Supporting Information

One-Pot Click Chemistry using Hydrazine as Azide Surrogate: Easy access to 1,2,3-Triazole Functionalities

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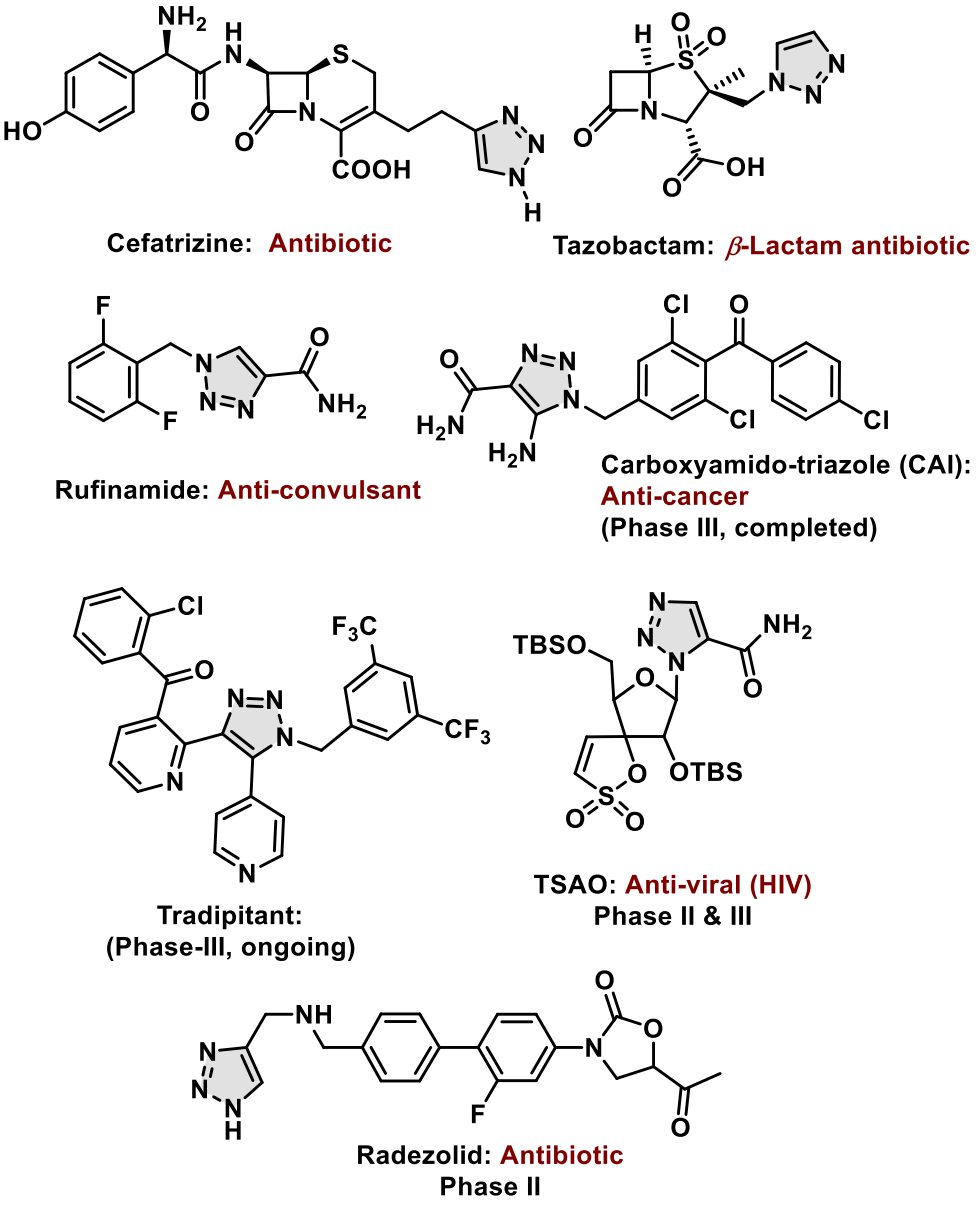


Figure S1: Representative picture of 1,2,3-triazole containing drugs and clinical candidates

EXPERIMENTAL SECTION

General Information

All reactions are carried out in round bottom flask in open atmosphere and reaction mixture was monitored by thin-layer chromatography (TLC). TLC pre-coated silica gel 60 F254 (20 × 20 cm). TLC plates are visualized by exposing UV light. Organic solvents are evaporated on rotary evaporator and all the compounds are purified on flash Column chromatography (230−400 mesh size). Mass spectra are obtained using an Agilent 6540 accurate mass Q-TOF LC/MS (135 eV) spectrometer, using electrospray ionization (ESI). ^{1}H NMR spectra are recorded on 400 and 500 MHz NMR instruments. Chemical data for protons are reported in parts per million (ppm, scale) downfield from tetramethylsilane as referenced to the residual proton in the NMR solvent ($CDCl_3$: δ 7.26, 1.56 $CDCl_3$ moisture and 1.25 grease peak, DMSO-d^6: δ 2.51, 3.33 DMSO-d^6 moisture or other solvents as mentioned). All the NMR spectras are processed with MestReNova software. The coupling constant *(J)* are in Hz. ESI-MS and HRMS spectra are recorded on LC-Q-TOF machines.

Precautionary note:

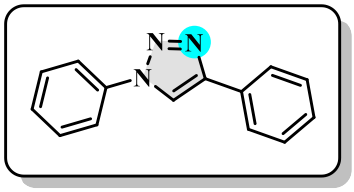
Although we have not experienced any problems in the handling of azides or diazo reagents, care should be taken when manipulating them due to their potentially explosive nature.

General Procedure for one pot conversion of aryl hydrazine hydrochloride to 1,2,3-triazoles (3a-3ac, Table 1, Scheme 1).

To an oven-dried 100 ml round bottom flask charged with a magnetic stir bar was added aryl hydrazine hydrochloride **1** (100 mg, 0.574-0.694 mmol, 1 equiv.) followed by *tert.* Butyl nitrite (1 equiv.) in PEG-400:H_2O (5 mL, 2:1) was stirred at 0 ^oC for 30 minutes. The progress of the reaction was observed using TLC to monitor the conversion of aryl hydrazine hydrochloride to phenyl azide (*in situ*) **2**. Then alkyne (1.0 equiv.) followed by $CuSO_4$. $5H_2O$ (0.1 equiv.) and Sod. Ascorbate (0.05 equiv.) were added to the reaction mixture. The reaction mixture was warmed to room temperature and the stirring was continued for 8-12 h overnight after the reaction was complete as monitored by TLC. The reaction mixture was diluted with H_2O, and the precipitate formed was filtered and dried in vacuo to afford the corresponding triazoles **3 (3a-3ac).**

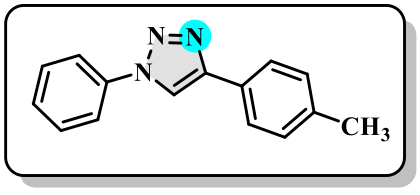
Experimental data:

1,4-Diphenyl-1*H*-1,2,3-triazole[1, 2](3a)



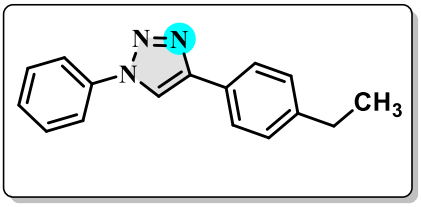
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.6; Yield 147 mg, 95%; yellow solid; m.p 185-190 ^oC; ^1H NMR (400 MHz, DMSO) δ 9.31 (s, 1H), 7.97 (m, 4H), 7.67 – 7.62 (m, 2H), 7.55 – 7.48 (m, 3H), 7.42 – 7.37 (m, 1H). ^{13}C NMR (101 MHz, DMSO) δ 147.8, 137.1, 130.7, 130.4, 129.4, 129.1, 128.7, 125.8, 120.4, 120.0; HRMS (ESI+TOF) calcd. for: $C_{14}H_{12}N_3$ 222.1031 $[M+H]^+$, found 222.1036.

1-Phenyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole[2, 3] (3b)



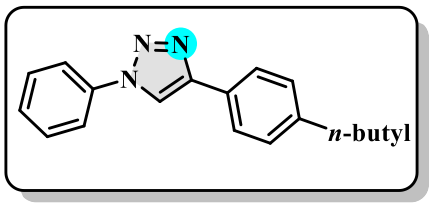
(Phenylhydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 158 mg, 96%; brown solid; m.p 142-148 ^oC; ^1H NMR (400 MHz, DMSO) δ 9.19 (s, 1H), 7.97 – 7.94 (m, 2H), 7.88 (d, *J* = 8.9 Hz, 2H), 7.64 (t, *J* = 7.9 Hz, 2H), 7.53 – 7.49 (m, 1H), 7.08 (d, *J* = 8.9 Hz, 2H), 3.82 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.7, 147.7, 137.1, 130.4, 129.0, 127.1, 123.2, 120.3, 119.0, 114.8, 55.6; HRMS (ESI+TOF) calcd. for: $C_{15}H_{14}N_3$ 236.1188 $[M+H]^+$, found 236.1196.

4-(4-Ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole (3c)



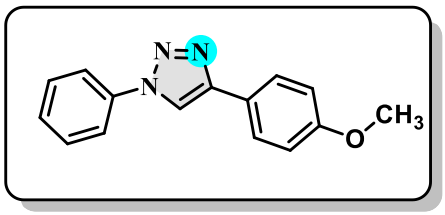
(Phenylhydrazine hydrogen chloride 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 161 mg, 93%; brown solid; m.p 145-150 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 9.26 (s, 1H), 7.98 – 7.94 (m, 2H), 7.89 – 7.85 (m, 2H), 7.68 – 7.61 (m, 2H), 7.53 (dd, *J* = 10.6, 4.3 Hz, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 2.66 (q, *J* = 7.6 Hz, 2H), 1.22 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 147.8, 144.4, 137.1, 130.4, 129.1, 128.8, 128.2, 125.8, 120.4, 119.6, 28.4, 15.9; HRMS (ESI+TOF) calcd. for: $C_{16}H_{16}N_3$ 250.1344 $[M+H]^+$, found 250.1345.

4-(4-Butylphenyl)-1-phenyl-1*H*-1,2,3-triazole (3d)



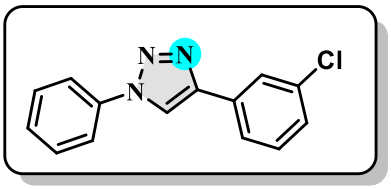
(Phenylhydrazine hydrogen chloride 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 176 mg, 91%; yellow solid; m.p 153-158 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 9.26 (s, 1H), 8.01 – 7.93 (m, 2H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.64 (t, *J* = 7.9 Hz, 2H), 7.52 (t, *J* = 7.4 Hz, 1H), 7.32 (d, *J* = 8.3 Hz, 2H), 2.67 – 2.58 (m, 2H), 1.59 (dq, *J* = 12.9, 7.5 Hz, 2H), 1.39 – 1.27 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 147.9, 143.0, 137.1, 130.4, 129.3, 129.1, 128.1, 125.7, 120.4, 119.6, 35.0, 33.5, 22.2, 14.2. HRMS (ESI+TOF) calcd. for: $C_{18}H_{20}N_3$ 278.1657 $[M+H]^+$, found 278.1652.

4-(4-Methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole (3e)



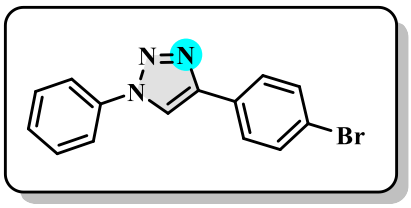
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4) R_f = 0.4; Yield 167 mg, 95%; yellow solid; m.p 141-147 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d^6) δ 9.19 (s, 1H), 7.95 (dd, *J* = 8.5, 1.0 Hz, 2H), 7.89 (d, *J* = 8.8 Hz, 2H), 7.67 – 7.58 (m, 2H), 7.51 (t, *J* = 8 Hz, 1H), 7.07 (d, *J* = 8.9 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.7, 147.7, 137.1, 130.3, 129.0, 127.1, 123.2, 120.3, 119.0, 114.8, 55.6; HRMS (ESI+TOF) calcd. for: $C_{15}H_{14}N_3O$ 252.1137 $[M+H]^+$, found 252.1135.

4-(3-Chlorophenyl)-1-phenyl-1*H*-1,2,3-triazole[2] (3f)



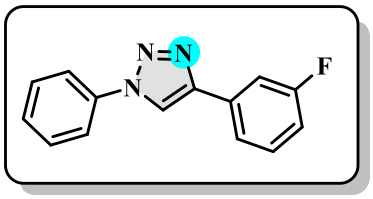
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 156 mg, 88%; pale yellow solid; m.p 142-147 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.39 (s, 1H), 7.99 (t, *J* = 1.7 Hz, 1H), 7.96 – 7.91 (m, 3H), 7.64 (dd, *J* = 8.5, 7.2 Hz, 2H), 7.57 – 7.51 (m, 2H), 7.45 (ddd, *J* = 8.0, 2.1, 1.1 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 146.4, 136.9, 134.2, 132.7, 131.4, 130.4, 129.3, 128.5, 125.3, 124.2, 120.8, 120.4; HRMS (ESI+TOF) calcd. for: $C_{14}H_{11}N_3Cl$ 256.0641 $[M+H]^+$, found 256.0641.

4-(4-Bromophenyl)-1-phenyl-1*H*-1,2,3-triazole (3g)



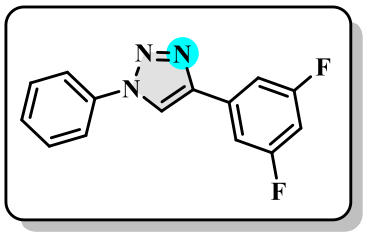
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 191 mg, 92%; pale yellow solid; m.p 135-139 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.35 (s, 1H), 7.96 – 7.89 (m, 4H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.64 (t, *J* = 7.9 Hz, 2H), 7.53 (ddd, *J* = 8.5, 2.2, 1.1 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 146.7, 136.9, 132.4, 130.4, 129.9, 129.3, 127.7, 121.7, 120.5, 120.4; HRMS (ESI+TOF) calcd. for: $C_{14}H_{11}N_3Br$ 300.0125 $[M+H]^+$, found 300.0125.

4-(3-Fluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3h)



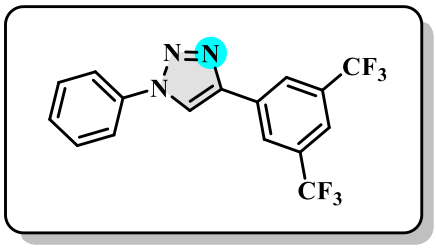
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 152 mg, 91%; white solid; m.p 146-152 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.39 (s, 1H), 7.97 – 7.94 (m, 2H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.75 (d, *J* = 9.2 Hz, 1H), 7.65 (t, *J* = 7.8 Hz, 2H), 7.55 (dd, *J* = 14.5, 6.9 Hz, 2H), 7.23 (t, *J* = 8.6 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 164.2, 161.8, 146.7, 137.0, 133.1, 133.0, 131.7, 131.6, 130.4, 129.3, 121.8, 121.8, 120.8, 120.5, 115.5, 115.3, 112.5, 112.2; ^{19}F NMR (400 MHz, DMSO) δ -112.5; HRMS (ESI+TOF) calcd. for: $C_{14}H_{11}N_3F$ 240.0942 $[M+H]^+$, found 240.0943.

4-(3,5-Difluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3i)



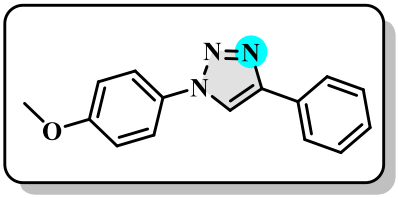
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 157 mg, 88%; pale yelow solid; m.p 202-207 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.26 (s, 1H), 7.77 – 7.74 (m, 2H), 7.48 (ddd, *J* = 5.5, 4.6, 3.5 Hz, 4H), 7.40 – 7.36 (m, 1H), 7.10 (ddd, *J* = 9.4, 5.9, 2.4 Hz, 1H); ^{19}F NMR (377 MHz, DMSO) δ -108.99; ^{13}C NMR (101 MHz, DMSO) δ 164.6, 164.5, 162.2, 162.1, 145.7, 136.8, 134.3-134.0 (t, *J* = 10 Hz), 130.4, 129.4, 121.5, 120.5, 108.8, 108.7, 108.67, 108.60, 104.1-103.6 (t, *J* = 2626 Hz); HRMS (ESI+TOF) calcd. for: $C_{14}H_{10}N_3O_2$ 258.0843 $[M+H]^+$, found 258.0839.

4-(3,5-Bis(trifluoromethyl)phenyl)-1-phenyl-1*H*-1,2,3-triazole (3j)



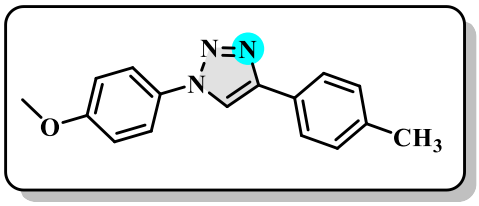
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 206 mg, 83%; white solid; m.p 223-228 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.46 (s, 1H), 8.36 (s, 2H), 7.89 (s, 1H), 7.77 – 7.74 (m, 2H), 7.49 – 7.45 (m, 2H), 7.38 – 7.34 (m, 1H); ^{19}F NMR (400 MHz, DMSO) δ -61.7; ^{13}C NMR (101 MHz, DMSO) δ 164.6, 164.5, 162.2, 162.1, 145.7, 136.8, 134.3, 134.2, 134.0, 130.4, 129.4, 121.5, 120.5, 108.8, 108.7, 108.6, 108.6, 104.1, 103.9, 103.6; HRMS (ESI+TOF) calcd. for: $C_{16}H_{10}N_3F_6$ 358.0779 $[M+H]^+$, found 358.0773.

1-(4-Methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole[1, 4] (3k)



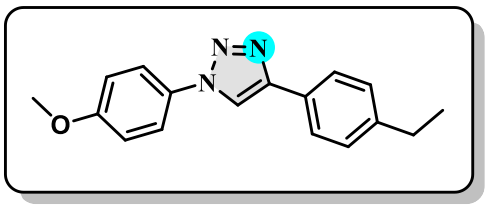
(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 129 mg, 92%; white solid; m.p 187—193 °C; ^{1}H NMR (400 MHz, DMSO) δ 9.21 (s, 1H), 7.97 – 7.93 (m, 2H), 7.87 (d, *J* = 9.1 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.41 – 7.36 (m, 1H), 7.18 (d, *J* = 9.1 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.7, 147.5, 130.8, 130.5, 129.4, 128.6, 125.7, 122.1, 120.0, 115.3, 56.0; HRMS (ESI+TOF) calcd. for: $C_{15}H_{14}N_3O$ 252.1137 $[M+H]^+$, found 252.1135.

1-(4-methoxyphenyl)-4-(*p*-tolyl)-1H-1,2,3-triazole (3l)



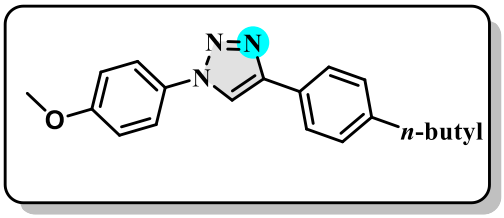
(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 130 mg, 85%; pale yellow solid; m.p 174-177 ^oC; ^1H NMR (400 MHz, DMSO) δ 9.14 (s, 1H), 7.84 (t, *J* = 8.8 Hz, 4H), 7.30 (d, *J* = 7.8 Hz, 2H), 7.17 (d, *J* = 9.0 Hz, 2H), 3.84 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.7, 147.6, 137.9, 130.5, 129.9, 128.0, 125.7, 122.0, 119.6, 115.3, 56.0, 21.3; HRMS (ESI+TOF) calcd. for: $C_{16}H_{16}N_3O$ 266.1293 $[M+H]^+$, found 266.1283.

4-(4-Ethylphenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3m)



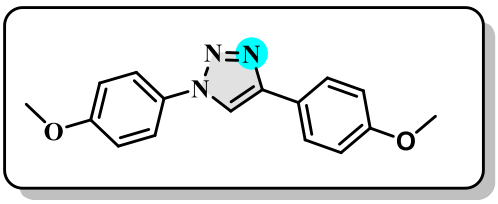
(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 145 mg, 90%; white solid; m.p 178-183 ^oC; ^1H NMR (400 MHz, DMSO) δ 9.14 (s, 1H), 7.86 (dd, *J* = 8.7, 2.2 Hz, 4H), 7.39 – 7.28 (m, 2H), 7.17 (d, *J* = 9.1 Hz, 2H), 3.84 (s, 3H), 2.64 (q, *J* = 8 Hz, 12 Hz, 2H), 1.21 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.7, 147.6, 144.2, 130.5, 128.8, 128.3, 125.7, 122.0, 119.6, 115.3, 56.0, 28.4, 15.9; HRMS (ESI+TOF) calcd. for: $C_{17}H_{18}N_3O$ 280.1450 $[M+H]^+$, found 280.1446.

4-(4-Butylphenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3n)



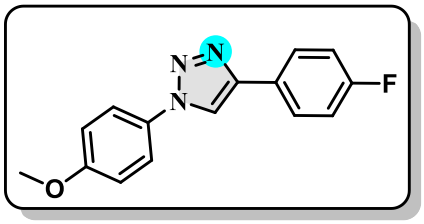
(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 165 mg, 93%; white solid; m.p 157-163 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.89 (s, 1H), 7.60 (t, *J* = 8.2 Hz, 4H), 7.06 (d, *J* = 8.3 Hz, 2H), 6.92 (d, *J* = 9.1 Hz, 2H), 3.59 (s, 3H), 2.39 – 2.34 (m, 2H), 1.37 – 1.30 (m, 2H), 1.08 (dd, *J* = 14.9, 7.4 Hz, 2H), 0.66 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.7, 147.6, 142.8, 130.5, 129.3, 128.3, 125.7, 122.07, 119.6, 115.3, 56.0, 35.0, 33.5, 22.2, 14.2; HRMS (ESI+TOF) calcd. for: $C_{19}H_{22}N_3O$ 308.1765 $[M+H]^+$, found 308.1763.

1,4-Bis(4-methoxyphenyl)-1*H*-1,2,3-triazole (3o)



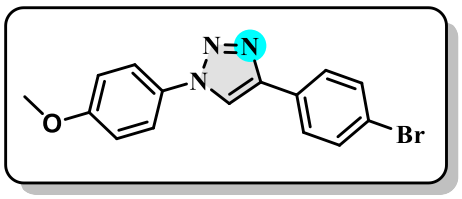
(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 156 mg, 96%; brown solid; m.p 153-158 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 9.09 (s, 1H), 7.86 (dd, *J* = 8.9, 6.1 Hz, 4H), 7.17 (d, *J* = 9.1 Hz, 2H), 7.06 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.6, 147.5, 130.6, 127.1, 123.4, 122.0, 119.0, 115.3, 114.8, 56.0, 55.6; HRMS (ESI+TOF) calcd. for: $C_{16}H_{16}N_3O_2$ 282.1245 $[M+H]^+$, found 282.1243.

