

## Supporting Information

### **Microwave assisted C-S cross-coupling reaction from thiols and 2-(4-bromo phenyl)-benzothiazole employed by CuI in acetonitrile**

Ramesh Katla,<sup>\*a</sup> and Rakhi Katla<sup>b</sup>

<sup>a</sup>Foreign Visiting Professor, **Organic Chemistry Laboratory-IV**, School of Chemistry and Food, Federal University of Rio Grande-FURG, Rio Grande, RS-Brazil. Tel.: +55(53) 3233-6959 and (53) 3233-6960. E-mail: [rameshkchem@gmail.com](mailto:rameshkchem@gmail.com)

<sup>b</sup>Organic Catalysis and Biocatalysis Laboratory - LACOB, Federal University of Grande Dourados-UFGD, Dourados/MS, Brazil. Tel.: +55(67) 3410 2081. E-mail: [rakhichowrasia147@gmail.com](mailto:rakhichowrasia147@gmail.com)

## **Supporting Information**

### **Contents**

<b>General Information.....</b>	<b>2</b>
<b>General Procedure.....</b>	<b>2</b>
<b>Spectral data of compounds.....</b>	<b>3-8</b>
<b>Copies of <sup>1</sup>HNMR and <sup>13</sup>CNMR of Compounds.....</b>	<b>9-25</b>

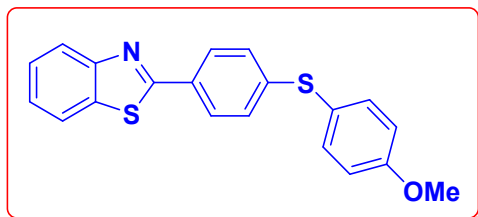
**General Information:**

All the chemicals were purchased from Sigma Aldrich with purity not less than 99.9%. Analytical Thin Layer Chromatography (TLC) was carried out by using silica gel 60 F254 pre-coated plates. Visualization was accomplished with UV lamp of I<sub>2</sub> stain. All the products were characterized by their NMR and Mass spectra. <sup>1</sup>H NMR and <sup>13</sup>C NMR were recorded on 400 MHz, in DMSO and CDCl<sub>3</sub>, and the chemical shifts were reported in parts per million (ppm, δ) downfield from the tetramethylsilane. FT-IR spectra were recorded on a Jasco FT/IR 4100 type A spectrophotometer of samples prepared as KBr pellets and are reported in wavenumbers (cm<sup>-1</sup>). All reactions were carried out in sealed glass tubes with a volume of 10 mL in a commercially available monomode microwave reactor (CEM, Matthews, NC, USA) equipped with infrared monitoring and a non-invasive pressure transducer

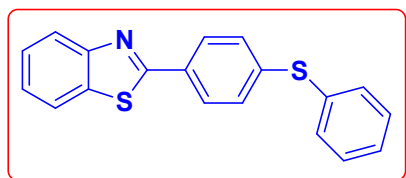
**General procedure for the synthesis of 5-phenylthio-2,1,3-benzothiadiazoles:**

Benzene thiols (0.45 mmol), 2-(4-bromo phenyl) benzothiazole (0.3 mmol), a catalytic amount of CuI (15 mol%), K<sub>2</sub>CO<sub>3</sub> (0.6 mmol) and CH<sub>3</sub>CN (2 mL) were added to a microwave reaction vessel armed with a magnetic stirrer bar. The reaction mixture was subjected to microwave irradiation (a CEM Discover MW reactor) (200W, 80 °C) for 25-35 min. The progress of the reaction was observed by TLC (eluent: EtOAc/hexane, 10:90). The reaction mixture was cooled to room temperature and the crude residue was extracted with ethyl acetate (3 x 10 mL) and water. Then, combined all the organic layers and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. The remaining solvent was evaporated under reduced pressure. Further, the crude product was purified by column chromatography over silica gel to afford the corresponding product, and yields were obtained in 64-84% as shown in **Table 3**.

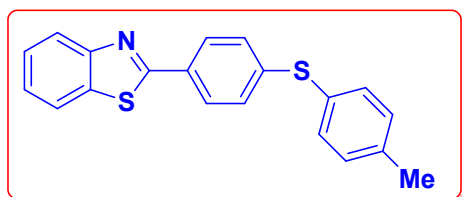
## SPECTRAL DATA OF COMPOUNDS:



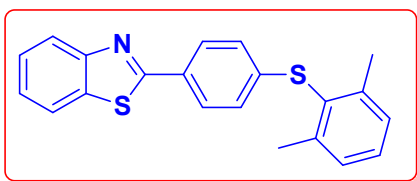
**2-(4-((4-methoxyphenyl)thio)phenyl)benzo[d]thiazole (3a):** Yield: 87.94 mg (84%); brown solid; mp 103-105°C. FT-IR (KBr): 3059, 2039, 1490, 1247, 1026  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 – 7.86 (m, 4H), 7.60 (d,  $J = 8.2$  Hz, 6H), 6.82 (d,  $J = 7.9$  Hz, 2H), 3.77 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.61, 159.85, 154.01, 132.58, 132.16, 128.83, 126.44, 125.39, 123.26, 121.61, 114.56, 55.29. MS (ESI):  $m/z = 350$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{20}\text{H}_{15}\text{NOS}_2$ ) C: 68.74, H: 4.33, N: 4.01, O: 4.58; S: 18.35; found C: 68.71, H: 4.27, N: 4.00, O: 4.51, S: 18.29.



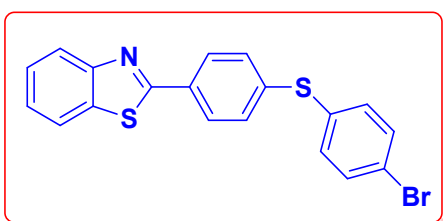
**2-(4-(phenylthio)phenyl)benzo[d]thiazole (3b):** Yield: 77.15 mg (81%); pale yellow solid; mp 93-95°C. FT-IR (KBr): 3057, 3030, 1475, 1068, 1012  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 8.1$  Hz, 1H), 7.99 – 7.94 (m, 2H), 7.91 (d,  $J = 8.0$  Hz, 1H), 7.67 – 7.59 (m, 2H), 7.51 (ddd,  $J_1 = 8.0$  Hz,  $J_2 = 6.1$  Hz,  $J_3 = 1.6$  Hz, 3H), 7.44 – 7.37 (m, 1H), 7.33 – 7.27 (m, 2H), 7.25 – 7.20 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.69, 154.08, 135.04, 132.56, 132.23, 128.98, 127.52, 127.14, 126.50, 125.45, 123.32, 121.66. MS (ESI):  $m/z = 320$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{19}\text{H}_{13}\text{NS}_2$ ) C: 71.44, H: 4.10, N: 4.38, S: 20.07; found C: 71.33, H: 4.04, N: 4.31, S: 20.01.



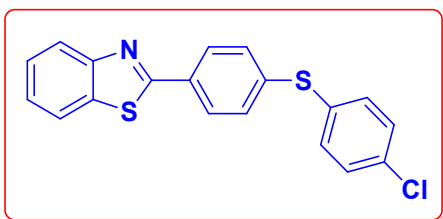
**2-(4-(p-tolylthio)phenyl)benzo[d]thiazole (3c):** Yield: 81.91 mg (82%); pale yellow solid; mp 174-176 °C. FT-IR (KBr): 3045, 1467, 1184, 1018, 900  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.08 (d,  $J = 8.1$  Hz, 1H), 7.93 (dd,  $J_1 = 24.2$  Hz,  $J_2 = 8.3$  Hz, 2H), 7.64 (s, 1H), 7.51 (dd,  $J_1 = 11.3$  Hz,  $J_2 = 4.1$  Hz, 1H), 7.41 (t,  $J = 7.0$  Hz, 4H), 7.11 (d,  $J = 8.0$  Hz, 3H), 2.33 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.62, 154.03, 137.38, 135.00, 133.86, 132.50, 132.17, 129.74, 128.85, 128.49, 126.45, 125.40, 123.28, 121.61, 21.01. MS (ESI):  $m/z = 334$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{20}\text{H}_{15}\text{NS}_2$ ) C: 72.04, H: 4.53, N: 4.20, S: 19.23; found C: 72.01, H: 4.47, N: 4.09, S: 19.18.



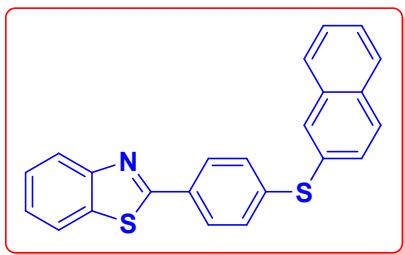
**2-(4-((2,6-dimethylphenyl)thio)phenyl)benzo[d]thiazole (3d):** Yield: 82.23 mg (79%); pale yellow solid; mp 98-100°C. FT-IR (KBr): 3057, 2922, 2731, 1165  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 8.1$  Hz, 1H), 7.93 (dd,  $J_1 = 22.3$  Hz,  $J_2 = 8.2$  Hz, 3H), 7.62 (d,  $J = 8.4$  Hz, 2H), 7.50 (t,  $J = 7.6$  Hz, 1H), 7.40 (t,  $J = 7.5$  Hz, 1H), 7.13 – 7.08 (m, 1H), 7.01 (d,  $J = 7.4$  Hz, 2H), 2.24 (s, 6H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.65, 154.06, 143.39, 135.02, 134.72, 132.53, 132.19, 129.23, 128.87, 128.02, 126.47, 125.40, 123.30, 121.63, 21.40. MS (ESI):  $m/z = 348$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{21}\text{H}_{17}\text{NS}_2$ ) C: 72.59, H: 4.93, N: 4.03, S: 18.45; found C: 72.51, H: 4.84, N: 3.90, S: 18.34.



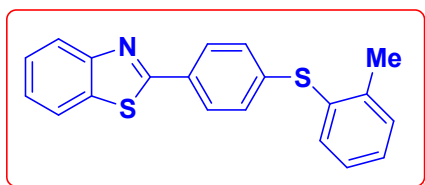
**2-(4-((4-bromophenyl)thio)phenyl)benzo[d]thiazole (3e):** Yield: 87.91 mg (74%); pale yellow solid; mp 126-128 °C. FT-IR (KBr): 3057, 3030, 2400, 1473, 1068, 1006  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 8.1$  Hz, 1H), 7.99 – 7.94 (m, 2H), 7.91 (d,  $J = 8.0$  Hz, 1H), 7.66 – 7.61 (m, 2H), 7.55 – 7.47 (m, 1H), 7.44 – 7.38 (m, 3H), 7.35 – 7.32 (m, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.70, 154.07, 135.73, 135.04, 132.56, 132.23, 129.41, 128.91, 126.50, 125.45, 123.32, 121.66. MS (ESI):  $m/z = 397$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{19}\text{H}_{12}\text{BrNS}_2$ ) C: 57.29, H: 3.04, Br: 20.06, N: 3.52, S: 16.10; found C: 57.21, H: 3.00, Br: 20.01, N: 3.43, S: 16.01.



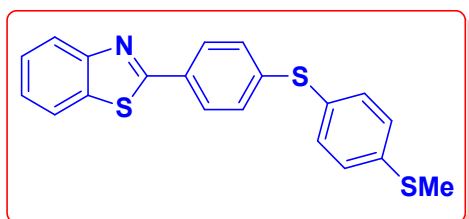
**2-(4-((4-chlorophenyl)thio)phenyl)benzo[d]thiazole (3f):** Yield: 75.18 mg (71%); pale yellow solid; mp 213-215°C. FT-IR (KBr): 3076, 3057, 2400, 1473, 1010  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.2$  Hz, 1H), 7.92 (t,  $J = 11.3$  Hz, 2H), 7.62 (s, 1H), 7.49 (t,  $J = 7.6$  Hz, 1H), 7.43 – 7.34 (m, 4H), 7.26 (d,  $J = 8.5$  Hz, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.64, 154.05, 135.07, 133.63, 132.52, 132.19, 129.29, 128.87, 126.46, 125.41, 123.30, 121.62. MS (ESI):  $m/z = 354$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{19}\text{H}_{12}\text{ClNS}_2$ ) C: 64.49, H: 3.42, Cl: 10.02, N: 3.96, S: 18.12; found C: 64.41, H: 3.38, Cl: 9.02, N: 3.90, S: 18.02.



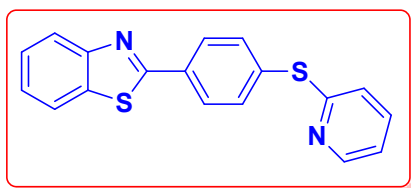
**2-(4-(naphthalen-2-ylthio)phenyl)benzo[d]thiazole (3g):** Yield: 88.56 mg (80%); pale yellow solid; mp 100-102°C. FT-IR (KBr): 3049, 2410, 1500, 1195, 1018  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.08 (d,  $J = 8.0$  Hz, 1H), 8.02 – 7.85 (m, 4H), 7.76 (dd,  $J_1 = 21.3$  Hz,  $J_2 = 7.5$  Hz, 3H), 7.62 (d,  $J = 7.8$  Hz, 3H), 7.55 – 7.35 (m, 4H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.61, 154.04, 135.01, 134.25, 133.44, 132.49, 132.16, 128.89, 127.72, 127.42, 126.87, 126.19, 125.63, 125.39, 123.29, 121.61. MS (ESI):  $m/z = 370$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{23}\text{H}_{15}\text{NS}_2$ ) C: 74.76, H: 4.09, N: 3.79, S: 17.35; found C: 74.66, H: 4.00, N: 3.70, S: 17.24.



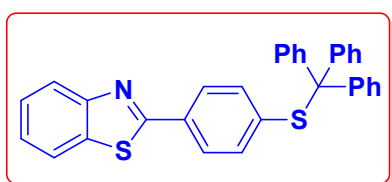
**2-(4-(o-tolylthio)phenyl)benzo[d]thiazole (3h):** Yield: 76.92 mg (77%); yellow solid; mp 135-137°C. FT-IR (KBr): 3045, 2900, 1467, 1184, 1018  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.08 (d,  $J = 8.1$  Hz, 1H), 7.93 (dd,  $J_1 = 23.0$  Hz,  $J_2 = 8.3$  Hz, 2H), 7.62 (d,  $J = 8.5$  Hz, 2H), 7.56 – 7.47 (m, 2H), 7.45 – 7.37 (m, 1H), 7.19 – 7.11 (m, 4H), 2.44 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.63, 154.04, 137.37, 135.39, 135.01, 132.51, 132.18, 130.27, 128.76, 127.29, 126.54, 125.39, 123.28, 121.61, 19.96. MS (ESI):  $m/z = 334$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{20}\text{H}_{15}\text{NS}_2$ ) C: 72.04, H: 4.53, N: 4.20, S: 19.23; found C: 72.01, H: 4.47, N: 4.09, S: 19.18.



