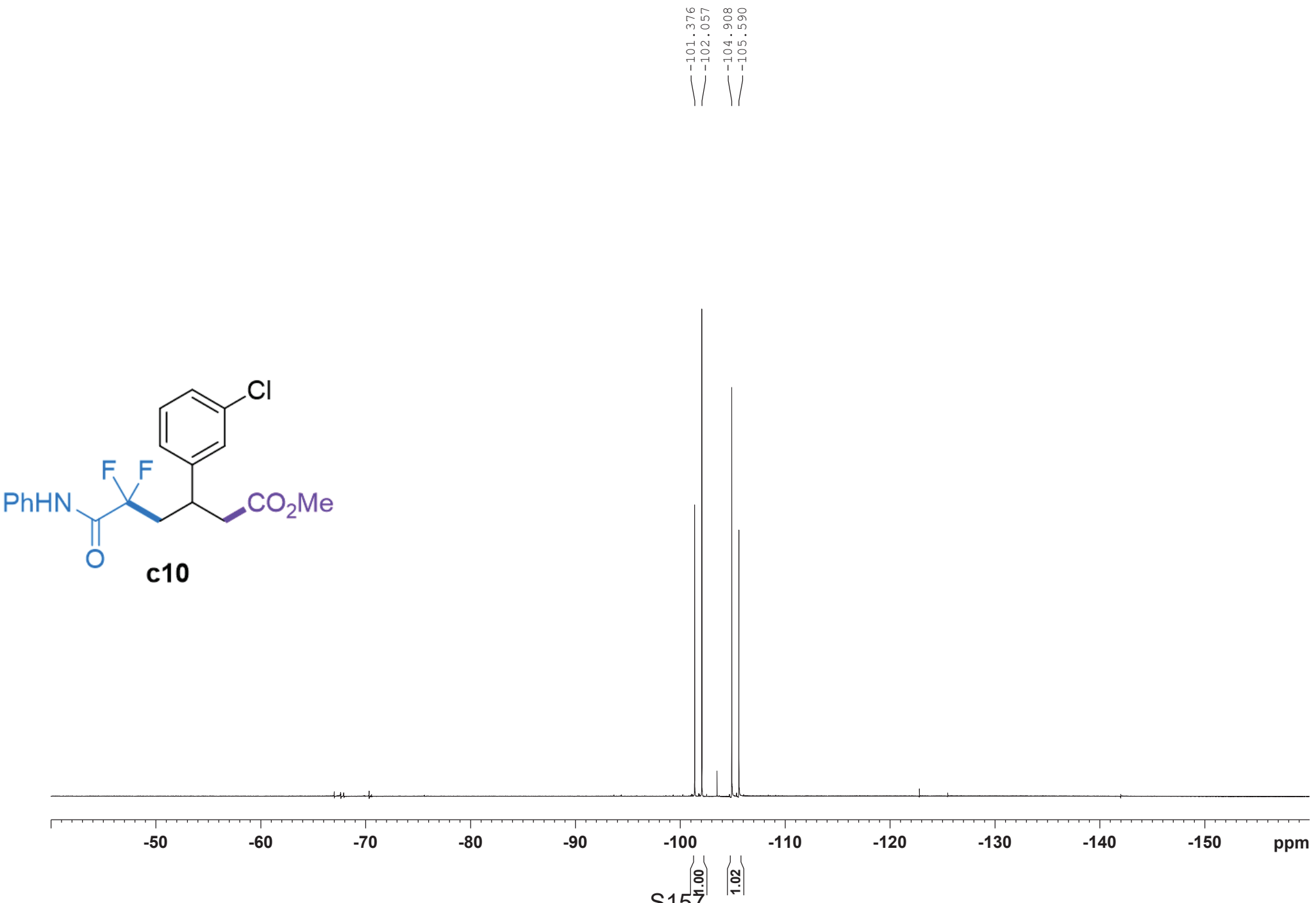

7.829
7.469
7.439
7.436
7.431
7.417
7.396
7.378
7.359
7.346
7.341
7.327
7.306
7.190
7.172
7.154
3.653
3.637
3.633
3.616
3.600
3.596
3.578
2.828
2.811
2.788
2.771
2.711
2.690
2.680
2.671
2.658
2.650
2.643
2.635
2.627
2.612
2.607
2.597
CF3
F
F
PhHN
CO2Me
O
c9
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
1.12
5.33
2.32
1.06
1.19
3.12
4.39


171.32
161.56
161.28
161.00
142.90
135.65
131.34
131.02
130.87
130.70
130.38
129.11
129.09
127.96
125.61
125.25
124.35
124.32
124.28
124.24
124.14
124.10
124.07
124.03
122.54
120.01
119.83
119.24
117.29
114.77
77.32
77.00
76.68
51.78
41.19
39.18
38.95
38.72
35.94
35.90
35.87
CF3
F
F
PhHN
CO2Me
O
c9
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

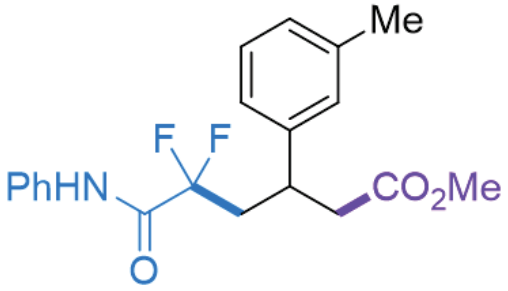

-62.571
-101.382
-102.067
-104.856
-105.540
CF3
F F
PhHN
CO2Me
O
c9
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
3.00
1.16
1.18


7.855
7.461
7.441
7.355
7.336
7.316
7.207
7.202
7.196
7.181
7.162
7.130
7.125
7.113
7.094
3.587
3.546
3.527
3.510
3.493
3.473
2.784
2.767
2.744
2.728
2.682
2.661
2.650
2.642
2.635
2.621
2.612
2.604
2.597
2.590
2.580
2.567
2.560
2.551
Cl
F
F
PhHN
CO2Me
O
c10
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.11
2.19
3.18
2.10
3.07
1.11
4.27


171.42
161.63
161.35
161.07
143.94
135.70
134.31
129.89
129.06
127.67
127.37
125.62
125.57
120.07
119.84
117.30
114.77
77.32
77.00
76.68
51.78
41.15
39.26
39.04
38.81
35.79
35.76
35.72
Cl
F
F
PhHN
O
CO2Me
c10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

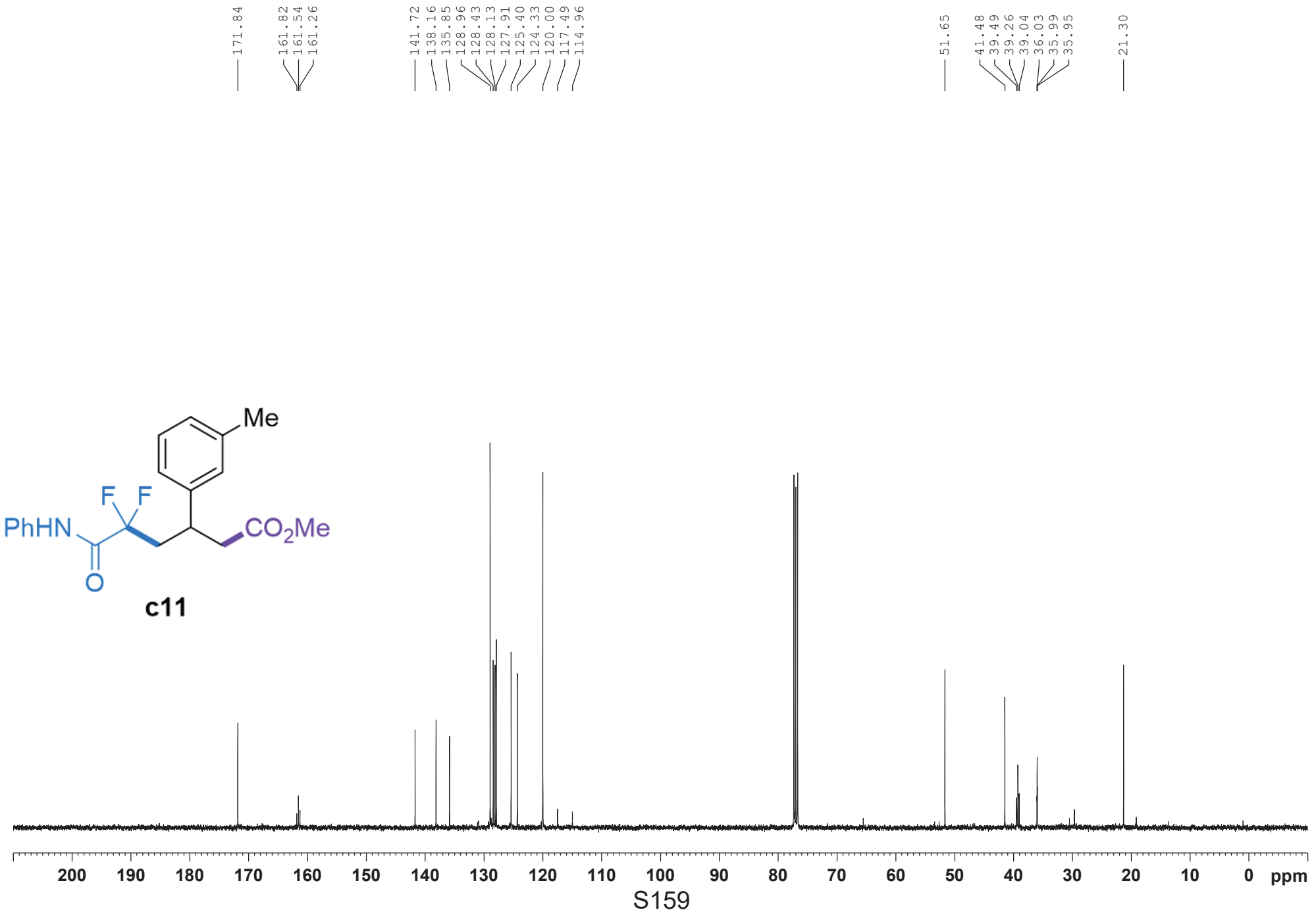

-101.376
-102.057
-104.908
-105.590
Cl
F
F
PhHN
O
CO2Me
c10
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.02

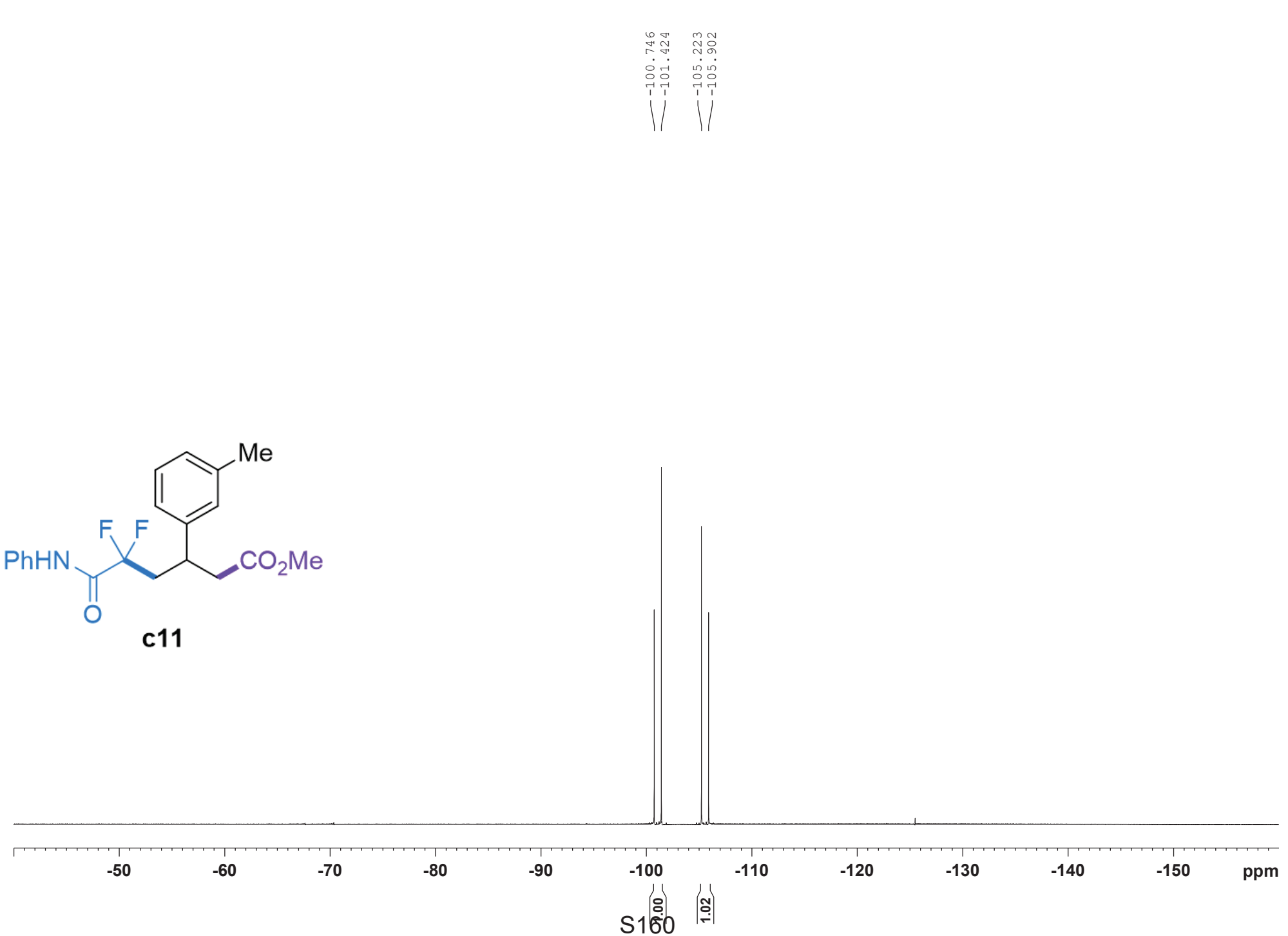

7.761
7.430
7.427
7.408
7.407
7.342
7.337
7.323
7.303
7.185
7.182
7.180
7.164
7.153
7.146
7.143
7.133
7.119
7.114
7.010
6.995
6.945
6.926
3.584
3.511
3.492
3.475
3.458
3.438
2.772
2.755
2.733
2.715
2.693
2.684
2.671
2.664
2.650
2.645
2.629
2.625
2.608
2.594
2.590
2.586
2.565
2.551
2.235

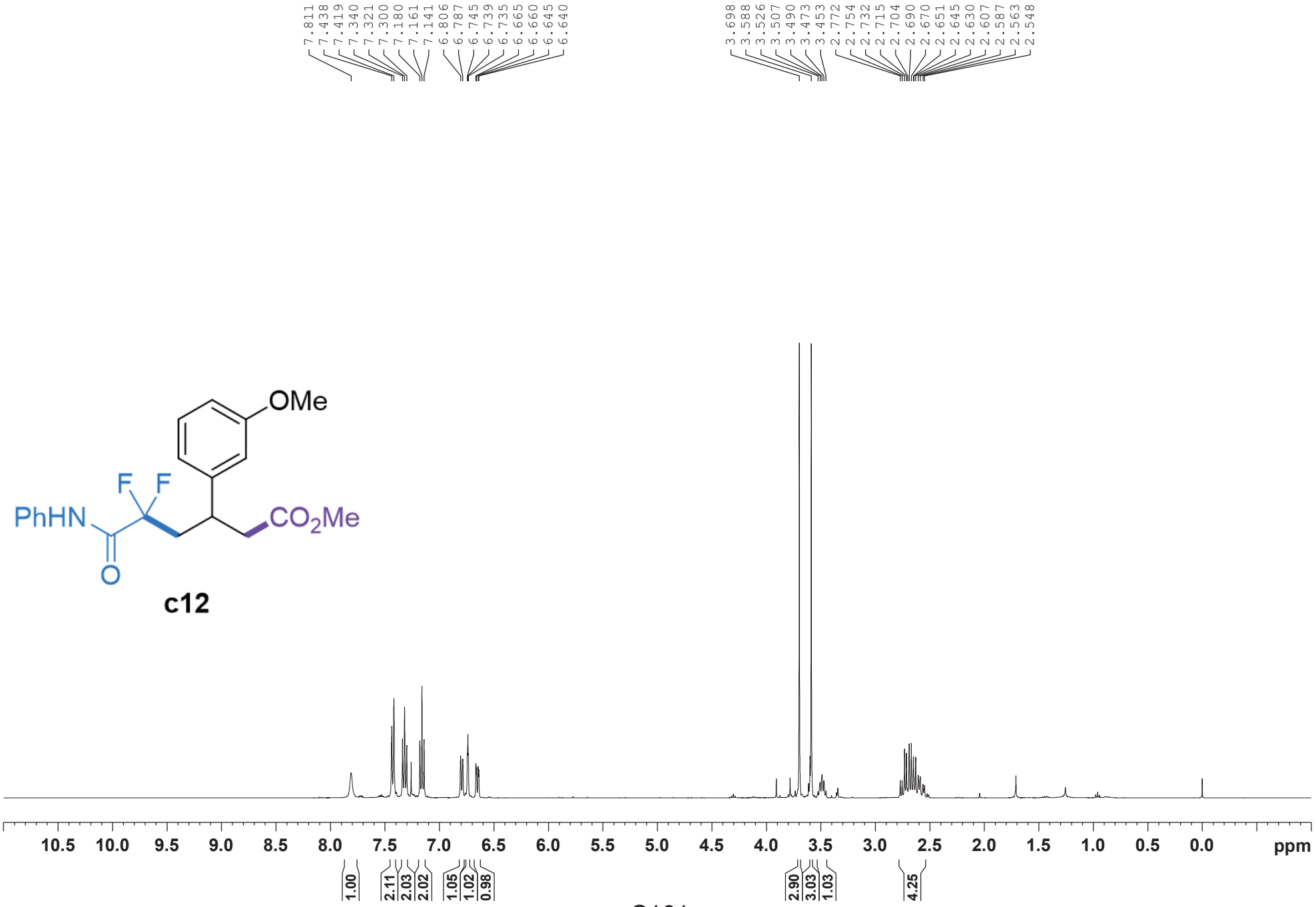

Me
F
F
PhHN
CO2Me
O

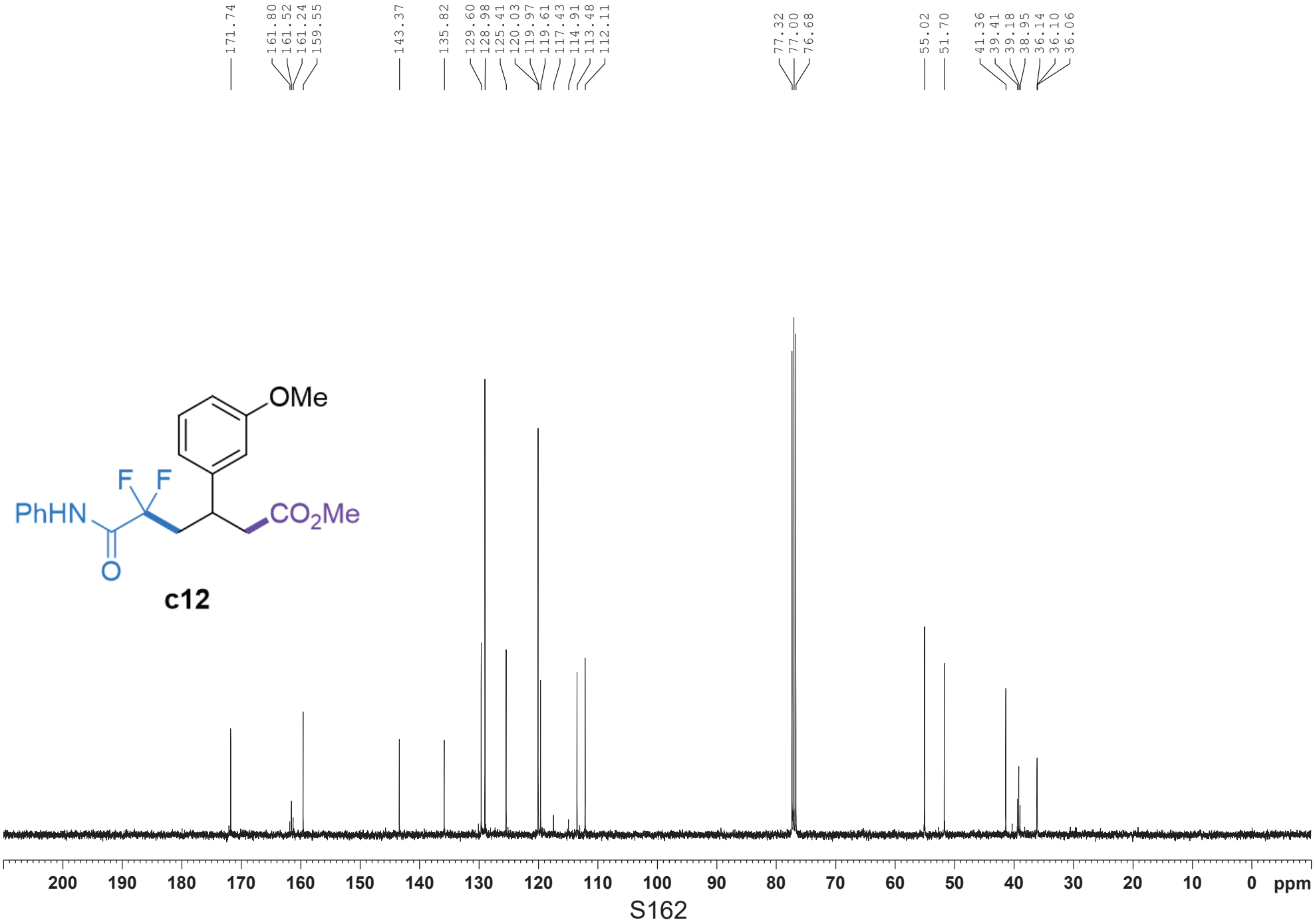
c11

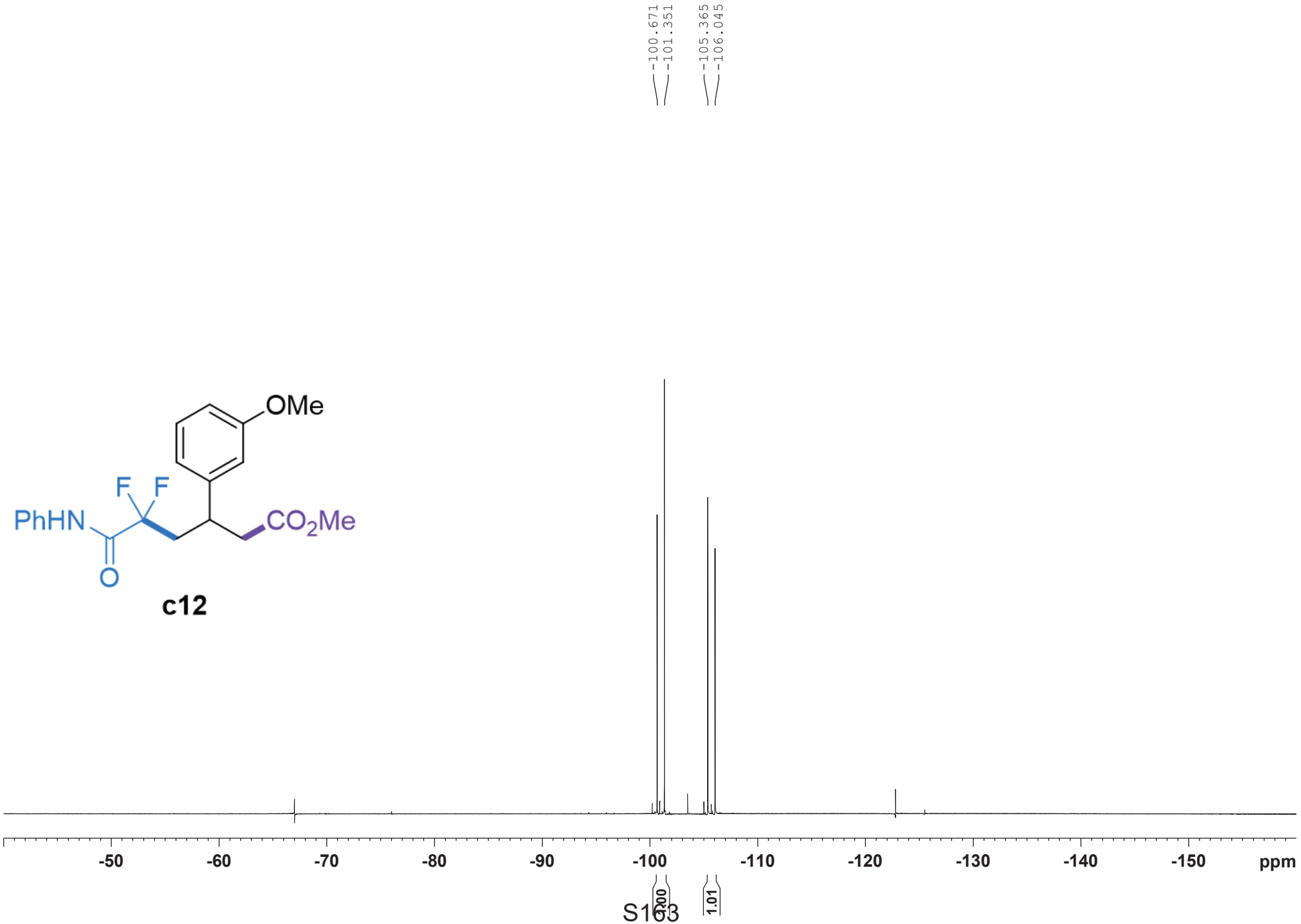
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.01
2.03
2.04
2.04
0.99
3.01
1.01
4.10
3.03

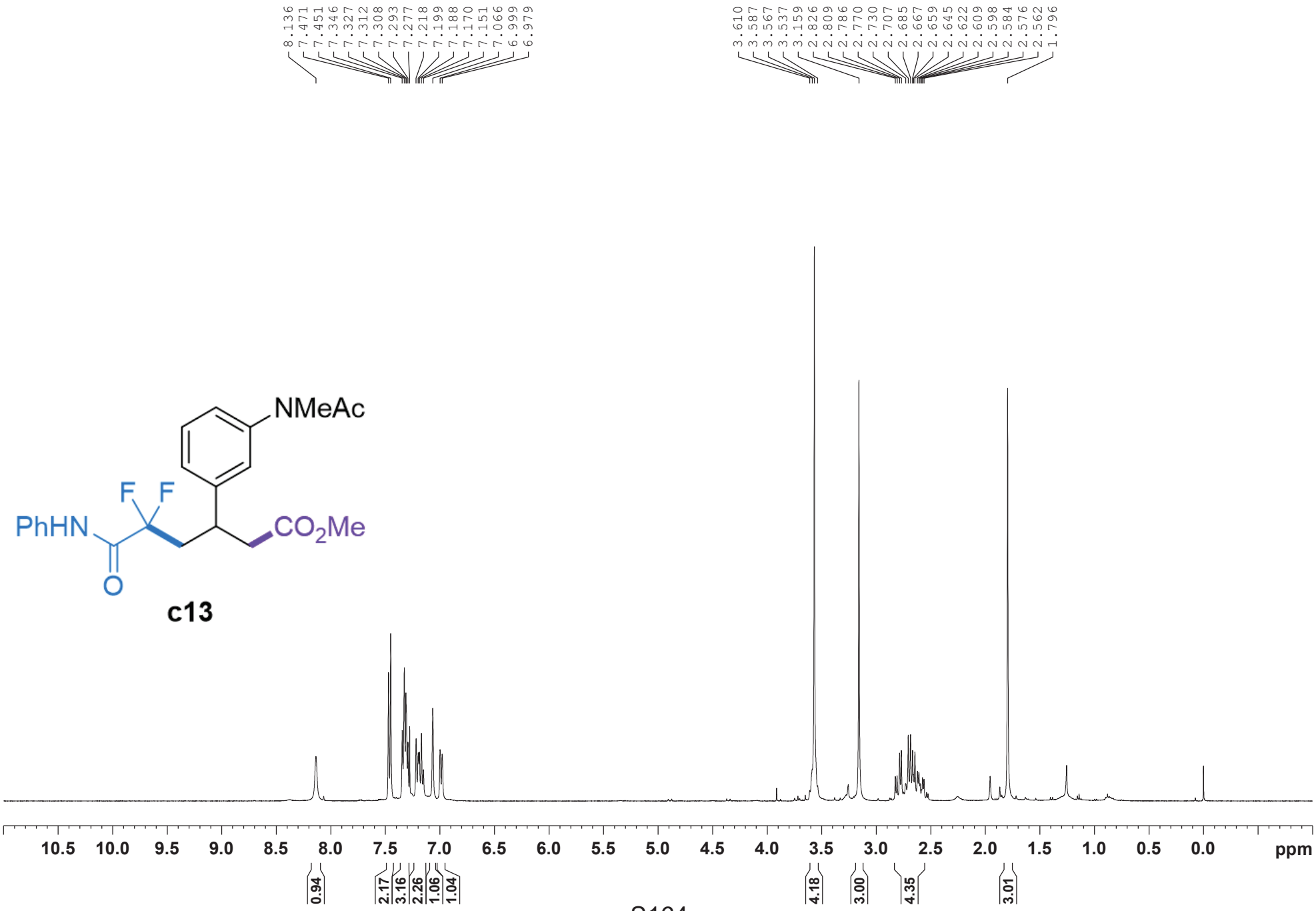

171.84
161.82
161.54
161.26
141.72
138.16
135.85
128.96
128.43
128.13
127.91
125.40
124.33
120.00
117.49
114.96
51.65
41.48
39.49
39.26
39.04
36.03
35.99
35.95
21.30
Me
F
F
PhHN
O
CO2Me
c11
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

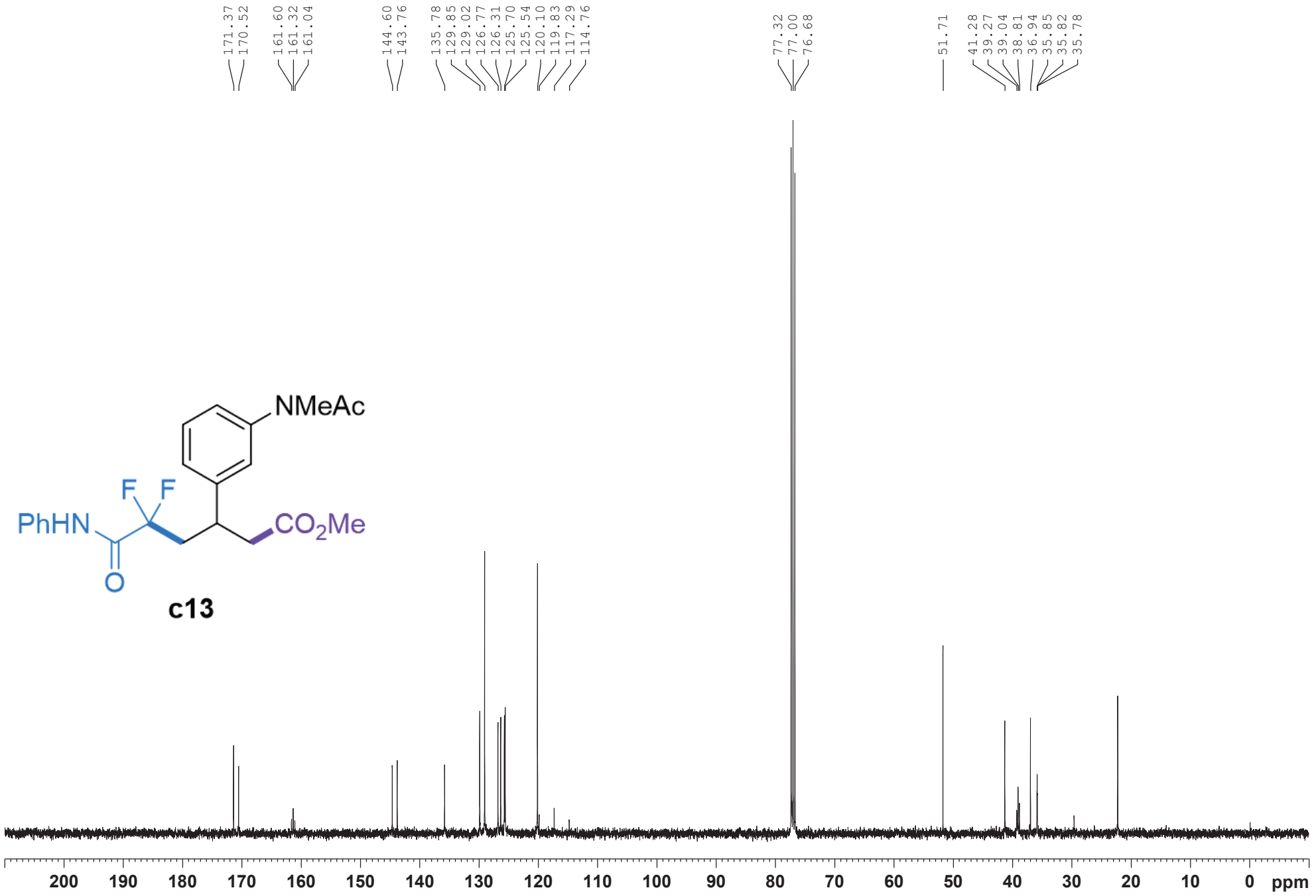

-100.746
-101.424
-105.223
-105.902
Me
F
F
PhHN
CO2Me
O
c11
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
2.00
1.02

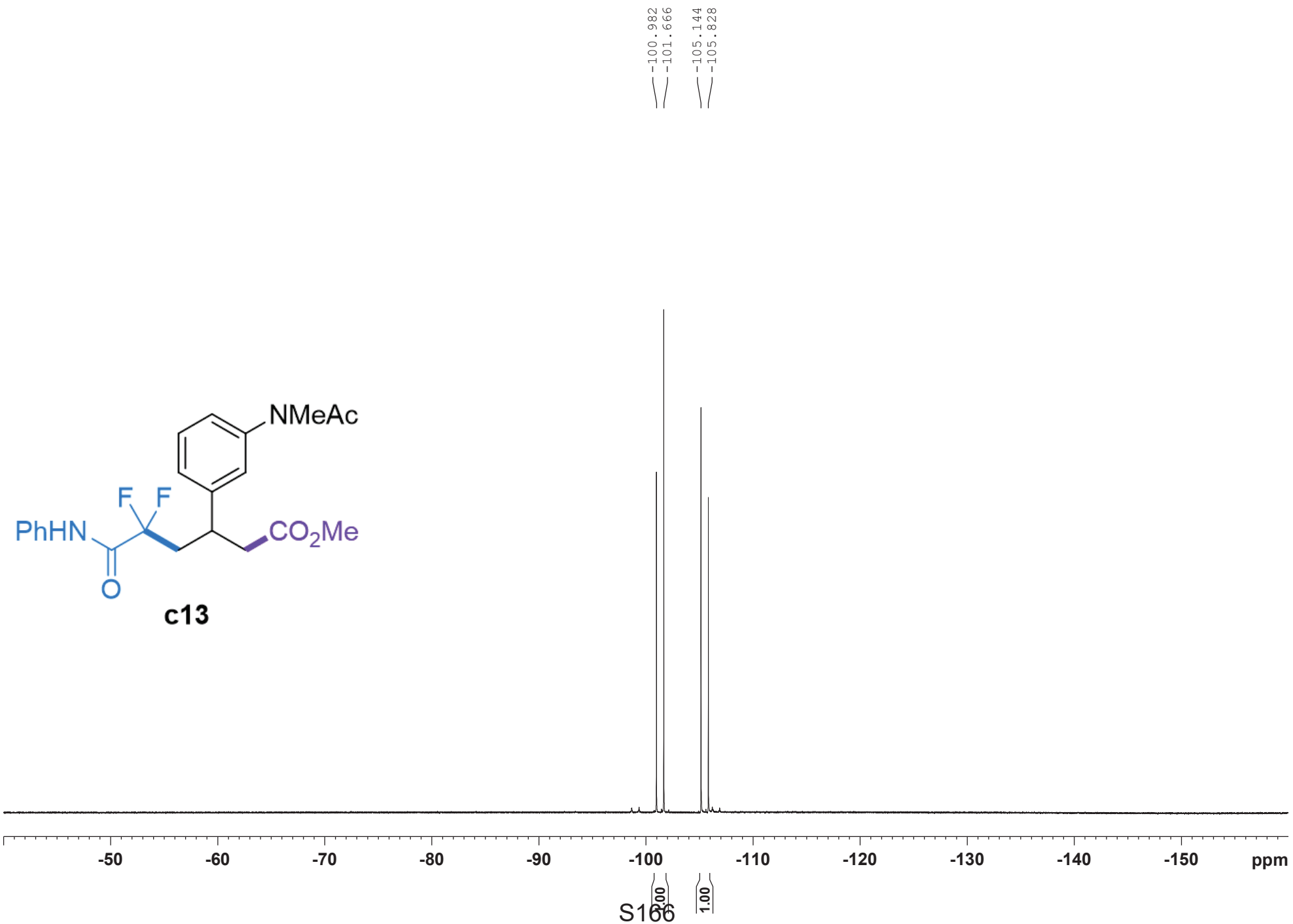

7.811
7.438
7.419
7.340
7.321
7.300
7.180
7.161
7.141
6.806
6.787
6.745
6.739
6.735
6.665
6.660
6.645
6.640
3.698
3.588
3.526
3.507
3.490
3.473
3.453
2.772
2.754
2.732
2.715
2.704
2.690
2.670
2.651
2.645
2.630
2.607
2.587
2.563
2.548
OMe
F
F
PhHN
CO2Me
O
c12
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.11
2.03
2.02
1.05
1.02
0.98
2.90
3.03
1.03
4.25

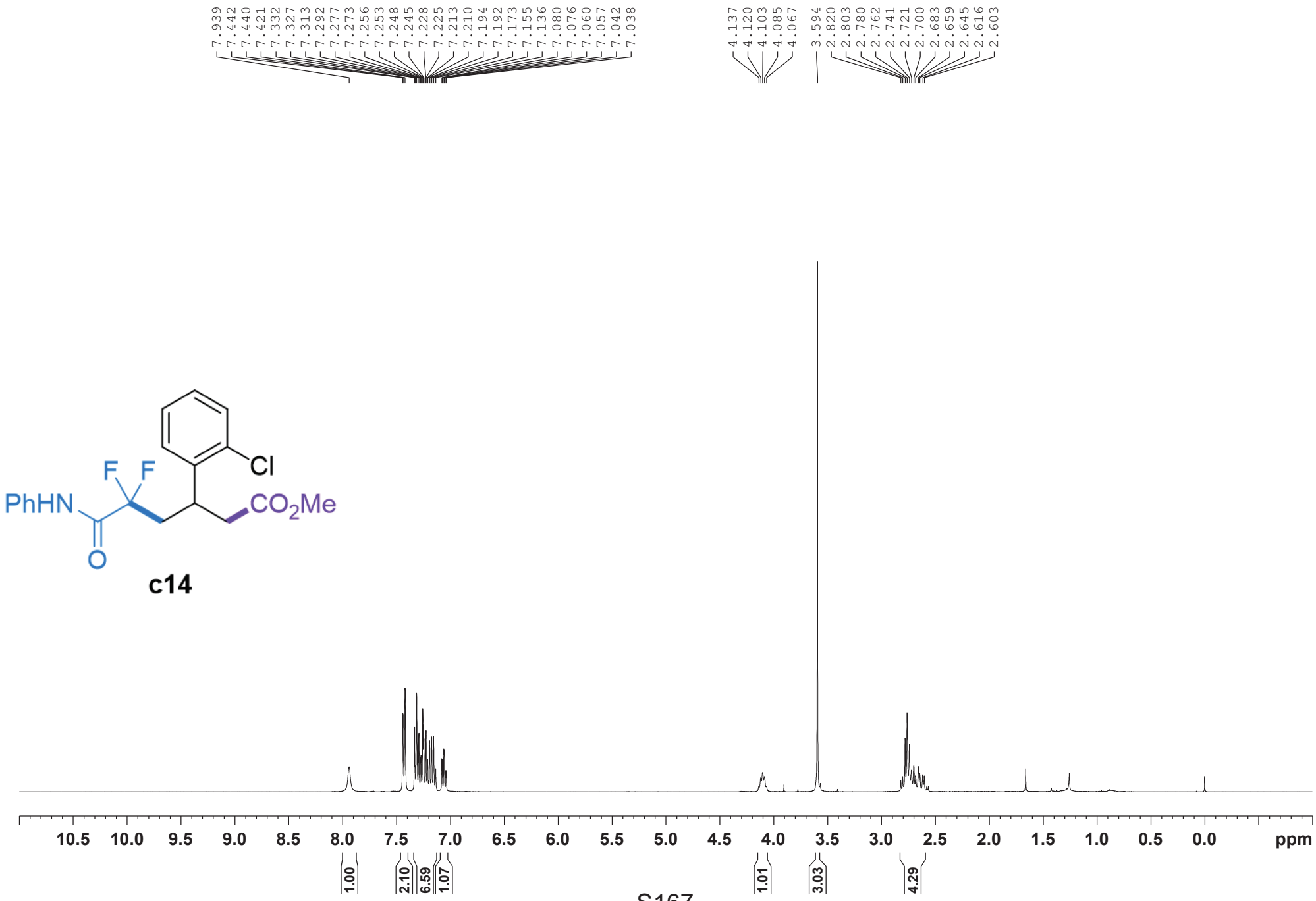

171.74
161.80
161.52
161.24
159.55
143.37
135.82
129.60
128.98
125.41
120.03
119.97
119.61
117.43
114.91
113.48
112.11
77.32
77.00
76.68
55.02
51.70
41.36
39.41
39.18
38.95
36.14
36.10
36.06
OMe
F
F
PhHN
CO2Me
O
c12
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

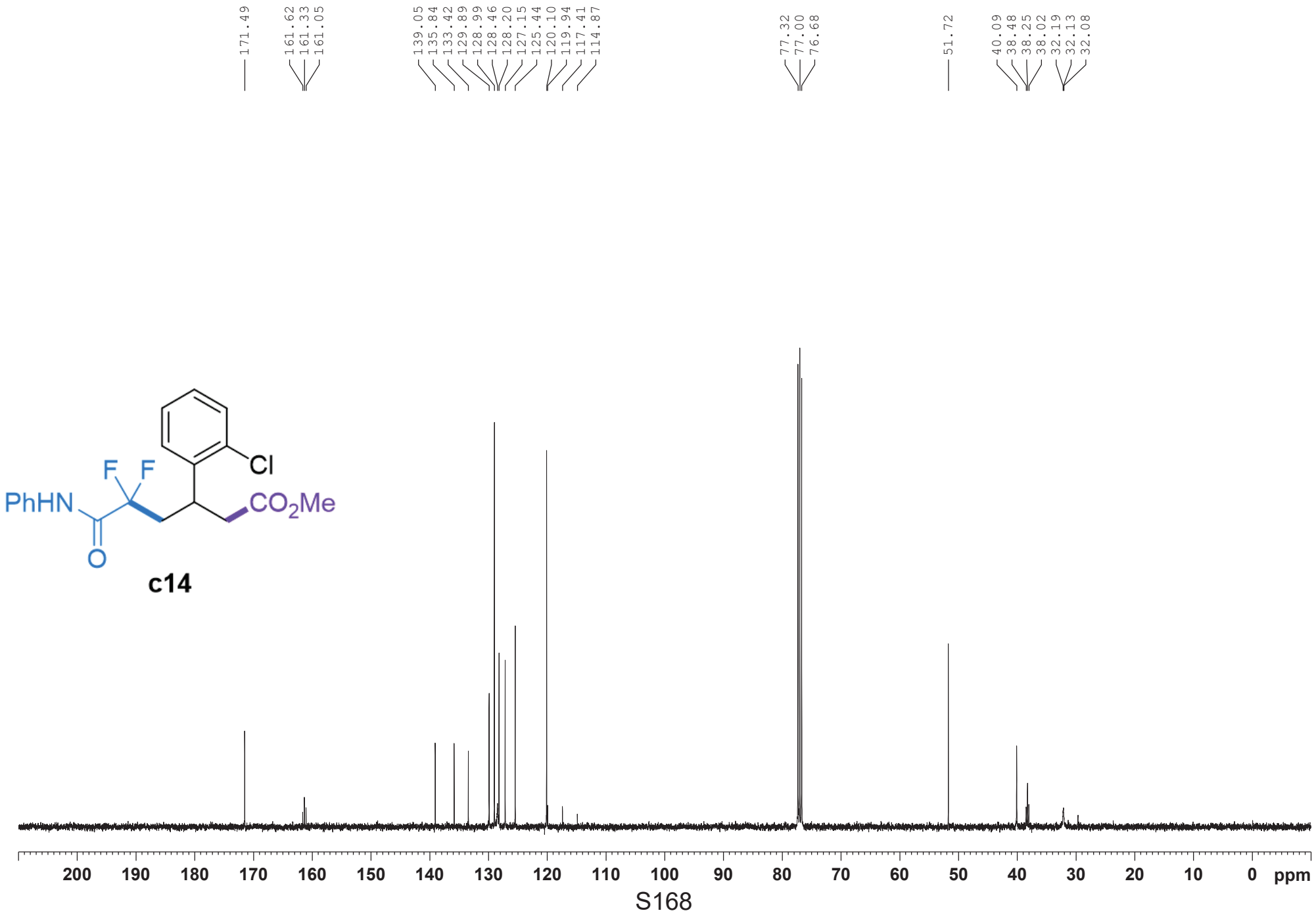

-100.671
-101.351
-105.365
-106.045
OMe
F
F
PhHN
CO2Me
O
c12
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

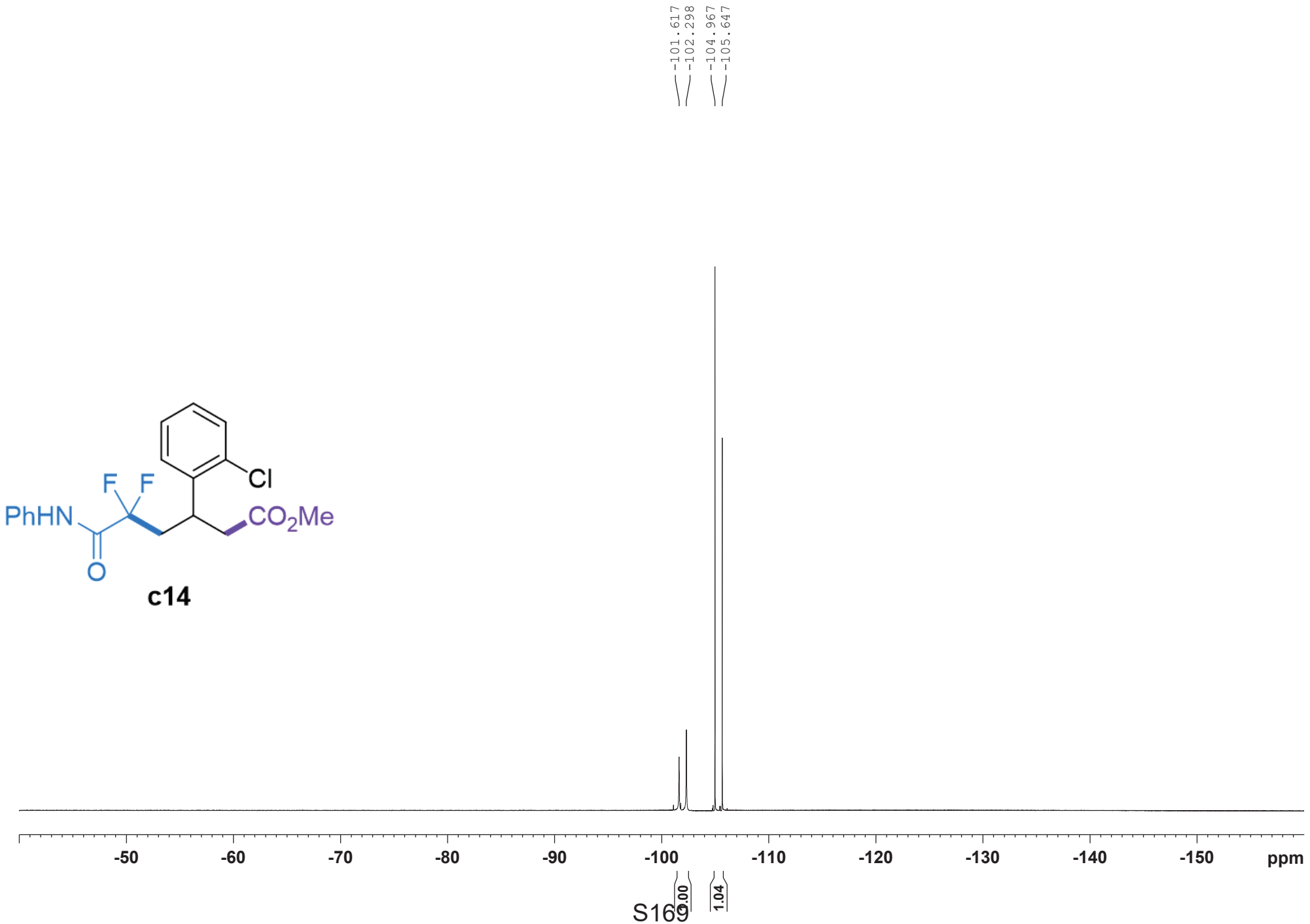

8.136
7.471
7.451
7.346
7.327
7.312
7.308
7.293
7.277
7.218
7.199
7.188
7.170
7.151
7.066
6.999
6.979
3.610
3.587
3.567
3.537
3.159
2.826
2.809
2.786
2.770
2.730
2.707
2.685
2.667
2.659
2.645
2.622
2.609
2.598
2.584
2.576
2.562
1.796
NMeAc
F F
PhHN
CO2Me
O
c13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.94
2.17
3.16
2.26
1.06
1.04
4.18
3.00
4.35
3.01


171.37
170.52
161.60
161.32
161.04
144.60
143.76
135.78
129.85
129.02
126.77
126.31
125.70
125.54
120.10
119.83
117.29
114.76
77.32
77.00
76.68
51.71
41.28
39.27
39.04
38.81
36.94
35.85
35.82
35.78
NMeAc
F F
PhHN
CO2Me
O
c13
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


-100.982
-101.666
-105.144
-105.828
NMeAc
F F
PhHN
CO2Me
O
c13
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
2.00
1.00

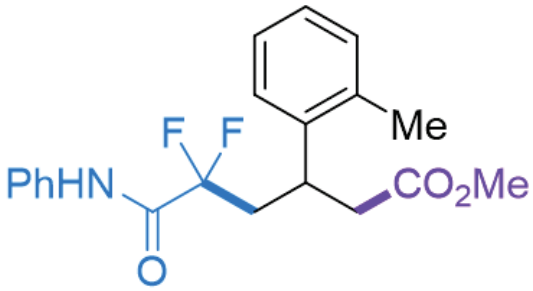

7.939
7.442
7.440
7.421
7.332
7.327
7.313
7.292
7.277
7.273
7.256
7.253
7.248
7.245
7.228
7.225
7.213
7.210
7.194
7.192
7.173
7.155
7.136
7.080
7.076
7.060
7.057
7.042
7.038
4.137
4.120
4.103
4.085
4.067
3.594
2.820
2.803
2.780
2.762
2.741
2.721
2.700
2.683
2.659
2.645
2.616
2.603
F
F
Cl
PhHN
CO2Me
O
c14
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.10
6.59
1.07
1.01
3.03
4.29


171.49
161.62
161.33
161.05
139.05
135.84
133.42
129.89
128.99
128.46
128.20
127.15
125.44
120.10
119.94
117.41
114.87
77.32
77.00
76.68
51.72
40.09
38.48
38.25
38.02
32.19
32.13
32.08
F
F
Cl
PhHN
CO2Me
O
c14
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

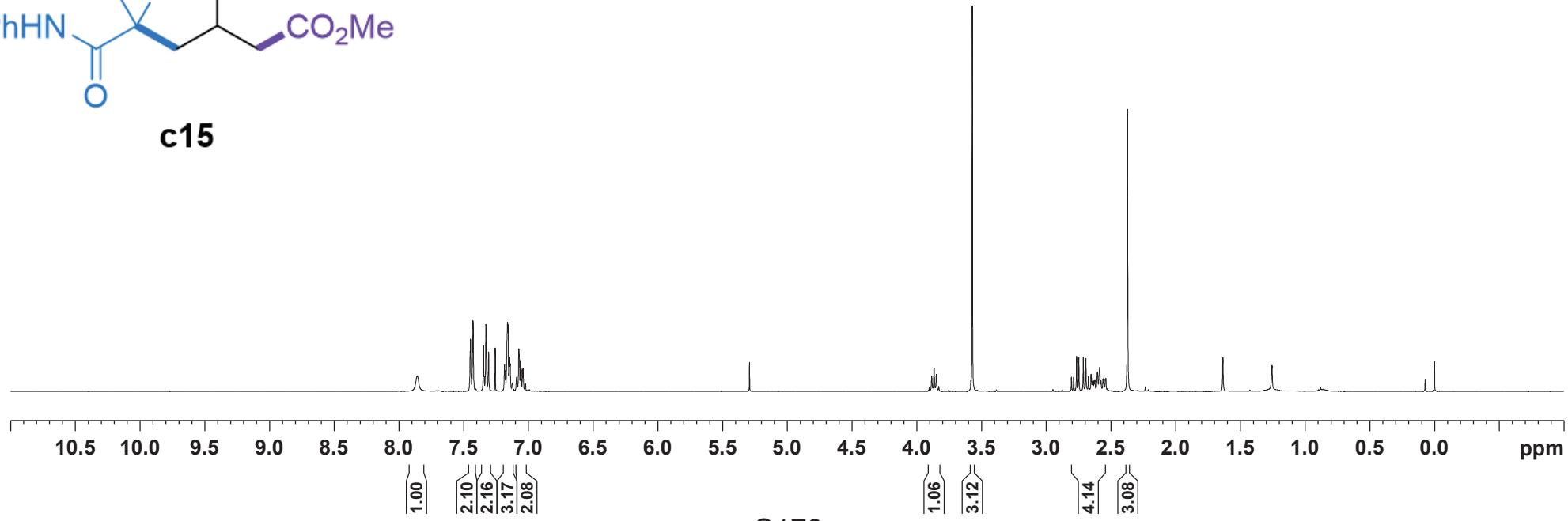

-101.617
-102.298
-104.967
-105.647
F
F
Cl
PhHN
CO2Me
O
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.04

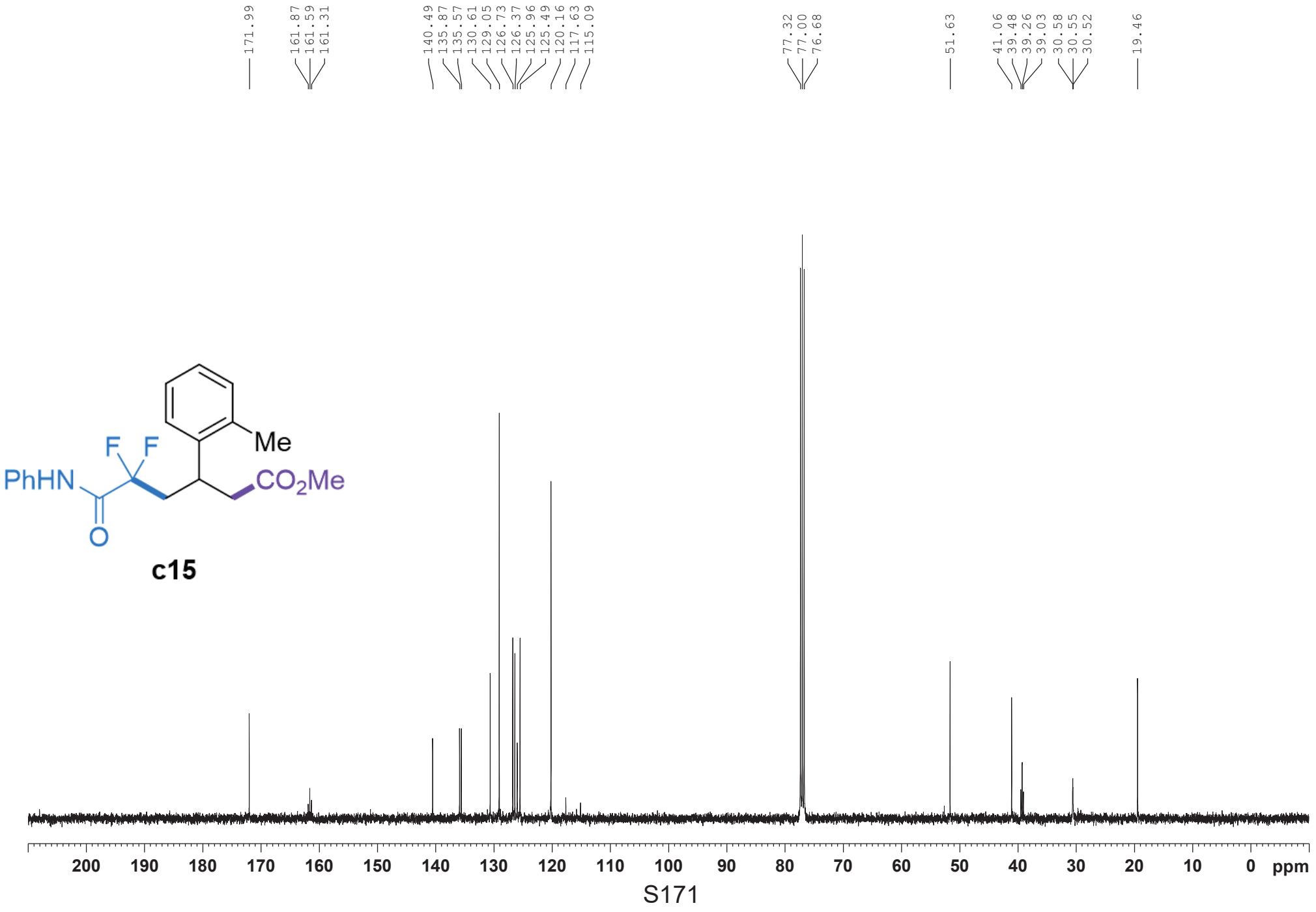
c14

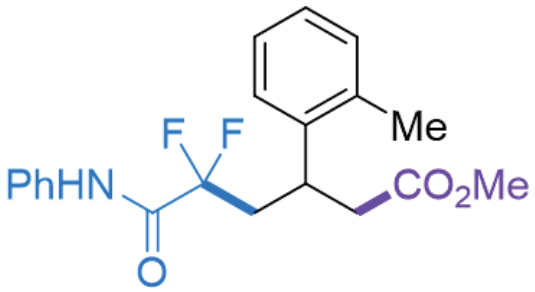

7.859
7.450
7.447
7.428
7.347
7.342
7.328
7.307
7.184
7.182
7.176
7.161
7.157
7.145
7.141
7.121
7.090
7.074
7.061
7.056
7.046
7.041
7.027
7.022
3.902
3.884
3.866
3.848
3.830
3.571
2.804
2.787
2.765
2.748
2.713
2.693
2.673
2.653
2.640
2.631
2.623
2.604
2.586
2.576
2.561
2.555
2.542
2.538
2.371


