Synthesis of 1,2,3-Triazole-Fused Heterocycles via Pd-Catalyzed Cyclization of 5-Iodotriazoles

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General Experimental Procedures

The palladium-catalyzed annulation reactions were performed in microwave vials under an atmosphere of nitrogen. All other reactions, unless otherwise indicated, were carried out under ambient atmosphere in single-neck, round bottom flasks fitted with a rubber septum, equipped with a magnetic stir bar. Air- or water-sensitive solvents were transferred via syringe. When required, solvents were degassed by bubbling of nitrogen through a needle. Organic solutions were concentrated by rotary evaporation at 25 – 40 °C under reduced pressure (15 – 30 torr, house vacuum). Analytical Thin Layer Chromatography (TLC) was performed using pre-coated UV 254 plates (0.2 mm) from EM Separations. Visualization was accomplished with a 254 nm UV light source, generally followed by immersion in potassium permanganate ($KMnO_4$) or anisaldehyde solutions, with subsequent heating with a heat gun. Flash chromatography was performed with Silicycle™ Ultra-Pure 230-400 mesh silica gel.

Instrumentation

Melting points (mp) were determined using a Fisher-Johns melting point apparatus. Infrared (IR) spectra were obtained using a Shimadzu FTIR-8400S FT-IR spectrometer on NaCl plates. High resolution mass spectra were obtained from SI2 Micromass 70S-250 mass spectrometer (EI) or an ABI/Sciex Qstar mass spectrometer (ESI). Proton nuclear magnetic resonance spectra (^{1}H NMR) and carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 23 °C with either a Bruker Avance III 400 MHz, Varian Mercury 400 MHz or Varian Mercury 300 MHz NMR spectrometer. Chemical shifts (δ) are expressed in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual NMR solvent ($CDCl_3$: δ 7.26 for ^{1}H NMR and δ 77.0 for ^{13}C NMR). Spectral data are represented in the following order: chemical shift; multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qn = quintuplet, sx = sextet, dd = doublet of doublets, m = multiplet, br = broad); coupling constant (*J*, Hz); number of protons.

Materials

Unless otherwise noted, all reagents, catalysts and ligands were purchased from commercial sources (Sigma-Aldrich, VWR, Alfa Aesar, Strem, Acros or TCI America) and used as received. Tetrahydrofuran and acetonitrile were purified by distillation under nitrogen from Na/benzophenone immediately prior to use. All other solvents were used as supplied without further purification. 4Å molecular sieves (MS) were dried in an oven at 120 °C prior to use.

Iodoalkynes were stored and reacted in the absence of light. All azides were prepared according to literature procedure.[1]

Experimental procedures and characterization data

General procedure A for the synthesis of terminal alkynes

The procedure was adapted from the literature.[2] To a round bottom flask was added the phenol (1 equiv.), followed by acetone (0.3 M). K_2CO_3 (1.3 equiv.) and propargyl bromide (1.2 equiv.) were added, and the heterogeneous mixture was heated to reflux overnight. After TLC analysis had shown complete conversion of the starting materials, the mixture was cooled to room temperature, and then quenched by the addition of sat. aq. NH_4Cl. The resulting mixture was partitioned with Et_2O, the organic layer separated, and the aqueous layer was extracted with Et_2O. The combined organic layers were dried over $MgSO_4$. Concentration under reduced pressure gave the desired target structure. The material was used without further purification.

General procedure B for the synthesis of terminal alkynes

The procedure was adapted from the literature.[3] To a round bottom flask was added the phenol (1 equiv.), followed by MeCN (0.5 M). K_2CO_3 (1.3 equiv.) and propargyl bromide (1.2 equiv.) were added, and the heterogeneous mixture was left stirring at room temperature. After TLC analysis had shown complete conversion of the starting materials, the mixture was quenched by the addition of sat. aq. NH_4Cl. The resulting mixture was partitioned with Et_2O, the organic layer separated, and the aqueous layer was extracted with Et_2O. The combined organic layers were dried over $MgSO_4$. Concentration under reduced pressure gave the desired target structure. The material was used without further purification.

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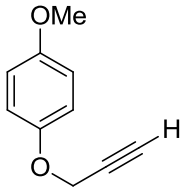
[1] Buckle, D. R.; Rockell, C. J.M. J. Chem. Soc., Perkin Trans. 1, **1982**, 627.

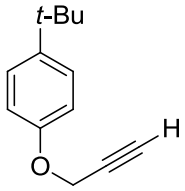
[2] Banday, A. H.; Shameem, S. A.; Gupta, B. D.; Kumar, H. M. S. *Steroids* **2010**, *75*, 801.

[3] Gomtsyan, A.; Bayburt, E. K.; Schmidt, R. G.; Lee, C.-H.; Brown, B. S.; Jinkerson, T. K.; Koenig, J. R.; Daanen, J. F.; Latshaw, S. P. US Patent 12,868, 2006.



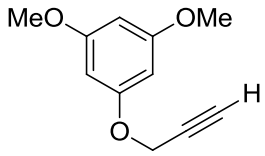
1-methoxy-4-(prop-2-yn-1-yloxy)benzene (S1).

According to general procedure A, the corresponding phenol (4.00 g, 32.2 mmol), propargyl bromide (4.30 mL, 48.3 mmol, 80% in toluene) and K_2CO_3 (7.13 g, 51.6 mmol) were reacted in acetone (120 mL) under reflux for 20 hours. Subsequent workup yielded **S1** as a brown oil (3.69 g, 71%). Characterization data were consistent with the literature.[4]



1-(tert-butyl)-4-(prop-2-yn-1-yloxy)benzene (S2).

According to general procedure A, the corresponding phenol (1.95 g, 13.0 mmol), propargyl bromide (1.72 mL, 16.0 mmol, 80% in toluene) and K_2CO_3 (2.40 g, 17.4 mmol) were reacted in acetone (50 mL) under reflux. Analysis by TLC after 24 hours suggested incomplete conversion of starting material, so additional propargyl bromide (0.43 mL, 4.0 mmol, 80% in toluene) was added. TLC after 55 hours showed complete consumption of starting material. Subsequent workup yielded **S2** as a yellow-orange oil (2.28 g, 93 %). Characterization data were consistent with the literature.[5]



1,3-dimethoxy-5-(prop-2-yn-1-yloxy)benzene (S3).

According to general procedure A, the corresponding phenol (1.96 g, 12.7 mmol), propargyl bromide (1.68 mL, 15.6 mmol, 80% in toluene) and K_2CO_3 (2.35 g, 17.0 mmol) were reacted in

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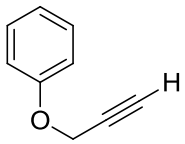
[4] Efe, C.; Lykakis, I. N.; Stratakis, M. *Chem. Commun.*, **2011**, *47*, 803.

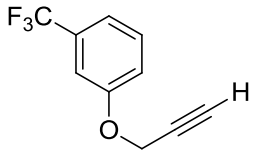
[5] Howell, S. J.; Spencer, N.; Douglas, P. *Tetrahedron* **2001**, *57*, 4945.

acetone (50 mL) under reflux for 20 hours. Subsequent workup yielded **S3** as an orange solid (2.45 g, 99%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 6.16 (d, *J* = 2.1 Hz , 2H), 6.13 (t, *J* = 2.1 Hz, 1H), 4.65 (d, *J* = 2.4 Hz, 2H), 3.77 (s, 6H), 2.53 (t, *J* = 2.4 Hz, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 161.6, 159.6, 93.9, 78.6, 75.7, 56.0, 55.5. **IR** (cm^{-1}, film) = 3290, 3241, 3012, 2961, 2842, 2123, 1597, 1478, 1378, 1208, 1154, 1065, 953, 810, 738, 675. **mp** = 37 – 39 °C. **HRMS** (ESI): Calc'd for $C_{11}H_{12}O_3^+$, 193.0865; found, 193.0860.



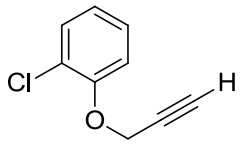
(prop-2-yn-1-yloxy)benzene (S4).

According to general procedure A, the corresponding phenol (1.51 g, 16.0 mmol), propargyl bromide (2.20 mL, 20.4 mmol, 80% in toluene) and K_2CO_3 (2.87 g, 20.8 mmol) were reacted in acetone (60 mL) under reflux overnight. Analysis by TLC the next morning suggested incomplete conversion of starting material, so additional propargyl bromide (0.35 mL, 3.25 mmol, 80% in toluene) was added. TLC after 48 hours still indicated starting material, so an additional 0.35 mL portion of propargyl bromide was added. TLC after 90 hours showed complete consumption of starting material.Subsequent workup yielded **S4** as a yellow-orange oil (1.34 g, 64 %). Characterization data were consistent with the literature.[4]



1-(prop-2-yn-1-yloxy)-3-(trifluoromethyl)benzene (S5).

According to general procedure B, the corresponding phenol (1.01 g, 6.2 mmol), propargyl bromide (0.80 mL, 7.4 mmol, 80% in toluene) and K_2CO_3 (1.10 g, 8.0 mmol) were reacted in MeCN (12 mL) at room temperature for 5 days. Subsequent workup yielded **S5** as a yellow-orange oil (757 mg, 60 %). Characterization data were consistent with the literature.[3]

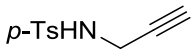


1-chloro-2-(prop-2-yn-1-yloxy)benzene (S6).

According to general procedure A, the corresponding phenol (1.19 g, 9.26 mmol), propargyl bromide (1.20 mL, 11.1 mmol, 80% in toluene) and K_2CO_3 (1.55 g, 11.2 mmol) were reacted in acetone (30 mL) under reflux overnight. Subsequent workup yielded **S6** as an amber oil (1.36 g, 88 %). Characterization data were consistent with the literature.[6]

General procedure for the protection of propargylamine

The procedure was adapted from literature.[7] To a round bottom flask containing a stirring solution of DCM (0.3 M) and *p*-toluenesulfonyl chloride (1 equiv.) was added propargylamine (1 equiv.), followed by Et_3N (2.2 equiv.) The reaction mixture was stirred at room temperature. After TLC analysis had shown complete conversion of the starting materials, the reaction mixture was diluted with DCM and washed with 1 M HCl. The combined organic layers were dried over $MgSO_4$. Concentration under reduced pressure gave the desired target structure. The material was used without further purification.



4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide (S7).

According to the general procedure, propargylamine (1.40 mL, 20.4 mmol), *p*-toluenesulfonyl chloride (3.82 g, 20.0 mmol) and Et_3N (6.00 mL, 44.0 mmol) were reacted in DCM (80 mL) at

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[6] Dinges, J.; Albert, D. H.; Arnold, L. D.; Ashworth, K. L.; Akritopouluo-Zance, I.; Bousquet, P. F.; Bouska, J. J.; Cunha, G. A.; Davidsen, S. K.; Diaz, G. J.; Djuric, S. W.; Gasiecki, A. F.; Gintant, G. A.; Gracias, V. J.; Harris, C. M.; Houseman, K. A.; Hutchins, C. W.; Johnson, E. F.; Li, H.; Marcotte, P. A.; Martin, R. L.; Michaelides, M. R.; Nyein, M.; Sowin, Z. S.; Tapang, P. H.; Xia, Z.; Zhang, H. Q.; *J. Med. Chem.* **2007**, *50*, 2011.

[7] Lo, M. M.-C.; Neumann, C. S.; Nagayama, S.; Perlstein, E. O.; Schreiber, S. L. *J. Am. Chem. Soc.* **2004**, 126, 16077.

room temperature for 20 hours. Subsequent workup yielded **S7** as an orange solid (4.06 g, 97 %). Characterization data were consistent with the literature.[8]

General procedure A for the synthesis of iodoalkynes

The procedure was adapted from literature.[9] To a round bottom flask containing 4 Å MS (~10 pieces), CuI (5 mol%) and *N*-iodomorpholine (1.2 equiv.) were added and dissolved in THF (0.1 M). The terminal alkyne (1 equiv.) was added and the reaction mixture was allowed to stir in the dark at room temperature. After TLC analysis had shown complete conversion of the starting materials, sat. aq. NH_4Cl was added and the mixture was extracted with Et_2O. The combined organic layers were washed with sat. aq. $Na_2S_2O_3$ solution and brine, and dried over $MgSO_4$. Concentration under reduced pressure gave the desired target structure. The material was used without further purification.

General procedure B for the synthesis of iodoalkynes

The procedure was adapted from literature.[10] In a round bottom flask, the propargyl species (1 equiv.) was dissolved in MeOH (0.7 M). A solution of KOH (3.5 equiv.) in H_2O (100 mL per mol of KOH) was cooled to 0 °C and added to the stirring reaction mixture. I_2 (0.9 equiv.) was added in one portion, and the solution was stirred at room temperature overnight. After TLC analysis had shown complete conversion of the starting materials, the reaction mixture was neutralized with 1M HCl and extracted with Et_2O. The combined organic layers were washed with sat. aq. $Na_2S_2O_3$ solution, and dried over Na_2SO_4. Concentration under reduced pressure gave the desired target structure. The material was used without further purification.

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[8] Ince, J.; Ross, T. M.; Shipman, M.; Slawin, A. M. Z.; Ennis, D. S. *Tetrahedron* **1996**, *52*, 7037.

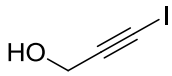
[9] Hein, J. E.; Tripp, J. C.; Krasnova, L. B.; Sharpless, K. B.; Fokin, V. V. *Angew. Chem., Int. Ed*. **2009**, *48*, 8018.

[10] Jahnke, E; Weiss, J.; Neuhaus, S; Hoheisel, T. N.; Frauenrath, H. *Chem. Eur. J.* **2009**, *15*, 388.

General procedure C for the synthesis of iodoalkynes

Method A: The procedure was adapted from literature.[11] To a round bottom flask containing a stirring solution of allyl bromide (1 equiv.) and iodopropargyl alcohol (1.25 equiv.) was added dropwise an aqueous solution of KOH (1.25 equiv.) in water (4 M) at 0 °C over 10 minutes. After the addition was completed, external cooling was removed and the reaction mixture was stirred under reflux. After TLC analysis had shown complete conversion of the starting materials, the reaction mixture was cooled and extracted with Et_2O. The combined organic layers were washed with water, and dried over Na_2SO_4. Concentration under reduced pressure gave the desired target structure. The material was used without further purification.

Method B: The procedure was adapted from literature.[12] To a round bottom flask containing a stirring solution of iodoalkyne (1 equiv.) and anhydrous K_2CO_3 (4 equiv.) in MeCN (0.1 M) was added dropwise allyl bromide (2 equiv.). After the addition was completed, the reaction mixture was heated to reflux overnight. After TLC analysis had shown complete conversion of the starting materials, the reaction mixture was cooled and the MeCN was removed *in vacuo*. $NaHCO_3$ was added to the residue and the aqueous solution was extracted with DCM. The combined organic layers were dried over $MgSO_4$ and concentrated under reduced pressure to yield the crude product. Purification by flash chromatography yielded the desired target structure.



3-iodoprop-2-yn-1-ol (S8).

According to general procedure B, propargyl alcohol (1.03 mL, 17.8 mmol) was dissolved in MeOH (25 mL) in a round bottom flask. A solution of KOH (3.50 g, 62.4 mmol) in H_2O (6 mL) was cooled to 0 °C and added to the stirring reaction mixture. I_2 (4.08 g, 16.1 mmol) was added in one portion, and the solution was stirred at room temperature for 24 hours. Subsequent workup yielded **S8** as a slightly orange solid (1.60 g, 49%). Characterization data were consistent with the literature.[10]

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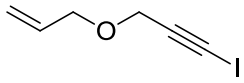
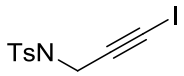
[11] Pandey, G.; Sekhar, B. B. V. S. *Tetrahedron* **1995**, *51*, 1483.

[12] Sylvester, K. T.; Chirik, P. J. *J. Am. Chem. Soc.* **2009**, 131, 8772.



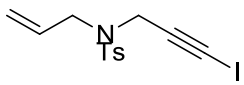
3-((3-iodoprop-2-yn-1-yl)oxy)prop-1-ene (S9).

According to method A of general procedure C, iodoalkyne **S8** (5.12 g, 28.2 mmol), allyl bromide (1.95 mL, 22.5 mmol) and an aqueous solution of KOH (1.59 g, 28.4 mmol) in water (7 mL) were reacted under reflux for 17 hours. Subsequent workup yielded **S9** as an orange oil (5.15 g, 83%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.83 – 5.96 (m, 1H), 5.31 (dq, *J* = 17.2, 4.4, 1.6 Hz, 1H), 5.23 (ddd, *J* = 10.4, 2.6, 1.2 Hz, 1H), 4.31 (s, 1H), 4.06 (dt, *J* = 5.8, 1.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 133.8, 118.1, 90.5, 70.8, 58.7, 2.8. **IR** (cm^{-1}, neat): 3080, 2852, 2185, 1647, 1438, 1425, 1350, 1264, 1248, 1078, 1026, 987, 931. **HRMS** (ESI): Calc'd for $C_6H_{11}NOI^+$, 239.98853; found, 239.98835.



N-(3-iodoprop-2-yn-1-yl)-4-methylbenzenesulfonamide (S10).

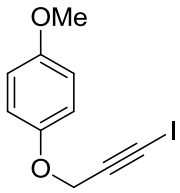
According to general procedure B, propargylamine **S7** (2.09 g, 10.0 mmol) was dissolved in MeOH (14 mL) in a round bottom flask. A solution of KOH (1.99 g, 35.4 mmol) in H_2O (3 mL) was cooled to 0 °C and added to the stirring reaction mixture. I_2 (2.58 g, 10.2 mmol) was added in one portion, and the solution was stirred at room temperature for 26 hours. Subsequent workup yielded **S10** as a yellow solid (2.81 g, 84%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.76 (d, *J* = 8.3 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 3.99 (d, *J* = 6.3 Hz, 2H), 2.44 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 142.4, 135.0, 128.2, 128.2, 125.9, 125.9, 86.5, 33.2, 20.1, 0.0. **IR** (cm^{-1}, neat): 3271, 1597, 1429, 1318, 1155, 1090, 1069, 989, 811, 647, 559, 536. **mp** = 143 – 145 °C. **HRMS** (ESI): Calc'd for $C_{10}H_{11}NO_2SI^+$, 335.95552; found, 335.95582.



N-allyl-N-(3-iodoprop-2-yn-1-yl)-4-methylbenzenesulfonamide (S11).

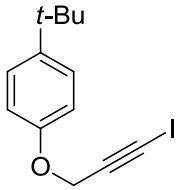
According to method B of general procedure C, iodoalkyne **S10** (1.50 g, 4.5 mmol), allyl bromide (1.08 g, 9.0 mmol) and K_2CO_3 (2.47 g, 17.9 mmol) were reacted in MeCN (47 mL) under reflux for 17 hours. Subsequent workup and flash column chromatography (gradient

petane:EtOAc 95:5 to 8:2) yielded **S11**. Due to major purification difficulties, the compound was carried on to the next step and fully characterized after the cycloaddition.



1-((3-iodoprop-2-yn-1-yl)oxy)-4-methoxybenzene (S12).

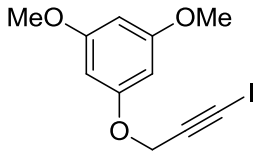
According to general procedure A, terminal alkyne **S1** (497 mg, 3.1 mmol), *N*-iodomorpholine (1.58 g, 4.6 mmol) and CuI (30 mg, 0.2 mmol) were reacted in the presence of 4 Å MS in THF (51 mL) in the dark at room temperature for 26 hours. Subsequent workup yielded **S12** as a dark brown oil (798 mg, 90%). Characterization data were consistent with the literature.[13]



1-(tert-butyl)-4-((3-iodoprop-2-yn-1-yl)oxy)benzene (S13).

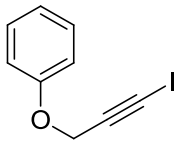
According to general procedure A, terminal alkyne **S2** (1.05 g, 5.6 mmol), *N*-iodomorpholine (3.62 g, 10.6 mmol) and CuI (57 mg, 0.3 mmol) were reacted in the presence of 4 Å MS in THF (90 mL) in the dark at room temperature overnight. Subsequent workup yielded **S13** as an amber oil (1.68 g, 96 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.36 (dd, *J* = 6.7 Hz, & 2.1 Hz, 2H), 6.93 (dd, *J* = 6.7 Hz, & 2.1 Hz, 2H), 4.83 (s, 2H), 1.35 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 155.4, 144.4, 126.4, 114.4, 89.5, 57.5, 34.2, 31.6, 4.8. **IR** (cm^{-1}, neat) = 2962, 2904, 2867, 2188, 1609, 1511, 1363, 1297, 1261, 1222, 1184, 1120, 1039, 982, 828. **HRMS** (ESI [M+NH_4^+]): Calc'd for $C_{13}H_{19}IN_1O_1^+$, 332.0511; found, 332.0512.

[13] Masters, K.-S.; Flynn, B. L.; *J. Org. Chem.* **2008**, *73*, 8081.



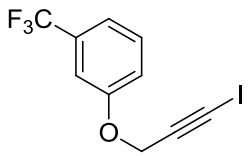
1-((3-iodoprop-2-yn-1-yl)oxy)-3,5-dimethoxybenzene (S14).

According to general procedure A, terminal alkyne **S3** (1.00 g, 5.2 mmol), *N*-iodomorpholine (2.66 g, 7.8 mmol) and CuI (57 mg, 0.3 mmol) were reacted in the presence of 4 Å MS in THF (80 mL) in the dark at room temperature for 4 days. Subsequent workup yielded **S14**. Due to major purification difficulties, the compound was carried on to the next step and fully characterized after the cycloaddition.



((3-iodoprop-2-yn-1-yl)oxy)benzene (S15).

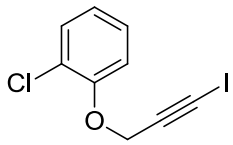
According to general procedure A, terminal alkyne **S4** (496 mg, 3.8 mmol), *N*-iodomorpholine (1.96 g, 5.8 mmol) and CuI (52 mg, 0.3 mmol) were reacted in the presence of 4 Å MS in THF (60 mL) in the dark at room temperature. TLC indicated some starting material left after 2 days, so additional *N*-iodomorpholine (151 mg, 0.4 mmol) and CuI (38 mg, 0.2 mmol) was added. TLC indicated complete consumption of starting material after an additional 3 days. Subsequent workup yielded **S15** as an amber oil (966 mg, 99%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.31 (m, 2H), 6.98 (m, 3H), 4.83 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 157.7, 129.7, 121.7, 115.0, 89.3, 57.4, 4.7. **IR** (cm^{-1}, neat) = 3063, 2914, 2858, 2189, 1598, 1587, 1496, 1489, 1372, 1366, 1303, 1212, 1173, 1080, 1042, 979, 884, 753, 690. **HRMS** (ESI): Calc'd for $C_9H_8IO^+$, 258.9620; found, 258.9624.



1-((3-iodoprop-2-yn-1-yl)oxy)-3-(trifluoromethyl)benzene (S16).

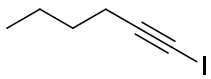
According to general procedure A, terminal alkyne **S5** (500 mg, 2.5 mmol), *N*-iodomorpholine (1.31 g, 3.8 mmol) and CuI (49 mg, 0.3 mmol) were reacted in the presence of 4 Å MS in THF (25 mL) in the dark at room temperature. TLC indicated some starting material left after 2 days,

so additional *N*-iodomorpholine (432 mg, 1.3 mmol) was added. TLC indicated complete consumption of starting material after an additional 1 day. Subsequent workup yielded **S16** as a red-brown oil (724 mg, 89%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.42 (t, *J* = 8.0 Hz, 1H), 7.26 (m, 1H), 7.19 (s, 1H), 7.14 (dd, *J* = 8.2 Hz & 2.5 Hz, 1H), 4.87 (s, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 157.7, 132.1 (q, *J* = 32.3 Hz), 130.2, 124.0 (q, *J* = 272.5 Hz), 118.5 (m), 118.3, 112.2, 88.5, 57.7, 5.8. **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -63.74. **IR** (cm^{-1}, film) = 3080, 2959, 2918, 2863, 2191, 1593, 1492, 1450, 1368, 1326, 1294, 1216, 1169, 1122, 1041, 882, 868, 794, 741, 696. **HRMS** (ESI): Calc'd for $C_{10}H_7F_3IO^+$, 326.9494; found, 326. 9486.



1-chloro-2-((3-iodoprop-2-yn-1-yl)oxy)benzene (S17).

According to general procedure A, terminal alkyne **S6** (517 mg, 3.1 mmol), *N*-iodomorpholine (1.54 g, 4.5 mmol) and CuI (38 mg, 0.2 mmol) were reacted in the presence of 4 Å MS in THF (40 mL) in the dark at room temperature. TLC indicated some starting material left after 4 days, so additional *N*-iodomorpholine (542 mg, 1.6 mmol) was added. TLC indicated complete consumption of starting material after an additional 1 day. Subsequent workup yielded **S17** as a yellow oil (902 mg, 99 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.39 (dd, *J* = 7.9 Hz & 1.6 Hz, 1H), 7.24 (m, 1H), 7.07 (dd, *J* = 8.3 Hz & 1.3 Hz, 1H), 6.95 (td, *J* = 7.7 Hz & 1.3 Hz, 1H), 4.91 (s, 2H). **^{13}C NMR** (100MHz, $CDCl_3$): δ = 153.3, 130.6, 127.8, 122.6, 114.6, 88.7, 58.5, 5.8. **IR** (cm^{-1}, film) = 3066, 2917, 2959, 2862, 2850, 2190, 1587, 1482, 1447, 1372, 1297, 1278, 1229, 1062, 1043, 1031, 982, 747. **HRMS** (ESI [$M+NH_4^+$]): Calc'd for $C_9H_{10}ClINO^+$, 309.9496; found, 309.9487.



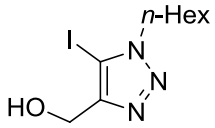
1-iodohex-1-yne (S18).

According to general procedure A, 1-hexyne (1.39 mL, 12.1 mmol), *N*-iodomorpholine (4.95 g, 14.5 mmol) and CuI (0.12 g, 0.6 mmol) were reacted in the presence of 4 Å MS in THF (200

mL) in the dark at room temperature for 28 hours. Subsequent workup yielded **S18** as a yellow oil (1.87 g, 74%). Characterization data were consistent with the literature.[14]

General procedure for the synthesis of 5-iodo-1,2,3-triazoles

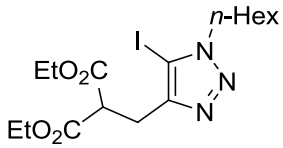
The procedure was adapted from literature.[9] CuI (0.1 equiv.) and TBTA (0.1 equiv.) were dissolved in THF (4.5 mL per mol of iodoalkyne) and stirred at room temperature for 20 minutes, after which a clear homogeneous solution was obtained. The iodoalkyne (1 equiv.) and the azide (1 equiv.) were dissolved in THF (0.5 mL per mol of iodoalkyne) and added to the catalyst solution. The reaction mixture was stirred at room temperature until TLC analysis had shown complete conversion of the starting materials. The solution was quenched with 10% NH_4OH and the volatile components were removed *in vacuo*. The resulting residue was extracted with DCM, washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure to yield the crude product. Purification by flash chromatography yielded the desired target structure.



(1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methanol (S19).

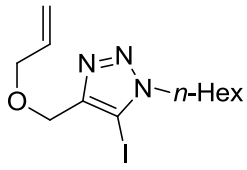
According to the general procedure, iodoalkyne **S8** (5.9 g, 32.6 mmol), *n*-hexylazide (5.0 g, 38.0 mmol), CuI (140 mg, 0.7 mmol) and TBTA (400 mg, 0.8 mmol) were reacted in THF (150 mL) at room temperature for 16 hours. Subsequent workup and flash column chromatography (gradient petane:EtOAc 6:4 to 1:1) yielded **S19** as an off-white solid (9.2 g, 84%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 4.73 (s, 4H), 4.37 (t, J = 7.34 Hz, 2H), 1.95–1.82 (m, 3H), 1.42 – 1.25 (m, 6H), 0.89 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 150.9, 78.7, 56.4, 50.9, 31.2, 29.9, 26.1, 22.5, 14.0. **IR** (cm^{-1}, neat): 3249, 2953, 2929, 2858, 1469, 1447, 1224, 1208, 1114, 1079, 1070, 1020. **mp** = 74 – 76 °C. **HRMS** (ESI): Calc'd for $C_9H_{17}N_3OI^+$, 310.0410; found, 310.0414.

[14] Usanov, D. L.; Yamamoto, H. *J. Am. Chem. Soc.* **2011**, *133*, 1286.



diethyl 2-((1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methyl)malonate (S20).

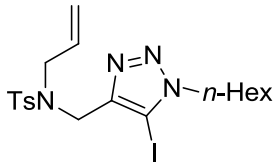
A solution of **S19** (1.24 g, 4 mmol) and Et_3N (0.56 mL, 4 mmol) in THF (7 mL) was cooled to 0 ^oC in an ice bath. Methanesulfonyl chloride (0.31 mL, 4 mmol) was added dropwise to the solution, which was allowed to warm up to room temperature thereafter. After 30 minutes at room temperature the reaction mixture was filtered through celite, washed with THF (6 mL), and was added to a solution of sodium diethyl malonate (4.4 mmol) at 0 $^{\circ}C$ (Note 1). The reaction was allowed to warm to room temperature and reacted for 16 hours. The reaction was quenched with aq. NH_4Cl, extracted with EtOAc, and dried over Mg_2SO_4. Concentration under reduced pressure gave the crude product. Purification by flash chromatography (gradient pentane:EtOAc 9:1 to 8:2) yielded **S20** as a colorless oil (902 mg, 50% yield). **Note 1:** Sodium malonate solution was prepared as follows: To a solution of diethyl malonate (0.67 mL, 4.4 mmol) in THF (7 mL) at 0 $^{\circ}C$ was added sodium hydride (220 mg, 5.5 mmol) in batches over 5 minutes. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 4.30 (t, *J* = 7.4 Hz, 2H), 4.24 – 4.08 (m, 4H), 4.00 (t, *J* = 7.7 Hz, 1H), 3.21 (d, *J* = 7.7 Hz, 2H), 1.94 – 1.76 (m, 2H), 1.34 – 1.26 (m, 6H), 1.22 (t, *J* = 7.1 Hz, 6H), 0.86 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 168.7, 148.2, 78.9, 61.7, 50.9, 31.2, 29.9, 26.1, 25.4, 22.5, 14.1, 14.0. **IR** (cm^{-1}, neat): 2956, 2918, 2871, 2857, 1750, 1739, 1722, 1448, 1370, 1332, 1231, 1155, 1097, 1053, 1034. **HRMS** (ESI): Calc'd for $C_{16}H_{27}IN_3O_4^+$, 452.1046; found, 452.1050.



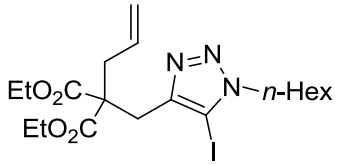
4-((allyloxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (1a).

According to the general procedure, iodoalkyne **S9** (1.50 g, 6.8 mmol), *n*-hexylazide (859 mg, 6.8 mmol), CuI (129 mg, 0.7 mmol) and TBTA (359 mg, 0.7 mmol) were reacted in THF (34 mL) at room temperature for 48 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **1a** as an off-white solid (1.87 g, 79%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.88 – 6.01 (m, 1H), 5.34 (ddd, *J* = 17.2, 4.8, 1.6 Hz, 1H), 5.22 (ddd, *J* = 10.4, 2.8, 1.2 Hz,

1H), 4.57 (s, 2H), 4.36 (t, *J* = 7.6 Hz, 2H), 4.07 (dt, *J* = 5.7, 1.4 Hz, 2H), 1.83 – 1.97 (m, 2H), 1.24 – 1.42 (m, 6H), 0.89 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 148.3, 134.3, 117.7, 79.9, 71.4, 63.2, 50.8, 31.2, 29.9, 26.1, 22.4, 14.0. **IR** (cm^{-1}, neat): 2931, 2858, 1453, 1331, 1221, 1089, 1058, 1010, 924, 792, 718. **mp** = 24 – 25 °C. **HRMS** (ESI): Calc'd for $C_{12}H_{21}N_3OI^+$, 350.0723; found, 350.0724.

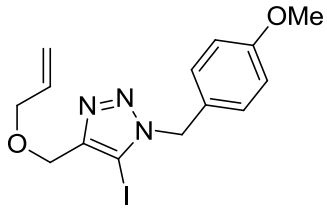


N-allyl-N-((1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methyl)-4-methylbenzenesulfonamide (1b). According to the general procedure, iodoalkyne **S11** (497 mg, 1.3 mmol), *n*-hexylazide (170 mg, 1.3 mmol), CuI (26 mg, 0.1 mmol) and TBTA (71 mg, 0.1 mmol) were reacted in THF (6.7 mL) at room temperature for 72 hours. Subsequent workup and flash column chromatography (gradient petane:EtOAc 8:2 to 6:4) yielded **1b** as an off-white solid (561 mg, 84%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.69 (d, *J* = 8.4 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 5.55 – 5.67 (m, 1H), 5.14 (dd, *J* = 17.1, 1.4 Hz, 1H), 5.06 (dd, *J* = 10.1, 1.3 Hz, 1H), 4.45 (s, 2H), 4.31 (t, *J* = 7.4 Hz, 2H), 3.87 (d, *J* = 6.3 Hz, 2H), 2.41 (s, 3H), 1.79 – 1.90 (m, 2H), 1.26 – 1.39 (m, 6H), 0.89 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 146.2, 143.3, 136.7, 132.5, 129.6, 127.4, 119.0, 79.9, 50.7, 50.1, 42.2, 31.1, 29.9, 26.0, 22.4, 21.5, 14.0. **IR** (cm^{-1}, neat): 2930, 2859, 1597, 1449, 1347, 1159, 1092, 1043, 902, 815, 757, 668, 547. **mp** = 81 – 82 °C. **HRMS** (ESI): Calc'd for $C_{19}H_{28}N_4O_2SI^+$, 503.09776; found, 503.09706.



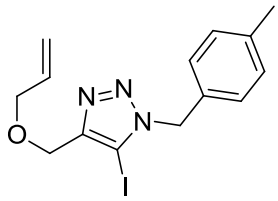
diethyl 2-allyl-2-((1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methyl)malonate (1c). A solution of diethyl **S20** (226 mg, 0.5 mmol) in THF (5 mL) was cooled to 0 °C in an ice bath. Sodium hydride (50 mg, 2.1 mmol) was added in a single portion. After stirring at 0 °C for 20 minutes, allyl bromide (0.065 mL, 0.8 mmol) was added and the reaction was allowed to warm to room temperature and stirred overnight. The mixture was quenched with aq. NH_4Cl, extracted with EtOAc, and dried over Mg_2SO_4. Concentration under reduced pressure gave the crude

product. Purification by flash chromatography (pentane:EtOAc 9:1) yielded **1c** as a colorless oil (180 mg, 73% yield). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.80 (dq, *J* = 9.8, 7.4 Hz, 1H), 5.10 (d, *J* = 11.1 Hz, 1H), 5.06 (d, *J* = 3.7 Hz, 1H), 4.28 (t, *J* = 7.3 Hz, 2H), 4.24 – 4.09 (m, 4H), 3.23 (s, 2H), 2.68 (d, *J* = 7.4 Hz, 2H), 1.89 – 1.75 (m, 2H), 1.32 – 1.24 (m, 6H), 1.21 (t, *J* = 7.1 Hz, 6H), 0.83 (t, *J* = 6.5 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 170.4, 147.0, 132.7, 119.4, 80.4, 61.5, 57.7, 50.8, 36.4, 31.1, 29.8, 28.4, 26.0, 22.4, 14.1, 13.9. **IR** (cm^{-1}, neat): 3078, 2979, 2956, 2919, 2871, 2858, 1747, 1732, 1720, 1641, 1464, 1445, 1367, 1287, 1190, 1065, 1037, 1011, 922, 862. **HRMS** (ESI): Calc'd for $C_{19}H_{31}IN_3O_4^+$, 492.13592; found, 492.13657.



4-((allyloxy)methyl)-5-iodo-1-(4-methoxybenzyl)-1H-1,2,3-triazole (1d).

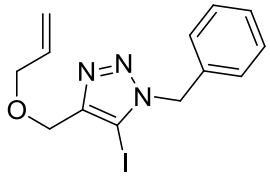
According to the general procedure, iodoalkyne **S9** (112 mg, 0.5 mmol), *p*-methoxybenzylazide (84 mg, 0.5 mmol), CuI (10 mg, 0.05 mmol) and TBTA (27 mg, 0.05 mmol) were reacted in THF (2.5 mL) at room temperature for 25 hours. Subsequent workup and flash column chromatography (pentane:EtOAc 8:2) yielded **1d** as an off-white solid (116 mg, 60%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.22 – 7.29 (m, 2H), 6.83 – 6.90 (m, 2H), 5.87 – 5.98 (m, 1H), 5.52 (s, 2H), 5.32 (ddd, *J* = 17.4, 5.0, 1.8 Hz, 1H), 5.20 (ddd, *J* = 10.4, 4.0, 1.6 Hz, 1H), 4.55 (s, 2H), 4.05 (dt, *J* = 5.7, 1.4 Hz, 2H), 3.79 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 159.8, 148.8, 134.3, 129.5, 126.3, 117.7, 114.2, 79.9, 71.4, 63.1, 55.3, 53.8. **IR** (cm^{-1}, neat): 2935, 2837, 1613, 1514, 1443, 1250, 1177, 1088, 1032, 927, 805, 668. **mp** = 45 – 46 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{17}N_3O_2I^+$, 386.03654; found, 386.03562.



4-((allyloxy)methyl)-5-iodo-1-(4-methylbenzyl)-1H-1,2,3-triazole (1e).

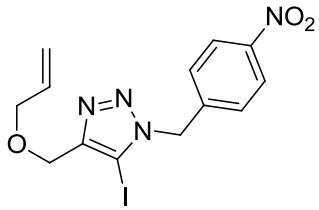
According to the general procedure, iodoalkyne **S9** (221 mg, 1.0 mmol), 4-methylbenzylazide (148 mg, 1.0 mmol), CuI (19 mg, 0.1 mmol) and TBTA (53 mg, 0.1 mmol) were reacted in THF

(5 mL) at room temperature for 47 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **1e** as an off-white solid (205 mg, 56%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.16 (q, *J* = 8.2 Hz, 4H), 5.86 – 5.99 (m, 1H), 5.55 (s, 2H), 5.32 (ddd, *J* = 17.4, 4.6, 1.8 Hz, 1H), 5.20 (ddd, *J* = 10.4, 2.7, 1.2 Hz, 1H), 4.56 (s, 2H), 4.06 (dt, *J* = 5.7, 1.3 Hz, 2H), 2.33 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 149.0, 138.6, 134.5, 131.4, 129.8, 128.1, 117.9, 80.3, 71.6, 63.3, 54.3, 21.4. **IR** (cm^{-1}, neat): 2855, 1515, 1420, 1219, 1089, 1055, 924, 797, 756, 668. **mp** = 63 – 65 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{17}N_3OI^+$, 370.04163; found, 370.04156.



4-((allyloxy)methyl)-1-benzyl-5-iodo-1H-1,2,3-triazole (1f).

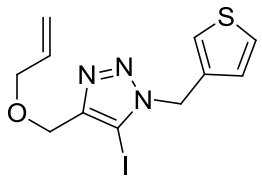
According to the general procedure, iodoalkyne **S9** (221 mg, 1.0 mmol), benzylazide (136 mg, 1.0 mmol), CuI (19 mg, 0.1 mmol) and TBTA (53 mg, 0.1 mmol) were reacted in THF (5 mL) at room temperature for 21 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **1f** as an off-white solid (191 mg, 54%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.24 – 7.38 (m, 5H), 5.86 – 6.00 (m, 1H), 5.59 (s, 2H), 5.32 (ddd, *J* = 17.2, 4.8, 1.6 Hz, 1H), 5.21 (dd, *J* = 10.4, 1.4 Hz, 1H), 4.57 (s, 2H), 4.06 (dt, *J* = 5.7, 1.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 148.9, 134.3, 134.2, 128.9, 128.5, 127.9, 117.7, 80.2, 71.4, 63.1, 54.2**.** **IR** (cm^{-1}, neat): 3032, 2854, 1497, 1456, 1444, 1420, 1358, 1331, 1217, 1090, 1056, 1002, 929, 823, 727, 699. **mp** = 38 – 40 °C. **HRMS** (ESI): Calc'd for $C_{13}H_{14}N_3OI^+$, 356.02598; found, 356.02602.



4-((allyloxy)methyl)-5-iodo-1-(4-nitrobenzyl)-1H-1,2,3-triazole (1g).

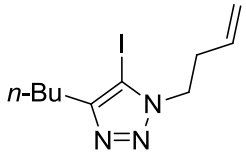
According to the general procedure, iodoalkyne **S9** (222 mg, 1.0 mmol), 4-nitrobenzylazide (180 mg, 1.0 mmol), CuI (19 mg, 0.1 mmol) and TBTA (53 mg, 0.1 mmol) were reacted in THF (5 mL) at room temperature for 21 hours. Subsequent workup and flash column chromatography

(gradient petane:EtOAc 8:2 to 6:4) yielded **1g** as a yellow solid (239 mg, 60%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.22 (d, *J* = 8.8 Hz, 2H), 7.42 (d, *J* = 8.7 Hz, 2H), 5.88 – 6.00 (m, 1H), 5.70 (s, 2H), 5.33 (ddd, *J* = 17.2, 4.8, 1.6 Hz, 1H), 5.23 (ddd, *J* = 10.4, 2.7, 1.2 Hz, 1H), 4.58 (s, 2H), 4.08 (dt, *J* = 5.7, 1.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 149.4, 141.0, 134.1, 128.6, 124.3, 124.2, 117.9, 80.4, 71.6, 63.0, 53.3**. IR** (cm^{-1}, neat): 2857, 1612, 1539, 1344, 1218, 1090, 1056, 1011, 859, 802, 730, 668. **mp** = 145 – 146 °C. **HRMS** (ESI): Calc'd for $C_{13}H_{14}N_4O_3I^+$, 401.01106; found, 401.01250.



4-((allyloxy)methyl)-5-iodo-1-(thiophen-3-ylmethyl)-1H-1,2,3-triazole (1h).