4-(4-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3p)



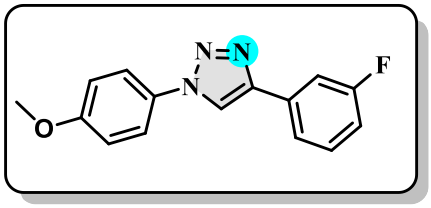
(4-Methoxyphenyl)phenylhydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 120 mg, 77 %; white solid; m.p 142-147 ^{o}C.: $^{;1}$H NMR (400 MHz, DMSO) δ 9.19 (s, 1H), 7.98 (dd, *J* = 8.9, 5.5 Hz, 2H), 7.85 (d, *J* = 9.1 Hz, 2H), 7.35 (t, *J* = 9.0 Hz, 2H), 7.18 (d, *J* = 9.1 Hz, 2H), 3.85 (s, 3H). ^{19}F NMR (400 MHz, DMSO) δ -113.69. ^{13}C NMR (101 MHz, DMSO) δ 163.6, 161.2, 159.8, 146.7, 130.5, 127.8-127.7(d, *J* = 8 Hz), 127.45-127.42 (d, *J* = 3 Hz), 122.1, 120.0, 116.5, 116.3, 115.4, 56.0. HRMS (ESI+TOF) calcd. for: $C_{15}H_{13}N_3OF$ 270.1043 $[M+H]^+$, found 270.1048.

4-(4-Bromophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole[5] (3q)



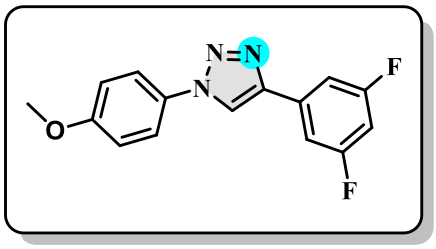
(4-Methoxyphenyl)hydrazine hydrogen chloride,100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 157 mg, 83 %; white solid; m.p 176-180 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 9.25 (s, 1H), 7.87 (dd, *J* = 17.8, 8.8 Hz, 4H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.18 (d, *J* = 9.1 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.8, 146.5, 132.4, 130.4, 130.1, 127.7, 122.2, 121.6, 120.5, 115.4, 56.0; HRMS (ESI+TOF) calcd. for: $C_{15}H_{13}N_3OF$ 330.0224 $[M+H]^+$, found 330.0242.

4-(3-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3r)



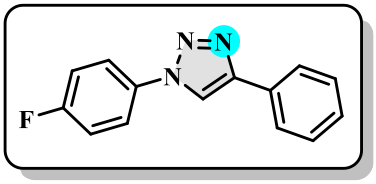
(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 120 mg, 77 %; white solid; m.p 163-168 ºC; ^{1}H NMR (400 MHz, DMSO) δ 9.27 (s, 1H), 7.84 (d, *J* = 9.1 Hz, 2H), 7.80 (d, *J* = 7.9 Hz, 1H), 7.73 (ddd, *J* = 10.3, 2.5, 1.5 Hz, 1H), 7.55 (td, *J* = 8.0, 6.2 Hz, 1H), 7.26 – 7.15 (m, 3H), 3.84 (s, 3H); ^{19}F NMR (377 MHz, DMSO) δ -112.64; ^{13}C NMR (101 MHz, DMSO) δ 164.2, 161.8, 159.8, 146.4, 146.4, 133.2, 133.1, 131.6, 131.5, 130.4, 122.1, 121.77, 121.75, 120.8, 115.4, 115.2, 112.4, 112.2, 56.0; HRMS (ESI+TOF) calcd. for: $C_{15}H_{13}N_3OF$ 270.1043 $[M+H]^+$, found 270.1037.

4-(3,5-Difluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3s)



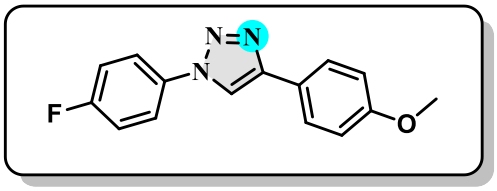
(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 160 mg, 86 %; pale yellow solid; m.p 207-211 ºC; ^{1}H NMR (400 MHz, DMSO) δ 9.16 (s, 1H), 7.70 – 7.64 (m, 2H), 7.51 – 7.44 (m, 2H), 7.10 (tt, *J* = 9.3, 2.2 Hz, 1H), 7.05 – 7.00 (m, 2H), 3.69 (s, 3H); ^{19}F NMR (377 MHz, DMSO) δ -109.03; ^{13}C NMR (101 MHz, DMSO) δ 164.6, 164.5, 162.2, 162.1, 159.9, 145.6, 145.58, 145.55, 134.4, 134.3, 134.2, 130.2, 122.2, 121.4, 115.4, 108.8, 108.7, 108.6, 108.5, 103.8, 56.0; HRMS (ESI+TOF) calcd. for: $C_{15}H_{12}N_3OF_2$ 288.0948 $[M+H]^+$, found 288.0951.

1-(4-Fluorophenyl)-4-phenyl-1*H*-1,2,3-triazole[4] (3t)



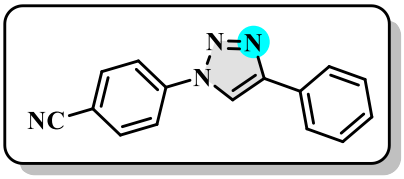
(4-fluorophenyl)hydrazine hydrogen chloride, 100 mg, 0.617 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.3; Yield 135 mg, 91 %; white solid; m.p 210-215 ºC; ^{1}H NMR (400 MHz, DMSO) δ 9.29 (s, 1H), 8.05 – 7.98 (m, 2H), 7.97 – 7.91 (m, 2H), 7.54 – 7.48 (m, 4H), 7.40 (m, 1H); ^{19}F NMR (377 MHz, DMSO) δ -113.06; ^{13}C NMR (101 MHz, DMSO) δ 163.3, 160.9, 147.8, 133.7, 133.6, 130.6, 129.5, 128.7, 125.8, 122.8, 122.8, 120.3, 117.4, 117.1; HRMS (ESI+TOF) calcd. for: $C_{14}H_{11}N_3F$ 240.0937 $[M+H]^+$, found 240.0919.

1-(4-Fluorophenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3u)



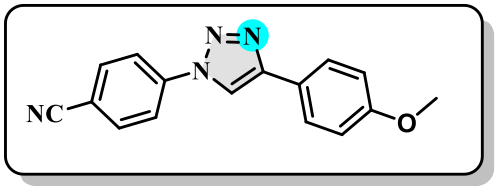
(4-fluorophenyl)hydrazine hydrogen chloride, 100 mg, 0.617 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.3; Yield 123 mg, 74%; white solid; m.p 187-194 ^oC; ^1H NMR (400 MHz, DMSO) δ 9.17 (s, 1H), 8.10 – 7.94 (m, 2H), 7.94 – 7.80 (m, 2H), 7.49 (t, *J* = 8.8 Hz, 2H), 7.20 – 6.97 (m, 2H), 3.81 (s, 3H); ^{19}F NMR (400 MHz, DMSO) δ -113.2; ^{13}C NMR (101 MHz, DMSO) δ 163.2, 160.8, 159.7, 147.7, 133.7, 133.7, 127.1, 123.1, 122.7, 122.6, 119.3, 117.3, 117.1, 114.8, 55.6; HRMS (ESI+TOF) calcd. for: $C_{15}H_{13}N_3OF$ 270.1043 $[M+H]^+$, found 270.1048.

4-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)benzonitrile (3v)



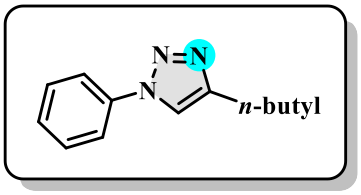
(4-Cyanophenyl)hydrazine hydrogen chloride, 100 mg, 0.591 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 140 mg, 96%; pale yellow solid; m.p 203-210 ^oC ; ^1H NMR (400 MHz, DMSO) δ 9.47 (s, 1H), 8.17 (dd, *J* = 22.1, 9.0 Hz, 4H), 7.98 – 7.93 (m, 2H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 148.1, 139.9, 134.8, 130.3, 129.5, 128.9, 125.8, 120.8, 120.2, 118.6, 111.5; HRMS (ESI+TOF) calcd. for: $C_{15}H_{11}N_4$ 247.0984 $[M+H]^+$, found 247.0981.

4-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3w)



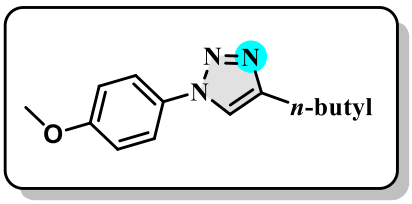
(4-Cyanophenyl)hydrazine hydrogen chloride, 100 mg, 0.591 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 139 mg, 95%; white solid; m.p 198-204 ^oC; ^1H NMR (400 MHz, DMSO) δ 9.31 (s, 1H), 8.13 (dd, *J* = 21.3, 9.0 Hz, 4H), 7.85 (d, *J* = 8.8 Hz, 2H), 7.15 – 7.00 (m, 2H), 3.80 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.90, 148.12, 139.99, 134.74, 127.24, 122.78, 120.60, 119.07, 118.62, 114.90, 111.31, 55.64, 40.15, 39.94, 39.73; HRMS (ESI+TOF) calcd. for: $C_{16}H_{13}N_4O$ 277.1089 $[M+H]^+$, found 277.1085.

4-Butyl-1-phenyl-1*H*-1,2,3-triazole (3x)



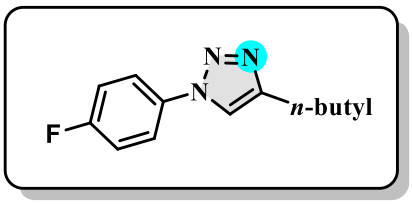
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.6; Yield 125 mg, 89 %; pale yellow solid ;^{1}H NMR (400 MHz, DMSO) δ 8.57 (s, 1H), 7.96 – 7.83 (m, 2H), 7.68 – 7.55 (m, 2H), 7.46 (m, 1H), 2.70 (t, *J* = 7.6 Hz, 2H), 1.74 – 1.60 (m, 2H), 1.37 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 148.6, 137.2, 130.3, 128.7, 120.4, 120.2, 31.40, 25.1, 22.1, 14.1; HRMS (ESI+TOF) calcd. for: $C_8H_7N_3$ 202.1343 $[M+H]^+$, found 202.1343 .

4-Butyl-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3y)



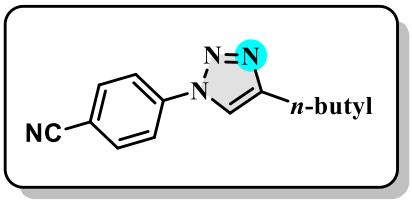
(4-Methoxyphenyl)hydrazine hydrogen chloride 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 107 mg, 80 %; yellow solid; ^{1}H NMR (400 MHz, DMSO) δ 8.46 (d, *J* = 1.0 Hz, 1H), 7.78 (d, *J* = 9.0 Hz, 2H), 7.20 – 7.02 (m, 2H), 3.82 (s, 3H), 2.69 (t, *J* = 7.6 Hz, 2H), 1.64 (ddd, *J* = 12.8, 8.6, 6.5 Hz, 2H), 1.47 – 1.32 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.4, 148.3, 130.7, 121.8, 120.4, 115.2, 55.9, 31.4, 25.1, 22.1, 14.1; HRMS (ESI+TOF) calcd. for: $C_{13}H_{18}N_3O$ 232.1450 $[M+H]^+$, found 232.1452.

4-Butyl-1-(4-fluorophenyl)-1*H*-1,2,3-triazole (3z)



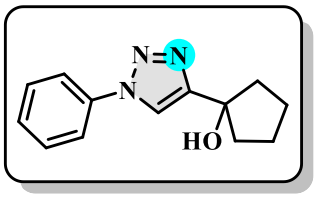
(4-Fluorophenyl)hydrazine hydrogen chloride, 100 mg, 0.617 mmol); TLC (Hexane/EtOAc, 6:4) R_f = 0.6; Yield 112 mg, 83 %; white solid; m.p 154-160 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 8.56 (s, 1H), 8.01 – 7.85 (m, 2H), 7.52 – 7.37 (m, 2H), 2.70 (t, *J* = 7.6 Hz, 2H), 1.72 – 1.57 (m, 2H), 1.37 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H); ^{19}F NMR (400 MHz, DMSO) δ -113.7; ^{13}C NMR (101 MHz, DMSO) δ 163.0, 160.6, 148.6, 133.8, 122.5, 122.4, 120.7, 117.2, 117.0, 31.3, 25.1, 22.1, 14.1; HRMS (ESI+TOF) calcd. for: $C_{12}H_{15}N_3F$ 220.1250 $[M+H]^+$, found 220.1255.

4-(4-Butyl-1*H*-1,2,3-triazol-1-yl)benzonitrile (3aa)



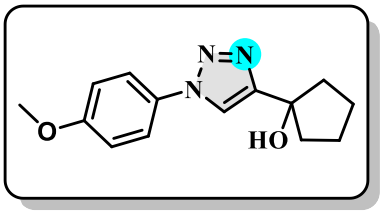
(4-Cyanophenyl)hydrazine hydrogen chloride, 100 mg, 0.591 mmol); TLC (Hexane/EtOAc, 6:4) R_f = 0.4; Yield 110 mg, 82 %; pale yellow liquid; ^{1}H NMR (400 MHz, DMSO) δ 8.75 (s, 1H), 8.18 – 8.04 (m, 4H), 2.81 – 2.64 (m, 2H), 1.74 – 1.58 (m, 2H), 1.37 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, DMSO) δ 149.1, 140.1, 134.7, 120.7, 120.5, 118.6, 111.0, 31.2, 25.0, 22.1, 14.1. HRMS (ESI+TOF) calcd. for: $C_{13}H_{15}N_4$ 227.1277 $[M+H]^+$, found 227.1276.

1-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ab)



Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 136 mg, 85 %; pale yellow solid; m.p 154-159 ^{o}C ; ^{1}H NMR (400 MHz, DMSO) δ 8.60 (s, 1H), 7.93 – 7.90 (m, 2H), 7.59 (dd, *J* = 8.5, 7.2 Hz, 2H), 7.49 – 7.45 (m, 1H), 5.15 (s, 1H), 2.09 – 2.00 (m, 2H), 1.95 – 1.83 (m, 4H), 1.73 (dd, *J* = 5.7, 2.2 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 156.1, 137.3, 130.3, 128.8, 120.3, 119.8, 77.8, 41.1, 23.7; HRMS (ESI+TOF) calcd. for: $C_{13}H_{16}N_3O$ 230.1293 $[M+H]^+$, found 230.1298.

1-(1-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ac)

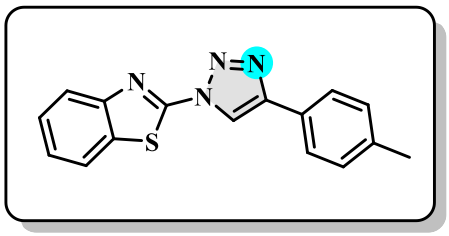


(4-Methoxyphenyl)hydrazine hydrogen chloride, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 129 mg, 86 %; pale yellow solid; m.p 171-176 ^{o}C; ^{1}H NMR (400 MHz, DMSO) δ 8.48 (s, 1H), 7.81 (d, *J* = 9.1 Hz, 2H), 7.12 (d, *J* = 9.1 Hz, 2H), 5.12 (s, 1H), 3.83 (s, 3H), 2.03 (d, *J* = 6.6 Hz, 2H), 2.00 – 1.81 (m, 4H), 1.78 – 1.68 (m, 2H); ^{13}C NMR (101 MHz, DMSO) δ 159.4, 155.8, 130.7, 121.9, 119.8, 115.2, 77.8, 55.9, 41.1, 23.7; HRMS (ESI+TOF) calcd. for: $C_{14}H_{18}N_3O_2$ 260.1399 $[M+H]^+$, found 260.1401.

General Procedure for one pot conversion of aryl hydrazine hydrochloride to 1,2,3-triazoles (4a-4f, Scheme 2).

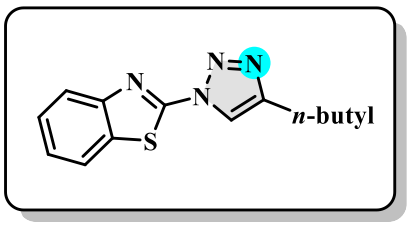
To an oven-dried 100 ml round bottom flask charged with a magnetic stir bar was added aryl hydrazine hydrochloride **1** (100 mg, 0.574-0.694 mmol, 1 equiv.) followed by *tert.* Butyl nitrite (1 equiv.) in PEG-400:H_2O (5 mL, 2:1) was stirred at 0 ^oC for 30 minutes. The progress of the reaction was observed using TLC to monitor the conversion of aryl hydrazine hydrochloride to phenyl azide (*in situ*) **2**. Then alkyne (1.0 equiv.) followed by $CuSO_4$. $5H_2O$ (0.1 equiv.) and Sod. Ascorbate (0.05 equiv.) were added to the reaction mixture. The reaction mixture was warmed to room temperature and the stirring was continued for 8-12 h overnight after the reaction was complete as monitored by TLC. The reaction mixture was diluted with H_2O, and the precipitate formed was filtered and dried in vacuo to afford the corresponding triazoles (**4a-4f**).

2-(4-(*p*-tolyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4a)



(2-Hydrazineylbenzo[*d*]thiazole, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 126 mg, 71%; white solid; m.p 193-197 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.73 (s, 1H), 8.00 (ddd, *J* = 8.2, 1.1, 0.6 Hz, 1H), 7.91 (ddd, *J* = 8.0, 1.2, 0.6 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 2H), 7.58 – 7.53 (m, 1H), 7.47 (ddd, *J* = 8.1, 7.3, 1.2 Hz, 1H), 7.30 (d, *J* = 7.9 Hz, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.4, 150.1, 148.9, 139.0, 133.1, 129.7, 127.0, 126.48, 126.1, 126.0, 123.1, 121.9, 116.7, 21.4; HRMS (ESI+TOF) calcd. for: $C_{16}H_{14}N_3S_2$ 293.0847 $[M+H]^+$, found 293.0847.

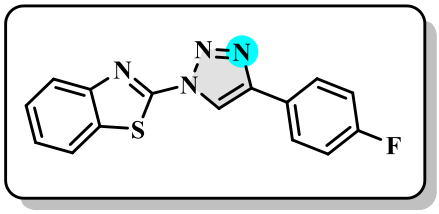
2-(4-butyl-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4b)



(2-Hydrazineylbenzo[*d*]thiazole, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 121 mg, 77%; pale yellow solid; m.p 198-205 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.98 – 7.96 (m, 1H), 7.91 – 7.89 (m, 1H), 7.56 – 7.52 (m, 1H), 7.48 – 7.43 (m, 1H), 2.84 (t, *J* = 7.5 Hz, 2H), 1.78 – 1.71 (m, 2H), 1.45 (dd, *J* = 15.0, 7.4 Hz,

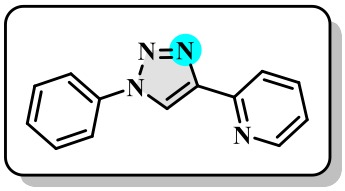
2H), 0.97 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.1, 149.8, 133.0, 126.9, 125.9, 123.0, 121.8, 118.6, 31.1, 30.9, 25.2, 22.2, 13.8; HRMS (ESI+TOF) calcd. for: $C_{13}H_{16}N_3S_2$ 259.1018 $[M+H]^+$, found 259.1018.

2-(4-(4-fluorophenyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4c)



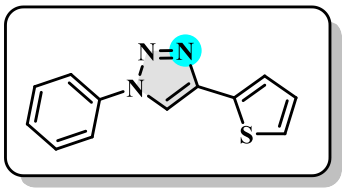
(2-Hydrazineylbenzo[*d*]thiazole, 100 mg, 0.574 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 119 mg, 68%; light brown solid; m.p 192-197 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (s, 1H), 7.93 (ddd, *J* = 8.1, 1.2, 0.6 Hz, 1H), 7.90 – 7.80 (m, 3H), 7.49 (ddd, *J* = 8.2, 7.3, 1.3 Hz, 1H), 7.40 (ddd, *J* = 8.4, 7.4, 1.2 Hz, 1H), 7.11 (t, *J* = 8.7 Hz, 2H); ^{19}F NMR (377 MHz, $CDCl_3$) δ -111.99; ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.41, 161.93, 156.28, 150.10, 147.95, 133.17, 127.98, 127.90, 127.16, 126.23, 125.58, 125.55, 123.26, 121.94, 116.91, 116.26, 116.05, 77.35, 77.04, 76.72; HRMS (ESI+TOF) calcd. for: $C_{15}H_{11}N_3S_2F$ 297.0617 $[M+H]^+$, found 297.0617.

2-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)pyridine (4d)



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 103 mg, 66 %; brown solid; m.p 179-184 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.62 (d, *J* = 4.3 Hz, 1H), 8.27 (d, *J* = 7.9 Hz, 1H), 7.82 (dd, *J* = 8.6, 1.2 Hz, 3H), 7.58 – 7.53 (m, 2H), 7.48 – 7.44 (m, 1H), 7.31 – 7.27 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.8, 149.3, 148.7, 137.2, 136.9, 129.8, 128.9, 123.1, 120.5, 120.4, 120.1; HRMS (ESI+TOF) calcd. for: $C_{13}H_{11}N_4$ 223.0984 $[M+H]^+$, found 223.0989.

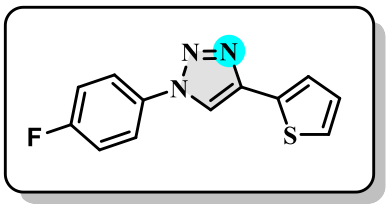
1-Phenyl-4-(thiophen-2-yl)-1*H*-1,2,3-triazole[6] (4e)



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 121 mg, 77%; pale yellow solid; m.p 132-138 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.72 – 7.68 (m, 2H), 7.49 – 7.44 (m, 2H), 7.41 – 7.36 (m, 2H), 7.27 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.04 (dd, *J* = 5.1, 3.6 Hz, 1H). ^{13}C NMR (101 MHz, CDCl3) δ 143.4,

136.8, 132.3, 129.8, 128.9, 127.7, 125.4, 124.6, 120.5, 117.1; HRMS (ESI+TOF) calcd. for: $C_{12}H_{10}N_3S$ 228.0595 $[M+H]^+$, found 228.0601.

1-(4-Fluorophenyl)-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4f)

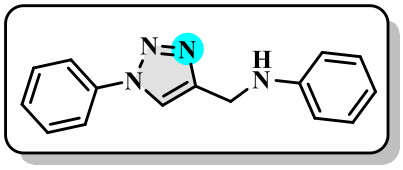


(4-Fluorophenyl)hydrazine hydrogen chloride 100 mg, 0.617 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 124 mg 82%; pale yellow solid; m.p 137-142 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.68 (dd, *J* = 9.0, 4.6 Hz, 2H), 7.40 (dd, *J* = 3.6, 1.0 Hz, 1H), 7.27 (dd, *J* = 5.1, 1.1 Hz, 1H), 7.16 (dd, *J* = 8.9, 8.1 Hz, 2H), 7.04 (dd, *J* = 5.1, 3.6 Hz, 1H). ^{19}F NMR (377 MHz, $CDCl_3$) δ -111.85. ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.7, 161.2, 143.6, 133.1, 132.2, 127.7, 125.5, 124.6, 122.5, 122.5, 117.2, 116.9, 116.6; HRMS (ESI+TOF) calcd. for: $C_{12}H_9N_3SF$ 246.0501 $[M+H]^+$, found 246.0508.

General Procedure for one pot conversion of aryl hydrazine hydrochloride to 1,2,3-triazoles (5a-5c), (Scheme 3).