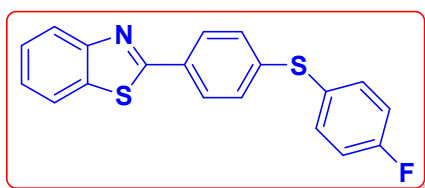
**2-(4-((4-methylthio)phenyl)thio)phenyl)benzo[d]thiazole (3i):** Yield: 85.64 mg (78%); yellow solid; mp 137-139°C. FT-IR (KBr): 3078, 3057, 3032, 2420, 1475, 1012  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 8.1$  Hz, 1H), 7.96 – 7.93 (m, 2H), 7.89 (d,  $J = 8.0$  Hz, 1H), 7.63 – 7.60 (m, 2H), 7.53 – 7.47 (m, 1H), 7.40 (ddd,  $J_1 = 8.4$  Hz,  $J_2 = 3.7$ ,  $J_3 = 1.5$  Hz, 3H), 7.21 – 7.12 (m, 2H), 2.45 (s, 3H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.63, 154.04, 138.55, 135.01, 133.42, 132.52, 132.18, 129.37, 128.86, 126.94, 126.45, 125.39, 123.29, 121.62, 15.69. MS (ESI):  $m/z = 366$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{20}\text{H}_{15}\text{NS}_3$ ) C: 65.72, H: 4.14, N: 3.83, S: 26.31; found C: 65.66, H: 4.08, N: 3.72, S: 26.22.



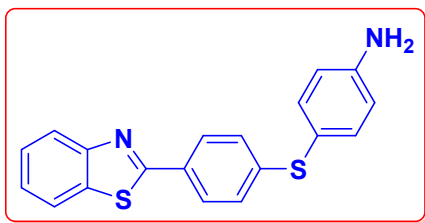
**2-(4-(pyridin-2-ylthio)phenyl)benzo[d]thiazole (3j):** Yield: 72 mg (75%); pale yellow solid; mp 109-111°C. FT-IR (KBr): 3047, 1595, 1415, 1112  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.46 (dd,  $J_1 = 3.5$  Hz,  $J_2 = 1.1$  Hz, 1H), 8.07 – 7.88 (m, 3H), 7.63 – 7.39 (m, 7H), 7.12 – 7.08 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.60, 158.87, 153.97, 149.49, 137.32, 132.15, 128.82, 126.43, 125.38, 123.23, 121.60, 121.04, 119.60. MS (ESI):  $m/z = 321$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{18}\text{H}_{12}\text{N}_2\text{S}_2$ ) C: 67.47, H: 3.7, N: 8.74, S: 20.01; found C: 67.38, H: 3.05, N: 8.68, S: 19.86.



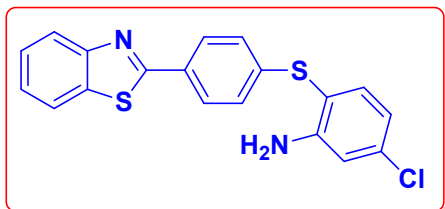
**2-(4-(tritylthio)phenyl)benzo[d]thiazole (3k):** Yield: 104.76 mg (72%); pale yellow solid; mp 112-114°C. FT-IR (KBr): 3057, 3022, 1477, 1068, 1012  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.13 (d,  $J = 8.0$  Hz, 1H), 8.02 – 7.99 (m, 1H), 7.94 (dd,  $J_1 = 8.0$  Hz,  $J_2 = 0.4$  Hz, 1H), 7.71 – 7.63 (m, 2H), 7.57 – 7.51 (m, 1H), 7.48 – 7.41 (m, 1H), 7.30 (dddd,  $J_1 = 9.4$  Hz,  $J_2 = 7.3$  Hz,  $J_3 = 6.0$  Hz,  $J_4 = 1.6$  Hz, 12H), 7.20 – 7.17 (m, 4H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.63, 154.05, 146.86, 144.50, 143.87, 143.49, 135.01, 132.51, 132.19, 130.34, 129.33, 128.87, 128.61, 128.29, 127.87, 127.16, 126.46, 126.25, 125.40, 123.29, 121.62, 56.82. MS (ESI):  $m/z = 486$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{32}\text{H}_{23}\text{NS}_2$ ) C: 79.14, H: 4.77, N: 2.88, S: 13.20; found C: 79.11, H: 4.67, N: 2.78, S: 13.12.



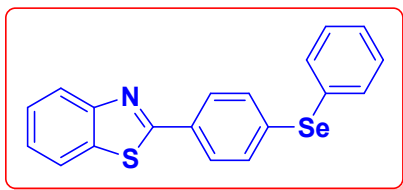
**2-(4-(4-fluorophenyl)thio)phenyl)benzo[d]thiazole (3l):** Yield: 69.75 mg (69%); pale yellow solid; mp 130-132 °C. FT-IR (KBr): 3056, 3020, 1494, 1068  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.1$  Hz, 1H), 7.96 – 7.88 (m, 4H), 7.63 – 7.60 (m, 2H), 7.52 – 7.367(m, 4H), 7.02 – 6.98 (m, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$   $\delta_{\text{C}}$  (101 MHz,  $\text{CDCl}_3$ ) 166.65, 163.80, 161.33 (d,  $J_1\text{C-F} = 249.47$  Hz), 154.02, 134.99, 132.50, 132.19, 131.28, 131.19 (d,  $J_3\text{C-F} = 9$  Hz), 128.86, 126.47, 125.41, 125.38, 123.28, 121.63, 116.36, 116.13 (d,  $J_2\text{C-F} = 23.23$  Hz). MS (ESI):  $m/z = 338$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{19}\text{H}_{12}\text{FNS}_2$ ) C: 67.63, H: 3.58, N: 4.15, S: 19.00; found C: 67.53, H: 4.05, N: 4.02, S: 18.89.



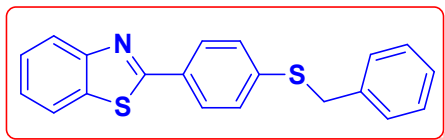
**4-((4-(benzo[d]thiazol-2-yl)phenyl)thio)aniline (3m):** Yield: 83.16 mg (83%); pale brown solid; mp 120-122°C. FT-IR (KBr): 3336, 3057, 3026, 1585, 1012  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.1$  Hz, 1H), 7.94 (d,  $J = 8.5$  Hz, 1H), 7.89 (d,  $J = 7.9$  Hz, 1H), 7.61 (d,  $J = 8.5$  Hz, 2H), 7.53 – 7.45 (m, 1H), 7.43 – 7.35 (m, 1H), 7.27 – 7.22 (m, 3H), 6.57 (d,  $J = 8.5$  Hz, 2H), 3.77 (s, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.63, 154.00, 147.05, 134.98, 133.85, 132.47, 132.16, 128.84, 126.45, 125.40, 123.24, 121.61, 115.30. MS (ESI):  $m/z = 335$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{19}\text{H}_{14}\text{N}_2\text{S}_2$ ) C: 68.23, H: 4.22, N: 8.38, S: 19.17; found C: 68.17, H: 4.12, N: 8.30, S: 19.10.



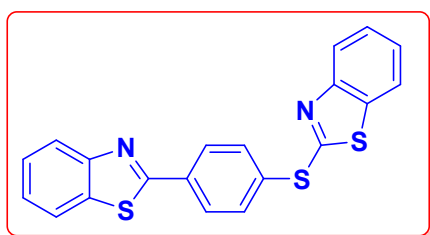
**2-((4-(benzo[d]thiazol-2-yl)phenyl)thio)-5-chloroaniline (3n):** Yield: 88.32 mg (80%); pale brown solid; mp 123-125°C. FT-IR (KBr): 3375, 3076, 3059, 3020, 1473, 1010  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 8.1$  Hz, 1H), 7.97 – 7.89 (m, 3H), 7.64 – 7.62 (m, 2H), 7.45 (ddd,  $J_1 = 15.2$  Hz,  $J_2 = 8.1$  Hz,  $J_3 = 1.0$  Hz, 2H), 7.02 (d,  $J = 8.2$  Hz, 1H), 6.71 (d,  $J = 2.1$  Hz, 1H), 6.55 (dd,  $J_1 = 8.2$  Hz,  $J_2 = 2.1$  Hz, 1H), 4.43 (s, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.69, 154.03, 149.42, 137.84, 135.01, 132.21, 128.88, 126.49, 125.43, 123.29, 121.65, 118.29, 116.57, 114.72. MS (ESI):  $m/z = 369$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{19}\text{H}_{13}\text{ClN}_2\text{S}_2$ ) C: 61.86, H: 3.55, Cl: 9.61, N: 7.59, S: 17.38; found C: 61.78, H: 3.49, Cl: 9.51, N: 7.50, S: 17.27.



**2-(4-(phenylselanyl)phenyl)benzo[d]thiazole (3o):** Yield: 85.64 mg (78%); yellow solid; mp 182-184°C. FT-IR (KBr): 3064, 3051, 1490, 1473, 1068  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.1$  Hz, 1H), 7.90 (dd,  $J_1 = 24.2$  Hz,  $J_2 = 8.2$  Hz, 2H), 7.59 (dd,  $J_1 = 7.6$  Hz,  $J_2 = 1.9$  Hz, 4H), 7.52 – 7.45 (m, 1H), 7.41 – 7.34 (m, 1H), 7.25 – 7.22 (m, 4H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.59, 154.01, 134.98, 132.92, 132.47, 132.15, 131.45, 131.40, 129.12, 128.83, 127.65, 126.43, 125.38, 123.26, 121.60. MS (ESI):  $m/z = 367$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{19}\text{H}_{13}\text{NSSe}$ ) C: 62.29, H: 3.58, N: 3.82, S: 8.75, Se: 21.55; found C: 62.21, H: 3.53, N: 3.74, S: 8.64, Se: 21.45.



**2-(4-(benzylthio)phenyl)benzo[d]thiazole (3p):** Yield: 75.92 mg (76%); pale yellow semi solid. IR (KBr): 3050, 3030, 2410, 1455, 1010  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.06 (d,  $J = 8.1$  Hz, 1H), 7.90 (dd,  $J_1 = 23.4$  Hz,  $J_2 = 8.2$  Hz, 2H), 7.60 (d,  $J = 8.5$  Hz, 1H), 7.49 (t,  $J = 7.3$  Hz, 1H), 7.42 – 7.16 (m, 8H), 3.58 (s, 2H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  166.61, 154.04, 137.33, 135.00, 132.51, 132.17, 129.36, 128.85, 128.43, 127.37, 126.45, 125.39, 123.28, 121.61, 43.26. MS (ESI):  $m/z = 334$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{20}\text{H}_{15}\text{NS}_2$ ) C: 72.04, H: 4.53, N: 4.20, S: 19.23; found C: 72.00, H: 4.42, N: 4.10, S: 19.13.

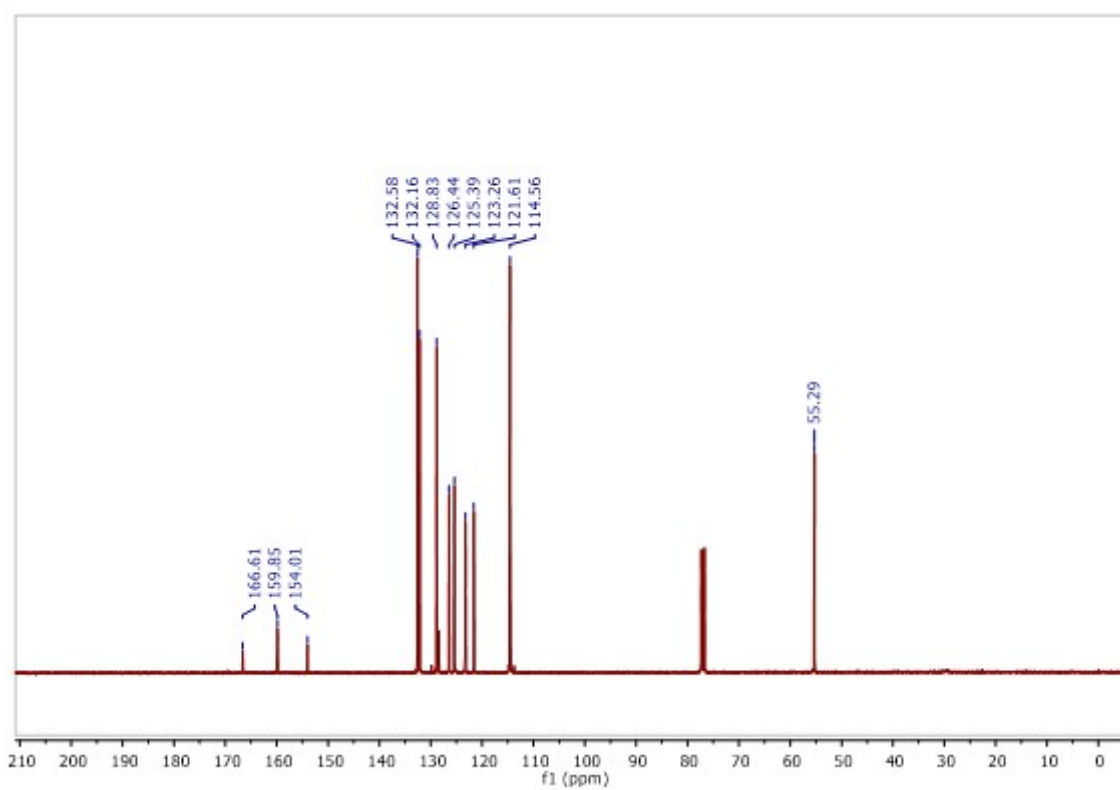
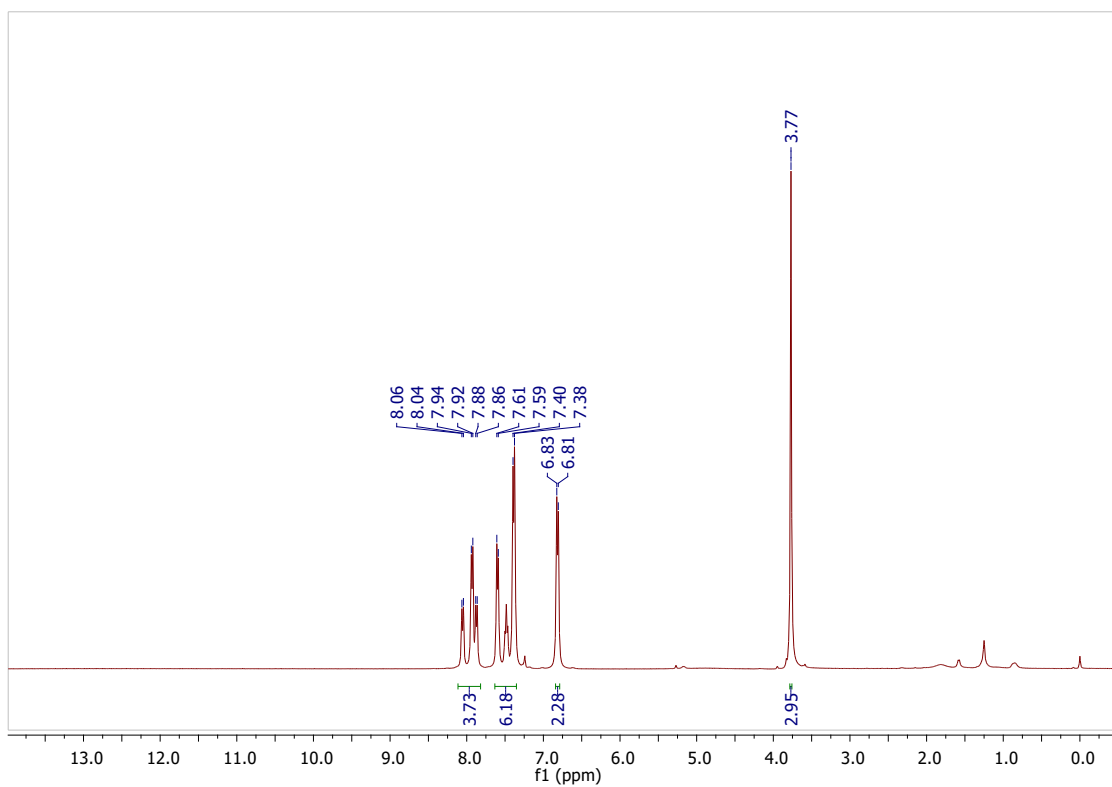


