

Supporting Information

for

Base-catalyzed switchable reactivity of *N*-acyl- α -aminonitriles: oxidative decyanation to imides and hydrolysis to amides in batch and flow

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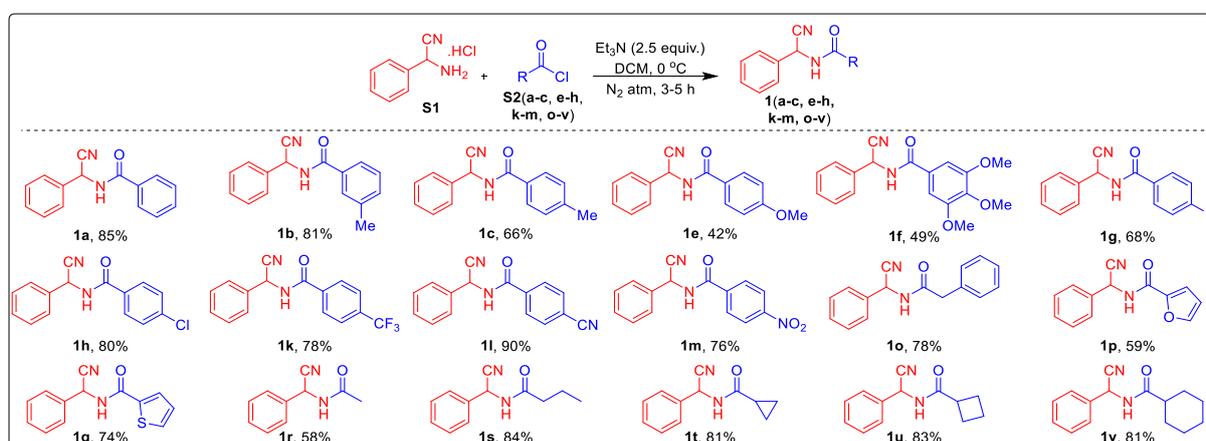
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1. General information

A Bruker 400 MHz, 500 MHz spectrometer and 400 MHz of Varian mercury and Jeol spectrometer was employed to acquire ^1H NMR spectra, while a Bruker 100 MHz, 125 MHz and 100 MHz of Varian mercury and Jeol spectrometer was utilized for ^{13}C NMR spectra. Parts per million (ppm) denotes chemical shift (δ) values, whereas hertz (Hz) indicates coupling constants (J). The spectra were obtained utilizing CDCl_3 as the solvent. ^1H NMR chemical shifts are calibrated to tetramethylsilane (TMS, 0 ppm), while ^{13}C NMR shifts are referenced to CDCl_3 (77.0 ppm). The reaction's development was tracked via TLC utilizing Merck pre-coated TLC sheets. The melting points of compounds were ascertained utilizing a digital melting point instrument (Model 935) from Deep Vision Electronics PVT. LTD and Fargo instruments. High Resolution Mass Spectrometry (HRMS) was analyzed using Agilent G6230B Accurate Mass TOF and HRMS (QTOF-ESI) on JMS-700 spectrometer. EPR studies were performed by using JEOL Model JES FA200 ESR Spectrometer. LC-MS studies were performed by using Thermo Scientific TSQ Quantum Ultra. Continuous flow setups such as T-shaped mixers were purchased from Sanko Seiki company, stainless tubes, and peeks were purchased from Idex Health & science. Harvard syringe pumps model-11 elite were used for the reaction and Alicat scientific for mass flow controller. Column chromatography was conducted on 100-120 mesh silica gel utilizing hexane/ethyl acetate as the eluent, with solvents employed without additional distillation. All commercial chemicals were acquired from Hyma, TCI and BLD.

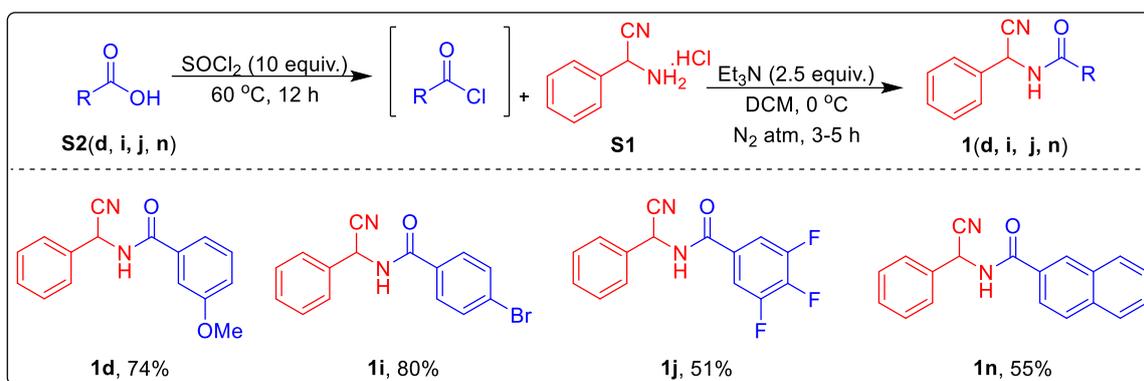
2. Experimental procedures

2.1. General experimental procedure (A) for synthesis of *N*-acyl α -aminonitriles



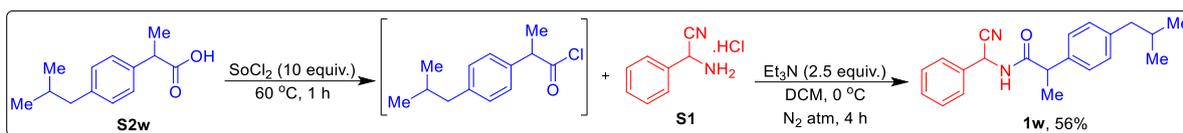
To a solution of 2-amino-2-phenylacetonitrile **S1** (1.0 equiv.) in DCM, triethylamine (2.5 equiv.) was added and stirred at 0-5 °C in nitrogen atmosphere for 10~15 mins. To this stirred reaction mixture acid chlorides **S2a-c**, **S2e-h**, **S2k-m** and **S2o-v** (1.5 equiv.) in DCM was added and continued stirring at 0~5 °C in nitrogen atmosphere for 3~5 h. After the completion of the reaction, DCM was evaporated under rotary vacuum. Then the crude product was diluted with water (30 mL) followed by extraction with ethyl acetate (3 x 20 mL). The obtained organic layer was given brine wash (20 mL), dried over Na₂SO₄ and concentrated under rotary vacuum. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 15-20% to obtain the pure *N*-acyl α -aminonitriles **1(a-c, e-h, k-m, o-v)** in 42-90% yields.

2.2. General experimental procedure (B) for synthesis of *N*-acyl α -aminonitriles



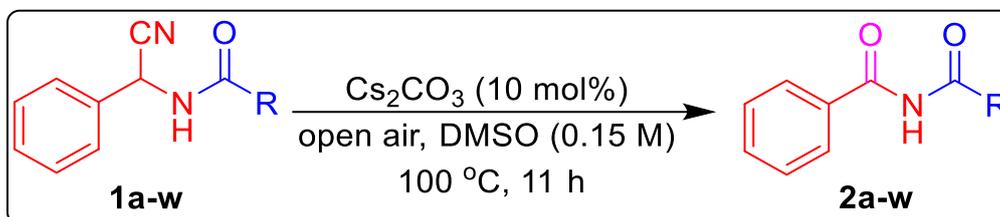
To a 100 mL round bottom flask charged with benzoic acid **S2d**, **S2i**, **S2j** and **S2n** in nitrogen atmosphere, thionyl chloride (10.0 equiv.) was added at 0 °C and stirred for 12 h in 60 °C. After complete formation of aroyl chloride confirmed by thin layer chromatography, excess SOCl₂ was removed in rotary vacuum under nitrogen atmosphere. To this reaction mixture 2-amino-2-phenylacetonitrile **S1** (1.0 equiv.) and triethylamine (2.5 equiv.) in DCM was added and stirred at 0~5 °C in nitrogen atmosphere for 3~5 h. After the completion of the reaction, DCM was evaporated under rotary vacuum. Then the crude product was diluted with water (30 mL) followed by extraction with ethyl acetate (3 x 20 mL). The obtained organic layer was given brine wash (20 mL), dried over Na₂SO₄ and concentrated under rotary vacuum. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 15-20% to obtain the pure *N*-acyl α -aminonitriles **1(d, i, j, n)** in 51-80% yields.

2.3. General experimental procedure (C) for synthesis of *N*-(cyano(phenyl)methyl)-2-(4-isobutylphenyl)propenamide (**1w**)



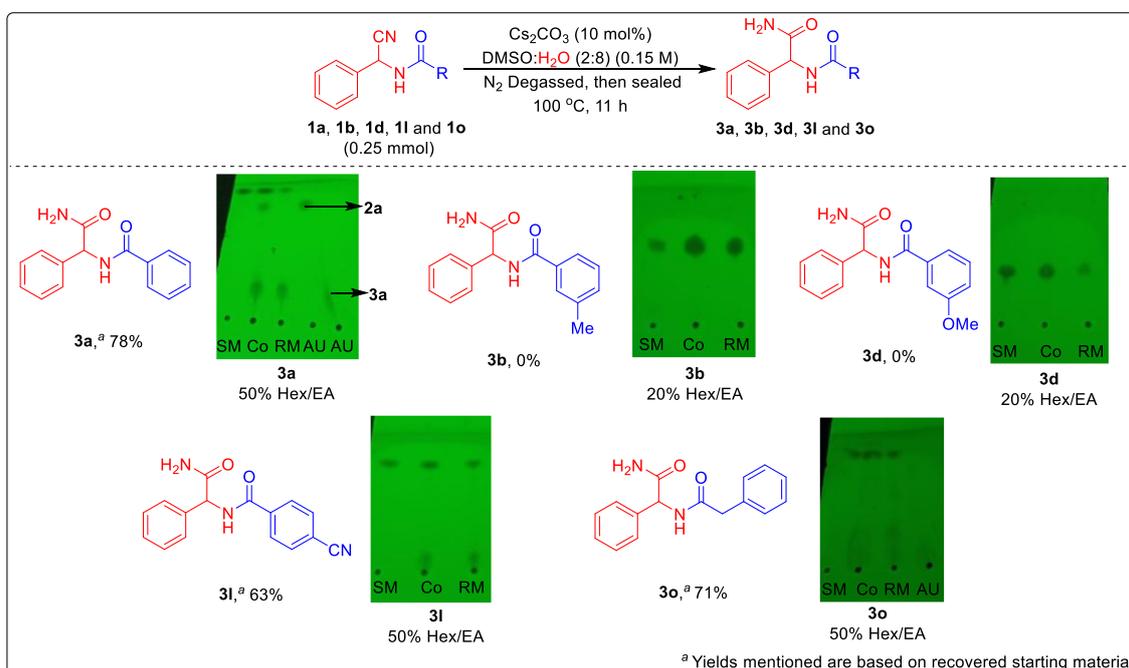
To a 100 mL round bottom flask charged with **S2w** in nitrogen atmosphere, thionyl chloride (10.0 equiv.) was added at 0 °C and stirred for 1 h in 60 °C. After complete formation of acyl chloride confirmed by thin layer chromatography, excess SOCl_2 was removed in rotary vacuum under nitrogen atmosphere. To this reaction mixture 2-amino-2-phenylacetonitrile **S1** (1.0 equiv.) and triethylamine (2.5 equiv.) in DCM was added and stirred at 0~5 °C in nitrogen atmosphere for 4 h. After the completion of the reaction, DCM was evaporated under rotary vacuum. Then the crude product was diluted with water (30 mL) followed by extraction with ethyl acetate (3 x 20 mL). The obtained organic layer was given brine wash (20 mL), dried over Na_2SO_4 and concentrated under rotary vacuum. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 15-20% to obtain the pure compound **1w** in 56% yield.

2.4. General experimental procedure (D) for synthesis of acyclic imides under batch process



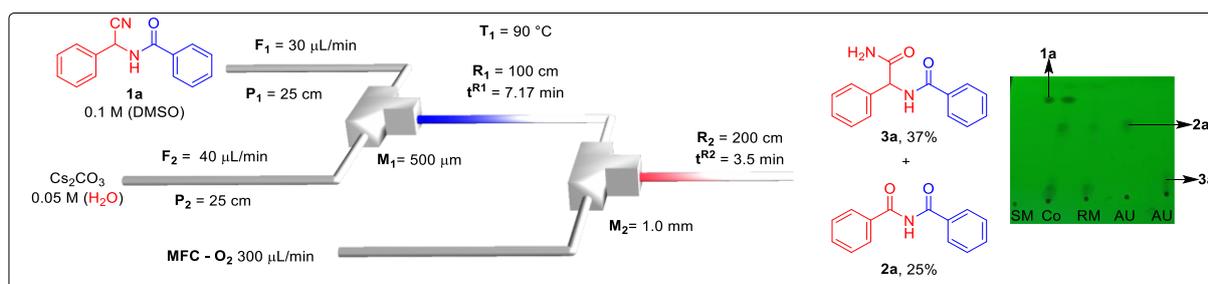
A 15 mL vial was charged with **1a-w** (0.5 mmol), DMSO (0.15 M) in 3.3 mL and Cs_2CO_3 (10 mol%). The reaction mixture was allowed to stir at 100 °C under open air until the completion of reaction by TLC chromatography (11 h). The reaction mixture was cooled to room temperature, diluted with 10 mL of water. The water layer was extracted with (3 x 15 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1 x 20 mL). The final ethyl acetate layer was dried over Na_2SO_4 and concentrated under reduced pressure to the get crude compound. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 20-25% to afford pure acyclic imides **2a-2w** in 48-89% yields.

2.5. General experimental procedure (E) for the synthesis of amides under batch process



A 15 mL sealed tube was charged with **1a**, **1b**, **1d**, **1l** and **1o** (0.25 mmol), DMSO (0.15 M) in 1.7 mL and Cs_2CO_3 (10 mol%). The reaction mixture was allowed to stir at 100 °C under sealed condition until 11 h. The reaction mixture was cooled to room temperature, diluted with 10 mL of water. The water layer was extracted with (3 x 15 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (1 x 20 mL). The final ethyl acetate layer was dried over Na_2SO_4 and concentrated under reduced pressure to get crude compound. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 60-70% to afford pure amides **3a**, **3l** and **3o** in 63-78% yields.

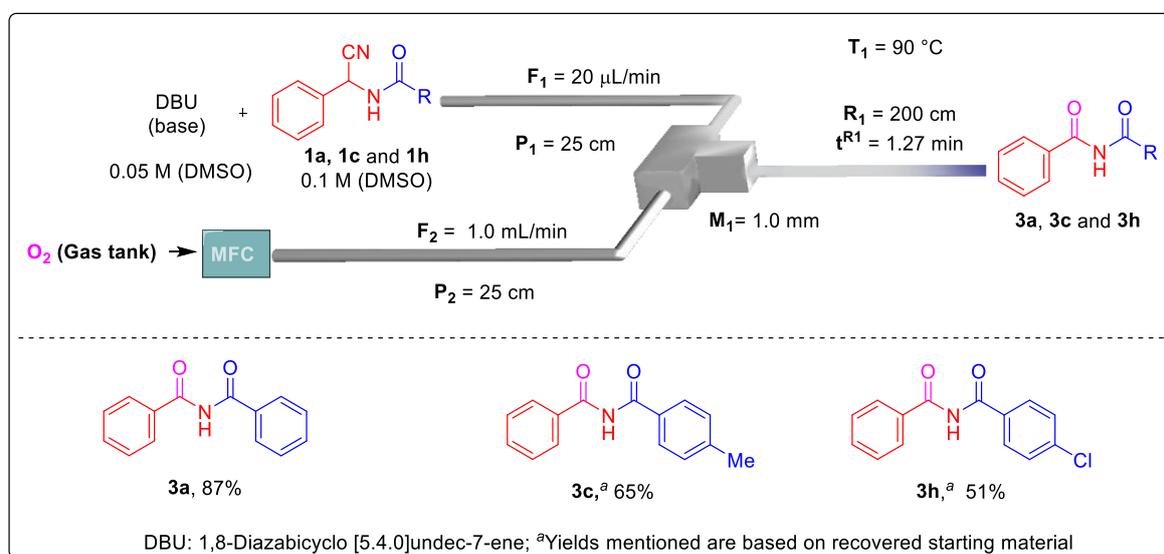
2.6. Investigation of imide synthesis under continuous-flow conditions with cat. Cs_2CO_3



A microreactor system consist of two T-shaped micromixers (M_1 , M_2), and two precooling units

P₁ (inner diameter = 800 μm, length L = 25 cm), P₂ (inner diameter = 800 μm, length L = 25 cm), A solution of **1a** (0.1 M in DMSO) (flow rate: F₁ = 20 μL/min) and a solution of Cs₂CO₃ (0.05 M in H₂O) (flow rate: F₂ = 40 μL/min) were introduced into M₁ (Φ = 500 μm). The resulting solution was passed through microtubing (R₁ = 100 cm, Φ = 800 μm) by syringe pumps, and was mixed with O₂ (flow rate: F₂ = 1.0 mL/min) were introduced into M₁ (Φ = 1.0 mm) by a mass flow controller. The resulting solution from R₁ and gas was passed through microtubing (R₁ = 200 cm, Φ = 1.0 mm, 1.3 mL) with a reaction temperature of 90 °C. After a steady state was reached, the solution was collected for 45 minutes in a vial. The resulting solution was extracted with ethyl acetate (3 mL x 5), and the organic layer was combined and washed with brine solution (5 mL). The organic layer was dried over anhydrous MgSO₄, filtered, and concentrated under a vacuum. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane to obtain **3a** in 37% and **2a** in 25% yields, respectively.

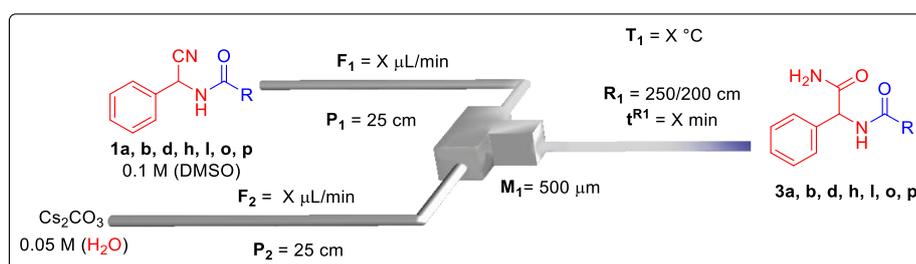
2.7. Investigation and scope of imides under continuous-flow conditions with cat. DBU



A microreactor system consists of one T-shaped micromixer (M₁), one microtube reaction (R₁), two precooling units P₁ (inner diameter Φ = 800 μm, length L = 25 cm), P₂ (Φ = 800 μm, length L = 25 cm). A solution of **1a** (0.1 M in DMSO), DBU (0.05 M in DMSO) (flow rate: F₁ = 20 μL/min) and O₂ (flow rate: F₂ = 1.0 mL/min) were introduced into M₁ (Φ = 1.0 mm) by syringe pumps and Mass flow controller. The resulting solution and gas was passed through microtubing (R₁ = 200 cm, Φ = 1.0 mm, 1.3 mL) with a reaction temperature of 90 °C. After a steady state was reached, the solution was collected for 45 minutes in a vial. The resulting

solution was extracted with ethyl acetate (3 mL x 5), and the organic layer was combined and washed with brine solution (5 mL). The organic layer was dried over anhydrous MgSO₄, filtered, and concentrated under a vacuum. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 20-25% to obtain **3a** in 87% yield. This methodology is also extended for the scope **1c** and **1h** to obtain **3c** and **3h** at 65% and 51% yields, respectively.

3. Table S1. Reaction parameter studies for amides under continuous-flow method^{ab}



entry	flow rate 1 (μL)	flow rate 2 (μL) Base	temperature ($^{\circ}\text{C}$)	residence time (min)	result ^b (%)
1	20	30	100	25.1	65
2	20	40	100	20.9	80 ^c
3	20	40	90	20.9	76^a
4	20	40	80	20.9	65
5	20	50	90	17.9	79 ^c
6	10	40	90	25.1	65

A continuous flow system consists of two reagents delivering units (P_1 , and P_2 , $\Phi = 800\mu\text{m}$, length $L = 25\text{ cm}$) T-shaped micromixer (M_1 , $\Phi = 500\mu\text{m}$), one microtube reactor ($R_1 = 250\text{ cm}$, $\Phi = 800\mu\text{m}$). ^aReaction was performed under standard optimized conditions ($F_1 = 20\mu\text{L}/\text{min}$, $F_2 = 40\mu\text{L}/\text{min}$) and the product was collected for 45 min. ^bIsolated yield. ^cClotting the reactor.

4. Experimental procedure (F) for amides (**3a**, **3d** and **3p**) under continuous-flow method

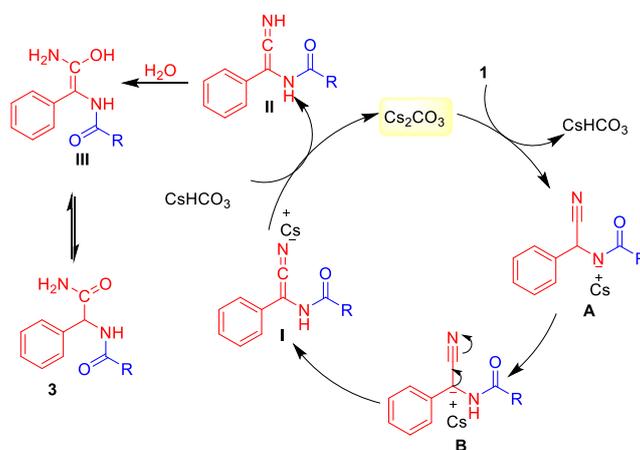
A microreactor system consists of one T-shaped micromixer (M_1), one microtube reaction (R_1), two precooling units P_1 (inner diameter $\Phi = 800\mu\text{m}$, length $L = 25\text{ cm}$), P_2 ($\Phi = 800\mu\text{m}$, length $L = 25\text{ cm}$). A solution of **1a**, **1d** and **1p** (0.1 M in DMSO) (flow rate: $F_1 = 20\mu\text{L}/\text{min}$) and a solution of Cs_2CO_3 (0.05 M in H_2O) (flow rate: $F_2 = 40\mu\text{L}/\text{min}$) were introduced into M_1 ($\Phi =$

500 μm) by syringe pumps. The resulting solution was passed through microtubing ($R_1= 250$ cm, $\Phi = 800$ μm , 1255 mL) with a reaction temperature of 90 $^\circ\text{C}$. After a steady state was reached, the solution was collected for 45 minutes in a vial. The resulting solution was extracted with ethyl acetate (3 mL x 5), and the organic layer was combined and washed with brine solution (5 mL). The organic layer was dried over anhydrous MgSO_4 , filtered, and concentrated under a vacuum. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 60-70% to afford **3a**, **3d**, and **3p** in 60-76% yields.

5. Experimental procedure (G) for amides (**3b**, **3h**, **3l** and **3o**) under Continuous-flow method

A microreactor system consists of one T-shaped micromixer (M_1), one microtube reaction (R_1), two precooling units P_1 (inner diameter $\Phi = 800$ μm , length $L = 25$ cm), P_2 ($\Phi = 800$ μm , length $L = 25$ cm). A solution of **1b**, **1h**, **1l** and **1o** (0.1 M in DMSO) (flow rate: $F_1 = 20$ $\mu\text{L}/\text{min}$) and a solution of Cs_2CO_3 (0.05 M in H_2O) (flow rate: $F_2 = 40$ $\mu\text{L}/\text{min}$) were introduced into M_1 ($\Phi = 500$ μm) by syringe pumps. The resulting solution was passed through microtubing ($R_1= 200$ cm, $\Phi = 1.0$ mm, 1.3 mL) with a reaction temperature of 90 $^\circ\text{C}$. After a steady state was reached, the solution was collected for 45 minutes in a vial. The reaction time will be 21.6 min. The resulting solution was extracted with ethyl acetate (3 mL x 5), and the organic layer was combined and washed with brine solution (5 mL). The organic layer was dried over anhydrous MgSO_4 , filtered, and concentrated under a vacuum. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 60-70% to afford **3b**, **3h**, **3l** and **3o** in 33-60% yields.

6. Plausible reaction mechanism for the synthesis of amides



Scheme S1. Plausible mechanism

7. TLC for substrate scope

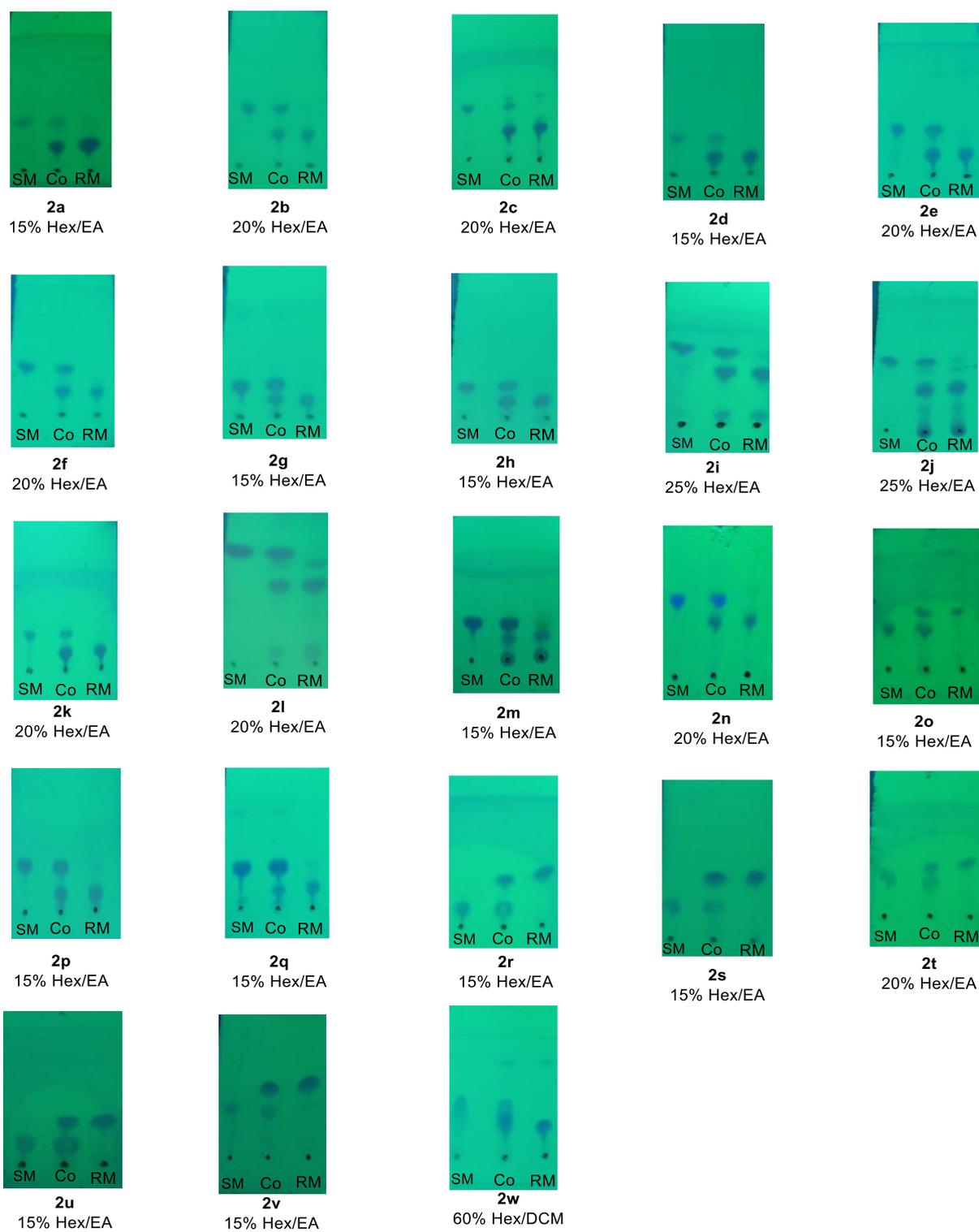
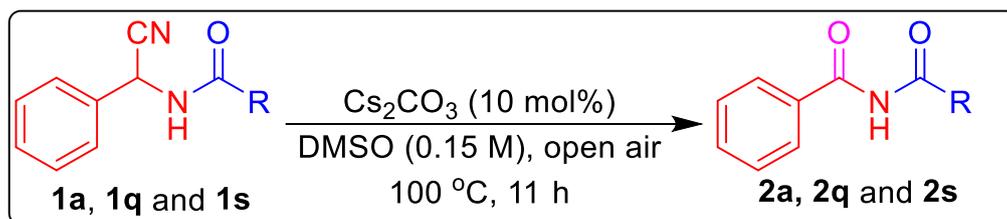


Fig. S1. TLCs for Substrate Scope **2a-2w**

8. Gram-scale synthesis of acyclic imides and experimental setup



A 100 mL RB flask was charged with **1a**, **1q** and **1s** (1.0 g), DMSO (0.15 M) and Cs_2CO_3 (10 mol%). The reaction mixture was allowed to stir at 100 °C under open air until the completion of reaction by TLC chromatography (11 h). The reaction mixture was cooled to room temperature, diluted with 100 mL of water. The water layer was extracted with (3 x 150 mL) of ethyl acetate and the combined ethyl acetate layer was given brine wash (2 x 100 mL). The final ethyl acetate layer was dried over Na_2SO_4 and concentrated under reduced pressure to get crude compound. The obtained crude was purified using column chromatography by eluting ethyl acetate/ hexane at 20-25% to afford pure acyclic imides **2a**, **2q** and **2s** in 82%, 72% and 85% yields.

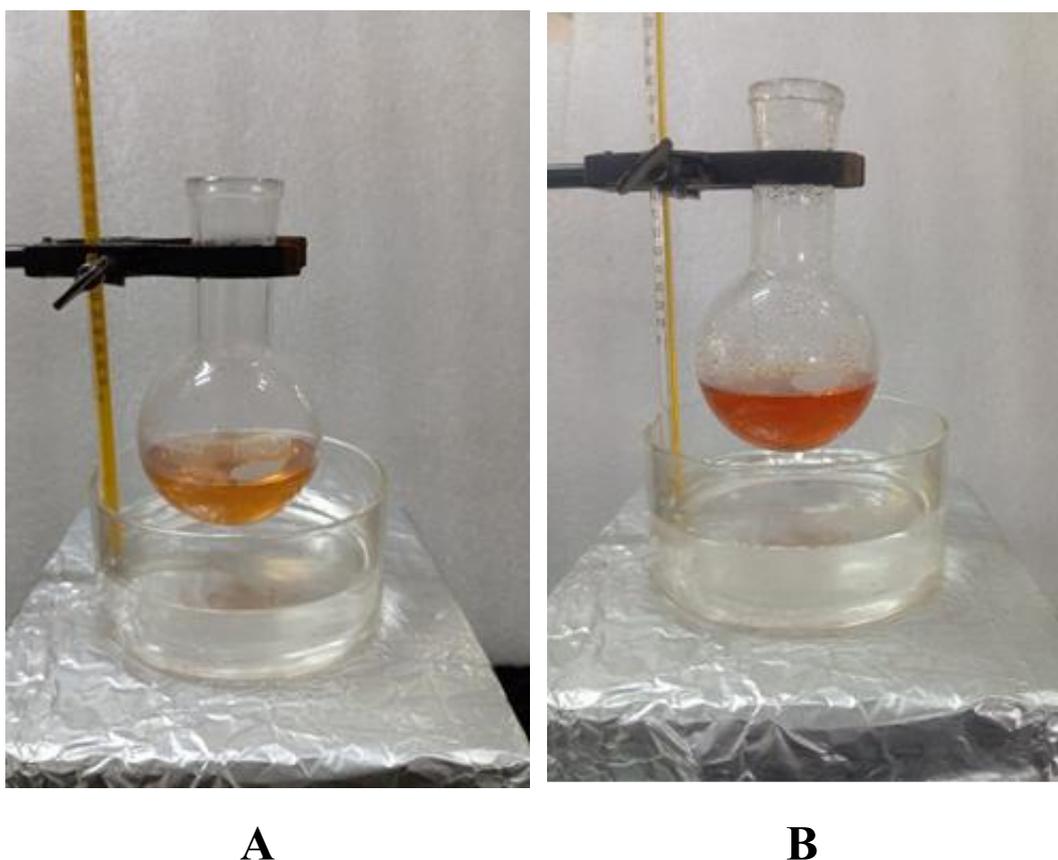


Fig. S2. Experimental setup for gram scale synthesis of acyclic imides. A) At the start of the reaction; B) after completion of the reaction.

9. EPR-studies

Spectra were recorded under three conditions: (i) DMPO in DMSO, (ii) DMPO with substrate **1a** and base in DMSO, and (iii) DMPO with substrate **1a** in DMSO. In the stacked spectra, the signal marked (*) corresponds to DMPO, while the feature labeled (Φ) arises from its oxidized adduct, consistent with trapping of superoxide species.

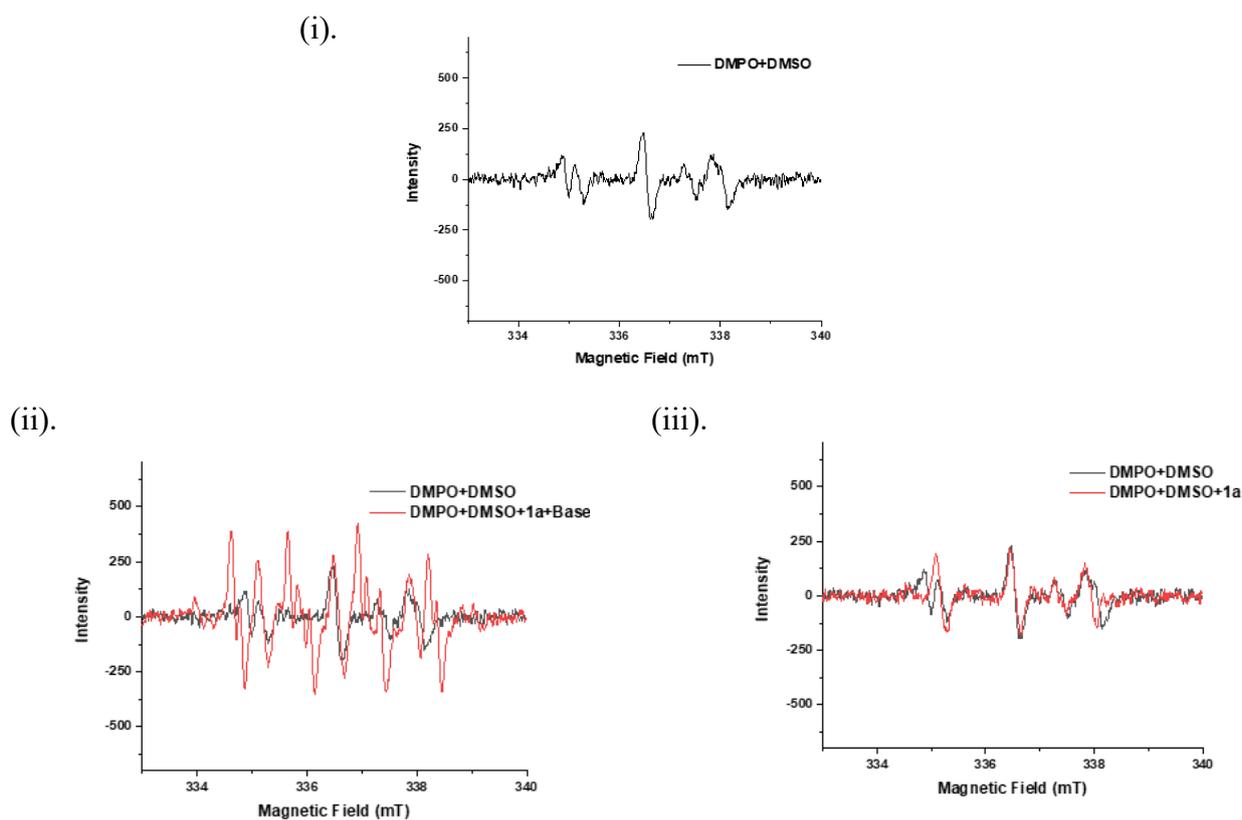


Fig. S3. EPR studies for trapping superoxide radical with DMPO

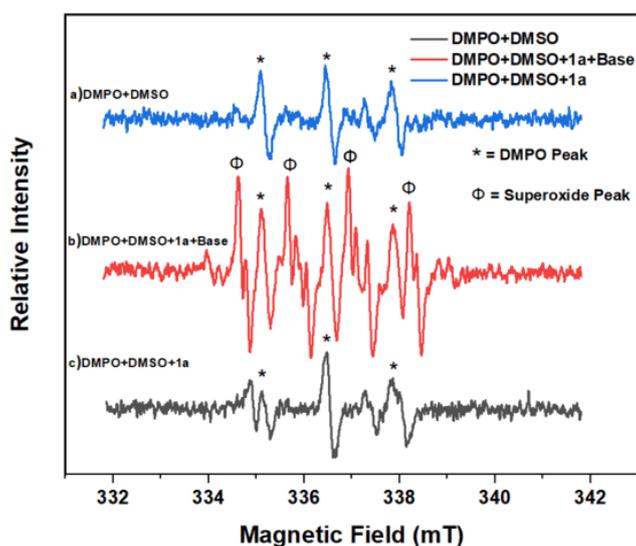


Fig. S4. Stacked EPR Spectra: ^a EPR spectra of DMSO heated for 1 h at 100 °C and cooled to room temperature and then added a solution of DMPO (0.1 mol/L). ^b EPR spectra of **1a** (0.1 mmol), Cs₂CO₃ (10 mol%) in 0.15 M of DMSO stirred and heated for 1 h at 100 °C and cooled to room temperature and then added a solution of DMPO (0.1 mol/L). ^c EPR spectra of **1a** (0.1 mmol) in 0.15 M of DMSO stirred and heated for 1 h at 100 °C and cooled to room temperature and then added a solution of DMPO (0.1 mol/L).

10. Isotopic labelling (H₂¹⁸O) experiments for amides under continuous-flow conditions

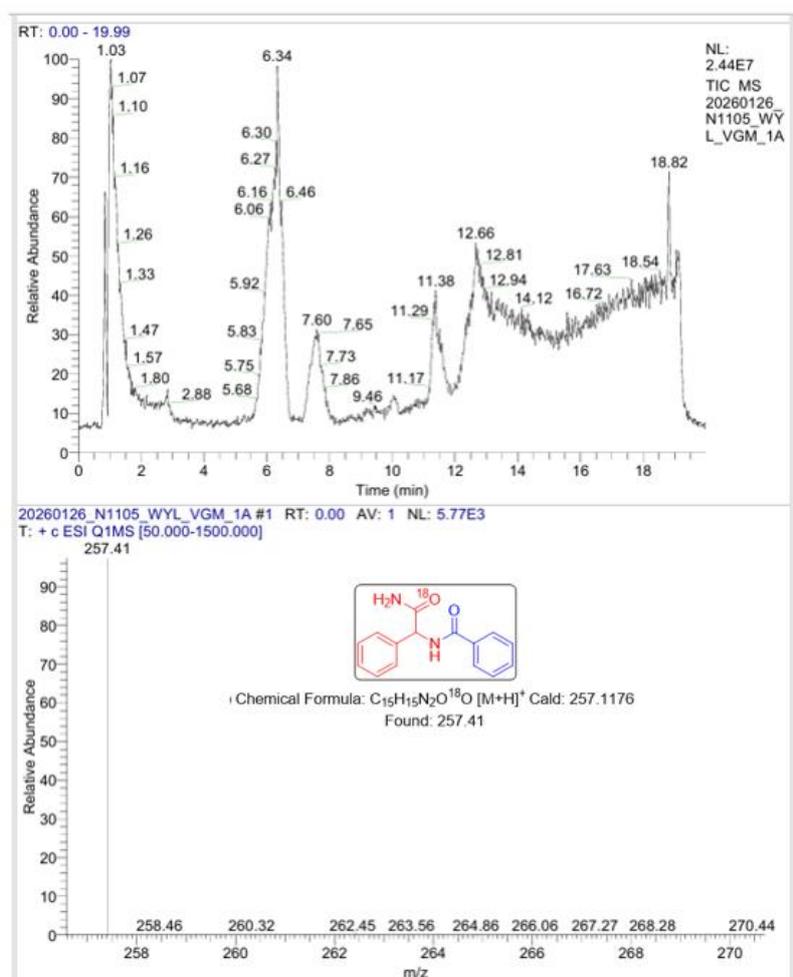
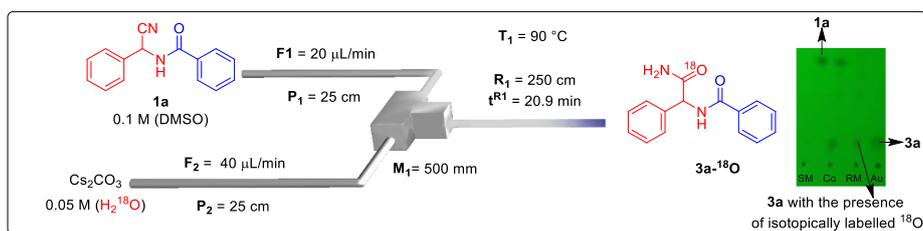


Fig. S5. LC-MS data for H₂¹⁸O-labelled reaction in the continuous-flow process.

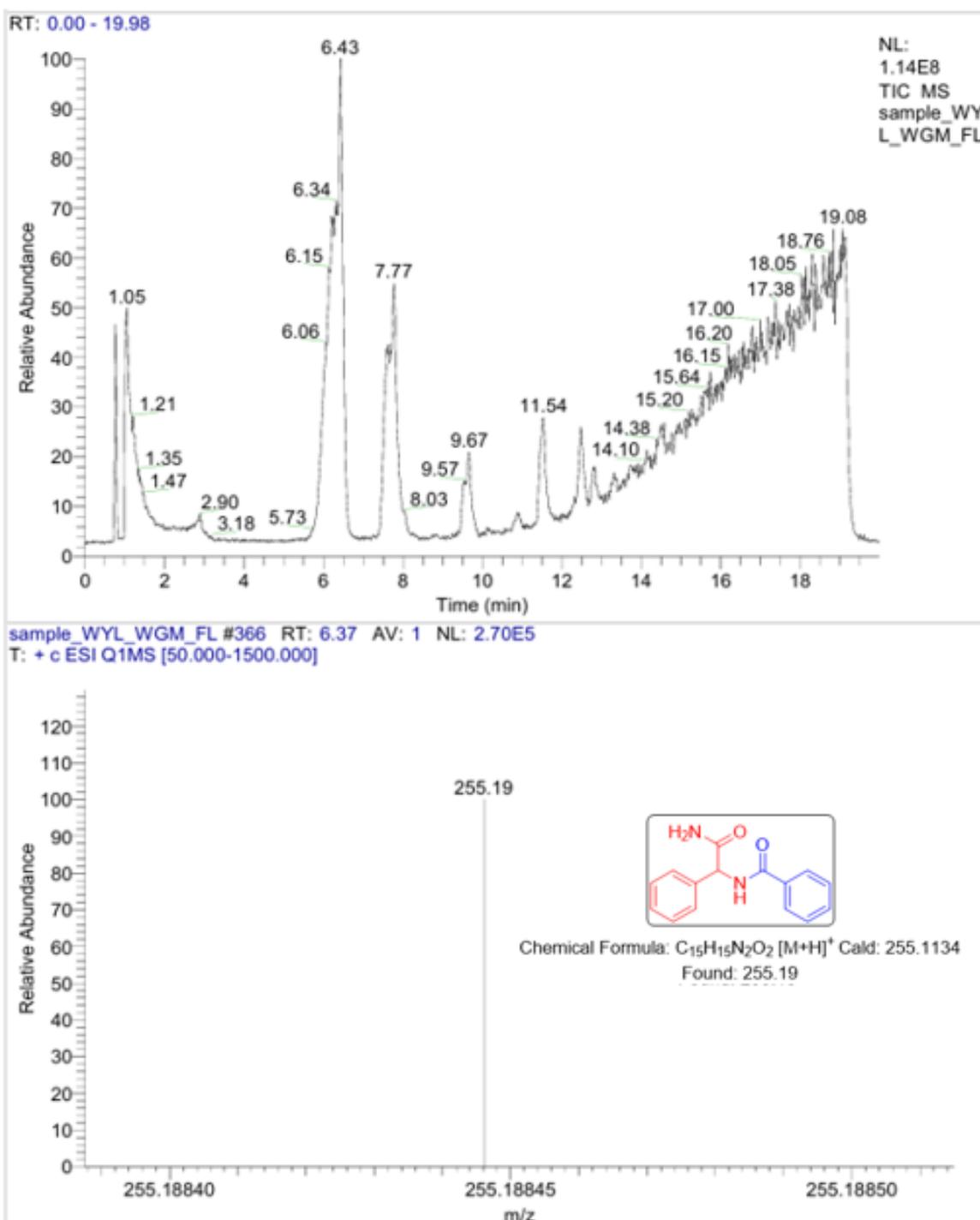
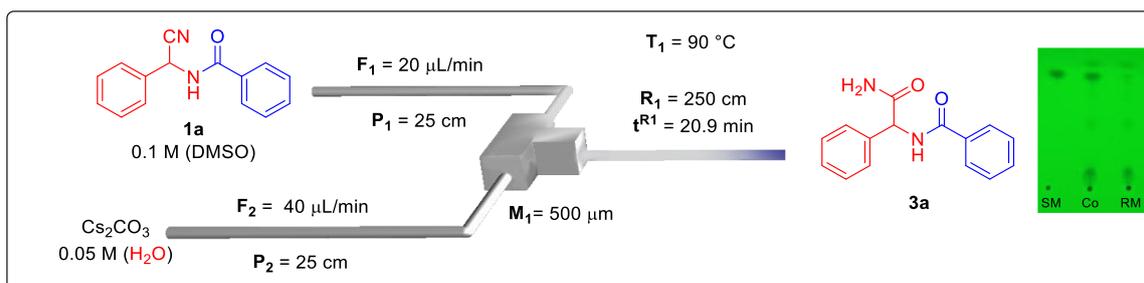


Fig. S6. LC-MS data of H_2O reaction in the continuous flow-process.

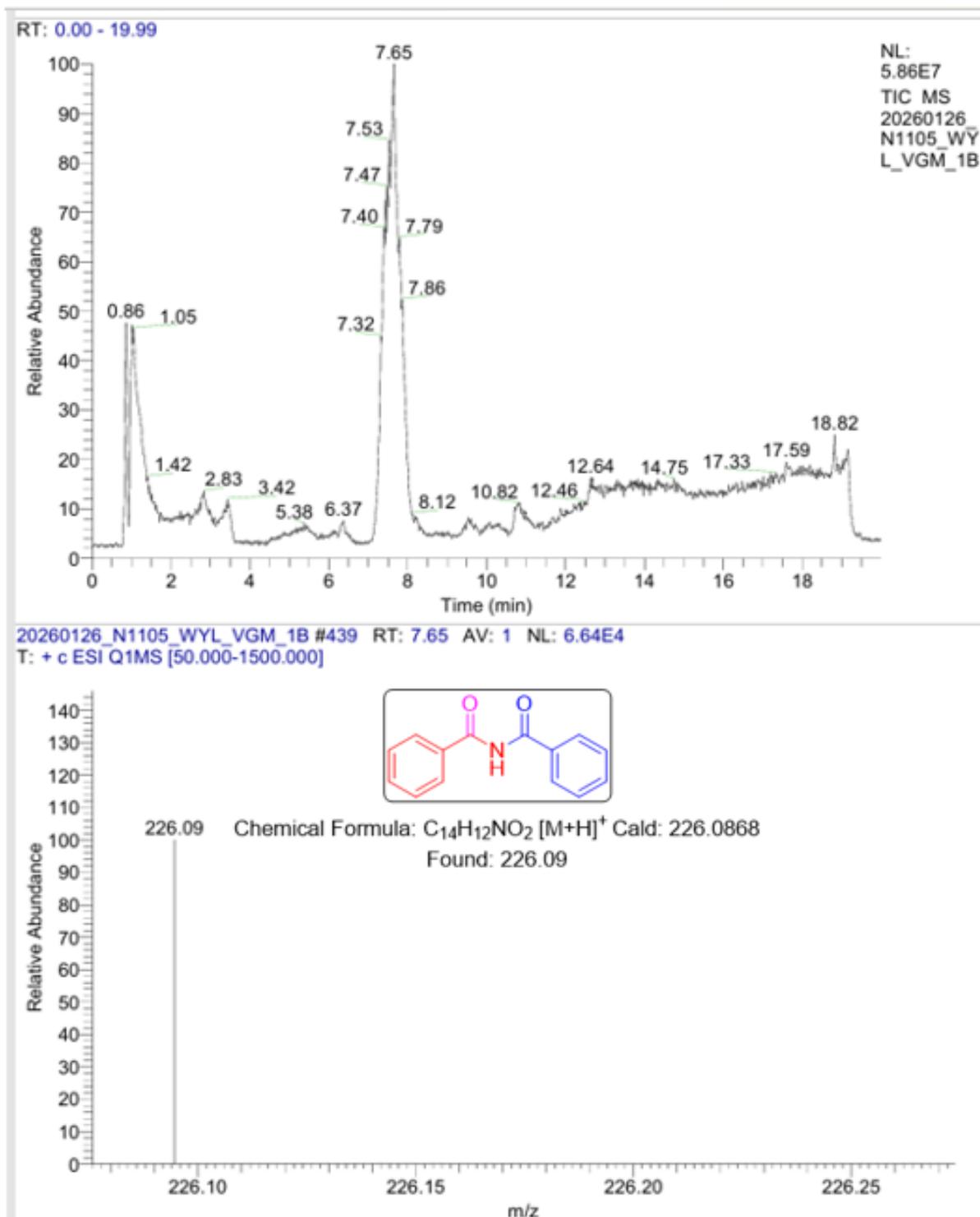
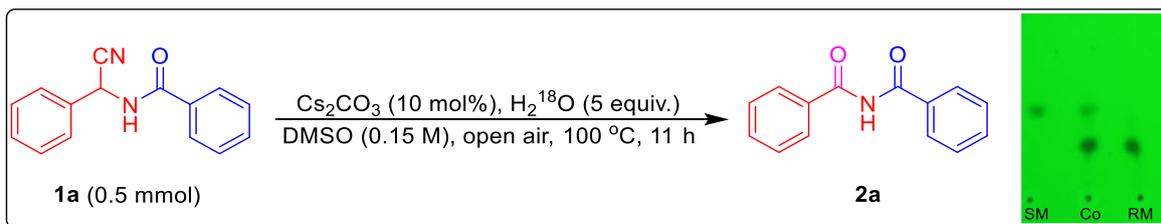


Fig. S7. LC-MS data for H_2^{18}O -labelled reaction in the batch process.

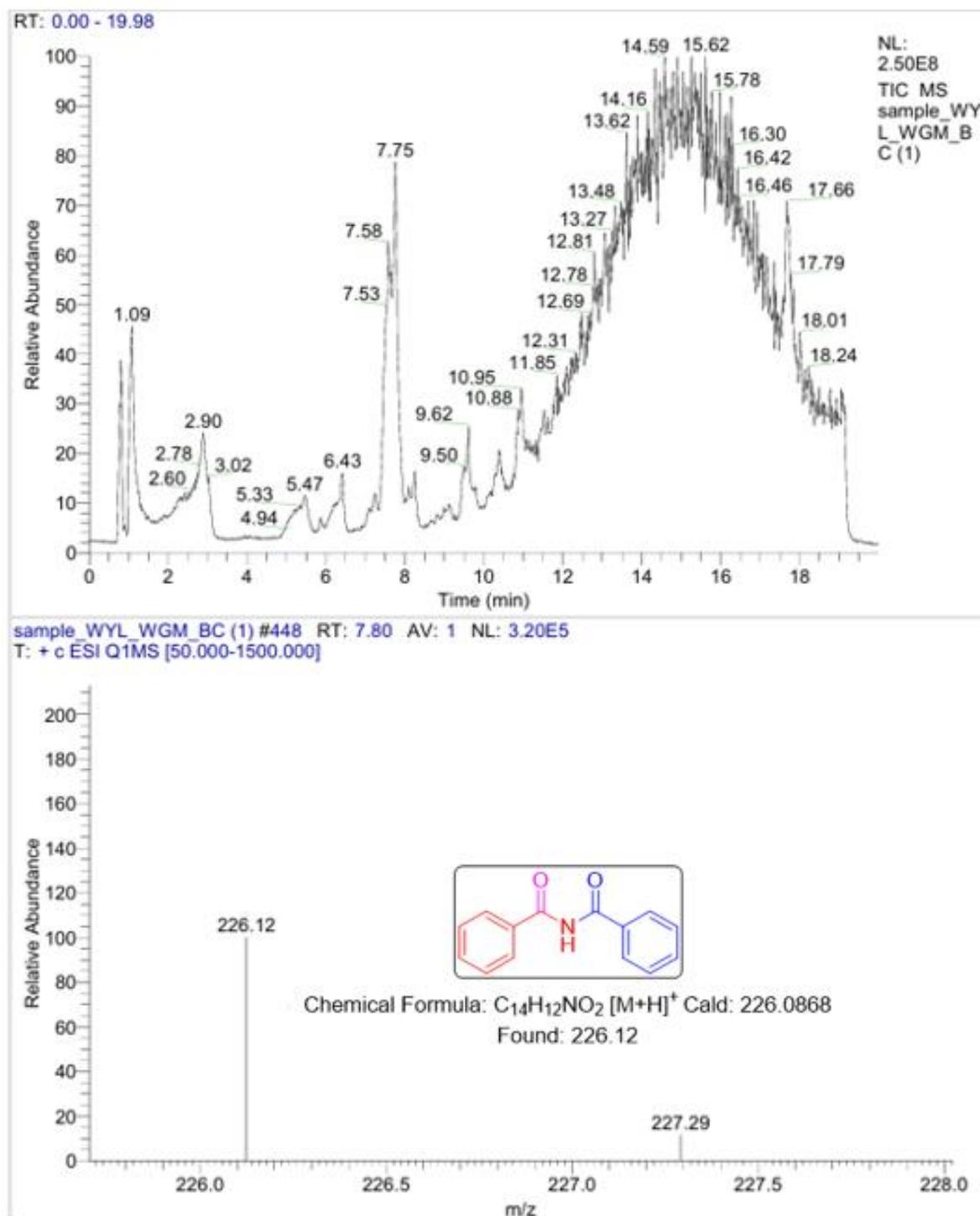
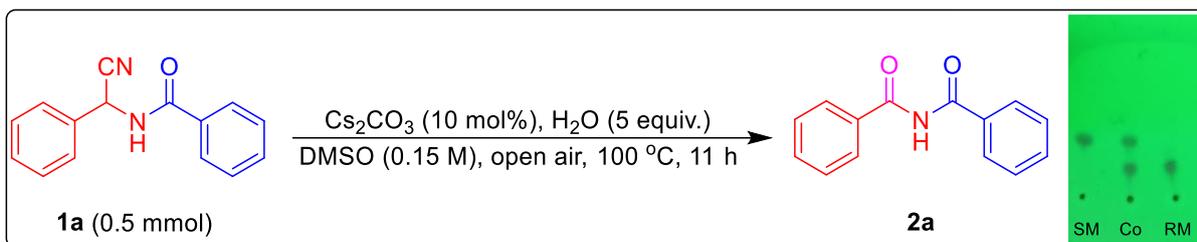
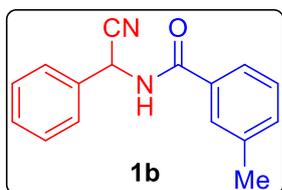


Fig. S8. LC-MS data of H₂O reaction in the batch process.

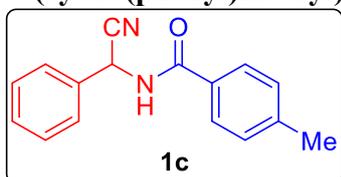
11. Spectral characterization

***N*-(cyano(phenyl)methyl)-3-methylbenzamide (1b).** The title compound was prepared



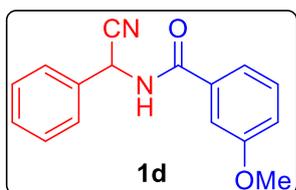
according to the general procedure (A) on a 2.0 mmol scale to obtain as a pale-yellow solid (406 mg, yield = 81%); Mp. 140-142 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.57 (s, 1H), 7.54 (d, *J* = 7.6 Hz, 1H), 7.50-7.48 (m, 2H), 7.40-7.35 (m, 3H), 7.33-7.22 (m, 3H), 6.26 (d, *J* = 8.4 Hz, 1H), 2.32 (s, 3H). ¹³C{¹H} NMR (CDCl₃, 100 MHz): δ 167.01, 138.77, 133.41, 133.32, 132.45, 129.59, 129.44, 128.70, 128.18, 127.16, 124.46, 117.68, 44.57, 21.34. HRMS (ESI) calculated for C₁₆H₁₄N₂O₂Na [M+Na]⁺: 273.1004 found 273.1003.

***N*-(cyano(phenyl)methyl)-4-methylbenzamide (1c).** The title compound was prepared



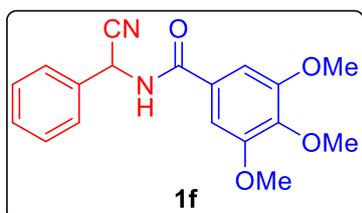
according to the general procedure (A) on a 2.0 mmol scale to obtain as a pale-yellow solid (331 mg, yield = 66%); Mp. 131-133 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.67 (d, *J* = 8 Hz, 2H), 7.49 (dd, *J* = 6.7, 2.7 Hz, 2H), 7.39-7.37 (m, 3H), 7.33-7.27 (m, 1H), 7.19 (d, *J* = 8 Hz, 2H), 6.27 (d, *J* = 8.5 Hz, 1H), 2.37 (s, 3H). ¹³C{¹H} NMR (126 MHz, CDCl₃) δ 166.71, 143.12, 133.34, 129.52, 129.44, 129.37, 129.31, 127.42, 127.07, 117.64, 44.44, 21.50. HRMS (ESI) calculated for C₁₆H₁₄N₂O₂Na [M+Na]⁺: 273.1004 found 273.1013.

***N*-(cyano(phenyl)methyl)-3-methoxybenzamide (1d).** The title compound was prepared



according to the general procedure (A) on a 2.0 mmol scale to obtain as a pale-yellow solid (395 mg, yield = 74%); Mp. 188-190 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.49-7.46 (m, 2H), 7.38-7.35 (m, 3H), 7.34-7.33 (m, 1H), 7.30-7.24 (m, 3H), 7.05-7.01 (m, 1H), 6.26 (d, *J* = 8.4 Hz, 1H), 3.76 (s, 3H). ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 166.67, 159.94, 133.88, 133.33, 129.85, 129.622, 129.44, 127.16, 119.30, 118.83, 117.65, 112.72, 55.54, 44.64. HRMS (ESI) calculated for C₁₆H₁₃N₂O₂ [M-H]⁻: 265.0977 found 265.0994.

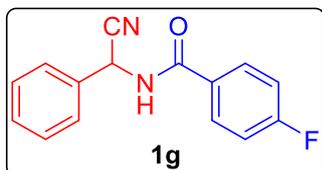
***N*-(cyano(phenyl)methyl)-3,4,5-trimethoxybenzamide (1f).** The title compound was



prepared according to the general procedure (A) on a 2.0 mmol scale to obtain as white solid (320 mg, yield = 49%); Mp. 192-194 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.56-7.53 (m, 2H), 7.47-7.42 (m, 3H), 7.01 (s, 2H), 6.81 (d, *J* = 8.4 Hz, 1H), 6.35 (d, *J* = 8.4 Hz, 1H), 3.88 (s, 6H), 3.87 (s, 3H). ¹³C{¹H} NMR (CDCl₃, 100 MHz): δ 166.22, 153.25,

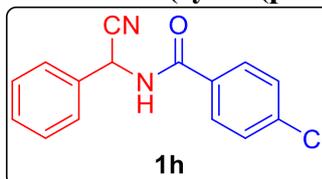
141.80, 133.30, 129.56, 129.38, 127.55, 127.07, 117.61, 104.88, 60.88, 56.37, 44.63. HRMS (ESI) calculated for $C_{18}H_{17}N_2O_4$ $[M-H]^-$: 325.1188 found 325.1199.

***N*-(Cyano(phenyl)methyl)-4-fluorobenzamide (1g)**. The title compound was prepared



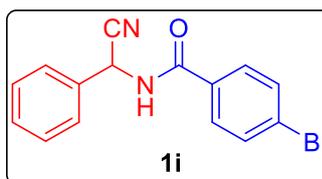
according to the general procedure (A) on a 2.0 mmol scale to obtain as a pale-yellow solid (346 mg, yield = 68%); Mp. 166-170 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.78 (dd, J = 8.4, 5.6 Hz, 2H), 7.49 (dd, J = 6.2, 2.2 Hz, 2H), 7.39 (d, J = 3.2 Hz, 4H), 7.05 (t, J = 8.4 Hz, 2H), 6.25 (d, J = 8 Hz, 1H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 166.12 (d, J_{CF} = 83.93 Hz), 164.02, 133.143, 129.92 (d, J_{CF} = 9.19 Hz), 129.63, 129.42, 128.58 (d, J_{CF} = 3.13 Hz), 127.11, 117.58, 115.88 (d, J_{CF} = 22.11), 44.63. ^{19}F NMR (376 MHz, $CDCl_3$) δ -106.06. HRMS (ESI) calculated for $C_{15}H_{11}N_2OFNa$ $[M+Na]^+$: 277.0747 found 277.0750.

4-Chloro-*N*-(cyano(phenyl)methyl)benzamide (1h). The title compound was prepared



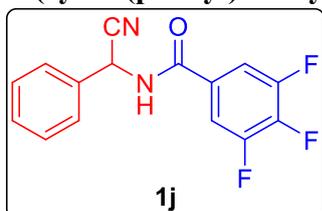
according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (435 mg, yield = 80%); Mp. 169-172 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8.4 Hz, 1H), 7.51-7.49 (m, 2H), 7.42-7.40 (m, 3H), 7.37 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8 Hz, 1H), 6.25 (d, J = 8 Hz, 1H). $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 165.72, 138.93, 133.01, 130.74, 129.71, 129.47, 129.07, 128.83, 127.12, 117.45. HRMS (ESI) calculated for $C_{15}H_{11}N_2OClNa$ $[M+Na]^+$: 293.0452 found 293.0452.

4-bromo-*N*-(cyano(phenyl)methyl)benzamide (1i). The title compound was prepared



according to the general procedure (B) on a 2.0 mmol scale to obtain as a white solid (507 mg, yield = 80%); Mp. 168-172 °C; 1H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, J = 8.5 Hz, 2H), 7.56 (d, J = 7.5 Hz, 2H), 7.51 (s, 2H), 7.42 (s, 3H), 7.02 (s, 1H), 6.27 (d, J = 8 Hz, 1H). $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 165.71, 132.95, 132.06, 131.17, 129.74, 129.49, 128.91, 127.45, 127.12, 117.35, 44.66. HRMS (ESI) calculated for $C_{15}H_{11}N_2OBrNa$ $[M+Na]^+$: 336.9947 found 336.9939.

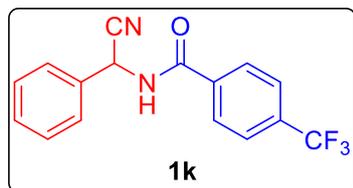
***N*-(cyano(phenyl)methyl)-3,4,5-trifluorobenzamide (1j)**. The title compound was prepared



according to the general procedure (B) on a 2.0 mmol scale to obtain as a white solid (297 mg, yield = 51%); Mp. 176-177 °C; 1H NMR (400 MHz, $CDCl_3$) δ 7.54-7.53 (m, 2H), 7.48-7.45 (m, 5H), 6.72 (d, J = 7.6 Hz, 1H), 6.26 (d, J = 8 Hz, 1H). $^{13}C\{^1H\}$ NMR

(CDCl₃, 100 MHz): δ 163.43, 152.50 (dd, J_{CF} = 10.4, 3.2 Hz), 149.97 (dd, J_{CF} = 10, 3.6 Hz), 143.90 (t, J_{CF} = 15 Hz), 141.31 (t, J_{CF} = 15 Hz), 132.58, 129.92, 129.57, 128.22, 127.08, 117.04, 112.20 (dd, J_{CF} = 16.2, 6.7 Hz), ¹⁹F NMR (376 MHz, CDCl₃) δ 44.89, -131.19, -152.73. HRMS (ESI) calculated for C₁₅H₈N₂OF₃ [M-H]⁻: 289.0589 found 289.0604.

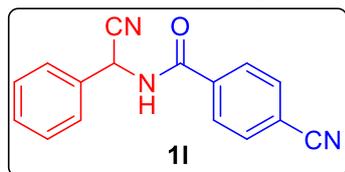
***N*-(cyano(phenyl)methyl)-4-(trifluoromethyl)benzamide (1k)**. The title compound was



prepared according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (475 mg, yield = 78%); Mp. 136-138 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.89 (d, J = 8.4 Hz, 2H), 7.69 (d, J = 8.4 Hz, 2H), 7.55-7.51 (m, 2H), 7.47-7.42 (m, 3H),

7.03 (d, J = 8 Hz, 1H), 6.30 (d, J = 8.4 Hz, 1H). ¹³C {¹H} NMR (CDCl₃, 100 MHz): δ 165.43, 135.73 (d, J_{CF} = 1.3 Hz), 134.46, 134.13, 133.80, 132.92, 130.57, 129.92, 129.63, 127.93, 127.20, 125.93 (q, J_{CF} = 3.7 Hz), 124.87, 122.15, 117.30, 44.84. ¹⁹F NMR (376 MHz, CDCl₃) δ -63.01. HRMS (ESI) calculated for C₁₆H₁₀N₂OF₃ [M-H]⁻: 303.0745 found 303.0764.

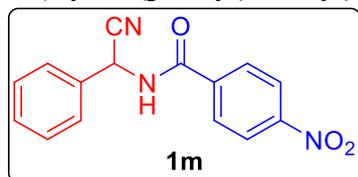
4-cyano-*N*-(cyano(phenyl)methyl)benzamide (1l). The title compound was prepared



according to the general procedure (A) on a 2.0 mmol scale to obtain as a yellow solid (471 mg, yield = 90%); Mp. 173-175 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.90 (d, J = 8.4 Hz, 2H), 7.73 (d,

J = 8.4 Hz, 2H), 7.55-7.51 (m, 2H), 7.46-7.43 (m, 3H), 7.08 (d, J = 8 Hz, 1H), 6.29 (d, J = 8 Hz, 1H). ¹³C {¹H} NMR (CDCl₃, 100 MHz): δ 164.77, 136.23, 132.69, 132.57, 129.88, 129.55, 128.04, 127.12, 117.63, 117.07, 116.05, 44.81. HRMS (ESI) calculated for C₁₆H₁₁N₃ONa [M+Na]⁺: 284.0800 found 284.0822.

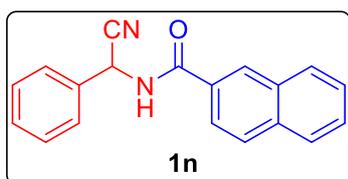
***N*-(Cyano(phenyl)methyl)-4-nitrobenzamide (1m)**. The title compound was prepared



according to the general procedure (A) on a 2.0 mmol scale to obtain as a yellow solid (428 mg, yield = 76%); Mp. 159-162 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.58 (d, J = 4 Hz, 1H), 7.54-7.50

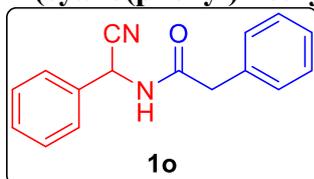
(m, 4H), 7.40 (d, J = 4 Hz, 3H), 7.07 (dd, J = 8.6, 4.6 Hz, 2H), 6.27 (d, J = 8.4, 1H). ¹³C {¹H} NMR (101 MHz, CDCl₃) δ 161.13, 136.69, 133.11, 131.70, 129.62, 129.59, 129.41, 127.98, 127.13, 117.47, 44.44. HRMS (ESI) calculated for C₁₅H₁₁N₃O₃Na [M+Na]⁺: 304.0692 found 304.0685.

***N*-(cyano(phenyl)methyl)-2-naphthamide (1n).** The title compound was prepared according



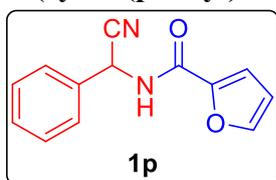
to the general procedure (B) on a 2.0 mmol scale to obtain as a white solid (317 mg, yield = 55%); Mp. 171-174 °C; ¹H NMR (400 MHz, CDCl₃) 8.28 (s, 1H), 7.83-7.78 (m, 4H), 7.57-7.53 (m, 3H), 7.51-7.47 (m, 1H), 7.43-7.29 (m, 4H), 6.36 (d, *J* = 8.4 Hz, 1H). ¹³C{¹H} NMR (CDCl₃, 100 MHz): δ 166.81, 135.08, 133.30, 132.41, 129.57, 129.54, 129.37, 129.01, 128.68, 128.27, 128.16, 127.74, 127.11, 126.95, 123.40, 117.58, 44.68. HRMS (ESI) calculated for C₁₉H₁₃N₂O [M-H]⁻: 285.1028 found 285.1023.

***N*-(cyano(phenyl)methyl)-2-phenylacetamide (1o).** The title compound was prepared



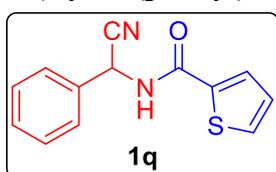
according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (392 mg, yield = 78%); Mp. 132-134 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.36-7.27 (m, 8H), 7.21 (d, *J* = 7 Hz, 2H), 6.67 (d, *J* = 8 Hz, 1H), 6.04 (d, *J* = 8.5 Hz, 1H), 3.55 (s, 2H). ¹³C{¹H} NMR (CDCl₃, 126 MHz) δ 170.56, 133.69, 133.06, 129.49, 129.34, 129.33, 129.13, 127.67, 126.83, 117.39, 44.07, 42.93. HRMS (ESI) calculated for C₁₆H₁₄N₂O₂Na [M+Na]⁺: 273.1004 found 273.1015.

***N*-(cyano(phenyl)methyl)furan-2-carboxamide (1p).** The title compound was prepared



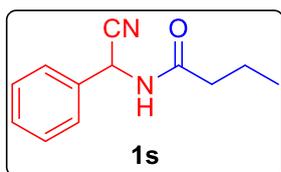
according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (268 mg, yield = 59%); Mp. 101-102 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.51-7.49 (m, 2H), 7.43 (s, 1H), 7.40-7.39 (m, 4H), 7.18 (d, *J* = 3.5, 1H), 6.50 (s, 1H), 6.26 (d, *J* = 8.5 Hz, 1H). ¹³C{¹H} NMR (126 MHz, CDCl₃) δ 157.34, 146.27, 145.01, 133.07, 129.55, 129.34, 127.08, 117.29, 116.26, 112.48, 43.66. HRMS (ESI) calculated for C₁₃H₉N₂O₂ [M-H]⁻: 225.0664 found 225.0659.

***N*-(Cyano(phenyl)methyl)thiophene-2-carboxamide (1q).** The title compound was prepared



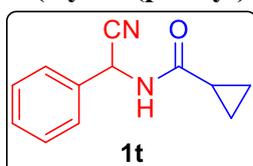
according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (380 mg, yield = 74%); Mp. 154-158 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.29 (d, *J* = 8, 2H), 7.97 (d, *J* = 8.4, 2H), 7.50 (d, *J* = 33.2, 4H), 6.94 (s, 1H), 6.30 (d, *J* = 7.6, 1H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 164.53, 150.19, 137.82, 132.57, 130.03, 129.67, 128.61, 127.20, 124.04, 117.02, 44.93. HRMS (ESI) calculated for C₁₃H₁₀N₂OSNa [M+Na]⁺: 265.0406 found 265.0400.

***N*-(Cyano(phenyl)methyl)butyramide (1s).** The title compound was prepared according to



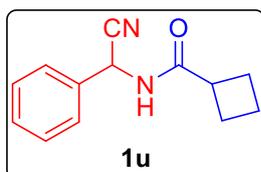
the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (340 mg, yield = 84%); Mp. 70-72 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.44-7.38 (m, 5H), 6.75 (d, *J* = 7.6 Hz, 1H), 6.05 (d, *J* = 8.4, 1H), 2.21-2.17 (m, 2H), 1.69-1.60 (m, 2H), 0.92 (t, *J* = 7.4, 3H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 172.54, 133.35, 129.47, 129.33, 126.97, 117.61, 43.90, 37.86, 18.85, 13.63. HRMS (ESI) calculated for C₁₂H₁₄N₂ONa [M+Na]⁺: 225.0998 found 225.0993.

***N*-(Cyano(phenyl)methyl)cyclopropanecarboxamide (1t).** The title compound was prepared



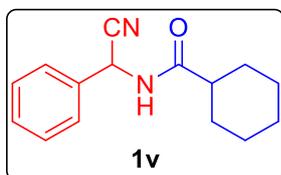
according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (325 mg, yield = 81%); Mp. 158-161 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.45-7.40 (m, 5H), 6.69 (d, *J* = 8, 1H), 6.08 (d, *J* = 8.4, 1H), 1.45-1.38 (m, 1H), 1.07-0.98 (m, 2H), 0.87-0.77 (m, 2H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 173.23, 133.38, 129.50, 129.36, 127.02, 117.62, 44.20, 14.42, 8.27, 8.11. HRMS (ESI) calculated for C₁₂H₁₂N₂ONa [M+Na]⁺: 223.0841 found 223.0834.

***N*-(Cyano(phenyl)methyl)cyclobutanecarboxamide (1u).** The title compound was prepared



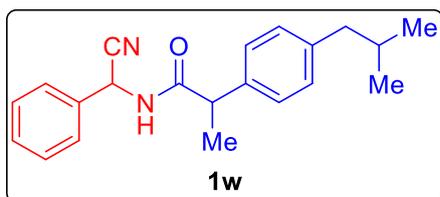
according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (357 mg, yield = 83%); Mp. 144-146 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.40-7.35 (m, 5H), 6.86 (d, *J* = 8 Hz, 1H), 6.01 (d, *J* = 8.4, 1H), 3.04 (p, *J* = 8.5, 1H), 2.28-2.17 (m, 2H), 2.16-2.06 (m, 2H), 1.99-1.90 (m, 1H), 1.87-1.82 (m, 1H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 174.54, 133.43, 129.39, 129.27, 126.94, 117.72, 43.89, 39.18, 25.13, 25.12, 18.20. HRMS (ESI) calculated for C₁₃H₁₄N₂ONa [M+Na]⁺: 237.0998 found 237.0994.

***N*-(Cyano(phenyl)methyl)cyclohexanecarboxamide (1v).** The title compound was prepared



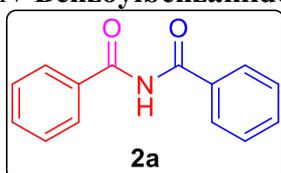
according to the general procedure (A) on a 2.0 mmol scale to obtain as a white solid (395 mg, yield = 81%); Mp. 159-163 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.42-7.39 (m, 5H), 6.61 (d, *J* = 7.6 Hz, 1H), 6.09 (d, *J* = 8.4, 1H), 2.16 (tt, *J* = 11.8, 3.3, 1H), 1.88-1.77 (m, 4H), 1.67 (s, 1H), 1.48-1.38 (m, 2H), 1.29-1.17 (m, 3H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 175.44, 133.51, 129.40, 129.31, 126.86, 117.67, 44.87, 43.72, 29.42, 29.25, 25.56, 25.52, 25.49. HRMS (ESI) calculated for C₁₅H₁₈N₂ONa [M+Na]⁺: 265.1311 found 265.1303.

