SUPPORTING INFORMATIONS

Synthesis of β-sulfinyl cyclobutane carboxylic amides via a formal α to β sulphoxide migration process

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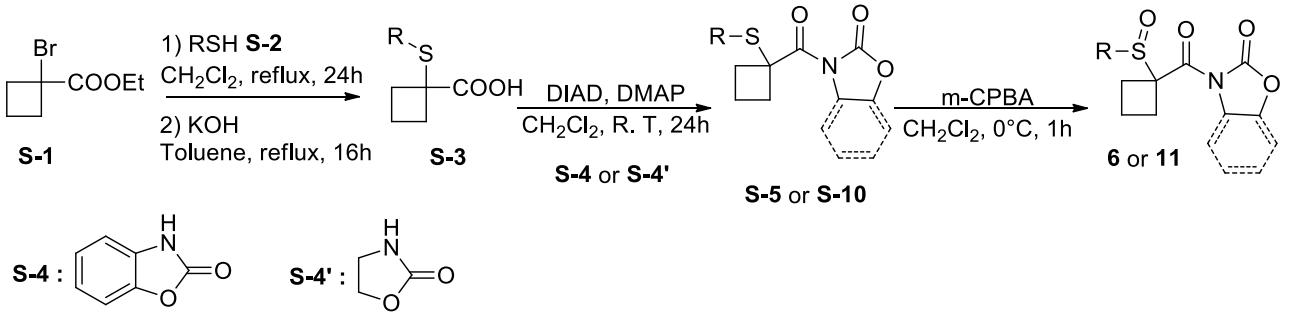
Table of Contents

General Methods

^{1}H NMR spectra were recorded on a Varian 500 and Bruker 600 spectrometers at ambient temperature with $CDCl_3$ as solvent. Data are reported as follows: chemical shifts (δ), multiplicity, coupling constants and integration. ^{13}C NMR spectra were recorded operating at 126 and 151 MHz at 27 °C with $CDCl_3$ as solvent. Infrared spectra were recorded on a FT–IR spectrophotometer. High resolution mass spectra (HRMS) were recorded on a spectrometer using Positive Electro Ionization (ESI) mode. Analytical thin layer chromatography was performed using 0.25 mm silica gel 60–F plates. Flash chromatography was performed using columns of 230 – 400 mesh silica gel 60 (0.040 – 0.063 mm).

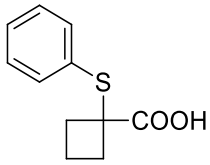
General Procedure for the synthesis of starting materials 6 and 11:



General Procedure for the synthesis of S-3

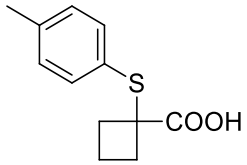
1) To a solution of thiol **S-2** (3.1 mmol) in ethanol (4 mL) was added potassium hydroxide (0.173 g, 3.1 mmol) slowly and the resulting suspension was heated at 60°C until all the potassium hydroxide was dissolved. The resulting solution was cooled to 0°C and ethyl 1-bromocyclobutanecarboxylate **S-1** (0.625 g, 3.1 mmol) was added dropwise. The mixture was then heated to reflux for 24 h before it was cooled to room temperature. Potassium bromide (white solid) was removed by filtration and the filtrate was concentrated under reduced pressure. The residue was dissolved in dichloromethane and the resulting solution was washed with water and brine, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The ethyl 1-(thio)cyclobutanecarboxylate derivative thus produced was pure enough for use in subsequent reactions.

2) Potassium hydroxide (0.755 g, 13.5 mmol) was dissolved in hot toluene (13 mL), and then the above crude ethyl 1-(thio)cyclobutanecarboxylate (3.1 mmol) was added. The mixture was refluxed for 16 h. After the mixture was cooled to 21°C, water (25 mL) was added, and the mixture was extracted with diethyl ether (15 mL) and ethyl acetate (15 mL). The aqueous phase was acidified with 1.0 M aqueous HCl to pH 1. The acidified aqueous layer was extracted with ethyl acetate, and the combined organic phases were washed with water and brine and dried over anhydrous Na_2SO_4. Flash column chromatography on silica gel, eluting with 1/1 petroleum ether/ethyl acetate, gave the corresponding acid. Yields refer to chromatographically pure materials.



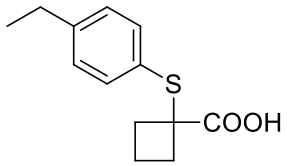
S-3a

1-(Phenylthio)cyclobutanecarboxylic acid **S-3a** –Yield 92% (0.58 g); white solid; m. p. = 56–59 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.47 (br s, 1H), 7.43 – 7.40 (m, 2H), 7.31 – 7.29 (m, 3H), 2.73 – 2.67 (m, 2H), 2.29 – 2.21 (m, 3H), 1.96 – 1.94 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 179.96, 133.33, 132.82, 129.05, 128.36, 52.90, 31.88, 15.99. **IR** (ATR) *cm^{-1}*: 2979, 2954, 1694, 1479, 1440, 1411, 1290, 1249, 1215, 1130, 922, 745, 690. **HRMS** (ESI) Calcd. for $C_{11}H_{13}O_2S$ ($M+H^+$) m/z 209,0485, found 209,0484.



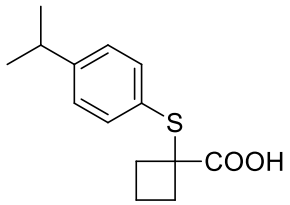
S-3b

1-(*p*-Tolylthio)cyclobutanecarboxylic acid **S-3b** – Yield 77% (0.52 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.07 (br s, 1H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 2.67 – 2.62 (m, 2H), 2.32 (s, 3H), 2.25 – 2.19 (m, 3H), 1.93 – 1.89 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.28, 138.91, 134.33, 129.82, 128.84, 53.10, 31.65, 21.31, 15.80. **IR** (ATR) *cm^{-1}*: 2962, 2870, 1699, 1408, 1292, 1251, 1212, 1130, 1053, 922, 828. **HRMS** (ESI) Calcd. for $C_{12}H_{15}O_2S$ ($M+H^+$) m/z 221,0642, found 221,0645.



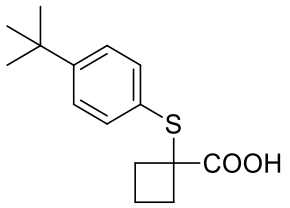
S-3c

1-((4-Ethylphenyl)thio)cyclobutanecarboxylic acid **S-3c** – Yield 70% (0.51 g); yellow solid; m. p. =54–57 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.1 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 2.70 – 2.61 (m, 4H), 2.27 – 2.20 (m, 3H), 1.97 – 1.91 (m, 1H), 1.22 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 179.84, 145.10, 134.20, 129.11, 128.65, 53.09, 31.70, 28.66, 15.87, 15.38. **IR** (ATR) *cm^{-1}*: 2966, 2875, 1696, 1495, 1408, 1295, 1249, 1210, 1128, 925, 830. **HRMS** (ESI) Calcd. for $C_{13}H_{17}O_2S$ ($M+H^+$) m/z 235,0798, found 235,0796.



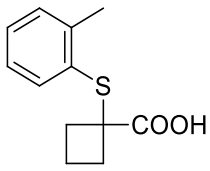
S-3d

1-((4-Isopropylphenyl)thio)cyclobutanecarboxylic acid **S-3d** – Yield 68% (0.52 g); white solid; m. p. = 66–68 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 11.27 (br s, 1H), 7.37 (d, *J* = 8.3 Hz, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 2.86 (hept, *J* = 6.9 Hz, 1H), 2.68 – 2.62 (m, 2H), 2.24 – 2.22 (m, 3H), 1.93 – 1.86 (m, 1H), 1.21 (d, *J* = 7.0 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.50, 149.42, 134.02, 129.26, 127.08, 52.89, 33.82, 31.58, 23.83, 15.74. **IR** (ATR) *cm^{-1}*: 2962, 2872, 1696, 1488, 1462, 1406, 1292, 1251, 1210, 1130, 1053, 927, 828. **HRMS** (ESI) Calcd. for $C_{14}H_{19}O_2S$ ($M+H^+$) m/z 249,0955, found 246,0951.



S-3e

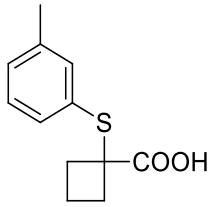
1-((4-(*Tert*-butyl)phenyl)thio)cyclobutanecarboxylic acid **S-3e** – Yield 66% (0.53 g); orange solid; m. p. = 75–79 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.48 (br s, 1H), 7.41 – 7.39 (m, 2H), 7.36 – 7.34 (m, 2H), 2.72 – 2.68 (m, 2H), 2.30 – 2.24 (m, 3H), 1.99 – 1.92 (m, 1H), 1.33 (s, *J* = 14.6 Hz, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.46, 151.72, 133.54, 129.12, 126.09, 52.89, 34.73, 31.70, 31.34, 15.87. **IR** (ATR) *cm^{-1}*: 2962, 2906, 2870, 1696, 1491, 1401, 1365, 1290, 1251, 1210, 1118, 927, 830, 755. **HRMS** (ESI) Calcd. for $C_{15}H_{21}O_2S$ ($M+H^+$) m/z 263,1111, found 263,1111.



S-3f

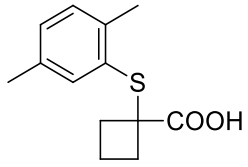
1-(*o*-Tolylthio)cyclobutanecarboxylic acid **S-3f** – Yield 79% (0.54 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.62 (br s, 1H), 7.28 – 7.26 (m, 1H), 7.19 – 7.09 (m, 3H), 2.76 – 2.70 (m, 2H), 2.41 (s, 3H), 2.30 – 2.20 (m, 3H), 1.98 – 1.91 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.42, 140.02, 132.63, 132.31, 130.53, 127.78, 126.49, 52.50, 32.07, 20.75, 16.28. **IR** (ATR) *cm^{-1}*: 2988, 2950, 2867,

1694, 1469, 1411, 1290, 1251, 1208, 1128, 1048, 927, 748, 698. **HRMS** (ESI) Calcd. for $C_{12}H_{15}O_2S$ ($M+H^+$) m/z 221,0642, found 221,0642.



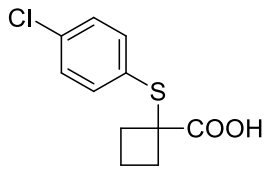
S-3g

1-(*m*-Tolylthio)cyclobutanecarboxylic acid **S-3g** – Yield 80% (0.54 g); white solid; m. p. = 62–68°C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.90 (br s, 1H), 7.24 – 7.16 (m, 3H), 7.11 (s, 1H), 2.70 – 2.65 (m, 2H), 2.31 (s, 3H), 2.28 – 2.17 (m, 3H), 1.96 – 1.91 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.20, 138.81, 134.04, 132.44, 130.37, 129.25, 128.86, 52.86, 31.82, 21.37, 15.95. **IR** (ATR) *cm^{-1}*: 2993, 2950, 2862, 1696, 1411, 1290, 1249, 1210, 1130,925, 779, 690. **HRMS** (ESI) Calcd. for $C_{12}H_{15}O_2S$ ($M+H^+$) m/z 221,0642, found 221,0644.



S-3h

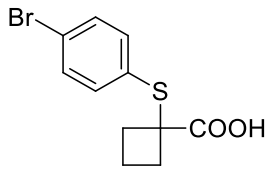
1-((2,5-Dimethylphenyl)thio)cyclobutanecarboxylic acid **S-3h** – Yield 72% (0.52 g); white solid; m. p. = 60–63 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.68 (s, 1H), 7.12 (s, 1H), 7.06 (d, *J* = 7.7 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 2.73 – 2.68 (m, 2H), 2.37 (s, 3H), 2.29 – 2.19 (m, 6H), 1.95 – 1.91 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.56, 137.29, 135.94, 133.62, 131.98, 130.34, 128.88, 52.62, 31.97, 20.90, 20.26, 16.20. **IR** (ATR) *cm^{-1}*: 2947, 2862, 1694, 1488, 1411, 1290, 1251, 1210, 1130, 925, 876, 811, 692. **HRMS** (ESI) Calcd. for $C_{13}H_{17}O_2S$ ($M+H^+$) m/z 235,0798, found 235,0795.



S-3i

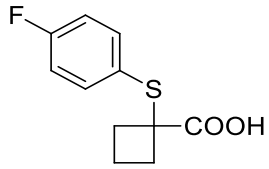
1-((4-Chlorophenyl)thio)cyclobutanecarboxylic acid **S-3i** – Yield 74% (0.55 g); yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.73 (br s, 1H), 7.35 (d, *J* = 8.6 Hz, 2H), 7.26 (d, *J* = 8.5 Hz, 2H), 2.72 – 2.66 (m, 2H), 2.26 – 2.20 (m, 3H), 1.98 – 1.90 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.22, 134.75, 134.68, 131.25, 129.19, 52.88, 31.77, 15.91. **IR** (ATR) *cm^{-1}*: 2995, 2947, 1696, 1479, 1411, 1389,

1295, 1249, 1212, 1130, 1096, 820. **HRMS** (ESI) Calcd. for $C_{11}H_{12}ClO_2S$ ($M+H^+$) m/z 241,0096, found 241,0098.



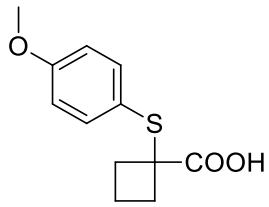
S-3j

1-((4-Bromophenyl)thio)cyclobutanecarboxylic acid **S-3j** – Yield 80% (0.7 g); yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 2.74 – 2.68 (m, 2H), 2.28 – 2.22 (m, 3H), 1.99 – 1.94 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 178.99, 134.67, 132.25, 132.02, 122.87, 52.81, 31.91, 16.04. **IR** (ATR) *cm^{-1}*: 2995, 2954, 2865, 1696, 1474, 1411, 1387, 1290, 1249, 1212, 1130, 1009, 816. **HRMS** (ESI) Calcd. for $C_{11}H_{12}BrO_2S$ ($M+H^+$) m/z 284,959, found 284,9587.



S-3k

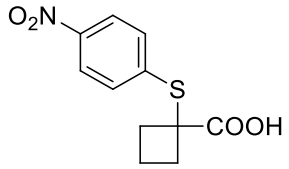
1-((4-Fluorophenyl)thio)cyclobutanecarboxylic acid **S-3k** – Yield 80% (0.55 g); white solid; m. p. = 76–80 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.94 (br s, 1H), 7.47 – 7.42 (m, 2H), 7.03 – 6.98 (m, 2H), 2.66 – 2.61 (m, 2H), 2.24 – 2.20 (m, 3H), 1.94 – 1.90 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.14, 163.39 (d, *J* = 249.5 Hz), 136.56 (d, *J* = 8.4 Hz), 127.62 (d, *J* = 3.3 Hz), 116.18 (d, *J* = 21.8 Hz), 53.25, 31.66, 15.79. **IR** (ATR) *cm^{-1}*: 2998, 2954, 1708, 1587, 1491, 1295, 1232, 1159, 835. **HRMS** (ESI) Calcd. for $C_{11}H_{12}FO_2S$ ($M+H^+$) m/z 225,0391, found 225,0387.



S-3l

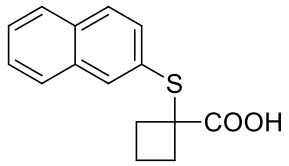
1-((4-Methoxyphenyl)thio)cyclobutanecarboxylic acid **S-3l** – Yield 98% (0.72 g); white solid; m. p. = 85–89 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 10.87 (br s, 1H), 7.43 (d, *J* = 8.9 Hz, 2H), 6.84 (d, *J* = 8.8 Hz, 2H), 3.78 (s, 3H), 2.62 – 2.59 (m, 2H), 2.23 – 2.17 (m, 3H), 1.91 – 1.88 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 180.35, 160.64, 136.99, 122.76, 114.57, 55.39, 53.45, 31.44, 15.65. **IR** (ATR)

cm^{-1}: 2995, 2945, 2836, 1701, 1595, 1493, 1411, 1290, 1254, 1174, 1033, 893, 830, 804. **HRMS** (ESI) Calcd. for $C_{12}H_{15}O_3S$ ($M+H^+$) m/z 237,0591, found 237,0594.



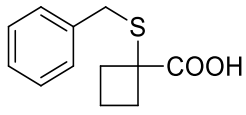
S-3m

1-((4-Nitrophenyl)thio)cyclobutanecarboxylic acid **S-3m** – (mix 75:25 of 2 rotamers according to NMR analysis in $CDCl_3$). Yield 47% (0.36 g); yellow solid; m. p. = 134–139 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.73 (br s, 1H), 8.12 (d, *J* = 8.8 Hz, 2H), 7.37 (d, *J* = 8.8 Hz, 2H), 2.92 – 2.87 (m, 2H), 2.36 – 2.31 (m, 3H), 2.09 – 2.05 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 179.06, 144.32, 128.75, 126.55, 124.13, 51.81, 32.16, 16.47. **IR** (ATR) *cm*$^{-1}$: 3102, 2995, 2954, 1701, 1597, 1580, 1515, 1479, 1401, 1341, 1285, 1217, 1089, 852. **HRMS** (ESI) Calcd. for $C_{11}H_{12}NO_4S$ ($M+H^+$) m/z 254,0482, found 254,0481.



S-3n

1-(Naphthalen-2-ylthio)cyclobutanecarboxylic acid **S-3n** – Yield 82% (0.65 g); yellow solid; m. p. = 122–127 °C. **^{1}H NMR** (500 MHz, CD_3OD) δ 7.88 (s, 1H), 7.79 – 7.73 (m, 3H), 7.44 – 7.42 (m, 3H), 2.70 – 2.64 (m, 2H), 2.26 – 2.15 (m, 3H), 1.91 – 1.86 (m, 1H). ^{13}C NMR (126 MHz, CD_3OD) δ 177.65, 134.92, 134.07, 133.06, 132.06, 131.10, 129.27, 128.62, 128.55, 127.54, 127.50, 54.37, 33.01, 16.68. **IR** (ATR) *cm*$^{-1}$: 3056, 2991, 2950, 1699, 1590, 1503, 1411, 1295, 1249, 1292, 1246, 1193, 1130, 857, 818, 745. **HRMS** (ESI) Calcd. for $C_{15}H_{15}O_2S$ ($M+H^+$) m/z 257,0642, found 257,0640.



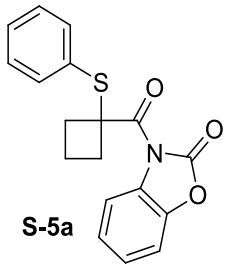
S-3o

1-(Benzylthio)cyclobutanecarboxylic acid **S-3o** – Yield 52% (0.35 g); white solid; m. p. = 95–97 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 9.86 (br s, 1H), 7.33 (d, *J* = 7.5 Hz, 2H), 7.30 – 7.27 (m, 2H), 7.23 – 7.20 (m, 1H), 3.82 (s, 2H), 2.69 – 2.64 (m, 2H), 2.19 – 2.12 (m, 3H), 1.93 – 1.90 (m, 1H). **^{13}C NMR**

(126 MHz, $CDCl_3$) δ 180.47, 137.32, 129.19, 128.55, 127.20, 50.49, 35.49, 31.71, 16.01. **IR** (ATR) *cm*$^{-1}$: 3029, 2988, 2950, 1689, 1495, 1411, 1295, 1256, 1210, 1125, 1072, 1026, 922, 796, 697. **HRMS** (ESI) Calcd. for $C_{12}H_{15}O_2S$ ($M+H^+$) m/z 221,0642, found 221,0639.

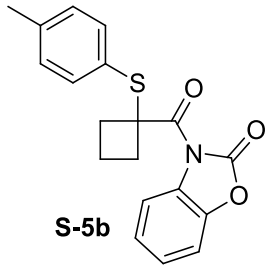
Procedure for the synthesis of S-5, S-10 and S-11

The carboxylic acid **S-3** (1.25 mmol), benzoxazolone **S-4** (0.152 g, 1.13 mmol) or oxazolidin-2-one **S-4'** (0.098 g, 1.13 mmol) or *p*-methoxyaniline (0.138 g, 1.13 mmol) and DMAP (0.023 g, 0.187 mmol) were dissolved in 2.5 mL of dry dichloromethane. Diisopropylcarbodimide (0.157 g, 1.25 mmol) was added and the resulting mixture was stirred for 24 h at room temperature. After completion of the reaction, the solid residue was filtered and washed with dichloromethane. The filtrate was washed with aqueous NH_4Cl, brine and dried over Na_2SO_4. The combined organic layer was concentrated in vacuo. The desired carboxylic amide was purified by column chromatography (silica gel, 5/1 petroleum ether/ethyl acetate). Yields refer to chromatographically pure materials.



S-5a

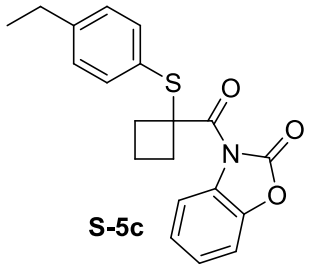
3-(1-(Phenylthio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5a** – Yield 64% (0.232 g); white solid; m. p. = 68–70 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 8.05 (m, 1H), 7.31 – 7.23 (m, 8H), 2.81 – 2.75 (m, 2H), 2.50 – 2.44 (m, 2H), 2.31 – 2.27 (m, 1H), 1.89 – 1.85 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.41, 149.84, 143.12, 134.43, 132.31, 128.99, 128.72, 128.65, 125.32, 124.77, 116.14, 110.03, 54.82, 31.38, 15.27. **IR** (ATR) *cm*$^{-1}$: 3124, 3058, 3005, 2952, 1800, 1704, 1479, 1312, 1287, 1254, 1145, 1026, 1002, 753. **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO_3S$ ($M+H^+$) m/z 326,0845, found 326,0844.



S-5b

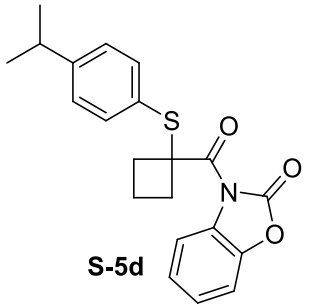
3-(1-(*p*-Tolylthio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5b** – Yield 63% (0.237 g); yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 8.08 (m, 1H), 7.30 – 7.25 (m, 3H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 2.79 – 2.73 (m, 2H), 2.50 – 2.45 (m, 2H), 2.36 – 2.27 (m, 1H), 2.34

(s, 3H), 1.92 – 1.84 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.36, 149.85, 143.14, 139.19, 135.19, 129.82, 128.76, 128.32, 125.28, 124.75, 116.14, 110.02, 55.07, 31.22, 21.32, 15.20. **IR** (ATR) *cm^{-1}*: 3020, 2950, 2920, 2870, 1800, 1704, 1600, 1479, 1350, 1307, 1285, 1249, 1145, 1024, 1002. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_3S$ ($M+H^+$) m/z 340,1002, found 340,0999.



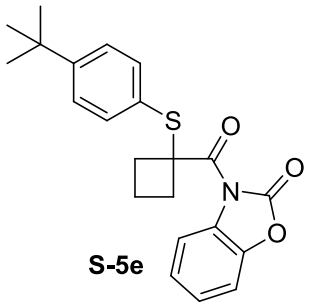
S-5c

3-(1-((4-Ethylphenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5c** – Yield 69% (0.272 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 8.04 (m, 1H), 7.27 – 7.21 (m, 5H), 7.09 (d, *J* = 7.9 Hz, 2H), 2.77 – 2.71 (m, 2H), 2.61 (q, *J* = 7.6 Hz, 2H), 2.48 – 2.42 (m, 2H), 2.29 (qt, *J* = 17.2, 8.6 Hz, 1H), 1.89 – 1.81 (m, 1H), 1.20 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.39, 149.82, 145.29, 143.11, 135.09, 128.74, 128.60, 128.56, 125.25, 124.72, 116.10, 109.99, 55.00, 31.23, 28.60, 15.28, 15.20. **IR** (ATR) *cm^{-1}*: 2964, 2933, 2872, 1803, 1706, 1479, 1348, 1309, 1290, 1251, 1145, 1024, 1002. **HRMS** (ESI) Calcd. for $C_{20}H_{20}NO_3S$ ($M+H^+$) m/z 354,1158, found 354,1156.



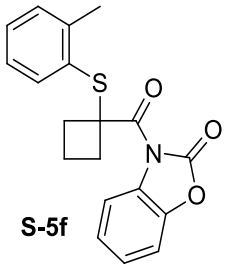
S-5d

3-(1-((4-Isopropylphenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5d** – Yield 62% (0.255 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 8.03 (m, 1H), 7.27 – 7.21 (m, 5H), 7.11 (d, *J* = 8.1 Hz, 2H), 2.89 – 2.83 (m, 1H), 2.78 – 2.72 (m, 2H), 2.47 – 2.43 (m, 2H), 2.33 – 2.24 (m, 1H), 1.89 – 1.81 (m, 1H), 1.21 (d, *J* = 7.0 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.49, 149.86, 149.82, 143.14, 134.96, 128.79, 128.77, 127.18, 125.27, 124.75, 116.12, 110.02, 54.98, 33.91, 31.30, 23.90, 15.23. **IR** (ATR) *cm^{-1}*: 2959, 2872, 1805, 1704, 1479, 1350, 1312, 1287, 1251, 1147, 1026, 1002. **HRMS** (ESI) Calcd. for $C_{21}H_{22}NO_3S$ ($M+H^+$) m/z 368,1315, found 368,1313.



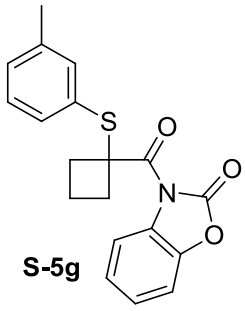
S-5e

3-(1-((4-(Tert-butyl)phenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5e** – Yield 60% (0.26 g); yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 8.03 (m, 1H), 7.28 – 7.21 (m, 7H), 2.79 – 2.73 (m, 2H), 2.46 (ddd, *J* = 13.6, 9.0, 4.4 Hz, 2H), 2.32 – 2.26 (m, 1H), 1.87 – 1.85 (m, 1H), 1.28 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.56, 152.03, 149.89, 143.16, 134.49, 128.79, 128.63, 126.08, 125.29, 124.77, 116.14, 110.04, 54.91, 34.76, 31.33 (2 C), 15.26. **IR** (ATR) *cm^{-1}*: 2959, 2906, 2870, 1803, 1704, 1479, 1350, 1307, 1285, 1251, 1142, 1024, 1002. **HRMS** (ESI) Calcd. for $C_{22}H_{24}NO_3S$ ($M+H^+$) m/z 382,1471, found 382,1472.



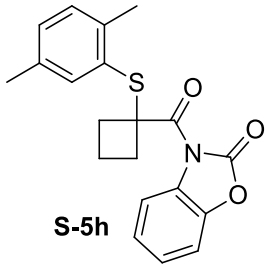
S-5f

3-(1-(*o*-Tolylthio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5f** – Yield 69% (0.26 g); white solid; m. p. = 72–74 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08 – 8.07 (m, 1H), 7.25 – 7.15 (m, 6H), 7.09 – 7.06 (m, 1H), 2.83 – 2.74 (m, 2H), 2.45 – 2.43 (m, 2H), 2.39 (s, 3H), 2.37 – 2.26 (m, 1H), 1.91 – 1.85 (m, 1H**). ^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.63, 149.89, 143.11, 141.61, 134.74, 131.89, 130.63, 128.71, 128.55, 126.41, 125.34, 124.81, 116.19, 110.04, 54.68, 31.33, 20.96, 15.53. **IR** (ATR) *cm^{-1}*: 3061, 3005, 2950, 1800, 1728, 1701, 1479, 1348, 1309, 1285, 1251, 1147, 1026, 1004. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_3S$ ($M+H^+$) m/z 338,0856, found 338,0855.



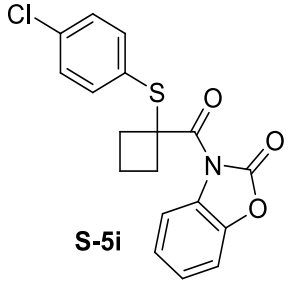
S-5g

3-(1-(*m*-Tolylthio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5g** – Yield 62% (0.235 g); yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 – 8.03 (m, 1H), 7.27 – 7.22 (m, 3H), 7.14 – 7.09 (m, 4H), 2.81 – 2.75 (m, 2H), 2.49 – 2.44 (m, 2H), 2.31 – 2.27 (m, 1H), 2.25 (s, 3H), 1.88 – 1.85 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.40, 149.83, 143.12, 138.74, 135.23, 131.84, 131.54, 129.56, 128.79, 128.74, 125.26, 124.72, 116.04, 110.01, 54.99, 31.35, 21.30, 15.26. **IR** (ATR) *cm^{-1}*: 2952, 2925, 2855, 1805, 1706, 1479, 1350, 1309, 1290, 1249, 1145, 1026, 1004. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_3S$ ($M+H^+$) m/z 340,1002, found 340,0980.



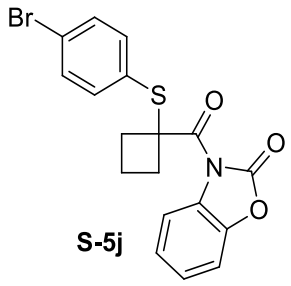
S-5h

3-(1-((2,5-Dimethylphenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5h** – Yield 50% (0.197 g); white solid; m. p. = 96–98 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08 – 8.06 (m, 1H), 7.27 – 7.23 (m, 3H), 7.08 (d, *J* = 7.6 Hz, 1H), 7.01 – 6.98 (m, 2H), 2.81 – 2.75 (m, 2H), 2.45 – 2.41 (m, 2H), 2.36 – 2.27 (m, 1H), 2.35 (s, 3H), 2.21 (s, 3H), 1.91 – 1.83 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.62, 149.92, 143.19, 138.86, 136.03, 135.92, 131.20, 130.47, 129.69, 128.81, 125.31, 124.80, 116.12, 110.07, 55.09, 31.34, 20.86, 20.49, 15.58. **IR** (ATR) *cm^{-1}*: 3015, 2952, 2920, 2865, 1803, 1704, 1479, 1348, 1307, 1285, 1254, 1145, 1027, 1002. **HRMS** (ESI) Calcd. for $C_{20}H_{20}NO_3S$ ($M+H^+$) m/z 354,1158, found 354,1156.



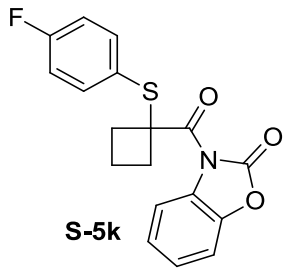
S-5i

3-(1-((4-Chlorophenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5i** – Yield 64% (0.255 g); white solid; m. p. = 95–97 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 8.04 (m, 1H), 7.27 – 7.22 (m, 7H), 2.81 – 2.72 (m, 2H), 2.47 – 2.42 (m, 2H), 2.31 – 2.23 (m, 1H), 1.90 – 1.84 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.15, 149.76, 143.05, 135.57, 135.02, 130.79, 129.18, 128.55, 125.40, 124.80, 116.08, 110.04, 54.77, 31.33, 15.21. **IR** (ATR) *cm^{-1}*: 3003, 2952, 1800, 1704, 1476, 1348, 1309, 1287, 1251, 1145, 1094, 1024, 1004. **HRMS** (ESI) Calcd. for $C_{18}H_{15}ClNO_3S$ ($M+H^+$) m/z 360,0456, found 360,0455.



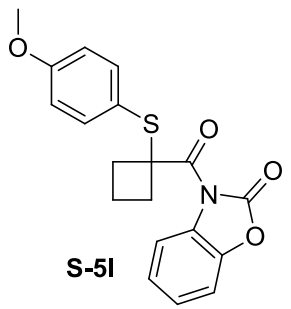
S-5j

3-(1-((4-Bromophenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5j** – Yield 76% (0.34 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 8.05 (m, 1H), 7.38 (d, *J* = 8.4 Hz, 2H), 7.28 – 7.23 (m, 3H), 7.16 (d, *J* = 8.4 Hz, 2H), 2.78 (dt, *J* = 13.8, 9.2 Hz, 2H), 2.45 – 2.43 (m, 2H), 2.31 – 2.22 (m, 1H), 1.91 – 1.83 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.20, 149.80, 143.09, 135.70, 132.16, 131.53, 128.58, 125.44, 124.84, 123.19, 116.13, 110.08, 54.69, 31.39, 15.25. **IR** (ATR) *cm^{-1}*: 3010, 2952, 1800, 1704, 1476, 1350, 1312, 1287, 1254, 1147, 1024, 1004. **HRMS** (ESI) Calcd. for $C_{18}H_{15}BrNO_3S$ ($M+H^+$) m/z 403,9951, found 403,9949.



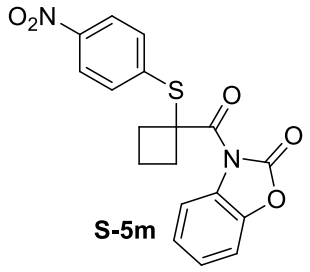
S-5k

3-(1-((4-Fluorophenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5k** – Yield 54% (0.207 g); white solid; m. p. = 81–83 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 8.05 (m, 1H), 7.31 – 7.23 (m, 5H), 6.98 – 6.95 (m, 2H), 2.77 – 2.71 (m, 2H), 2.46 – 2.41 (m, 2H), 2.32 – 2.23 (m, 1H), 1.90 – 1.82 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.18, 163.44 (d, *J* = 249.6 Hz), 149.83, 143.12, 137.21 (d, *J* = 8.4 Hz), 128.63, 127.20 (d, *J* = 3.4 Hz), 125.42, 124.84, 116.29, 116.12 (d, *J* = 0.9 Hz), 110.09, 55.11, 31.24, 15.18. **IR** (ATR) *cm^{-1}*: 3003, 2952, 2865, 1800, 1704, 1587, 1491, 1479, 1348, 1307, 1285, 1251, 1225, 1147, 1024, 1002. **HRMS** (ESI) Calcd. for $C_{18}H_{15}FNO_3S$ ($M+H^+$) m/z 344,0751, found 344,0752.



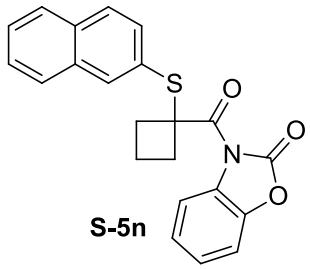
S-5l

3-(1-((4-Methoxyphenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5l** – Yield 75% (0.397 g); yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 – 8.03 (m, 1H), 7.25 – 7.22 (m, 5H), 6.79 (d, *J* = 8.8 Hz, 2H), 3.76 (s, 3H), 2.73 – 2.66 (m, 2H), 2.43 – 2.42 (m, 2H), 2.29 – 2.26 (m, 1H), 1.86 – 1.80 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.18, 160.64, 149.77, 143.07, 137.40, 128.69, 125.22, 124.69, 122.22, 116.05, 114.52, 109.96, 55.36, 55.33, 31.01, 15.09. **IR** (ATR) *cm^{-1}*: 2945, 2838, 1803, 1706, 1495, 1476, 1314, 1285, 1251, 1145, 1024, 1002. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 356,0951.



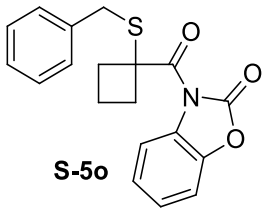
S-5m

3-(1-((4-Nitrophenyl)thio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5m** – Yield 49% (0.202 g); yellow solid; m. p. = 151–153 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.11 – 8.09 (m, 3H), 7.37 (d, *J* = 8.9 Hz, 2H), 7.29 – 7.23 (m, 3H), 3.04 – 2.98 (m, 2H), 2.61 – 2.56 (m, 2H), 2.31 – 2.29 (m, 1H), 2.00 – 1.97 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.06, 149.78, 146.37, 144.00, 143.06, 130.09, 128.38, 125.72, 124.99, 124.01, 116.25, 110.19, 53.79, 31.85, 15.48. **IR** (ATR) *cm^{-1}*: 3010, 2952, 1803, 1704, 1597, 1578, 1515, 1479, 1341, 1314, 1290, 1251, 1145, 1026, 1004. **HRMS** (ESI) Calcd. for $C_{18}H_{15}N_2O_5S$ ($M+H^+$) m/z 371,0696, found 371,0695.



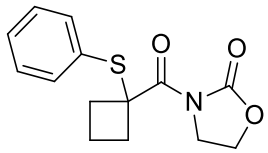
S-5n

3-(1-(Naphthalen-2-ylthio)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **S-5n** – Yield 71% (0.297 g); white solid; m. p. = 83–86 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.09 – 8.06 (m, 1H), 7.83 (s, 1H), 7.78 – 7.76 (m, 1H), 7.71 – 7.69 (m, 2H), 7.48 – 7.44 (m, 2H), 7.31 (d, *J* = 8.5 Hz, 1H), 7.28 – 7.22 (m, 3H), 2.81 (dt, *J* = 13.9, 9.2 Hz, 2H), 2.55 – 2.49 (m, 2H), 2.34 – 2.29 (m, 1H), 1.91 – 1.85 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.51, 149.94, 143.17, 133.98, 133.57, 133.00, 131.03, 129.77, 128.76, 128.54, 127.85, 127.78, 126.81, 126.62, 125.36, 124.81, 116.15, 110.08, 55.03, 31.48, 15.36. **IR** (ATR) *cm^{-1}*: 3058, 2951, 1819, 1803, 1704, 1479, 1349, 1312, 1286, 1252, 1145, 1027, 1003. **HRMS** (ESI) Calcd. for $C_{22}H_{18}NO_3S$ ($M+H^+$) m/z 376,1002, found 376,1002.



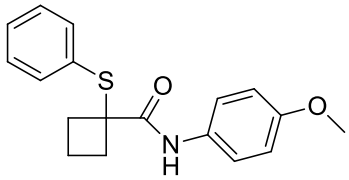
S-5o

3-(1-(Benzylthio)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **S-5o** – Yield 66% (0.25 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.89 – 7.88 (m, 1H), 7.23 – 7.15 (m, 5H), 7.11 – 7.08 (m, 2H), 7.05 – 7.04 (m, 1H), 3.65 (s, 2H), 2.85 (dt, *J* = 13.8, 9.4 Hz, 2H), 2.55 – 2.50 (m, 2H), 2.30 – 2.24 (m, 1H), 1.90 – 1.85 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.91, 149.51, 143.00, 137.15, 128.90, 128.53, 128.41, 127.02, 125.11, 124.46, 116.25, 109.76, 53.06, 34.28, 31.60, 15.46. **IR** (ATR) *cm^{-1}*: 3029, 3000, 2950, 1800, 1699, 1604, 1479, 1348, 1312, 1285, 1251, 1145, 1024, 1002. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_3S$ ($M+H^+$) m/z 340,1002, found 340,1003.



S-10

3-(1-(Phenylthio)cyclobutanecarbonyl)oxazolidin-2-one **S-10 –** Yield 63% (0.195 g); white solid; m. p. = 128–133 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.32 – 7.26 (m, 5H), 4.45 (t, *J* = 8.1 Hz, 2H), 4.07 (t, *J* = 8.0 Hz, 2H), 2.72 – 2.66 (m, 2H), 2.39 – 2.35 (m, 2H), 2.22 – 2.20 (m, 1H), 1.84 – 1.76 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.40, 152.11, 133.46, 133.32, 128.88, 128.04, 62.51, 53.58, 43.65, 31.67, 15.38. **IR** (ATR) *cm^{-1}*: 3057, 2957, 2928, 2859, 1776, 1680, 1476, 1446, 1388, 1361, 1313, 1219, 1150, 1121, 1042. **HRMS** (ESI) Calcd. for $C_{14}H_{16}NO_3S$ ($M+H^+$) m/z 278,0845, found 278,0842.



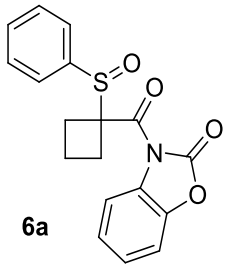
S-11

N-(4-methoxyphenyl)-1-(phenylthio)cyclobutanecarboxamide **S-11 –** Yield 71% (0.250 g); orange oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.33 (br s, 1H), 7.30 (d, *J* = 9.0 Hz, 2H), 7.22 – 7.17 (m, 2H), 7.15 (d, *J* = 7.3 Hz, 3H), 6.77 (d, *J* = 9.0 Hz, 2H), 3.71 (s, 3H), 2.88 (dt, *J* = 12.6, 9.4 Hz, 2H), 2.28 – 2.21 (m, 1H), 2.16 – 2.11 (m, 2H), 2.03 – 1.97 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.42, 156.63, 133.59, 131.08, 129.85, 129.37, 127.24, 121.74, 114.29, 55.64, 54.61, 31.69, 16.74. **IR** (ATR) *cm^{-1}*:

3330, 3059, 2993, 2952, 1666, 1512, 1439, 1244, 1181, 1035, 829, 743. **HRMS** (ESI) Calcd. for $C_{18}H_{20}NO_2S$ ($M+H^+$) m/z 314,1209, found 314,1209.

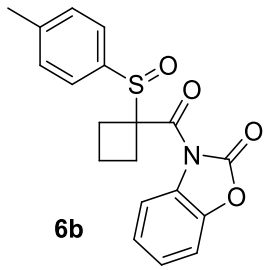
Procedure for the synthesis of 6, 10, 11 and 13

The α-sulfinyl cyclobutane carboxylic derivative **S-5** or **S-10** or **6a** or **S-11** (0.425 mmol) was dissolved in dichloromethane (2.6 mL) with 1 equiv of sodium bicarbonate (0.036 g). m-CPBA (0.066 g, 0.9 equiv.) was dissolved in dichloromethane (1.5 mL) in an addition funnel and added dropwise to the sulfide solution for 15 min at 0°C. The solution was then stirred for an additional 45 min. The product was washed with distilled water; the organic layer was dried over Na_2SO_4 and purified on a silica gel column using 1:1 petroleum ether/ethyl acetate. Yields refer to chromatographically pure materials.



6a

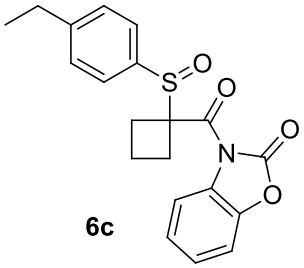
3-(1-(Phenylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6a** – Yield 80% (0.115 g); white solid; m. p. = 122–124 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 – 8.04 (m, 1H), 7.55 – 7.46 (m, 5H), 7.34 – 7.26 (m, 3H), 3.11 – 3.04 (m, 1H), 2.79 – 2.74 (m, 1H), 2.64 – 2.57 (m, 1H), 2.37 – 2.33 (m, 1H), 1.80 – 1.73 (m, 1H), 1.59 – 1.54 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.40, 150.12, 143.05, 139.82, 131.87, 128.95, 128.10, 126.02, 125.24, 125.17, 116.34, 110.32, 71.75, 25.91, 23.73, 14.81. **IR** (ATR) *cm^{-1}*: 3061, 3012, 2952, 1798, 1706, 1479, 1348, 1309, 1290, 1251, 1147, 1029, 1007. **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO_4S$ ($M+H^+$) m/z 342,0794, found 342,0798.



6b

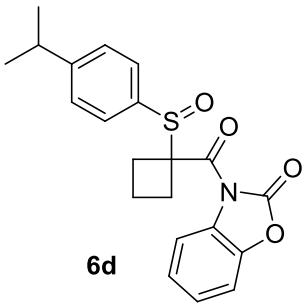
3-(1-(*p*-Polylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6b** – Yield 87% (0.131 g); orange oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 – 8.02 (m, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.26 (m, 5H), 3.07 – 3.04 (m, 1H), 2.76 – 2.75 (m, 1H), 2.63 – 2.57 (m, 1H), 2.40 (s, 3H), 2.36 – 2.35 (m, 1H), 1.79 – 1.74 (m, 1H), 1.58 – 1.55 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.52, 150.10, 143.05, 142.44, 136.51, 129.69, 125.98, 125.21, 125.14, 116.35, 110.30, 71.77, 71.77, 25.88, 23.71, 21.62,

14.82. **IR** (ATR) *cm*$^{-1}$: 3061, 3010, 2950, 1803, 1706, 1479, 1348, 1312, 1287, 1251, 1147, 1026, 1007. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 348,0647.



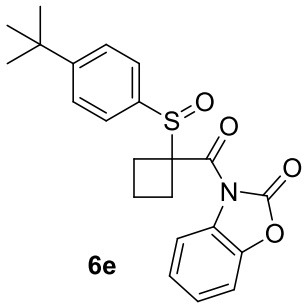
6c

3-(1-((4-Ethylphenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6c** – Yield 73% (0.114 g); white solid; m. p. = 87–90 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 – 8.03 (m, 1H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.26 (m, 5H), 3.08 – 3.05 (m, 1H), 2.78 – 2.75 (m, 1H), 2.70 (q, *J* = 7.6 Hz, 2H), 2.65 – 2.58 (m, 1H), 2.38 – 2.35 (m, 1H), 1.78 – 1.74 (m, 1H), 1.62 – 1.56 (m, 1H), 1.25 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.55, 150.13, 148.64, 143.06, 136.70, 128.52, 128.15, 125.98, 125.33, 125.15, 116.36, 110.31, 71.75, 28.90, 25.86, 23.84, 15.30, 14.84. **IR** (ATR) *cm*$^{-1}$: 3058, 2964, 2877, 1798, 1706, 1479, 1348, 1309, 1287, 1254, 1145, 1029, 1006. **HRMS** (ESI) Calcd. for $C_{20}H_{20}NO_4S$ ($M+H^+$) m/z 370,1107, found 370,1105.



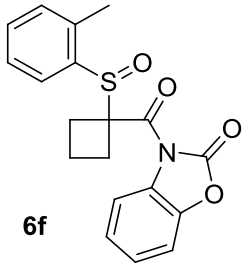
6d

3-(1-((4-Isopropylphenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6d** – Yield 75% (0.122 g); yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.05 – 8.03 (m, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.33 – 7.27 (m, 5H), 3.07 – 3.03 (m, 1H), 2.98 – 2.92 (m, 1H), 2.80 – 2.75 (m, 1H), 2.65 – 2.59 (m, 1H), 2.39 – 2.36 (m, 1H), 1.80 – 1.74 (m, 1H), 1.58 – 1.54 (m, 1H), 1.26 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.48, 153.21, 150.08, 143.01, 136.77, 128.10, 127.09, 125.92, 125.34, 125.08, 116.29, 110.24, 71.69, 34.17, 25.82, 23.86, 23.80, 14.80. **IR** (ATR) *cm*$^{-1}$: 3061, 2962, 2870, 1798, 1706, 1479, 1348, 1309, 1290, 1251, 1145, 1029, 1002. **HRMS** (ESI) Calcd. for $C_{21}H_{22}NO_4S$ ($M+H^+$) m/z 384.1264, found 384.1264.



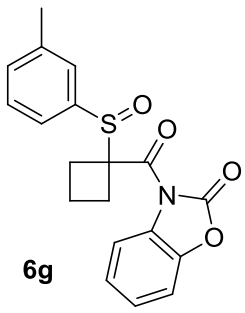
6e

3-(1-((4-(*Tert*-butyl)phenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6e** – Yield 75% (0.126 g); white solid; m. p. = 120–122 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 8.02 (m, 1H), 7.49 – 7.47 (m, 4H), 7.32 – 7.26 (m, 3H), 3.07 – 3.05 (m, 1H), 2.79 – 2.76 (m, 1H), 2.65 – 2.59 (m, 1H), 2.40 – 2.37 (m, 1H), 1.80 – 1.74 (m, 1H), 1.57 – 1.54 (m, 1H), 1.32 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.35, 155.38, 149.98, 142.88, 136.32, 127.99, 125.87, 125.84, 124.99 (2 C), 116.17, 110.14, 71.53, 35.03, 31.18, 25.72, 23.87, 14.72. **IR** (ATR) *cm^{-1}*: 3061, 2959, 2870, 1798, 1706, 1479, 1348, 1307, 1290, 1251, 1147, 1029, 1004. **HRMS** (ESI) Calcd. for $C_{22}H_{24}NO_4S$ ($M+H^+$) m/z 398,1420, found 398,1418.



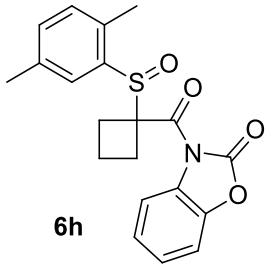
6f

3-(1-(*o*-Tolylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6f** – Yield 84% (0.126 g); white solid; m. p. = 110–113 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.88 – 7.86 (m, 1H), 7.39 – 7.36 (m, 2H), 7.32 – 7.29 (m, 1H), 7.27 – 7.24 (m, 2H), 7.11 – 7.09 (m, 1H), 3.21 (dt, *J* = 13.6, 9.1 Hz, 1H), 2.87 (dt, *J* = 12.7, 9.3 Hz, 1H), 2.74 – 2.69 (m, 1H), 2.38 (ddd, *J* = 12.8, 8.3, 4.0 Hz, 1H), 2.11 (s, 3H), 1.85 – 1.76 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 168.50, 149.94, 142.94, 138.51, 136.28, 131.57, 130.85, 127.94, 126.67, 126.00, 125.79, 125.13, 116.32, 110.25, 71.87, 28.58, 22.46, 18.23, 15.27. **IR** (ATR) *cm^{-1}*: 3061, 2954, 1800, 1706, 1479, 1350, 1312, 1287, 1251, 1145, 1031, 1004. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 356,0949.



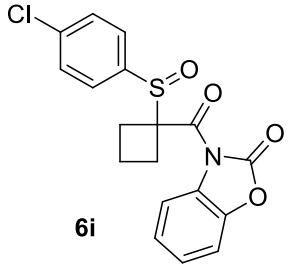
6g

3-(1-(*m*-Tolylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6g** – Yield 98% (0.147 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03 – 8.01 (m, 1H), 7.36 – 7.27 (m, 7H), 3.07 (dt, *J* = 13.5, 9.2 Hz, 1H), 2.79 – 2.77 (m, 1H), 2.66 – 2.60 (m, 1H), 2.39 – 2.35 (m, 1H), 2.34 (s, 3H), 1.83 – 1.74 (m, 1H), 1.63 – 1.57 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.30, 150.07, 143.03, 139.54, 139.13, 132.72, 128.76, 128.09, 125.99, 125.38, 125.13, 122.32, 116.24, 110.31, 71.72, 26.12, 23.40, 21.48, 14.83. **IR** (ATR) *cm^{-1}*: 3012, 2950, 1800, 1706, 1479, 1350, 1309, 1287, 1251, 1145, 1053, 1029, 1004. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 356,0950.



6h

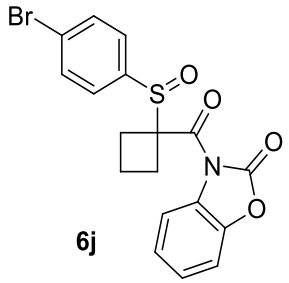
3-(1-((2,5-Dimethylphenyl)sulfinyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **6h** – Yield 81% (0.127 g); white solid; m. p. = 153–155 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.02 – 8.01 (m, 1H), 7.66 (s, 1H), 7.34 – 7.25 (m, 3H), 7.18 (d, *J* = 7.7 Hz, 1H), 7.00 (d, *J* = 7.7 Hz, 1H), 3.22 (dt, *J* = 13.7, 9.1 Hz, 1H), 2.90 (dt, *J* = 12.9, 9.4 Hz, 1H), 2.77 – 2.72 (m, 1H), 2.45 – 2.39 (m, 1H), 2.37 (s, 3H), 2.08 (s, 3H), 1.87 – 1.80 (m, 2H). **^{13}C NMR** (126 MHz $CDCl_3$) δ 168.55, 149.96, 142.99, 138.05, 136.63, 133.23, 132.57, 130.82, 128.03, 125.99, 125.89, 125.14, 116.38, 110.26, 71.84, 28.68, 22.66, 21.19, 17.82, 15.34. **IR** (ATR) *cm^{-1}*: 3063, 2954, 1803, 1696, 1479, 1348, 1310, 1290, 1251, 1145, 1033, 1007. **HRMS** (ESI) Calcd. for $C_{20}H_{20}NO_4S$ ($M+H^+$) m/z 370,1107, found 370,1108.



6i

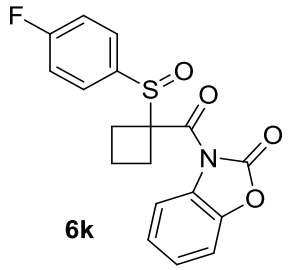
3-(1-((4-Chlorophenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6i** – Yield 77% (0.122 g); white solid; m. p. = 153–156 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.46 (m, 4H), 7.34 – 7.29 (m, 3H), 3.08 – 3.02 (m, 1H), 2.78 – 2.75 (m, 1H), 2.57 – 2.51 (m, 1H), 2.37 – 2.34 (m, 1H), 1.82 – 1.77 (m, 1H), 1.61 – 1.56 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.25, 150.14, 143.04, 138.34, 138.27, 129.31, 127.99, 126.66, 126.15, 125.27, 116.34, 110.39, 71.84, 25.77, 23.95, 14.79. **IR** (ATR) *cm^{-1}*: 3058, 2954, 1798, 1706, 1476, 1348, 1312, 1287, 1254,

1145, 1079, 1031, 1004. **HRMS** (ESI) Calcd. for $C_{18}H_{15}ClNO_4S$ ($M+H^+$) m/z 376,0404, found 376,0401.



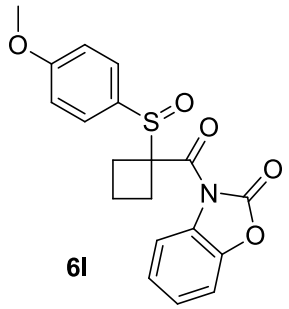
6j

3-(1-((4-Bromophenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6j** – Yield 77% (0.136 g); white solid; m. p. = 154–156 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 8.05 (m, 1H), 7.65 – 7.61 (m, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.35 – 7.27 (m, 3H), 3.07 – 3.01 (m, 1H), 2.79 – 2.74 (m, 1H), 2.56 – 2.50 (m, 1H), 2.38 – 2.34 (m, 1H), 1.82 – 1.75 (m, 1H), 1.60 – 1.56 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.19, 150.10, 143.00, 138.97, 132.19, 127.96, 126.79, 126.56, 126.13, 125.24, 116.30, 110.36, 71.74, 25.76, 23.88, 14.77. **IR** (ATR) *cm^{-1}*: 3056, 2981, 2889, 1800, 1706, 1479, 1348, 1312, 1251, 1145, 1055, 1031, 1007. **HRMS** (ESI) Calcd. for $C_{18}H_{15}BrNO_4S$ ($M+H^+$) m/z 419,9899, found 419,9890.



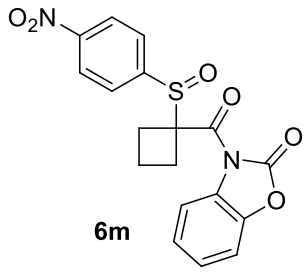
6k

3-(1-((4-Fluorophenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6k** – Yield 74% (0.113 g); white solid; m. p. = 135–138 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.55 (m, 2H), 7.33 – 7.27 (m, 3H), 7.20 – 7.17 (m, 2H), 3.03 – 3.01 (m, 1H), 2.78 – 2.76 (m, 1H), 2.55 – 2.53 (m, 1H), 2.38 – 2.35 (m, 1H), 1.83 – 1.74 (m, 1H), 1.57 – 1.54 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.26, 164.93 (d, *J* = 252.5 Hz), 150.07, 142.96, 135.18 (d, *J* = 3.0 Hz), 127.95, 127.49 (d, *J* = 8.9 Hz), 126.05, 125.17, 116.43, 116.25, 110.30, 71.78, 25.65, 23.89, 14.70. **IR** (ATR) *cm^{-1}*: 3063, 3012, 2950, 1795, 1706, 1590, 1479, 1350, 1312, 1251, 1145, 1053, 1029, 1007. **HRMS** (ESI) Calcd. for $C_{18}H_{15}FNO_4S$ ($M+H^+$) m/z 360,0700, found 360,0700.



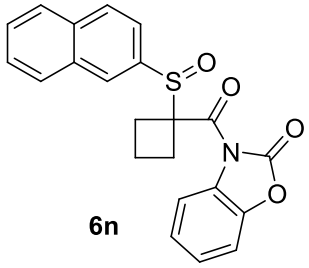
6l

3-(1-((4-Methoxyphenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6l** – Yield 98% (0.154 g); white solid; m. p. = 134–136 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 8.02 (m, 1H), 7.49 (d, *J* = 8.7 Hz, 2H), 7.32 – 7.26 (m, 3H), 6.98 (d, *J* = 8.8 Hz, 2H), 3.84 (s, 3H), 3.02 (dt, *J* = 13.5, 9.2 Hz, 1H), 2.78 – 2.75 (m, 1H), 2.61 (ddd, *J* = 13.1, 10.0, 9.0 Hz, 1H), 2.39 – 2.38 (m, 1H), 1.77 (ddd, *J* = 19.0, 9.5, 1.6 Hz, 1H), 1.58 – 1.52 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.51, 162.60, 150.05, 142.95, 130.40, 128.04, 126.96, 125.89, 125.06, 116.26, 114.48, 110.20, 71.82, 55.56, 25.46, 23.94, 14.72. **IR** (ATR) *cm^{-1}*: 3058, 3010, 2945, 2838, 1795, 1706, 1592, 1495, 1479, 1348, 1307, 1249, 1145, 1082, 1026, 1002. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_5S$ ($M+H^+$) m/z 372,0900, found 372,0901.



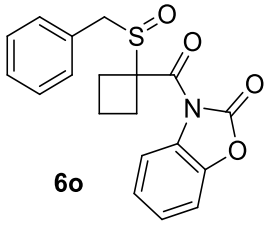
6m

3-(1-((4-Nitrophenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **6m** – Yield 85% (0.139 g); yellow solid; m. p. = 140–144 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.7 Hz, 2H), 8.09 – 8.07 (m, 1H), 7.72 (d, *J* = 8.6 Hz, 2H), 7.37 – 7.31 (m, 3H), 3.12 (dd, *J* = 22.8, 9.3 Hz, 1H), 2.78 (td, *J* = 9.6, 4.7 Hz, 1H), 2.53 – 2.47 (m, 1H), 2.34 (td, *J* = 9.5, 4.7 Hz, 1H), 1.87 – 1.78 (m, 1H), 1.65 – 1.63 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.90, 150.21, 150.14, 147.55, 143.09, 127.86, 126.46, 126.44, 125.48, 123.99, 116.37, 110.57, 72.12, 29.85, 14.92. **IR** (ATR) *cm^{-1}*: 3102, 3017, 2918, 2850, 1798, 1706, 1527, 1479, 1348, 1312, 1254, 1145, 1031, 1004. **HRMS** (ESI) not stable.



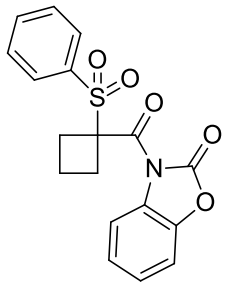
6n

3-(1-(Naphthalen-2-ylsulfinyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **6n** – Yield 97% (0.16 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.93 (d, *J* = 7.7 Hz, 1H), 7.80 (t, *J* = 8.6 Hz, 2H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.44 (m, 2H), 7.40 (d, *J* = 8.4 Hz, 1H), 7.24 – 7.17 (m, 3H), 3.04 (dd, *J* = 15.7, 6.8 Hz, 1H), 2.74 – 2.70 (m, 1H), 2.69 – 2.54 (m, 1H), 2.25 (dd, *J* = 12.9, 4.7 Hz, 1H), 1.70 – 1.65 (m, 1H), 1.49 – 1.47 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.36, 150.15, 143.03, 137.06, 134.88, 132.67, 128.89, 128.69, 128.14, 128.08, 127.35, 126.02, 126.01, 125.15, 120.90, 116.27, 110.31, 71.90, 25.97, 23.76, 14.83. **IR** (ATR) *cm^{-1}*: 3056, 3012, 2950, 1800, 1708, 1479, 1348, 1309, 1287, 1249, 1145, 1029, 1000. **HRMS** (ESI) Calcd. for $C_{22}H_{18}NO_4S$ ($M+H^+$) m/z 392,0951, found 392,0948.



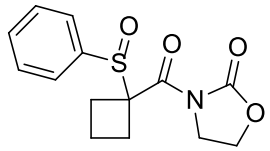
6o

3-(1-(Benzylsulfinyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **6o** – Yield 70% (0.105 g); white solid; m. p. = 103–105 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.88 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.28 – 7.17 (m, 5H), 7.14 (t, *J* = 7.4 Hz, 2H), 7.09 – 7.06 (m, 1H), 3.84 (d, *J* = 13.2 Hz, 1H), 3.76 (d, *J* = 13.2 Hz, 1H), 3.21 (dt, *J* = 13.7, 9.4 Hz, 1H), 3.06 – 3.02 (m, 1H), 2.97 – 2.93 (m, 1H), 2.66 – 2.63 (m, 1H), 2.00 – 1.95 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.44, 149.63, 142.79, 130.05, 129.74, 128.87, 128.21, 127.75, 125.88, 124.74, 116.44, 110.03, 69.10, 54.92, 28.41, 21.72, 15.56. **IR** (ATR) *cm^{-1}*: 3061, 3034, 3008, 2947, 1798, 1699, 1476, 1348, 1309, 1287, 1251, 1145, 1048, 1029, 1007. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 356,0951.



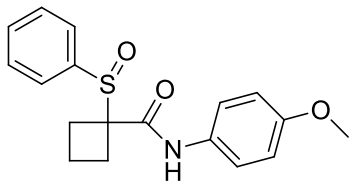
10

3-(1-(phenylsulfonyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **10** – Yield 81% (0.123 g); white semi-solid; **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 8.04 (m, 1H), 7.81 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.68 – 7.64 (m, 1H), 7.53 – 7.50 (m, 2H), 7.32 – 7.26 (m, 2H), 7.25 – 7.22 (m, 1H), 3.02 – 2.94 (m, 2H), 2.92 – 2.88 (m, 2H), 2.15 – 2.09 (m, 1H), 1.85 – 1.79 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 167.68, 149.38, 143.01, 136.57, 134.34, 129.73, 129.11, 128.29, 126.01, 124.94, 116.21, 110.23, 73.28, 30.08, 15.42. **IR** (ATR) *cm^{-1}*: 2961, 1816, 1701, 1476, 1357, 1316, 1251, 1149, 1079, 1031, 754, 690, 548. **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO_5S$ ($M+H^+$) m/z 358,0743, found 358,0744.



11

3-(1-(Phenylsulfinyl)cyclobutanecarbonyl)oxazolidin-2-one **11** – Yield 74% (0.092 g); white solid; m. p. = 134–139 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.60 – 7.49 (m, 5H), 4.53 (t, *J* = 8.1 Hz, 2H), 4.16 (dt, *J* = 11.1, 8.0 Hz, 1H), 4.14 – 4.04 (m, 1H), 2.93 – 2.90 (m, 1H), 2.69 – 2.60 (m, 1H), 2.50 – 2.47 (m, 1H), 2.28 – 2.27 (m, 1H), 1.73 – 1.64 (m, 1H), 1.45 – 1.40 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.98, 152.39, 140.01, 131.62, 128.75, 125.22, 70.46, 62.83, 43.57, 25.35, 24.33, 14.72. **IR** (ATR) *cm^{-1}*: 3057, 2955, 1775, 1680, 1476, 1444, 1386, 1361, 1311, 1219, 1121, 1082, 1042. **HRMS** (ESI) Calcd. for $C_{14}H_{16}NO_4S$ ($M+H^+$) m/z 294,0795, found 294,0796.



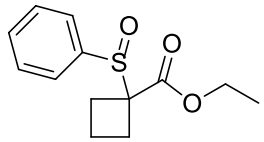
13

N-(4-methoxyphenyl)-1-(phenylsulfinyl)cyclobutanecarboxamide **13** – Yield 65% (0.090 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.56 (br s, 1H), 7.48 – 7.46 (m, 2H), 7.41 – 7.35 (m, 1H), 7.33 – 7.19 (m, 4H), 6.77 – 6.76 (m, 2H), 3.71 (s, 3H), 2.92 – 2.86 (m, 1H), 2.83 – 2.77 (m, 1H), 2.57 – 2.51 (m, 1H), 2.22 – 2.12 (m, 2H), 2.10 – 2.03 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 166.20, 156.50, 138.82, 132.10, 131.10, 129.28, 124.91, 121.83, 114.27, 64.95, 55.59, 29.66, 24.15, 15.91. **IR** (ATR) *cm^{-1}*: 3773 2917 2958 1676 1602 1513 1454 1413 1240 1033 831 786. **HRMS** (ESI) Calcd. for $C_{18}H_{20}NO_3S$ ($M+H^+$) m/z 330,1158, found 330,1158.

Procedure for the synthesis of 12

1) To a solution of benzenethiol (0.170 g, 1.55 mmol) in ethanol (2 mL) was added potassium hydroxide (0.0865 g, 1.55 mmol) slowly and the resulting suspension was heated at 60°C until all the potassium hydroxide was dissolved. The resulting solution was cooled to 0°C and ethyl 1-bromocyclobutanecarboxylate **S-1** (0.312 g, 1.55 mmol) was added dropwise. The mixture was then heated to reflux for 24 h before it was cooled to room temperature. Potassium bromide (white solid) was removed by filtration and the filtrate was concentrated under reduced pressure. The residue was dissolved in dichloromethane and the resulting solution was washed with water and brine, dried over anhydrous sodium sulfate, and concentrated under reduced pressure. The residue was purified by flash chromatography (5:1 petroleum ether/ethyl acetate) to afford the corresponding ethyl 1-(phenylthio)cyclobutanecarboxylate derivative – Yield 81% (0.315 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.40 – 7.38 (m, 2H), 7.31 – 7.26 (m, 3H), 4.13 (q, *J* = 7.1 Hz, 2H), 2.69 – 2.66 (m, 2H), 2.26 – 2.23 (m, 3H), 1.92 – 1.88 (m, 1H), 1.19 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 174.13, 133.39, 133.27, 128.89, 128.10, 61.37, 53.13, 32.22, 16.10, 14.21. **IR** (ATR) *cm^{-1}*: 2983, 2950, 1728, 1713, 1442, 1287, 1208, 1128, 1082, 750, 685. The ethyl 1-(thio)cyclobutanecarboxylate derivative thus produced was used in the subsequent reaction:

2) The ethyl 1-(phenylthio)cyclobutanecarboxylate (0.1 g, 0.425 mmol) was dissolved in dichloromethane (2.55 mL) with 1 equiv of sodium bicarbonate (0.036 g). m-CPBA (0.066 g, 0.9 equiv.) was dissolved in dichloromethane (1.5 mL) in an addition funnel and added dropwise to the sulfide solution for 15 min at 0°C. The solution was then stirred for an additional 45 min. The product was washed with water; the organic layer was dried over Na_2SO_4 and purified on a silica gel column using 1:1 petroleum ether/ethyl acetate.

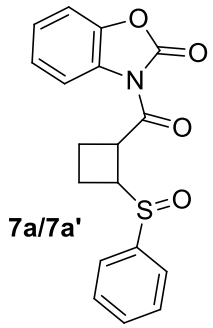


12

Ethyl 1-(phenylsulfinyl)cyclobutanecarboxylate **12** – Yield 70% (0.074 g); orange oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.54 – 7.43 (m, 5H), 4.14 – 4.08 (m, 2H), 2.90 (dt, *J* = 12.4, 9.2 Hz, 1H), 2.79 – 2.77 (m, 1H), 2.44 – 2.41 (m, 1H), 2.12 – 1.90 (m, 3H), 1.21 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 170.13, 140.47, 131.65, 128.83, 124.89, 68.91, 61.73, 28.32, 20.03, 15.82, 14.04. **IR** (ATR) *cm^{-1}*: 3061, 2990, 2951, 1728, 1446, 1226, 1207, 1130, 1086, 1015, 751. **HRMS** (ESI) Calcd. for $C_{13}H_{17}O_3S$ ($M+H^+$) m/z 253,0892, found 253,0892.

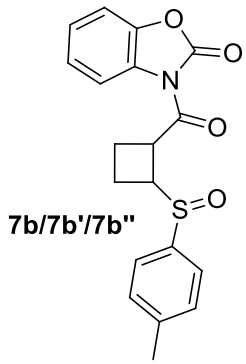
Procedure for the synthesis of 7, 8a and 8b

The sulphoxide **6** or **10** (0.225 mmol) in toluene (1.38 mL) was heated at 80°C for 4 days under argon. The solvent was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, 1/1 petroleum ether/ethyl acetate). Yields refer to chromatographically pure materials.



7a/7a'

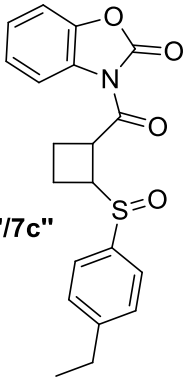
3-(2-(Phenylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7a/7a'** – Yield 70% (0.054 g). Pure **7a** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 151–157 °C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.68 – 7.66 (m, 1H), 7.55 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.32 (t, *J* = 7.8 Hz, 2H), 7.24 – 7.13 (m, 4H), 4.77 – 4.71 (m, 1H), 4.16 – 4.11 (m, 1H), 2.66 – 2.52 (m, 2H), 2.26 – 2.17 (m, 1H), 2.13 – 2.05 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.24, 150.56, 142.37, 141.46, 130.84, 129.02, 127.44, 125.47, 124.74, 123.93, 115.73, 109.97, 57.31, 34.99, 22.61, 18.70. **IR** (ATR) cm^{-1}: 3061, 2996, 2956, 1793, 1714, 1477, 1444, 1377, 1303, 1282, 1253, 1174, 1138, 1086, 1038, 995. **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO_4S$ ($M+H^+$) m/z 342,0795, found 342,0797. The following data are attributed to **7a'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 5.7, 1.7 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.54 – 7.44 (m, 4H), 7.14 – 7.07 (m, 2H), 4.61 (q, *J* = 9.3 Hz, 1H), 4.10 (dd, *J* = 15.1, 6.8 Hz, 1H), 1.61 (dd, *J* = 16.9, 9.3 Hz, 1H), other signals masked. **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.39, 150.64, 142.64, 141.29, 131.11, 129.28, 127.68, 125.74, 125.03, 124.17, 115.97, 110.18, 56.48, 39.69, 22.61, 14.30.



7b/7b'/7b''

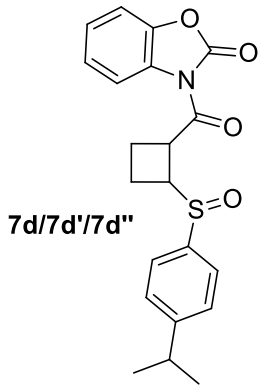
3-(2-(*p*-Tolylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7b/7b'/7b''** – Yield 88% (0.07 g). Pure **7b** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 127–133°C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.9 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 2H),

7.25 – 7.14 (m, 3H), 7.07 (d, *J* = 8.0 Hz, 2H), 4.73 (q, *J* = 9.0 Hz, 1H), 4.07 (q, *J* = 8.8 Hz, 1H), 2.62 – 2.55 (m, 1H), 2.52 – 2.45 (m, 1H), 2.23 – 2.17 (m, 1H), 2.13 – 2.06 (m, 1H), 1.99 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.45, 150.49, 142.23, 141.49, 138.08, 129.56, 127.40, 125.37, 124.71, 123.84, 115.62, 109.91, 57.96, 34.60, 22.32, 21.00, 18.60. **IR** (ATR) *cm^{-1}*: 2951, 1793, 1717, 1477, 1372, 1307, 1283, 1249, 1139, 1084, 1037, 920. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 356,0950. The following data are attributed to **7b'** and **7b''** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 6.0 Hz, 1H), 8.06 – 7.96 (m, 1H), 7.49 (d, *J* = 8.1 Hz, 2H), 4.57 (q, *J* = 9.3 Hz, 1H), 4.50 (q, *J* = 8.4 Hz, 1H), 4.03 – 3.96 (m, 1H), 2.90 – 2.78 (m, 1H), 2.70 – 2.63 (m, 1H), 2.42 – 2.37 (m, 1H), 2.34 (s, 3H), 2.30 (s, 3H), 1.96 – 1.89 (m, 1H), 1.66 (dd, *J* = 17.1, 9.0 Hz, 1H), other signals masked.



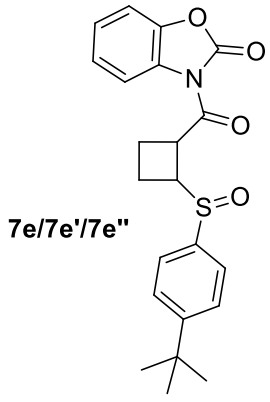
7c/7c'/7c''

3-(2-((4-Ethylphenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7c/7c'/7c''** – Yield 87% (0.072 g). Pure **7c** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 167–170 °C – **^{1}HNMR** (500 MHz, $CDCl_3$) δ 7.67 – 7.66 (m, 1H), 7.45 (d, *J* = 8.2 Hz, 2H), 7.22 – 7.11 (m, 5H), 4.75 (q, *J* = 8.7 Hz, 1H), 4.09 (q, *J* = 8.9 Hz, 1H), 2.62 – 2.58 (m, 1H), 2.50 (ddd, *J* = 19.5, 9.7, 2.3 Hz, 1H), 2.32 (q, *J* = 7.6 Hz, 2H), 2.21 – 2.19 (m, 1H), 2.11 – 2.07 (m, 1H), 0.96 (t, *J* = 7.6 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.43, 150.54, 147.72, 142.31, 138.33, 128.44, 127.48, 125.44, 124.74, 123.99, 115.73, 109.95, 57.71, 34.69, 28.44, 22.46, 18.62, 15.00. **IR** (ATR) *cm^{-1}*: 2967, 2875, 1800, 1720, 1482, 1375, 1307, 1286, 1252, 1142, 1040. **HRMS** (ESI) Calcd. for $C_{20}H_{20}NO_4S$ ($M+H^+$) m/z 370,1108, found 370,1108. The following data are attributed to **7c'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 7.99 (m, 1H), 7.52 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.05 (d, *J* = 7.6 Hz, 1H), 4.58 (q, *J* = 9.5 Hz, 1H), 4.07 (dd, *J* = 16.3, 7.8 Hz, 1H), 1.74 – 1.63 (m, 1H), 1.21 (t, *J* = 7.6 Hz, 3H), other signals masked.



7d/7d'/7d"

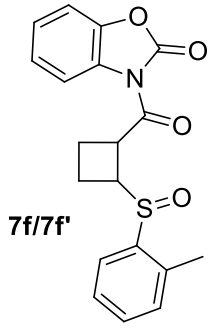
3-(2-((4-Isopropylphenyl)sulfinyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **7d/7d'/7d''** – Yield 58% (0.05 g). Pure **7d** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 160–165 °C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 – 7.68 (m, 1H), 7.46 (d, *J* = 8.3 Hz, 2H), 7.22 – 7.11 (m, 5H), 4.79 – 4.74 (m, 1H), 4.14 – 4.08 (m, 1H), 2.66 – 2.51 (m, 3H), 2.21 – 2.17 (m, 1H), 2.09 – 2.05 (m, 1H), 0.99 (d, *J* = 10.2 Hz, 3H), 0.98 (d, *J* = 10.2 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.30, 152.32, 150.54, 142.35, 138.40, 127.45, 127.11, 125.47, 124.76, 124.02, 115.79, 109.97, 57.28, 34.75, 33.87, 23.64, 23.54, 22.57, 18.58. **IR** (ATR) *cm^{-1}*: 2964, 2870, 1793, 1715, 1474, 1372, 1304, 1283, 1249, 1137, 1048, 1035. **HRMS** (ESI) Calcd. for $C_{21}H_{22}NO_4S$ ($M+H^+$) m/z 384,1264, found 384,1261. The following data are attributed to **7d'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 8.00 (m, 1H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.1 Hz, 2H), 4.59 (q, *J* = 9.0 Hz, 1H), 4.08 (dd, *J* = 14.3, 5.4 Hz, 1H), 1.73 – 1.64 (m, 1H), 1.22 (dd, *J* = 6.9, 2.7 Hz, 6H), other signals masked.



7e/7e'/7e"

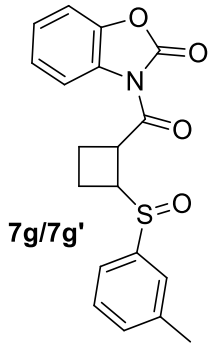
3-(2-((4-(*Tert*-butyl)phenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7e/7e'/7e''** – Yield 56% (0.049 g). Pure **7e** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 151–155 °C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 – 7.68 (m, 1H), 7.48 – 7.46 (m, 2H), 7.35 – 7.33 (m, 2H), 7.20 – 7.12 (m, 3H), 4.81 – 4.76 (m, 1H), 4.14 – 4.09 (m, 1H), 2.63 – 2.50 (m, 2H), 2.22 – 2.17 (m, 1H), 2.11 – 2.05 (m, 1H), 1.06 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.25, 154.64, 150.53, 142.30, 137.98, 125.96, 125.49, 124.78, 123.74, 115.82, 109.98, 57.14, 34.83, 34.59, 31.03, 22.57, 18.54. **IR** (ATR) *cm^{-1}*: 2963, 2907, 2873, 1796, 1719, 1478, 1373, 1303, 1284, 1251,

1142, 1082, 1040. **HRMS** (ESI) Calcd. for $C_{22}H_{24}NO_4S$ ($M+H^+$) m/z 398,1421, found 398,1421. The following data are attributed to **7e'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08 – 7.96 (m, 1H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 2H), 4.59 (q, *J* = 9.2 Hz, 1H), 4.08 (q, *J* = 8.4 Hz, 1H), 1.71 – 1.66 (m, 1H), 1.29 (s, 9H), other signals masked.



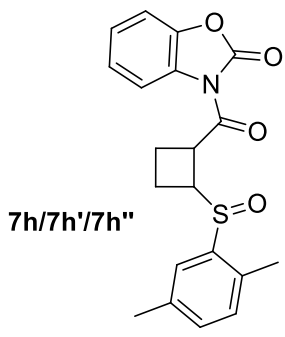
7f/7f'

3-(2-(*o*-Tolylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7f**/**7f'** – Yield 76% (0.061 g); orange oil. NMR data were obtained from a not separable d.r.: 57:43 mixture: **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.07 – 8.06 (m, 1H), 7.81 – 7.80 (m, 1H), 7.77 (d, *J* = 7.7 Hz, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.39 – 7.35 (m, 2H), 7.28 – 7.26 (m, 1H), 7.24 – 7.19 (m, 3H), 7.18 – 7.08 (m, 4H), 7.04 – 6.97 (m, 2H), 4.67 (q, *J* = 9.2 Hz, 1H), 4.58 (q, *J* = 9.5 Hz, 1H), 4.26 (q, *J* = 9.0 Hz, 1H), 4.18 (q, *J* = 8.5 Hz, 1H), 2.69 – 2.61 (m, 3H), 2.53 (qd, *J* = 9.8, 2.3 Hz, 1H), 2.47 (s, 3H), 2.41 (s, 3H), 2.22 (td, *J* = 10.7, 1.6 Hz, 1H), 2.09 – 2.03 (m, 2H), 1.50 – 1.49 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.46, 171.01, 150.55, 150.51, 142.62, 142.28, 139.71, 139.42, 134.58, 134.34, 130.86, 130.74, 130.71, 130.47, 127.65, 127.32, 126.84, 126.33, 125.67, 125.37, 124.95, 124.63, 124.11, 123.50, 115.93, 115.59, 110.13, 109.88, 53.54, 53.47, 39.98, 34.43, 22.75, 22.60, 18.59, 18.27, 18.16, 13.36. **IR** (ATR) cm^{-1}: 3059, 3011, 2950, 1796, 1717, 1478, 1371, 1307, 1286, 1251, 1142, 1036, 757. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 356,0951. The structure of diastereoisomeric compounds **7f** and **7f'** were further supported by oxidation with m-CPBA which gave the same sulfone **9f**: white solid; m. p. = 164–169 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.93 – 7.90 (m, 1H), 7.86 – 7.83 (m, 1H), 7.34 (t, *J* = 6.8 Hz, 1H), 7.24 – 7.13 (m, 5H), 4.61– 4.57 (m, 2H), 2.70 (s, 3H), 2.66 – 2.61 (m, 2H), 2.17 – 2.10 (m, 1H), 2.05 – 2.00 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 170.40, 150.59, 142.53, 138.84, 135.75, 133.88, 132.97, 130.69, 127.48, 126.55, 125.76, 124.99, 115.94, 110.15, 55.00, 40.38, 22.49, 20.61, 19.24. **IR** (ATR) cm^{-1}: 3064, 2959, 2922, 2692, 1798, 1720, 1602, 1479, 1312, 1252, 1147, 1048, 758, 609. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_5S$ ($M+H^+$) m/z 372,0900, found 372,0900.



7g/7g'

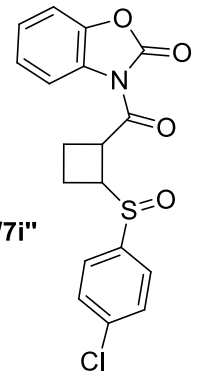
3-(2-(*m*-Tolylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7g/7g'** – Yield 45% (0.036 g); orange oil. NMR data were obtained from a not separable d.r. 74:26 mixture: **7g** – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.67 – 7.66 (m, 1H), 7.36 (s, 1H), 7.30 – 7.29 (m, 1H), 7.23 – 7.21 (m, 1H), 7.18 – 7.15 (m, 3H), 6.90 (d, *J* = 7.5 Hz, 1H), 4.77 – 4.72 (m, 1H), 4.10 (q, *J* = 8.9 Hz, 1H), 2.62 – 2.55 (m, 1H), 2.50 (ddd, *J* = 19.8, 9.8, 2.4 Hz, 1H), 2.24 – 2.18 (m, 1H), 2.19 (s, 3H), 2.14 – 2.08 (m, 1H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.48, 150.53, 142.32, 141.24, 139.31, 131.63, 128.83, 127.41, 125.47, 124.69, 124.11, 121.08, 115.66, 109.89, 57.74, 34.84, 22.47, 21.27, 18.71. **7g'** – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.04 – 8.03 (m, 1H), 7.42 (s, 1H), 7.42 – 7.34 (m, 2H), 7.28 – 7.23 (m, 3H), 7.15 – 7.14 (m, 1H), 4.62 – 4.57 (m, 1H), 4.08 (q, *J* = 8.8 Hz, 1H), 2.61 (ddd, *J* = 30.1, 16.3, 14.4 Hz, 2H), 2.40 (s, 3H), 2.14 – 2.08 (m, 1H), 1.65 – 1.60 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.46, 150.62, 142.62, 141.52, 139.46, 131.89, 129.07, 127.67, 125.71, 125.01, 124.45, 121.26, 115.95, 110.16, 56.52, 39.64, 22.64, 21.53, 14.41. **IR** (ATR) *cm^{-1}*: 3059, 3011, 2950, 1796, 1717, 1478, 1371, 1307, 1286, 1251, 1142, 1036, 757. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356.0951, found 355.0950. The structure of diastereoisomeric compounds **7g** and **7g'** were further supported by oxidation with m-CPBA which gave the same sulfone **9g**: white solid; m. p. = 143–148 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.65 – 7.63 (m, 2H), 7.34 – 7.30 (m, 2H), 7.20 – 7.13 (m, 3H), 4.67 – 4.62 (m, 1H), 4.47 – 4.42 (m, 1H), 2.66 – 2.53 (m, 2H), 2.32 (s, 3H), 2.16 – 2.10 (m, 1H), 2.05 – 2.00 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 170.40, 150.66, 142.54, 139.78, 137.59, 134.80, 129.30, 128.80, 127.50, 125.79, 125.66, 125.04, 56.07, 40.25, 22.47, 21.41, 19.60. **IR** (ATR) *cm^{-1}*: 2959, 1978, 1800, 1720, 1599, 1479, 1377, 1312, 1254, 1140, 1045, 755. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_5S$ ($M+H^+$) m/z 372,0900, found 372,0902.



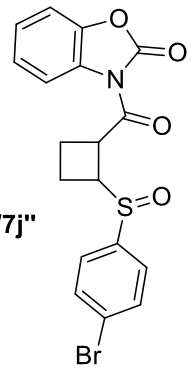
7h/7h'/7h"

3-(2-((2,5-Dimethylphenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7h/7h'/7h''** – Yield 84% (0.069 g). Pure **7h** diastereomer was obtained by recrystallization from diethyl ether; white semi-solid;– **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.58 – 7.55 (m, 2H), 7.24 – 7.21 (m, 1H), 7.14 (dd, *J* = 12.2, 4.5 Hz, 2H), 6.86 (d, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 7.4 Hz, 1H), 4.69 (q, *J* = 8.9 Hz, 1H), 4.21 (q, *J* = 9.1 Hz, 1H), 2.64 (dq, *J* = 19.7, 9.8 Hz, 1H), 2.49 (qd, *J* = 9.7, 2.0 Hz, 1H), 2.33 (s, 3H), 2.19 (dt, *J* = 10.3, 5.1 Hz, 1H), 2.07 (dd, *J* = 19.3, 10.0 Hz, 1H), 2.03 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.31, 150.54, 142.34, 139.19, 136.55, 131.33, 131.28, 130.72, 127.31, 125.44, 124.66, 123.74, 115.65, 109.83, 54.12, 34.27, 22.56, 20.68, 18.67, 17.68. **IR** (ATR) *cm^{-1}*: 2951, 2879, 2805, 1754, 1482, 1401, 1308, 1253, 1143, 1059, 1007, 923. **HRMS** (ESI) Calcd. for $C_{20}H_{20}NO_4S$ ($M+H^+$) m/z 370,1108, found 370,1108. The following data are attributed to **7h'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 1H), 4.58 (dd, *J* = 18.2, 9.5 Hz, 1H), 4.17 (dd, *J* = 16.7, 7.9 Hz, 1H), 2.41 (s, 3H), 2.38 (s, 3H), 1.56 – 1.51 (m, 1H), other signals masked.

7i/7i'/7i"

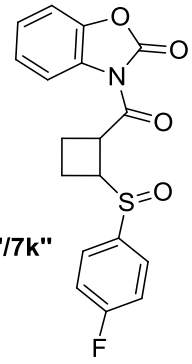


3-(2-((4-Chlorophenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7i/7i'/7i''** – Yield 80% (0.067 g). Pure **7i** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 148–153°C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.70 – 7.66 (m, 1H), 7.52 – 7.48 (m, 2H), 7.33 – 7.29 (m, 2H), 7.27 – 7.17 (m, 3H), 4.69 (q, *J* = 9.2 Hz, 1H), 4.11 (q, *J* = 8.5 Hz, 1H), 2.64 – 2.54 (m, 2H), 2.28 – 2.21 (m, 1H), 2.15 – 2.07 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.09, 150.57, 142.35, 140.04, 137.38, 129.32, 127.30, 125.63, 125.39, 125.01, 115.63, 110.13, 57.30, 35.03, 22.66, 18.77. **IR** (ATR) *cm^{-1}*: 3082, 3063, 2951, 1798, 1715, 1476, 1369, 1309, 1284, 1253, 1140, 1080, 1042, 1013. **HRMS** (ESI) Calcd. for $C_{18}H_{15}ClNO_4S$ ($M+H^+$) m/z 376,0405, found 376,0405. The following data are attributed to **7i'** in the mixture – ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 – 8.03 (m, 1H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 7.30 – 7.27 (m, 2H), 7.17 – 7.05 (m, 1H), 4.60 (dt, *J* = 9.7, 4.8 Hz, 1H), 4.08 (dd, *J* = 17.3, 8.8 Hz, 1H), 1.65 – 1.56 (m, 1H), other signals masked.



7j/7j'/7j''

3-(2-((4-Bromophenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7j/7j'/7j''** – Yield 68% (0.064 g). Pure **7j** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 149–154°C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 – 7.68 (m, 1H), 7.47 – 7.41 (m, 4H), 7.25 – 7.18 (m, 3H), 4.71 – 4.66 (m, 1H), 4.14 – 4.09 (m, 1H), 2.64 – 2.53 (m, 2H), 2.27 – 2.19 (m, 1H), 2.15 – 2.06 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.09, 150.58, 142.36, 140.67, 132.24, 127.29, 125.64, 125.62, 125.58, 125.07, 115.68, 110.17, 57.27, 35.02, 22.67, 18.78. **IR** (ATR) *cm^{-1}*: 3080 - 2951, 1798, 1717, 1476, 1375, 1307, 1284, 1251, 1140, 1042, 1007. **HRMS** (ESI) Calcd. for $C_{18}H_{15}BrNO_4S$ ($M+H^+$) m/z 419,9900, found 419,9899. The following data are attributed to **7j'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.08 – 8.00 (m, 1H), 7.64 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 2H), 4.63 – 4.52 (m, 1H), 4.06 (dd, *J* = 17.3, 8.8 Hz, 1H), 1.60 (dd, *J* = 18.9, 7.7 Hz, 1H), other signals masked.

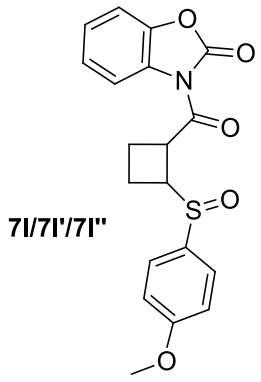


7k/7k'/7k''

3-(2-((4-Fluorophenyl)sulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7k/7k'/7k''** – Yield 80% (0.065 g). Pure **7k** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 160–164 °C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.2 Hz, 1H), 7.57 – 7.54 (m, 2H), 7.25 – 7.16 (m, 3H), 7.06 – 7.02 (m, 2H), 4.69 (q, *J* = 9.4 Hz, 1H), 4.11 (q, *J* = 8.8 Hz, 1H), 2.61 – 2.54 (m, 2H), 2.25 – 2.19 (m, 1H), 2.12 – 2.06 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.06, 164.34 (d, *J* = 251.5 Hz), 150.57, 142.34, 136.81 (d, *J* = 3.0 Hz), 127.32, 126.16 (d, *J* = 8.9 Hz), 125.64, 124.94, 116.43 (d, *J* = 22.6 Hz), 115.61, 110.11, 57.11, 35.10, 22.64, 18.69. **IR** (ATR) *cm^{-1}*: 3098, 3069, 2996, 2950, 1798, 1719, 1588, 1480, 1371, 1307, 1286, 1251, 1225, 1142, 1084, 1042. **HRMS** (ESI) Calcd. for $C_{18}H_{15}FNO_4S$ ($M+H^+$) m/z 360,0700, found 360,0700. The following data

are attributed to **7k'** and **7k''** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 6.0, 3.2 Hz, 1H), 8.07 – 8.00 (m, 1H), 7.62 (dd, *J* = 8.8, 5.1 Hz, 2H), 7.54 – 7.45 (m, 2H), 4.61 – 4.55 (m, 1H), 4.51 (dd, *J* = 16.9, 8.6 Hz, 1H), 4.06 (q, *J* = 8.4 Hz, 1H), 3.99 (dd, *J* = 16.3, 8.6 Hz, 1H), 1.69 – 1.58 (m, 1H), other signals masked. The mother liquor from the above mentioned crystallization was concentrated to give a 24:4:54 mixture of **7k**:**7k'**:**7k''** isomers and unreacted starting material **6k** (18%). This mixture was treated with m-CPBA to give a mixture of sulfones **9k** (*trans*) and **9k'** (*cis*) and 3-(1-((4-fluorophenyl)sulfonyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **10k**. Careful column chromatography of this mixture gave **9k** contaminated with minor impurities and a highly enriched sample of compound **9k'**: white solid; m. p. = 128–132 °C – **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.07 – 8.05 (m, 1H), 7.72 – 7.69 (m, 2H), 7.23 – 7.19 (m, 2H), 7.14 – 7.11 (m, 1H), 6.94 (t, *J* = 8.5 Hz, 2H), 4.49 (dd, *J* = 18.4, 9.2 Hz, 1H), 4.45 – 4.42 (m, 1H), 3.14 – 3.07 (m, 1H), 2.41 – 2.35 (m, 2H), 2.10 – 2.04 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 168.06, 165.93 (d, *J* = 257.5 Hz), 151.22, 142.46, 134.21, 131.28 (d, *J* = 9.3 Hz), 127.70, 125.65, 125.21, 116.60, 116.26 (d, *J* = 58.6 Hz), 110.03, 61.44, 41.89, 20.66, 20.34. **IR** (ATR) *cm^{-1}*: 3400, 2958, 2924, 1796, 1590, 1556, 1478, 1373, 1316, 1290, 1144, 1086, 843, 757, 671. **HRMS** (ESI) Calcd. for $C_{18}H_{15}FNO_5S$ ($M+H^+$) m/z 376,0649, found 376,0648.

9k: white semi-solid – **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.89 – 7.85 (m, 3H), 7.23 – 7.17 (m, 1H), 7.16 – 7.11 (m, 4H), 4.61 (dt, *J* = 9.7, 4.8 Hz, 1H), 4.44 (q, *J* = 8.7 Hz, 1H), 2.66 (tdd, *J* = 13.2, 9.8, 4.5 Hz, 1H), 2.63 – 2.55 (m, 1H), 2.18 – 2.12 (m, 1H), 2.06 – 1.99 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 170.23, 166.15 (d, *J* = 257.1 Hz), 150.66, 142.57, 133.90, 131.42 (d, *J* = 9.8 Hz), 127.44, 125.90, 125.13, 116.86 (d, *J* = 22.9 Hz), 115.96, 110.24, 56.07, 40.52, 22.48, 19.49. **IR** (ATR) *cm^{-1}*: 3356, 2959, 2922, 2852, 1801, 1722, 1592, 1479, 1375, 1317, 1241, 1145, 1045, 758, 590. **HRMS** (ESI) Calcd. for $C_{18}H_{15}FNO_5S$ ($M+H^+$) m/z 376,0649, found 376,0649.

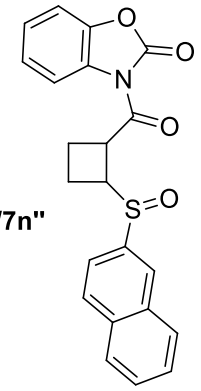


7l/7l'/7l''

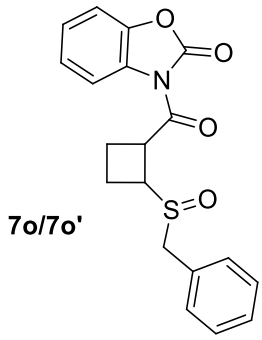
3-(2-((4-Methoxyphenyl)sulfinyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **7l/7l'/7l''** – Yield 88% (0.073 g). Pure **7l** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 153–157 °C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 – 7.69 (m, 1H), 7.45 (d, *J* = 8.8 Hz, 2H),

7.25 – 7.15 (m, 3H), 6.81 – 6.78 (m, 2H), 4.75 – 4.69 (m, 1H), 4.06 (q, *J* = 8.8 Hz, 1H), 3.52 (s, 3H), 2.60 – 2.48 (m, 2H), 2.22 – 2.16 (m, 1H), 2.11 – 2.06 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.45, 161.83, 150.58, 142.33, 132.20, 127.48, 125.59, 125.42, 124.77, 115.70, 114.50, 109.95, 57.86, 55.29, 34.93, 22.37, 18.60. **IR** (ATR) *cm^{-1}*: 3003, 2944, 1796, 1719, 1594, 1496, 1478, 1376, 1307, 1284, 1250, 1178, 1140, 1088, 1038. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_5S$ ($M+H^+$) m/z 372,0900, found 372,0900. The following data are attributed to **7l'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.01 (dd, *J* = 6.6, 2.4 Hz, 1H), 7.54 (d, *J* = 8.8 Hz, 1H), 6.97 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.9 Hz, 55H), 4.56 (t, *J* = 8.4 Hz, 1H), 3.73 (s, 3H), 1.71 (q, *J* = 9.5 Hz, 17H), other signals masked.

7n/7n'/7n''

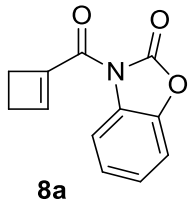


3-(2-(Naphthalen-2-ylsulfinyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one **7n/7n'/7n''** – Yield 30% (0.027 g). Pure **7n** diastereomer was obtained by recrystallization from diethyl ether; white solid; m. p. = 174–177°C – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.64 (d, *J* = 8.6 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.33 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.29 (dd, *J* = 11.0, 4.0 Hz, 1H), 7.24 – 7.19 (m, 2H), 7.00 (td, *J* = 8.1, 1.1 Hz, 1H), 6.89 – 6.87 (m, 2H), 4.73 (q, *J* = 9.1 Hz, 1H), 4.11 (q, *J* = 9.0 Hz, 1H), 2.58 (dq, *J* = 19.4, 9.7 Hz, 1H), 2.42 (qd, *J* = 9.8, 2.3 Hz, 1H), 2.18 (dt, *J* = 18.5, 5.6 Hz, 1H), 2.05 – 1.98 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 171.28, 150.44, 141.93, 138.66, 134.28, 132.60, 129.12, 128.11, 127.69, 127.66, 127.28, 126.88, 125.09, 124.53, 124.32, 119.90, 115.30, 109.70, 57.96, 34.43, 22.35, 18.78. **IR** (ATR) *cm^{-1}*: 3063, 2950, 2878, 2805, 1773, 1757, 1723, 1480, 1373, 1307, 1251, 1142, 1069, 1036, 923. **HRMS** (ESI) Calcd. for $C_{22}H_{18}NO_4S$ ($M+H^+$) m/z 392.0951, found 392.0951. The following data are attributed to **7n'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 – 7.97 (m, 1H), 7.95 – 7.92 (m, 2H), 7.59 (dd, *J* = 8.6, 1.6 Hz, 1H), 7.57 – 7.54 (m, 2H), 4.71 – 4.60 (m, 1H), 1.67 – 1.59 (m, 1H), other signals masked.



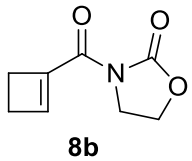
7o/7o'

3-(2-(Benzylsulfinyl)cyclobutanecarbonyl)benzo[*d*]oxazol-2(3*H*)-one **7o**/**7o'** – Yield 45% (0.036 g); colorless oil. **7o – ^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.12 – 8.09 (m, 1H), 7.42 (d, *J* = 7.1 Hz, 2H), 7.36 (t, *J* = 7.3 Hz, 2H), 7.33 – 7.25 (m, 4H), 4.89 – 4.83 (m, 1H), 4.20 (q, *J* = 8.5 Hz, 1H), 3.92 (d, *J* = 12.9 Hz, 1H), 3.82 (d, *J* = 12.9 Hz, 1H), 2.79 – 2.72 (m, 1H), 2.45 – 2.38 (m, 1H), 2.22 – 2.11 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 172.20, 150.47, 142.71, 130.31, 130.24, 129.07, 128.39, 127.76, 125.75, 125.00, 116.07, 110.21, 56.69, 50.93, 36.75, 23.85, 19.40. **IR** (ATR) *cm^{-1}*: 3063, 2982, 2953, 1798, 1715, 1480, 1367, 1307, 1253, 1144, 1038, 761. **HRMS** (ESI) Calcd. for $C_{19}H_{18}NO_4S$ ($M+H^+$) m/z 356,0951, found 356,0954. The following data are attributed to **7o'** in the mixture – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 4.66 – 4.60 (m, 1H), 1.82 – 1.67 (m, 1H), other signals masked.



8a

3-(cyclobut-1-enecarbonyl)benzo[d]oxazol-2(3H)-one **8a –** White solid; m. p. = 79–81 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.98 – 7.96 (m, 1H), 7.25 – 7.20 (m, 4H), 3.00 – 2.99 (m, 2H), 2.62 – 2.60 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 160.37, 152.63, 150.83, 142.86, 138.05, 128.31, 125.30, 124.78, 115.79, 110.02, 30.60, 28.07. **IR** (ATR) *cm^{-1}*: 2973, 2923, 1821, 1801, 1673, 1480, 1348, 1321, 1251, 1148, 1032, 1005. **HRMS** (ESI) Calcd. for $C_{12}H_{10}NO_3$ ($M+H^+$) m/z 216,0655, found 216,0657.



8b

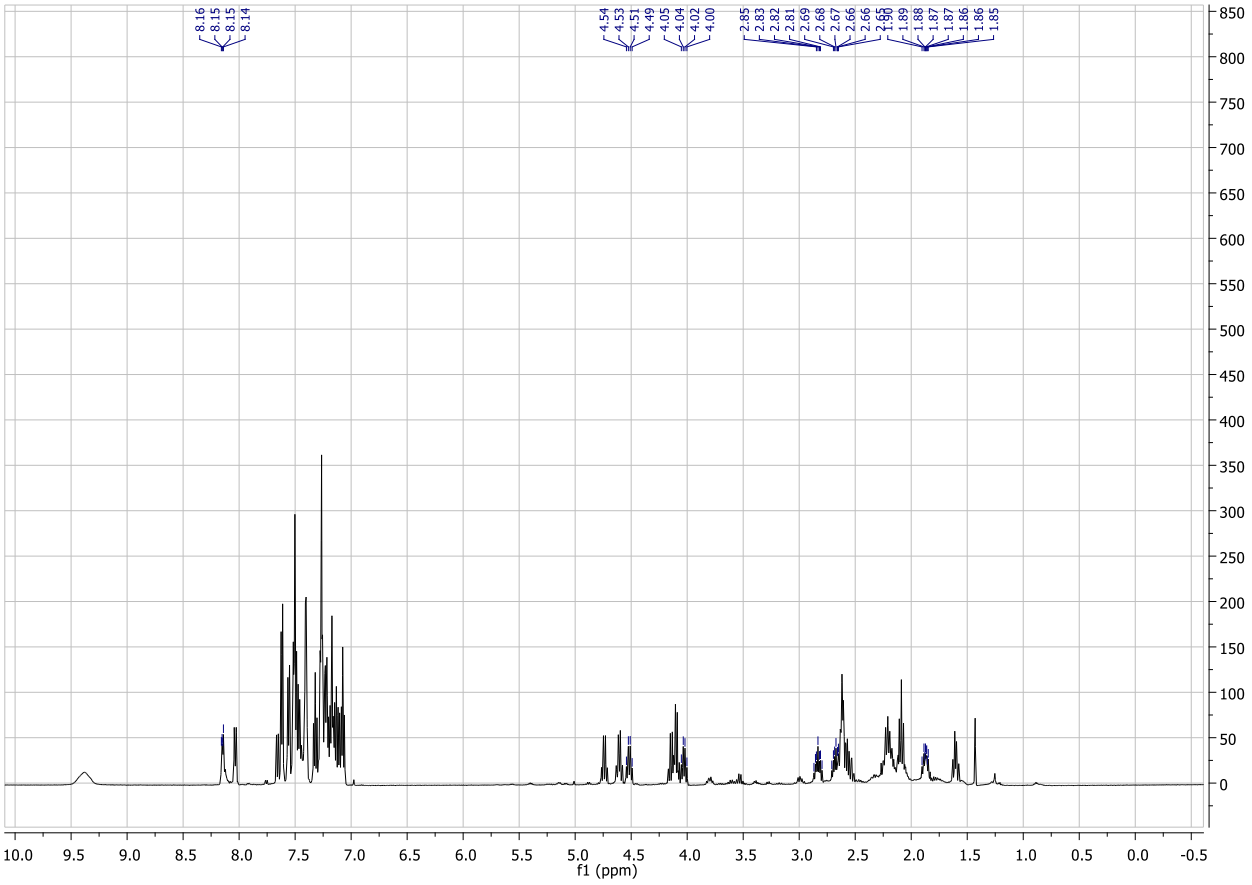
3-(cyclobut-1-enecarbonyl)oxazolidin-2-one **8b** – Yield 90% (0.034 g); colorless oil. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.04 (t, *J* = 1.2 Hz, 1H), 4.44 (t, *J* = 7.9 Hz, 2H), 4.05 (t, *J* = 8.0 Hz, 2H), 2.89 – 2.87 (m, 2H), 2.53 – 2.51 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.75, 152.97, 150.19, 138.00, 62.64,

43.27, 30.63, 27.78. **IR** (ATR) cm^{-1}: 2976, 2925, 1776, 1651, 1586, 1478, 1384, 1361, 1325, 1200, 1098, 1040, 1000. **HRMS** (ESI) Calcd. for $C_8H_{10}NO_3$ ($M+H^+$) m/z 168,0655, found 168,0656.

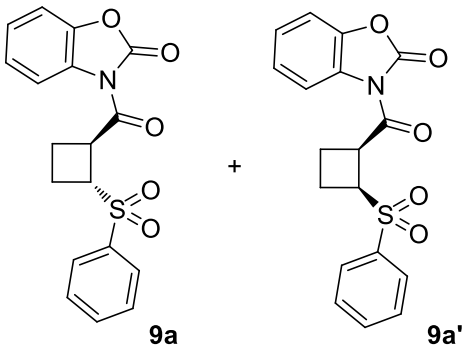
Charaterization of the third diastereomer 7a'' (from Table 1, entry 10)

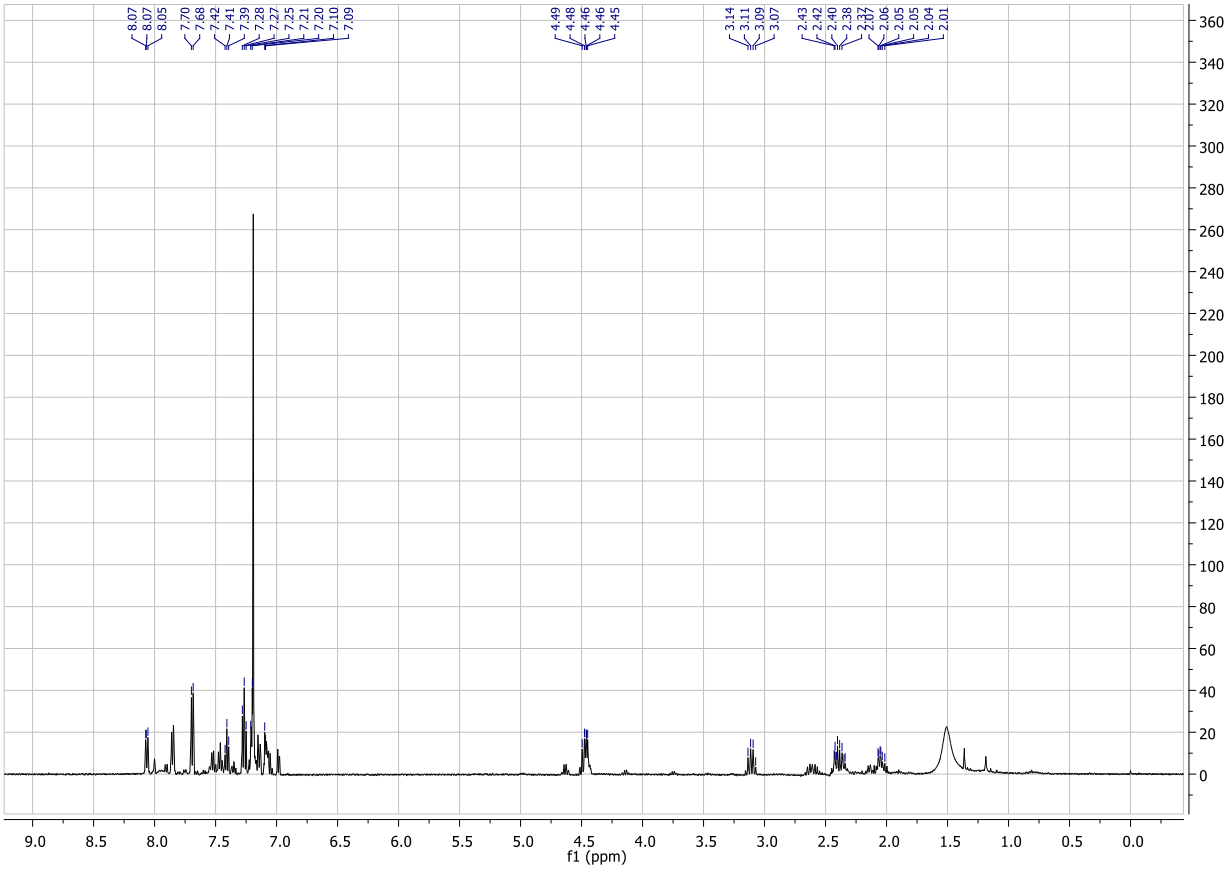
The sulphoxide **6a** (0.225 mmol) in toluene (1.4 mL) was heated at 60°C for 4 days under argon. The solvent was removed under reduced pressure, and the residue contained a 31:8:16:20 mixture of **7a**, **7a**', **7a''**, **8a** and unreacted **6a** (25%). Fractionation of the crude product by column chromatography (silica gel, 1/1 petroleum ether/ethyl acetate) gave a 30:37:33 mixture of **7a**:**7a**':**7a''**, a mixture of **7a**:**8a** and a mixture of **7a**:**7a'**. The following data are attributed to **7a''** in the mixture (since some peaks for diastereomer **7a''** are indiscriminate from diastereomers **7a** and **7a'**, only representative peaks for diastereomer **7a''** are listed): **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.16 – 8.14 (m, 1H), 4.52 (dd, *J* = 16.9, 8.6 Hz, 1H), 4.03 (dd, *J* = 16.3, 8.6 Hz, 1H), 2.85 – 2.81 (m, 1H), 2.69 – 2.65 (m, 1H), 1.90 – 1.85 (m, 1H) other signals masked.

Mixture **7a**:**7a'**:**7a''**=30:37:33



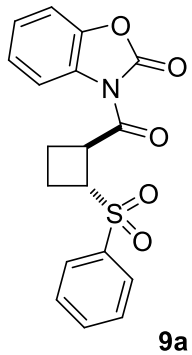
Oxidation of the above mentioned mixture with m-CPBA gave, after column chromatography, pure compound **9a** (*trans*) and a 16:84 mixture of sulfones **9a** (*trans*) and **9a'** (*cis*).





Careful column chromatography of this mixture allowed the preparation of a sample of the compound **9a'** contaminated with minor impurities. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 6.6, 2.6 Hz, 1H), 7.69 (d, *J* = 7.3 Hz, 2H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.26 (t, *J* = 7.8 Hz, 2H), 7.21 – 7.20 (m, 2H), 7.09 – 7.08 (m, 1H), 4.47 – 4.43 (m, 2H), 3.13 – 3.07 (m, 1H), 2.43 – 2.36 (m, 2H), 2.09 – 2.01 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 168.14, 151.19, 142.47, 138.15, 138.83, 129.14, 128.33, 127.75, 125.51, 125.12, 116.11, 109.92, 61.23, 41.86, 20.61, 20.37. **IR** (ATR) *cm^{-1}*: 3225, 3019, 2951, 2880, 2800, 2666, 1776, 1727, 1477, 1307, 1143, 741. **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO_5S$ (M+H+) m/z 358,0744, found 358.0741.

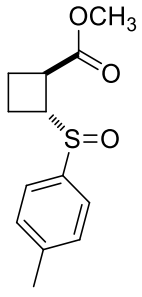
Procedure for the synthesis of 3-(2-(phenylsulfonyl)cyclobutanecarbonyl)benzo[d]oxazol-2(3H)-one 9a



9a

The 50:50 mixture of sulphoxides **7a** and **7a'** (0.025 g, 0.07 mmol) was dissolved in dichloromethane (1 mL) with 1 equiv. of sodium bicarbonate (0.006 g). m-CPBA (0.013 g, 0.077 mmol) was dissolved in dichloromethane in an addition funnel and added dropwise to the solution of sulphoxides for 15 min at room temperature. The solution was then stirred for an additional 15 h. The product was washed with distilled water; the organic layer was dried over Na_2SO_4 and purified on a silica gel column using 1:1 hexane/ethyl acetate. Yield 83% (0.021 g); white solid; m. p. = 170–173 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.86 – 7.84 (m, 3H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.19 – 7.13 (m, 4H), 4.63 (q, *J* = 8.6 Hz, 1H), 4.46 (q, *J* = 8.7 Hz, 1H), 2.67 – 2.55 (m, 2H), 2.17 – 2.11 (m, 1H), 2.02 (dd, *J* = 19.2, 8.8 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 170.29, 150.65, 142.56, 137.82, 134.01, 129.46, 128.54, 127.50, 125.80, 125.04, 115.98, 110.17, 56.01, 40.39, 22.51, 19.52. **IR** (ATR) *cm^{-1}*: 3063, 2976, 1798, 1719, 1480, 1376, 1313, 1251, 1146, 1048. **HRMS** (ESI) Calcd. for $C_{18}H_{16}NO_5S$ ($M+H^+$) m/z 358,0743, found 358.0740.

Procedure for the synthesis of methyl 2-(p-tolylsulfinyl)cyclobutanecarboxylate 14b and 14b'

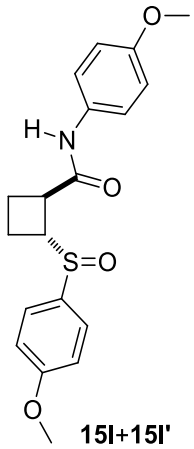


14b+14b'

The 50:50 mixture of sulphoxides **7b** and **7b'** (0.036 g, 0.1 mmol) was dissolved in 2 mL of MeOH and sodium carbonate (0.021 g, 0.2 mmol) was added. The mixture was stirred at room temperature for 48 h. After completion of the reaction, the solvent was removed in vacuo and the crude product was purified over silica gel by column chromatography (silica gel, 5/1 hexanes/ethyl acetate). Yield 80% (0.02 g); colorless oil. It was obtained as a not separable 50:50 mixture of diastereoisomers. **^{1}H**

NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.40 (m, 4H), 7.30 – 7.26 (m, 4H), 3.76 – 3.70 (m, 1H), 3.71 (s, 3H), 3.65 (q, *J* = 8.9 Hz, 1H), 3.58 – 3.53 (m, 2H), 3.28 (s, 3H), 2.51 – 2.46 (m, 2H), 2.40 (s, 3H), 2.38 (s, 3H), 2.20 – 2.09 (m, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 173.39, 173.19, 141.41, 141.20, 138.44, 138.03, 129.94, 129.72, 124.09, 124.04, 58.85 (2 C), 52.21, 51.67, 37.58, 33.39, 21.55, 21.52, 21.48, 21.13, 19.18, 13.98. **IR** (ATR) *cm^{-1}*: 2951, 1732, 1496, 1436, 1361, 1244, 1203, 1086, 1048, 813. **HRMS** (ESI) Calcd. for $C_{13}H_{17}O_3S$ ($M+H^+$) m/z 253.0892, found 253.0890.

Procedure for the synthesis of N-(4-methoxyphenyl)-2-((4-methoxyphenyl)sulfinyl)cyclobutanecarboxamide 15l and 15l'



15l+15l'

A mixture of **7l** and **7l'** (d. r. 88:12; 0.041 g, 0.11 mmol), *para*-methoxy aniline (0.0015 g, 0.12 mmol) in dichloromethane (0.5 mL) was stirred for 72h at room temperature. After completion of the reaction, the solvent was removed in vacuo and the crude product was purified over silica gel by column chromatography (silica gel, 1/1 hexanes/ethyl acetate). Yield 75% (0.029 g); yellow oil. It was obtained as a not separable 91:9 mixture of diastereoisomers **15l** and **15l'**. **15l** – **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.60 (br s, 1H), 7.56 (d, *J* = 8.8 Hz, 2H), 7.39 (d, *J* = 9.0 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 9.0 Hz, 2H), 3.78 (s, 3H), 3.76 (s, 3H), 3.75 – 3.69 (m, 1H), 3.67 – 3.64 (m, 1H), 2.44 – 2.38 (m, 1H), 2.28 – 2.22 (m, 2H), 1.95 – 1.90 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 169.65, 162.55, 156.18, 132.29, 131.74, 125.94, 121.12, 115.18, 114.12, 61.35, 55.62 (2 C), 41.34, 20.37, 19.03. **IR** (ATR) *cm^{-1}*: 3300, 3071, 2946, 2838, 1659, 1598, 1544, 1509, 1301, 146, 1176, 1088, 1034. **HRMS** (ESI) Calcd. for $C_{19}H_{22}NO_4S$ ($M+H^+$) m/z 360.1264, found 360.1262.

X-ray diffraction data for compound 7a

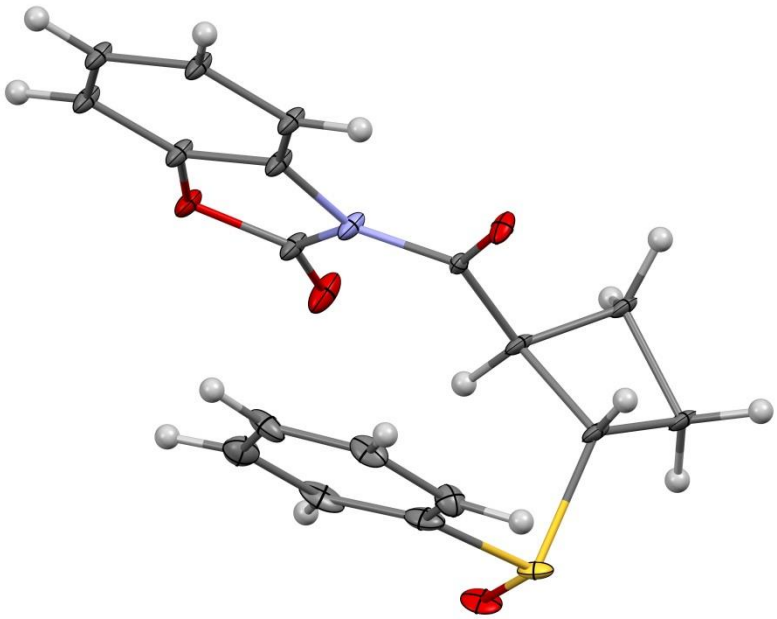


Fig. 1. ORTEP diagram of **7a** shows only one molecule of the eight in the asymmetric unit. Thermal ellipsoids are shown at the 30% level.

X-ray diffraction data for compound **7a** was collected by using a Kappa X8 APPEX II Bruker diffractometer with graphite-monochromated MoKα radiation. Crystals were mounted on a CryoLoop (Hampton Research) with Paratone-N (Hampton Research) as cryoprotectant and then flashfrozen in a nitrogen-gas stream at 100 K. For compound, the temperature of the crystal was maintained at the selected value by means of a 700 series Cryostream cooling device to within an accuracy of ±1K. The data were corrected for Lorentz polarization, and absorption effects. The structures were solved by direct methods using SHELXS-97[1] and refined against F^2 by full-matrix least-squares techniques using SHELXL-2018[2] with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were located on a difference Fourier map and introduced into the calculations as a riding model with isotropic thermal parameters. All calculations were performed by using the Crystal Structure crystallographic software package WINGX.[3]

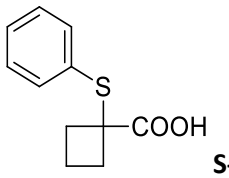
The crystal data collection and refinement parameters are given in Table X1.

1) Sheldrick, G. M. SHELXS-97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, Germany, **1997**.
2) G. M. Sheldrick, Acta Crystallogr., Sect. A: Found. Crystallogr., **2008**, 64, 112-122
3) Farrugia, L. J. *J. Appl. Cryst.*, **1999**, *32*, 837.

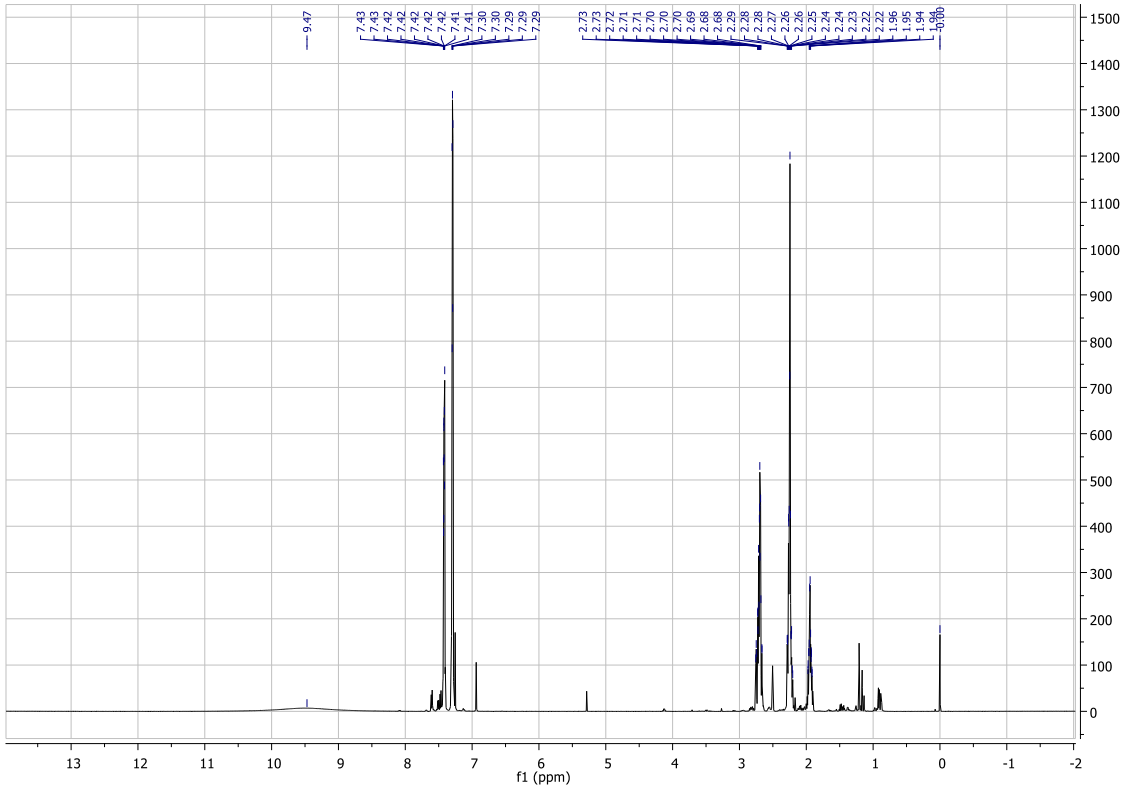
CCDC 1902949 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/Community/Requestastructure.

Table X1. Crystallographic data and structure refinement details.

Compound	**7a**
CCDC	1902949
Empirical Formula	C_{18} H_{15} N O_4 S
M_r	341.37
Crystal size, mm^3	0.22 x 0.06 x 0.03
Crystal system	monoclinic
Space group	*P c*
a, Å	11.4012(8)
b, Å	24.6145(17)
c, Å	21.8613(17
α, °	90
β, °	90.414(3)
γ, °	90
Cell volume, $Å^3$	6134.9(8)
Z ; Z’	16 ; 8
T, K	100(1)
Radiation type ; wavelength Å	MoKα ; 0.71073
F_{000}	2848
μ, mm^{-1}	0.234
θ range, °	0.827 - 28.499
Reflection collected	113 139
Reflections unique	28 680
R_{int}	0.0874
GOF	1.032
Refl. obs. (I>2σ(I))	20 189
Parameters	1286
wR_2 (all data)	0.1932
R value (I>2σ(I))	0.0885
Largest diff. peak and hole (e-.$Å^{-3}$)	0.652 ; -1.171


S
COOH

S-3a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7.42
7.42
7.42
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7.42
7.41
7.41
7.30
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7.29
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7.29
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2.25
2.24
2.24
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2.23
2.23
2.22
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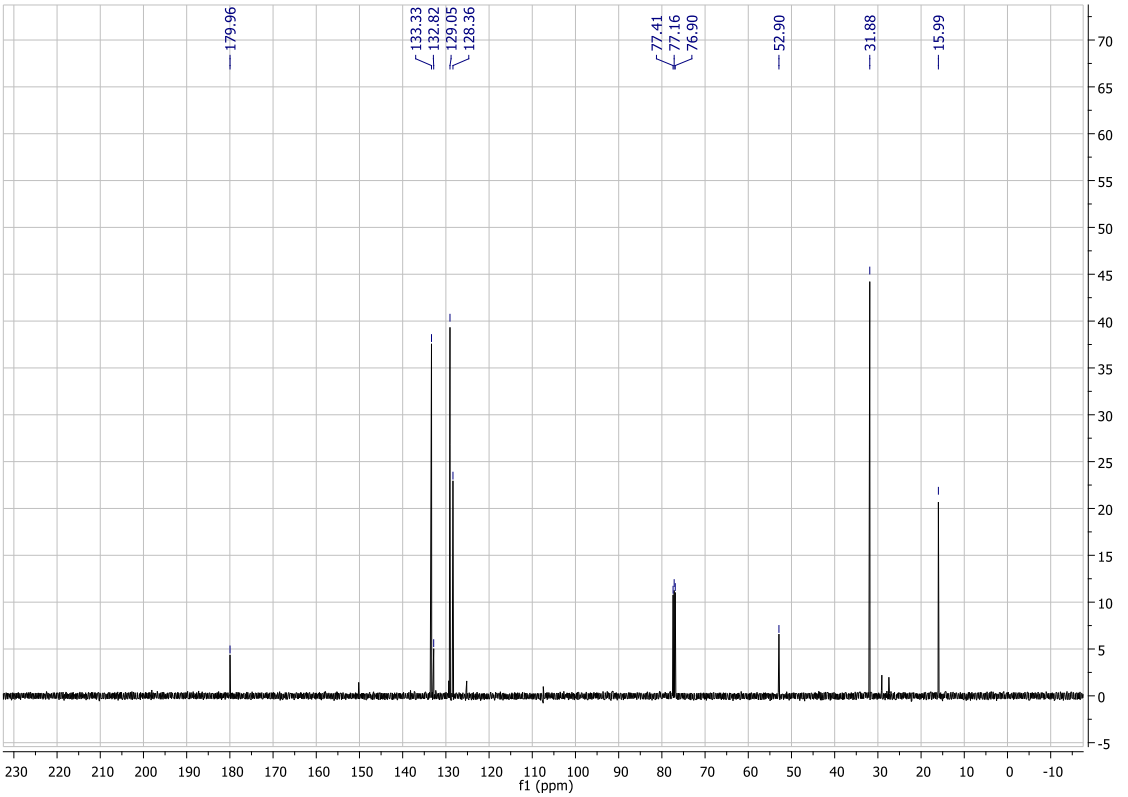
1.95
1.94
1.94
0.00
f1 (ppm)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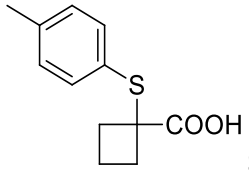
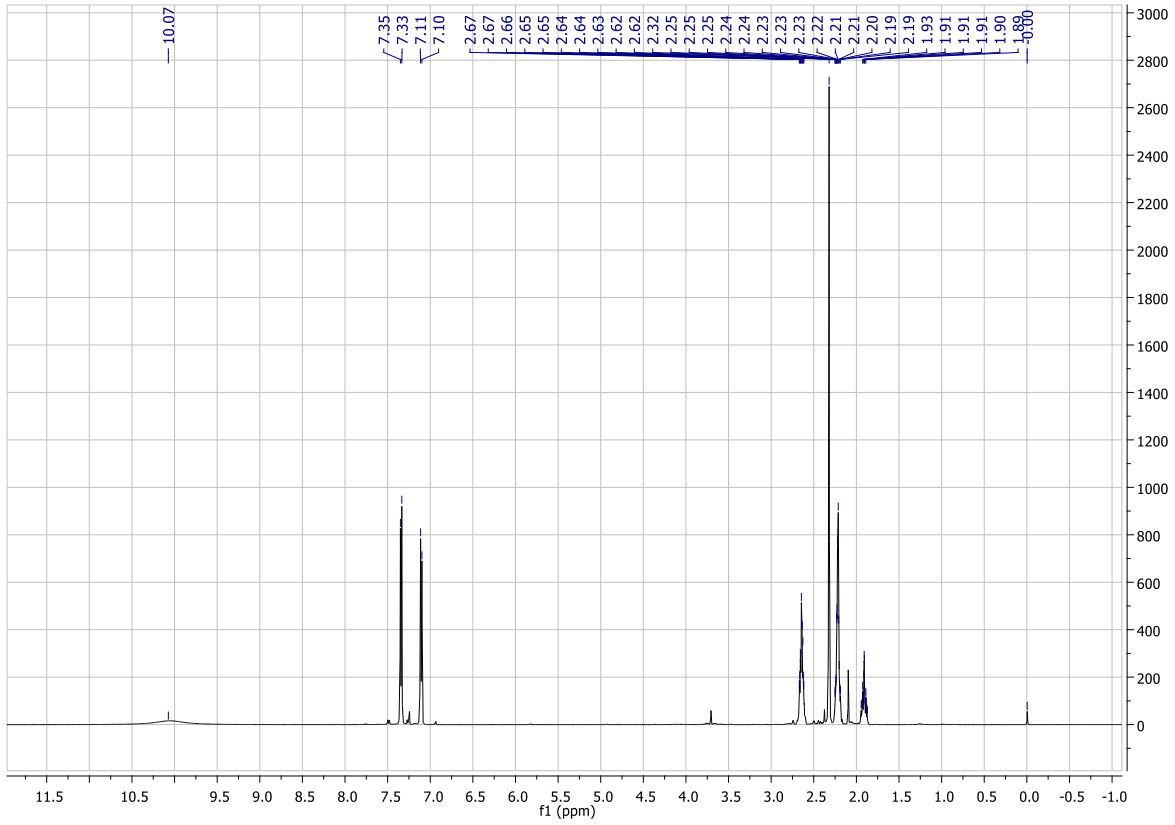
132.82
129.05
128.36
77.41
77.16
76.90
52.90
31.88
15.99
f1 (ppm)


S
COOH

S-3b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2.32
2.25
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2.23
2.22
2.21
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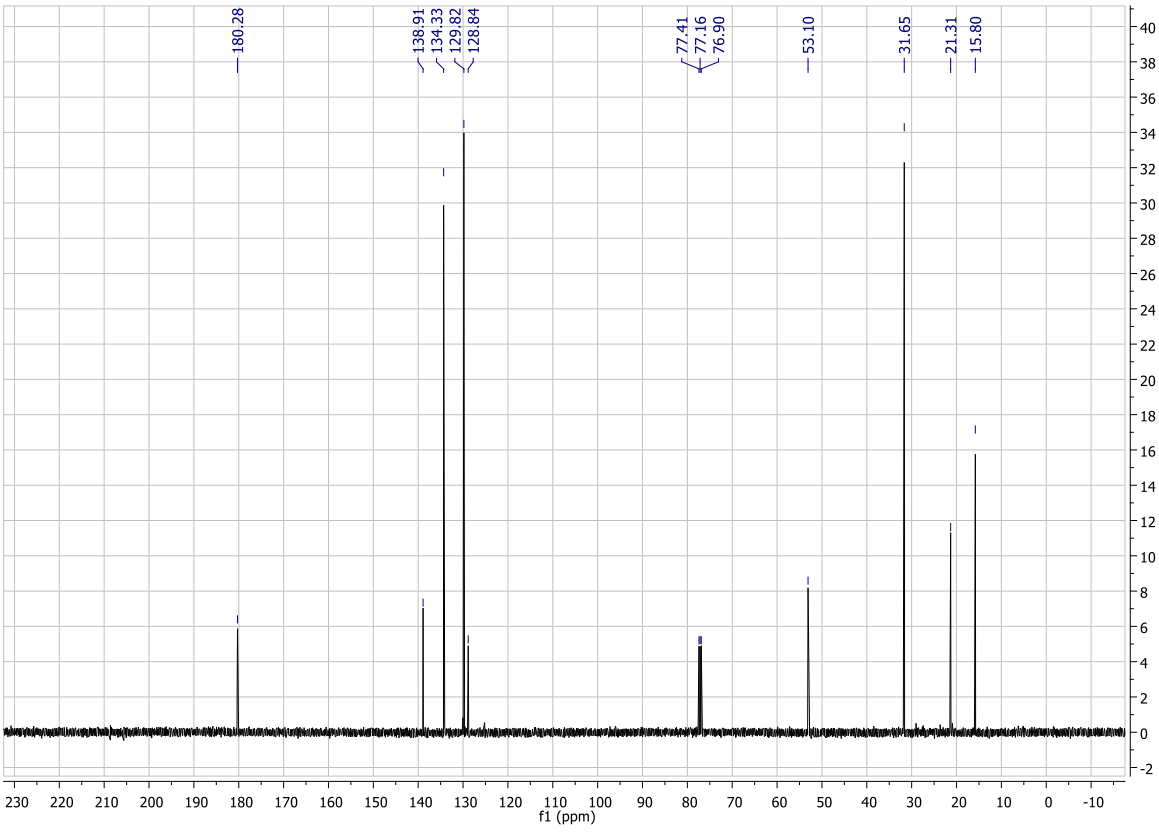
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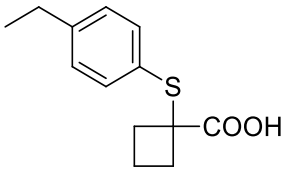
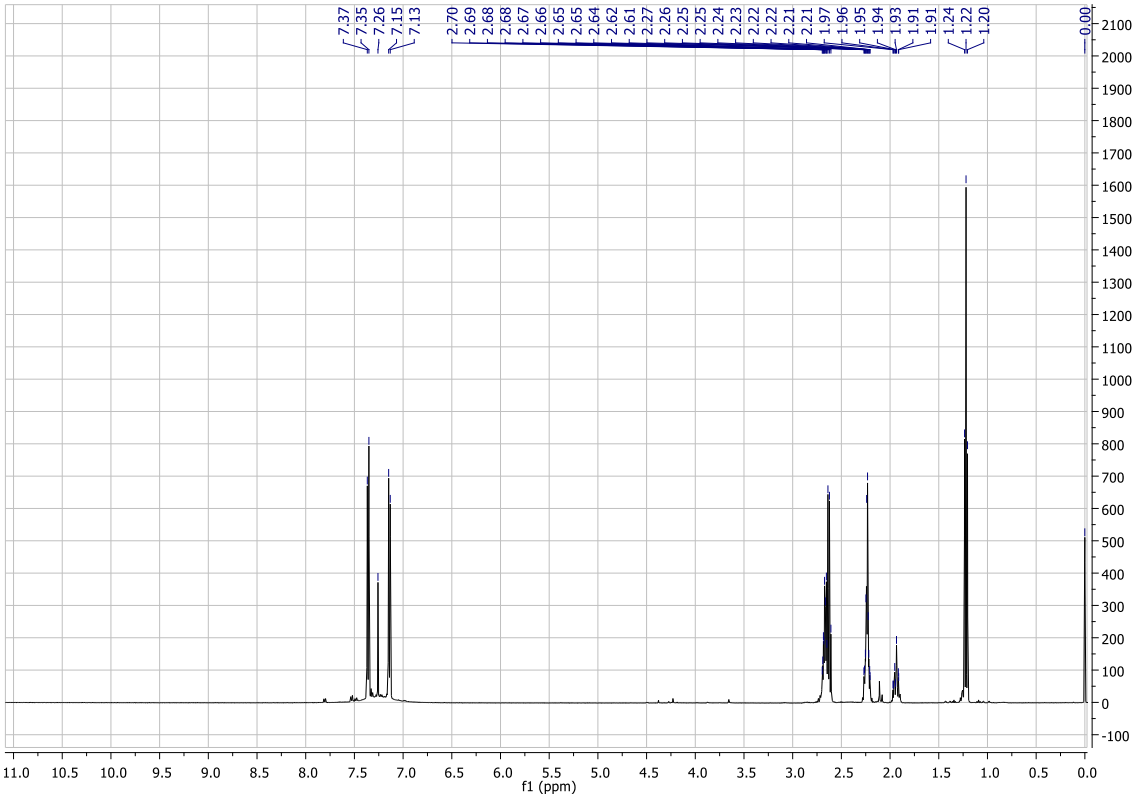
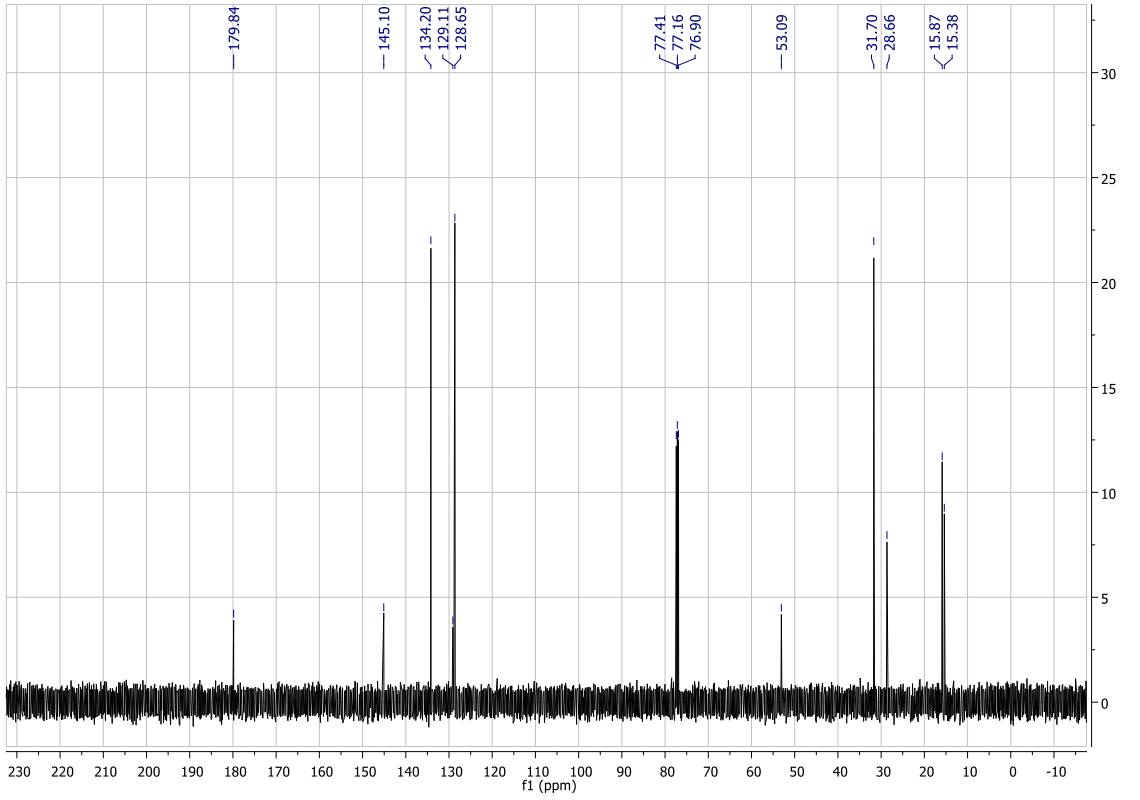
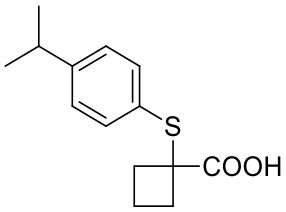
77.41
77.16
76.90
53.10
31.65
21.31
15.80
f1 (ppm)


S
COOH

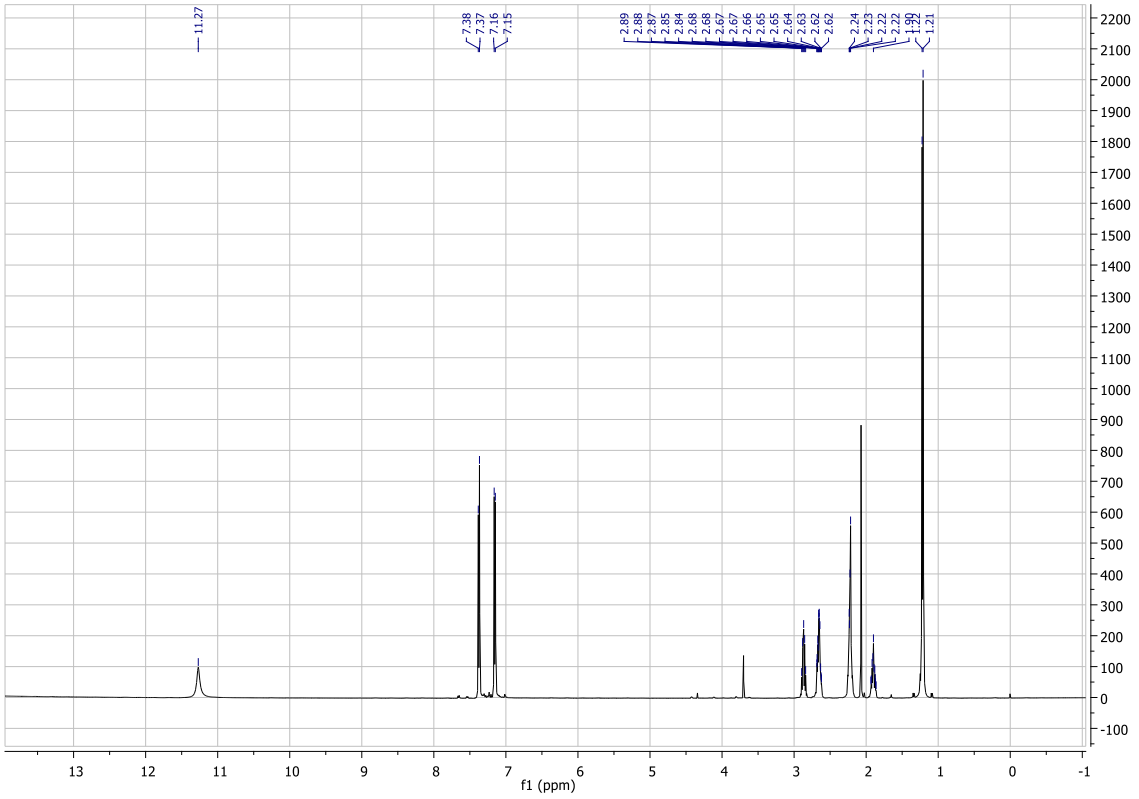
S-3c

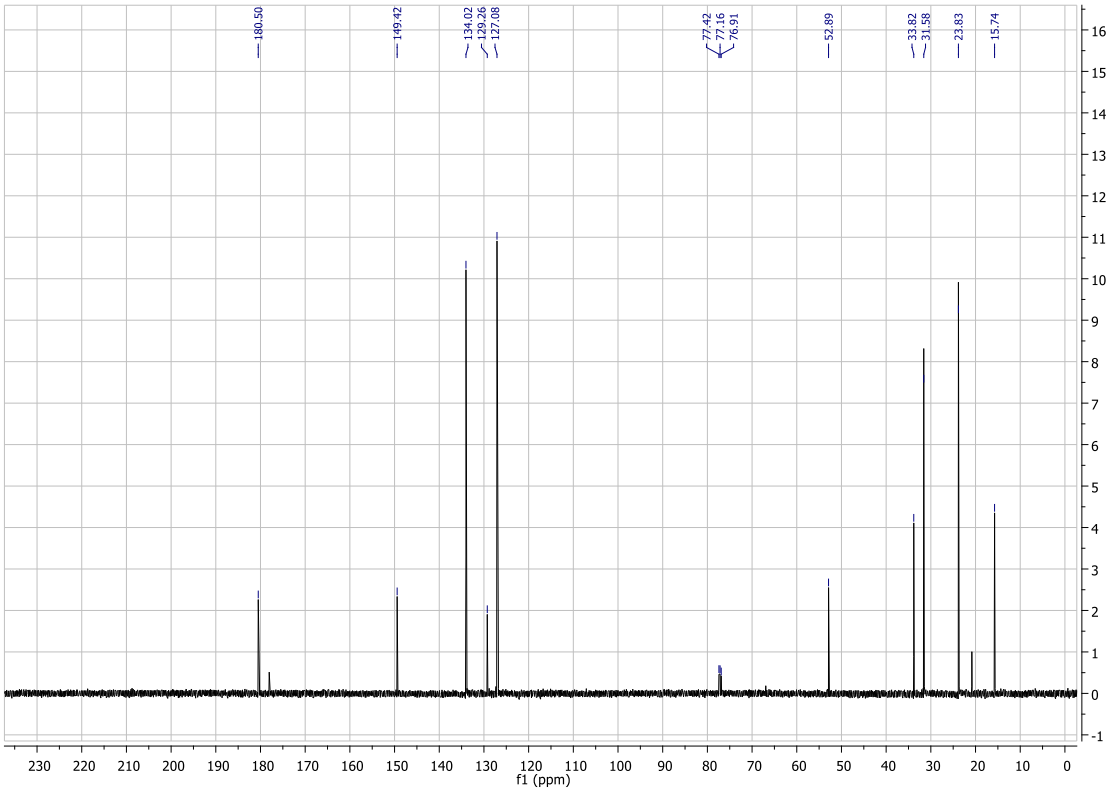

7.37
7.35
7.26
7.15
7.13
2.70
2.69
2.68
2.68
2.67
2.66
2.65
2.65
2.64
2.62
2.61
2.27
2.26
2.25
2.25
2.24
2.23
2.22
2.22
2.21
2.21
1.97
1.96
1.95
1.94
1.93
1.91
1.91
1.24
1.22
1.20
0.00
f1 (ppm)

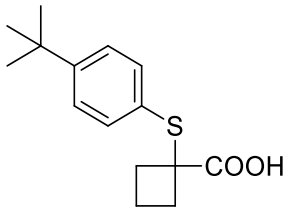

179.84
145.10
134.20
129.11
128.65
77.41
77.16
76.90
53.09
31.70
28.66
15.87
15.38
f1 (ppm)


S
COOH

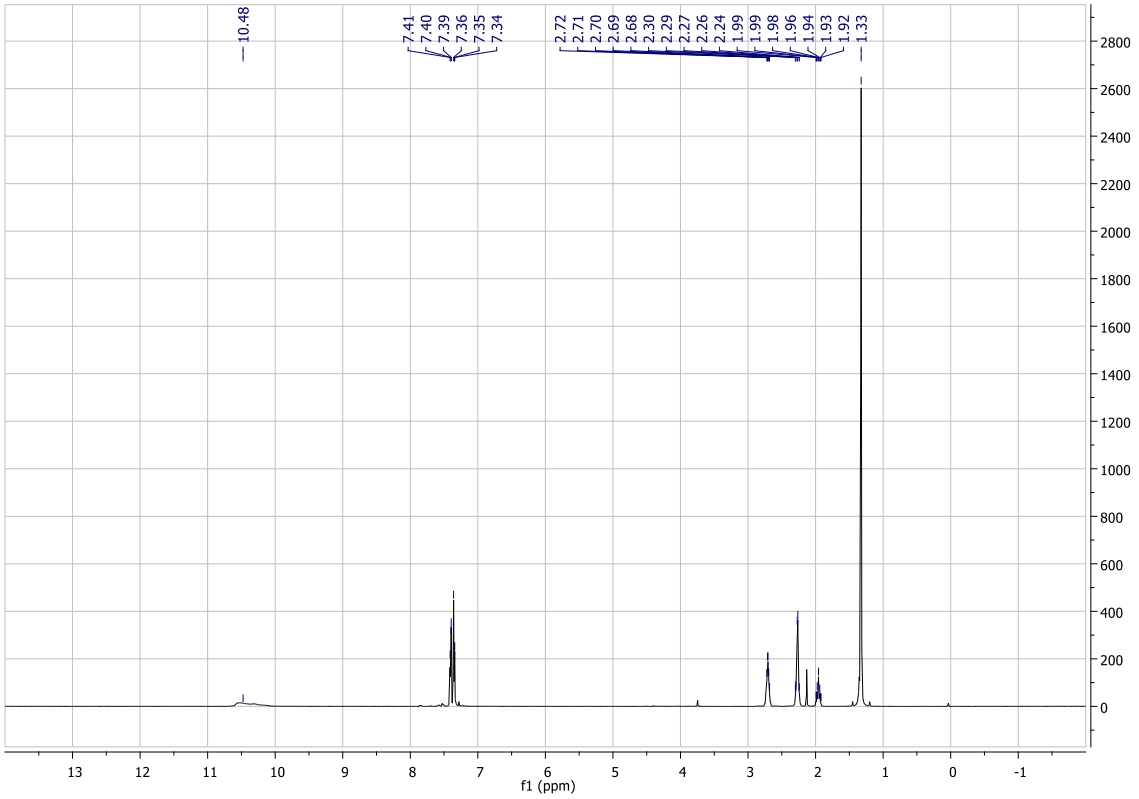
S-3d

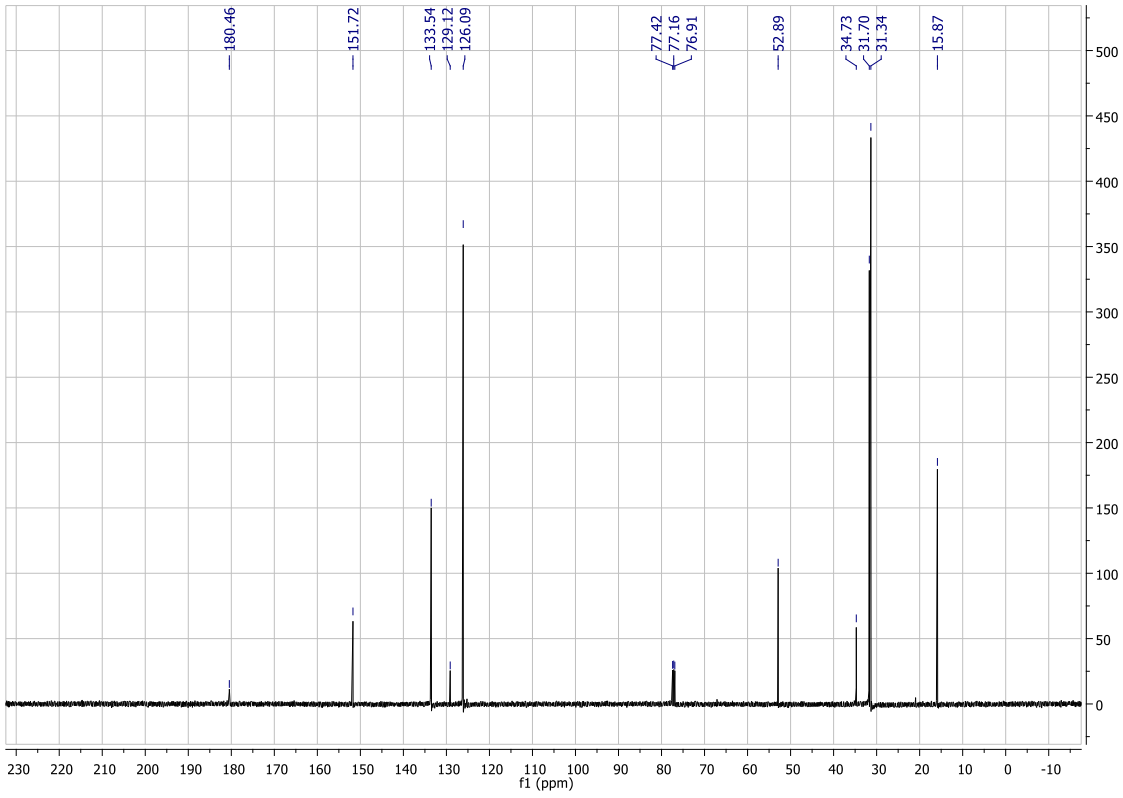

11.27
7.38
7.37
7.16
7.15
2.89
2.88
2.87
2.85
2.84
2.68
2.68
2.67
2.67
2.66
2.65
2.65
2.64
2.63
2.62
2.62
2.24
2.23
2.22
2.22
1.90
1.22
1.21
f1 (ppm)

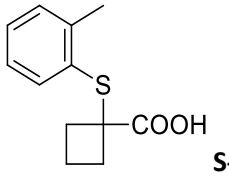

180.50
149.42
134.02
129.26
127.08
77.42
77.16
76.91
52.89
33.82
31.58
23.83
15.74
f1 (ppm)


S
COOH

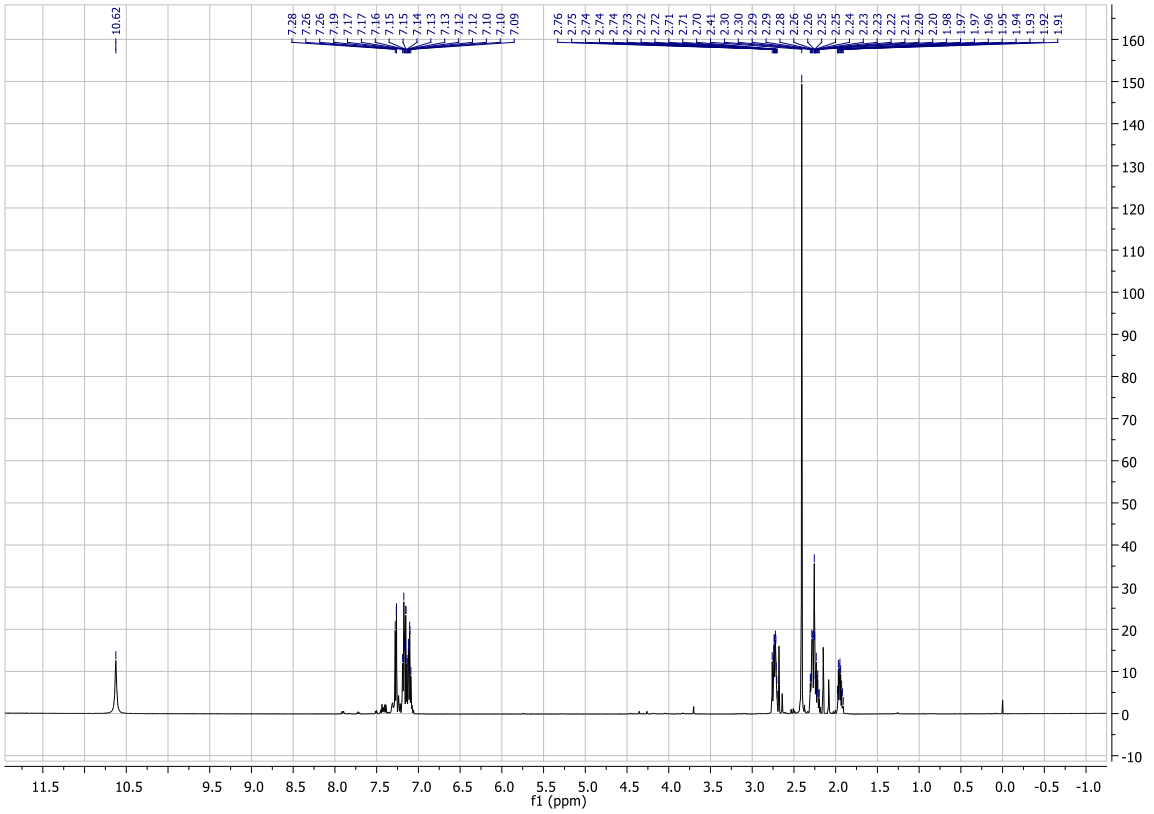
S-3e


10.48
7.41
7.40
7.39
7.36
7.35
7.34
2.72
2.71
2.70
2.69
2.68
2.30
2.29
2.27
2.26
2.24
1.99
1.99
1.98
1.96
1.94
1.93
1.92
1.33
f1 (ppm)


180.46
151.72
133.54
129.12
126.09
77.42
77.16
76.91
52.89
34.73
31.70
31.34
15.87
f1 (ppm)


S
COOH

S-3f


10.62
7.28
7.26
7.26
7.19
7.17
7.17
7.16
7.15
7.15
7.14
7.13
7.13
7.12
7.12
7.10
7.10
7.09
2.76
2.75
2.74
2.74
2.74
2.73
2.72
2.72
2.71
2.71
2.70
2.41
2.30
2.30
2.29
2.29
2.28
2.26
2.26
2.25
2.25
2.24
2.23
2.23
2.22
2.21
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1.97
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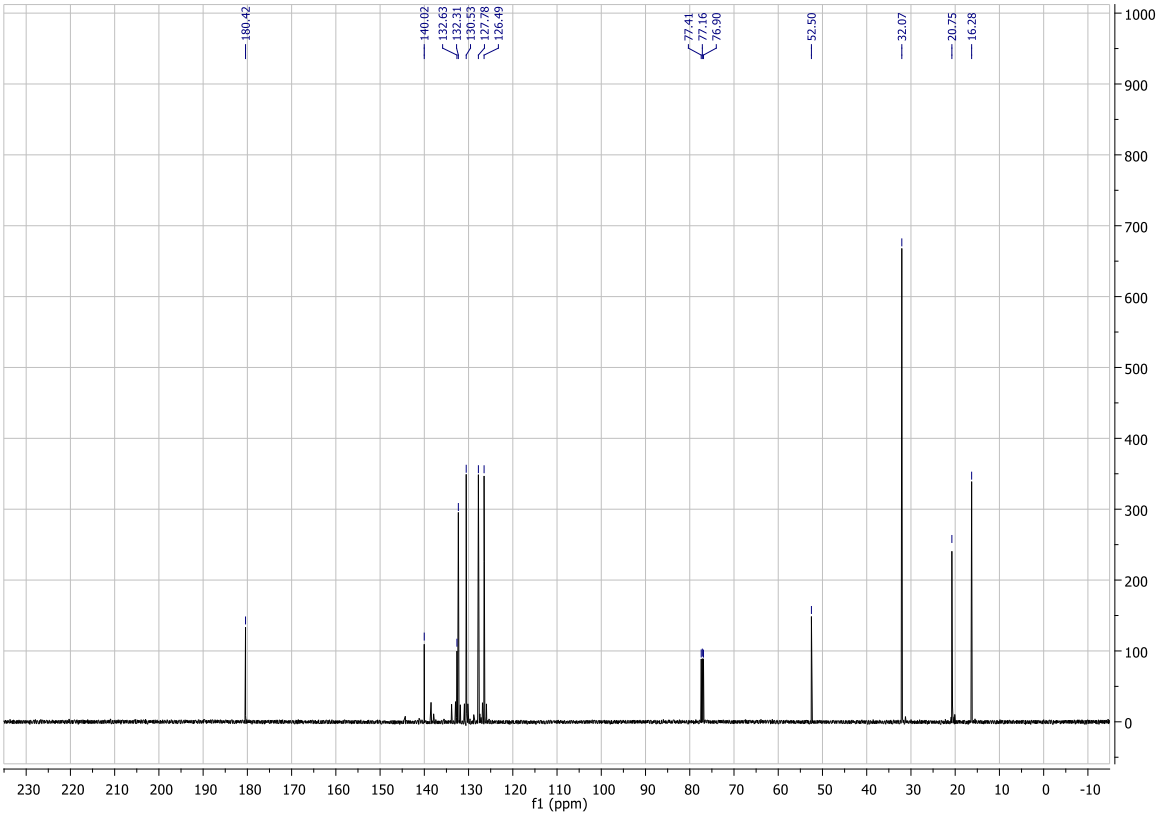
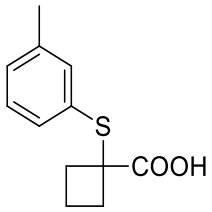
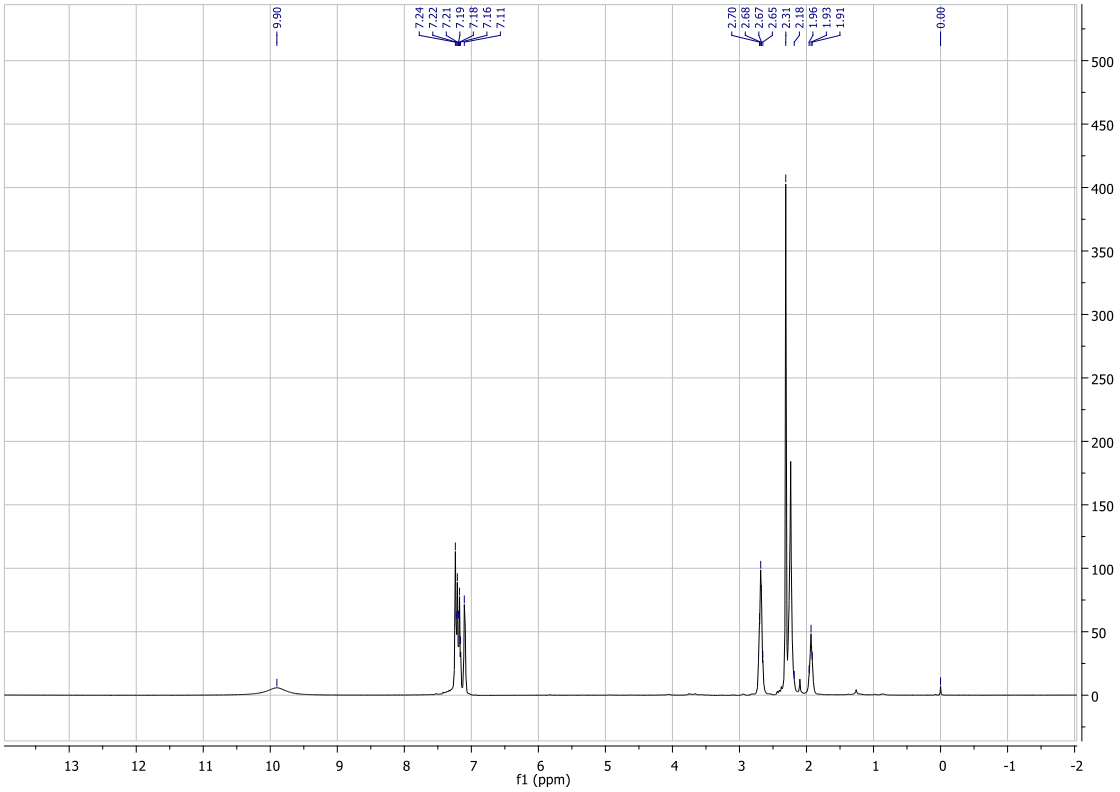
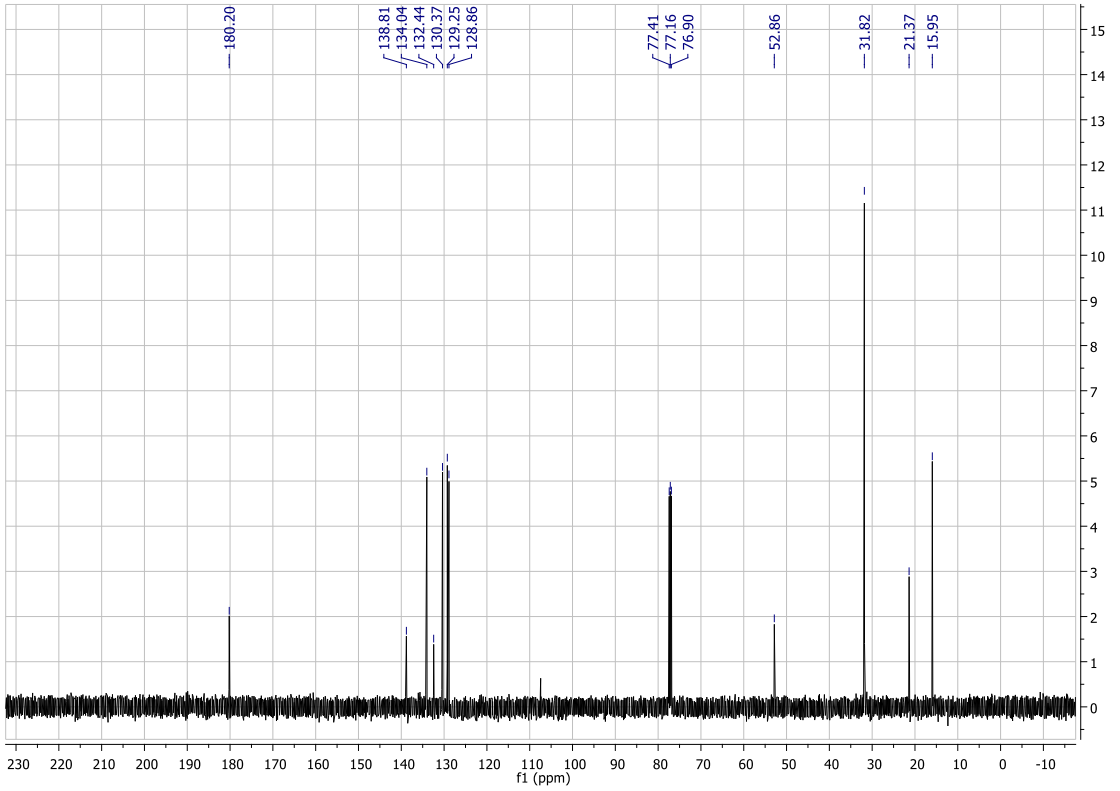
1.95
1.94
1.93
1.92
1.91
f1 (ppm)

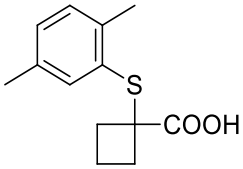

180.42
140.02
132.63
132.31
130.53
127.78
126.49
77.41
77.16
76.90
52.50
32.07
20.75
16.28
f1 (ppm)


S
COOH

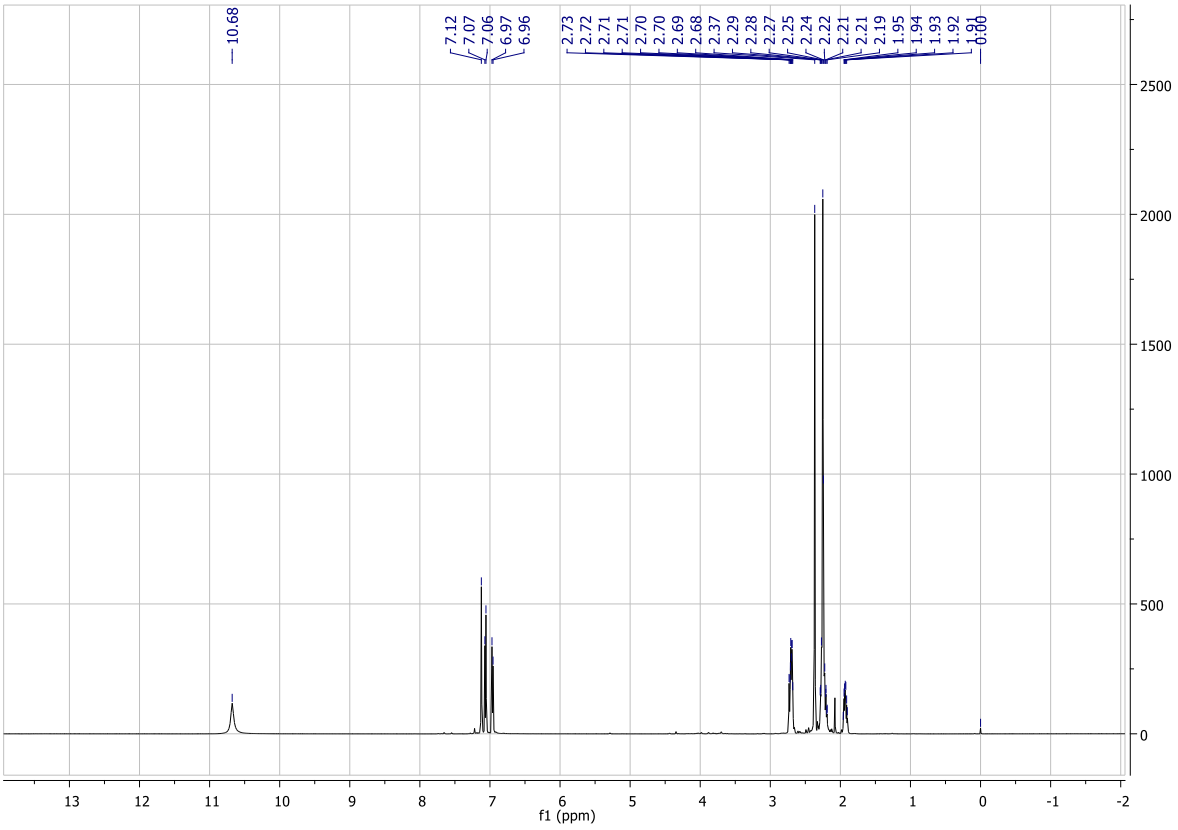
S-3g

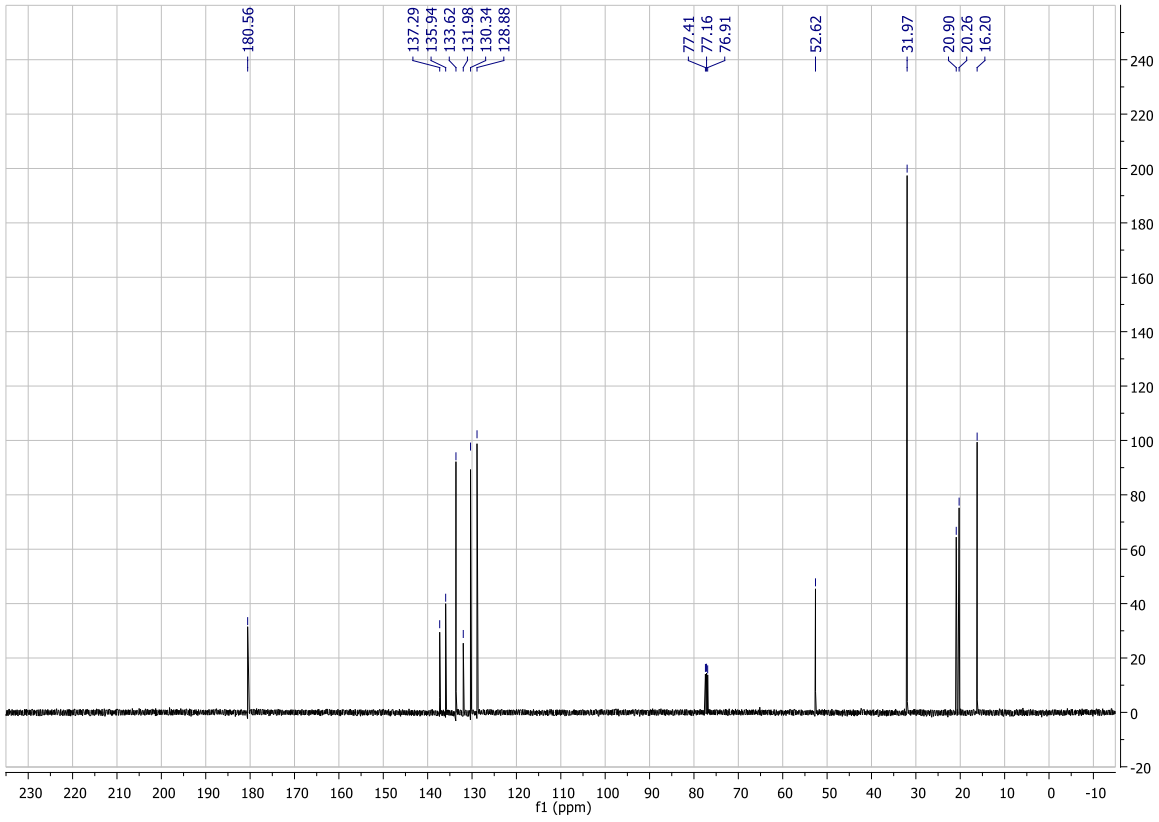

9.90
7.24
7.22
7.21
7.19
7.18
7.16
7.11
2.70
2.68
2.67
2.65
2.31
2.18
1.96
1.93
1.91
0.00
f1 (ppm)

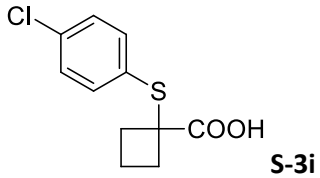

180.20
138.81
134.04
132.44
130.37
129.25
128.86
77.41
77.16
76.90
52.86
31.82
21.37
15.95
f1 (ppm)


S
COOH

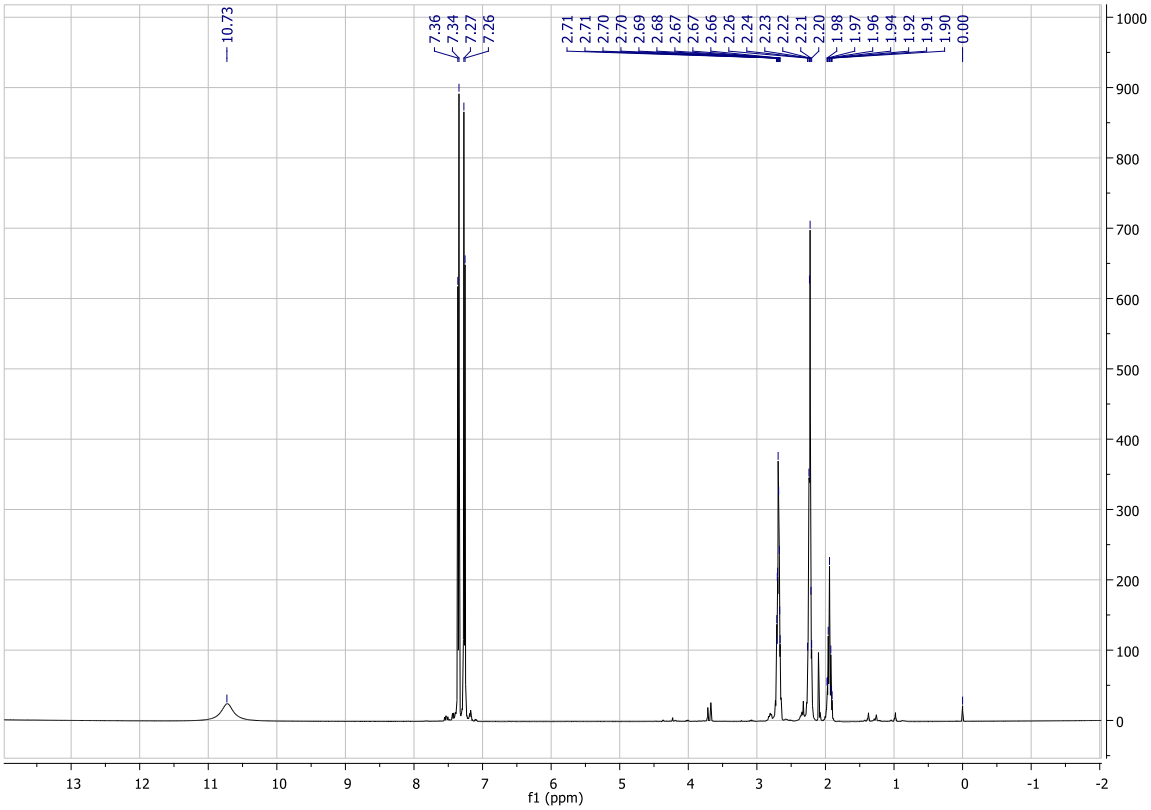
S-3h

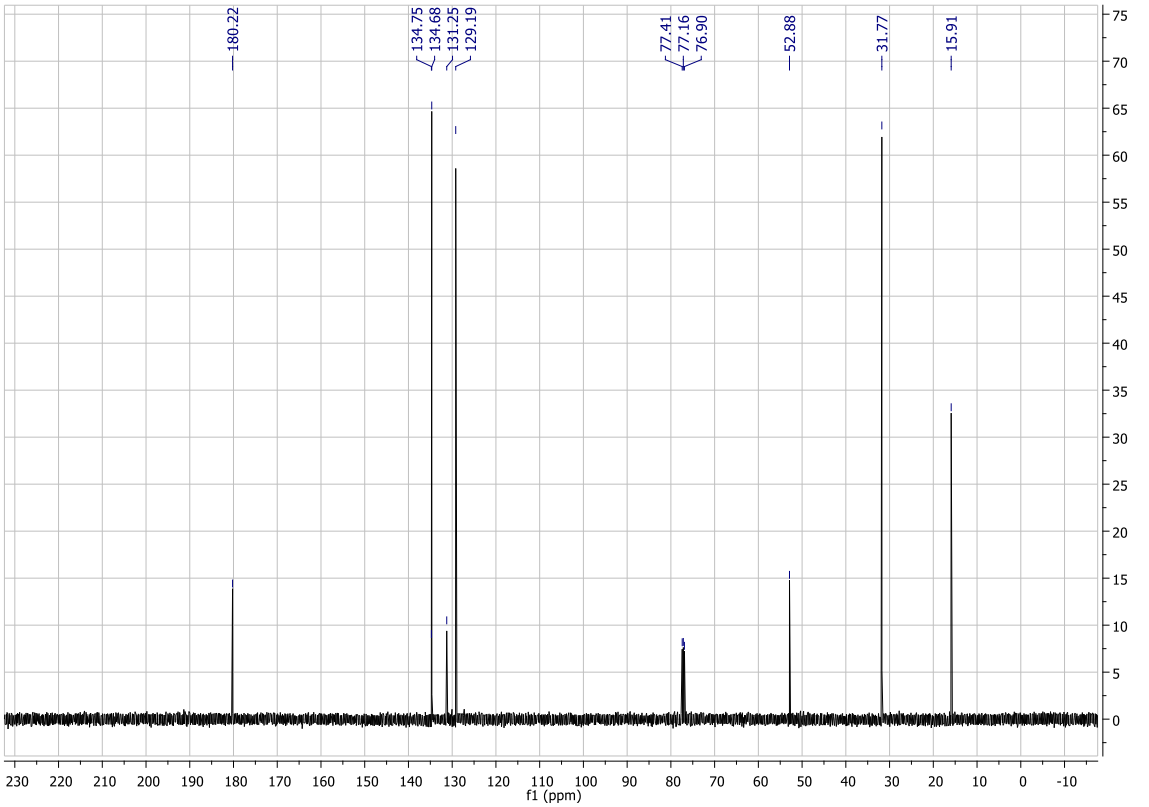

10.68
7.12
7.07
7.06
6.97
6.96
2.73
2.72
2.71
2.71
2.70
2.70
2.69
2.68
2.37
2.29
2.28
2.27
2.25
2.24
2.22
2.21
2.21
2.19
1.95
1.94
1.93
1.92
1.91
0.00
f1 (ppm)

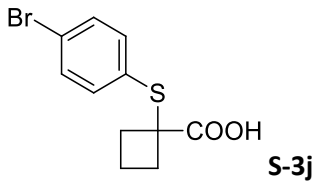

180.56
137.29
135.94
133.62
131.98
130.34
128.88
77.41
77.16
76.91
52.62
31.97
20.90
20.26
16.20
f1 (ppm)


Cl
S
COOH

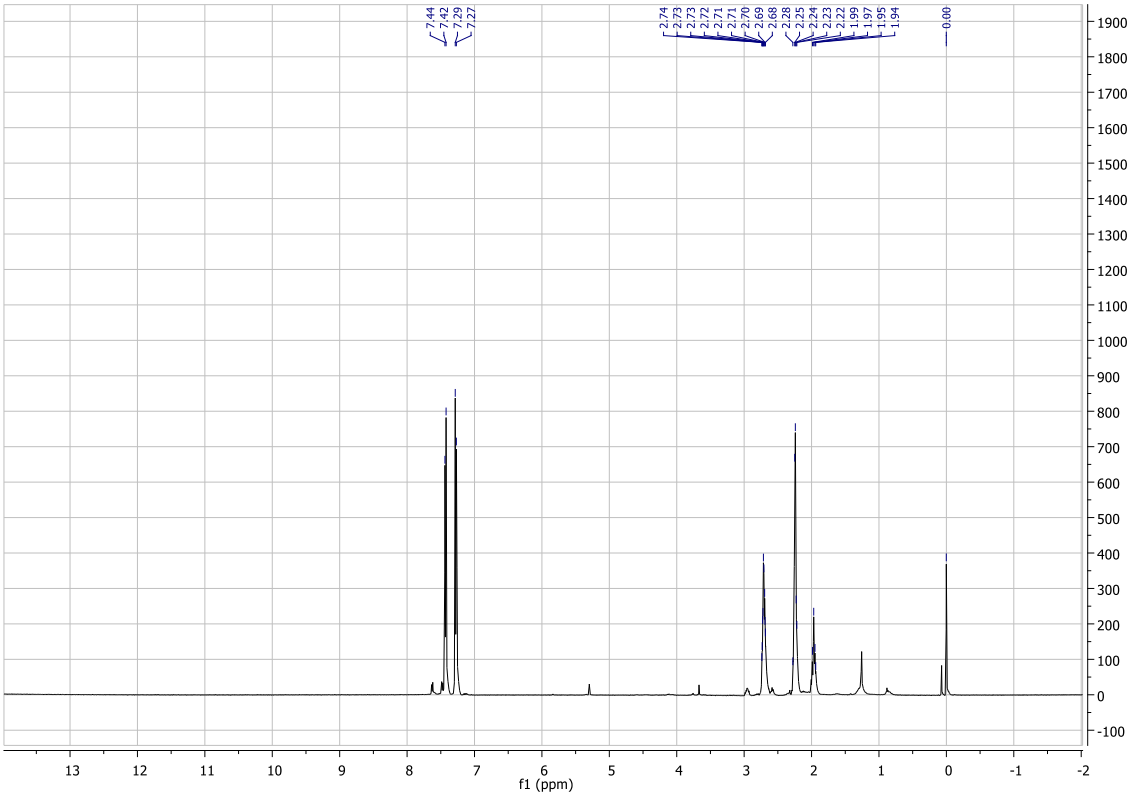
S-3i

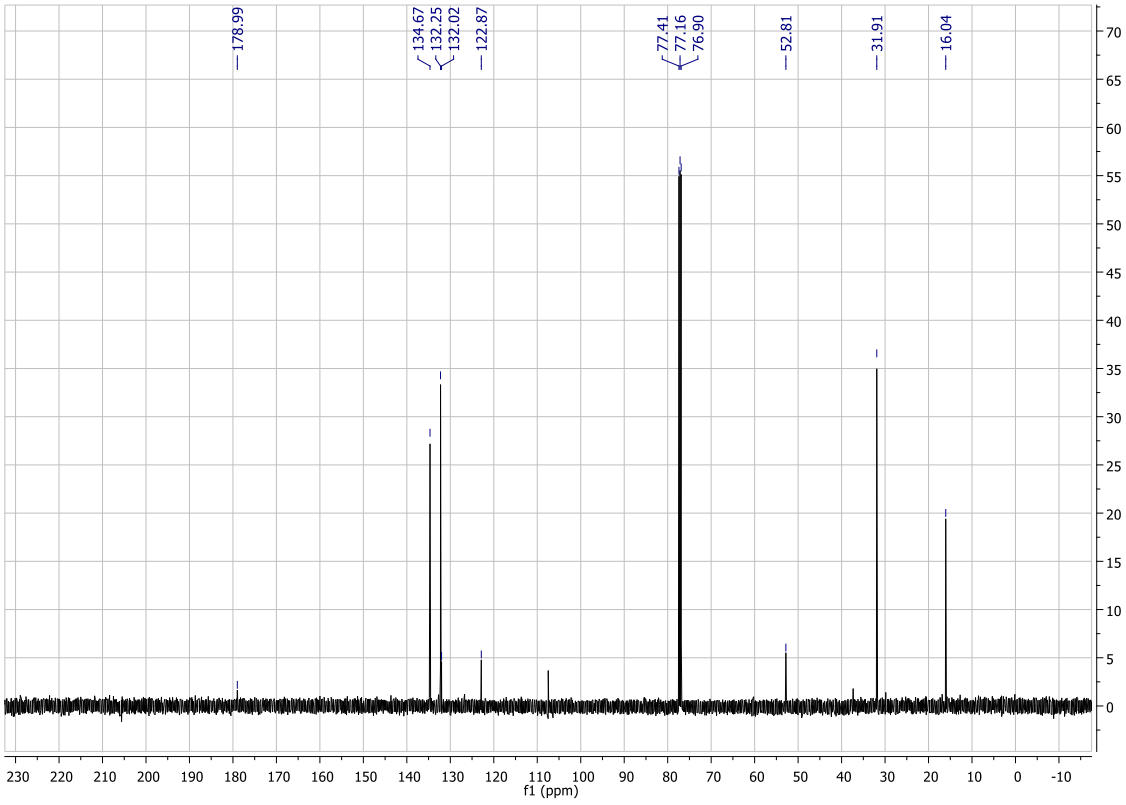

10.73
7.36
7.34
7.27
7.26
2.71
2.71
2.70
2.70
2.69
2.68
2.67
2.67
2.66
2.26
2.24
2.23
2.22
2.21
2.20
1.98
1.97
1.96
1.94
1.92
1.91
1.90
0.00
f1 (ppm)

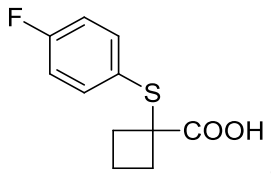

180.22
134.75
134.68
131.25
129.19
77.41
77.16
76.90
52.88
31.77
15.91
f1 (ppm)


Br
S
COOH

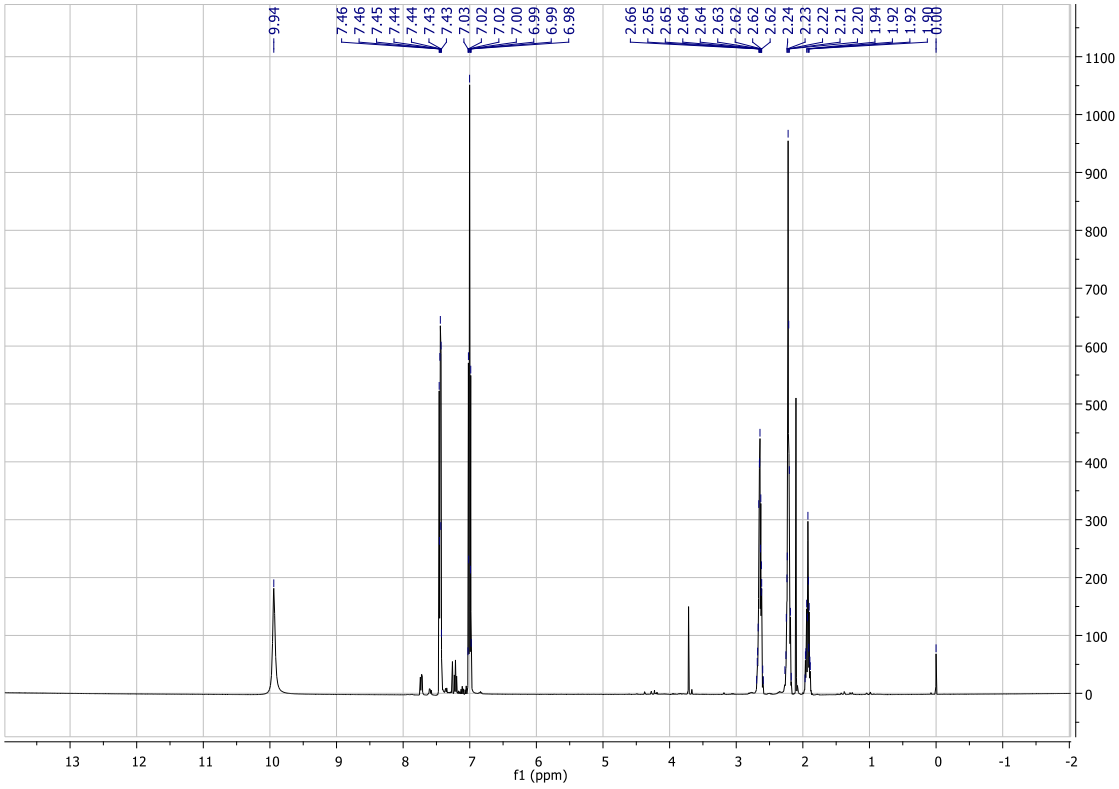
S-3j

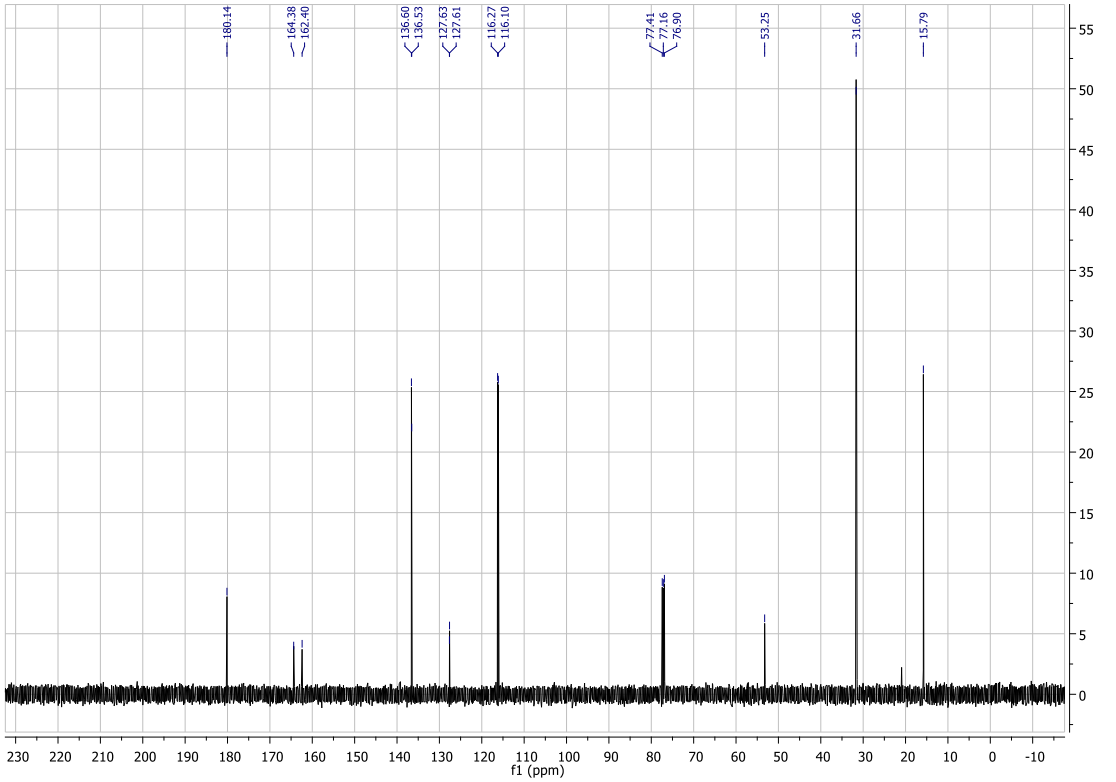

7.44
7.42
7.29
7.27
2.74
2.73
2.73
2.72
2.71
2.71
2.70
2.69
2.68
2.28
2.25
2.24
2.23
2.22
1.99
1.97
1.95
1.94
0.00
f1 (ppm)

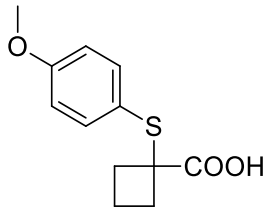

178.99
134.67
132.25
132.02
122.87
77.41
77.16
76.90
52.81
31.91
16.04
f1 (ppm)


F
S
COOH

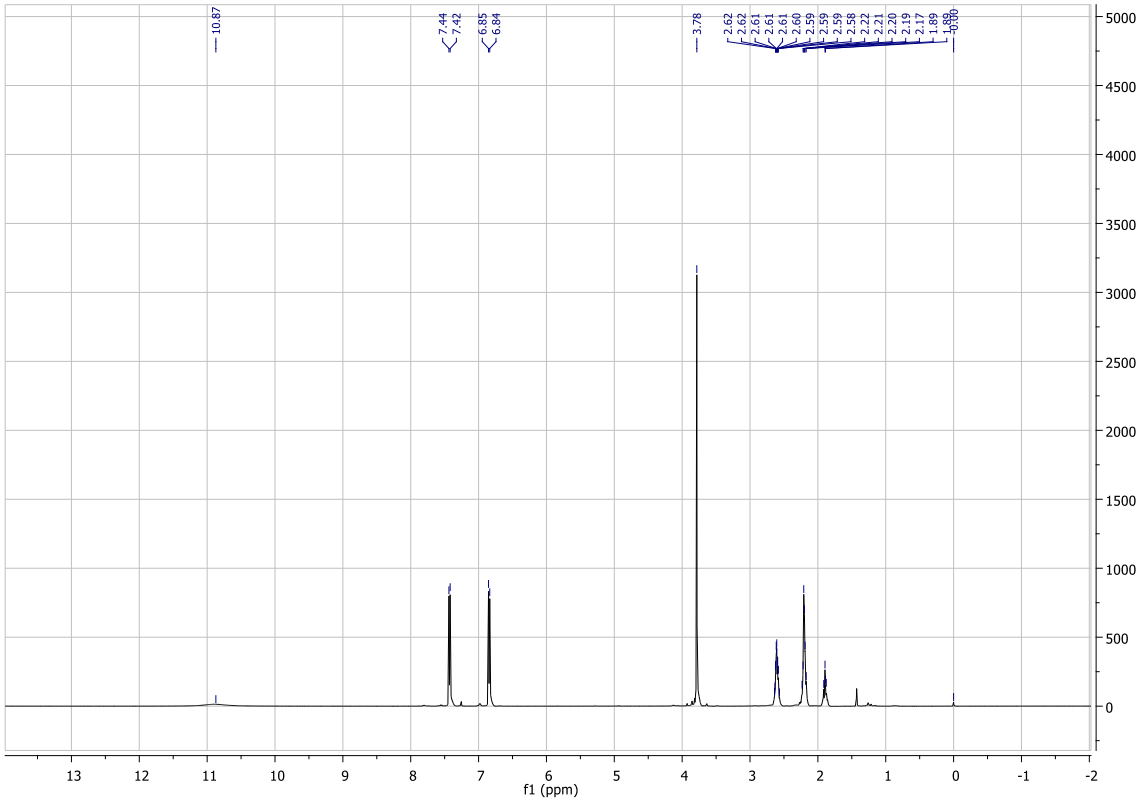
S-3k

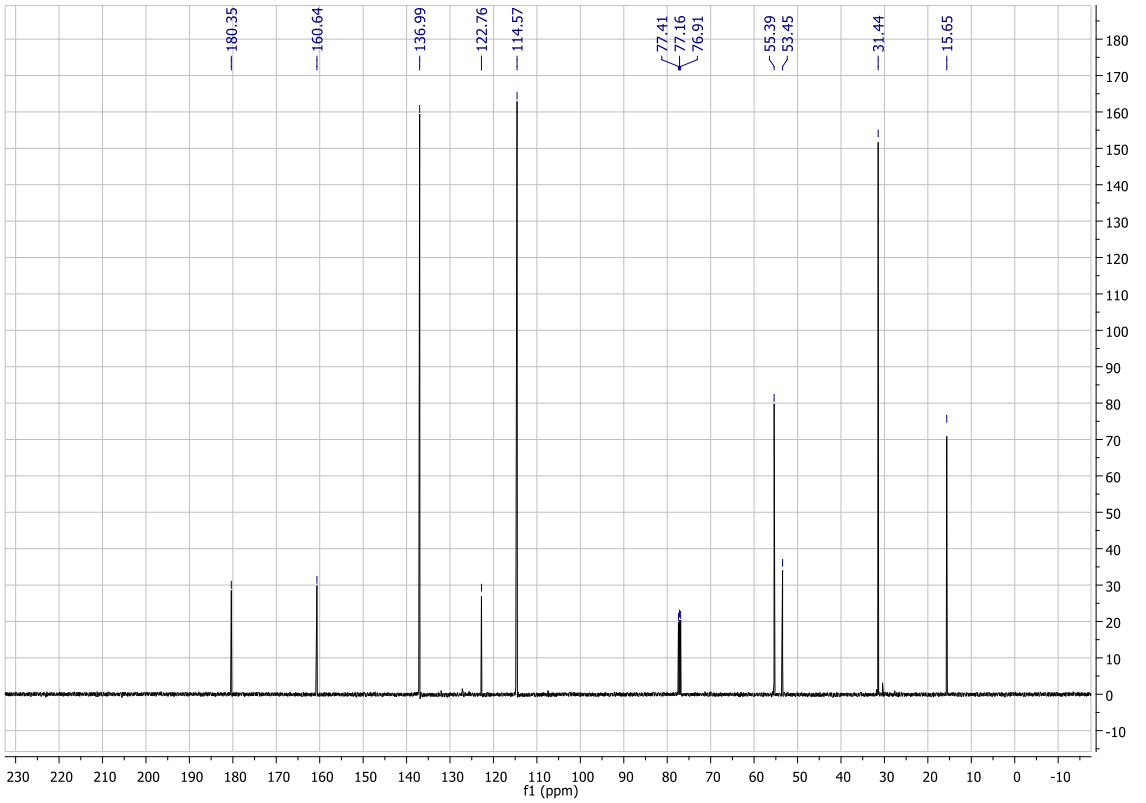

9.94
7.46
7.46
7.45
7.44
7.44
7.43
7.43
7.03
7.02
7.02
7.00
6.99
6.99
6.98
2.66
2.65
2.65
2.64
2.64
2.63
2.62
2.62
2.62
2.24
2.23
2.22
2.21
2.20
1.94
1.92
1.92
1.90
0.00
f1 (ppm)

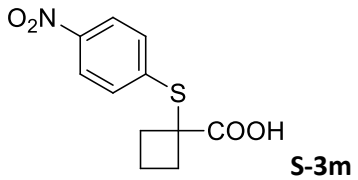

180.14
164.38
162.40
136.60
136.53
127.63
127.61
116.27
116.10
77.41
77.16
76.90
53.25
31.66
15.79
f1 (ppm)


O
S
COOH

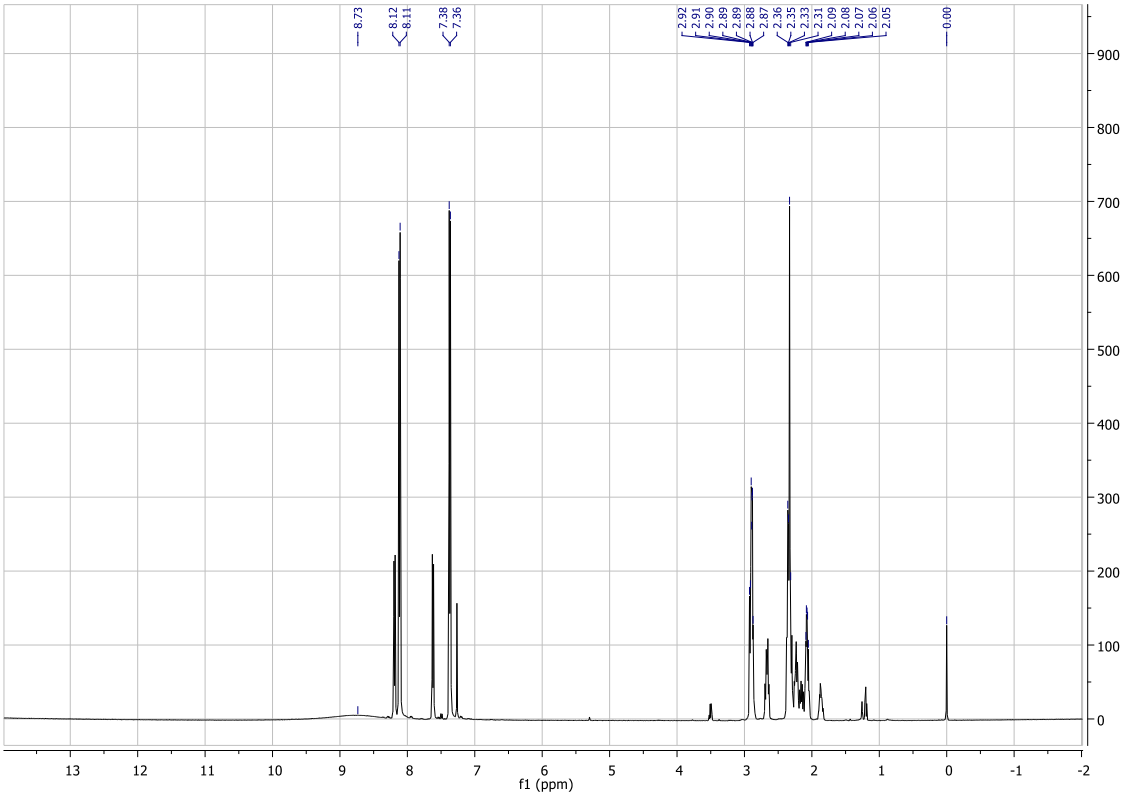
S-3l

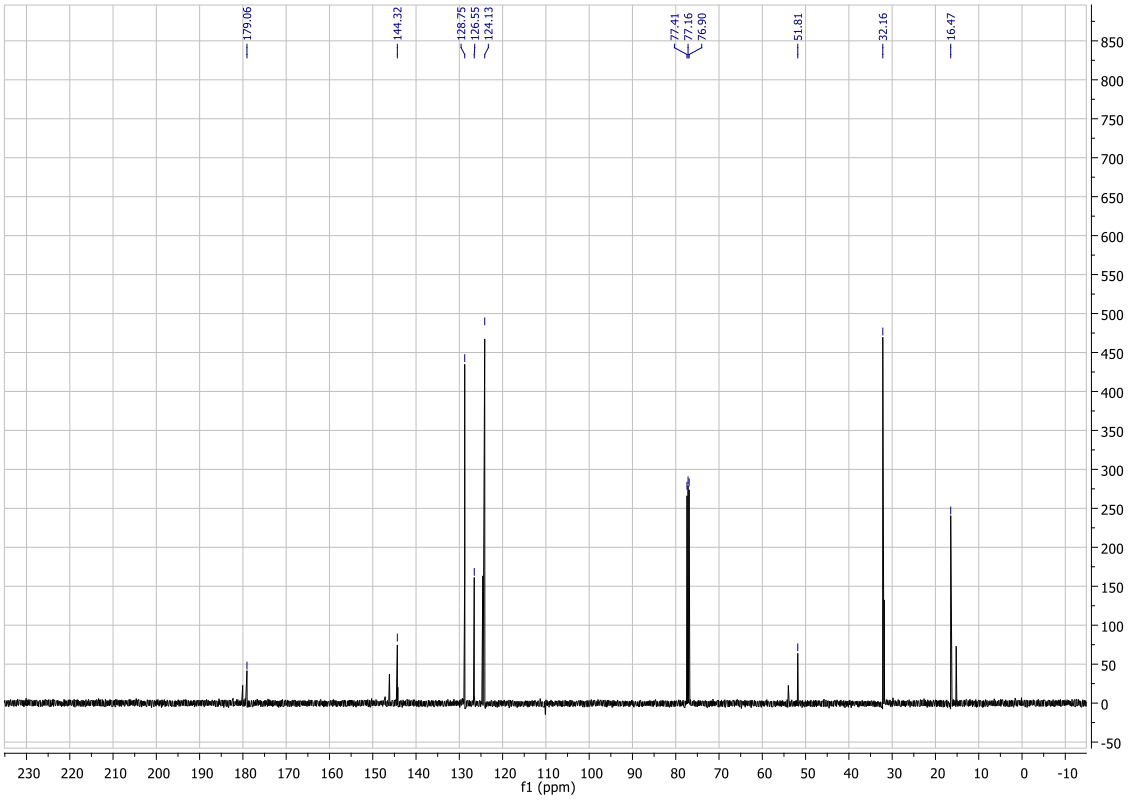

10.87
7.44
7.42
6.85
6.84
3.78
2.62
2.62
2.61
2.61
2.61
2.60
2.59
2.59
2.59
2.58
2.22
2.21
2.20
2.19
2.17
1.89
1.88
1.880
f1 (ppm)

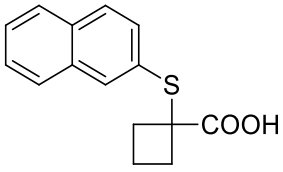

180.35
160.64
136.99
122.76
114.57
77.41
77.16
76.91
55.39
53.45
31.44
15.65
f1 (ppm)


O2N
S
COOH

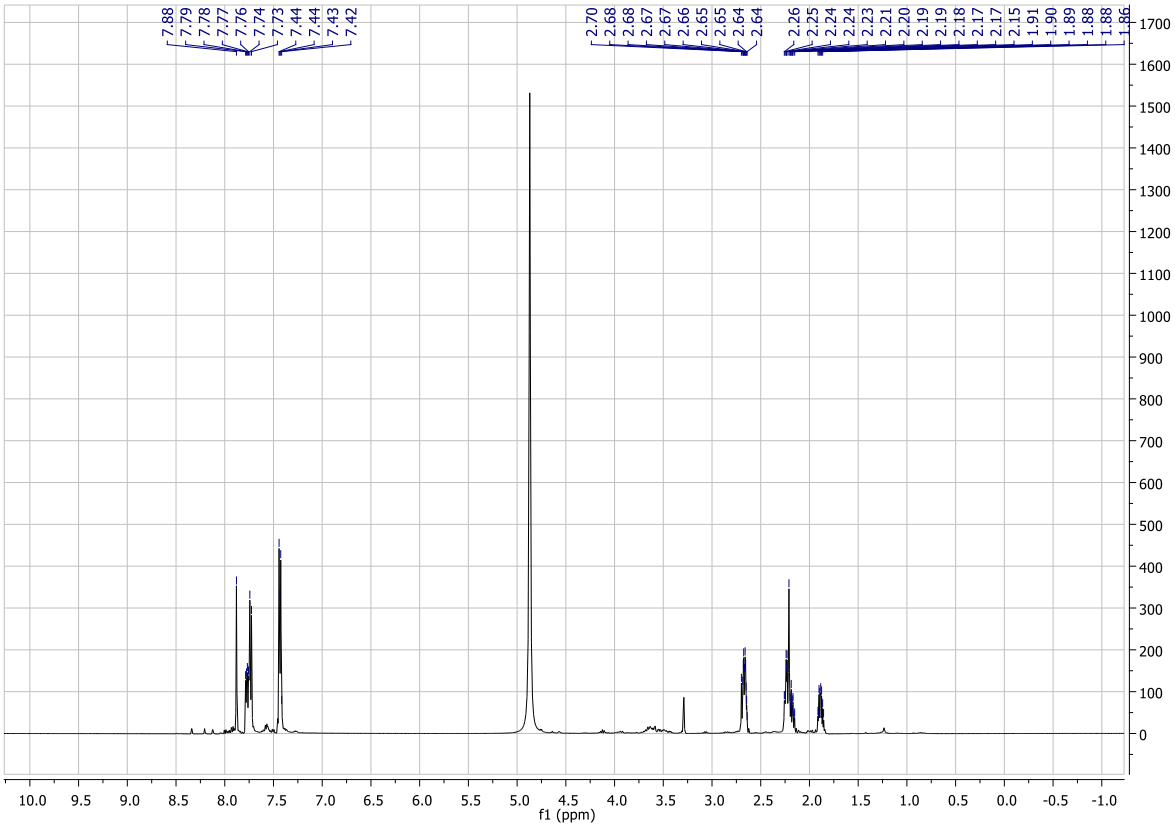
S-3m

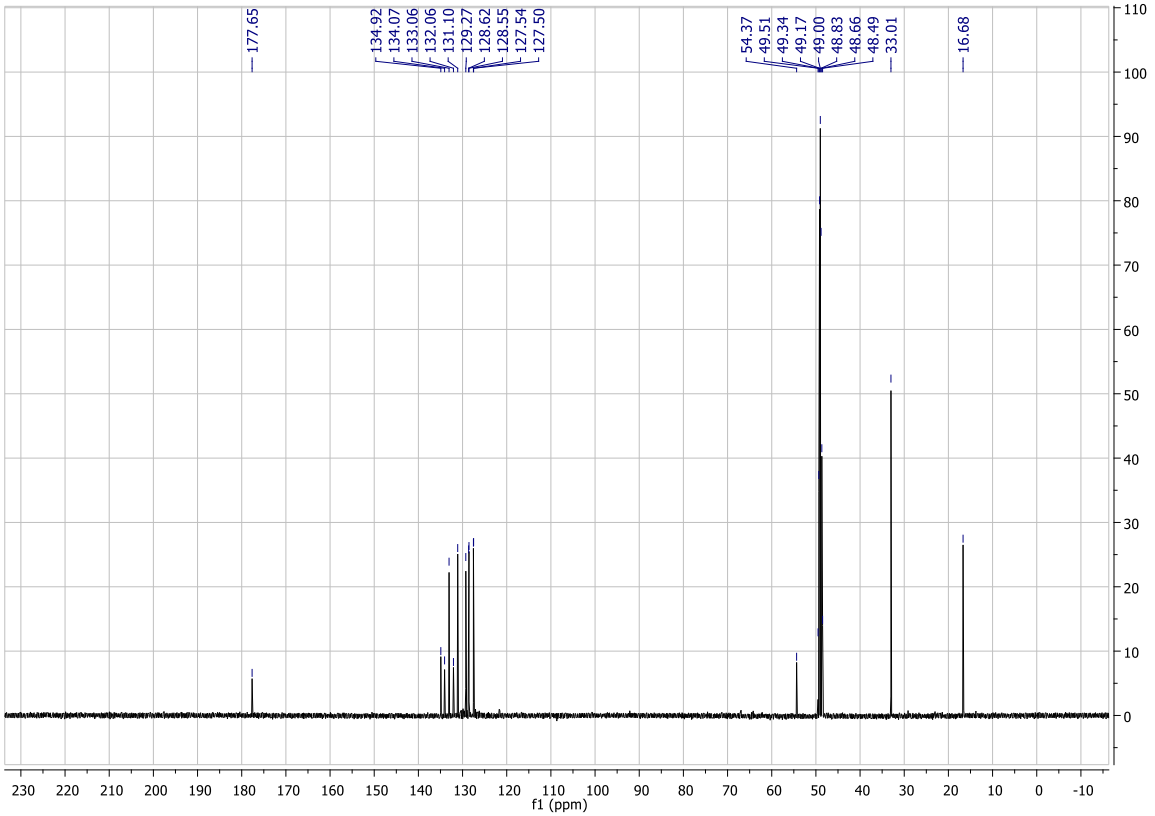

8.73
8.12
8.11
7.38
7.36
2.92
2.91
2.90
2.89
2.89
2.88
2.87
2.36
2.35
2.33
2.31
2.09
2.08
2.07
2.06
2.05
0.00
f1 (ppm)


179.06
144.32
128.75
126.55
124.13
77.41
77.16
76.90
51.81
32.16
16.47
f1 (ppm)


S
COOH

S-3n


7.88
7.79
7.78
7.77
7.76
7.74
7.73
7.44
7.44
7.43
7.42
2.70
2.68
2.68
2.67
2.67
2.66
2.65
2.65
2.64
2.64
2.26
2.25
2.24
2.24
2.23
2.21
2.20
2.19
2.19
2.18
2.17
2.17
2.15
1.91
1.90
1.89
1.88
1.88
1.86
f1 (ppm)


177.65
134.92
134.07
133.06
132.06
131.10
129.27
128.62
128.55
127.54
127.50
54.37
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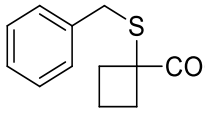
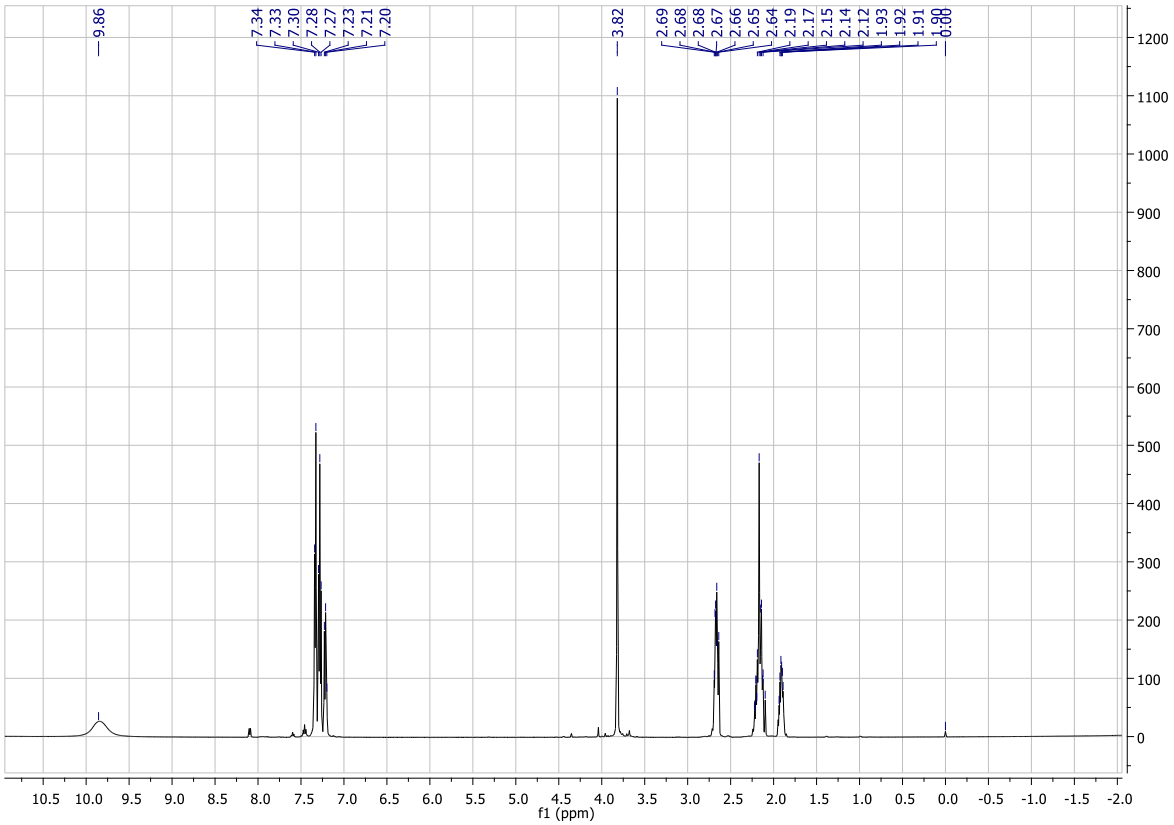
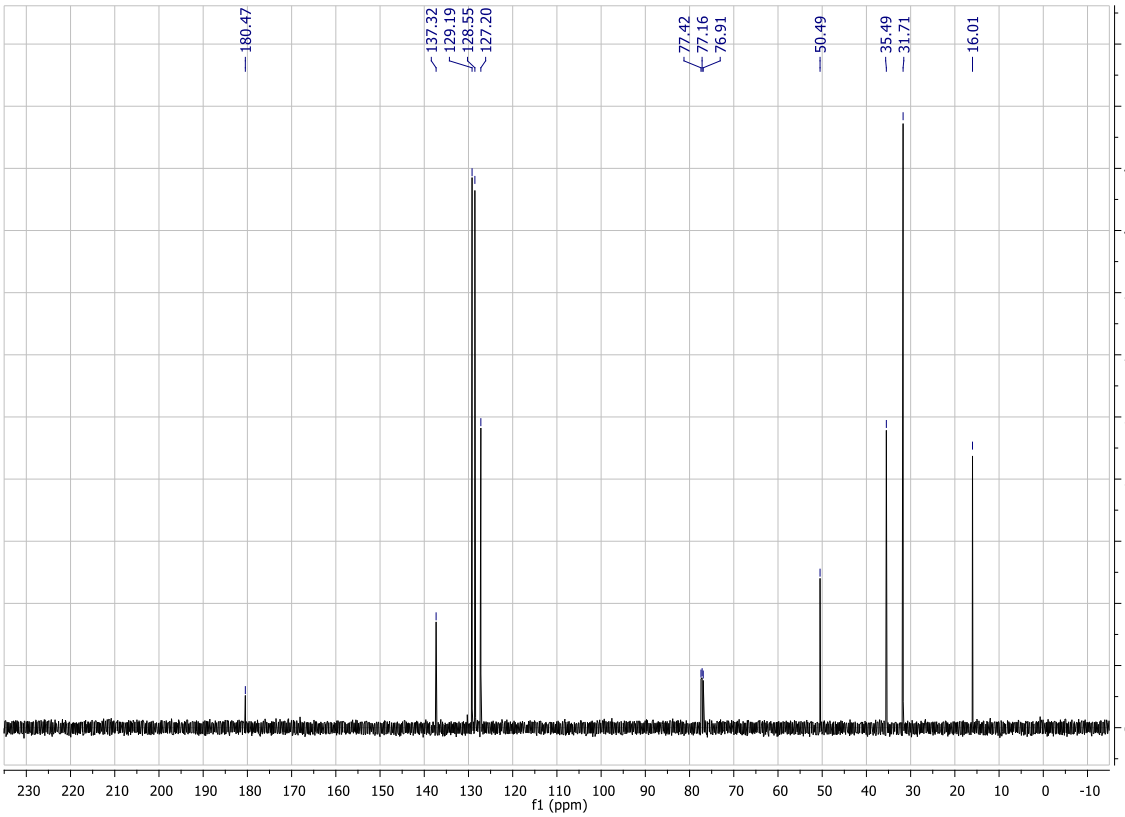
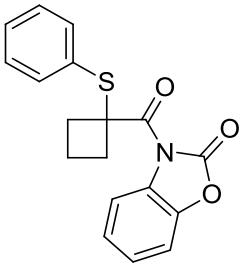
48.83
48.66
48.49
33.01
16.68
f1 (ppm)


S
COOH

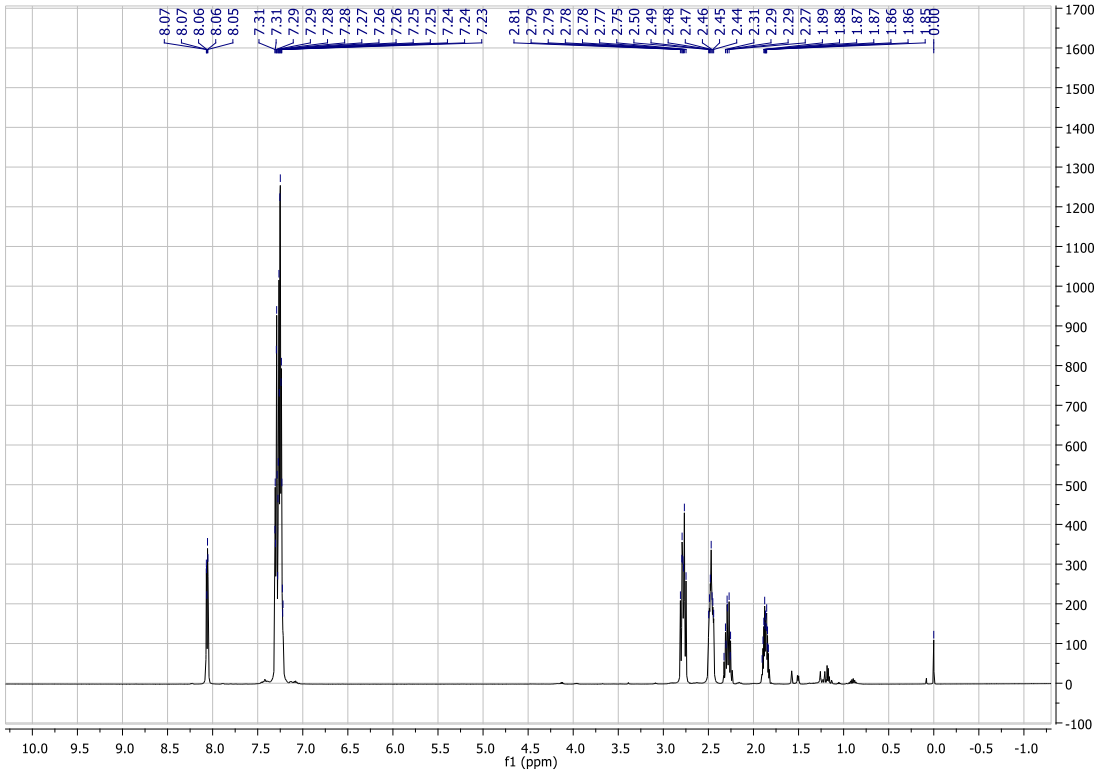
S-3o


9.86
7.34
7.33
7.30
7.28
7.27
7.23
7.21
7.20
3.82
2.69
2.68
2.68
2.67
2.66
2.65
2.64
2.19
2.17
2.15
2.14
2.12
1.93
1.92
1.91
0.00
f1 (ppm)


180.47
137.32
129.19
128.55
127.20
77.42
77.16
76.91
50.49
35.49
31.71
16.01
f1 (ppm)



S-5a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8.07
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8.06
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7.29
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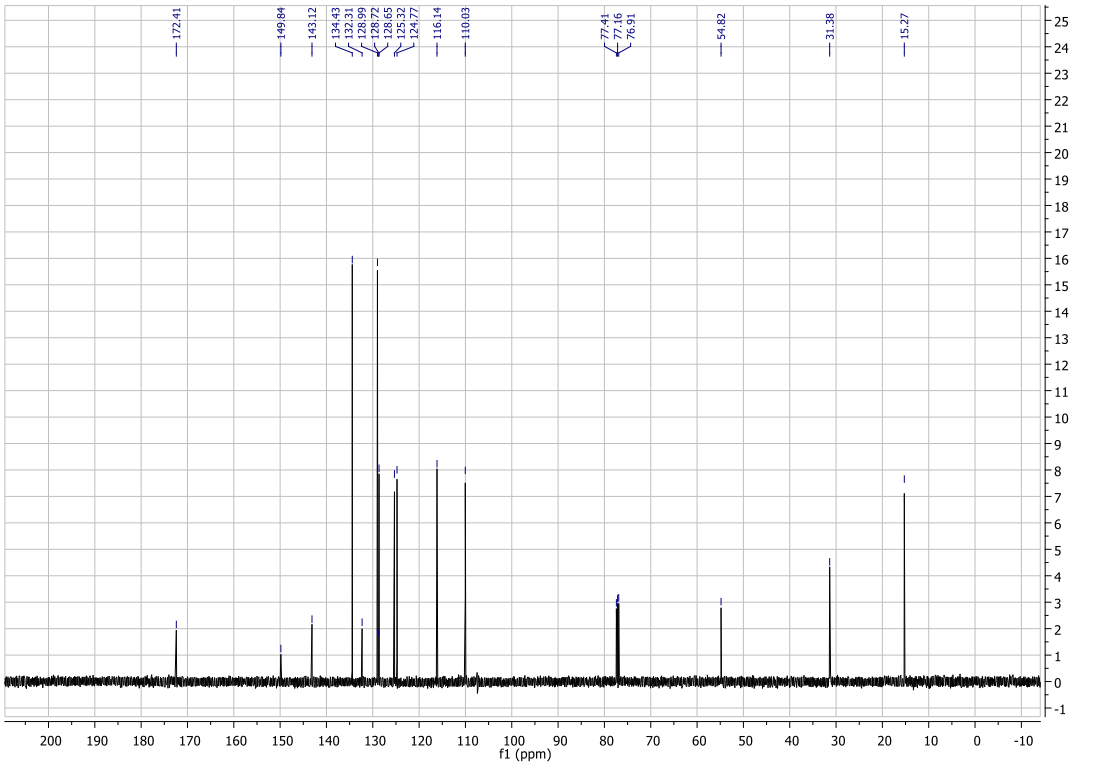
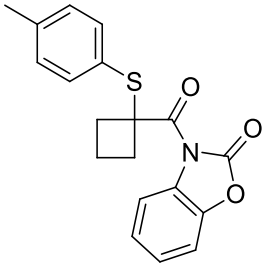
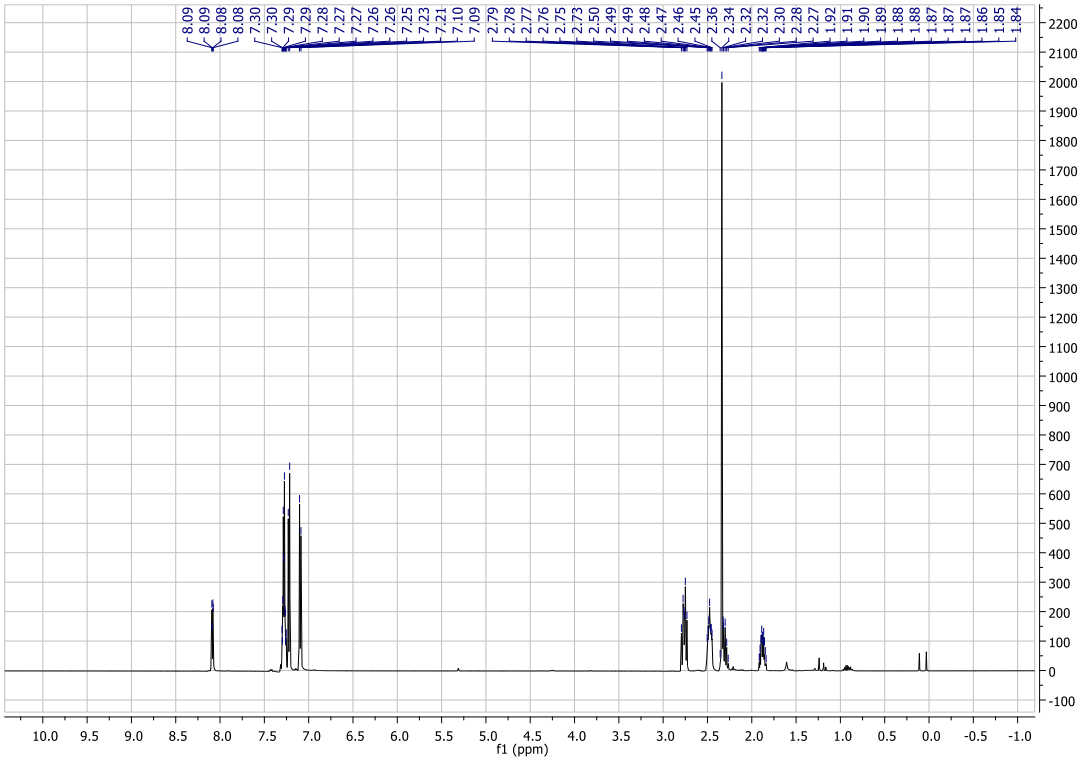
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.23
2.81
2.79
2.79
2.78
2.78
2.77
2.75
2.50
2.49
2.48
2.47
2.46
2.45
2.44
2.31
2.29
2.29
2.27
1.89
1.88
1.87
1.87
1.86
1.86
0.00
f1 (ppm)