F
F
Me
PhHN
CO2Me
O

c15

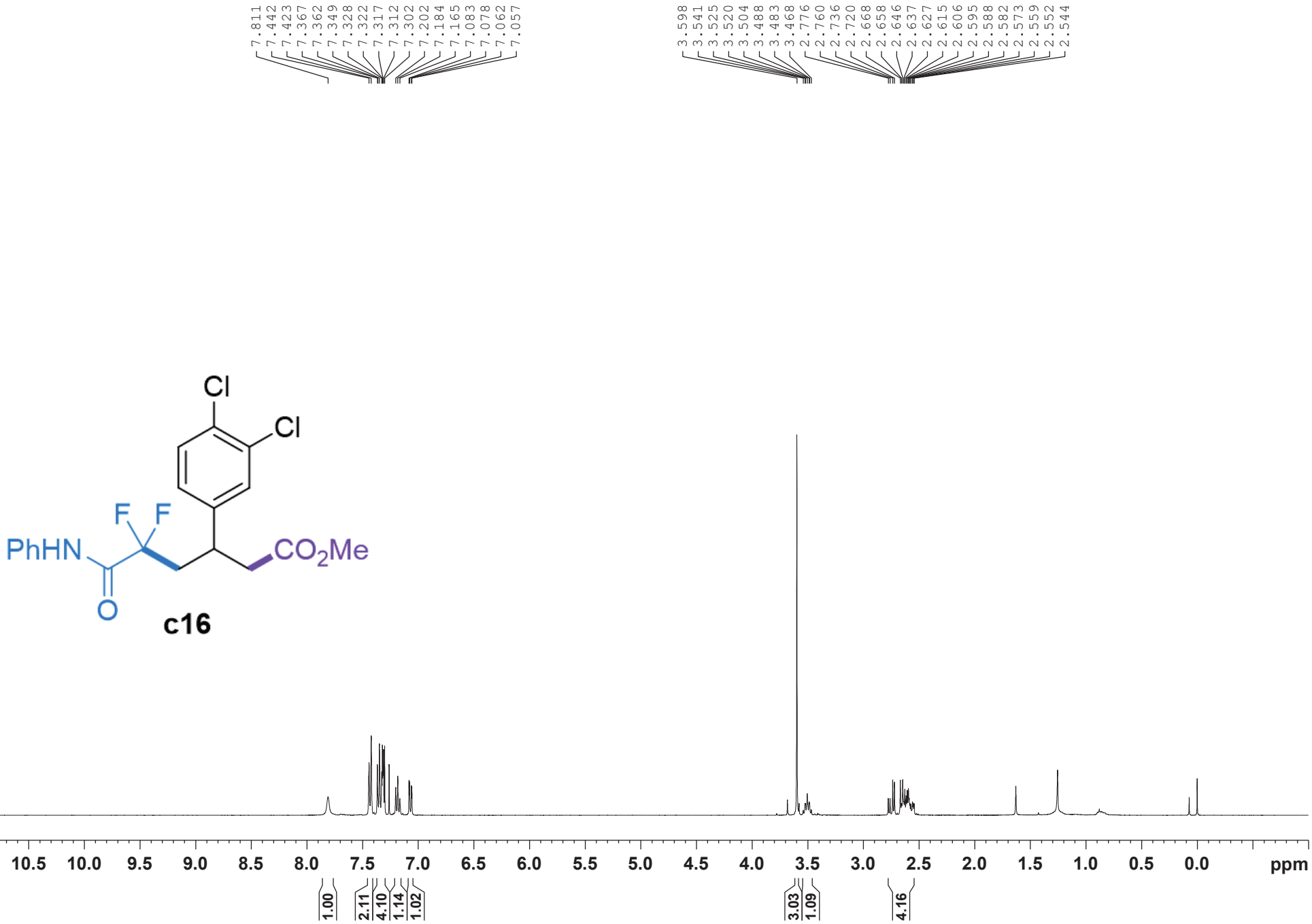

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.10
2.16
3.17
2.08
1.06
3.12
4.14
3.08

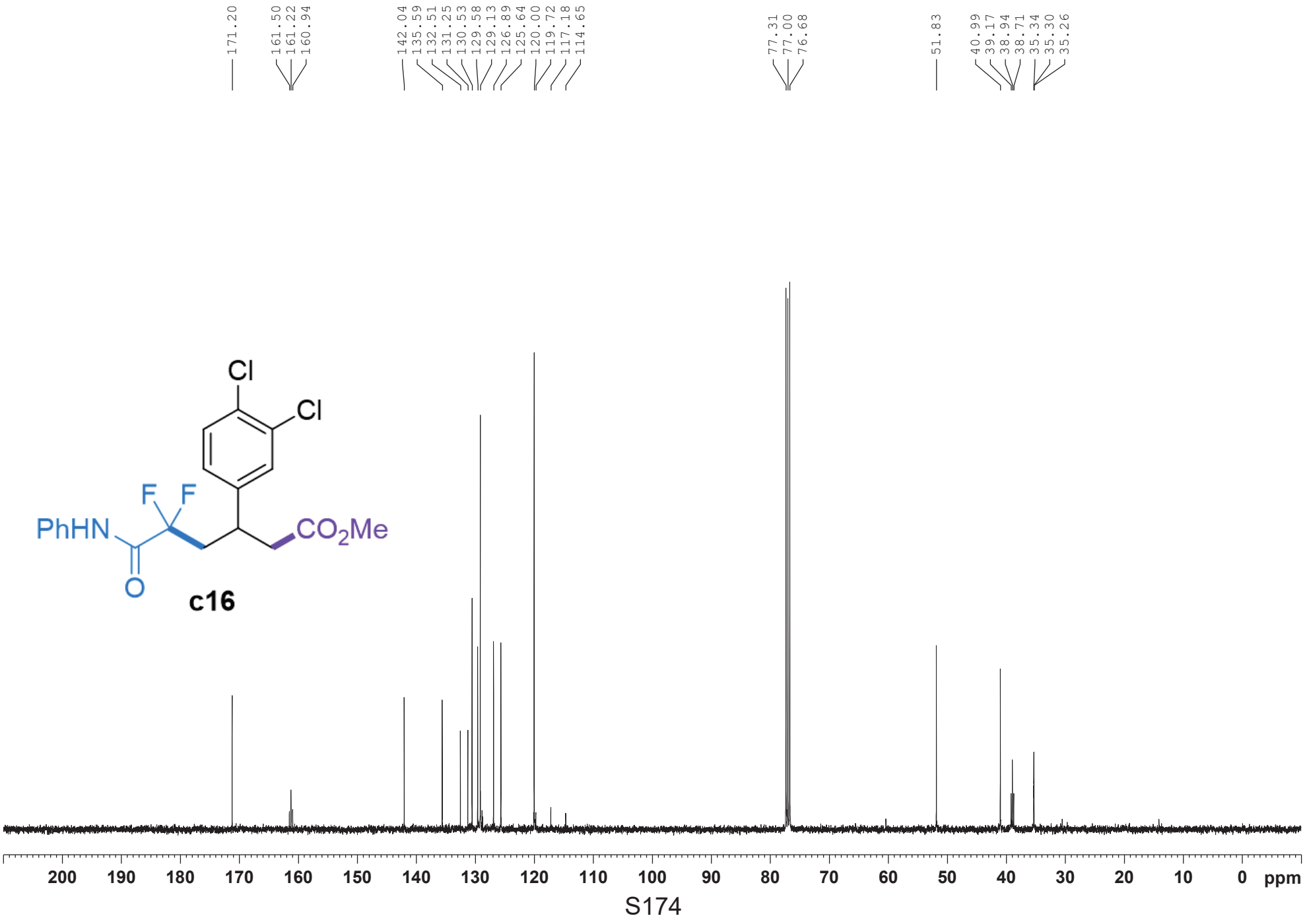

171.99
161.87
161.59
161.31
140.49
135.87
135.57
130.61
129.05
126.73
126.37
125.96
125.49
120.16
117.63
115.09
77.32
77.00
76.68
51.63
41.06
39.48
39.26
39.03
30.58
30.55
30.52
19.46
F
F
Me
PhHN
CO2Me
O
c15
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

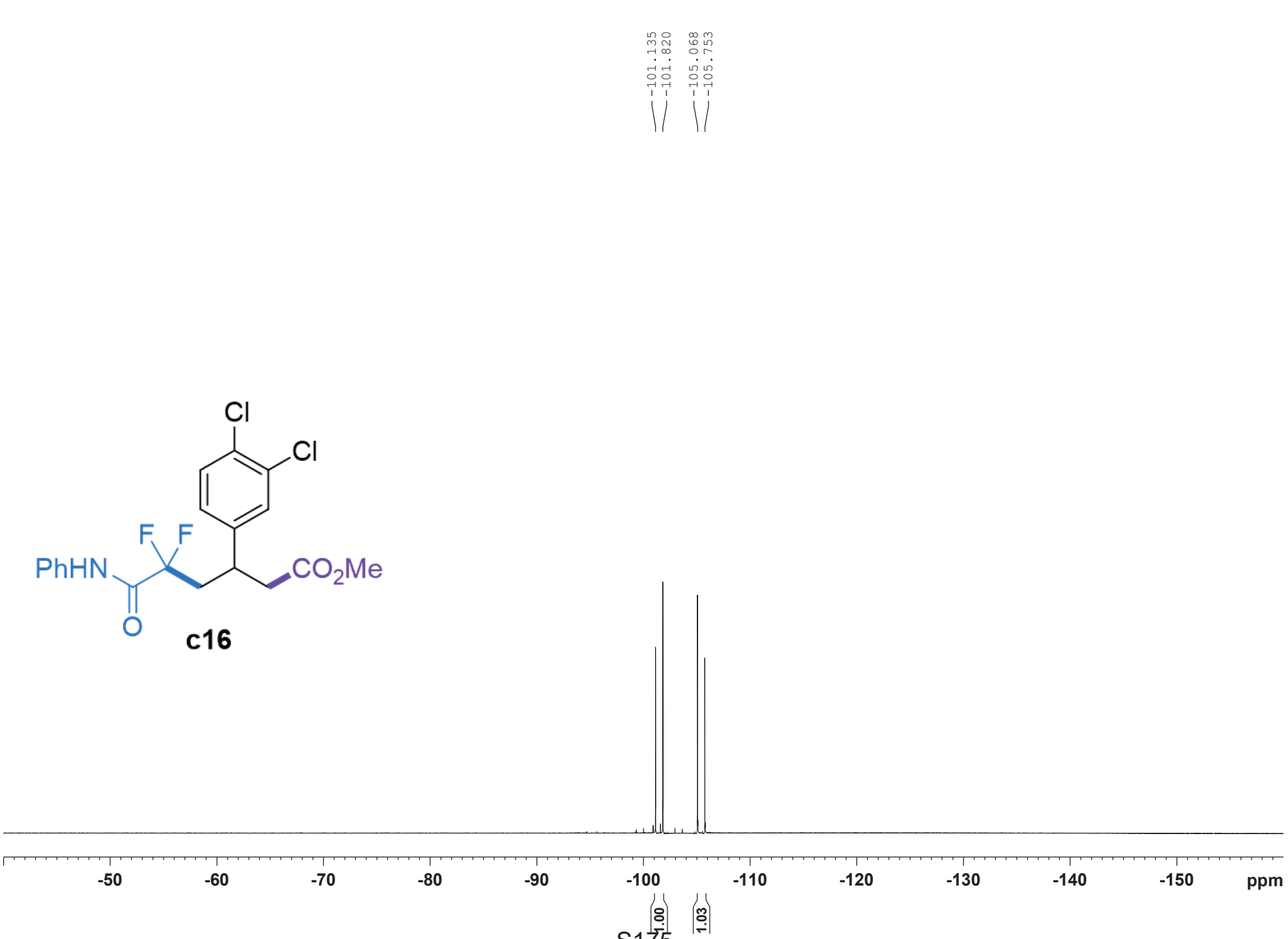

F
F
Me
PhHN
CO_2Me
O

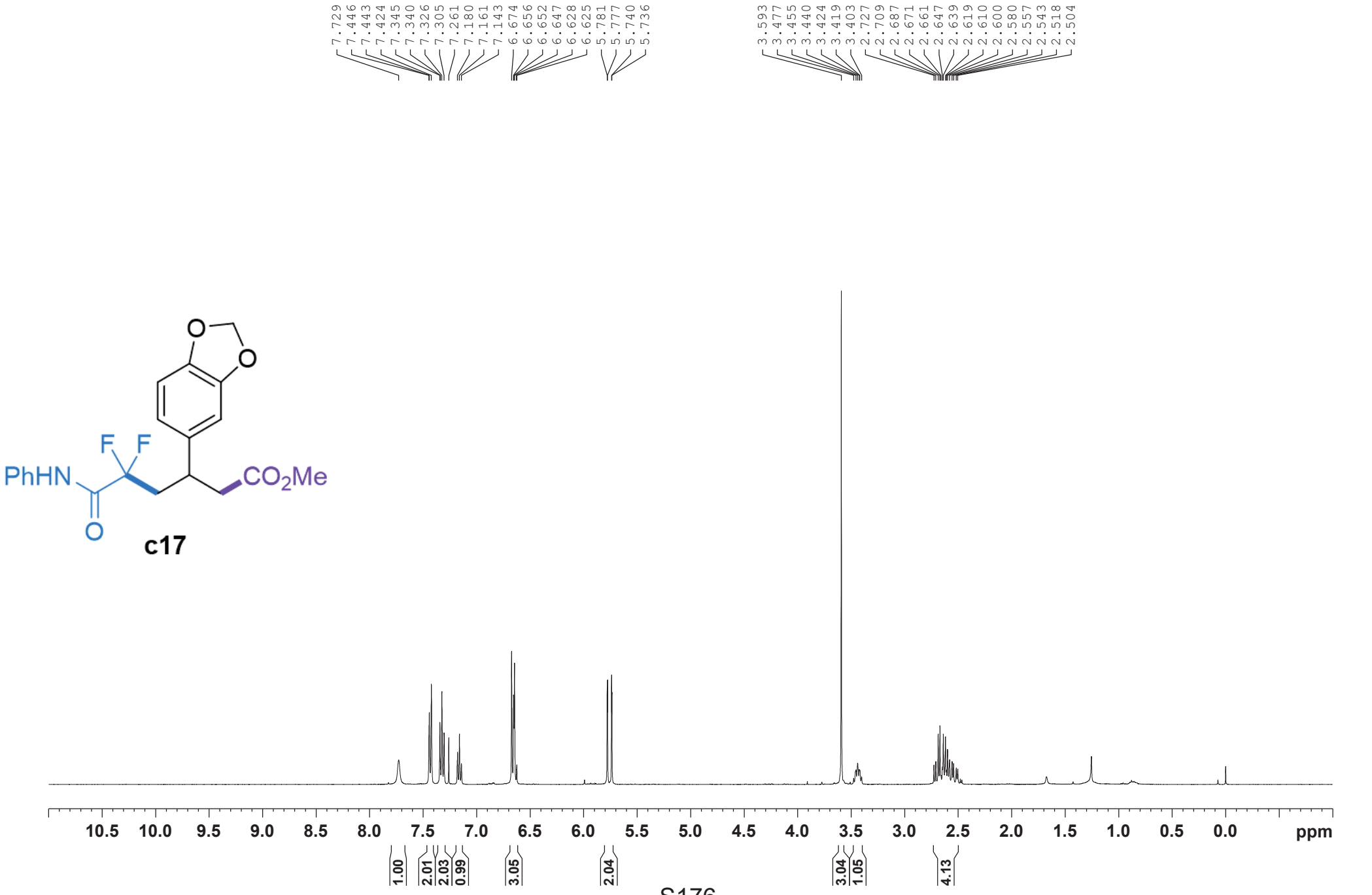
c15

-101.312
-101.992
-105.464
-106.143
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.00

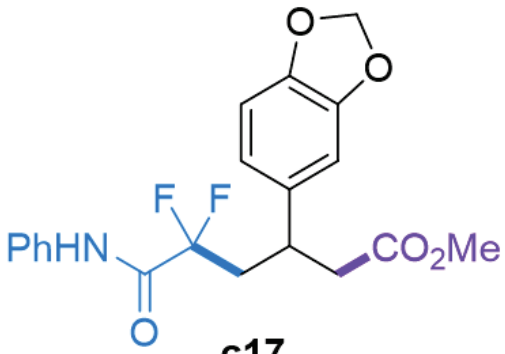

7.811
7.442
7.423
7.367
7.362
7.349
7.328
7.322
7.317
7.312
7.302
7.202
7.184
7.165
7.083
7.078
7.062
7.057
3.598
3.541
3.525
3.520
3.504
3.488
3.483
3.468
2.776
2.760
2.736
2.720
2.668
2.658
2.646
2.637
2.627
2.615
2.606
2.595
2.588
2.582
2.573
2.559
2.552
2.544
Cl
Cl
F
F
PhHN
O
CO2Me
c16
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.11
4.10
1.14
1.02
3.03
1.09
4.16


171.20
161.50
161.22
160.94
142.04
135.59
132.51
131.25
130.53
129.58
129.13
126.89
125.64
120.00
119.72
117.18
114.65
77.31
77.00
76.68
51.83
40.99
39.17
38.94
38.71
35.34
35.30
35.26
Cl
Cl
F
F
PhHN
O
CO2Me
c16
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

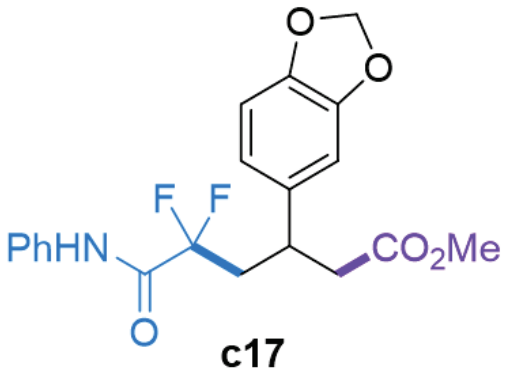

-101.135
-101.820
-105.068
-105.753
Cl
Cl
F
F
PhHN
O
CO2Me
c16
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.03


7.729
7.446
7.443
7.424
7.345
7.340
7.326
7.305
7.261
7.180
7.161
7.143
6.674
6.656
6.652
6.647
6.628
6.625
5.781
5.777
5.740
5.736
3.593
3.477
3.455
3.440
3.424
3.419
3.403
2.727
2.709
2.687
2.671
2.661
2.647
2.639
2.619
2.610
2.600
2.580
2.557
2.543
2.518
2.504
PhHN
F
F
O
O
O
CO2Me
c17
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.01
2.03
0.99
3.05
2.04
3.04
1.05
4.13

171.67
161.81
161.52
161.25
147.70
146.58
135.89
135.20
129.01
125.38
120.80
119.96
119.91
117.45
114.90
108.24
107.70
100.94
77.32
77.00
76.68
51.69
41.59
39.65
39.43
39.20
36.06
36.02
35.98



c17

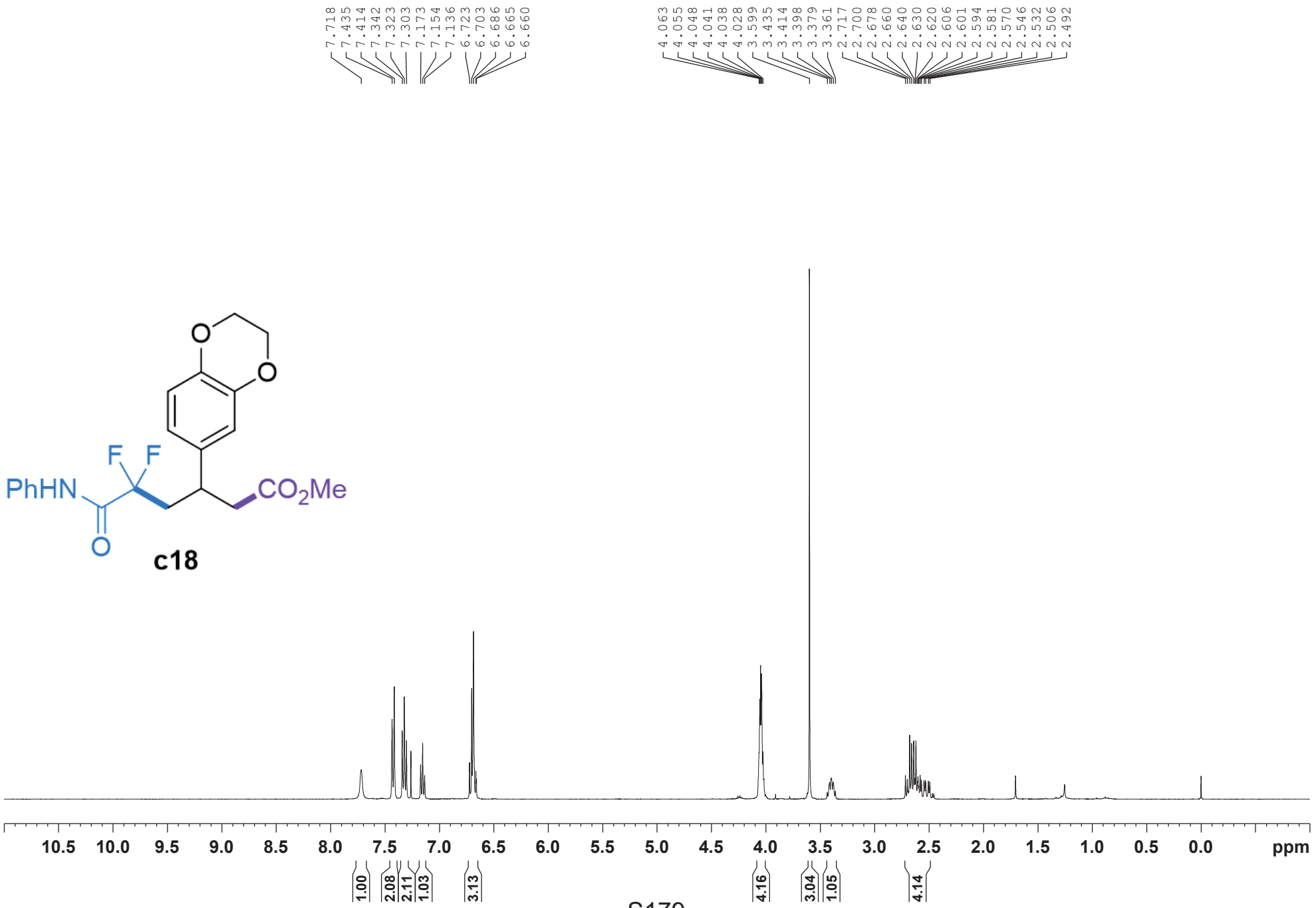


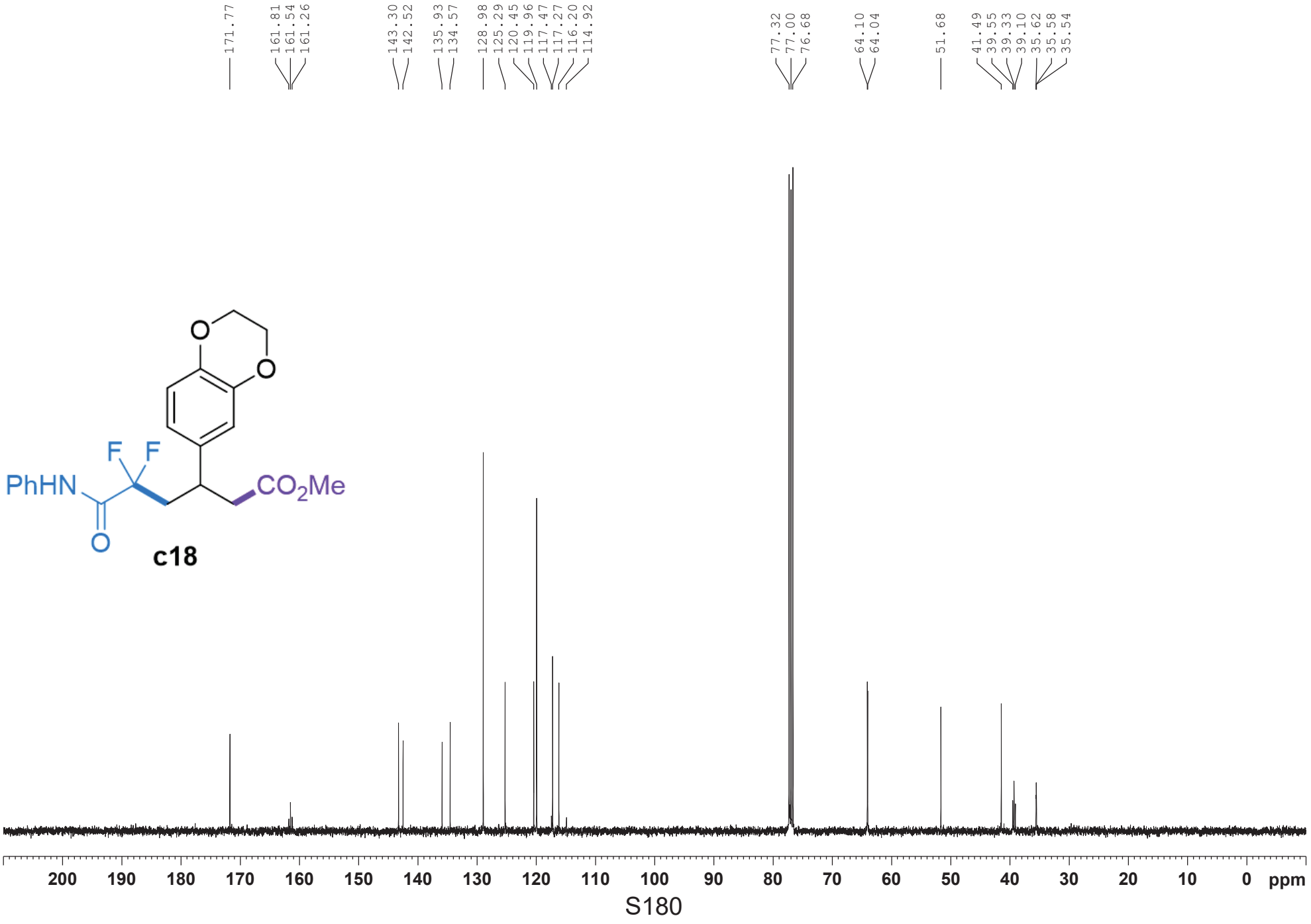
c17

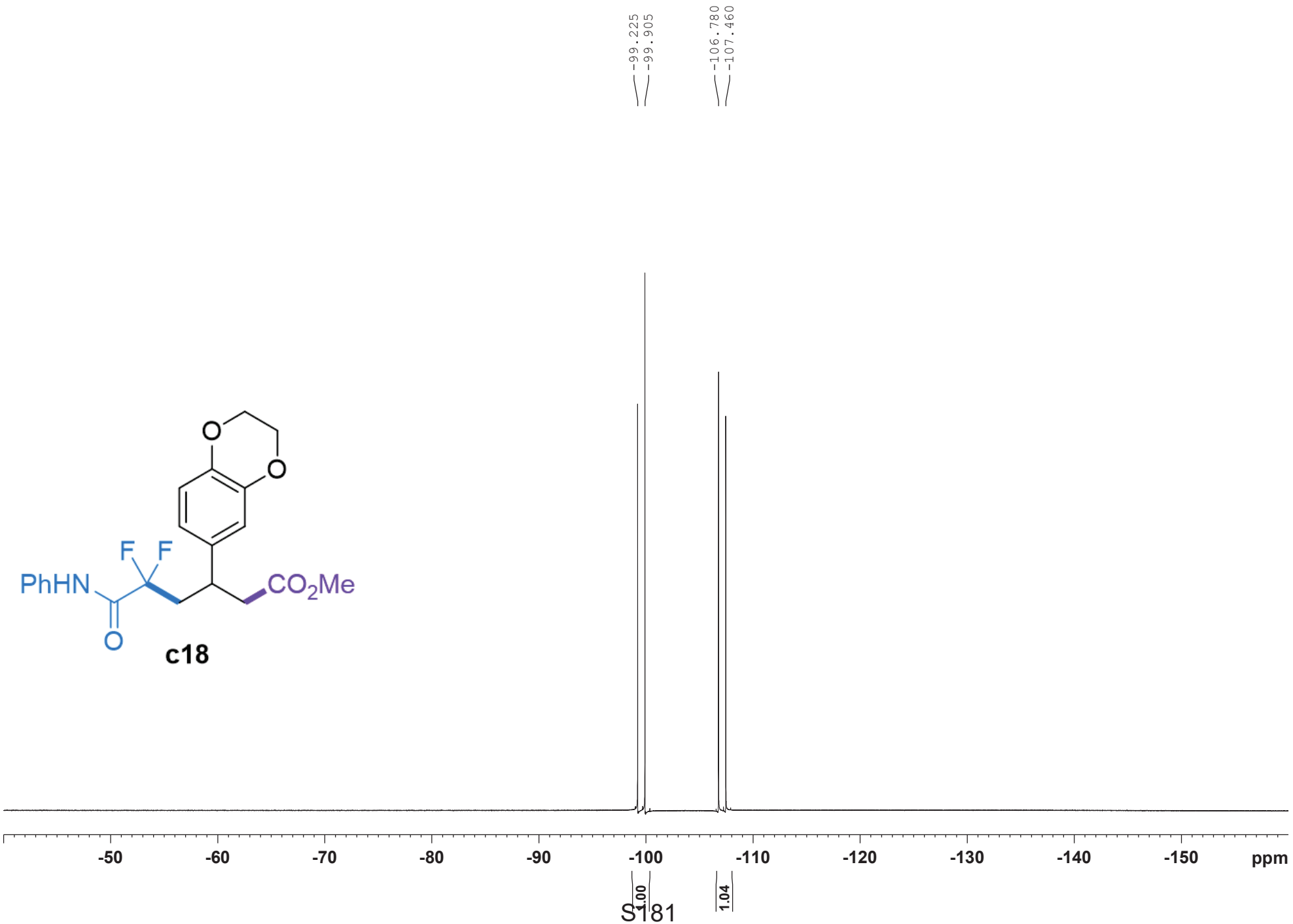
-99.708
-100.389
-106.466
-107.147

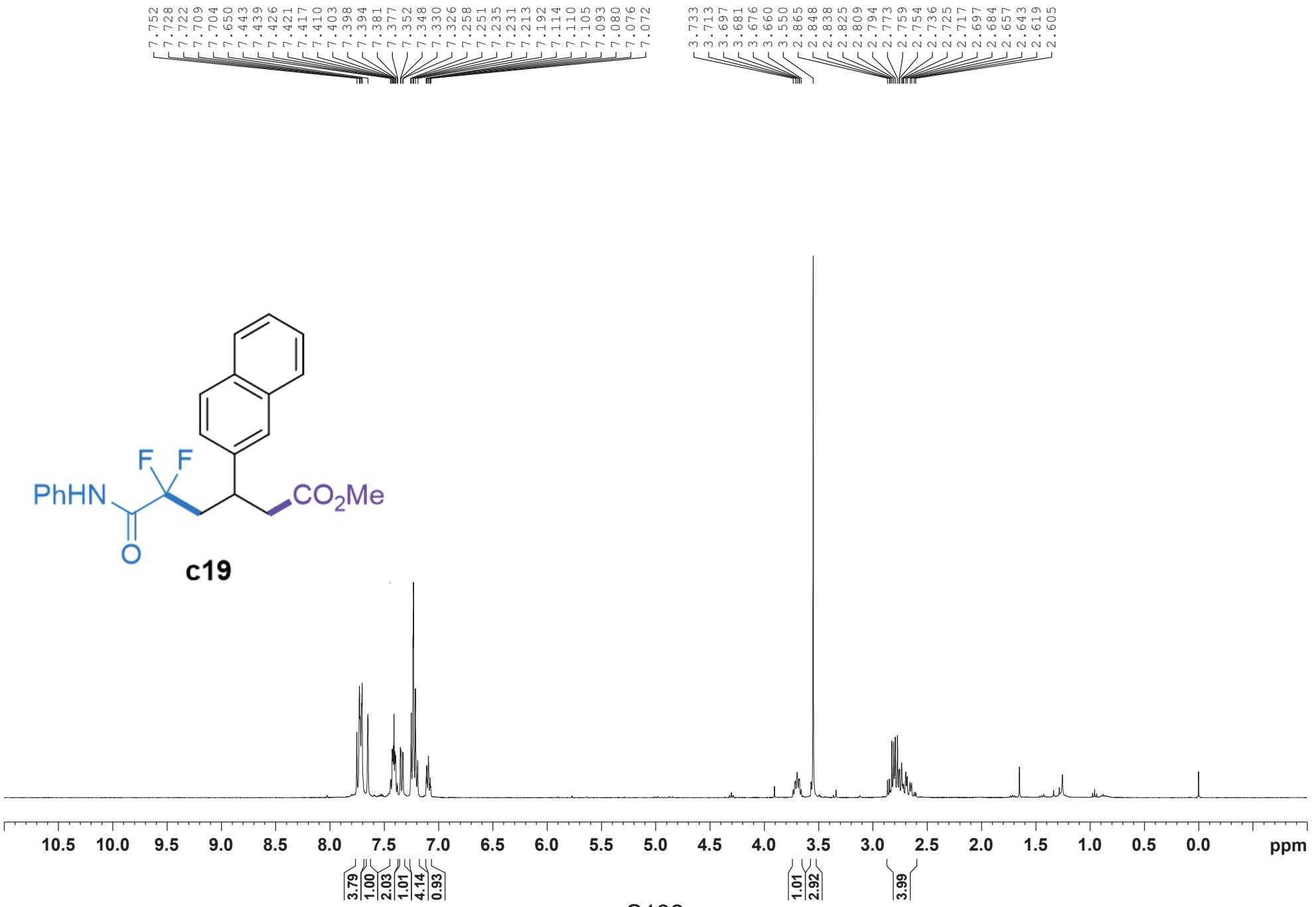
-50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 ppm

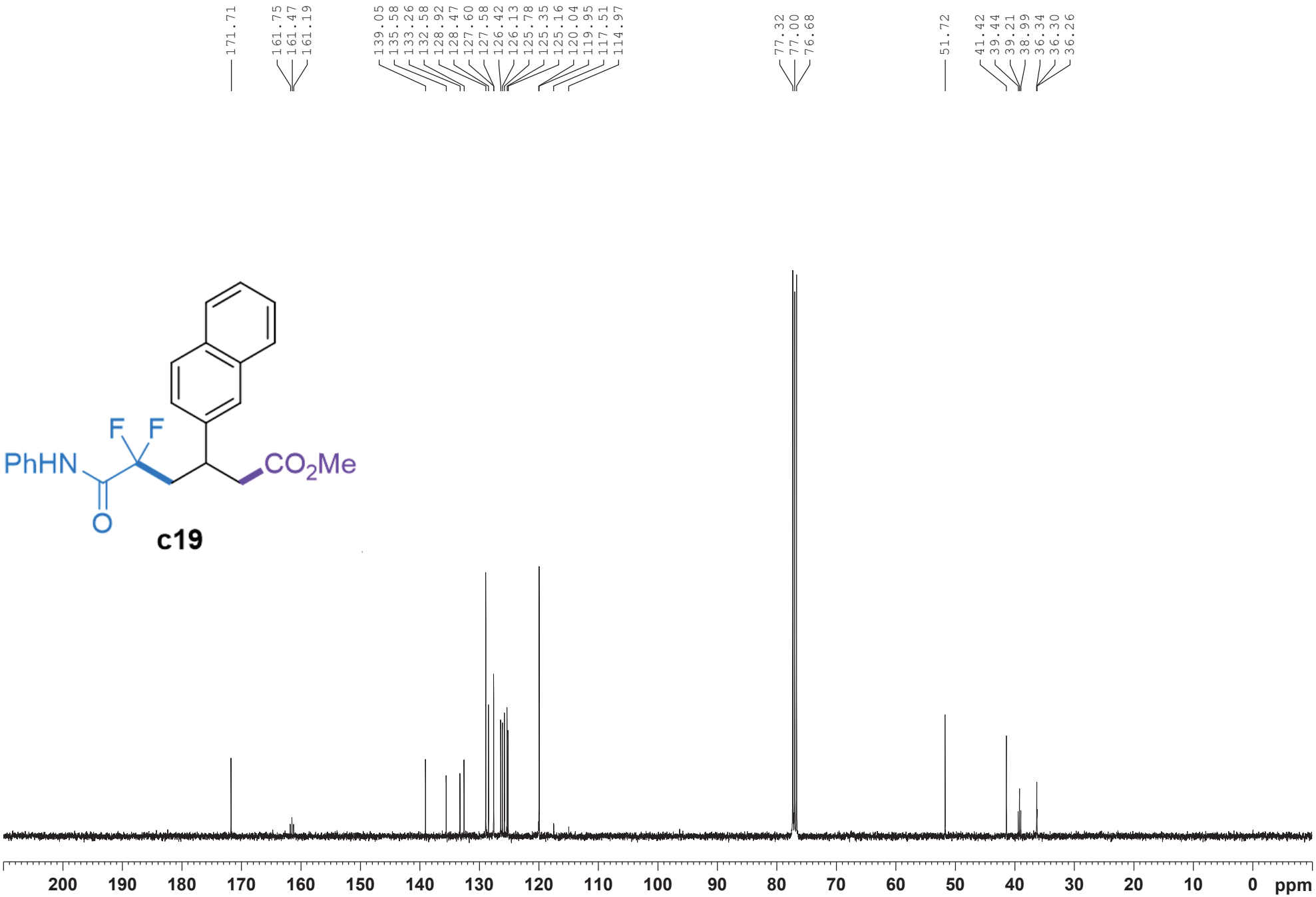
1.00
1.01

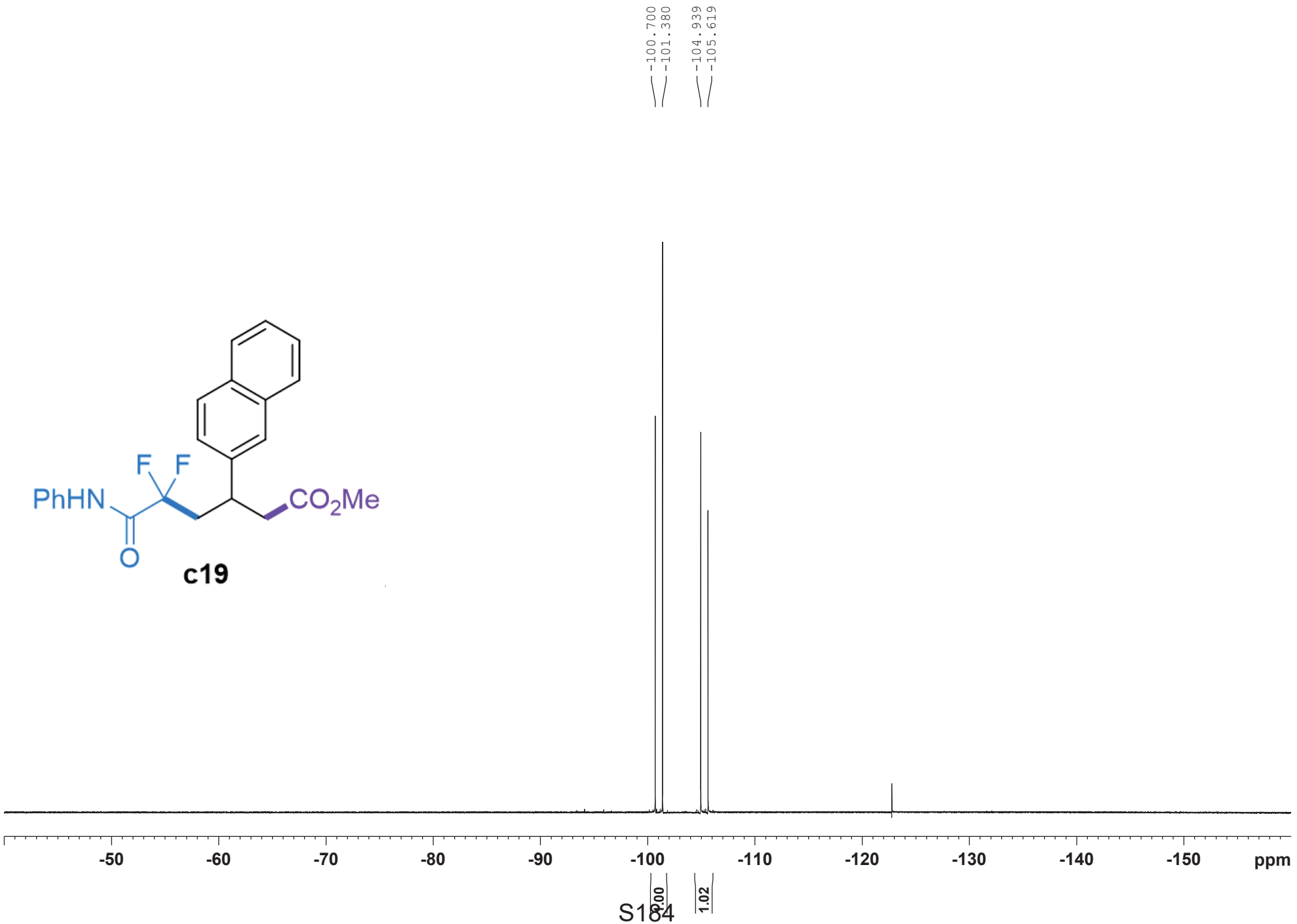

7.718
7.435
7.414
7.342
7.323
7.303
7.173
7.154
7.136
6.723
6.703
6.686
6.665
6.660
4.063
4.055
4.048
4.041
4.038
4.028
3.599
3.435
3.414
3.398
3.379
3.361
2.717
2.700
2.678
2.660
2.640
2.630
2.620
2.606
2.601
2.594
2.581
2.570
2.546
2.532
2.506
2.492
PhHN
F
F
O
O
O
CO2Me
c18
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.08
2.11
1.03
3.13
4.16
3.04
1.05
4.14

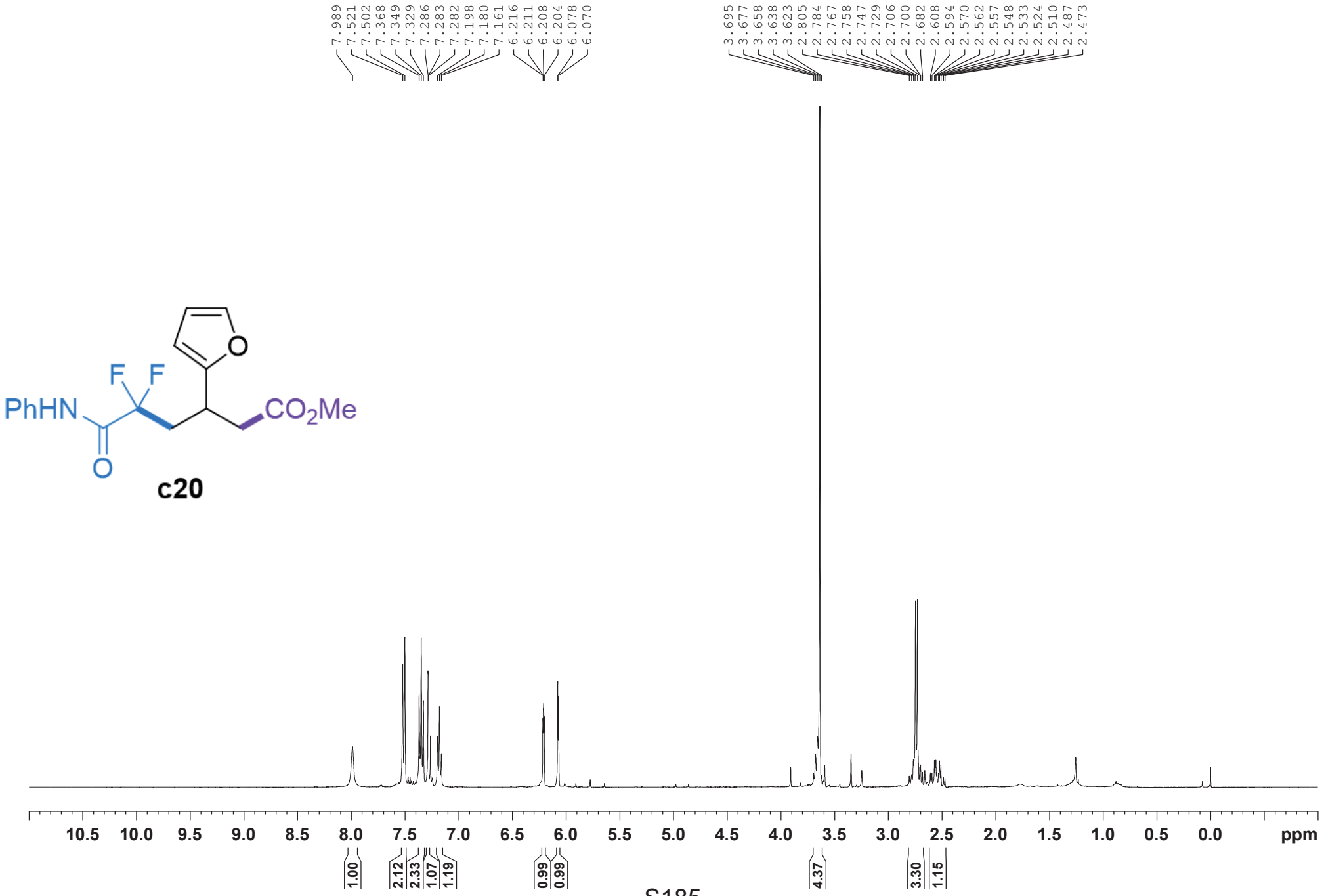

171.77
161.81
161.54
161.26
143.30
142.52
135.93
134.57
128.98
125.29
120.45
119.96
117.47
117.27
116.20
114.92
77.32
77.00
76.68
64.10
64.04
51.68
41.49
39.55
39.33
39.10
35.62
35.58
35.54
PhHN
F
F
O
O
O
CO2Me
c18
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

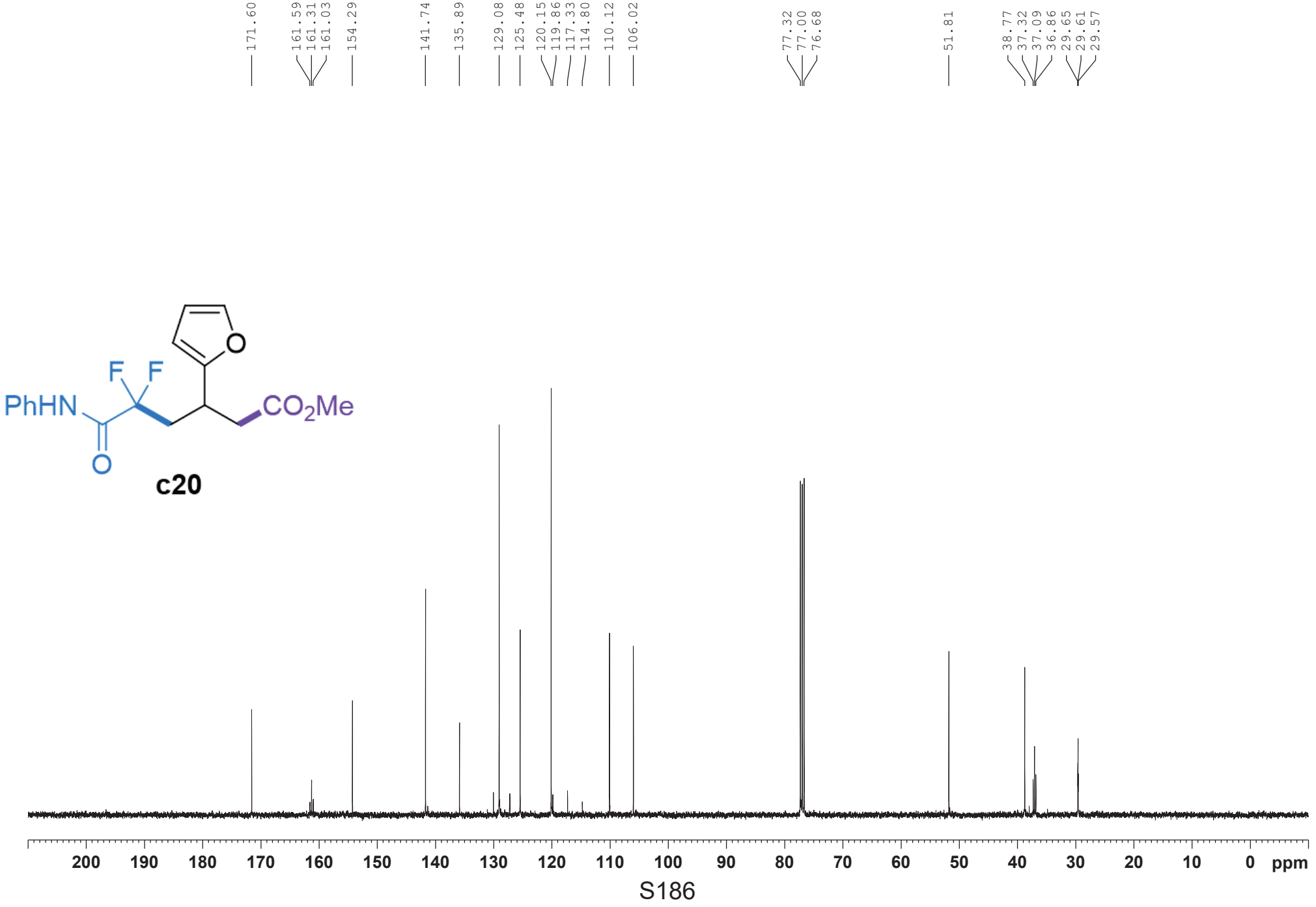

-99.225
-99.905
-106.780
-107.460
PhHN
F
F
O
O
O
CO2Me
c18
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.04

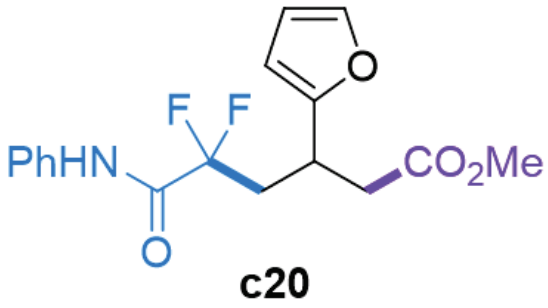

7.752
7.728
7.722
7.709
7.704
7.650
7.443
7.439
7.426
7.421
7.417
7.410
7.403
7.398
7.394
7.381
7.377
7.352
7.348
7.330
7.326
7.258
7.251
7.235
7.231
7.213
7.192
7.114
7.110
7.105
7.093
7.080
7.076
7.072
3.733
3.713
3.697
3.681
3.676
3.660
3.550
2.865
2.848
2.838
2.825
2.809
2.794
2.773
2.759
2.754
2.736
2.725
2.717
2.697
2.684
2.657
2.643
2.619
2.605
F
F
PhHN
CO2Me
O
c19
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
3.79
1.00
2.03
1.01
4.14
0.93
1.01
2.92
3.99


171.71
161.75
161.47
161.19
139.05
135.58
133.26
132.58
128.92
128.47
127.60
127.58
126.42
126.13
125.78
125.35
125.16
120.04
119.95
117.51
114.97
77.32
77.00
76.68
51.72
41.42
39.44
39.21
38.99
36.34
36.30
36.26
F
F
PhHN
CO2Me
O
c19
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-100.700
-101.380
-104.939
-105.619
F
F
PhHN
O
CO2Me
c19
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
2.00
1.02

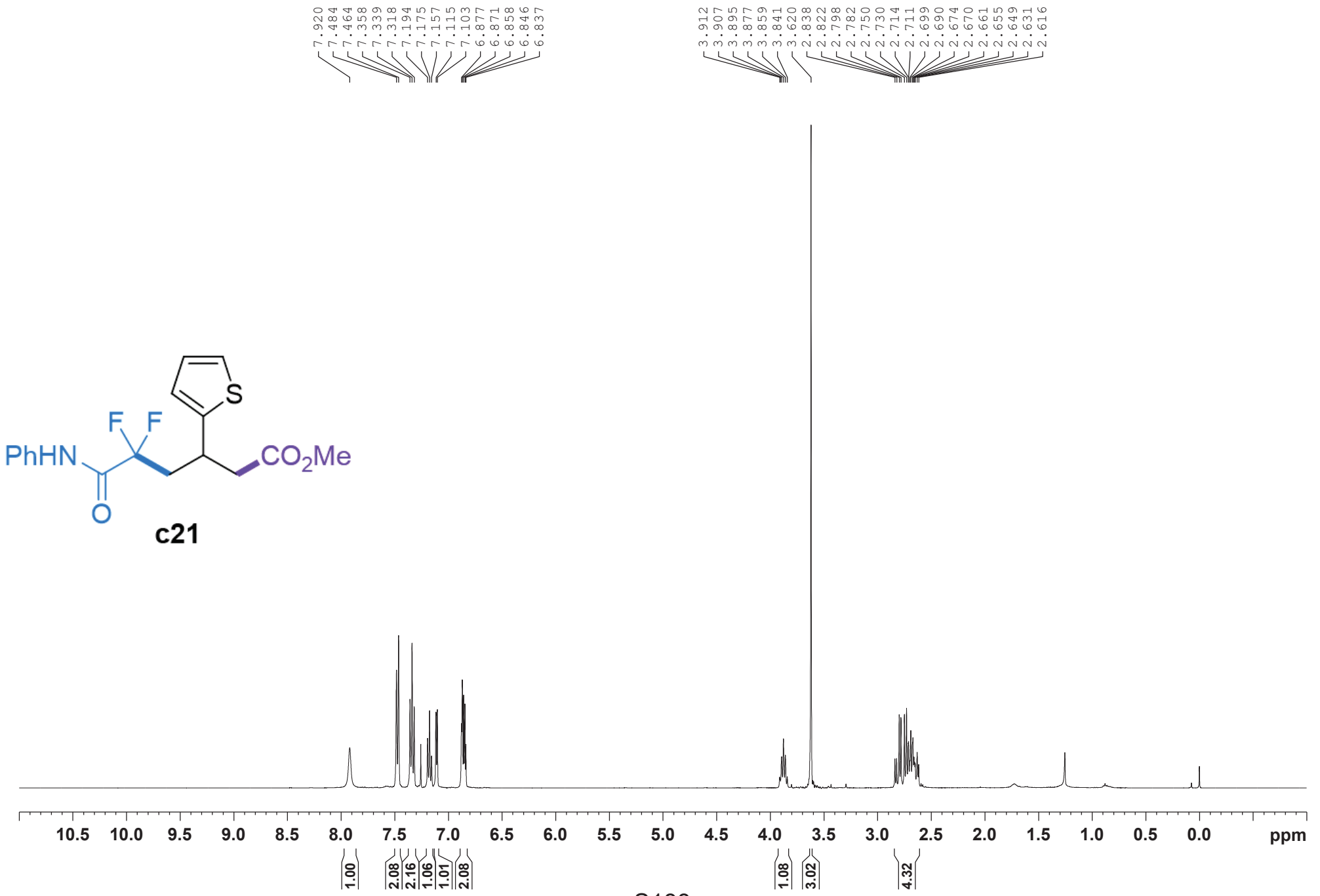

7.989
7.521
7.502
7.368
7.349
7.329
7.286
7.283
7.282
7.198
7.180
7.161
6.216
6.211
6.208
6.204
6.078
6.070
3.695
3.677
3.658
3.638
3.623
2.805
2.784
2.767
2.758
2.747
2.729
2.706
2.700
2.682
2.608
2.594
2.570
2.562
2.557
2.548
2.533
2.524
2.510
2.487
2.473
PhHN
F
F
O
O
CO2Me
c20
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.12
2.33
1.07
1.19
0.99
0.99
4.37
3.30
1.15

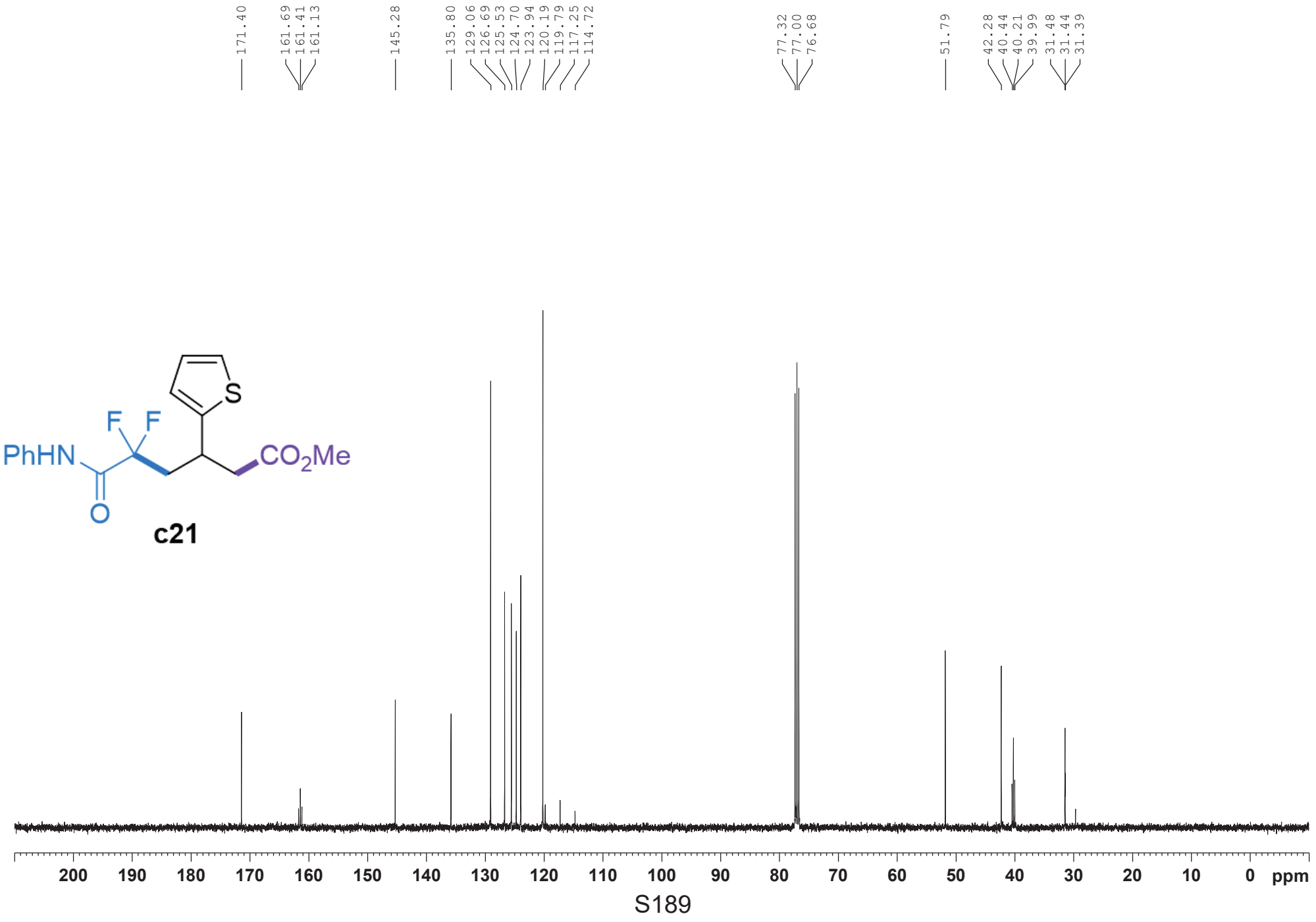

171.60
161.59
161.31
161.03
154.29
141.74
135.89
129.08
125.48
120.15
119.86
117.33
114.80
110.12
106.02
77.32
77.00
76.68
51.81
38.77
37.32
37.09
36.86
29.65
29.61
29.57
F
F
PhHN
O
O
CO2Me
c20
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