***N*-(cyano(phenyl)methyl)-2-(4-isobutylphenyl)propenamide (1w).** The title compound was



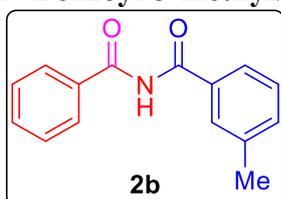
prepared according to the general procedure (C) on a 2.0 mmol scale to obtain as a white solid (362 mg, yield = 56%); Mp. 88-90 °C; ^1H NMR (500 MHz, CDCl_3) δ 7.35-7.33 (m, 2H), 7.31-7.26 (m, 2H), 7.21-7.20 (m, 1H), 7.18-7.08 (m, 4H), 6.50 (s, 1H), 6.06-6.02 (m, 1H), 3.60 (q, $J = 7$, 1H), 2.44 (dd, $J = 7$, 2.5 Hz, 2H), 1.88-1.79 (m, 1H), 1.51-1.49 (m, 3H), 0.90-0.87 (m, 6H). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CDCl_3) δ 173.98, 173.88, 141.07, 141.04, 137.54, 137.25, 133.19, 133.13, 129.78, 129.72, 129.34, 129.22, 129.19, 129.09, 127.19, 127.18, 126.74, 126.43, 117.51, 117.29, 30.13, 30.11, 22.34, 22.32, 22.28. HRMS (ESI) calculated for $\text{C}_{21}\text{H}_{23}\text{N}_2\text{O}$ $[\text{M}-\text{H}]^-$: 319.1810 found 319.1811.

***N*-Benzoylbenzamide (2a).**¹ The title compound was prepared according to the general



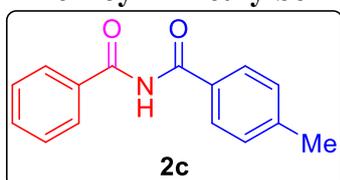
procedure (D) on a 0.5 mmol scale to obtain as a white solid (98 mg, yield = 87%); Mp. 156-157 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.29 (s, 1H), δ 7.84 (d, $J = 8$ Hz, 4H), 7.56 (t, $J = 7.4$ Hz, 2H), 7.45 (t, $J = 7.6$ Hz, 4H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.69, 133.39, 133.04, 128.80, 128.05.

***N*-Benzoyl-3-methylbenzamide (2b).**² The title compound was prepared according to the



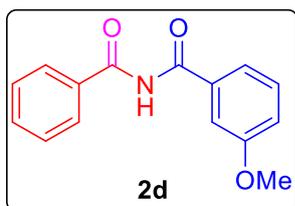
general procedure (D) on a 0.5 mmol scale to obtain as a white solid (91 mg, yield = 76%); Mp. 133-134 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.13 (s, 1H), δ 7.85 (d, $J = 7.2$ Hz, 2H), 7.67 (s, 1H), 7.63 (d, $J = 7.2$ Hz, 1H), 7.58 (t, $J = 7.4$ Hz, 1H), 7.47 (t, $J = 7.6$ Hz, 2H), 7.40-7.33 (m, 2H), 2.40 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.58, 138.86, 133.87, 133.46, 133.36, 133.02, 128.82, 128.70, 128.64, 128.00, 124.92, 21.36.

***N*-Benzoyl-4-methylbenzamide (2c).**² The title compound was prepared according to the



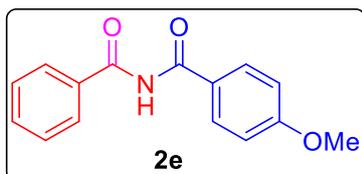
general procedure (D) on a 0.5 mmol scale to obtain as a white solid (100 mg, yield = 83%); Mp. 121-123 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.00 (s, 1H), δ 7.85 (d, $J = 7.6$ Hz, 2H), 7.76 (d, $J = 8.4$ Hz, 2H), 7.59 (t, $J = 7.4$ Hz, 1H), 7.49 (t, $J = 7.6$ Hz, 2H), 7.27 (t, $J = 7.2$ Hz, 2H), 2.42 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.57, 166.27, 144.01, 133.51, 133.01, 130.49, 129.55, 128.84, 128.07, 127.96, 21.66.

N-Benzoyl-3-methoxybenzamide (2d).³ The title compound was prepared according to the



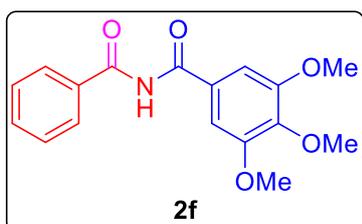
general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid (96 mg, yield = 75%); Mp. 132-134 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.24 (s, 1H), δ 7.83 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.39-7.33 (m, 3H), 7.09 (d, *J* = 7.2 Hz, 1H), 3.81 (s, 3H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 166.68, 166.19, 159.93, 134.75, 133.41, 133.02, 129.84, 128.78, 128.03, 119.72 119.25, 113.21, 55.52.

N-Benzoyl-4-methoxybenzamide (2e).² The title compound was prepared according to the



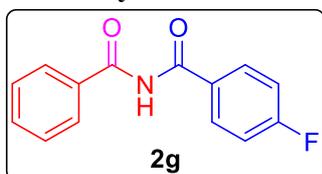
general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid (102 mg, yield = 80%); Mp. 122-123 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.20 (s, 1H), δ 7.83 (t, *J* = 4.4 Hz, 4H), 7.54 (t, *J* = 7.4 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.83 (s, 3H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 167.01, 166.05, 163.52, 133.61, 132.88, 130.39, 128.72, 128.03, 125.40, 114.01, 55.43.

N-Benzoyl-3,4,5-trimethoxybenzamide (2f). The title compound was prepared according to



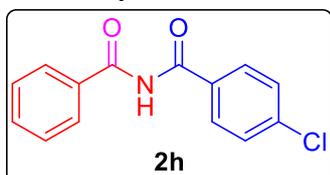
the general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid (90 mg, yield = 57%); Mp. 174-175 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.24 (s, 1H), δ 7.82 (d, *J* = 7.6 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.10 (s, 2H), 3.89 (s, 3H), 3.87 (s, 6H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 167.81, 166.08, 153.25, 142.37, 133.60, 132.92, 128.70, 128.28, 128.12, 105.61, 60.97, 56.39. HRMS (ESI) calculated for C₁₇H₁₇NO₅Na [M+Na]⁺: 338.0998 found 338.0990.

N-Benzoyl-4-fluorobenzamide (2g).¹ The title compound was prepared according to the



general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid (90 mg, yield = 74%); Mp. 137-140 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.30 (s, 1H), δ 7.90-7.83 (m, 4H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.12 (t, *J* = 8.4 Hz, 2H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 166.85 (d, *J*_{CF} = 3.53 Hz), 166.09, 164.34, 133.20, 133.14, 130.92, 130.83, 129.54 (d, *J*_{CF} = 3.13 Hz), 128.80, 128.08, 115.90 (d, *J*_{CF} = 22.22). ¹⁹F NMR (376 MHz, CDCl₃) δ -104.9.

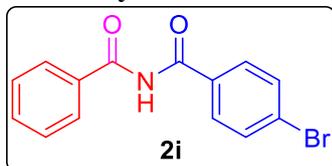
N-Benzoyl-4-chlorobenzamide (2h).² The title compound was prepared according to the



general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid (86 mg, yield = 66%); Mp. 140-141 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.19 (s, 1H), δ 7.84 (d, *J* = 7.6 Hz, 2H), 7.78 (d, *J* = 8.4

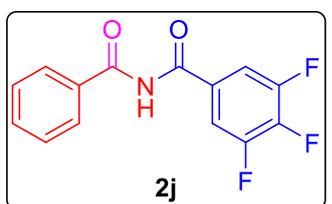
Hz, 2H), 7.58 (t, $J = 7.4$ Hz, 1H), 7.49-7.42 (m, 4H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.57, 166.22, 139.42, 133.19, 133.04, 131.70, 129.60, 129.01, 128.82, 128.02.

***N*-Benzoyl-4-bromobenzamide (2i).**² The title compound was prepared according to the



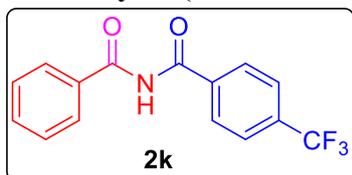
general procedure (D) on a 0.5 mmol scale to obtain as a white solid (95 mg, yield = 62%); Mp. 132-134 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.07 (s, 1H), 7.85 (d, $J = 7.6$ Hz, 2H), 7.71 (d, $J = 8$ Hz, 2H), 7.62-7.59 (m, 3H), 7.49 (t, $J = 7.6$ Hz, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.46, 166.38, 133.29, 133.03, 132.21, 132.06, 129.70, 128.92, 128.07, 128.02.

***N*-Benzoyl-3,4,5-trifluorobenzamide (2j).** The title compound was prepared according to the



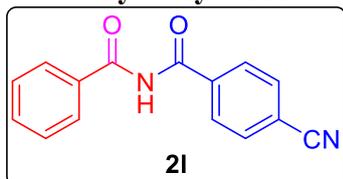
general procedure (D) on a 0.5 mmol scale to obtain as a white solid (73 mg, yield = 52%); Mp. 165-169 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.18 (s, 1H), 7.85 (d, $J = 7.6$ Hz, 2H), 7.63 (t, $J = 7.4$ Hz, 1H), 7.53-7.50 (m, 4H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.62, 164.72, 152.38 (dd, $J_{\text{CF}} = 10.45, 3.4$ Hz), 149.86 (dd, $J_{\text{CF}} = 10.40, 3.5$ Hz), 144.21 (t, $J_{\text{CF}} = 15.3$ Hz), 141.62 (t, $J_{\text{CF}} = 15.2$ Hz), 133.54, 132.57, 128.93, 128.11, 113.19 (dd, $J_{\text{CF}} = 16.46, 6.66$ Hz). ^{19}F NMR (376 MHz, CDCl_3) δ -131.57, -152.09. HRMS (ESI) calculated for $\text{C}_{14}\text{H}_8\text{NO}_2\text{F}_3\text{Na}$ $[\text{M}+\text{Na}]^+$: 302.0399 found 302.0398.

***N*-Benzoyl-4-(trifluoromethyl)benzamide (2k).**³ The title compound was prepared according



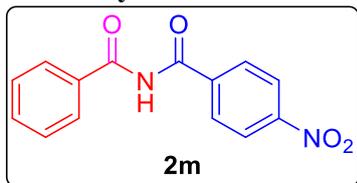
to the general procedure (D) on a 0.5 mmol scale to obtain as a white solid (93 mg, yield = 63%); Mp. 135-138 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.09 (s, 1H), 7.94 (d, $J = 8$ Hz, 2H), 7.88 (d, $J = 7.6$ Hz, 2H), 7.74 (t, $J = 8.4$ Hz, 2H), 7.62 (t, $J = 7.4$ Hz, 1H), 7.51 (t, $J = 7.6$ Hz, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.62, 166.21, 136.80, 134.36 (q, $J_{\text{CF}} = 33.0$ Hz), 132.72, 129.00, 128.57, 128.02, 125.76 (q, $J_{\text{CF}} = 3.7$ Hz), 123.46 (q, $J_{\text{CF}} = 273.7$ Hz). ^{19}F NMR (376 MHz, CDCl_3) δ -63.14.

***N*-Benzoyl-4-cyanobenzamide (2l).**⁴ The title compound was prepared according to the



general procedure (D) on a 0.5 mmol scale to obtain as a white solid (67 mg, yield = 53%); Mp. 130-133 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.27 (s, 1H), 7.89 (dd, $J = 14.2, 7.8$ Hz, 4H), 7.75 (d, $J = 7.6$ Hz, 2H), 7.62 (t, $J = 7.2$ Hz, 1H), 7.50 (t, $J = 7.4$ Hz, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.85, 166.31, 137.48, 133.62, 132.47, 132.39, 129.01, 128.81, 128.10, 117.79, 116.14.

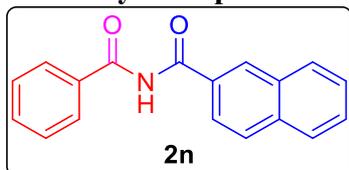
N-Benzoyl-4-nitrobenzamide (2m).² The title compound was prepared according to the



general procedure **(D)** on a 0.5 mmol scale to obtain as a bright yellow solid (65 mg, yield = 48%); Mp. 178-181 °C; ¹H NMR

(400 MHz, CDCl₃) δ 9.16 (s, 1H), 8.31 (d, *J* = 8.8 Hz, 2H), 7.96 (d, *J* = 8.8 Hz, 2H), 7.88 (d, *J* = 7.6 Hz, 2H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.52 (t, *J* = 7.6 Hz, 2H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 166.88, 166.06, 150.07, 139.18, 133.73, 132.31, 129.32, 129.09, 128.05, 123.79.

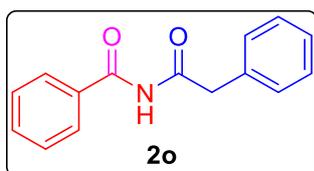
N-Benzoyl-2-naphthamide (2n).¹ The title compound was prepared according to the general



procedure **(D)** on a 0.5 mmol scale to obtain as a white solid (82 mg, yield = 59%); Mp. 158-160 °C; ¹H NMR (400 MHz, CDCl₃)

δ 9.17 (s, 1H), 8.38 (s, 1H), 7.95-7.87 (m, 6H), 7.59 (dt, *J* = 15, 7.2 Hz, 3H), 7.51 (t, *J* = 7.6 Hz, 2H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 166.60, 166.56, 135.44, 133.42, 133.11, 132.42, 130.54, 129.27, 129.11, 128.89, 127.15, 123.90.

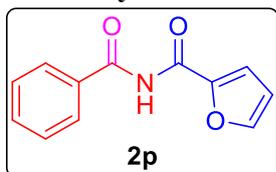
N-(2-Phenylacetyl)benzamide (2o).⁵ The title compound was prepared according to the



general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid

(95 mg, yield = 79%); Mp. 140-144 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.13 (s, 1H), 7.85 (d, *J* = 7.2 Hz, 2H), 7.58 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.37-7.27 (m, 5H), 4.31 (s, 2H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 174.23, 165.66, 133.75, 133.25, 132.62, 129.84, 128.95, 128.61, 127.81, 127.21, 43.97.

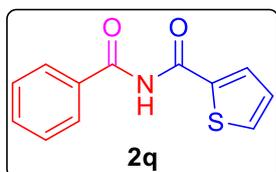
N-Benzoylfuran-2-carboxamide (2p).² The title compound was prepared according to the



general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid

(78 mg, yield = 72%); Mp. 128-131 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.36 (s, 1H), 7.87 (d, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 9.4 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.37 (d, *J* = 3.6 Hz, 1H), 6.60 (dd, *J* = 3.2, 1.6 Hz, 1H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 165.19, 155.00, 146.57, 145.37, 133.33, 133.13, 128.92, 127.78, 118.05, 113.30.

N-Benzoylthiophene-2-carboxamide (2q).² The title compound was prepared according to

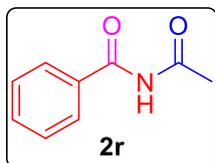


the general procedure **(D)** on a 0.5 mmol scale to obtain as a white solid

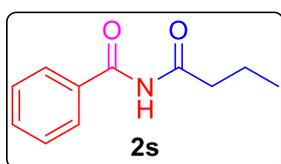
(90 mg, yield = 77%); Mp. 128-130 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.28 (s, 1H), 7.84 (d, *J* = 3.6 Hz, 1H), 7.63 (d, *J* = 4.8 Hz, 1H), 7.54 (t,

$J = 7.2$ Hz, 1H), 7.43 (t, $J = 7.6$ Hz, 2H), 7.12 (t, $J = 4.4$ Hz, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 166.68, 160.16, 137.68, 133.51, 133.42, 132.97, 131.36, 128.71, 128.18, 128.06.

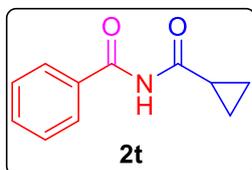
***N*-Acetylbenzamide (2r).**² The title compound was prepared according to the general procedure (D) on a 0.5 mmol scale to obtain as a white solid (73 mg, yield = 89%); Mp. 130-133 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.18 (s, 1H), 7.89 (d, $J = 7.2$ Hz, 2H), 7.59 (t, $J = 7.4$ Hz, 1H), 7.48 (t, $J = 7.6$ Hz, 2H), 2.60 (s, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 173.91, 165.90, 133.24, 132.68, 128.95, 127.82, 25.65.



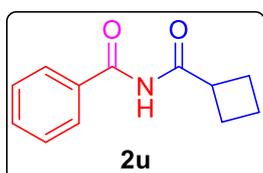
***N*-Butyrylbenzamide (2s).**⁶ The title compound was prepared according to the general procedure (D) on a 0.5 mmol scale to obtain as a white solid (84 mg, yield = 87%); Mp. 121-123 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.14 (s, 1H), 7.91 (d, $J = 8$ Hz, 2H), 7.59 (t, $J = 7.4$ Hz, 1H), 7.49 (t, $J = 7.8$ Hz, 2H), 2.99 (t, $J = 7.2$ Hz, 2H), 1.74 (dd, $J = 14.6, 7.4$ Hz, 2H), 1.02 (t, 7.6 Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 176.64, 165.73, 133.13, 132.87, 128.90, 127.80, 39.50, 17.55, 13.73.



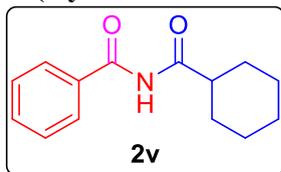
***N*-(Cyclopropanecarbonyl)benzamide (2t).**⁷ The title compound was prepared according to the general procedure (D) on a 0.5 mmol scale to obtain as a white solid (75 mg, yield = 79%); Mp. 146-150 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.25 (s, 1H), 7.90 (d, $J = 7.6$ Hz, 2H), 7.59 (t, $J = 7.4$ Hz, 1H), 7.49 (t, $J = 7.4$ Hz, 2H), 3.13-3.07 (m, 1H), 1.20-1.19 (m, 2H), 1.11-1.02 (m, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 177.66, 166.22, 133.11, 128.84, 127.89, 14.55, 11.13.



***N*-(Cyclobutanecarbonyl)benzamide (2u).** The title compound was prepared according to the general procedure (D) on a 0.5 mmol scale to obtain as a white solid (86 mg, yield = 84%); Mp. 152-154 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.86 (s, 1H), 7.88 (d, $J = 8$ Hz, 2H), 7.59 (t, $J = 7.2$ Hz, 1H), 7.49 (t, $J = 7.6$ Hz, 2H), 4.07 (p, $J = 8.4$ Hz, 1H), 2.43-2.30 (m, 4H), 2.10-1.98 (m, 2H), 1.96-1.86 (m, 1H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl_3) δ 178.23, 165.39, 133.07, 132.83, 128.83, 127.89, 40.60, 24.59, 17.97. HRMS (ESI) calculated for $\text{C}_{12}\text{H}_{13}\text{NO}_2\text{Na}$ $[\text{M}+\text{Na}]^+$: 226.0838 found 226.0833.

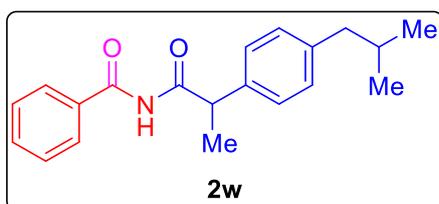


N-(Cyclohexanecarbonyl)benzamide (2v).⁵ The title compound was prepared according to



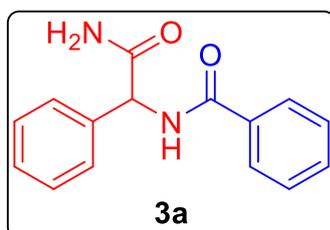
the general procedure (D) on a 0.5 mmol scale to obtain as a white solid (96 mg, yield = 83%); Mp. 158-162 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.81 (s, 1H), 7.87 (d, *J* = 7.2 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 2H), 3.39 (tt, *J* = 11.2, 3.2 Hz, 1H), 1.99 (d, *J* = 12.4 Hz, 2H), 1.84-1.80 (m, 2H), 1.72 (d, *J* = 12.8 Hz, 2H), 1.54-1.21 (m, 4H), 1.30-1.21 (m, 1H). ¹³C{¹H} NMR (101 MHz, CDCl₃) δ 179.19, 165.42, 133.08, 128.92, 127.73, 44.54, 28.93, 25.88, 25.60.

N-(2-(4-isobutylphenyl)propanoyl)benzamide (2w). The title compound was prepared



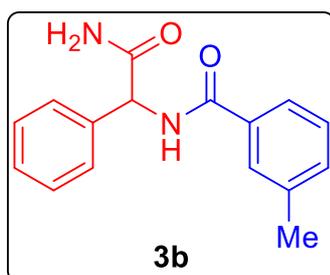
according to the general procedure (D) on a 0.5 mmol scale to obtain as a white solid (113 mg, yield = 73%); Mp. 128-130 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.66 (s, 1H), 7.70-7.68 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 2H), 7.30 (d, *J* = 8 Hz, 2H), 7.12 (d, *J* = 8 Hz, 2H), 4.67 (q, *J* = 7 Hz, 1H), 2.45 (d, *J* = 7.2 Hz, 2H), 1.90-1.80 (m, 1H), 1.55 (d, *J* = 7.2 Hz, 3H), 0.89 (d, *J* = 6.4 Hz, 6H). ¹³C{¹H} NMR (100 MHz, CDCl₃) δ 176.03, 165.05, 140.91, 137.38, 133.00, 132.97, 129.59, 128.79, 127.77, 127.60, 46.10, 45.02, 30.13, 22.36, 18.69. HRMS (ESI) calculated for C₂₀H₂₂NO₂ [M-H]⁻: 308.1651 found 308.1674.

N-(2-amino-2-oxo-1-phenylethyl)benzamide (3a). The title compound was prepared



according to the general procedure (F) on a 0.09 mmol scale to obtain as a white solid (17.4 mg, yield = 76%); Mp. 189-191 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.68 (d, *J* = 8 Hz, 1H), 7.92-7.86 (m, 2H), 7.68 (s, 1H), 7.53-7.51 (m, 3H), 7.46 (t, *J* = 7.4 Hz, 2H), 7.35 (t, *J* = 7.2 Hz, 2H), 7.31-7.27 (m, 1H), 7.23 (s, 1H), 5.62 (d, *J* = 8 Hz, 1H). ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 171.64, 165.91, 138.77, 133.92, 131.38, 128.23, 128.20, 127.59, 127.49, 127.46, 56.80. HRMS (ESI) calculated for C₁₅H₁₄N₂O₂Na [M+Na]⁺: 277.0947 found 277.0941.

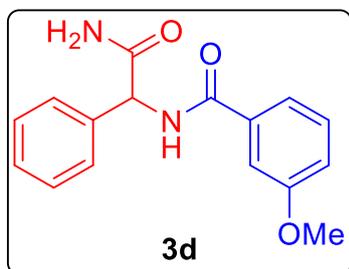
N-(2-amino-2-oxo-1-phenylethyl)-3-methylbenzamide (3b). The title compound was



prepared according to the general procedure (G) on a 0.09 mmol scale to obtain as a white solid (14.6 mg, yield = 60%); Mp. 185-187 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.58 (d, *J* = 8 Hz, 1H), 7.71 (s, 1H), 7.67-7.63 (m, 2H), 7.50-7.47 (m, 2H), 7.35-7.24 (m, 5H), 7.20 (s, 1H), 5.58 (d, *J* = 8 Hz, 1H), 2.33 (s, 3H). ¹³C{¹H}

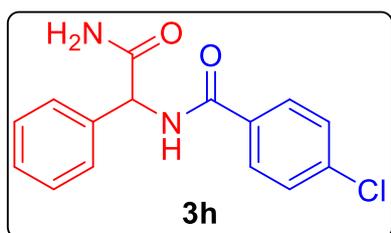
NMR (101 MHz, DMSO-*d*₆) δ 172.14, 166.44, 139.20, 137.96, 134.29, 132.41, 128.69, 128.57, 128.46, 127.96, 127.88, 125.18, 57.19, 21.30. HRMS (ESI) calculated for C₁₆H₁₆N₂O₂Na [M+Na]⁺: 291.1109 found 291.1096.

***N*-(2-amino-2-oxo-1-phenylethyl)-3-methoxybenzamide (3d)**. The title compound was



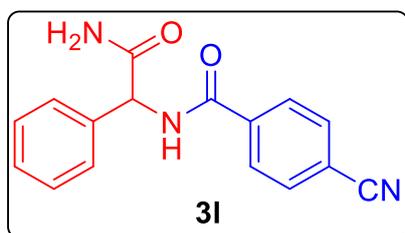
prepared according to the general procedure (F) on a 0.09 mmol scale to obtain as a white solid (17.5 mg, yield = 68%); Mp. 134-136 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.72 (d, *J* = 8 Hz, 1H), 7.69 (s, 1H), 7.50 (td, *J* = 8.1, 1.2 Hz, 3H), 7.45-7.44 (m, 1H), 7.39-7.33 (m, 3H), 7.31-7.27 (m, 1H), 7.26 (s, 1H), 7.09 (ddd, *J* = 8.2, 2.6, 0.8 Hz, 1H), 5.62 (d, *J* = 8 Hz, 1H), 3.80 (s, 3H). ¹³C {¹H} NMR (101 MHz, DMSO-*d*₆) δ 171.62, 165.69, 159.08, 138.72, 135.37, 129.33, 128.22, 127.49, 119.83, 117.35, 112.67, 56.84, 55.28. HRMS (ESI) calculated for C₁₆H₁₆N₂O₃Na [M+Na]⁺: 307.1053 found 307.1046.

***N*-(2-amino-2-oxo-1-phenylethyl)-4-chlorobenzamide (3h)**. The title compound was



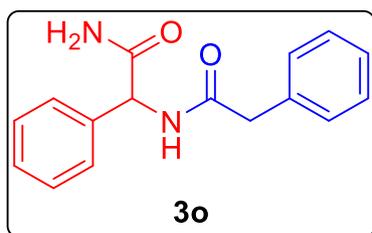
prepared according to the general procedure (G) on a 0.09 mmol scale to obtain as a white solid (10.4 mg, yield = 33%); Mp. 237-238 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.80 (d, *J* = 8 Hz, 1H), 7.90-7.88 (m, 2H), 7.65 (s, 1H), 7.50-7.47 (m, 3H), 7.46 (s, 1H), 7.33-7.29 (m, 2H), 7.27-7.23 (m, 1H), 7.19 (s, 1H), 5.56 (d, *J* = 8 Hz, 1H). ¹³C {¹H} NMR (101 MHz, DMSO-*d*₆) δ 171.97, 165.43, 139.01, 136.60, 133.12, 130.09, 129.82, 128.72, 128.66, 127.98, 57.36. HRMS (ESI) calculated for C₁₅H₁₃ClN₂O₂Na [M+Na]⁺: 311.0563 found 311.0549.

***N*-(2-amino-2-oxo-1-phenylethyl)-4-cyanobenzamide (3i)**. The title compound was prepared



according to the general procedure (G) on a 0.09 mmol scale to obtain as a white solid (10.1 mg, yield = 40%); Mp. 220-221 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.05 (d, *J* = 8 Hz, 1H), 8.05-7.98 (m, 2H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.69 (s, 1H), 7.49 (d, *J* = 7.2 Hz, 2H), 7.35-7.26 (m, 3H), 7.22 (s, 1H), 5.59 (d, *J* = 8 Hz, 1H). ¹³C {¹H} NMR (101 MHz, DMSO-*d*₆) δ 171.82, 165.26, 138.78, 138.43, 132.82, 132.68, 129.05, 128.70, 128.05, 118.79, 114.11, 57.52. HRMS (ESI) calculated for C₁₆H₁₃N₃O₂Na [M+Na]⁺: 302.0905 found 302.0892.

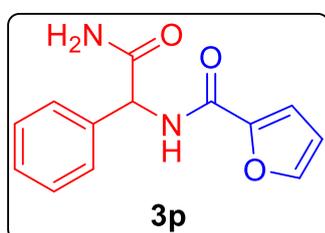
***N*-(2-amino-2-oxo-1-phenylethyl)-2-phenylacetamide (3o).** The title compound was



prepared according to the general procedure (G) on a 0.09 mmol scale to obtain as a white solid (13.3 mg, yield = 55%); Mp. 235-236 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.59 (d, *J* = 8 Hz, 1H), 7.65 (s, 1H), 7.36 (d, *J* = 7.2 Hz, 2H), 7.27 (t, *J* = 7.4 Hz, 2H), 7.21-7.20 (m, 4H), 7.16-7.13 (m, 1H), 7.09

(s, 1H), 5.35 (d, *J* = 8 Hz, 1H), 3.50 (s, 1H). ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 172.11, 170.15, 139.61, 136.88, 129.52, 128.66, 128.58, 127.44, 126.73, 56.49, 42.27. HRMS (ESI) calculated for C₁₆H₁₆N₂O₂Na [M+Na]⁺: 291.1109 found 291.1109.

***N*-(2-amino-2-oxo-1-phenylethyl)furan-2-carboxamide (3p).** The title compound was



prepared according to the general procedure (F) on a 0.09 mmol scale to obtain as a white solid (13.1 mg, yield = 60%); Mp. 184-186 °C; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.33 (d, *J* = 7.6 Hz, 1H), 7.85 (s, 1H), 7.74 (s, 1H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.30-7.27 (m, 2H), 7.24 (d, *J* = 3.2 Hz, 1H), 6.63-6.62 (m,

1H), 5.54 (d, *J* = 7.6 Hz, 1H). ¹³C{¹H} NMR (101 MHz, DMSO-*d*₆) δ 171.27, 156.87, 147.18, 145.37, 138.72, 128.31, 127.59, 127.17, 114.14, 111.93, 55.77. HRMS (ESI) calculated for C₁₃H₁₂N₂O₃Na [M+Na]⁺: 267.0740 found 267.0731.

12. References

- 1 T. Ye, Y. Li, Y. Ma, S. Tan and F. Li, *J. Org. Chem.*, 2024, **89**, 534-540.
- 2 L. Ran, Z.-H. Ren, Y.-Y. Wang and Z.-H. Guan, *Chem. Asian J.*, 2014, **9**, 577-583.
- 3 K. Kataoka, K. Wachi, X. Jin, K. Suzuki, Y. Sasano, Y. Iwabuchi, J.-Y Hasegawa, N. Mizuno and K. Yamaguchi, *Chem. Sci.*, 2018, **9**, 4756-4768.
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- 6 F. Wang, H. Liu, H. Fu, Y. Jiang and Y. Zhao, *Adv. Synth. Catal.*, 2009, **351**, 246-252.
- 7 L. Xu, S. Zhang and M. L. Trudell, *Chem. Commun.*, 2004, 1668-1669.

13. Copies of ^1H , ^{13}C , ^{19}F spectra and HRMS data

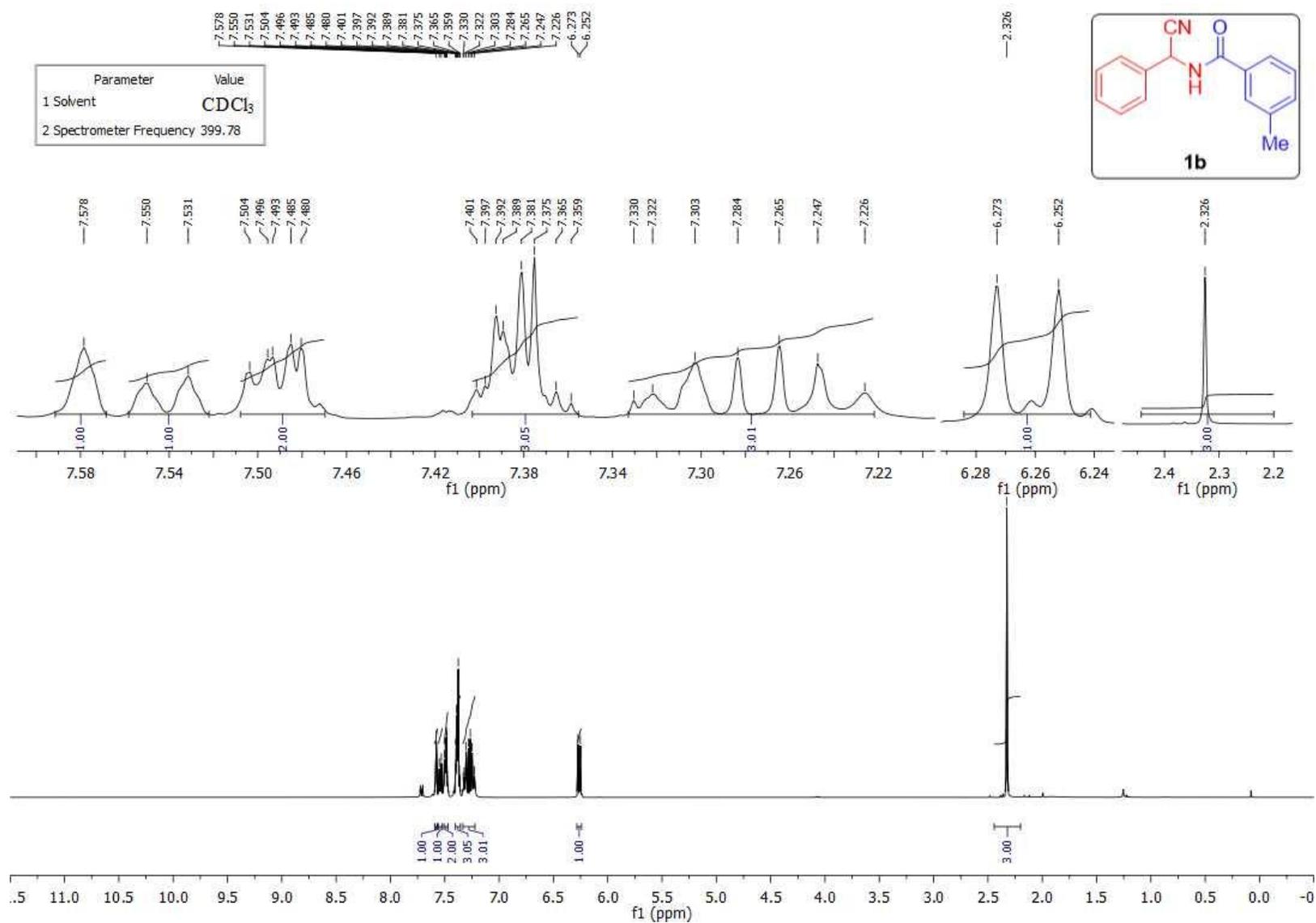


Fig. S9. ^1H NMR spectra of *N*-(cyano(phenyl)methyl)-3-methylbenzamide (**1b**).

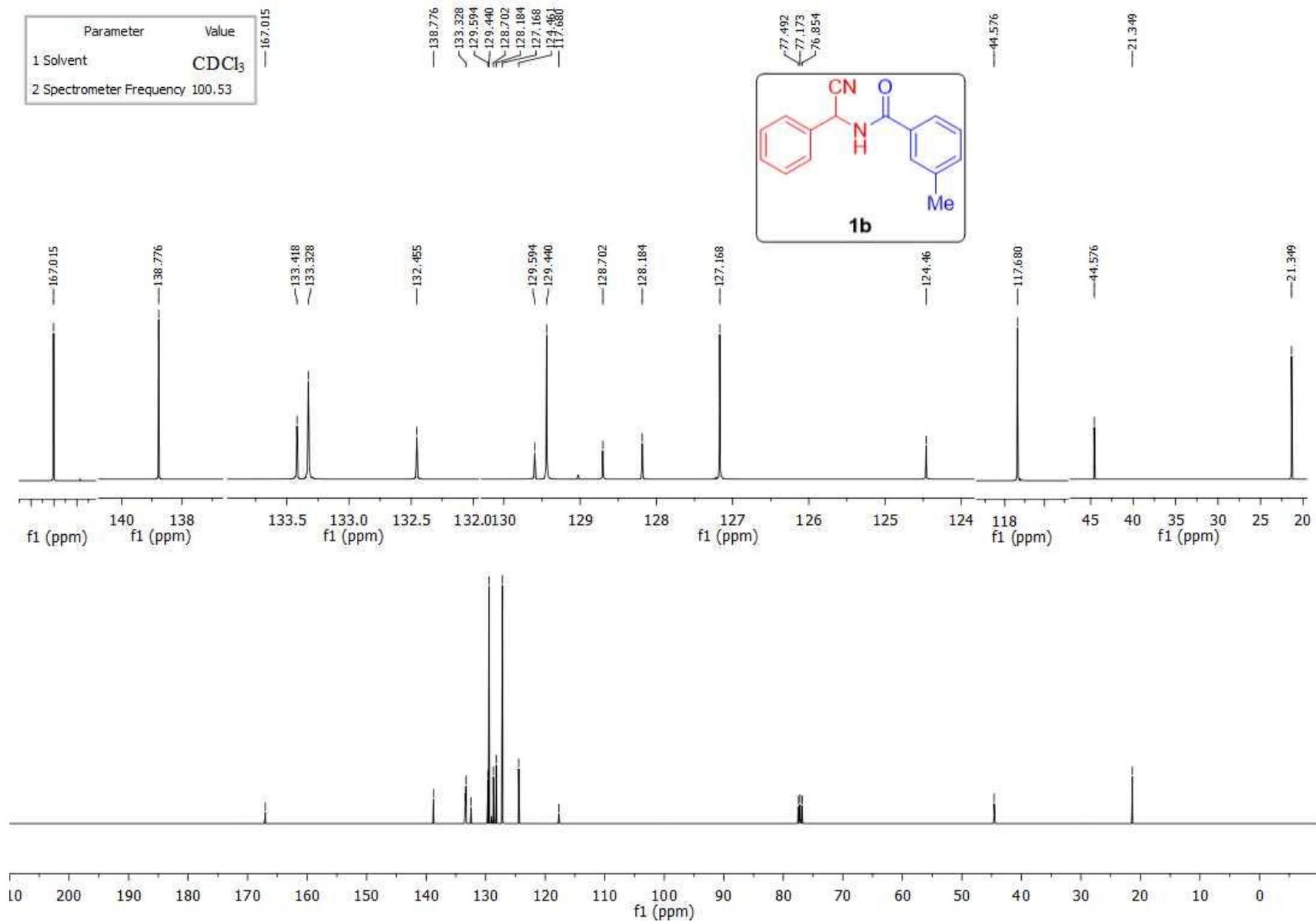


Fig. S10. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-3-methylbenzamide (**1b**).

Sample Name	VG P2 35_MeOH_Positive	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 35_MeOH_Positive.d
ACQ Method	TEST.m	Comment		Acquired Time	10/4/2025 11:48:49 AM (UTC+05:30)

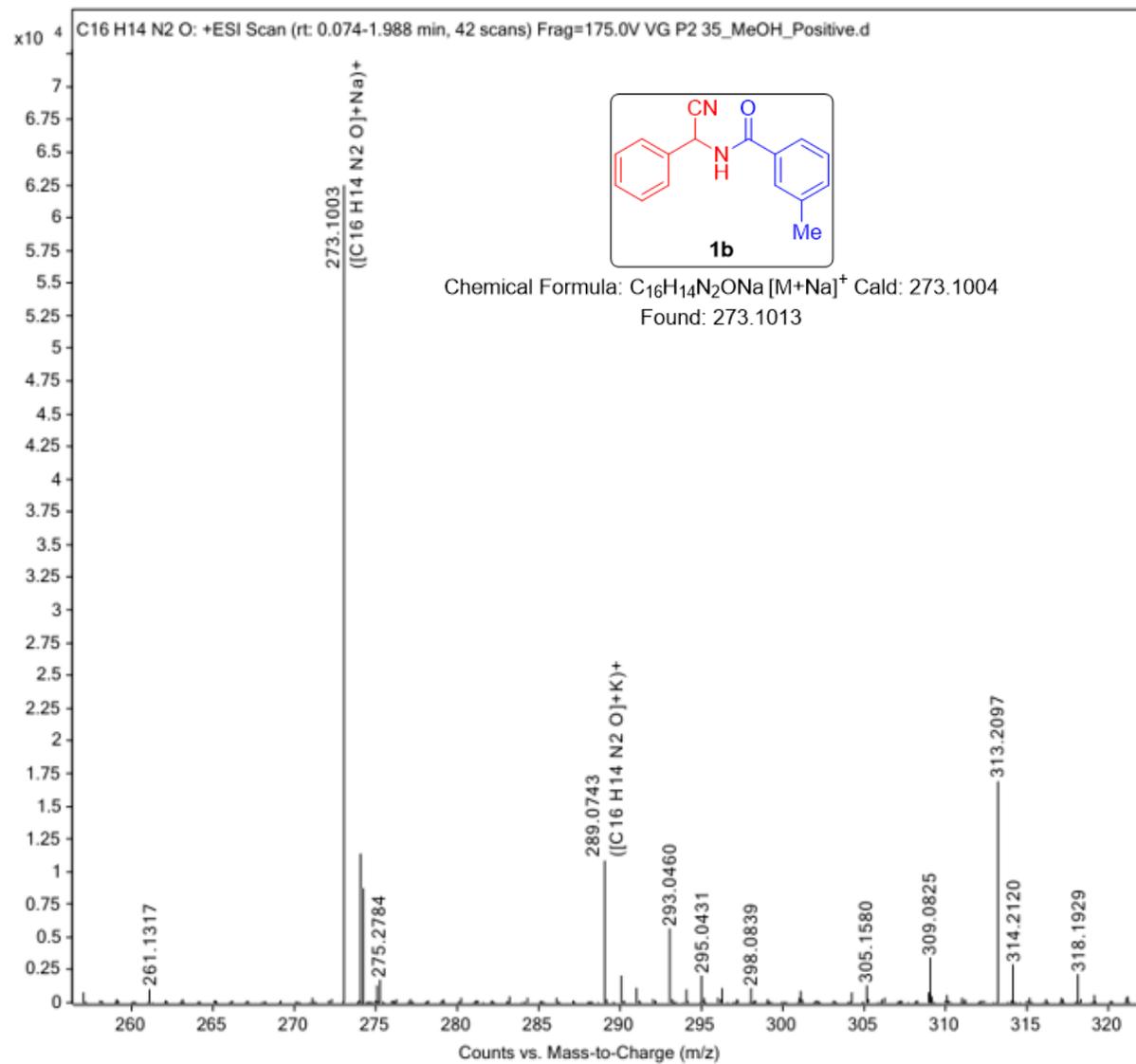


Fig. S11. HRMS data of *N*-(cyano(phenyl)methyl)-3-methylbenzamide (**1b**).

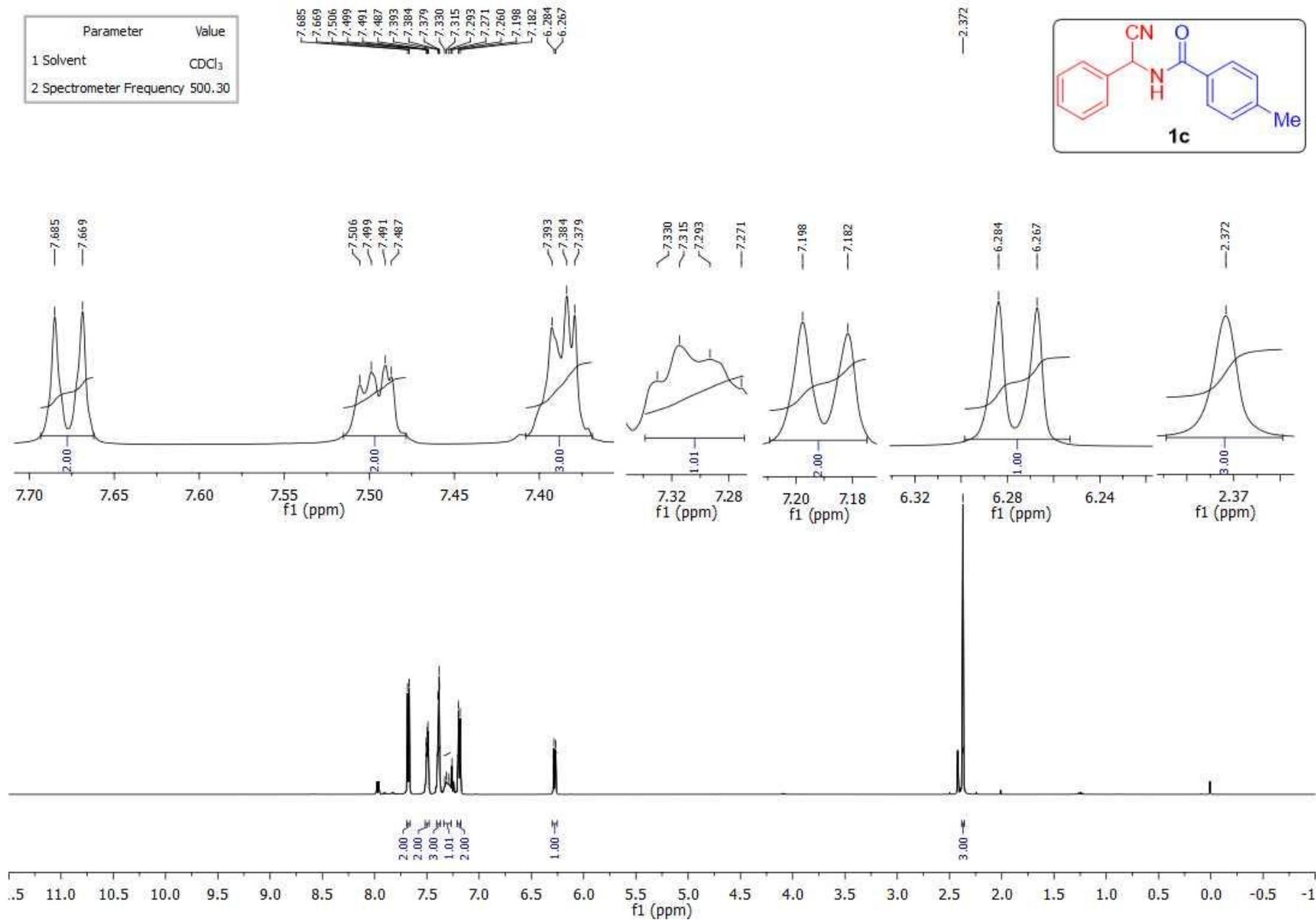


Fig. S12. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-4-methylbenzamide (**1c**).

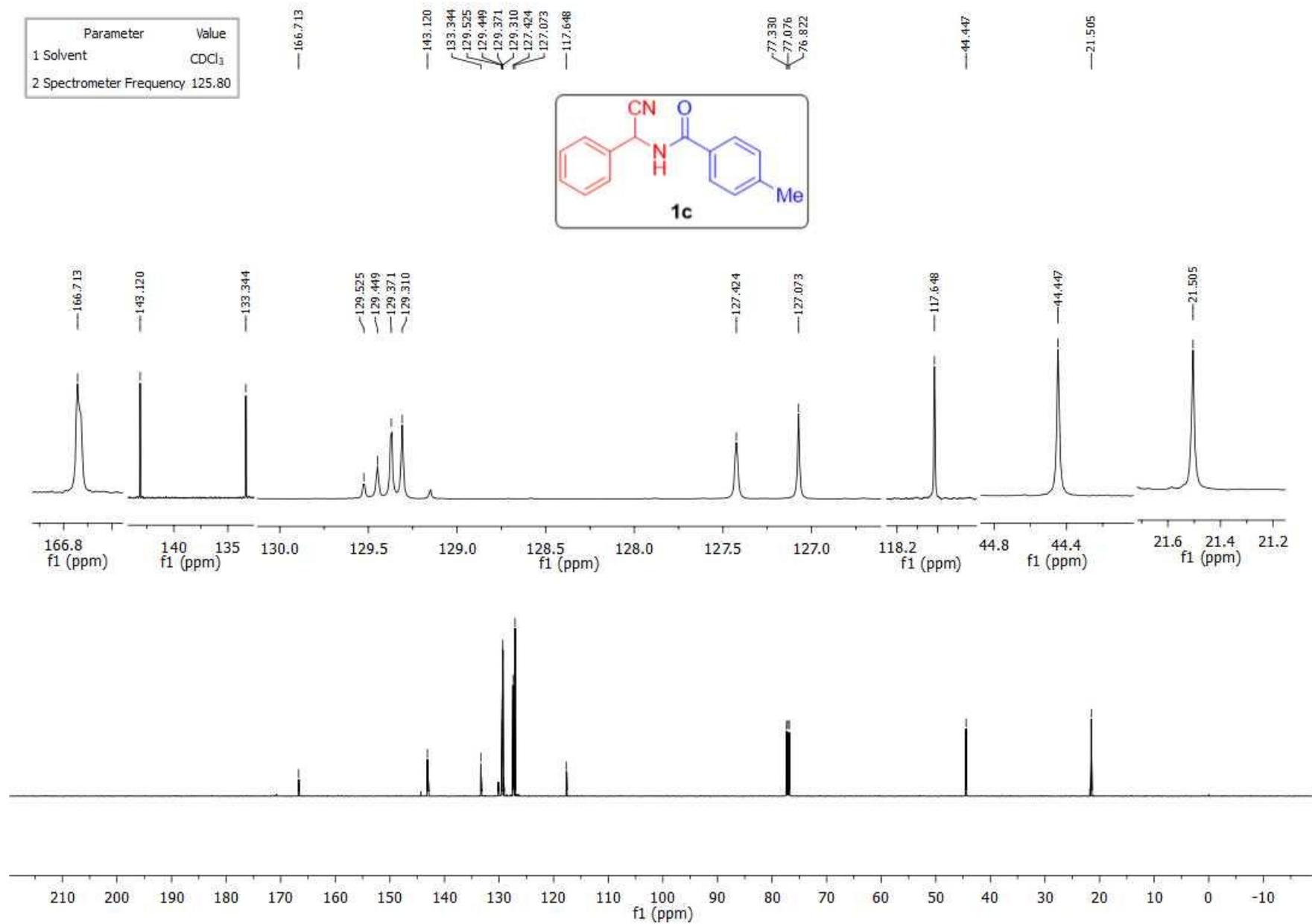


Fig. S13. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-4-methylbenzamide (**1c**).

Sample Name	VG P2 37_MeOH_Positive	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 37_MeOH_Positive.d
ACQ Method	TEST.m	Comment		Acquired Time	10/8/2025 10:24:09 AM (UTC+05:30)

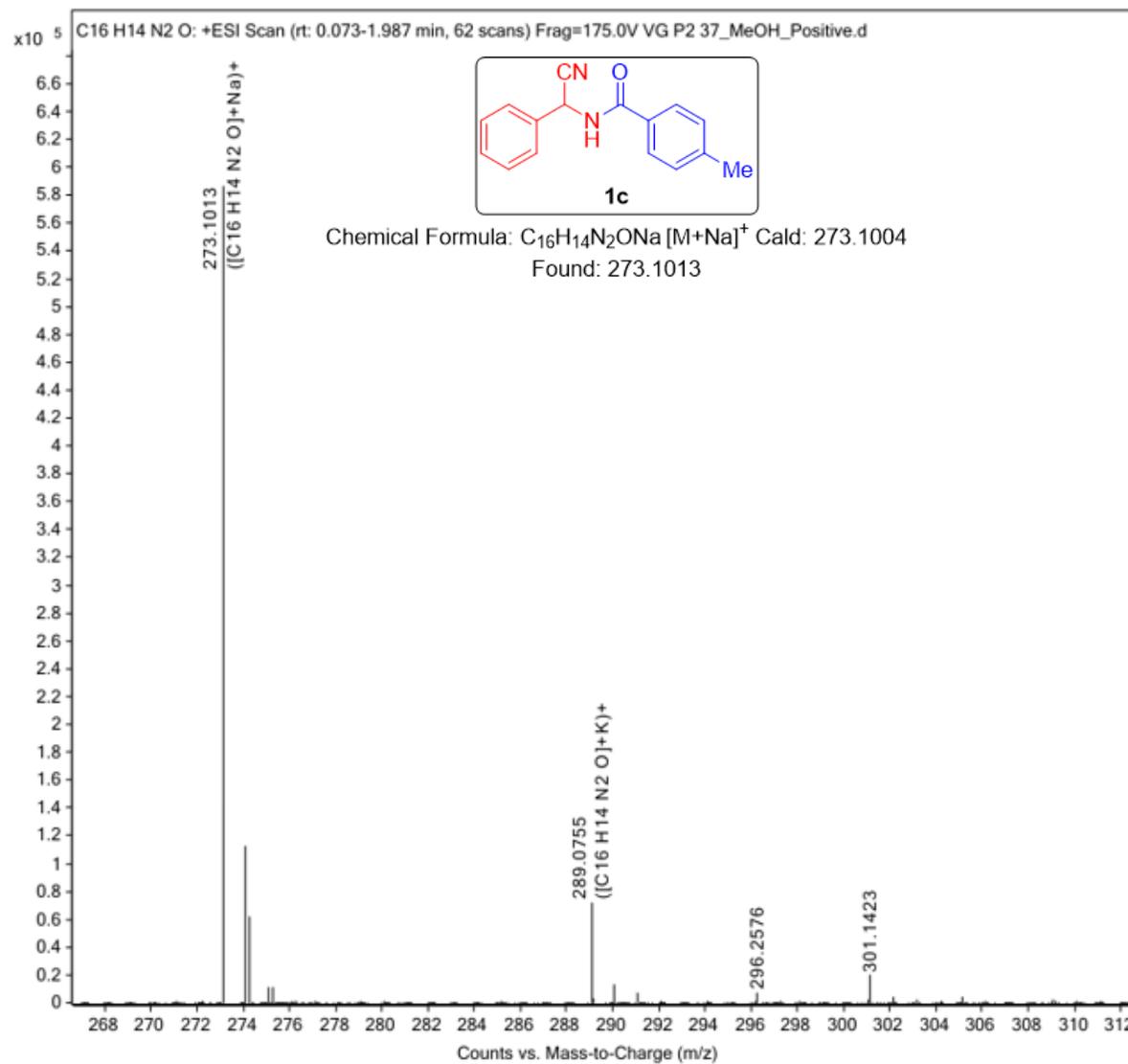


Fig. S14. HRMS data of *N*-(cyano(phenyl)methyl)-4-methylbenzamide (**1c**).

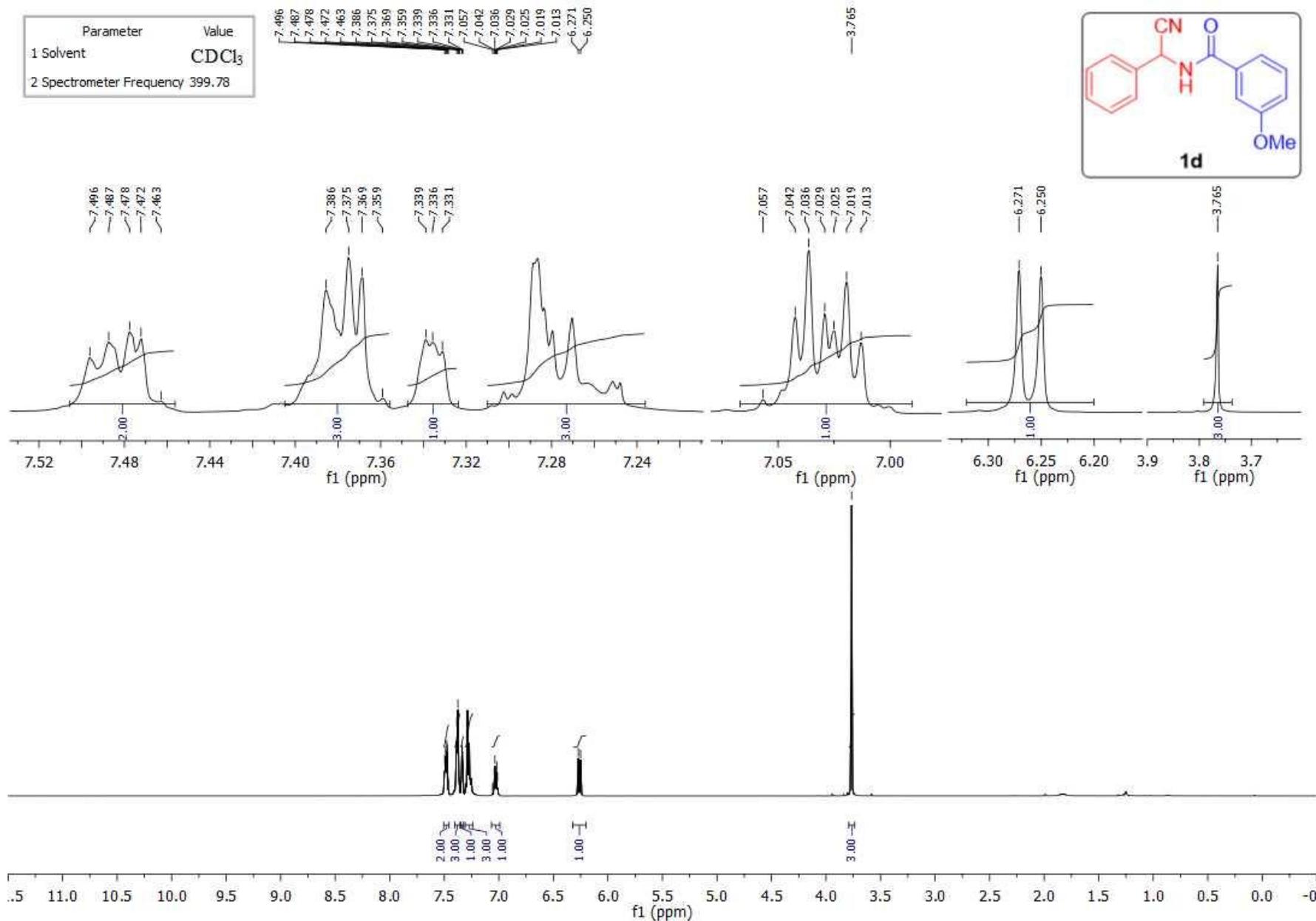


Fig. S15. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-3-methoxybenzamide (**1d**).

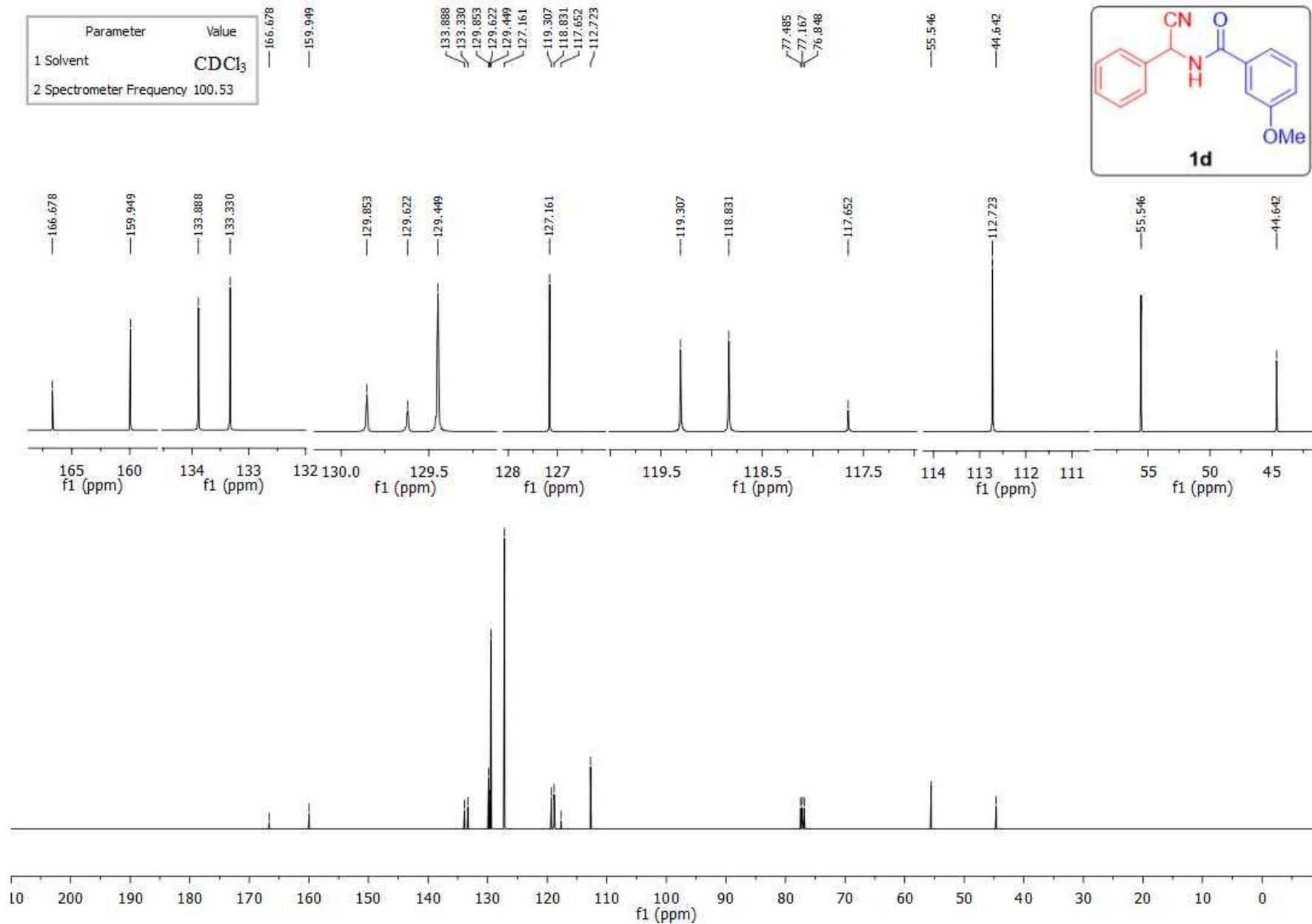


Fig. S16. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-3-methoxybenzamide (**1d**).

Sample Name	VG P2 36_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 36_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/4/2025 2:54:27 PM (UTC+05:30)

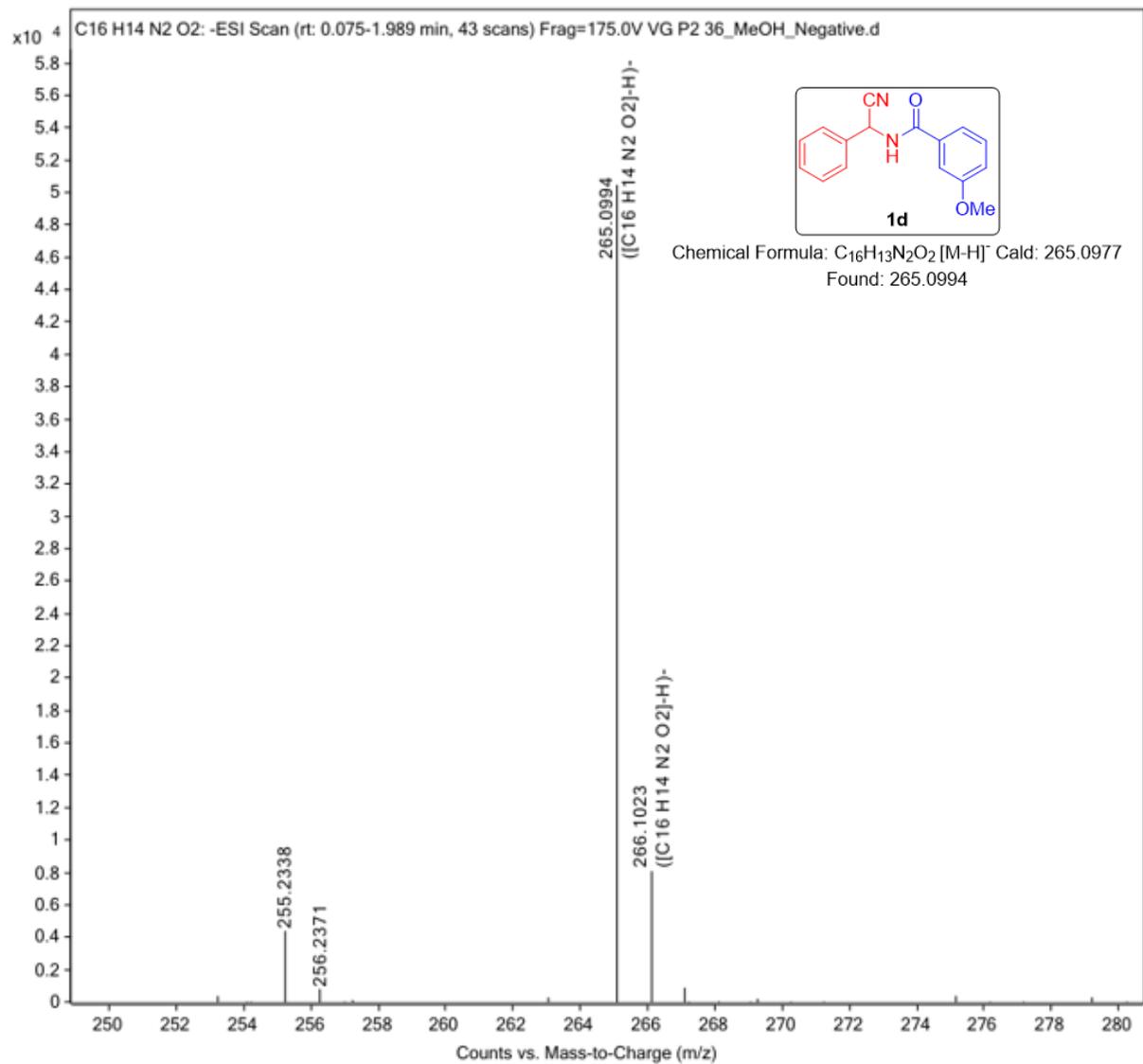


Fig. S17. HRMS data of *N*-(cyano(phenyl)methyl)-3-methoxybenzamide (**1d**).

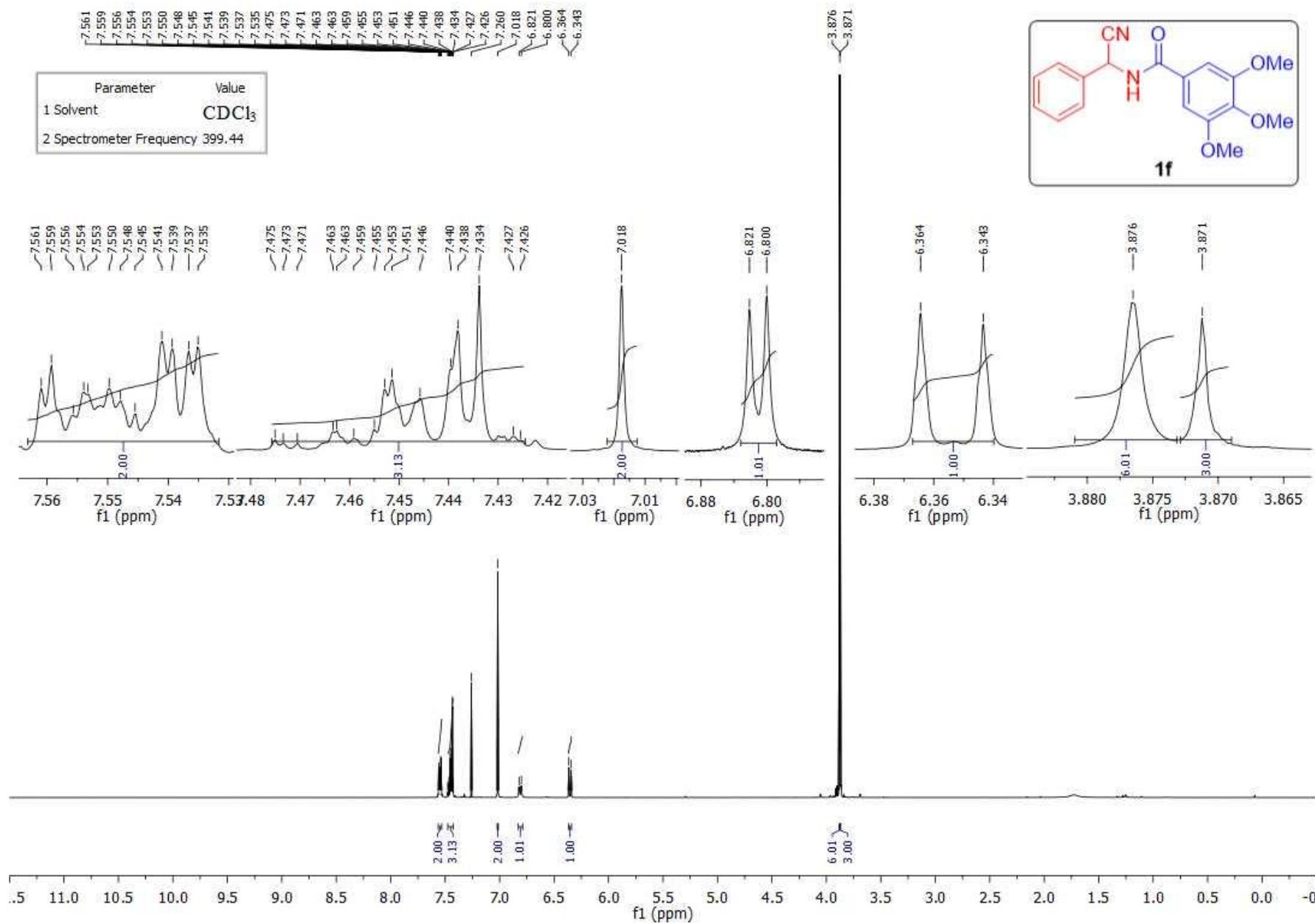


Fig. S18. ^1H NMR spectra of *N*-(cyano(phenyl)methyl)-3,4,5-trimethoxybenzamide (**1f**).

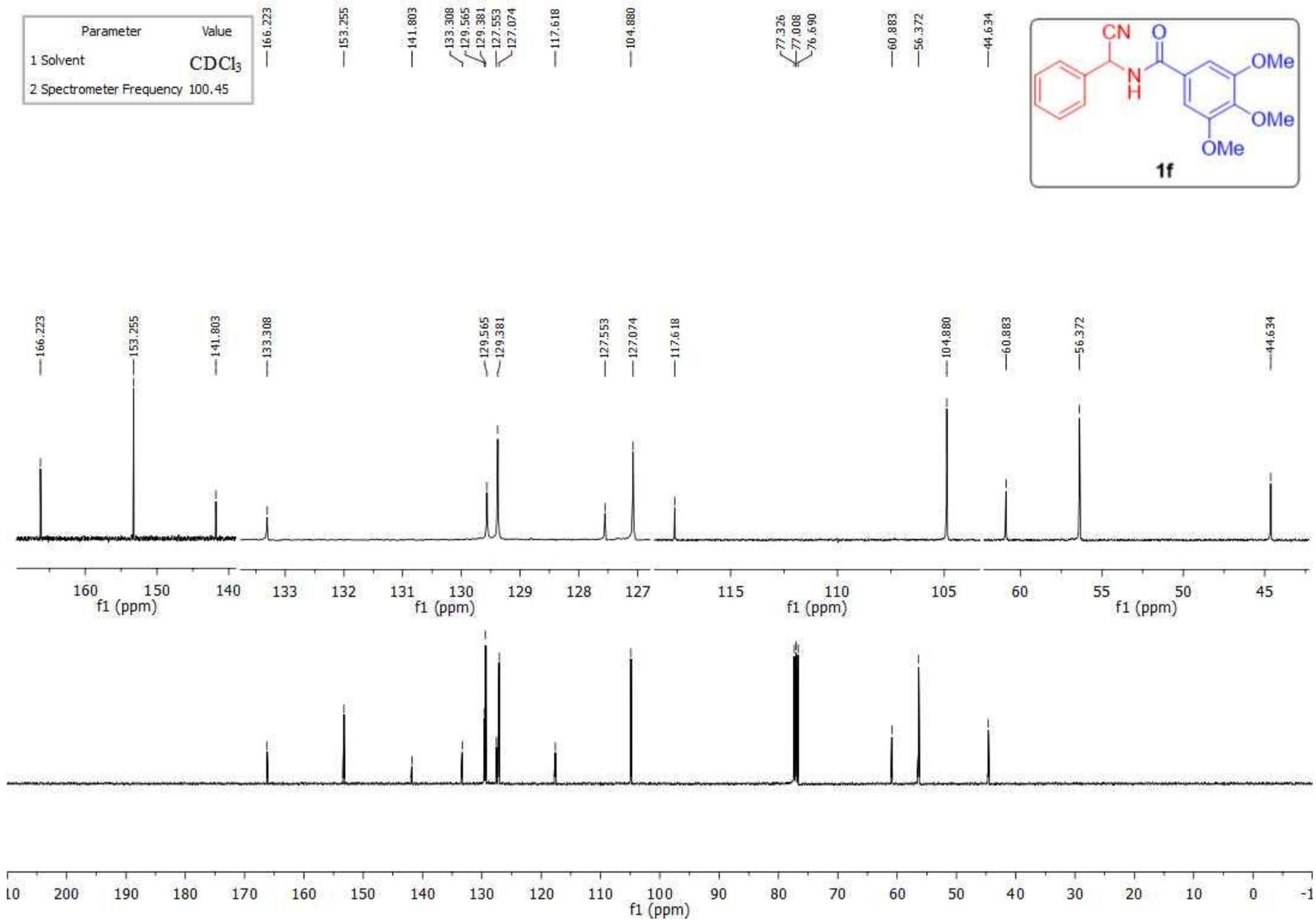


Fig. S19. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-3,4,5-trimethoxybenzamide (**1f**).

Sample Name	VG P2 33_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 33_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/7/2025 2:58:27 PM (UTC+05:30)

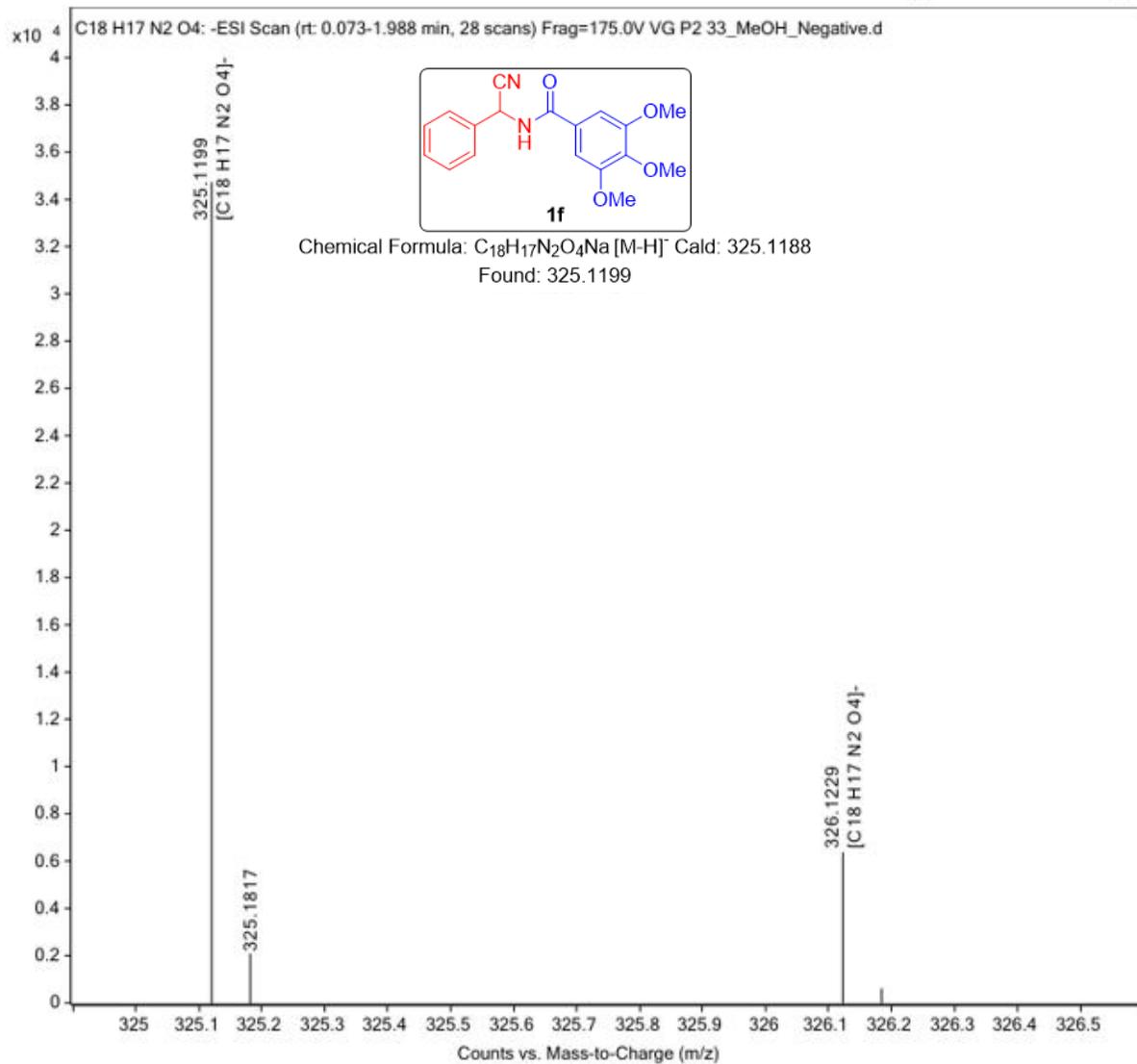


Fig. S20. HRMS data of *N*-(cyano(phenyl)methyl)-3,4,5-trimethoxybenzamide (**1f**).