**2-((4-(benzo[d]thiazol-2-yl)phenyl)thio)benzo[d]thiazole (3q):** Yield: 72.19 mg (64%); pale yellow solid; mp 133-135  $^{\circ}\text{C}$ . IR (KBr): 3059, 3030, 1550, 1500, 1068  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR (400 MHz, DMSO)  $\delta$  8.08 – 7.90 (m, 4H), 7.64 (d,  $J = 8.5$  Hz, 2H), 7.54 – 7.26 (m, 4H), 7.04 (t,  $J = 7.4$  Hz, 1H), 6.89 (t,  $J = 7.4$  Hz, 1H).  $^{13}\text{C}$  NMR (101 MHz,  $\text{CDCl}_3$ )  $\delta$  164.31, 153.99, 151.95, 135.63, 132.97, 130.46, 127.14, 124.77, 123.79, 123.23, 122.31, 121.26, 120.25, 118.69, 117.21, 115.63. MS (ESI):  $m/z = 377$   $[\text{M} + \text{H}]^+$ . Anal. Calcd for: ( $\text{C}_{20}\text{H}_{12}\text{N}_2\text{S}_3$ ) C: 63.80, H: 3.21, N: 7.44, S: 25.55; found C: 63.70, H: 3.12, N: 7.34, S: 25.45.

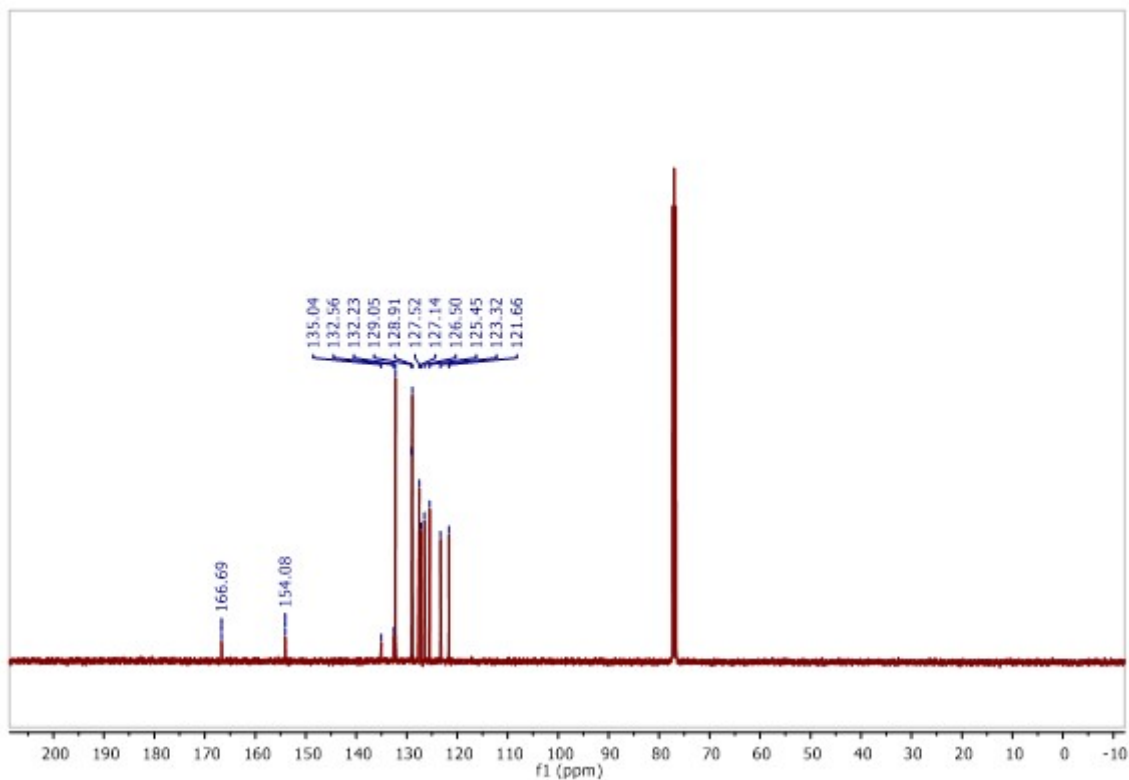
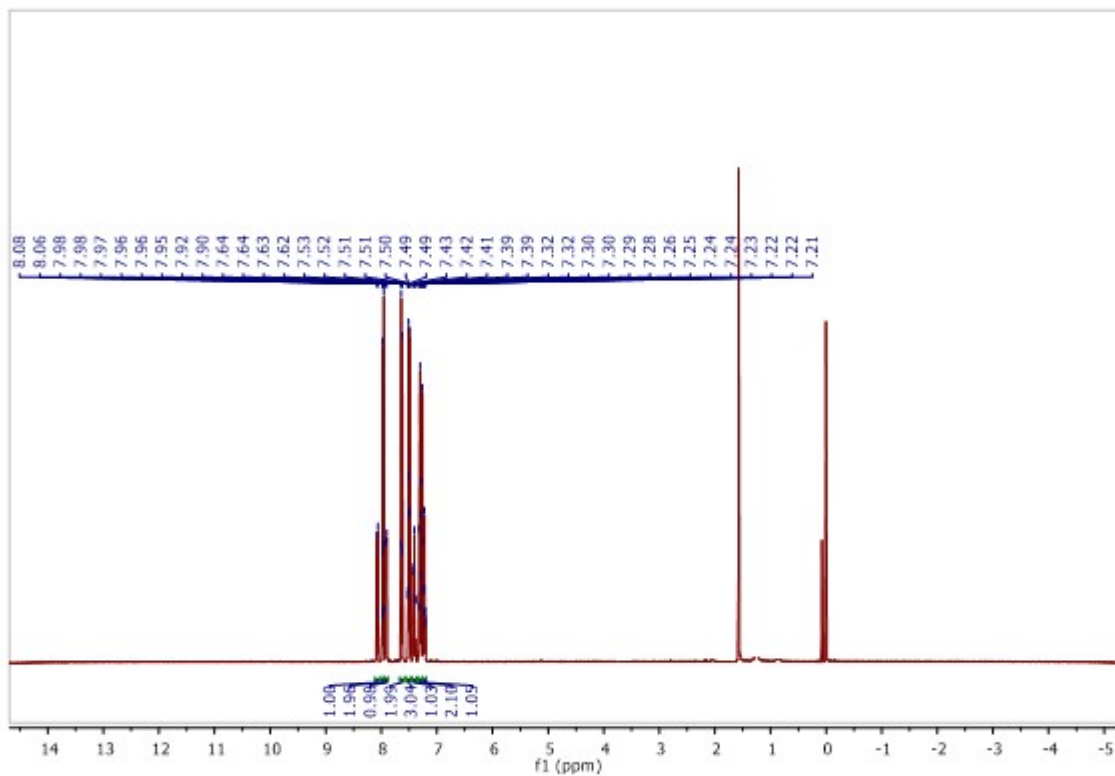


# $^1\text{H}$ AND $^{13}\text{C}$ SPECTRAS OF THE COMPOUNDS:

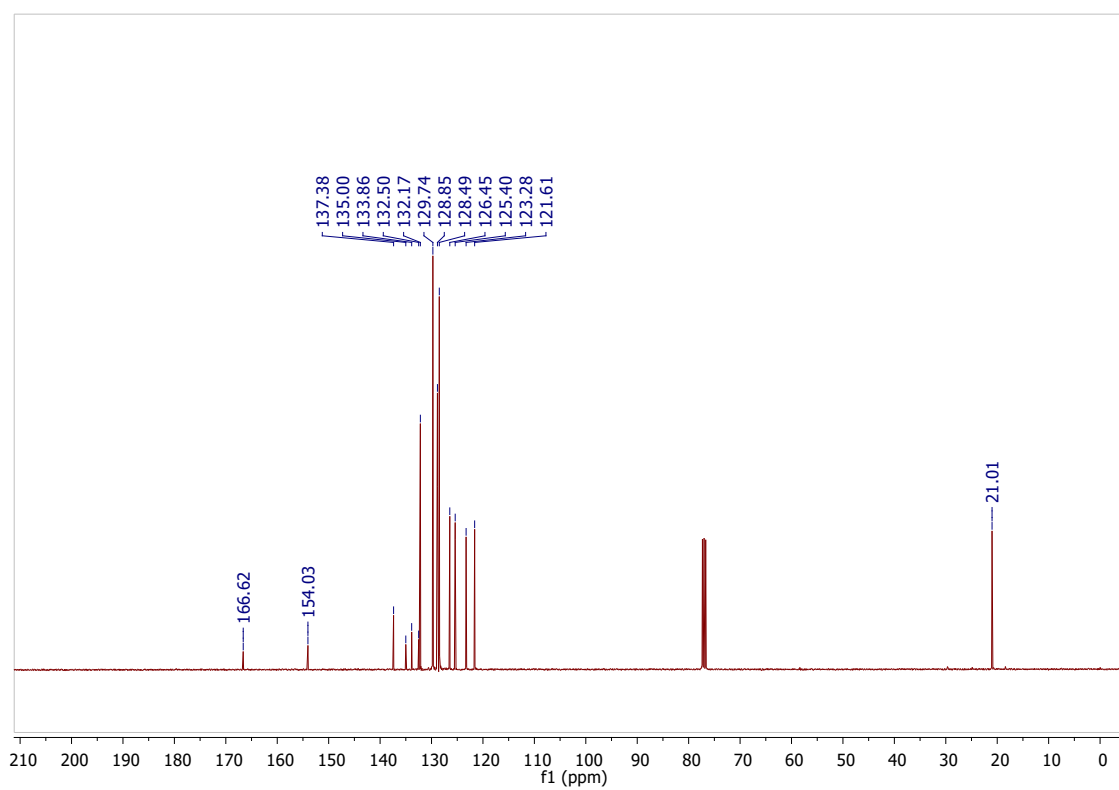
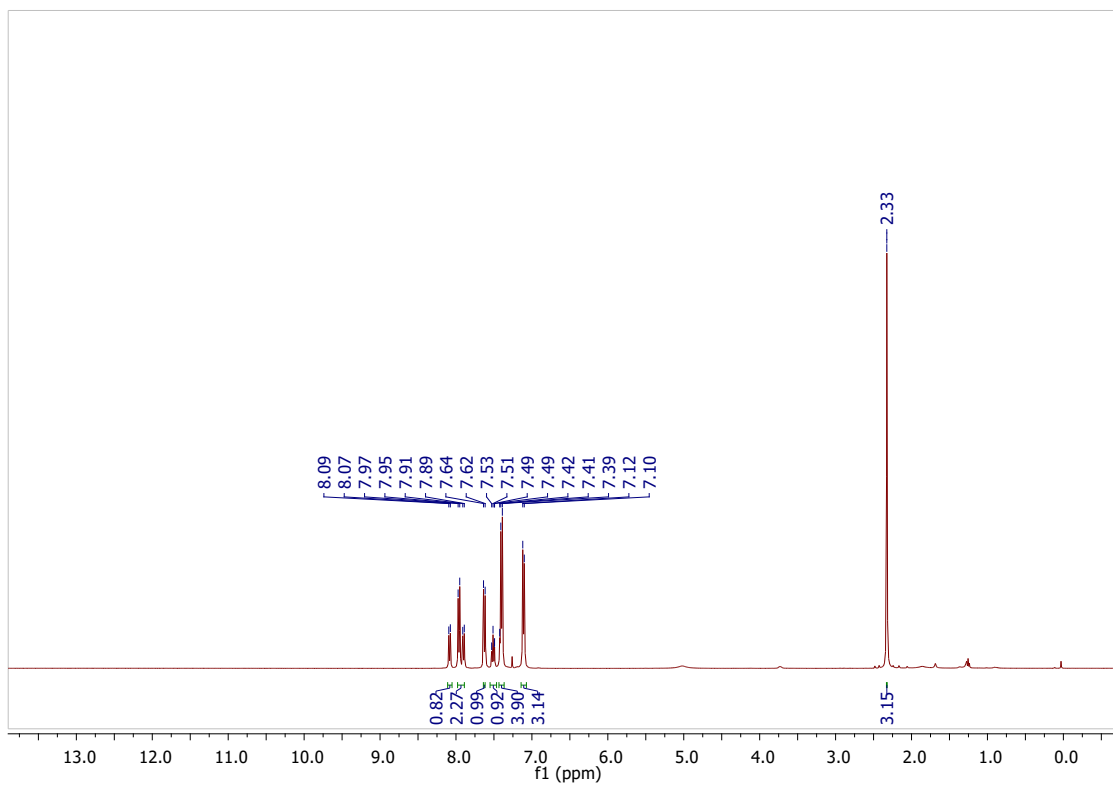
3a:



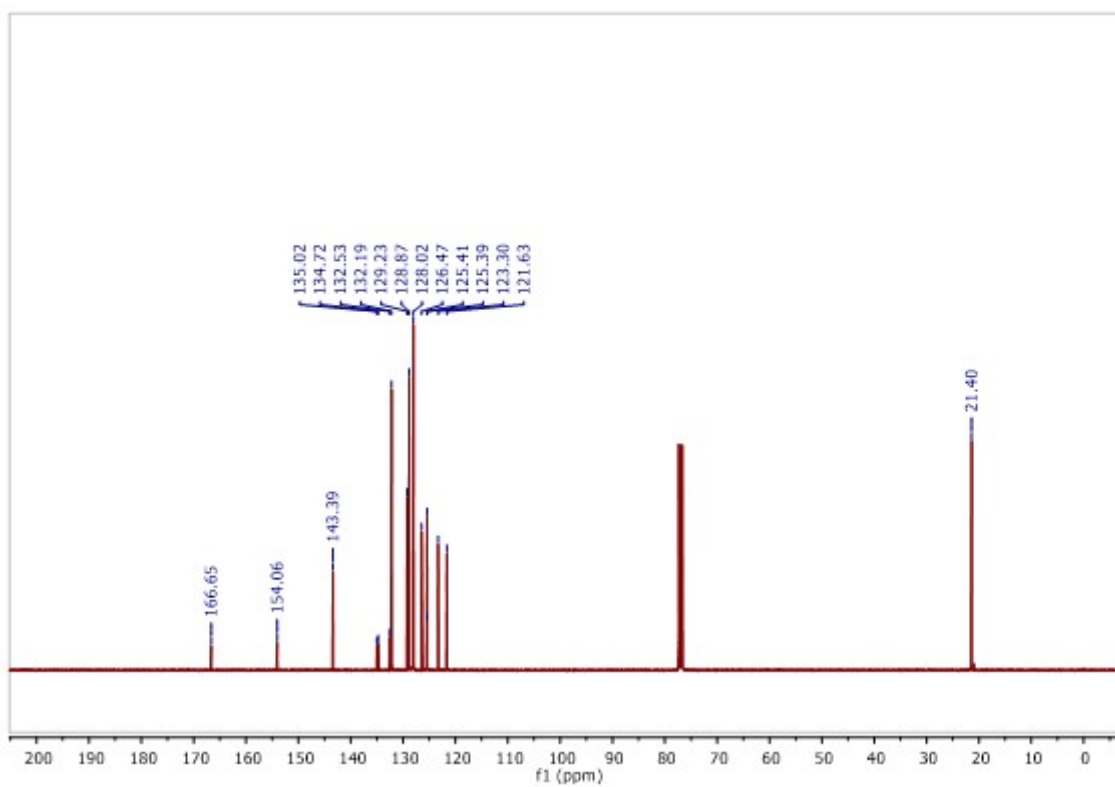
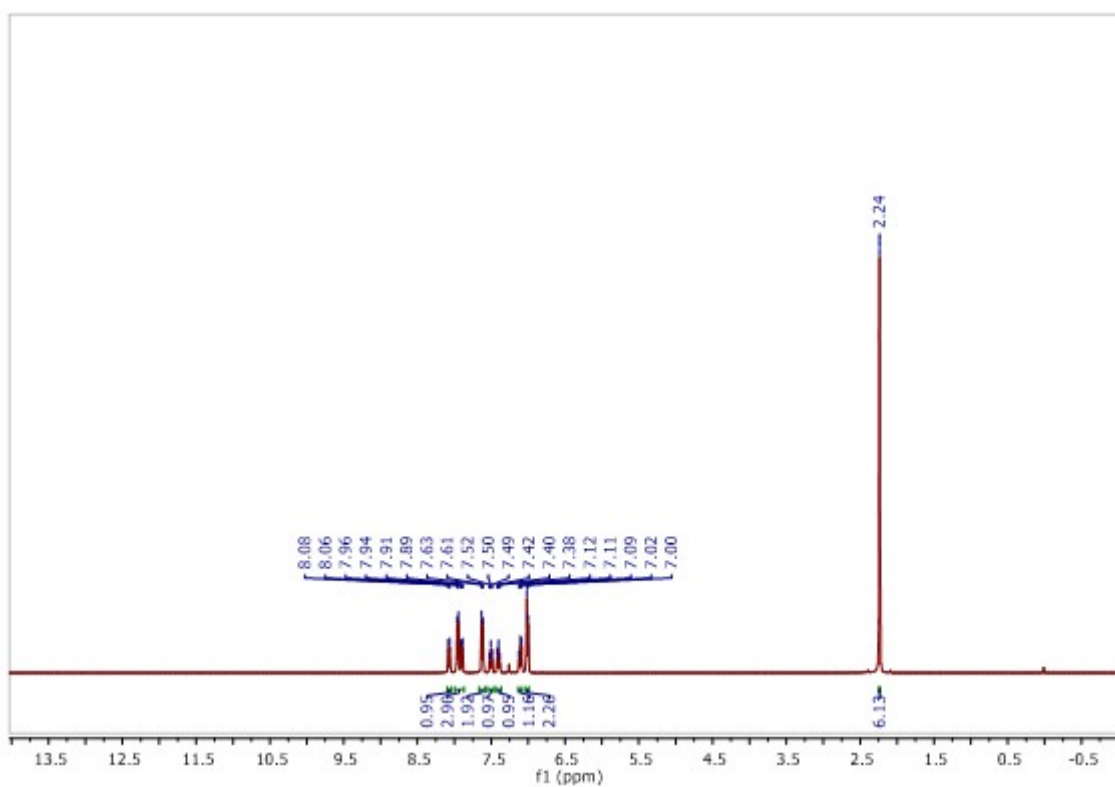
3b:



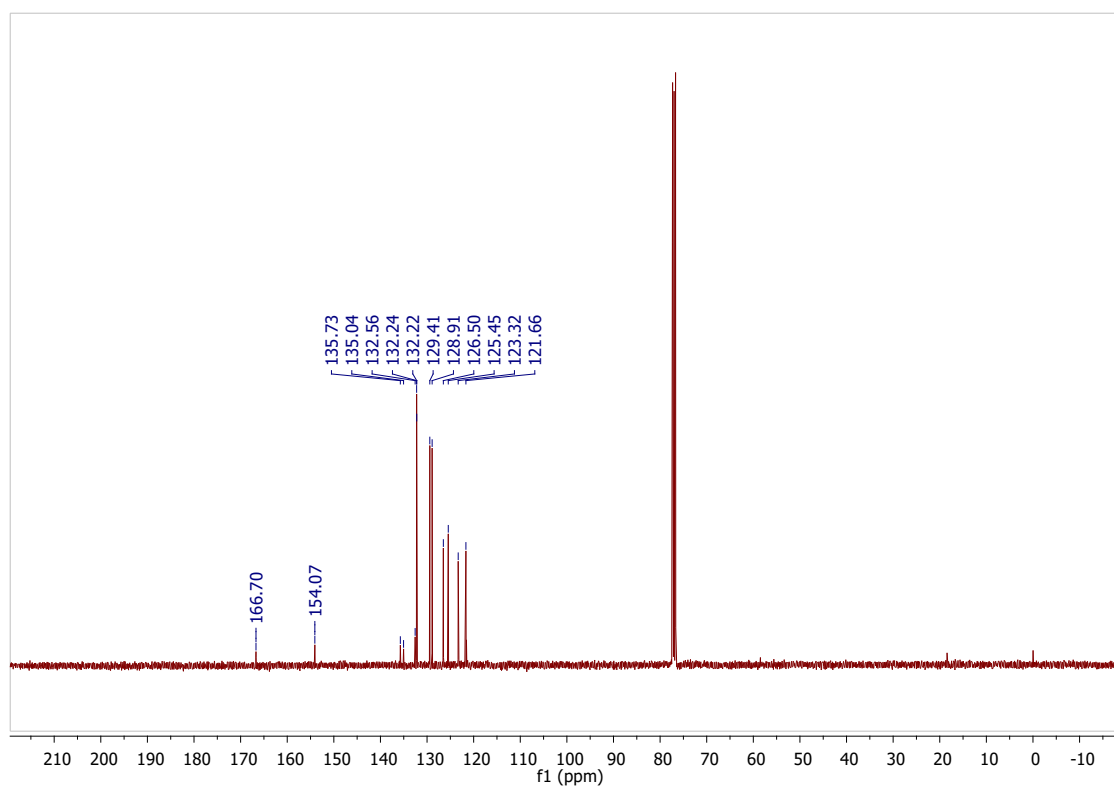
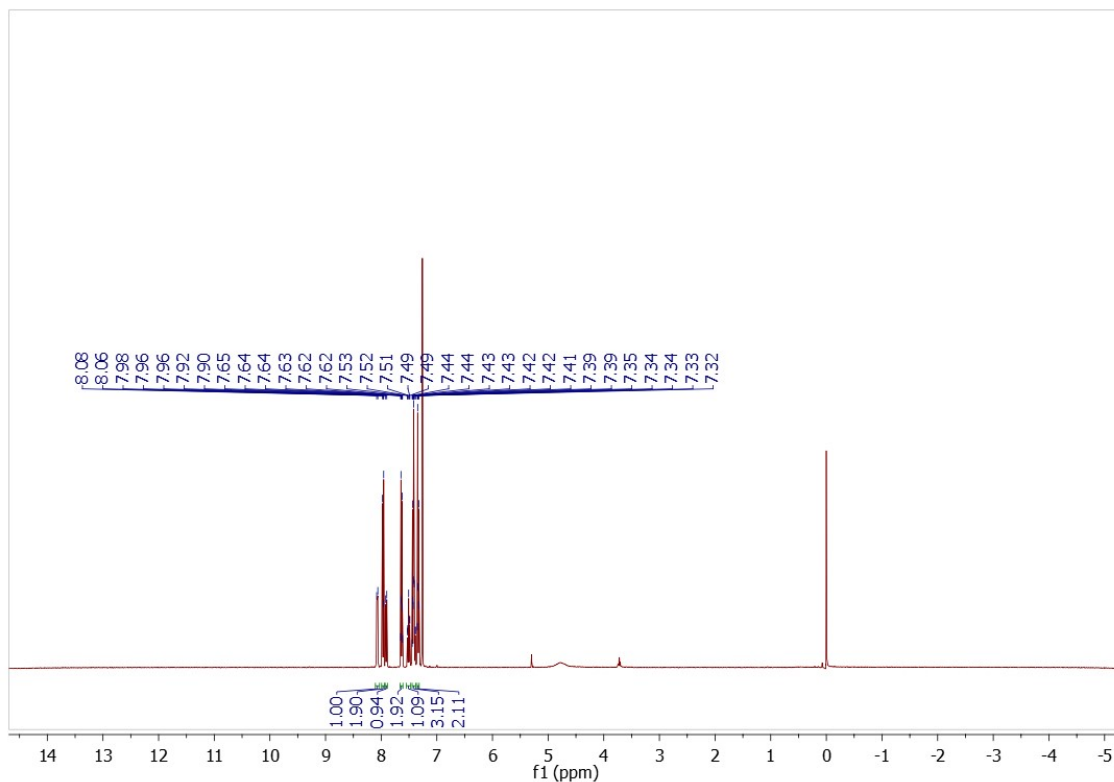
3c:



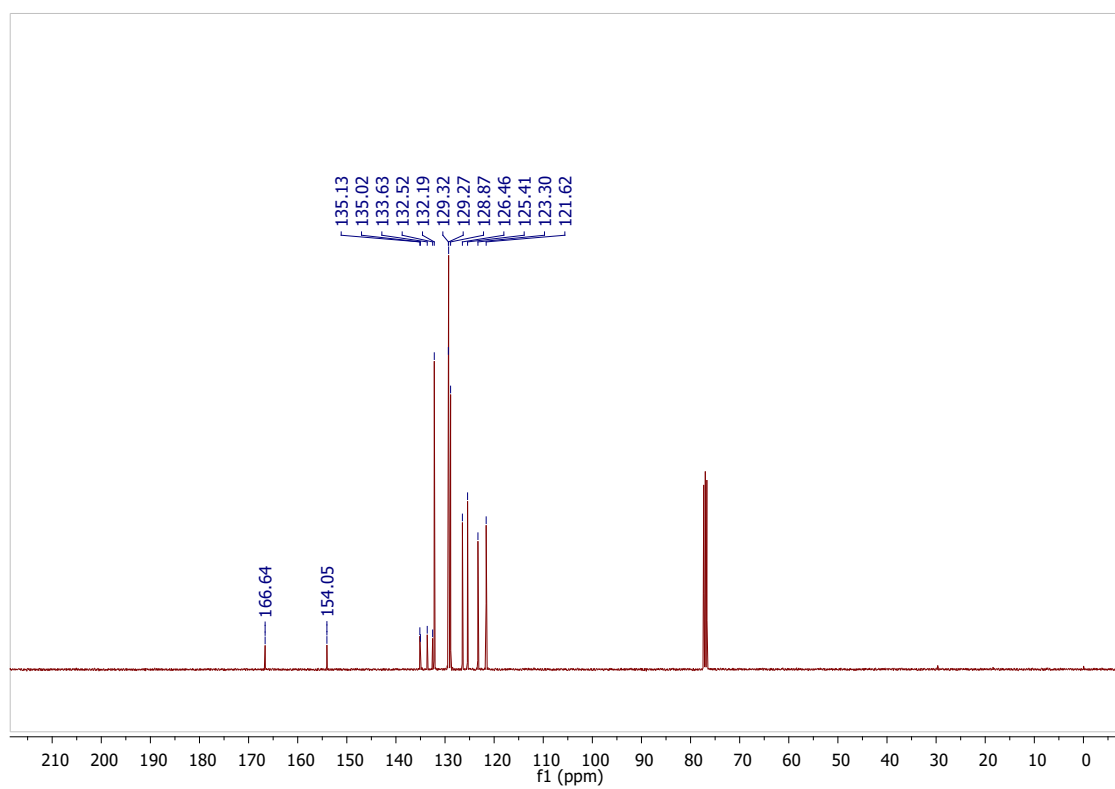
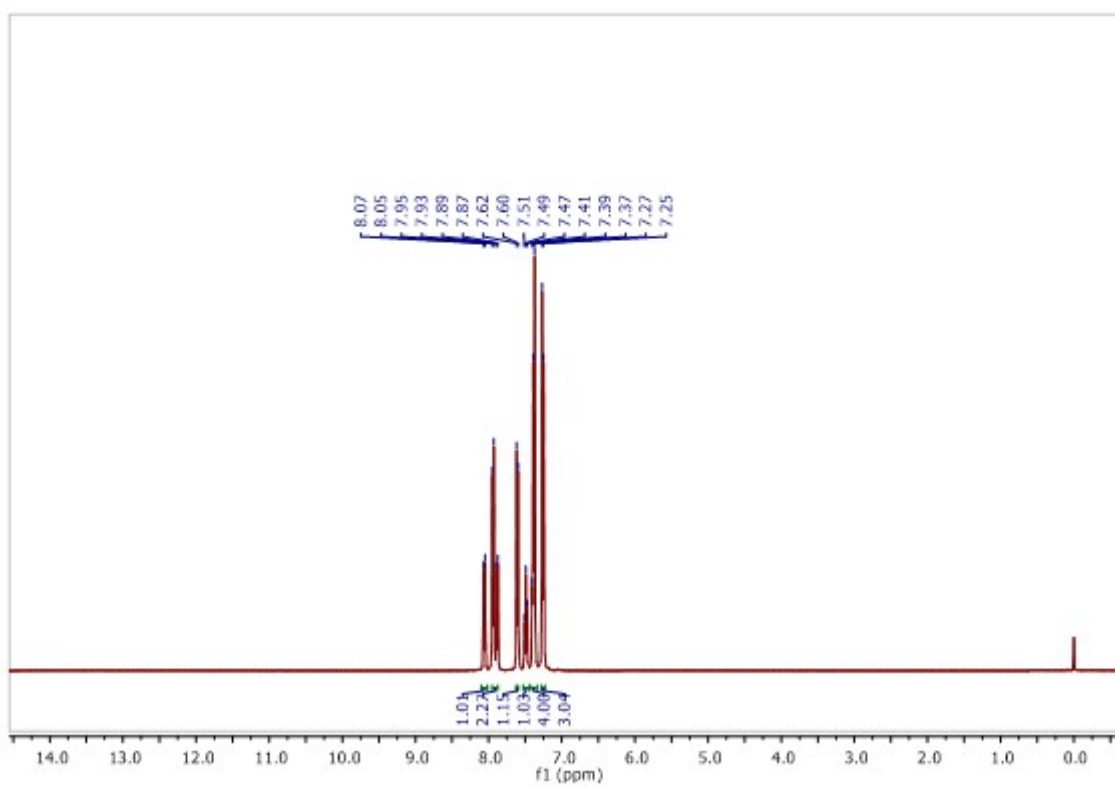
3d:



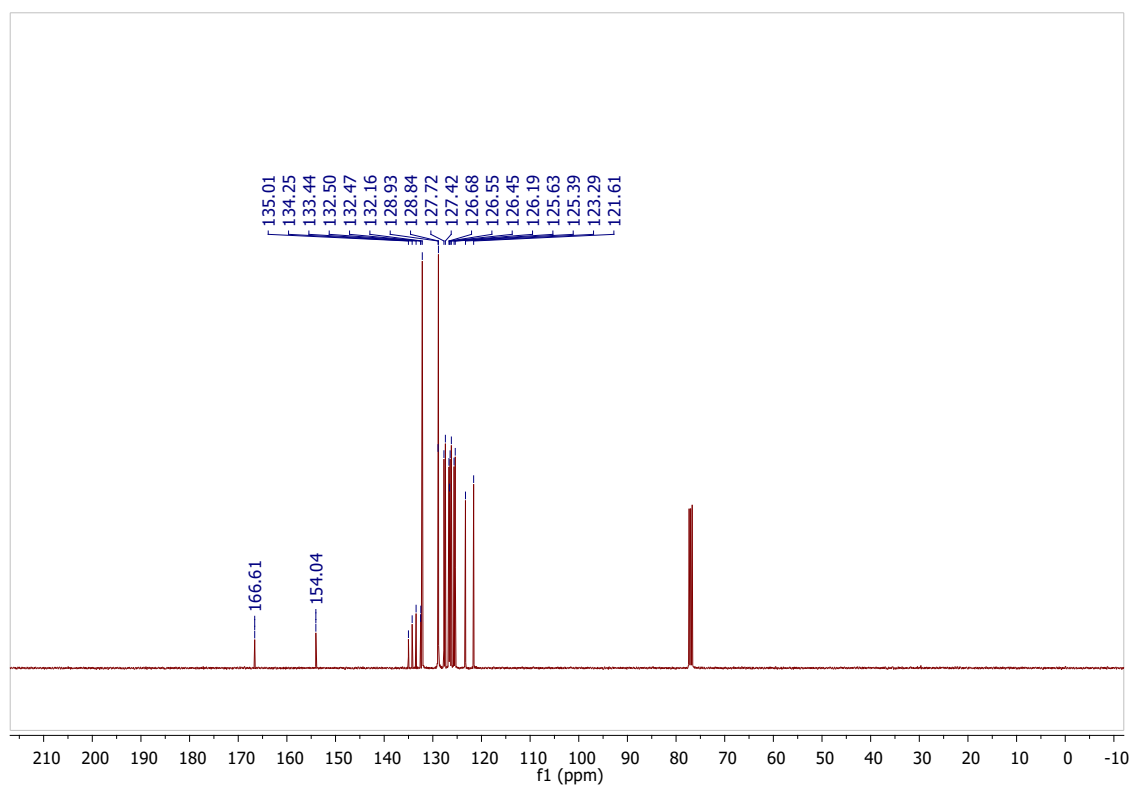
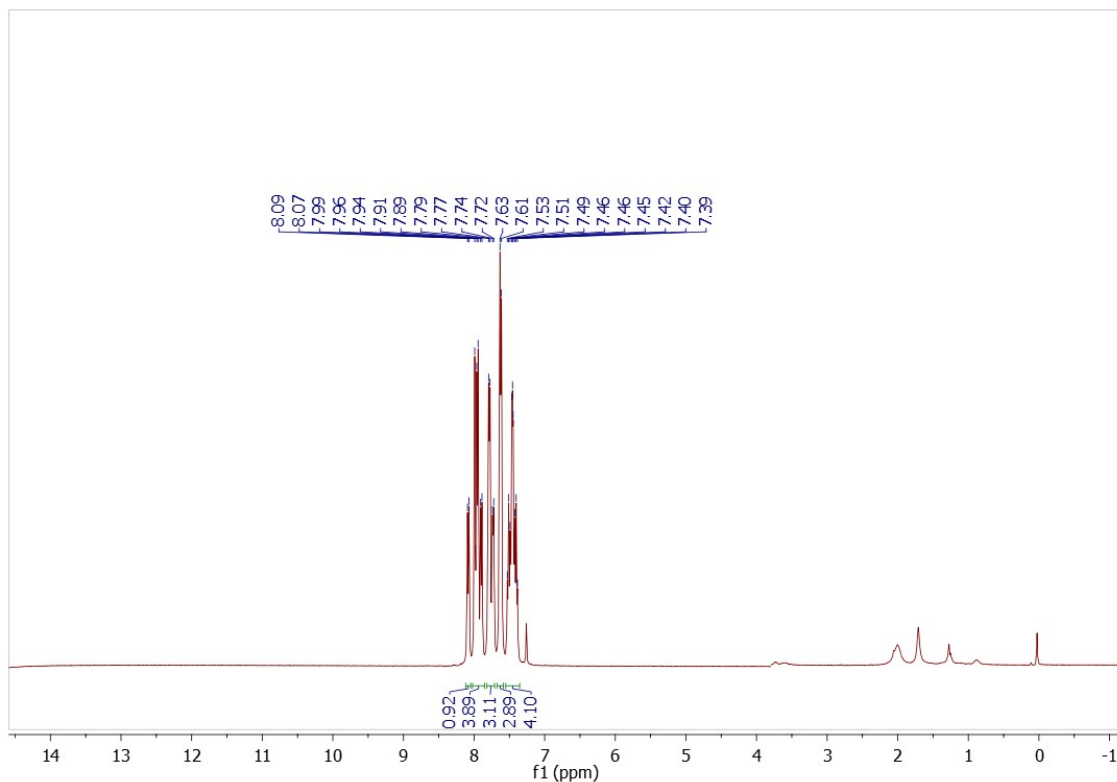
3e:



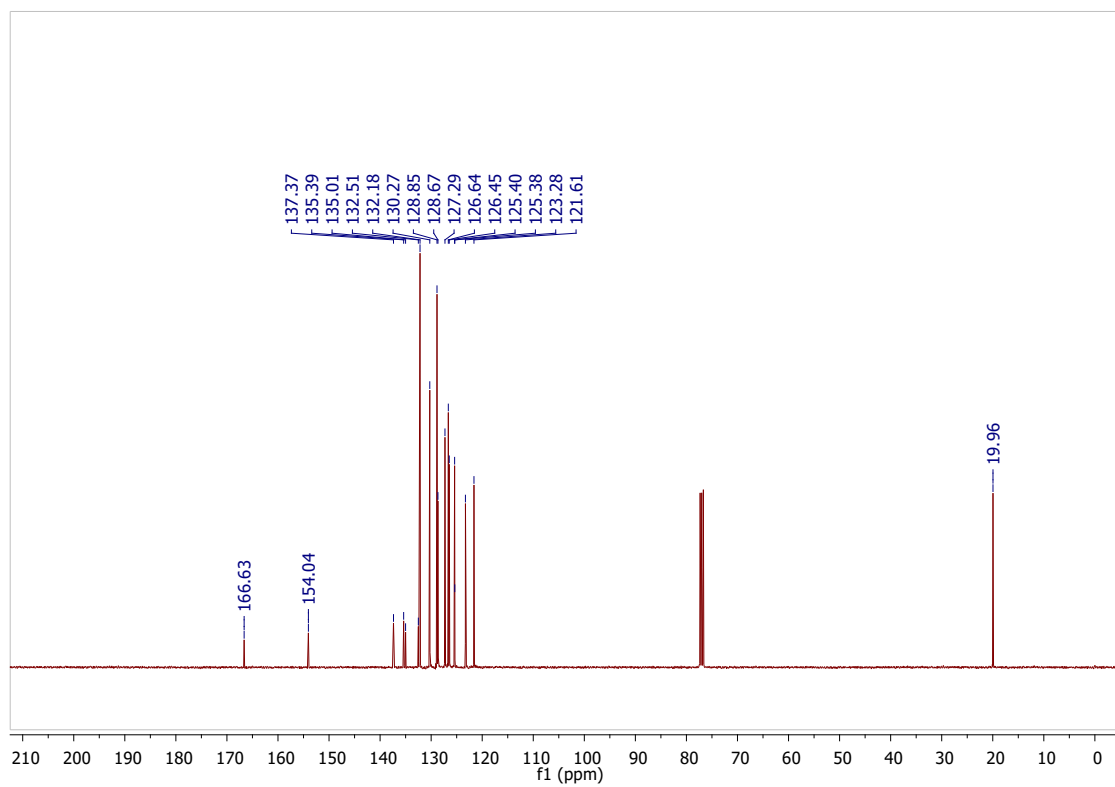
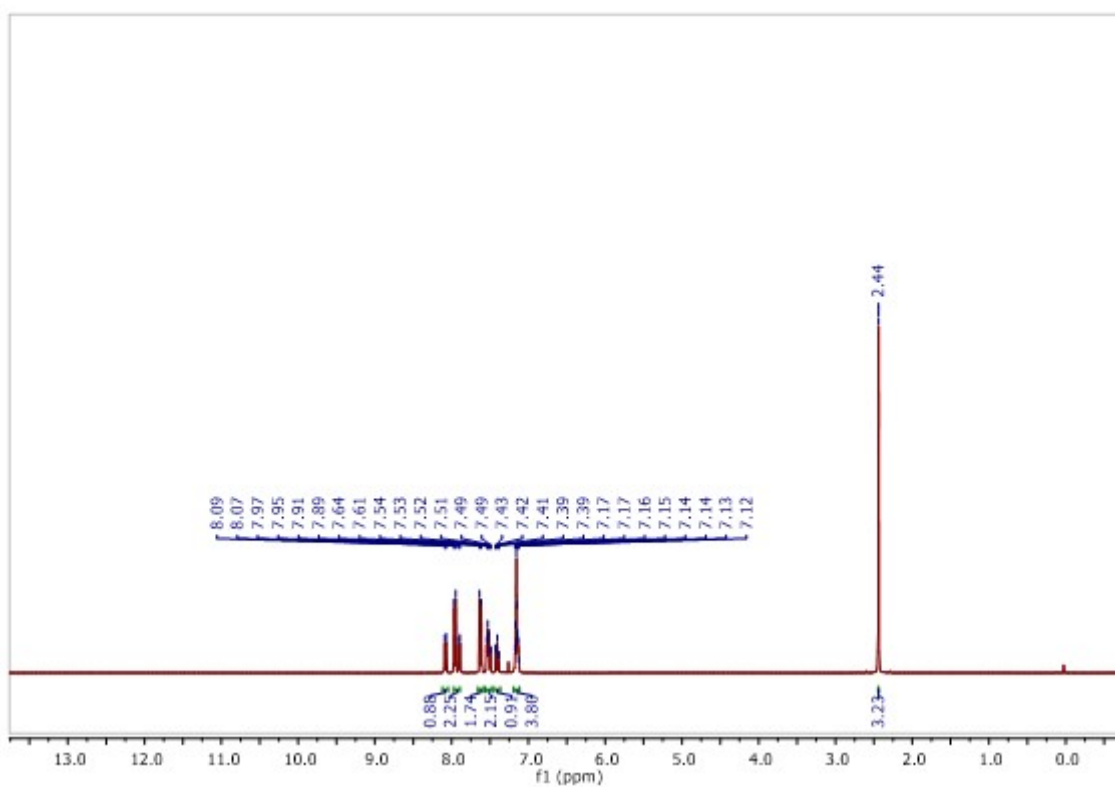
3f:



3g:

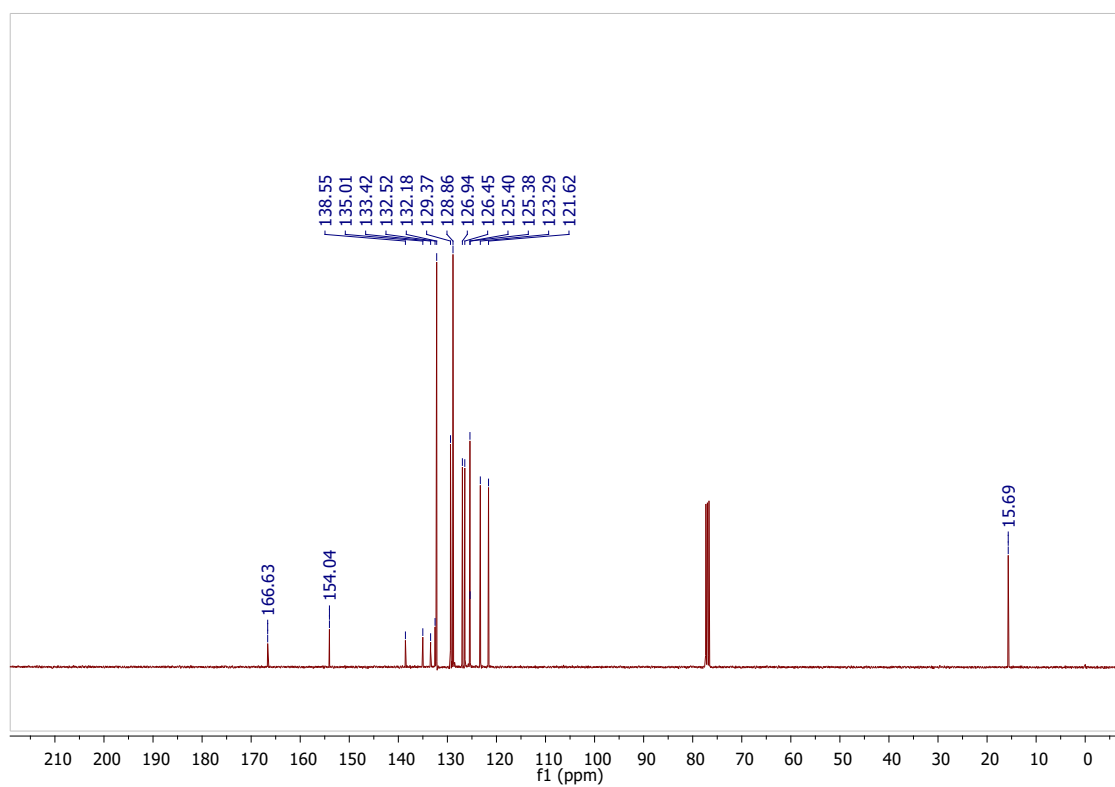
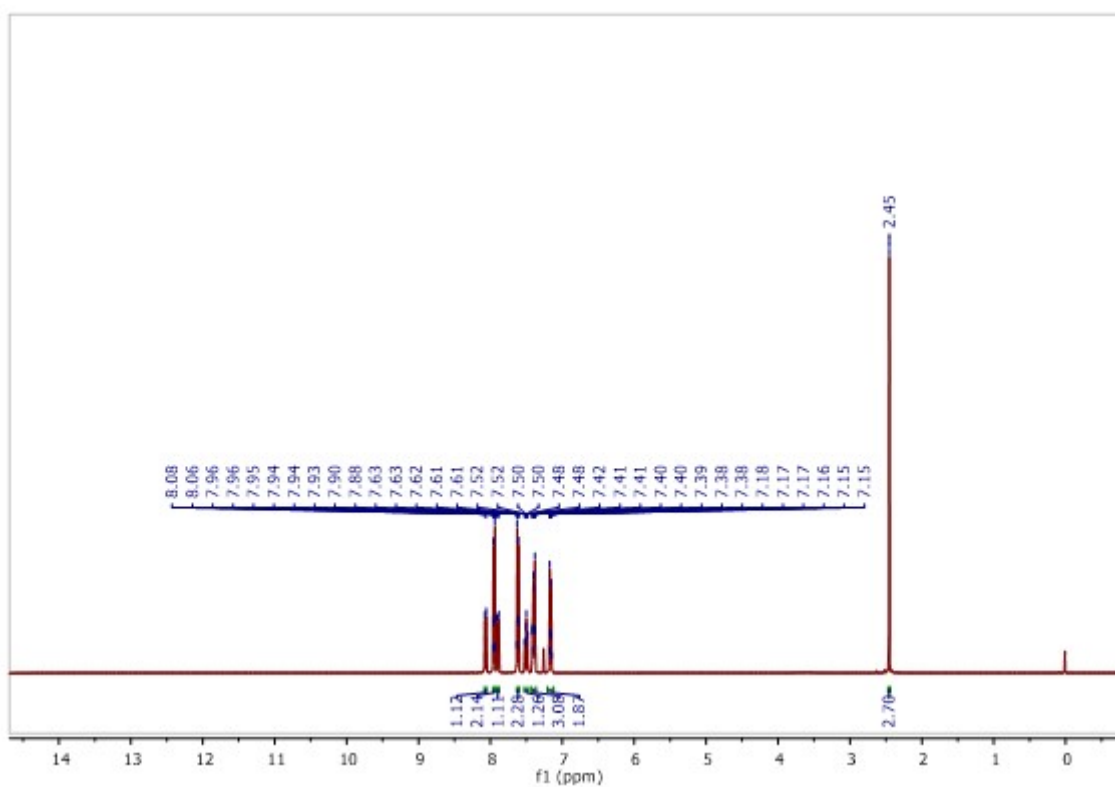


3h:

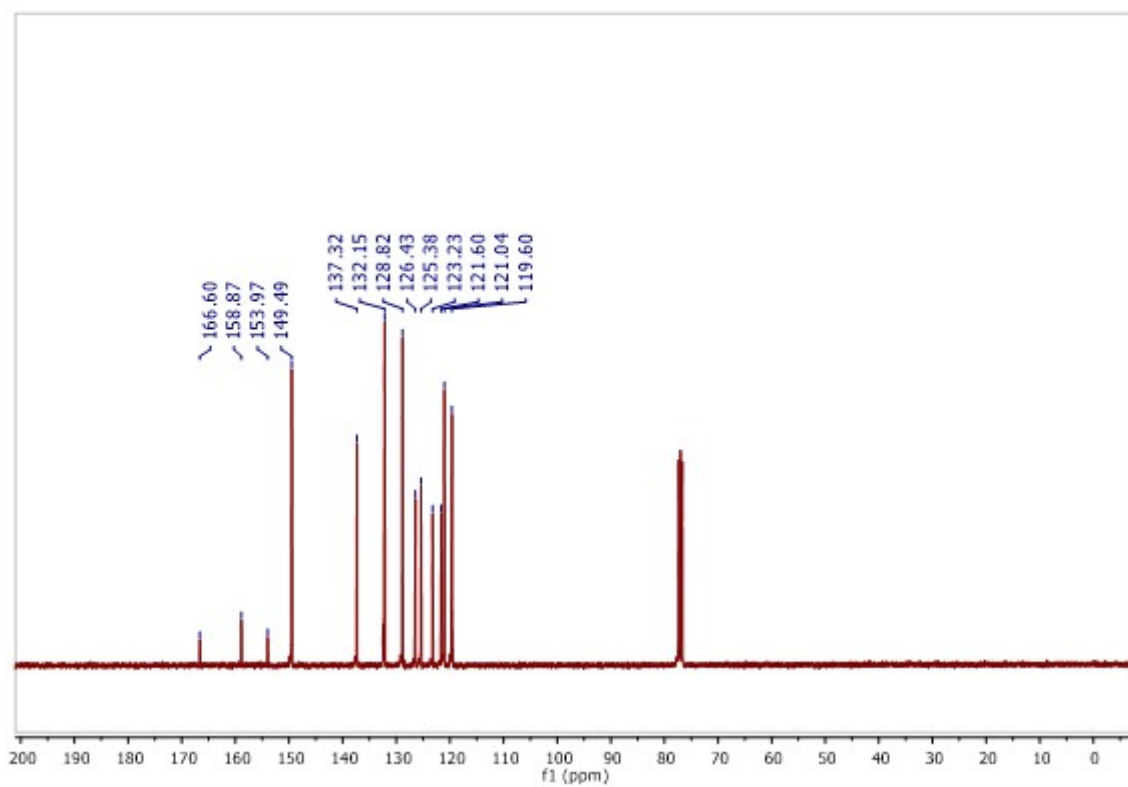
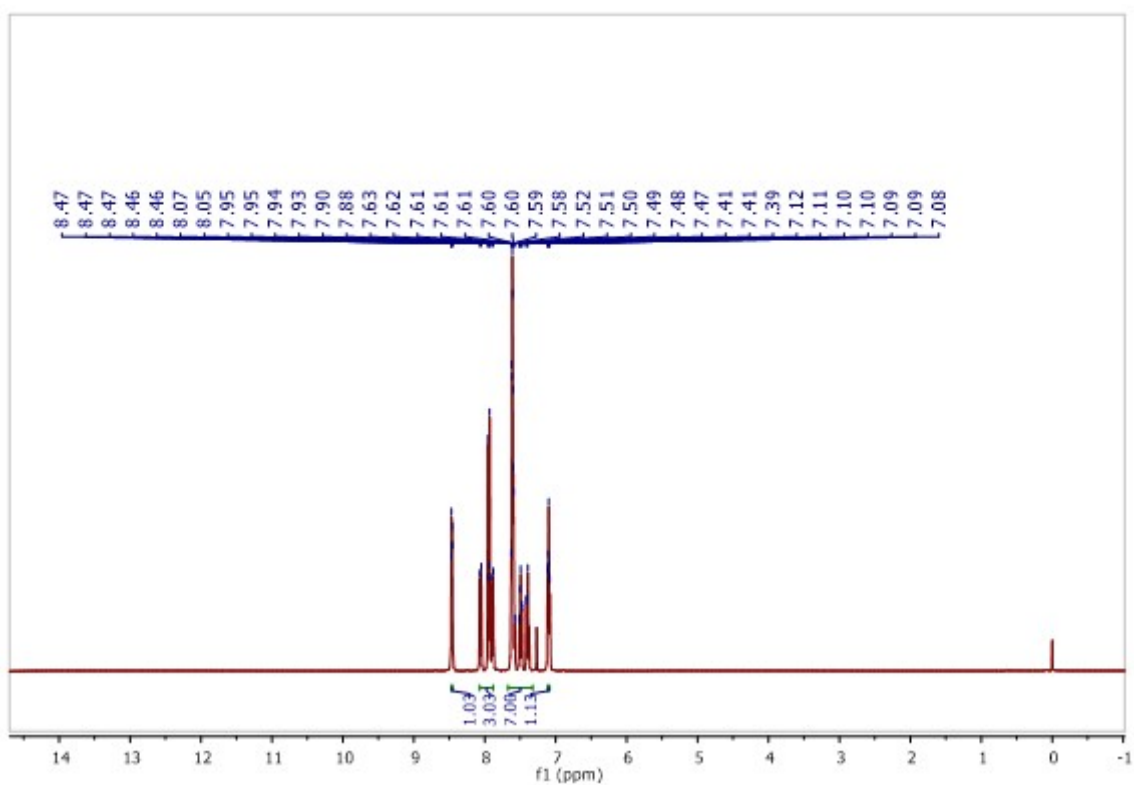




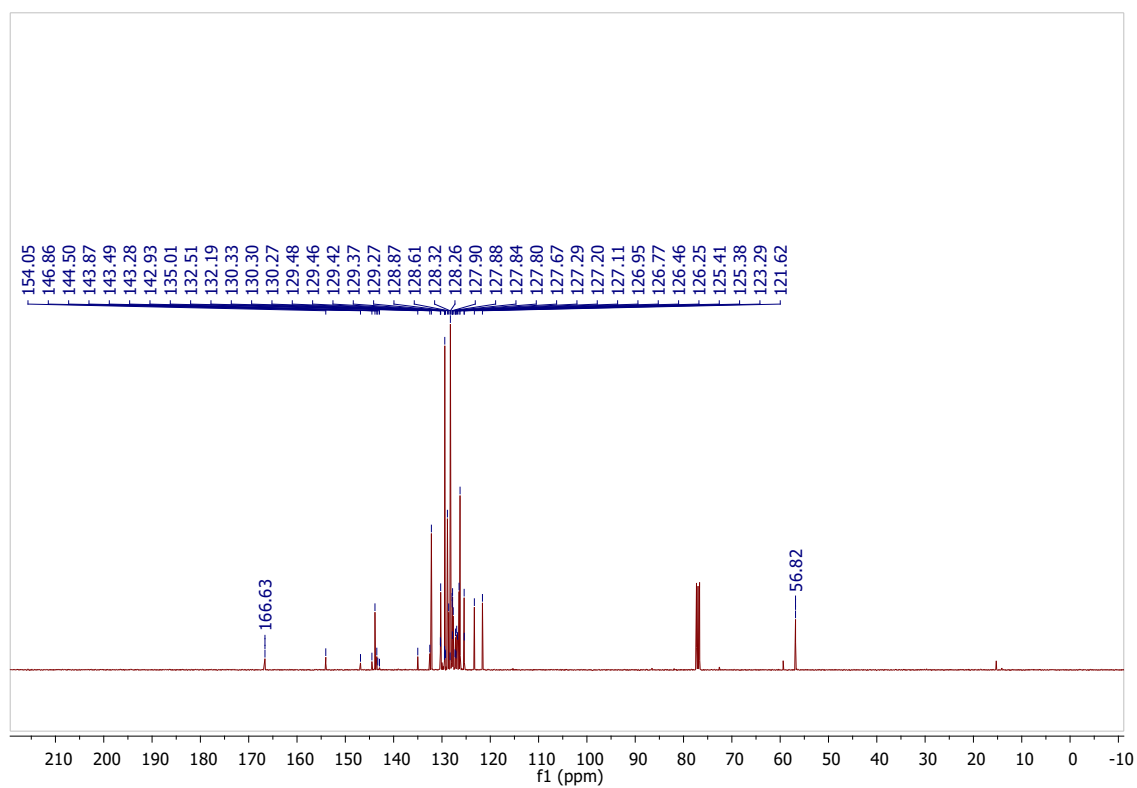
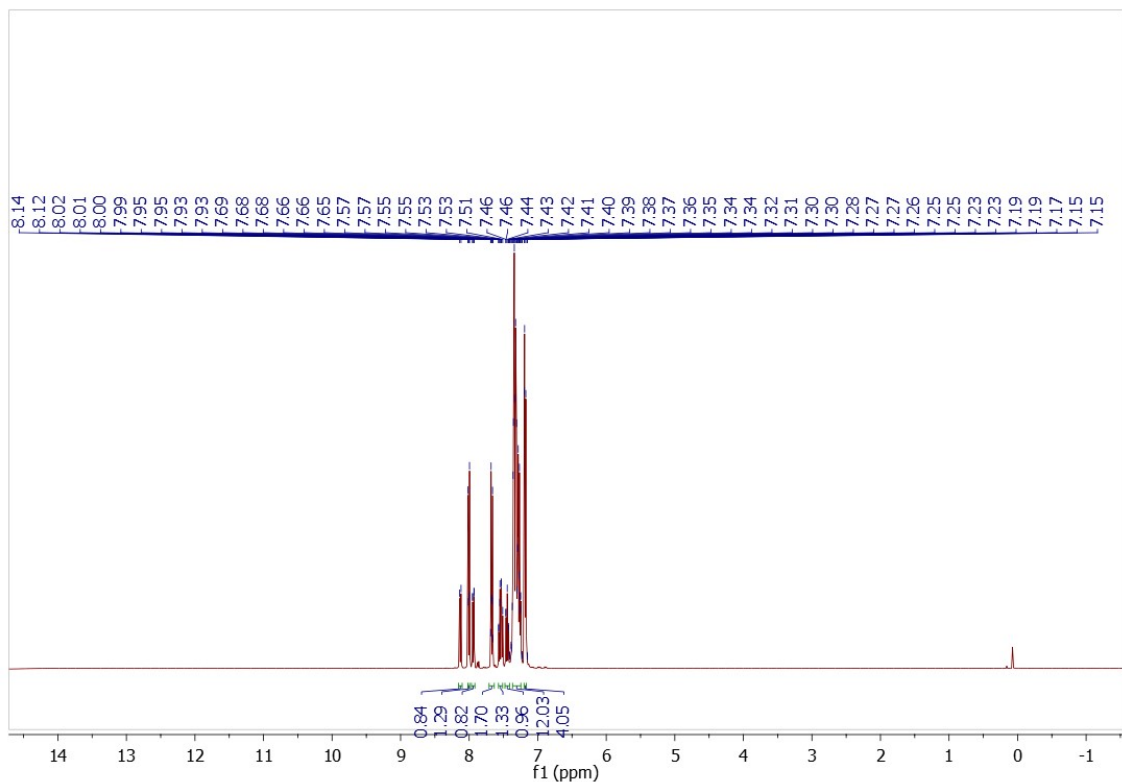
3i:



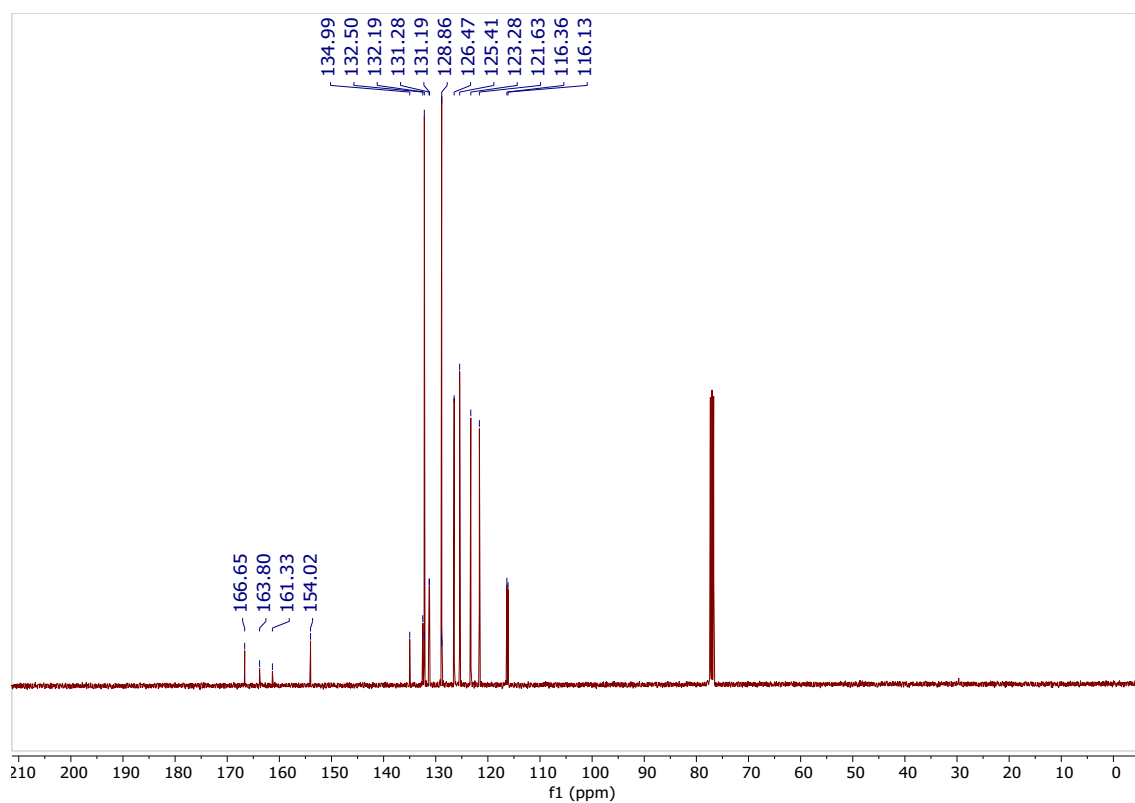
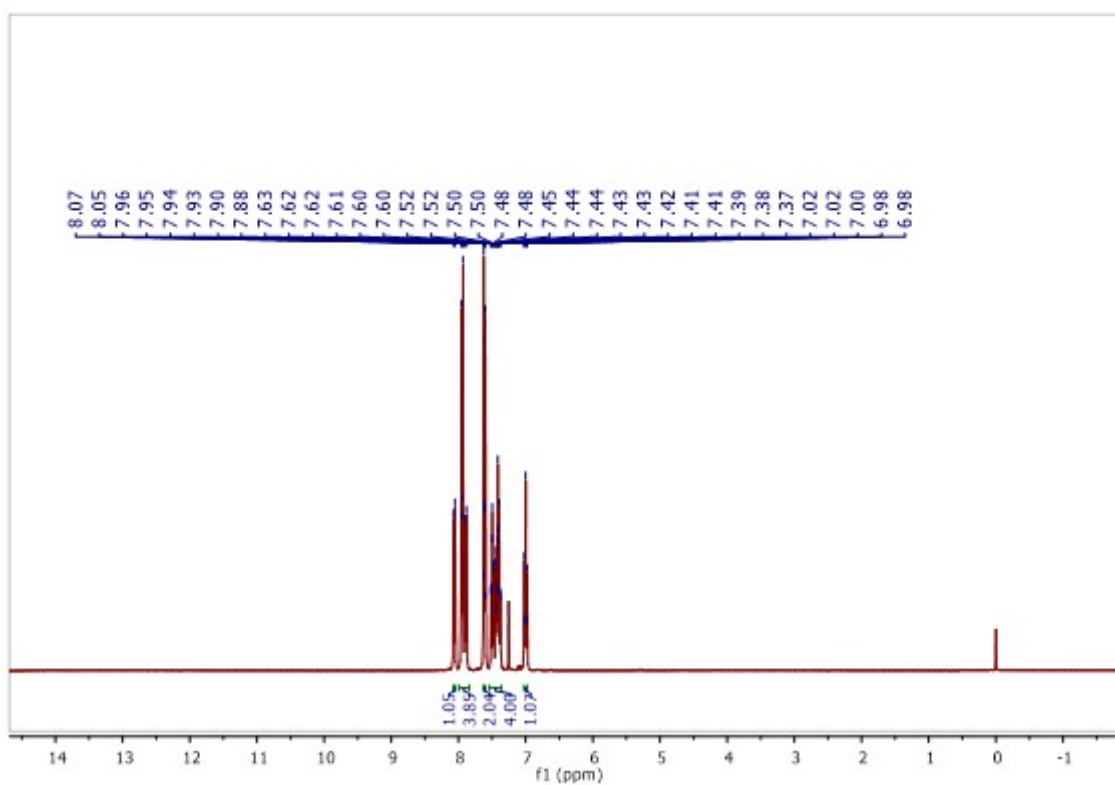
3j:



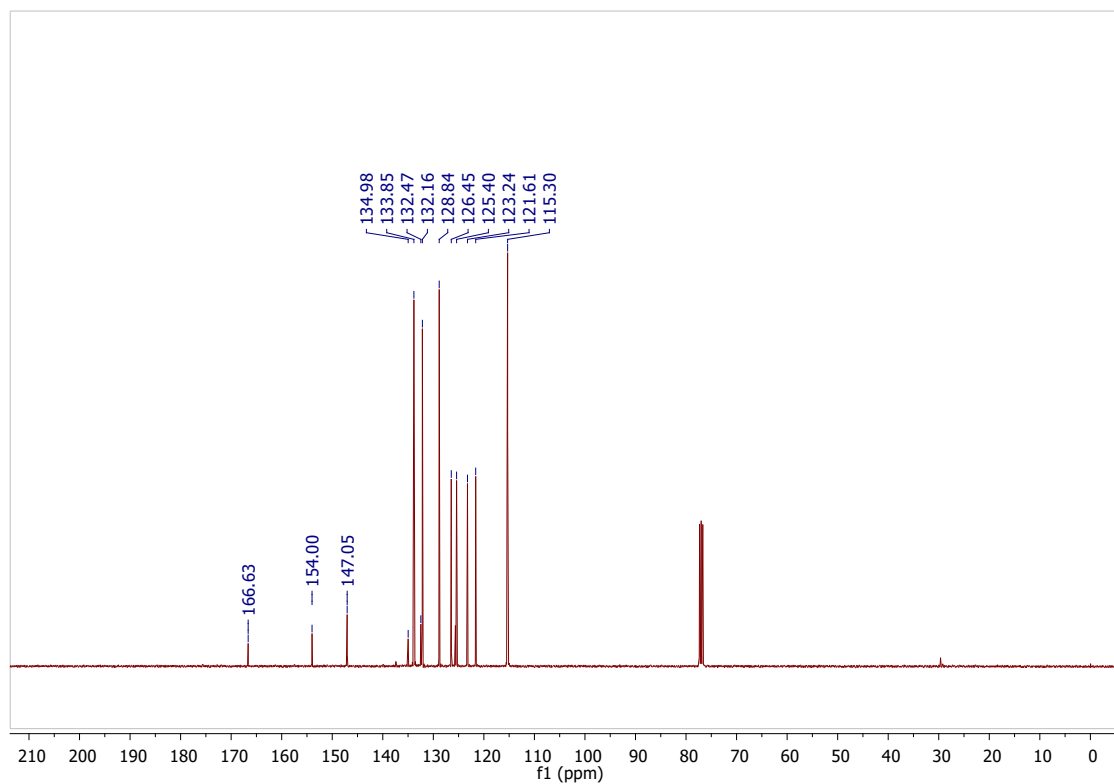
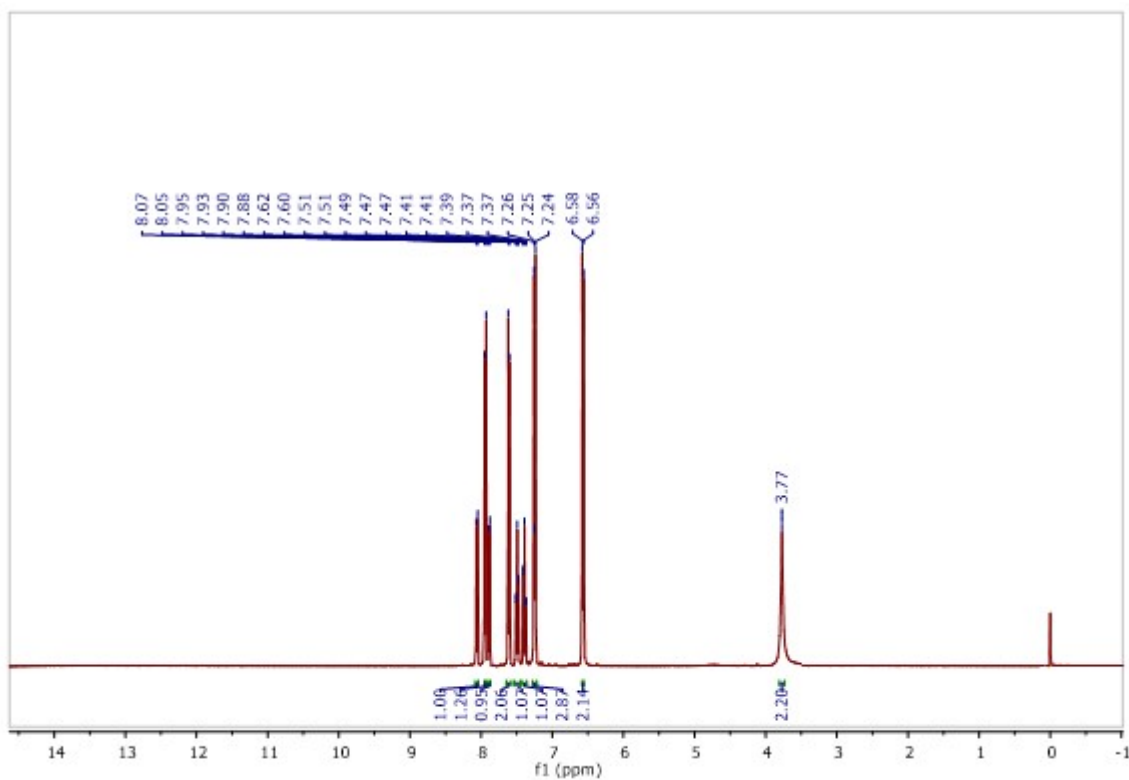
3k:



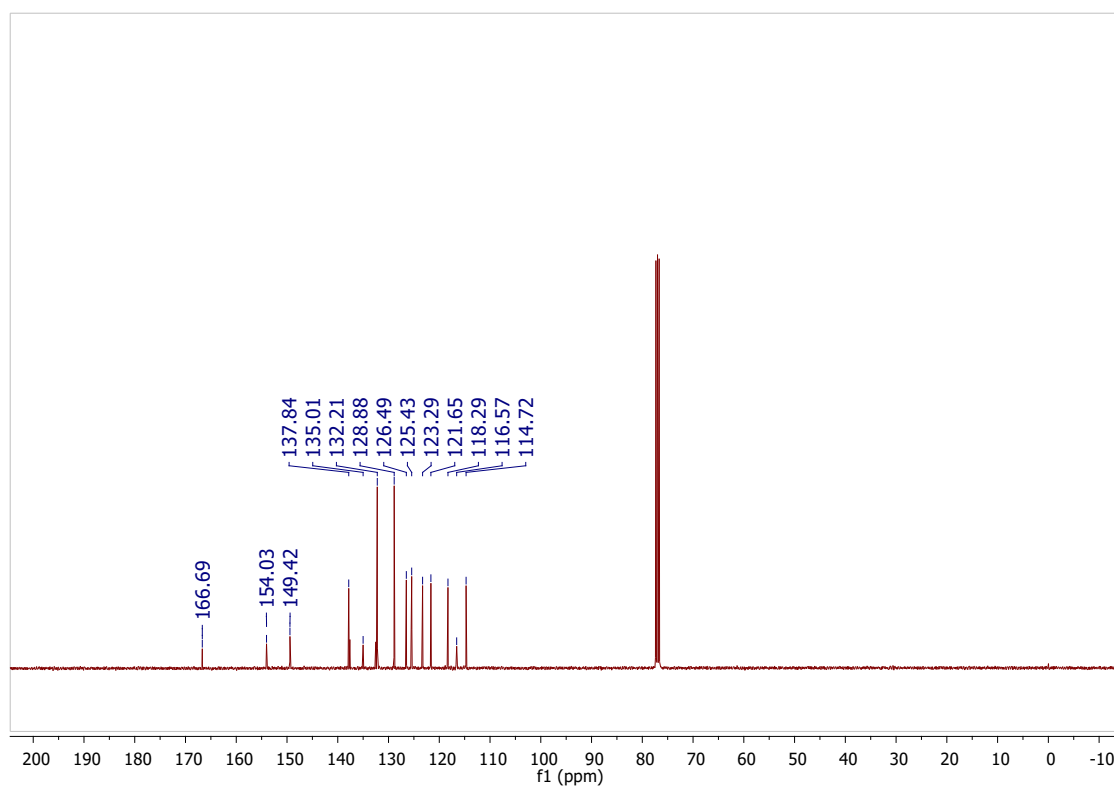
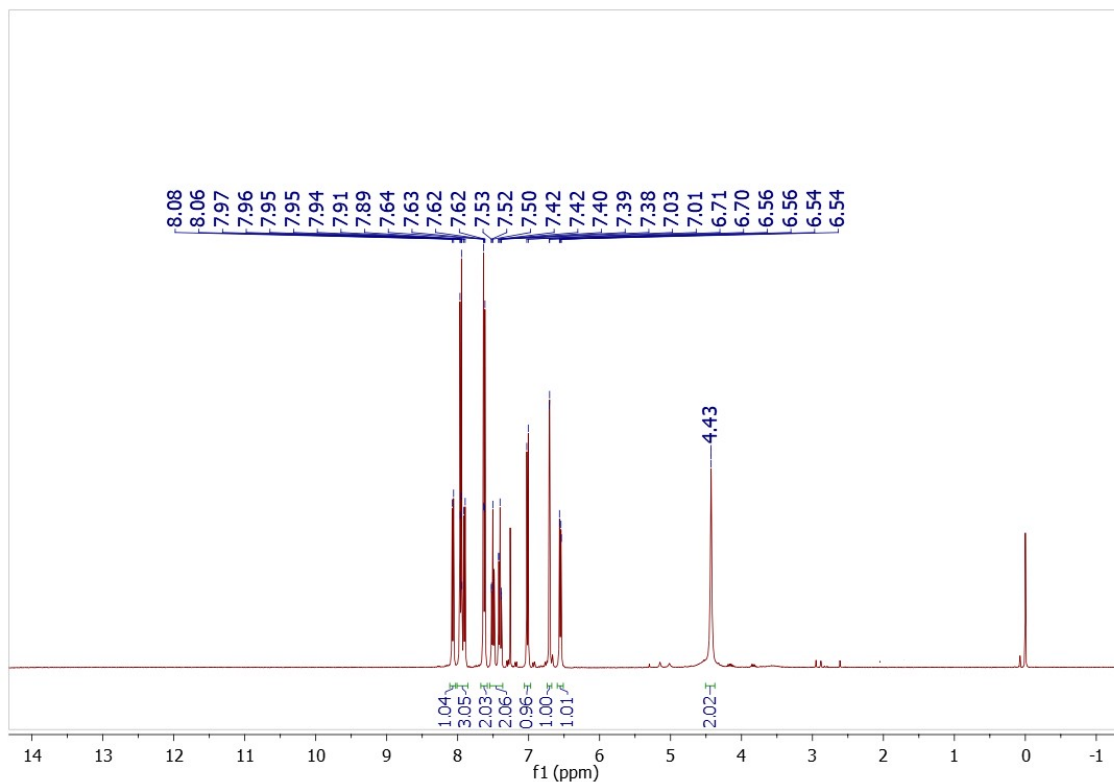
3l:



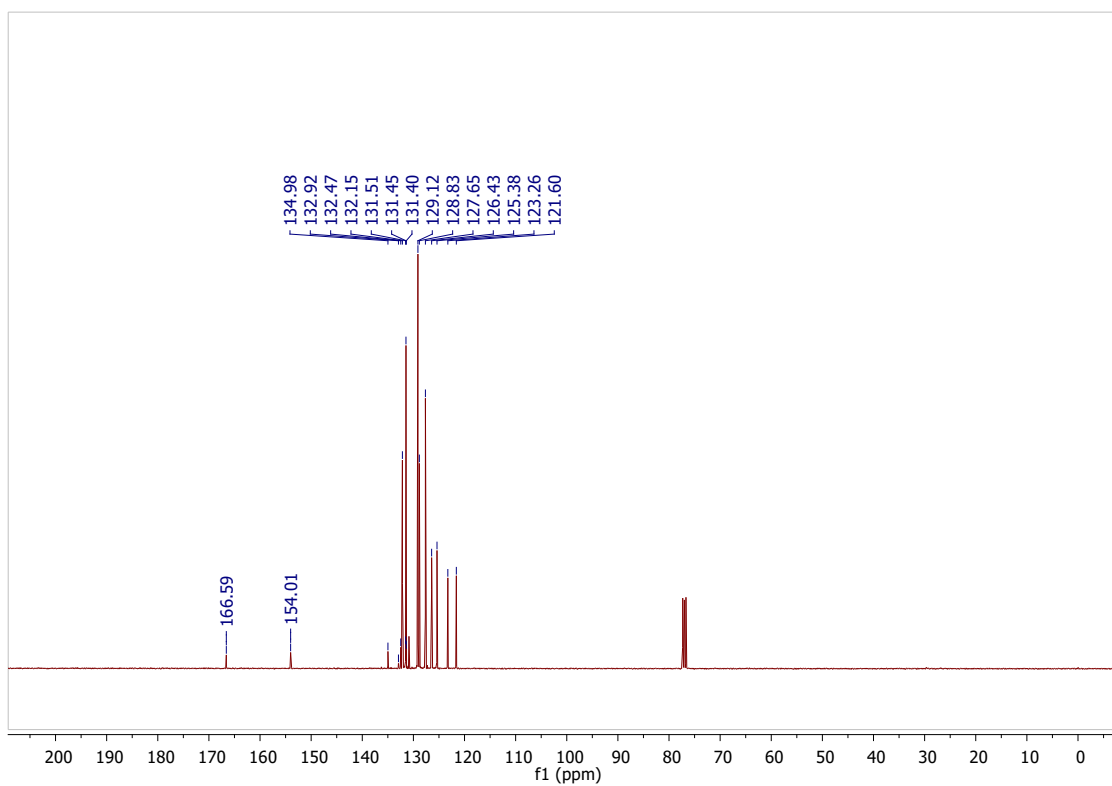
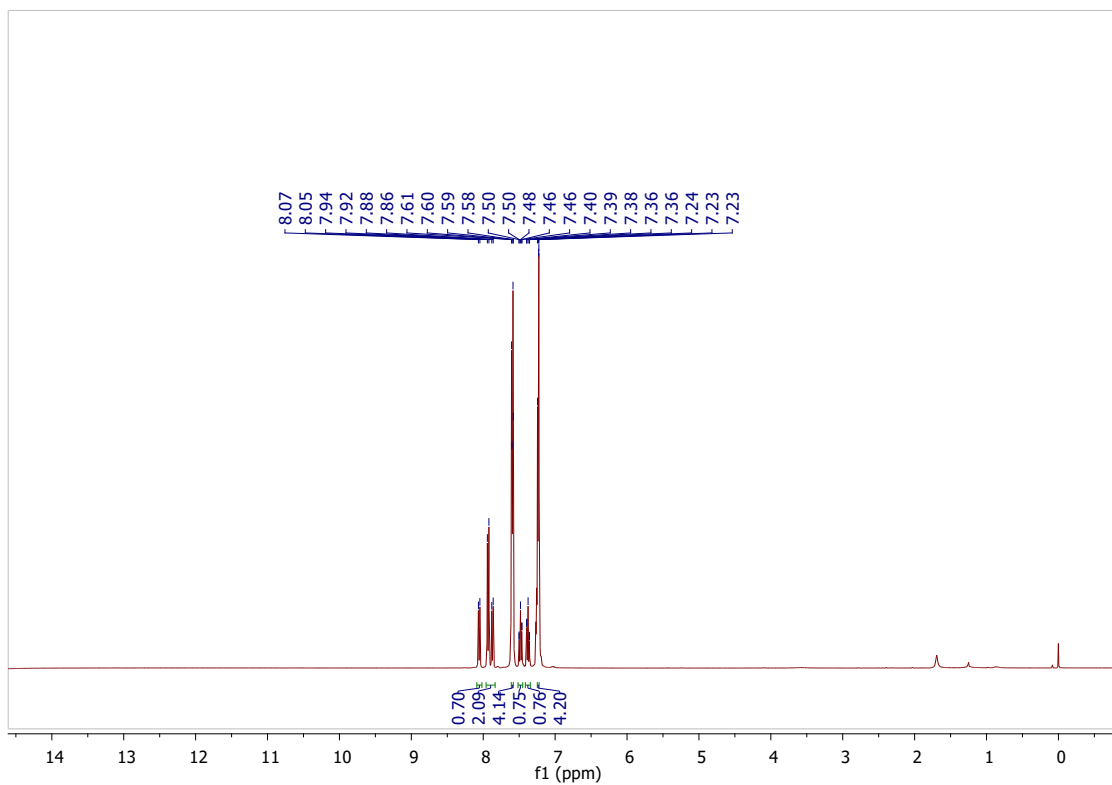
3m:



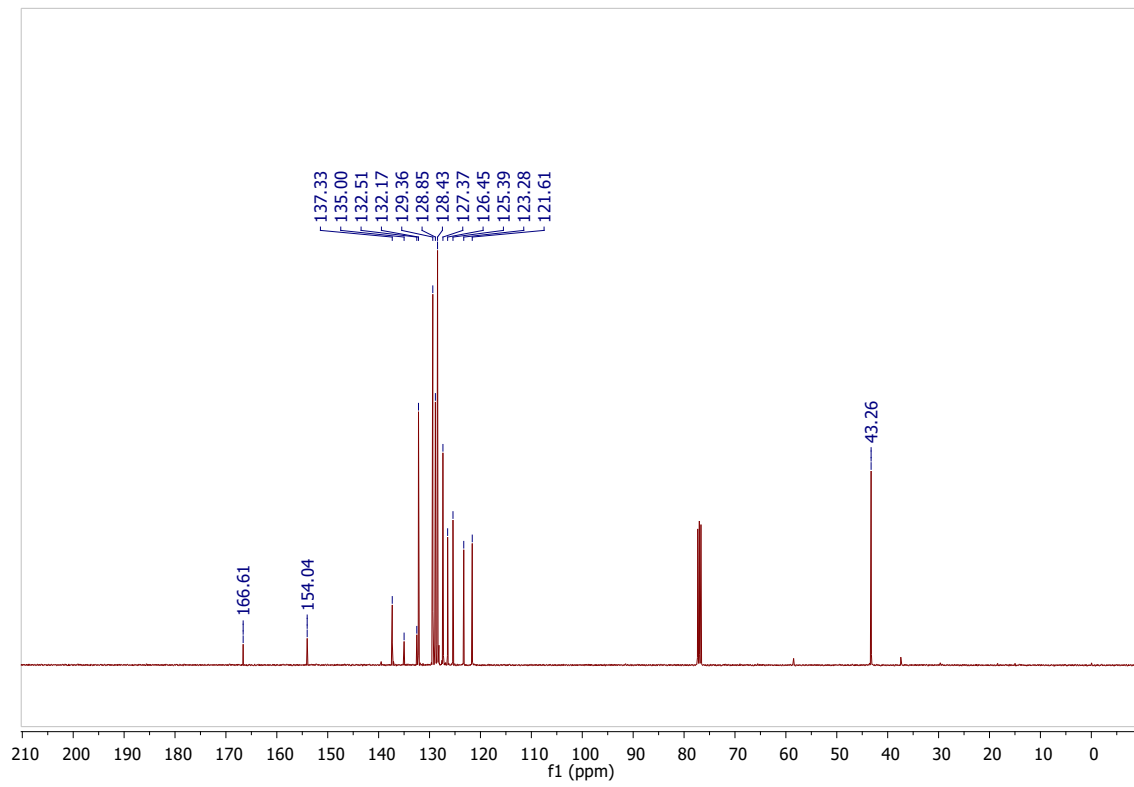
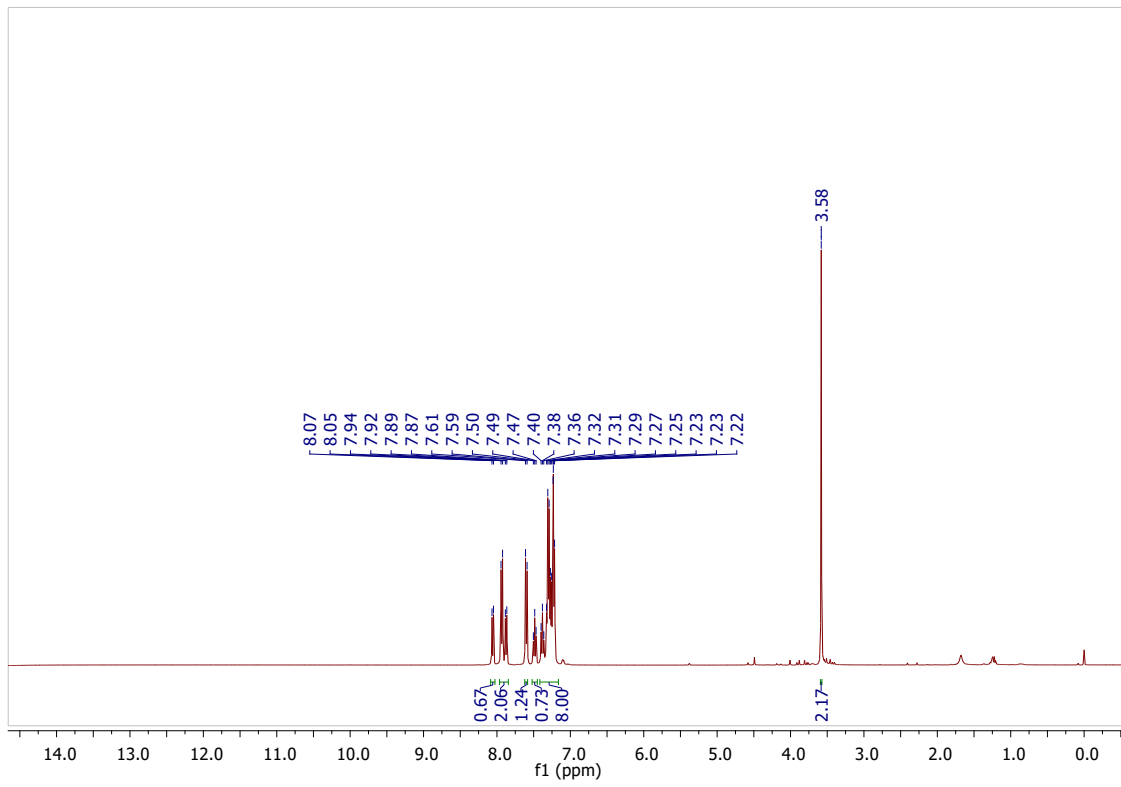
3n:



30:



3p:





3q:

