Supporting Information

Replacing Sulfuric Acid with Water in Electrochemical Metal-Free Mild Aromatic C-H Amidation: a Direct Route to *N*-Phenylamides

Alexander I. Kononov,[a‡] Sofia O. Strekalova*,[a‡] Vladimir I. Morozov,[a] Konstantin V. Boyko,[b,c] Vladimir I. Timashev,[b,d] Michael G. Medvedev*,[b,e] Olga B. Bazanova[a] Ekaterina V. Kobeleva,[a] Kamil A. Ivshin[a], Vasily M. Babaev[a] and Yulia H. Budnikova[a]

[a]Arbuzov Institute of Organic and Physical Chemistry, Kazan, 420088 Russia
[b]Zelinsky Institute of Organic Chemistry, Moscow, 119991, Russia
[c]Mendeleev University of Chemical Technology of Russia, Moscow, 125047 Russia
[d]Lomonosov Moscow State University, Moscow, 119991 Russia
[e]National Research University Higher School of Economics, Moscow, 101000 Russia
E-mail: strekalova@iopc.ru, medvedev.m.g@gmail.com

‡ These authors contributed equally to this work

Table of Contents:

1. General Information

1.1 Method

Preparative electrolysis was performed in galvanostatic mode with simultaneous control of the working electrode potential in thermostatically controlled, cylindrical 30 mL cell with separate anodic and cathodic compartments using a B5-49 direct current source at a current of 35 mA. A ceramic plate with the pore size 900 nm was used as a membrane. The potential of the working electrode was detected by a V7-27 DC voltmeter using Ag/AgCl as a reference electrode. The platinum cylindrical anode with a surface area of 20 cm^2 was used as a working electrode and the platinum rod (10 cm^2) was used as the cathode. The distance between two Pt electrodes is 1.5 cm. The catholyte was a saturated solution of the $PyHBF_4$ in the RCN (R = Me, Et). During electrolysis, the electrolyte was stirred using a magnetic stirrer. Preparative chromatography BUCHI system including Pump Module C-601, ELS Detector C-605, Fraction Collector C-660, Control Unit C-620, Sepacore Control Package and software program were used for products isolation.

1.2 Materials

Chemicals were obtained from commercial sources and used without further purification: 1,4-Bis(trifluoromethyl)benzene (Sigma Aldrich, 98%), 1,3-Bis(trifluoromethyl)benzene (Sigma Aldrich, 98%), 1,3,5-Tris(trifluoromethyl)benzene (Sigma Aldrich, 97%), Benzotrifluoride (Sigma Aldrich, ≥99%), Chlorobenzene (Sigma Aldrich, ≥99%), Fluorobenzene (Sigma Aldrich, 99%), Nitrobenzene (Sigma Aldrich, ≥99%), Benzene (Sigma Aldrich, ≥99%), Benzonitrile (Sigma Aldrich, 99+%), 1,2-Dichlorobenzene (Sigma Aldrich, anhydrous, 99%), 1-Chloro-4-nitrobenzene (Sigma Aldrich, 99%), 1-Chloro-2-nitrobenzene (Sigma Aldrich, 99%), 1-Fluoro-4-nitrobenzene (Sigma Aldrich, 99%), 1-Bromo-4-nitrobenzene (Sigma Aldrich, 99%), 4-Chloro-1-(trifluoromethyl)benzene (Sigma Aldrich, 99%), 1-Bromo-4-fluorobenzene (Sigma Aldrich, 99%), 1-Chloro-4-fluorobenzene (Sigma Aldrich, 99%), Ethyl benzoate (Sigma Aldrich, 99%), Dimethyl isophthalate (Sigma Aldrich, 99%), Phenol (Acros Organics, 99+%), 2,6-Dimethylphenol (Acros Organics, 99%), 2-Methylphenol (Acros Organics, 99%), Acetonitrile (Acros Organics, CHROMASOLV® Plus, ≥99.9%, «extra pure»), Propionitrile (Sigma Aldrich, 99%), Butyronitrile (Sigma Aldrich, 99%). Methyl salicylate and Ethyl salicylate were obtained by the known method.[1]

1.3 NMR and Mass measurements

NMR measurements were performed in the NMR department (A.E. Arbuzov Institute Organic and Physical Chemistry) of the Federal Collective Spectral Analysis Center for physical and

chemical studies on the structure, properties, and composition of matter and materials. NMR experiments were conducted using Bruker spectrometers AVANCE-400 (399.85 MHz (^{1}H), 100.6 MHz (^{13}C), 376 MHz (^{19}F)), AVANCE-600 (600.1 MHz (^{1}H), 150.9 MHz (^{13}C)) and AVANCE-500 (500.13 MHz (^{1}H), 125.77 MHz (^{13}C)) equipped with a pulsed gradient unit capable of producing magnetic field pulse gradients in the z-direction of 53.5 G/cm. All spectra were acquired in a 5 mm gradient inverse broad band probe head. As a result, chemical shifts were reported on the δ (ppm) scale relative to the residual ^{1}H and ^{13}C $CDCl_3$ and CD_3CN signal resulting in external NMR spectra. The ^{1}H and ^{13}C NMR spectra of synthesized compounds were completely assigned by using a combination of 2D NMR experiments, which included ^{1}H-^{1}H COSY, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC sequences.

Mass spectrometric studies (electrospray ionization) of the samples was carried out on a Bruker Daltonik GmbH AmazonX (Germany). Nitrogen was used as a drying gas in the source with a temperature of 220°C. The source voltage was 4.5 kV. Solutions of the samples were diluted with acetonitrile to a concentration of ~10–3 mg mL^{-1}. The samples were injected using an autosampler of an Agilent 1260 Infinity liquid chromatograph (Agilent Technologies, USA).

HPLC-MS experiment. Samples were analysed using an Impact II mass spectrometer with an Elute UHPLC system («Bruker Daltonik GmbH», Germany). The column used was a YMC-Triart C18 (50×2.0 mm; 3 μm). The temperature of the column thermostat was set at 40°C, and the temperature of the autosampler at 12°C. Elution solvents used were Milli-Q water + 0.1% FA (A) and HPLC-grade acetonitrile + 0.1% FA (B) and elution gradient was the following: 0 min at 5% B, 3 min at 95% B, 4 min at 95% B, 4.1 min at 5% B, 6 min at 5% B with a flow rate of 0.3 mL/min. The injection volume was 2 μL. Analytes were ionized by electrospray in positive polarity. ESI conditions were set with the capillary temperature at 220 °C, capillary voltage at 4.5 kV, and a sheath gas flow rate of 6 L/min. Measurements were made in the range *m*/*z* 50-1900. The solution of analyte (1 mg/mL, HPLC acetonitrile) was diluted in acetonitrile:water (5%:95%) solvent mixture to a concentration of 0.005 mg/mL. The solution of sodium iodide in Milli-Q water at concentration 2 mg/mL was used as a calibrant. The relative error in determining the masses was no more than 3.0 ppm. For instrument control and data acquiring the otofControl software (Bruker Daltonik GmbH, Version 5.2) was used. Data processing was performed by DataAnalysis software (Bruker Daltonik GmbH, Version 5.3).

2. Synthesis

2.1 Electrolysis setup

Figure S1. Electrolysis setup: cylindrical cell with divided anodic and cathodic compartments. **1** - anodic compartment; **2** - cathodic compartment; **3** - membrane: ceramic plate with the pore size of 900 nm; **4** – platinum cylindrical working electrode with a surface area of 20 cm^2 (anode); **5** - platinum rod (10 cm^2) (cathode); **6** - stir bar. The cell can be thermostatted.

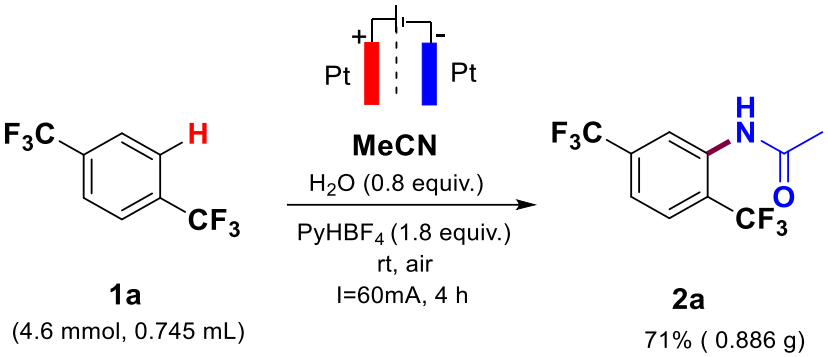
2.2 General electrolysis procedure

Arene (1.2 mmol), H_2O (0.8 equiv., 0.96 mmol, 17 ul) and nitrile (20 mL) as solvent were placed into anodic compartment **1** of the electrochemical divided cell equipped with a stir bar **6**. Saturated solution of $PyHBF_4$ (3.0 equiv., 3.6 mmol, 0.6 g) in nitrile was placed into cathodic compartment **2**. The electrolysis was carried out at room temperature (23-25 °C) and a constant current of 35 mA in air for the specified time. At the end of electrolysis as monitored by TLC, the solvent (nitrile) was evaporated on rotary evaporator to give the residue; nitrile was collected (≈16 ml). The distilled off nitrile can be reused in the following reactions. Then, chloroform (≈15 ml) was added to the residue to separate the supporting electrolyte by filtration, since $PyHBF_4$ is not soluble in chloroform. The mixture with product was filtered and chloroform was evaporated to give the crude product. The crude product was further purified by silica gel (mesh size 230–400) column chromatography (ethyl acetate/hexane = 1:1 or 1:2).

The chloroform-insoluble pyridinium salt $PyHBF_4$ was collected after electrolysis and washed with ethanol to remove the gum. Recovered (≈ 0.48 g) and purified salt can be used in the following synthesis.

2.3 Gram scale synthesis

1,4-Bis(trifluoromethyl)benzene **1a** (4.6 mmol, 0.745 mL), MeCN (30 mL), $PyHBF_4$ (1.1 equiv., 5 mmol, 0.84 g) in acetonitrile were placed in the cylindrical divided cell (as described in 2.2) and the solution was electrolyzed at a constant current of 60 mA at room temperature for 4 h. After the reaction was terminated, the solvent was evaporated to give the residue. Then chloroform (≈20 ml) was added to the residue to separate the supporting electrolyte by filtration. The mixture with product was filtered and chloroform was evaporated to give the crude product. The procedure was repeated at least 3 times Then the crude product was purified by silica gel (230-400 mesh) column chromatography (ethyl acetate/hexane = 1:1).



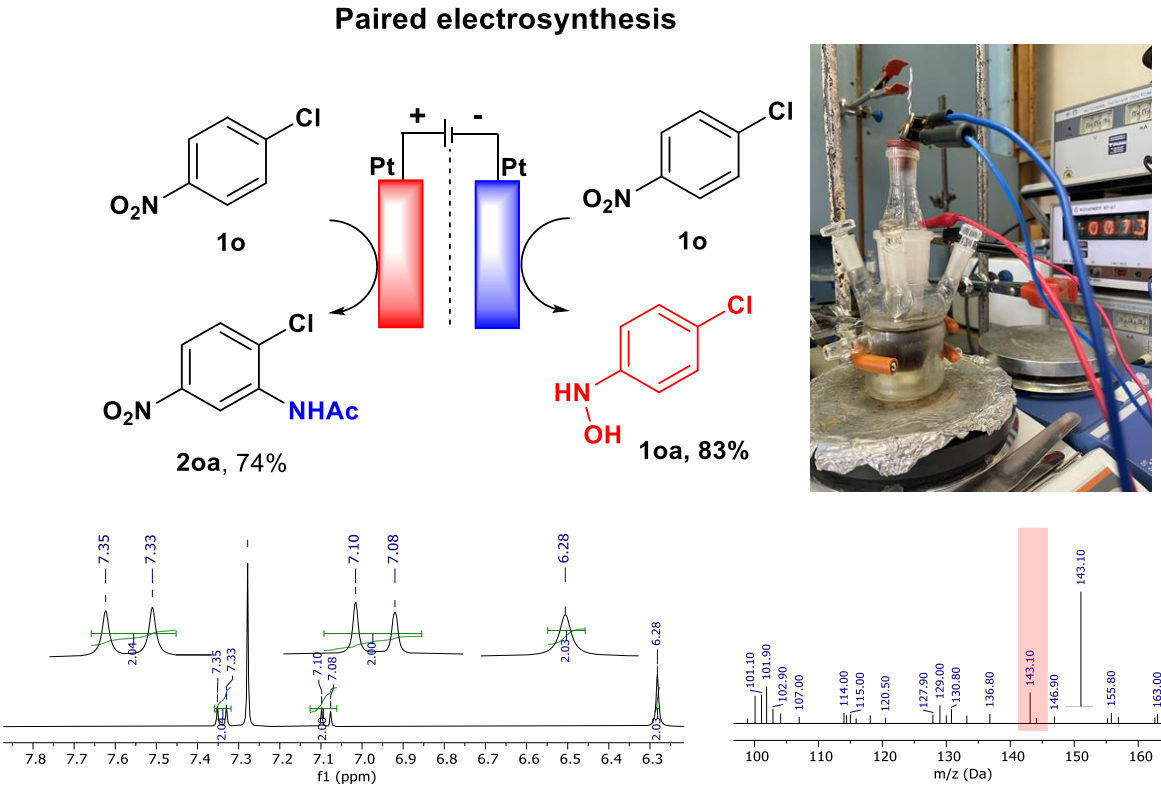
The anilide **2a** was obtained in 71% yield as a white solid.

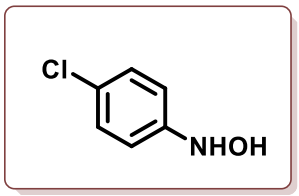
2.4 Paired electrosynthesis experiment

Oxidation process: 1-Chloro-4-nitrobenzene (**1o**) (1.8 mmol, 0.285 g), H_2O (0.8 equiv., 1.44 mmol, 33 ul), Et_4NBF_4 (2.4 mmol, 0.53 g) as background salt and acetonitrile (30 mL) as solvent were placed into anodic compartment **1** of the electrochemical divided cell equipped with a stir bar **6**. The electrolysis was carried out at room temperature (23-25 °C) and a constant current of 35 mA for 6 hours. At the end of electrolysis, as monitored by TLC, acetonitrile was evaporated on rotary evaporator to give the residue. Ethanol (≈7 mL) was then added to the residue, since Et4NBF4 is very poorly soluble in ethanol and, therefore, the supporting electrolyte can be separated from the reaction mixture. The mixture with product was filtered and ethanol was evaporated to give the crude product. The crude product was further purified by silica gel (mesh size 230–400) column chromatography (ethyl acetate/hexane = 1:1) to give **2oa** in 74% as a yellow solid.

Reduction process: 1-Chloro-4-nitrobenzene (**1o**) (0.6 mmol, 0.095 g), Et_4NBF_4 (0.8 mmol, 0.12 g) as background salt and acetonitrile (7 mL) as solvent were placed into cathodic compartment **2** of the electrochemical divided cell. The electrolysis was carried out at room temperature (23-25 °C) and a constant current of 35 mA for 3 hours. Note that due to different

volumes of the cathodic and anodic compartments and different substrate loadings, the synthesis was stopped after 3 hours to remove the reaction mixture from the cathodic compartment and replace it with a saturated solution of Et_4NBF_4 in acetonitrile to continue the oxidation synthesis, which required more time (6 hours). At the end of electrolysis, as monitored by TLC, acetonitrile was evaporated on rotary evaporator to give the residue. Ethanol (≈3 mL) was then added to the residue. The mixture with product was filtered and ethanol was evaporated to give the crude product. The crude product was further purified by silica gel (mesh size 230–400) column chromatography (ethyl acetate/hexane = 1:1) to give **1oa** in 83% as a white solid. We also recorded the formation of 3-aminocrotononitrile occurring during the reduction of acetonitrile.





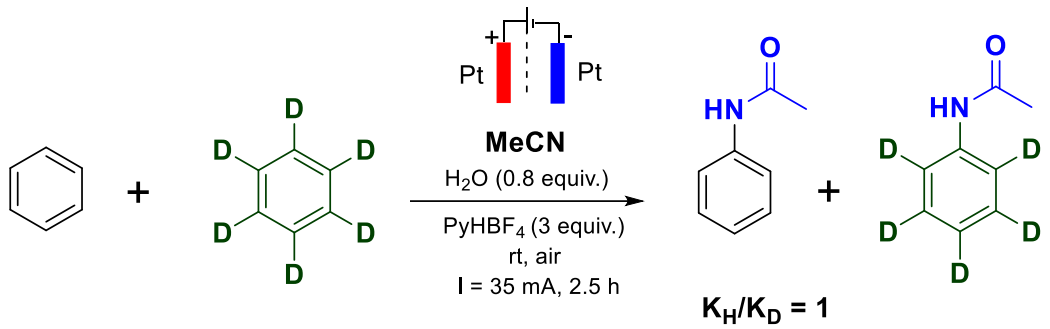
N-(4-chlorophenyl)hydroxylamine **(1oa)**. Yield: 83%, 0.07 g. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.35 – 7.33 (d, *J* = 8.6 Hz, 2H), 7.10 – 7.08 (d, *J* = 8.6 Hz, 2H), 6.28 (s, 2H). MS (ESI) m/z: calcd for C_6H_6ClNO $[M]^+$: 143.01; found: 143.10.

2.5 Kinetic isotope effect experiment

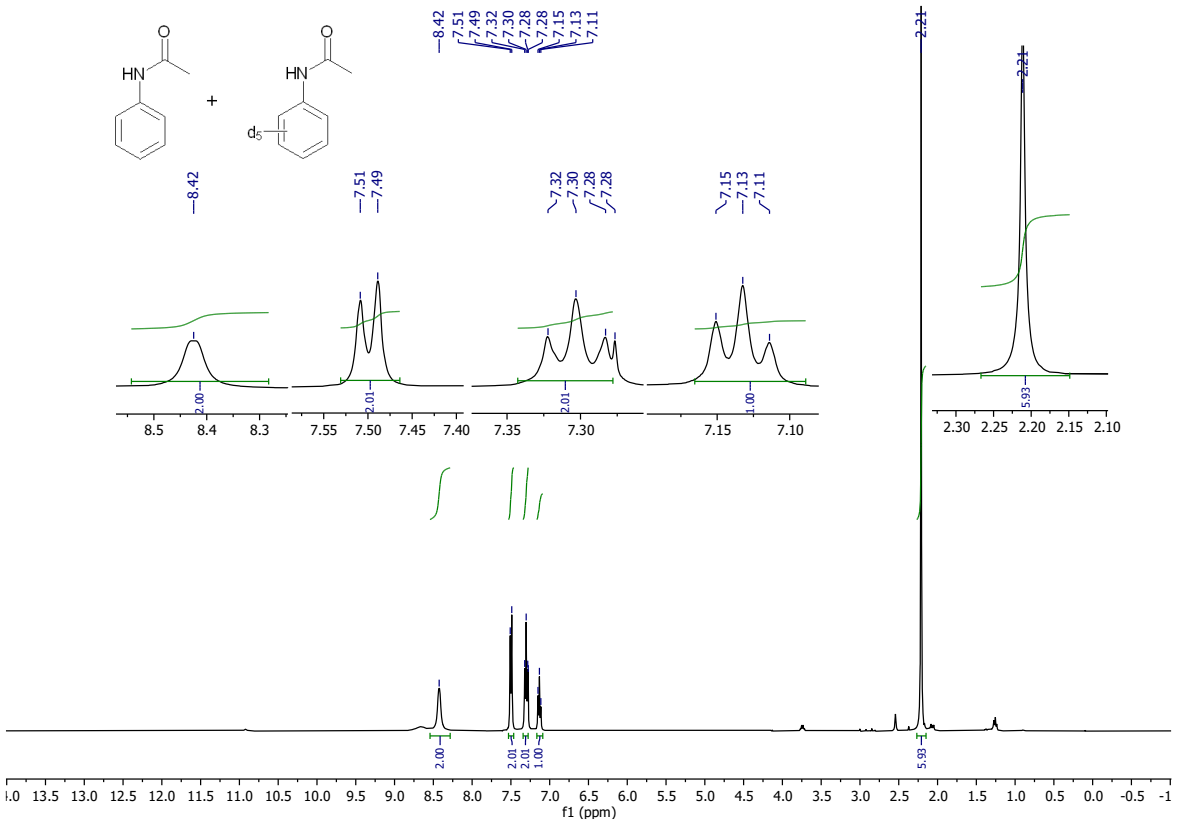
To gain additional mechanistic insight a KIE experiment with one equimolar mixture of benzene and d6-benzene was conducted (Scheme S1).

Benzene (0.6 mmol, 55 ul), Benzene-d6 (0.6 mmol, 53 ul), H_2O (0.8 equiv., 0.96 mmol, 17 ul) and nitrile (20 mL) as solvent, were placed into anodic compartment **1** of the electrochemical

divided cell equipped with a stir bar **6** (Figure S1). Saturated solution of $PyHBF_4$ (3.0 equiv., 3.6 mmol, 0.6 g) in MeCN was placed into cathodic compartment **2**. The electrolysis was carried out at room temperature (23-25 °C) and a constant current of 35 mA in air. The experiment was carried out for 2.5 hours. Then, chloroform (≈15 ml) was added to the residue to separate the supporting electrolyte by filtration. The mixture with products was filtered and chloroform was evaporated to give the crude products. The crude products was further purified by silica gel (mesh size 230–400) column chromatography (ethyl acetate/hexane = 1:1). The ratio of KH/KD is 1:1 indicating that C−H cleavage is not the rate-determining step.



Scheme S1 Kinetic Isotope Effect Experiment



3. EPR experiments

The measurements were carried out on an apparatus program complex including an analog electrochemical system with a potentiostat and a PWR-3 programmer, an ELEXSYS E500 ESR spectrometer of the X-range, and an E14-440 analog-to-digital and digital-to-analog modulus (LCard), a fourth-generation computer, and a unique three-electrode helical cell. ESR spectra were simulated using the WinSim 0.96 program (developed by NIEHS). The material of the auxiliary electrode was platinum, the reference electrode was Pt wire, and the working electrode was platinum. Electrochemical experiments were carried out at 293 K using 0.1 M Et_4NBF_4 as a supporting electrolyte; the potential sweep E(t) being 0.1 V s^{-1}.

Table S1 Values of ***g*** and hyperfine coupling constants (a_{iso}) of PBN spin-adduct radicals

Spin-adduct	g	a_{iso}	Line width, G
A	2.001	a_N = 13.9 G, a_H= 2.3 G	1.2
B	2.009	a_{N1} = 5.19 G, a_{N2}= 4.36 G, a_{H1}= 5.25 G, a_{H2}= 9.20 G	1.5
C	2.006	a_{N1} = 5.24 G, a_{N2}= 4.32 G, a_{H1}= 5.15 G, a_{H2}= 9.24 G	1.5

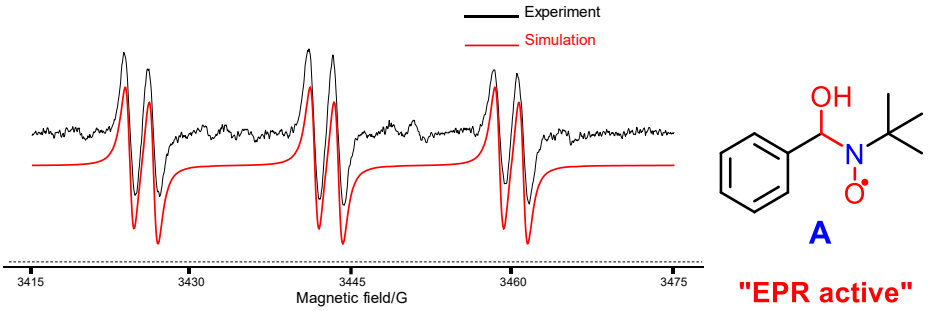


Figure S2 EPR spectrum of PBN-OH• recorded during oxidation of solution of MeCN (2 ml) with water (100 ul) at +2.2 V and 293 K with simulations. g = 2.001, a_N = 13.9 G, a_H = 2.3 G. C (PBN) = 0.5 mg/ml.

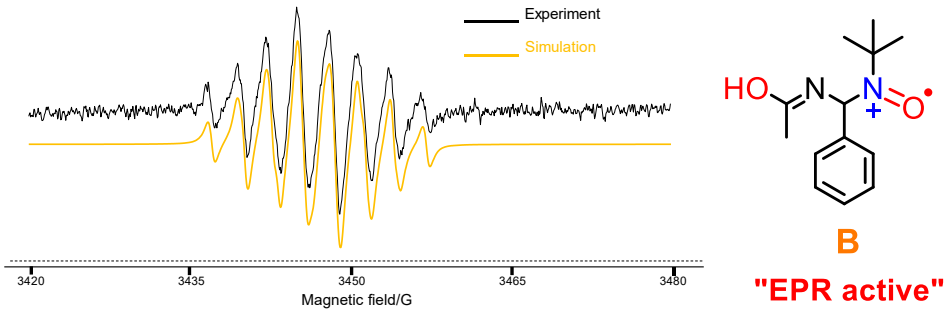


Figure S3. EPR spectrum of spin-adduct **B** recorded during oxidation of benzene solution in MeCN with water (0.8 equiv.) at +2.2 V and 293 K with simulations. g = 2.021, a_{N1} = 5.2 G, a_{N2} = 4.4 G, a_{H1} = 5.3 G, a_{H2} = 9.2 G. C (PBN) = 1.5 mg/ml.

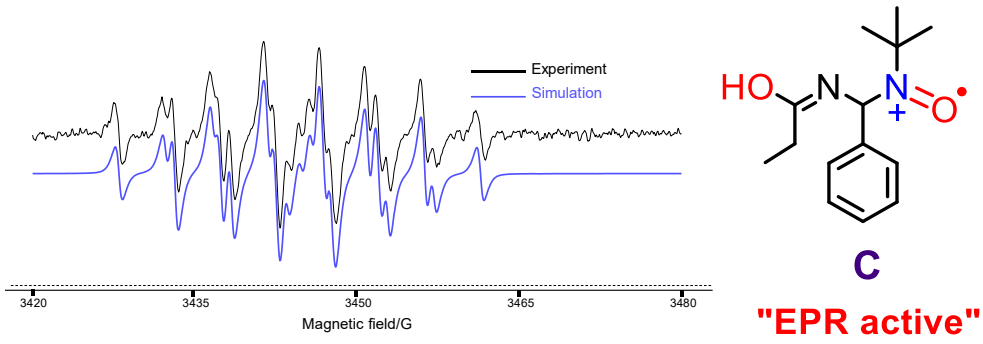
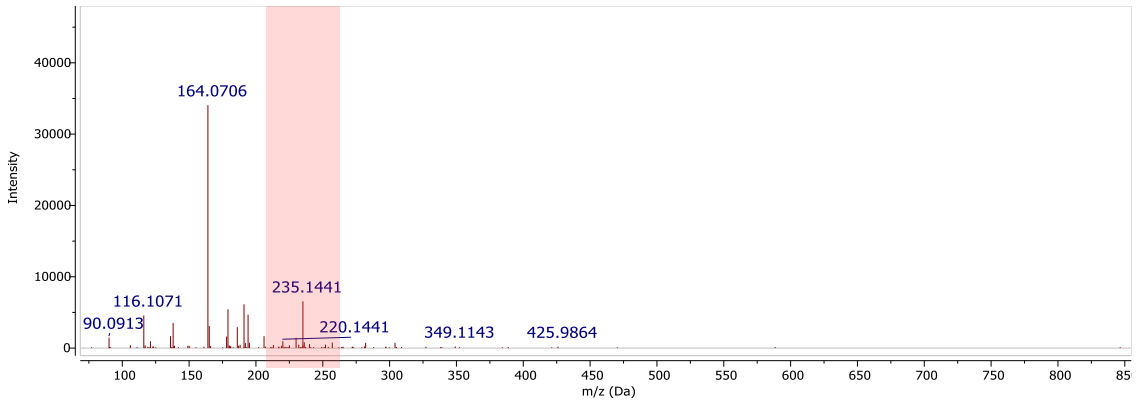
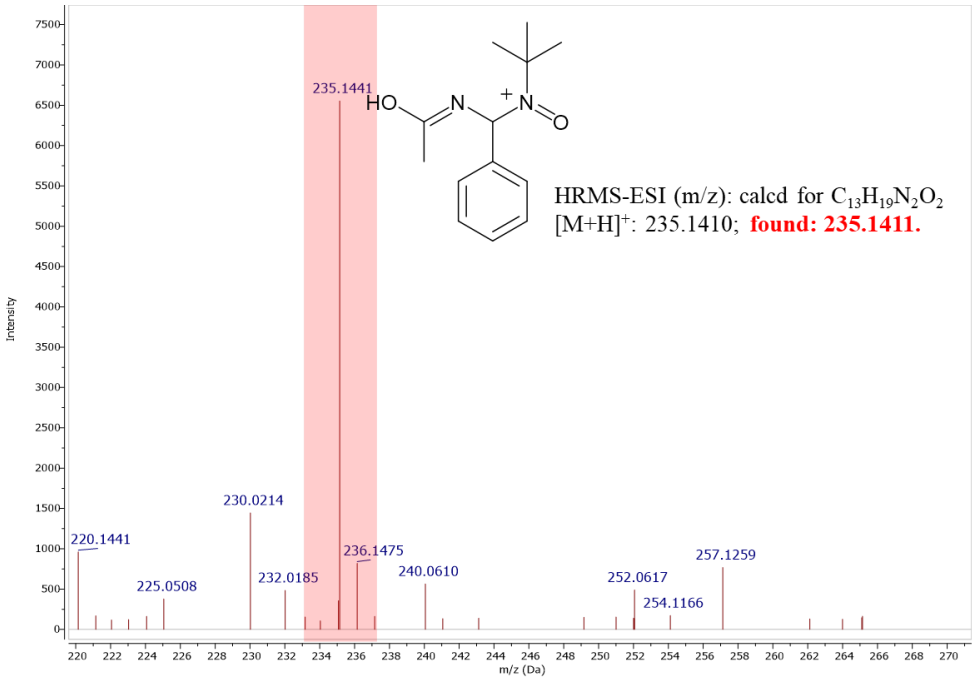


Figure S4 EPR spectrum of spin-adduct **C** recorded during oxidation of benzene solution in EtCN with water (0.8 equiv.) at +2.2 V and 293 K with simulations. g = 2.021, a_{N1} = 5.24 G, a_{N2} = 4.32 G, a_{H1} = 5.15 G, a_{H2} = 9.24 G. C (PBN) = 1.5 mg/ml.

HRMS of spin-adduct B





4. Cyclic voltammetry

Cyclic voltammograms (CVs) have been recorded in MeCN solution in three-electrode cell with 5 mM substrate concentration, Bu_4NBF_4 was used as a supporting electrolyte (0.1 M) and a glassy carbon electrode as a working electrode (6 mm^2), auxiliary electrode was platinum rod. All potentials are referenced against the Ag/AgCl (0.01 M KCl) in MeCN. The reference electrode was connected with the cell solution by a modified Luggin capillary filled with the 0.1 M Bu_4NBF_4 in MeCN electrolyte solution. Thus, the reference electrode assembly had two compartments, each terminated with an ultra-fine glass frit to separate the AgCl from the analyte. CVs were recorded using BASi Epsilon potentiostat (USA) and P-30S potentiostat Elins (Russia).

4.1 Electrochemical potentials

Table S2 Redox potentials (V) of arenes; ***(a)*** our results, conditions: WE- GC, RE – Ag/AgCl, Bu_4NBF_4, CH_3CN; ***(b)*** literature data, conditions: WE- Pt, RE – $Ag/AgNO_3$, perchlorate salts ($LiClO_4$, $NaClO_4$, $(C_2H_5)_4NClO_4$, $(n\text{-}C_8H_7)_4NClO_4$, $(n\text{-}C_4H_9)_4NClO_4$)), CH_3CN

№	Compound	E_{ox}^{a}, V	E_{ox}^{b}, V	Ref.
1a	1,4-Bis(trifluoromethyl)benzene	> 3.2		
1b	1,3-Bis(trifluoromethyl)benzene	> 3.2		
1c	1,3,5-Tris(trifluoromethyl)benzene	> 3.2		
1d	Trifluoromethyl benzene	> 3.2		
1e	4-Chloro-1-(trifluoromethyl)benzene	> 3.2		
1f	Fluorobenzene	> 3.2		
1g	Chlorobenzene	2.63	2.07	[2]
1h	1,2-Chlorobenzene	2.75		
1i	1-Chloro-4-fluorobenzene	2.49		
1j	1-Bromo-4-fluorobenzene	2.46		
1k	Benzene	2.56	2.08	[2]
1l	Benzonitrile	2.35	1.8 **vs SCE**	[3]
1m	Nitrobenzene	> 3.2		
1n	1-Chloro-2-nitrobenzene	> 3.2		
1o	1-Chloro-4-nitrobenzene	> 3.2		
1p	1-Fluoro-4-nitrobenzene	> 3.2		
1q	1-Bromo-4-nitrobenzene	> 3.2		

1r	Ethyl benzoate	> 3.2		
1s	Dimethyl isophthalate	> 3.2		
1t	Phenol	1.80	1.04	[2]
1u	2,6-Dimethylphenol	1.76		
1v	2-Methylphenol	1.78		
1w	Methyl salicylate	1.85		
1x	Ethyl salicylate	2.16		
2a	*N*-(2,5-bis(trifluoromethyl)phenyl) acetamide	2.45		
2k	Acetanilide	1.65		
2t	Paracetamol	1.32		

4.2 Cyclic voltammograms

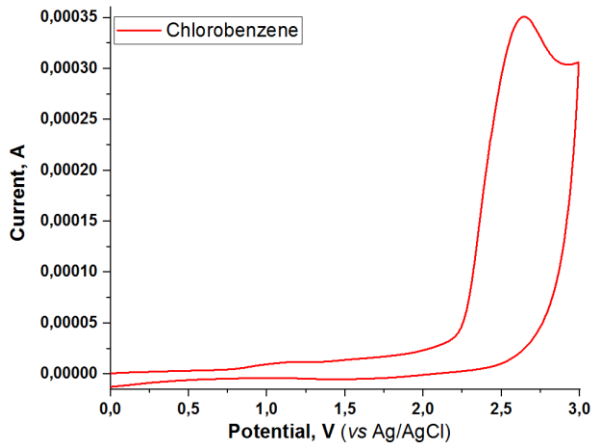


Figure S2: Oxidation of Chlorobenzene (**1g**)

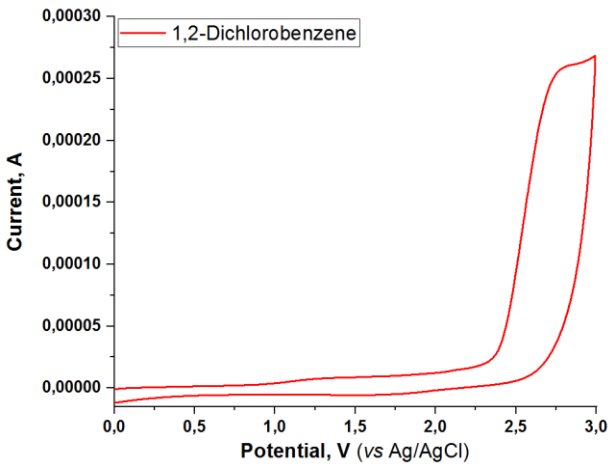


Figure S3: Oxidation of 1,2-Dichlorobenzene (**1h**)

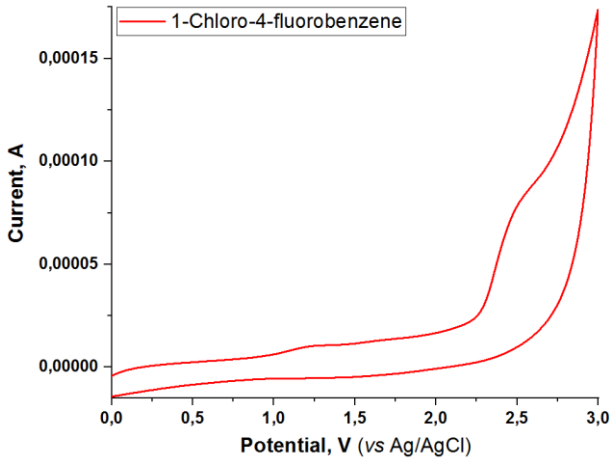


Figure S4: Oxidation of 1-Chloro-4-fluorobenzene (**1i**)

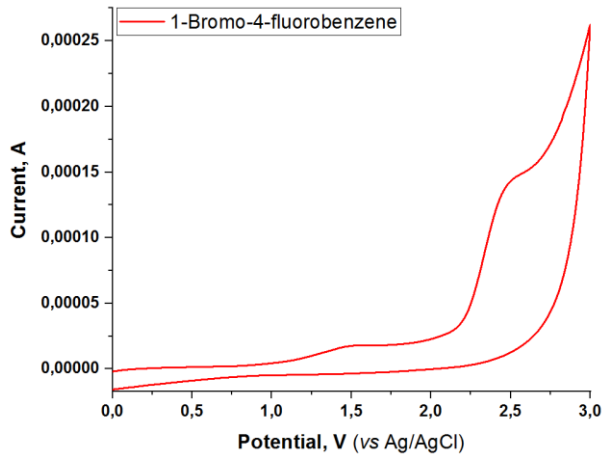


Figure S5: Oxidation of 1-Bromo-4-fluorobenzene (**1j**)

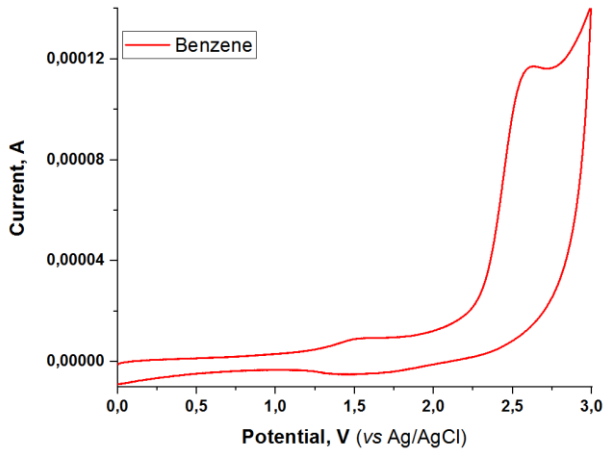


Figure S6: Oxidation of Benzene (**1k**)

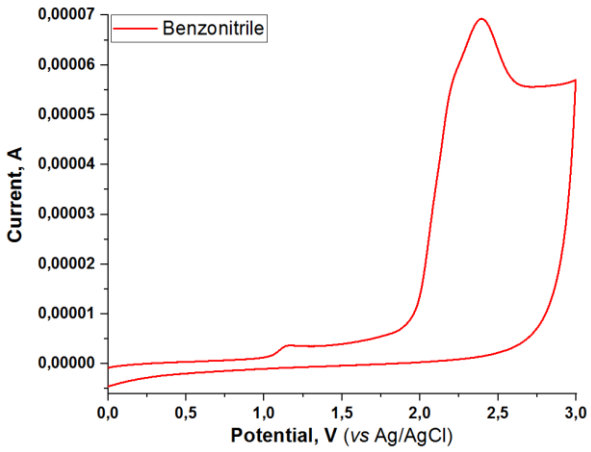


Figure S7: Oxidation of Benzonitrile (**1l**)

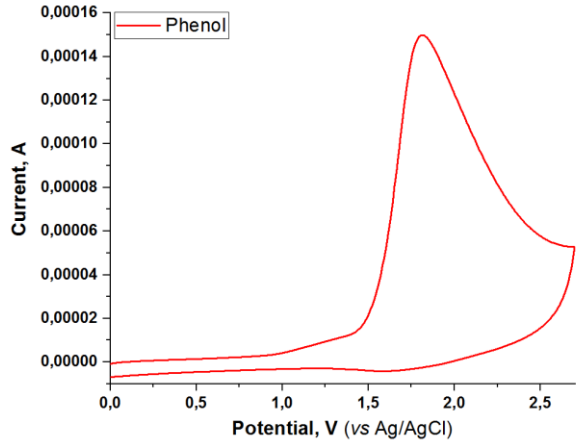


Figure S8: Oxidation of Phenol **(1t)**

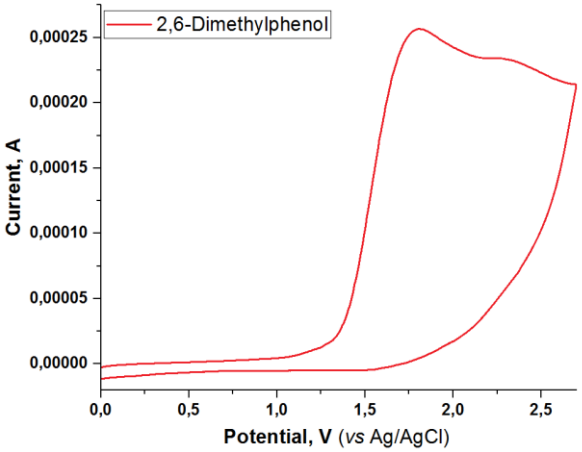


Figure S9: Oxidation of 2,6-Dimethylphenol (**1u**)

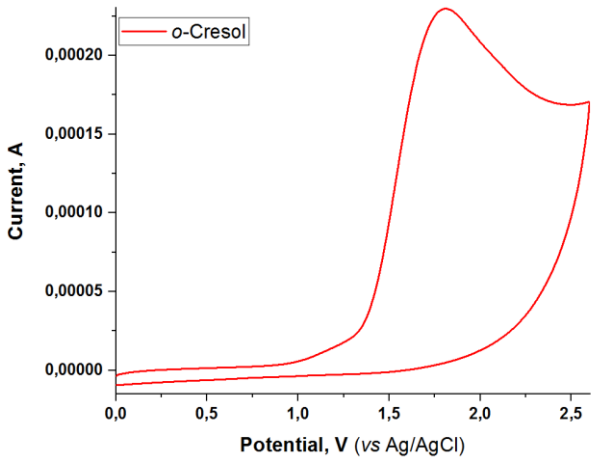


Figure S10: Oxidation of 2-Methylphenol **(1v)**

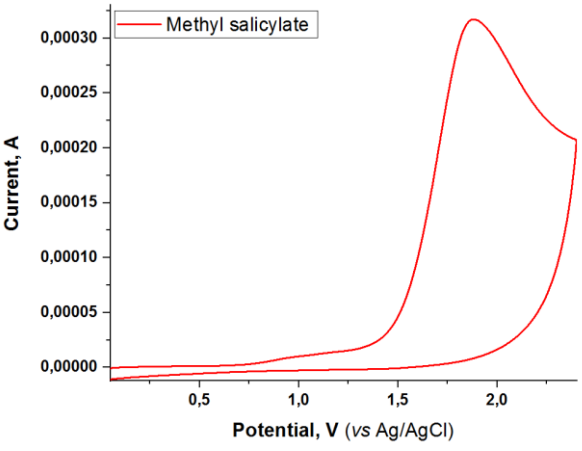


Figure S11: Oxidation of Methyl salicylate **(1w)**

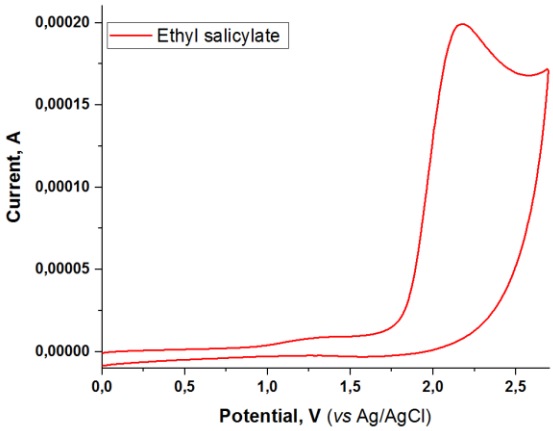


Figure S12: Oxidation of Ethyl salicylate **(1x)**

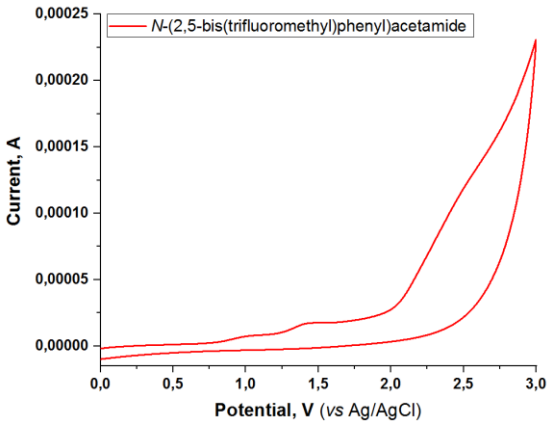


Figure S13: Oxidation of *N*-(2,5-bis(trifluoromethyl)phenyl)acetamide **(2a)**

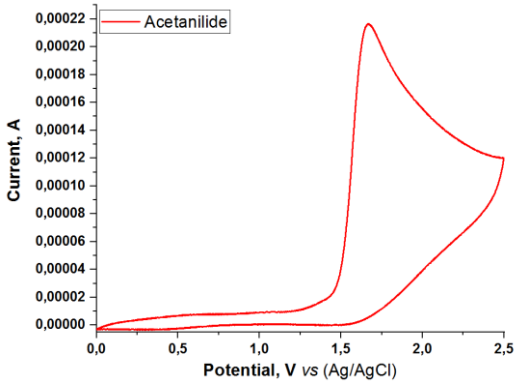


Figure S14: Oxidation of Acetanilide **(2k)**

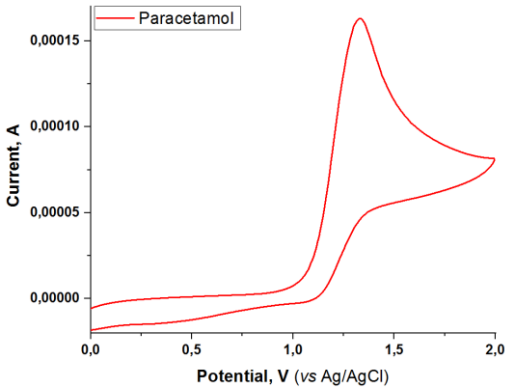


Figure S15: Oxidation of Paracetamol **(2t)**

5. Quantum chemical calculations

5.1 General notes

Conformational searches were performed for **TS1** and **TS2** using CREST (Conformer-Rotamer Ensemble Sampling Tool)[4] software with GFN2-xTB[5] method, implicit accounting for solvation effects (**alpb**[6]), and correct system charge and multiplicity. The following CREST controls were used to constrain the breaking/forming bond lengths, as proposed in[7]:

```
$constrain
distance: 15, 2, auto
force constant=2.0
$end
```

These conformational searches yielded 5 and 6 different conformers for TS1 and TS2, respectively, from which the most stable ones (**TS1_4** and **TS2_0**) were selected.

The obtained conformers were optimized in ORCA 5.0.4 at the B3LYP[8,9]-D3BJ[10,11]/def2-TZVP/CPCM(CH_3CN)[12] level of theory, and harmonic frequencies were calculated to ascertain the types of located stationary points and compute free energies corrections.

All transition-state optimizations were performed in two steps: (1) first, we minimized their energies with constraints fixing the changing bonds at their "partially formed lengths": 1.4 Å for C…H, and 2.0 Å for C…C (we call this step "preoptimization"[7]); (2) the second step is an unconstrained transition-state search from the preoptimized structure.

To further refine the computed free energies, we have computed electronic energies of all located stationary points at DLPNO-CCSD(T)[13]/def2-TZVPP[14]/CPCM(CH_3CN) level of theory and recalculated the free energies using the following formula:

$$G'CCSD(T) = ECCSD(T) + (GDFT - EDFT),$$

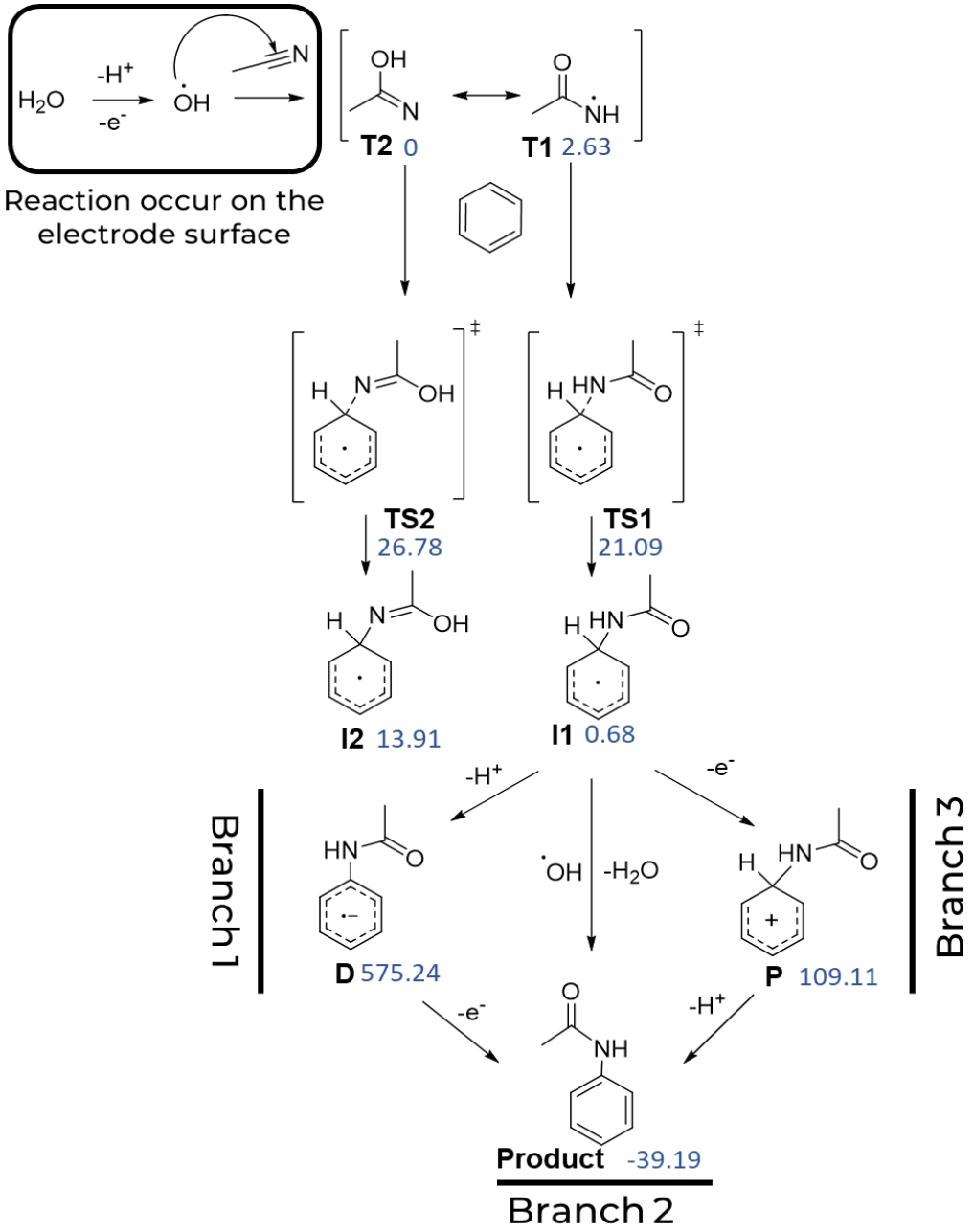
where G_{DFT} and E_{DFT} are the free and electronic energies obtained from DFT calculations; $E_{CCSD(T)}$ is the electronic energy obtained from calculations of the same geometry by the coupled cluster method.

During the clarification of the mechanism, it was necessary to determine the presence of an energy barrier in the last reaction - detachment of a hydrogen radical from **I1** by an OH radical. For this purpose, a relaxed scan of the potential energy surface ("Scan" keyword in ORCA) was carried out.

5.2 Mechanism

Scheme S2 shows the starting molecule **T2**, the **Product**, and all intermediate and transition states that were studied during the molecular modelling procedure. All the located structures

corresponding to stationary points on the PES, as well as their charges, multiplicities, total electronic energies (E_B3LYP, E_CCSD(T)), Gibbs free energies (G(298K)_B3LYP, G(298K)_CCSD(T)), imaginary frequency counts (NumImFreq), and perturbative triples (PT) are available in the file "supplementary.xyz".



Scheme S2 Detailed reaction mechanism showing the three pathways of reaction product formation from the **I1**. Numbers in blue show the energies in kcal/mol relative to the initial **T2** structure

After obtaining the intermediate **I1**, further transformations into the product are divided into three branches:

Branch 1: the solvated proton is cleaved from the intermediate compound **I1** followed by oxidation on the anode. The energy of the acetonitrile-solvated proton was taken from the literature[15].

Branch 2: cleavage of hydrogen atom by OH radical from **I1** to form the target product and water. In order to prove that this reaction occurs without an energy barrier, a relaxed scan of the potential energy surface was performed, see Figure 6. The curve does not contain a maximum, indicating the absence of an energy barrier.

Branch 3: pre-oxidation of intermediate **I1** followed by proton elimination.

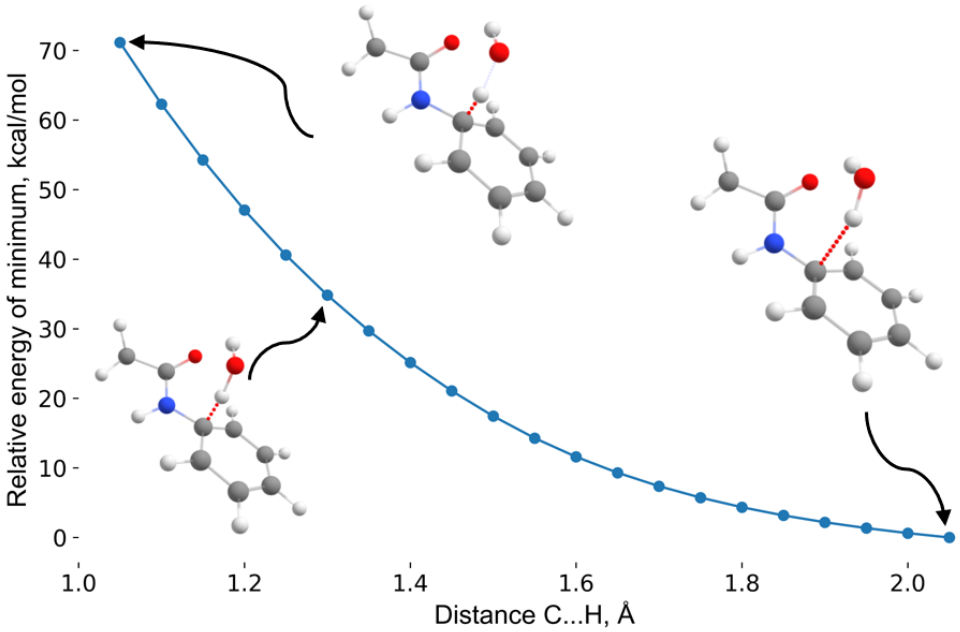
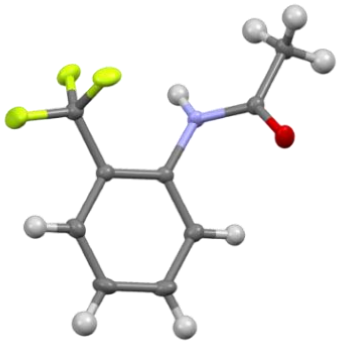


Figure S16. Relaxed scan of the potential energy surface along the distance between hydrogen atom and carbon atom of the benzene ring. Different elements are shown in different colors: red - oxygen, grey - carbon, white - hydrogen and blue - nitrogen.

6. X-ray crystallography

The X-ray diffraction data for the single crystals **2da** and **3o** were collected on a Bruker AXS D8 Venture diffractometer at 101(2) K in the ω and φ-scan models using Mo radiation (λ = 0.71073Å). The structures were solved by direct methods using APEX3[16] for data collection, SAINT[17] for data reduction, SHELXT[18] for structure solution, SHELXL[18] for structure refinement by full-matrix least-squares against F^2, and SADABS[19] and TWINABS[20] for multi-scan absorption corrections for **2da** and **3o** respectively. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms at carbon atoms were placed into calculated positions and refined as "riding" atoms. Crystal data and structure refinement data are presented in table 1 and table 2. CCDC 2336800, 2336823 contain the supplementary crystallographic data for this paper.

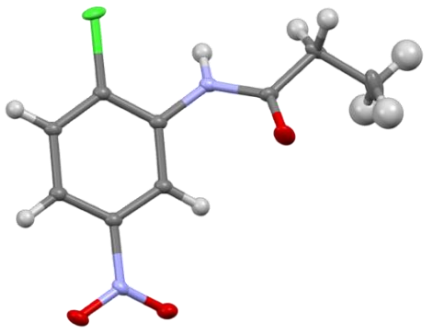
Table S2 Crystal data and structure refinement for **2da**



Identification code	**bud_ks_a_57_fr8_16_0m**	
Empirical formula	$C_9H_8F_3NO$	
Formula weight (g/mol)	203.16	
Temperature (K)	101(2)	
Wavelength (Å)	0.71073	
Crystal system, space group	Monoclinic, $P2_1/n$	
Unit cell dimensions (Å, deg)	a = 4.7728(4)	a= 90
	b = 13.3728(12)	b= 92.480(3)
	c = 13.9438(13)	g = 90
Volume (Å^3)	889.14(14)	
Z	4	
Density (calculated) (g/cm^3)	1.518	
Absorption coefficient (mm^{-1})	0.142	

F(000)	416
Crystal size (mm^3)	0.454 x 0.194 x 0.140
θ range for data collection (deg)	2.111 to 28.739
Index ranges	$-6 \leq h \leq 6$, $-18 \leq k \leq 18$, $-18 \leq l \leq 18$
Reflections collected	32558
Independent reflections	2312 [R_{int} = 0.0651]
Completeness to θ = 25.242°	99.9 %
Absorption correction	multi-scan
Max. and min. transmission	0.7458 and 0.7012
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2312 / 1 / 132
Goodness-of-fit on F^2	1.059
Final R indices [I>2sigma(I)]	R_1 = 0.0365, wR_2 = 0.0845
R indices (all data)	R_1 = 0.0468, wR_2 = 0.0895
Largest diff. peak and hole ($eÅ^{-3}$)	0.353 and -0.286

Table S3 Crystal data and structure refinement for **3o**

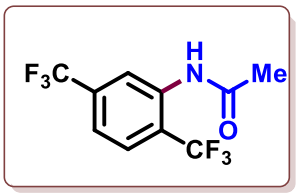


Identification code	**bud_ks_55_t5**
Empirical formula	$C_9H_9ClN_2O_3$
Formula weight (g/mol)	228.63

Temperature (K)	101(2)
Wavelength (Å)	0.71073
Crystal system, space group	Monoclinic, $P2_1$
Unit cell dimensions (Å, deg)	a = 5.8609(7) a= 90 b = 4.8745(5) b= 93.312(4) c = 17.4671(18) g = 90
Volume ($Å^3$)	498.18(9) E^3
Z	2
Density (calculated) (g/cm^3)	1.524
Absorption coefficient (mm^{-1})	0.371
F(000)	236
Crystal size (mm^3)	0.623 x 0.488 x 0.056
θ range for data collection (deg)	3.482 to 28.806°.
Index ranges	$-7 \leq h \leq 7$, $-6 \leq k \leq 6$, $-23 \leq l \leq 23$
Reflections collected	8089
Independent reflections	5355 [R_{int} = 0.0553]
Completeness to θ = 25.242°	99.4 %
Absorption correction	multi-scan
Max. and min. transmission	0.745757 and 0.570774
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2686 / 1 / 142
Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R_1 = 0.0529, wR_2 = 0.1403
R indices (all data)	R_1 = 0.0560, wR_2 = 0.1426
Absolute structure parameter	0.07(12)
Largest diff. peak and hole ($eÅ^{-3}$)	0.602 and -0.637

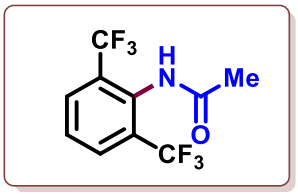
7. Characterization of the products

N-(2,5-bis(trifluoromethyl)phenyl)acetamide (2a)



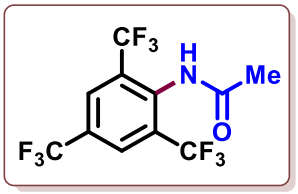
Known compound.[21] Yield: 87%, 0.28 g. White solid, mp 120-122 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.63 (s, 1H), 7.76 (d, *J* = 8.2 Hz, 1H). 7.50 (d, *J* = 8.4 Hz, 2H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.94, 136.60, 136.04, 135.71, 135.38, 135.05, 127.92, 127.60, 127.37, 127.32, 127.27, 127.21, 125.20, 124.88, 122.48, 122.16, 121.73, 121.50, 119.76, 119.45, 25.18. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -61.21, -63.40. MS (ESI) m/z: $[M+H]^+$ 272.0. HRMS (ESI) m/z $[M+H]^+$: calcd for $C_{10}H_8F_6NO$, 272.0505; found, 272.0504.

N-(2,6-bis(trifluoromethyl)phenyl)acetamide (2b)



Unknown compound. Yield: 81%, 0.264 g. White solid, mp 118-122 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 7.92 (d, *J* = 8.03 Hz, 2H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.22 (s, 1H), 2.21 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 170.02, 132.80, 131.26, 131.01, 130.77, 130.53, 130.00, 129.96, 129.92, 129.88, 128.24, 125.46, 123.29, 121.11, 118.93, 22.41. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -61.47. MS (ESI) m/z: $[M+H]^+$ 272.0. HRMS (ESI) m/z $[M+H]^+$: calcd for $C_{10}H_8F_6NO$, 272.0505; found, 272.0507.

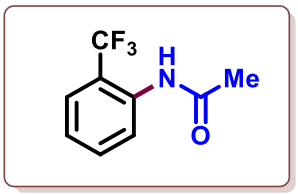
N-(2,4,6-tris(trifluoromethyl)phenyl)acetamide (2c)



Unknown compound. Yield: 63%, 0.256 g. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.56 (s, 2H), 8.13 (s, 1H), 2.34 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 166.76, 132.66, 132.50, 132.24, 131.85, 130.24, 128.67, 123.93, 121.75, 24.90. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -60.97, -62.52. MS (ESI) m/z: $[M+H]^+$ 340.0. HRMS (ESI) m/z $[M+H]^+$: calcd for $C_{11}H_7F_9NO$, 340.0378; found, 340.0380.

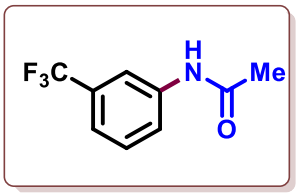
Compounds **2d**, yield 83%, 0.202 g, ratio **2d-*a*:2d-*b*:2d-*c*** 3:3:1

***N*-(2-(trifluoromethyl)phenyl)acetamide (2d-*a*)**



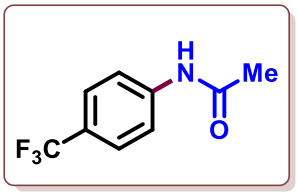
Known compound.[22] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H =8.55 (s, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.25 (t, *J* = 7.4 Hz, 1H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.31, 135.09, 132.71, 125.96, 125.91, 125.87, 125.82, 125.23, 124.61, 124.42, 122.53, 120.78, 120.30, 120.00, 119.82, 24.49. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -60.62. MS (ESI) m/z: $[M+H]^+$ 204.06. HRMS-ESI (m/z): calcd for $C_9H_9F_3NO$ $[M+H]^+$: 204.0631; found: 204.0634.

N-(3-(trifluoromethyl)phenyl)acetamide (2d-*b*)



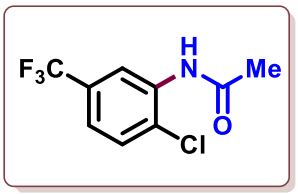
Known compound.[22] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.51 (s, 1H), 7.83 (s, 1H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.39 –7.31 (m, 2H), 2.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 169.05, 138.54, 131.89, 131.57, 131.25, 130.93, 129.66, 128.03, 125.33, 123.12, 122.63, 121.07, 121.03, 120.99, 120.95, 119.93, 116.78, 116.74, 116.70, 116.66, 24.63. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -62.77. MS (ESI) m/z: $[M+H]^+$ 204.06. HRMS-ESI (m/z): calcd for $C_9H_9F_3NO$ $[M+H]^+$: 204.0631; found: 204.0634.

N-(4-(trifluoromethyl)phenyl)acetamide (2d-*c*)



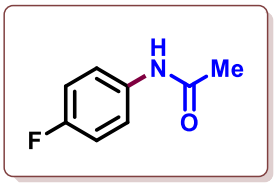
Known compound.[22] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.51 (s, 1H), 7.62 (d, *J* = 7.9 Hz, 2H), 7.50 (d, *J* = 7.8 Hz, 2H), 2.15 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.90, 140.98, 128.68, 126.48-126.36, 125.97, 125.93, 123.25, 120.54, 119.45, 24.78. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -62.11. MS (ESI) m/z: $[M+H]^+$ 204.06. HRMS-ESI (m/z): calcd for $C_9H_9F_3NO$ $[M+H]^+$: 204.0631; found: 204.0634.

N-(2-chloro-5-(trifluoromethyl)phenyl)acetamide (2e)



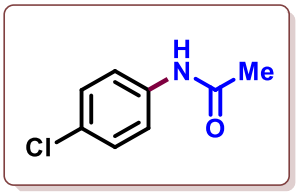
Unknown compound. 89%, 0.25 g. White solid, mp 94-96 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.77 (s, 1H), 7.70 (s, 1H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.32 (dd, *J* = 8.5 Hz, 1H), 2.29 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 167.81, 134.68, 129.93, 129.67, 128.88, 125.04, 124.05, 121.89, 120.54, 117.85, 24.32. ^{19}F NMR (376 MHz, $CDCl_3$) δ = -62.73. MS (ESI) m/z: $[M+H]^+$ 238.02. HRMS-ESI (m/z): calcd for $C_9H_8ClF_3NO$ $[M+H]^+$: 238.0241; found: 238.0241.

N-(4-fluorophenyl)acetamide (2f)



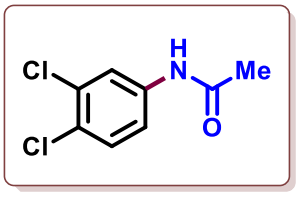
Known compound.[23] Yield: 73%, 0.13 g. White solid, mp 152-153 °C. ^{1}H NMR (400 MHz, $CDCl_3$: δ_H = 7.62 (s, 1H), 7.47 (dd, *J* = 8.6, 3.5 Hz, 2H), 7.05 (t, *J* = 8.6 Hz, 2H), 2.17 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.01, 159.77, 158.10, 133.44, 121.42, 121.38, 115.16, 115.06, 23.85. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -119.69. MS (ESI) m/z: $[M+H]^+$ 154.06. HRMS-ESI (m/z): calcd for C_8H_9FNO $[M+H]^+$: 154.0663, found 154.0665.

N-(4-chlorophenyl)acetamide (2g)



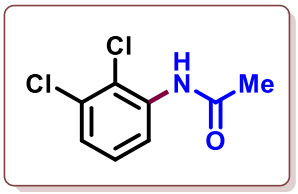
Known compound.[23] Yield: 44%, 0.089 g. Brown solid, mp 176-179 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H =7.91 (s, 1H), 7.45 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.69, 136.47, 129.61-129.33, 121.03, 24.29. MS (ESI) m/z: $[M+H]^+$ 170.03. HRMS-ESI (m/z): calcd for $C_8H_9ClNO[M+H]^+$: 170.0367; found: 170.0369.

N-(3,4-dichlorophenyl)acetamide (2h-*a*)



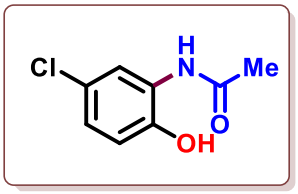
Known compound.[24] Yield: 48%, 0.118 g. White solid, mp 120-122°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.58 (s, 1H), 8.14 (d, *J* = 2.5 Hz, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.48 (dd, *J* = 8.0, 2.4 Hz, 1H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C =169.28, 139.84, 131.46, 131.03, 124.80, 120.53, 119.42, 24.48. MS (ESI) m/z: $[M+H]^+$ 203.99. HRMS-ESI (m/z): calcd for $C_8H_8Cl_2NO$ $[M+H]^+$: 203.9977; found:203.9978.

N-(2,3-dichlorophenyl)acetamide (2h-*b*)



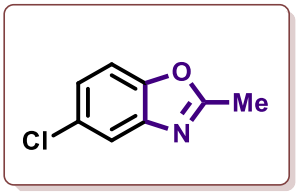
Known compound.[25] Yield: 16%, 0.04 g. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.99 (s, 1H), 7.89 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.39 (dd, *J* = 7.8, 2.2 Hz, 1H), 7.32 (t, *J* = 8.0 Hz, 1H), 2.20 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C =168.27, 136.75, 131.69, 126.96, 125.53, 124.21, 123.27, 23.14. MS (ESI) m/z: $[M+H]^+$ 203.9. HRMS-ESI (m/z): calcd for $C_8H_8Cl_2NO$ $[M+H]^+$: 203.9977; found: 203.9979.

N-(5-chloro-2-hydroxyphenyl)acetamide (2i)



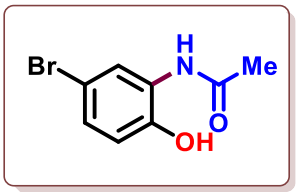
Known compound.[26] Yield: 13%, 0.029 g. White solid. ^{1}H NMR (400 MHz, CD_3CN): δ_H = 8.46 (s, 1H), 8.34 (s, 1H), 7.49 (dd, *J* = 2.6 Hz, 1H), 7.05 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.90 (d, *J* = 8.7 Hz, 1H), 2.18 (s, 3H). ^{13}C NMR (100 MHz, CD_3CN): δ_C = 169.16, 146.29, 127.86, 123.50, 122.12, 121.08, 116.39, 23.86. MS (ESI) m/z: $[M+H]^+$ 186.02. HRMS-ESI (m/z): calcd for $C_8H_9ClNO_2$ $[M+H]^+$: 186.0316; found: 186.0318.

5-chloro-2-methylbenzo[d]oxazole (2ii)



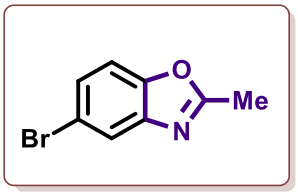
Known compound.[26] Yield: 53%, 0.106 g. White crystals, mp 52-54 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.65 (d, *J* = 2.5 Hz, 1H), 7.40 (d, *J* = 8.6 Hz, 1H), 7.28 (dd, *J* = 8.5, 2.5 Hz, 1H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 165.75, 149.97, 143.13, 129.98, 125.20, 119.85, 111.36, 14.94. MS (ESI) m/z: $[M+H]^+$ 168.02. HRMS-ESI (m/z): calcd for C_8H_7ONCl $[M+H]^+$: 168.0211; found: 168.0211.

***N*-(5-bromo-2-hydroxyphenyl)acetamide (2j)**



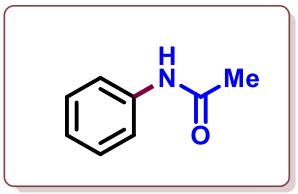
Known compound.[26] Yield: 23%, 0.064 g. White solid. ^{1}H NMR (400 MHz, CD_3CN): δ_H = 8.75 (s, 1H), 8.44 (s, 1H), 7.61 (d, *J* = 2.4 Hz, 1H), 7.18 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.84 (d, *J* = 8.6 Hz, 1H), 2.16 (s, 3H). ^{13}C NMR (100 MHz, CD_3CN): δ_C = 169.09, 146.76, 128.04, 126.40, 123.82, 116.88, 109.64, 23.85. MS (ESI) m/z: $[M+H]^+$ 230.0. HRMS-ESI (m/z): calcd for $C_8H_9BrNO_2$ $[M+H]^+$: 229.9811; found: 229.9814.

5-bromo-2-methylbenzo[d]oxazole (2jj)



Known compound.[26] Yield: 45%, 0.114 g. White solid, mp 65-67 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.80 (d, *J* = 1.9 Hz, 1H), 7.42 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.35 (d, *J* = 8.5 Hz, 1H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 164.65, 149.48, 142.61, 127.00, 121.98, 110.93, 14.00. MS (ESI) m/z: $[M+H]^+$ 211.97. HRMS-ESI (m/z): calcd for C_8H_7ONBr $[M+H]^+$: 211.9705; found: 211.9710.

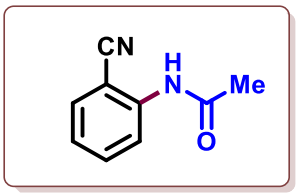
***N*-phenylacetamide (2k)**



Known compound.[23] Yield: 72%, 0.115 g. Light brown solid, mp 113-115 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.48 (s, 1H), 7.54 (d, *J* = 7.8 Hz, 2H), 7.29 (t, *J* = 7.9 Hz, 2H), 7.10 (t, *J* = 7.4 Hz, 1H), 2.14 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 169.83, 138.71, 129.40, 124.82, 120.86, 24.84. MS (ESI) m/z: $[M+H]^+$ 136.07. HRMS-ESI (m/z): calcd for $C_8H_{10}NO$ $[M+H]^+$: 136.0762; found: 136.0761.

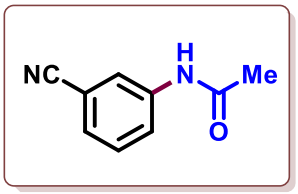
Compounds **2l**, yield 79%, 0.152 g, ratio **2l**-*a*:**2l**-*b*:**2l**-*c* = 1.3:1:1.3

***N*-(2-cyanophenyl)acetamide (2l-*a*)**



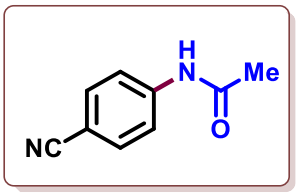
Known compound.[27] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 10.99 (s, 1H), 8.72 (d, *J* = 8.7 Hz, 1H), 8.12 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.13 (t, *J* = 7.7 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 167.84, 141.44, 134.71, 131.53, 124.76, 121.66, 115.68, 24.82. MS (ESI) m/z: $[M+H]^+$ 161.07. HRMS-ESI (m/z): calcd for $C_9H_9N_2O$ $[M+H]^+$: 161.0709; found: 161.0709.

***N*-(3-cyanophenyl)acetamide** (**2l**-*b*)



Known compound.[21] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.93 (s, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.55 (s, 1H), 7.51 – 7.42 (m, 2H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 169.31, 139.02, 129.91, 127.64, 124.11, 123.01, 118.70, 112.69, 24.43. MS (ESI) m/z: $[M+H]^+$ 161.07. HRMS-ESI (m/z): calcd for $C_9H_9N_2O$ $[M+H]^+$: 161.0709; found: 161.0709.

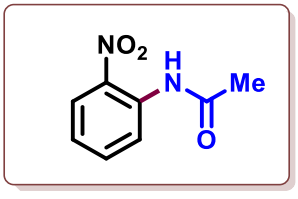
***N*-(4-cyanophenyl)acetamide** (**2l**-*c*)



Known compound.[28] White solid. ^{1}H NMR (400 MHz, CDCl3): δ_H = 7.67 (d, *J* = 9.0 Hz, 2H), 7.62 (d, *J* = 8.2 Hz, 2H), 7.59 (s, 1H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 169.21, 143.54, 133.21, 119.12, 104.67, 24.26. MS (ESI) m/z: $[M+H]^+$ 161.07. HRMS-ESI (m/z): calcd for $C_9H_9N_2O$ $[M+H]^+$: 161.0709; found: 161.0709.

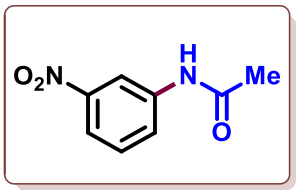
Compounds **2m,** yield 64%, 0.138 g, ratio **2m**-*a*:**2m**-*b* :**2m**-*c*= 3.5:1.3:1

***N*-(2-nitrophenyl)acetamide** (**2m**-*a*)



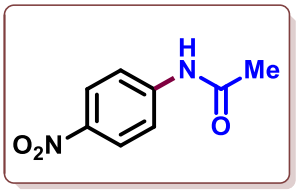
Known compound.[29] Yield: 39%, 0.084 g. Yellow solid, mp 91-93 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 10.34 (s, 1H), 8.79 (d, *J* = 8.7 Hz, 1H), 8.23 (dd, *J* = 8.5 Hz, 1H), 7.69 – 7.65 (m, 1H), 7.20 (t, *J* = 7.9 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 169.97, 135.94, 134.87, 134.51, 127.70, 123.19, 122.20, 25.60. MS (ESI) m/z: $[M+H]^+$ 180.06. HRMS-ESI (m/z): calcd for $C_8H_9N_2O_3$ $[M+H]^+$: 181.0608; found: 181.0608.

***N*-(3-nitrophenyl)acetamide (2m-*b*)**



Known compound.[30] Yield: 14%, 0.03 g. Yellow solid, mp 103-105 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.38 (s, 1H), 7.97 (dd, *J* = 8.0, 2.1 Hz, 2H), 7.71 (s, 1H), 7.50 (t, *J* = 8.2 Hz, 1H), 2.25 (s, 3H).
. ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.39, 148.03, 138.59, 129.31, 125.08, 118.32, 114.03, 24.04. MS (ESI) m/z: $[M+H]^+$ 180.06. HRMS-ESI (m/z): calcd for $C_8H_9N_2O_3$ $[M+H]^+$: 181.0608; found: 181.0607.

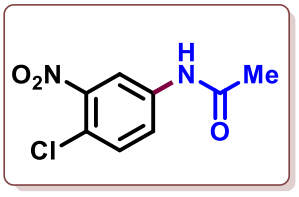
***N*-(4-nitrophenyl)acetamide (2m-*c*)**



Known compound.[31] Yield: 11%, 0.023 g. Yellow solid, mp 96-98 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.22 (d, *J* = 9.2 Hz, 1H), 7.71 (d, *J* = 9.1 Hz, 2H), 6.33 (s, 1H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 170.31, 145.32, 142.75, 124.56, 118.73, 23.56. MS (ESI) m/z: $[M+H]^+$ 180.06. HRMS-ESI (m/z): calcd for $C_8H_9N_2O_3$ $[M+H]^+$: 181.0608; found: 181.0608.

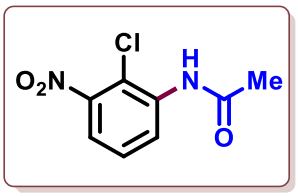
Compounds **2n,** yield 82%, 0.211 g, ratio **2n-*a*:2n-*b*** = 1.2:1

***N*-(4-chloro-3-nitrophenyl)acetamide (2n-*a*)**



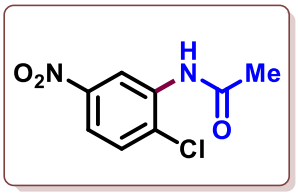
Known compound.[32] Yield: 49%. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.15 (d, *J* = 2.24, 1H), 7.72 (dd, *J* = 8.74, 2.24 Hz, 1H), 7.51 (s, 1H), 7.49 (d, *J* = 8.74 Hz, 2H), 2.23 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 167.99, 147.45, 136.91, 131.62, 123.25, 120.89, 115.74, 24.01. MS (ESI) m/z: $[M+H]^+$ 215.02. HRMS-ESI (m/z): calcd for $C_8H_8ClN_2O_3$ $[M+H]^+$: 215.0218; found: 215.0220

***N*-(2-chloro-3-nitrophenyl)acetamide (2n-*b*)**



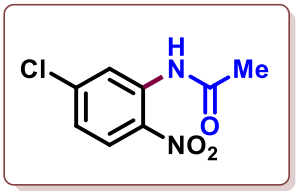
Unknown compound. Yield: 33%. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.67 (d, *J* = 8.41 Hz, 1H), 7.81 (s, 1H), 7.60 (dd, *J* = 8.15, 1.45 Hz, 1H), 7.44 (t, *J* = 8.2 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 167.99, 148.02, 136.05, 127.32, 124.28, 119.41, 113.58, 24.39. MS (ESI) m/z: $[M+H]^+$ 215.02. HRMS-ESI (m/z): calcd for $C_8H_8ClN_2O_3$ $[M+H]^+$: 215.0218; found: 215.0220

***N*-(2-chloro-5-nitrophenyl)acetamide (2o-*a*)**



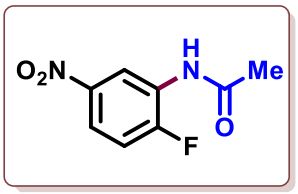
Known compound.[33] Yield: 77%, 0.198 g. Yellow solid, mp 155-158 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 9.13 (d, *J* = 2.6 Hz, 1H), 8.10 (s, 1H), 7.98 (dd, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 2.37 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 170.13, 148.33, 135.21, 130.06, 128.55, 119.14, 117.13, 24.21. MS (ESI) m/z: $[M+H]^+$ 215.02. HRMS-ESI (m/z): calcd for $C_8H_8ClN_2O_3$ $[M+H]^+$: 215.0218; found: 215.0218.

***N*-(5-chloro-2-nitrophenyl)acetamide** (2o-*b*)



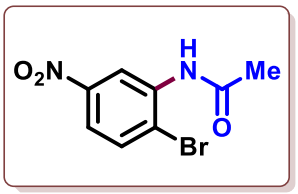
Known compound.[34] Yield: 11%, 0.028 g. Yellow solid, mp 115-118 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 10.45 (s, 1H), 8.78 (d, *J* = 2.3 Hz, 1H), 8.19 (d, *J* = 9.1 Hz, 1H), 7.20 (dd, *J* = 9.0, 2.2 Hz, 1H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 169.20, 142.95, 135.93, 134.46, 127.05, 123.54, 121.77, 25.75. MS (ESI) m/z: $[M+H]^+$ 215.02. HRMS-ESI (m/z): calcd for $C_8H_8ClN_2O_3$ $[M+H]^+$: 215.0218; found: 215.0218.

***N*-(2-fluoro-5-nitrophenyl)acetamide (2p)**



Known compound.[35] Yield: 68%, 0.159 g. Pale orange solid, mp 177-178 °C. ^{1}H NMR (400 MHz, CD_3CN): δ_H = 9.15 (dd, *J* = 6.9, 2.9 Hz, 1H), 8.49 (s, 1H), 7.99 (ddd, *J* = 9.1, 4.2, 2.9 Hz, 1H), 7.36 (dd, *J* = 10.2, 9.1 Hz, 1H), 2.19 (s, 3H). ^{13}C NMR (100 MHz, CD_3CN): δ_C = 169.57, 157.44, 154.78, 143.73, 135.93, 127.62, 127.54, 120.13, 120.05, 116.61, 116.43, 23.69. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -118.17. MS (ESI) m/z: $[M+H]^+$ 199.05. HRMS-ESI (m/z): calcd for $C_8H_8FN_2O_3$ $[M+H]^+$: 199.0513; found: 199.0513.

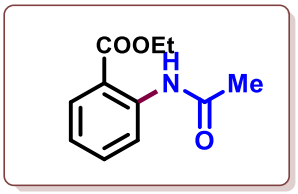
N-(2-bromo-5-nitrophenyl)acetamide (2q)



Known compound.[36] Yield: 64%, 0.198 g. Yellow solid, mp 182-183 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 9.19 (s, 1H), 8.11 (d, *J* = 8.9 Hz, 1H), 7.88 (dd, *J* = 9.1, 2.6 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 1169.30, 147.47, 137.78, 134.53, 120.97, 120.17, 23.98. MS (ESI) m/z: $[M+H]^+$ 258.97. HRMS-ESI (m/z): calcd for $C_8H_8BrN_2O_3$ $[M+H]^+$: 258.9713; found: 258.9713.

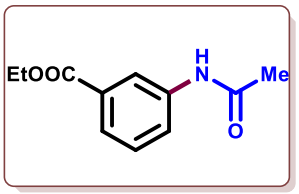
Compounds **2r,** yield 78%, 0.196 g, ratio **2r**-*a*:**2r**-*b*:**2r**-*c* = 2.2:1.7:1

Ethyl 2-acetamidobenzoate (2r-*a*)



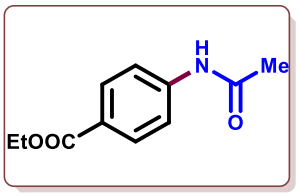
Known compound.[37] ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 11.10 (s, 1H), 8.71 (d, *J* = 8.7 Hz, 1H), 8.05 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 7.7 Hz, 1H), 4.39 (q, *J* = 7.5 Hz, 2H), 2.24 (s, 3H), 1.41 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 169.57, 168.87, 142.17, 135.07, 130.06, 122.88, 120.84, 115.62, 61.90, 25.99, 14.70. MS (ESI) m/z: $[M+H]^+$ 208.09. HRMS-ESI (m/z): calcd for $C_{11}H_{14}NO_3$ $[M+H]^+$: 208.0968; found: 208.0968.

Ethyl 3-acetamidobenzoate (2r-*b*)



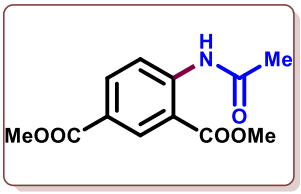
Known compound.[38] ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.03 (s, 1H), 8.00 (s, 1H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.79 (d, *J* = 6.9 Hz, 1H), 7.39 (t, *J* = 8.0 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 6H), 2.21 (s, 3H), 1.39 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.74, 165.81, 137.82, 130.42, 128.41, 125.01, 124.61, 124.11, 60.31, 23.80, 13.67. MS (ESI) m/z: $[M+H]^+$ 208.09. HRMS-ESI (m/z): calcd for $C_{11}H_{14}NO_3$ $[M+H]^+$: 208.0968; found: 208.09670.

Ethyl 4-((methoxycarbonyl)amino)benzoate (**2r**-*c*)



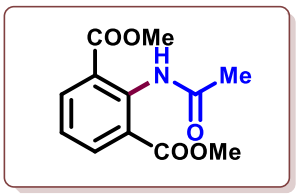
Known compound.[38] ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.02 (d, *J* = 4.8 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H), 4.37 (q, *J* = 7.1 Hz, 2H), 2.21 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H).^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 168.80, 165.83, 141.91, 130.02, 120.41, 118.31, 60.61, 24.00, 13.67. MS (ESI) m/z: $[M+H]^+$ 208.09. HRMS-ESI (m/z): calcd for $C_{11}H_{14}NO_3$ $[M+H]^+$: 208.0968; found: 208.0970.

Dimethyl 4-acetamidoisophthalate (2s-*a*)



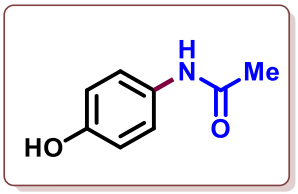
Unknown compound. Yield: 42%, 0.126 g. White solid, mp 156.8 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 11.27 (s, 1H), 8.80 (d, *J* = 8.9 Hz, 1H), 8.72 (d, *J* = 2.1 Hz, 1H), 8.18 (dd, *J* = 8.9, 2.2 Hz, 1H), 3.97 (s, 3H), 3.93 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 169.81, 168.80, 166.38, 145.68, 136.12, 133.31, 124.50, 120.36, 114.90, 53.08, 52.71, 26.08. MS (ESI) m/z: $[M+H]^+$ 252.08. HRMS-ESI (m/z): calcd for $C_{12}H_{14}NO_5$ $[M+H]^+$: 252.0867; found: 252.0868.

Dimethyl 2-acetamidoisophthalate (2s-*b*)



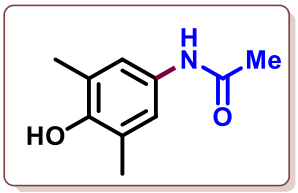
Unknown compound. Yield: 33%, 0.099 g. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 10.54 (s, 1H), 8.04 (d, *J* = 7.8 Hz, 2H), 7.24 (t, *J* = 7.8 Hz, 1H), 3.93 (s, 6H), 2.23 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 169.02, 167.47, 137.44, 134.13, 123.87, 123.49, 52.50, 24.41. MS (ESI) m/z: $[M+H]^+$ 252.08. HRMS-ESI (m/z): calcd for $C_{12}H_{14}NO_5$ $[M+H]^+$: 252.0867; found: 252.0868.

N-(4-hydroxyphenyl)acetamide (2t)



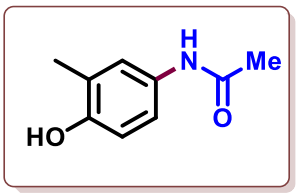
Known compound.[39] Yield: 74%, 0.132 g. White solid, mp 167-170 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 9.61 (s, 1H), 9.09 (s, 1H), 7.33 (d, *J* = 8.8 Hz, 2H), 6.67 (d, *J* = 8.8 Hz, 2H), 1.97 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d6): δ_C = 168.47, 154.11, 132.04, 121.81, 115.98, 24.72. MS (ESI) m/z: $[M+H]^+$ 152.07. HRMS-ESI (m/z): calcd for $C_8H_{10}NO_2$ $[M+H]^+$: 152.0706; found: 152.0709.

N-(4-hydroxy-3,5-dimethylphenyl)acetamide (2u)



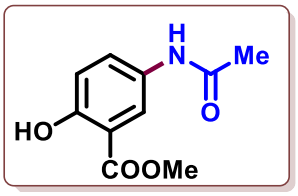
Known compound.[39] Yield: 67%, 0.144 g. Brown solid, mp 141-144 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 9.21 (s, 1H), 7.94 (s, 1H), 7.31 (s, 2H), 2.13 (s, 6H), 1.98 (s, 3H). ^{13}C NMR (100 MHz, DMSO-d6): δ_C = 168.23, 149.65, 131.82, 125.06, 120.28, 24.56, 17.57. MS (ESI) m/z: $[M+H]^+$ 180.10. HRMS-ESI (m/z): calcd for $C_{10}H_{14}NO_2$ $[M+H]^+$: 180.1019; found: 180.1018.

N-(4-hydroxy-3-methylphenyl)acetamide (2v)



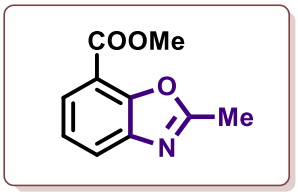
Known compound.[39] Yield: 68%, 0.135 g. White solid, mp 160-163 °C. ^{1}H NMR (400 MHz, CD_3CN): δ_H = 9.17 (s, 1H), 8.85 (s, 1H), 7.17 (dq, *J* = 4.6, 2.1 Hz, 2H), 6.66 (d, *J* = 9.0 Hz, 1H), 2.16 (s, 3H), 2.03 (s, 3H). ^{13}C NMR (100 MHz, CD_3CN): δ_C = 169.82, 152.10, 130.04, 124.42, 123.24, 119.24, 114.12, 22.16, 14.97. MS (ESI) m/z: $[M+H]^+$ 166.08. HRMS-ESI (m/z): calcd for $C_9H_{12}NO_2$ $[M+H]^+$: 166.0868; found: 166.0868.

Methyl 5-acetamido-2-hydroxybenzoate (2w)



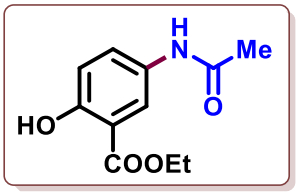
Known compound.[40] Yield: 42%, 0.105 g. Brown solid, mp 143-145 °C. ^{1}H NMR (400 MHz, CD_3CN): δ_H = 8.64 (s, 1H), 8.04 (d, *J* = 2.3 Hz, 1H), 7.60 (s, 1H), 7.54 (dd, *J* = 9.0, 2.8 Hz, 1H), 6.93 (d, *J* = 9.0 Hz, 1H), 3.93 (s, 3H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, CD_3CN): δ_C = 170.83, 170.60, 158.70, 130.38, 129.25, 121.94, 118.13, 112.65, 52.86, 23.07. MS (ESI) m/z: $[M+H]^+$ 210.07. HRMS-ESI (m/z): calcd for $C_{10}H_{12}NO_4$ $[M+H]^+$: 210.0761; found: 210.0762.

Methyl 2-methylbenzo[d]oxazole-7-carboxylate (2ww)



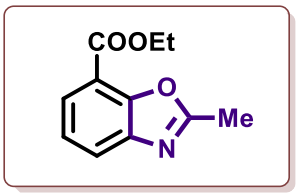
Unknown compound. Yield: 35%, 0.08 g. Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.95 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.86 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 4.02 (s, 3H), 2.73 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 165.09, 164.70, 135.70, 124.29, 123.95, 119.16, 117.59, 111.60, 52.26, 14.59. MS (ESI) m/z: $[M+H]^+$ 192.06. HRMS-ESI (m/z): calcd for $C_{10}H_{10}NO_3$ $[M+H]^+$: 192.0655; found: 192.0655.

Ethyl 5-acetamido-2-hydroxybenzoate (2x)



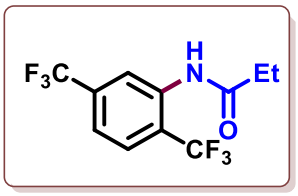
Unknown compound. Yield: 41%, 0.11 g. Brown solid, mp 121-124 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 10.69 (s, 1H), 7.98 (d, *J* = 2.7 Hz, 1H), 7.54 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.29 (s, 1H), 6.94 (d, *J* = 8.9 Hz, 1H), 4.41 (q, *J* = 7.3 Hz, 2H), 2.16 (s, 1H), 1.41 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 170.30, 168.97, 159.16, 129.87, 129.40, 122.33, 118.46, 112.89, 62.15, 24.71, 14.69. MS (ESI) m/z: $[M+H]^+$ 224.09. HRMS-ESI (m/z): calcd for $C_{11}H_{14}NO_4$ $[M+H]^+$: 224.0917; found: 224.0919.

Ethyl 2-methylbenzo[d]oxazole-7-carboxylate (2xx)



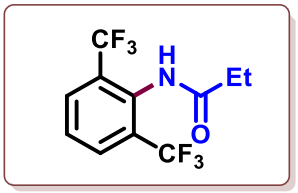
Unknown compound. Yield: 34%, 0.084 g. Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.95 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.85 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 4.49 (q, *J* = 7.1 Hz, 2H), 2.72 (s, 1H), 1.46 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 165.57, 164.73, 150.58, 143.42, 127.02, 124.67, 124.38, 115.59, 61.86, 15.12, 14.86. MS (ESI) m/z: $[M+H]^+$ 206.08. HRMS-ESI (m/z): calcd for $C_{11}H_{12}NO_3$ $[M+H]^+$: 206.0812; found: 206.0814.

N-(2,5-bis(trifluoromethyl)phenyl)propionamide (3a)



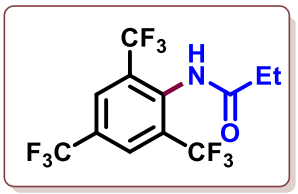
Known compound.[21] Yield: 85%, 0.287 g. White solid, mp 83-85 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.69 (s, 1H), 7.75 (d, *J* = 8.0 Hz, 1H). 7.55 (d, *J* = 7.5 Hz, 2H), 2.50 (q, *J* = 7.5 Hz, 2H), 1.30 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.62, 136.77, 136.06, 135.73, 135.40, 135.06, 128.00, 127.94, 127.89, 127.66, 127.37, 127.31, 127.26, 127.21, 125.30, 124.95, 122.58, 122.23, 121.54, 121.50, 121.29, 121.25, 119.85, 119.51, 31.38, 9.72. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -61.22, -63.41. MS (ESI) m/z: $[M+H]^+$ 286.06. HRMS-ESI (m/z): calcd for $C_{11}H_{10}F_6NO$ $[M+H]^+$: 286.0661; found: 286.0662.

N-(2,6-bis(trifluoromethyl)phenyl)propionamide (3b)



Unknown compound. Yield: 75%, 0.257 g. White solid, mp 82-85 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 7.93 (d, *J* = 8.0 Hz, 2H), 7.61 (t, *J* = 7.9 Hz, 1H), 7.08 (s, 1H), 2.48 (q, *J* = 7.6 Hz, 2H), 1.29 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 173.78, 132.77, 131.24, 131.00, 130.75, 130.51, 130.01, 129.98, 129.94, 129.90, 128.20, 123.30, 121.12, 118.94, 29.16, 8.93. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -61.39. MS (ESI) m/z: $[M+H]^+$ 286.06. HRMS (ESI) m/z $[M+H]^+$: calcd for $C_{11}H_{10}F_6NO$, 286.0661; found, 286.0664.

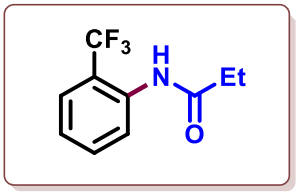
N-(2,4,6-tris(trifluoromethyl)phenyl)propionamide (3c)



Unknown compound. Yield: 45%, 0.263 g. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.41 (s, 2H), 7.98 (s, 1H), 2.36 (q, *J* = 7.2 Hz, 2H), 1.31 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 171.36, 132.99, 132.57, 132.05, 130.54, 129.36, 124.67, 123.41, 29.28, 9.59. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -60.77, -62.41. MS (ESI) m/z: $[M+H]^+$ 340.0. HRMS (ESI) m/z $[M+H]^+$: calcd for $C_{12}H_9F_9NO$, 354.05349; found, 354.05350.

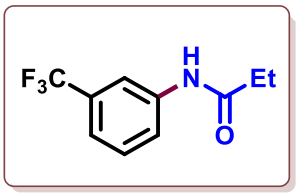
Compounds **3d**, yield 82%, 0.211 g, ratio **3d-*a*:3d-*b*:3d-**c = 3:3:2

N*-(2-(trifluoromethyl)phenyl)propionamide** (**3d-*a)



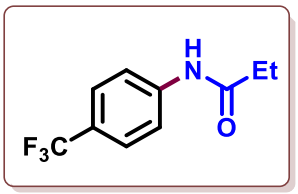
Known compound.[41] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.34 (s, 1H), 8.03 (d, *J* = 7.8 Hz, 1H), 7.64 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.23 (t, *J* = 7.4 Hz, 1H), 2.46 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 173.70, 135.50, 133.24, 128.52, 126.71, 126.66, 126.62, 126.57, 126.18, 125.79, 125.59, 123.08, 120.34, 30.95, 10.00. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -60.68. MS (ESI) m/z: [M+H]+ 218.1. HRMS-ESI (m/z): calcd for $C_{10}H_{11}F_3NO$ [M+H]+ : 218.0787; found: 218.0790.

N*-(3-(trifluoromethyl)phenyl)propionamide** (**3d-*b)



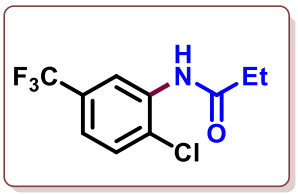
Known compound.[21] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.85 (s, 1H), 7.70 (d, *J* = 7.8 Hz, 1H), 7.52 (s, 1H), 7.34 (m, 2H), 2.37 (q, *J* = 7.6 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 173.70, 139.29, 132.17, 131.84, 131.52, 131.20, 128.72, 127.73, 126.08, 123.57, 123.32, 121.06, 120.62, 117.25, 31.03, 10.00. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -62.79. MS (ESI) m/z: $[M+H]^+$ 218.1. HRMS-ESI (m/z): calcd for $C_{10}H_{11}F_3NO$ $[M+H]^+$: 218.0787; found: 218.0790.

N*-(4-(trifluoromethyl)phenyl)propionamide** (**3d-*c)



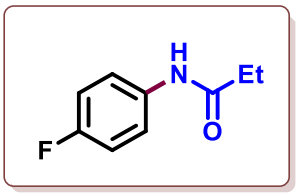
Known compound.[42] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.32 (s, 1H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 7.9 Hz, 2H), 2.38 (q, *J* = 7.5 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 173.40, 141.88, 128.57, 126.67, 126.61, 126.56, 126.48, 126.03, 125.84, 123.13, 120.38, 120.05, 31.15, 9.96. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -62.34. MS (ESI) m/z: $[M+H]^+$ 218.1. HRMS-ESI (m/z): calcd for $C_{10}H_{11}F_3NO$ [M+H]+ : 218.0787; found: 218.0790.

N-(2-chloro-5-(trifluoromethyl)phenyl)propionamide (3e)



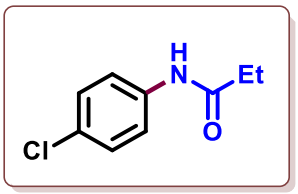
Unknown compound. 87%, 0.263 g. White solid, mp 79-82 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.77 (s, 1H), 7.77 (s, 1H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.29 (dd, *J* = 8.5 Hz, 1H), 2.52 (q, *J* = 7.5 Hz, 2H), 1.29 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 171.77, 134.64, 130.08, 129.82, 129.56, 129.29, 128.86, 126.22, 125.25, 124.05, 121.89, 120.44, 120.41, 117.90, 30.37, 8.78. ^{19}F NMR (376 MHz, $CDCl_3$) δ = -62.77. MS (ESI) m/z: $[M+H]^+$ 252.0. HRMS-ESI (m/z): calcd for $C_{10}H_{10}ClF_3NO$ $[M+H]^+$: 252.0397; found: 252.0394.

N-(4-fluorophenyl)propionamide (3f)



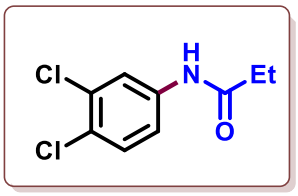
Known compound.[42] Yield: 72%, 0.144 g. Brown solid, mp 132-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.69 (s, 1H), 7.42 (dd, *J* = 8.9 Hz, 3.5 Hz, 2H), 6.97 – 6.92 (m, 2H), 2.36 (q, *J* = 7.6 Hz, 2H), 1.24 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.59, 160.25, 157.70, 134.00, 121.93, 121.81, 115.55, 115.26, 30.37, 9.66. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -120.78. MS (ESI) m/z: $[M+H]^+$ 168.08. HRMS-ESI (m/z): calcd for $C_9H_{11}FNO$ $[M+H]^+$: 168.0819, found 168.0817.

N-(4-chlorophenyl)propionamide (3g)



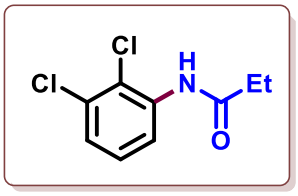
Known compound.[23] Yield: 45%, 0.099 g. Brown solid, mp 134-137 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.70 (s, 1H), 7.51 (d, *J* = 8.9 Hz, 2H), 7.30 (d, *J* = 8.9 Hz, 2H), 2.43 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.61, 136.82, 129.33, 129.13, 121.41, 30.82, 9.83. MS (ESI) m/z: $[M+H]^+$ 184.05. HRMS-ESI (m/z): calcd for $C_9H_{11}ClNO$ [M+H]+: 184.0524; found: 184.0522.

N-(3,4-dichlorophenyl)propionamide (3h-*a*)



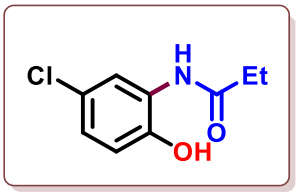
Known compound.[43] Yield: 51%, 0.133 g. White solid, mp 90-92°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.78 (s, 1H), 7.35 – 7.34 (m, 1H), 7.32 (s, 2H), 2.42 (q, *J* = 7.5 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.39, 136.66, 132.08, 129.77, 120.73, 118.24, 28.94, 8.75. MS (ESI) m/z: $[M+H]^+$ 218.01. HRMS-ESI (m/z): calcd for $C_9H_{10}Cl_2NO$ $[M+H]^+$: 218.0134; found: 218.0134.

N-(2,3-dichlorophenyl)propionamide (3h-*b*)



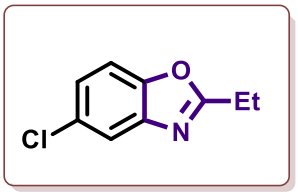
Unknown compound. Yield: 17%, 0.044 g. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.88 (s, 1H), 7.70 (dd, *J* = 8.1, 2.2 Hz, 1H), 7.37 (dd, *J* = 8.0, 2.2 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 2.53 (q, *J* = 7.6 Hz, 2H), 1.17 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.13, 137.12, 134.84, 128.59, 124.84, 123.51, 119.98, 31.31, 9.78. MS (ESI) m/z: $[M+H]^+$ 218.01. HRMS-ESI (m/z): calcd for $C_9H_{10}Cl_2NO$ $[M+H]^+$: 218.0134; found: 218.0136.

N-(5-chloro-2-hydroxyphenyl)propionamide (3i)



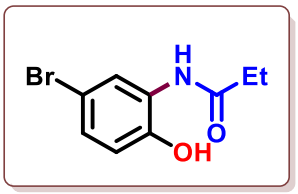
Unknown compound. Yield: 25%, 0.055 g. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.29 (s, 1H), 7.15 (d, *J* = 2.5 Hz, 1H), 7.08 (dd, *J* = 8.7, 2.5 Hz, 1H), 7.02 (s, 1H), 6.94 (d, *J* = 8.5 Hz, 1H), 2.51 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.15, 147.80, 126.90, 124.06, 122.95, 120.96, 116.11, 30.68, 9.57. MS (ESI) m/z: $[M+H]^+$ 200.0. HRMS-ESI (m/z): calcd for $C_9H_{11}ClNO_2$ $[M+H]^+$: 200.0473; found: 200.0475.

5-chloro-2-ethylbenzo[d]oxazole (3ii)



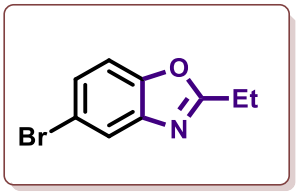
Known compound.[26] Yield: 49%, 0.107 g. White solid, mp 35-38°C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 7.67 (d, *J* = 2.1 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.29 (dd, *J* = 8.6, 2.1 Hz, 1H), 2.98 (q, *J* = 7.6 Hz, 2H), 1.47 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 169.11, 148.93, 142.04, 129.06, 124.23, 119.09, 110.46, 21.71, 10.29. MS (ESI) m/z: $[M+H]^+$ 182.0. HRMS-ESI (m/z): calcd for C_9H_9ONCl $[M+H]^+$: 182.0367; found: 182.0366.

N-(5-bromo-2-hydroxyphenyl)propionamide (3j)



Unknown compound. 12%, 0.035 g. Brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.78 (s, 1H), 7.43 (dd, *J* = 4.6, 2.2 Hz, 1H), 7.17 (dd, *J* = 8.7, 2.4 Hz, 1H), 7.16 (s, 1H), 6.86 (d, *J* = 8.6 Hz, 1H), 2.50 (q, *J* = 7.5 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.00, 147.84, 129.69, 127.68, 124.96, 117.50, 112.43, 30.68, 10.21. MS (ESI) m/z: $[M+H]^+$ 244.0. HRMS-ESI (m/z): calcd for $C_9H_{11}BrNO_2$ $[M+H]^+$: 243.9967; found: 243.9967.

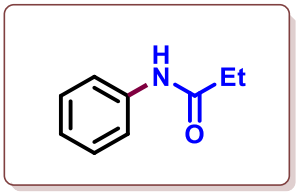
5-bromo-2-ethylbenzo[d]oxazole (3jj)



Known compound.[26] Yield: 61%, 0.165 g. White solid, mp 46-48 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 7.83 (d, *J* = 8.7 Hz, 1H), 7.44 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.38 (d, *J* = 8.6 Hz, 1H), 2.99 (q, *J* = 7.6 Hz, 2H), 1.47 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 169.79, 149.76, 143.237, 127.82, 122.94, 117.19, 111.90, 22.60, 10.98. ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 169.16, 149.24, 141.99, 127.16, 121.93,

116.49, 111.07, 21.64, 10.25. MS (ESI) m/z: $[M+H]^+$ 226.0. HRMS-ESI (m/z): calcd for C_9H_9ONBr $[M+H]^+$: 225.9862; found: 225.9862.

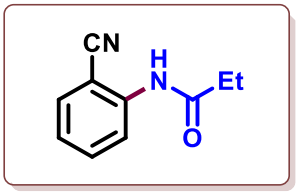
***N*-phenylpropionamide (3k-*a*)**



Known compound.[42] Yield: 71%, 0.125 g. White solid, mp 101-104 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.54 (d, *J* = 7.6 Hz, 2H), 7.40 (s, 1H), 7.35 (t, *J* = 7.9 Hz, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 2.40 (q, *J* = 7.6, 2H), 1.15 (t, *J* = 7.6, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.24, 138.09, 129.13, 124.22, 120.03, 30.80, 9.77. MS (ESI) m/z: $[M+H]^+$ 150.1. HRMS-ESI (m/z): calcd for $C_9H_{12}NO$ $[M+H]^+$: 159.0913; found: 159.0914.

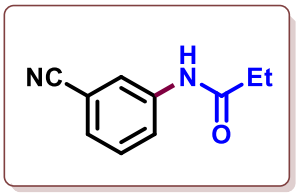
Compounds **3l**, yield 73%, 0.152 g, ratio **3l-*a*:3l-*b*:3l-*c*** = 3:1:2

***N*-(2-cyanophenyl)propionamide (3l-*a*)**



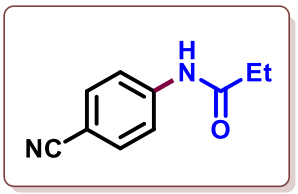
Known compound.[21] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 11.17 (s, 1H), 8.71 (dd, *J* = 8.5 Hz, 1H), 8.06 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.12 – 7.08 (m, 1H), 2.51 (q, *J* = 7.6 Hz, 2H), 1.43 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 173.70, 142.64, 135.91, 132.21, 123.08, 118.98, 114.52, 32.25, 10.10. MS (ESI) m/z: $[M+H]^+$ 175.1. HRMS-ESI (m/z): calcd for $C_{10}H_{11}N_2O$ $[M+H]^+$: 175.0866; found: 175.0867.

***N*-(3-cyanophenyl)propionamide (3l-*b*)**



Known compound.[21] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.95 (s, 1H), 7.74 (d, *J* = 8 Hz, 1H), 7.44 – 7.37 (m, 3H), 2.45 (q, *J* = 7.6 Hz, 2H), 1.30 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = δ 171.34, 139.34, 130.41, 128.14, 121.00, 119.35, 118.31, 113.56, 29.23, 9.97. MS (ESI) m/z: $[M+H]^+$ 175.1. HRMS-ESI (m/z): calcd for $C_{10}H_{11}N_2O$ $[M+H]^+$: 175.0866; found: 175.0867.

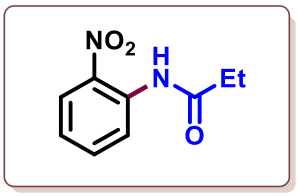
***N*-(4-cyanophenyl)propionamide (3l-*c*)**



Known compound.[44] White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.68 (d, *J* = 8.9, 2H), 7.62 (d, *J* = 8.9 Hz, 2H), 7.45 (s, 1H), 2.46 (q, *J* = 7.6 Hz, 2H), 1.28 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.97, 142.57, 133.83, 120.01, 107.55, 31.36, 9.90. MS (ESI) m/z: $[M+H]^+$ 175.1. HRMS-ESI (m/z): calcd for $C_{10}H_{11}N_2O$ $[M+H]^+$: 175.0866; found: 175.0867.

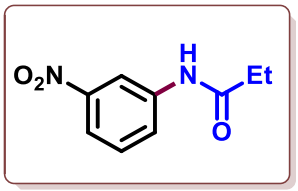
Compounds **3m,** yield 68%, 0.159 g, ratio **3m-*a*:3m-*b*:3m-*c*=** 3.2:1:1

N*-(2-nitrophenyl)propionamide** (**3m-*a)



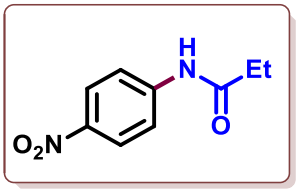
Known compound.[42] Yield: 42%, 0.098 g. Yellow solid, mp 63-65 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 9.47 (s, 1H), 8.80 (dd, *J* = 9.7, 1.8 Hz, 1H), 8.21 (dd, *J* = 9.5, 1.7 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 2.56 (q, *J* = 7.5 Hz, 2H), 1.31 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.75, 136.14, 135.93, 134.89, 125.61, 122.95, 120.01, 30.80, 9.78. MS (ESI) m/z: $[M+H]^+$ 195.1. HRMS-ESI (m/z): calcd for $C_9H_{11}N_2O_3$ $[M+H]^+$: 195.0764; found: 195.0764.

N*-(3-nitrophenyl)propionamide** (**3m-*b)



Known compound.[45] Yield: 13%, 0.033 g. Yellow solid, mp 100-102 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.39 (s, 1H), 7.98 – 7.94 (m, 2H), 7.83 (s, 1H), 7.48 (t, *J* = 8.2 Hz, 1H), 2.47 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 173.30, 148.17, 139.14, 129.55, 125.56, 118.42, 114.39, 30.36, 9.34. MS (ESI) m/z: $[M+H]^+$ 195.1. HRMS-ESI (m/z): calcd for $C_9H_{11}N_2O_3$ $[M+H]^+$: 195.0764; found: 195.0765.

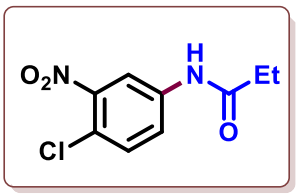
N*-(4-nitrophenyl)propionamide** (**3m-*c)



Known compound.[46] Yield: 13%, 0.03 g. Yellow solid, mp 69-72 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.20 (d, *J* = 9.2 Hz, 2H), 7.78 (s, 1H), 7.73 (d, *J* = 9.2 Hz, 2H), 2.47 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 173.69, 145.90, 142.47, 125.48, 118.83, 30.17, 9.67. MS (ESI) m/z: $[M+H]^+$ 195.1. HRMS-ESI (m/z): calcd for $C_9H_{11}N_2O_3$ $[M+H]^+$: 195.0764; found: 195.0765.

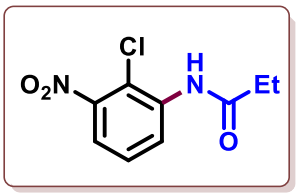
Compounds **3n,** yield 80%, 0.217 g, ratio **3n-*a*:3n-*b* =** 2.2:1

***N*-(4-chloro-3-nitrophenyl)propionamide (3n-*a*)**



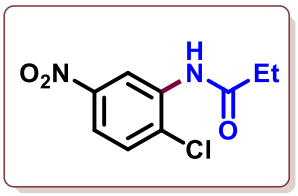
Unknown compound. Yield: 58%. Brown solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.18 (d, *J* = 2.43 Hz, 1H), 7.73 (dd, *J* = 8.78, 2.43 Hz, 1H), 7.54 (s, 1H), 7.48 (d, *J* = 8.78 Hz, 1H), 2.45 (q, *J* = 7.58 Hz, 2H), 1.28 (t, *J* = 7.58 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 171.82, 147.40, 137.04, 131.59, 123.26, 120.71, 115.75, 30.12, 8.80. MS (ESI) m/z: $[M+H]^+$ 229.0. HRMS-ESI (m/z): calcd for $C_9H_{10}ClN_2O_3$ $[M+H]^+$:229.0375; found: 229.0375.