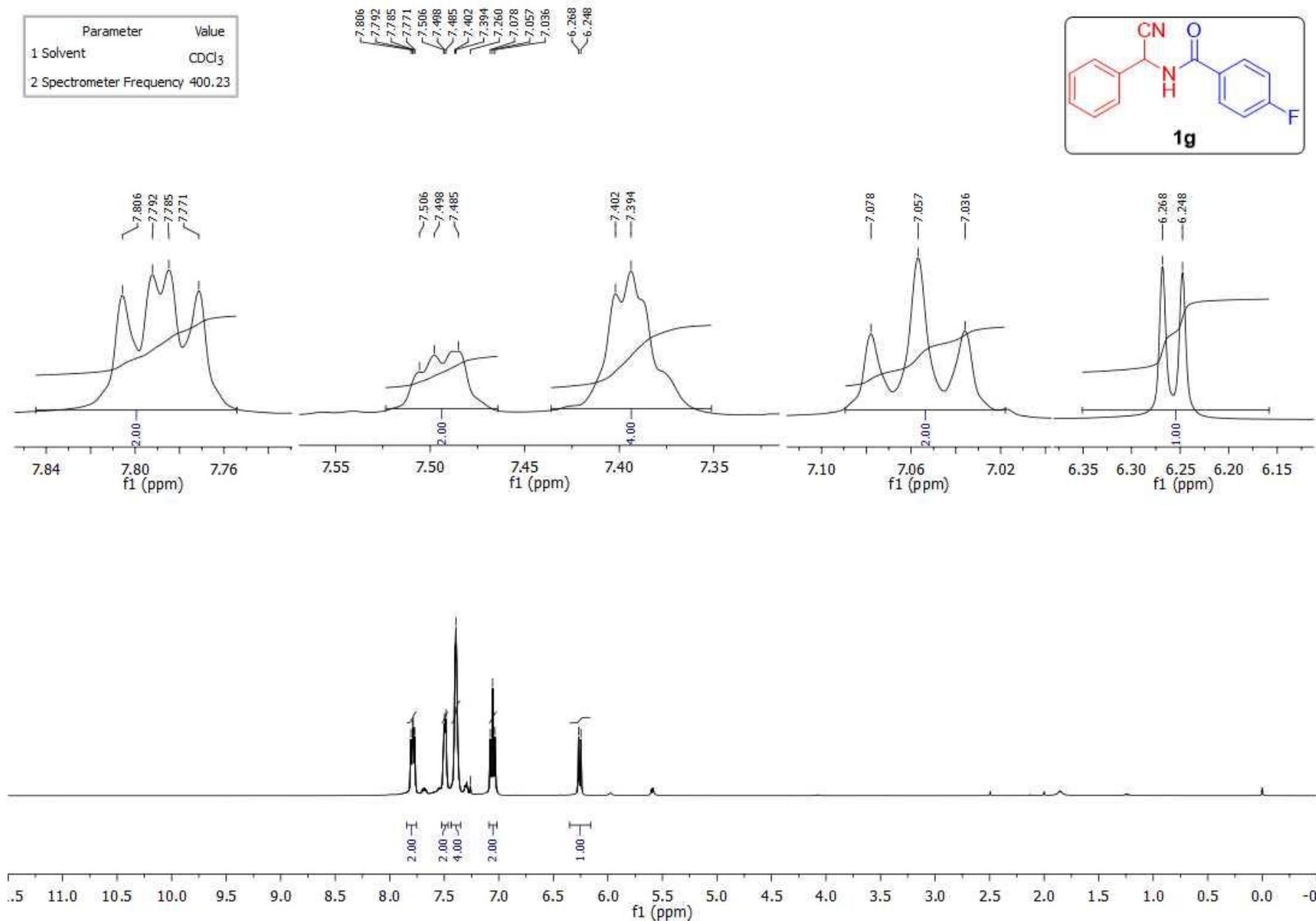


Fig. S21. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-4-fluorobenzamide (**1g**).

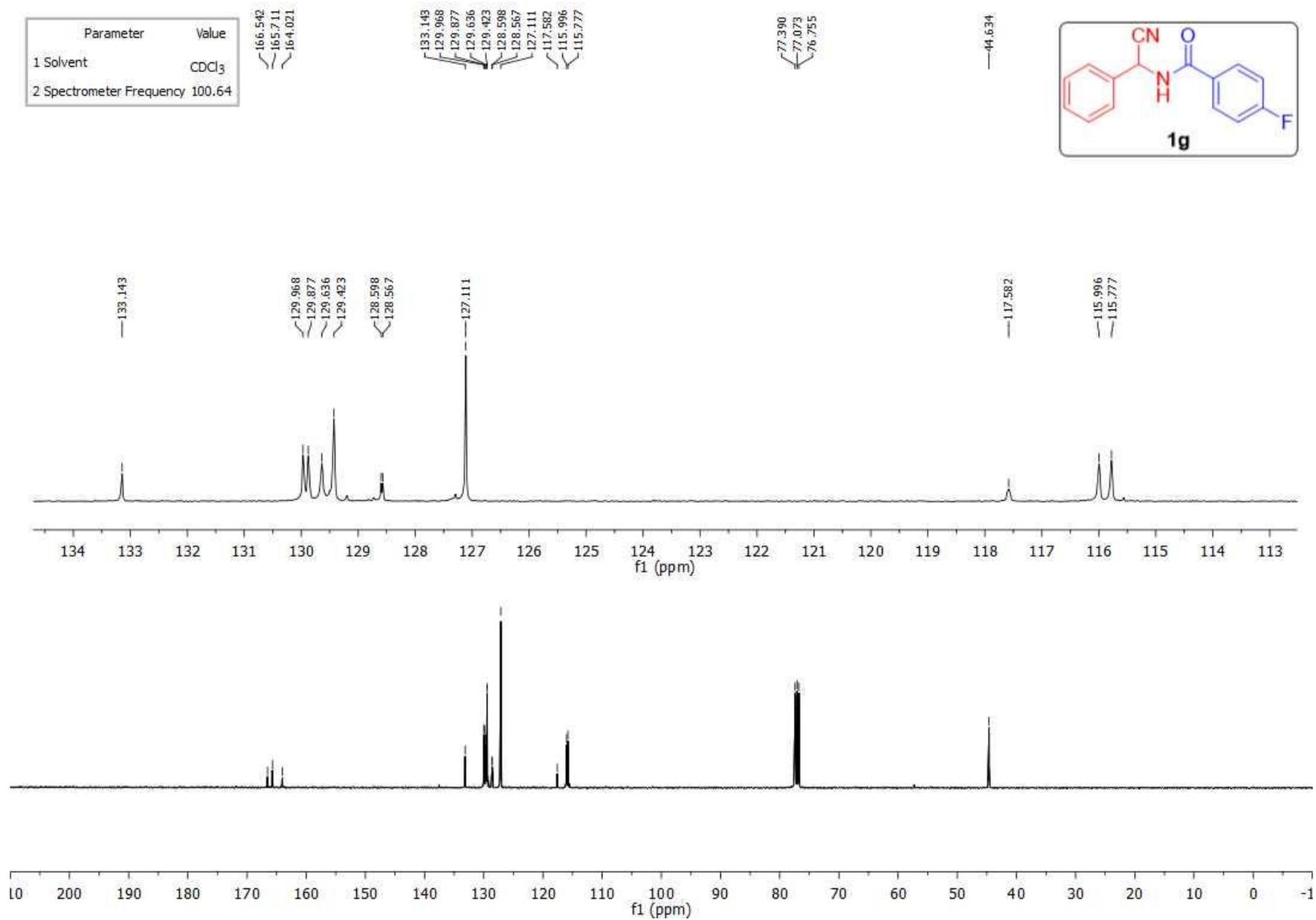


Fig. S22. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-4-fluorobenzamide (**1g**).

Parameter	Value
1 Solvent	CDCl ₃
2 Spectrometer Frequency	376.59

106.064

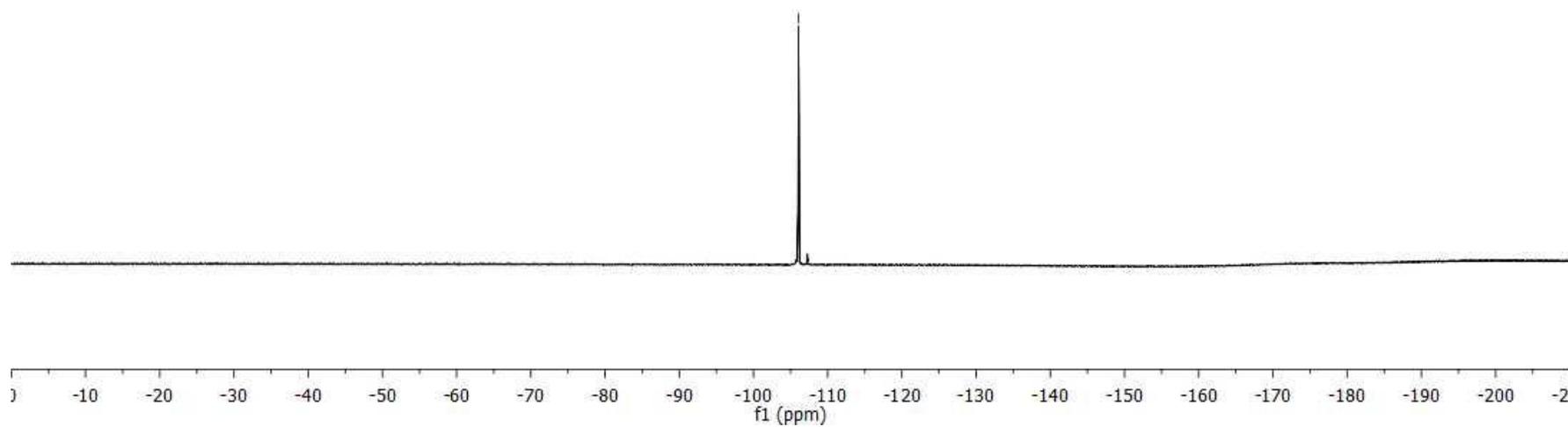
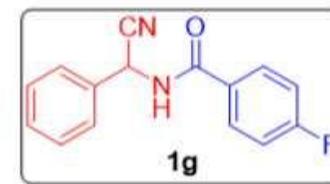
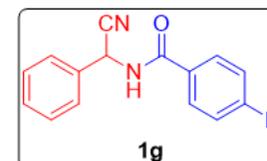


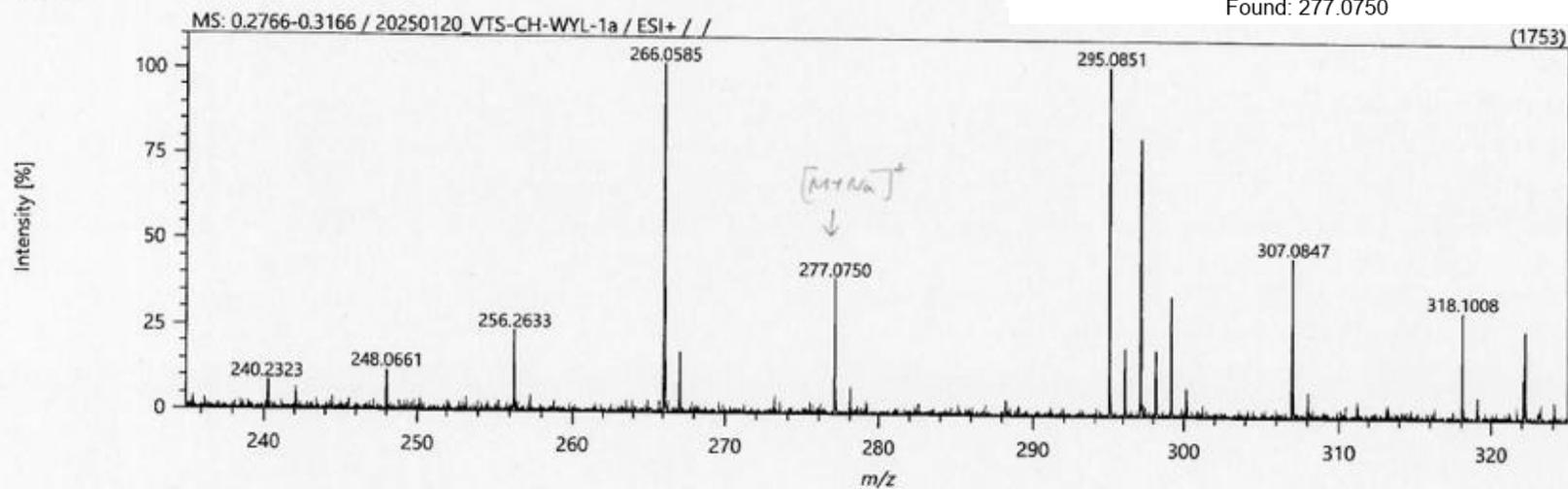
Fig. S23. ¹⁹F NMR spectra of *N*-(cyano(phenyl)methyl)-4-fluorobenzamide (**1g**).

VTS-CH-WYL-1a HR-ESI



Chemical Formula: $C_{15}H_{11}FN_2ONa$ $[M+Na]^+$ Calcd: 277.0753
Found: 277.0750

Spectrum



Elemental Composition

Parameters

Tolerance: ± 3.00 ppm

Electron: Odd/Even

Charge: +1

DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	F	Na
Min	0	0	1	2	1	0
Max	400	1000	1	2	1	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
277.07504	$C_{15}H_{11}N_2OFNa$	277.07476	0.28	1.00	10.5

Fig. S24. HRMS data of *N*-(cyano(phenyl)methyl)-4-fluorobenzamide (**1g**).

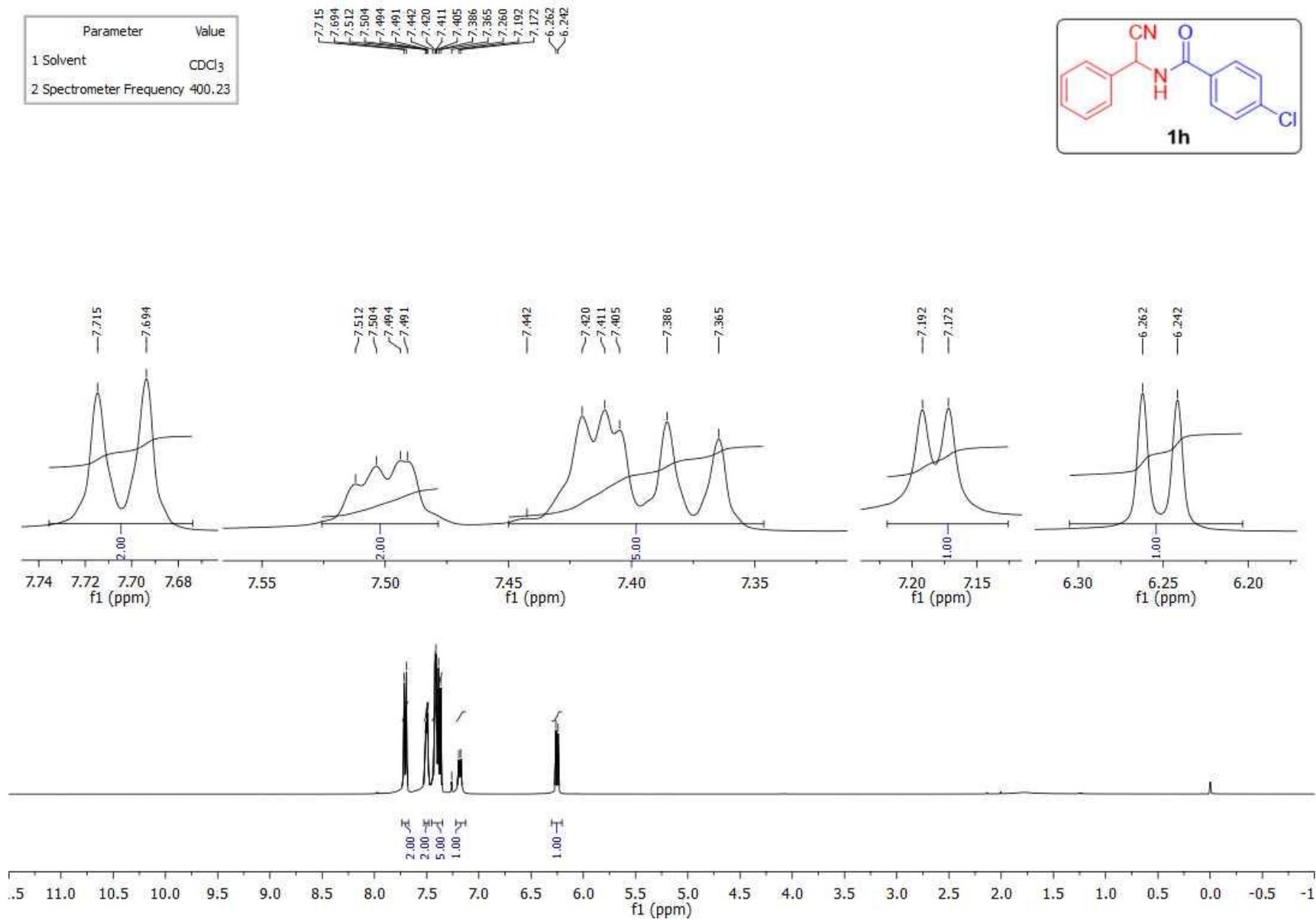


Fig. S25. ¹H NMR spectra of 4-chloro-*N*-(cyano(phenyl)methyl)benzamide (**1h**).

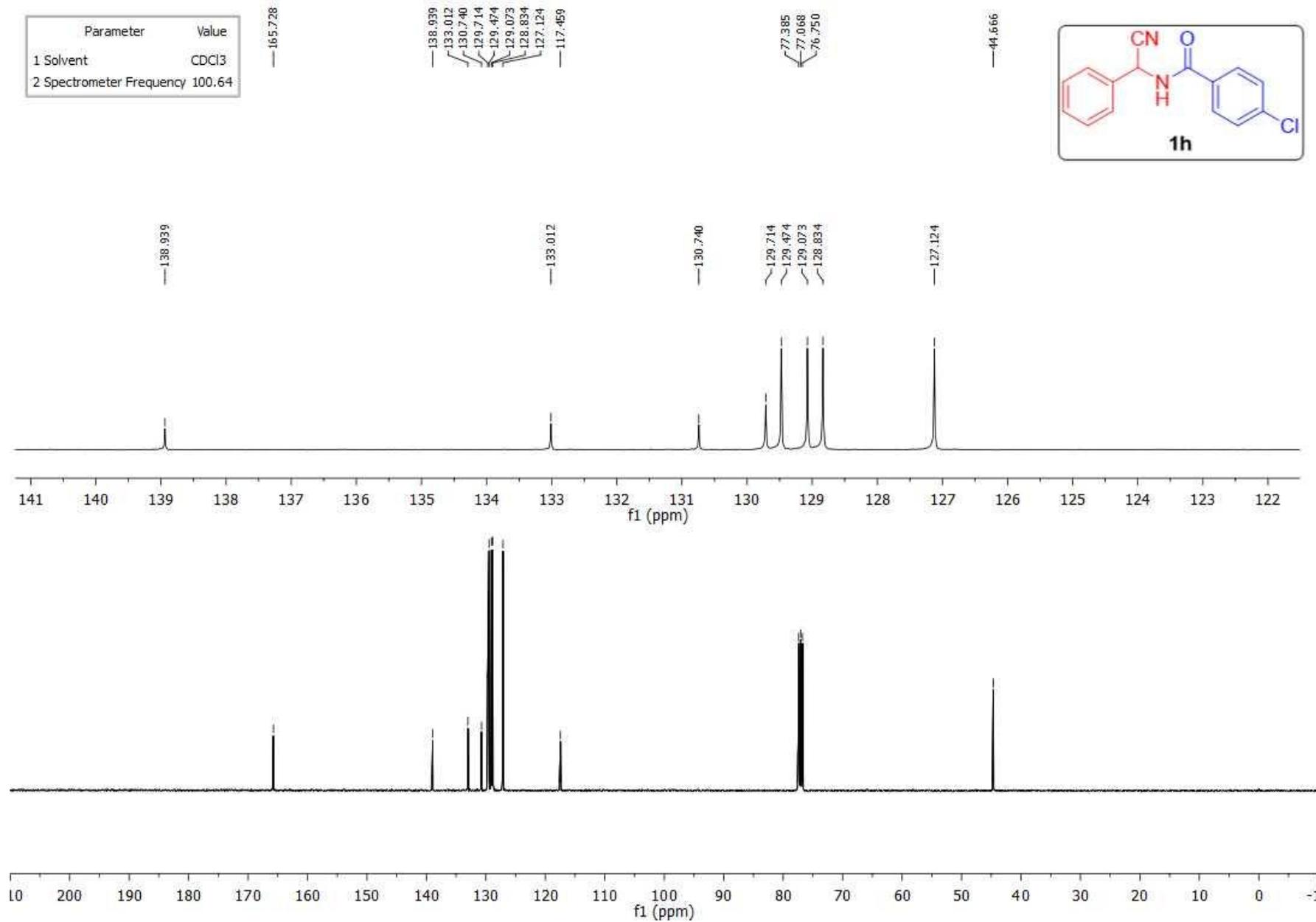
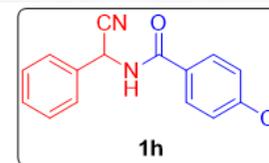


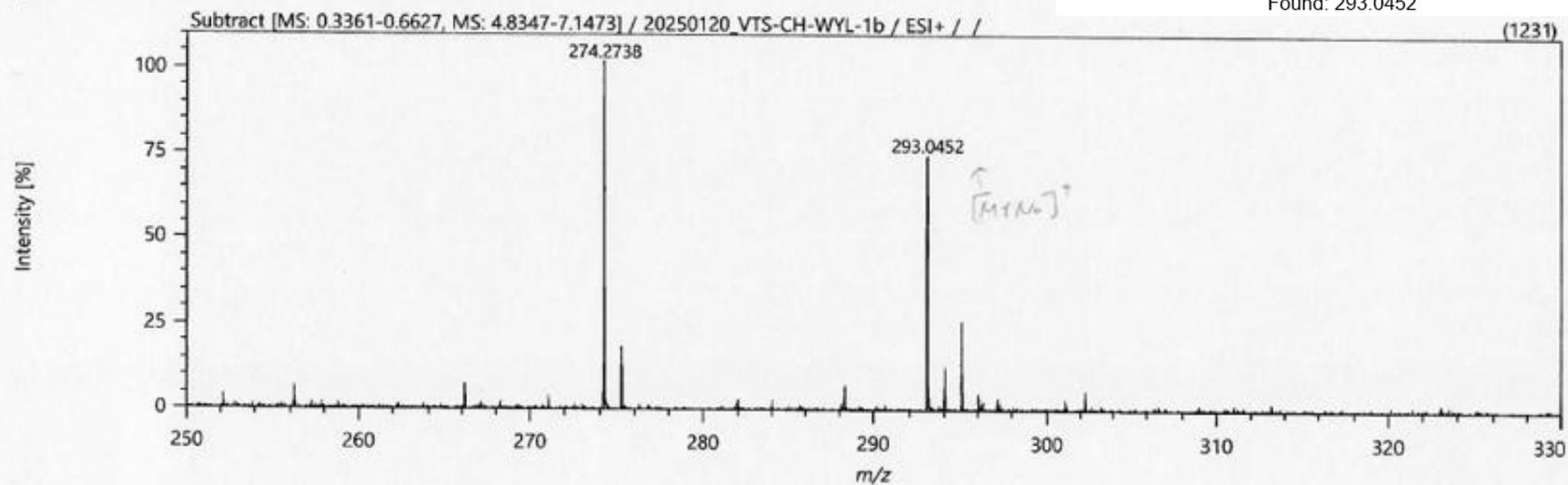
Fig. S26. ¹³C NMR spectra of 4-chloro-*N*-(cyano(phenyl)methyl)benzamide (**1h**).

VTS-CH-WYL-1b (HR-ESI)



Chemical Formula: C₁₅H₁₁ClN₂O₂Na [M+Na]⁺ Calcd: 293.0458
Found: 293.0452

Spectrum



Elemental Composition

Parameters

Tolerance: ±3.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Cl	Na
Min	0	0	1	2	1	0
Max	400	1000	1	2	1	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
293.04523	C ₁₅ H ₁₁ N ₂ O Na Cl	293.04521	0.02	0.07	10.5

Fig. S27. HRMS data of 4-chloro-*N*-(cyano(phenyl)methyl)benzamide (**1h**).

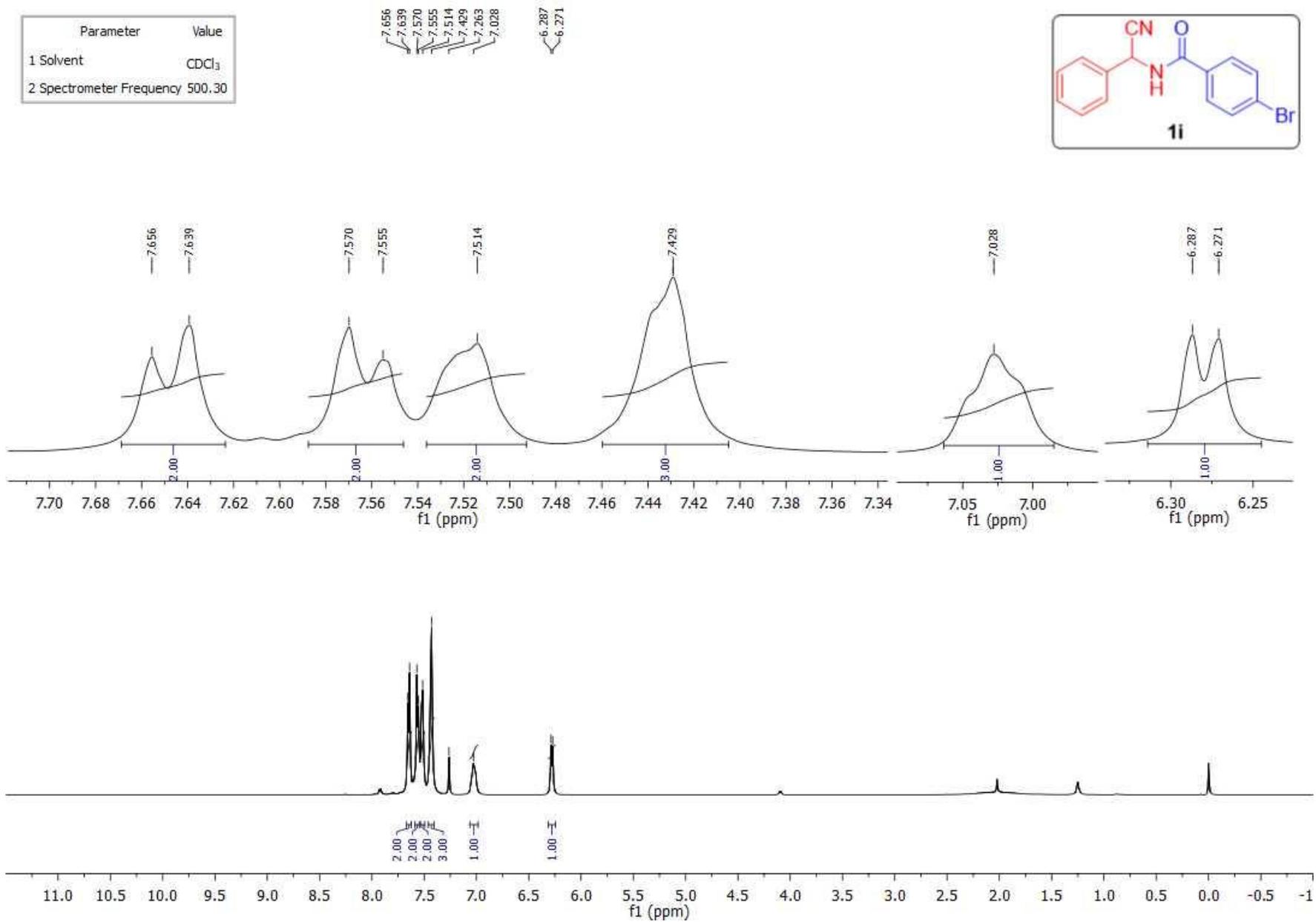


Fig. S28. ¹H NMR spectra of 4-bromo-*N*-(cyano(phenyl)methyl)benzamide (**1i**).

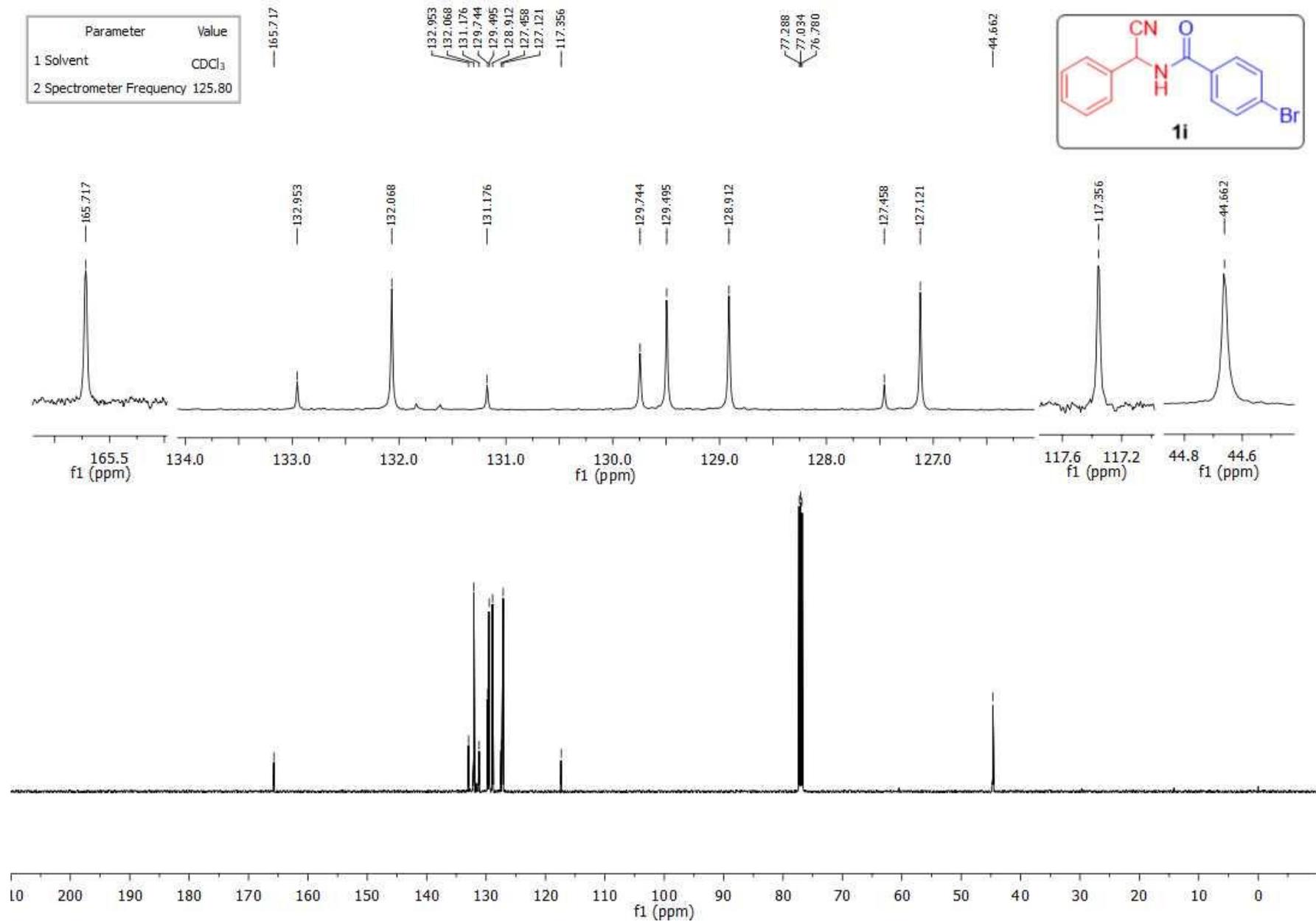
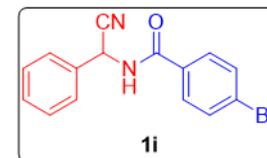


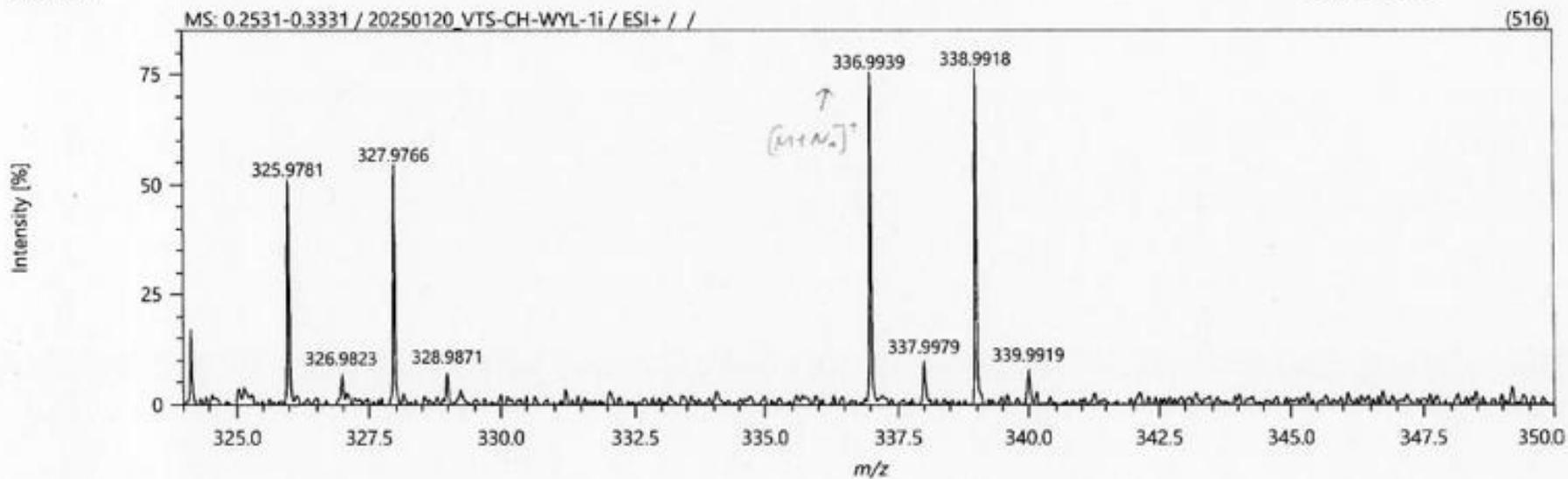
Fig. S29. ¹³C NMR spectra of 4-bromo-*N*-(cyano(phenyl)methyl)benzamide (**1i**).

VTS-CH-WYL-1i (HR-ESI)



Chemical Formula: C₁₅H₁₁BrN₂O_{Na} [M+Na]⁺ Calcd: 336.9952
Found: 336.9939

Spectrum



Elemental Composition

Parameters

Tolerance: ±5.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na	Br
Min	0	0	1	2	0	1
Max	400	1000	1	2	1	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
336.99386	C ₁₅ H ₁₁ N ₂ O Na Br	336.99470	-0.83	-2.47	10.5

Fig. S30. HRMS data of 4-bromo-*N*-(cyano(phenyl)methyl)benzamide (**1i**).

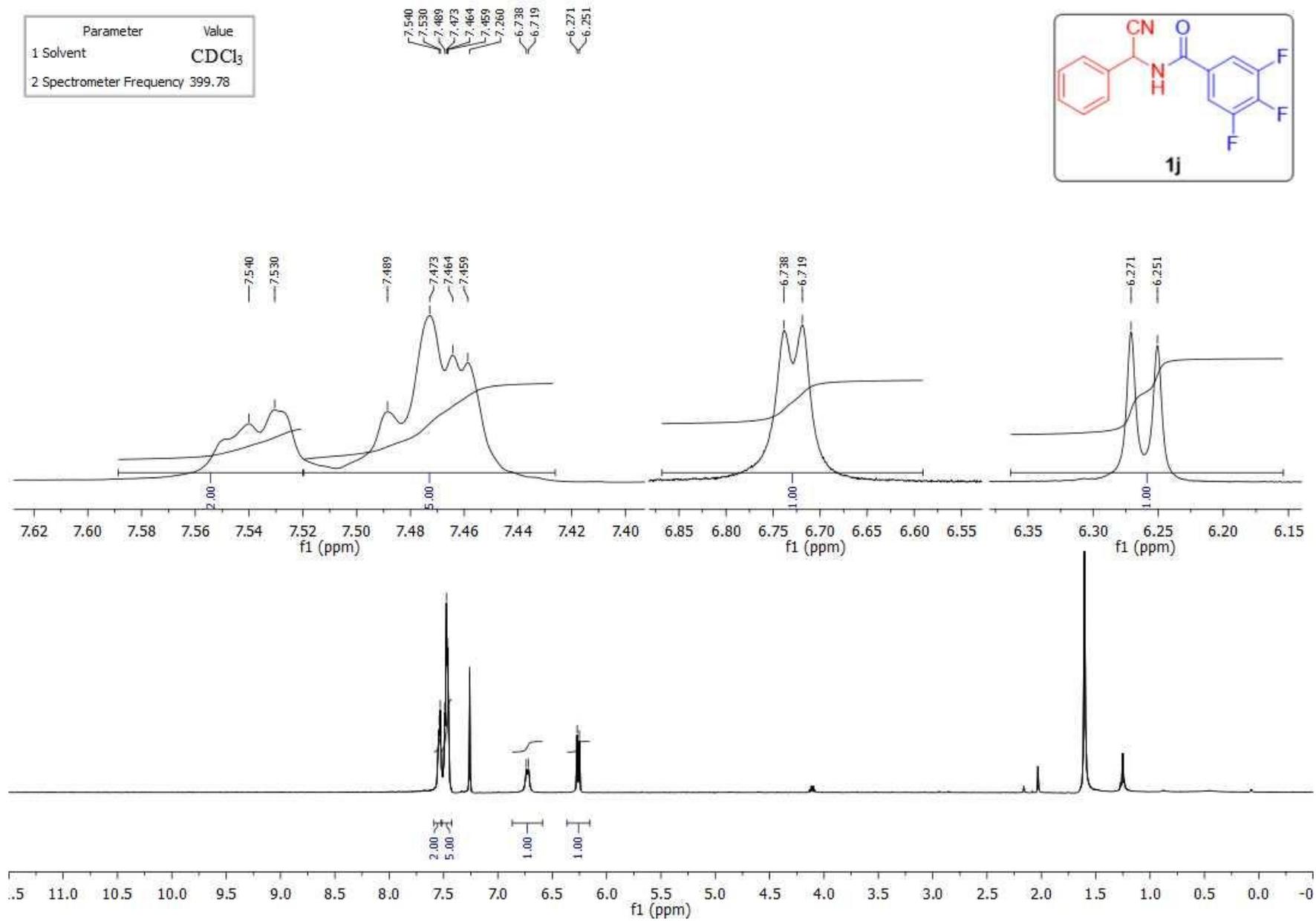


Fig. S31. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-3,4,5-trifluorobenzamide (**1j**).

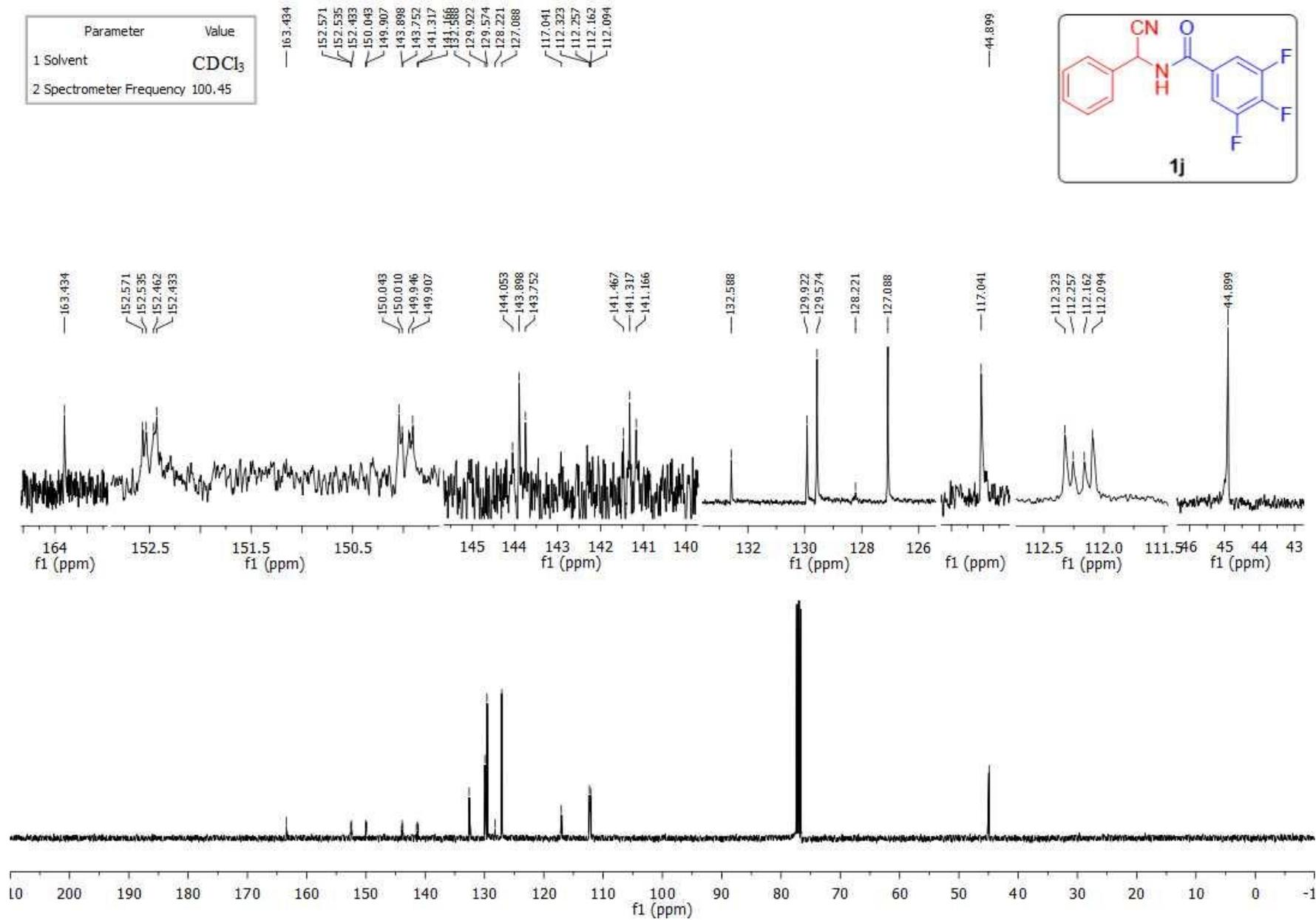


Fig. S32. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-3,4,5-trifluorobenzamide (**1j**).

Parameter	Value
1 Solvent	CDCl ₃
2 Spectrometer Frequency	376.17

131.165
131.230

152.667
152.730
152.793

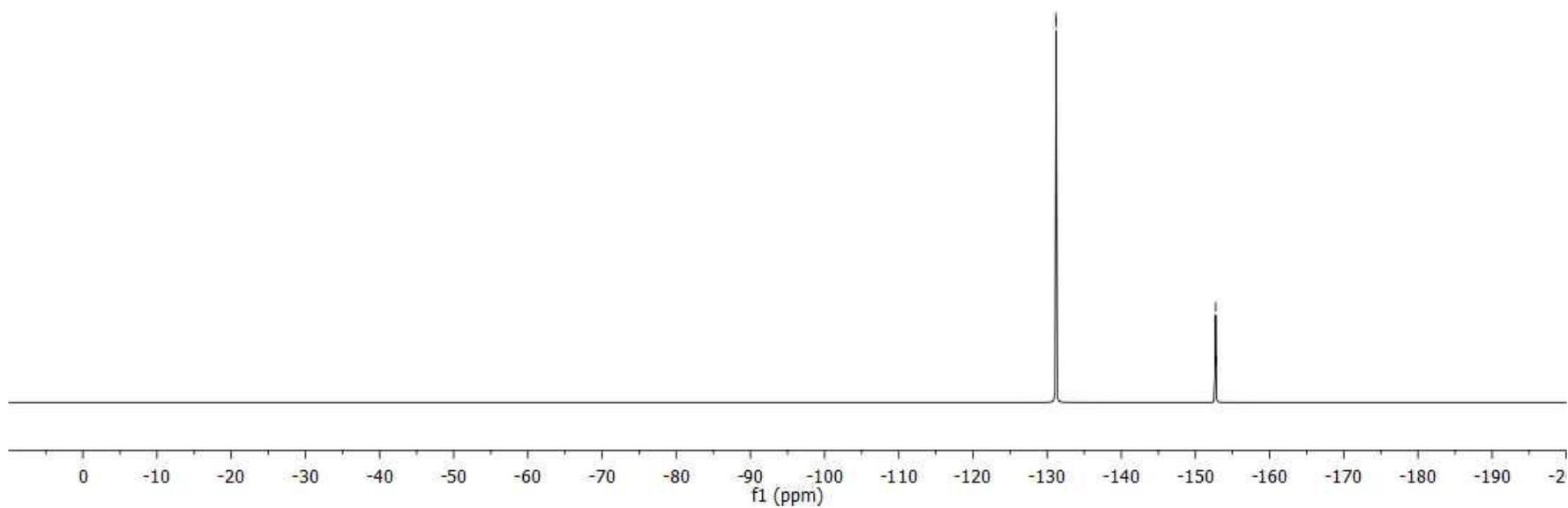
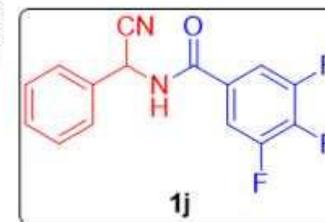


Fig. S33. ¹⁹F NMR spectra of *N*-(cyano(phenyl)methyl)-3,4,5-trifluorobenzamide (**1j**).

Sample Name	VG P2 38_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 38_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/8/2025 11:47:37 AM (UTC+05:30)

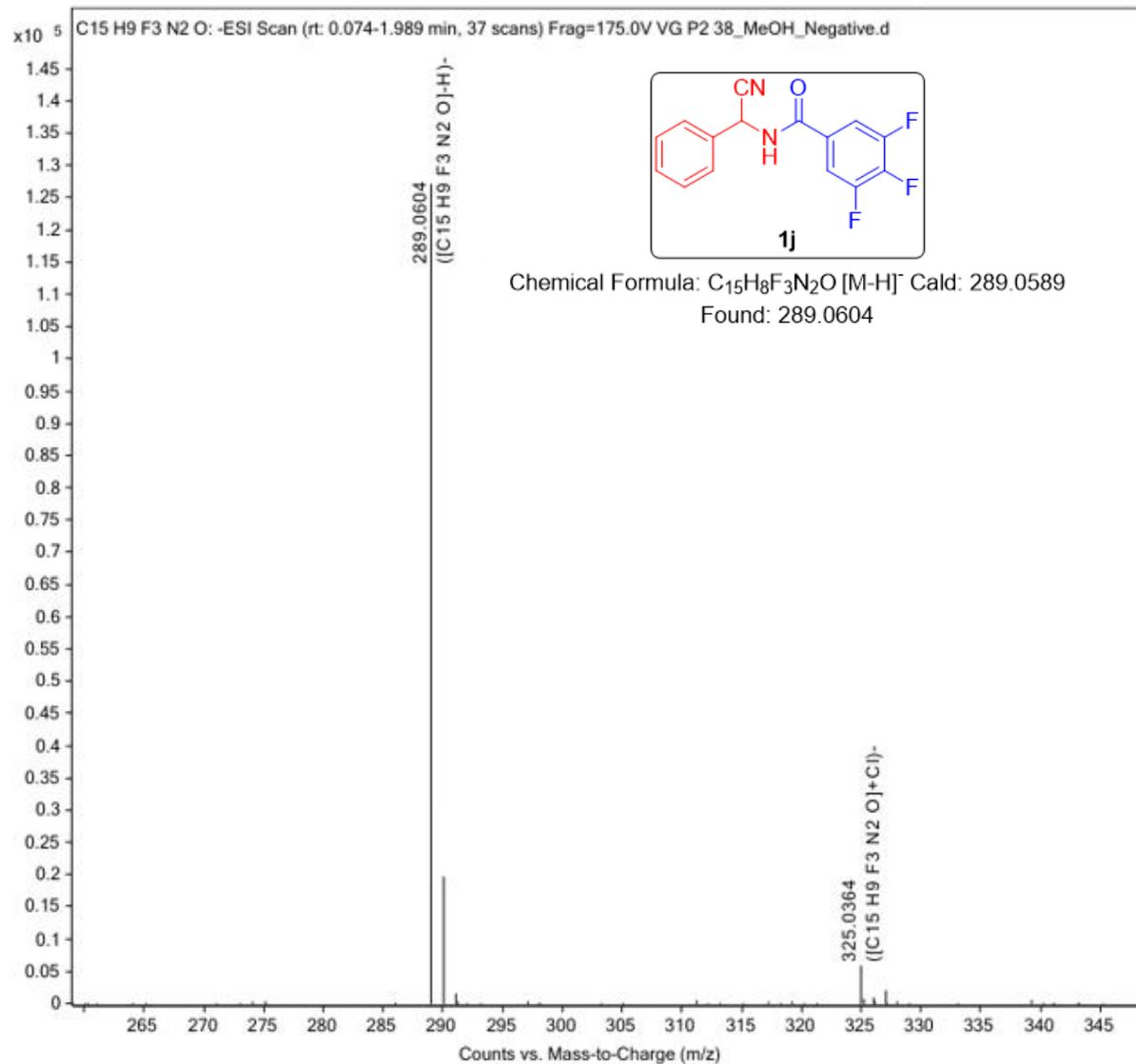


Fig. S34. HRMS data of *N*-(cyano(phenyl)methyl)-3,4,5-trifluorobenzamide (**1j**).

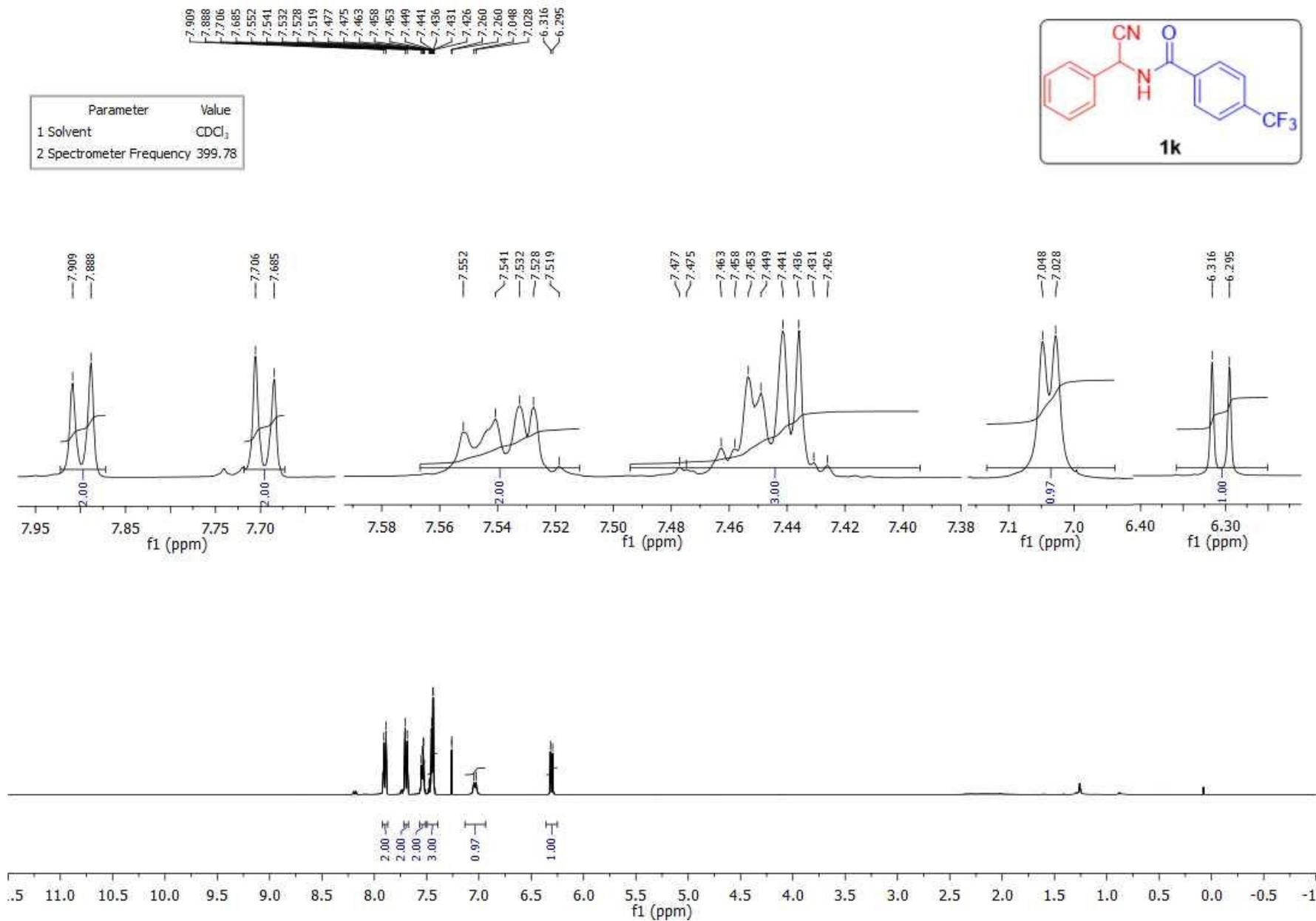


Fig. S35. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-4-(trifluoromethyl)benzamide (**1k**).

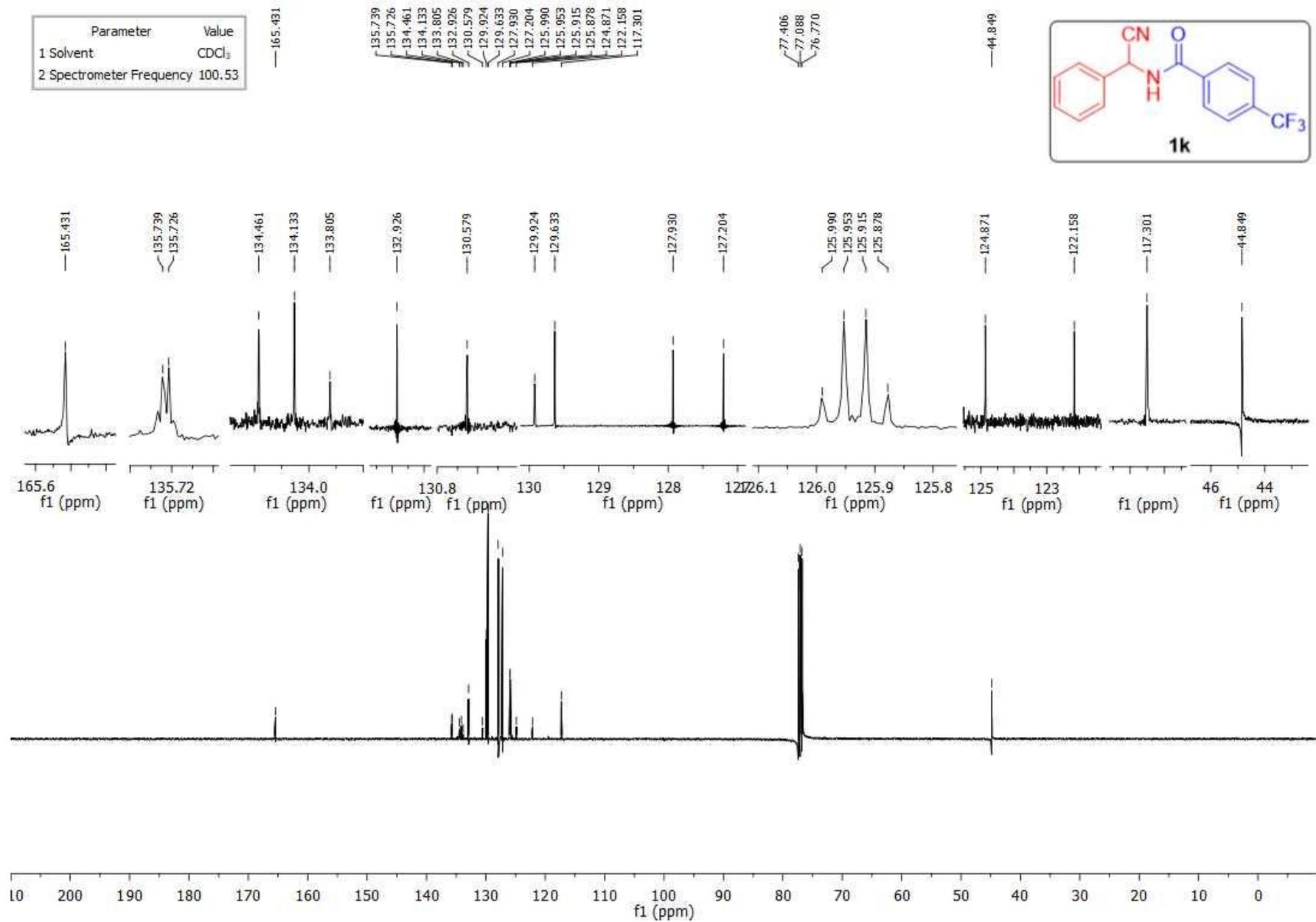


Fig. S36. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-4-(trifluoromethyl)benzamide (**1k**).

Parameter	Value
1 Solvent	CDCl ₃
2 Spectrometer Frequency	376.17

-63.014

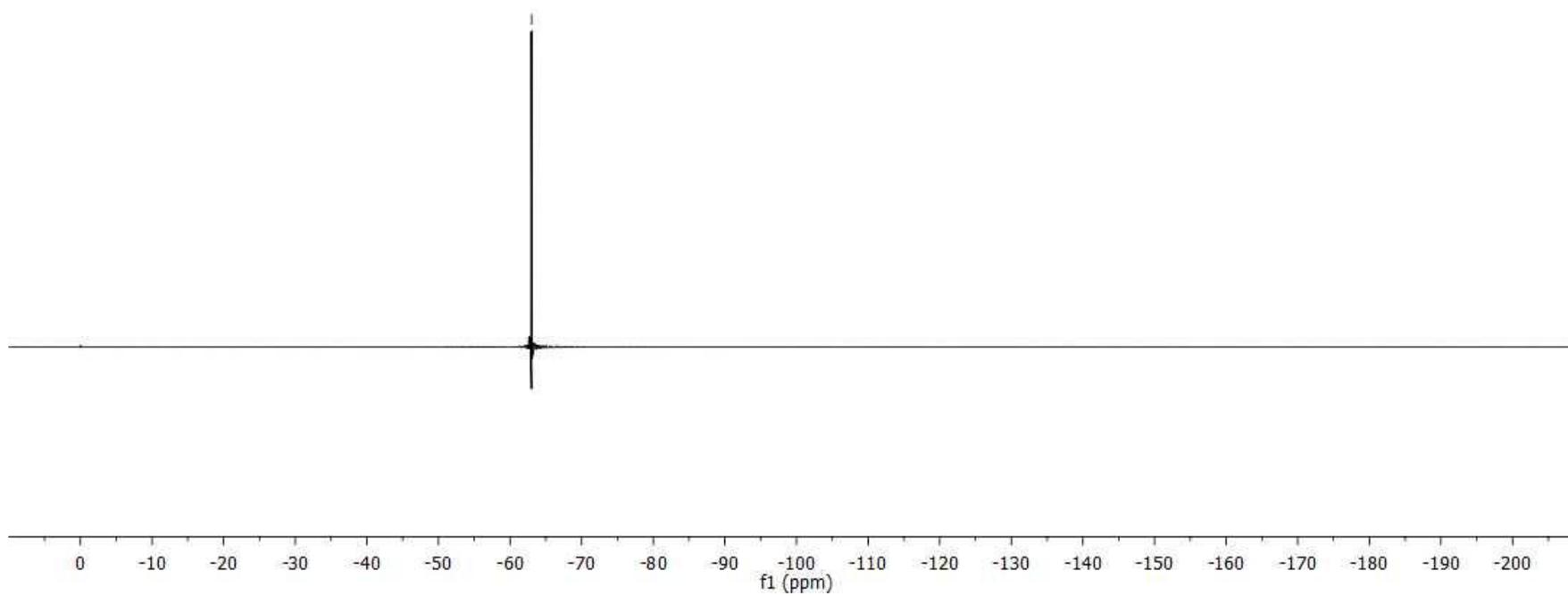
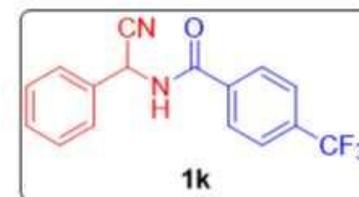


Fig. S37. ¹⁹F NMR spectra of *N*-(cyano(phenyl)methyl)-4-(trifluoromethyl)benzamide (**1k**).

Sample Name	VG P2 39_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 39_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/8/2025 3:01:11 PM (UTC+05:30)

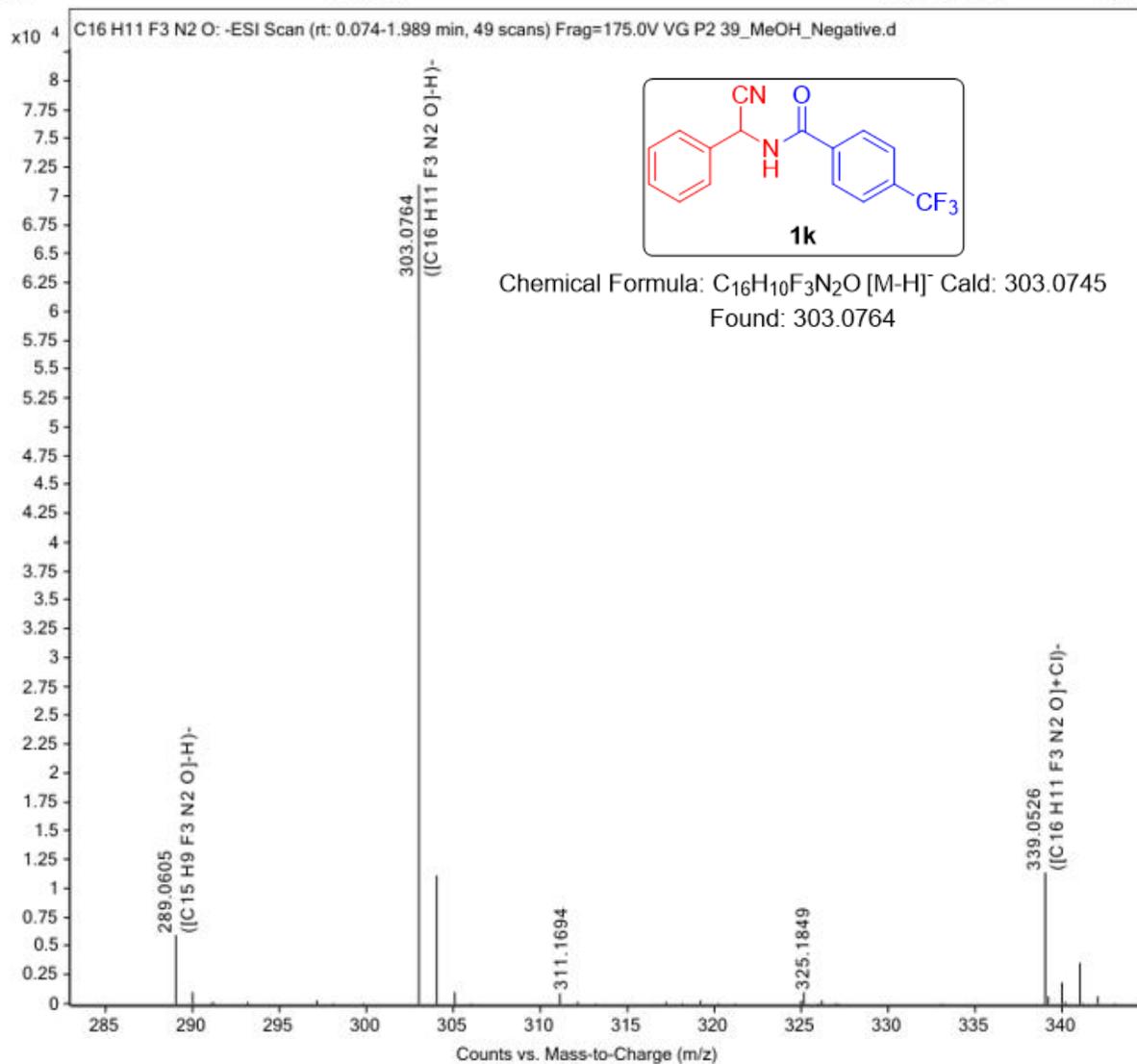


Fig. S38. HRMS data of *N*-(cyano(phenyl)methyl)-4-(trifluoromethyl)benzamide (**1k**).

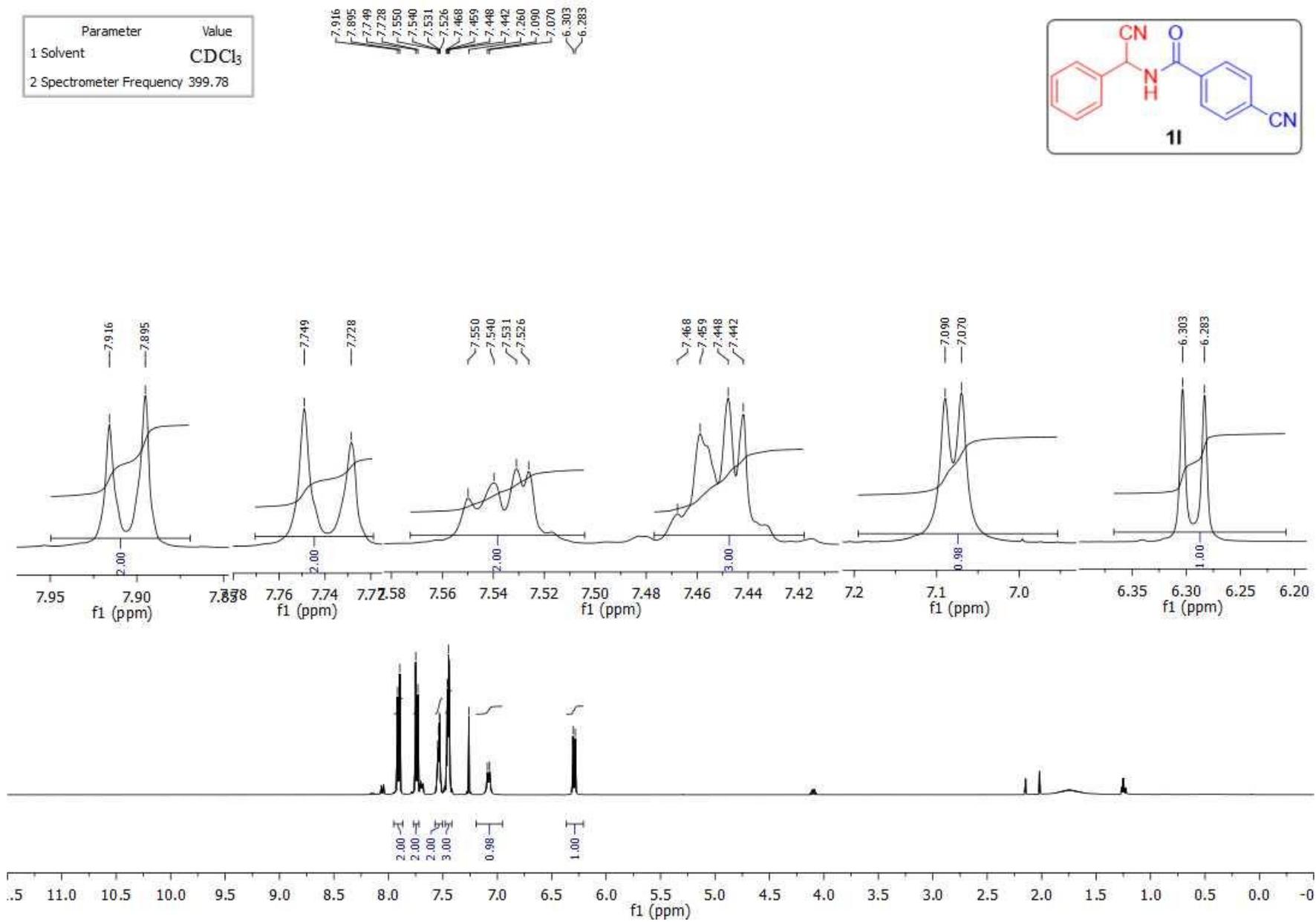


Fig. S39. ¹H NMR spectra of 4-cyano-*N*-(cyano(phenyl)methyl)benzamide (**11**).

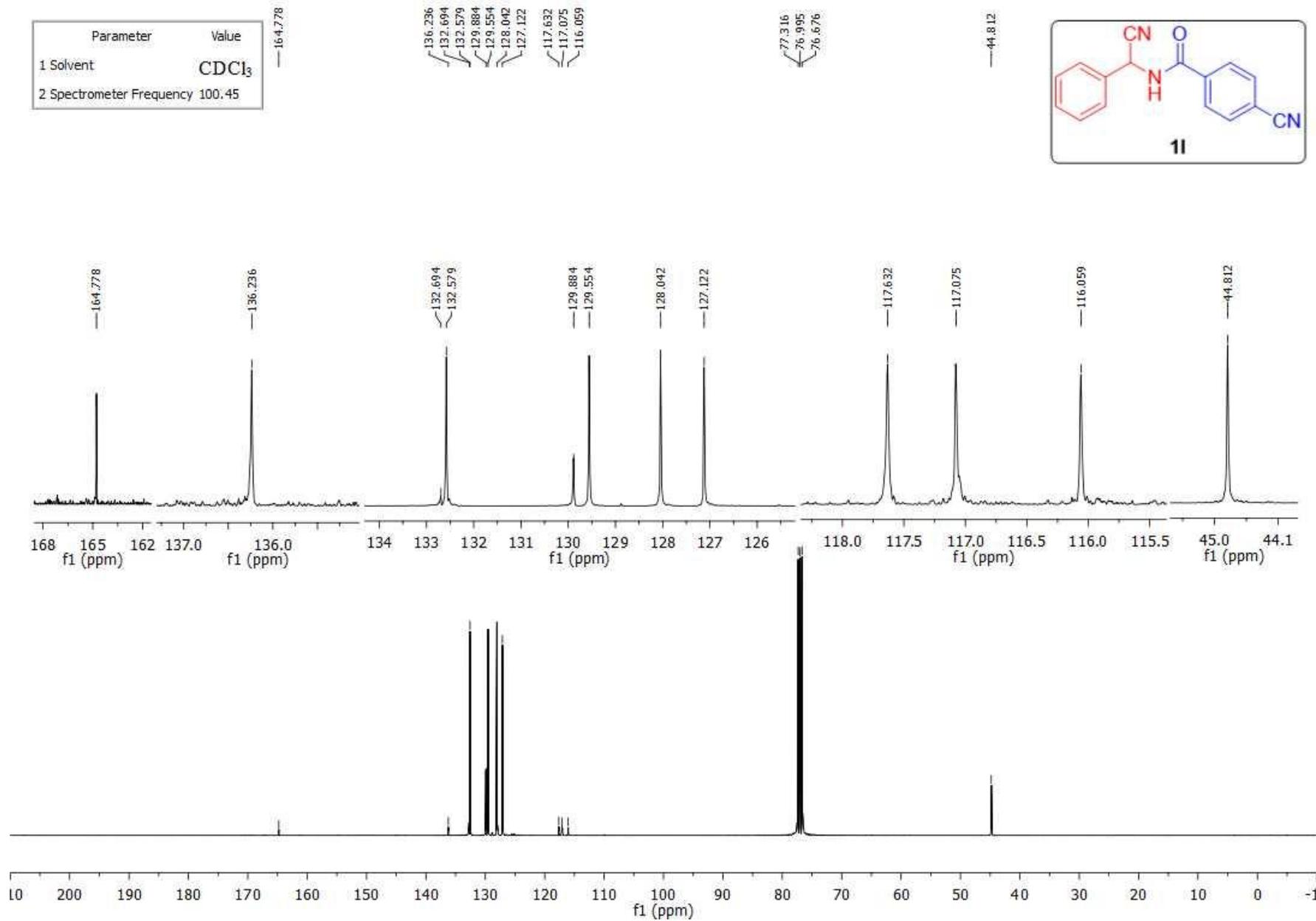


Fig. S40. ¹³C NMR spectra of 4-cyano-*N*-(cyano(phenyl)methyl)benzamide (**11**).