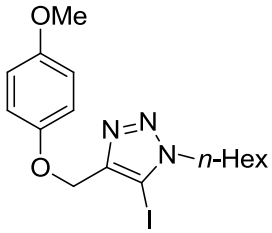
According to the general procedure, iodoalkyne **S9** (111 mg, 0.5 mmol), 3-(azidomethyl)thiophene (70 mg, 0.5 mmol), CuI (10 mg, 0.05 mmol) and TBTA (27 mg, 0.05 mmol) were reacted in THF (2.5 mL) at room temperature for 25 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **1h** as a colourless oil (100 mg, 55%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.28 – 7.33 (m, 1H), 7.24 – 7.28 (m, 1H), 7.06 (dd, *J* = 5.0, 1.2 Hz, 1H) 5.87 – 5.99 (m, 1H), 5.59 (s, 2H), 5.32 (ddd, *J* = 17.3, 4.6, 1.6 Hz, 1H), 5.21 (ddd, *J* = 10.4, 2.6, 1.1 Hz, 1H), 4.56 (s, 2H), 4.06 (dt, *J* = 5.7, 1.3 Hz, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 148.8, 134.7, 134.3, 127.0, 126.9, 124.4, 117.8, 80.0, 71.4, 63.1, 49.6. **IR** (cm^{-1}, neat): 3097, 2922, 2854, 1444, 1420, 1333, 1294, 1215, 1089, 1056, 1010, 928, 831, 788, 745, 668. **HRMS** (ESI): Calc'd for $C_{11}H_{13}N_3OSI^+$, 361.98240; found, 361.98288.



1-(but-3-en-1-yl)-4-butyl-5-iodo-1H-1,2,3-triazole (1i).

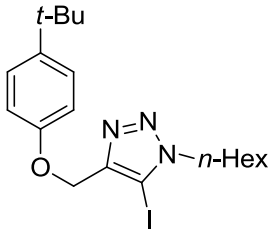
According to the general procedure, iodoalkyne **S18** (205 mg, 1.0 mmol), homoallyl azide (104 mg, 1.1 mmol), CuI (19 mg, 0.1 mmol) and TBTA (53 mg, 0.1 mmol) were reacted in THF (5 mL) at room temperature for 17 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **1i** as a colourless oil (259 mg, 86%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ

= 5.73 – 5.86 (m, 1H), 5.05 – 5.15 (m, 2H), 4.41 (t, *J* = 7.4 Hz, 2H), 2.60 – 2.71 (m, 4H), 1.61 – 1.74 (m, 2H), 1.37 (sx, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 151.9, 133.0, 118.3, 77.9, 49.9, 34.2, 31.1, 25.8, 22.3, 13.8. **IR** (cm^{-1}, neat): 2956, 2859, 1520, 1456, 1213, 1061, 993, 921, 668. **HRMS** (ESI): Calc'd for $C_{10}H_{17}N_3I^+$, 306.04671; found, 306.04763.



1-hexyl-5-iodo-4-((4-methoxyphenoxy)methyl)-1H-1,2,3-triazole (3a).

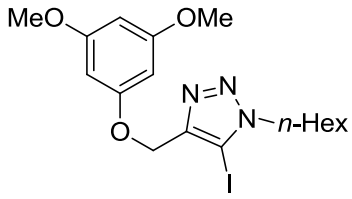
According to the general procedure, iodoalkyne **S12** (257 mg, 0.9 mmol), *n*-hexylazide (135 mg, 1.1 mmol), CuI (19 mg, 0.1 mmol) and TBTA (54 mg, 0.1 mmol) were reacted in THF (5 mL) at room temperature for 20 hours. Subsequent workup and flash column chromatography (petane:EtOAc 85:15) yielded **3a** as an off-white solid (294 mg, 79%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 6.96 (d, *J* = 9.0 Hz, 2H), 6.82 (d, *J* = 9.0 Hz, 2H), 5.05 (s, 2H), 4.35 (t, *J* = 7.4 Hz, 2H), 3.75 (s, 3H) 1.84 – 1.94 (m, 2H), 1.23 – 1.39 (m, 6H), 0.88 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 154.5, 152.7, 147.6, 116.5, 114.8, 80.5, 62.9, 55.9, 51.0, 31.4, 30.1, 26.3, 22.6, 14.2. **IR** (cm^{-1}, neat): 2930, 2858, 1592, 1505, 1461, 1227, 1108, 1037, 864, 825, 707. **mp** = 49 – 50 °C. **HRMS** (ESI): Calc'd for $C_{16}H_{23}N_3O_2I^+$, 416.0829; found, 416.0821.



4-((4-(tert-butyl)phenoxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (3b).

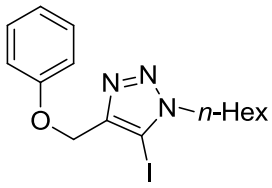
According to the general procedure, iodoalkyne **S13** (509 mg, 1.6 mmol), *n*-hexylazide (247 mg, 1.9 mmol), CuI (35 mg, 0.2 mmol) and TBTA (87 mg, 0.2 mmol) were reacted in THF (12 mL) at room temperature for 40 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **3b** as a pale orange solid (552 mg, 77%). **^{1}H NMR** (300 MHz, $CDCl_3$): δ = 7.32 (d, *J* = 8.9 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 5.10 (s, 2H), 4.37 (t, *J* = 7.4 Hz,

2H), 1.91 (qn, *J* = 7.3 Hz, 2H), 1.22 – 1.42 (m, 15H), 0.89 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (100MHz, $CDCl_3$): δ = 156.3, 147.5, 144.1, 126.4, 114.6, 80.3, 61.9, 51.0, 34.2, 31.7, 31.3, 30.0, 26.2, 22.6, 14.1. **IR** (cm^{-1}, film) = 2960, 2925, 2871, 1606, 1514, 1363, 1336, 1293, 1218, 1184, 1112, 1018, 867, 827, 819, 738, 729. **mp** = 72 – 73 °C. **HRMS** (ESI): Calc'd for $C_{19}H_{29}IN_3O^+$, 442.1355; found, 442.1348.



4-((3,5-dimethoxyphenoxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (3c).

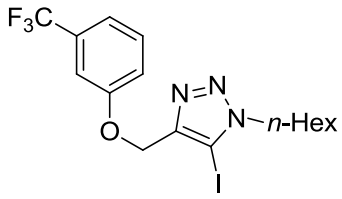
According to the general procedure, iodoalkyne **S14** (508 mg, 1.6 mmol), *n*-hexylazide (244 mg, 1.9 mmol), CuI (38 mg, 0.2 mmol) and TBTA (85 mg, 0.2 mmol) were reacted in THF (12 mL) at room temperature for 20 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **3c** as a pink solid (423 mg, 59%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 6.23 (d, *J* = 2.1 Hz, 2H), 6.12 (t, *J* = 2.1 Hz , 1H), 5.28 (s, 2H), 4.37 (t, *J* = 7.4 Hz, 2H), 3.77 (s, 6H), 1.91 (qn, *J* = 7.4 Hz, 2H), 1.34 (br m, 6H), 0.89 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 161.6, 160.4, 147.2, 93.9, 93.7, 80.3, 62.0, 55.2, 51.0, 31.3, 30.0, 26.2, 22.6, 14.1. **IR** (cm^{-1}, film) = 2998, 2955, 2933, 2858, 1598, 1478, 1466, 1205, 1193, 1152, 1063, 1030, 820, 681. **mp** = 58 – 60 °C. **HRMS** (ESI): Calc'd for $C_{17}H_{24}IN_3O_3^+$, 446.0941; found, 446.0944.



1-hexyl-5-iodo-4-(phenoxymethyl)-1H-1,2,3-triazole (3d).

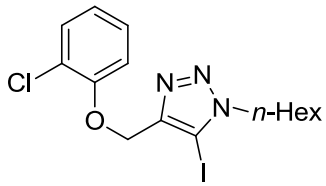
According to the general procedure, iodoalkyne **S15** (499 mg, 1.9 mmol), *n*-hexylazide (281 mg, 2.2 mmol), CuI (40 mg, 0.2 mmol) and TBTA (105 mg, 0.2 mmol) were reacted in THF (12 mL) at room temperature for 22 hours. Subsequent workup and flash column chromatography (petane:EtOAc 9:1) yielded **3d** as an off-white solid (608 mg, 81%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.31 (m, 2H), 7.05 (m, 2H), 6.98 (tt, *J* = 7.3 Hz & 1.0 Hz, 1H), 5.13 (s, 2H), 4.37 (t, *J* = 7.4 Hz, 2H), 1.93 (qn, *J* = 7.4 Hz, 2H), 1.33 (br m, 6H), 0.89 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR**

(100 MHz, $CDCl_3$): δ = 158.5, 147.4, 129.6, 121.5, 115.2, 80.2, 61.9, 51.0, 31.3, 30.0, 26.2, 22.6, 14.1. **IR** (cm^{-1}, film) = 2954, 2930, 2859, 1599, 1587, 1495, 1458, 1239, 1173, 1031, 1013, 854, 754, 692. **mp** = 43 – 44 °C. **HRMS** (ESI): Calc'd for $C_{15}H_{21}IN_3O^+$, 386.0729 ; found, 386.0737 .



1-hexyl-5-iodo-4-((3-(trifluoromethyl)phenoxy)methyl)-1H-1,2,3-triazole (3e).

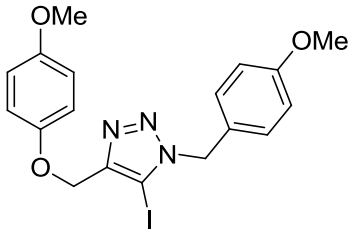
According to the general procedure, iodoalkyne **S16** (406 mg, 1.3 mmol), *n*-hexylazide (175 mg, 1.4 mmol), CuI (37 mg, 0.2 mmol) and TBTA (74 mg, 0.1 mmol) were reacted in THF (12 mL) at room temperature for 27 hours. Subsequent workup and flash column chromatography (petane:EtOAc 9:1) yielded **3e** as a yellow solid (408 mg, 72 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.40 (t, *J* = 7.9 Hz, 1H), 7.23 (m, 3H), 5.16 (s, 2H), 4.38 (t, *J* = 7.4 Hz, 3H), 1.91 (qn, *J* = 7.4 Hz, 2H), 1.34 (br m, 6H), 0.88 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 158.5, 146.8, 132.1 (q, *J* = 32.3 Hz), 130.2, 124.0 (q, *J* = 272.4 Hz), 118.5 (m), 118.1 (q, *J* = 3.9 Hz), 112.3 (q, *J* = 3.9 Hz), 80.5, 62.1, 51.1, 31.3, 30.0, 26.2, 22.5, 14.1. **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -63.10. **IR** (cm^{-1}, film) = 2956, 2932, 2860, 1593, 1492, 1447, 1326, 1292, 1225, 1168, 1126, 1067, 1018, 794, 697. **mp** = 65 – 67 °C. **HRMS** (ESI): Calc'd for $C_{16}H_{19}F_3IN_3O^+$, 454.0603; found, 454.0621.



4-((2-chlorophenoxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (3f).

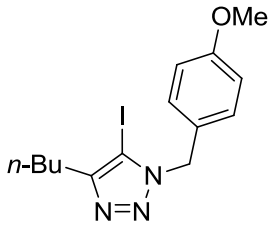
According to the general procedure, iodoalkyne **S17** (417 mg, 1.4 mmol), *n*-hexylazide (330 mg, 2.6 mmol), CuI (48 mg, 0.2 mmol) and TBTA (78 mg, 0.2 mmol) were reacted in THF (12 mL) at room temperature for 20 hours. Subsequent workup and flash column chromatography (petane:EtOAc 9:1) yielded **3f** as an off-white solid (399 mg, 67 %). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.35 (dd, *J* = 7.9 Hz & 1.5 Hz, 1H), 7.21 (ddd, *J* = 8.2 Hz, 7.2 Hz & 1.5 Hz, 1H), 7.16 (dd, *J* = 8.2 Hz & 1.7 Hz, 1H), 6.92 (ddd, *J* = 7.9 Hz, 7.2 Hz, & 1.7 Hz, 1H), 5.22 (s, 2H),

4.37 (t, *J* = 7.4 Hz, 2H), 1.91 (qn, *J* = 7.4 Hz, 2H), 1.33 (br m, 6H), 0.89 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 153.8, 146.9, 130.6, 127.8, 123.8, 123.4, 115.2, 80.4, 63.1, 51.0, 31.3, 30.0, 26.2, 22.6, 14.1; **IR** (cm^{-1}, film) = 2954, 2931, 2869, 2859, 1589, 1484, 1447, 1277, 1245, 1060, 1007, 855, 749; **mp** = 63 – 64 °C. **HRMS** (ESI): Calc'd for $C_{15}H_{19}ClIN_3O^+$, 420.0340; found, 420.0327.



5-iodo-1-(4-methoxybenzyl)-4-((4-methoxyphenoxy)methyl)-1H-1,2,3-triazole (3g).

According to the general procedure, iodoalkyne **S12** (401 mg, 1.4 mmol), *p*-methoxybenzylazide (227 mg, 1.4 mmol), CuI (13 mg, 0.07 mmol) and TBTA (37 mg, 0.07 mmol) were reacted in THF (7.5 mL) at room temperature for 40 hours. Subsequent workup and flash column chromatography (pentane:EtOAc 65:35) yielded **3g** as an off-white solid (314 mg, 50%). Characterization data were consistent with the literature.[15] **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.24 (d, *J* = 8.8 Hz, 2H), 6.95 (d, *J* = 9.1 Hz, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.82 (d, *J* = 9.1 Hz, 2H), 5.51 (s, 2H), 5.05 (s, 2H), 3.78 (s, 3H), 3.75 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 160.0, 154.5, 152.6, 148.1, 129.7, 126.4, 116.6, 114.8, 114.5, 80.5, 62.9, 55.9, 55.5, 54.1. **mp** = 80 – 81 °C.

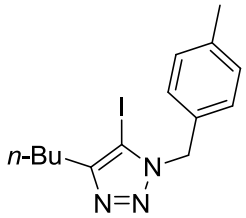


4-butyl-5-iodo-1-(4-methoxybenzyl)-1H-1,2,3-triazole (5a).

According to the general procedure, iodoalkyne **S18** (1.50 g, 7.2 mmol), *p*-methoxybenzylazide (1.18 g, 7.2 mmol), CuI (137 mg, 0.7 mmol) and TBTA (383 mg, 0.7 mmol) were reacted in THF (36 mL) at room temperature. TLC analysis indicated some starting material left after 19

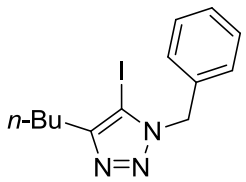
[15] Smith, N. W.; Polenz, B. P.; Johnson, S. B.; Dzyuba, S. V. *Tetrahedron Letters* **2010**, *51*, 550.

hours, so additional CuI (27 mg, 0.1 mmol) and TBTA (77 mg, 0.1 mmol) was added. TLC indicated complete consumption of starting material after an additional 24 hours. Subsequent workup and flash column chromatography (gradient petane:EtOAc 8:2 to 6:4) yielded **5a** as an off-white solid (2.32 g, 87%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.23 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 5.49 (s, 2H), 3.79 (s, 3H), 2.63 (t, *J* = 7.6 Hz, 2H), 1.66 (qn, *J* = 7.6 Hz, 2H), 1.37 (sx, *J* = 7.6 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 159.6, 152.4, 129.3, 126.6, 114.2, 77.8, 55.3, 53.7, 31.1, 25.8, 22.3, 13.8. **IR** (cm^{-1}, neat): 2930, 2858, 1612, 1586, 1514, 1464, 1456, 1304, 1250, 1213, 1177, 1110, 1033, 801. **mp** = 65 – 67 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{19}N_3OI^+$, 372.0567; found, 372.0559.



4-butyl-5-iodo-1-(4-methylbenzyl)-1H-1,2,3-triazole (5b).

According to the general procedure, iodoalkyne **S18** (204 mg, 1.0 mmol), 4-methylbenzylazide (150 mg, 1.0 mmol), CuI (19 mg, 0.1 mmol) and TBTA (53 mg, 0.1 mmol) were reacted in THF (5 mL) at room temperature for 27 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **5b** as a white solid (291 mg, 82%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.11 – 7.18 (m, 4H), 5.52 (s, 2H), 2.64 (t, *J* = 7.8 Hz, 2H), 2.33 (s, 3H), 1.67 (qn, *J* = 7.6 Hz, 2H), 1.37 (sx, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 152.5, 138.2, 131.5, 129.5, 127.8, 77.9, 54.0, 31.1, 25.8, 22.3, 21.2, 13.8. **IR** (cm^{-1}, neat): 2953, 2930, 2859, 1513, 1434, 1349, 1312, 1217, 1179, 1142, 1064, 794, 754. **mp** = 86 – 89 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{18}N_3I^+$, 356.06236; found, 356.06214.



1-benzyl-4-butyl-5-iodo-1H-1,2,3-triazole (5c).

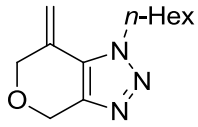
According to the general procedure, iodoalkyne **S18** (199 mg, 1.0 mmol), benzylazide (171 mg, 1.3 mmol), CuI (18 mg, 0.1 mmol) and TBTA (51 mg, 0.1 mmol) were reacted in THF (5 mL) at

room temperature for 38 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **5c** as a white solid (277 mg, 85%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.21 – 7.38 (m, 5H), 5.56 (s, 2H), 2.65 (t, *J* = 7.8 Hz, 2H), 1.67 (qn, *J* = 7.6 Hz, 2H), 1.37 (sx, *J* = 7.4 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 152.5, 134.6, 128.8, 128.4, 127.7, 78.1, 54.1, 31.1, 25.8, 22.3, 13.8. **IR** (cm^{-1}, neat): 3032, 2955, 2858, 1521, 1497, 1456, 1331, 1212, 1139, 1061, 820, 726, 697, 668. **mp** = 92 – 93 °C. **HRMS** (ESI): Calc'd for $C_{13}H_{17}N_3I^+$, 342.04671; found, 342.04571.

General procedure for the synthesis of fused 1,2,3-triazoles

Method A: To a microwave vial equipped with a magnetic stir bar, the corresponding 5-iodo-1,2,3-triazole (1 equiv.), $PdCl_2(MeCN)_2$ (5 mol%), PPh_3 (10 mol%) and CsOPiv (2 equiv.) were added. The reaction mixture was purged with nitrogen, after which MeCN (0.06 M) was added. The vial was capped and immersed in an oil bath pre-heated to 100 °C. After TLC analysis had shown complete conversion of the starting materials, the reaction mixture was cooled to room temperature, passed through a silica plug and concentrated under reduced pressure. Purification by flash chromatography yielded the desired target structure.

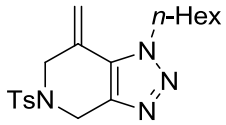
Method B: To a microwave vial equipped with a magnetic stir bar, the corresponding 5-iodo-1,2,3-triazole (1 equiv.), $PdCl_2(MeCN)_2$ (5 mol%), $P(p\text{-}FC_6H_4)_3$ (5 mol%), K_2CO_3 (3 equiv.) and PivOH (30 mol%) were added. The reaction mixture was purged with nitrogen, after which DMA (0.26 M) was added. The vial was capped and immersed in an oil bath pre-heated to 130 °C. After TLC analysis had shown complete conversion of the starting materials, the reaction mixture was cooled to room temperature, passed through a silica plug and concentrated under reduced pressure. Purification by flash chromatography yielded the desired target structure.



1-hexyl-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2a).

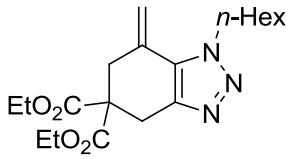
According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1a** (174 mg, 0.5 mmol), $PdCl_2(MeCN)_2$ (7 mg, 0.025 mmol), PPh_3 (14 mg, 0.05 mmol) and CsOPiv (237 mg, 1.0 mmol)

were reacted in MeCN (8 mL) at 100 °C for 6 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2a** as a yellow oil (101 mg, 92%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.34 (s, 1H), 5.22 (s, 1H), 4.89 (s, 2H), 4.47 (t, *J* = 7.4 Hz, 2H), 4.32 (s, 2H), 1.89 (qn, *J* = 7.5 Hz, 2H), 1.17 – 1.45 (m, 6H), 0.89 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 143.8, 130.9, 127.6, 108.8, 70.5, 64.3, 50.0, 31.2, 29.1, 26.2, 22.5, 14.0. **IR** (cm^{-1}, neat): 2931, 2857, 1652, 1493, 1456, 1345, 1314, 1200, 1104, 1083, 1034, 929, 904, 836. **HRMS** (ESI): Calc'd for $C_{12}H_{20}N_3O^+$, 222.1600; found, 222.1602.



1-hexyl-7-methylene-5-tosyl-4,5,6,7-tetrahydro-1H-[1,2,3]triazolo[4,5-c]pyridine (2b).

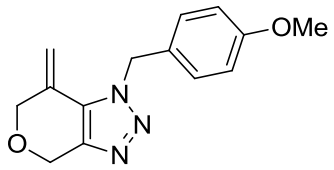
According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1b** (50 mg, 0.1 mmol), $PdCl_2(MeCN)_2$ (1 mg, 0.005 mmol), PPh_3 (3 mg, 0.01 mmol) and CsOPiv (47 mg, 0.2 mmol) were reacted in MeCN (1.6 mL) at 100 °C for 6 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2b** as a yellow oil (37 mg, 99%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.59 (d, *J* = 8.3 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 5.29 (s, 1H), 5.25 (s, 1H), 4.56 (s, 2H), 4.28 (t, *J* = 7.4 Hz, 2H), 4.07 (s, 2H), 2.34 (s, 3H), 1.56 – 1.79 (m, 2H), 1.16 – 1.38 (m, 6H), 0.87 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 143.8, 141.3, 134.3, 130.1, 129.5, 127.9, 127.7, 111.6, 50.8, 49.9, 43.8, 31.2, 29.0, 26.1, 22.4, 21.5, 13.9. **IR** (cm^{-1}, neat): 2931, 2859, 1652, 1597, 1456, 1348, 1164, 1090, 1049, 934, 815, 666, 594, 549. **HRMS** (ESI): Calc'd for $C_{19}H_{27}N_4O_2S^+$, 375.18547; found, 375.18573.



diethyl 1-hexyl-7-methylene-6,7-dihydro-1H-benzo[d][1,2,3]triazole-5,5(4H)-dicarboxylate (2c).

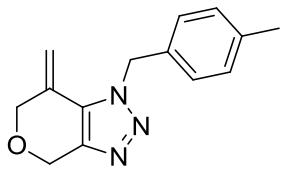
According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1c** (98 mg, 0.20 mmol), $Pd(PPh_3)_2Cl_2$ (7 mg, 0.01 mmol) and CsOPiv (94 mg, 0.4 mmol) were reacted in MeCN (2 mL) at 100 °C for 16 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **2c** as a colorless oil (65 mg, 89%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.30 (s, 1H),

5.25 (s, 1H), 4.38 (t, *J* = 7.4 Hz, 2H), 4.22 – 4.04 (m, 4H), 3.36 (s, 2H), 2.99 (s, 2H), 1.92 – 1.73 (m, 2H), 1.38 – 1.21 (m, 6H), 1.17 (t, *J* = 7.1 Hz, 6H), 0.83 (t, *J* = 6.5 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 169.9, 143.4, 129.1, 128.9, 112.4, 61.9, 55.0, 50.1, 39.1, 31.2, 29.0, 28.6, 26.1, 22.5, 14.0, 13.9. **IR** (cm^{-1}, neat): 2977, 2958, 2933, 2871, 1748, 1729, 1722, 1714, 1645, 1464, 1446, 1367, 1301, 1238, 1190, 1095, 1070, 1049, 1012. **HRMS** (ESI): Calc'd for $C_{19}H_{30}N_3O_4^+$, 364.22363; found, 364.22415.



1-(4-methoxybenzyl)-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2d).

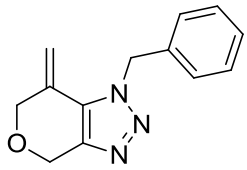
According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1d** (50 mg, 0.13 mmol), $PdCl_2(MeCN)_2$ (2 mg, 0.006 mmol), PPh_3 (3 mg, 0.013 mmol) and CsOPiv (61 mg, 0.26 mmol) were reacted in MeCN (2.1 mL) at 100 °C for 6 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2d** as an off-white solid (30 mg, 92%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.05 (d, *J* = 8.7 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 5.65 (s, 2H), 5.24 (s, 1H), 5.10 (s, 1H), 4.92 (s, 2H), 4.27 (s, 2H), 3.79 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 159.5, 144.0, 130.1, 128.2, 127.9, 126.4, 114.4, 110.0, 70.4, 64.3, 55.3, 52.8. **IR** (cm^{-1}, neat): 2928, 2837, 1612, 1515, 1443, 1293, 1250, 1178, 1077, 1033, 903, 816. **mp** = 53 – 56 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{16}N_3O_2^+$, 258.12425; found, 258.12527.



1-(4-methylbenzyl)-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2e).

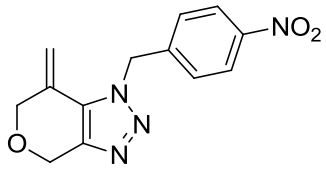
According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1e** (50 mg, 0.13 mmol), $PdCl_2(MeCN)_2$ (2 mg, 0.006 mmol), PPh_3 (3 mg, 0.013 mmol) and CsOPiv (63 mg, 0.27 mmol) were reacted in MeCN (2.2 mL) at 100 °C for 6 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2e** as a white solid (32 mg, 99%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.14 (d, *J* = 7.9 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 5.68 (s, 2H), 5.21 (s, 1H), 5.08 (s, 1H), 4.92 (s, 2H), 4.27 (s, 2H), 2.33 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 144.0,

138.1, 131.4, 130.1, 129.7, 128.3, 126.5, 110.0, 70.3, 64.3, 53.0, 21.1. **IR** (cm^{-1}, neat): 2923, 2844, 1653, 1517, 1449, 1314, 1204, 1077, 928, 898, 844, 805. **mp** = 89 – 91 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{16}N_3O^+$, 242.12934; found, 242.12934.



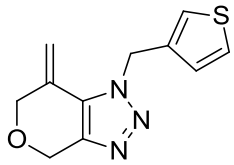
1-benzyl-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2f).

According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1f** (50 mg, 0.14 mmol), $PdCl_2(MeCN)_2$ (2 mg, 0.007 mmol), PPh_3 (4 mg, 0.014 mmol) and CsOPiv (66 mg, 0.28 mmol) were reacted in MeCN (2.3 mL) at 100 °C for 6 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2f** as an off-white solid (32 mg, 99%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.27 – 7.38 (m, 3H), 7.10 (d, *J* = 6.8 Hz, 2H), 5.72 (s, 2H), 5.19 (s, 1H), 5.08 (s, 1H), 4.93 (s, 2H), 4.28 (s, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 144.1, 134.4, 130.1, 129.1, 128.4, 128.3, 126.5, 110.0, 70.4, 64.3, 53.2. **IR** (cm^{-1}, neat): 2961, 2847, 1652, 1498, 1456, 1314, 1204, 1079, 1032, 900, 841, 717. **mp** = 84 – 87 °C. **HRMS** (ESI): Calc'd for $C_{13}H_{14}N_3O^+$, 228.11369; found, 228.11320.



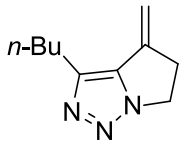
7-methylene-1-(4-nitrobenzyl)-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2g).

According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1g** (50 mg, 0.13 mmol), $PdCl_2(MeCN)_2$ (2 mg, 0.006 mmol), PPh_3 (3 mg, 0.013 mmol) and CsOPiv (58 mg, 0.26 mmol) were reacted in MeCN (2 mL) at 100 °C for 23 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2g** as an orange solid (21 mg, 61%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.23 (d, *J* = 8.8 Hz, 2H), 7.27 (d, *J* = 8.8 Hz, 2H), 5.84 (s, 2H), 5.11 (s, 1H), 5.09 (s, 1H), 4.94 (s, 2H), 4.30 (s, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 148.0, 144.5, 141.4, 130.2, 128.4, 127.4, 124.4, 109.9, 70.2, 64.2, 52.4. **IR** (cm^{-1}, neat): 2926, 2854, 1652, 1539, 1346, 1207, 1077, 901, 839, 720, 668. **mp** = 126 – 127 °C. **HRMS** (ESI): Calc'd for $C_{13}H_{13}N_4O_3^+$, 273.0982; found, 273.0978.



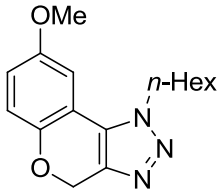
7-methylene-1-(thiophen-3-ylmethyl)-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2h).

According to Method A of the general procedure, 5-iodo-1,2,3-triazole **1h** (44 mg, 0.12 mmol), $PdCl_2(MeCN)_2$ (2 mg, 0.006 mmol), PPh_3 (3 mg, 0.012 mmol) and CsOPiv (56 mg, 0.24 mmol) were reacted in MeCN (1.9 mL) at 100 °C for 24 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2h** as an orange oil (24 mg, 84%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.33 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.02 – 7.06 (m, 1H), 6.94 (dd, *J* = 5.0, 1.2 Hz, 1H), 5.71 (s, 2H), 5.27 (s, 1H), 5.14 (s, 1H), 4.92 (s, 2H), 4.30 (s, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 144.0, 135.2, 130.2, 128.1, 127.3, 126.1, 122.6, 109.9, 70.4, 64.2, 49.2. **IR** (cm^{-1}, neat): 3100, 2925, 2852, 1652, 1456, 1307, 1202, 1075, 900, 836, 796, 668. **HRMS** (ESI): Calc'd for $C_{11}H_{12}N_3OS^+$, 234.0695; found, 234.0698.



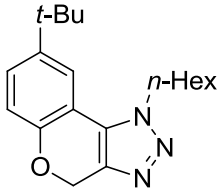
3-butyl-4-methylene-5,6-dihydro-4H-pyrrolo[1,2-c][1,2,3]triazole (2i).

According to Method A of the general procedure, but using $Pd(OAc)_2$ instead of $PdCl_2(MeCN)_2$, 5-iodo-1,2,3-triazole **1i** (53 mg, 0.17 mmol), $Pd(OAc)_2$ (2 mg, 0.008 mmol), PPh_3 (4 mg, 0.017 mmol) and CsOPiv (80 mg, 0.34 mmol) were reacted in MeCN (2.7 mL) at 100 °C for 6 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **2i** as an orange oil (31 mg, 99%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 5.38 (t, *J* = 2.5 Hz, 1H), 5.19 (t, *J* = 2.1 Hz, 1H), 4.40 (t, *J* = 7.0 Hz, 2H), 3.40 – 3.47 (m, 2H), 2.78 (t, *J* = 7.6 Hz, 2H), 1.69 (qn, *J* = 7.6 Hz, 2H), 1.40 (sx, *J* = 7.4 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 140.9, 138.2, 132.7, 108.2, 45.2, 35.2, 31.1, 25.4, 22.4, 13.8. **IR** (cm^{-1}, neat): 2956, 2859, 1653, 1574, 1434, 1315, 1166, 1085, 877, 798, 668, 626. **HRMS** (ESI): Calc'd for $C_{10}H_{16}N_3^+$, 178.13442; found, 178.13354.



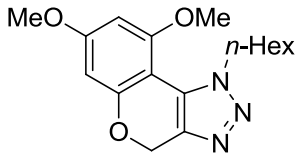
1-hexyl-8-methoxy-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4a).

According to Method B of the general procedure, 5-iodo-1,2,3-triazole **3a** (153 mg, 0.4 mmol), $PdCl_2(MeCN)_2$ (5 mg, 0.02 mmol), $P(p\text{-}FC_6H_4)_3$ (6 mg, 0.02 mmol), K_2CO_3 (152 mg, 1.20 mmol) and PivOH (11 mg, 0.12 mmol) were reacted in DMA (1.40 mL) at 130 ºC for 4 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **4a** as an off white solid (94 mg, 88%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 6.99 (d, *J* = 8.9 Hz, 1H), 6.96 (d, *J* = 2.9 Hz, 1H), 6.82 (dd, *J* = 8.9 Hz & 2.9 Hz, 1H), 5.37 (s, 2H), 4.58 (t, *J* = 7.4 Hz, 2H), 3.82 (s, 3H), 1.96 (qn, *J* = 7.4 Hz, 2H), 1.45 – 1.30 (br m, 6H), 0.88 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 154.7, 147.6, 140.3, 127.2, 118.7, 115.1, 114.7, 108.5, 64.4, 55.9, 49.9, 31.3, 29.9, 26.3, 22.6, 14.0. **IR** (cm^{-1}, film) = 2955, 2929, 2858, 1521, 1469, 1310, 1224, 1193, 1045, 1003, 837. **mp** = 69 – 71 °C. **HRMS** (ESI): Calc'd for $C_{16}H_{22}N_3O_2^+$, 288.1712; found, 288.1704.



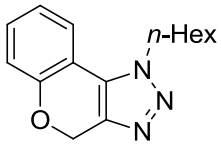
8-(tert-butyl)-1-hexyl-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4b).

According to Method B of the general procedure, 5-iodo-1,2,3-triazole **3b** (103 mg, 0.2 mmol), $PdCl_2(MeCN)_2$ (4 mg, 0.01 mmol), $P(p\text{-}FC_6H_4)_3$ (4 mg, 0.01 mmol), K_2CO_3 (95 mg, 0.6 mmol) and PivOH (7 mg, 0.06 mmol) were reacted in DMA (0.9 mL) at 130 ºC for 4 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **4b** as a yellow oil (68 mg, 93%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.44 (d, *J* = 2.3 Hz, 1H), 7.30 (dd, *J* = 8.6 Hz & 2.4 Hz, 1H), 6.99 (d, *J* = 8.6 Hz, 1H), 5.42 (s, 2H), 4.61 (t, *J* = 7.6 Hz, 2H), 1.98 (qn, *J* = 7.6 Hz, 2H), 1.50 – 1.32 (m, 15H), 0.89 (3 H, t, 7.1 Hz). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 151.5, 145.1, 139.6, 127.6, 127.5, 126.4, 119.0, 117.6, 113.7, 64.5, 50.2, 34.5, 31.5, 29.6, 26.4, 22.6, 14.0. **IR** (cm^{-1}, film) = 2957, 2931, 2860, 1522, 1467, 1363, 1330, 1258, 1232, 1209, 1139, 1036, 1002, 825. **HRMS** (ESI): Calc'd for $C_{19}H_{28}N_3O_3^+$, 314.2232; found, 318.2246.



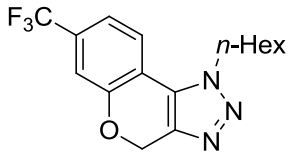
1-hexyl-7,9-dimethoxy-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4c).

According to Method B of the general procedure, 5-iodo-1,2,3-triazole **3c** (99 mg, 0.2 mmol), $PdCl_2(MeCN)_2$ (3 mg, 0.01 mmol), P(*p*-$FC_6H_4)_3$ (4 mg, 0.01 mmol), K_2CO_3 (95 mg, 0.6 mmol) and PivOH (7 mg, 0.06 mmol) were reacted in DMA (0.9 mL) at 130 ºC for 4 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **4c** as an off-white solid (68 mg, 75%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 6.31 (d, *J* = 2.4 Hz, 1H), 6.21 (d, *J* = 2.4 Hz, 1H), 5.25 (s, 2H), 4.67 (t, *J* = 7.5 Hz, 2H), 3.90 (s, 2H), 3.82 (s, 3H), 1.76 (qn, *J* = 7.4 Hz, 2H), 1.28 (br m, 6H), 0.85 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 162.1, 156.7, 155.9, 139.2, 127.1, 99.3, 95.8, 93.5, 64.7, 55.7, 55.5, 52.0, 31.5, 30.3, 26.6, 22.6, 14.0. **IR** (cm^{-1}, film) = 2955, 2918, 2857, 1589, 1448, 1417, 1303, 1222, 1201, 1158, 1108, 1084, 1073, 998, 935, 926, 834, 807. **mp** = 79 – 80 °C. **HRMS** (ESI): Calc'd for $C_{17}H_{24}N_3O_3^+$, 318.1818; found, 318.1822.



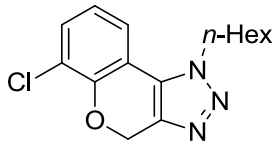
1-hexyl-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4d).

According to Method B of the general procedure, 5-iodo-1,2,3-triazole **3d** (100 mg, 0.3 mmol), $PdCl_2(MeCN)_2$ (4 mg, 0.015 mmol), P(*p*-$FC_6H_4)_3$ (4 mg, 0.015 mmol), K_2CO_3 (109 mg, 0.9 mmol) and PivOH (8 mg, 0.09 mmol) were reacted in DMA (1 mL) at 130 ºC for 22 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **4d** as a yellow oil (46 mg, 68%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.42 (dd, *J* = 8.0 Hz & 1.6 Hz, 1H), 7.29 (m, 1H), 7.06 (m, 2H), 5.46 (s, 2H), 4.60 (t, *J* = 7.4 Hz, 2H), 1.96 (qn, *J* = 7.5 Hz, 2H), 1.33 (m, 6H), 0.89 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 153.8, 139.6, 130.6, 127.1, 122.3, 122.2, 118.3, 114.4, 64.6, 50.1, 31.3, 29.8, 26.3, 22.6, 14.1. **IR** (cm^{-1}, film) = 2956, 2931, 2859, 1522, 1467, 1447, 1336, 1229, 1197, 1125, 1041, 1023, 990, 841, 755. **HRMS** (ESI): Calc'd for $C_{15}H_{19}N_3O^+$, 258.1606; found, 258.1610.



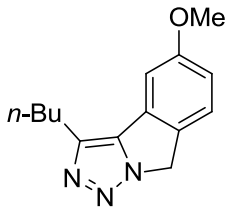
1-hexyl-7-(trifluoromethyl)-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4e).

According to Method B of the general procedure, 5-iodo-1,2,3-triazole **3e** (99 mg, 0.2 mmol), $PdCl_2(MeCN)_2$ (3 mg, 0.01 mmol), $P(p\text{-}FC_6H_4)_3$ (4 mg, 0.01 mmol), K_2CO_3 (94 mg, 0.6 mmol) and PivOH (7 mg, 0.06 mmol) were reacted in DMA (0.9 mL) at 130 ºC for 22 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **4e** as a colourless oil (36 mg, 51%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.50 (1 H, d, *J* = 7.9 Hz), 7.30 (2 H, m), 5.51 (2 H, s), 4.61 (2 H, t, *J* = 7.4 Hz), 1.95 (2 H, qn, *J* = 7.4 Hz), 1.38 (6 H, br m), 0.88 (3 H, t, *J* = 7.1 Hz). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 153.9, 140.2, 132.3 (q, *J* = 33.1 Hz), 126.1, 123.5 (q, *J* = 272.4 Hz), 122.4, 118.9 (q, *J* = 3.9 Hz), 117.4 (m), 115.5 (q, *J* = 3.9 Hz), 65.0, 50.3, 31.3, 29.8, 26.3, 22.6, 14.0. **^{19}F NMR** (376 MHz, $CDCl_3$): δ = -63.63. **IR** (cm^{-1}, film) = 2959, 2932, 2858, 1423, 1336, 1172, 1138, 1129, 1067, 1023, 882, 870, 823. **HRMS** (ESI): Calc'd for $C_{16}H_{19}F_3N_3O^+$, 326.1480; found, 326.1481.



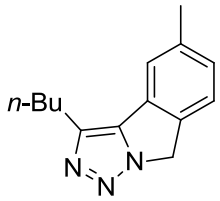
6-chloro-1-hexyl-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4f).

According to Method B of the general procedure, 5-iodo-1,2,3-triazole **3f** (95 mg, 0.2 mmol), $PdCl_2(MeCN)_2$ (3 mg, 0.01 mmol), $P(p\text{-}FC_6H_4)_3$ (4 mg, 0.01 mmol), K_2CO_3 (108 mg, 0.6 mmol) and PivOH (8 mg, 0.06 mmol) were reacted in DMA (0.9 mL) at 130 ºC for 4 hours. Subsequent workup and flash column chromatography (petane:EtOAc 8:2) yielded **4f** as an off-white solid (52 mg, 79%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.34 (m, 2H), 6.99 (t, *J* = 7.9 Hz, 1H), 5.57 (s, 2H), 4.59 (t, *J* = 7.4 Hz, 2H), 1.94 (qn, *J* = 7.4 Hz, 2H), 1.36 (br m, 6H), 0.88 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 149.5, 139.6, 131.1, 126.6, 123.6, 122.4, 120.5, 115.8, 65.3, 50.1, 31.3, 29.8, 26.2, 22.5, 14.0. **IR** (cm^{-1}, film) = 2956, 2919, 2859, 1511, 1456, 1425, 1331, 1278, 1229, 1198, 1082, 1007, 853, 781, 734. **mp** = 59 – 61 °C. **HRMS** (ESI): Calc'd for $C_{15}H_{19}ClN_3O^+$, 292.1217; found, 292.1222.



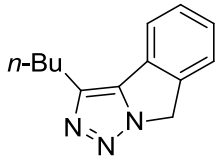
3-butyl-5-methoxy-8H-[1,2,3]triazolo[5,1-a]isoindole (6a).

According to Method A of the general procedure, but using $Pd(OAc)_2$ instead of $PdCl_2(MeCN)_2$, 5-iodo-1,2,3-triazole **5a** (50 mg, 0.14 mmol), $Pd(OAc)_2$ (2 mg, 0.007 mmol), PPh_3 (4 mg, 0.014 mmol) and CsOPiv (63 mg, 0.28 mmol) were reacted in MeCN (2.2 mL) at 100 °C for 27 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **6a** as a slightly yellow solid (29 mg, 87%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.31 (d, *J* = 8.4 Hz, 1H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.82 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.15 (s, 2H), 3.81 (s, 3H), 2.87 (t, *J* = 7.6 Hz, 2H), 1.72 (qn, *J* = 7.6 Hz, 2H), 1.37 (sx, *J* = 7.4 Hz, 2H), 0.89 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 159.3, 138.3, 138.3, 131.4, 128.7, 123.9, 112.0, 106.0, 54.7, 49.6, 30.7, 24.6, 21.3, 12.8. **IR** (cm^{-1}, neat): 2927, 2855, 1622, 1489, 1464, 1338, 1303, 1220, 1032, 859, 812, 669. **mp** = 74 – 75 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{18}N_3O^+$, 244.1444; found, 244.1441.



3-butyl-5-methyl-8H-[1,2,3]triazolo[5,1-a]isoindole (6b).