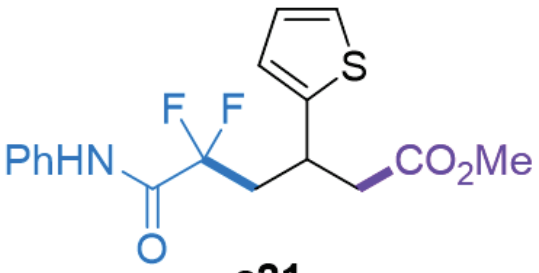

F
F
PhHN
O
O
CO_2Me

c20

-102.541
-103.225
-105.117
-105.799
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
0.97

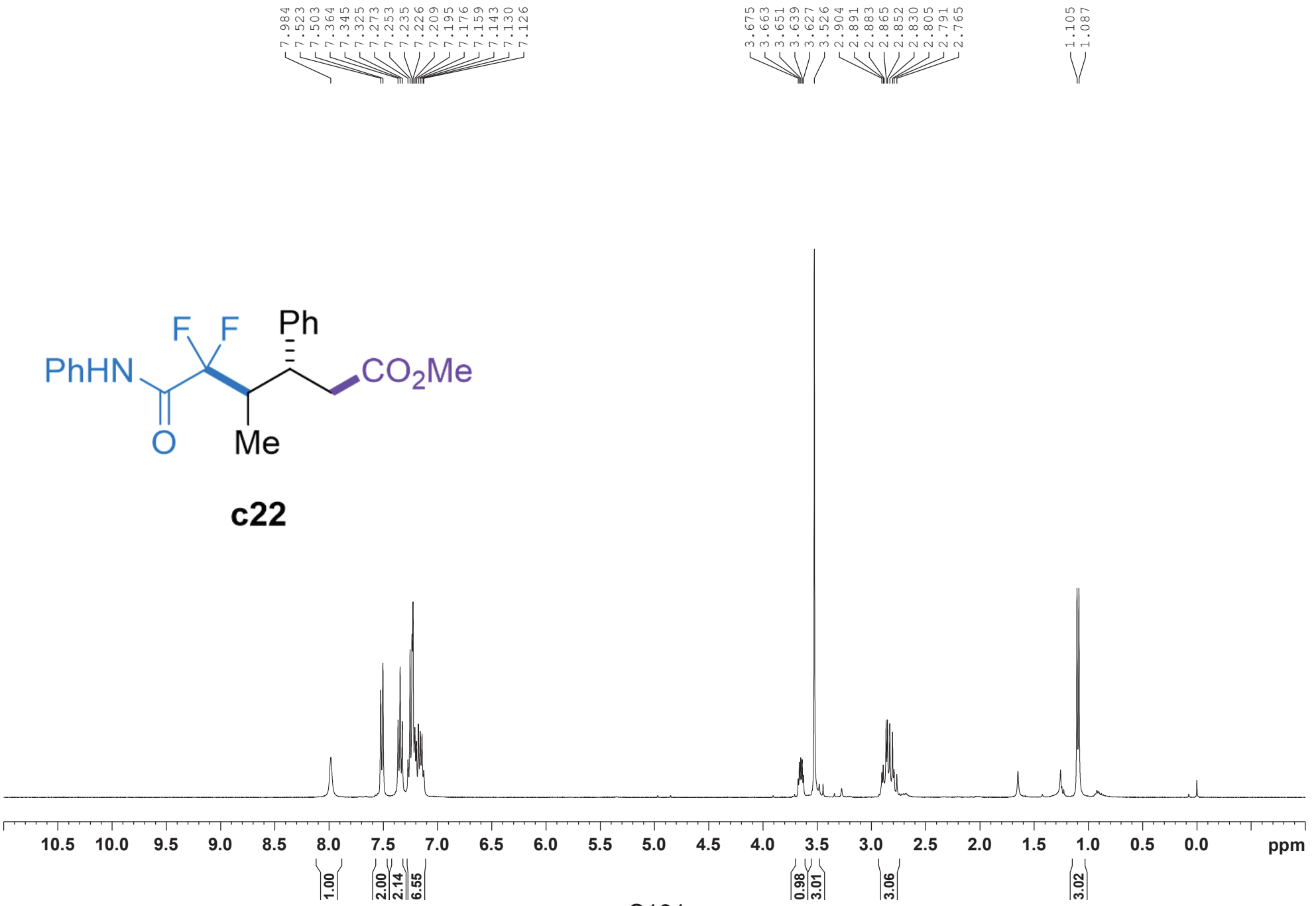

7.920
7.484
7.464
7.358
7.339
7.318
7.194
7.175
7.157
7.115
7.103
6.877
6.871
6.858
6.846
6.837
3.912
3.907
3.895
3.877
3.859
3.841
3.620
2.838
2.822
2.798
2.782
2.750
2.730
2.714
2.711
2.699
2.690
2.674
2.670
2.661
2.655
2.649
2.631
2.616
S
F
F
PhHN
CO2Me
O
c21
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.08
2.16
1.06
1.01
2.08
1.08
3.02
4.32

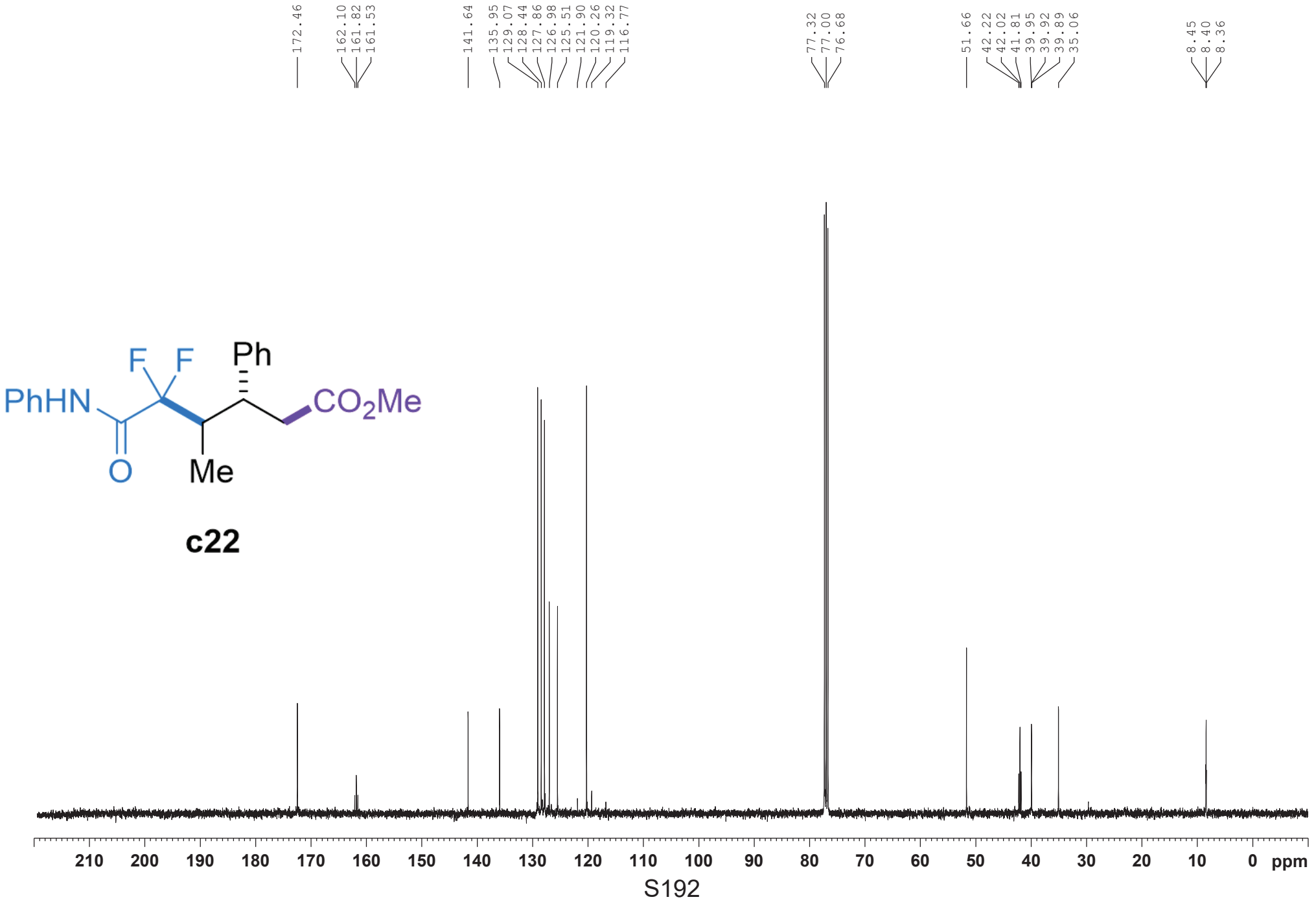

171.40
161.69
161.41
161.13
145.28
135.80
129.06
126.69
125.53
124.70
123.94
120.19
119.79
117.25
114.72
77.32
77.00
76.68
51.79
42.28
40.44
40.21
39.99
31.48
31.44
31.39
S
F
F
PhHN
O
CO2Me
c21
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

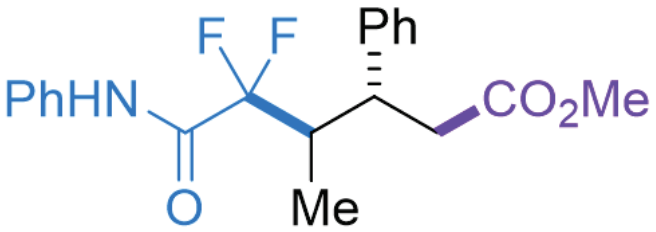

S
F
F
PhHN
O
CO2Me

c21

-101.632
-102.314
-105.067
-105.751
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.00

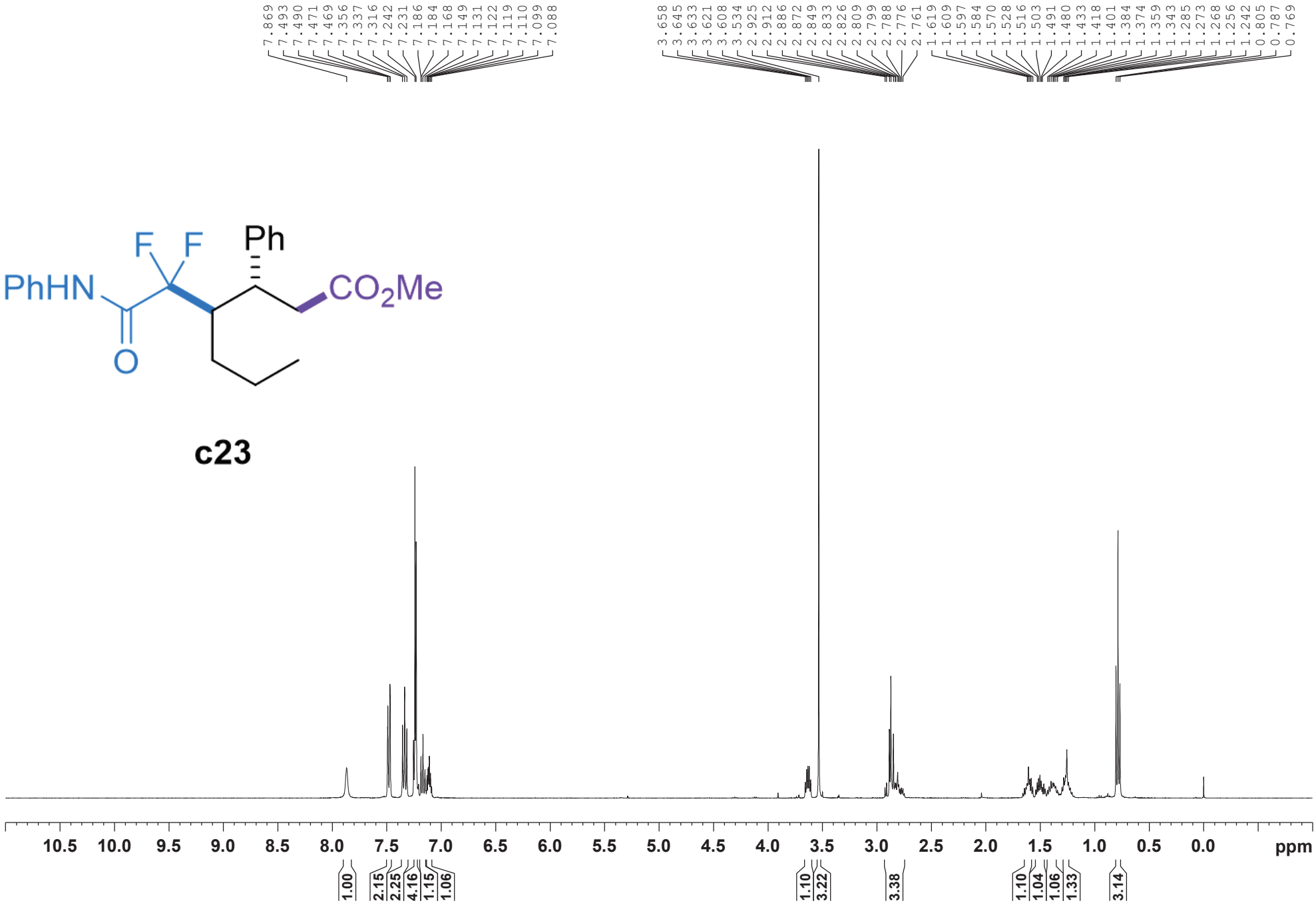

7.984
7.523
7.503
7.364
7.345
7.325
7.273
7.253
7.235
7.226
7.209
7.195
7.176
7.159
7.143
7.130
7.126
3.675
3.663
3.651
3.639
3.627
3.526
2.904
2.891
2.883
2.865
2.852
2.830
2.805
2.791
2.765
1.105
1.087
F
F
Ph
PhHN
CO2Me
O
Me
c22
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.00
2.14
6.55
0.98
3.01
3.06
3.02

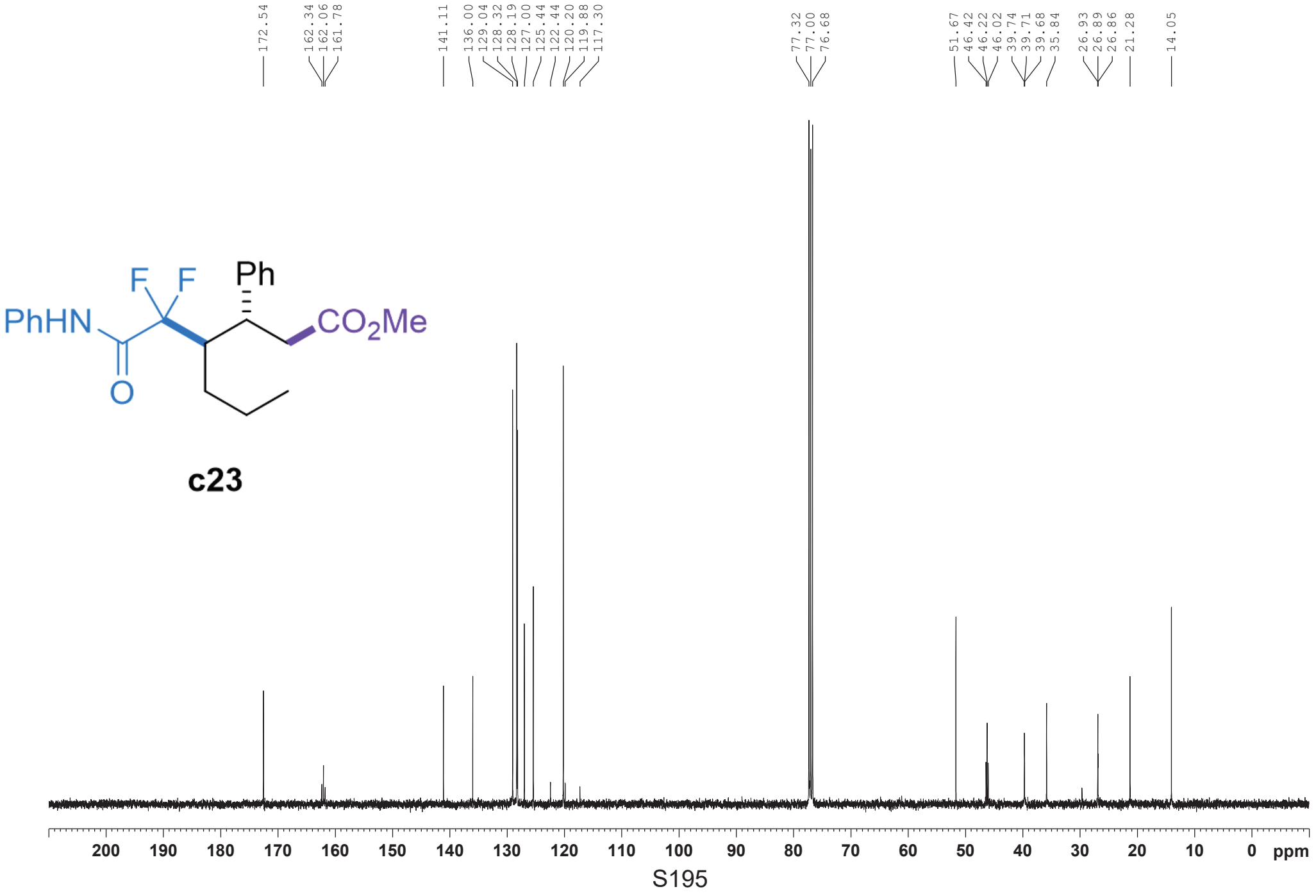

172.46
162.10
161.82
161.53
141.64
135.95
129.07
128.44
127.86
126.98
125.51
121.90
120.26
119.32
116.77
77.32
77.00
76.68
51.66
42.22
42.02
41.81
39.95
39.92
39.89
35.06
8.45
8.40
8.36
F
F
Ph
PhHN
CO2Me
O
Me
c22
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

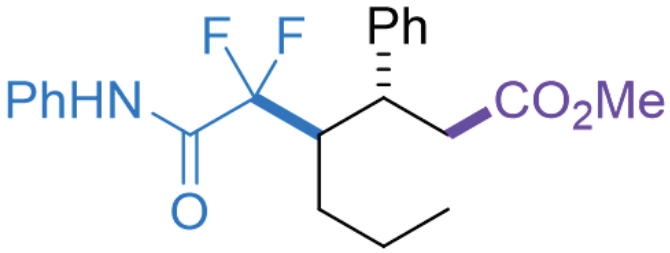

F
F
Ph
PhHN
CO2Me
O
Me

c22

-107.323
-107.999
-111.191
-111.868
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

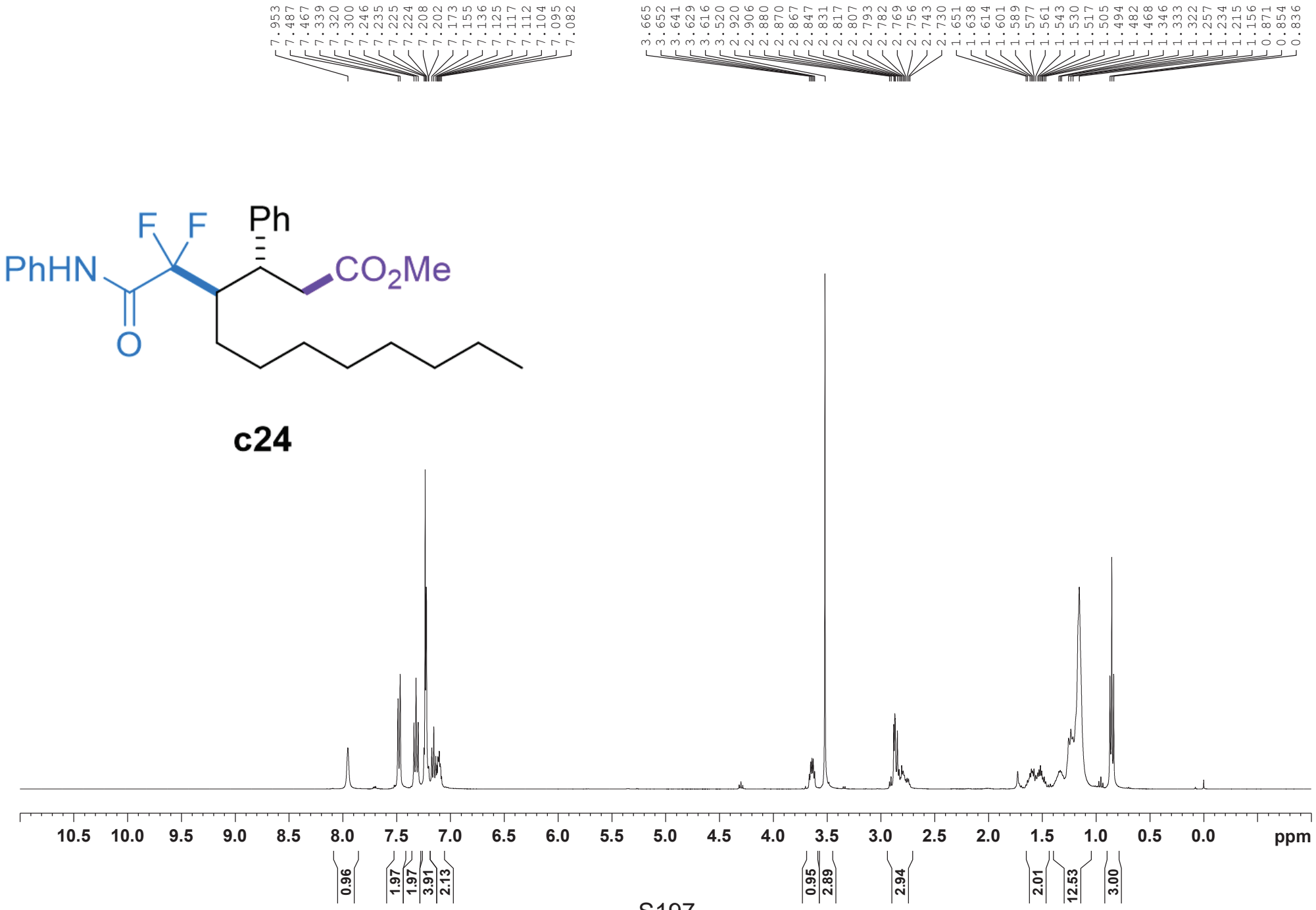

7.869
7.493
7.490
7.471
7.469
7.356
7.337
7.316
7.242
7.231
7.186
7.184
7.168
7.149
7.131
7.122
7.119
7.110
7.099
7.088
3.658
3.645
3.633
3.621
3.608
3.534
2.925
2.912
2.886
2.872
2.849
2.833
2.826
2.809
2.799
2.788
2.776
2.761
1.619
1.609
1.597
1.584
1.570
1.528
1.516
1.503
1.491
1.480
1.433
1.418
1.401
1.384
1.374
1.359
1.343
1.285
1.273
1.268
1.256
1.242
0.805
0.787
0.769
F
F
Ph
PhHN
CO2Me
O
c23
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.15
2.25
4.16
1.15
1.06
1.10
3.22
3.38
1.10
1.04
1.06
1.33
3.14

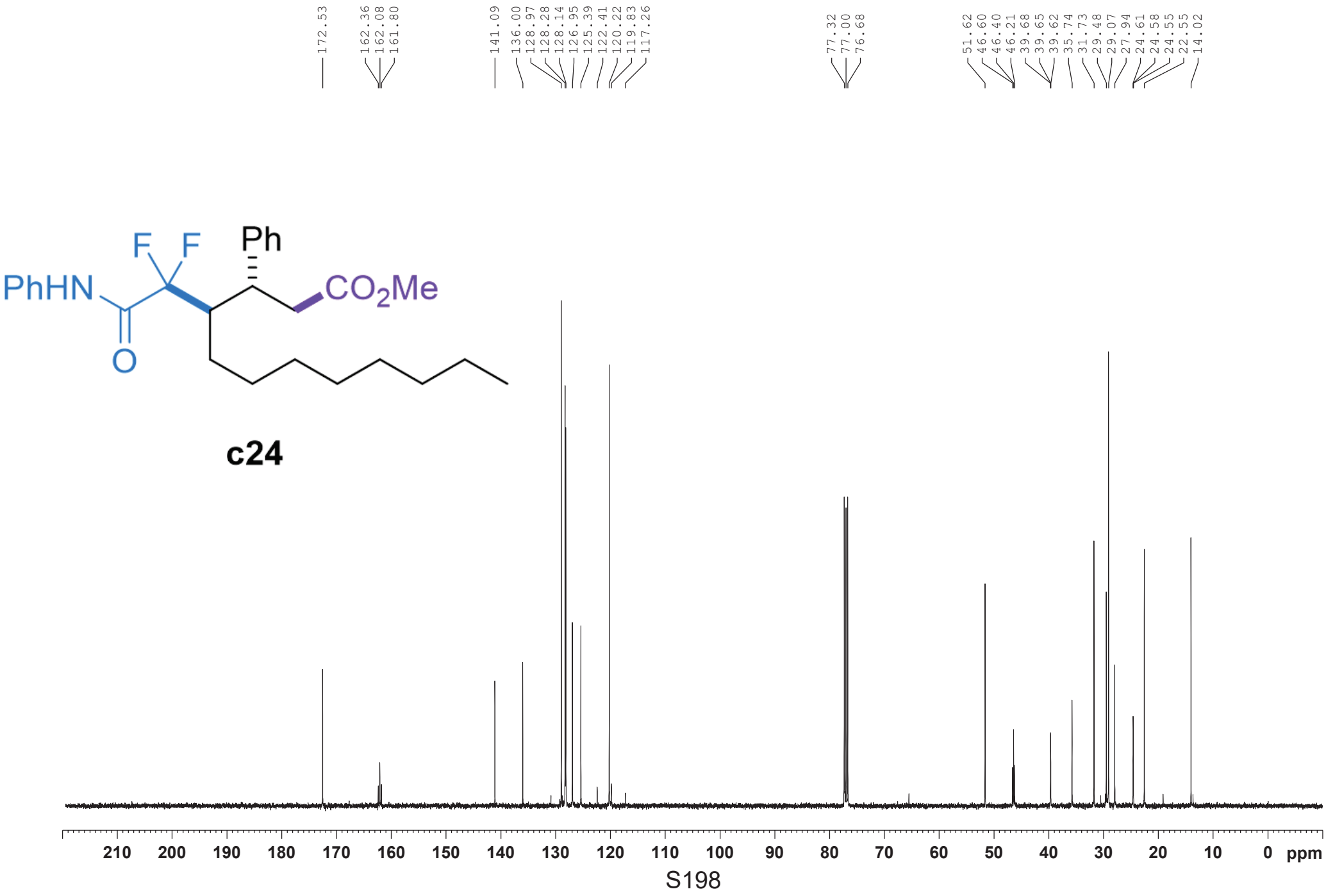

172.54
162.34
162.06
161.78
141.11
136.00
129.04
128.32
128.19
127.00
125.44
122.44
120.20
119.88
117.30
77.32
77.00
76.68
51.67
46.42
46.22
46.02
39.74
39.71
39.68
35.84
26.93
26.89
26.86
21.28
14.05
F
F
Ph
PhHN
CO2Me
O
c23
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

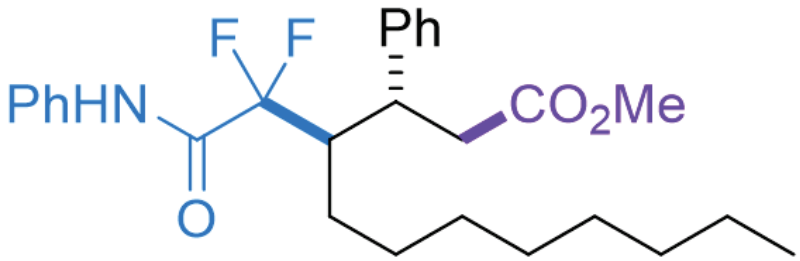

F
F
Ph
PhHN
CO2Me
O

c23

-104.605
-105.289
-109.142
-109.825
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.02

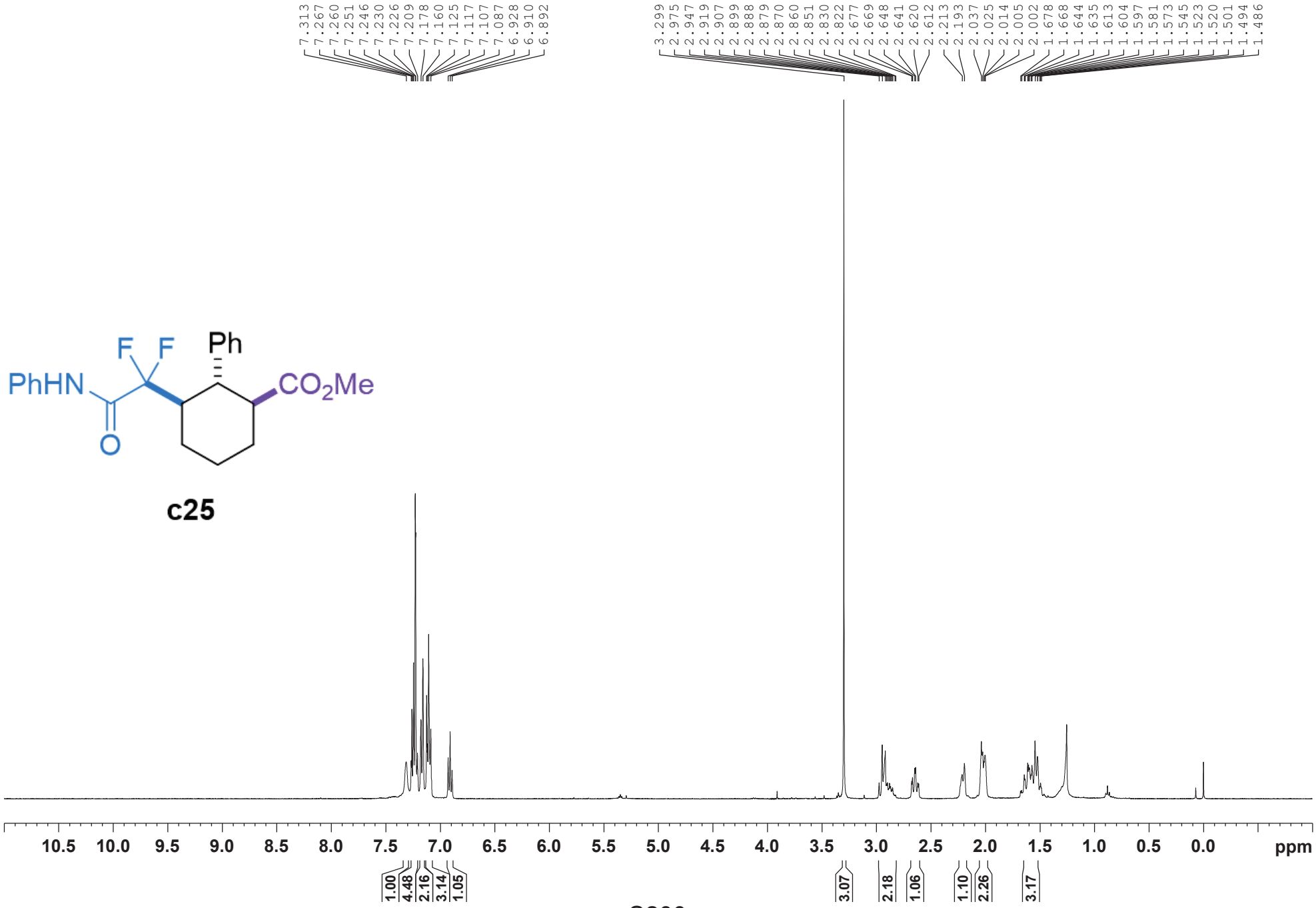

7.953
7.487
7.467
7.339
7.320
7.300
7.246
7.235
7.225
7.224
7.208
7.202
7.173
7.155
7.136
7.125
7.117
7.112
7.104
7.095
7.082
3.665
3.652
3.641
3.629
3.616
3.520
2.920
2.906
2.880
2.870
2.867
2.847
2.831
2.817
2.807
2.793
2.782
2.769
2.756
2.743
2.730
1.651
1.638
1.614
1.601
1.589
1.577
1.561
1.543
1.530
1.517
1.505
1.494
1.482
1.468
1.346
1.333
1.322
1.257
1.234
1.215
1.156
0.871
0.854
0.836
F
F
Ph
PhHN
CO2Me
O
c24
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.96
1.97
1.97
3.91
2.13
0.95
2.89
2.94
2.01
12.53
3.00

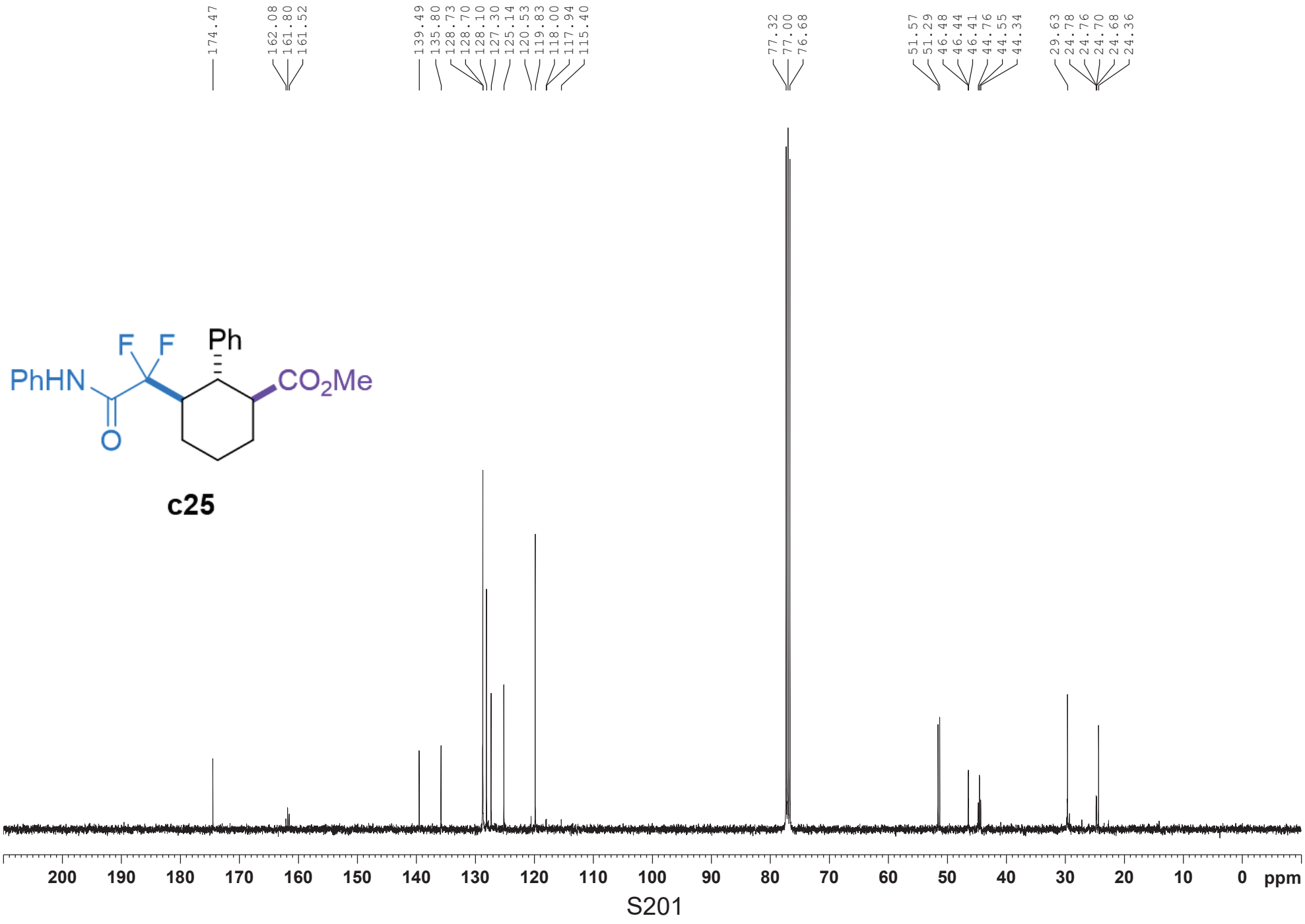

172.53
162.36
162.08
161.80
141.09
136.00
128.97
128.28
128.14
126.95
125.39
122.41
120.22
119.83
117.26
77.32
77.00
76.68
51.62
46.60
46.40
46.21
39.68
39.65
39.62
35.74
31.73
29.48
29.07
27.94
24.61
24.58
24.55
22.55
14.02
F
F
Ph
PhHN
CO2Me
O
c24
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

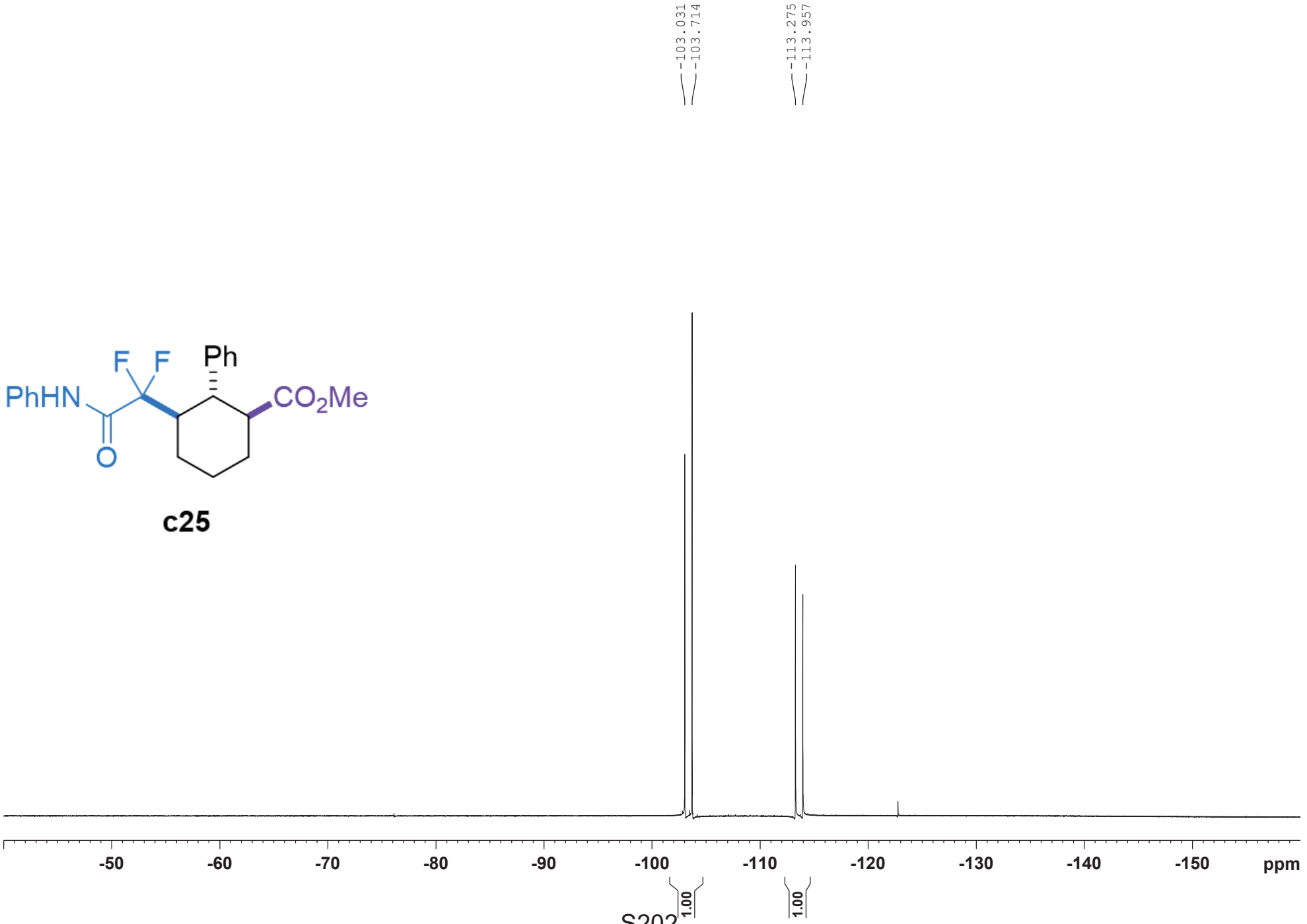

F
F
Ph
PhHN
CO2Me
O

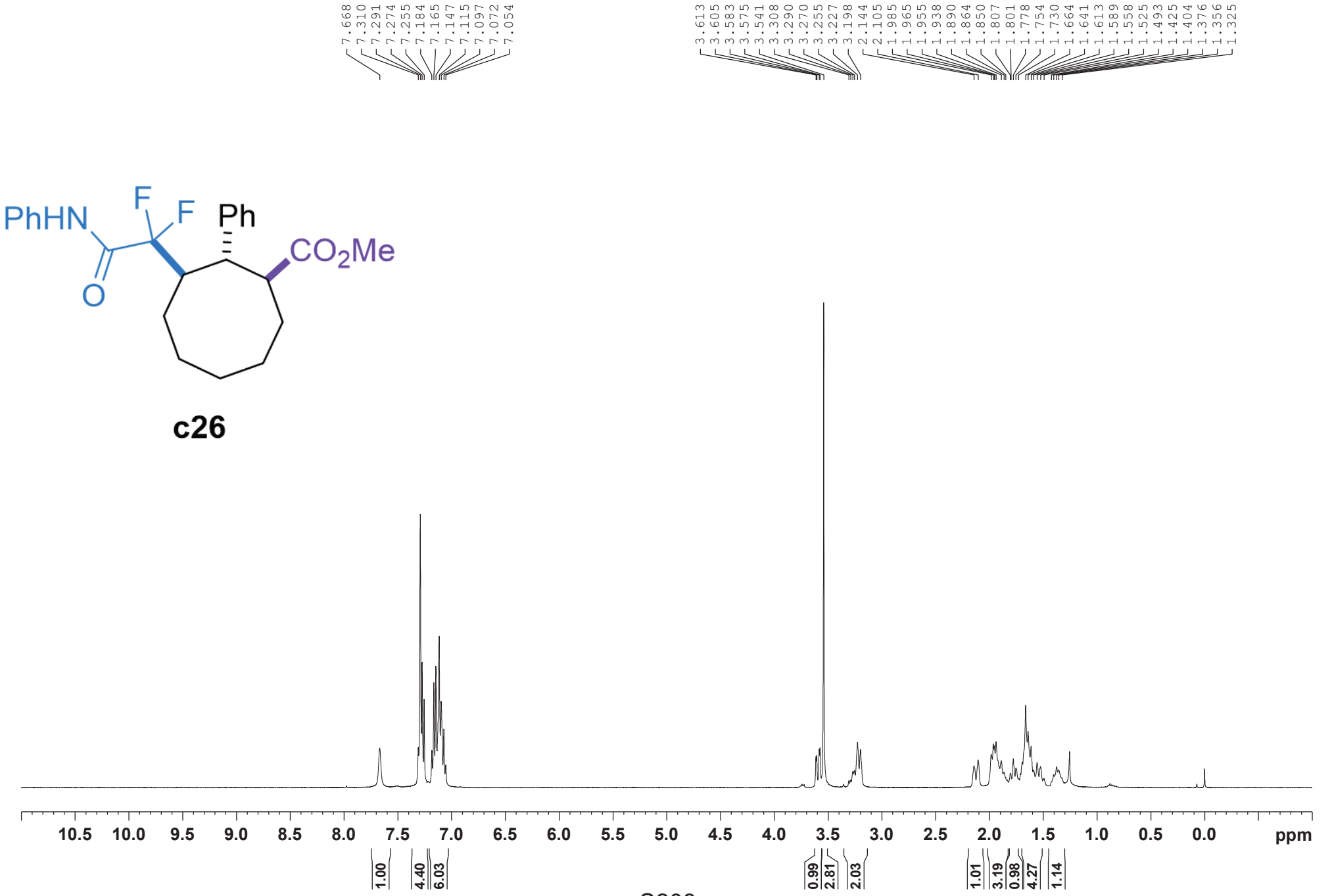
c24

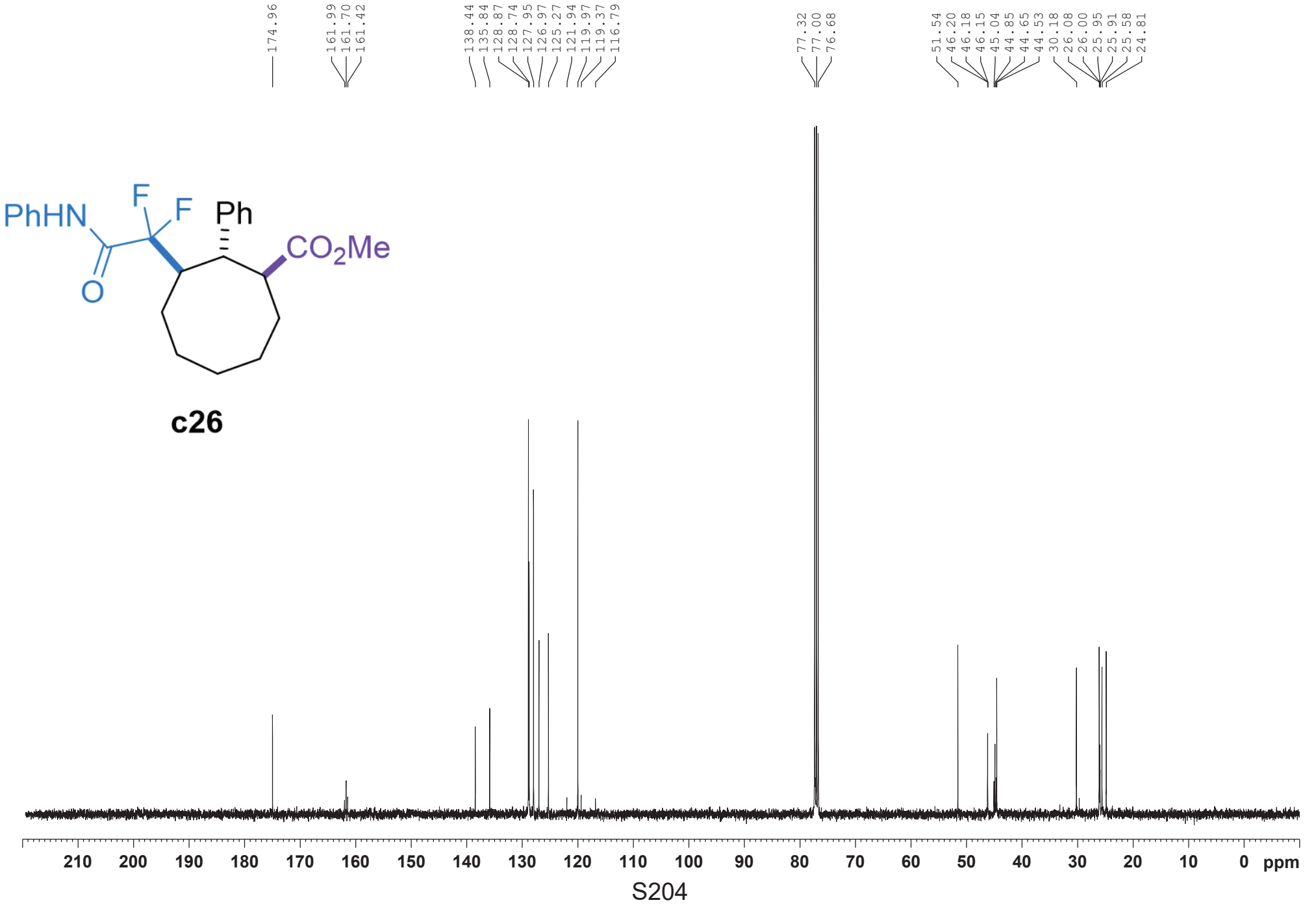
-104.862
-105.544
-108.950
-109.633
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.00

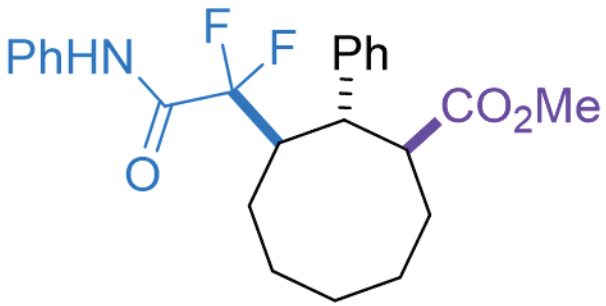

7.313
7.267
7.260
7.251
7.246
7.230
7.226
7.209
7.178
7.160
7.125
7.117
7.107
7.087
6.928
6.910
6.892
3.299
2.975
2.947
2.919
2.907
2.899
2.888
2.879
2.870
2.860
2.851
2.830
2.822
2.677
2.669
2.648
2.641
2.620
2.612
2.213
2.193
2.037
2.025
2.014
2.005
2.002
1.678
1.668
1.644
1.635
1.613
1.604
1.597
1.581
1.573
1.545
1.523
1.520
1.501
1.494
1.486
F
F
Ph
PhHN
CO2Me
O
c25
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.48
2.16
3.14
1.05
3.07
2.18
1.06
1.10
2.26
3.17


174.47
162.08
161.80
161.52
139.49
135.80
128.73
128.70
128.10
127.30
125.14
120.53
119.83
118.00
117.94
115.40
77.32
77.00
76.68
51.57
51.29
46.48
46.44
46.41
44.76
44.55
44.34
29.63
24.78
24.76
24.70
24.68
24.36
F
F
Ph
PhHN
CO2Me
O
c25
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-103.031
-103.714
-113.275
-113.957
F
F
Ph
PhHN
CO2Me
O
c25
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.00

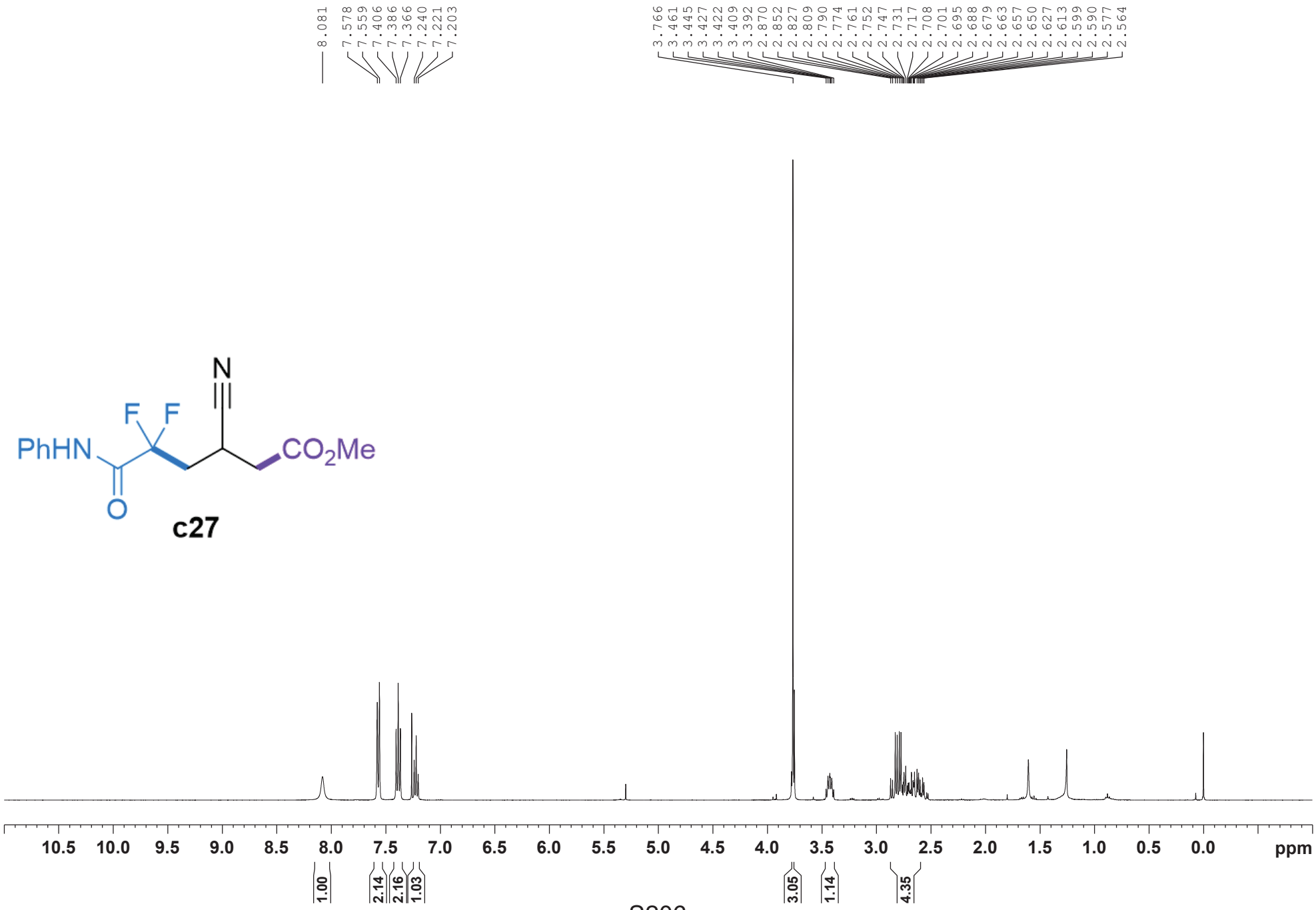

7.668
7.310
7.291
7.274
7.255
7.184
7.165
7.147
7.115
7.097
7.072
7.054
3.613
3.605
3.583
3.575
3.541
3.308
3.290
3.270
3.255
3.227
3.198
2.144
2.105
1.985
1.965
1.955
1.938
1.890
1.864
1.850
1.807
1.801
1.778
1.754
1.730
1.664
1.641
1.613
1.589
1.558
1.525
1.493
1.425
1.404
1.376
1.356
1.325
PhHN
F
F
Ph
CO2Me
O
c26
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
4.40
6.03
0.99
2.81
2.03
1.01
3.19
0.98
4.27
1.14

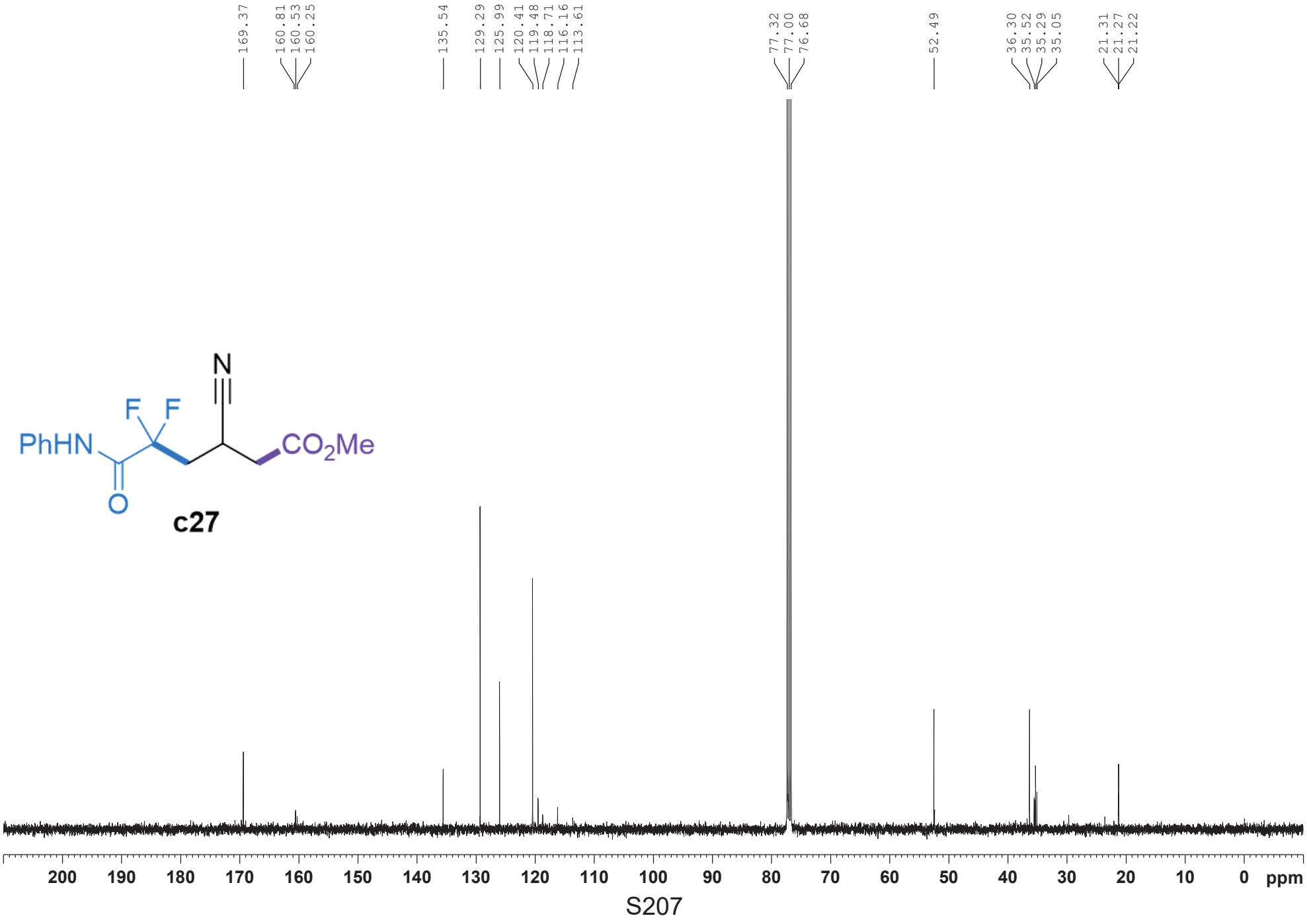

174.96
161.99
161.70
161.42
138.44
135.84
128.87
128.74
127.95
126.97
125.27
121.94
119.97
119.37
116.79
77.32
77.00
76.68
51.54
46.20
46.18
46.15
45.04
44.85
44.65
44.53
30.18
26.08
26.00
25.95
25.91
25.58
24.81
PhHN
F
F
Ph
CO2Me
O
c26
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