Sample Name	VG P2 40_MeOH_Positive	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 40_MeOH_Positive.d
ACQ Method	TEST.m	Comment		Acquired Time	10/8/2025 3:46:14 PM (UTC+05:30)

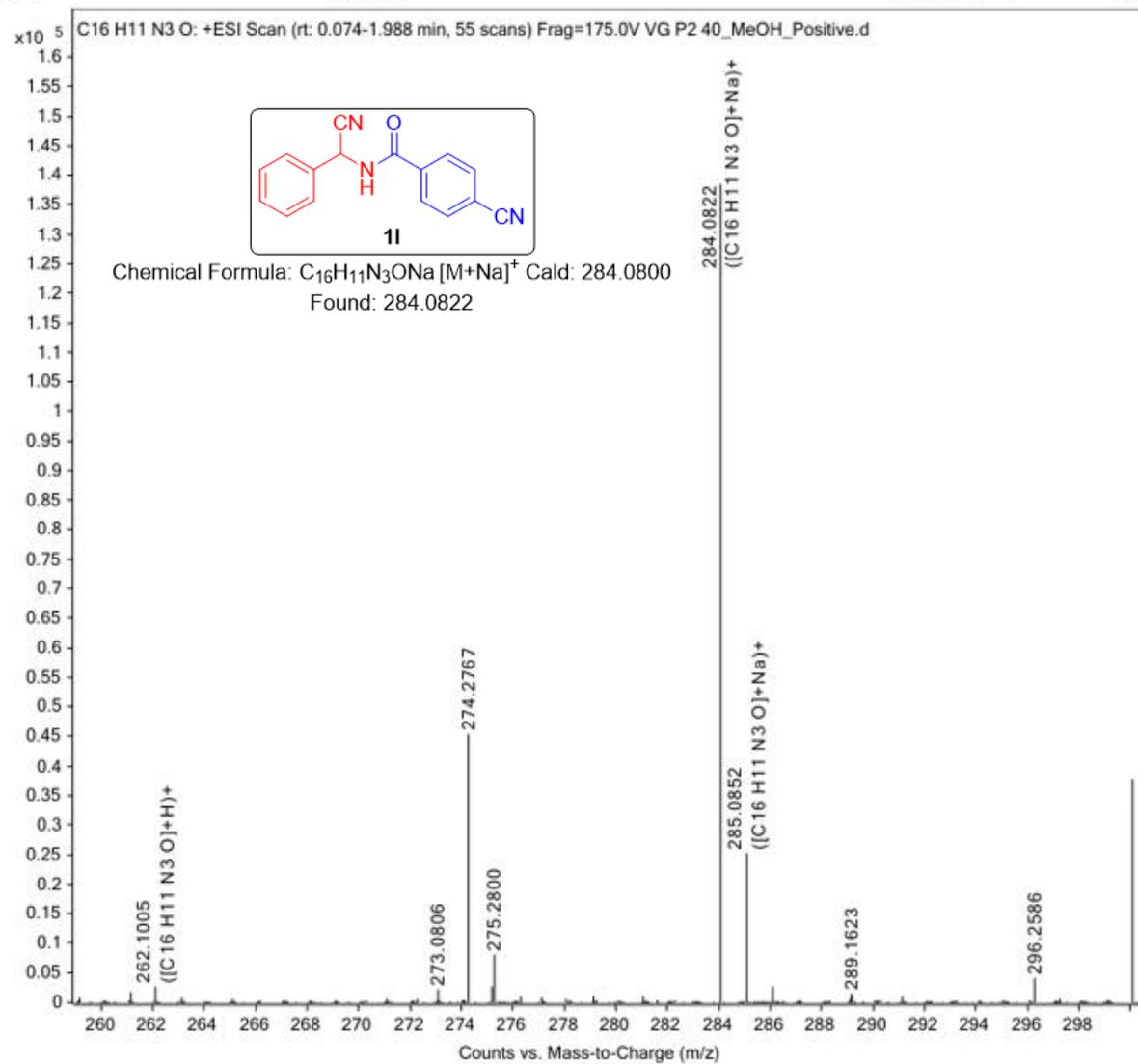


Fig. S41. HRMS data of 4-cyano-*N*-(cyano(phenyl)methyl)benzamide (**11**).

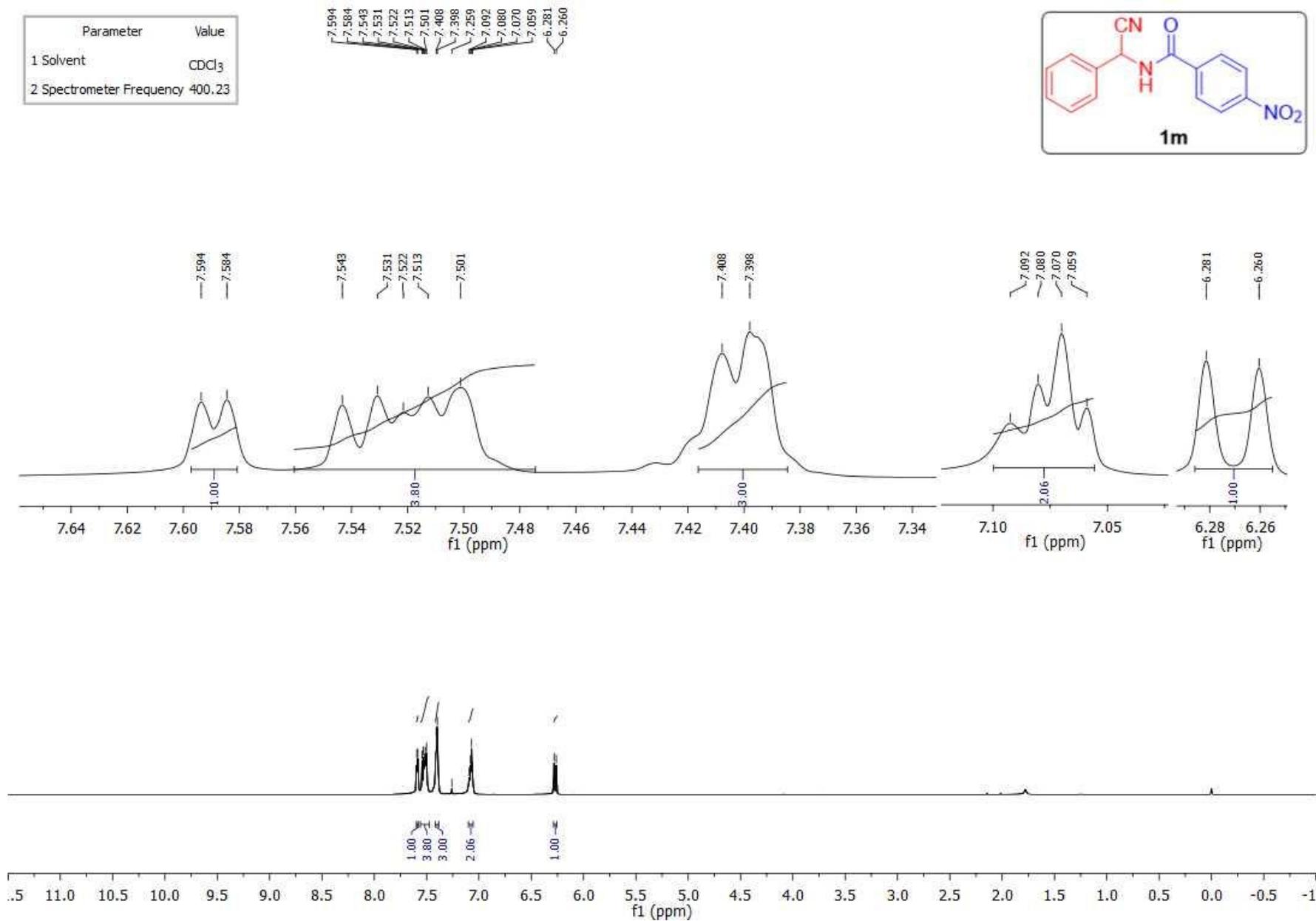


Fig. S42. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-4-nitrobenzamide (**1m**).

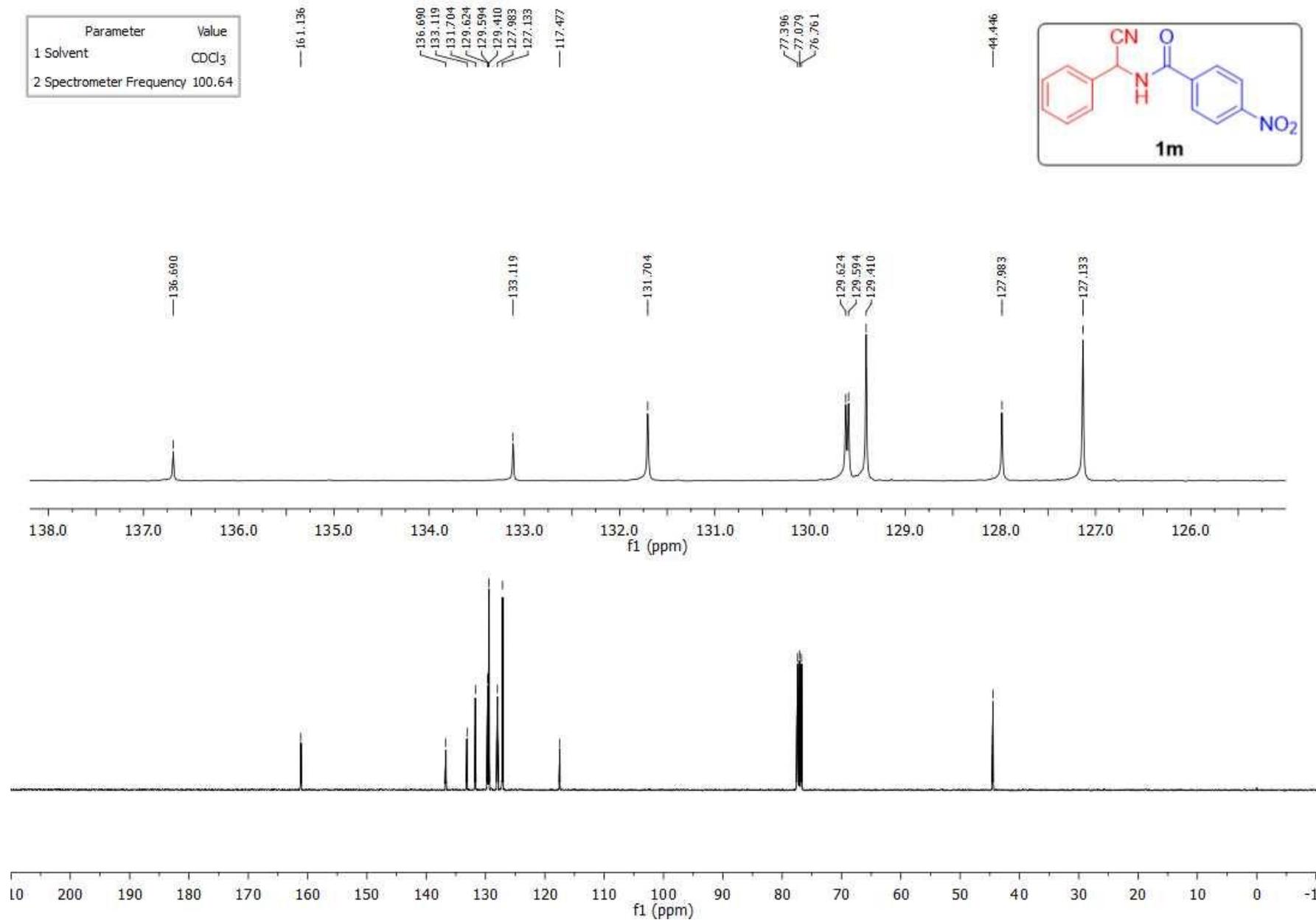
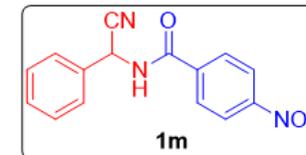


Fig. S43. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-4-nitrobenzamide (**1m**).

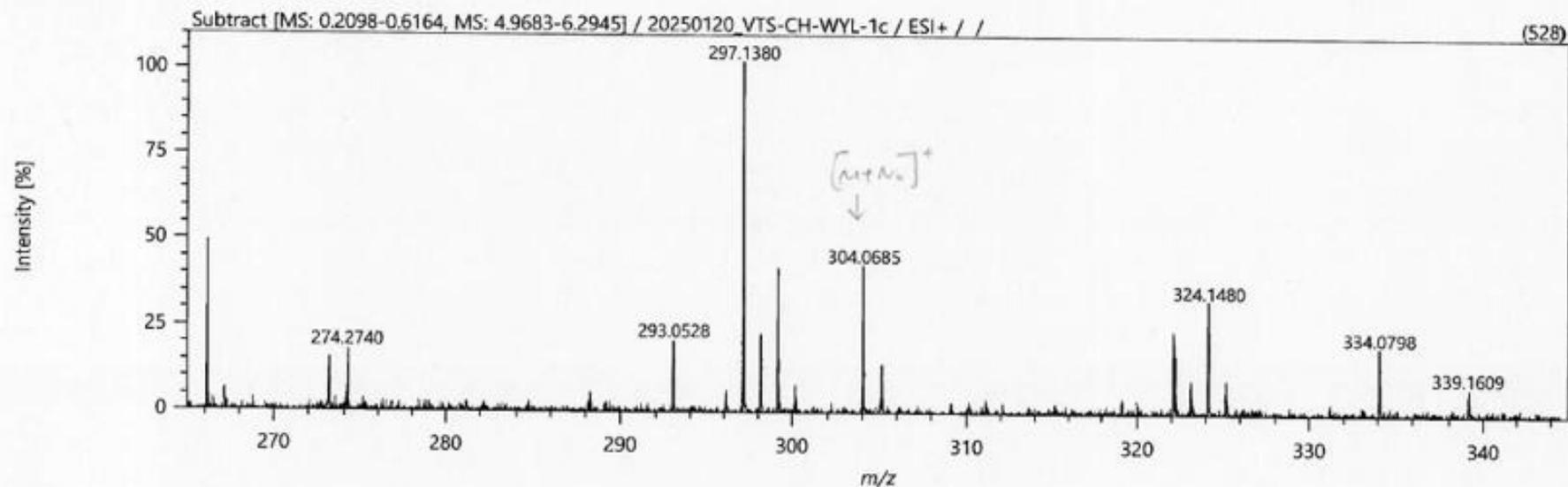
VTS-CH-WYL-1c (HR-ESI)



Chemical Formula: $C_{15}H_{11}N_3O_3Na$ $[M+Na]^+$ Calcd: 304.0698

Found: 304.0685

Spectrum



Elemental Composition

Parameters

Tolerance: ± 3.00 ppm

Electron: Odd/Even

Charge: +1

DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	3	3	0
Max	400	1000	3	3	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
304.06853	$C_{15}H_{11}N_3O_3Na$	304.06926	-0.74	-2.42	11.5

Fig. S44. HRMS data of *N*-(cyano(phenyl)methyl)-4-nitrobenzamide (**1m**).

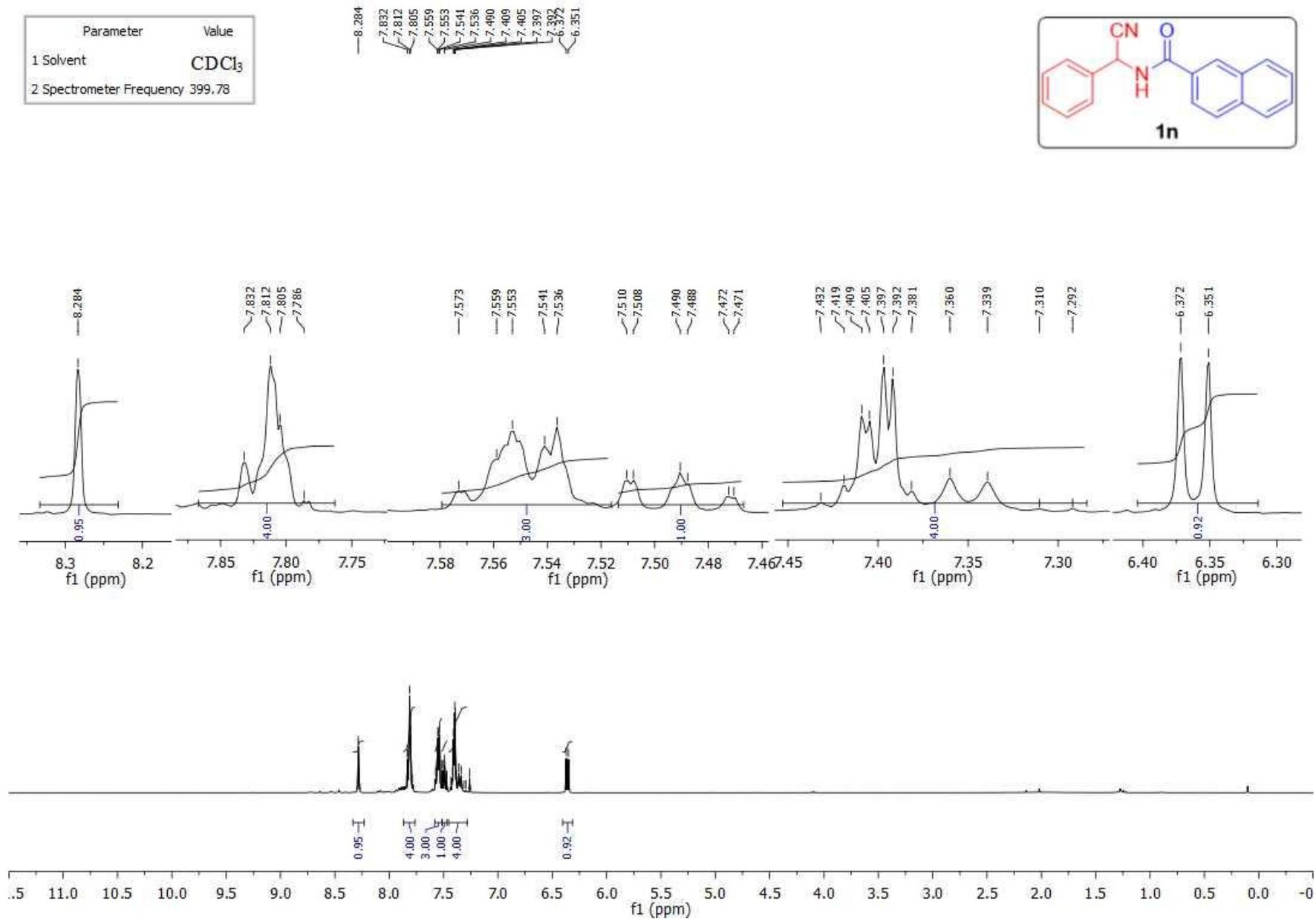


Fig. S45. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-2-naphthamide (**1n**).

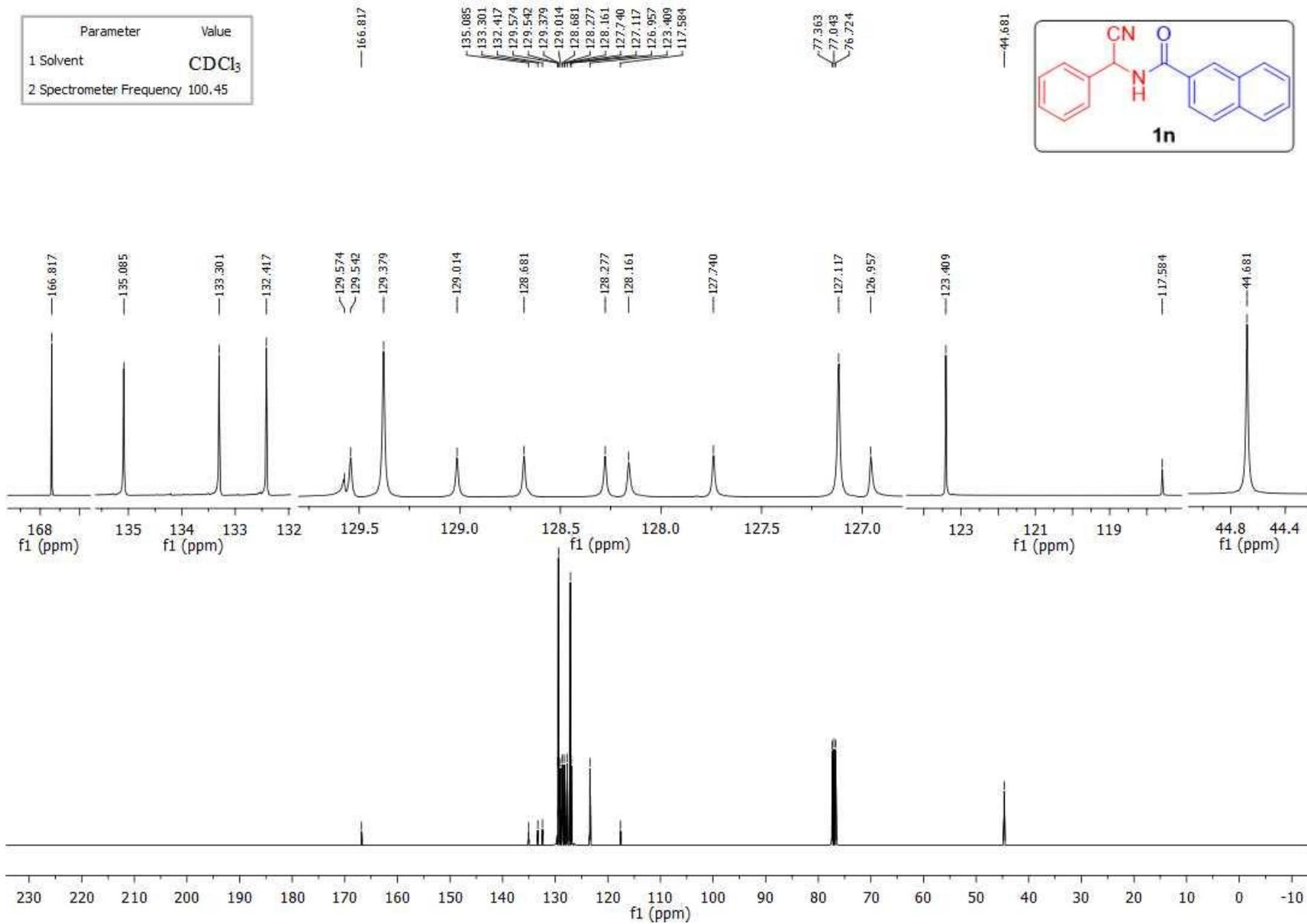


Fig. S46. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-2-naphthamide (**1n**).

Sample Name	VG P2 32_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 32_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/7/2025 11:52:29 AM (UTC+05:30)

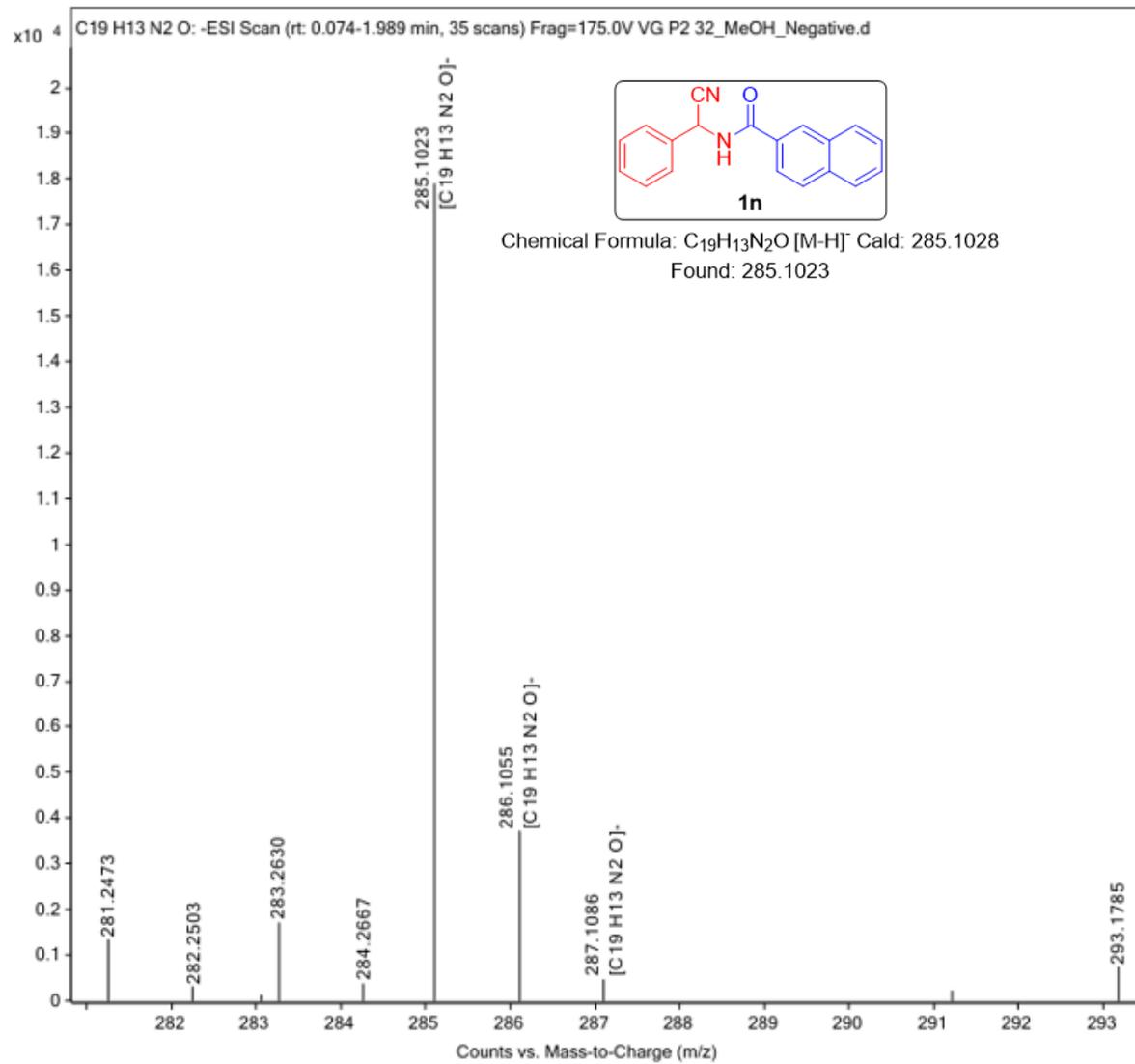


Fig. S47. HRMS data of *N*-(cyano(phenyl)methyl)-2-naphthamide (**1n**).

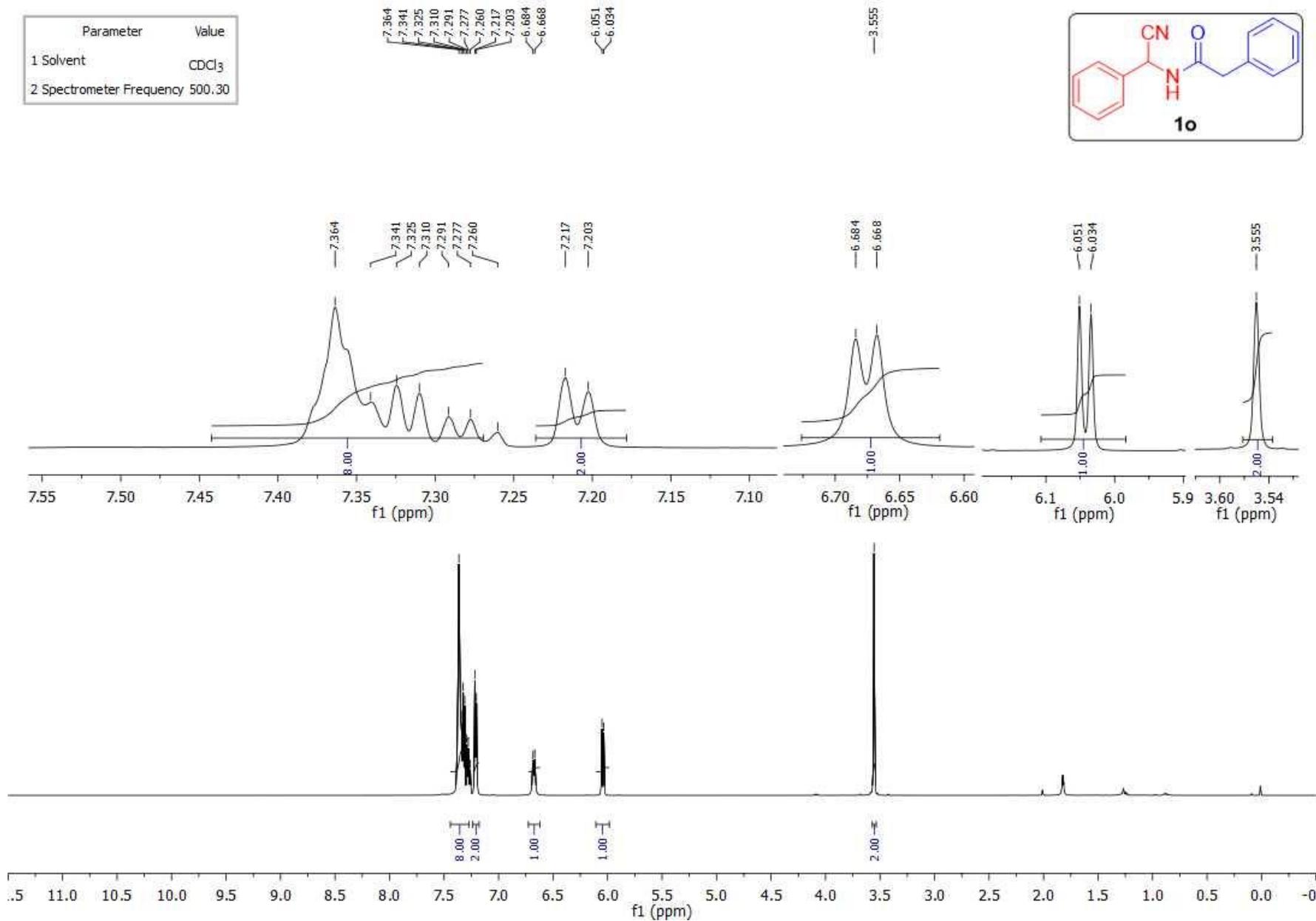


Fig. S48. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-2-phenylacetamide (**1o**).

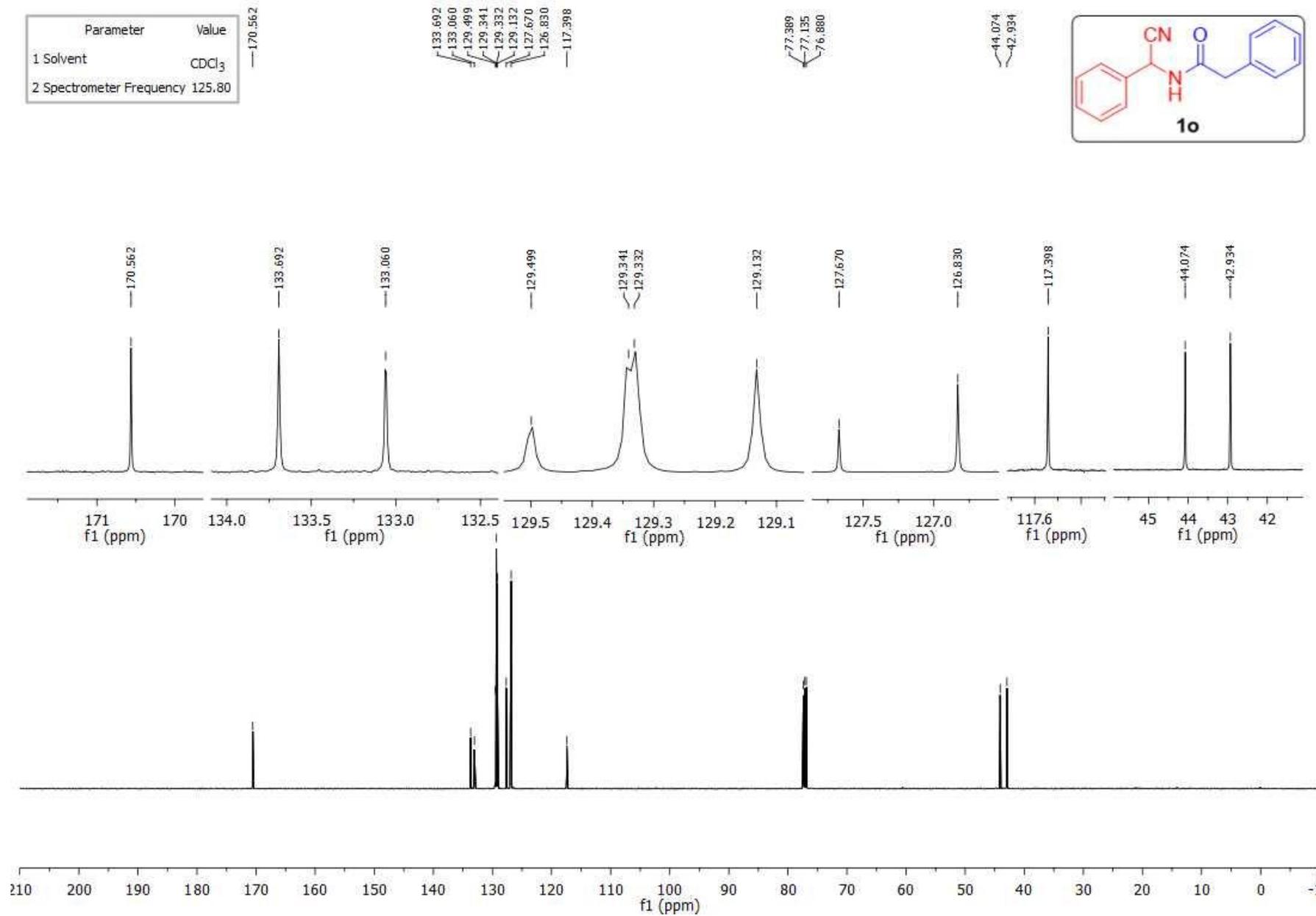


Fig. S49. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-2-phenylacetamide (**1o**).

Sample Name	VG P2 42_MeOH_Positive	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 42_MeOH_Positive.d
ACQ Method	TEST.m	Comment		Acquired Time	10/9/2025 11:43:04 AM (UTC+05:30)

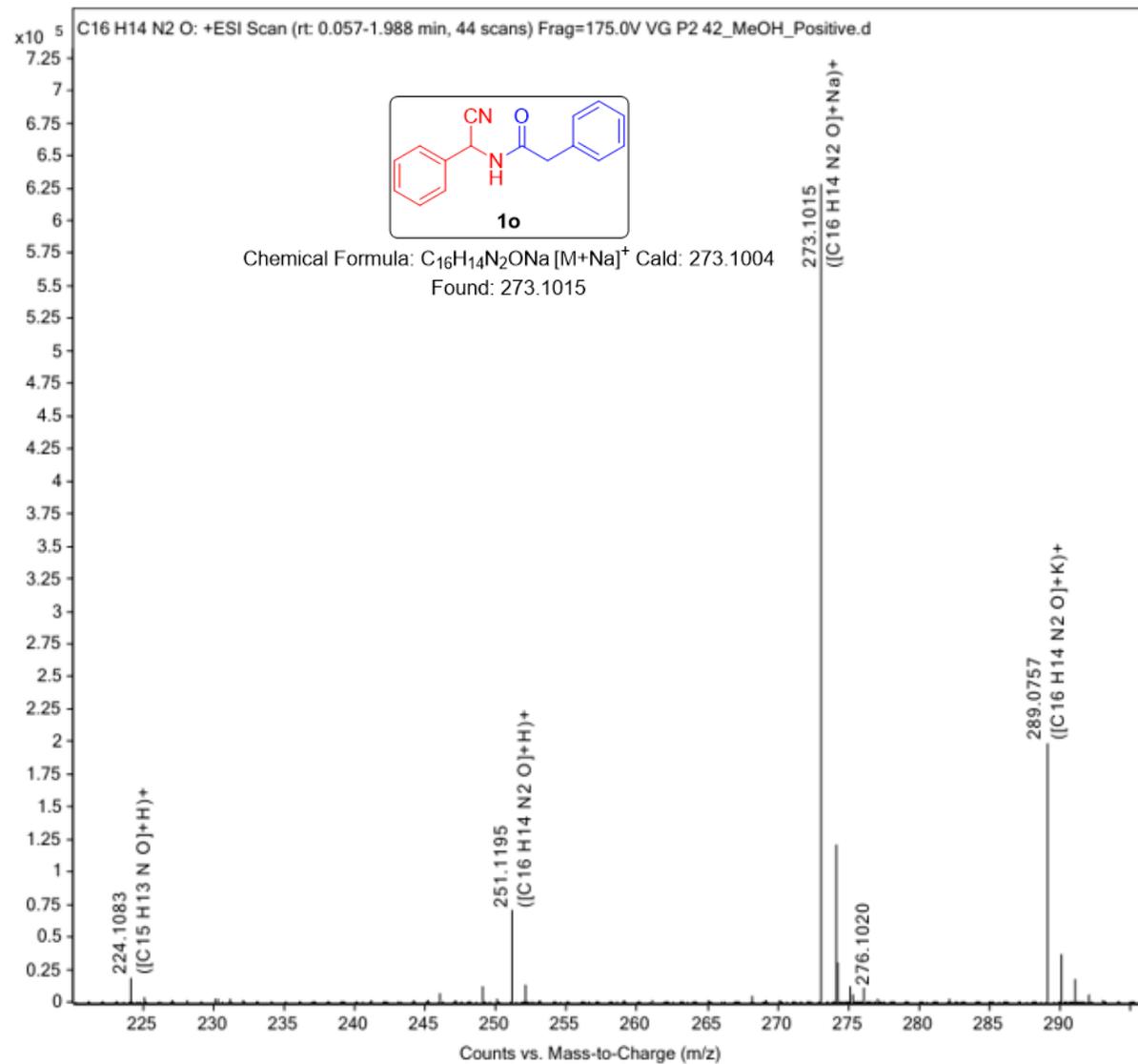


Fig. S50. HRMS data of *N*-(cyano(phenyl)methyl)-2-phenylacetamide (**1o**).

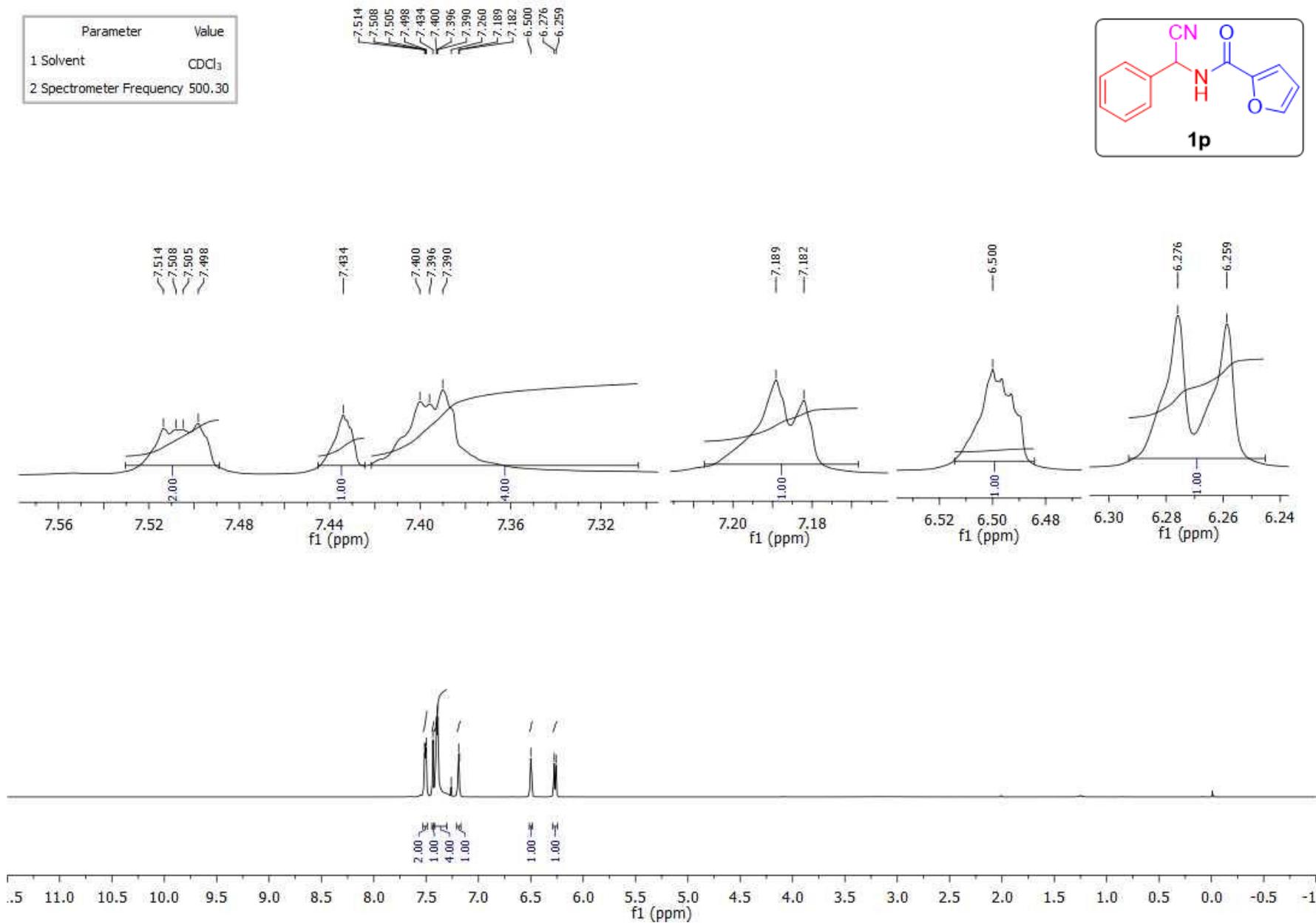


Fig. S51. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)furan-2-carboxamide (**1p**).

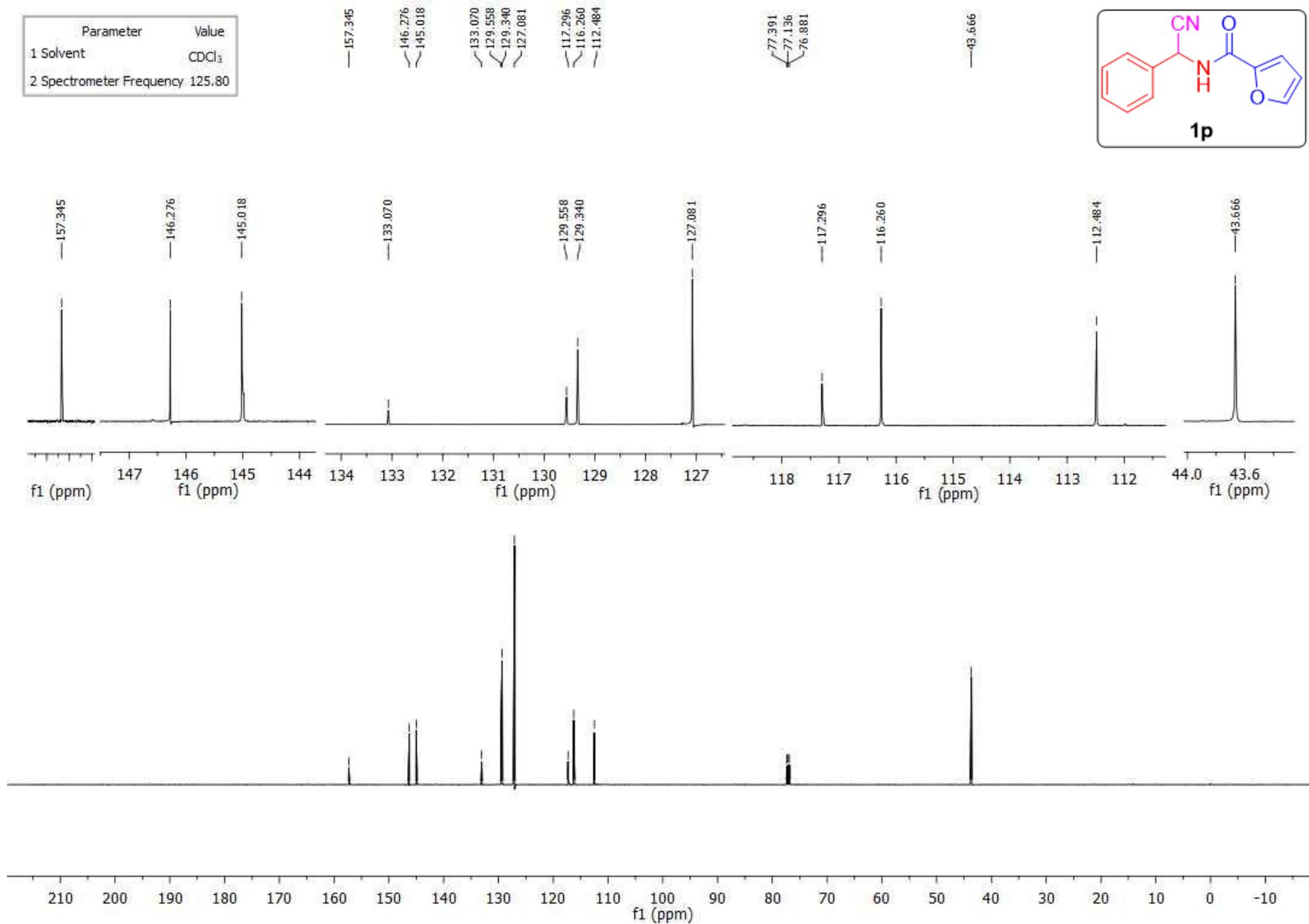


Fig. S52. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)furan-2-carboxamide (**1p**).

Sample Name	VG P2 41_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 41_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/9/2025 9:51:53 AM (UTC+05:30)

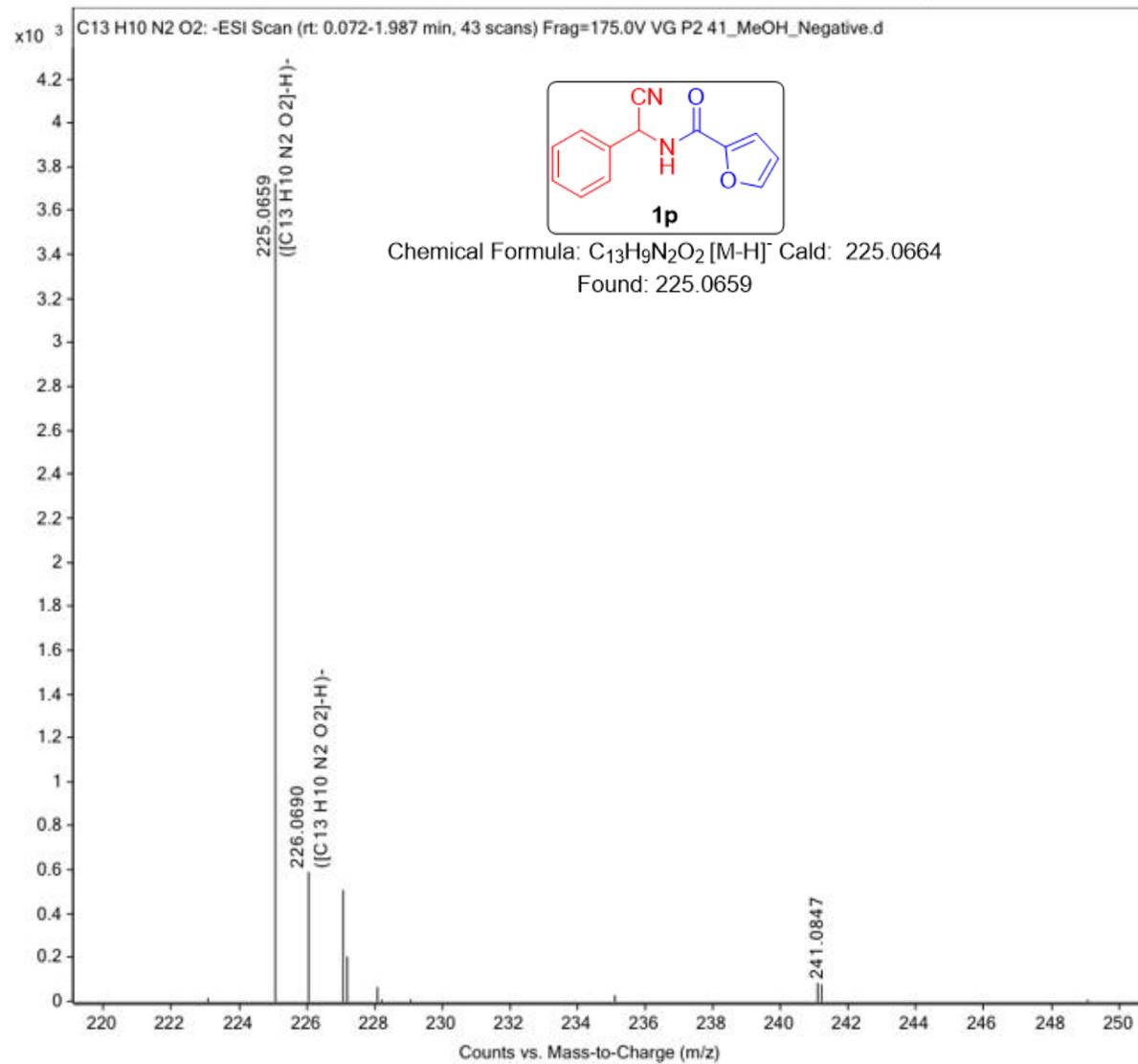


Fig. S53. HRMS data of *N*-(cyano(phenyl)methyl)furan-2-carboxamide (**1p**).

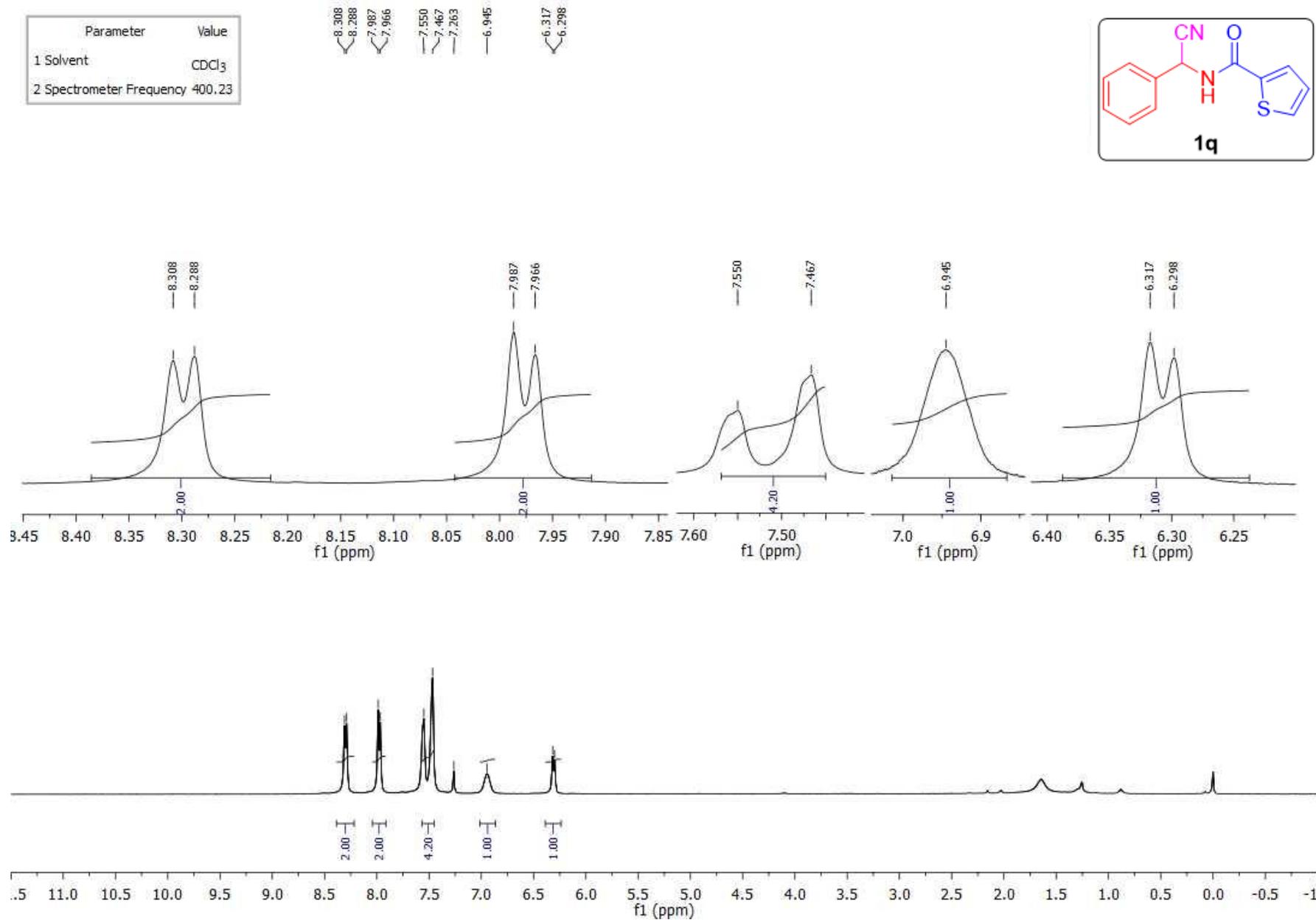


Fig. S54. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)thiophene-2-carboxamide (**1q**).

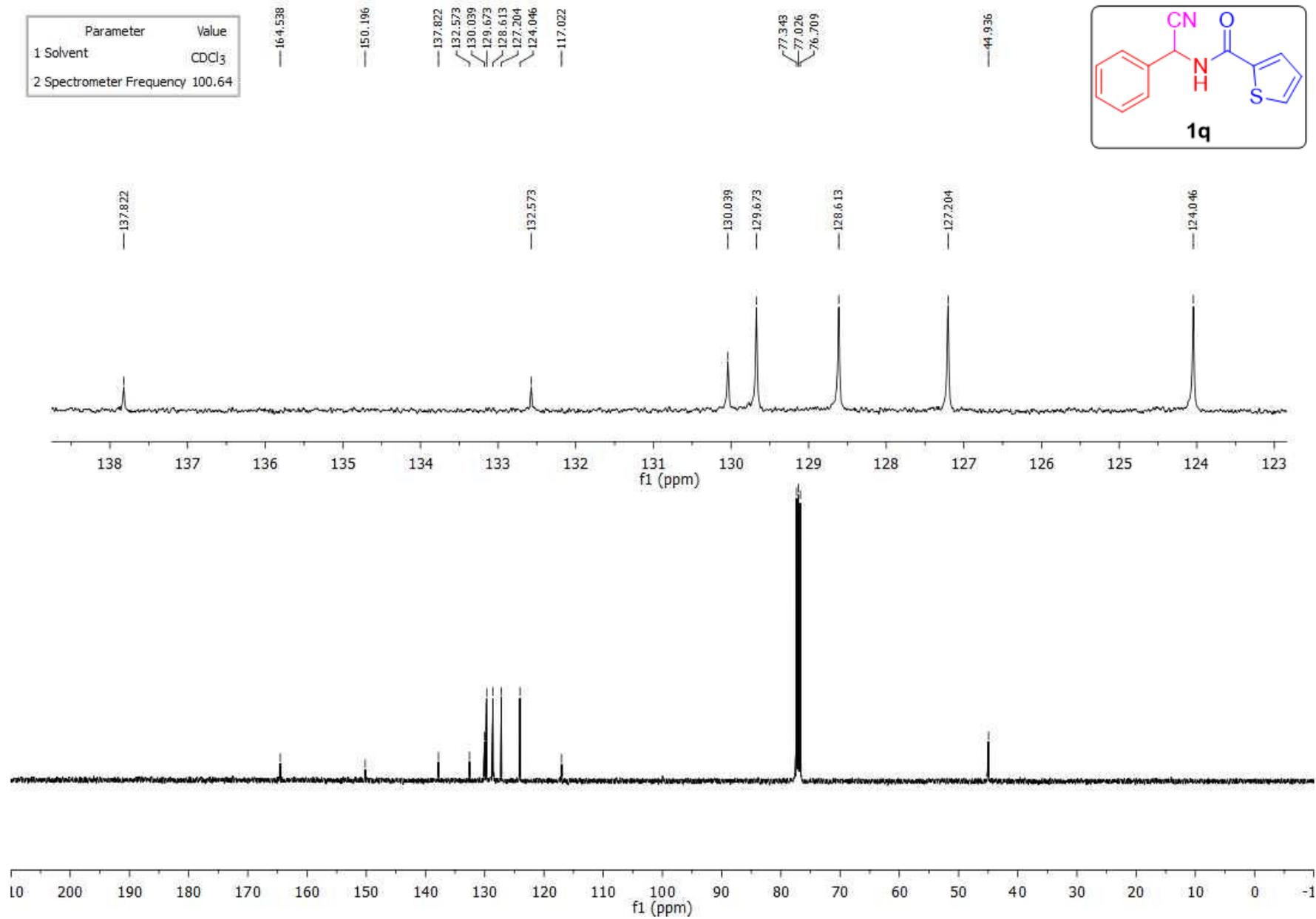
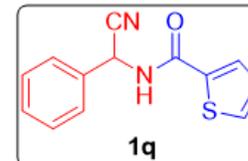


Fig. S55. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)thiophene-2-carboxamide (**1q**).

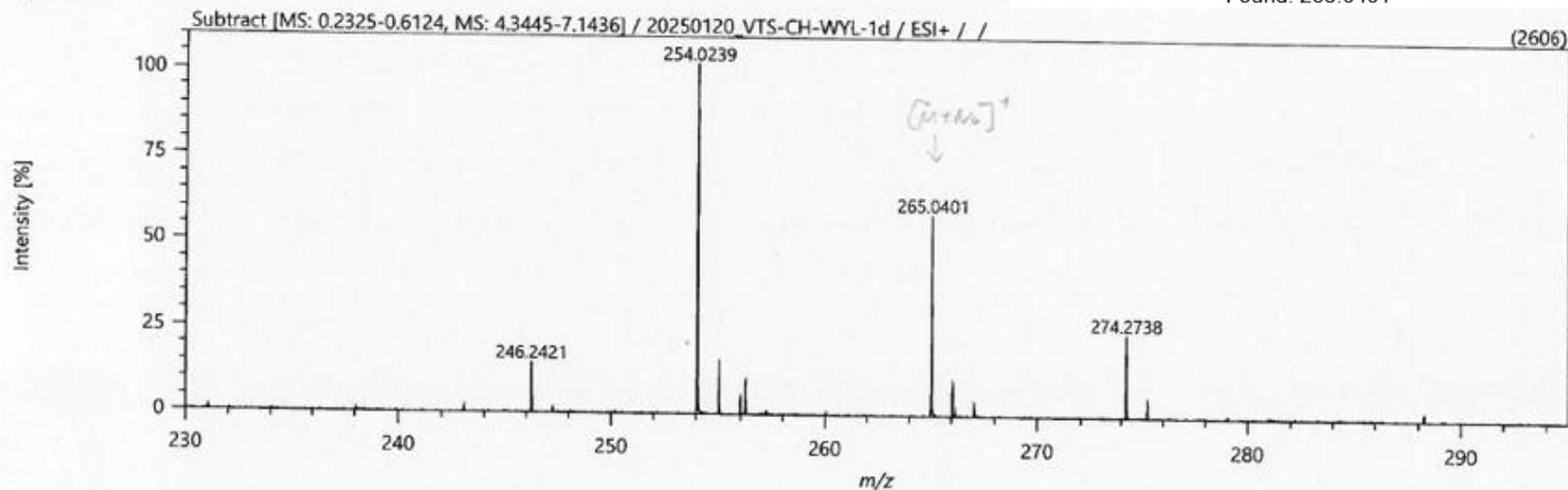
VTS-CH-WYL-1d (HR-ESI)



1q

Chemical Formula: C₁₃H₁₀N₂OSNa [M+Na]⁺ Calcd: 265.0412
Found: 265.0401

Spectrum



Elemental Composition

Parameters

Tolerance: ±3.00 ppm

Electron: Odd/Even

Charge: +1

DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na	S
Min	0	0	1	2	0	1
Max	400	1000	1	2	1	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
265.04008	C ₁₃ H ₁₀ N ₂ O Na S	265.04060	-0.52	-1.97	9.5

Fig. S56. HRMS data of *N*-(cyano(phenyl)methyl)thiophene-2-carboxamide (**1q**).

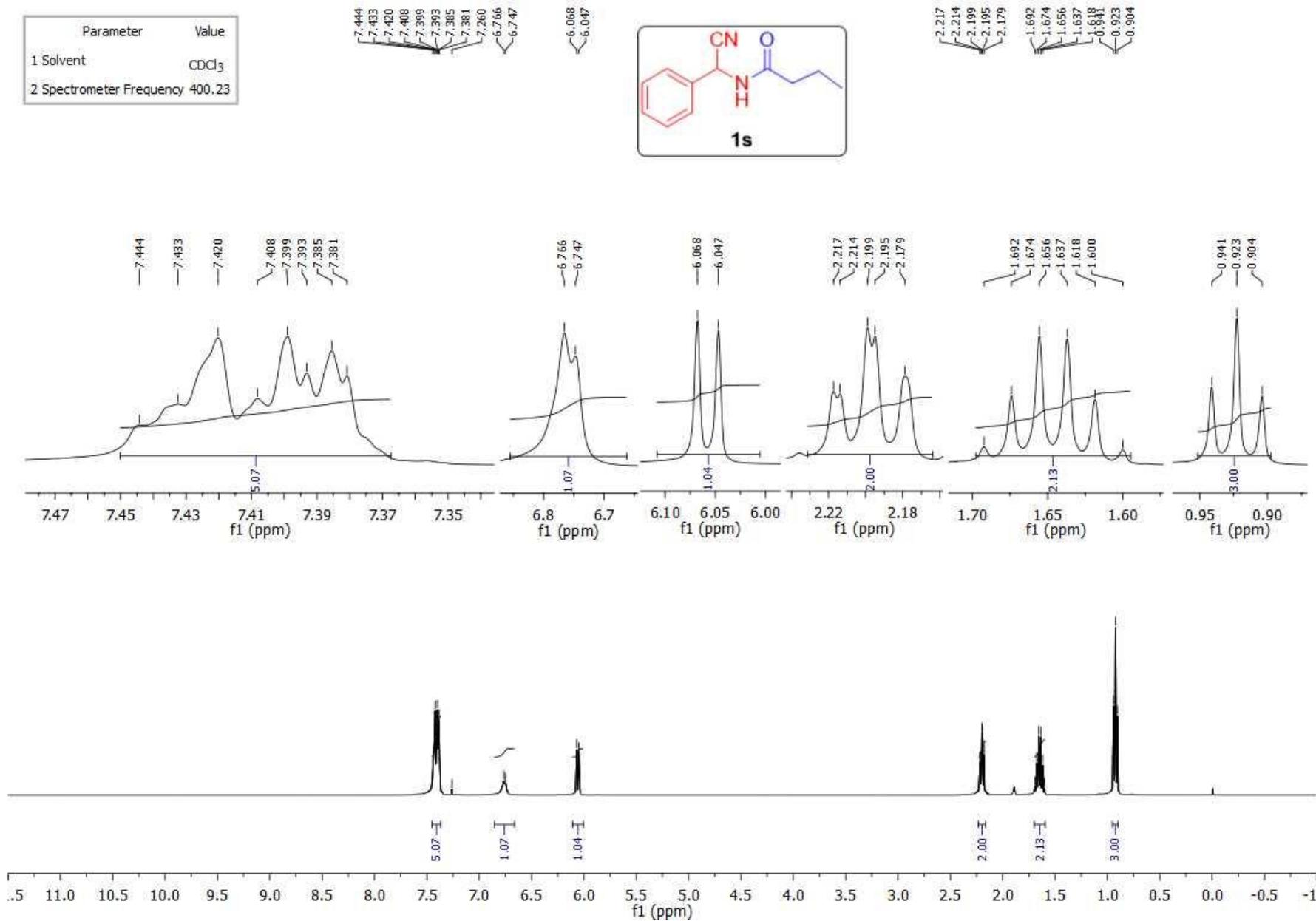


Fig. S57. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)butyramide (**1s**).

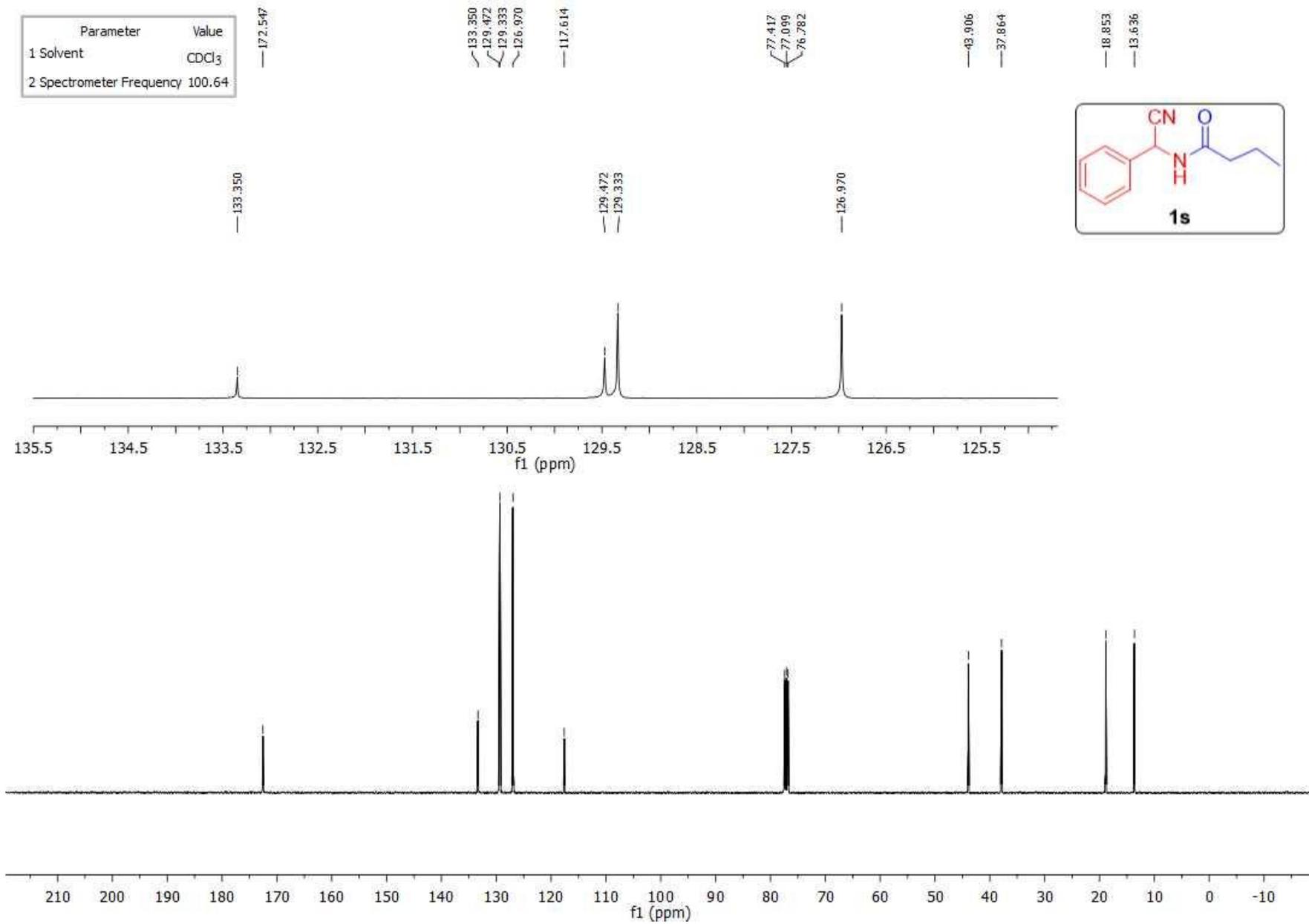
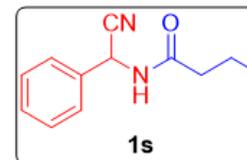


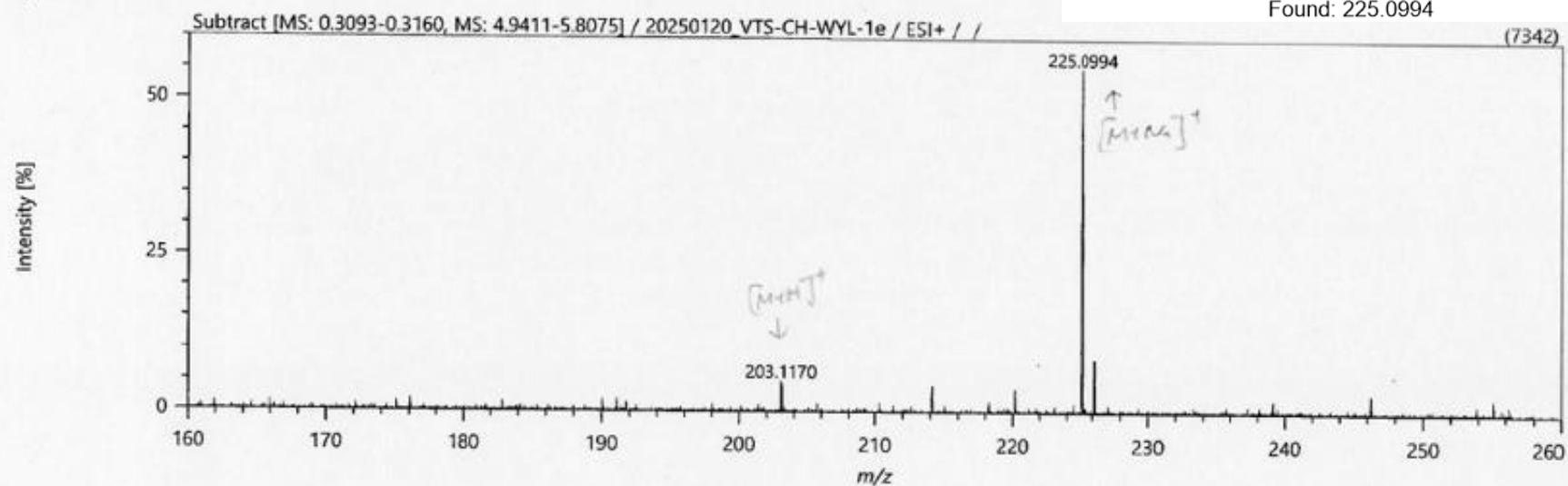
Fig. S58. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)butyramide (**1s**).

VTS-CH-WYL-1e (HR-ESI)



Chemical Formula: C₁₂H₁₄N₂O_{Na} [M+Na]⁺ Calcd: 225.1004
Found: 225.0994

Spectrum



Elemental Composition

Parameters

Tolerance: ±5.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	1	2	0
Max	400	1000	1	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
203.11701	C ₁₂ H ₁₅ N ₂ O	203.11789	-0.88	-4.33	6.5
225.09938	C ₁₂ H ₁₄ N ₂ O Na	225.09983	-0.46	-2.04	6.5

Fig. S59. HRMS data of *N*-(cyano(phenyl)methyl)butyramide (**1s**).

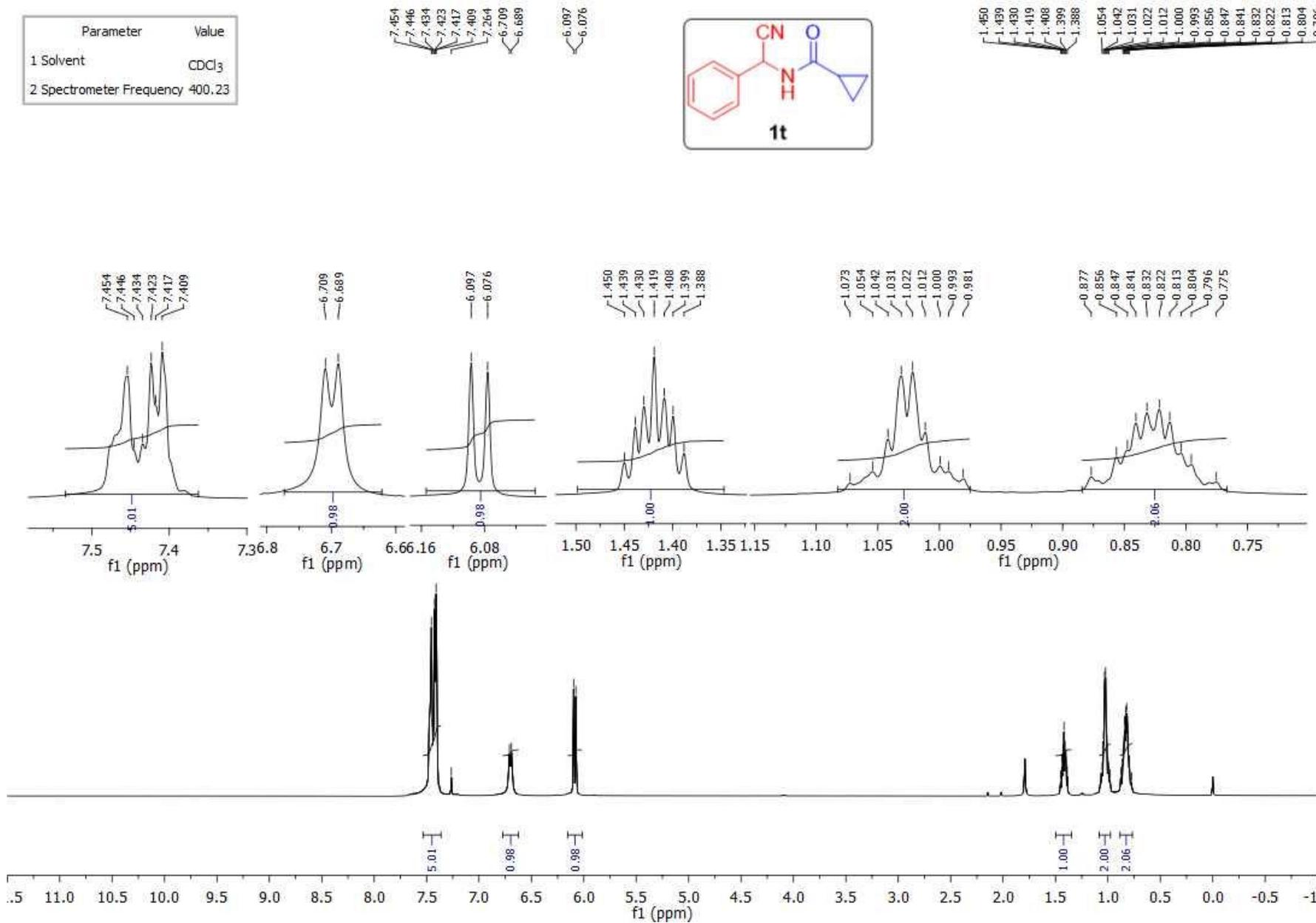


Fig. S60. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)cyclopropanecarboxamide (**1t**).

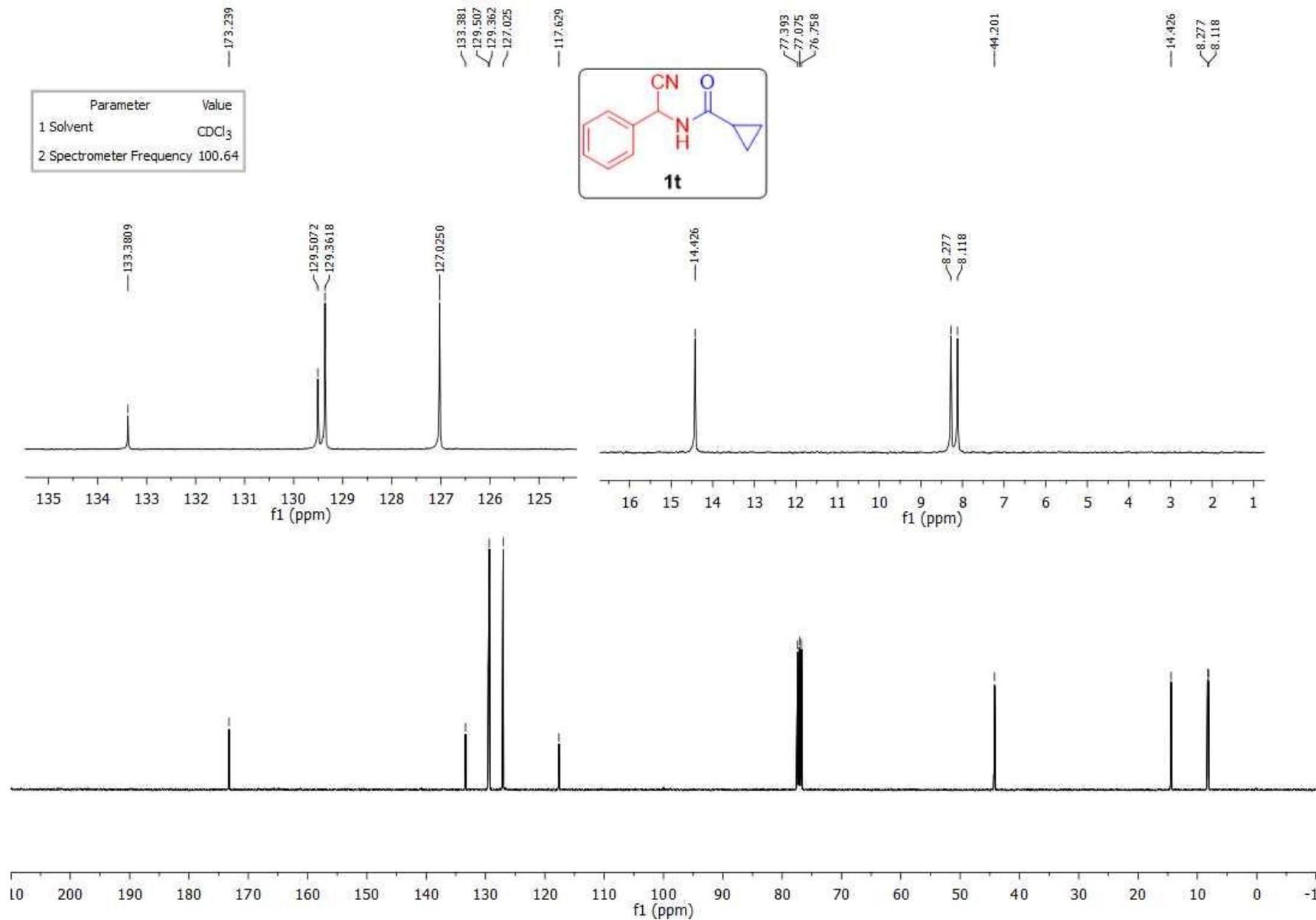
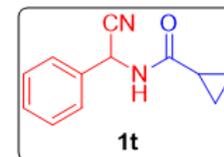


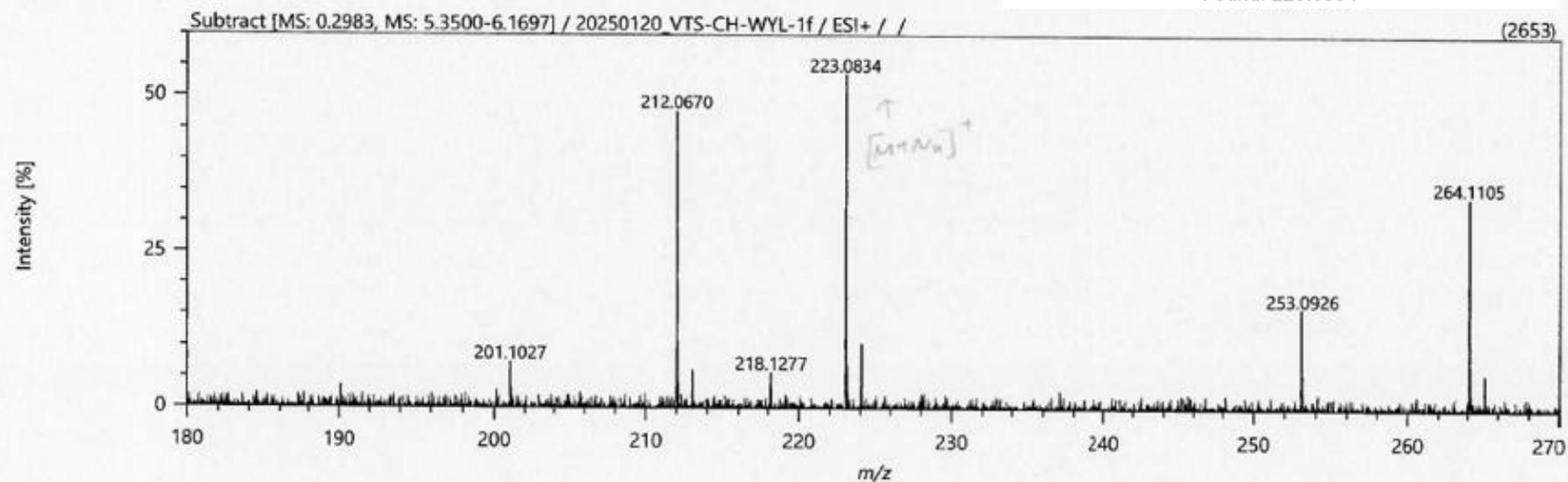
Fig. S61. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)cyclopropanecarboxamide (**1t**).

VTS-CH-WYL-1f (HR-ESI)



Chemical Formula: C₁₂H₁₂N₂O_{Na} [M+Na]⁺ Calcd: 223.0847
Found: 223.0834

Spectrum



Elemental Composition

Parameters

Tolerance: ±5.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	1	2	0
Max	400	1000	1	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
223.08344	C ₁₂ H ₁₂ N ₂ O Na	223.08418	-0.75	-3.36	7.5

Fig. S62. HRMS data of *N*-(cyano(phenyl)methyl)cyclopropanecarboxamide (**1t**).

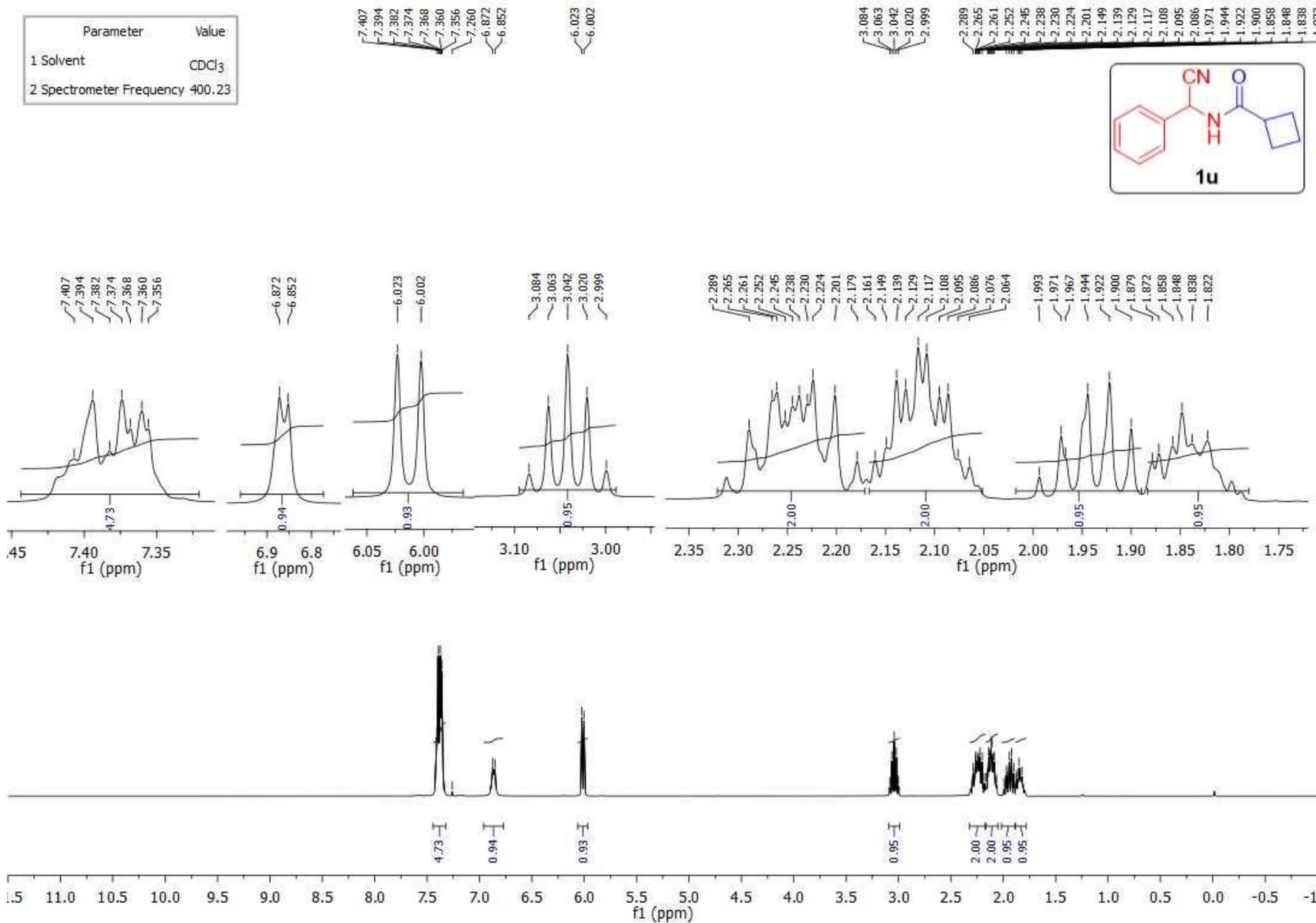


Fig. S63. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)cyclobutanecarboxamide (**1u**).

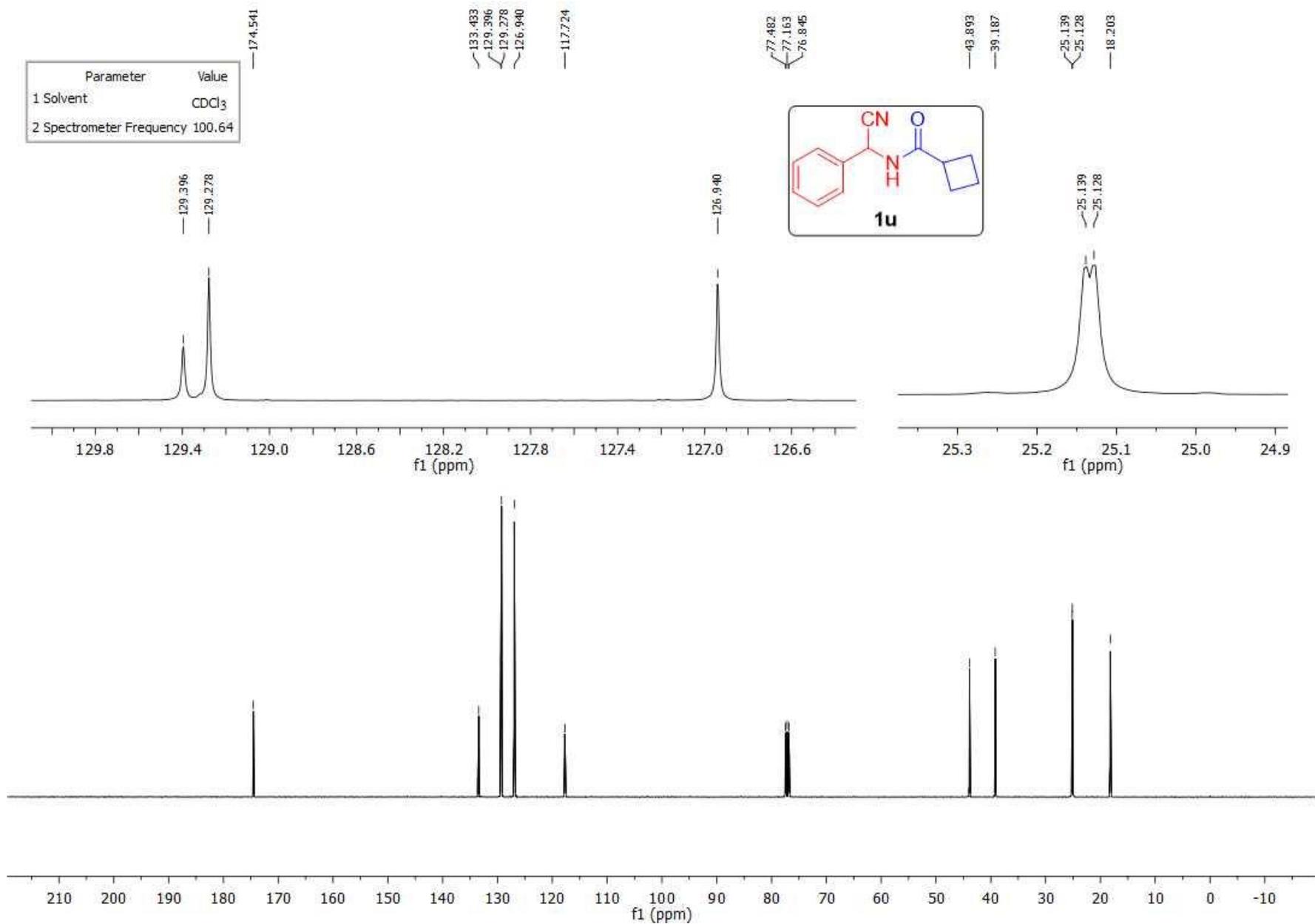
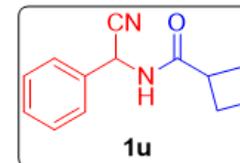


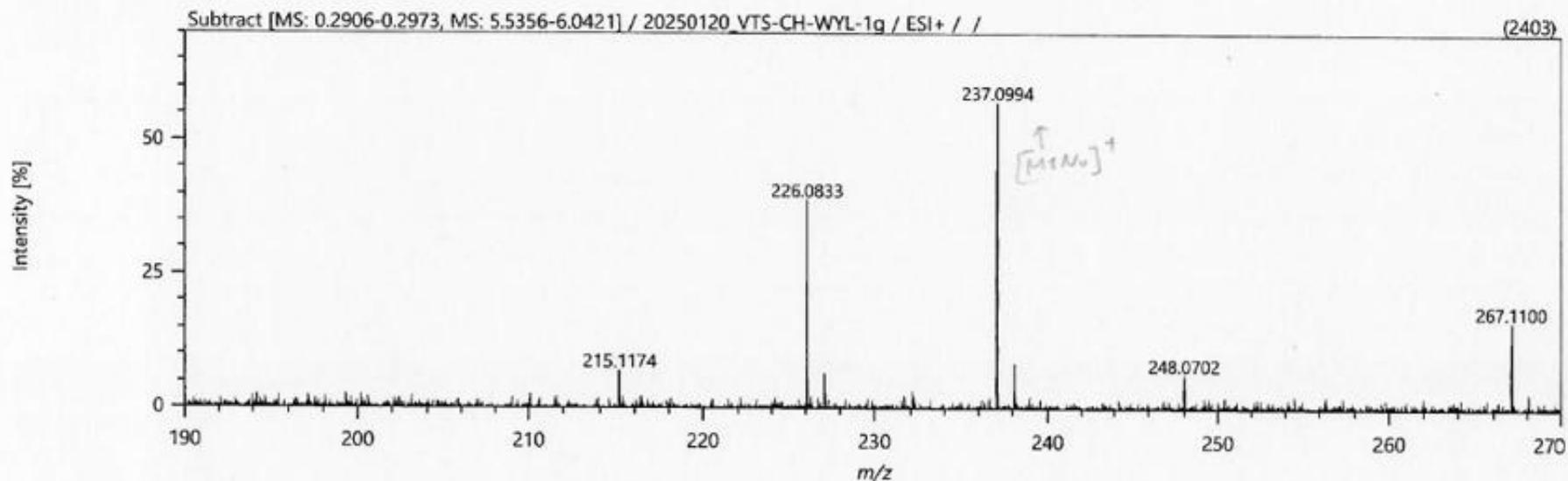
Fig. S64. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)cyclobutanecarboxamide (**1u**).

VTS-CH-WYL-1g (HR-ESI)



Chemical Formula: C₁₃H₁₄N₂ONa [M+Na]⁺ Calcd: 237.1004
Found: 237.0994

Spectrum



Elemental Composition

Parameters

Tolerance: ±5.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	1	2	0
Max	400	1000	1	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
237.09942	C ₁₃ H ₁₄ N ₂ O Na	237.09983	-0.41	-1.75	7.5

Fig. S65. HRMS data of *N*-(cyano(phenyl)methyl)cyclobutanecarboxamide (**1u**).

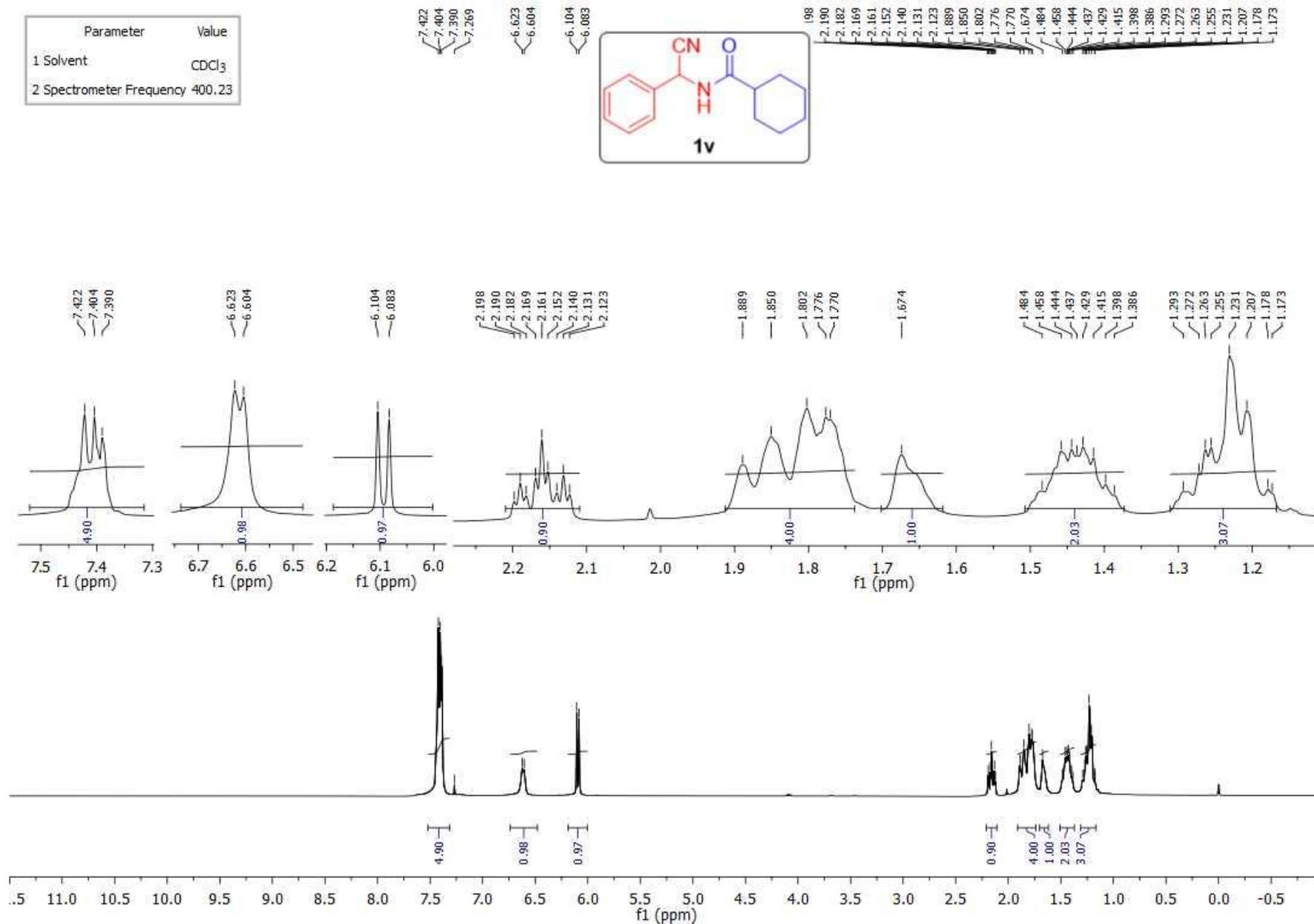


Fig. S66. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)cyclohexanecarboxamide (**1v**).

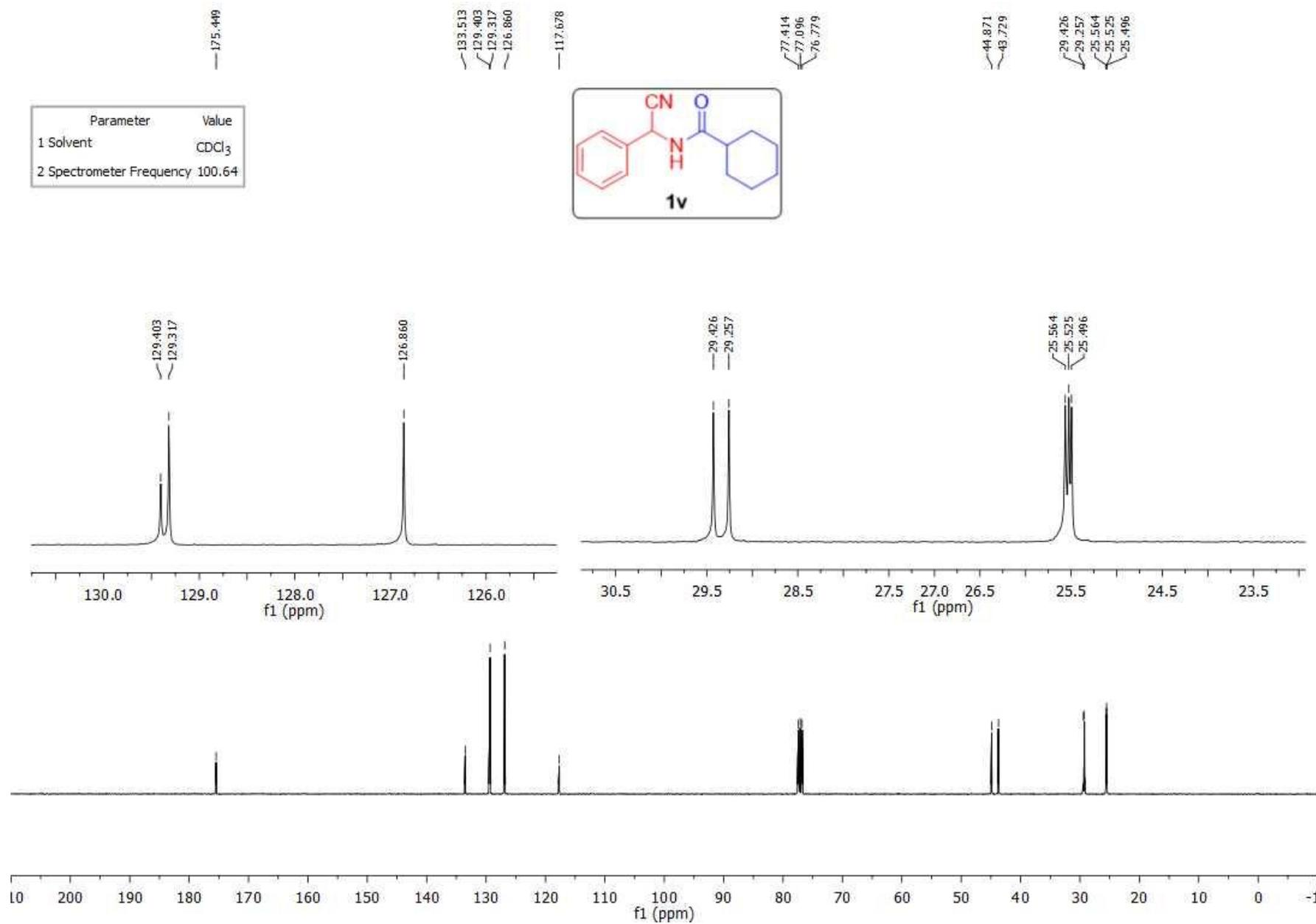
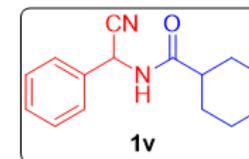


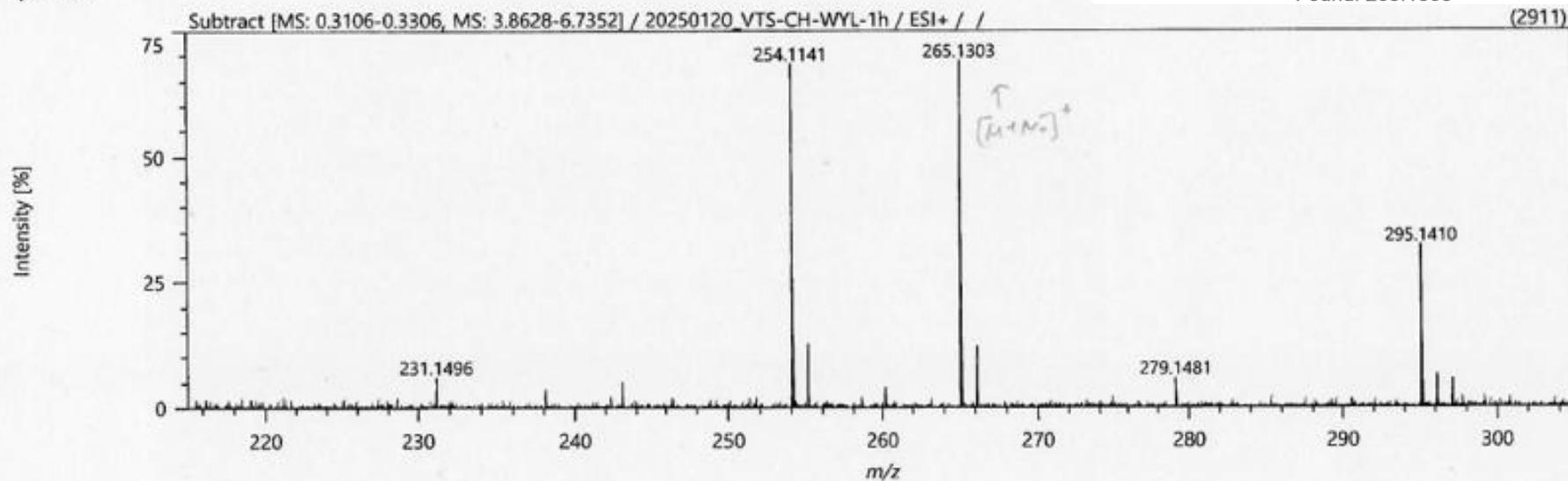
Fig. S67. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)cyclohexanecarboxamide (**1v**).

VTS-CH-WYL-1h (HR-ESI)



Chemical Formula: C₁₅H₁₈N₂ONa [M+Na]⁺ Calcd: 265.1317
Found: 265.1303

Spectrum



Elemental Composition

Parameters

Tolerance: ±5.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	1	2	0
Max	400	1000	1	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
265.13034	C ₁₅ H ₁₈ N ₂ O Na	265.13113	-0.79	-2.99	7.5

Fig. S68. HRMS data of *N*-(cyano(phenyl)methyl)cyclohexanecarboxamide (**1v**).

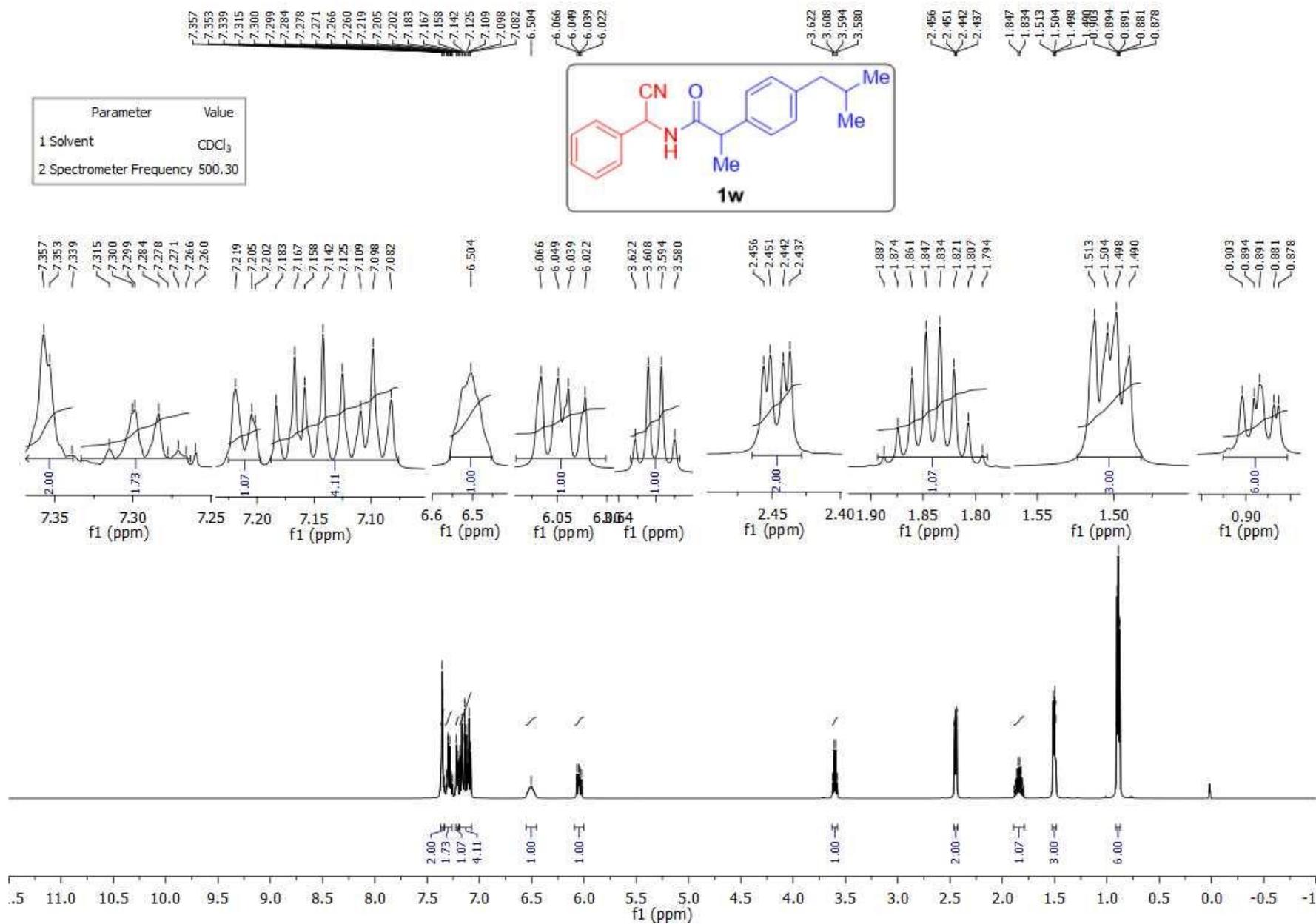


Fig. S69. ¹H NMR spectra of *N*-(cyano(phenyl)methyl)-2-(4-isobutylphenyl)propanamide (**1w**).

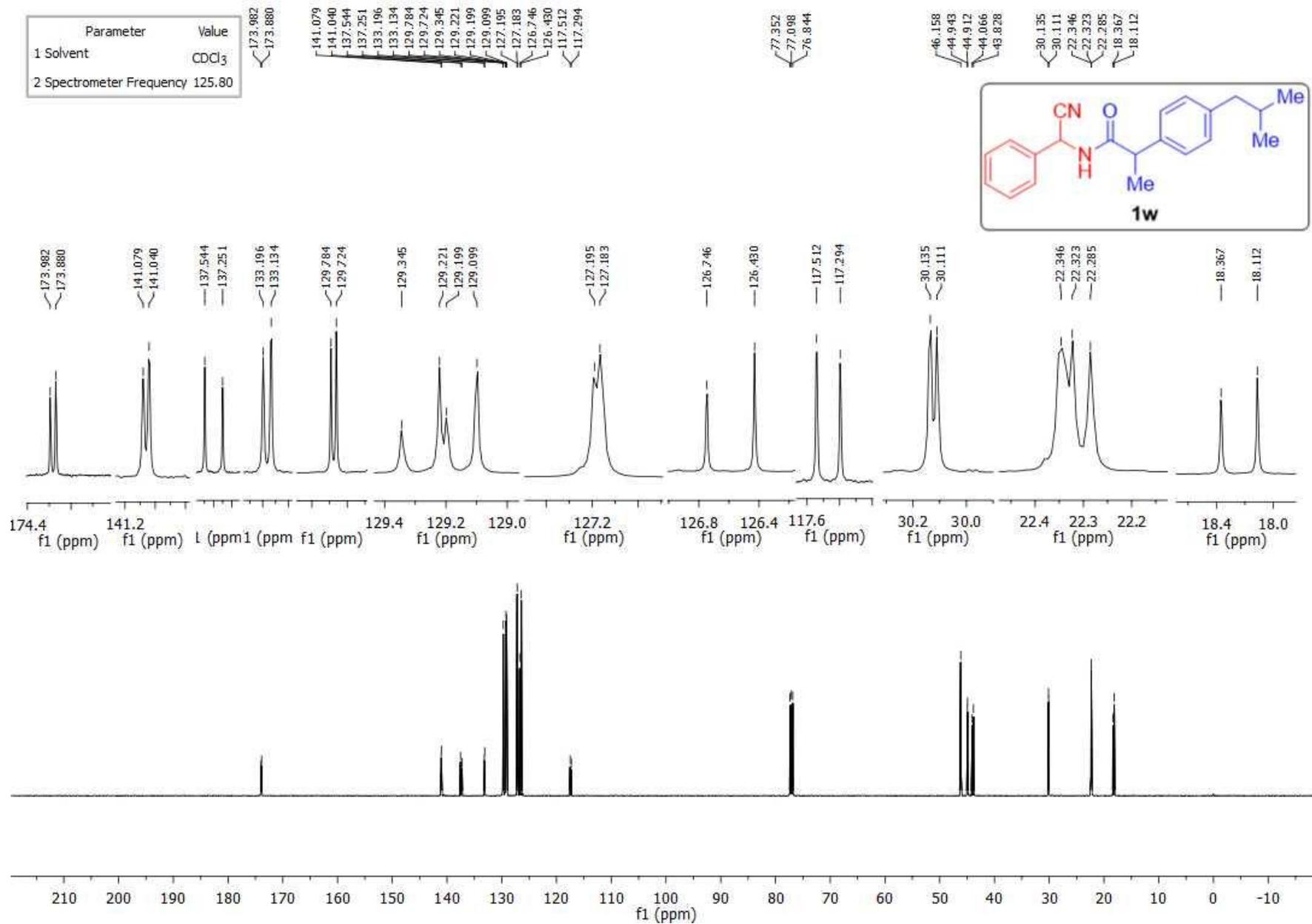


Fig. S70. ¹³C NMR spectra of *N*-(cyano(phenyl)methyl)-2-(4-isobutylphenyl)propanamide (**1w**).

Sample Name	VG P2 34_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 34_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/4/2025 9:58:15 AM (UTC+05:30)

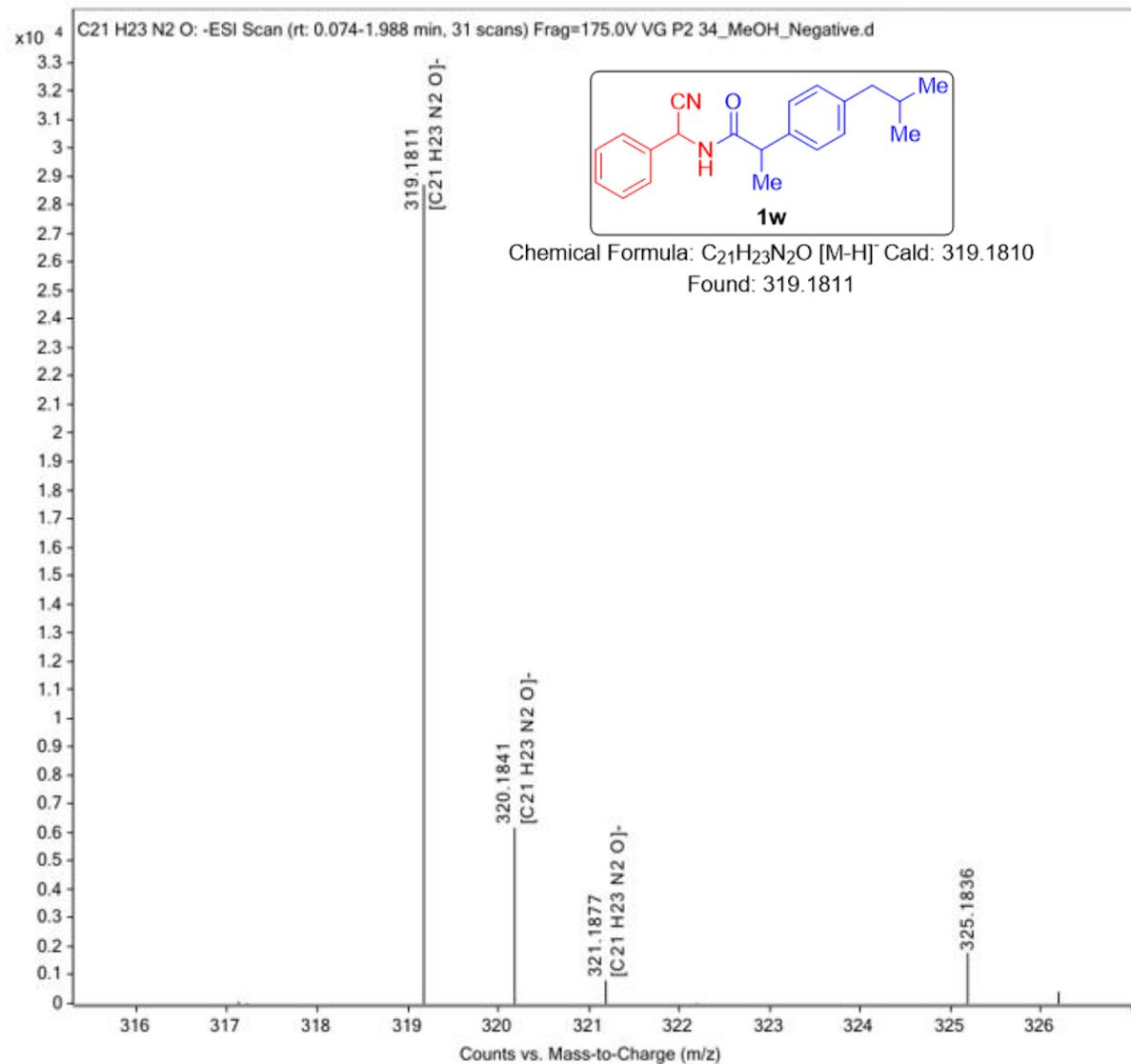


Fig. S71. HRMS data of *N*-(cyano(phenyl)methyl)-2-(4-isobutylphenyl)propanamide (**1w**).

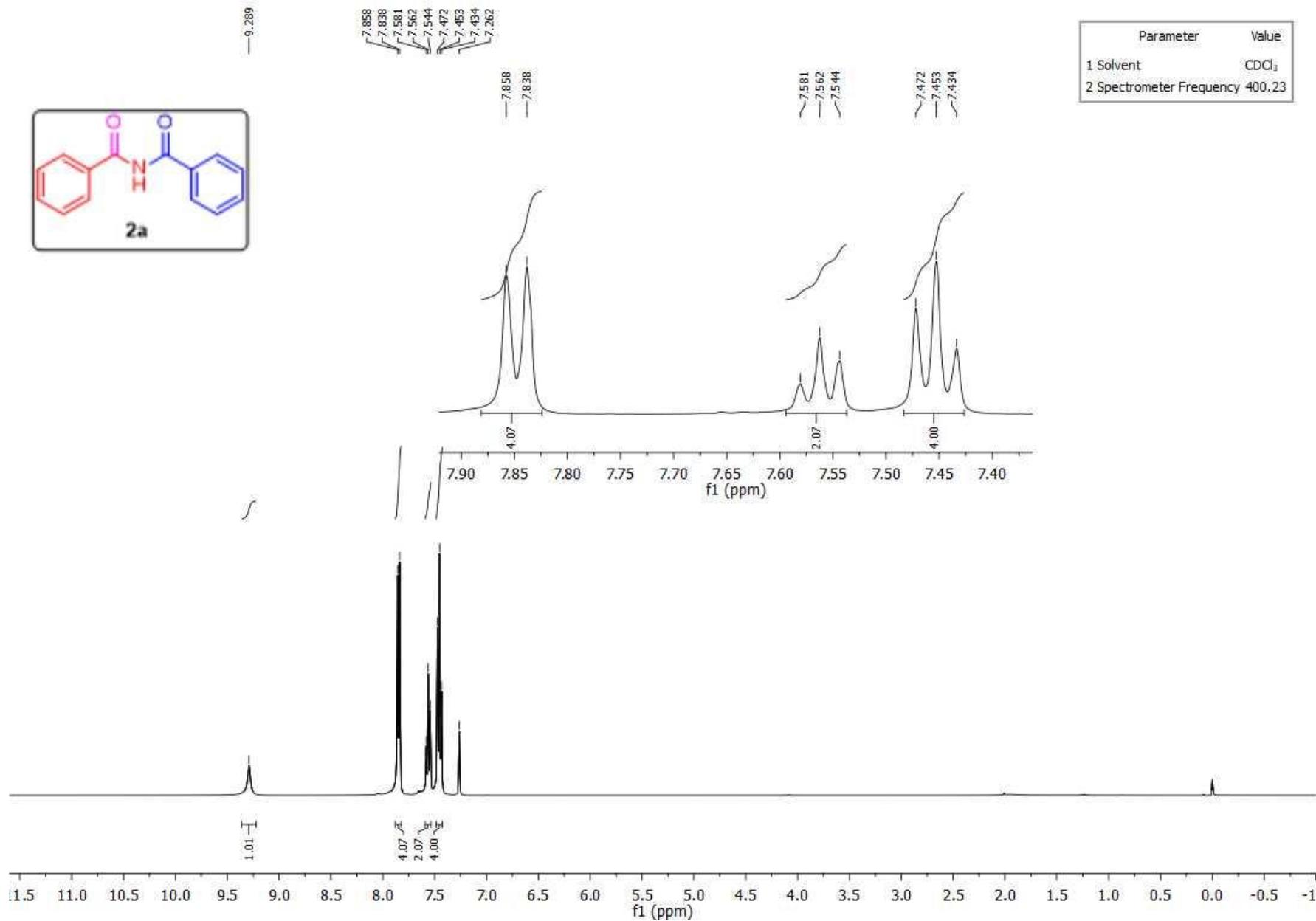


Fig. S72. ¹H NMR spectra of *N*-benzoylbenzamide (**2a**).

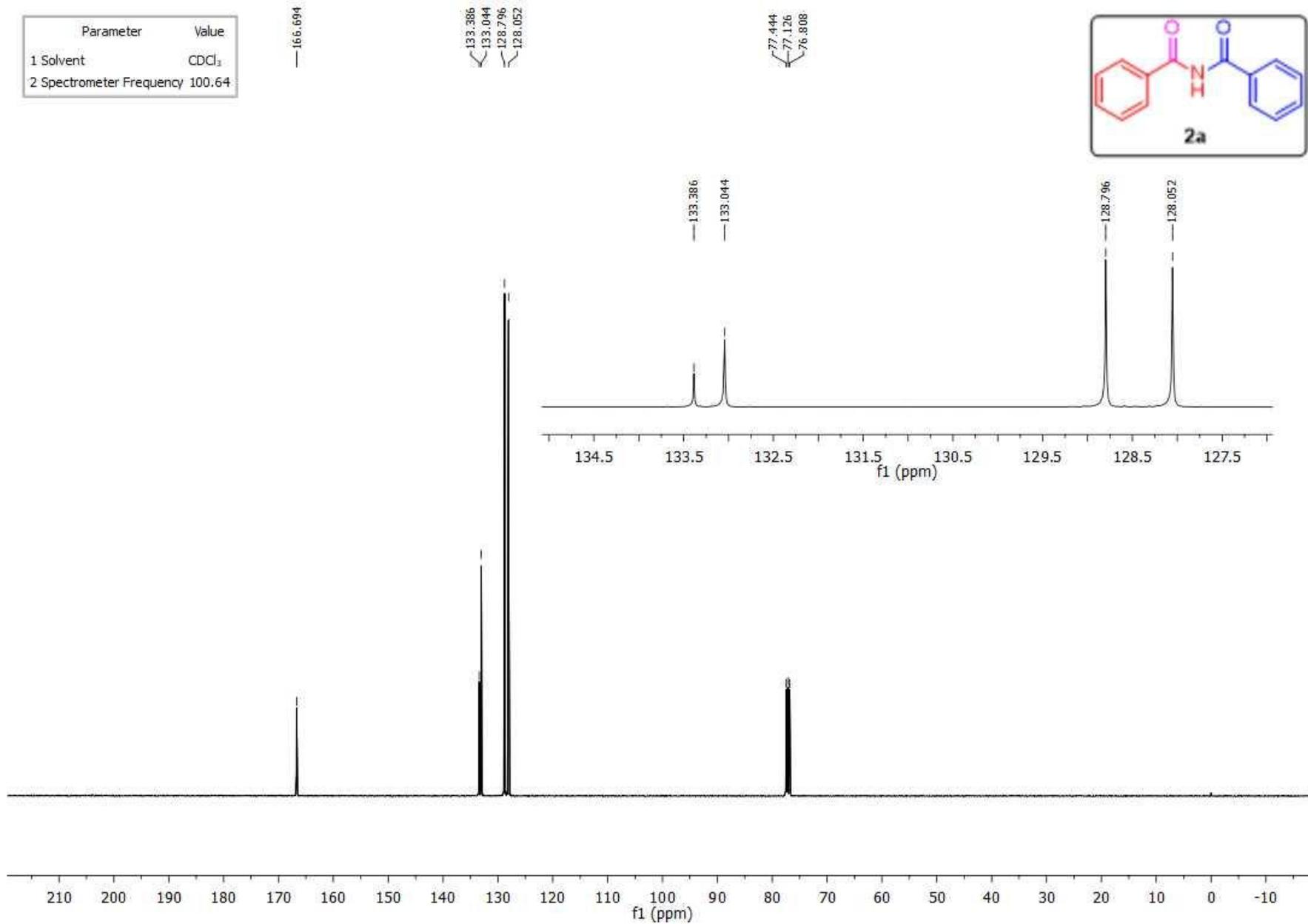


Fig. S73. ¹³C NMR spectra of *N*-benzoylbenzamide (2a).

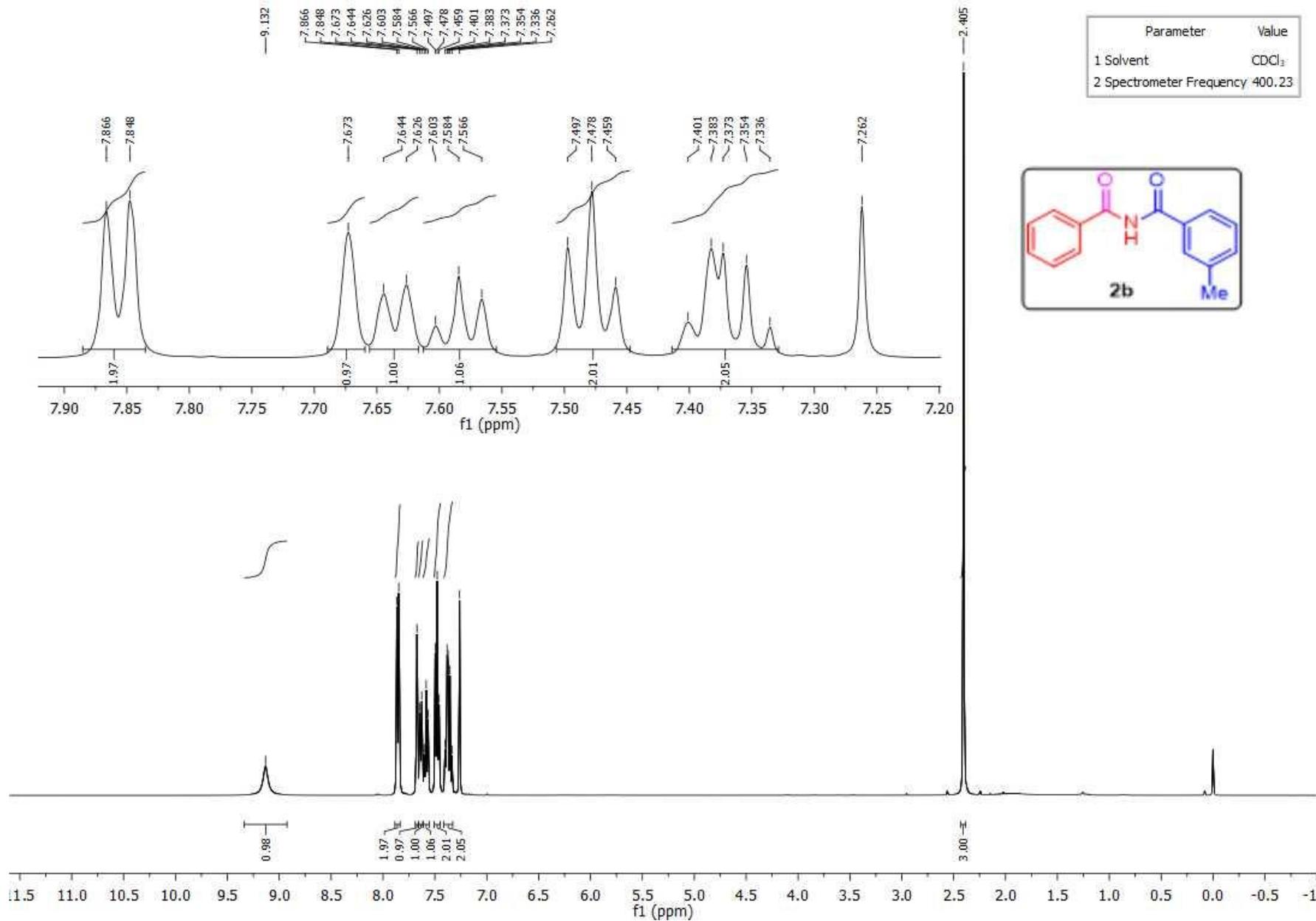


Fig. S74. ¹H NMR spectra of *N*-benzoyl-3-methylbenzamide (**2b**).

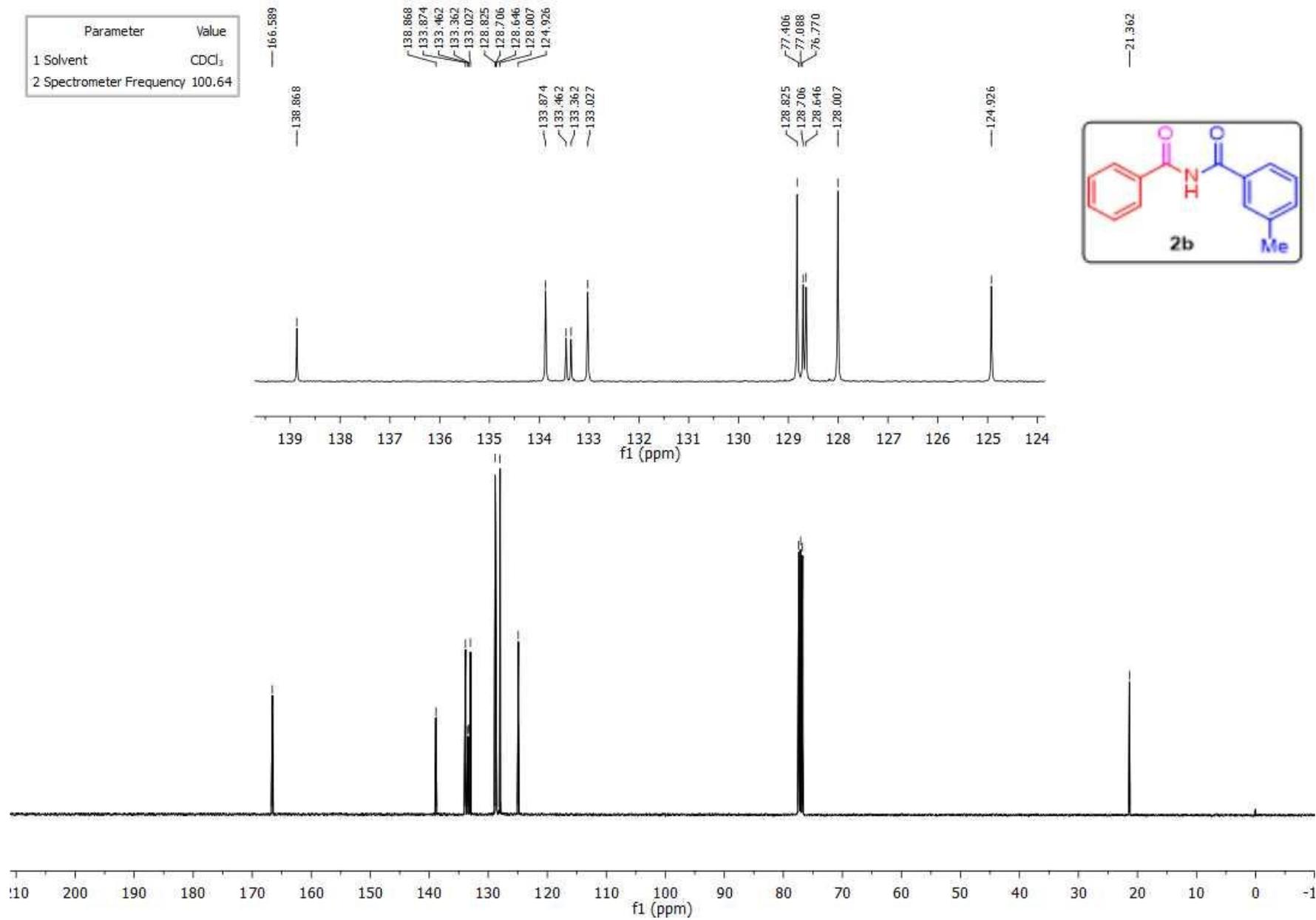


Fig. S75. ¹³C NMR spectra of *N*-benzoyl-3-methylbenzamide (**2b**).

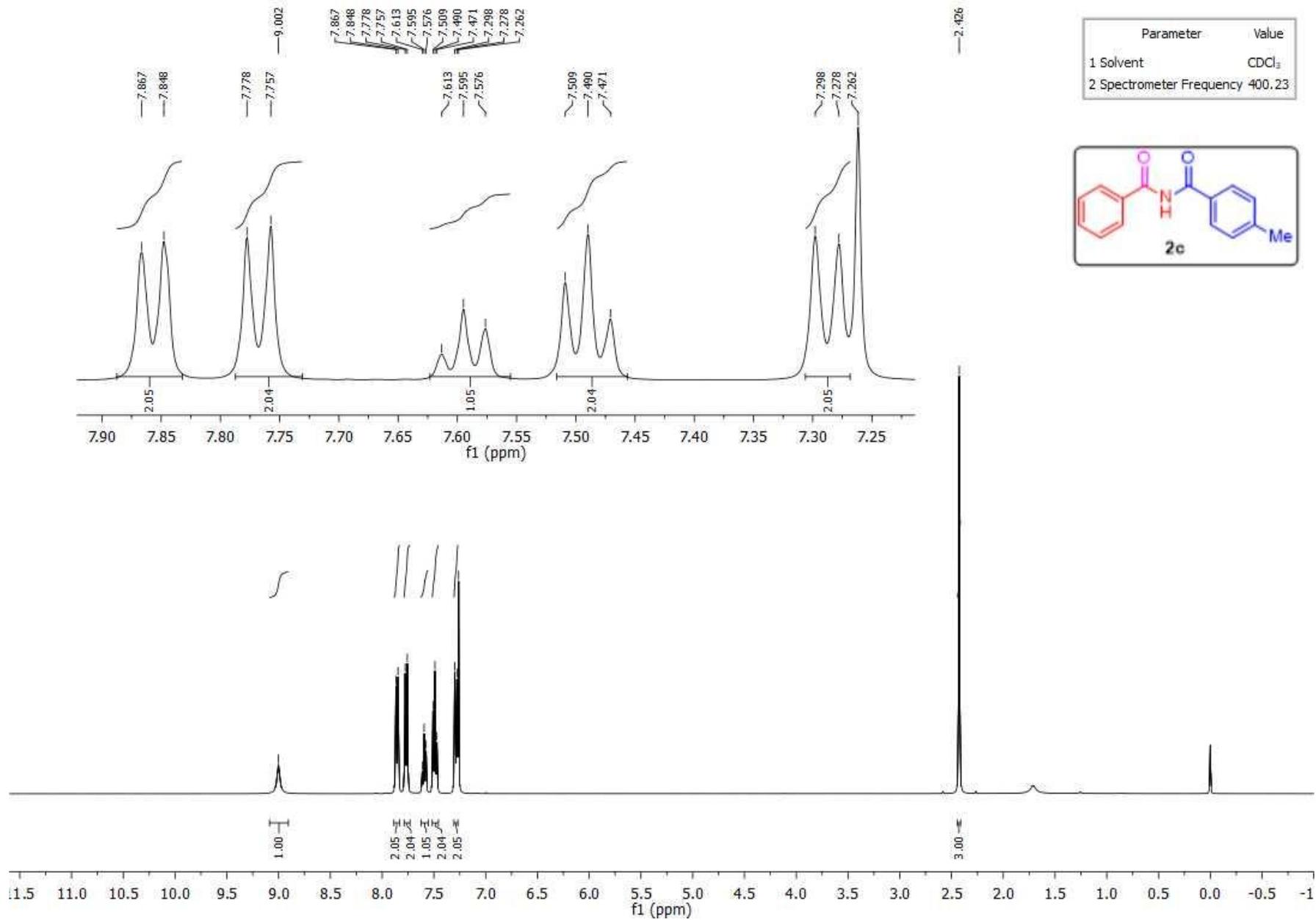


Fig. S76. ¹H NMR spectra of *N*-benzoyl-4-methylbenzamide (**2c**).

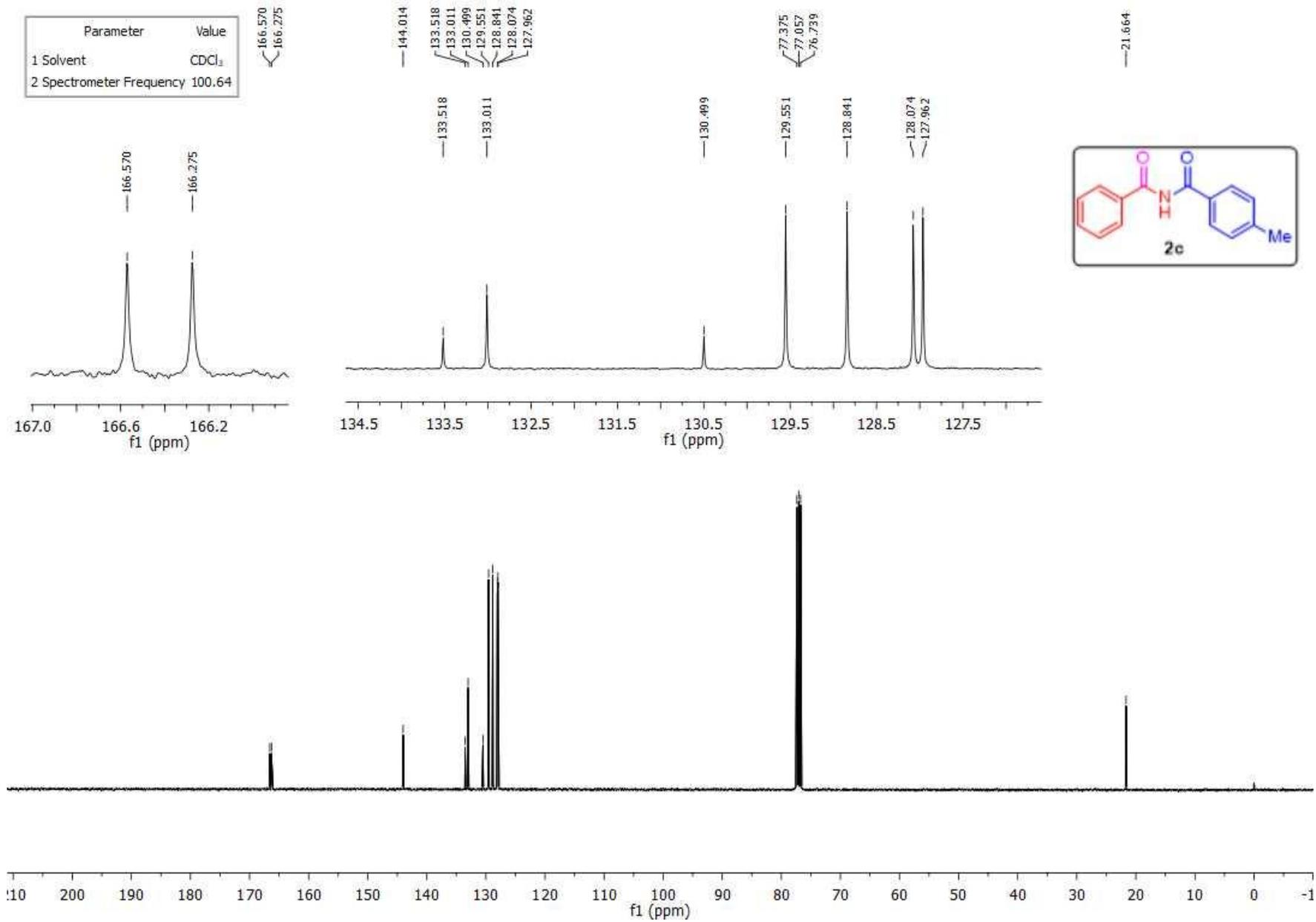


Fig. S77. ¹³C NMR spectra of *N*-benzoyl-4-methylbenzamide (**2c**).

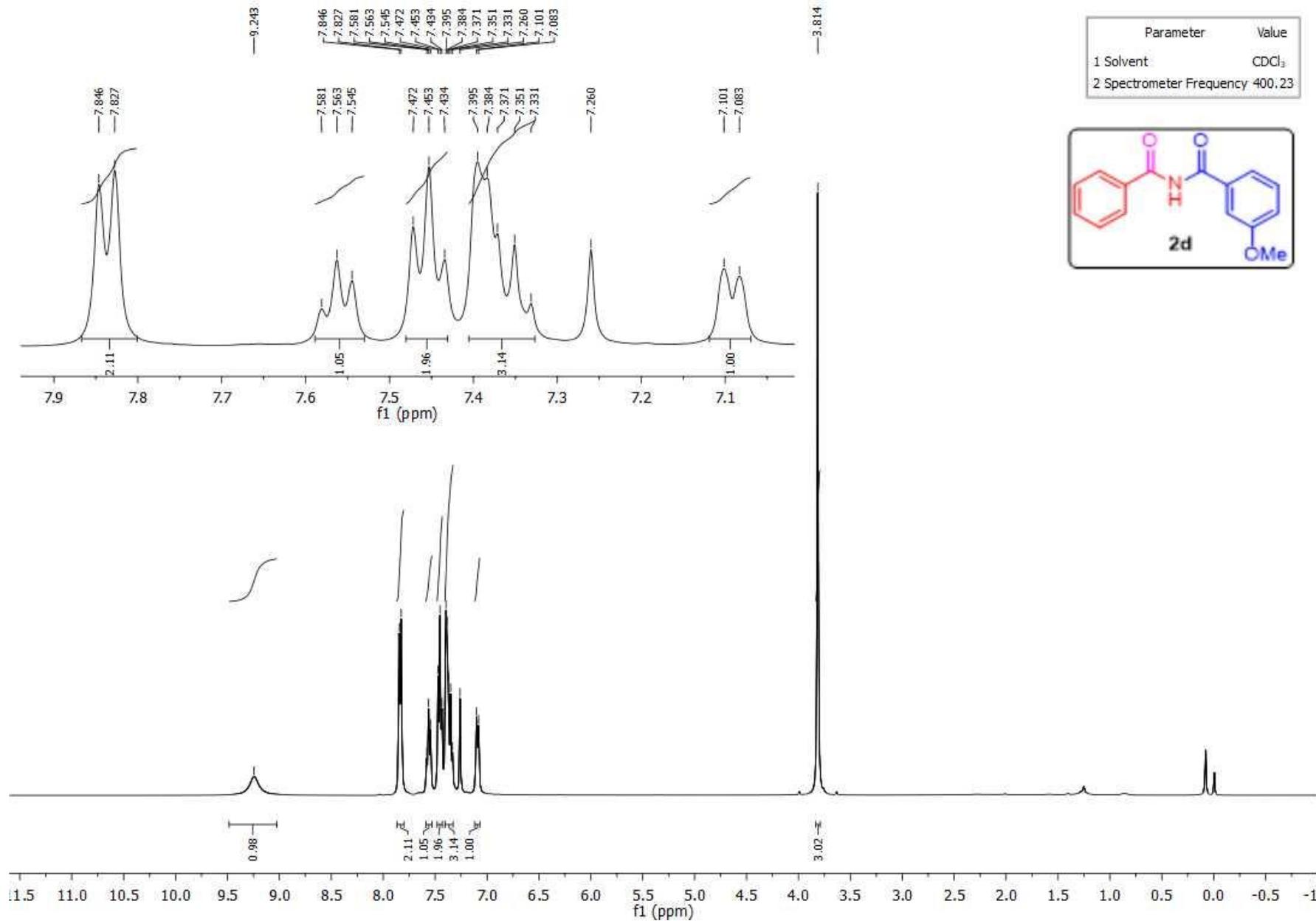


Fig. S78. ¹H NMR spectra of *N*-benzoyl-3-methoxybenzamide (**2d**).

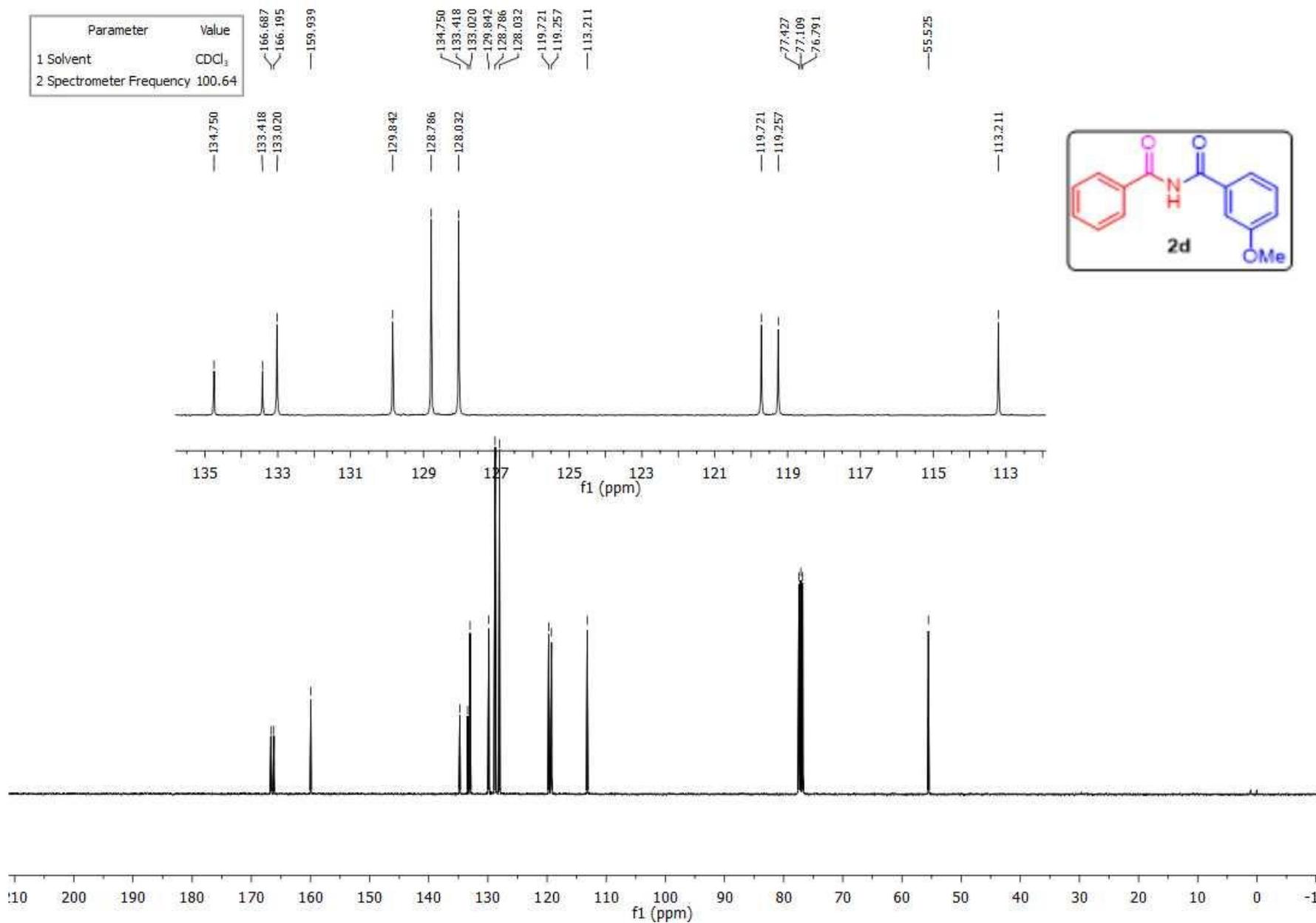


Fig. S79. ¹³C NMR spectra of *N*-benzoyl-3-methoxybenzamide (**2d**).

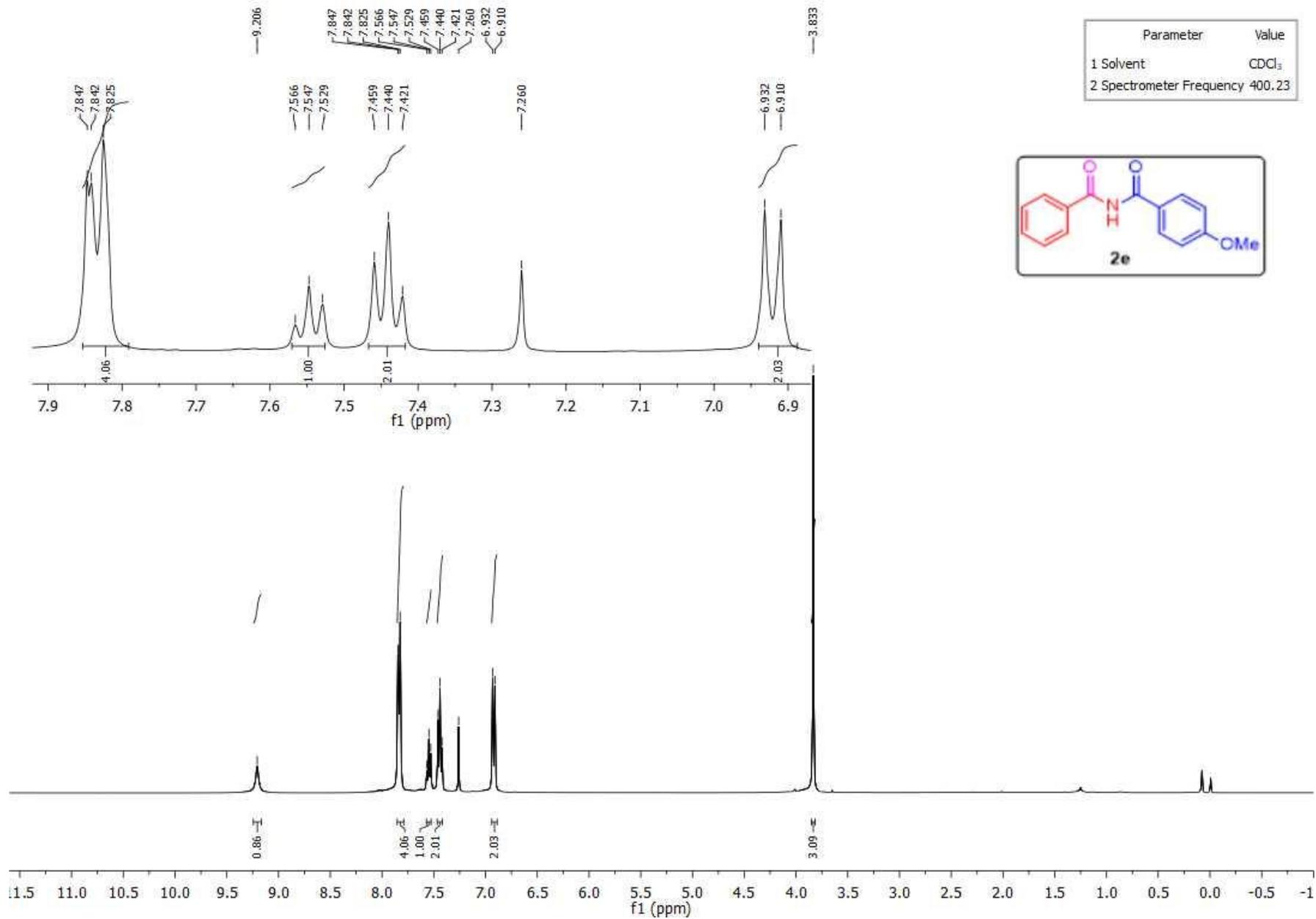


Fig. S80. ¹H NMR spectra of *N*-benzoyl-4-methoxybenzamide (**2e**).

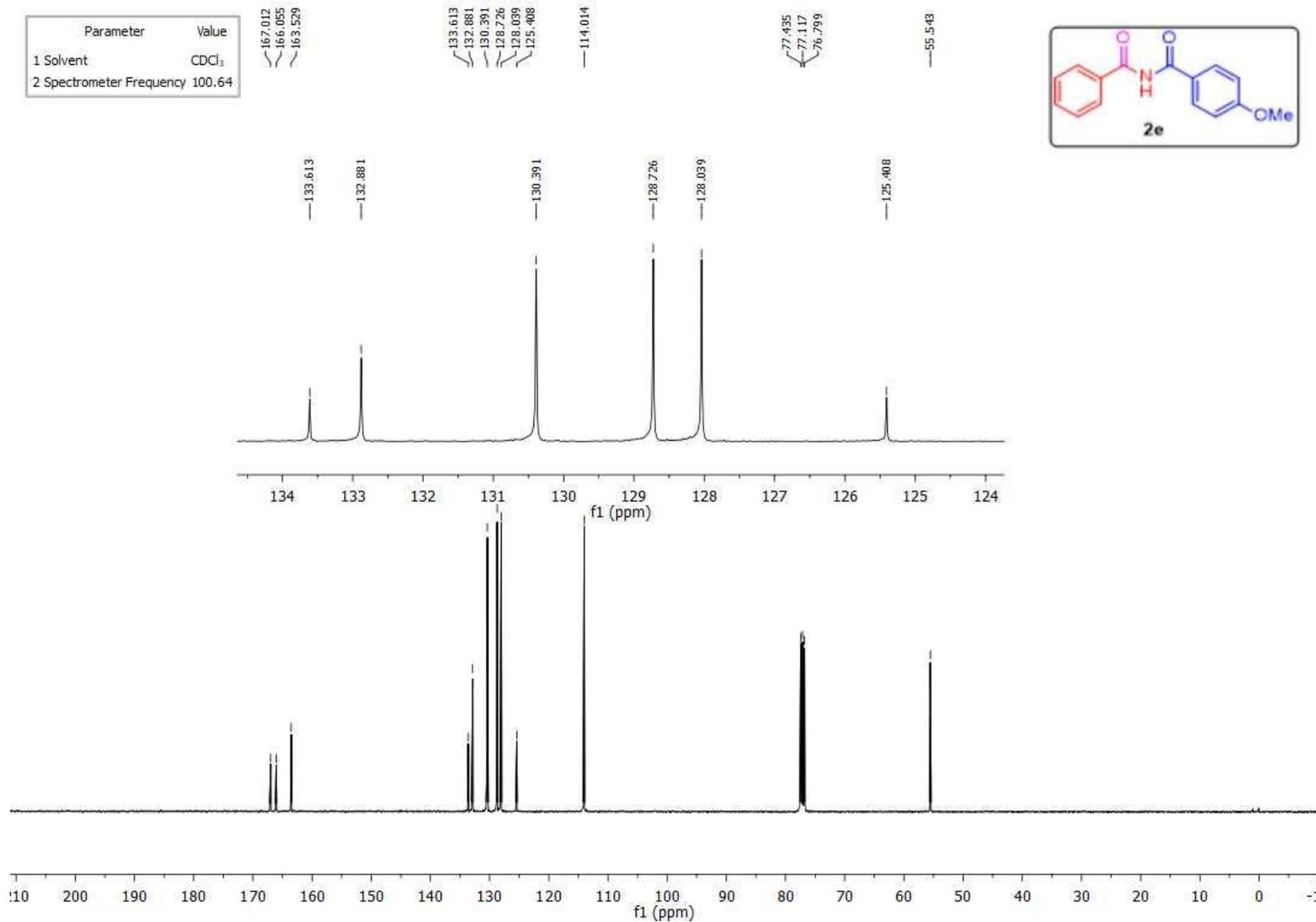


Fig. S81. ¹³C NMR spectra of *N*-benzoyl-4-methoxybenzamide (**2e**).