According to Method A of the general procedure, but using $Pd(OAc)_2$ instead of $PdCl_2(MeCN)_2$, 5-iodo-1,2,3-triazole **5b** (50 mg, 0.14 mmol), $Pd(OAc)_2$ (2 mg, 0.007 mmol), PPh_3 (4 mg, 0.014 mmol) and CsOPiv (66 mg, 0.28 mmol) were reacted in MeCN (2.3 mL) at 100 °C for 27 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **6b** as an orange solid (29 mg, 89%). **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.39 (s, 1H), 7.36 (d, *J* = 7.8 Hz, 1H), 7.17 (d, *J* = 7.8 Hz, 1H), 5.23 (s, 2H), 2.94 (t, *J* = 7.6 Hz, 2H), 2.45 (s, 3H), 1.79 (qn, *J* = 7.6 Hz, 2H), 1.45 (sx, *J* = 7.4 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 139.4, 139.2, 138.8, 137.8, 128.6, 128.5, 123.8, 121.5, 50.8, 31.7, 25.6, 22.4, 21.6, 13.9. **IR** (cm^{-1}, neat): 2927, 2858, 1653, 1631, 1486, 1457, 1305, 1086, 878, 808, 695. **mp** = 74 – 77 °C. **HRMS** (ESI): Calc'd for $C_{14}H_{18}N_3^+$, 228.15007; found, 228.15074.



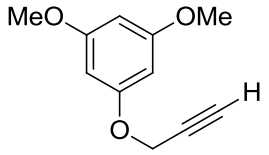
3-butyl-8H-[1,2,3]triazolo[5,1-a]isoindole (6c).

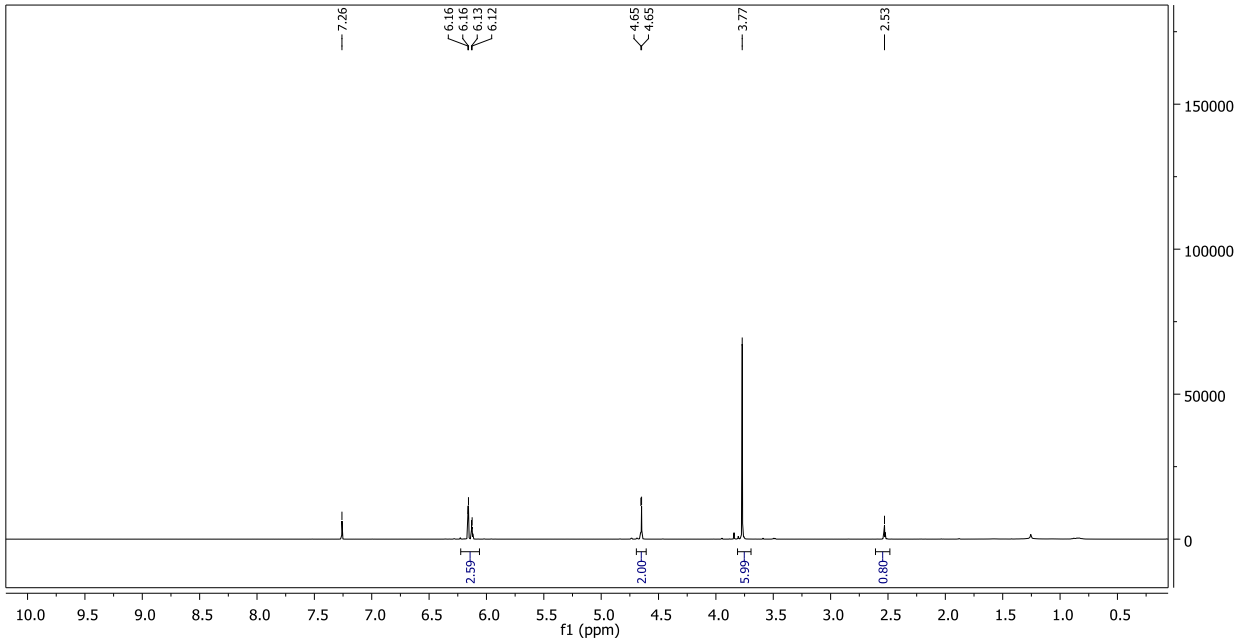
According to Method A of the general procedure, but using $Pd(OAc)_2$ instead of $PdCl_2(MeCN)_2$, 5-iodo-1,2,3-triazole **5c** (50 mg, 0.15 mmol), $Pd(OAc)_2$ (2 mg, 0.007 mmol), PPh_3 (4 mg, 0.015 mmol) and CsOPiv (69 mg, 0.30 mmol) were reacted in MeCN (2.4 mL) at 100 °C for 27 hours. Subsequent workup and flash column chromatography (petane:EtOAc 6:4) yielded **6c** as a slightly brown solid (277 mg, 85%). Characterization data were consistent with the literature.[16] **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.62 (d, *J* = 7.6 Hz, 1H), 7.35 – 7.53 (m, 3H), 5.30 (s, 2H), 2.96 (t, *J* = 7.6 Hz, 2H), 1.80 (qn, *J* = 7.6 Hz, 2H), 1.45 (sx, *J* = 7.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 140.7, 139.4, 139.3, 128.8, 128.6, 127.7, 124.2, 120.9, 51.0, 31.7, 25.7, 22.4, 13.9. **mp** = 73 – 75 °C.

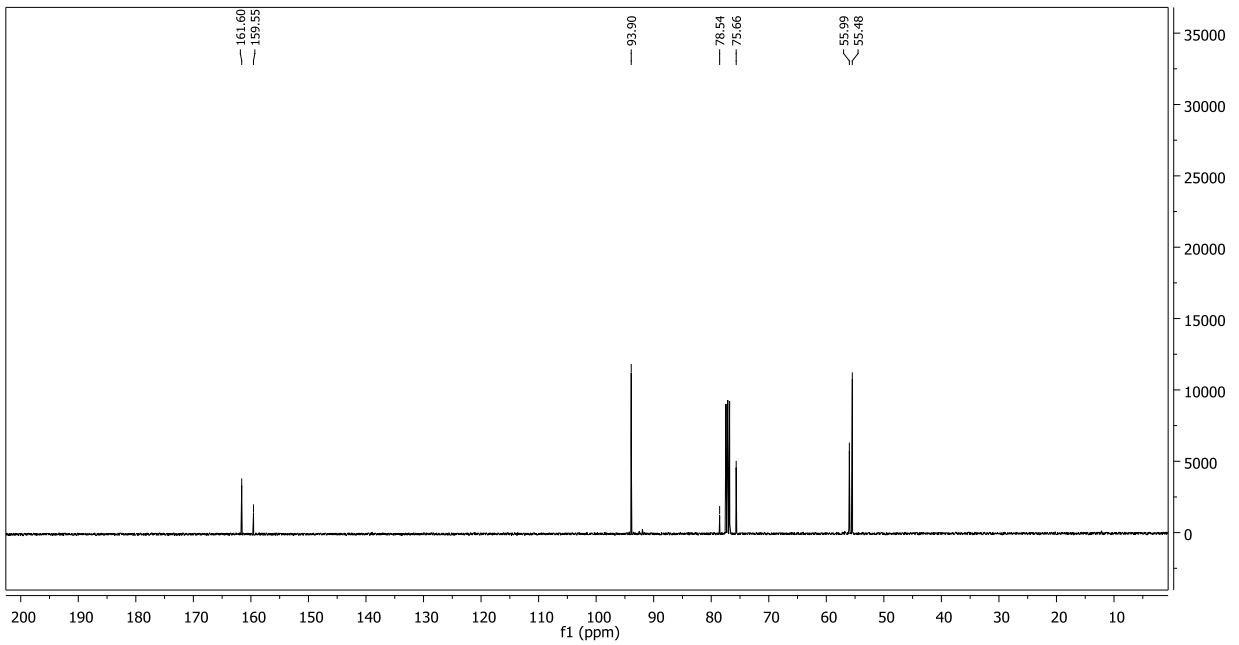
[16] Chowdhury, C.; Mandal, S. B.; Achari, B. *Tetrahedron Lett.* **2005**, *46*, 8531.

Spectra

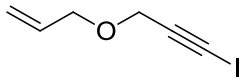
1,3-dimethoxy-5-(prop-2-yn-1-yloxy)benzene (S3)

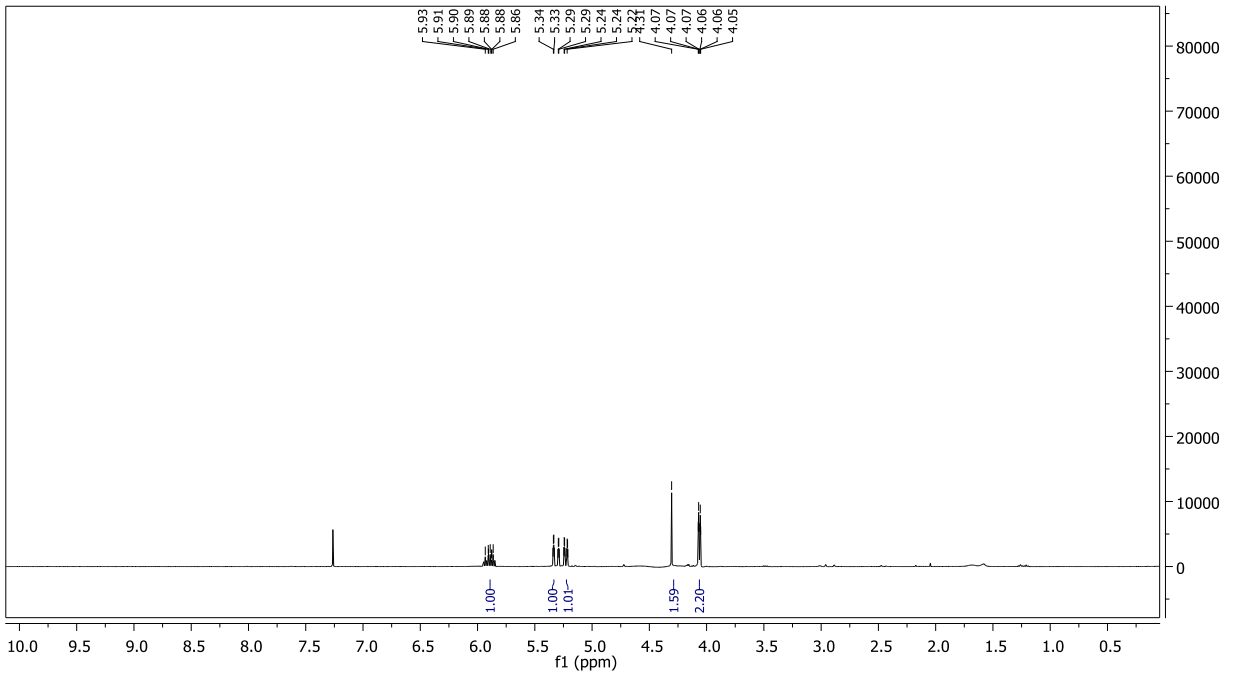


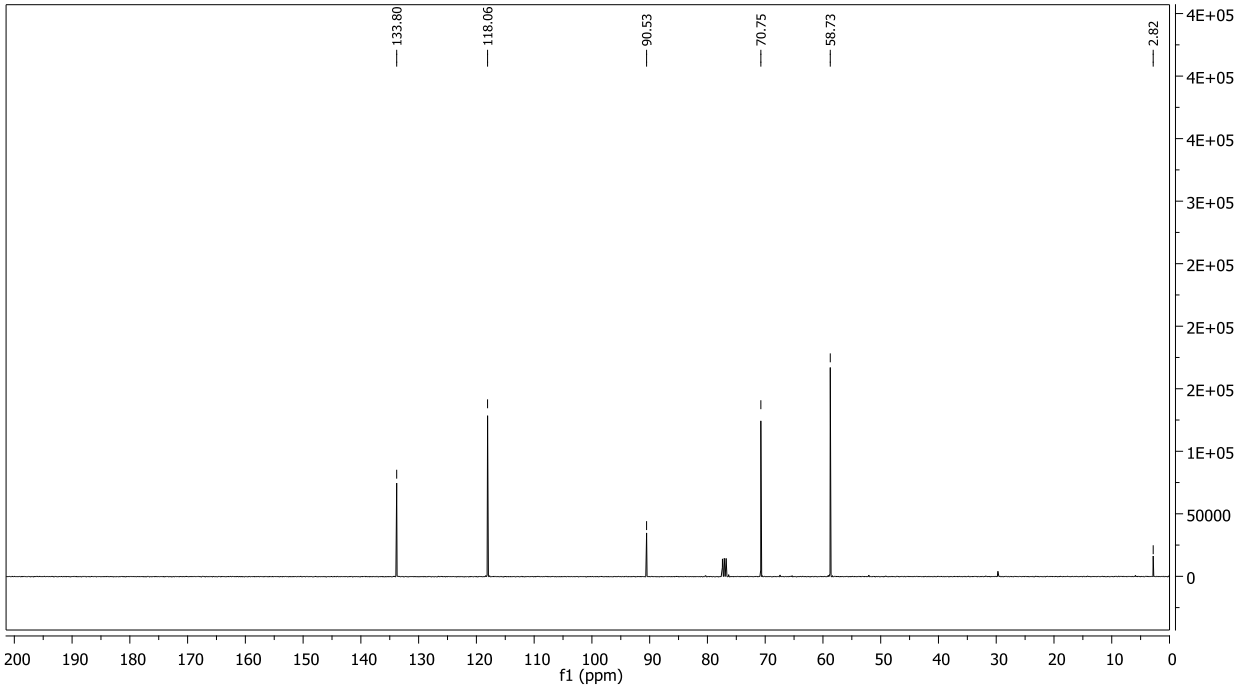




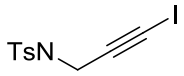
3-((3-iodoprop-2-yn-1-yl)oxy)prop-1-ene (S9)

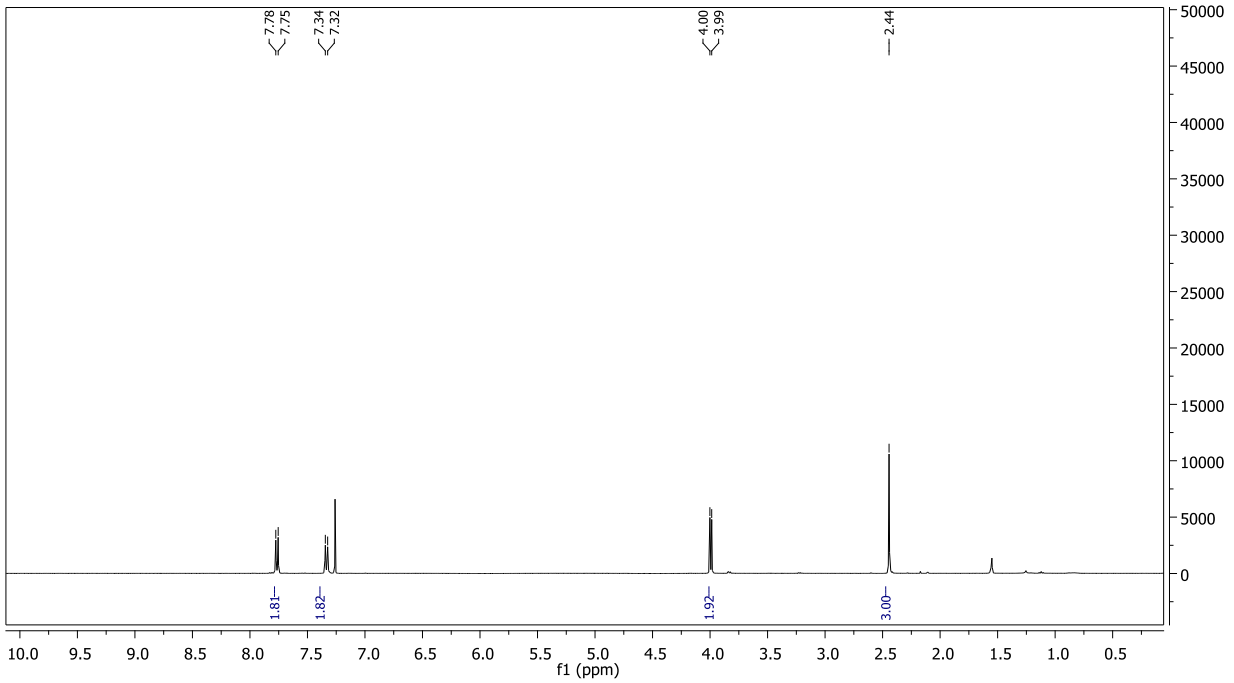


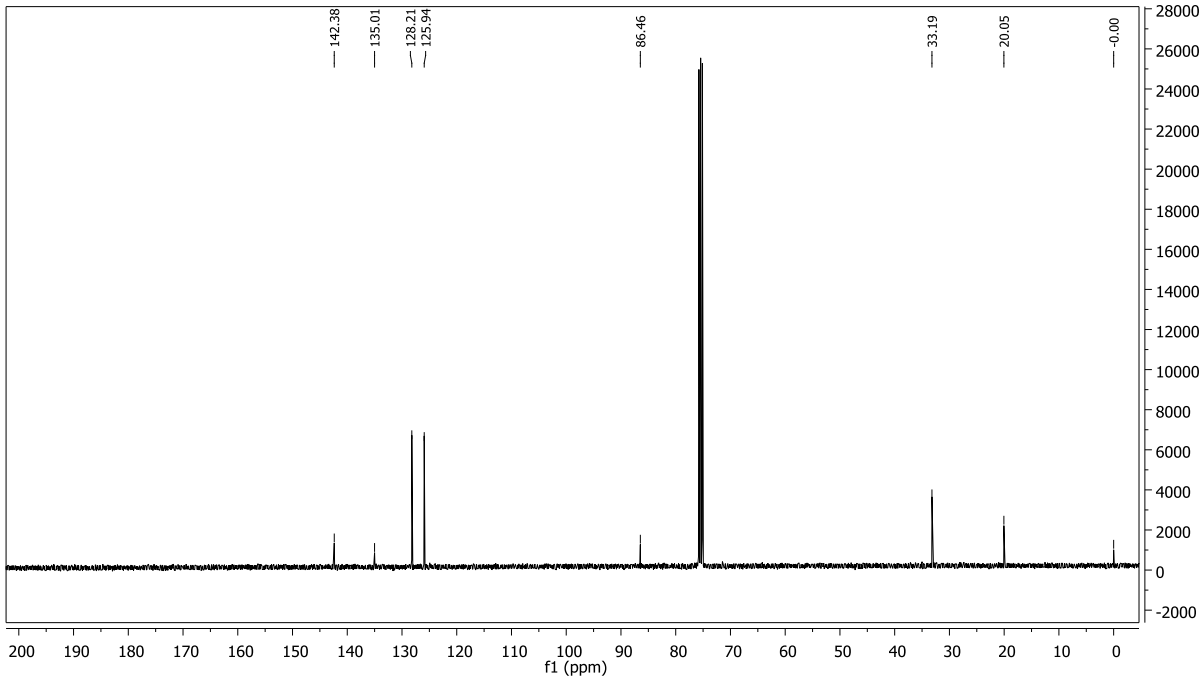




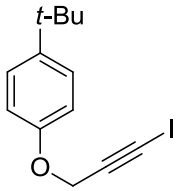
N-(3-iodoprop-2-yn-1-yl)-4-methylbenzenesulfonamide (S10)

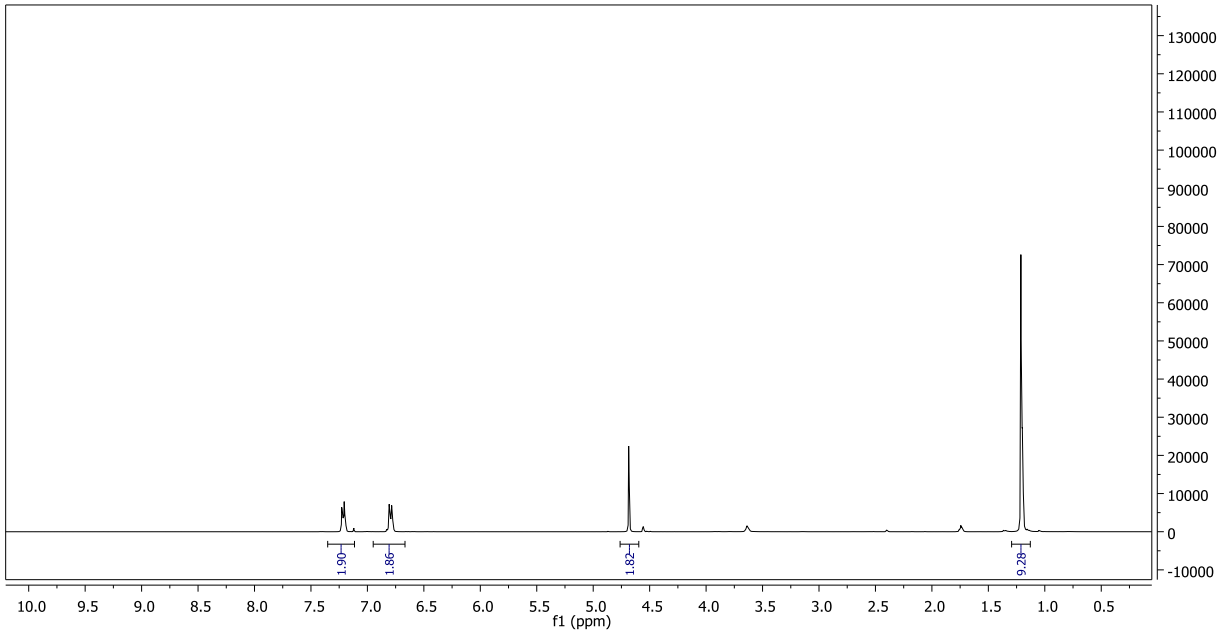


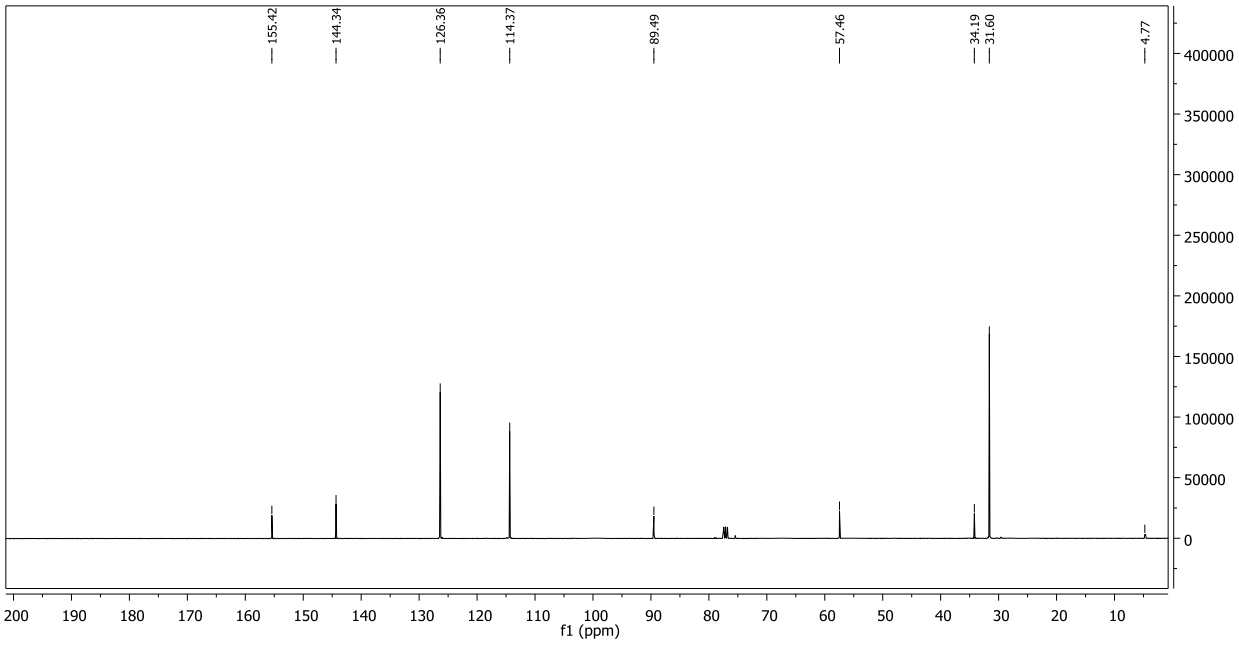




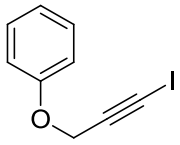
1-(tert-butyl)-4-((3-iodoprop-2-yn-1-yl)oxy)benzene (S13)

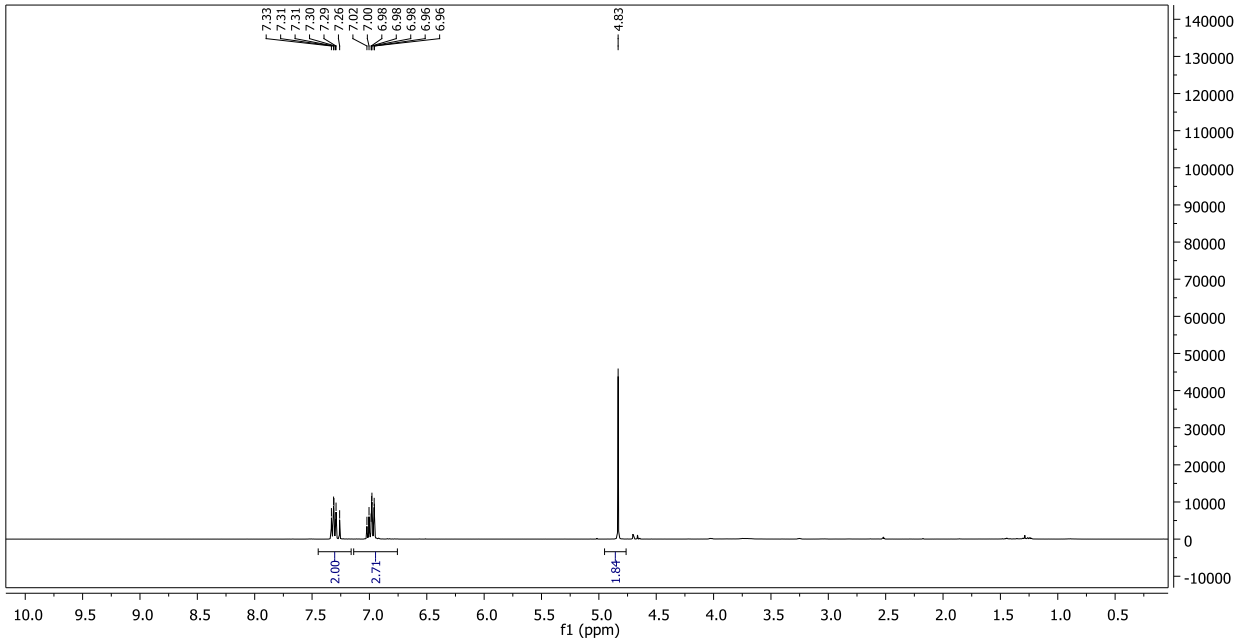


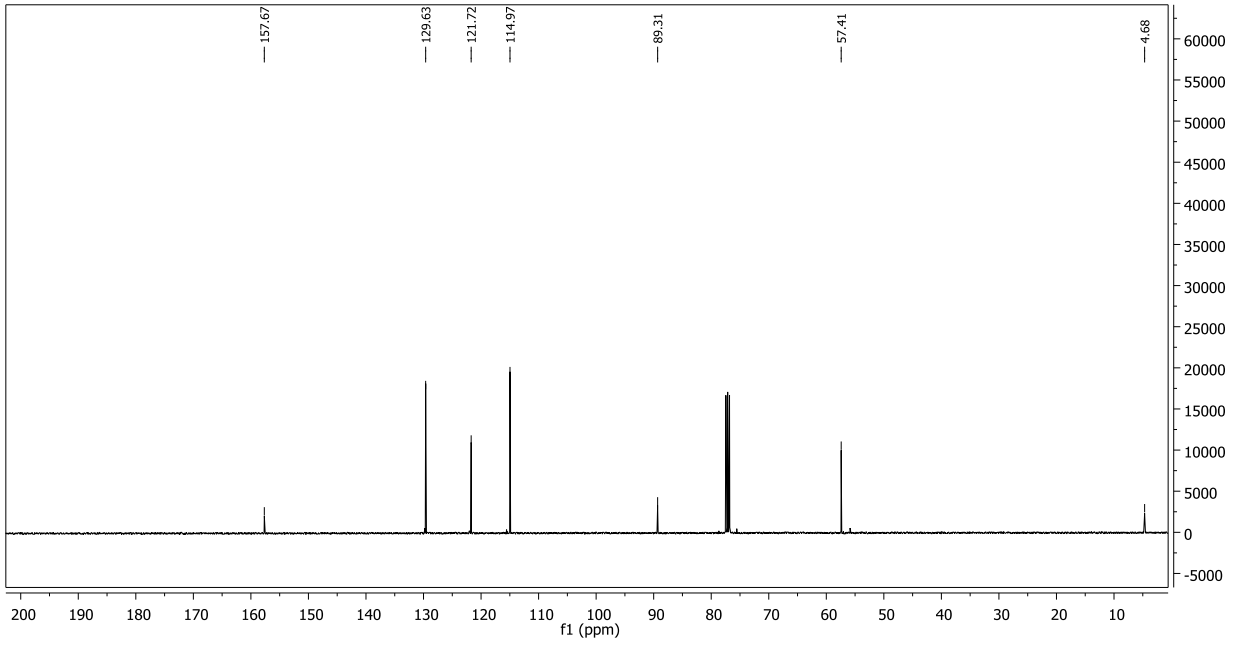




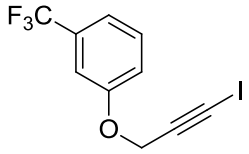
((3-iodoprop-2-yn-1-yl)oxy)benzene (S15)

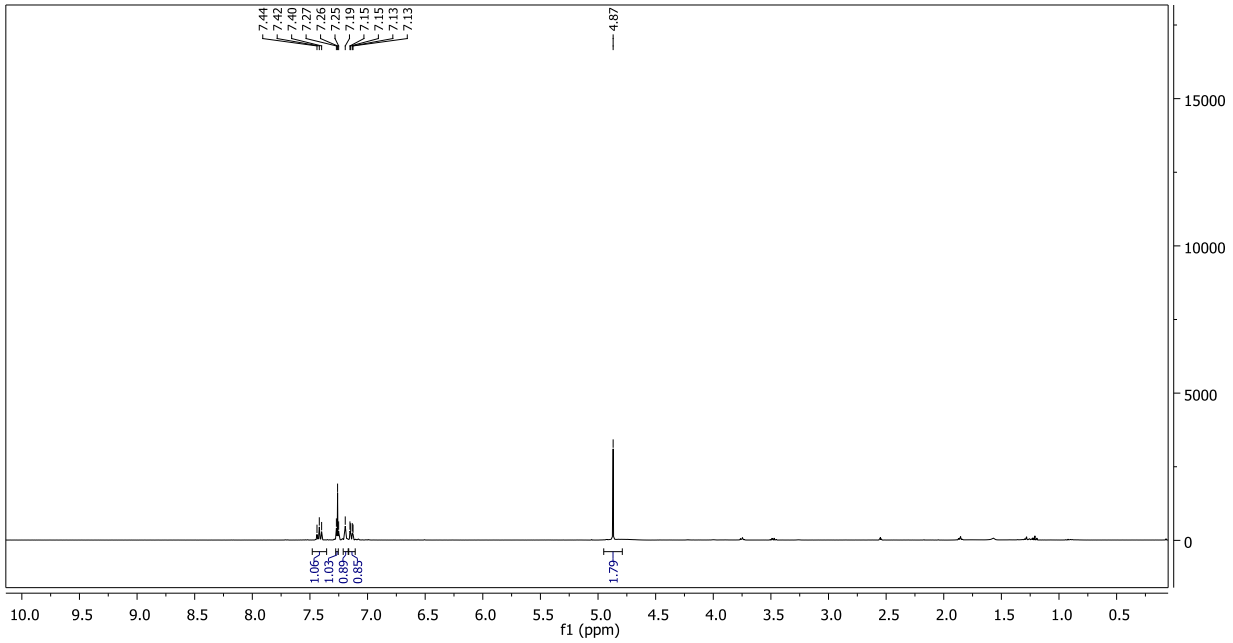


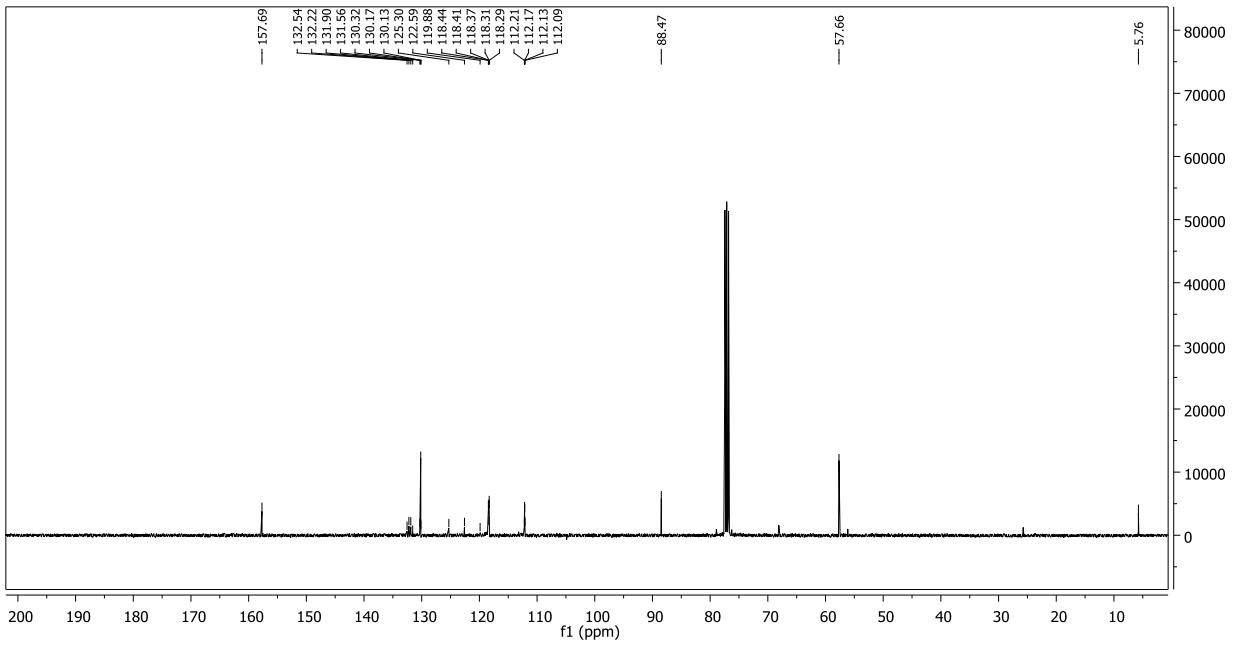


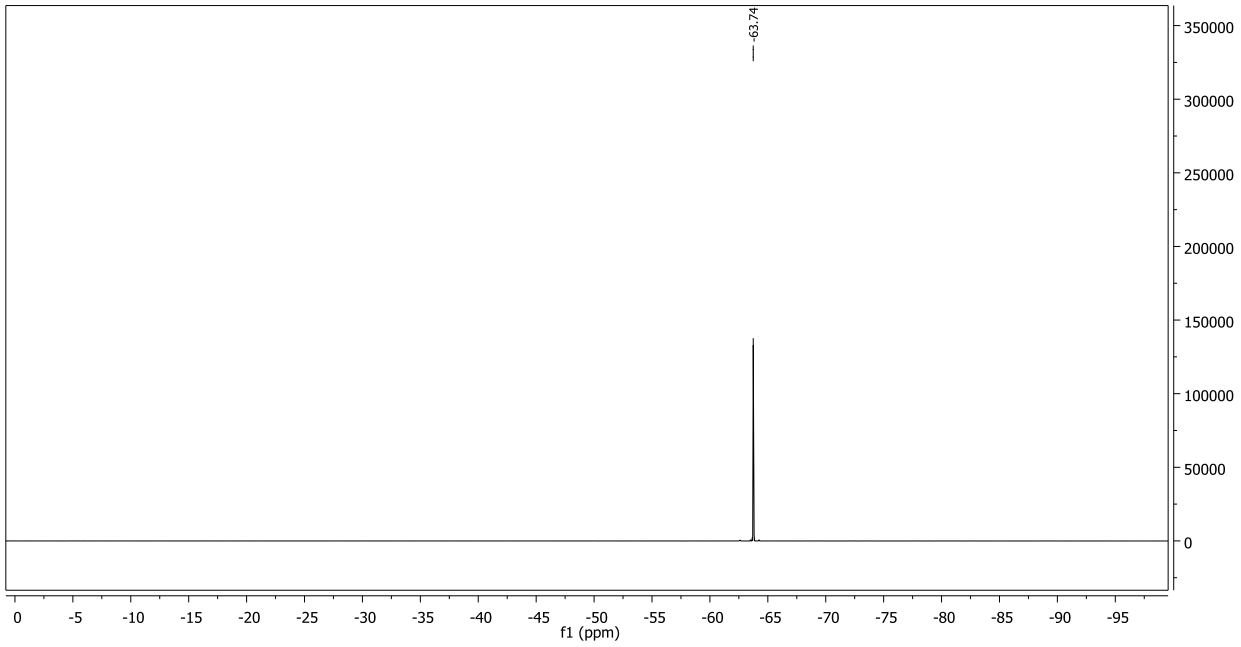


1-((3-iodoprop-2-yn-1-yl)oxy)-3-(trifluoromethyl)benzene (S16)





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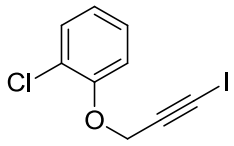
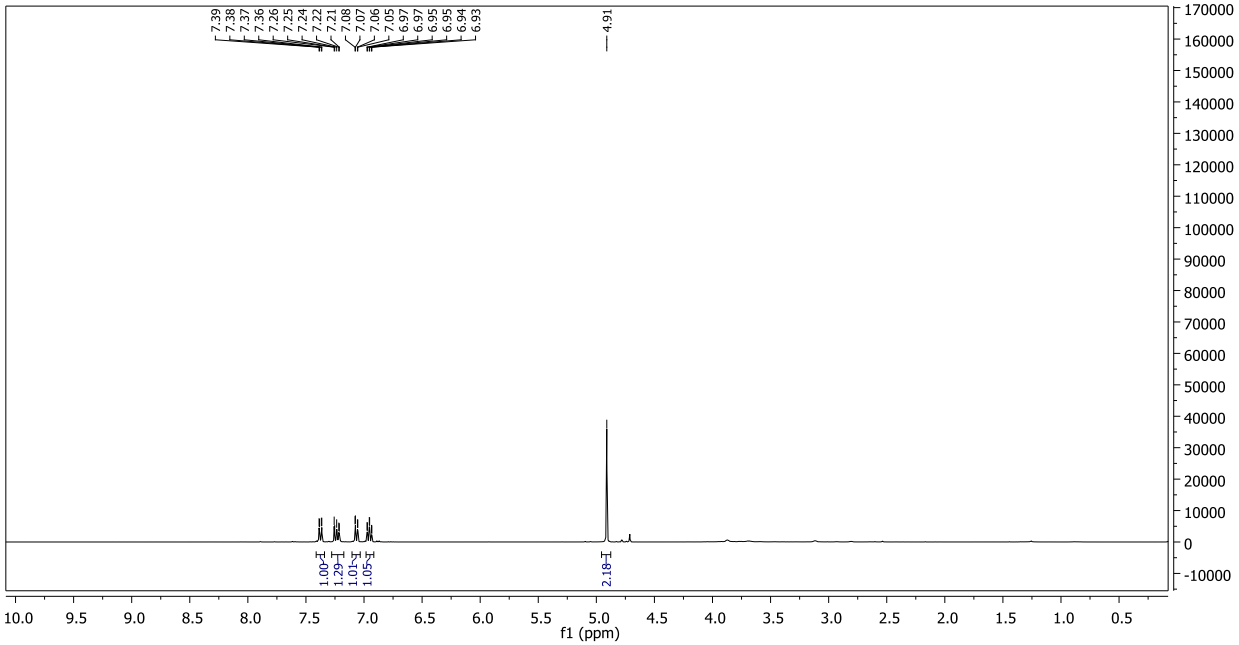
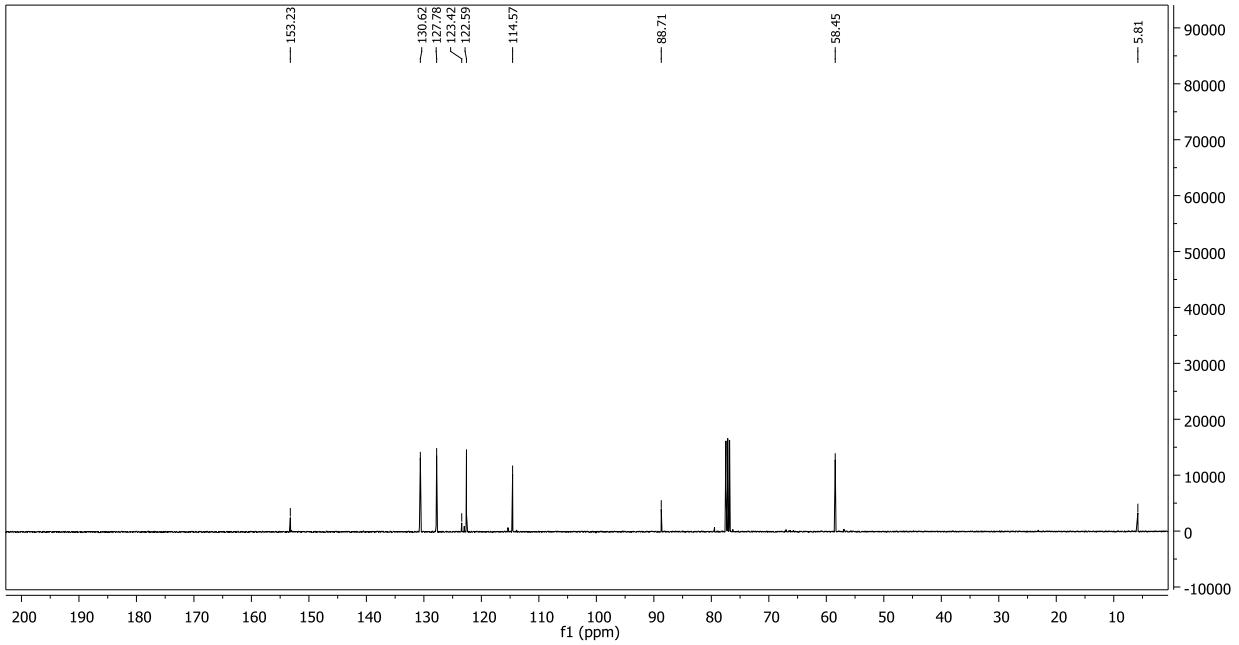
f1 (ppm)