172.41
149.84
143.12
134.43
132.31
128.99
128.72
128.65
125.32
124.77
116.14
110.03
77.41
77.16
76.91
54.82
31.38
15.27
f1 (ppm)


S
O
N
O
O

S-5b


8.09
8.09
8.08
8.08
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7.30
7.29
7.29
7.29
7.28
7.27
7.27
7.26
7.26
7.25
7.23
7.21
7.10
7.09
2.79
2.78
2.77
2.77
2.76
2.75
2.73
2.50
2.49
2.49
2.48
2.47
2.46
2.45
2.36
2.34
2.32
2.32
2.30
2.28
2.27
1.92
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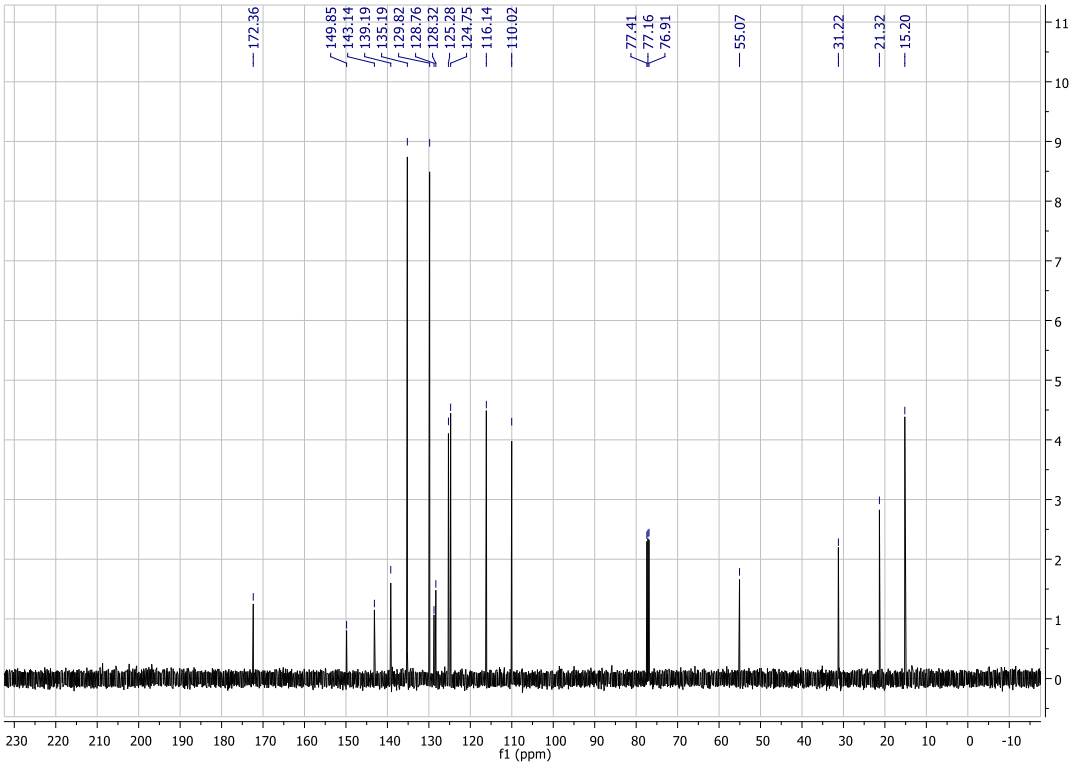
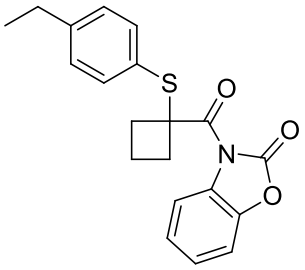
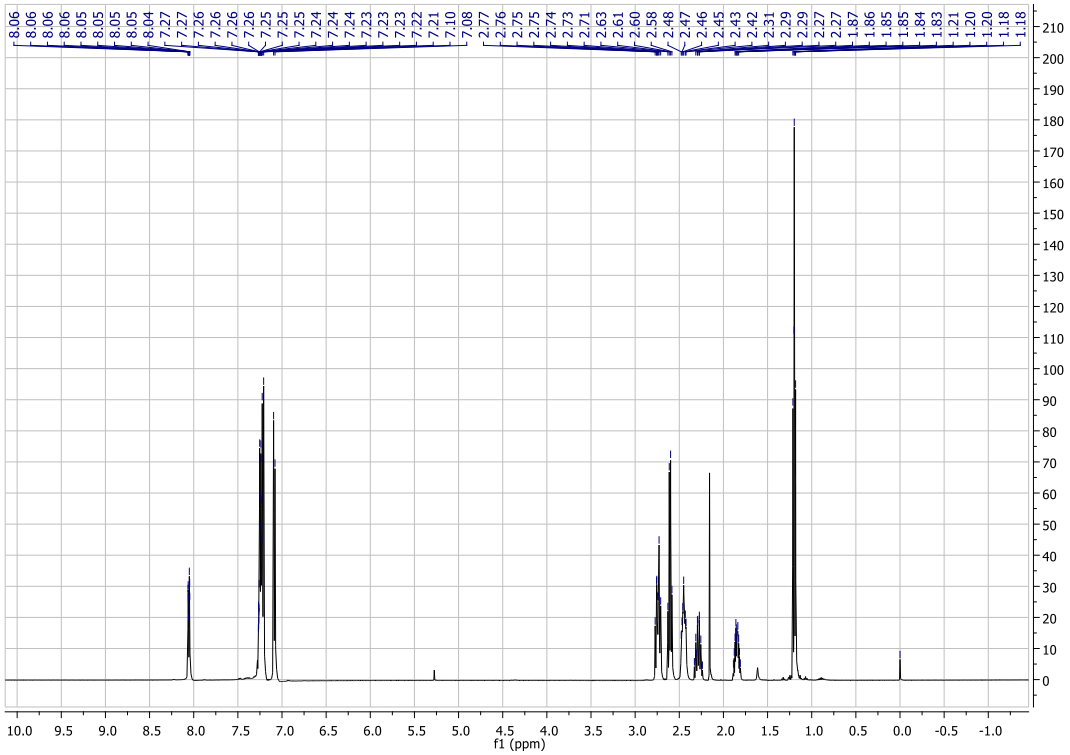
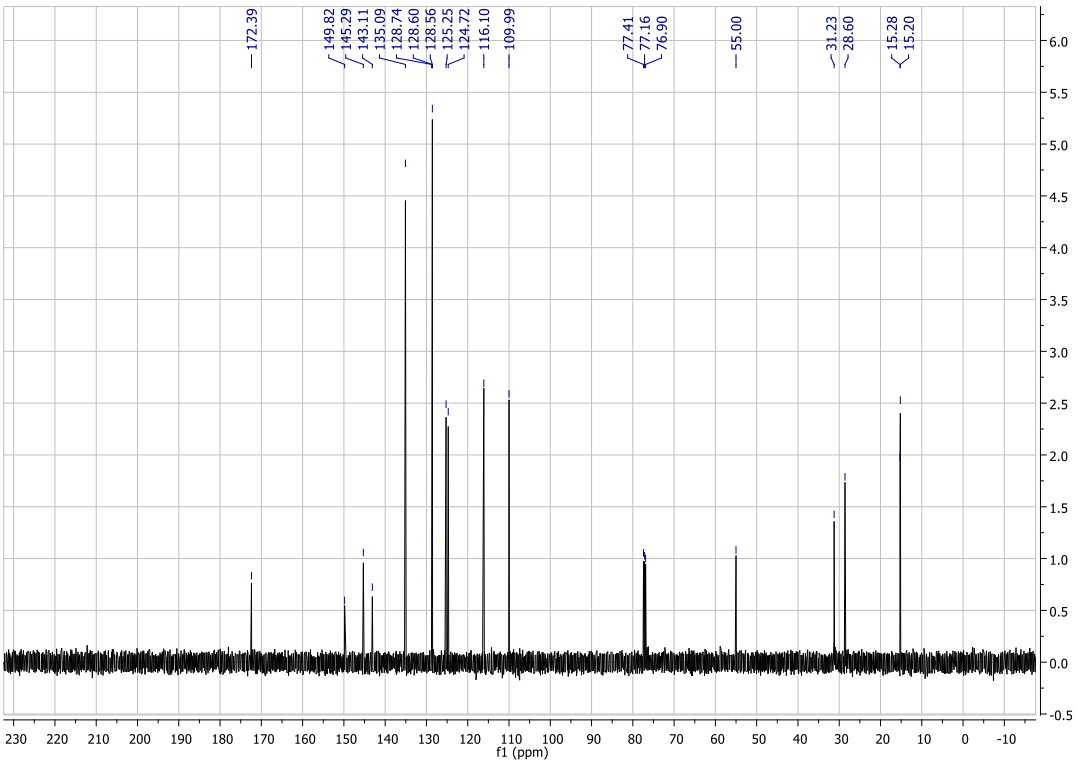
1.87
1.86
1.85
1.84
f1 (ppm)


172.36
149.85
143.14
139.19
135.19
129.82
128.76
128.32
125.28
124.75
116.14
110.02
77.41
77.16
76.91
55.07
31.22
21.32
15.20
f1 (ppm)



S-5c


f1 (ppm)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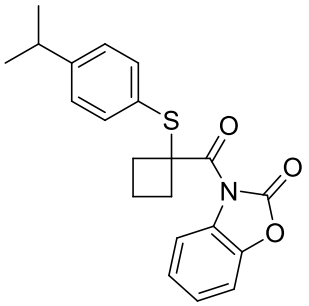
145.29
143.11
135.09
128.74
128.60
128.56
125.25
124.72
116.10
109.99
77.41
77.16
76.90
55.00
31.23
28.60
15.28
15.20
f1 (ppm)


S
O
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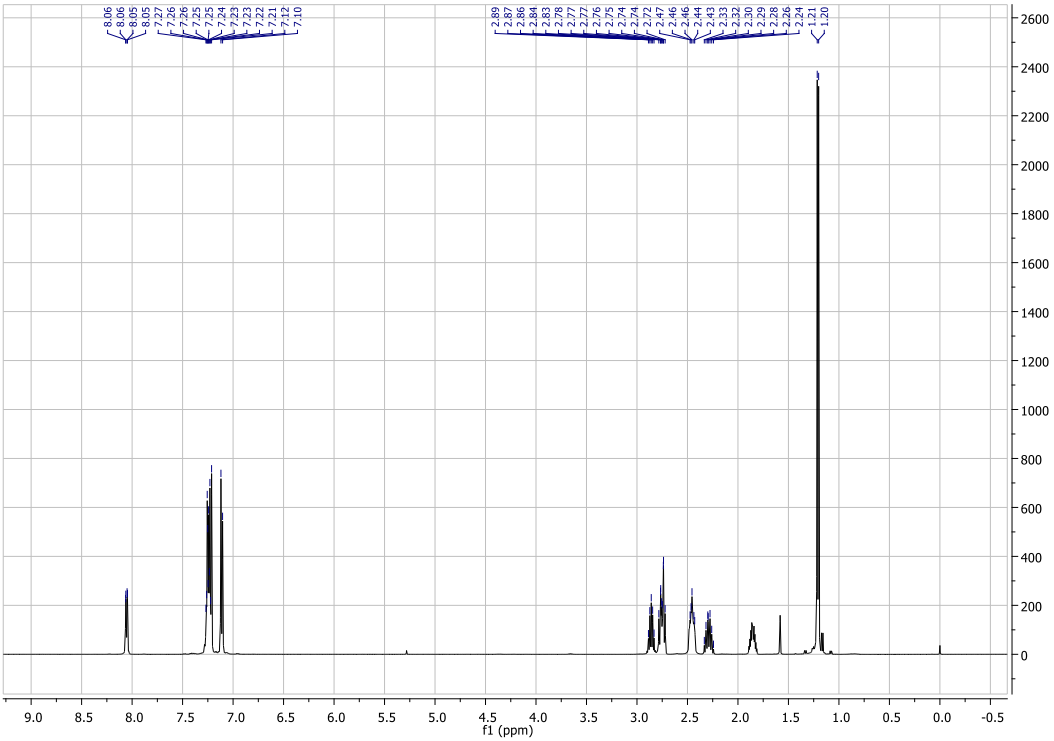
N
O

S-5d


8.06
8.06
8.05
8.05
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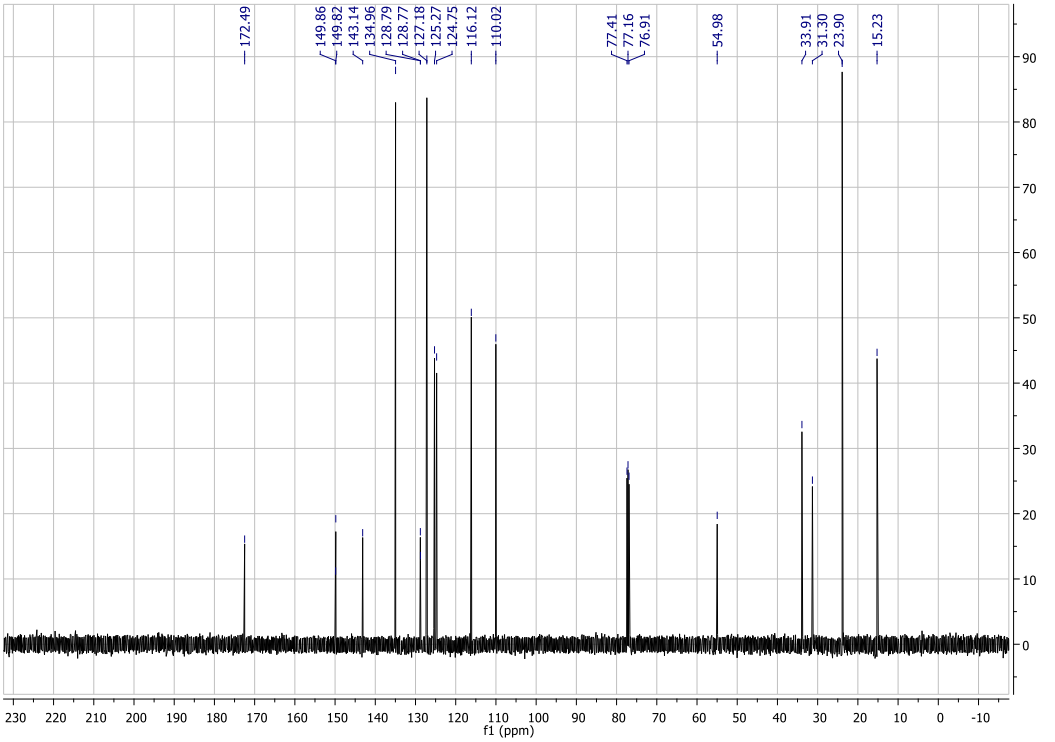
7.26
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.12
7.10
2.89
2.87
2.86
2.84
2.83
2.78
2.77
2.77
2.76
2.75
2.74
2.74
2.72
2.47
2.46
2.46
2.44
2.43
2.33
2.32
2.30
2.29
2.28
2.26
2.24
1.21
1.20
f1 (ppm)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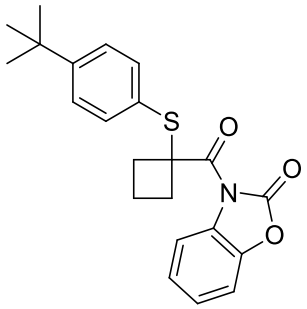
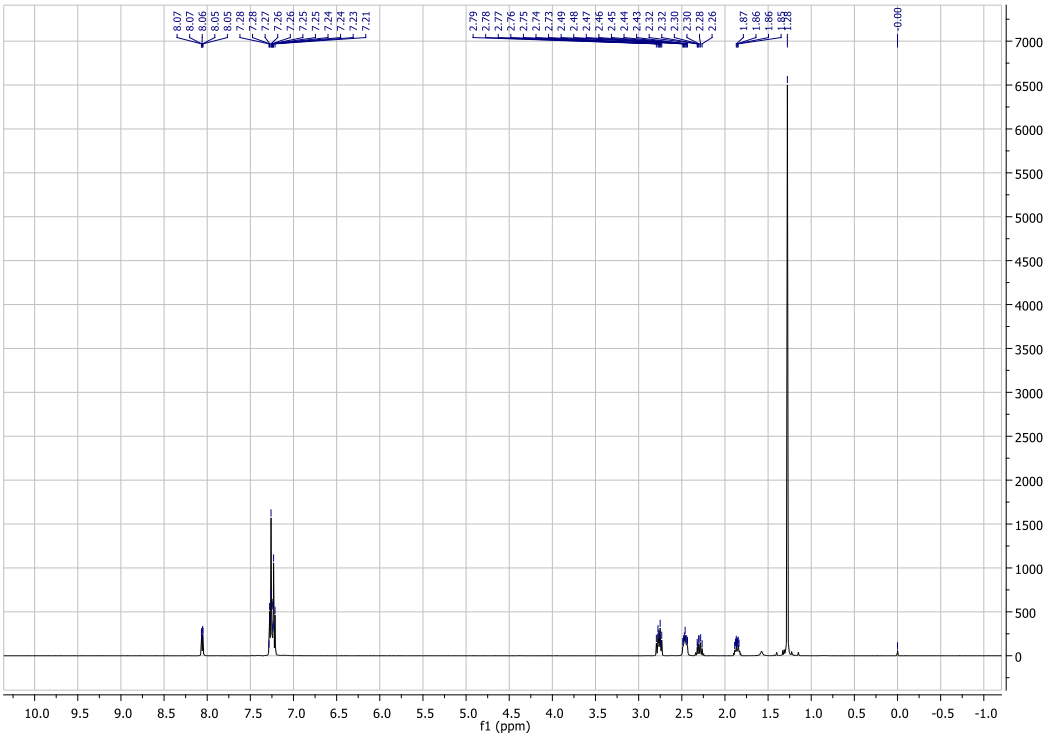
149.86
149.82
143.14
134.96
128.79
128.77
127.18
125.27
124.75
116.12
110.02
77.41
77.16
76.91
54.98
33.91
31.30
23.90
15.23
f1 (ppm)


S
O
O
N
O

S-5e


8.07
8.07
8.06
8.05
8.05
7.28
7.28
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.21
2.79
2.78
2.77
2.76
2.75
2.74
2.73
2.49
2.48
2.47
2.46
2.45
2.44
2.43
2.32
2.32
2.30
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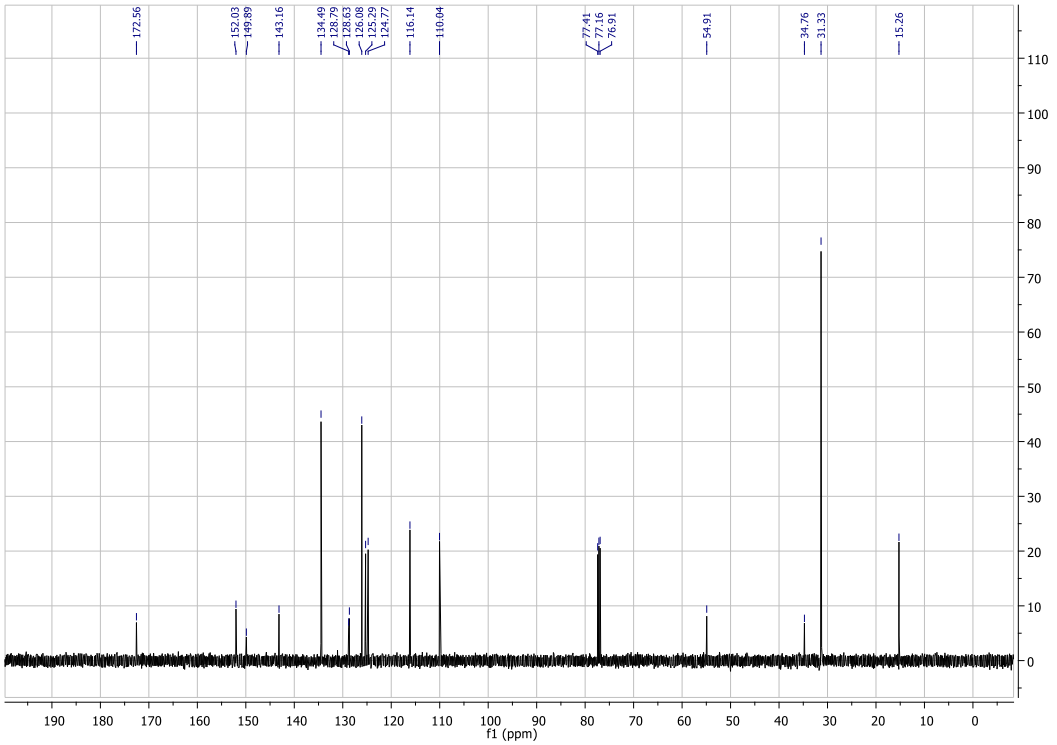
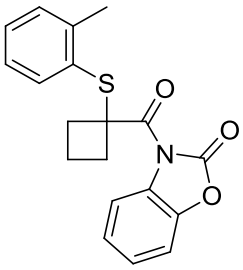
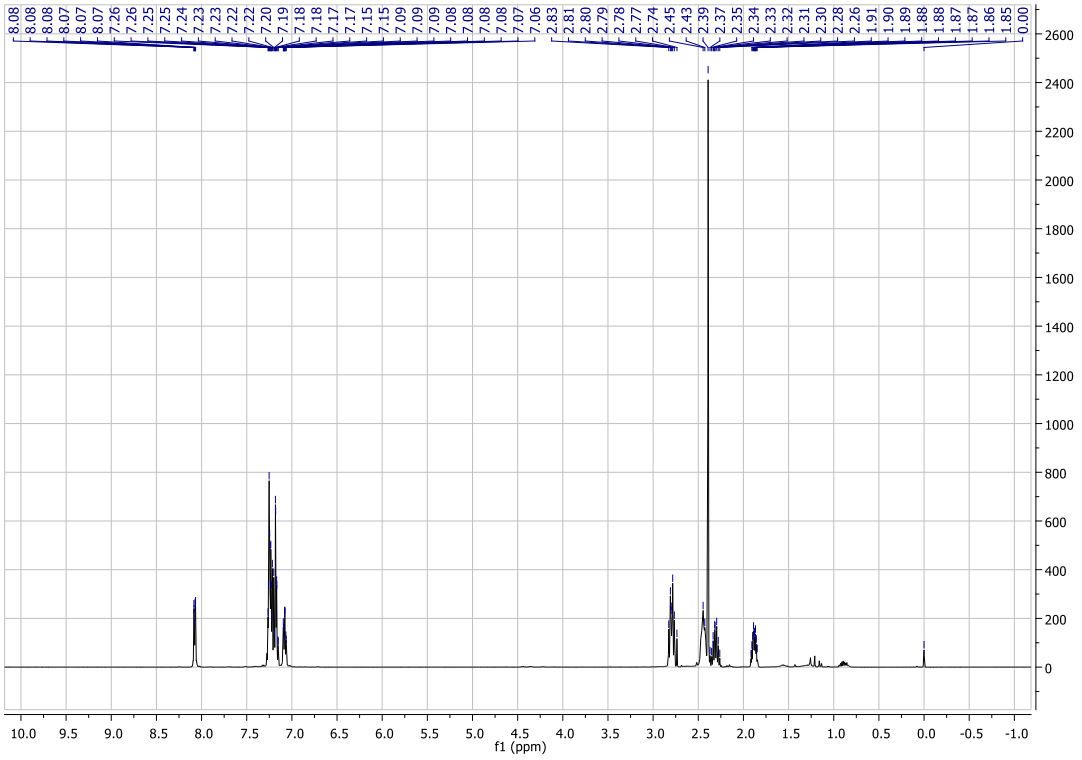
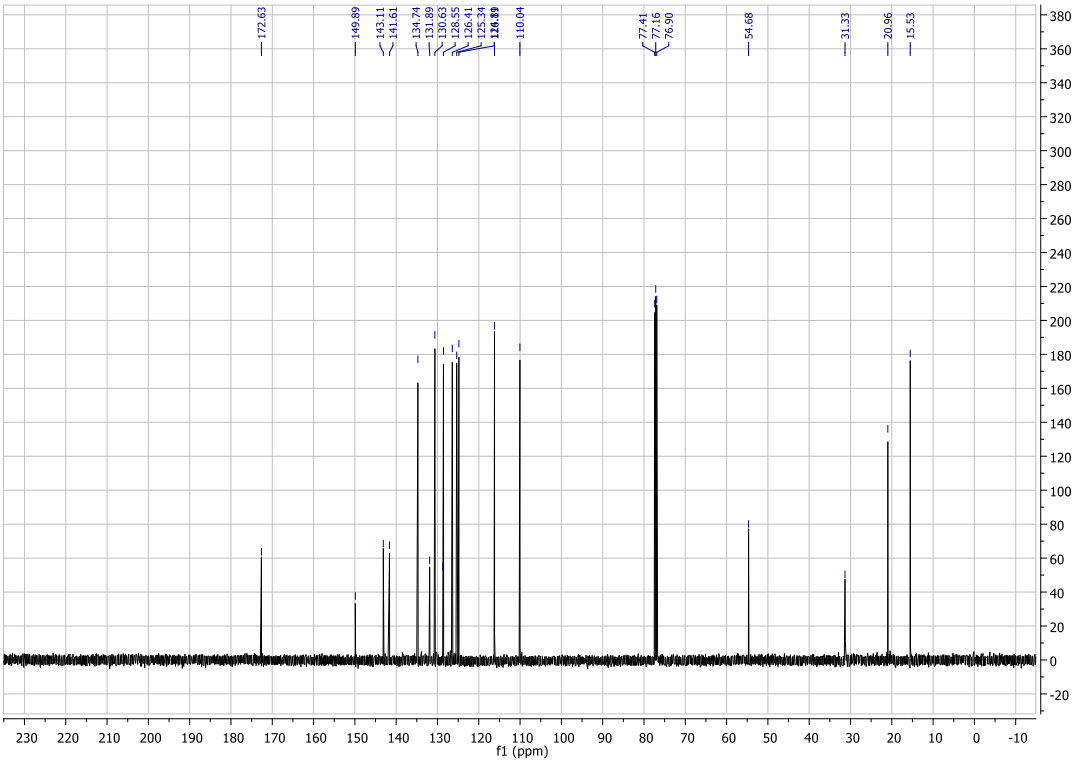
2.28
2.26
1.87
1.86
1.86
1.85
1.28
0.00
f1 (ppm)

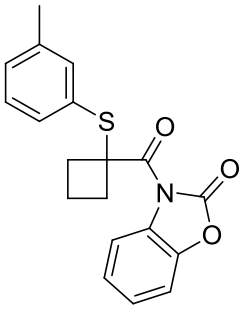

172.56
152.03
149.89
143.16
134.49
128.79
128.63
126.08
125.29
124.77
116.14
110.04
77.41
77.16
76.91
54.91
34.76
31.33
15.26
f1 (ppm)



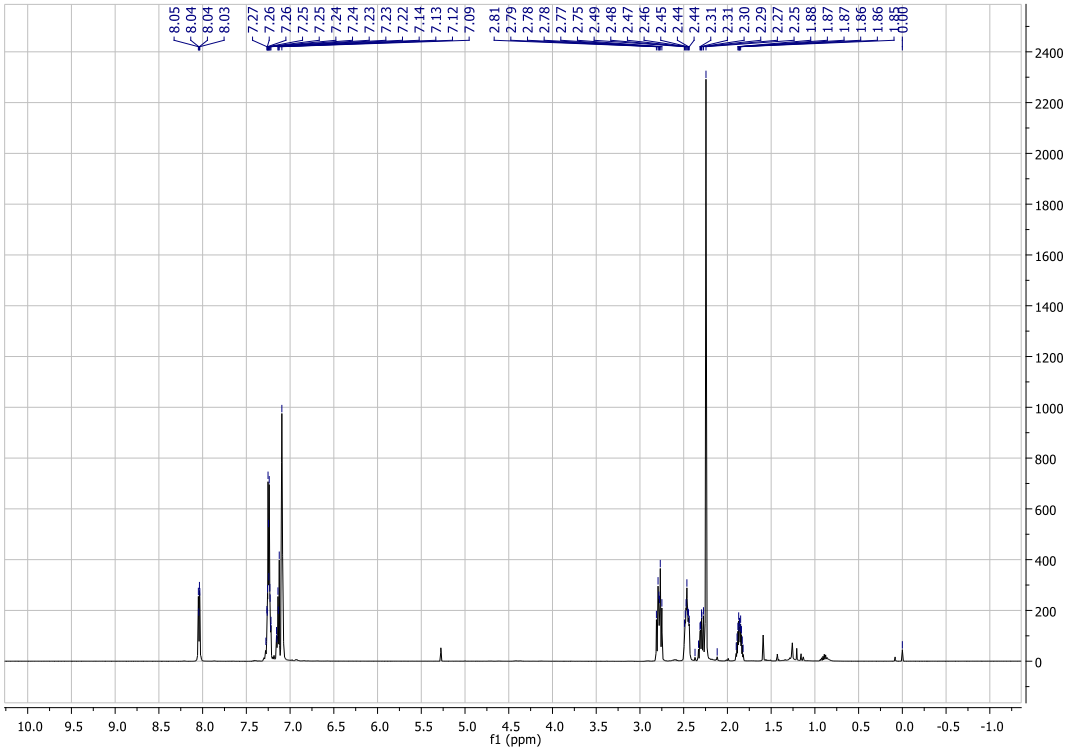
S-5f

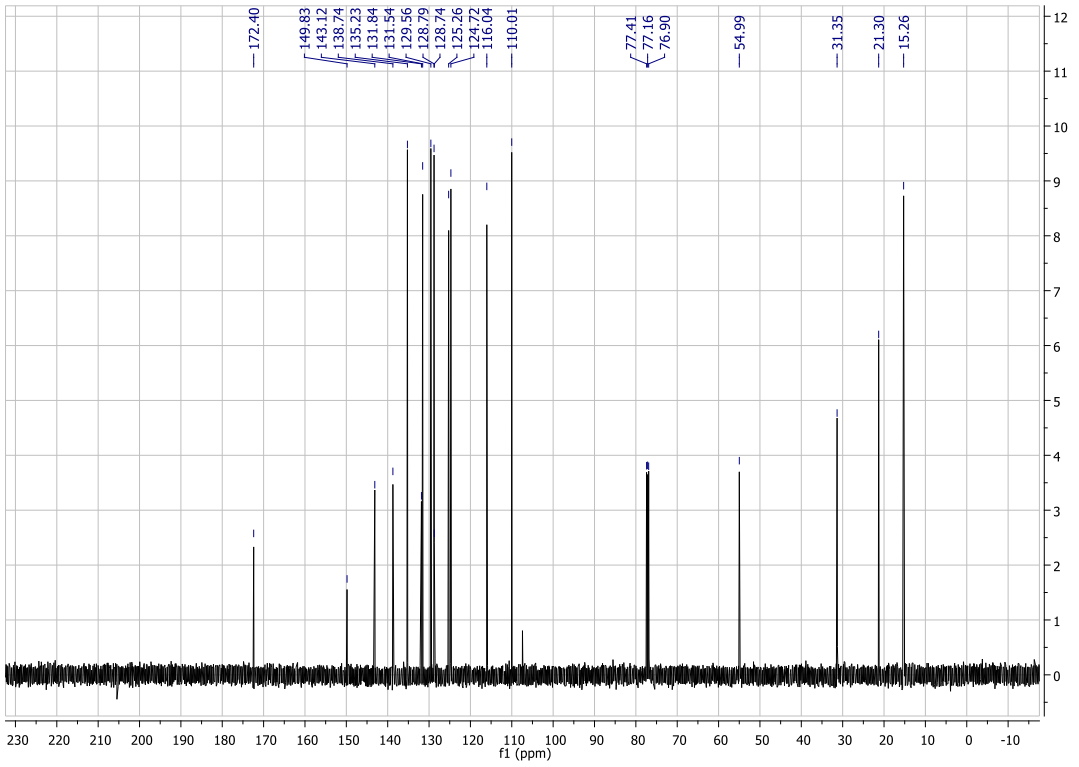





S
O
O
N
O

S-5g


8.05
8.04
8.04
8.03
7.27
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.22
7.14
7.13
7.12
7.09
2.81
2.79
2.78
2.78
2.77
2.75
2.49
2.48
2.47
2.46
2.45
2.44
2.44
2.31
2.31
2.30
2.29
2.27
2.25
1.88
1.87
1.87
1.86
1.86
1.85
0.00
f1 (ppm)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135.23
131.84
131.54
129.56
128.79
128.74
125.26
124.72
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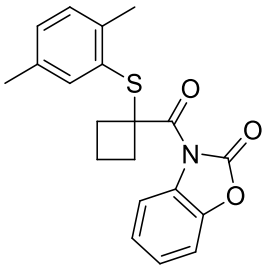
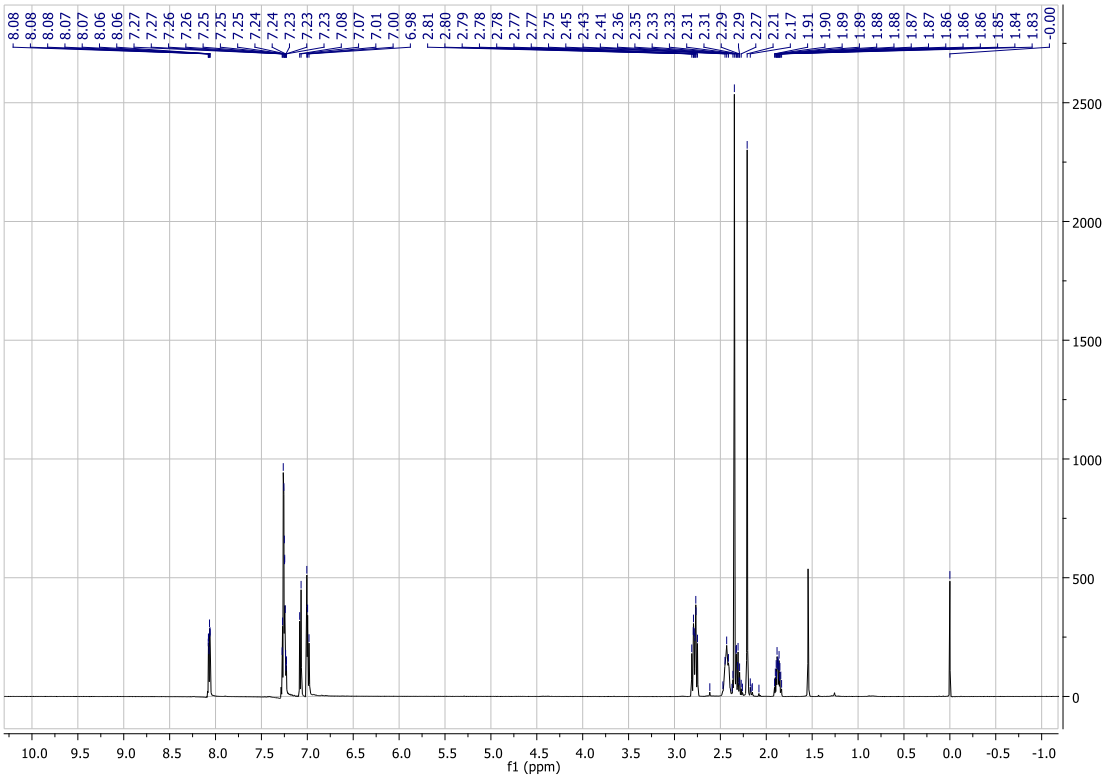
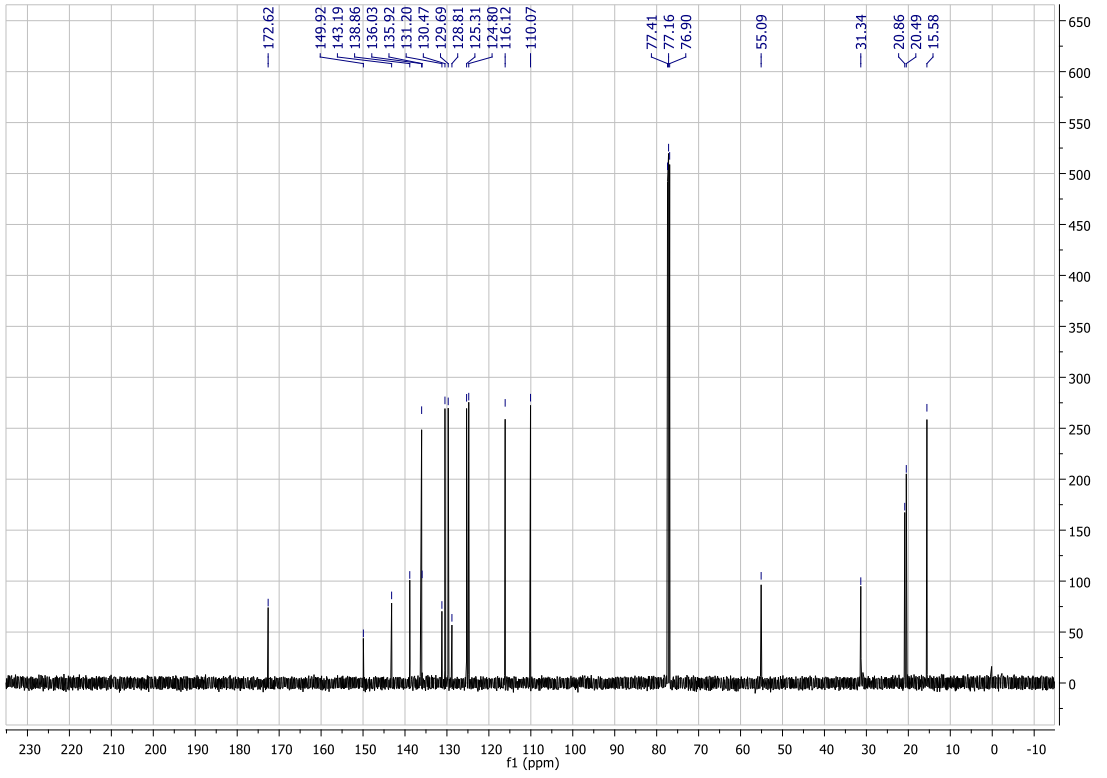
110.01
77.41
77.16
76.90
54.99
31.35
21.30
15.26
f1 (ppm)


S
O
N
O
O

S-5h


8.08 8.08 8.08 8.07 8.07 8.06 8.06 7.27 7.27 7.26 7.26 7.25 7.25 7.25 7.24 7.24 7.23 7.23 7.23 7.08 7.07 7.01 7.00 6.98 2.81 2.80 2.79 2.78 2.78 2.77 2.77 2.75 2.45 2.43 2.41 2.36 2.35 2.33 2.33 2.31 2.31 2.29 2.29 2.27 2.21 2.17 1.91 1.90 1.89 1.89 1.88 1.88 1.87 1.87 1.86 1.86 1.86 1.85 1.84 1.83 -0.00
2500
2000
1500
1000
500
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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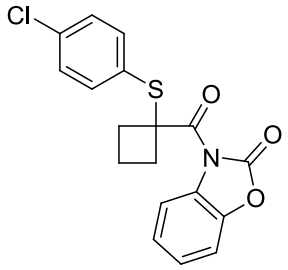
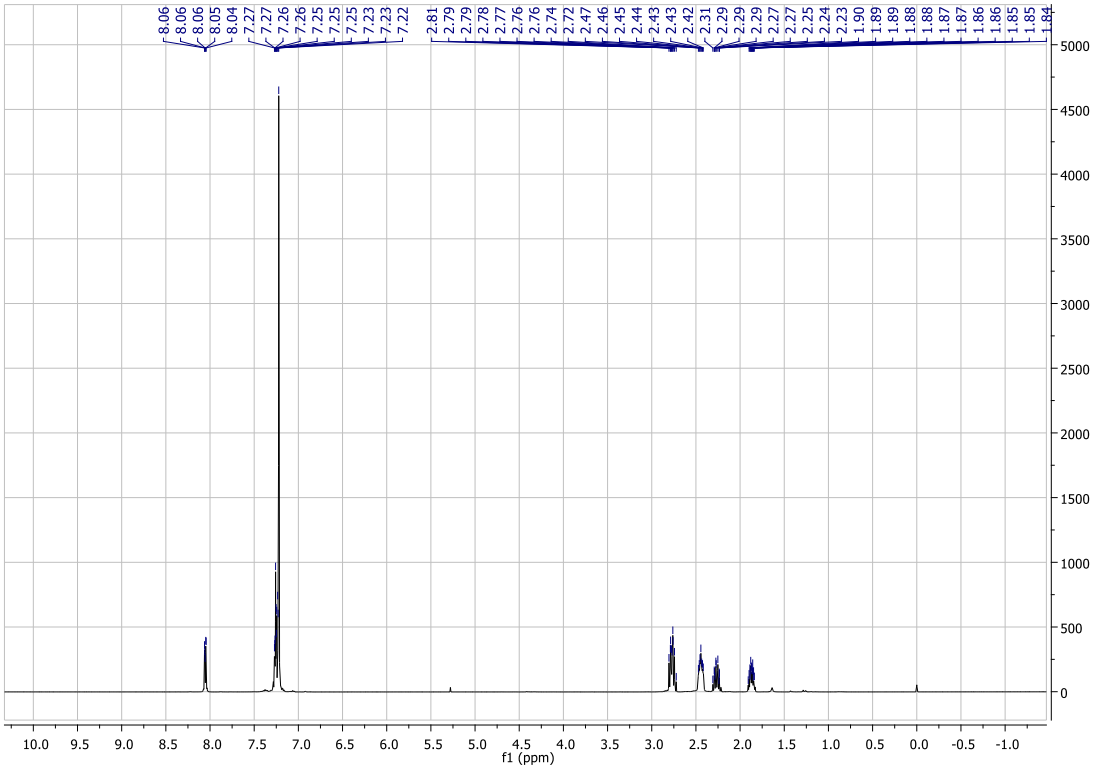
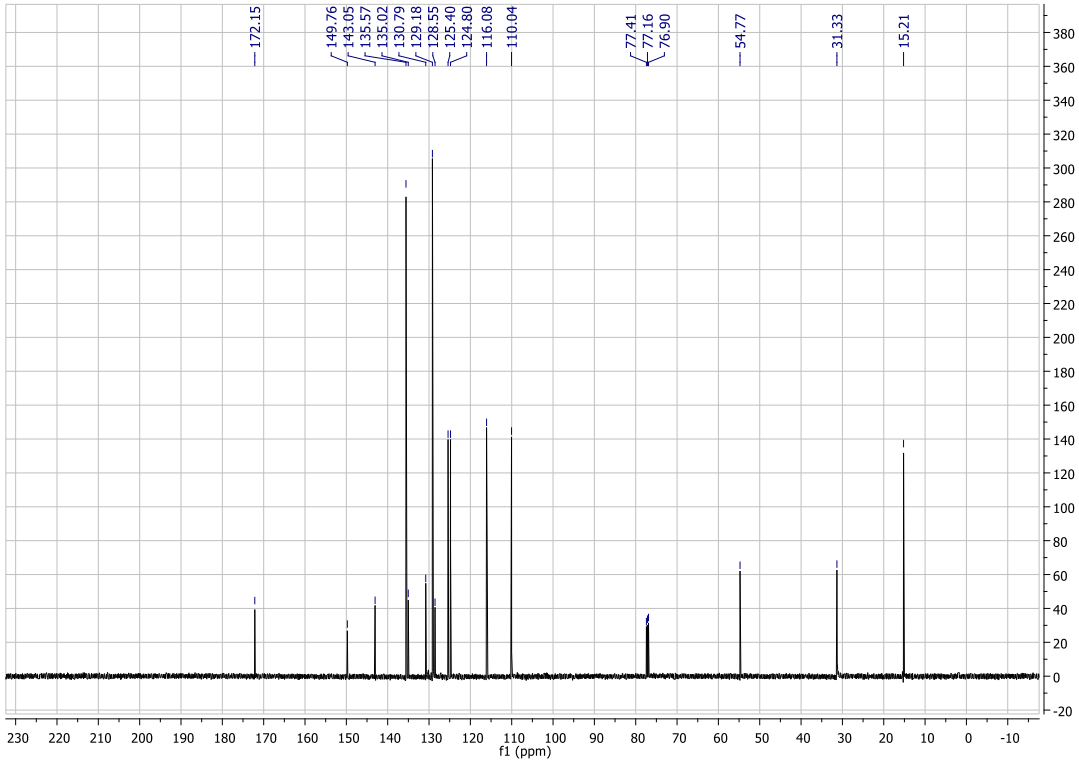
138.86
136.03
135.92
131.20
130.47
129.69
128.81
125.31
124.80
116.12
110.07
77.41
77.16
76.90
55.09
31.34
20.86
20.49
15.58
650
600
550
500
450
400
350
300
250
200
150
100
50
0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Cl
S
O
N
O
O

S-5i


8.06
8.06
8.06
8.05
8.04
7.27
7.27
7.26
7.26
7.25
7.25
7.25
7.23
7.23
7.22
2.81
2.79
2.79
2.78
2.77
2.76
2.76
2.74
2.72
2.47
2.46
2.45
2.44
2.43
2.43
2.42
2.31
2.29
2.29
2.29
2.27
2.27
2.25
2.24
2.23
1.90
1.89
1.89
1.88
1.88
1.87
1.87
1.86
1.86
1.85
1.85
1.84
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)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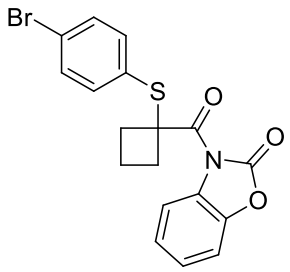
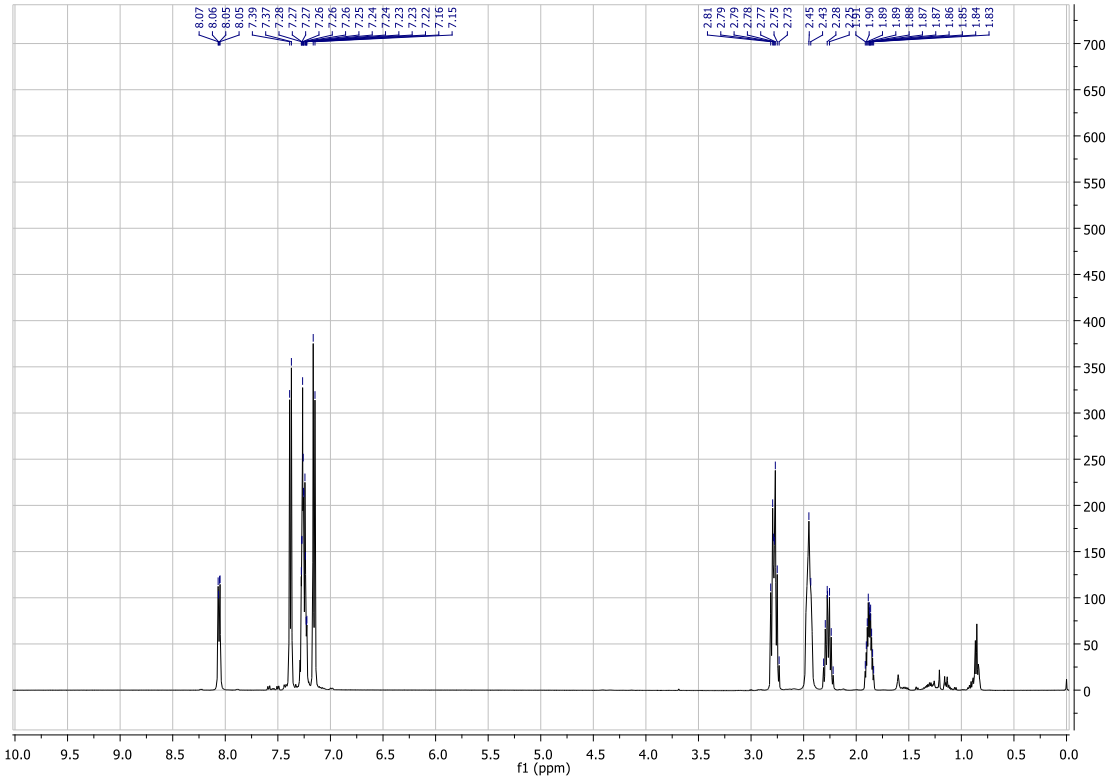
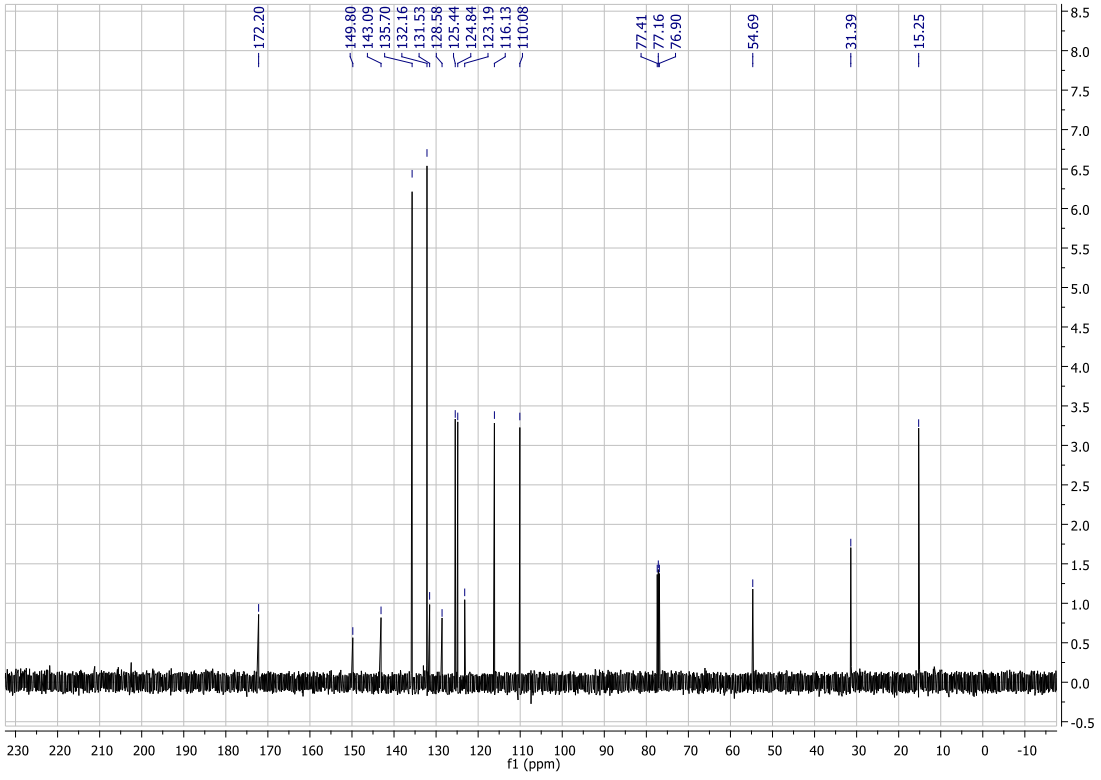
135.57
135.02
130.79
129.18
128.55
125.40
124.80
116.08
110.04
77.41
77.16
76.90
54.77
31.33
15.21
380
360
340
320
300
280
260
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Br
S
O
O
N
O

S-5j


8.07
8.06
8.05
8.05
7.39
7.37
7.28
7.27
7.27
7.26
7.26
7.26
7.25
7.24
7.24
7.23
7.23
7.22
7.16
7.15
2.81
2.79
2.79
2.78
2.77
2.75
2.73
2.45
2.43
2.28
2.25
1.91
1.90
1.89
1.89
1.88
1.87
1.87
1.86
1.85
1.84
1.83
f1 (ppm)


172.20
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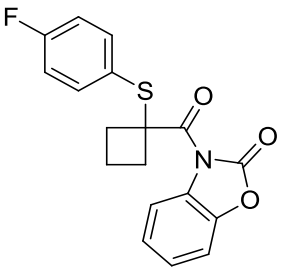
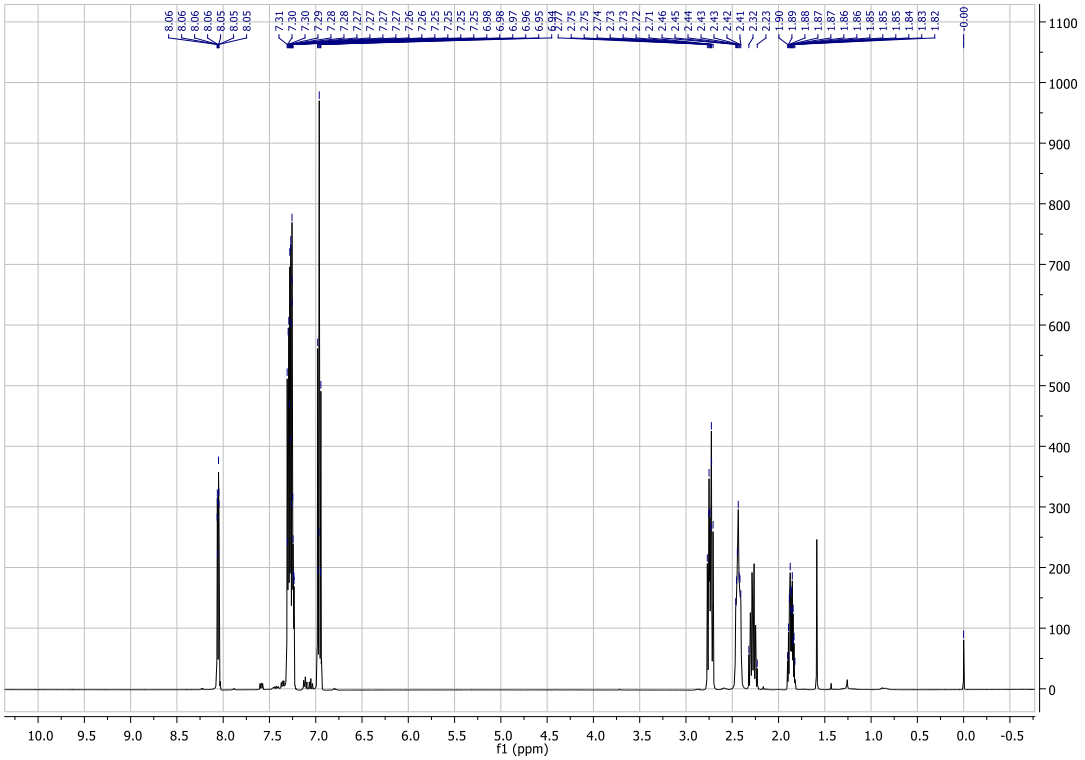
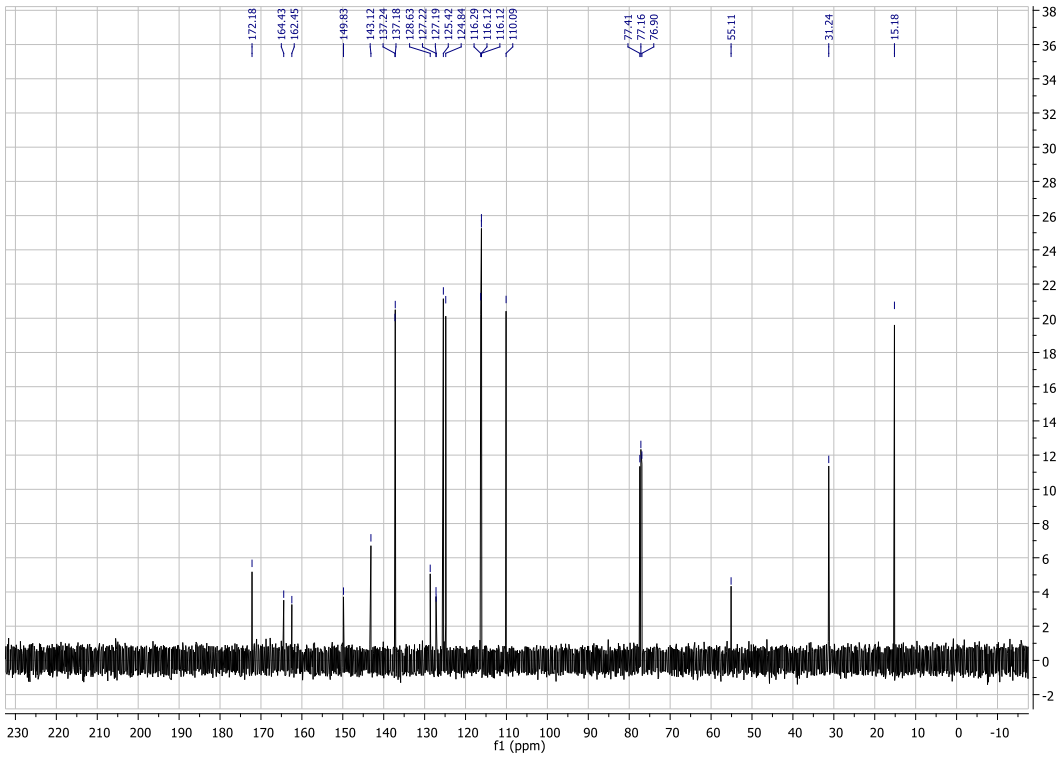
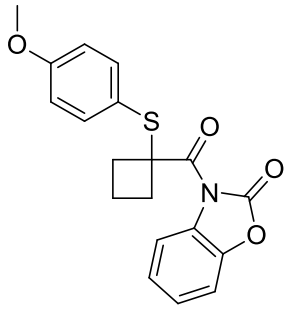
143.09
135.70
132.16
131.53
128.58
125.44
124.84
123.19
116.13
110.08
77.41
77.16
76.90
54.69
31.39
15.25
f1 (ppm)


F
S
O
N
O
O

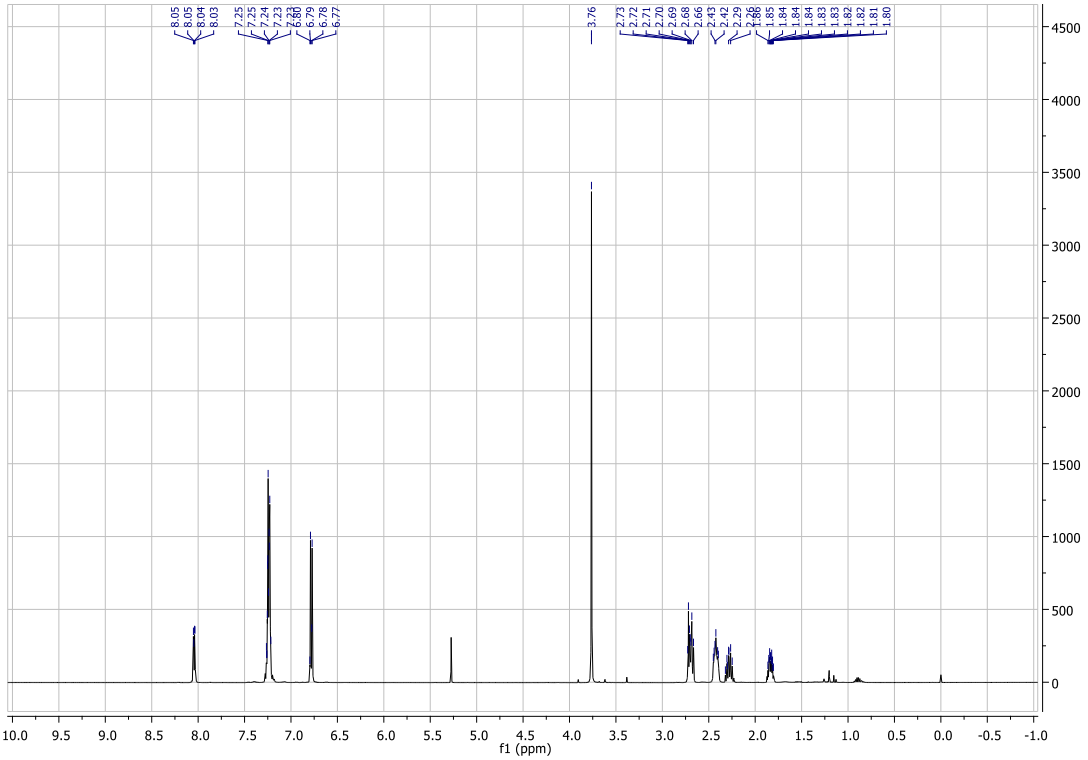
S-5k

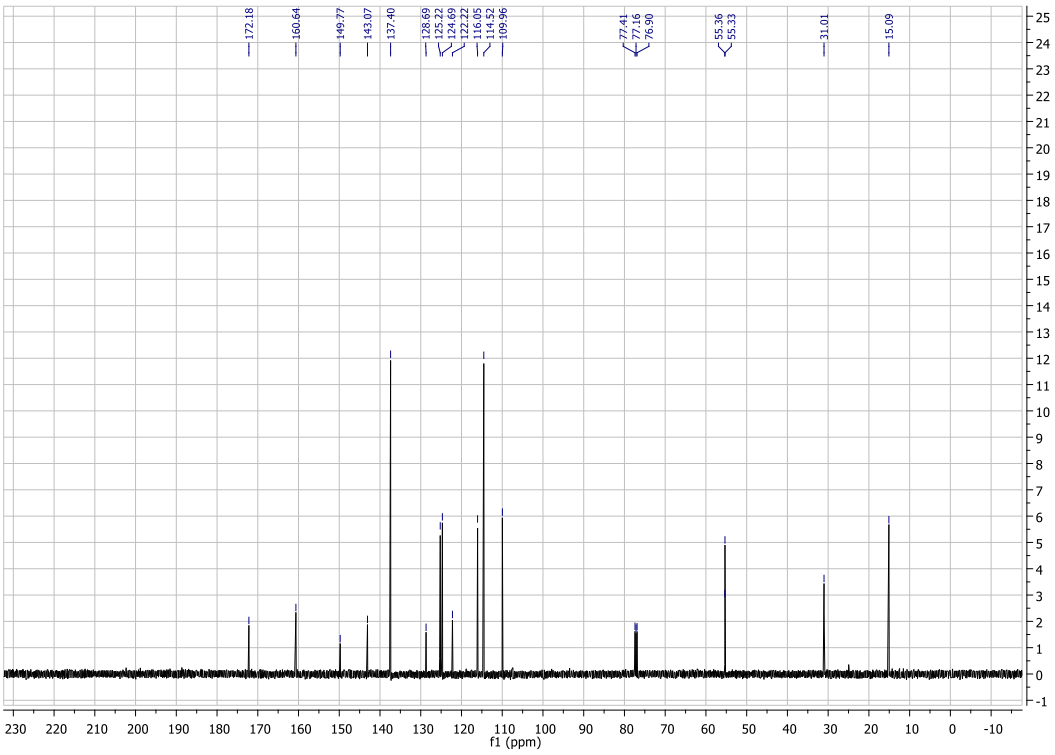

8.06
8.06
8.06
8.06
8.05
8.05
8.05
7.31
7.30
7.30
7.29
7.28
7.28
7.27
7.27
7.27
7.27
7.26
7.26
7.25
7.25
7.25
7.25
6.98
6.98
6.97
6.96
6.95
2.75
2.75
2.74
2.73
2.73
2.72
2.71
2.46
2.45
2.44
2.43
2.42
2.41
2.32
2.23
1.90
1.89
1.88
1.87
1.87
1.86
1.85
1.85
1.85
1.84
1.83
1.82
-0.00
f1 (ppm)


172.18
164.43
162.45
149.83
143.12
137.24
137.18
128.63
127.22
127.19
125.42
124.84
116.29
116.12
116.12
110.09
77.41
77.16
76.90
55.11
31.24
15.18
f1 (ppm)



S-5l


8.05
8.05
8.04
8.03
7.25
7.25
7.24
7.23
6.80
6.79
6.78
6.77
3.76
2.73
2.72
2.71
2.70
2.69
2.68
2.66
2.43
2.42
2.29
1.88
1.85
1.84
1.84
1.84
1.83
1.83
1.82
1.82
1.81
1.80
f1 (ppm)


172.18
160.64
149.77
143.07
137.40
128.69
125.22
124.69
122.22
116.05
114.52
109.96
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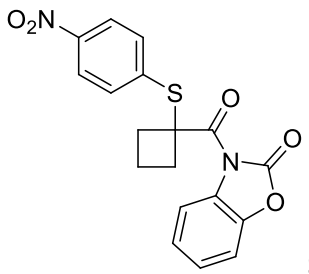
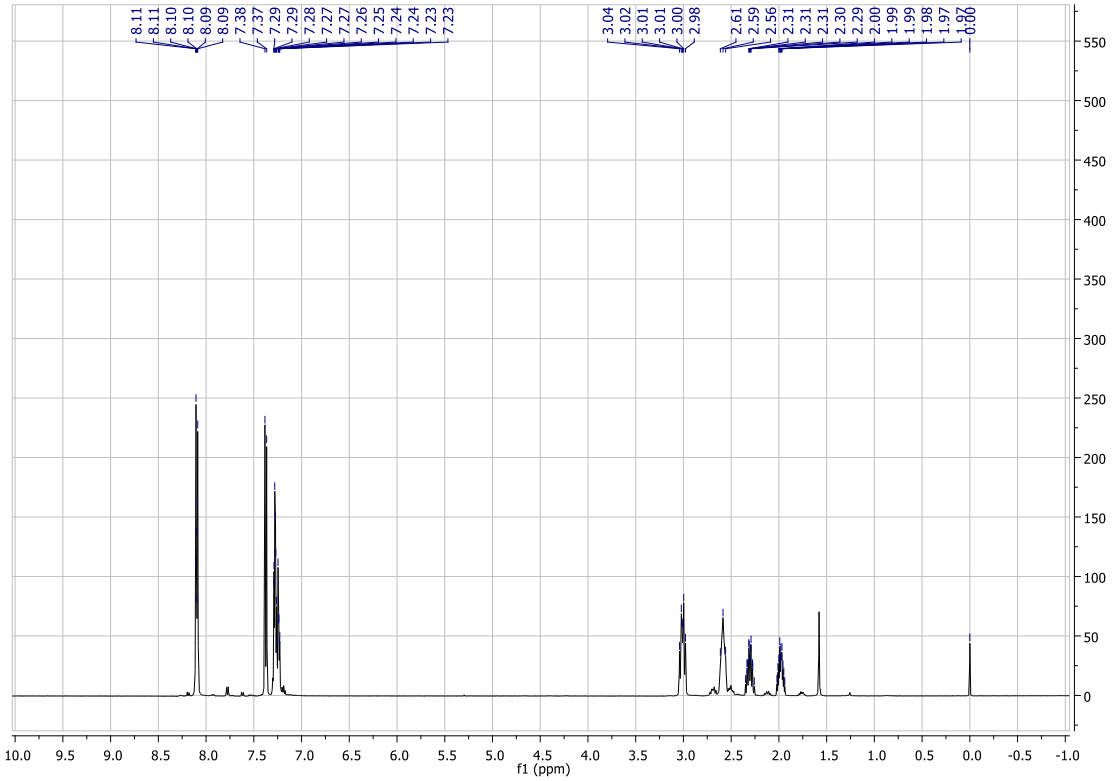
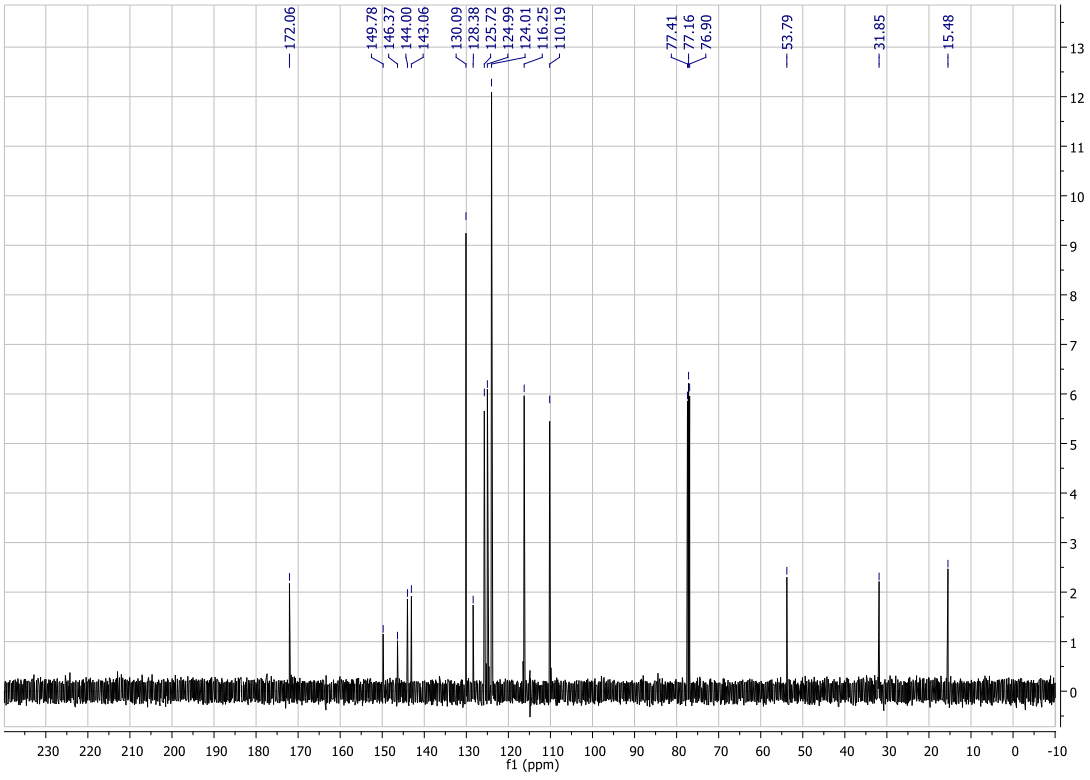
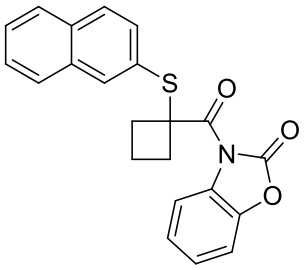
76.90
55.36
55.33
31.01
15.09
f1 (ppm)



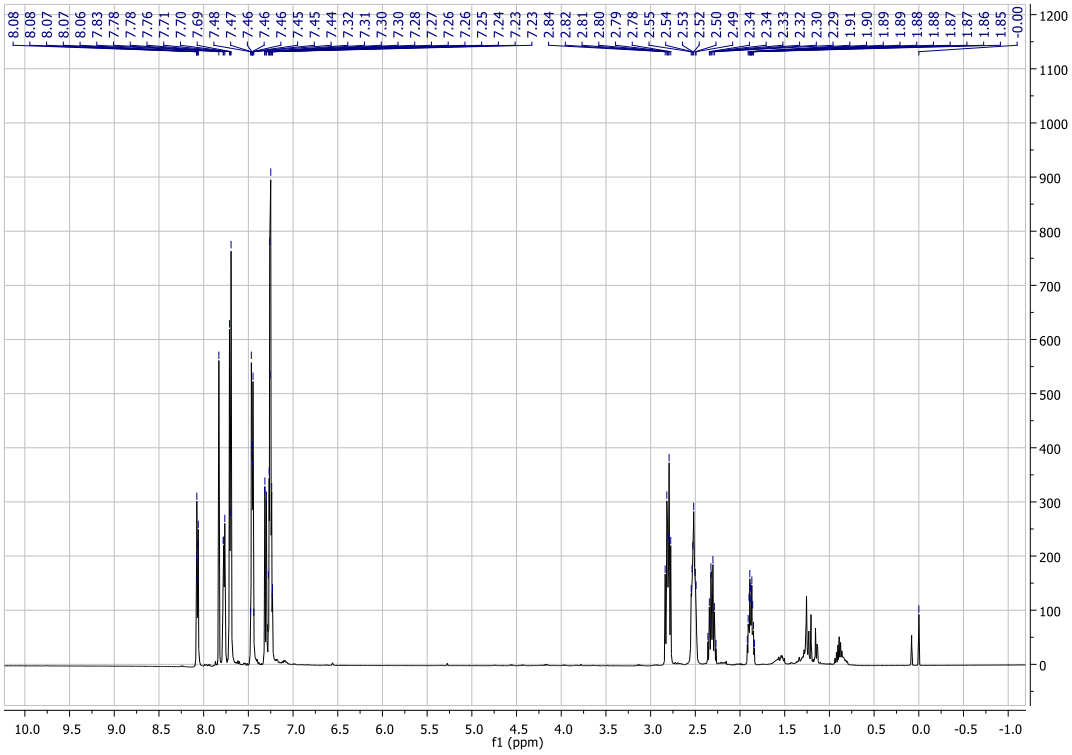
S-5m

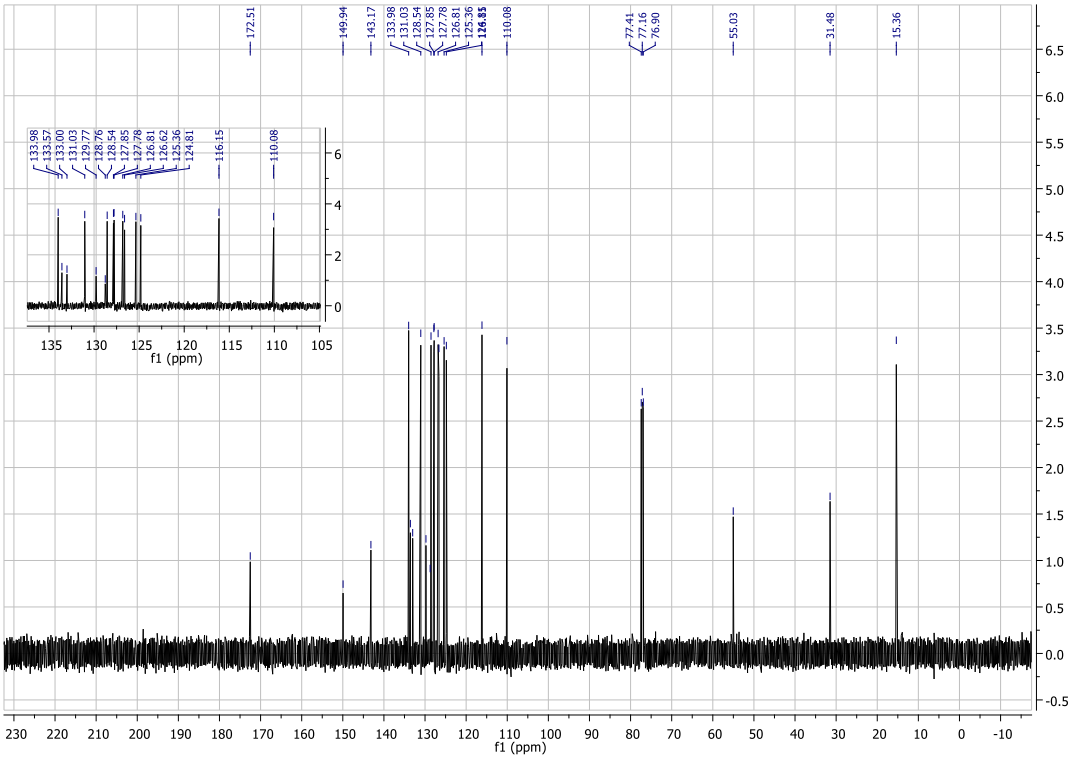

8.11
8.11
8.10
8.10
8.09
8.09
7.38
7.37
7.29
7.29
7.28
7.27
7.27
7.26
7.25
7.24
7.24
7.23
7.23
3.04
3.02
3.01
3.01
3.00
2.98
2.61
2.59
2.56
2.31
2.31
2.31
2.30
2.29
2.00
1.99
1.99
1.98
1.97
1.97
0.00
f1 (ppm)

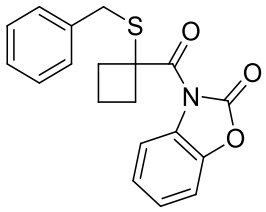

172.06
149.78
146.37
144.00
143.06
130.09
128.38
125.72
124.99
124.01
116.25
110.19
77.41
77.16
76.90
53.79
31.85
15.48
f1 (ppm)



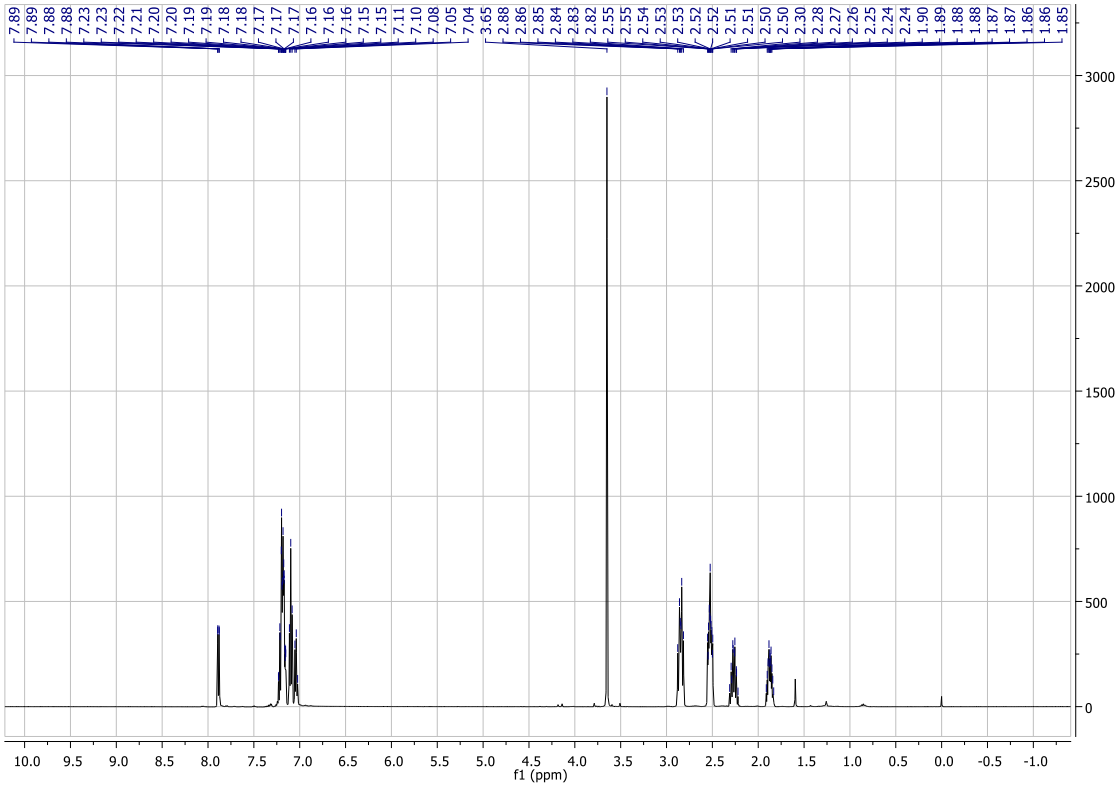
S-5n

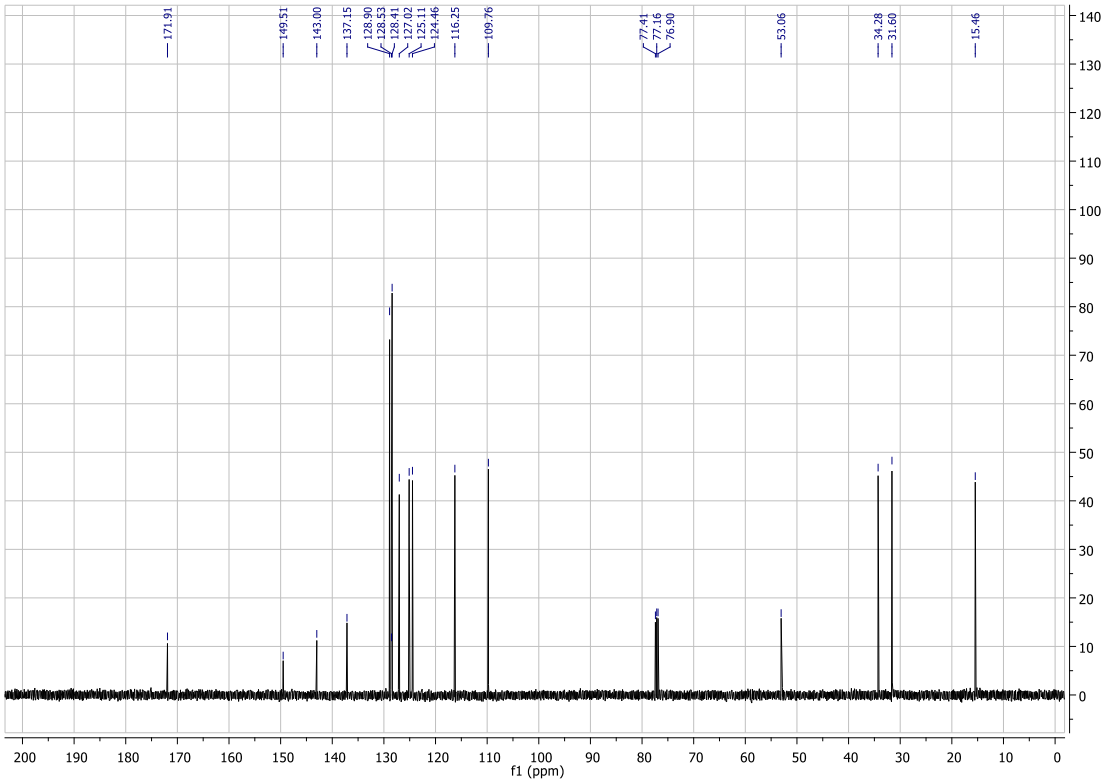


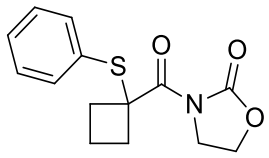



S
O
O
N
O

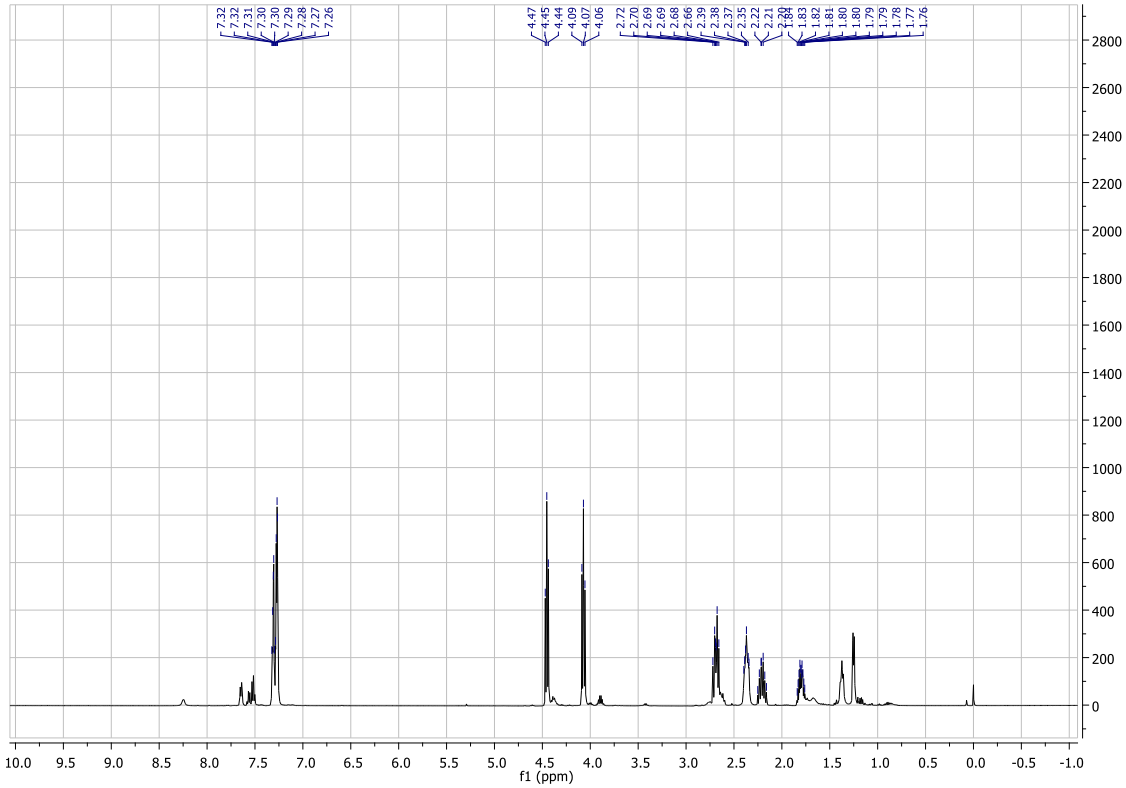
S-5o

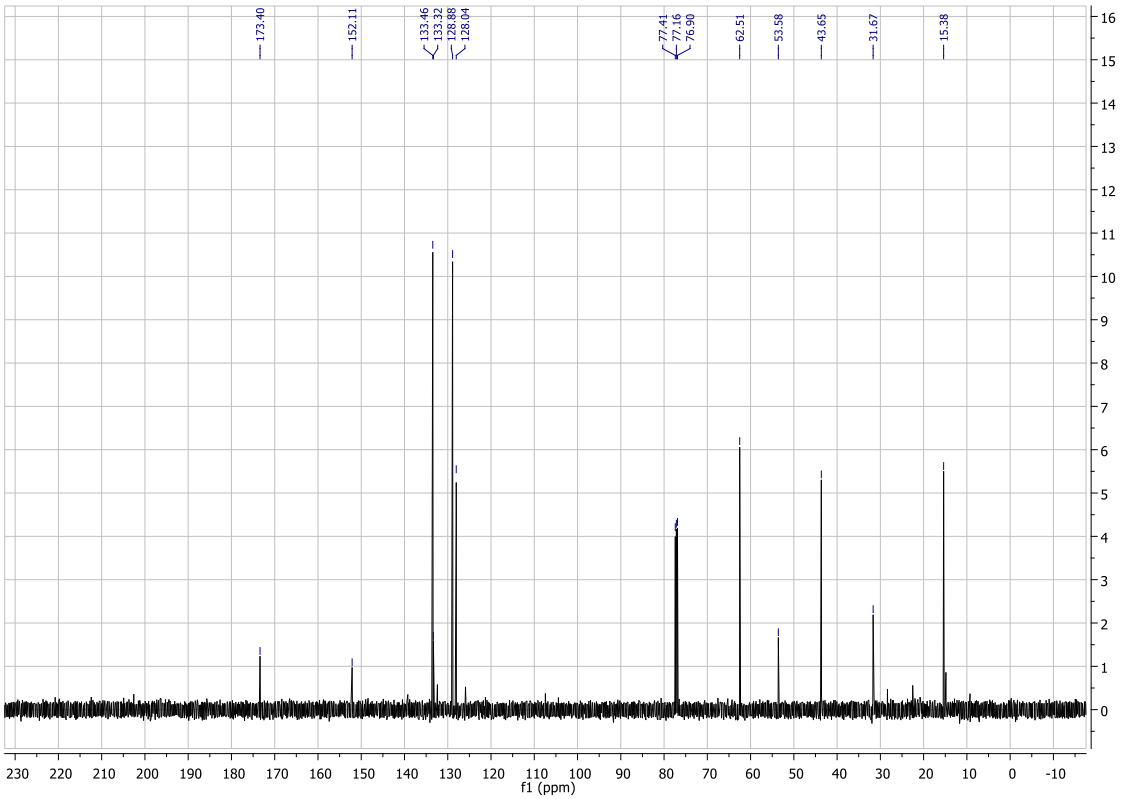

7.89 7.89 7.88 7.88 7.23 7.23 7.22 7.21 7.20 7.20 7.19 7.19 7.18 7.18 7.17 7.17 7.17 7.16 7.16 7.16 7.15 7.15 7.11 7.10 7.08 7.05 7.04
3.65 2.88 2.86 2.85 2.84 2.83 2.82 2.55 2.55 2.54 2.53 2.53 2.52 2.52 2.51 2.51 2.50 2.50 2.30 2.28 2.27 2.26 2.25 2.24 2.24 1.90 1.89 1.88 1.88 1.87 1.87 1.86 1.86 1.85
3000
2500
2000
1500
1000
500
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

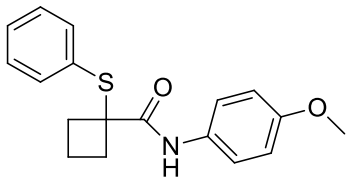

171.91
149.51
143.00
137.15
128.90
128.53
128.41
127.02
125.11
124.46
116.25
109.76
77.41
77.16
76.90
53.06
34.28
31.60
15.46
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


S
O
O
N
O

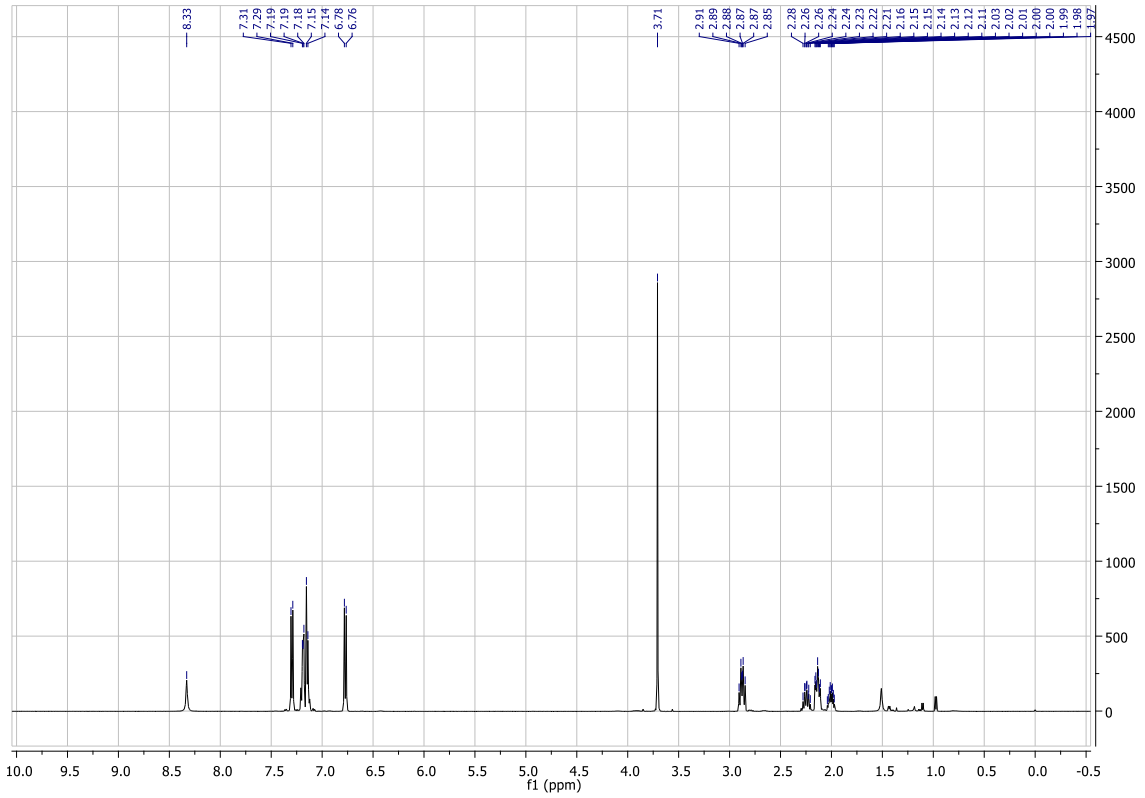
S-10

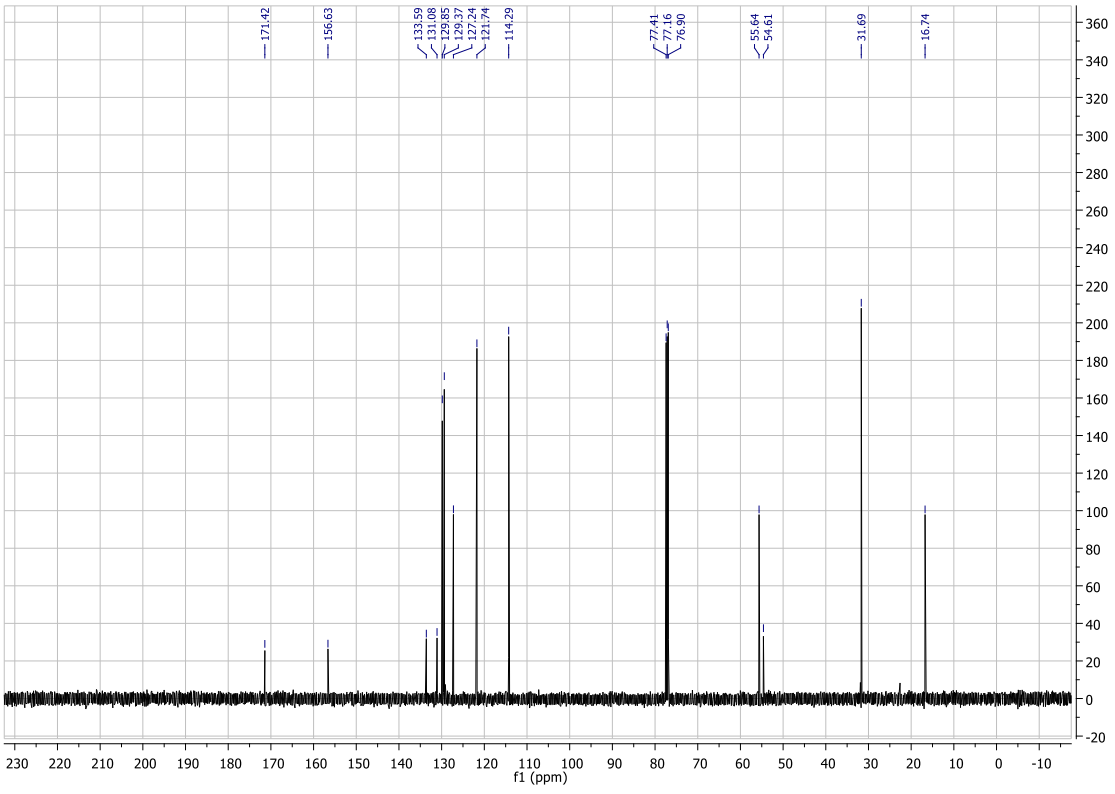

7.32
7.32
7.31
7.30
7.30
7.29
7.28
7.27
7.26
4.47
4.45
4.44
4.09
4.07
4.06
2.72
2.70
2.69
2.69
2.68
2.66
2.39
2.38
2.37
2.35
2.22
2.21
2.20
1.84
1.83
1.82
1.81
1.80
1.80
1.79
1.79
1.78
1.77
1.76
f1 (ppm)

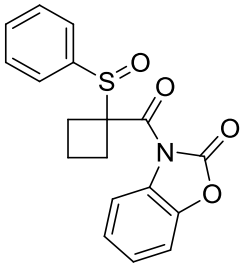

173.40
152.11
133.46
133.32
129.88
128.04
77.41
77.16
76.90
62.51
53.58
43.65
31.67
15.38
f1 (ppm)



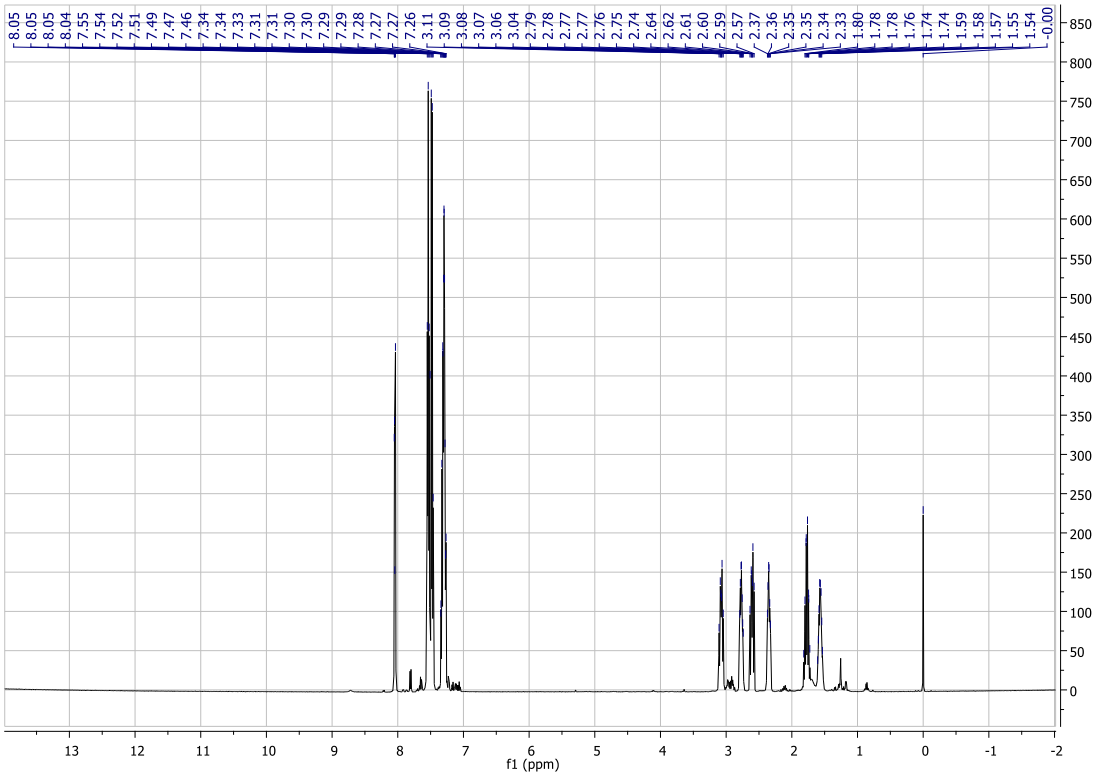
S-11

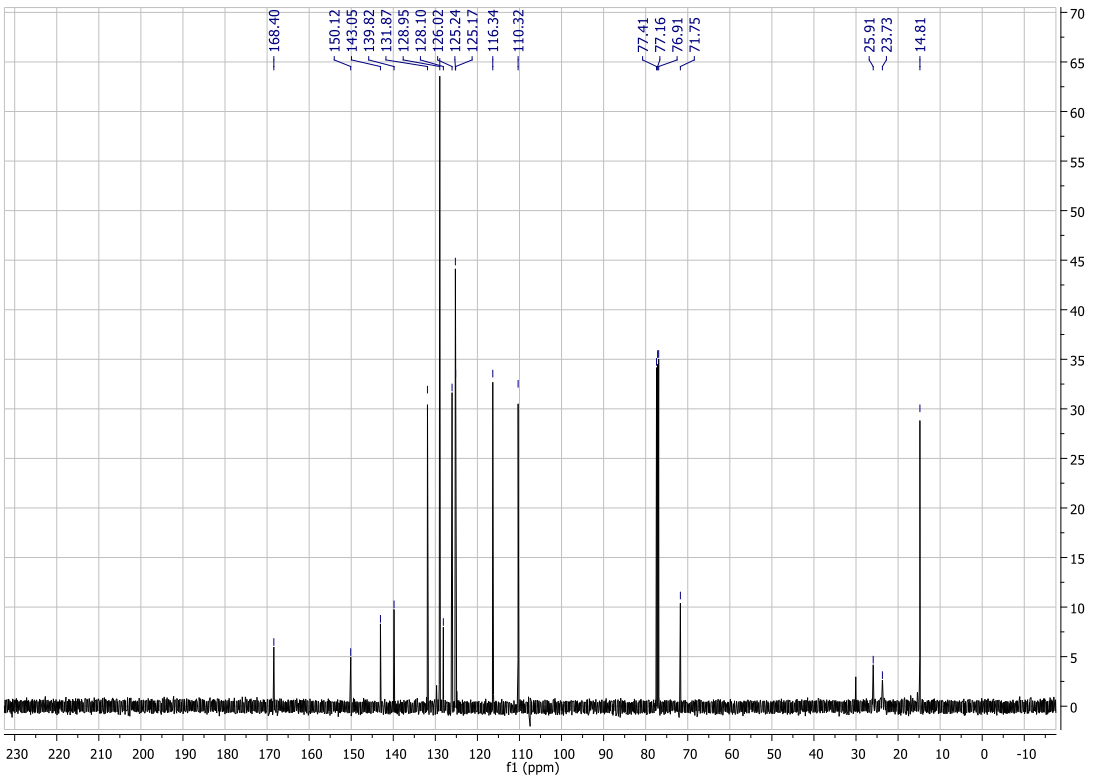

8.33
7.31
7.29
7.19
7.19
7.18
7.15
7.14
6.78
6.76
3.71
2.91
2.89
2.88
2.87
2.87
2.85
2.28
2.26
2.26
2.24
2.24
2.23
2.22
2.21
2.16
2.15
2.15
2.14
2.13
2.12
2.11
2.03
2.02
2.01
2.00
2.00
1.99
1.98
1.97
f1 (ppm)

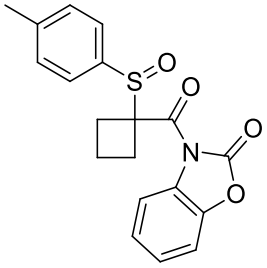

171.42
156.63
133.59
131.08
129.85
129.37
127.24
121.74
114.29
77.41
77.16
76.90
55.64
54.61
31.69
16.74
f1 (ppm)



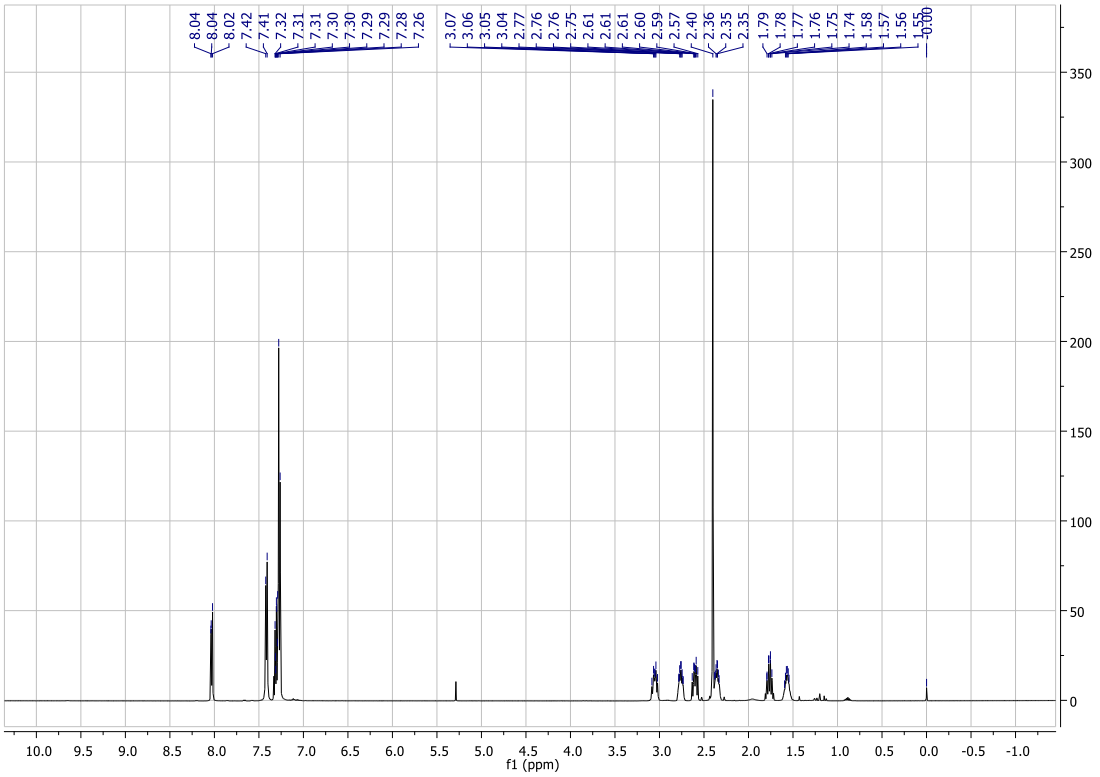
6a


8.05 8.05 8.05 8.04 7.55 7.54 7.52 7.51 7.49 7.47 7.46 7.34 7.34 7.33 7.31 7.31 7.30 7.30 7.29 7.29 7.28 7.27 7.27 7.26 3.11 3.09 3.08 3.07 3.06 3.04 2.79 2.78 2.77 2.77 2.76 2.75 2.74 2.64 2.62 2.61 2.60 2.59 2.57 2.37 2.36 2.35 2.35 2.34 2.33 1.80 1.78 1.78 1.76 1.74 1.74 1.59 1.58 1.57 1.55 1.54 -0.00
f1 (ppm)


168.40 150.12 143.05 139.82 131.87 128.95 128.10 126.02 125.24 125.17 116.34 110.32 77.41 77.16 76.91 71.75 25.91 23.73 14.81
f1 (ppm)



6b


8.04
8.04
8.02
7.42
7.41
7.32
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.26
3.07
3.06
3.05
3.04
2.77
2.76
2.76
2.75
2.61
2.61
2.61
2.60
2.59
2.57
2.40
2.36
2.35
2.35
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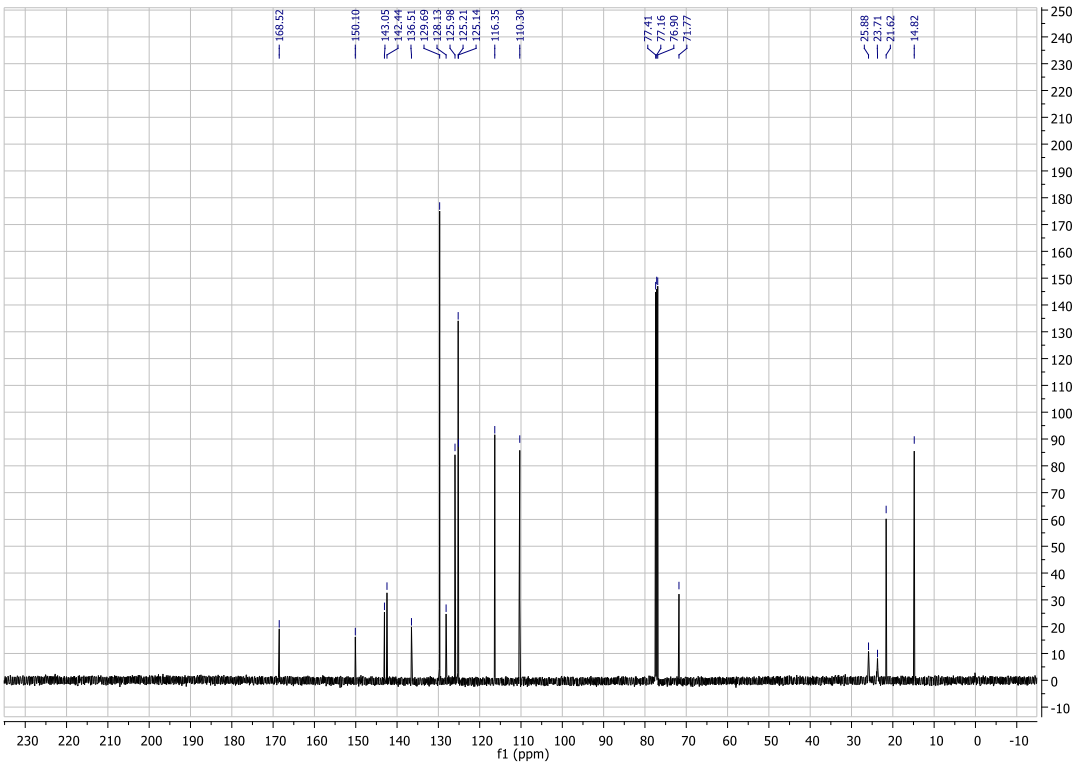
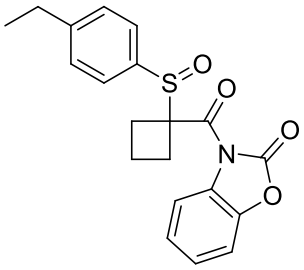
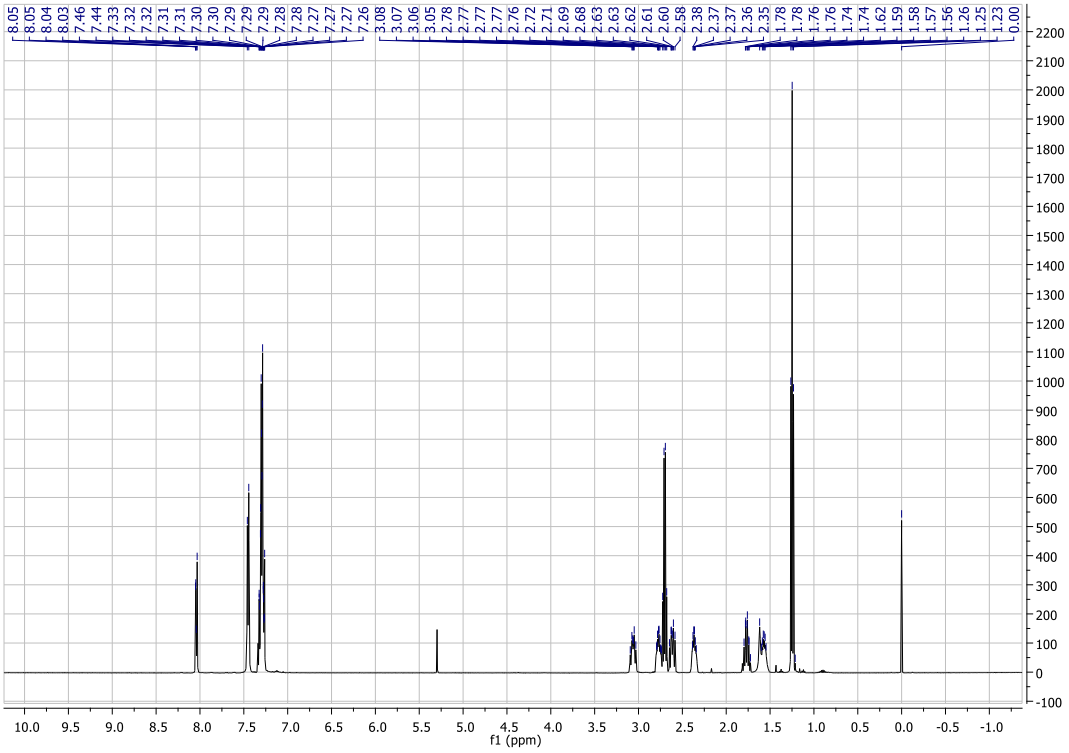
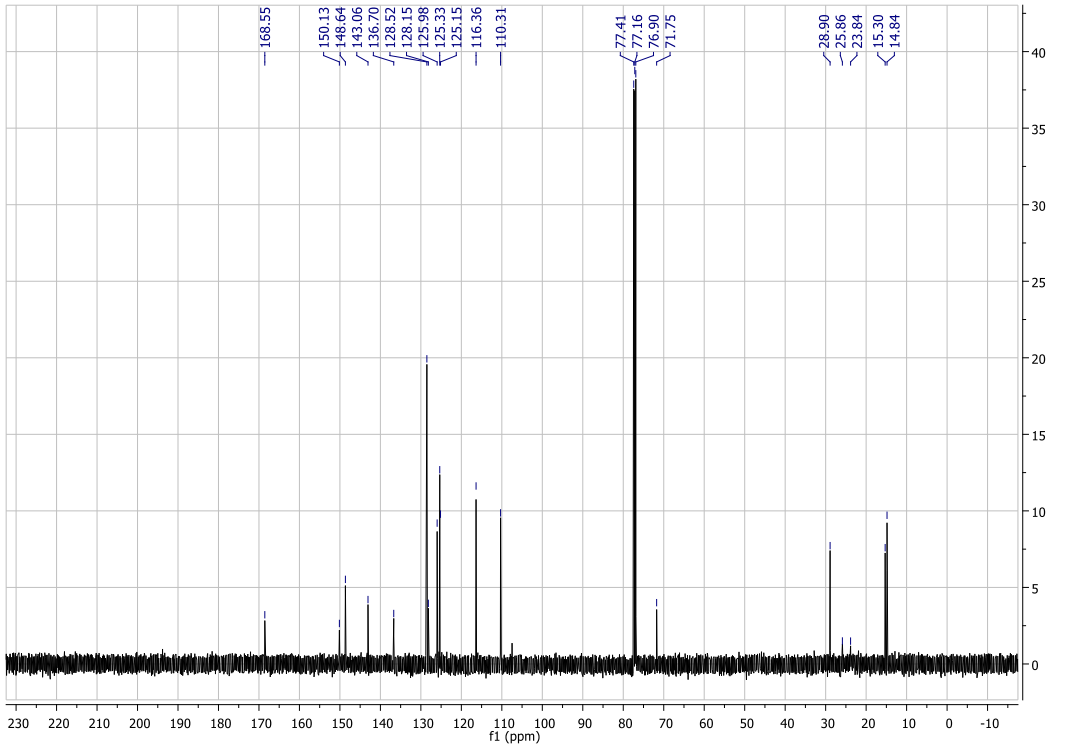
1.57
1.56
1.55
0.00
f1 (ppm)

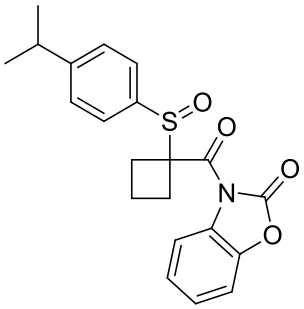

168.52
150.10
143.05
142.44
136.51
129.69
128.13
125.98
125.21
125.14
116.35
110.30
77.41
77.16
76.90
71.77
25.88
23.71
21.62
14.82
f1 (ppm)



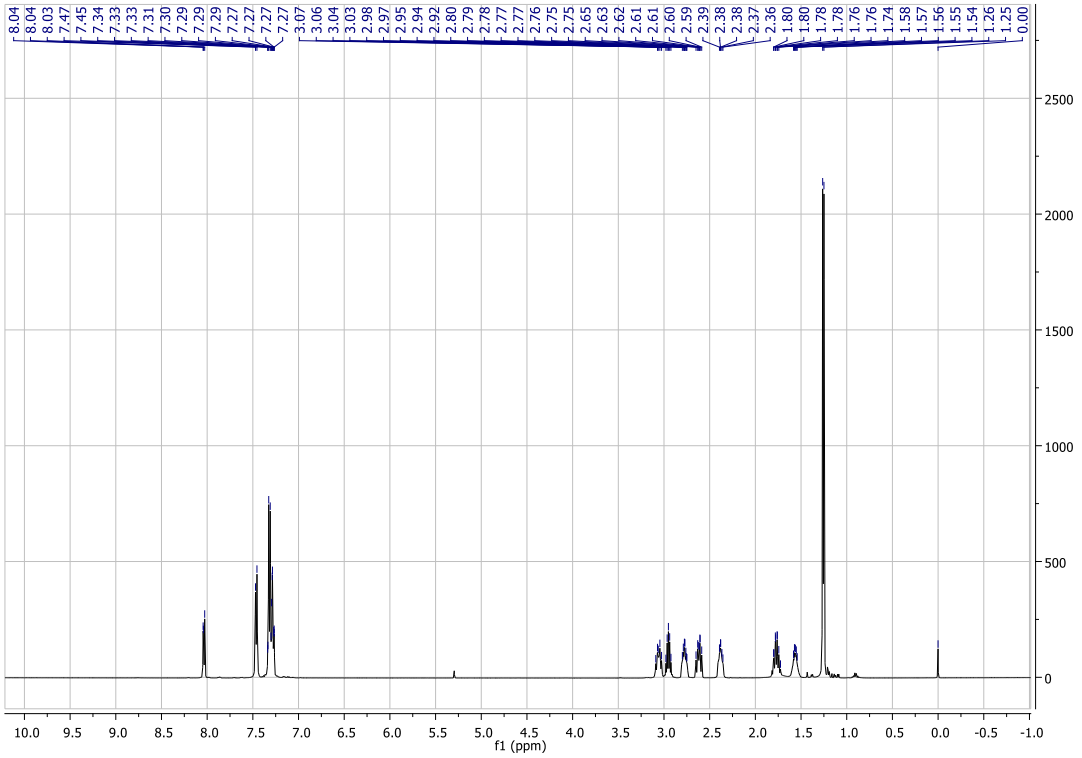
6c

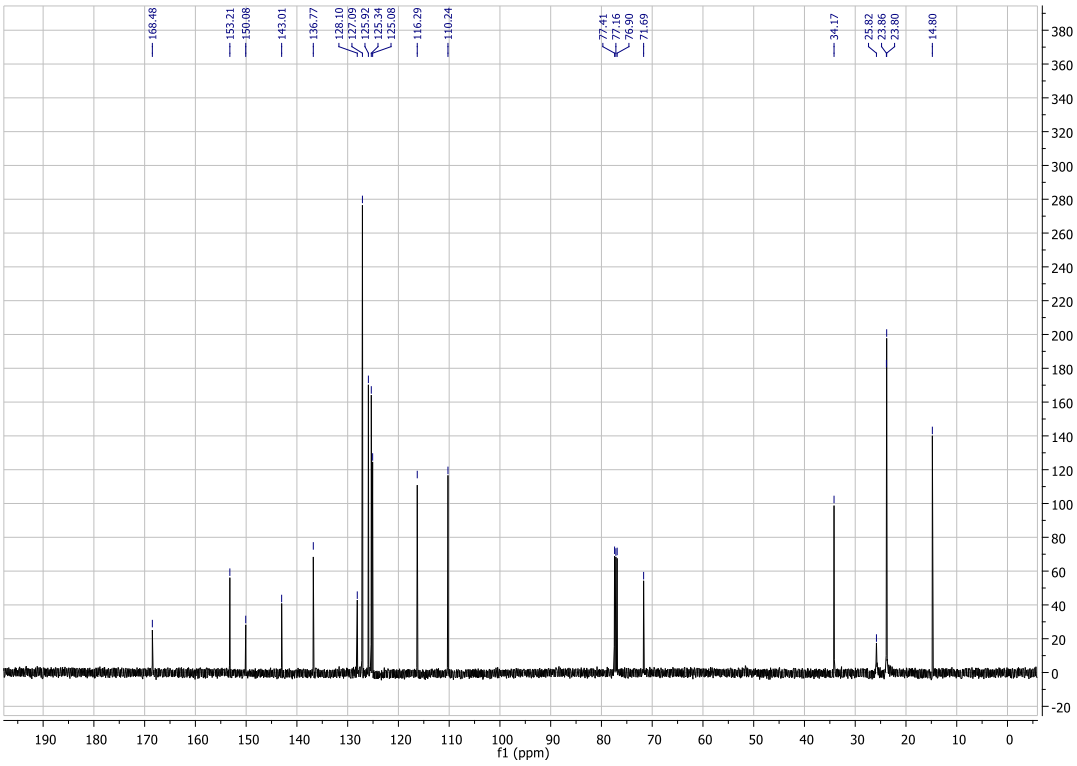

8.05 8.05 8.04 8.03 7.46 7.44 7.33 7.32 7.32 7.31 7.31 7.30 7.30 7.29 7.29 7.29 7.28 7.28 7.27 7.27 7.27 7.26
3.08 3.07 3.06 3.05 2.78 2.77 2.77 2.77 2.76 2.72 2.71 2.69 2.68 2.63 2.63 2.62 2.61 2.60 2.58 2.38 2.37 2.37 2.36 2.35 1.78 1.78 1.76 1.76 1.74 1.74 1.62 1.59 1.58 1.57 1.56 1.26 1.25 1.23 0.00
f1 (ppm)

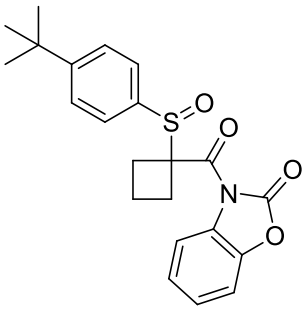

168.55 150.13 148.64 143.06 136.70 128.52 128.15 125.98 125.33 125.15 116.36 110.31 77.41 77.16 76.90 71.75 28.90 25.86 23.84 15.30 14.84
f1 (ppm)



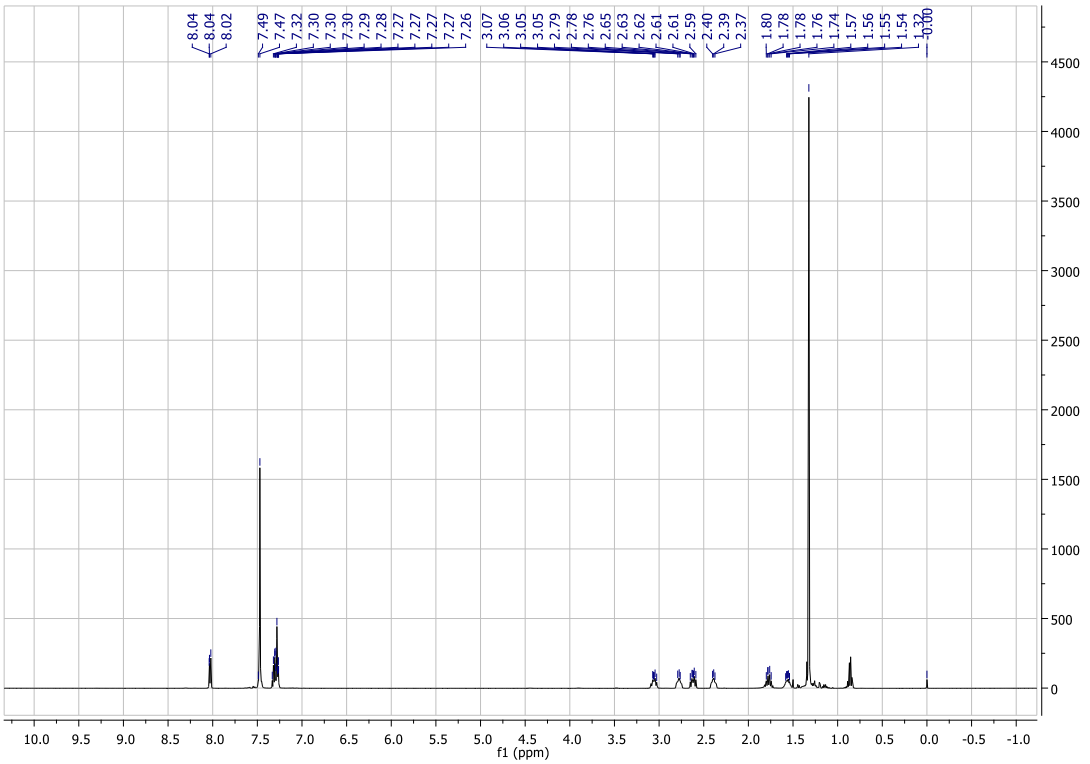
6d


8.04 8.04 8.03 7.47 7.45 7.34 7.33 7.33 7.31 7.30 7.29 7.29 7.27 7.27 7.27 7.27
3.07 3.06 3.04 3.03 2.98 2.97 2.95 2.94 2.92 2.80 2.79 2.78 2.77 2.77 2.76 2.75 2.75 2.65 2.63 2.62 2.61 2.61 2.60 2.59 2.39 2.38 2.38 2.37 2.36
1.80 1.80 1.78 1.78 1.76 1.76 1.74 1.58 1.57 1.56 1.55 1.54 1.26 1.25 0.00
2500
2000
1500
1000
500
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


168.48
153.21
150.08
143.01
136.77
128.10
127.09
125.92
125.34
125.08
116.29
110.24
77.41
77.16
76.90
71.69
34.17
25.82
23.86
23.80
14.80
f1 (ppm)


S
O
O
N
O
O

6e


8.04
8.04
8.02
7.49
7.47
7.32
7.30
7.30
7.30
7.29
7.28
7.27
7.27
7.27
7.27
7.26
3.07
3.06
3.05
3.05
2.79
2.78
2.76
2.65
2.63
2.62
2.61
2.61
2.59
2.40
2.39
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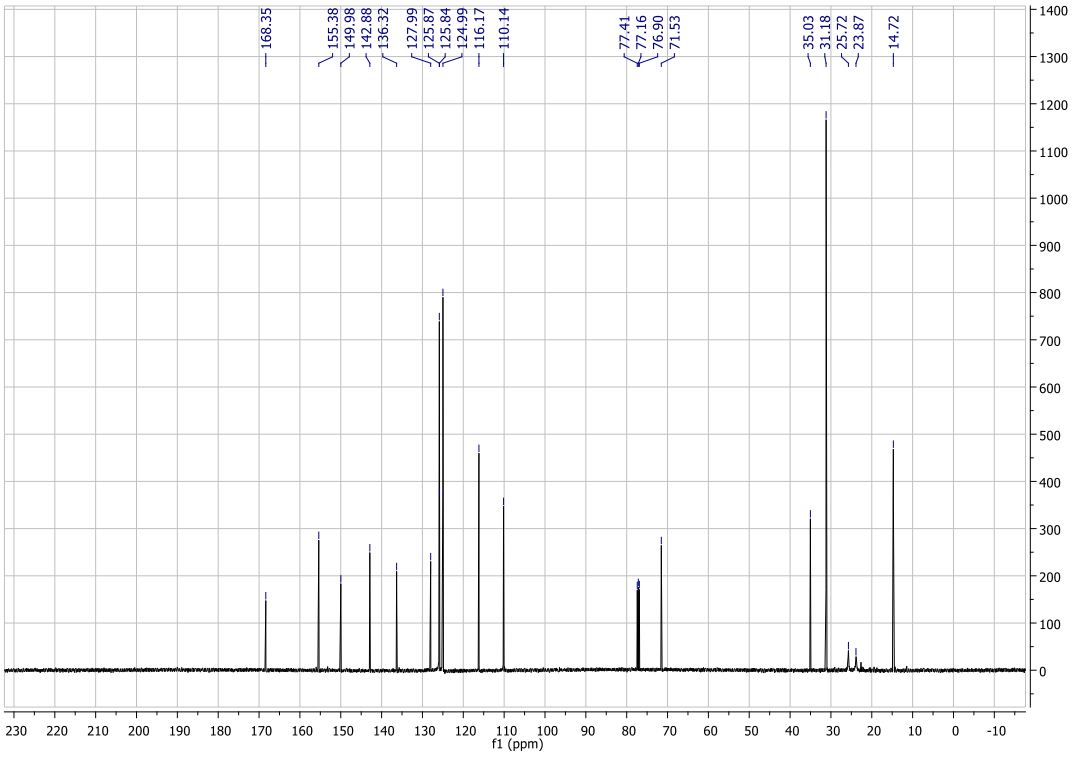
1.76
1.74
1.57
1.56
1.55
1.54
0.00
f1 (ppm)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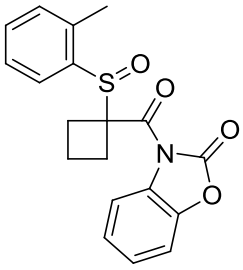
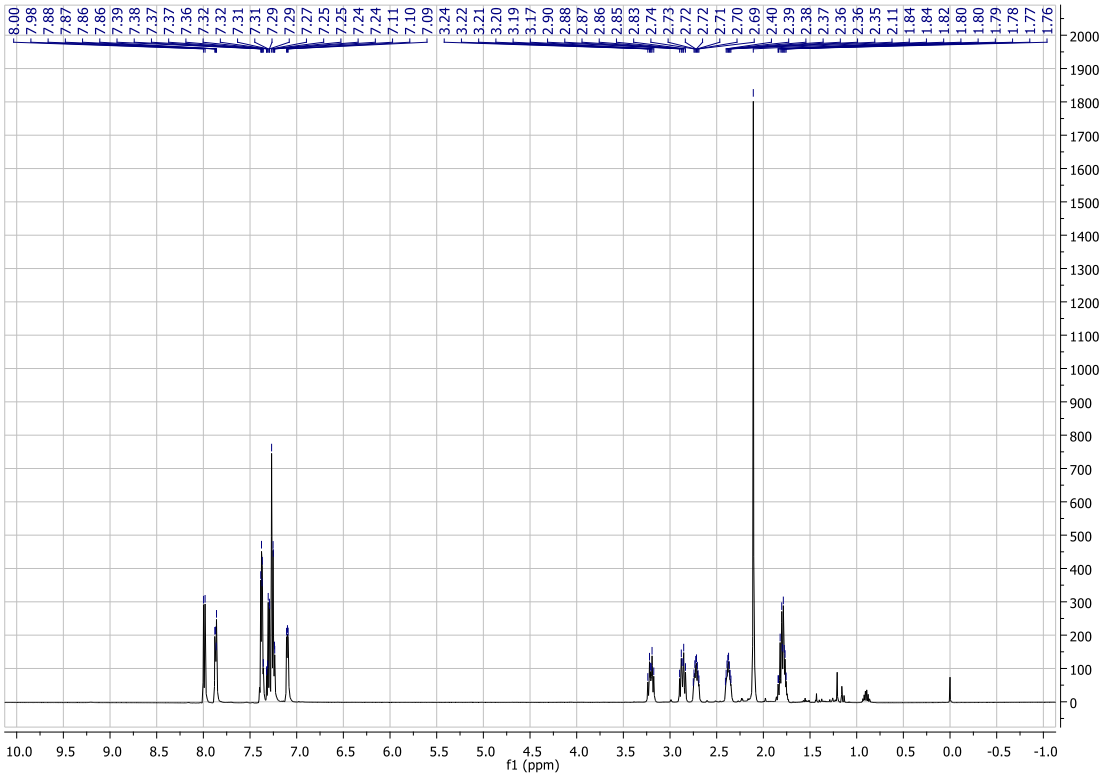
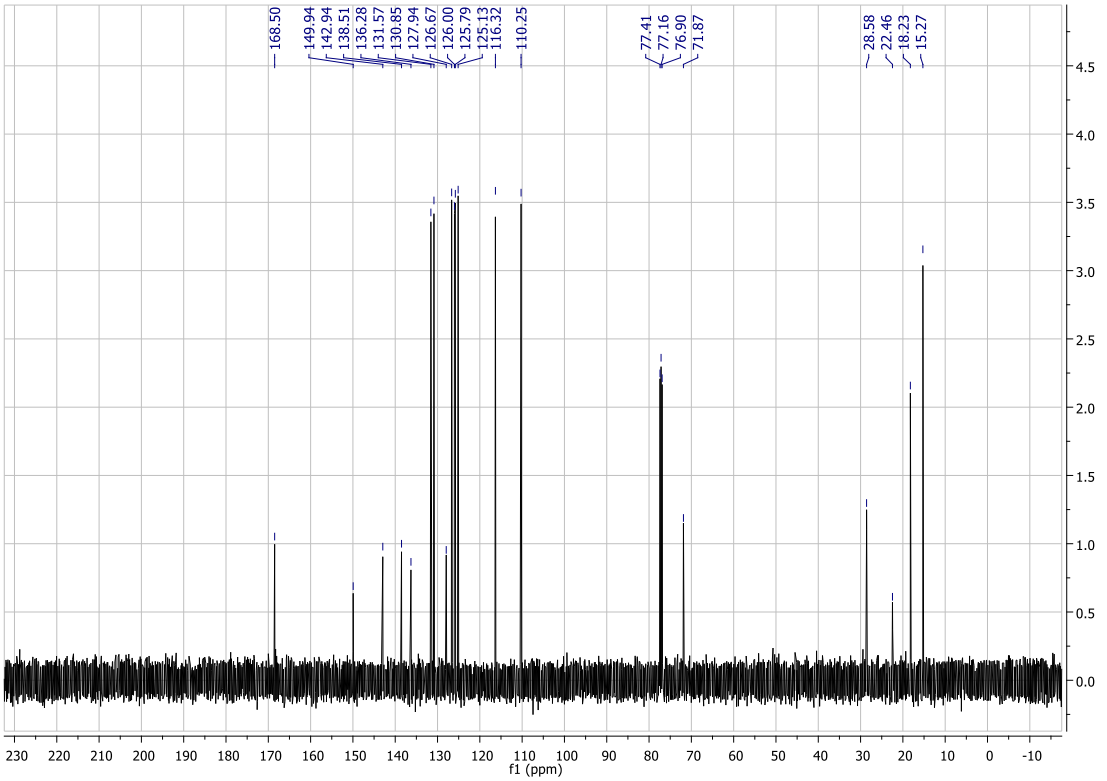
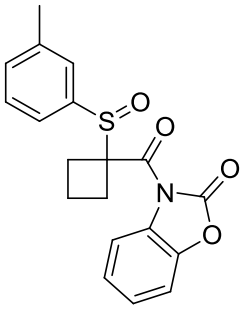
155.38
149.98
142.88
136.32
127.99
125.87
125.84
124.99
116.17
110.14
77.41
77.16
76.90
71.53
35.03
31.18
25.72
23.87
14.72
f1 (ppm)



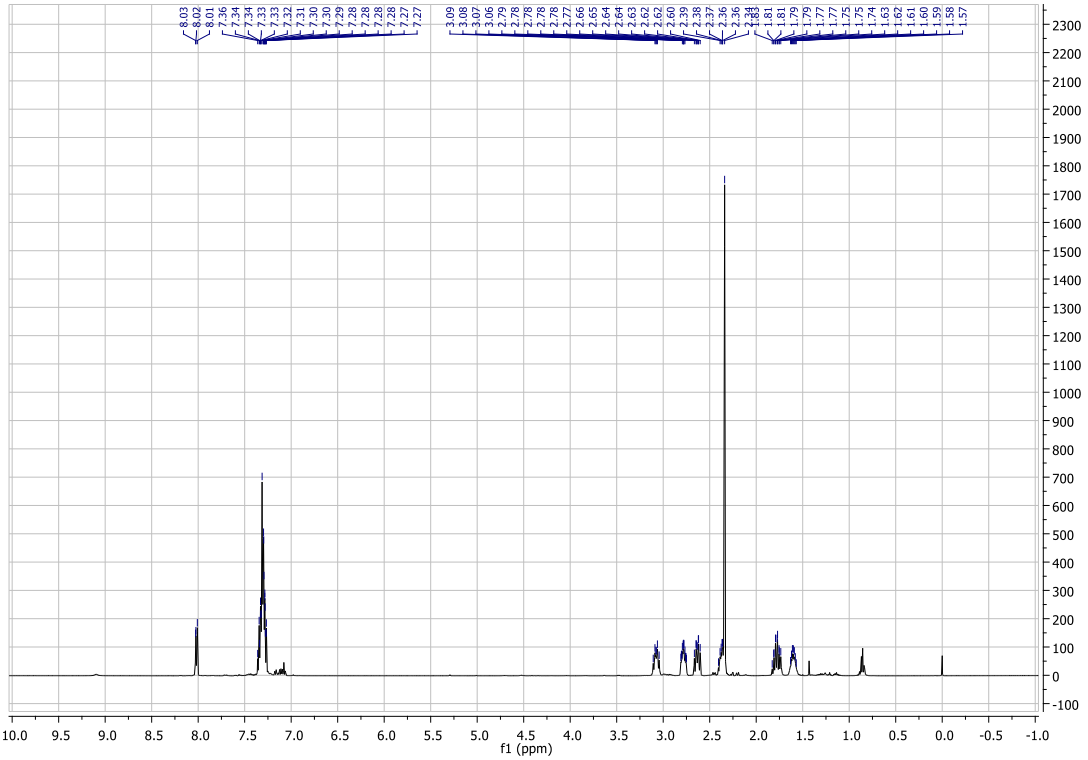
6f


8.00 7.98 7.88 7.87 7.86 7.86 7.39 7.38 7.37 7.37 7.36 7.32 7.32 7.31 7.31 7.29 7.29 7.27 7.25 7.25 7.24 7.24 7.11 7.10 7.09
3.24 3.22 3.21 3.20 3.19 3.17 2.90 2.88 2.87 2.86 2.85 2.83 2.74 2.73 2.72 2.72 2.71 2.70 2.69 2.40 2.39 2.38 2.37 2.36 2.35 2.11 1.84 1.84 1.82 1.80 1.80 1.79 1.78 1.77 1.76
f1 (ppm)


168.50 149.94 142.94 138.51 136.28 131.57 130.85 127.94 126.67 126.00 125.79 125.13 116.32 110.25
77.41 77.16 76.90 71.87
28.58 22.46 18.23 15.27
f1 (ppm)



6g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8.02
8.01
7.36
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7.34
7.33
7.33
7.32
7.31
7.30
7.30
7.29
7.28
7.28
7.28
7.27
7.27
3.09
3.08
3.07
3.06
2.79
2.78
2.78
2.78
2.78
2.77
2.77
2.66
2.65
2.64
2.64
2.63
2.62
2.62
2.60
2.39
2.38
2.37
2.36
2.36
1.83
1.81
1.81
1.79
1.79
1.79
1.77
1.77
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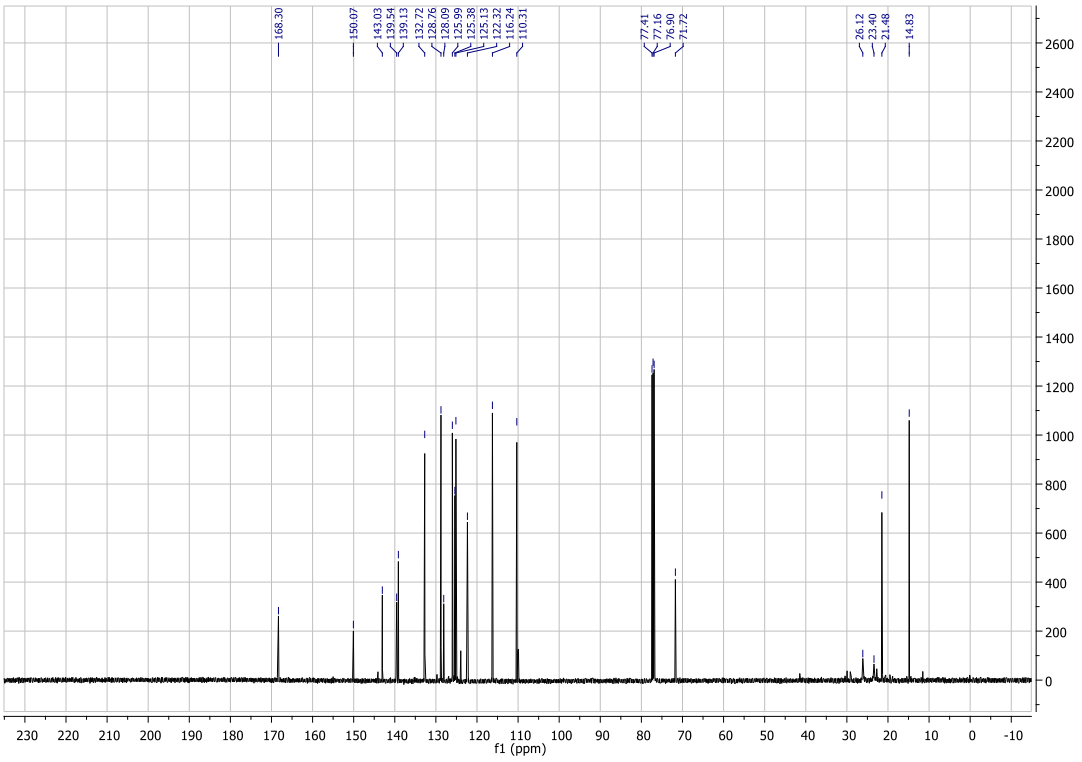
1.63
1.62
1.61
1.60
1.59
1.58
1.57
f1 (ppm)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132.72
128.76
128.09
125.99
125.38
125.13
122.32
116.24
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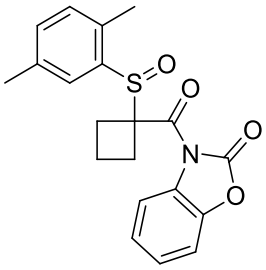
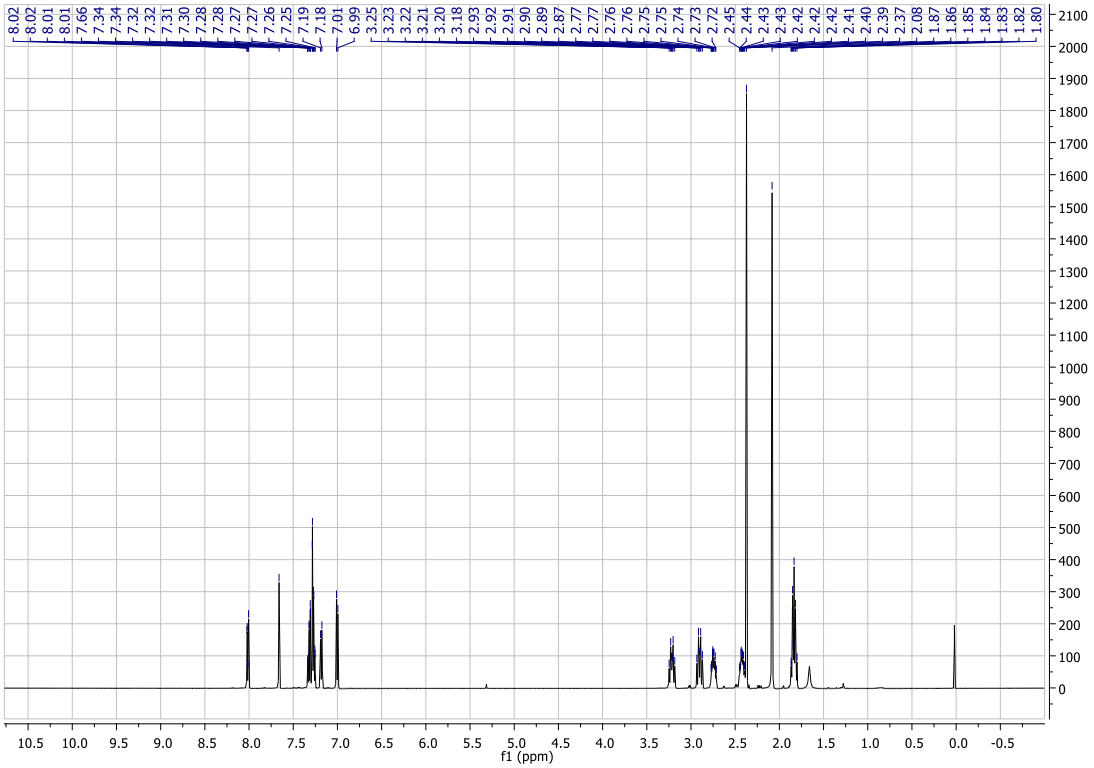
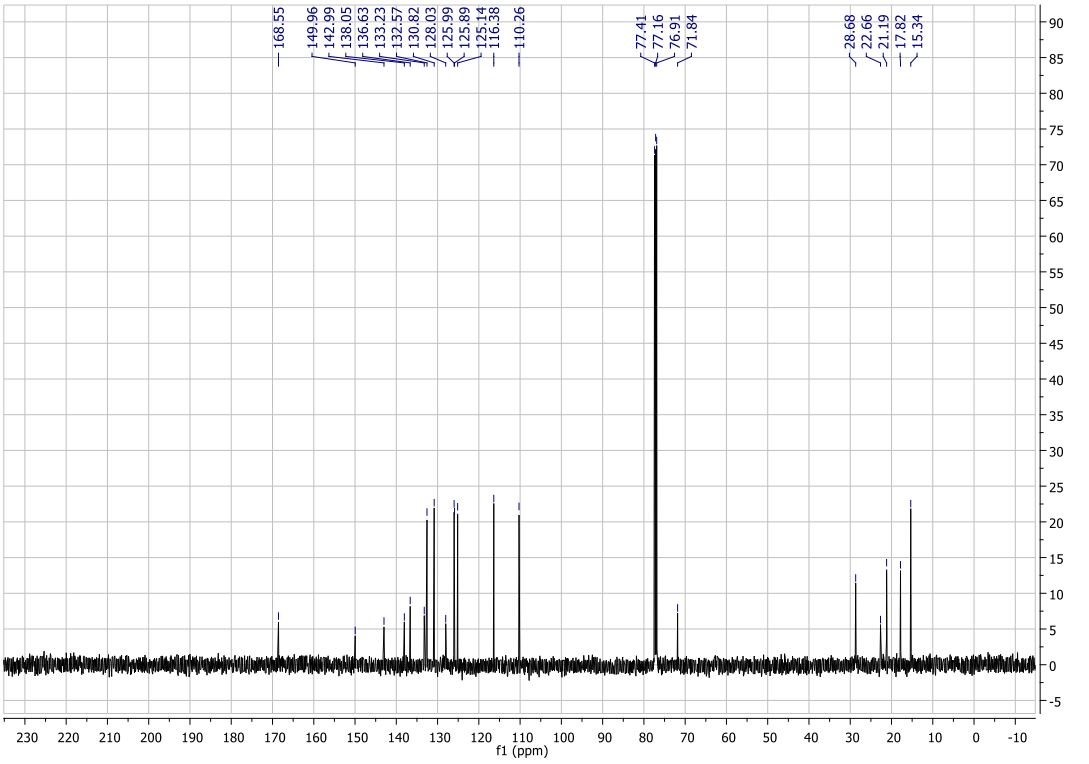
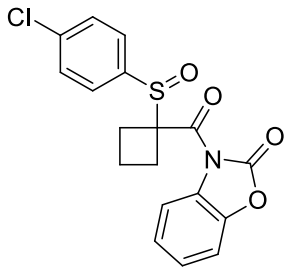
77.41
77.16
76.90
71.72
26.12
23.40
21.48
14.83
f1 (ppm)



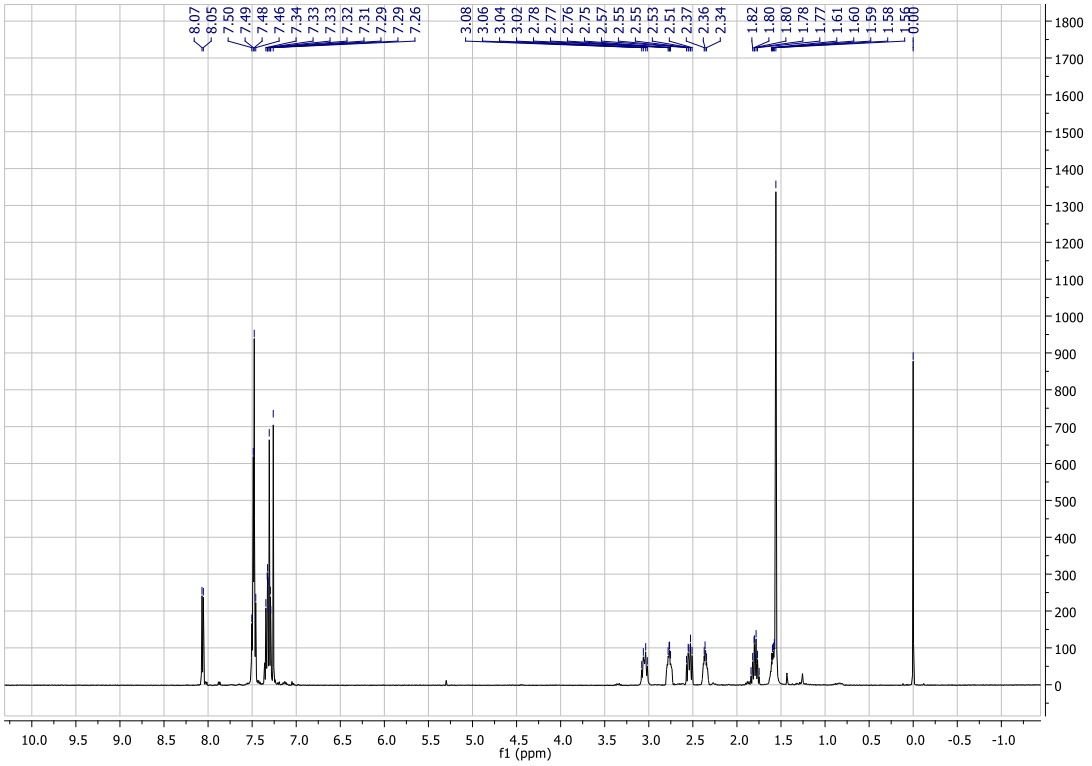
6h


8.02 8.02 8.01 8.01 7.66 7.34 7.34 7.32 7.32 7.31 7.30 7.28 7.28 7.27 7.27 7.26 7.25 7.19 7.18 7.01 6.99 3.25 3.23 3.22 3.21 3.20 3.18 2.93 2.92 2.91 2.90 2.89 2.87 2.77 2.77 2.76 2.76 2.75 2.75 2.74 2.73 2.72 2.45 2.44 2.43 2.43 2.42 2.42 2.42 2.41 2.40 2.39 2.37 2.08 1.87 1.86 1.85 1.84 1.83 1.82 1.80
f1 (ppm)