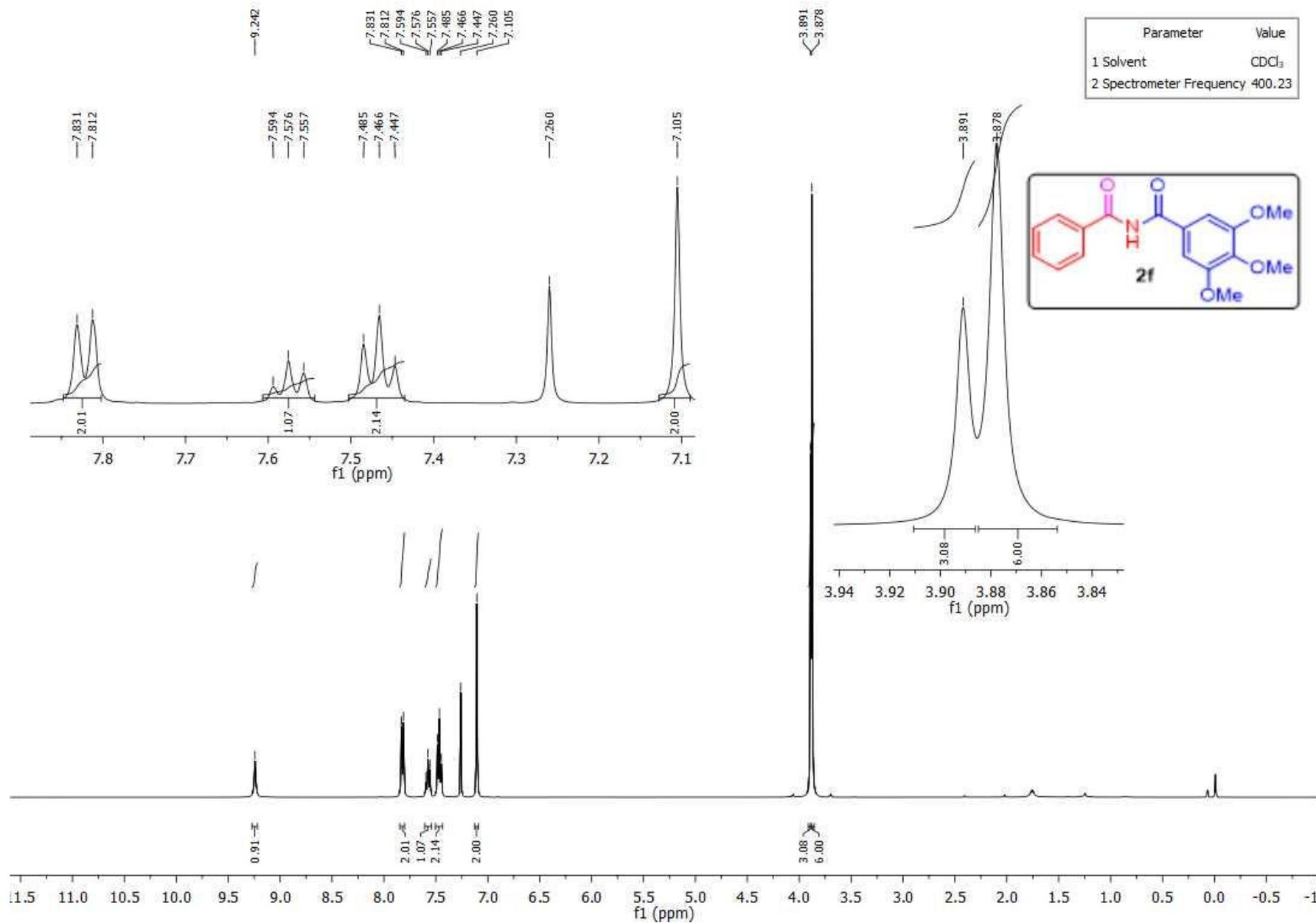


Fig. S82. ¹H NMR spectra of *N*-benzoyl-3,4,5-trimethoxybenzamide (**2f**).

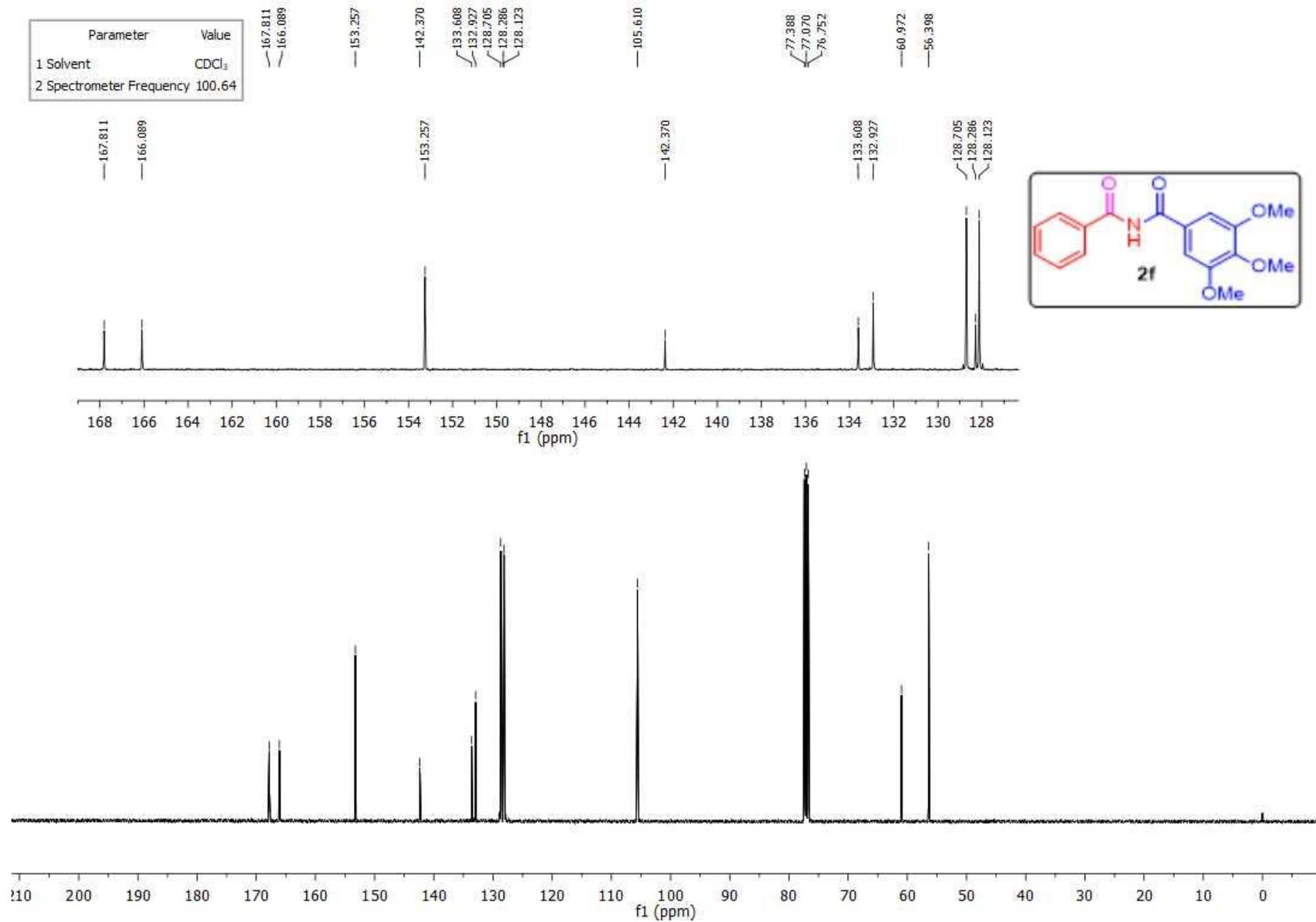
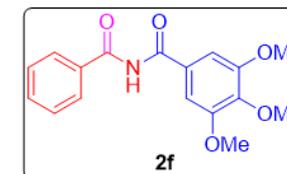


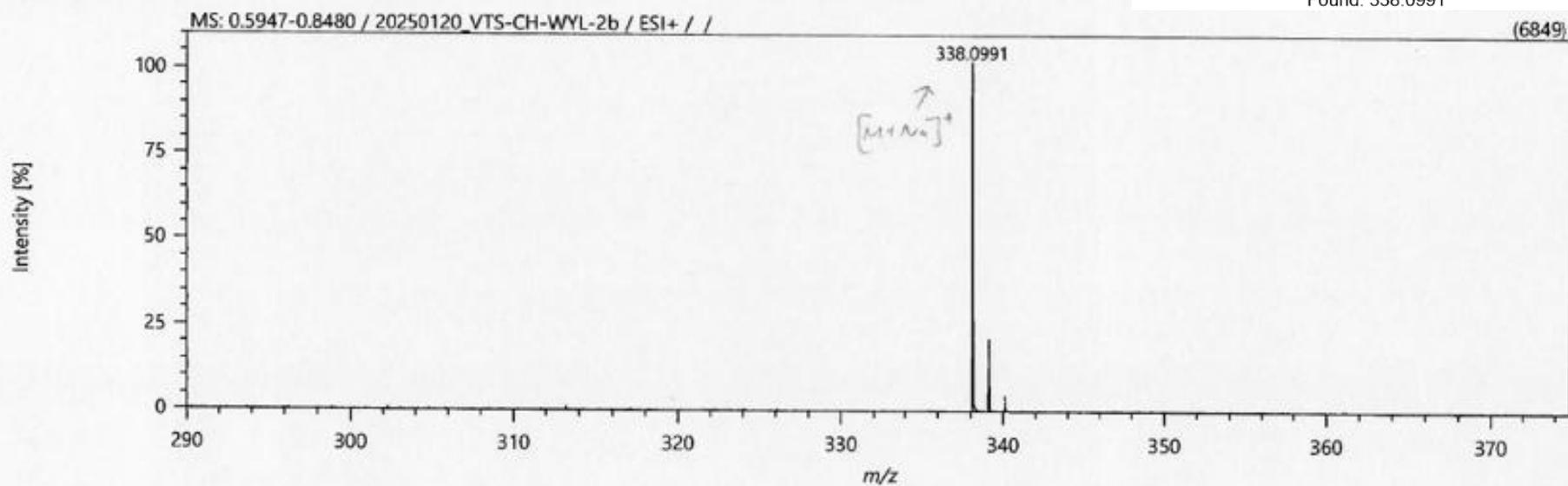
Fig. S83. ¹³C NMR spectra of *N*-benzoyl-3,4,5-trimethoxybenzamide (**2f**).

VTS-CH-WYL-2b (HR. ESI)



Chemical Formula: $C_{17}H_{17}NO_5Na$ $[M+Na]^+$ Calcd: 338.1004
Found: 338.0991

Spectrum



Elemental Composition

Parameters

Tolerance: ± 5.00 ppm

Electron: Odd/Even

Charge: +1

DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	5	1	0
Max	400	1000	5	1	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
338.09906	$C_{17}H_{17}NO_5Na$	338.09989	-0.83	-2.46	9.5

Fig. S84. HRMS data of *N*-benzoyl-3,4,5-trimethoxybenzamide (**2f**).

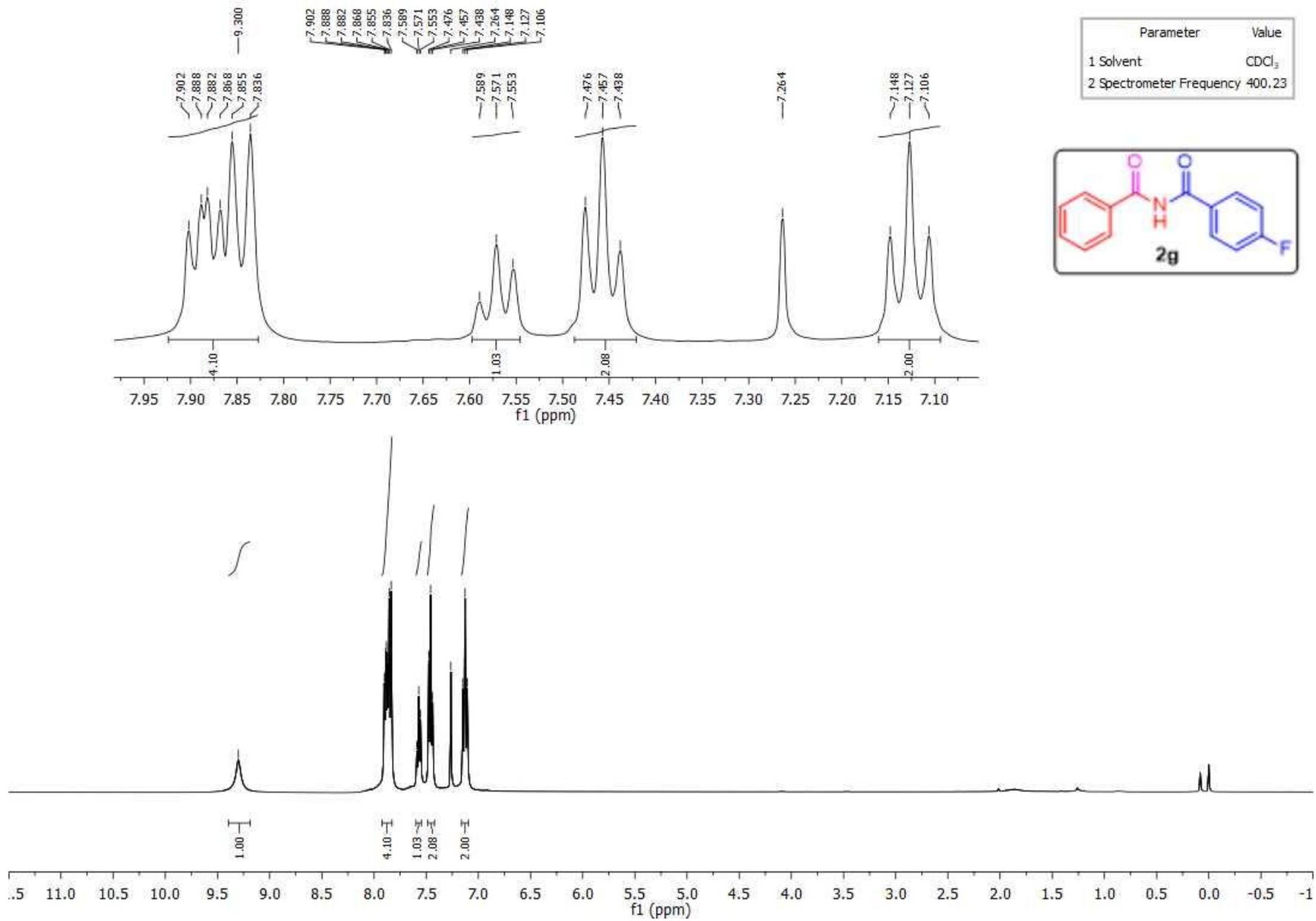


Fig. S85. ¹H NMR spectra of *N*-benzoyl-4-fluorobenzamide (**2g**).

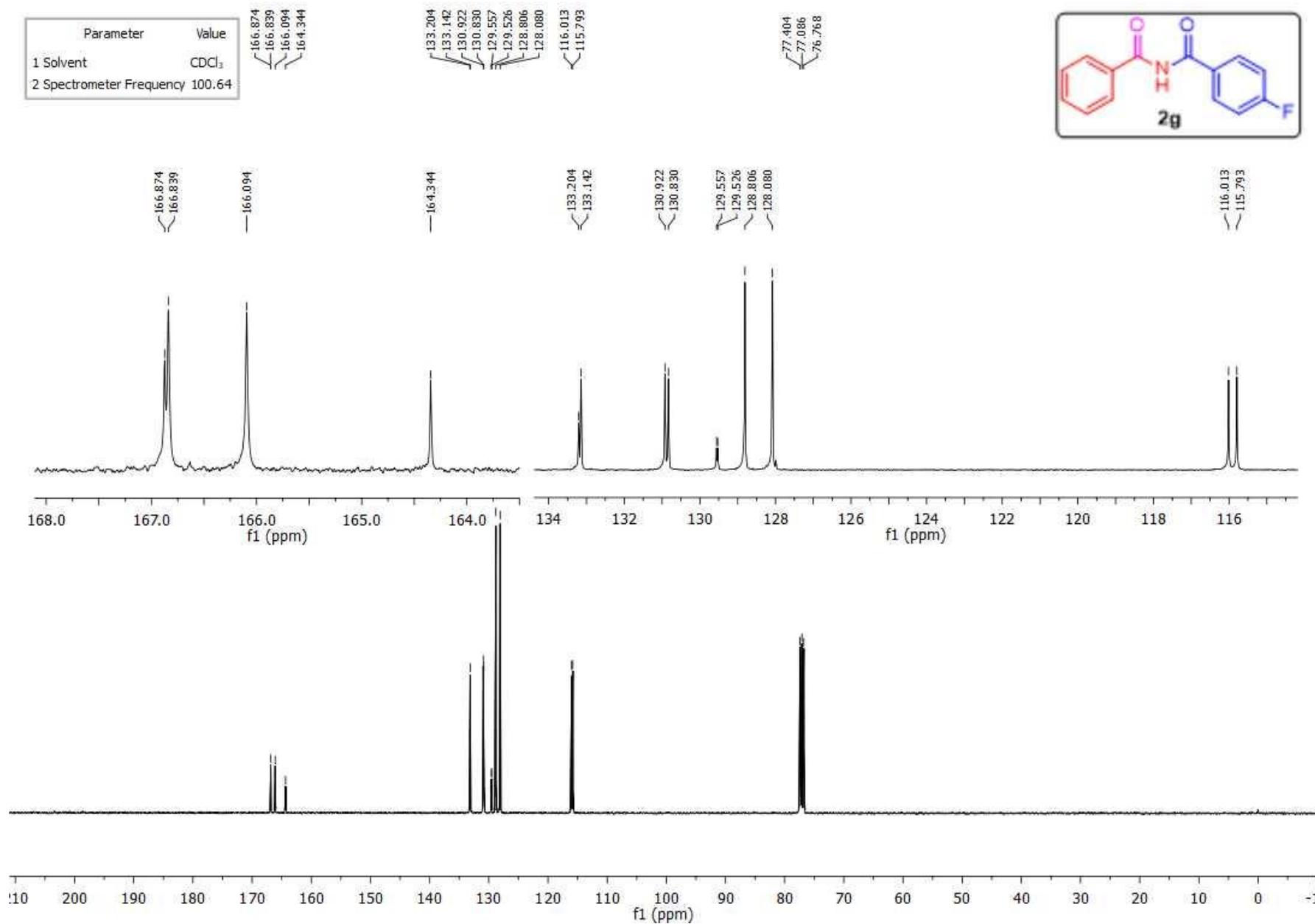
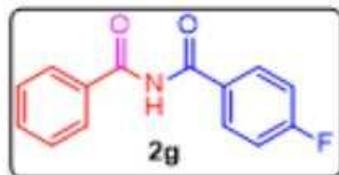


Fig. S86. ¹³C NMR spectra of *N*-benzoyl-4-fluorobenzamide (**2g**).

Parameter	Value
1 Solvent	CDCl ₃
2 Spectrometer Frequency	376.59



104.970
104.979
104.992
105.006
105.014

104.970
104.979
104.992
105.006
105.014

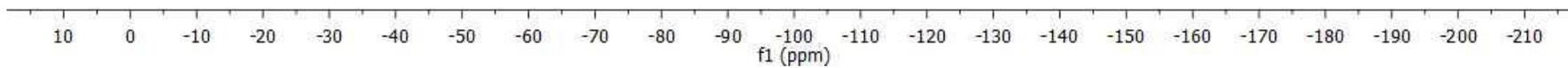
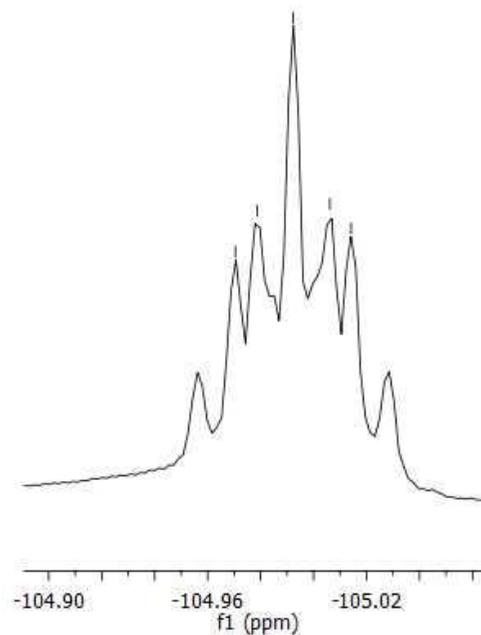


Fig. S87. ¹⁹F NMR spectra of *N*-benzoyl-4-fluorobenzamide (**2g**).

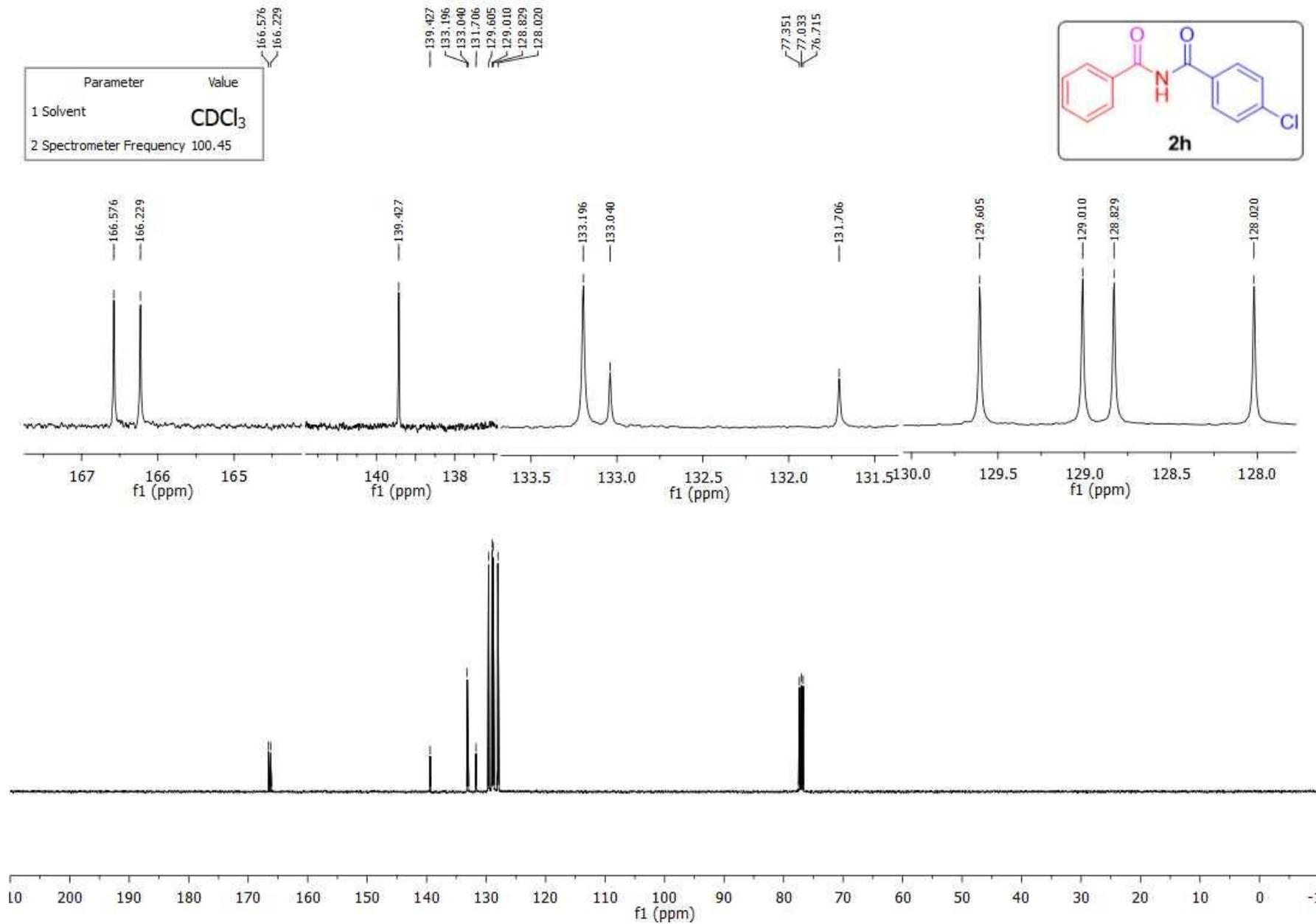


Fig. S89. ¹³C NMR spectra of *N*-benzoyl-4-chlorobenzamide (**2h**).

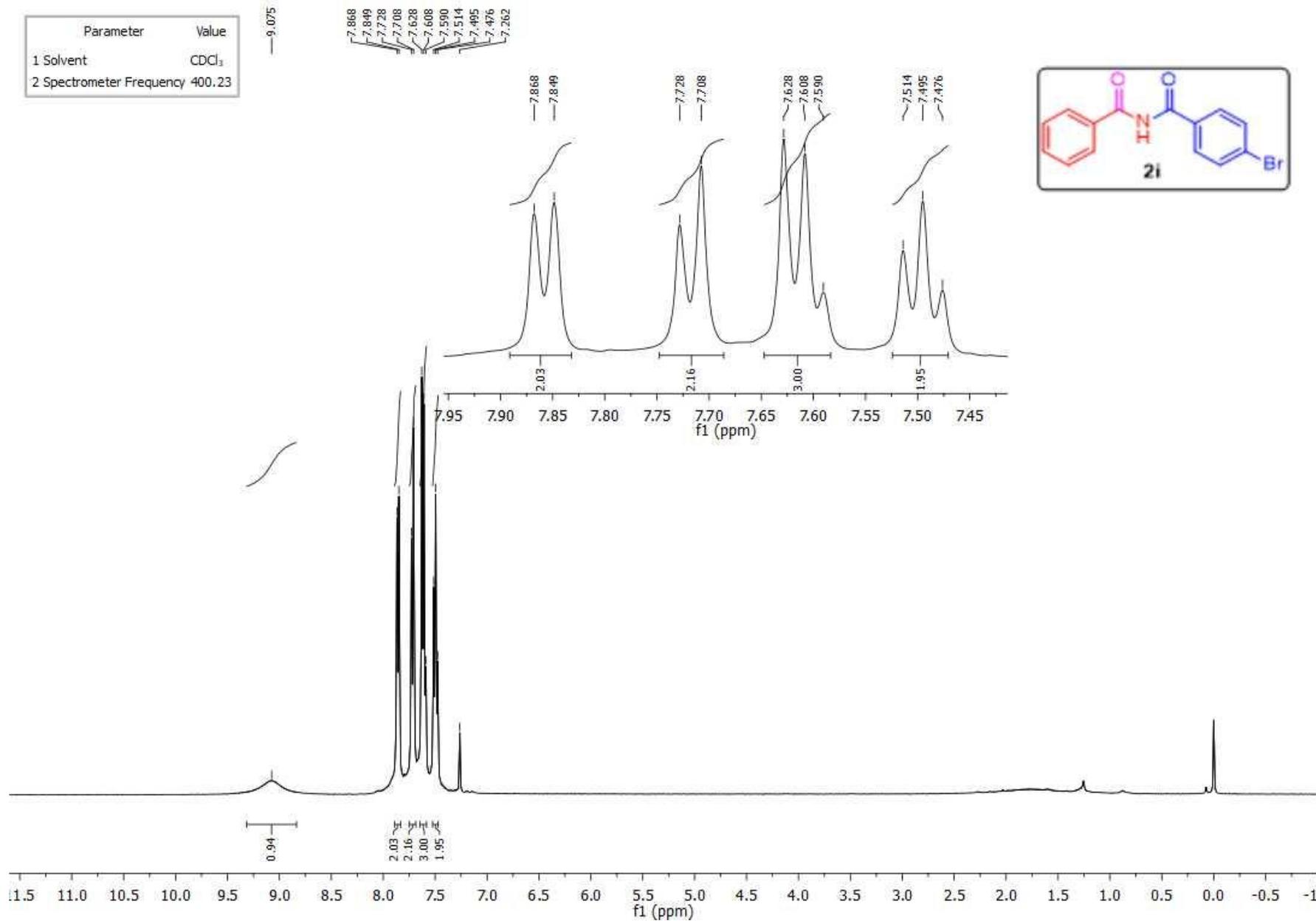


Fig. S90. ¹H NMR spectra of *N*-benzoyl-4-bromobenzamide (**2i**).

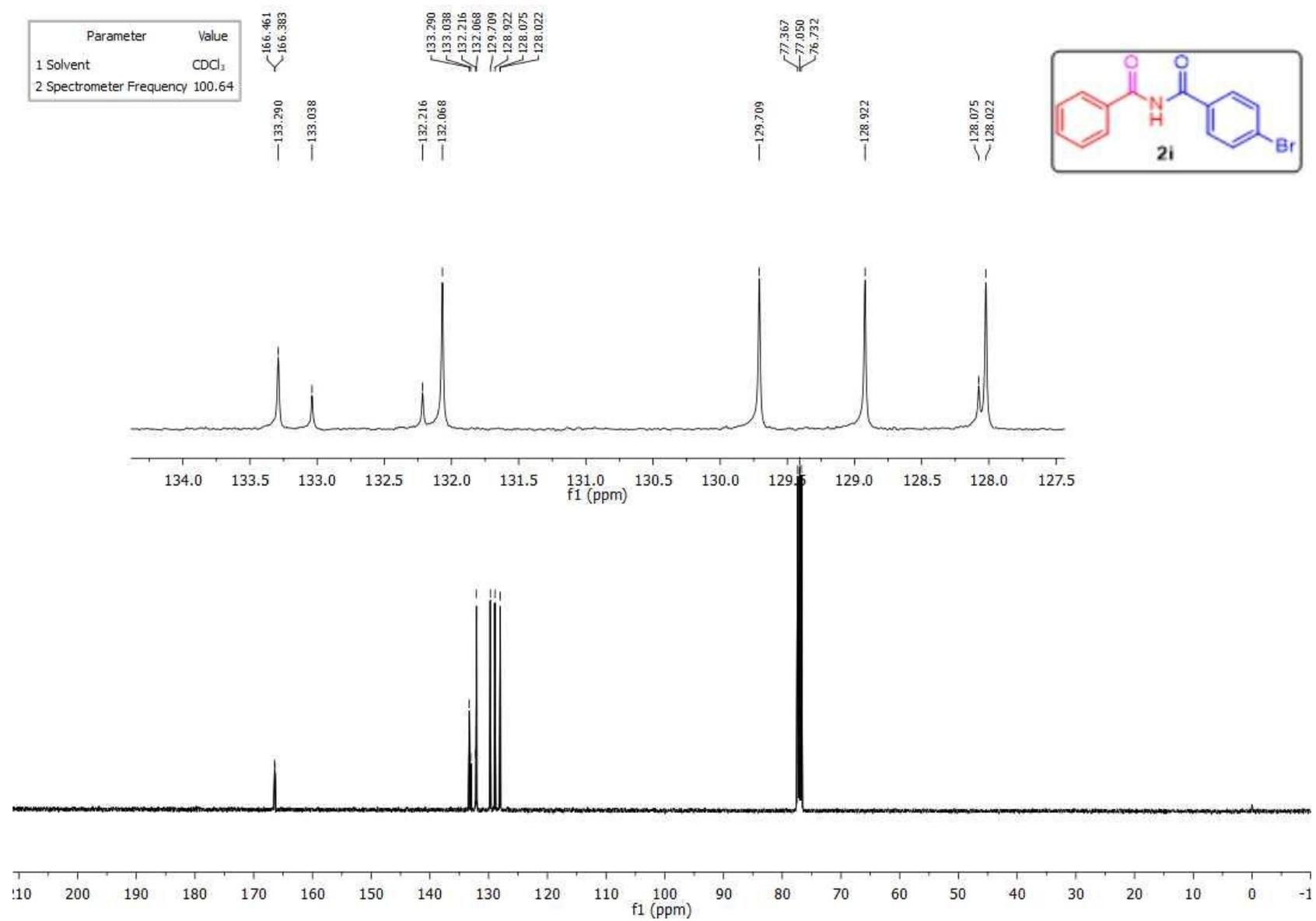


Fig. S91. ¹³C NMR spectra of *N*-benzoyl-4-bromobenzamide (**2i**).

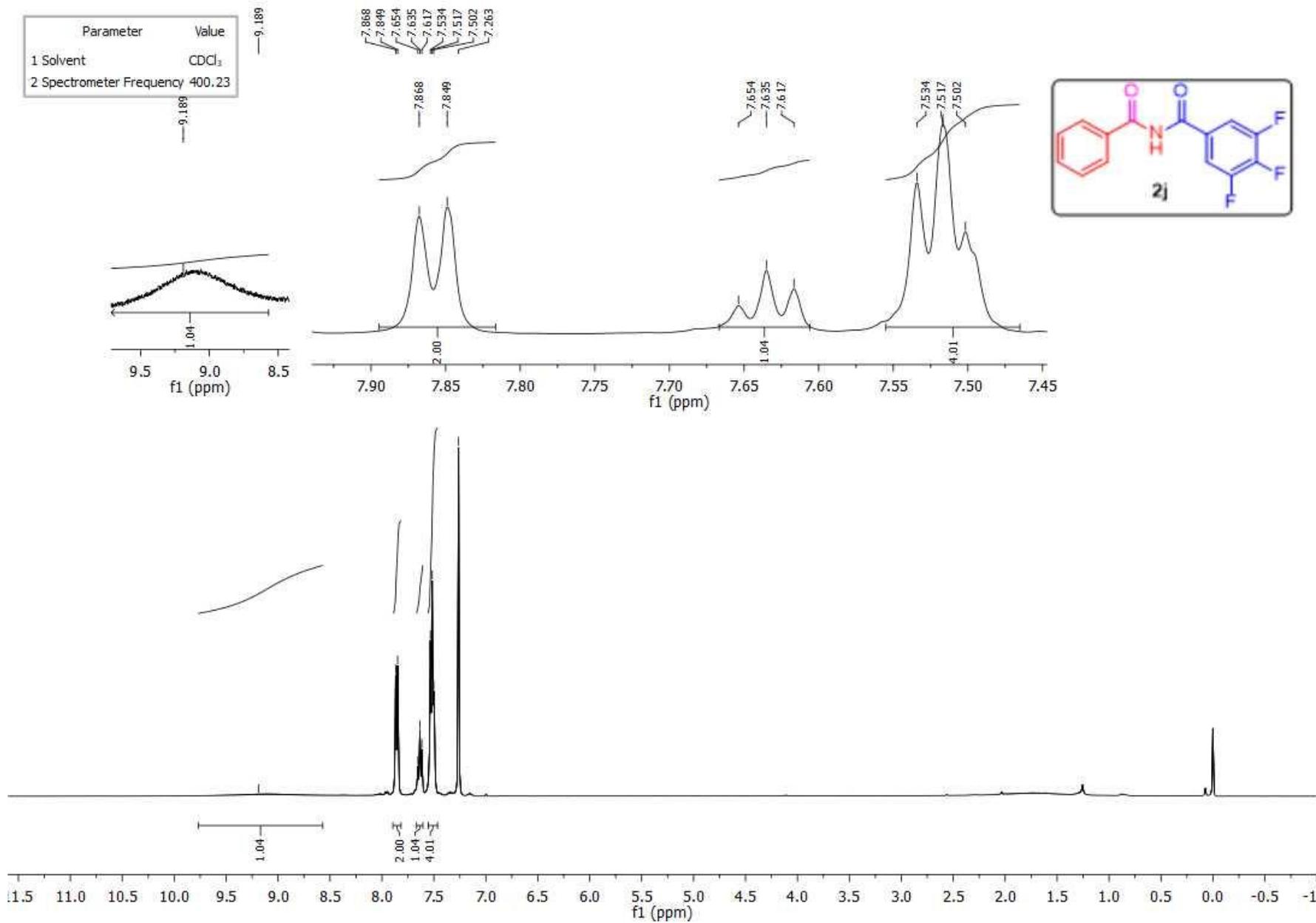


Fig. S92. ¹H NMR spectra of *N*-benzoyl-3,4,5-trifluorobenzamide (**2j**).

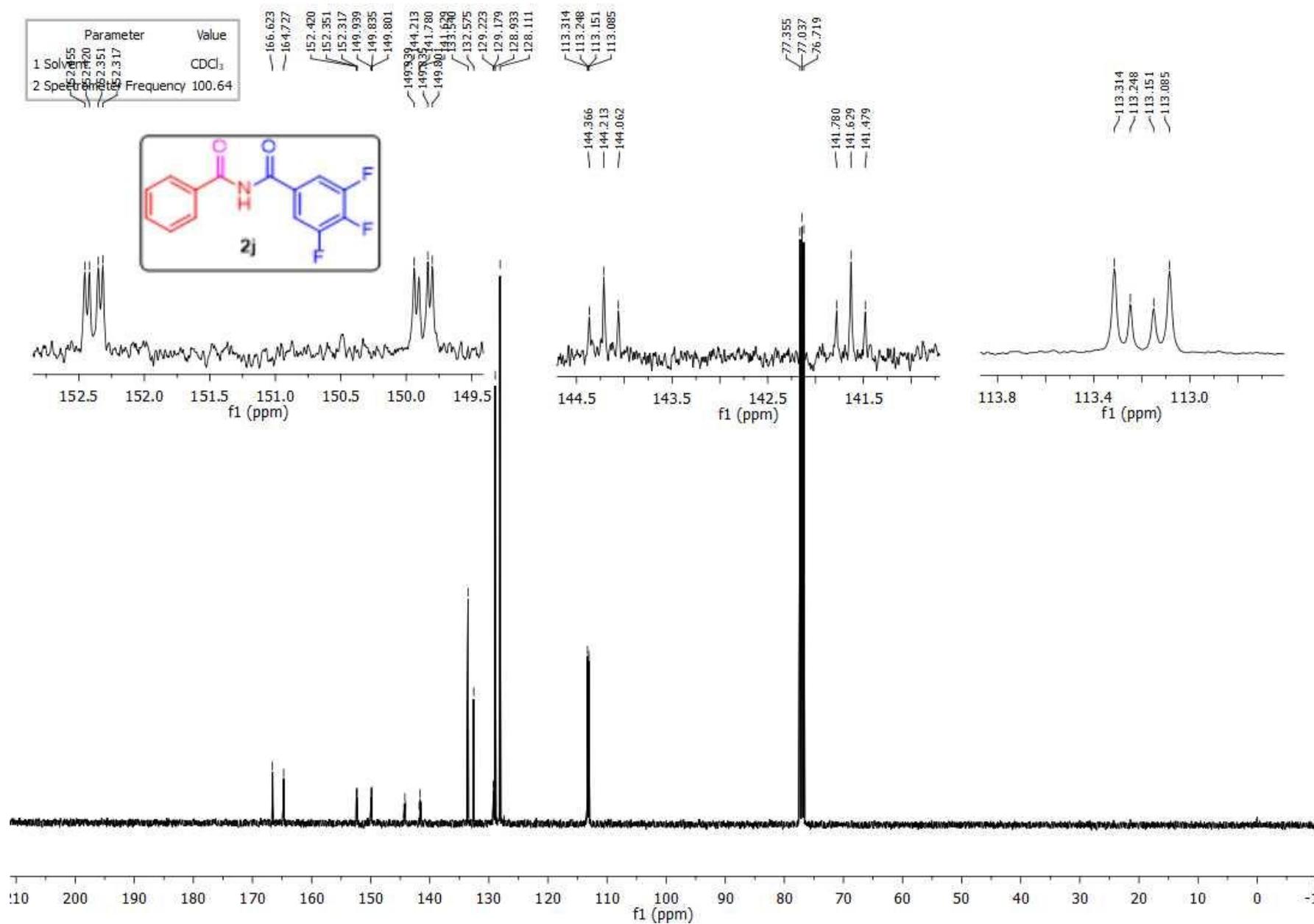


Fig. S93. ¹³C NMR spectra of *N*-benzoyl-3,4,5-trifluorobenzamide (**2j**).

Parameter	Value
1 Solvent	CDCl ₃
2 Spectrometer Frequency	376.59

131.537
131.556
131.590
131.610

152.098

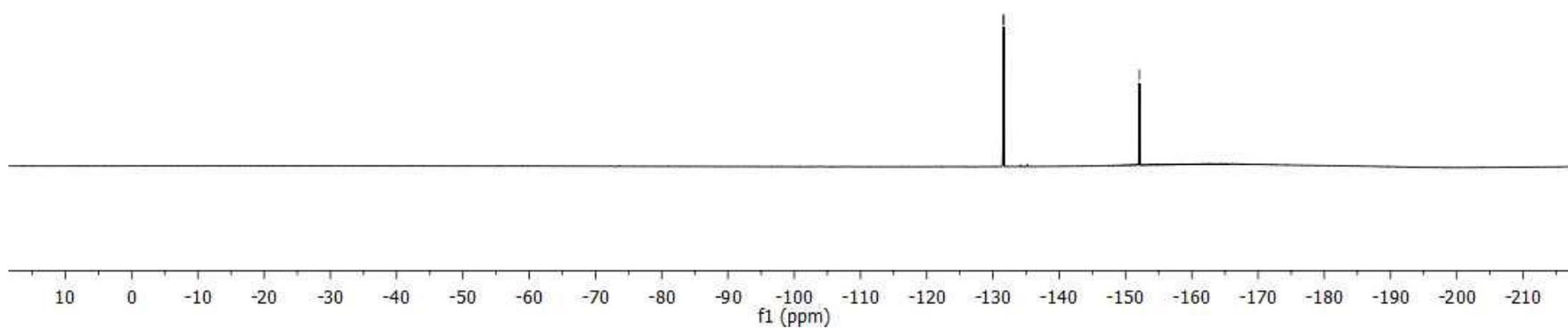
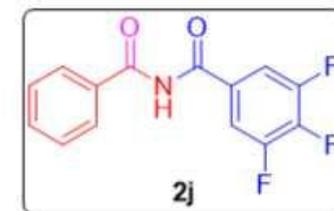
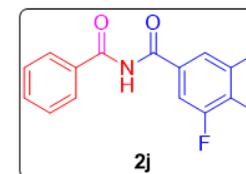


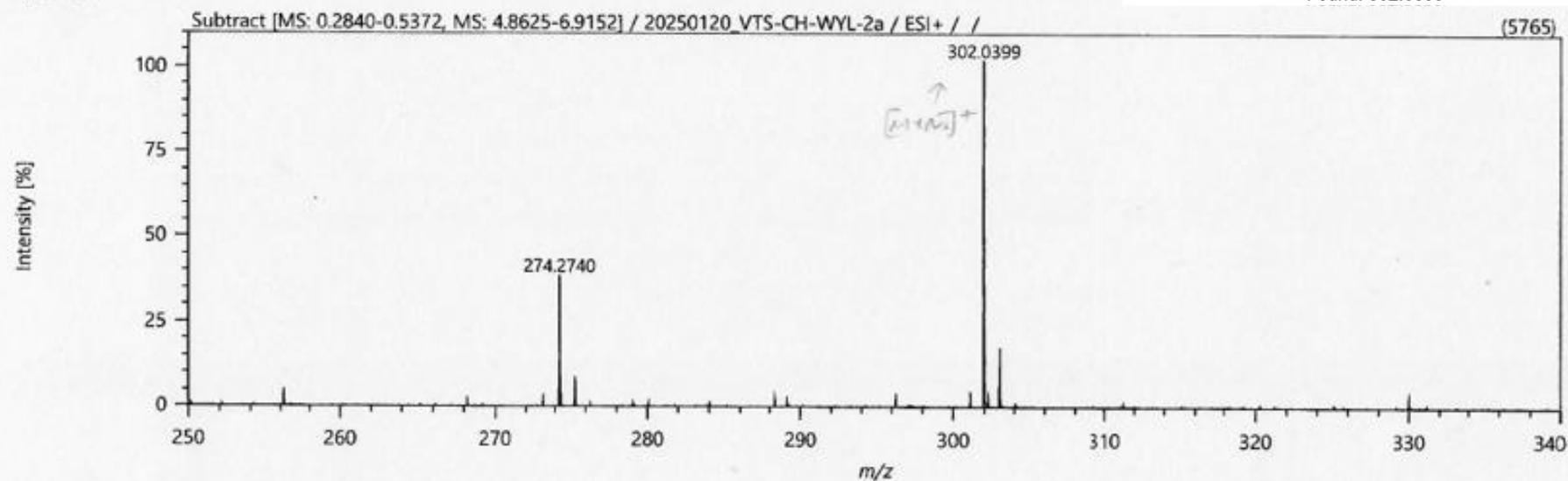
Fig. S94. ¹⁹F NMR spectra of *N*-benzoyl-3,4,5-trifluorobenzamide (**2j**).

VTS-CH-WYL-2a (HR-ESI)



Chemical Formula: $C_{14}H_8F_3NO_2Na$ $[M+Na]^+$ Calcd: 302.0405
Found: 302.0399

Spectrum



Elemental Composition

Parameters

Tolerance: ± 5.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na	F
Min	0	0	2	1	0	3
Max	400	1000	2	1	1	3

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
302.03987	$C_{14}H_8N O_2 F_3 Na$	302.03993	-0.06	-0.21	9.5

Fig. S95. HRMS data of *N*-benzoyl-3,4,5-trifluorobenzamide (**2j**).

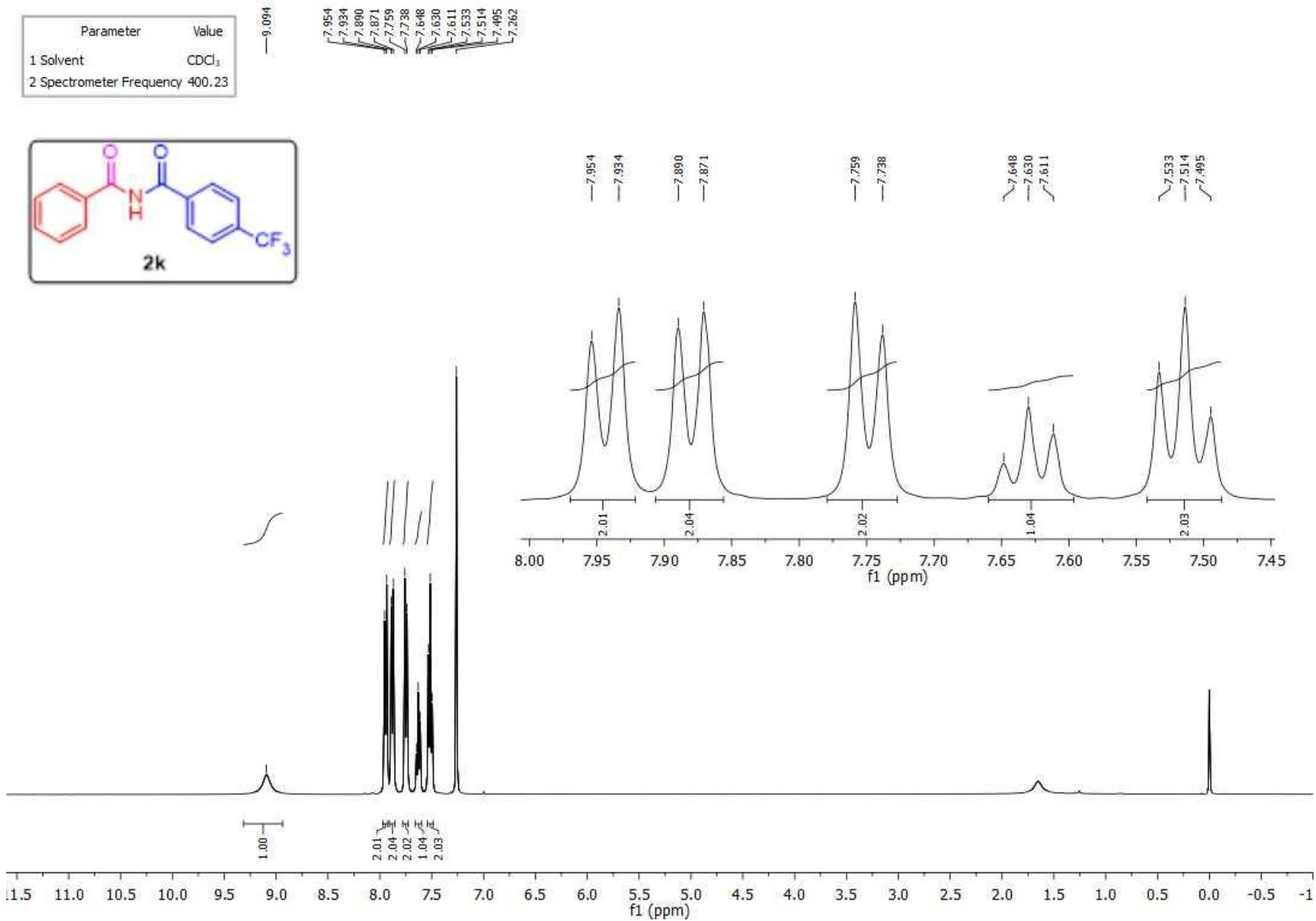


Fig. S96. ¹H NMR spectra of *N*-benzoyl-4-(trifluoromethyl)benzamide (**2k**).

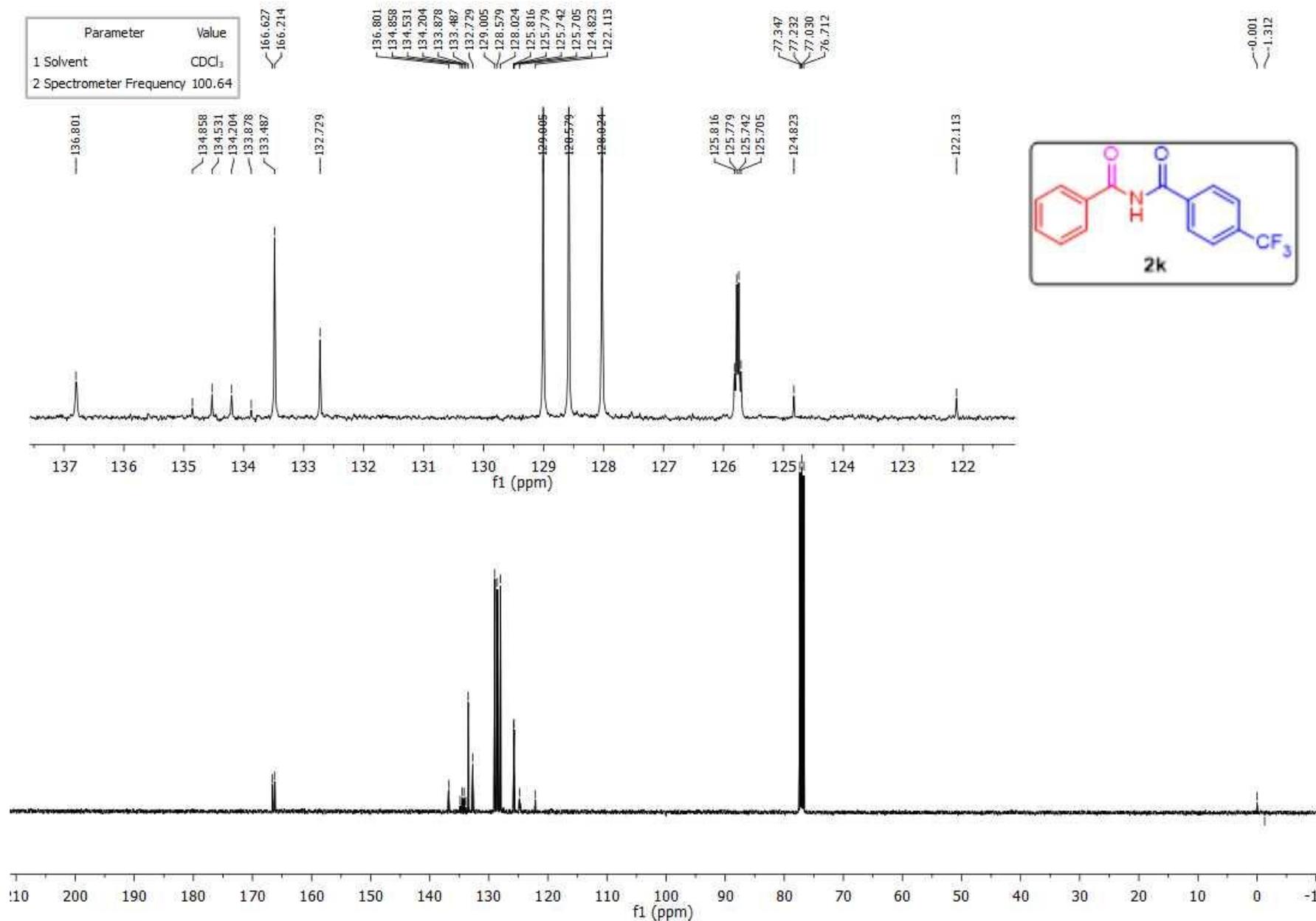


Fig. S97. ¹³C NMR spectra of *N*-benzoyl-4-(trifluoromethyl)benzamide (**2k**).

Parameter	Value
1 Solvent	CDCl ₃
2 Spectrometer Frequency	376.59

63.141

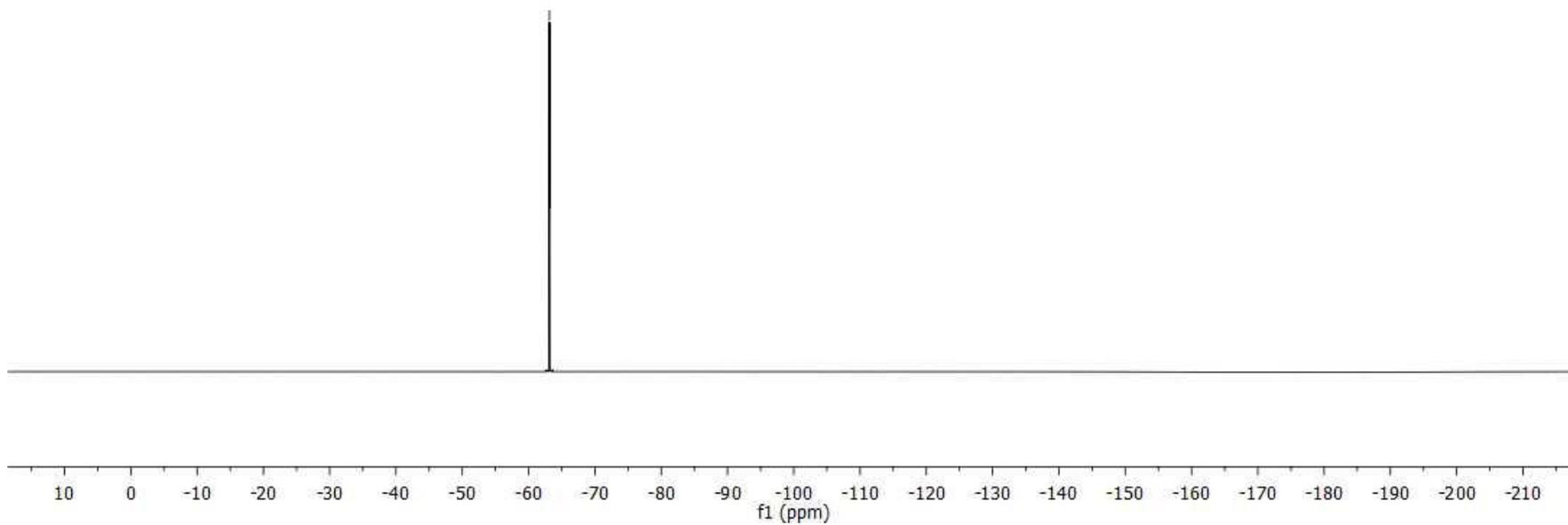
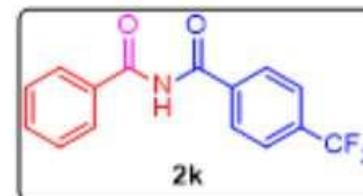


Fig. S98. ¹⁹F NMR spectra of *N*-benzoyl-4-(trifluoromethyl)benzamide (**2k**).

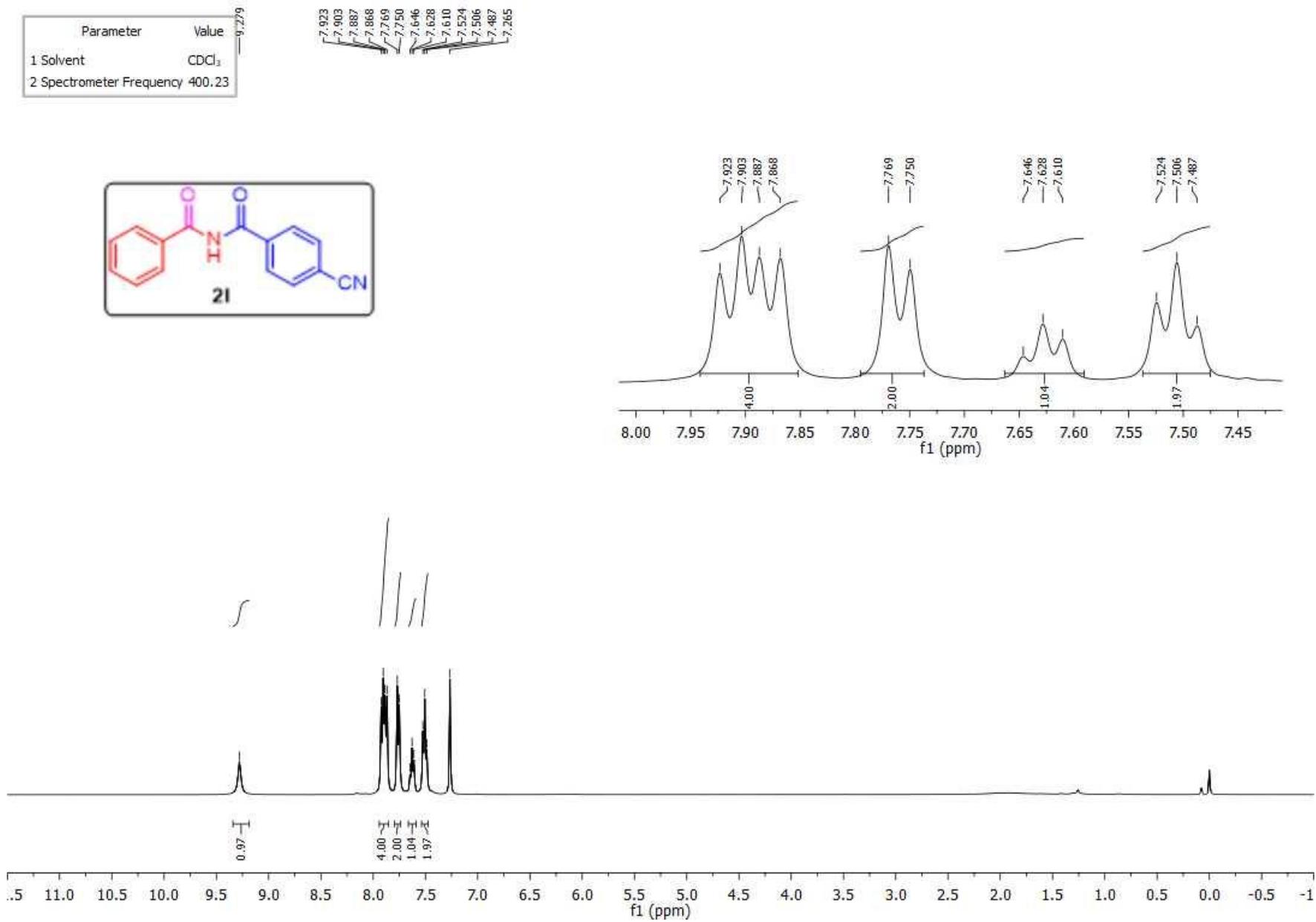


Fig. S99. ¹H NMR spectra of *N*-benzoyl-4-cyanobenzamide (**21**).

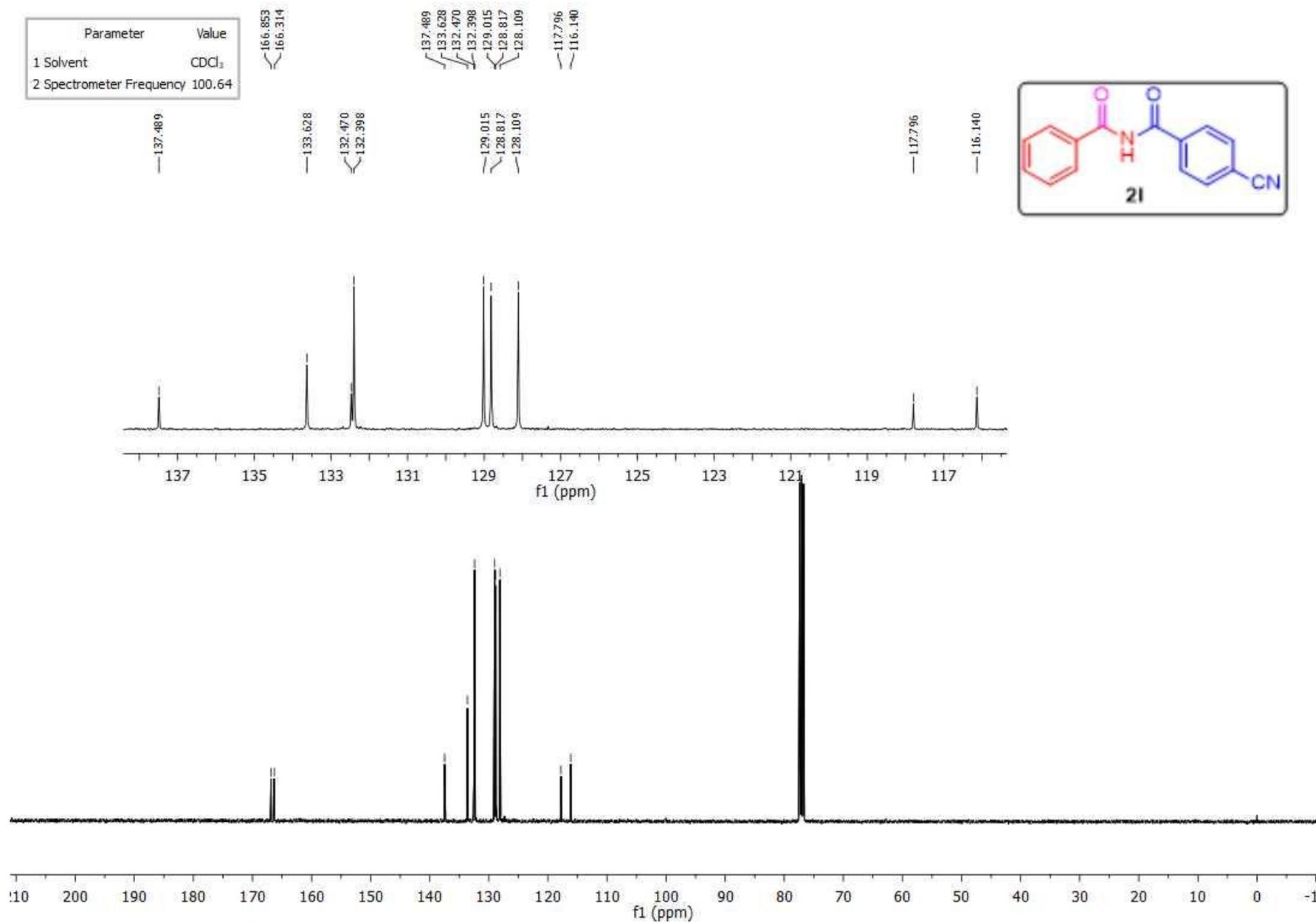


Fig. S100. ¹³C NMR spectra of *N*-benzoyl-4-cyanobenzamide (**2I**).

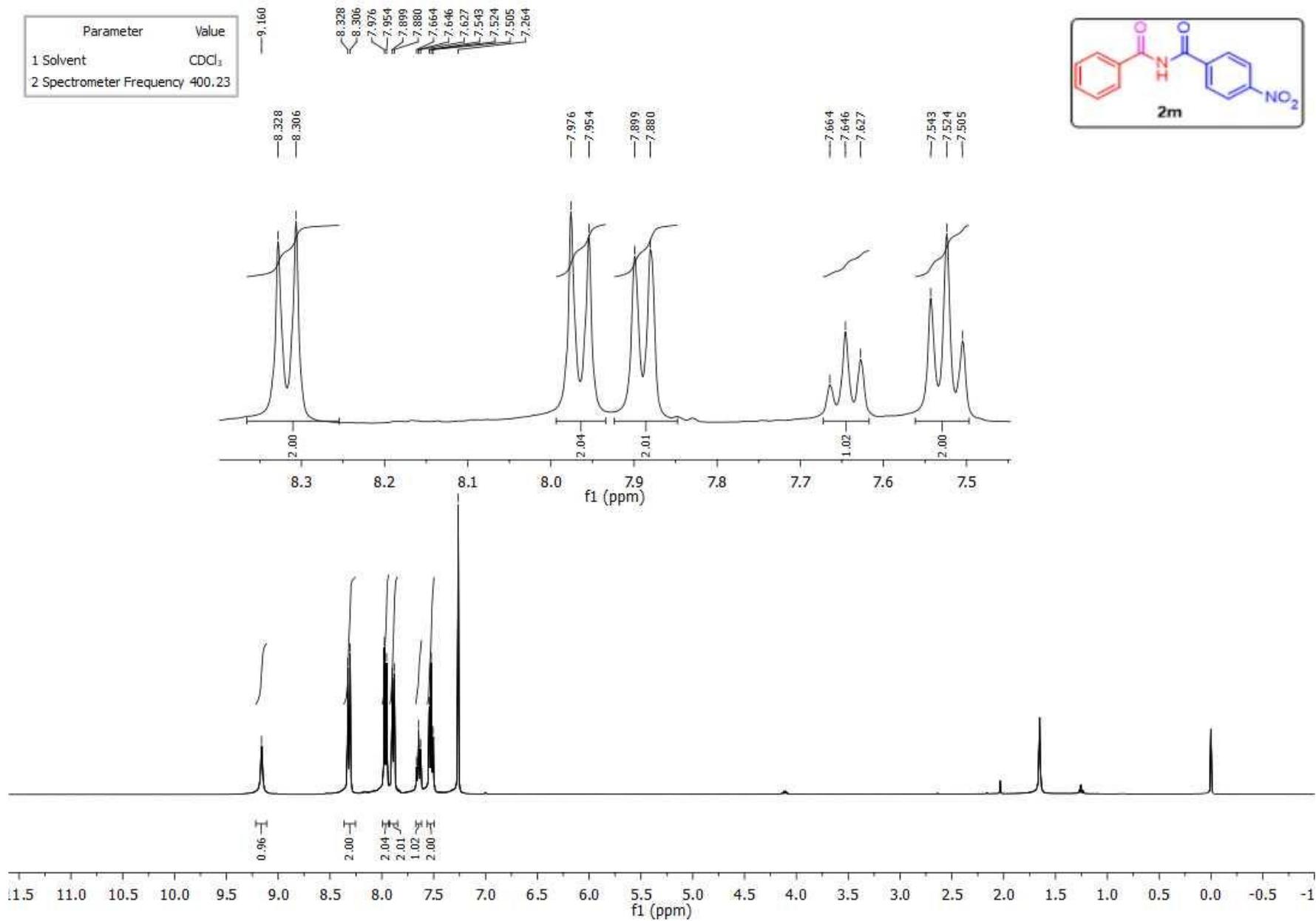


Fig. S101. ¹H NMR spectra of *N*-benzoyl-4-nitrobenzamide (**2m**).

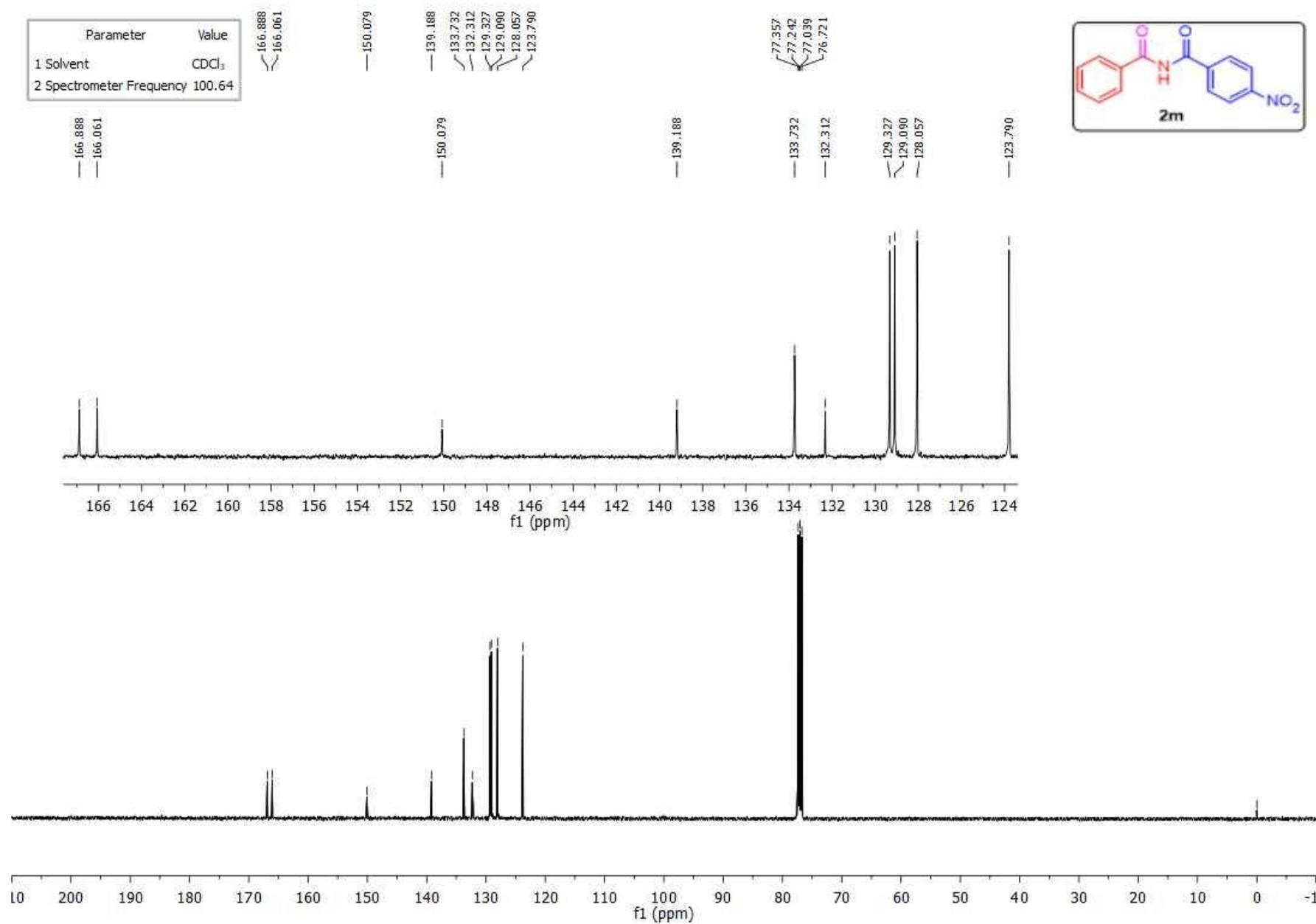


Fig. S102. ¹³C NMR spectra of *N*-benzoyl-4-nitrobenzamide (**2m**).

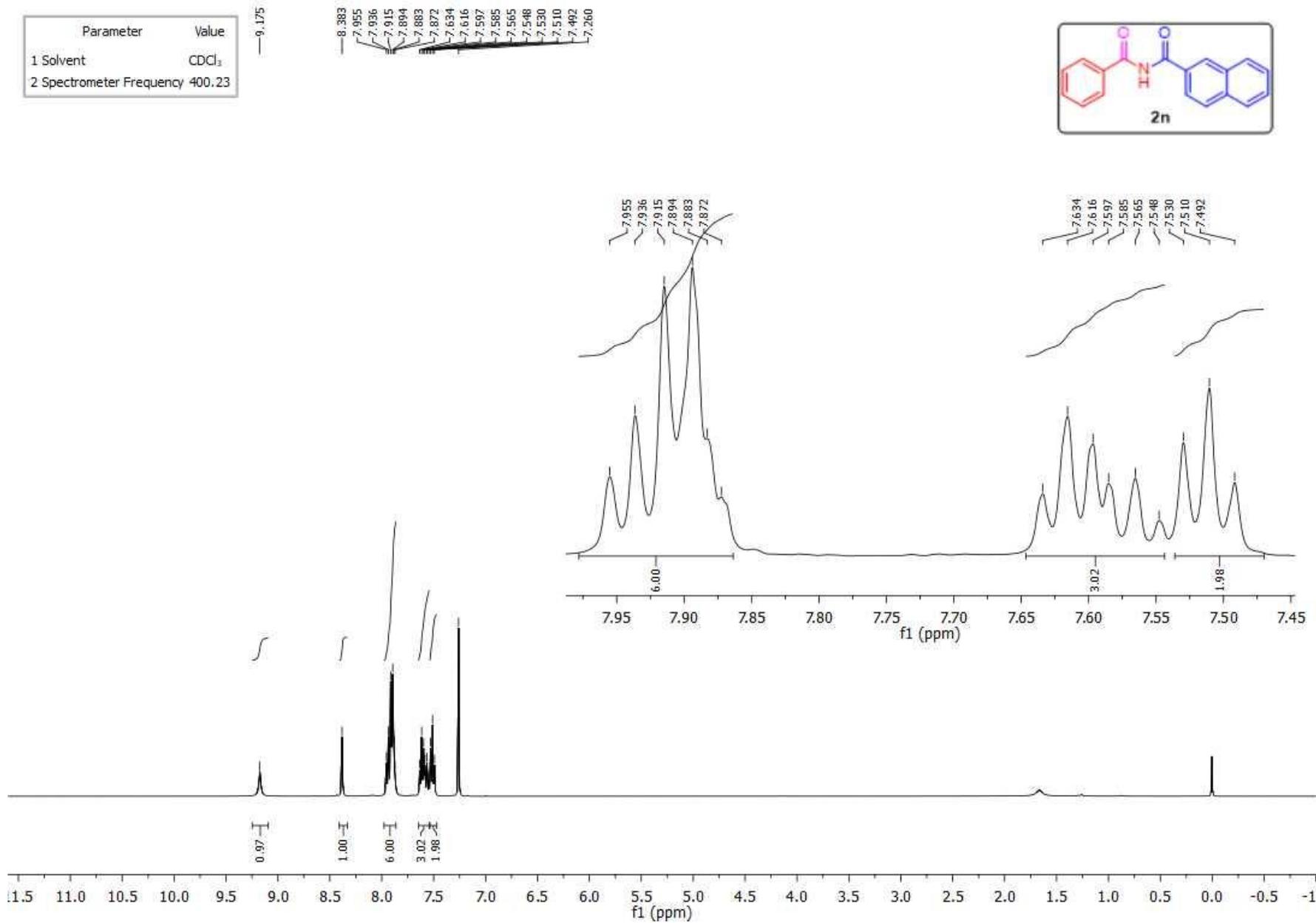


Fig. S103. ¹H NMR spectra of *N*-benzoyl-2-naphthamide (**2n**).