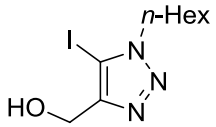
1-chloro-2-((3-iodoprop-2-yn-1-yl)oxy)benzene (S17)

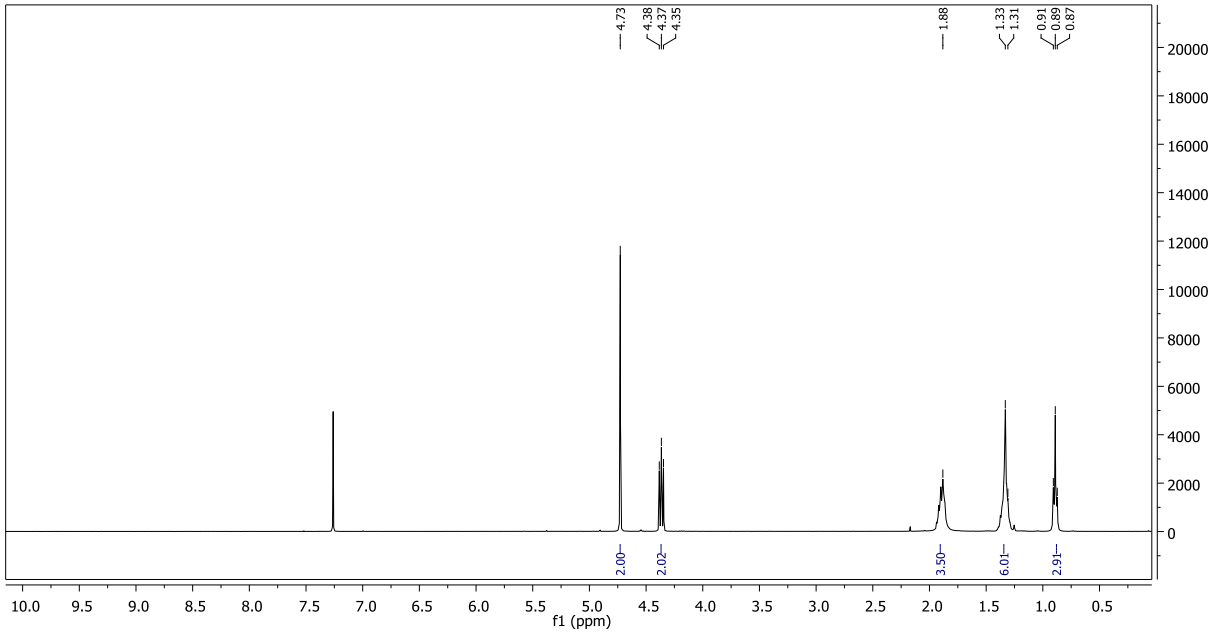


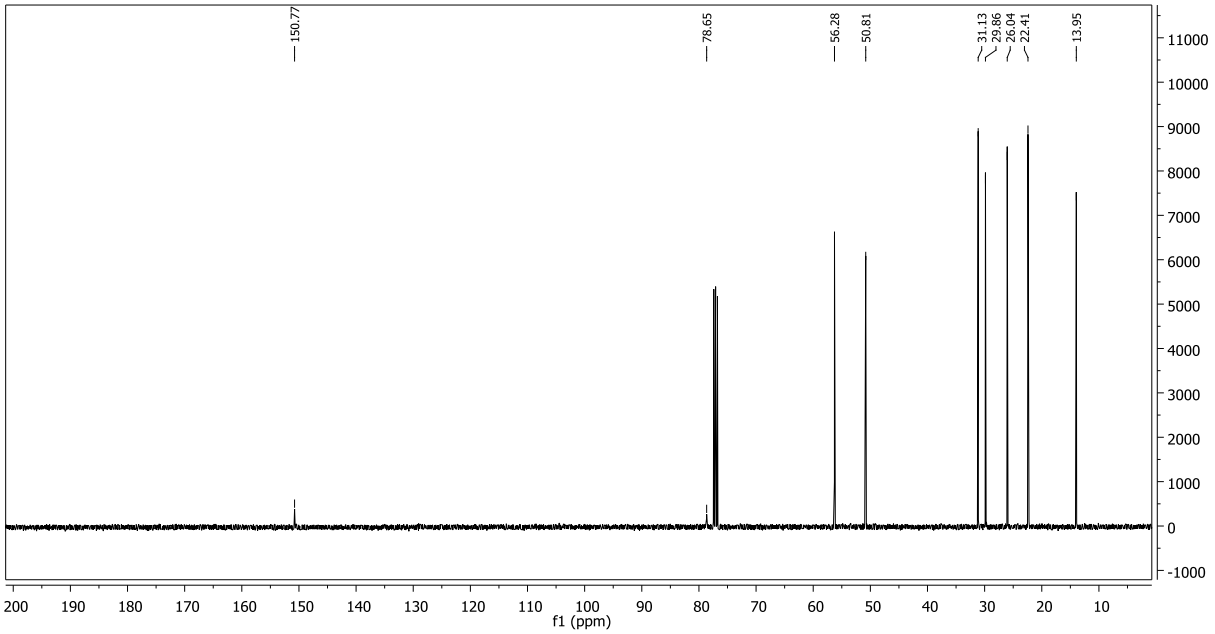




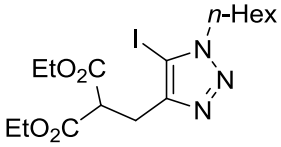
(1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methanol (S19)

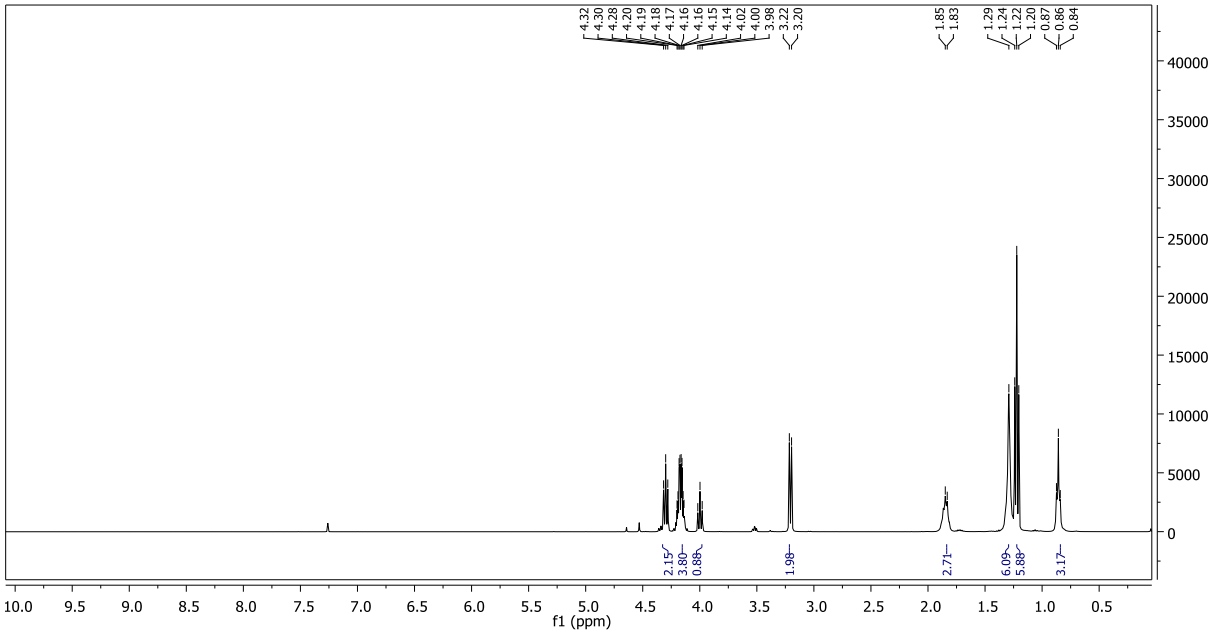


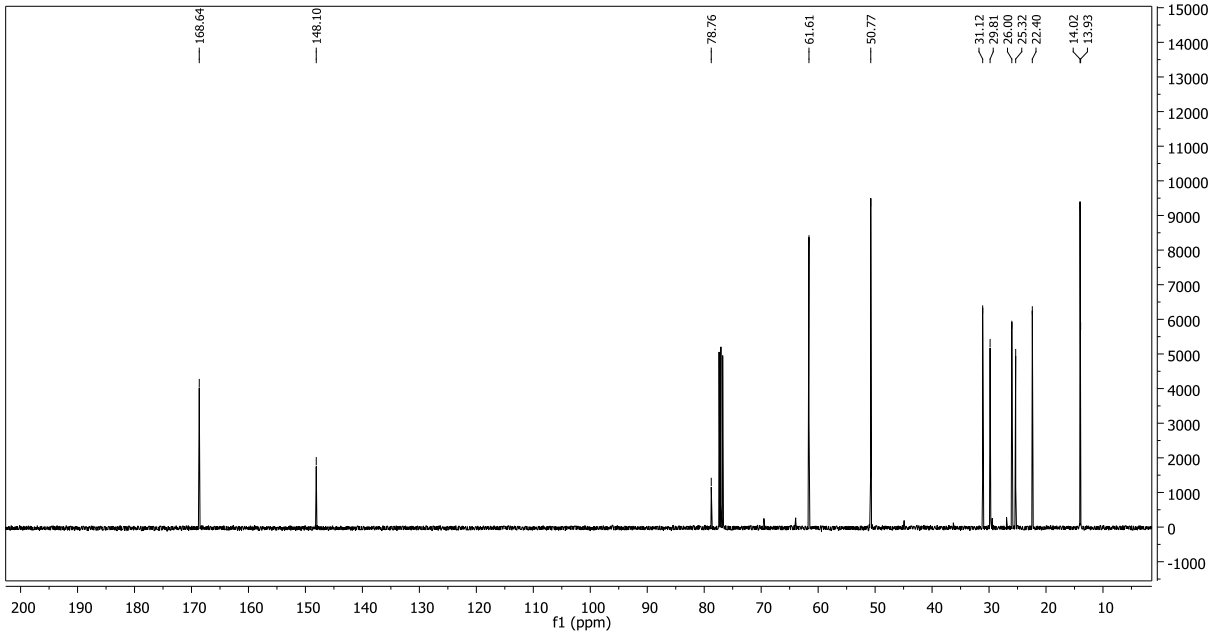




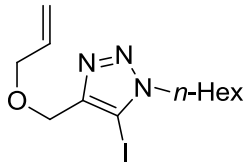
diethyl 2-((1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methyl)malonate (S20)

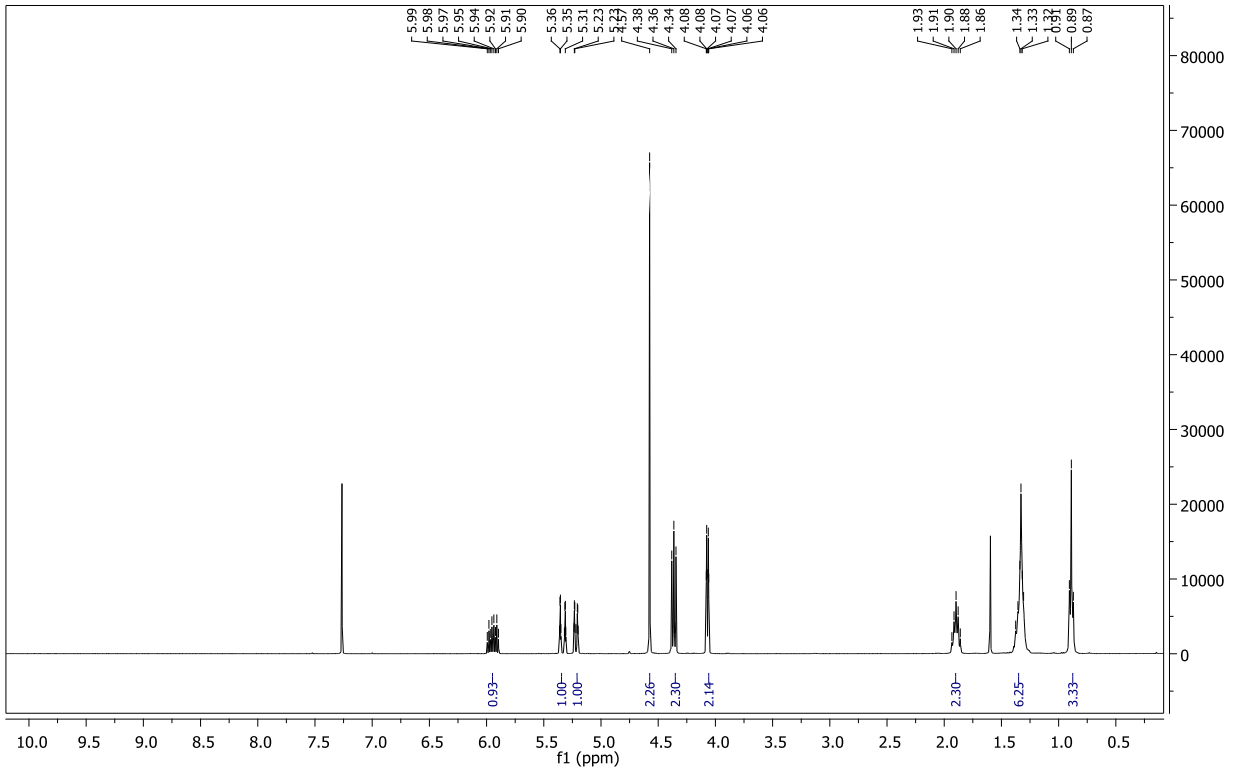


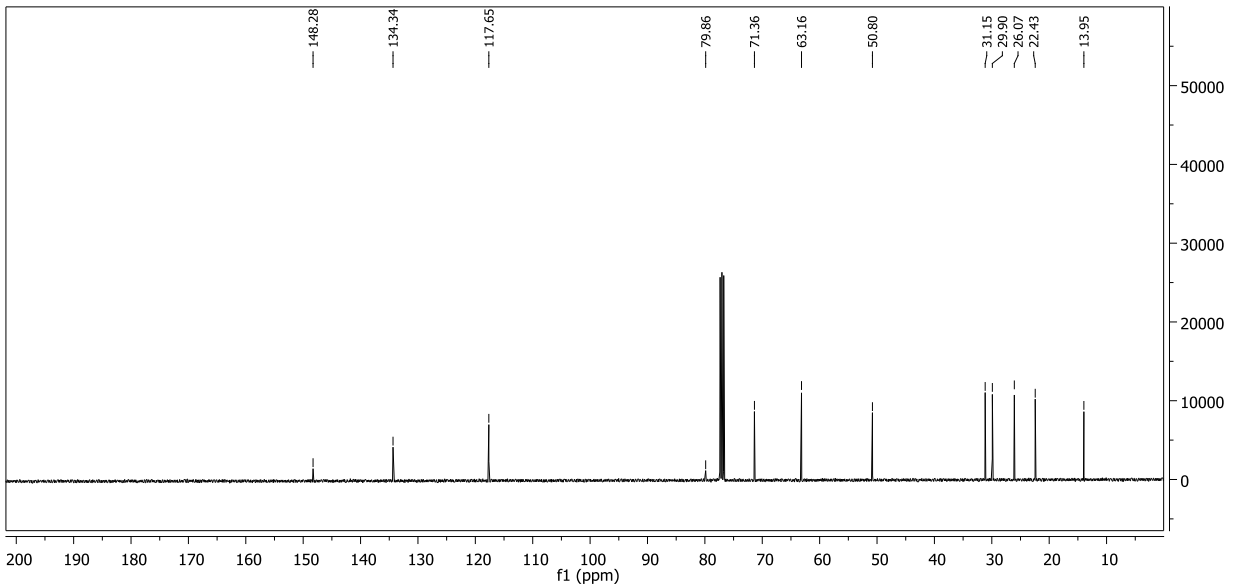




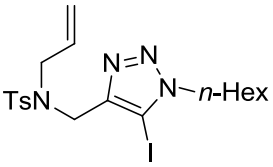
4-((allyloxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (1a)

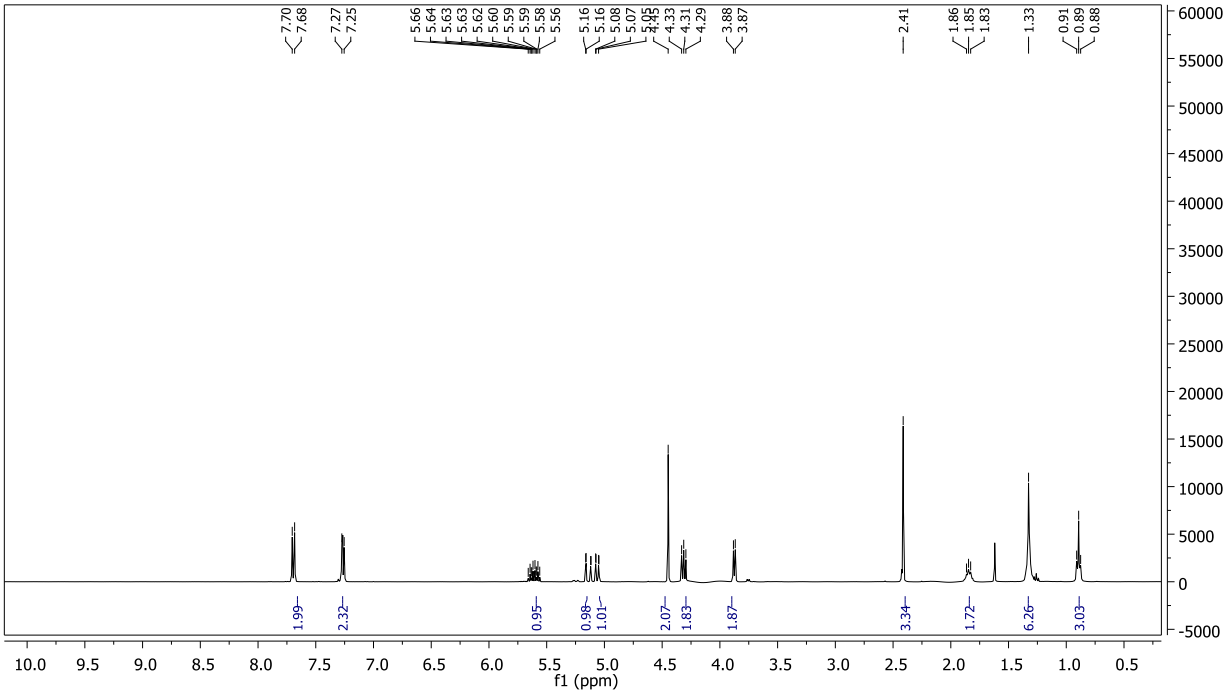


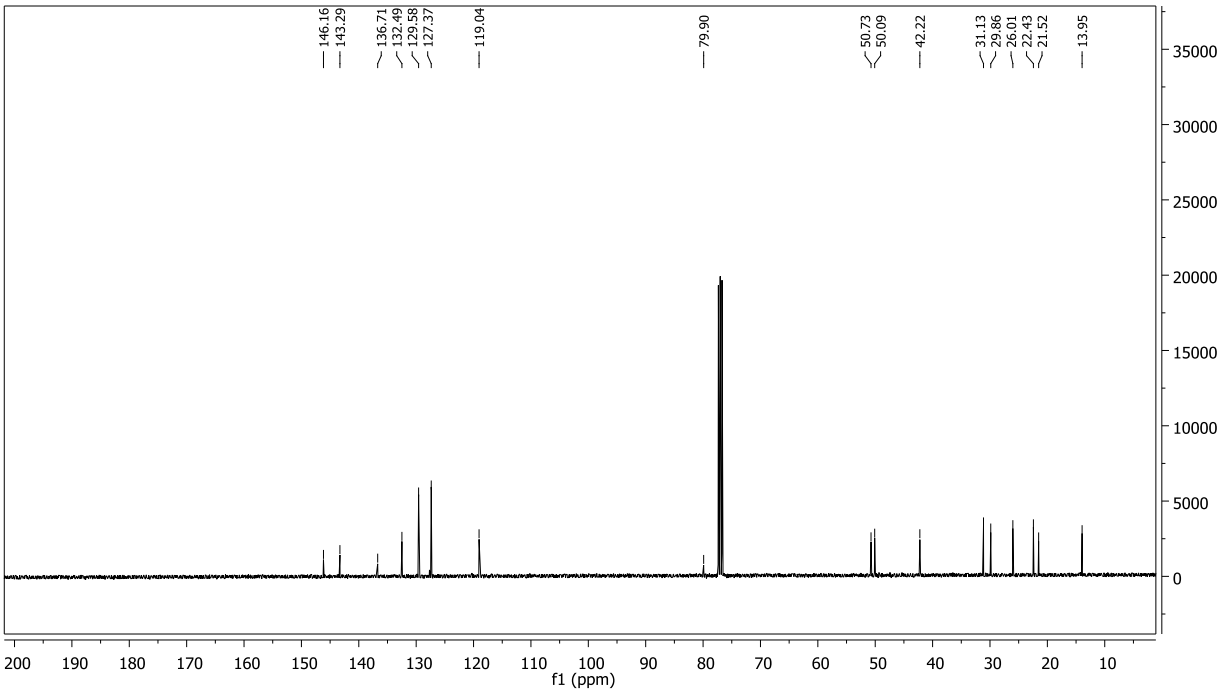




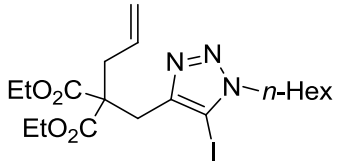
N-allyl-N-((1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methyl)-4-methylbenzenesulfonamide (1b)

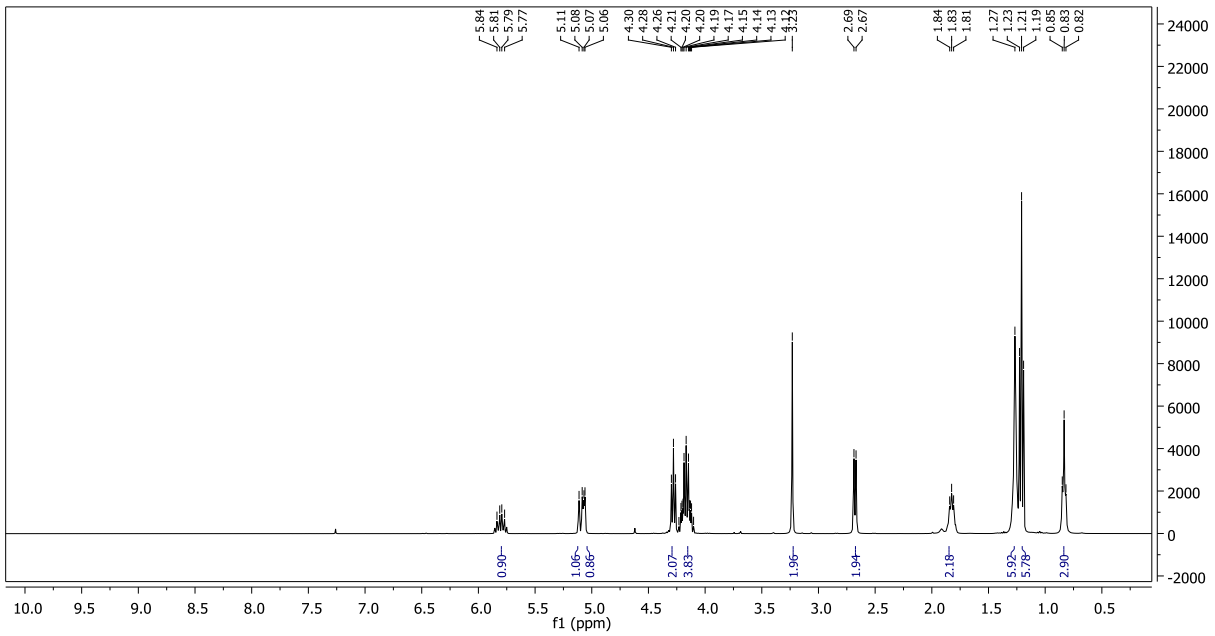


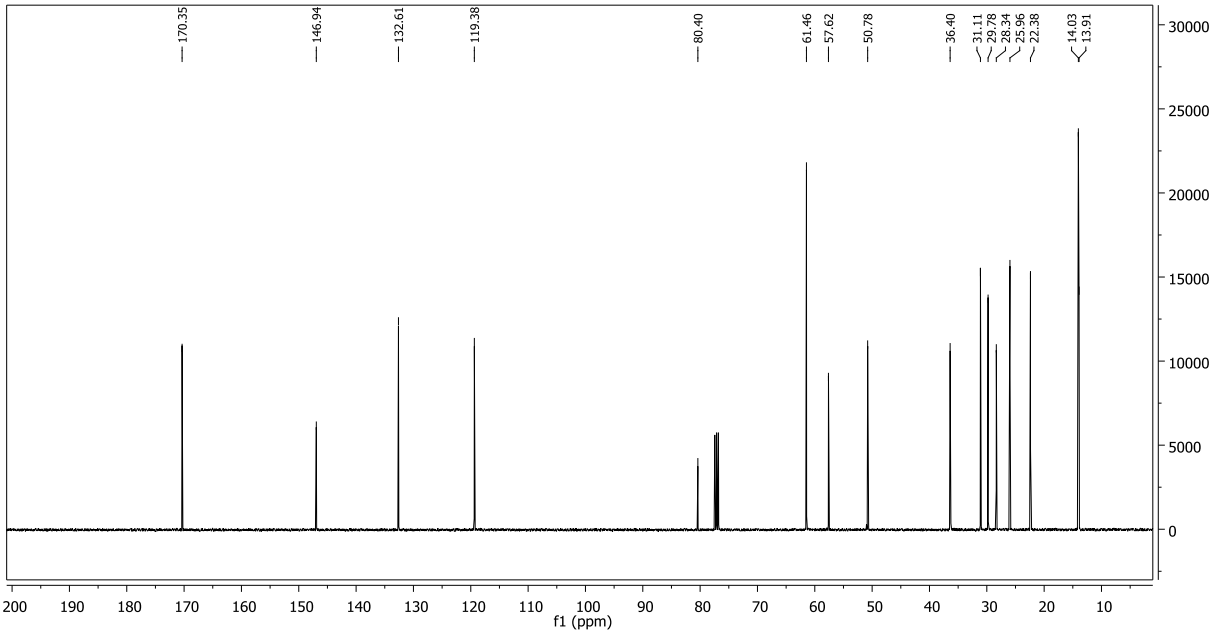




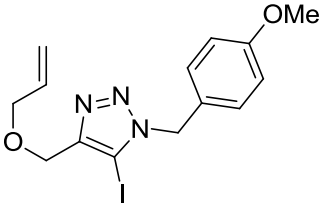
diethyl 2-allyl-2-((1-hexyl-5-iodo-1H-1,2,3-triazol-4-yl)methyl)malonate (1c)

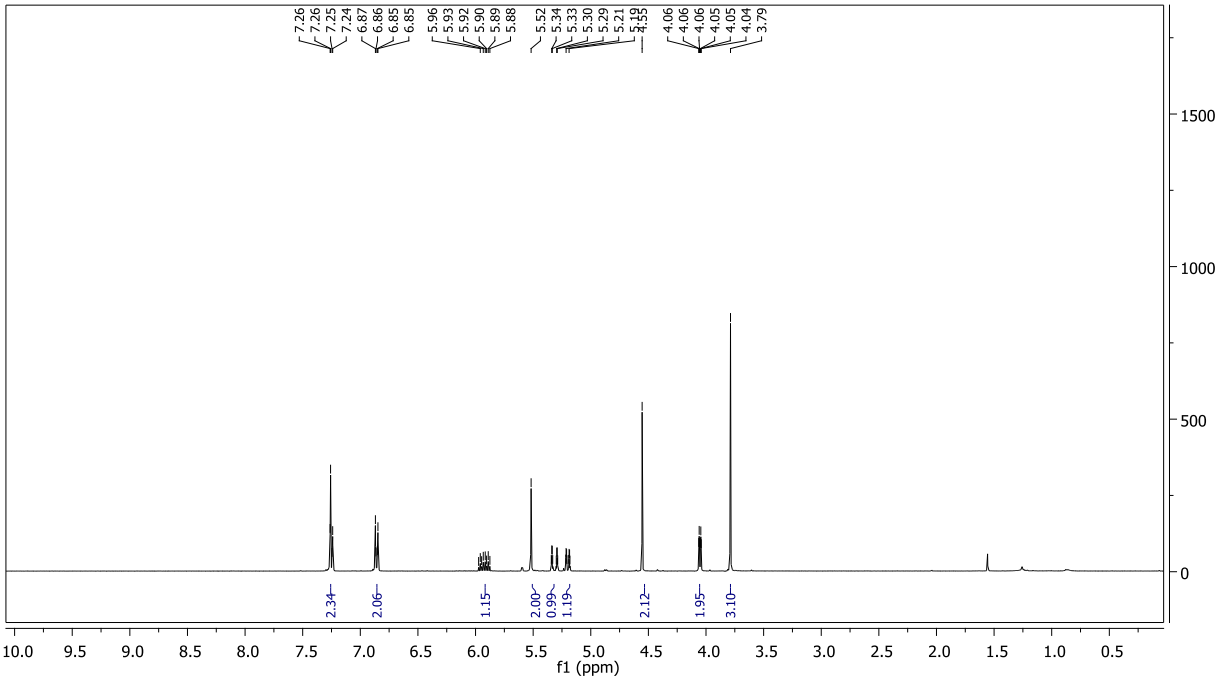


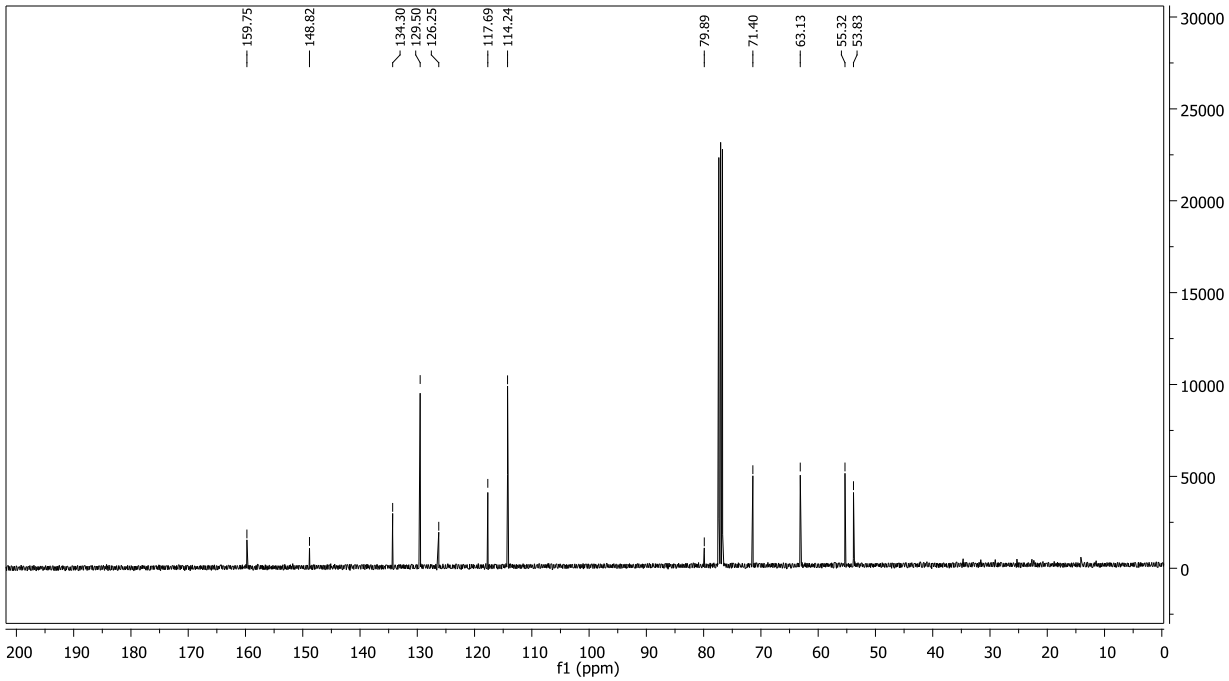




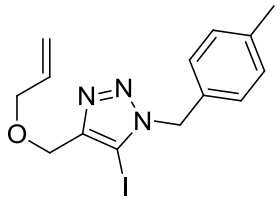
4-((allyloxy)methyl)-5-iodo-1-(4-methoxybenzyl)-1H-1,2,3-triazole (1d)

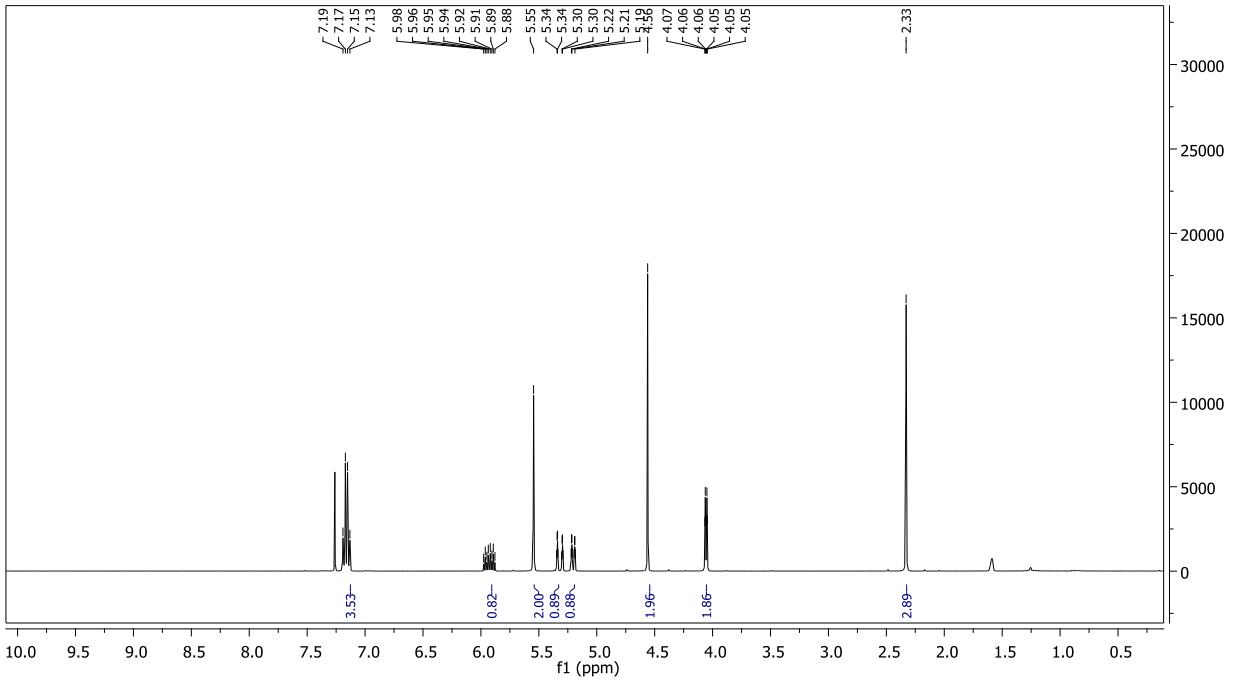


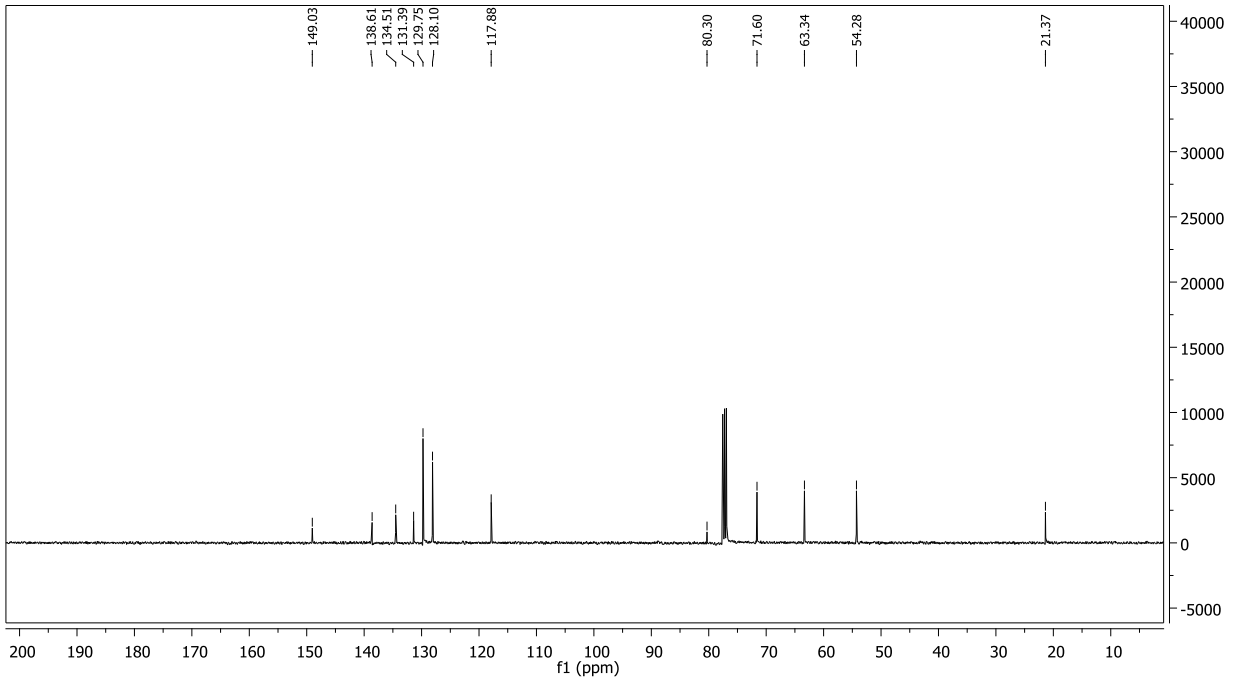




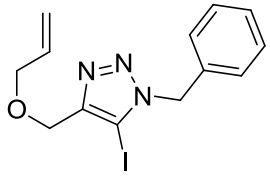
4-((allyloxy)methyl)-5-iodo-1-(4-methylbenzyl)-1H-1,2,3-triazole (1e)

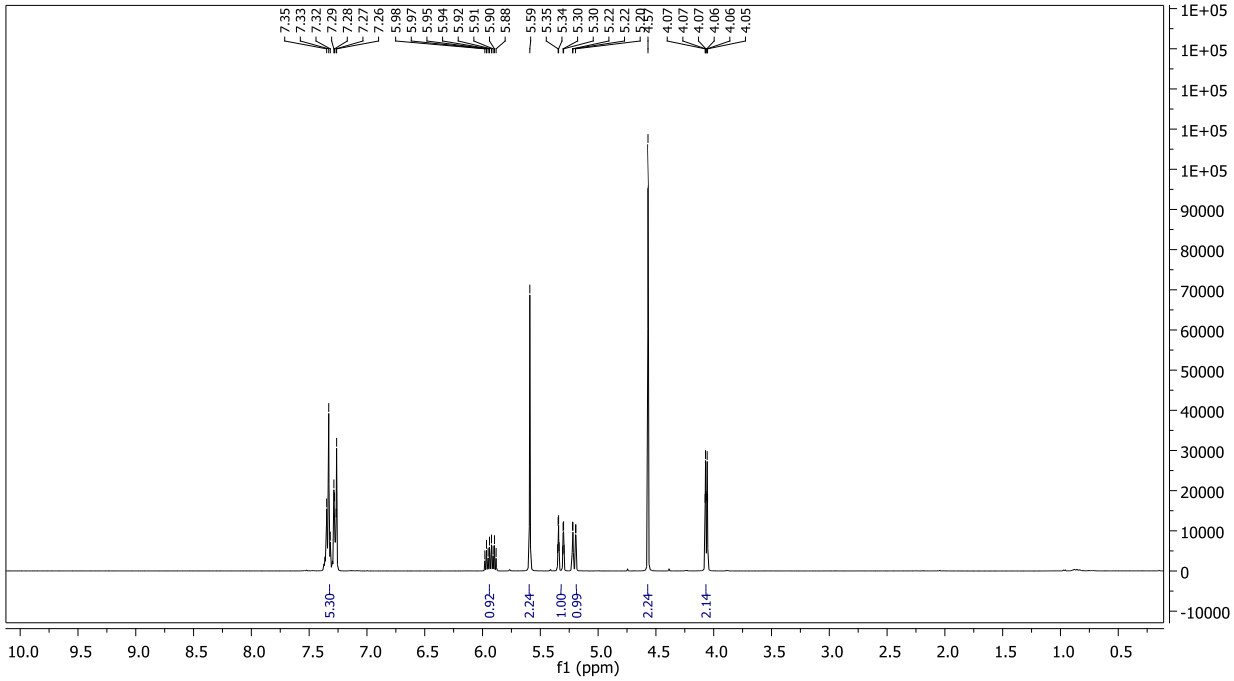


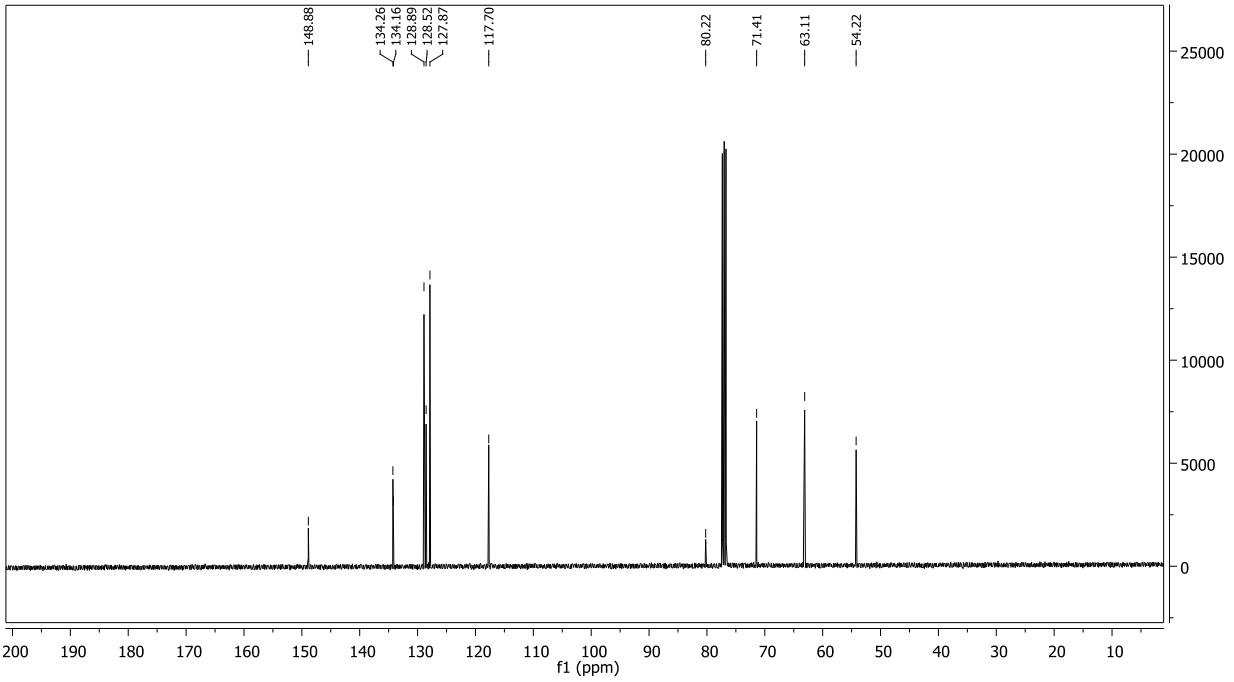




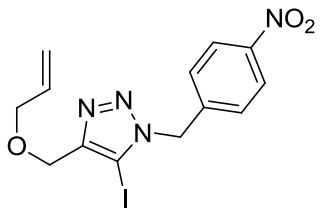
4-((allyloxy)methyl)-1-benzyl-5-iodo-1H-1,2,3-triazole (1f)

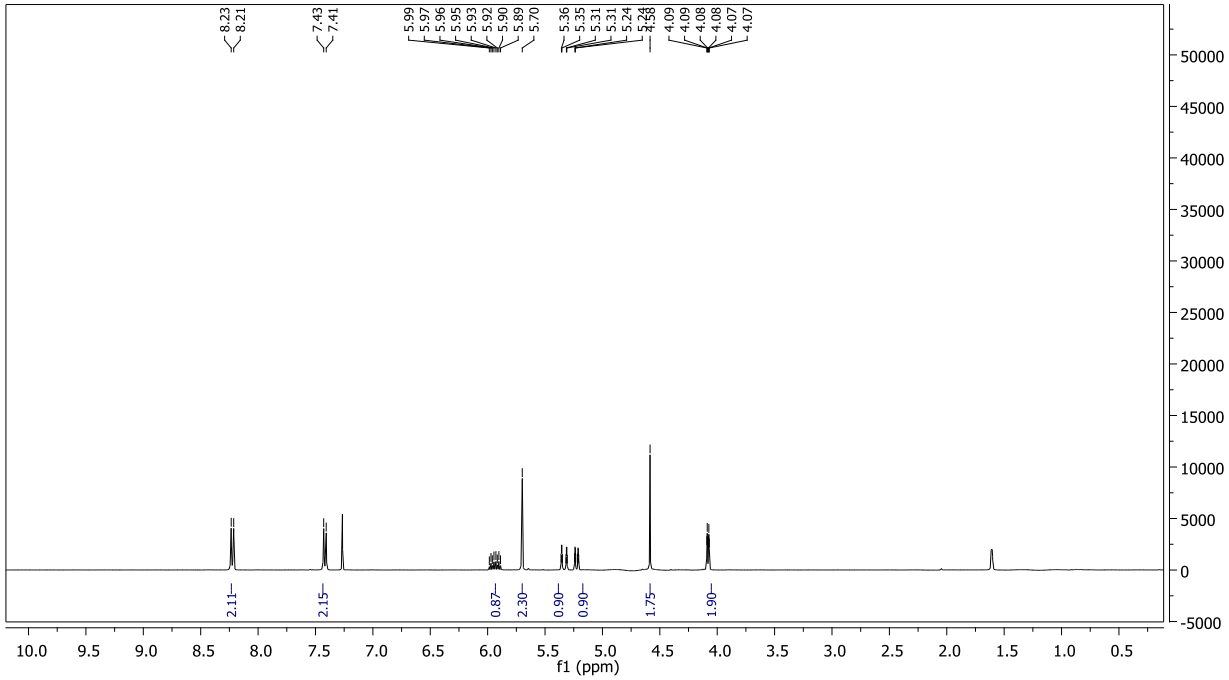


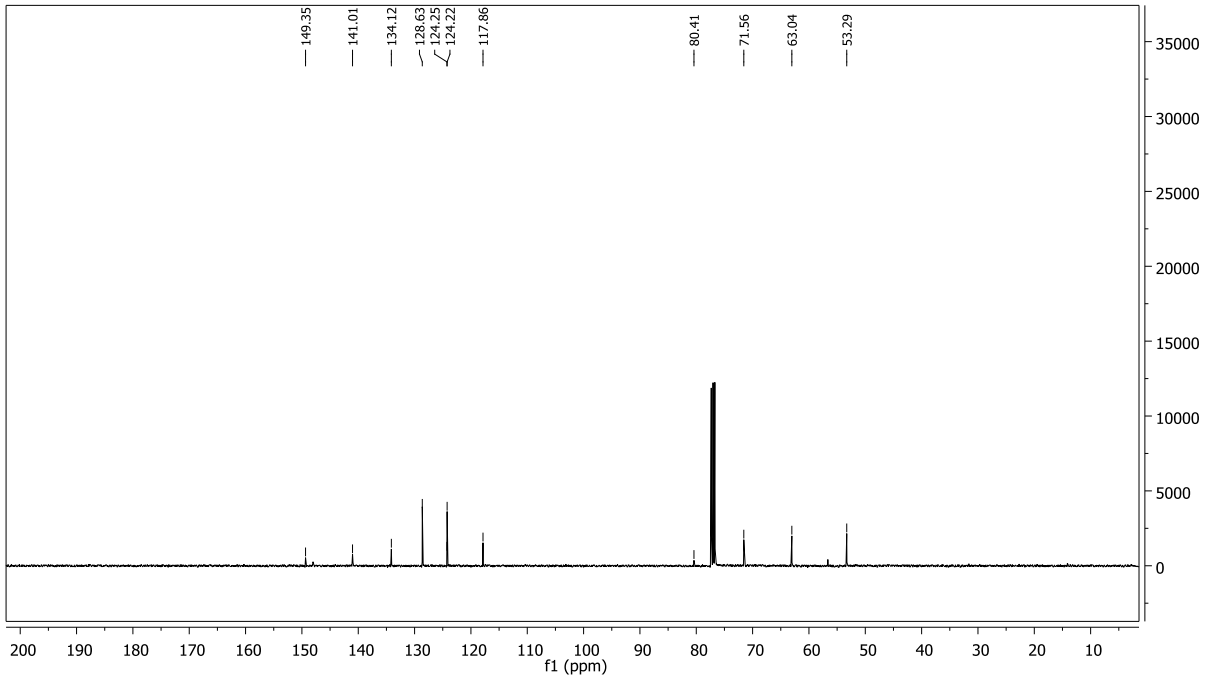




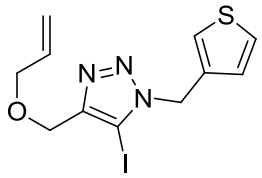
4-((allyloxy)methyl)-5-iodo-1-(4-nitrobenzyl)-1H-1,2,3-triazole (1g)

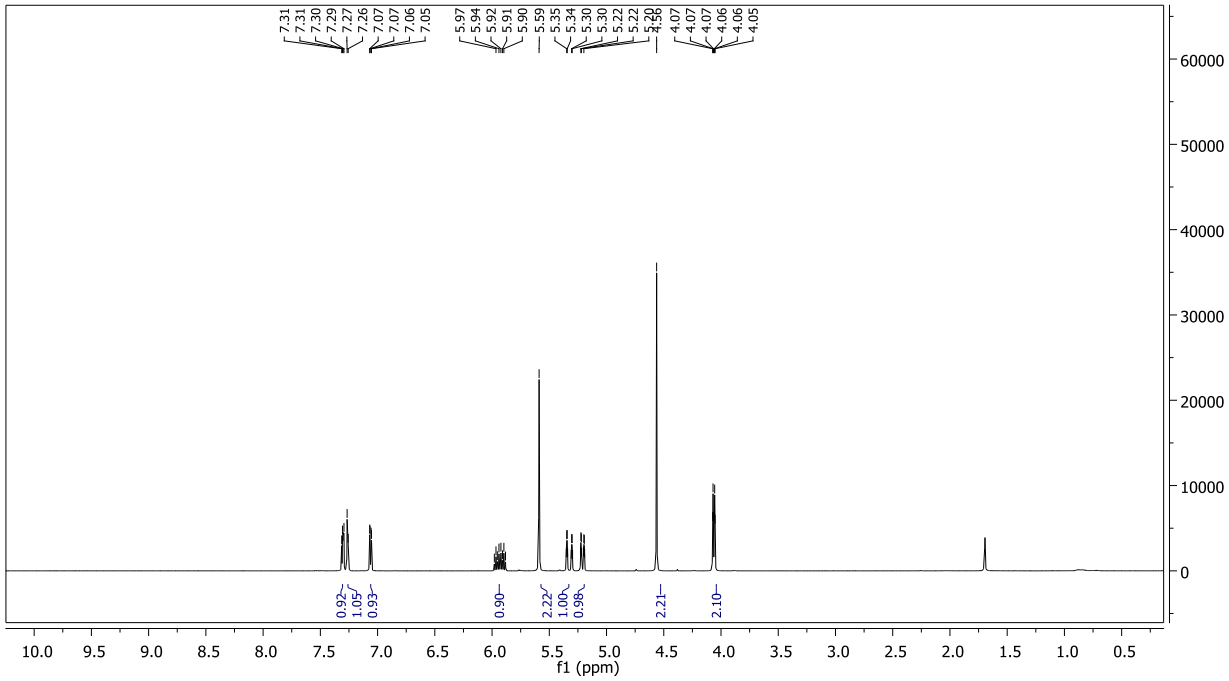


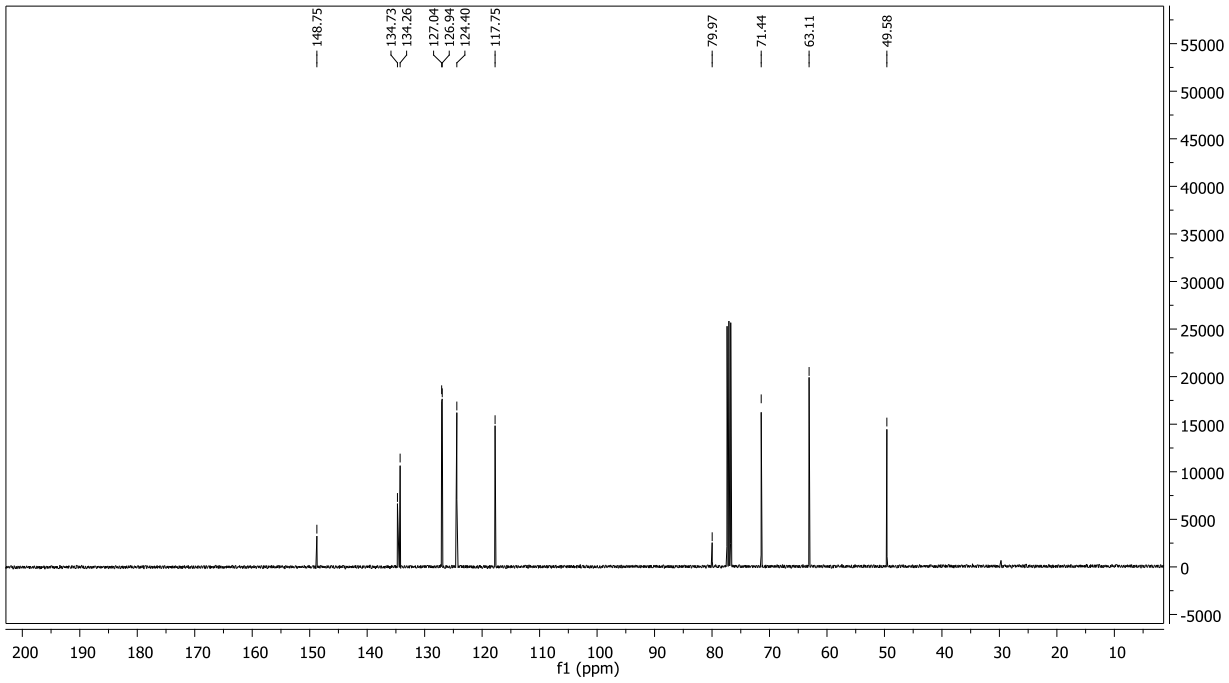




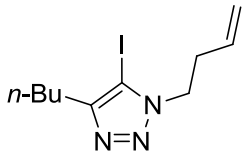
4-((allyloxy)methyl)-5-iodo-1-(thiophen-3-ylmethyl)-1H-1,2,3-triazole (1h)

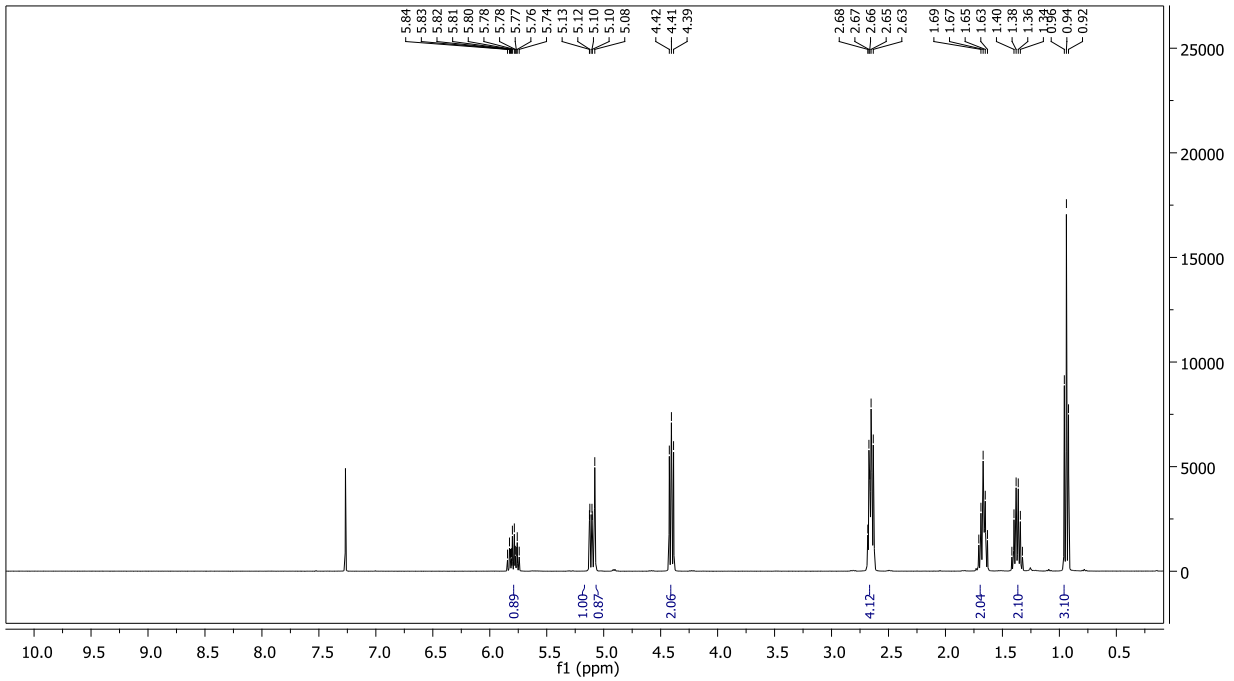


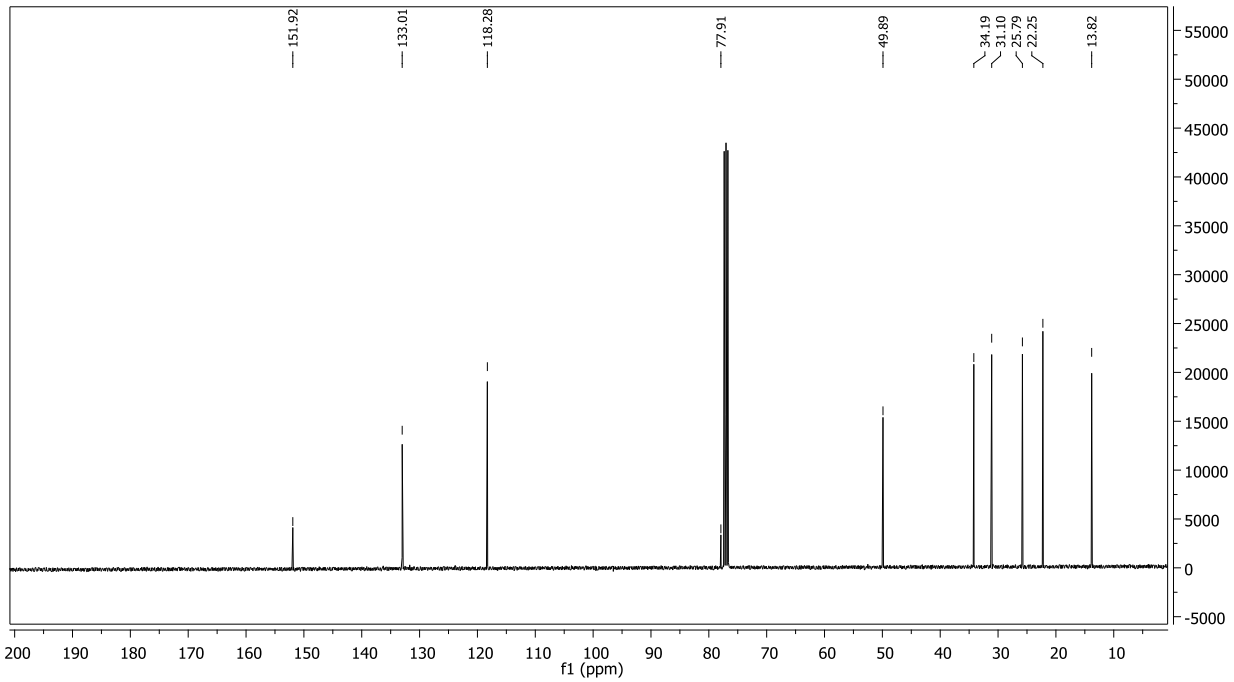




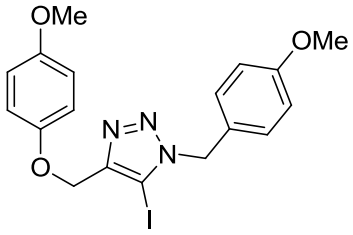
1-(but-3-en-1-yl)-4-butyl-5-iodo-1H-1,2,3-triazole (1i)

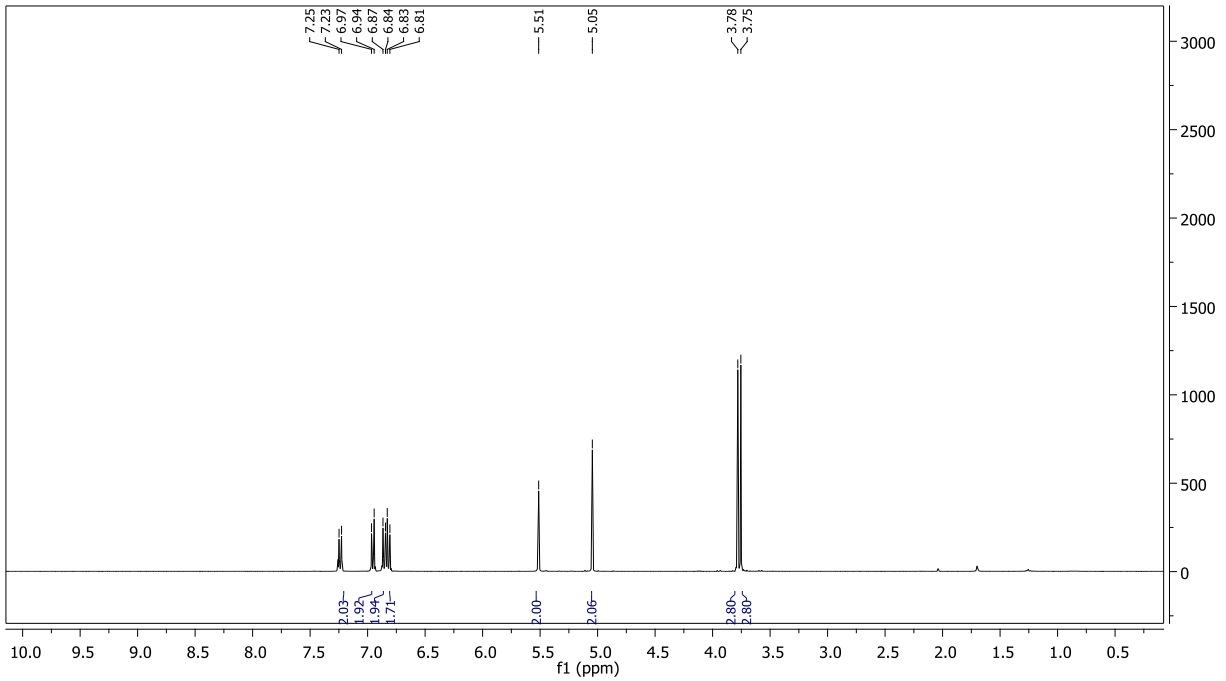


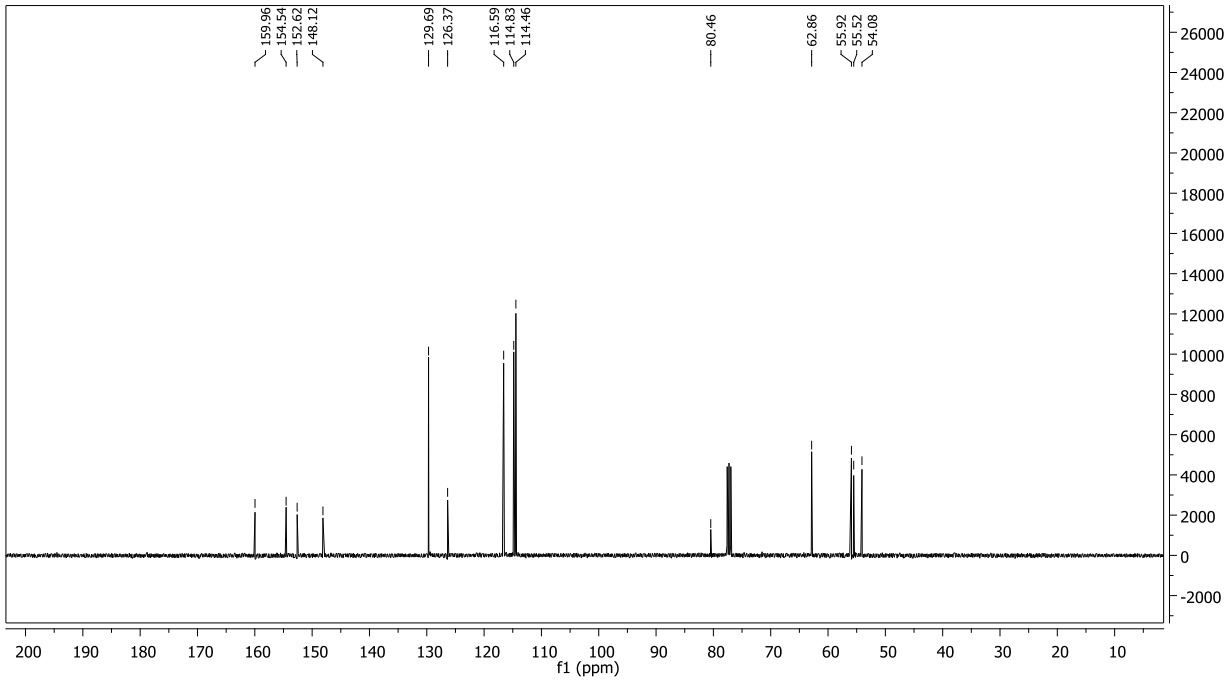




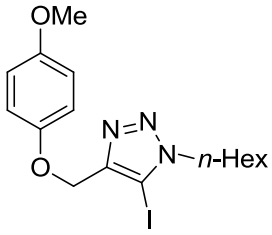
5-iodo-1-(4-methoxybenzyl)-4-((4-methoxyphenoxy)methyl)-1H-1,2,3-triazole (3g)

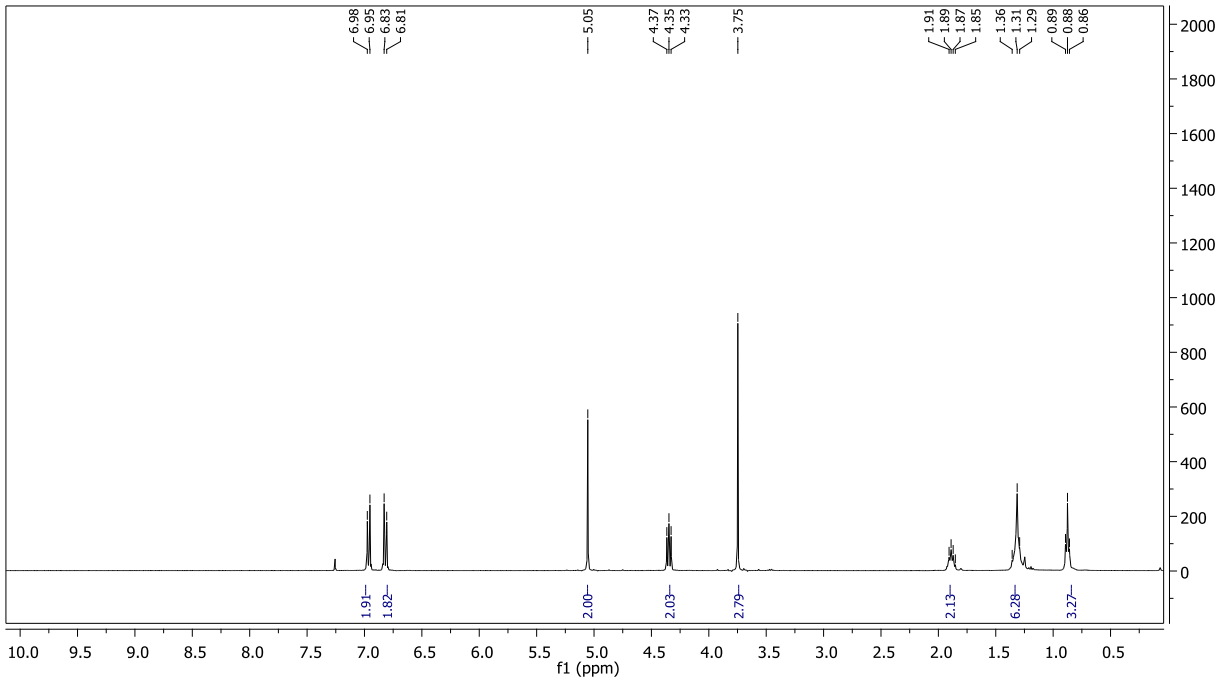


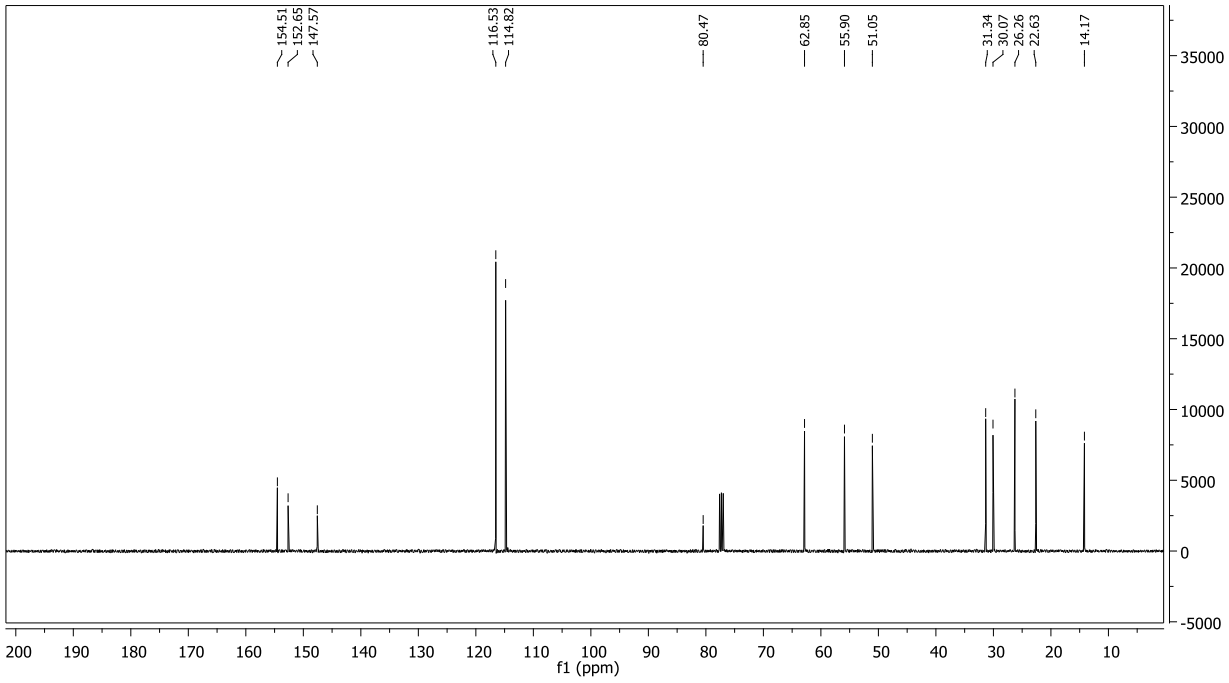




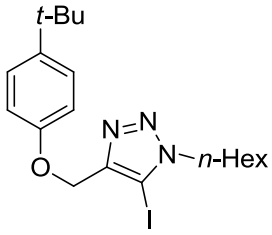
1-hexyl-5-iodo-4-((4-methoxyphenoxy)methyl)-1H-1,2,3-triazole (3a)

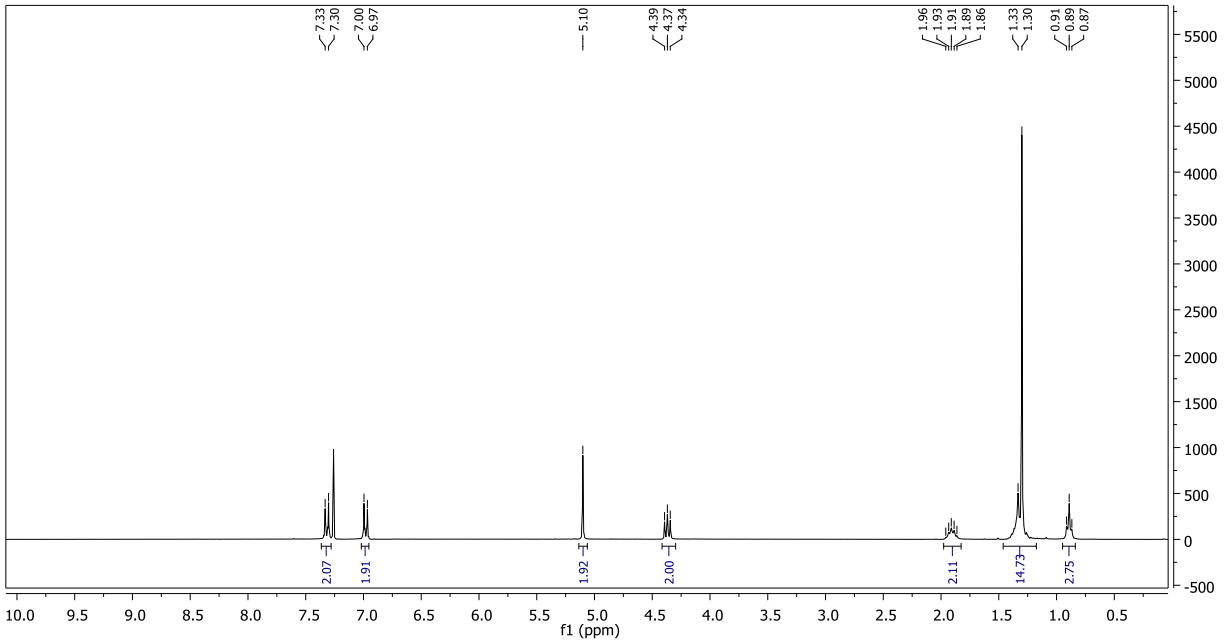


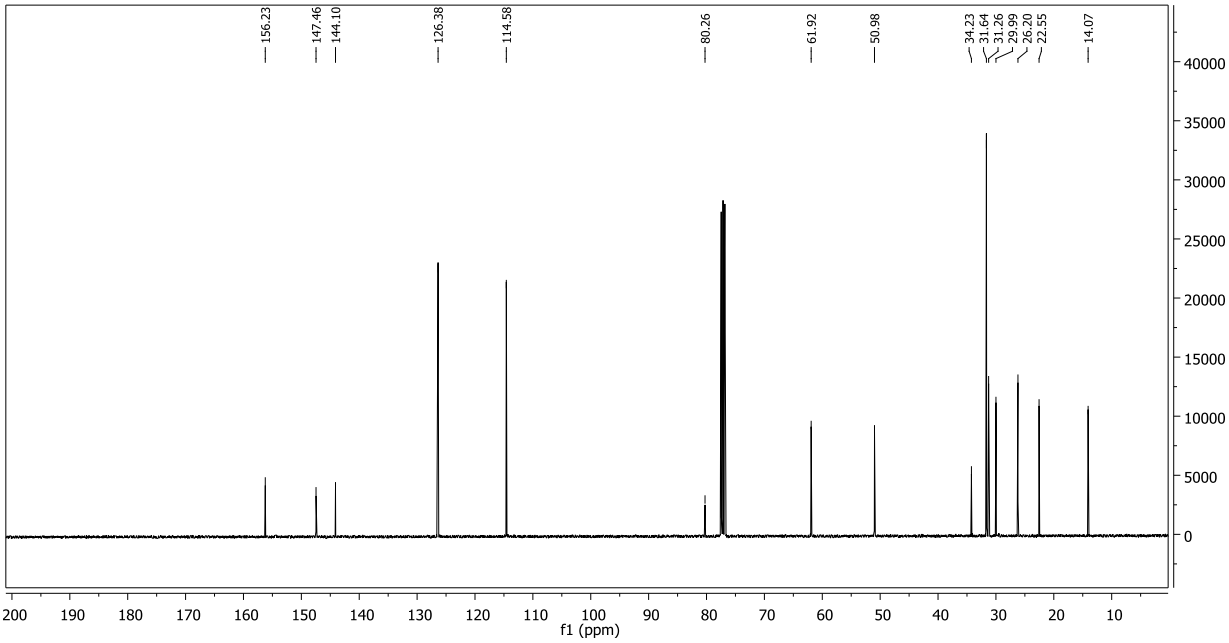




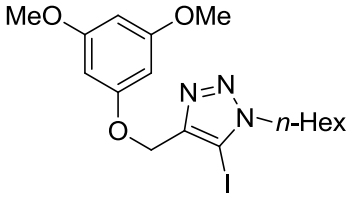
4-((4-(tert-butyl)phenoxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (3b)

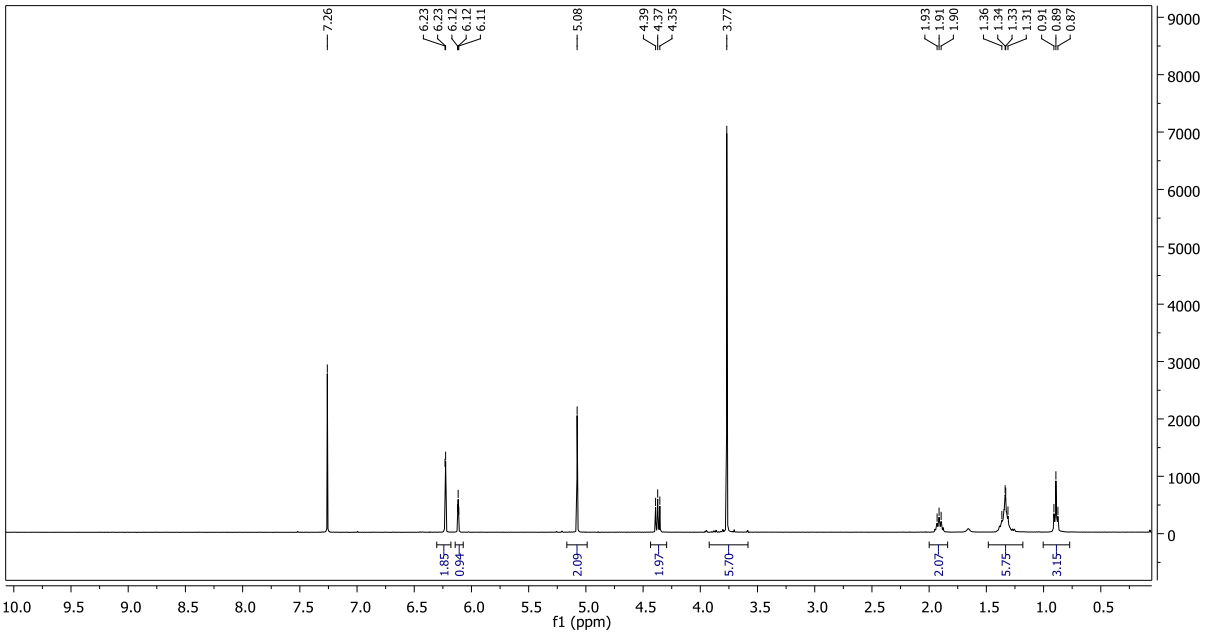


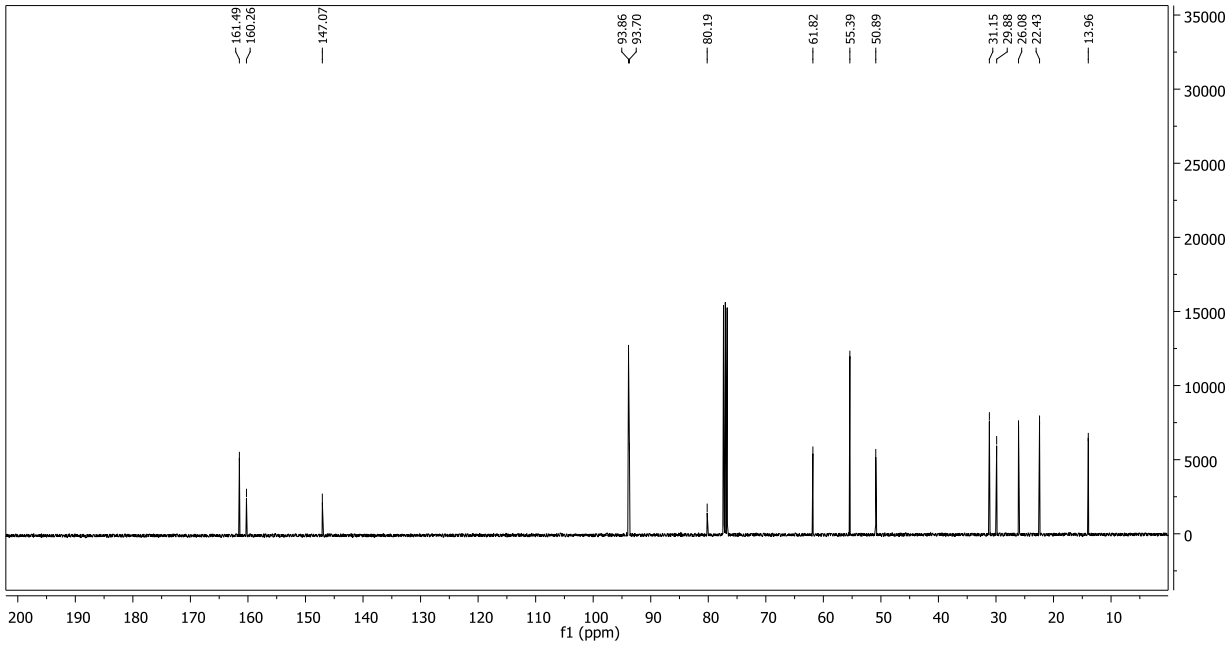




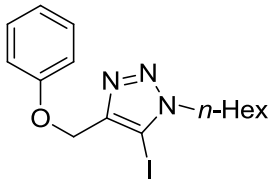
4-((3,5-dimethoxyphenoxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (3c)

