Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Copper-Catalysed α-Selective Allylic Alkylation of Heteroaryllithium reagents

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General methods:

All reactions were carried out under a nitrogen atmosphere using oven dried glassware and using standard Schlenk techniques. THF, TBME and toluene were dried and distilled over sodium. All copper salts ($CuBr \cdot SMe_2$, CuI and CuCl) were purchased from Aldrich and used without further purification. ^{n}BuLi (1.6 M solution in hexane) was purchased from Acros. Furan, benzofuran, benzothiophene, cinnamyl bromide, cinnamyl chloride, 3-bromocyclohexene and trans-1,4-dibromo-2-butene were purchased from Aldrich. Allyl bromides **2b**,[1] **2c**,[1] **2d**,[1] **2e**,[1] **2f**,[2] **2h**,[3] **2j**[4] and **2o**[1] were prepareded following a literature procedure. The branched:linear ratio was determined by 1H NMR analysis and GC and mass spectra analysis of each compound.

Chromatography: Merck silica gel type 9385 230-400 mesh, TLC: Merck silica gel 60, 0.25 mm. Components were visualized by UV and cerium/molybdenum or potassium permanganate staining. Progress and conversion of the reaction were determined by GC-MS (GC, HP6890: MS HP5973) with an HP1 or HP5 column (Agilent Technologies, Palo Alto, CA). Mass spectra were recorded on an AEI-MS-902 mass spectrometer (EI+) or a LTQ Orbitrap XL (ESI+). ^{1}H- and ^{13}C-NMR were recorded on a Varian AMX400 (400 and 100.59 MHz, respectively) using $CDCl_3$ as solvent. Chemical shift values are reported in ppm with the solvent resonance as the internal standard ($CHCl_3$: δ 7.26 for ^{1}H, δ 77.0 for ^{13}C). Data are reported as follows: chemical shifts, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, br = broad, m = multiplet), coupling constants (Hz), and integration. Carbon assignments are based on APT ^{13}C-NMR experiments. Melting points were measured using a Büchi Melting Point B-545.

General Procedures for the allylic alkylation

Method A: General procedure for allylic alkylation with 2-thienyllithium.

In a dry Schlenk flask $CuBr \cdot SMe_2$ (2 mol%, 0.01 mmol, 2.04 mg) and the allyl bromide (0.2 mmol) were dissolved in 2 mL of dry THF at -5 °C. 2-Thienyllithium (1.5 equiv or 1.1 equiv, 0.3 mmol,) was diluted with THF to reach the concentration of 0.3 M; this solution was slowly added over 1 h by the use of a syringe pump. After the addition was completed the reaction mixture was stirred for 2 additional hours. After that a saturated aqueous solution of NH_4Cl was added and the mixture was extracted three times with ether. The organic phases were collected, dried over Na_2SO_4 and filtered. The solvent evaporated under reduced pressure afforded the crude product that was then purified by column chromatography.

Method B: General procedure for allylic alkylation with 2-heteroaryllithium reagents.

In a dry Schlenk flask $CuBr \cdot SMe_2$ (2 mol%, 0.01 mmol, 2.04 mg) and the allyl bromide (0.2 mmol) were dissolved in 2 mL of dry THF at -5 °C. 2-heteroaryllithium reagent (1.5 equiv, 0.3 mmol, 0.3 M in THF) was slowly added over 1 h by the use of a syringe pump. After the addition was completed the reaction mixture was stirred for 2 additional hours. After that a saturated aqueous solution of NH_4Cl was added and the mixture was extracted three times with ether. The organic phases were collected, dried over Na_2SO_4 and filtered. The solvent evaporated under reduced pressure afforded the crude product that was then purified by column chromatography.

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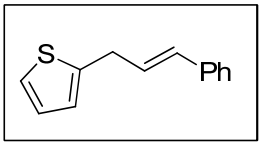
[1] Vyas, D.J., Oestreich, M., *Chem. Commun*., **2010**, 568-570.
[2] Armstrong, A. Gethin, D.M., Wheelhouse, C.J. *Synlett*, **2004**, 350-352.
[3] Ellwood, A.R., Mortimer, A.J.P., Tocher, D.A., Porter, M.J. Synlett, 2008, 2199-2203.
[4] Teichert, J.T., Zhang, S., van Zijl, A.W., Slaa, J.W., Minnaard, A.J., Feringa, B.L., *Org. Lett.* **2010**, *12*, 4658-4660.

Preparation of organolithium reagents:

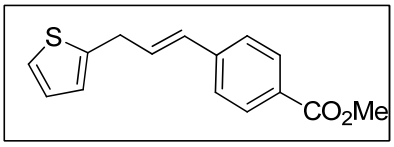
A. benzo[b]thiophen-2-yllithium, 2-furanyllithium and 2-benzofuranyllithium reagents

In a dry Schlenk flask, heteroarene (3.0 mmol) was dissolved in dry THF (8 mL) and the solution was cooled to 0 ºC. *n*-BuLi (1 equiv.) was added slowly and the solution was stirred for 10 min. Then the solution was allowed to reach room temperature and stirred for 1h.

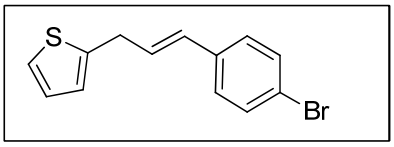
Spectral data of compounds 3a-3o:



2-Cinnamylthiophene (3a): Synthesized according to **Method A**. [86% yield, 98:2 regioselectivity, starting from (*E*)-(3-bromoprop-1-en-1-yl)benzene] [93% yield, 98:2 regioselectivity, starting from (*E*)-(3-chloroprop-1-en-1-yl)benzene] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.25 (t, *J* = 7.2 Hz, 1H), 7.19 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.99 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.92-6.88 (m, 1H), 6.54 (d, *J* = 15.8 Hz, 1H), 6.40 (dt, *J* = 15.7, 6.8 Hz, 1H), 3.77 (d, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.1, 137.2, 131.4, 128.6, 128.2, 127.3, 127.0, 126.3, 124.7, 123.8, 33.4 ppm. The physical data were identical in all respects to those previously reported.[5]



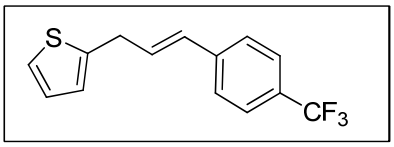
(*E*)-Methyl 4-(3-(thiophen-2-yl)prop-1-en-1-yl)benzoate (3b): Synthesized according to **Method A**. [60% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.18 (dd, *J* = 5.1, 0.9 Hz, 1H), 6.97 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.87 (d, *J* = 2.6 Hz, 1H), 6.62-6.39 (m, 2H), 3.91 (s, 3H), 3.77 (d, *J* = 5.5 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 142.3, 141.7, 131.1, 130.5, 129.9, 128.8, 127.0, 126.1, 124.9, 123.9, 52.0, 33.4 ppm. HRMS (APCI+, *m/z*): calcd for $C_{12}H_{15}OS$ $[M+H]^+$: 259.0787; found: 259.0787.



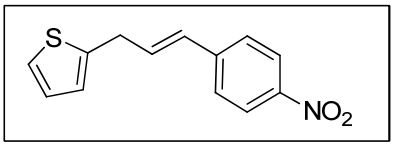
(*E*)-2-(3-(4-Bromophenyl)allyl)thiophene (3c): Synthesized according to **Method A**. [81% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.4 Hz, 2H), 7.23 (t, *J* = 8.5

[5] G. W. Kabalka, G. Dong, B. Venkataiah, *Org. Lett.* **2003**, *5*, 893.

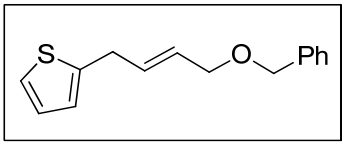
Hz, 2H), 7.18 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.97 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.86 (dd, *J* = 3.3, 0.9 Hz, 1H), 6.45 (d, *J* = 15.9 Hz, 1H), 6.36 (dt, *J* = 15.7, 6.4 Hz, 1H), 3.73 (d, *J* = 6.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 136.1, 131.6, 130.2, 129.1, 127.8, 127.0, 124.8, 123.9, 121.0, 33.3 ppm. HRMS (APCI+, *m/z*): calcd for $C_{13}H_{12}BrS$ $[M+H]^+$: 278.9838; found: 278.9839.



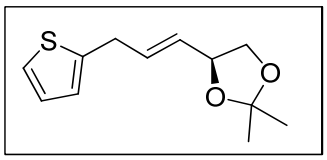
(*E*)-2-(3-(4-(Trifluoromethyl)phenyl)allyl)thiophene (3d): Synthesized according to **Method A**. [91% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.2 Hz, 2H), 7.46 (d, *J* = 8.2 Hz, 2H), 7.20 (dd, *J* = 5.2, 0.7 Hz, 1H), 6.98 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.89 (d, *J* = 3.1 Hz, 1H), 6.55 (d, *J* = 15.9 Hz, 1H), 6.48 (dt, *J* = 15.7, 6.0 Hz, 1H), 3.78 (d, *J* = 6.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 140.6 (q, $J_{C\text{-}F}$ = 1.2 Hz), 131.0, 130.1, 129.1 (q, $J_{C\text{-}F}$ = 32.5 Hz), 127.0, 126.4, 125.5 (q, $J_{C\text{-}F}$ = 5.5 Hz), 125.0, 124.2 (q, $J_{C\text{-}F}$ = 271.6 Hz), 124.0, 33.3 ppm. HRMS (APCI+, *m/z*): calcd for $C_{14}H_{12}F_3S$ $[M+H]^+$: 269.0606; found: 269.0608.



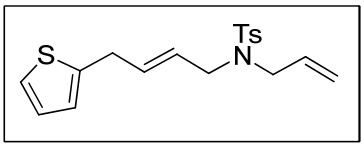
(*E*)-2-(3-(4-Nitrophenyl)allyl)thiophene (3e): Synthesized according to **Method A**. [83% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.8 Hz, 2H), 7.48 (d, *J* = 8.8 Hz, 2H), 7.20 (dd, *J* = 5.1, 0.8 Hz, 1H), 6.98 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.88 (d, *J* = 2.9 Hz, 1H), 6.61-6.49 (m, 2H), 3.80 (d, *J* = 4.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 141.6, 133.4, 129.4, 127.1, 126.7, 125.2, 124.2, 124.0, 123.8, 33.4 ppm. HRMS (APCI+, *m/z*): calcd for $C_{13}H_{12}NO_2S$ $[M+H]^+$: 246.0583; found: 246.0583.



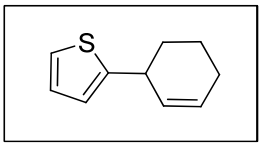
(*E*)-2-(4-(Benzyloxy)but-2-en-1-yl)thiophene (3f): Synthesized according to **Method A**. [78% yield, 96:4 regioselectivity]. Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.28 (m, 5H), 7.16 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.95 (dd, *J* = 5.1, 3.4 Hz, 1H), 6.85-6.81 (m, 1H), 5.97-5.88 (m, 1H), 5.80-5.71 (m, 1H), 4.54 (s, 2H), 4.04 (dd, *J* = 6.0, 1.1 Hz, 2H), 3.61 (d, *J* = 6.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 138.3, 132.0, 128.4, 128.2, 127.8, 127.6, 126.9, 124.7, 123.8, 72.0, 70.4, 32.8 ppm. HRMS (APCI+, *m/z*): calcd for $C_{15}H_{17}OS$ $[M+H]^+$: 245.0995; found: 245.0989.



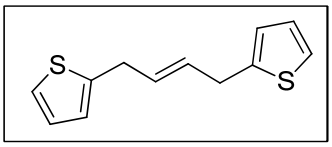
(*S,E*)-2,2-Dimethyl-4-(3-(thiophen-2-yl)prop-1-en-1-yl)-1,3-dioxolane (3g): Synthesized according to **Method A**. [90% yield, 92:8 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.93 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.82-6.79 (m, 1H), 5.96 (dt, *J* = 14.1, 6.7 Hz, 1H), 5.58 (ddt, *J* = 15.2, 7.6, 1.3 Hz, 1H), 4.52 (dd, *J* = 14.8, 7.4 Hz, 1H), 4.09 (dd, *J* = 8.1, 6.2 Hz, 1H), 3.61-3.57 (m, 3H), 1.43 (s, 3H), 1.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 132.8, 129.2, 126.9, 124.8, 123.7, 109.2, 76.8, 69.4, 32.6, 26.7, 25.9 ppm. MS-EI: *m/z* (%) 224 (M^+, 25), 209 (45), 166 (30), 149 (80), 135 (60), 115 (50), 97 (77), 72 (100).



(*E*)-*N*-allyl-4-methyl-N-(4-(thiophen-2-yl)but-2-en-1-yl)benzenesulfonamide (3h): Synthesized according to **Method A**. [68% yield, 96:4 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.3 Hz, 2H), 7.13 (dd, *J* = 5.1, 1.1 Hz, 1H), 6.92 (dd, *J* = 5.1, 3.5 Hz, 1H), 6.75-6.72 (m, 1H), 5.72 (dt, *J* = 14.8, 6.7 Hz, 1H), 5.61 (ddt, *J* = 16.1, 9.8, 6.3 Hz, 1H), 5.38 (dt, *J* = 15.0, 6.6 Hz, 1H), 5.18-5.08 (m, 2H), 3.80-3.79 (m, 4H), 3.50 (d, *J* = 6.7 Hz, 2H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 142.5, 137.5, 133.3, 132.7, 129.6, 127.2, 126.9, 126.0, 124.6, 123.7, 119.9, 49.2, 48.3, 32.6, 21.5 ppm. HRMS (APCI+, *m/z*): calcd for $C_{18}H_{21}NOSNa$ $[M+Na]^+$: 370.0906; found: 370.0905.

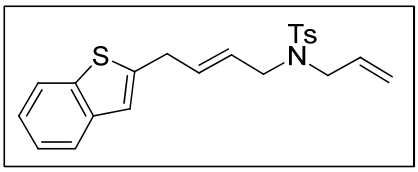


2-(cyclohex-2-en-1-yl)thiophene (3i): Synthesized according to **Method A**. [96% yield] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/Ether 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (dd, *J* = 5.1, 0.7 Hz, 1H), 6.95 (dd, *J* = 5.0, 3.5 Hz, 1H), 6.84 (d, *J* = 3.4 Hz, 1H), 5.88-5.80 (m, 2H), 3.71 (br s, 1H), 2.11-2.06 (m, 3H), 1.82-1.71 (m, 2H), 1.67-1.60 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 129.7, 128.3, 126.5, 123.3, 122.9, 36.7, 32.5, 24.9, 20.7 ppm. HRMS (APCI+, *m/z*): calcd for $C_{10}H_{13}S$ $[M+H]^+$: 165.0732; found: 165.0732.

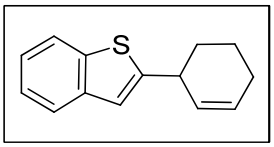


(E)-1,4-di(thiophen-2-yl)but-2-ene (3j): Synthesized according to **Method A**. [70% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/EtOAc 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (d, *J* = 4.9 Hz, 2H), 6.95 (s, 2H),

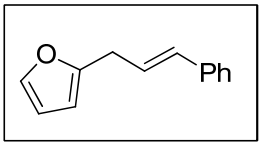
6.83 (s, 2H), 6.07 (br s, 2H), 3.88 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.8, 130.3, 127.1, 124.7, 123.9, 33.1 ppm. HRMS (APCI+, *m/z*): calcd for $C_{12}H_{13}S_2$ $[M+H]^+$: 221.0453; found: 221.0454.



(*E*)-*N*-allyl-N-(4-(benzo[b]thiophen-2-yl)but-2-en-1-yl)-4-methylbenzenesulfonamide (3k): Synthesized according to **Method B**. [78% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/Ether 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.8 Hz, 1H), 7.70 (d, *J* = 8.3 Hz, 2H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.29-7.22 (m, 3H), 6.97 (s, 1H), 5.83-5.72 (m, 1H), 5.63 (ddt, *J* = 16.6, 10.2, 6.3 Hz, 1H), 5.46 (dt, *J* = 14.9, 6.6Hz, 1H), 5.16 (dd, *J* = 8.5, 1.1 Hz, 1H), 5.13 (s, 1H), 3.85-3.82 (m, 4H), 3.57 (d, *J* = 6.7 Hz, 2H), 2.38 (s, 3H).^{13}C NMR (100 MHz, $CDCl_3$) δ 143.6, 143.2, 140.1, 139.5, 137.4, 132.8, 132.4, 129.6, 127.2, 126.8, 124.2, 123.7, 122.9, 122.1, 121.2, 120.0, 49.3, 48.3, 33.5, 21.5 ppm.

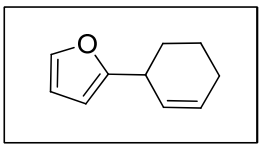


2-(cyclohex-2-en-1-yl)benzo[b]thiophene (3l): Synthesized according to **Method B**. [82% yield] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/Ether 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.6 Hz, 1H), 7.89 (d, *J* = 7.3 Hz, 1H), 7.60-7.40 (m, 3H), 6.26-6.01 (m, 2H), 3.96 (br s, 1H), 2.32 (br s, 3H), 2.10-1.96 (m, 2H), 1.93-1.82 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.2, 140.0, 139.2, 129.0, 128.9, 124.0, 123.4, 122.8, 122.2, 120.0 37.3, 31.9, 24.9, 20.6 ppm.

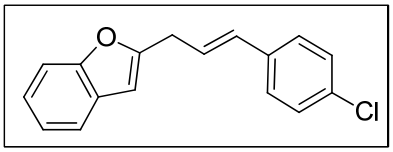


2-cinnamylfuran (3m): Synthesized according to **Method B**. [94% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/Ether 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.37 (m, 3H), 7.19 (t, *J* = 7.5 Hz, 2H), 7.23 (t, *J* = 7.2 Hz, 1H), 6.52 (d, *J* = 15.8 Hz, 1H), 6.40-6.27 (m, 2H), 6.09 (d, *J* = 2.4 Hz, 1H), 3.58 (d, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 141.3, 137.2, 132.0, 128.5, 127.3, 126.2, 125.6, 110.3, 105.6, 31.8 ppm. The physical data were identical in all respects to those previously reported.[6]

[6] R. Riveiros, R. Tato, J. Perez-Sestelo, L. A. Sarandeses, *Eur. J. Org. Chem.* **2012**, 3018-3023.

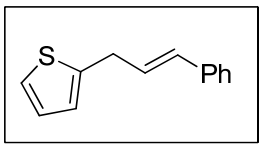


2-(cyclohex-2-en-1-yl)furan (3o): Synthesized according to **Method B**. [65% yield] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 0.9 Hz, 1H), 6.29 (dd, *J* = 3.0, 1.9 Hz, 1H), 5.99 (d, *J* = 3.1 Hz, 1H), 5.90-5.82 (m, 1H), 5.77 (dd, *J* = 10.1, 2.5 Hz, 1H), 3.48 (br s, 1H), 2.06-1.95 (m, 3H), 1.80-1.70 (m, 2H), 1.66-1.58 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 140.9, 128.7, 127.1, 109.9, 104.4, 35.0, 28.2, 24.9, 20.4 ppm. HRMS (APCI+, *m/z*): calcd for $C_{10}H_{13}O$ $[M+H]^+$: 149.0961; found: 149.0960.

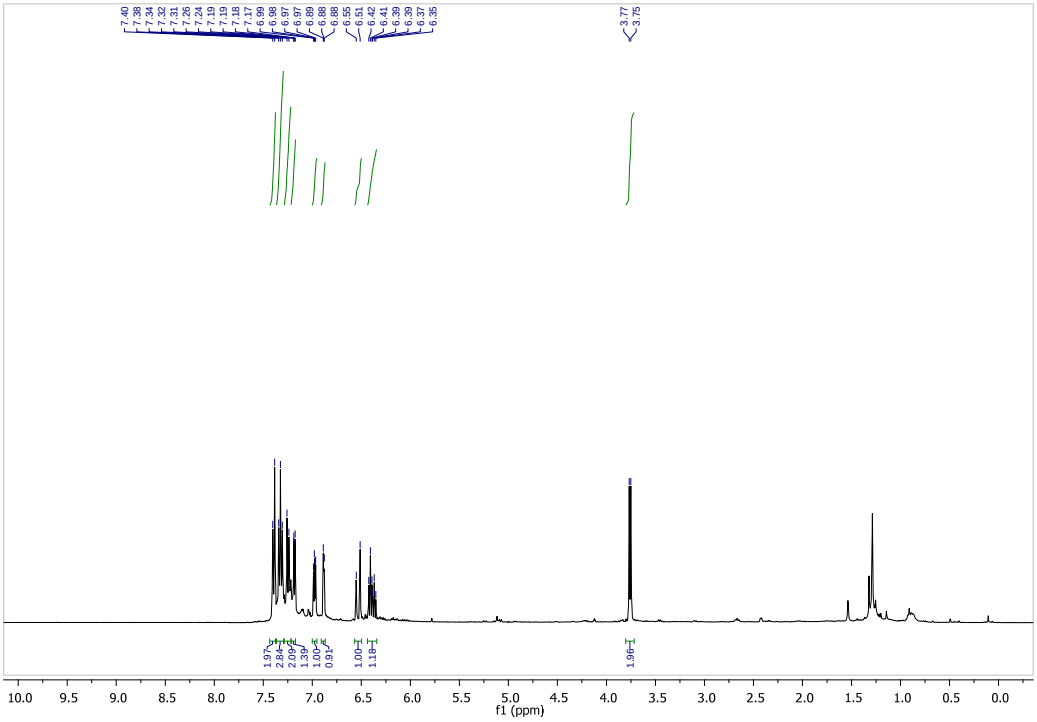


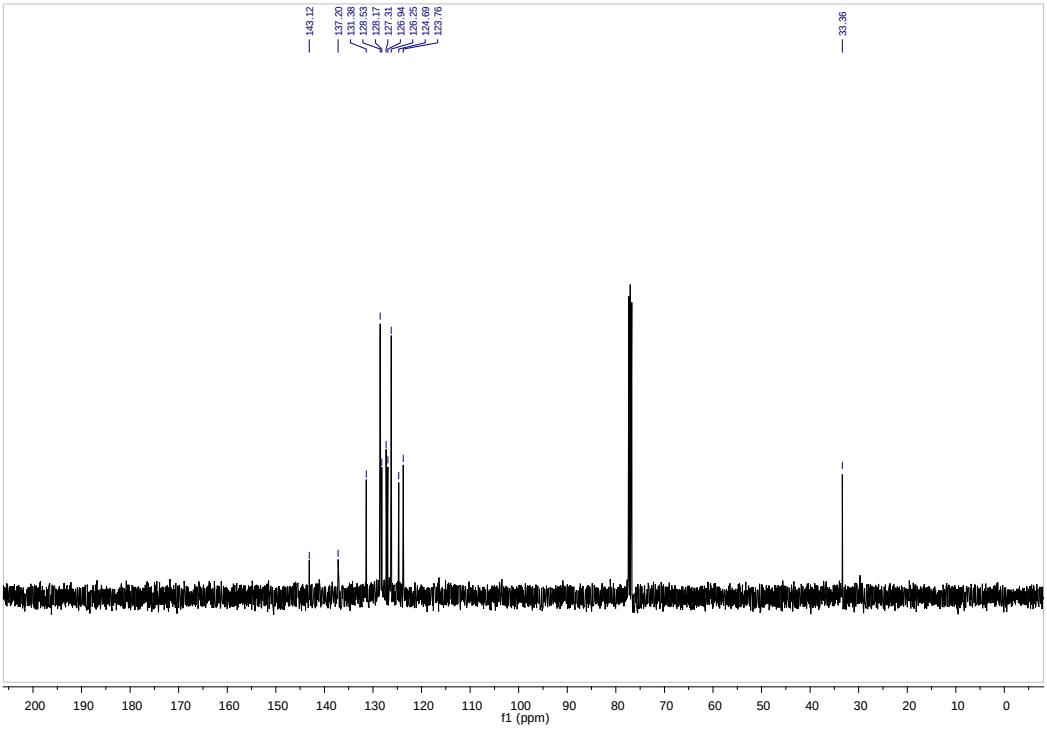
(E)-2-(3-(4-chlorophenyl)allyl)benzofuran (3n): Synthesized according to **Method B**. [72% yield, 95:5 regioselectivity] Colorless oil obtained after column chromatography (SiO_2, *n*-pentane/Ether 100:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 6.8, 1.6 Hz, 1H), 7.44 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.24-7.18 (m, 2H), 6.53 (d, *J* = 15.8 Hz, 1H), 6.48 (d, *J* = 0.8 Hz, 1H), 6.36 (dt, *J* = 15.8, 6.7 Hz, 1H), 3.70 (d, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 154.9, 135.5, 133.0, 131.5, 128.8, 128.7, 127.4, 125.4, 123.5, 122.6, 120.4, 110.9, 102.9, 32.1 ppm.

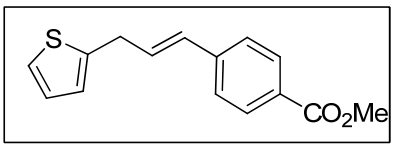
^{1}H and ^{13}C NMR of isolated compounds



3a



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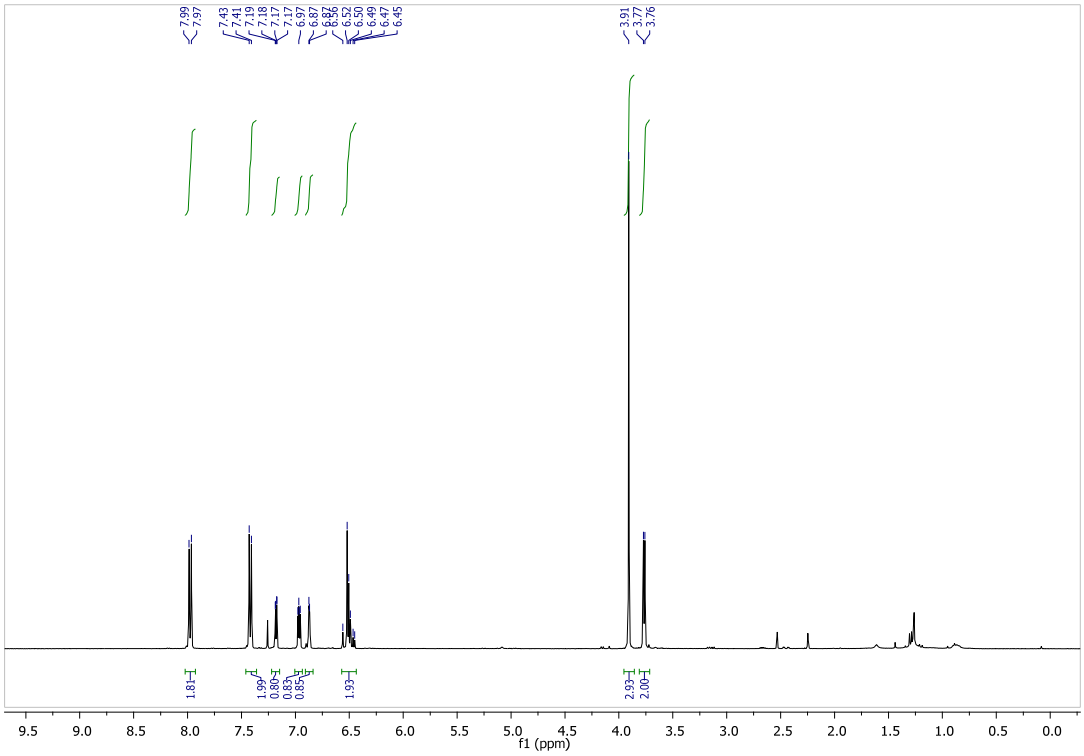
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6.47
6.45
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0.85
1.93
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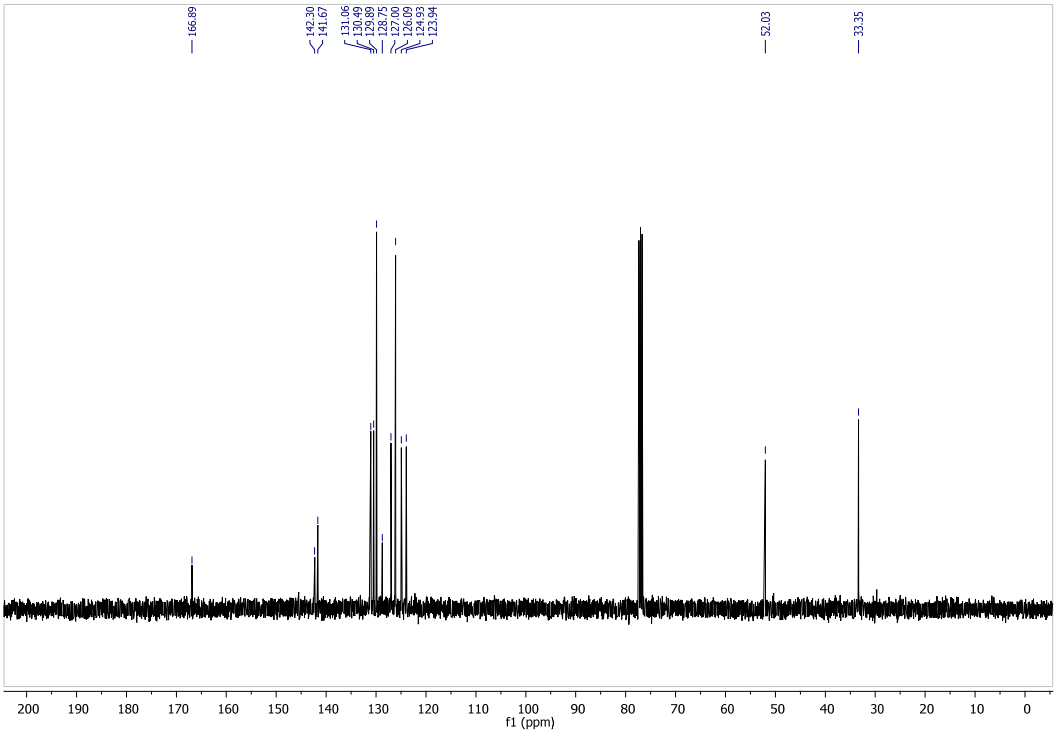
2.00
f1 (ppm)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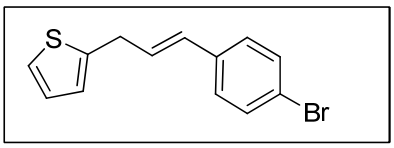
f1 (ppm)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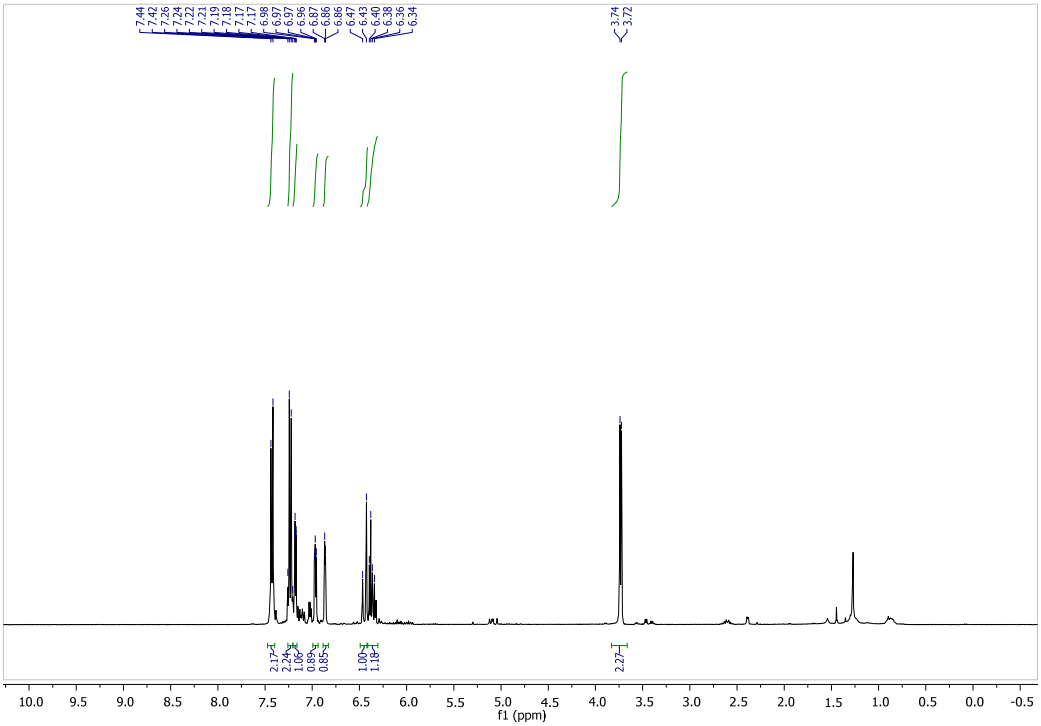
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6.86
6.47
6.43
6.40
6.38
6.36
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1.00
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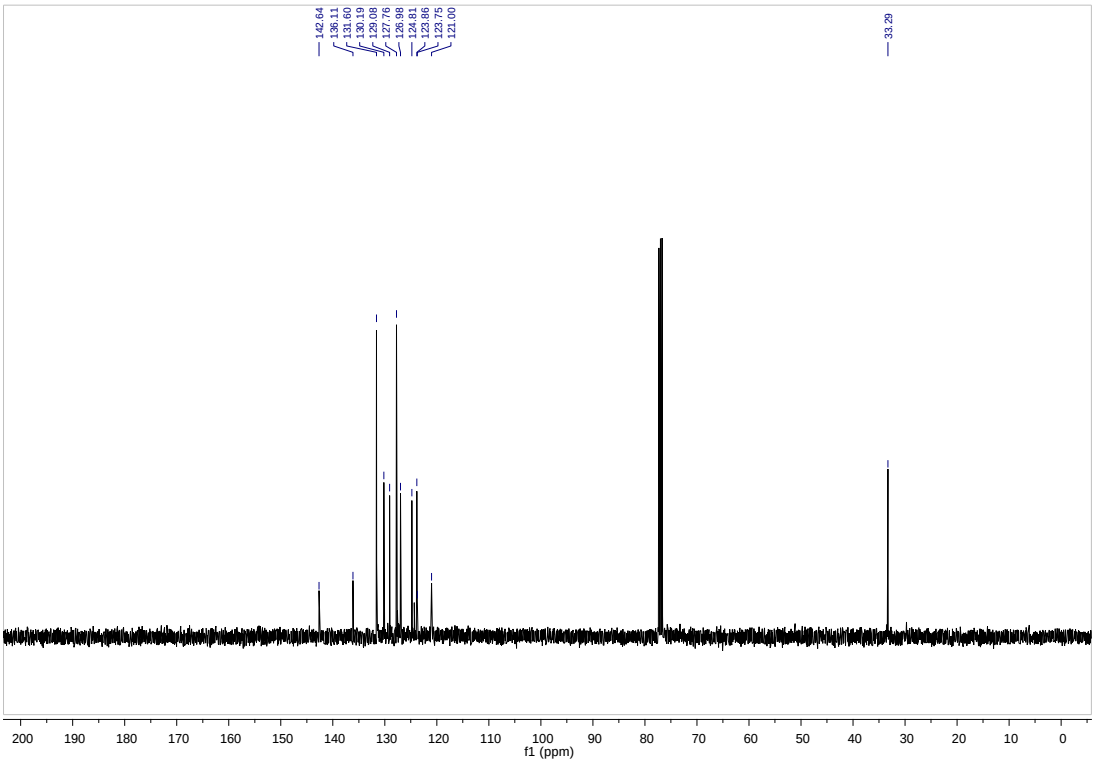
f1 (ppm)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123.75
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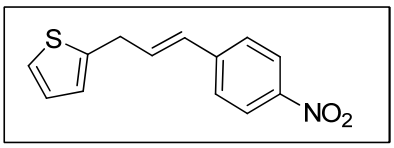
33.29
f1 (ppm)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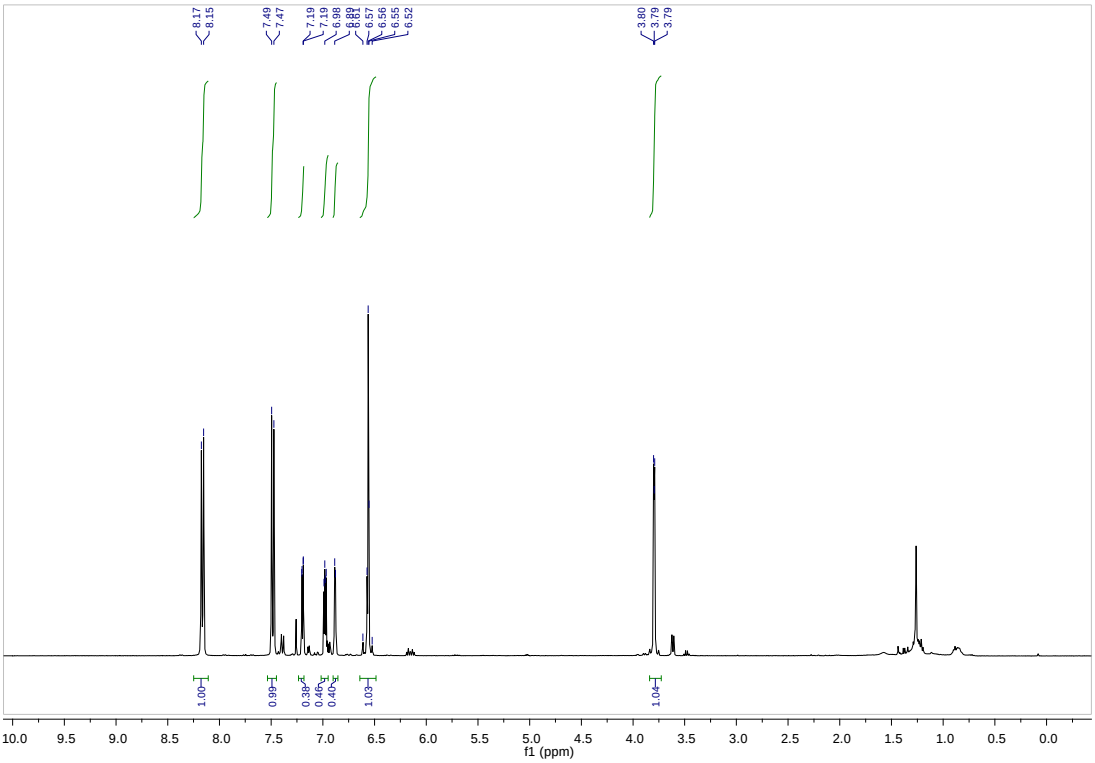
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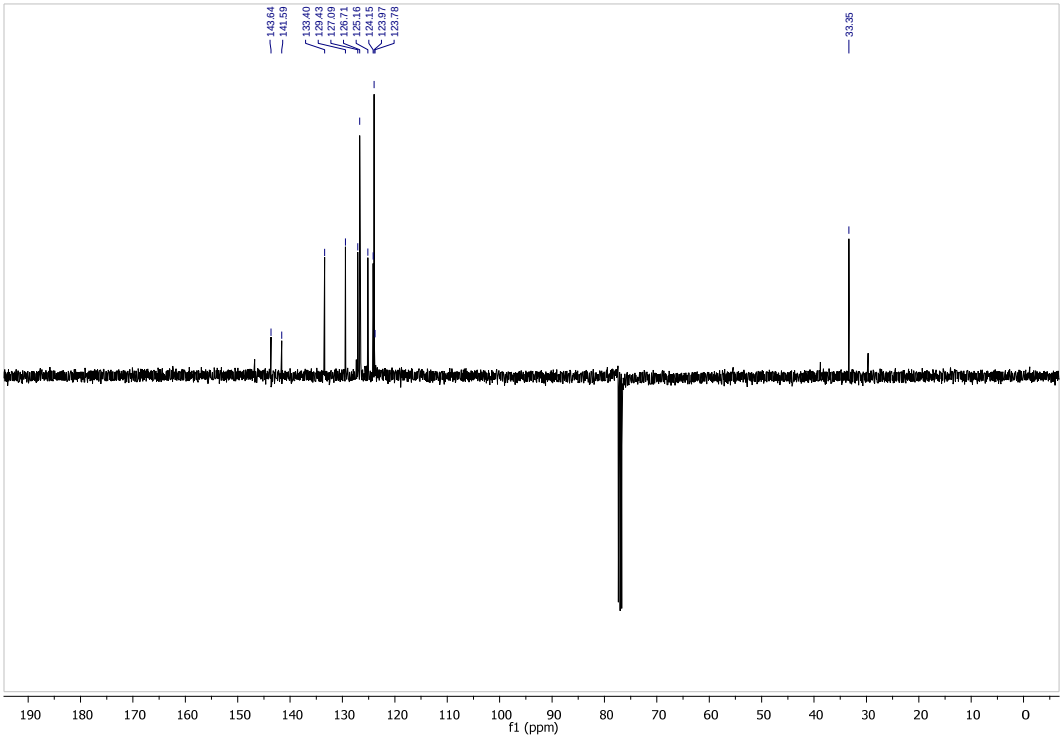
6.55
6.52
3.80
3.79
3.79
1.00
0.99
0.38
0.46
0.40
1.03
1.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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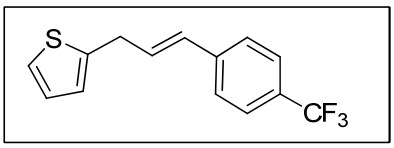
f1 (ppm)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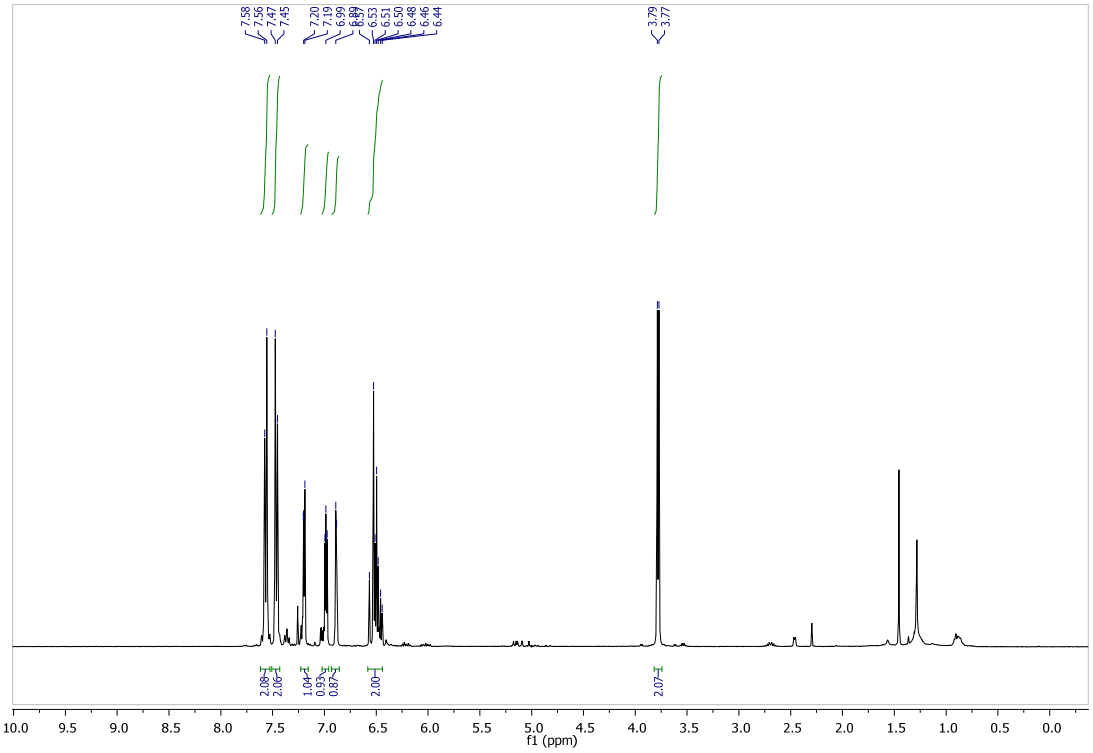
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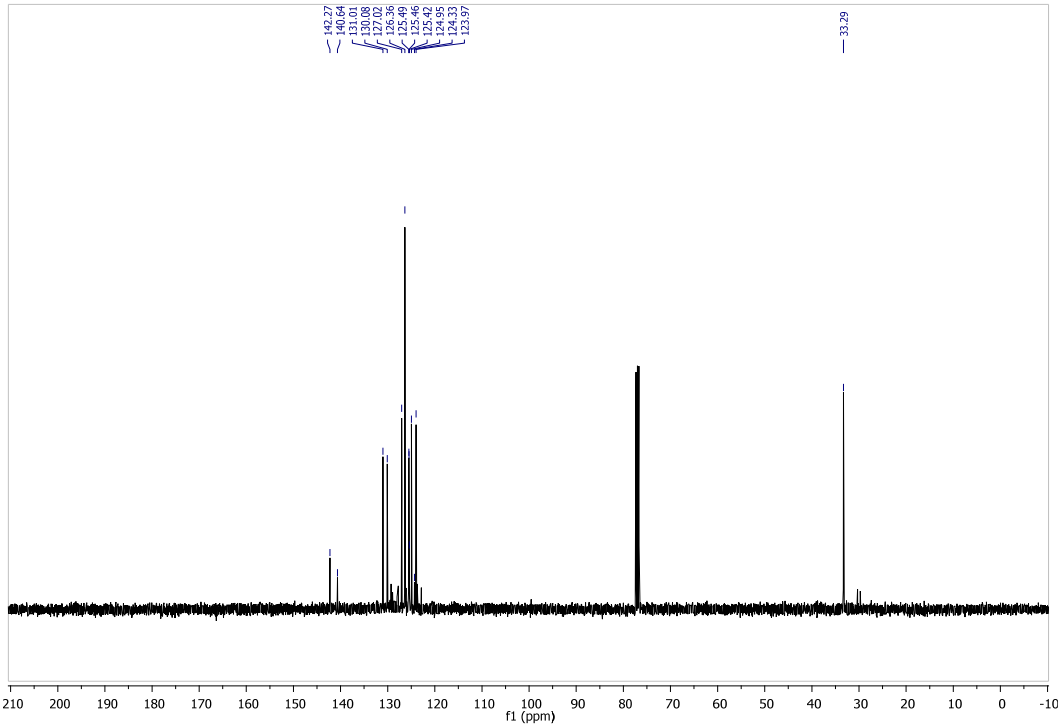
f1 (ppm)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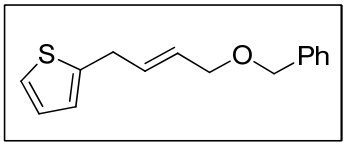
f1 (ppm)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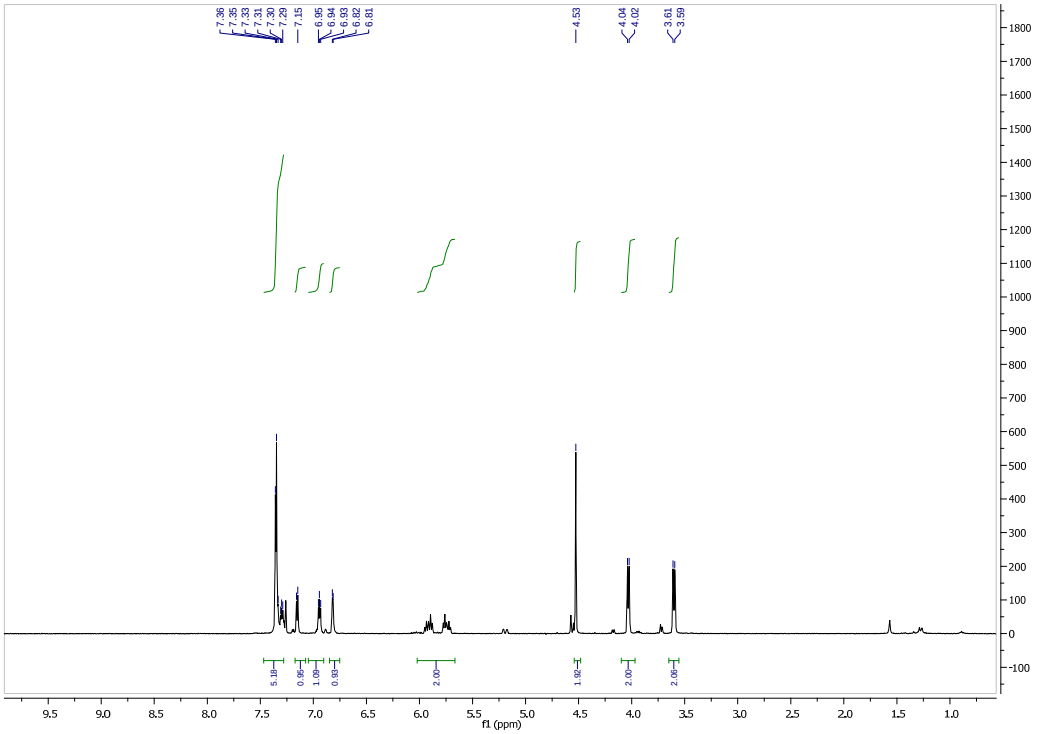
O
Ph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4.04
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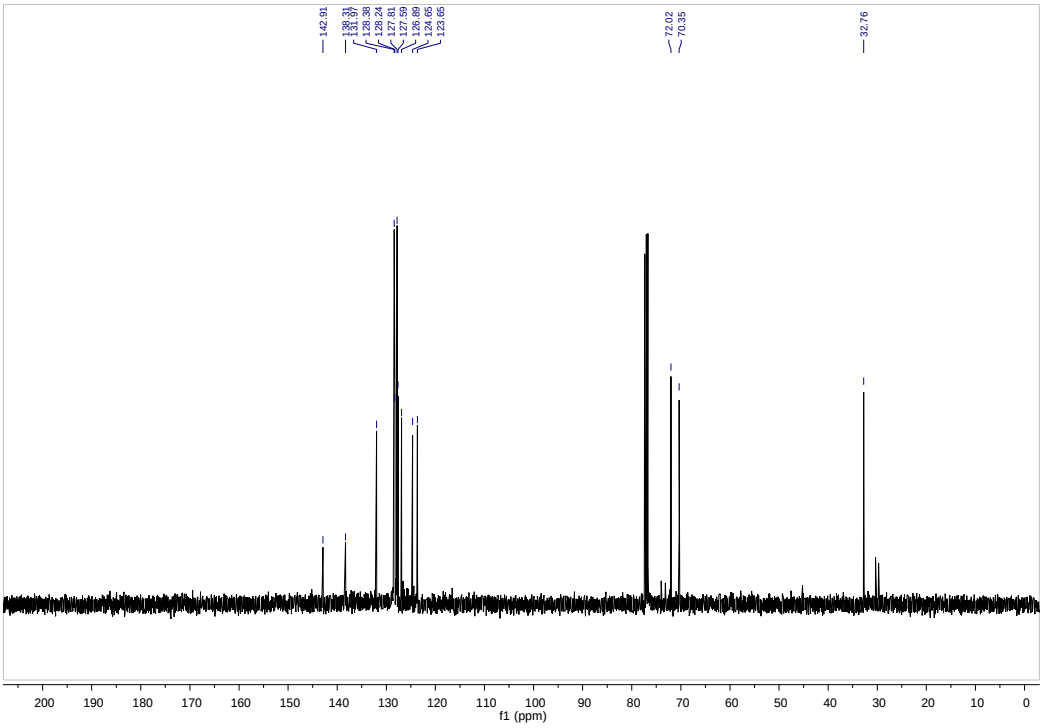
f1 (ppm)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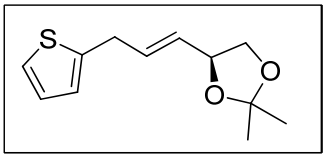
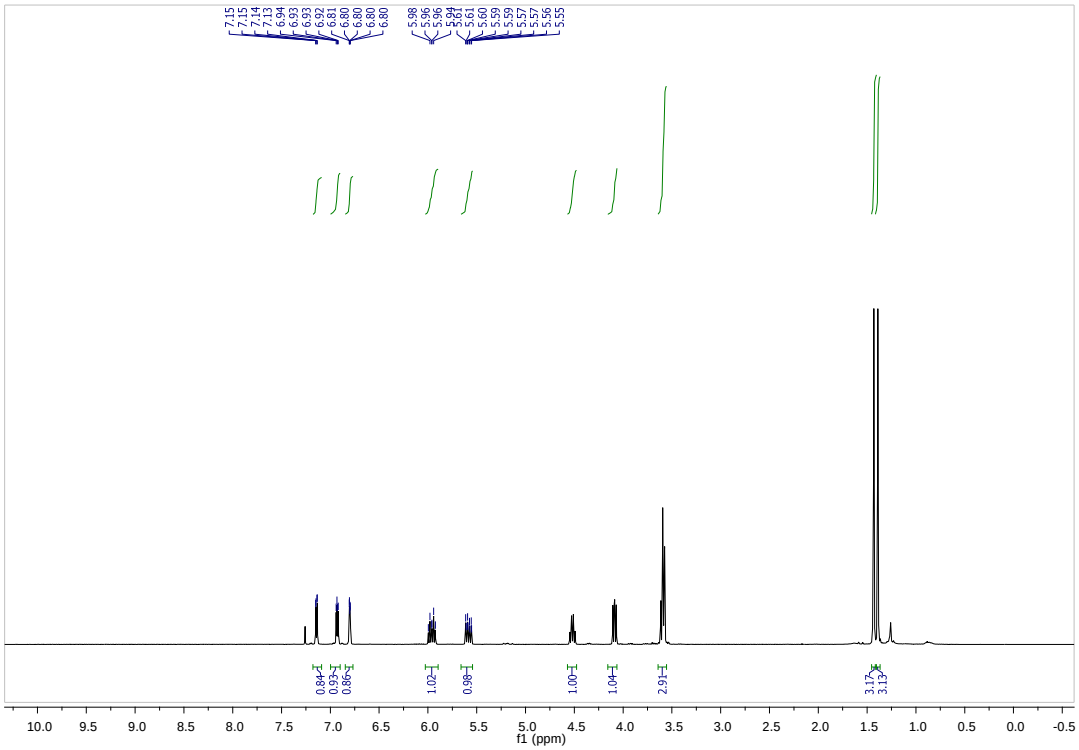
f1 (ppm)


S
O
O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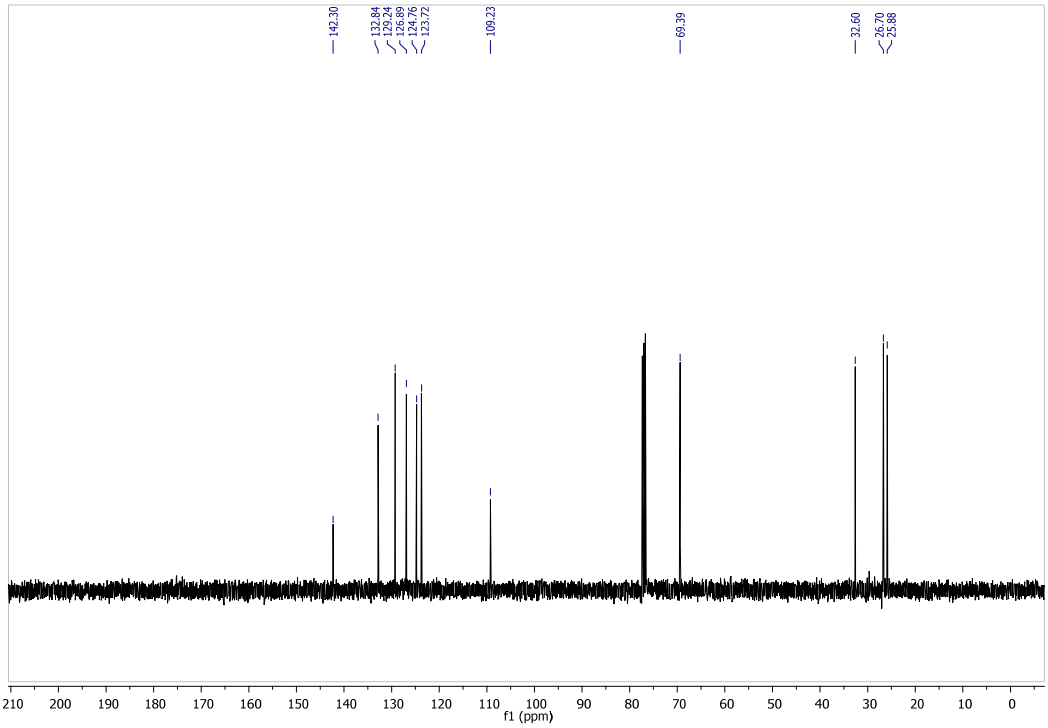
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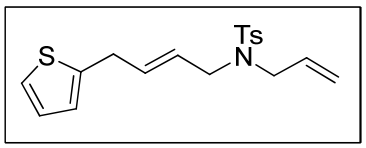
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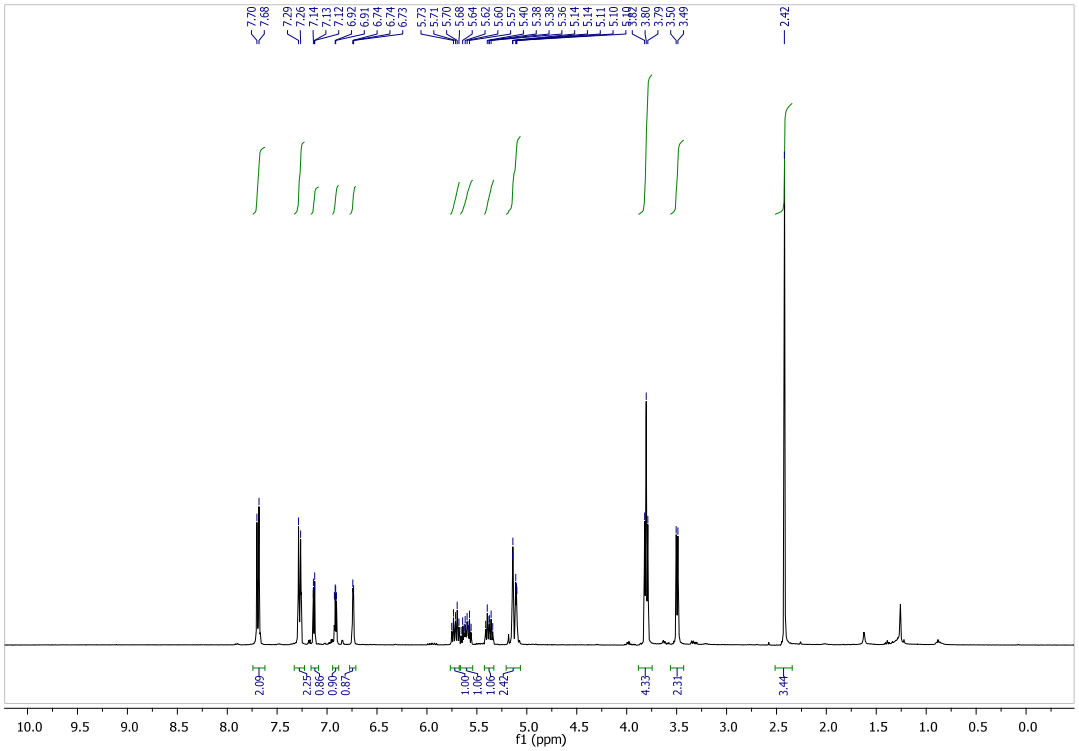
S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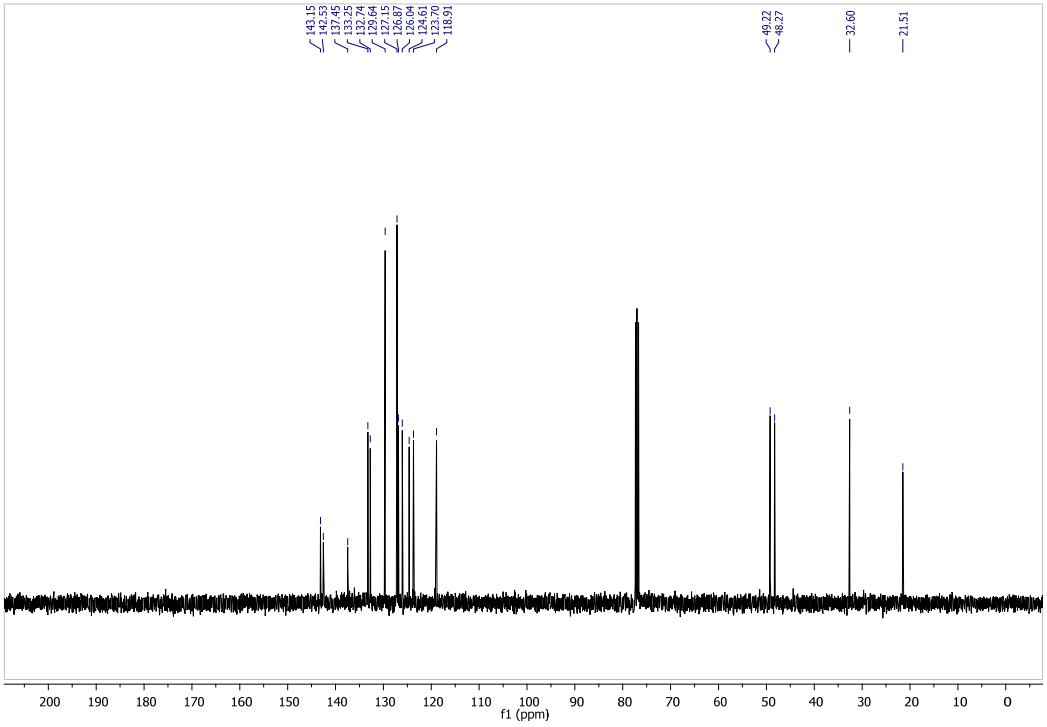
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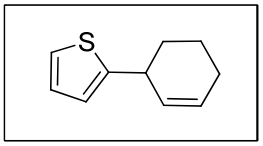
f1 (ppm)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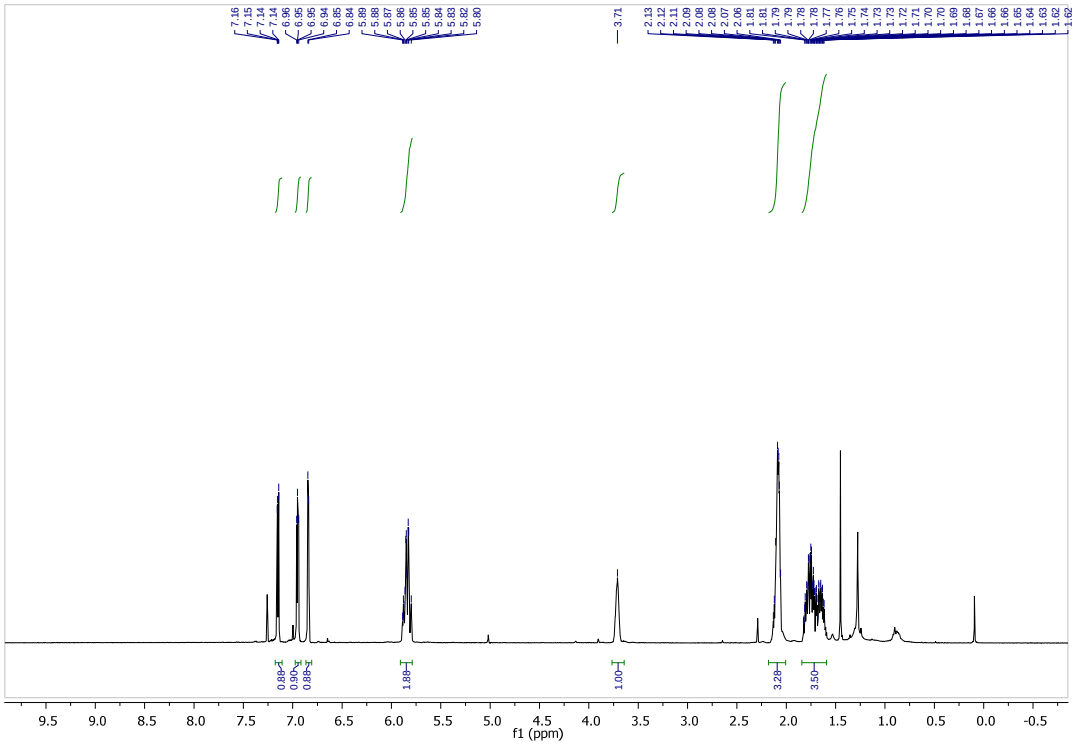
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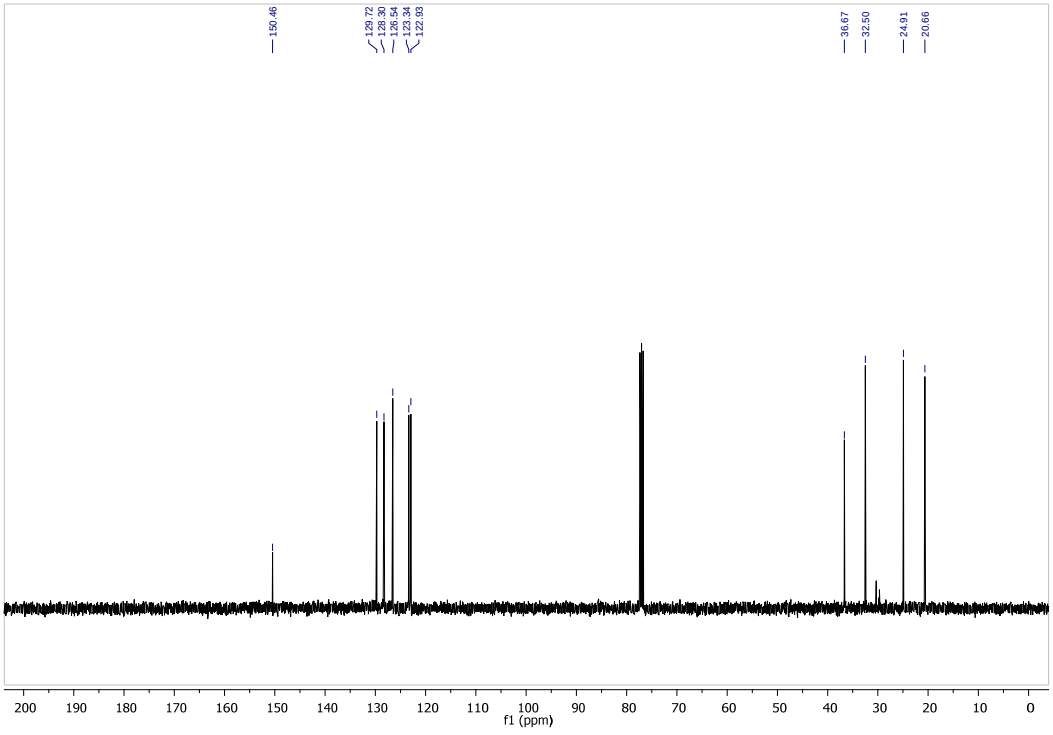
1.65
1.64
1.63
1.62
1.62
0.89
0.90
0.88
1.89
1.00
3.26
3.50
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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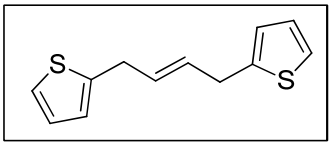
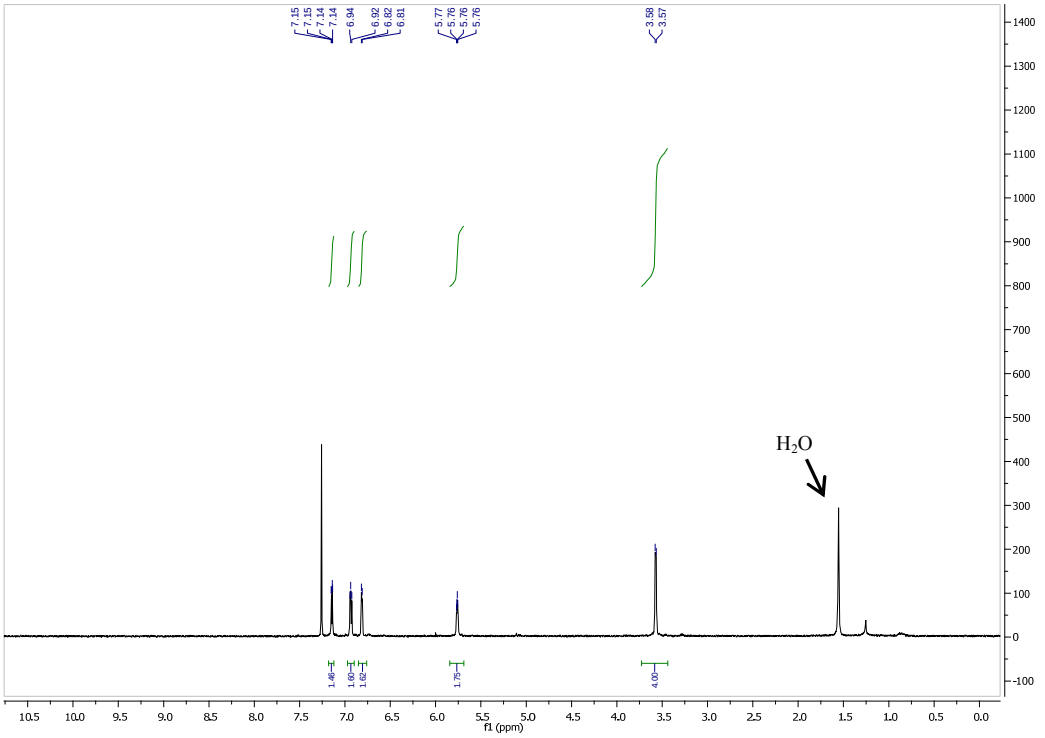
f1 (ppm)


S
S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6.92
6.82
6.81
5.77
5.76
5.76
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3.58
3.57
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1.62
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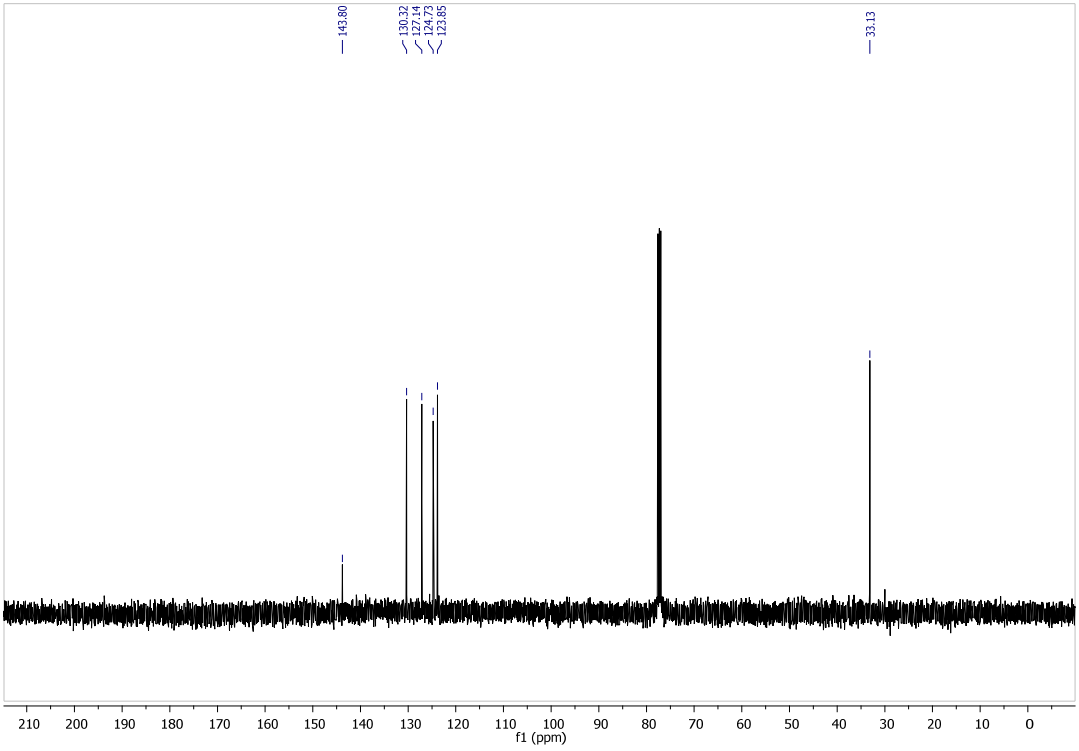
f1 (ppm)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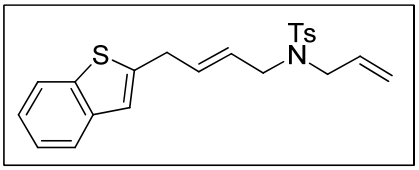
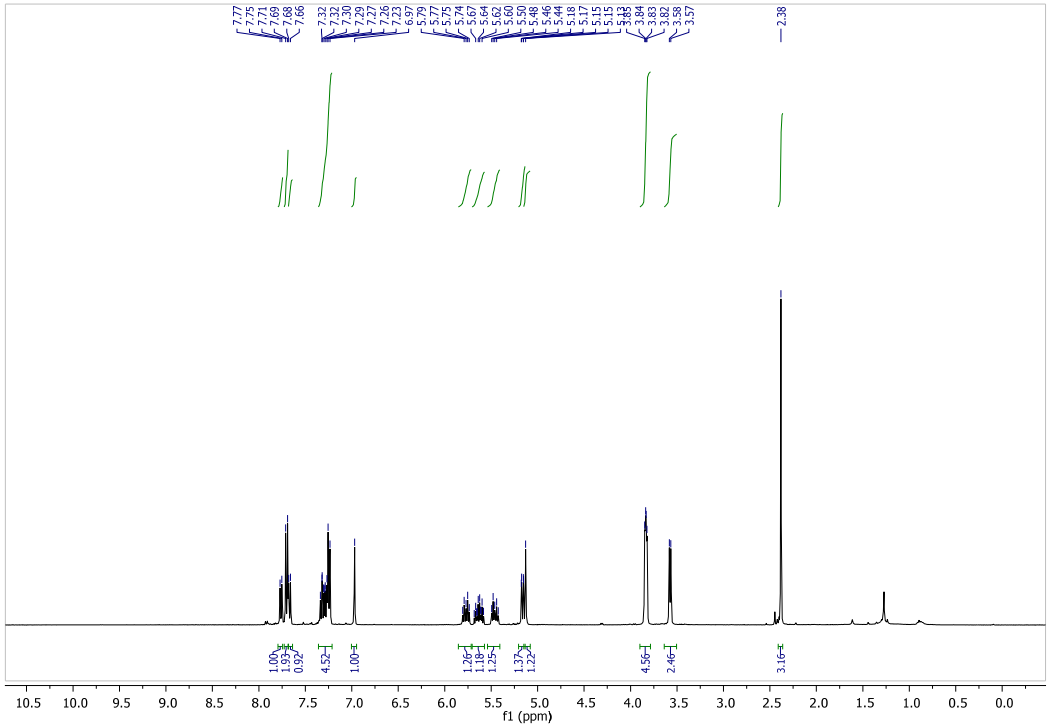
123.85
33.13
f1 (ppm)


Ts
N
S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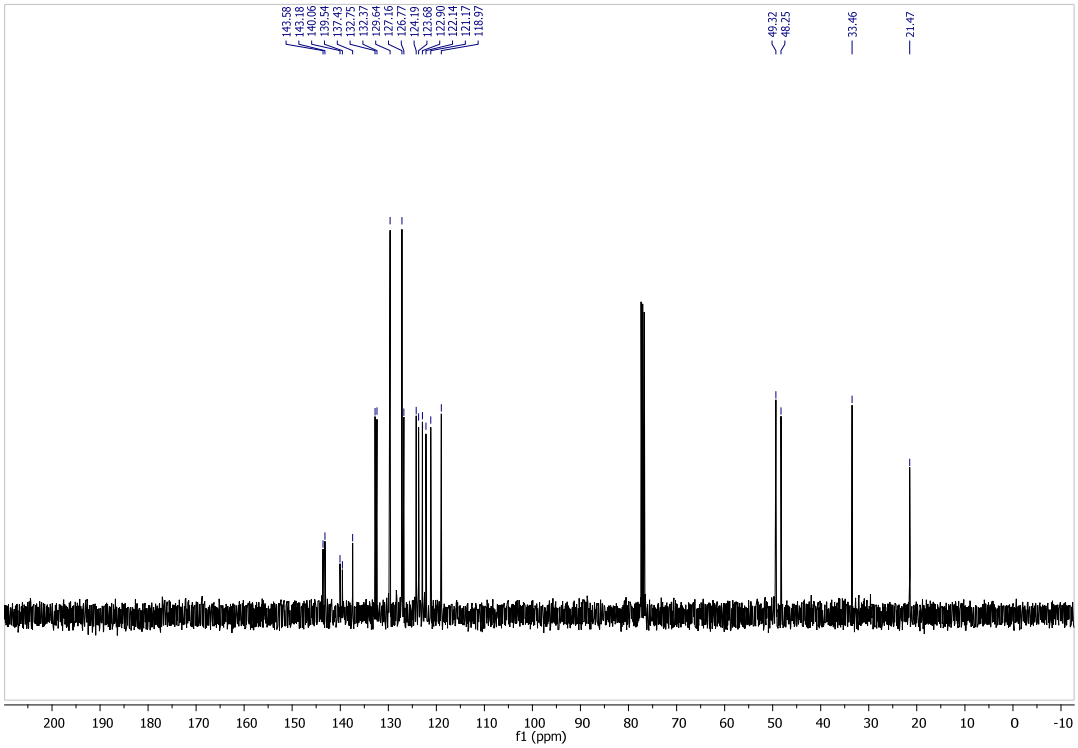
7.75
7.71
7.69
7.68
7.66
7.32
7.32
7.30
7.29
7.27
7.26
7.23
6.97
5.79
5.77
5.75
5.74
5.67
5.64
5.62
5.60
5.50
5.48
5.46
5.44
5.18
5.17
5.15
5.13
3.84
3.83
3.82
3.58
3.57
2.38
1.00
1.93
0.92
4.52
1.00
1.26
1.18
1.25
1.37
1.22
4.56
2.46
3.16
f1 (ppm)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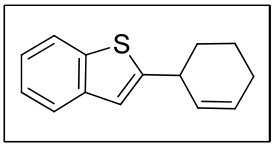
143.18
140.06
139.54
137.43
132.75
132.37
129.64
127.76
126.77
124.19
123.68
122.90
122.14
121.17
118.97
49.32
48.25
33.46
21.47
f1 (ppm)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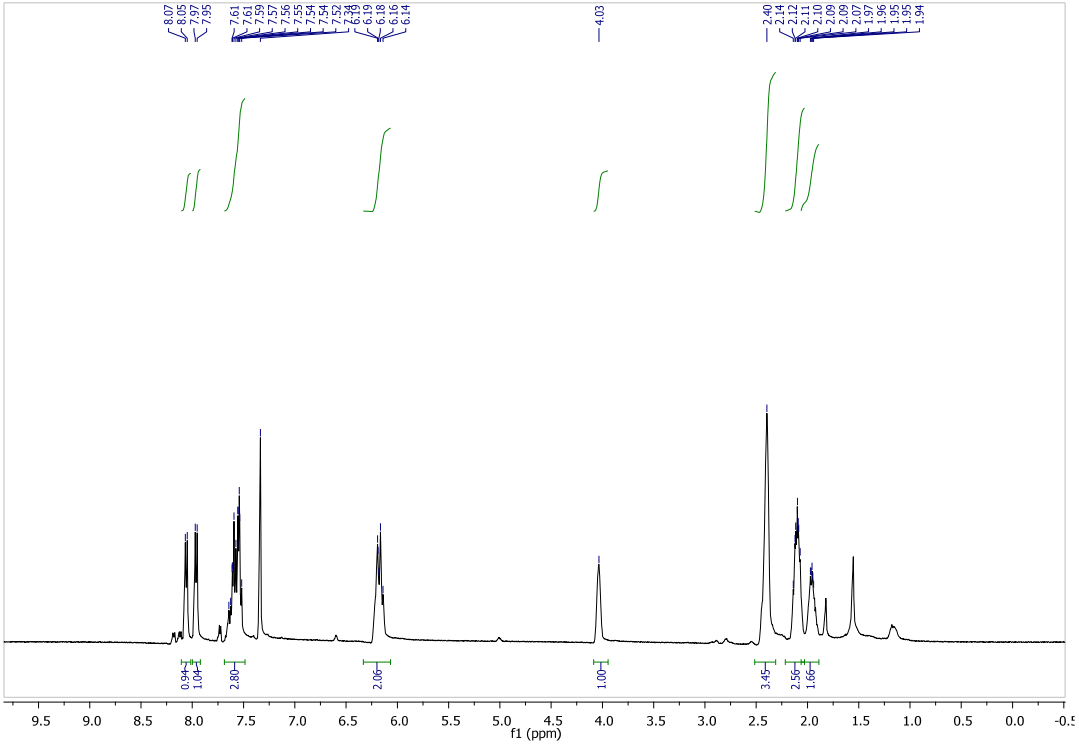
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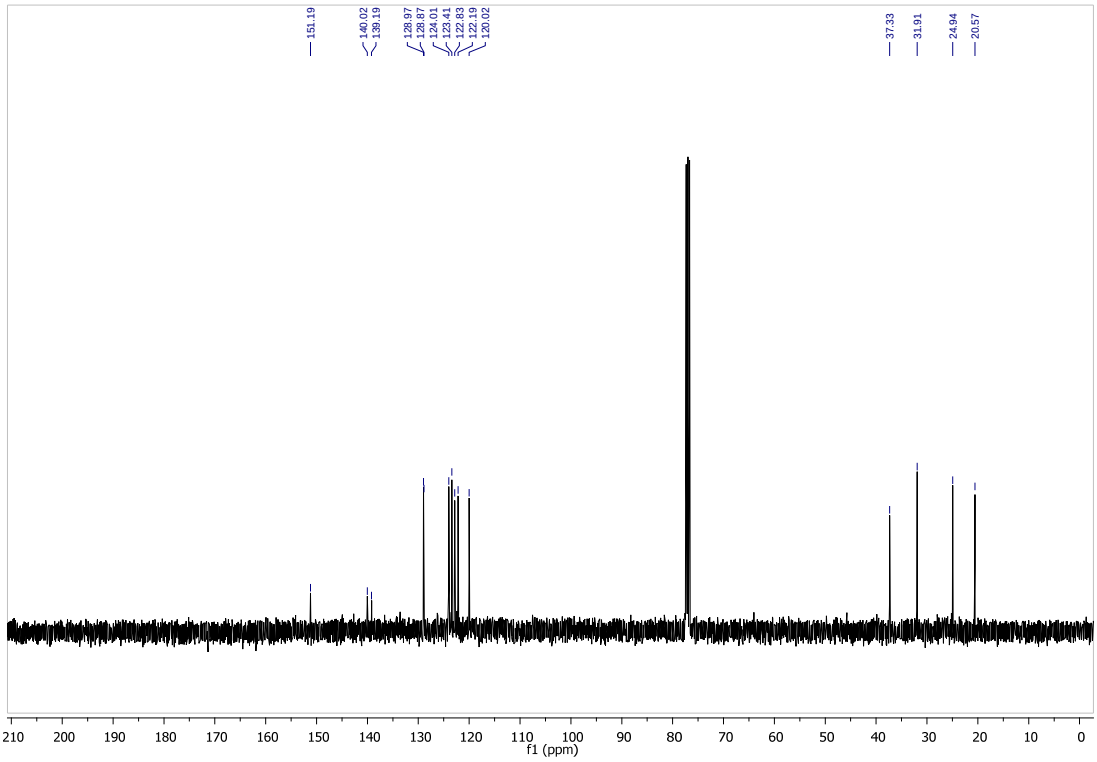
8.05
7.97
7.95
7.61
7.61
7.59
7.57
7.56
7.55
7.54
7.54
7.52
6.34
6.19
6.18
6.16
6.14
4.03
2.40
2.14
2.12
2.11
2.10
2.09
2.09
2.07
1.97
1.96
1.95
1.95
1.94
0.94
1.04
2.80
2.06
1.00
3.45
2.56
1.66
f1 (ppm)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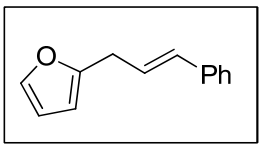
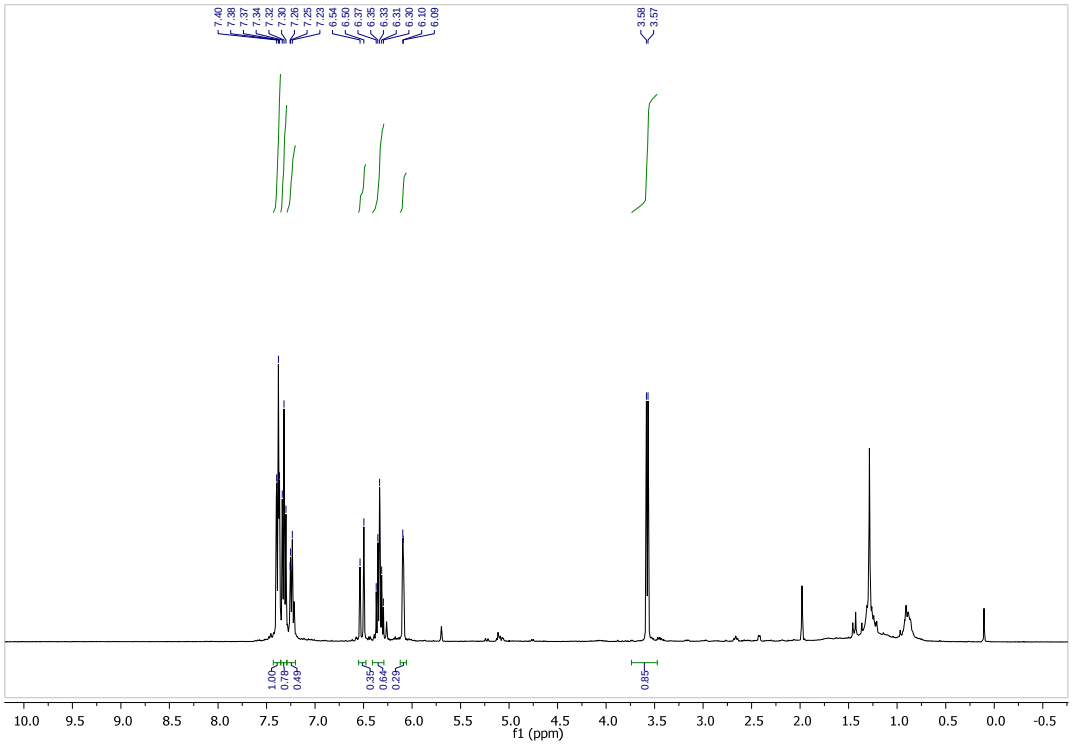
140.02
138.19
128.97
128.87
124.01
123.41
122.83
122.19
120.02
37.33
31.91
24.94
20.57
f1 (ppm)


O
Ph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7.38
7.37
7.34
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7.30
7.26
7.25
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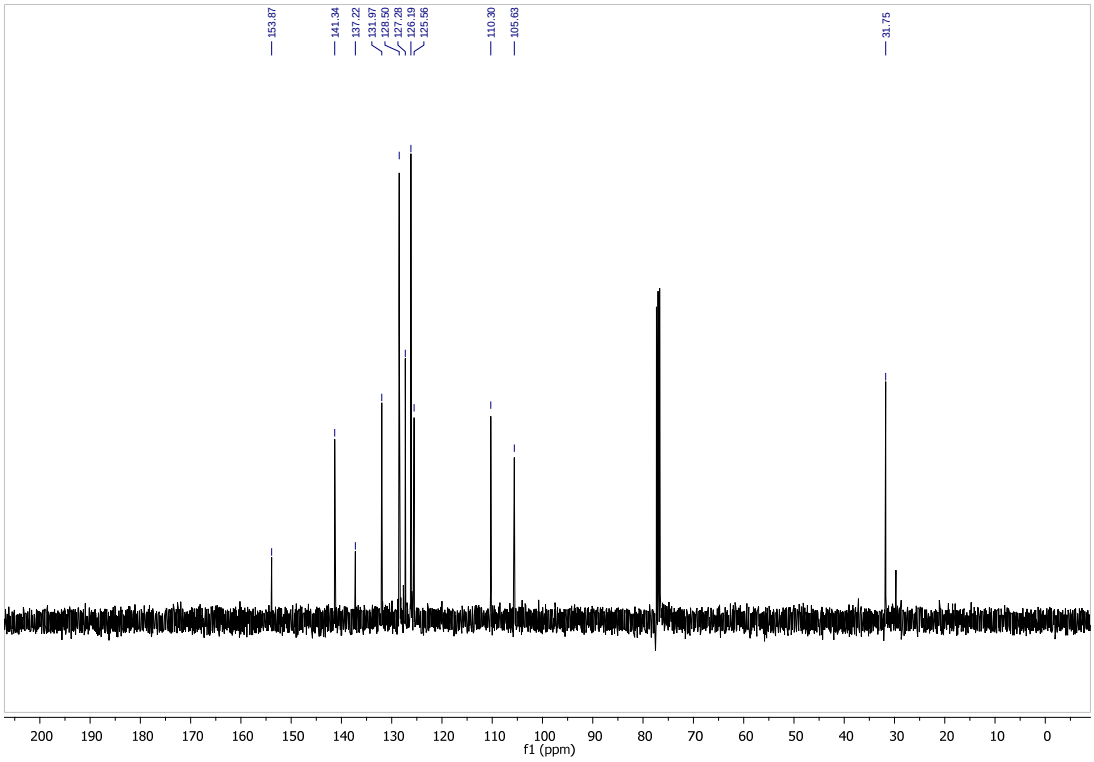
6.54
6.50
6.37
6.35
6.33
6.31
6.30
6.10
6.09
3.58
3.57
1.00
0.78
0.49
0.35
0.64
0.29
0.85
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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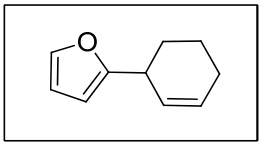
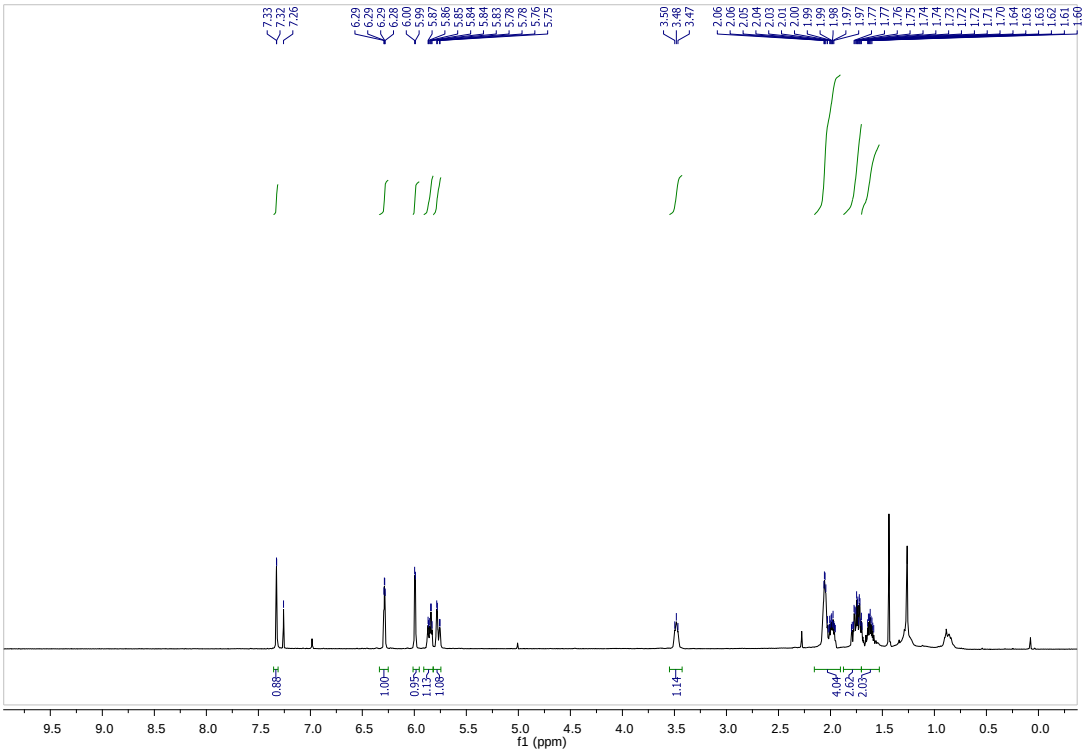
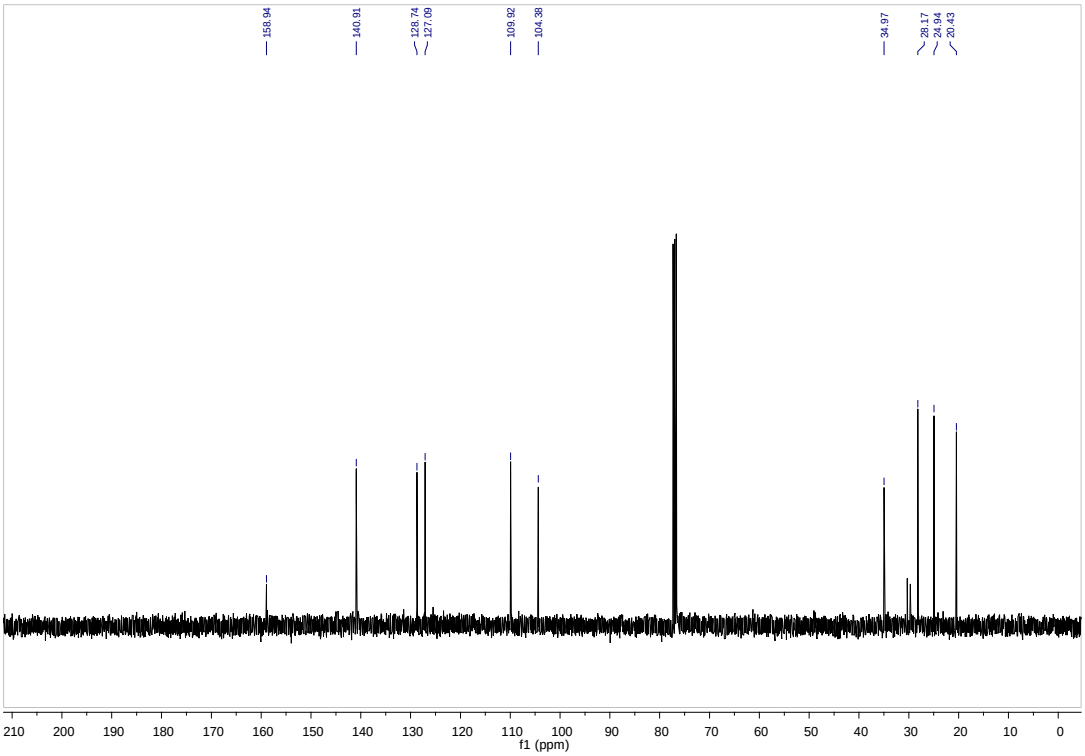
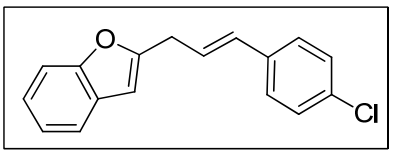
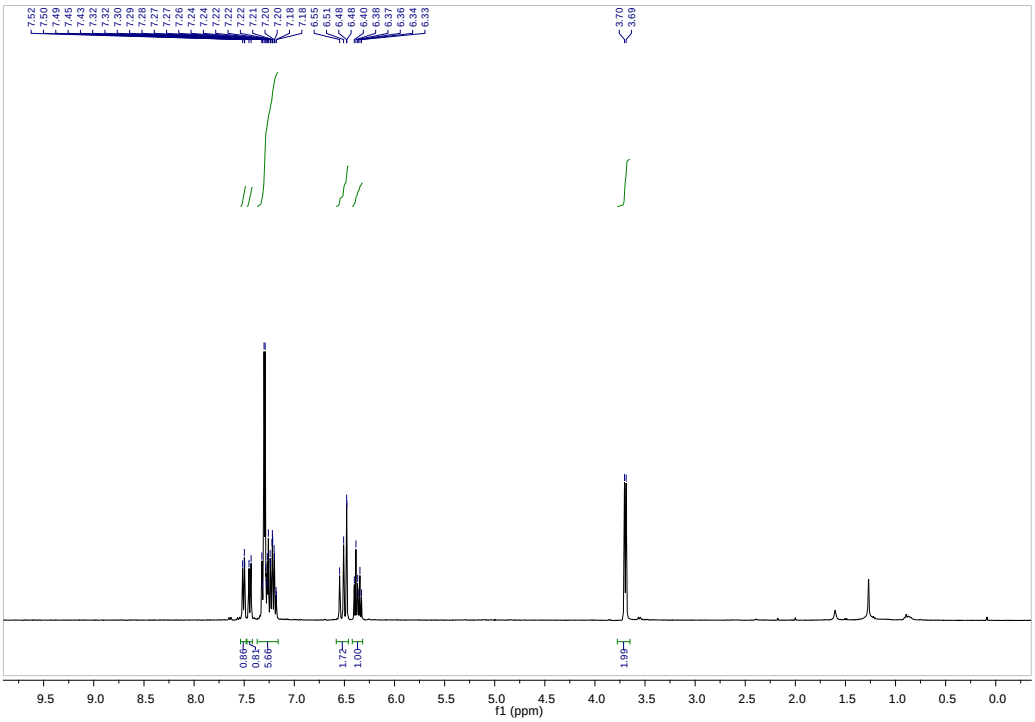
141.34
137.22
131.97
128.50
127.28
126.19
125.56
110.30
105.63
31.75
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

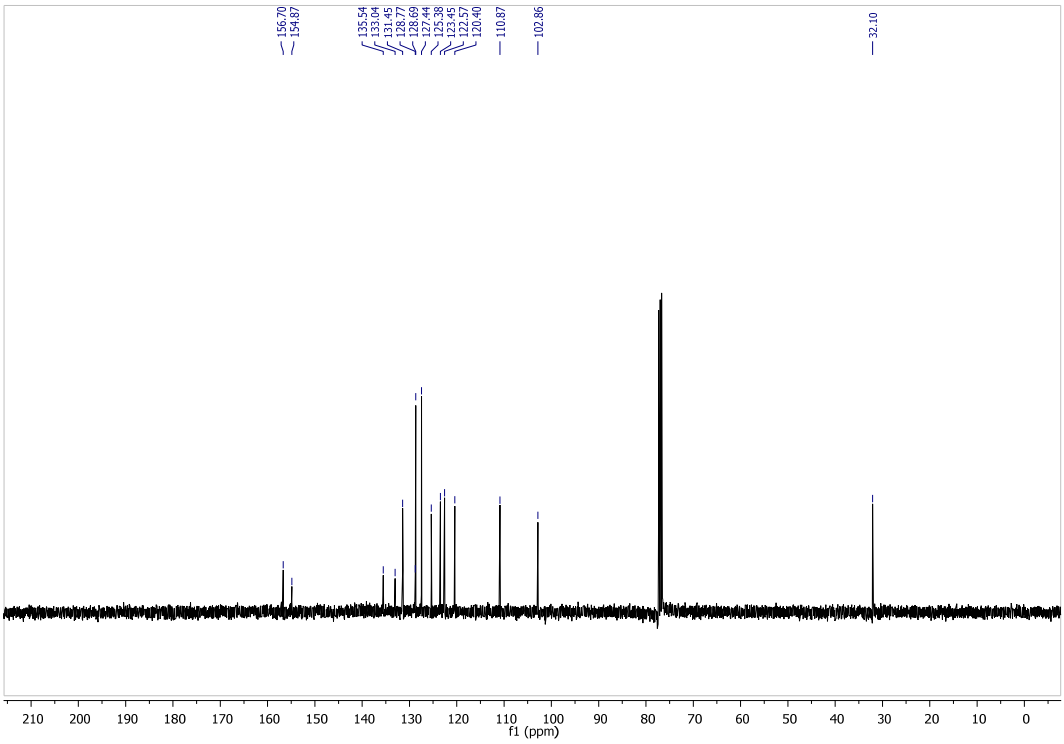



7.33
7.32
7.26
6.29
6.29
6.29
6.28
6.00
5.99
5.87
5.86
5.85
5.84
5.84
5.83
5.78
5.78
5.76
5.75
3.50
3.48
3.47
2.06
2.06
2.05
2.04
2.03
2.01
2.00
1.99
1.99
1.98
1.97
1.97
1.77
1.77
1.76
1.75
1.74
1.74
1.73
1.72
1.72
1.71
1.70
1.64
1.63
1.63
1.62
1.61
1.60
0.88
1.00
0.95
1.13
1.08
1.14
4.04
2.62
2.03
f1 (ppm)


158.94
140.91
128.74
127.09
109.92
104.38
34.97
28.17
26.44
20.43
f1 (ppm)


O
Cl


7.52
7.50
7.49
7.45
7.43
7.32
7.32
7.30
7.29
7.28
7.27
7.27
7.26
7.24
7.24
7.22
7.22
7.22
7.21
7.20
7.20
7.18
6.55
6.51
6.48
6.46
6.40
6.38
6.37
6.36
6.34
6.33
3.70
3.69
0.86
0.81
5.66
1.72
1.00
1.99
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
f1 (ppm)


156.70
154.87
135.54
133.04
131.45
128.77
128.69
127.44
125.38
123.45
122.57
120.40
110.87
102.86
32.10
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)