To an oven-dried 100 ml round bottom flask charged with a magnetic stir bar was added aryl hydrazine hydrochloride **1** (100 mg, 0.574-0.694 mmol, 1 equiv.) followed by *tert.* Butyl nitrite (1 equiv.) in PEG-400:H_2O (5 mL, 2:1) was stirred at 0 ^oC for 30 minutes. The progress of the reaction was observed using TLC to monitor the conversion of aryl hydrazine hydrochloride to phenyl azide (*in situ*) **2**. Then alkyne (1.0 equiv.) followed by $CuSO_4$. $5H_2O$ (0.1 equiv.) and Sod. Ascorbate (0.05 equiv.) were added to the reaction mixture. The reaction mixture was warmed to room temperature and the stirring was continued for 8-12 h overnight after the reaction was complete as monitored by TLC. The reaction mixture was diluted with H_2O, and the precipitate formed was filtered and dried in vacuo to afford the corresponding triazoles (**5a-5c**).

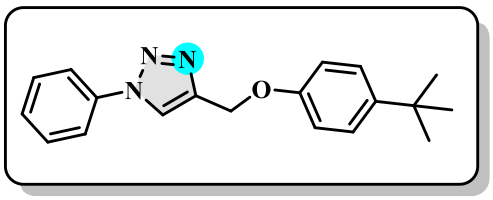
***N*-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)aniline[7] (5a)**



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 145 mg, 83 %; yellow solid; m.p 137-143 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.90 – 7.82 (m, 2H), 7.76 – 7.69 (m, 2H), 7.53 (dt, *J* = 8.3, 7.2 Hz, 4H), 7.49 – 7.38 (m,

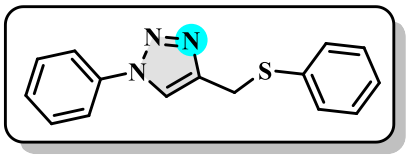
2H);^{13}C NMR (101 MHz, $CDCl_3$) δ 141.6, 136.8, 129.8, 129.7, 129.6, 128.9, 127.6, 123.7, 120.5, 119.7, 77.3, 77.0, 76.7, 40.7; HRMS (ESI+TOF) calcd. for: $C_{15}H_{15}N_4$ 251.1240 $[M+H]^+$, found 251.1240.

4-((4-(Tert-butyl)phenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (5b)



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 160 mg, 75%; brown solid; m.p 178-184 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.75 (dd, *J* = 8.4, 1.1 Hz, 2H), 7.57 – 7.52 (m, 2H), 7.46 (ddd, *J* = 7.4, 3.8, 1.2 Hz, 1H), 7.34 (d, *J* = 8.9 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 5.31 (s, 2H), 1.32 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9, 144.1, 136.99, 129.8, 128.9, 126.4, 120.6, 114.2, 62.0, 34.1, 31.5. HRMS (ESI+TOF) calcd. for: $C_{19}H_{22}N_3O$ 308.1763 $[M+H]^+$, found 308.1769.

1-Phenyl-4-((phenylthio)methyl)-1*H*-1,2,3-triazole[8] (5c)

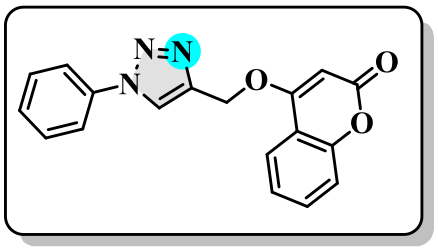


(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 146 mg, 78%; yellow solid; m.p 165-170 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.53 – 7.48 (m, 2H), 7.37 – 7.32 (m, 2H), 7.28 – 7.21 (m, 3H), 7.15 – 7.11 (m, 2H), 7.05 (ddd, *J* = 7.3, 3.9, 1.3 Hz, 1H), 4.16 (d, *J* = 0.6 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 136.0, 134.3, 129.2, 128.7, 127.9, 125.7, 119.2, 27.2; HRMS (ESI+TOF) calcd. for: $C_{15}H_{14}N_3S$ 268.0908 $[M+H]^+$, found 268.0918.

General procedure for late-stage functionalization of natural products (6a-6e), (Scheme 4).

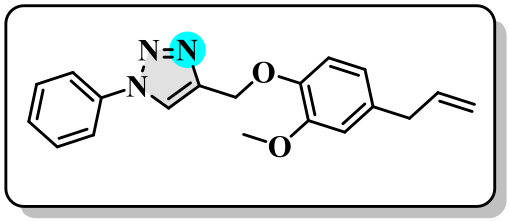
To an oven-dried 100 ml round bottom flask charged with a magnetic stir bar was added aryl hydrazine hydrochloride **1** (100 mg, 0.574-0.694 mmol, 1 equiv.) followed by *tert.* Butyl nitrite (1 equiv.) in PEG-400:H_2O (5 mL, 2:1) was stirred at 0 ^oC for 30 minutes. The progress of the reaction was observed using TLC to monitor the conversion of aryl hydrazine hydrochloride to phenyl azide (*in situ*) **2**. Then alkyne (1.0 equiv.) followed by $CuSO_4$. $5H_2O$ (0.1 equiv.) and Sod. Ascorbate (0.05 equiv.) were added to the reaction mixture. The reaction mixture was warmed to room temperature and the stirring was continued for 8-12 h overnight after the reaction was complete as monitored by TLC. The reaction mixture was diluted with H_2O, and the precipitate formed was filtered and dried in vacuo to afford the corresponding triazoles (**6a-6e**).

4-((1-Phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one[9] (6a)



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 154 mg, 69%; pale yellow solid; m.p 164-170 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.85 – 7.77 (m, 3H), 7.60 – 7.48 (m, 4H), 7.33 (dd, *J* = 8.4, 0.7 Hz, 1H), 7.26 (dd, *J* = 8.0, 0.9 Hz, 1H), 5.93 (s, 1H), 5.44 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.9, 162.6, 153.3, 142.1, 136.7, 132.6, 129.9, 129.2, 123.9, 123.1, 121.7, 120.7, 116.7, 115.4, 91.2, 62.6, 30.9; HRMS (ESI+TOF) calcd. for: $C_{18}H_{14}N_3O_3$ 320.1035 $[M+H]^+$, found 320.1038.

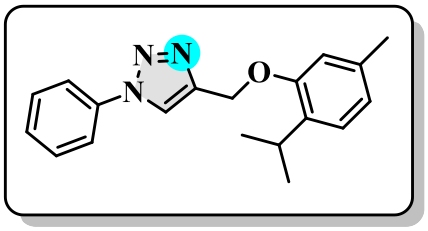
4-((4-Allyl-2-methoxyphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6b)



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 188 mg, 80%; yellow solid; ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.68 – 7.62 (m, 2H), 7.50 – 7.34 (m, 3H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.65 (dt, *J* = 8.0, 1.9 Hz, 2H), 5.88 (ddt, *J* = 16.8, 10.1, 6.7 Hz, 1H), 5.34 – 5.23 (m, 2H), 5.17 – 4.85 (m, 2H), 3.80 (s, 3H), 3.26 (d, *J* = 6.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.4, 145.8, 145.2, 137.5, 137.0, 133.9, 129.8, 129.7, 128.8, 121.1, 120.6, 120.6, 120.5,

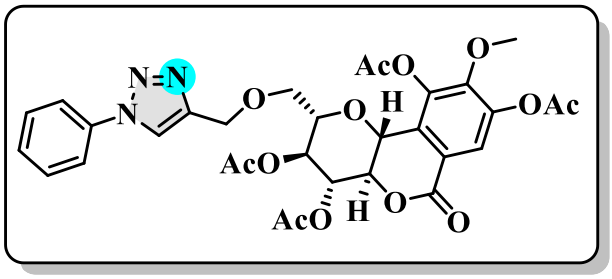
115.7, 114.3, 112.2, 63.3, 55.8, 39.8; HRMS (ESI+TOF) calcd. for: $C_{19}H_{20}N_3O_2$ 322.1556 $[M+H]^+$, found 322.1557.

4-((2-Isopropyl-5-methylphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole[10] (6c)



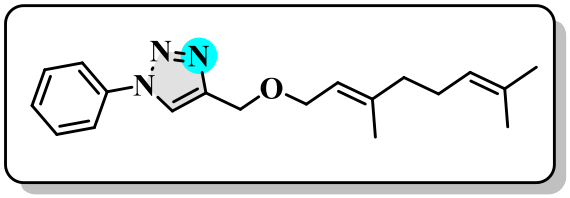
(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.5; Yield 171 mg, 80%; white solid; m.p 124-130 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.76 – 7.72 (m, 2H), 7.52 (m, 2H), 7.46 – 7.41 (m, 1H), 7.12 (d, *J* = 7.7 Hz, 1H), 6.83 (s, 1H), 6.79 (d, *J* = 7.7 Hz, 1H), 5.30 (s, 2H), 3.32 (dt, *J* = 13.8, 6.9 Hz, 1H), 2.33 (s, 3H), 1.22 (s, 3H), 1.20 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.2, 145.6, 137.0, 136.5, 134.2, 129.8, 128.8, 126.1, 121.9, 120.6, 120.5, 112.8, 62.4, 26.63, 22.8, 21.4; HRMS (ESI+TOF) calcd. for: $C_{19}H_{22}N_3O$ 308.1763 $[M+H]^+$, found 308.1771.

9-Methoxy-6-methylene-2-(((1-phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)methyl)-2,3,4,4a,6,10b-hexahydropyrano[3,2-c]isochromene-3,4,8,10-tetrayl tetraacetate (6d)



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 350 mg, 77%; white solid; m.p 238-242 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.67 (d, *J* = 7.4 Hz, 3H), 7.42 (dt, *J* = 31.0, 7.3 Hz, 3H), 5.40 (t, *J* = 9.5 Hz, 1H), 5.28 (s, 2H), 5.07 – 4.99 (m, 1H), 4.74 (d, *J* = 10.5 Hz, 1H), 4.30 – 4.19 (m, 2H), 4.71 – 3.83 (m, 6H), 4.07 (dd, *J* = 12.6, 3.9 Hz, 1H), 3.85 (s, 3H), 3.77 (dd, *J* = 10.0, 1.4 Hz, 1H), 2.24 (s, 3H), 2.02 (d, *J* = 3.9 Hz, 6H), 1.99 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 165.7, 165.3, 164.9, 163.4, 157.6, 147.2, 142.7, 136.4, 125.1, 124.2, 120.1, 115.9, 113.6, 108.9, 71.8, 67.8, 67.3, 63.5, 57.9, 57.2, 56.6, 16.04, 16.01, 15.8, 15.7; HRMS (ESI+TOF) calcd. for: $C_{31}H_{32}N_3O_{13}$ 654.1935 $[M+H]^+$, found 654.1947.

(Z)-4-(((3,7-dimethylocta-2,6-dien-1-yl)oxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6e)



(Phenylhydrazine hydrogen chloride, 100 mg, 0.694 mmol); TLC (Hexane/EtOAc, 6:4); R_f = 0.4; Yield 121 mg, 56%; pale yellow solid;^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 4H), 7.68 – 7.65 (m, 8H), 7.48 – 7.44 (m, 8H), 7.38 (dt, *J* = 4.1, 1.6 Hz, 4H), 5.38 – 5.28 (m, 5H), 5.06 – 4.98 (m, 5H), 4.65 (s, 9H), 4.08 (d, *J* = 6.8 Hz, 9H), 2.06 – 1.97 (m, 16H), 1.62 (s, 11H), 1.61 (d, *J* = 1.0 Hz, 14H), 1.53 (s, 14H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.1, 137.0, 131.7, 129.7, 128.7, 123.9, 120.5, 120.2, 67.1, 63.3, 39.6, 26.3, 25.7, 17.7, 16.5; HRMS (ESI+TOF) calcd. for: $C_{19}H_{26}N_3O$ 312.2076 $[M+H]^+$, found 312.2077.

General Procedure for gram scale reaction.

To an oven-dried 100 ml round bottom flask charged with a magnetic stir bar was added aryl hydrazine hydrochloride **1** (100 mg, 0.574-0.694 mmol, 1 equiv.) followed by *tert.* Butyl nitrite (1 equiv.) in PEG-400:H_2O (5 mL, 2:1) was stirred at 0 ^oC for 30 minutes. The progress of the reaction was observed using TLC to monitor the conversion of aryl hydrazine hydrochloride to phenyl azide (*in situ*) **2**. Then alkyne (1.0 equiv.) followed by $CuSO_4$. $5H_2O$ (0.1 equiv.) and Sod. Ascorbate (0.05 equiv.) were added to the reaction mixture. The reaction mixture was warmed to room temperature and the stirring was continued for 8-12 h overnight after the reaction was complete as monitored by TLC. The reaction mixture was diluted with H_2O, and the precipitate formed was filtered and dried in vacuo to afford the corresponding triazoles.

Calculation of Green Metrics and Formulas Used

1. Yield (%)

The efficiency of a reaction in converting starting materials into the desired product.

$$\text{Formula: Yield (\%)} = \frac{\text{Mass of product obtained}}{\text{Theoretical mass of product}} \times 100 \qquad \text{……Eq. 1}$$

2. E-factor

The mass of waste generated per mass of product.

$$\text{Formula: E-factor} = \frac{\text{Total waste generated}}{\text{Mass of product}} \qquad \text{……Eq. 2}$$

3. PMI (Process Mass Intensity)

The total mass of all materials used per mass of product.

$$\text{Formula: PMI} = \frac{\text{Total mass input (including solvents,water,reagents)}}{\text{Mass of product}} \qquad \text{……Eq. 3}$$

4. WWI (Water Waste Intensity)

The mass of water used per mass of product.

$$\text{Formula: WWI} = \frac{\text{Total water used}}{\text{Mass of product}} \qquad \text{……Eq. 4}$$

Calculation of the Green Chemistry Metrics for the gram-scale synthesis of 1,4-diphenyl-1H-1,2,3-triazole (3a)

Reaction Stoichiometry

Entry	Reagent	Formula	MW (g/mol)	Mass (g)	mmol	Equiv.
1	Phenylhydrazine hydrochloride	$C_6H_5NHNH_2 \cdot HCl$	144.60	5.0	34.5781	1.0
2	*tert*-Butyl nitrite	$C_4H_9NO_2$	103.12	3.56	34.5781	1.0
3	Phenylacetylene	C_8H_6	102.13	3.53	34.5781	1.0
4	Sodium ascorbate	$C_6H_7NaO_6$	198.11	0.68	3.4578	0.1
5	Copper sulfate pentahydrate	$CuSO_4 \cdot 5H_2O$	249.69	0.43	1.728	0.05

Solvents & Processing Conditions

Solvent	Total Volume Used (mL)	Type	Amount Considered (g)	Note
PEG-400*	50	Recyclable	5	10% loss considered per cycle [11-17]
Water	60	Recyclable	6	10% loss considered per cycle

**** PEG-400 was considered a recyclable solvent based on literature reports.*** [11-17]

Product & Yield

Product	Formula	MW	Isolated Yield (g)	Yield (%)
1,4-Diphenyl-1*H*-1,2,3-triazole **(3a)**	$C_{14}H_{11}N_3$	221.26	7.5	98

Green Chemistry Metrics

Metric	Calculation	Value
E-factor (Eq. 2)	10.7*÷7.50	1.42
PMI (Eq. 3)	(5.0 + 3.56 + 3.53 + 0.68 + 0.43 + 50 + 60) ÷7.50 g	16.42
Water Intensity (Eq. 4)	50÷7.5 g	6.6

*****Amount of waste = (Amount of reagents - Amount of final product) + Solvent loss = {(5.0+3.56+3.53+0.68+0.43) – 7.5}g + 5 = 10.7 g

Calculation of Green Metrics of Literature Reports

Literature 1: Kaboudin *et al.*[18]

Reaction Stoichiometry

Entry	Reagent	Formula	MW (g/mol)	Mass (g)	mmol	Equiv.
1	Phenylboronic acid	$C_6H_7BO_2$	121.93	0.122	1.0	1.0
2	Sodium azide	NaN_3	65.01	0.195	3.0	1.0
3	Phenylacetylene	C_8H_6	102.13	0.102	1.0	1.0
4	Cu_2-β-CD complex	-	1198.6	0.065	0.05	0.1
5	Sodium sulfate	Na_2SO_4	142.03	10	-	-
6	NaOH	NaOH	40.0	1.0	1.0	1.0
7	β-Cyclodextrin	-	1134.98	1.1	1.0	1.0
8	$CuSO_4 \cdot 5H_2O$	-	249.69	2.5	3.0	3.0

Solvents & Processing Conditions

Solvent	Total Volume Used (mL)	Type	Amount Considered (g)	Note
DCM	50	Recyclable	5	10% loss considered
Hexane	10	Recyclable	1	10% loss considered
Ethanol	400	Recyclable	40	10% loss considered
Water	124	Recyclable	12.4	10% loss considered

Product & Yield

Product	Formula	MW	Isolated Yield (g)	Yield (%)
1,4-Diphenyl-1H-1,2,3-triazole	$C_{14}H_{11}N_3$	221.26	0.21	94

Green Chemistry Metrics

Metric	Calculation	Value
E-factor (Eq. 2)	61.87*****÷0.210	294.62
PMI (Eq. 3)	(0.122+0.195+0.102+0.065+40+10+10+47.5+5+50+400+72.5) ÷0.210 g	3026.11
Water Intensity (Eq. 4)	(49+3+72.5) ÷0.210	592.85

*****Amount of waste = (Amount of reagents - Amount of final product) + Solvent loss = {(0.122+0.195+0.102+0.065+10+1+1.1+2.5) – 0.21}g + (5 + 1 + 40) = 60.87 g

Literature-2 *Fokin et al*[19]

Reaction Stoichiometry

Entry	Reagent	Formula	MW (g/mol)	Mass (g)	mmol	Equiv.
1	Iodobenzene	C_6H_5I	204.01	0.102	1.0	1.0
2	1-Chloro-4-prop-2-ynyloxy-benzene	C_9H_7ClO	166.60	0.084	3.0	1.0
3	L-Proline	$C_5H_9NO_2$	115.13	0.012	0.1	0.2
4	Sodium Carbonate	Na_2CO_3	105.98	0.012	0.1	0.2
5	Sodium Azide	NaN_3	65.01	0.039	0.6	1.2
6	Sodium Ascorbate	$C_6H_7NaO_6$	198.11	0.020	0.05	0.1
7	Copper Sulfate pentahydrate	$CUSO_4.5H_2O$	249.69	0.013	0.025	0.05
8	Ammonium Hydroxide	NH_4OH	35.04	4.0	-	
9	Sodium Chloride	NaCl	58.43	5.0	-	

Solvents & Processing Conditions

Solvent	Total Volume Used (mL)	Type	Amount Considered (g)	Note
DMSO	50	Recyclable	5	10% loss considered
Ethyacetate	60	Recyclable	6	10% loss considered
Water	100.1	Recyclable	10.01	10% loss considered

Product & Yield

Product	Formula	MW	Isolated Yield (g)	Yield (%)
4-((4-methoxyphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole	$C_{16}H_{15}N_3O_2$	281.31	0.211	83

Green Chemistry Metrics

Metric	Calculation	Value
E-factor (Eq. 2)	20.071*****÷ 0.211	95.12
PMI (Eq. 3)	(0.282+0.10+60+40+30+30+5+4+1+1.1)÷ 0.211 g	807.48
Water Intensity (Eq. 4)	(60 +0.1+40)÷ 0.211 g	474.40

*****Amount of waste = (Amount of reagents - Amount of final product) + Solvent loss = {(0.102+0.084+0.012+0.012+0.39+0.020+0.013+4+5– 0.21 }g + (5 + 6) = 20.071 g

Literature-3 Ranu *et. al*[20]

Reaction Stoichiometry

Entry	Reagent	Formula	MW (g/mol)	Mass (g)	mmol	Equiv.
1	Phenylboronic Acid	$C_6H_7BO_2$	121.93	0.122	1.0	1.0
2	Potassium Carbonate	K_2CO_3	138.20	0.138	1.0	-
3	Sodium Azide	NaN_3	65.01	0.195	3.0	-
4	Cu/Al_2O_3	$CuAl_2O_4$	181.51	0.400	0.01	0.1
5	Phenylacetylene	C_8H_6	102.13	0.102	1.0	1.0
6	Copper Sulfate pentahydrate	$CUSO_4.5H_2O$	249.69	1.0	4.0	-
7	Sodium Chloride	NaCl	58.43	5.0		
8	Alumina	Al_2O_3	101.96	15.0		-

Solvents & Processing Conditions

Solvent	Total Volume Used (mL)	Type	Amount Considered (g)	Note
Ethanol	10	Recyclable	1.0	10% loss considered
Hexane	20	Recyclable	2.0	10% loss considered
Ethyacetate	20	Recyclable	2.0	10% loss considered
Water	68	Recyclable	6.8	10% loss considered

Product & Yield

Product	Formula	MW	Isolated Yield (g)	Yield (%)
1,4-Diphenyl-1*H*-1,2,3-triazole	$C_{14}H_{11}N_3$	221.26	0.203	91

Green Chemistry Metrics

Metric	Calculation	Value
E-factor (Eq. 2)	26.754***** ÷ 0.203	131.79
PMI (Eq. 3)	(26.754+38+30+20+10+10+30)÷ 0.203 g	811.59
Water Intensity (Eq. 4)	(38+30) ÷ 0.203 g	334.97

*****Amount of waste = (Amount of reagents - Amount of final product) + Solvent loss = {(0.122+0.138+0.195+0.400+0.102+1+5+15)- 0.203 }g + (1+2+2) = 26.754 g

Literature-4- Portilla *et al.*[21]

Reaction Stoichiometry

Entry	Reagent	Formula	MW (g/mol)	Mass (g)	mmol	Equiv.
1	Benzyl Bromide	C_7H_7Br	171.03	2.97	1.0	-
2	1-nitro-4-(prop-2-yn-1-yloxy)benzene	$C_9H_7NO_3$	177.15	4.429	3.0	-
3	Sodium Azide	NaN_3	65.01	1.625	1.0	-
4	CuI Ligand	$C_{29}H_{31}CUIN_4P$	657.00	3.20	0.05	0.1
5	$CuI(PPh_3)_4$	$C_{72}H_{60}Cu_4I_4P_4$	1810.88	0.129	-	1.0
6	Cesium Carbonate	Cs_2CO_3	325.81	2.20	-	
7	Silica Gel		In large amount			

Solvents & Processing Conditions

Solvent	Total Volume Used (mL)	Type	Amount Considered (g)	Note
DCM	120	Recyclable	12	10% loss considered
Ethyl Acetate	20	Recyclable	2	10% loss considered
Methanol	20	Recyclable	2	10% loss considered
Water	132	Recyclable	13.2	10% loss considered

Product & Yield

Product	Formula	MW	Isolated Yield (g)	Yield (%)
1,4-diphenyl-1*H*-1,2,3-triazole	$C_{14}H_{11}N_3$	221.26	6.98	91