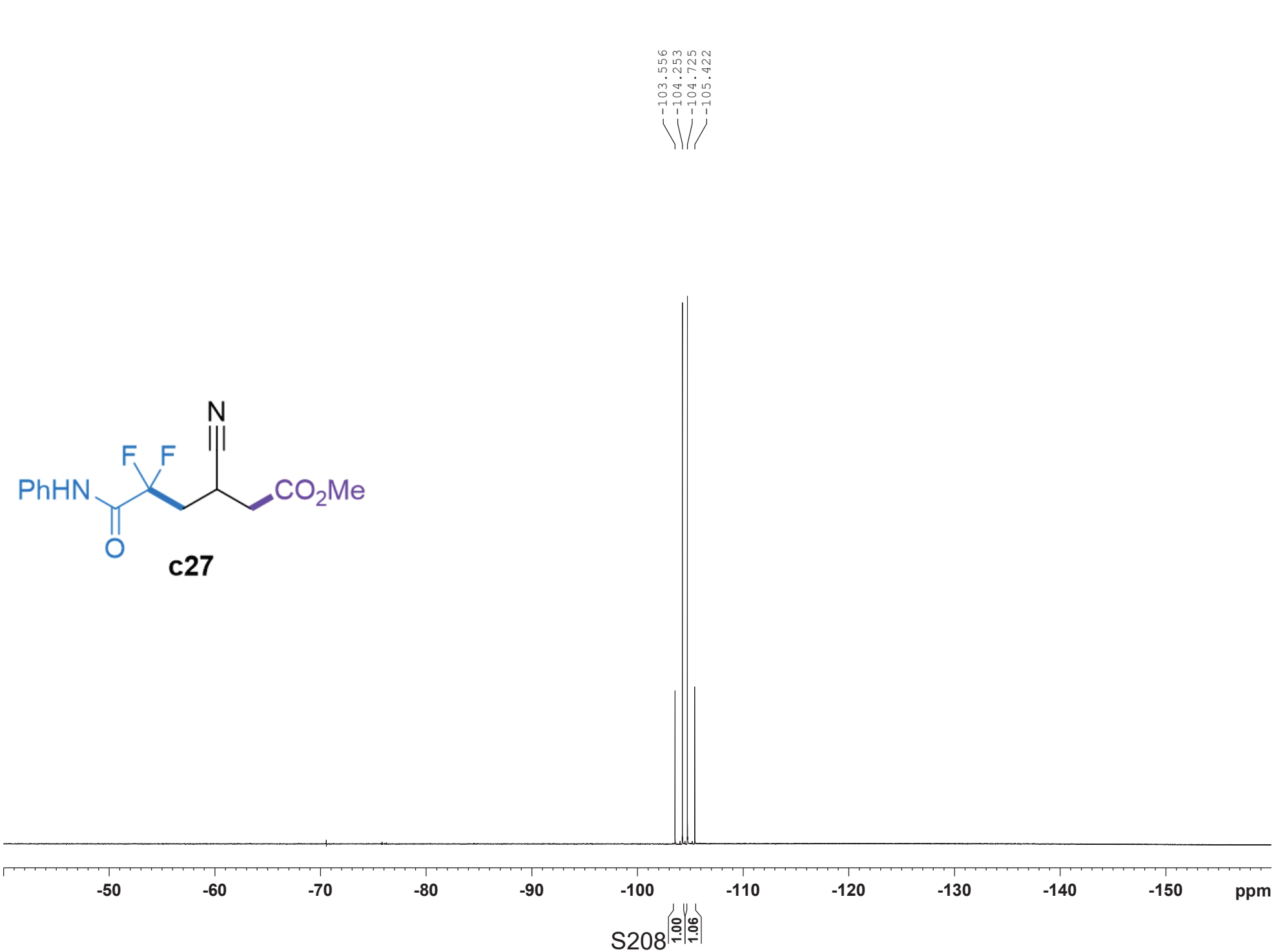

PhHN
F
F
Ph
CO2Me
O

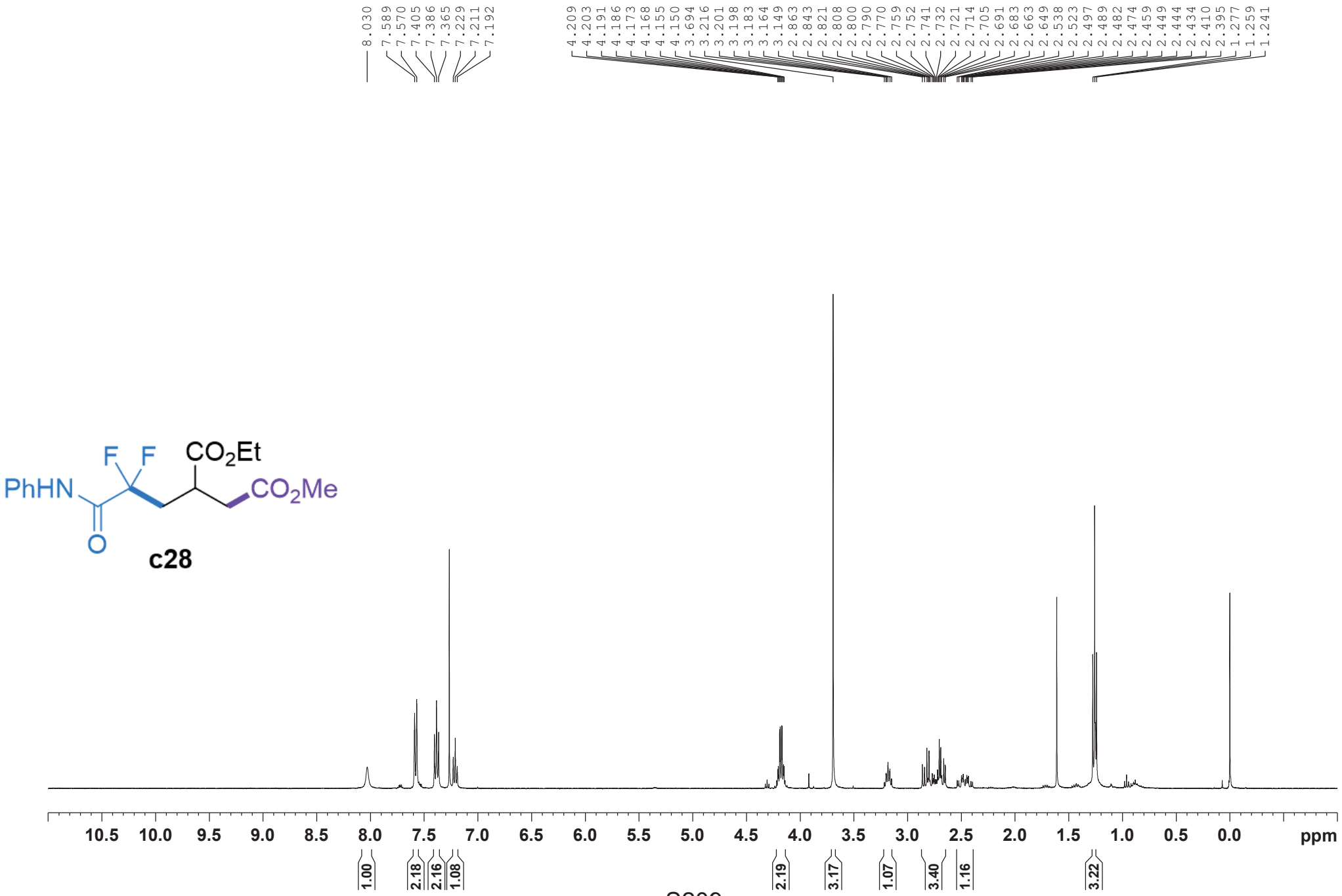
c26

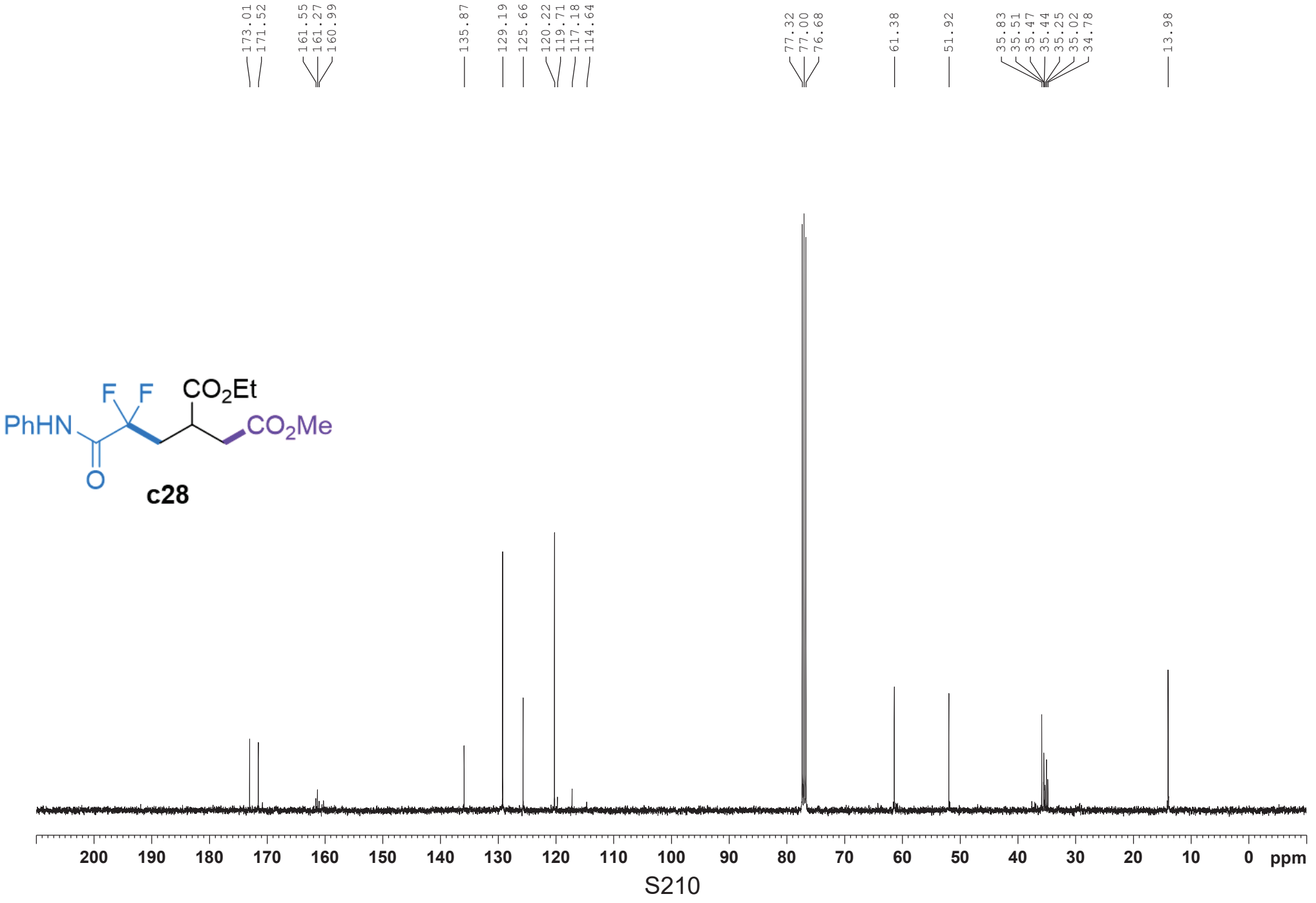
-106.308
-106.982
-107.939
-108.613
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
0.95

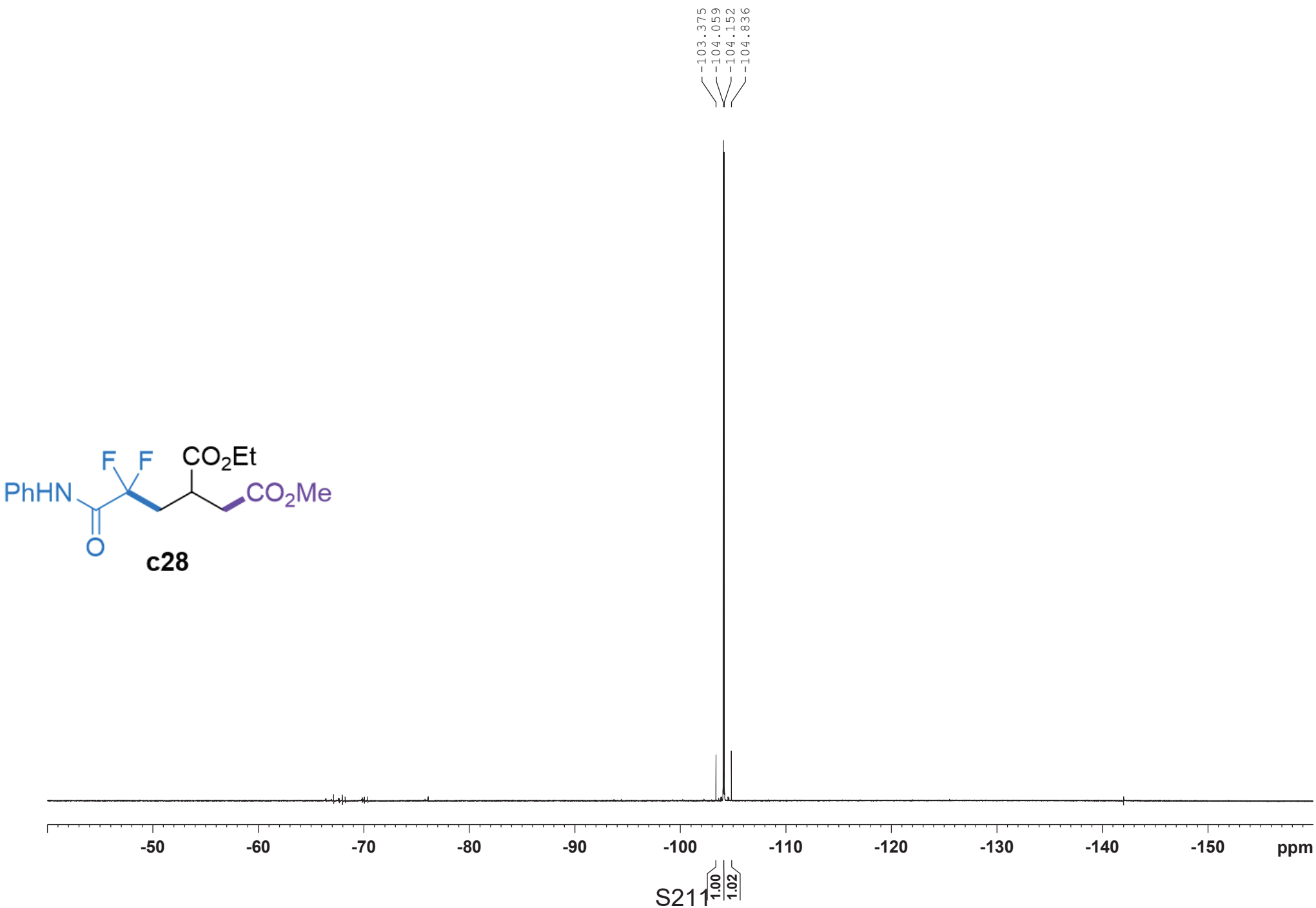

8.081
7.578
7.559
7.406
7.386
7.366
7.240
7.221
7.203
3.766
3.461
3.445
3.427
3.422
3.409
3.392
2.870
2.852
2.827
2.809
2.790
2.774
2.761
2.752
2.747
2.731
2.717
2.708
2.701
2.695
2.688
2.679
2.663
2.657
2.650
2.627
2.613
2.599
2.590
2.577
2.564
N
F
F
PhHN
CO2Me
O
c27
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.14
2.16
1.03
3.05
1.14
4.35

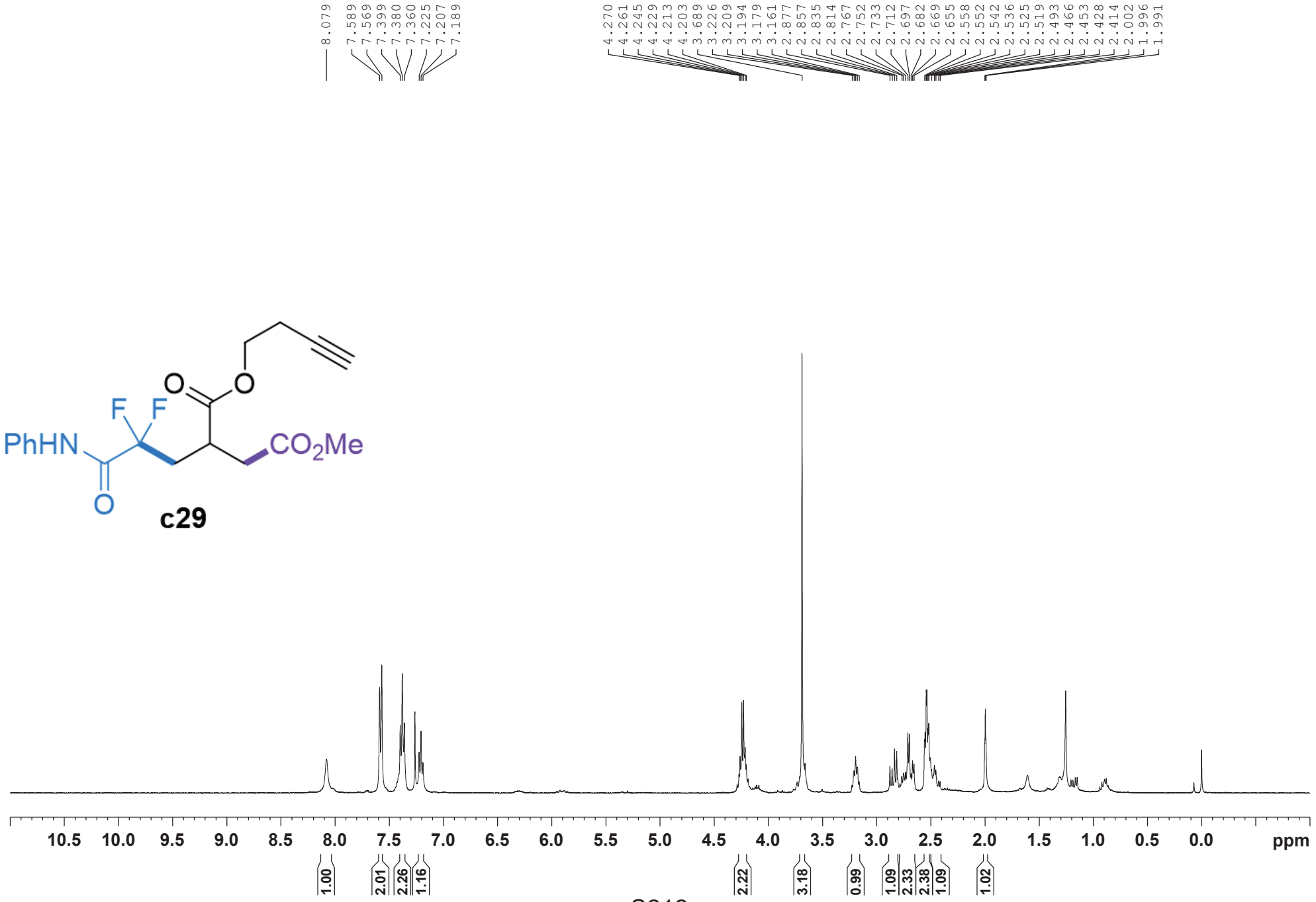

169.37
160.81
160.53
160.25
135.54
129.29
125.99
120.41
119.48
118.71
116.16
113.61
77.32
77.00
76.68
52.49
36.30
35.52
35.29
35.05
21.31
21.27
21.22
N
F
F
PhHN
CO2Me
O
c27
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

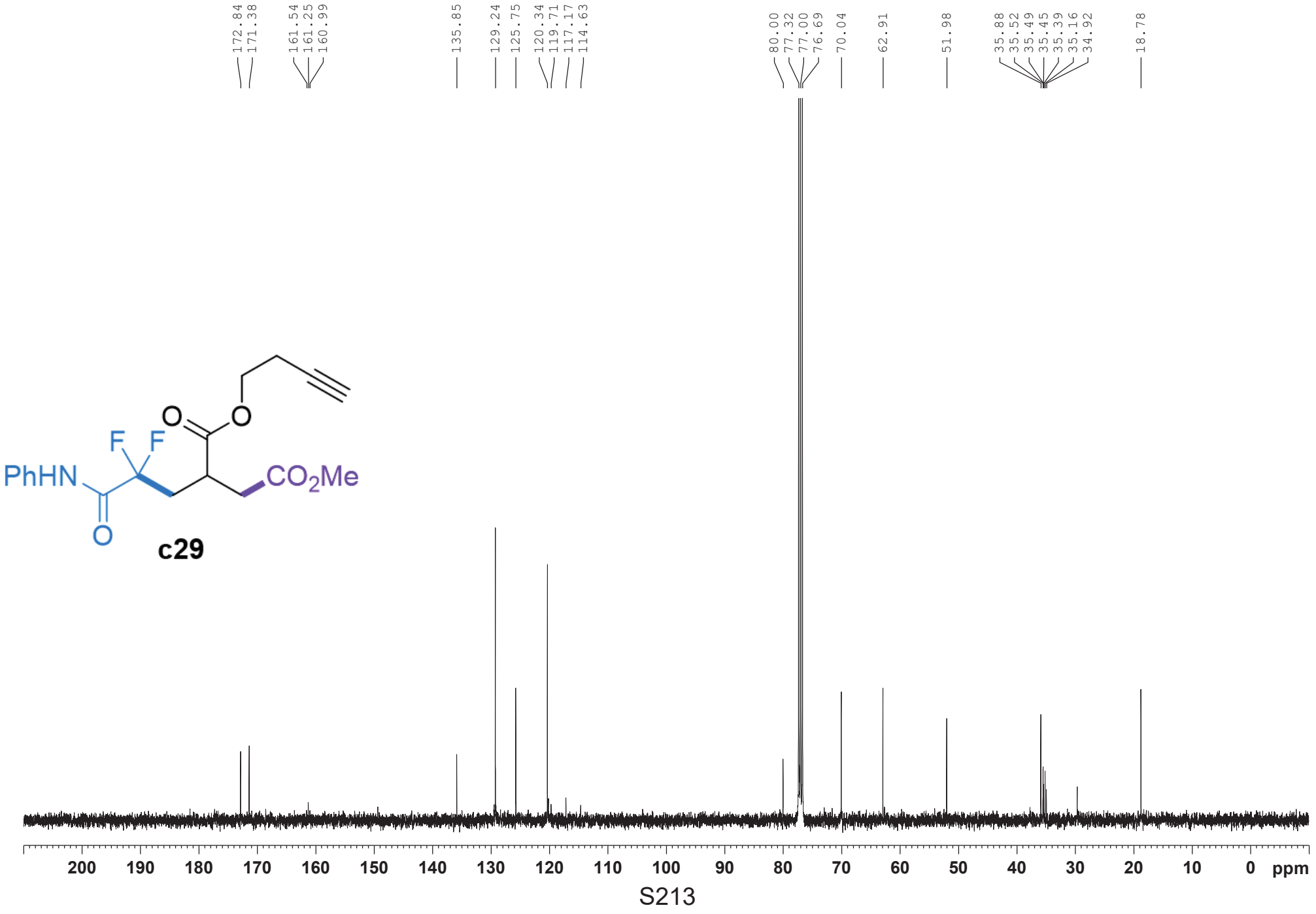

-103.556
-104.253
-104.725
-105.422
N
F F
PhHN
O
CO2Me
c27
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.06

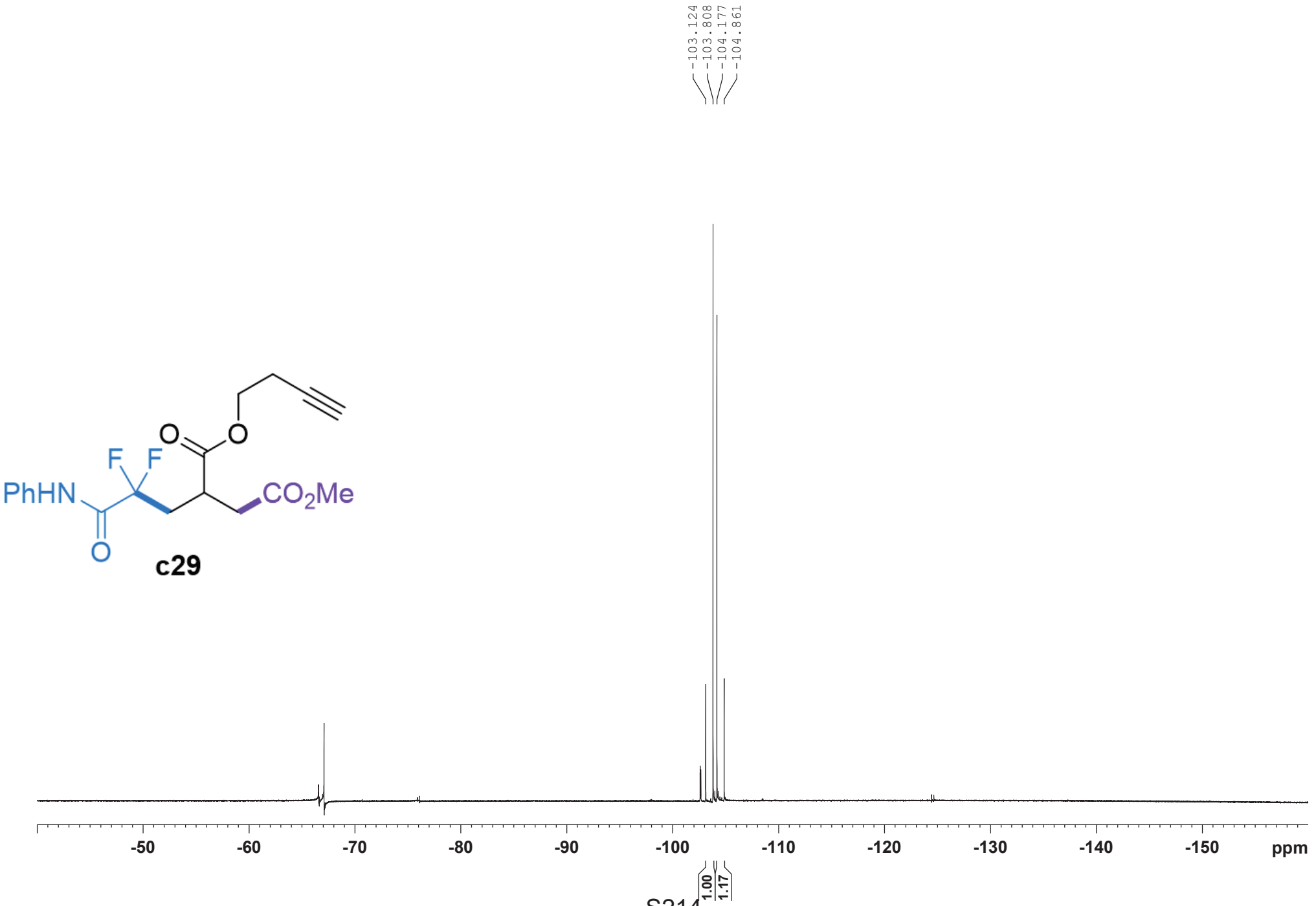

8.030
7.589
7.570
7.405
7.386
7.365
7.229
7.211
7.192
4.209
4.203
4.191
4.186
4.173
4.168
4.155
4.150
3.694
3.216
3.201
3.198
3.183
3.164
3.149
2.863
2.843
2.821
2.808
2.800
2.790
2.770
2.759
2.752
2.741
2.732
2.721
2.714
2.705
2.691
2.683
2.663
2.649
2.538
2.523
2.497
2.489
2.482
2.474
2.459
2.449
2.444
2.434
2.410
2.395
1.277
1.259
1.241
F
F
CO2Et
PhHN
CO2Me
O
c28
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.18
2.16
1.08
2.19
3.17
1.07
3.40
1.16
3.22

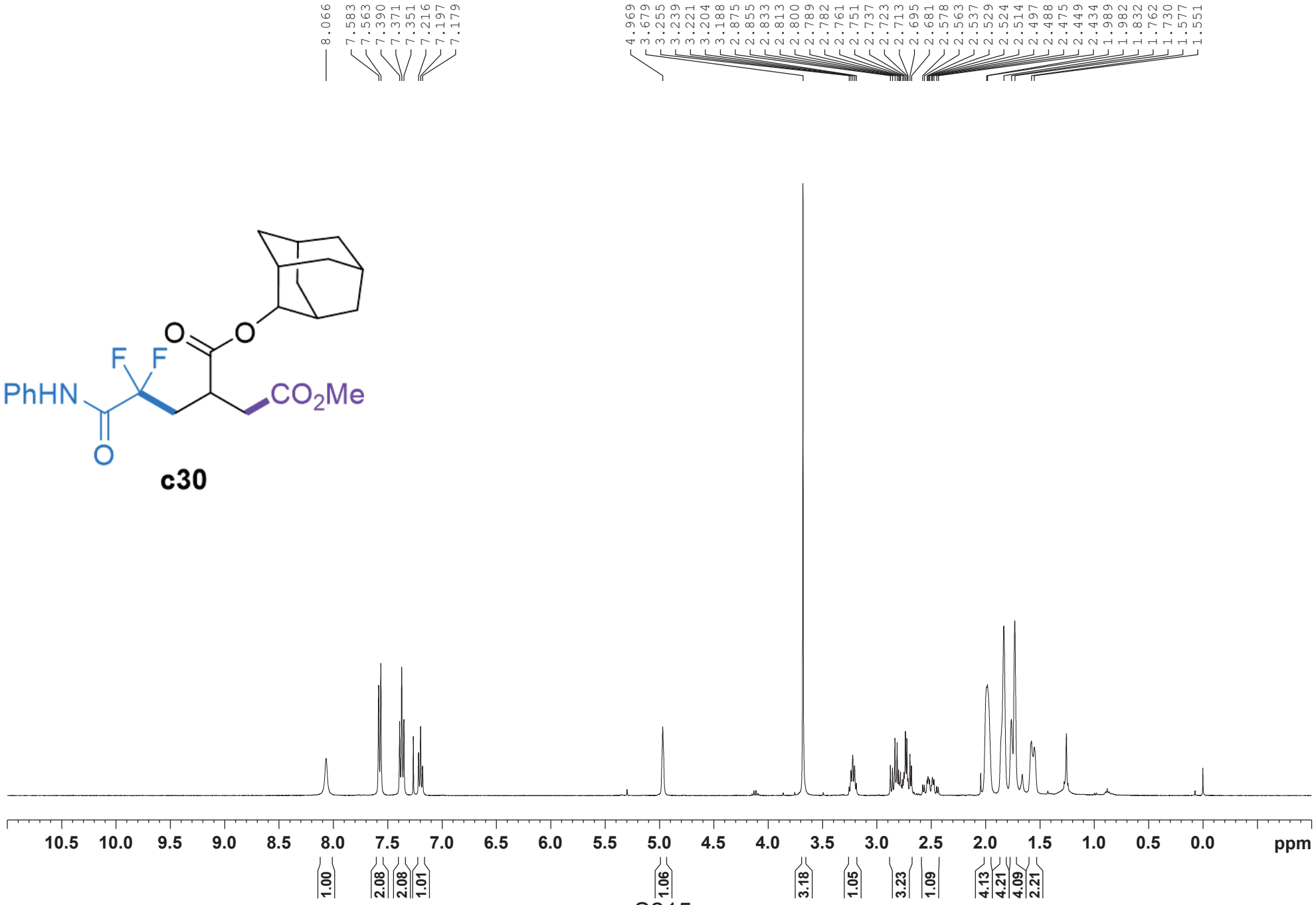

173.01
171.52
161.55
161.27
160.99
135.87
129.19
125.66
120.22
119.71
117.18
114.64
77.32
77.00
76.68
61.38
51.92
35.83
35.51
35.47
35.44
35.25
35.02
34.78
13.98
F
F
CO2Et
PhHN
CO2Me
O
c28
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

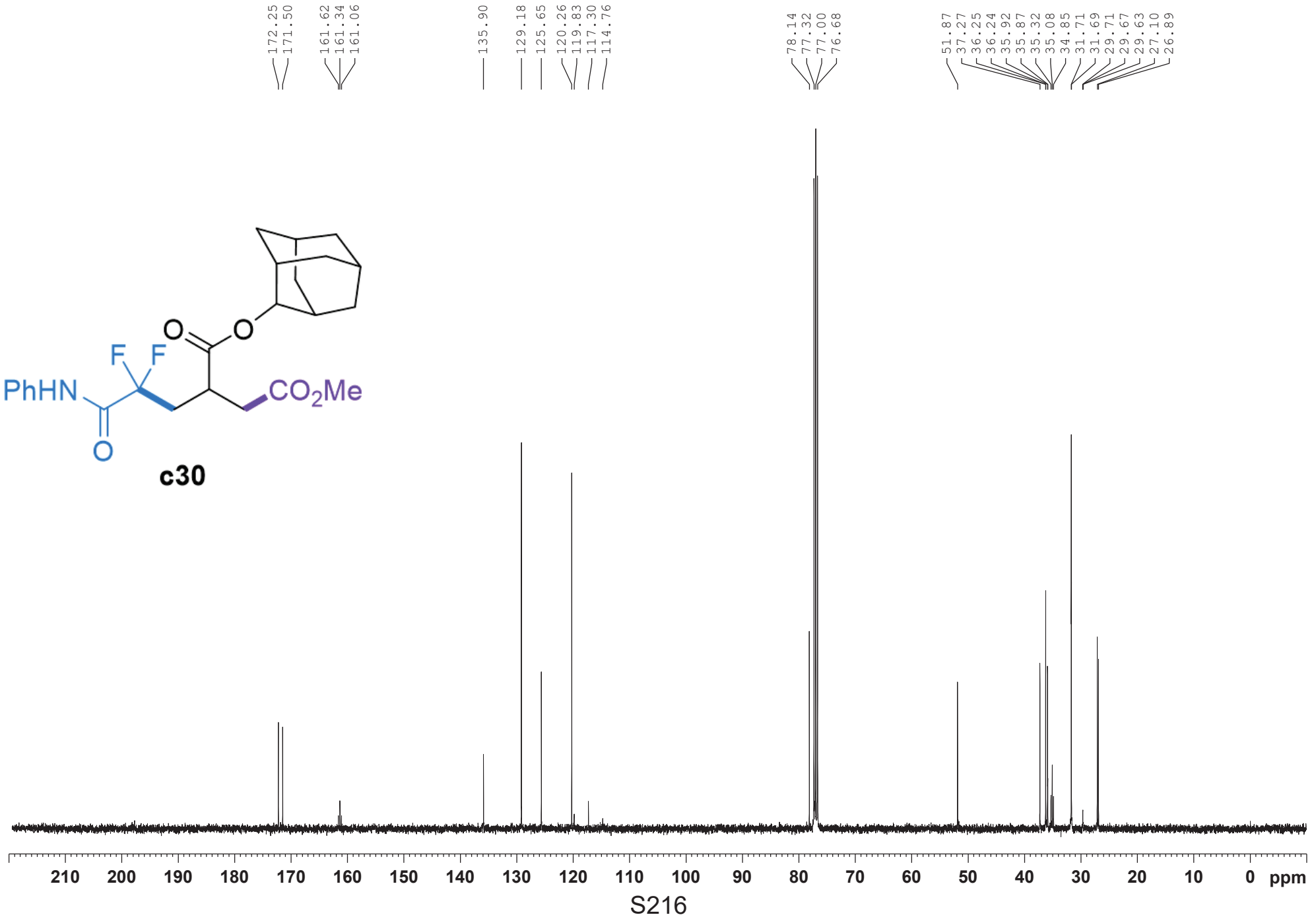

-103.375
-104.059
-104.152
-104.836
F
F
CO2Et
PhHN
CO2Me
O
c28
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.02

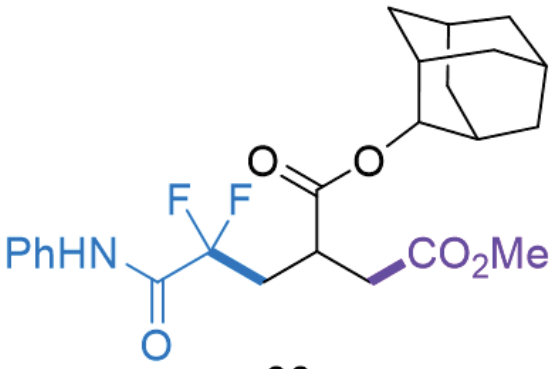

8.079
7.589
7.569
7.399
7.380
7.360
7.225
7.207
7.189
4.270
4.261
4.245
4.229
4.213
4.203
3.689
3.226
3.209
3.194
3.179
3.161
2.877
2.857
2.835
2.814
2.767
2.752
2.733
2.712
2.697
2.682
2.669
2.655
2.558
2.552
2.542
2.536
2.525
2.519
2.493
2.466
2.453
2.428
2.414
2.002
1.996
1.991
PhHN
F
F
O
O
O
CO2Me
c29
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.01
2.26
1.16
2.22
3.18
0.99
1.09
2.33
2.38
1.09
1.02


172.84
171.38
161.54
161.25
160.99
135.85
129.24
125.75
120.34
119.71
117.17
114.63
80.00
77.32
77.00
76.69
70.04
62.91
51.98
35.88
35.52
35.49
35.45
35.39
35.16
34.92
18.78
PhHN
F
F
O
O
O
CO2Me
c29
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-103.124
-103.808
-104.177
-104.861
PhHN
F
F
O
O
O
CO2Me
c29
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.17

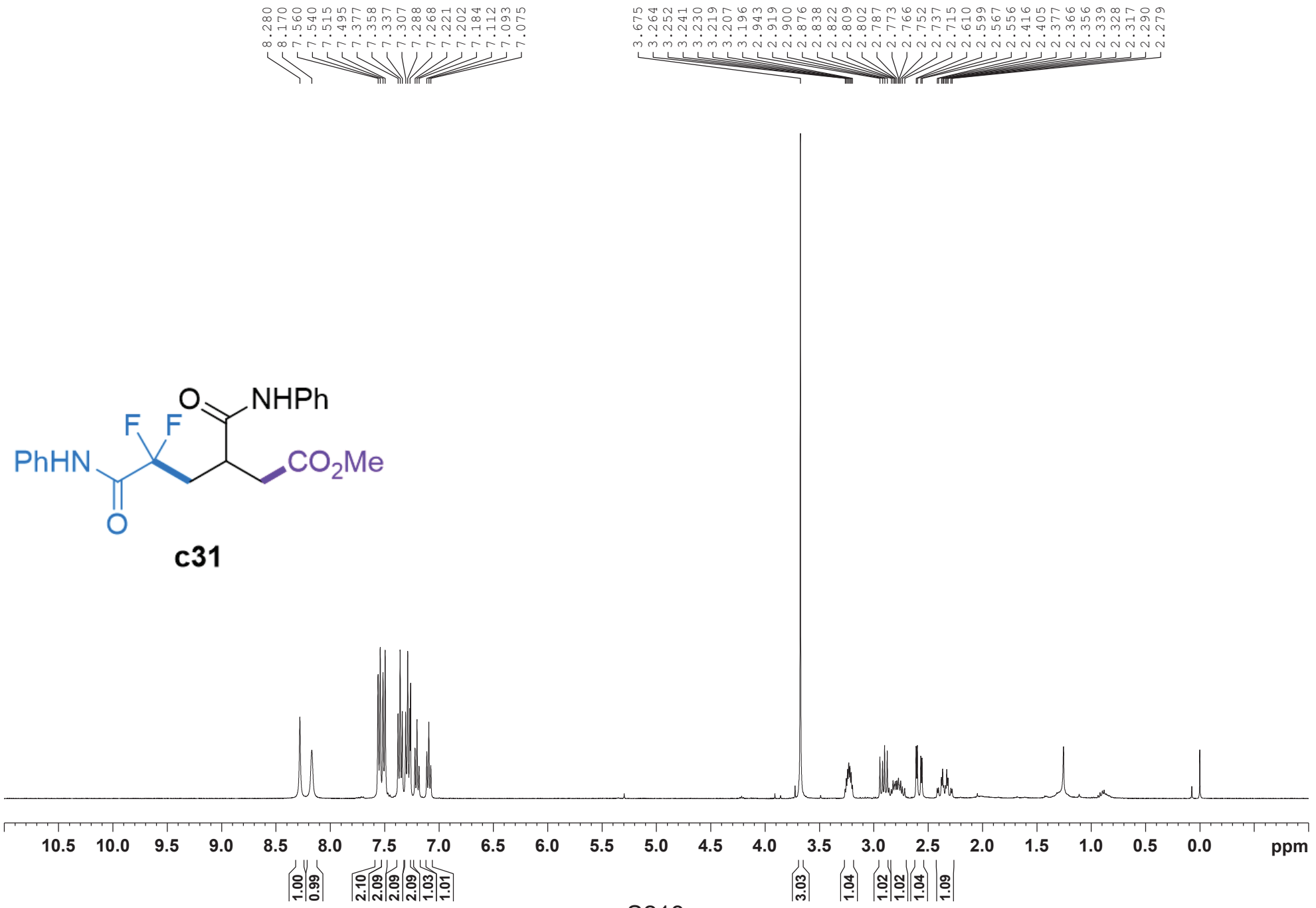

8.066
7.583
7.563
7.390
7.371
7.351
7.216
7.197
7.179
4.969
3.679
3.255
3.239
3.221
3.204
3.188
2.875
2.855
2.833
2.813
2.800
2.789
2.782
2.761
2.751
2.737
2.723
2.713
2.695
2.681
2.578
2.563
2.537
2.529
2.524
2.514
2.497
2.488
2.475
2.449
2.434
1.989
1.982
1.832
1.762
1.730
1.577
1.551
PhHN
F
F
O
O
O
CO2Me
c30
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.08
2.08
1.01
1.06
3.18
1.05
3.23
1.09
4.13
4.21
4.09
2.21

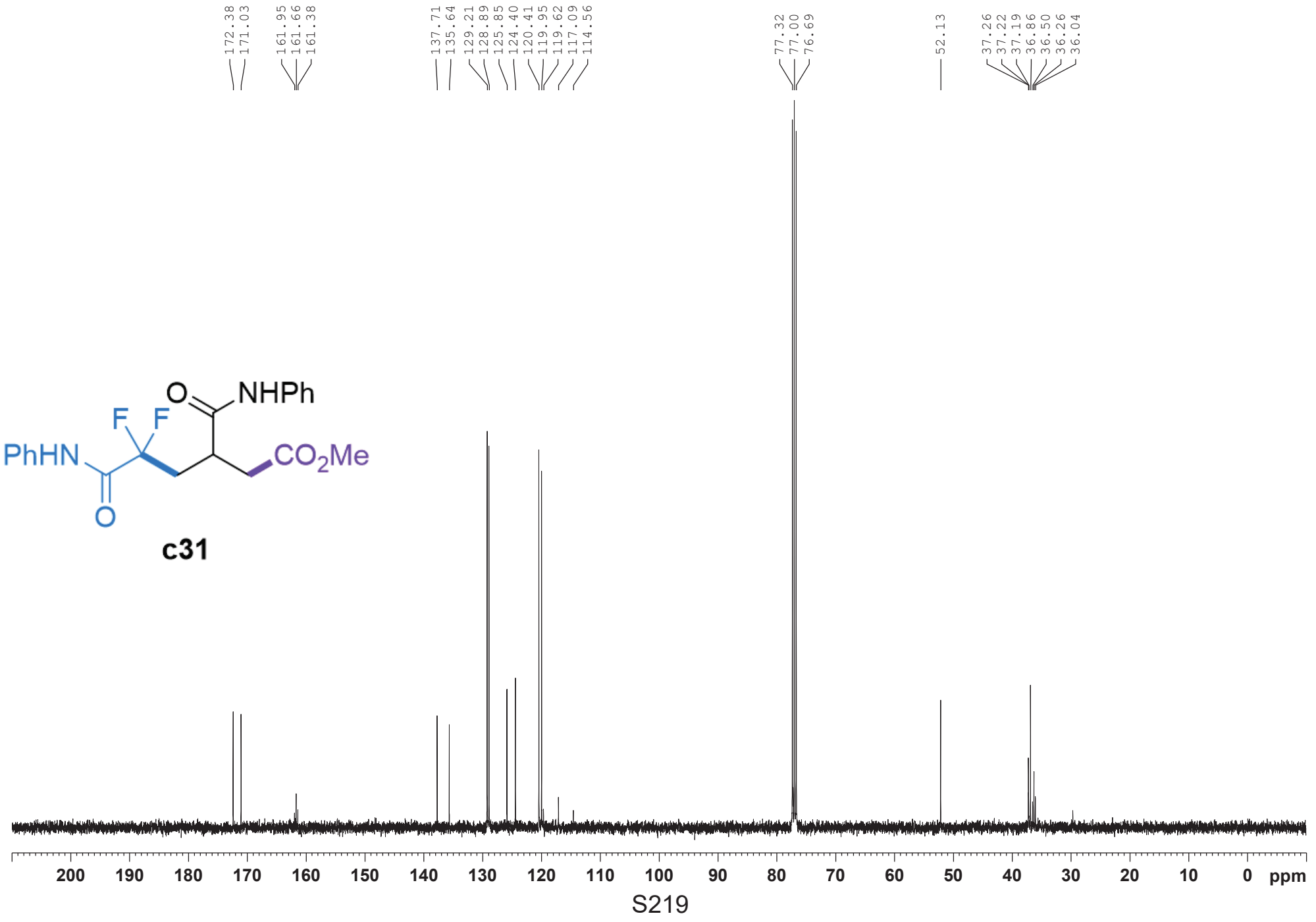

172.25
171.50
161.62
161.34
161.06
135.90
129.18
125.65
120.26
119.83
117.30
114.76
78.14
77.32
77.00
76.68
51.87
37.27
36.25
36.24
35.92
35.87
35.32
35.08
34.85
31.71
31.69
29.71
29.67
29.63
27.10
26.89
PhHN
F
F
O
O
O
CO2Me
c30
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

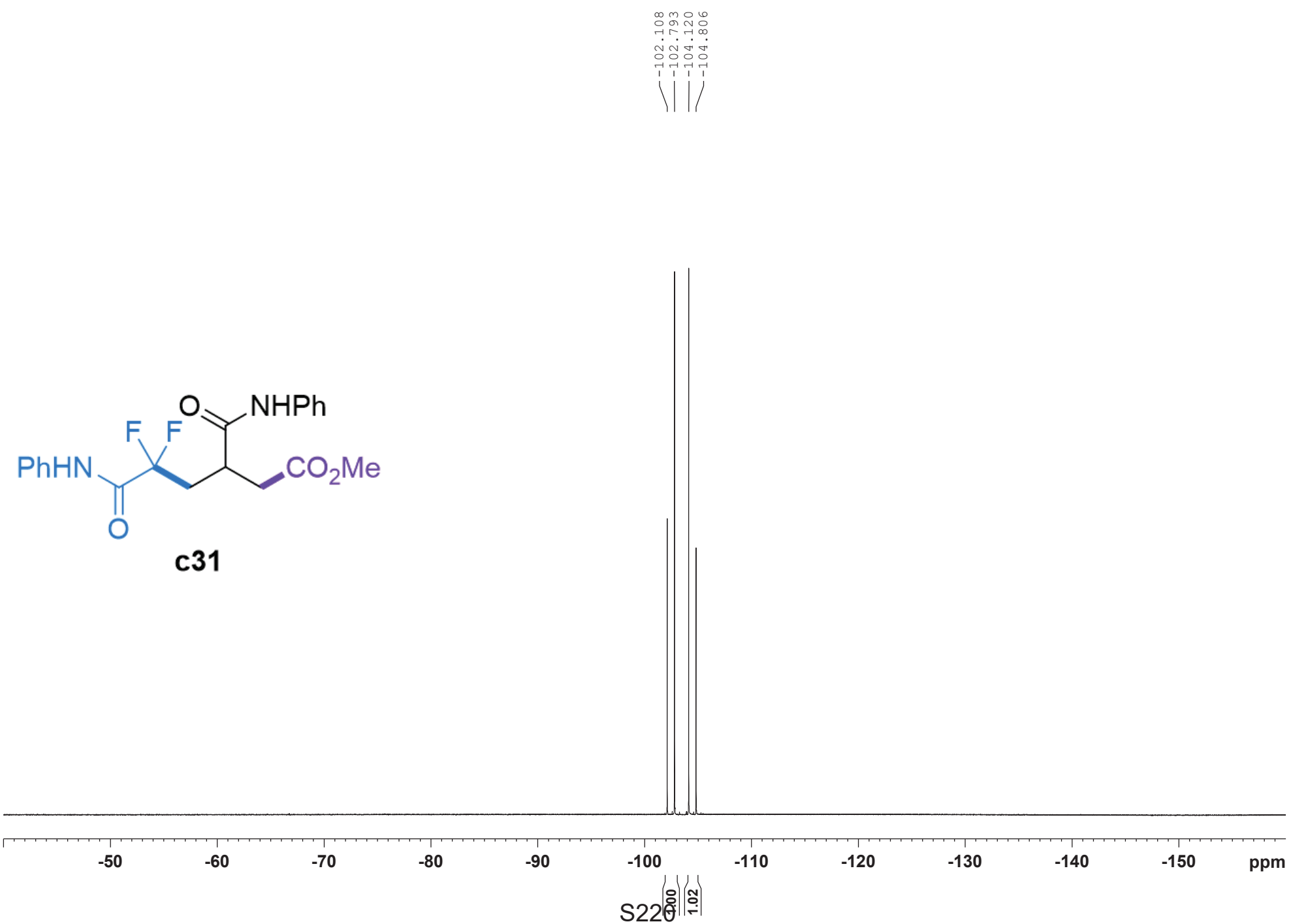

PhHN
F
F
O
O
O
CO2Me

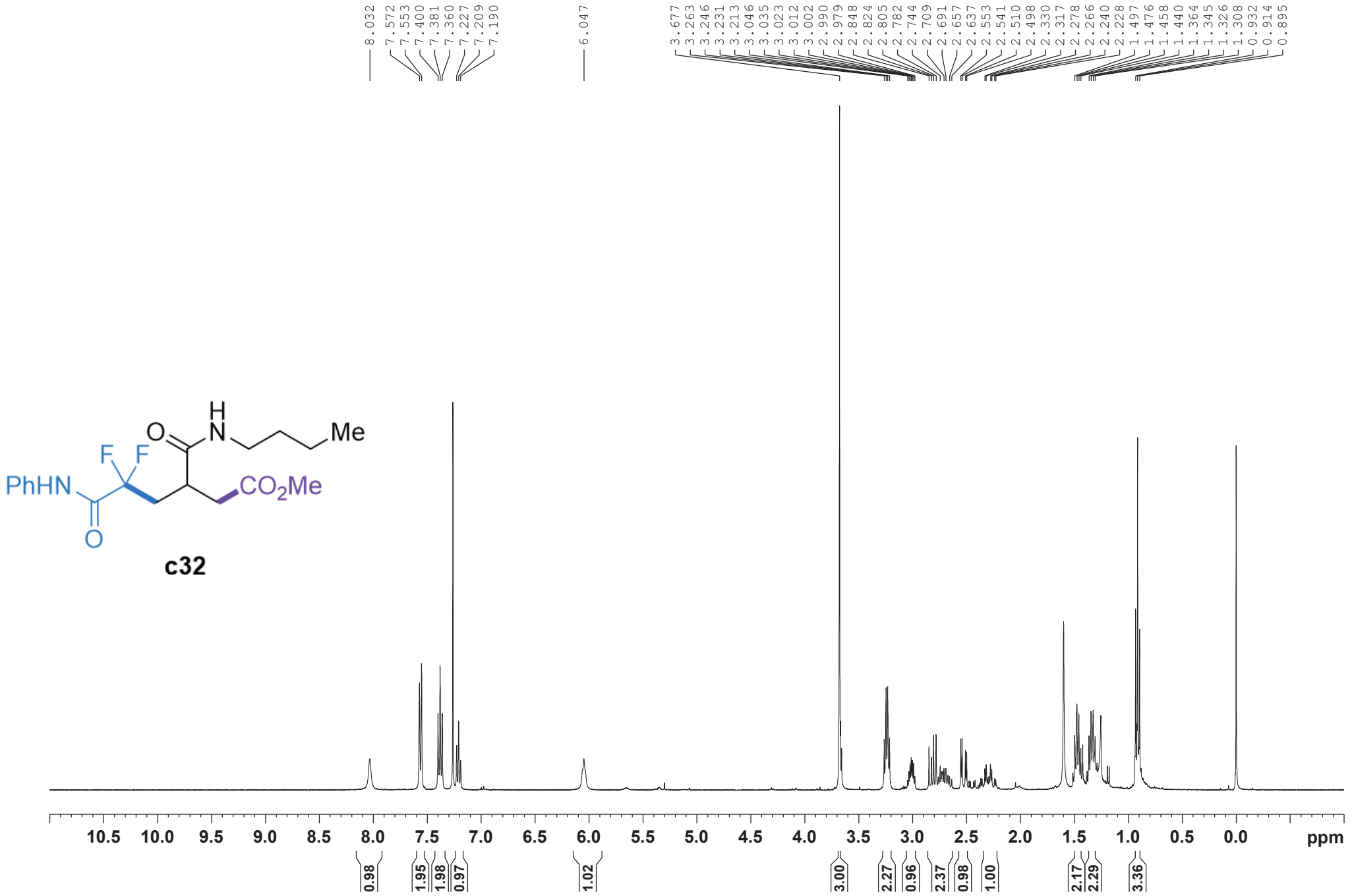
c30

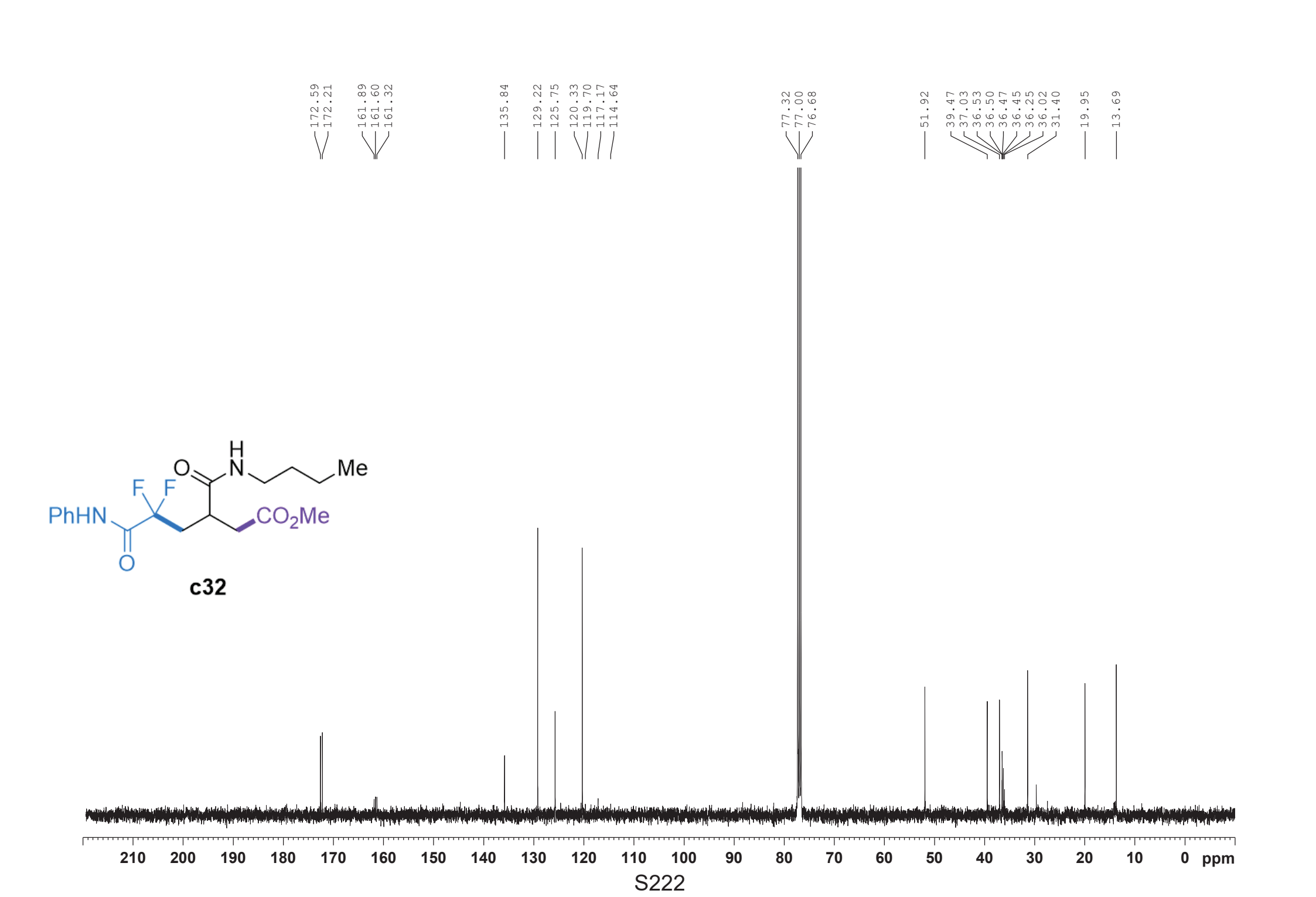
-103.299
-103.982
-104.046
-104.728
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
0.95

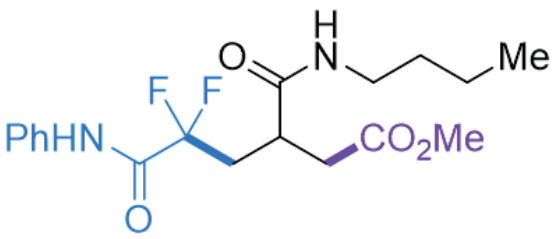

8.280
8.170
7.560
7.540
7.515
7.495
7.377
7.358
7.337
7.307
7.288
7.268
7.221
7.202
7.184
7.112
7.093
7.075
3.675
3.264
3.252
3.241
3.230
3.219
3.207
3.196
2.943
2.919
2.900
2.876
2.838
2.822
2.809
2.802
2.787
2.773
2.766
2.752
2.737
2.715
2.610
2.599
2.567
2.556
2.416
2.405
2.377
2.366
2.356
2.339
2.328
2.317
2.290
2.279
O
NHPh
F
F
PhHN
CO2Me
O
c31
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
0.99
2.10
2.09
2.09
2.09
1.03
1.01
3.03
1.04
1.02
1.02
1.04
1.09


172.38
171.03
161.95
161.66
161.38
137.71
135.64
129.21
128.89
125.85
124.40
120.41
119.95
119.62
117.09
114.56
77.32
77.00
76.69
52.13
37.26
37.22
37.19
36.86
36.50
36.26
36.04
O
NHPh
F
F
PhHN
CO2Me
O
c31
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-102.108
-102.793
-104.120
-104.806
O
NHPh
F
F
PhHN
CO2Me
O
c31
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.02