168.55 149.96 142.99 138.05 136.63 133.23 132.57 130.82 128.03 125.99 125.89 125.14 116.38 110.26 77.41 77.16 76.91 71.84 28.68 22.66 21.19 17.82 15.34
f1 (ppm)


Cl
S
O
O
O
N
O
O

6i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8.05
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7.34
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7.32
7.31
7.29
7.29
7.26
3.08
3.06
3.04
3.02
2.78
2.77
2.76
2.75
2.57
2.55
2.55
2.53
2.51
2.37
2.36
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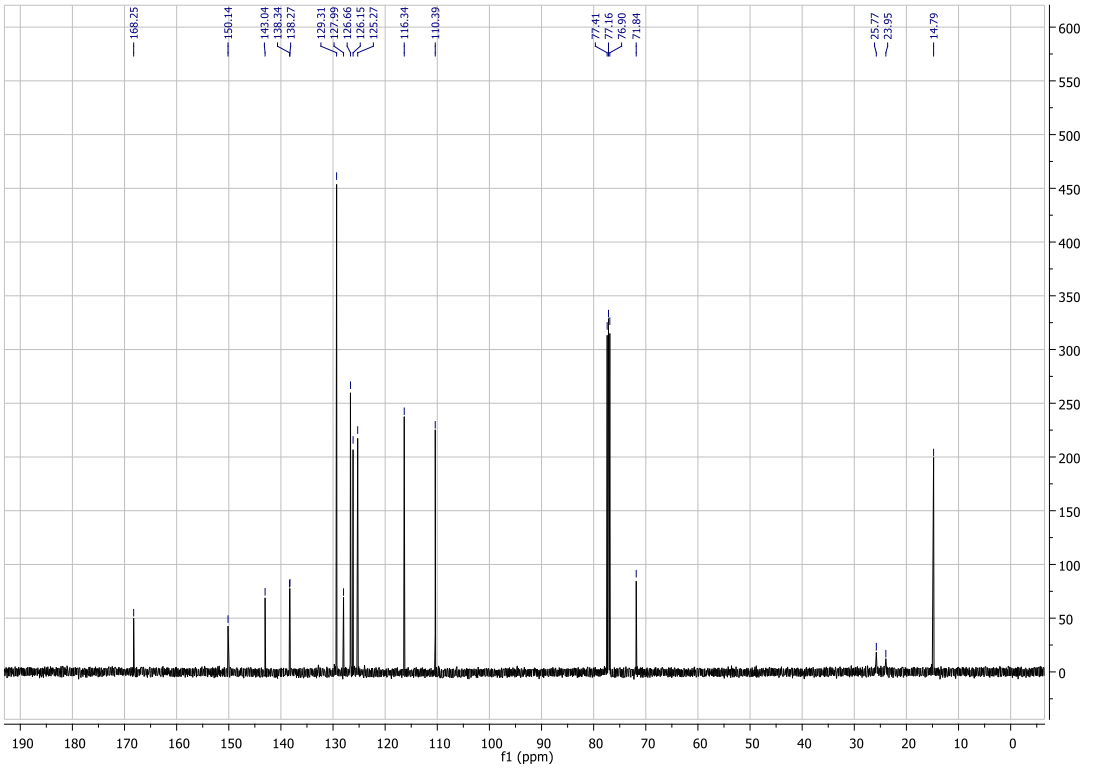
1.60
1.59
1.58
0.00
f1 (ppm)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129.31
127.99
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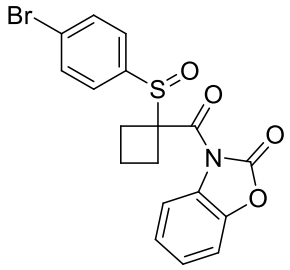
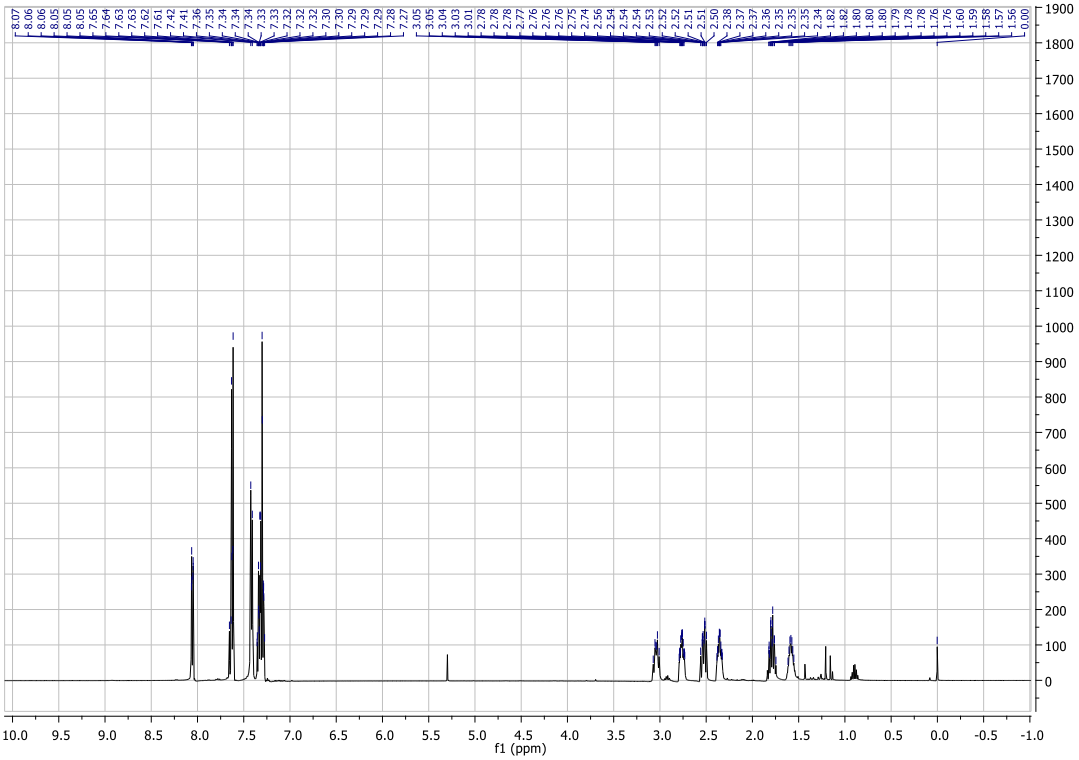
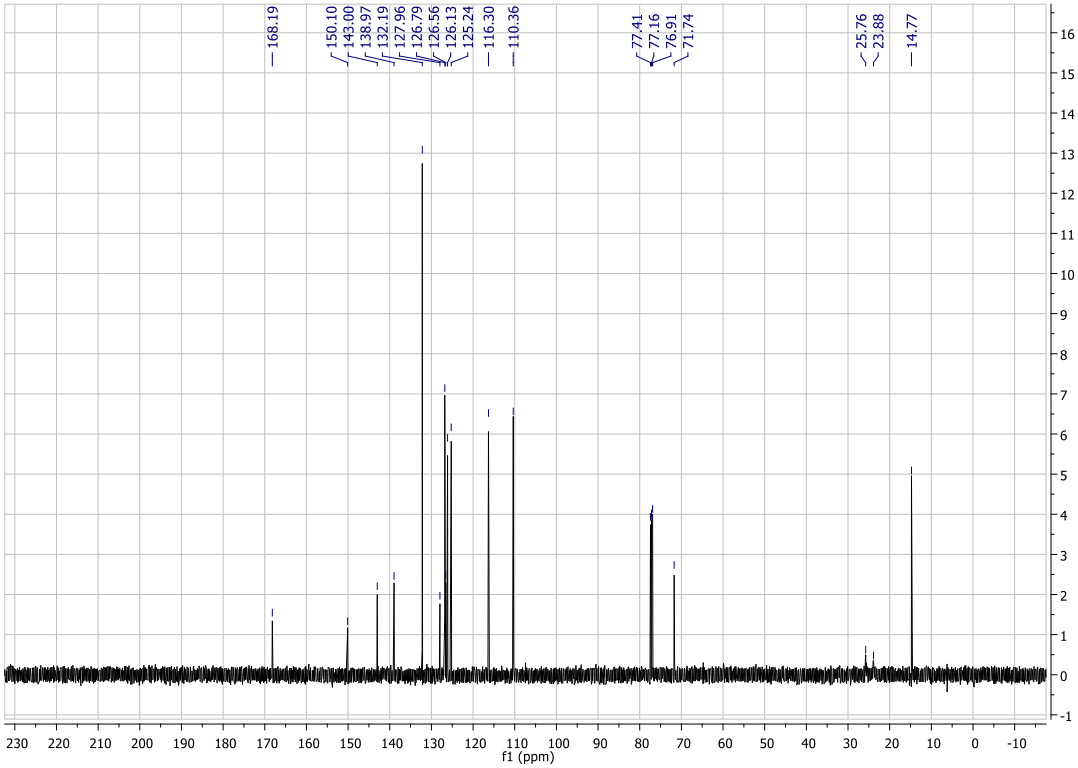
126.15
125.27
116.34
110.39
77.41
77.16
76.90
71.84
25.77
23.95
14.79
f1 (ppm)


Br
S
O
O
O
N
O
O

6j


f1 (ppm)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132.19
127.96
126.79
126.56
126.13
125.24
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110.36
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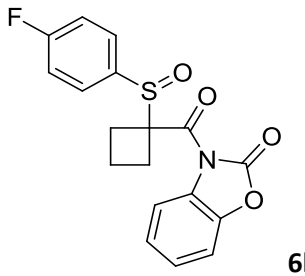
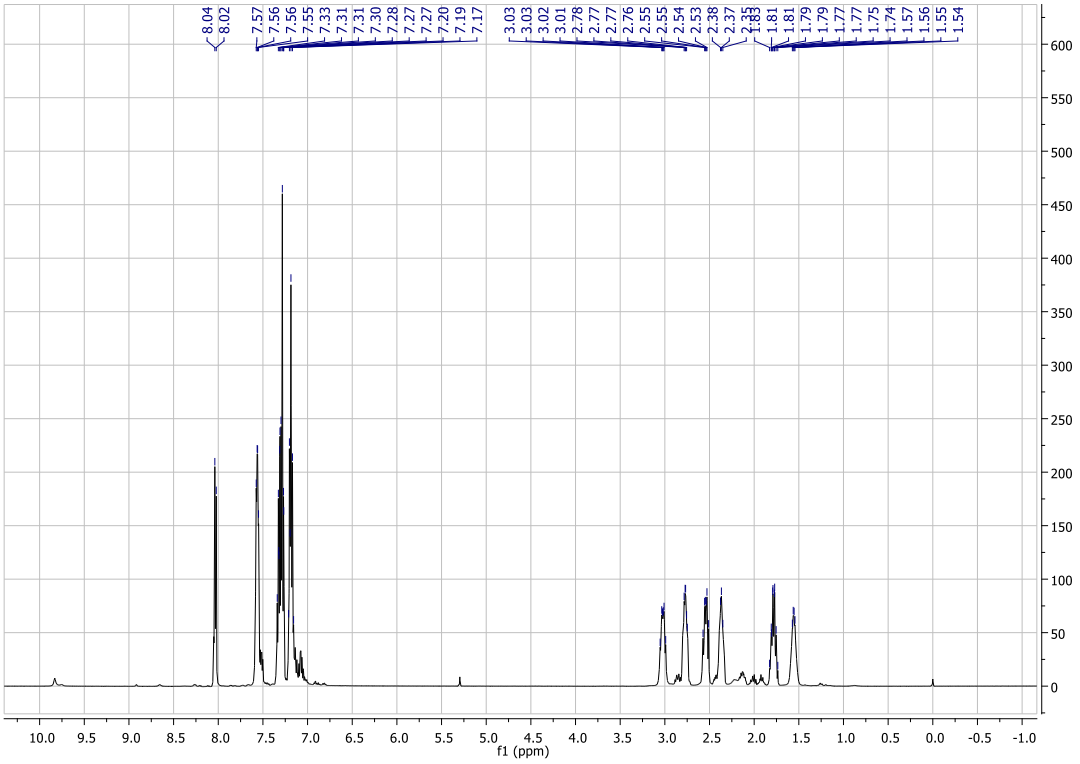
71.74
25.76
23.88
14.77
f1 (ppm)


F
S
O
O
N
O
O

6k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8.02
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7.56
7.56
7.55
7.33
7.31
7.31
7.30
7.28
7.27
7.27
7.20
7.19
7.17
3.03
3.03
3.02
3.01
2.78
2.77
2.77
2.76
2.55
2.55
2.54
2.53
2.38
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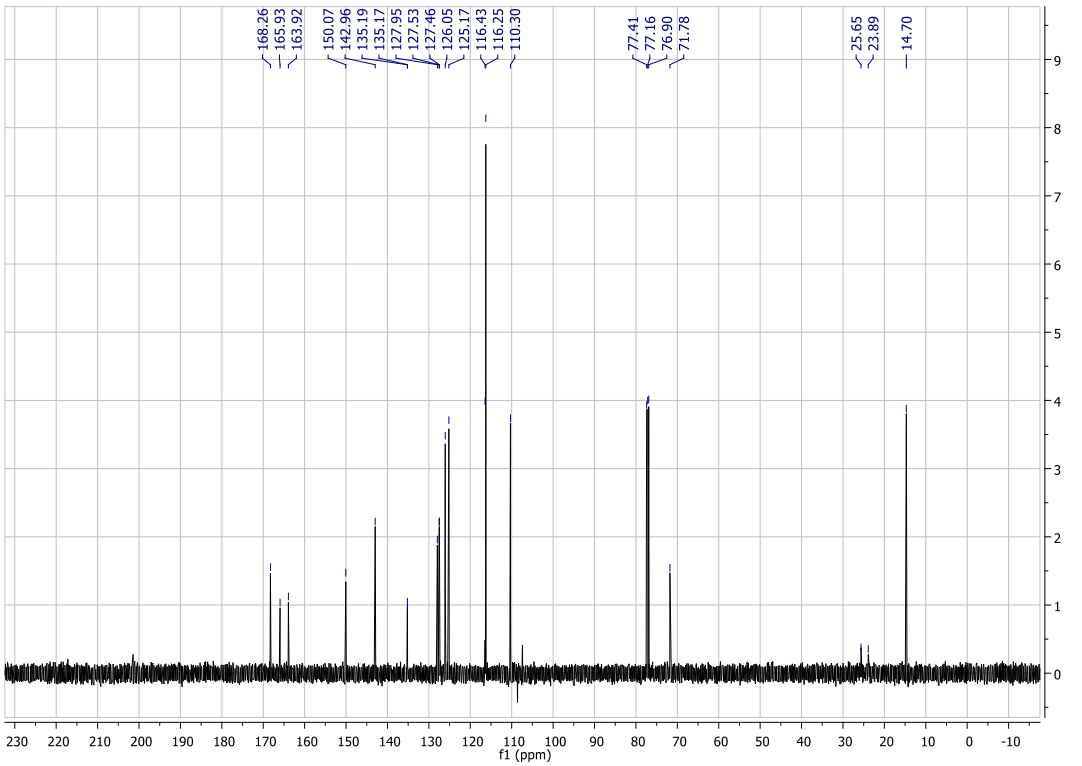
1.57
1.56
1.55
1.54
f1 (ppm)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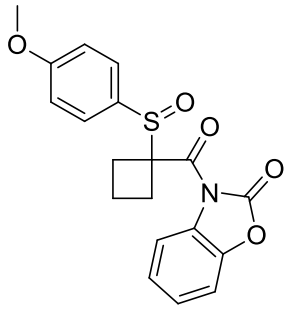
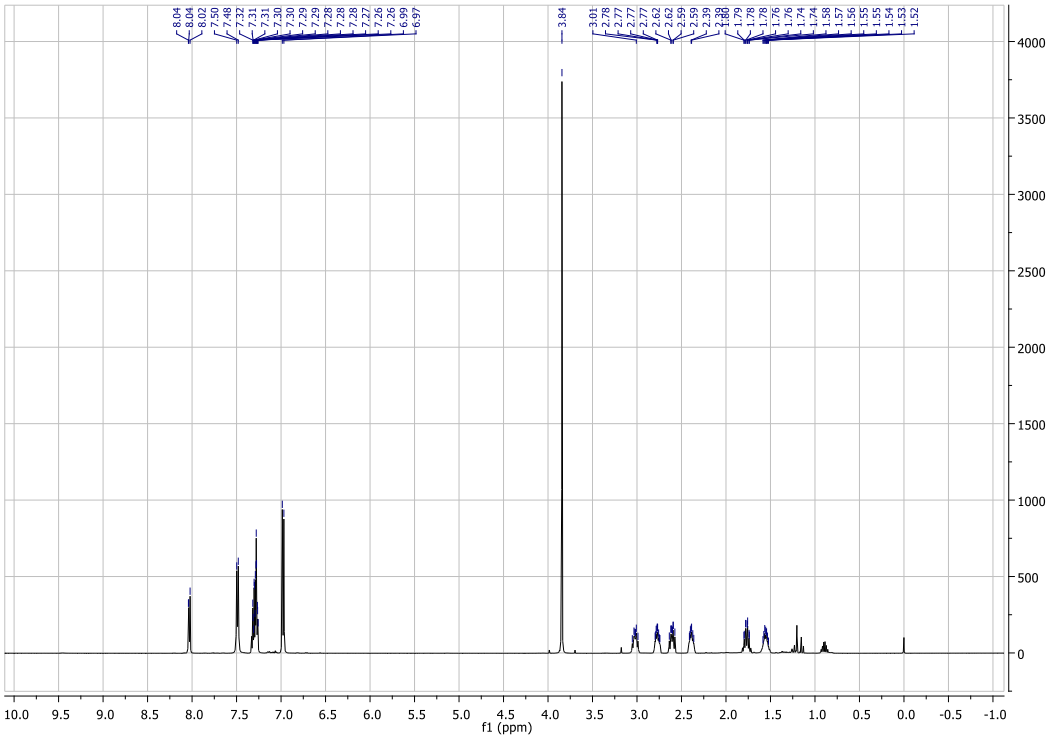
135.19
135.17
127.95
127.53
127.46
126.05
125.17
116.43
116.25
110.30
77.41
77.16
76.90
71.78
25.65
23.89
14.70
f1 (ppm)



6l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8.04
8.02
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7.48
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.28
7.27
7.27
7.26
6.99
6.97
3.84
3.01
2.78
2.77
2.77
2.62
2.62
2.59
2.59
2.39
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1.78
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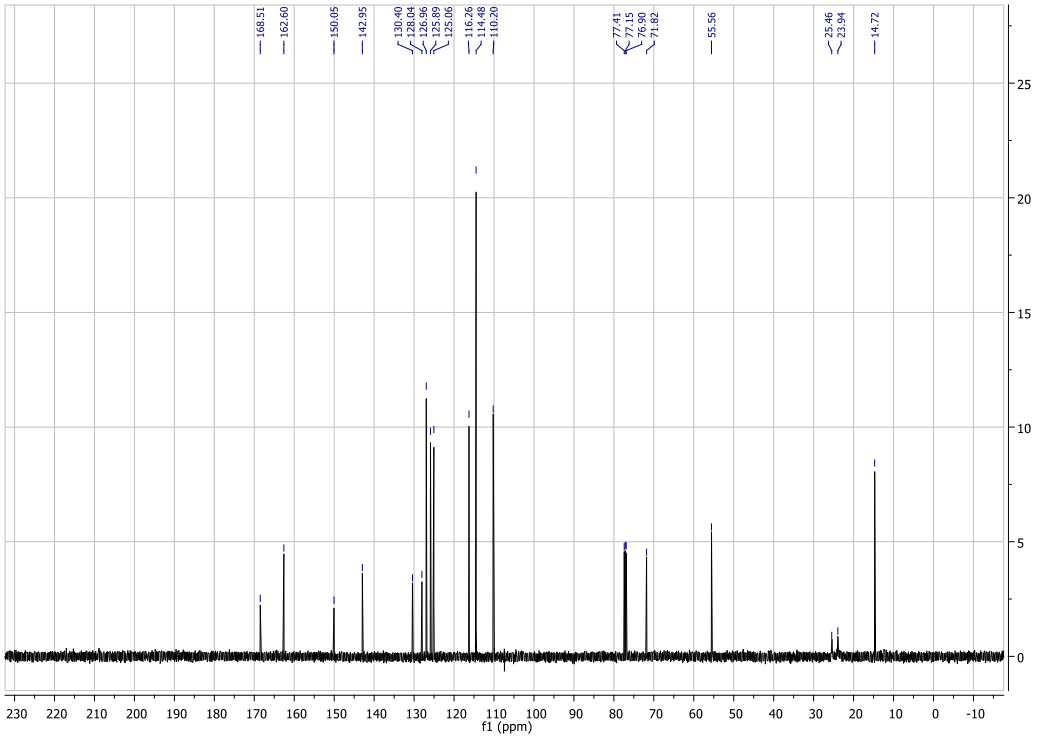
1.54
1.53
1.52
f1 (ppm)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162.60
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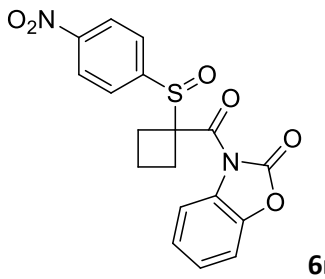
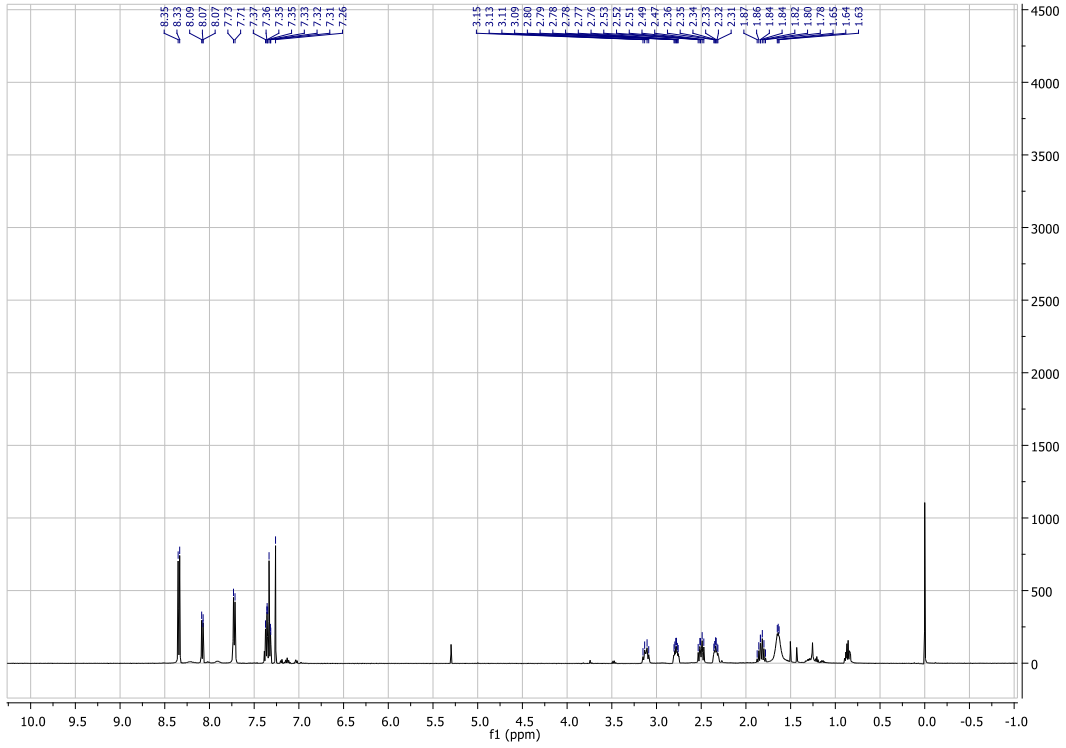
142.95
130.40
128.04
126.96
125.88
125.06
116.26
114.48
110.20
77.41
77.15
76.90
71.82
55.56
25.46
23.94
14.72
f1 (ppm)



6m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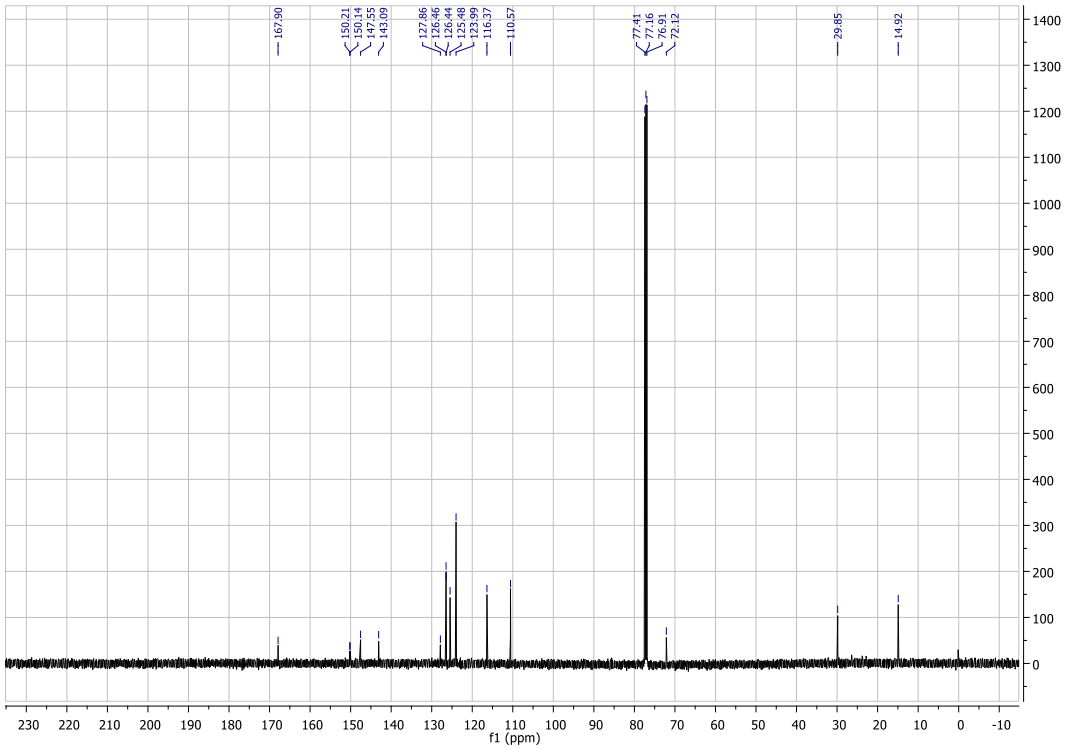
8.07
8.07
7.73
7.71
7.37
7.36
7.35
7.33
7.32
7.31
7.26
3.15
3.13
3.11
3.09
2.80
2.79
2.78
2.78
2.77
2.76
2.53
2.52
2.51
2.49
2.47
2.36
2.35
2.34
2.33
2.32
2.31
1.87
1.86
1.84
1.84
1.82
1.80
1.78
1.65
1.64
1.63
f1 (ppm)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147.55
143.09
127.86
126.46
126.44
125.48
123.99
116.37
110.57
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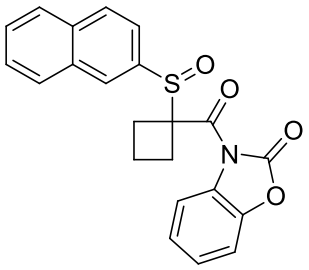
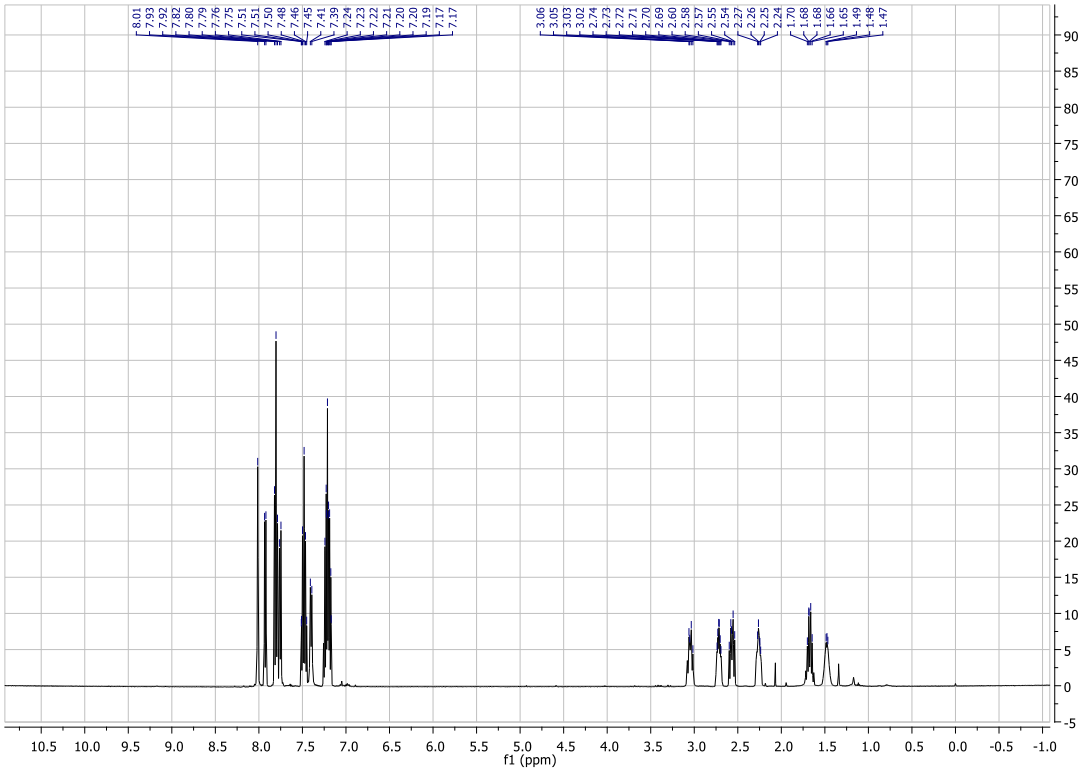
76.91
72.12
29.85
14.92
f1 (ppm)



6n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7.76
7.75
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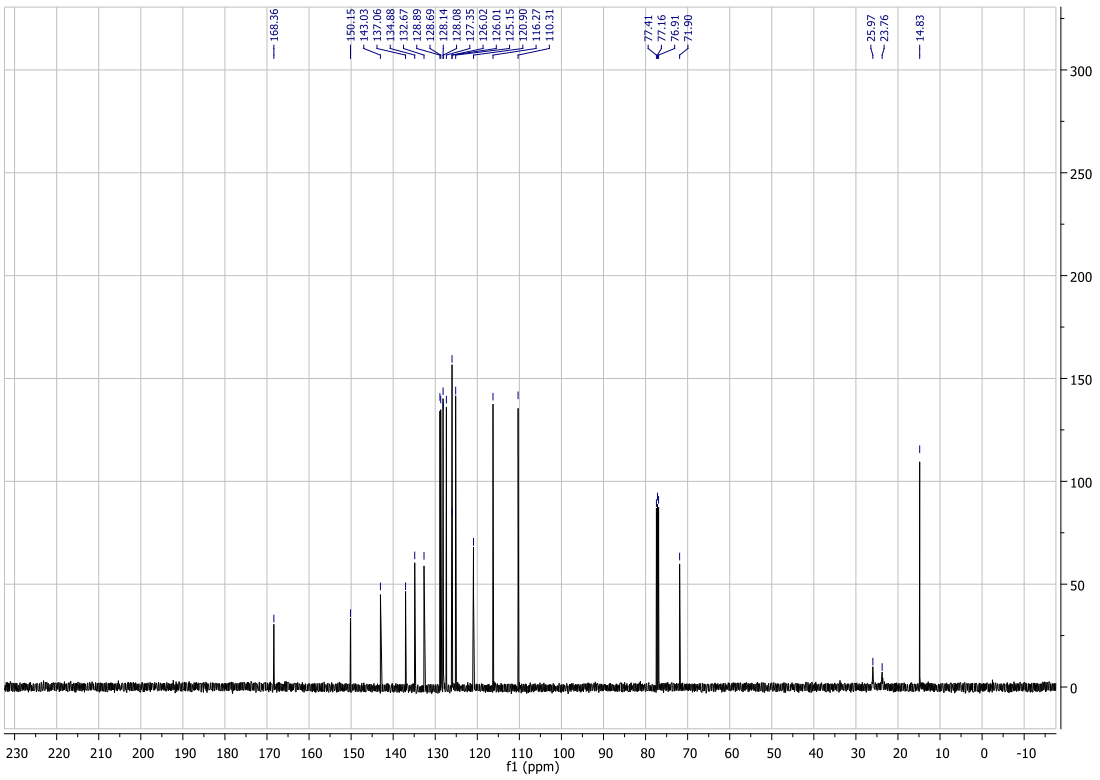
7.50
7.48
7.46
7.45
7.41
7.39
7.24
7.23
7.22
7.21
7.20
7.20
7.19
7.17
7.17
3.06
3.05
3.03
3.02
2.74
2.73
2.72
2.71
2.70
2.69
2.60
2.58
2.57
2.55
2.54
2.27
2.26
2.25
2.24
1.70
1.68
1.68
1.66
1.65
1.49
1.48
1.47
f1 (ppm)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150.15
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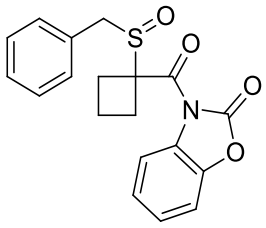
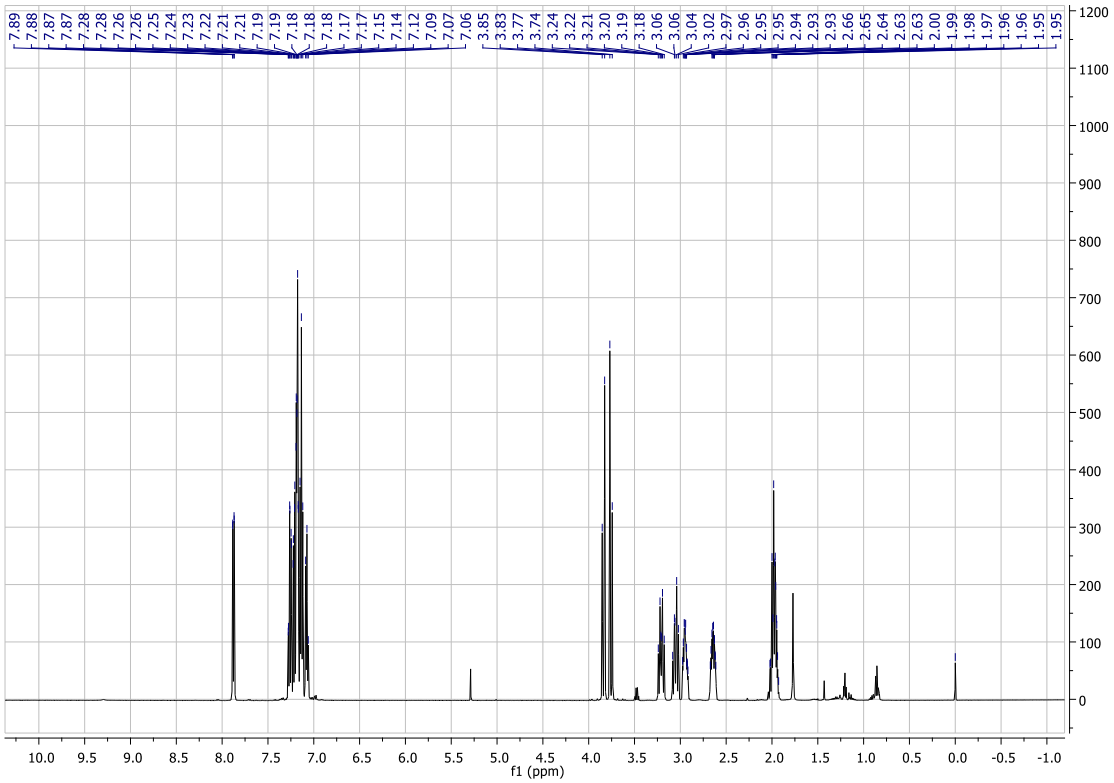
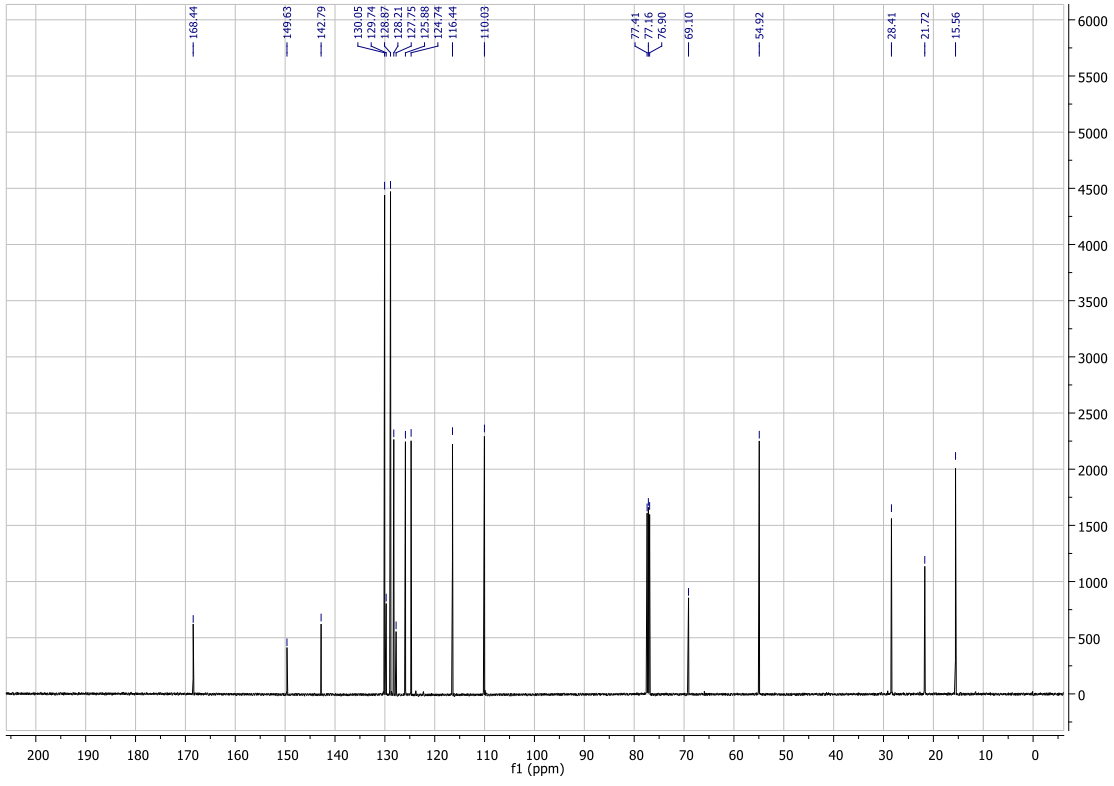
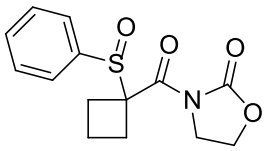
137.06
134.88
132.67
128.89
128.69
128.14
128.08
127.35
126.02
126.01
125.15
120.90
116.27
110.31
77.41
77.16
76.91
71.90
25.97
23.76
14.83
f1 (ppm)



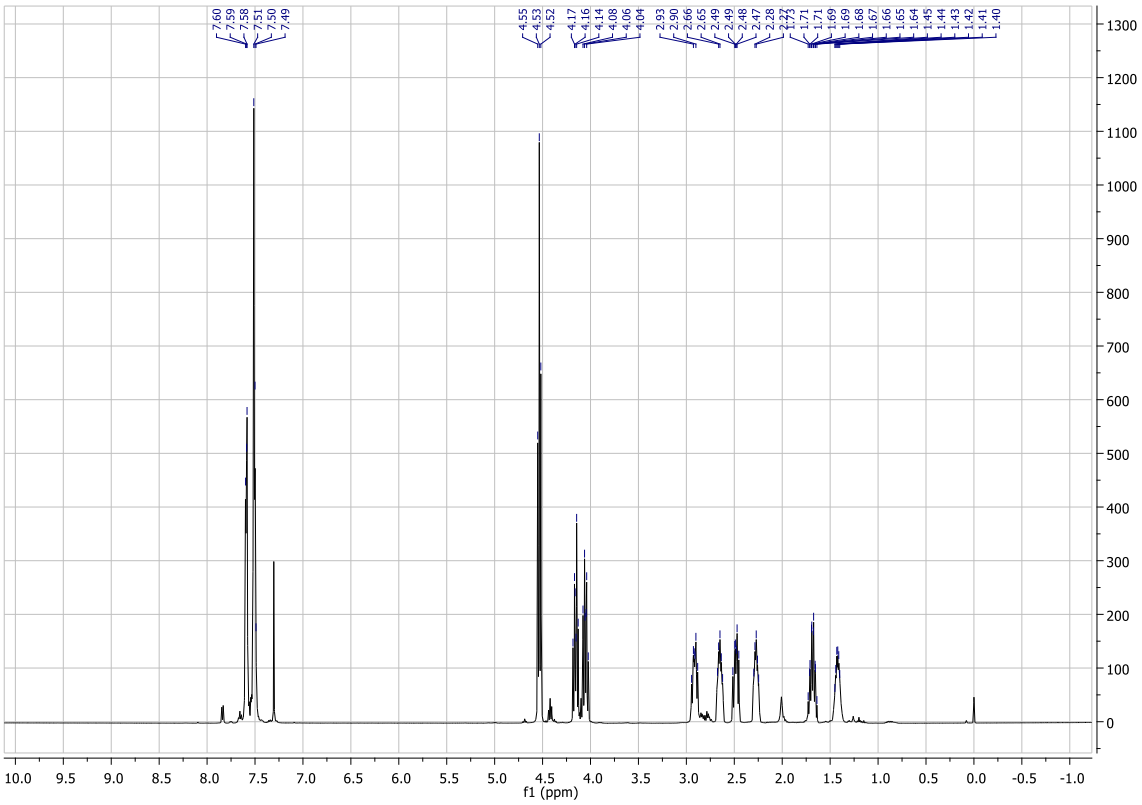
6o


7.89 7.88 7.87 7.87 7.28 7.28 7.26 7.26 7.25 7.24 7.23 7.22 7.21 7.21 7.19 7.19 7.18 7.18 7.18 7.17 7.17 7.15 7.14 7.12 7.09 7.07 7.06 3.85 3.83 3.77 3.74 3.24 3.22 3.21 3.20 3.19 3.18 3.06 3.06 3.04 3.02 2.97 2.96 2.95 2.95 2.94 2.93 2.93 2.66 2.65 2.64 2.63 2.63 2.00 1.99 1.98 1.97 1.96 1.96 1.95 1.95
f1 (ppm)


168.44 149.63 142.79 130.05 129.94 128.97 128.21 127.75 125.88 124.74 116.44 110.03 77.41 77.16 76.90 69.10 54.92 28.41 21.72 15.56
f1 (ppm)



11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4.06
4.04
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2.23
1.71
1.71
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1.69
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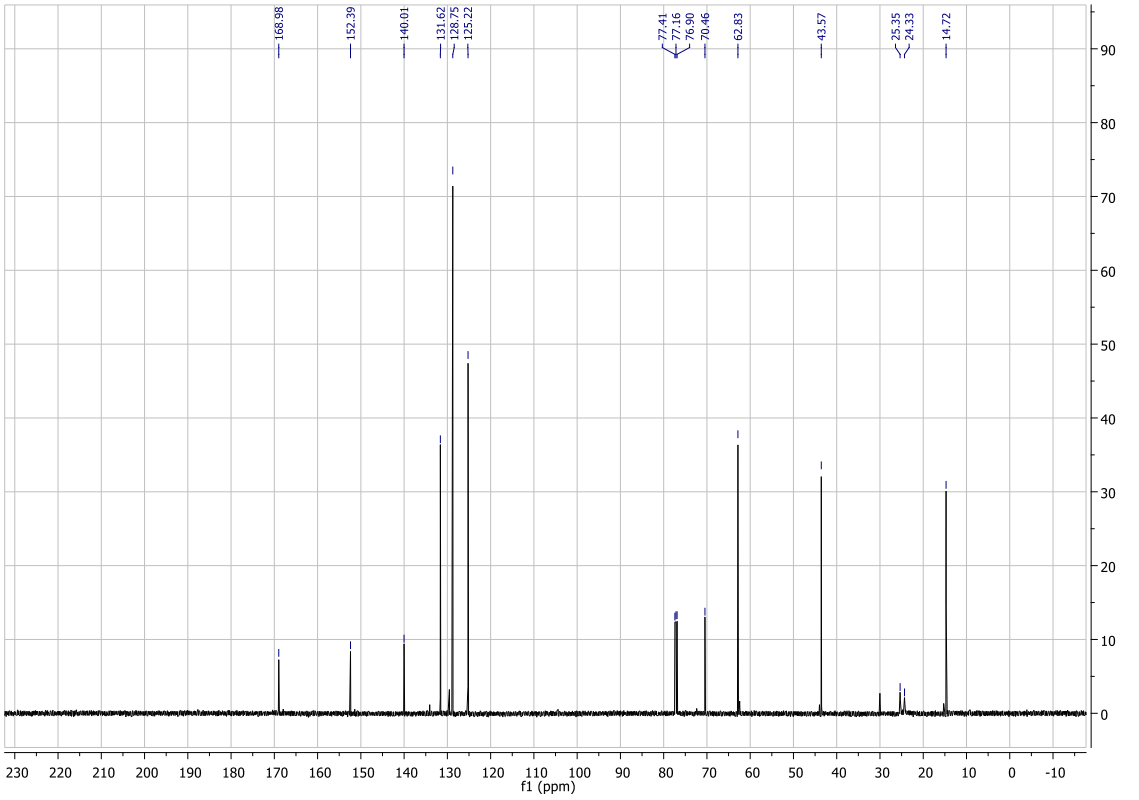
1.43
1.42
1.41
1.40
f1 (ppm)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125.22
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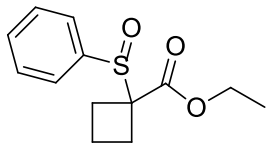
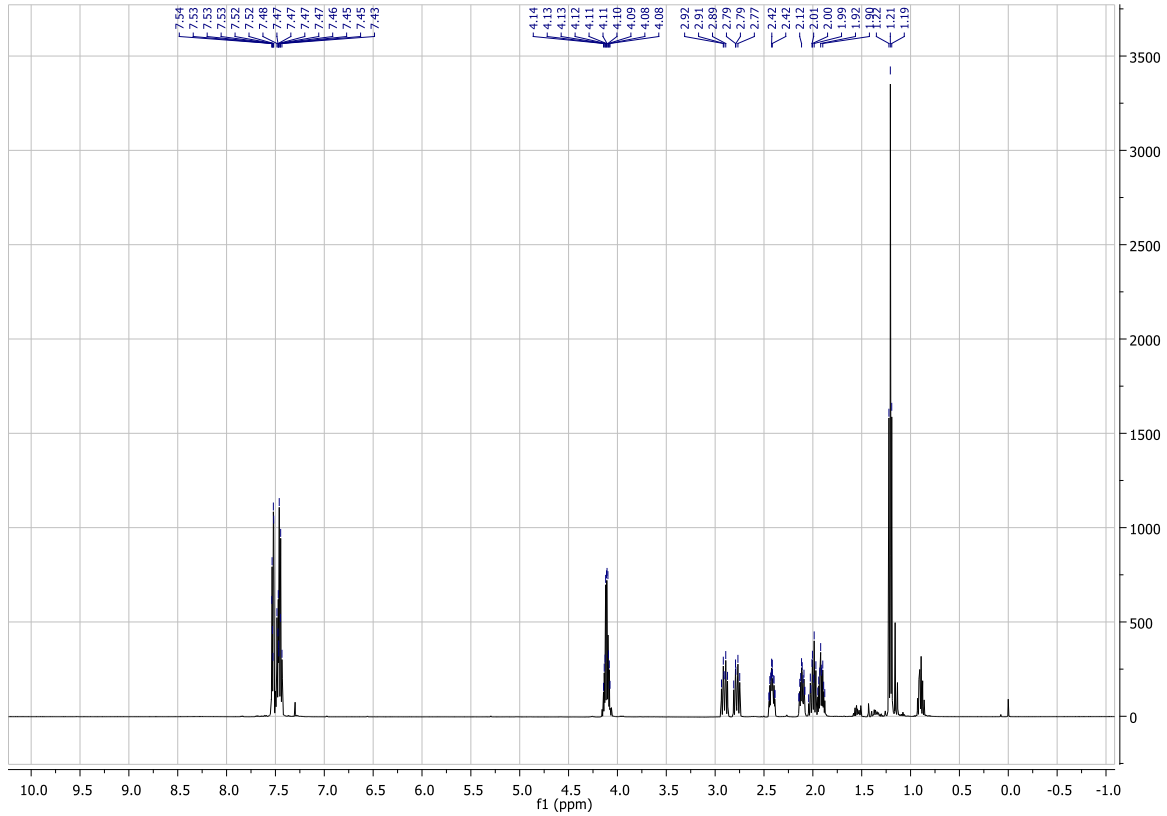
77.16
76.90
70.46
62.83
43.57
25.35
24.33
14.72
f1 (ppm)



12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7.47
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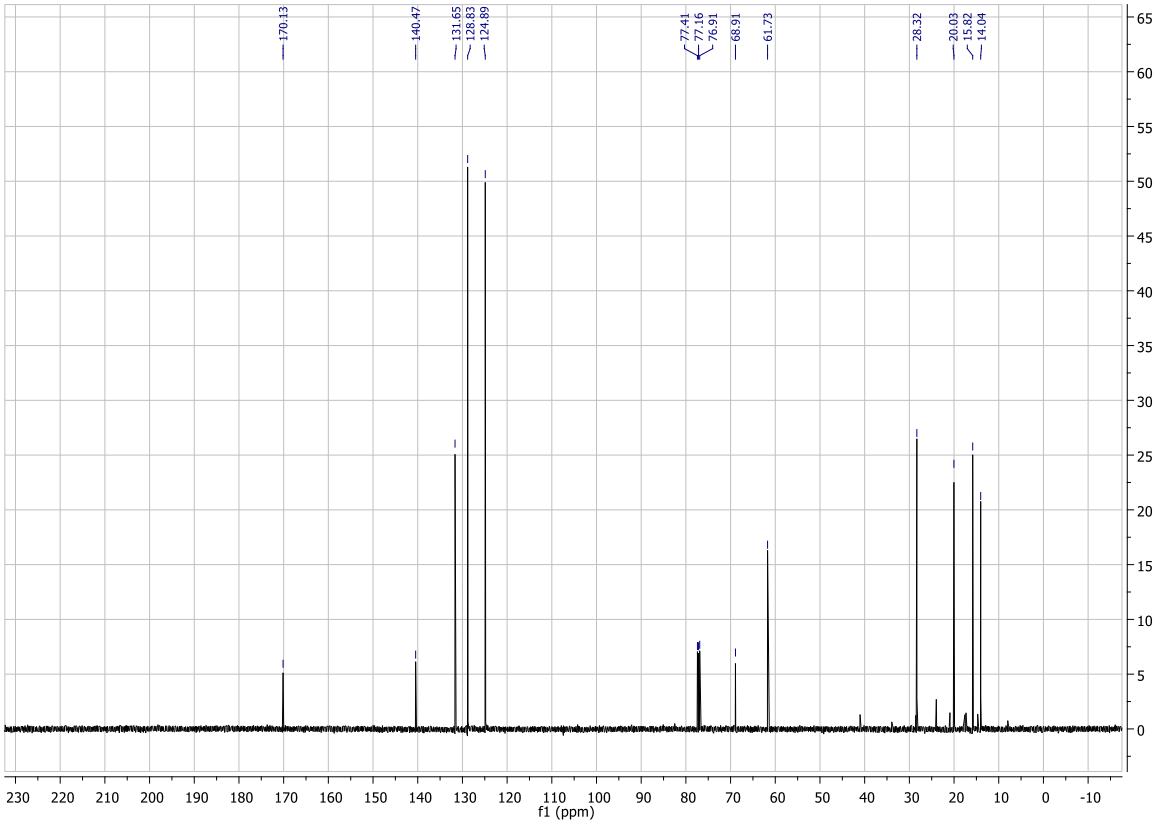
1.90
1.22
1.21
1.19
f1 (ppm)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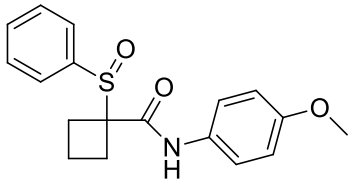
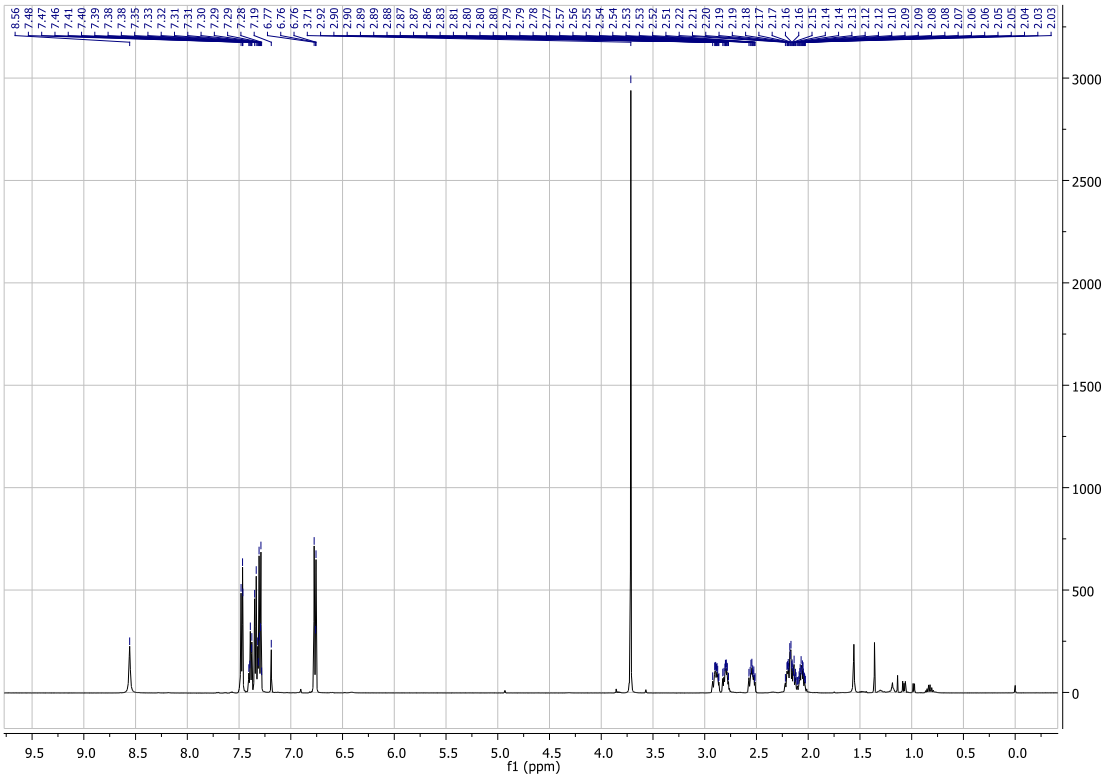
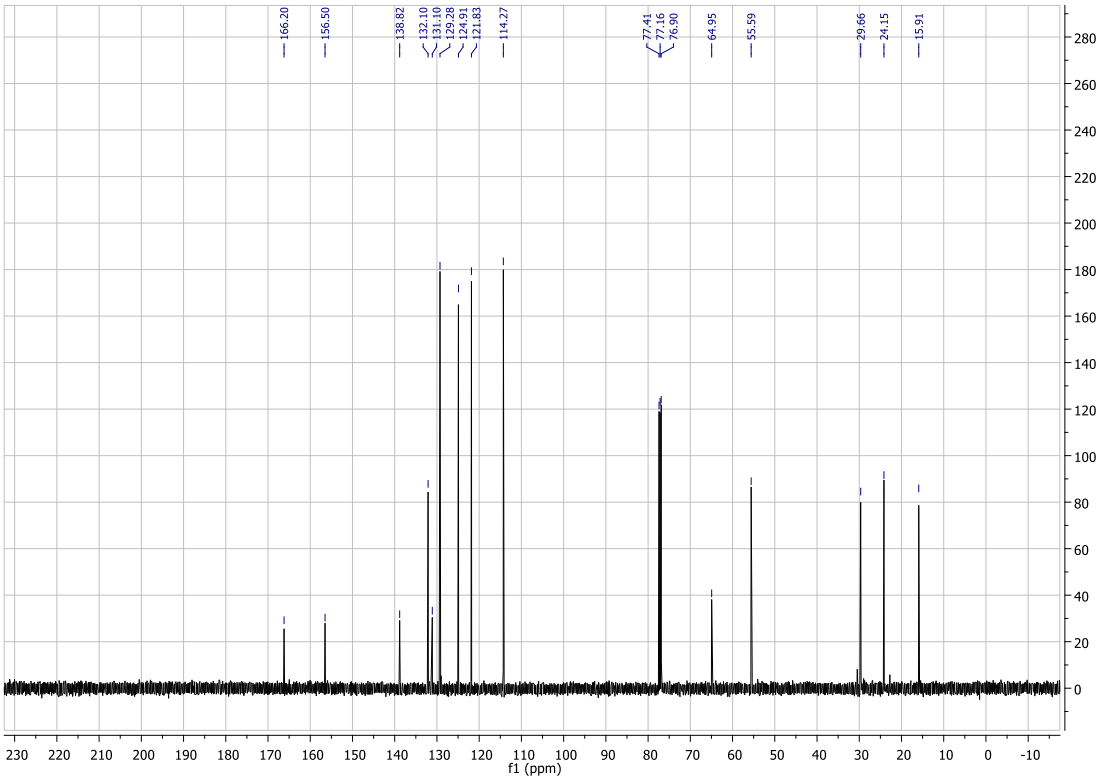
128.83
124.89
77.41
77.16
76.91
68.91
61.73
28.32
20.03
15.82
14.04
f1 (ppm)



13


f1 (ppm)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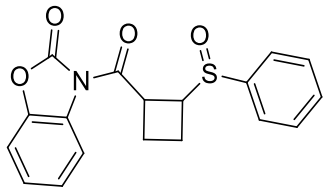
76.90
64.95
55.59
29.66
24.15
15.91
f1 (ppm)



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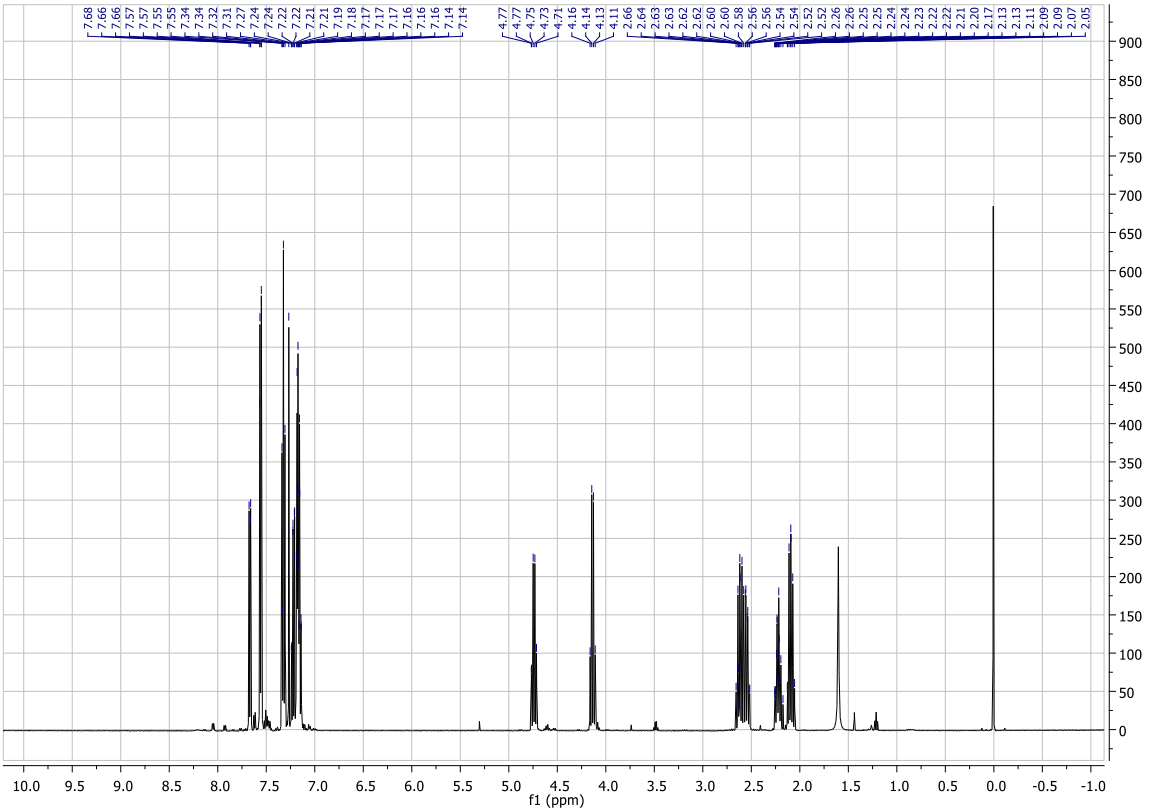
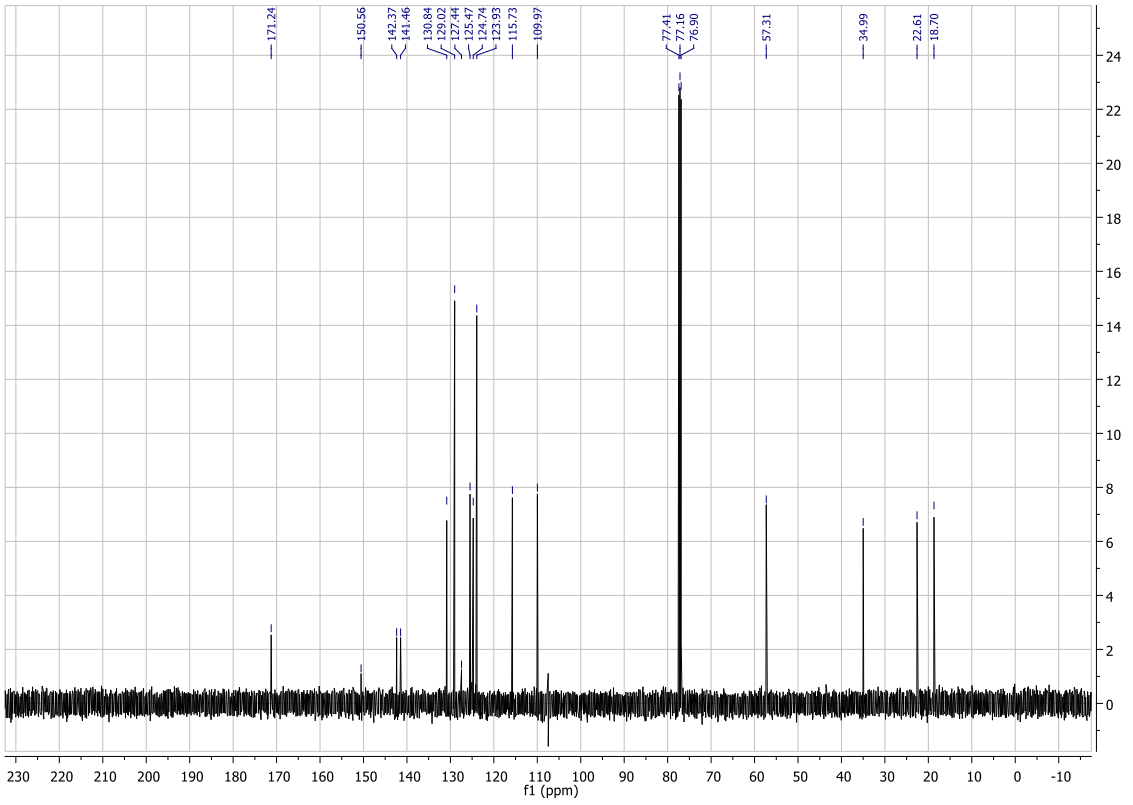
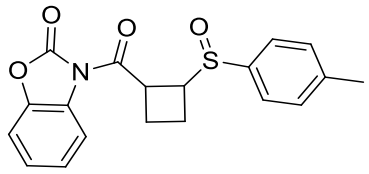
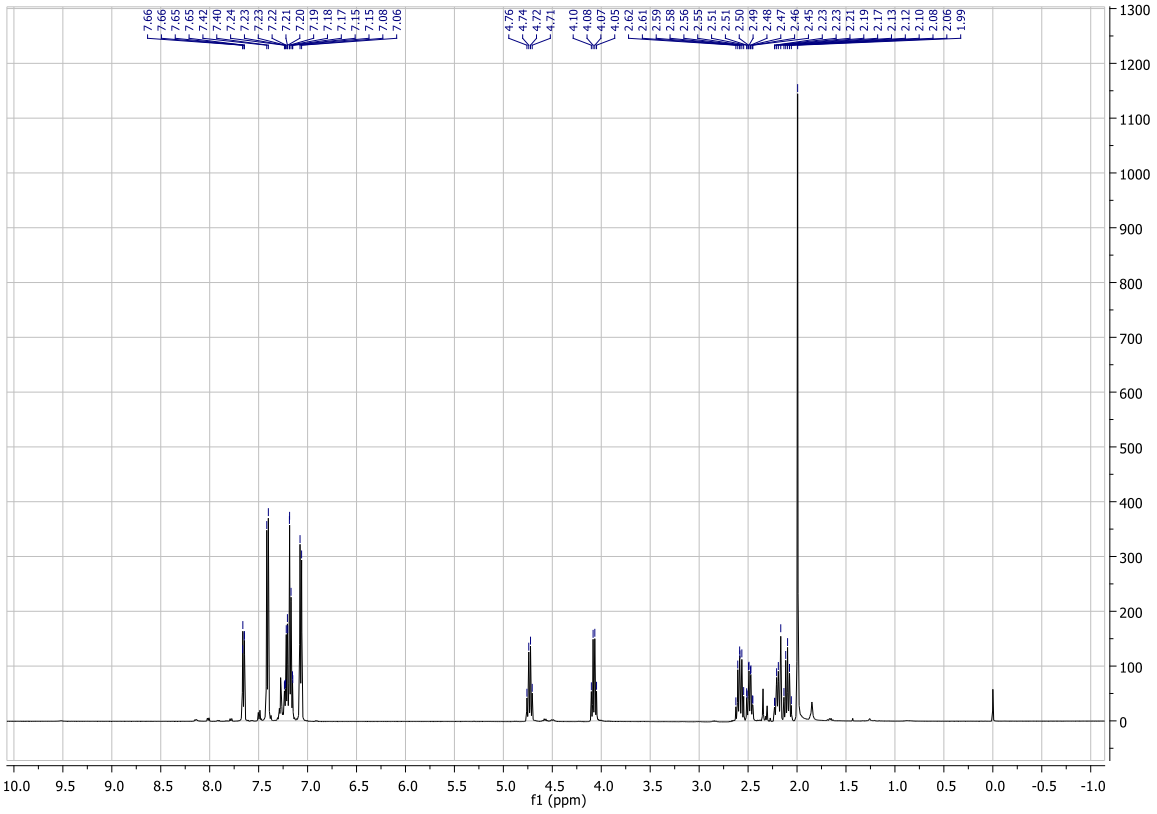

7.68 7.66 7.66 7.57 7.57 7.55 7.55 7.34 7.34 7.32 7.31 7.27 7.24 7.24 7.22 7.22 7.21 7.21 7.19 7.18 7.17 7.17 7.17 7.16 7.16 7.16 7.14 7.14
4.77 4.77 4.75 4.73 4.71 4.16 4.14 4.13 4.11 2.66 2.64 2.63 2.62 2.62 2.60 2.60 2.58 2.56 2.56 2.54 2.54 2.52 2.52 2.26 2.26 2.25 2.25 2.24 2.24 2.23 2.22 2.22 2.21 2.20 2.17 2.13 2.13 2.11 2.09 2.09 2.07 2.05
f1 (ppm)


171.24 150.56 142.37 141.46 130.84 129.02 127.44 125.47 124.74 123.93 115.73 109.97 77.41 77.16 76.90 57.31 34.99 22.61 18.70
f1 (ppm)



7b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7.23
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7.22
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7.20
7.19
7.18
7.17
7.15
7.15
7.08
7.06
4.76
4.74
4.72
4.71
4.10
4.08
4.07
4.05
2.62
2.61
2.59
2.58
2.56
2.55
2.51
2.51
2.50
2.49
2.48
2.47
2.46
2.45
2.23
2.23
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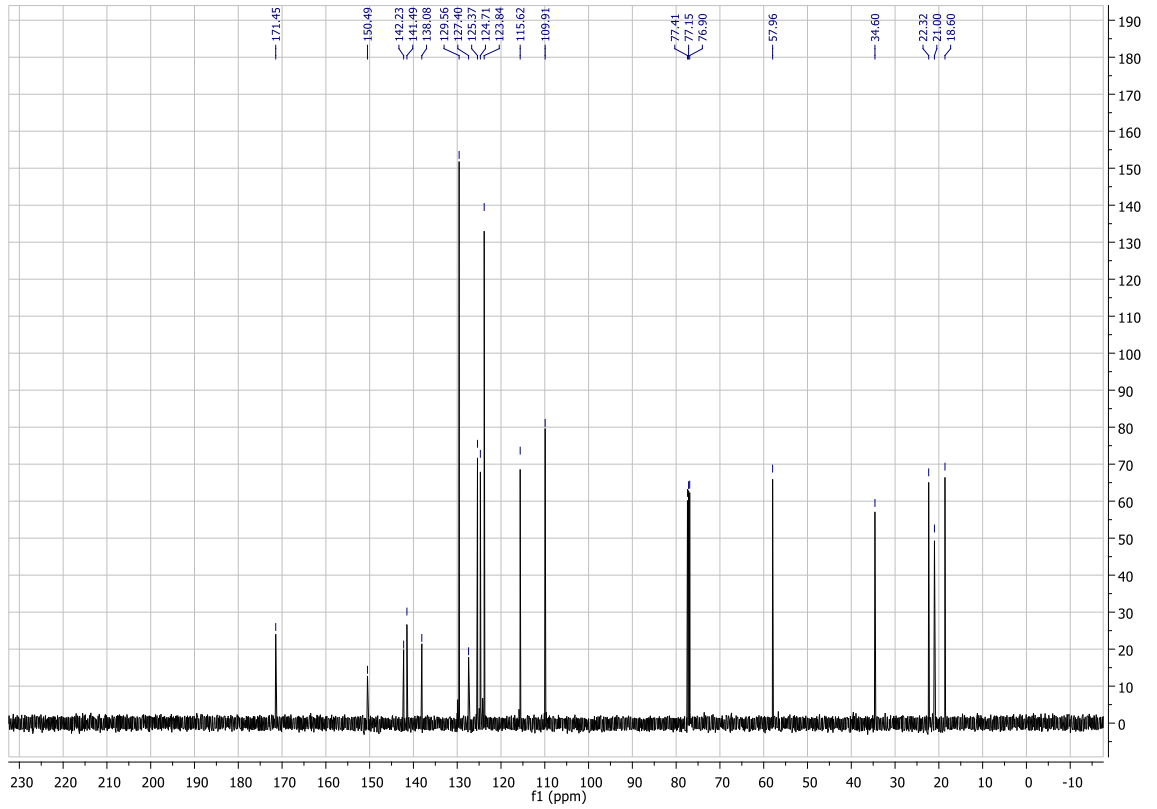
2.19
2.17
2.13
2.12
2.10
2.08
2.06
1.99
f1 (ppm)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109.91
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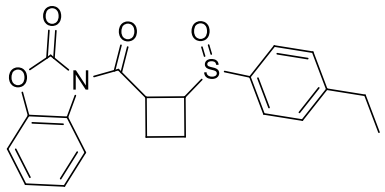
34.60
22.32
21.00
18.60
f1 (ppm)