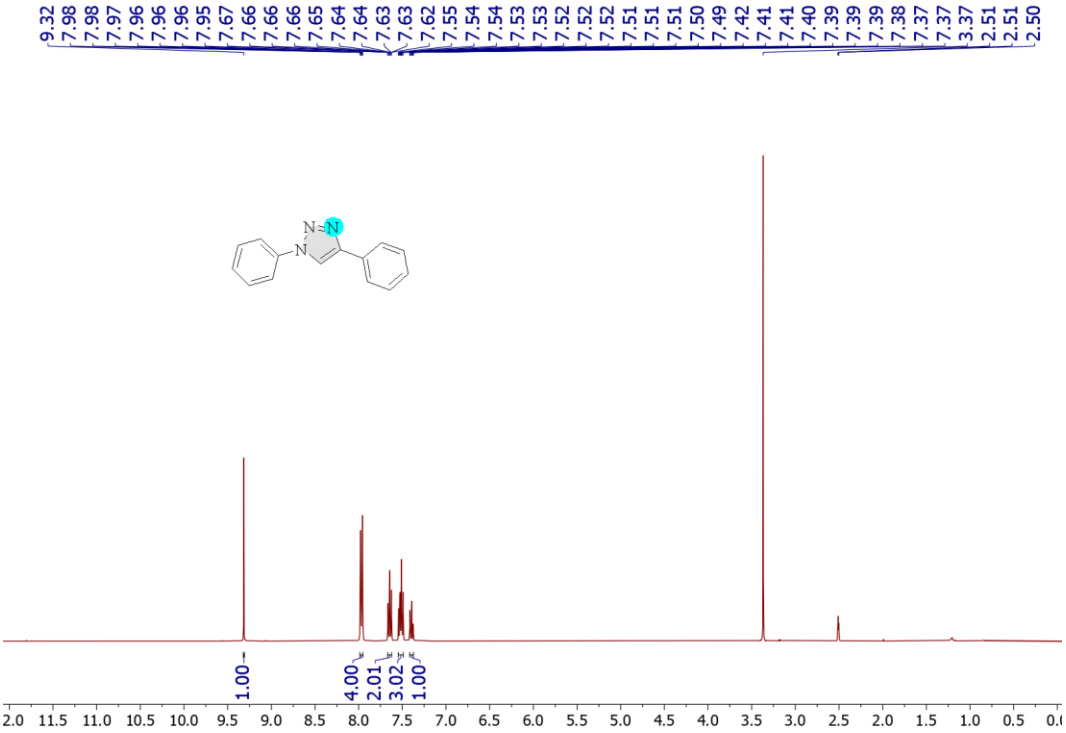
Green Chemistry Metrics

Metric	Calculation	Value
E-factor (Eq. 2)	23.56*****÷ 6.98	3.37
PMI (Eq. 3)	(23.56+20+30+30+100+5+5+5)÷6.98 g	31.31
Water Intensity (Eq. 4)	(30+102) ÷6.98	18.91

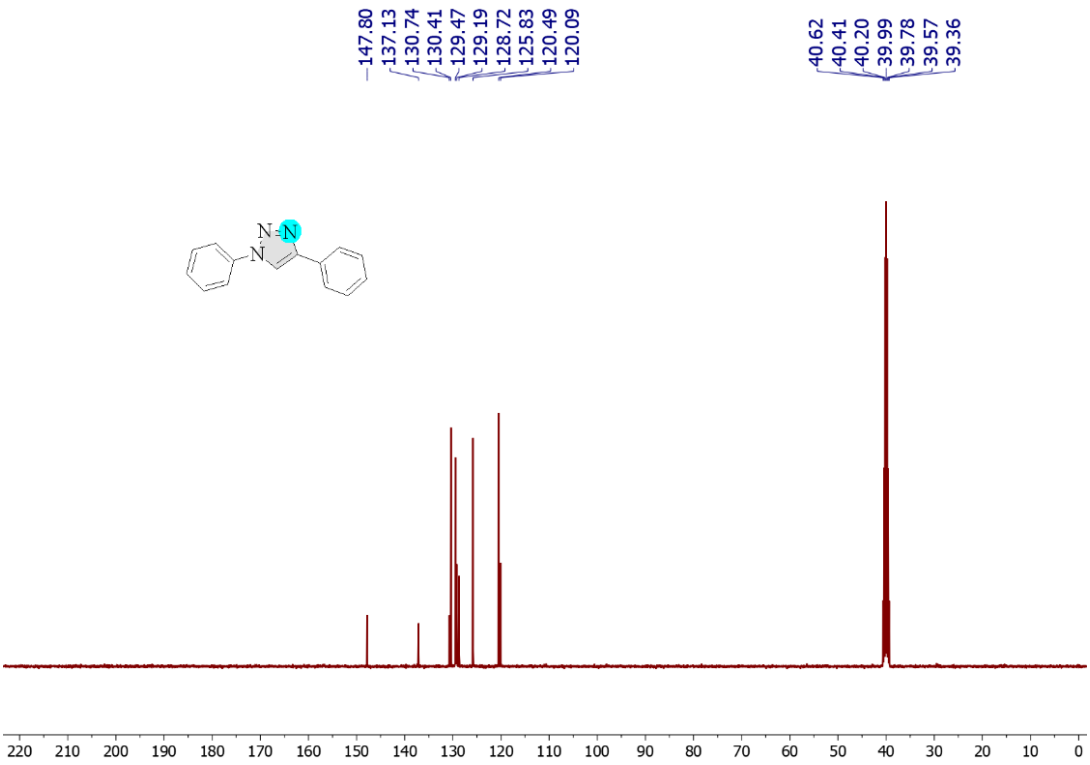
*****Amount of waste = (Amount of reagents - Amount of final product) + Solvent loss = {(2.97+4.42+1.62+3.20+0.13+2.20)- 6.98 }g + (12+2+2) = 23.56 g

Spectral copies of compounds

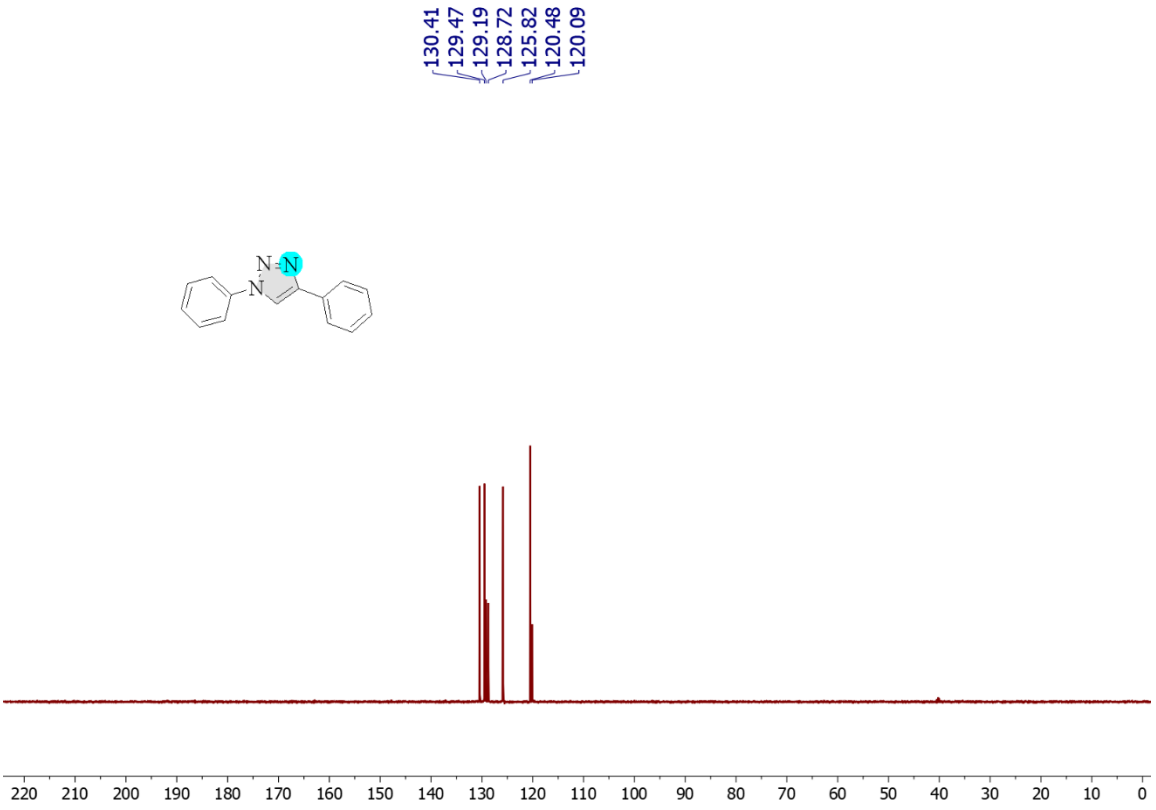
^{1}H-NMR of 1,4-Diphenyl-1*H*-1,2,3-triazole (3a)



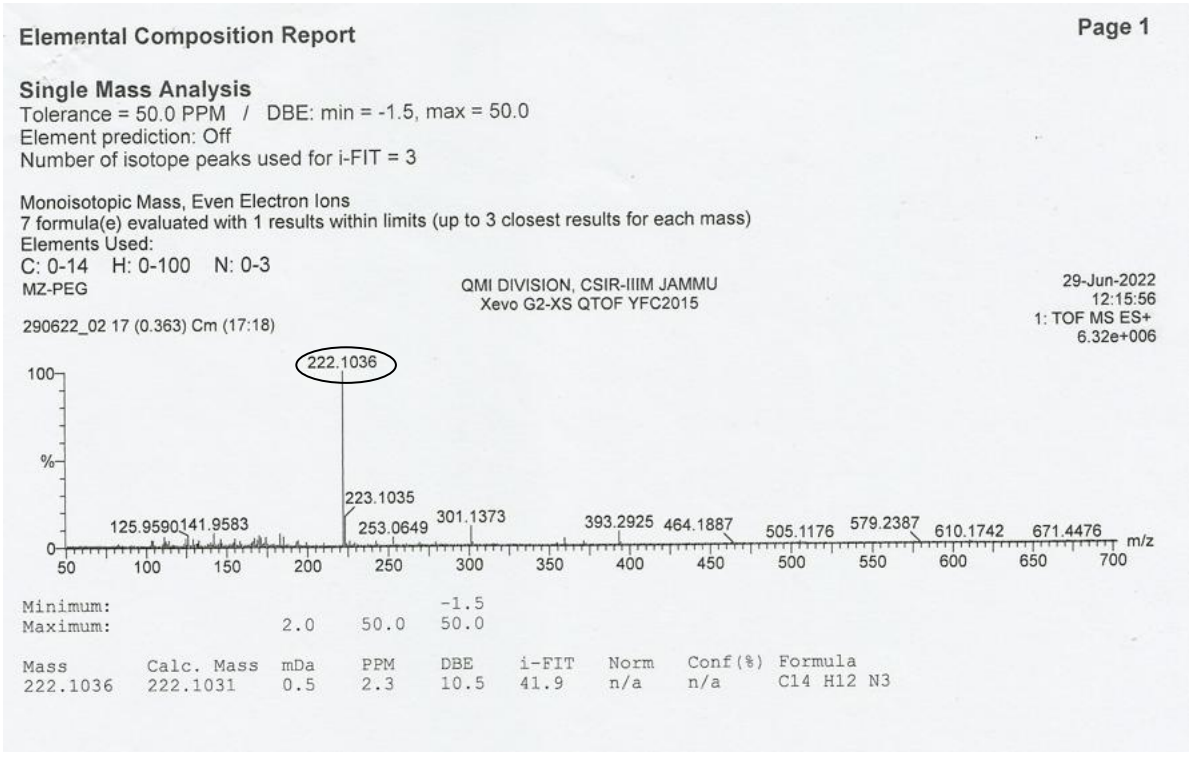
^{13}C-NMR of 1,4-Diphenyl-1*H*-1,2,3-triazole (3a)



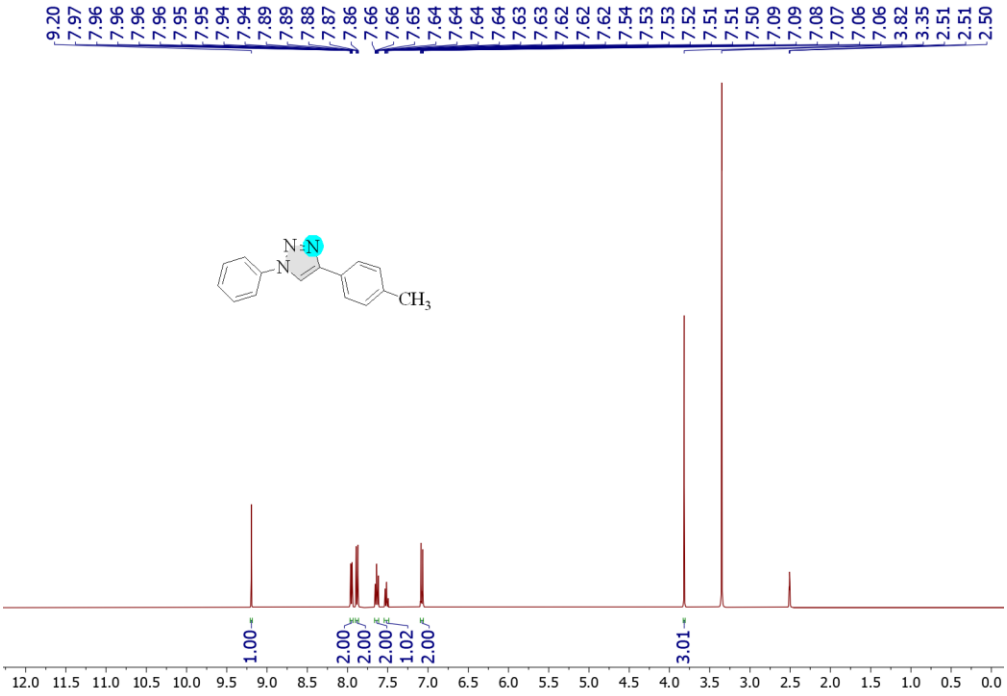
DEPT of 1,4-Diphenyl-1*H*-1,2,3-triazole (3a)



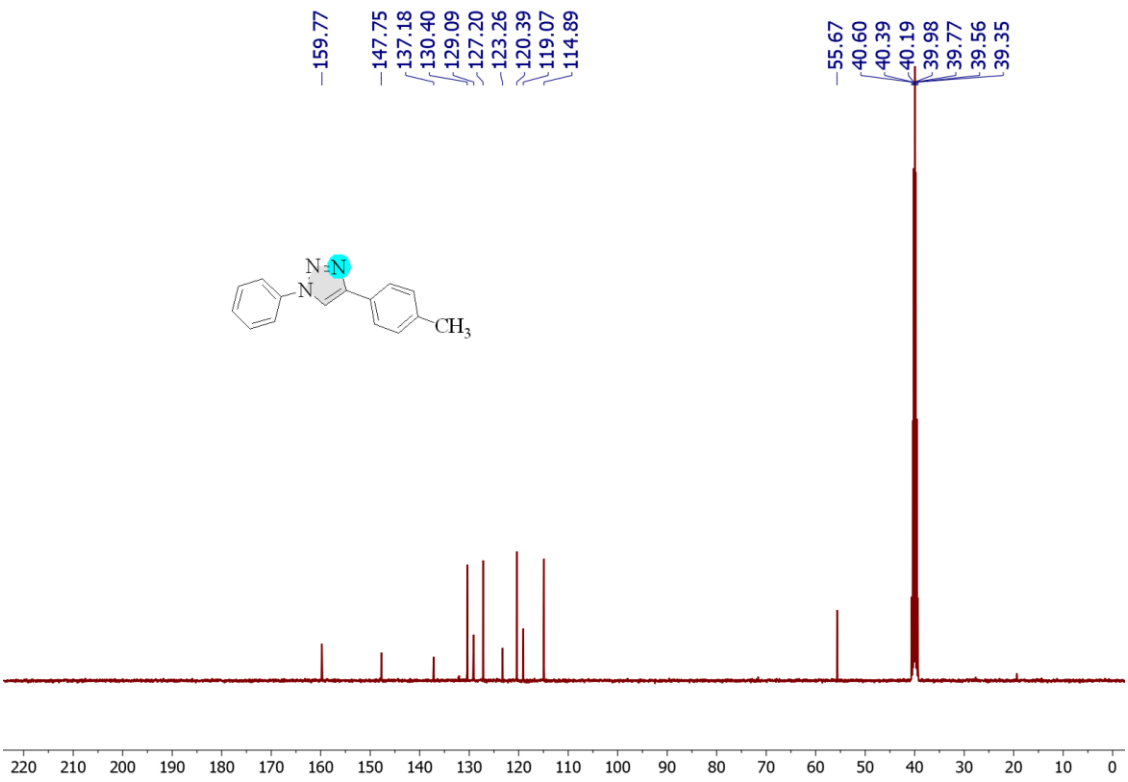
HRMS of 1,4-Diphenyl-1*H*-1,2,3-triazole (3a)



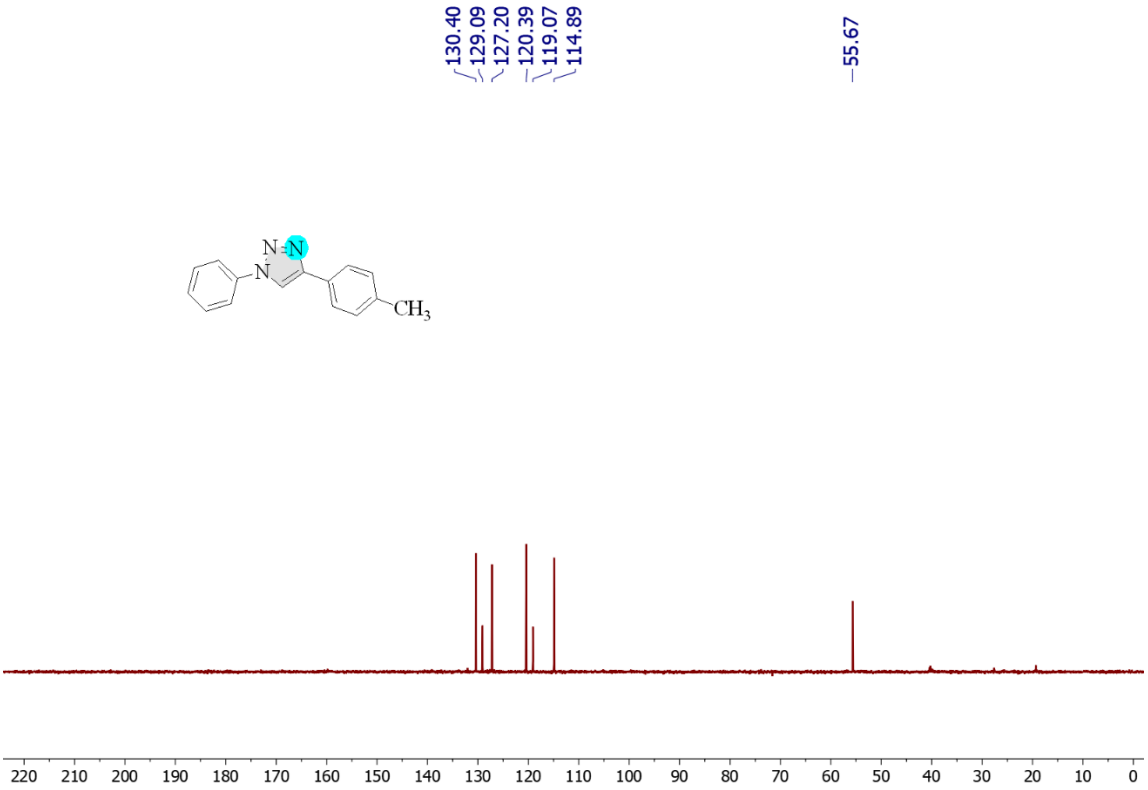
^{1}H-NMR of 1-Phenyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3b)



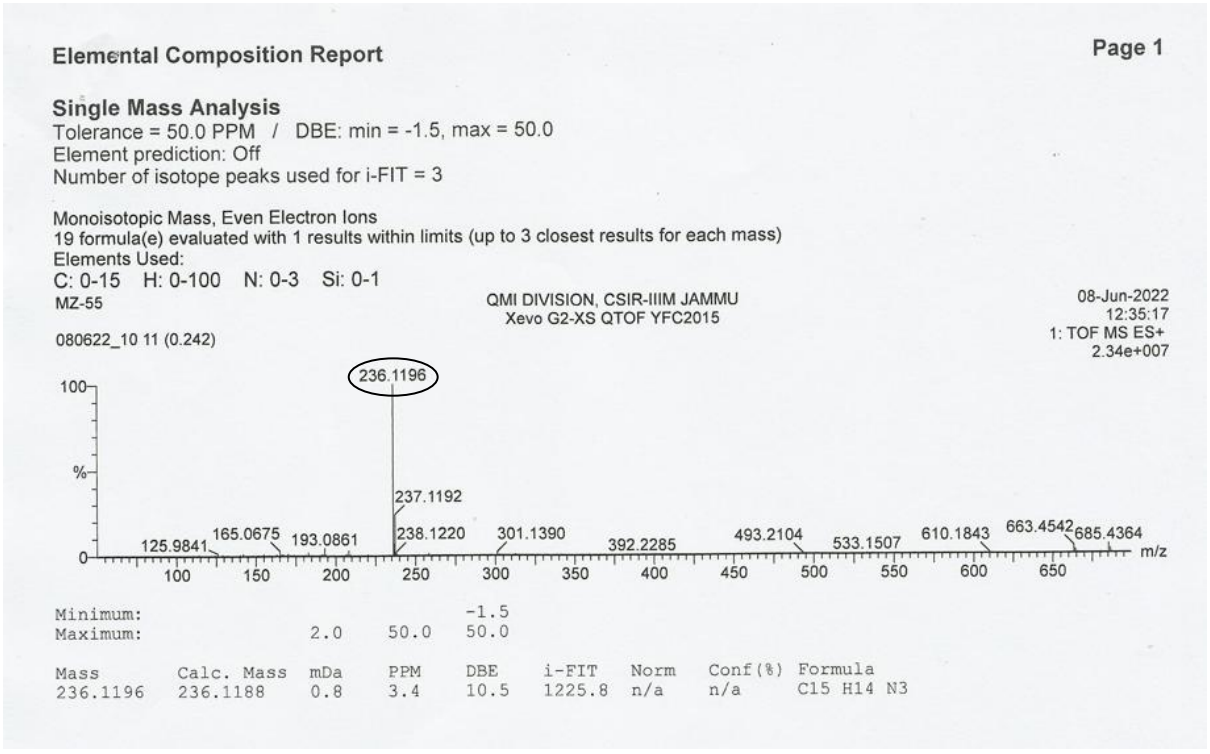
^{13}C-NMR of 1-Phenyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3b)



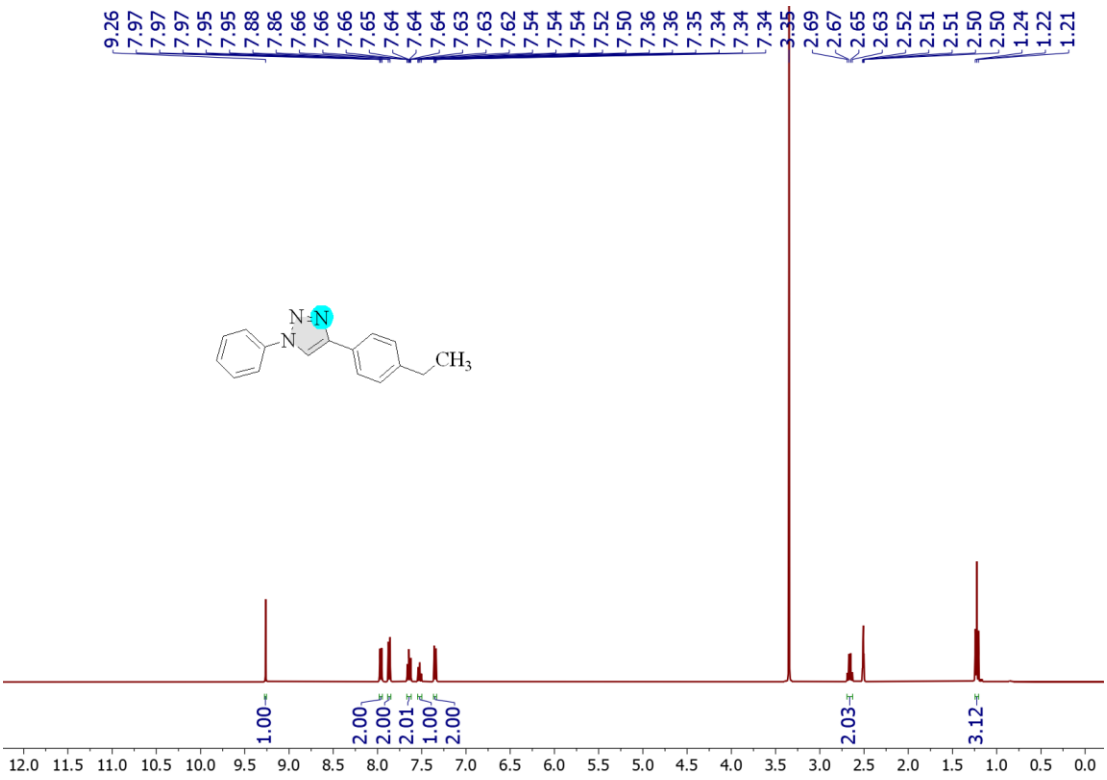
DEPT of 1-Phenyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3b)



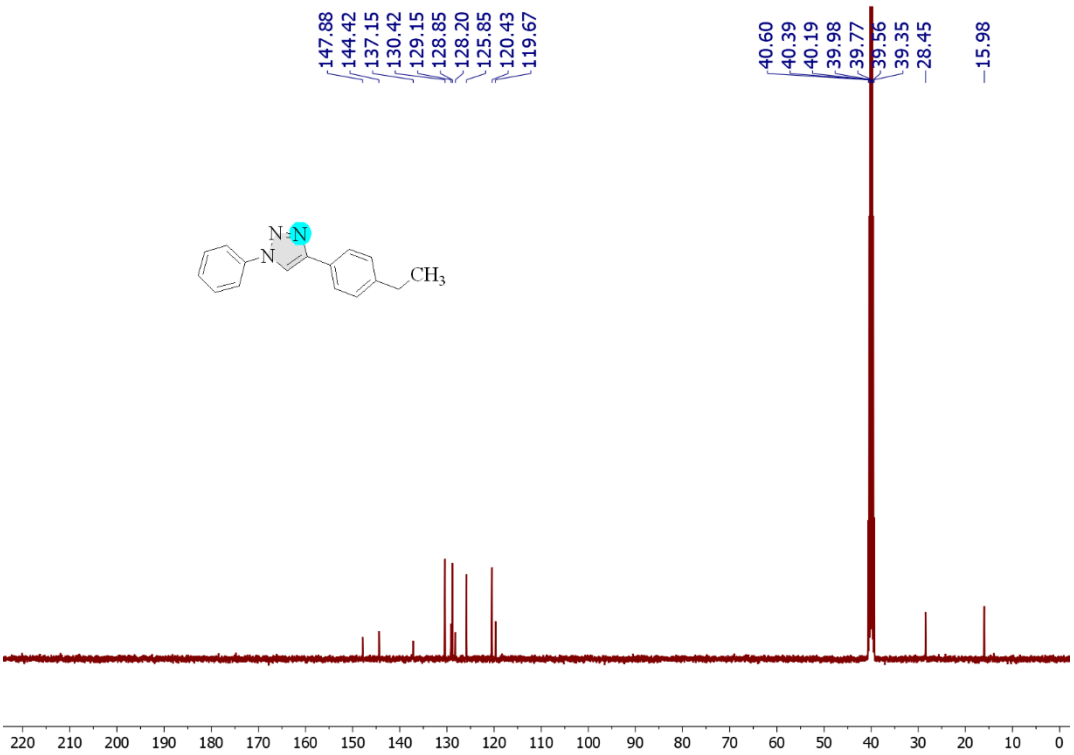
HRMS of 1-Phenyl-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3b)



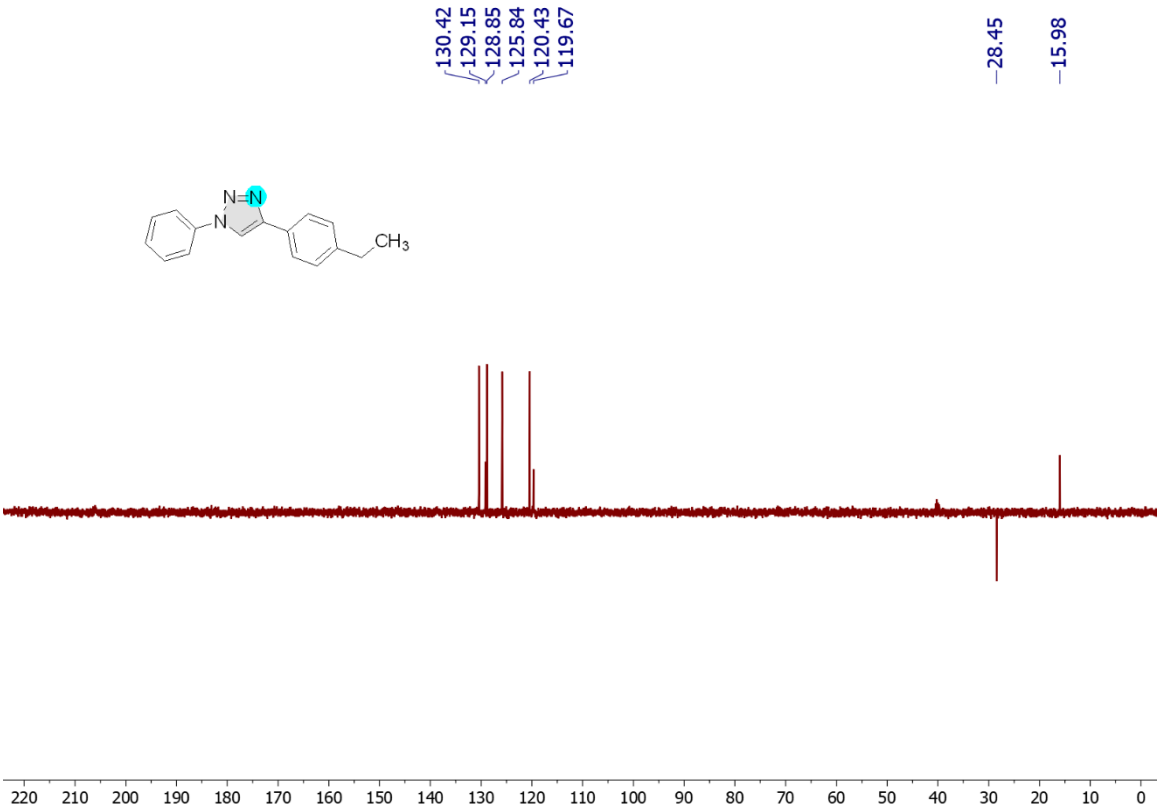
^{1}H-NMR of 4-(4-Ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole (3c)



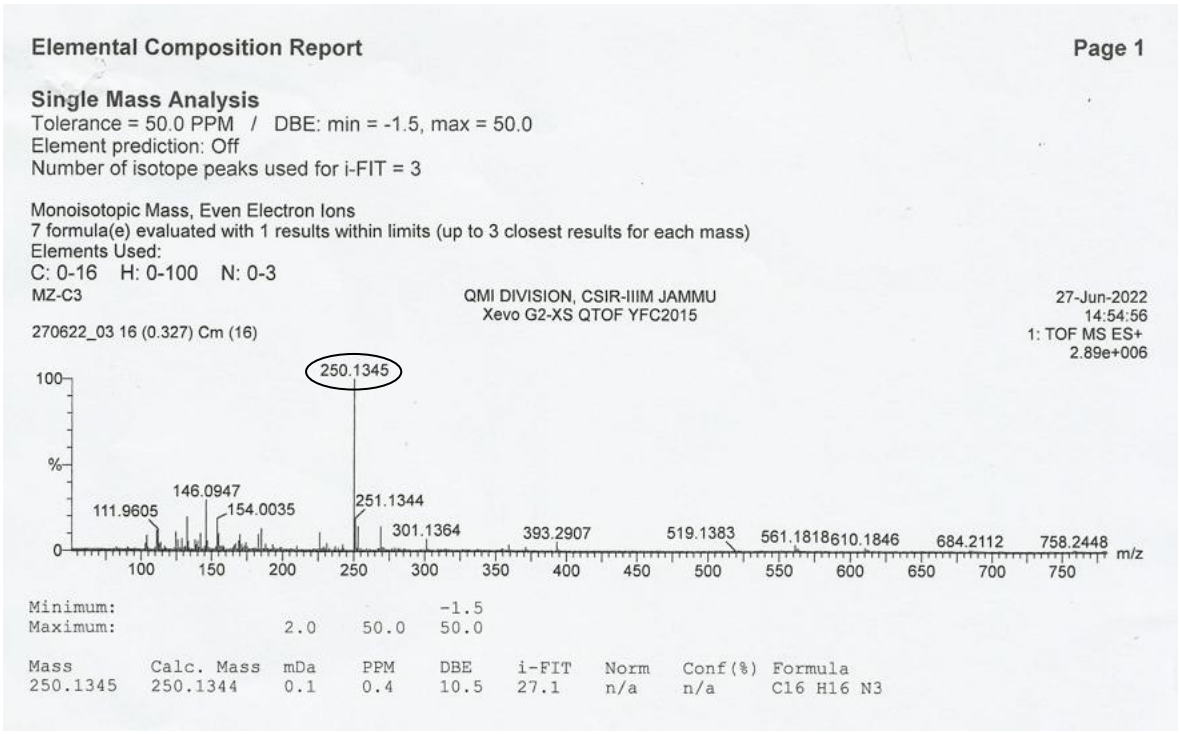
^{13}C-NMR of 4-(4-Ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole (3c)



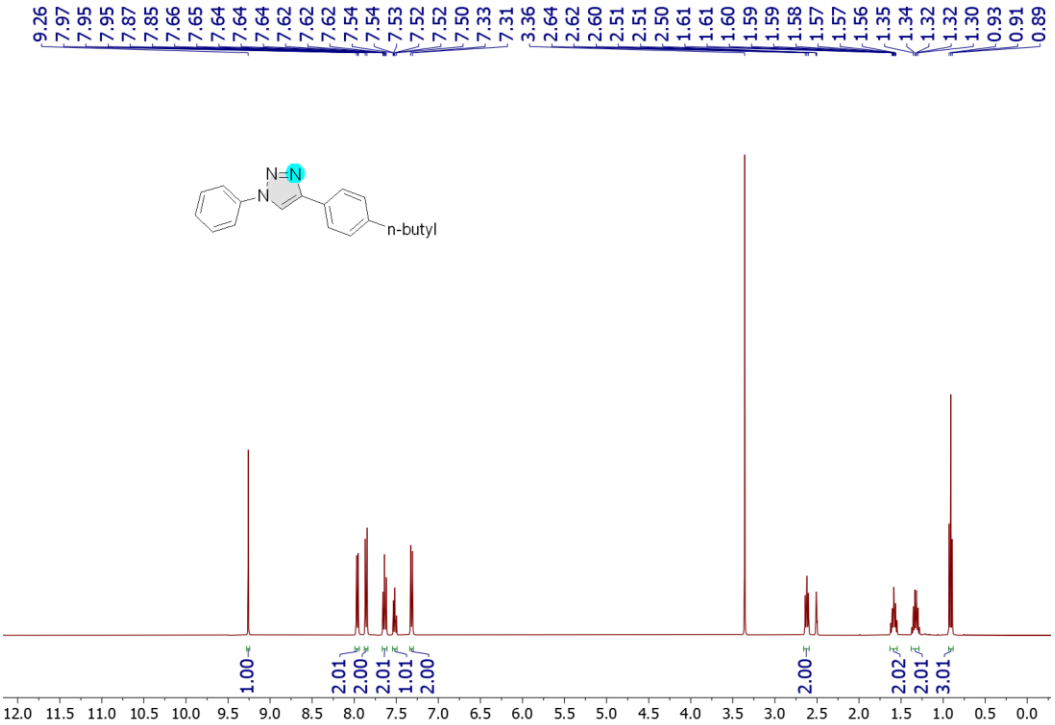
DEPT of 4-(4-Ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole (3c)



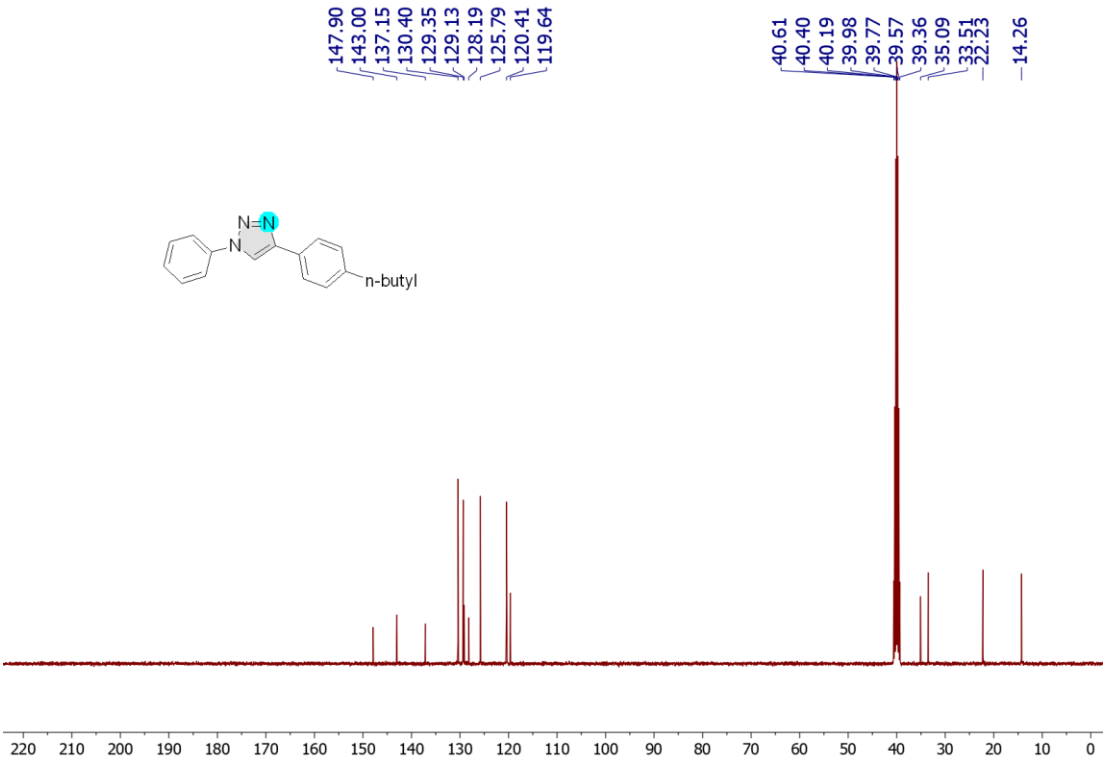
HRMS of 4-(4-Ethylphenyl)-1-phenyl-1*H*-1,2,3-triazole (3c)



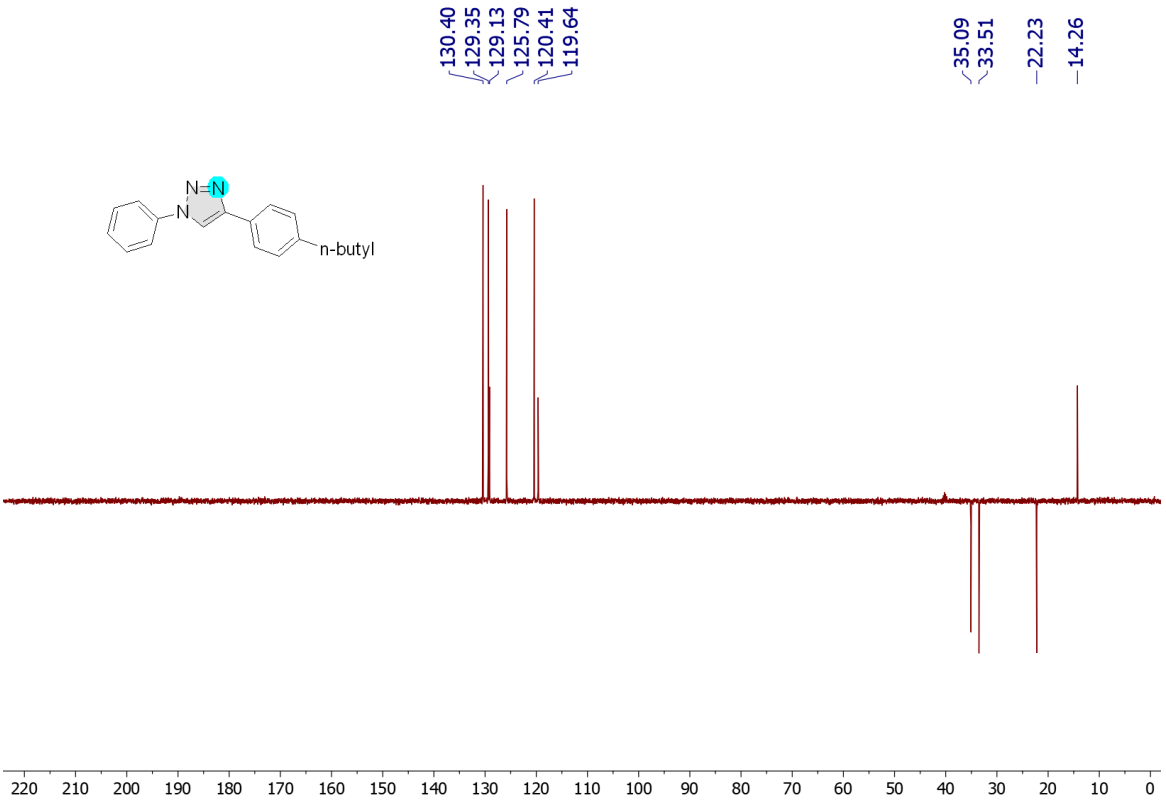
[1]H-NMR of 4-(4-Butylphenyl)-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3d)



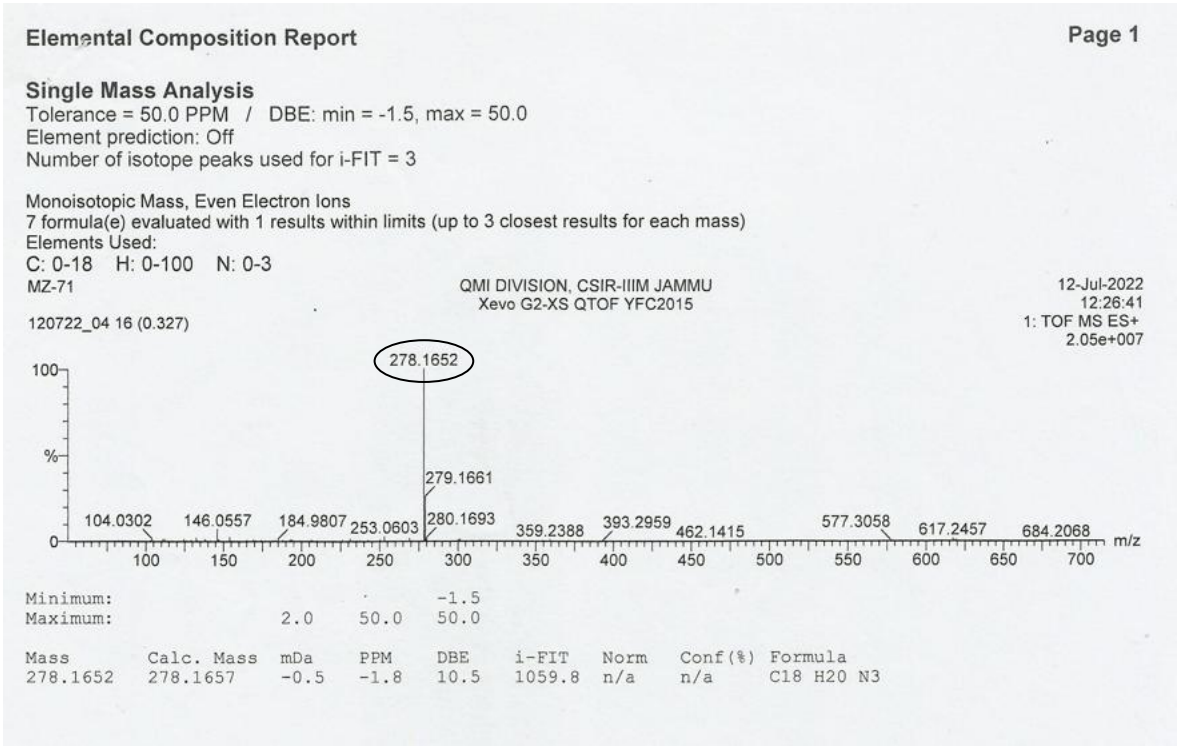
[13]C-NMR of 4-(4-Butylphenyl)-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3d)



DEPT of 4-(4-Butylphenyl)-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3d)



HRMS of 4-(4-Butylphenyl)-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3d)



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-18 H: 0-100 N: 0-3

MZ-71
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
12-Jul-2022
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2.05e+007
120722_04 16 (0.327)