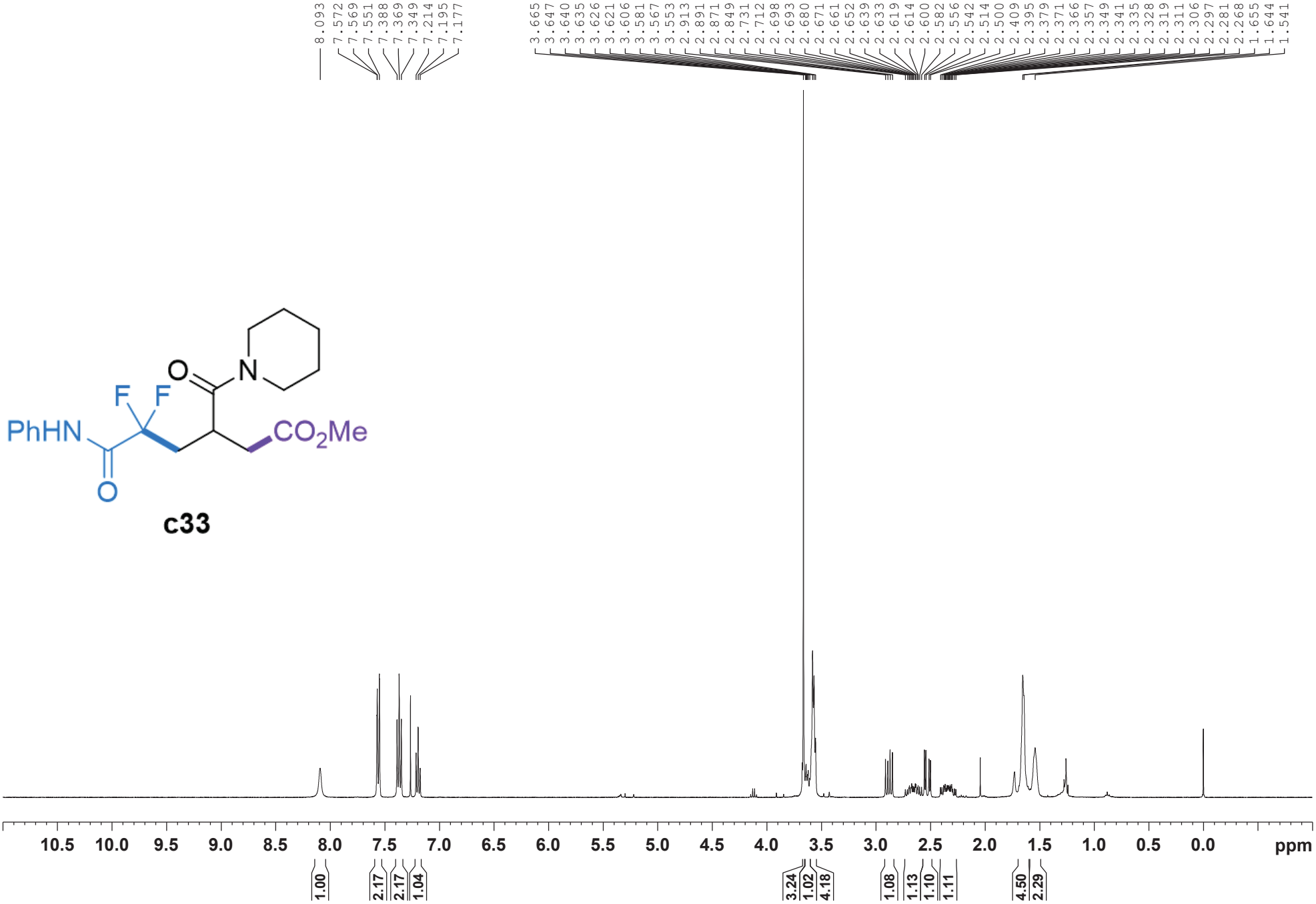

8.032
7.572
7.553
7.400
7.381
7.360
7.227
7.209
7.190
6.047
3.677
3.263
3.246
3.231
3.213
3.046
3.035
3.023
3.012
3.002
2.990
2.979
2.848
2.824
2.805
2.782
2.744
2.709
2.691
2.657
2.637
2.553
2.541
2.510
2.498
2.330
2.317
2.278
2.266
2.240
2.228
1.497
1.476
1.458
1.440
1.364
1.345
1.326
1.308
0.932
0.914
0.895
PhHN
F
F
O
H
N
Me
CO2Me
O
c32
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
0.98
1.95
1.98
0.97
1.02
3.00
2.27
0.96
2.37
0.98
1.00
2.17
2.29
3.36

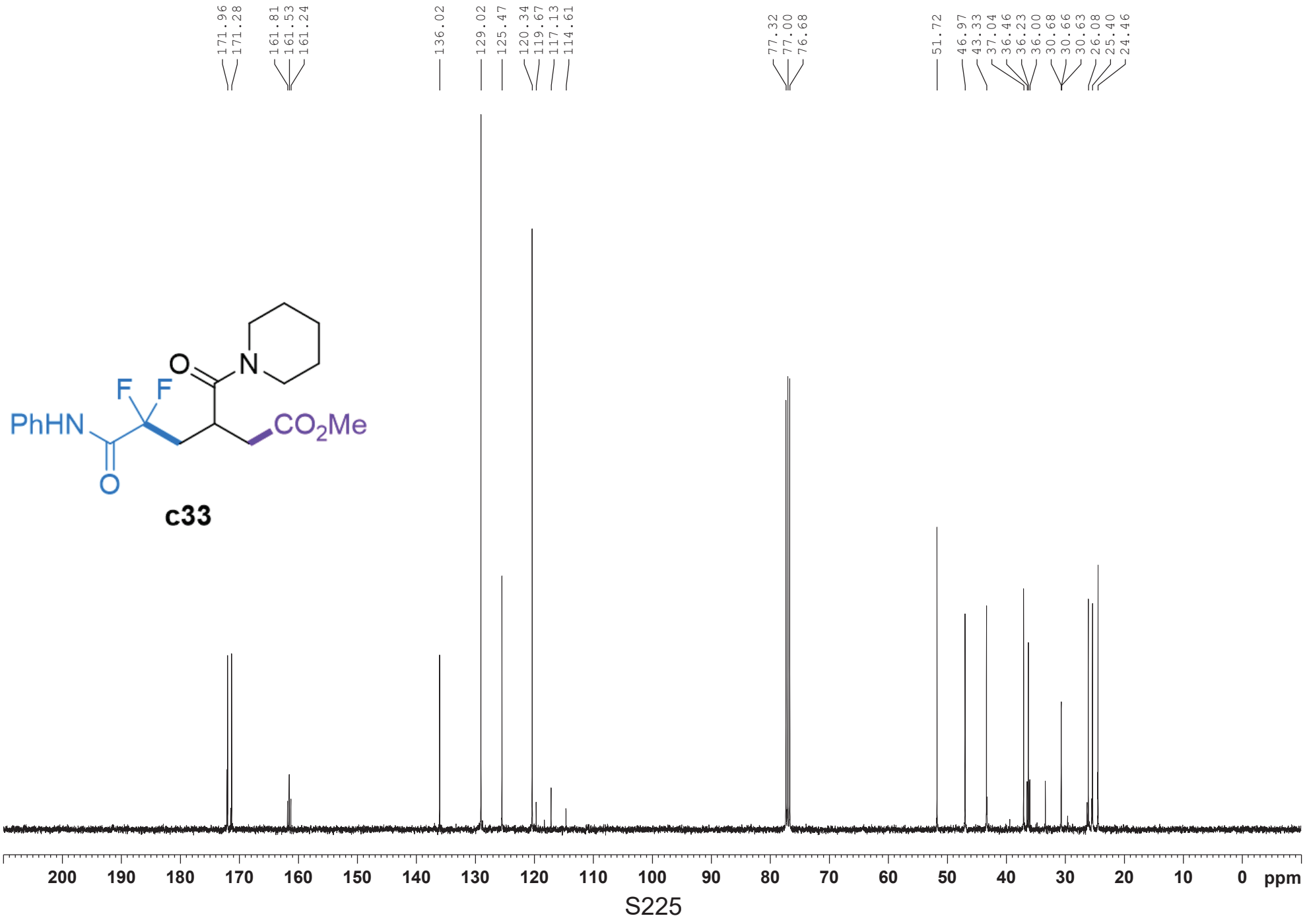

172.59
172.21
161.89
161.60
161.32
135.84
129.22
125.75
120.33
119.70
117.17
114.64
77.32
77.00
76.68
51.92
39.47
37.03
36.53
36.50
36.47
36.45
36.25
36.02
31.40
19.95
13.69
PhHN
F
F
O
H
N
Me
CO2Me
O
c32
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

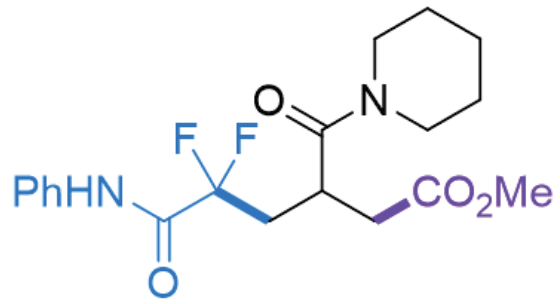

PhHN
F
F
O
H
N
Me
CO2Me
O

c32

-102.824
-103.507
-104.393
-105.075
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
0.91

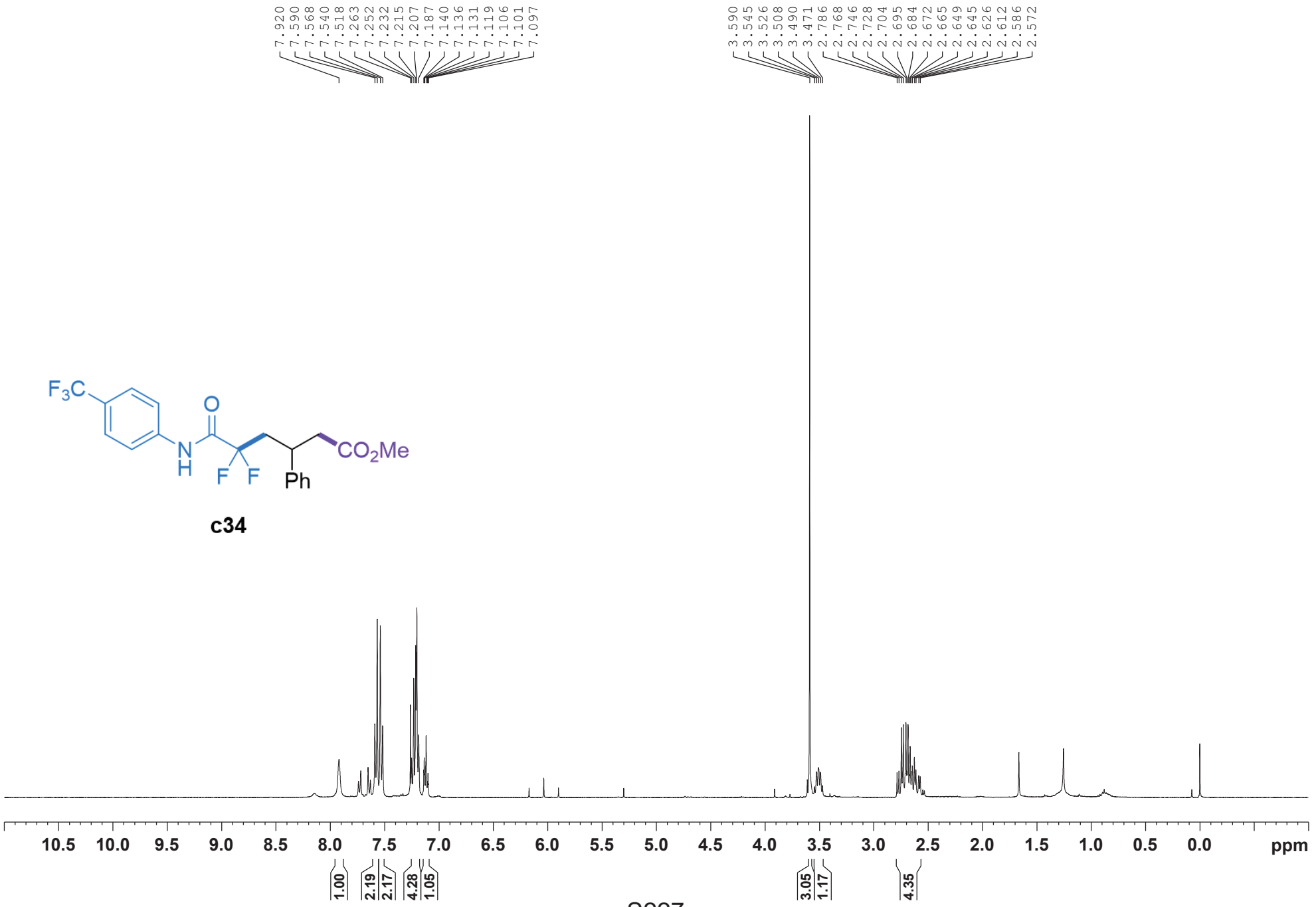

8.093
7.572
7.569
7.551
7.388
7.369
7.349
7.214
7.195
7.177
3.665
3.647
3.640
3.635
3.626
3.621
3.606
3.581
3.567
3.553
2.913
2.891
2.871
2.849
2.731
2.712
2.698
2.693
2.680
2.671
2.661
2.652
2.639
2.633
2.619
2.614
2.600
2.582
2.556
2.542
2.514
2.500
2.409
2.395
2.379
2.371
2.366
2.357
2.349
2.341
2.335
2.328
2.319
2.311
2.306
2.297
2.281
2.268
1.655
1.644
1.541
O
N
F
F
PhHN
CO2Me
O
c33
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.17
2.17
1.04
3.24
1.02
4.18
1.08
1.13
1.10
1.11
4.50
2.29

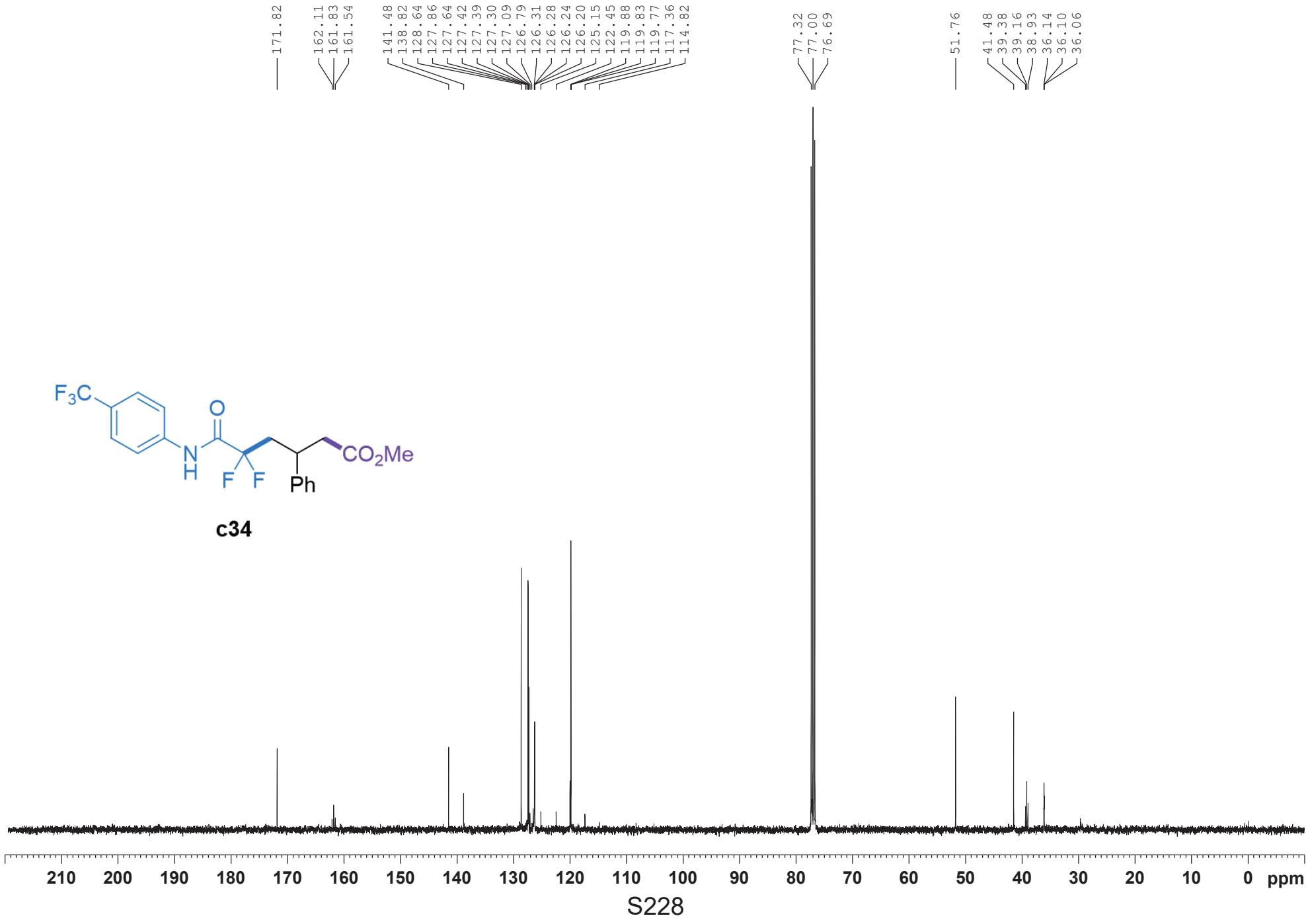

171.96
171.28
161.81
161.53
161.24
136.02
129.02
125.47
120.34
119.67
117.13
114.61
77.32
77.00
76.68
51.72
46.97
43.33
37.04
36.46
36.23
36.00
30.68
30.66
30.63
26.08
25.40
24.46
O
N
F
F
PhHN
O
CO2Me
c33
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

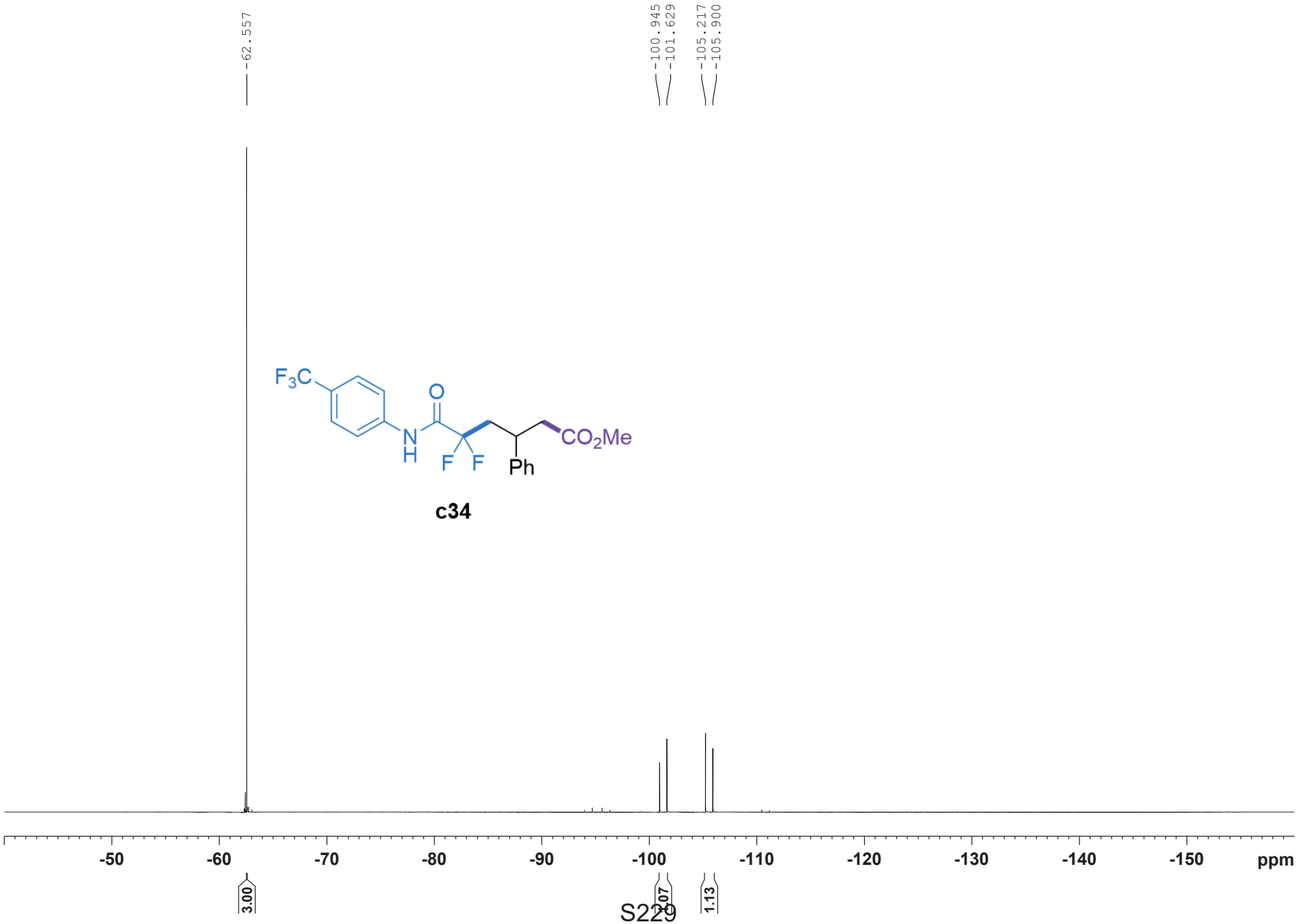

PhHN
F
F
O
O
N
CO2Me

c33

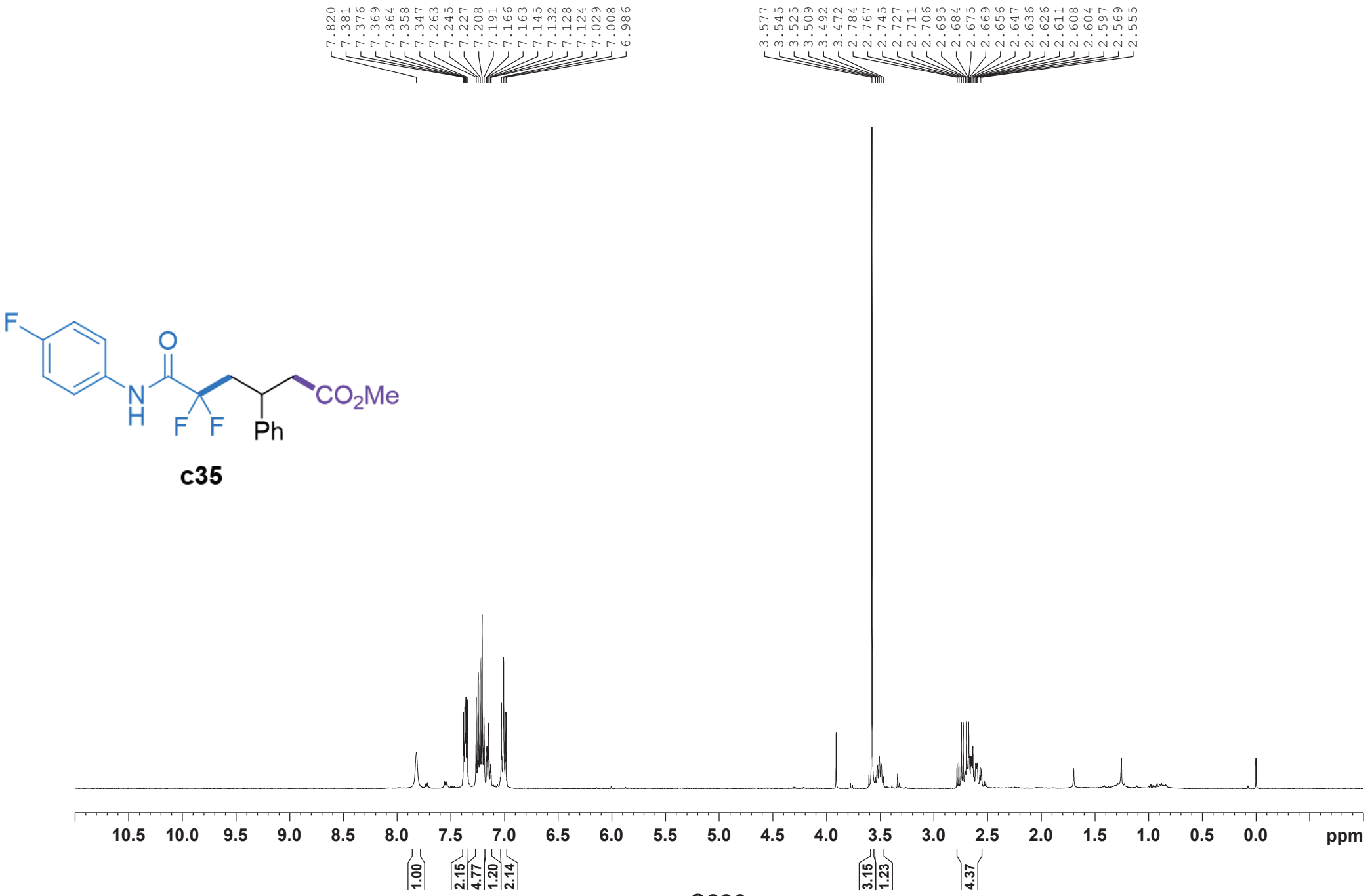
-103.116
-103.794
-105.051
-105.729
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.03

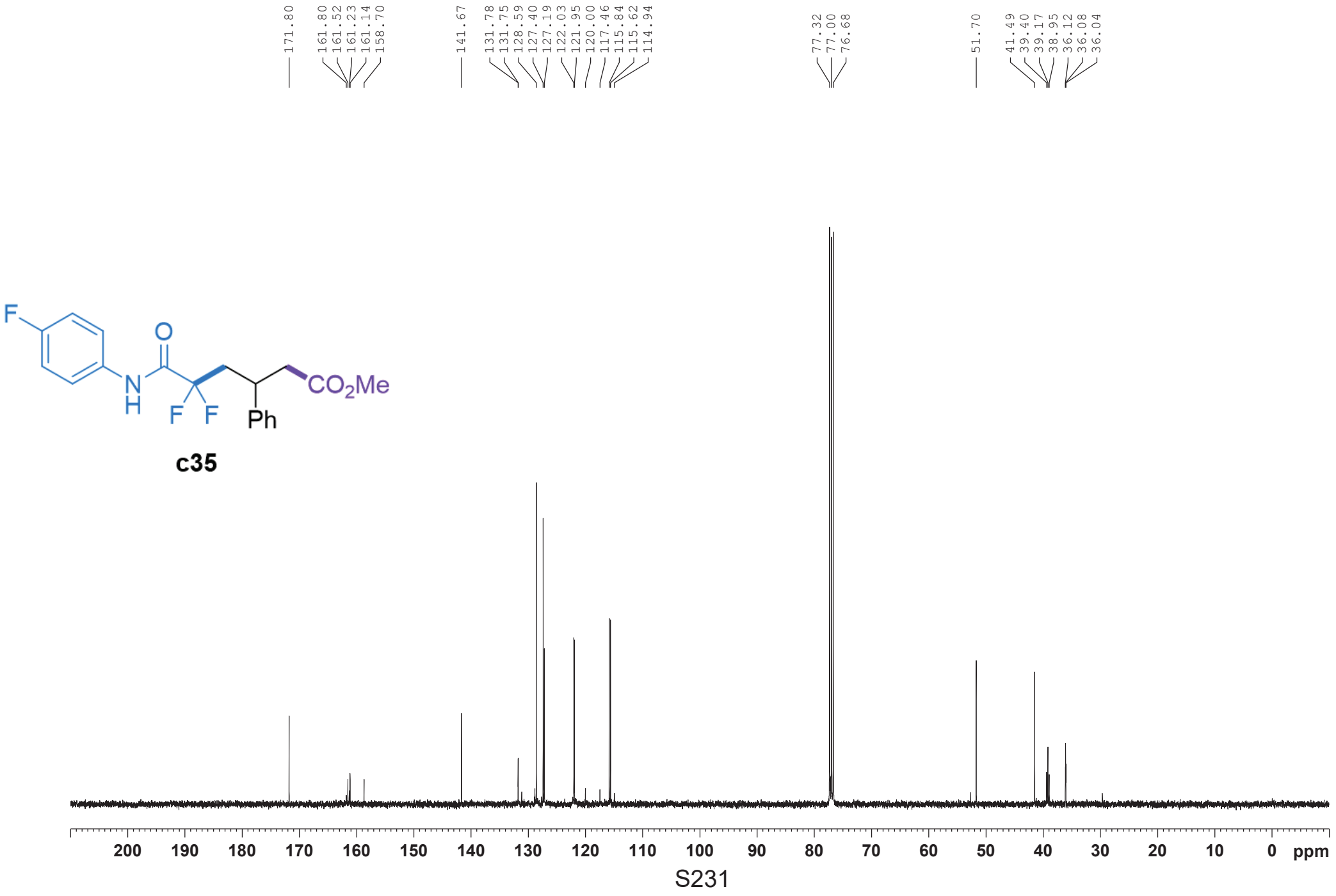

7.920
7.590
7.568
7.540
7.518
7.263
7.252
7.232
7.215
7.207
7.187
7.140
7.136
7.131
7.119
7.106
7.101
7.097
3.590
3.545
3.526
3.508
3.490
3.471
2.786
2.768
2.746
2.728
2.704
2.695
2.684
2.672
2.665
2.649
2.645
2.626
2.612
2.586
2.572
F3C
O
N
H
F F
Ph
CO2Me
c34
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
2.19
2.17
4.28
1.05
3.05
1.17
4.35

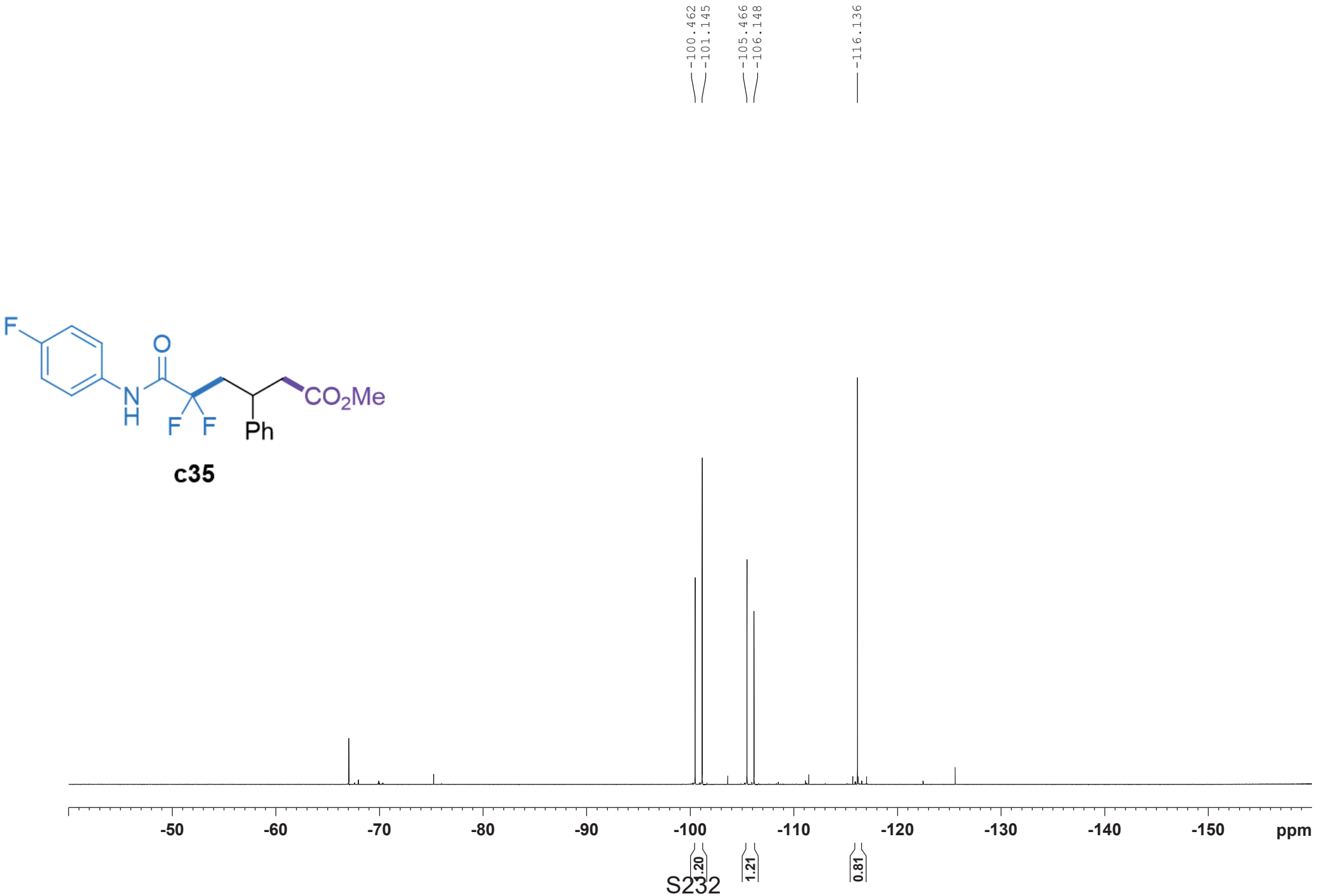

171.82
162.11
161.83
161.54
141.48
138.82
128.64
127.86
127.64
127.42
127.39
127.30
127.09
126.79
126.31
126.28
126.24
126.20
125.15
122.45
119.88
119.83
119.77
117.36
114.82
77.32
77.00
76.69
51.76
41.48
39.38
39.16
38.93
36.14
36.10
36.06
F3C
O
N
H
F F
Ph
CO2Me
c34
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

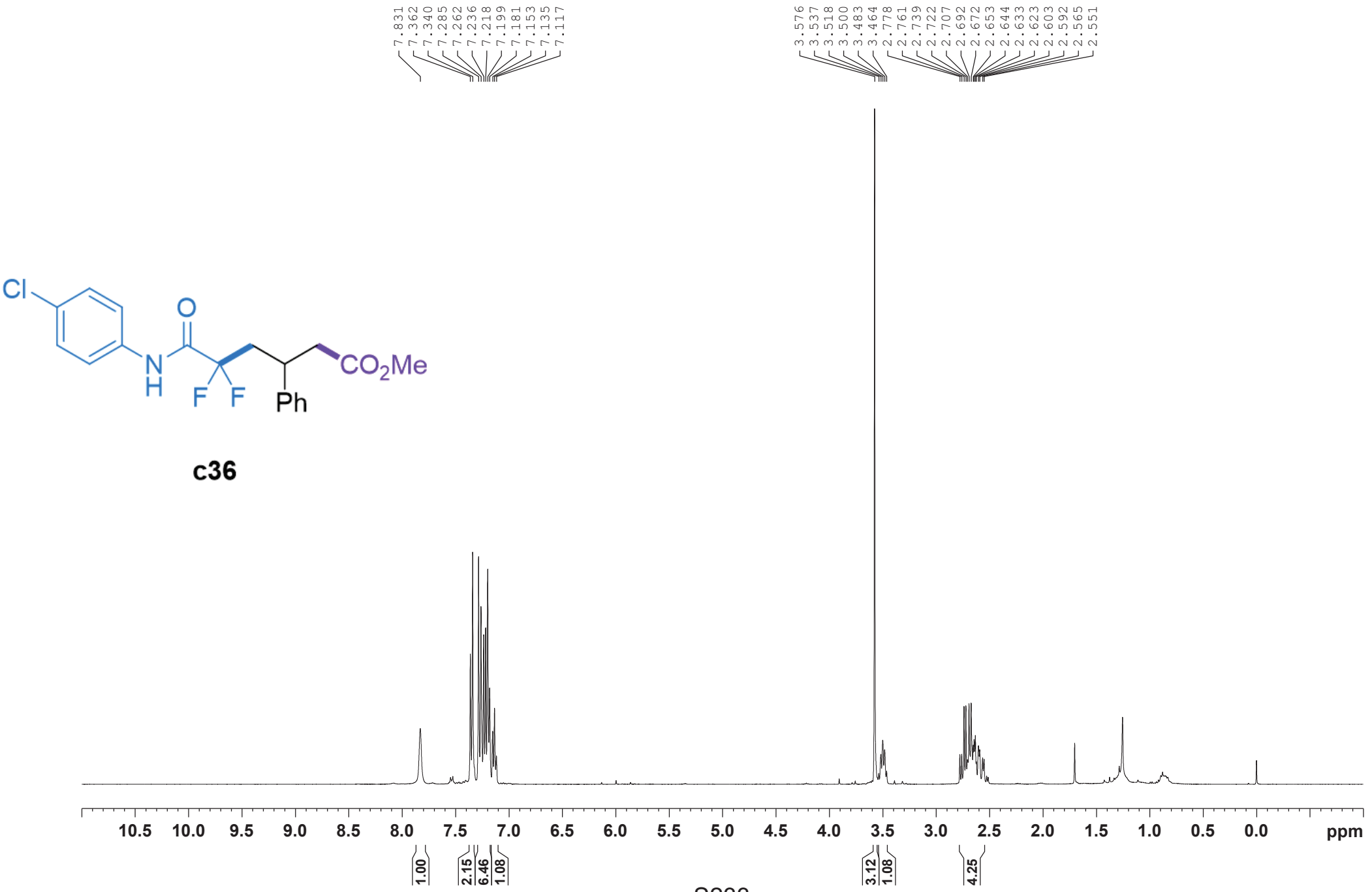

-62.557
-100.945
-101.629
-105.217
-105.900
F3C
O
N
H
F F
Ph
CO2Me
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
3.00
1.07
1.13

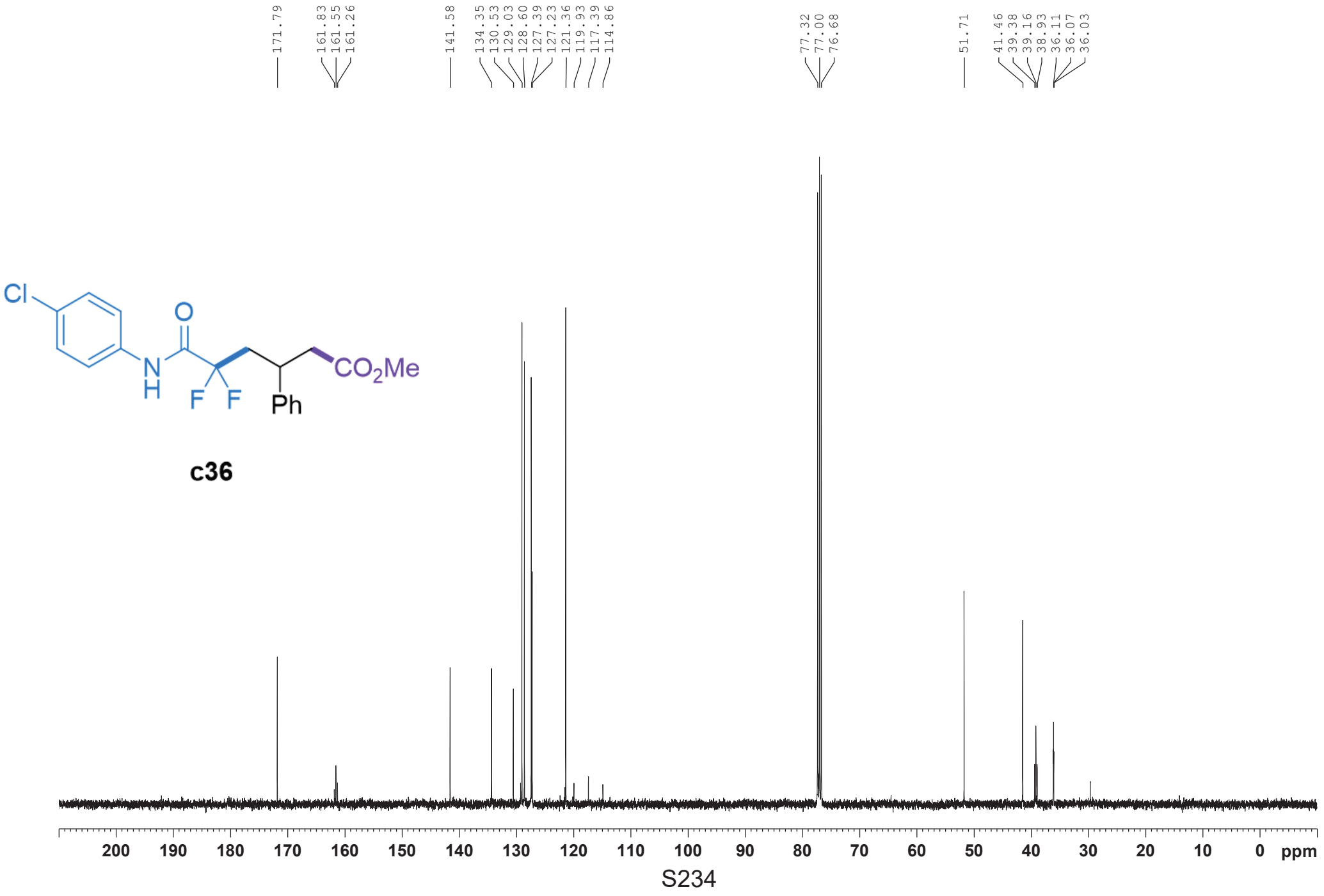
c34

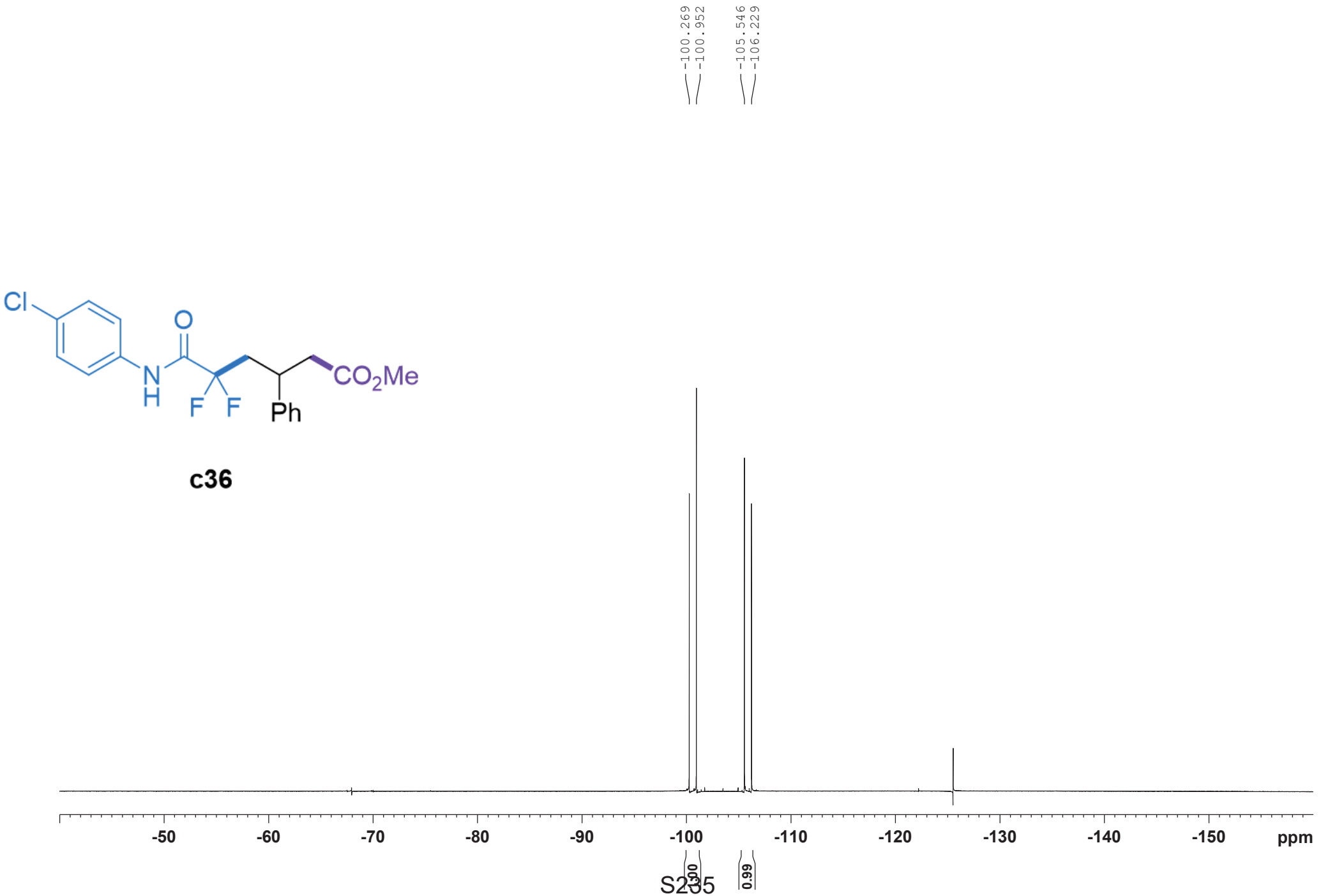

7.820
7.381
7.376
7.369
7.364
7.358
7.347
7.263
7.245
7.227
7.208
7.191
7.166
7.163
7.145
7.132
7.128
7.124
7.029
7.008
6.986
3.577
3.545
3.525
3.509
3.492
3.472
2.784
2.767
2.745
2.727
2.711
2.706
2.695
2.684
2.675
2.669
2.656
2.647
2.636
2.626
2.611
2.608
2.604
2.597
2.569
2.555
F
O
N
H
F F
Ph
CO2Me
c35
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
2.15
4.77
1.20
2.14
3.15
1.23
4.37

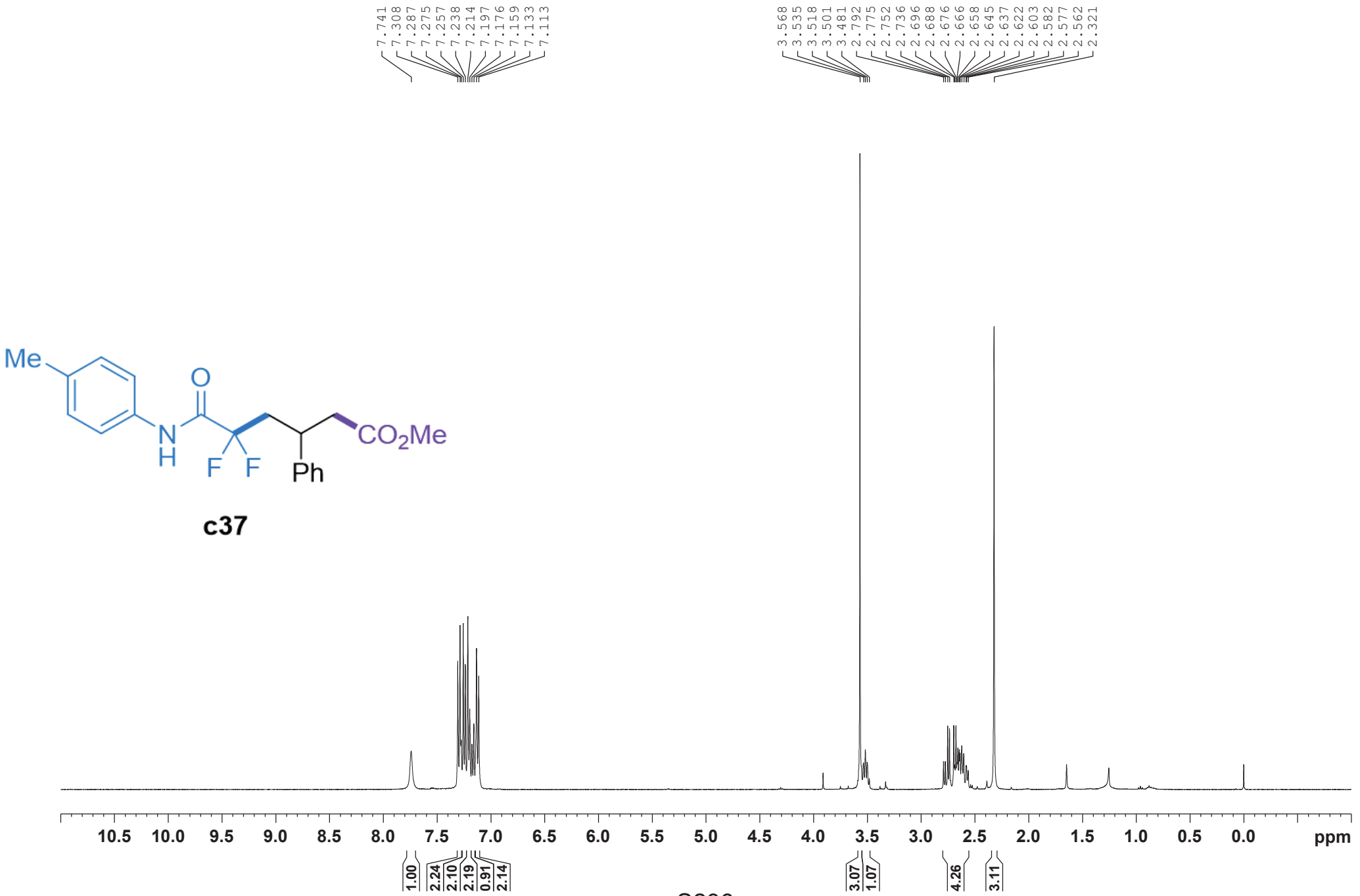

171.80
161.80
161.52
161.23
161.14
158.70
141.67
131.78
131.75
128.59
127.40
127.19
122.03
121.95
120.00
117.46
115.84
115.62
114.94
77.32
77.00
76.68
51.70
41.49
39.40
39.17
38.95
36.12
36.08
36.04
F
O
N
H
F F
Ph
CO2Me
c35
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

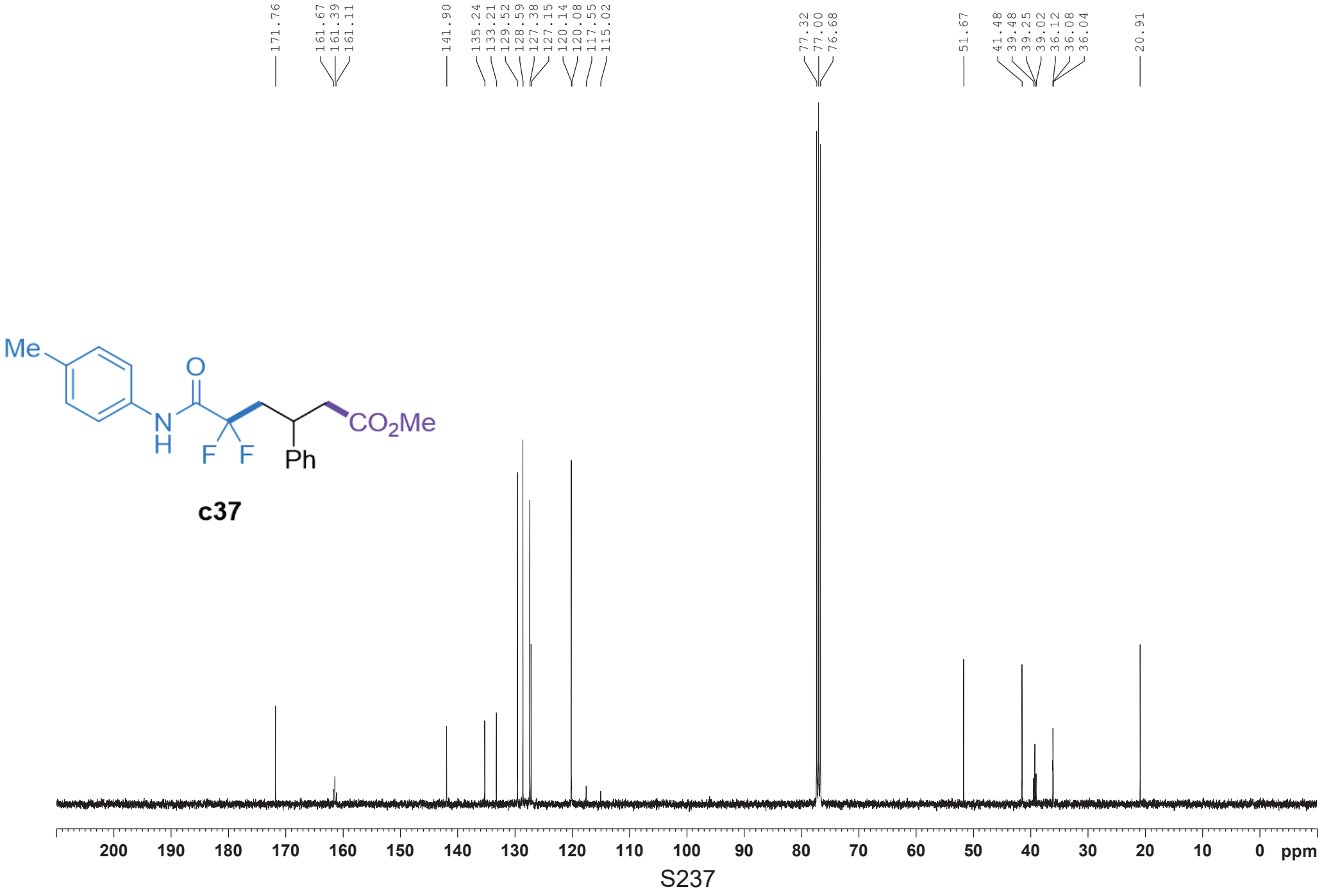

-100.462
-101.145
-105.466
-106.148
-116.136
F
O
N
H
F F
Ph
CO2Me
c35
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.20
1.21
0.81

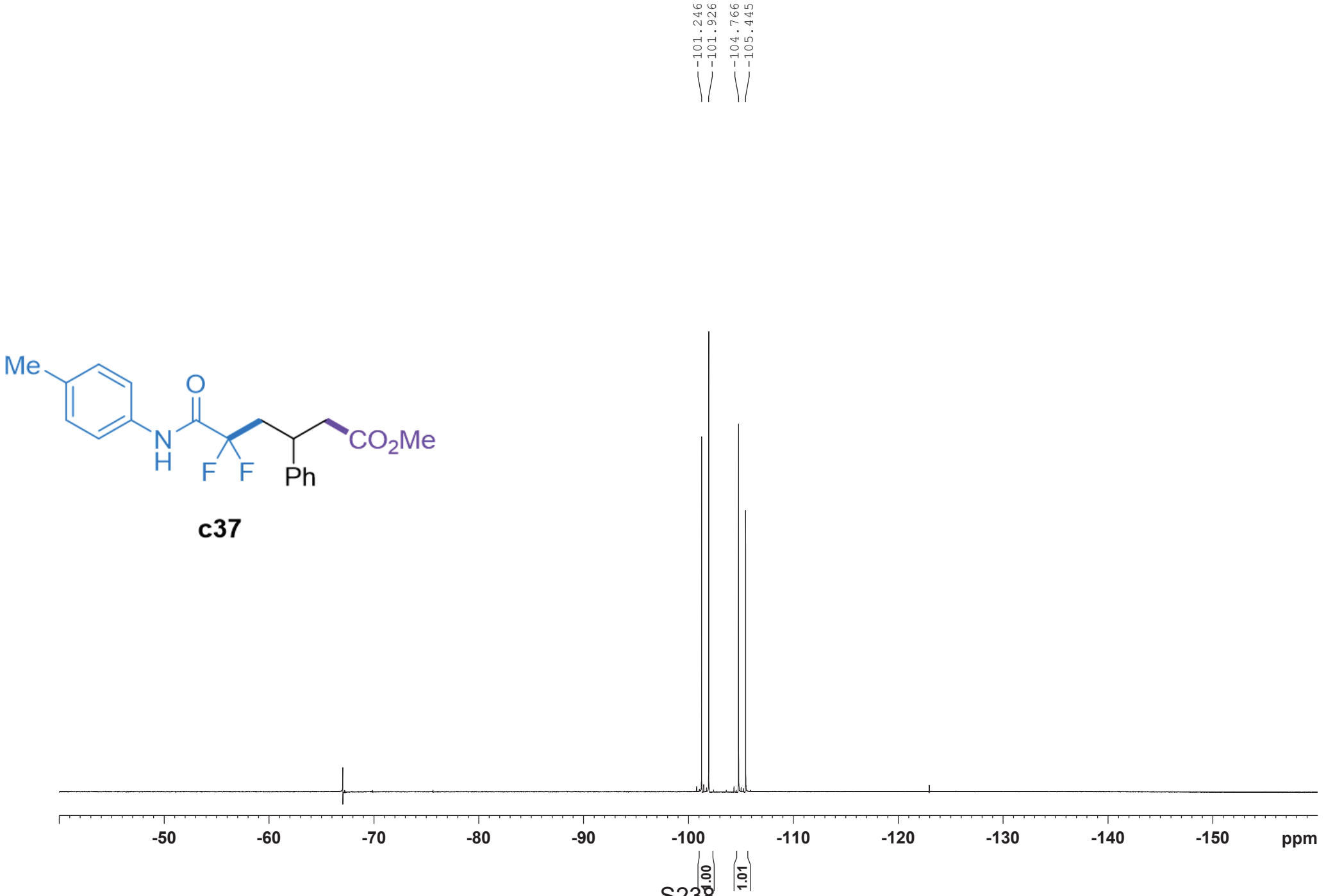

7.831
7.362
7.340
7.285
7.262
7.236
7.218
7.199
7.181
7.153
7.135
7.117
3.576
3.537
3.518
3.500
3.483
3.464
2.778
2.761
2.739
2.722
2.707
2.692
2.672
2.653
2.644
2.633
2.623
2.603
2.592
2.565
2.551
Cl
O
N
H
F
F
Ph
CO2Me
c36
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.15
6.46
1.08
3.12
1.08
4.25

