

Supporting Information

n-Bu₄Ni/K₂S₂O₈ Mediated Csp²-Csp² Bond Cleavage – Transformylation from *p*-Anisaldehyde to Primary Amides

Xiaochen Liu,^{[a],[b]} Samuel Hee,^{[a],[b]} Netanel G. Sapir,^[a] Alvin Li,^[a] Jianbo Liu,^{*[a],[b]} Yu

Chen^{*[a],[b]}

[a] Department of Chemistry and Biochemistry, Queens College of the City University of New York, 65-30 Kissena Blvd., Queens, New York 11367, United States

[b] Ph.D. Program in Chemistry, The Graduate Center of the City University of New York, 365 Fifth Ave., New York, New York 10016, United States

yu.chen1@qc.cuny.edu; jianbo.liu@qc.cuny.edu

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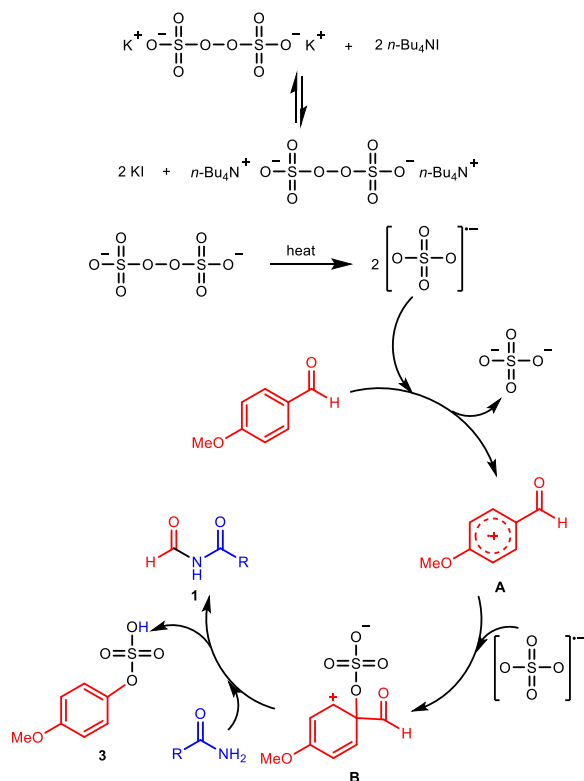
1. Density Functional Theory (DFT) Electronic Structure Calculations of the Proposed *n*-Bu₄NI/K₂S₂O₈ Mediated Transformylation Mechanism

Computational Methods

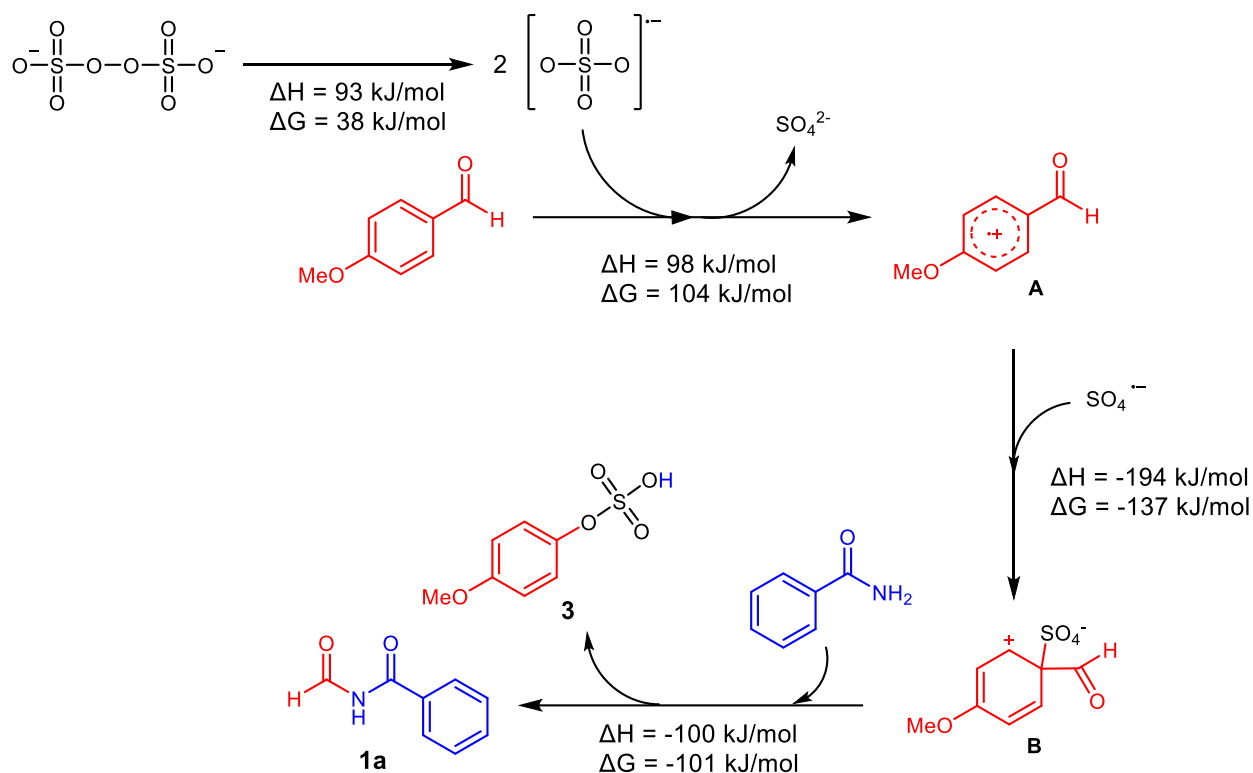
DFT electronic structure calculations were performed using the ω B97XD^[1] functional coupled with the 6-31+G(d,p) basis set, except for the reactions involving the iodine species for which the LANL2DZ basis set (which uses D95V on first row^[2] and Los Alamos ECP plus DZ on Na-La and Hf-Bi^[3]) was used. Geometries of reactants and products were fully optimized by calculating force constants at every step. Thermal corrections, reaction enthalpies (ΔH) and changes of Gibbs free energy (ΔG) were calculated by the standard statistical thermodynamical methods using the unscaled ω B97XD vibrational frequencies and the rigid rotor and harmonic oscillator approximations. All reactions were calculated in the acetonitrile solvent using the SMD solvation model.^[4] Reaction enthalpy and change of Gibbs free energy reported for each product pathway include zero-point energies (ZPEs) and thermal corrections to 298 K.

The calculations were accomplished at a Linux computational cluster equipped with 20 nodes of dual Intel Xeon 28-core 2.7 GHz processors and using the Gaussian 16 suite of program.^[5]

Scheme SI.1. Proposed Mechanism for the *n*-Bu₄NI and K₂S₂O₈ Mediated Transformylation from *p*-Anisaldehyde to Benzamide.

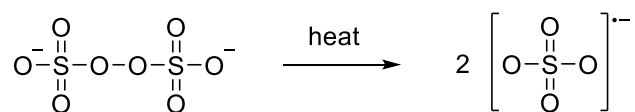


Scheme SI.2. Reaction Flow Chart for the *n*-Bu₄NI and K₂S₂O₈ Mediated Transformylation from *p*-Anisaldehyde to Benzamide.*



* The reaction enthalpies and Gibbs free energy changes were calculated at 298 K using the ω B97XD/6-31+G(d,p) method.

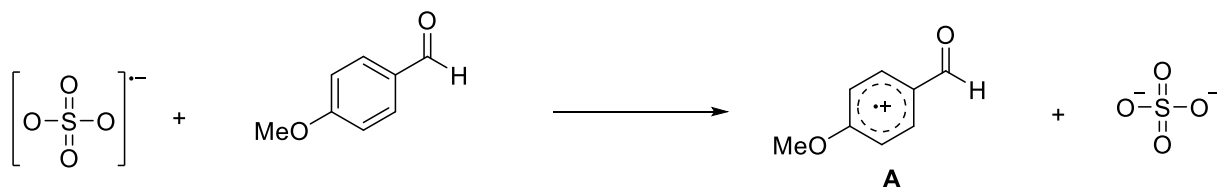
Elementary reaction (1)



ΔH (298 K) = 93 kJ/mol

ΔG (298 K) = 38 kJ/mol

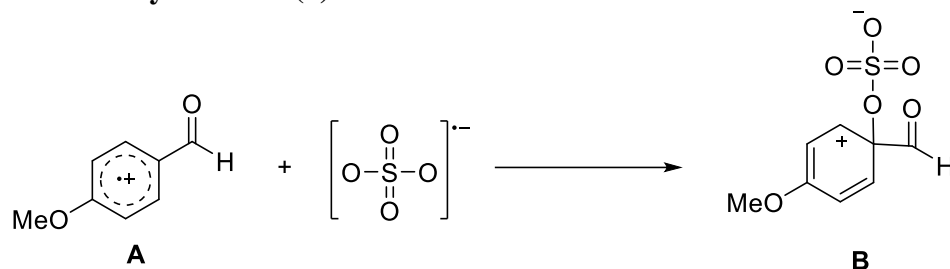
Elementary reaction (2)



$$\Delta H (298 \text{ K}) = 98 \text{ kJ/mol}$$

$$\Delta G (298 \text{ K}) = 104 \text{ kJ/mol}$$

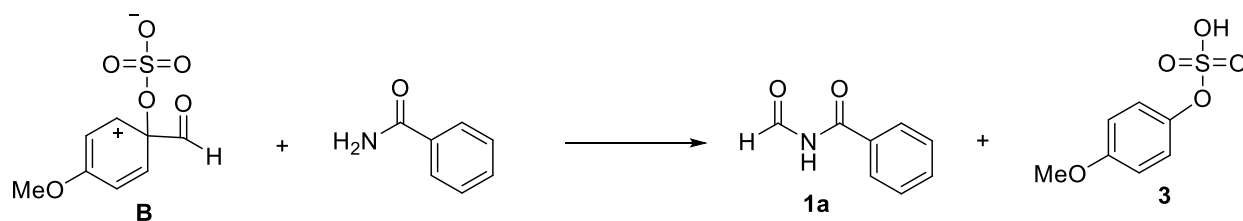
Elementary reaction (3)



$$\Delta H (298 \text{ K}) = -194 \text{ kJ/mol}$$

$$\Delta G (298 \text{ K}) = -137 \text{ kJ/mol}$$

Elementary reaction (4)



$$\Delta H (298 \text{ K}) = -100 \text{ kJ/mol}$$

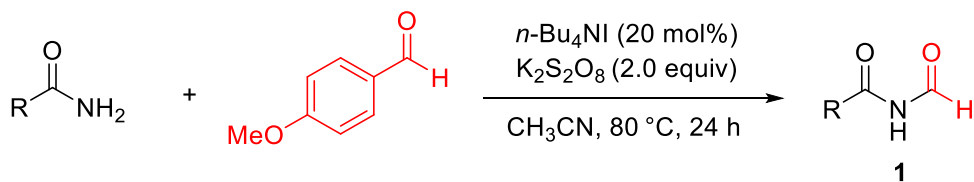
$$\Delta G (298 \text{ K}) = -101 \text{ kJ/mol}$$

2. General information.

All reactions were carried out in sealed 20 mL glass vials, unless otherwise indicated. All commercially available chemicals were used as received without further purification, unless otherwise noted. Acetonitrile is dried over 4Å molecular sieves overnight before use. Molecular sieves (4Å) were activated at 200 °C at 0.5 mmHg for a week before use. All ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded at 400 or 500 MHz and 100 or 125 MHz, respectively, using either CDCl_3 or $\text{DMSO-}d_6$ as solvent. The chemical shifts of all ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra are referenced to the residual signal of CDCl_3 (δ 7.26 ppm for the ^1H NMR spectra and δ 77.23 ppm for the $^{13}\text{C}\{^1\text{H}\}$ NMR spectra) and the residual signal of $\text{DMSO-}d_6$ (δ 2.50 ppm for the ^1H NMR

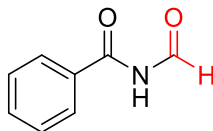
spectra and δ 39.52 ppm for the $^{13}\text{C}\{^1\text{H}\}$ NMR spectra). $^{19}\text{F}\{^1\text{H}\}$ NMR spectra were recorded at 376 MHz with fluorobenzene as the internal standard and CDCl_3 as solvent. The chemical shifts of the ^{19}F NMR spectra are referenced to fluorobenzene (δ -112.96 ppm). The high-resolution mass analysis was carried out on high resolution mass spectrometers using electrospray ionization (ESI) or heated electrospray ionization (HESI) method. Samples were dissolved in methanol or acetonitrile and analyzed via flow injection into the mass spectrometer at a flow rate of 200 $\mu\text{L}/\text{min}$. The mobile phase was 90:10 methanol:water, with 0.1% formic acid or 90:10 acetonitrile:water, with 0.1% formic acid. The melting points are uncorrected.

3. General Procedure for *n*-Bu₄NI/K₂S₂O₈ Mediated Transformylation and ^1H , ^{13}C , and ^{19}F NMR Data



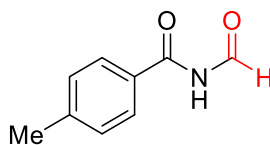
An oven dried 20 mL glass reaction vial was charged with amides (1.0 mmol, 1.0 equiv), *p*-anisaldehyde (1.2 mmol, 1.2 equiv, 163.4 mg), tetrabutylammonium iodide (0.2 mmol, 73.8 mg), potassium persulfate (2.0 mmol, 540.6 mg), and anhydrous acetonitrile (7 mL). The reaction mixture was stirred at 80 °C for 24 h. The reaction mixture was diluted with 20 mL of ethyl acetate and washed with saturated aqueous NaHCO_3 solution (20 mL). The aqueous phase was extracted with diethyl ether (2×15 mL). The combined organic layers were dried over anhydrous MgSO_4 and concentrated using a rotary evaporator under reduced pressure (20 mmHg). The subsequent residue was purified by flash column chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the corresponding product.

N-formylbenzamide (1a)



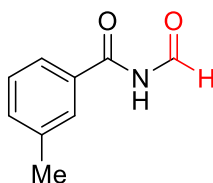
This product was obtained as a yellow solid (119.3 mg, 80% yield): m.p. 98.2-100.3 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.46$; ^1H NMR (500 MHz, CDCl_3) δ 9.81 (s, 1H), 9.40 (d, $J = 9.4$ Hz, 1H), 7.97-7.99 (m, 2H), 7.64-7.68 (m, 1H), 7.53-7.57 (m, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 166.7, 164.4, 134.2, 131.3, 129.3, 128.2. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[6]

***N*-formyl-4-methylbenzamide (1b)**



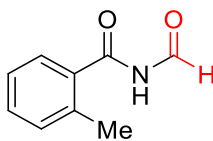
This product was obtained as a beige solid (128.9 mg, 79% yield): m.p. 129.7-129.9 °C; flash column chromatography eluent: 1/1 ethyl acetate/hexanes, $R_f = 0.68$; ^1H NMR (500 MHz, CDCl_3) δ 10.37 (d, $J = 9.69$ Hz, 1H), 9.38 (d, $J = 9.54$ Hz, 1H), 7.92 (d, $J = 8.20$ Hz, 2H), 7.33 (d, $J = 7.98$ Hz, 2H), 2.44 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 166.9, 165.4, 145.1, 129.9, 128.39, 128.35, 21.8. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[6]

***N*-formyl-3-methylbenzamide (1c)**



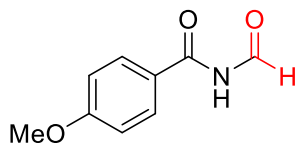
This product was obtained as a white solid (130.5 mg, 80% yield): m.p. 121.0-121.9 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.46$; ^1H NMR (500 MHz, CDCl_3) δ 9.57 (s, 1H), 9.38 (d, $J = 9.7$ Hz, 1H), 7.77 (s, 1H), 7.72 (d, $J = 7.4$ Hz, 1H), 7.40-7.47 (m, 2H), 2.44 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 166.6, 163.4, 139.5, 135.0, 131.3, 129.3, 128.7, 125.0, 21.6. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[6]

***N*-formyl-2-methylbenzamide (1d)**



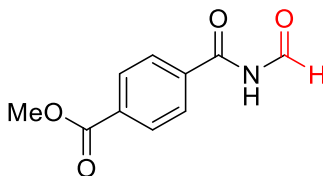
This product was obtained as a beige solid (71.8 mg, 44% yield): m.p. 101.7-102.9 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.37$; ^1H NMR (500 MHz, CDCl_3) δ 9.24 (d, $J = 10.1$ Hz, 1H), 8.77 (s, 1H), 7.49-7.51 (m, 1H), 7.44-7.47 (m, 1H), 7.29-7.32 (m, 2H), 2.53 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 168.7, 163.4, 138.6, 132.5, 132.3, 132.1, 127.4, 126.4, 20.6. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[6,10]

***N*-formyl-4-methoxybenzamide (1e)**



This product was obtained as an orange solid (157.7 mg, 88% yield): m.p. 195.5-196.4 °C; flash column chromatography eluent: 1/1 ethyl acetate/hexanes, $R_f = 0.54$; ^1H NMR (500 MHz, CDCl_3) δ 9.36 (d, $J = 9.8$ Hz, 1H), 9.16 (s, 1H), 7.89 (d, $J = 9.8$ Hz, 2H), 7.01 (d, $J = 9.8$ Hz, 2H), 3.90 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, $\text{DMSO}-d_6$) δ 166.7, 164.6, 163.5, 130.7, 123.5, 114.1, 55.6. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[7,10]

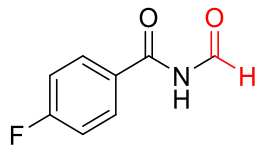
methyl 4-(formylcarbamoyl)benzoate (1f)



This product was obtained as a beige solid (128.5 mg, 62% yield): m.p. 181.2-181.6 °C; flash column chromatography eluent: 1/1 ethyl acetate/hexanes, $R_f = 0.62$; ^1H NMR (500 MHz, CDCl_3) δ 9.38 (d, $J = 8.9$ Hz, 1H), 9.31 (s, 1H), 8.20 (d, $J = 8.9$ Hz, 2H), 7.99 (d, $J = 8.4$ Hz, 2H), 3.97 (s,

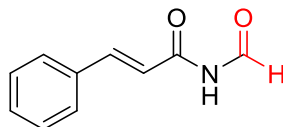
3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 166.0, 165.9, 163.9, 135.0, 134.9, 130.5, 128.2, 52.9; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd for $(\text{C}_{10}\text{H}_9\text{NO}_4\text{Na})^+$ 230.0424, found 230.0421.