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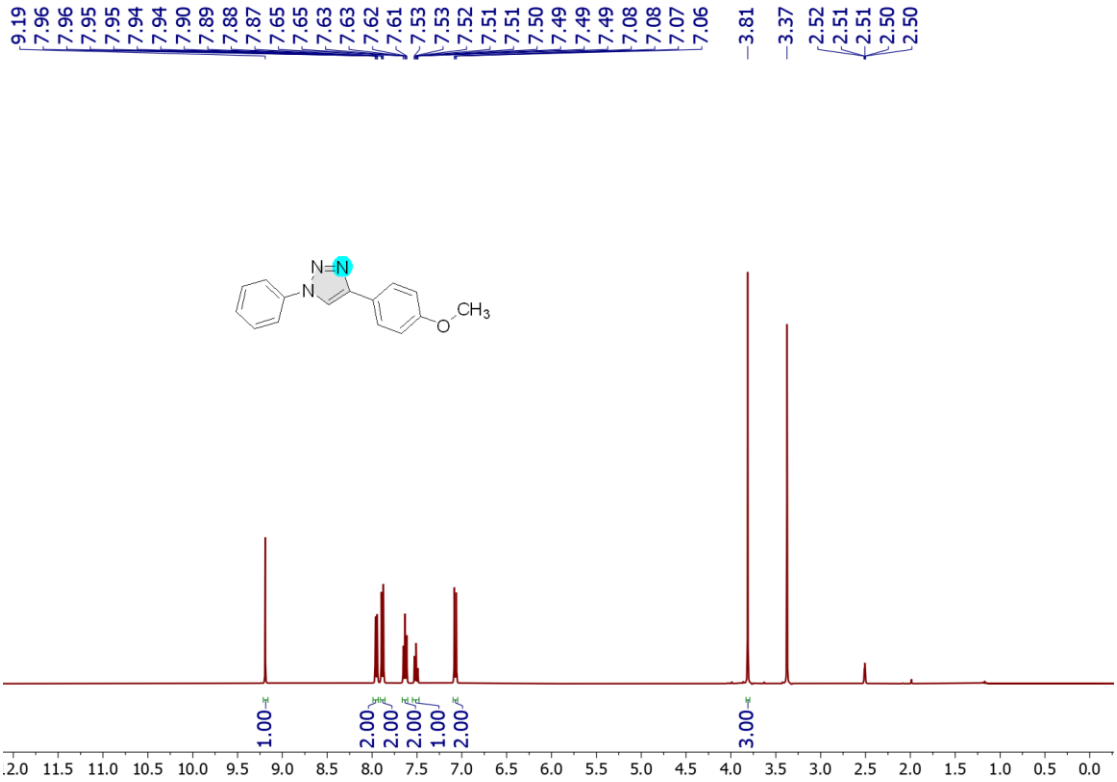
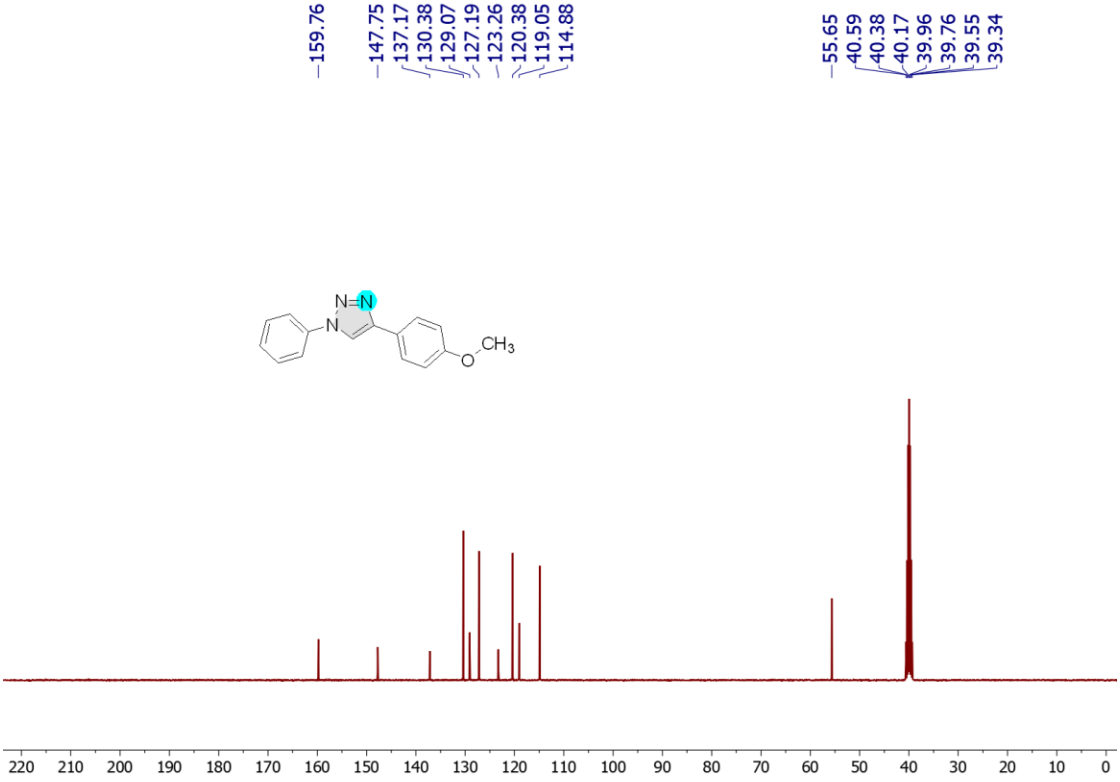
279.1661
280.1693
104.0302 146.0557 184.9807 253.0603 359.2388 393.2959 462.1415 577.3058 617.2457 684.2068
100 150 200 250 300 350 400 450 500 550 600 650 700 m/z

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
278.1652	278.1657	-0.5	-1.8	10.5	1059.8	n/a	n/a	C18 H20 N3

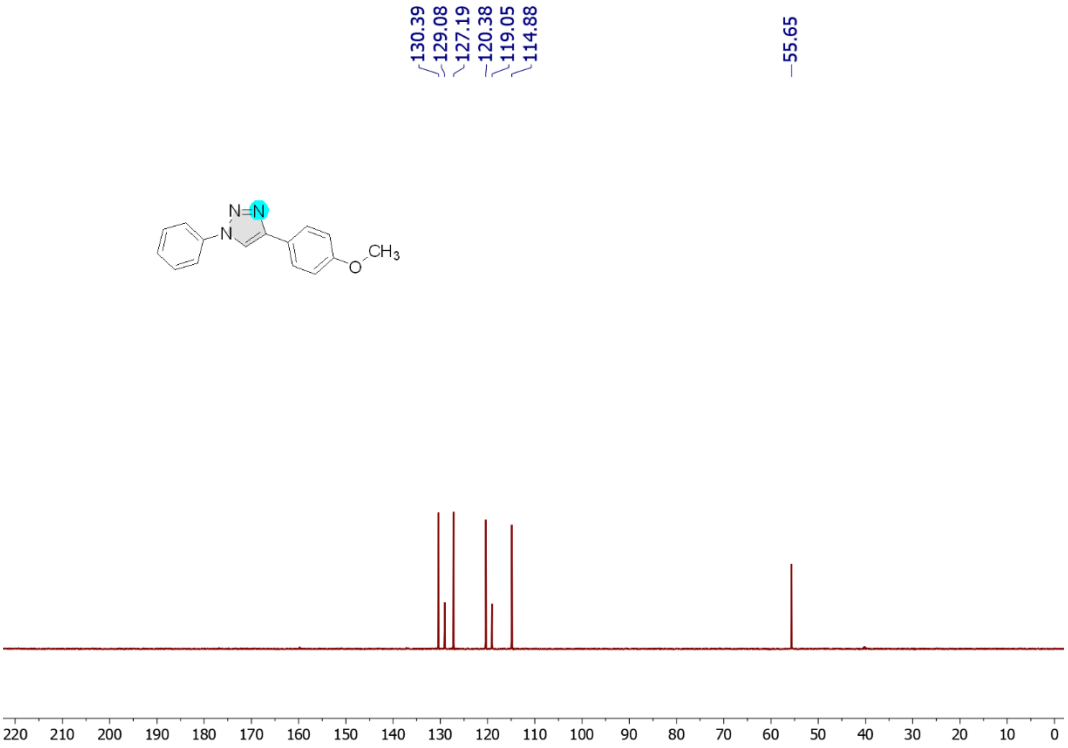
^{1}H-NMR of 4-(4-Methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole (3e)



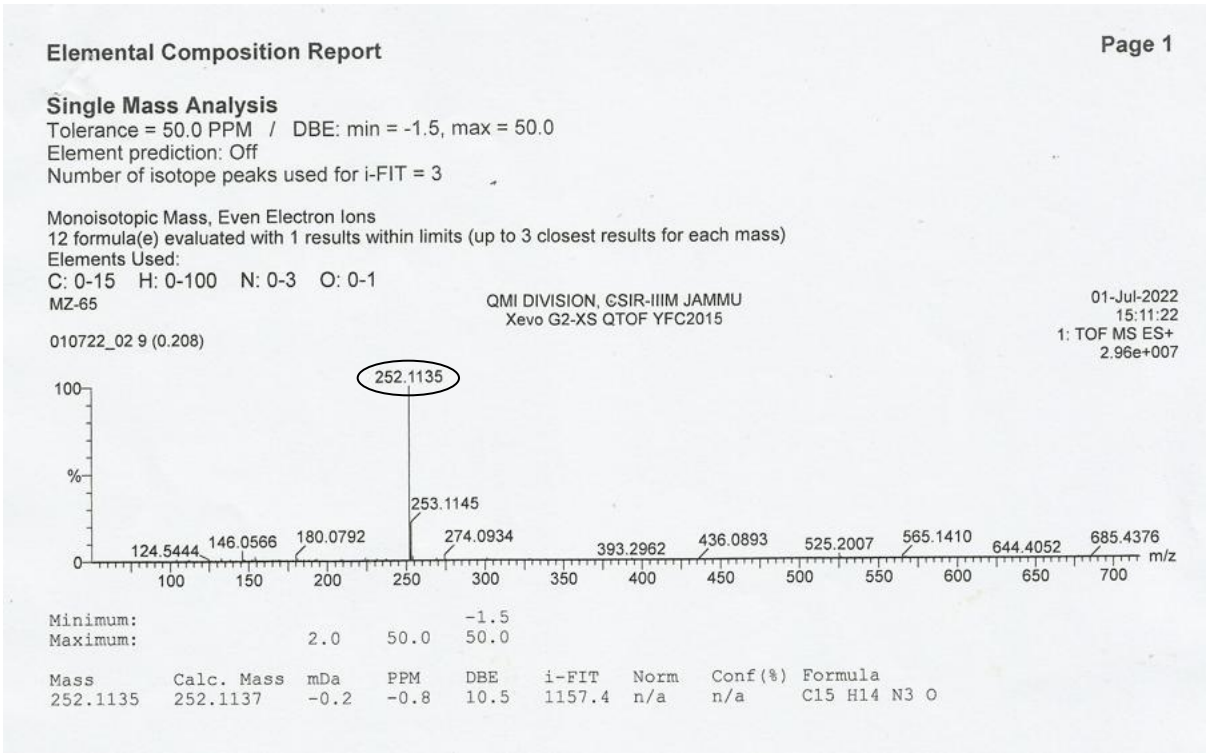
^{13}C-NMR of 4-(4-Methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole (3e)



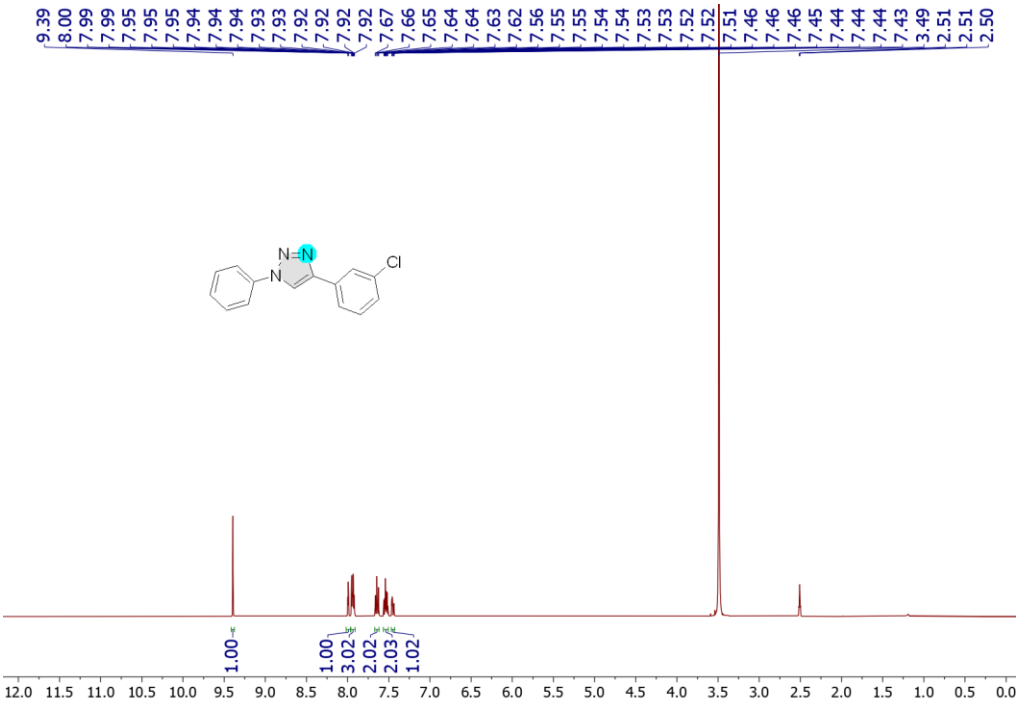
DEPT of 4-(4-Methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole (3e)



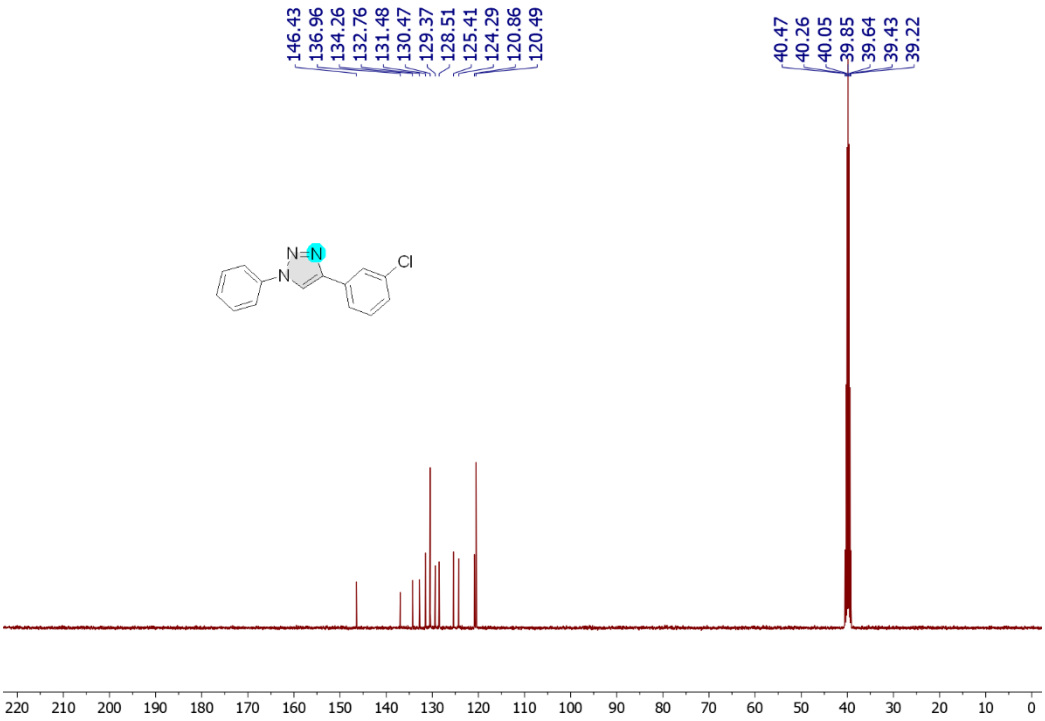
HRMS of 4-(4-Methoxyphenyl)-1-phenyl-1*H*-1,2,3-triazole (3e)



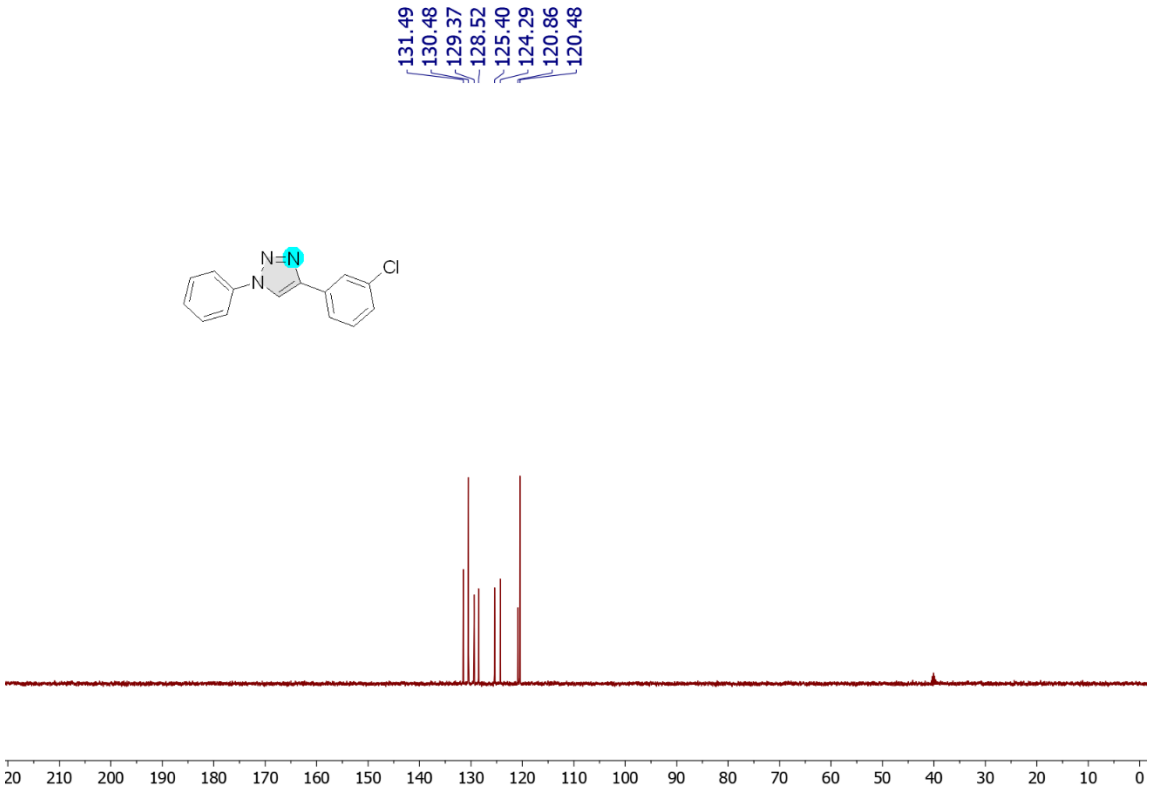
^{1}H- NMR of 4-(3-Chlorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3f)



^{13}C-NMR of 4-(3-Chlorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3f)



DEPT of 4-(3-Chlorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3f)



HRMS of 4-(3-Chlorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3f)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 Cl: 0-1

MZ-3Cl
220424_02 7 (0.155)

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

22-Apr-2024
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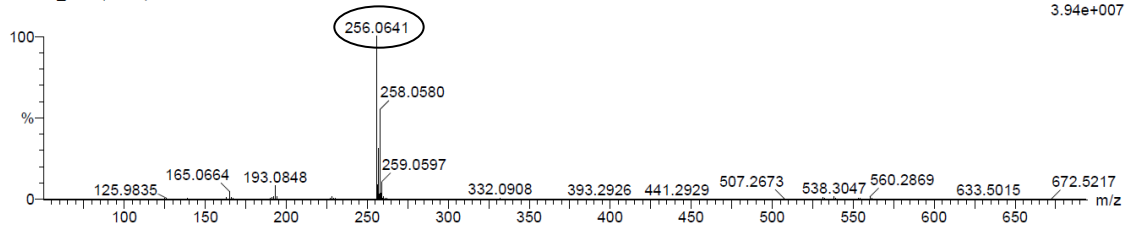
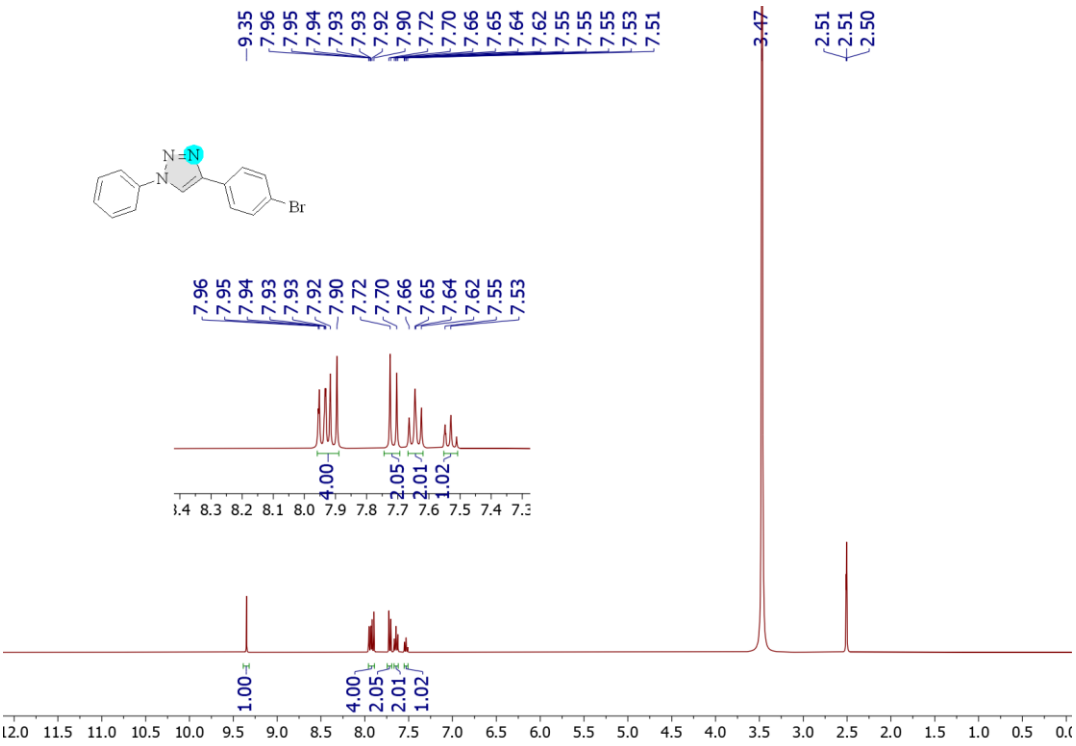
3.94e+007

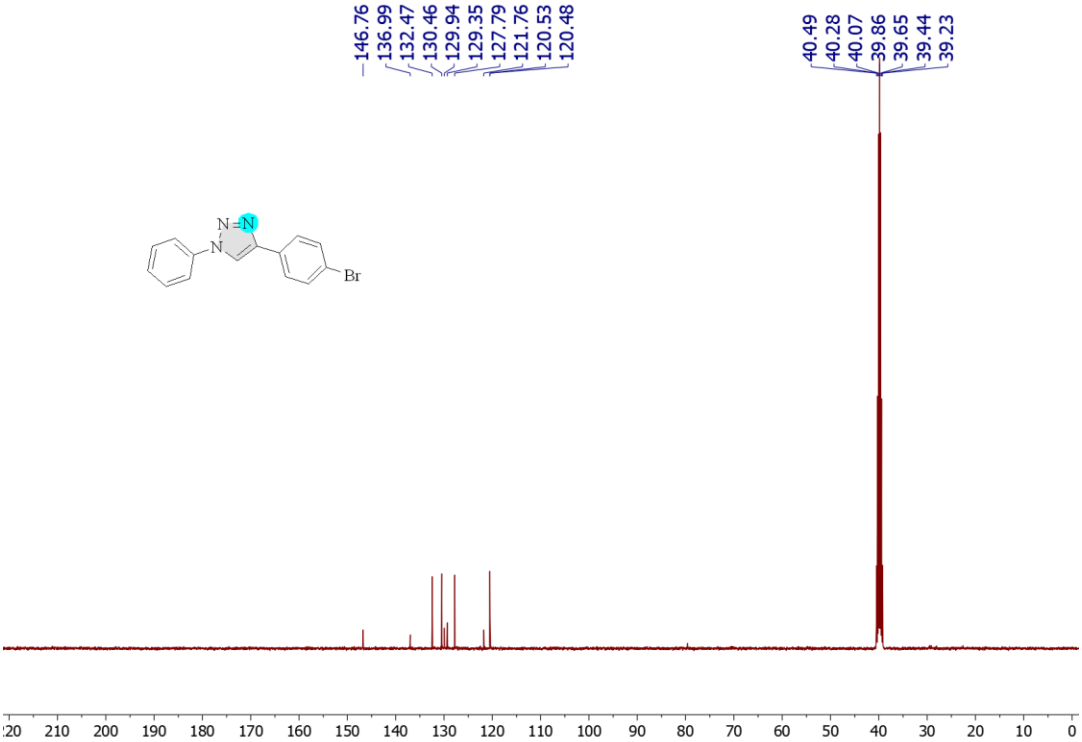


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
256.0641	256.0642	-0.1	-0.4	10.5	1265.4	n/a	n/a	C14 H11 N3 Cl