***N*-(2-chloro-3-nitrophenyl)propionamide (3n-*b*)**



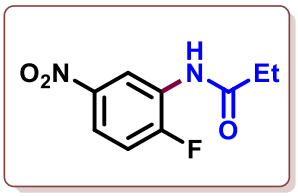
Unknown compound. Yield: 22%. Brown solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 8.69 (dd, *J* = 8.38, 1.43 Hz, 1H), 7.84 (s, 1H), 7.59 (dd, *J* = 8.16, 1.43 Hz, 1H), 7.44 (t, *J* = 8.4 Hz, 1H), 2.55 (q, *J* = 7.52 Hz, 2H), 1.32 (t, *J* = 7.52 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 171.73, 147.96, 136.09, 127.31, 124.25, 119.26, 114.51, 30.55, 8.87. MS (ESI) m/z: $[M+H]^+$ 229.0. HRMS-ESI (m/z): calcd for $C_9H_{10}ClN_2O_3$ $[M+H]^+$:229.0375; found: 229.0377.

***N*-(2-chloro-5-nitrophenyl)propionamide (3o)**



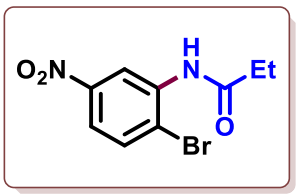
Unknown compound. Yield: 85%, 0.233 g. Yellow solid, mp 116-120 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.39 (d, *J* = 2.59 Hz, 1H), 7.93 (dd, *J* = 8.75 Hz, 1H), 7.75 (s, 1H), 7.56 (d, *J* = 8.74 Hz, 1H), 2.55 (q, *J* = 7.54 Hz, 2H), 1.33 (t, *J* = 7.54 Hz). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 171.50, 146.73, 135.04, 128.92, 127.79, 118.30, 115.70, 30.45, 8.76. MS (ESI) m/z: $[M+H]^+$ 229.0. HRMS-ESI (m/z): calcd for $C_9H_{10}ClN_2O_3$ $[M+H]^+$: 229.0375; found: 229.0378.

N-(2-fluoro-5-nitrophenyl)propionamide (3p)



Unknown compound. Yield: 72%, 0.255 g. Yellow solid, mp 98-102 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.35 (dd, *J* = 6.82, 2.79 Hz, 1H), 8.00 (ddd, *J* = 9.07, 4.65, 2.79 Hz, 1H), 7.47 (s, 1H), 7.25 (dd, *J* = 9.93, 9.07 Hz, 1H), 2.52 (q, *J* = 7.53 Hz, 2H), 1.31 (t, *J* = 7.53 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 171.57, 155.67, 153.66, 144.08, 126.85, 126.76, 119.13, 119.06, 116.75, 114.82, 114.63, 30.24, 8.73. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -121.72. MS (ESI) m/z: $[M+H]^+$ 213.1. HRMS-ESI (m/z): calcd for $C_9H_{10}FN_2O_3$ $[M+H]^+$: 213.0670; found: 213.0669.

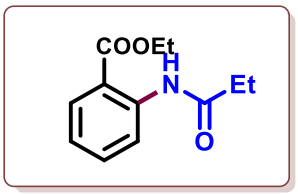
N-(2-bromo-5-nitrophenyl)propionamide (3q)



Unknown compound. Yield: 57%, 0.186 g. Yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 9.30 (d, *J* = 2.7 Hz, 1H), 7.84 (dd, *J* = 8.8, 2.7 Hz, 1H), 7.77 (s, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 2.54 (q, *J* = 7.5 Hz, 2H), 1.31 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.73, 148.39, 137.26, 133.27, 119.92, 119.70, 116.84, 31.52, 9.84. MS (ESI) m/z: $[M+H]^+$ 273.0. HRMS-ESI (m/z): calcd for $C_9H_{10}BrN_2O_3$ $[M+H]^+$: 272.9869; found: 272.9870.

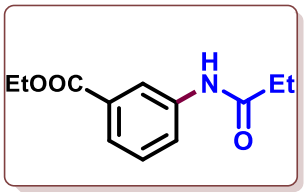
Compounds **3r,** yield 82%, 0.218 g, ratio **3r**-*a*:**3r**-*b*:**3r**-*c* = 2:2:1

Ethyl 2-propionamidobenzoate (3r-*a*)



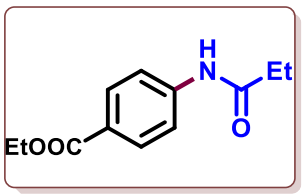
Unknown compound. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 11.17 (s, 1H), 8.74 (d, *J* = 8.5 Hz, 1H), 8.12 (dd, *J* = 8.0, 1.7 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.10 (td, *J* = 7.7, 1.2 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 2.49 (q, *J* = 7.6 Hz, 2H), 1.39 (t, *J* = 6.7 Hz, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.91, 170.81, 140.94, 134.55, 131.72, 122.79, 119.55, 116.41, 62.08, 31.09, 14.61, 9.82. MS (ESI) m/z: $[M+H]^+$ 222.1. HRMS-ESI (m/z): calcd for $C_{12}H_{16}NO_3$ $[M+H]^+$: 222.1125; found: 222.1124.

Ethyl 3-propionamidobenzoate (**3r**-*b*)



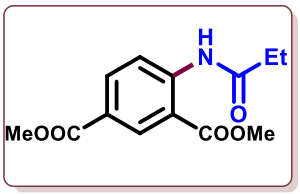
Unknown compound. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.44 (s, 1H), 8.03 (d, *J* = 6.4 Hz, 1H), 7.95 (s, 1H), 7.82 (d, *J* = 6.2 Hz, 1H), 7.45 (t, *J* = 6.3 Hz, 1H), 4.39 (q, *J* = 5.1 Hz, 2H), 2.44 (q, *J* = 5.7 Hz, 2H), 1.40 (t, *J* = 5.1 Hz, 3H), 1.19 (t, *J* = 5.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.06, 166.20, 138.59, 130.98, 127.87, 125.50, 124.79, 124.41, 60.83, 30.50, 14.06, 9.91. MS (ESI) m/z: $[M+H]^+$ 222.1. HRMS-ESI (m/z): calcd for $C_{12}H_{16}NO_3$ $[M+H]^+$: 222.1125; found: 222.1126.

Ethyl 4-propionamidobenzoate (**3r**-*c*)



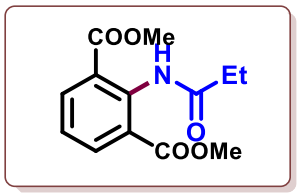
Unknown compound. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.00 (d, *J* = 6.9 Hz, 1H), 7.94 (s, 1H), 7.67 (d, *J* = 6.8 Hz, 1H), 4.39 (q, *J* = 5.1 Hz, 2H), 2.39 (q, *J* = 5.7 Hz, 2H), 1.40 (t, *J* = 5.1 Hz, 3H), 1.15 (t, *J* = 5.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.98, 166.15, 142.09, 130.53, 120.74, 118.51, 60.62, 30.36, 14.06, 9.44. MS (ESI) m/z: $[M+H]^+$ 222.1. HRMS-ESI (m/z): calcd for $C_{12}H_{16}NO_3$ $[M+H]^+$: 222.1125; found: 222.1126.

Dimethyl 4-propionamidoisophthalate (3s-*a*)



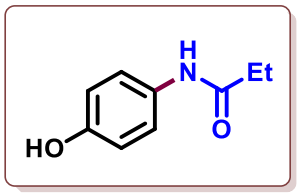
Unknown compound. Yield: 38%, 0.121 g. Orange solid, mp 158-160 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 11.33 (s, 1H), 8.81 (d, *J* = 8.9 Hz, 1H), 8.71 (d, *J* = 2.1 Hz, 1H), 8.17 (dd, *J* = 8.9, 2.2 Hz, 1H), 3.96 (s, 3H), 3.92 (s, 3H), 2.47 (q, *J* = 7.6 Hz, 4H), 1.39 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 172.58, 168.82, 166.80, 144.69, 135.72, 133.54, 125.02, 120.73, 115.75, 52.74, 52.45, 30.24, 9.65. MS (ESI) m/z: $[M+H]^+$ 266.1. HRMS-ESI (m/z): calcd for $C_{13}H_{16}NO_5$ $[M+H]^+$: 266.1023; found: 266.1023.

Dimethyl 2-propionamidoisophthalate (3s-*b*)



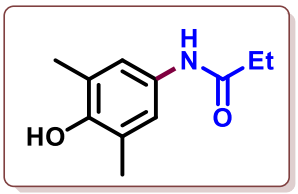
Unknown compound. Yield: 26%, 0.083 g. Orange solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 11.31 (s, 1H), 8.06 (d, *J* = 7.8 Hz, 2H), 6.53 (t, *J* = 7.8 Hz, 1H), 3.93 (s, 6H), 2.50 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 172.76, 169.30, 138.80, 133.84, 121.94, 121.23, 52.84, 29.28, 9.89. MS (ESI) m/z: $[M+H]^+$ 266.1. HRMS-ESI (m/z): calcd for $C_{13}H_{16}NO_5$ $[M+H]^+$: 266.1023; found: 266.1023.

N-(4-hydroxyphenyl)propionamide (3t)



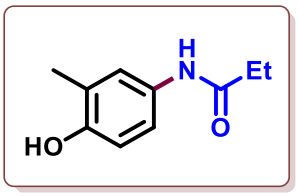
Known compound.[47] Yield: 73%, 0.145 g. White solid, mp 170-173 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 8.21 (s, 1H), 7.70 (s, 1H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.23 (d, *J* = 8.7 Hz, 2H), 2.26 (q, *J* = 7.5 Hz, 2H), 1.09 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 171.32, 153.11, 131.14, 120.88, 115.08, 27.60, 9.89. MS (ESI) m/z: $[M+H]^+$ 166.1. HRMS-ESI (m/z): calcd for $C_9H_{12}NO_2$ $[M+H]^+$: 166.0826; found: 166.0827.

N-(4-hydroxy-3,5-dimethylphenyl)propionamide (3u)



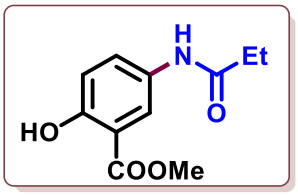
Known compound.[48] Yield: 65%, 0.151 g. White solid, mp 206-210 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ_H = 9.41 (s, 1H), 7.99 (s, 1H), 7.16 (s, 2H), 2.45 (q, *J* = 7.5 Hz, 2H), 2.15 (s, 6H), 1.15 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d6): δ_C = 171.41, 148.99, 131.16, 124.47, 119.88, 29.58, 16.87, 9.94. MS (ESI) m/z: $[M+H]^+$ 194.1. HRMS-ESI (m/z): calcd for $C_{11}H_{16}NO_2$ $[M+H]^+$: 194.1176; found: 194.1176.

N-(4-hydroxy-3-methylphenyl)propionamide (3v)



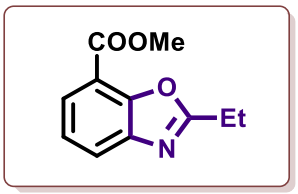
Unknown compound. Yield: 66%, 0.141 g. White solid, mp 137-139 °C. ^{1}H NMR (400 MHz, CD_3CN): δ_H = 8.91 (s, 1H), 8.49 (s, 1H), 7.26 (dd, *J* = 8.7, 2.1 Hz, 2H), 6.81 (d, *J* = 8.5 Hz), 2.42 (q, *J* = 7.5 Hz, 2H), 2.15 (s, 3H), 1.13 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, CD_3CN): δ_C = 172.13, 147.33, 132.49, 125.34, 122.78, 120.28, 117.27, 30.88, 16.32, 9.78. MS (ESI) m/z: $[M+H]^+$ 180.1. HRMS-ESI (m/z): calcd for $C_{10}H_{14}NO_2$ $[M+H]^+$: 180.1019; found: 180.1019.

Methyl 2-hydroxy-5-propionamidobenzoate (3w)



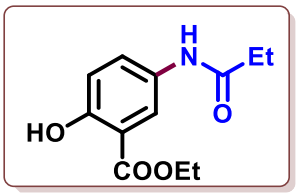
Unknown compound. Yield: 36%, 0.096 g. Brown solid, mp 121-124 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.72 (s, 1H), 8.06 (d, *J* = 1.2 Hz, 1H), 7.87 (s, 1H), 7.56 (dd, *J* = 7.9 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 3.93 (s, 3H), 2.46 (q, *J* = 7.3 Hz, 2H), 1.12 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.78, 168.57, 159.12, 131.07, 125.82, 121.84, 116.14, 115.02, 52.98, 31.46, 11.14. MS (ESI) m/z: $[M+H]^+$ 224.1. HRMS-ESI (m/z): calcd for $C_{11}H_{14}NO_4$ $[M+H]^+$: 224.0917; found: 224.0917.

Methyl 2-ethylbenzo[d]oxazole-7-carboxylate (3ww)



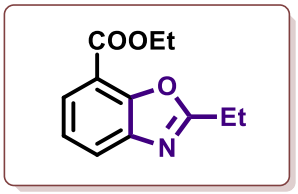
Unknown compound. Yield: 32%, 0.079 g. Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.98 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.88 (dd, *J* = 7.9 Hz, 1H), 7.49 (t, *J* = 8.0 Hz, 1H), 3.91 (s, 3H), 3.01 (q, *J* = 7.3 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 170.20, 168.02, 148.98, 139.52, 127.98, 126.54, 118.75, 115.22, 52.67, 22.29, 11.19. MS (ESI) m/z: $[M+H]^+$ 206.1. HRMS-ESI (m/z): calcd for $C_{11}H_{12}NO_3$ $[M+H]^+$: 206.0811; found: 206.0813.

Ehyl 2-hydroxy-5-propionamidobenzoate (3x)



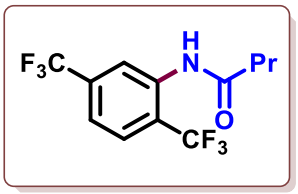
Unknown compound. Yield: 34%, 0.097 g. Brown solid, mp 97-100 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 10.70 (s, 1H), 8.04 (d, *J* = 2.7 Hz, 1H), 7.54 (dd, *J* = 8.9, 2.7 Hz, 1H), 7.19 (s, 1H), 6.95 (d, *J* = 8.9 Hz, 1H), 4.42 (q, *J* = 7.3 Hz, 2H), 2.40 (q, *J* = 7.3 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.06, 169.85, 158.51, 129.51, 128.63, 121.51, 117.90, 112.36, 61.61, 30.44, 29.69, 14.19, 9.63. MS (ESI) m/z: $[M+H]^+$ 238.1. HRMS-ESI (m/z): calcd for $C_{12}H_{16}NO_4$ $[M+H]^+$: 238.1074; found: 238.1073.

Ethyl 2-ethylbenzo[d]oxazole-7-carboxylate (3xx)



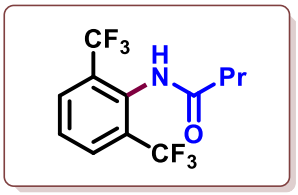
Unknown compound. Yield: 33%, 0.087 g. Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.97 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.88 (dd, *J* =7.9, 1.2 Hz, 1H), 7.40 (t, *J* = 8.1 Hz, 1H), 4.48 (q, *J* = 7.2 Hz, 2H), 3.06 (q, *J* = 7.2 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.33 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.06, 169.85, 158.52, 129.51, 128.63, 121.51, 117.90, 112.36, 61.61, 30.44, 14.19, 9.63. MS (ESI) m/z: $[M+H]^+$ 220.1. HRMS-ESI (m/z): calcd for $C_{12}H_{14}NO_3$ $[M+H]^+$: 220.0968; found: 220.0971.

N-(2,5-bis(trifluoromethyl)phenyl)butyramide (4a)



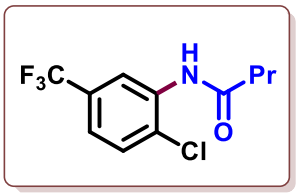
Unknown compound. Yield: 82%, 0.294 g. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.54 (s, 1H), 7.80 (d, *J* = 9.1 Hz, 1H), 7.50 (d, *J* = 8.9 Hz, 2H), 2.47 (t, *J* = 7.5 Hz, 2H), 1.77 (h, *J* = 7.5 Hz, 2H), 0.97 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.77, 138.45, 136.89, 136.82, 136.75, 134.97, 134.65, 134.33, 134.01, 130.87, 128.13, 127.35, 125.40, 122.69, 121.18, 39.08, 20.76, 14.17. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -61.17, -63.11. MS (ESI) m/z: $[M+H]^+$ 300.1. HRMS-ESI (m/z): calcd for $C_{12}H_{12}F_6NO$ $[M+H]^+$: 300.0817; found: 300.0818.

N-(2,6-bis(trifluoromethyl)phenyl)butyramide (4b)



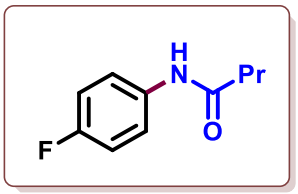
Unknown compound. Yield: 74%, 0.253 g. Brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.83 (s, 1H), 8.03 (d, *J* = 8.5 Hz, 2H), 7.70 (t, *J* = 8.4 Hz, 1H), 2.44 (t, *J* = 7.4 Hz, 2H), 1.75 (h, *J* = 7.5 Hz, 2H), 0.98 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.60, 140.47, 140.43, 140.40, 133.12, 132.79, 132.47, 132.41, 132.08, 130.07, 130.04, 130.00, 129.97, 129.93, 129.09, 129.06, 129.02, 128.98, 128.95, 127.94, 125.19, 122.46, 119.72, 38.18, 19.94, 14.06. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -61.28. MS (ESI) m/z: $[M+H]^+$ 300.1. HRMS (ESI) m/z $[M+H]^+$: calcd for $C_{12}H_{12}F_6NO$, 300.0817; found, 300.0818.

N-(2-chloro-5-(trifluoromethyl)phenyl)butyramide (4e)



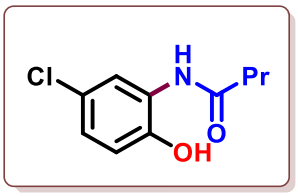
Unknown compound. 85%, 0.271 g. Brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.57 (s, 1H), 8.18 (s, 1H), 7.52 (d, *J* = 8.5 Hz, 1H), 7.33 (d, *J* = 8.2 Hz, 1H), 2.46 (t, *J* = 7.5 Hz, 2H), 1.73 (h, *J* = 7.5 Hz, 2H), 1.00 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 172.41, 134.35, 130.31, 130.04, 129.78, 129.52, 129.19, 126.16, 125.16, 124.03, 122.05, 119.99, 118.29, 39.31, 20.20, 14.40. ^{19}F NMR (376 MHz, $CDCl_3$) δ = -62.65. MS (ESI) m/z: $[M+H]^+$ 266.1. HRMS-ESI (m/z): calcd for $C_{11}H_{12}ClF_3NO$ $[M+H]^+$: 266.0554; found: 266.0554.

N-(4-fluorophenyl)butyramide (4f)



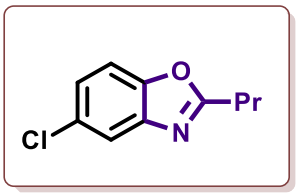
Known compound.[49] Yield: 67%, 0.146 g. Brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.48 (dd, *J* = 8.8 Hz, 3.5 Hz, 2H), 7.14 (s, 1H), 7.05 – 7.00 (m, 2H), 2.34 (t, *J* = 7.6 Hz, 2H), 1.72 (h, *J* = 7.5 Hz, 2H), 1.00 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.67, 160.39, 157.92, 134.36, 134.34, 121.73, 115.70, 115.48, 38.81, 21.14, 13.80. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -118.05. MS (ESI) m/z: $[M+H]^+$ 182.1. HRMS-ESI (m/z): calcd for $C_{10}H_{13}FNO$ $[M+H]^+$: 182.0976, found 182.0977.

N-(5-chloro-2-hydroxyphenyl)butyramide (4i)



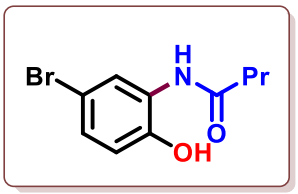
Known compound.[50] Yield: 23%, 0.059 g. White solid. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 10.04 (s, 1H), 9.12 (s, 1H), 8.01 (d, *J* = 1.9 Hz, 1H), 6.98 (dd, *J* = 6.4, 1.8 Hz, 1H), 6.89 (d, *J* = 6.4 Hz, 1H), 2.39 (t, *J* = 5.5 Hz, 2H), 1.63 (h, *J* = 5.5 Hz, 2H), 0.96 (t, *J* = 5.6 Hz, 3H).^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 172.99, 147.30, 128.84, 124.45, 123.21, 122.06, 117.35, 38.92, 19.69, 14.49. MS (ESI) m/z: $[M+H]^+$ 214.1. HRMS-ESI (m/z): calcd for $C_{10}H_{13}ClNO_2$ $[M+H]^+$: 214.0629; found: 214.0628.

5-chloro-2-propylbenzo[d]oxazole (4ii)



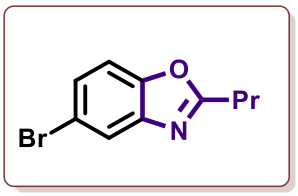
Unknown compound. Yield: 50%, 0.117 g. White solid, mp 41-44 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.70 (d, *J* = 1.6 Hz, 1H), 7.47 (d, *J* = 6.5 Hz, 1H), 7.33 (dd, *J* = 6.4, 1.6 Hz, 1H), 2.95 (t, *J* = 5.5 Hz, 2H), 1.94 (h, *J* = 5.6 Hz, 2H), 1.02 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 169.58, 149.87, 142.26, 130.22, 124.98, 119.33, 110.77, 30.68, 20.25, 13.64. MS (ESI) m/z: $[M+H]^+$ 196.1. HRMS-ESI (m/z): calcd for $C_{10}H_{11}ONCl$ $[M+H]^+$: 196.0524; found: 196.0524.

N-(5-bromo-2-hydroxyphenyl)butyramide (4j)



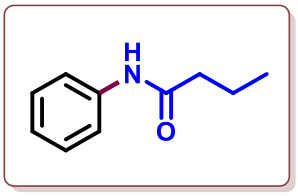
Unknown compound. 11%, 0.034 g. Brown solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.78 (s, 1H), 8.40 (s, 1H), 7.92 (d, *J* = 2.5 Hz, 1H), 7.18 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.89 (d, *J* = 8.4 Hz, 1H), 2.44 (t, *J* = 7.4 Hz, 2H), 1.68 (h, *J* = 7.4 Hz, 2H), 0.97 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 172.38, 147.71, 129.78, 126.95, 123.58, 117.93, 113.13, 38.84, 20.39, 14.24. MS (ESI) m/z: $[M+H]^+$ 258.0. HRMS-ESI (m/z): calcd for $C_{10}H_{13}BrNO_2$ $[M+H]^+$: 258.0124; found: 258.0124.

5-bromo-2- propylbenzo[d]oxazole (4jj)



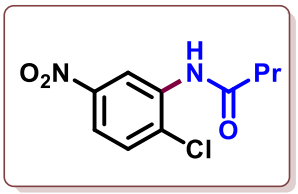
Unknown compound. Yield: 63%, 0.182 g. White solid, mp 51-53 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.81 (d, *J* = 1.6 Hz, 1H), 7.49 (dd, *J* = 6.4, 1.5 Hz, 1H), 7.39 (d, *J* = 6.4 Hz, 1H), 2.93 (t, *J* = 5.6 Hz, 2H), 1.97 (h, *J* = 5.6 Hz, 2H), 1.08 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 169.12, 149.96, 143.10, 128.15, 121.89, 117.32, 111.65, 30.65, 22.11, 13.53. MS (ESI) m/z: $[M+H]^+$ 240.0. HRMS-ESI (m/z): calcd for $C_{10}H_{11}BrNO$ $[M+H]^+$: 240.0019; found: 240.0018.

N-phenylbutyramide (4k)



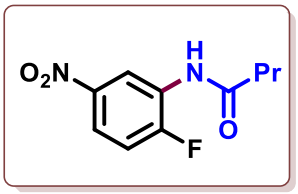
Known compound.[51] Yield: 68%, 0.133 g. Brown solid, mp 99-103 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.67 (d, *J* = 7.9 Hz, 2H), 7.60 (s, 1H), 7.33 (t, *J* = 7.9 Hz, 2H), 7.12 (t, *J* = 7.4 Hz, 1H), 2.25 (t, *J* = 5.6 Hz, 2H), 1.66 (h, *J* = 5.6 Hz, 2H), 0.97 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.40, 138.09, 129.09, 124.18, 119.88, 39.72, 20.20, 13.72. MS (ESI) m/z: $[M+H]^+$ 164.1. HRMS-ESI (m/z): calcd for $C_{10}H_{14}NO$ $[M+H]^+$: 164.1070; found: 164.1072.

N-(2-chloro-5-nitrophenyl)butyramide (4o)



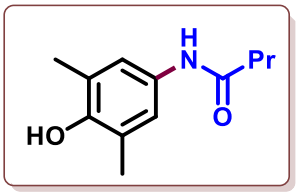
Unknown compound. Yield: 82%, 0.239 g. Yellow solid, mp 126.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ_H = 9.37 (d, *J* = 2.59 Hz, 1H), 7.92 (dd, *J* = 8.75 Hz, 1H), 7.74 (s, 1H), 7.56 (d, *J* = 8.74 Hz, 1H), 2.49 (t, *J* = 5.6 Hz, 2H), 1.83 (h, *J* = 5.6 Hz, 2H), 1.07 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ_C = 171.35, 147.21, 135.52, 129.44, 128.37, 118.84, 116.29, 116.27, 39.74, 18.76, 13.65. MS (ESI) m/z: $[M+H]^+$ 243.0. HRMS-ESI (m/z): calcd for $C_{10}H_{12}ClN_2O_3$ $[M+H]^+$: 243.0531; found: 243.0531.

N-(2-fluoro-5-nitrophenyl)butyramide (4p)



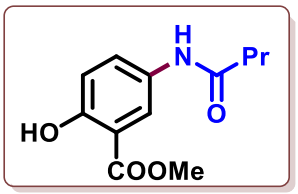
Unknown compound. Yield: 70%, 0.190 g. Yellow solid, mp 103.6 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 9.31 (dd, *J* = 6.9, 2.8 Hz, 1H), 7.97 (ddd, *J* = 9.0, 4.4, 2.9 Hz, 1H), 7.65 (s, 1H), 7.28 – 7.19 (m, 1H), 2.46 (t, *J* = 7.4 Hz, 2H), 1.79 (h, *J* = 7.4 Hz, 2H), 1.03 (t, *J* = 7.4 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.64, 171.23, 156.35, 154.33, 144.51, 127.38, 127.28, 119.68, 119.61, 117.42, 115.38, 115.20, 39.26, 17.83, 13.57. ^{19}F NMR (376 MHz, $CDCl_3$): δ_F = -119.93. MS (ESI) m/z: $[M+H]^+$ 227.1. HRMS-ESI (m/z): calcd for $C_{10}H_{12}FN_2O_3$ $[M+H]^+$: 227.0827; found: 227.0829.

N-(4-hydroxy-3,5-dimethylphenyl)butyramide (4u)



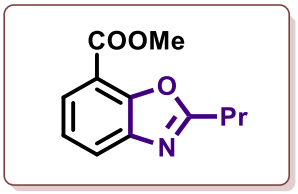
Known compound.[48] Yield: 64%, 0.159 g. White solid, mp 138-140 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ_H = δ 8.75 (s, 1H), 8.09 (s, 1H), 7.12 (s, 2H), 2.22 (t, *J* = 7.6 Hz, 2H), 2.15 (s, 6H), 1.59 (h, *J* = 7.6 Hz, 2H), 0.92 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d6): δ_C = 170.29, 149.61, 131.82, 124.83, 119.90, 38.42, 19.11, 17.14, 13.72. MS (ESI) m/z: $[M+H]^+$ 208.1. HRMS-ESI (m/z): calcd for $C_{12}H_{18}NO_2$ $[M+H]^+$: 208.1332; found: 208.1331.

Methyl 5-butyramido-2-hydroxybenzoate (4w)



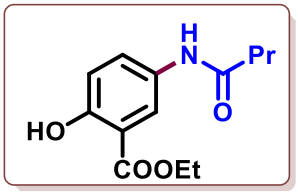
Unknown compound. Yield: 34%, 0.097 g. Brown solid, mp 127-130 °C. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 9.10 (s, 1H), 8.37 (s, 1H), 8.05 (d, *J* = 1.4 Hz, 1H), 7.56 (dd, *J* = 6.5, 1.4 Hz, 1H), 6.98 (d, *J* = 6.4 Hz, 1H), 3.92 (s, 3H), 2.41 (t, *J* = 5.6 Hz, 2H), 1.66 (h, *J* = 5.6 Hz, 2H), 1.03 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 171.94, 170.60, 158.82, 128.18, 116.61, 113.50, 53.09, 39.27, 20.42, 13.72. MS (ESI) m/z: $[M+H]^+$ 238.1. HRMS-ESI (m/z): calcd for $C_{12}H_{16}NO_4$ $[M+H]^+$: 238.1074; found: 238.1074.

Methyl 2-propylbenzo[d]oxazole-7-carboxylate (4ww)



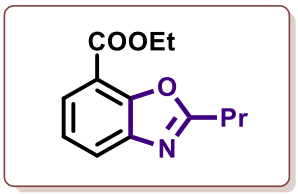
Unknown compound. Yield: 33%, 0.087 g. Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.98 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.72 (dd, *J* = 8.4, 1.8 Hz, 1H), 7.50 (t, *J* = 8.6 Hz, 1H), 3.98 (s, 3H), 2.95 (t, *J* = 7.4 Hz, 2H), 1.99 (h, *J* = 7.5 Hz, 2H), 0.99 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.59, 169.50, 151.05, 139.74, 127.13, 126.13, 119.84, 115.76, 52.33, 30.32, 20.21, 13.35. MS (ESI) m/z: $[M+H]^+$ 220.1. HRMS-ESI (m/z): calcd for $C_{12}H_{14}NO_3$ $[M+H]^+$: 220.0968; found: 220.0968.

Ethyl 5-butyramido-2-hydroxybenzoate (4x)



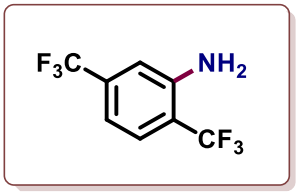
Unknown compound. Yield: 31%, 0.093 g. Orange solid, mp 105-108 °C. ^{1}H NMR (400 MHz, CD_3CN): δ_H = 10.18 (s, 1H), 8.51 (s, 1H), 8.08 (d, *J* = 1.7 Hz, 1H), 7.63 (dd, *J* = 6.3, 1.6 Hz, 1H), 6.95 (d, *J* = 6.4 Hz, 1H), 4.36 (q, *J* = 5.5 Hz, 2H), 2.47 (t, *J* = 5.7 Hz, 2H), 1.66 (h, *J* = 5.7 Hz, 2H), 1.43 (t, *J* = 5.5 Hz, 3H), 0.97 (t, *J* = 5.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 171.69, 170.49, 159.17, 130.33, 128.81, 121.31, 115.43, 114.28, 62.12, 39.84, 20.17, 14.12 MS (ESI) m/z: $[M+H]^+$ 252.12. HRMS-ESI (m/z): calcd for $C_{13}H_{18}NO_4$ $[M+H]^+$: 252.1230; found: 252.1231.

Ethyl 2-propylbenzo[d]oxazole-7-carboxylate (4xx)



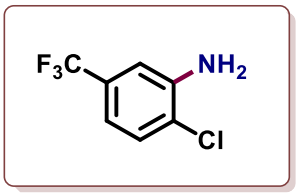
Unknown compound. Yield: 35%, 0.098 g. Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.04 (dd, *J* = 12.9, 3.0 Hz, 1H), 7.69 (dd, *J* = 12.9, 2.9 Hz, 1H), 7.50 (t, *J* = 13.0 Hz, 1H), 4.45 (q, *J* = 10.8 Hz, 2H), 2.96 (t, *J* = 11.4 Hz, 2H), 2.07 (h, *J* = 11.5 Hz, 2H), 1.41 (t, *J* = 10.8 Hz, 3H), 0.96 (t, J = 11.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 170.84, 169.54, 157.80, 130.52, 128.95, 123.08, 118.31, 113.33, 61.96, 30.03, 20.07, 14.19, 13.59. MS (ESI) m/z: $[M+H]^+$ 234.11. HRMS-ESI (m/z): calcd for $C_{13}H_{16}NO_3$ $[M+H]^+$: 234.1125; found: 234.1124.

2,5-bis(trifluoromethyl)aniline (5a)



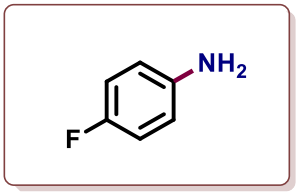
Yield: 78%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.55 (d, *J* = 7.6 Hz, 1H), 7.02 (d, *J* = 7.8 Hz, 2H), 4.38 (s, 2H).

2-chloro-5-(trifluoromethyl)aniline (5e)



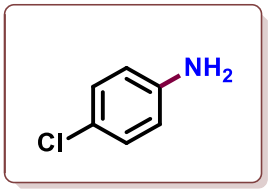
Yield: 80%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.53 (q, *J* = 4.5 Hz, 1H), 7.21 (d, *J* = 7.9 Hz, 2H), 5.72 (s, 2H).

4-fluoroaniline (5f)



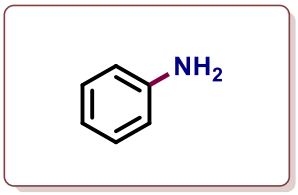
Yield: 64%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 6.90 – 6.85 (m, 1H), 6.65 – 6.62 (m, 1H), 3.55 (s, 1H).

4-chloroaniline (5g)



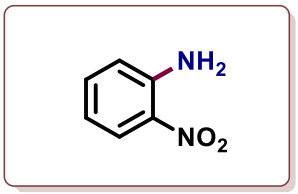
Yield: 38%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 6.95 – 6.87 (m, 1H), 6.67 – 6.63 (m, 1H), 3.65 (s, 1H).

aniline (5k)



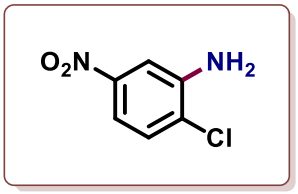
Yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.22 – 7.17 (m, 1H), 6.80 (tt, *J* = 7.5, 1.0 Hz, 1H), 6.74 – 6.70 (m, 1H), 3.66 (s, 1H).

2-nitroaniline (5m)



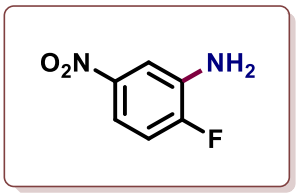
Yield: 31%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 8.14 (dd, *J* = 8.6, 1.4 Hz, 1H), 7.40 – 7.35 (m, 1H), 6.82 (dd, *J* = 8.4, 1.2 Hz, 1H), 6.73 (ddd, *J* = 8.5, 7.0, 1.3 Hz, 1H), 6.05 (s, 2H).

2-chloro-5-nitroaniline (5o)



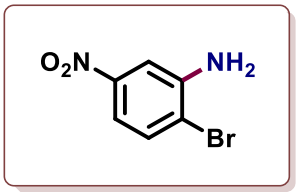
Yield: 63%. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.63 (d, *J* = 2.6 Hz, 1H), 7.55 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.40 (d, *J* = 8.7 Hz, 1H), 4.39 (s, 2H).

2-fluoro-5-nitroaniline (5p)



^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.70-7.67 (m, 1H), 7.45 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 7.7 Hz, 1H), 4.38 (s, 2H).

2-bromo-5-nitroaniline (5q)



^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 7.80 (dd, *J* = 8.7, 2.6 Hz, 1H), 7.69 (d, *J* = 8.7 Hz, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 4.56 (s, 2H).

8. References

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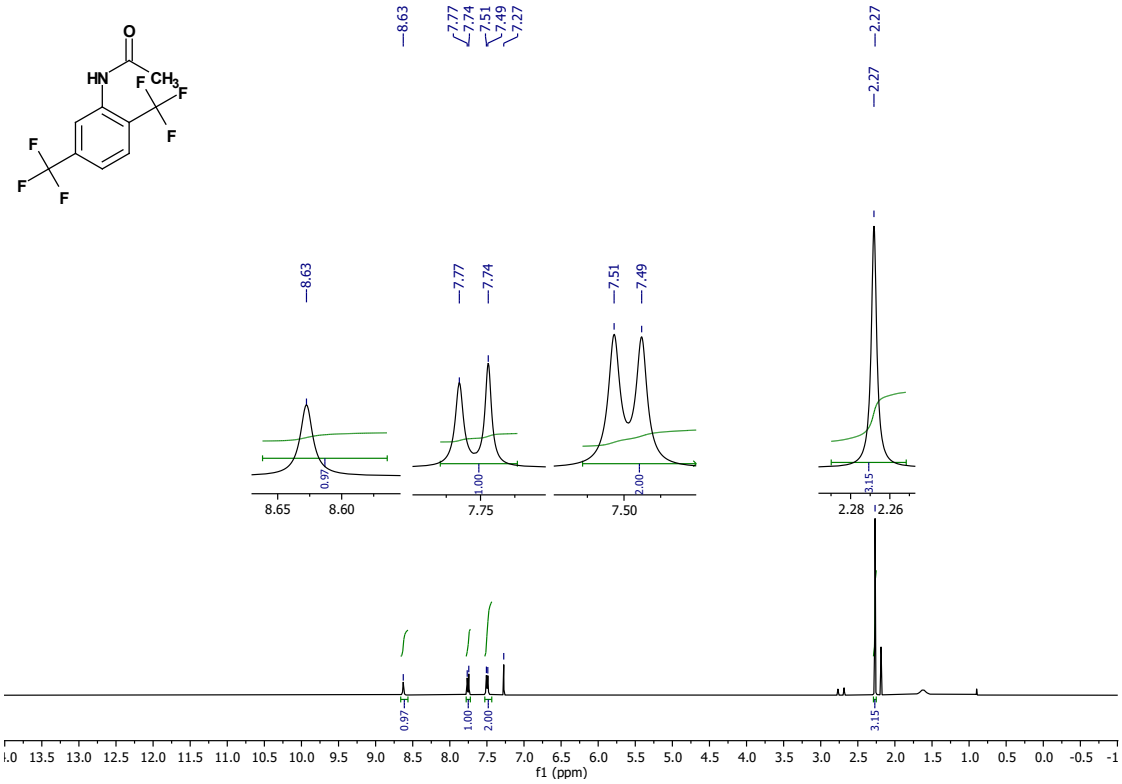
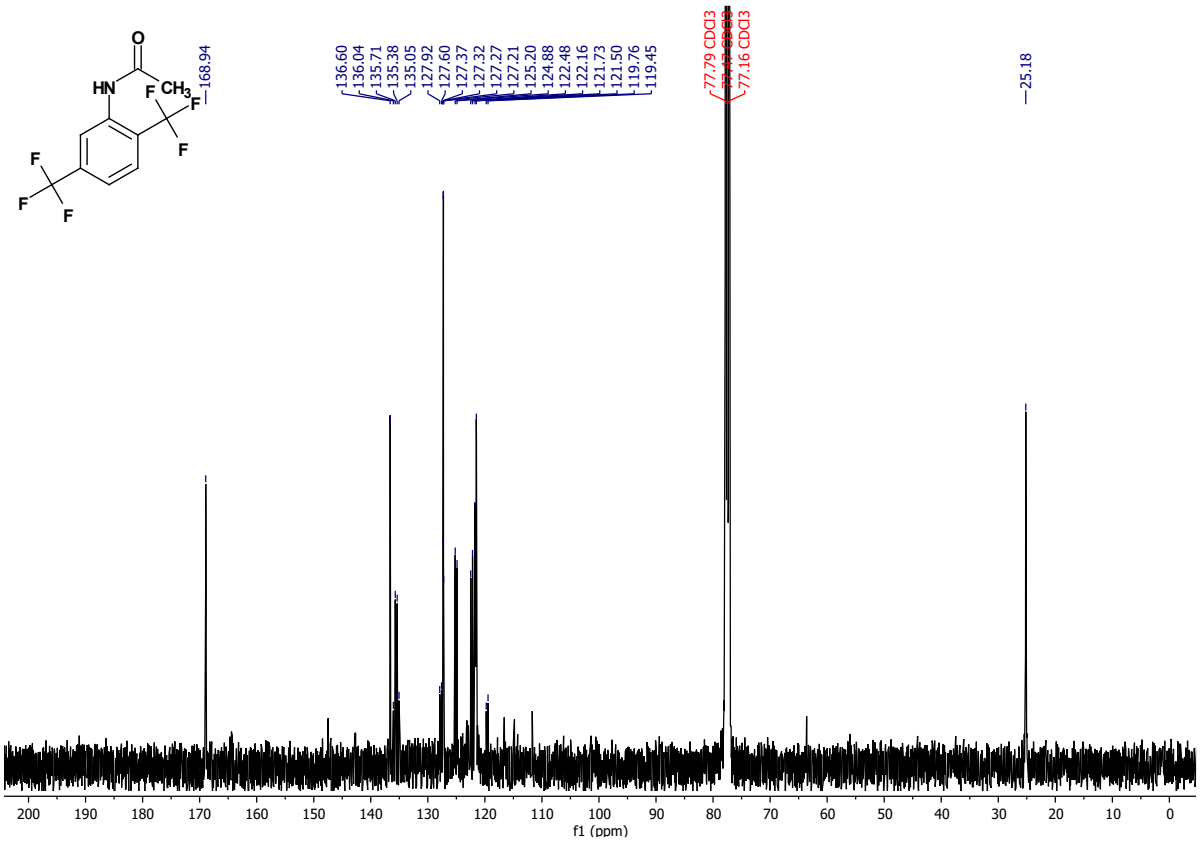
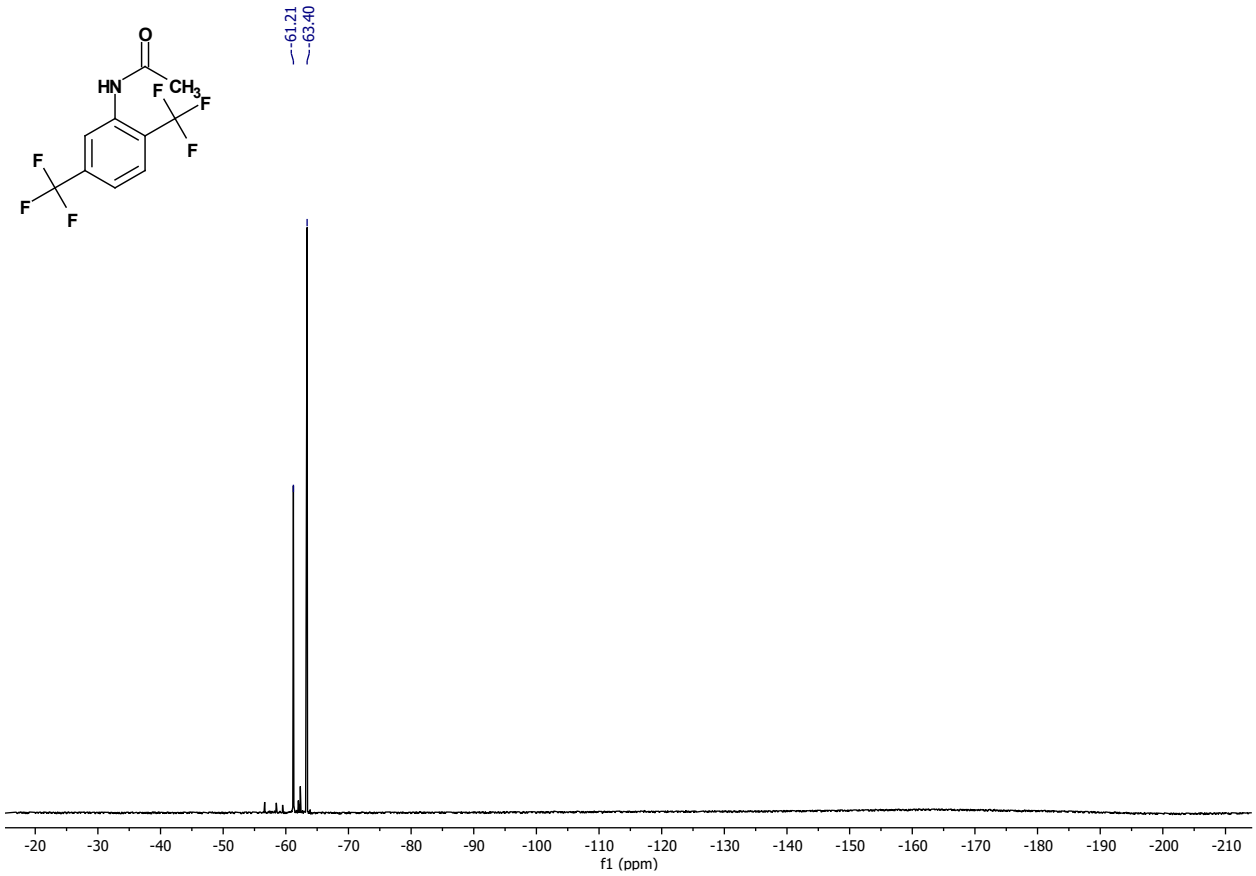
9. Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra of Products

^{1}H and ^{13}C NMR *N*-(2,5-bis(trifluoromethyl)phenyl)acetamide (**2a**)

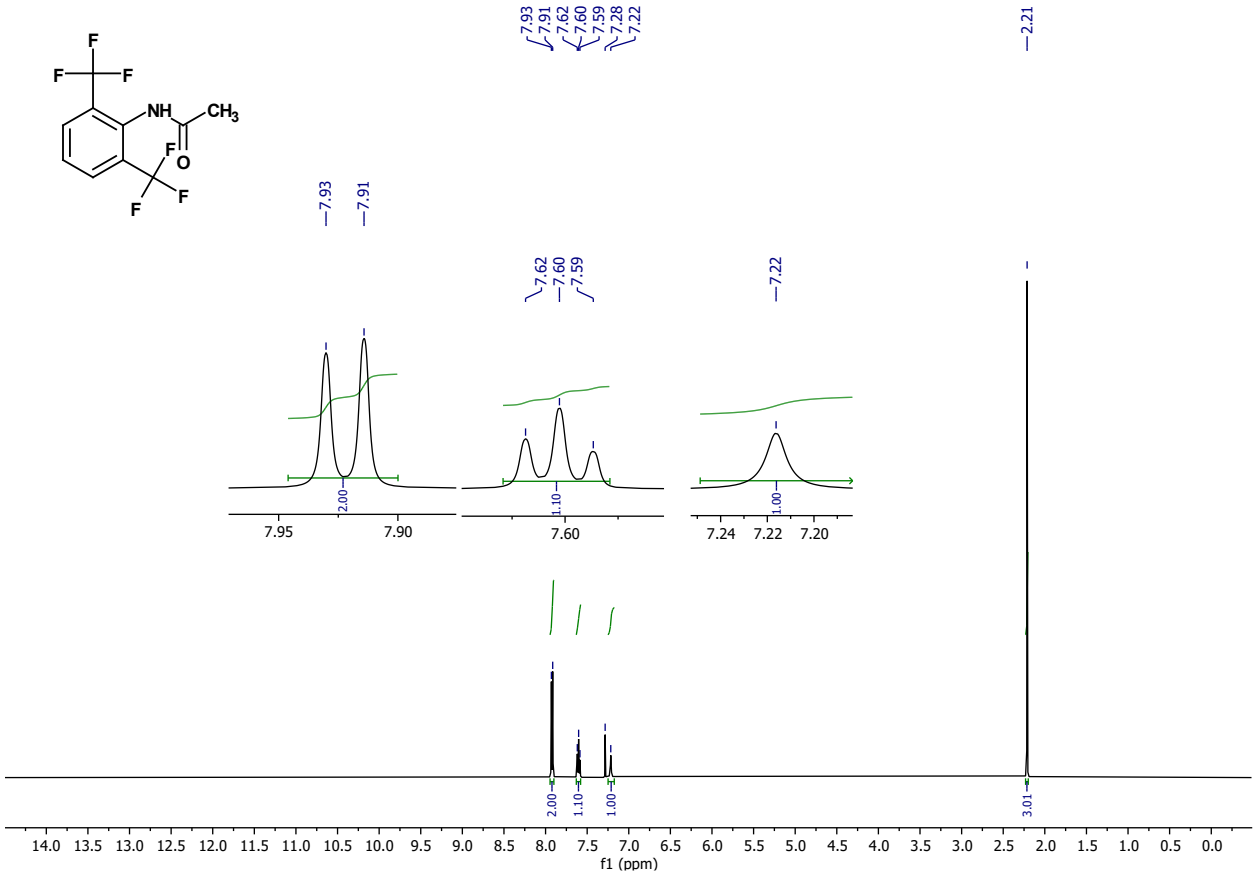


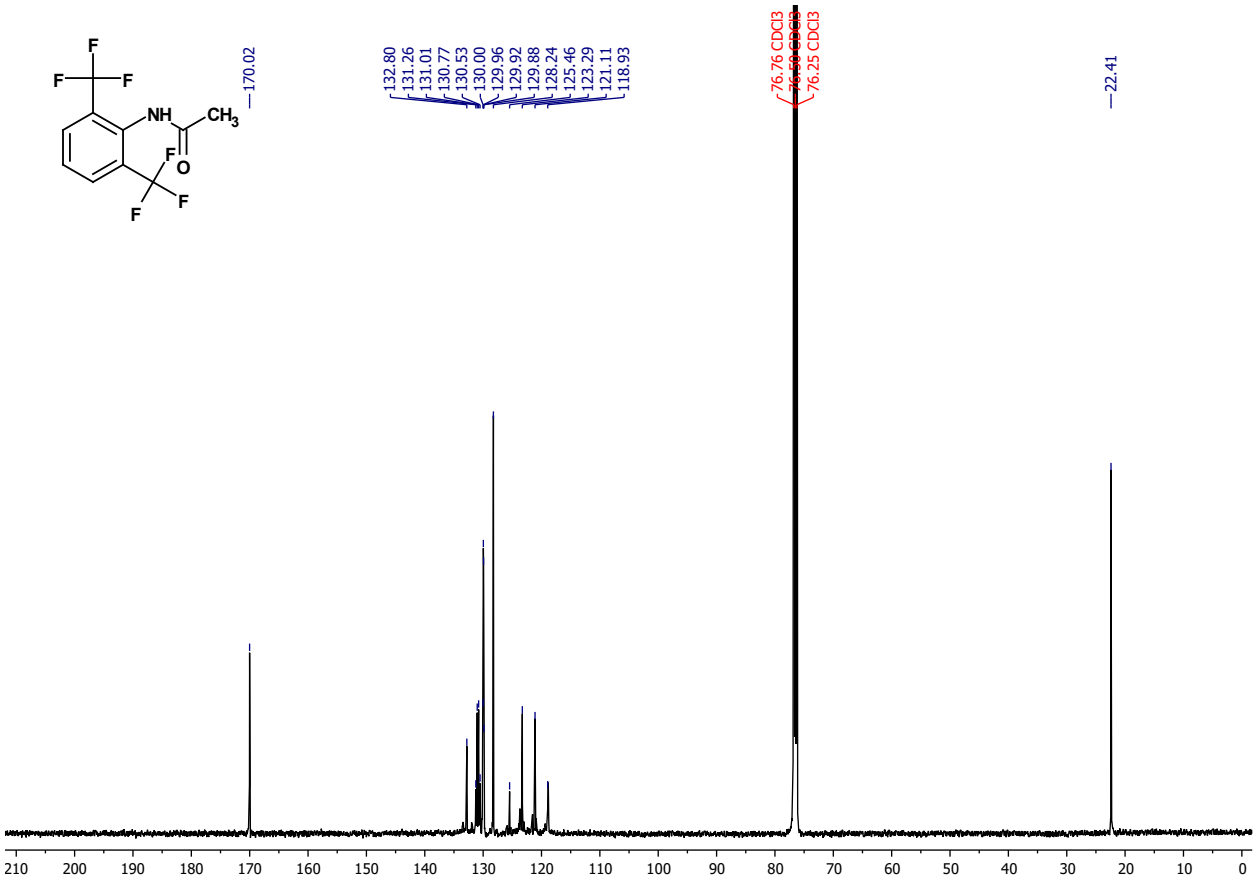


^{19}F NMR *N*-(2,5-bis(trifluoromethyl)phenyl)acetamide (**2a**)



^{1}H and ^{13}C NMR *N*-(2,6-bis(trifluoromethyl)phenyl)acetamide (**2b**)





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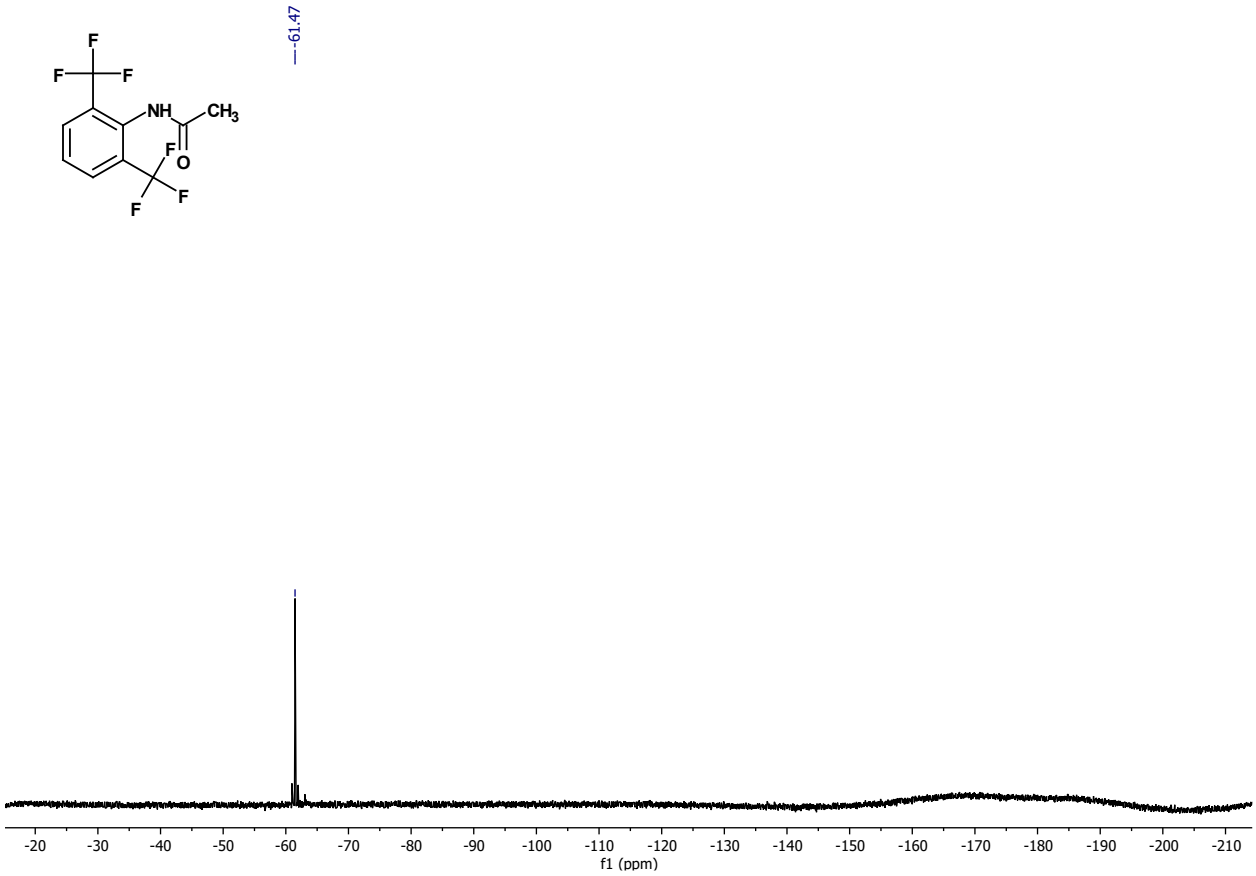
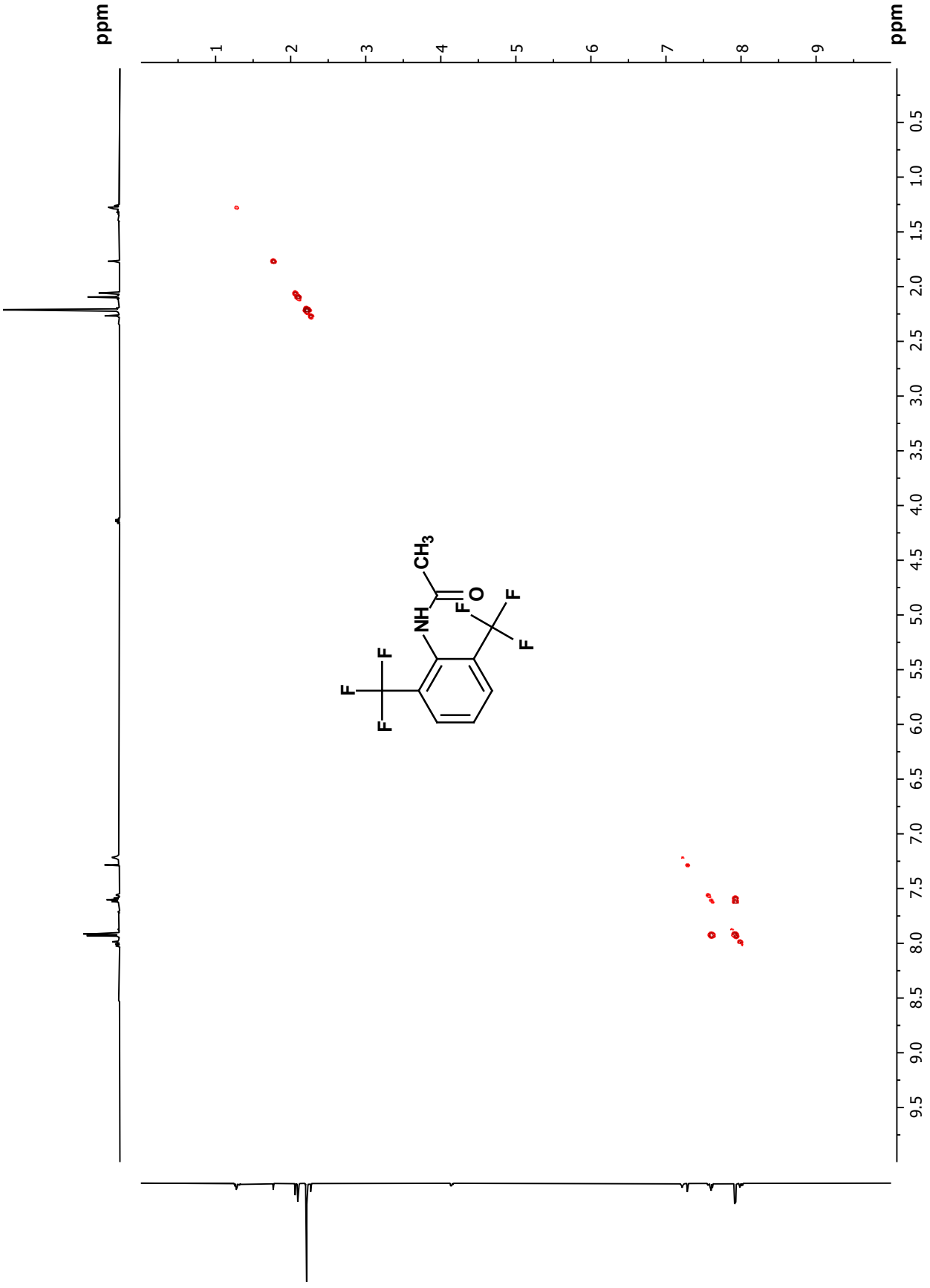
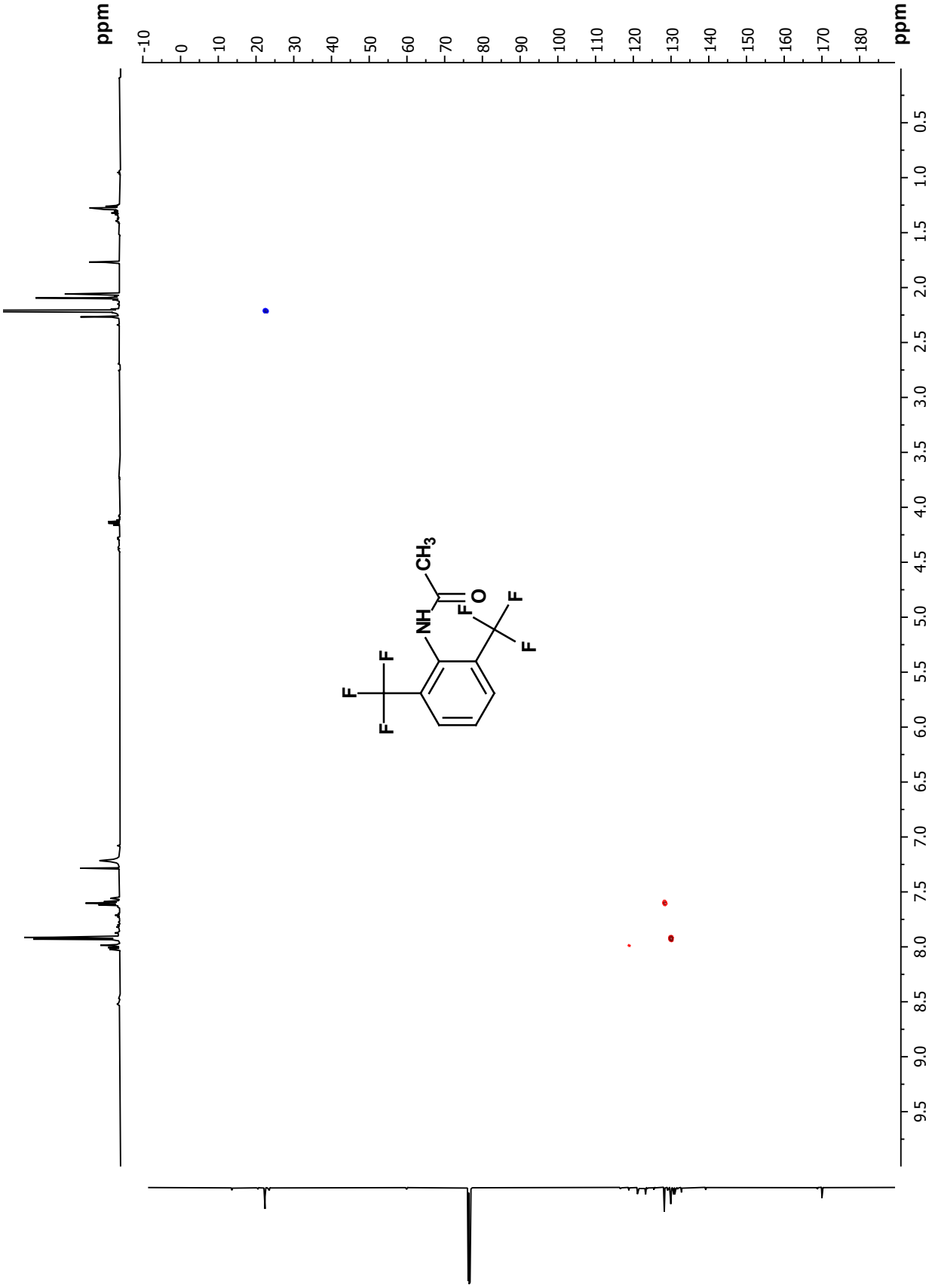


COSY NMR *N*-(2,6-bis(trifluoromethyl)phenyl)acetamide (**2b**)



HSQC NMR *N*-(2,6-bis(trifluoromethyl)phenyl)acetamide (**2b**)



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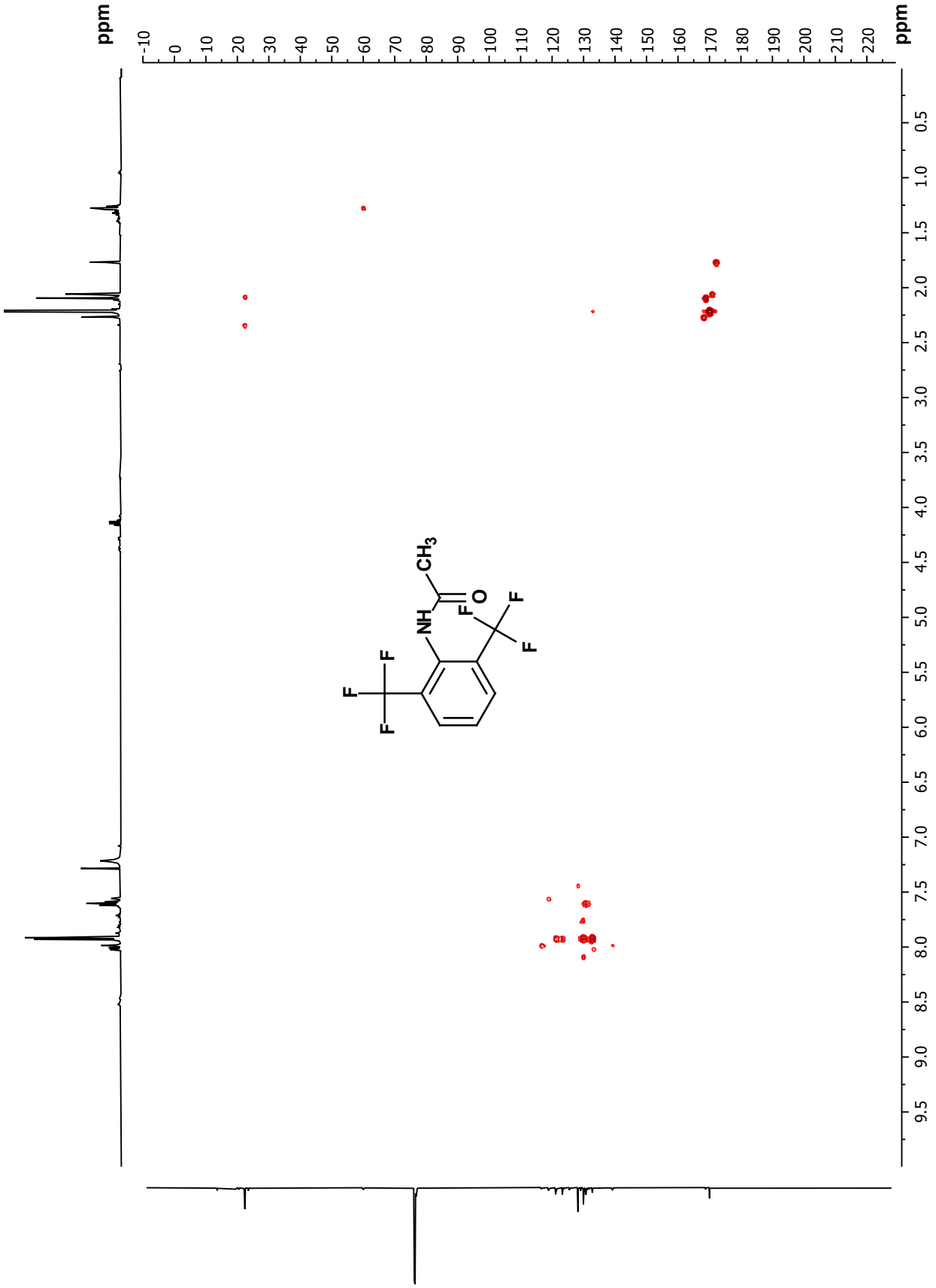
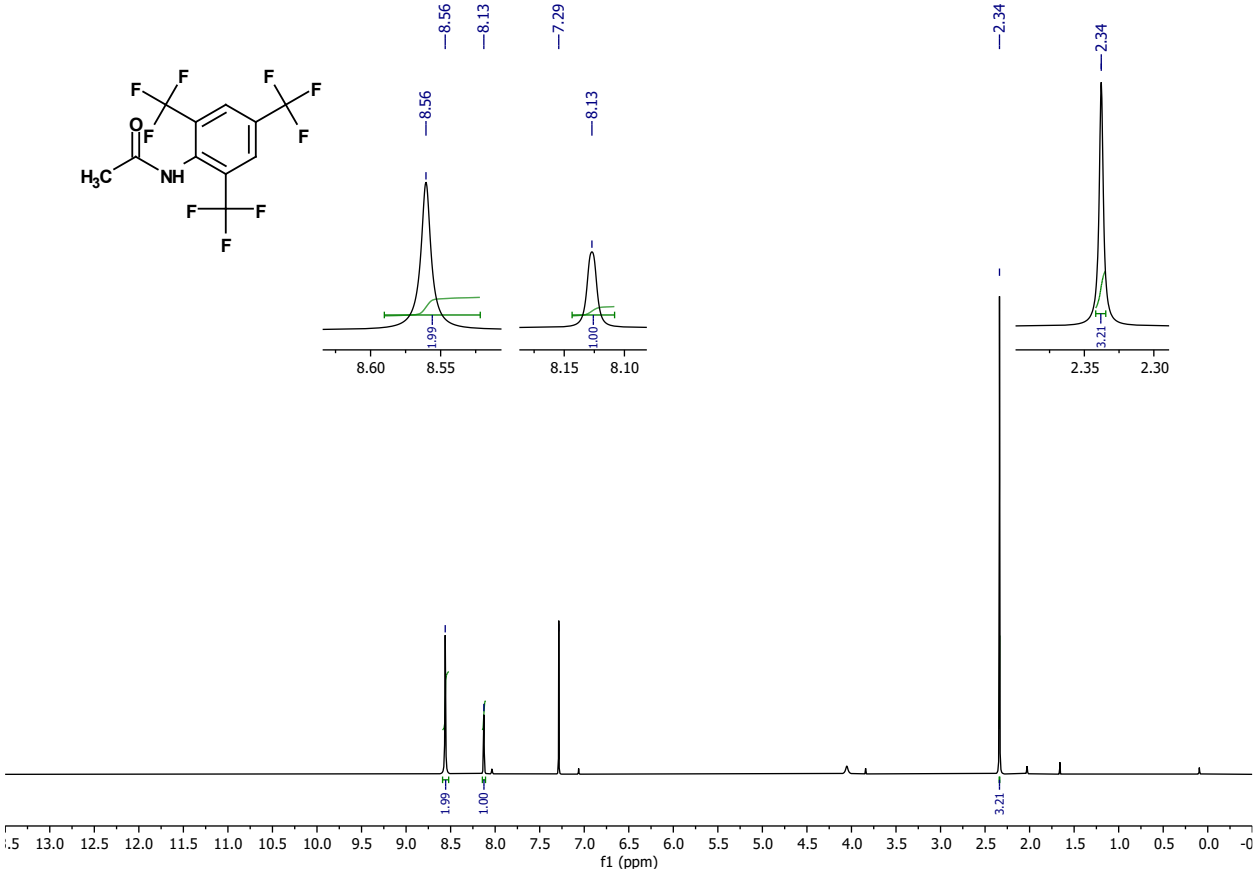
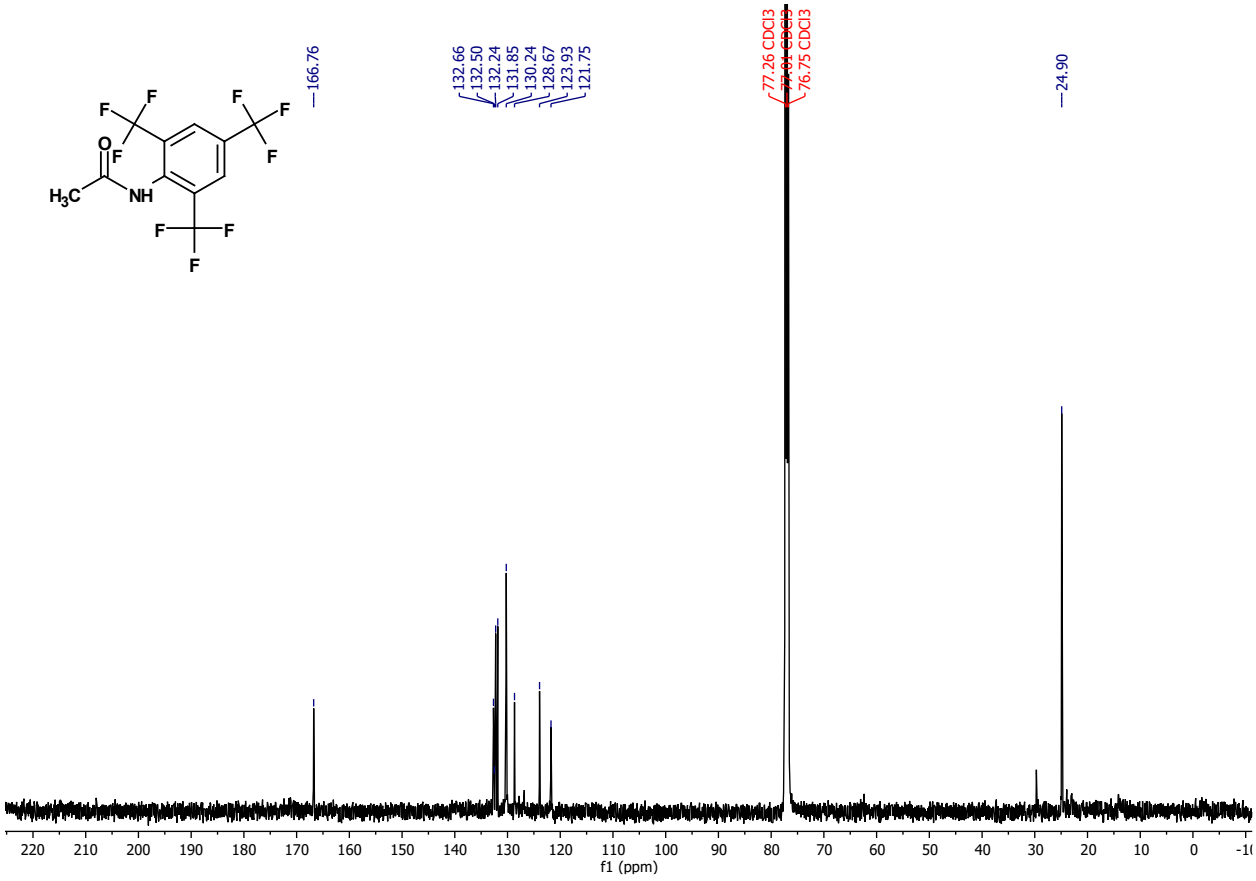
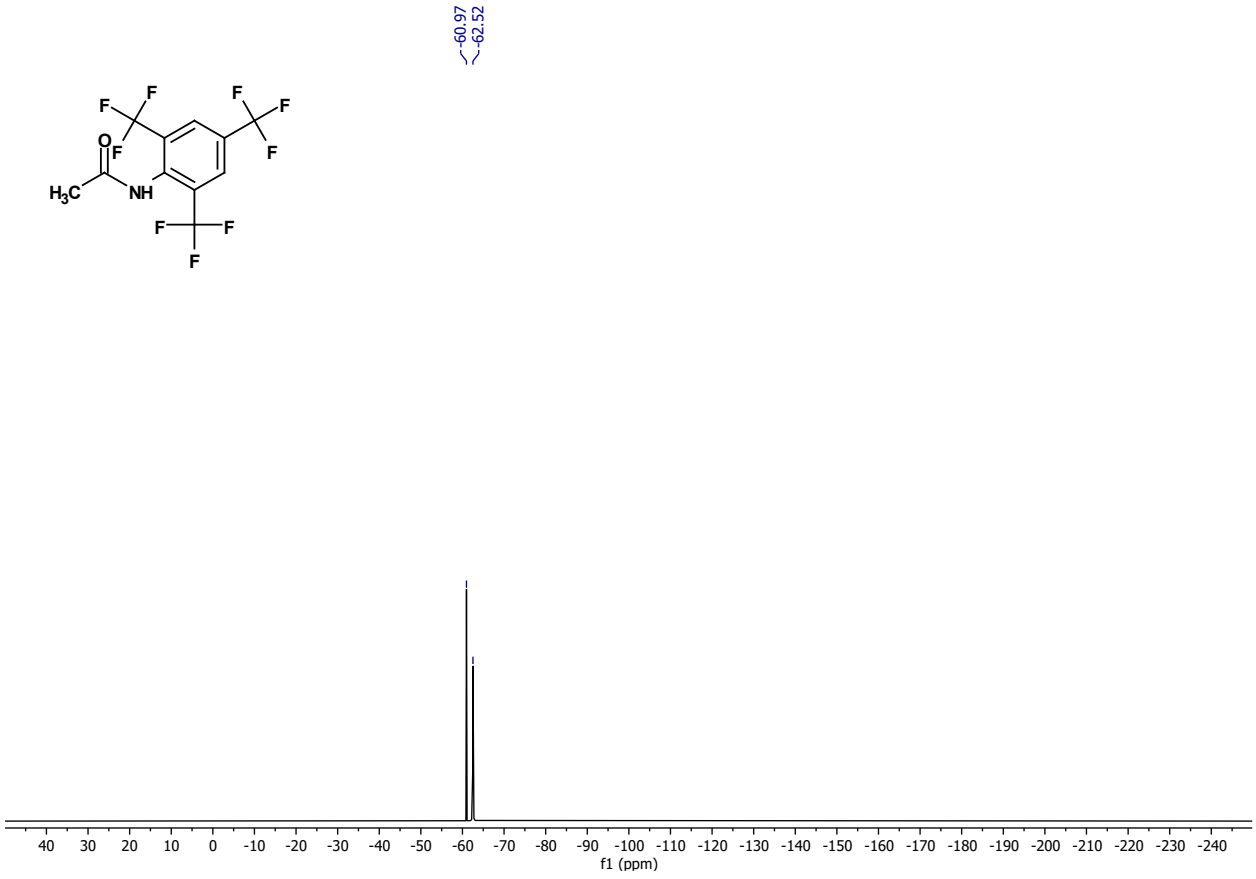


^{1}H and ^{13}C NMR *N*-(2,4,6-tris(trifluoromethyl)phenyl)acetamide **(2c)**





^{19}F NMR *N*-(2,4,6-tris(trifluoromethyl)phenyl)acetamide **(2c)**



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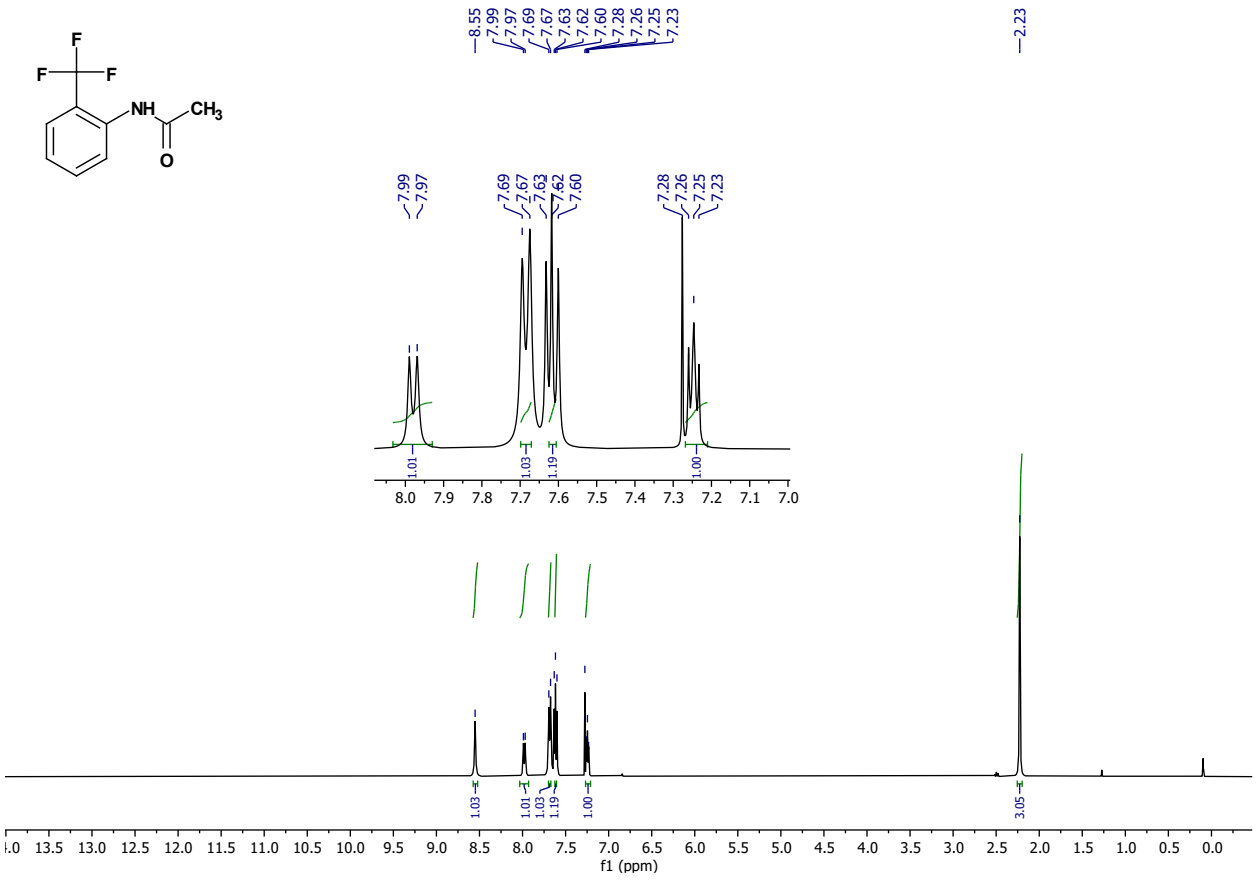

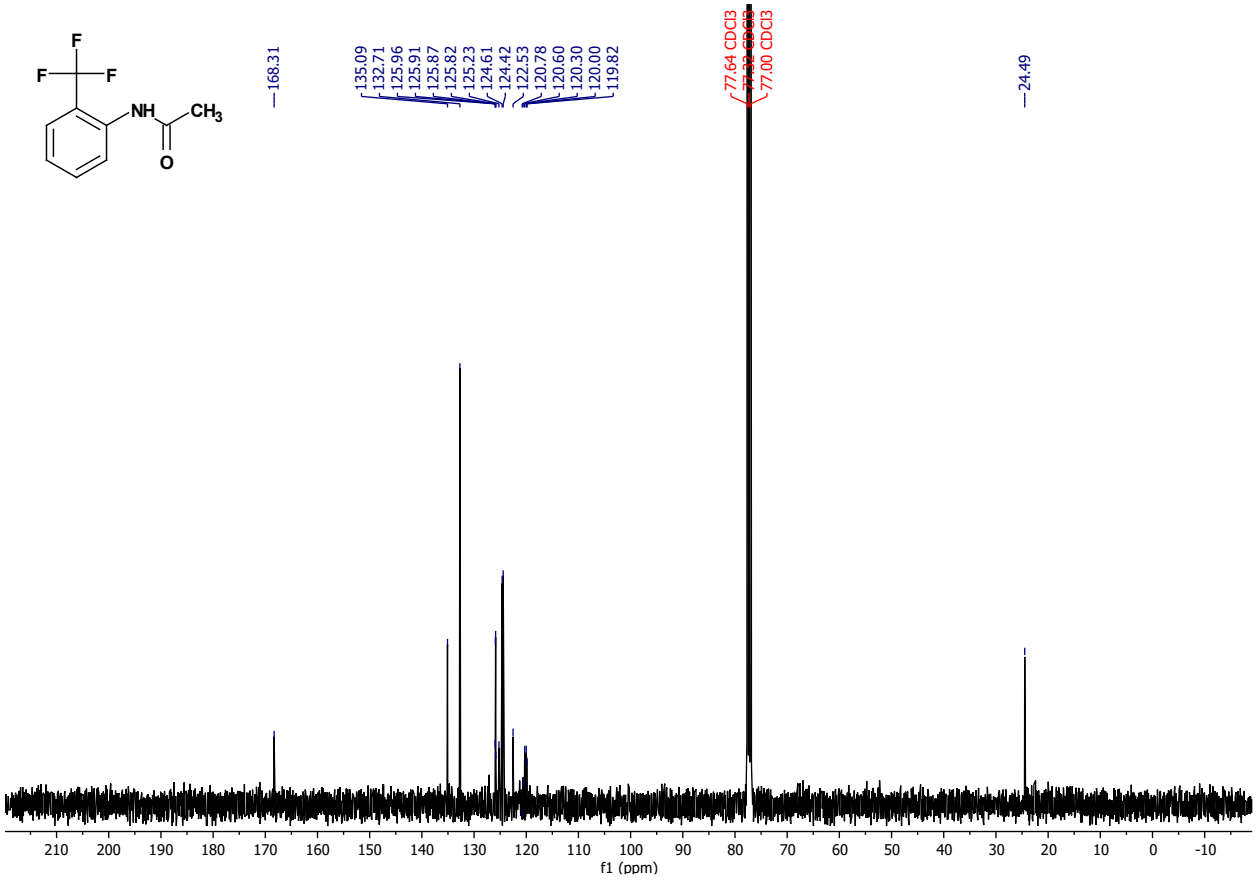

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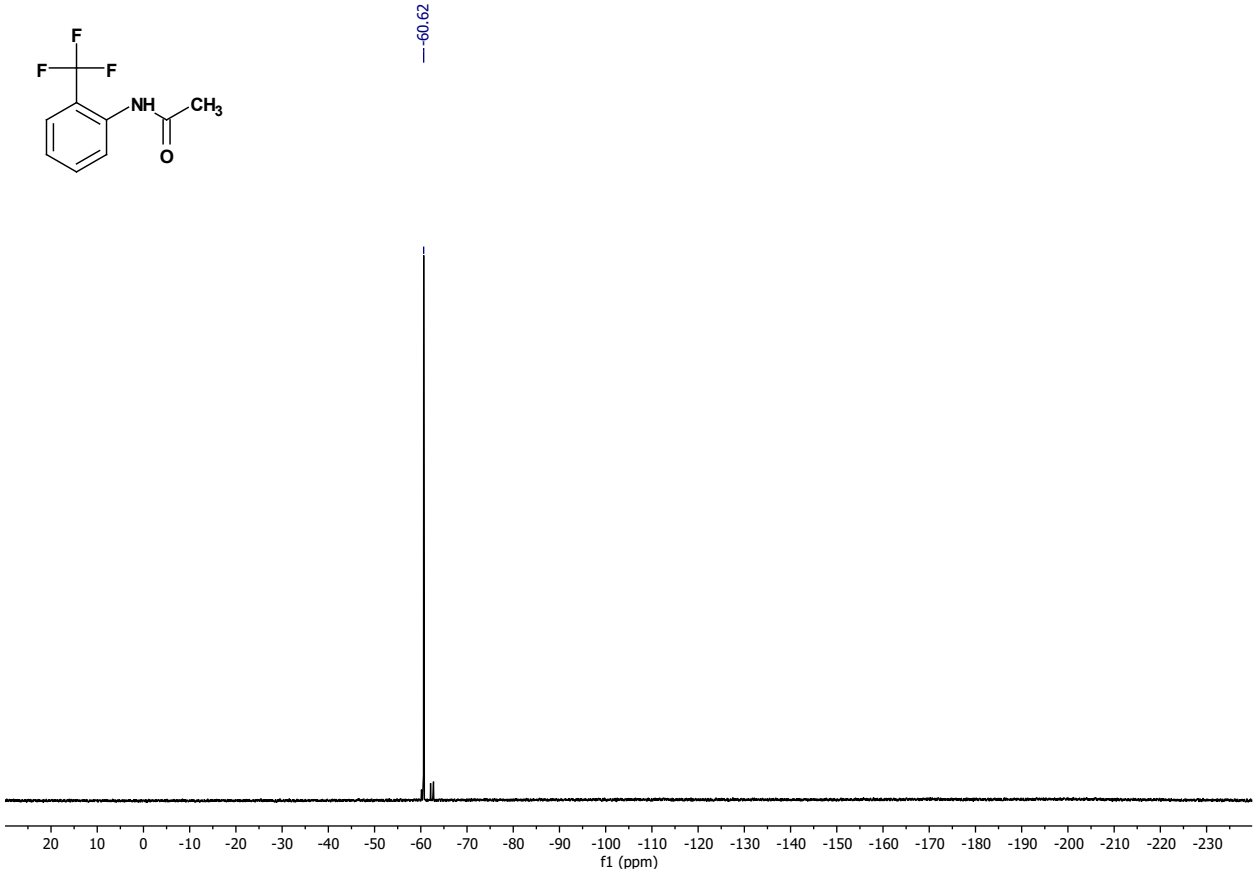
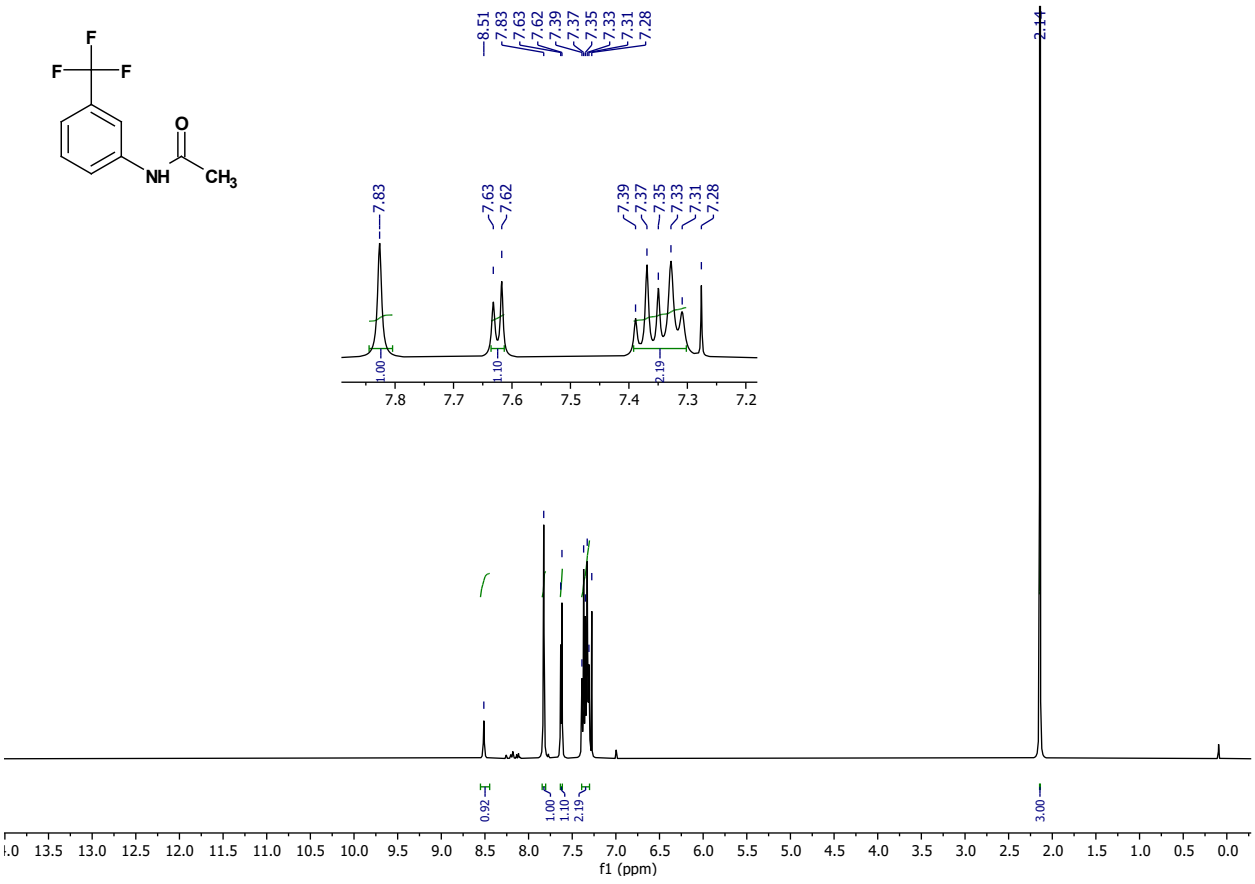
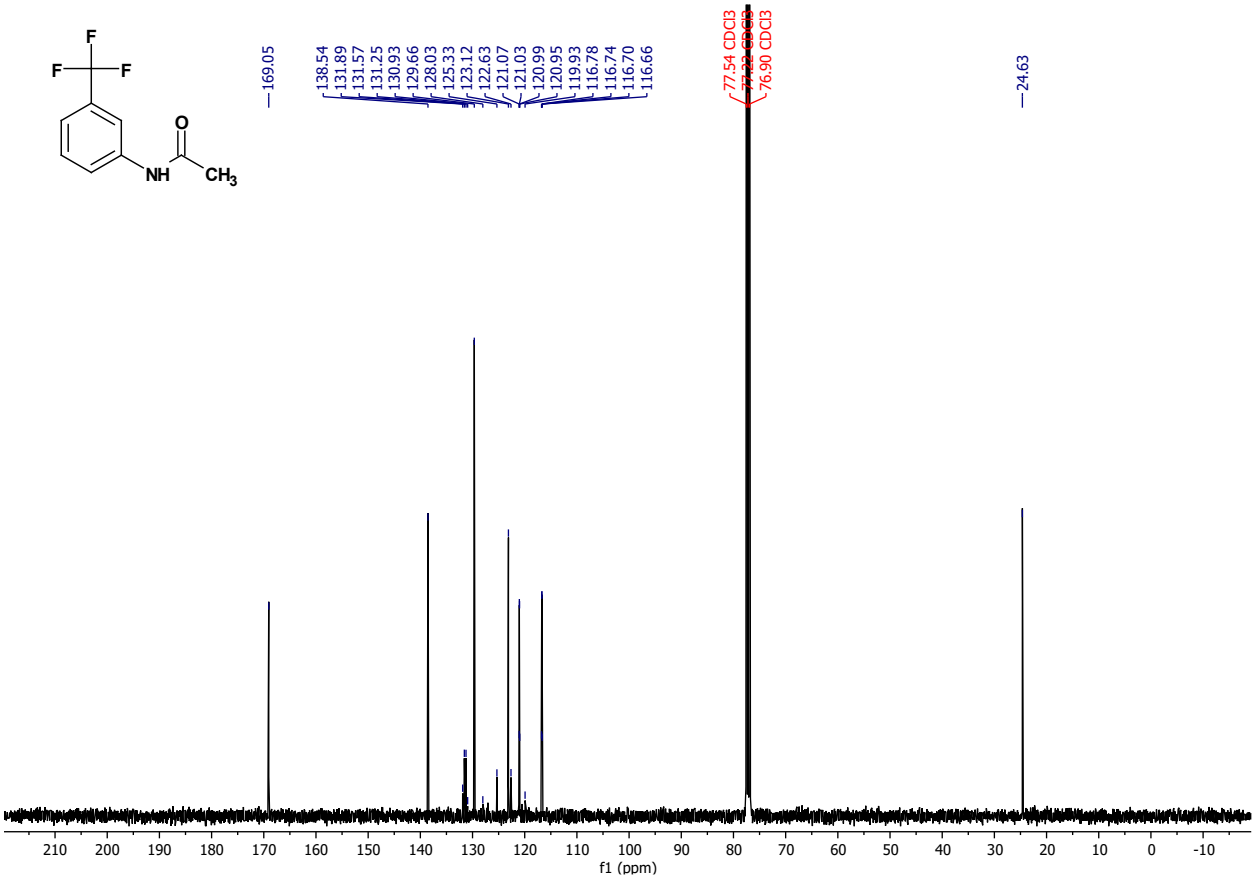
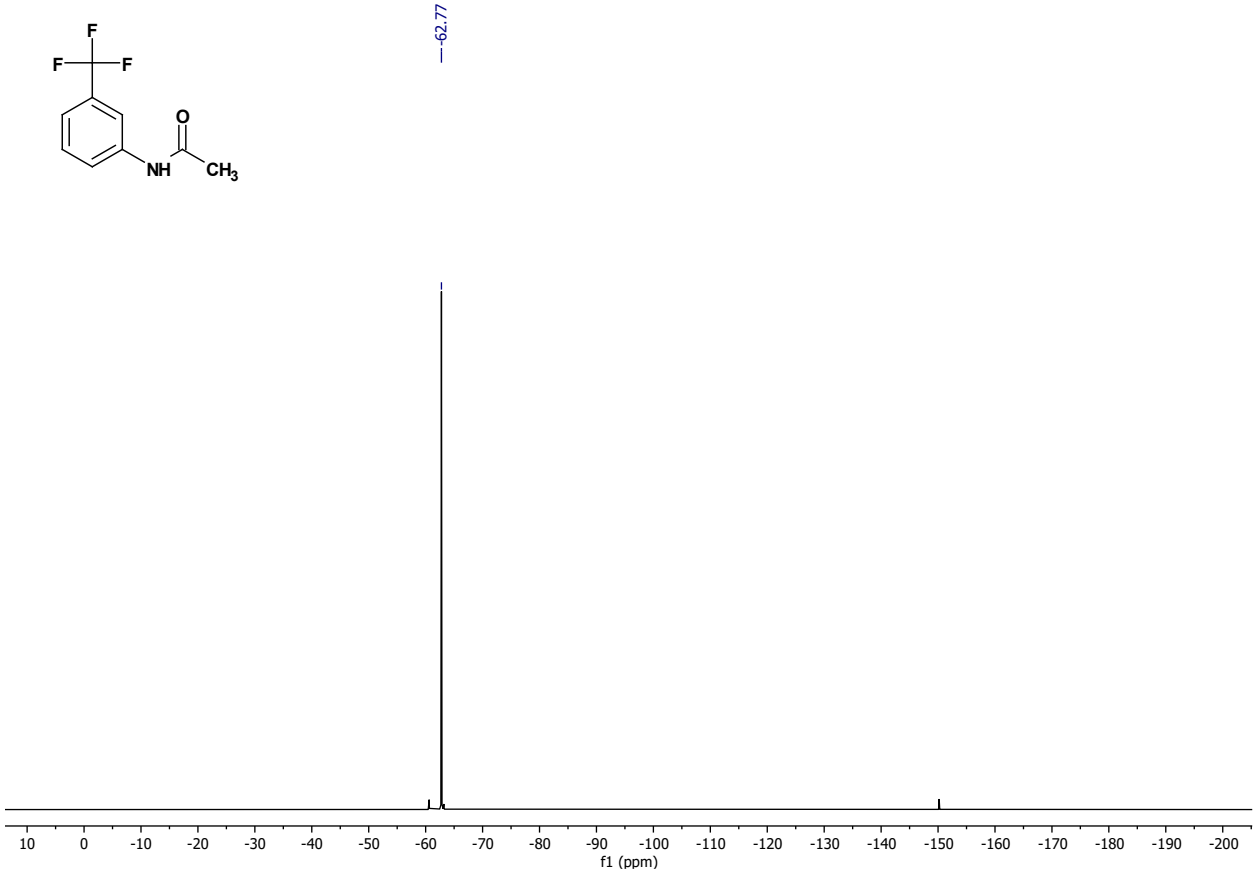


^{1}H and ^{13}C NMR *N*-(3-(trifluoromethyl)phenyl)acetamide (**2d**-*b*)

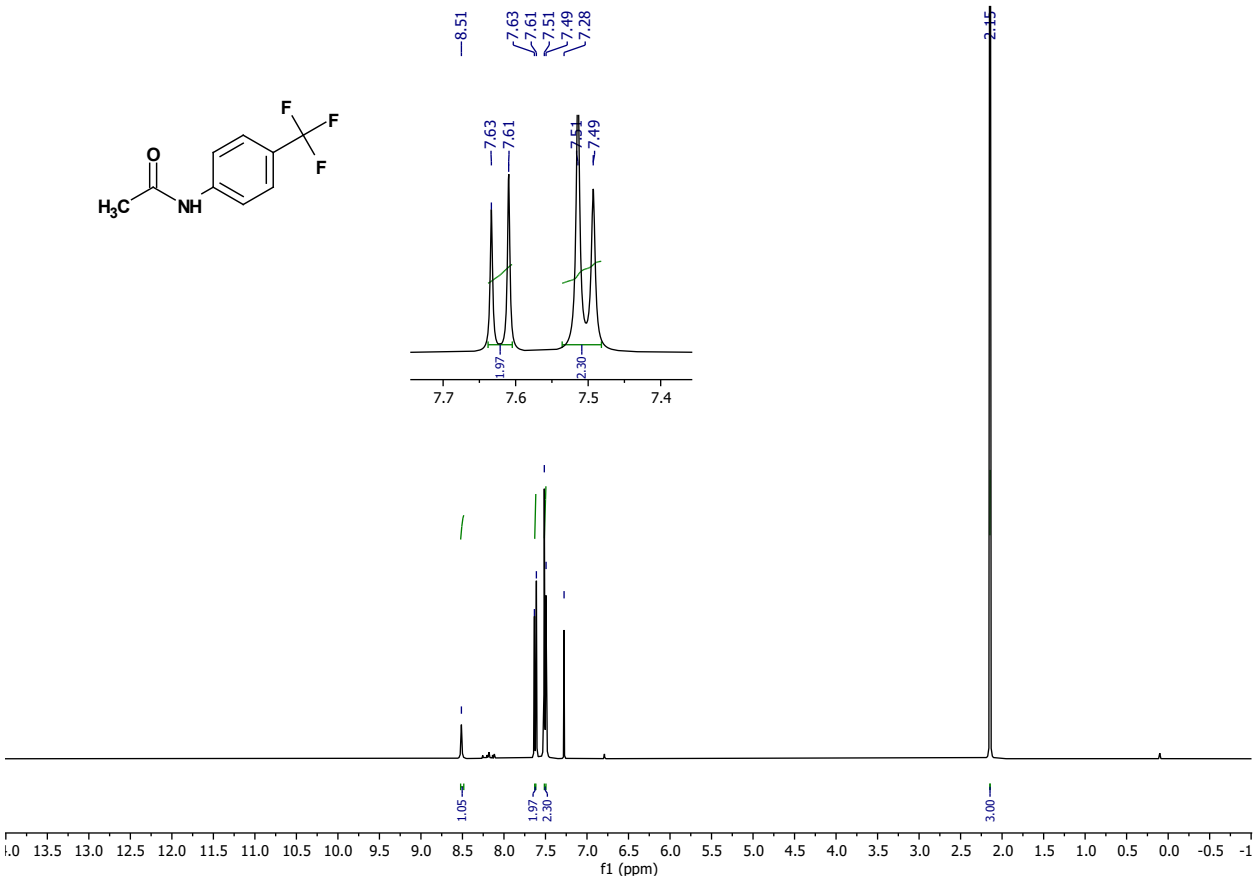


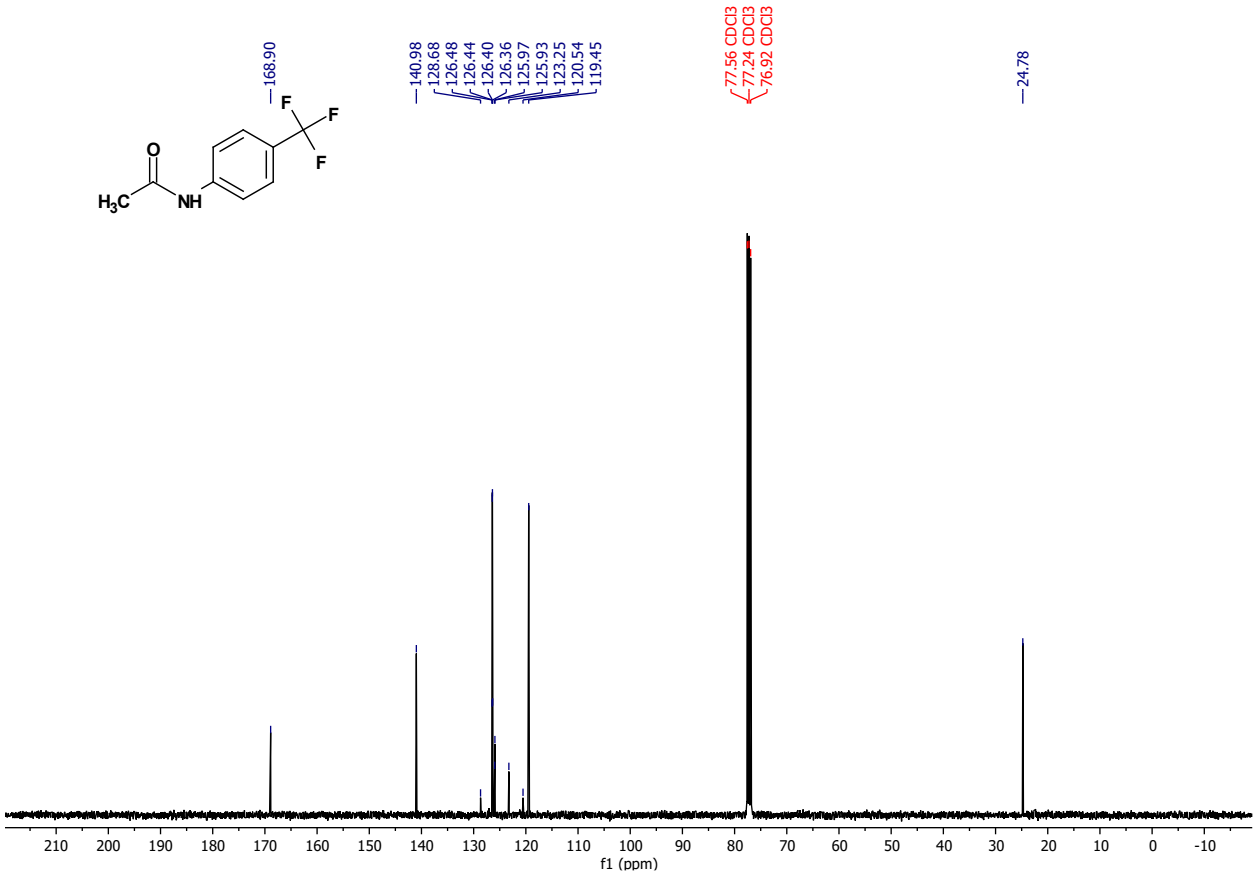


^{19}F NMR *N*-(3-(trifluoromethyl)phenyl)acetamide (**2d**-*b*)



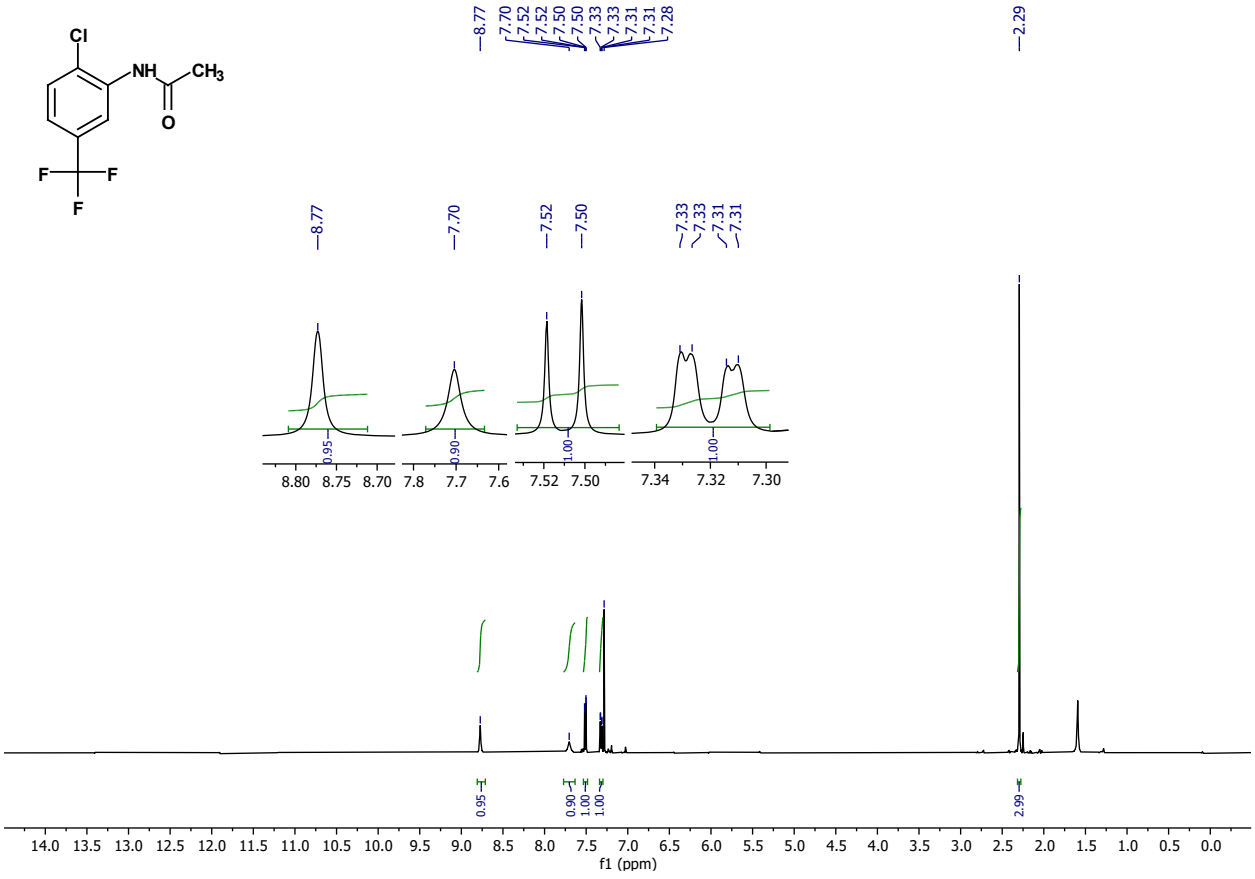
^{1}H and ^{13}C NMR *N*-(4-(trifluoromethyl)phenyl)acetamide (**2d-*c***)

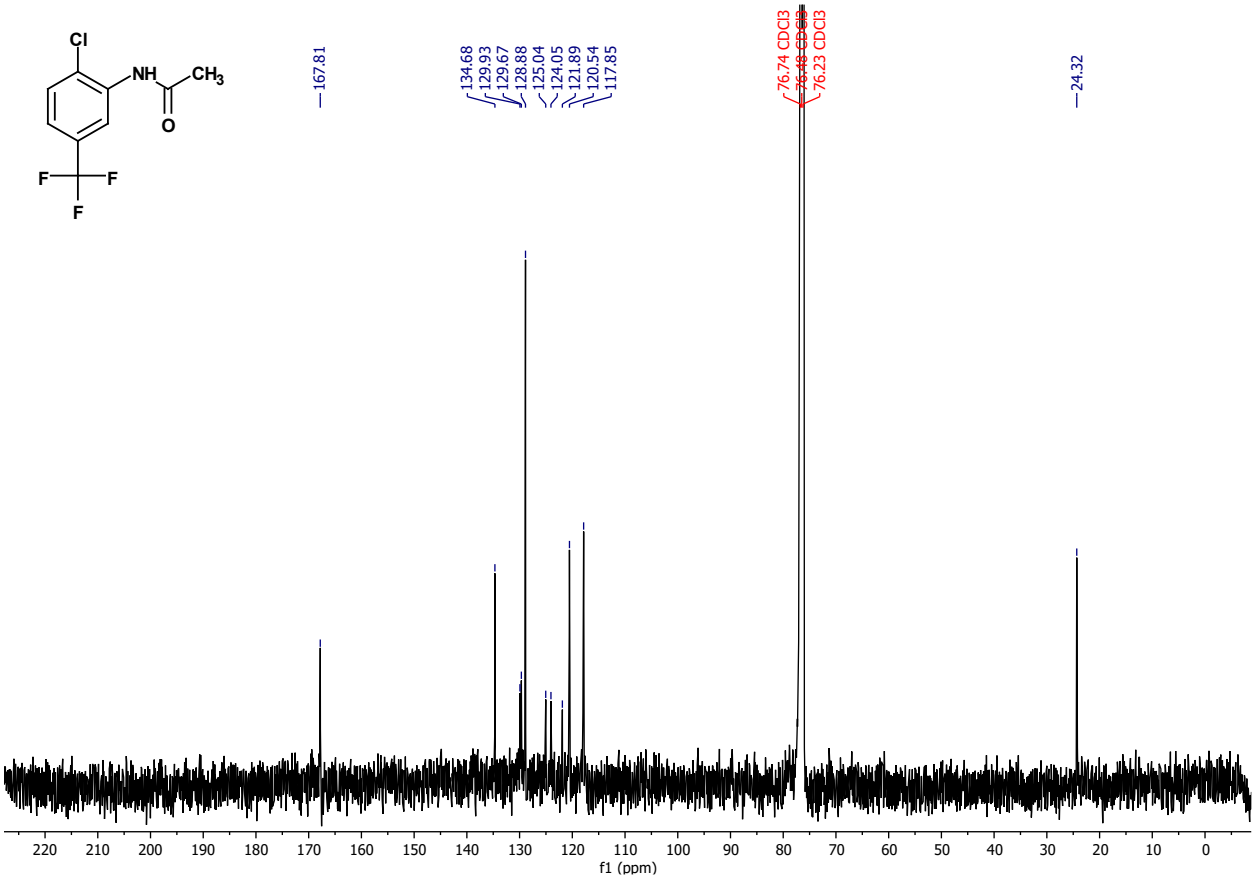




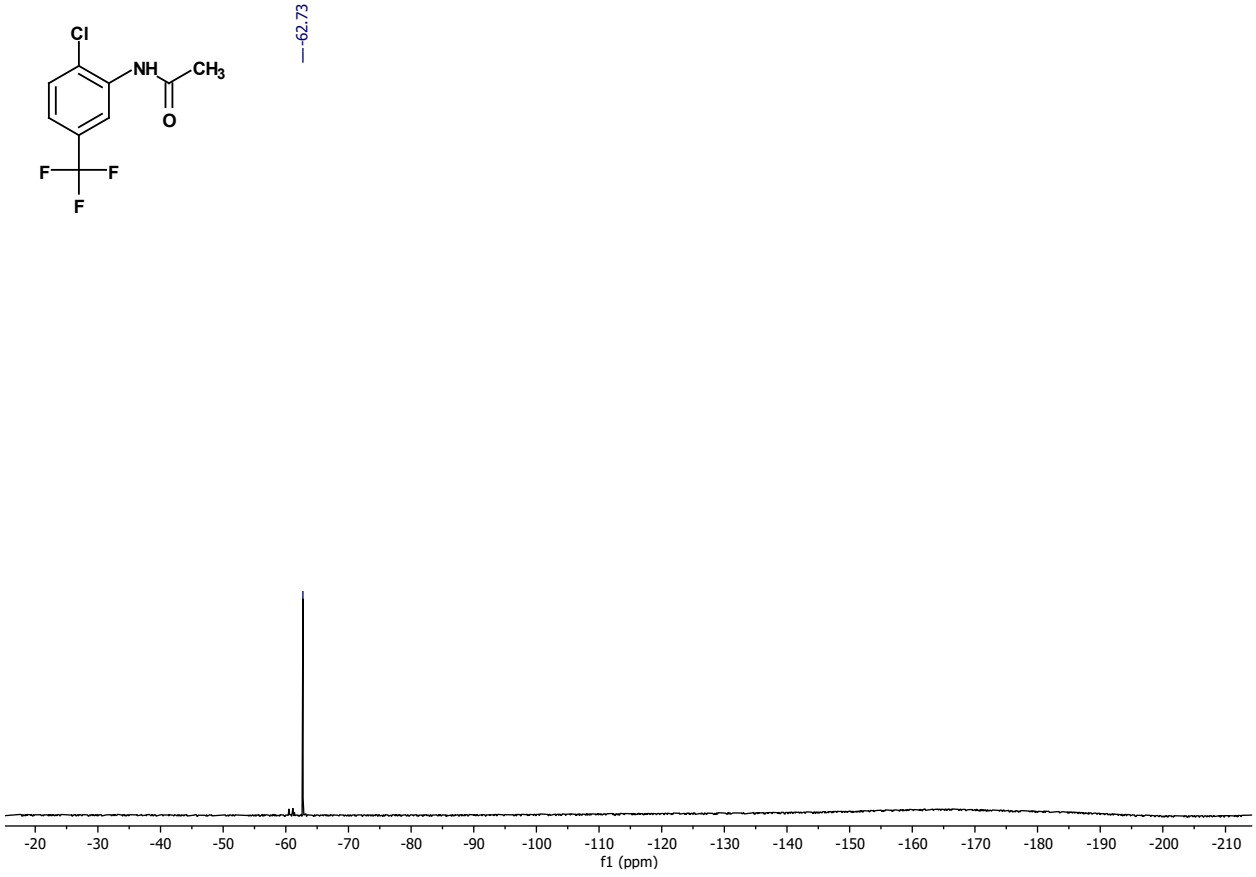
^{19}F NMR *N*-(4-(trifluoromethyl)phenyl)acetamide (**2d-***c*)