4-fluoro-*N*-formylbenzamide (1g)



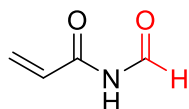
This product was obtained as an orange solid (83.6 mg, 50% yield): m.p. 159.1-159.4 °C; flash column chromatography eluent: 1/1 ethyl acetate/hexanes, $R_f = 0.58$; ^1H NMR (500 MHz, CDCl_3) δ 9.64 (s, 1H), 9.38 (d, $J = 9.5$ Hz, 1H), 7.99-8.02 (m, 2H), 7.22-7.26 (m, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 166.4 ($J_{\text{C-F}} = 256.1$ Hz), 165.5, 164.3, 130.9 ($J_{\text{C-F}} = 9.7$ Hz), 127.5 ($J_{\text{C-F}} = 2.9$ Hz), 116.7 ($J_{\text{C-F}} = 22.1$ Hz); $^{19}\text{F}\{^1\text{H}\}$ NMR (376 MHz, CDCl_3) δ -103.20. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[7, 11]

N-formylcinnamamide (1h)



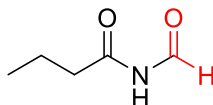
This product was obtained as a yellow solid (152.4 mg, 87% yield): m.p. 137.4-137.7 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.63$; ^1H NMR (400 MHz, CDCl_3) δ 9.79 (d, $J = 7.4$ Hz, 1H), 9.30 (d, $J = 9.4$ Hz, 1H), 7.90 (d, $J = 15.6$ Hz, 1H), 7.57-7.60 (m, 2H), 7.40-7.45 (m, 3H), 6.56 (d, $J = 15.7$ Hz, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 165.7, 164.9, 146.8, 133.8, 131.4, 129.3, 128.8, 118.2. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[6]

N-formylacrylamide (1i)



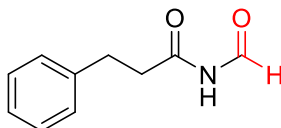
This product was obtained as an orange solid (45.6 mg, 46% yield): m.p. 81.1-81.4 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.31$; ^1H NMR (400 MHz, CDCl_3) δ 9.74 (s, 1H), 9.21 (d, $J = 9.7$ Hz, 1H), 6.57 (dd, $J = 17.2, 0.6$ Hz, 1H), 6.26 (dd, $J = 17.4, 10.7$ Hz, 1H), 5.98 (dd, $J = 10.5, 0.6$ Hz, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 165.2, 164.6, 132.3, 129.3; HRMS (HESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $(\text{C}_{10}\text{H}_{11}\text{NO}_2+\text{H})^+$ 100.03930, found 100.03920.

***N*-formylbutyramide (1j)**



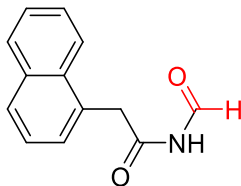
This product was obtained as a yellow oil (99.0 mg, 86% yield); flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.38$; ^1H NMR (400 MHz, CDCl_3) δ 9.30 (s, 1H), 9.11 (s, 1H), 2.37 (t, $J = 7.3$ Hz, 2H), 1.71 (sextet, $J = 7.3$ Hz, 2H), 0.98 (t, $J = 7.4$ Hz, 3H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 173.7, 163.8, 38.6, 17.9, 13.7. HRMS (HESI) m/z : $[\text{M}+\text{H}]^+$ calcd for $(\text{C}_{10}\text{H}_{11}\text{NO}_2+\text{H})^+$ 116.07061, found 116.07053.

***N*-formyl-3-phenylpropanamide (1k)**



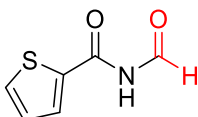
This product was obtained as a white solid (148.8 mg, 84% yield): m.p. 76.1-76.4 °C; flash column chromatography eluent: 1/1 ethyl acetate/hexanes, $R_f = 0.52$; ^1H NMR (400 MHz, CDCl_3) δ 9.16 (s, 1H), 9.10 (s, 1H), 7.29-7.32 (m, 2H), 7.20-7.24 (m, 3H), 3.01 (t, $J = 7.6$ Hz, 2H), 2.71 (t, $J = 7.6$ Hz, 2H). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 172.8, 163.5, 139.8, 128.9, 128.5, 126.8, 38.4, 30.2. HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd for $(\text{C}_{10}\text{H}_{11}\text{NO}_2\text{Na})^+$ 200.0682, found 200.0680.

***N*-formyl-2-(naphthalen-1-yl)acetamide (1l)**



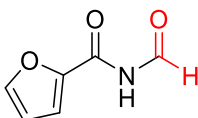
This product was obtained as a yellow solid (91.7 mg, 43% yield): m.p. 147.8-148.8 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.54$; ^1H NMR (500 MHz, CDCl_3) δ 9.07 (d, $J = 10.0$ Hz, 2H), 8.26 (s, 1H), 7.87-7.92 (m, 3H), 7.54-7.60 (m, 2H), 7.47 (t, $J = 7.1$ Hz, 1H), 7.42 (d, $J = 6.9$ Hz, 1H), 4.13 (s, 2H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 171.4, 162.5, 134.2, 132.0, 129.6, 129.3, 129.0, 128.4, 127.5, 126.7, 125.8, 123.3, 42.3; HRMS (ESI-TOF) m/z : $[\text{M}+\text{Na}]^+$ calcd for $(\text{C}_{13}\text{H}_{11}\text{NO}_2\text{Na})^+$ 236.0682, found 236.0678.

***N*-formylthiophene-2-carboxamide (1m)**



This product was obtained as a beige solid (93.1 mg, 60% yield): m.p. 151.7-152.2 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.56$; ^1H NMR (500 MHz, CDCl_3) δ 10.26 (d, $J = 7.12$ Hz, 1H), 9.36 (d, $J = 9.63$ Hz, 1H), 7.96 (dd, $J = 3.80, 0.95$ Hz, 1H), 7.74 (dd, $J = 4.96, 0.96$ Hz, 1H), 7.21 (dd, $J = 4.9, 4.0$ Hz, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 164.6, 161.1, 136.2, 134.9, 132.0, 128.8. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[6,10]

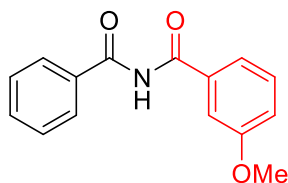
***N*-formylfuran-2-carboxamide (1n)**



This product was obtained as a beige solid (45.9 mg, 33% yield): m.p. 156.7-157.5 °C; flash column chromatography eluent: 1/3 ethyl acetate/hexanes, $R_f = 0.62$; ^1H NMR (500 MHz, $\text{DMSO}-d_6$) δ 11.66 (s, 1H), 9.17 (s, 1H), 8.06 (dd, $J = 1.5, 0.5$ Hz, 1H), 7.67 (dd, $J = 3.7, 0.5$ Hz, 1H), 6.75

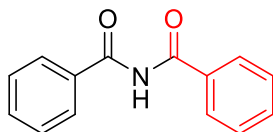
(dd, $J = 3.7, 1.7$ Hz, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, DMSO- d_6) δ 163.7, 157.6, 148.5, 145.0, 118.6, 112.6. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[7,12]

***N*-benzoyl-3-methoxybenzamide (2a)**



Benzamide (1.0 mmol, 1.0 equiv, 121.1 mg) and *m*-anisaldehyde (1.2 mmol, 1.2 equiv, 163.4 mg) were used. This product was obtained as a yellow solid (53.6 mg, 21% yield): m.p. 121.1-121.9 °C; ^1H NMR (400 MHz, CDCl_3) δ 9.09 (s, 1H), 7.84-7.87 (m, 2H), 7.58-7.62 (m, 1H), 7.49 (t, $J = 7.9$ Hz, 2H), 7.39-7.42 (m, 3H), 7.11-7.14 (m, 1H), 3.85 (s, 3H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 166.7, 166.2, 160.2, 134.9, 133.6, 133.3, 130.1, 129.0, 128.1, 119.7, 119.5, 113.3, 55.7. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[8]

***N*-benzoylbenzamide (2b)**

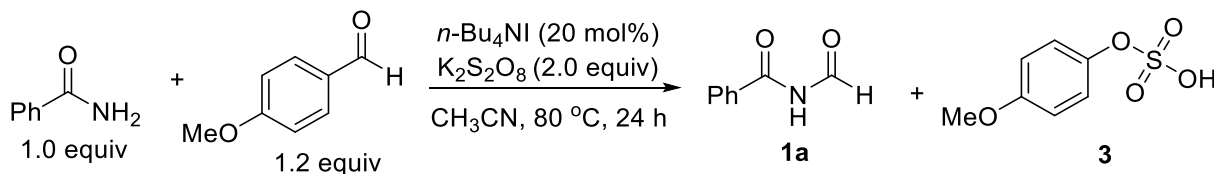


Benzamide (1.0 mmol, 1.0 equiv, 121.1 mg) and benzaldehyde (1.2 mmol, 1.2 equiv, 127.3 mg) were used. This product was obtained as a white solid (177.8 mg, 79% yield): m.p. 140.5-141.2 °C; ^1H NMR (500 MHz, CDCl_3) δ 8.89 (s, 1H), 7.87 (d, $J = 7.4$ Hz, 4H), 7.62 (t, $J = 6.5$ Hz, 2H), 7.52 (t, $J = 7.8$ Hz, 4H); $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, CDCl_3) δ 166.5, 133.5, 133.4, 129.1, 128.1. The ^1H and ^{13}C NMR spectral data are in good agreement with the literature data.^[9]

4. Procedure of *n*-Bu₄NI and K₂S₂O₈ Mediated Transformylation from *p*-Anisaldehyde to Benzamide at Gram Scale

An oven dried 250 mL two-necked round bottom flask was charged with benzamide (8.0 mmol, 1.0 equiv, 0.968 g), *p*-anisaldehyde (9.6 mmol, 1.2 equiv, 1.307 g), tetrabutylammonium iodide (1.6 mmol, 0.2 equiv, 0.590 g), potassium persulfate (16.0 mmol, 4.325 g), anhydrous acetonitrile (55 mL), and equipped with a reflux condenser and a rubber septum. The reaction mixture was stirred at 80 °C for 8 h. Then, potassium persulfate (8.0 mmol, 2.160 g) was added to the reaction mixture, and the mixture was stirred at 80 °C for another 16 h. The mixture was cooled to room temperature and diluted with 150 mL of ethyl acetate and washed with saturated aqueous NaHCO₃ solution (150 mL). The aqueous phase was extracted with diethyl ether (2 × 100 mL). The combined organic layers were dried over anhydrous MgSO₄ and concentrated using a rotary evaporator under reduced pressure (20 mmHg). The subsequent residue was purified by flash column chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the corresponding product *N*-formylbenzamide (**1a**). This product was obtained as a yellow solid (0.901 g, 76% yield).

5. High Resolution Accurate Mass Measurement of the Reaction Mixture of Benzamide and *p*-Anisaldehyde



Sample Format

The samples (reaction mixture) were submitted in liquid form and stored at room temperature. They are soluble in water and methanol. They are not air, acid, or light sensitive.

Analysis

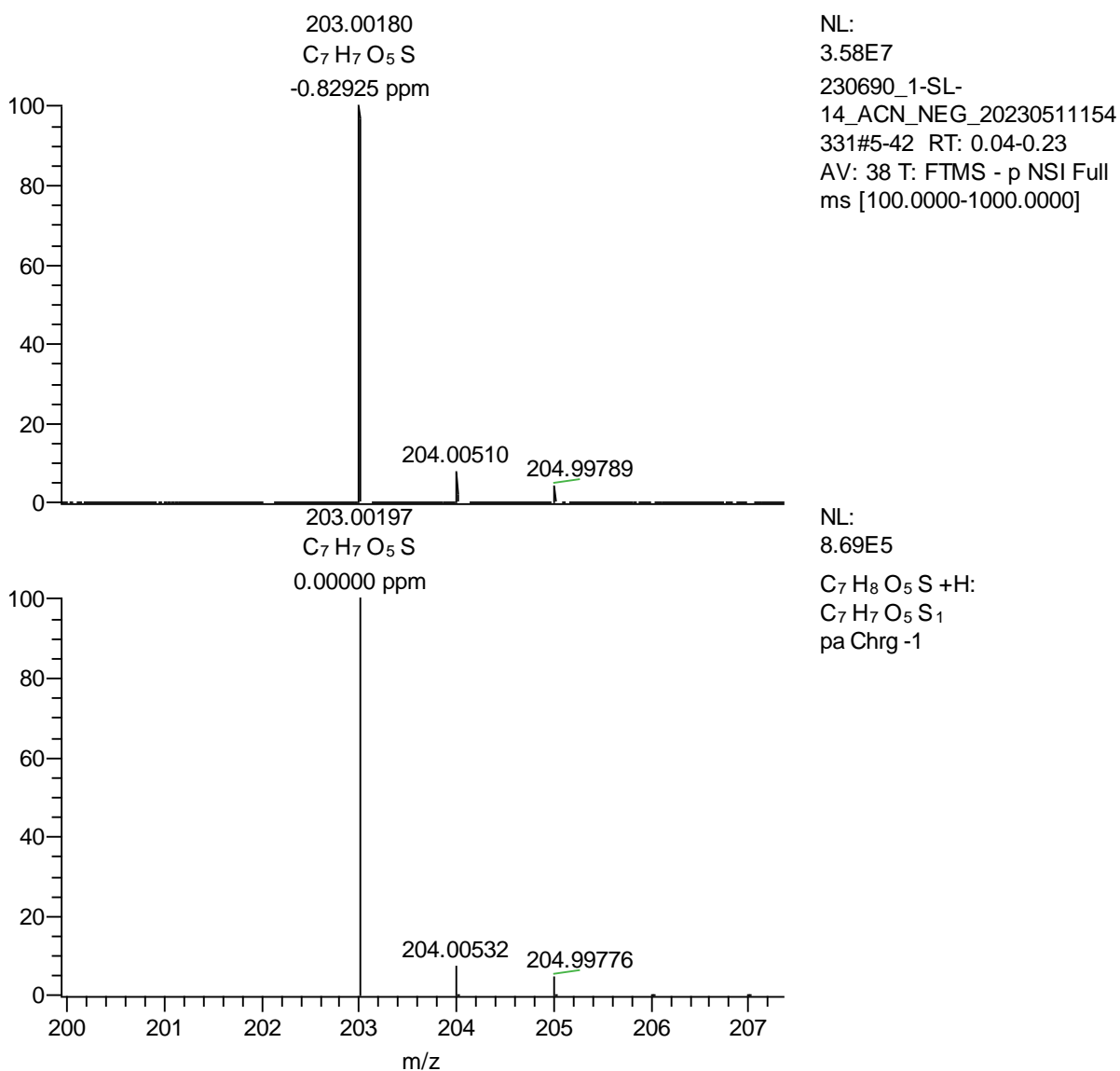
Analysis was carried out on a high-resolution mass spectrometer – the *Thermo Fisher Scientific Exactive Plus MS*, a benchtop full-scan Orbitrap™ mass spectrometer – using Heated Electrospray Ionization (HESI). Samples were diluted in acetonitrile and methanol and analyzed via Nanomate

into the mass spectrometer. The mass spectrometer was operated in positive and negative ion mode.

| HESI Source Parameters | |
|-------------------------------|--------------|
| Spray voltage | 1.45 kV |
| Capillary temperature | 250 C |
| Heater Temp | 350 C |
| S Lens RF level | 55 V |
| Sheath gas flow rate | 0 |
| Resolution | 70,000 |
| Scan Range | 100-1000 m/z |

| Sample | M_{Theoretical} | M_{Experimental} | ΔM (ppm) | Elemental Composition |
|----------------------------------|---------------------------------|---------------------------------|-----------------|--|
| 3 in the reaction Mixture | 203.00197 [M-H] ⁻ | 203.00180 [M-H] ⁻ | -0.82925 | C ₇ H ₇ O ₅ S |

Experimental and Theoretical Isotopic Distribution [M-H]⁻



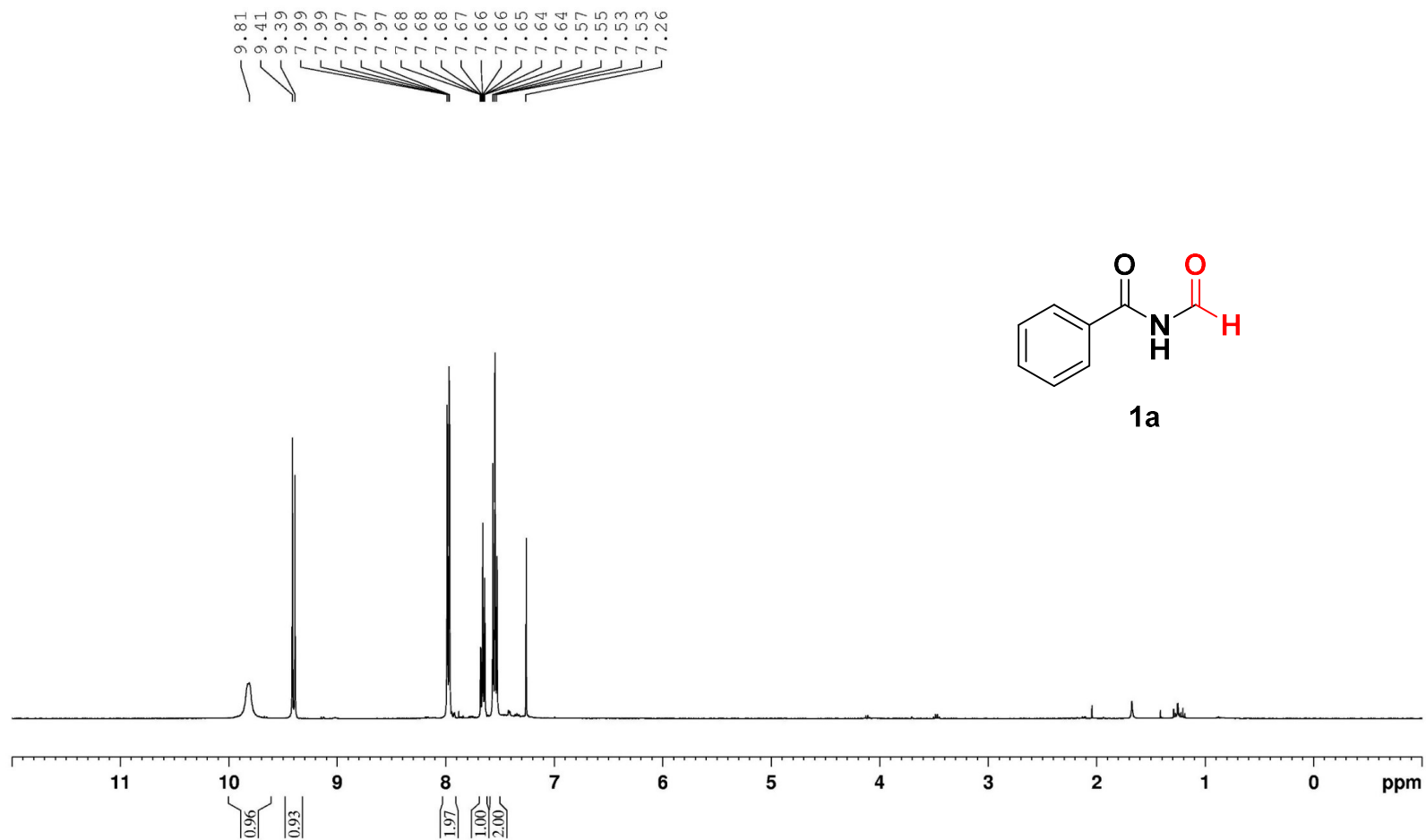
6. Reference:

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

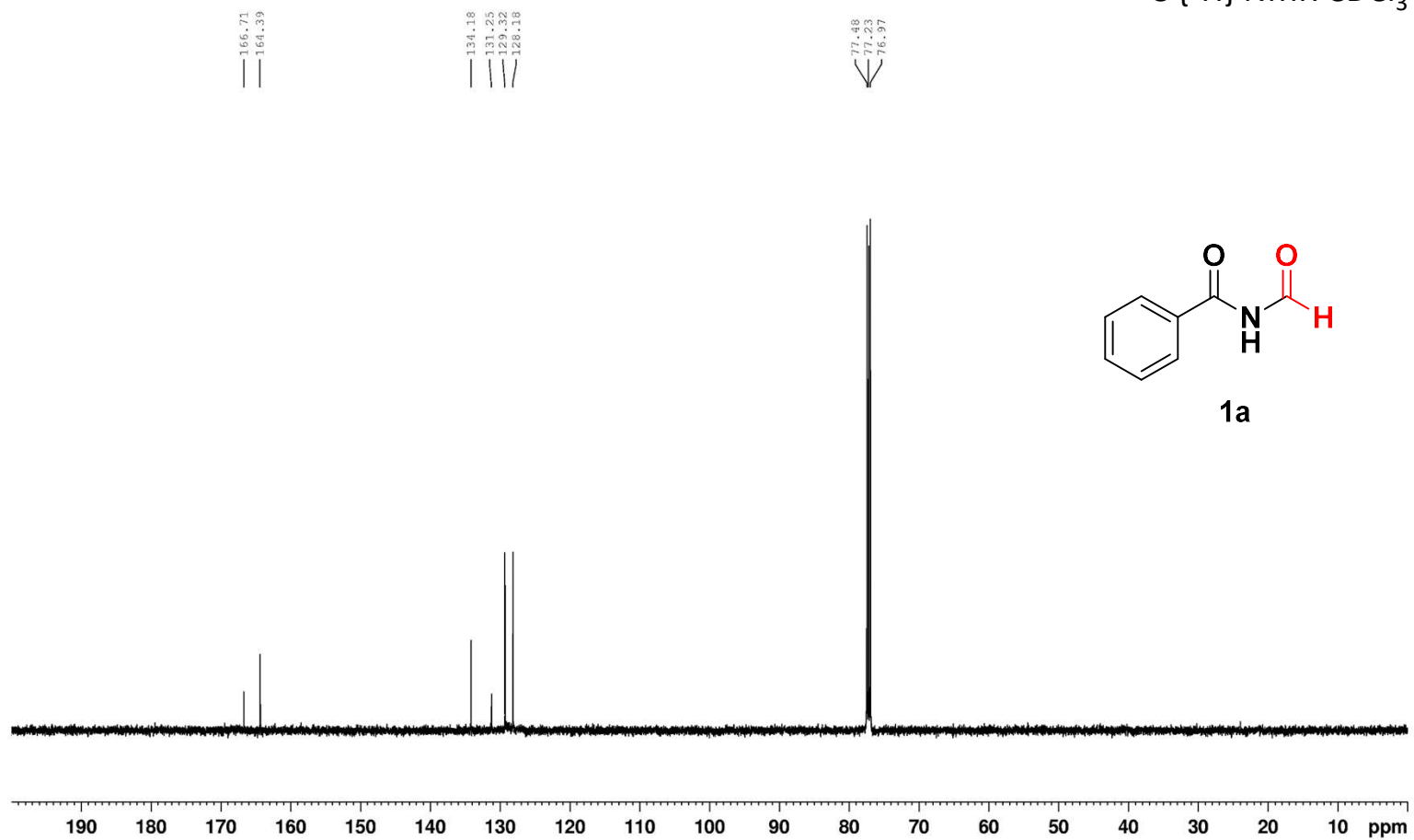
^1H NMR CDCl_3 / 500 MHz



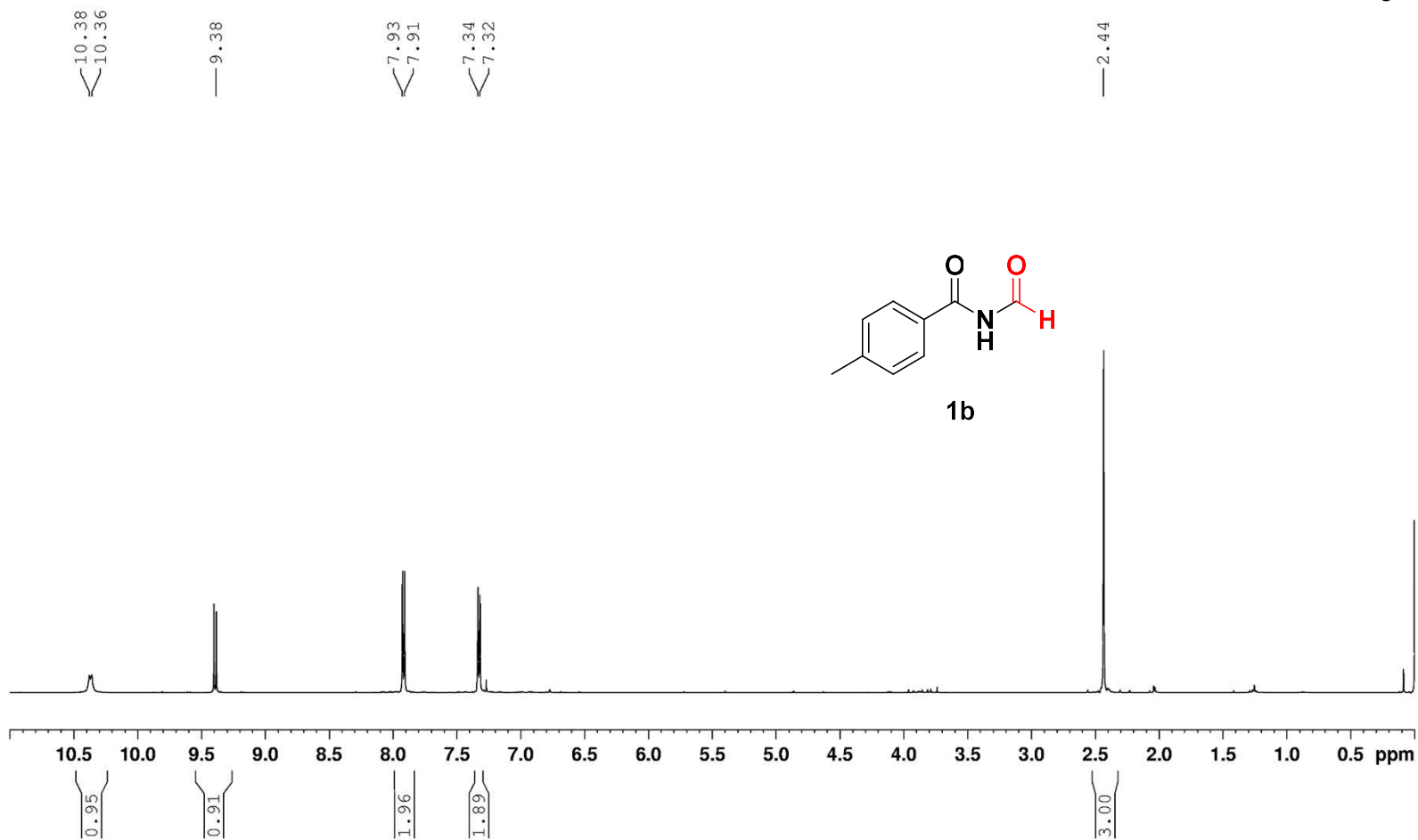
S

16

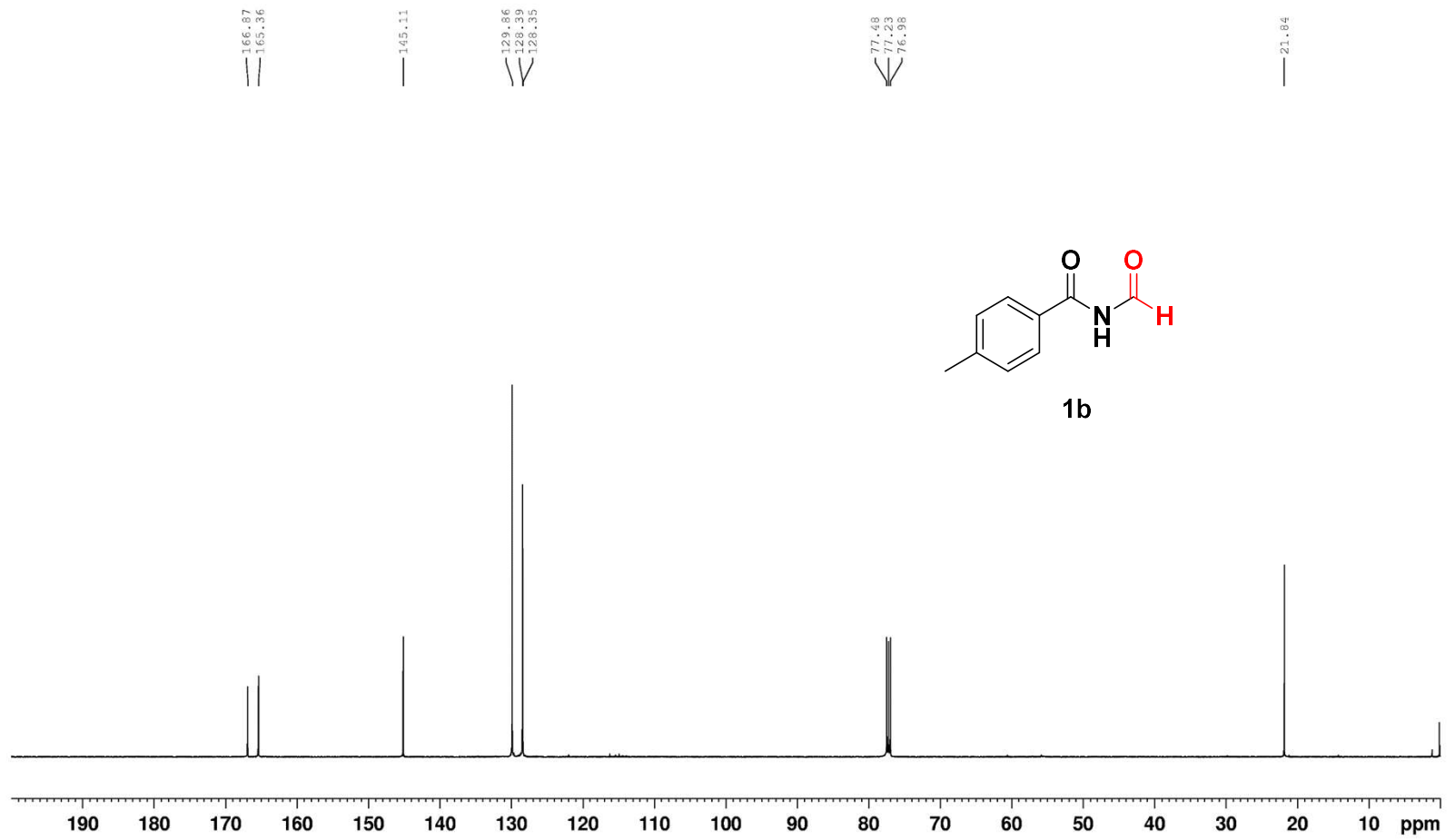
^{13}C $\{^1\text{H}\}$ NMR CDCl_3 / 125 MHz



^1H NMR CDCl_3 / 500 MHz



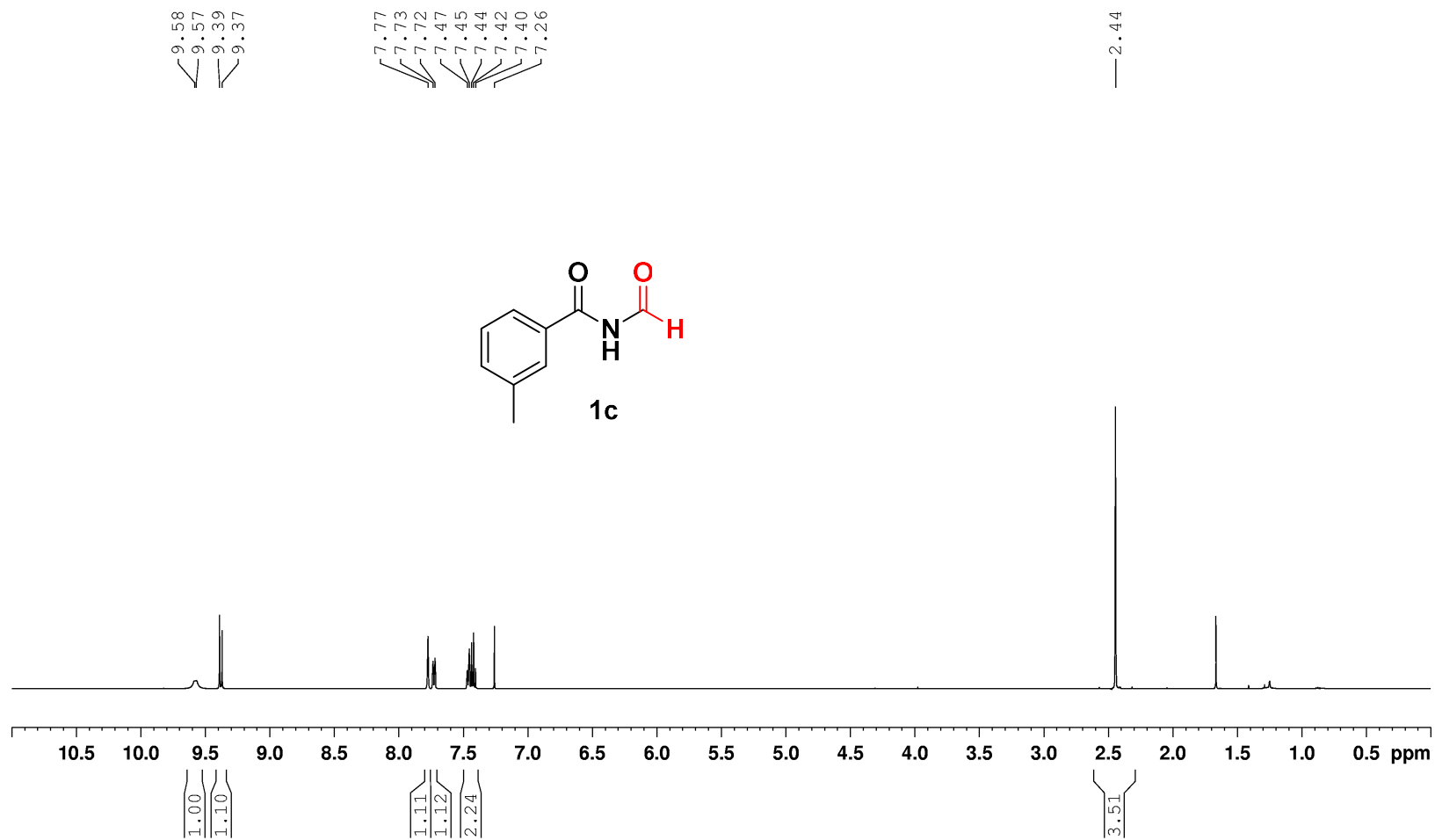
$^{13}\text{C} \{^1\text{H}\}$ NMR CDCl_3 / 125 MHz