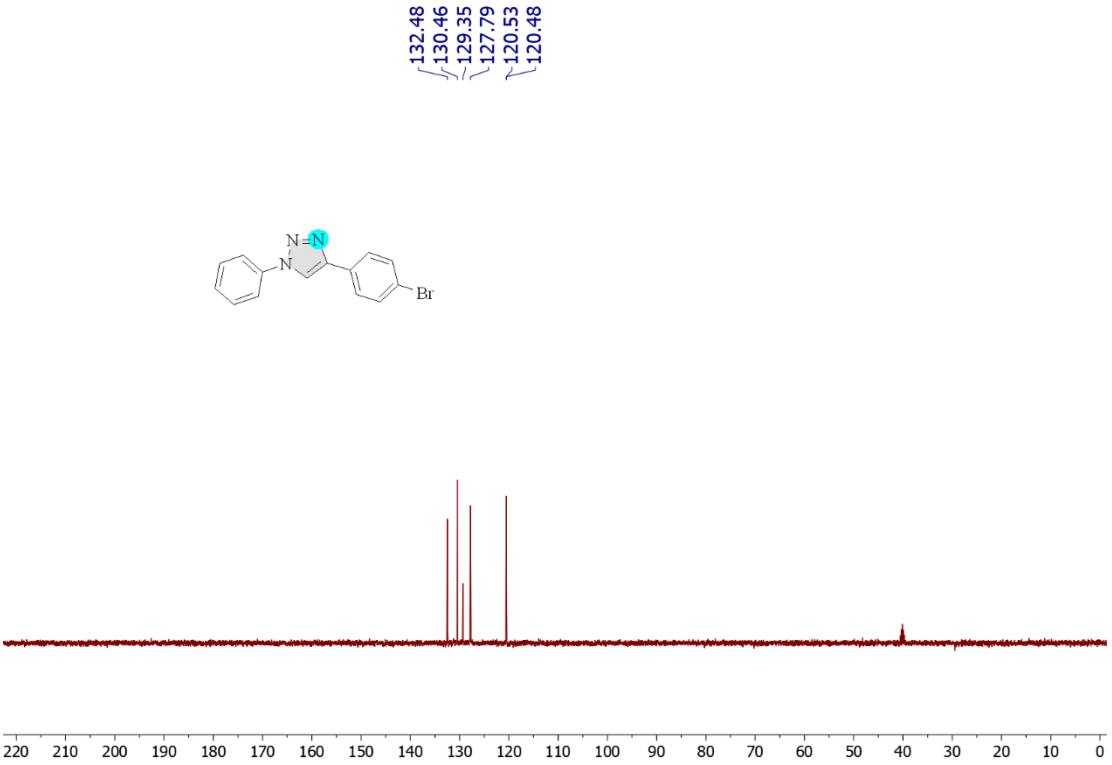
^{1}H-NMR of 4-(4-Bromophenyl)-1-phenyl-1*H*-1,2,3-triazole (3g)



^{13}C-NMR of 4-(4-Bromophenyl)-1-phenyl-1*H*-1,2,3-triazole (3g)



DEPT of 4-(4-Bromophenyl)-1-phenyl-1*H*-1,2,3-triazole (3g)



HRMS of 4-(4-Bromophenyl)-1-phenyl-1*H*-1,2,3-triazole (3g)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 Br: 0-1

MZ-4Br
230424_25 4 (0.104)

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

23-Apr-2024
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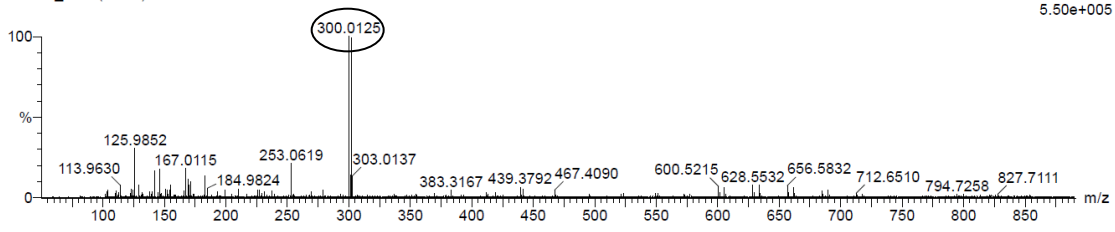
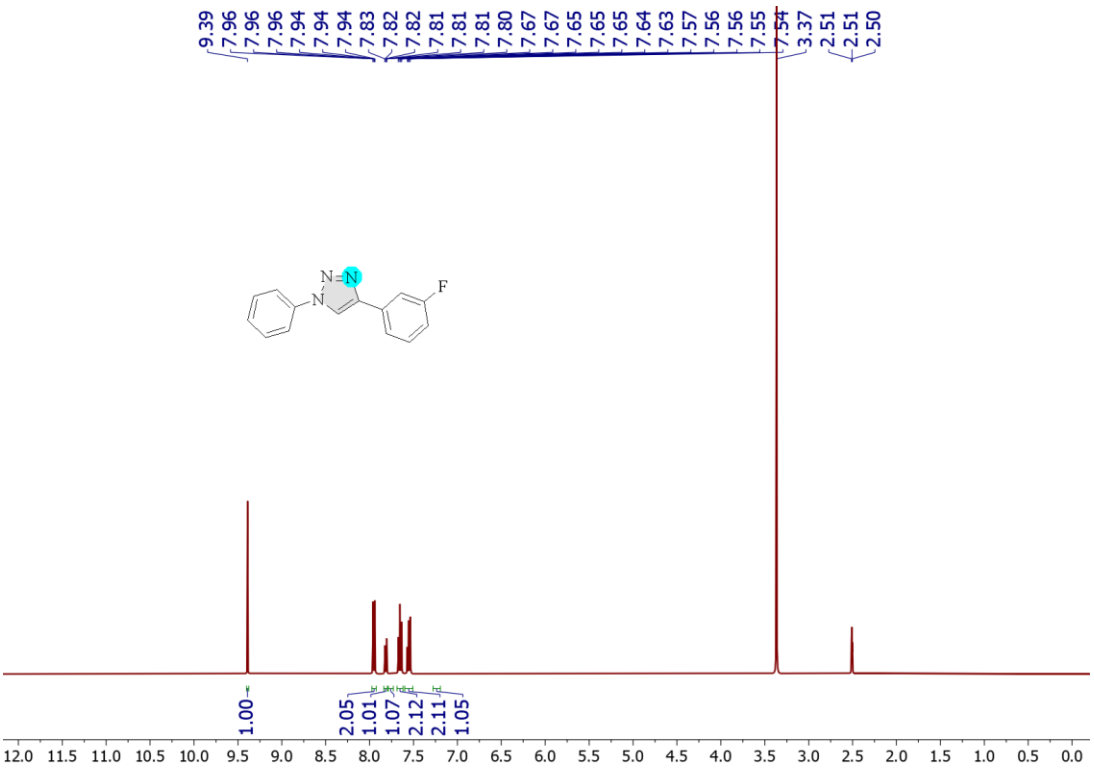
5.50e+005

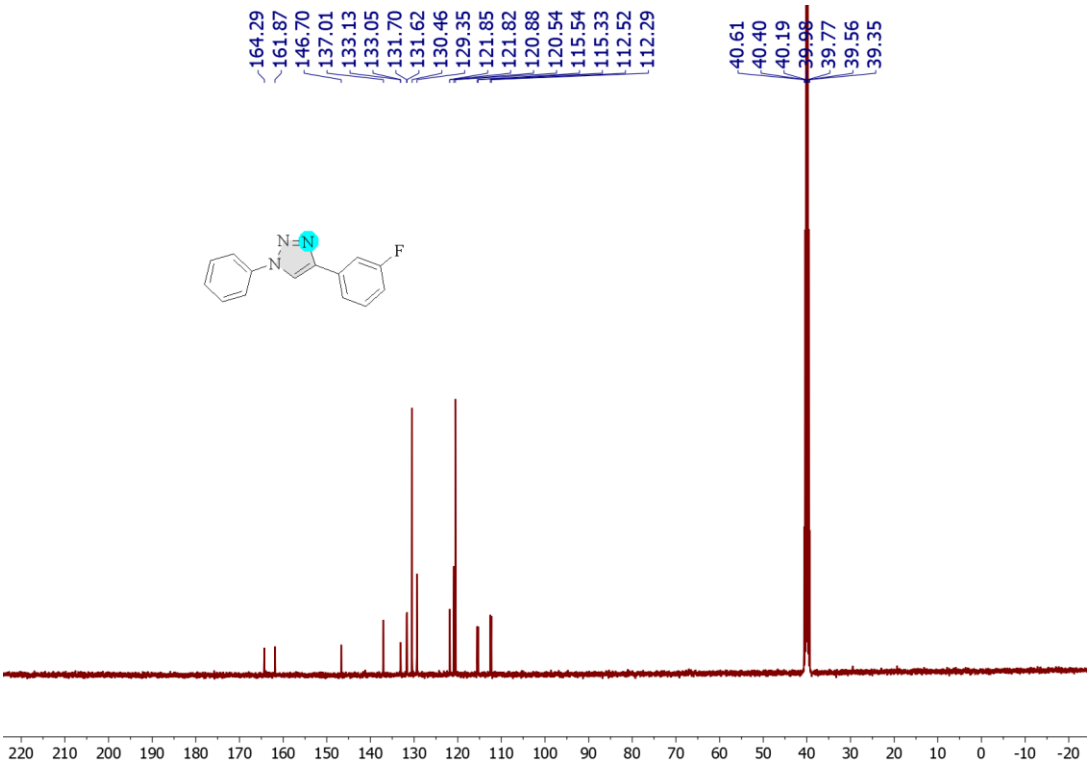


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
300.0125	300.0136	-1.1	-3.7	10.5	1187.6	n/a	n/a	C14 H11 N3 Br

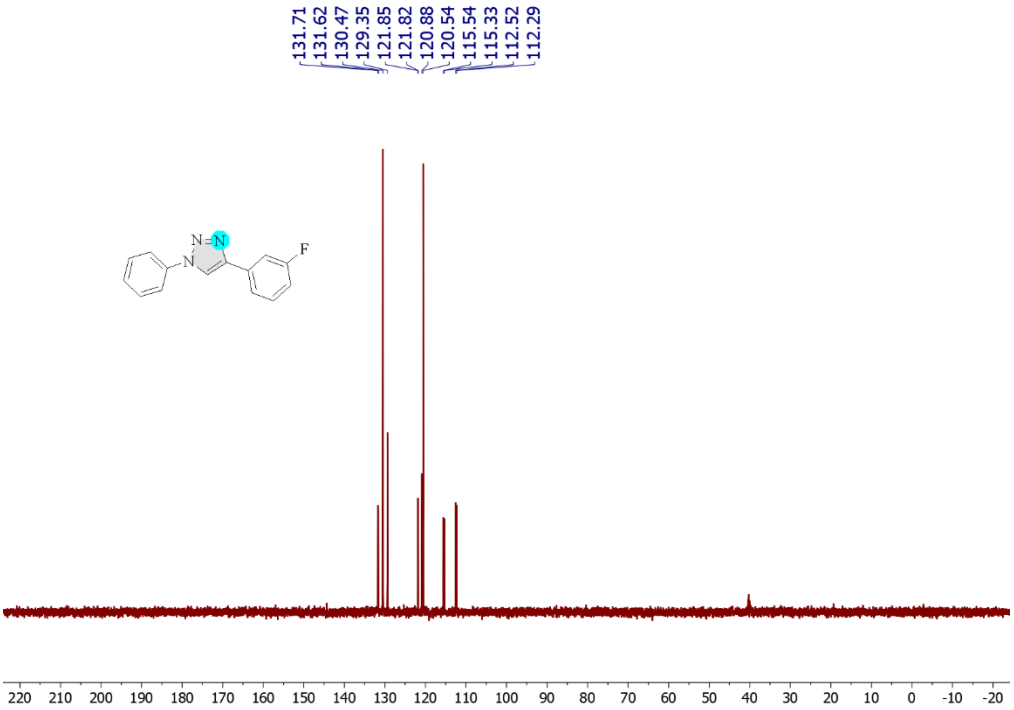
[1]H- NMR of 4-(3-Fluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3h)



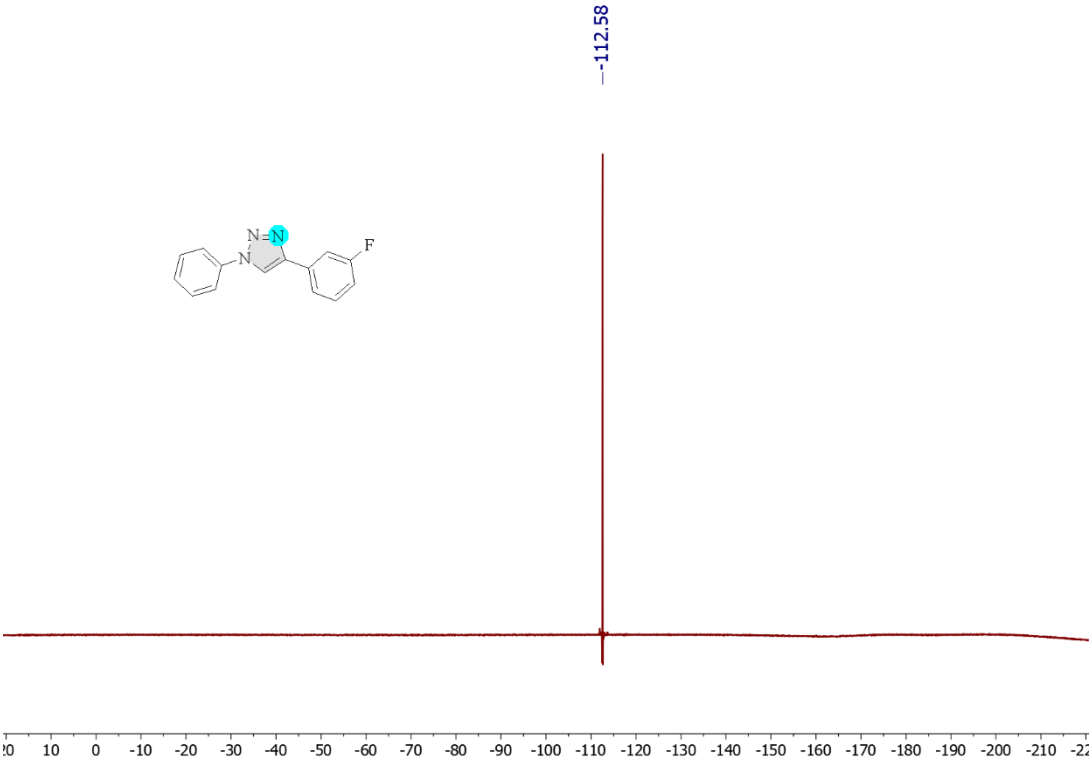
[13]C- NMR of 4-(3-Fluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3h)



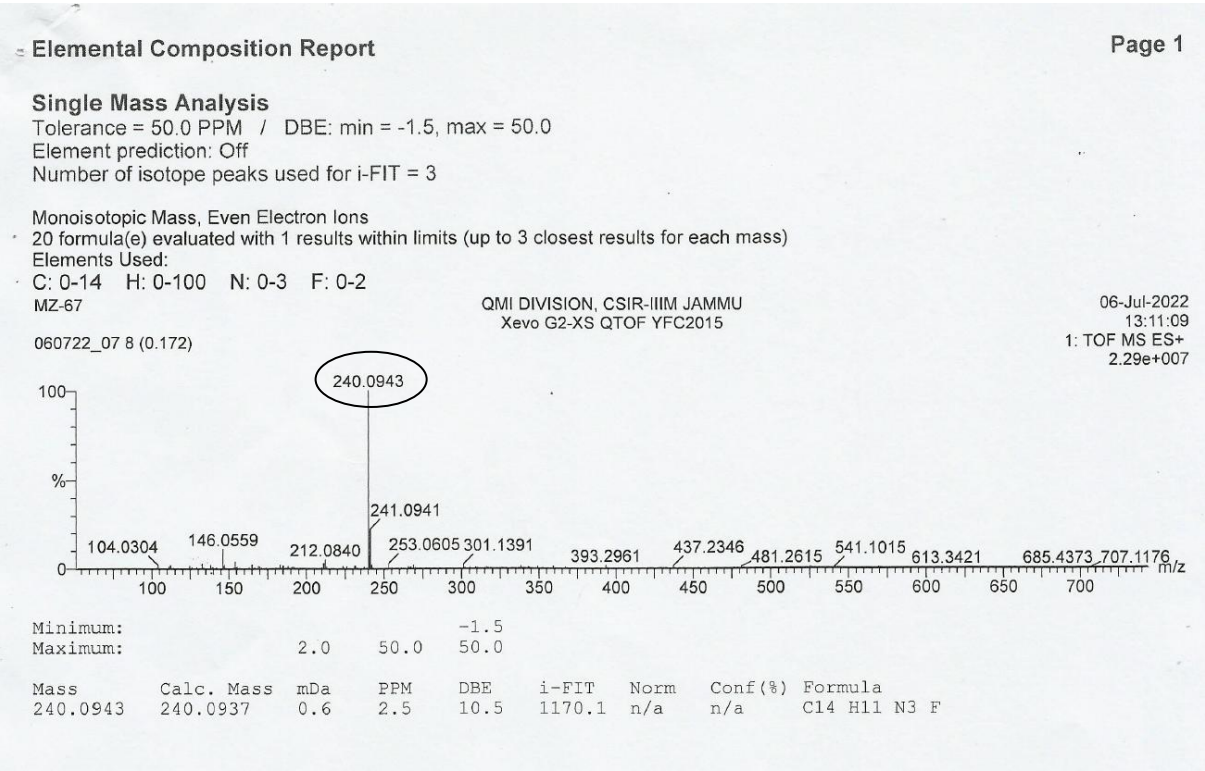
DEPT of 4-(3-Fluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3h)



^{19}F-NMR of 4-(3-Fluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3h)



HRMS of 4-(3-Fluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3h)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 F: 0-2

MZ-67

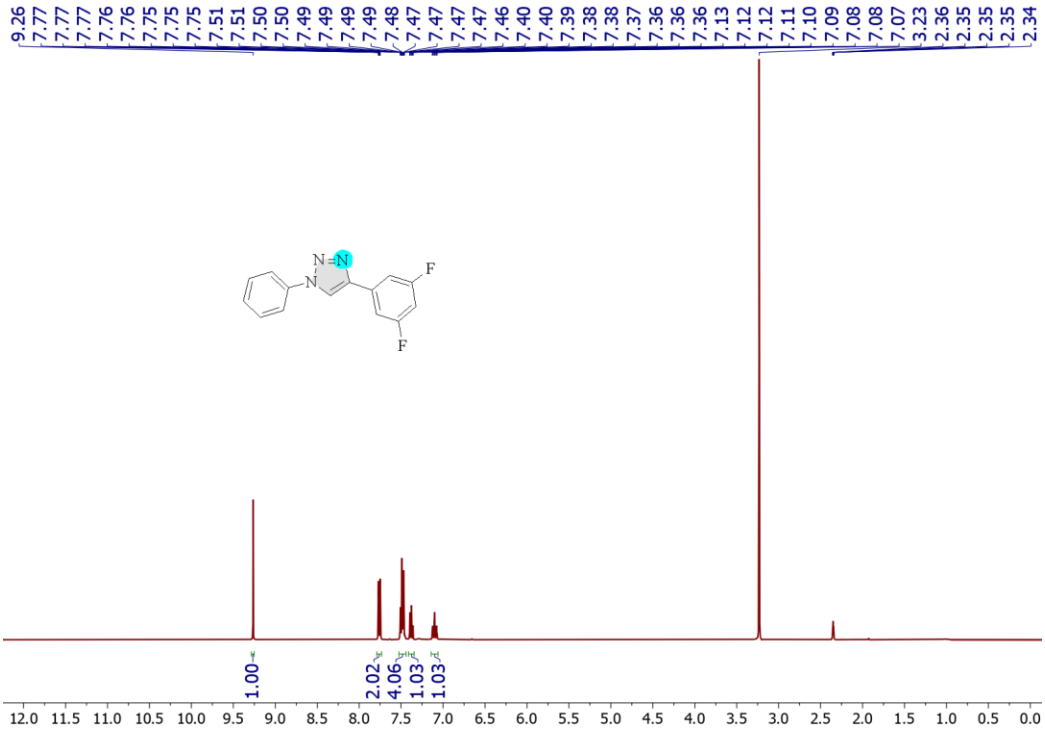
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

06-Jul-2022
13:11:09
1: TOF MS ES+
2.29e+007

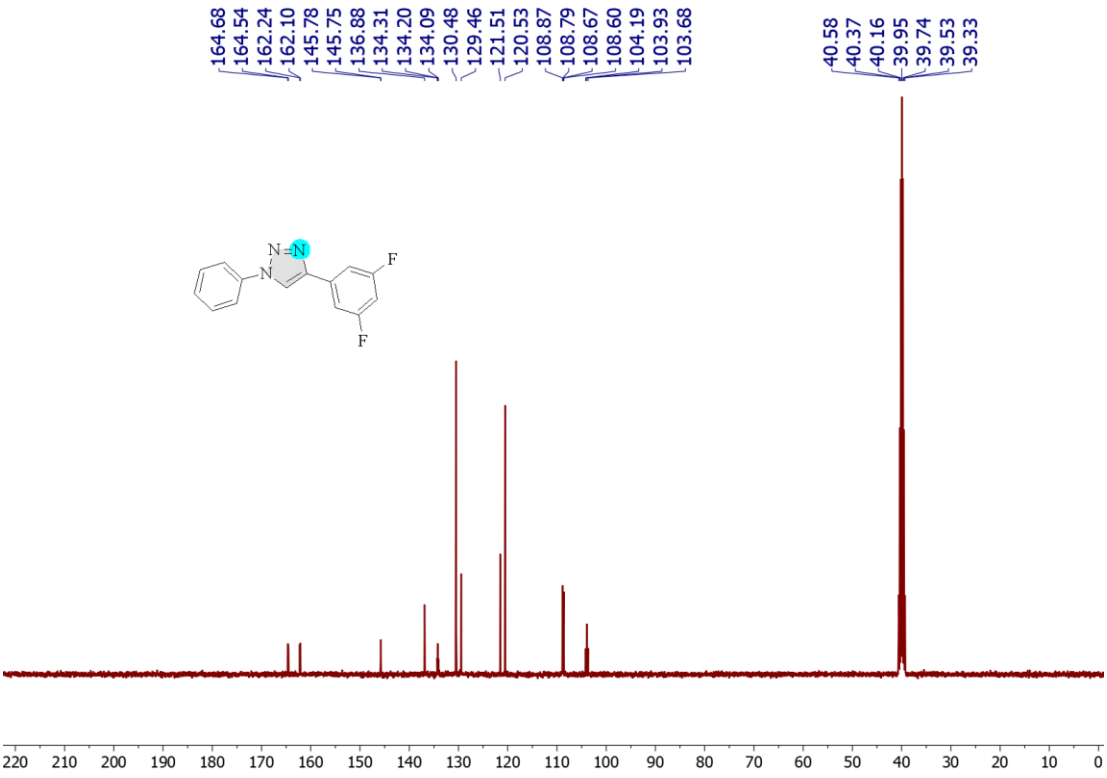
060722_07 8 (0.172)

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
240.0943	240.0937	0.6	2.5	10.5	1170.1	n/a	n/a	C14 H11 N3 F