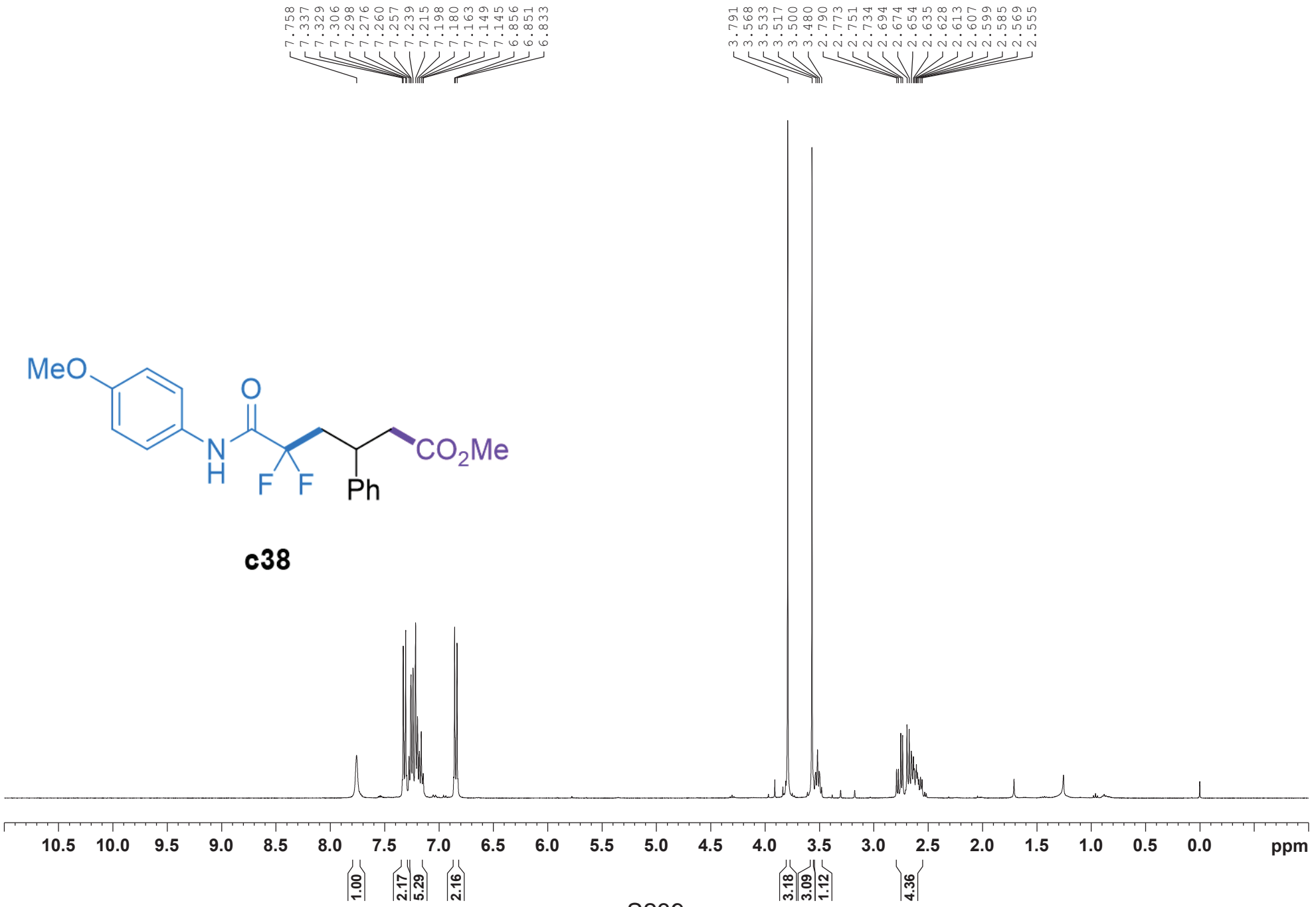

171.79
161.83
161.55
161.26
141.58
134.35
130.53
129.03
128.60
127.39
127.23
121.36
119.93
117.39
114.86
77.32
77.00
76.68
51.71
41.46
39.38
39.16
38.93
36.11
36.07
36.03
Cl
O
N
H
F F
Ph
CO2Me
c36
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

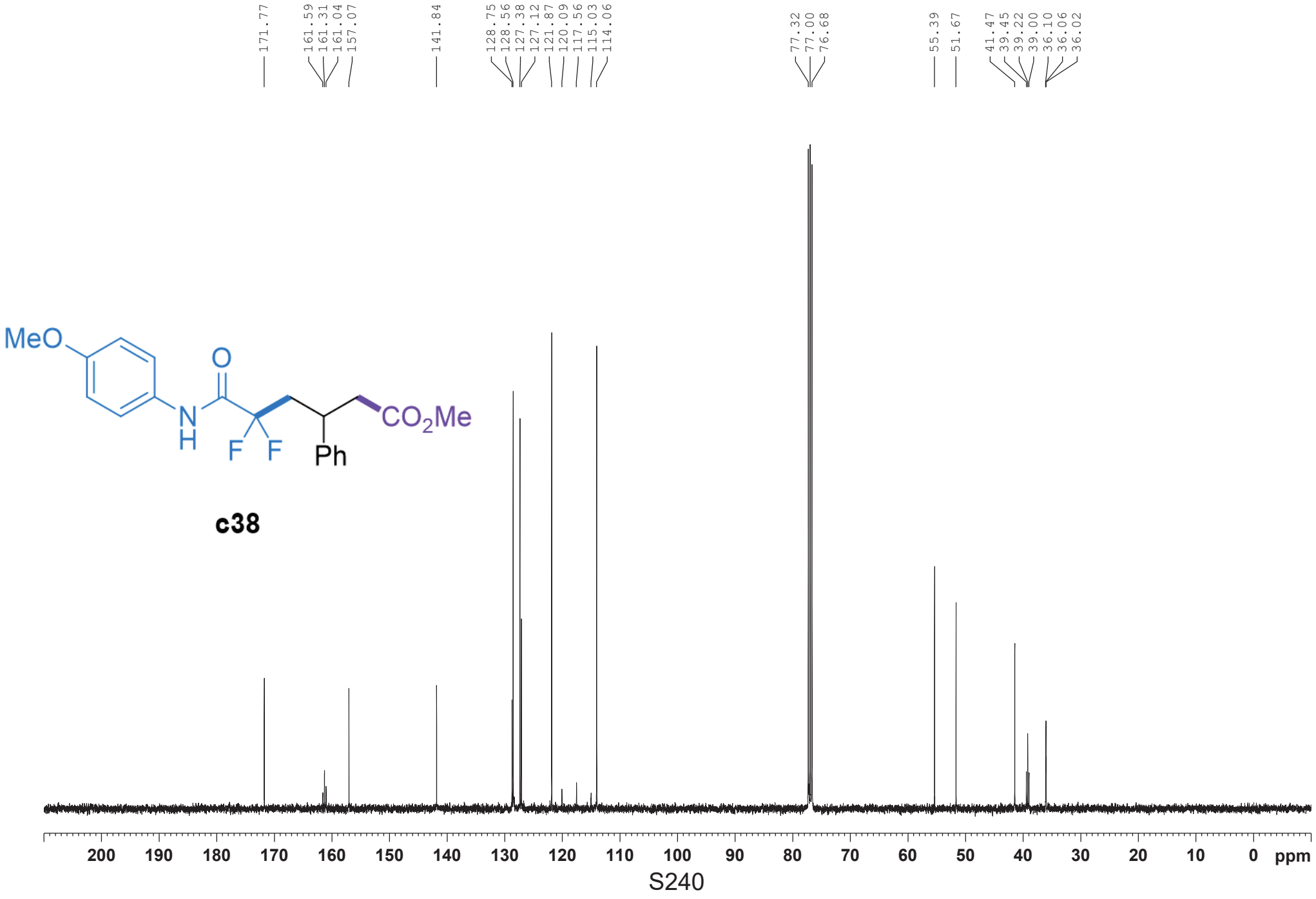

-100.269
-100.952
-105.546
-106.229
Cl
O
N
H
F F
Ph
CO2Me
c36
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
0.99

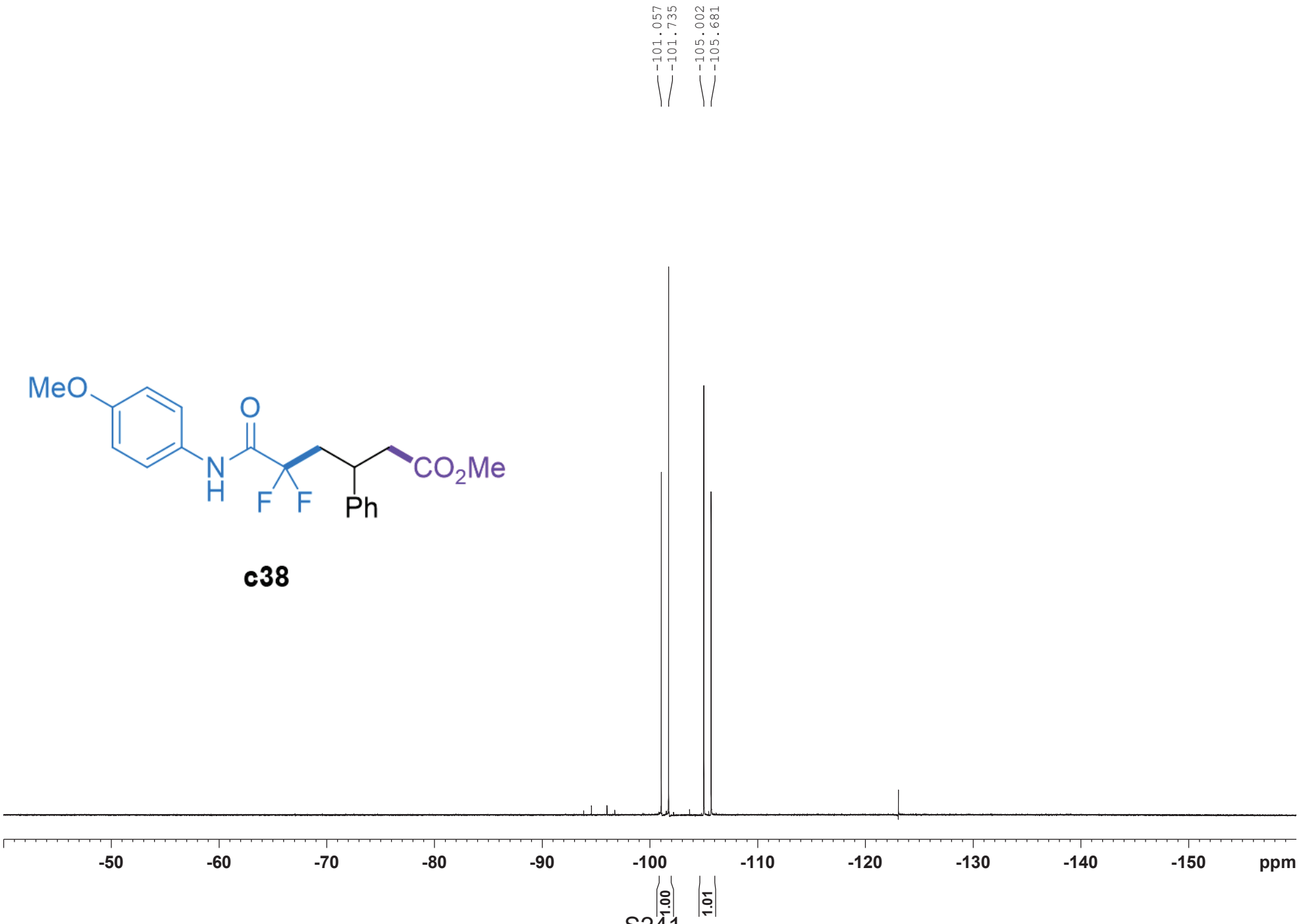

7.741
7.308
7.287
7.275
7.257
7.238
7.214
7.197
7.176
7.159
7.133
7.113
3.568
3.535
3.518
3.501
3.481
2.792
2.775
2.752
2.736
2.696
2.688
2.676
2.666
2.658
2.645
2.637
2.622
2.603
2.582
2.577
2.562
2.321
Me
O
N
H
F F
Ph
CO2Me
c37
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00 2.24 2.10 2.19 0.91 2.14 3.07 1.07 4.26 3.11

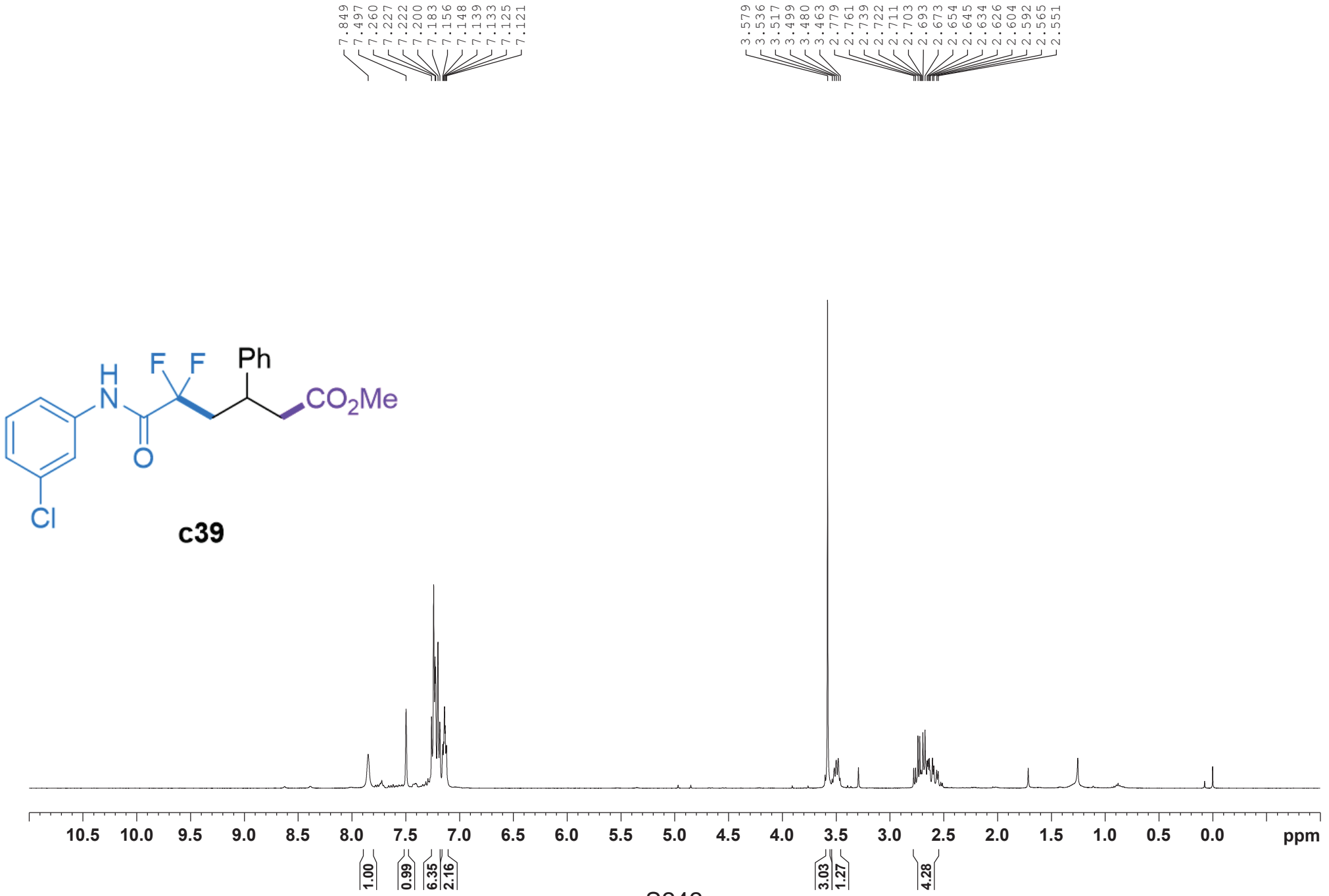

171.76
161.67
161.39
161.11
141.90
135.24
133.21
129.52
128.59
127.38
127.15
120.14
120.08
117.55
115.02
77.32
77.00
76.68
51.67
41.48
39.48
39.25
39.02
36.12
36.08
36.04
20.91
Me
O
N
H
F F
Ph
CO2Me
c37
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

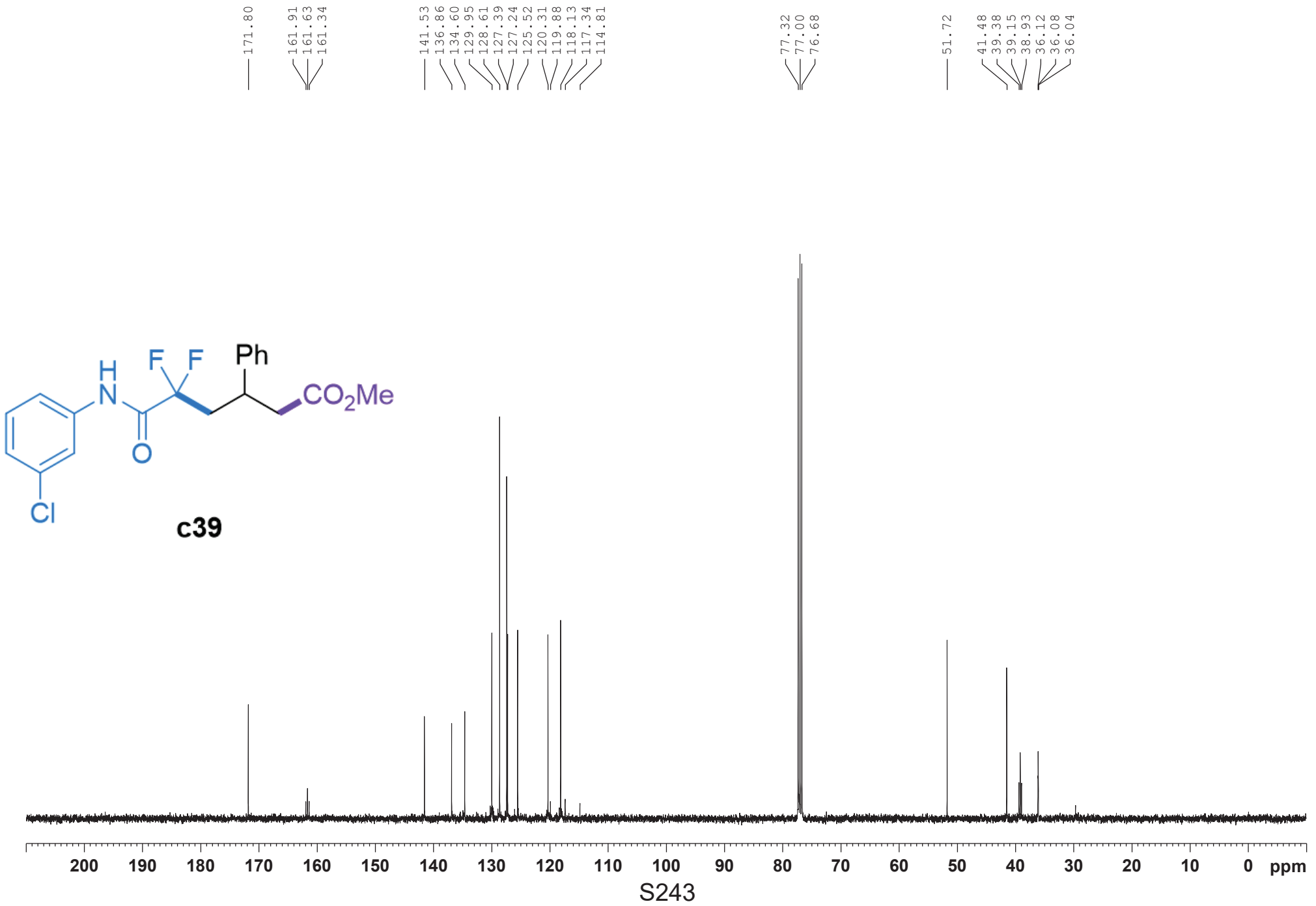

-101.246
-101.926
-104.766
-105.445
Me
O
N
H
F F
Ph
CO2Me
c37
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

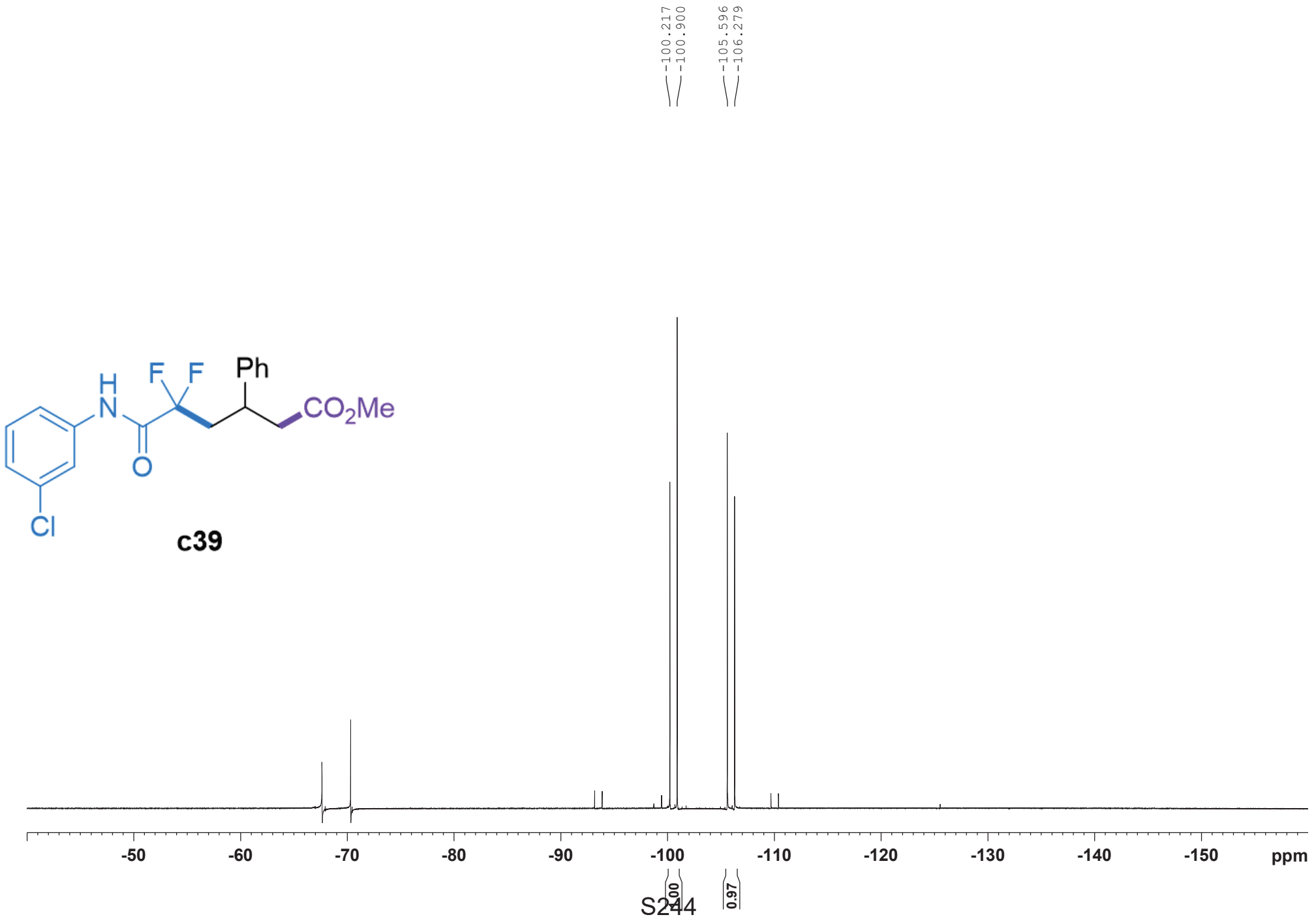

7.758
7.337
7.329
7.306
7.298
7.276
7.260
7.257
7.239
7.215
7.198
7.180
7.163
7.149
7.145
6.856
6.851
6.833
3.791
3.568
3.533
3.517
3.500
3.480
2.790
2.773
2.751
2.734
2.694
2.674
2.654
2.635
2.628
2.613
2.607
2.599
2.585
2.569
2.555
MeO
O
N
H
F
F
Ph
CO2Me
c38
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.17
5.29
2.16
3.18
3.09
1.12
4.36

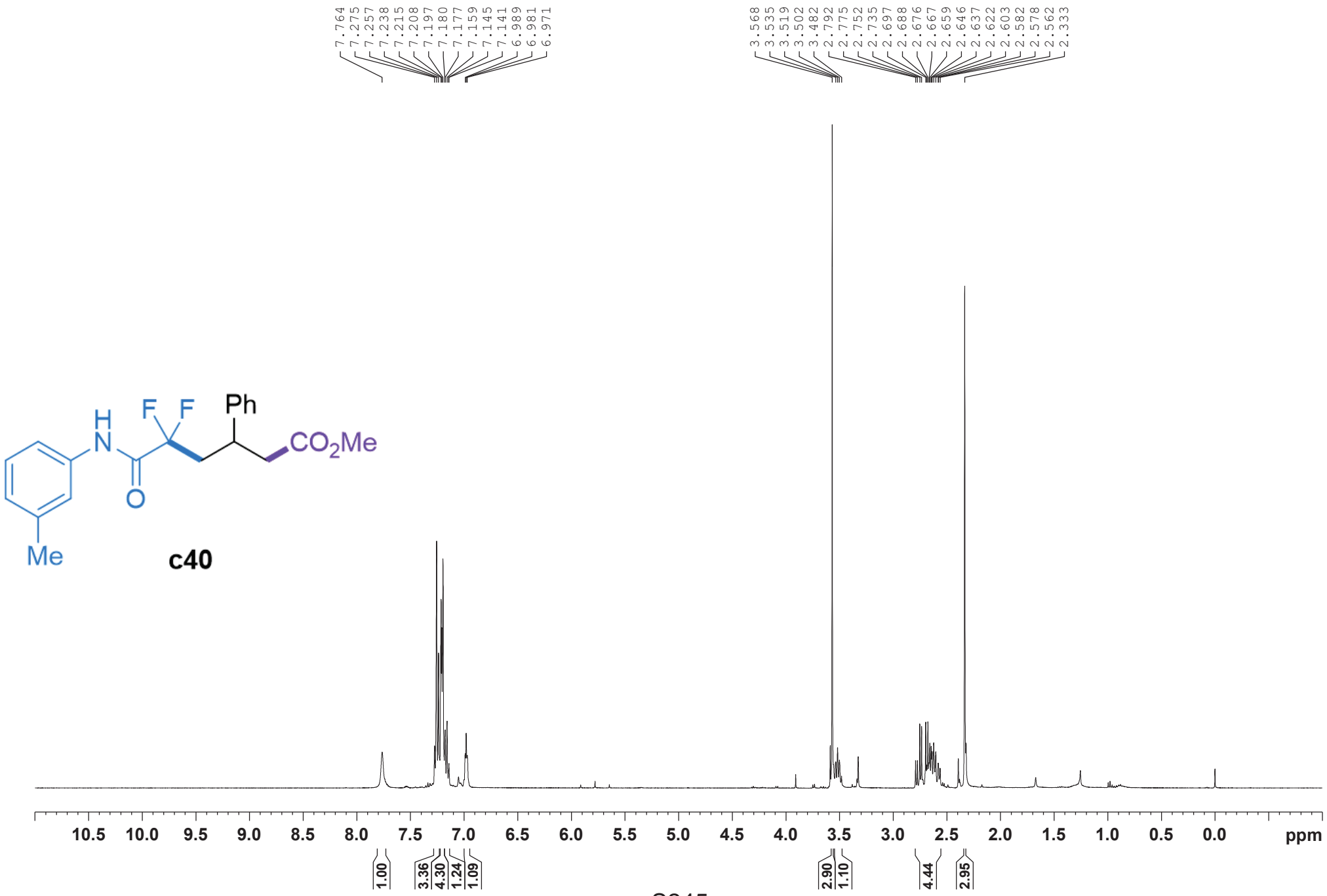

171.77
161.59
161.31
161.04
157.07
141.84
128.75
128.56
127.38
127.12
121.87
120.09
117.56
115.03
114.06
77.32
77.00
76.68
55.39
51.67
41.47
39.45
39.22
39.00
36.10
36.06
36.02
MeO
O
N
H
F F
Ph
CO2Me
c38
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

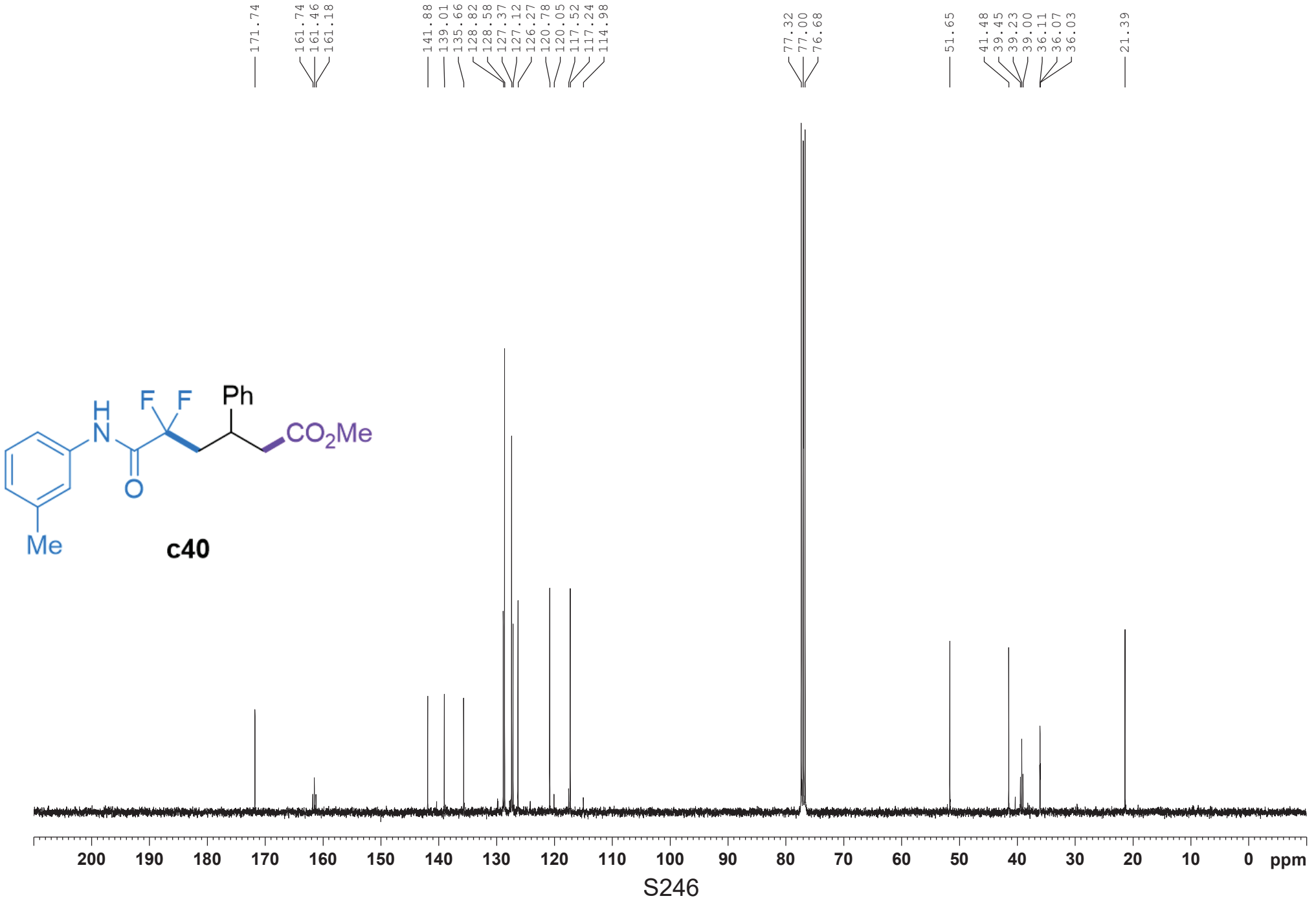

-101.057
-101.735
-105.002
-105.681
MeO
O
N
H
F
F
Ph
CO2Me
c38
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

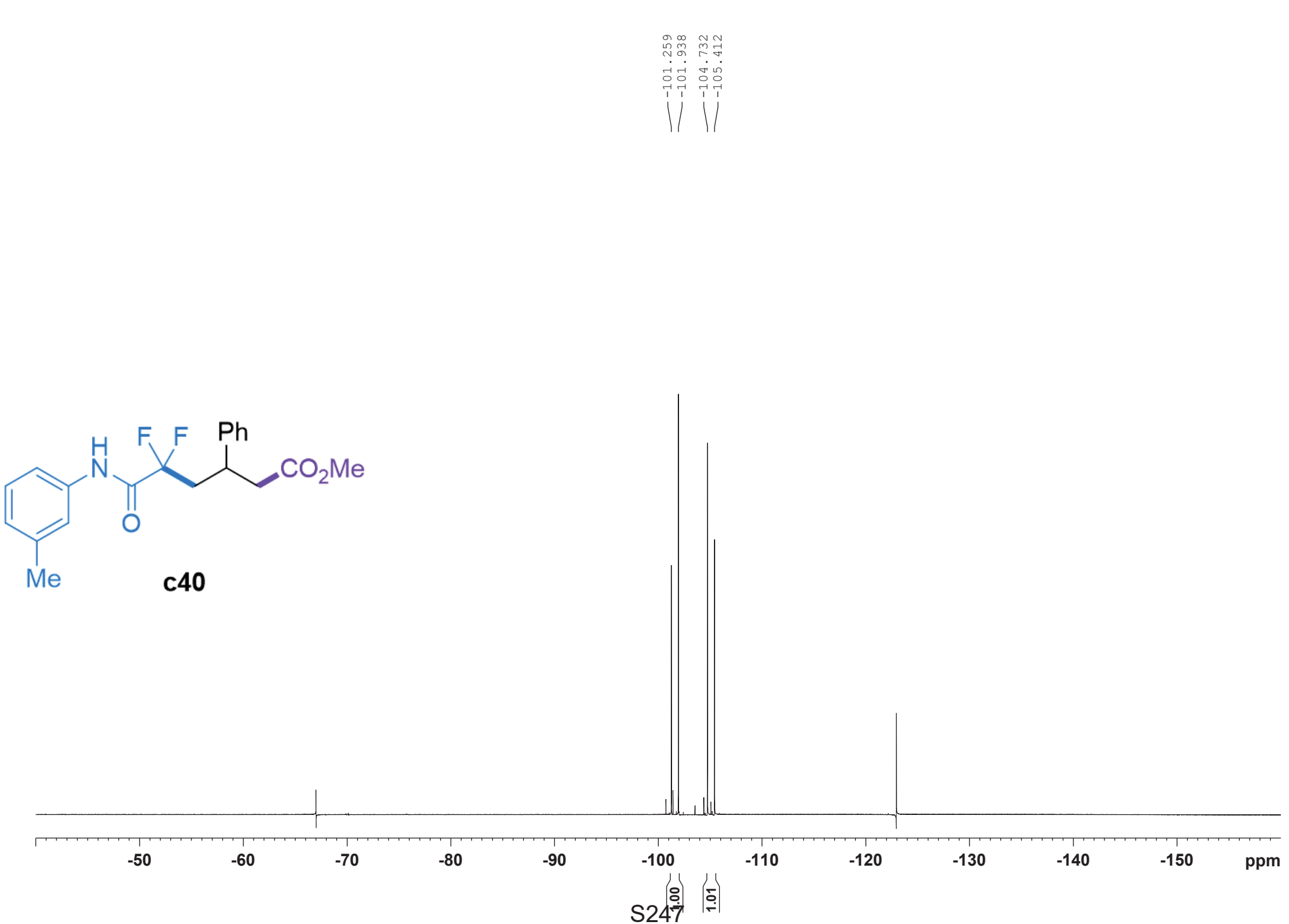

7.849
7.497
7.260
7.227
7.222
7.200
7.183
7.156
7.148
7.139
7.133
7.125
7.121
3.579
3.536
3.517
3.499
3.480
3.463
2.779
2.761
2.739
2.722
2.711
2.703
2.693
2.673
2.654
2.645
2.634
2.626
2.604
2.592
2.565
2.551
H
N
F
F
Ph
CO2Me
O
Cl
c39
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
0.99
6.35
2.16
3.03
1.27
4.28

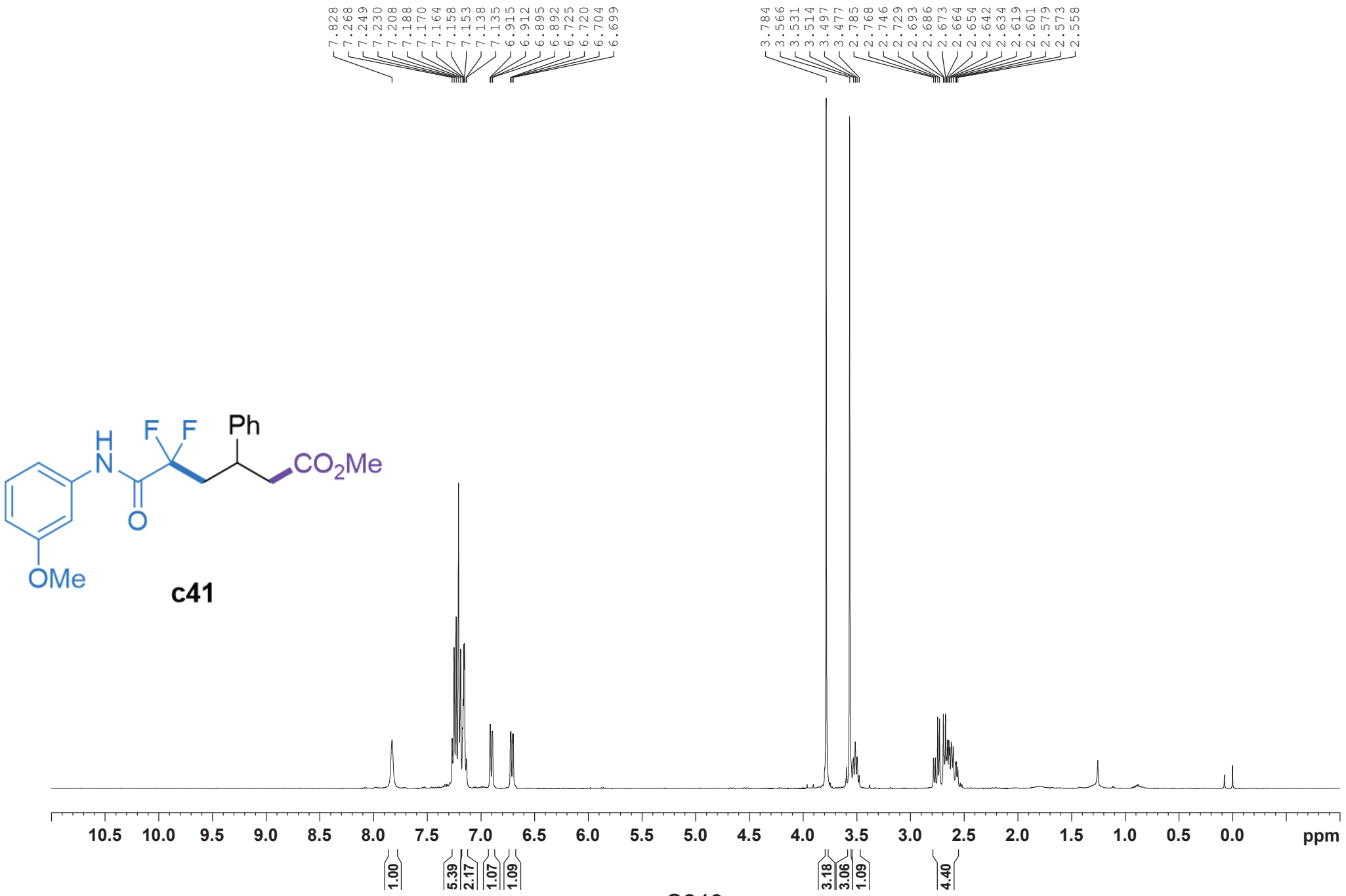

171.80
161.91
161.63
161.34
141.53
136.86
134.60
129.95
128.61
127.39
127.24
125.52
120.31
119.88
118.13
117.34
114.81
77.32
77.00
76.68
51.72
41.48
39.38
39.15
38.93
36.12
36.08
36.04
H
N
F
F
Ph
CO2Me
O
Cl
c39
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

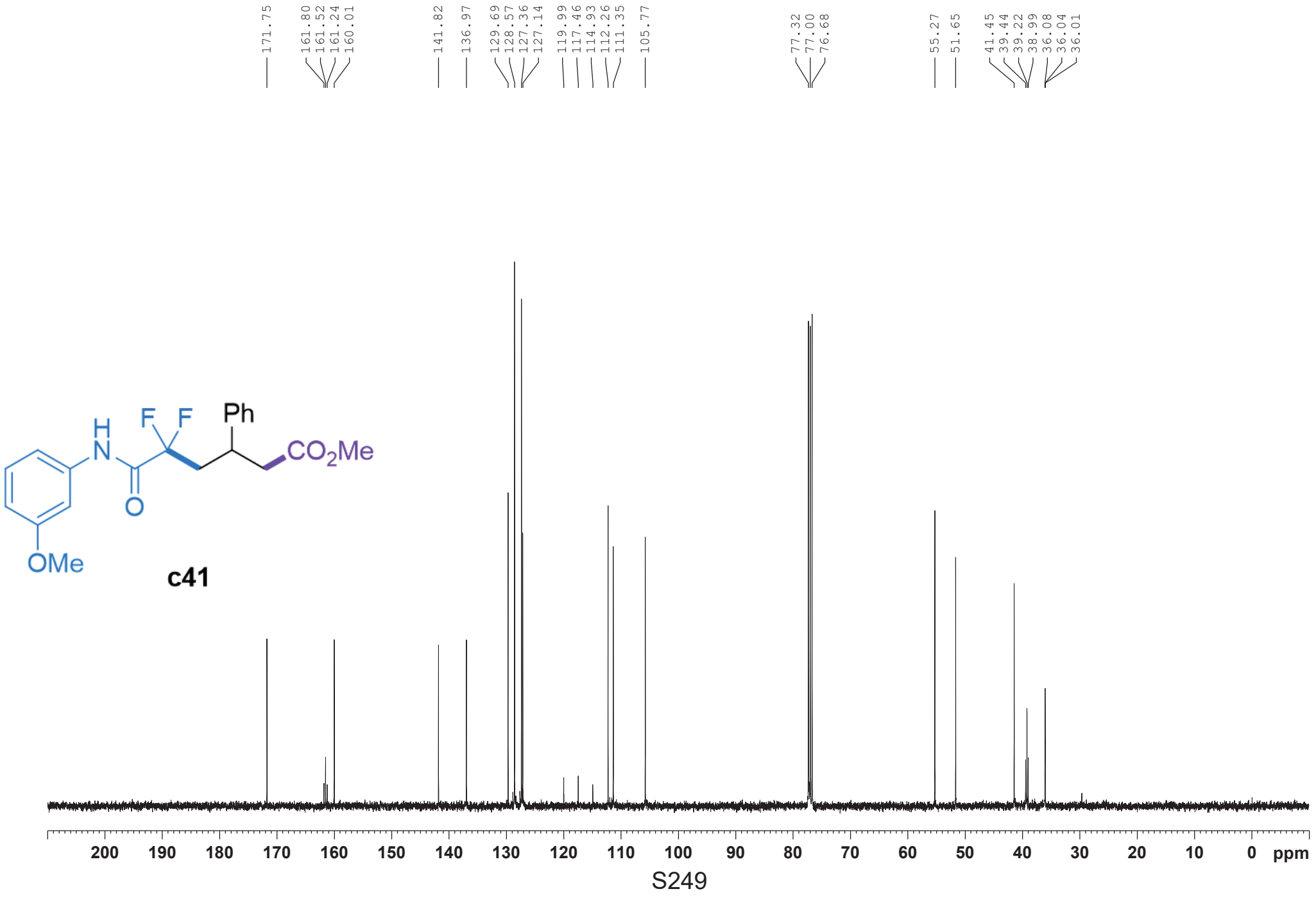

-100.217
-100.900
-105.596
-106.279
H
N
F
F
Ph
CO2Me
O
Cl
c39
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
0.97

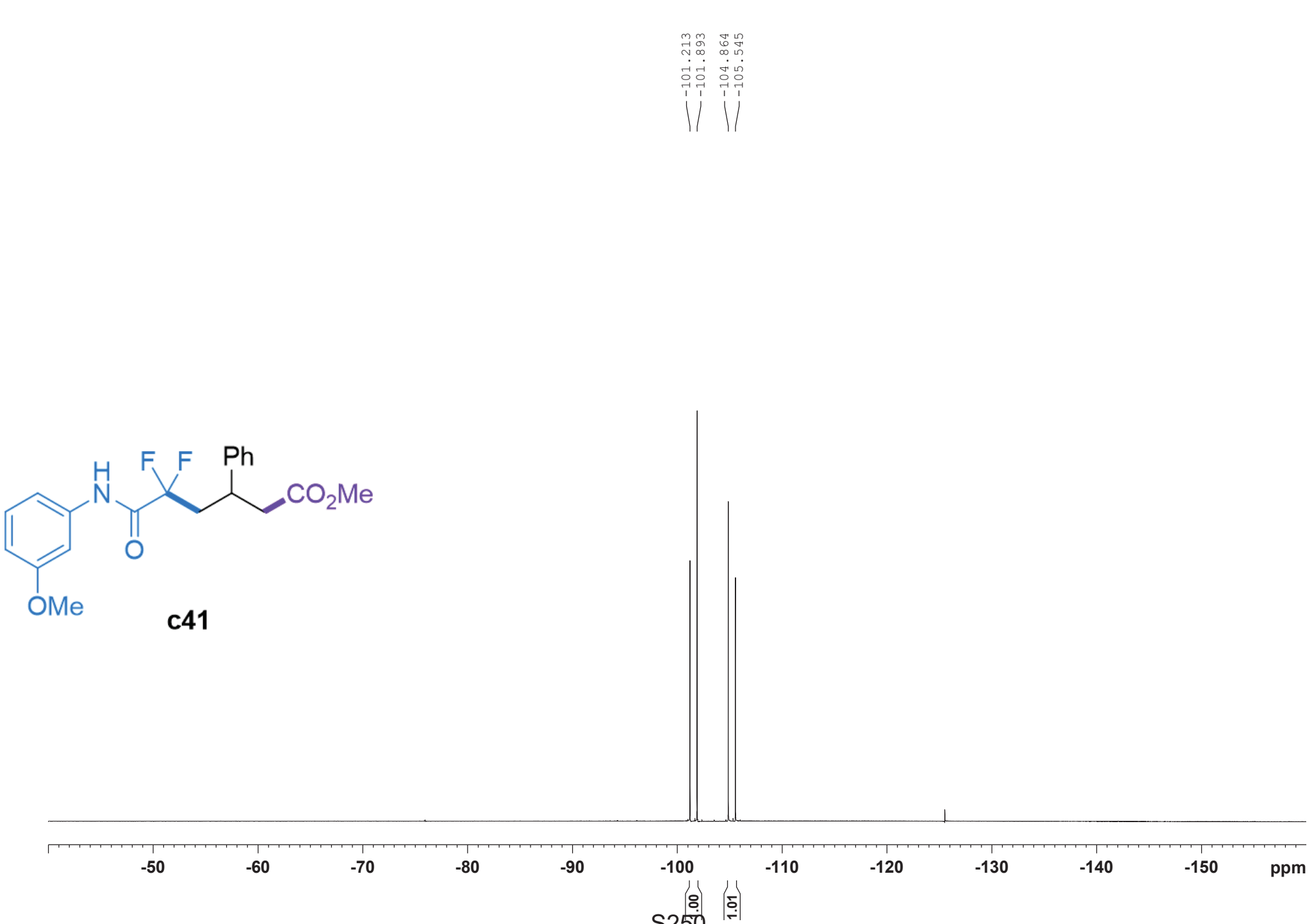

7.764
7.275
7.257
7.238
7.215
7.208
7.197
7.180
7.177
7.159
7.145
7.141
6.989
6.981
6.971
3.568
3.535
3.519
3.502
3.482
2.792
2.775
2.752
2.735
2.697
2.688
2.676
2.667
2.659
2.646
2.637
2.622
2.603
2.582
2.578
2.562
2.333
H
N
F
F
Ph
CO2Me
O
Me
c40
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
3.36
4.30
1.24
1.09
2.90
1.10
4.44
2.95

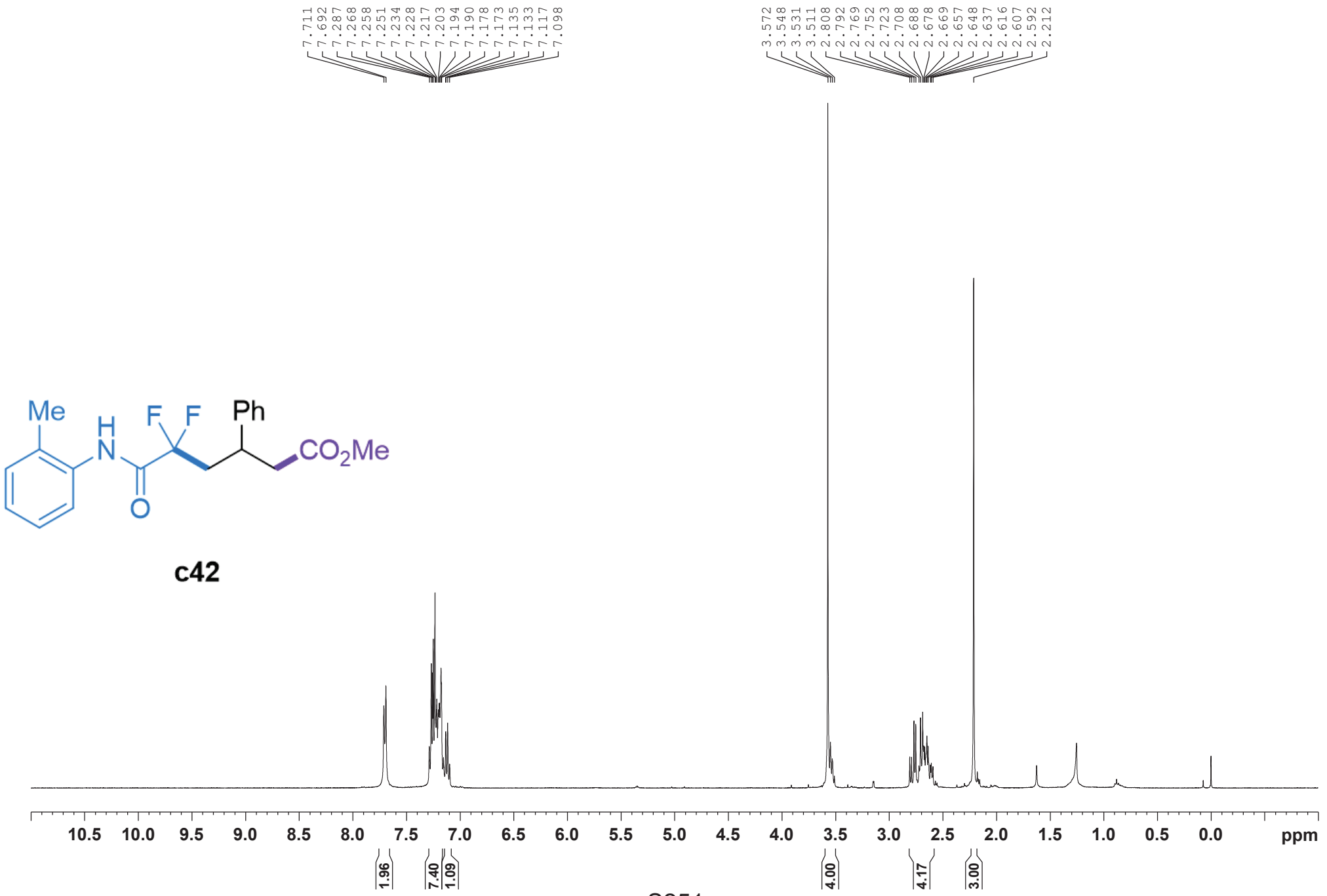

171.74
161.74
161.46
161.18
141.88
139.01
135.66
128.82
128.58
127.37
127.12
126.27
120.78
120.05
117.52
117.24
114.98
77.32
77.00
76.68
51.65
41.48
39.45
39.23
39.00
36.11
36.07
36.03
21.39
H
N
F
F
Ph
CO2Me
O
Me
c40
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

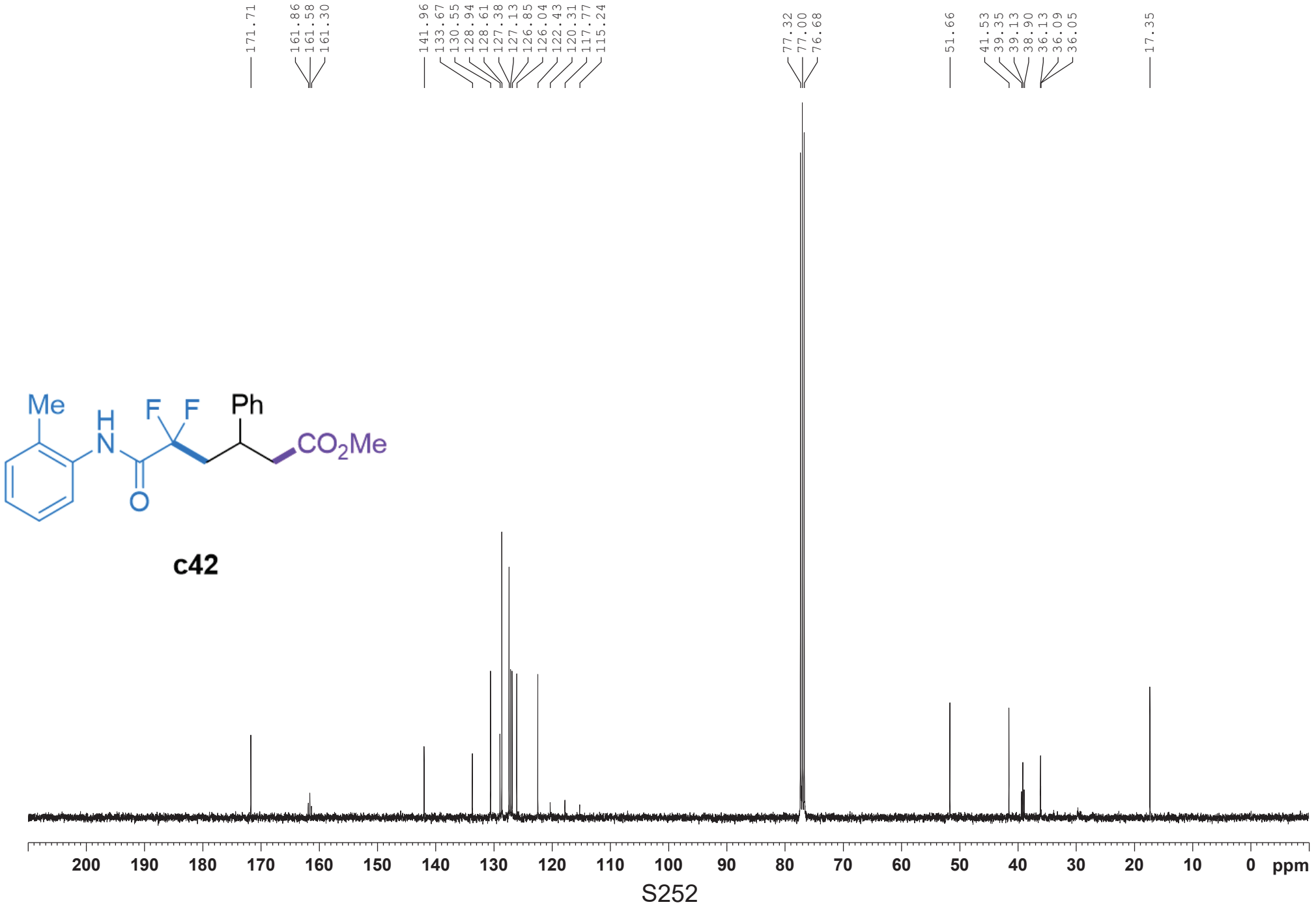

-101.259
-101.938
-104.732
-105.412
H
N
F
F
Ph
CO2Me
O
Me
c40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

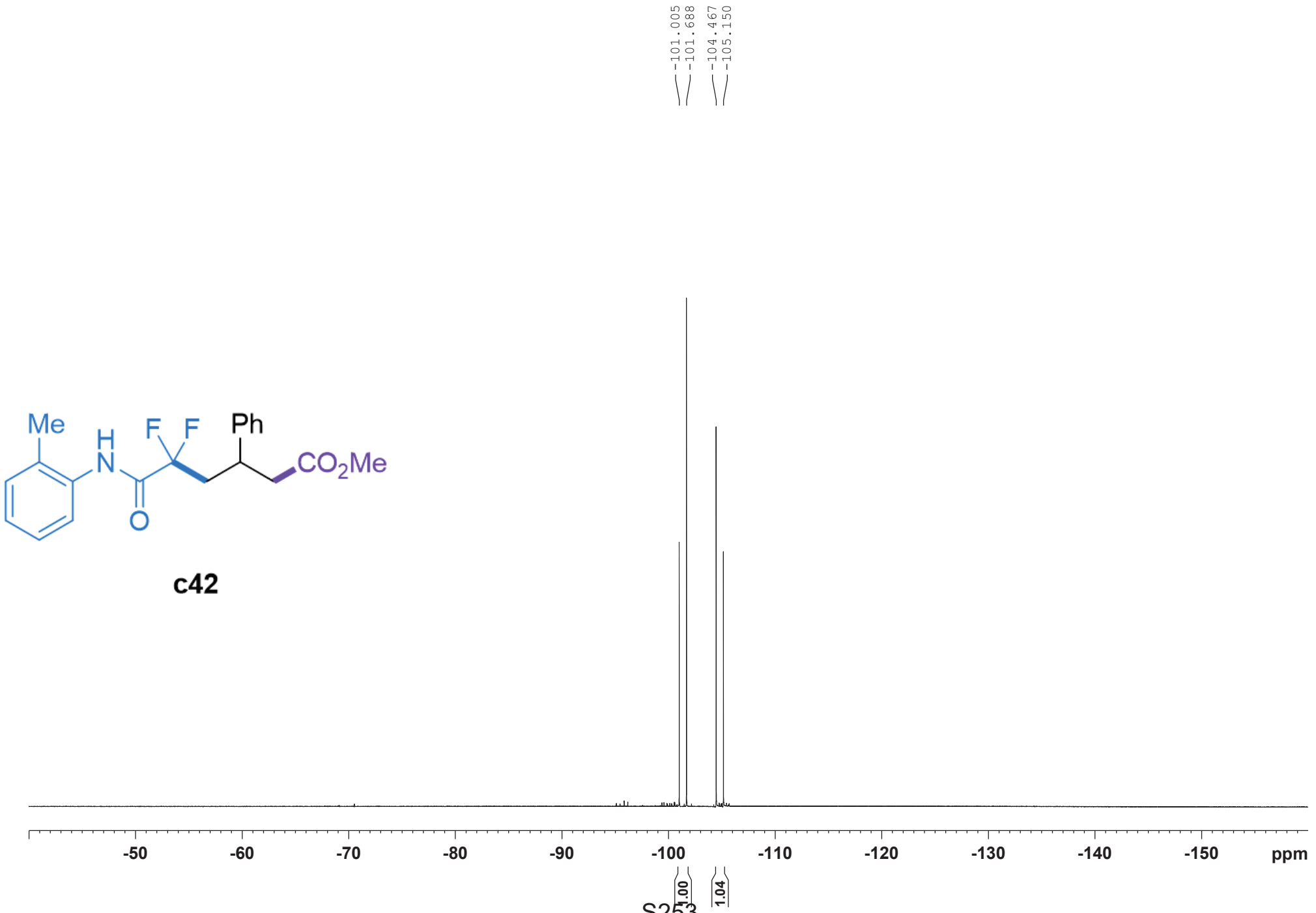

7.828
7.268
7.249
7.230
7.208
7.188
7.170
7.164
7.158
7.153
7.138
7.135
6.915
6.912
6.895
6.892
6.725
6.720
6.704
6.699
3.784
3.566
3.531
3.514
3.497
3.477
2.785
2.768
2.746
2.729
2.693
2.686
2.673
2.664
2.654
2.642
2.634
2.619
2.601
2.579
2.573
2.558
H
N
F
F
Ph
CO2Me
O
OMe
c41
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
5.39
2.17
1.07
1.09
3.18
3.06
1.09
4.40