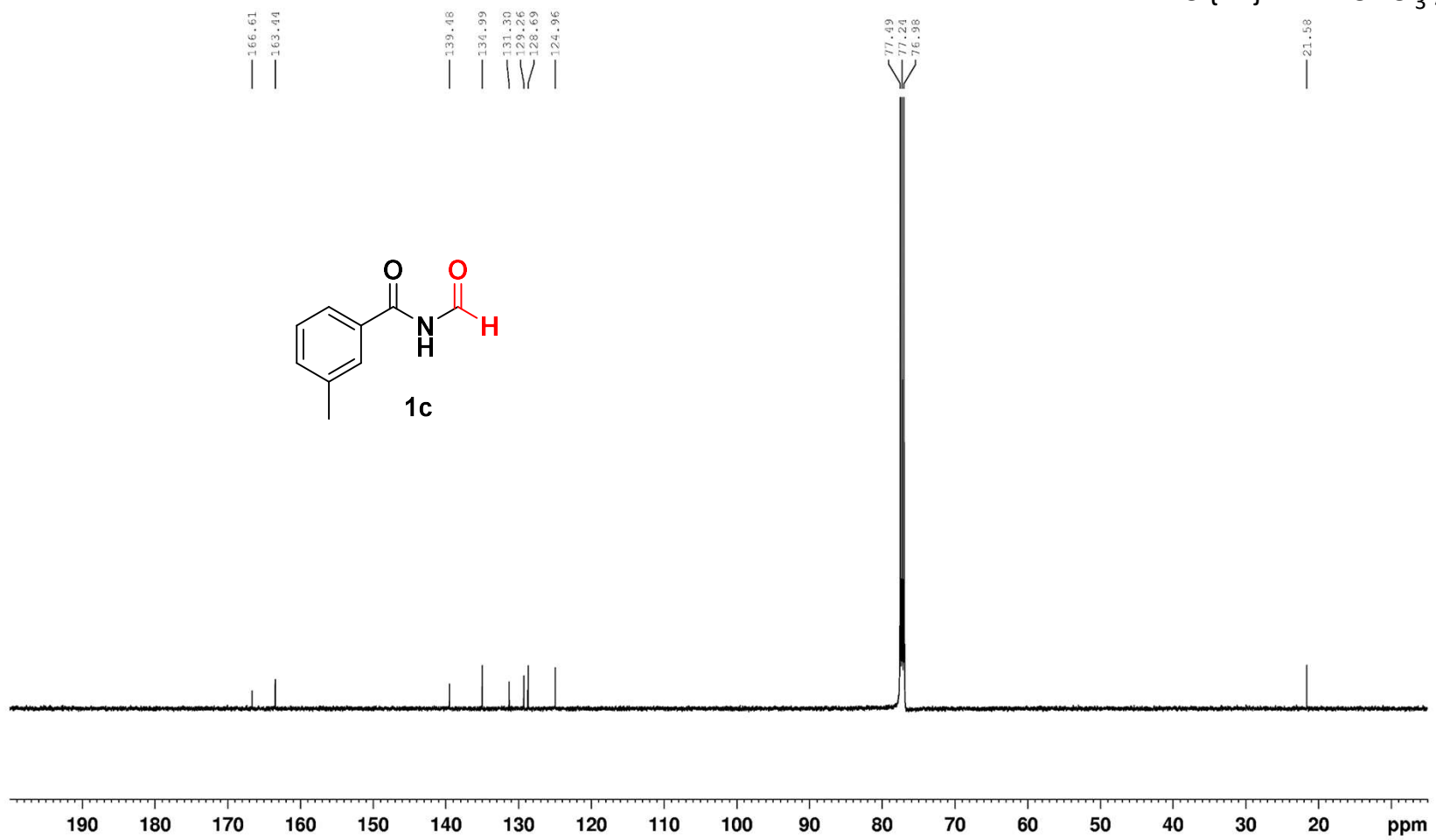
S

19

^1H NMR CDCl_3 / 500 MHz

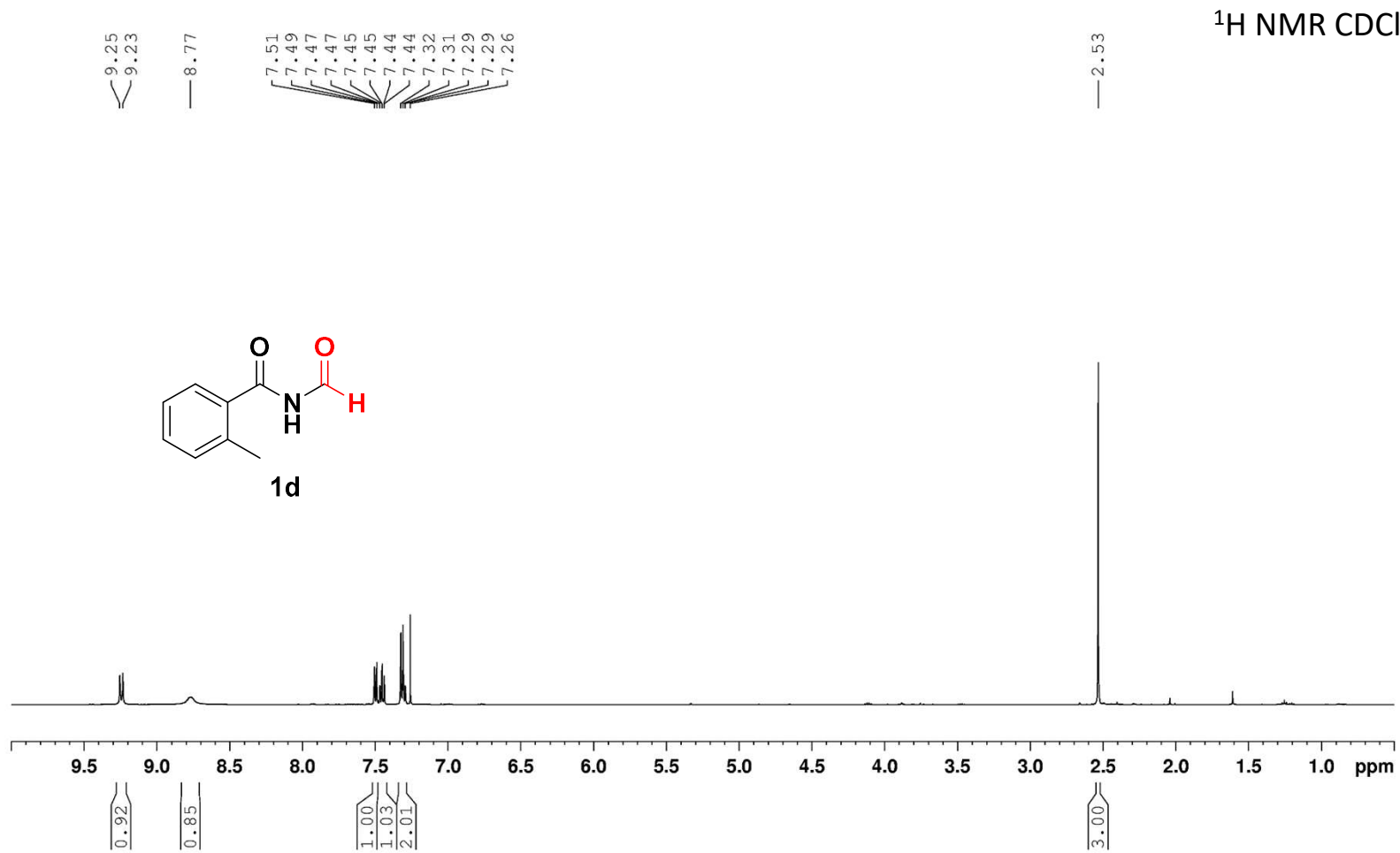


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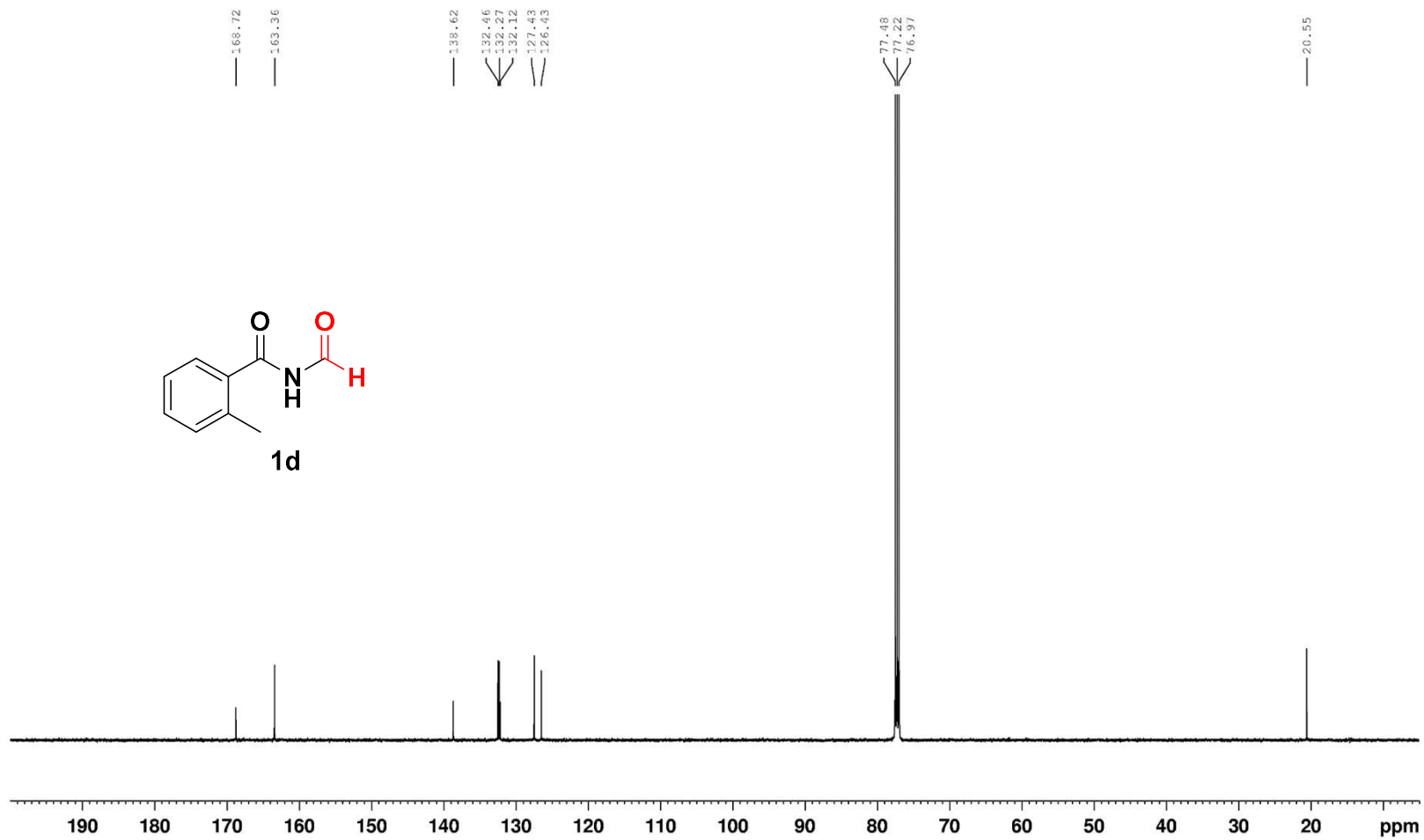


S

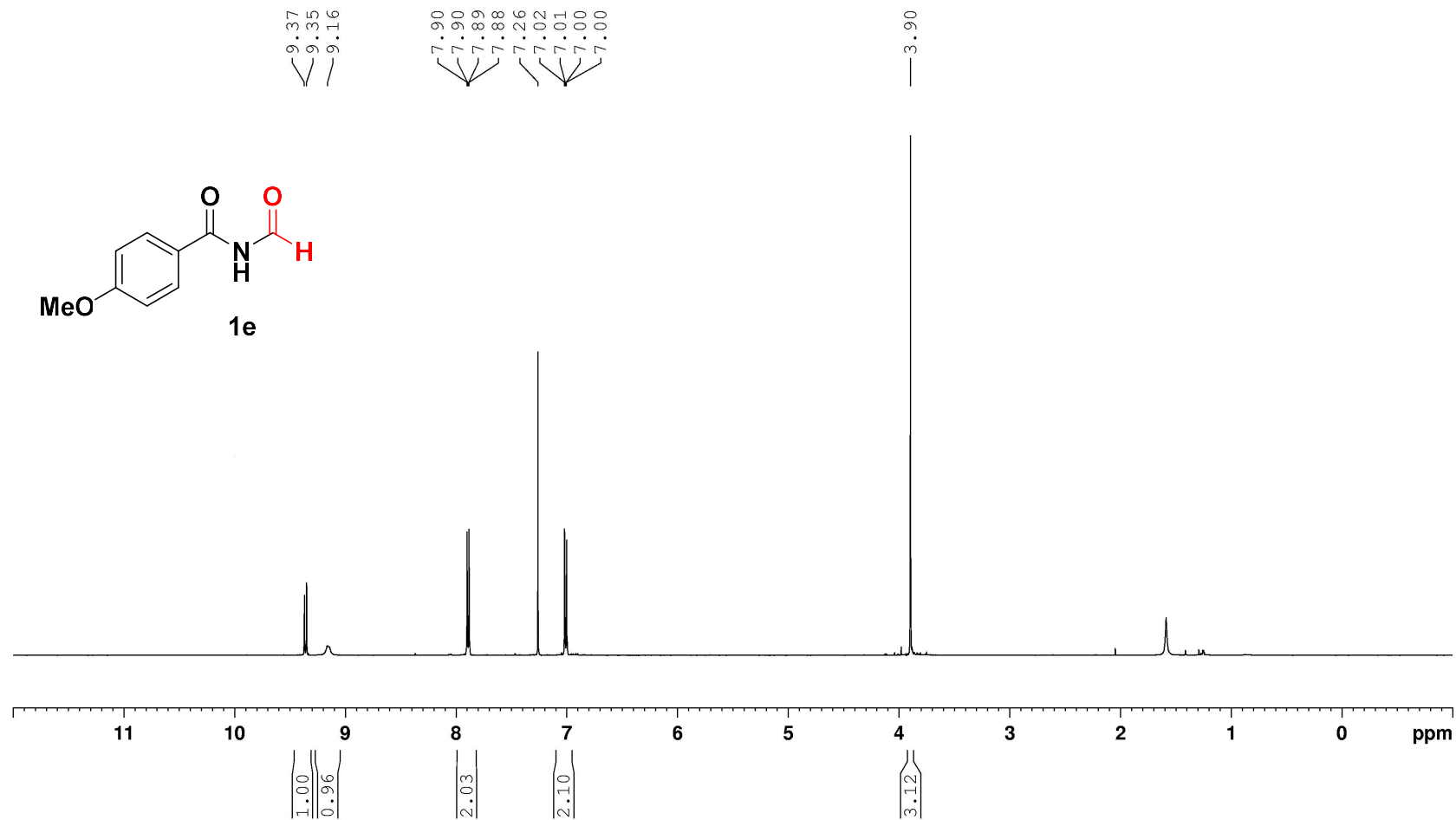
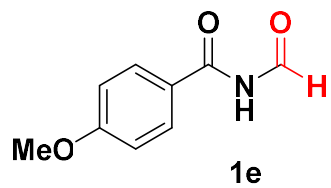
21