^{1}H and ^{13}C NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)acetamide **(2e)**

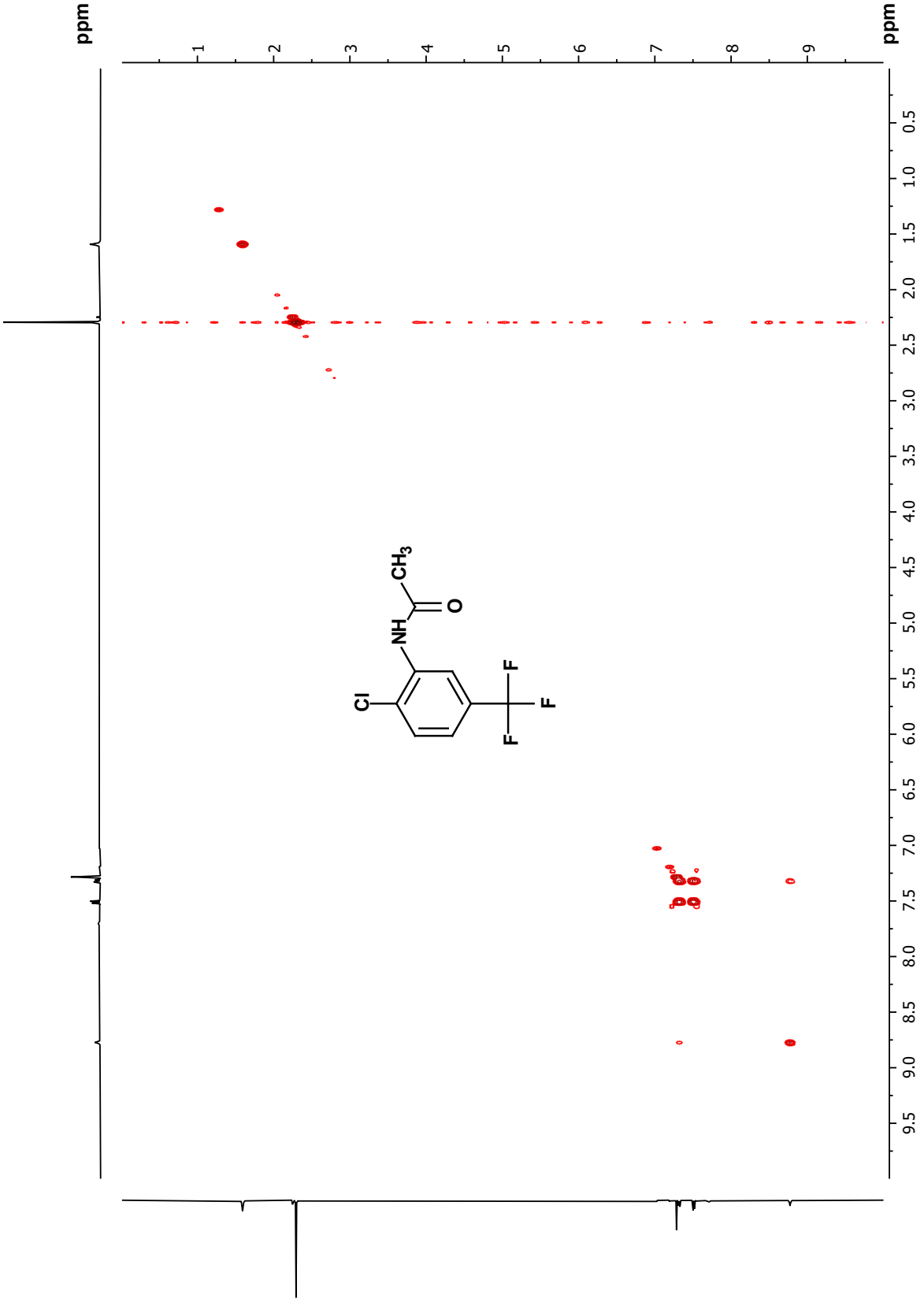




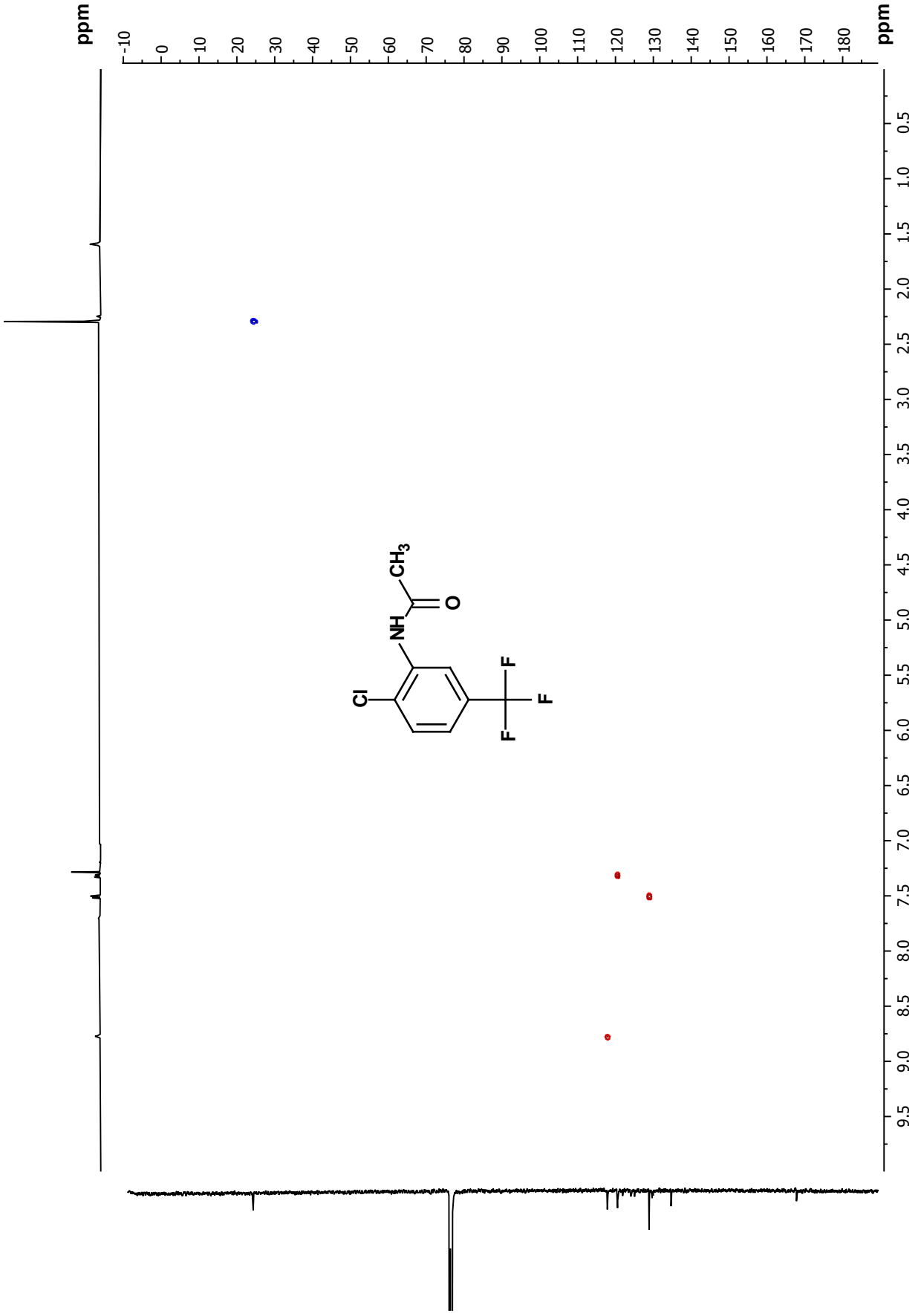
^{19}F NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)acetamide **(2e)**



COSY NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)acetamide **(2e)**



HSQC NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)acetamide **(2e)**



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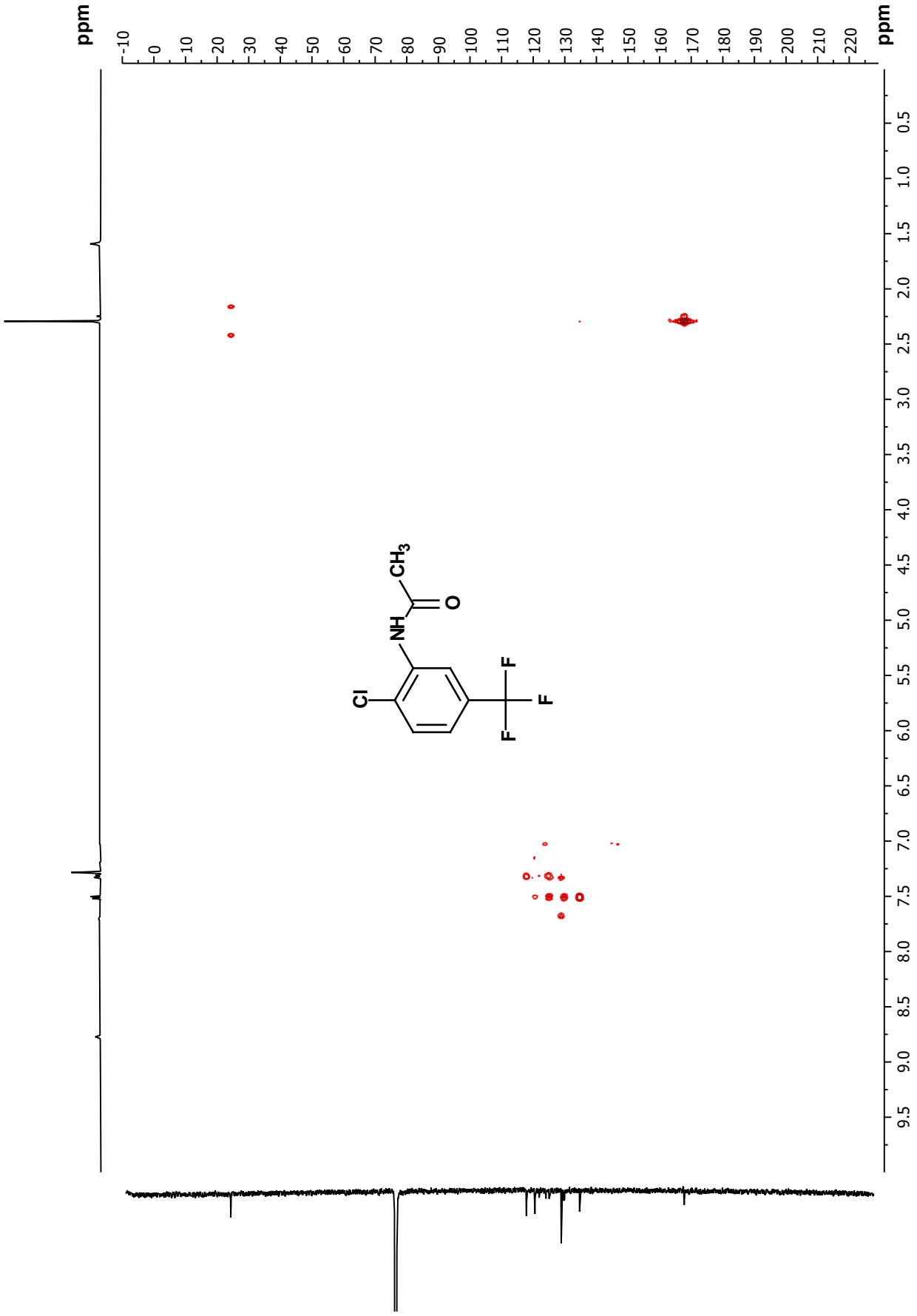
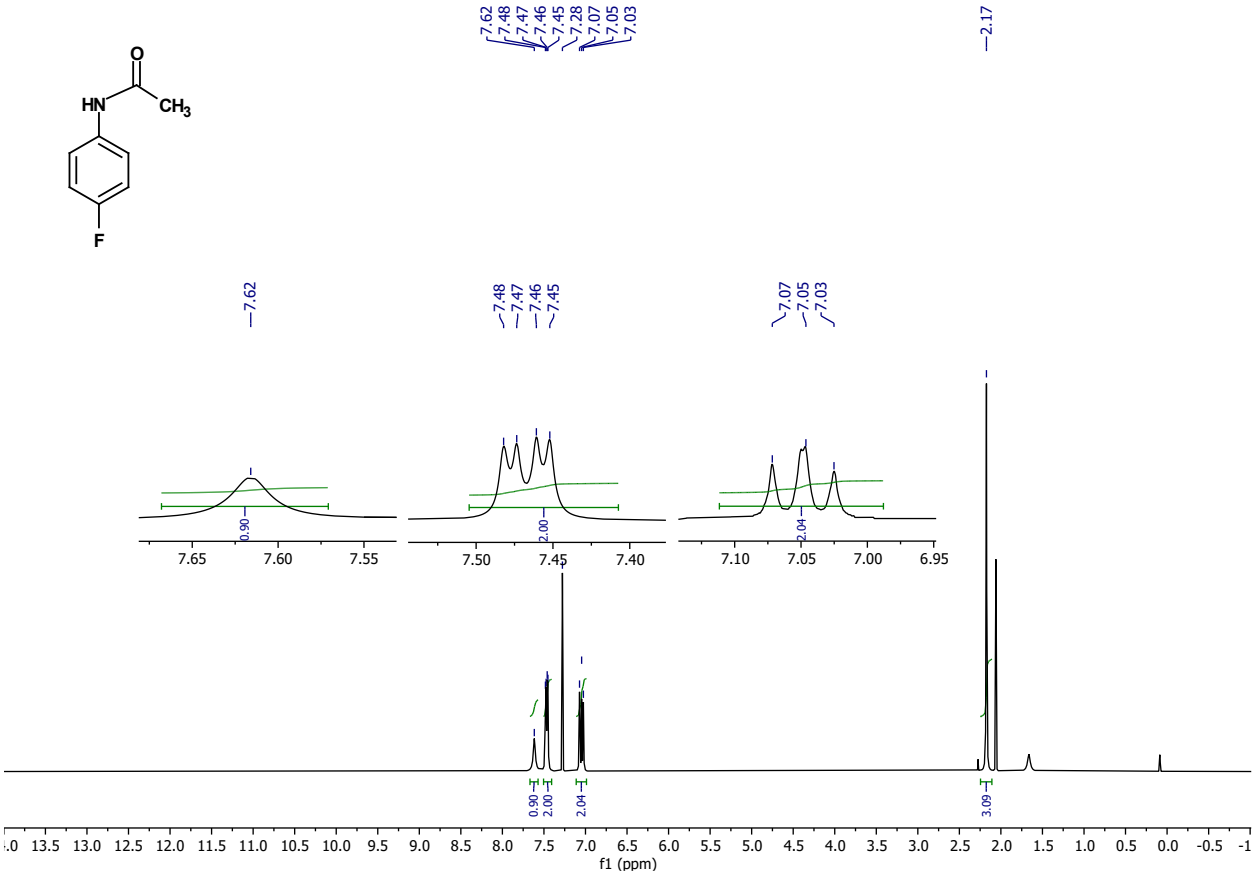
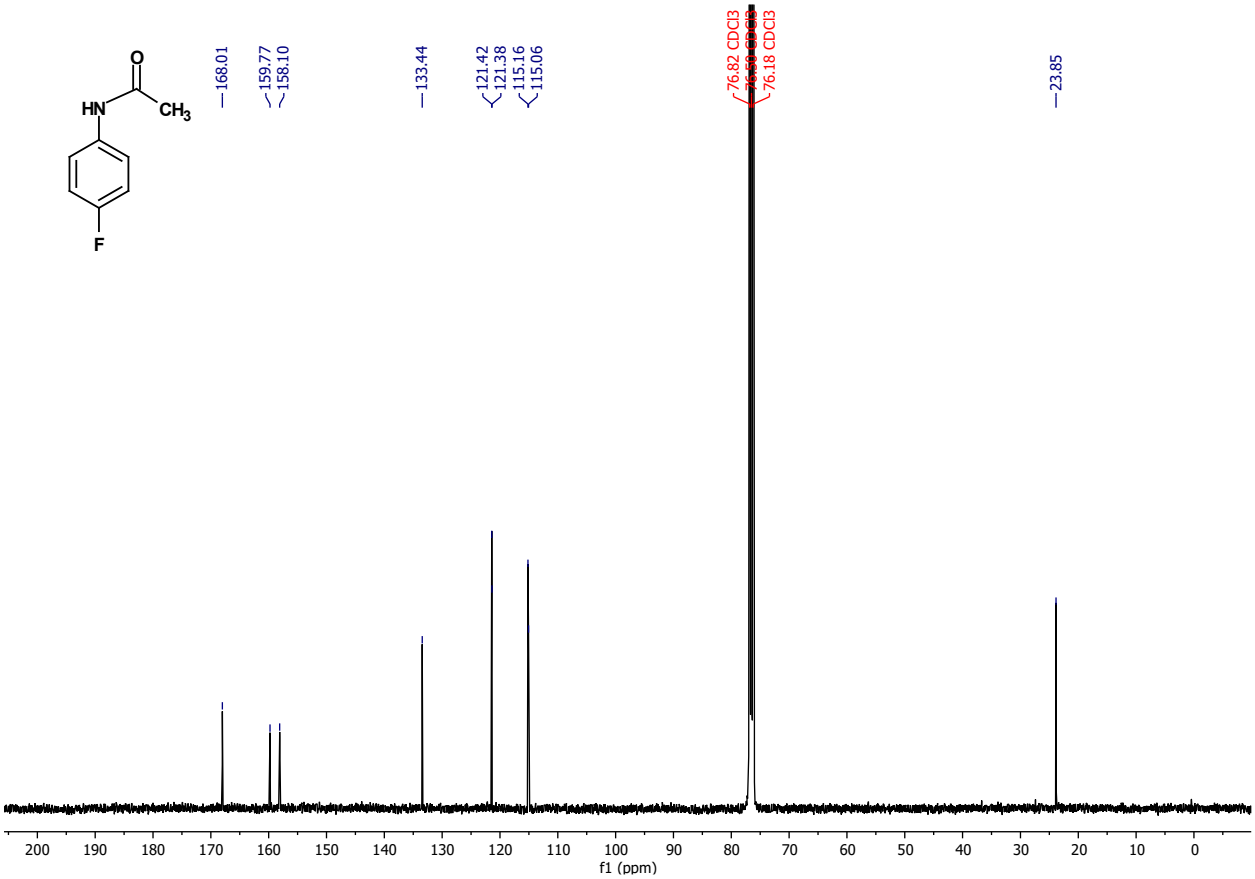
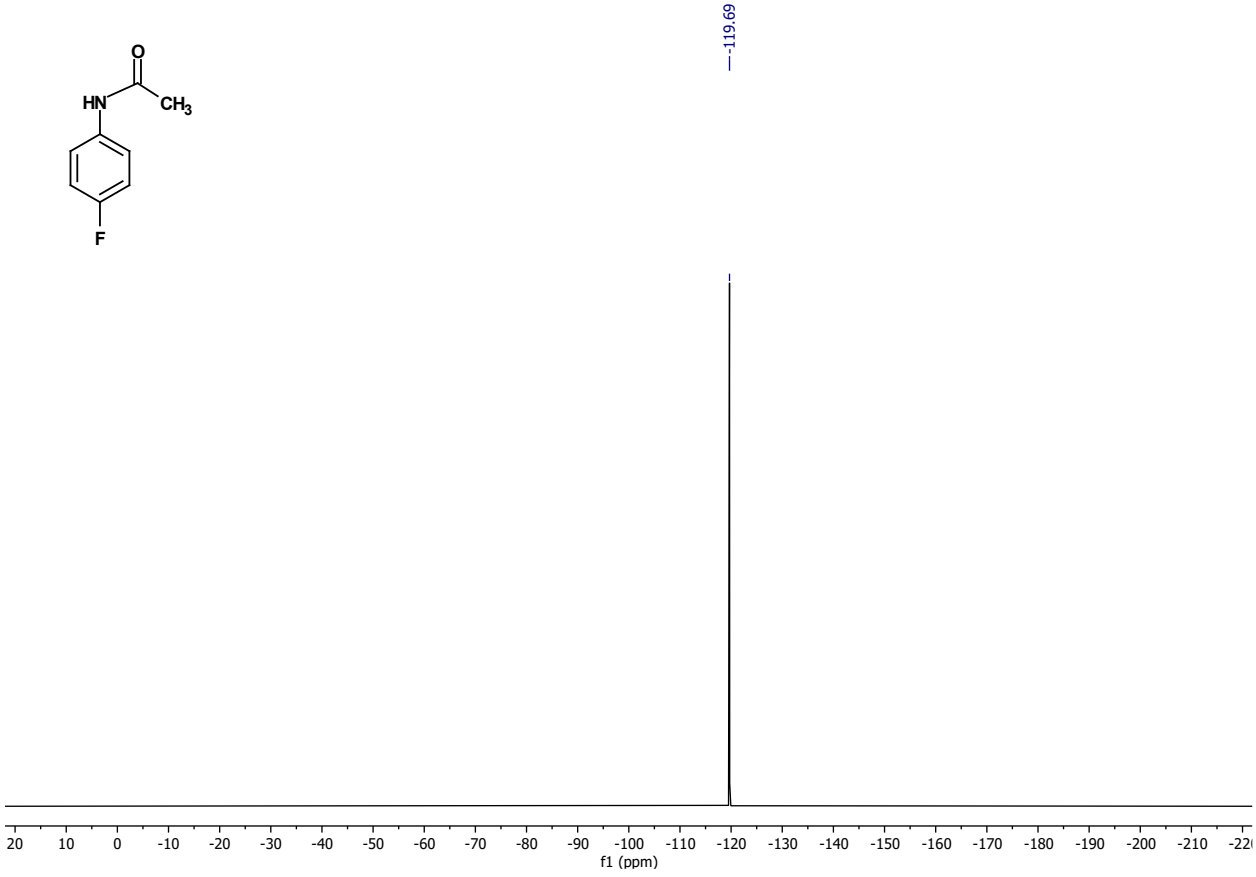


^{1}H and ^{13}C NMR *N*-(4-fluorophenyl)acetamide (**2f**)

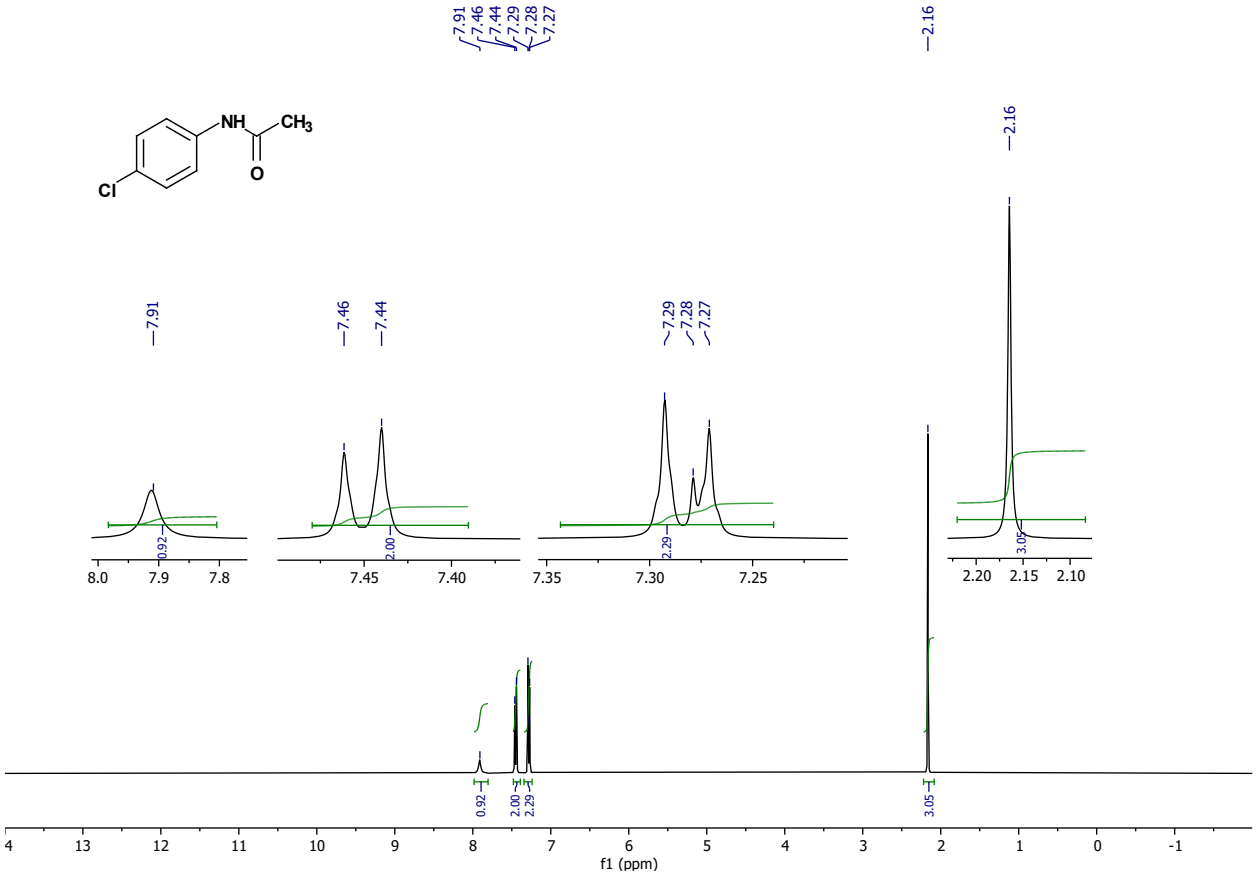


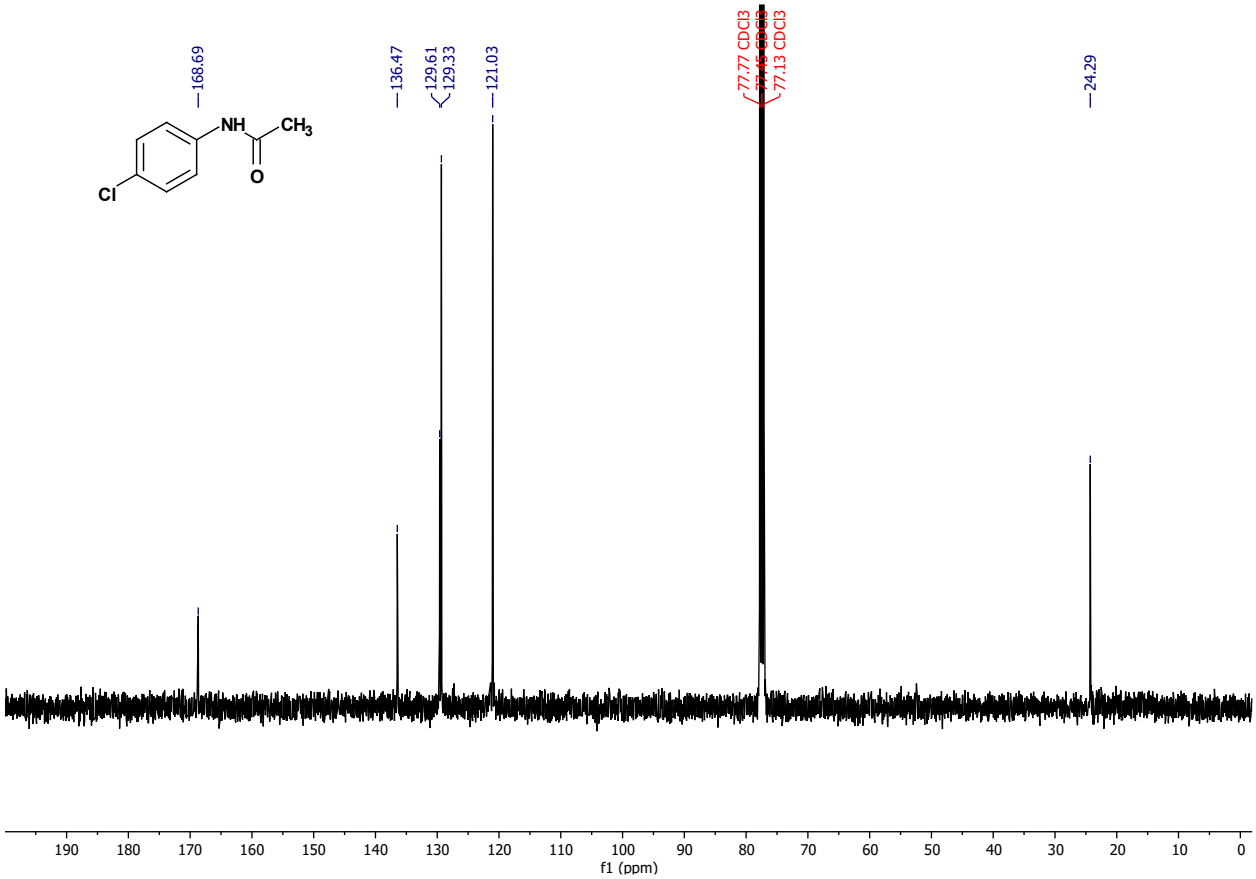


^{19}F NMR *N*-(4-fluorophenyl)acetamide (**2f**)

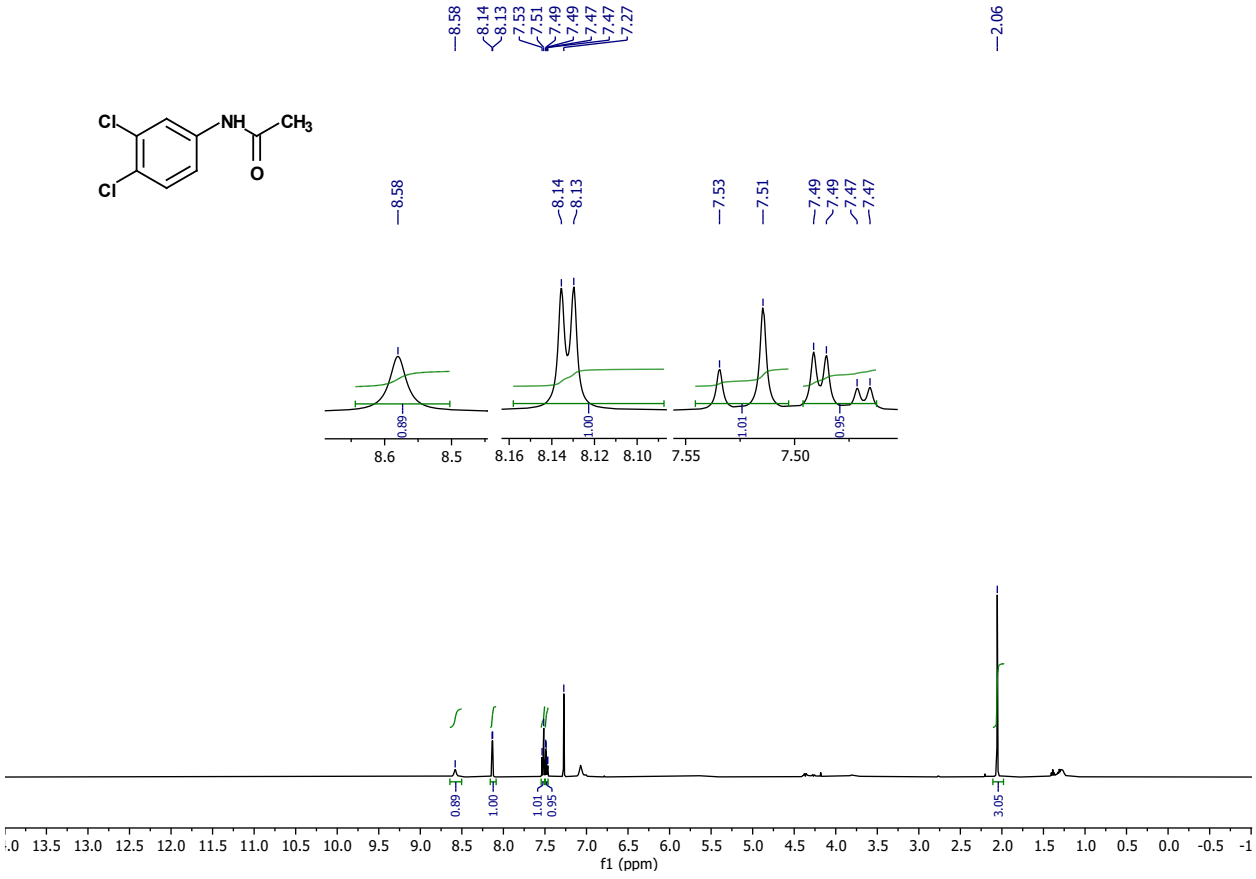


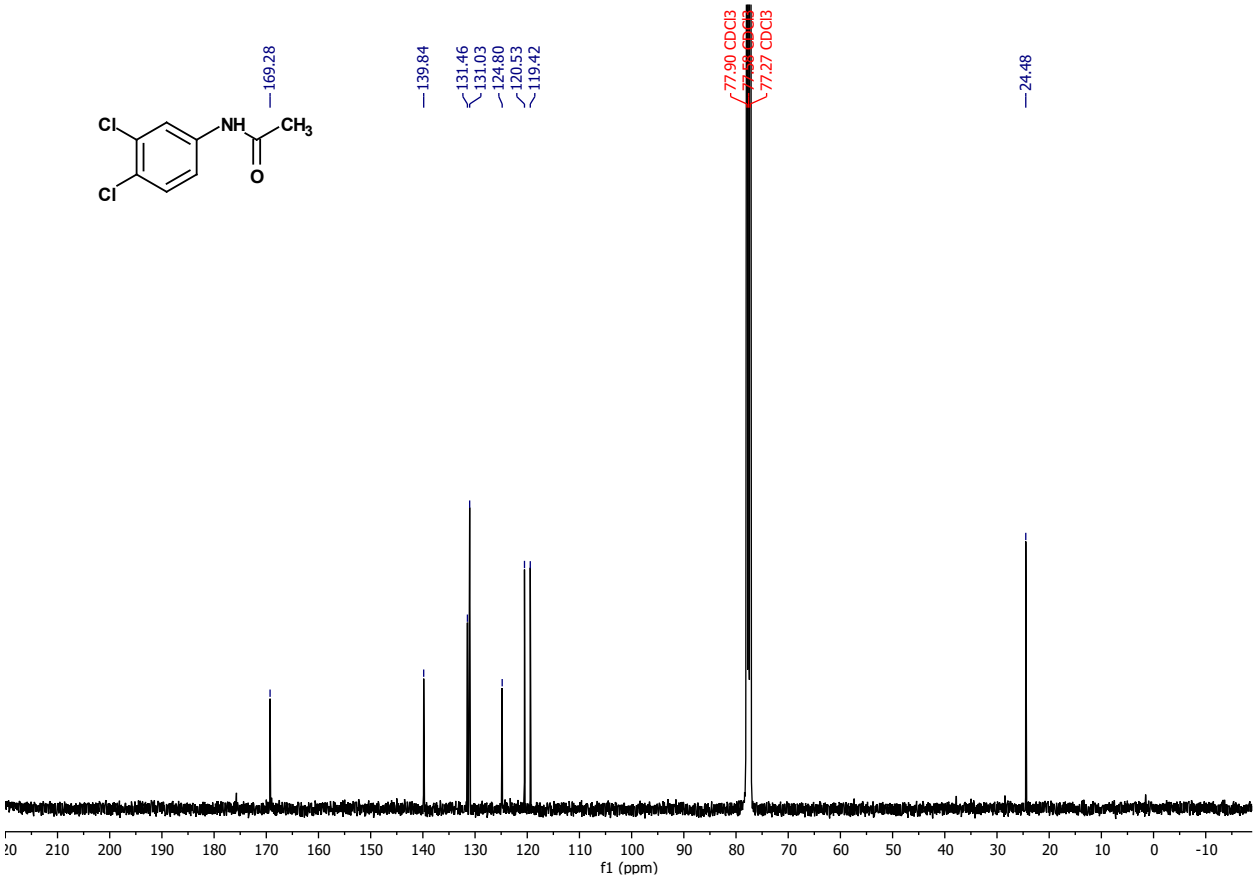
^{1}H and ^{13}C NMR *N*-(4-chlorophenyl)acetamide (**2g**)





^{1}H and ^{13}C NMR *N*-(3,4-dichlorophenyl)acetamide **(2h-*a*)**





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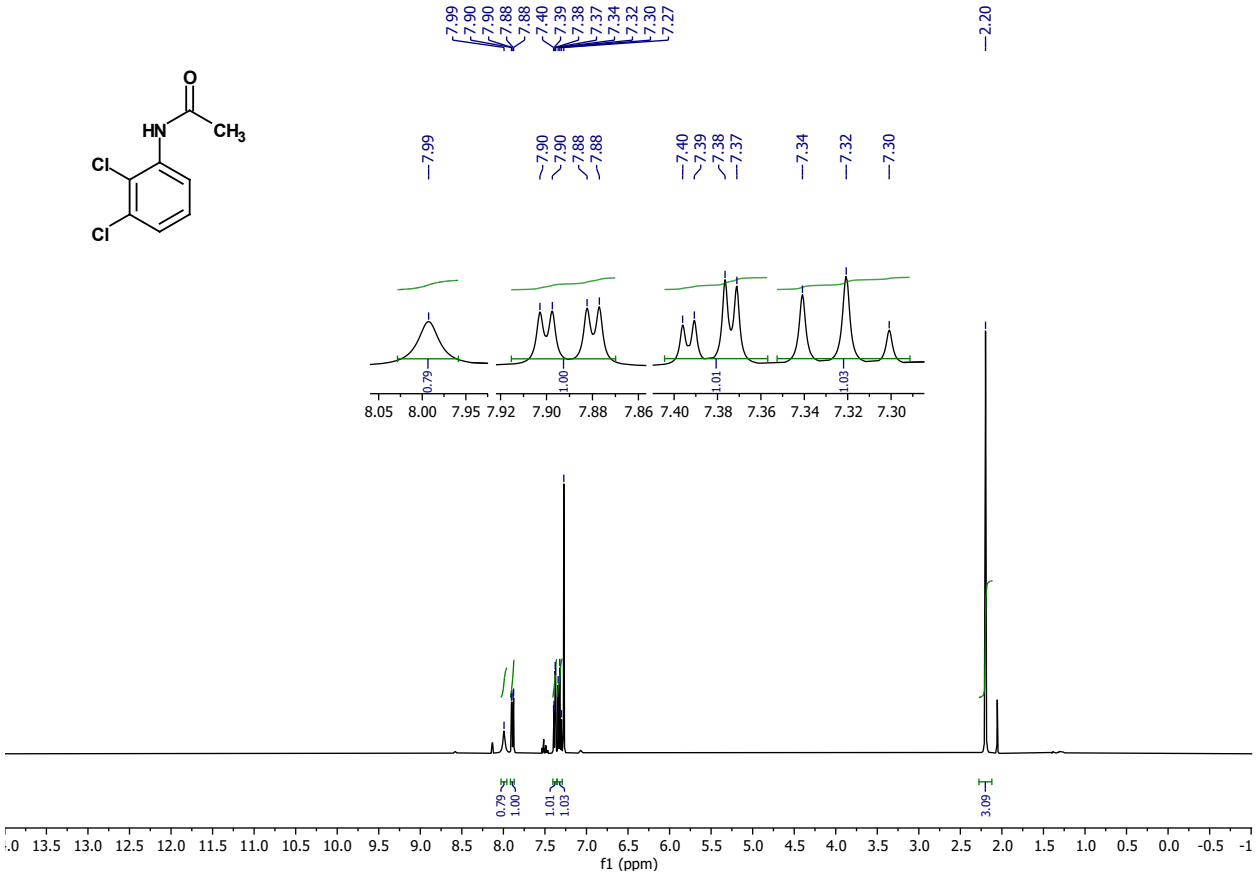
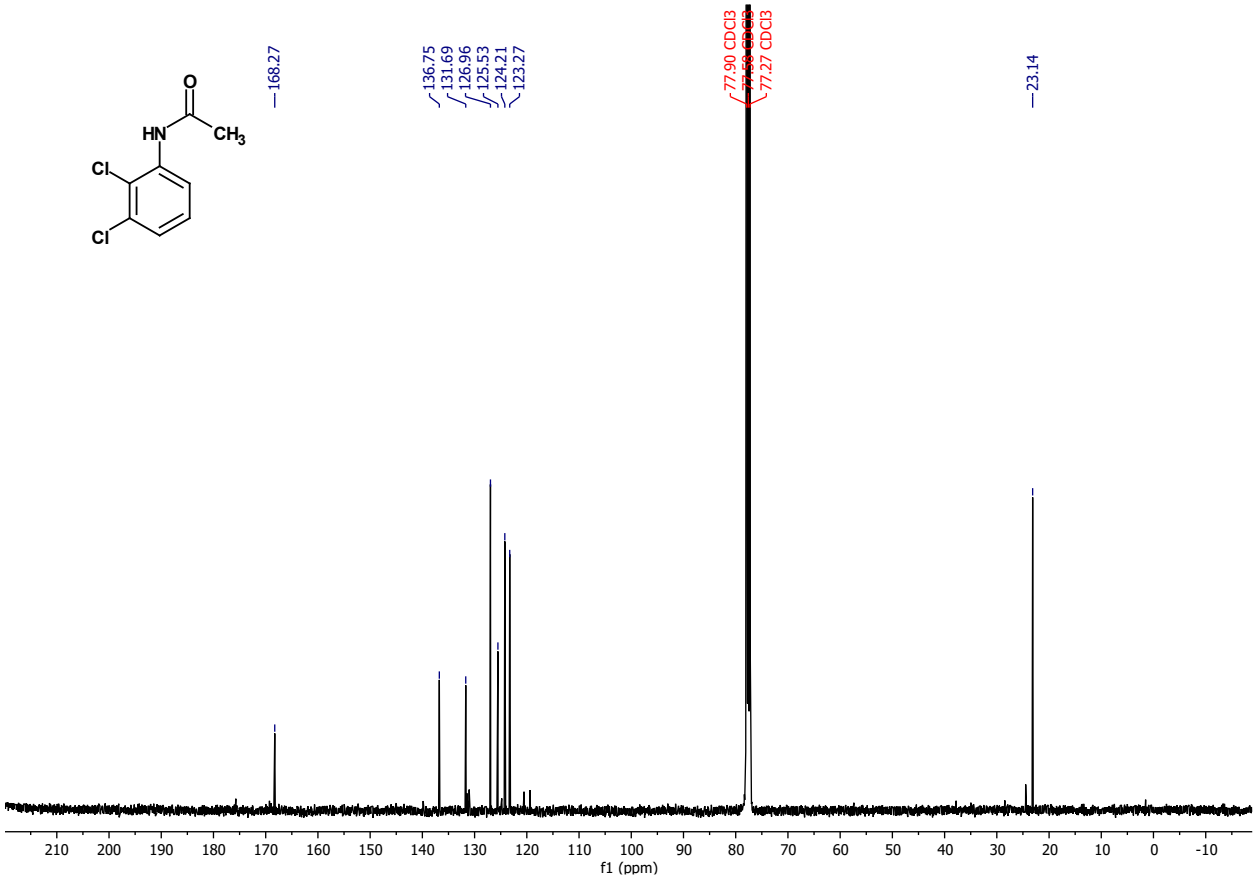
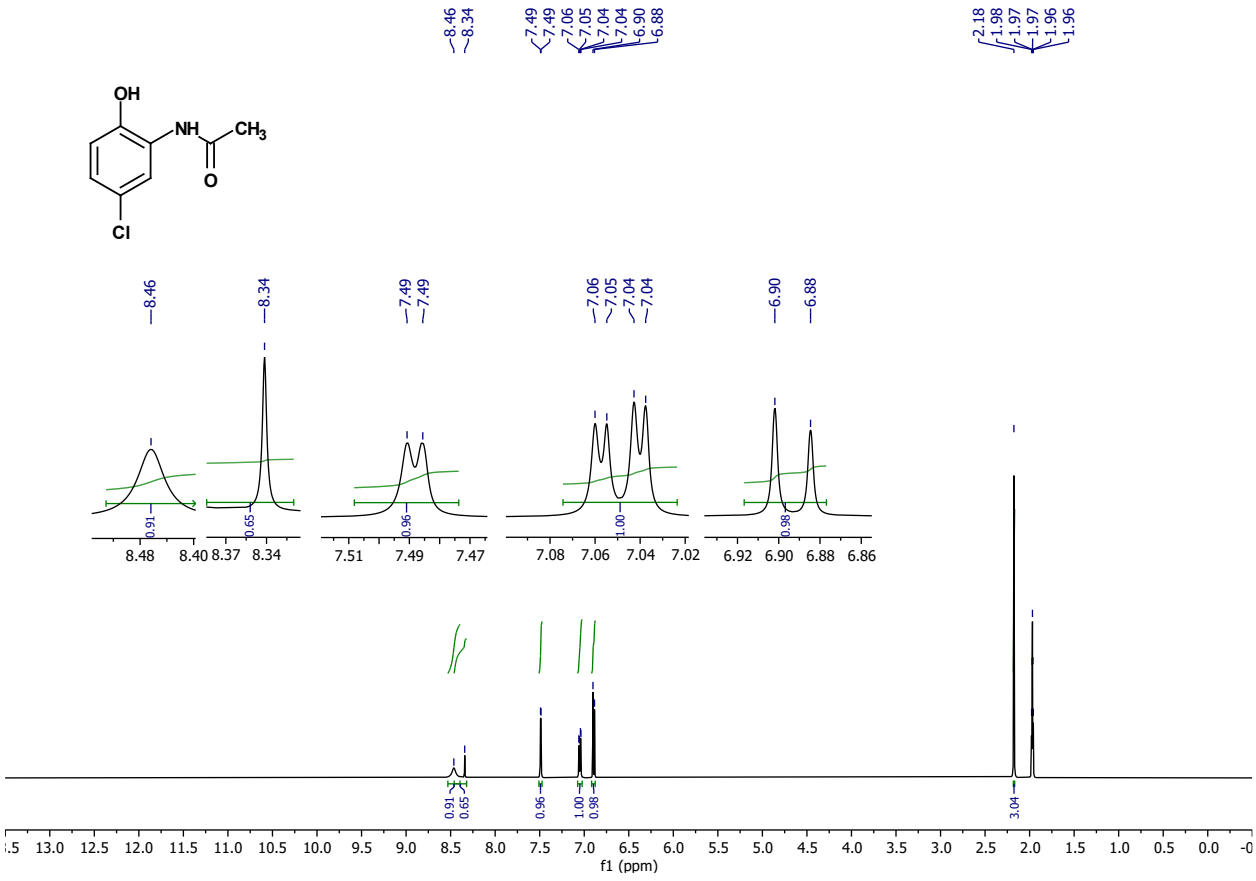
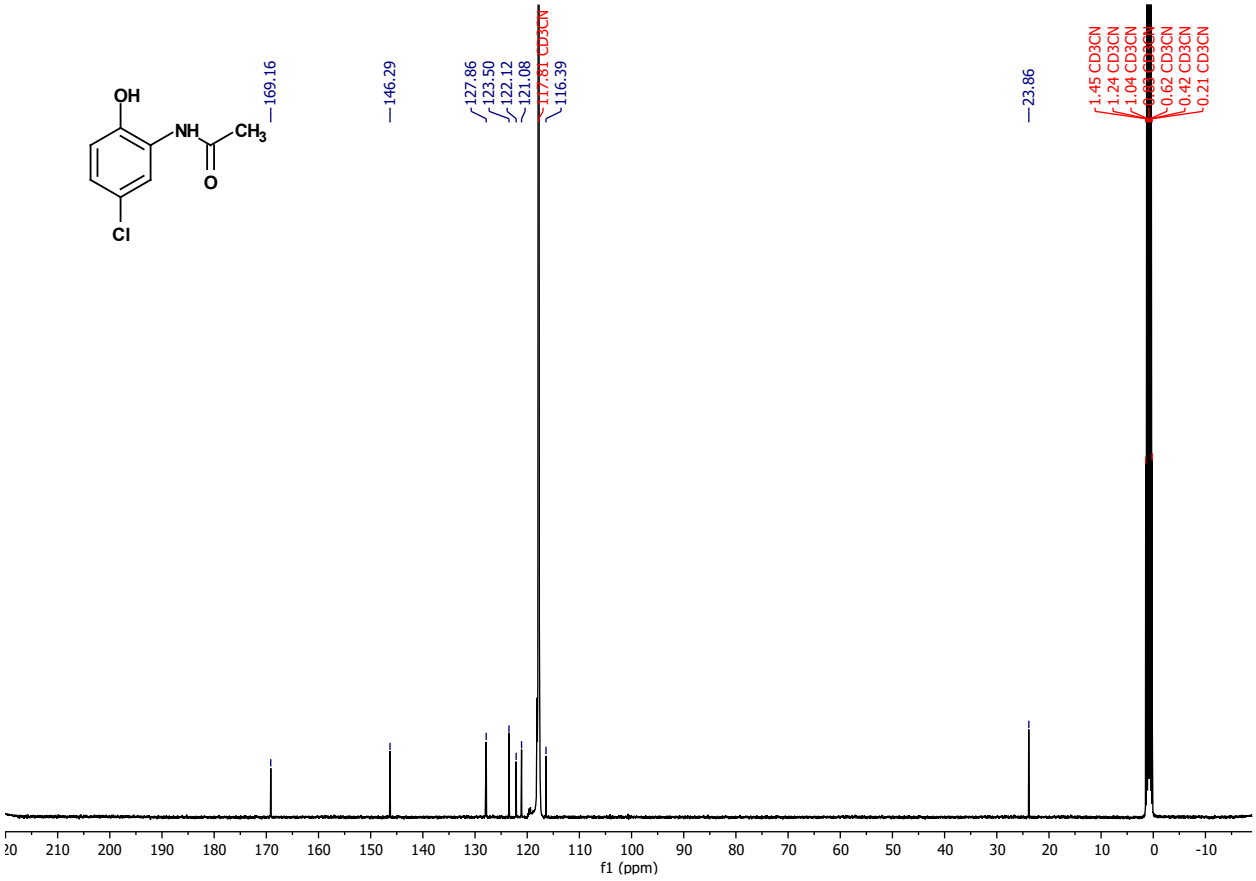


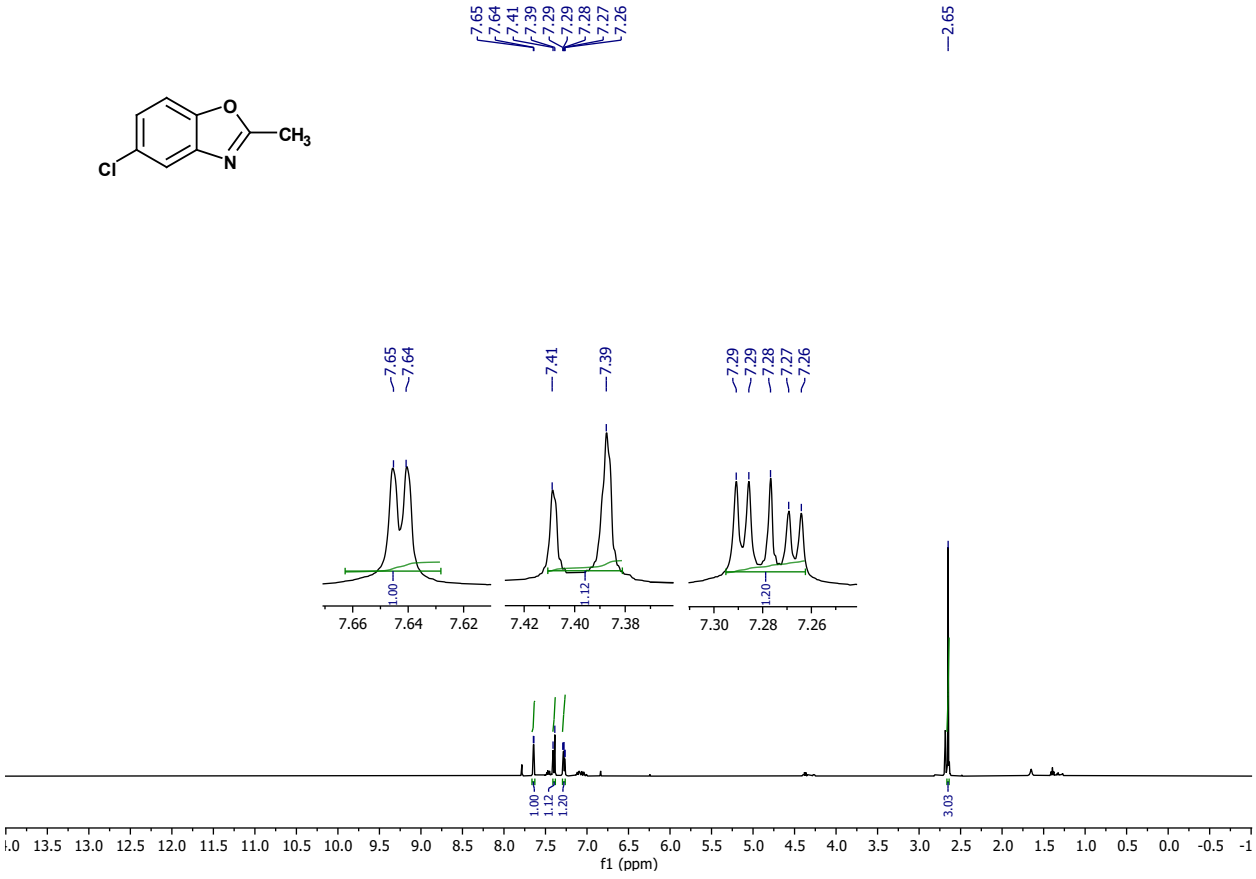


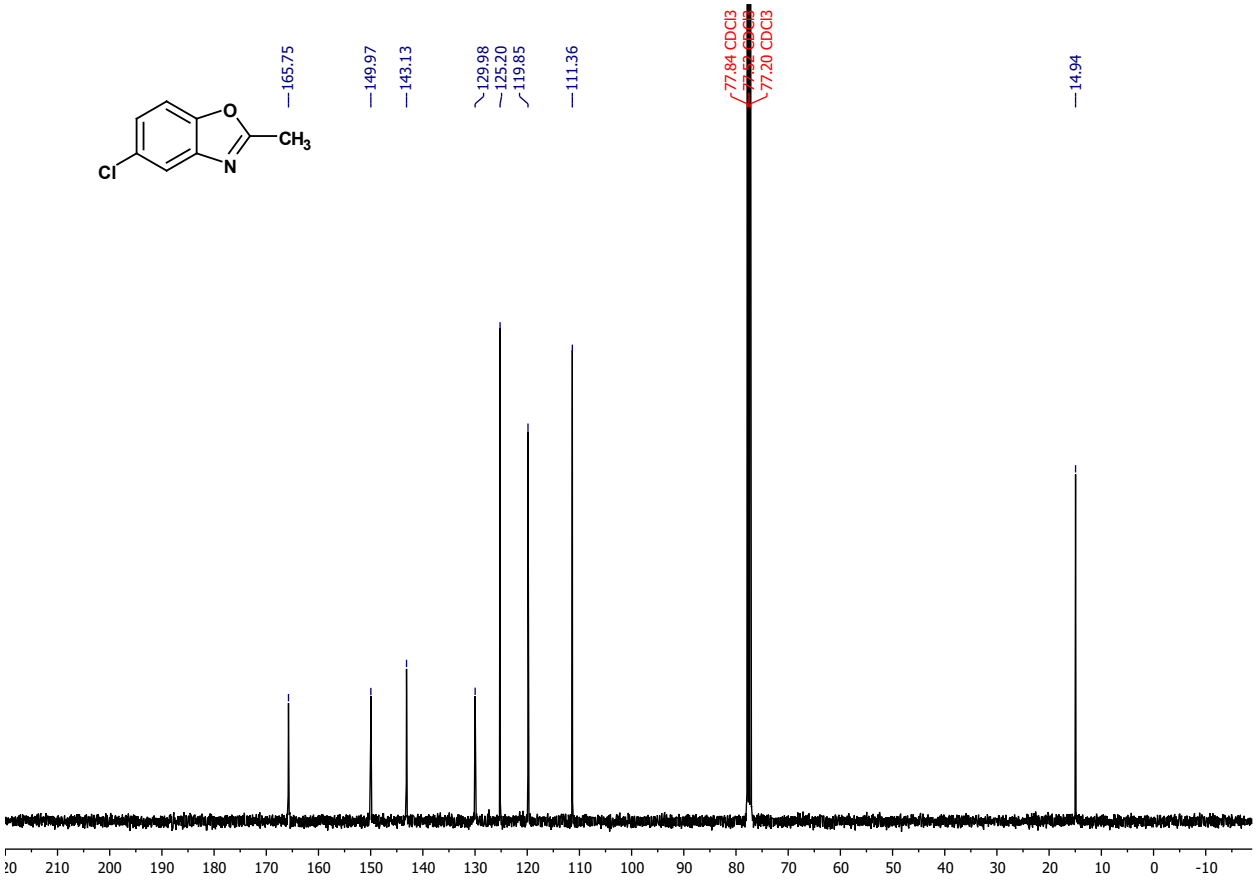
^{1}H and ^{13}C NMR *N*-(5-chloro-2-hydroxyphenyl)acetamide (**2i**)



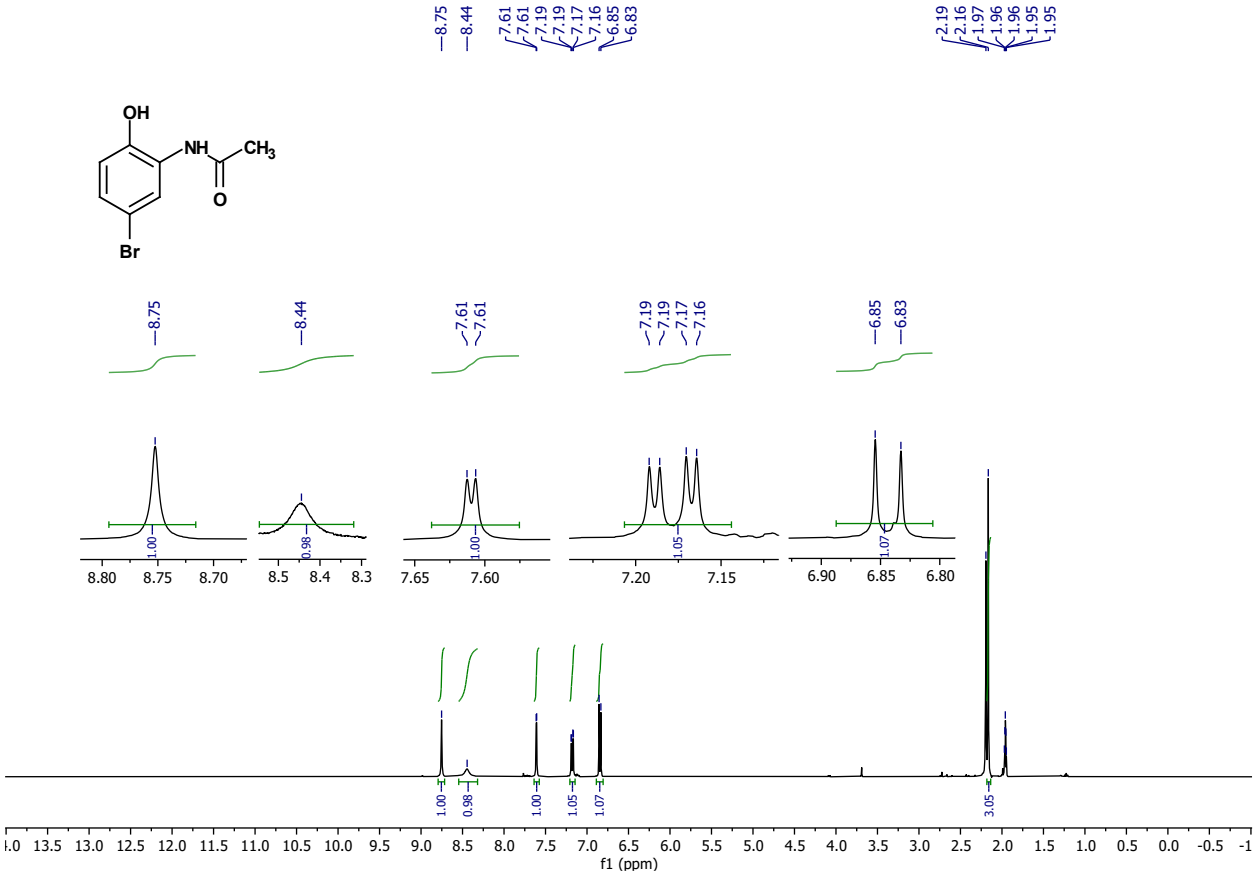


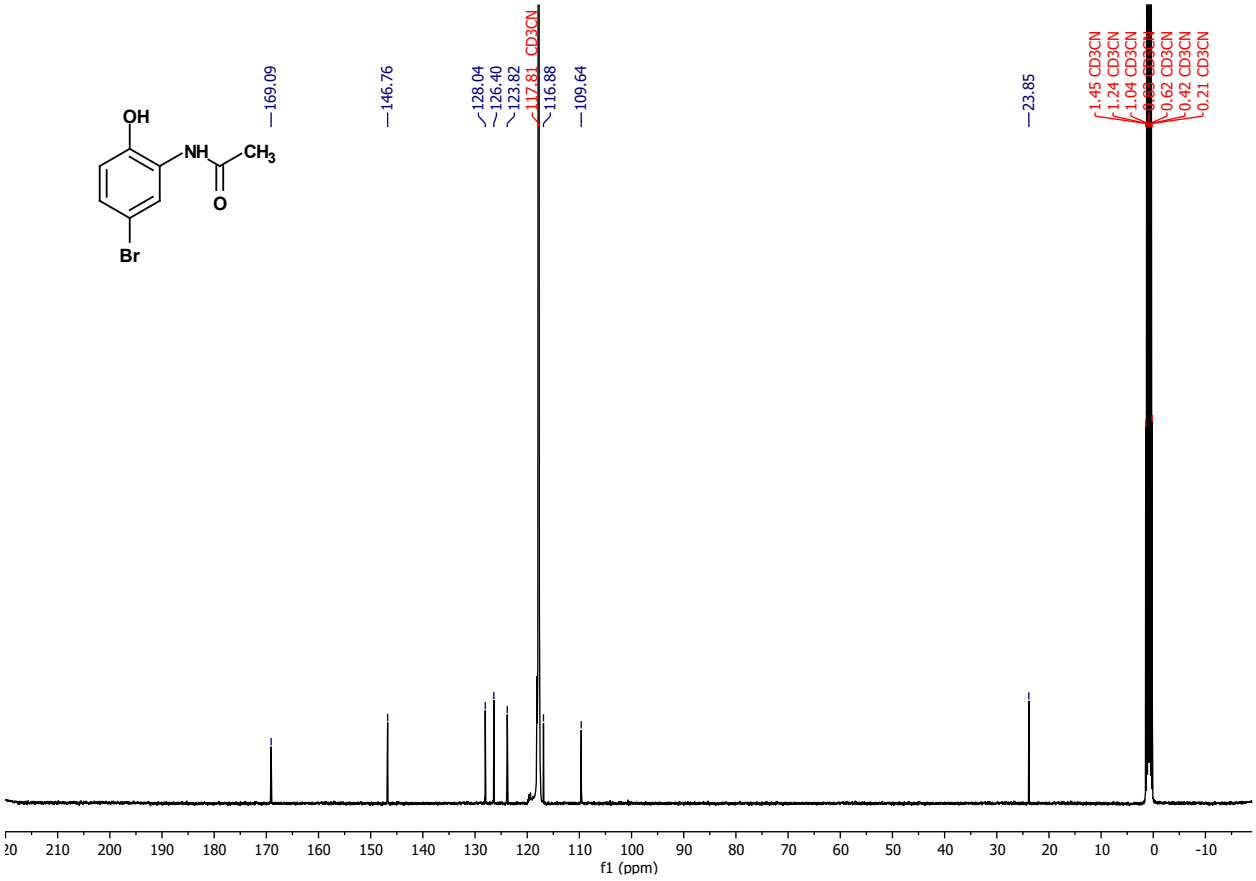
^{1}H and ^{13}C NMR 5-chloro-2-methylbenzo[d]oxazole **(2ii)**



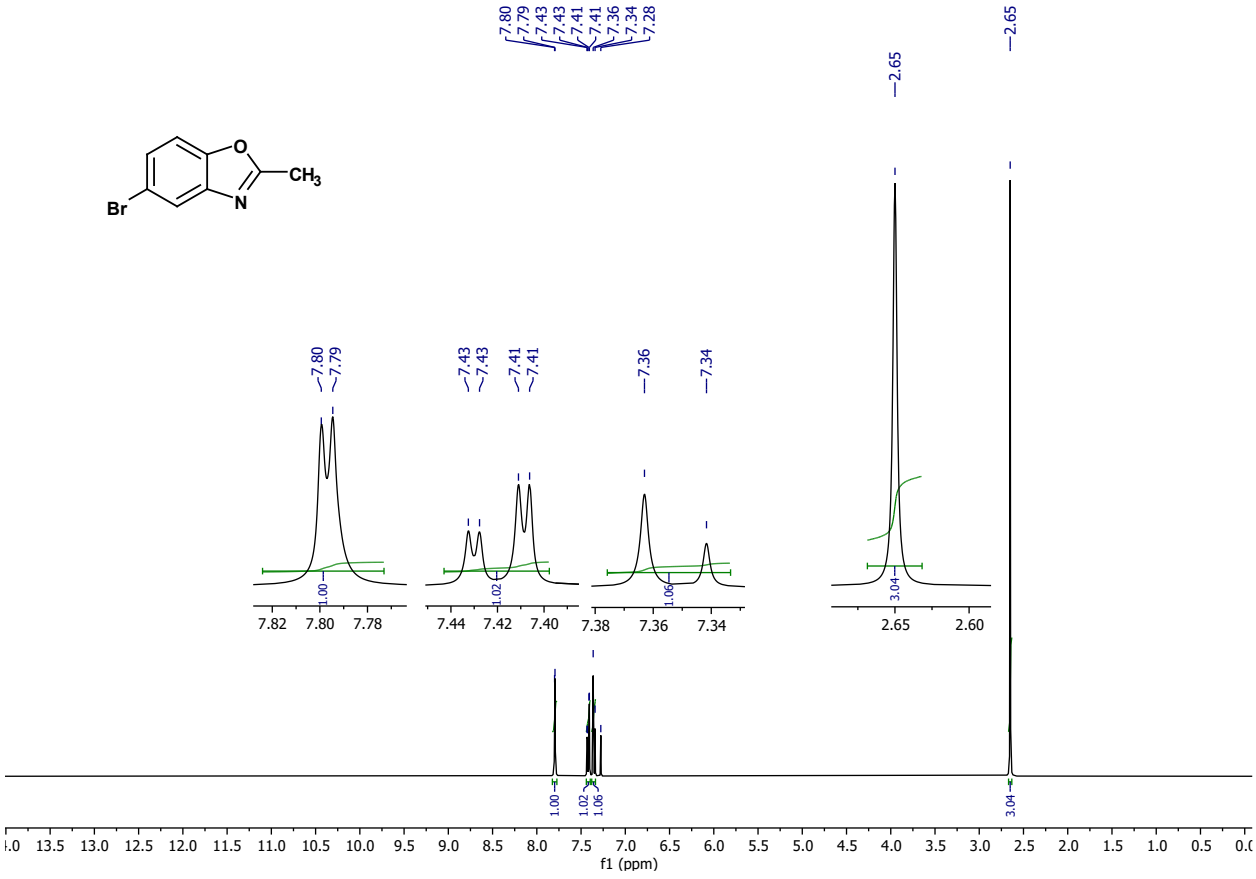


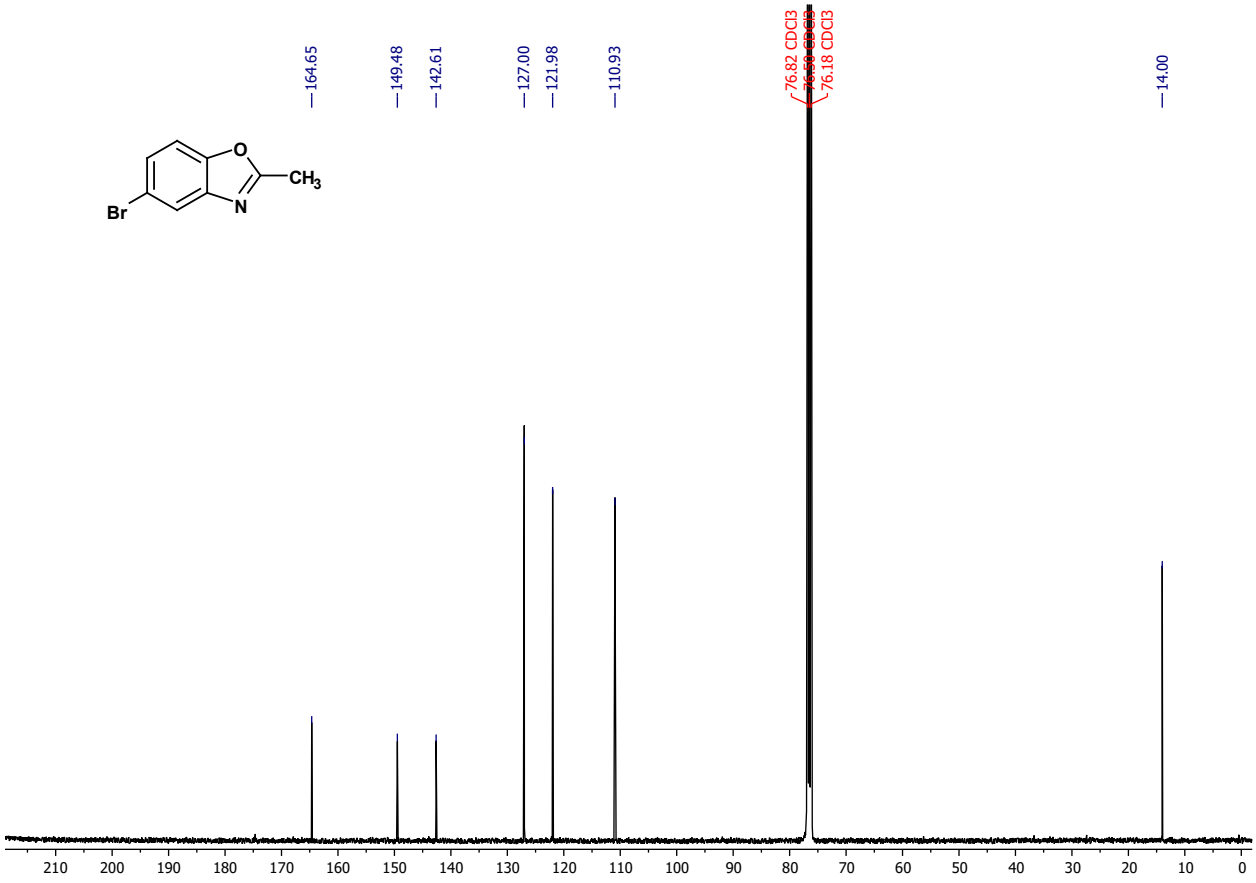
^{1}H and ^{13}C NMR *N*-(5-bromo-2-hydroxyphenyl)acetamide **(2j)**



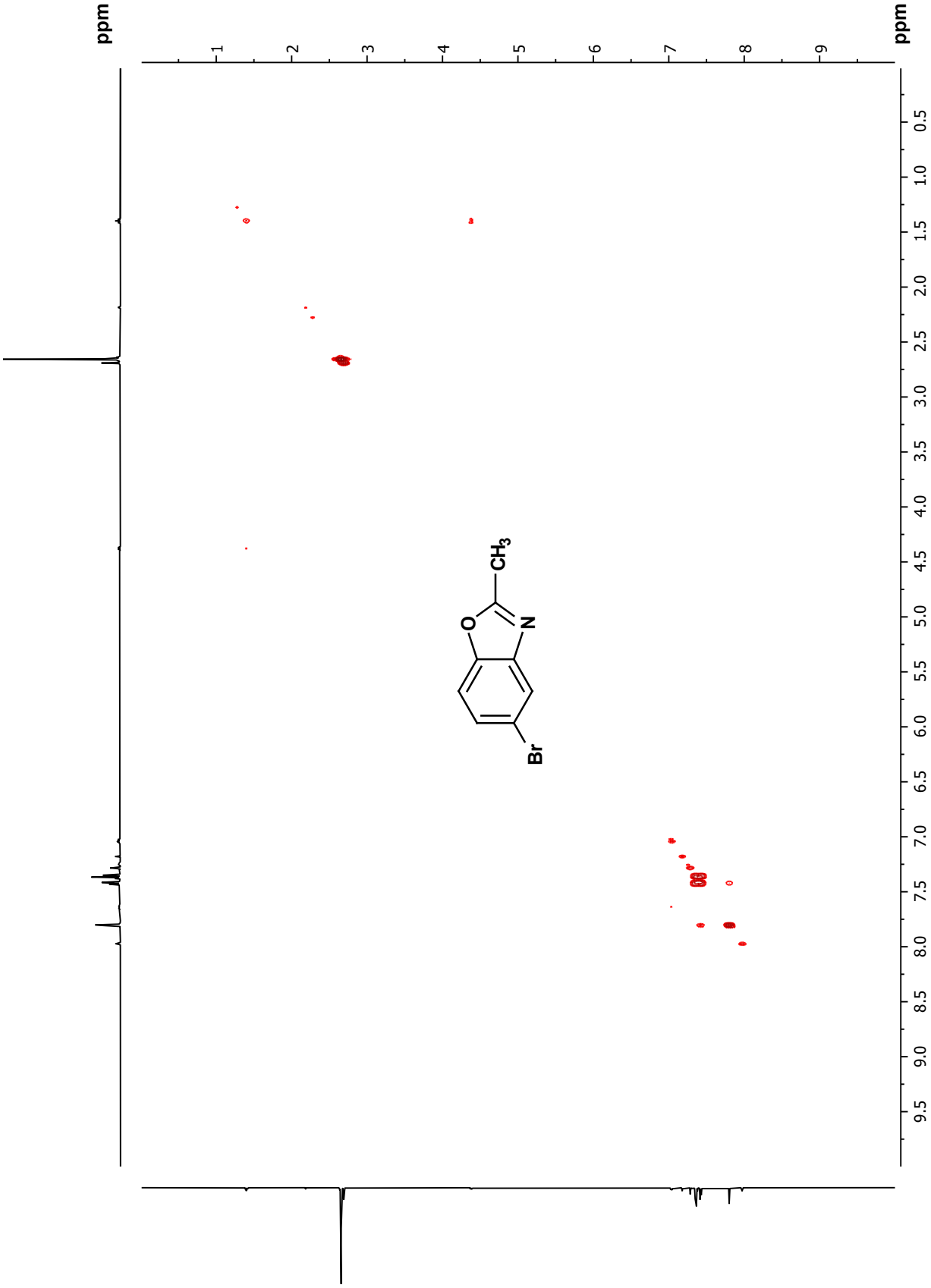


^{1}H and ^{13}C NMR 5-bromo-2-methylbenzo[d]oxazole **(2jj)**

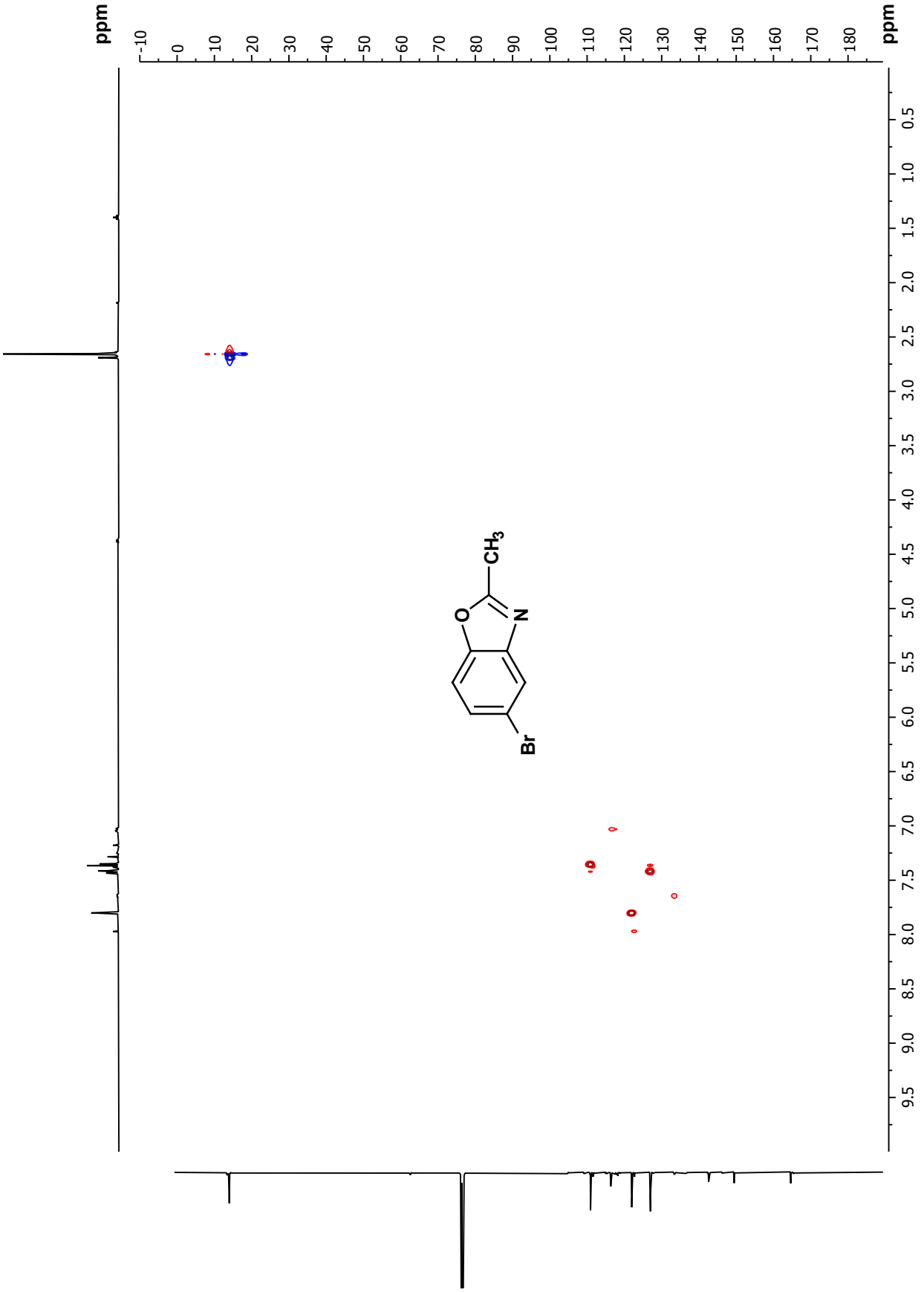




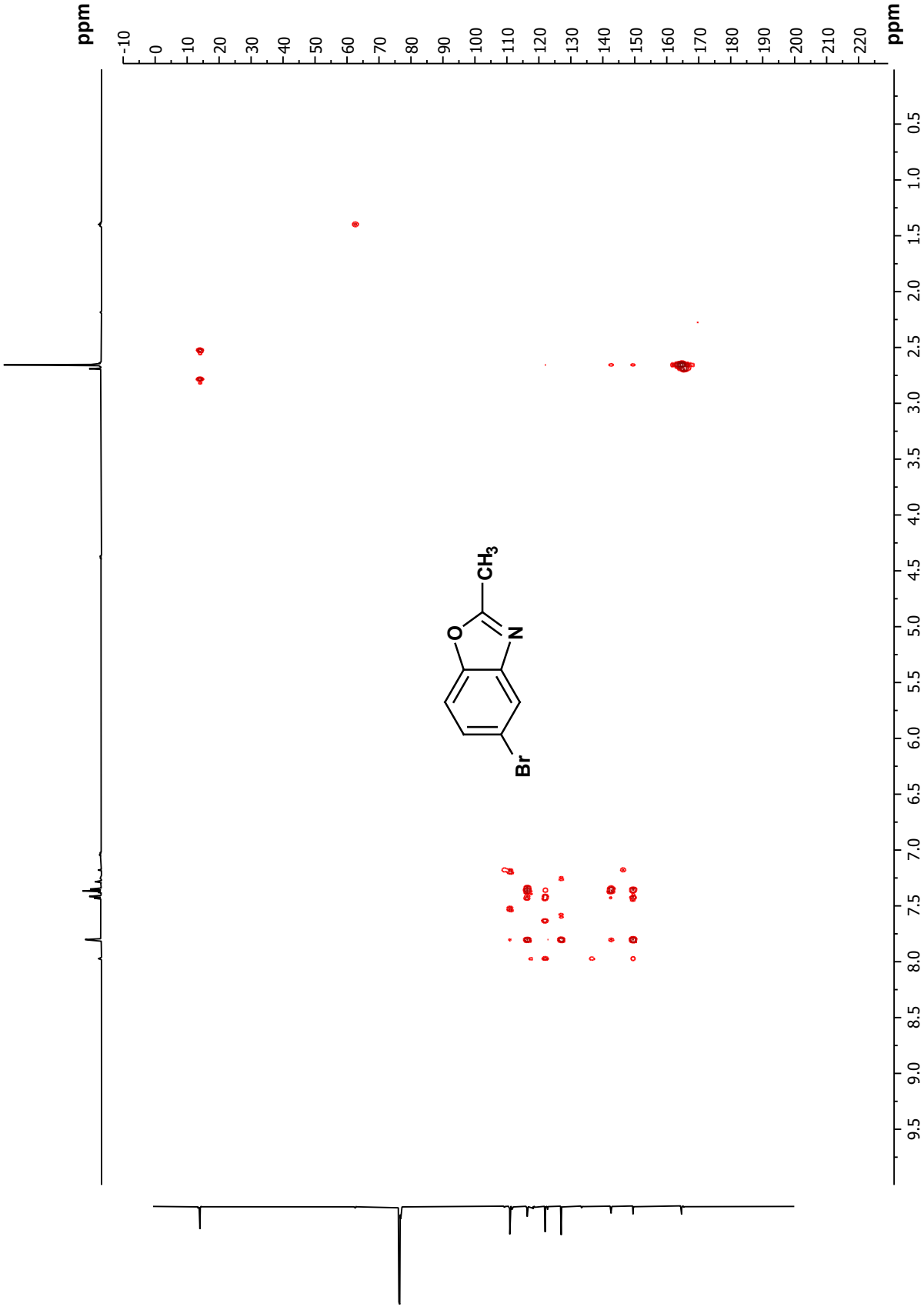
COSY NMR 5-bromo-2-methylbenzo[d]oxazole **(2jj)**



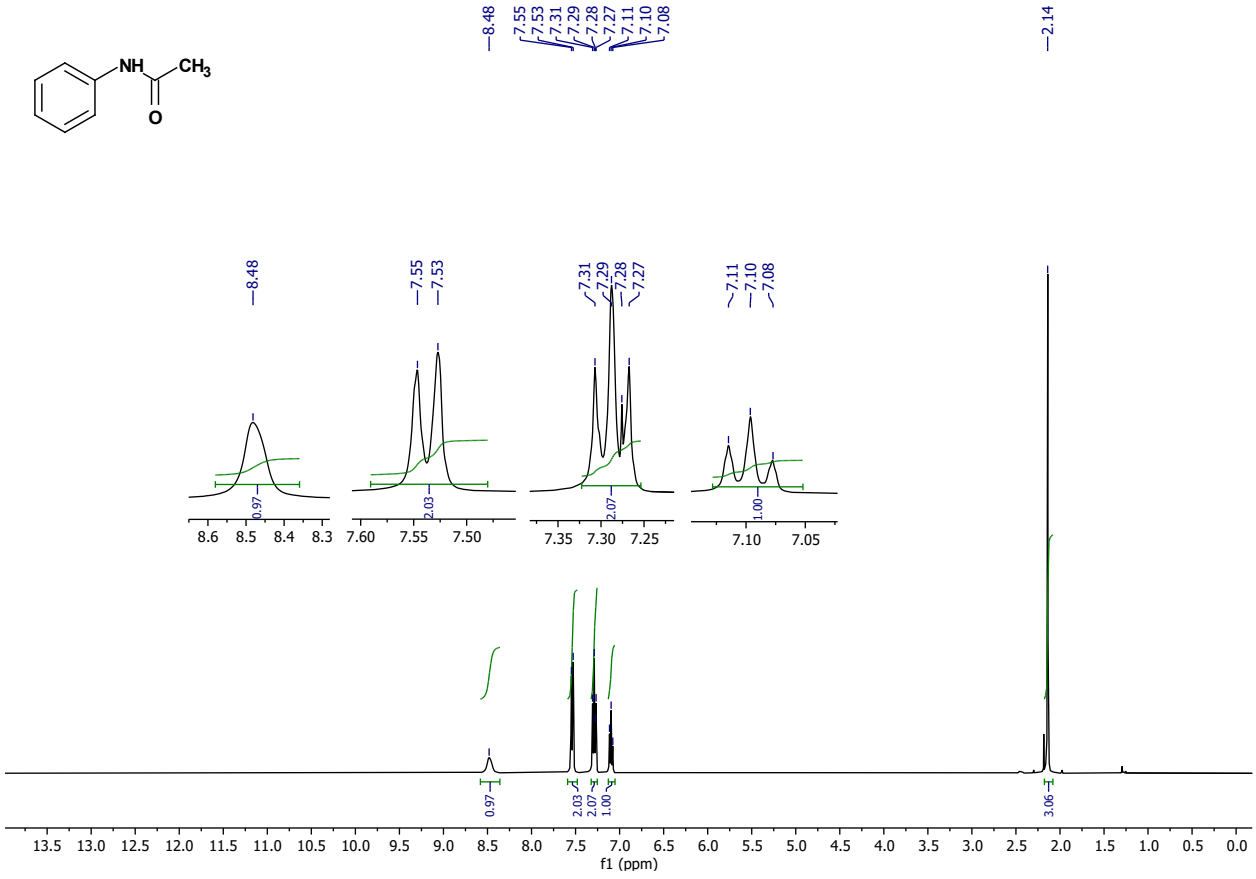
HSQC NMR 5-bromo-2-methylbenzo[d]oxazole **(2jj)**

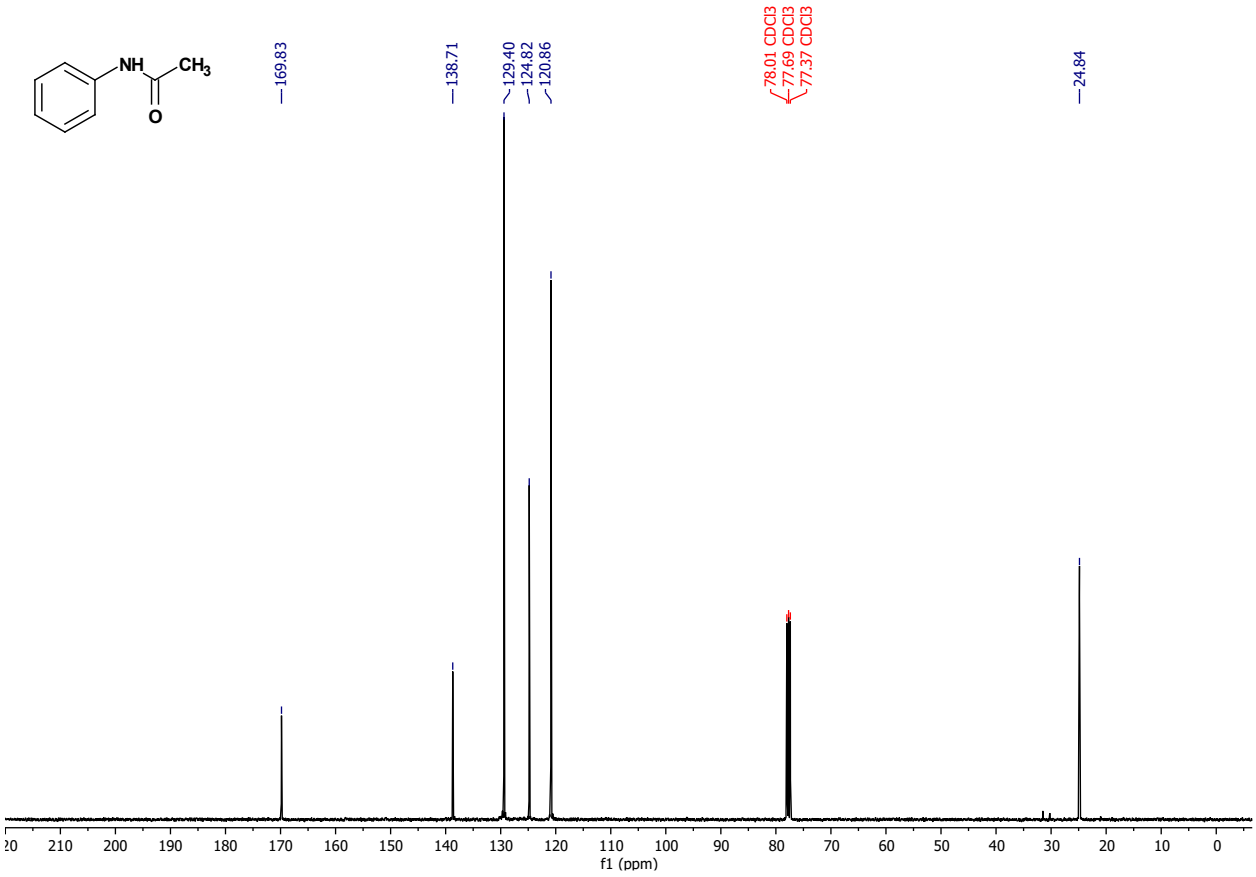


HMBC NMR 5-bromo-2-methylbenzo[d]oxazole **(2jj)**

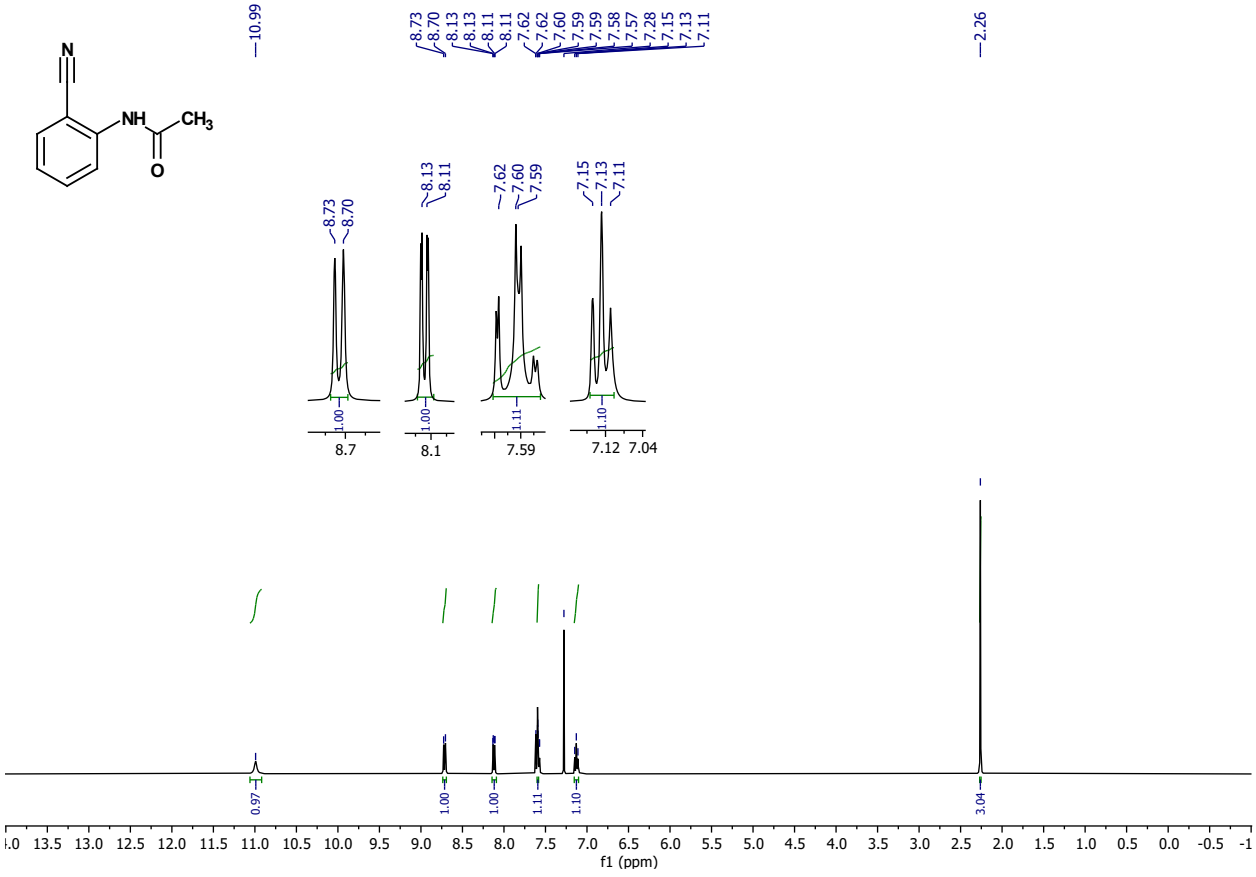


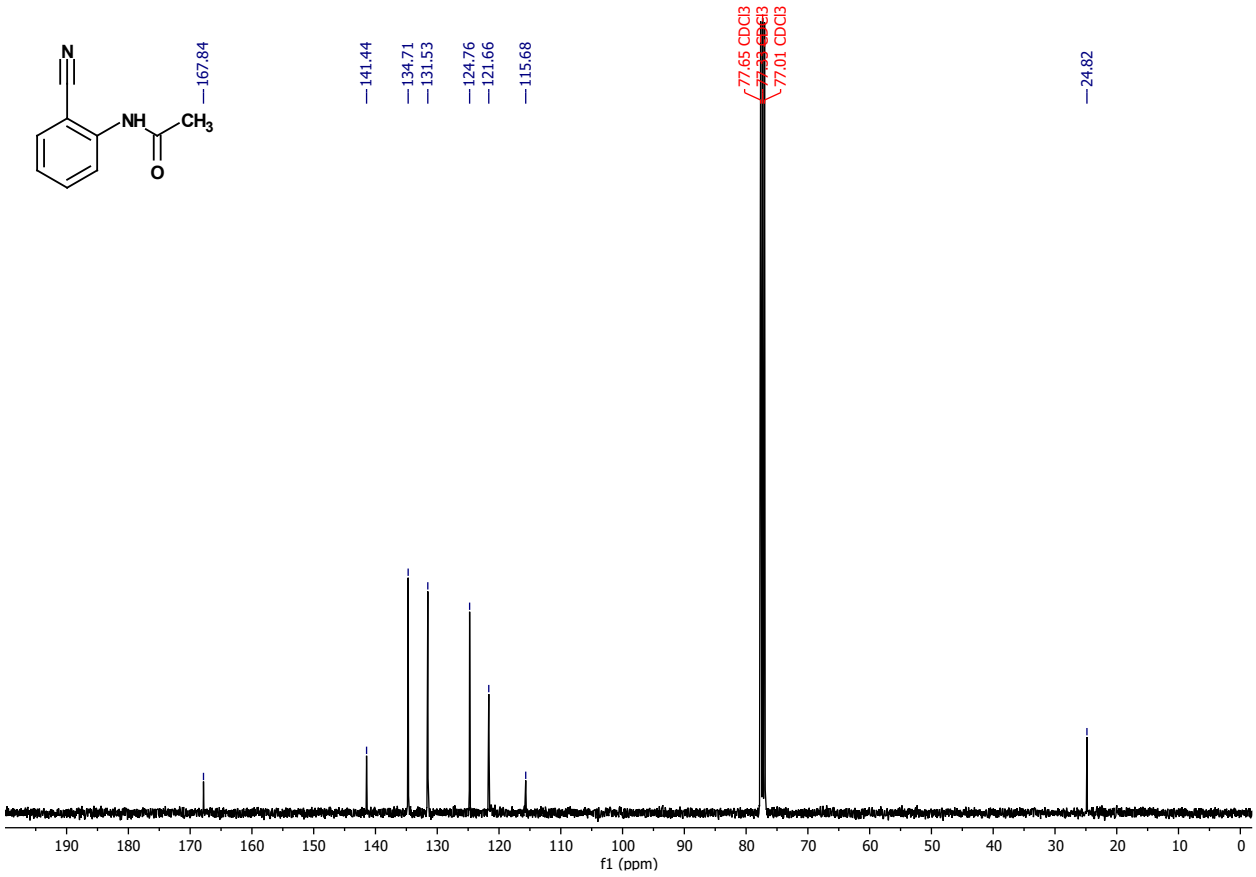
^{1}H and ^{13}C NMR *N*-phenylacetamide (**2k**)



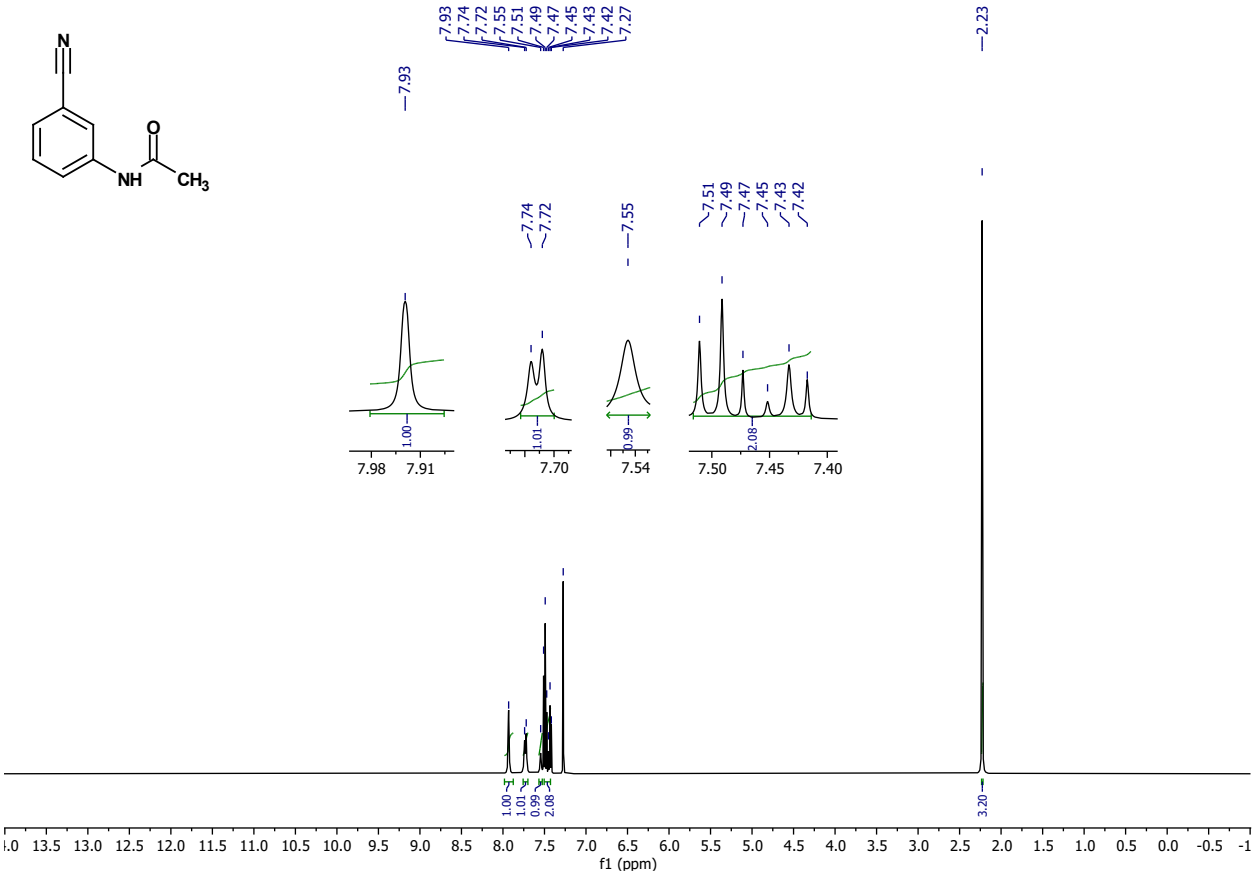


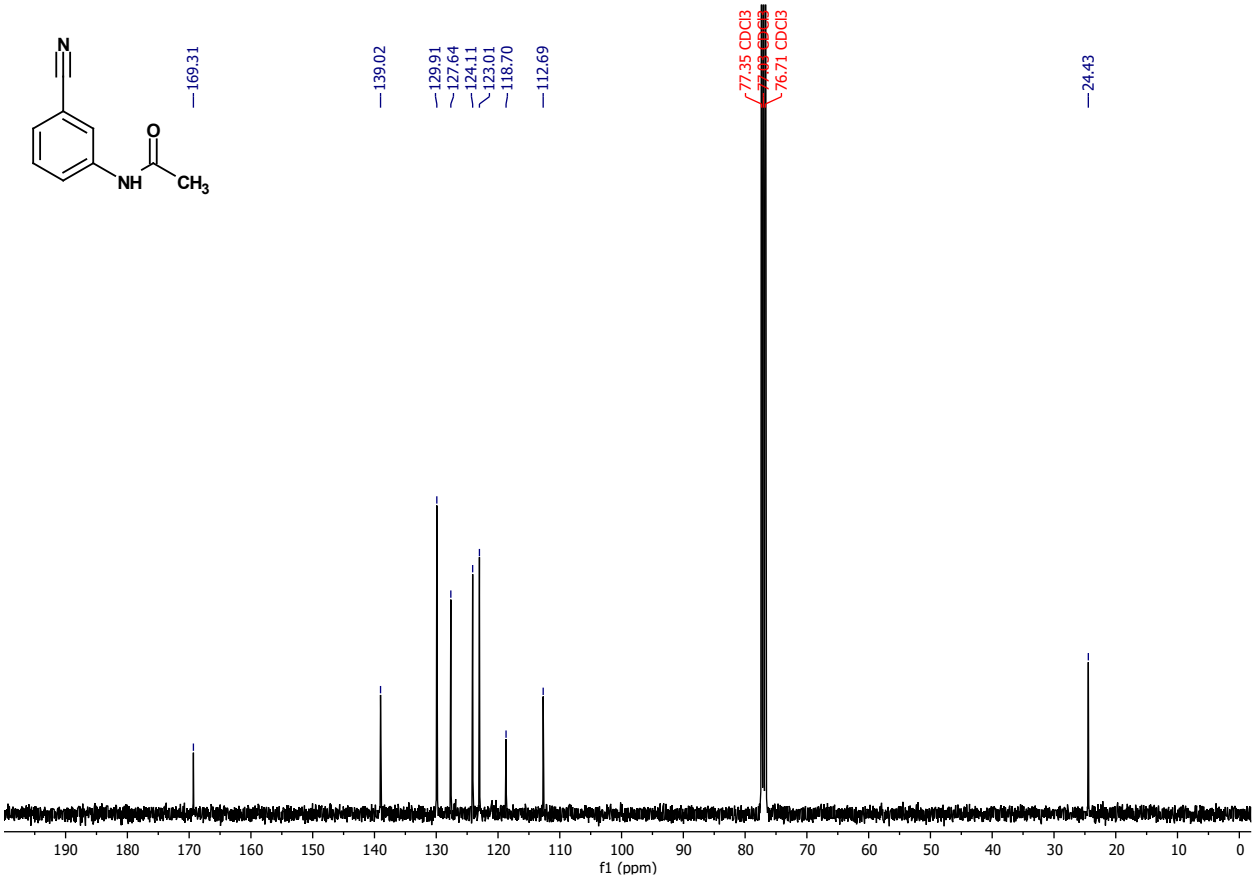
^{1}H and ^{13}C NMR *N*-(2-cyanophenyl)acetamide (**2l**-*a*)



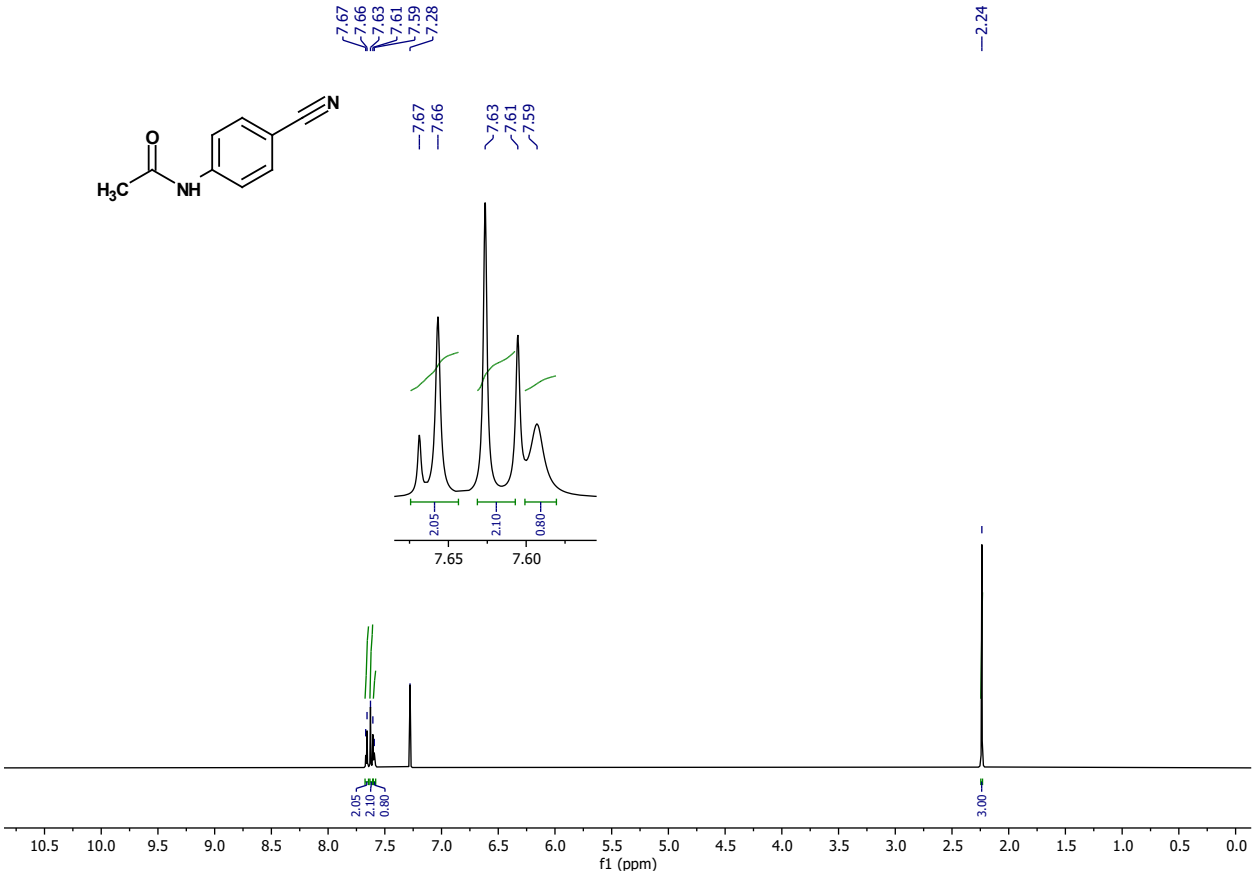


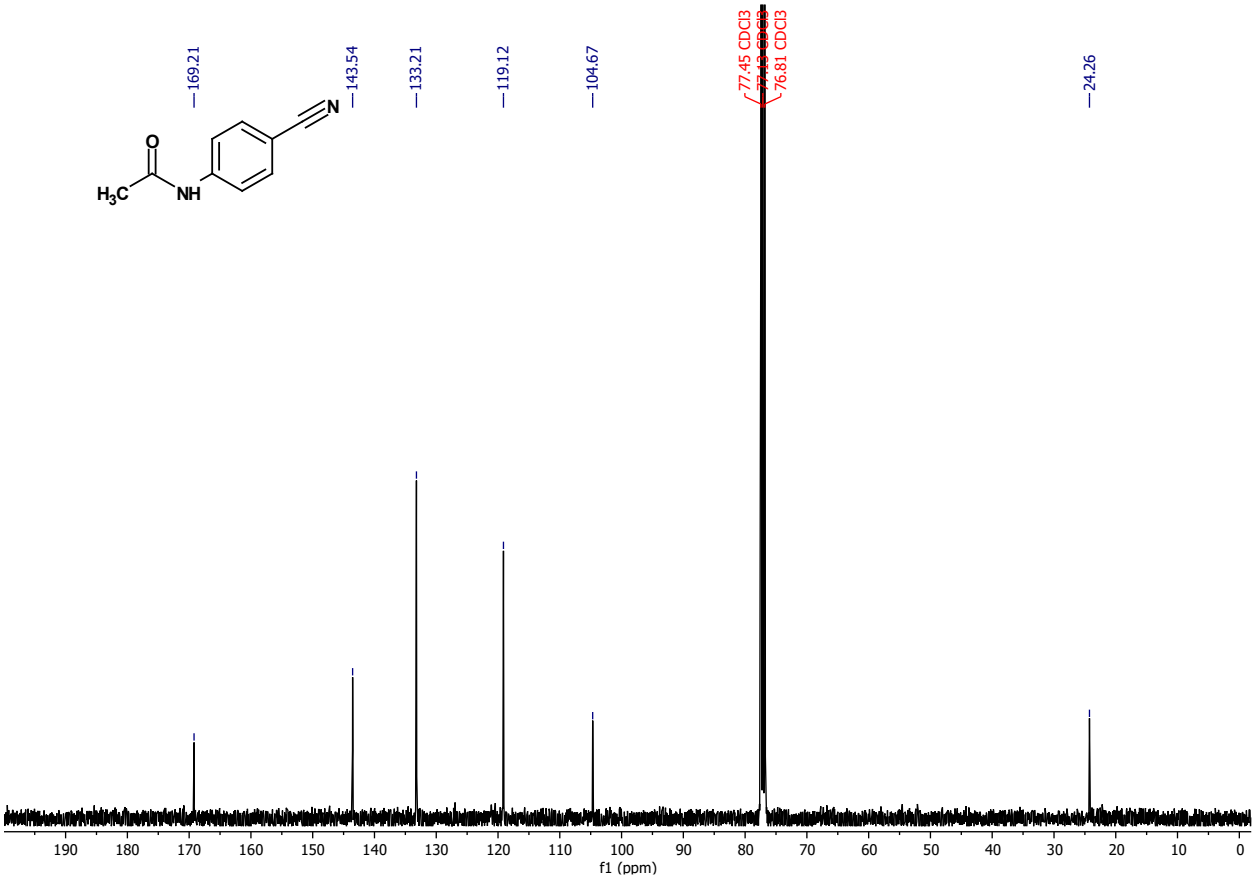
^{1}H and ^{13}C NMR *N*-(3-cyanophenyl)acetamide (**2l**-*b*)