171.75
161.80
161.52
161.24
160.01
141.82
136.97
129.69
128.57
127.36
127.14
119.99
117.46
114.93
112.26
111.35
105.77
77.32
77.00
76.68
55.27
51.65
41.45
39.44
39.22
38.99
36.08
36.04
36.01
H
N
F
F
Ph
CO2Me
O
OMe
c41
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

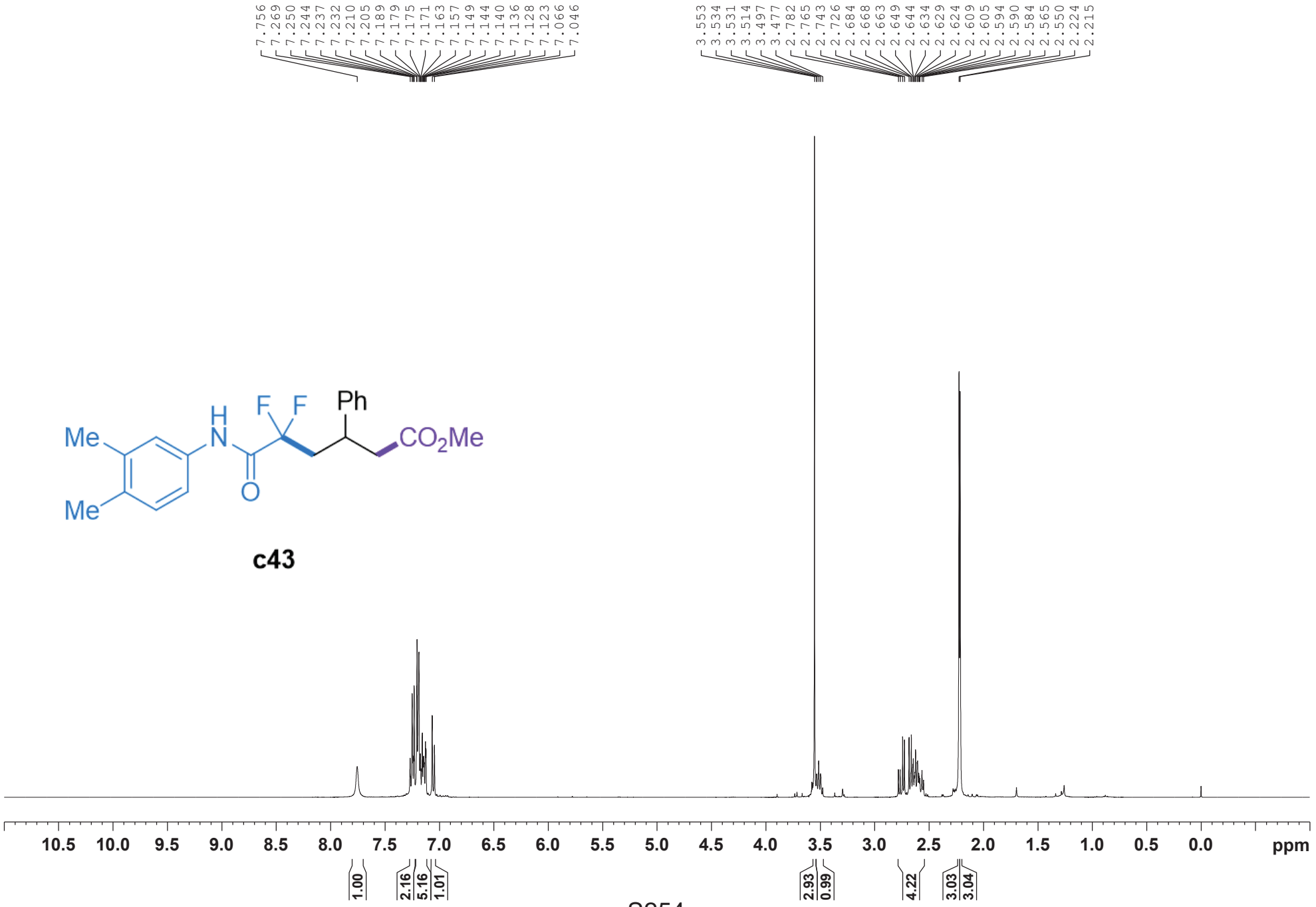

-101.213
-101.893
-104.864
-105.545
H
N
F
F
Ph
CO2Me
O
OMe
c41
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01

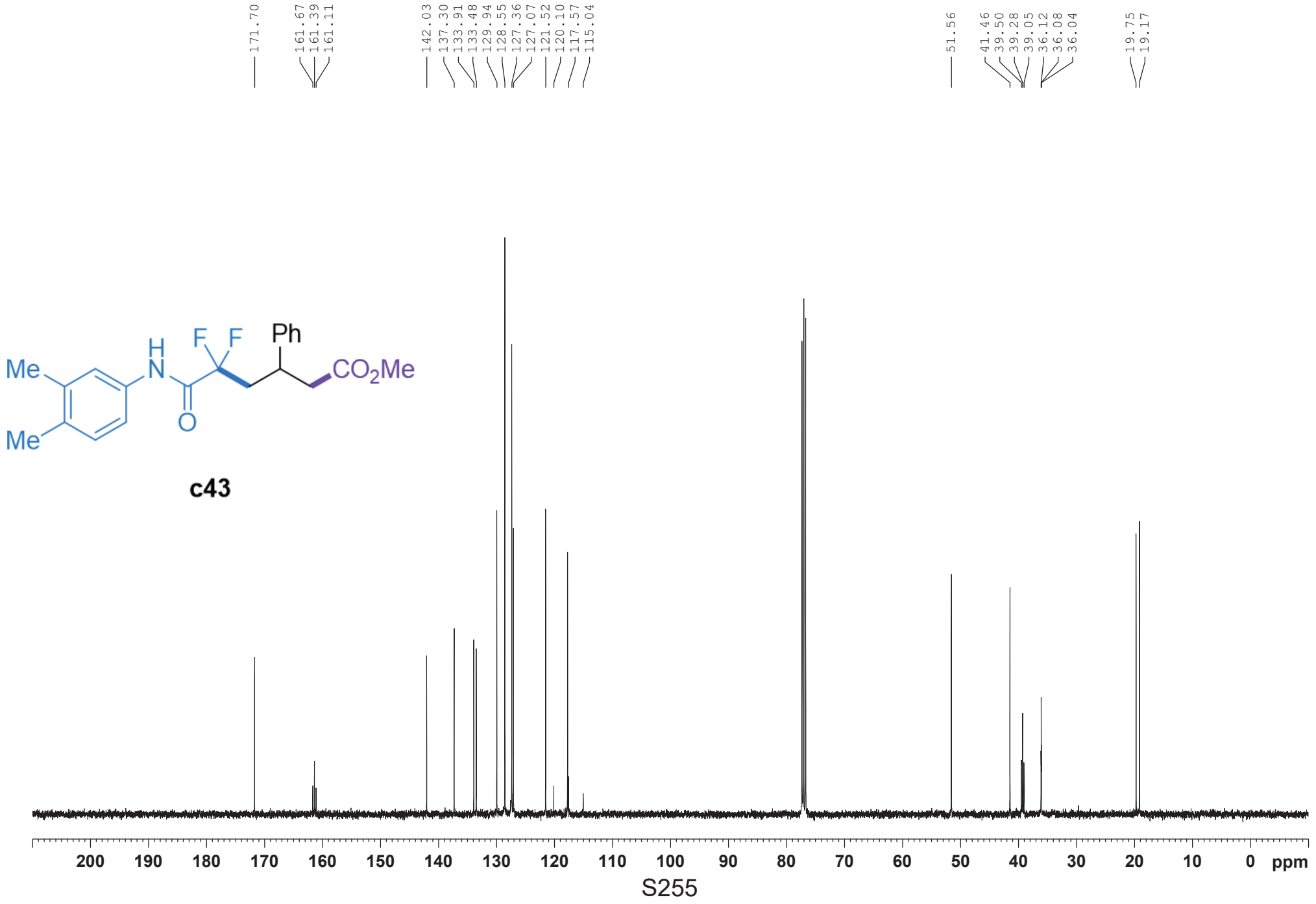

7.711
7.692
7.287
7.268
7.258
7.251
7.234
7.228
7.217
7.203
7.194
7.190
7.178
7.173
7.135
7.133
7.117
7.098
3.572
3.548
3.531
3.511
2.808
2.792
2.769
2.752
2.723
2.708
2.688
2.678
2.669
2.657
2.648
2.637
2.616
2.607
2.592
2.212
Me
H
N
F
F
Ph
CO2Me
O
c42
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.96
7.40
1.09
4.00
4.17
3.00

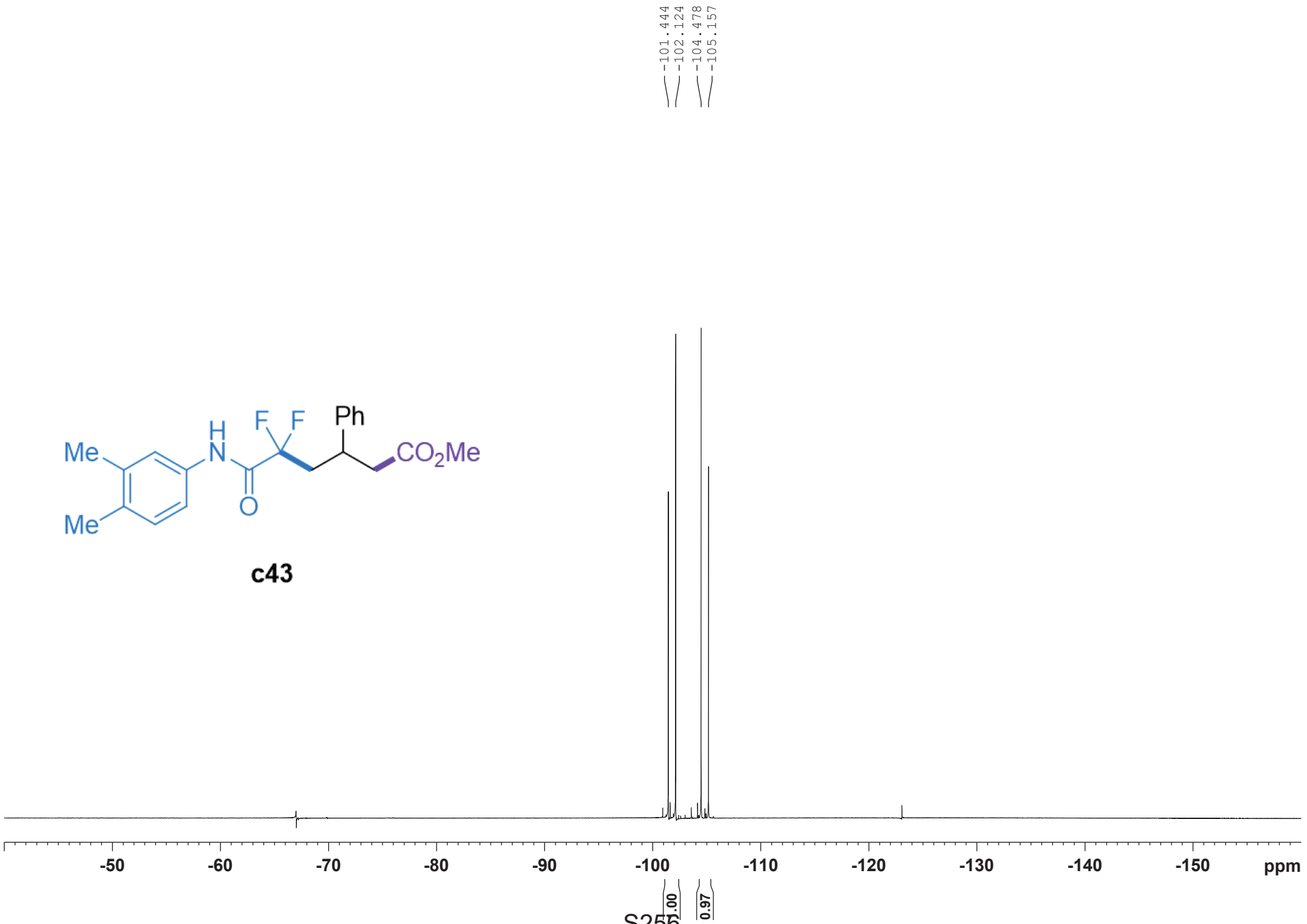

171.71
161.86
161.58
161.30
141.96
133.67
130.55
128.94
128.61
127.38
127.13
126.85
126.04
122.43
120.31
117.77
115.24
77.32
77.00
76.68
51.66
41.53
39.35
39.13
38.90
36.13
36.09
36.05
17.35
Me
H
N
F
F
Ph
CO2Me
O
c42
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

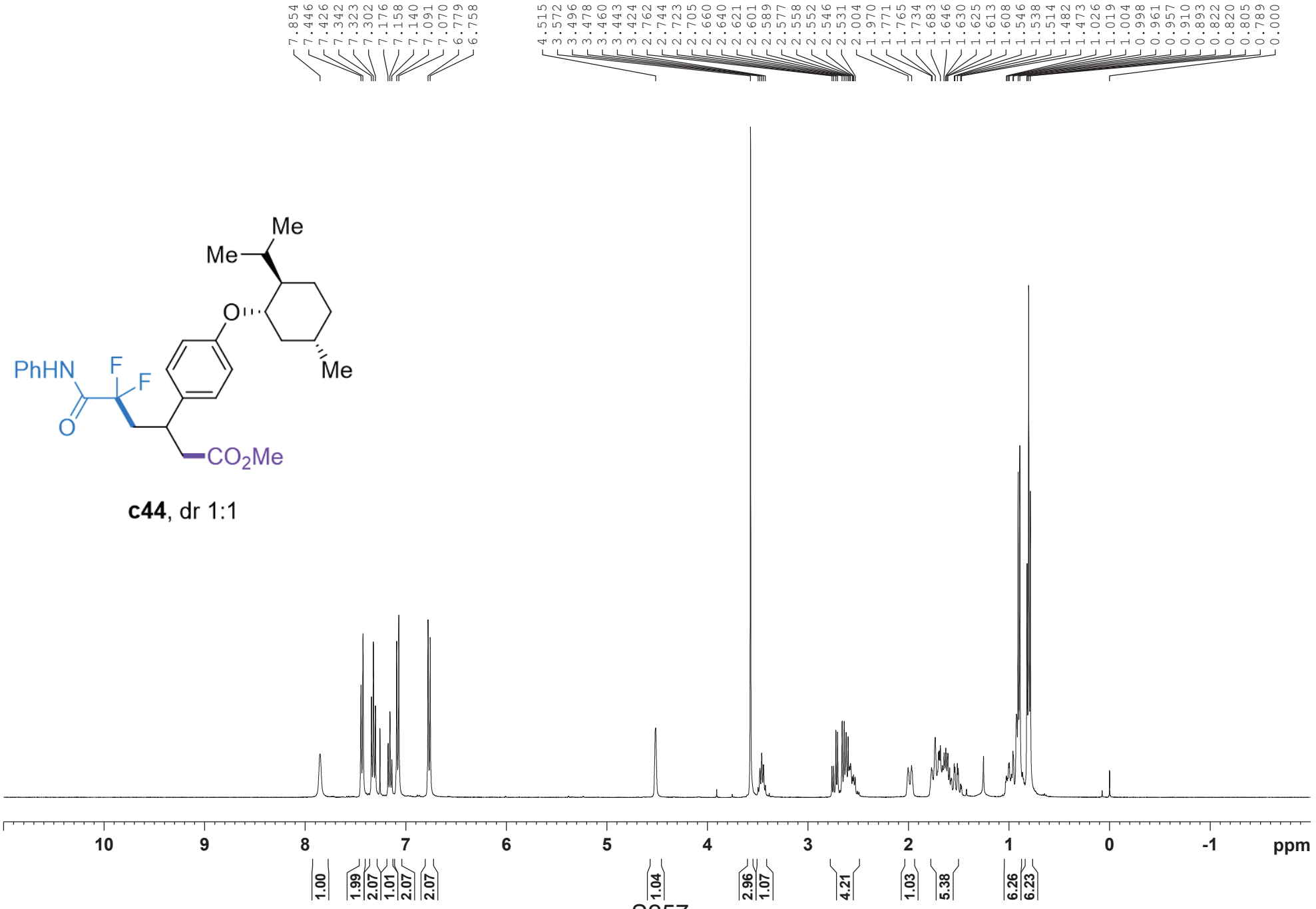

-101.005
-101.688
-104.467
-105.150
Me
H
N
F F
Ph
CO2Me
O
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.04

c42

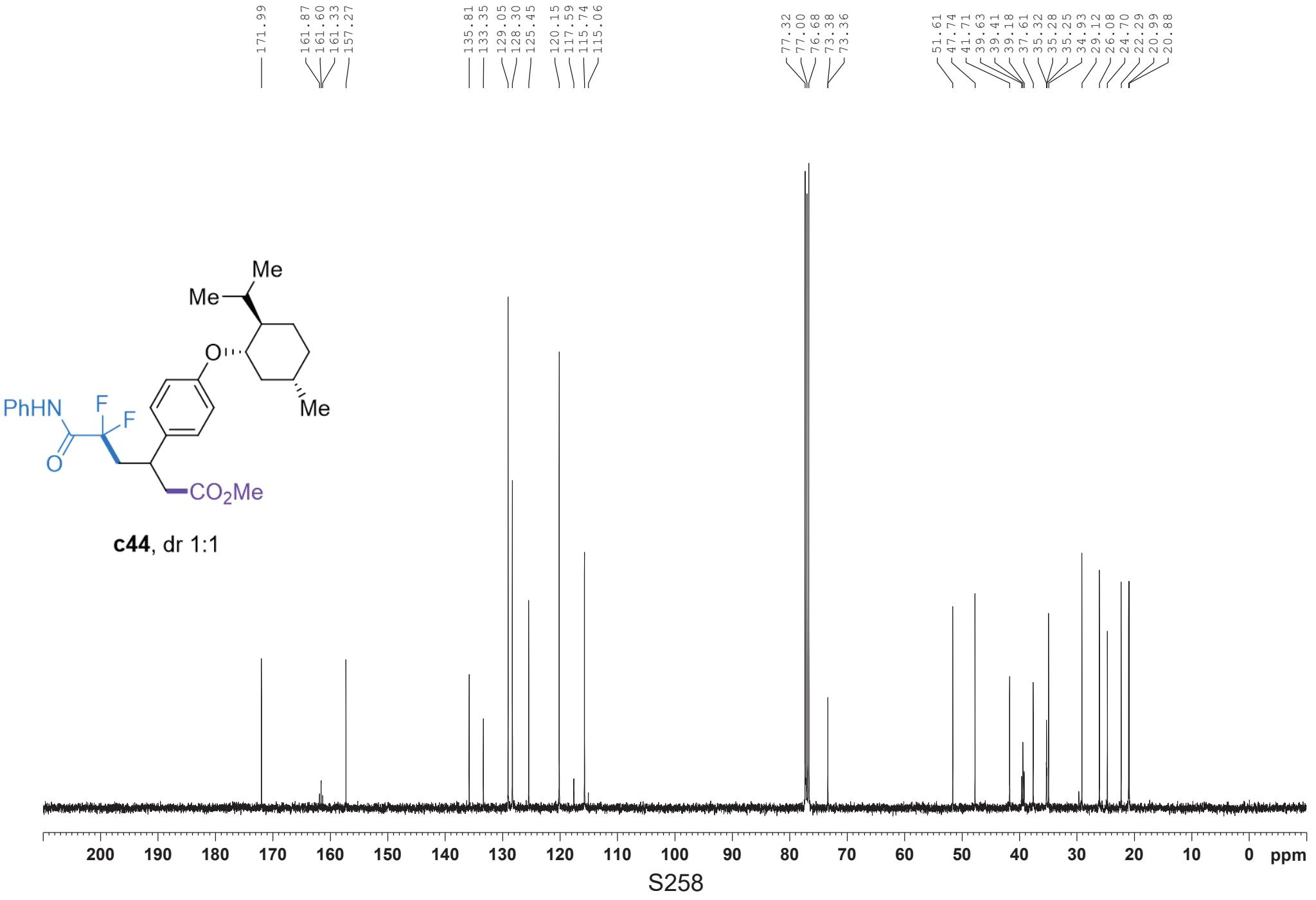

7.756
7.269
7.250
7.244
7.237
7.232
7.210
7.205
7.189
7.179
7.175
7.171
7.163
7.157
7.149
7.144
7.140
7.136
7.128
7.123
7.066
7.046
3.553
3.534
3.531
3.514
3.497
3.477
2.782
2.765
2.743
2.726
2.684
2.668
2.663
2.649
2.644
2.634
2.629
2.624
2.609
2.605
2.594
2.590
2.584
2.565
2.550
2.224
2.215
Me
Me
H
N
O
F
F
Ph
CO2Me
c43
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.16
5.16
1.01
2.93
0.99
4.22
3.03
3.04


171.70
161.67
161.39
161.11
142.03
137.30
133.91
133.48
129.94
128.55
127.36
127.07
121.52
120.10
117.57
115.04
51.56
41.46
39.50
39.28
39.05
36.12
36.08
36.04
19.75
19.17
Me
Me
H
N
O
F
F
Ph
CO2Me
c43
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

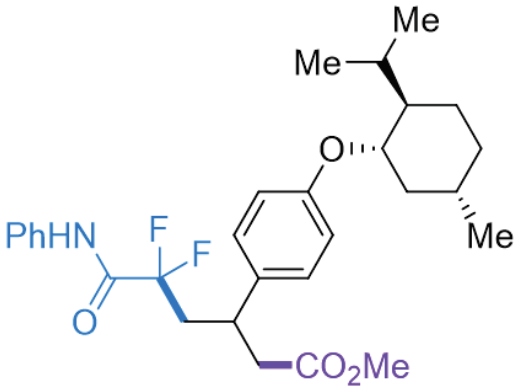

-101.444
-102.124
-104.478
-105.157
Me
Me
H
N
O
F
F
Ph
CO2Me
c43
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
0.97


7.854
7.446
7.426
7.342
7.323
7.302
7.176
7.158
7.140
7.091
7.070
6.779
6.758
4.515
3.572
3.496
3.478
3.460
3.443
3.424
2.762
2.744
2.723
2.705
2.660
2.640
2.621
2.601
2.589
2.577
2.558
2.552
2.546
2.531
2.004
1.970
1.771
1.765
1.734
1.683
1.646
1.630
1.625
1.613
1.608
1.546
1.538
1.514
1.482
1.473
1.026
1.019
1.004
0.998
0.961
0.957
0.910
0.893
0.822
0.820
0.805
0.789
0.000
Me
Me
O
Me
PhHN
F
F
O
CO2Me
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
1.00
1.99
2.07
1.01
2.07
2.07
1.04
2.96
1.07
4.21
1.03
5.38
6.26
6.23

c44, dr 1:1

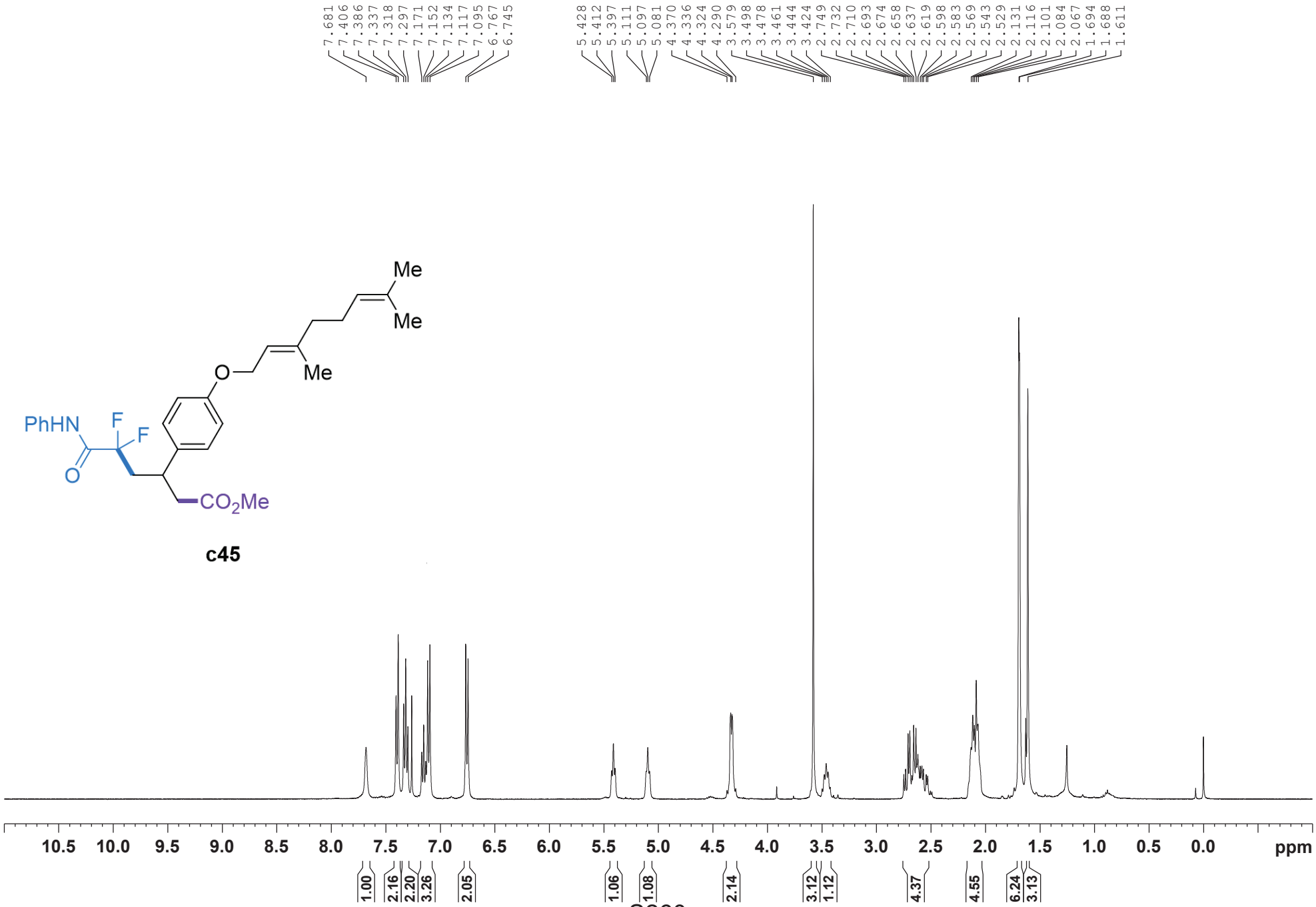

171.99
161.87
161.60
161.33
157.27
135.81
133.35
129.05
128.30
125.45
120.15
117.59
115.74
115.06
77.32
77.00
76.68
73.38
73.36
51.61
47.74
41.71
39.63
39.41
39.18
37.61
35.32
35.28
35.25
34.93
29.12
26.08
24.70
22.29
20.99
20.88
Me
Me
O
Me
PhHN
F
F
O
CO2Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

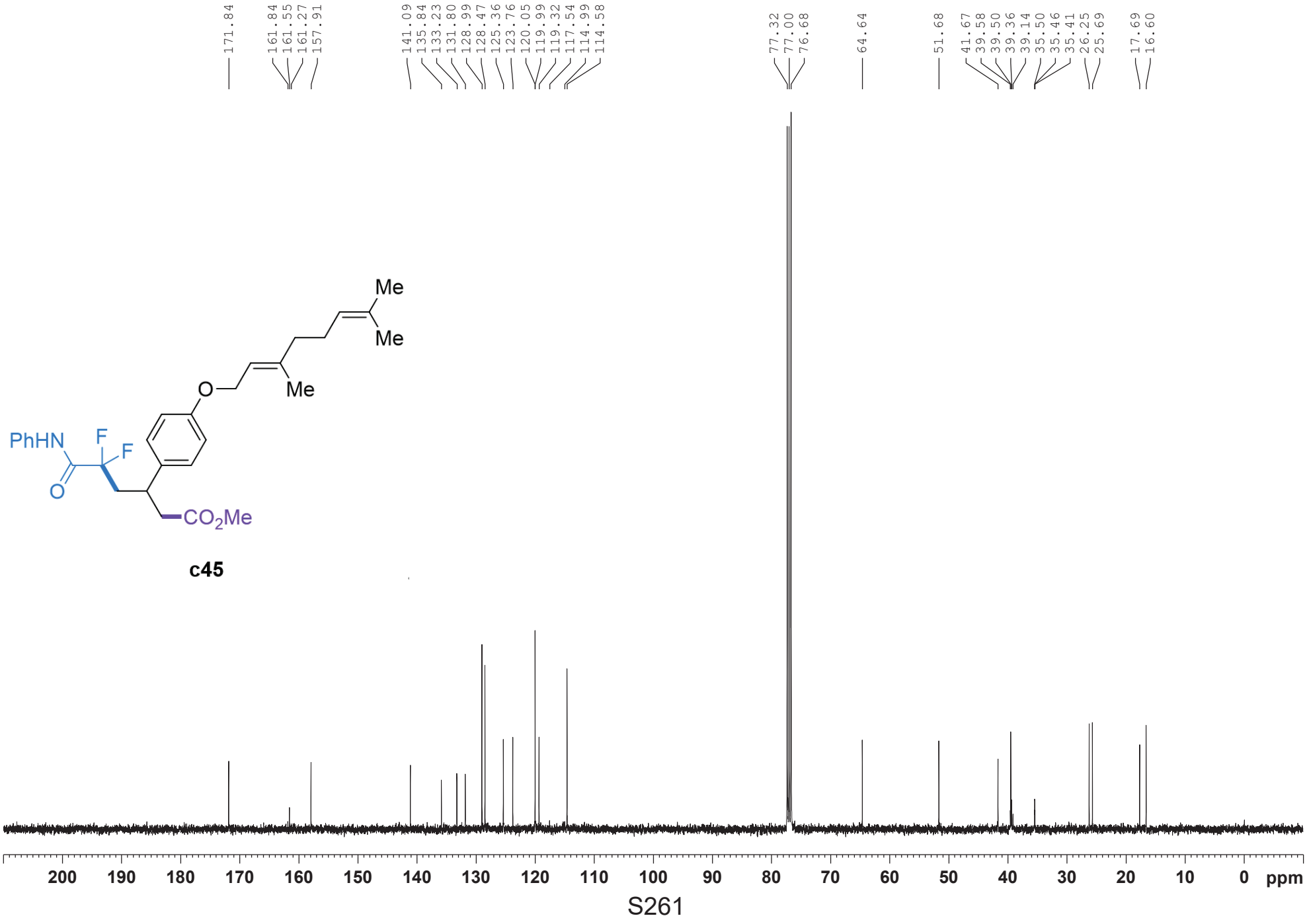
c44, dr 1:1


Me
Me
O
Me
PhHN
F
F
O
CO2Me

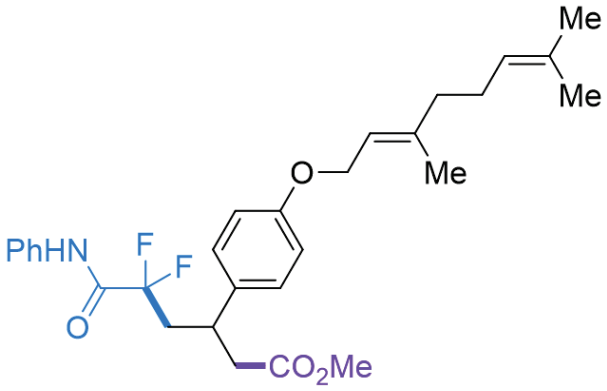
c44, dr 1:1

-101.033
-101.039
-101.711
-101.718
-104.886
-104.927
-105.565
-105.607
-101.7
ppm
-104.9
ppm
-101.0
ppm
-105.6
ppm
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.01
0.28
0.28
0.19
0.20


7.681
7.406
7.386
7.337
7.318
7.297
7.171
7.152
7.134
7.117
7.095
6.767
6.745
5.428
5.412
5.397
5.111
5.097
5.081
4.370
4.336
4.324
4.290
3.579
3.498
3.478
3.461
3.444
3.424
2.749
2.732
2.710
2.693
2.674
2.658
2.637
2.619
2.598
2.583
2.569
2.543
2.529
2.131
2.116
2.101
2.084
2.067
1.694
1.688
1.611
Me
Me
Me
O
PhHN
F
F
O
CO2Me
c45
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.16
2.20
3.26
2.05
1.06
1.08
2.14
3.12
1.12
4.37
4.55
6.24
3.13

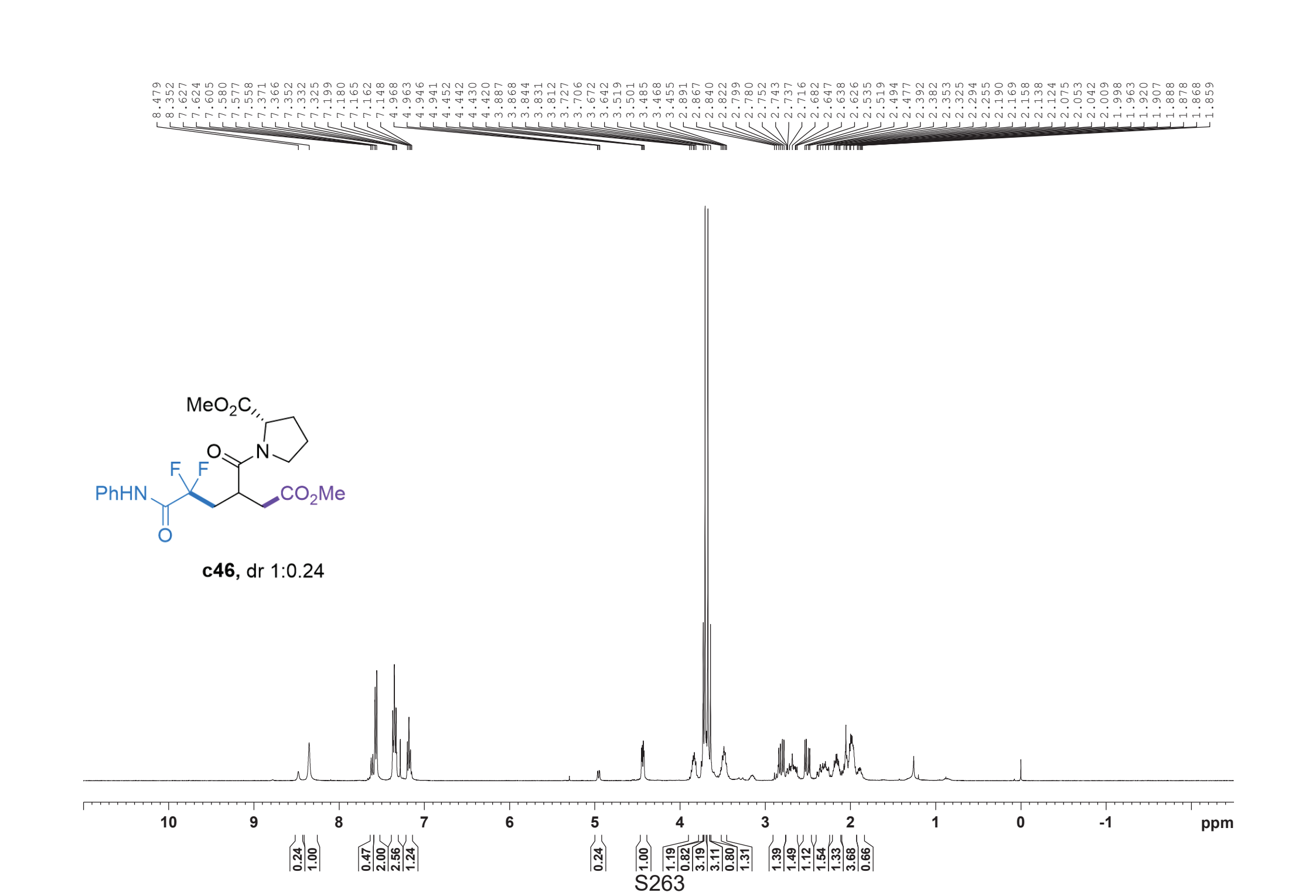

171.84
161.84
161.55
161.27
157.91
141.09
135.84
133.23
131.80
128.99
128.47
125.36
123.76
120.05
119.99
119.32
117.54
114.99
114.58
77.32
77.00
76.68
64.64
51.68
41.67
39.58
39.50
39.36
39.14
35.50
35.46
35.41
26.25
25.69
17.69
16.60
Me
Me
Me
O
PhHN
F
F
O
CO2Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

c45

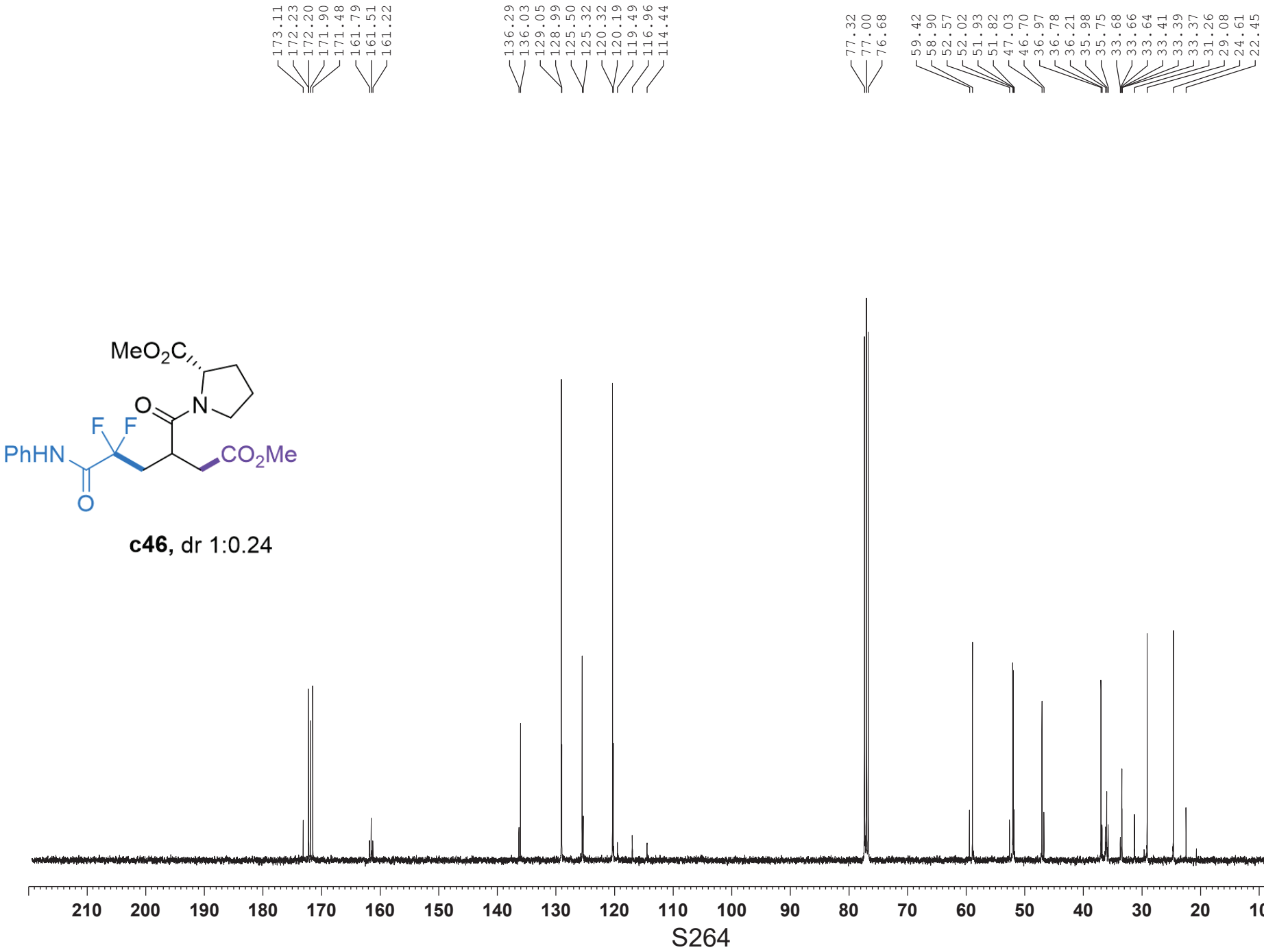

Me
Me
Me
O
PhHN
F
F
O
CO2Me

c45

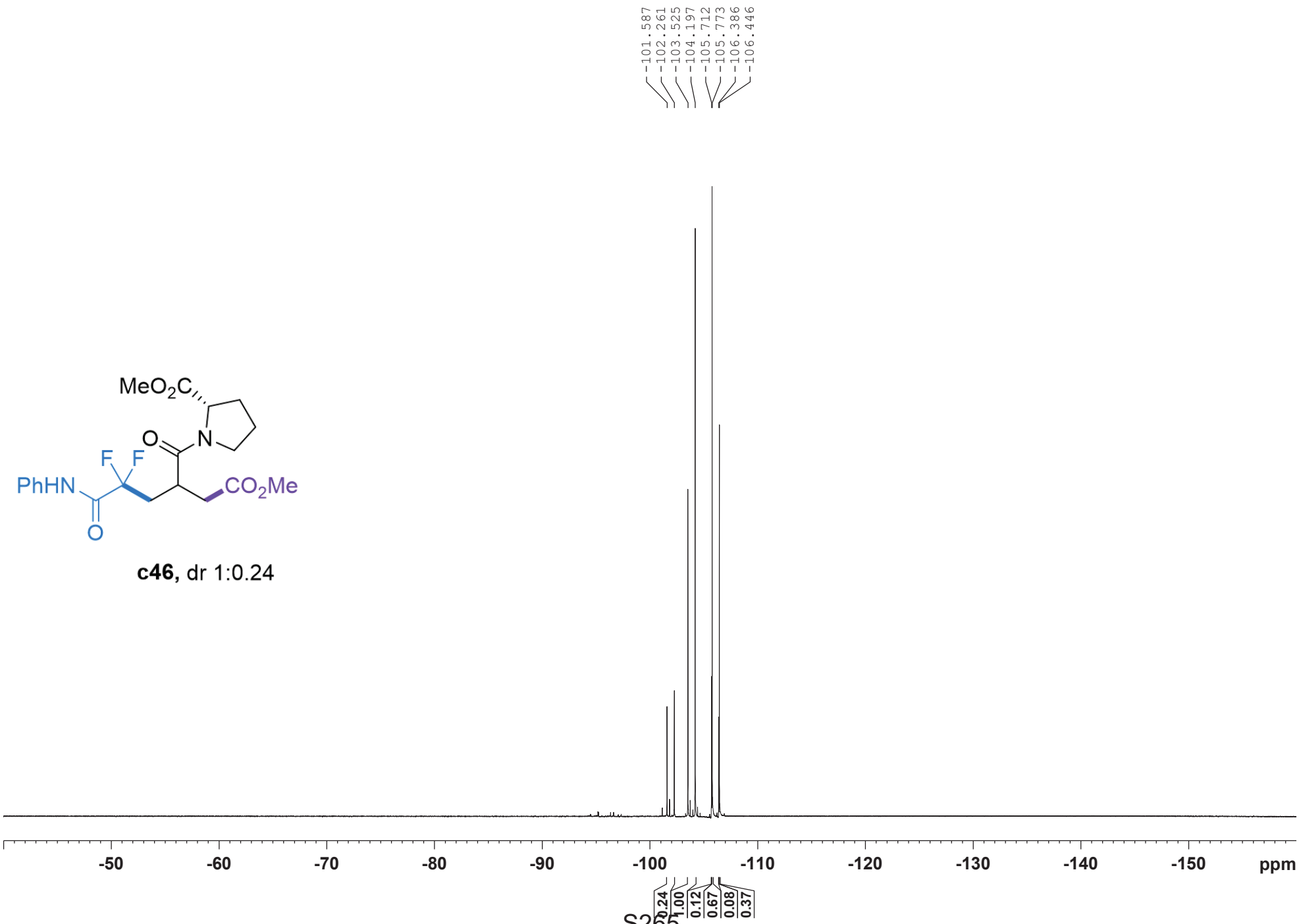
-99.768
-100.448
-106.084
-106.764
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.03


8.479
8.352
7.627
7.624
7.605
7.580
7.577
7.558
7.371
7.366
7.352
7.332
7.325
7.199
7.180
7.165
7.162
7.148
4.968
4.963
4.946
4.941
4.452
4.442
4.430
4.420
3.887
3.868
3.844
3.831
3.812
3.727
3.706
3.672
3.642
3.519
3.501
3.485
3.468
3.455
2.891
2.867
2.840
2.822
2.799
2.780
2.752
2.743
2.737
2.716
2.682
2.647
2.638
2.626
2.535
2.519
2.494
2.477
2.392
2.382
2.353
2.325
2.294
2.255
2.190
2.169
2.158
2.138
2.124
2.075
2.053
2.042
2.009
1.998
1.963
1.920
1.907
1.888
1.878
1.868
1.859
MeO2C
O
N
F
F
PhHN
CO2Me
O
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
0.24
1.00
0.47
2.00
2.56
1.24
0.24
1.00
1.19
0.82
3.19
3.11
0.80
1.31
1.39
1.49
1.12
1.54
1.33
3.68
0.66

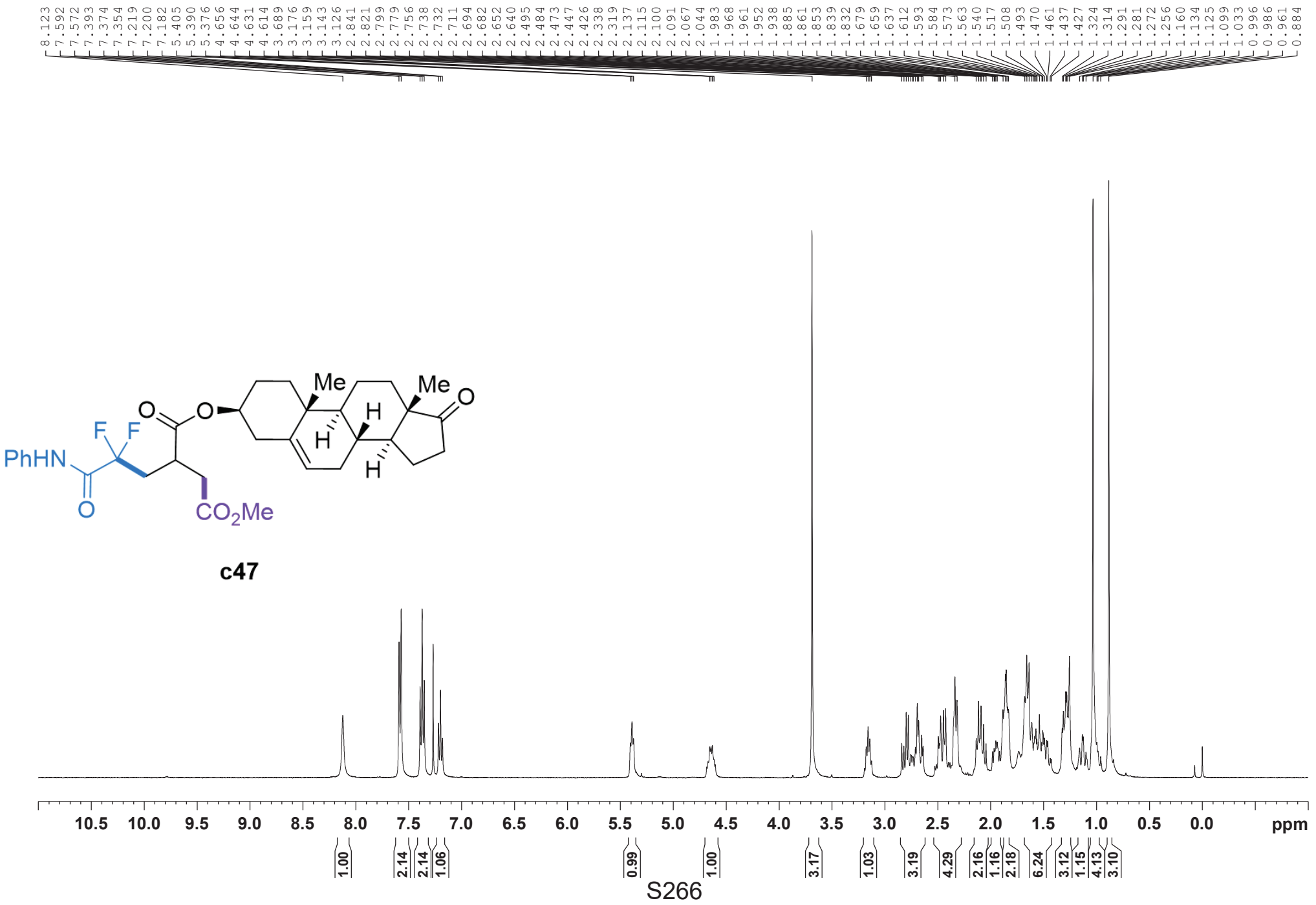
c46, dr 1:0.24

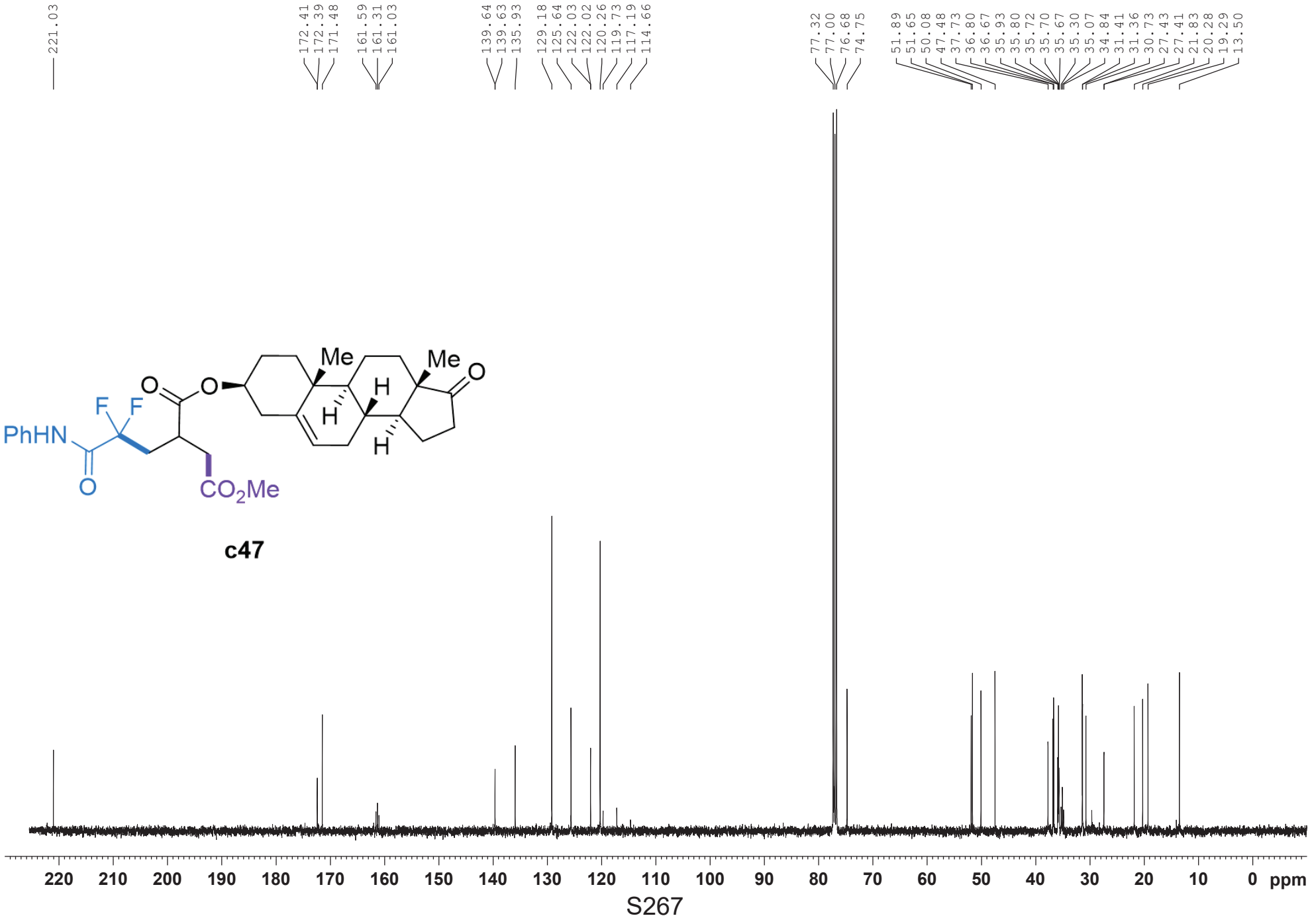

173.11
172.23
172.20
171.90
171.48
161.79
161.51
161.22
136.29
136.03
129.05
128.99
125.50
125.32
120.32
120.19
119.49
116.96
114.44
77.32
77.00
76.68
59.42
58.90
52.57
52.02
51.93
51.82
47.03
46.70
36.97
36.78
36.21
35.98
35.75
33.68
33.66
33.64
33.41
33.39
33.37
31.26
29.08
24.61
22.45
MeO2C
O
N
F
F
PhHN
CO2Me
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

c46, dr 1:0.24

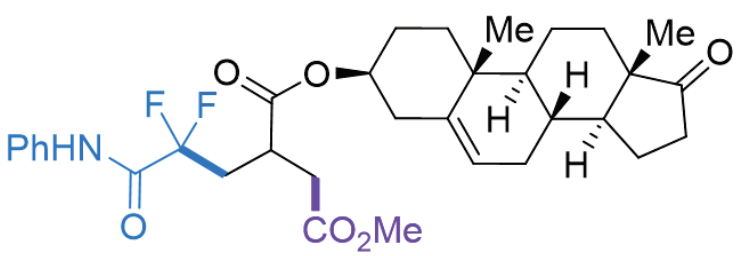

-101.587
-102.261
-103.525
-104.197
-105.712
-105.773
-106.386
-106.446
MeO2C
O
N
F
F
PhHN
CO2Me
O
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
0.24
1.00
0.12
0.67
0.08
0.37

c46, dr 1:0.24


8.123
7.592
7.572
7.393
7.374
7.354
7.219
7.200
7.182
5.405
5.390
5.376
4.656
4.644
4.631
4.614
3.689
3.176
3.159
3.143
3.126
2.841
2.821
2.799
2.779
2.756
2.738
2.732
2.711
2.694
2.682
2.652
2.640
2.495
2.484
2.473
2.447
2.426
2.338
2.319
2.137
2.115
2.100
2.091
2.067
2.044
1.983
1.968
1.961
1.952
1.938
1.885
1.861
1.853
1.839
1.832
1.679
1.659
1.637
1.612
1.593
1.584
1.573
1.563
1.540
1.517
1.508
1.493
1.470
1.461
1.437
1.427
1.324
1.314
1.291
1.281
1.272
1.256
1.160
1.134
1.125
1.099
1.033
0.996
0.986
0.961
0.884
PhHN
F
F
O
O
O
O
Me
Me
H
H
H
O
CO2Me
c47
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.14
2.14
1.06
0.99
1.00
3.17
1.03
3.19
4.29
2.16
1.16
2.18
6.24
3.12
1.15
4.13
3.10

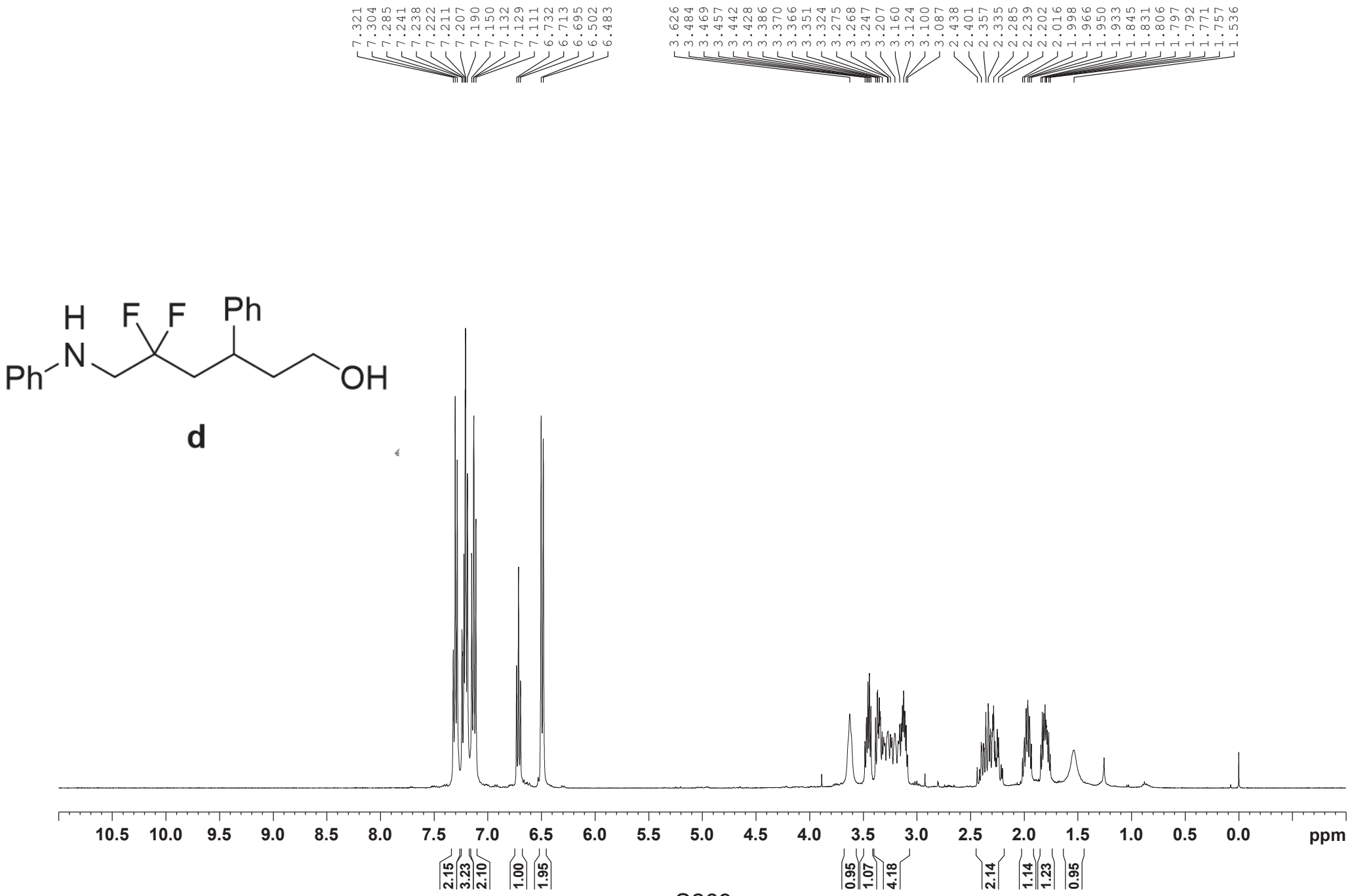

221.03
172.41
172.39
171.48
161.59
161.31
161.03
139.64
139.63
135.93
129.18
125.64
122.03
122.02
120.26
119.73
117.19
114.66
77.32
77.00
76.68
74.75
51.89
51.65
50.08
47.48
37.73
36.80
36.67
35.93
35.80
35.72
35.70
35.67
35.30
35.07
34.84
31.41
31.36
30.73
27.43
27.41
21.83
20.28
19.29
13.50
PhHN
F
F
O
O
O
O
Me
Me
H
H
H
O
CO2Me
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