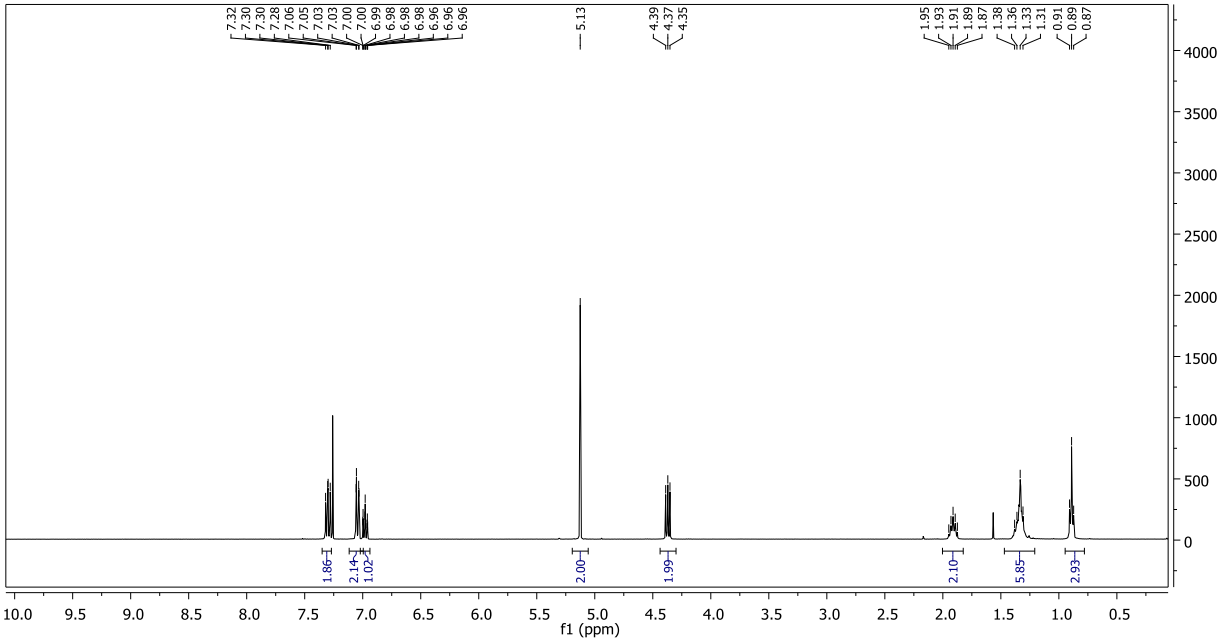


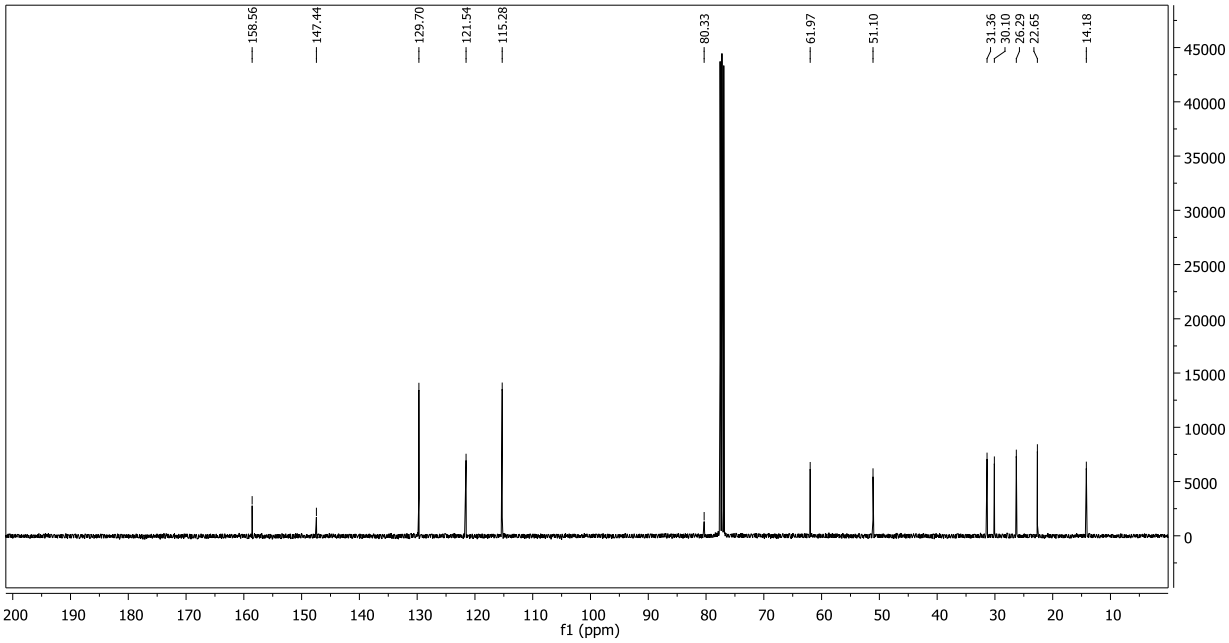




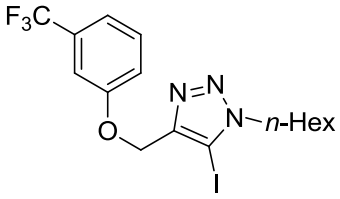
1-hexyl-5-iodo-4-(phenoxymethyl)-1H-1,2,3-triazole (3d)

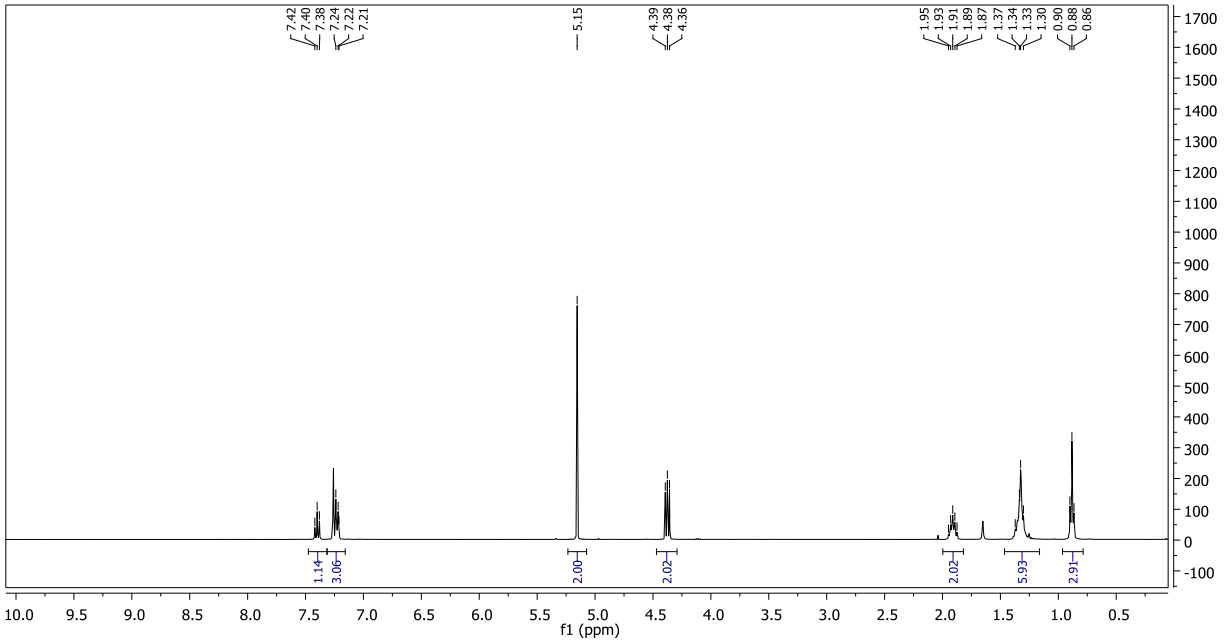


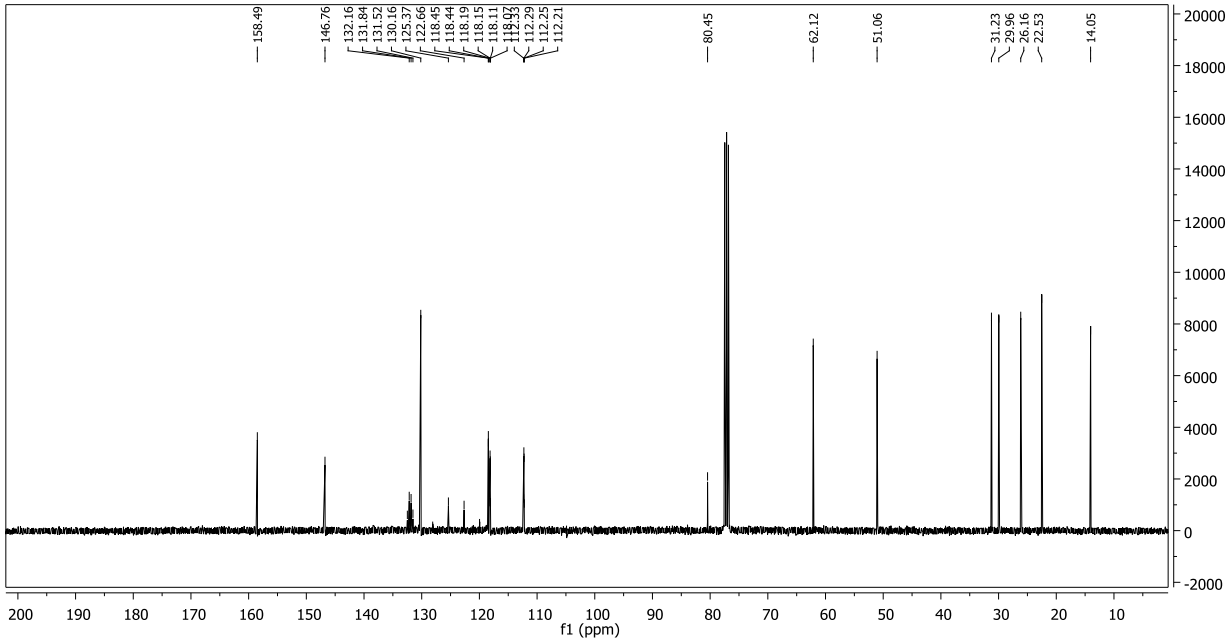


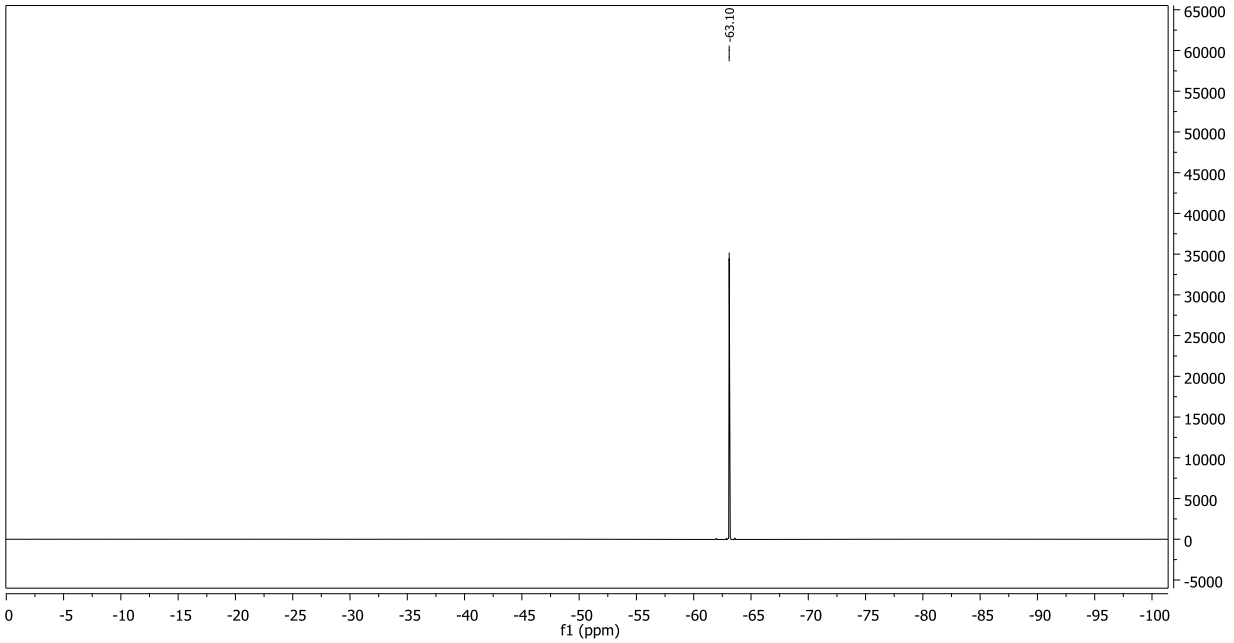


1-hexyl-5-iodo-4-((3-(trifluoromethyl)phenoxy)methyl)-1H-1,2,3-triazole (3e)

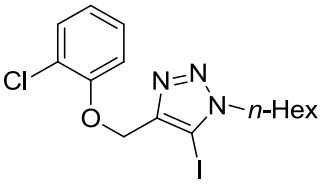


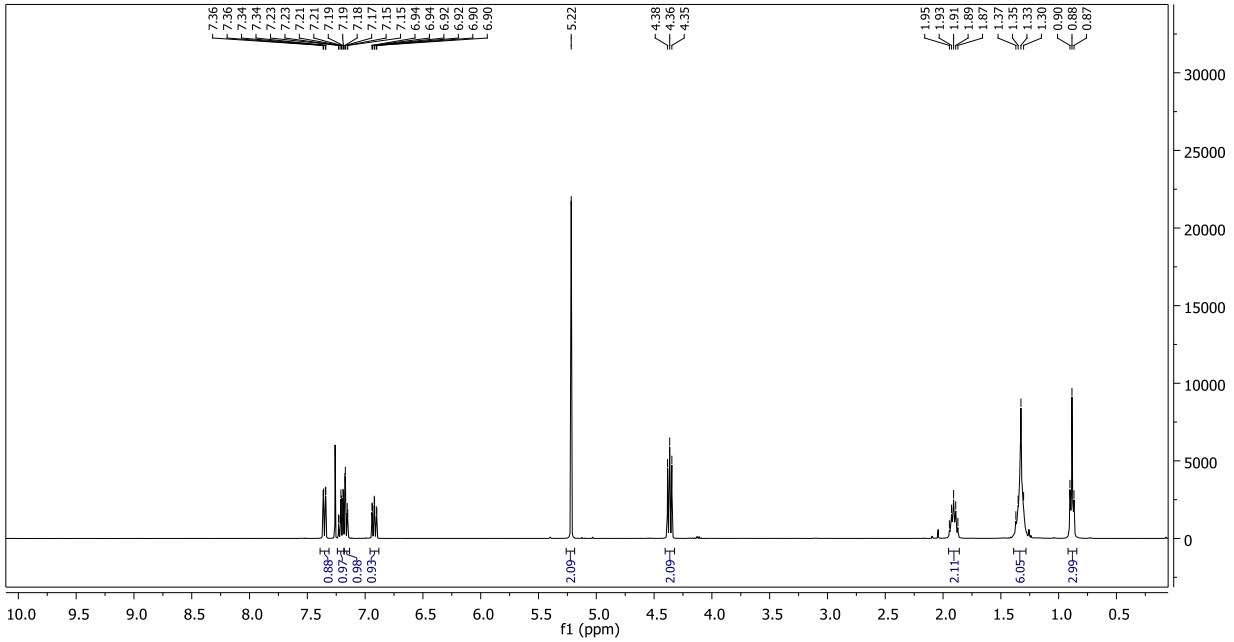


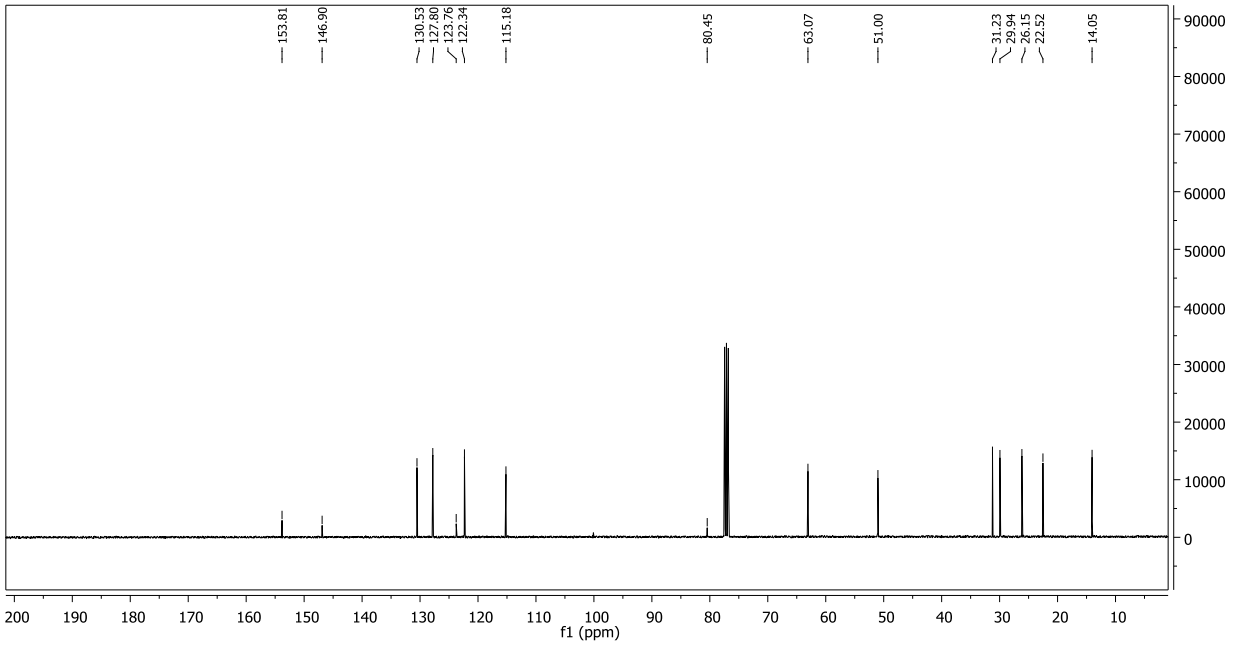




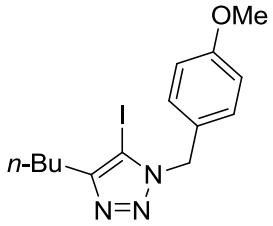
4-((2-chlorophenoxy)methyl)-1-hexyl-5-iodo-1H-1,2,3-triazole (3f)

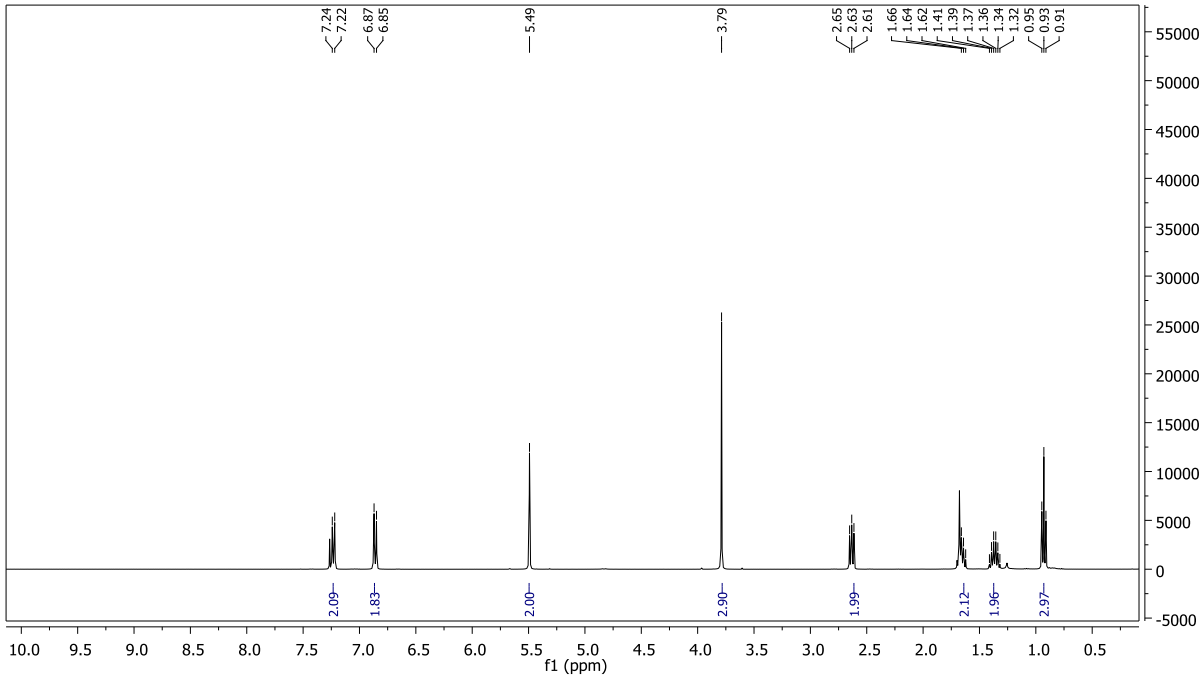


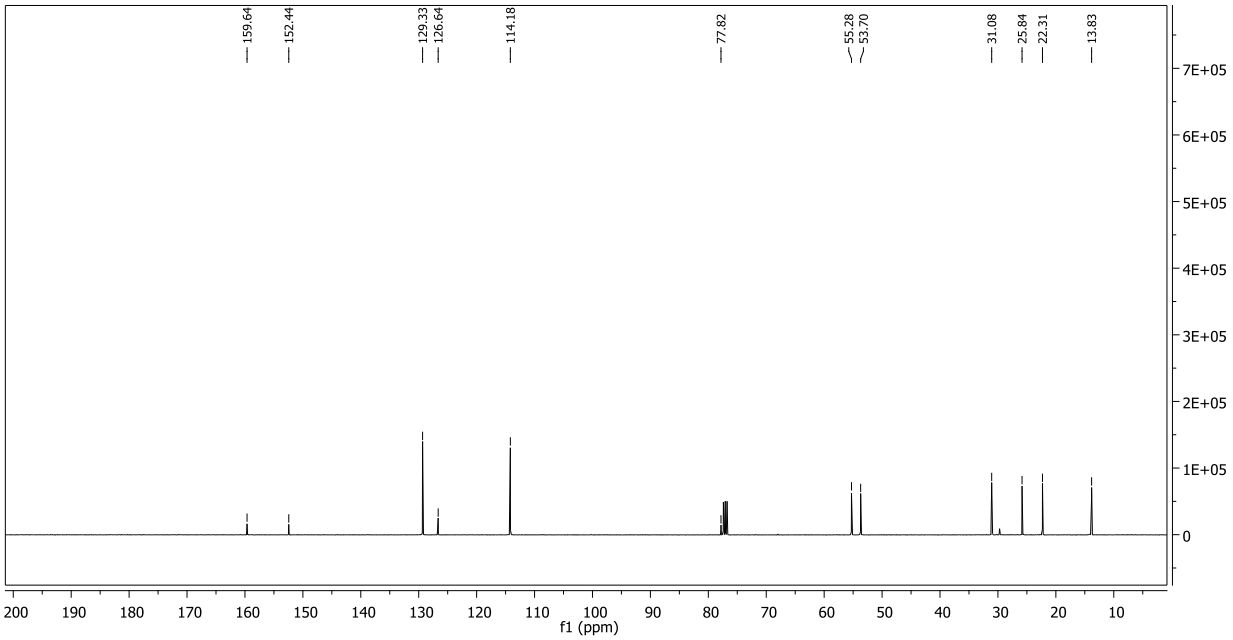




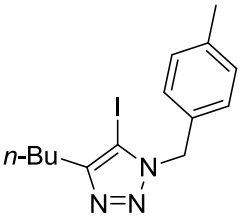
4-butyl-5-iodo-1-(4-methoxybenzyl)-1H-1,2,3-triazole (5a)

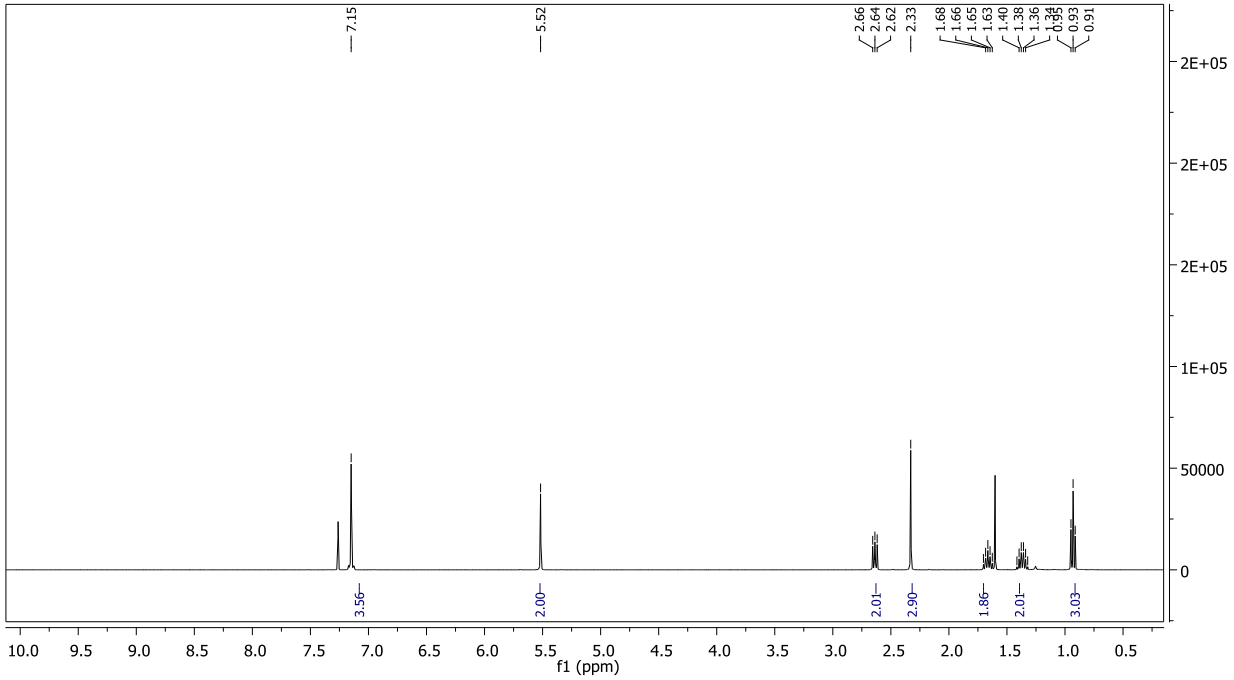


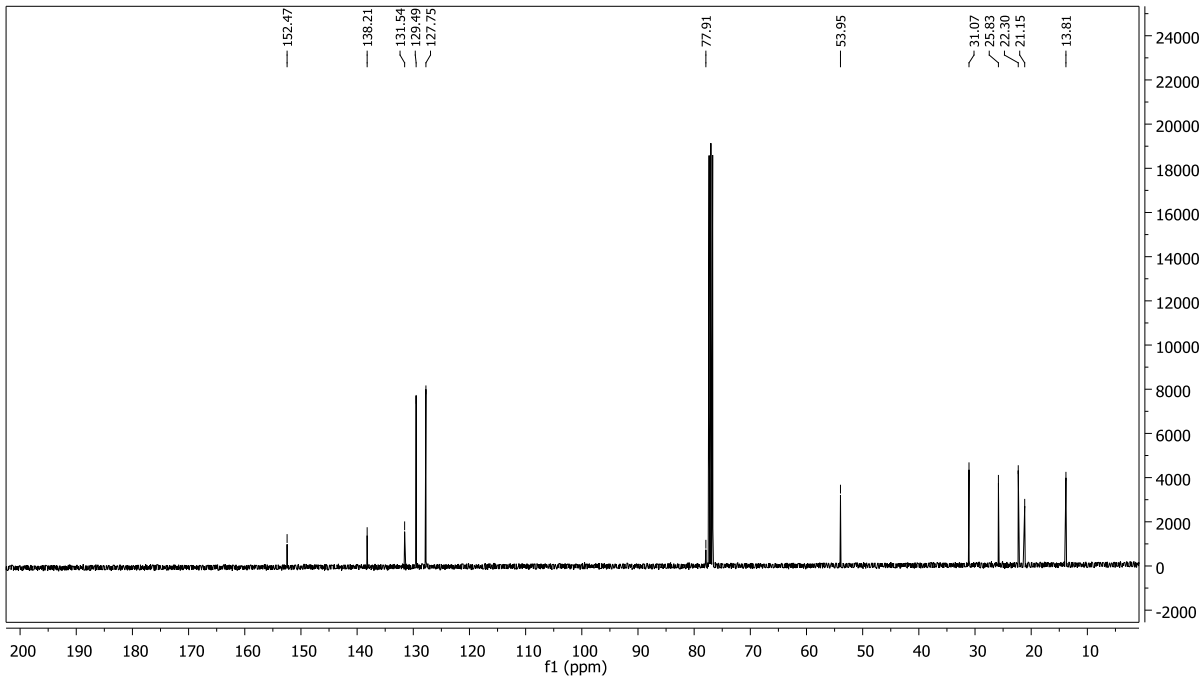




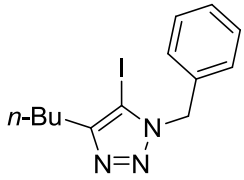
4-butyl-5-iodo-1-(4-methylbenzyl)-1H-1,2,3-triazole (5b)

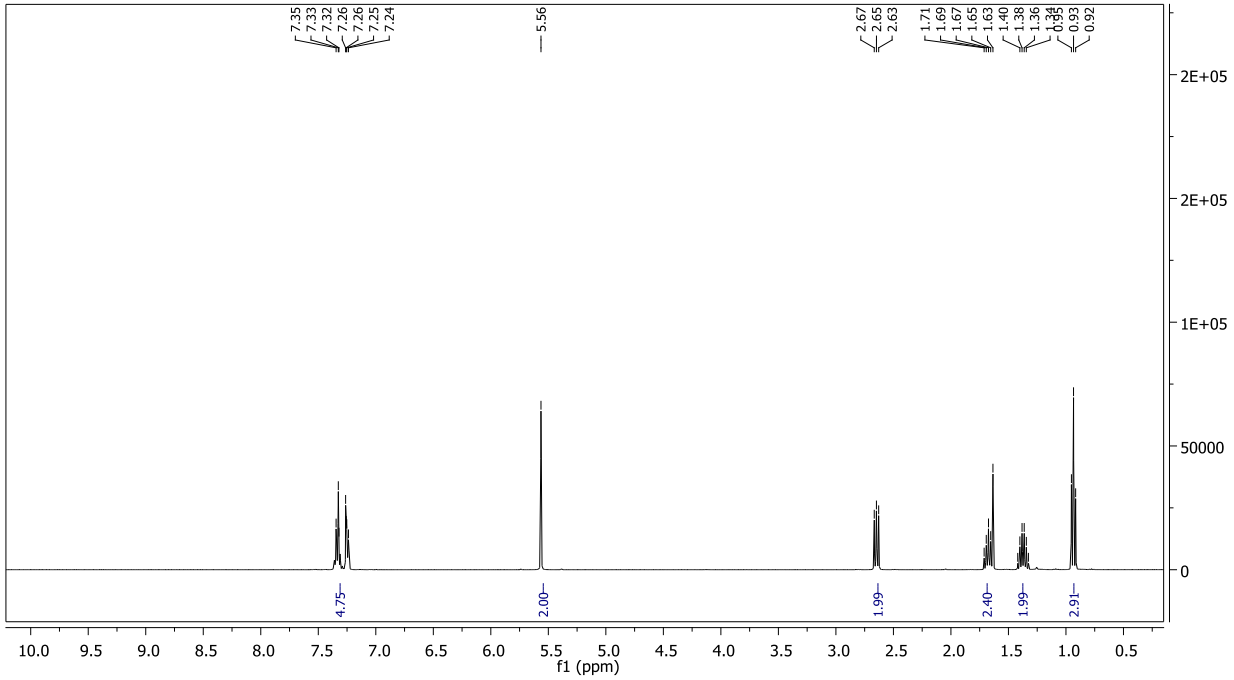


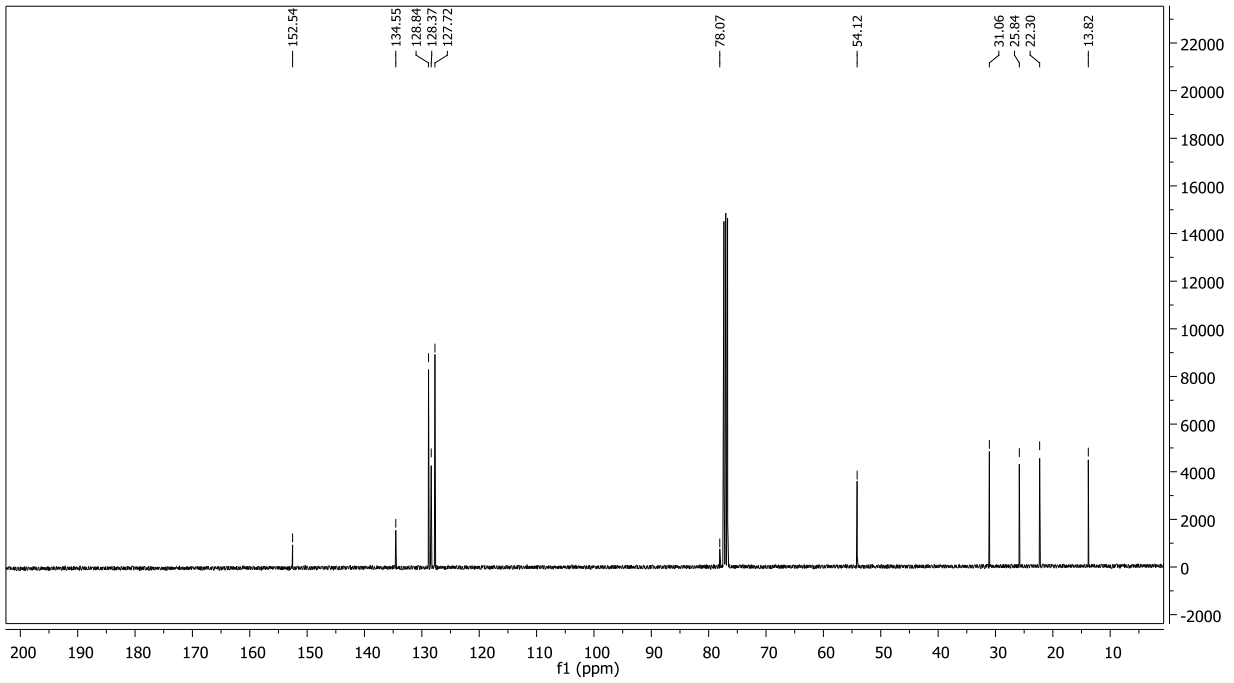




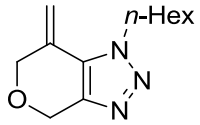
1-benzyl-4-butyl-5-iodo-1H-1,2,3-triazole (5c)

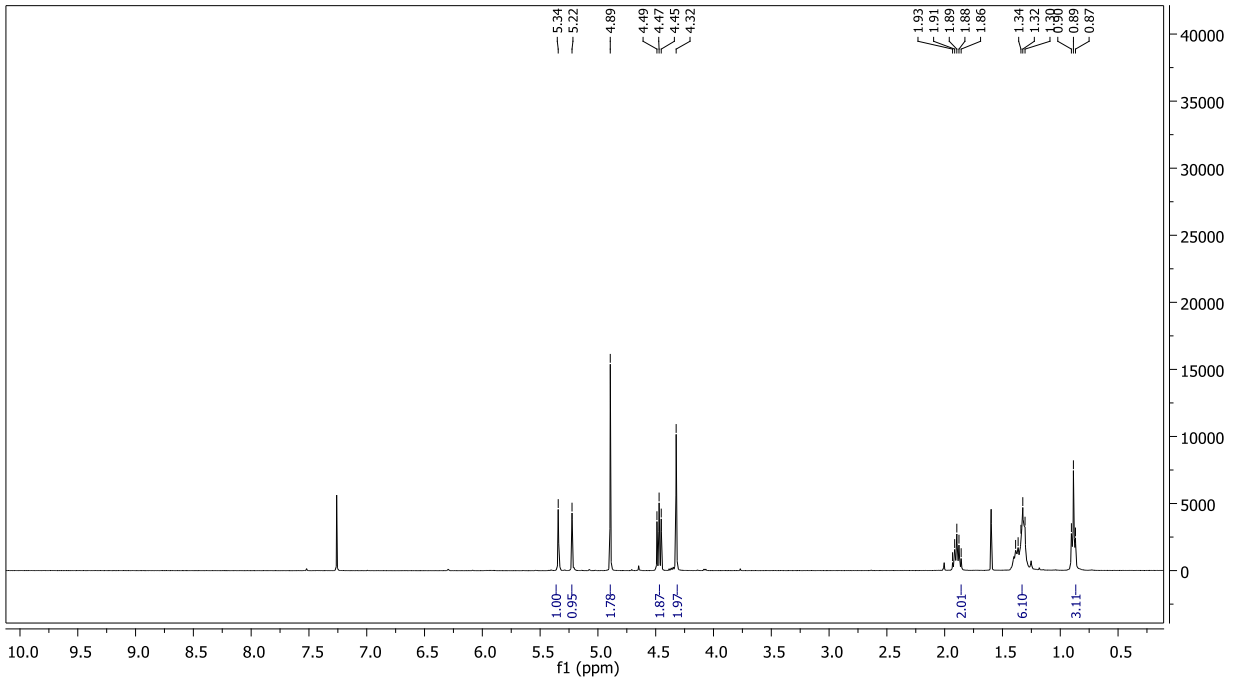


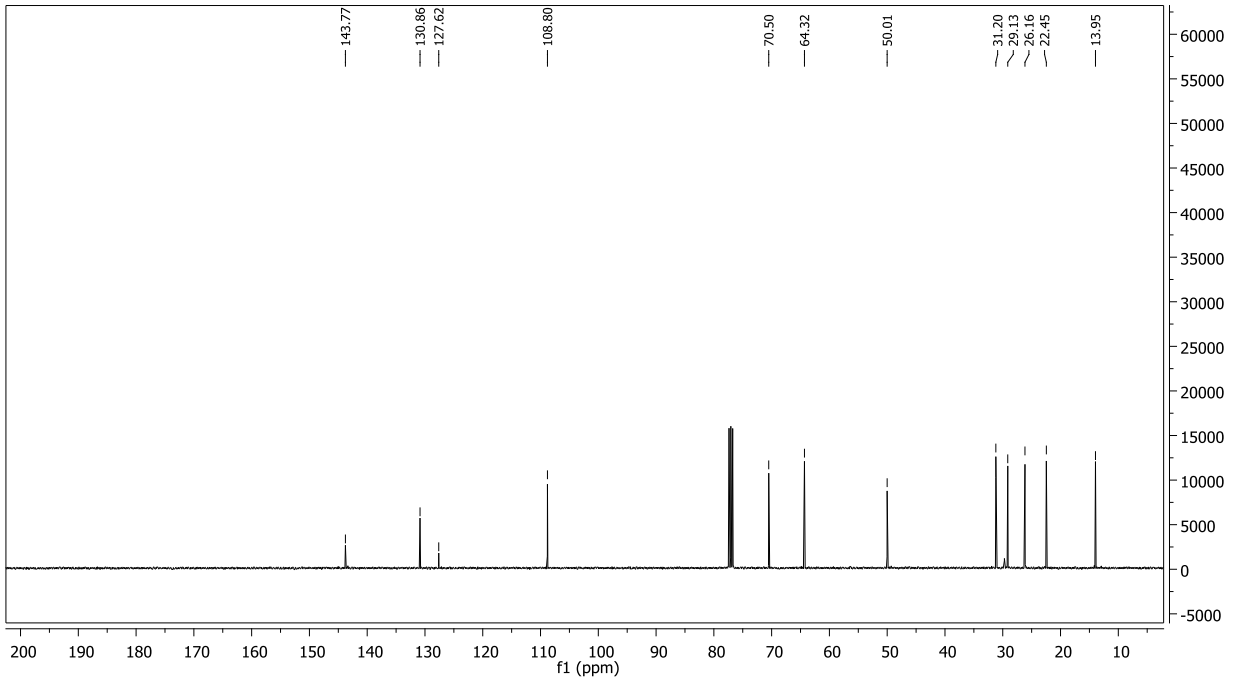




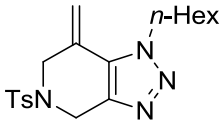
1-hexyl-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2a)

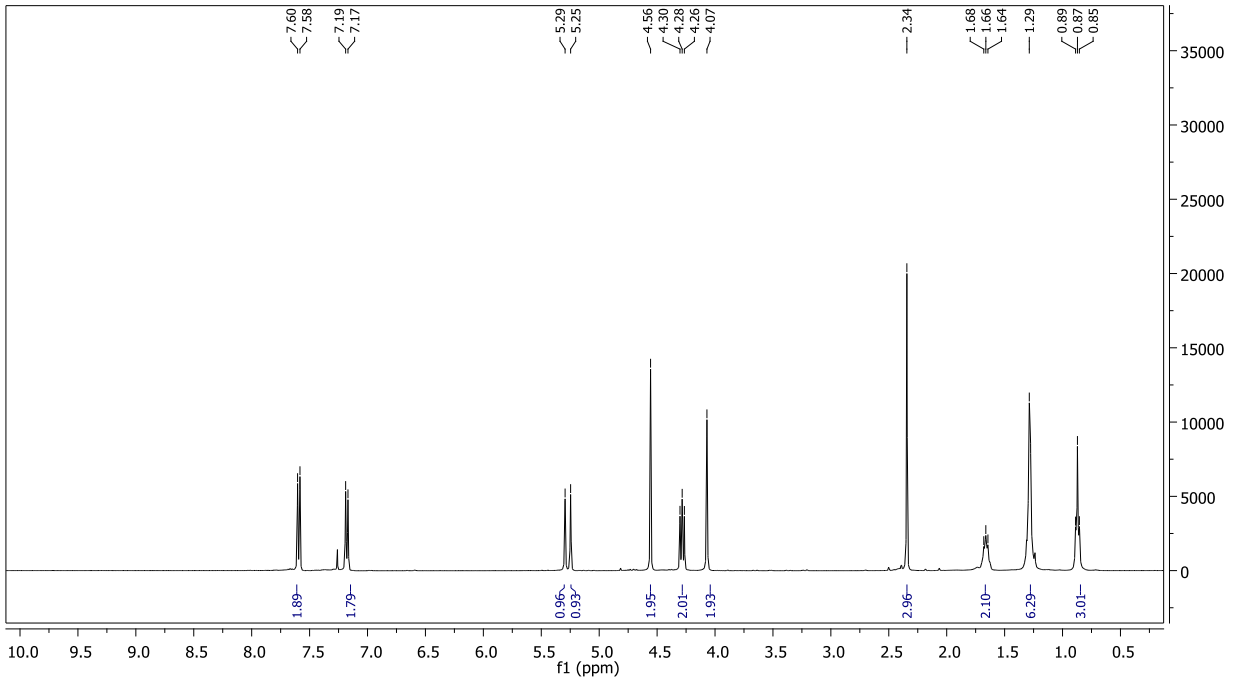


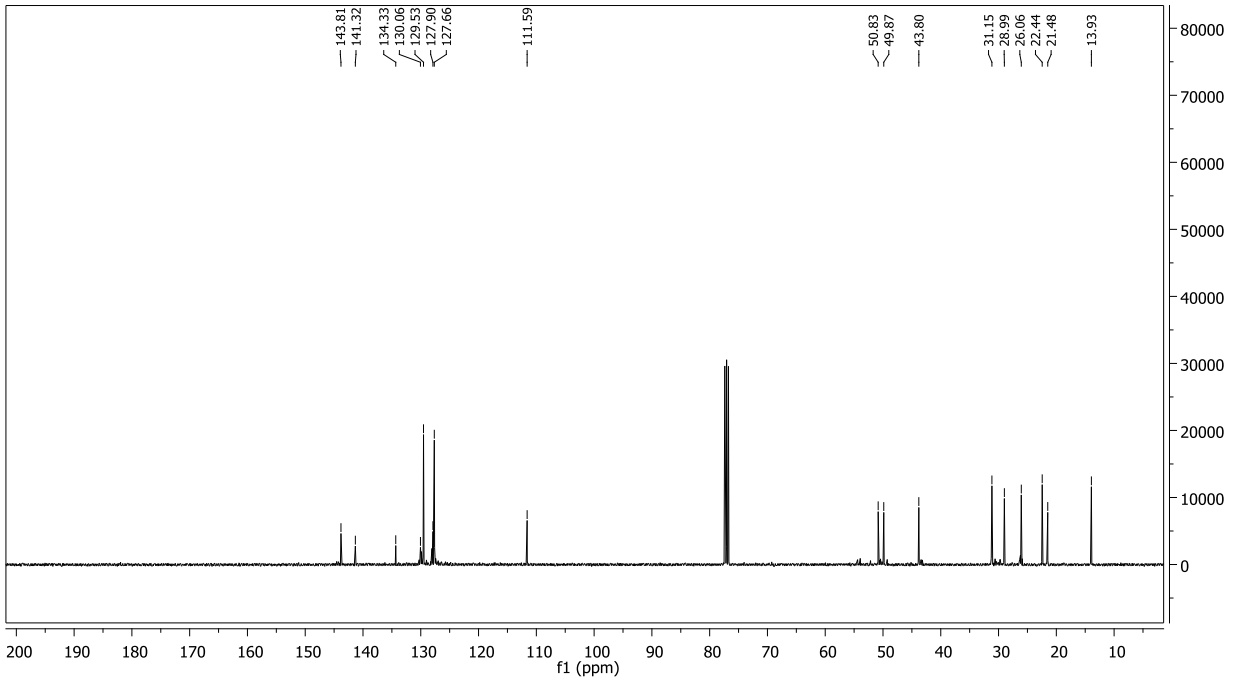




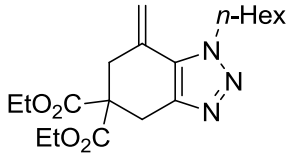
1-hexyl-7-methylene-5-tosyl-4,5,6,7-tetrahydro-1H-[1,2,3]triazolo[4,5-c]pyridine (2b)