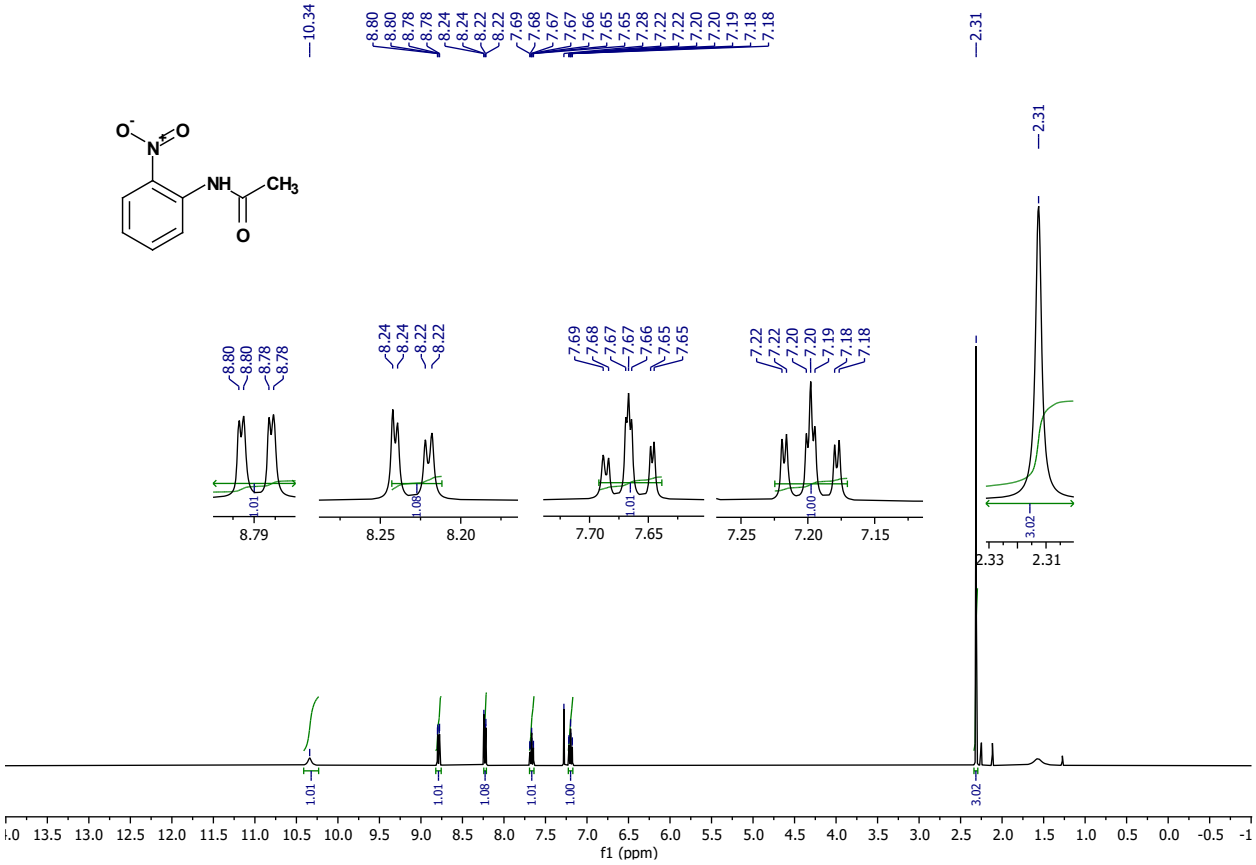


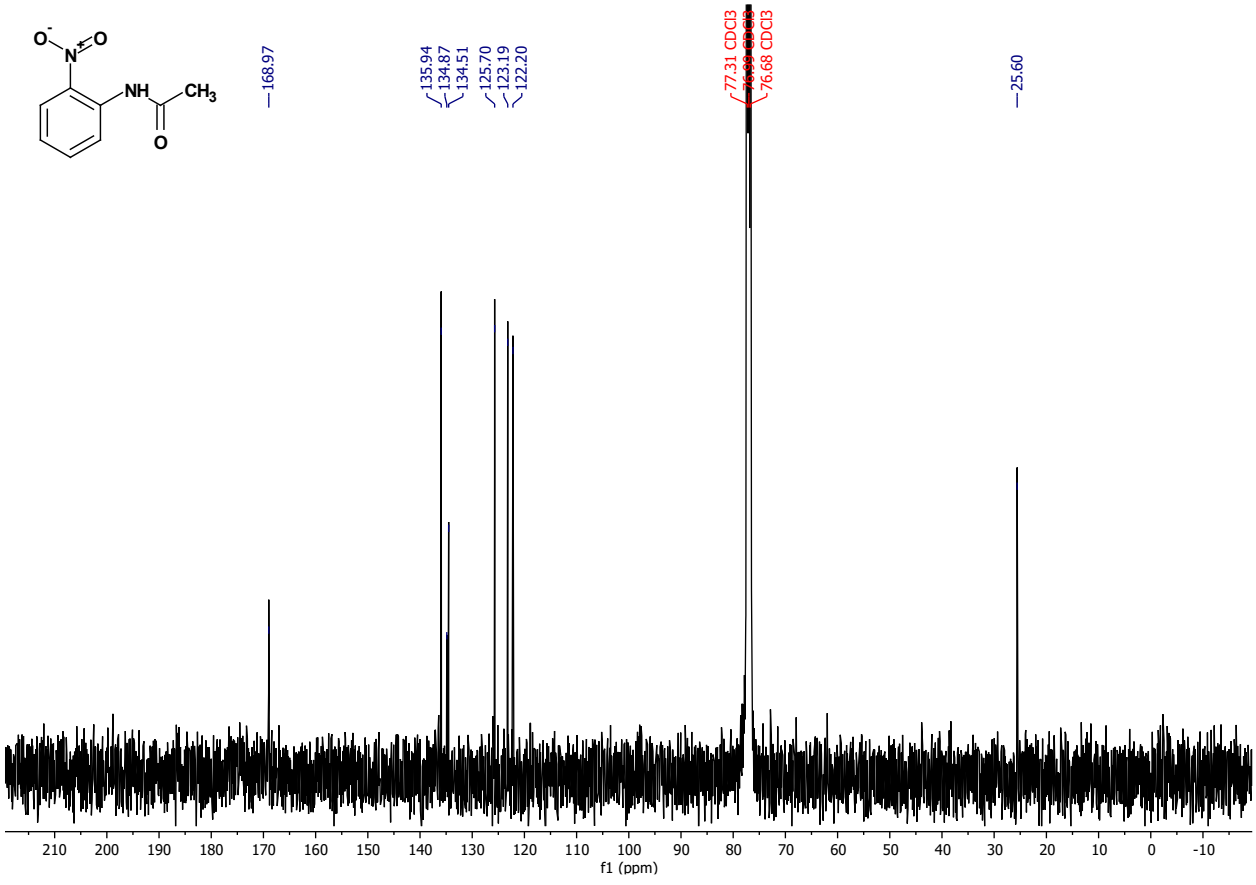
^{1}H and ^{13}C NMR *N*-(4-cyanophenyl)acetamide (**2l**-*c*)



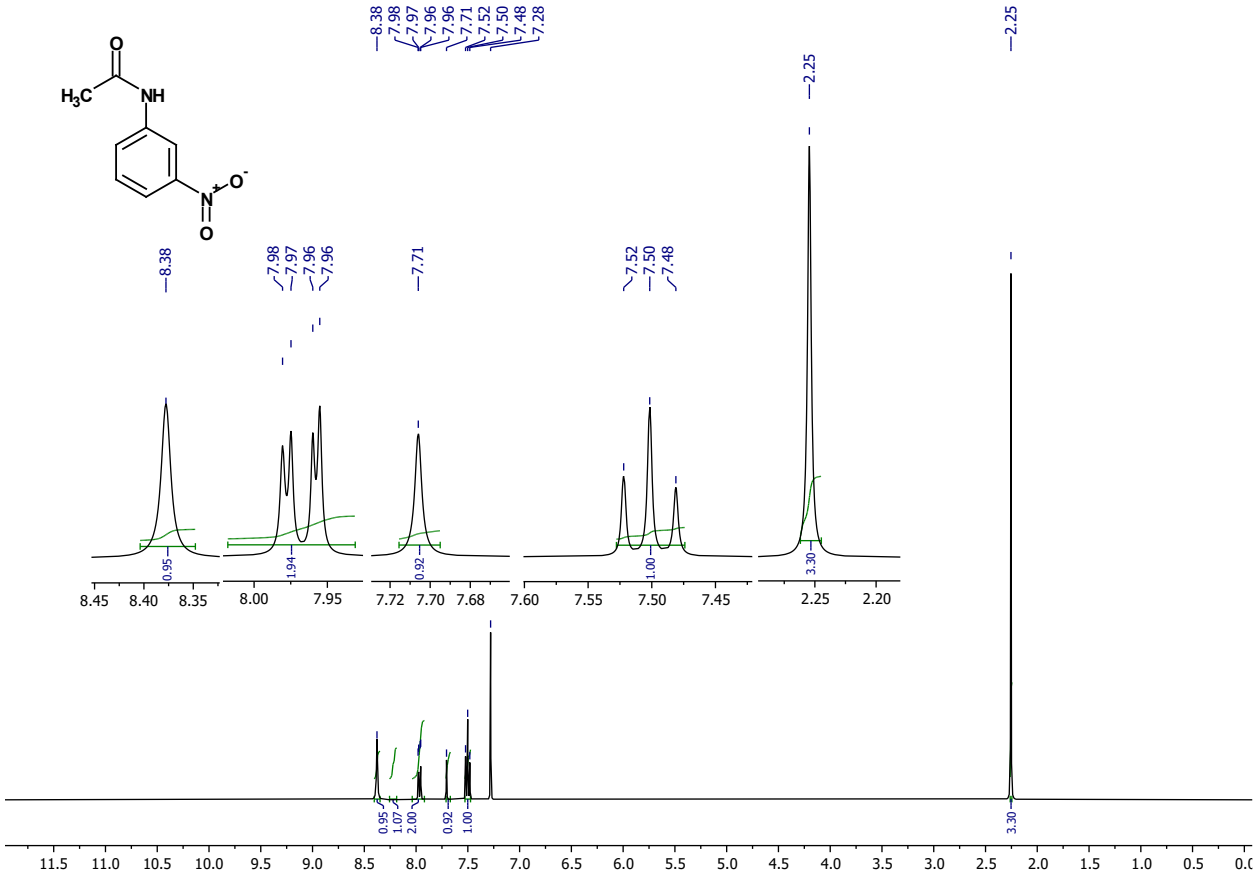


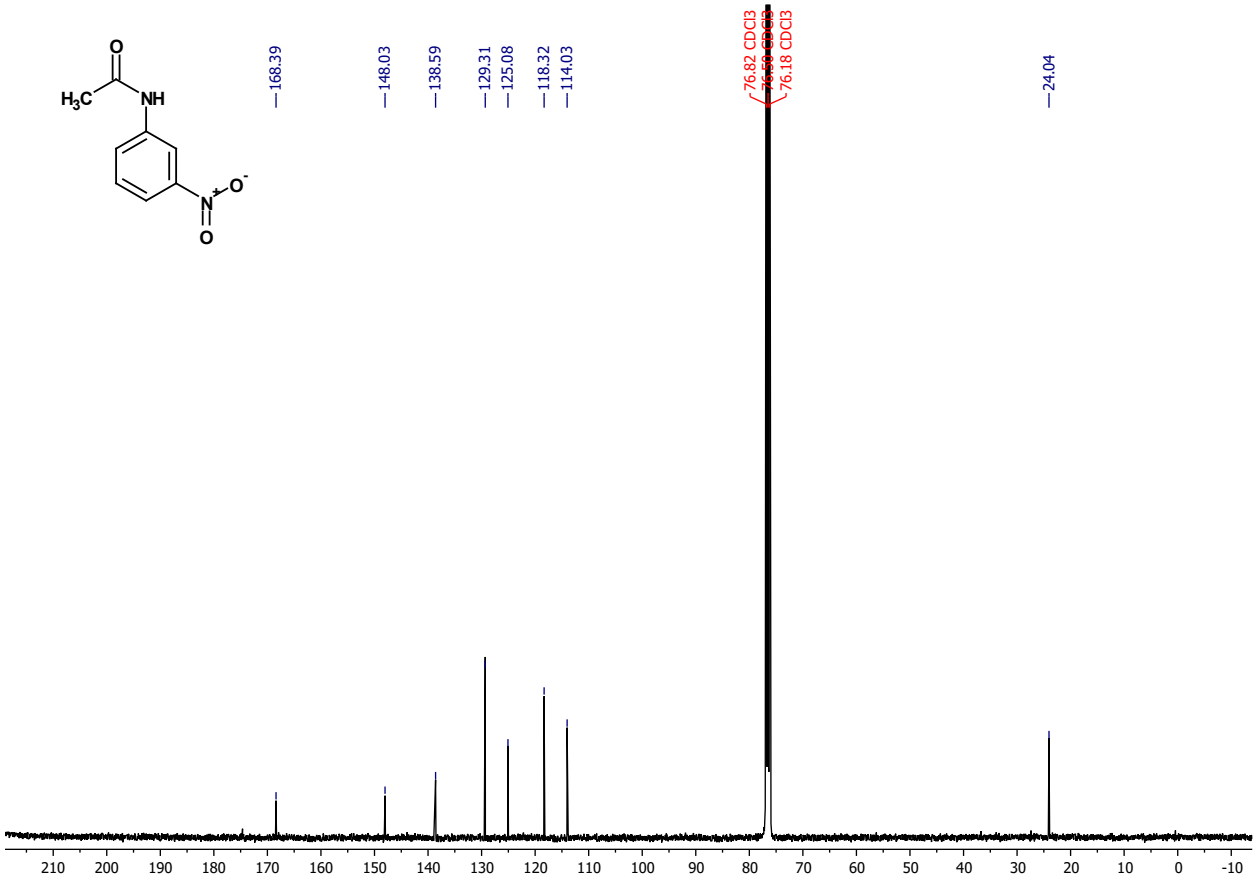
^{1}H and ^{13}C NMR *N*-(2-nitrophenyl)acetamide (**2m**-*a*)



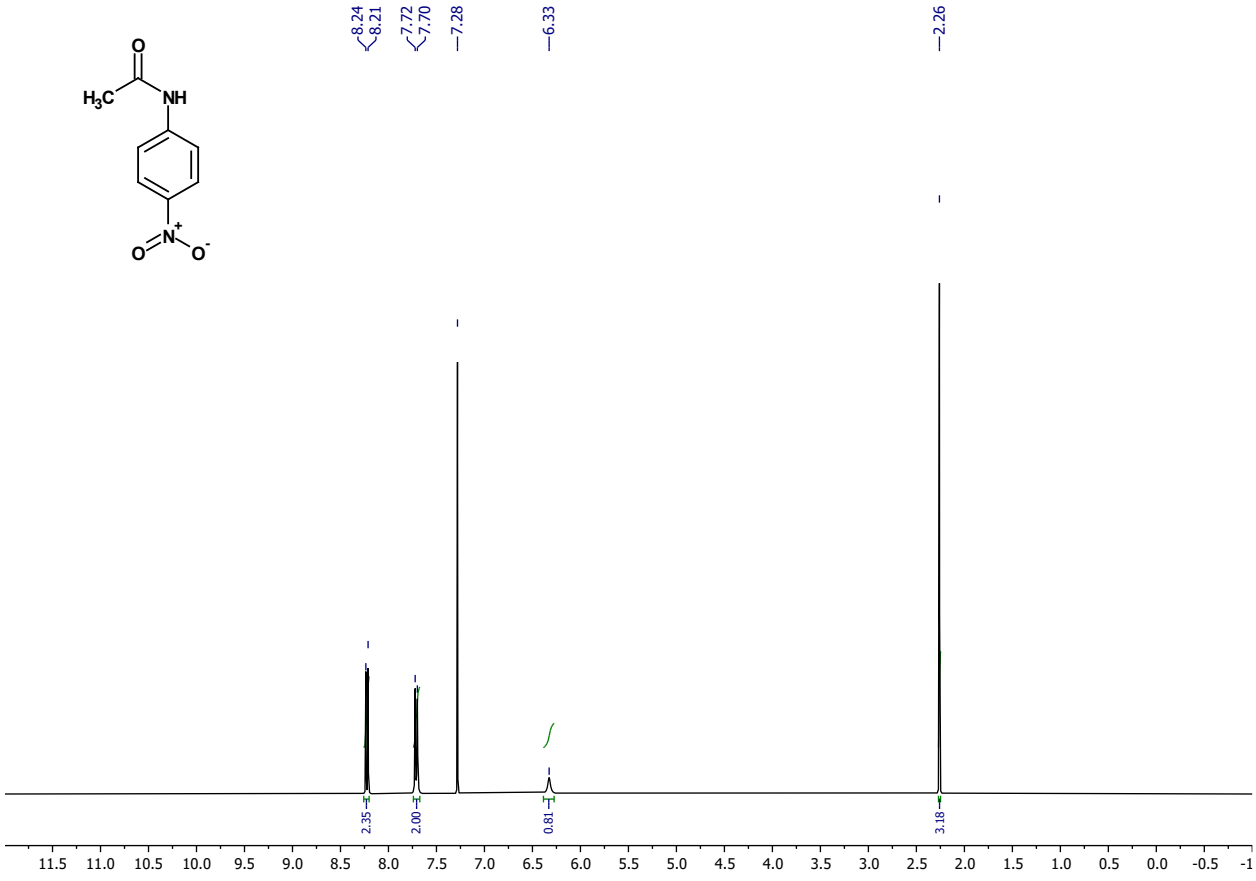


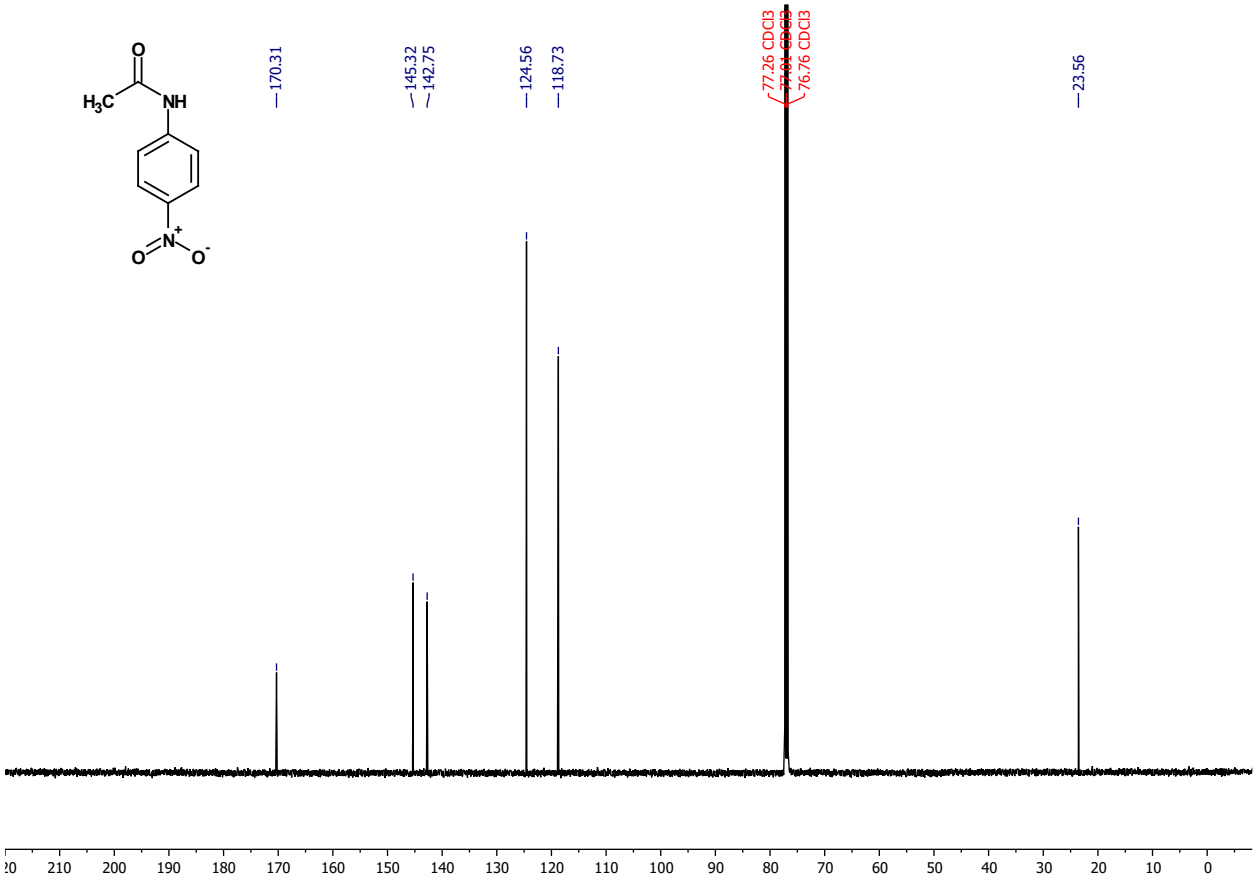
^{1}H and ^{13}C NMR *N*-(3-nitrophenyl)acetamide (**2m**-*b*)



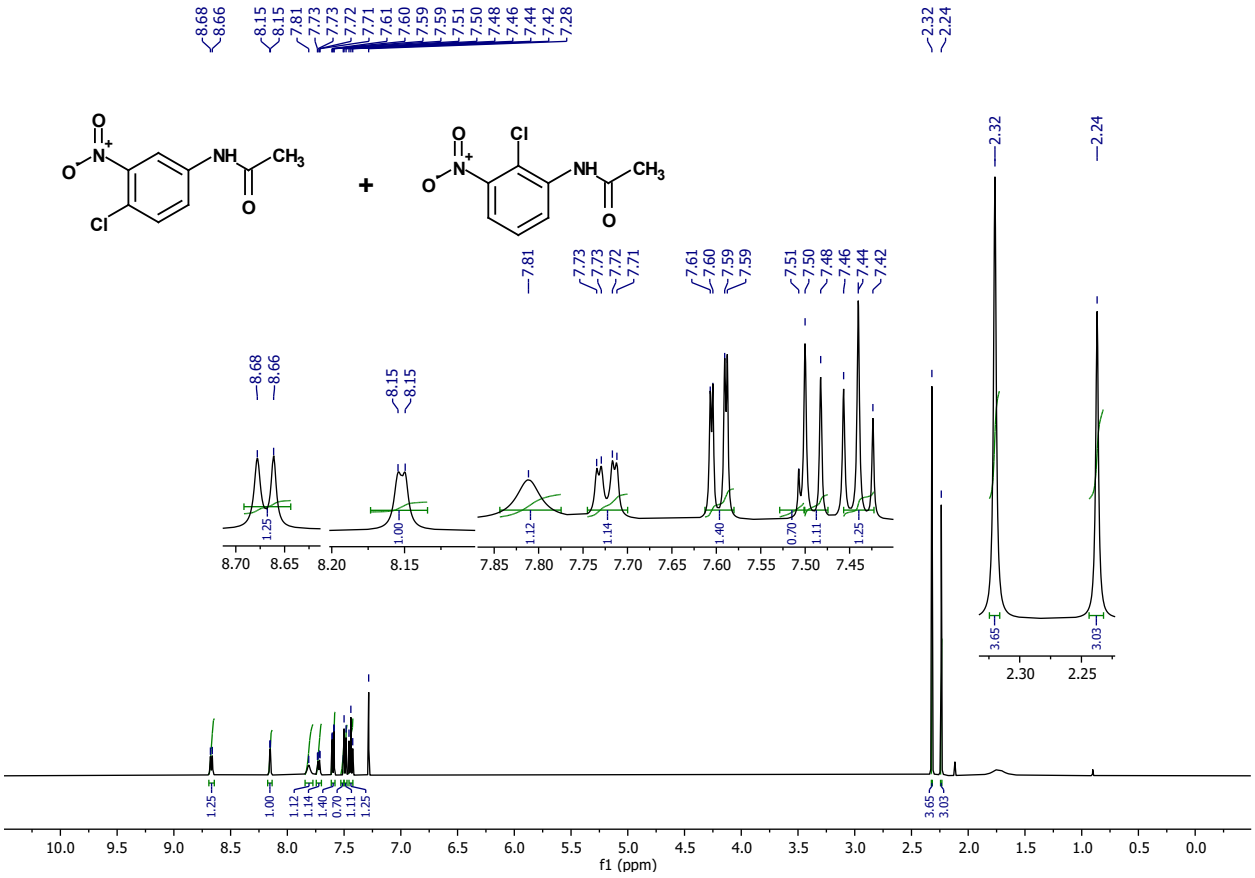


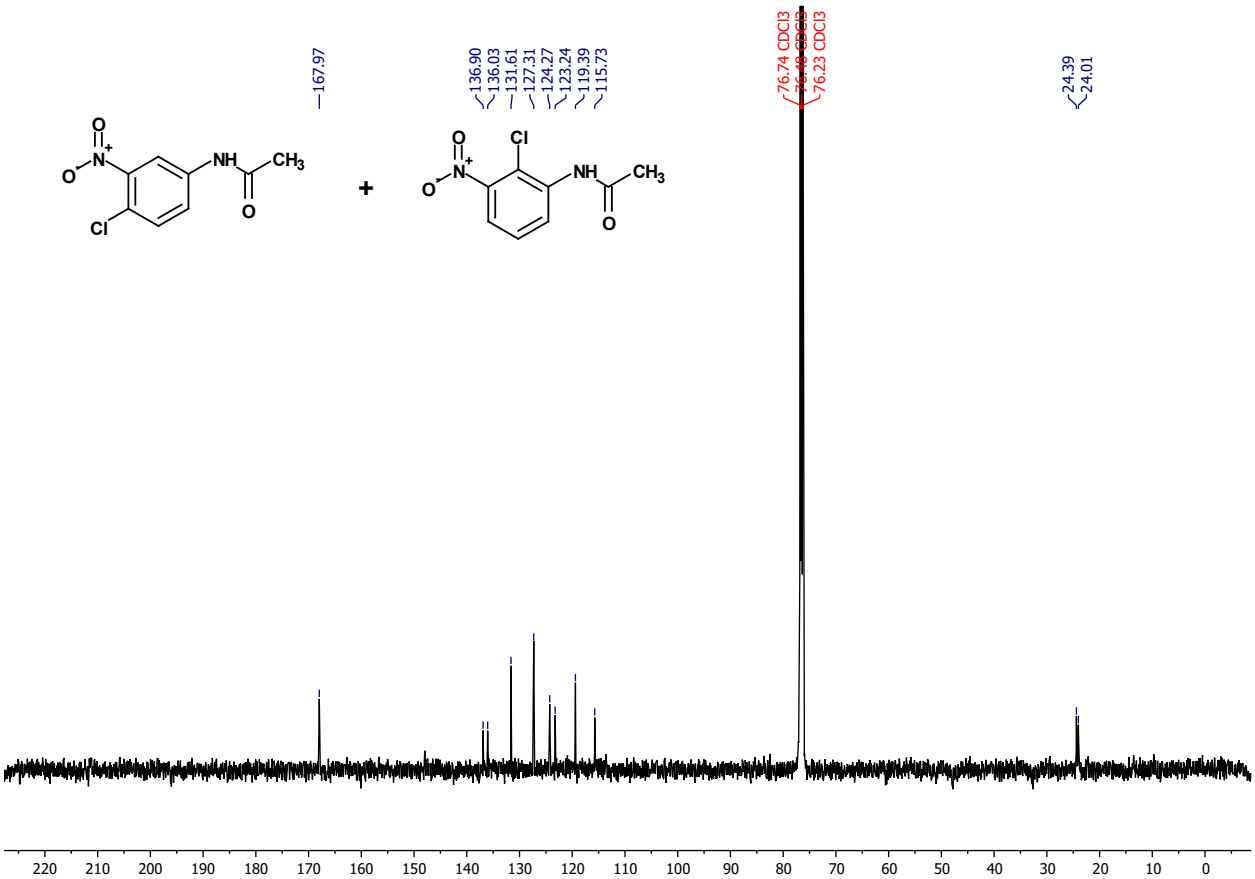
^{1}H and ^{13}C NMR *N*-(4-nitrophenyl)acetamide (**2m**-*c*)



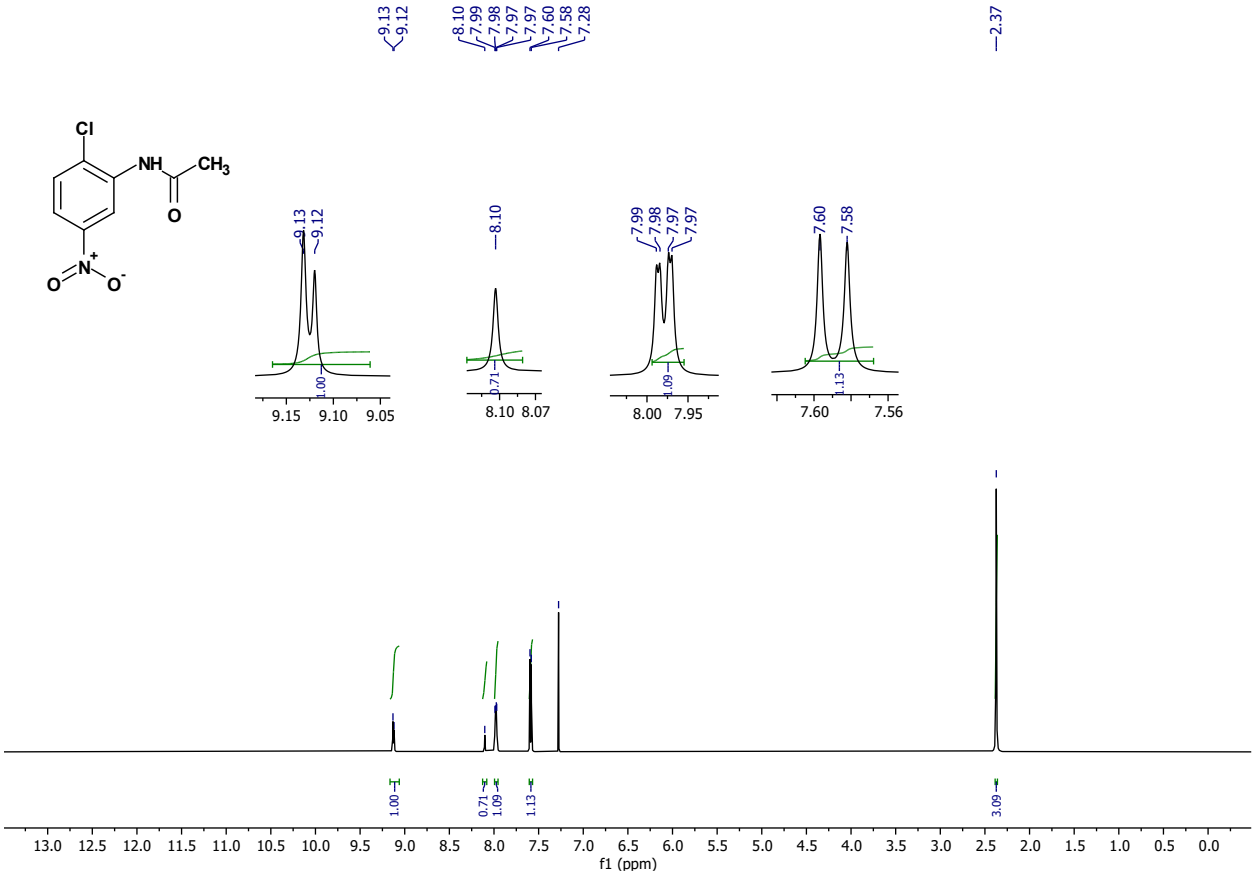


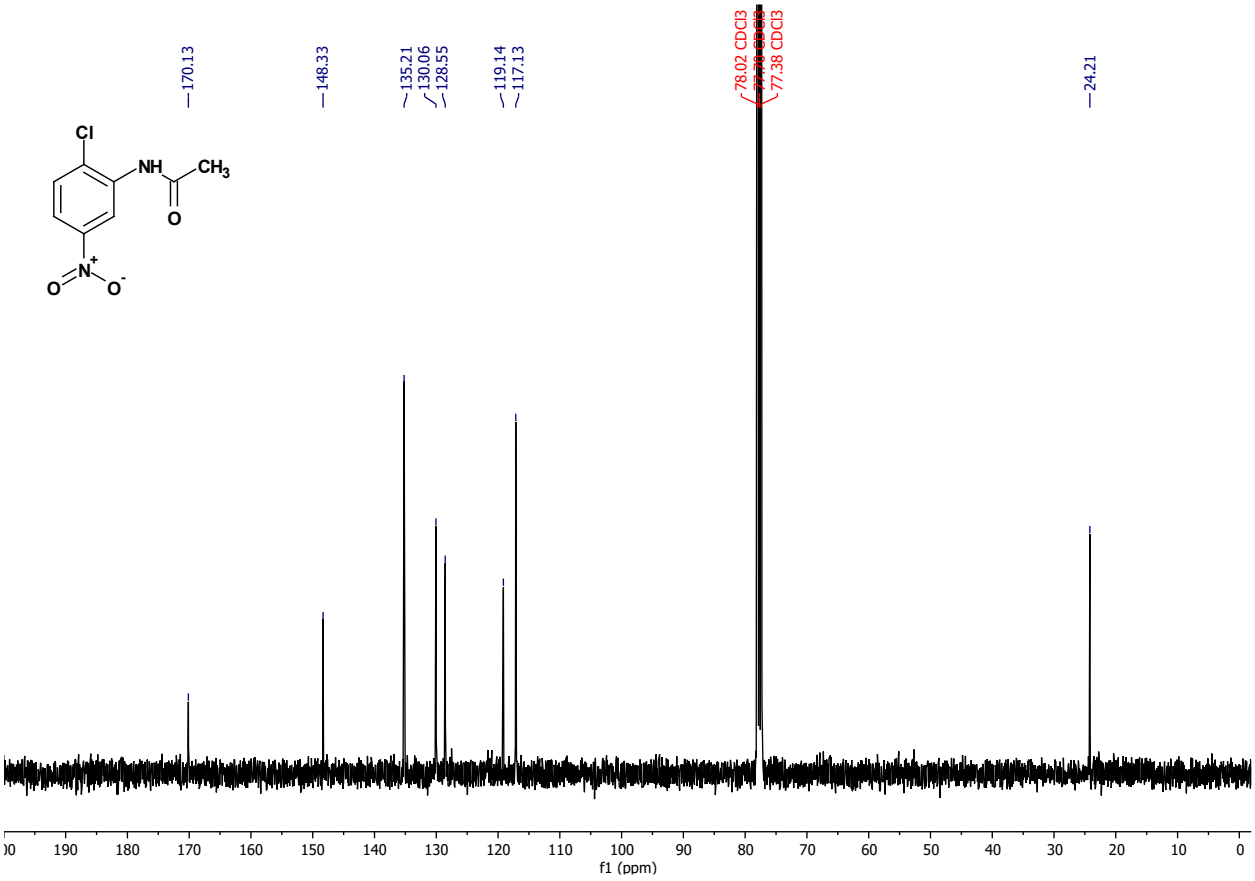
^{1}H and ^{13}C NMR *N*-(4-chloro-3-nitrophenyl)acetamide (**2n**-*a*) + *N*-(2-chloro-3-nitrophenyl)acetamide **(2n**-*b***)**



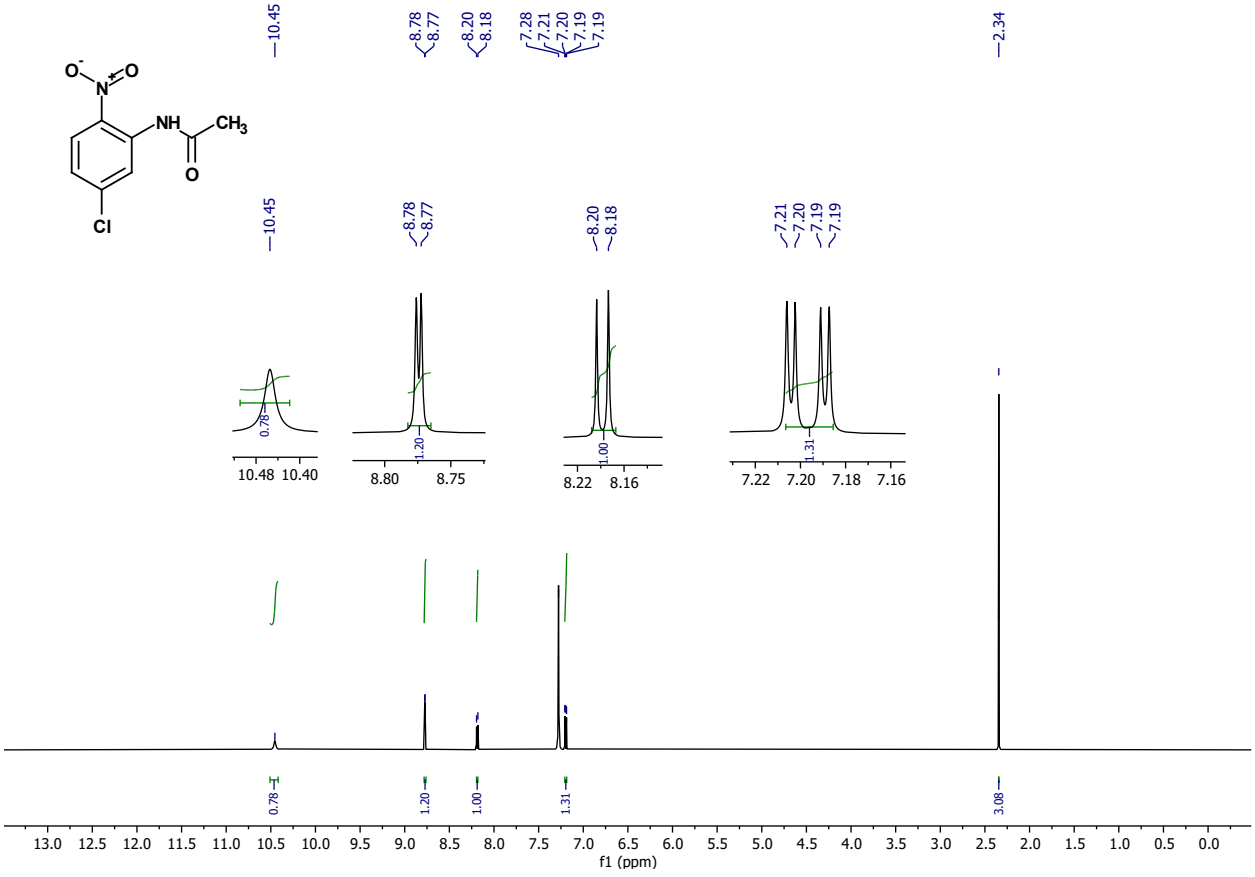


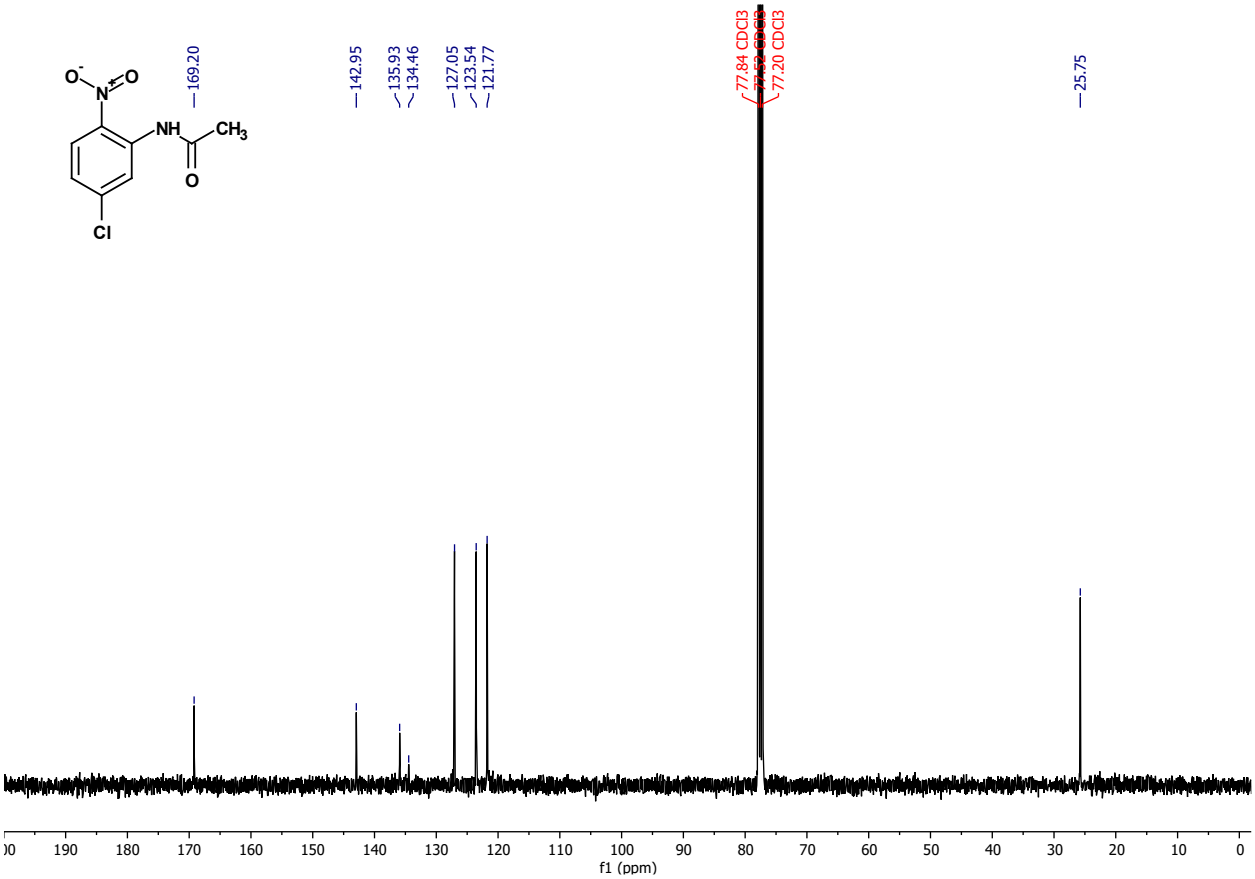
^{1}H and ^{13}C NMR *N*-(2-chloro-5-nitrophenyl)acetamide **(2o-*a*)**



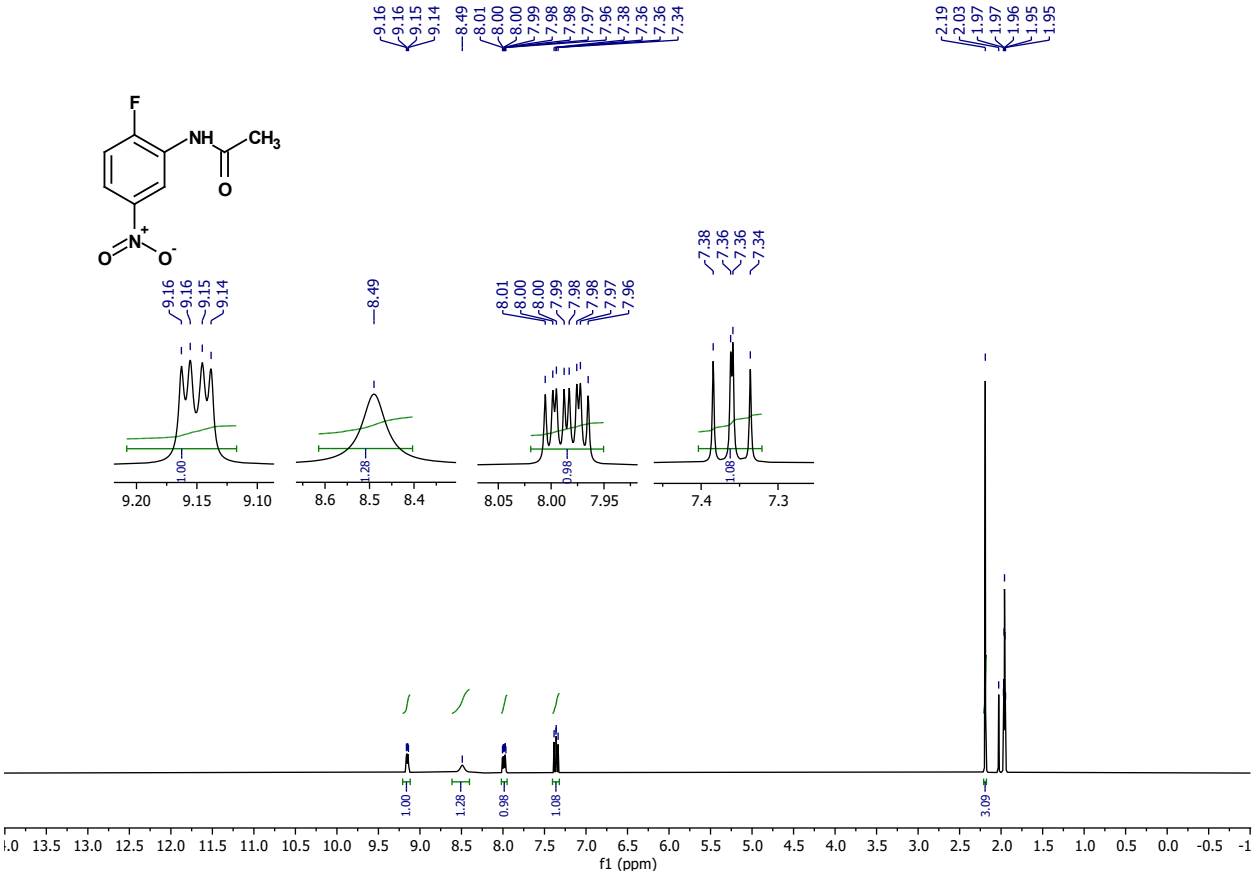


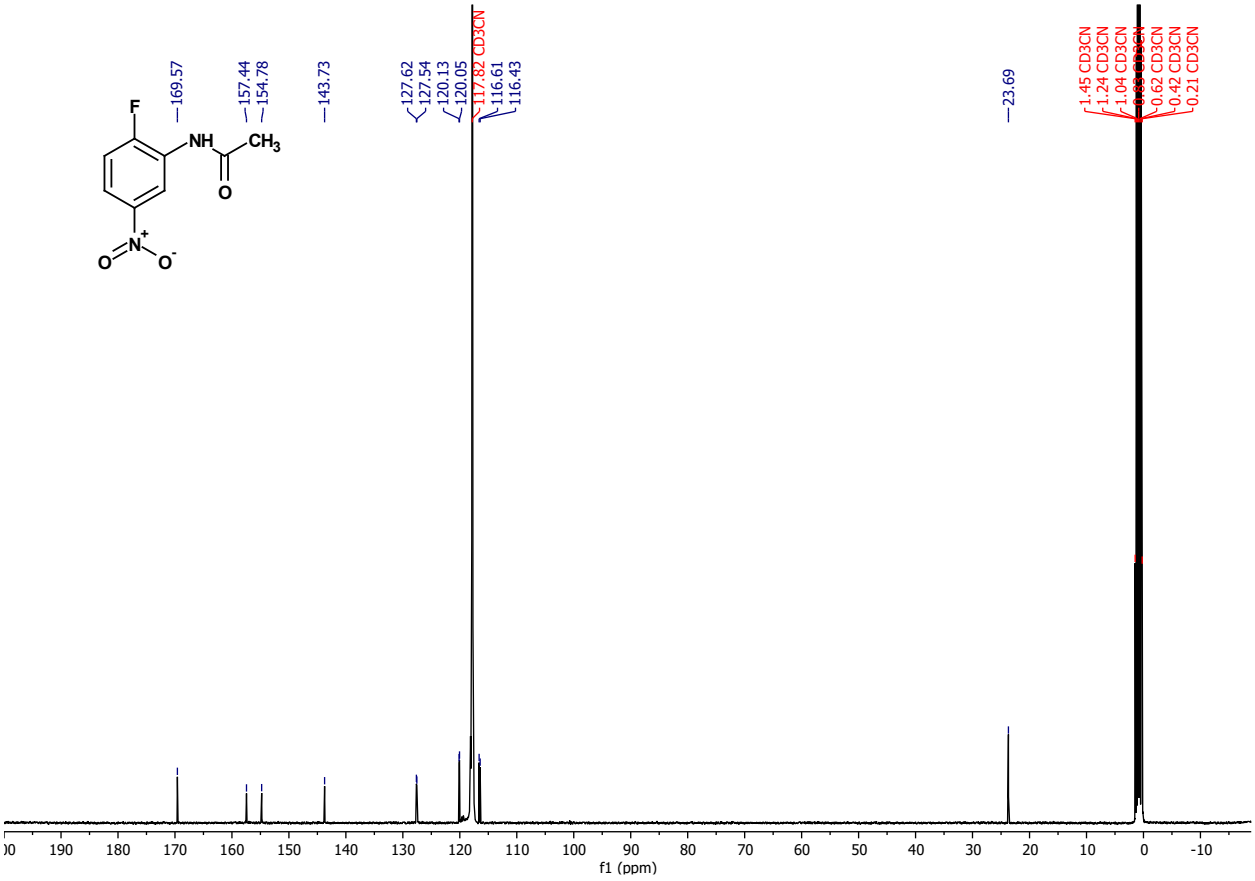
^{1}H and ^{13}C NMR *N*-(5-chloro-2-nitrophenyl)acetamide (**2o**-*b*)



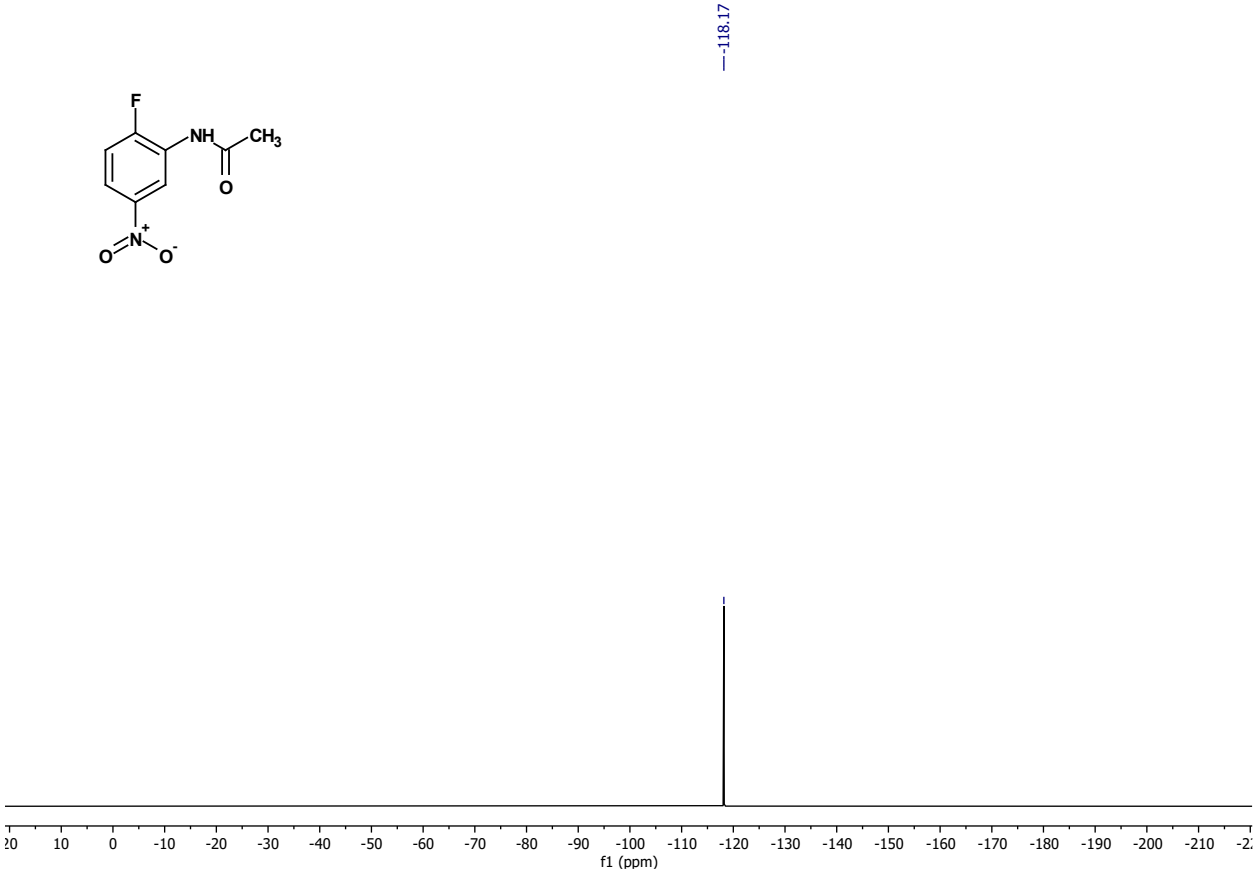


^{1}H and ^{13}C NMR *N*-(2-fluoro-5-nitrophenyl)acetamide **(2p)**

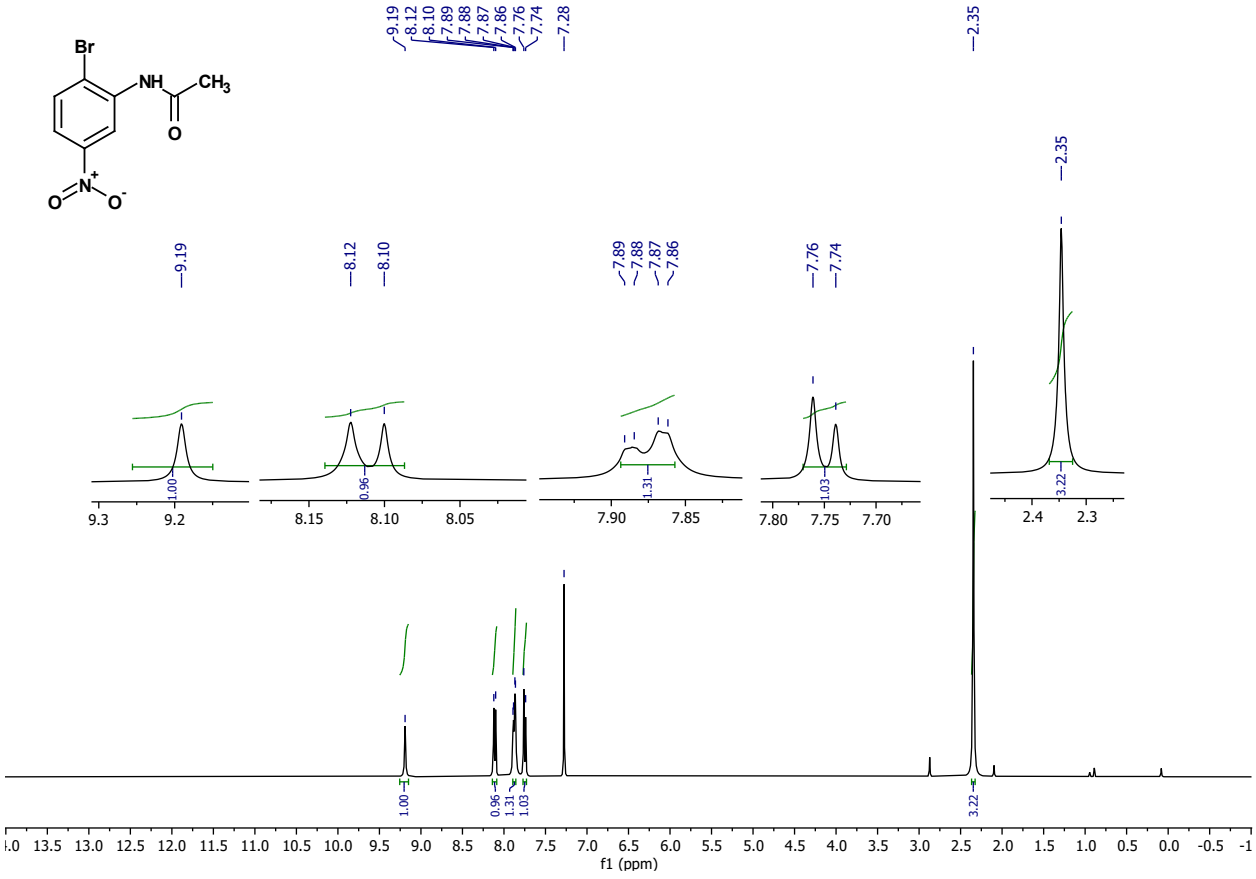


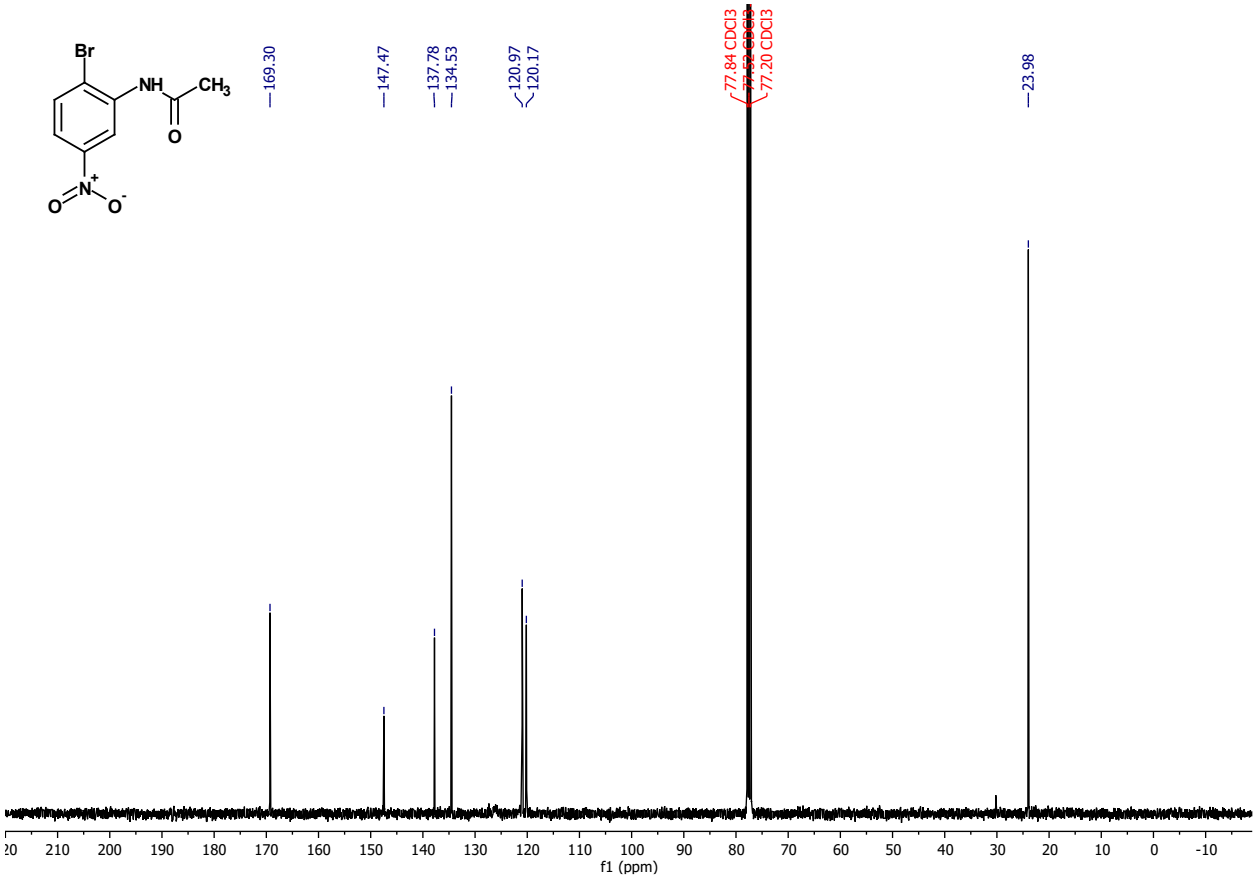


^{19}F NMR *N*-(2-fluoro-5-nitrophenyl)acetamide **(2p)**

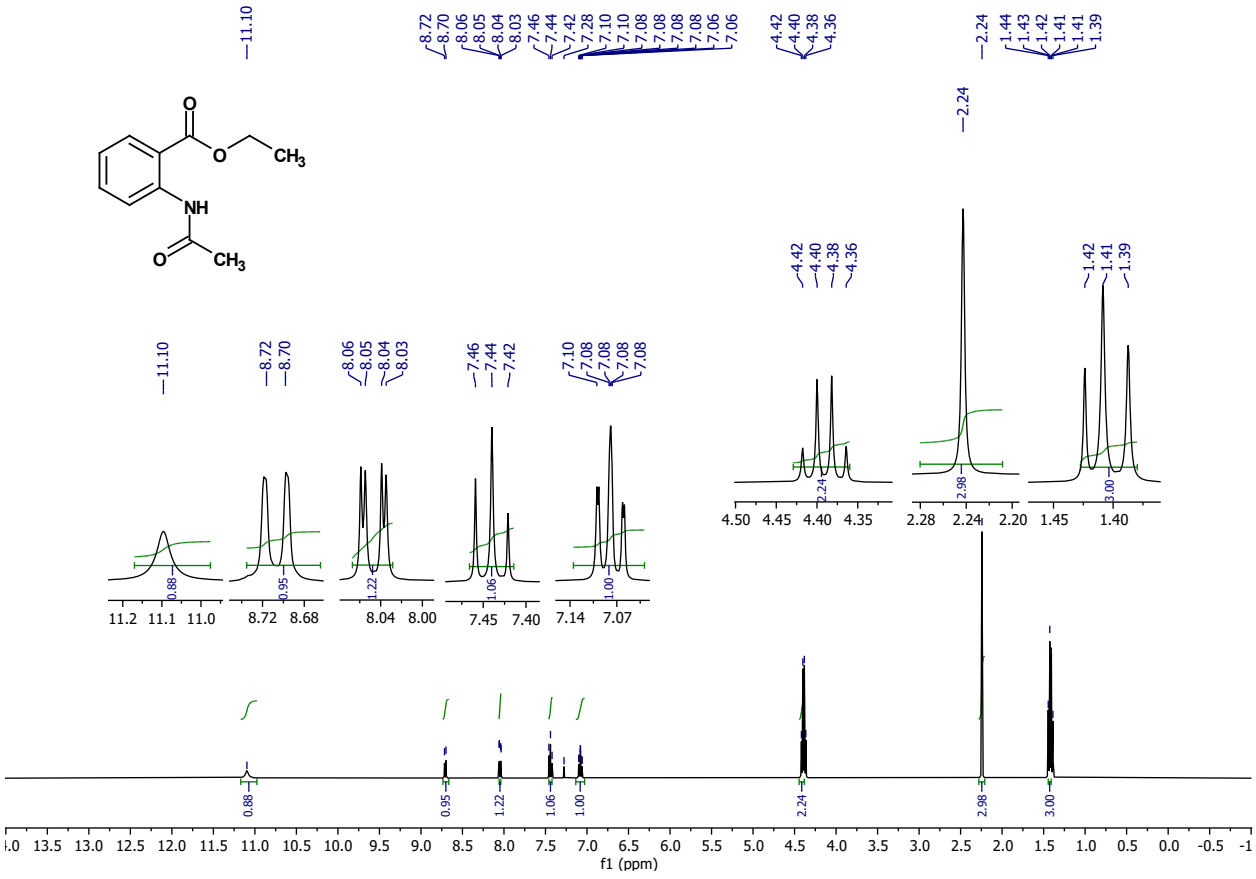


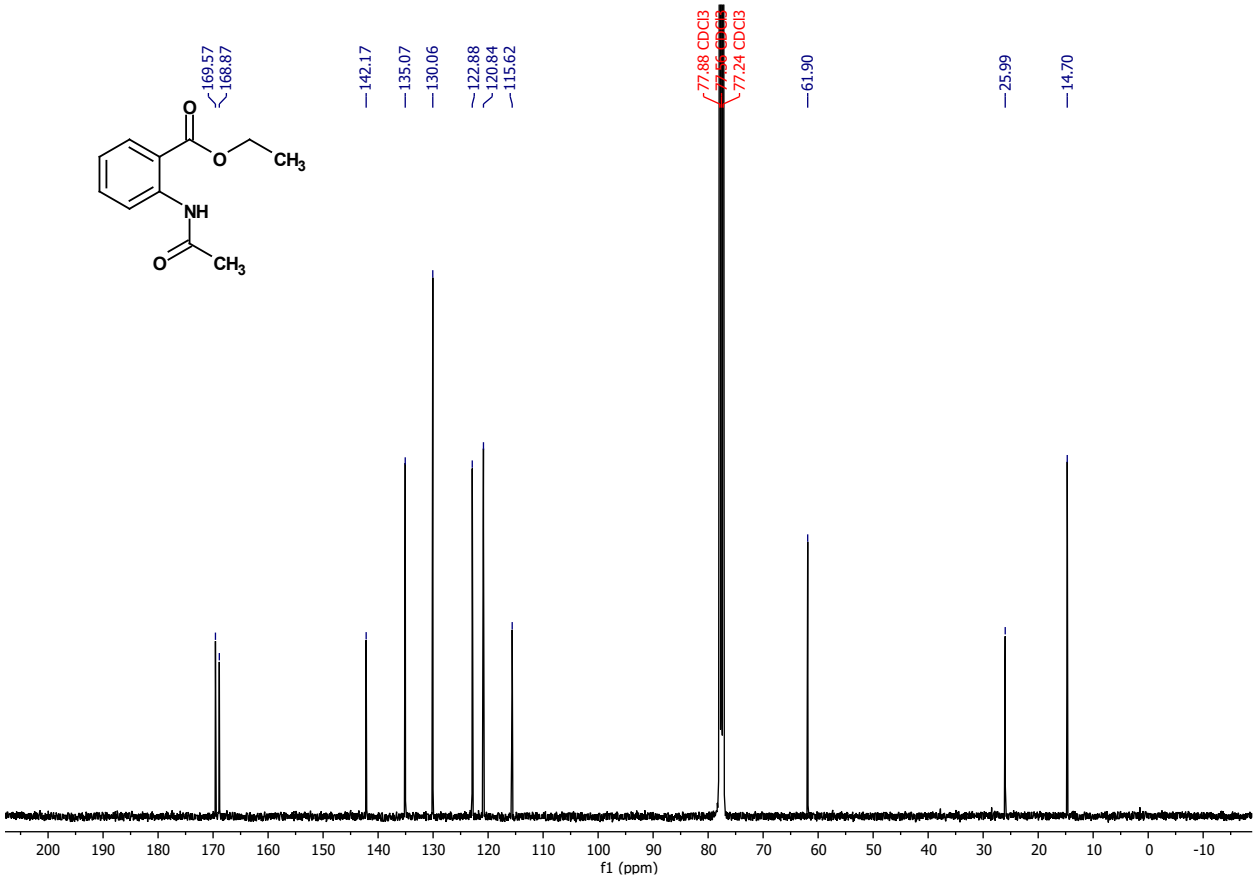
^{1}H and ^{13}C NMR *N*-(2-bromo-5-nitrophenyl) acetamide **(2q)**



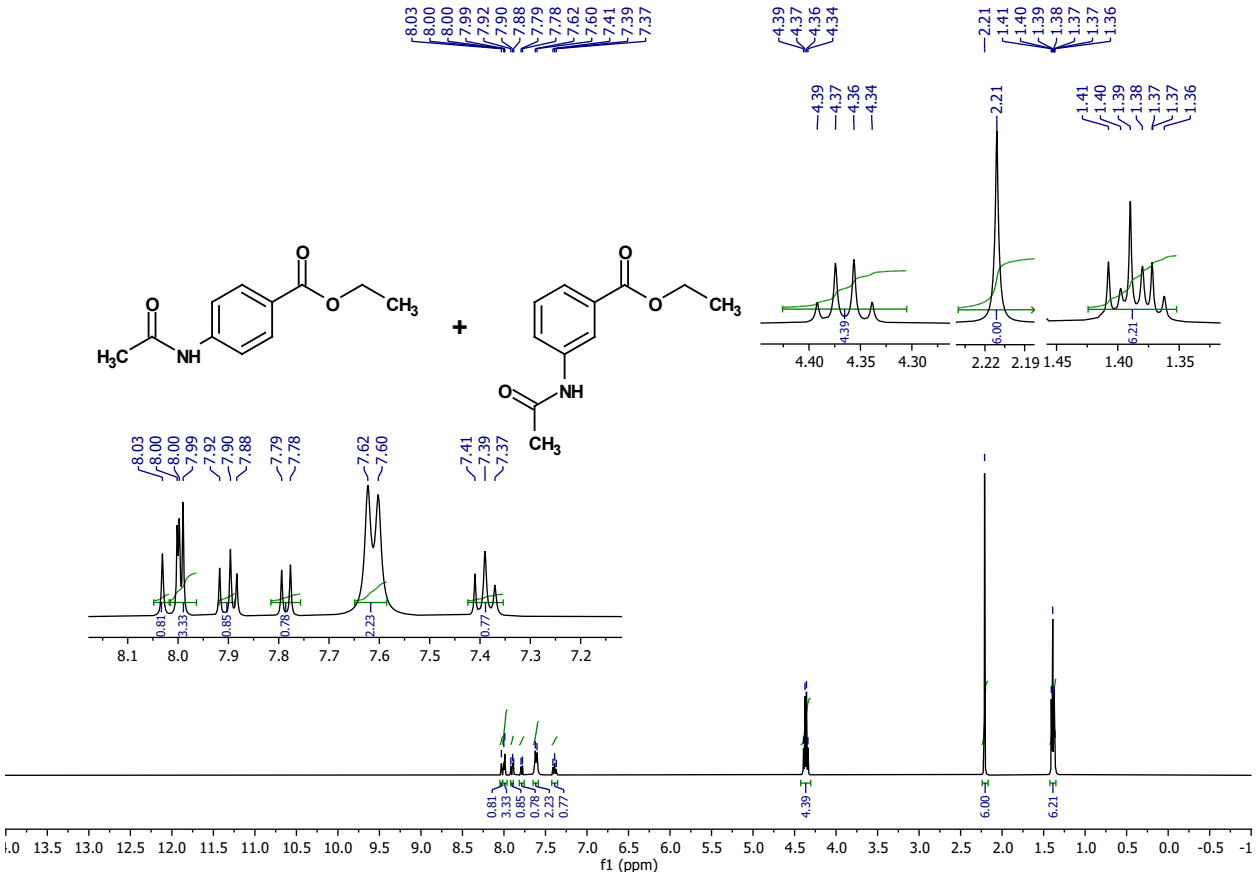


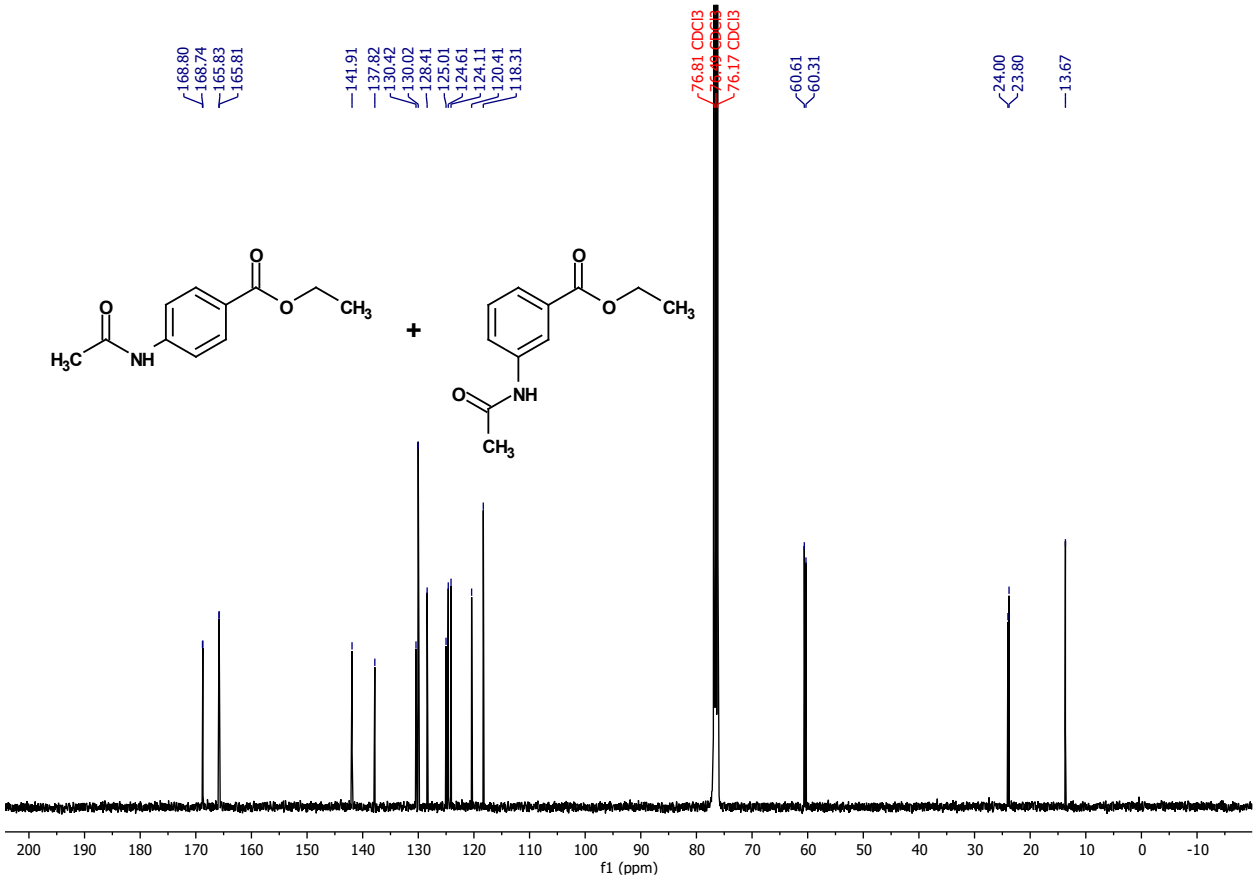
^{1}H and ^{13}C NMR Ethyl 2-acetamidobenzoate (**2r**-*a*)



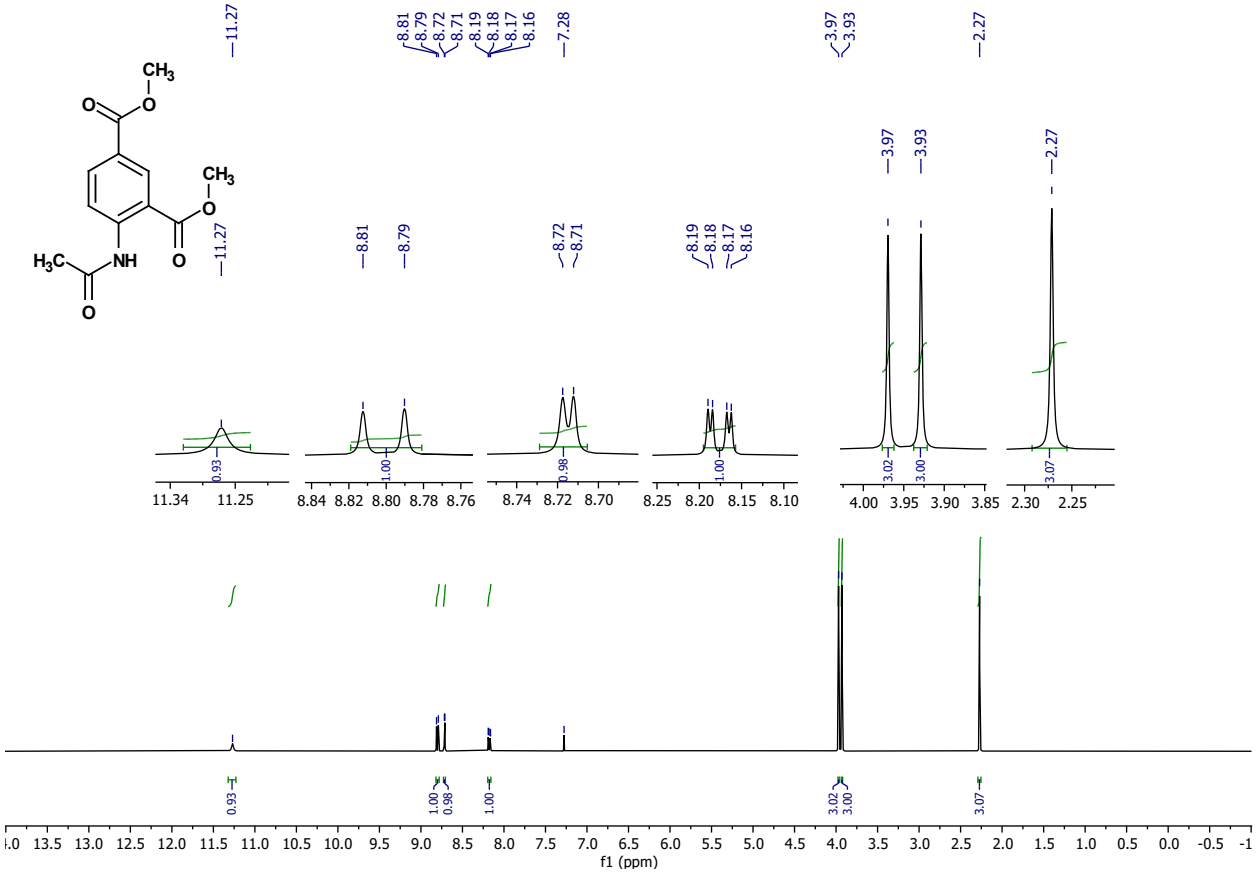


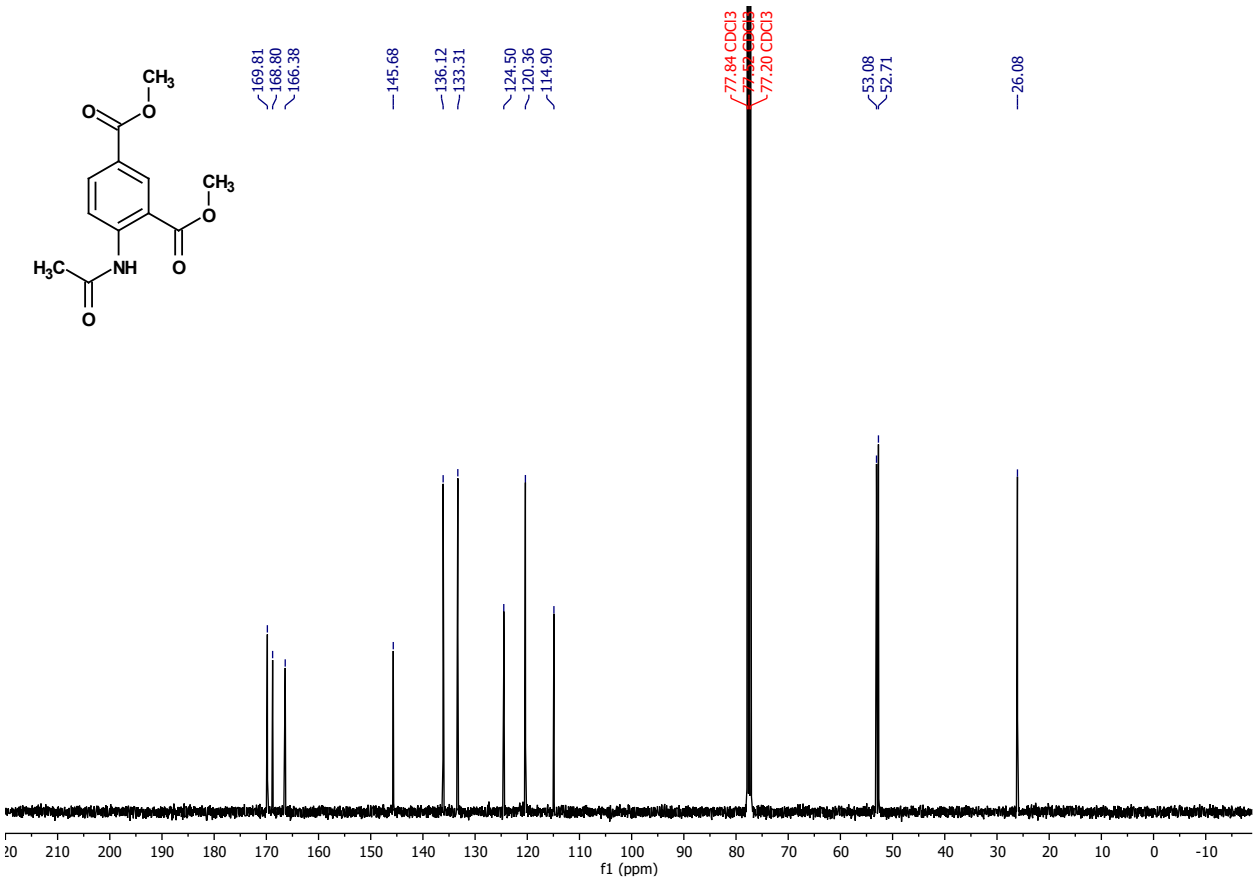
^{1}H and ^{13}C NMR Ethyl 3-acetamidobenzoate (**2r**-*b*) + Ethyl 4-((methoxycarbonyl)amino)benzoate (**2r**-*c*)



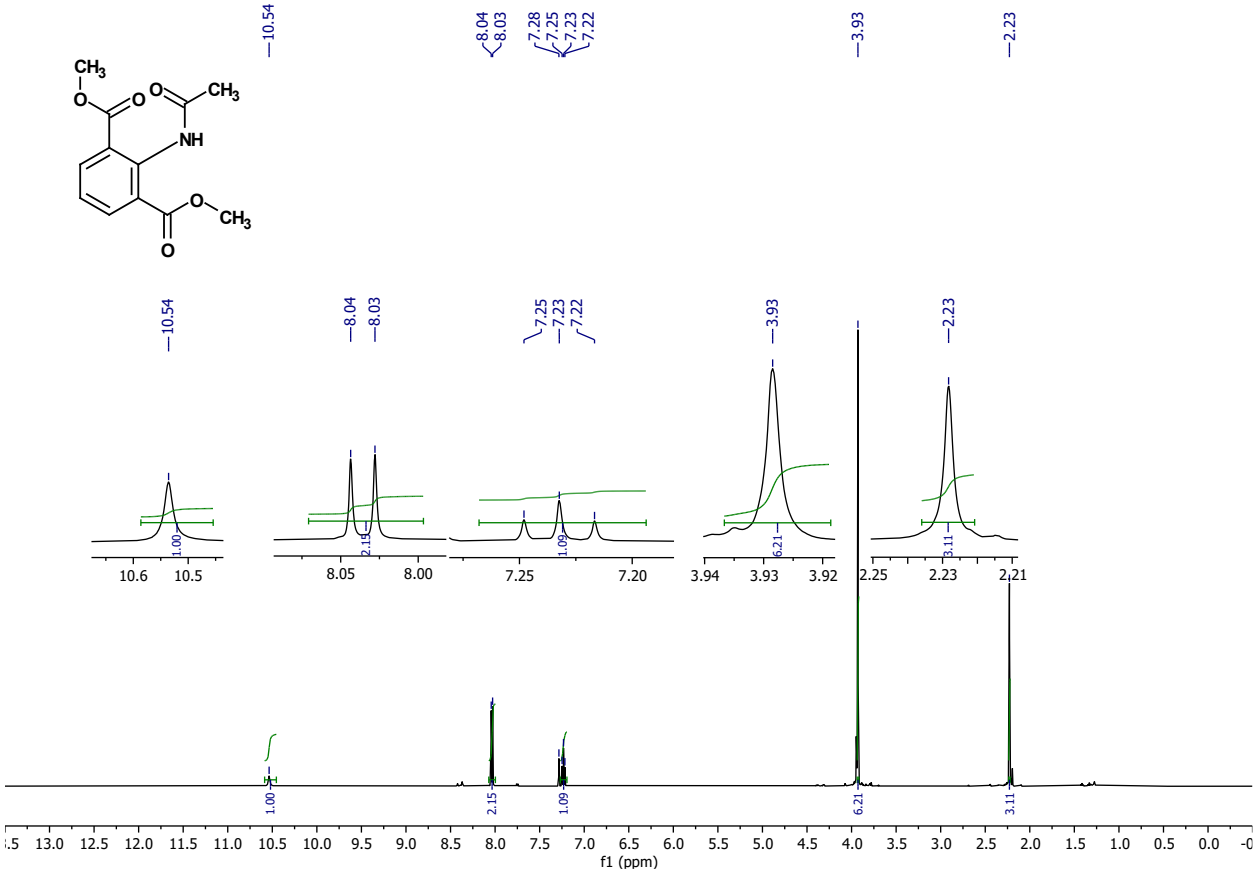


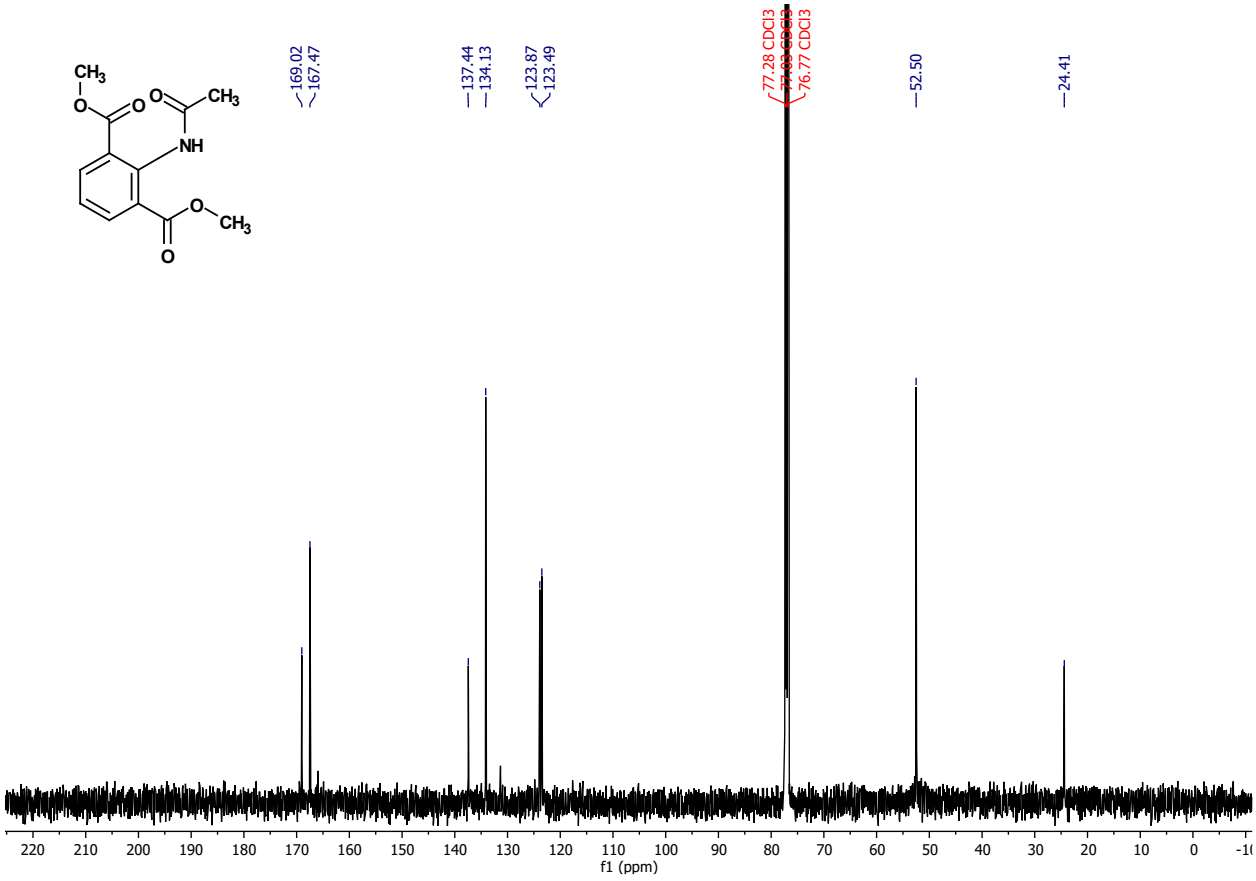
^{1}H and ^{13}C NMR Dimethyl 4-acetamidoisophthalate **(2s-*a*)**



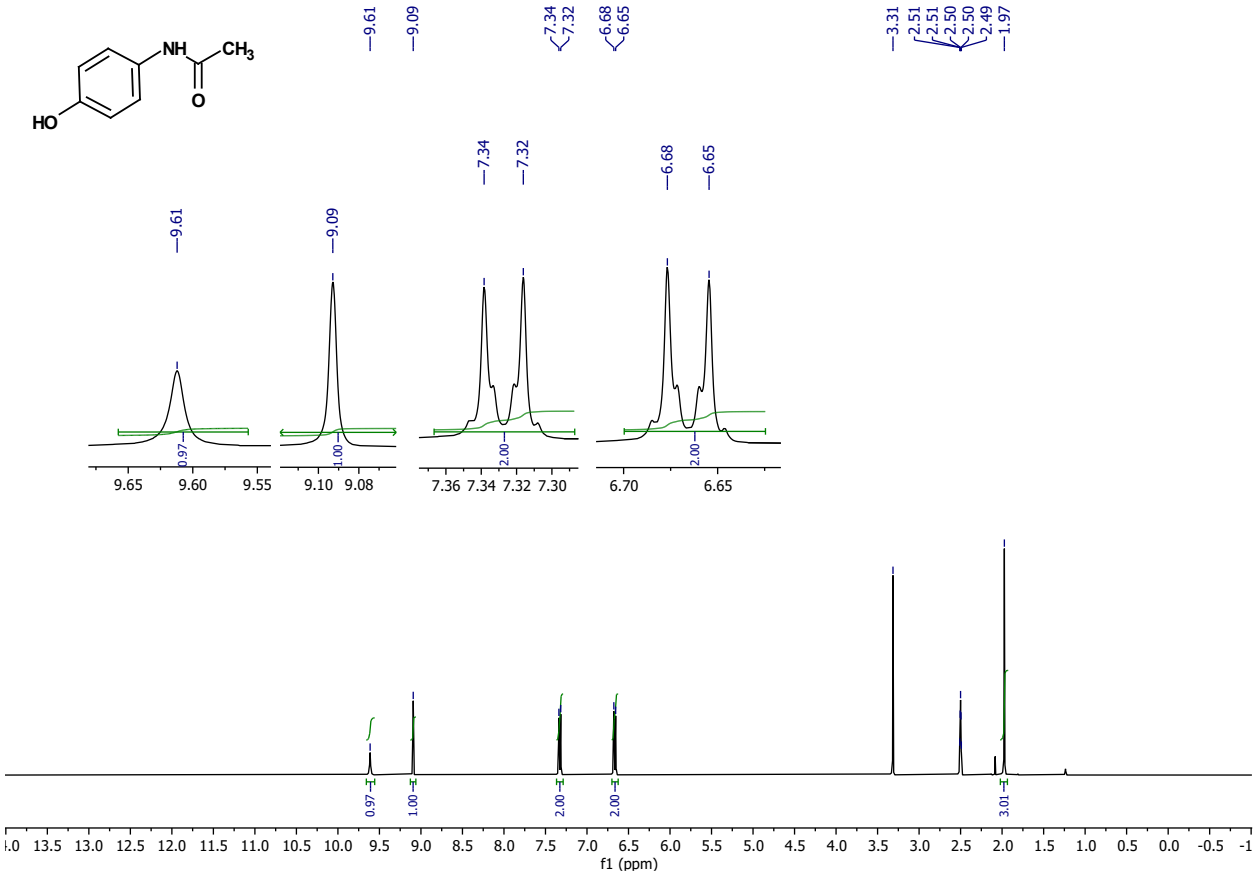


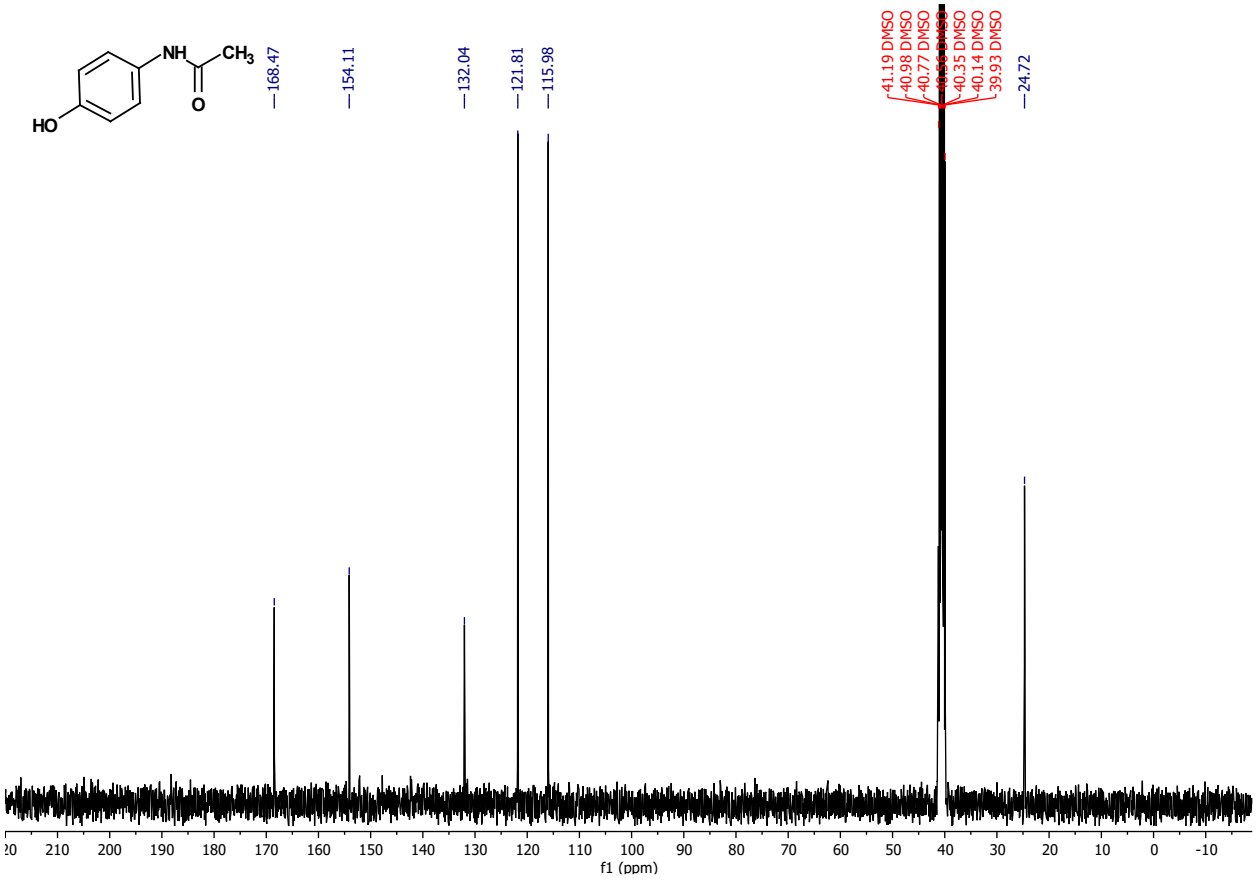
^{1}H and ^{13}C NMR Dimethyl 2-acetamidoisophthalate **(2s-*b*)**



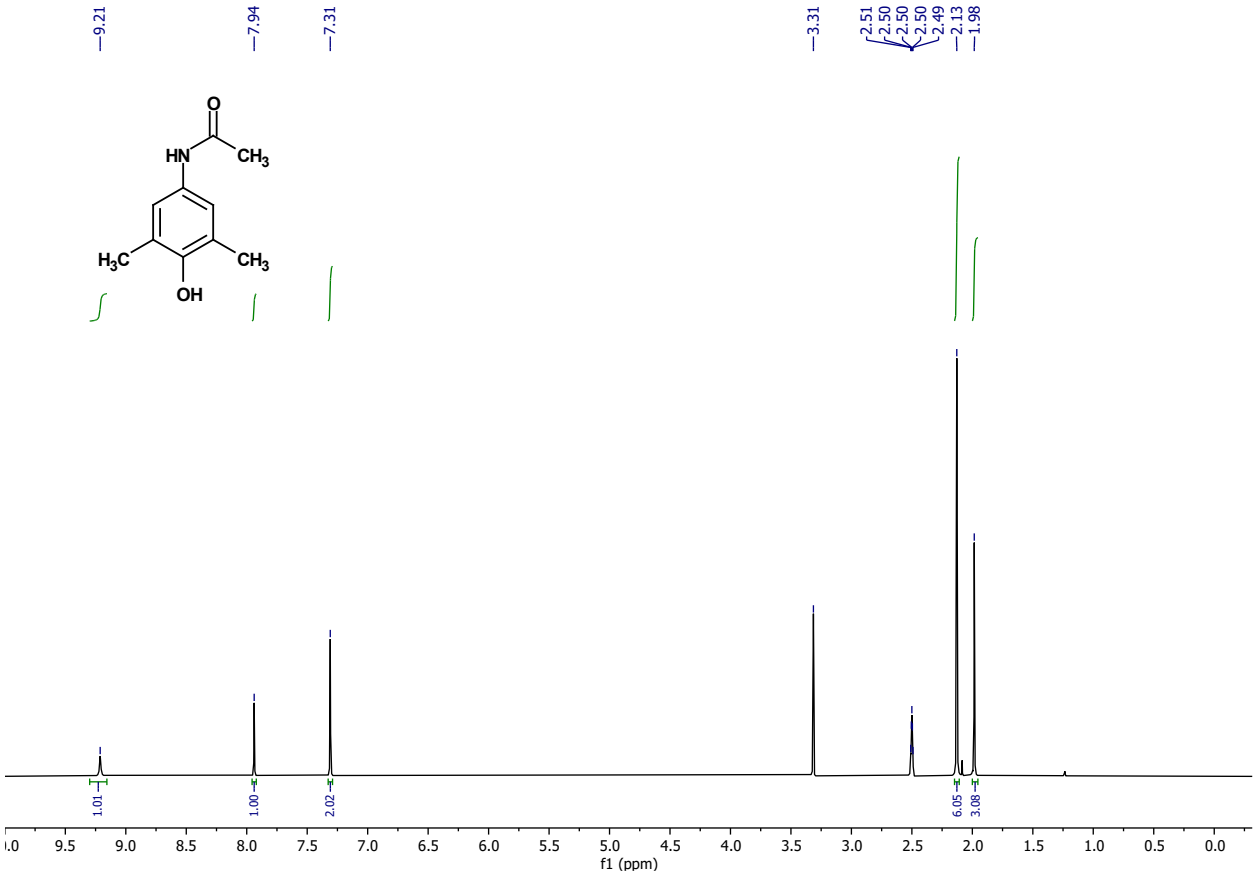


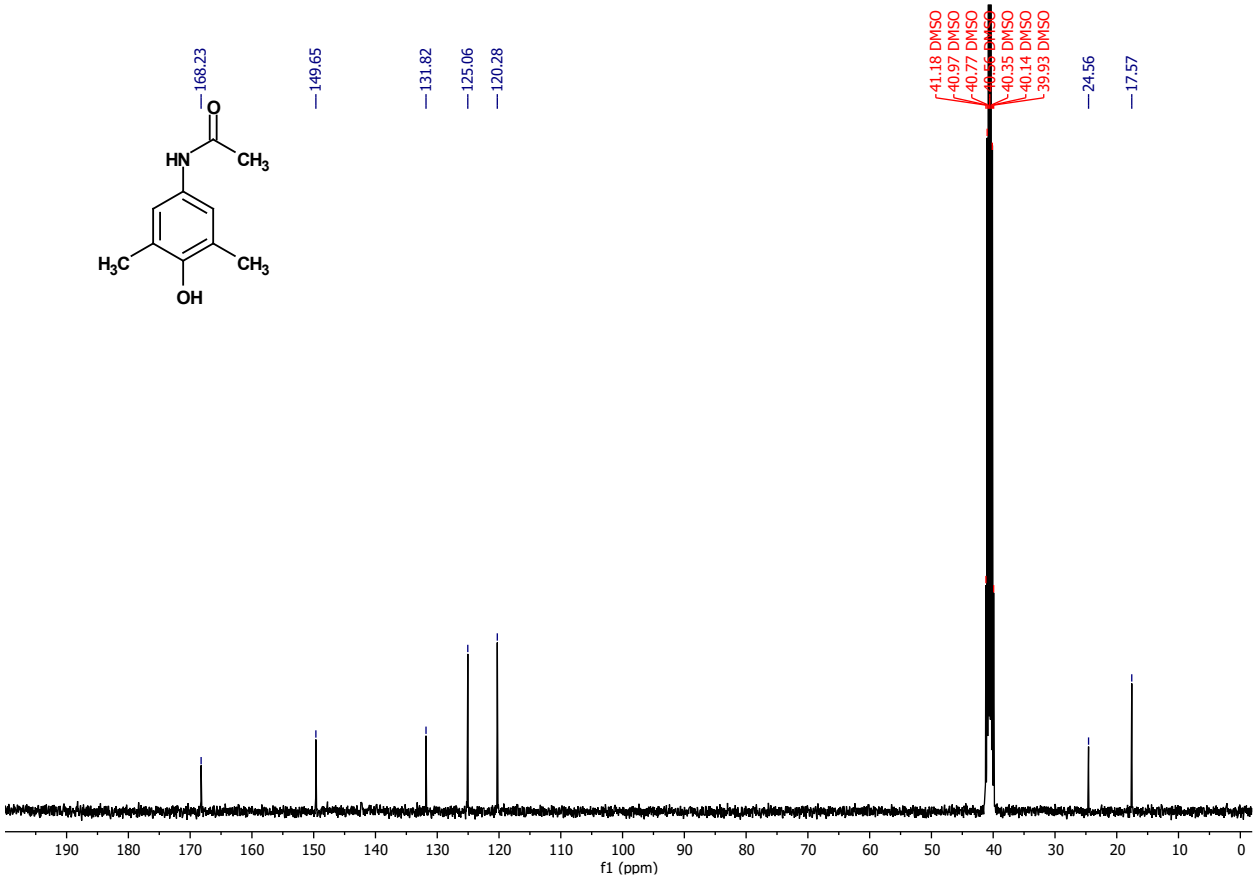
^{1}H and ^{13}C NMR *N*-(4-hydroxyphenyl)acetamide (**2t**)



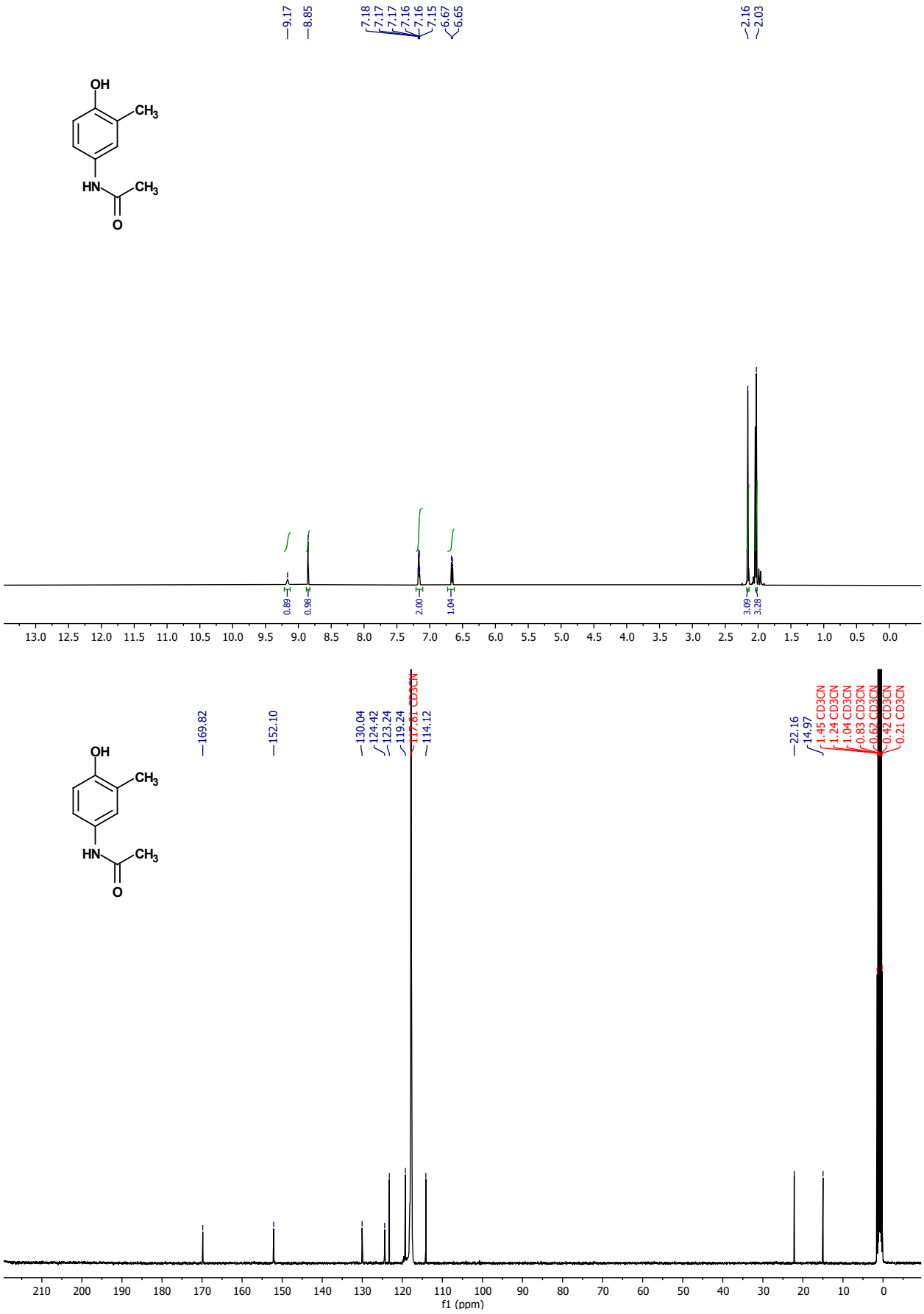


^{1}H and ^{13}C NMR *N*-(4-hydroxy-3,5-dimethylphenyl)acetamide **(2u)**

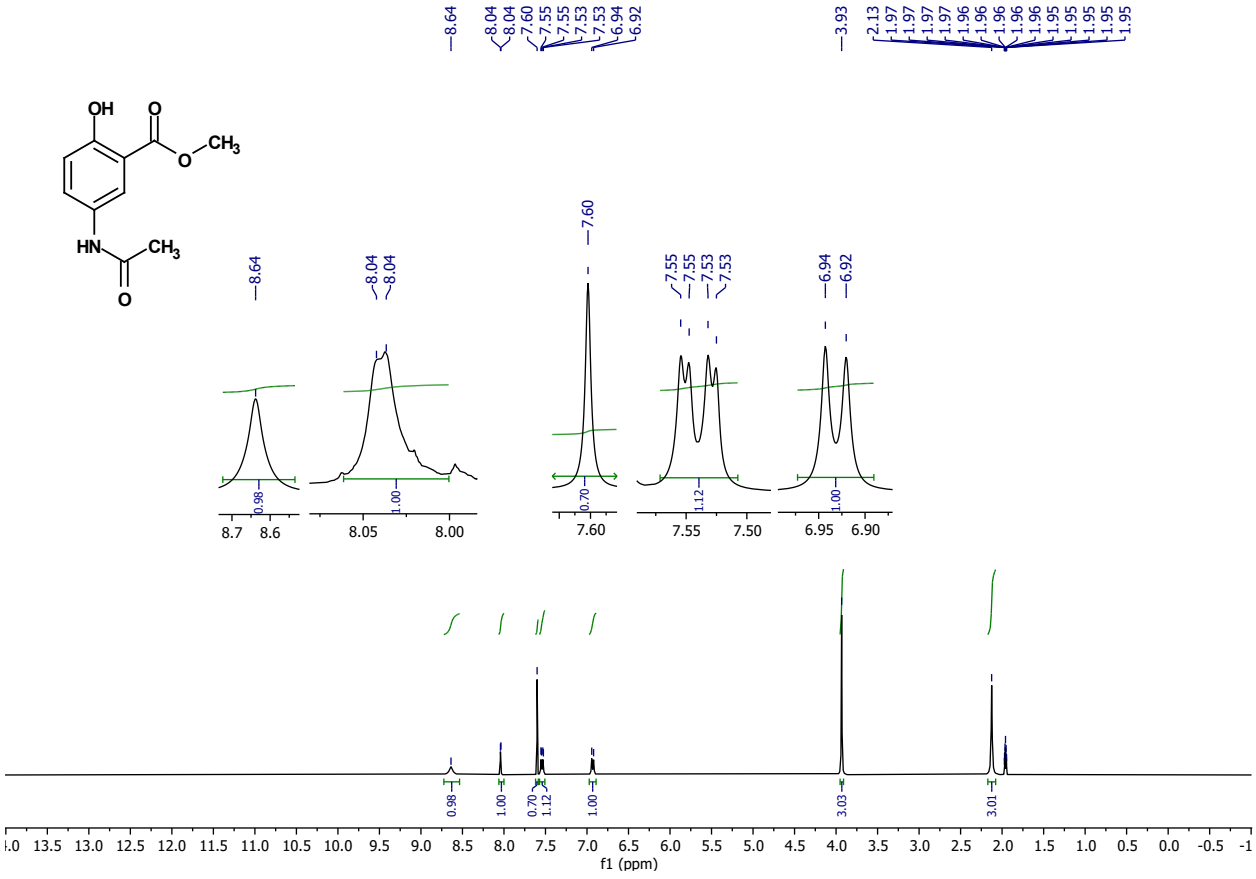


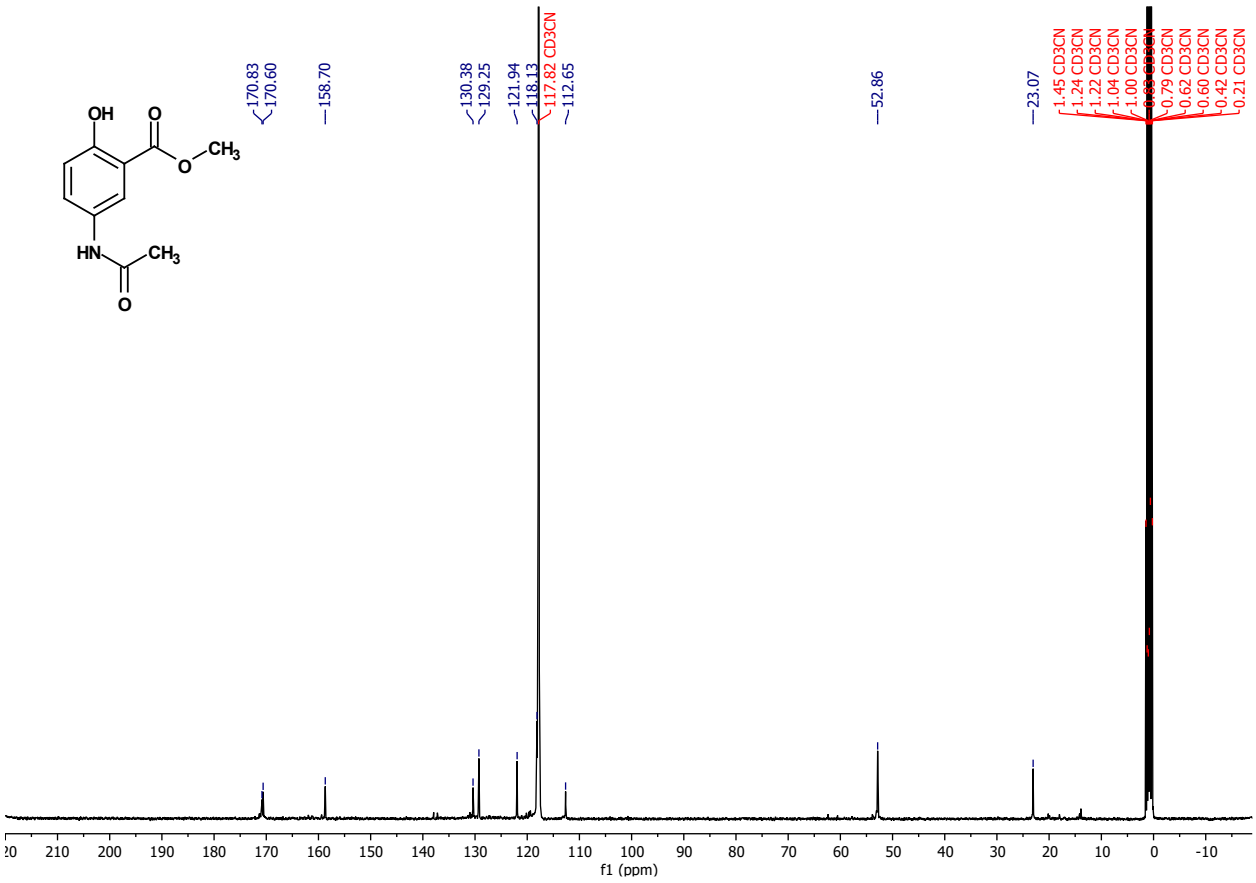


^{1}H and ^{13}C NMR *N*-(4-hydroxy-3-methylphenyl)acetamide **(2v)**

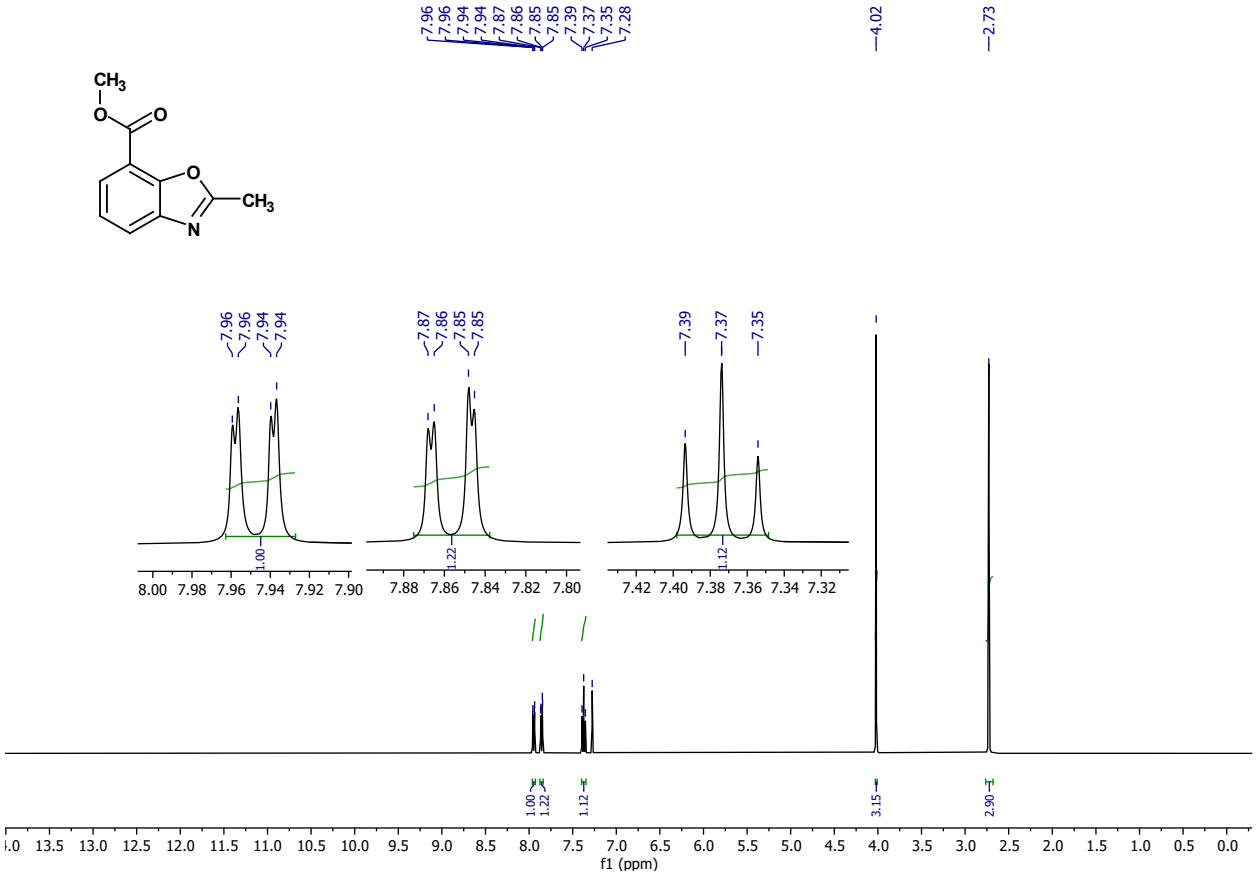


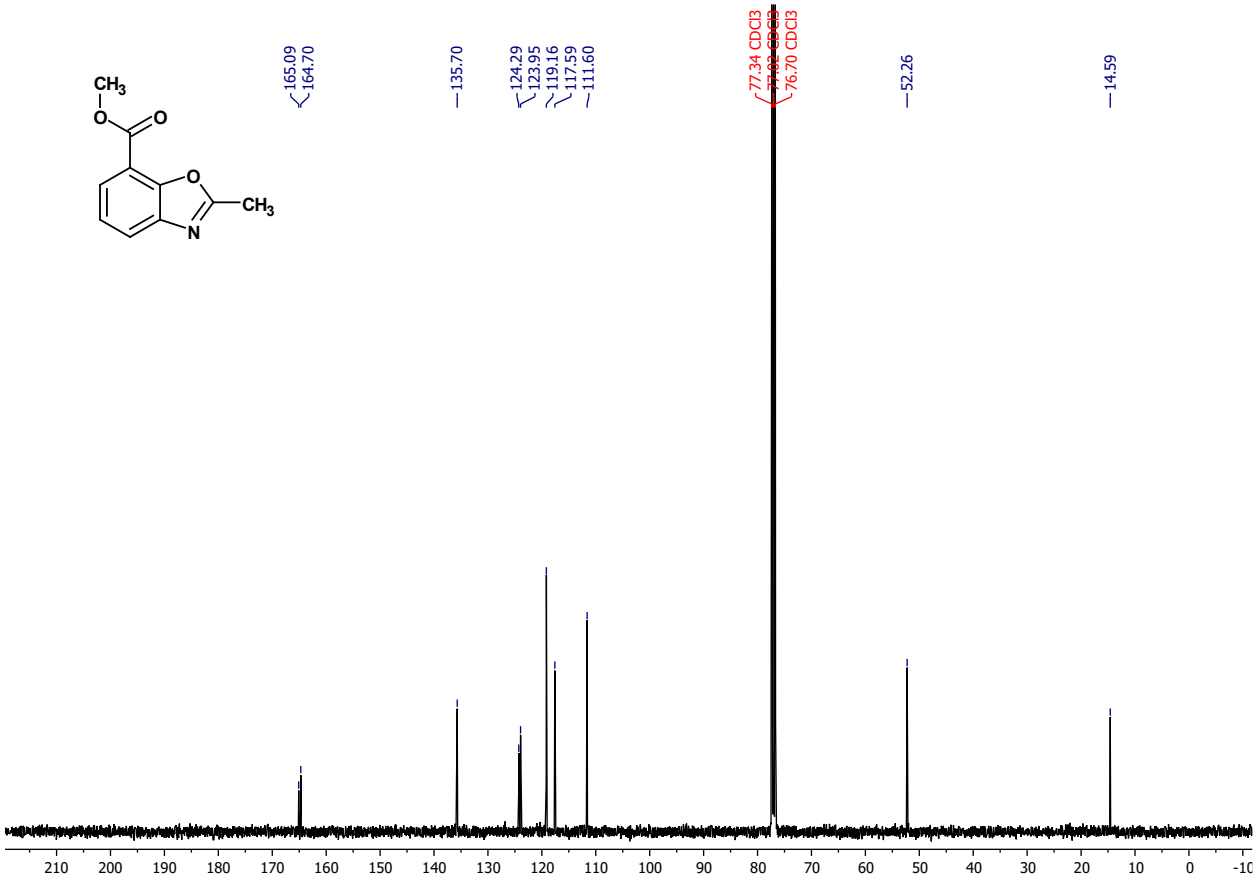
^{1}H and ^{13}C NMR Methyl 5-acetamido-2-hydroxybenzoate **(2w)**