^{13}C $\{^1\text{H}\}$ NMR CDCl_3 / 125 MHz

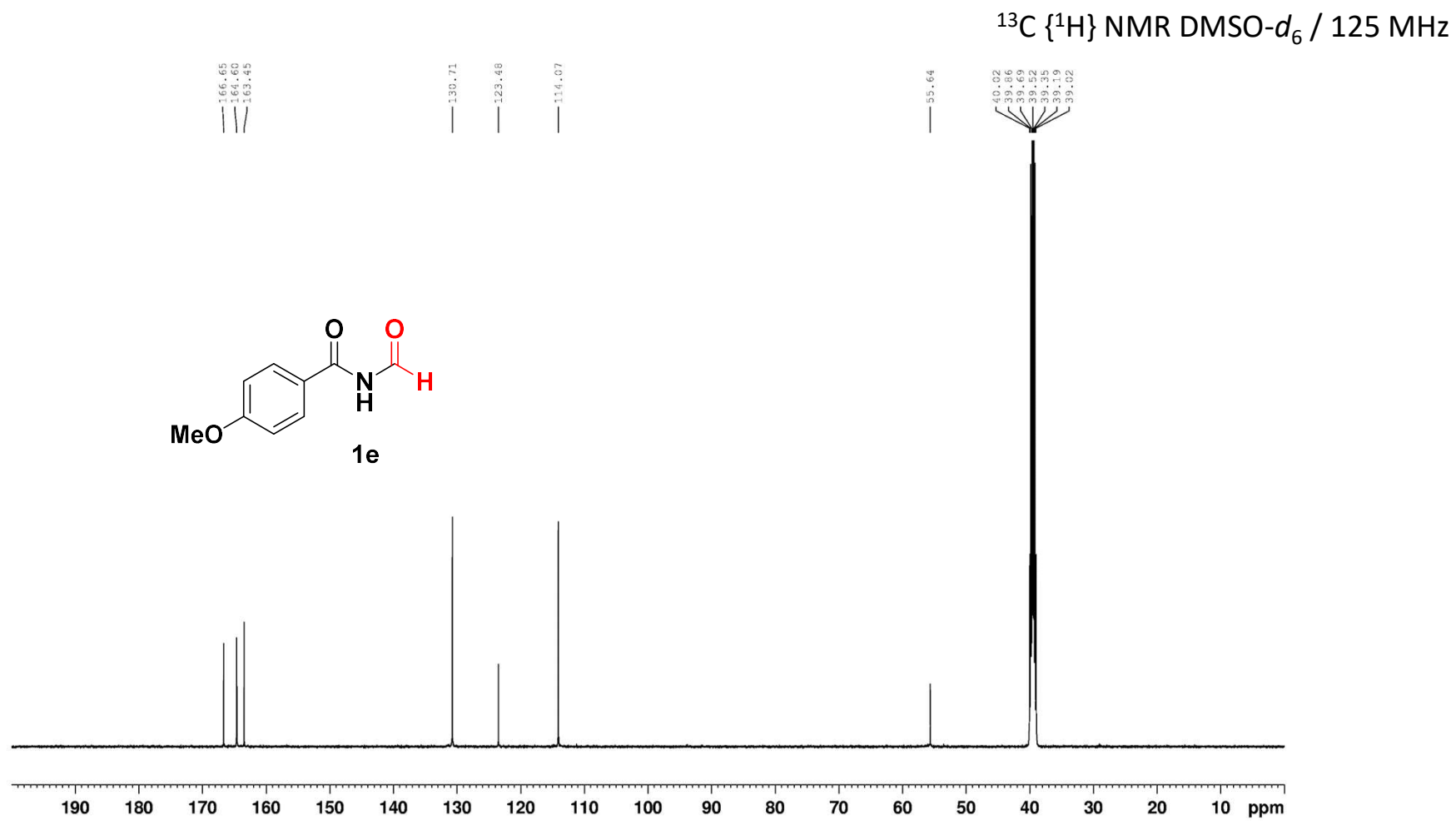


^1H NMR CDCl_3 / 500 MHz

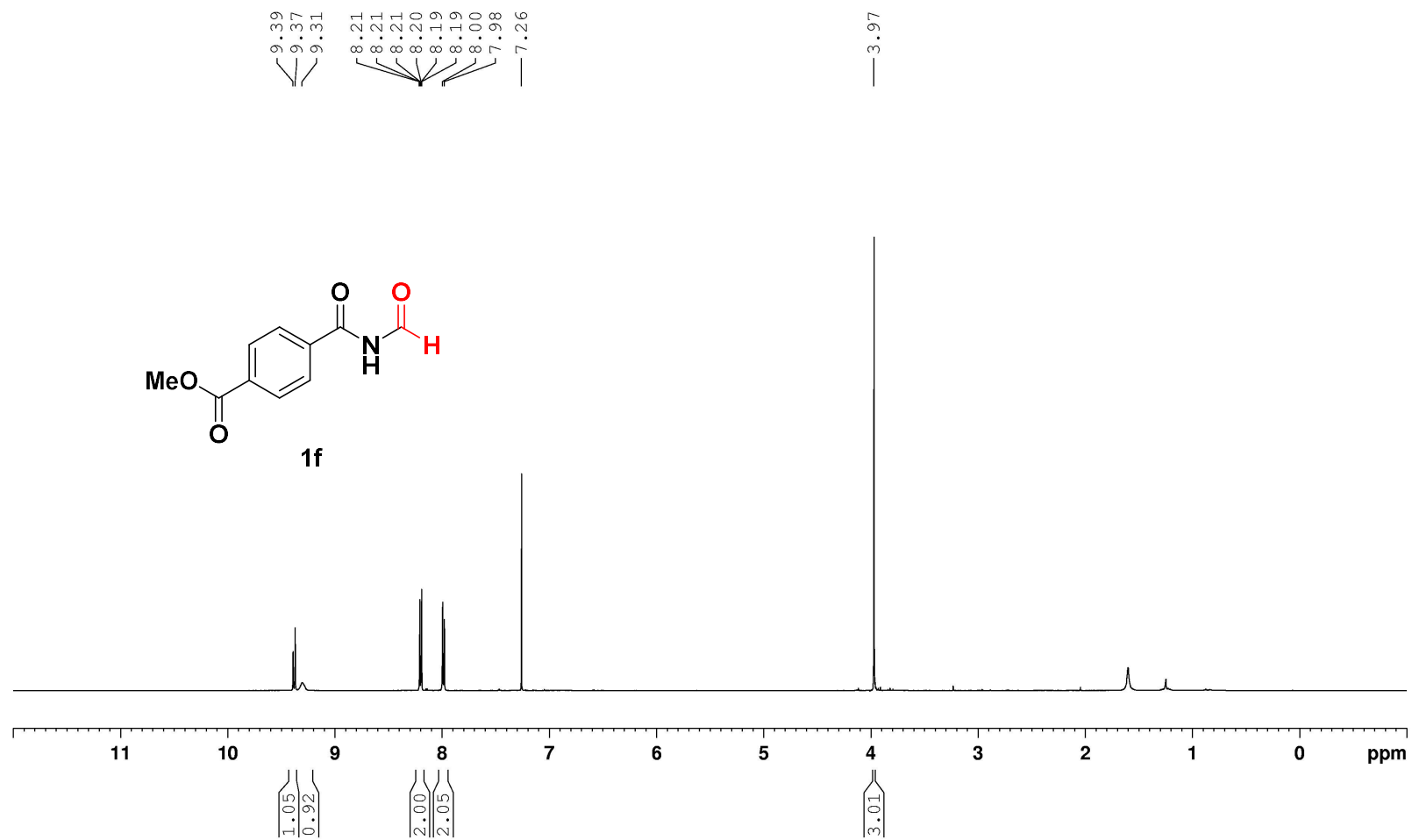


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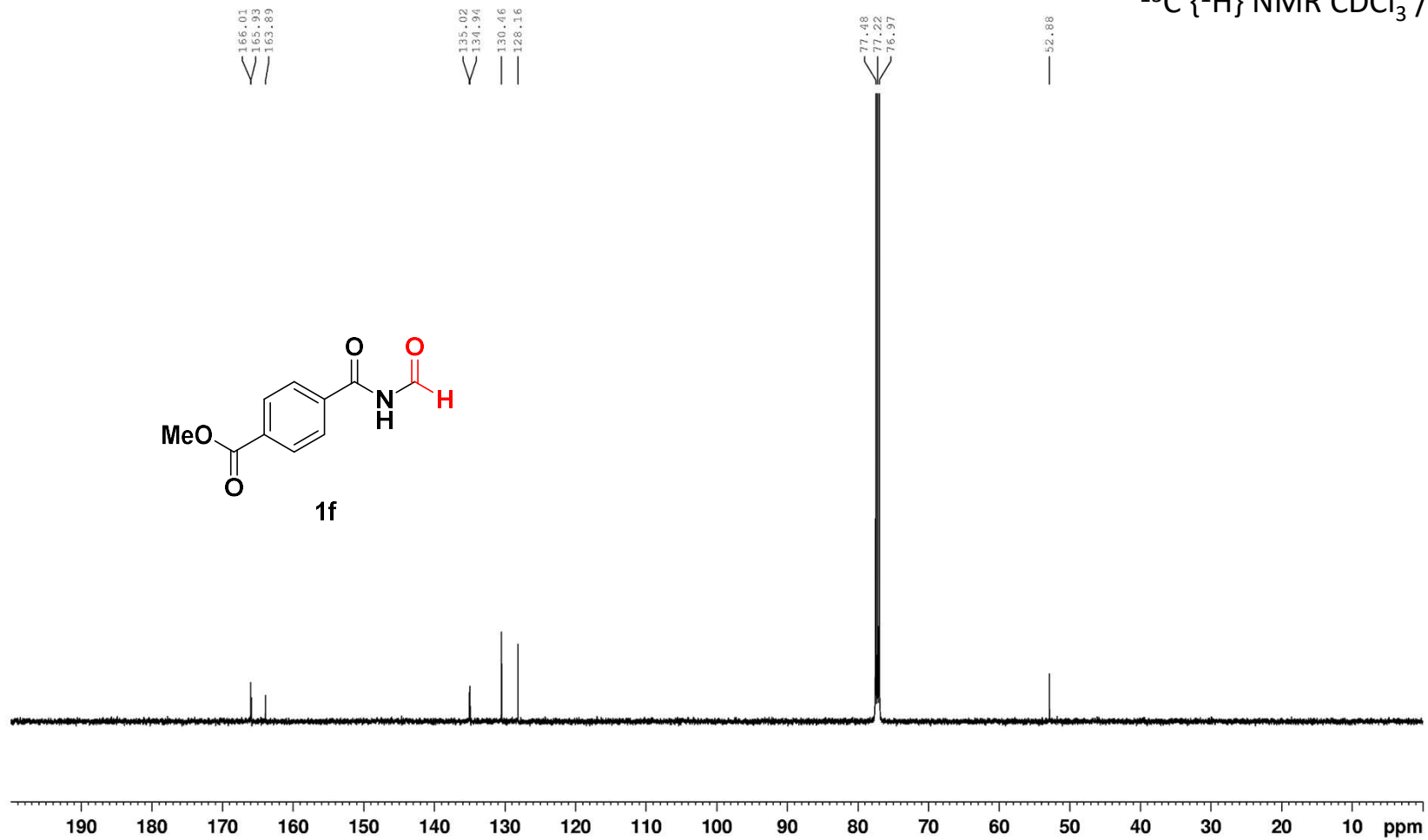
24



^1H NMR CDCl_3 / 500 MHz



^{13}C $\{^1\text{H}\}$ NMR CDCl_3 / 125 MHz

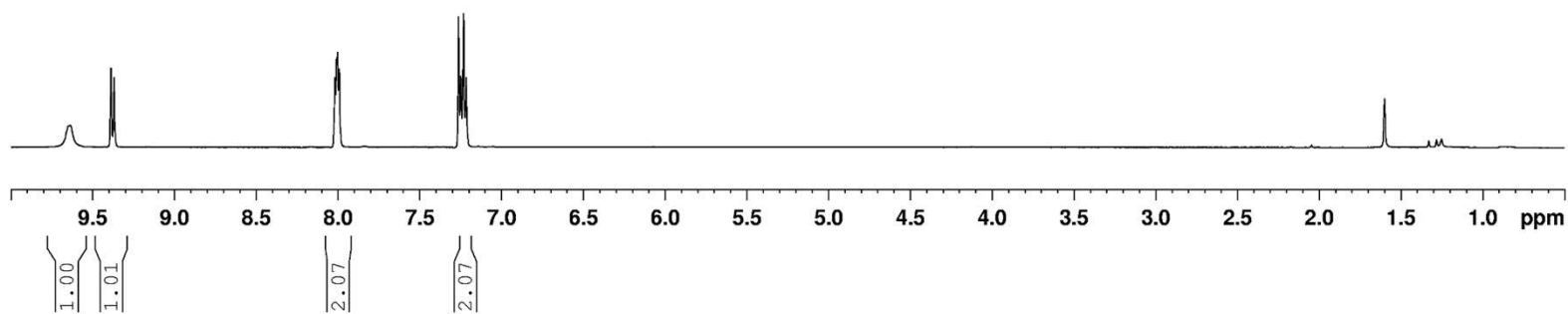
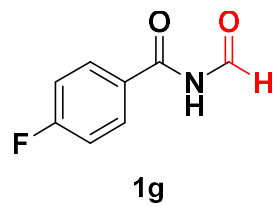


^1H NMR CDCl_3 / 500 MHz

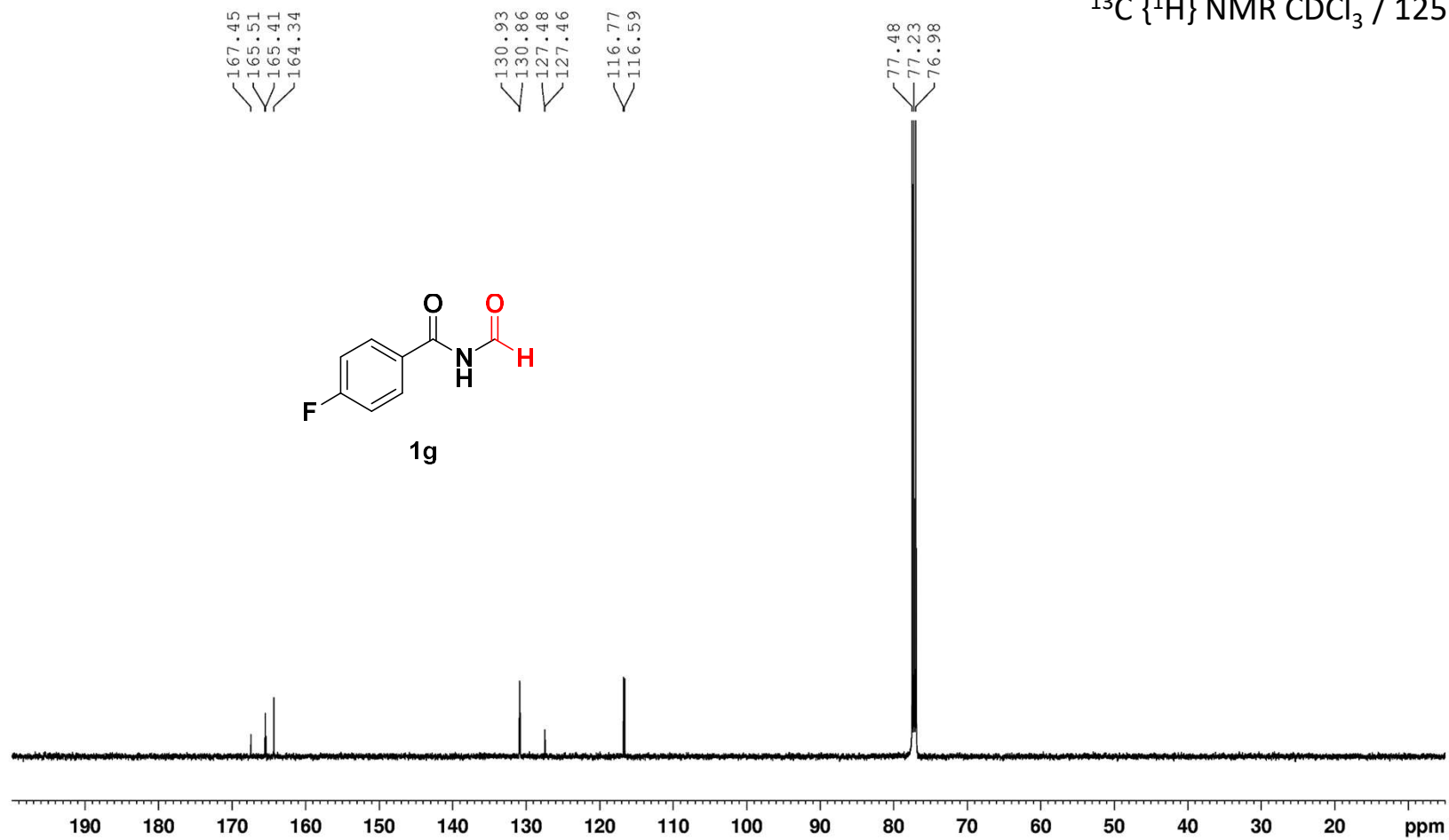
9.64
9.39
9.37

8.02
8.01
8.00
7.99

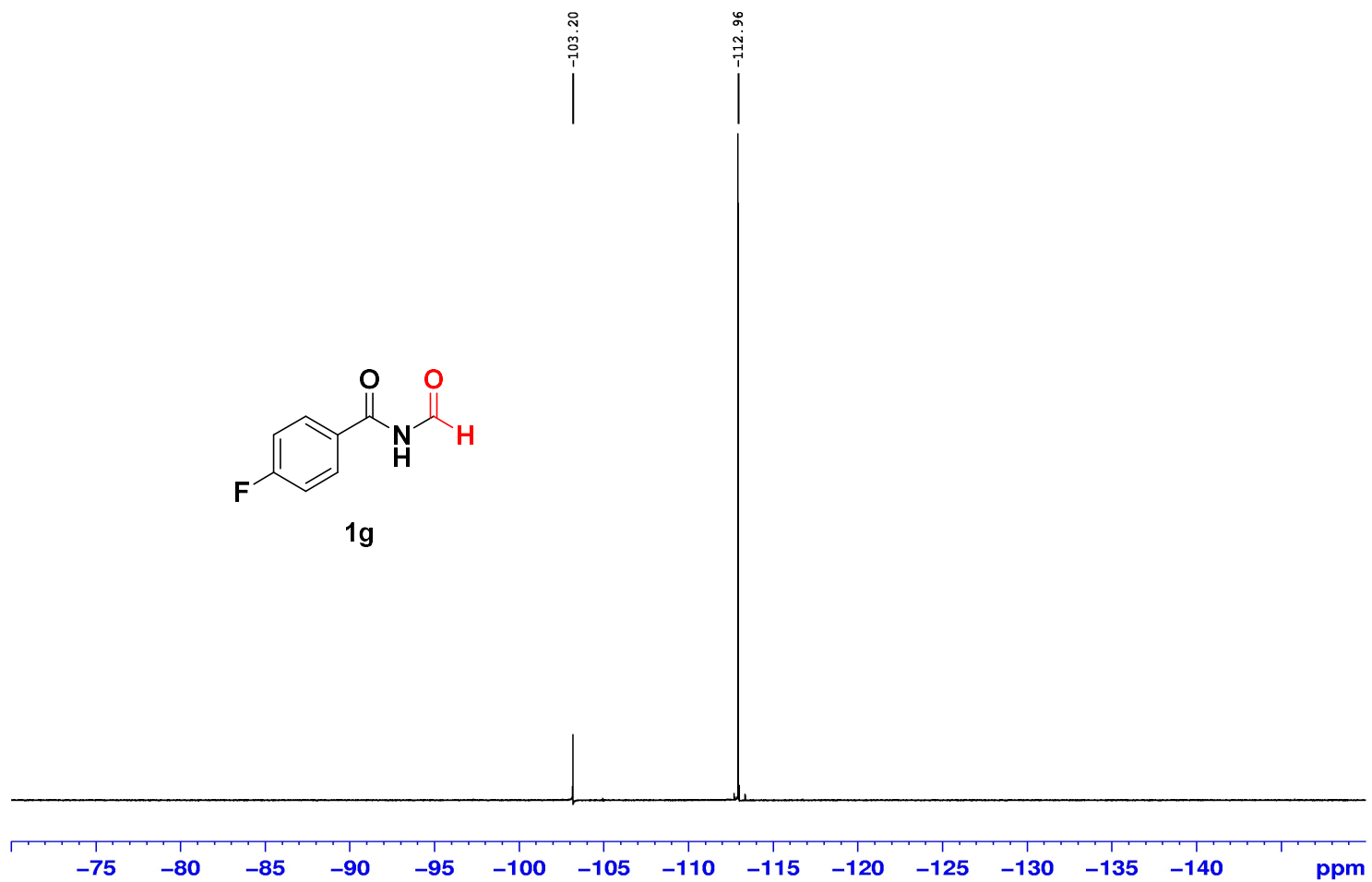
7.26
7.25
7.23
7.22



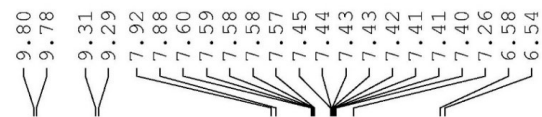
^{13}C $\{^1\text{H}\}$ NMR CDCl_3 / 125 MHz