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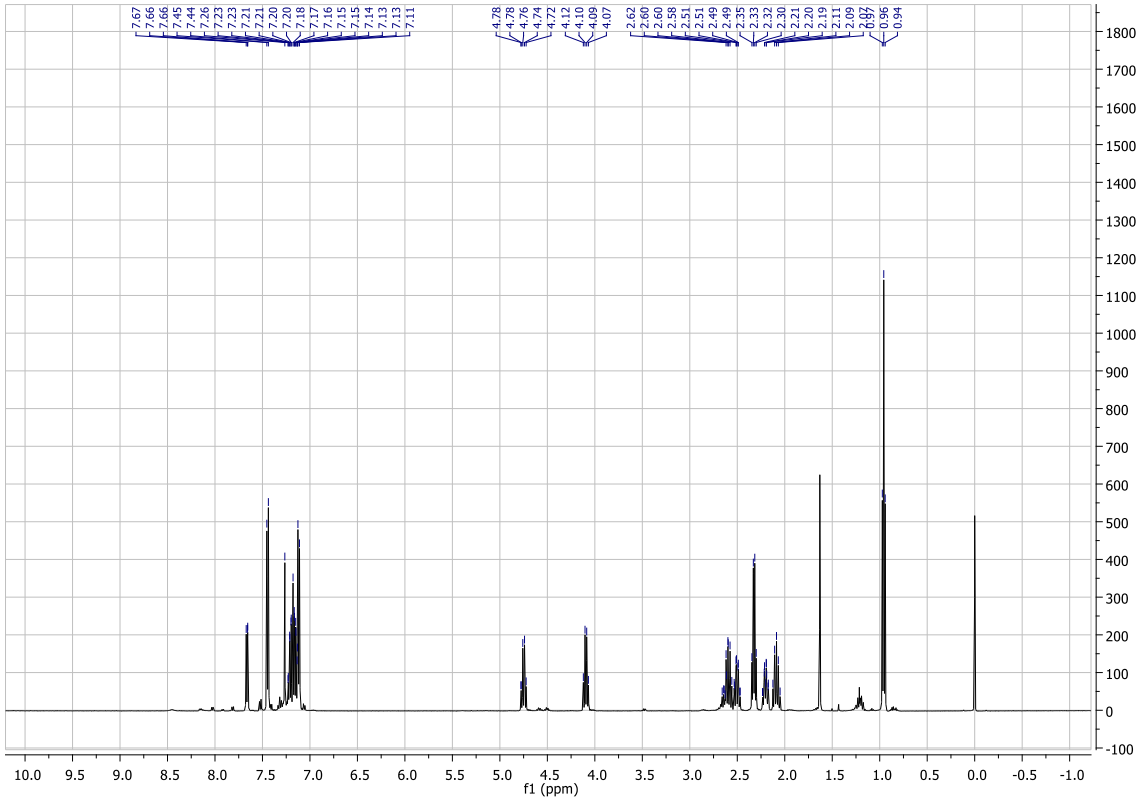
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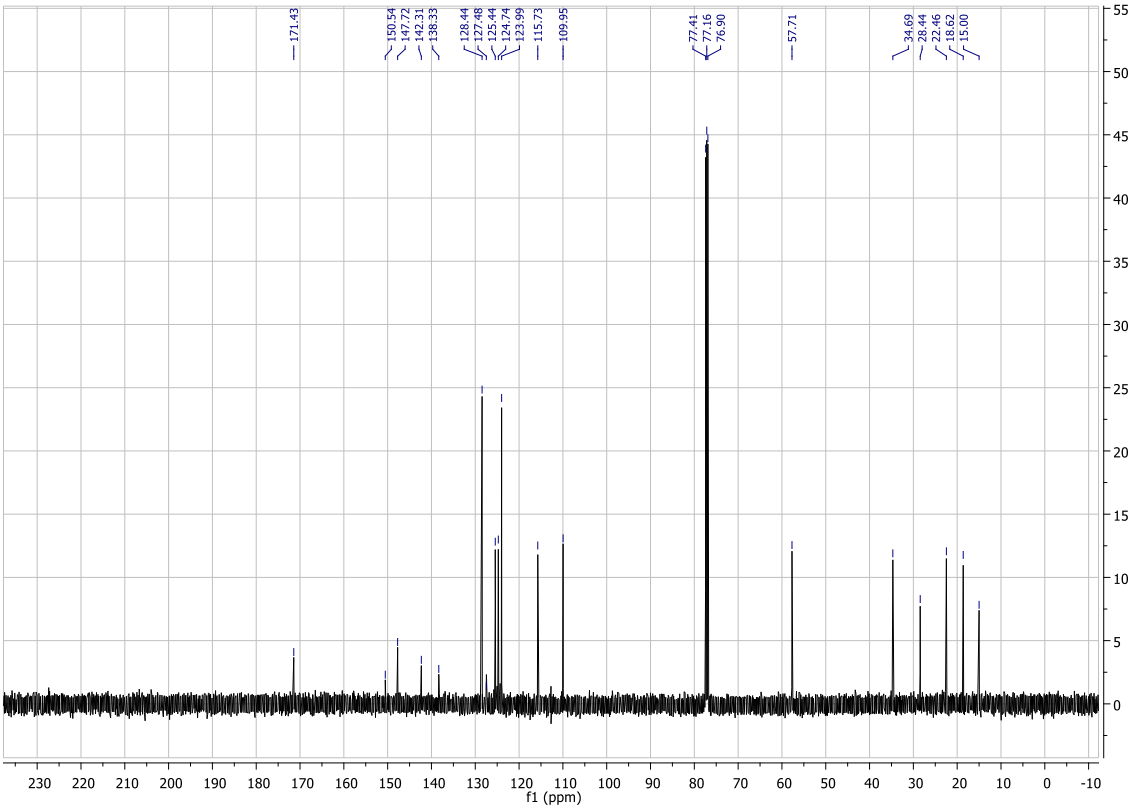
7.20
7.19
7.17
7.16
7.15
7.15
7.14
7.13
7.13
7.11
4.78
4.78
4.76
4.74
4.72
4.12
4.10
4.09
4.07
2.62
2.60
2.60
2.58
2.51
2.51
2.49
2.49
2.35
2.33
2.32
2.30
2.21
2.20
2.19
2.11
2.09
0.97
0.96
0.94
f1 (ppm)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125.44
124.74
123.99
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109.95
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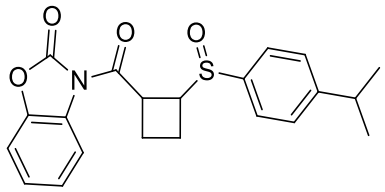
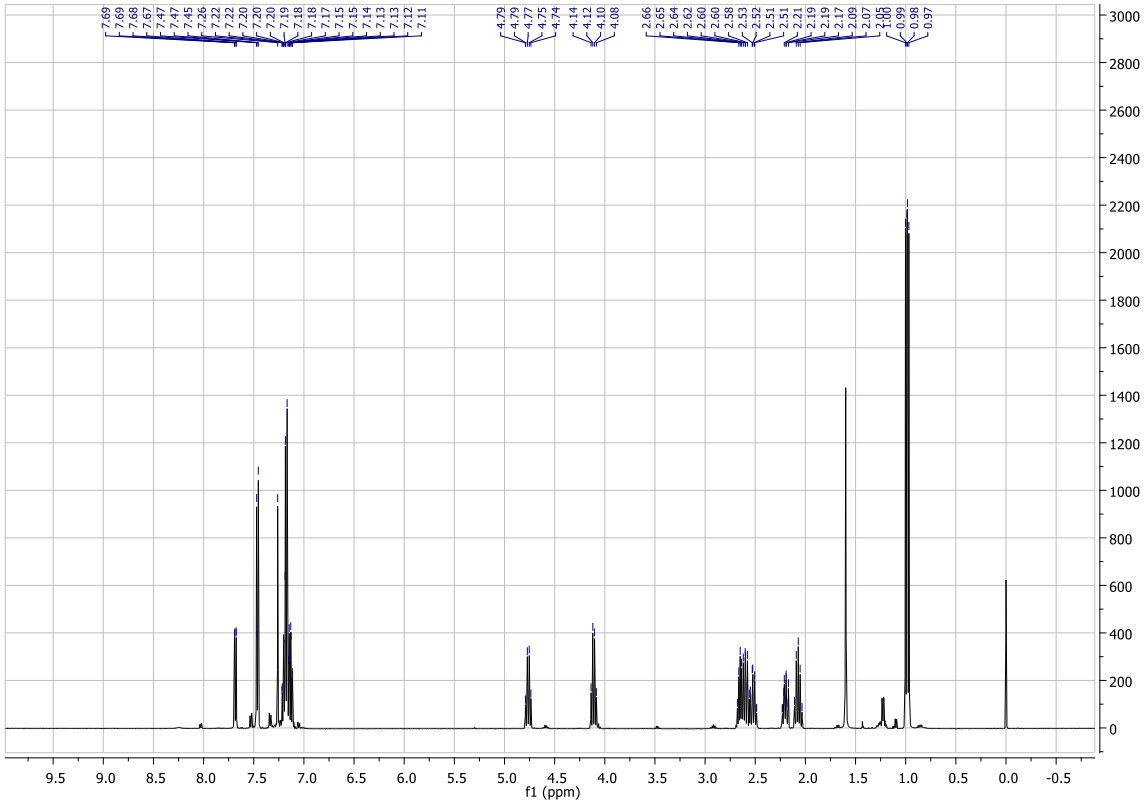
28.44
22.46
18.62
15.00
f1 (ppm)



7d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7.20
7.19
7.18
7.18
7.17
7.15
7.14
7.13
7.13
7.12
7.11
4.79
4.79
4.77
4.75
4.74
4.14
4.12
4.10
4.08
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2.65
2.64
2.62
2.60
2.60
2.58
2.53
2.52
2.51
2.51
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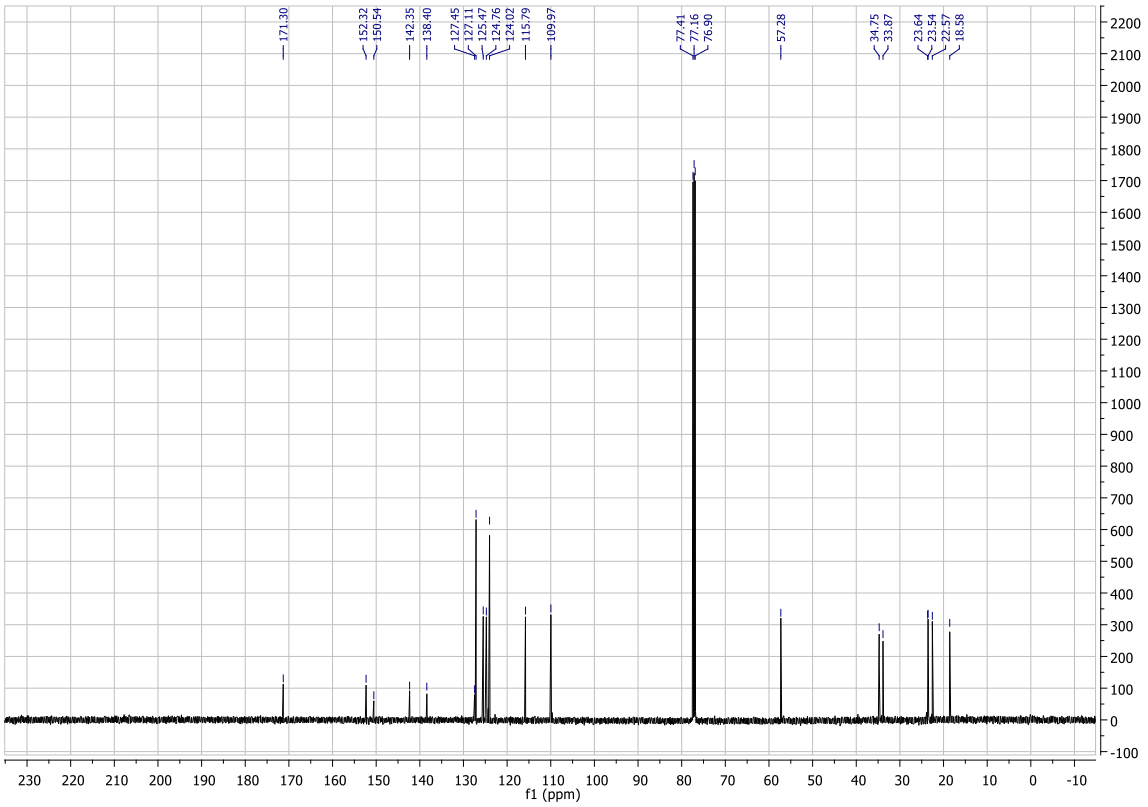
2.19
2.17
2.09
2.07
1.00
0.99
0.98
0.97
f1 (ppm)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127.45
127.11
125.47
124.76
124.02
115.79
109.97
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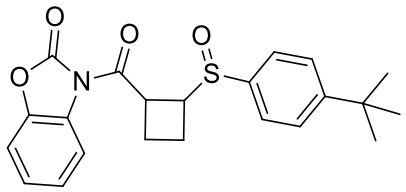
23.64
23.54
22.57
18.58
f1 (ppm)



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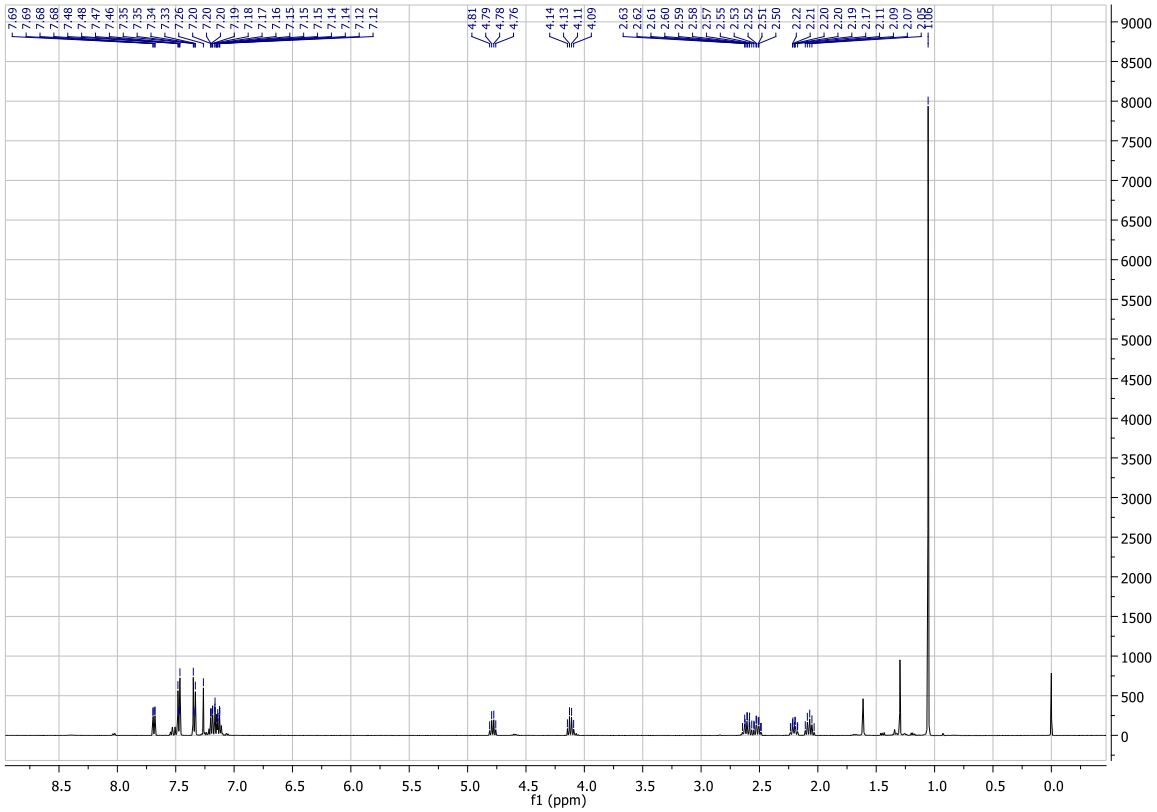
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7.34
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7.26
7.20
7.20
7.19
7.18
7.17
7.16
7.15
7.15
7.14
7.12
7.12
4.81
4.79
4.78
4.76
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4.13
4.11
4.09
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2.60
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2.52
2.51
2.50
2.22
2.21
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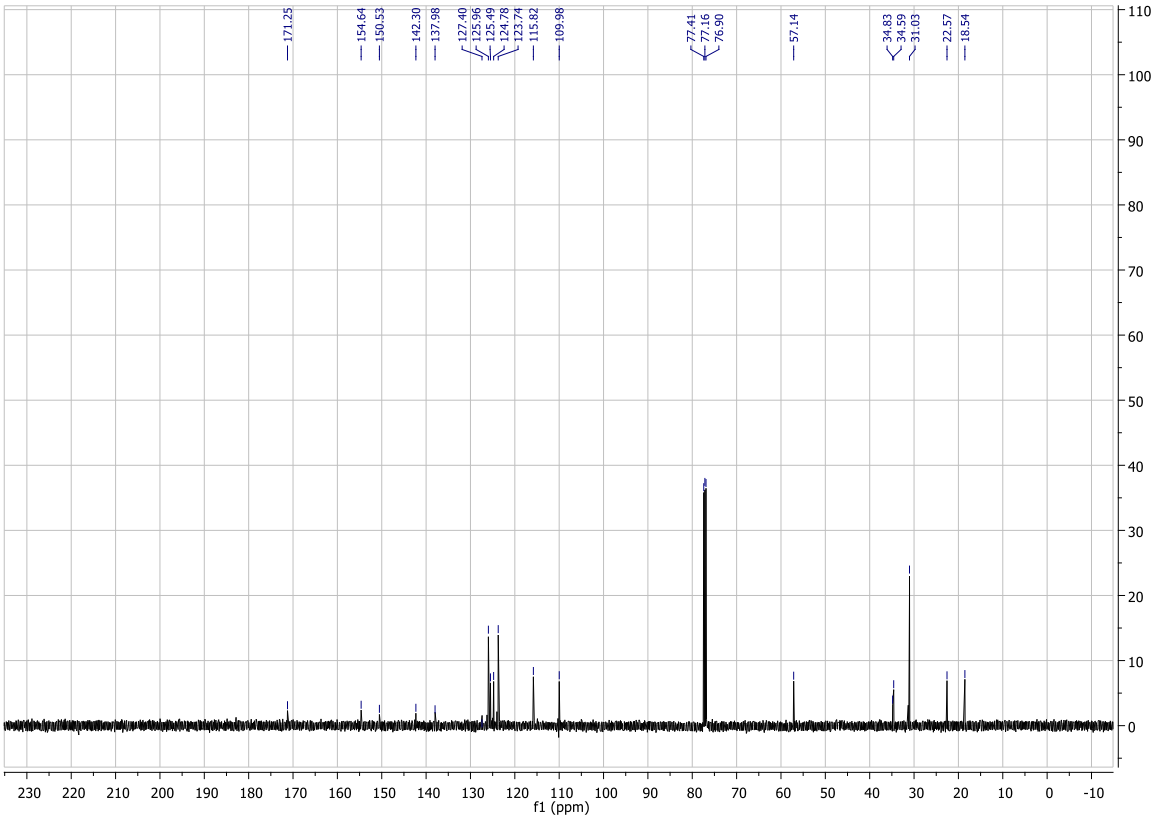
2.20
2.19
2.17
2.11
2.09
2.07
2.05
1.00
f1 (ppm)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124.78
123.74
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109.98
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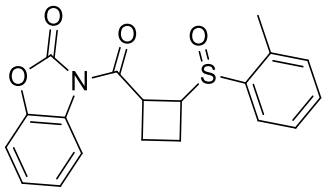
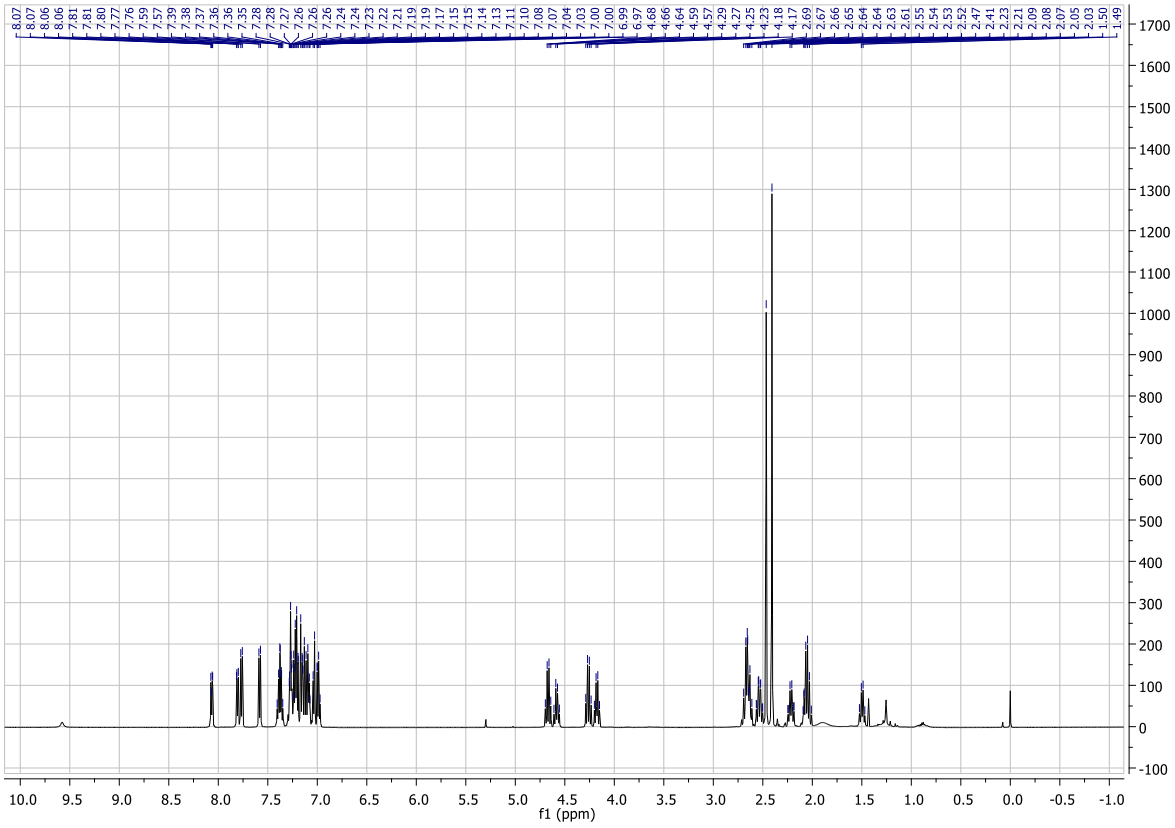
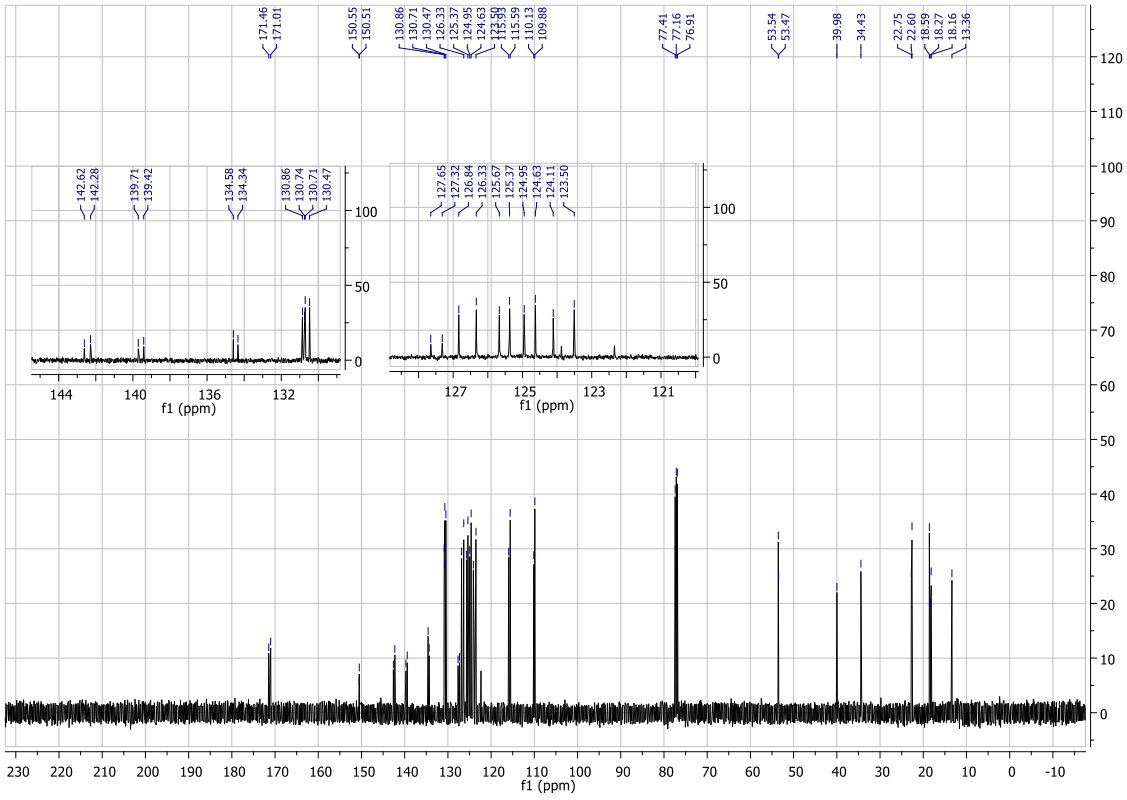
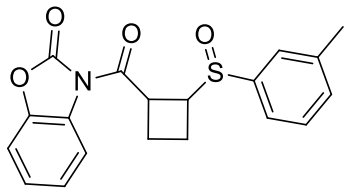
34.59
31.03
22.57
18.54
f1 (ppm)



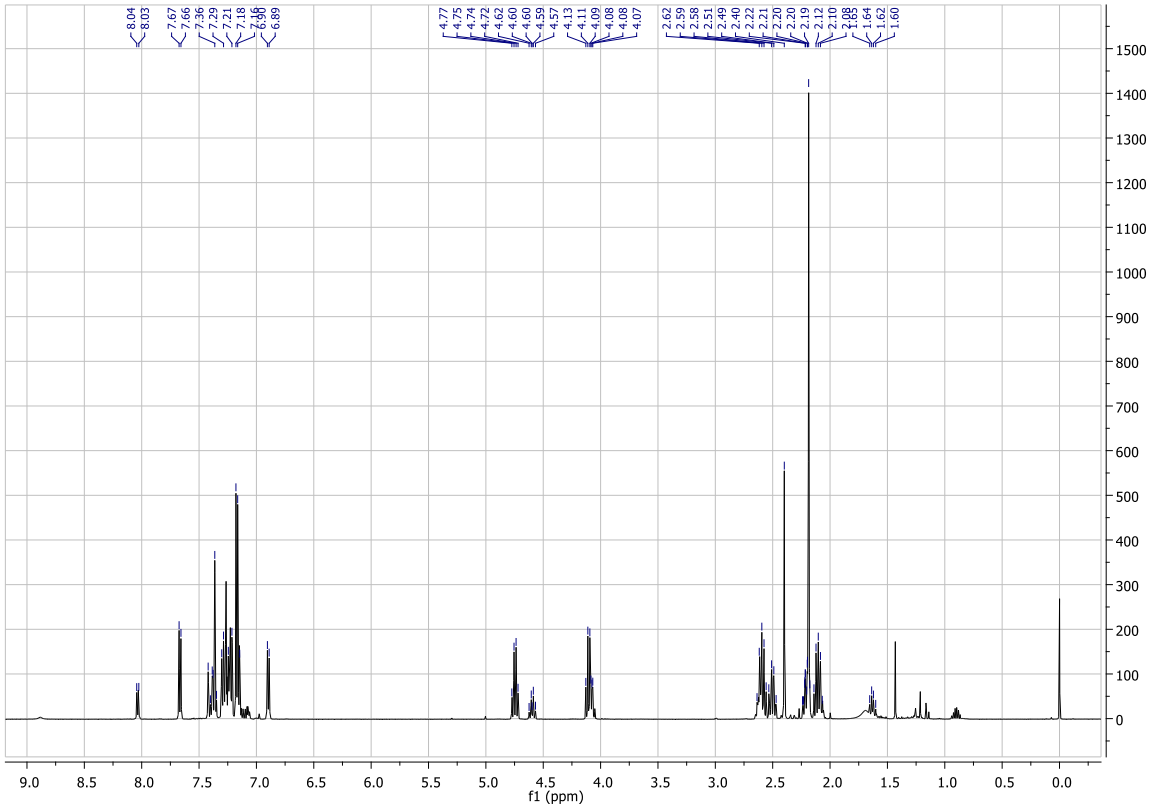
7f+7f'







7g+7g'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4.62
4.60
4.59
4.57
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4.11
4.09
4.08
4.08
4.07
2.62
2.59
2.58
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2.49
2.40
2.22
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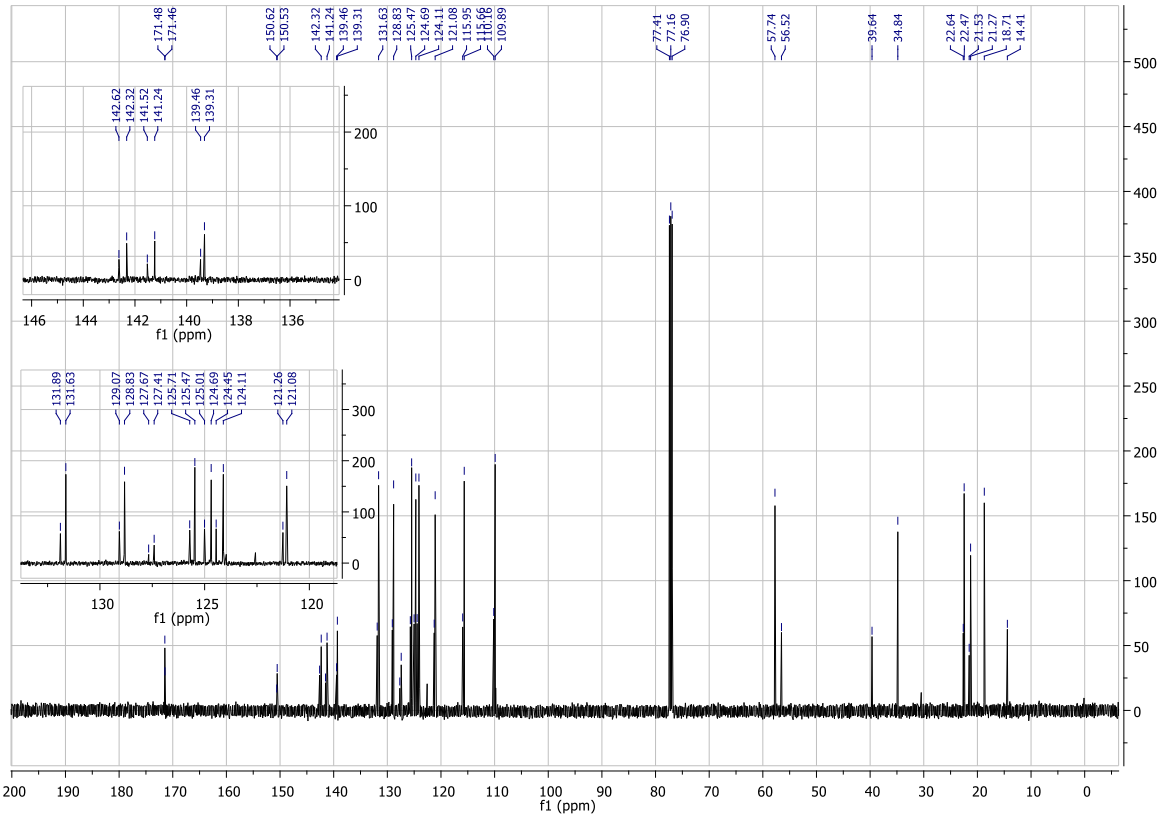
2.19
2.12
2.10
2.08
1.65
1.64
1.62
1.60
f1 (ppm)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121.08
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115.66
110.16
109.89
77.41
77.16
76.90
57.74
56.52
39.64
34.84
22.64
22.47
21.53
21.27
18.71
14.41
142.62
142.32
141.52
141.24
139.46
139.31
f1 (ppm)
131.89
131.63
129.07
128.83
127.67
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125.01
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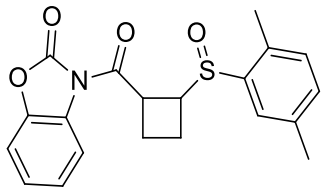
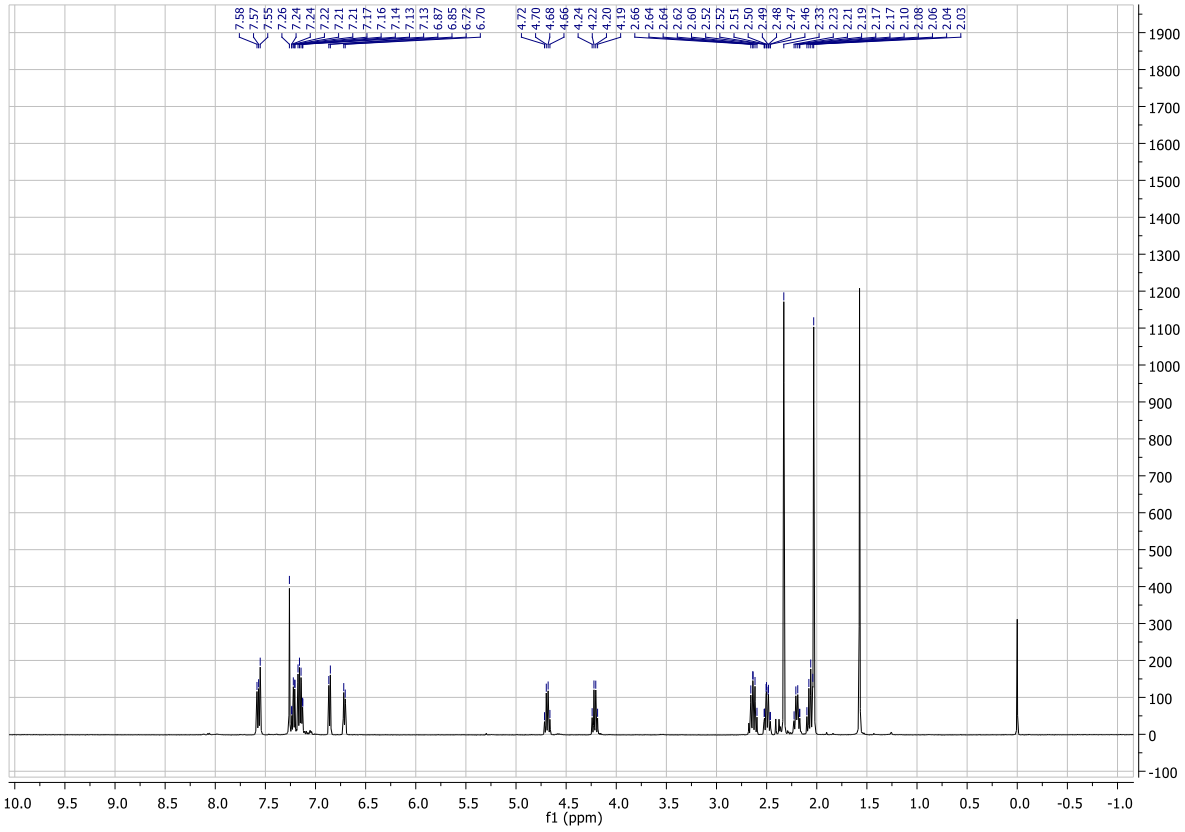
124.45
124.11
121.26
121.08
f1 (ppm)
f1 (ppm)



7h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7.13
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6.85
6.72
6.70
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4.70
4.68
4.66
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4.22
4.20
4.19
2.66
2.64
2.64
2.62
2.60
2.52
2.52
2.51
2.50
2.49
2.48
2.47
2.46
2.33
2.23
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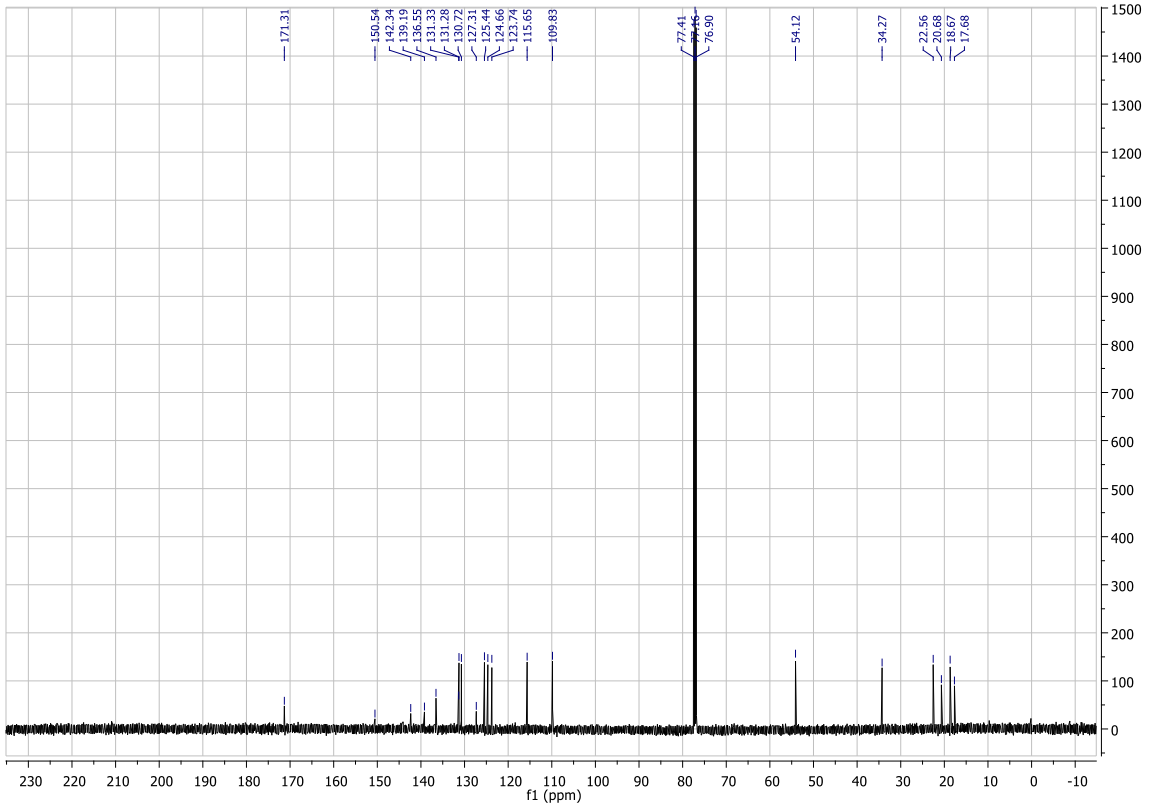
2.19
2.17
2.17
2.10
2.08
2.06
2.04
2.03
f1 (ppm)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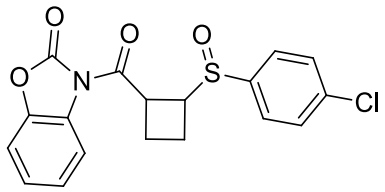
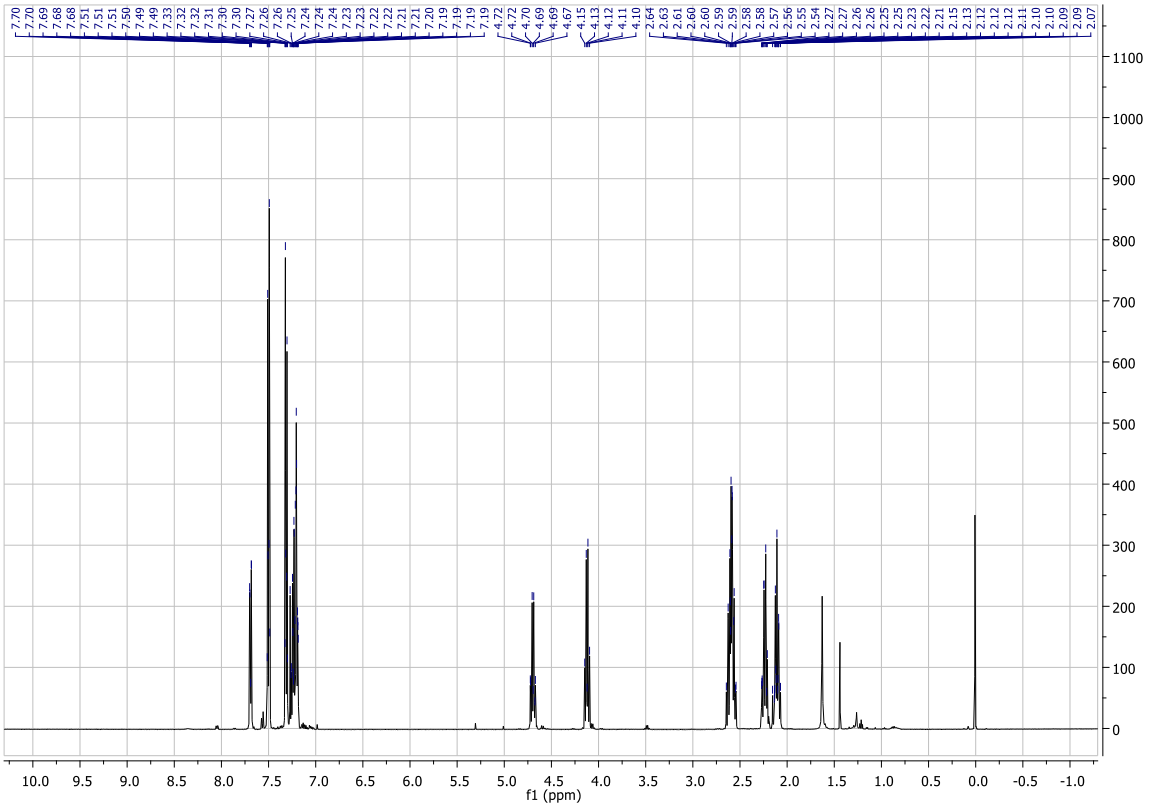
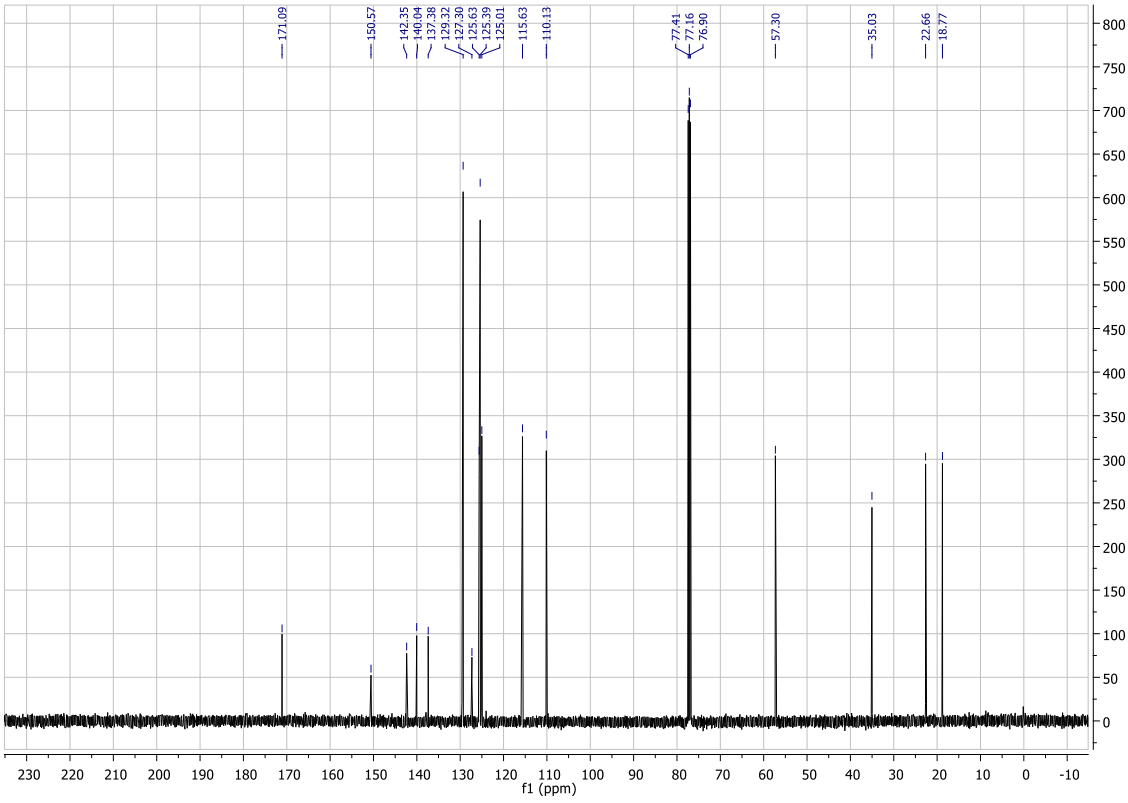
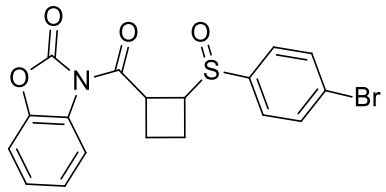
76.90
54.12
34.27
22.56
20.68
18.67
17.68
f1 (ppm)



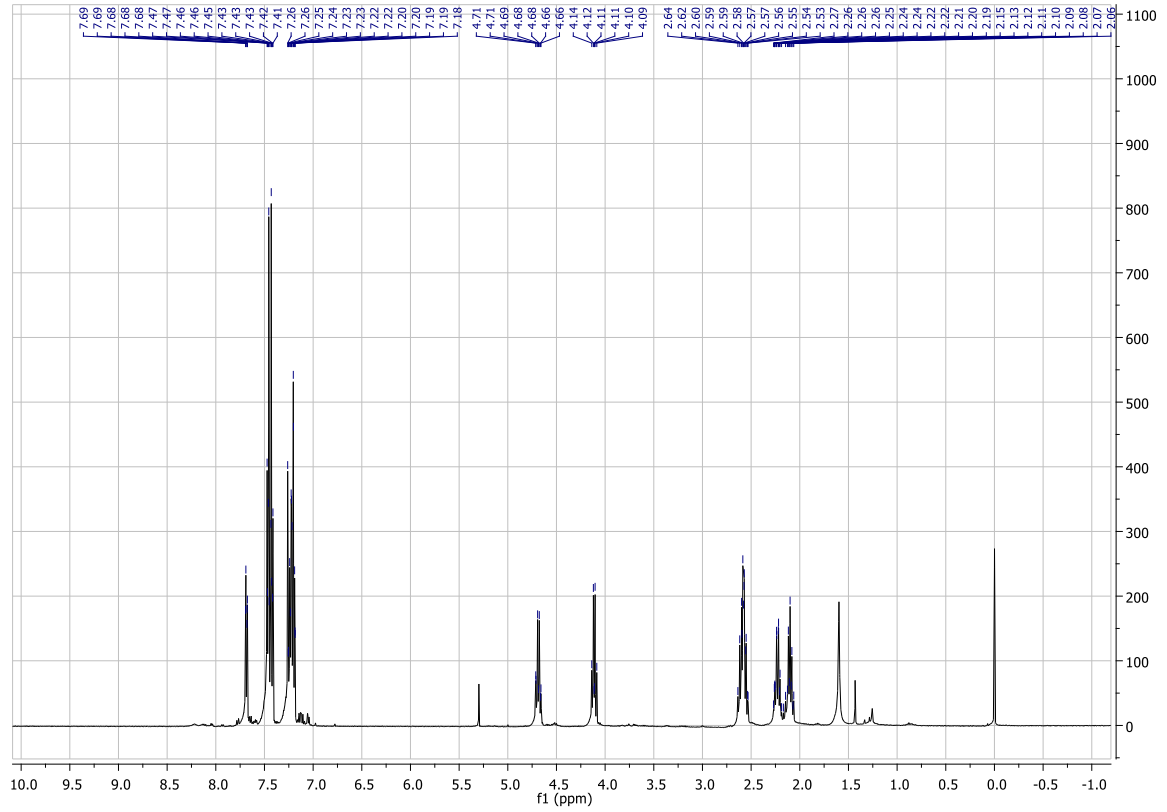
7i






O
O
O
O
N
S
Br

7j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4.09
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2.58
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2.56
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2.53
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2.26
2.25
2.24
2.22
2.21
2.20
2.19
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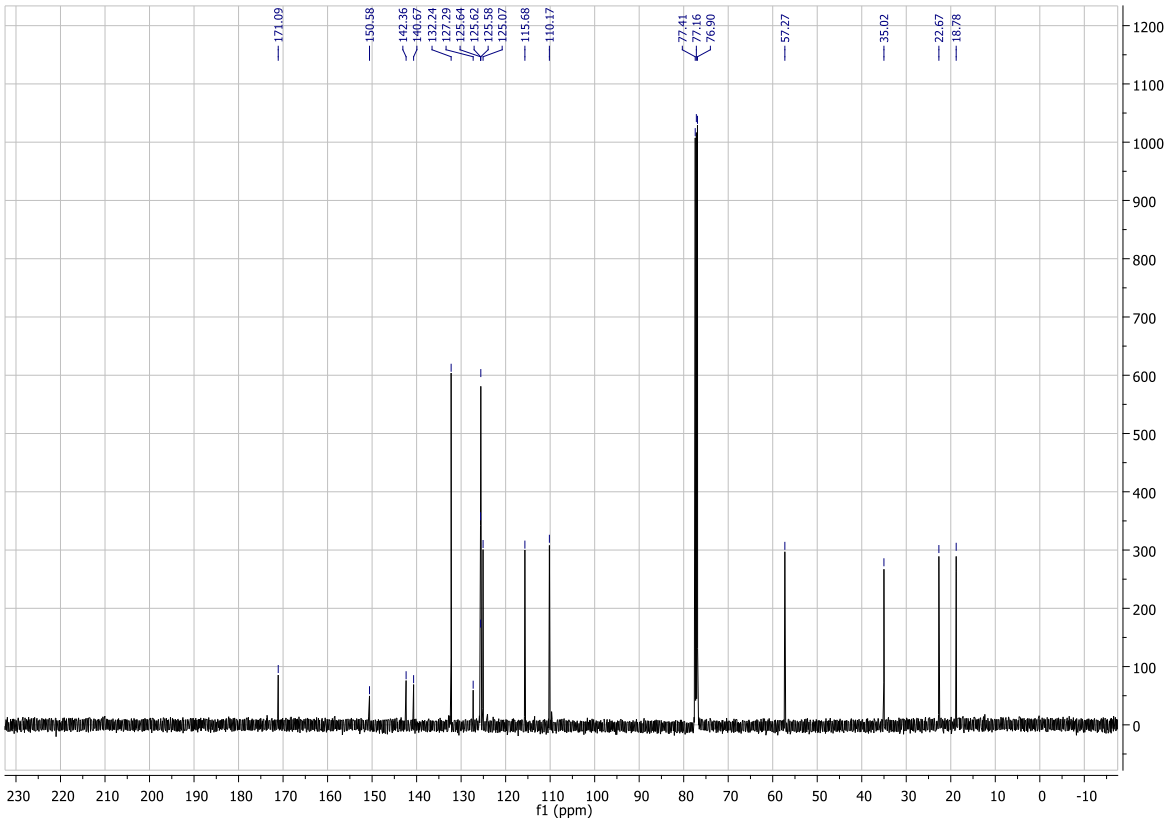
2.13
2.12
2.11
2.10
2.09
2.08
2.07
2.06
f1 (ppm)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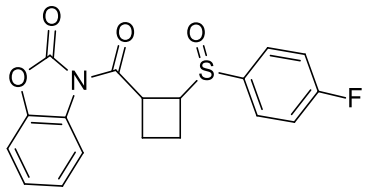
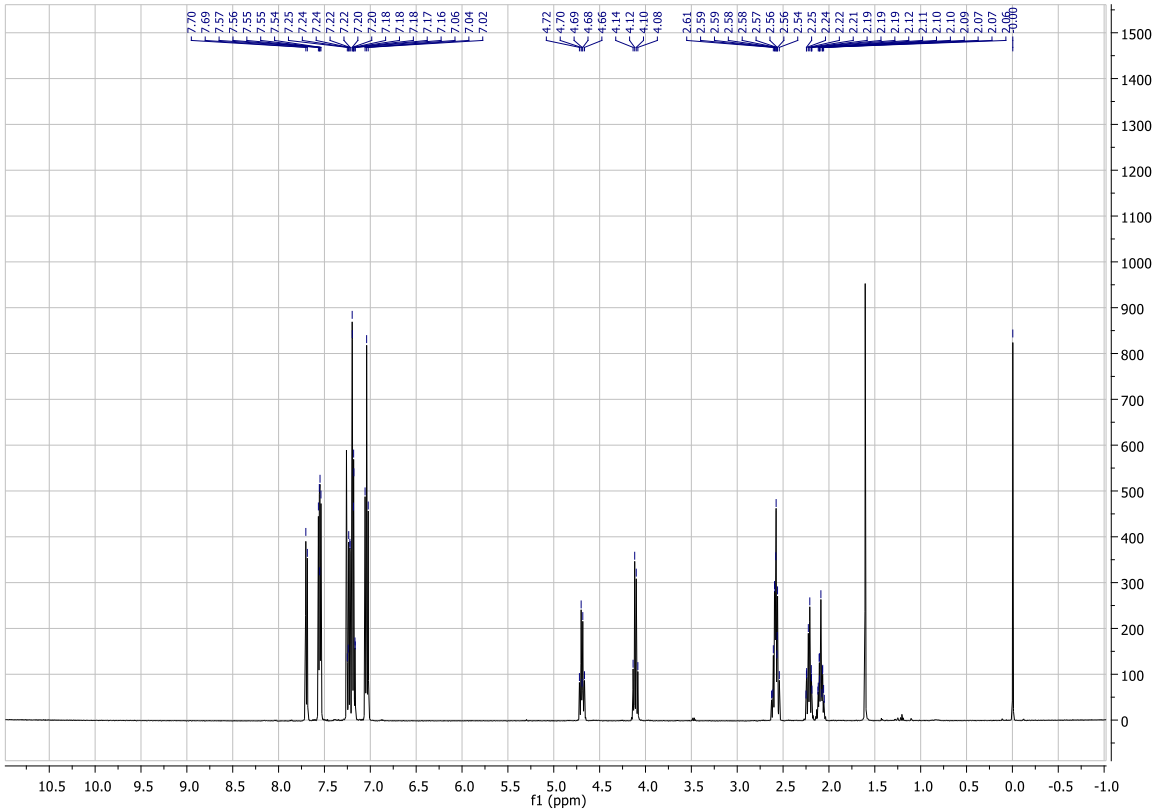
57.27
35.02
22.67
18.78
f1 (ppm)



7k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7.18
7.18
7.17
7.16
7.06
7.04
7.02
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4.69
4.68
4.66
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4.10
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2.24
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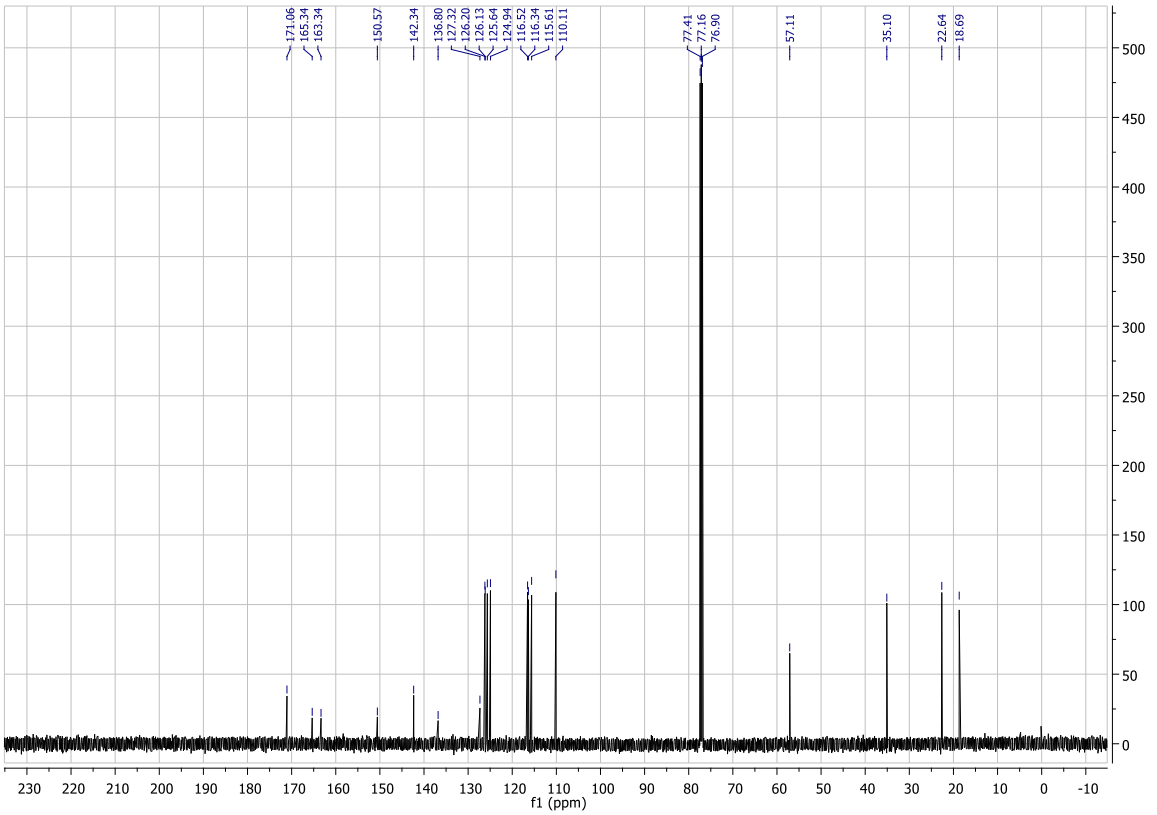
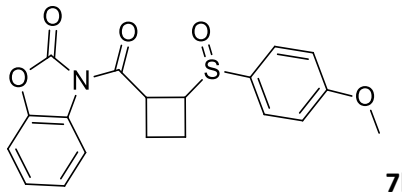
2.21
2.19
2.19
2.12
2.11
2.10
2.10
2.09
2.07
2.07
2.06
0.00
f1 (ppm)


171.06
165.34
163.34
150.57
142.34
136.80
127.32
126.20
126.13
125.64
124.94
116.52
116.34
115.61
110.11
77.41
77.16
76.90
57.11
35.10
22.64
18.69
f1 (ppm)



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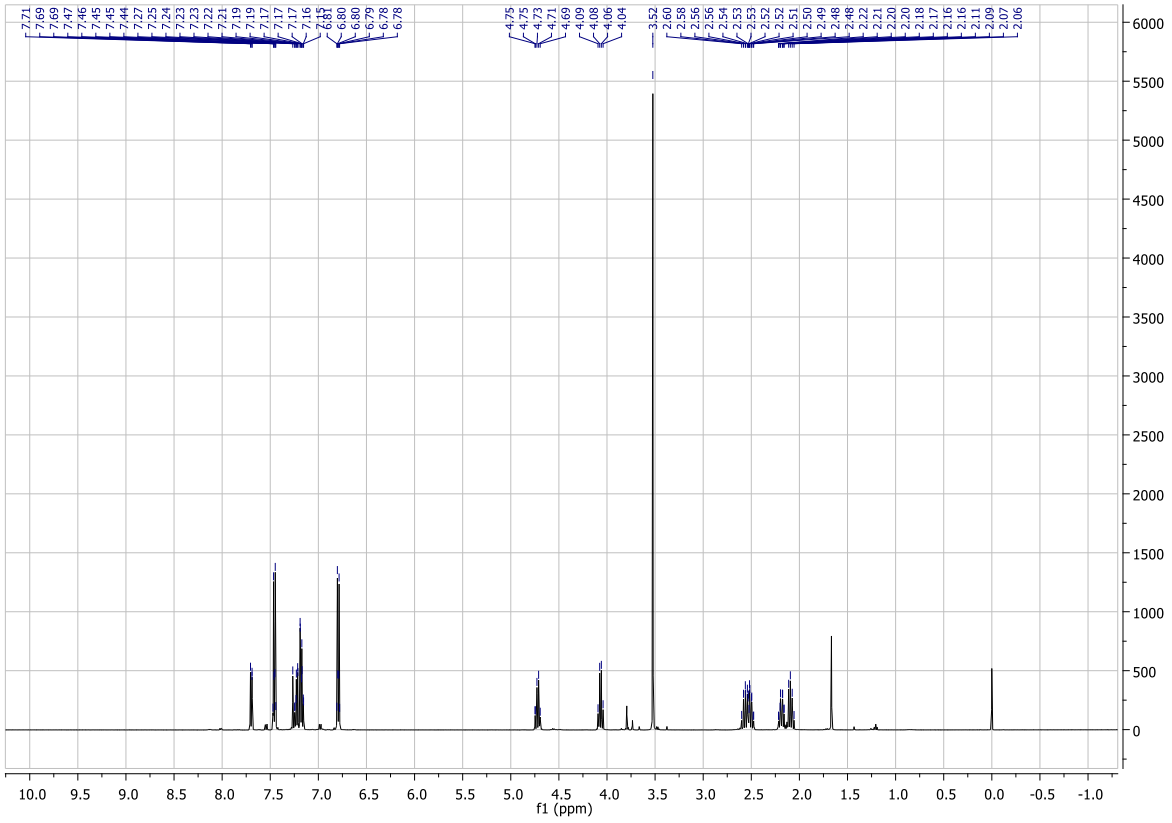
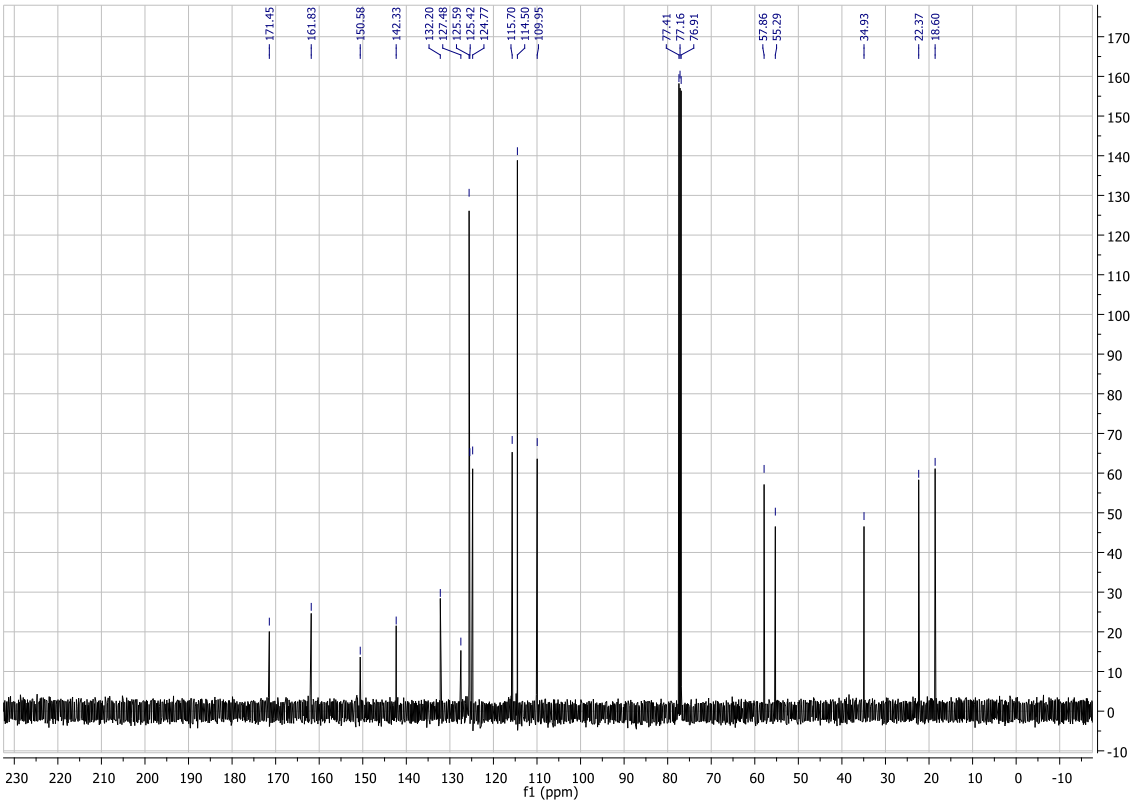
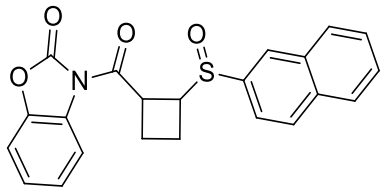

7.71 7.69 7.69 7.47 7.46 7.45 7.45 7.44 7.27 7.25 7.24 7.23 7.23 7.22 7.21 7.19 7.19 7.17 7.17 7.17 7.16 6.81 6.80 6.80 6.79 6.78 6.78
4.75 4.75 4.73 4.71 4.69 4.09 4.08 4.06 4.04
3.52
2.60 2.58 2.56 2.56 2.54 2.53 2.53 2.52 2.52 2.51 2.50 2.49 2.48 2.48 2.22 2.21 2.20 2.20 2.18 2.17 2.16 2.16 2.11 2.09 2.07 2.06
6000 5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


171.45 161.83 150.58 142.33 132.20 127.48 125.59 125.42 124.77 115.70 114.50 109.95 77.41 77.16 76.91 57.86 55.29 34.93 22.37 18.60
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



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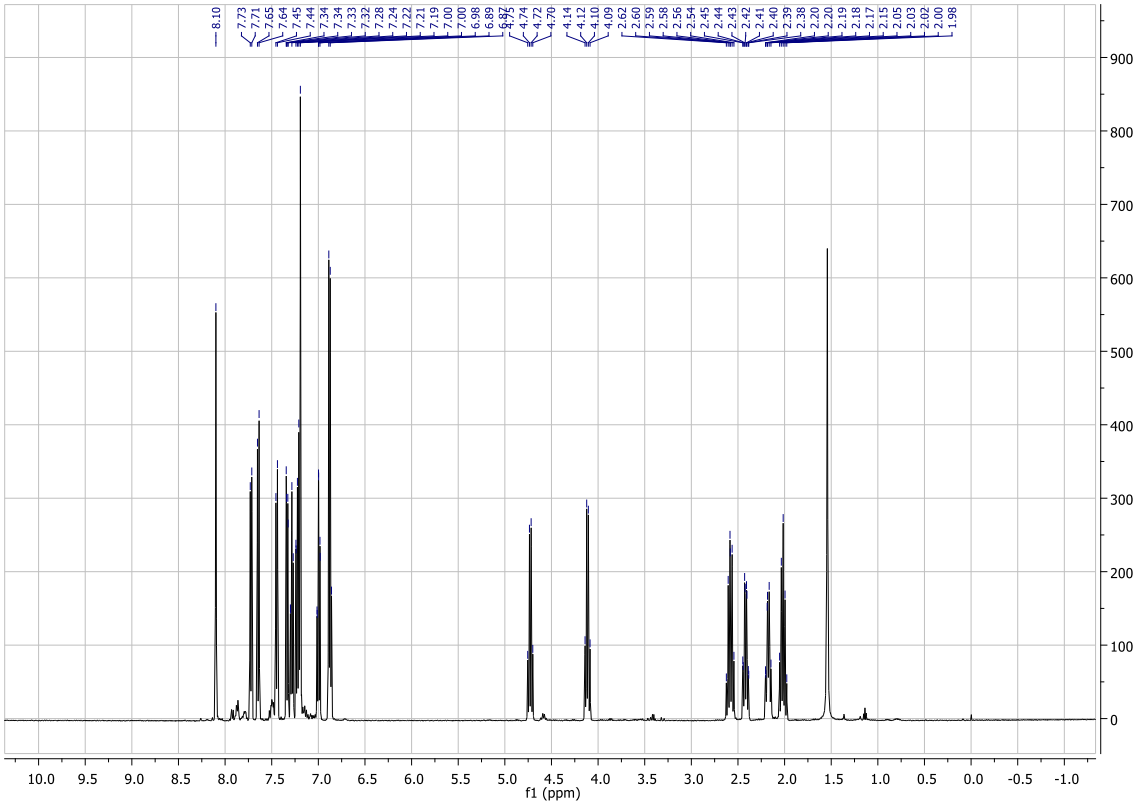
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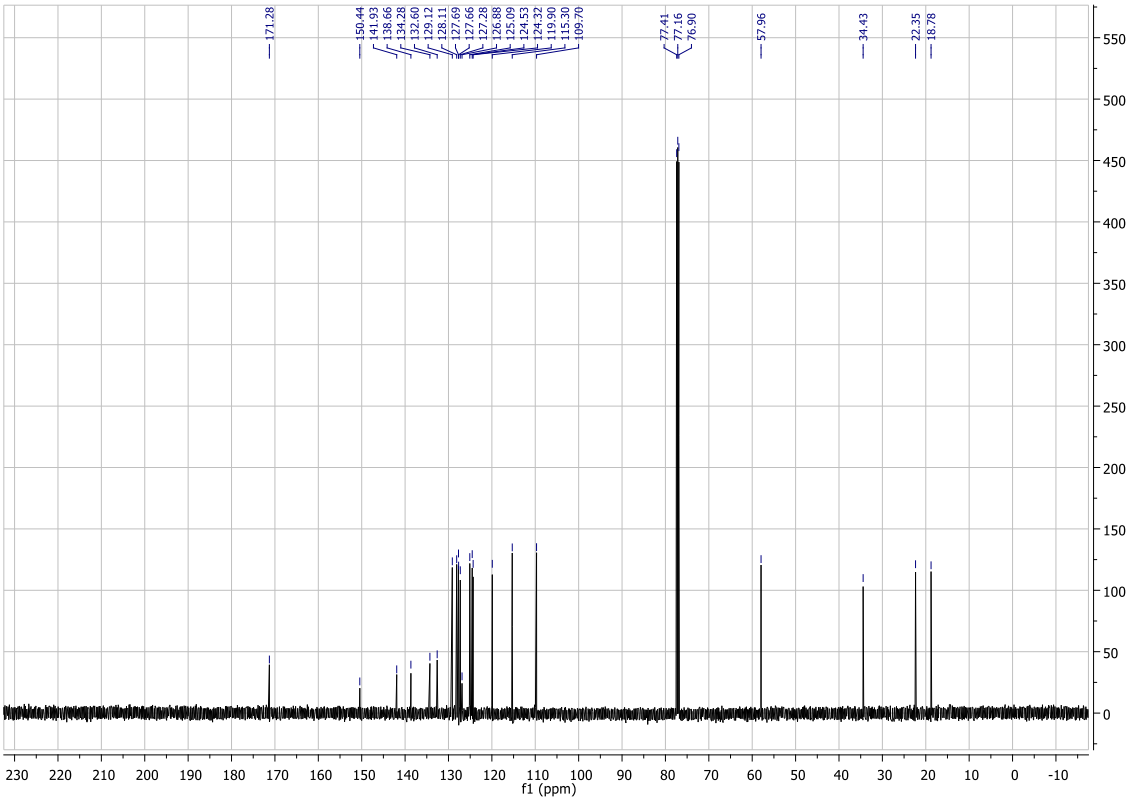
7.73
7.71
7.65
7.64
7.45
7.44
7.34
7.34
7.33
7.32
7.28
7.24
7.22
7.21
7.19
7.00
7.00
6.98
6.89
6.87
4.74
4.72
4.70
4.14
4.12
4.10
4.09
2.62
2.60
2.59
2.58
2.56
2.54
2.45
2.44
2.43
2.42
2.41
2.40
2.39
2.38
2.20
2.20
2.19
2.18
2.17
2.15
2.05
2.03
2.02
2.00
1.98
f1 (ppm)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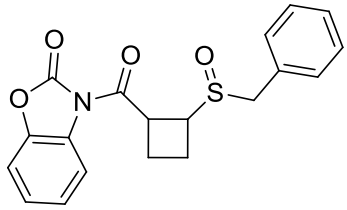
150.44
141.93
138.66
134.28
132.60
129.12
128.11
127.69
127.66
127.28
126.88
125.09
124.53
124.32
119.90
115.30
109.70
77.41
77.16
76.90
57.96
34.43
22.35
18.78
f1 (ppm)