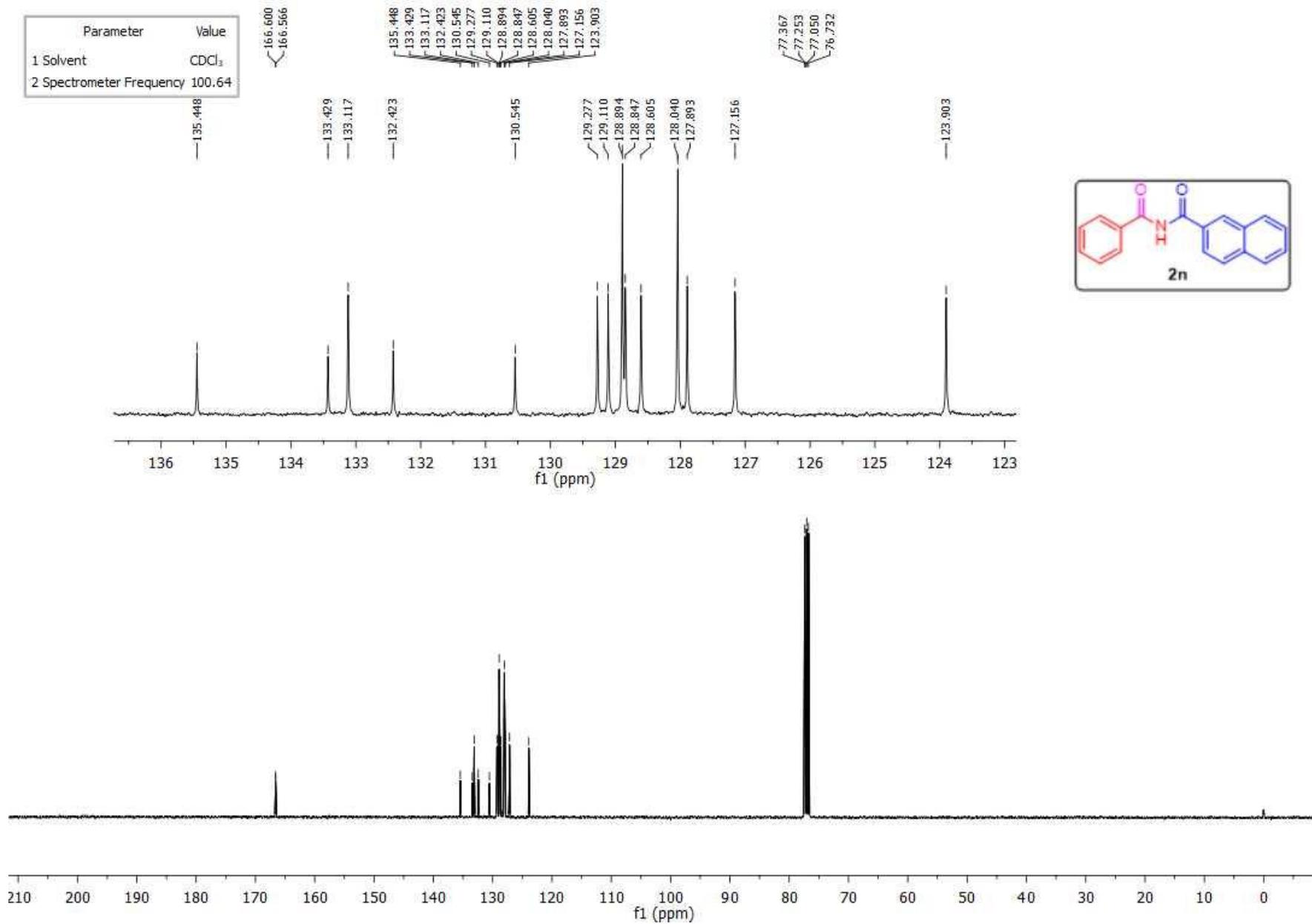


Fig. S104. ¹³C NMR spectra of *N*-benzoyl-2-naphthamide (**2n**).

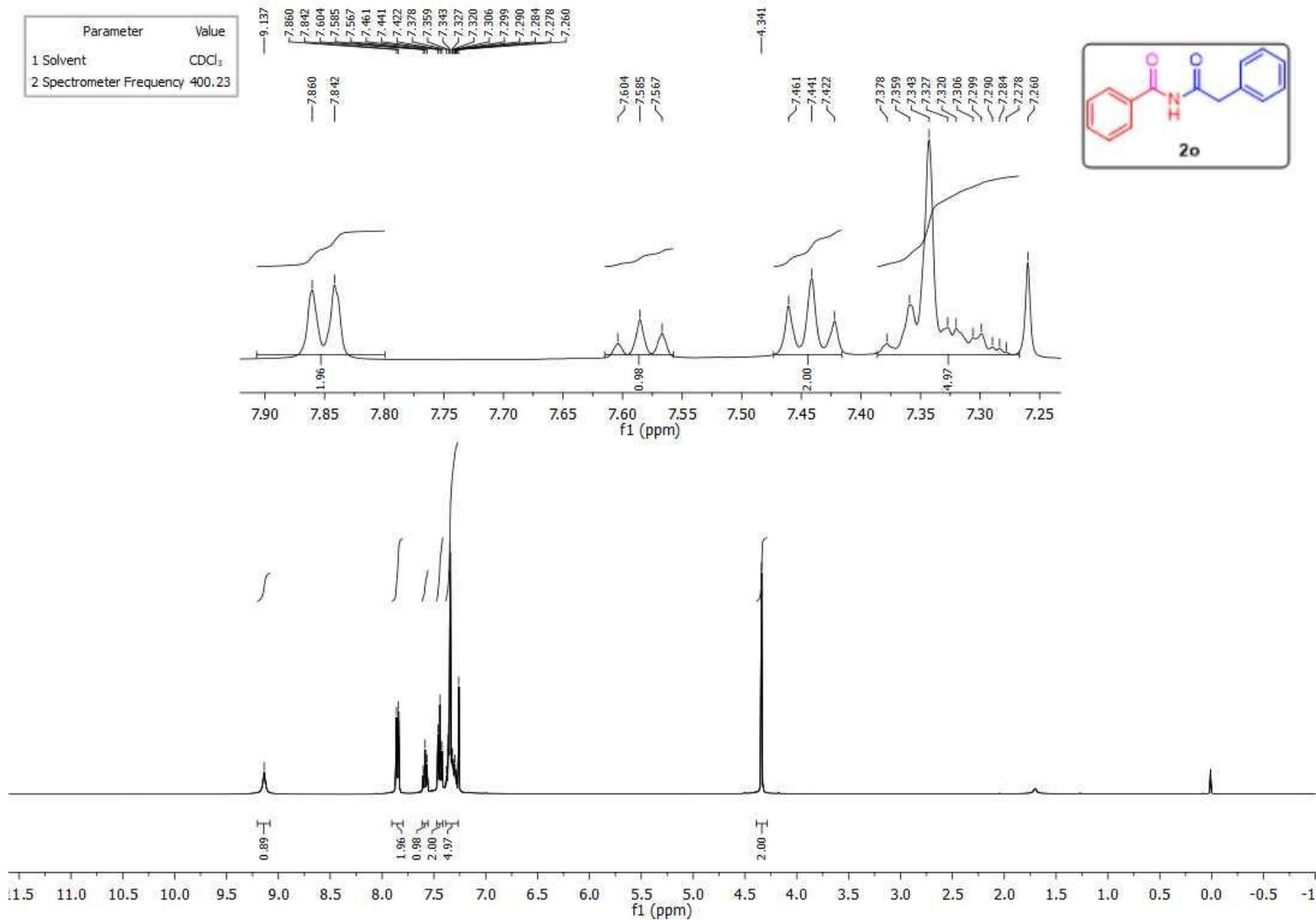


Fig. S105. ¹H NMR spectra of *N*-(2-phenylacetyl)benzamide (**2o**).

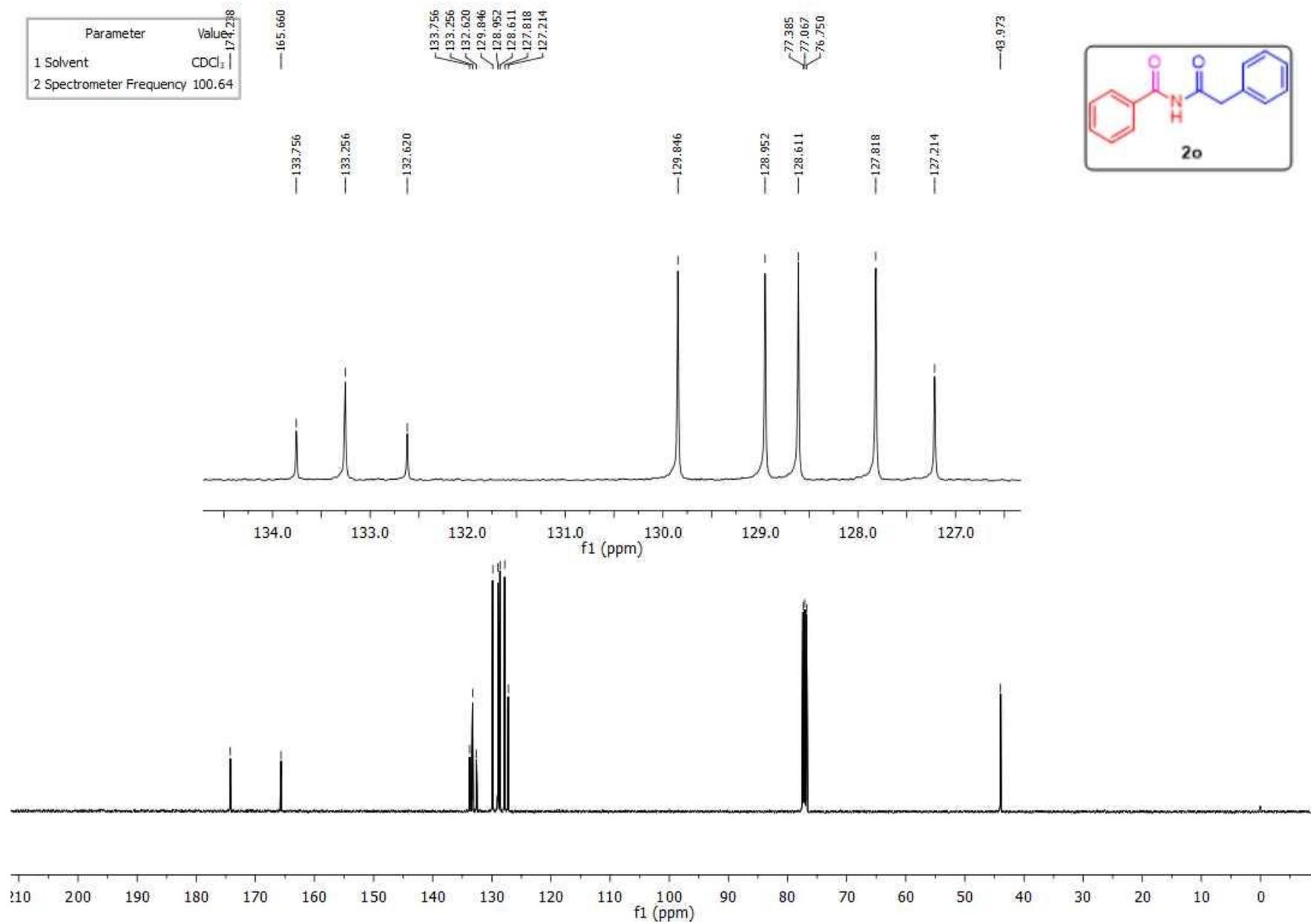


Fig. S106. ¹³C NMR spectra of *N*-(2-phenylacetyl)benzamide (**2o**).

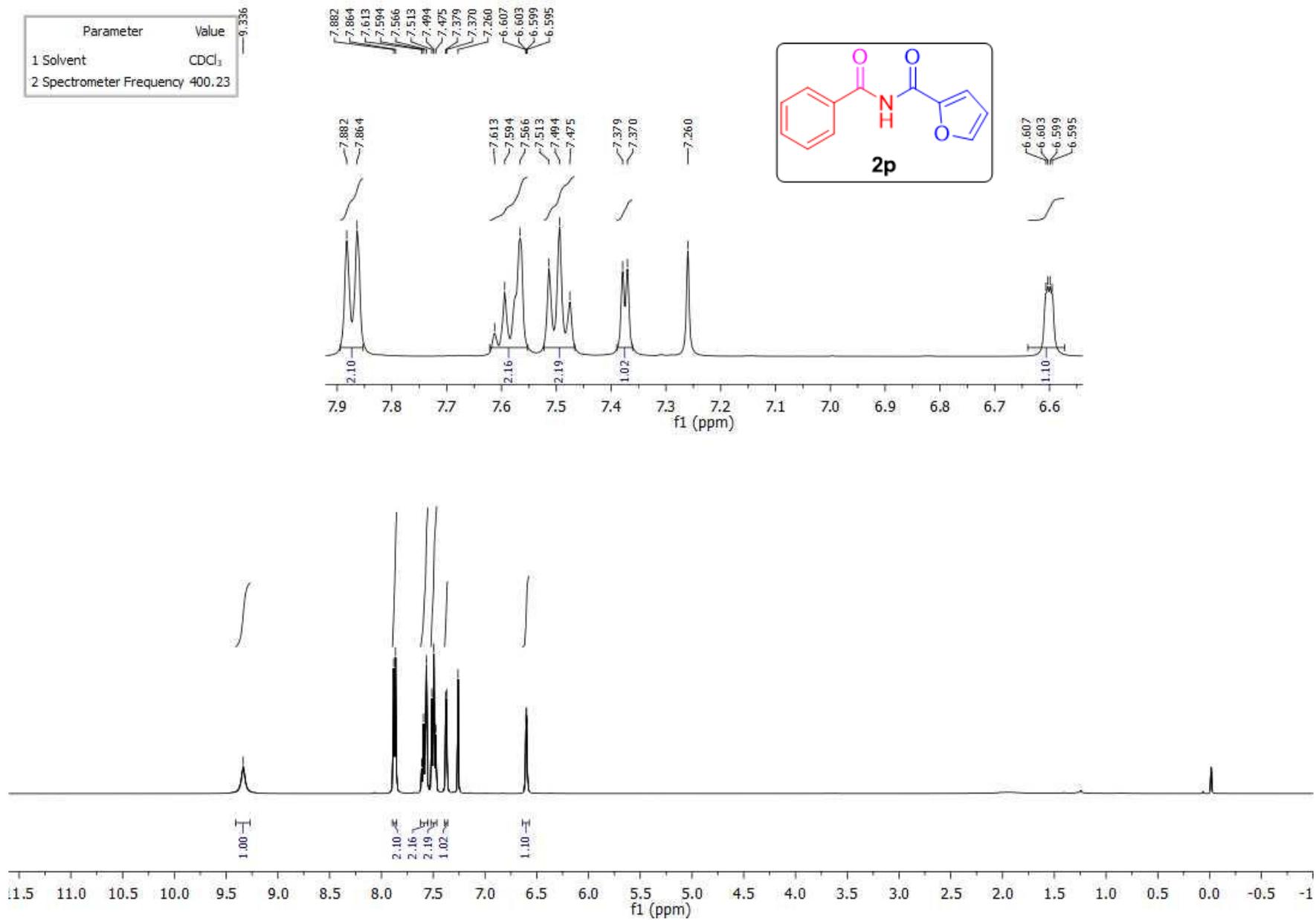


Fig. S107. ¹H NMR spectra of *N*-benzoylfuran-2-carboxamide (**2p**).

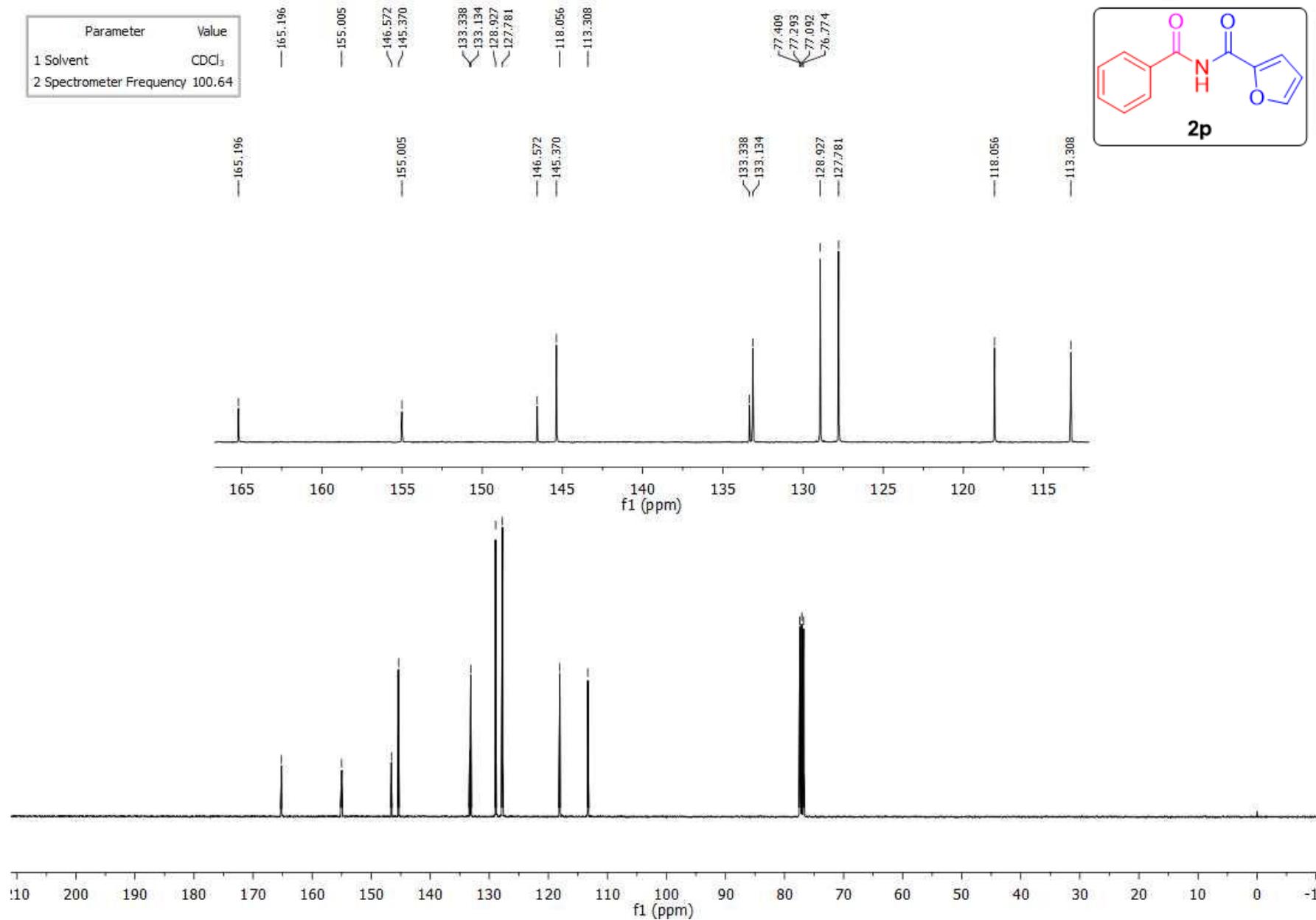


Fig. S108. ¹³C NMR spectra of *N*-benzoylfuran-2-carboxamide (**2p**).

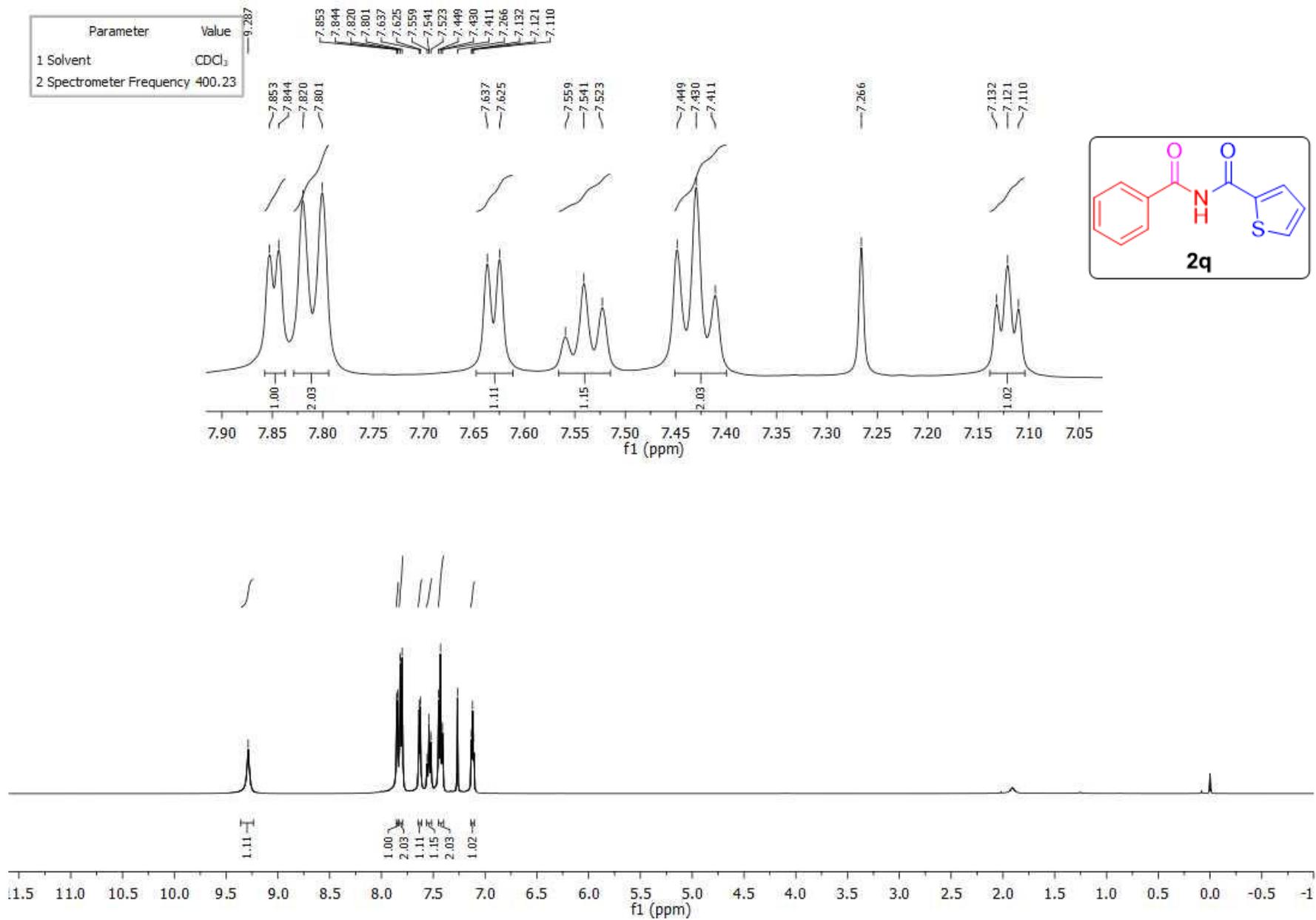


Fig. S109. ¹H NMR spectra of *N*-benzoylthiophene-2-carboxamide (**2q**).

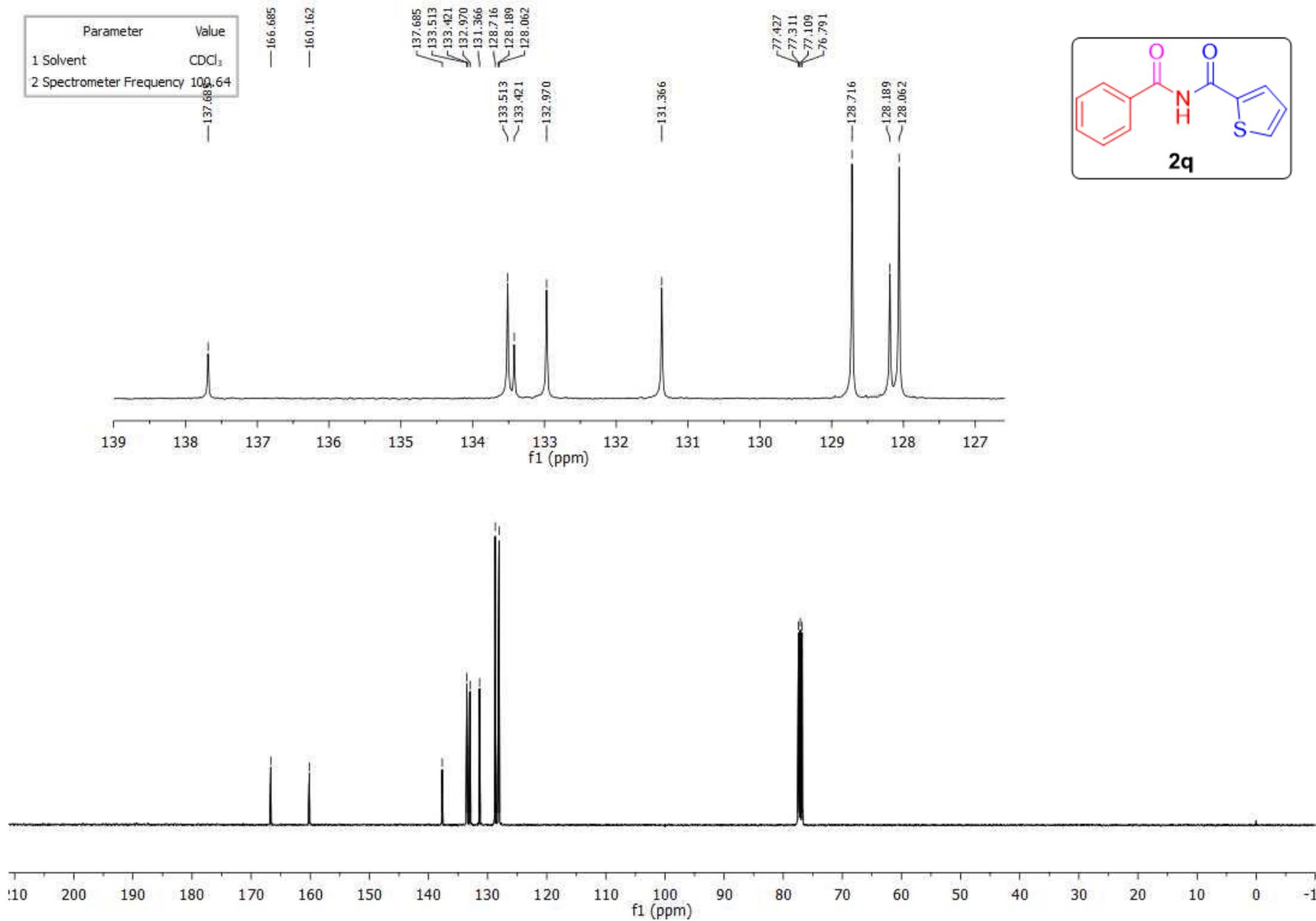


Fig. S110. ¹³C NMR spectra of N-benzoylthiophene-2-carboxamide (**2q**).

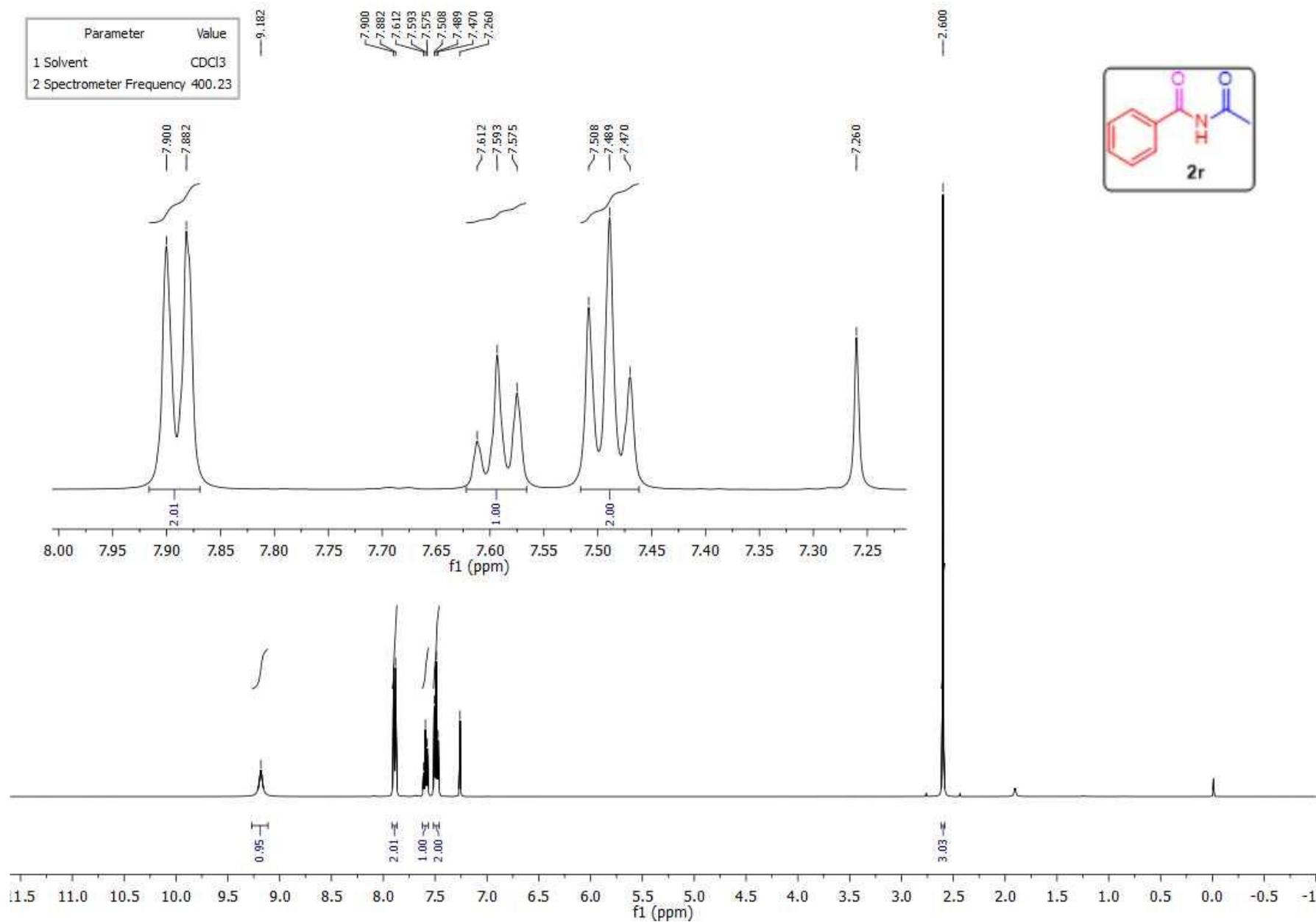


Fig. S111. ¹H NMR spectra of *N*-acetylbenzamide (**2r**).

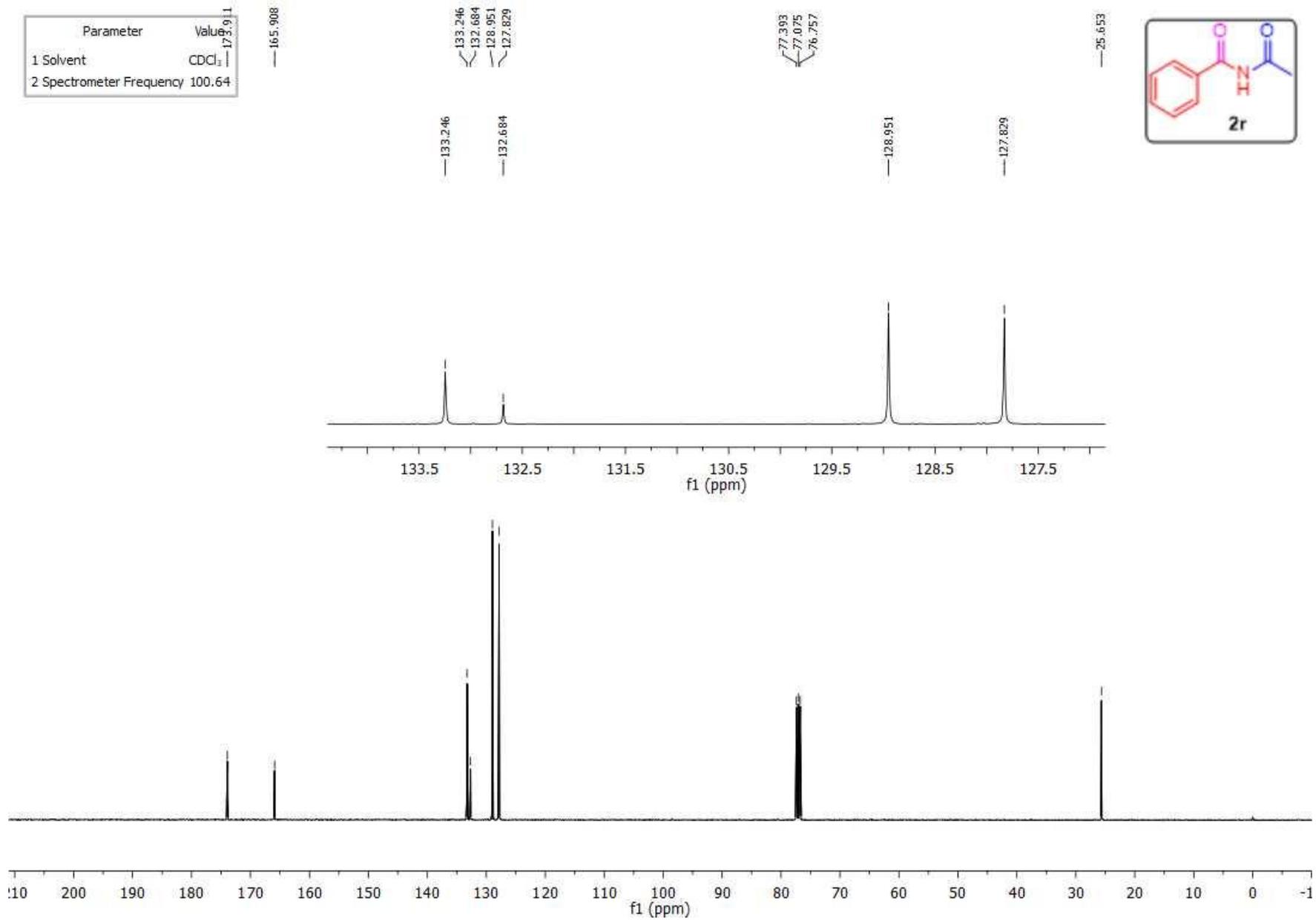


Fig. S112. ¹³C NMR spectra of *N*-acetylbenzamide (**2r**).

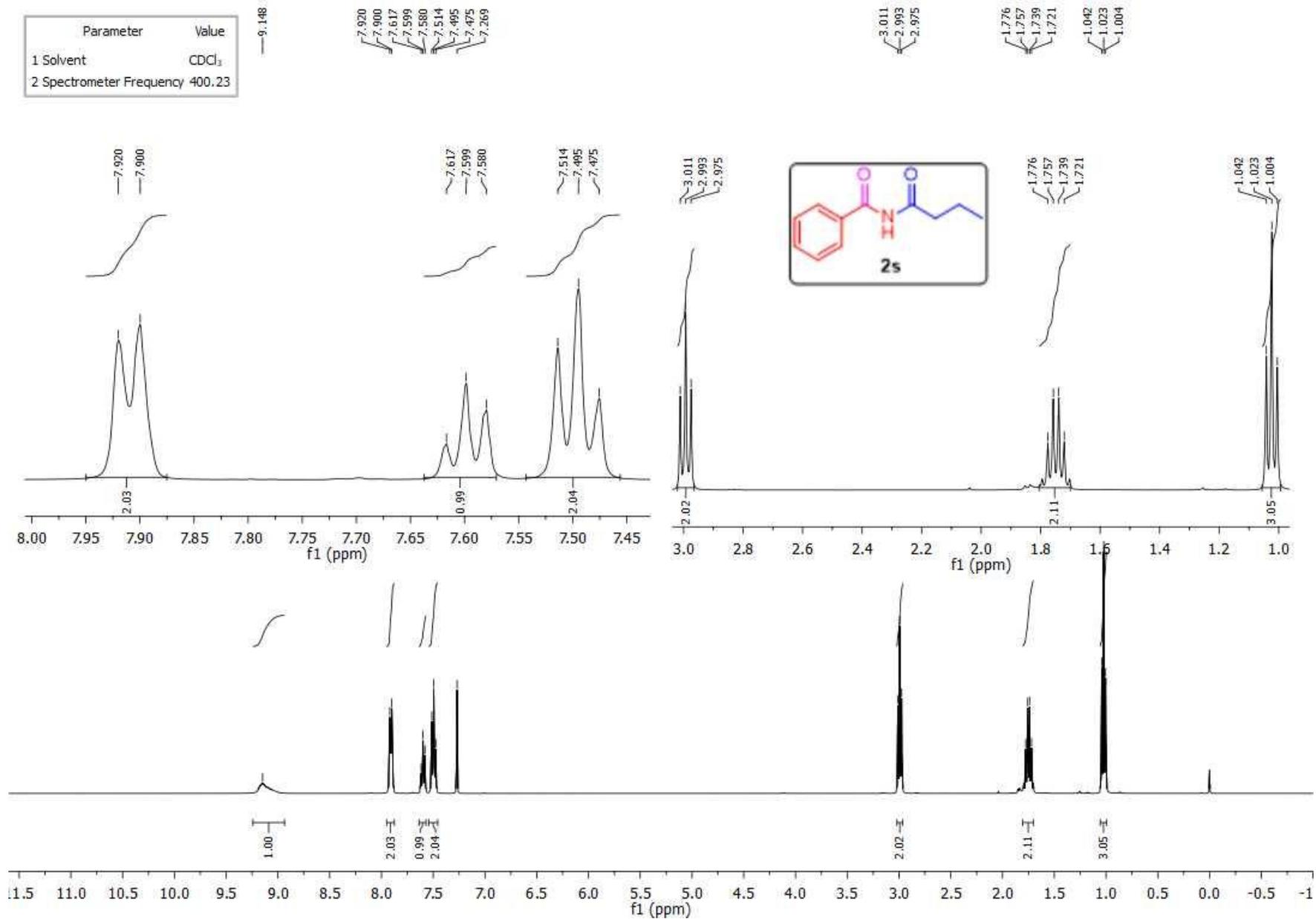


Fig. S113. ¹H NMR spectra of *N*-butyrylbenzamide (**2s**).

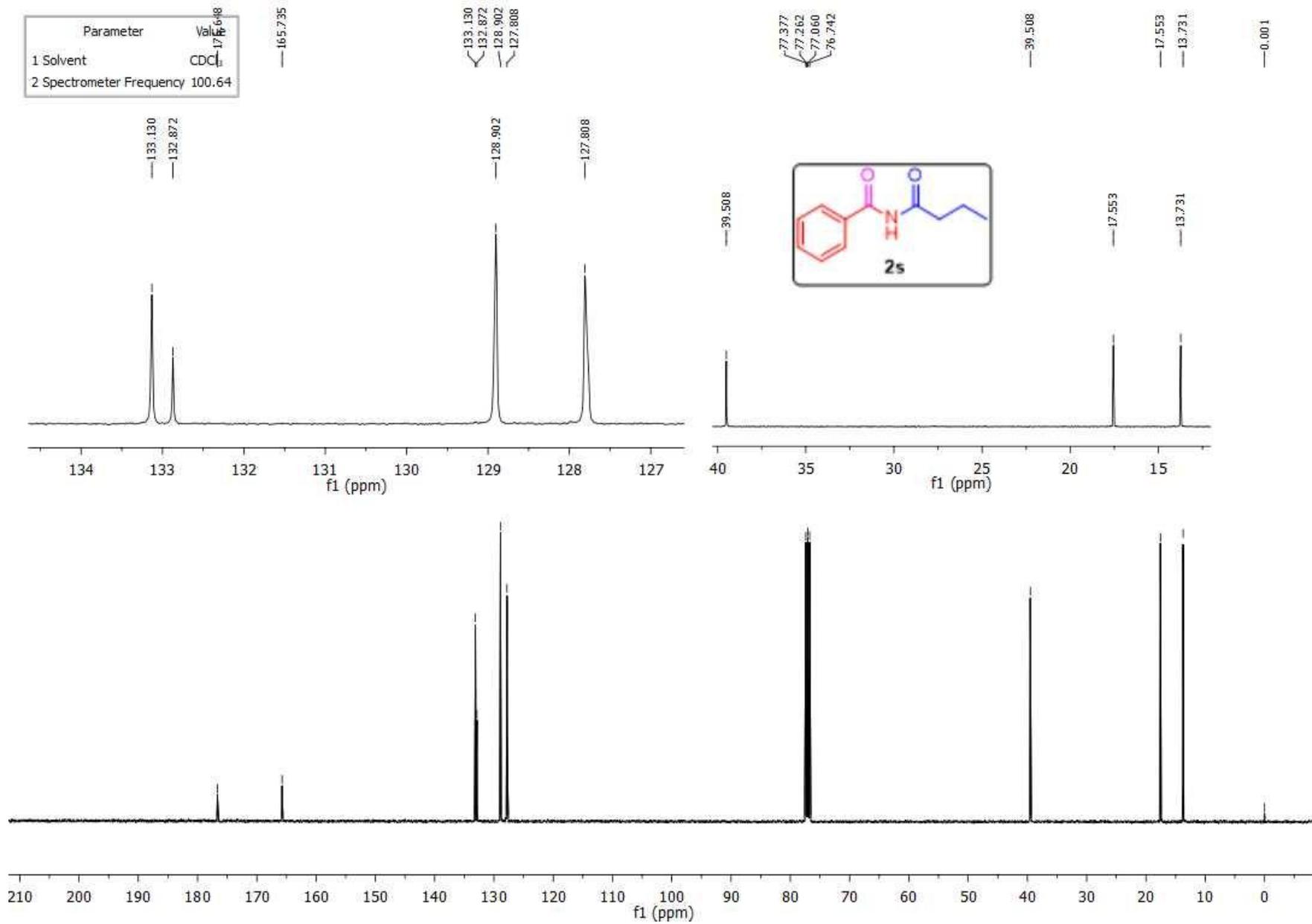


Fig. S114. ¹³C NMR spectra of *N*-butyrylbenzamide (**2s**).

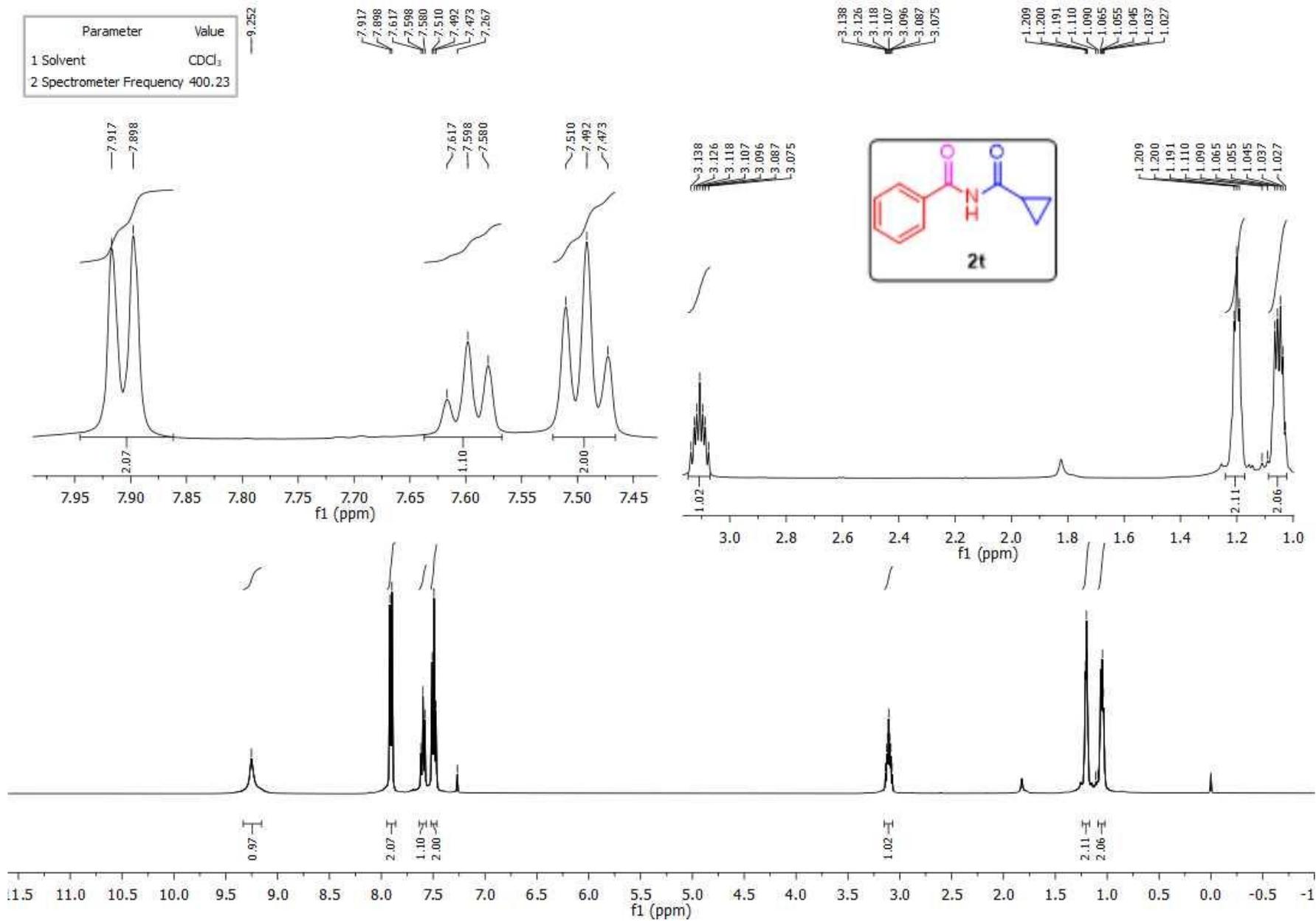


Fig. S115. ¹H NMR spectra of *N*-(cyclopropanecarbonyl)benzamide (**2t**).

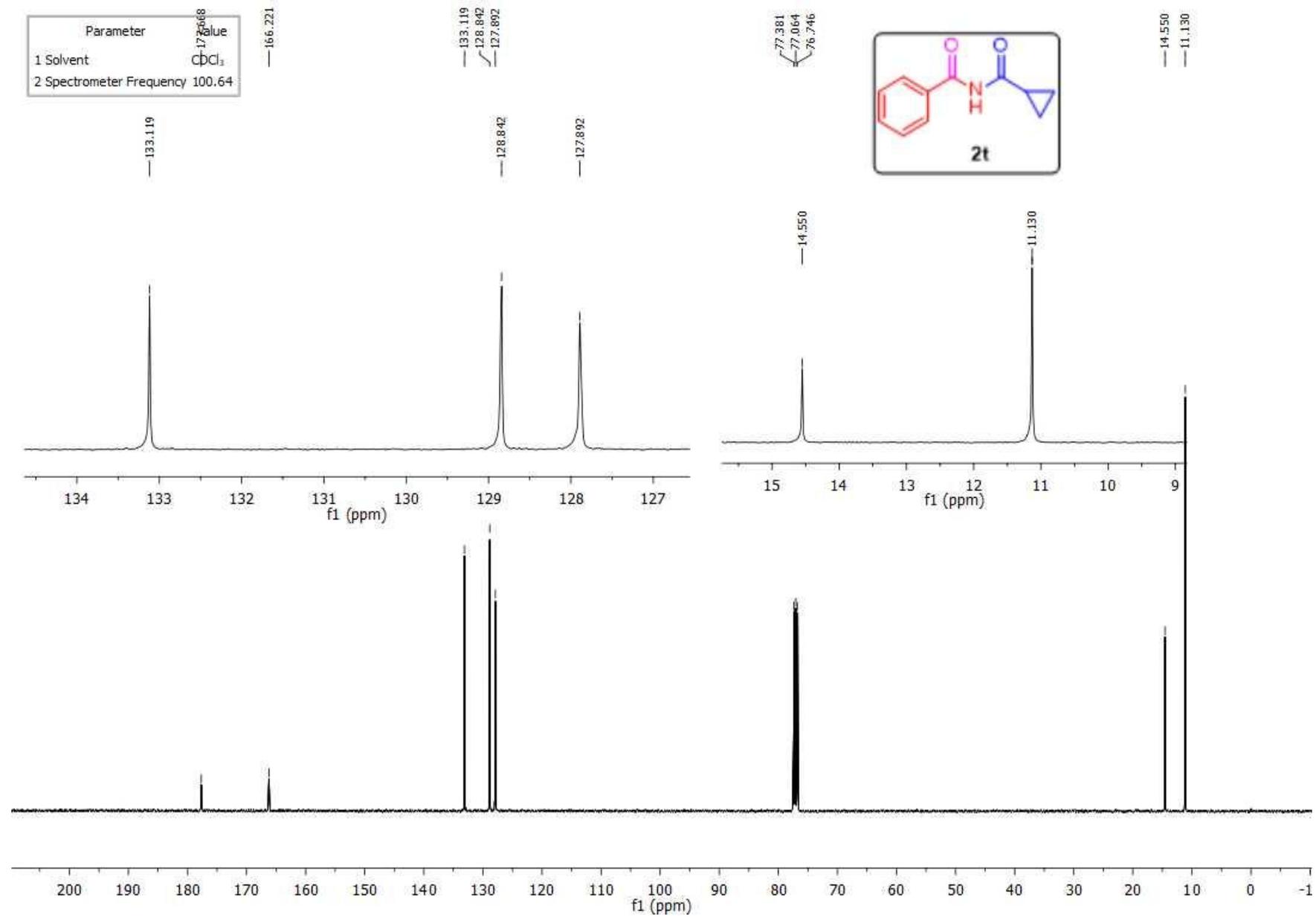


Fig. S116. ^{13}C NMR spectra of *N*-(cyclopropanecarbonyl)benzamide (**2t**).

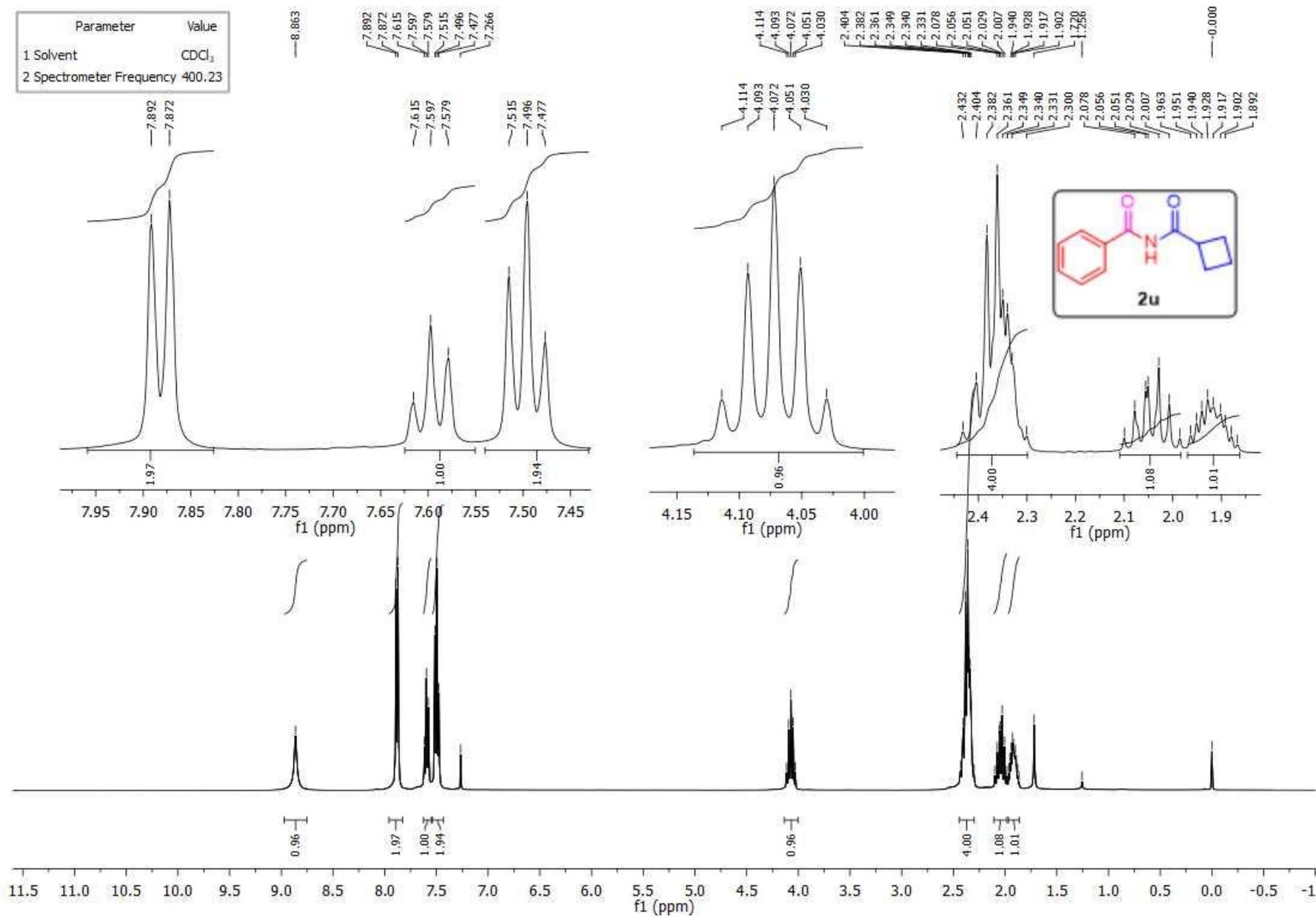


Fig. S117. ¹H NMR spectra of *N*-(cyclobutanecarbonyl)benzamide (**2u**).

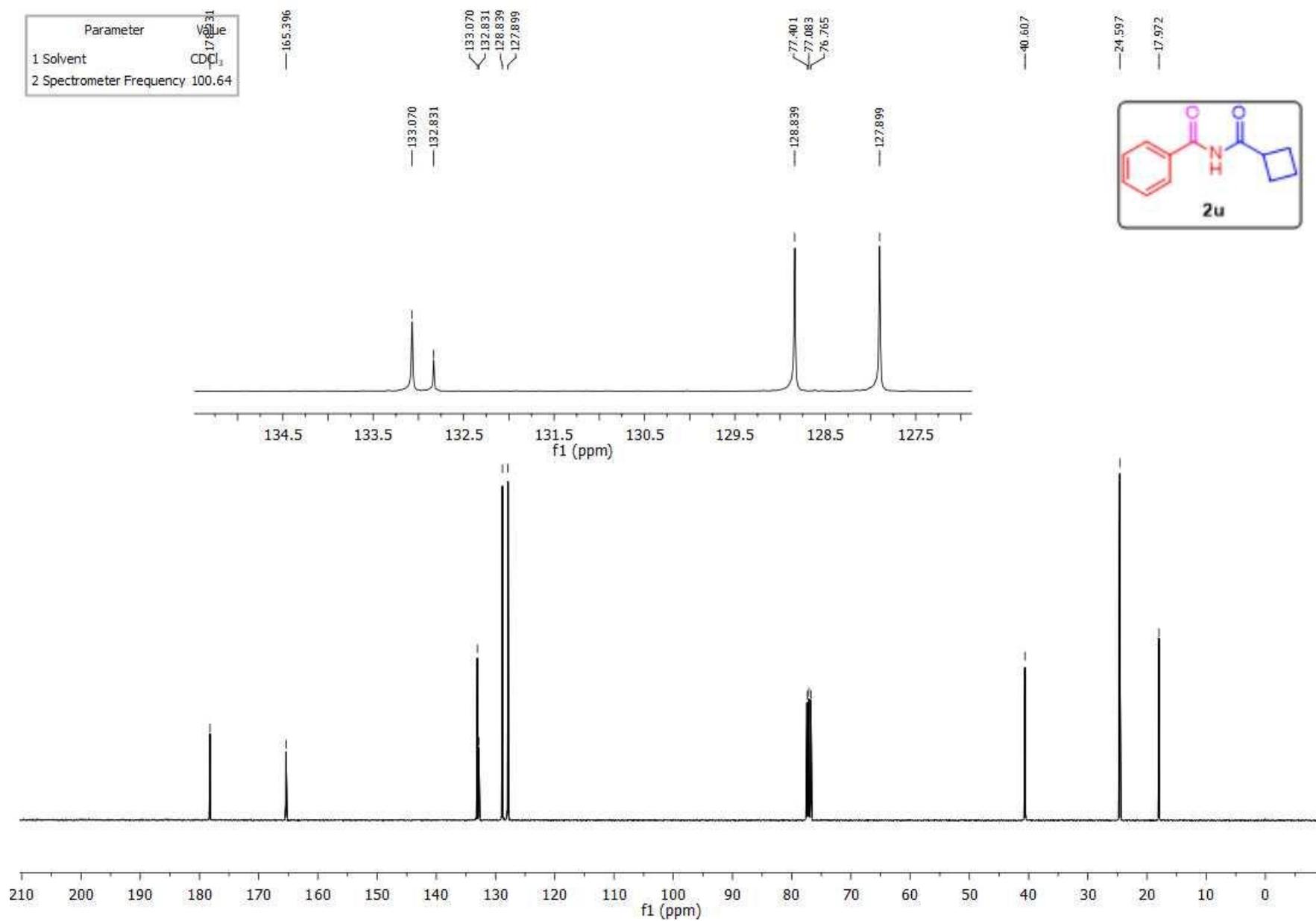
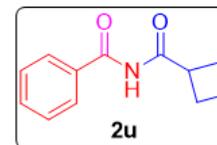


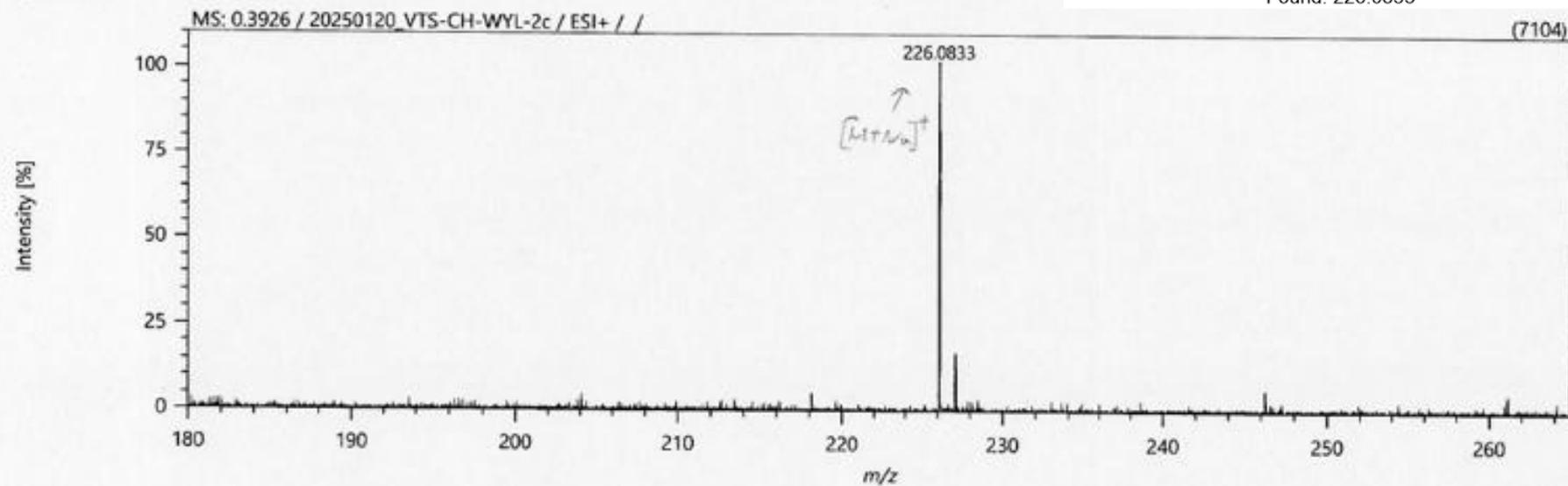
Fig. S118. ¹³C NMR spectra of *N*-(cyclobutanecarbonyl)benzamide (**2u**).

VTS-CH-WYL-2c (HR-ESI)



Chemical Formula: C₁₂H₁₃NO₂Na [M+Na]⁺ Calcd: 226.0844
Found: 226.0833

Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	2	1	1
Max	400	1000	2	1	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
226.08333	C ₁₂ H ₁₃ N O ₂ Na	226.08385	-0.52	-2.29	6.5

Fig. S119. HRMS data of *N*-(cyclobutanecarbonyl)benzamide (2u).

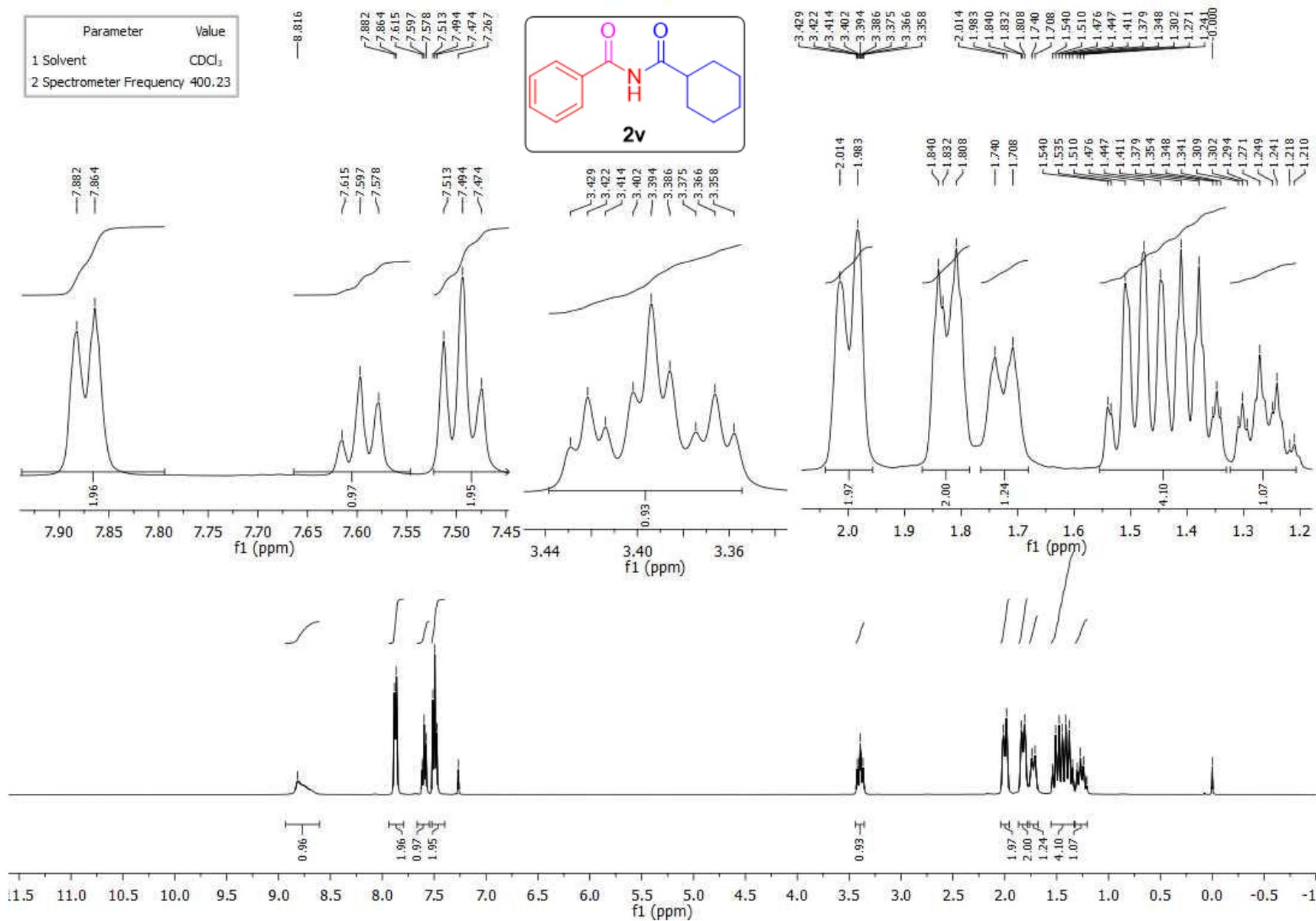


Fig. S120. ¹H NMR spectra of *N*-(cyclohexanecarbonyl)benzamide (**2v**).

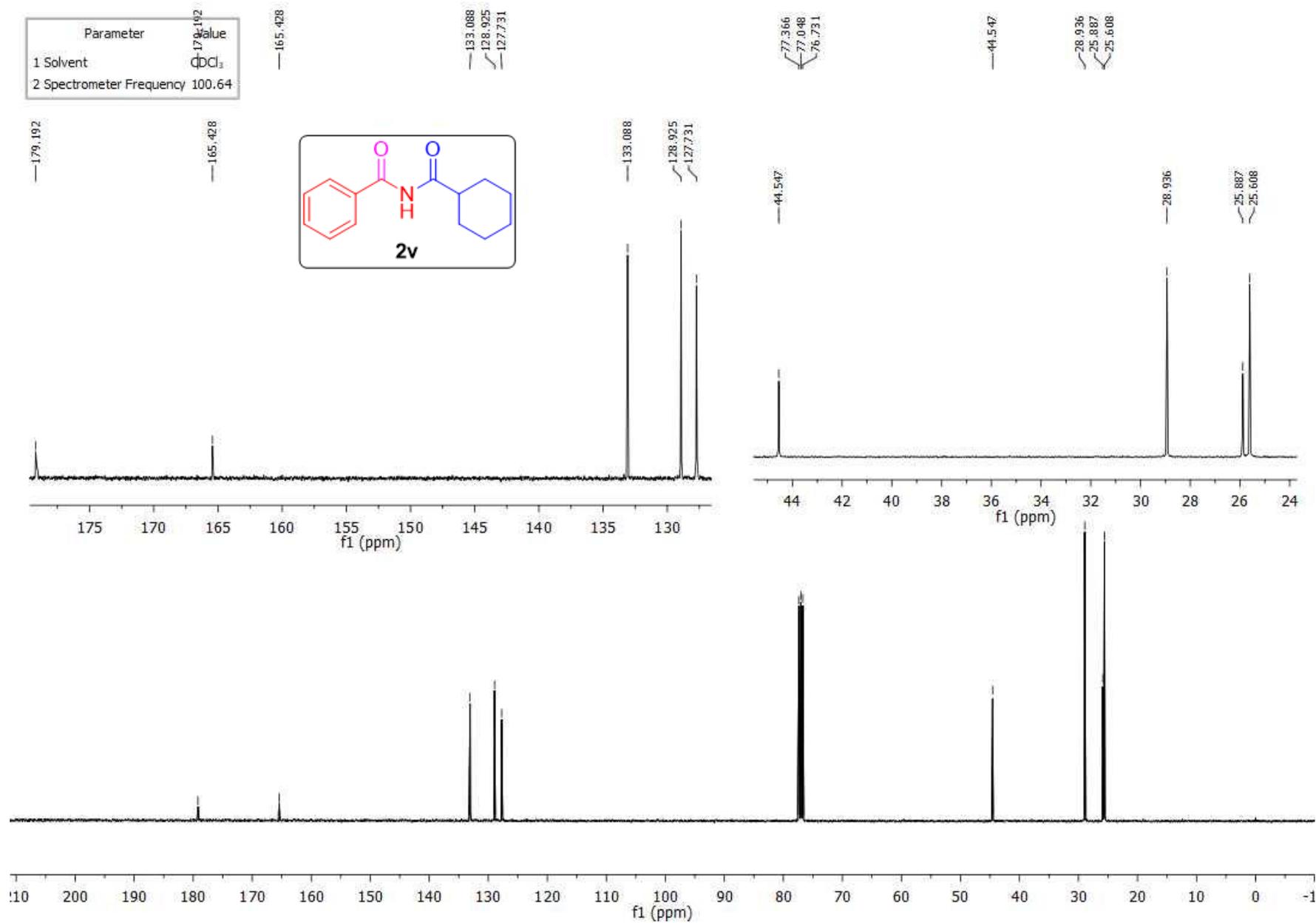


Fig. S121. ^{13}C NMR spectra of *N*-(cyclohexanecarbonyl)benzamide (**2v**).

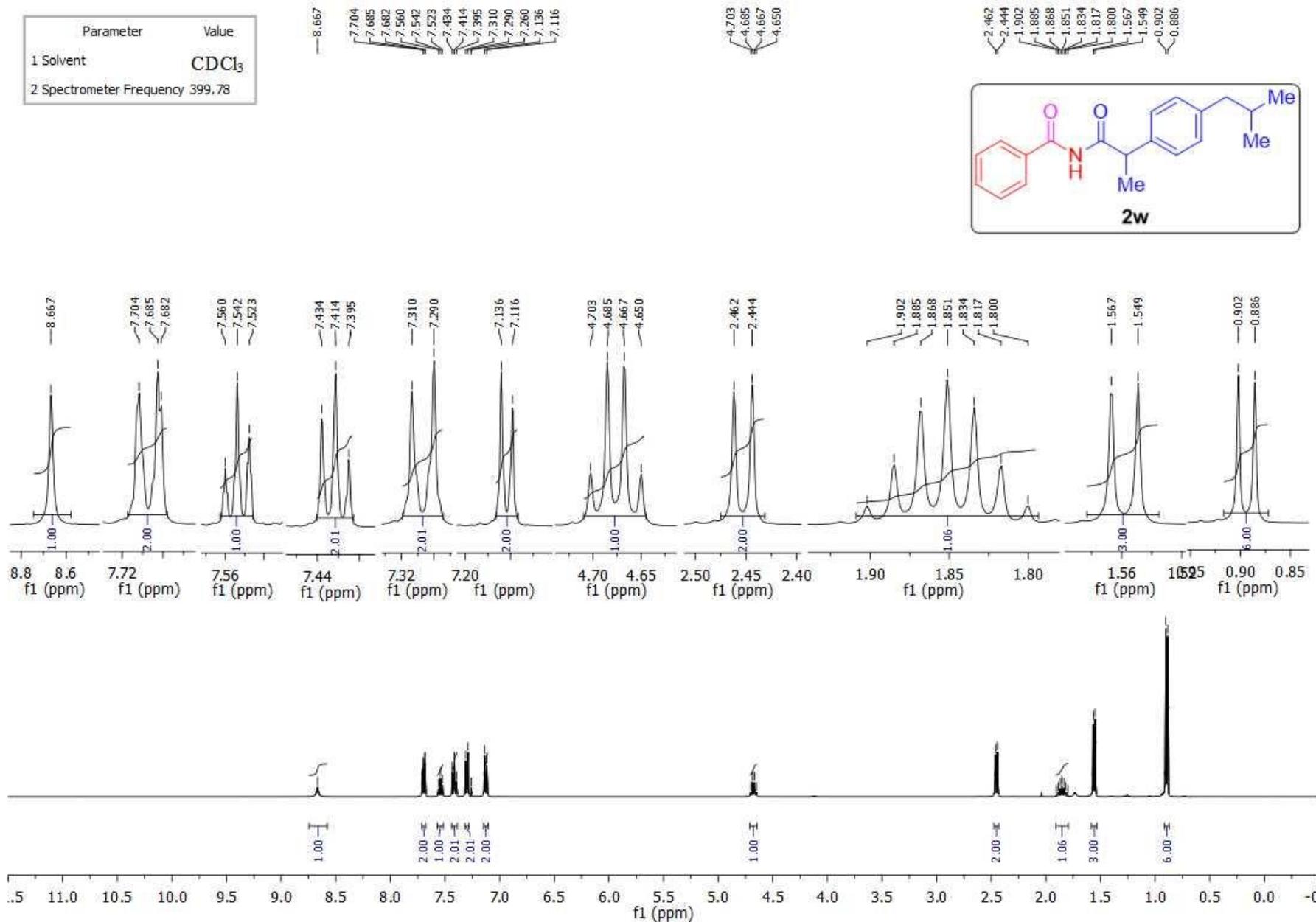


Fig. S122. ¹H NMR spectra of *N*-(2-(4-isobutylphenyl)propanoyl)benzamide (**2w**).

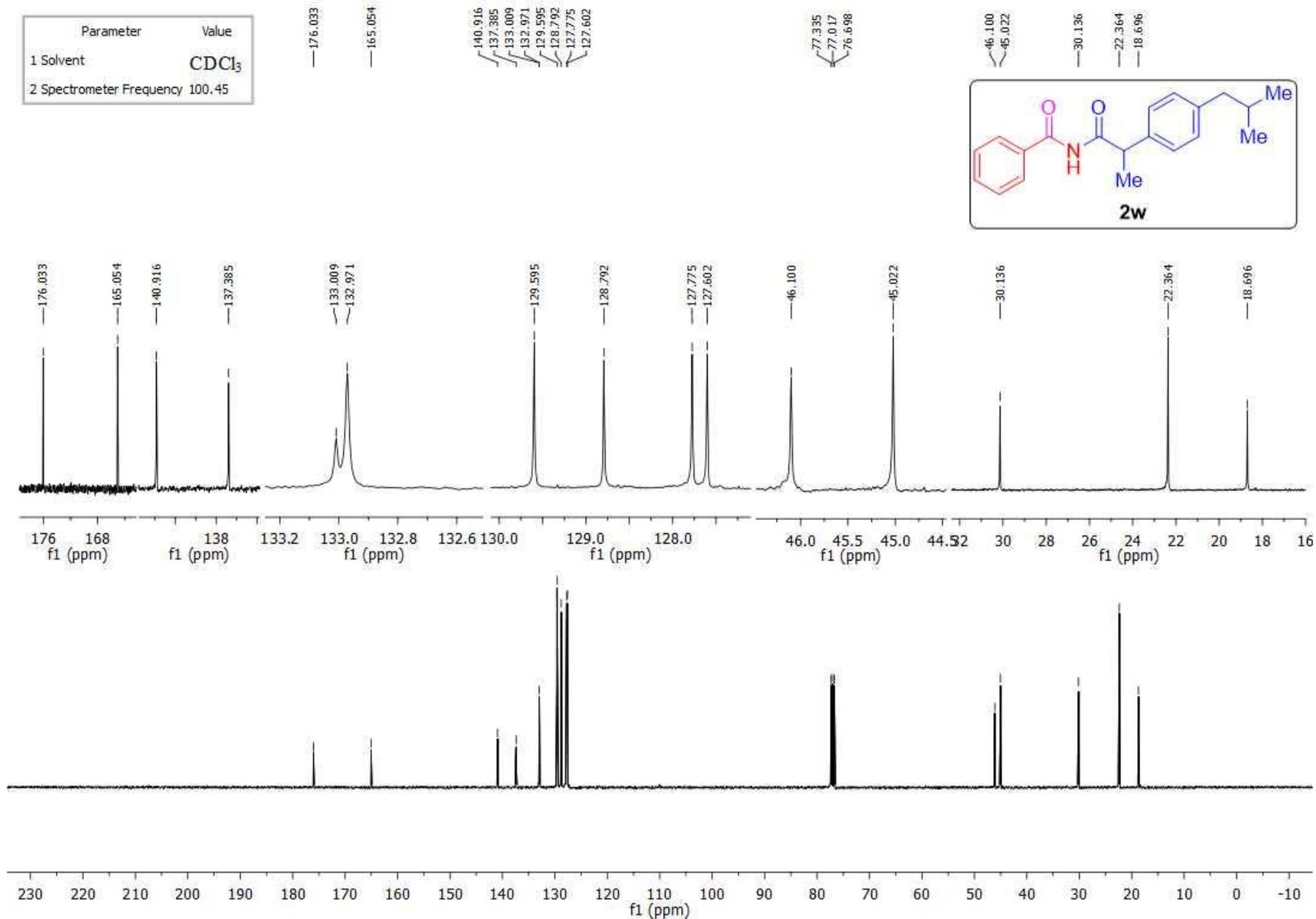


Fig. S123. ¹³C NMR spectra of *N*-(2-(4-isobutylphenyl)propanoyl)benzamide (**2w**).