^{19}F { ^1H } NMR CDCl_3 / 376 MHz

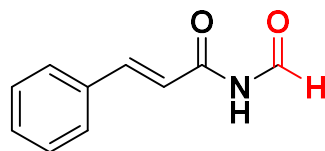


$^1\text{H NMR CDCl}_3 / 400 \text{ MHz}$

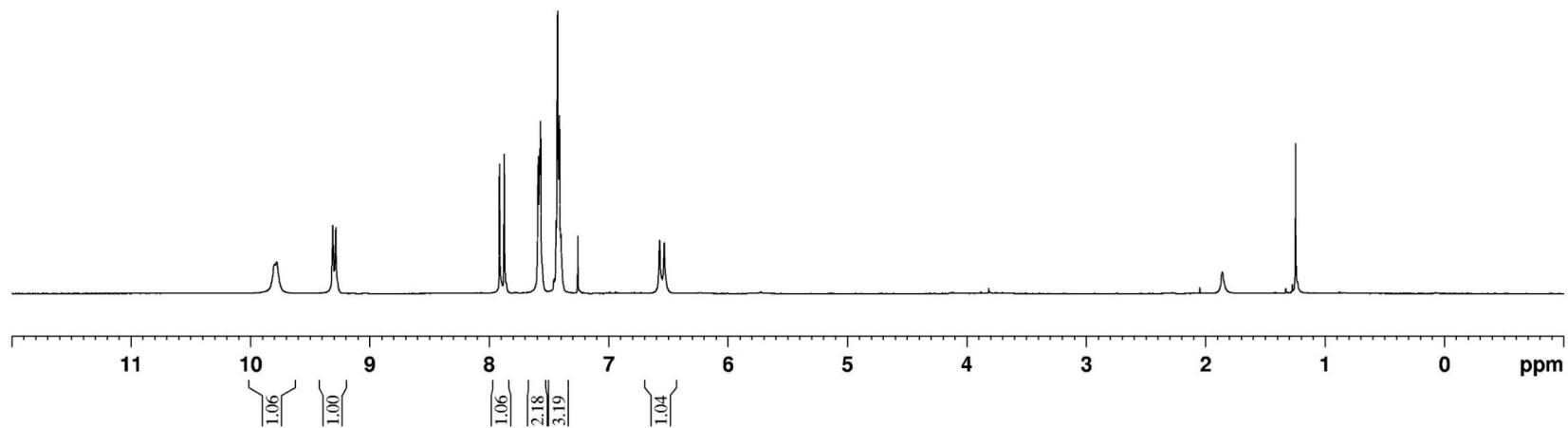


— 1.86

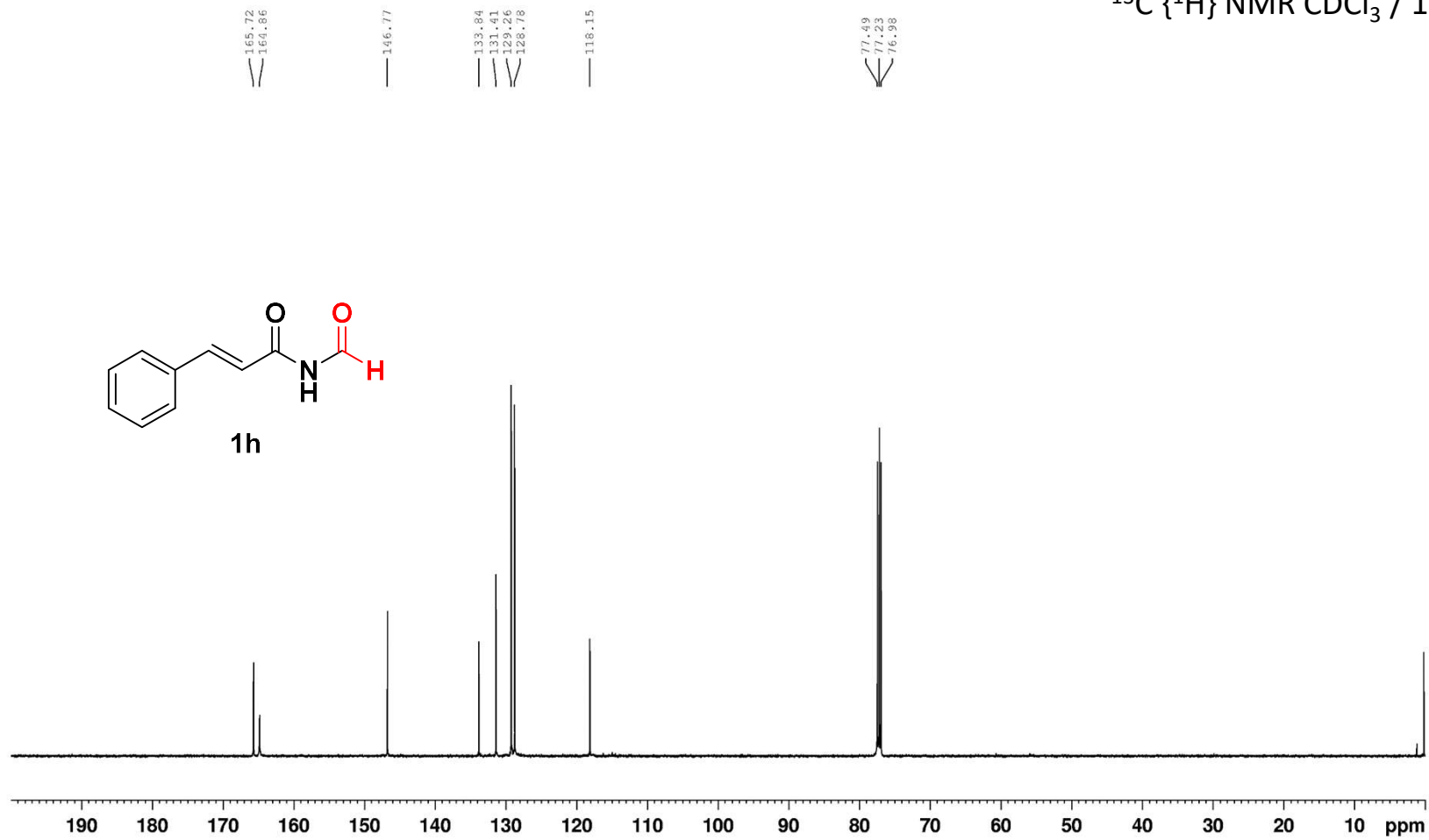
— 1.25



1h



$^{13}\text{C} \{^1\text{H}\}$ NMR CDCl_3 / 125 MHz



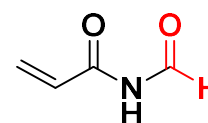
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9.74

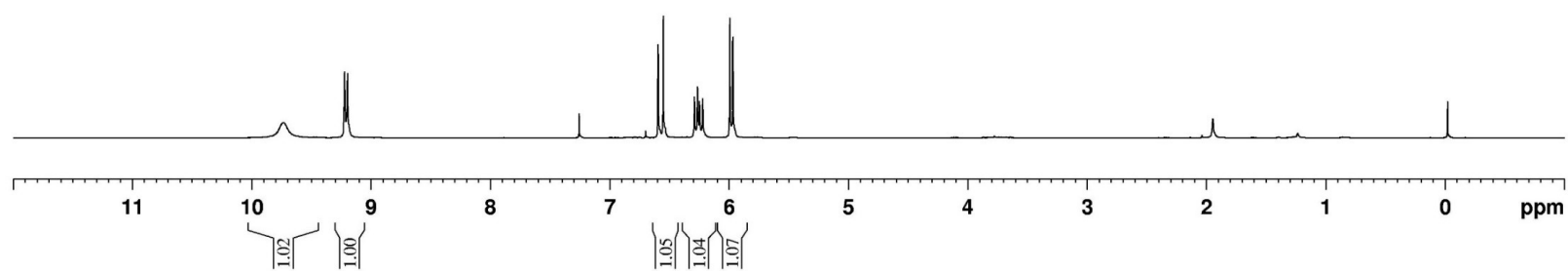
9.22
9.20

7.26
6.60
6.60
6.55
6.55
6.29
6.27
6.25
6.22
6.00
6.00
5.97

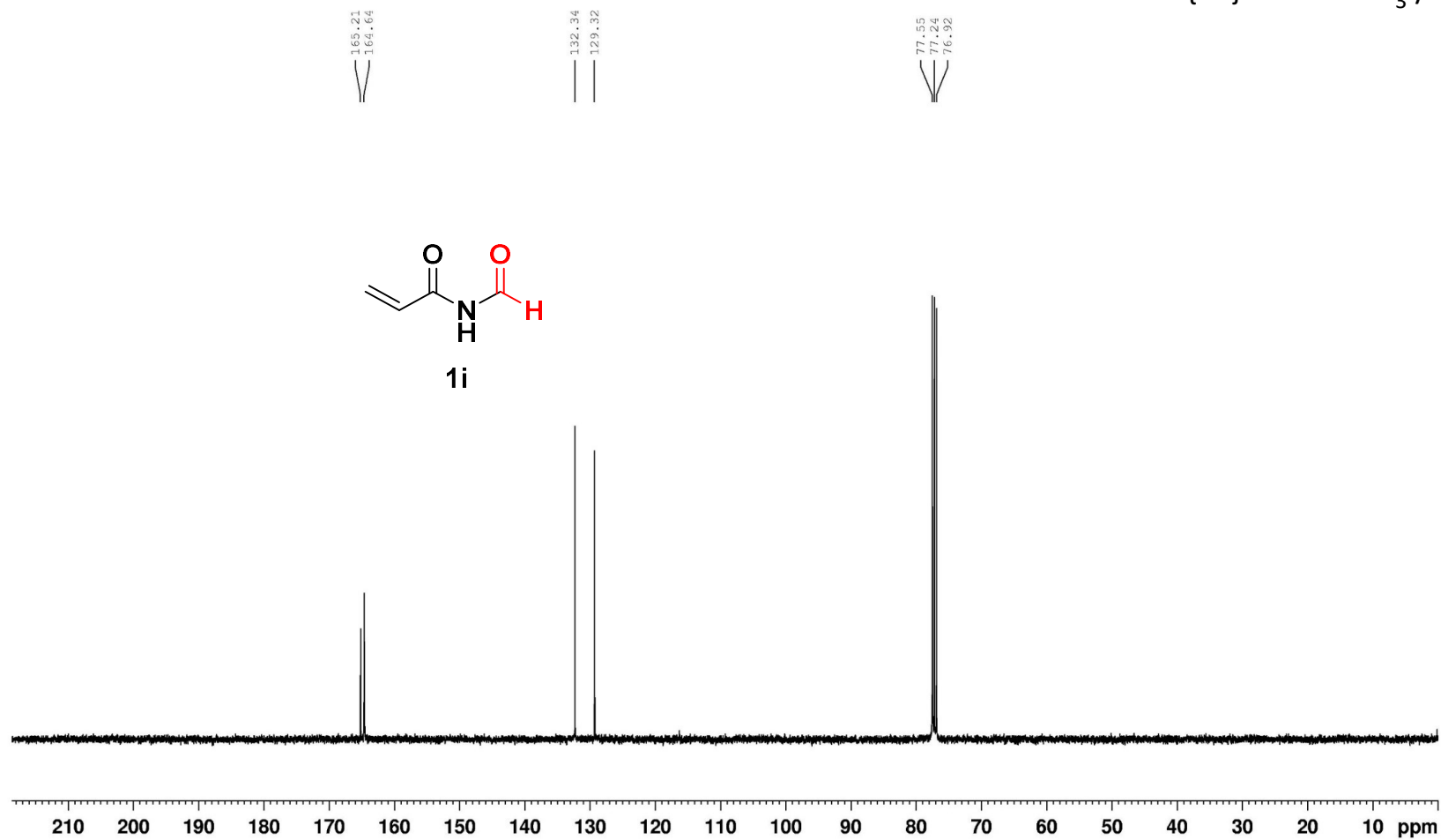
-0.02

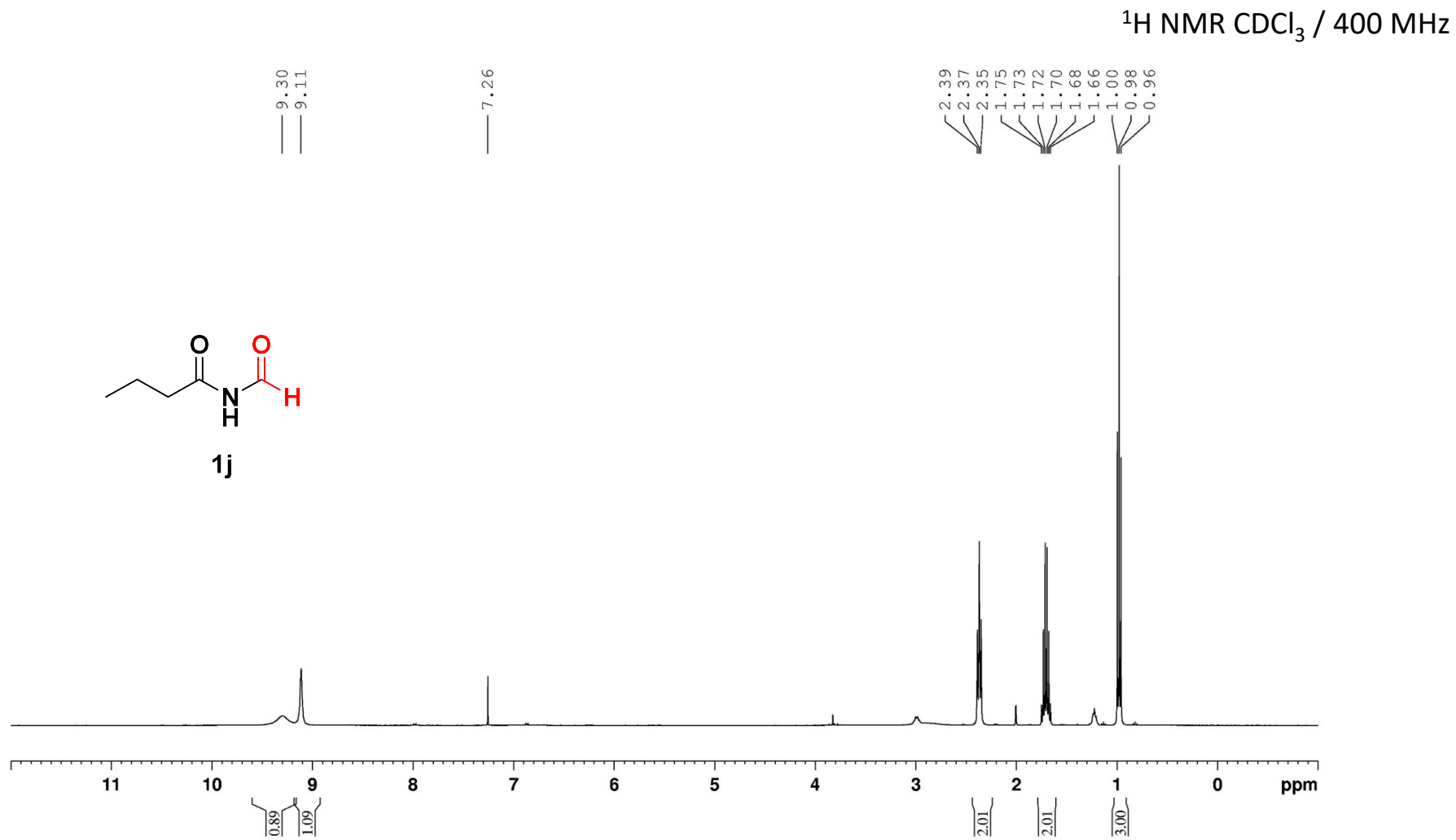
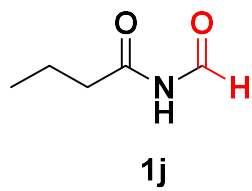


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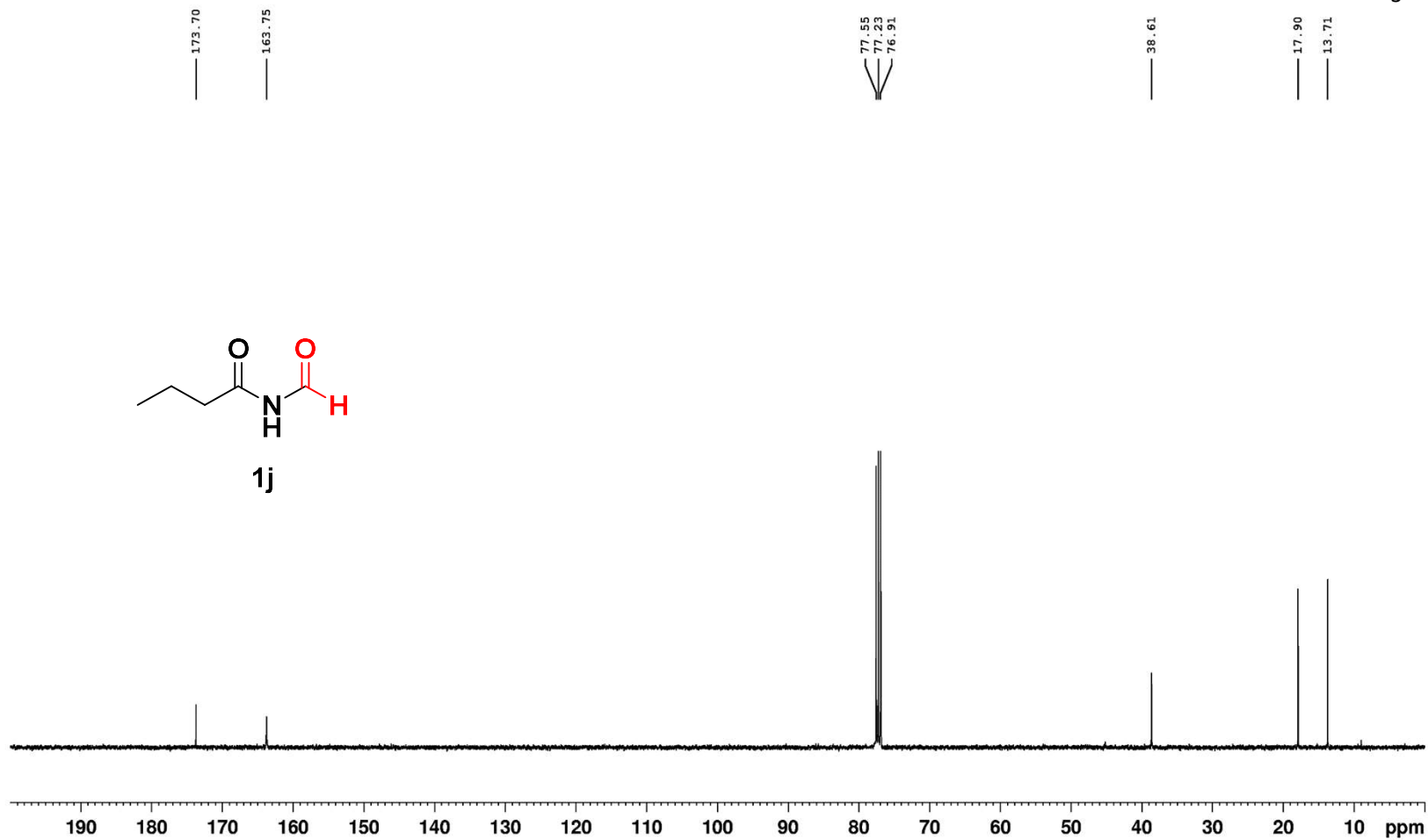
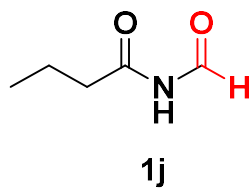


^{13}C $\{^1\text{H}\}$ NMR CDCl_3 / 100 MHz





$^{13}\text{C} \{^1\text{H}\}$ NMR CDCl_3 / 100 MHz

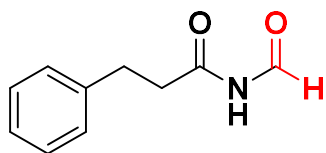


^1H NMR CDCl_3 / 400 MHz

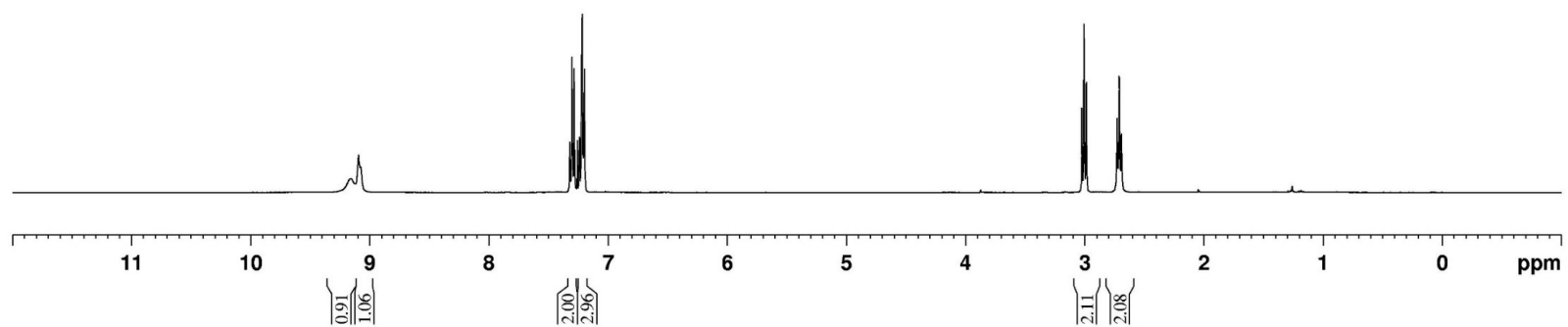
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9.10