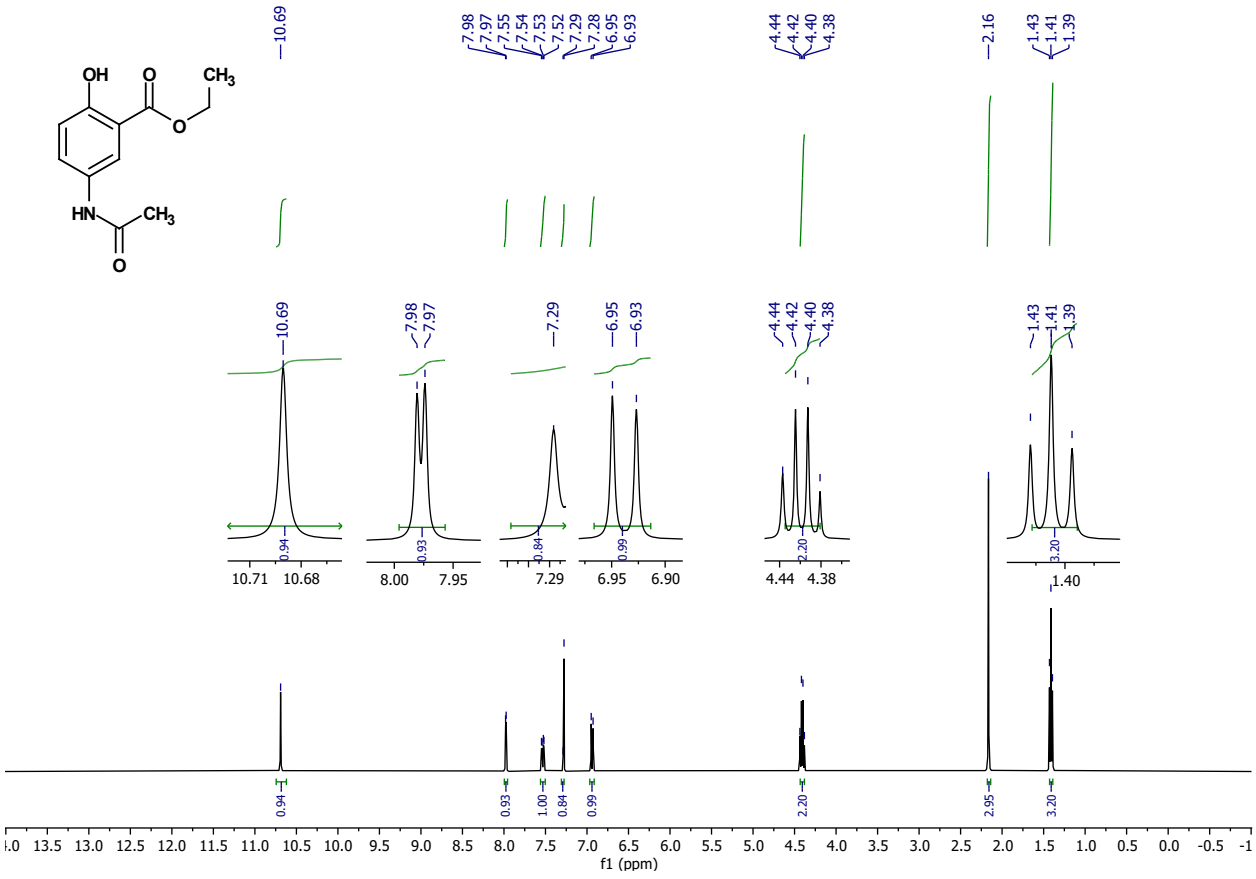


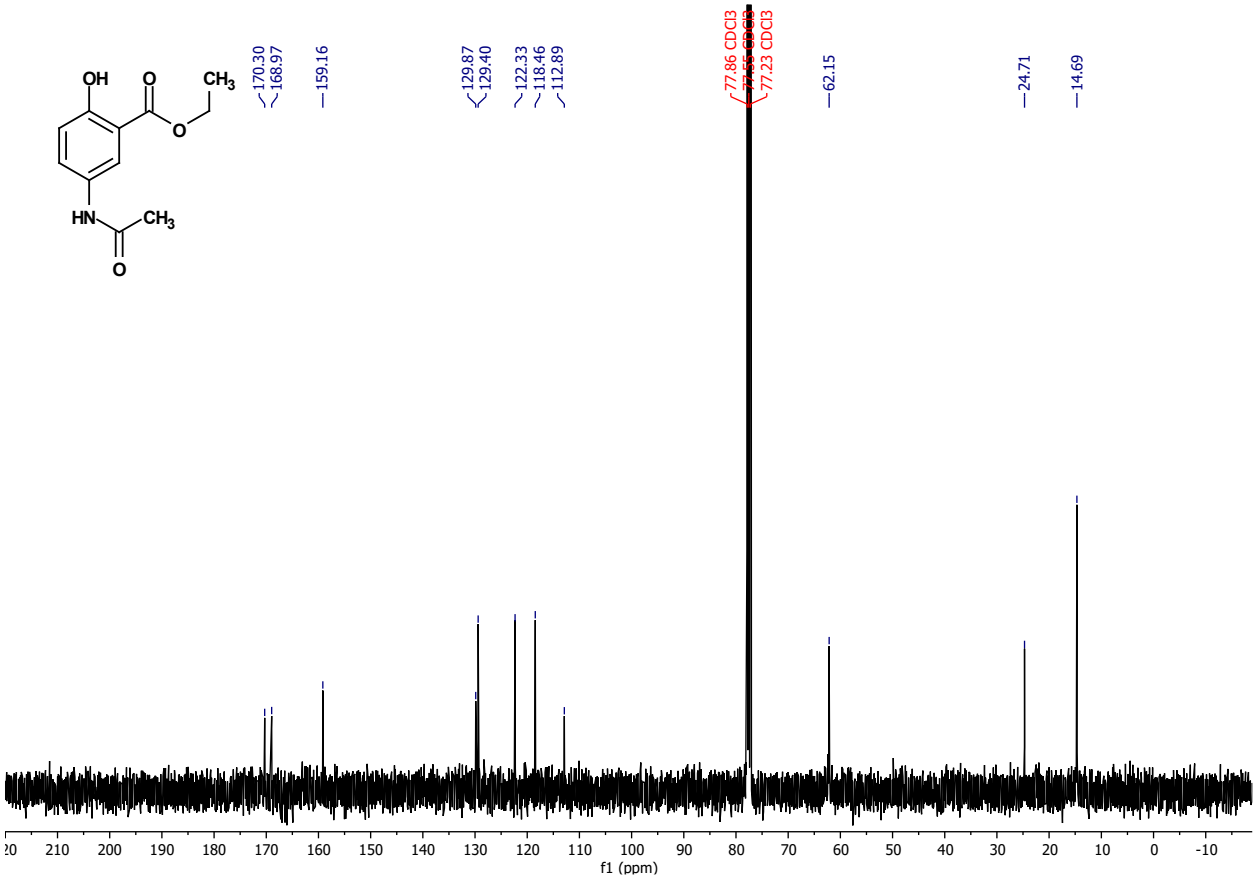
^{1}H and ^{13}C NMR Methyl 2-methylbenzo[d]oxazole-7-carboxylate **(2ww)**



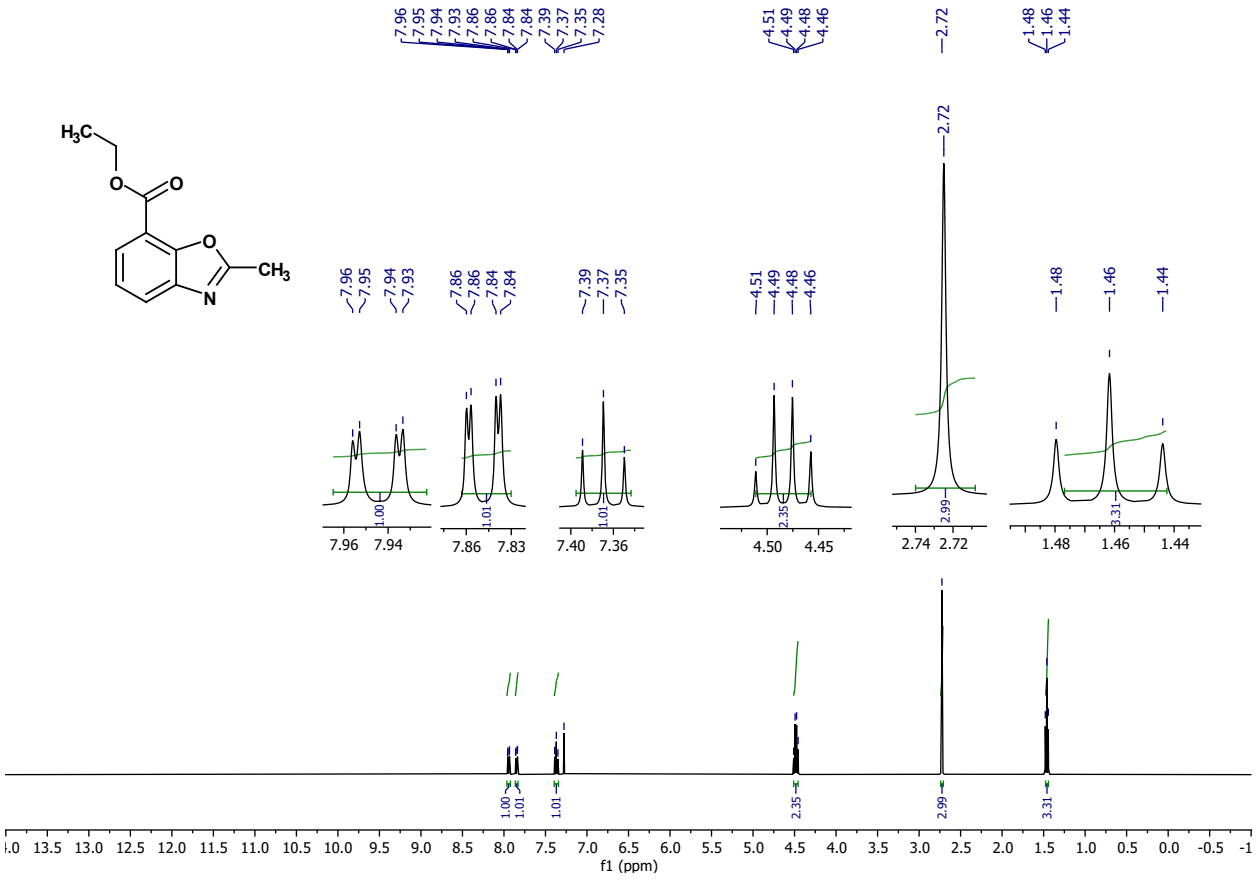


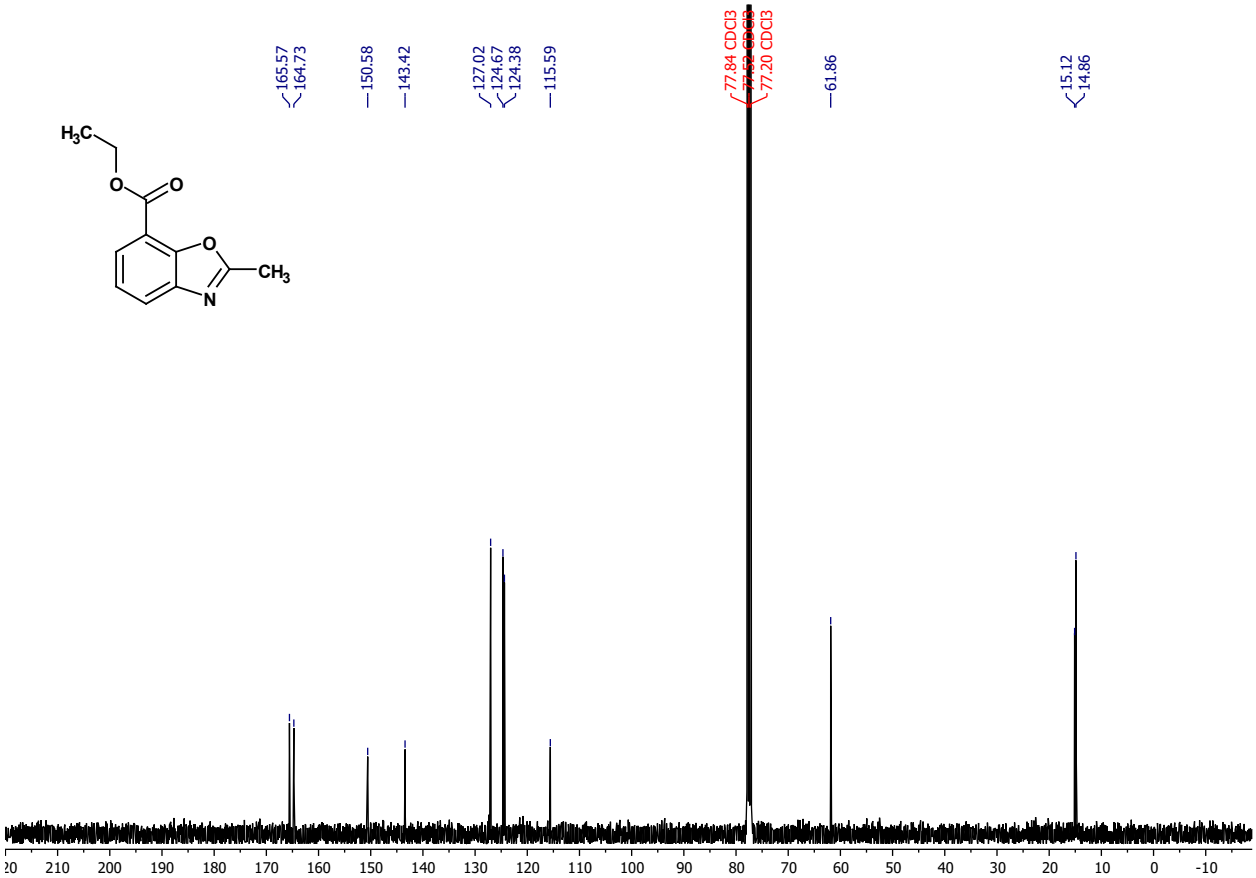
^{1}H and ^{13}C NMR Ethyl 5-acetamido-2-hydroxybenzoate **(2x)**



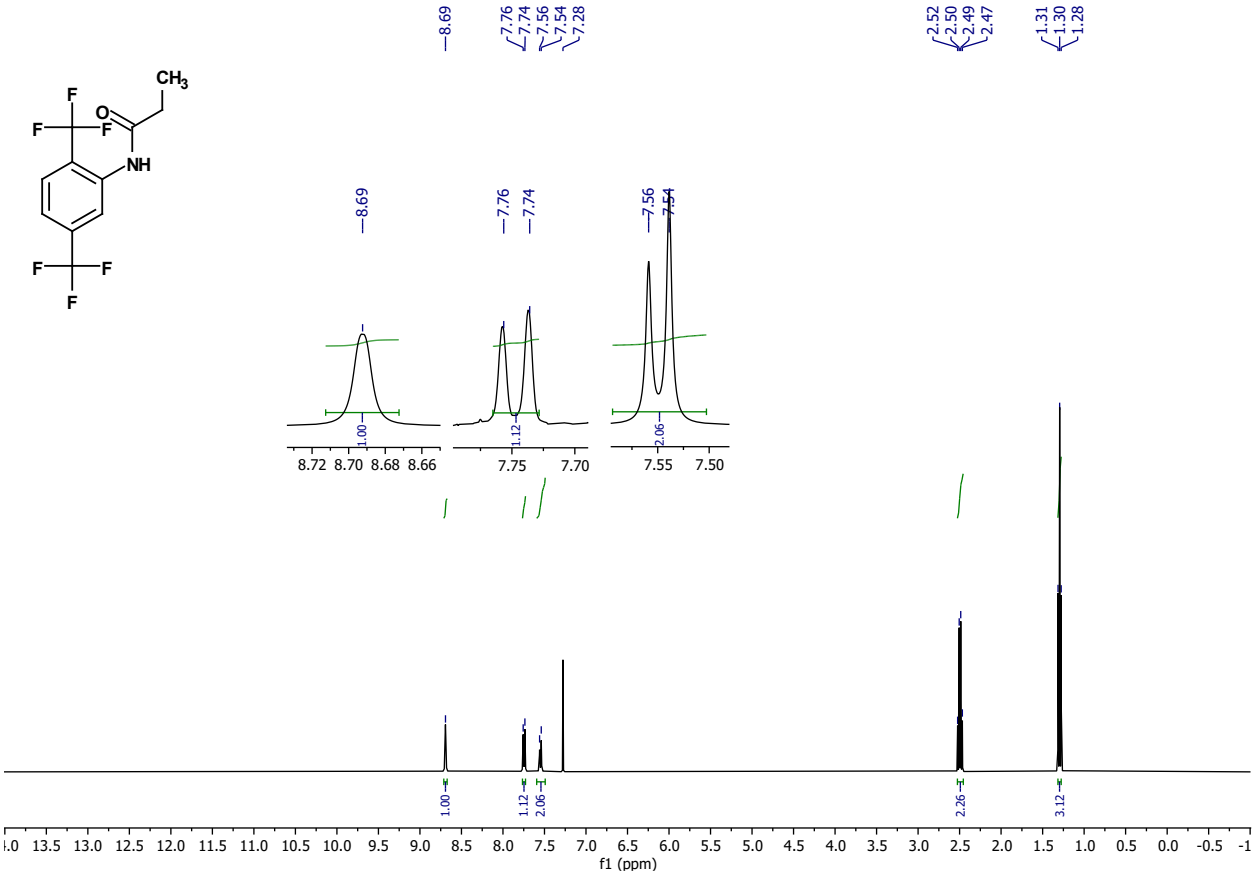


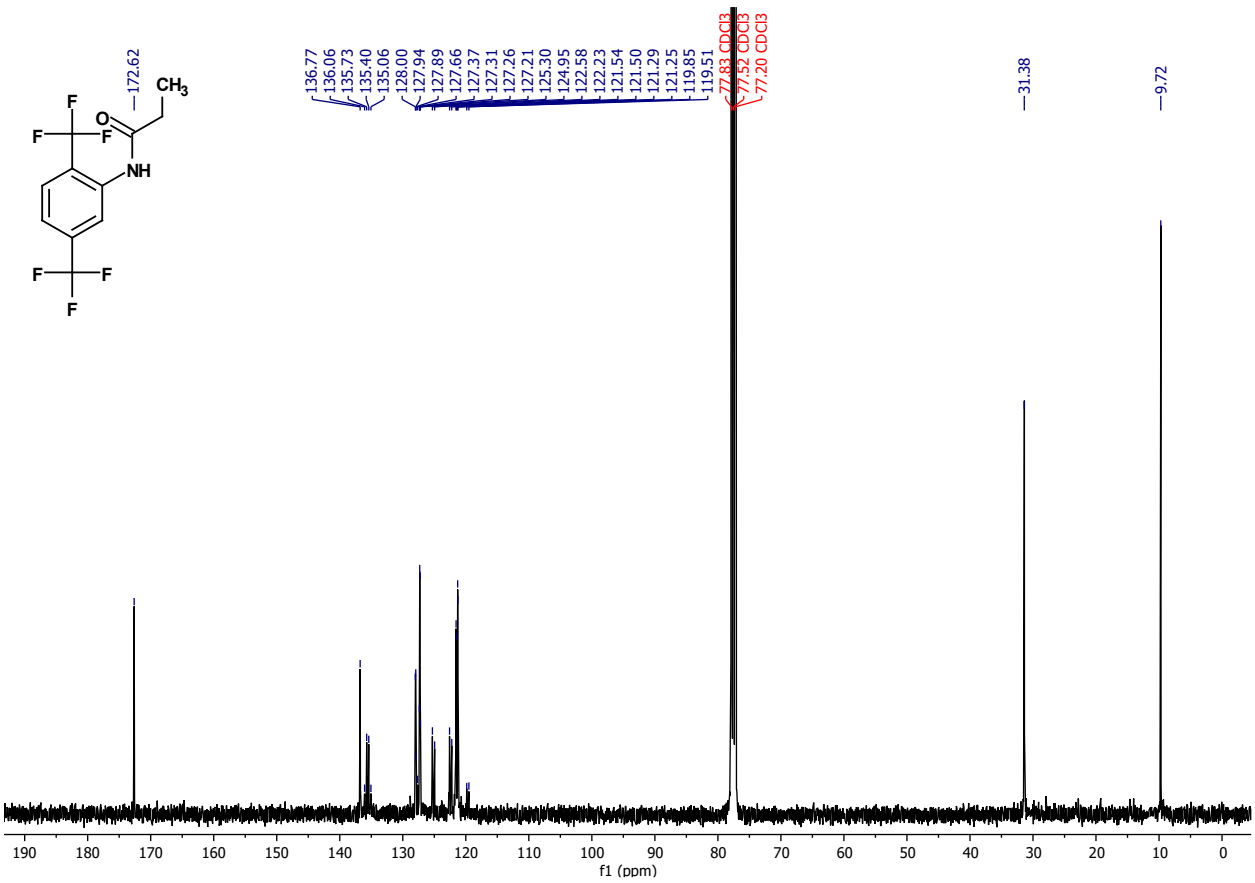
^{1}H and ^{13}C NMR Ethyl 2-methylbenzo[d]oxazole-7-carboxylate **(2xx)**



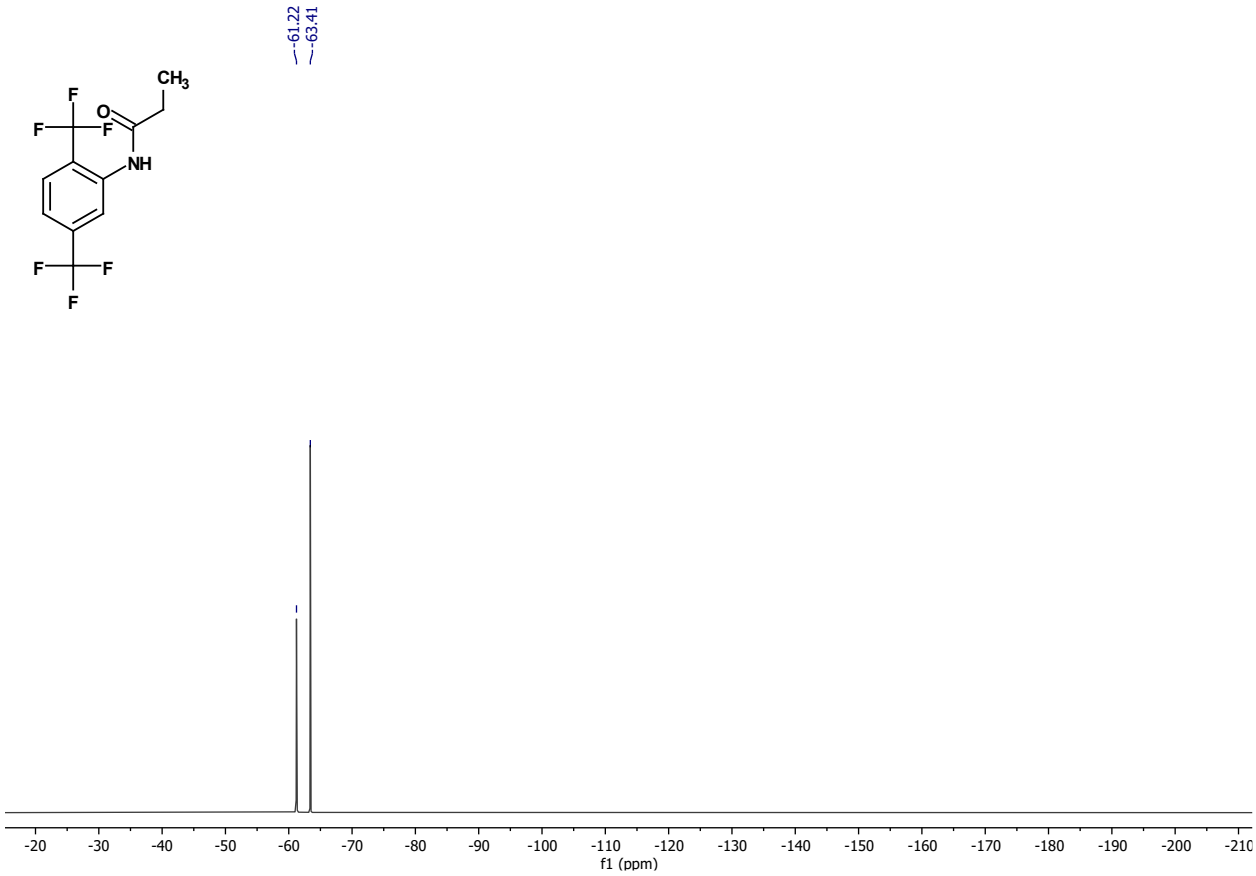


^{1}H and ^{13}C NMR *N*-(2,5-bis(trifluoromethyl)phenyl)propionamide **(3a)**

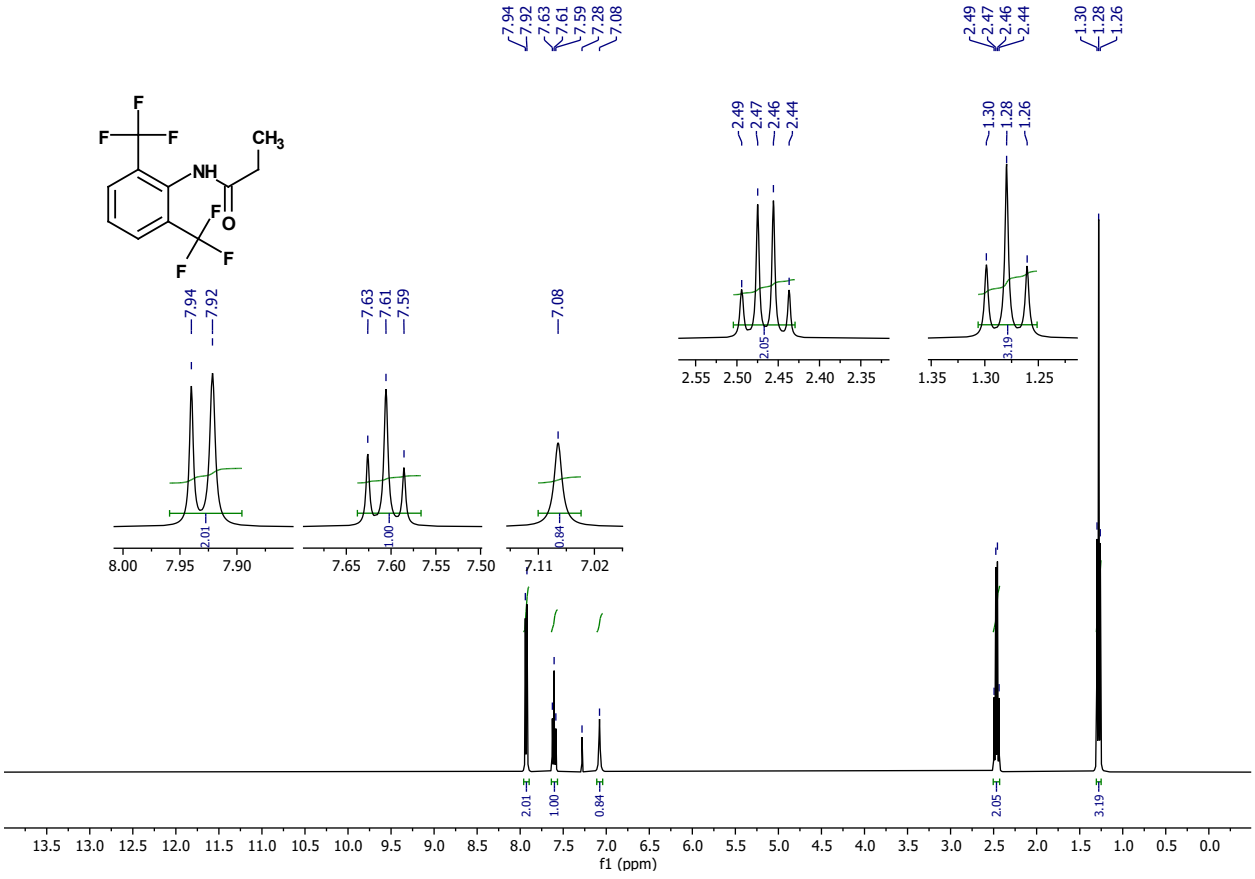


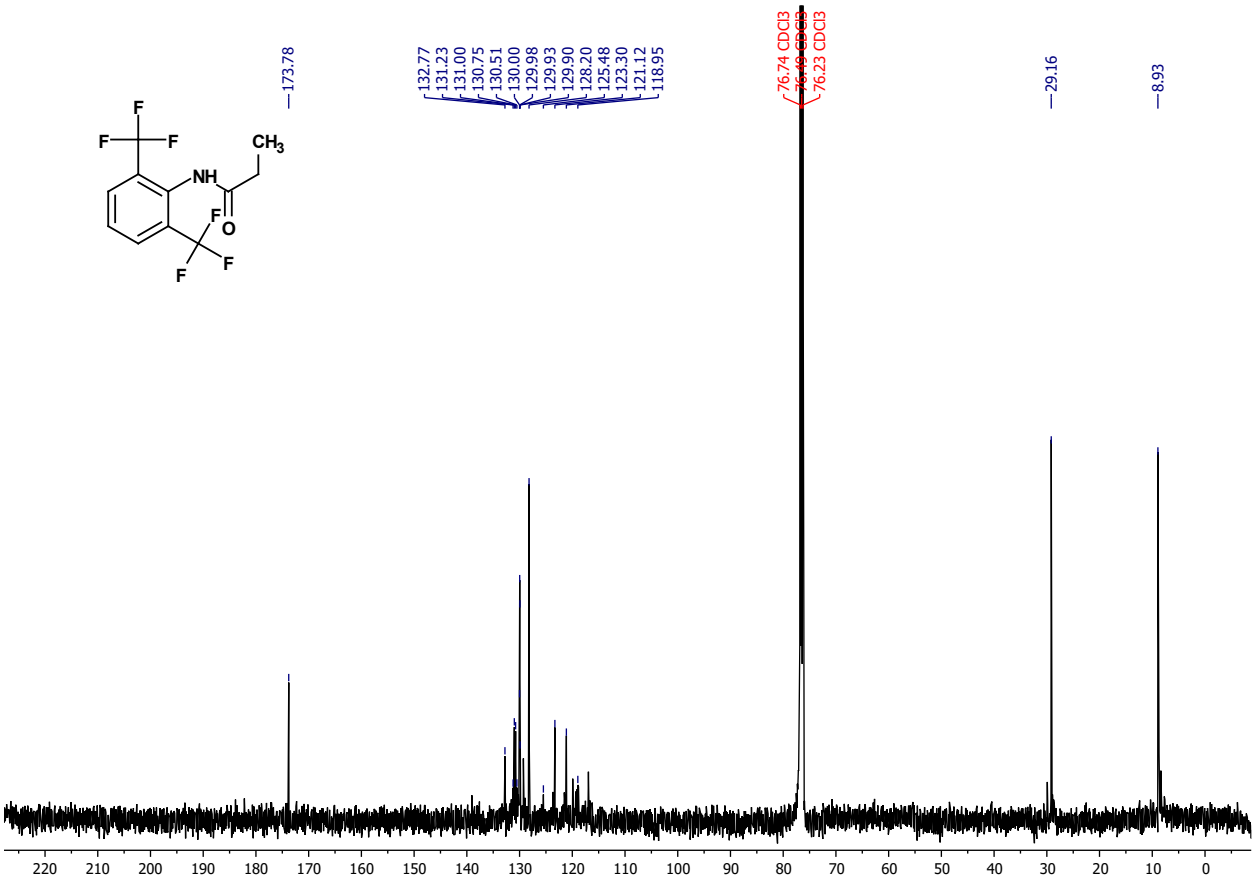


^{19}F NMR *N*-(2,5-bis(trifluoromethyl)phenyl)propionamide **(3a)**

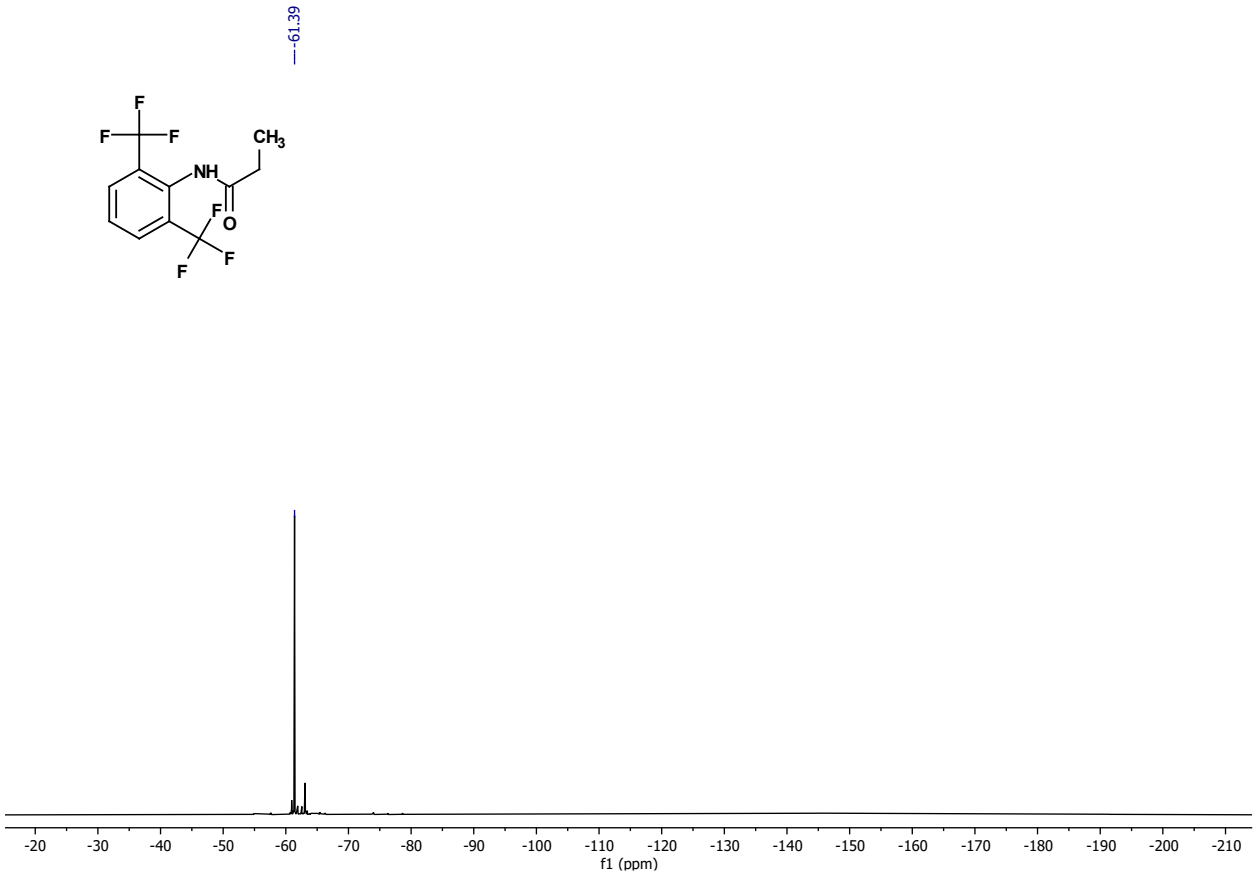


^{1}H and ^{13}C NMR *N*-(2,6-bis(trifluoromethyl)phenyl)propionamide **(3b)**

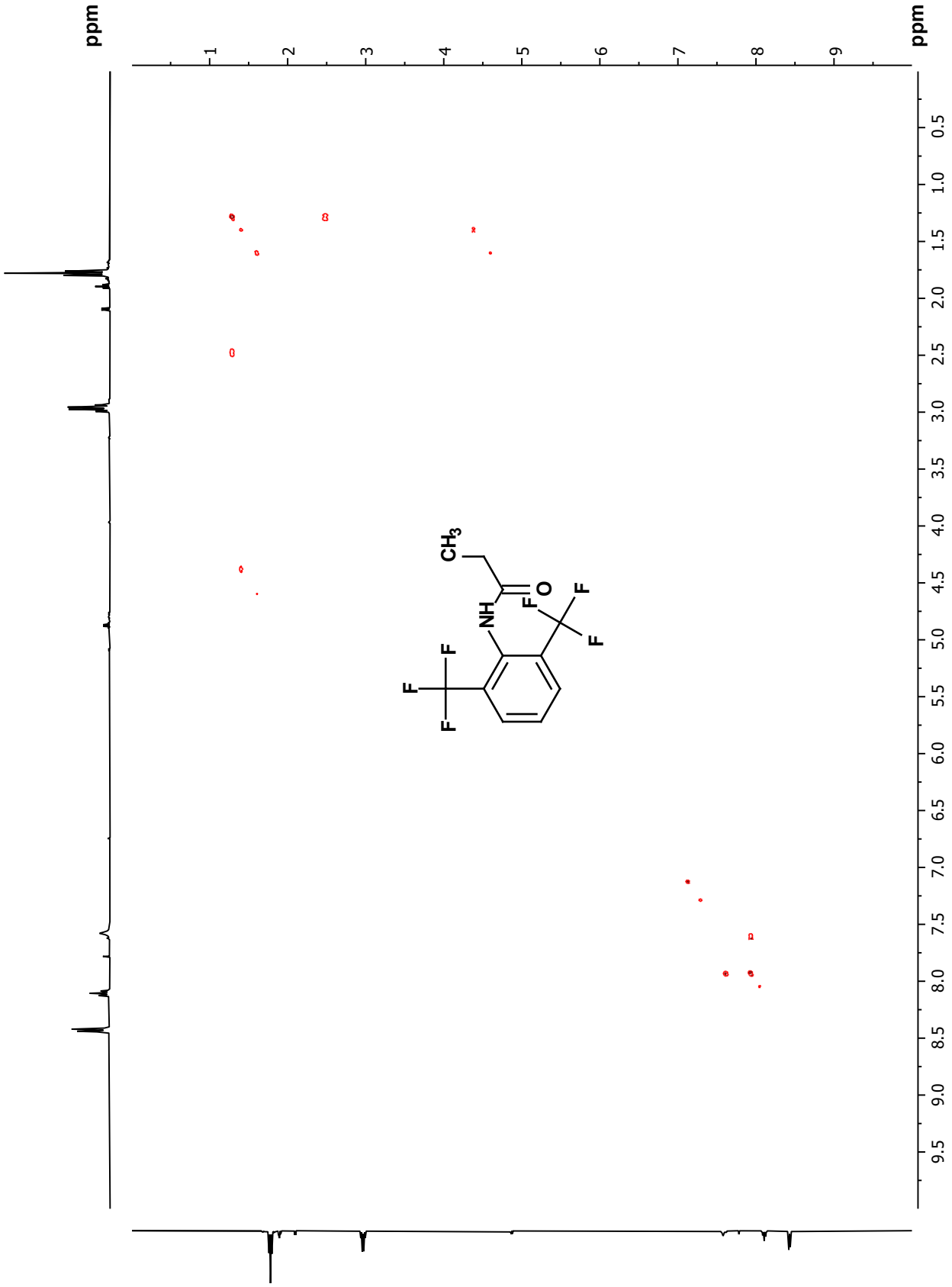




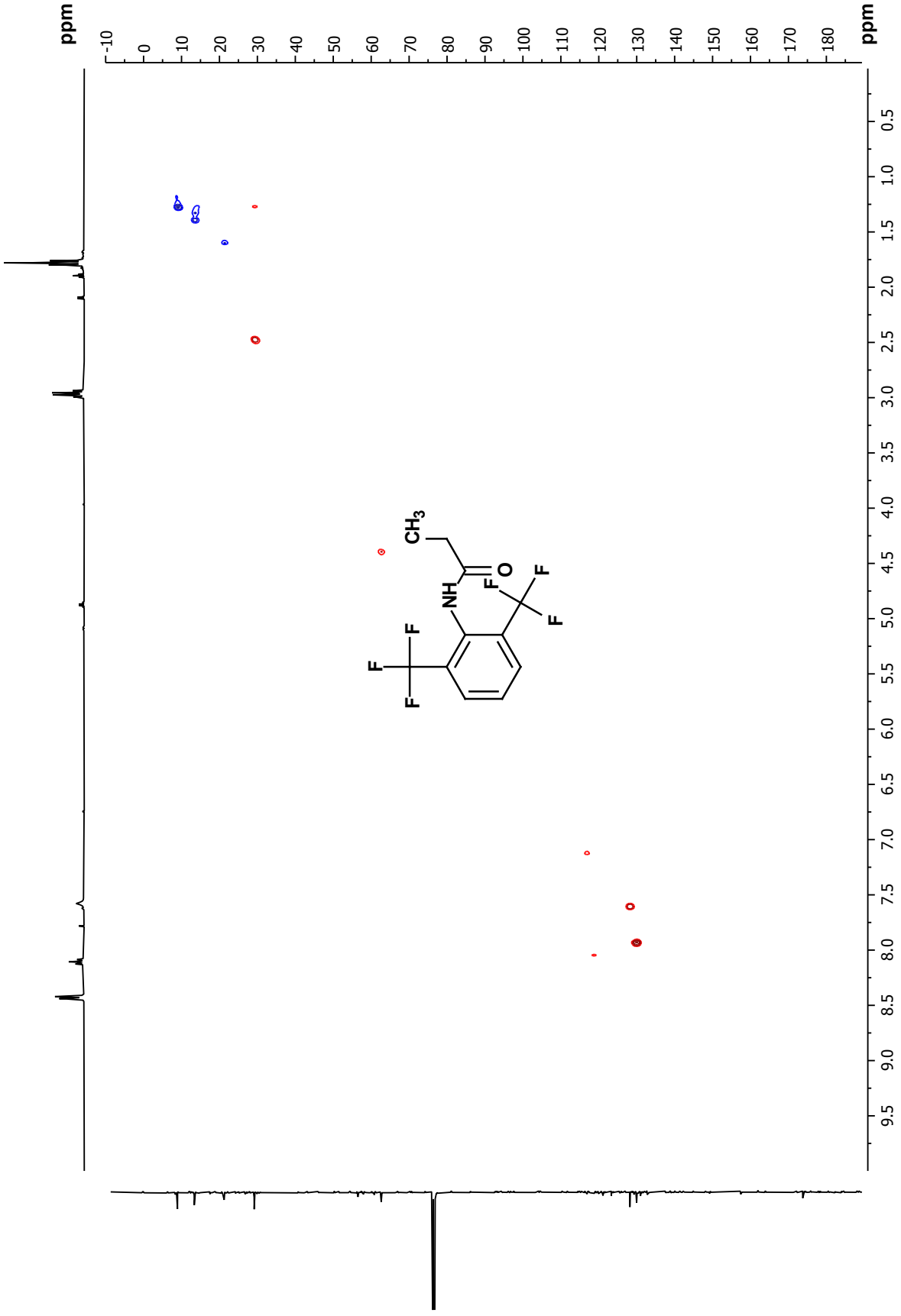
^{19}F NMR *N*-(2,6-bis(trifluoromethyl)phenyl)propionamide **(3b)**



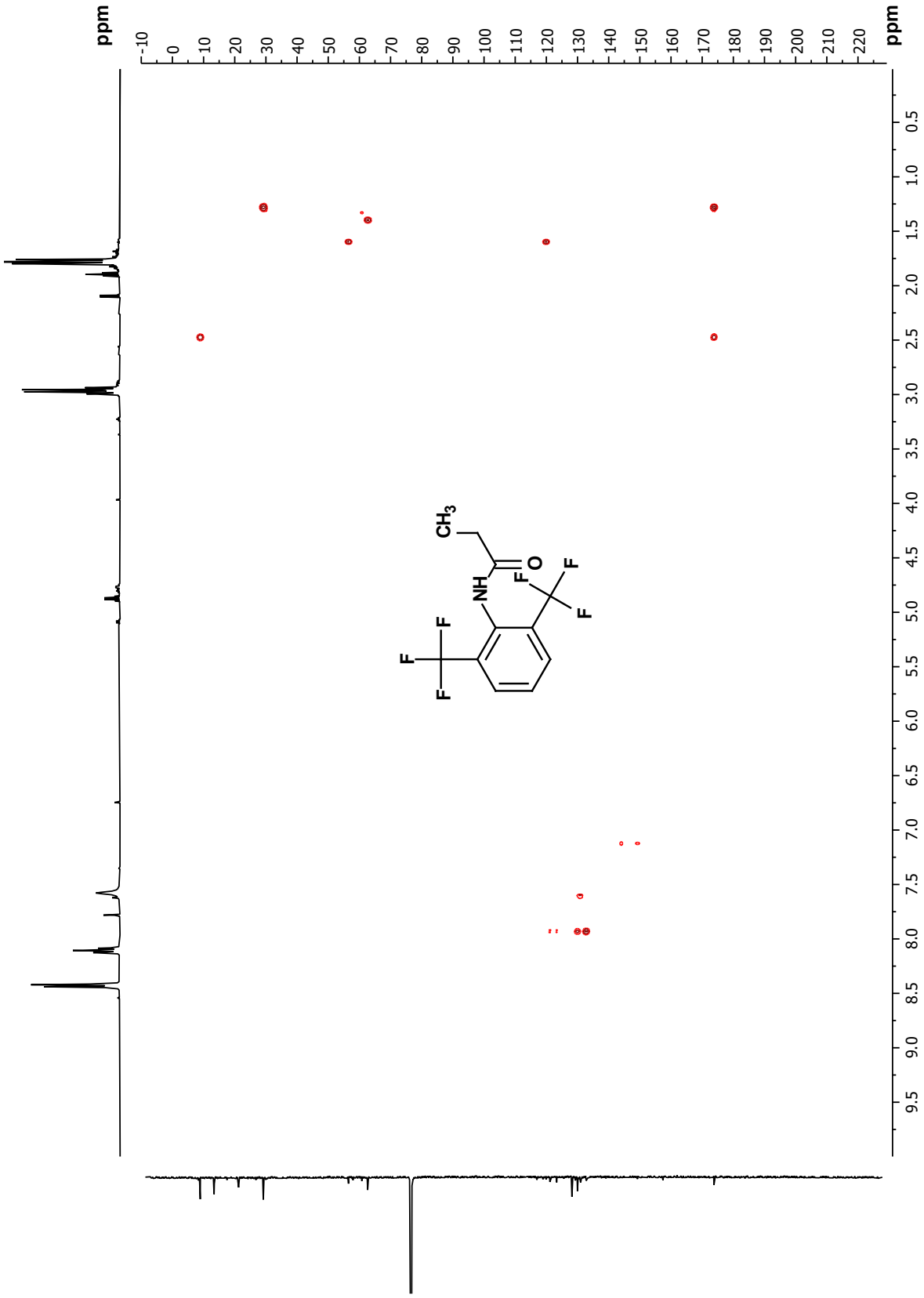
COSY NMR *N*-(2,6-bis(trifluoromethyl)phenyl)propionamide **(3b)**



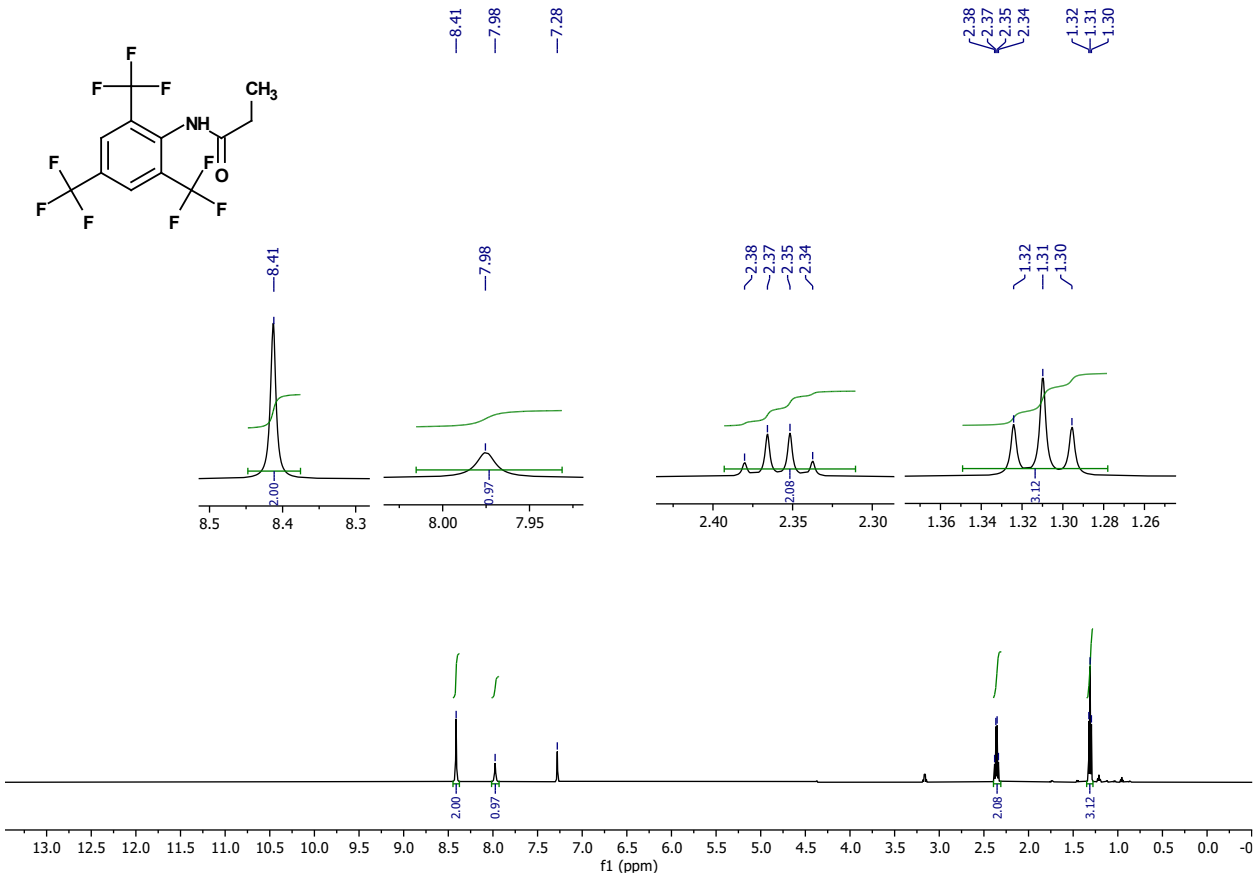
HSQC NMR *N*-(2,6-bis(trifluoromethyl)phenyl)propionamide **(3b)**

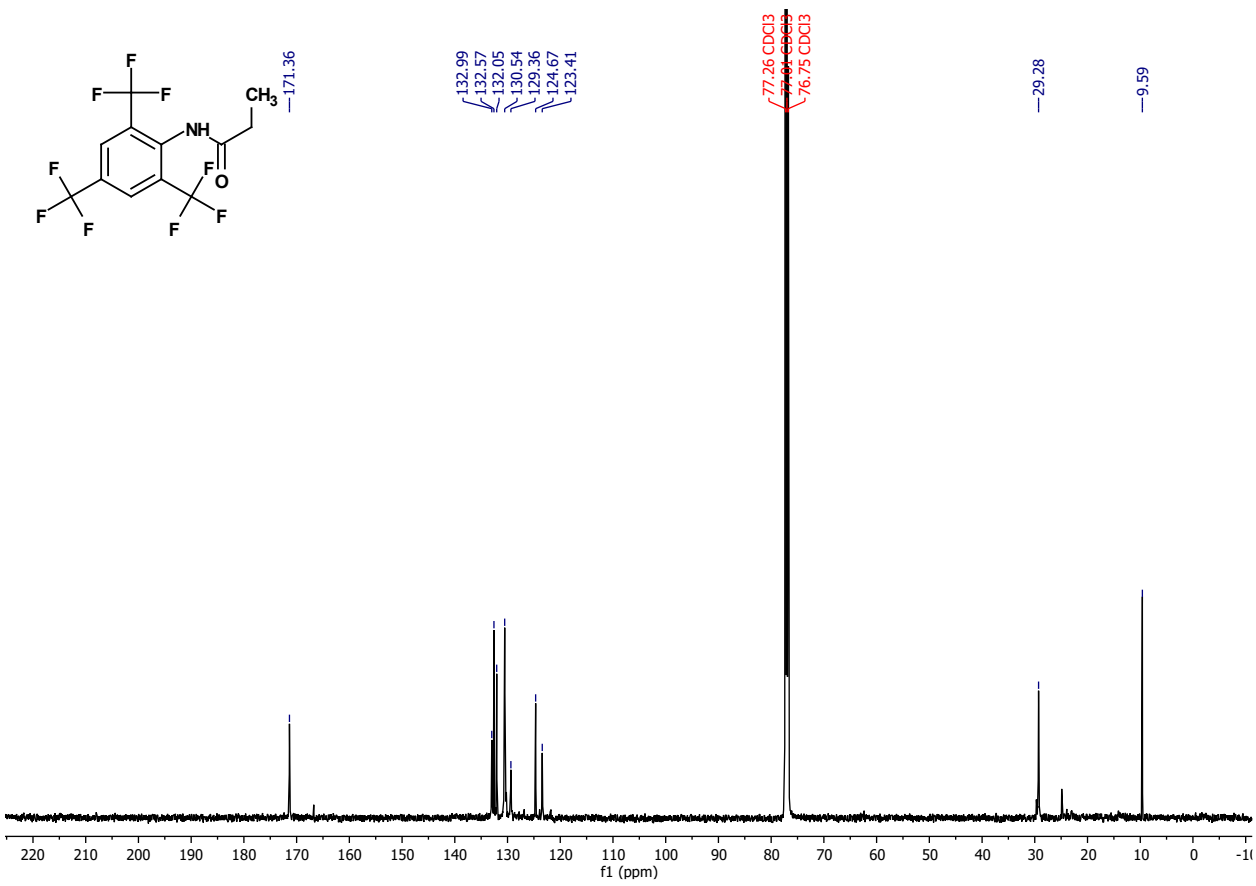


HMBC NMR *N*-(2,6-bis(trifluoromethyl)phenyl)propionamide **(3b)**

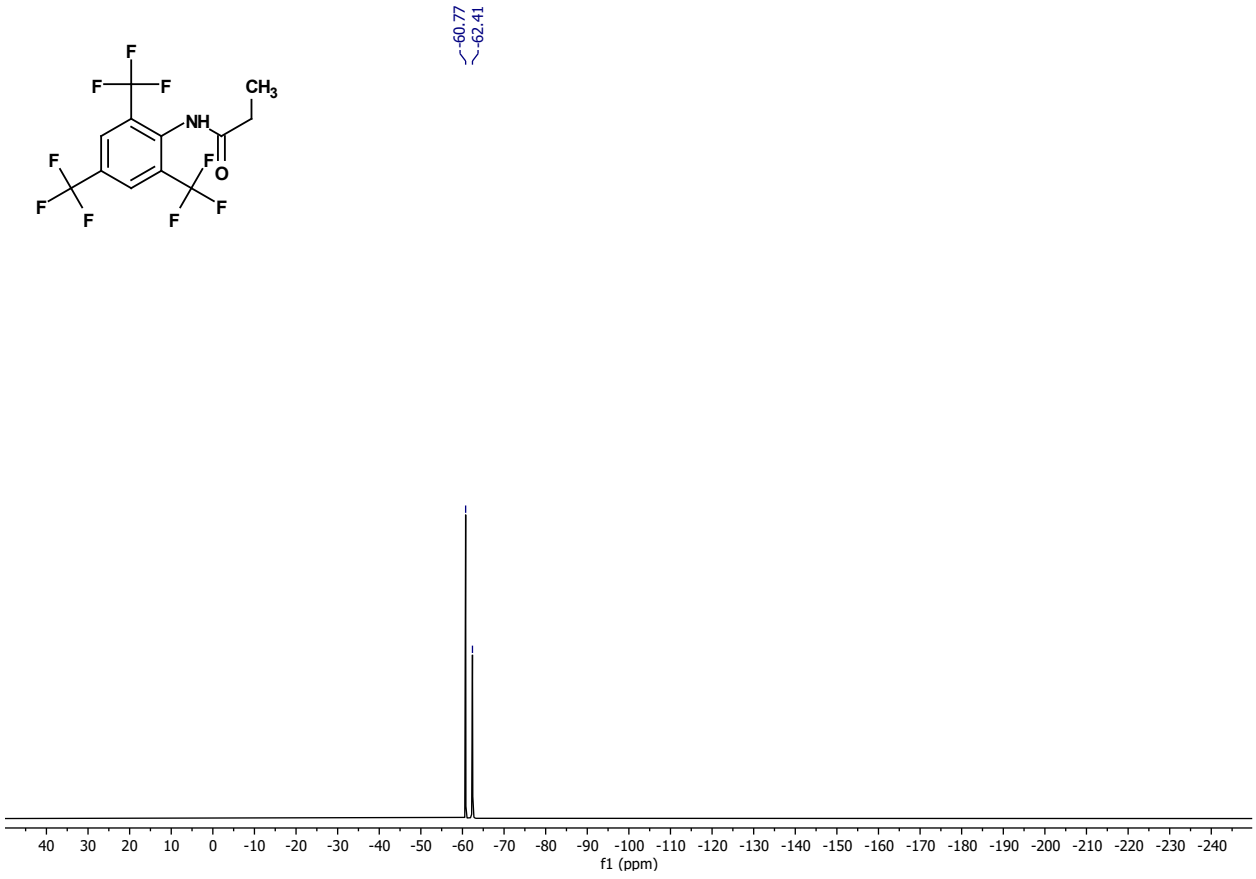


^{1}H and ^{13}C NMR *N*-(2,4,6-tris(trifluoromethyl)phenyl)propionamide **(3c)**

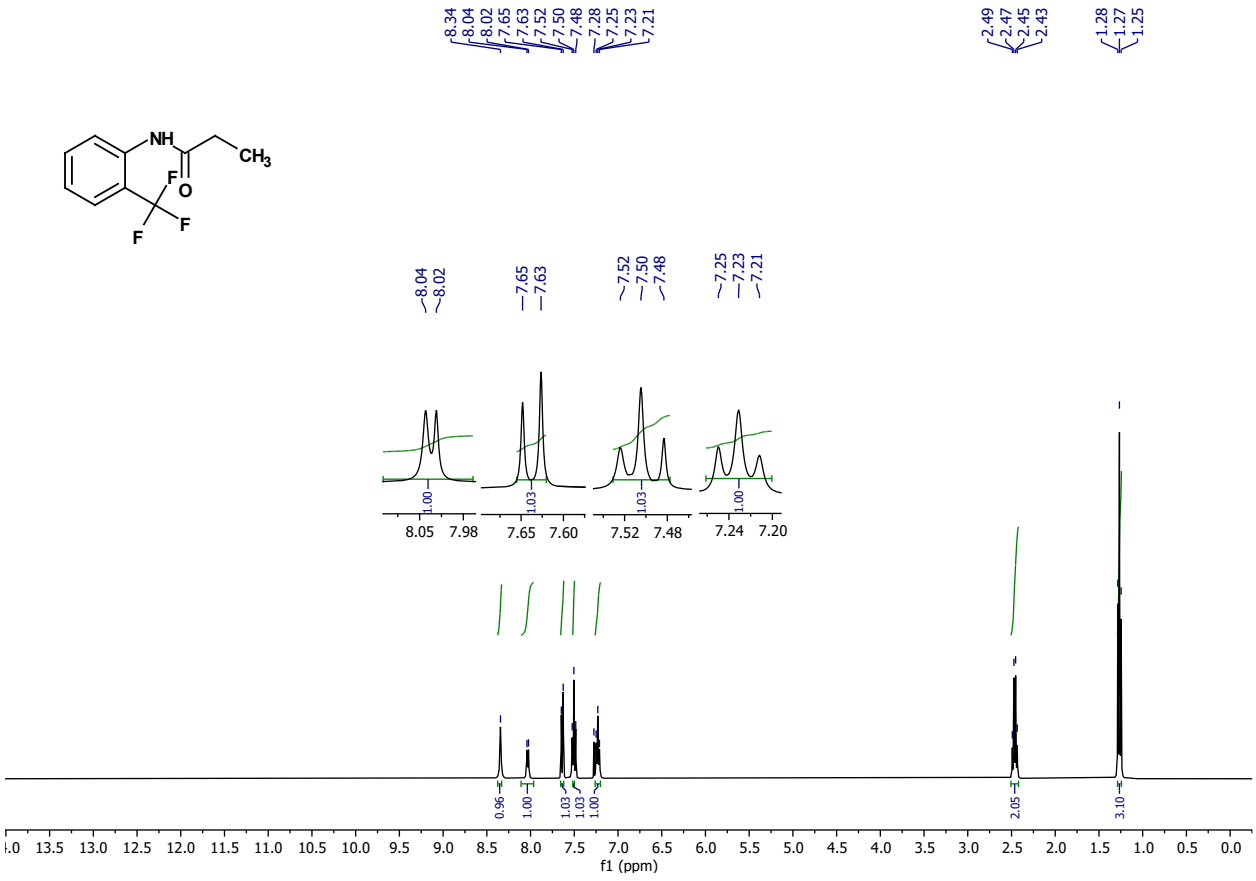


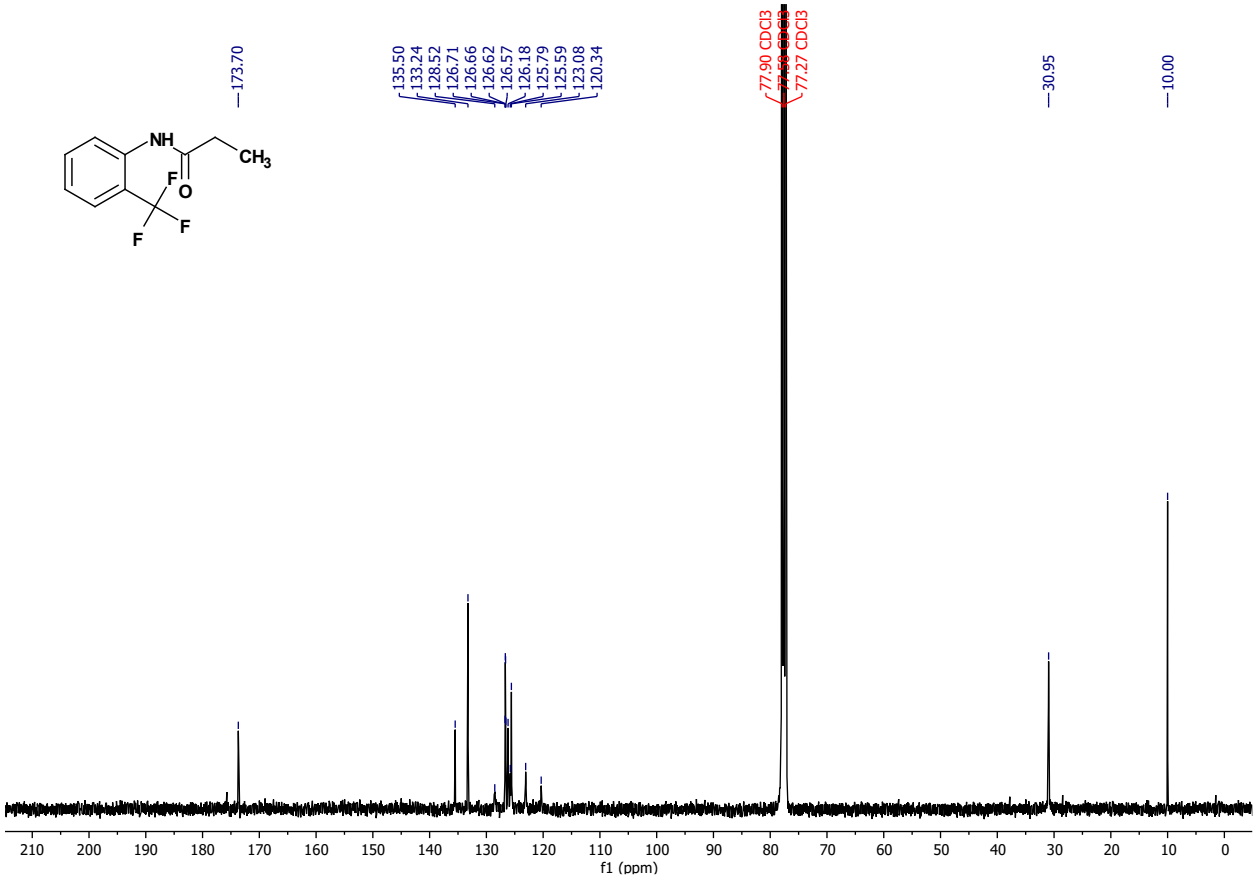


^{19}F NMR *N*-(2,4,6-tris(trifluoromethyl)phenyl)propionamide **(3c)**

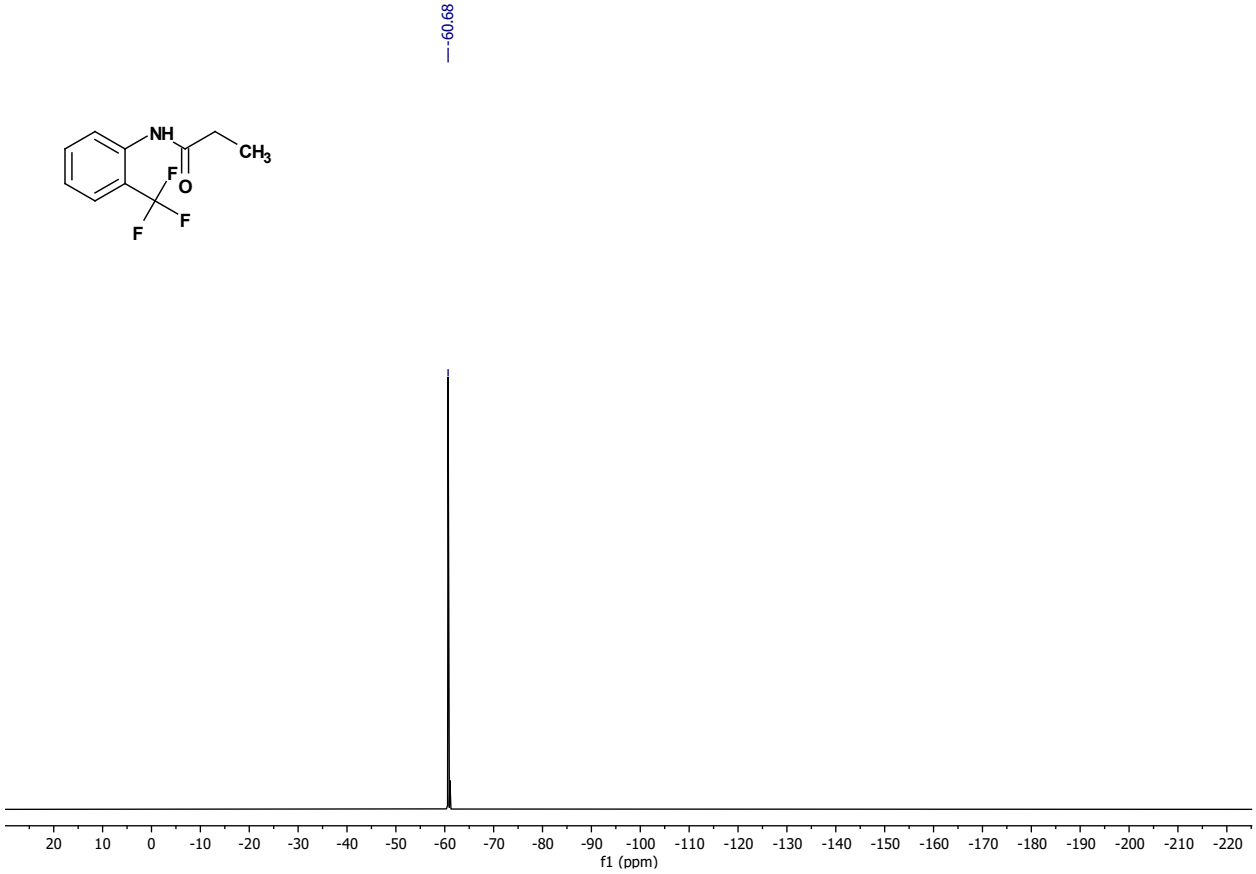


^{1}H and ^{13}C NMR *N*-(2-(trifluoromethyl)phenyl)propionamide (**3d**-*a*)

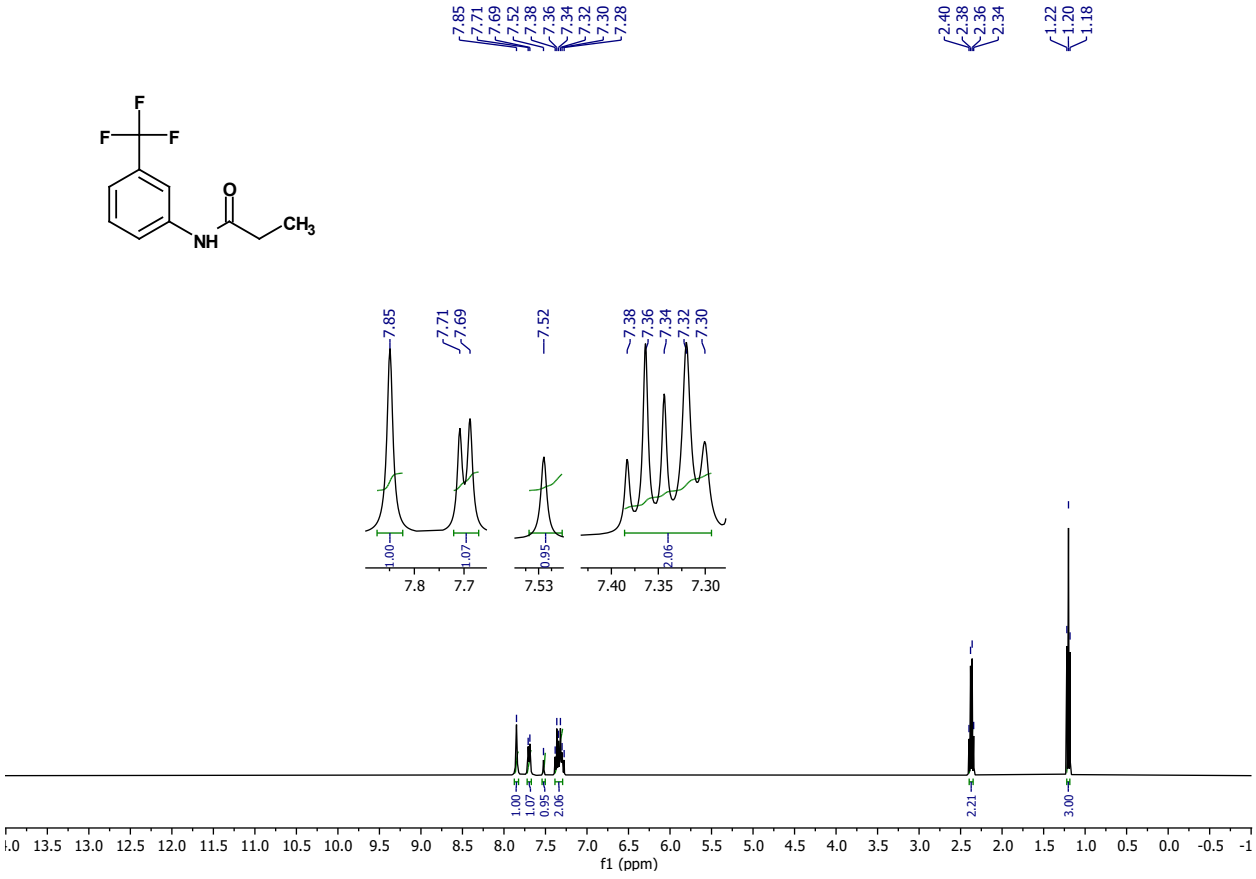


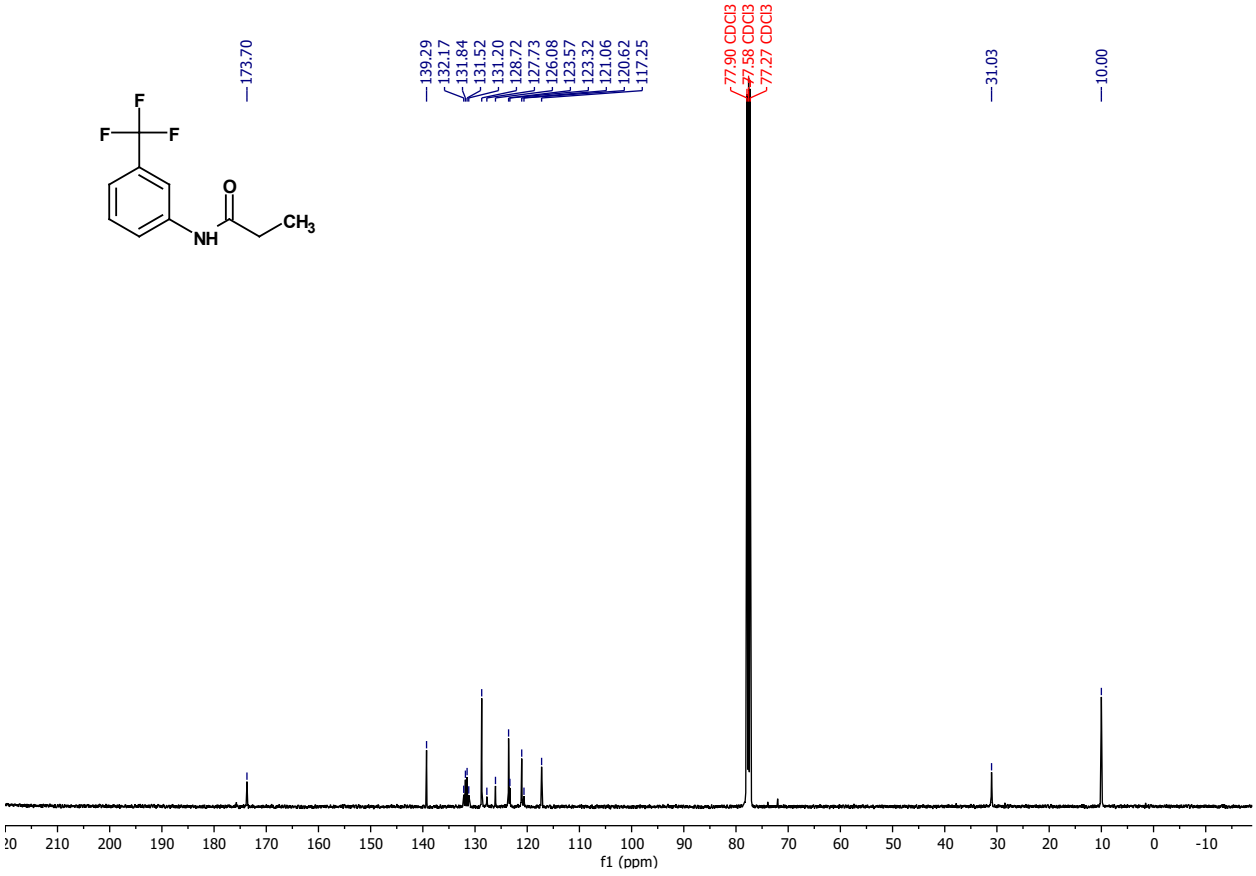


^{19}F NMR *N*-(2-(trifluoromethyl)phenyl)propionamide (**3d**-*a*)

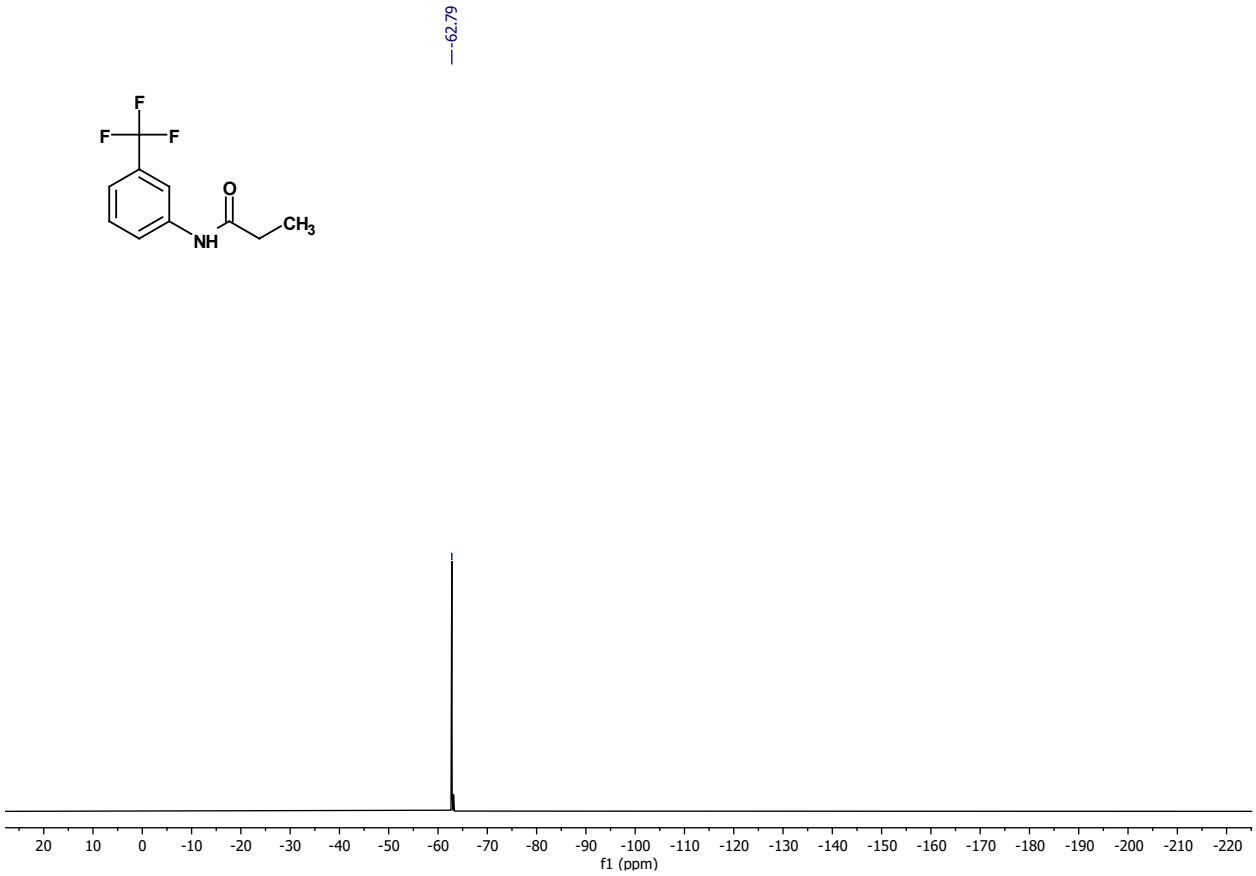


^{1}H and ^{13}C NMR *N*-(3-(trifluoromethyl)phenyl)propionamide (**3d**-*b*)

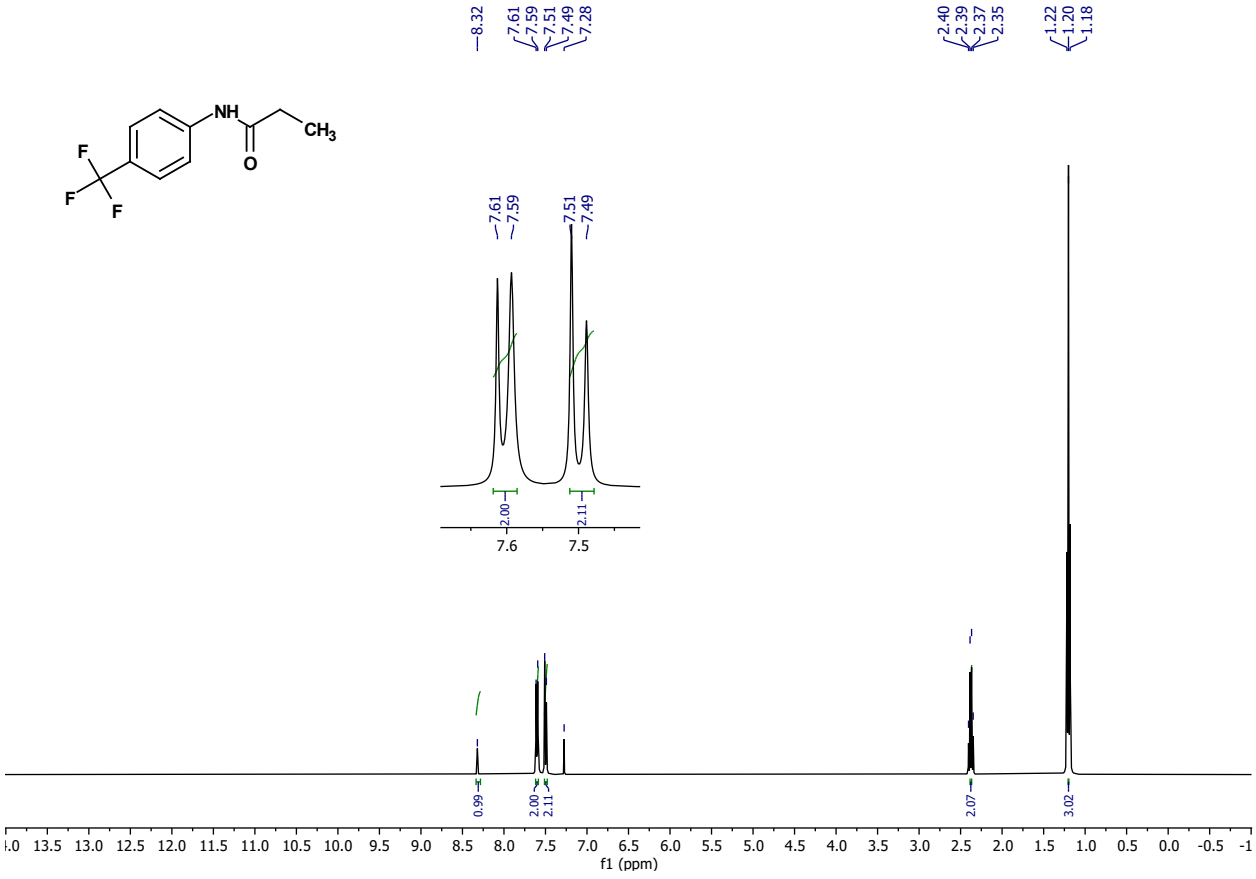


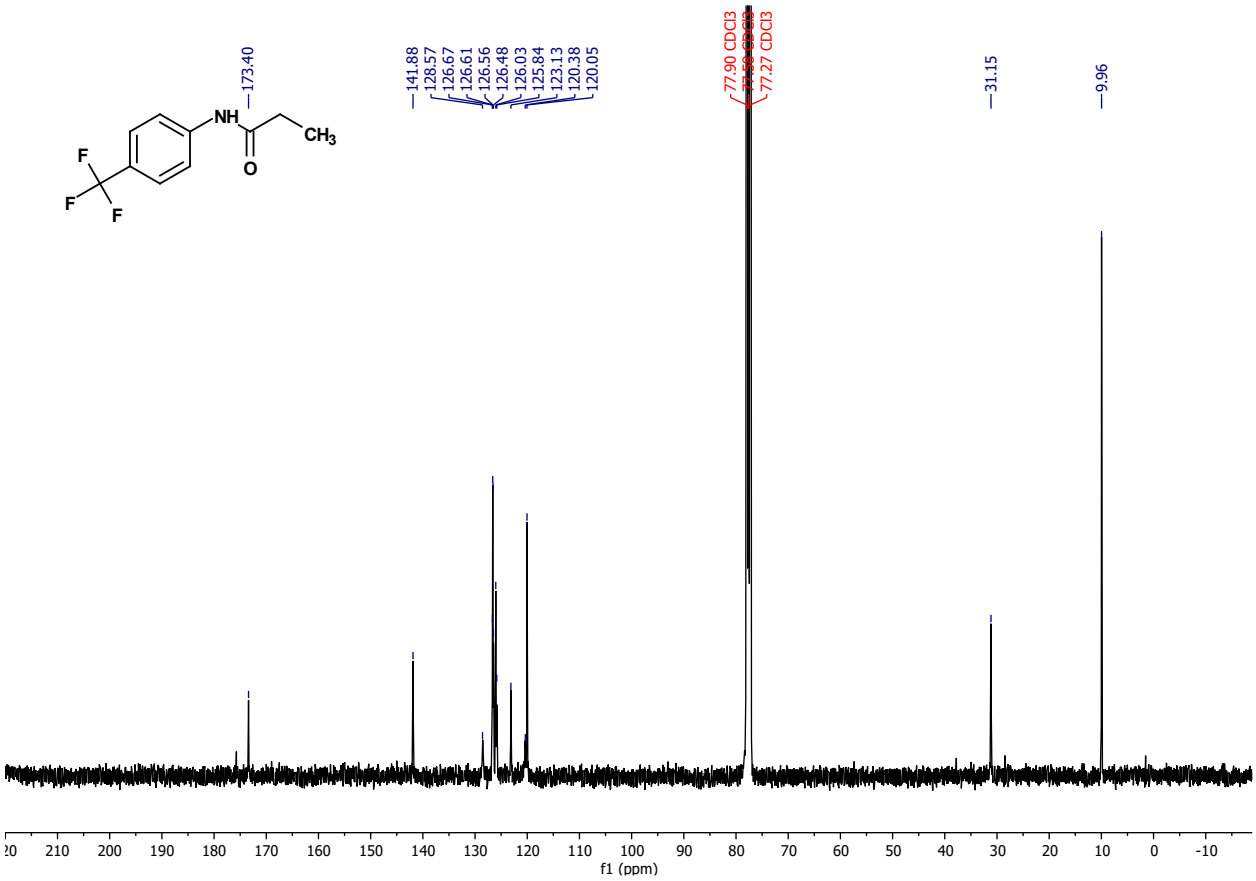


^{19}F NMR *N*-(3-(trifluoromethyl)phenyl)propionamide (**3d**-*b*)

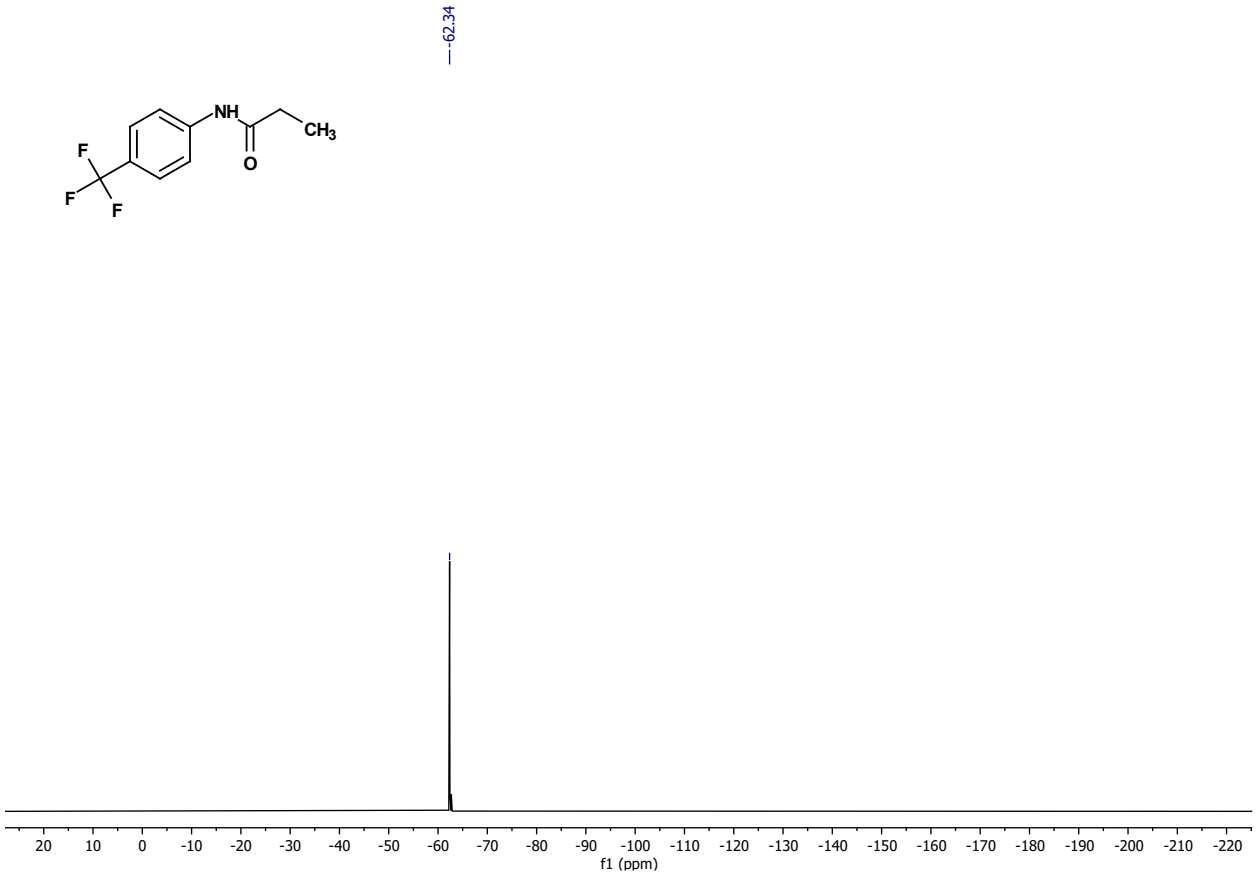


^{1}H and ^{13}C NMR *N*-(4-(trifluoromethyl)phenyl)propionamide (**3d**-*c*)

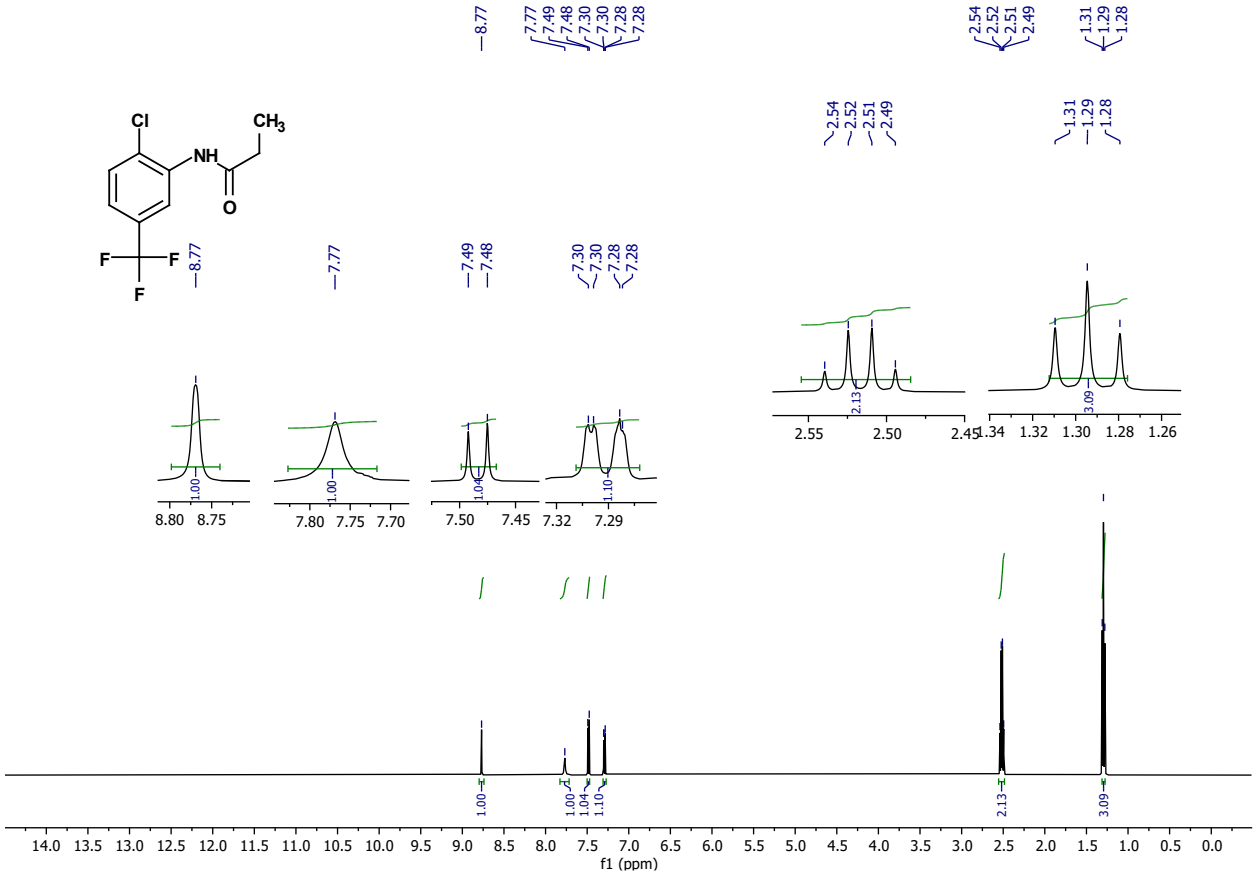


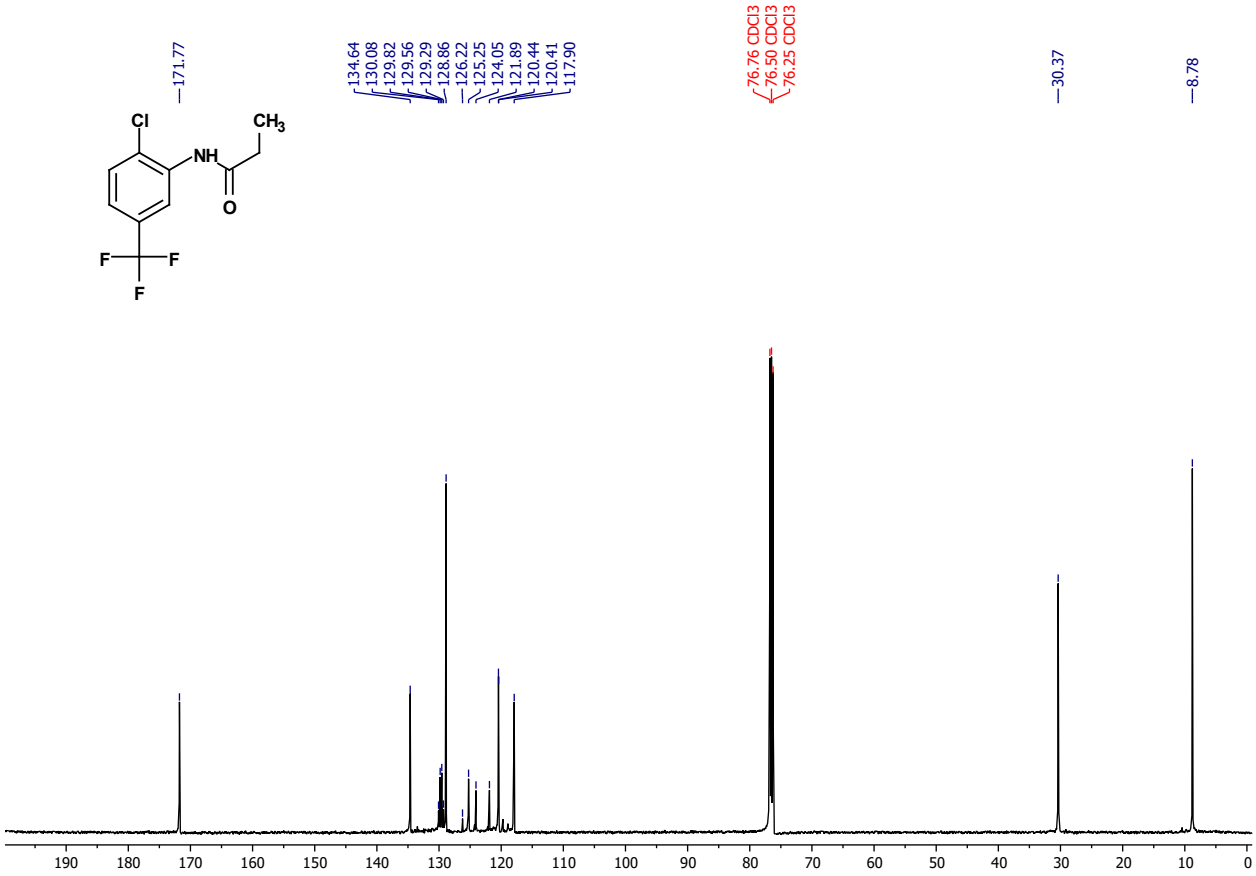


^{19}F NMR *N*-(4-(trifluoromethyl)phenyl)propionamide (**3d**-*c*)

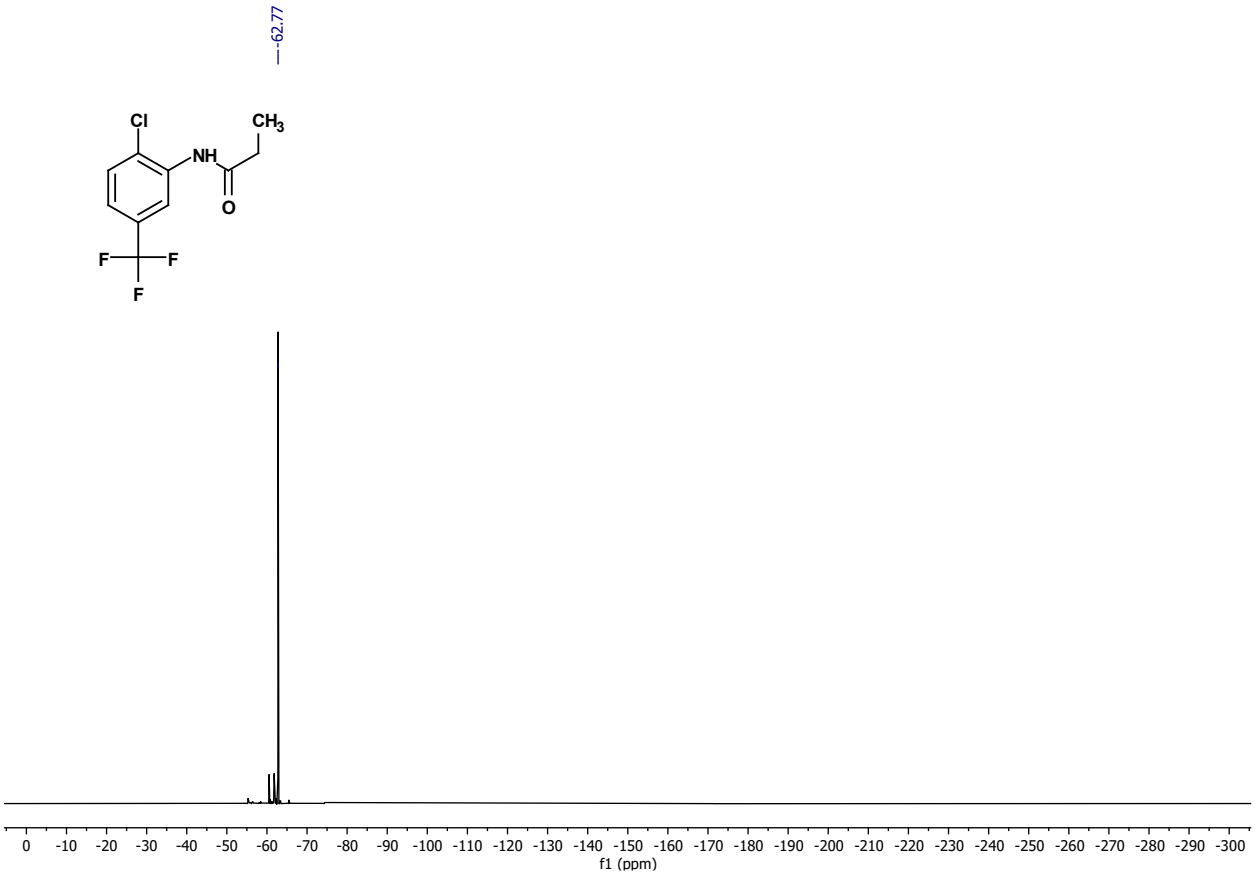


^{1}H and ^{13}C NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)propionamide (**3e**)

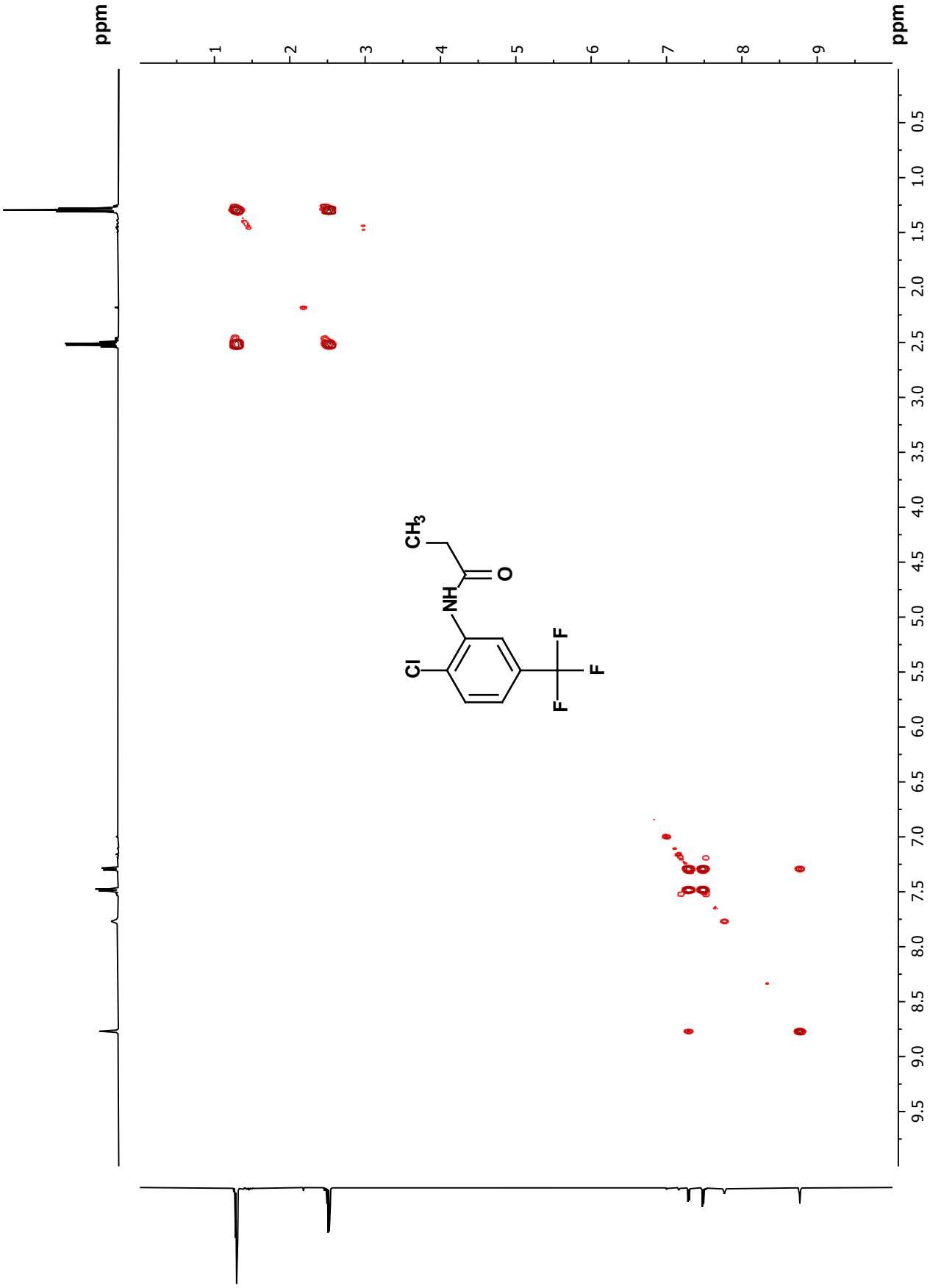




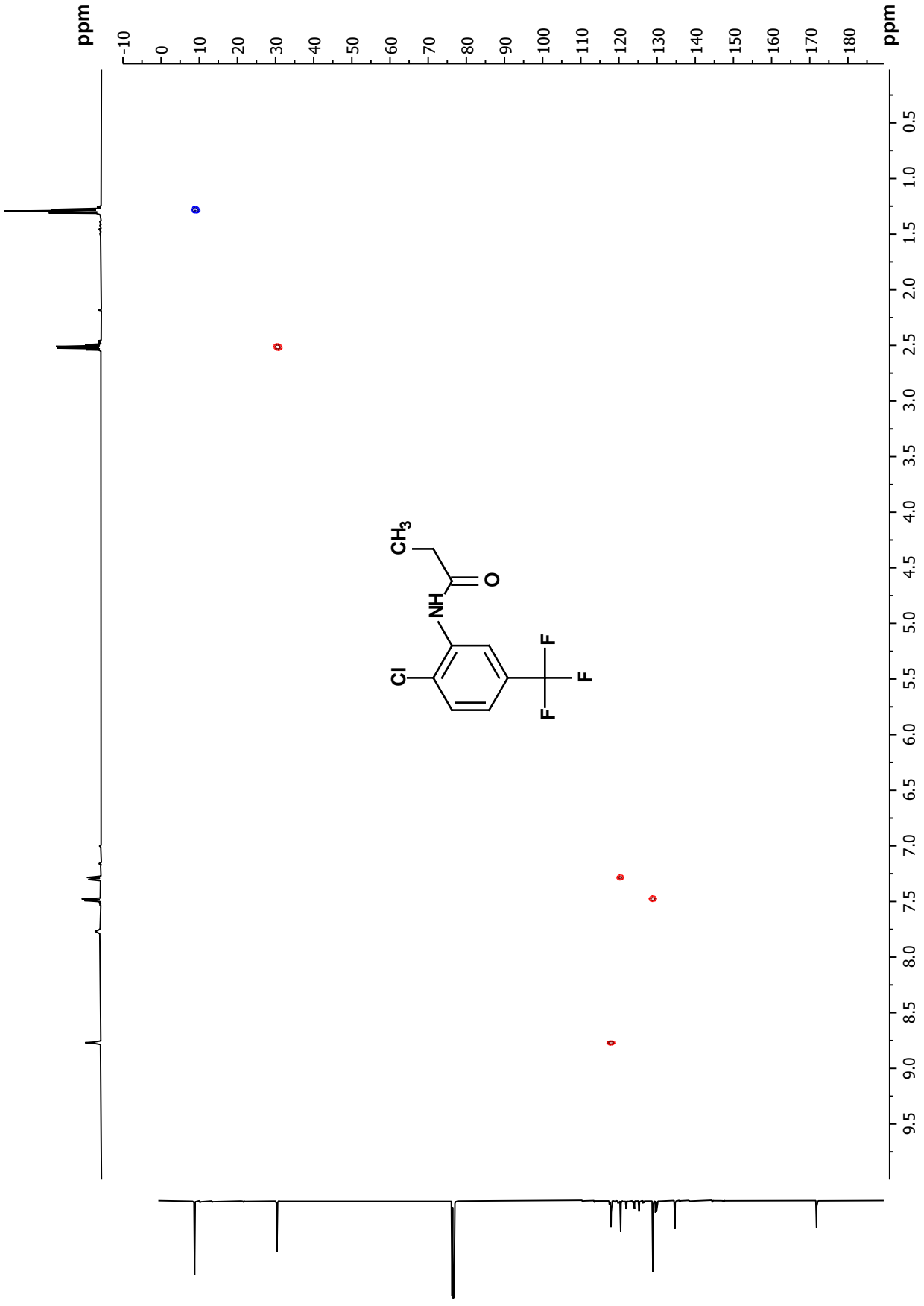
^{19}F NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)propionamide (**3e**)



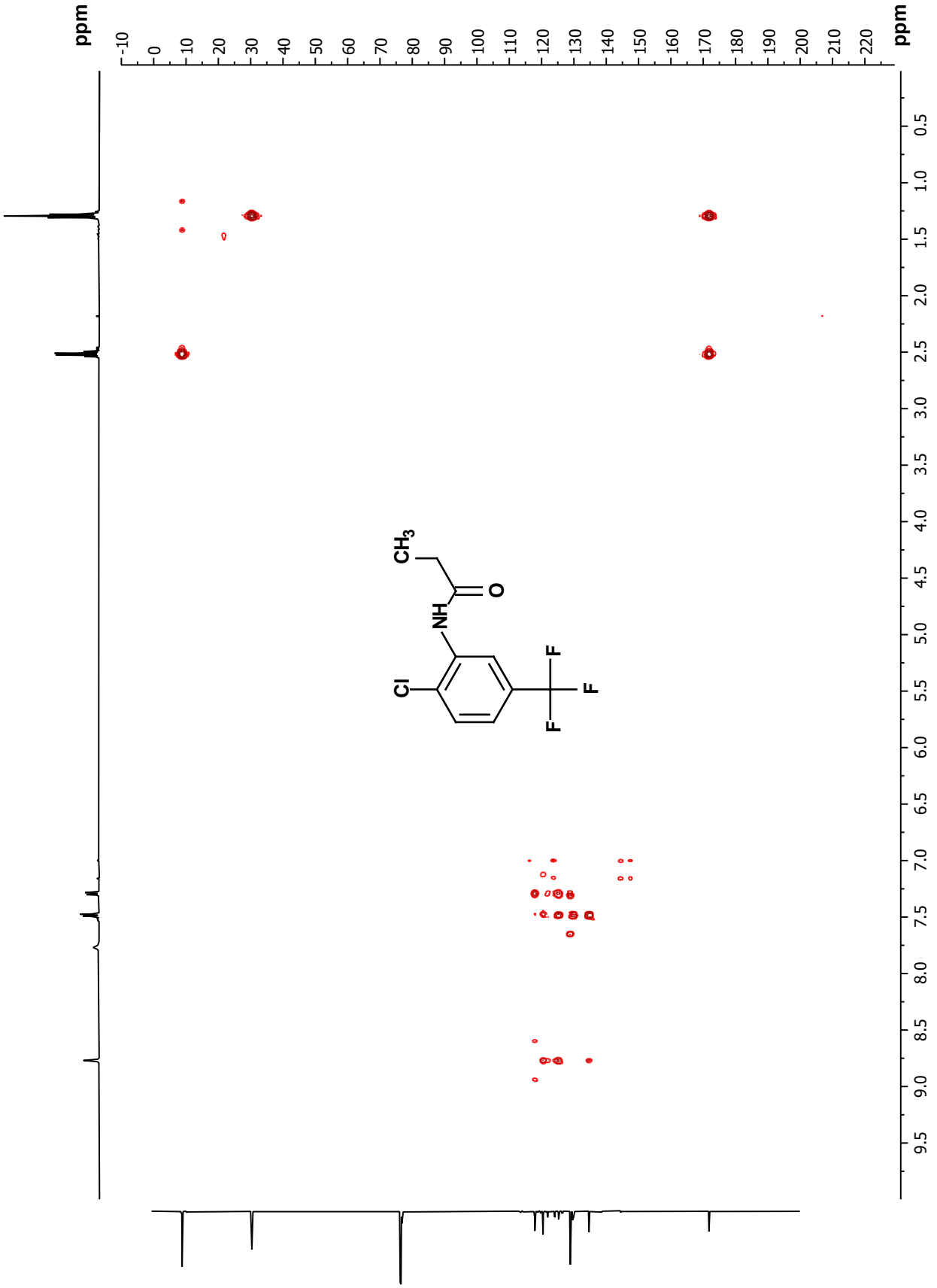
COSY NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)propionamide (**3e**)