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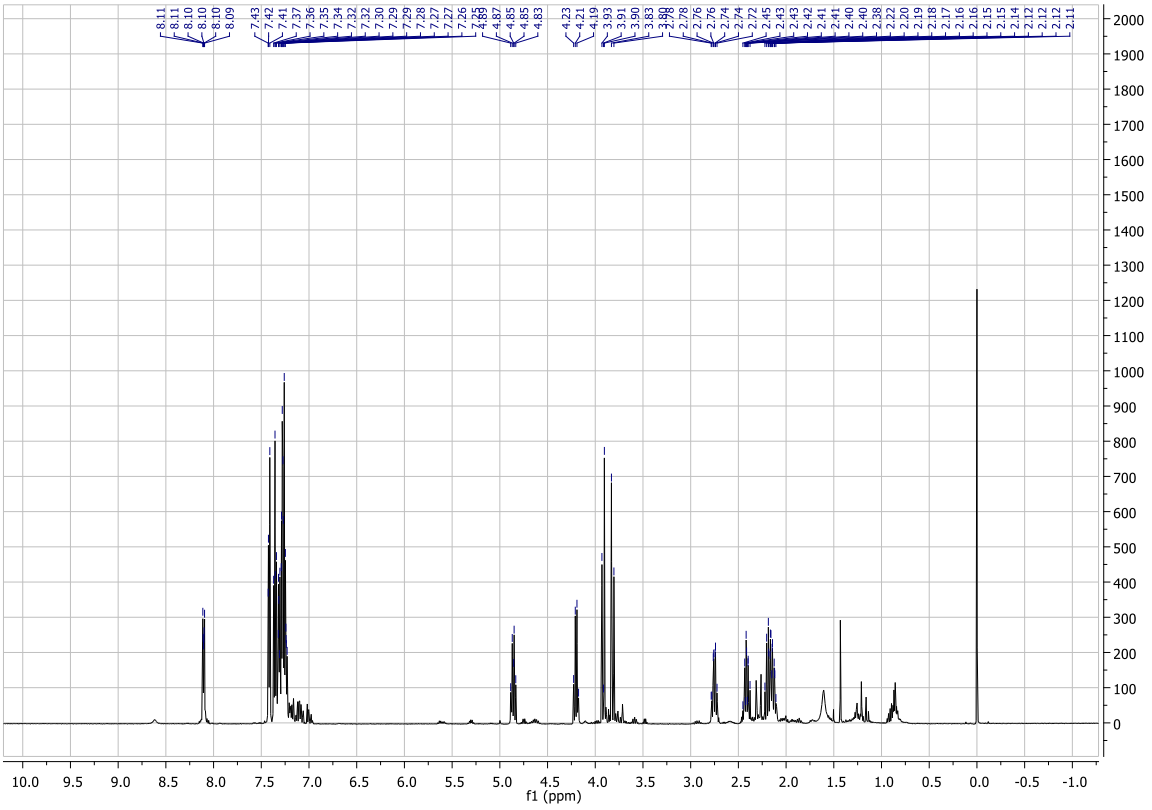
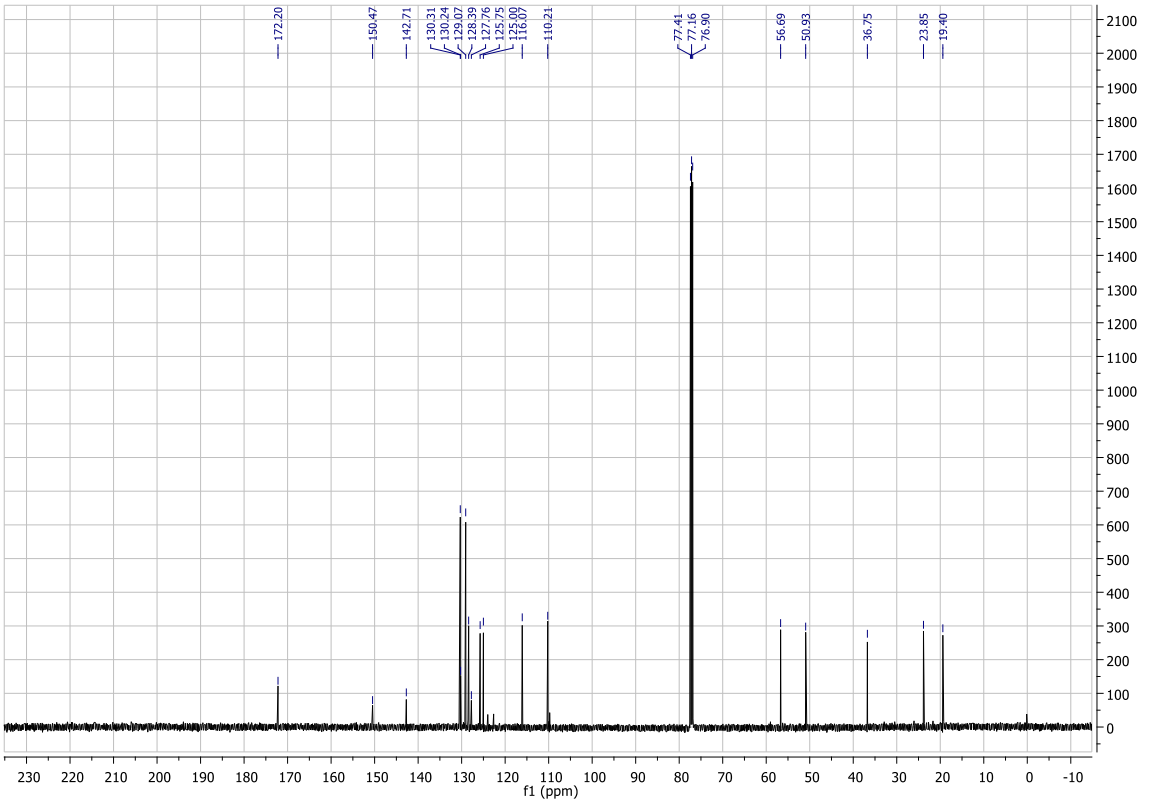
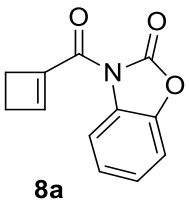
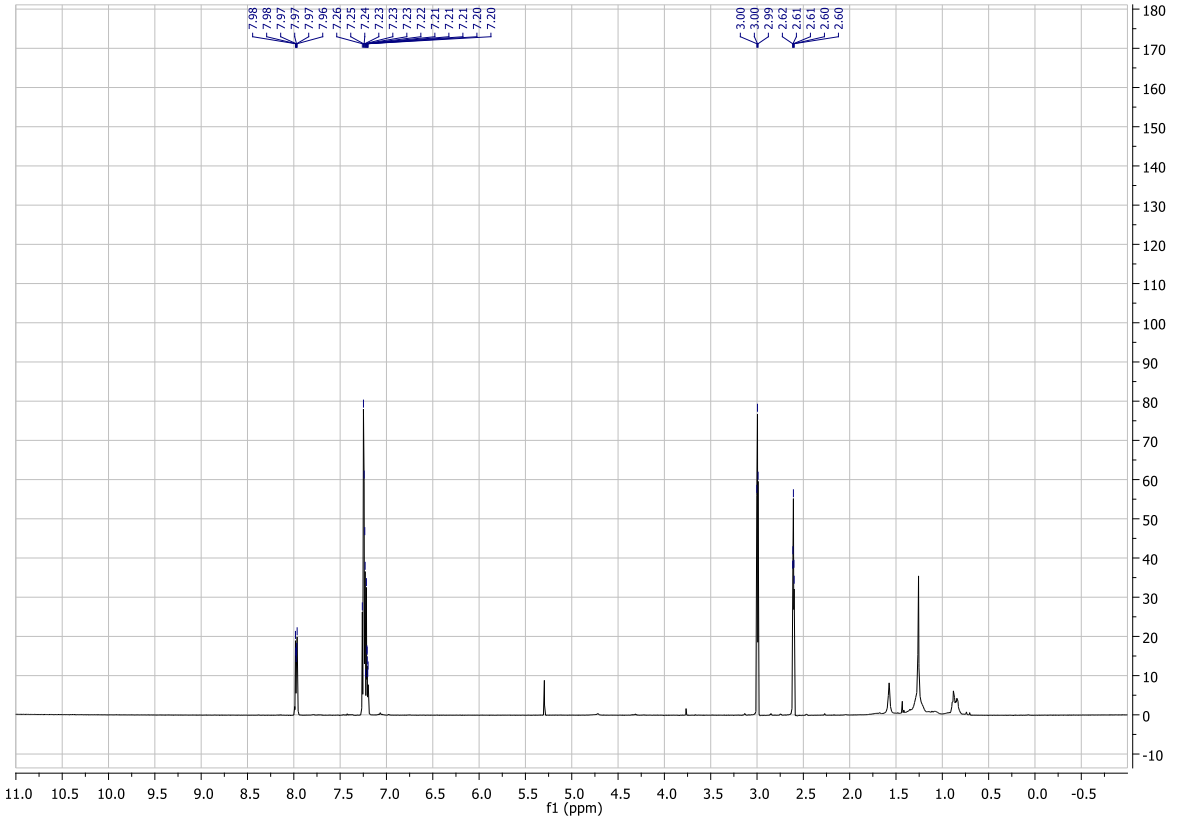
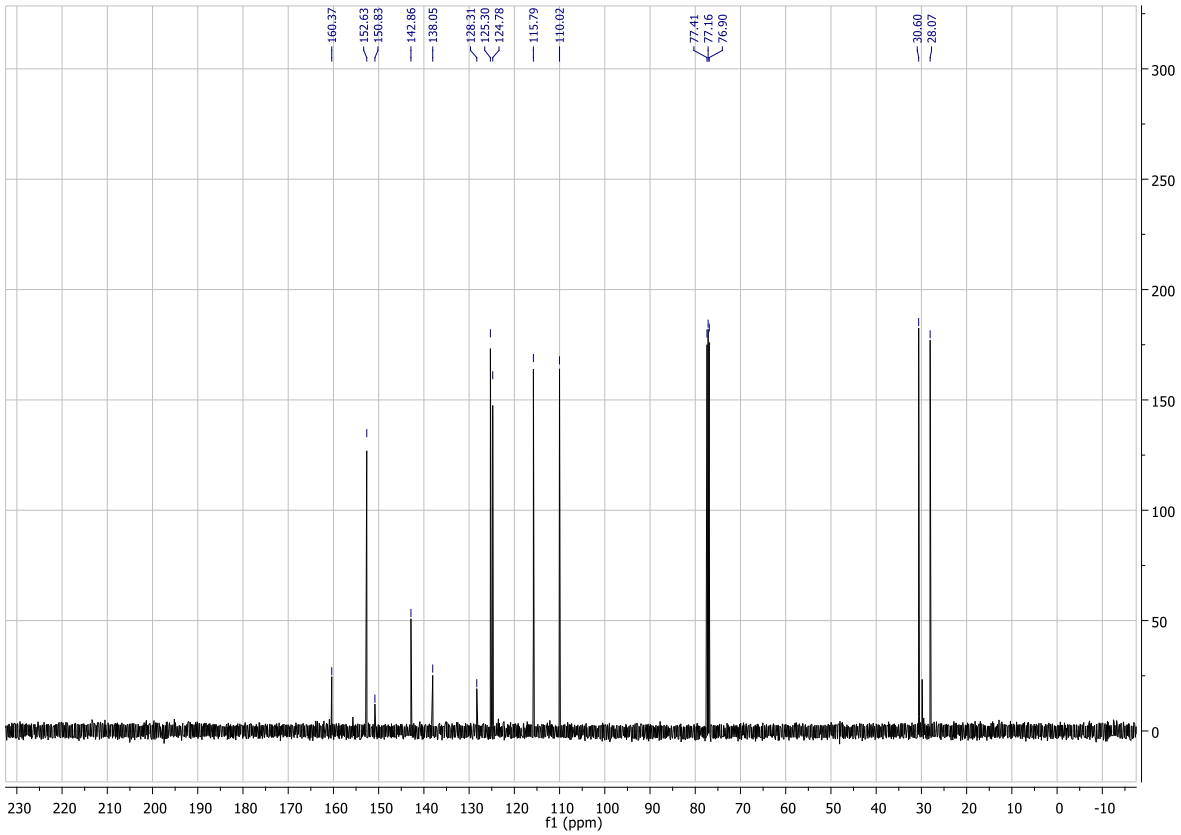


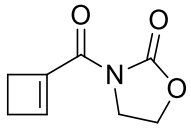




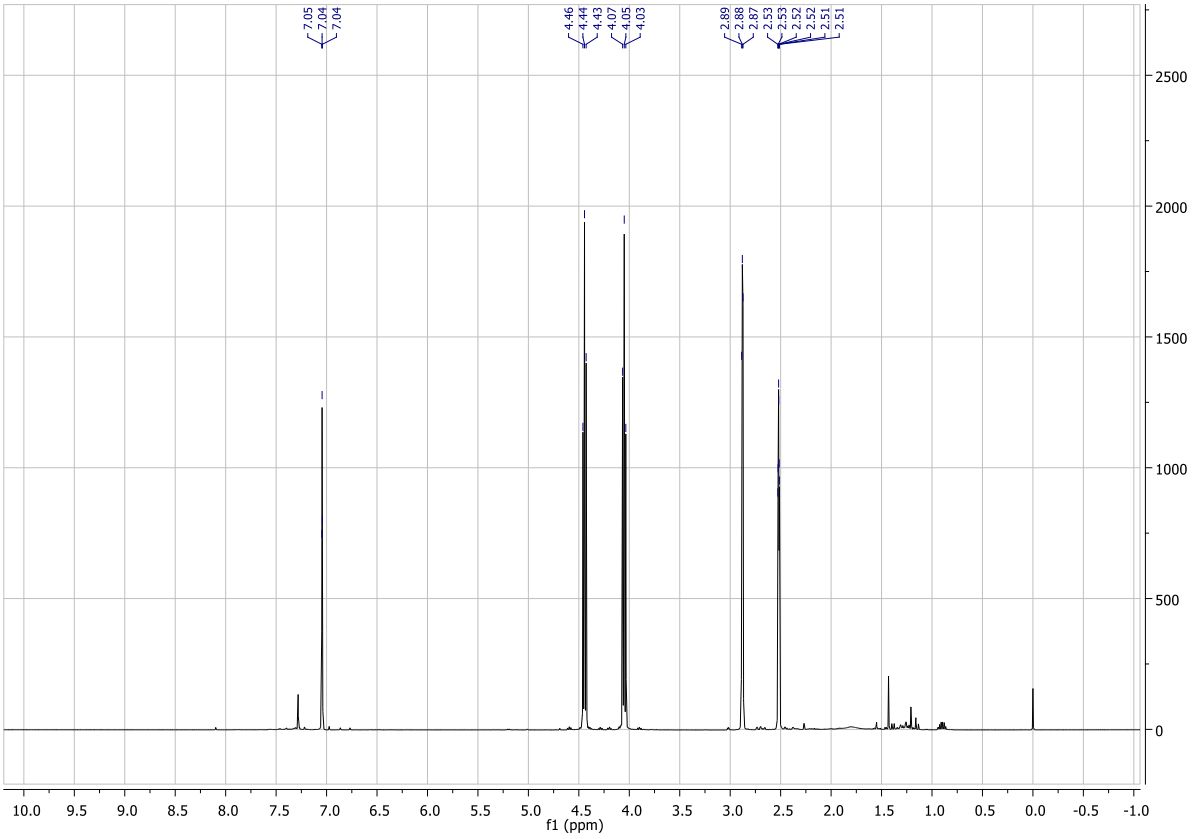
8a

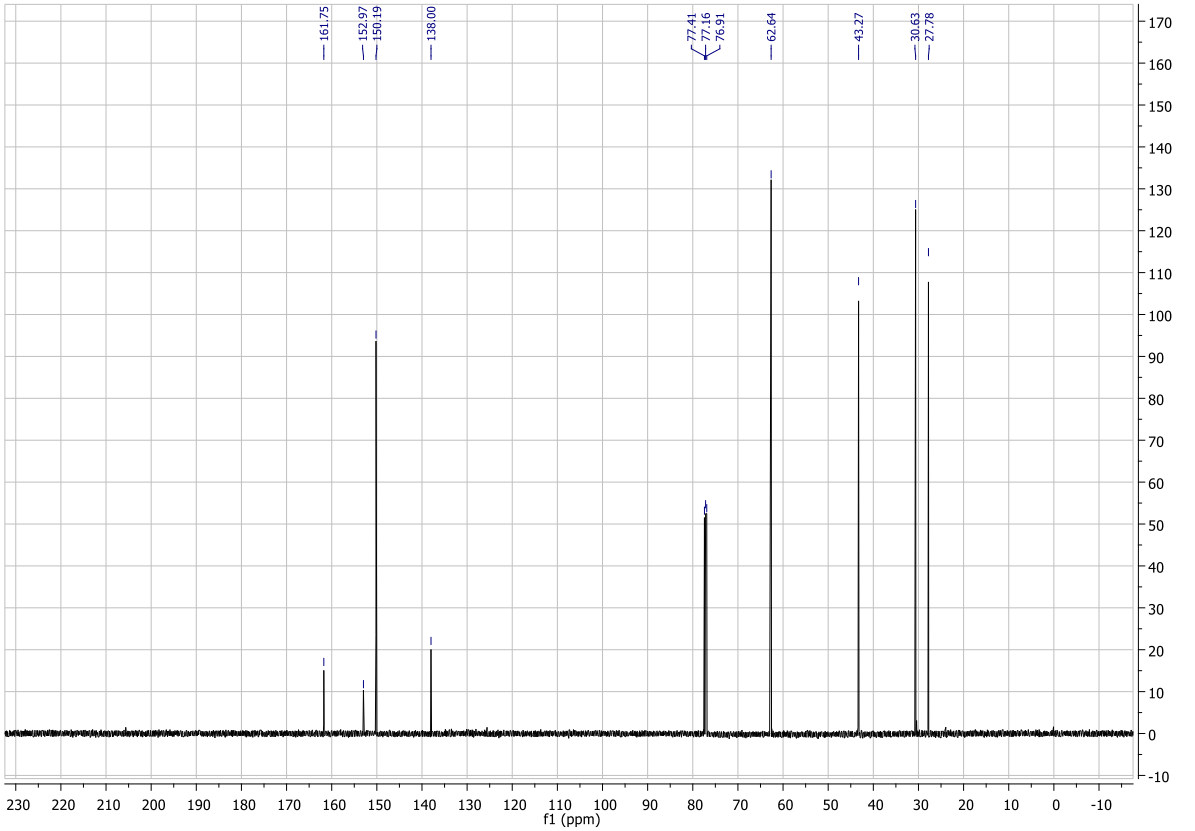

7.98
7.98
7.97
7.97
7.97
7.96
7.26
7.25
7.24
7.23
7.23
7.23
7.22
7.21
7.21
7.21
7.20
7.20
3.00
3.00
2.99
2.62
2.61
2.61
2.60
2.60
f1 (ppm)


160.37
152.63
150.83
142.86
138.05
128.31
125.30
124.78
115.79
110.02
77.41
77.16
76.90
30.60
28.07
f1 (ppm)



8b


7.05
7.04
7.04
4.46
4.44
4.43
4.07
4.05
4.03
2.89
2.88
2.87
2.53
2.53
2.52
2.52
2.51
2.51
2500
2000
1500
1000
500
0
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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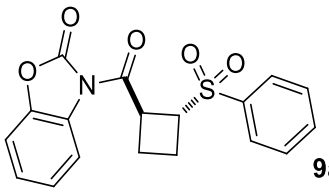
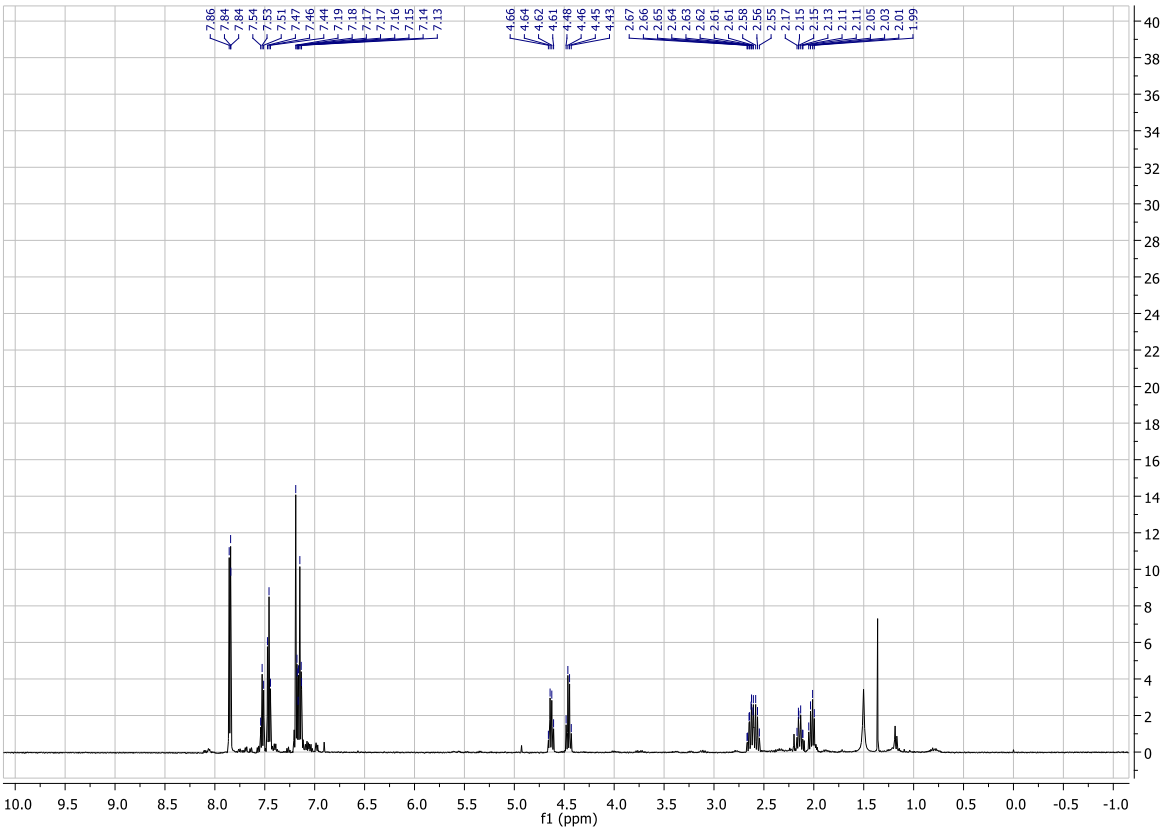
77.16
76.91
62.64
43.27
30.63
27.78
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



9a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7.84
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7.19
7.18
7.17
7.17
7.16
7.15
7.14
7.13
4.66
4.64
4.62
4.61
4.48
4.46
4.45
4.43
2.67
2.66
2.65
2.64
2.63
2.62
2.61
2.61
2.58
2.56
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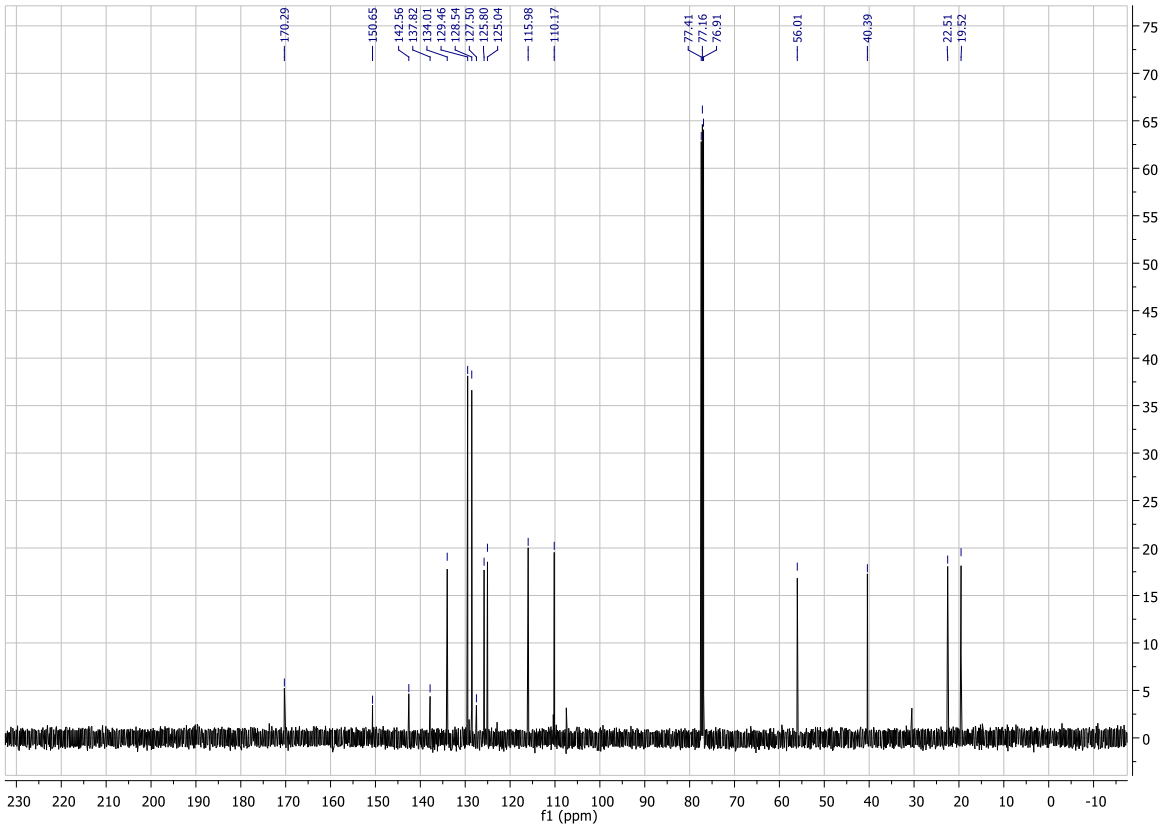
2.15
2.13
2.11
2.11
2.05
2.03
2.01
1.99
f1 (ppm)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128.54
127.50
125.80
125.04
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110.17
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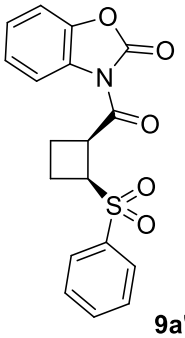
76.91
56.01
40.39
22.51
19.52
f1 (ppm)



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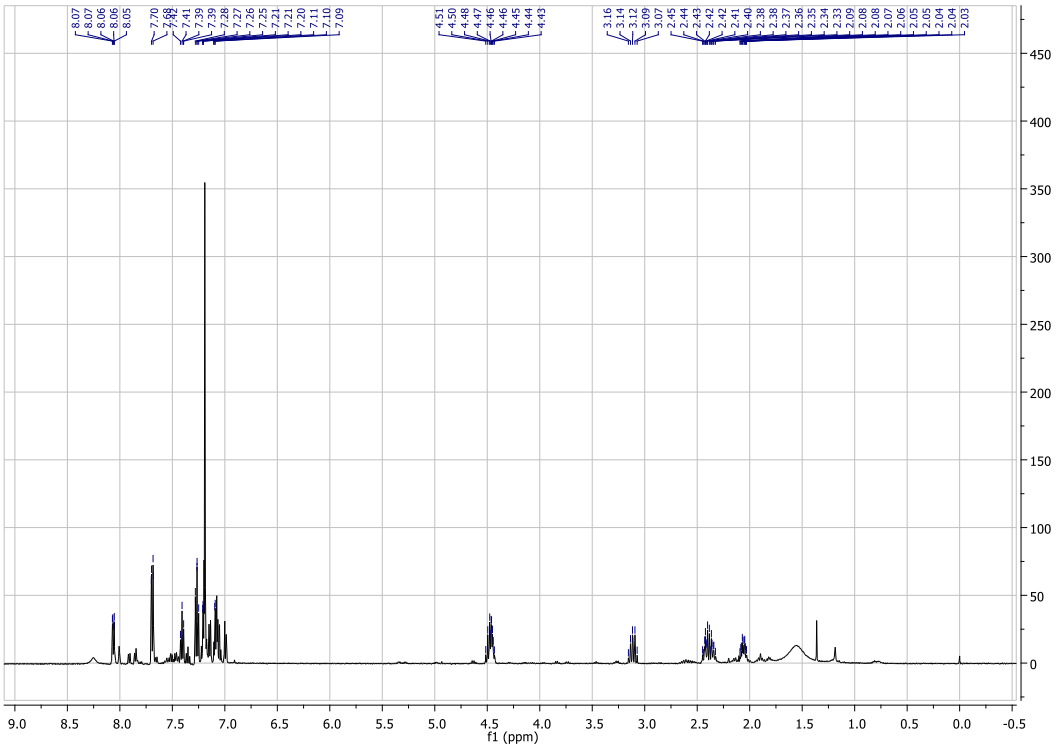
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8.07
8.06
8.06
8.05
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7.68
7.41
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7.39
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7.27
7.26
7.25
7.21
7.21
7.20
7.11
7.10
7.09
4.51
4.50
4.48
4.47
4.46
4.46
4.45
4.44
4.43
3.16
3.14
3.12
3.09
3.07
2.45
2.44
2.43
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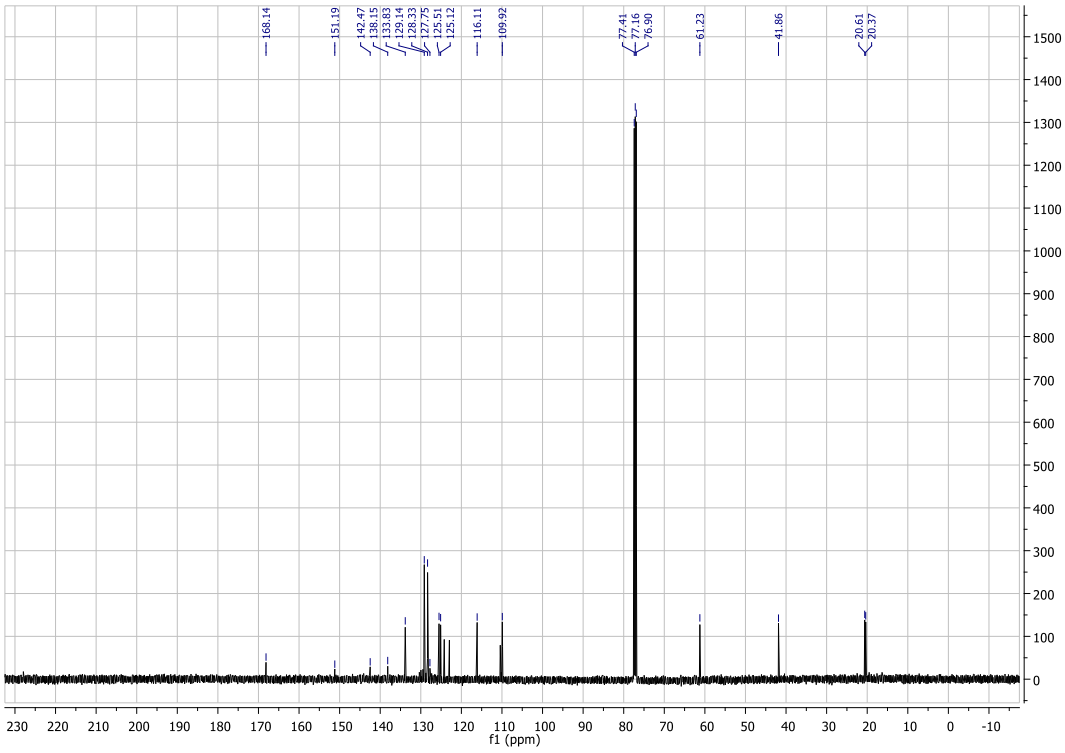
2.41
2.40
2.38
2.38
2.37
2.36
2.35
2.34
2.33
2.09
2.08
2.08
2.07
2.06
2.05
2.05
2.04
2.04
2.03
f1 (ppm)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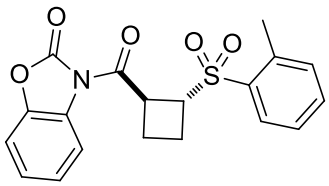
138.15
133.83
129.14
128.33
127.75
125.51
125.12
116.11
109.92
77.41
77.16
76.90
61.23
41.86
20.61
20.37
f1 (ppm)



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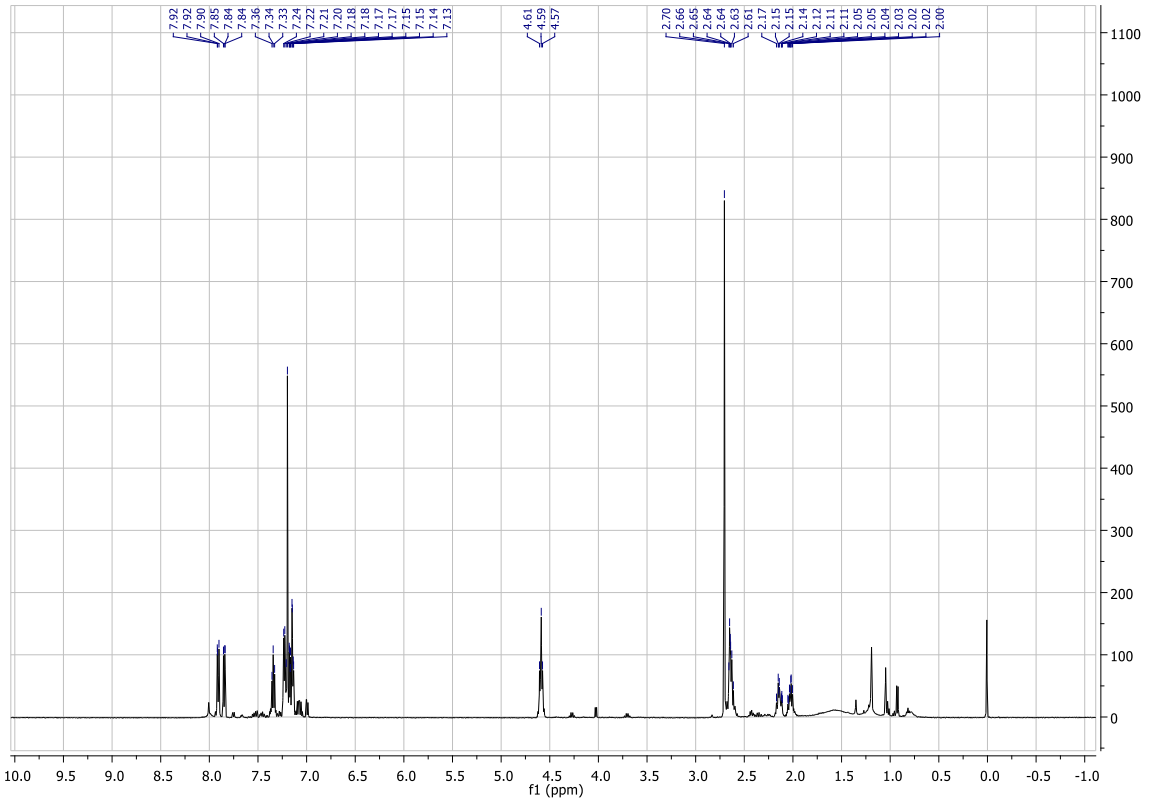
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7.84
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7.18
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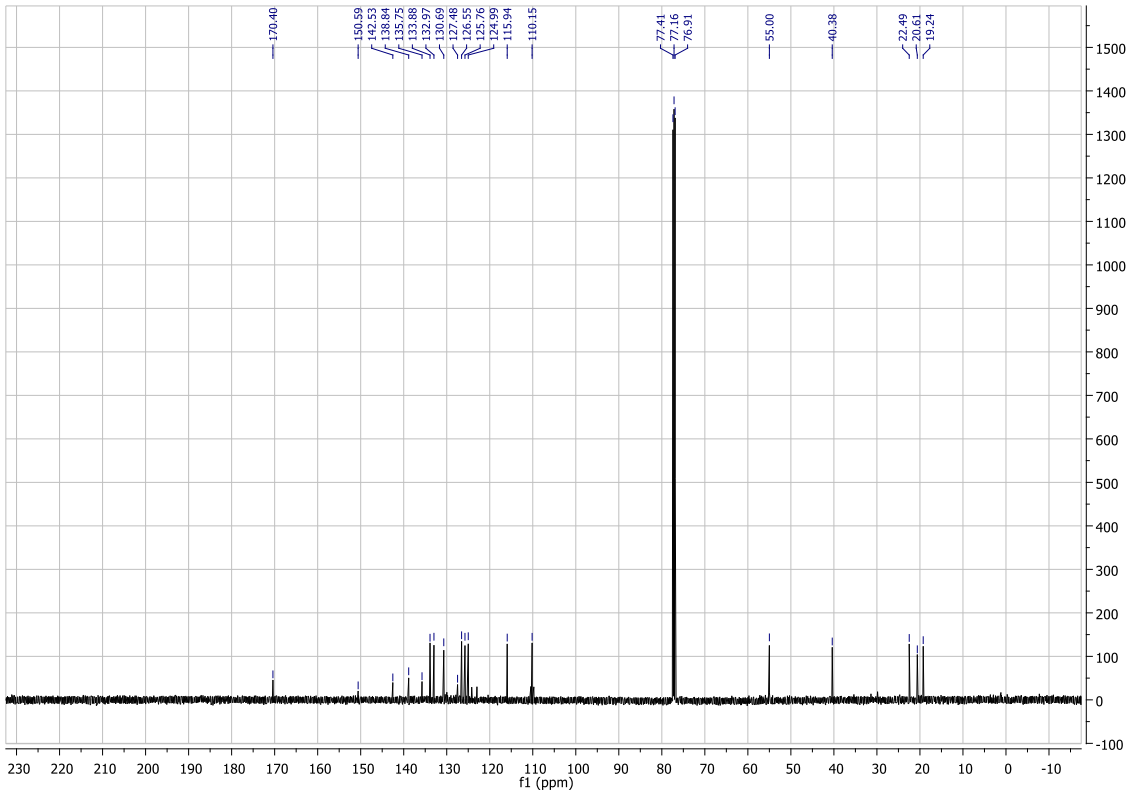
7.17
7.17
7.15
7.15
7.14
7.13
4.61
4.59
4.57
2.70
2.66
2.65
2.64
2.64
2.63
2.61
2.17
2.15
2.15
2.14
2.12
2.11
2.11
2.05
2.05
2.04
2.03
2.02
2.02
2.00
f1 (ppm)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127.48
126.55
125.76
124.99
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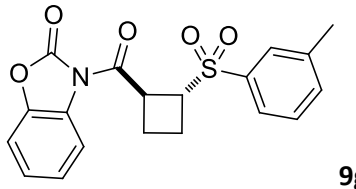
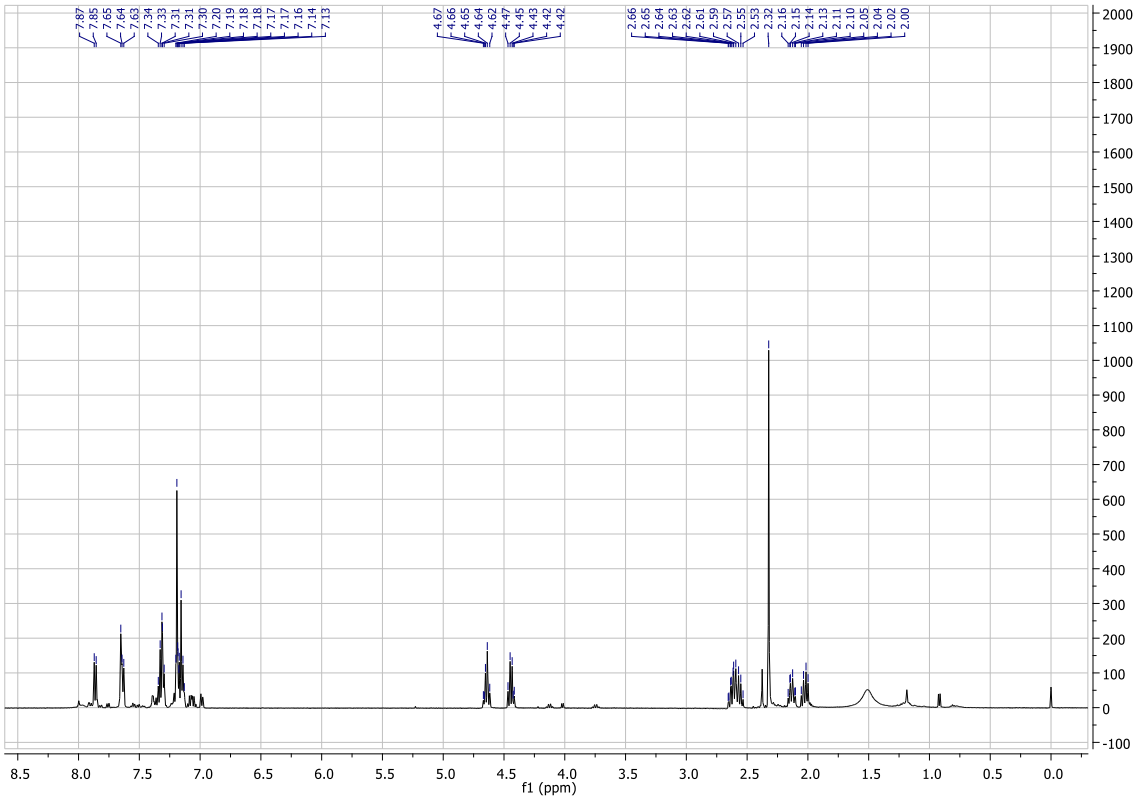
40.38
22.49
20.61
19.24
f1 (ppm)



9g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7.18
7.17
7.17
7.16
7.14
7.13
4.67
4.66
4.65
4.64
4.62
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4.45
4.43
4.42
4.42
2.66
2.65
2.64
2.63
2.62
2.61
2.59
2.57
2.55
2.53
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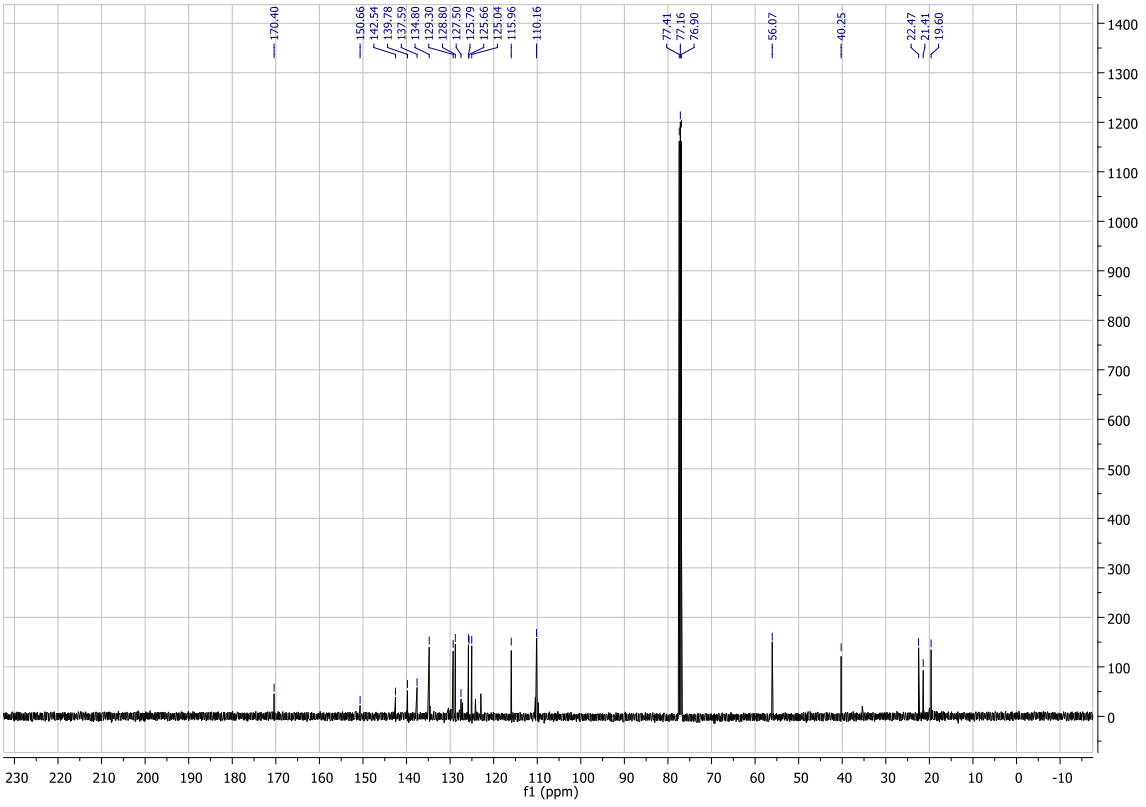
2.14
2.13
2.11
2.10
2.05
2.04
2.02
2.00
f1 (ppm)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125.79
125.66
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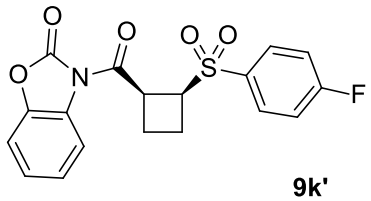
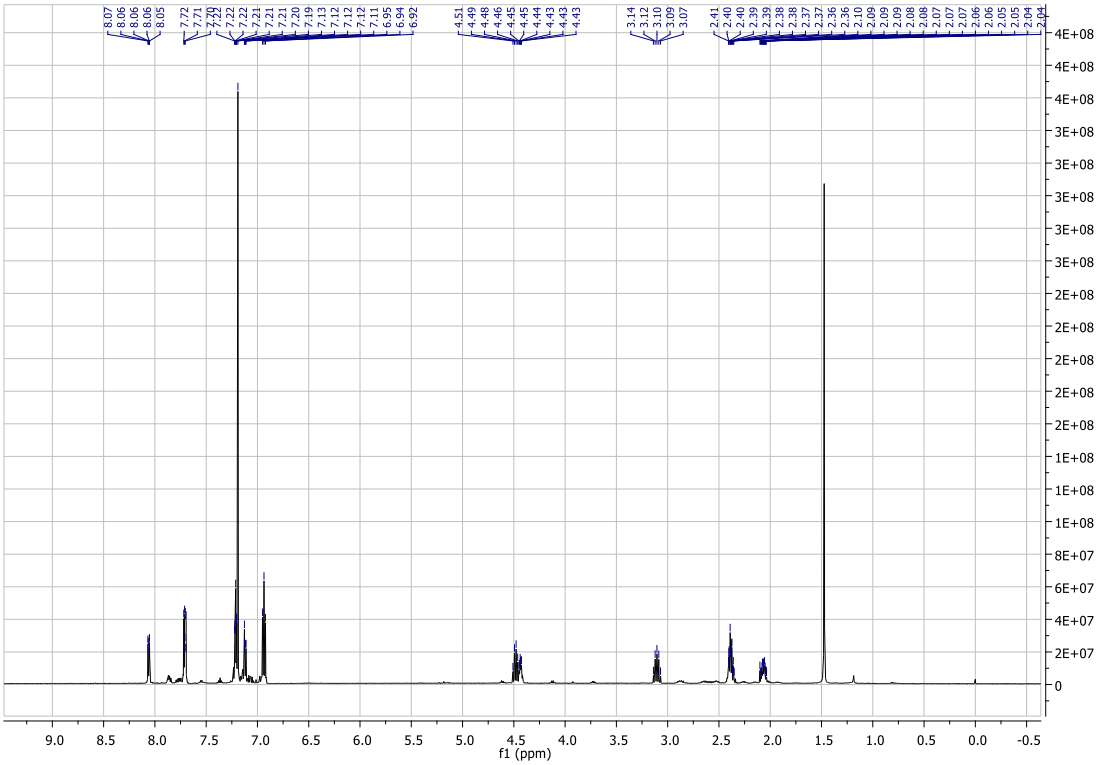
40.25
22.47
21.41
19.60
f1 (ppm)



9k'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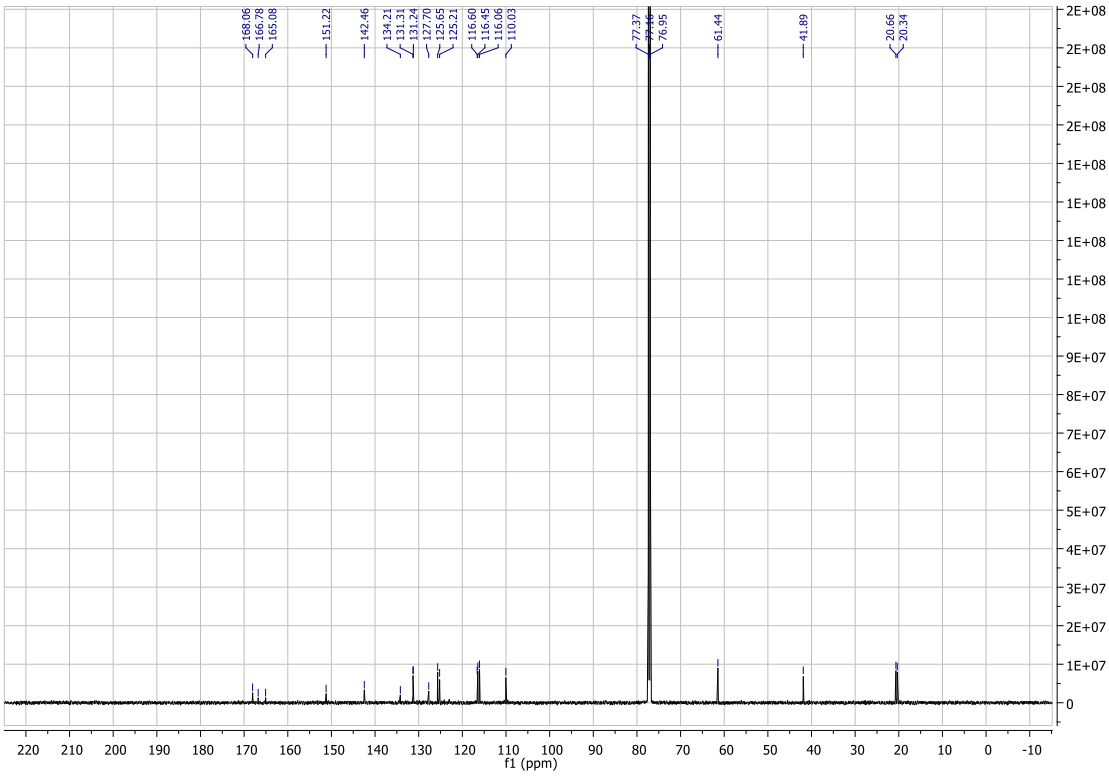
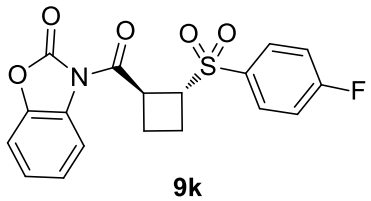
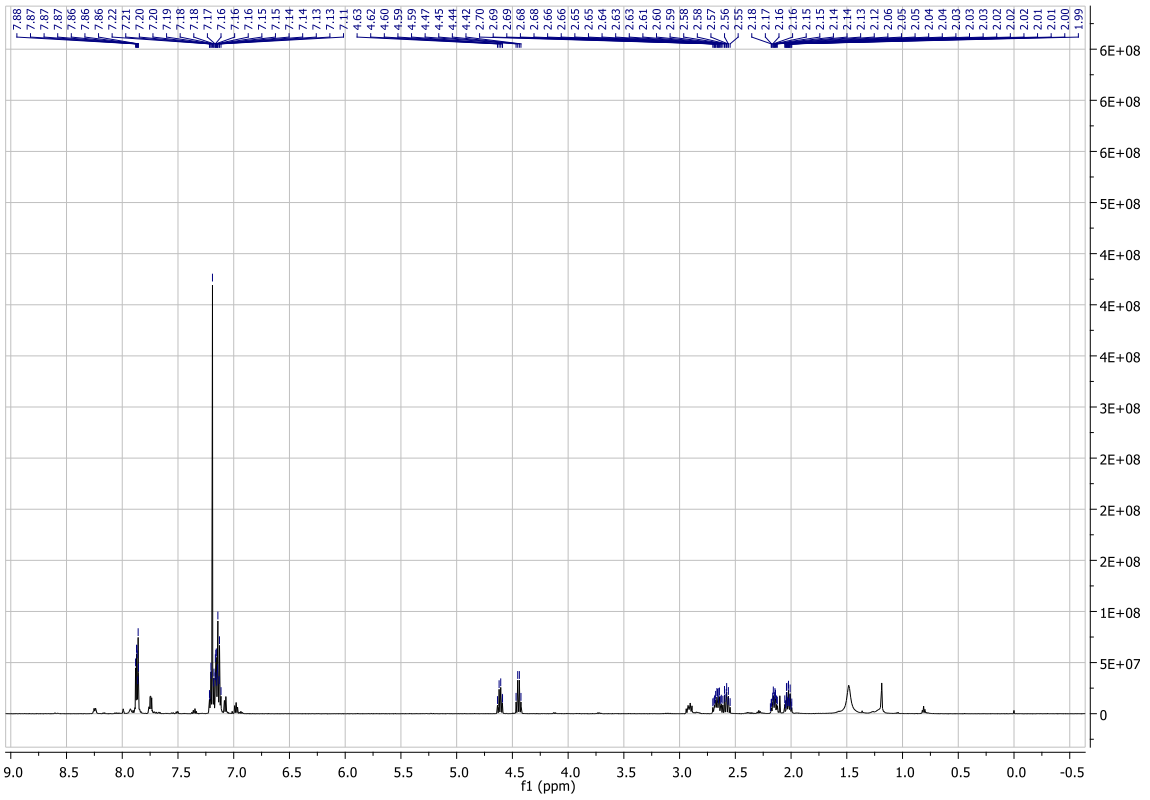
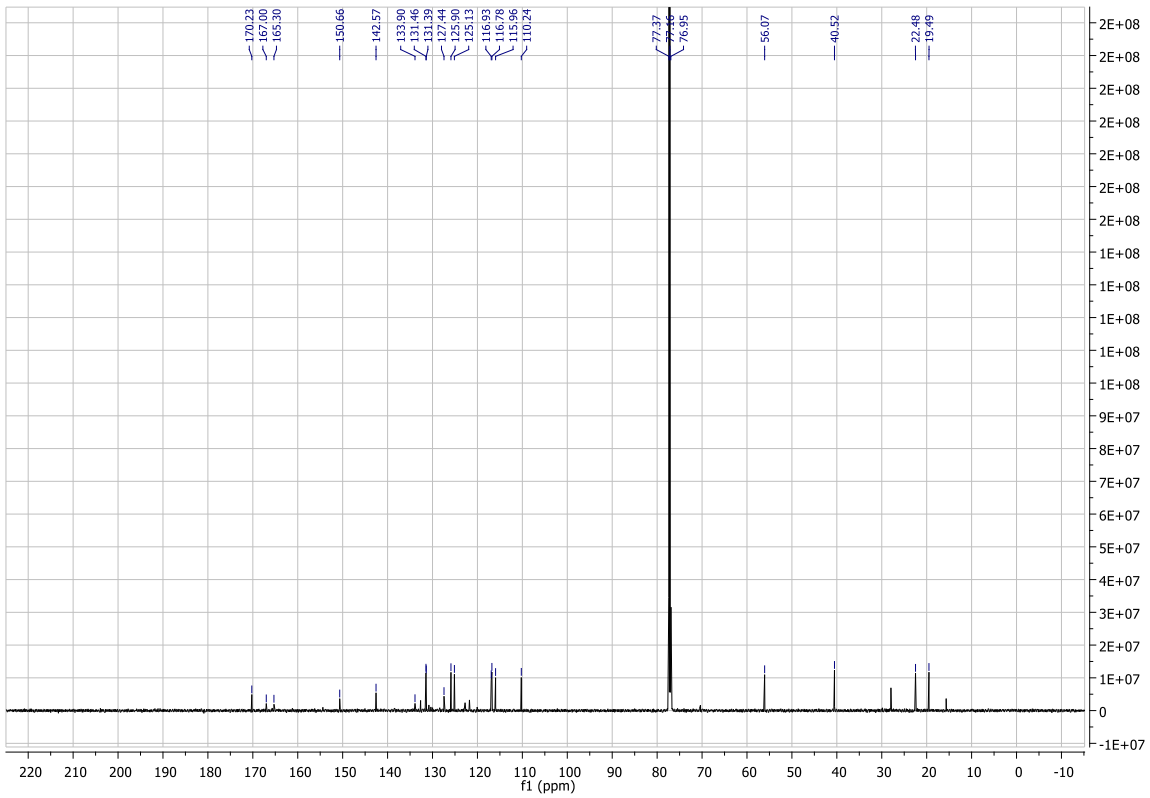
7.72 7.71 7.70 7.22 7.22 7.21 7.21 7.21 7.20 7.19 7.13 7.12 7.12 7.11 6.95 6.94 6.92
4.51 4.49 4.48 4.46 4.45 4.45 4.44 4.43 4.43 4.43
3.14 3.12 3.10 3.09 3.07
2.41 2.40 2.40 2.39 2.39 2.38 2.38 2.37 2.37 2.36 2.36 2.10 2.09 2.09 2.09 2.08 2.08 2.07 2.07 2.07 2.06 2.06 2.05 2.05 2.04 2.04
4E+08 4E+08 4E+08 3E+08 3E+08 3E+08 3E+08 3E+08 3E+08 2E+08 2E+08 2E+08 2E+08 2E+08 2E+08 1E+08 1E+08 1E+08 8E+07 6E+07 4E+07 2E+07 0
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

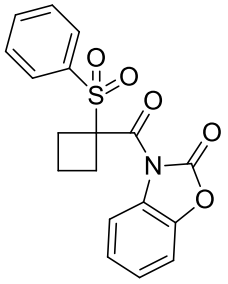

168.06 166.78 165.08 151.22 142.46 134.21 131.31 131.24 127.70 125.65 125.21 116.60 116.45 116.06 110.03 77.37 77.16 76.95 61.44 41.89 20.66 20.34
2E+08 2E+08 2E+08 2E+08 1E+08 1E+08 1E+08 1E+08 1E+08 9E+07 8E+07 7E+07 6E+07 5E+07 4E+07 3E+07 2E+07 1E+07 0
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



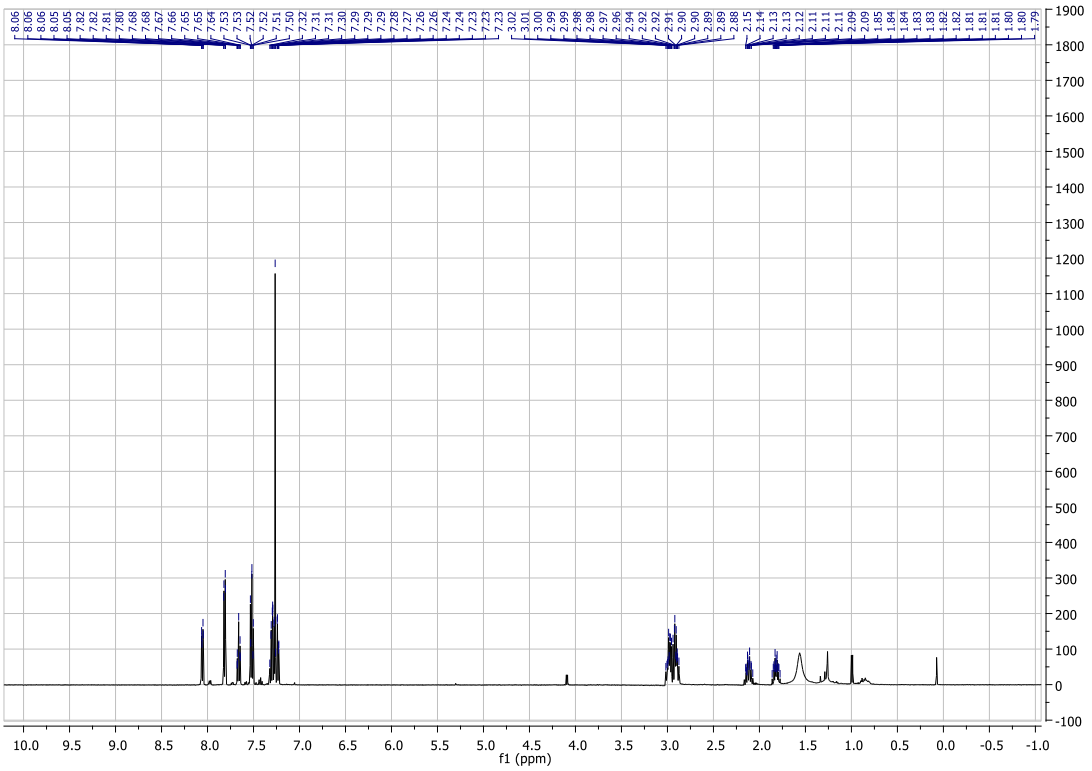
9k

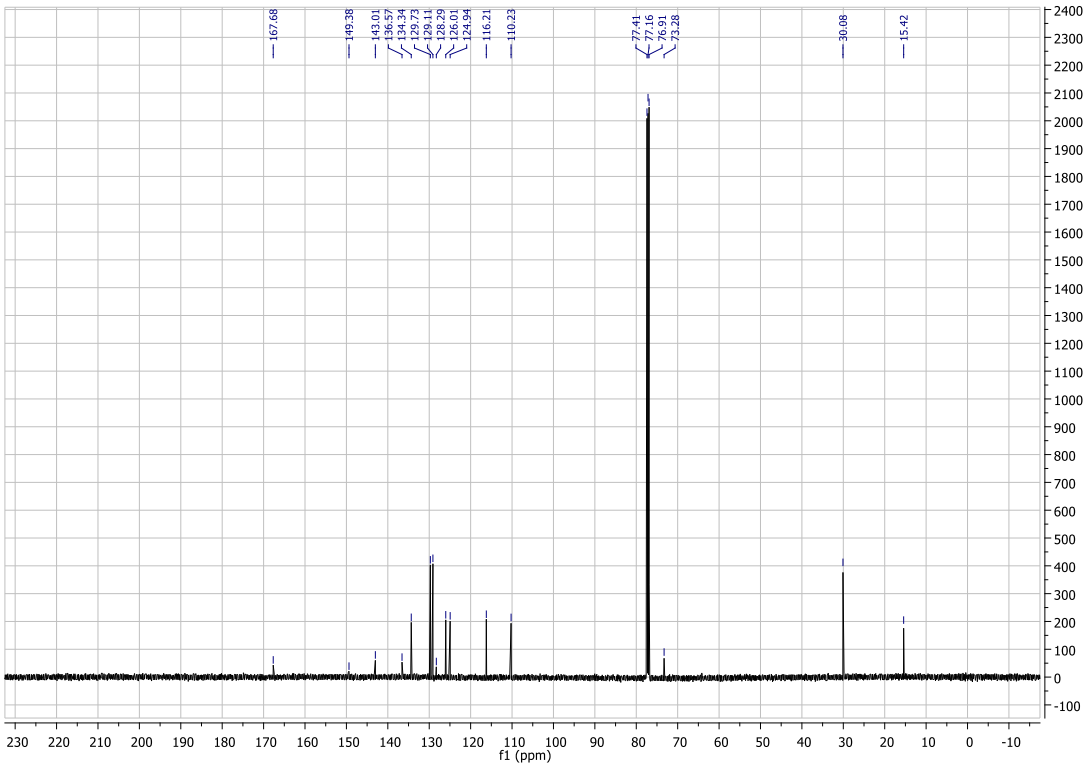

7.88 7.87 7.87 7.87 7.86 7.86 7.86 7.22 7.21 7.20 7.20 7.19 7.18 7.18 7.17 7.16 7.16 7.16 7.15 7.15 7.14 7.14 7.13 7.13 7.11 4.63 4.62 4.60 4.59 4.59 4.47 4.45 4.44 4.42 2.70 2.69 2.69 2.68 2.68 2.66 2.66 2.65 2.65 2.64 2.63 2.63 2.61 2.60 2.59 2.58 2.58 2.57 2.56 2.55 2.18 2.17 2.16 2.16 2.15 2.15 2.14 2.14 2.13 2.12 2.06 2.05 2.05 2.04 2.04 2.03 2.03 2.02 2.02 2.02 2.01 2.01 2.00 1.99
6E+08 6E+08 6E+08 5E+08 4E+08 4E+08 4E+08 3E+08 2E+08 2E+08 2E+08 2E+08 1E+08 5E+07 0
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

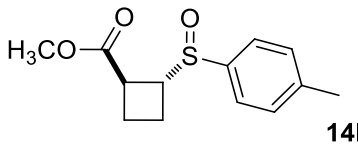

170.23 167.00 165.30 150.66 142.57 133.90 131.46 131.39 127.44 125.90 125.13 116.93 116.78 115.96 110.24 77.37 77.16 76.95 56.07 40.52 22.48 19.49
2E+08 2E+08 2E+08 2E+08 2E+08 2E+08 2E+08 2E+08 1E+08 1E+08 1E+08 1E+08 1E+08 1E+08 9E+07 8E+07 7E+07 6E+07 5E+07 4E+07 3E+07 2E+07 1E+07 0 -1E+07
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



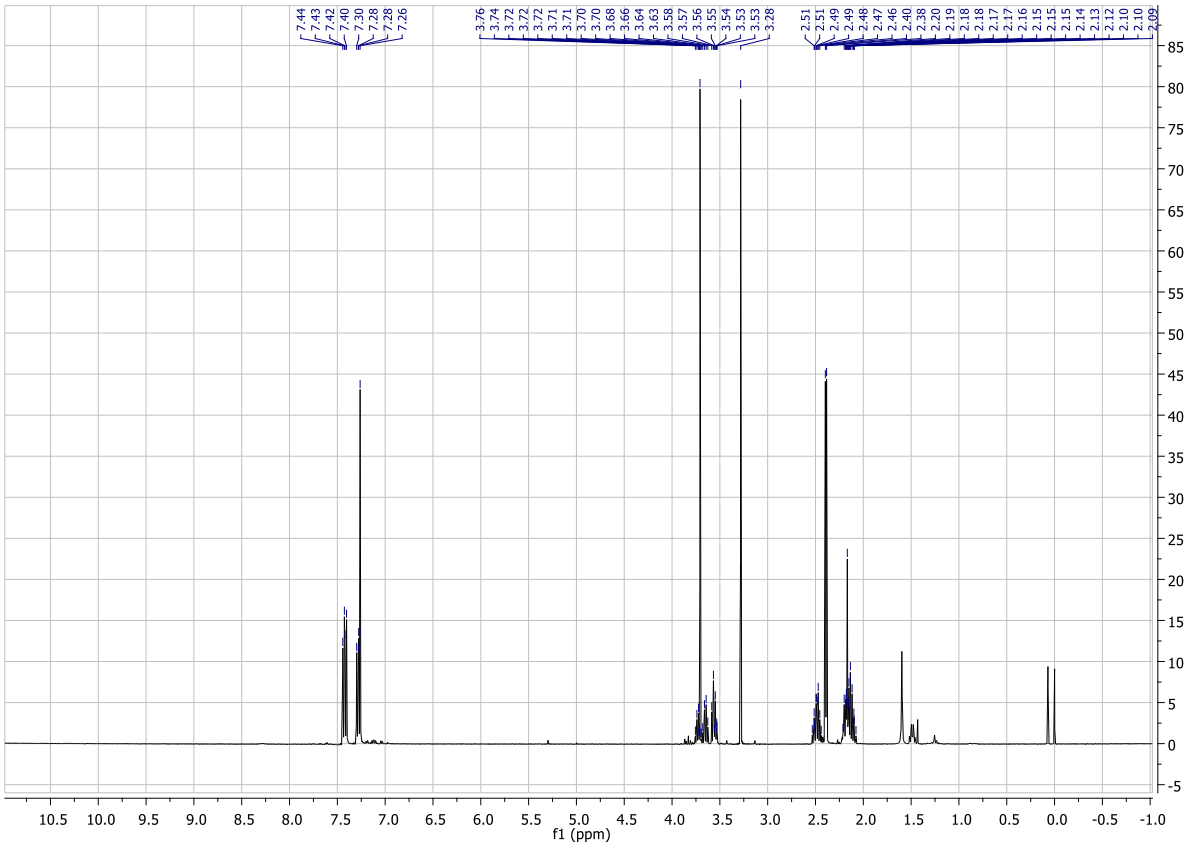
10

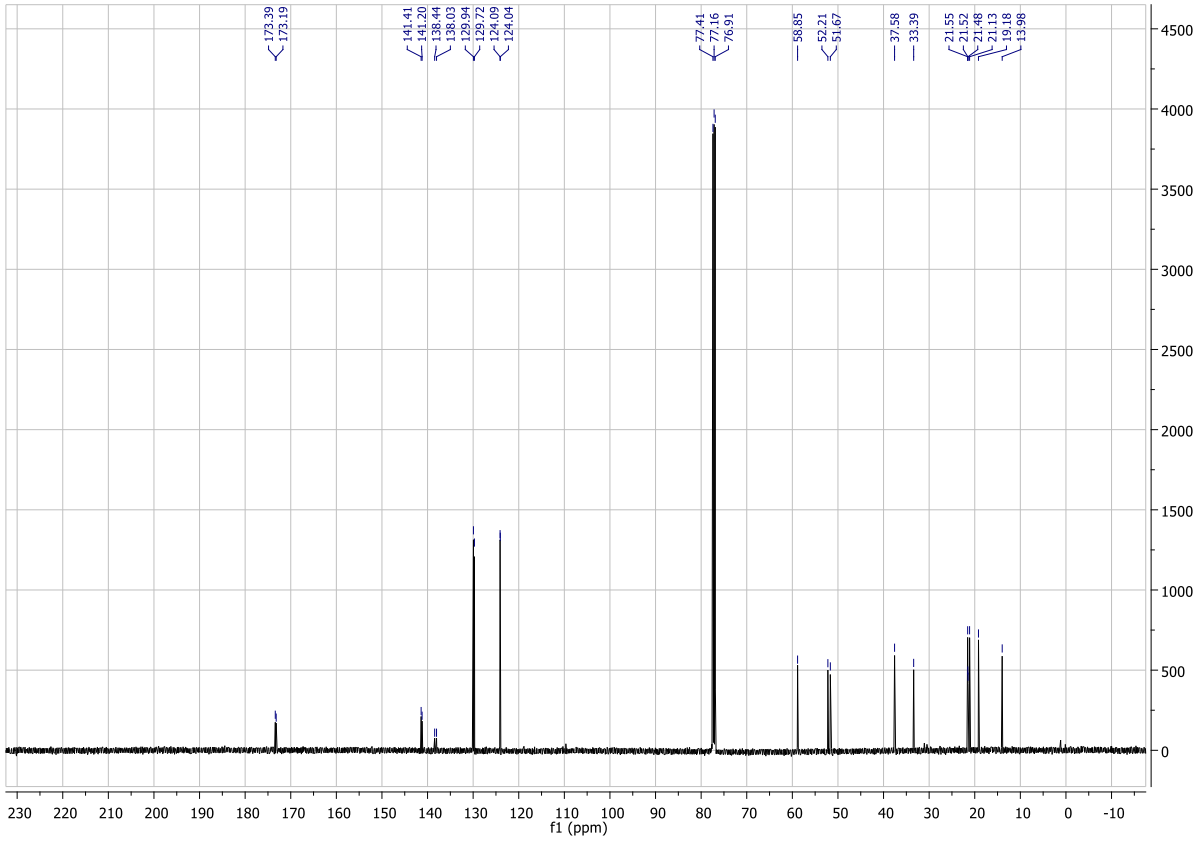

f1 (ppm)

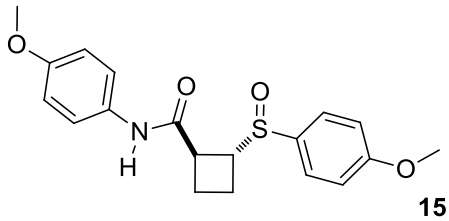

167.68
149.38
143.01
136.57
134.34
129.73
129.11
128.29
126.01
124.94
116.21
110.23
77.41
77.16
76.91
73.28
30.08
15.42
f1 (ppm)


O
O
H3CO
S

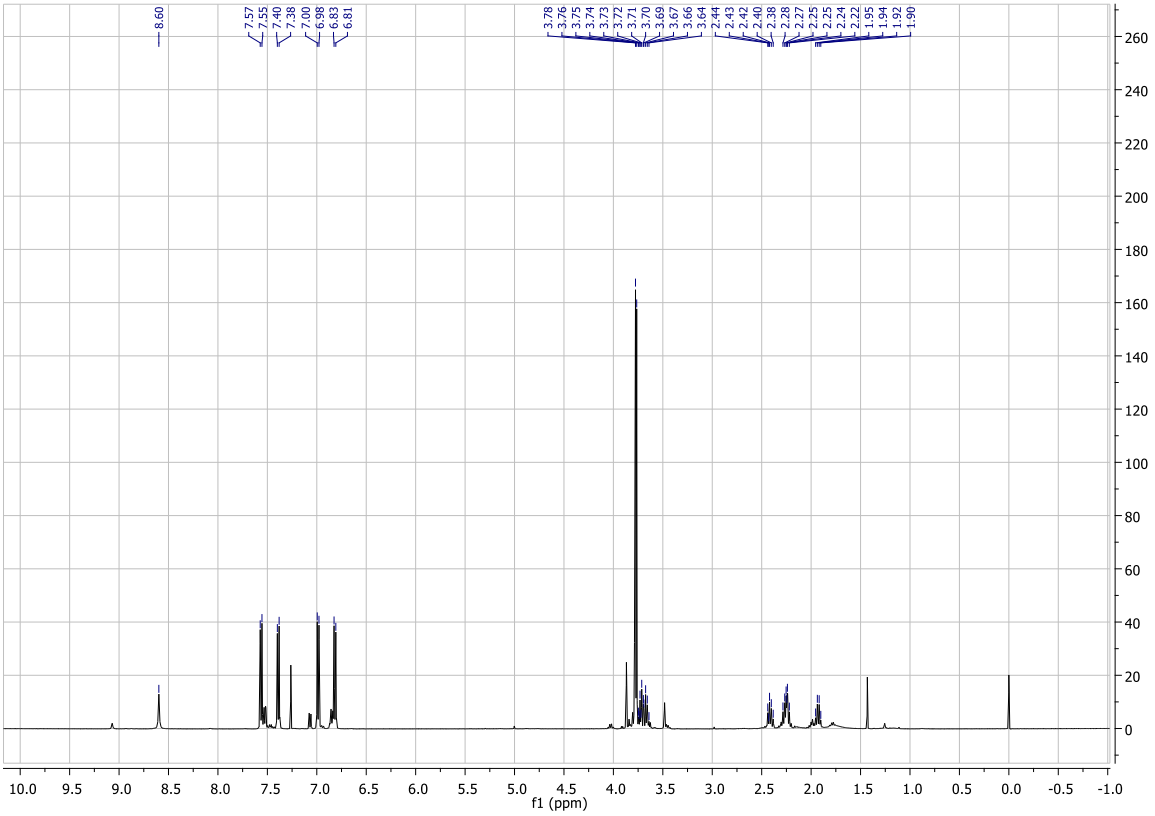
14b+14b'


7.44
7.43
7.42
7.40
7.30
7.28
7.28
7.26
3.76
3.74
3.72
3.72
3.72
3.71
3.71
3.70
3.70
3.68
3.66
3.64
3.63
3.58
3.57
3.56
3.55
3.54
3.53
3.53
3.28
2.51
2.51
2.49
2.49
2.48
2.47
2.46
2.40
2.38
2.20
2.19
2.18
2.18
2.17
2.17
2.16
2.15
2.15
2.15
2.14
2.13
2.12
2.10
2.10
2.09
f1 (ppm)


173.39
173.19
141.41
141.20
138.44
138.03
129.94
129.72
124.09
124.04
77.41
77.16
76.91
58.85
52.21
51.67
37.58
33.39
21.55
21.52
21.48
21.13
19.18
13.98
f1 (ppm)



15l+15l'


8.60
7.57
7.55
7.40
7.38
7.00
6.98
6.83
6.81
3.78
3.76
3.75
3.74
3.73
3.72
3.71
3.70
3.69
3.67
3.66
3.64
2.44
2.43
2.42
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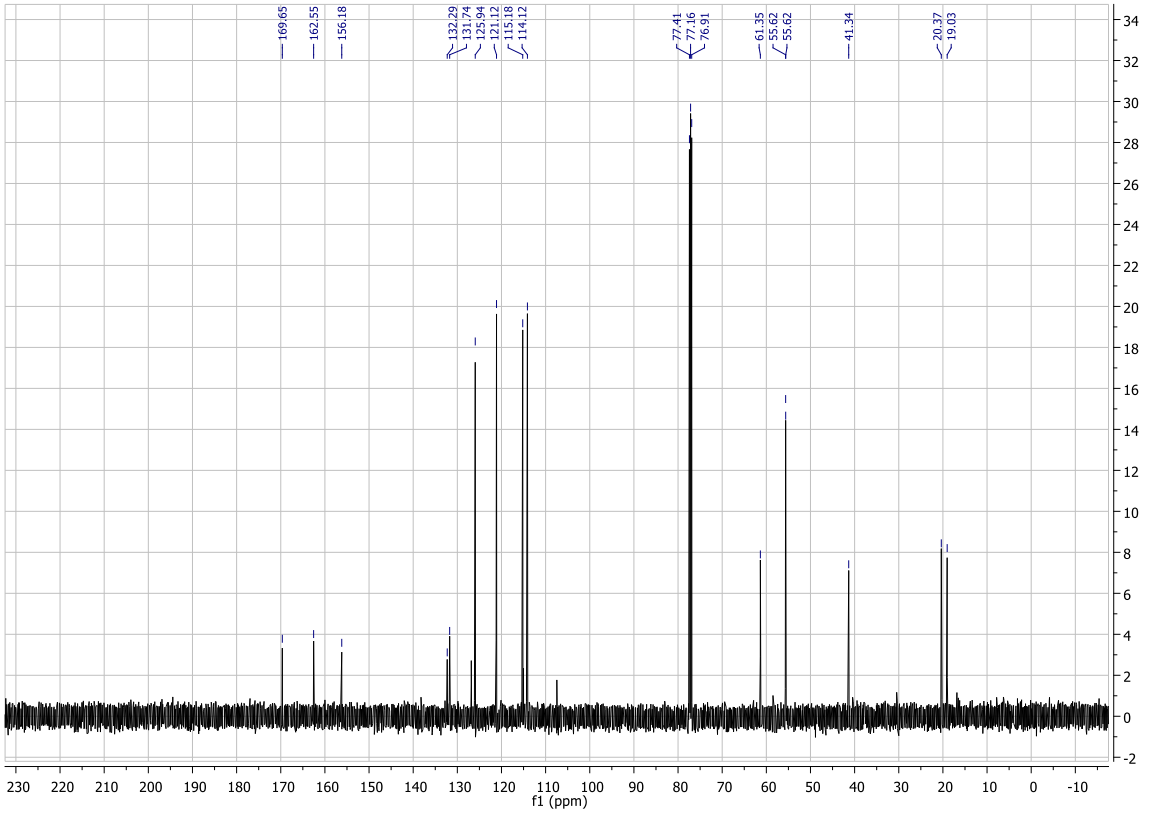
2.22
1.95
1.94
1.92
1.90
f1 (ppm)


169.65
162.55
156.18
132.29
131.74
125.94
121.12
115.18
114.12
77.41
77.16
76.91
61.35
55.62
55.62
41.34
20.37
19.03
f1 (ppm)