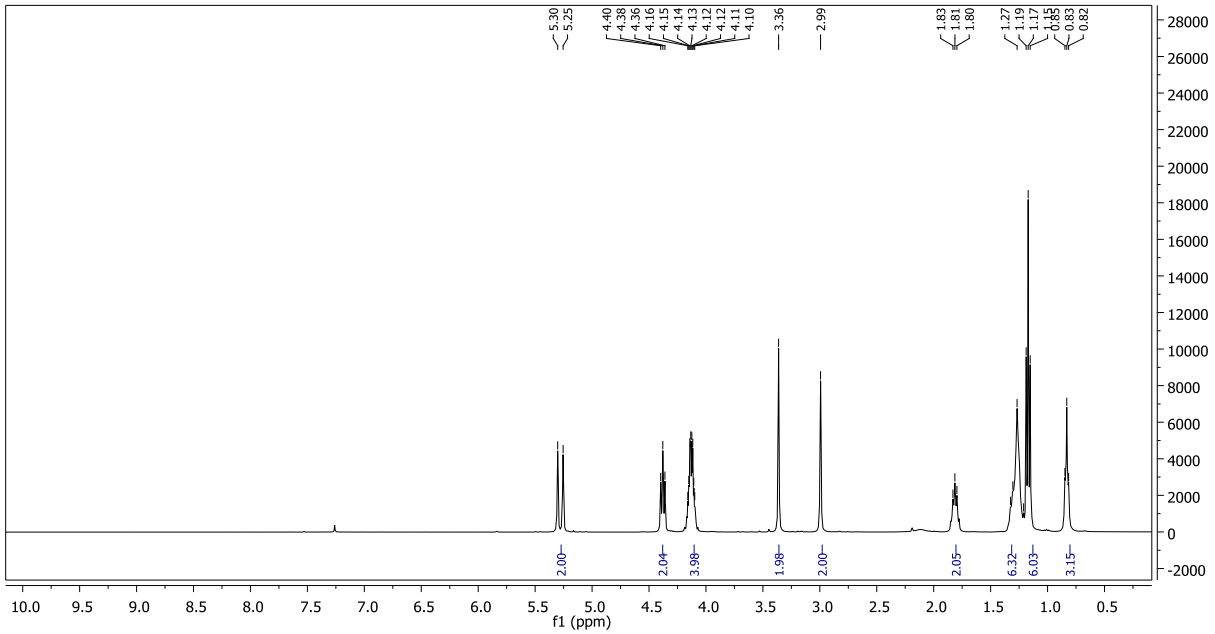


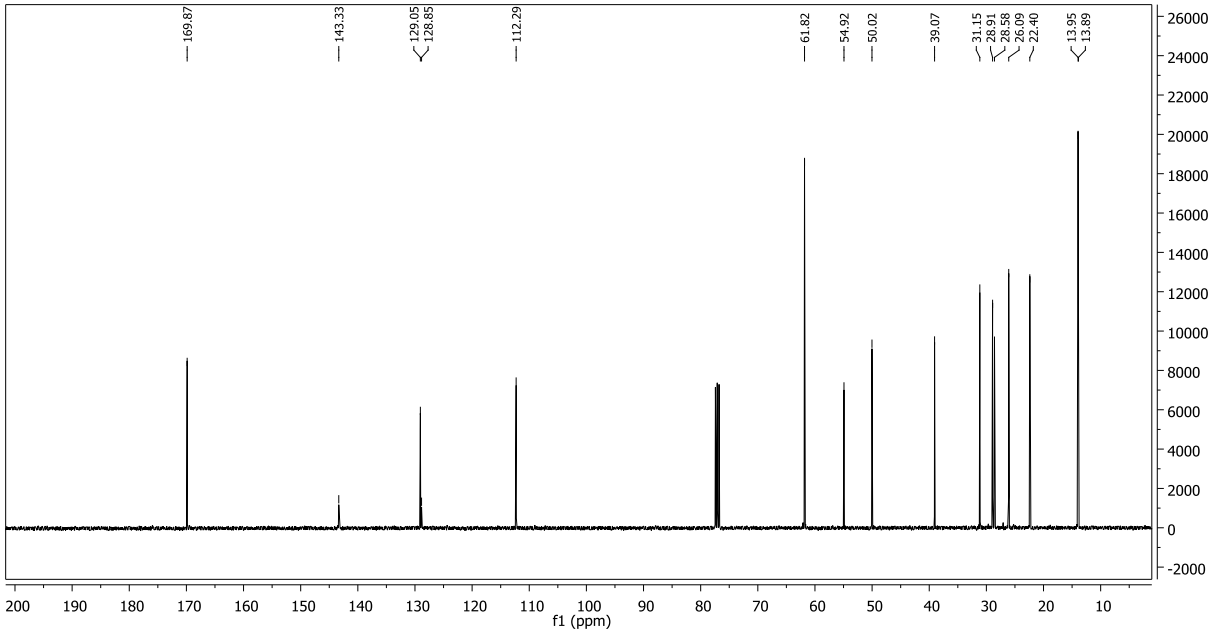




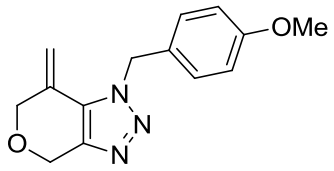
diethyl 1-hexyl-7-methylene-6,7-dihydro-1H-benzo[d][1,2,3]triazole-5,5(4H)-dicarboxylate (2c)

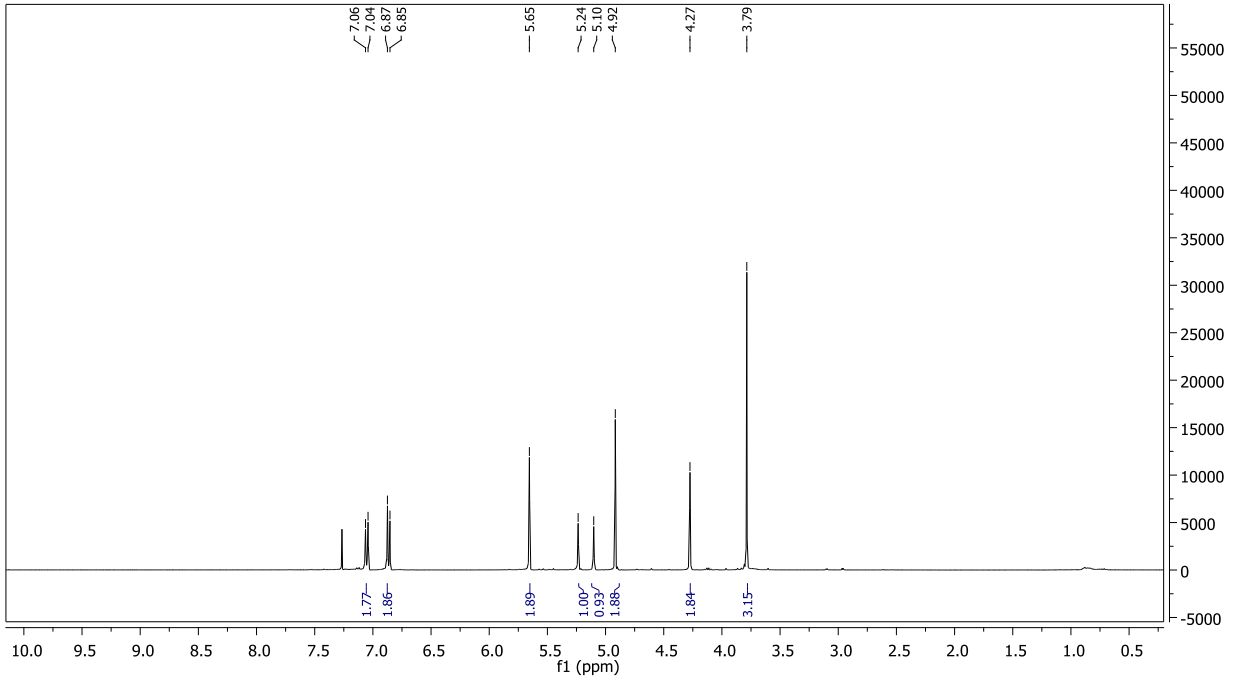


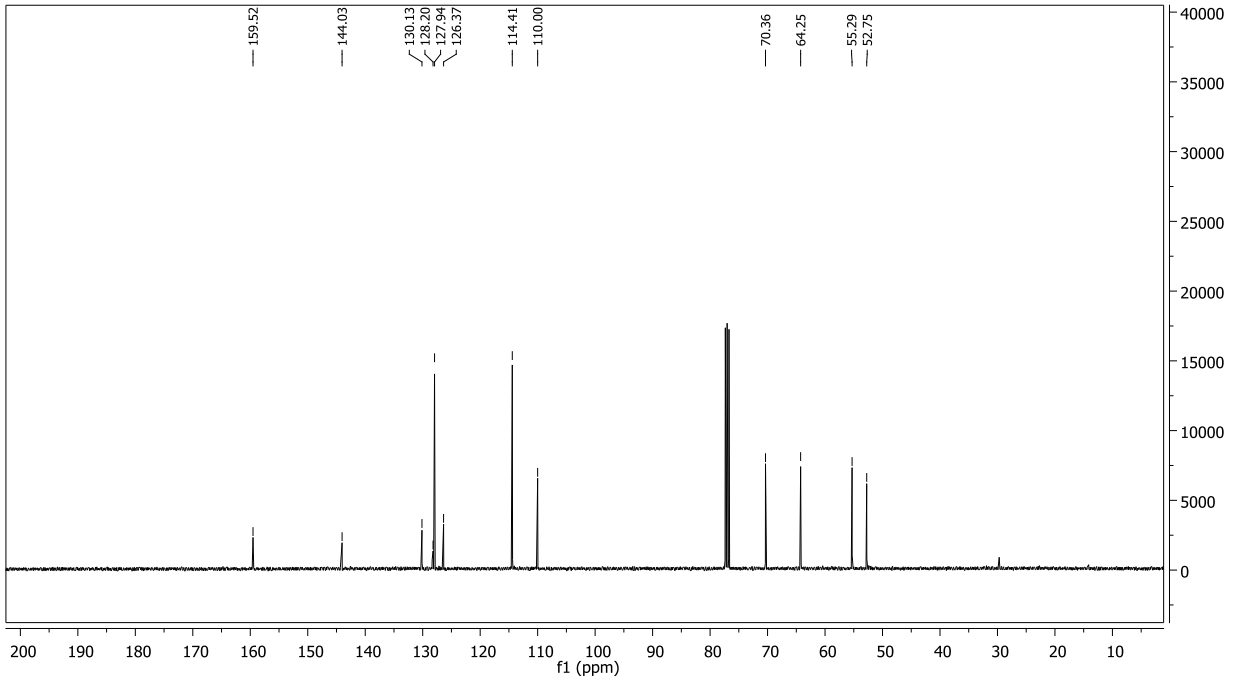




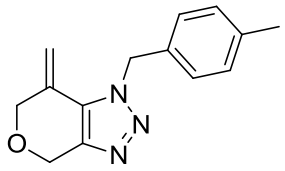
1-(4-methoxybenzyl)-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2d)

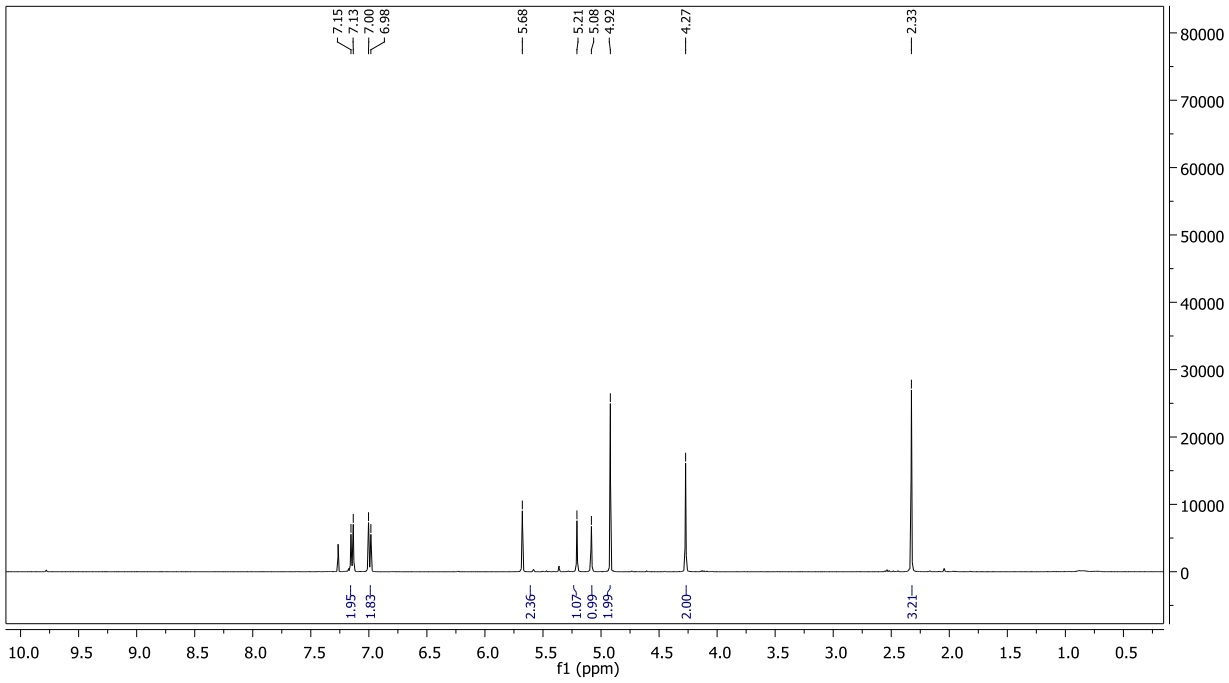


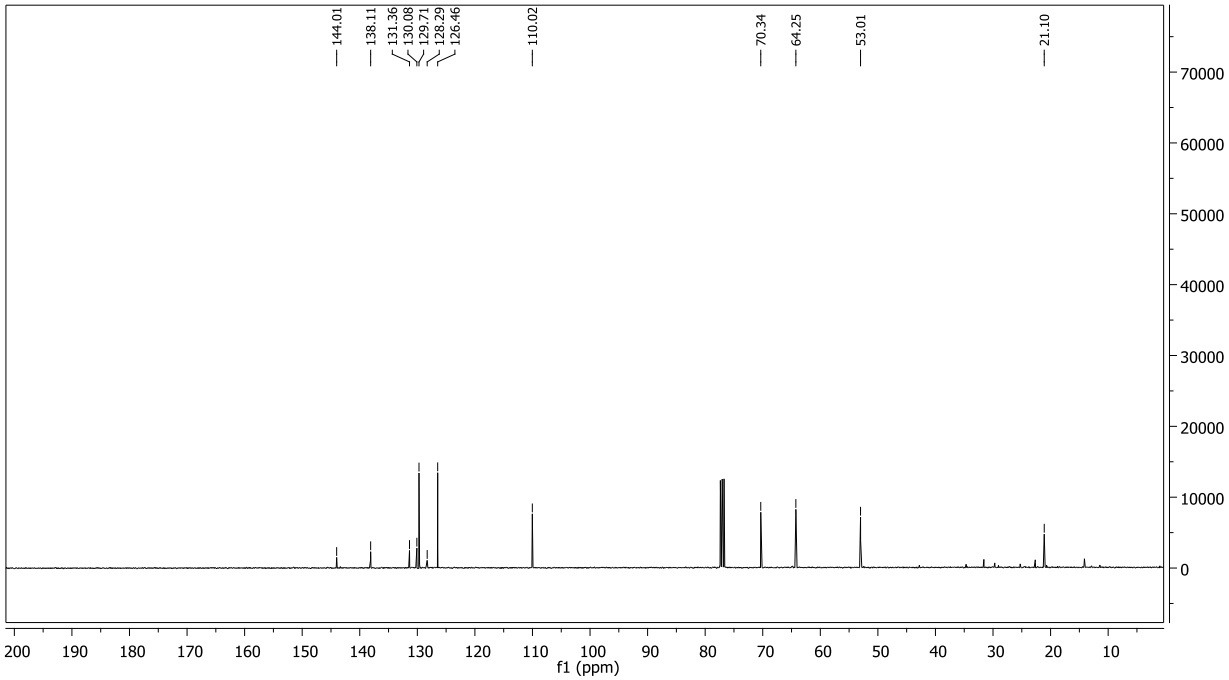




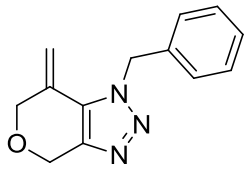
1-(4-methylbenzyl)-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2e)

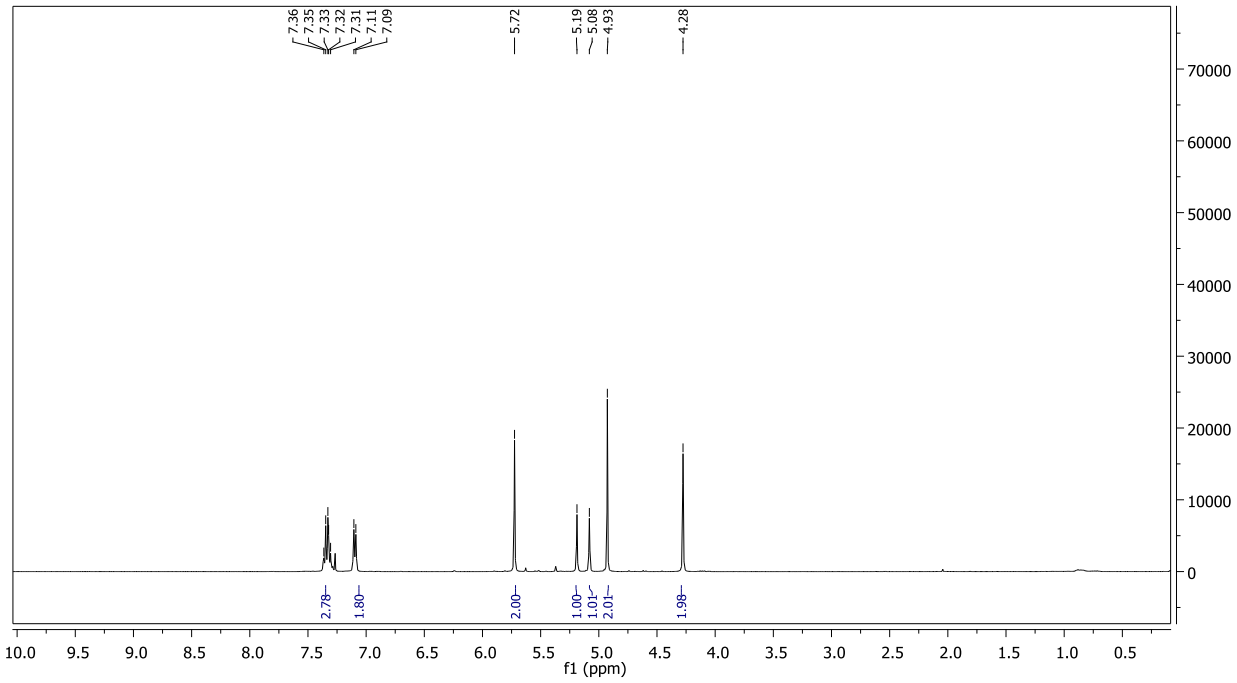


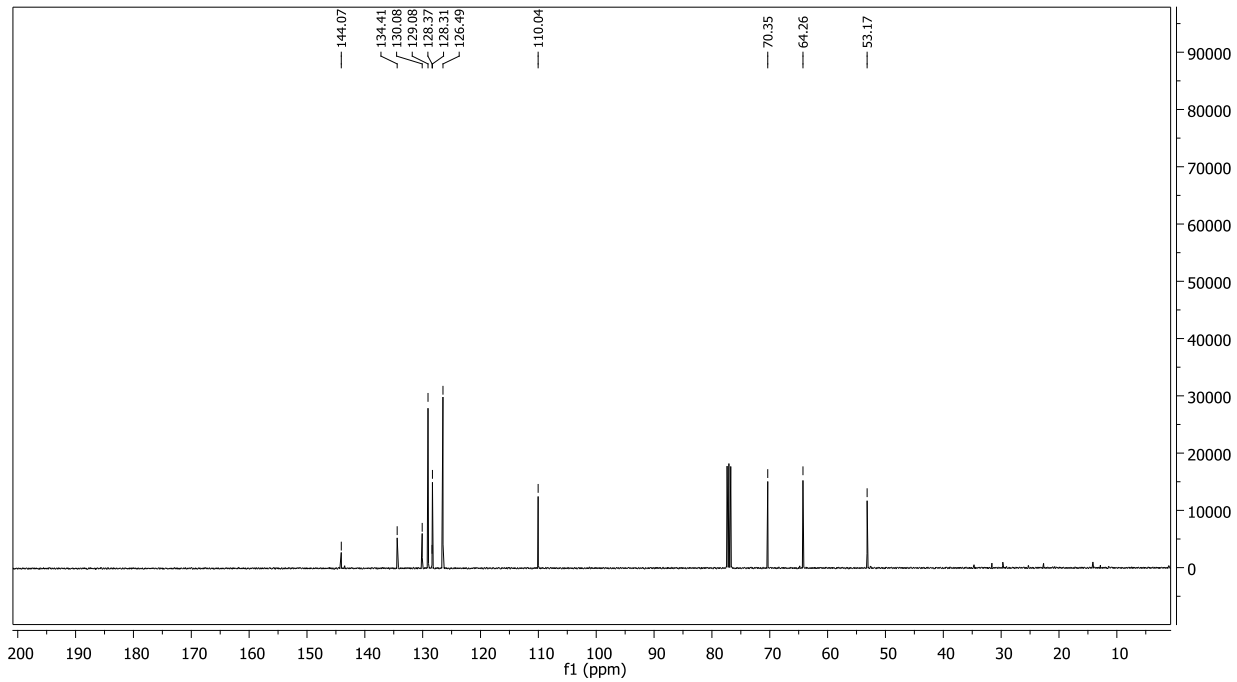




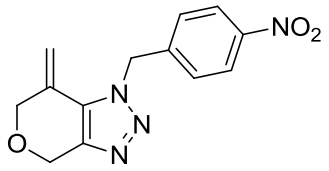
1-benzyl-7-methylene-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2f)

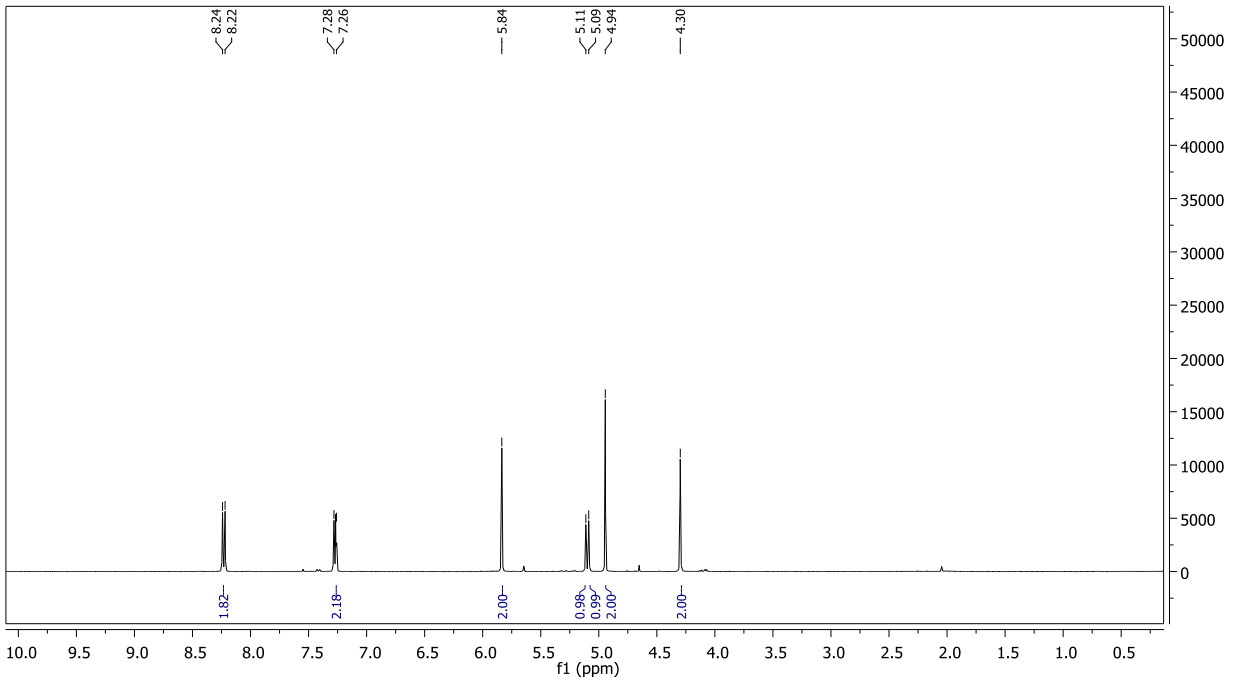


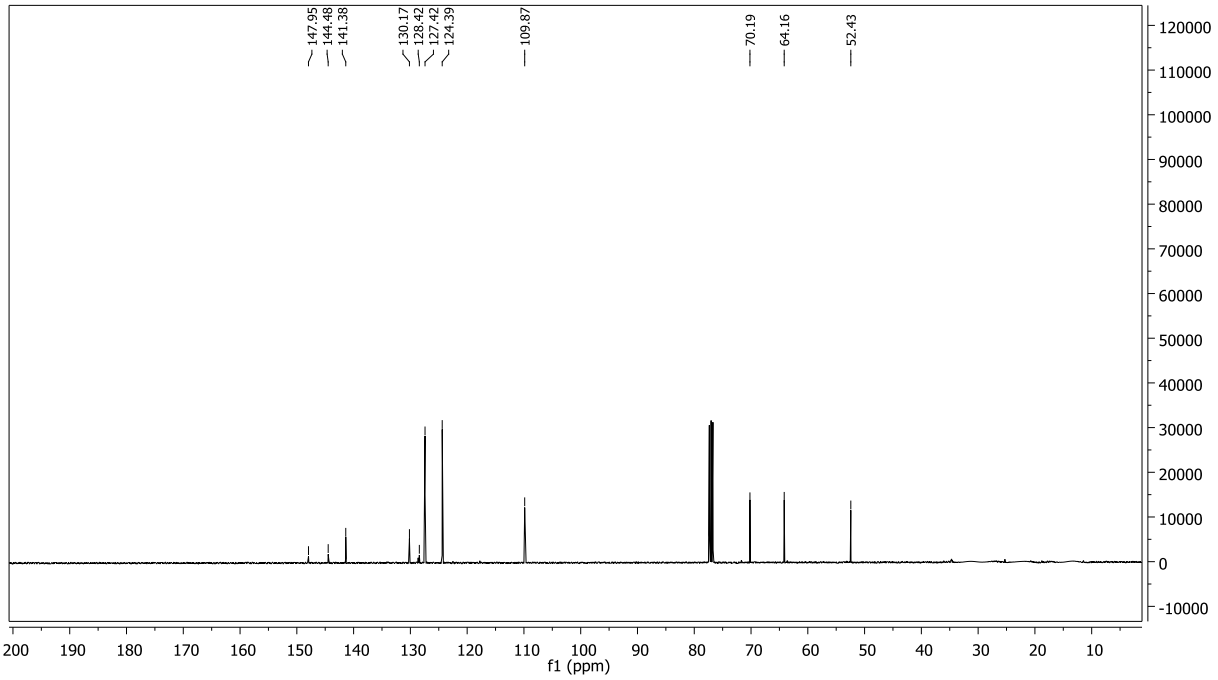




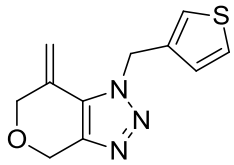
7-methylene-1-(4-nitrobenzyl)-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2g)

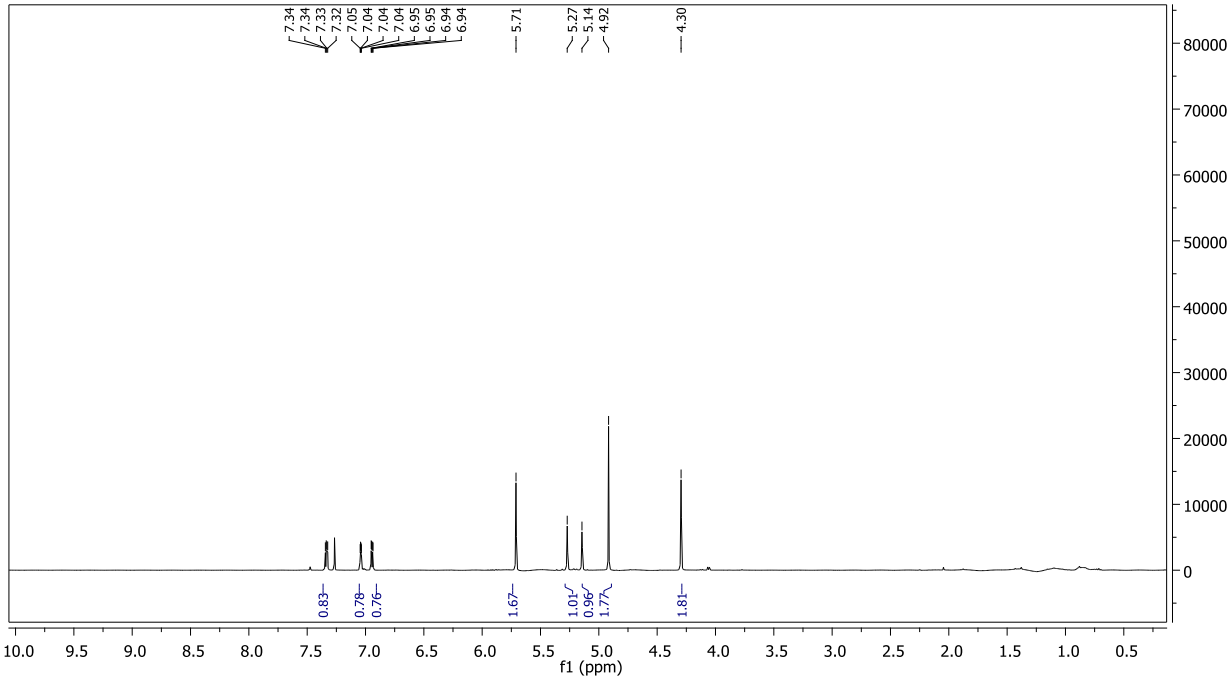


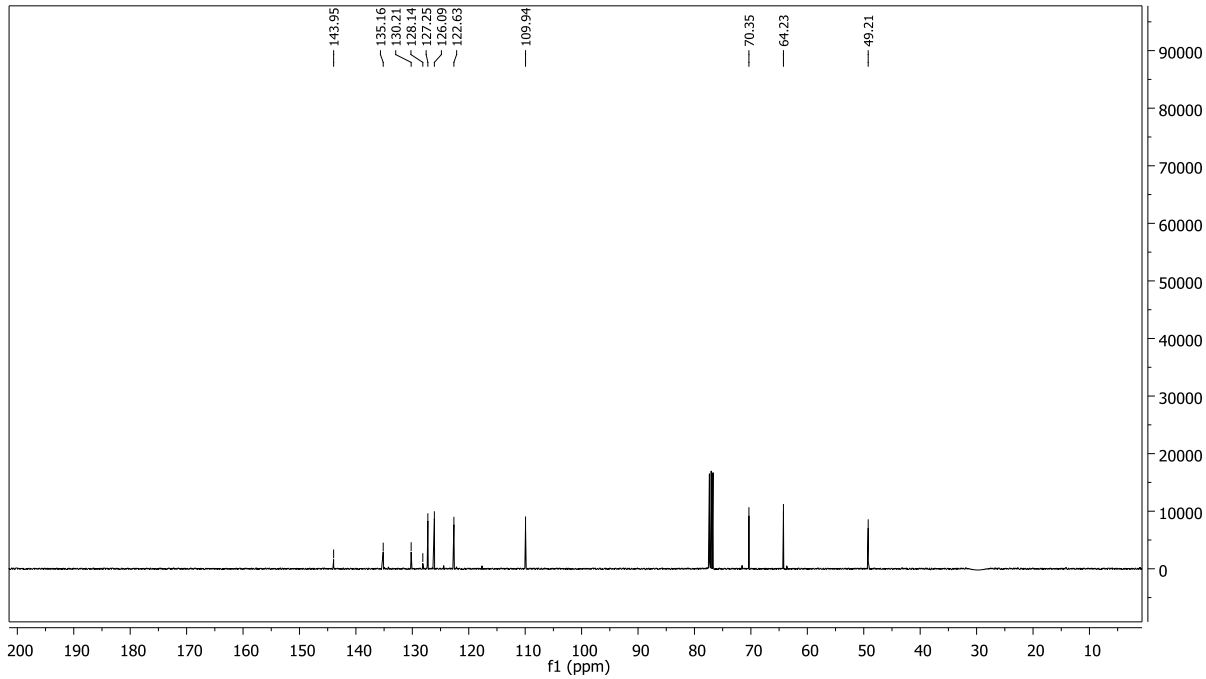




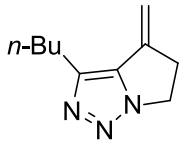
7-methylene-1-(thiophen-3-ylmethyl)-1,4,6,7-tetrahydropyrano[3,4-d][1,2,3]triazole (2h)

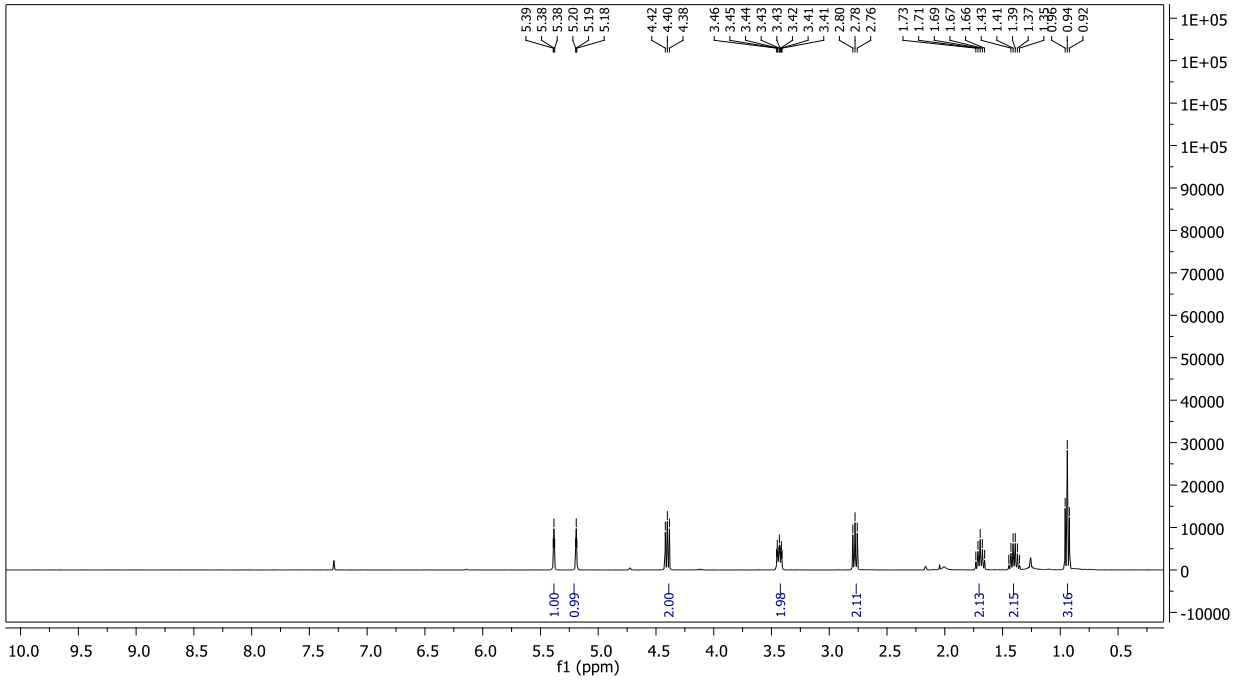


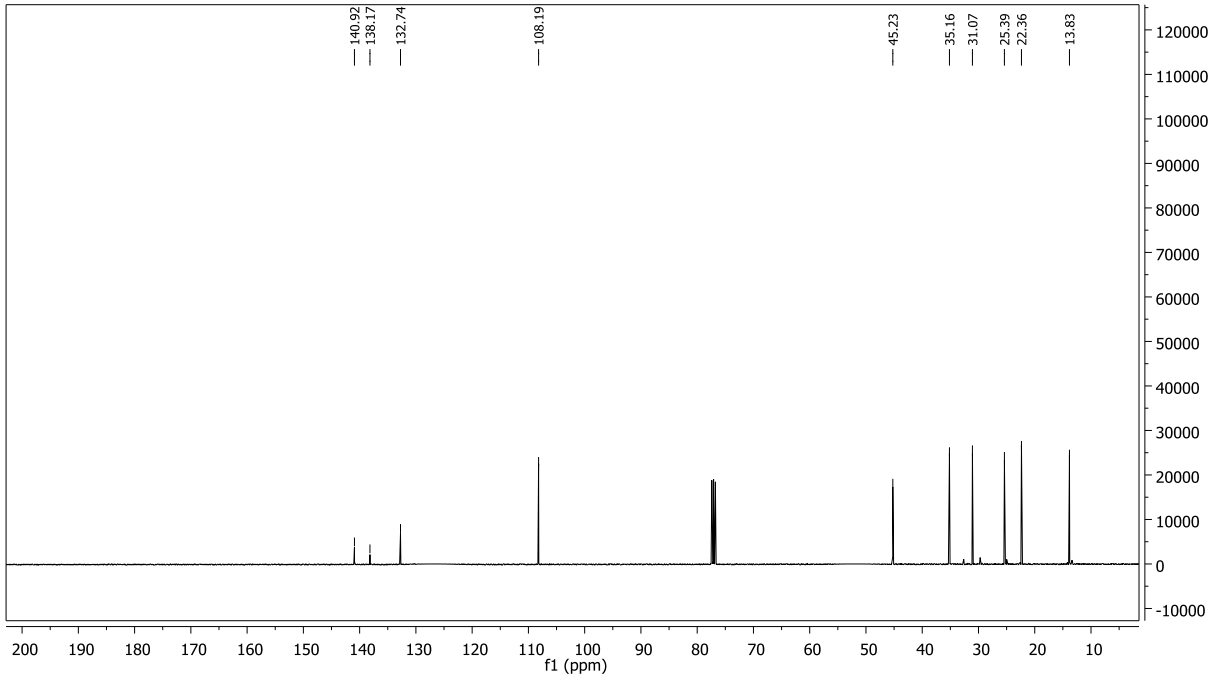




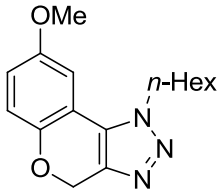
3-butyl-4-methylene-5,6-dihydro-4H-pyrrolo[1,2-c][1,2,3]triazole (2i)