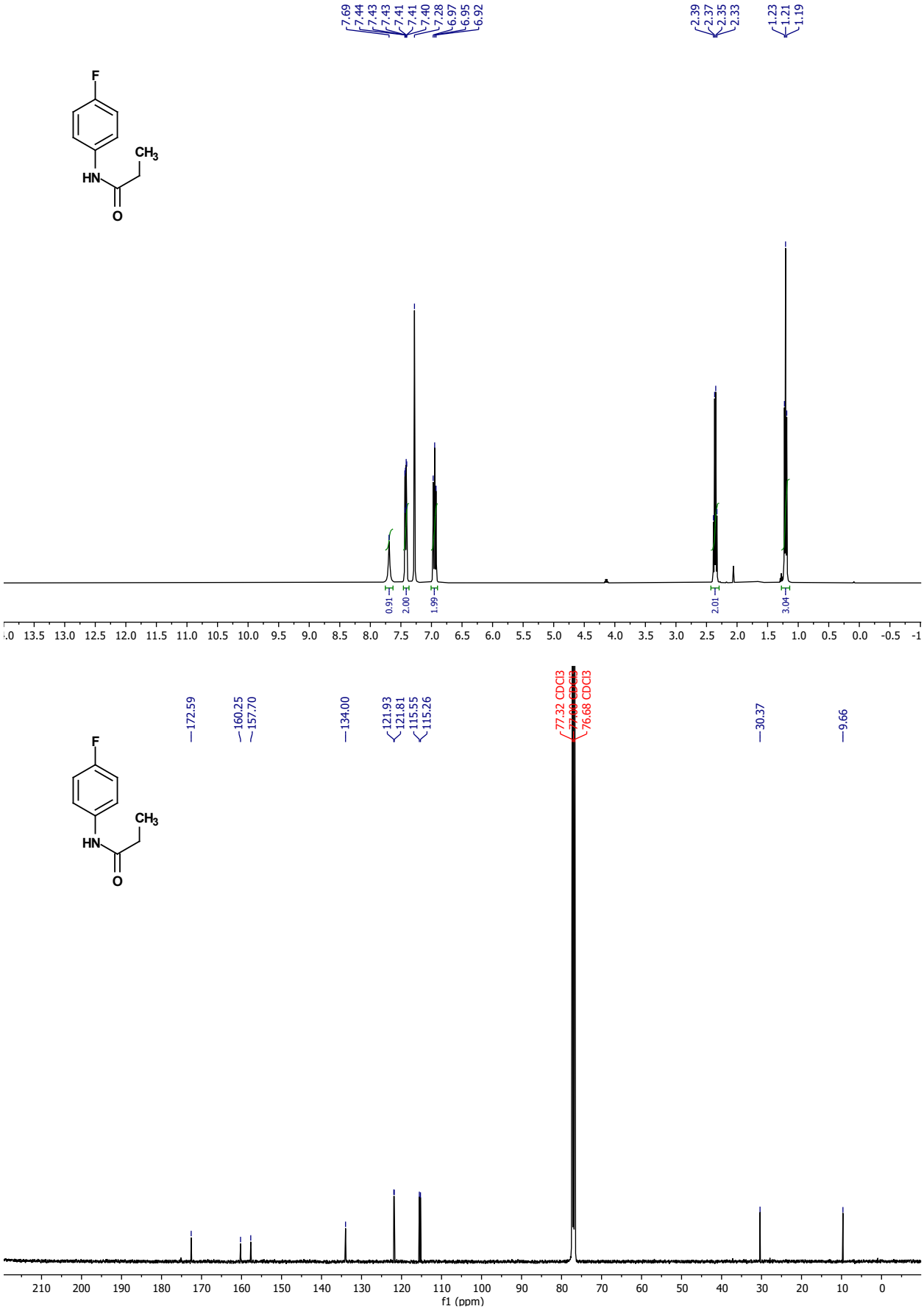
HSQC NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)propionamide (**3e**)



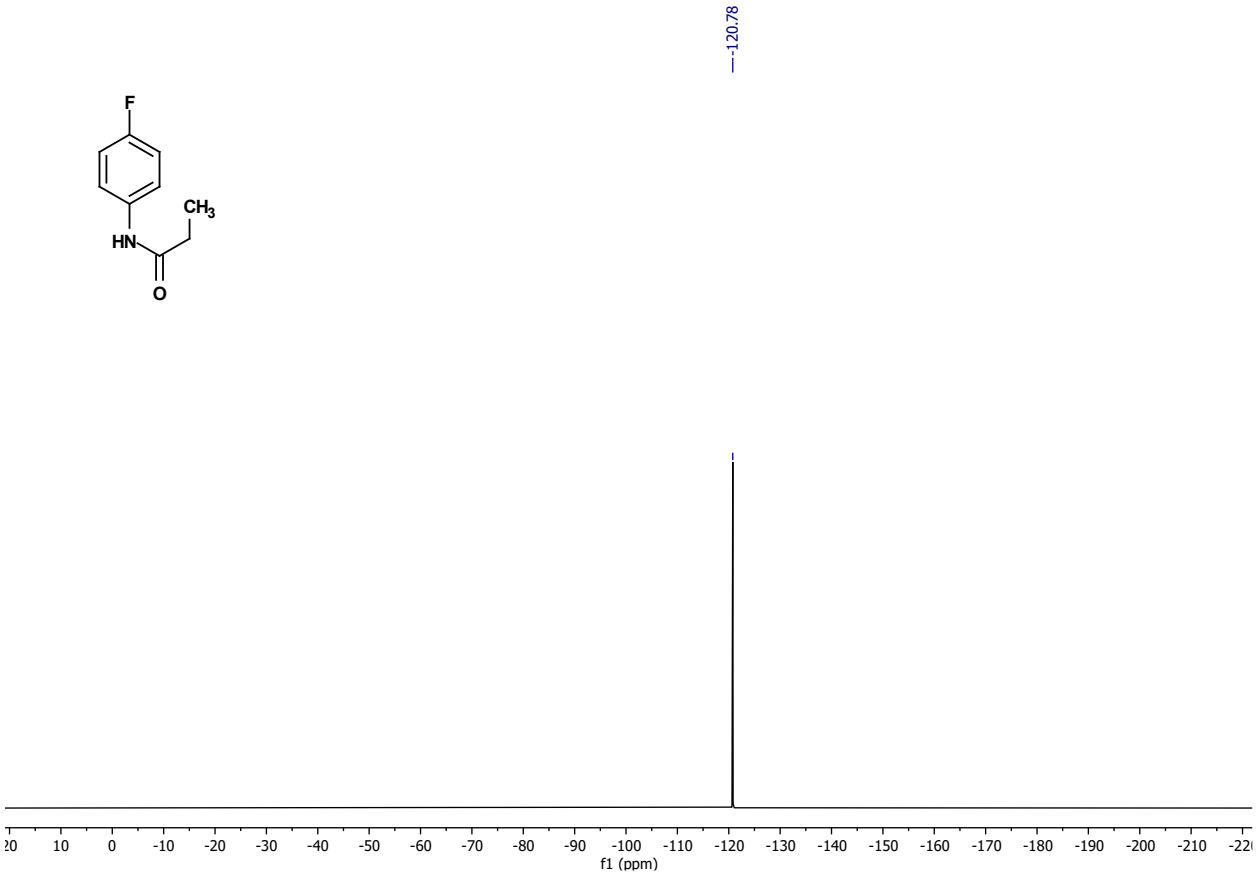
HMBC NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)propionamide (**3e**)



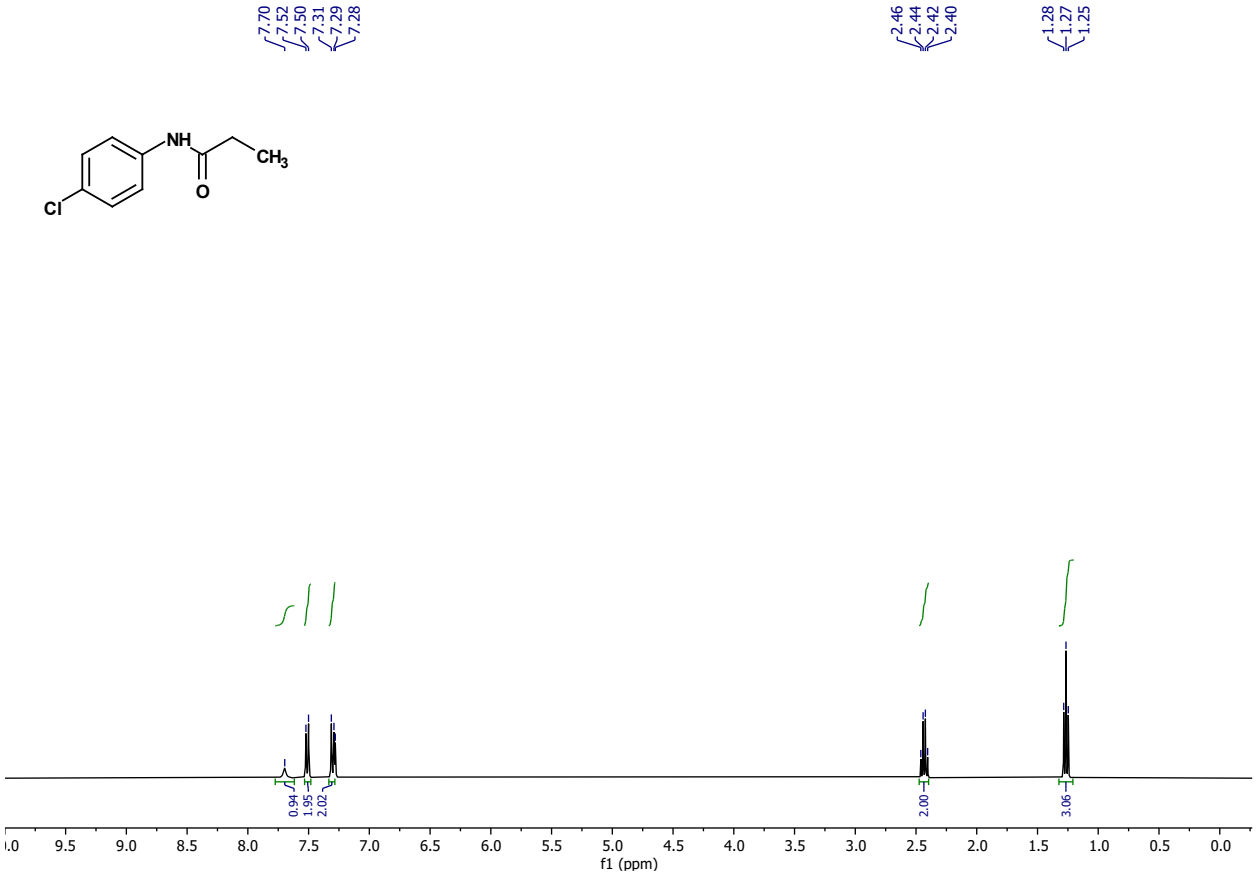
^{1}H and ^{13}C NMR *N*-(4-fluorophenyl)propionamide (**3f**)

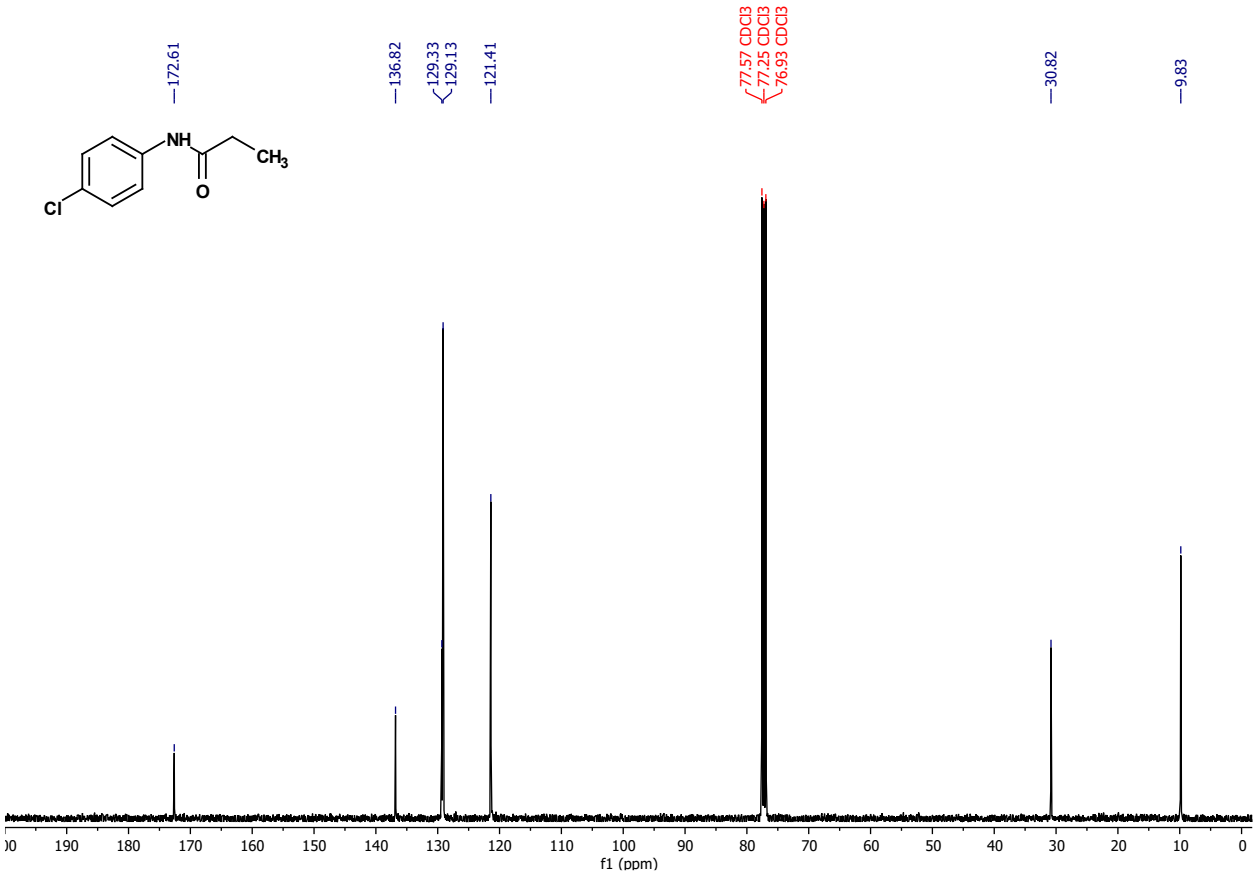


^{19}F NMR *N*-(4-fluorophenyl)propionamide (**3f**)

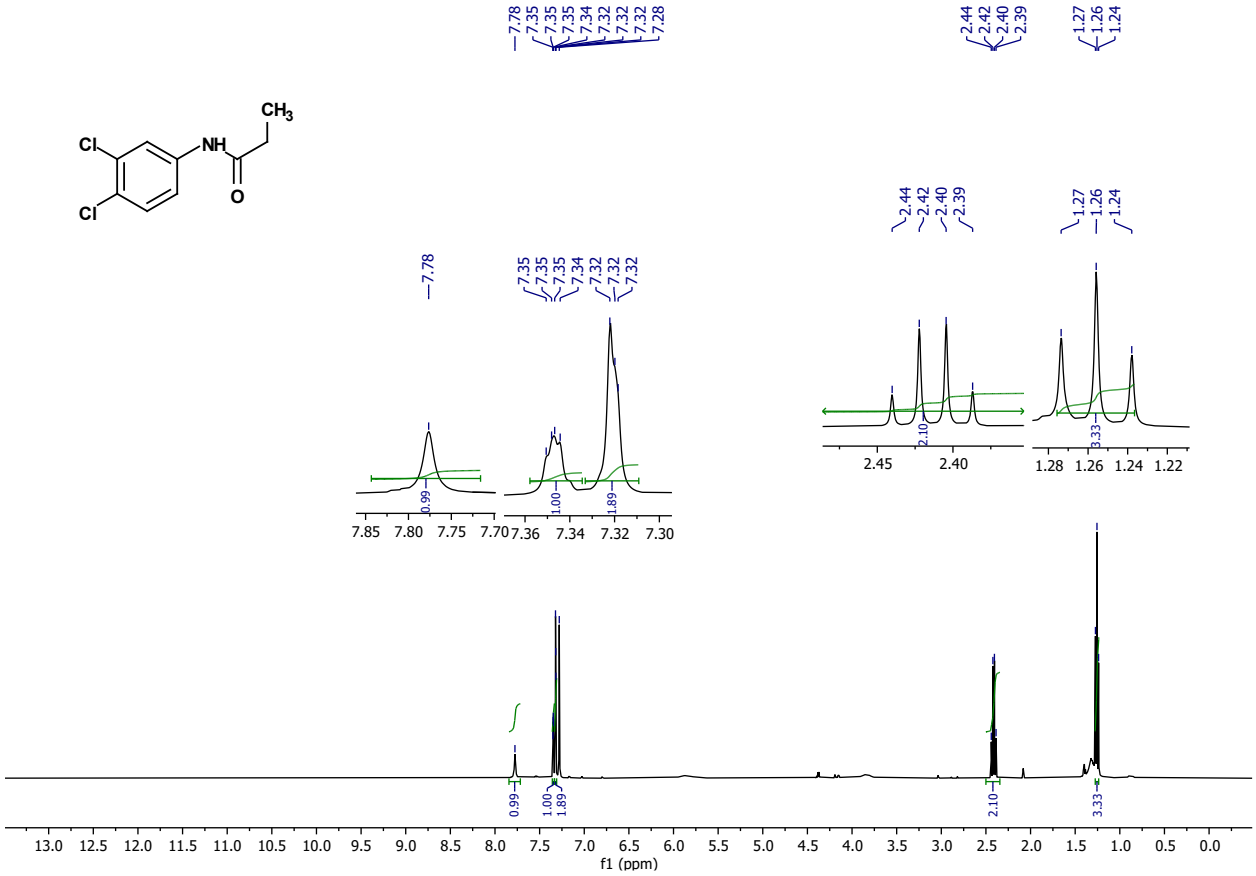


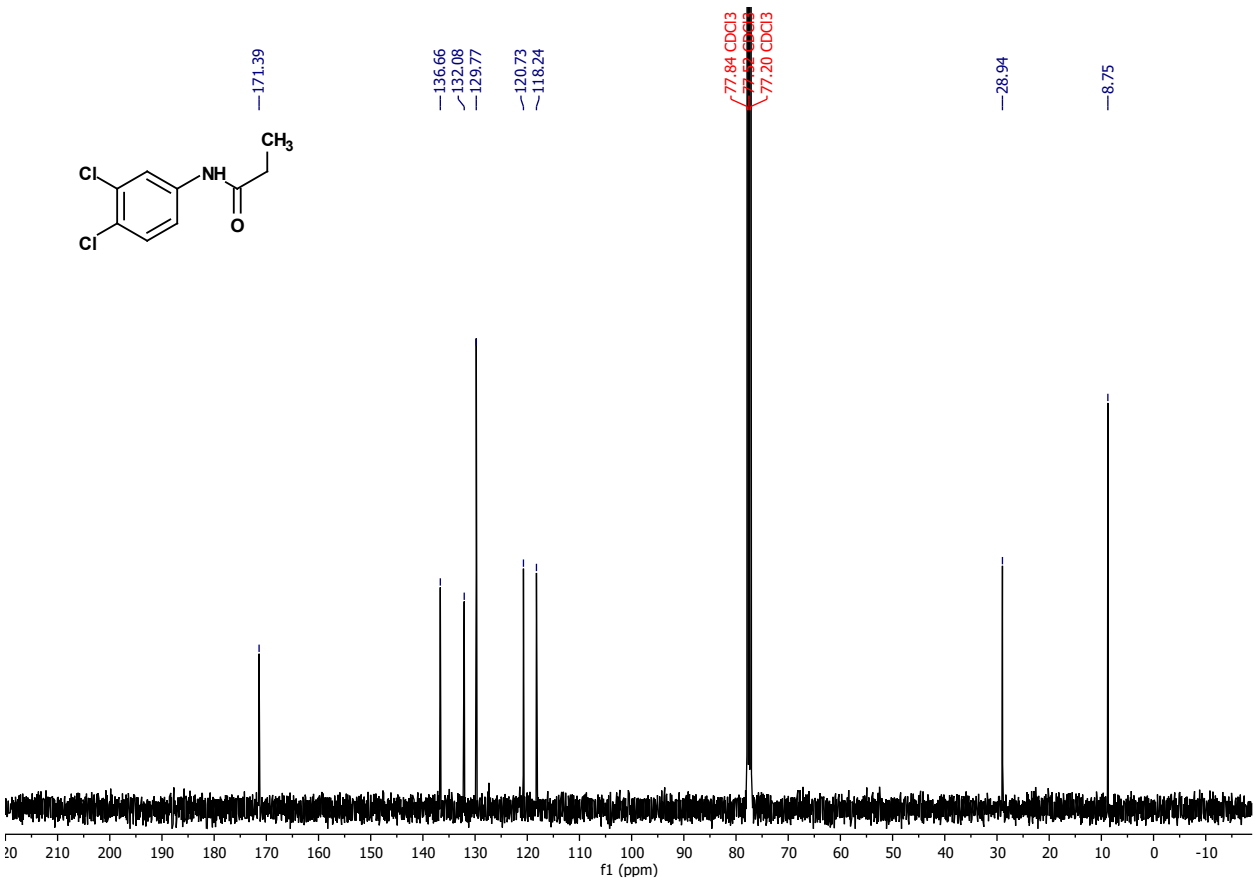
^{1}H and ^{13}C NMR *N*-(4-chlorophenyl)propionamide (**3g**)



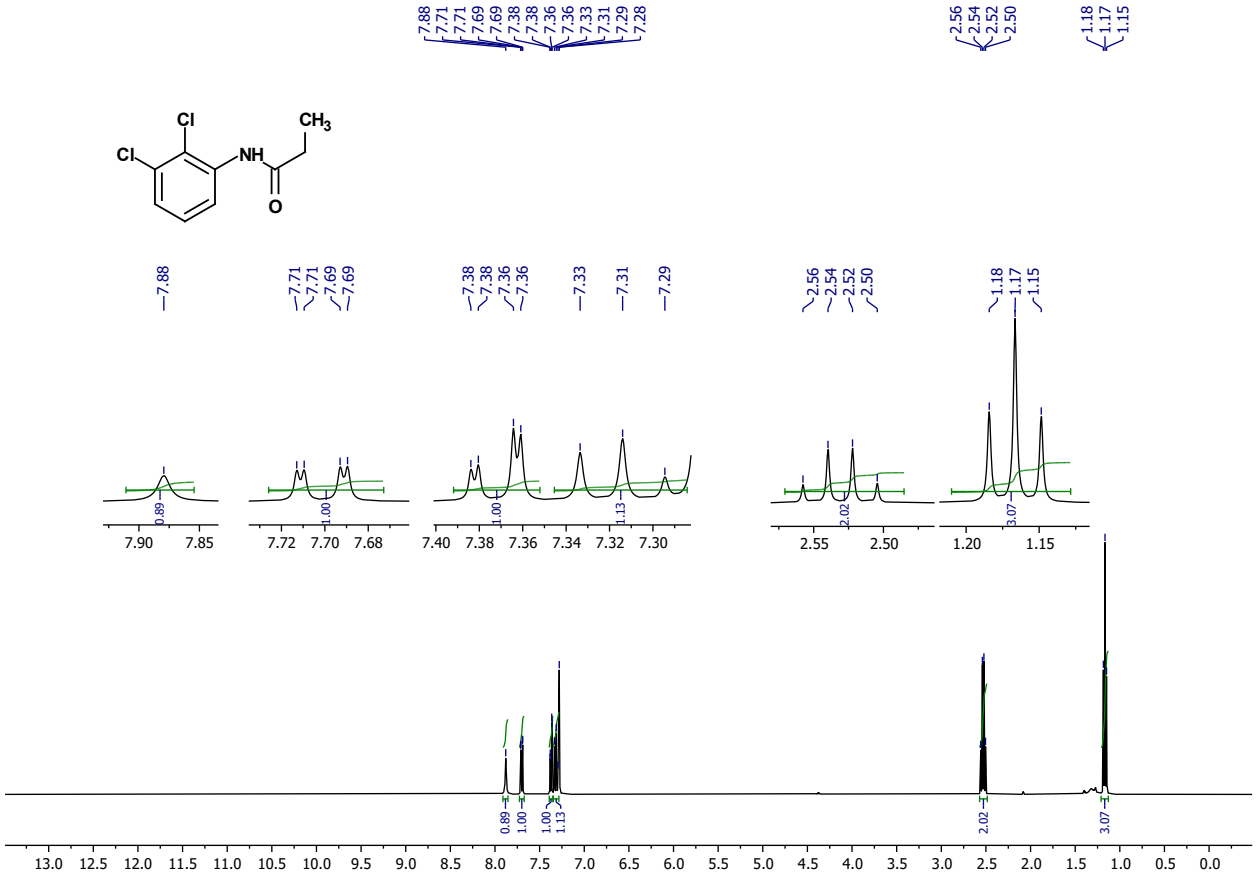


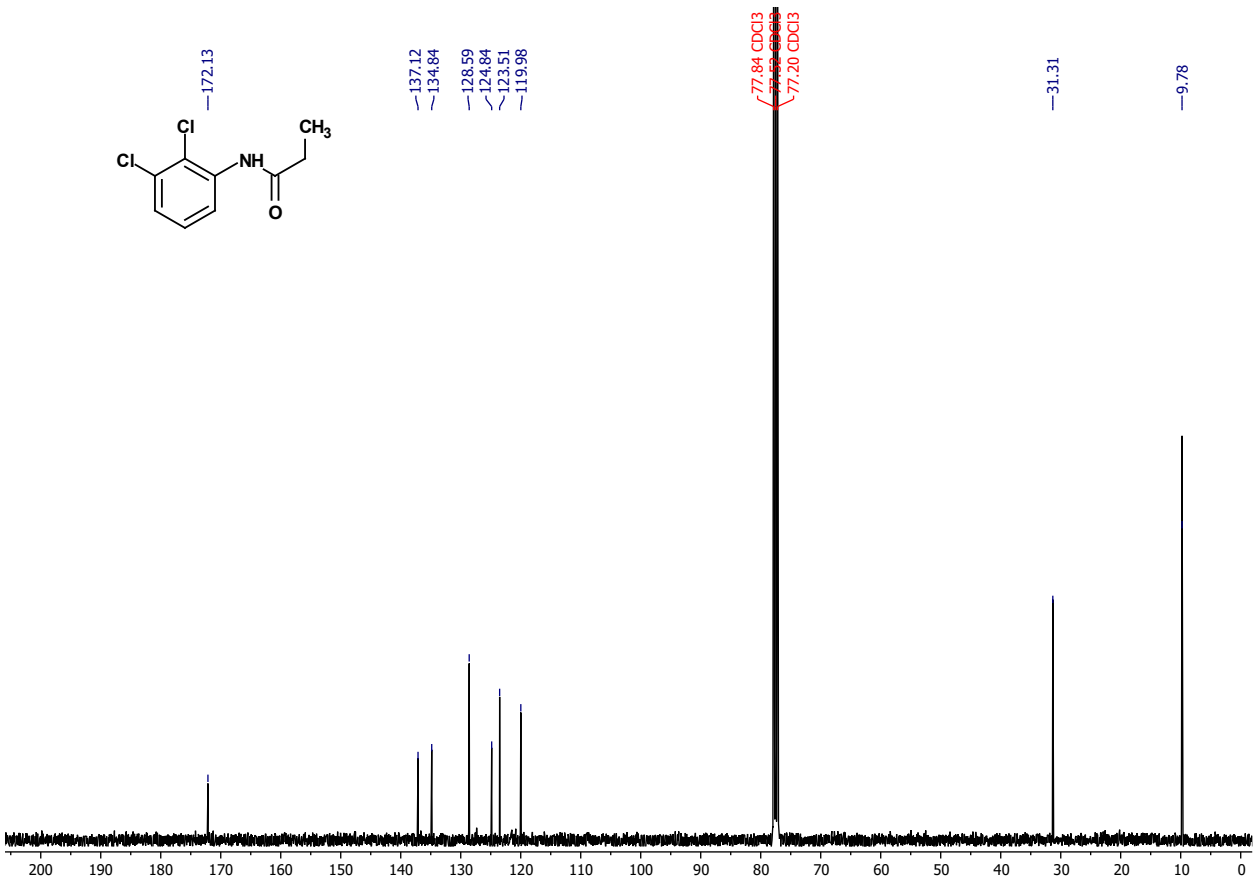
^{1}H and ^{13}C NMR *N*-(3,4-dichlorophenyl)propionamide (**3h**-*a*)



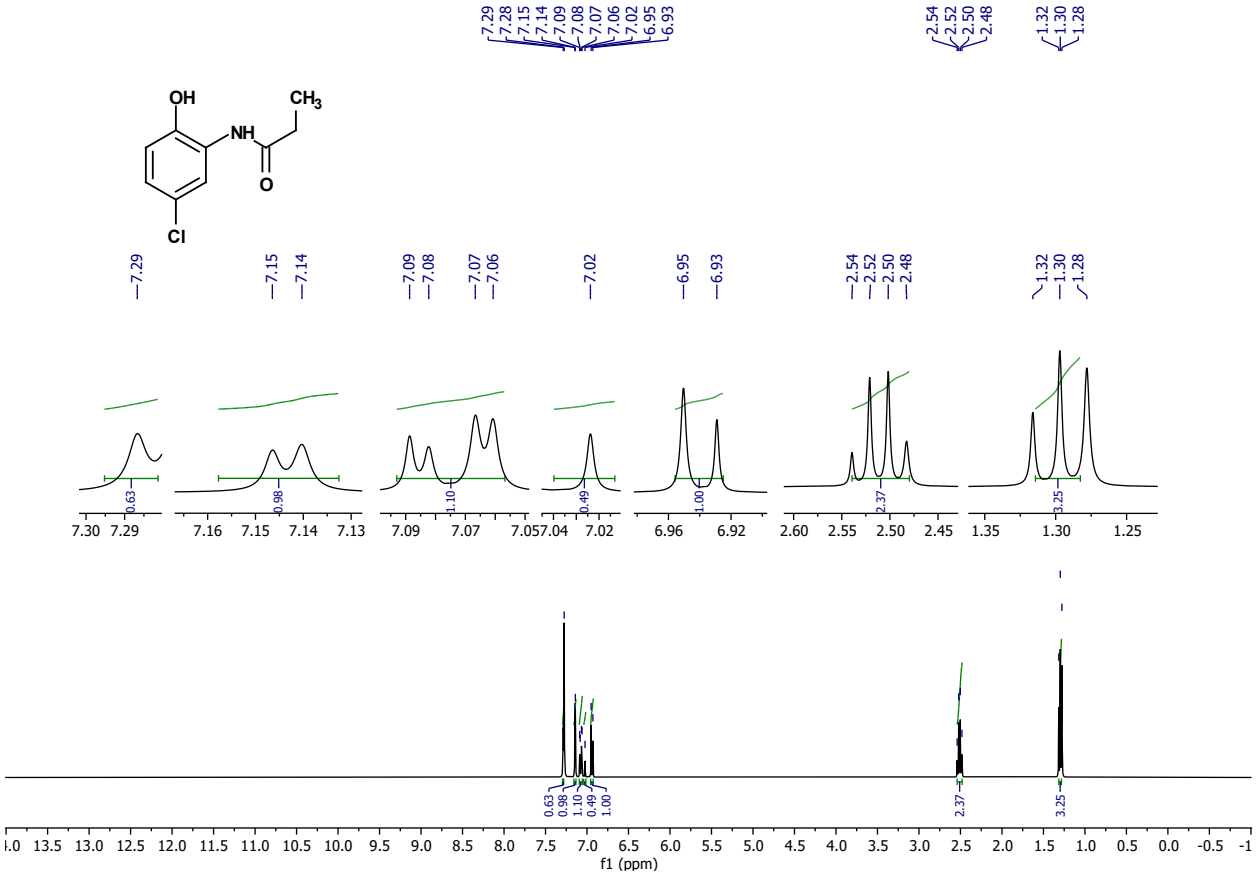


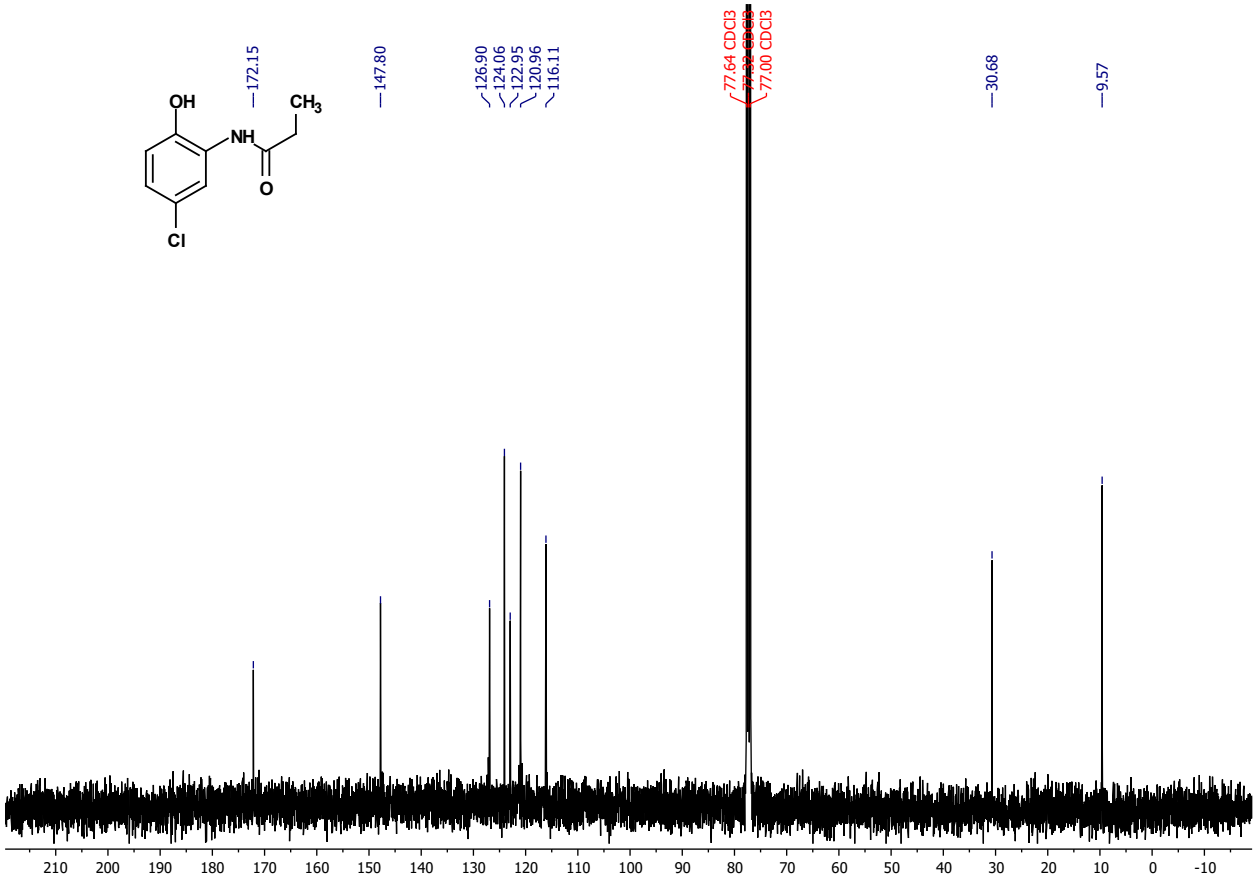
^{1}H and ^{13}C NMR *N*-(3,4-dichlorophenyl)propionamide (**3h**-*b*)



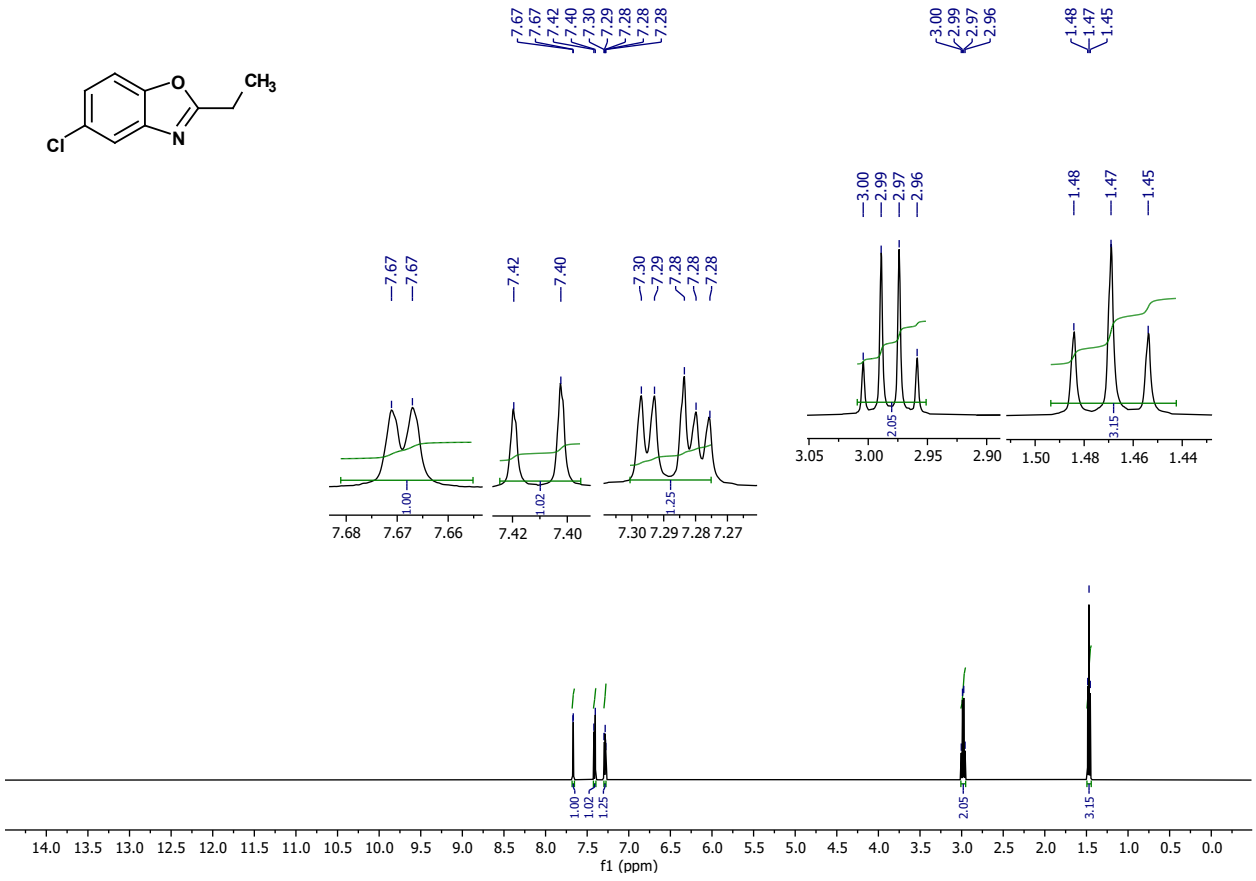


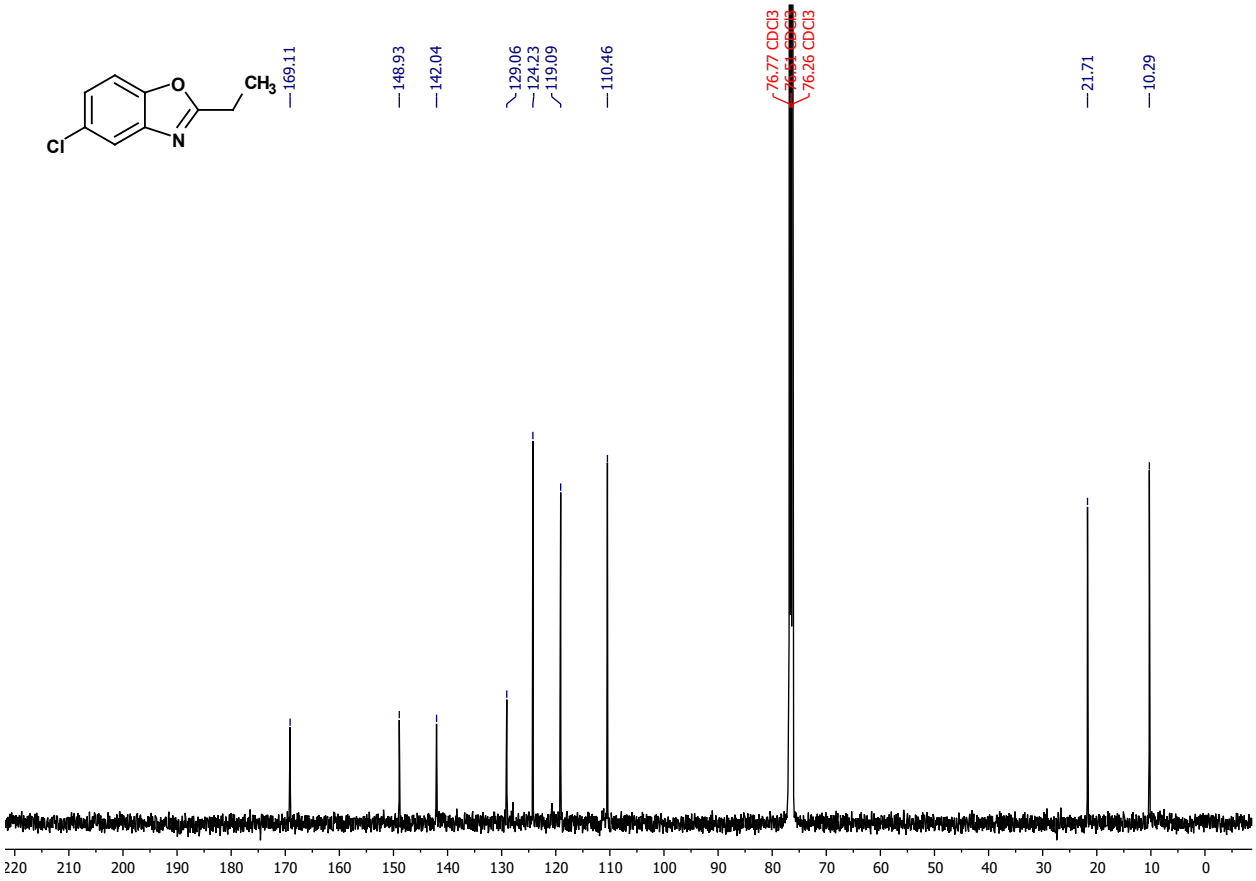
^{1}H and ^{13}C NMR *N*-(5-chloro-2-hydroxyphenyl)propionamide (**3i**)



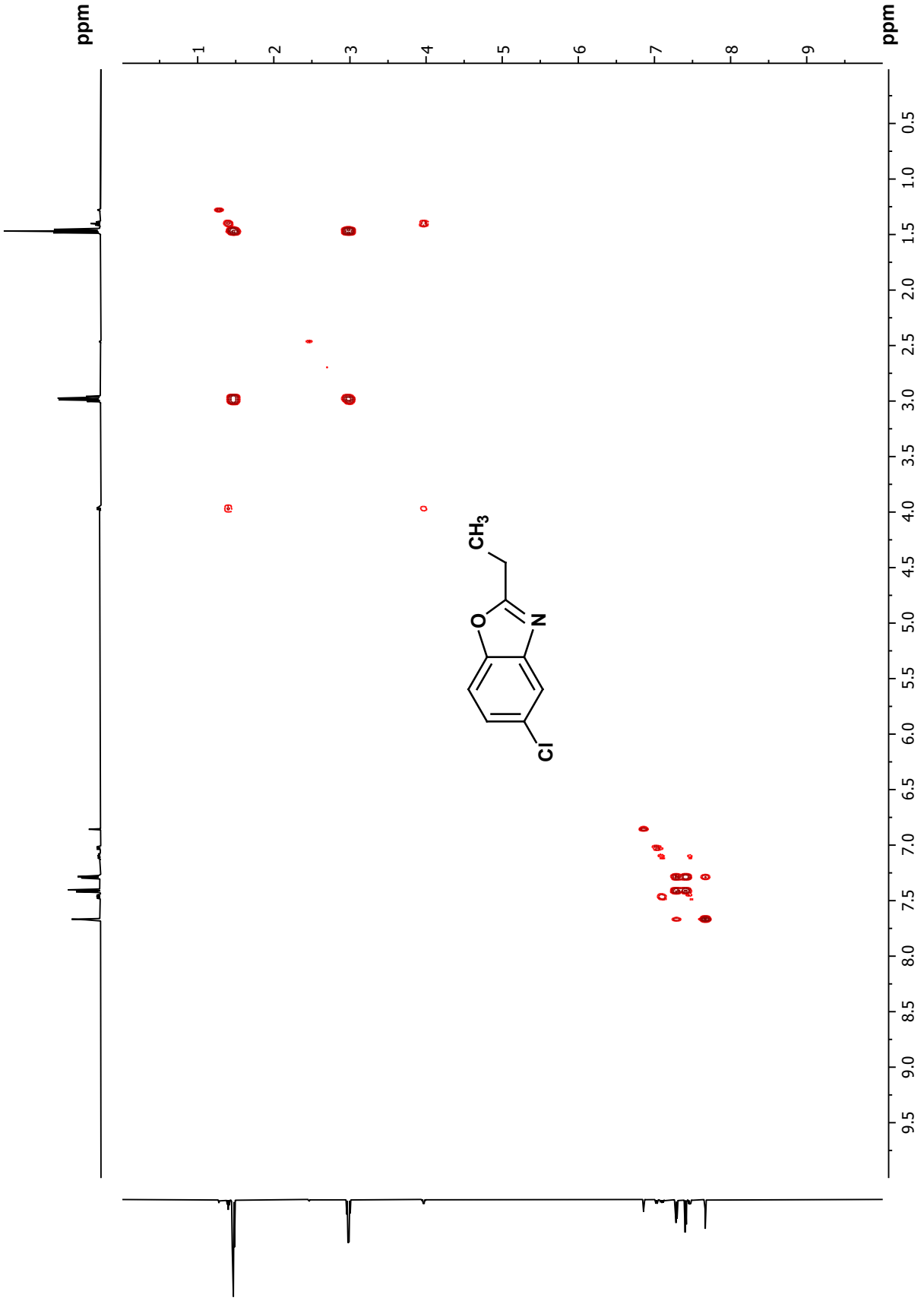


^{1}H and ^{13}C NMR 5-chloro-2-ethylbenzo[d]oxazole **(3ii)**

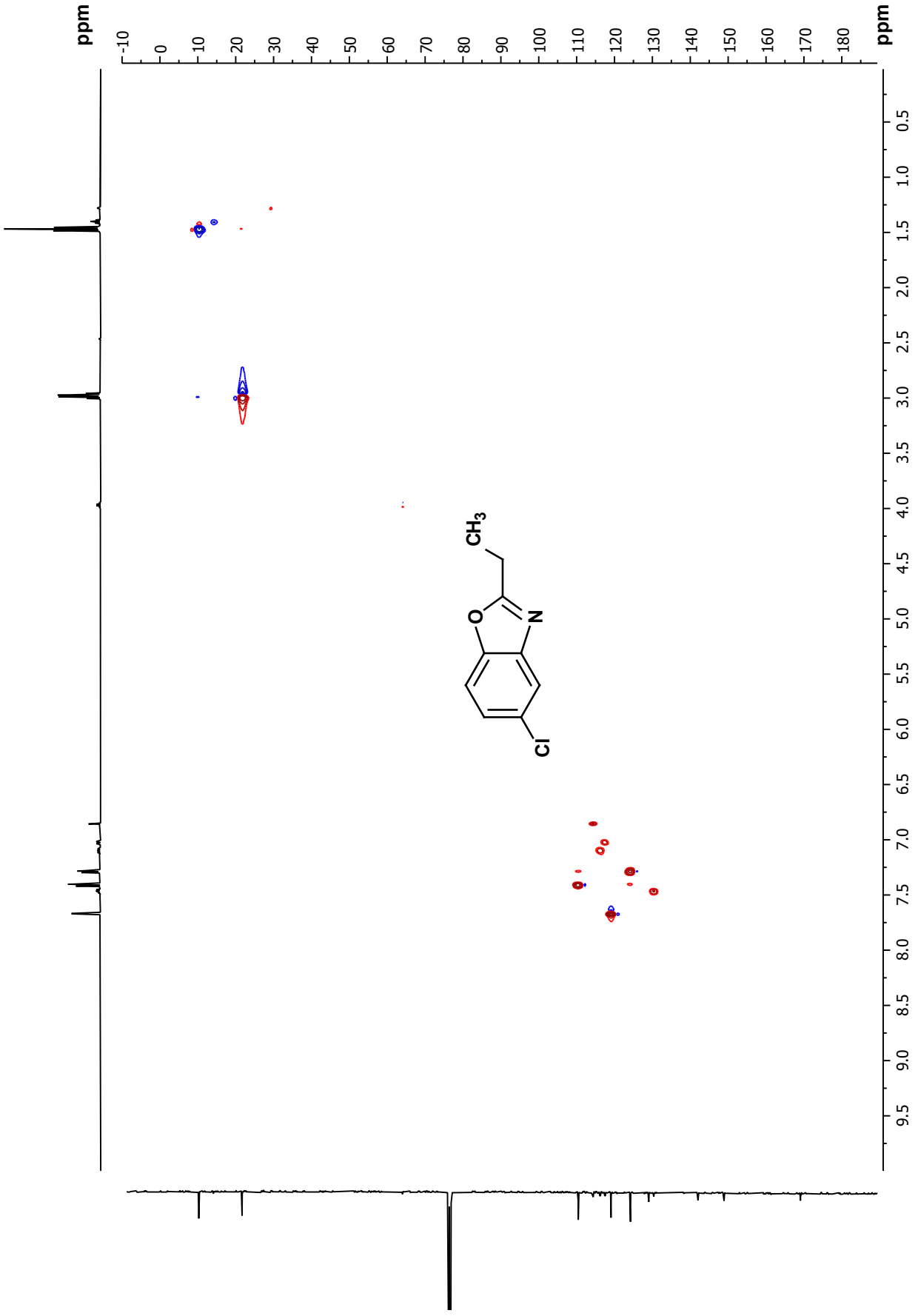




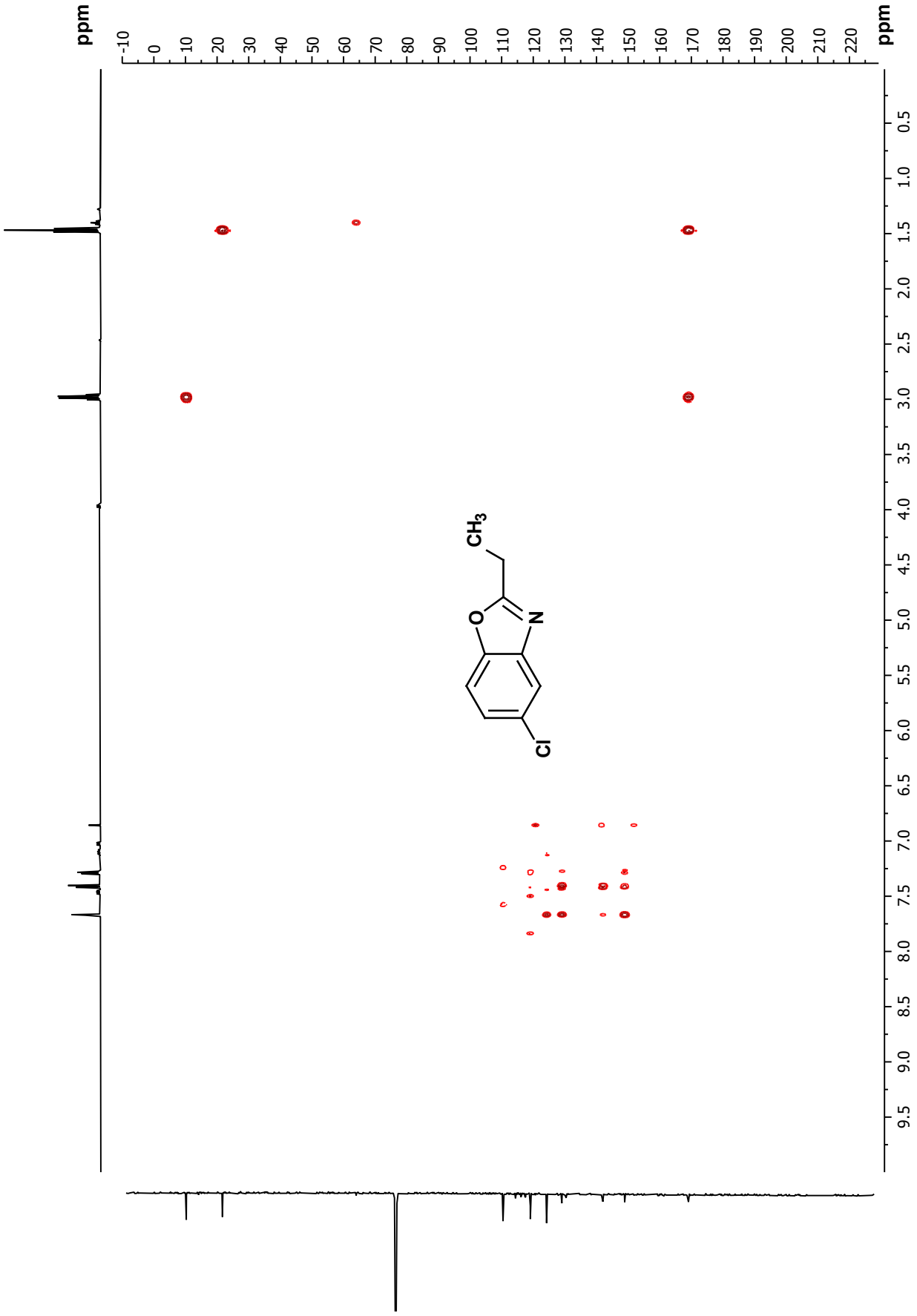
COSY NMR 5-chloro-2-ethylbenzo[d]oxazole **(3ii)**



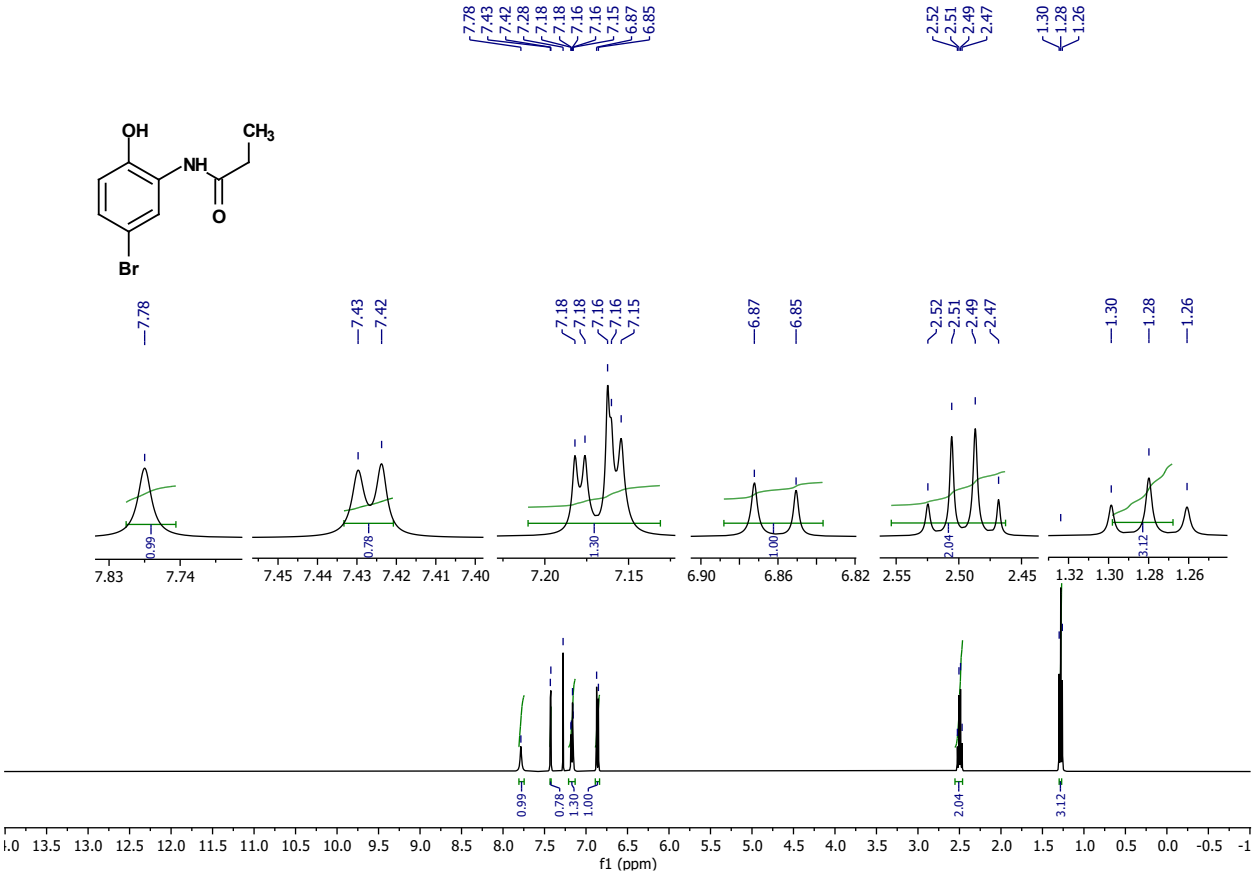
HSQC NMR 5-chloro-2-ethylbenzo[d]oxazole **(3ii)**

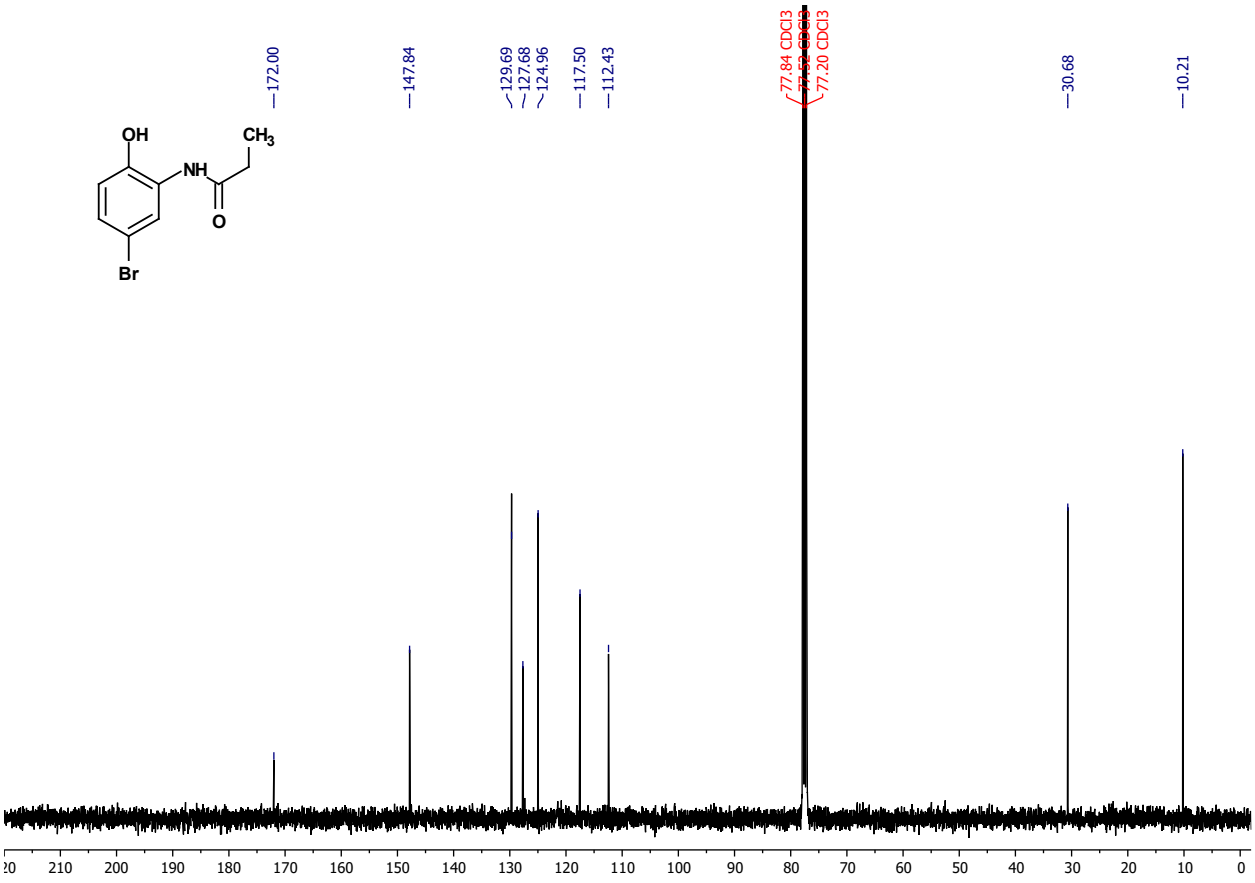


HMBC NMR 5-chloro-2-ethylbenzo[d]oxazole **(3ii)**

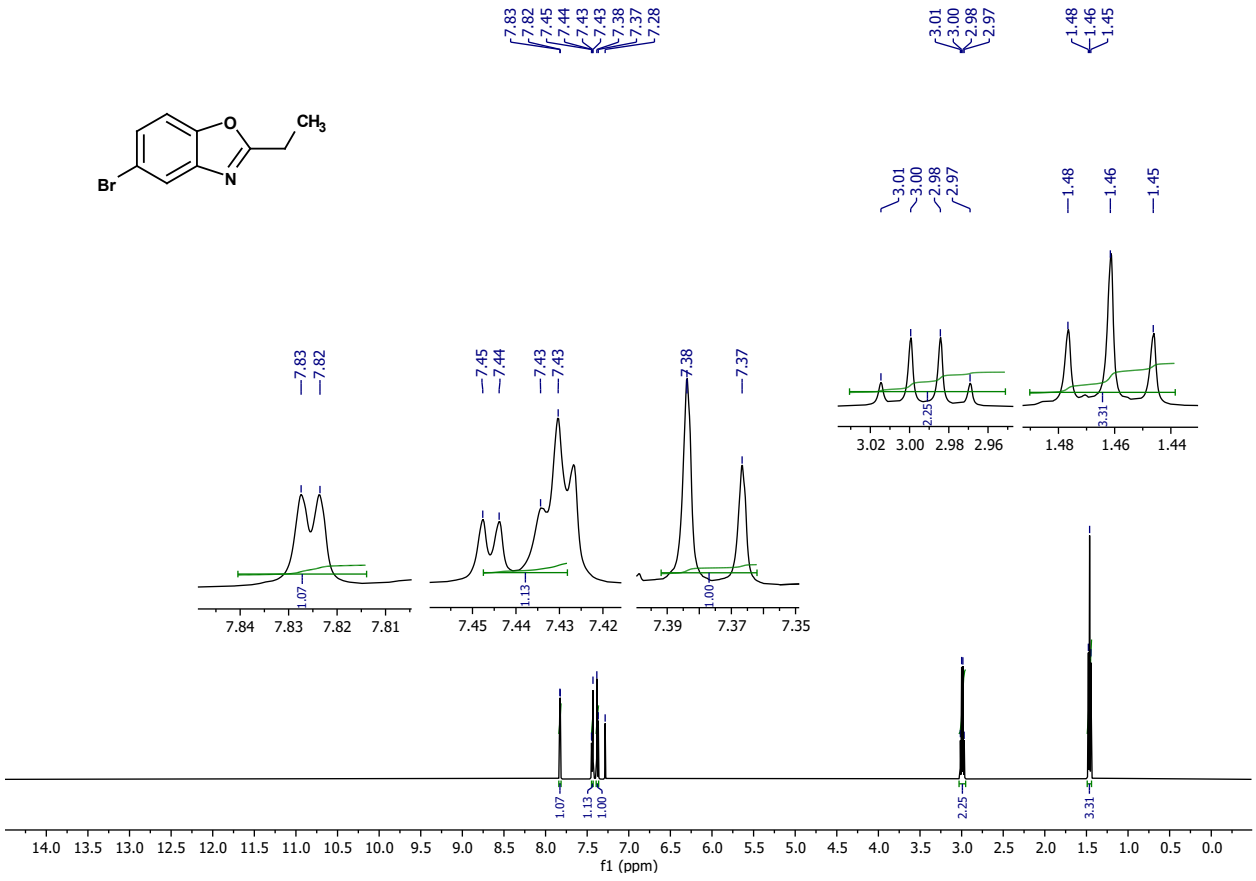


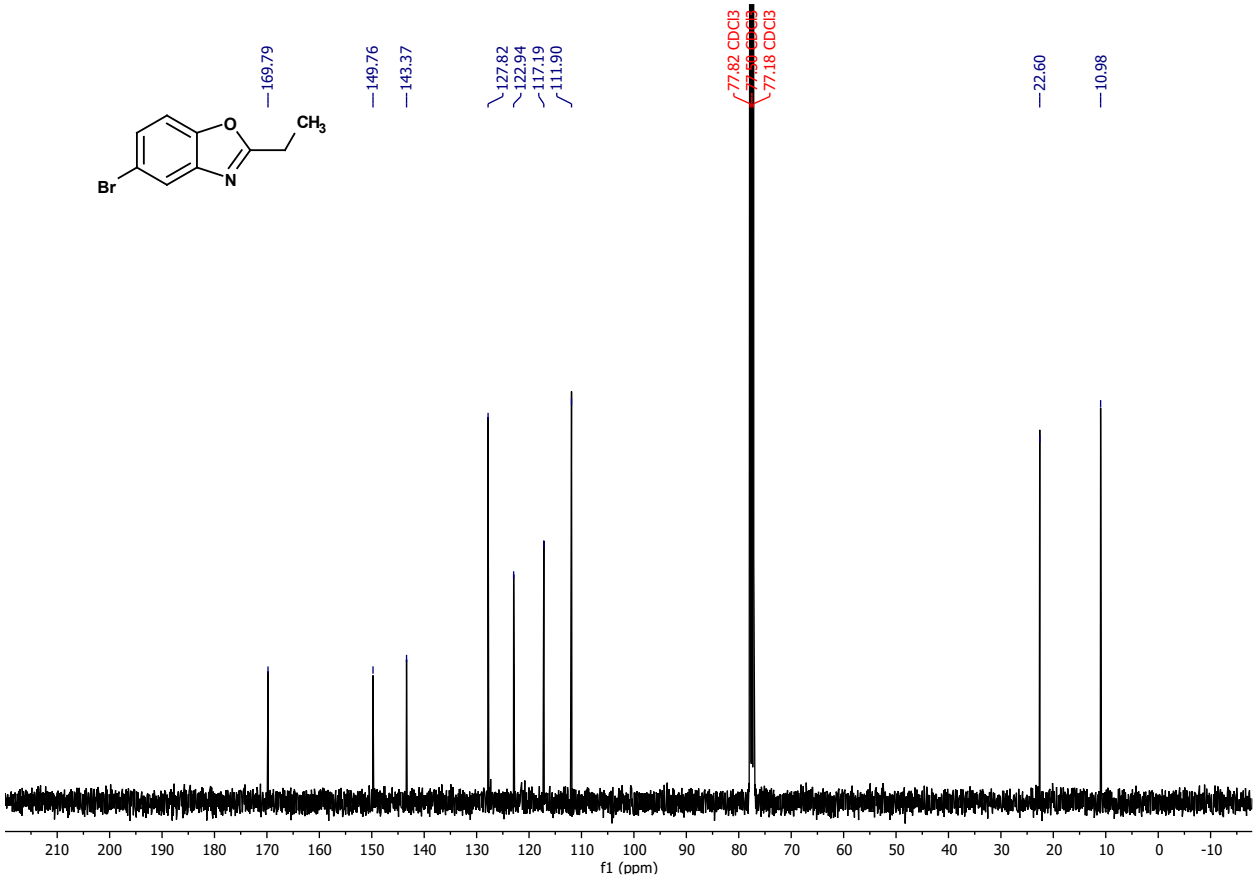
^{1}H and ^{13}C NMR *N*-(5-bromo-5-hydroxyphenyl)propionamide (**3j**)



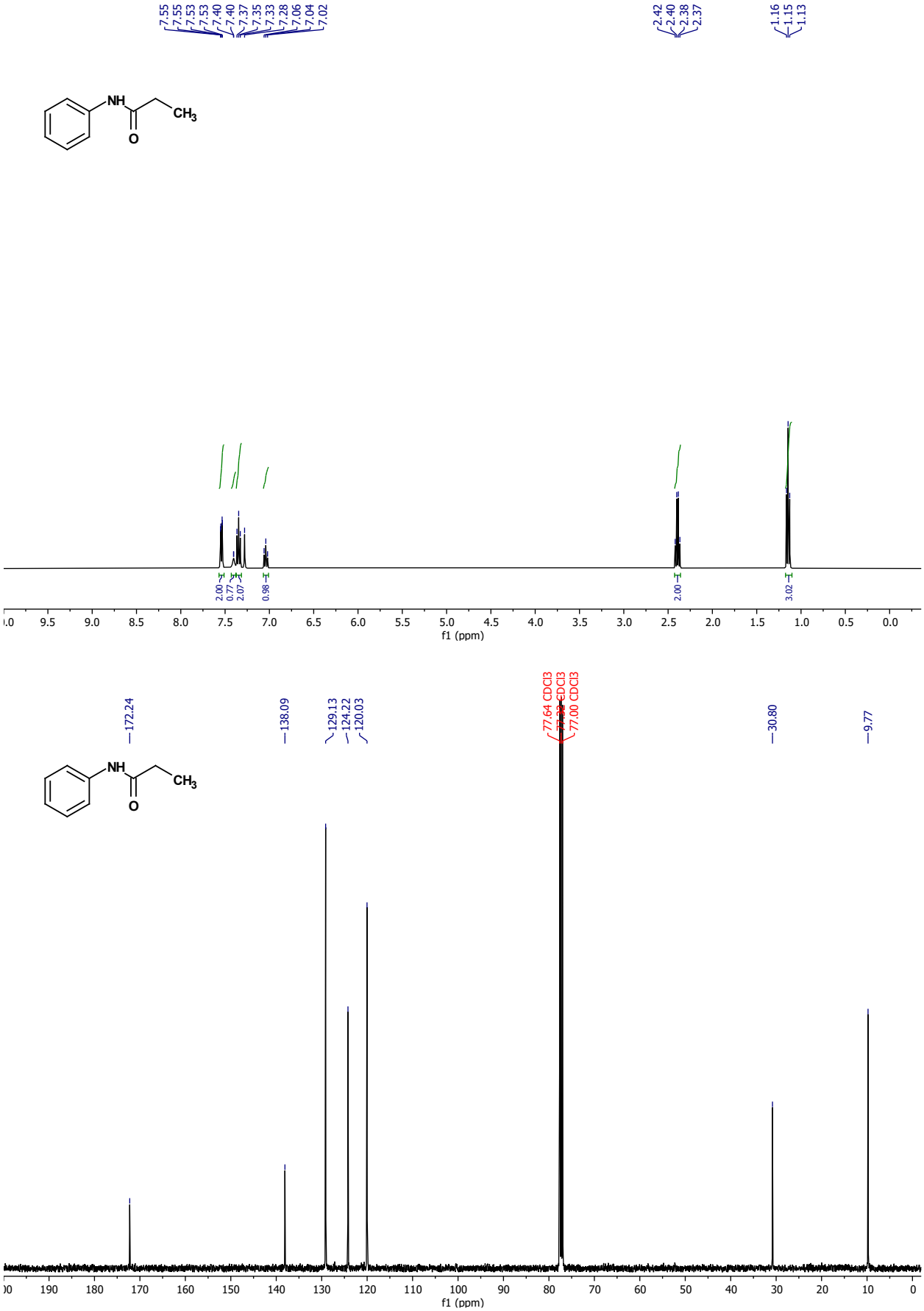


^{1}H and ^{13}C NMR 5-bromo-2-ethylbenzo[d]oxazole **(3jj)**

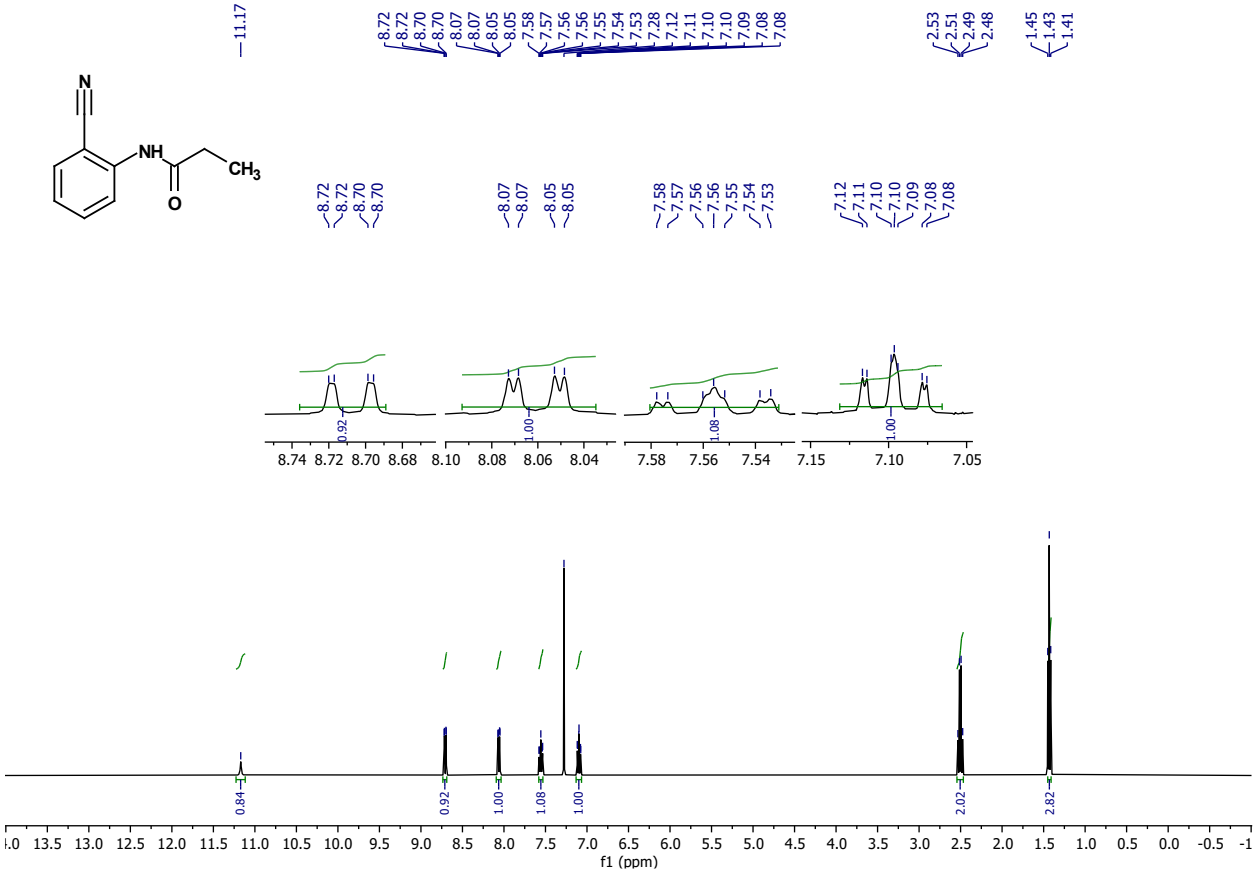


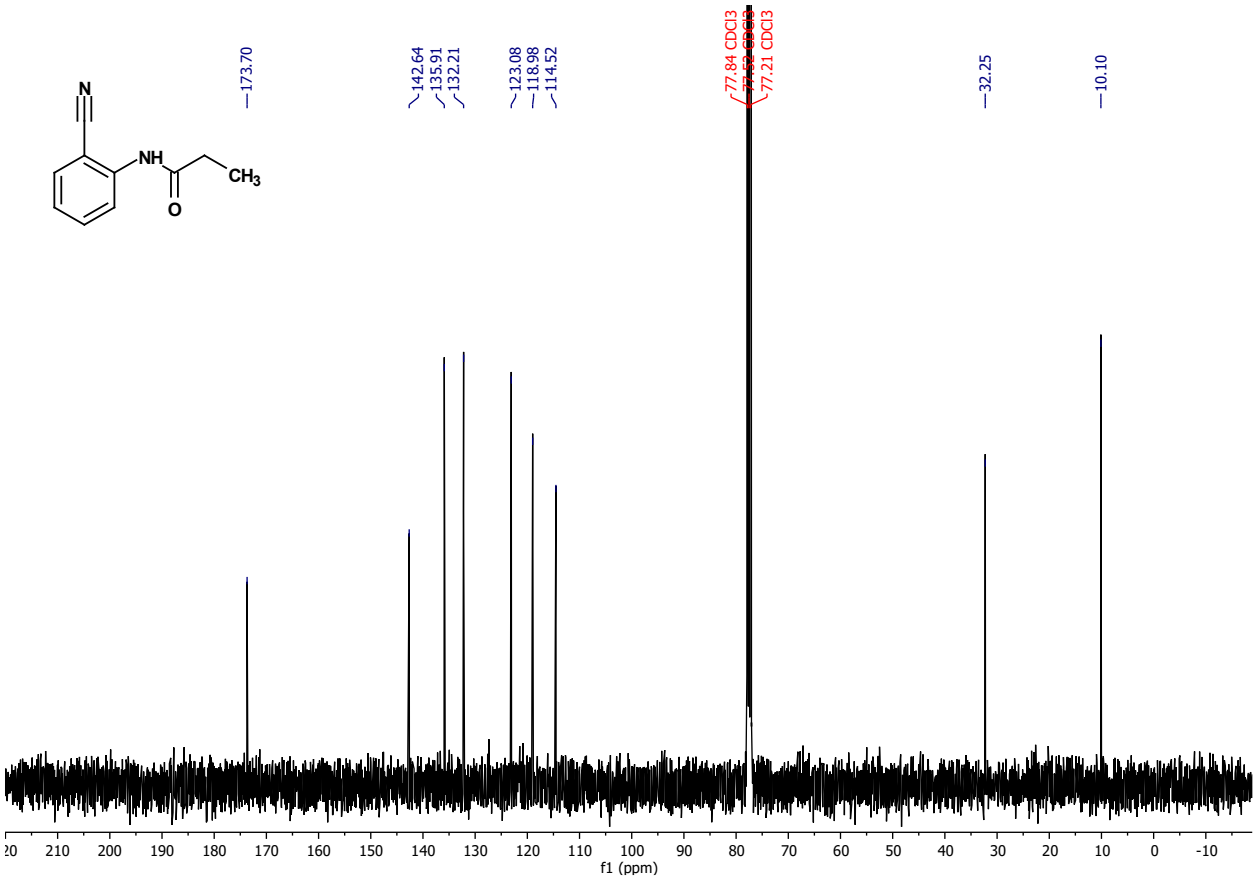


^{1}H and ^{13}C NMR *N*-phenylpropionamide (**3k**)

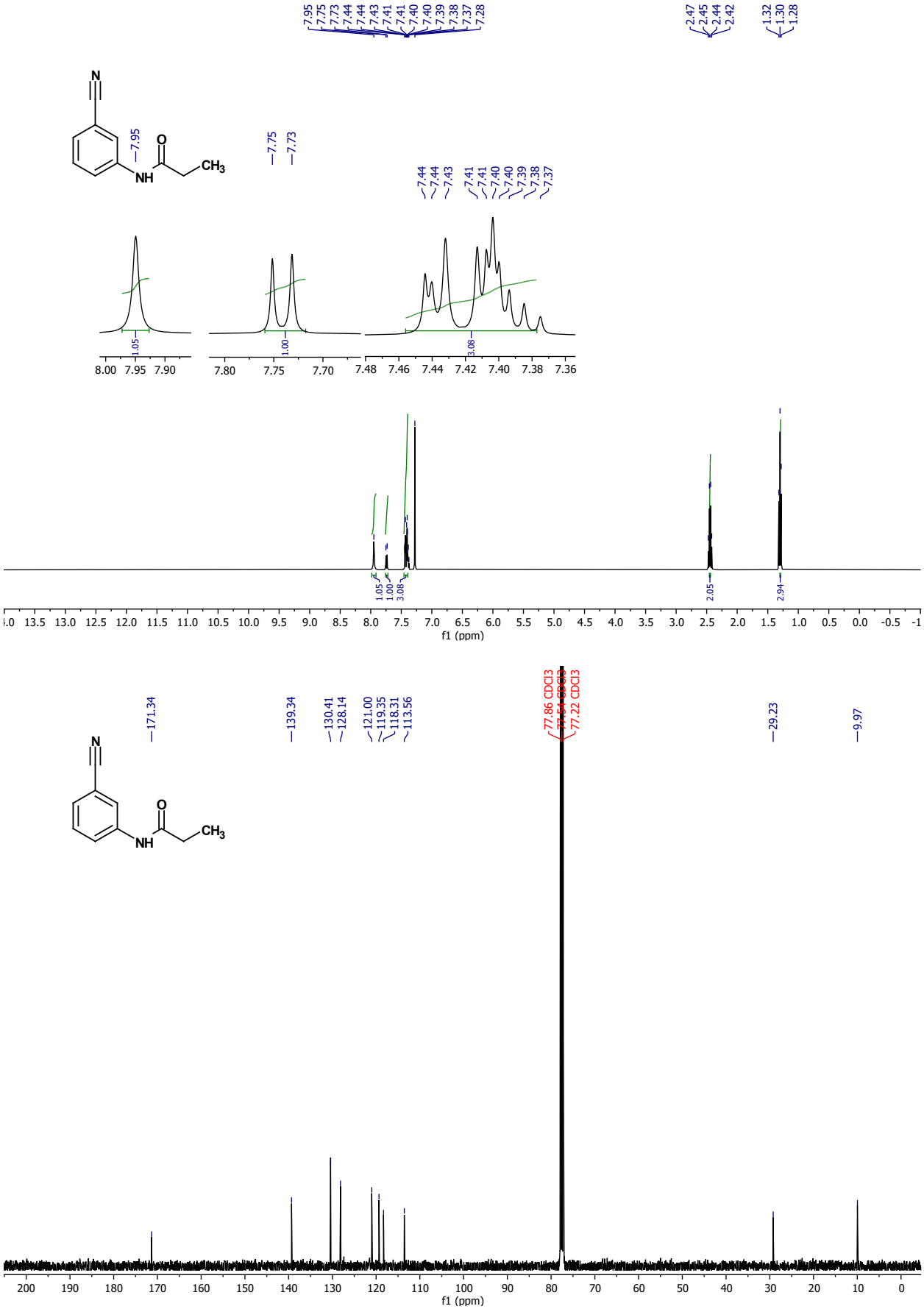


^{1}H and ^{13}C NMR *N*-(2-cyanophenyl)propionamide (**3l**-*a*)

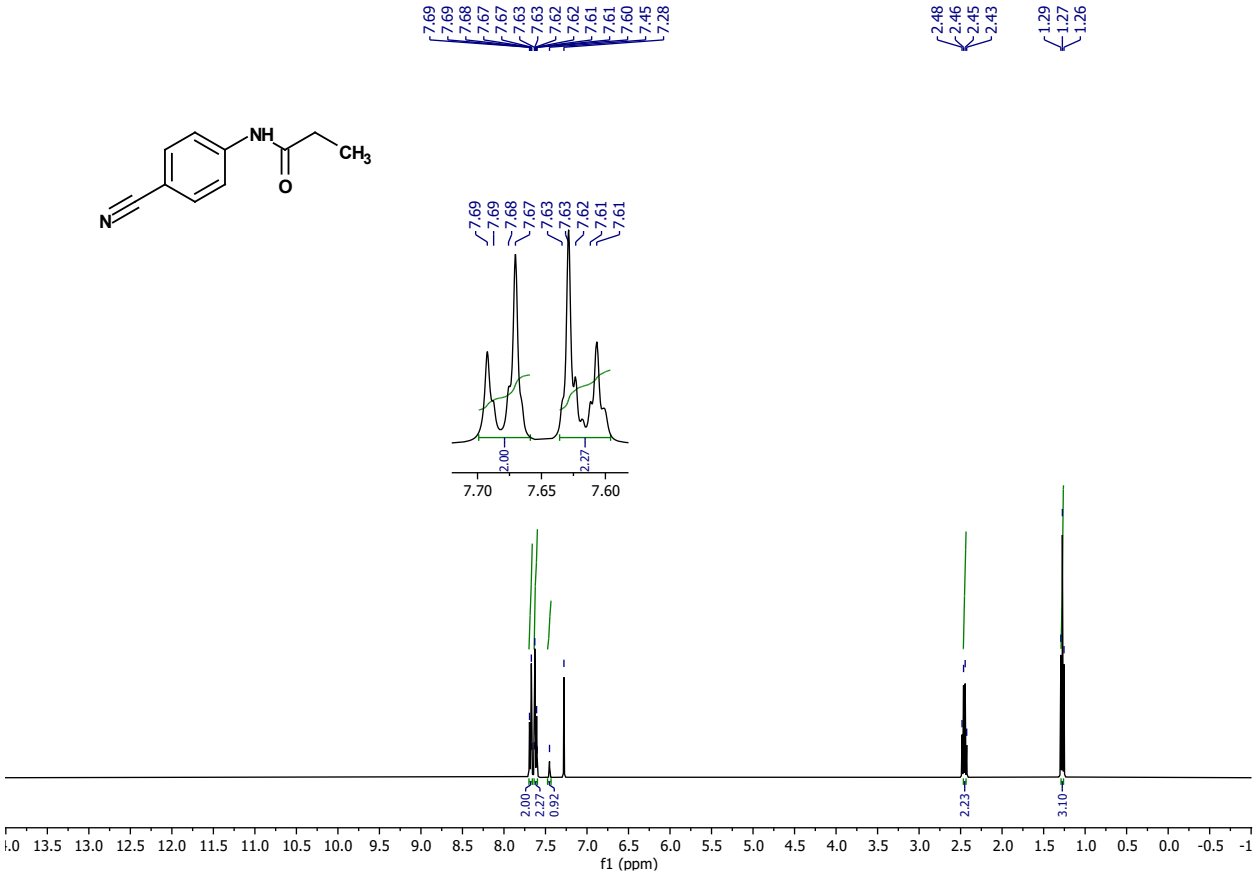


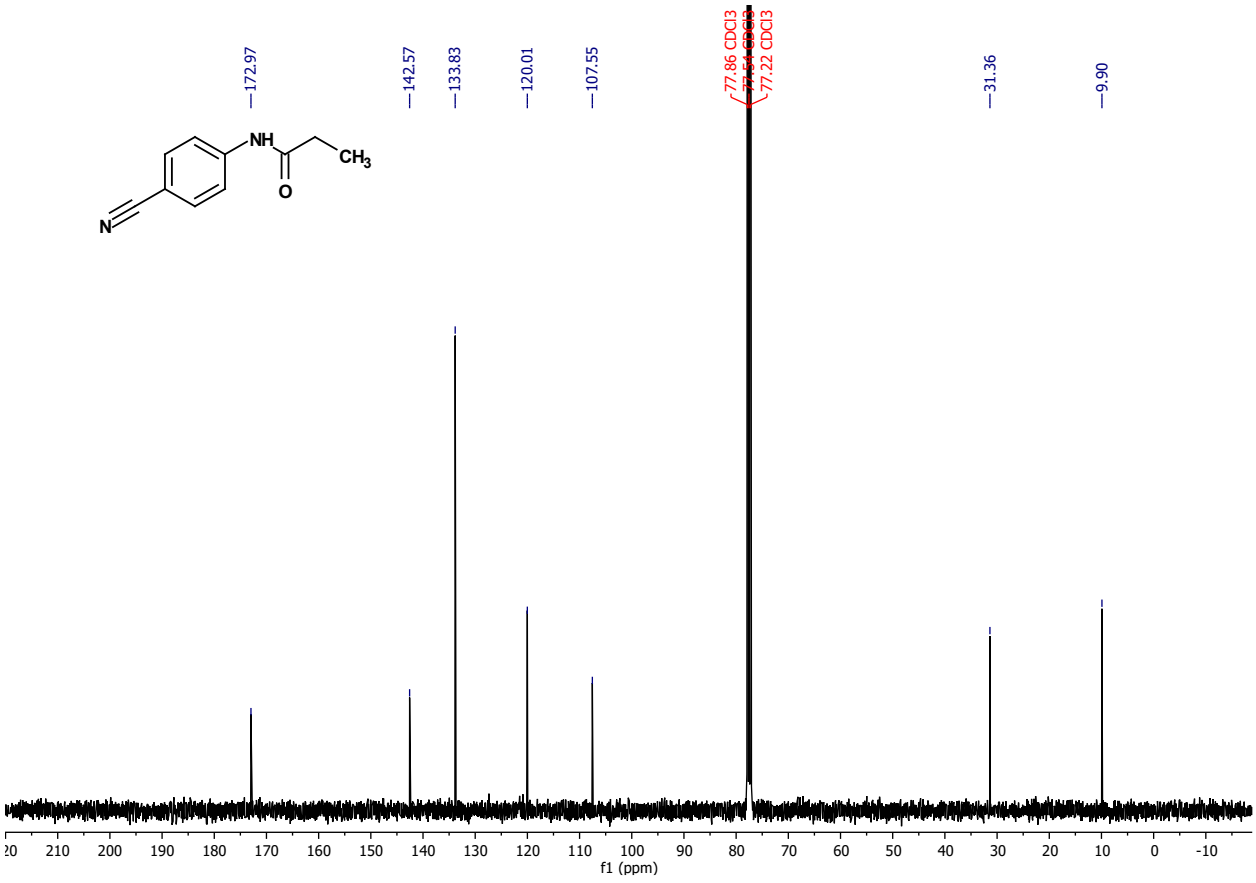


^{1}H and ^{13}C NMR *N*-(3-cyanophenyl)propionamide (**3l**-*b*)

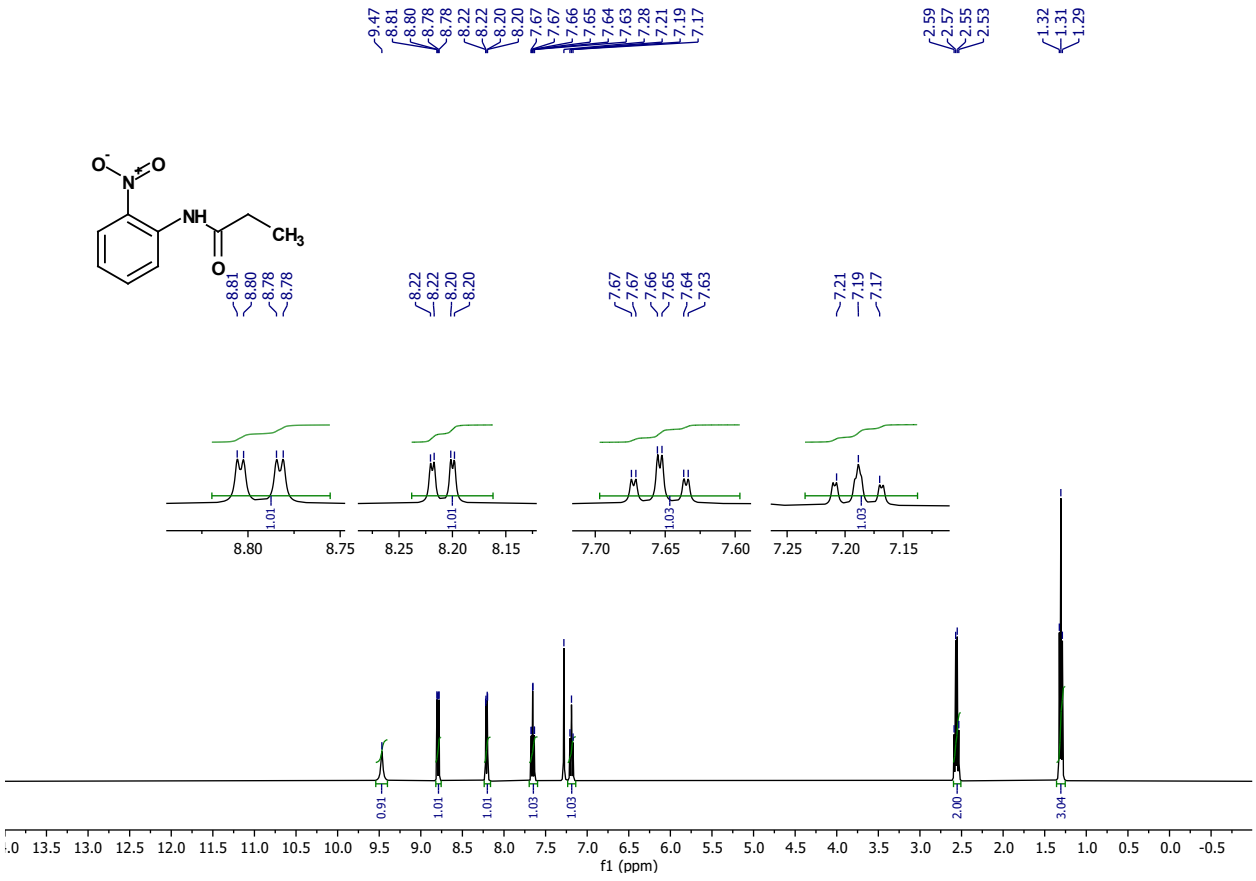


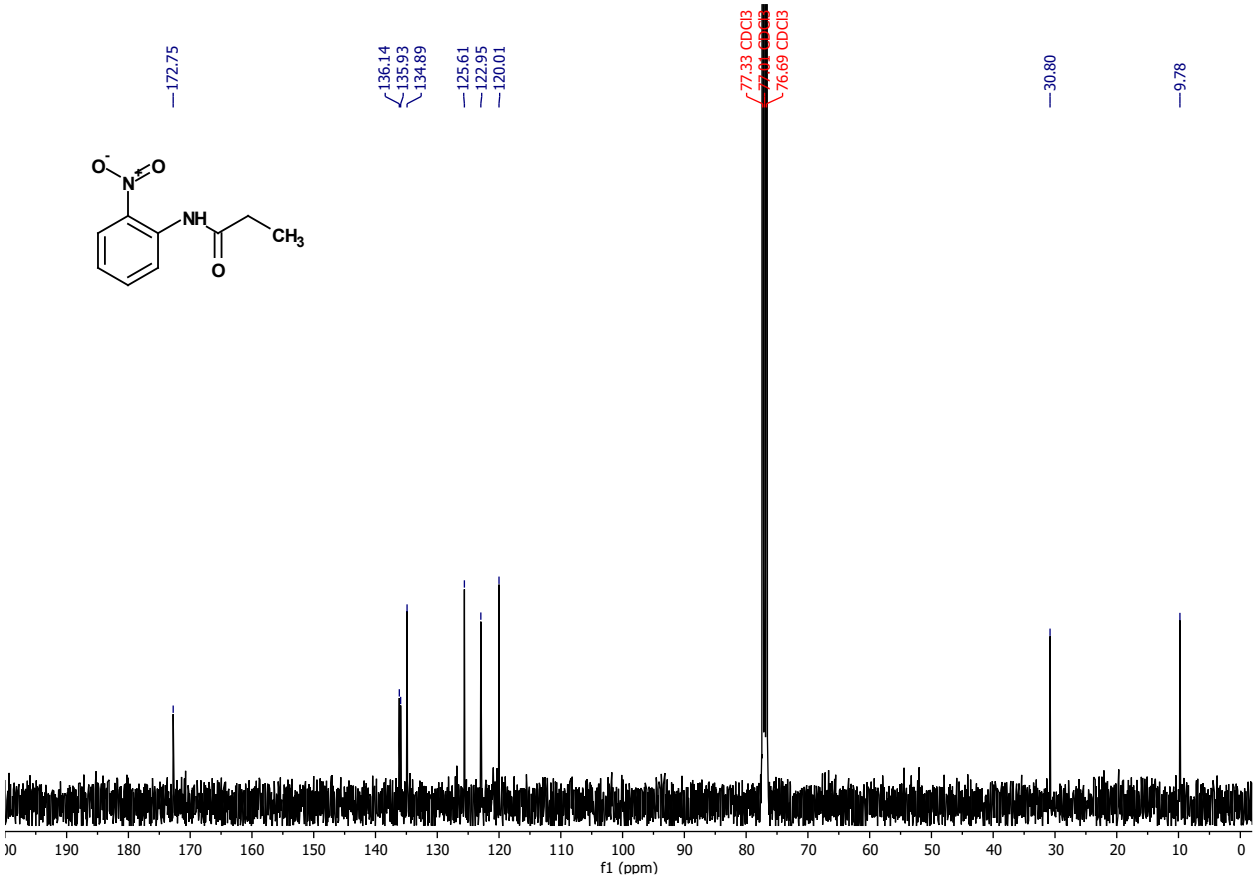
^{1}H and ^{13}C NMR *N*-(4-cyanophenyl)propionamide (**3l**-*c*)



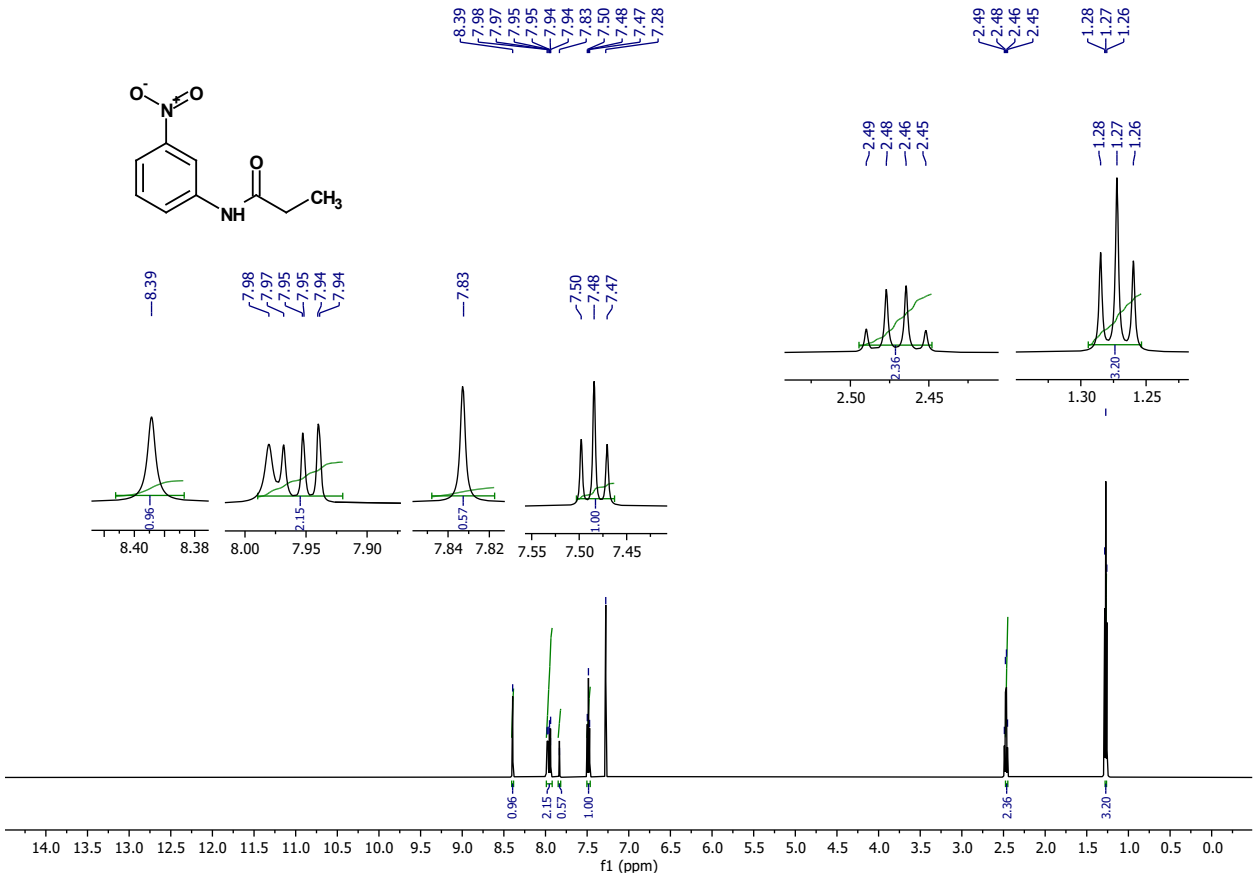


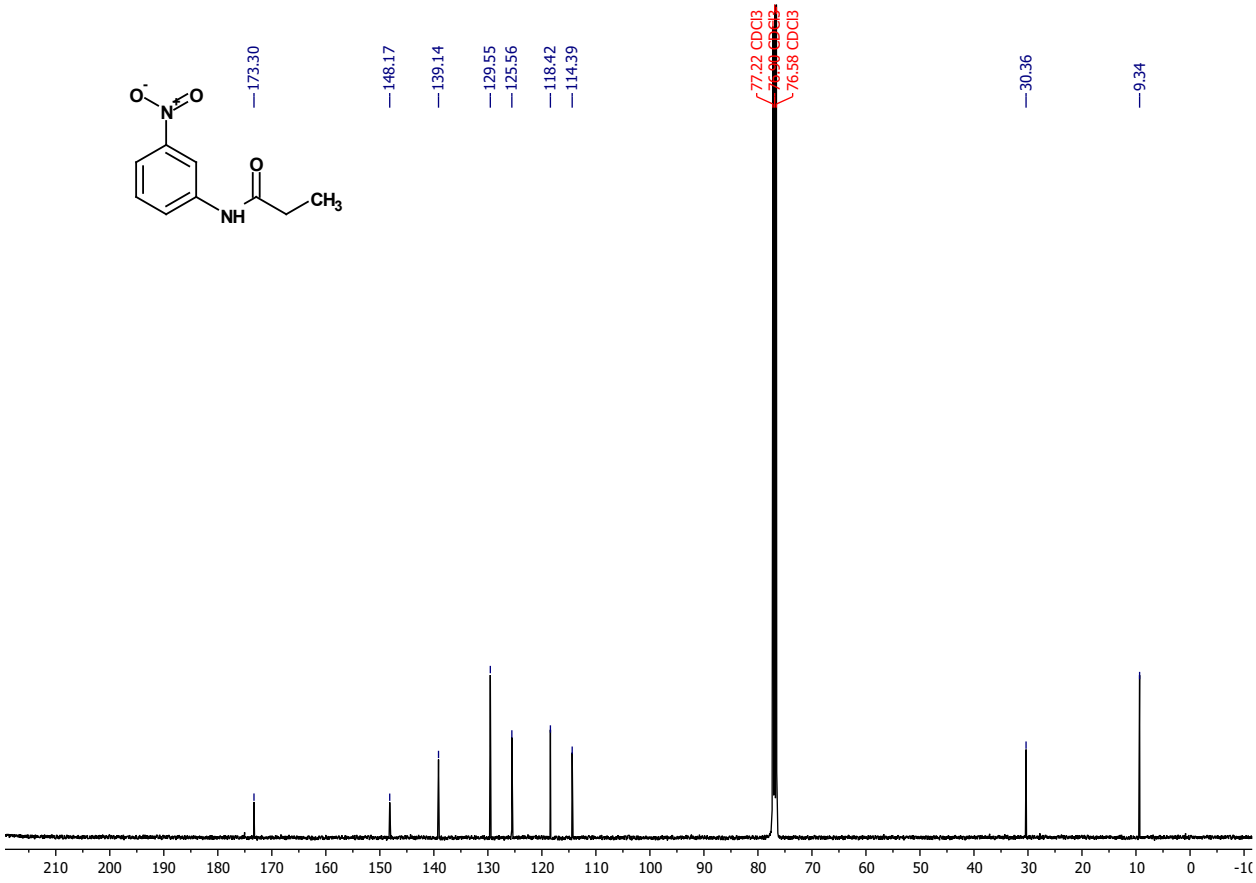
^{1}H and ^{13}C NMR *N*-(2-nitrophenyl)propionamide (**3m**-*a*)



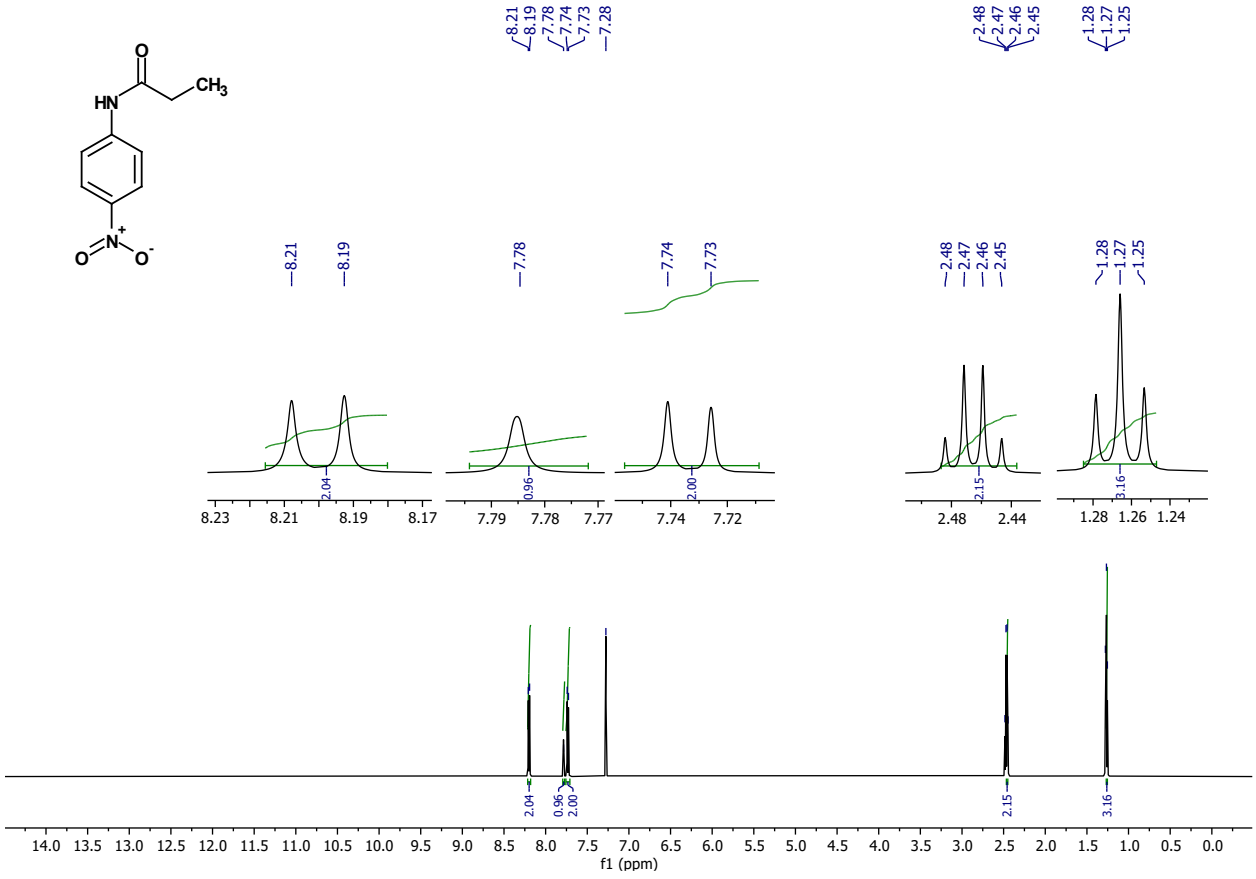


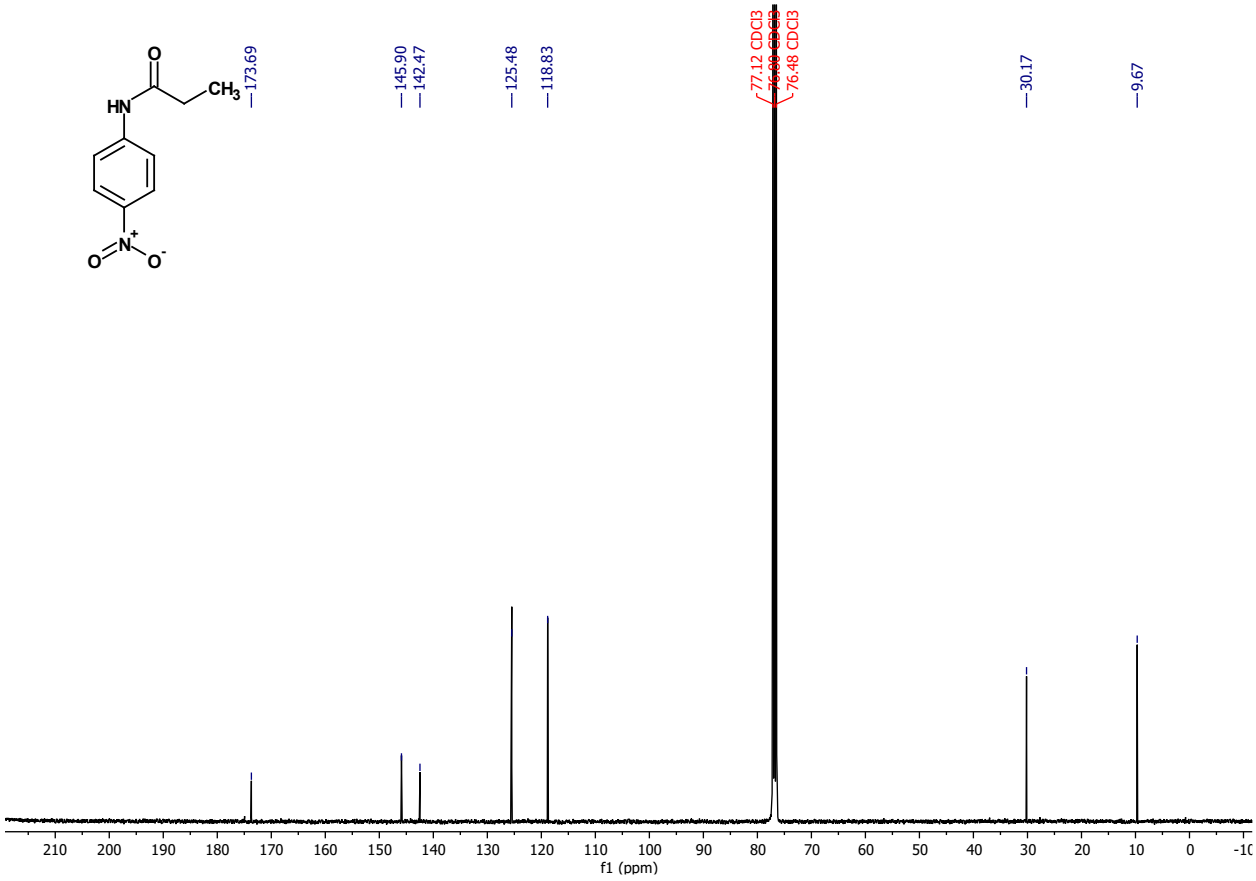
^{1}H and ^{13}C NMR *N*-(3-nitrophenyl)propionamide (**3m**-*b*)



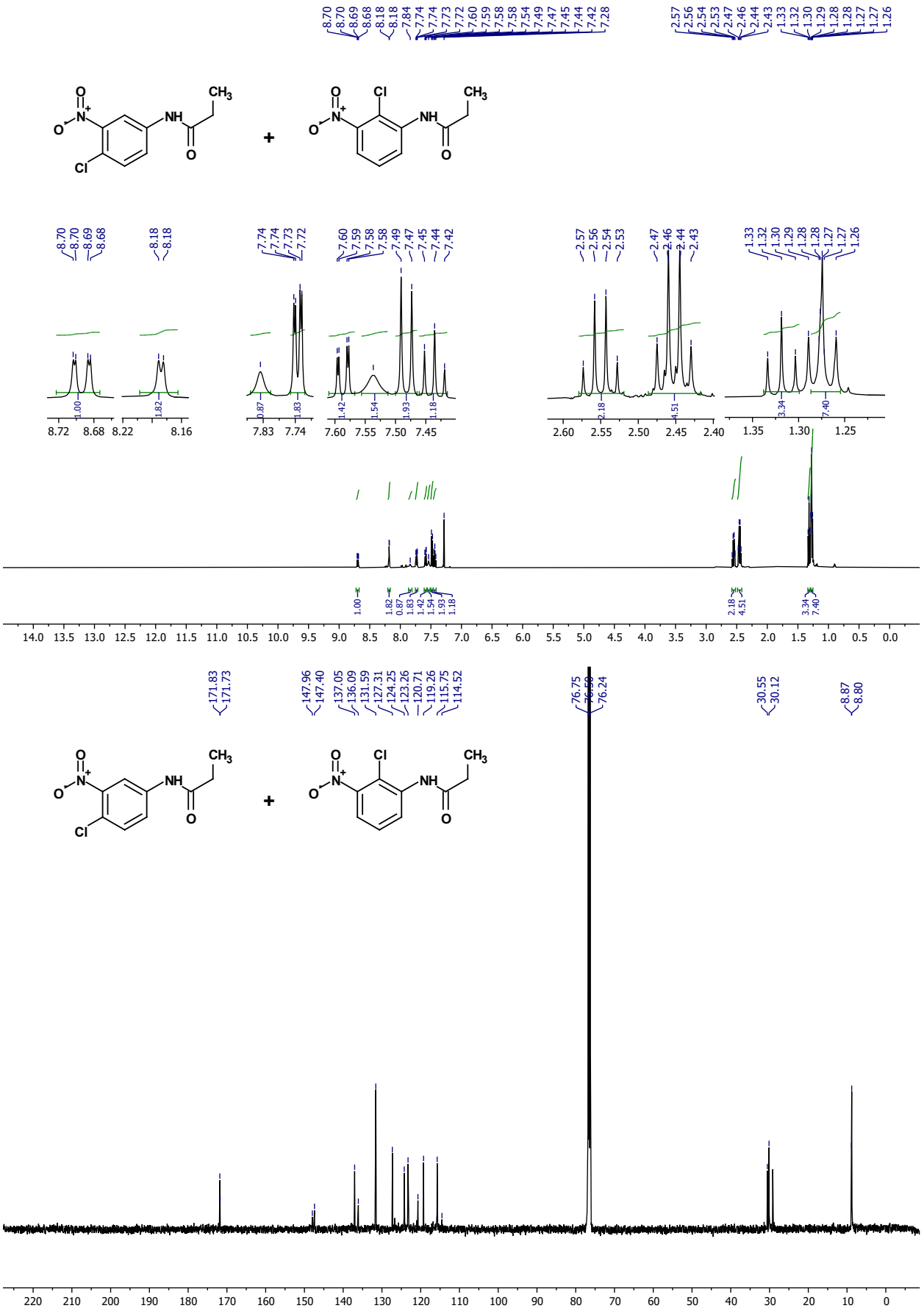


^{1}H and ^{13}C NMR *N*-(4-nitrophenyl)propionamide (**3m**-*c*)