7.32
7.31
7.31
7.29
7.26
7.24
7.24
7.22
7.20

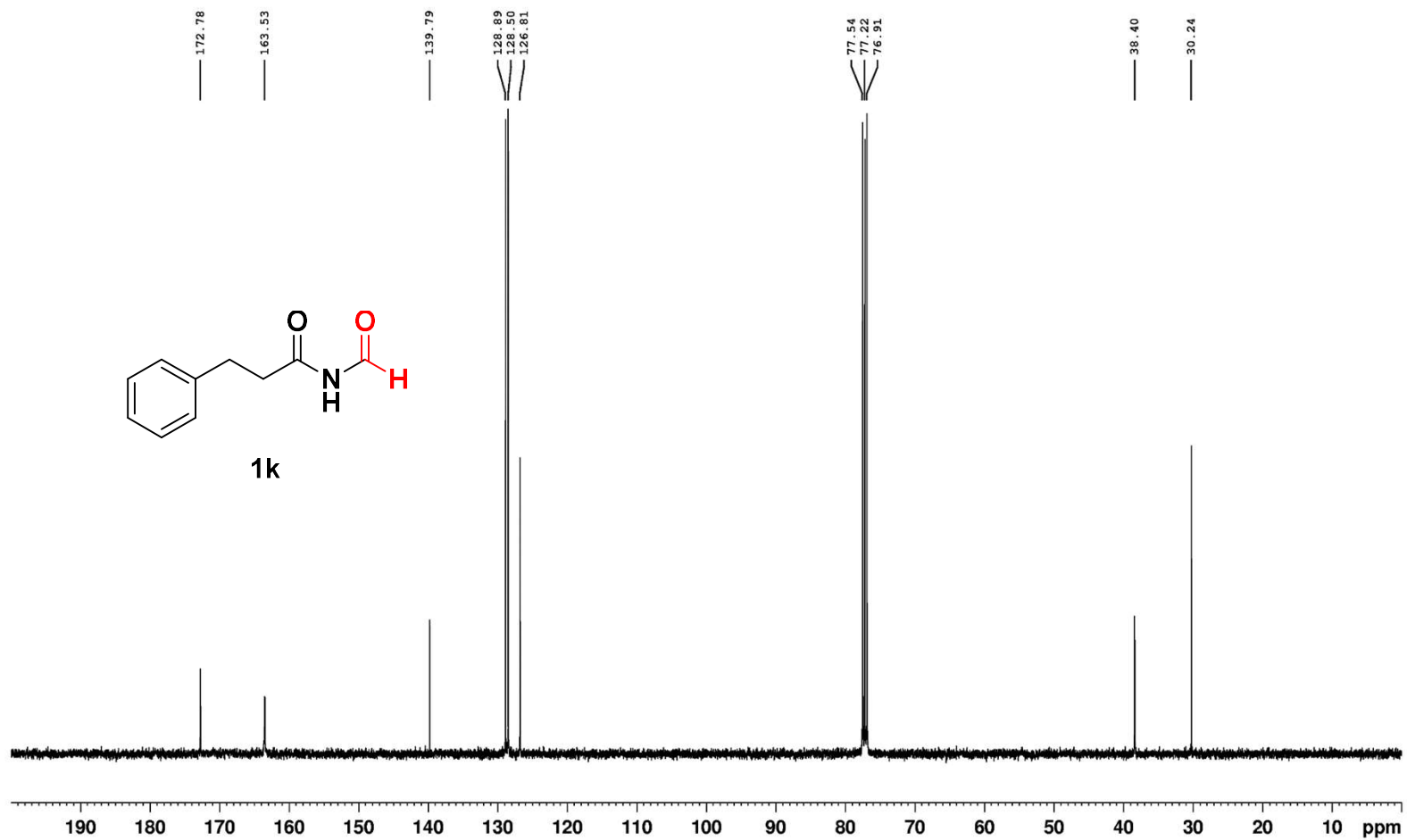
3.03
3.01
2.99
2.73
2.71
2.69



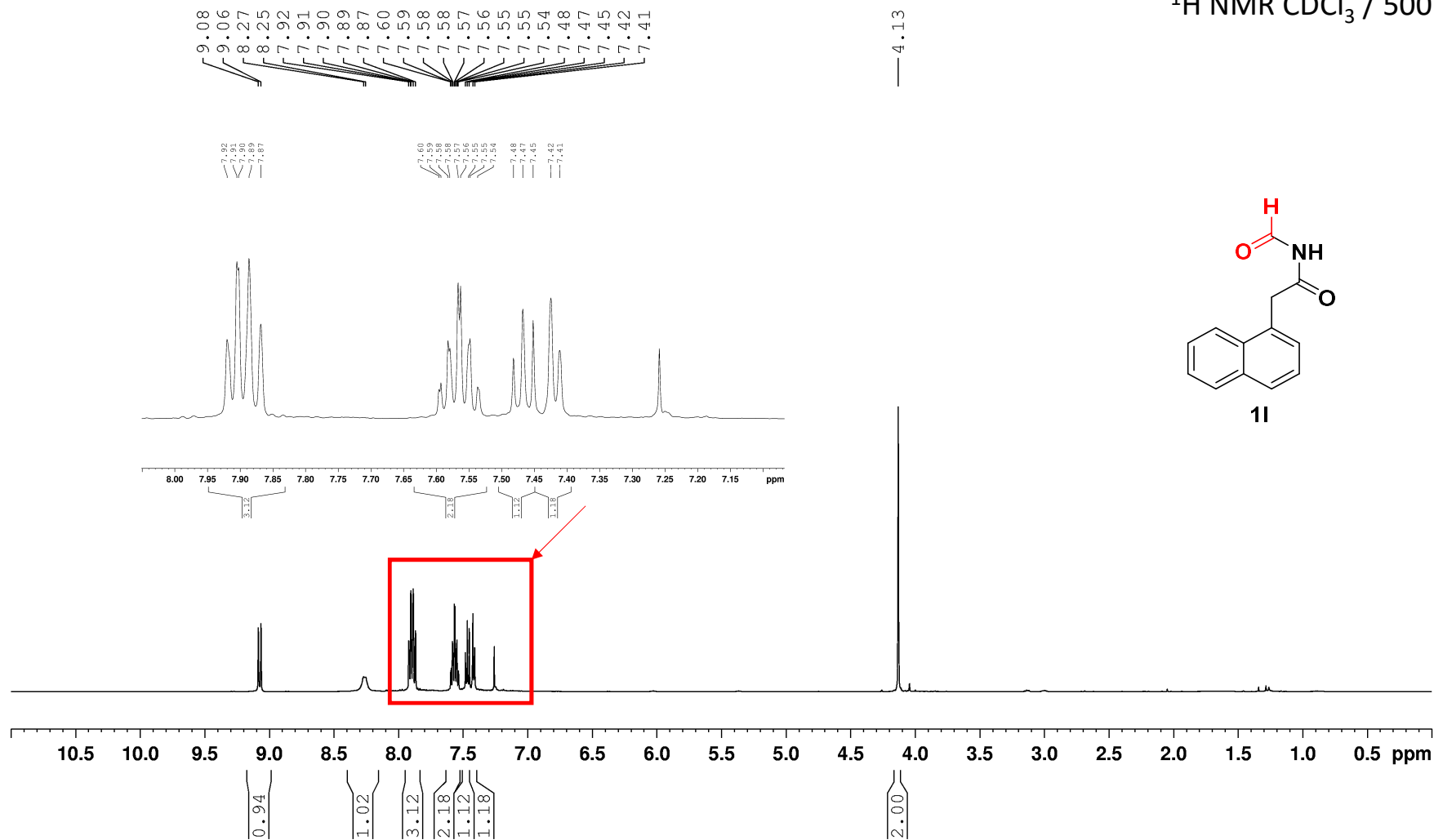
1k



^{13}C $\{^1\text{H}\}$ NMR CDCl_3 / 100 MHz



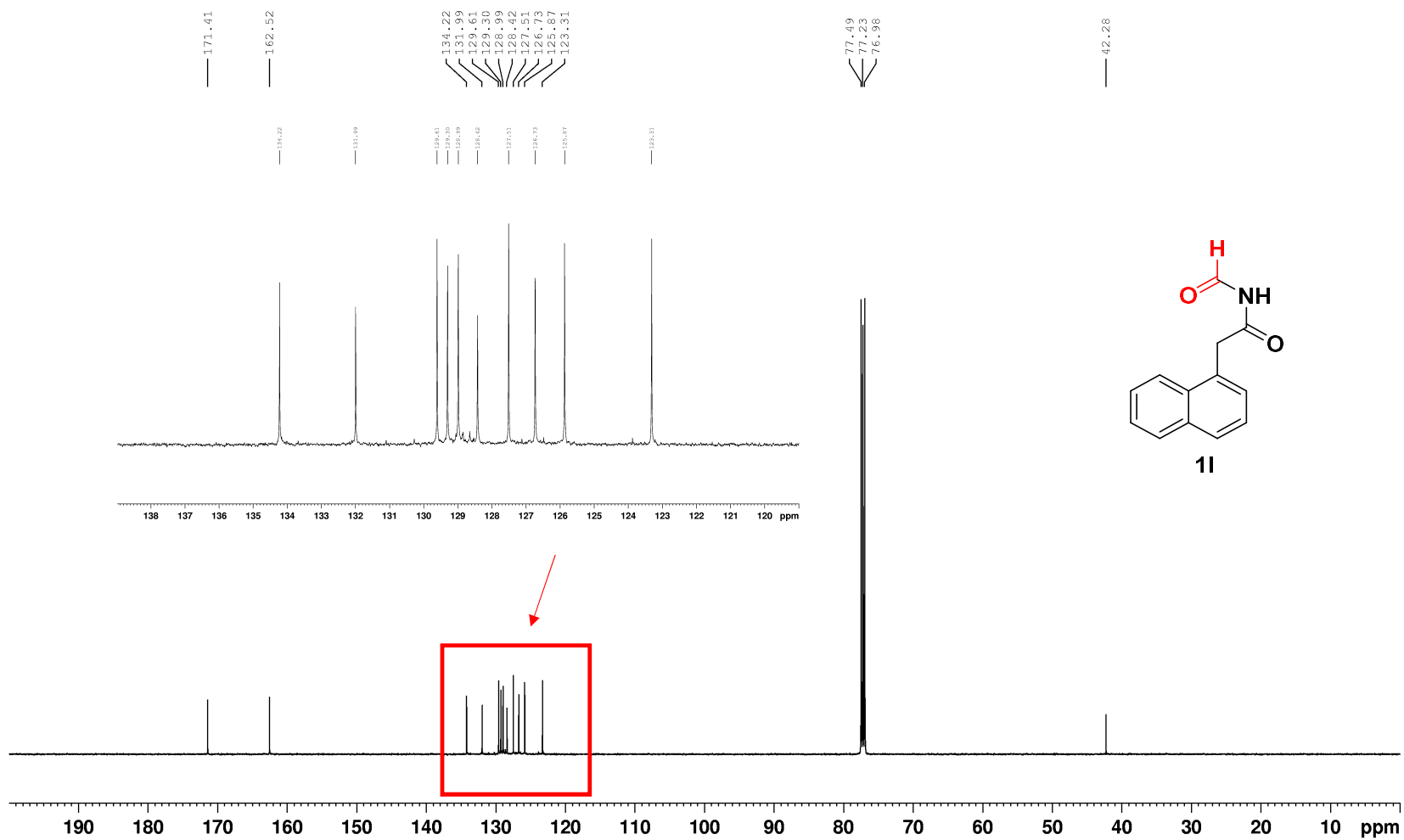
^1H NMR CDCl_3 / 500 MHz



S

39

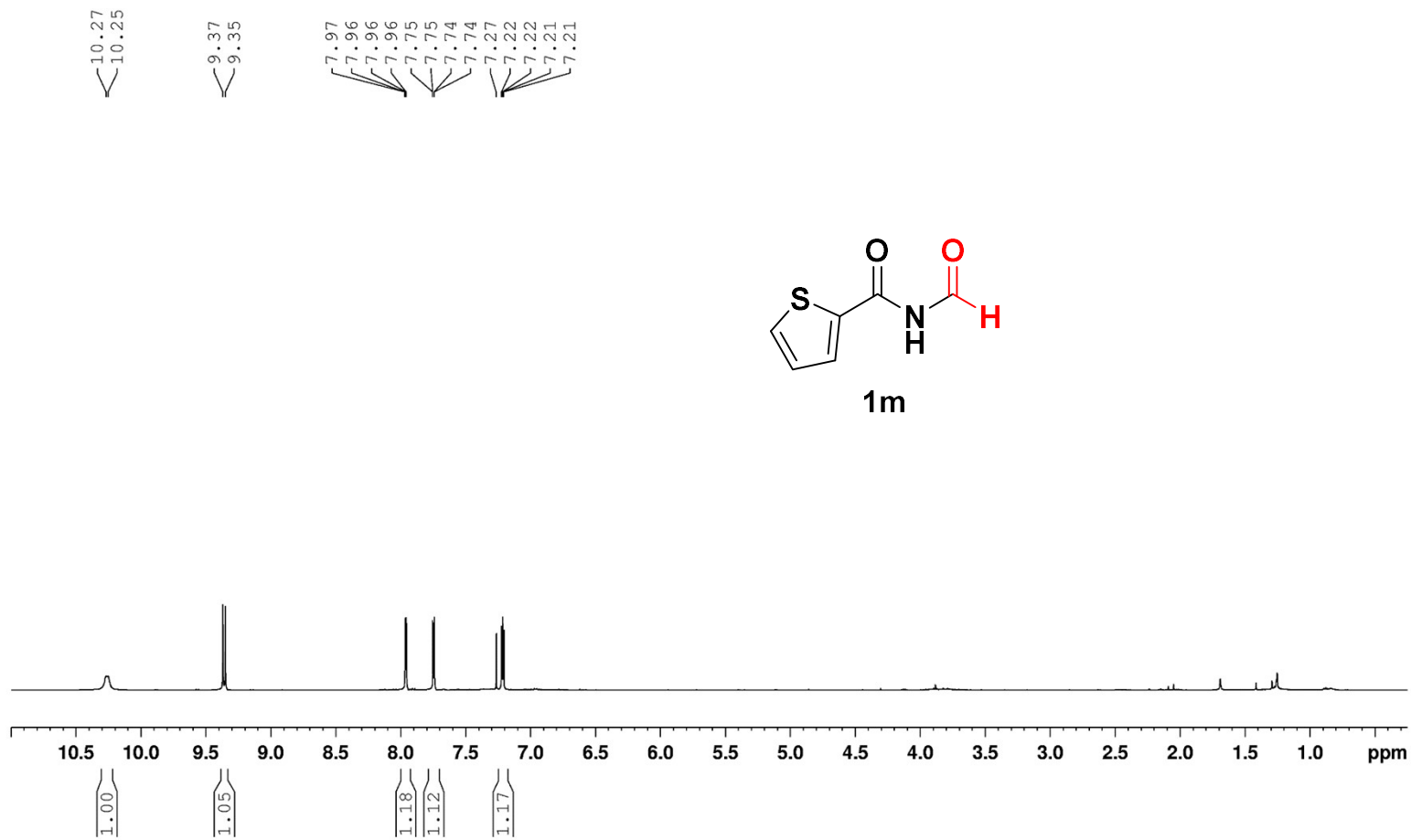
$^{13}\text{C} \{^1\text{H}\}$ NMR CDCl_3 / 125 MHz