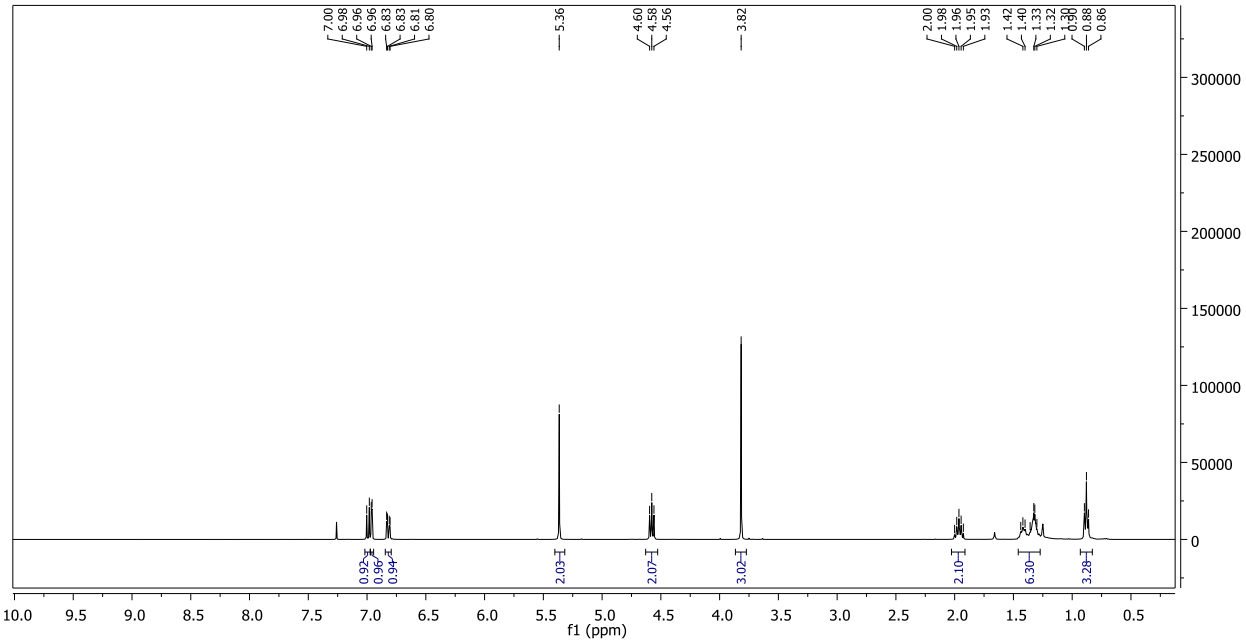


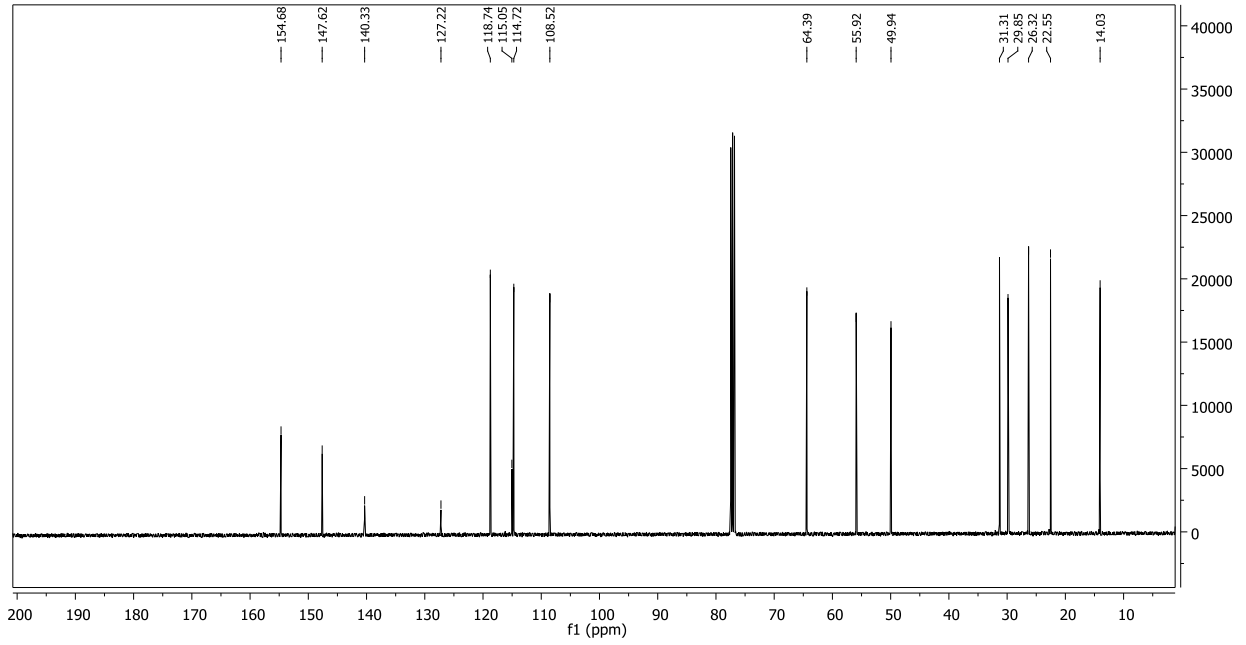




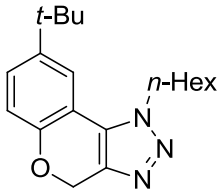
1-hexyl-8-methoxy-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4a)

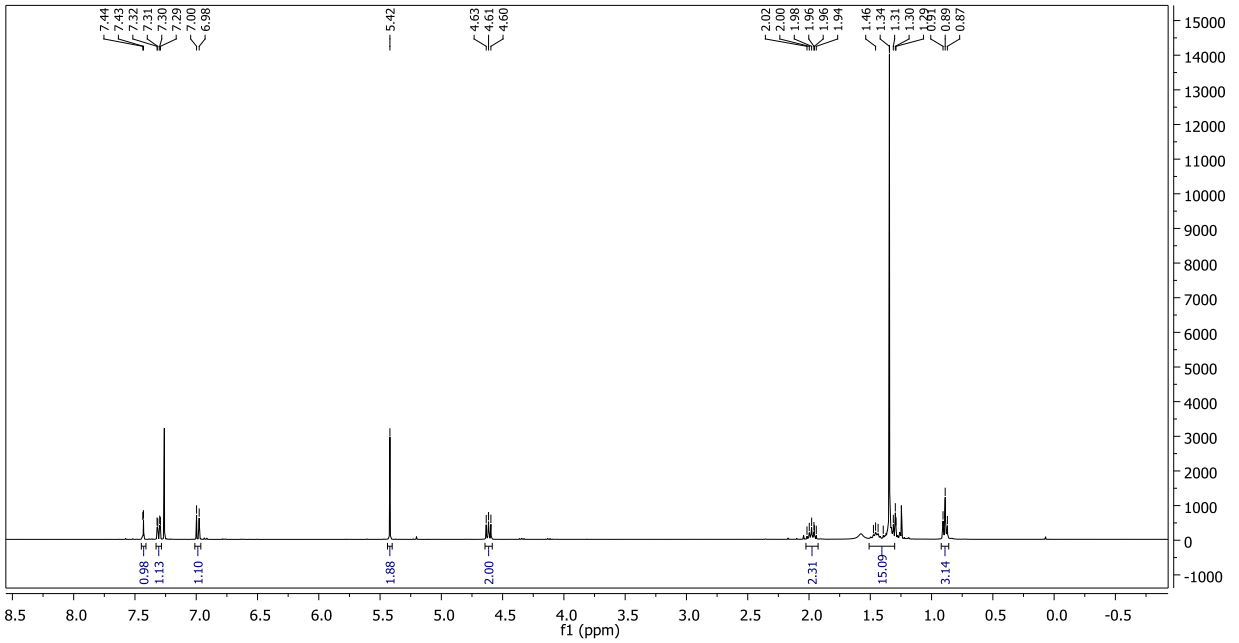


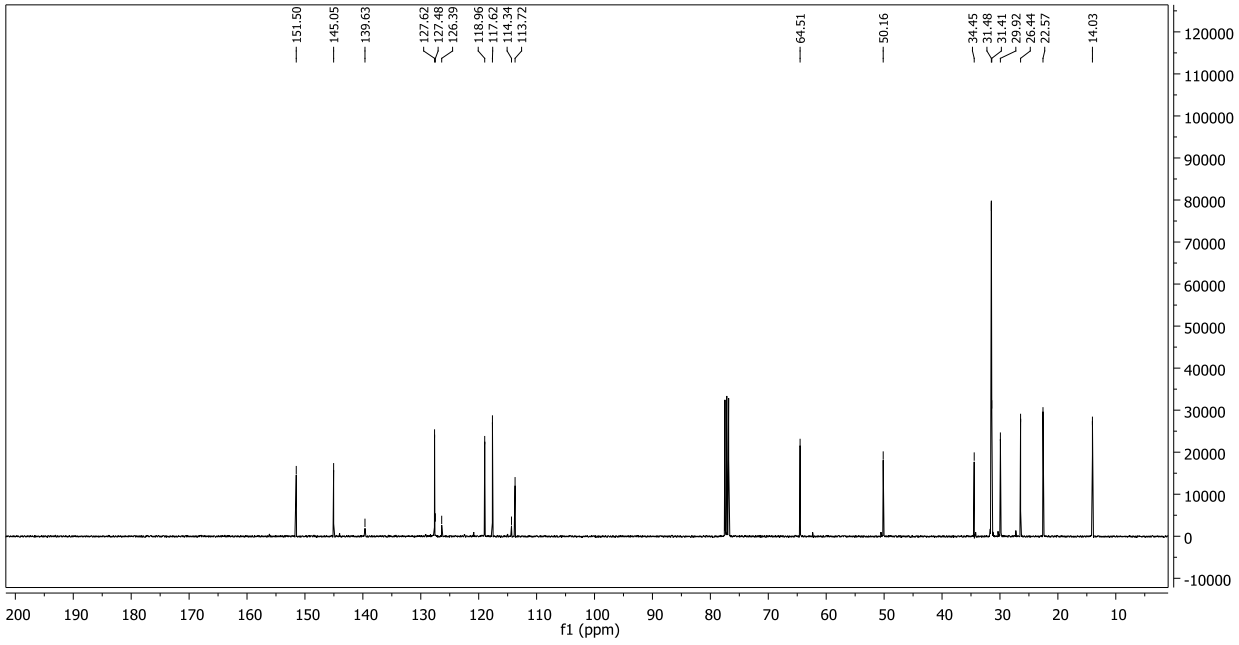




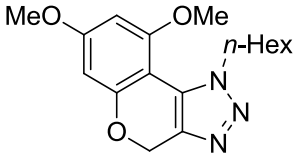
8-(tert-butyl)-1-hexyl-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4b)

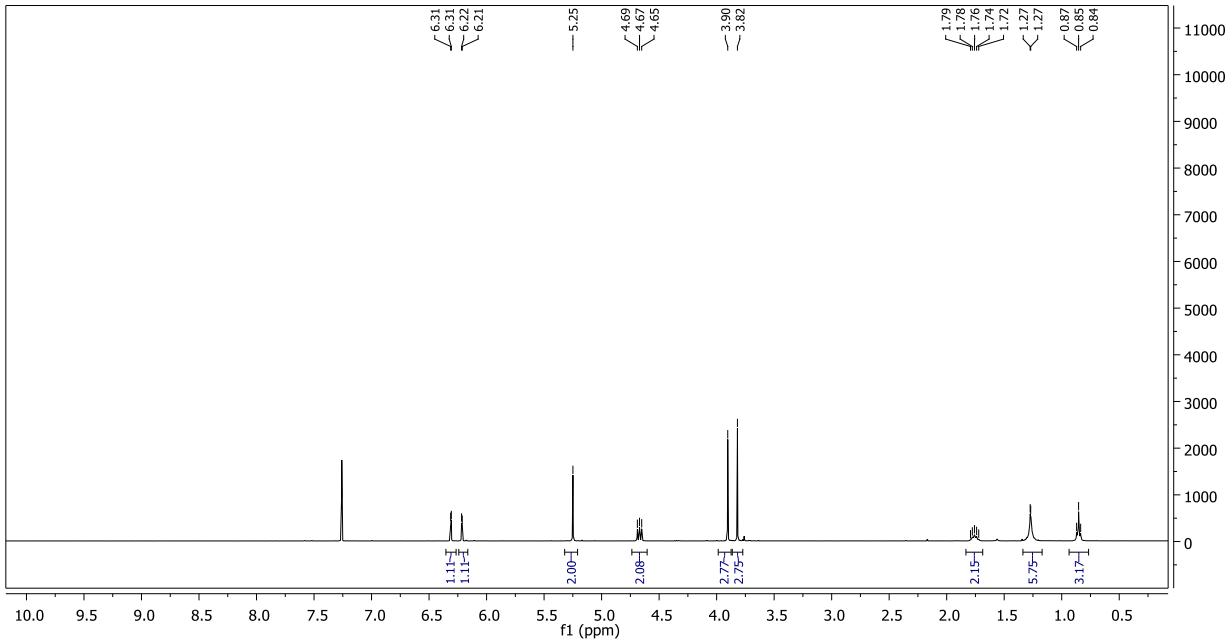


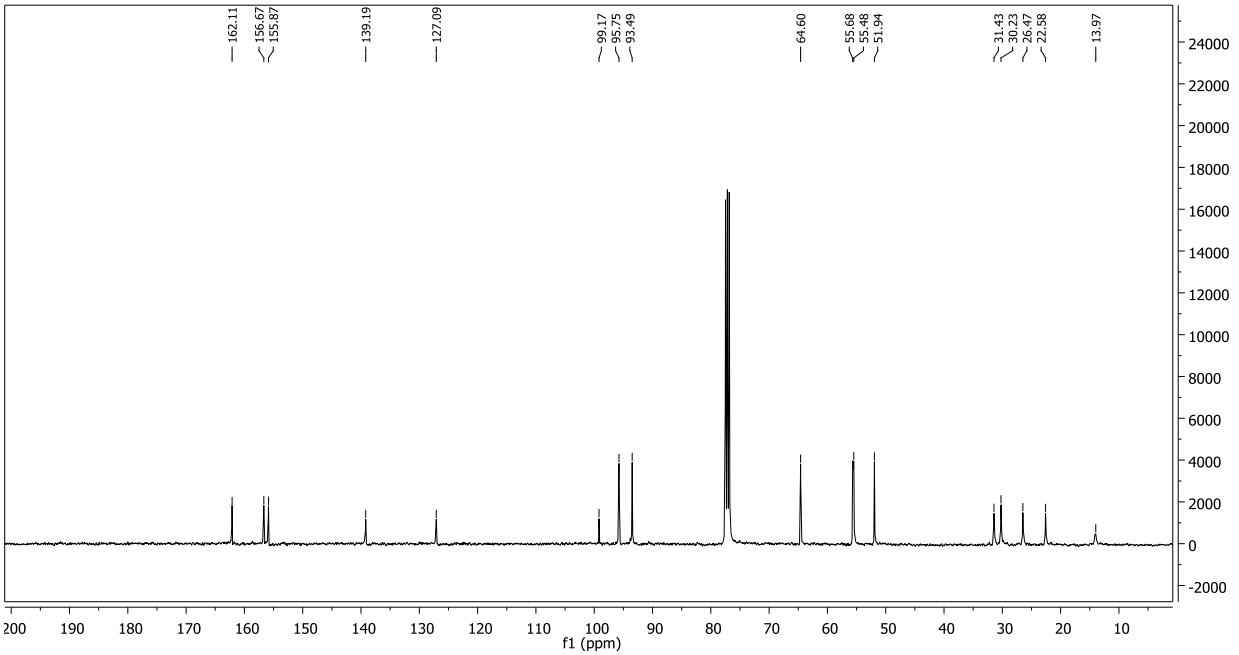




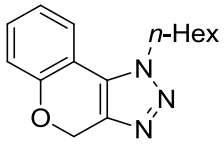
1-hexyl-7,9-dimethoxy-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4c)

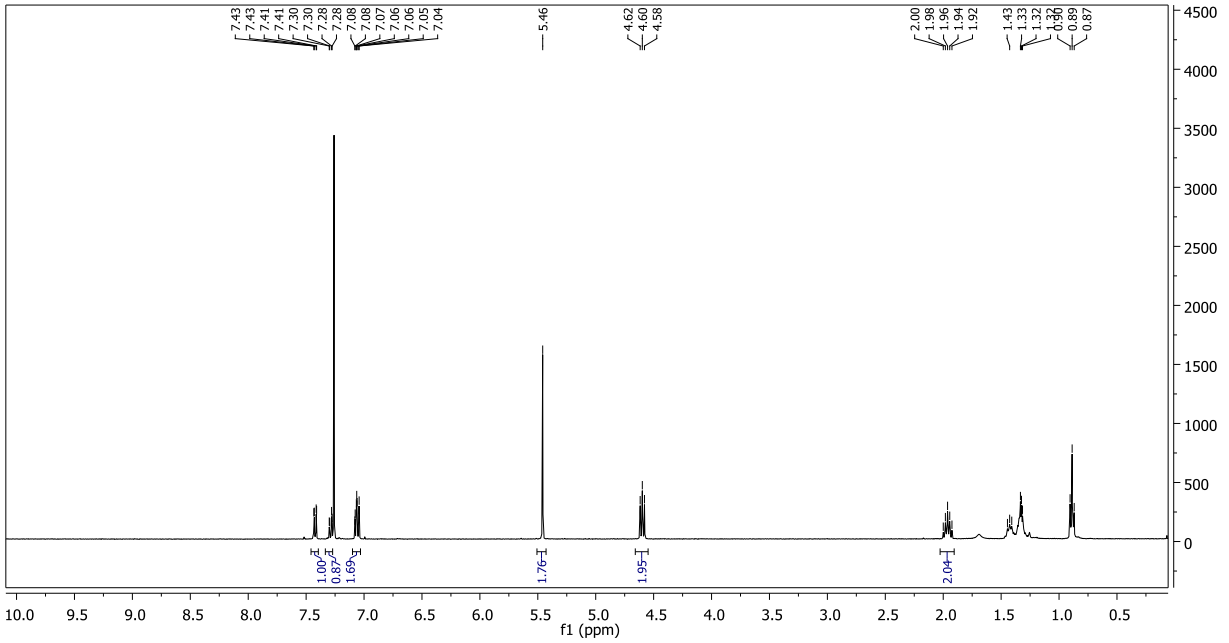


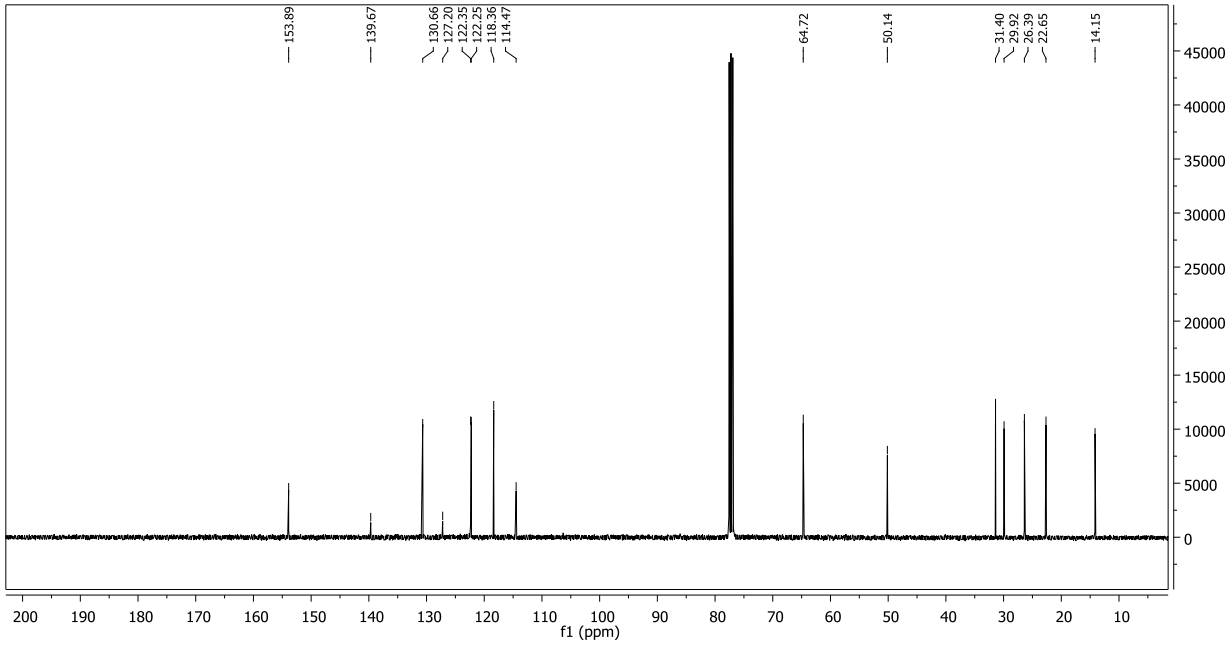




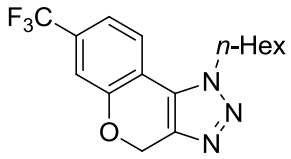
1-hexyl-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4d)

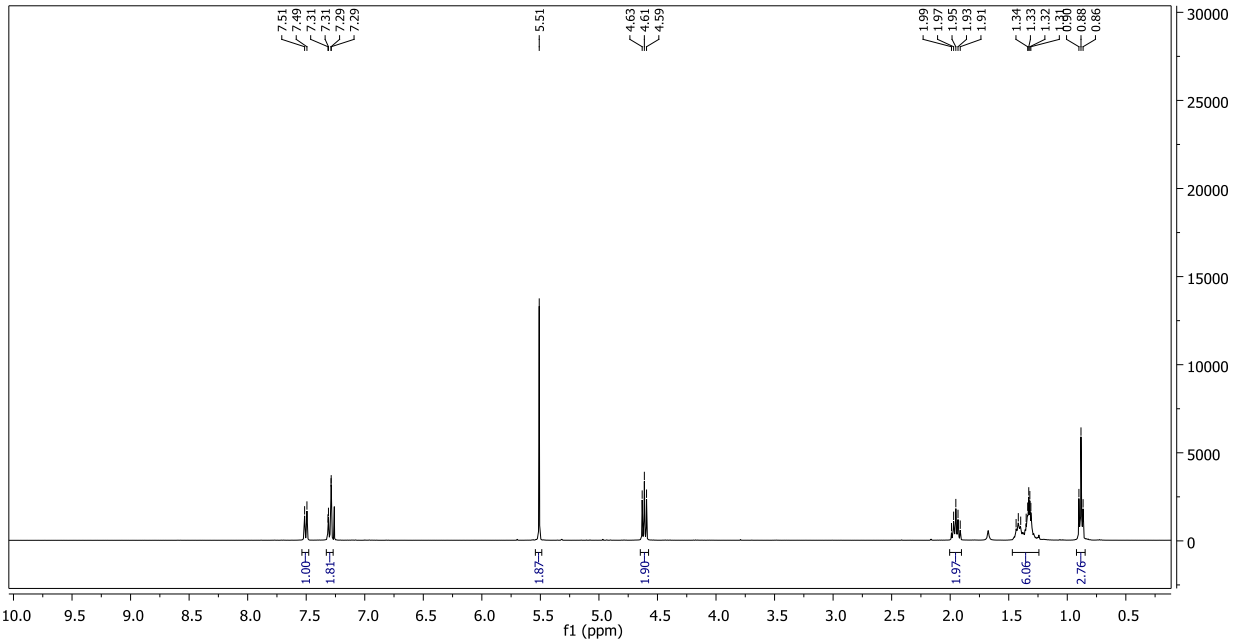


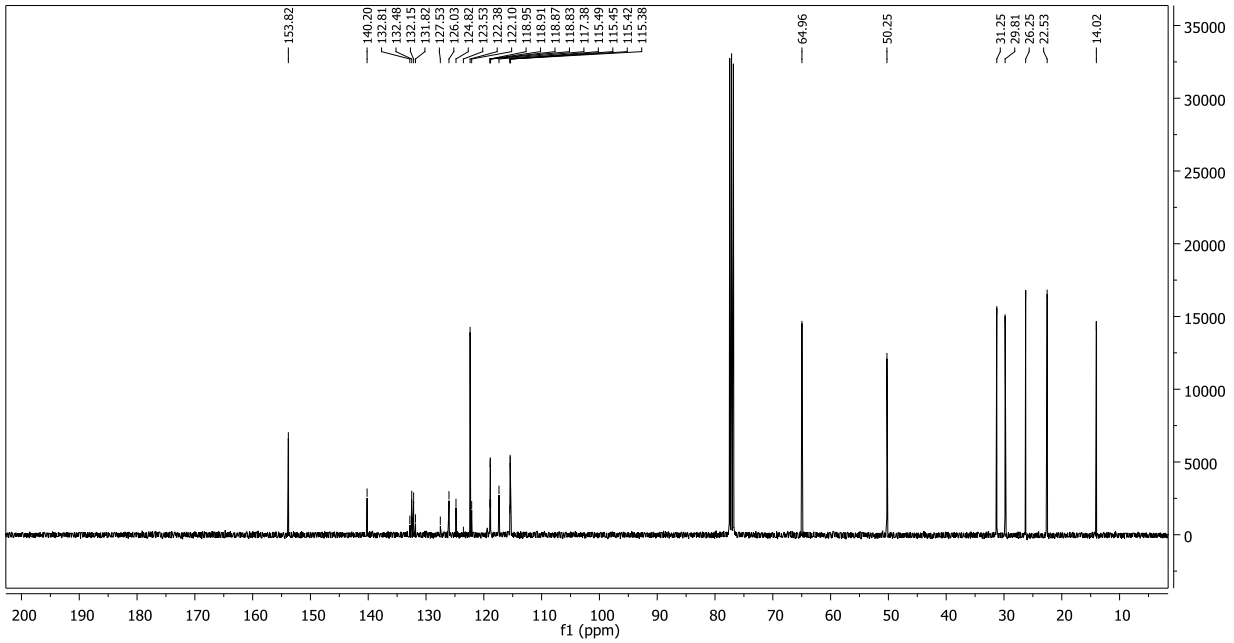


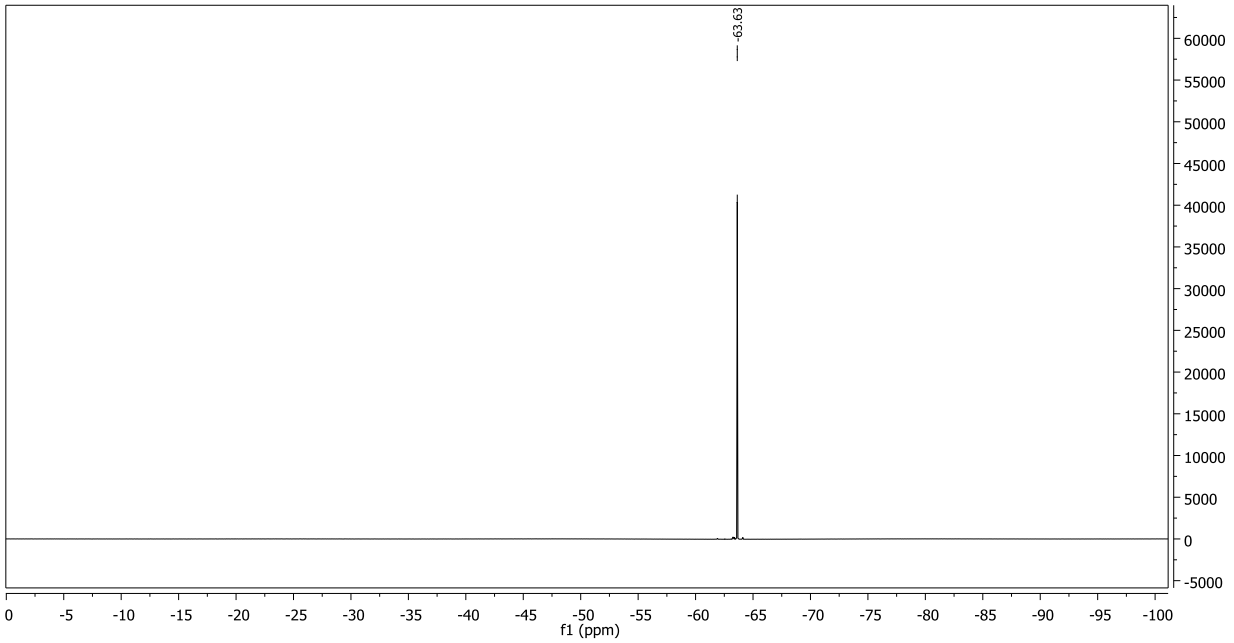


1-hexyl-7-(trifluoromethyl)-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4e)

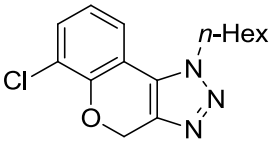


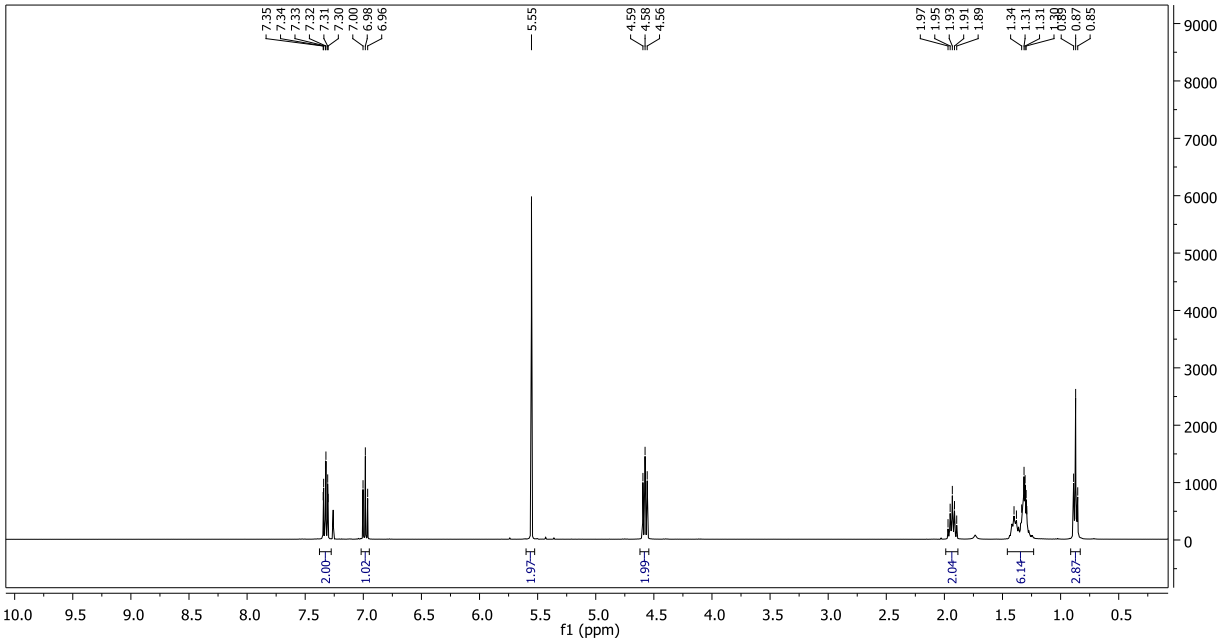


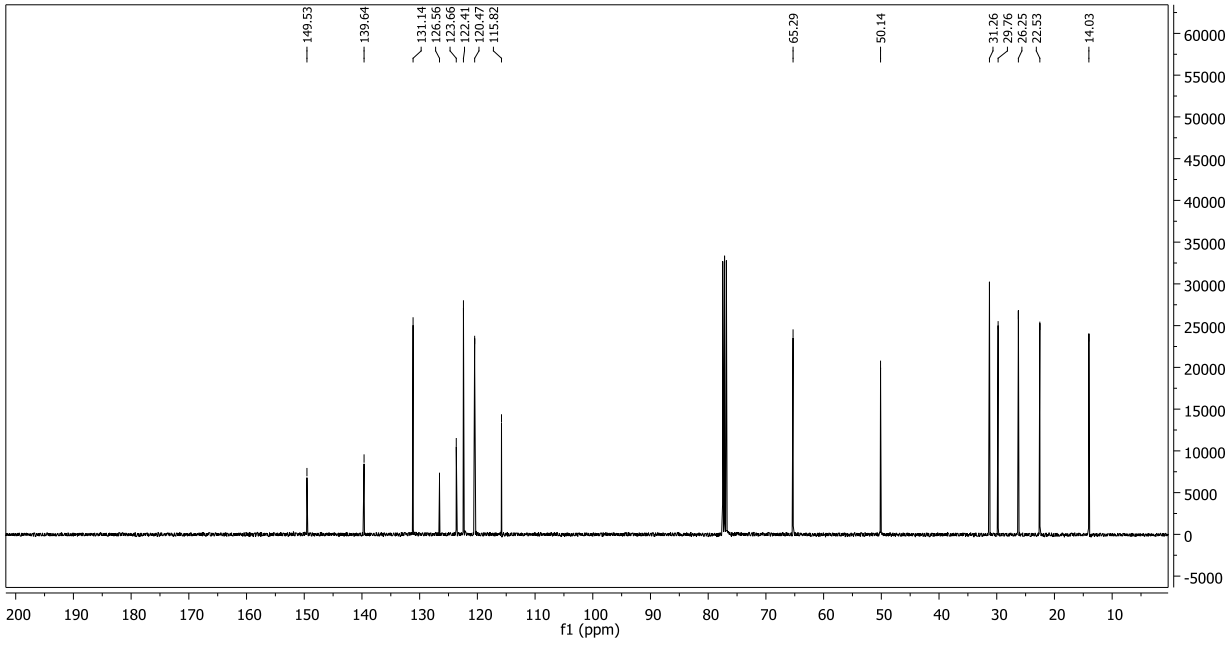




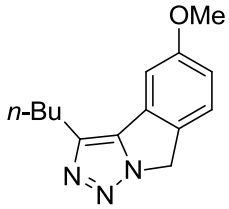
6-chloro-1-hexyl-1,4-dihydrochromeno[3,4-d][1,2,3]triazole (4f)

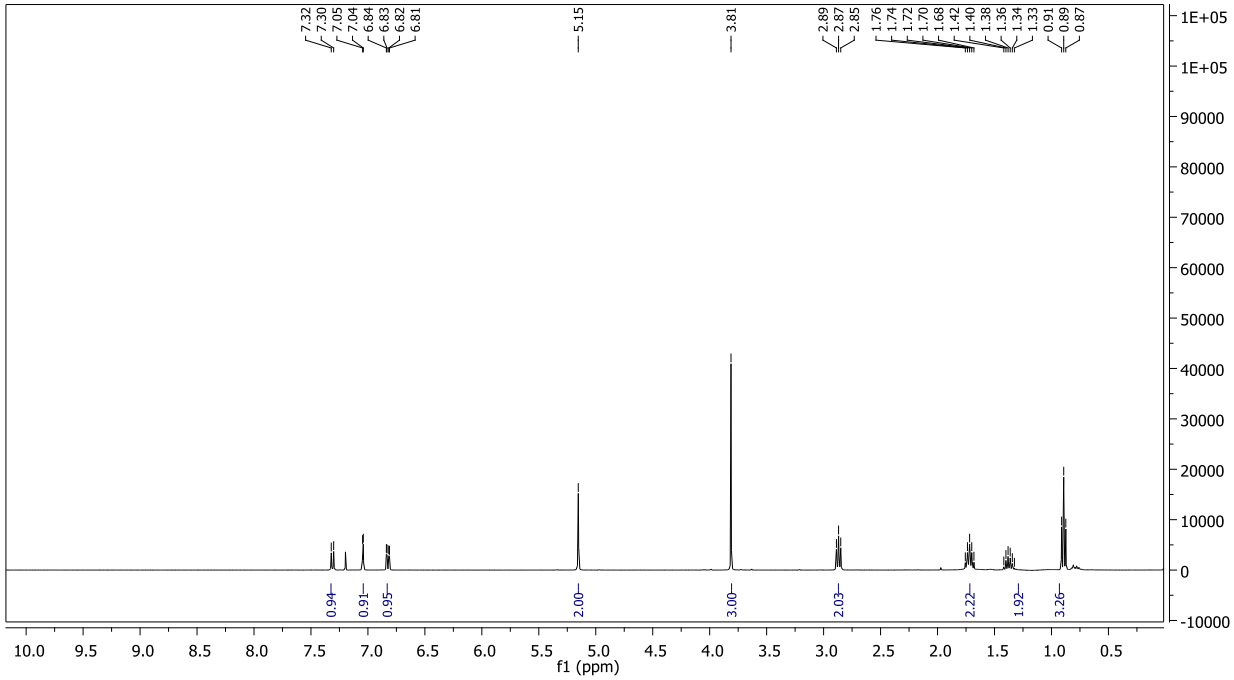


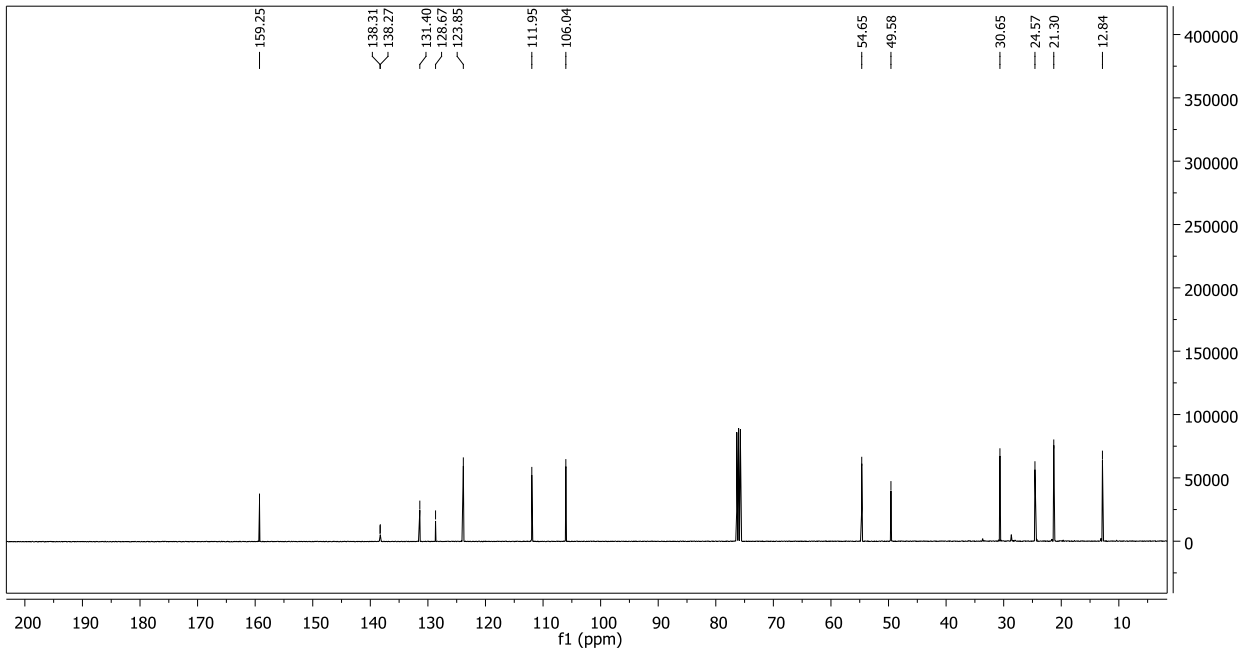




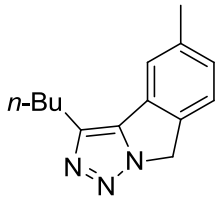
3-butyl-5-methoxy-8H-[1,2,3]triazolo[5,1-a]isoindole (6a)

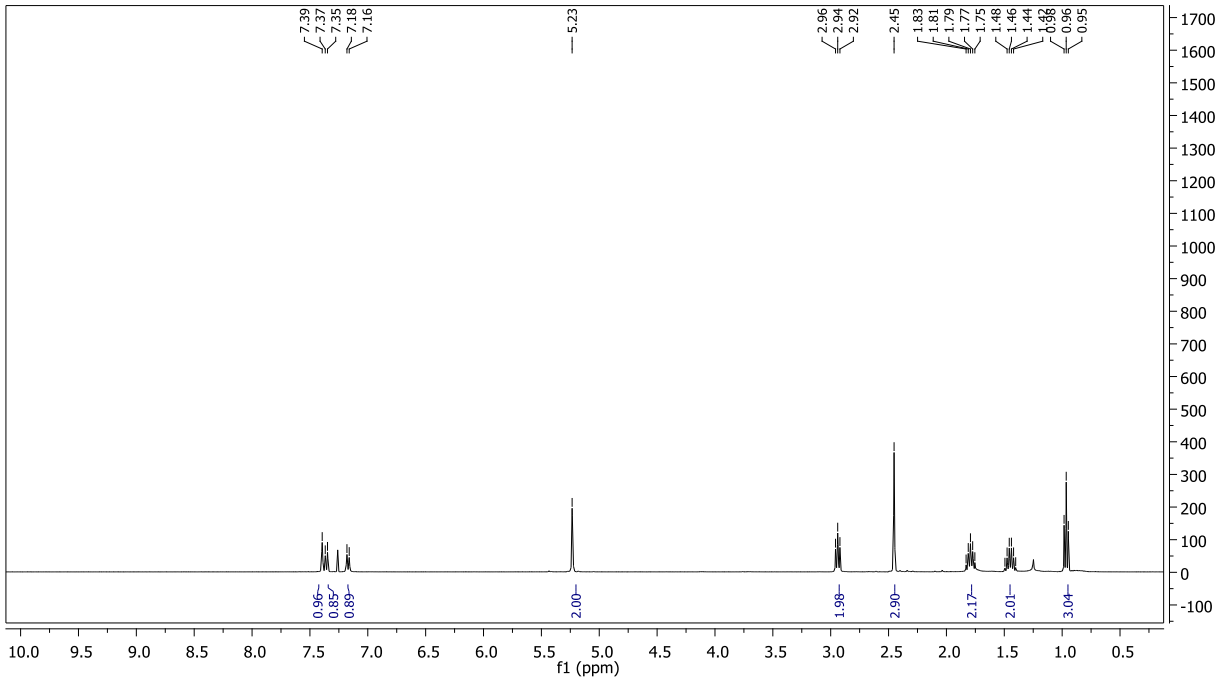


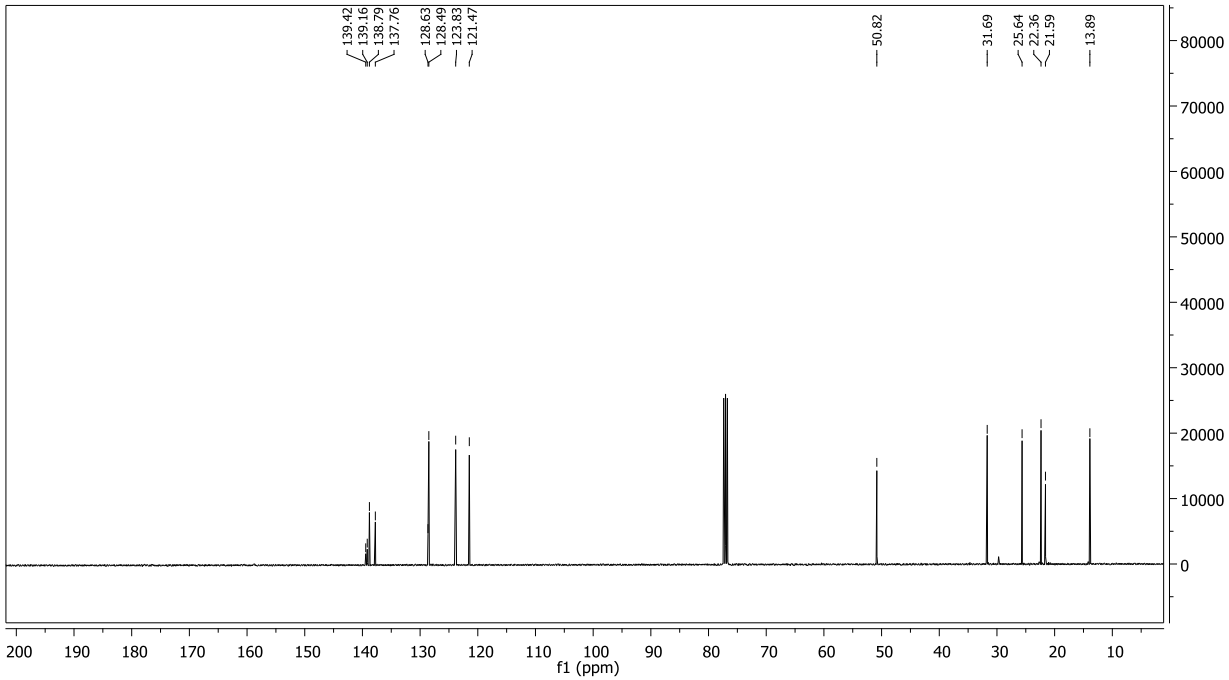




3-butyl-5-methyl-8H-[1,2,3]triazolo[5,1-a]isoindole (6b)







3-butyl-8H-[1,2,3]triazolo[5,1-a]isoindole (6c)