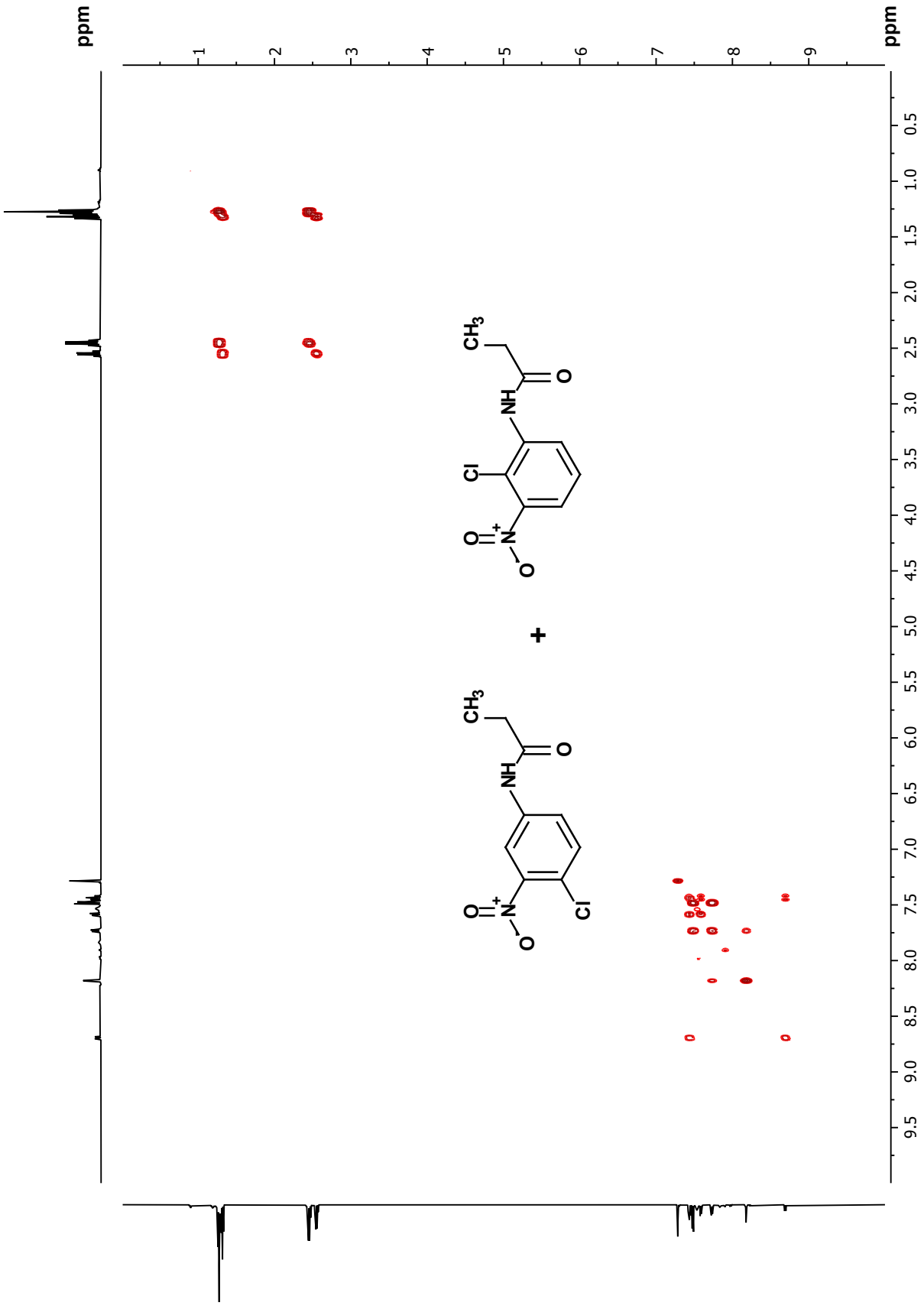




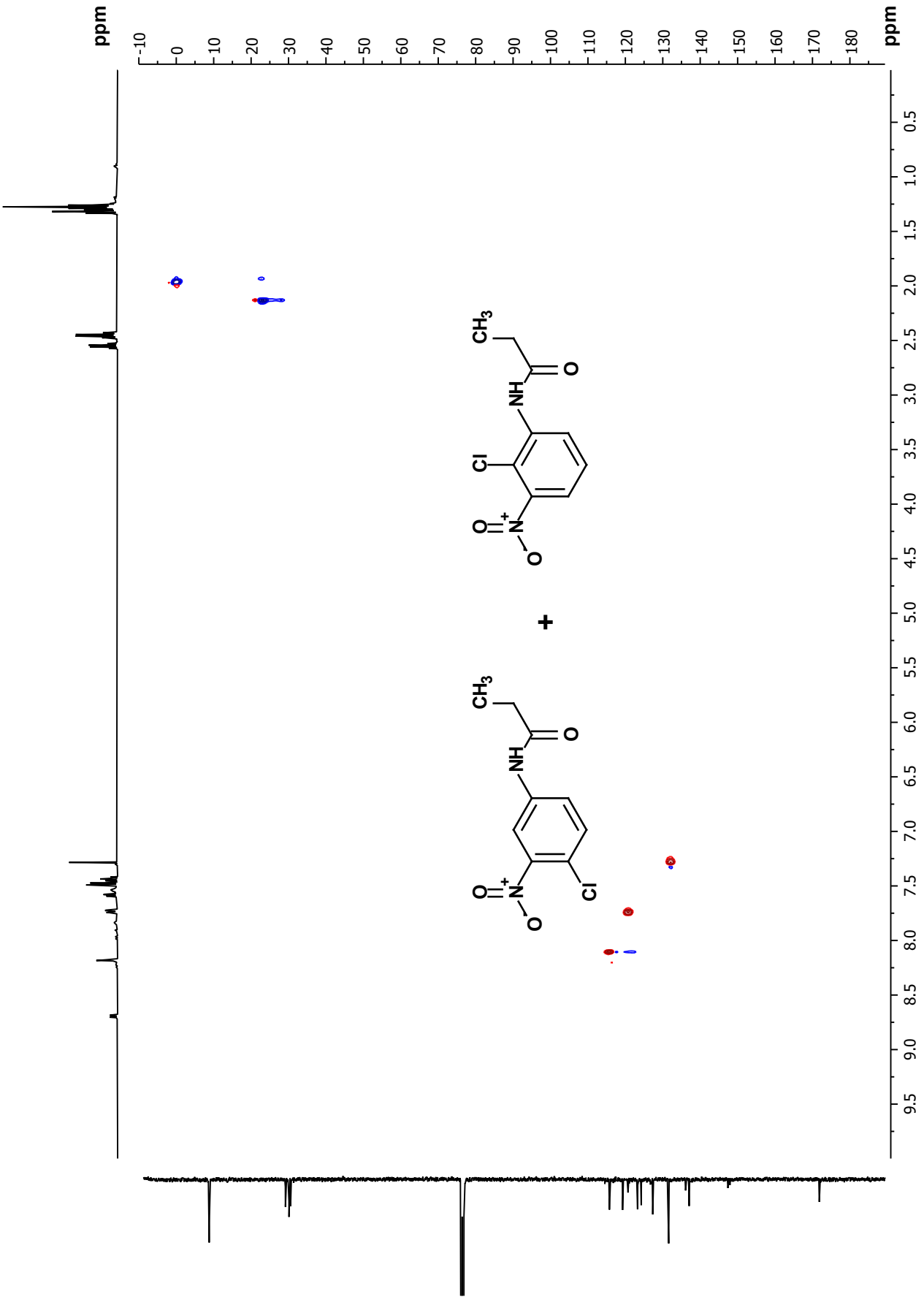
^{1}H and ^{13}C NMR *N*-(4-chloro-3-nitrophenyl)propionamide **(3n-*a*)** + *N*-(2-chloro-3-nitrophenyl)propionamide **(3n-*b*)**



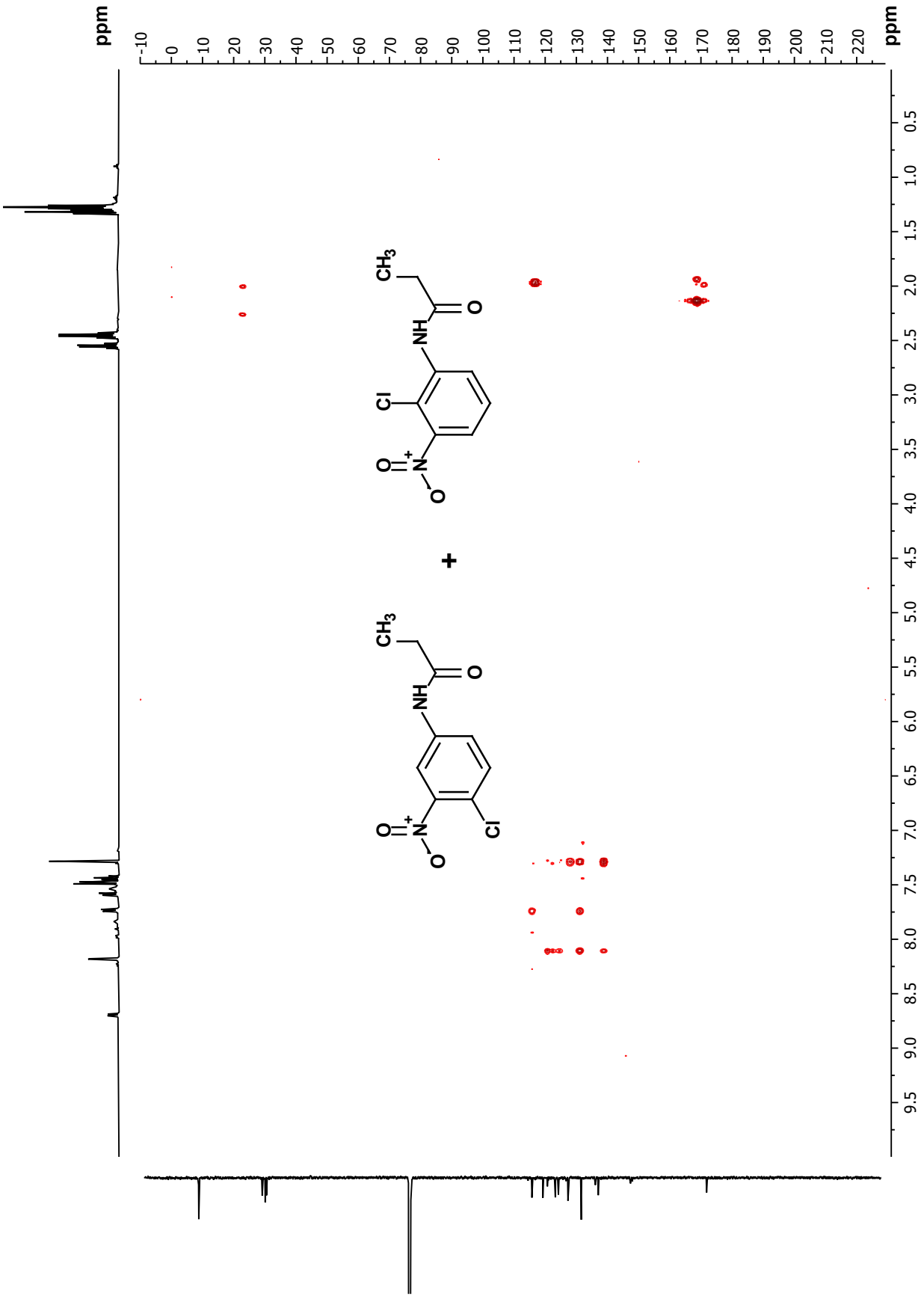
COSY NMR *N*-(4-chloro-3-nitrophenyl)propionamide **(3n-*a*)** + *N*-(2-chloro-3-nitrophenyl)propionamide **(3n-*b*)**



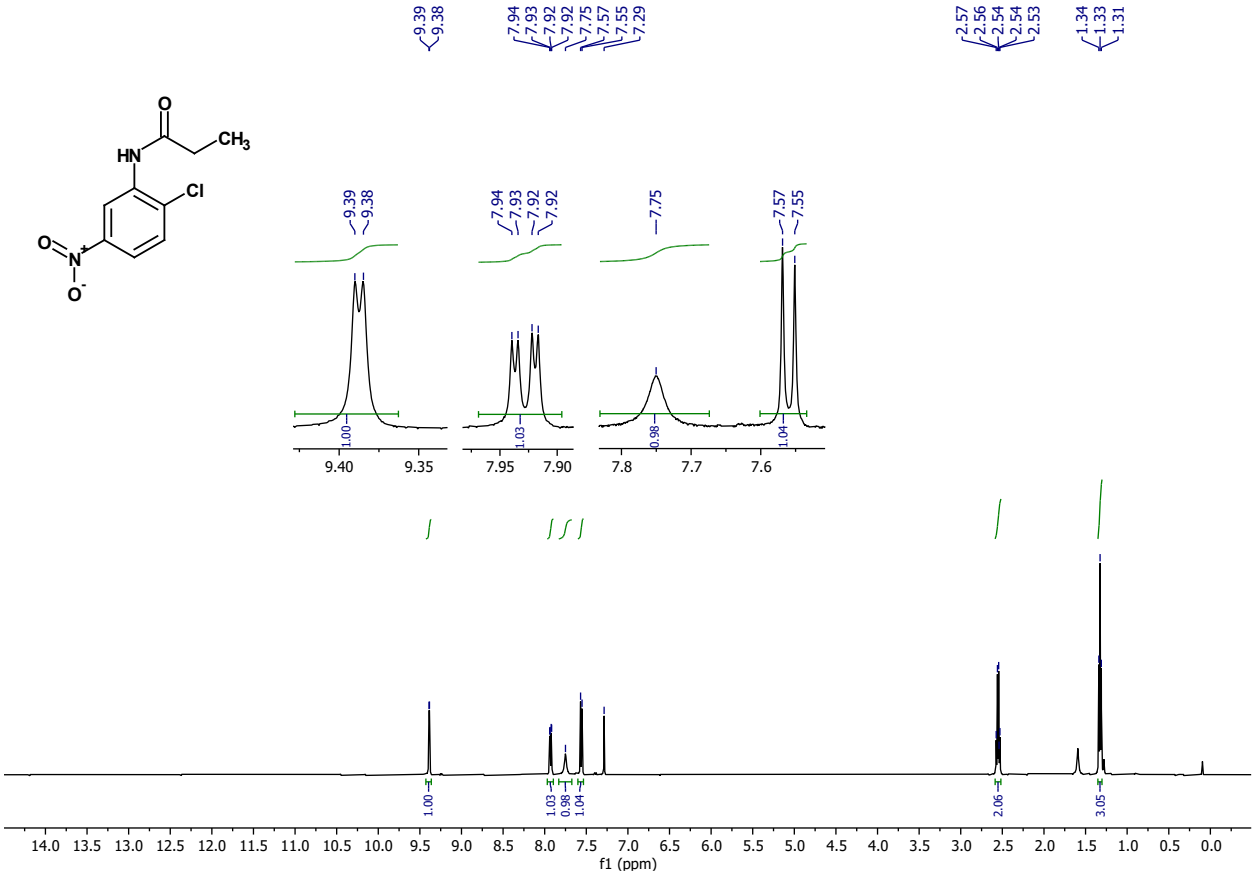
HSQC NMR *N*-(4-chloro-3-nitrophenyl)propionamide **(3n-*a*)** + *N*-(2-chloro-3-nitrophenyl)propionamide **(3n-*b*)**

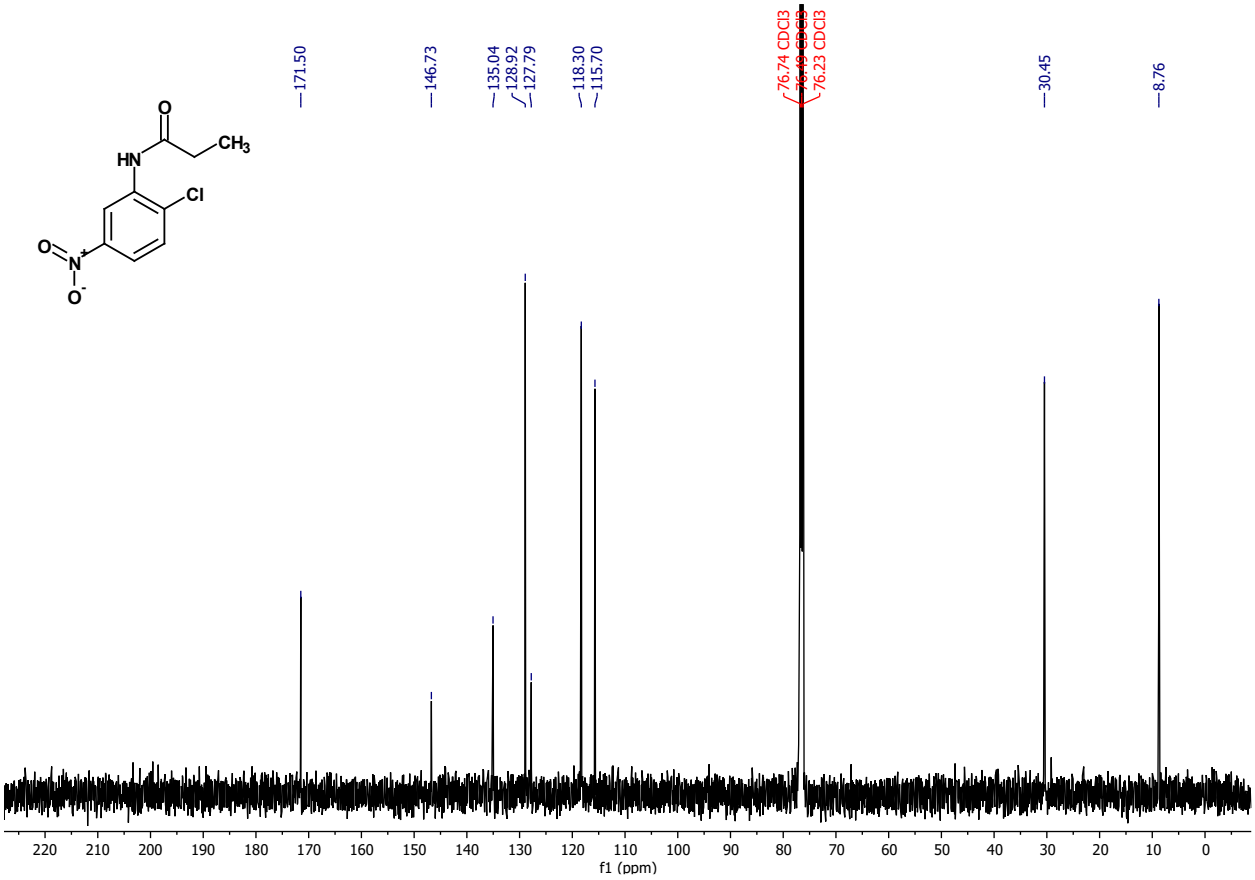


HMBC NMR *N*-(4-chloro-3-nitrophenyl)propionamide **(3n-*a*)** + *N*-(2-chloro-3-nitrophenyl)propionamide **(3n-*b*)**

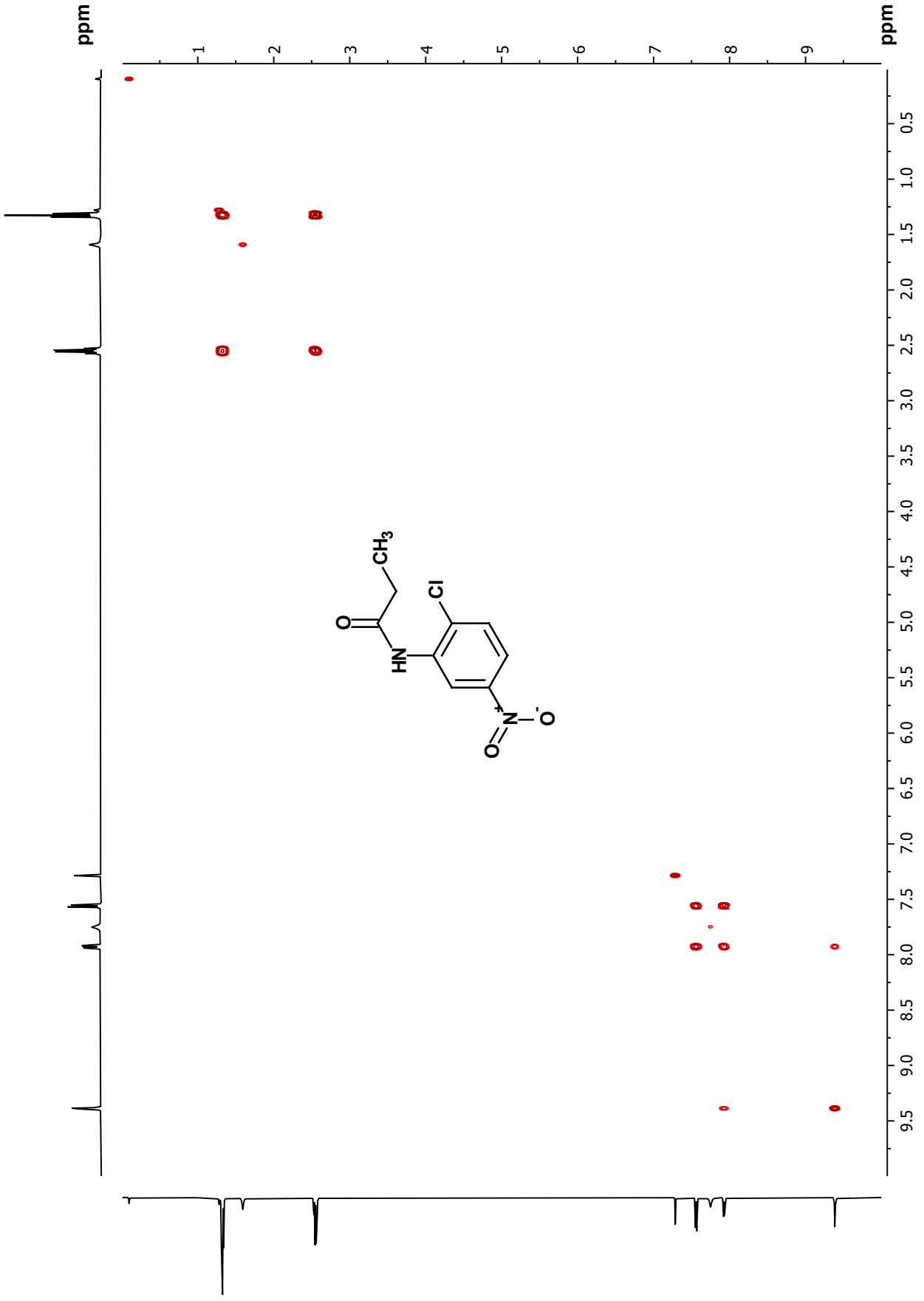


^{1}H and ^{13}C NMR *N*-(2-chloro-5-nitrophenyl)propionamide (**3o**)

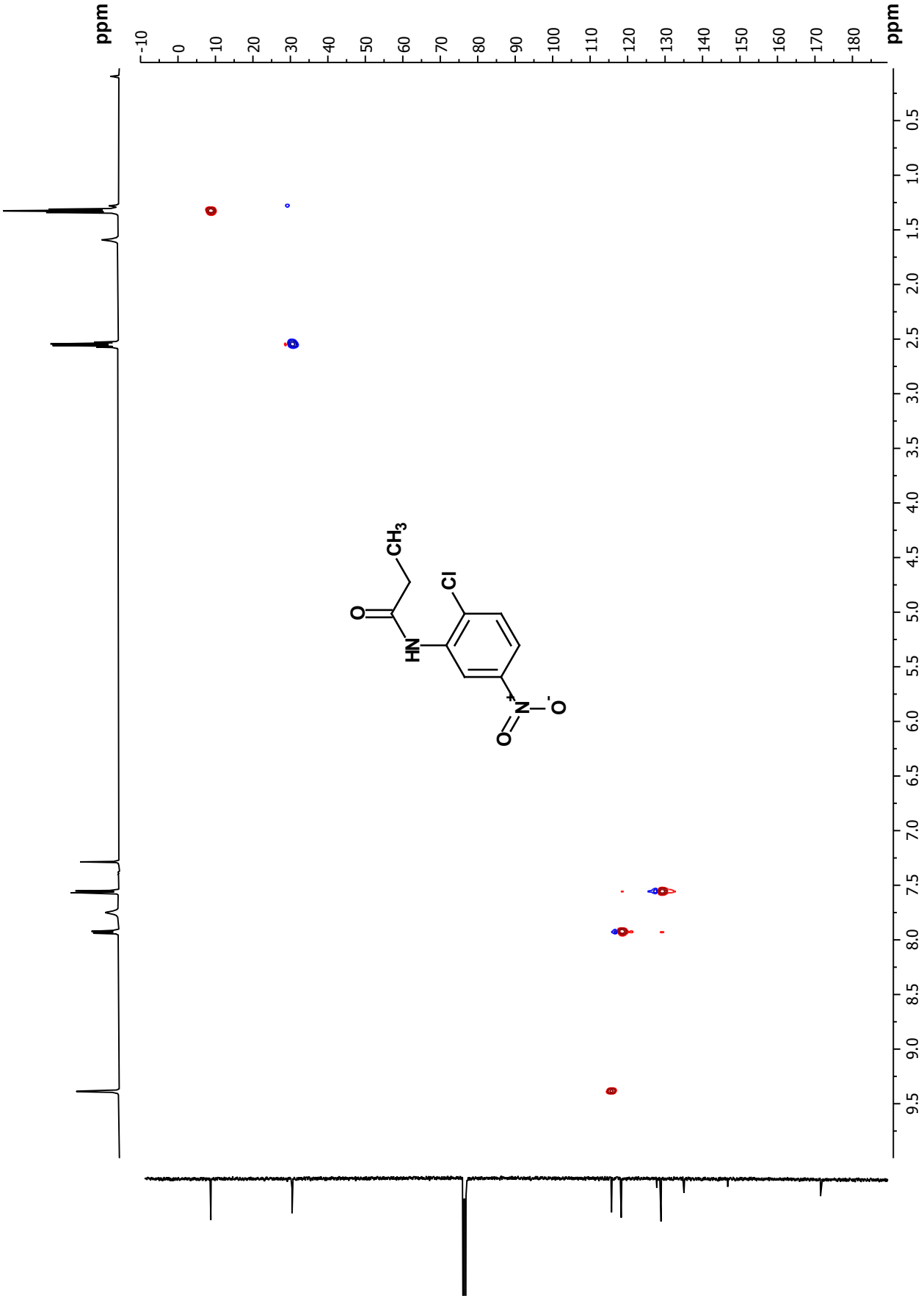




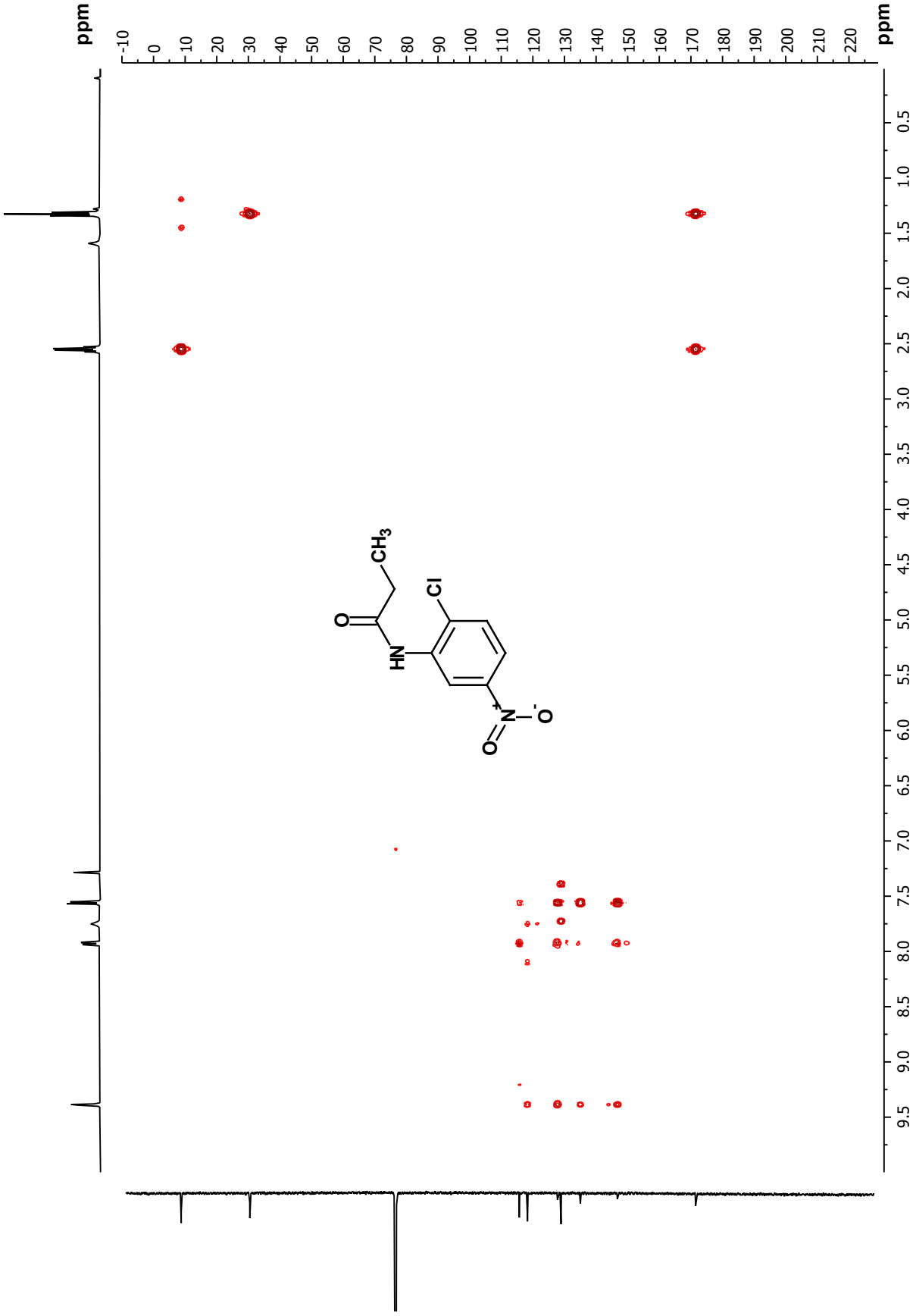
COSY NMR *N*-(2-chloro-5-nitrophenyl)propionamide (**3o**)



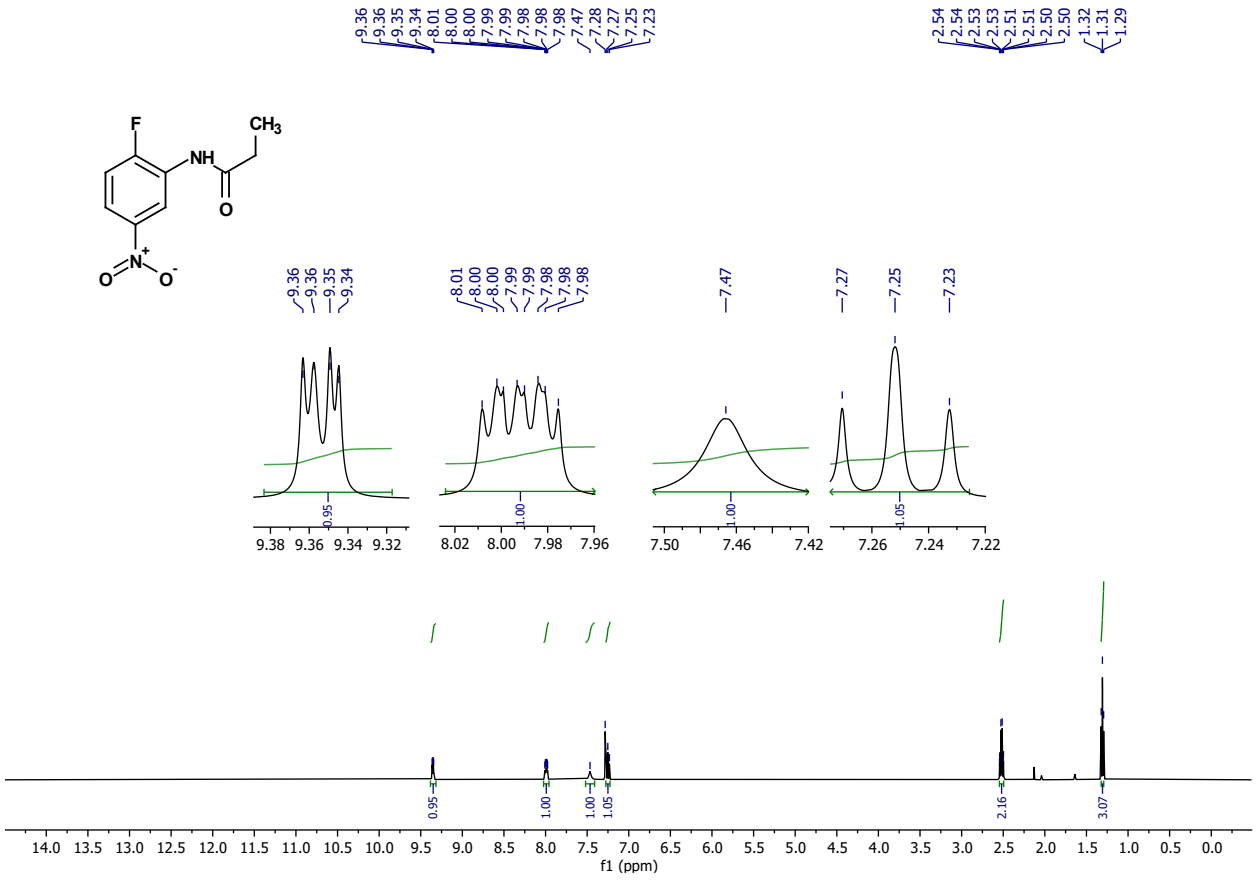
HSQC NMR *N*-(2-chloro-5-nitrophenyl)propionamide (**3o**)

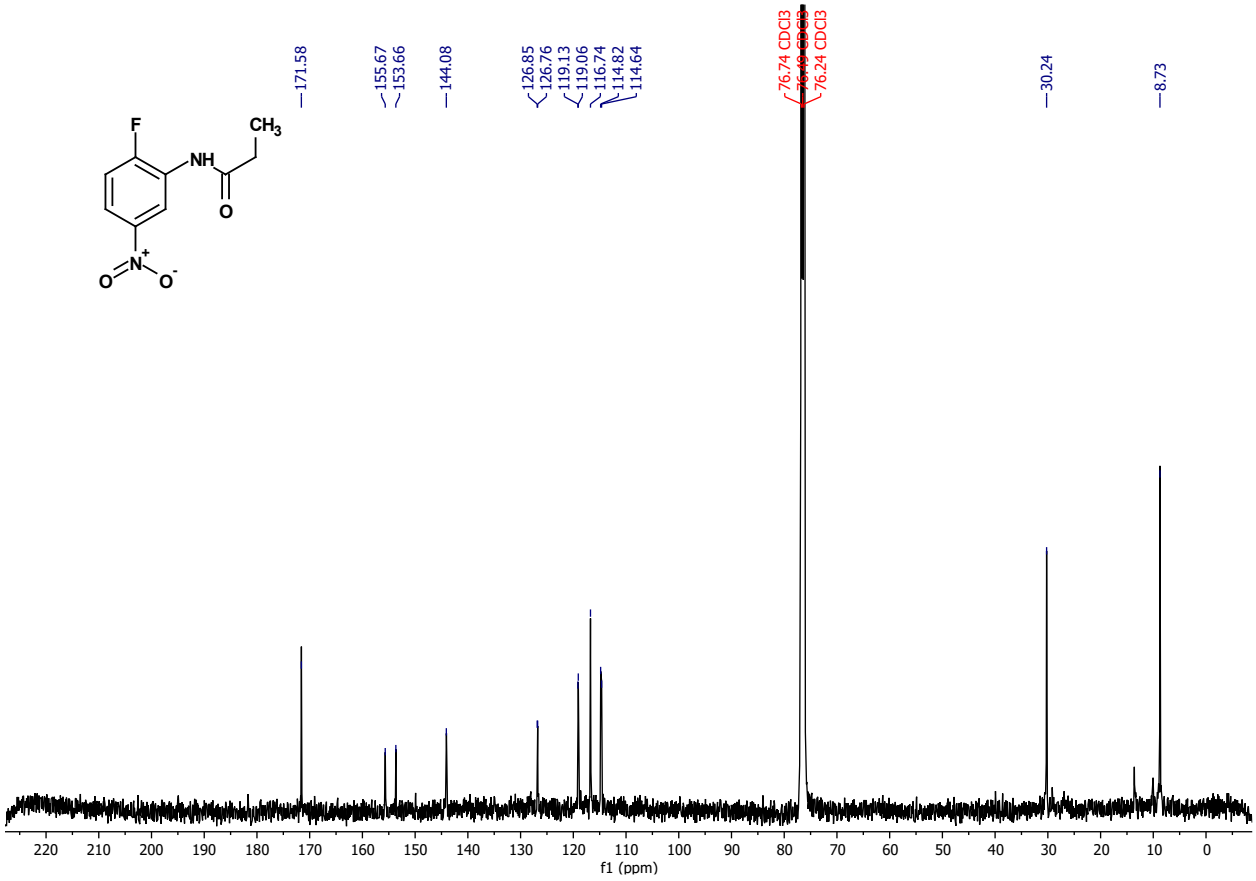


HMBC NMR *N*-(2-chloro-5-nitrophenyl)propionamide (**3o**)

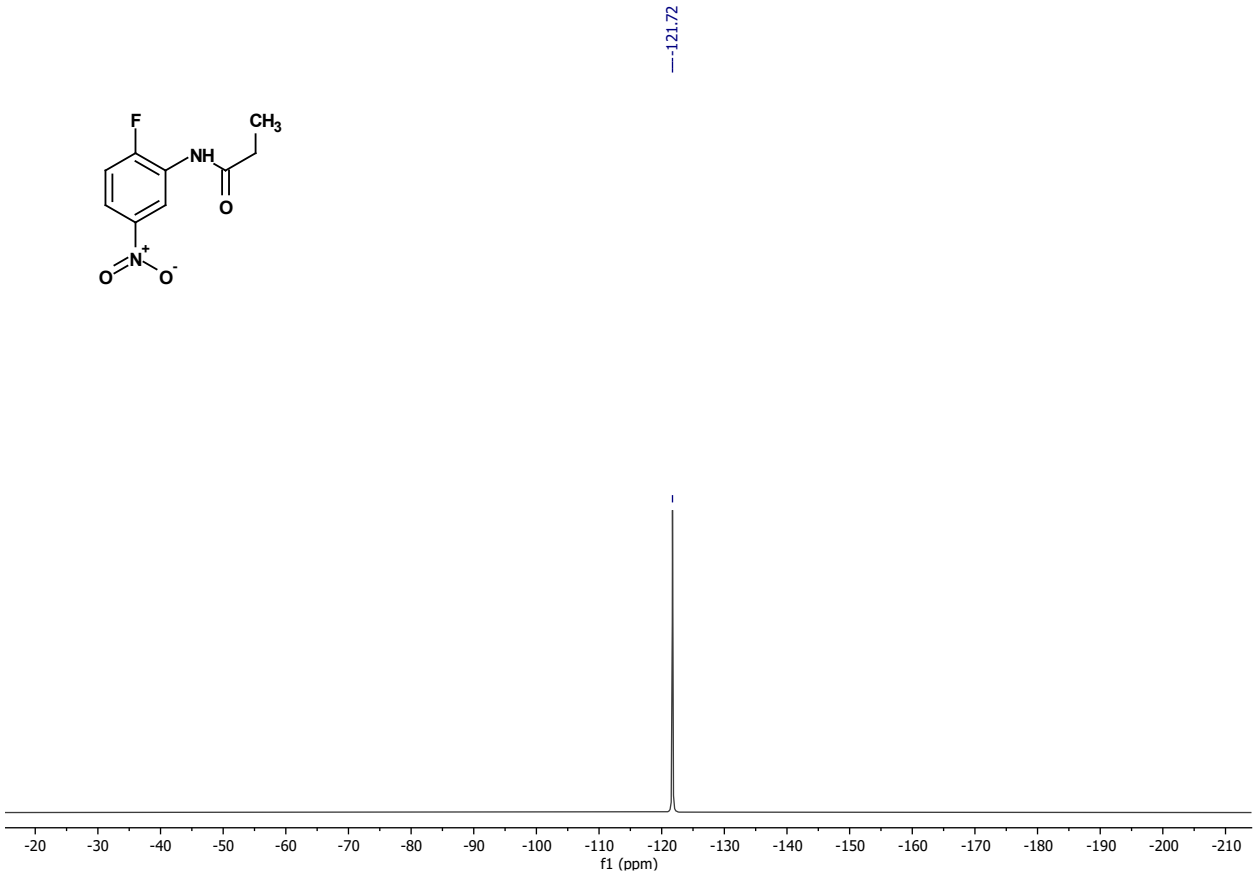


^{1}H and ^{13}C NMR *N*-(2-fluoro-5-nitrophenyl)propionamide **(3p)**

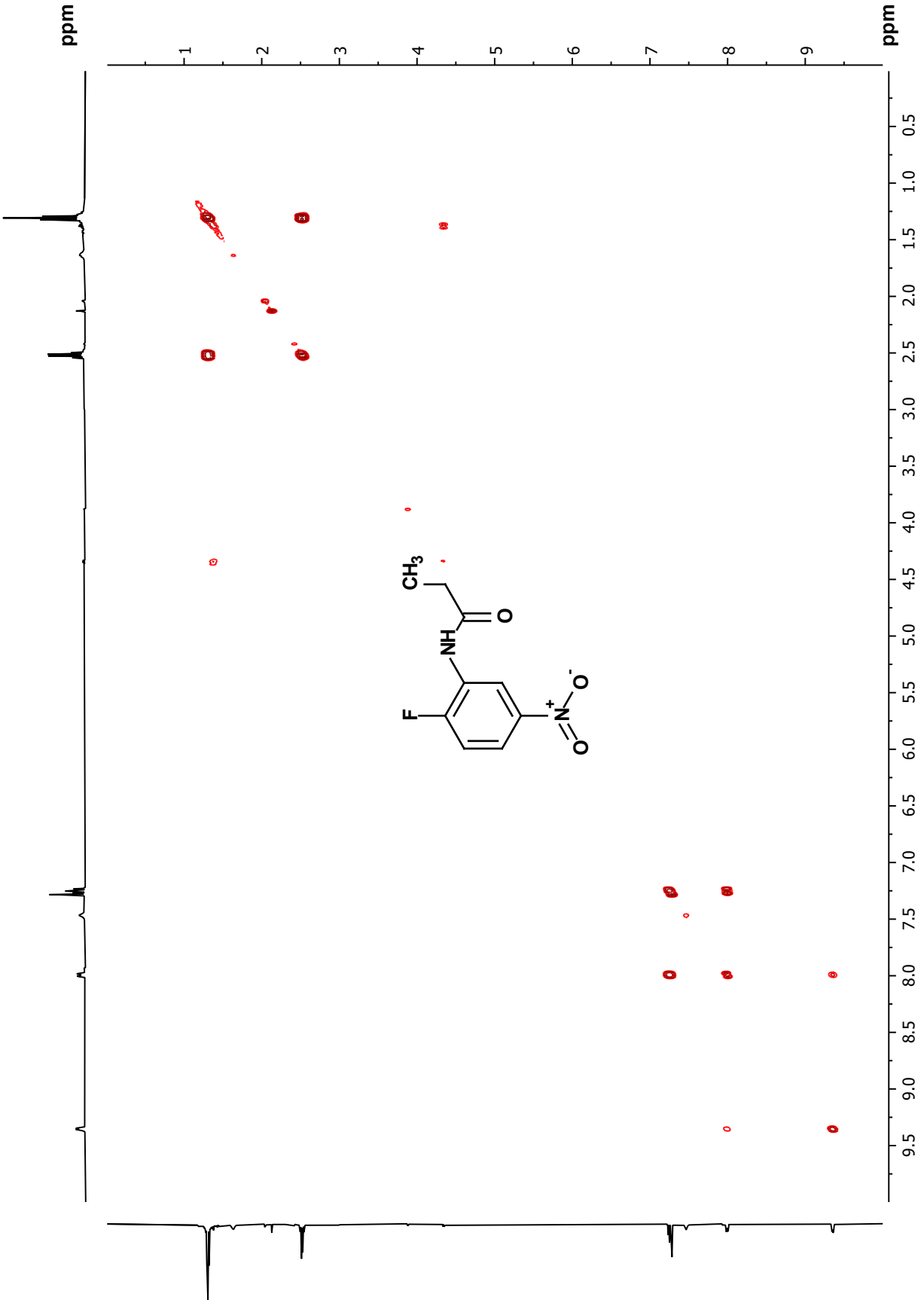




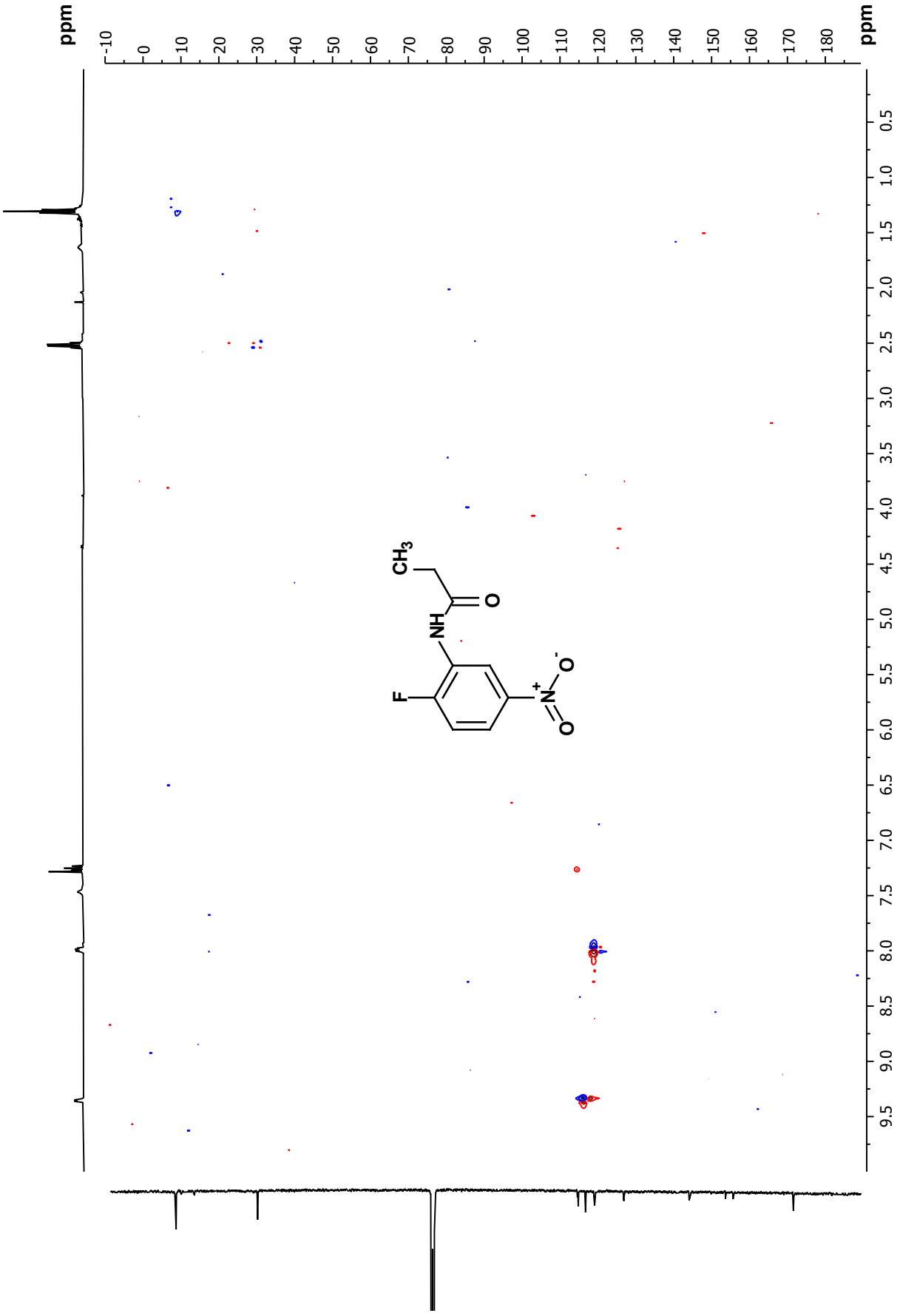
^{19}F NMR *N*-(2-fluoro-5-nitrophenyl)propionamide **(3p)**



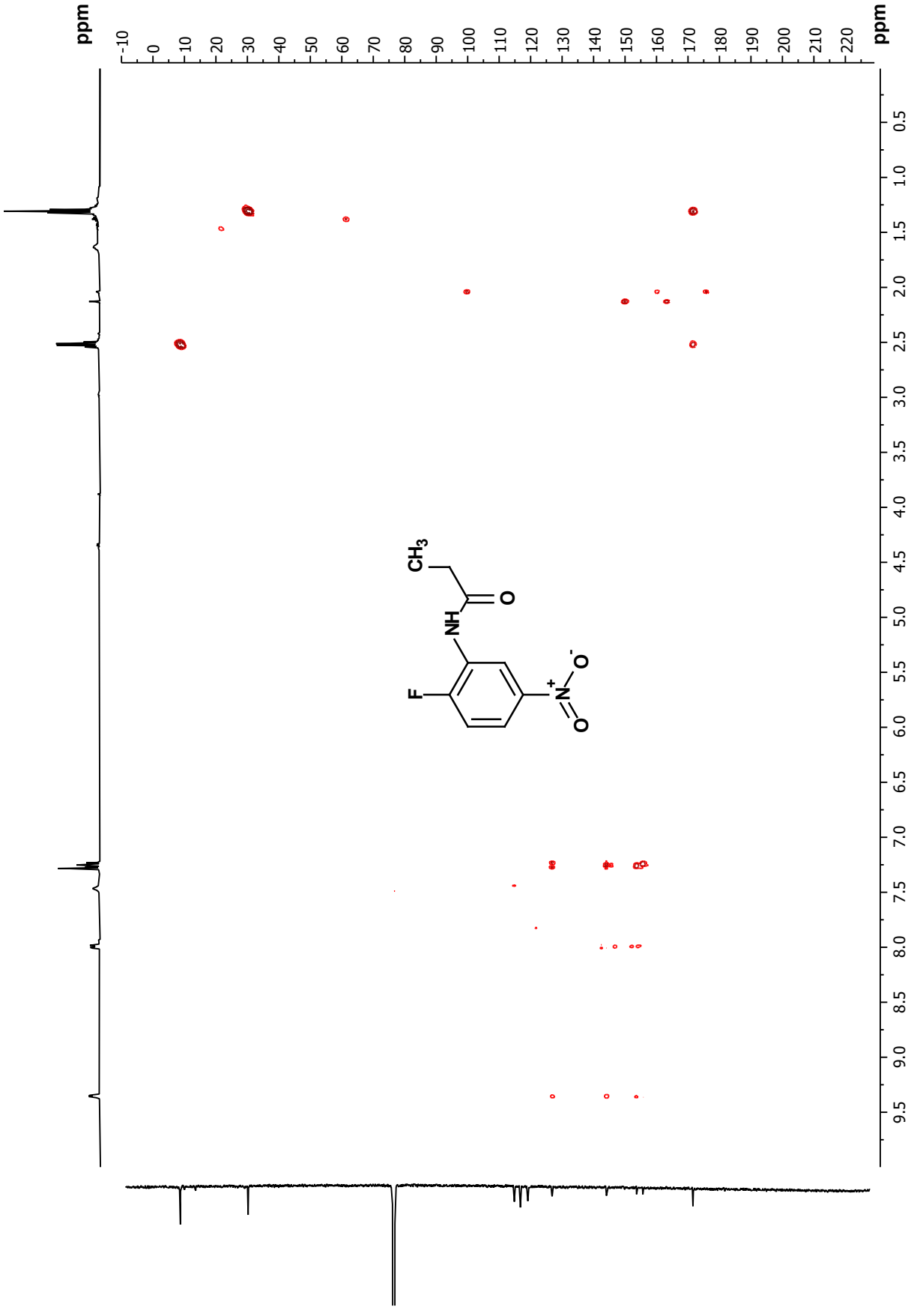
COSY NMR *N*-(2-fluoro-5-nitrophenyl)propionamide **(3p)**



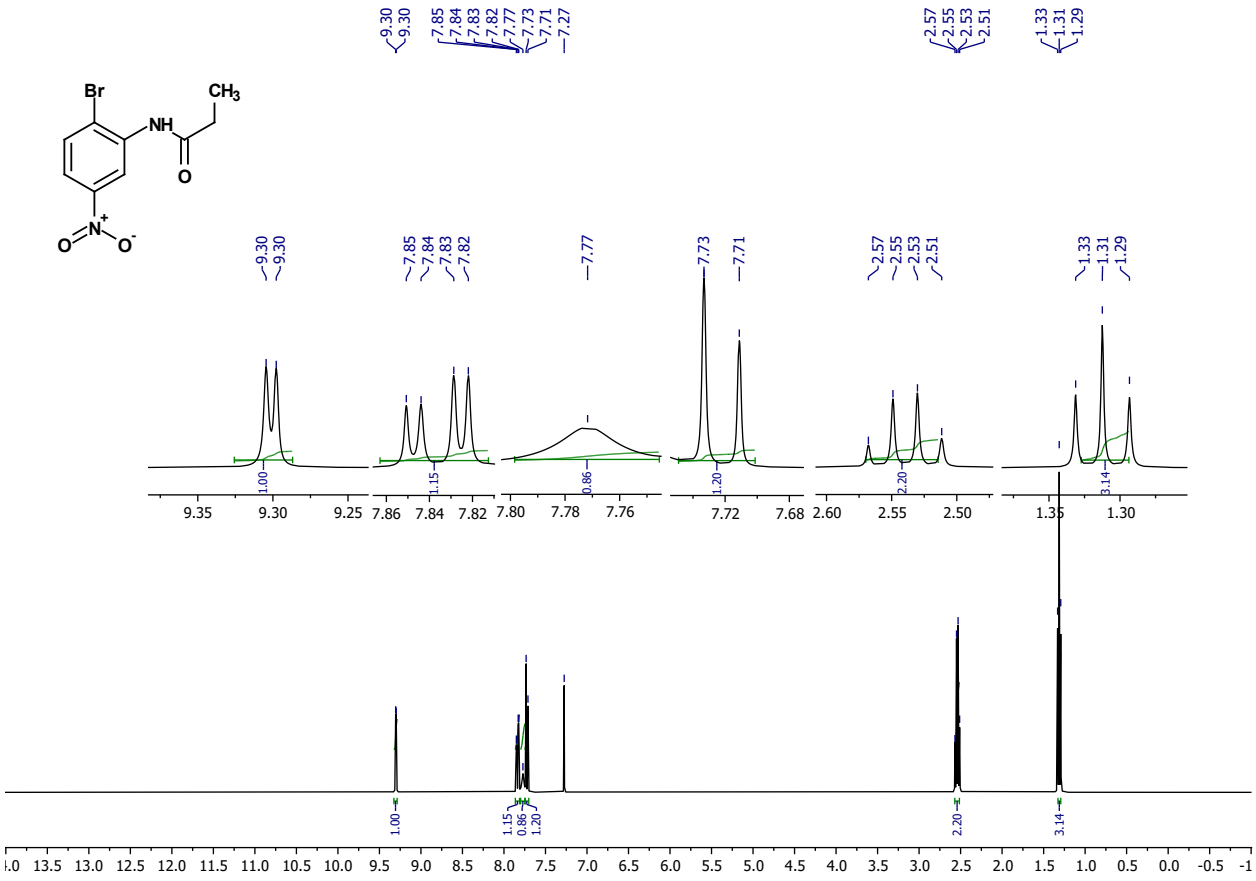
HSQC NMR *N*-(2-fluoro-5-nitrophenyl)propionamide **(3p)**

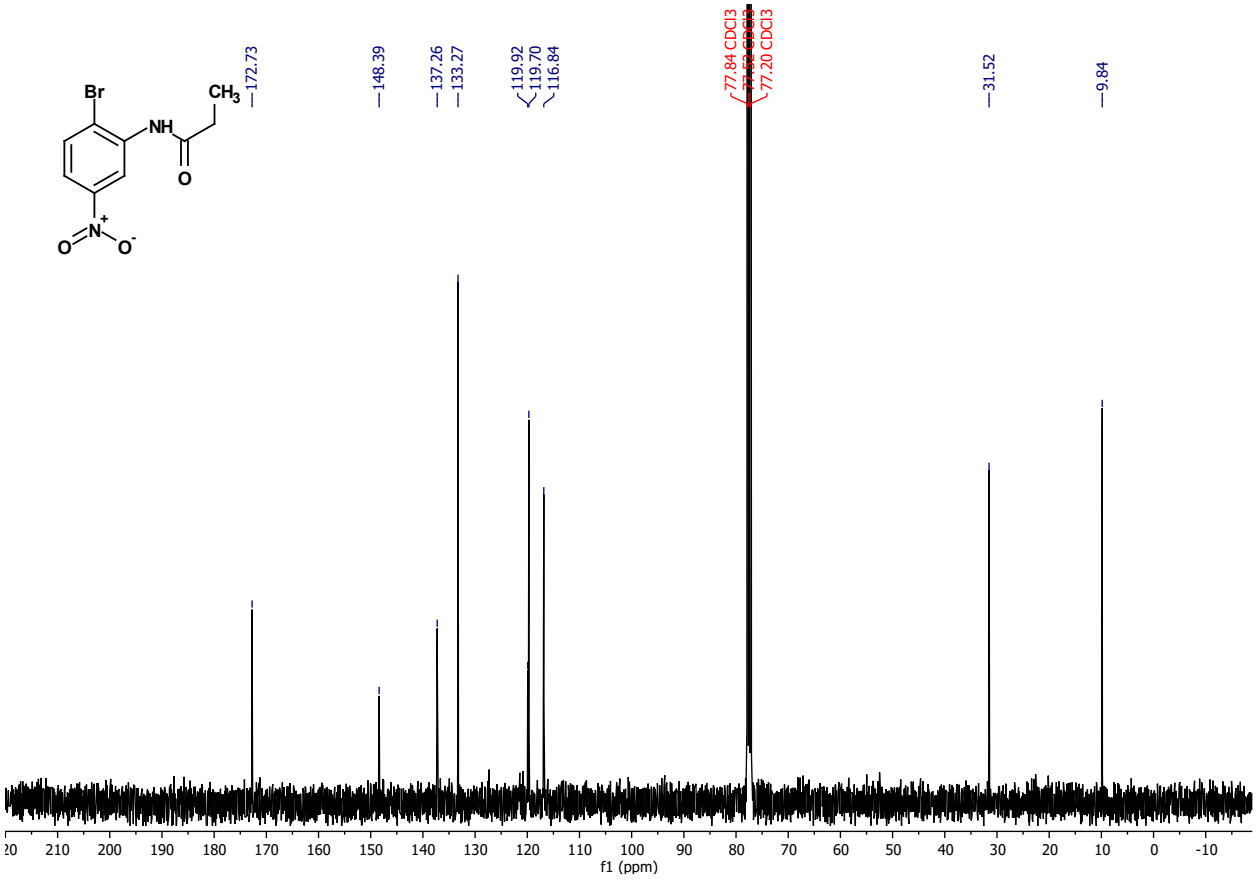


HMBC NMR *N*-(2-fluoro-5-nitrophenyl)propionamide **(3p)**

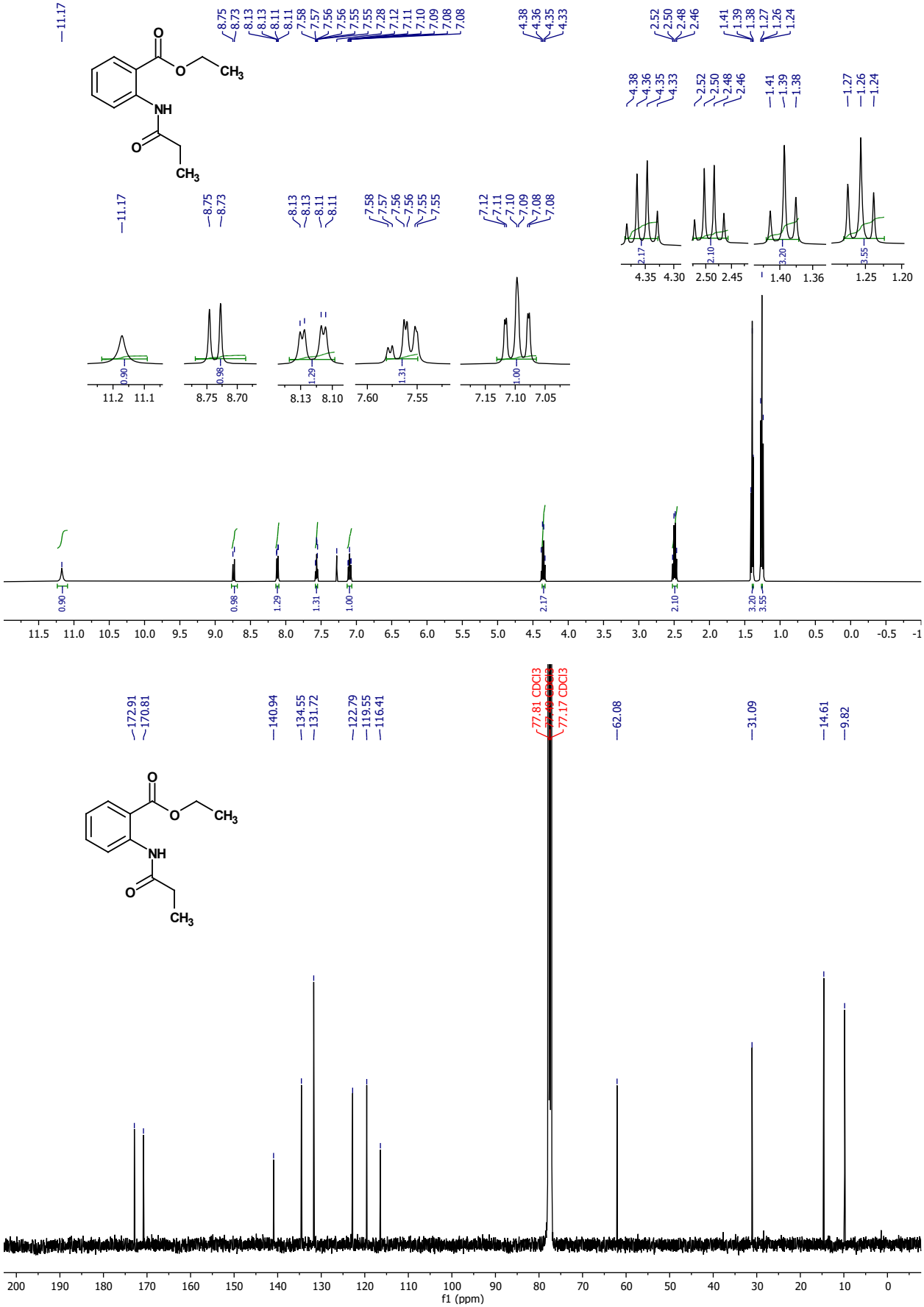


^{1}H and ^{13}C NMR *N*-(2-bromo-5-nitrophenyl) propionamide **(3q)**

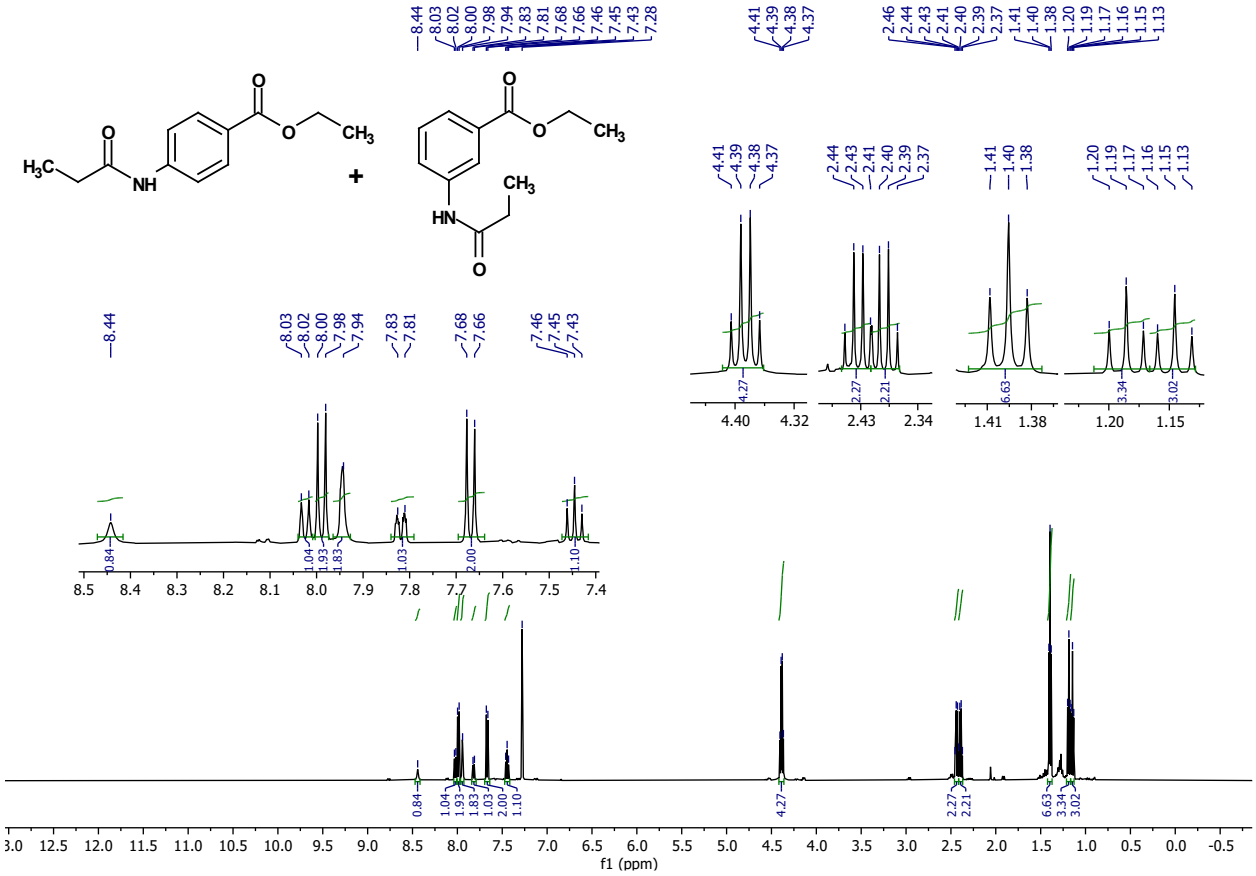


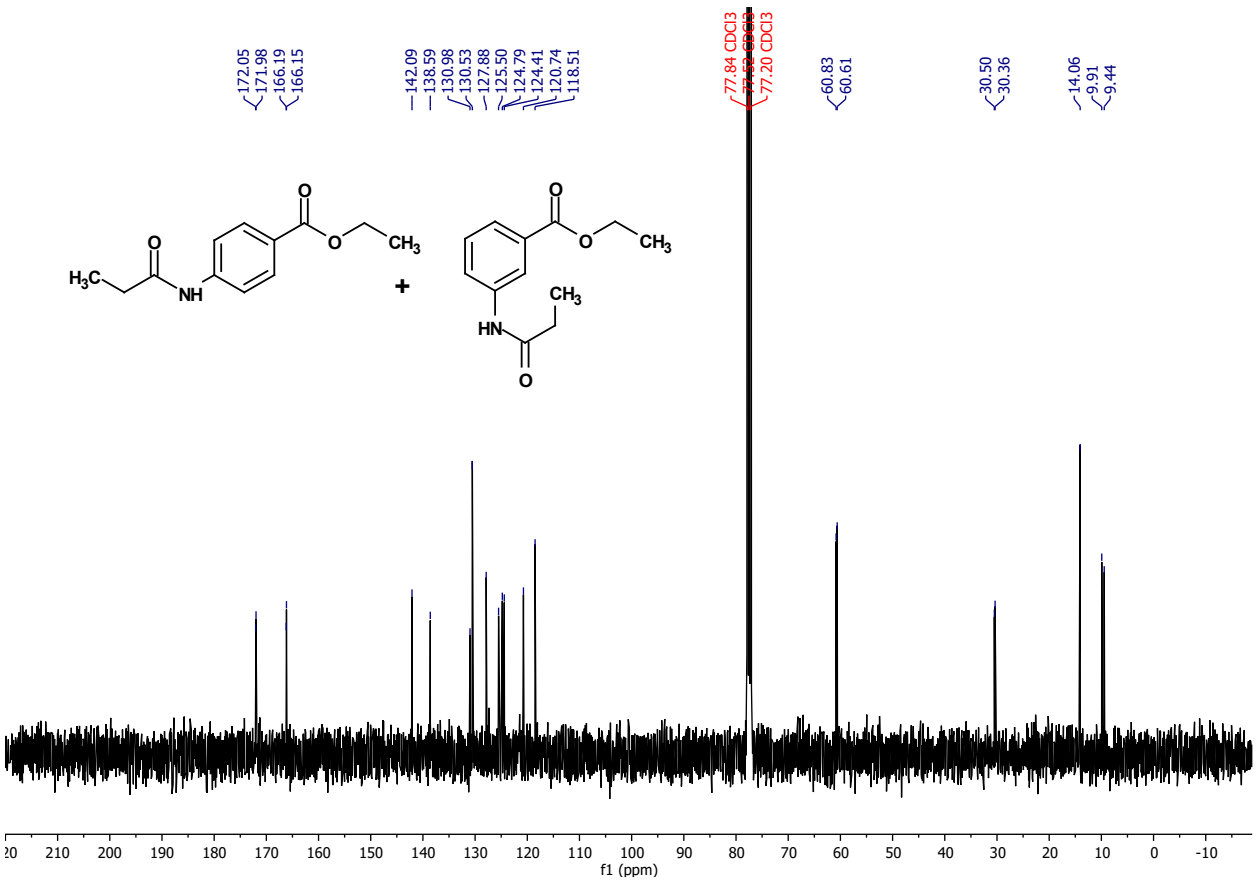


^{1}H and ^{13}C NMR ethyl 2-propionamidobenzoate (**3r**-*a*)

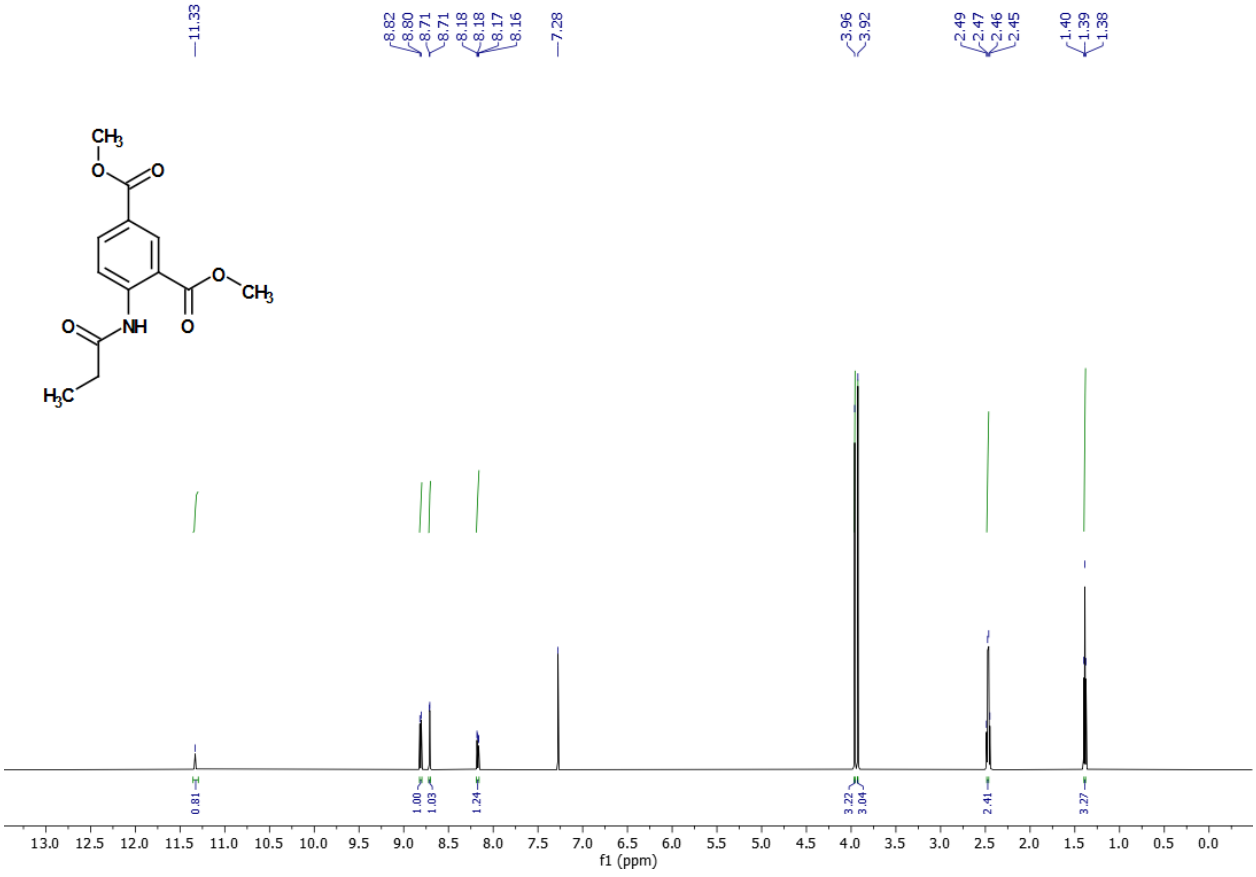


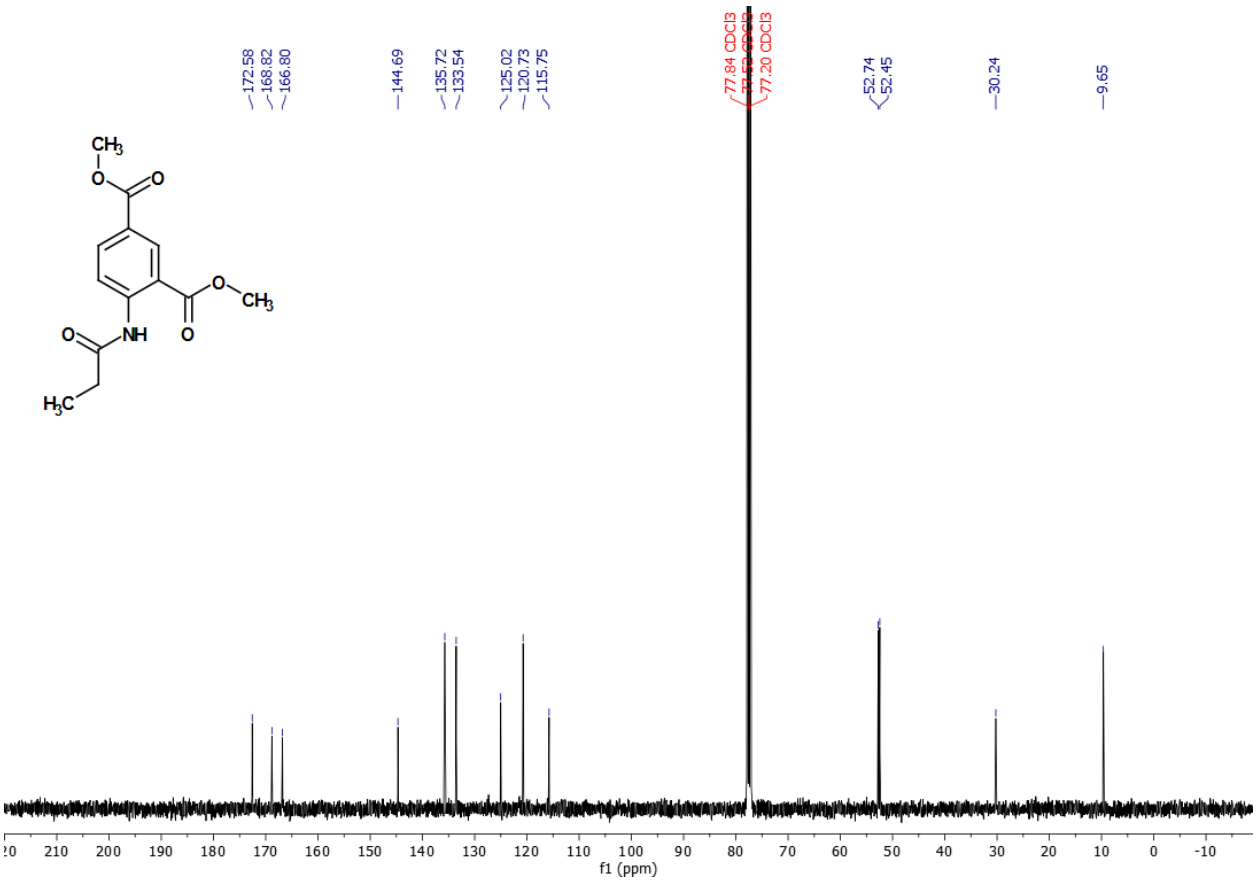
^{1}H and ^{13}C NMR Ethyl 3-propionamidobenzoate (**3r**-*b*) + Ethyl 4-propionamidobenzoate (**3r**-*c*)



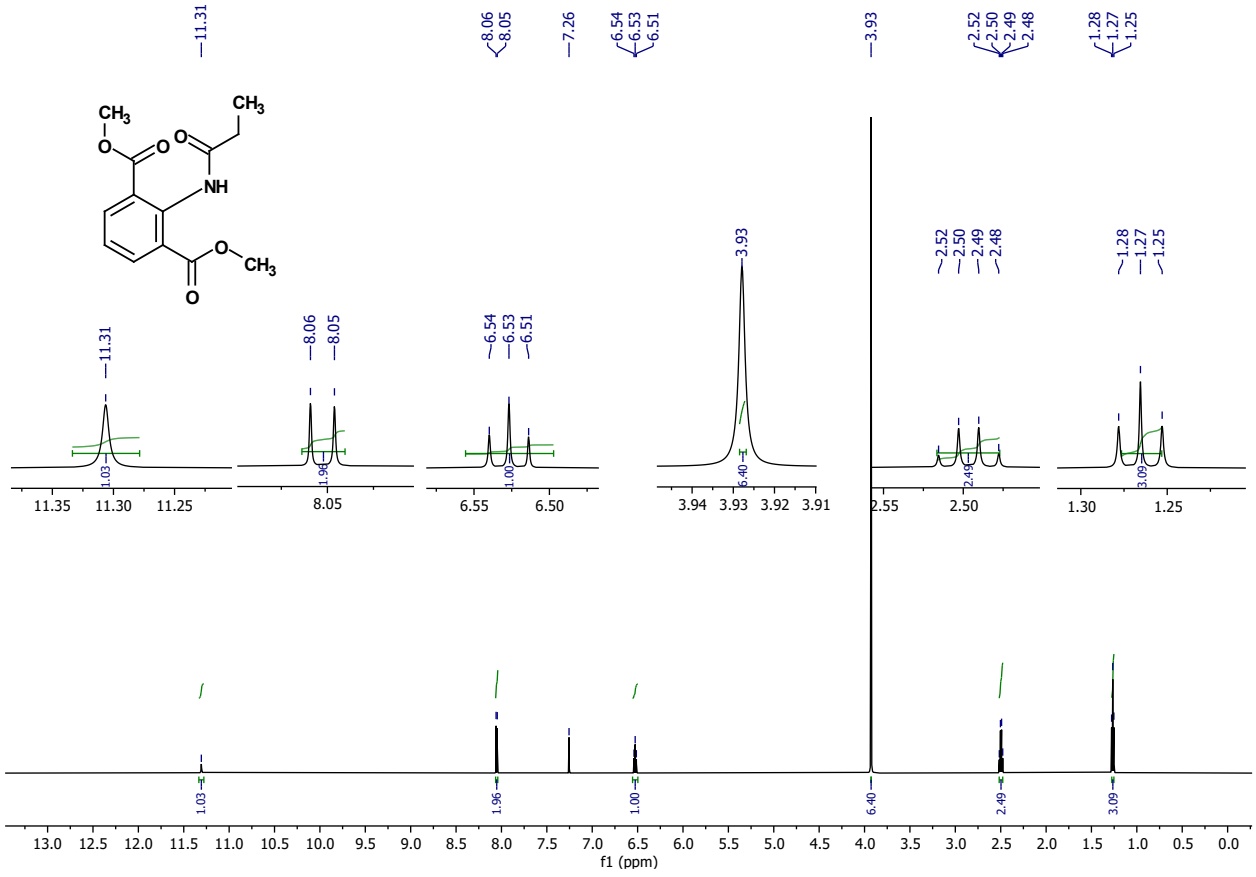


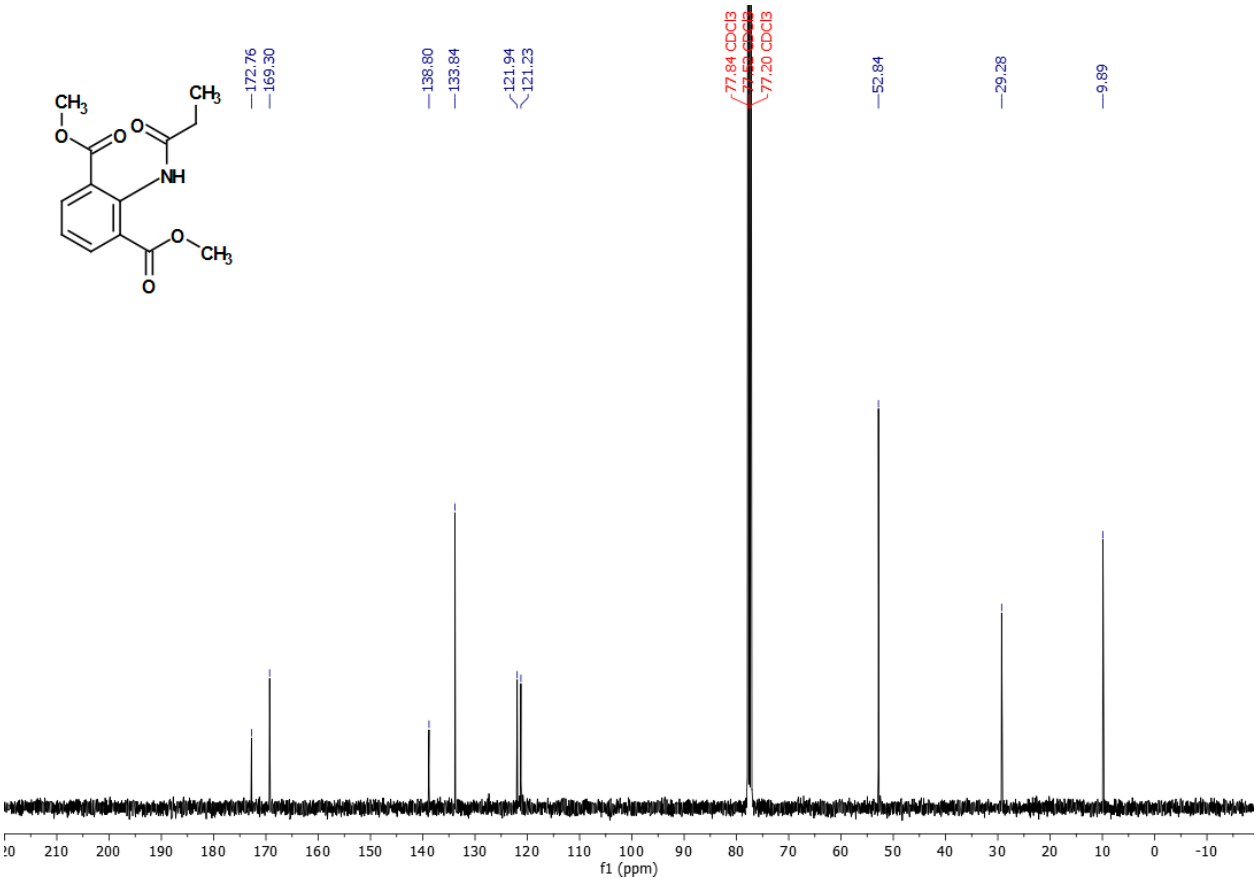
^{1}H and ^{13}C NMR Dimethyl 4-propionamidoisophthalate **(3s-*a*)**



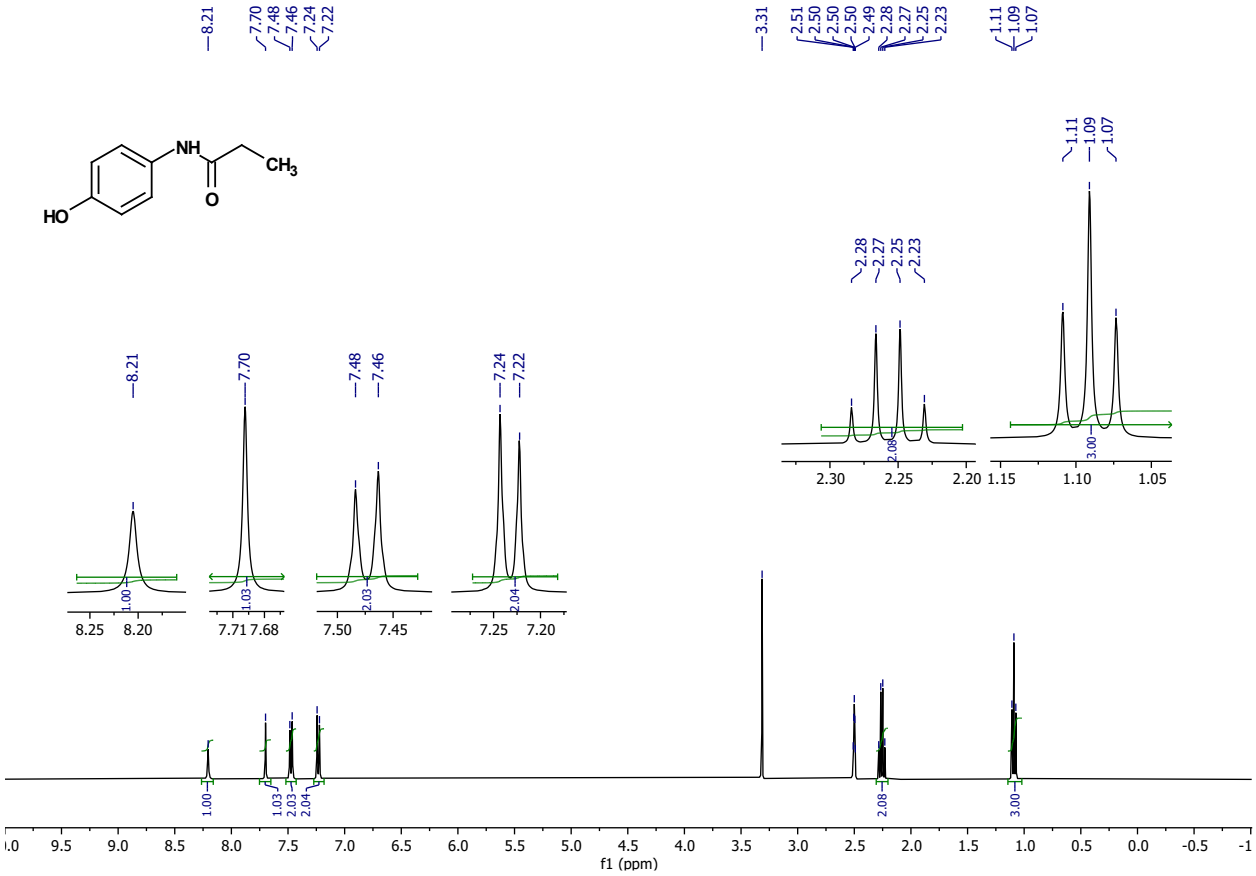


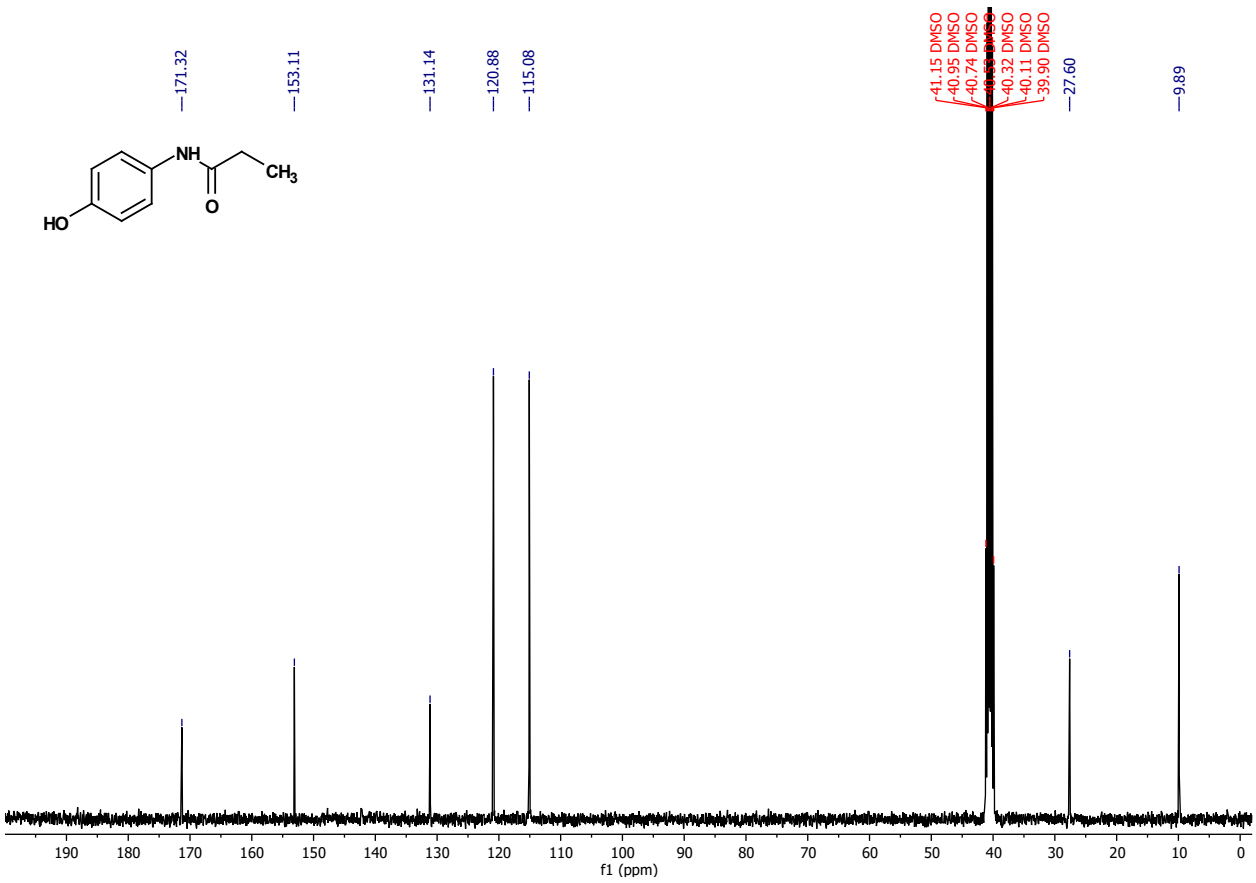
^{1}H and ^{13}C NMR Dimethyl 2-propionamidoisophthalate **(3s-*b*)**



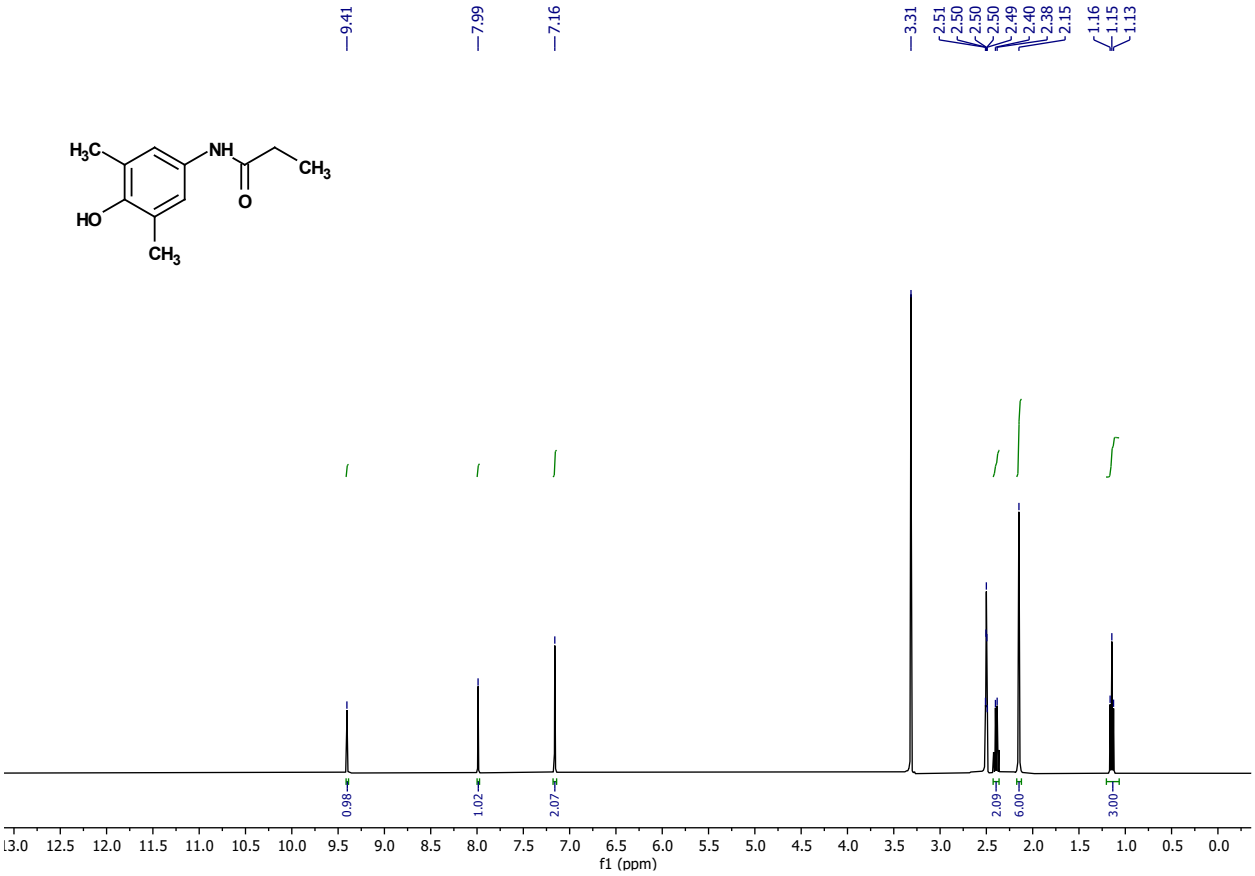


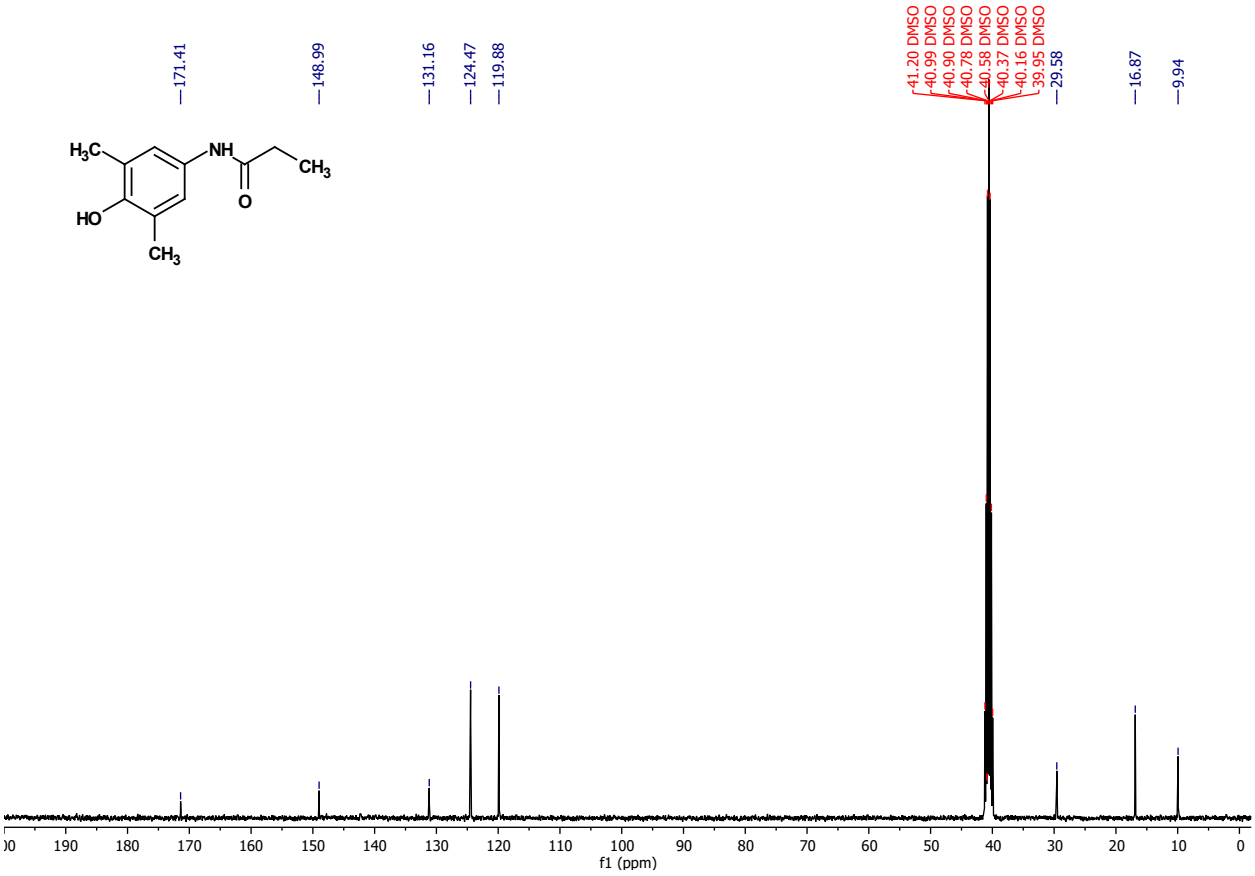
^{1}H and ^{13}C NMR *N*-(4-hydroxyphenyl)propionamide (**3t**)



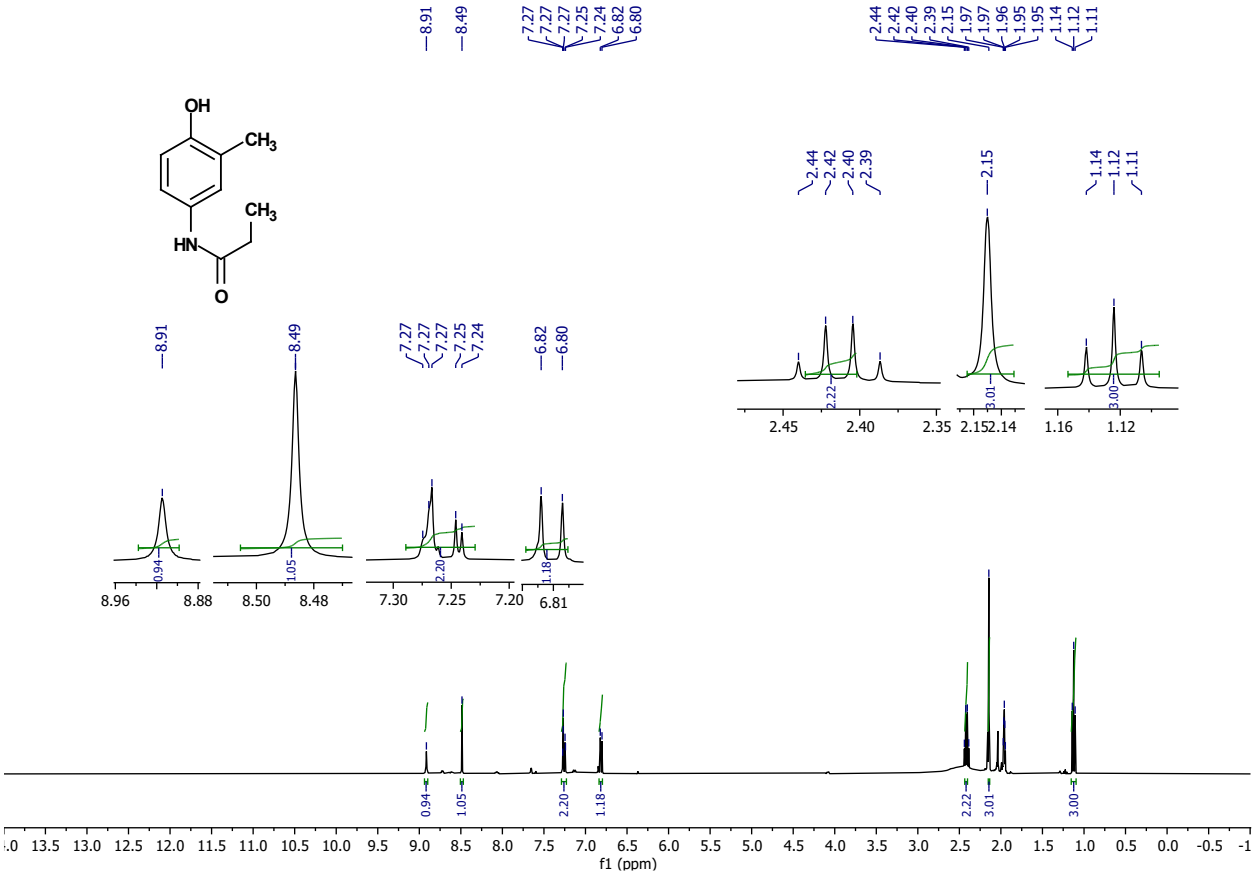


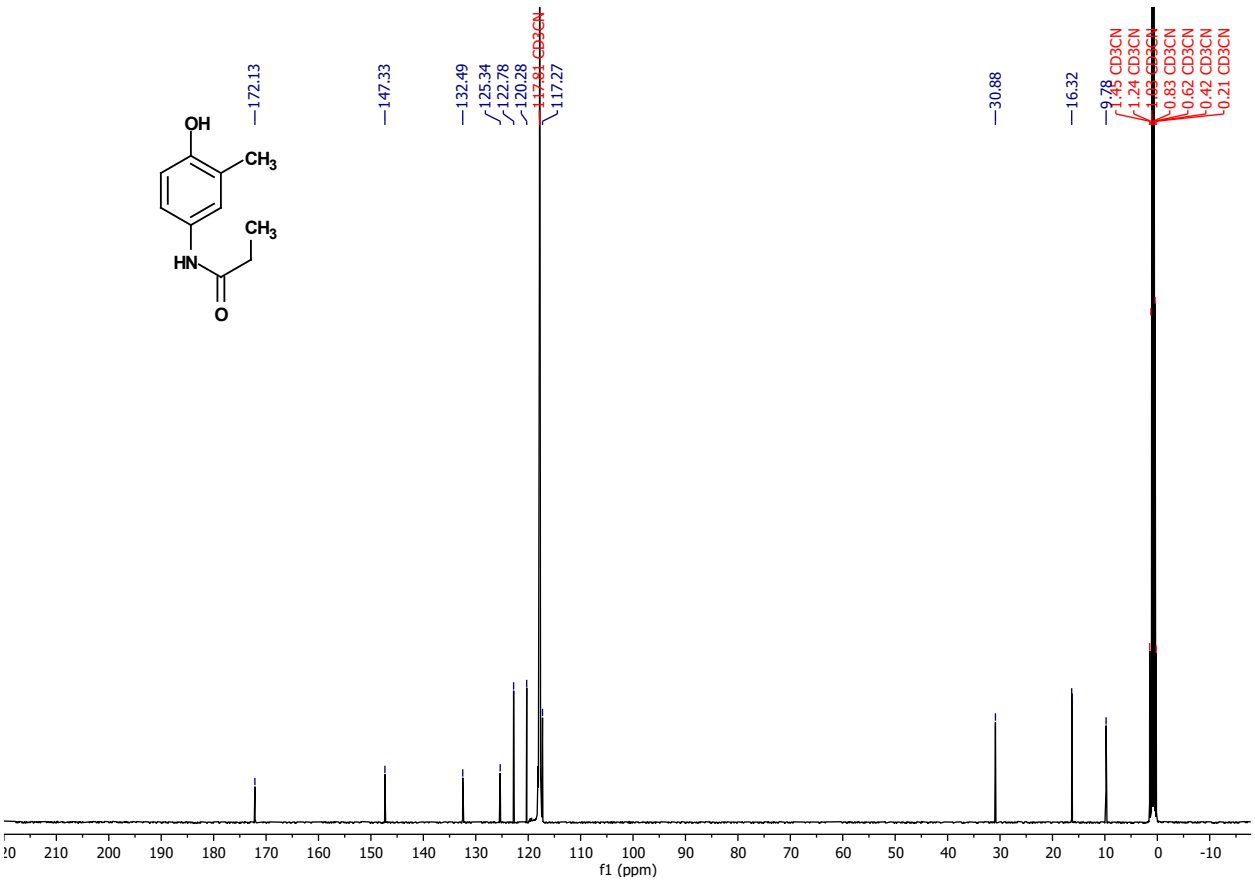
^{1}H and ^{13}C NMR *N*-(4-hydroxyphenyl)propionamide (**3u**)



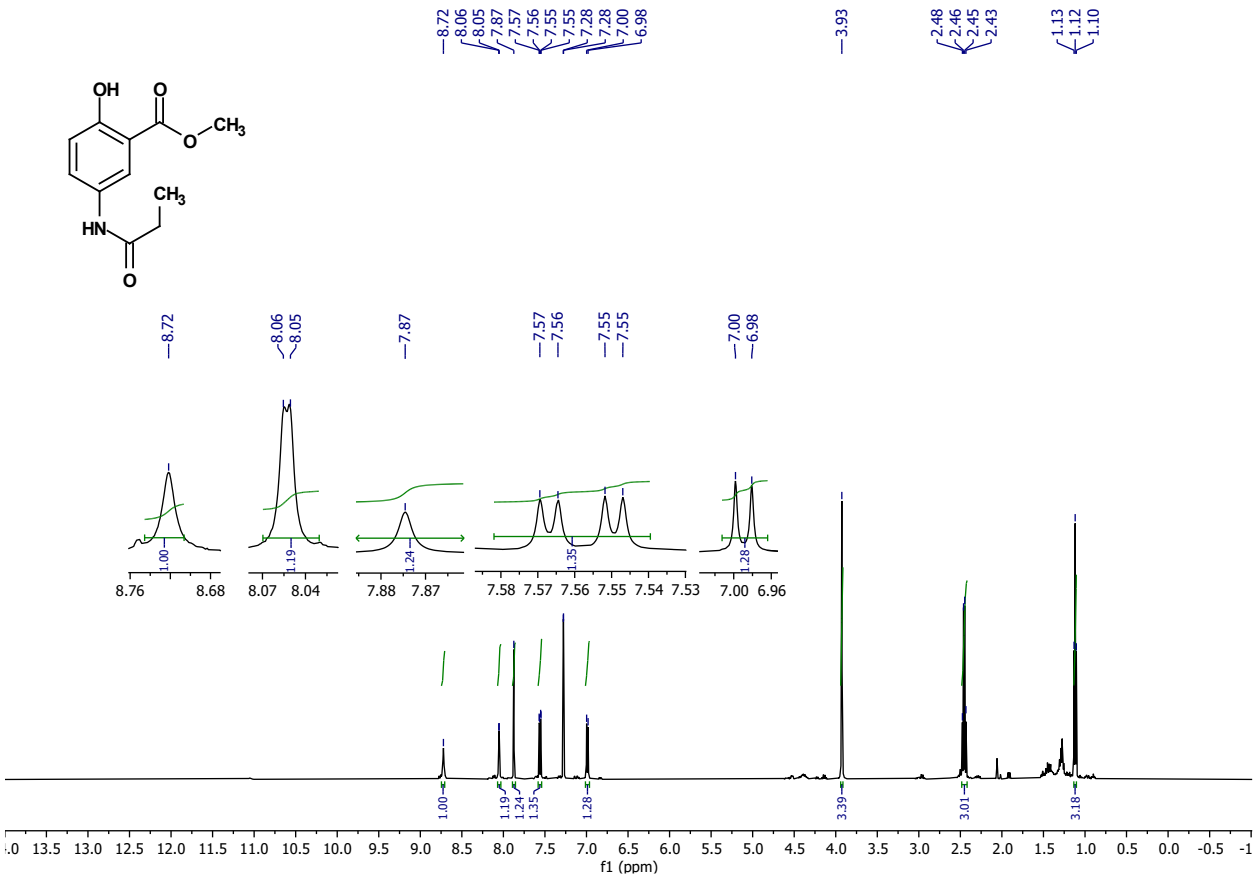


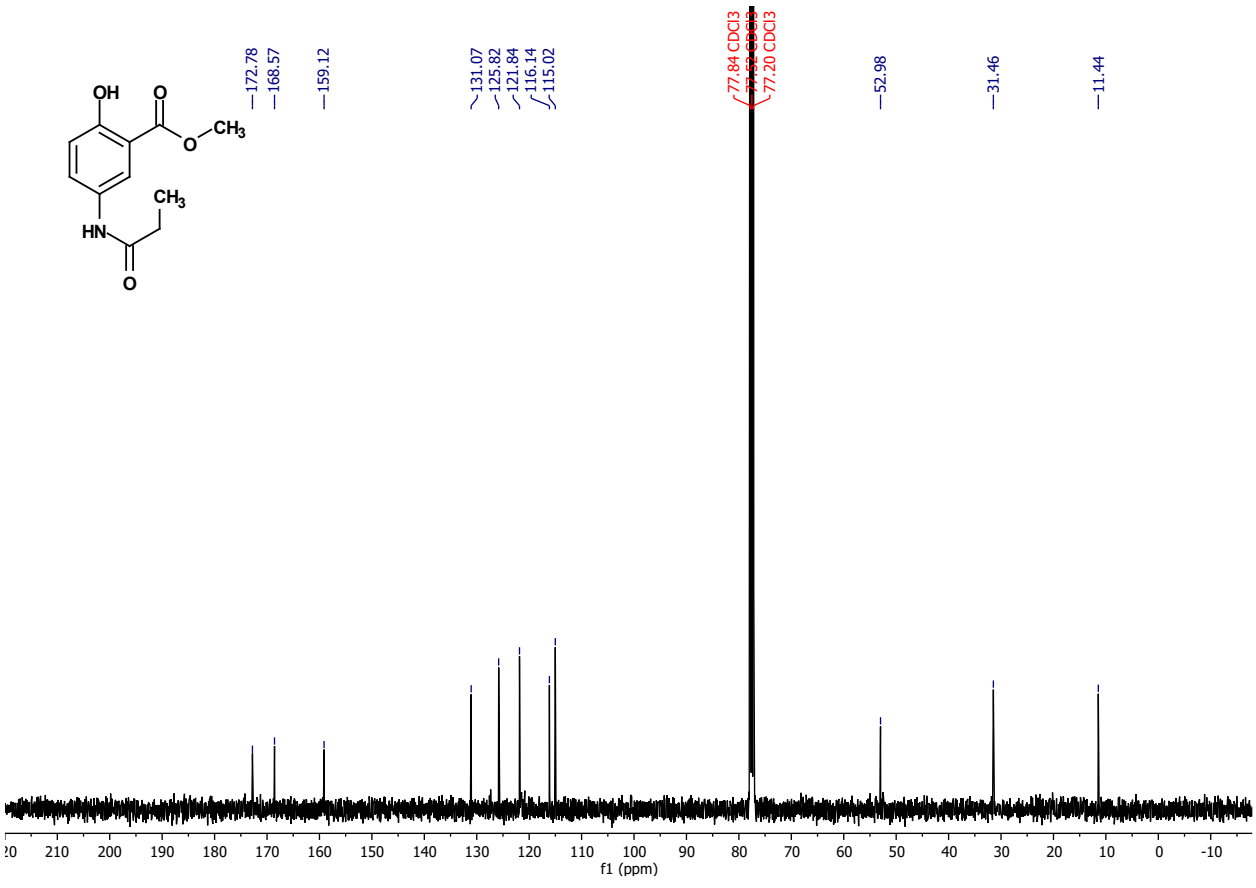
^{1}H and ^{13}C NMR *N*-(4-hydroxy-3-methylphenyl)propionamide (**3v**)