Sample Name	VG P2 31_MeOH_Negative	Position		Instrument Name	CY-E-HRMS-01
User Name		Inj Vol	Unknown / Injection Program	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	VG P2 31_MeOH_Negative.d
ACQ Method	TEST.m	Comment		Acquired Time	10/3/2025 3:53:32 PM (UTC+05:30)

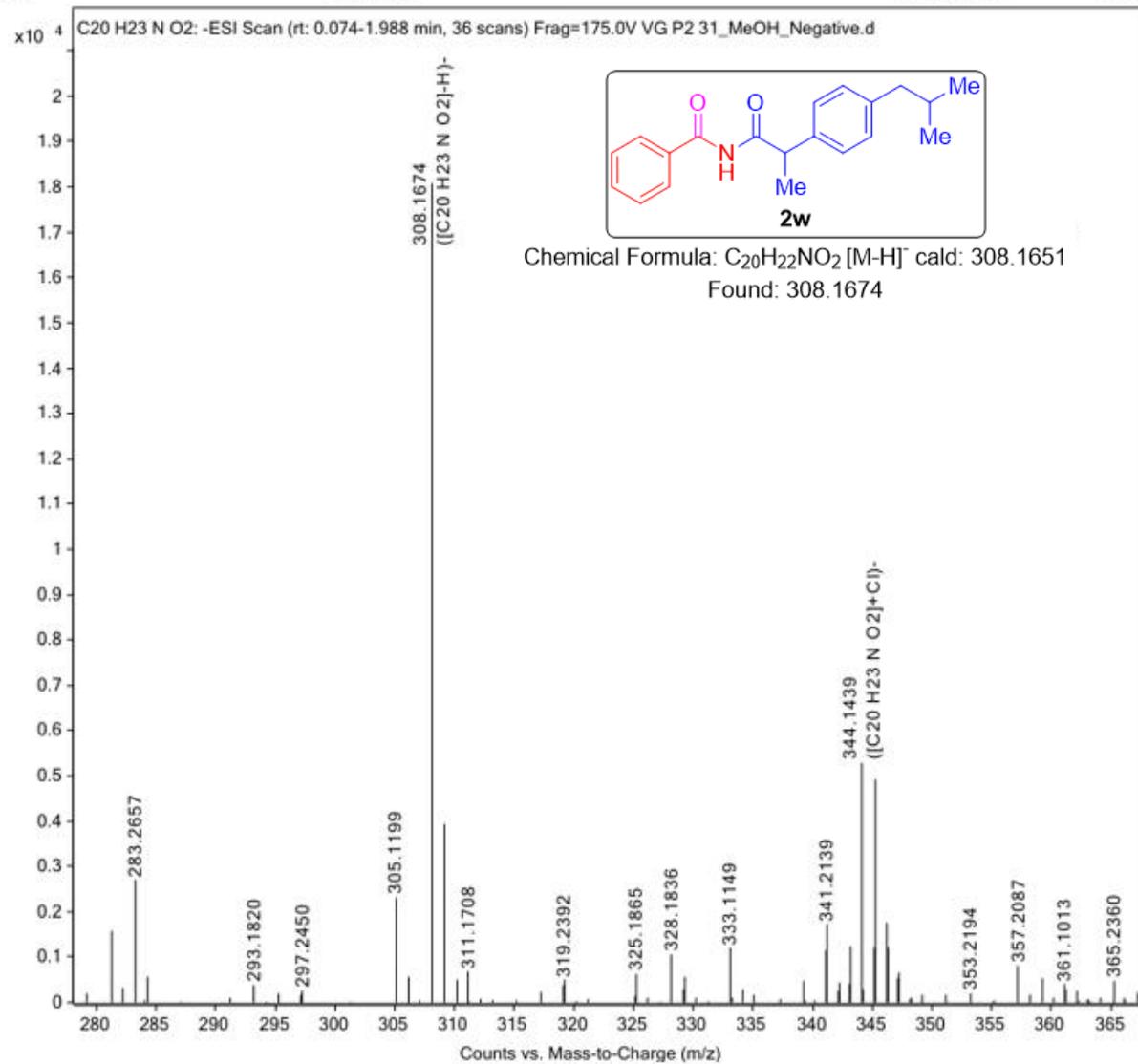


Fig. S124. HRMS data of *N*-(2-(4-isobutylphenyl)propanoyl)benzamide (**2w**).

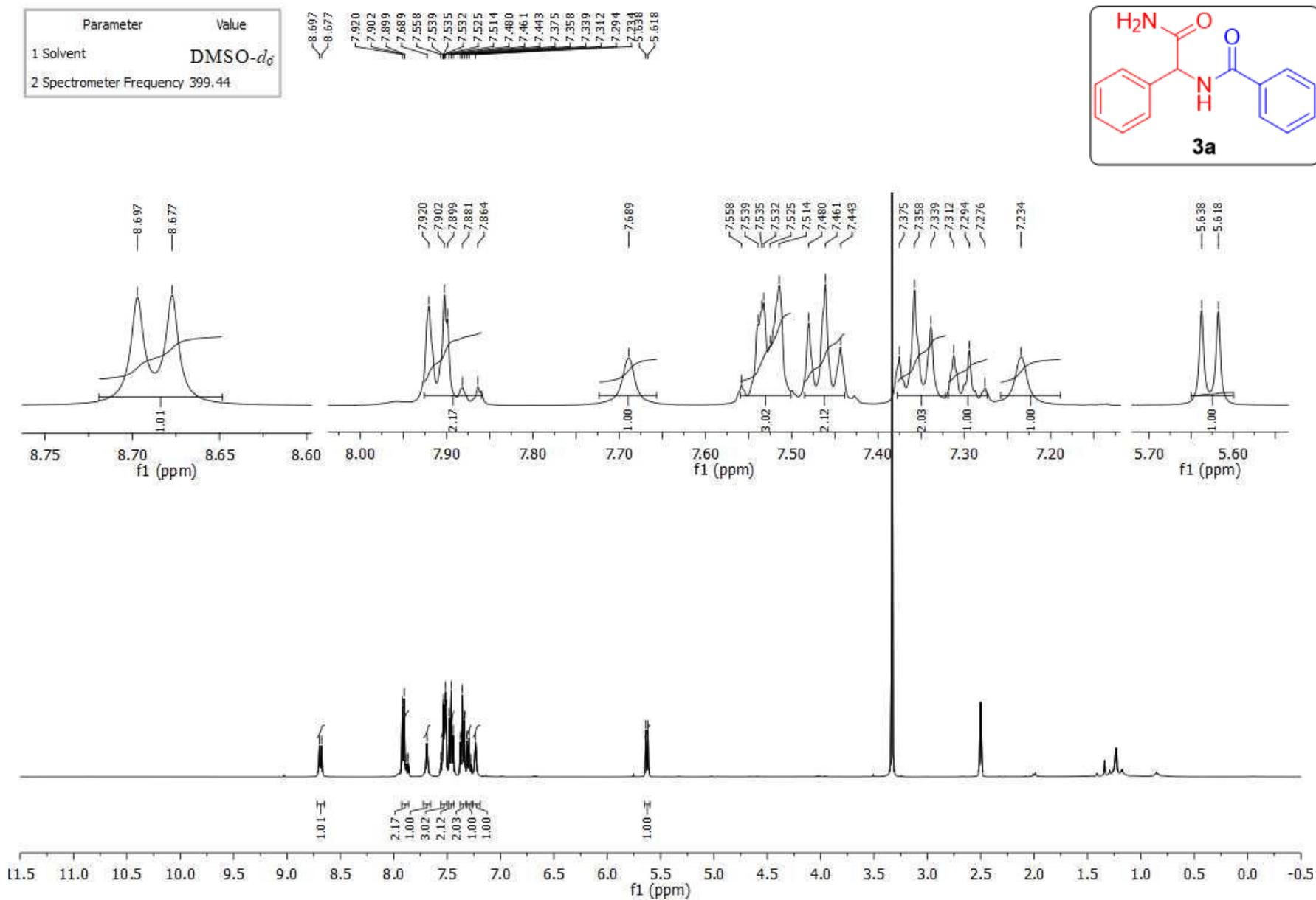


Fig. S125. ¹H NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)benzamide (**3a**).

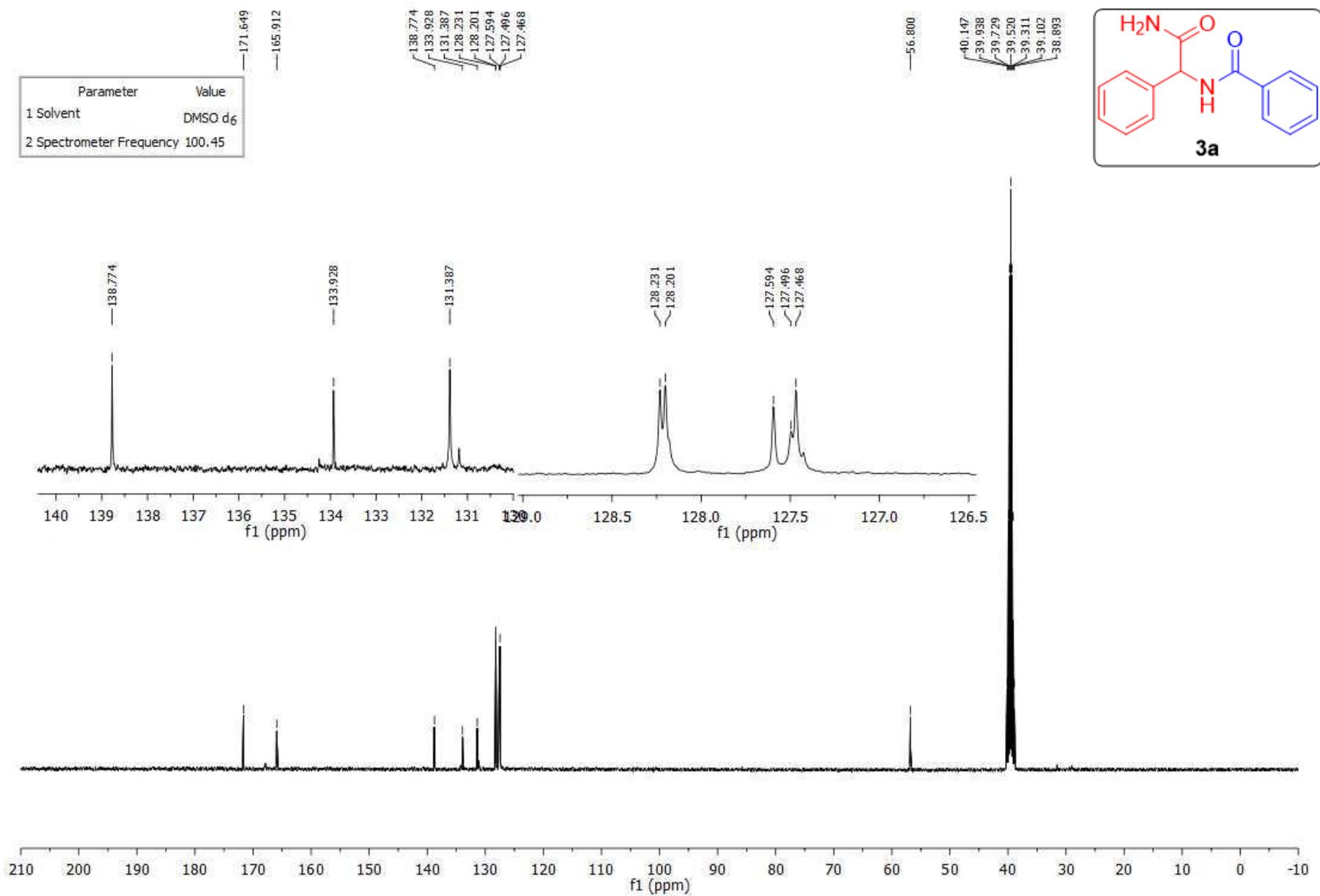
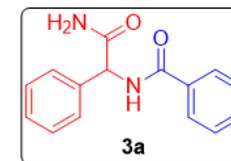


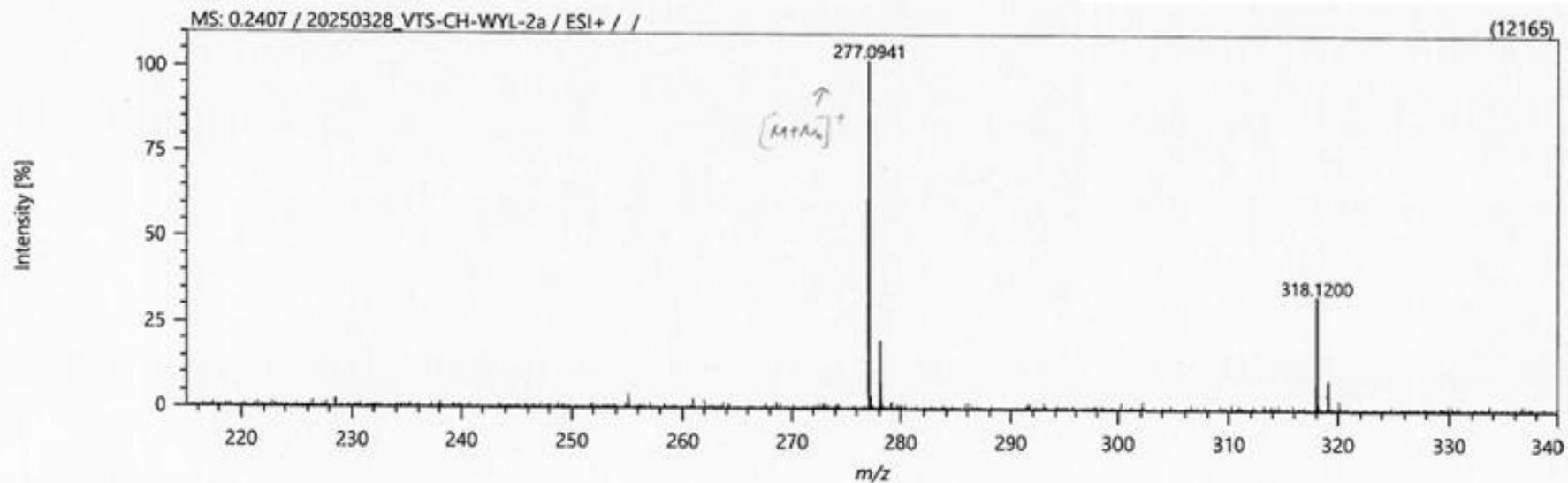
Fig. S126. ^{13}C NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)benzamide (**3a**).

VTS-CH-WYS-2a (HR-ESI)



Chemical Formula: C₁₅H₁₄N₂O₂Na [M+Na]⁺ Calcd: 277.0953
Found: 277.0941

Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	2	2	1
Max	400	1000	2	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
277.09413	C ₁₅ H ₁₄ N ₂ O ₂ Na	277.09475	-0.62	-2.23	9.5

Fig. S127. HRMS data of *N*-(2-amino-2-oxo-1-phenylethyl)benzamide (**3a**).

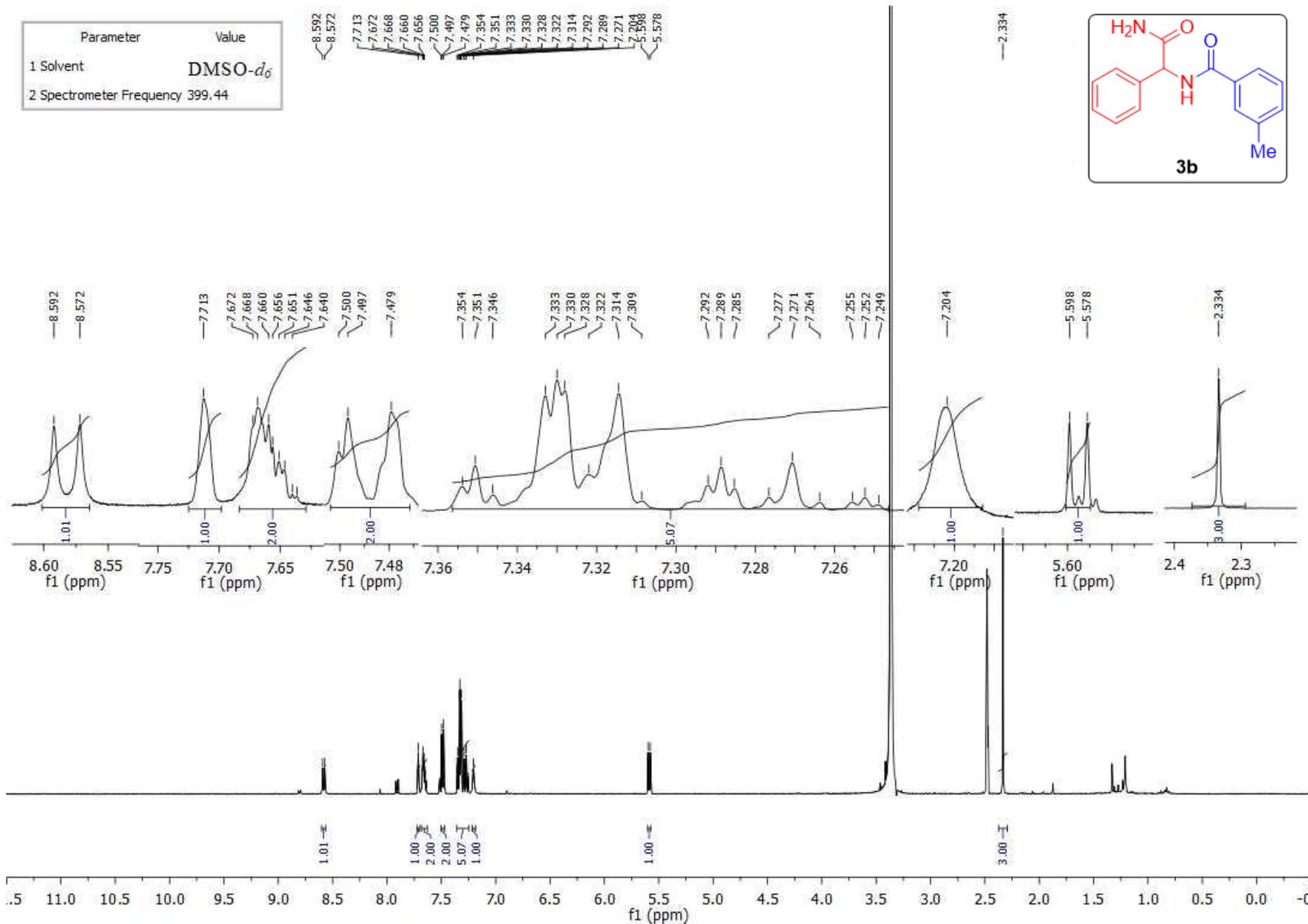


Fig. S128. ¹H NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-3-methylbenzamide (**3b**).

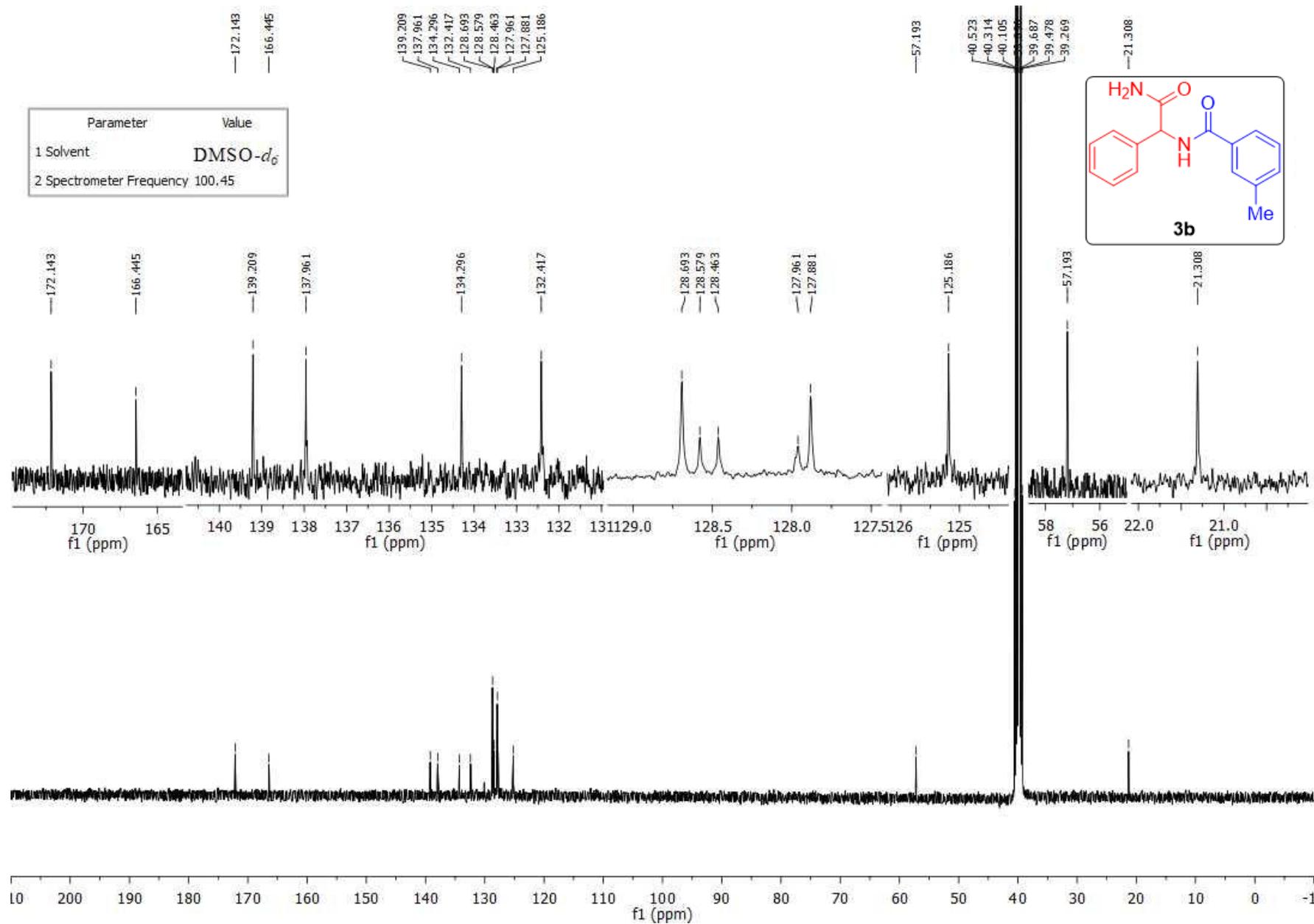
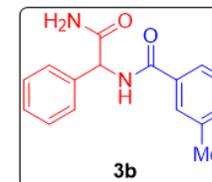
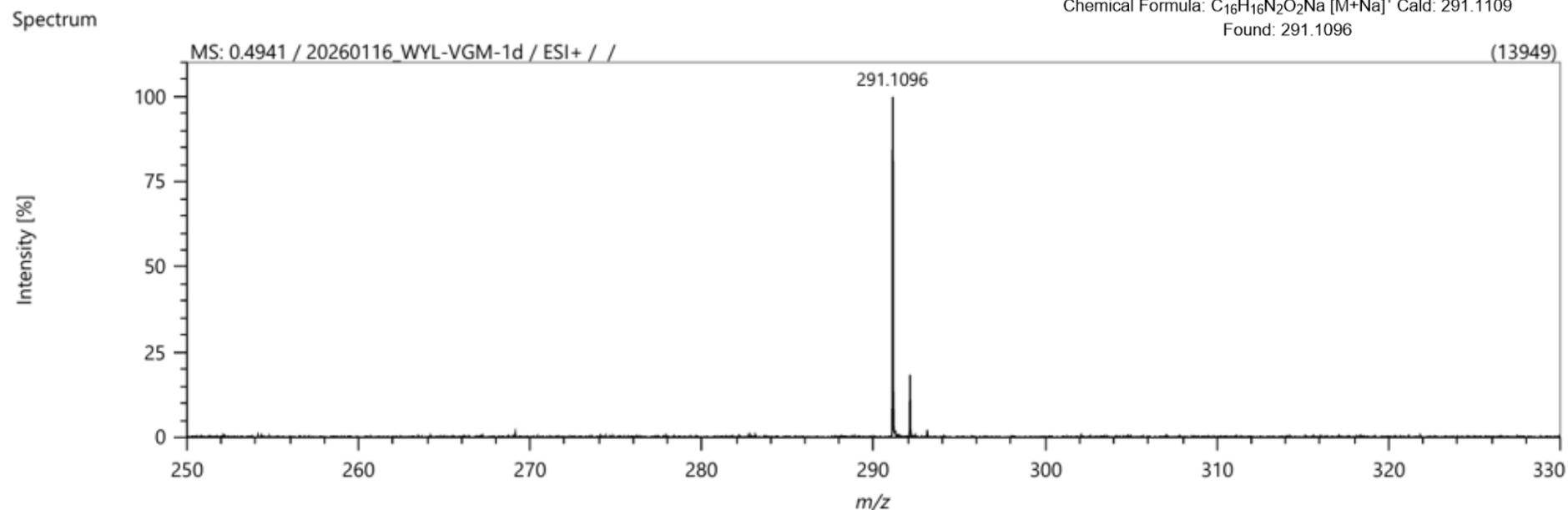


Fig. S129. ¹³C NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-3-methylbenzamide (**3b**).



Chemical Formula: C₁₆H₁₆N₂O₂Na [M+Na]⁺ Calcd: 291.1109
 Found: 291.1096



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
 Electron: Odd/Even
 Charge: +1
 DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	1	0	2	2	1
Max	400	1000	2	3	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
291.10957	C ₁₆ H ₁₆ N ₂ O ₂ Na	291.11040	-0.83	-2.83	9.5

Fig. S130. HRMS data of *N*-(2-amino-2-oxo-1-phenylethyl)-3-methylbenzamide (**3b**).

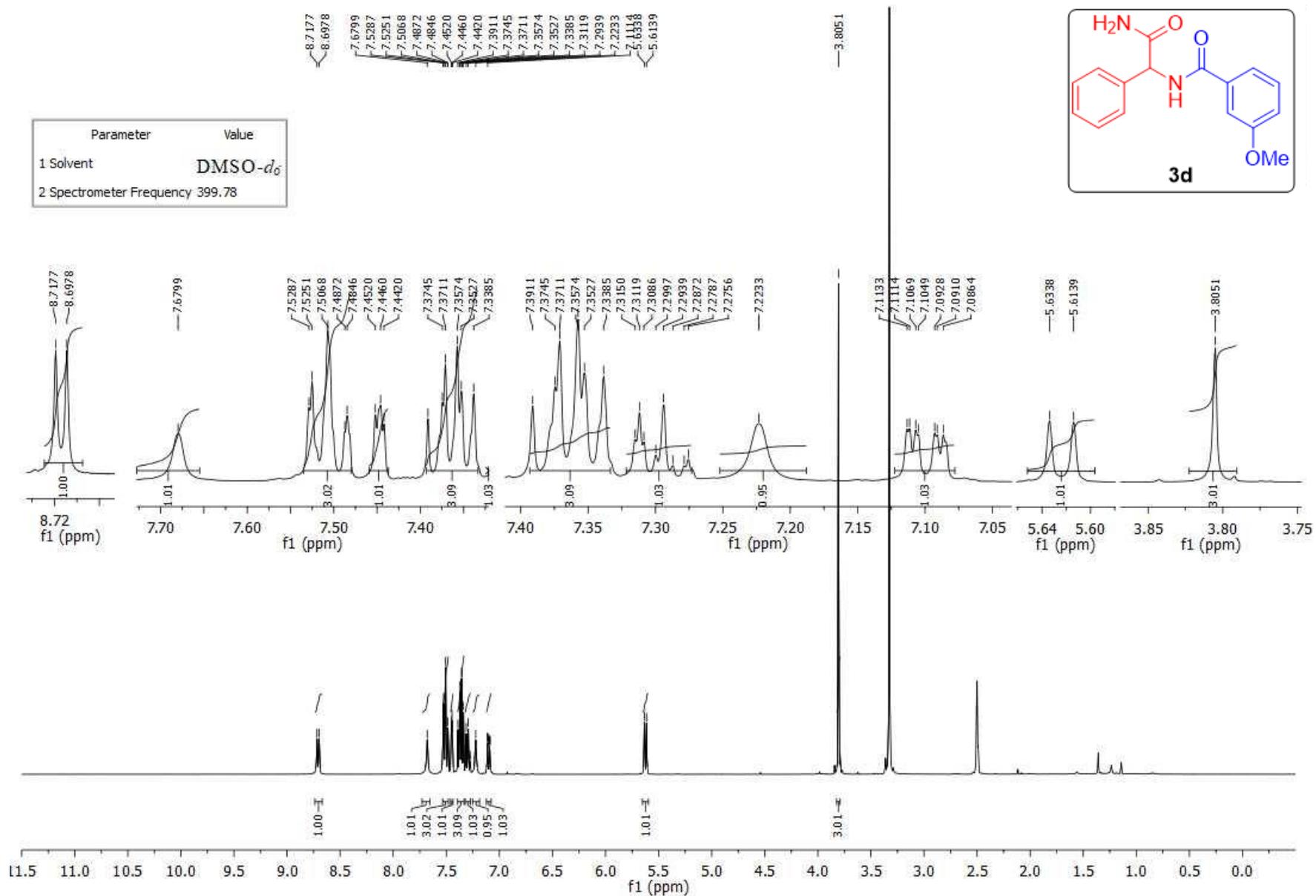


Fig. S131. ¹H NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-3-methoxybenzamide (**3d**).

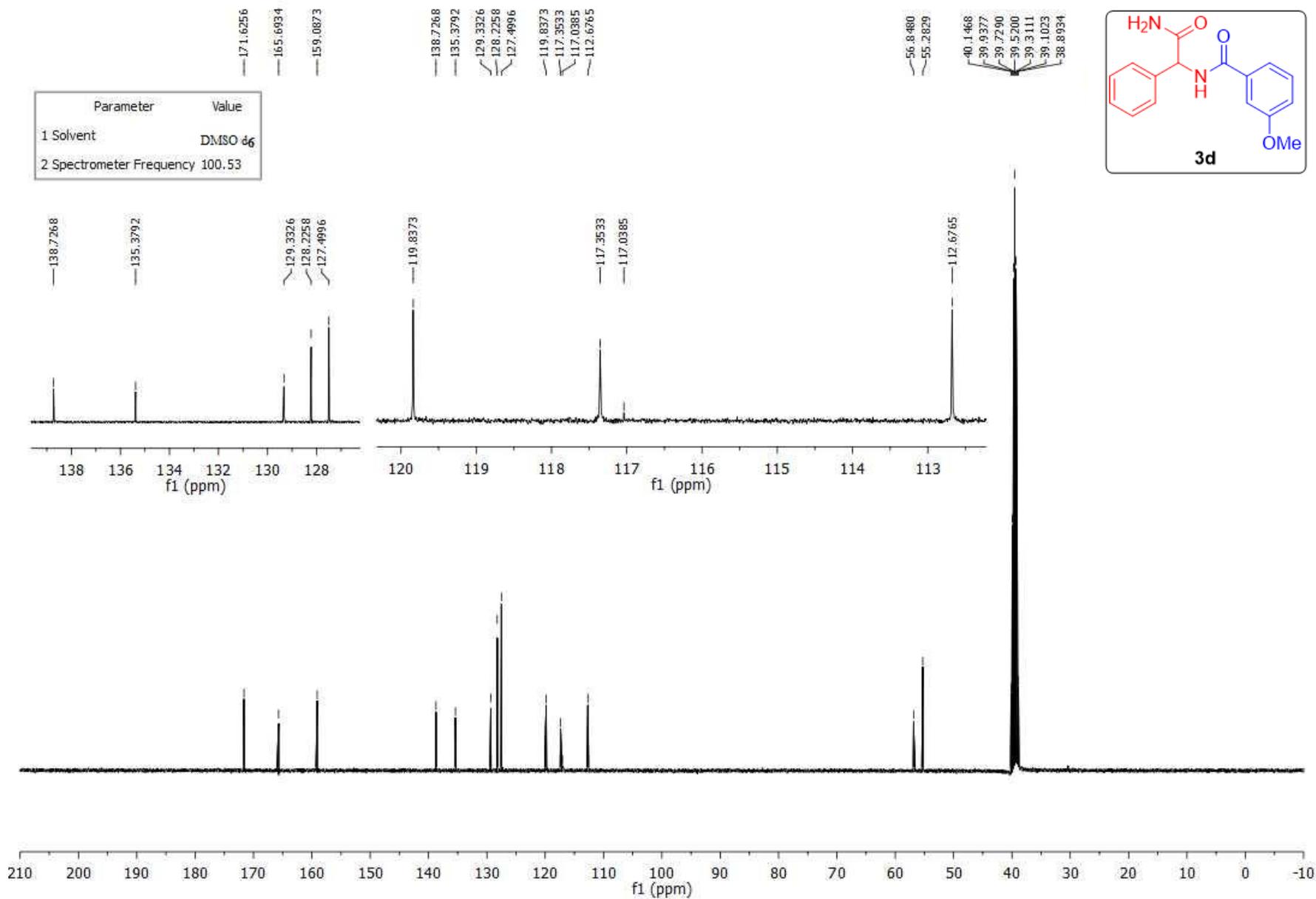
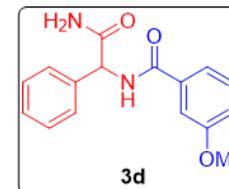


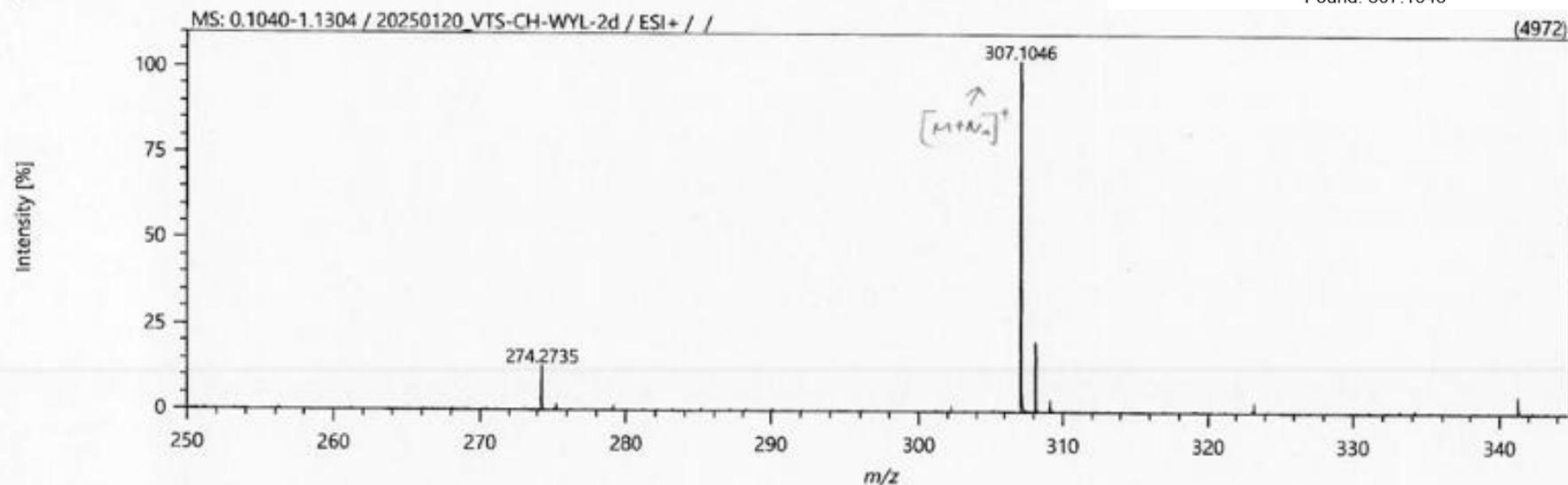
Fig. S132. ^{13}C NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-3-methoxybenzamide (**3d**).

VTS-CH-WYL-2d (HR-ESI)



Chemical Formula: $C_{16}H_{16}N_2O_3Na$ $[M+Na]^+$ Calcd: 307.1059
Found: 307.1046

Spectrum



Elemental Composition

Parameters

Tolerance: ± 10.00 ppm

Electron: Odd/Even

Charge: +1

DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	3	2	1
Max	400	1000	3	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
307.10463	$C_{16}H_{16}N_2O_3Na$	307.10531	-0.68	-2.23	9.5

Fig. S133. HRMS data of *N*-(2-amino-2-oxo-1-phenylethyl)-3-methoxybenzamide (**3d**).

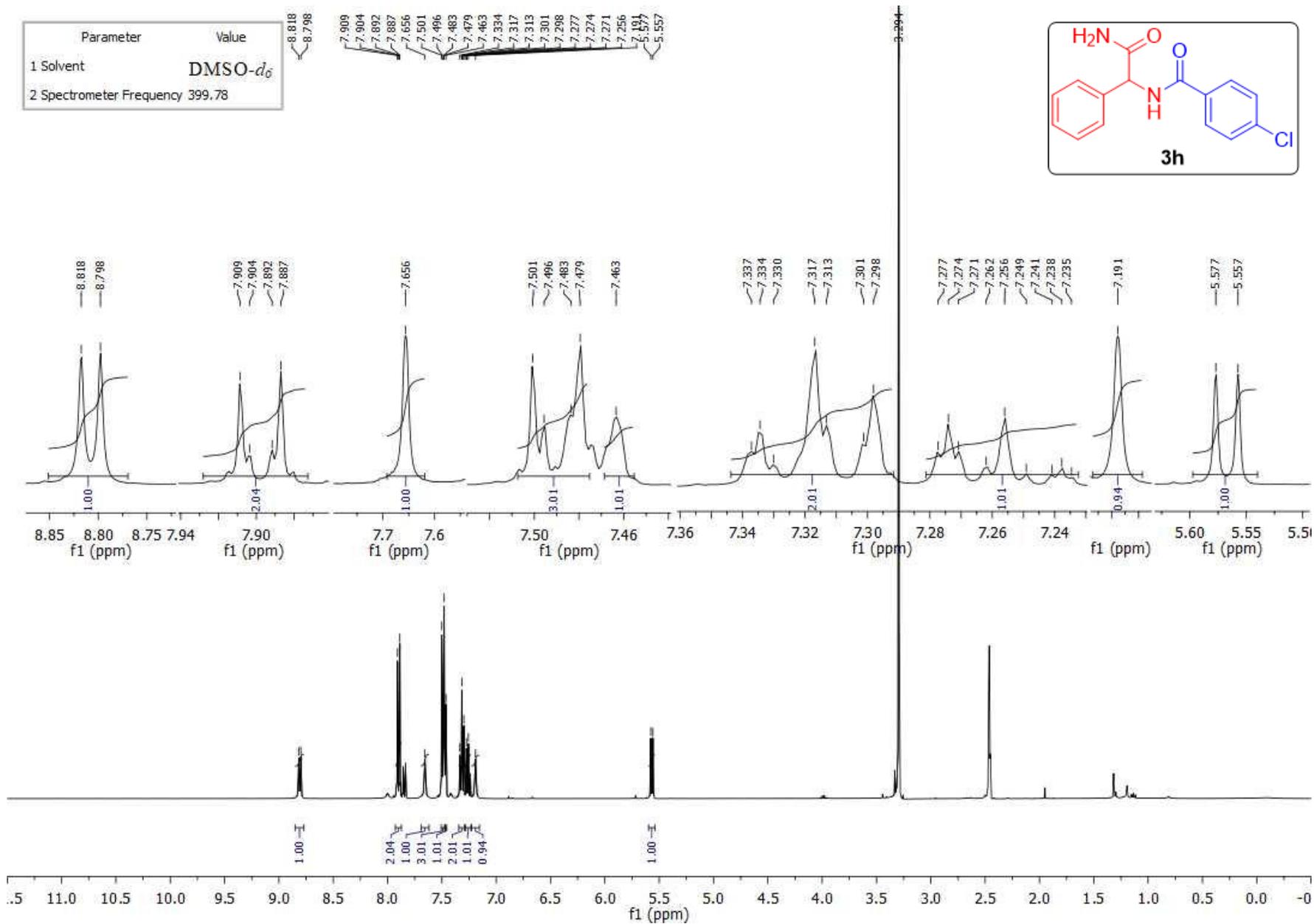


Fig. S134. ¹H NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-4-chlorobenzamide (**3h**).

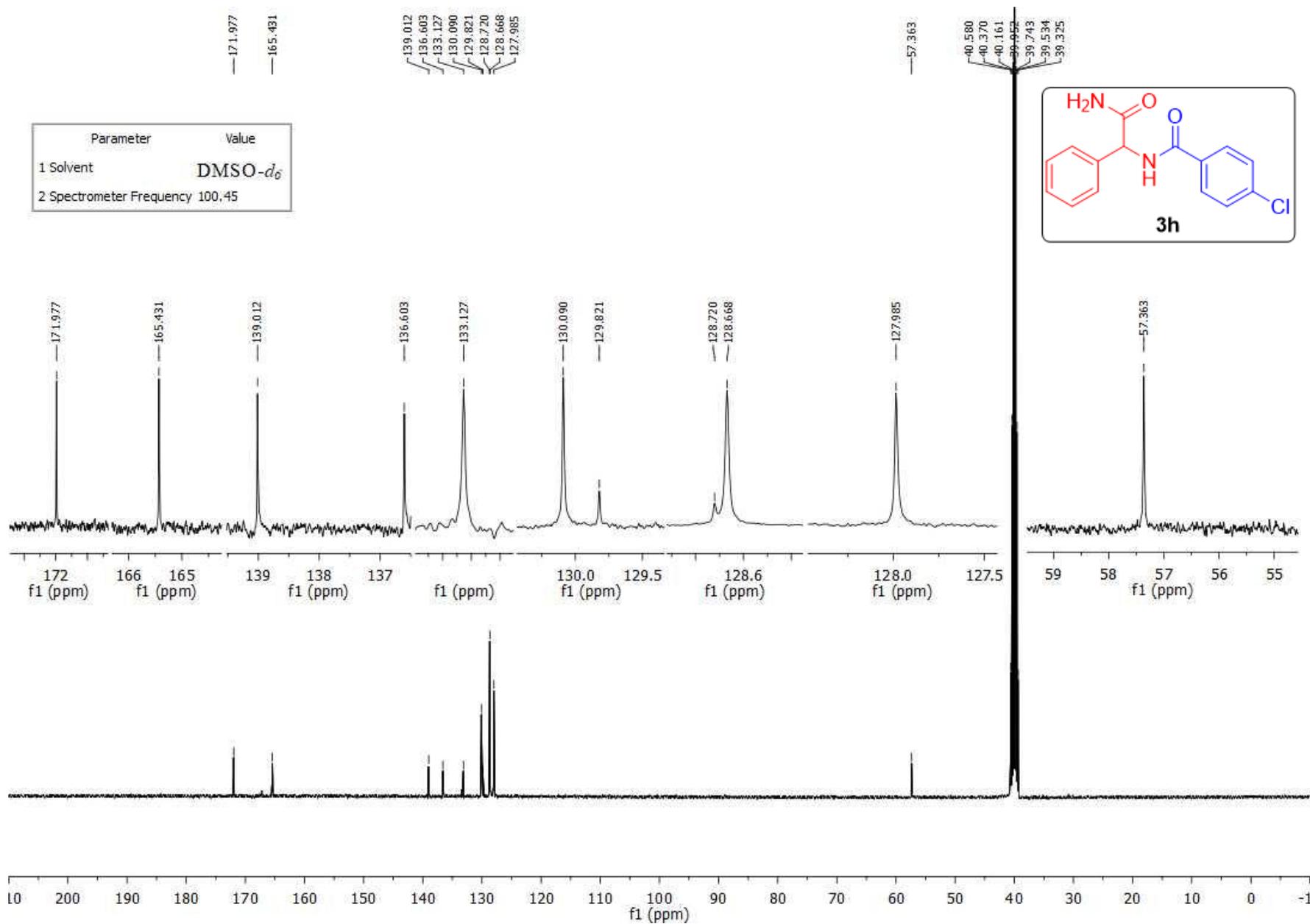
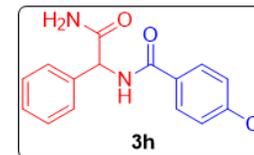


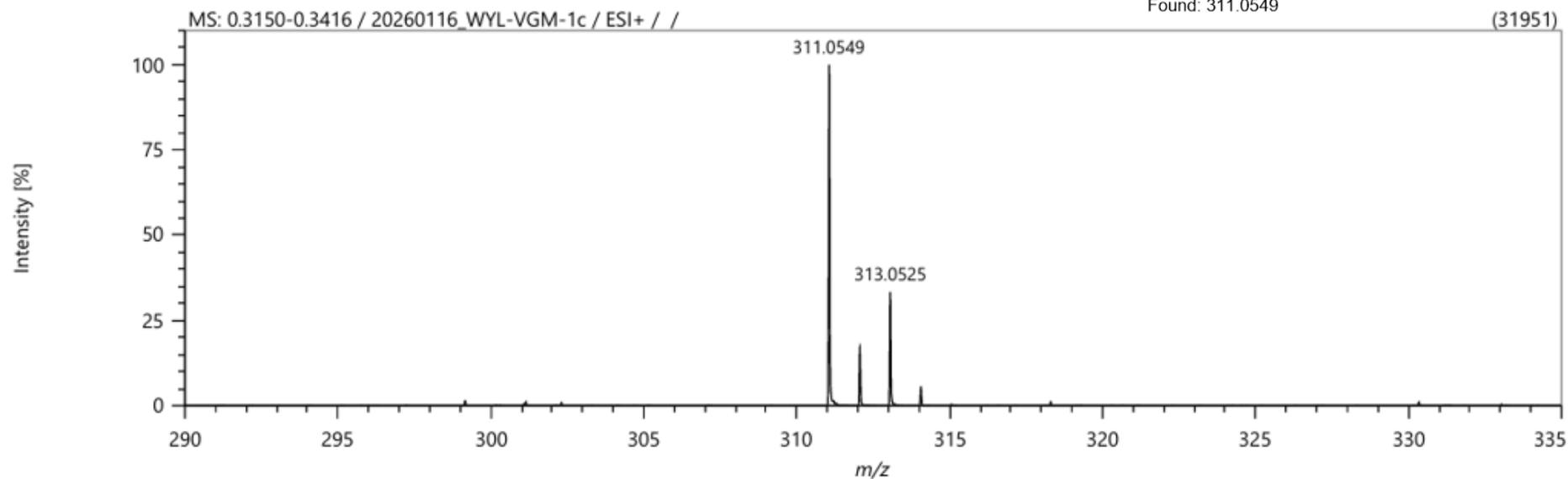
Fig. S135. ¹³C NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-4-chlorobenzamide (**3h**).



Chemical Formula: C₁₅H₁₃ClN₂O₂Na [M+Na]⁺ Calcd: 311.0563

Found: 311.0549

Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
 Electron: Odd/Even
 Charge: +1
 DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na	Cl
Min	1	0	2	2	1	1
Max	400	1000	2	3	1	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
311.05491	C ₁₅ H ₁₃ N ₂ O ₂ Na Cl	311.05578	-0.86	-2.78	9.5

Fig. S136. HRMS data of *N*-(2-amino-2-oxo-1-phenylethyl)-4-chlorobenzamide (**3h**).

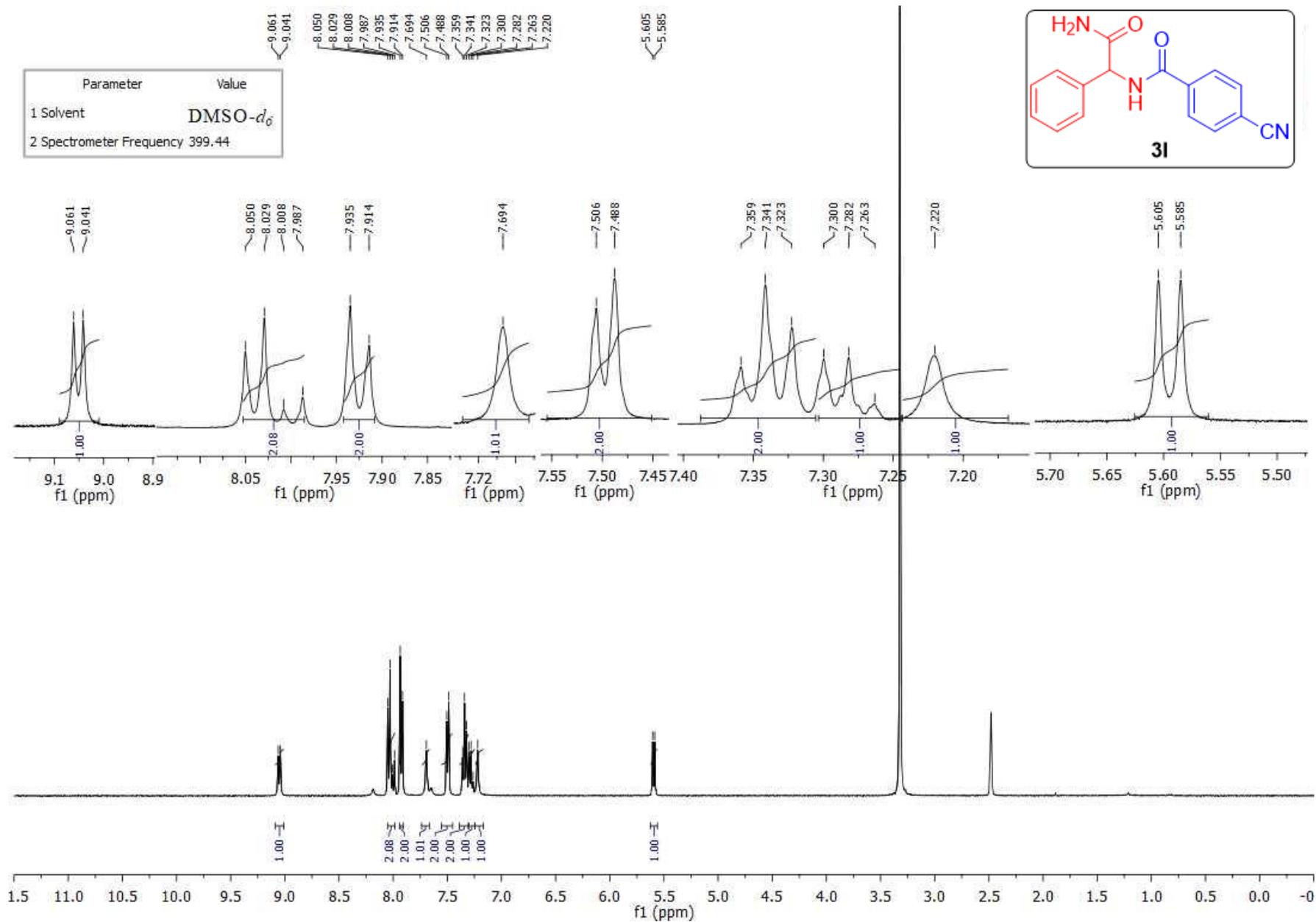


Fig. S137. ¹H NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-4-cyanobenzamide (**31**).

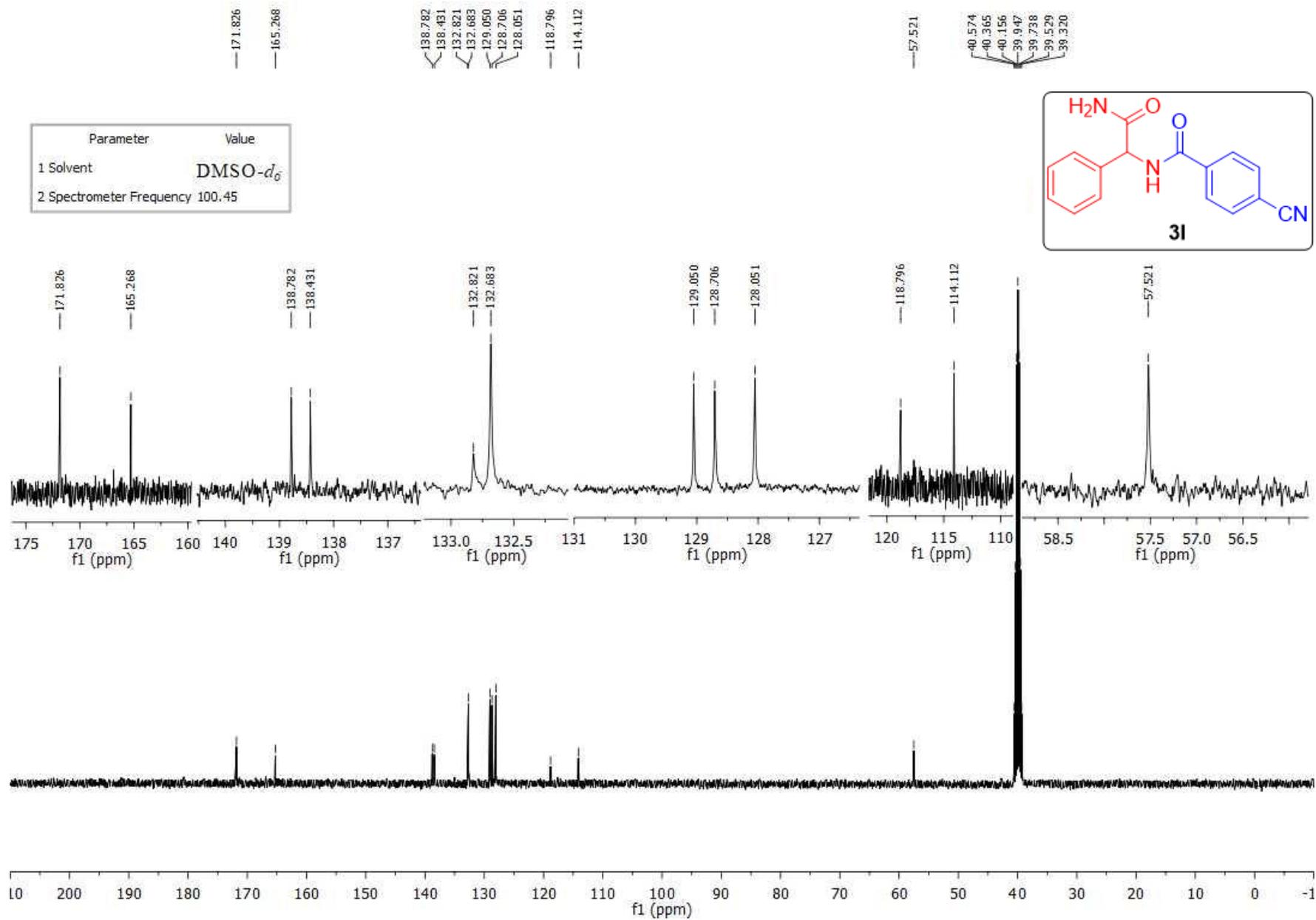
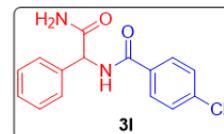
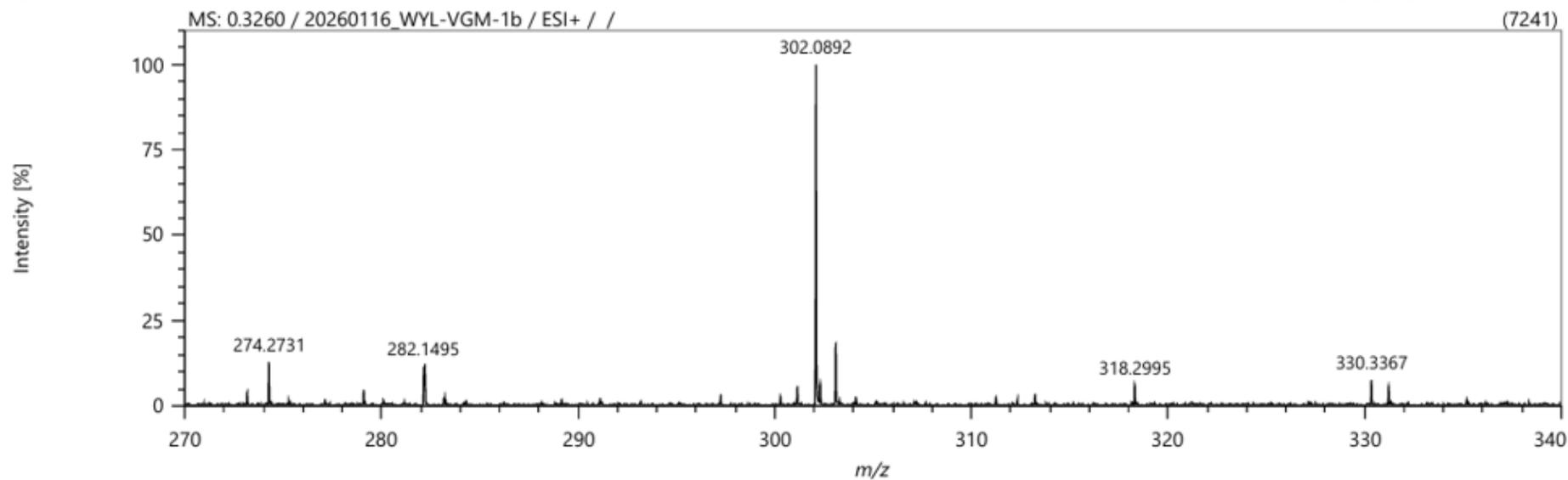


Fig. S138. ^{13}C NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-4-cyanobenzamide (**31**).



Chemical Formula: C₁₆H₁₃N₃O₂Na [M+Na]⁺ Calcd: 302.0905
Found: 302.0892

Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	1	0	2	3	1
Max	400	1000	2	3	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
302.08924	C ₁₆ H ₁₃ N ₃ O ₂ Na	302.09000	-0.76	-2.52	11.5

Fig. S139. HRMS data of *N*-(2-amino-2-oxo-1-phenylethyl)-4-cyanobenzamide (**31**).

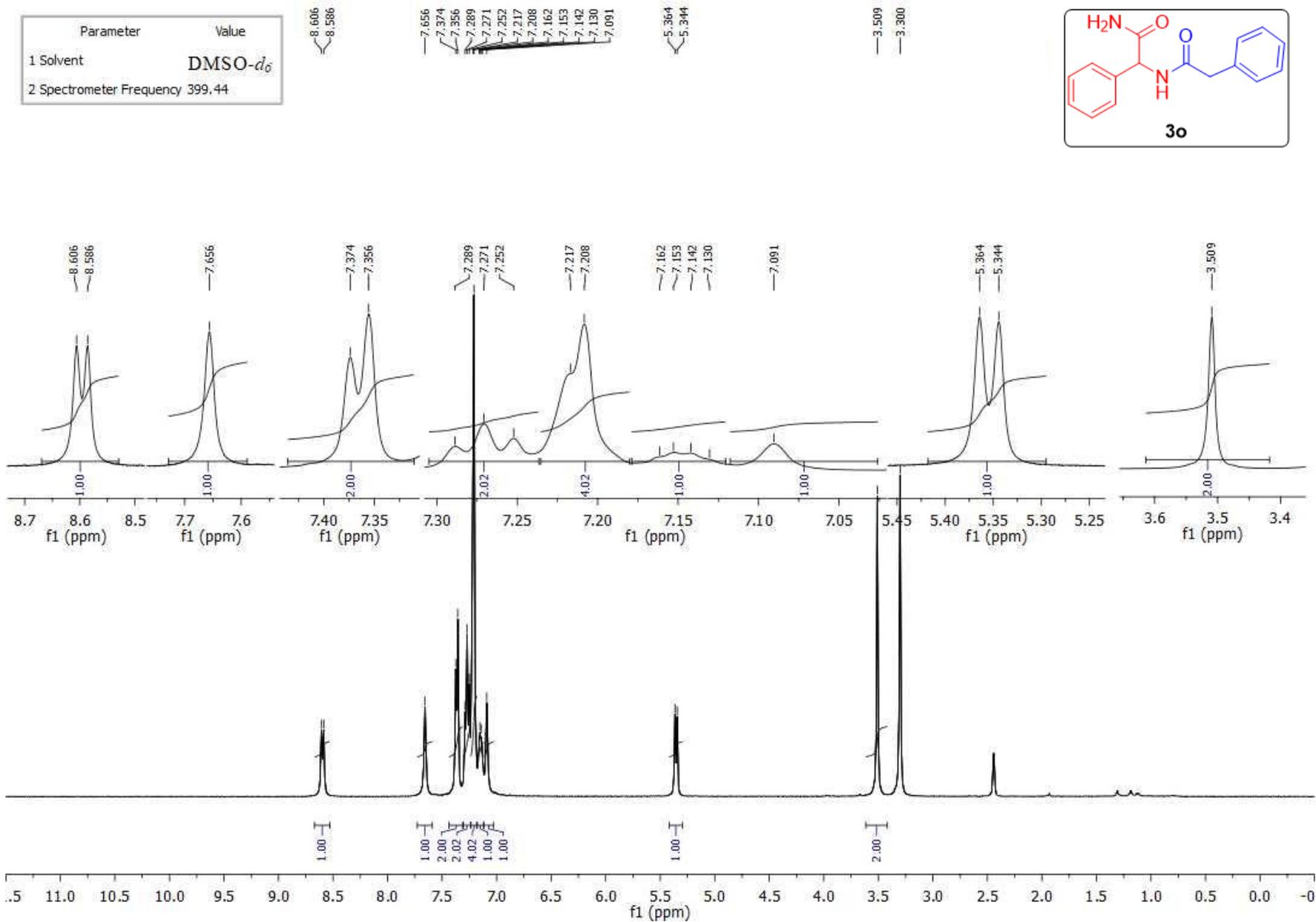


Fig. S140. ¹H NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-2-phenylacetamide (**3o**).

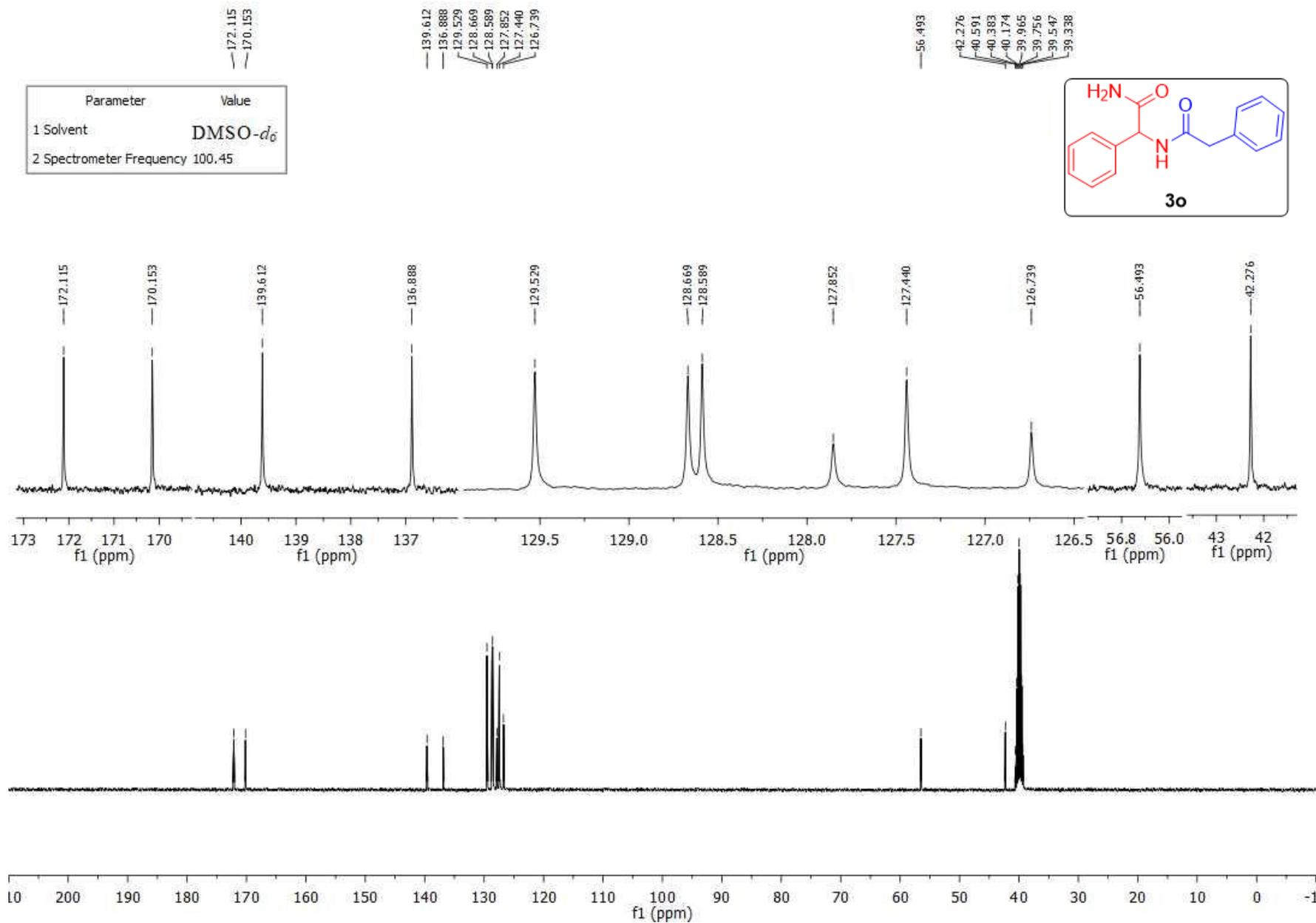
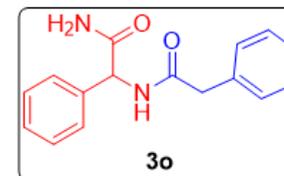
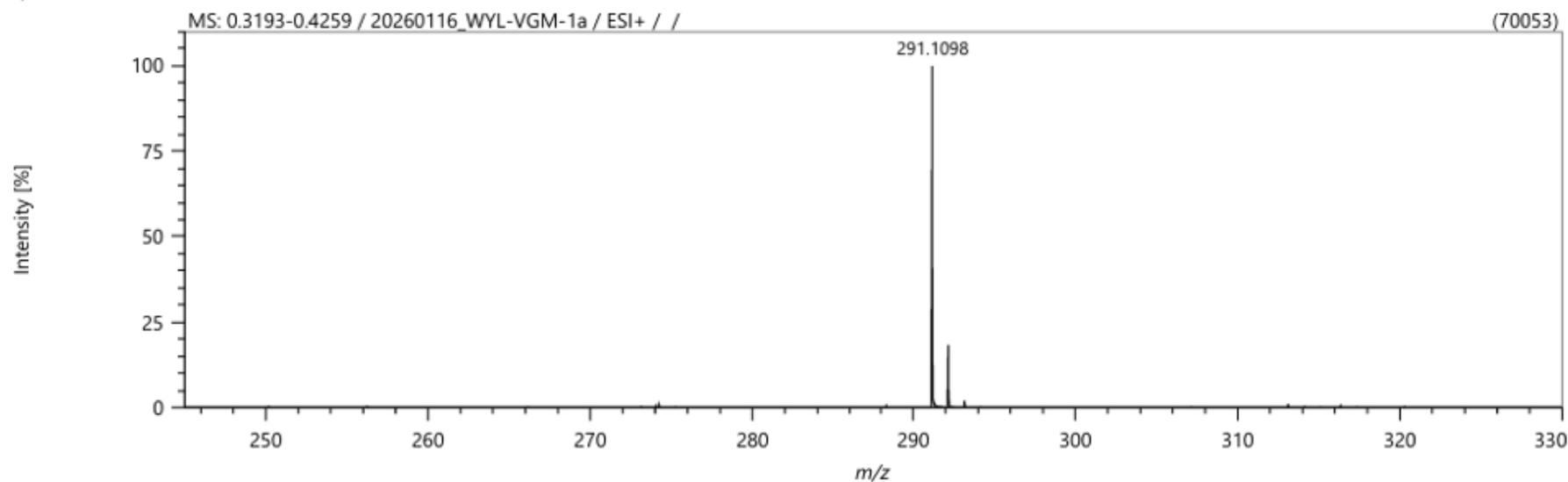


Fig. S141. ¹³C NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)-2-phenylacetamide (**3o**).



Chemical Formula: C₁₆H₁₆N₂O₂Na [M+Na]⁺ Cald: 291.1109
Found: 291.1098

Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	1	0	2	2	1
Max	400	1000	2	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
291.10978	C ₁₆ H ₁₆ N ₂ O ₂ Na	291.11040	-0.62	-2.12	9.5

Fig. S142. HRMS data of *N*-(2-amino-2-oxo-1-phenylethyl)-2-phenylacetamide (**3o**).

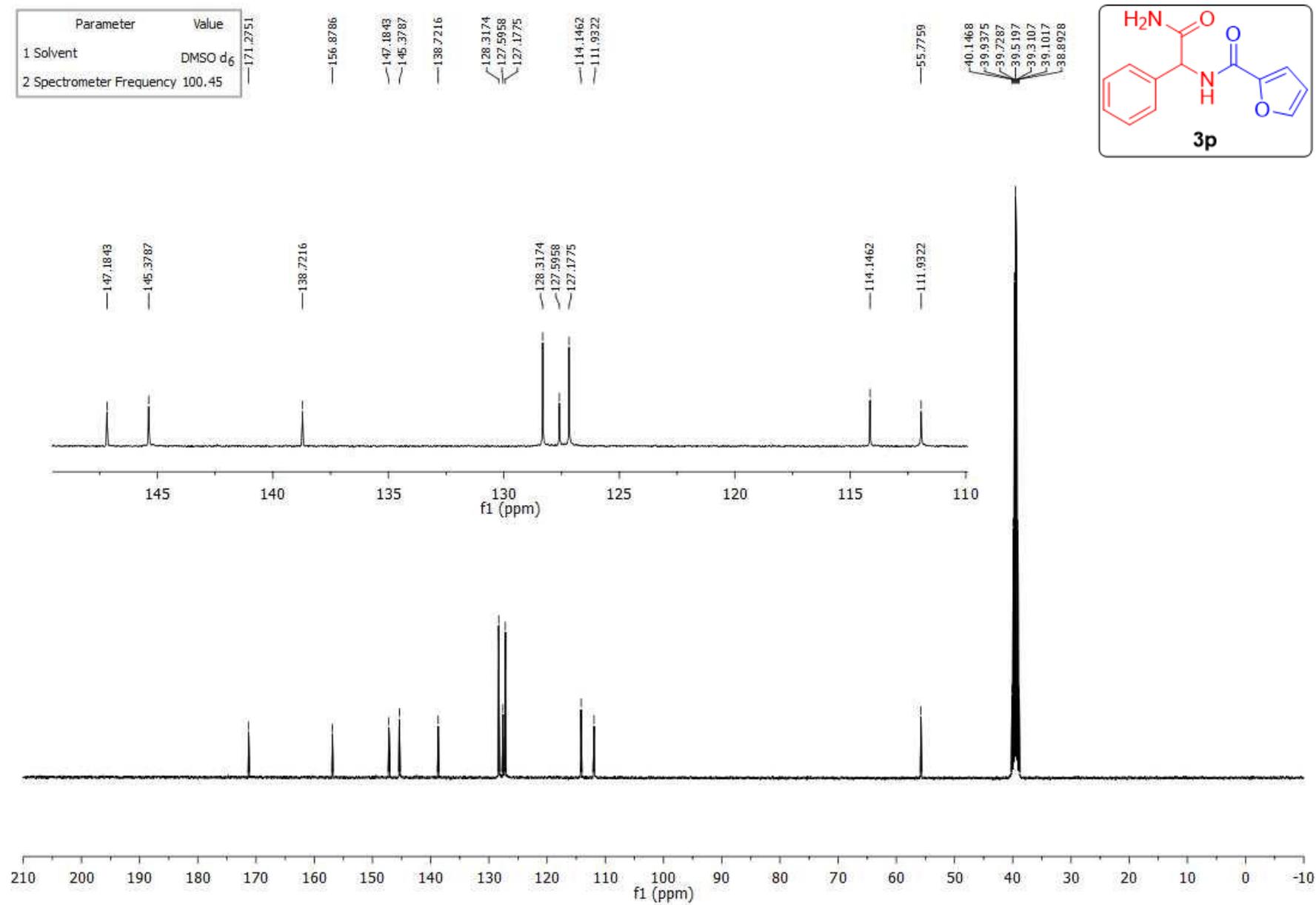
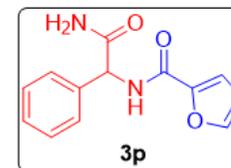


Fig. S144. ¹³C NMR spectra of *N*-(2-amino-2-oxo-1-phenylethyl)furan-2-carboxamide (**3p**).

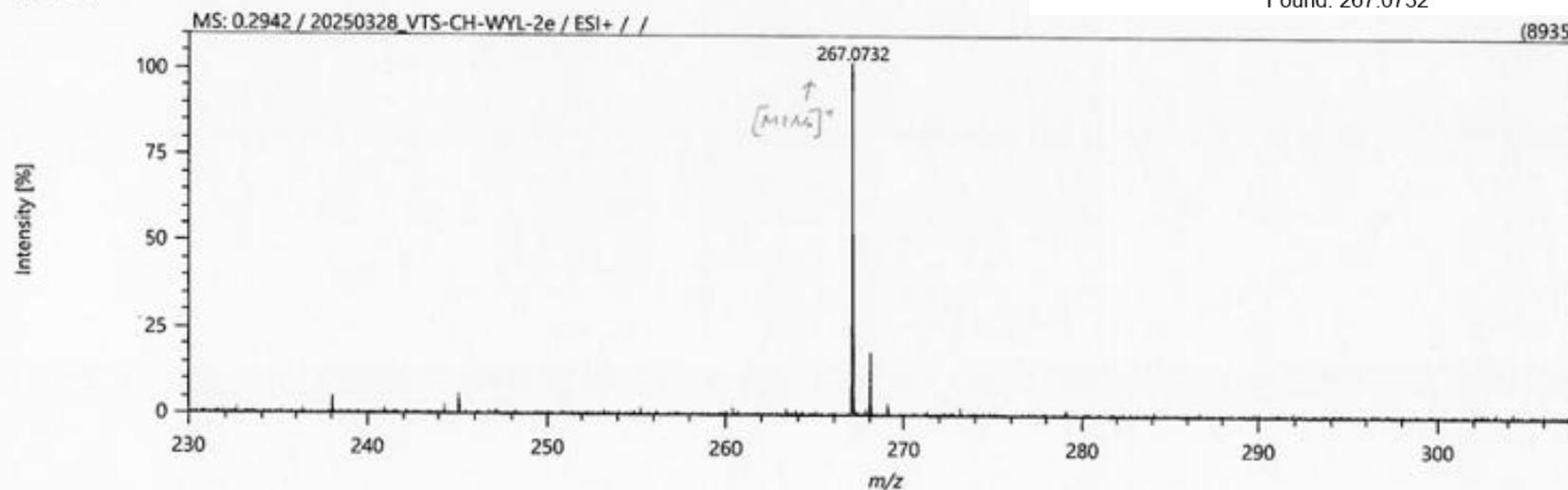
VTS-CH-WYL-2e (HR-ESI)



3p

Chemical Formula: C₁₃H₁₂N₂O₃Na [M+Na]⁺ Calcd: 267.0746
Found: 267.0732

Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 ppm
Electron: Odd/Even
Charge: +1
DBE: -99.0 - 999.0

Elements Set 2:

Symbol	C	H	O	N	Na
Min	0	0	3	2	1
Max	400	1000	3	2	1

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
267.07318	C ₁₃ H ₁₂ N ₂ O ₃ Na	267.07401	-0.84	-3.13	8.5

Fig. S145. HRMS data of *N*-(2-amino-2-oxo-1-phenylethyl)furan-2-carboxamide (**3p**).