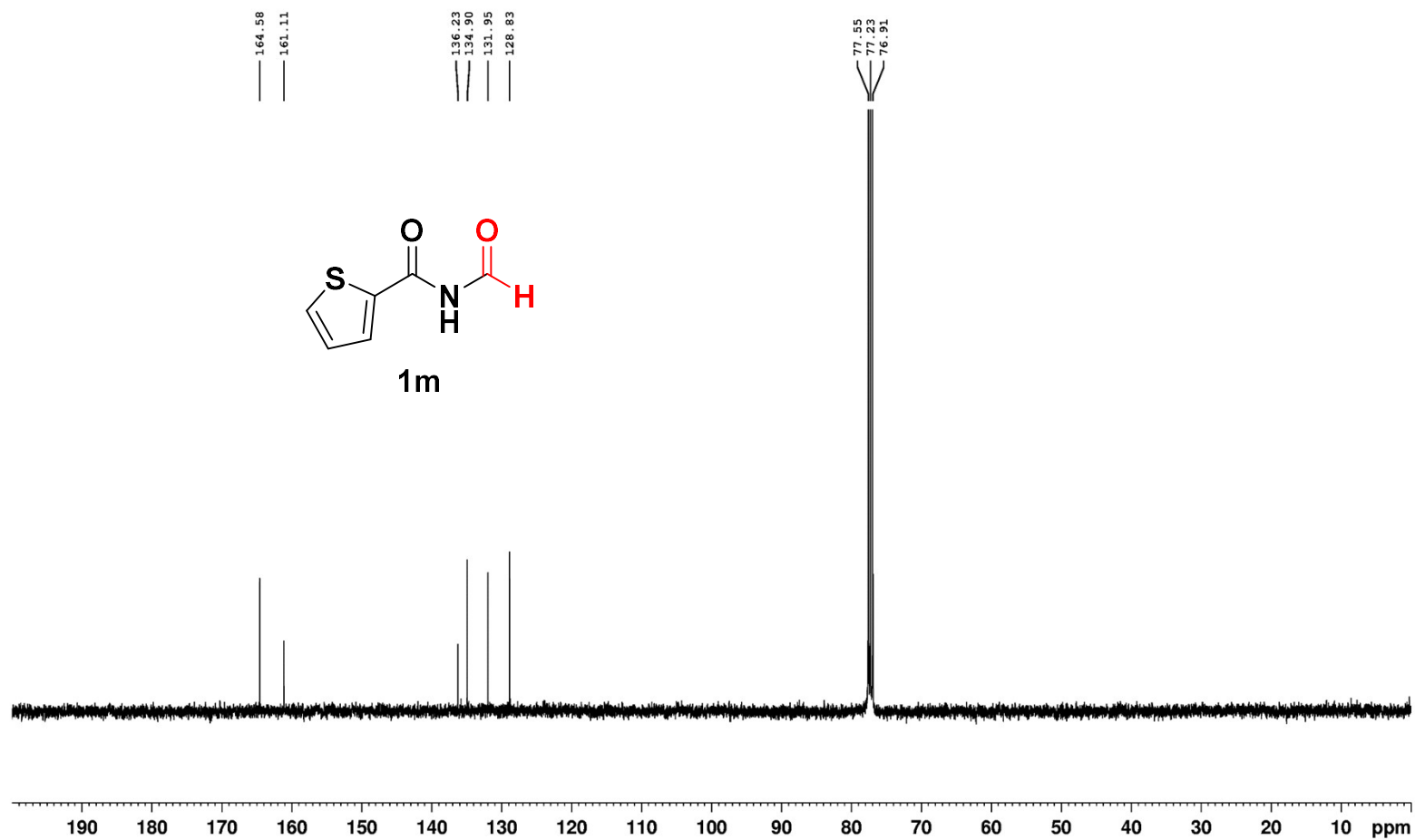
S

40

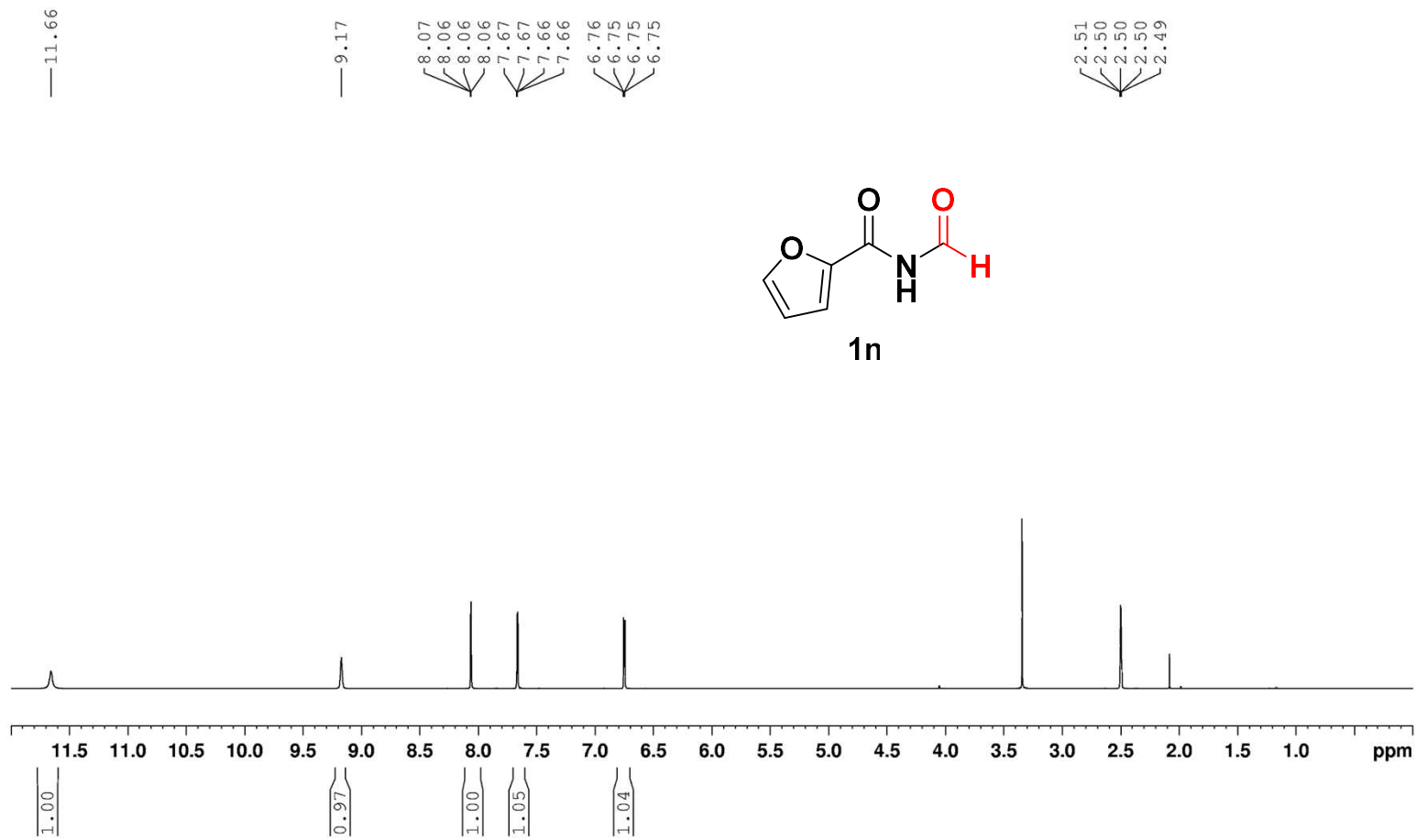
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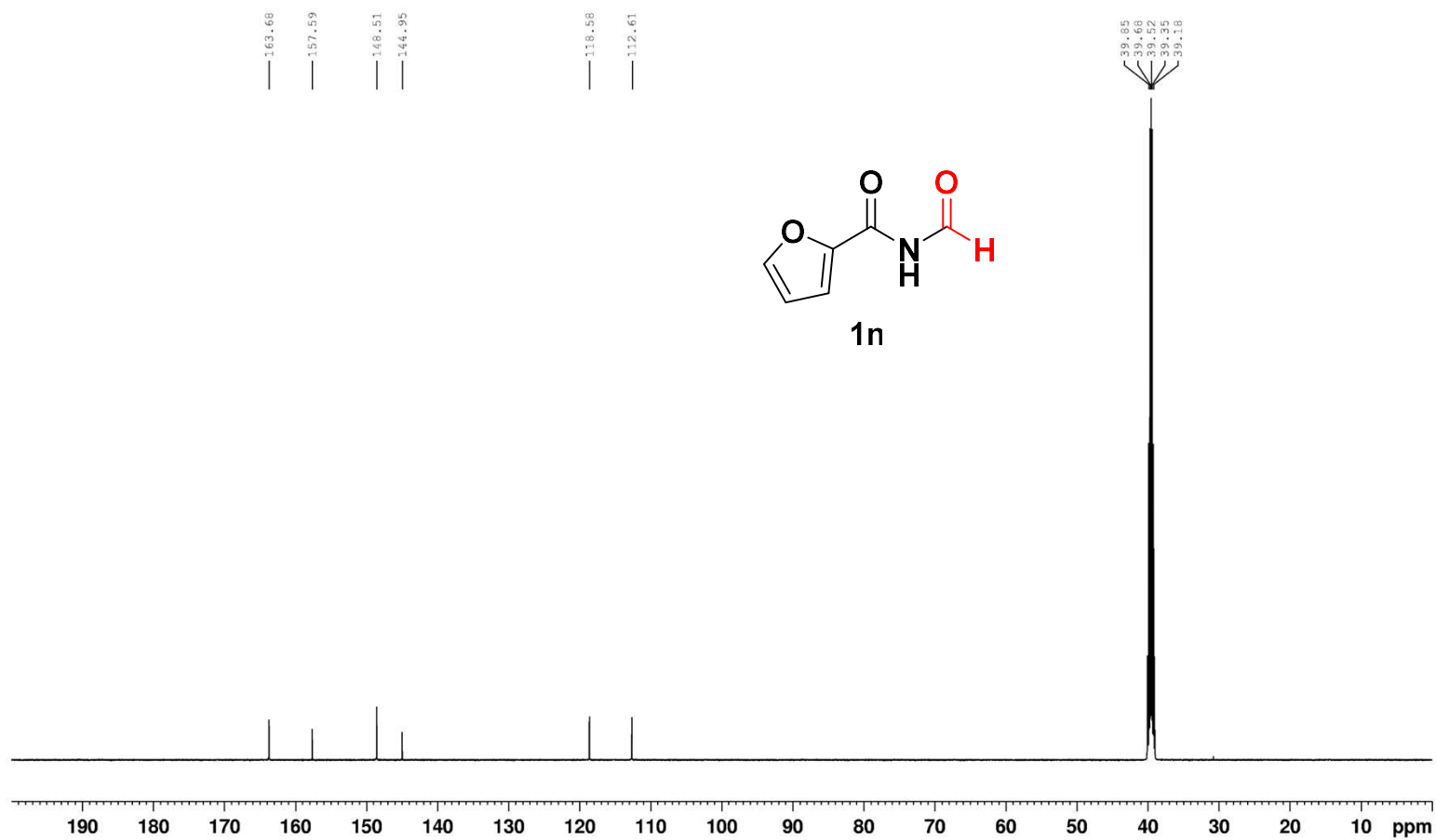
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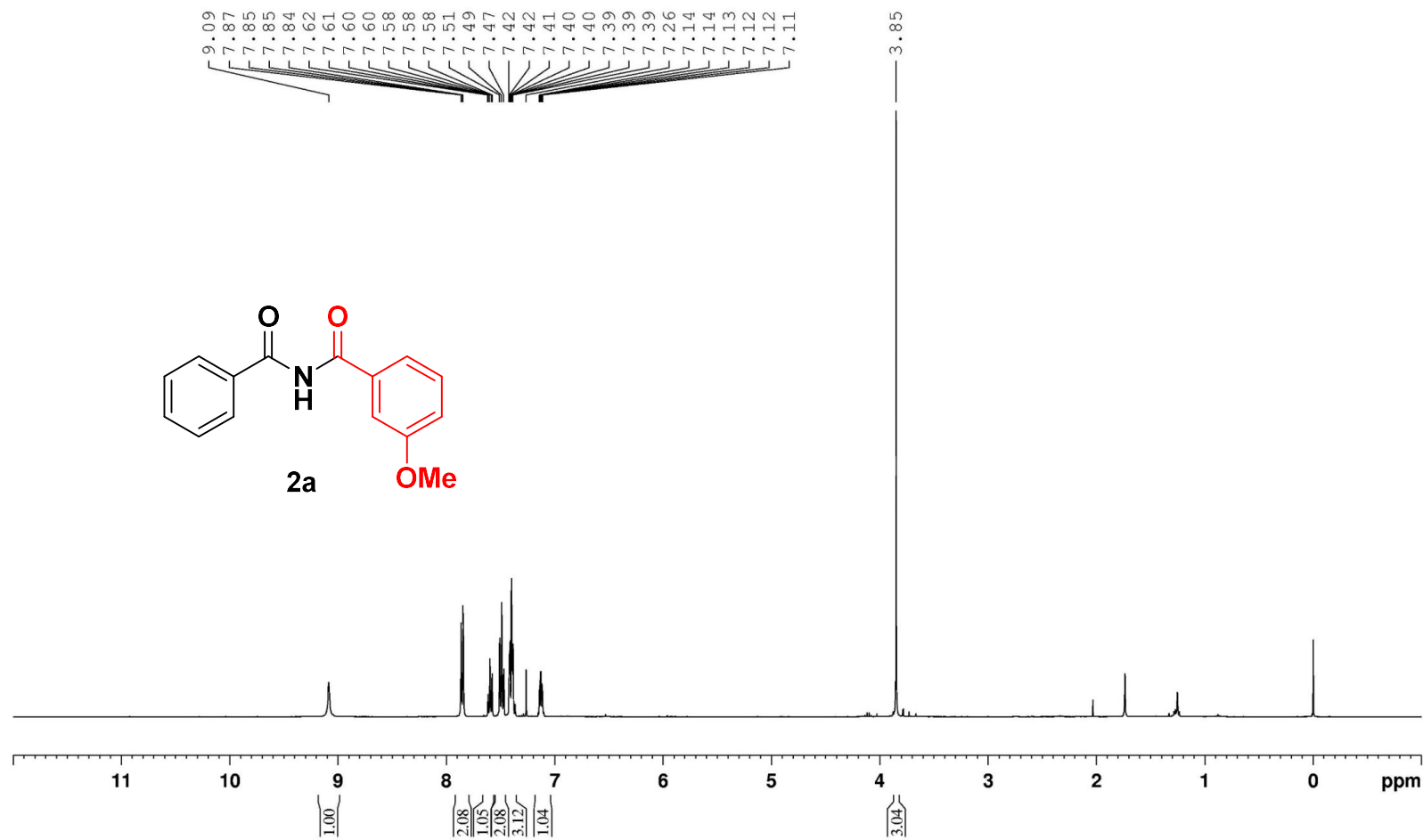
^1H NMR DMSO- d_6 / 500 MHz



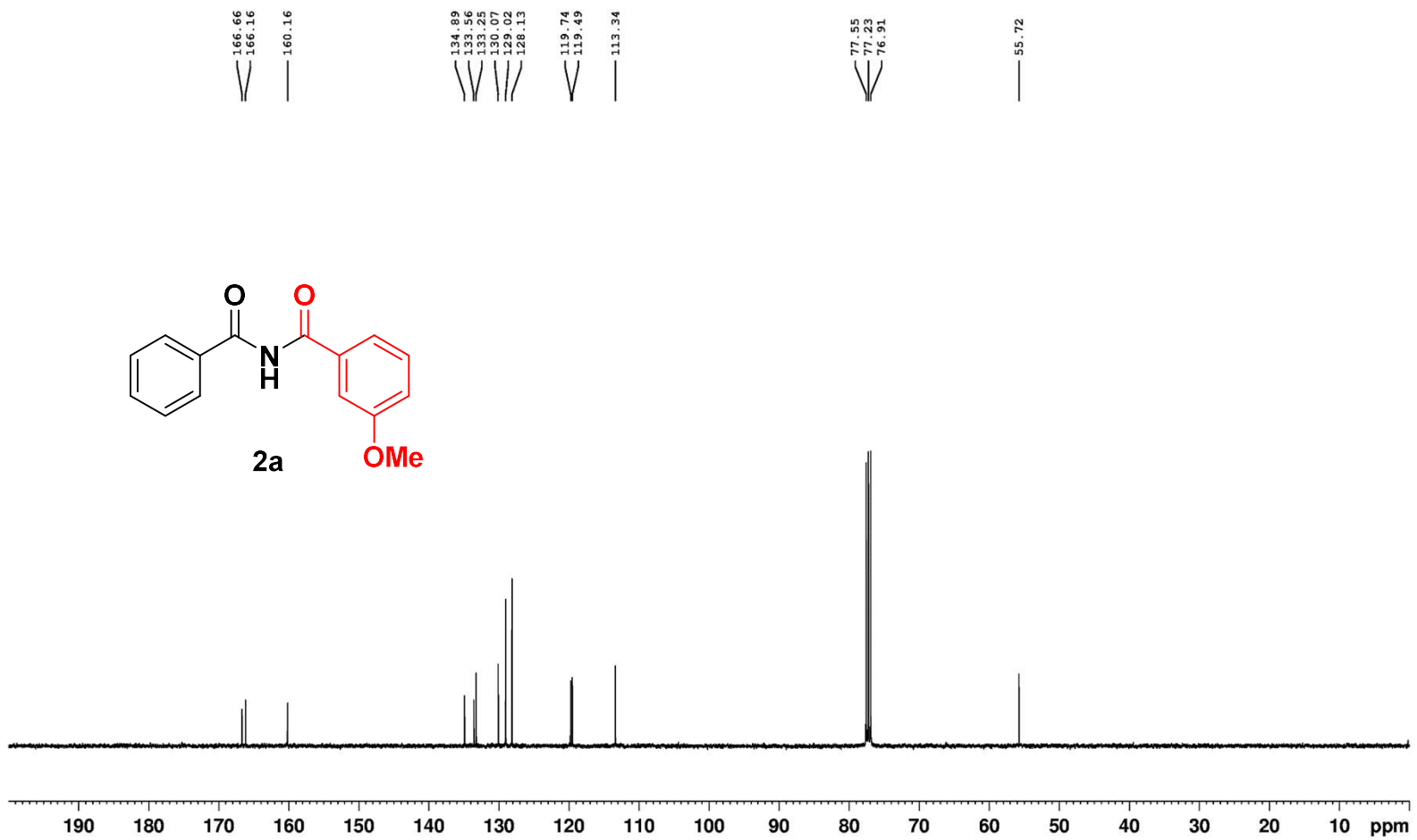
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^1H NMR CDCl_3 / 400 MHz

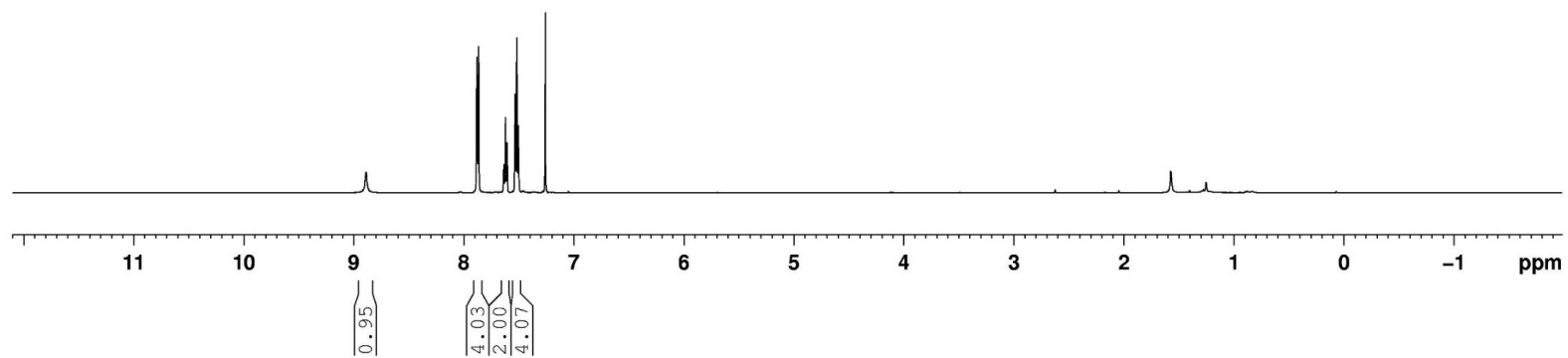
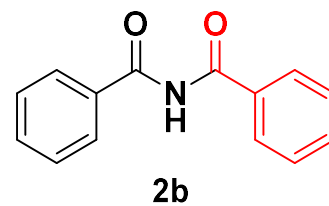


$^{13}\text{C} \{^1\text{H}\}$ NMR CDCl_3 / 100 MHz



^1H NMR CDCl_3 / 500 MHz

8.89
7.88
7.87
7.64
7.62
7.61
7.53
7.52
7.50
7.26



$^{13}\text{C} \{^1\text{H}\}$ NMR CDCl_3 / 125 MHz