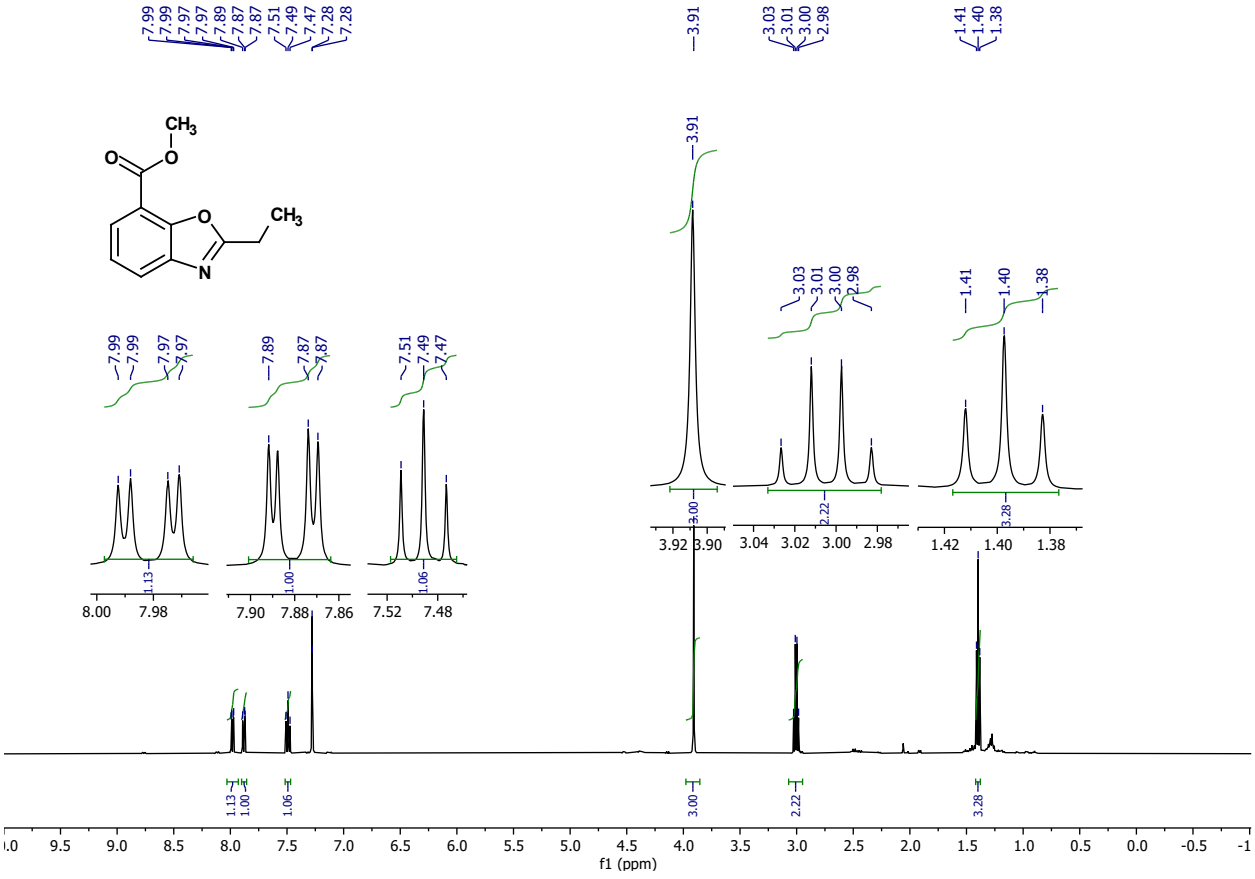


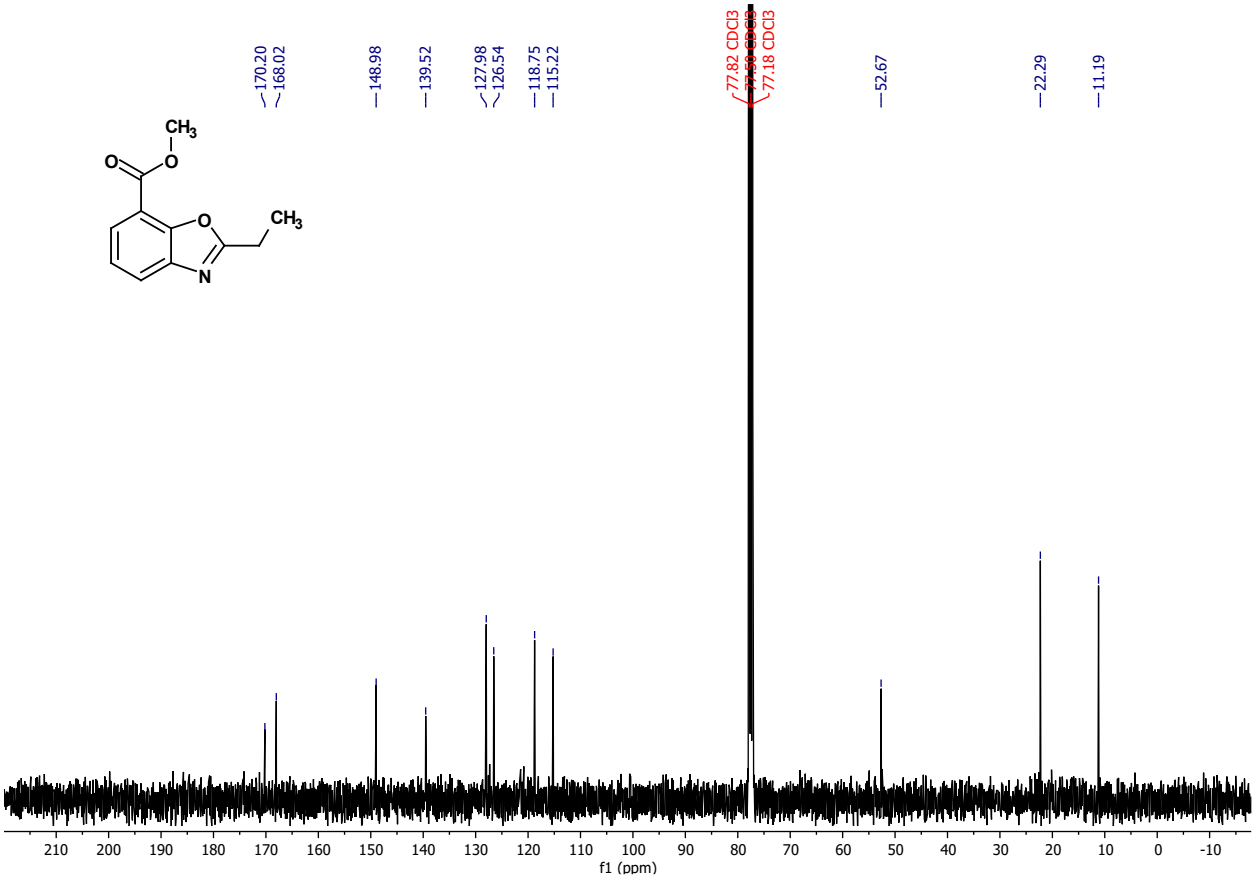
^{1}H and ^{13}C NMR Methyl 2-hydroxy-5-propionamidobenzoate (**3w**)



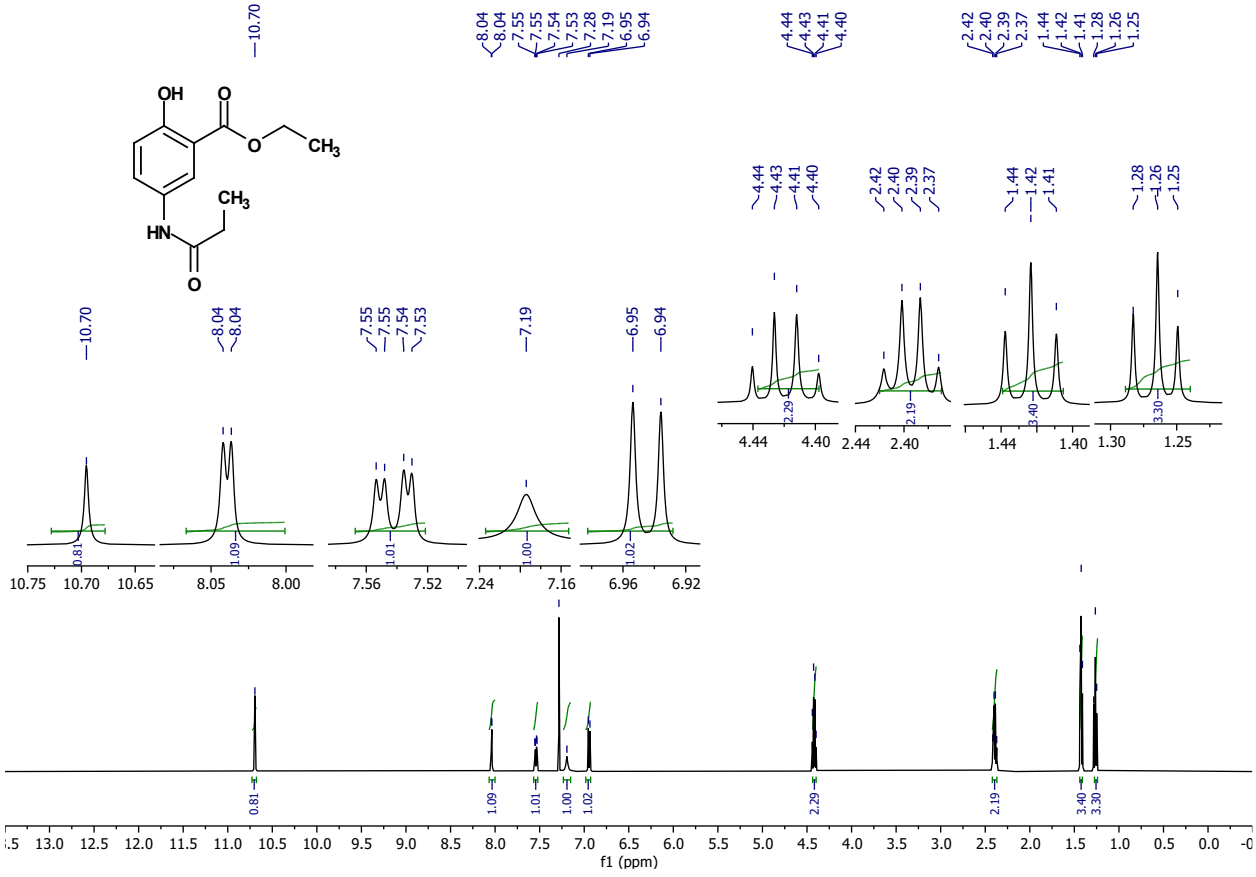


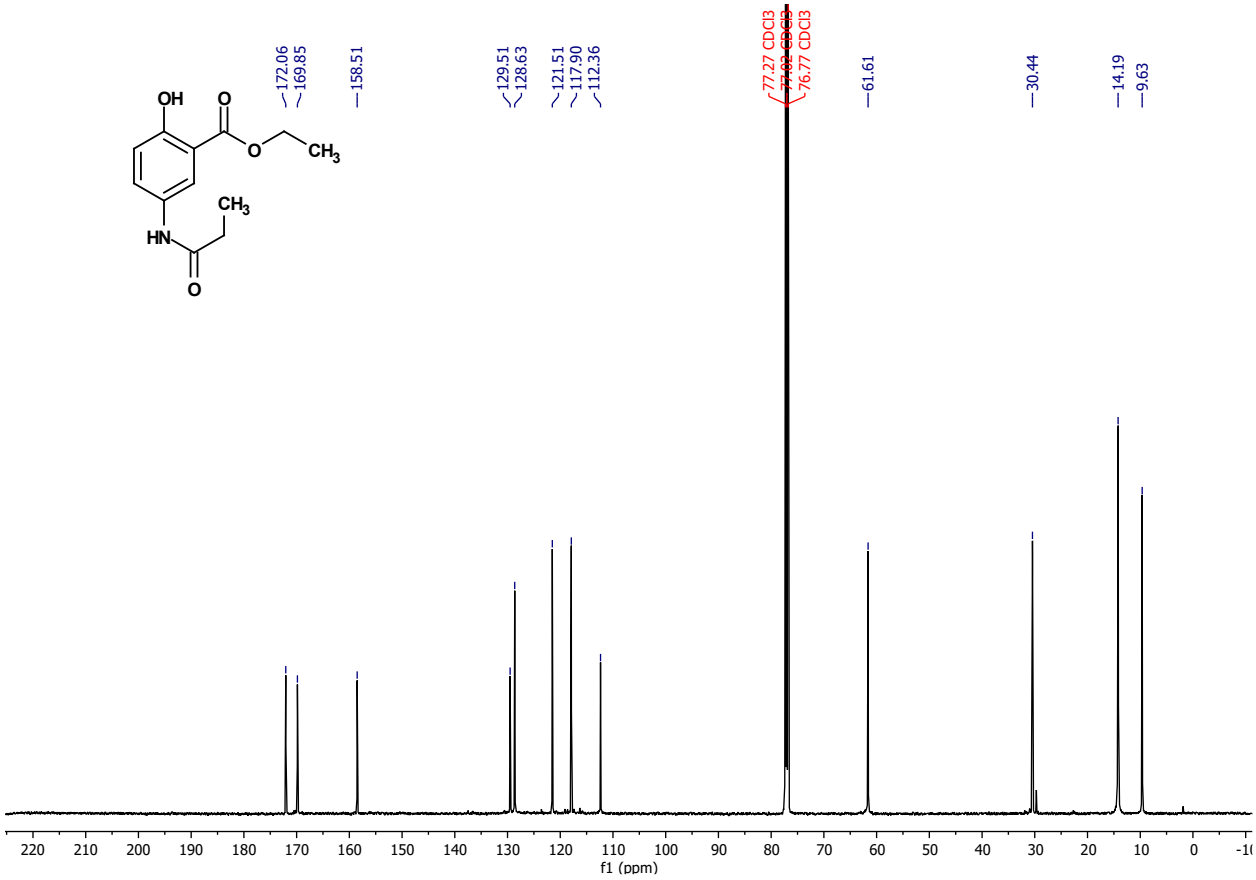
^{1}H and ^{13}C NMR Methyl 2-ethylbenzo[d]oxazole-7-carboxylate **(3ww)**



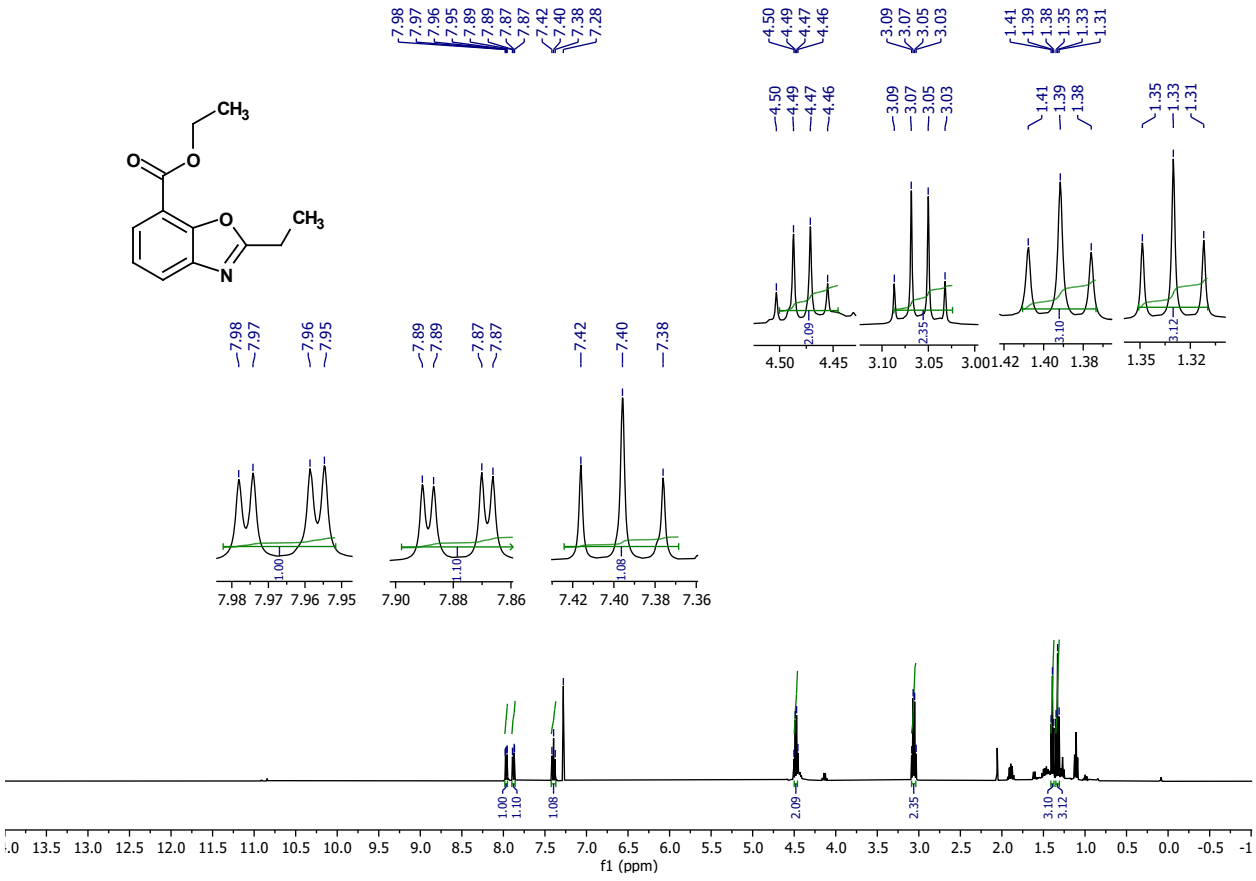


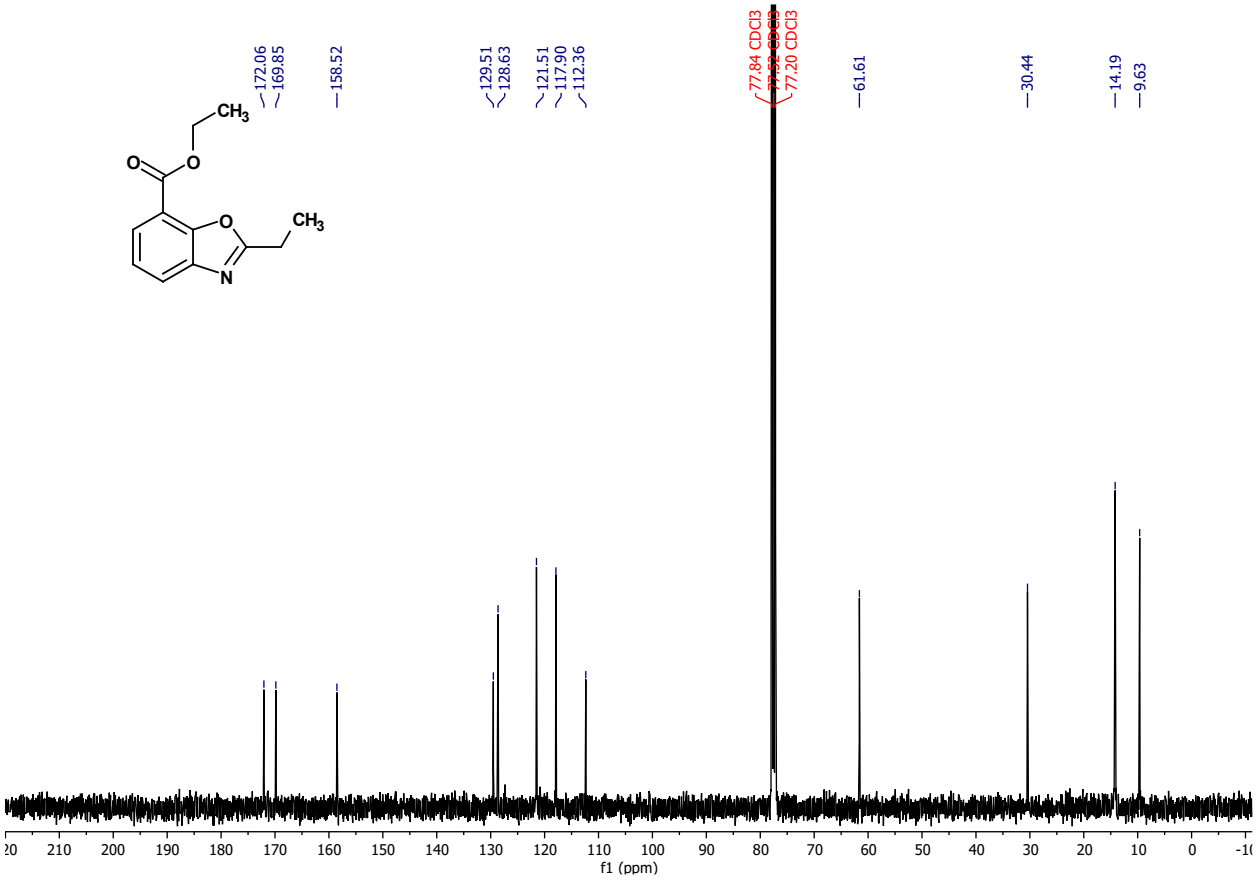
^{1}H and ^{13}C NMR Ehyl 2-hydroxy-5-propionamidobenzoate **(3x)**



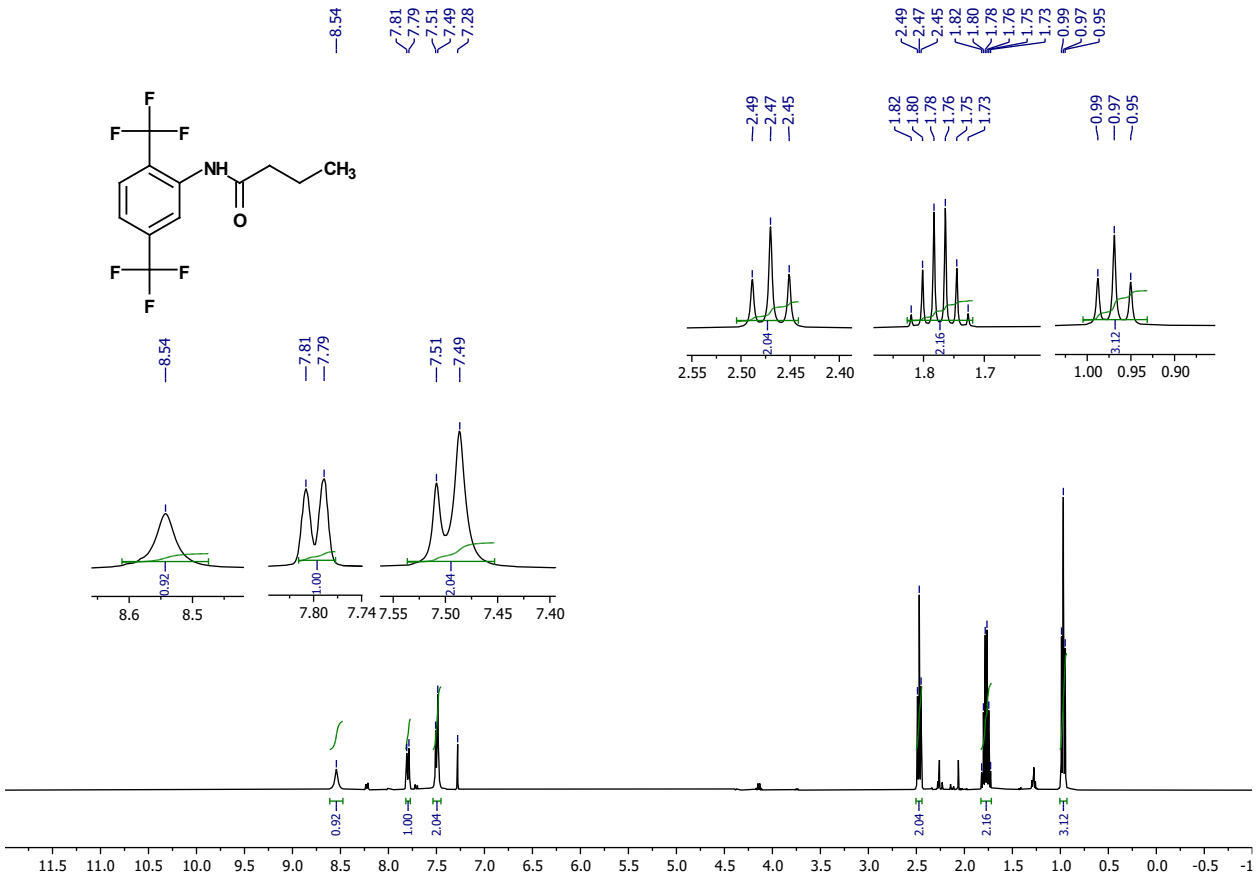


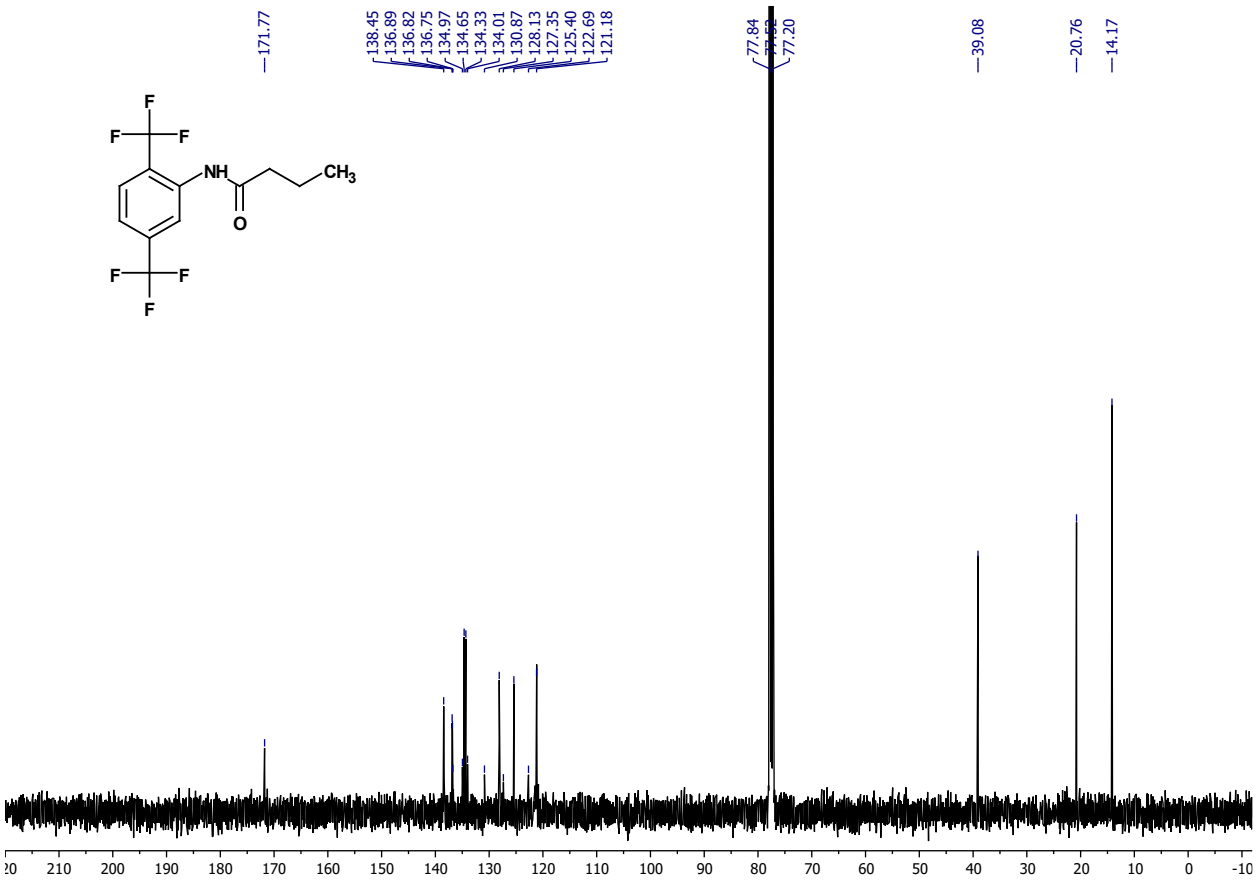
^{1}H and ^{13}C NMR Ethyl 2-ethylbenzo[d]oxazole-7-carboxylate **(3xx)**



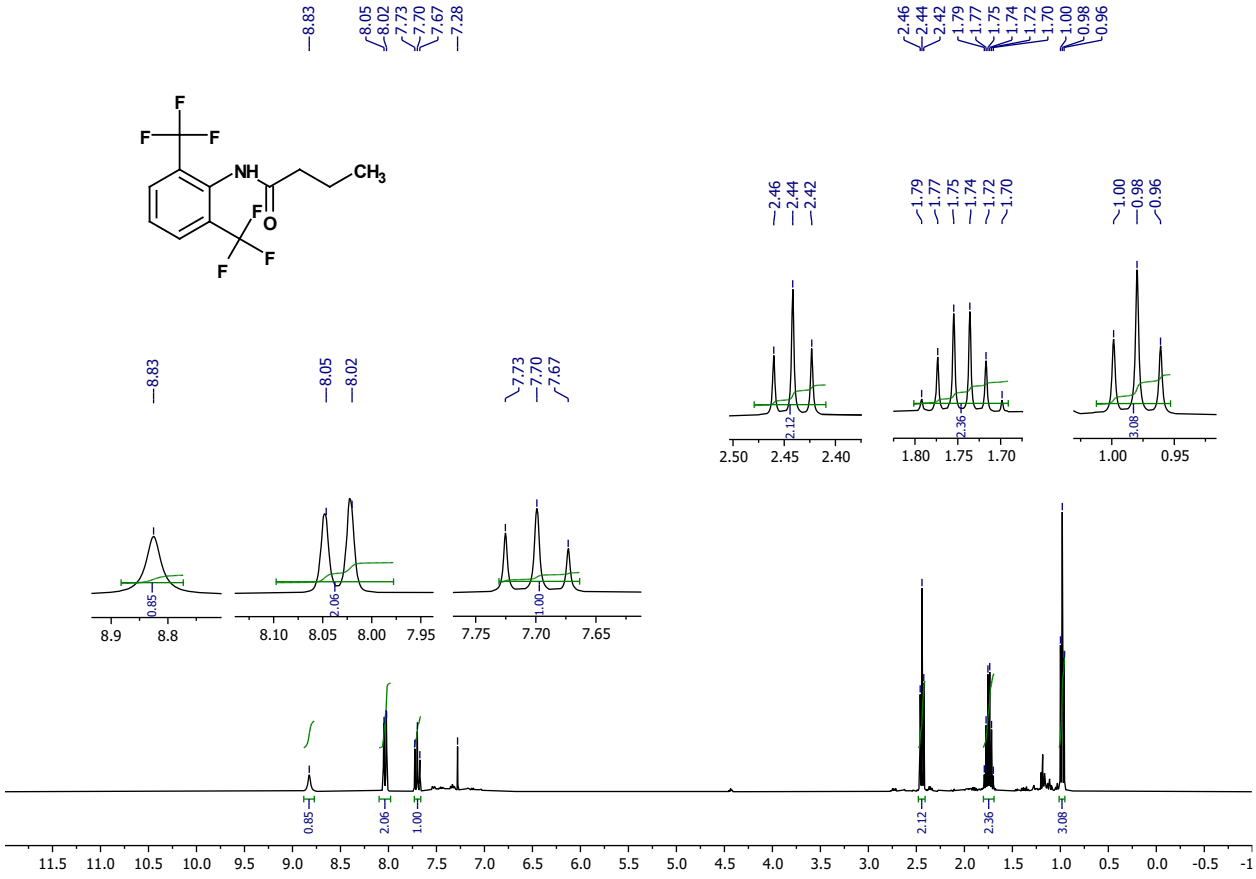


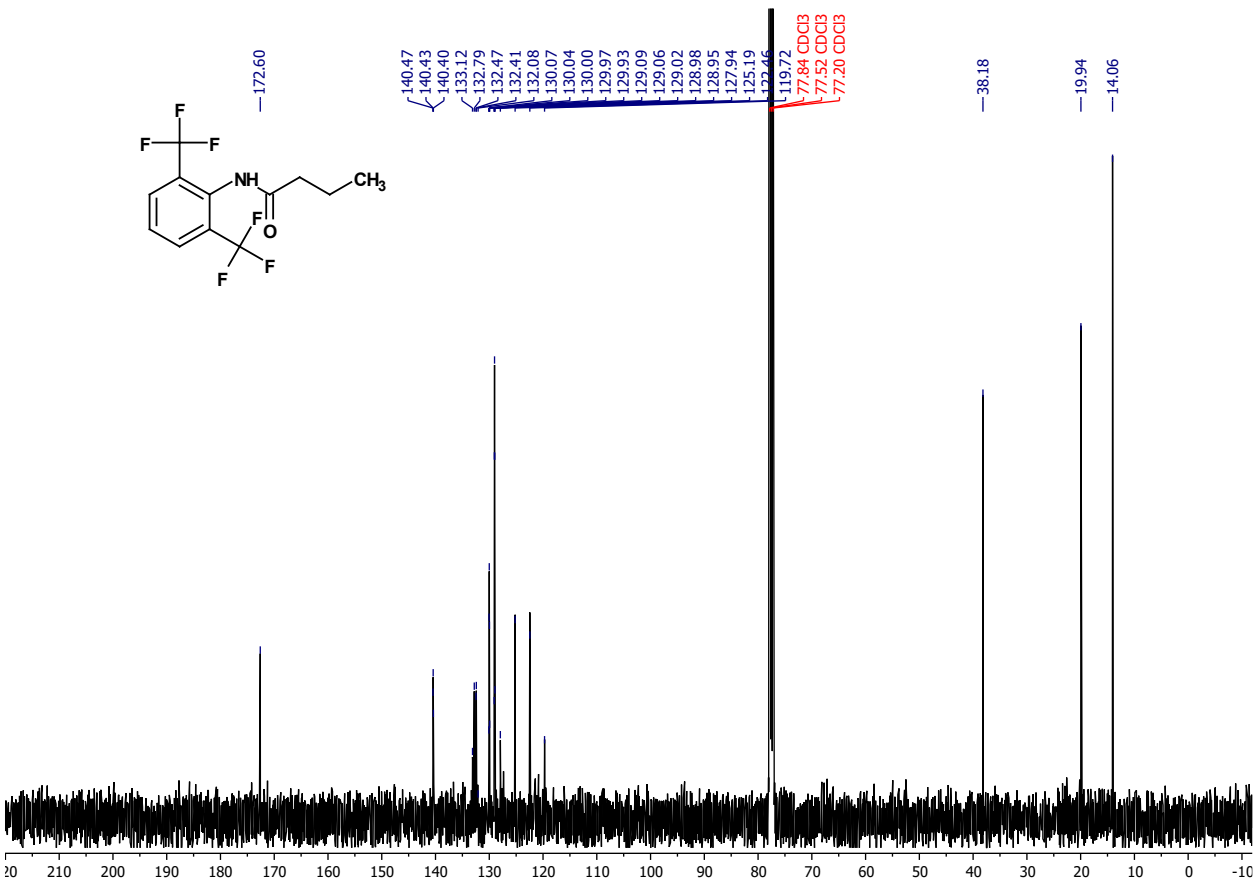
^{1}H and ^{13}C NMR *N*-(2,5-bis(trifluoromethyl)phenyl)butyramide **(4a)**



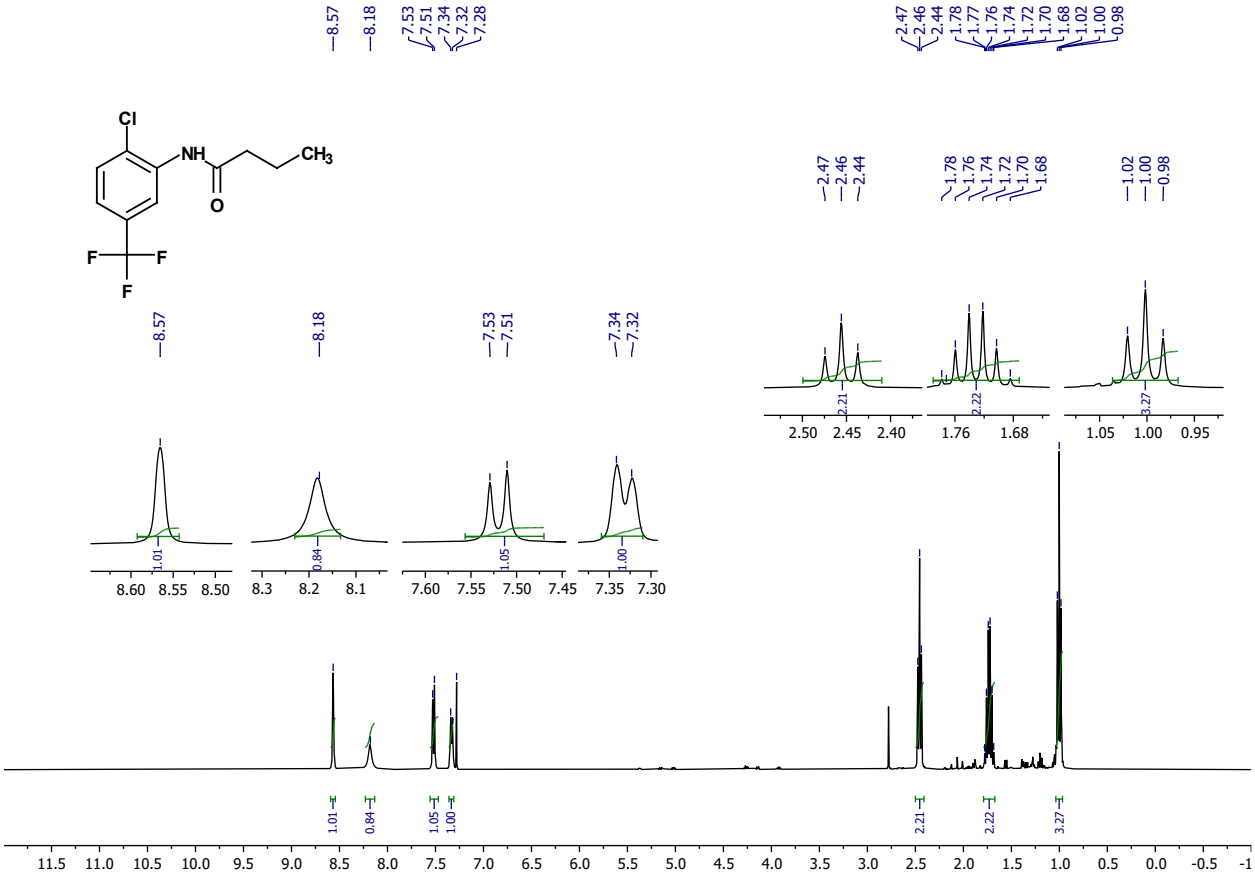


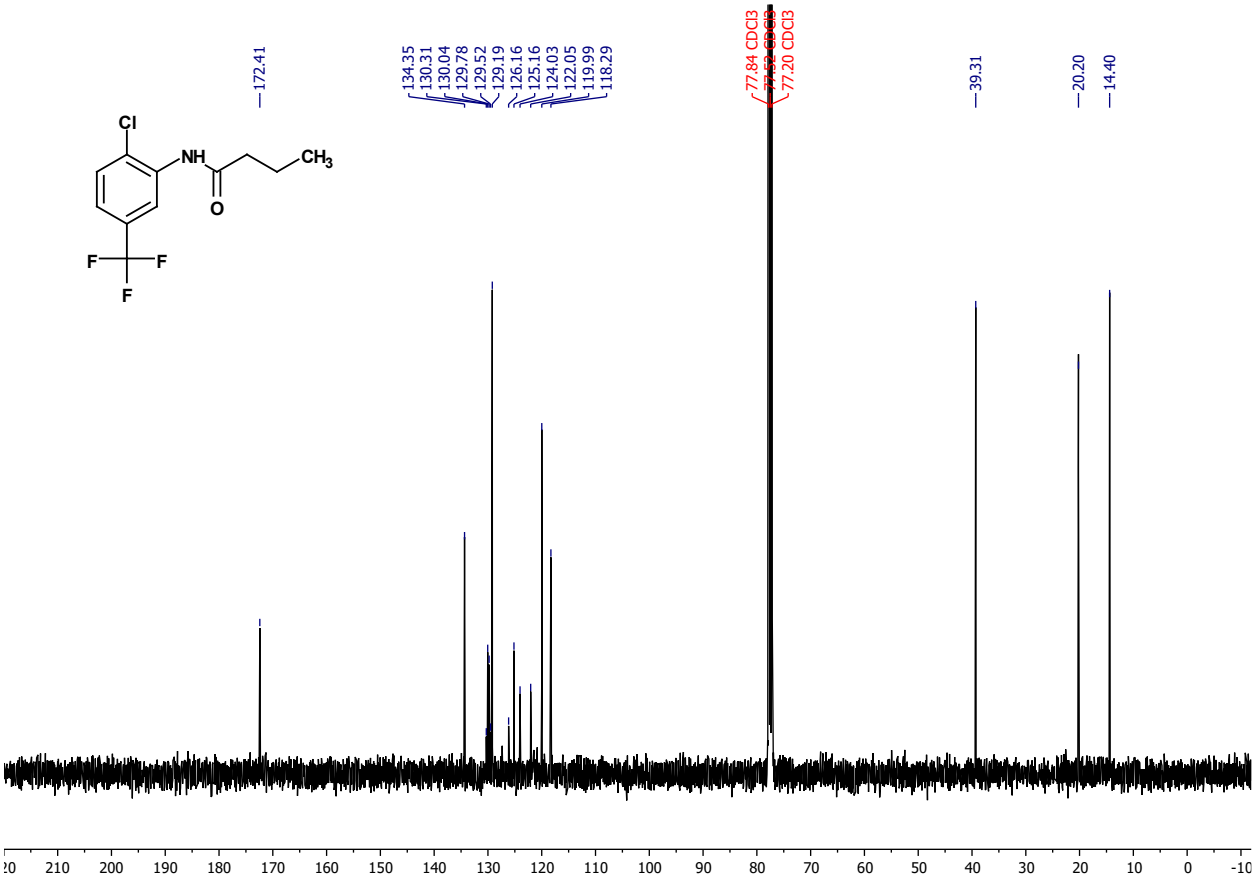
^{1}H and ^{13}C NMR *N*-(2,6-bis(trifluoromethyl)phenyl)butyramide **(4b)**



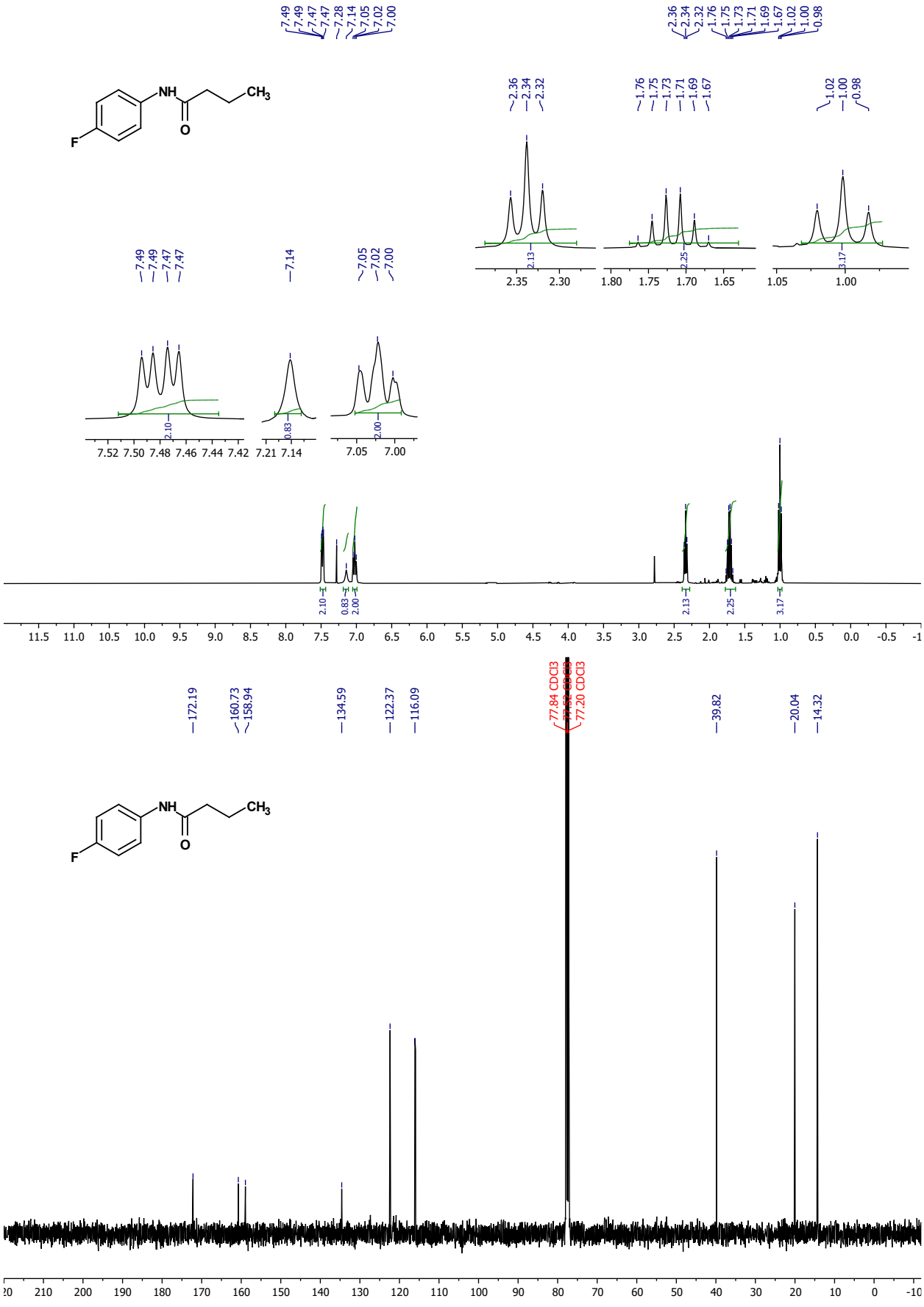


^{1}H and ^{13}C NMR *N*-(2-chloro-5-(trifluoromethyl)phenyl)butyramide **(4e)**

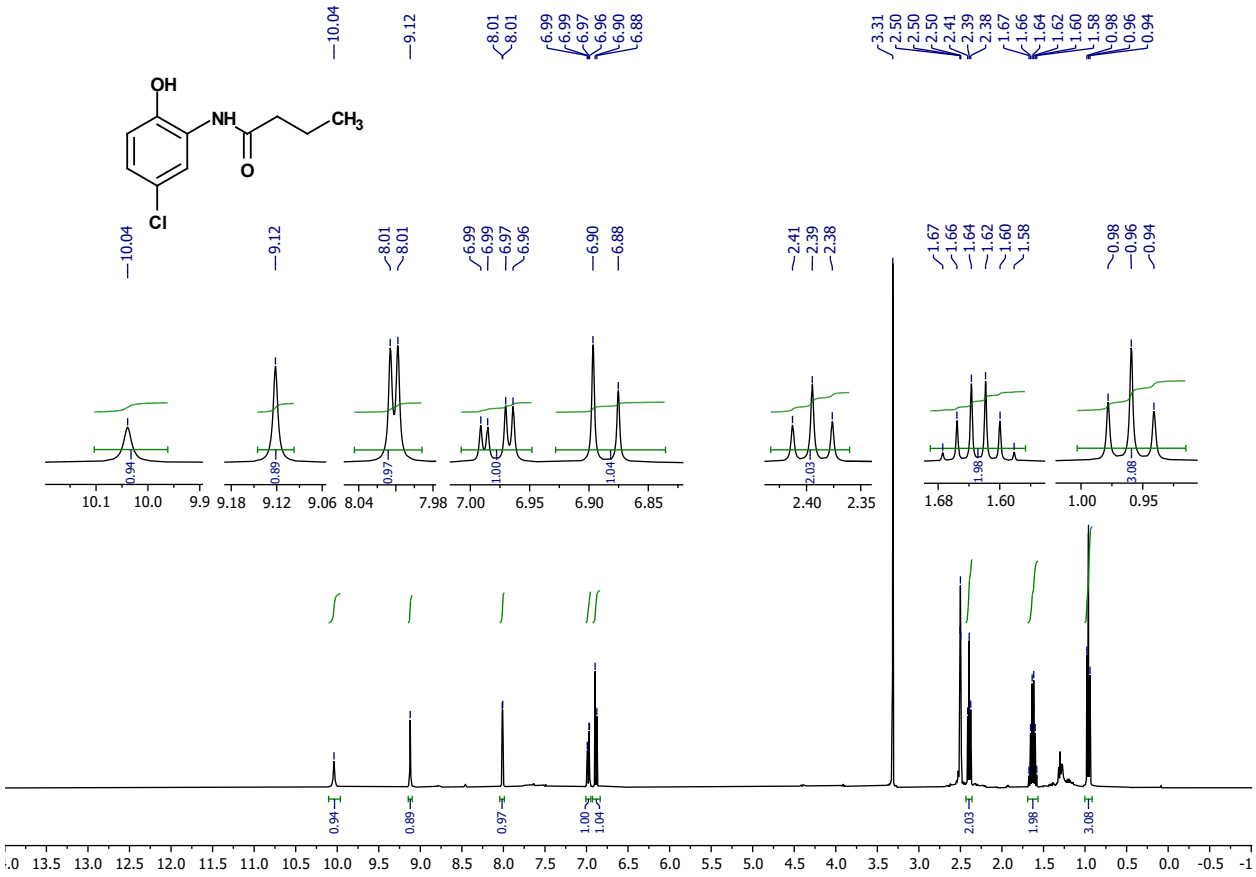


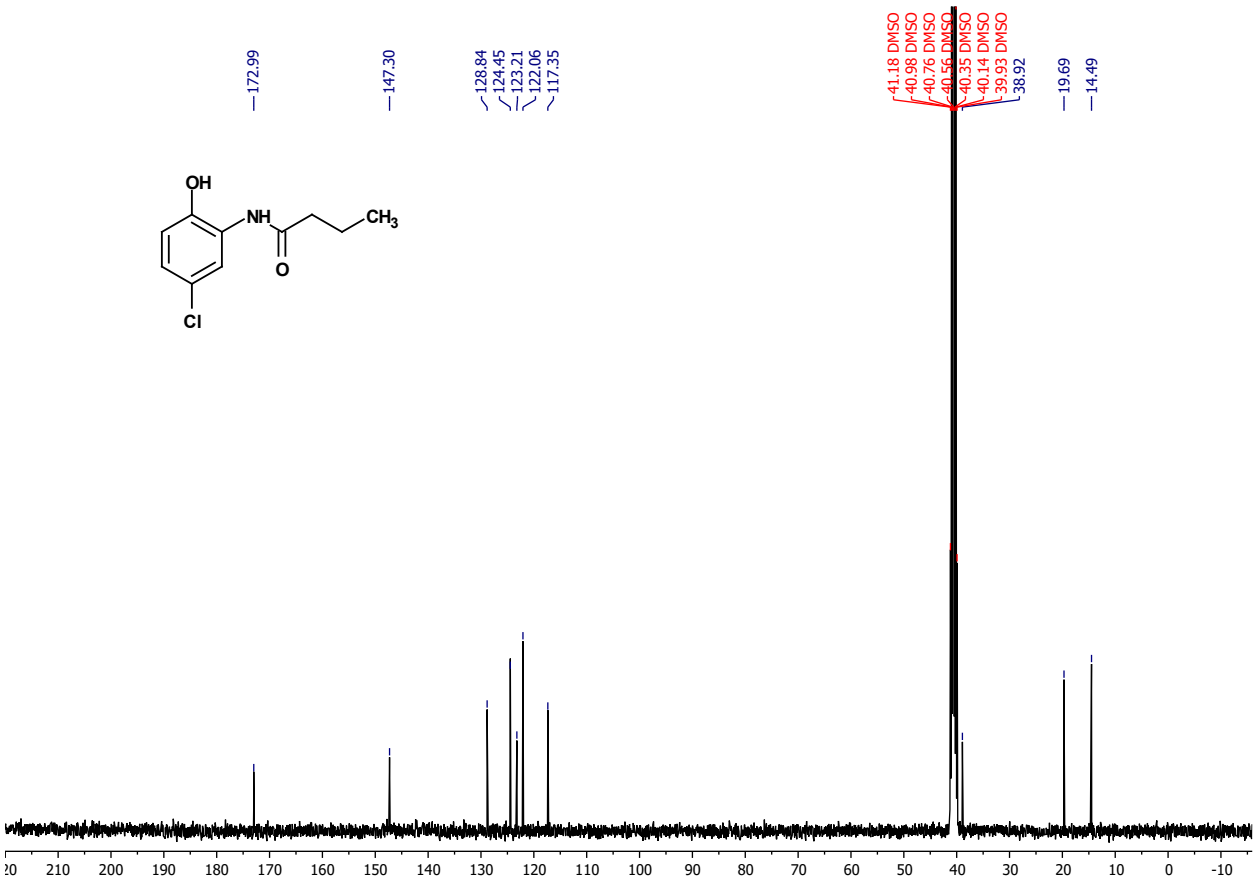


^{1}H and ^{13}C NMR *N*-(4-fluorophenyl)butyramide (**4f**)

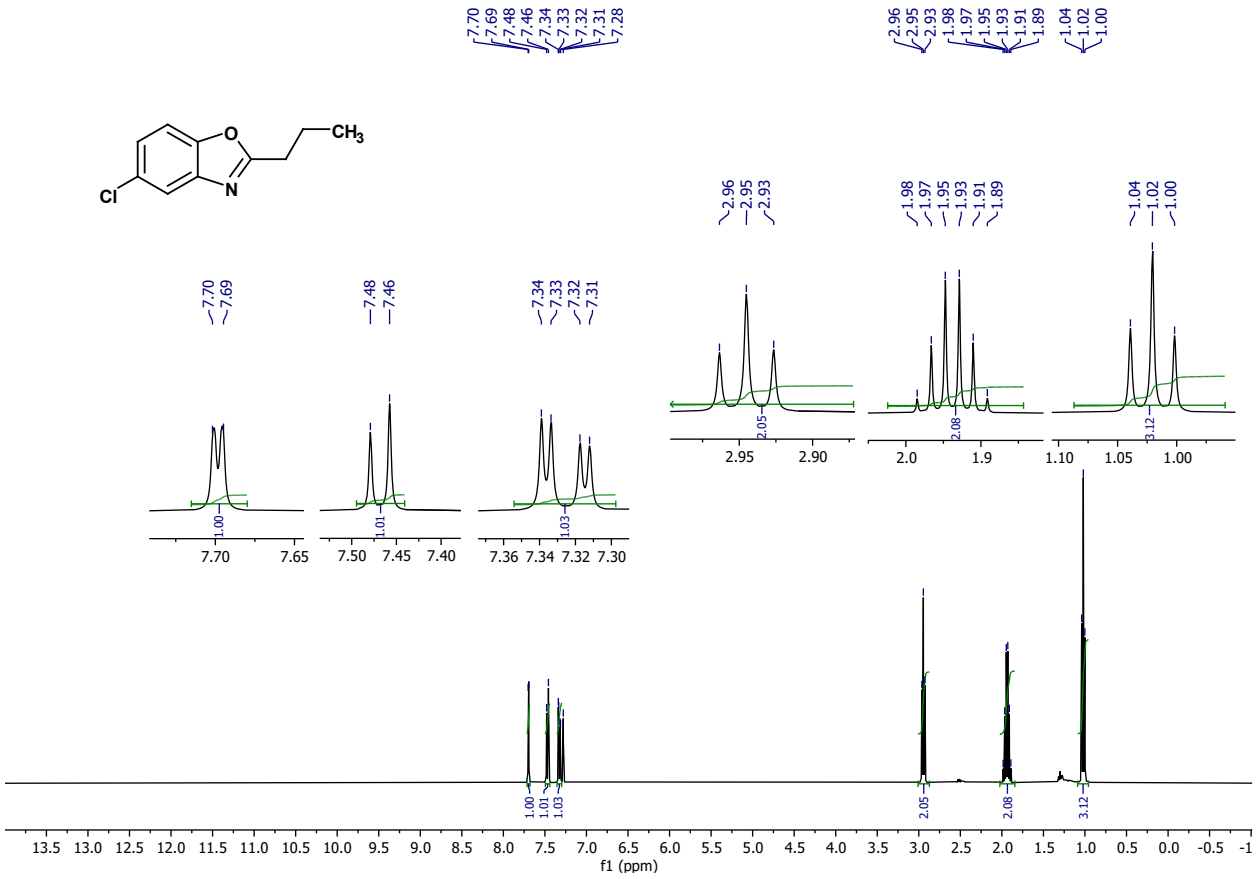


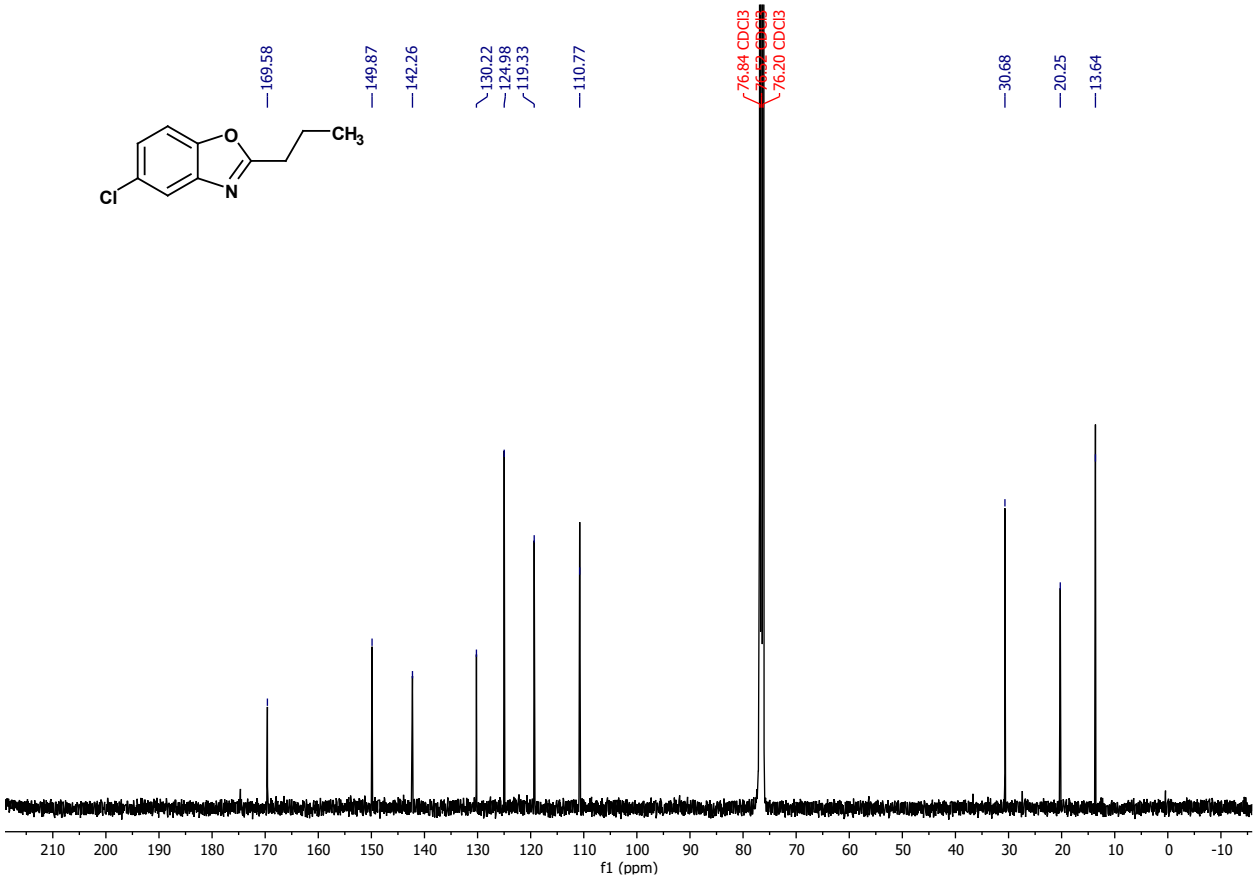
^{1}H and ^{13}C NMR *N*-(5-chloro-2-hydroxyphenyl)butyramide (**4i**)



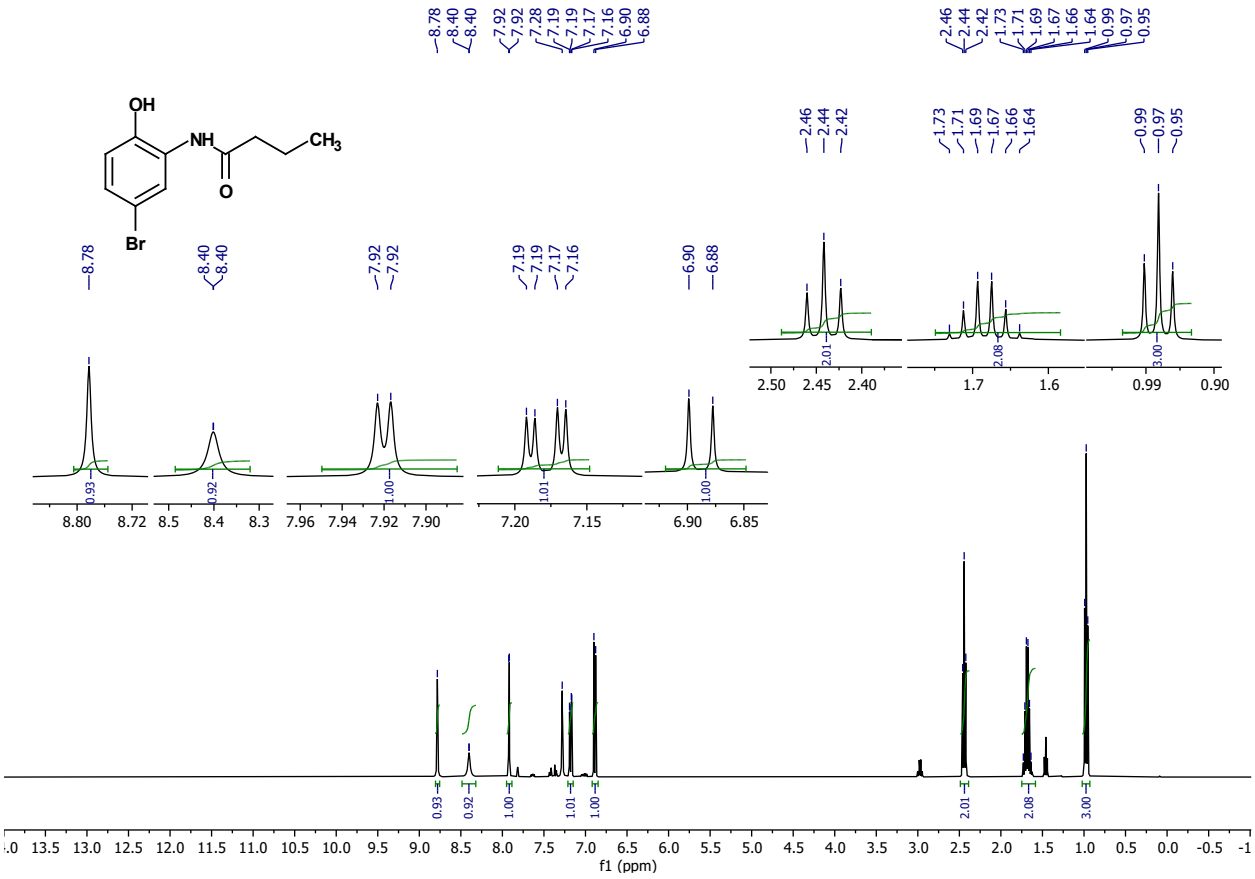


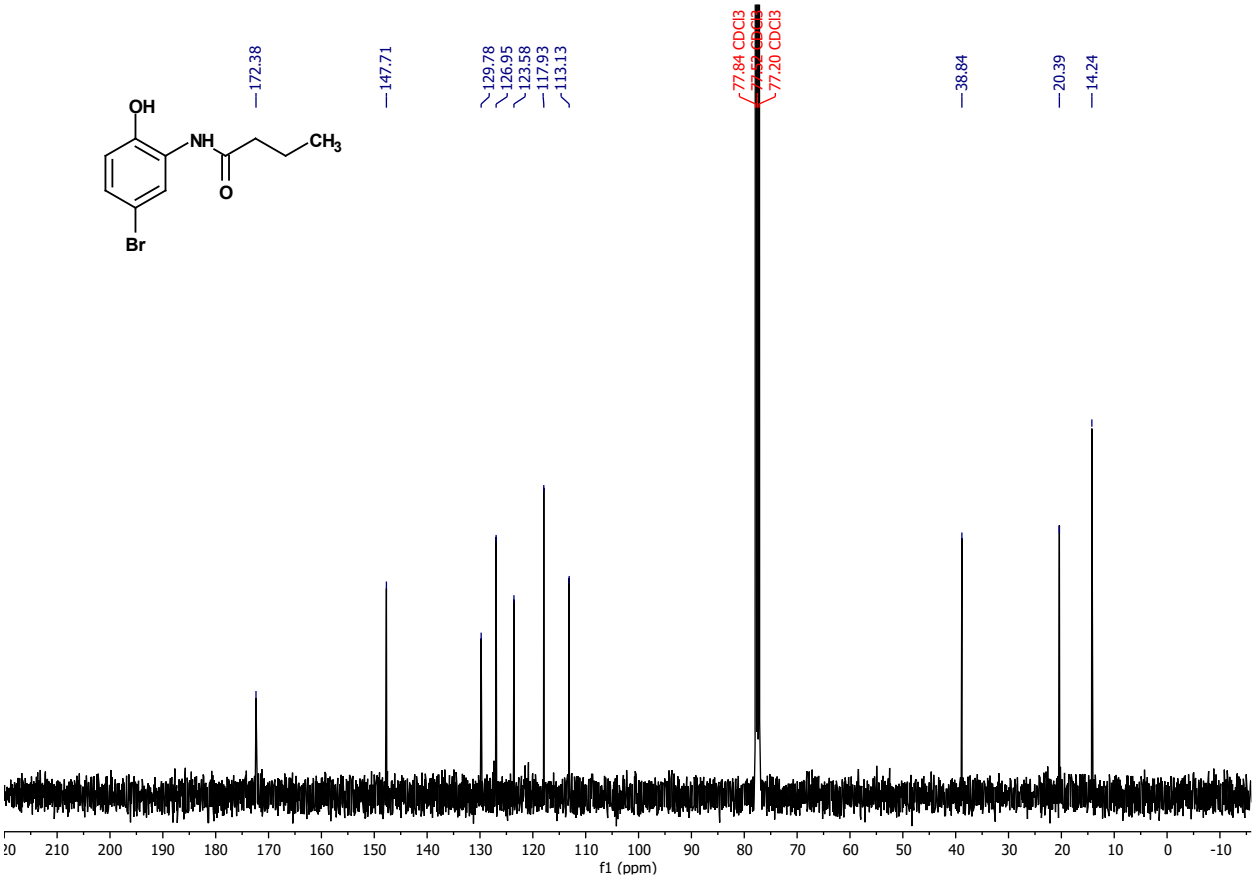
^{1}H and ^{13}C NMR 5-chloro-2-propylbenzo[d]oxazole **(4ii)**



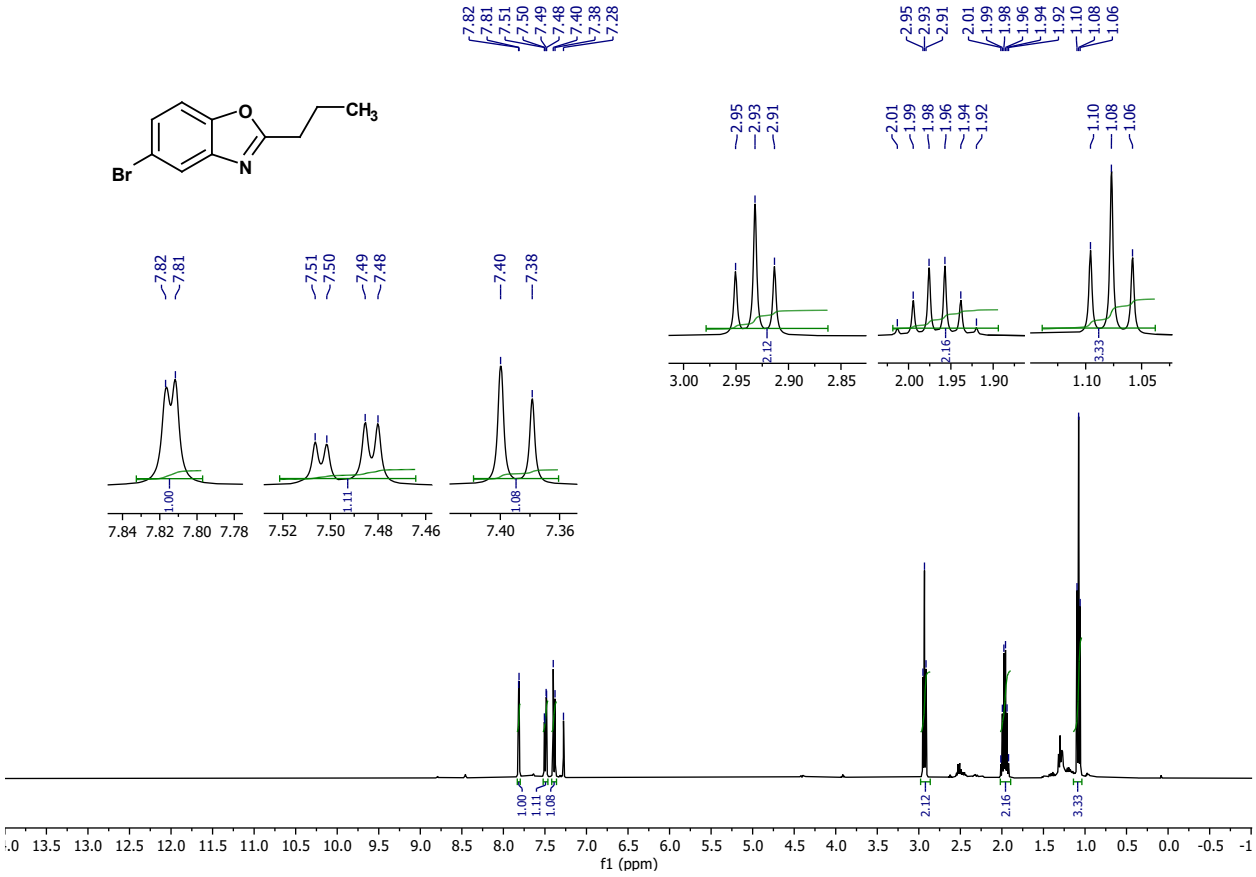


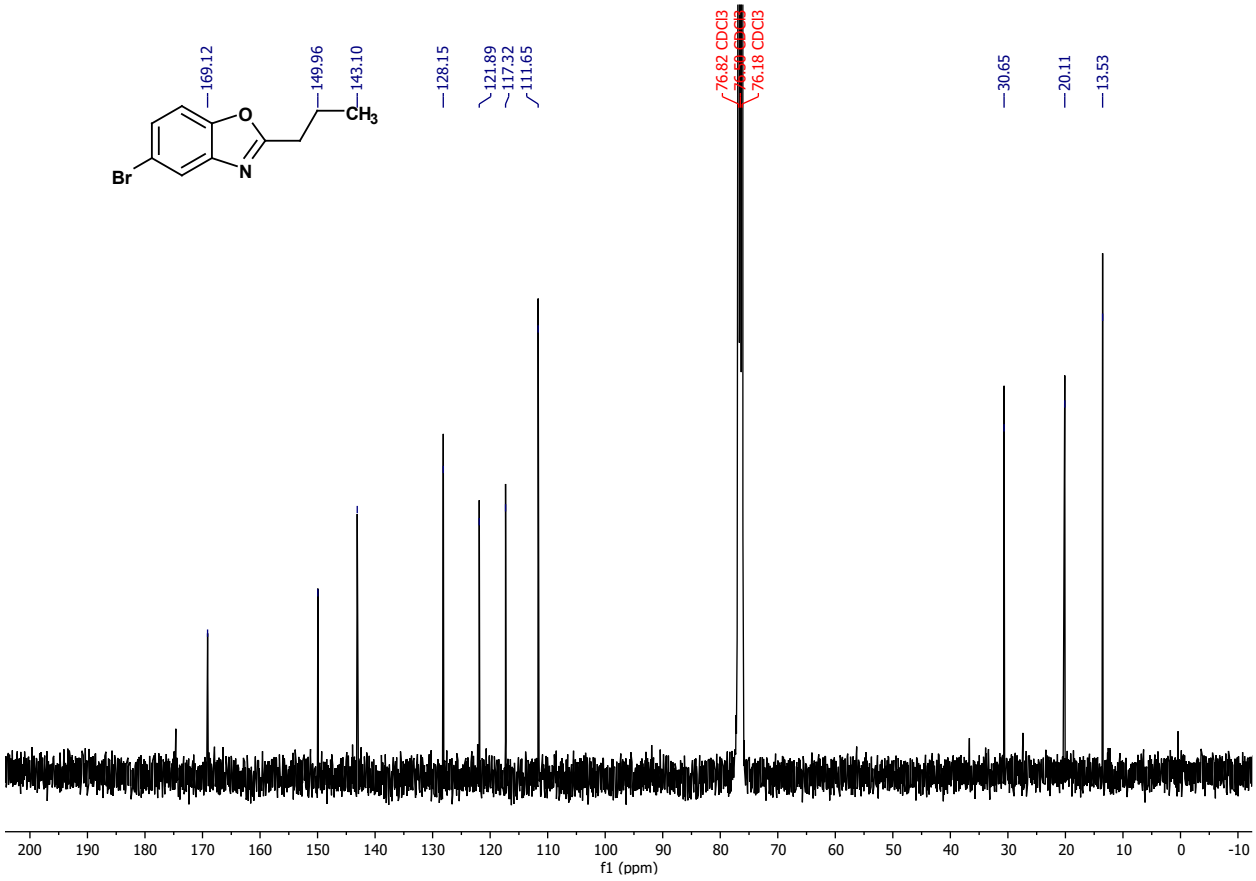
^{1}H and ^{13}C NMR *N*-(5-bromo-2-hydroxyphenyl)butyramide **(4j)**



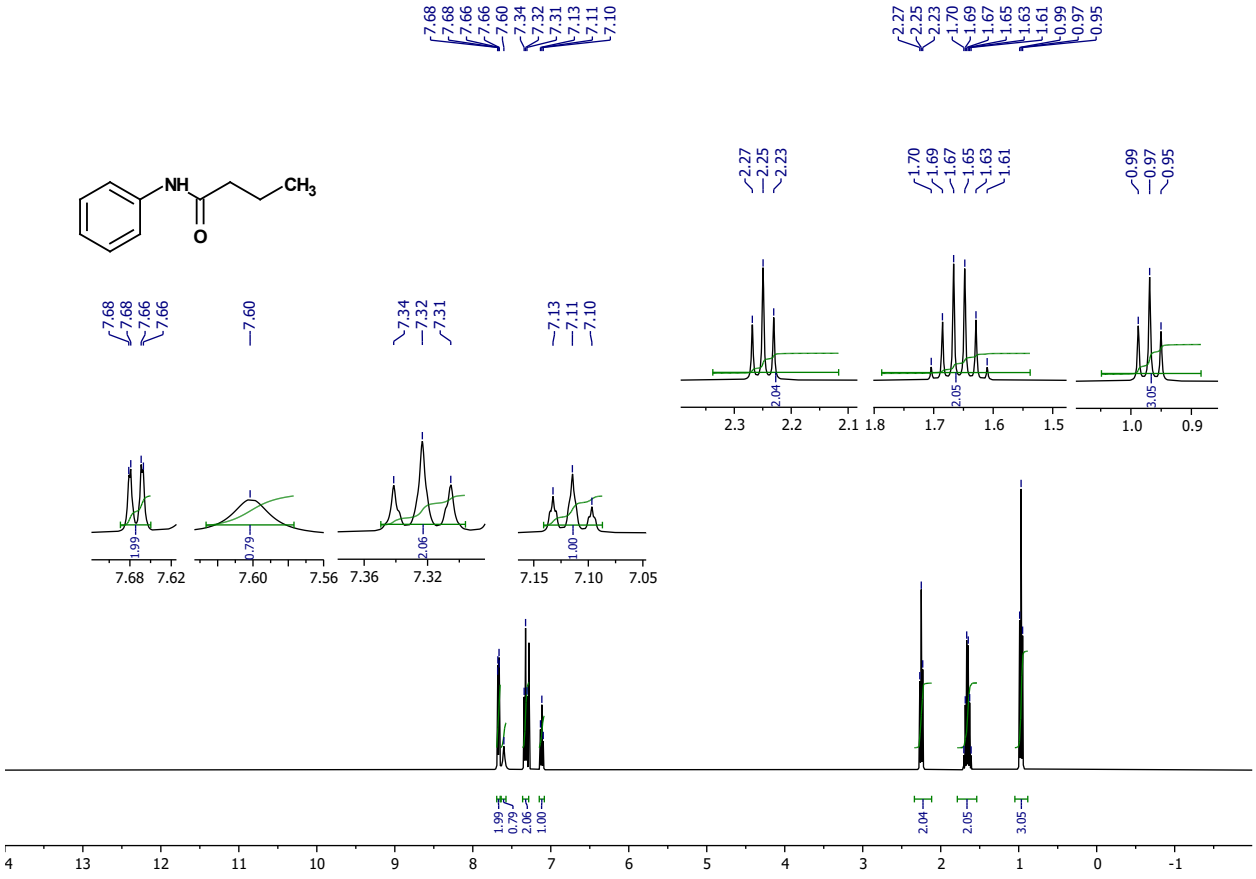


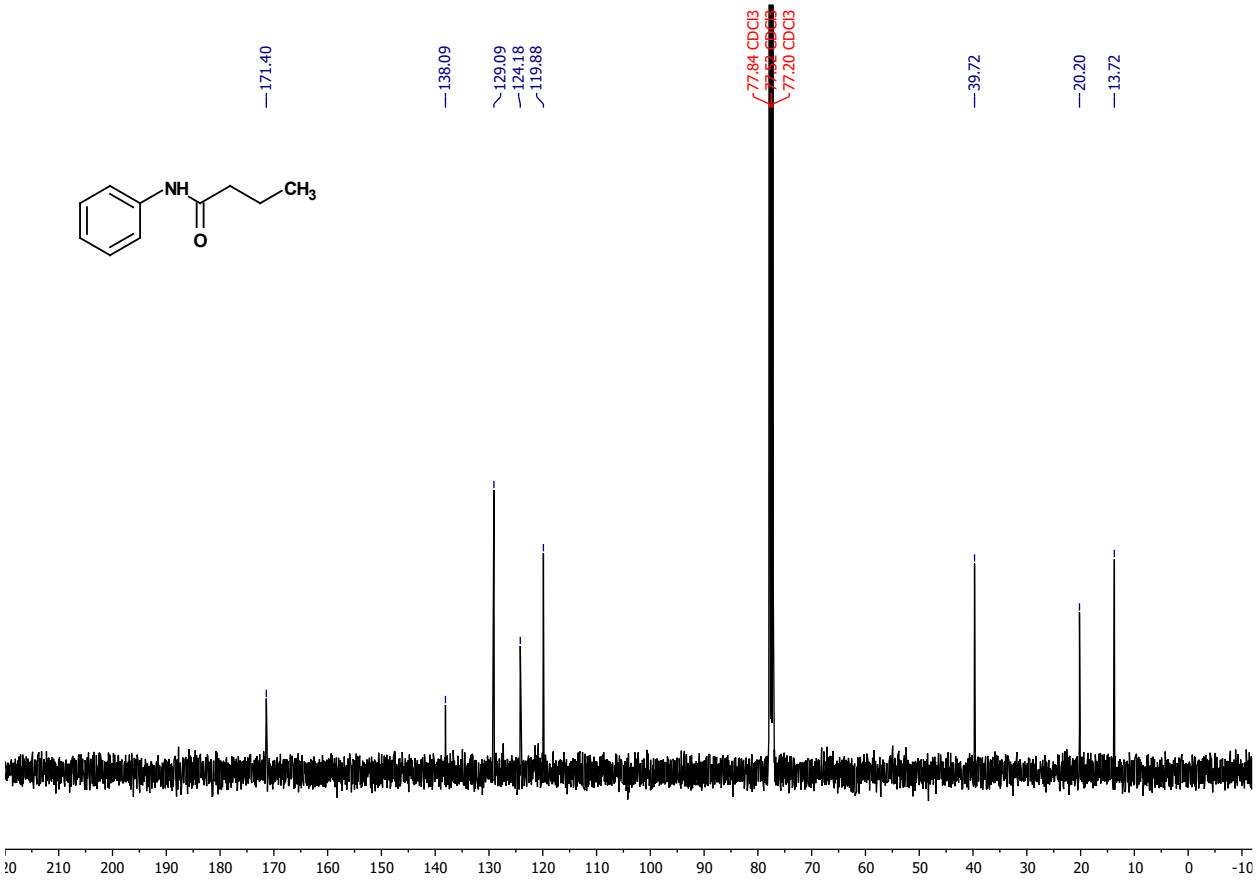
^{1}H and ^{13}C NMR 5-bromo-2- propylbenzo[d]oxazole **(4jj)**



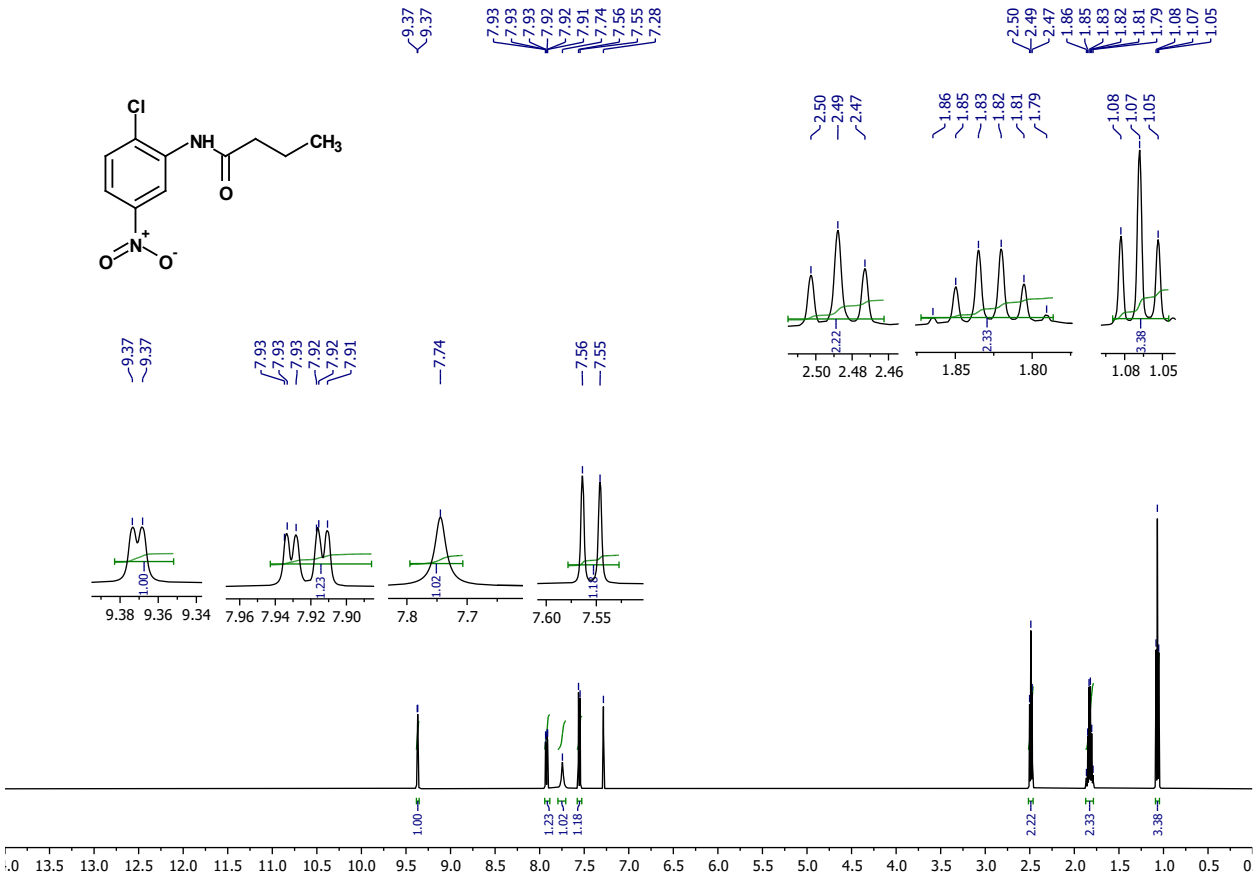


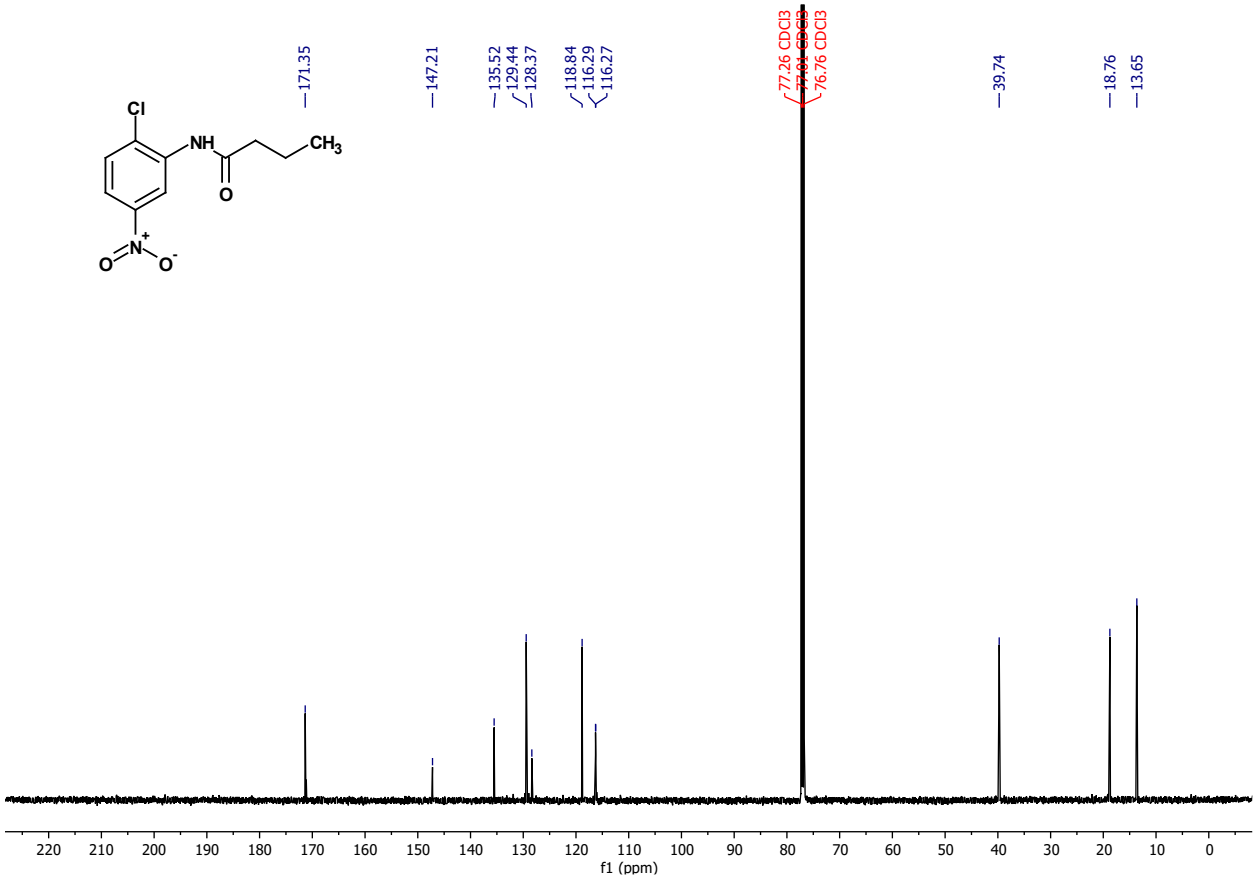
^{1}H and ^{13}C NMR *N*-phenylbutyramide (**4k**)



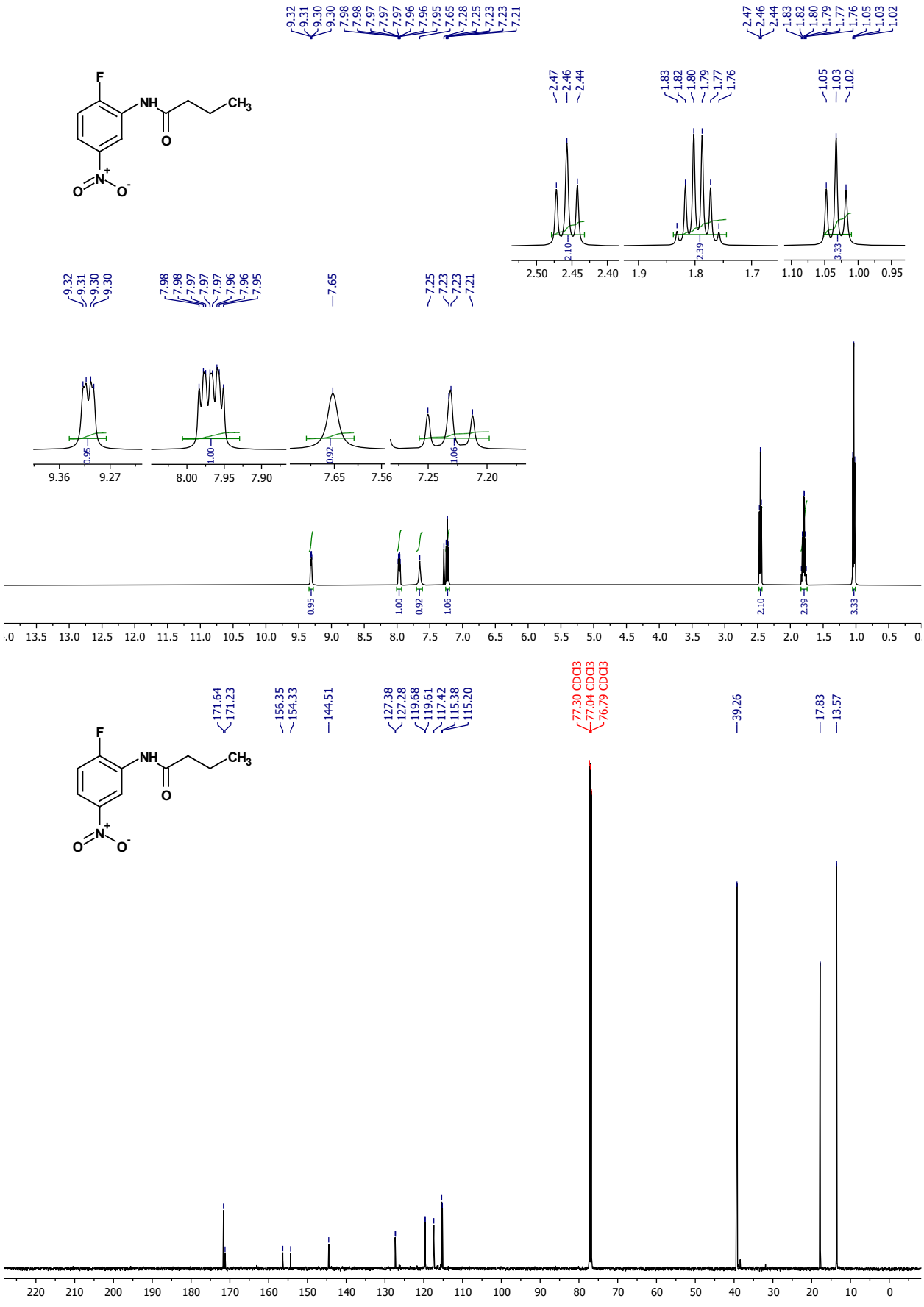


^{1}H and ^{13}C NMR *N*-(2-chloro-5-nitrophenyl)butyramide **(4o)**

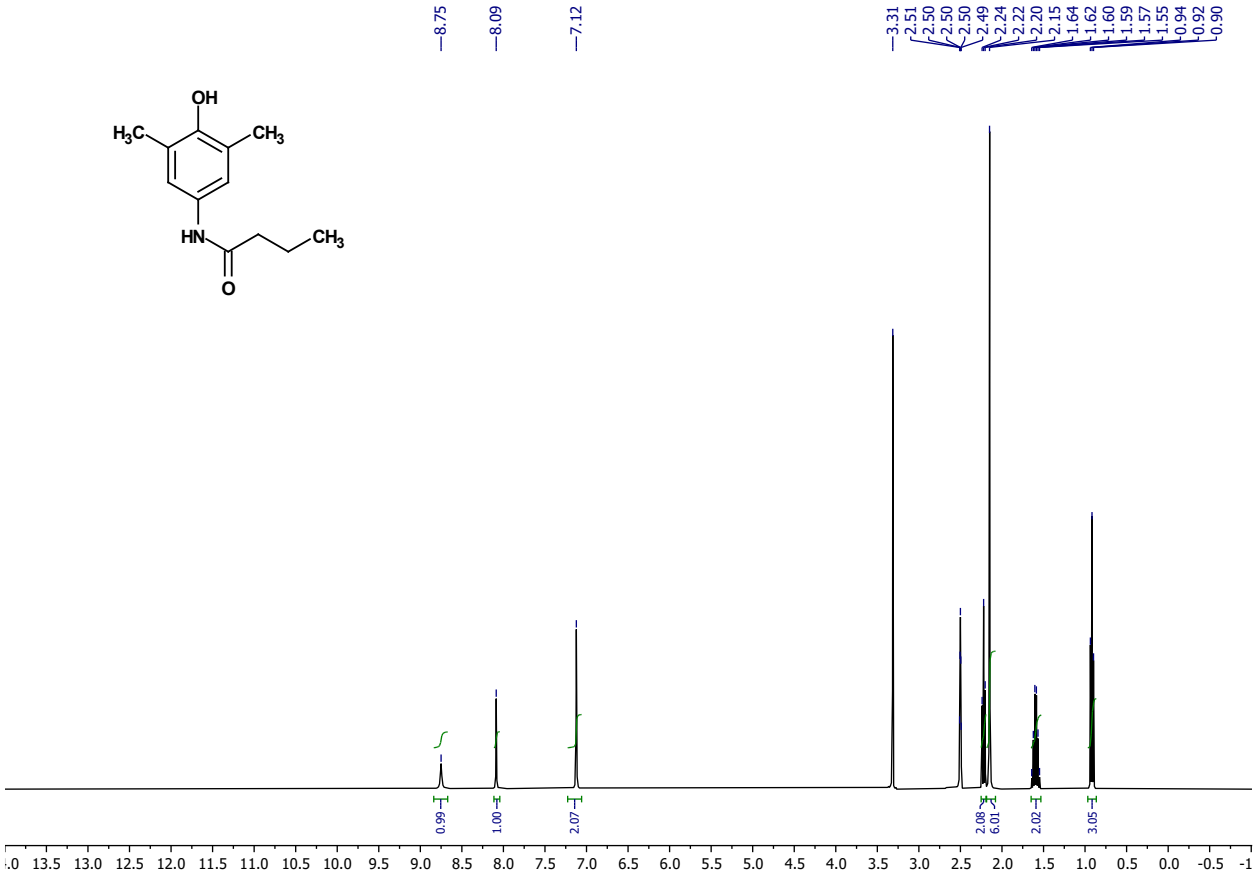


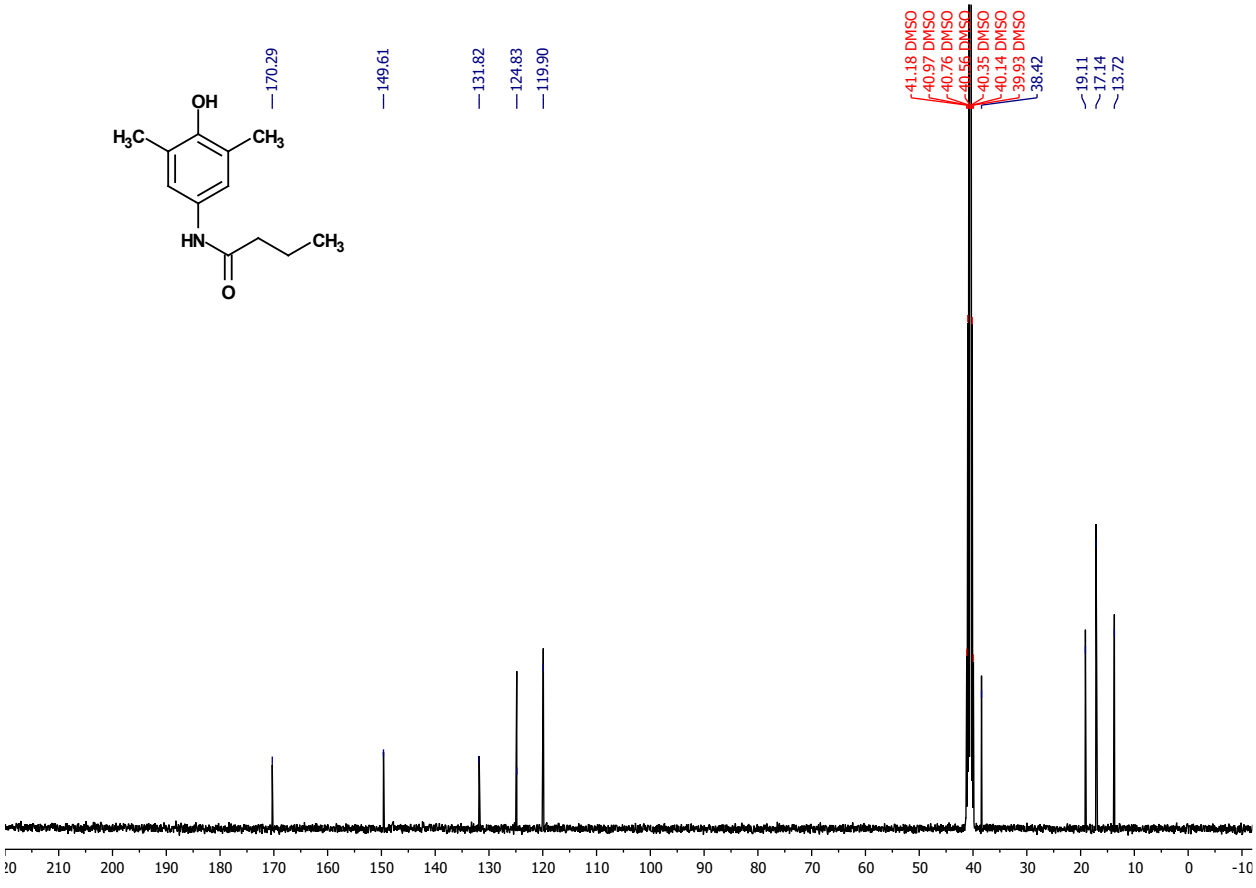


^{1}H and ^{13}C NMR *N*-(2-fluoro-5-nitrophenyl)butyramide **(4p)**

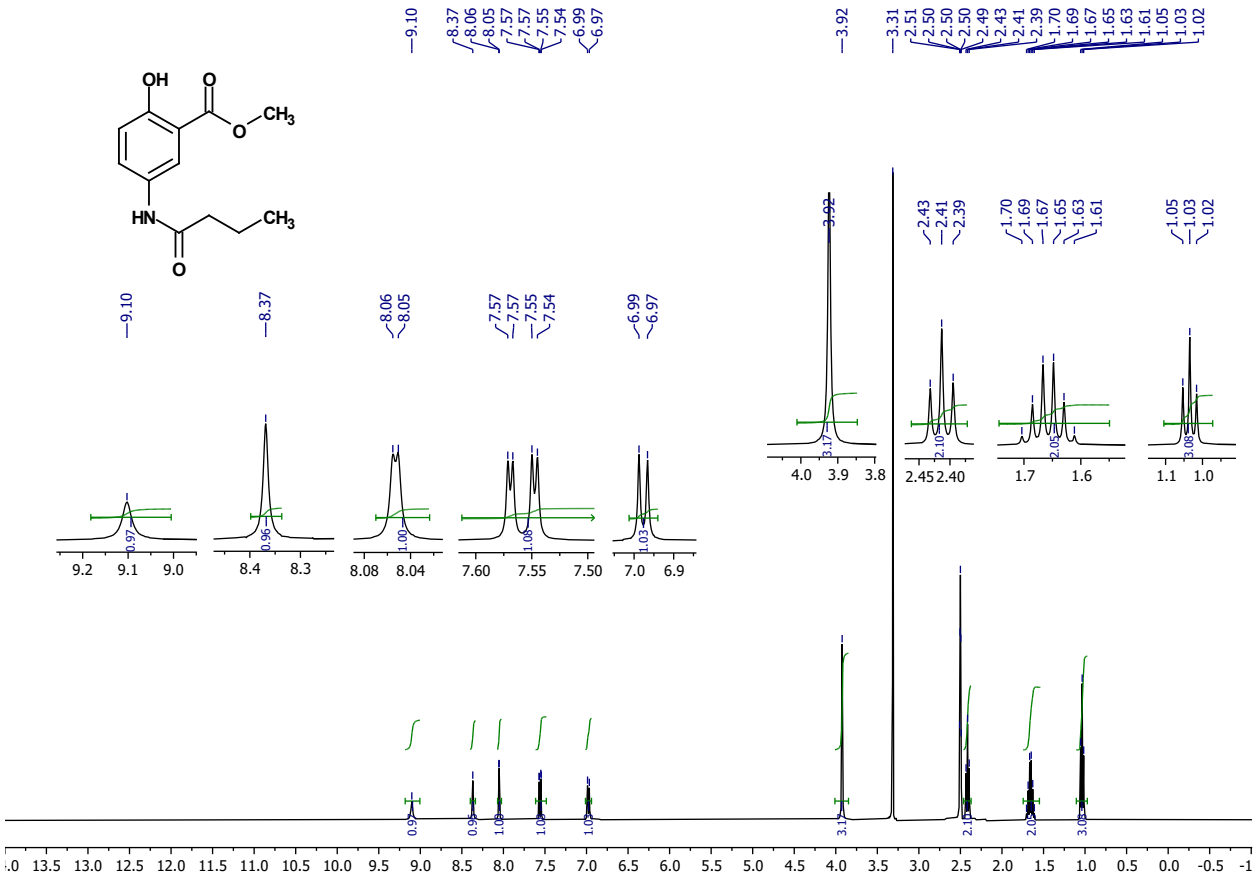


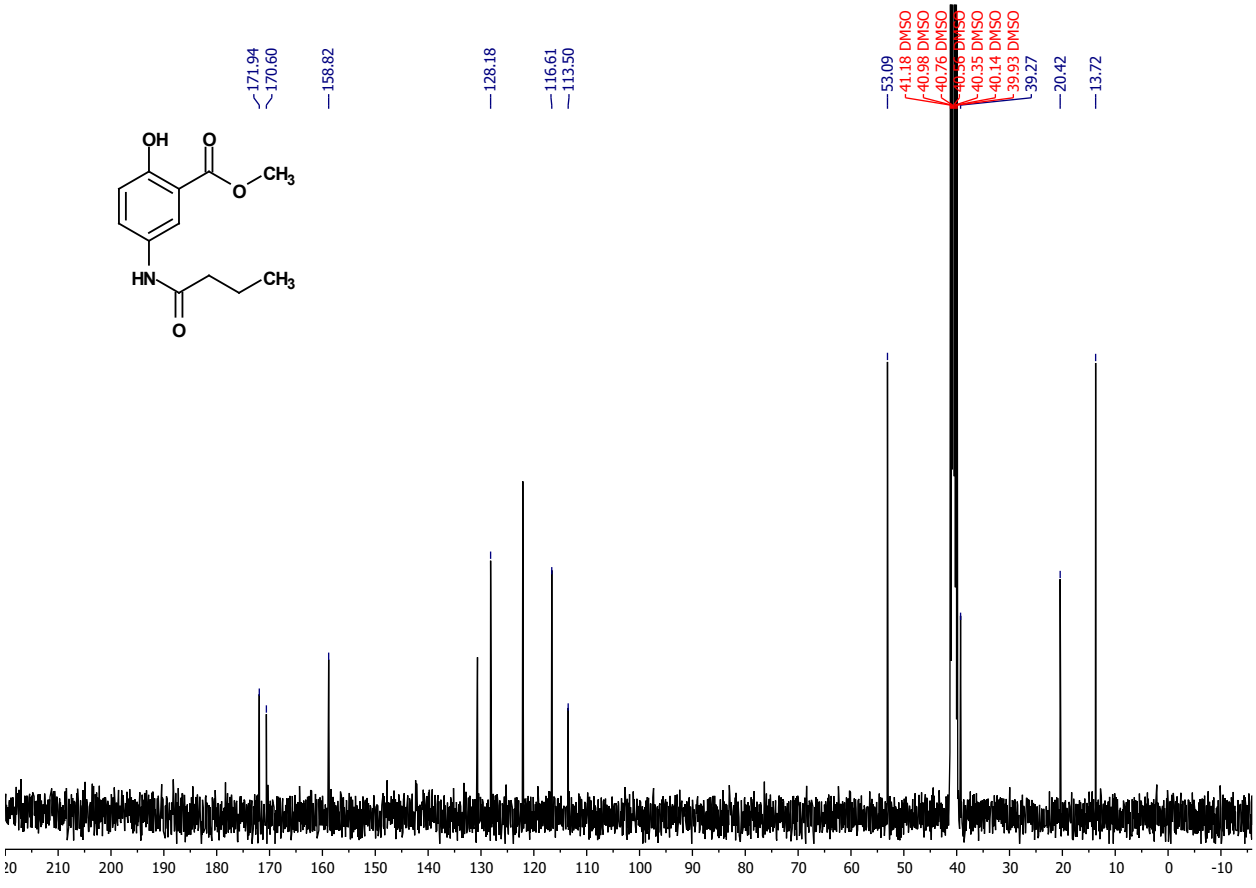
^{1}H and ^{13}C NMR *N*-(4-hydroxy-3,5-dimethylphenyl)butyramide **(4u)**



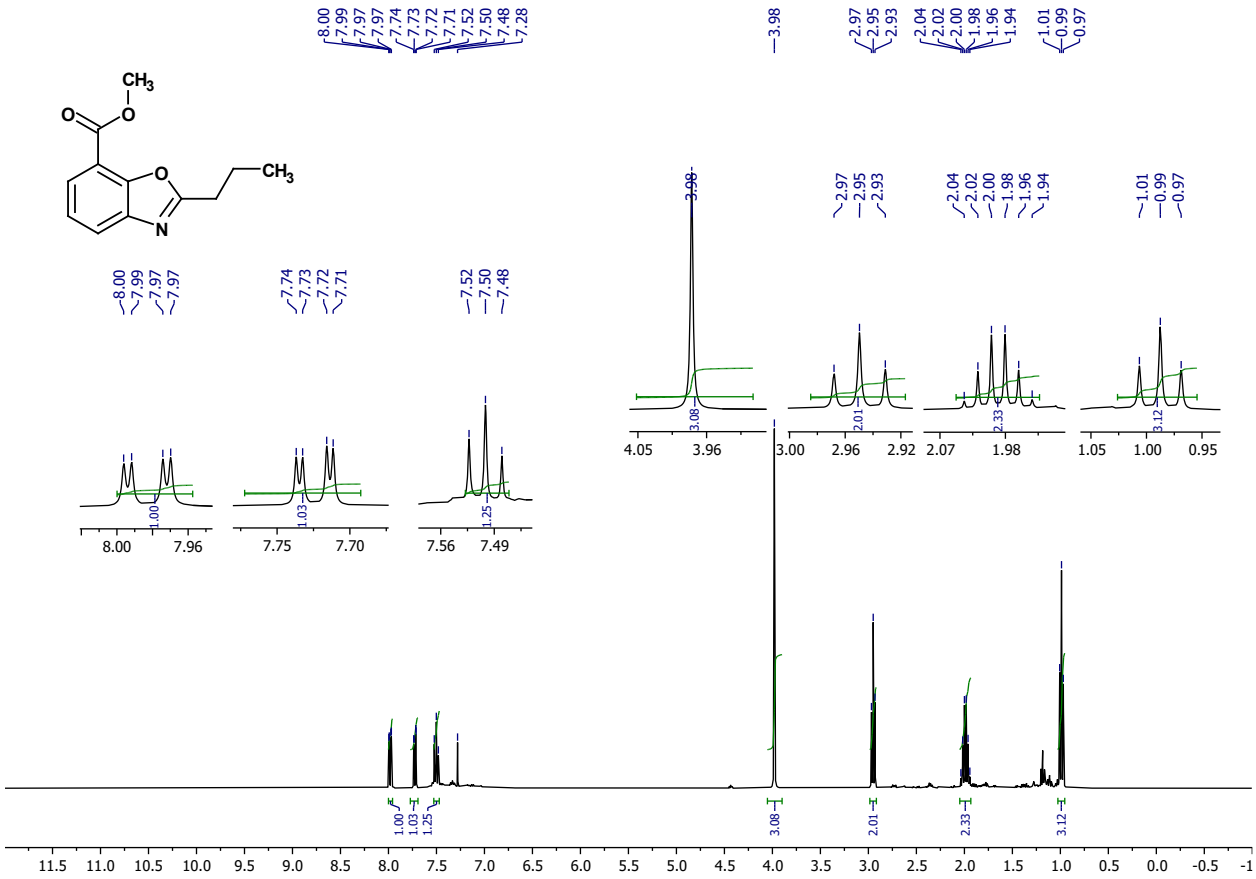


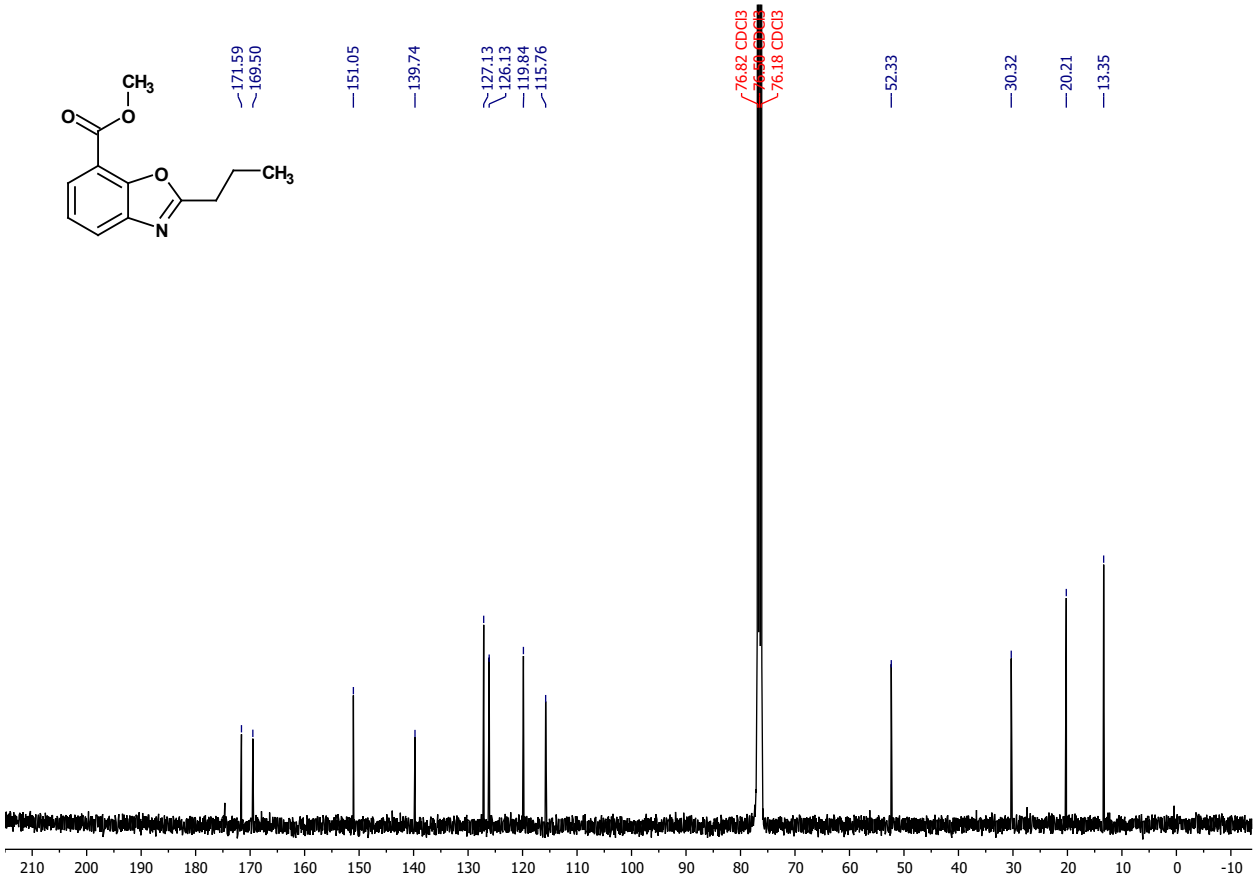
^{1}H and ^{13}C NMR Methyl 5-butyramido-2-hydroxybenzoate **(4w)**



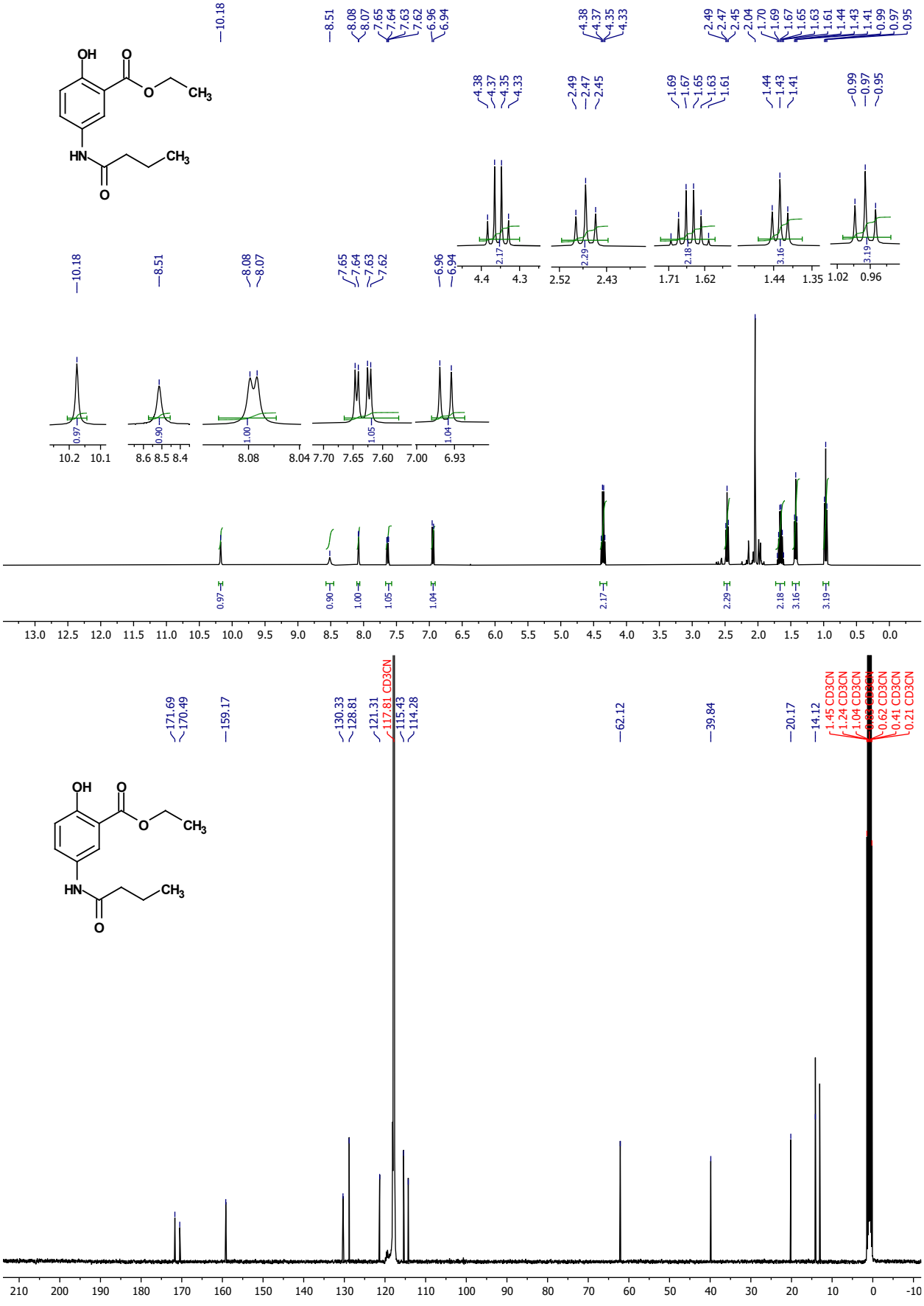


^{1}H and ^{13}C NMR Methyl 2-propylbenzo[d]oxazole-7-carboxylate **(4ww)**





^{1}H and ^{13}C NMR Ethyl 5-butyramido-2-hydroxybenzoate **(4x)**



^{1}H and ^{13}C NMR Ethyl 2-propylbenzo[d]oxazole-7-carboxylate **(4xx)**