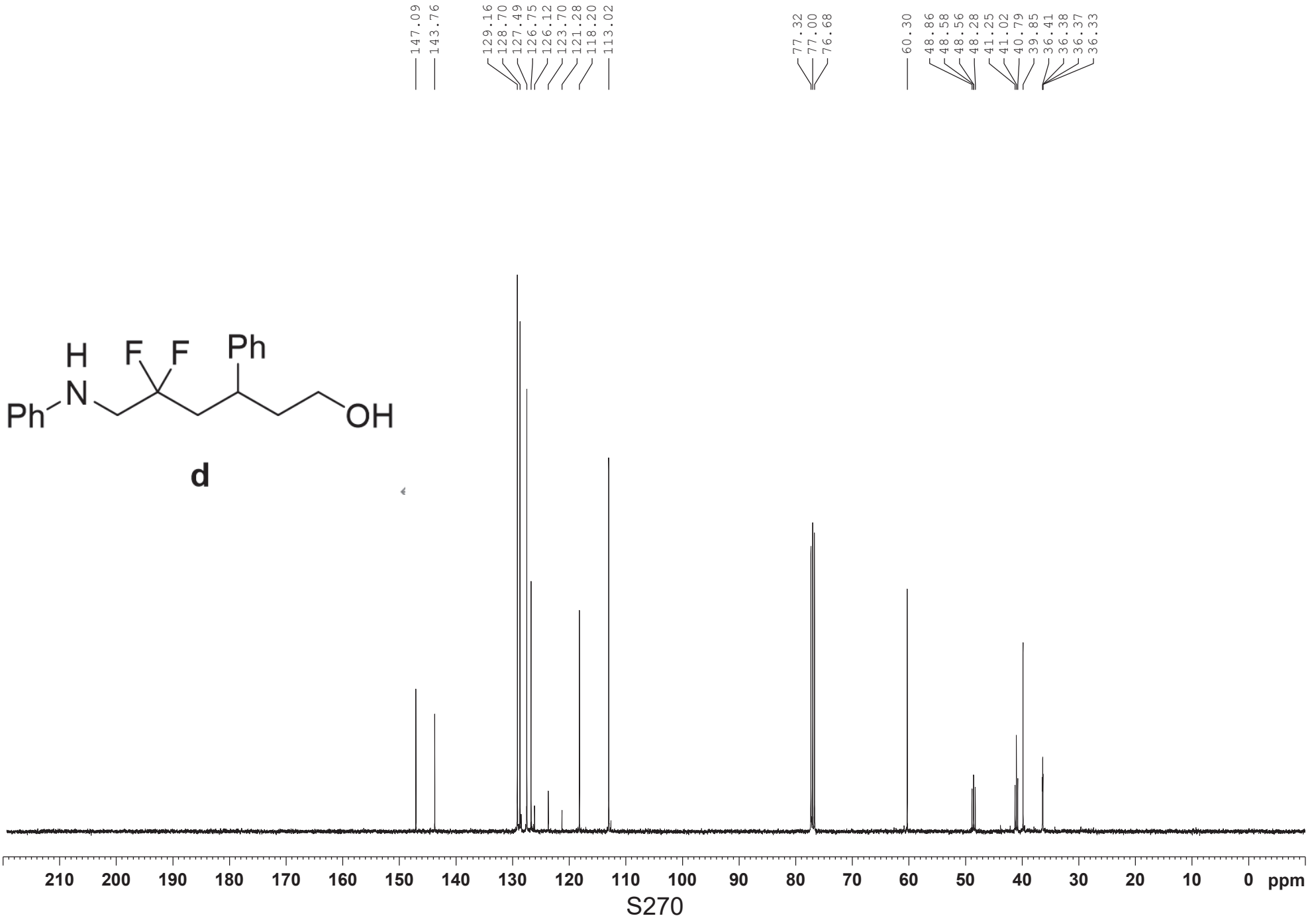
c47

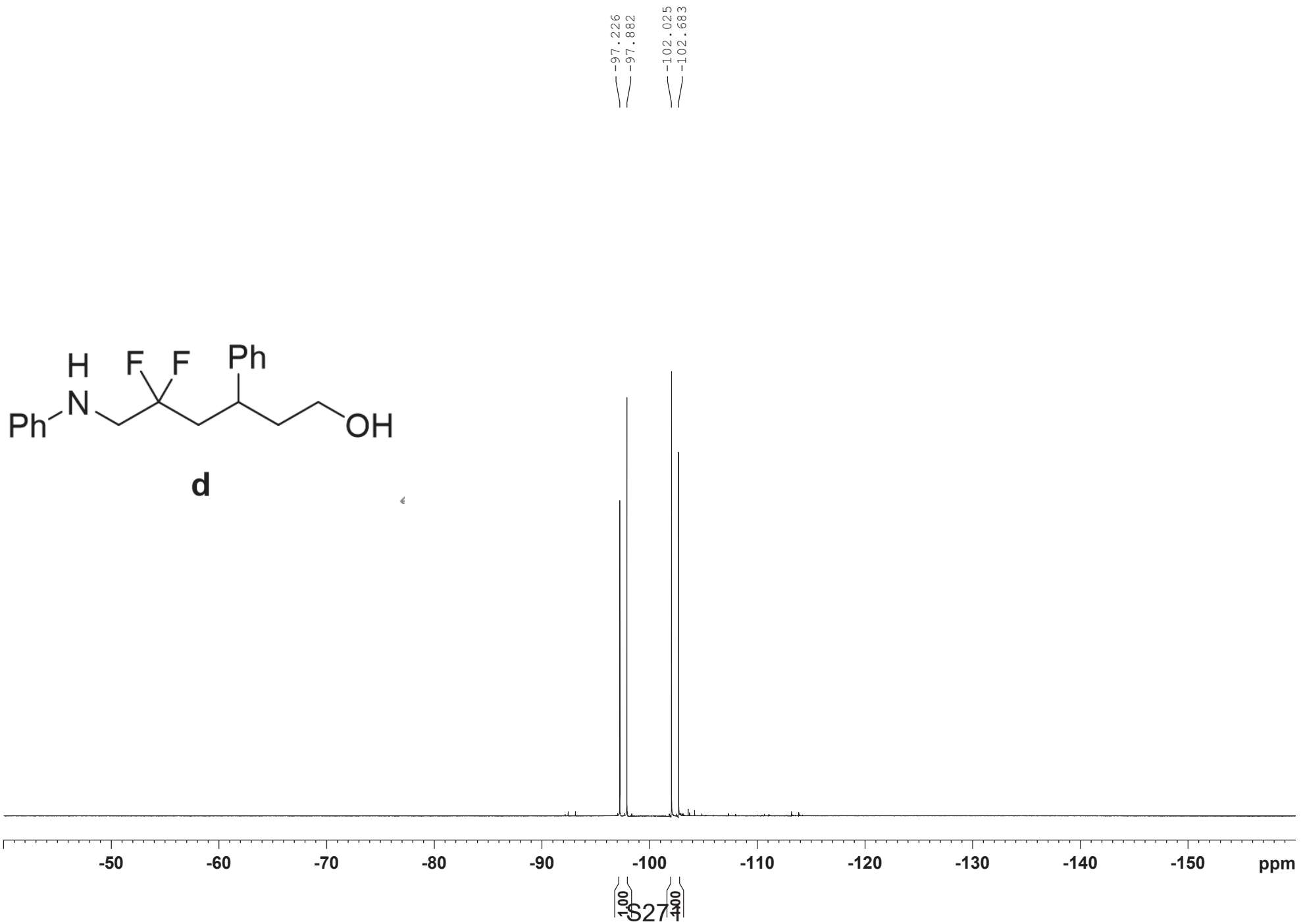

PhHN
F
F
O
O
O
CO2Me
Me
Me
H
H
H
O

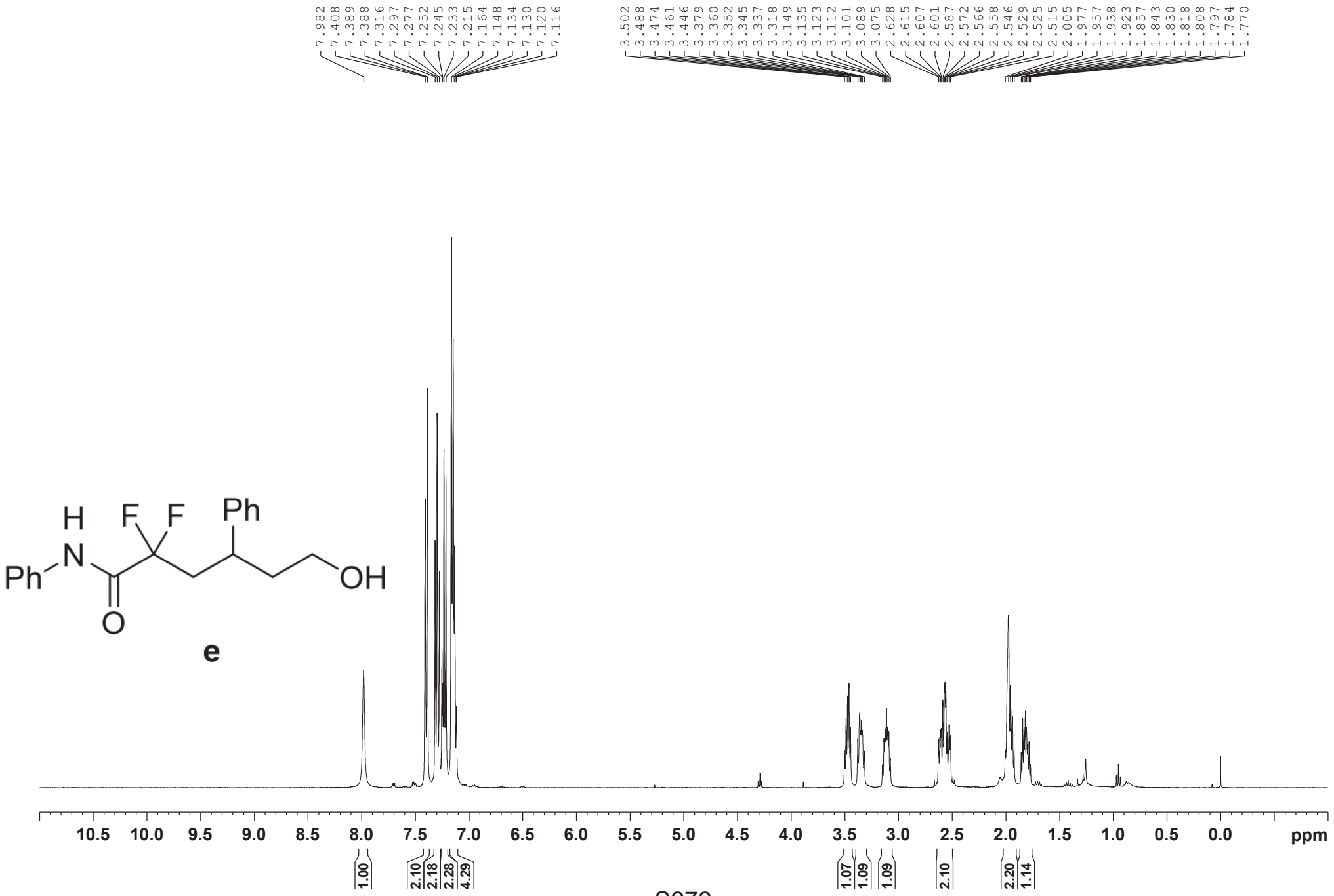
c47

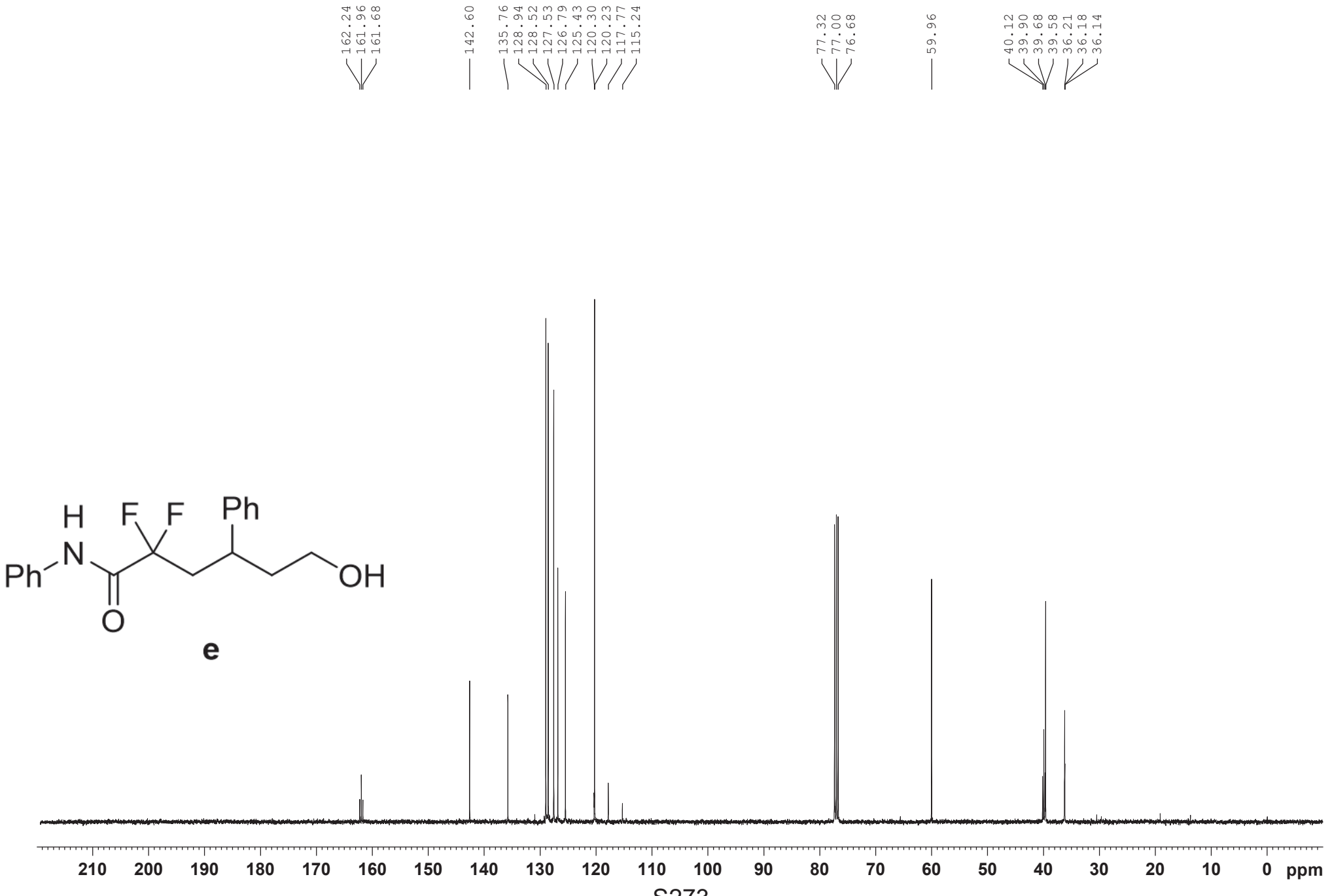
-103.947
-103.968
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
2.00

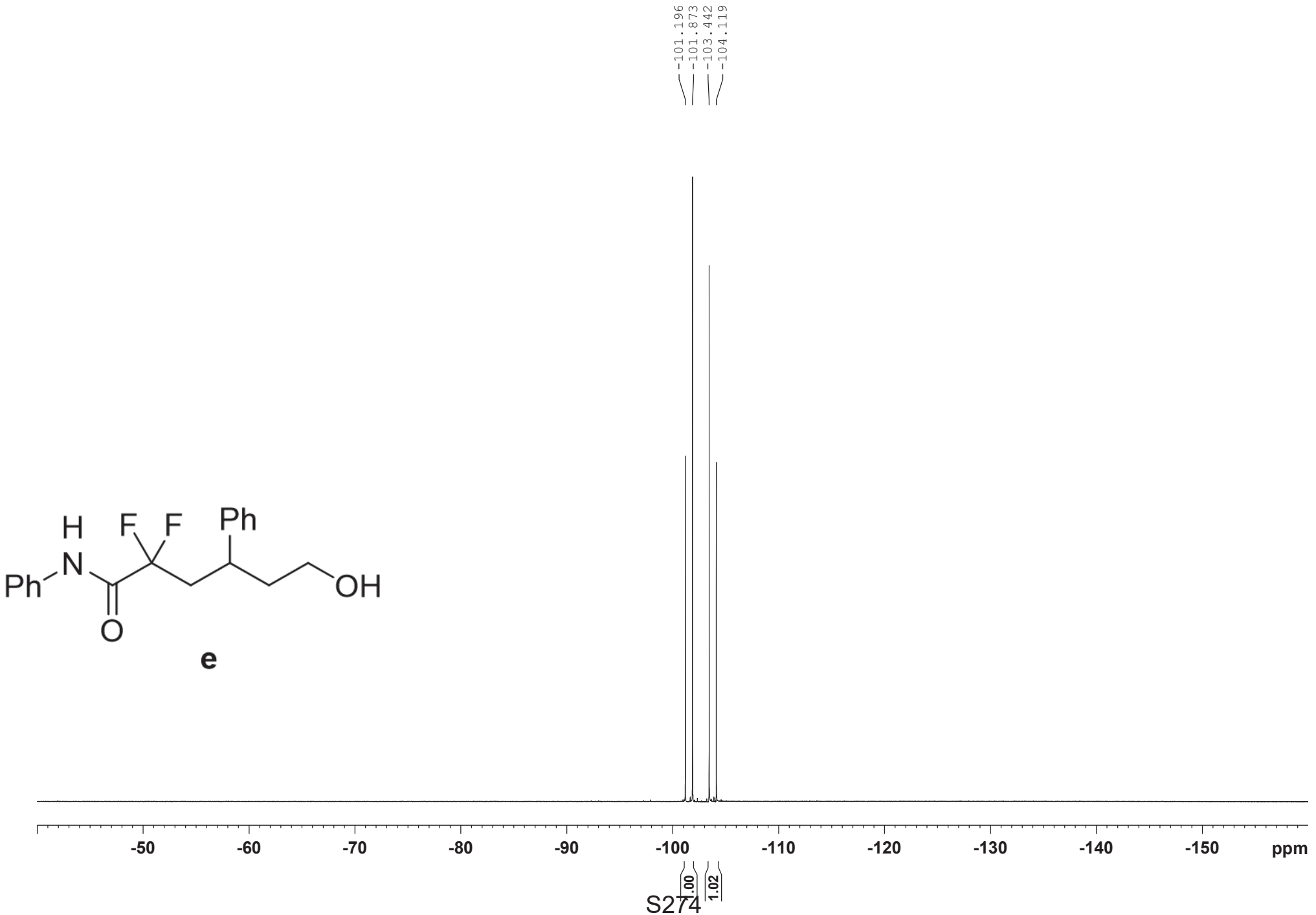

7.321
7.304
7.285
7.241
7.238
7.222
7.211
7.207
7.190
7.150
7.132
7.129
7.111
6.732
6.713
6.695
6.502
6.483
3.626
3.484
3.469
3.457
3.442
3.428
3.386
3.370
3.366
3.351
3.324
3.275
3.268
3.247
3.207
3.160
3.124
3.100
3.087
2.438
2.401
2.357
2.335
2.285
2.239
2.202
2.016
1.998
1.966
1.950
1.933
1.845
1.831
1.806
1.797
1.792
1.771
1.757
1.536
H
F
F
Ph
N
Ph
OH
d
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.15
3.23
2.10
1.00
1.95
0.95
1.07
4.18
2.14
1.14
1.23
0.95

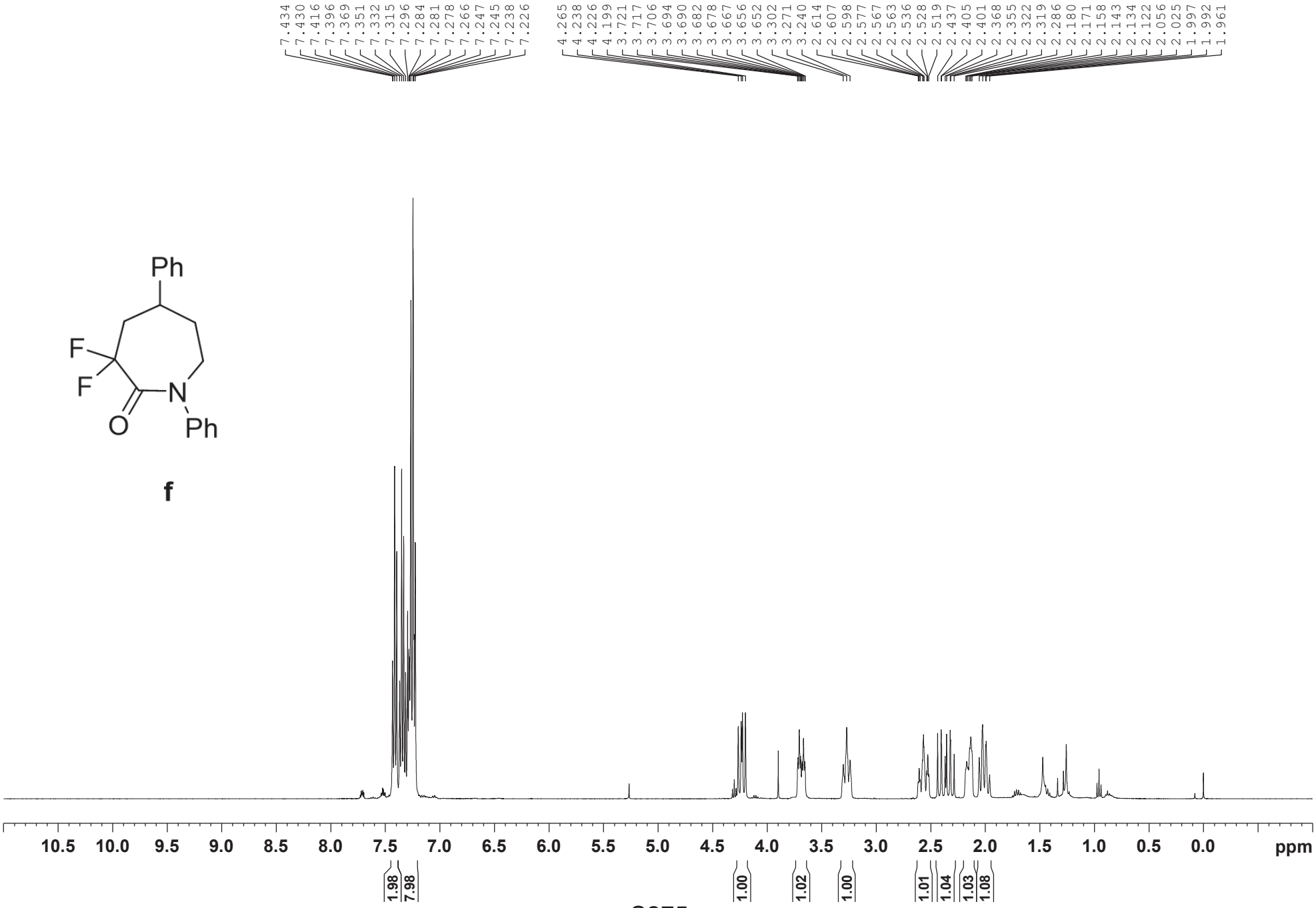

147.09
143.76
129.16
128.70
127.49
126.75
126.12
123.70
121.28
118.20
113.02
77.32
77.00
76.68
60.30
48.86
48.58
48.56
48.28
41.25
41.02
40.79
39.85
36.41
36.38
36.37
36.33
H
F
F
Ph
N
Ph
OH
d
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

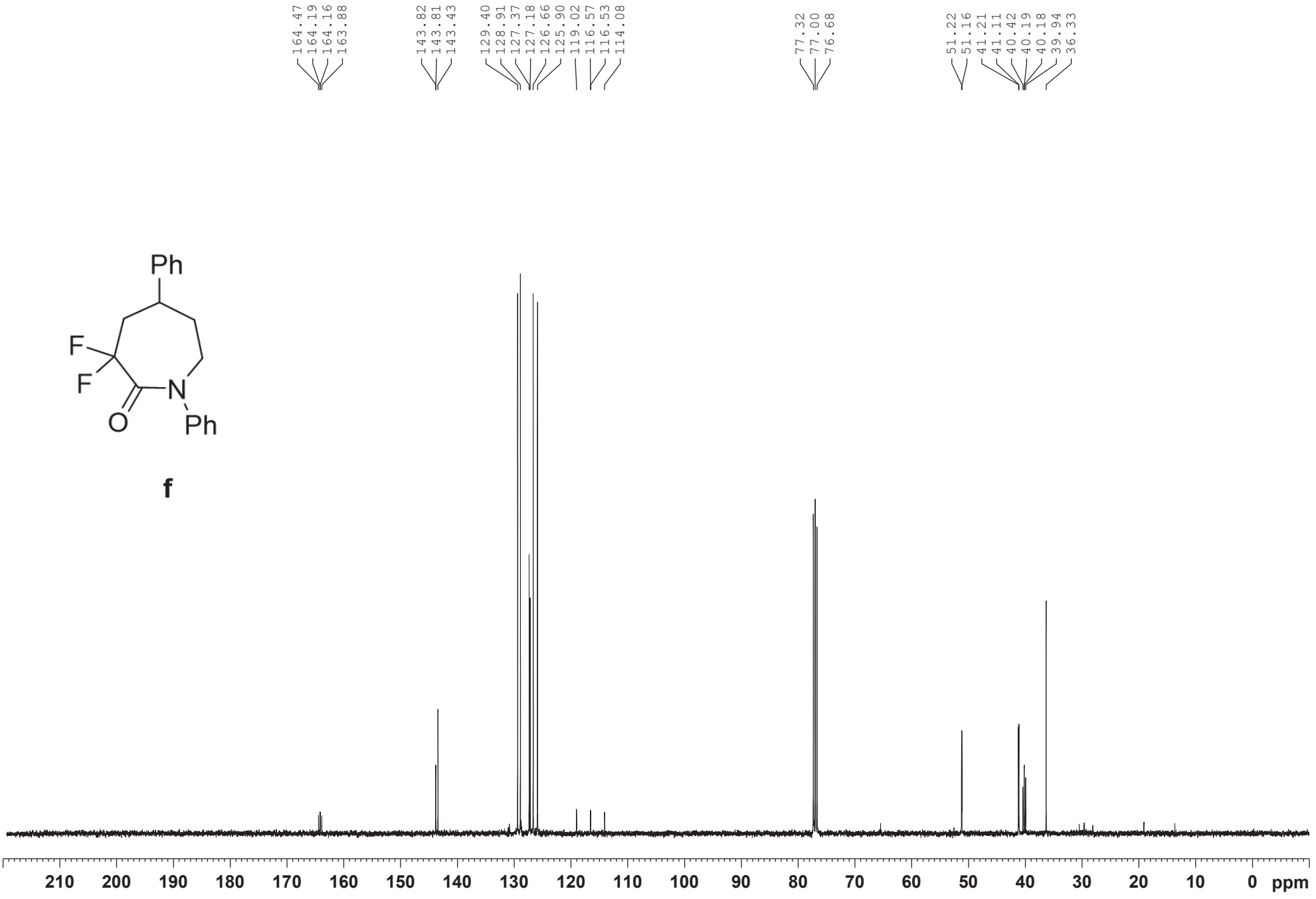

-97.226
-97.882
-102.025
-102.683
H
F
F
Ph
N
Ph
OH
d
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.00

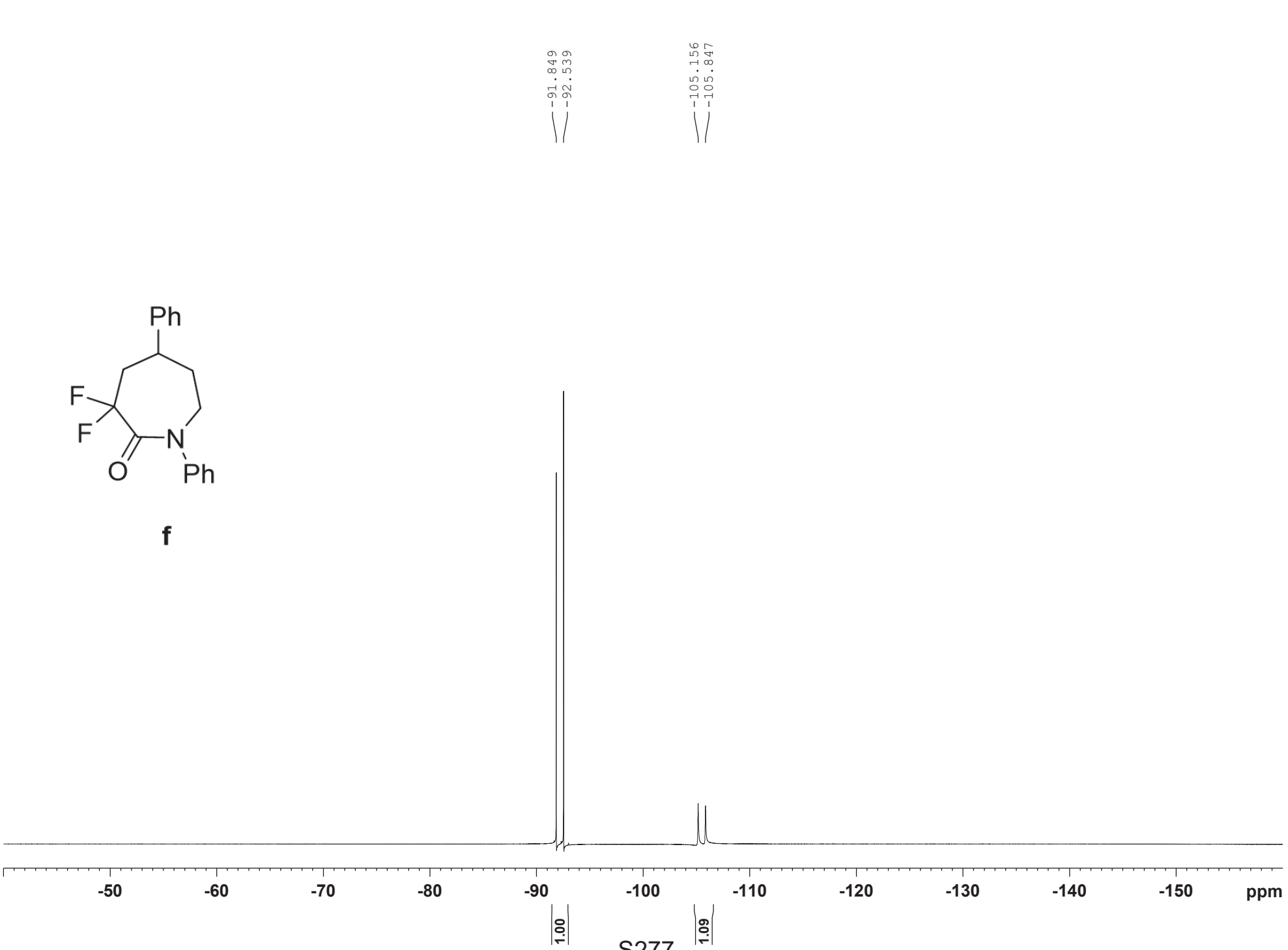

7.982
7.408
7.389
7.388
7.316
7.297
7.277
7.252
7.245
7.233
7.215
7.164
7.148
7.134
7.130
7.120
7.116
3.502
3.488
3.474
3.461
3.446
3.379
3.360
3.352
3.345
3.337
3.318
3.149
3.135
3.123
3.112
3.101
3.089
3.075
2.628
2.615
2.607
2.601
2.587
2.572
2.566
2.558
2.546
2.529
2.525
2.515
2.005
1.977
1.957
1.938
1.923
1.857
1.843
1.830
1.818
1.808
1.797
1.784
1.770
H
F
F
Ph
N
Ph
OH
O
e
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.00
2.10
2.18
2.28
4.29
1.07
1.09
1.09
2.10
2.20
1.14

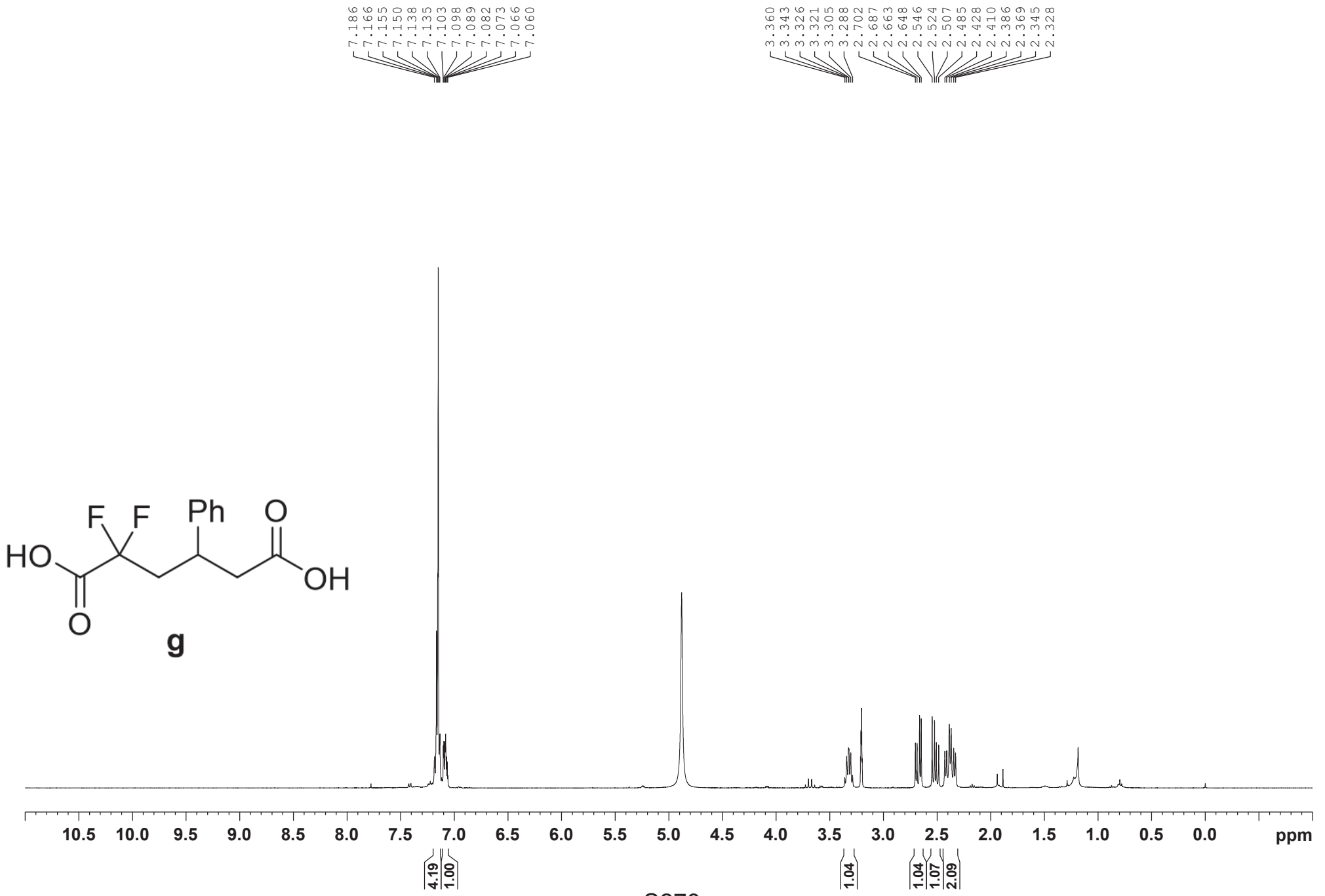

162.24
161.96
161.68
142.60
135.76
128.94
128.52
127.53
126.79
125.43
120.30
120.23
117.77
115.24
77.32
77.00
76.68
59.96
40.12
39.90
39.68
39.58
36.21
36.18
36.14
H
F
F
Ph
N
Ph
OH
O
e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

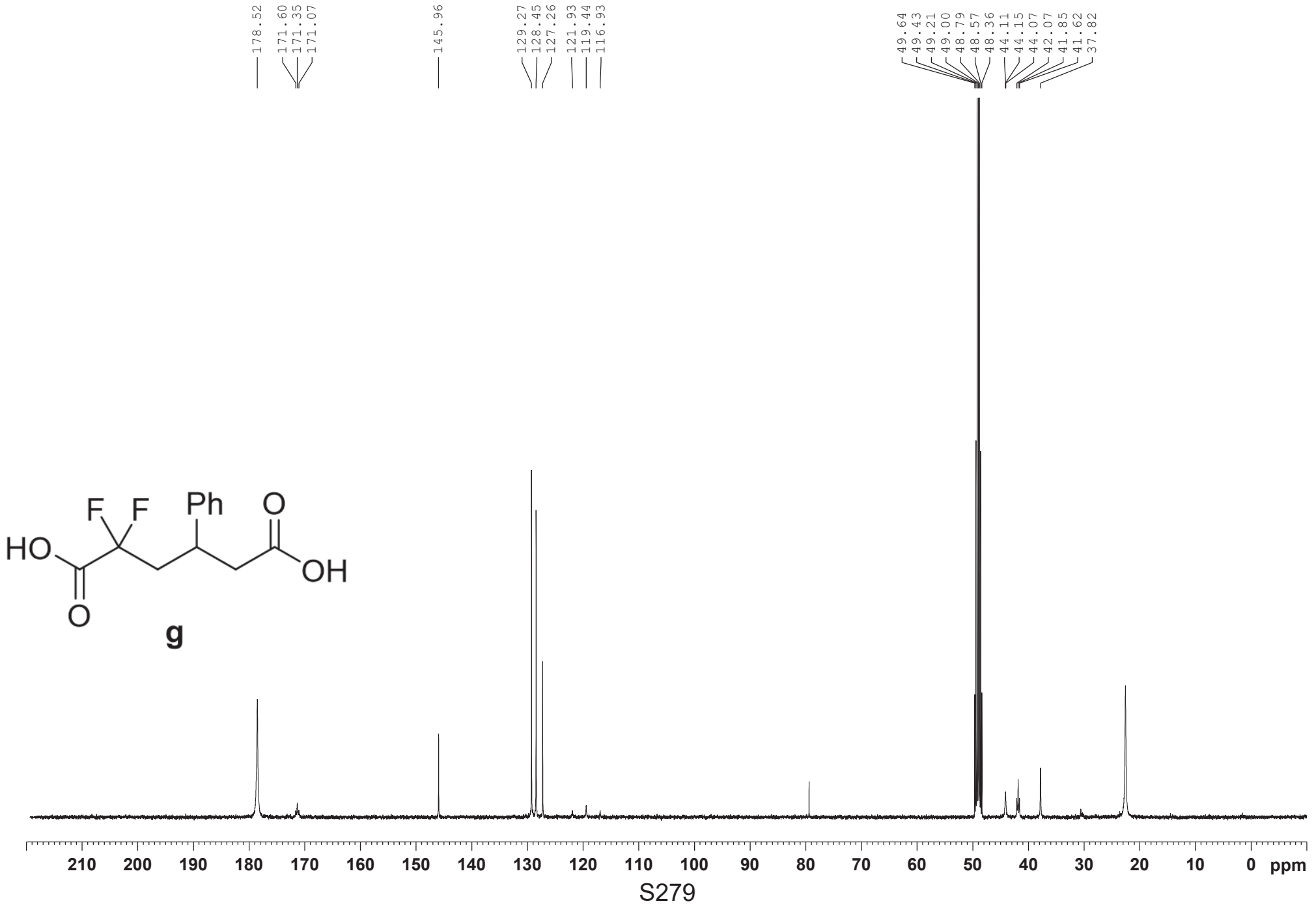

-101.196
-101.873
-103.442
-104.119
H
N
F
F
Ph
Ph
OH
O
e
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.02

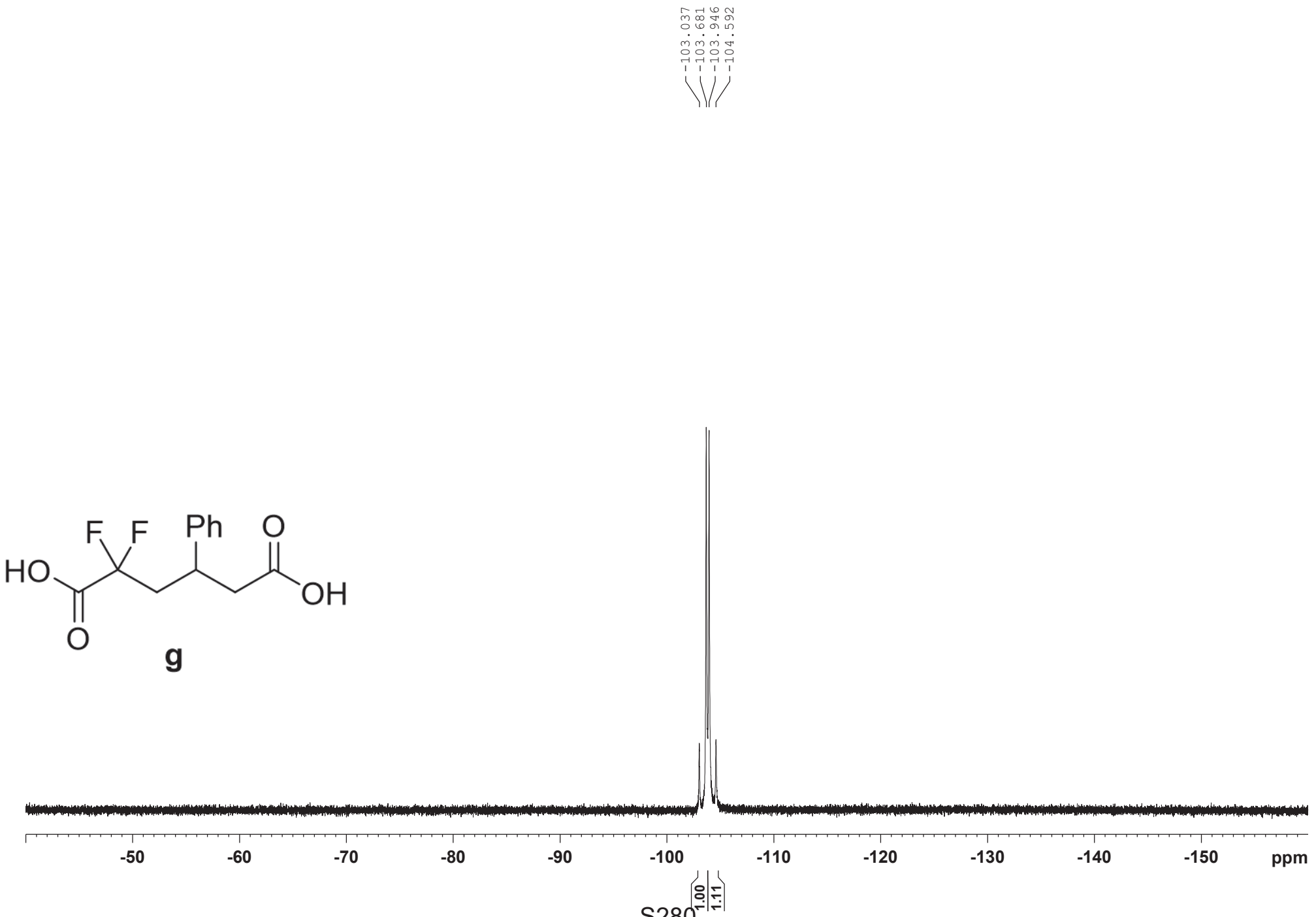

7.434
7.430
7.416
7.396
7.369
7.351
7.332
7.315
7.296
7.284
7.281
7.278
7.266
7.247
7.245
7.238
7.226
4.265
4.238
4.226
4.199
3.721
3.717
3.706
3.694
3.690
3.682
3.678
3.667
3.656
3.652
3.302
3.271
3.240
2.614
2.607
2.598
2.577
2.567
2.563
2.536
2.528
2.519
2.437
2.405
2.401
2.368
2.355
2.322
2.319
2.286
2.180
2.171
2.158
2.143
2.134
2.122
2.056
2.025
1.997
1.992
1.961
Ph
F
F
O
N
Ph
f
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
1.98
7.98
1.00
1.02
1.00
1.01
1.04
1.03
1.08

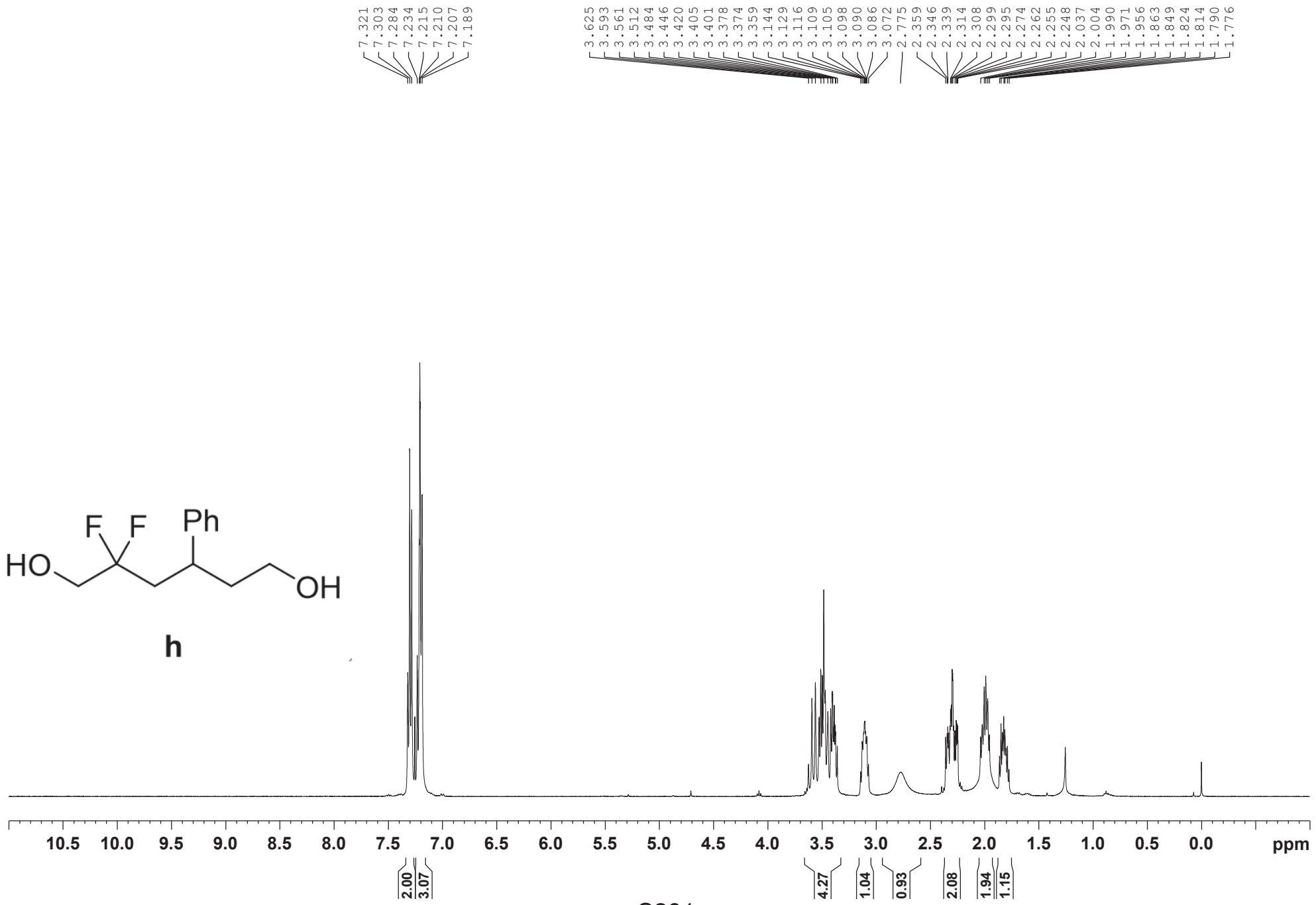

164.47
164.19
164.16
163.88
143.82
143.81
143.43
129.40
128.91
127.37
127.18
126.66
125.90
119.02
116.57
116.53
114.08
77.32
77.00
76.68
51.22
51.16
41.21
41.11
40.42
40.19
40.18
39.94
36.33
Ph
F
F
O
N
Ph
f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

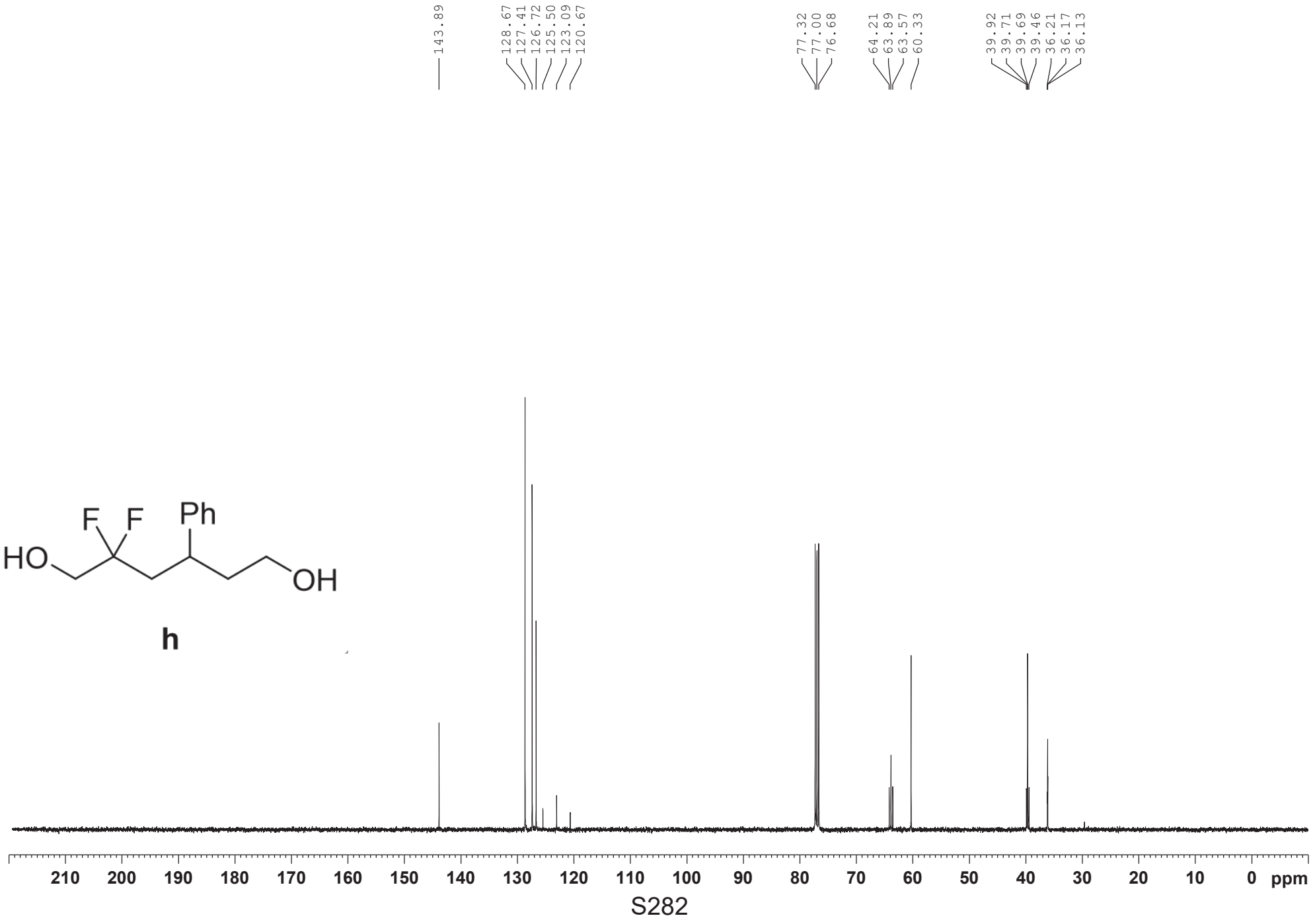

-91.849
-92.539
-105.156
-105.847
Ph
F
F
N
O
Ph
f
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.09

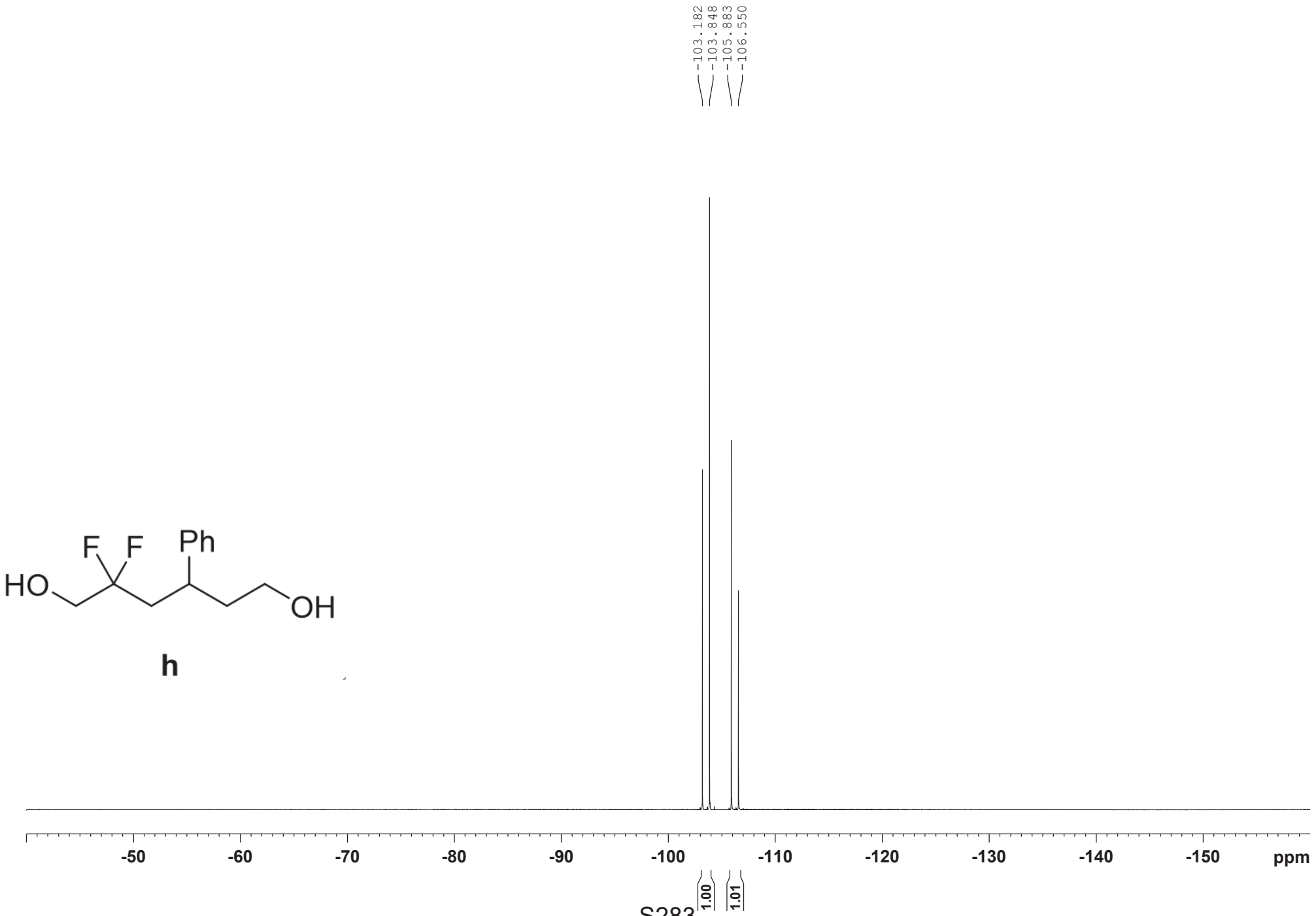

7.186
7.166
7.155
7.150
7.138
7.135
7.103
7.098
7.089
7.082
7.073
7.066
7.060
3.360
3.343
3.326
3.321
3.305
3.288
2.702
2.687
2.663
2.648
2.546
2.524
2.507
2.485
2.428
2.410
2.386
2.369
2.345
2.328
F
F
Ph
O
HO
OH
O
g
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
4.19
1.00
1.04
1.04
1.07
2.09


178.52
171.60
171.35
171.07
145.96
129.27
128.45
127.26
121.93
119.44
116.93
49.64
49.43
49.21
49.00
48.79
48.57
48.36
44.11
44.15
44.07
42.07
41.85
41.62
37.82
F
F
Ph
O
HO
OH
O
g
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-103.037
-103.681
-103.946
-104.592
F
F
Ph
O
HO
OH
O
g
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.11


7.321
7.303
7.284
7.234
7.215
7.210
7.207
7.189
3.625
3.593
3.561
3.512
3.484
3.446
3.420
3.405
3.401
3.378
3.374
3.359
3.144
3.129
3.116
3.109
3.105
3.098
3.090
3.086
3.072
2.775
2.359
2.346
2.339
2.314
2.308
2.299
2.295
2.274
2.262
2.255
2.248
2.037
2.004
1.990
1.971
1.956
1.863
1.849
1.824
1.814
1.790
1.776
F
F
Ph
HO
OH
h
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
3.07
4.27
1.04
0.93
2.08
1.94
1.15


143.89
128.67
127.41
126.72
125.50
123.09
120.67
77.32
77.00
76.68
64.21
63.89
63.57
60.33
39.92
39.71
39.69
39.46
36.21
36.17
36.13
F
F
Ph
HO
OH
h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


-103.182
-103.848
-105.883
-106.550
F
F
Ph
HO
OH
h
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
ppm
1.00
1.01