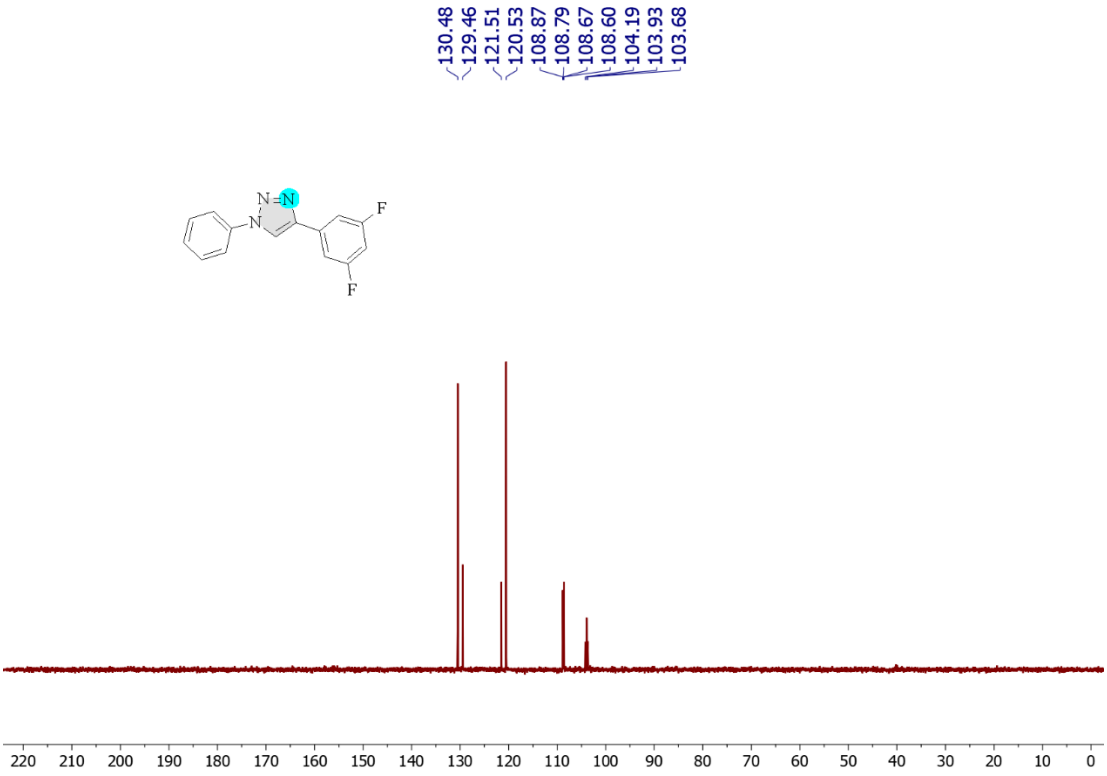
^{1}H-NMR of 4-(3,5-Difluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3i)



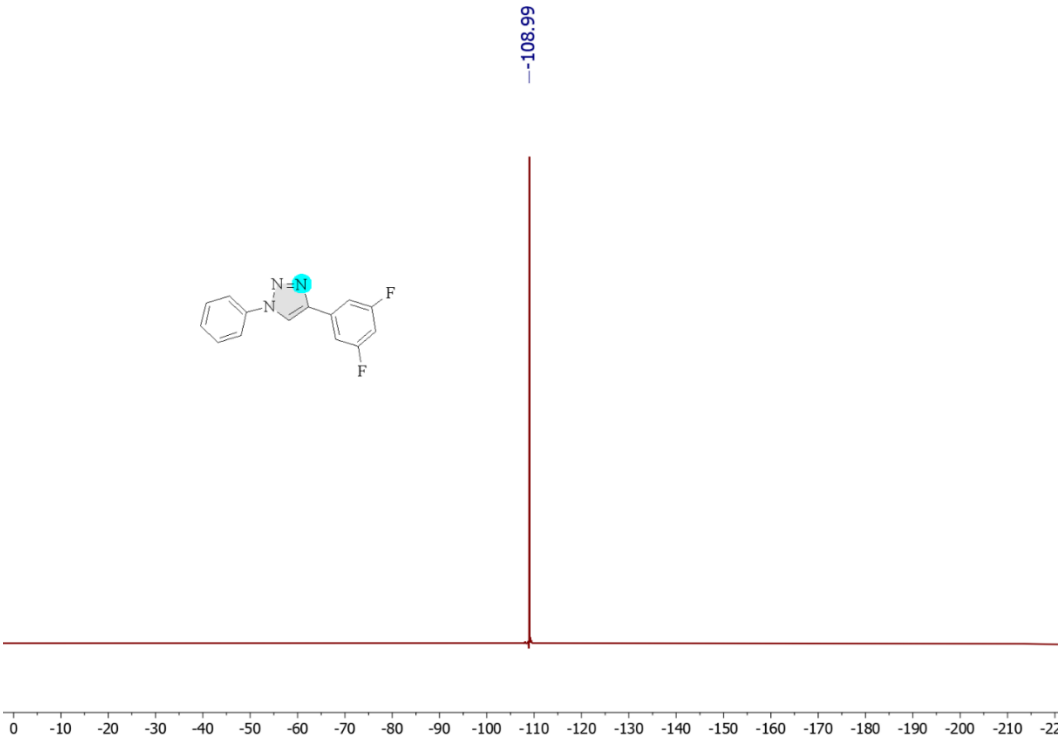
^{13}C-NMR of 4-(3,5-Difluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3i)



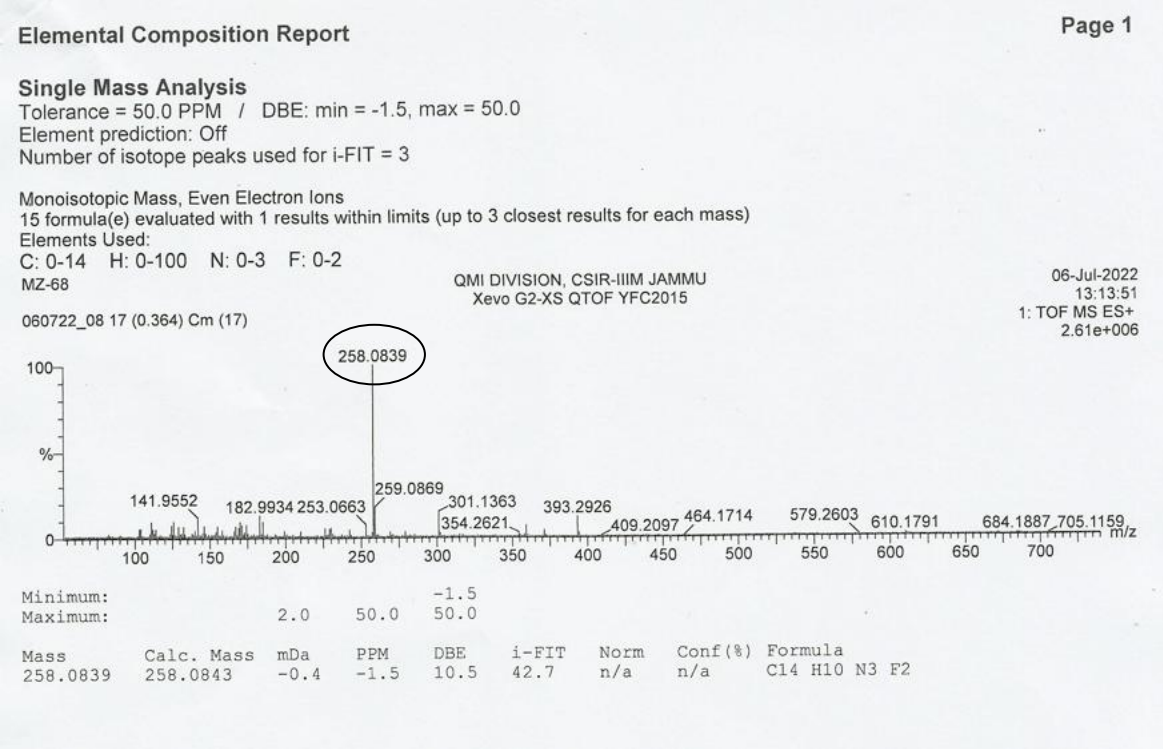
DEPT of 4-(3,5-Difluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3i)



^{19}F-NMR of 4-(3,5-Difluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3i)



HRMS of 4-(3,5-Difluorophenyl)-1-phenyl-1*H*-1,2,3-triazole (3i)



Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
15 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 F: 0-2

MZ-68

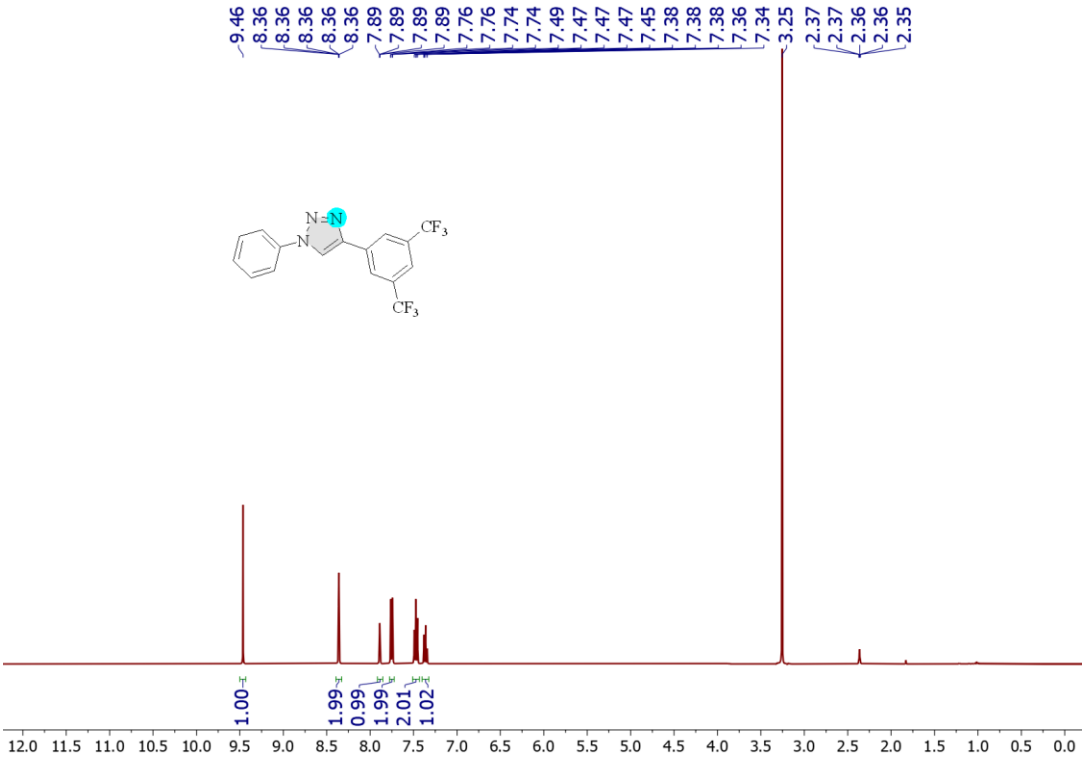
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

06-Jul-2022
13:13:51
1: TOF MS ES+
2.61e+006

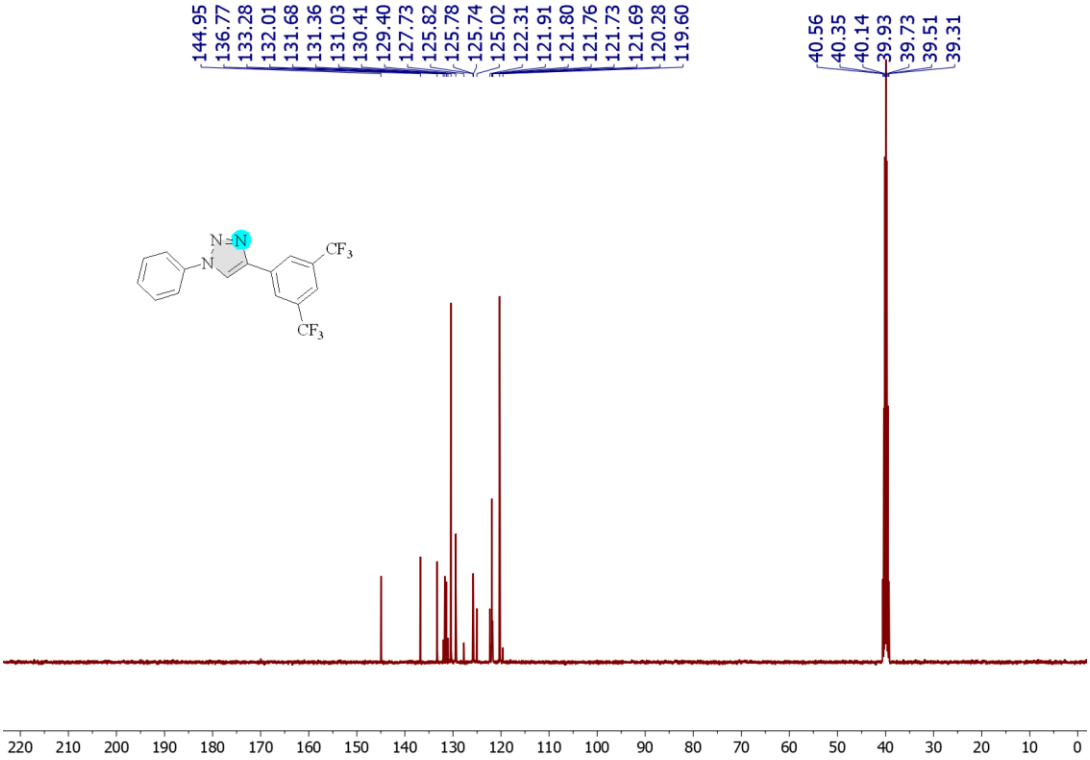
060722_08 17 (0.364) Cm (17)

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
258.0839	258.0843	-0.4	-1.5	10.5	42.7	n/a	n/a	C14 H10 N3 F2

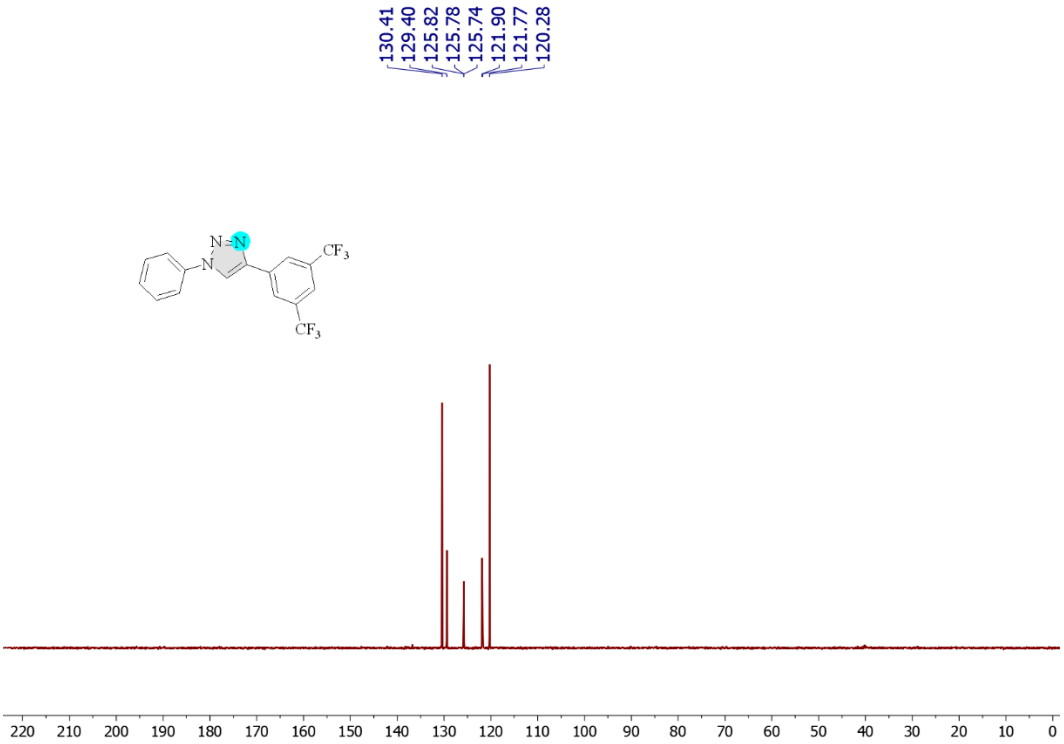
^{1}H-NMR of 4-(3,5-Bis(trifluoromethyl)phenyl)-1-phenyl-1*H*-1,2,3-triazole (3j)



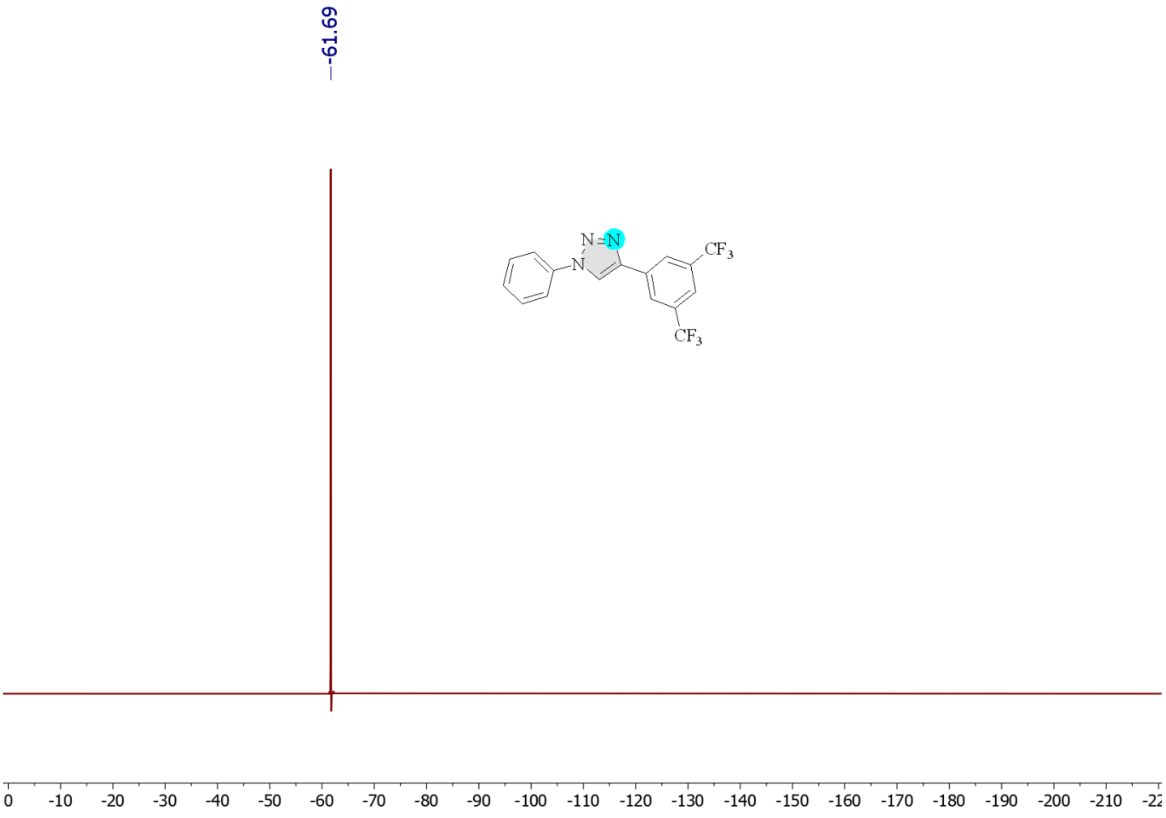
^{13}C-NMR of 4-(3,5-Bis(trifluoromethyl)phenyl)-1-phenyl-1*H*-1,2,3-triazole (3j)



DEPT of 4-(3,5-Bis(trifluoromethyl)phenyl)-1-phenyl-1*H*-1,2,3-triazole (3j)



^{19}F-NMR of 4-(3,5-Bis(trifluoromethyl)phenyl)-1-phenyl-1*H*-1,2,3-triazole (3j)



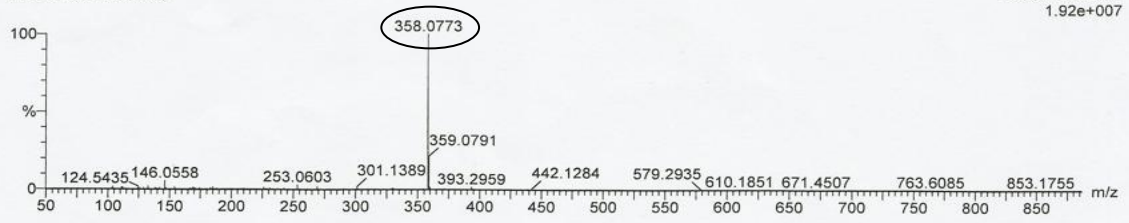
HRMS of 4-(3,5-Bis(trifluoromethyl)phenyl)-1-phenyl-1*H*-1,2,3-triazole (3j)

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

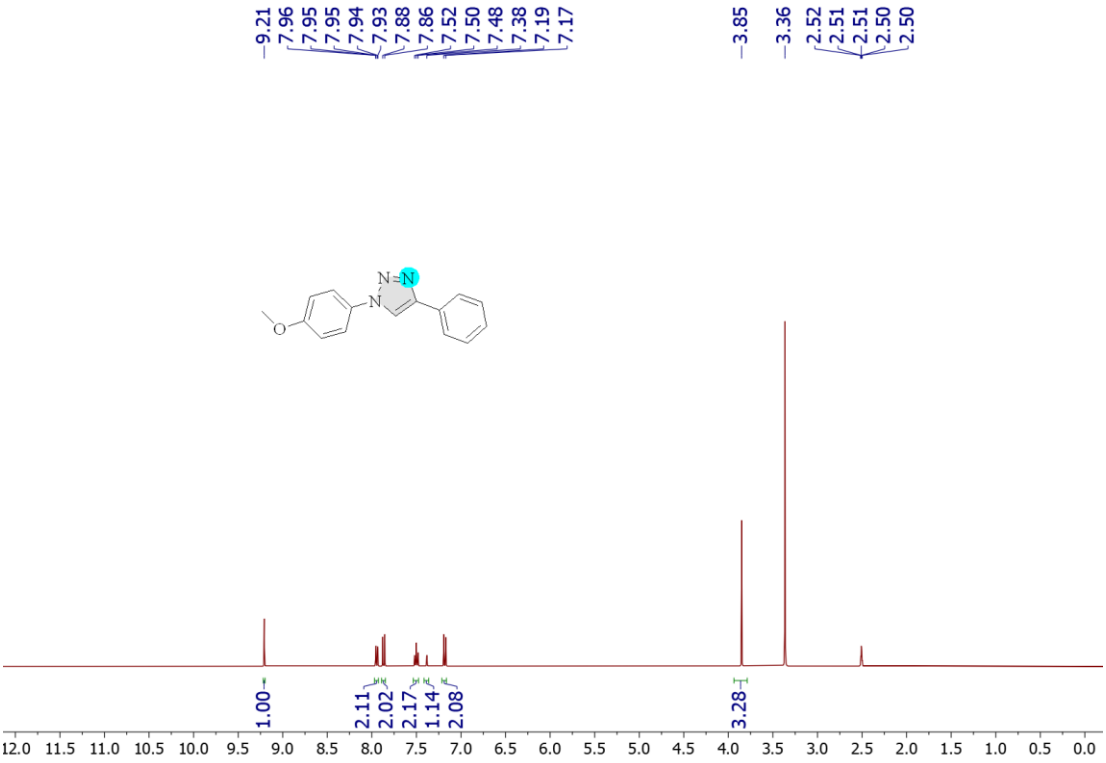
Monoisotopic Mass, Even Electron Ions
31 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-16 H: 0-100 N: 0-3 F: 0-6

MZ-69
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
06-Jul-2022
13:08:27
060722_06 12 (0.259)
1: TOF MS ES+
1.92e+007

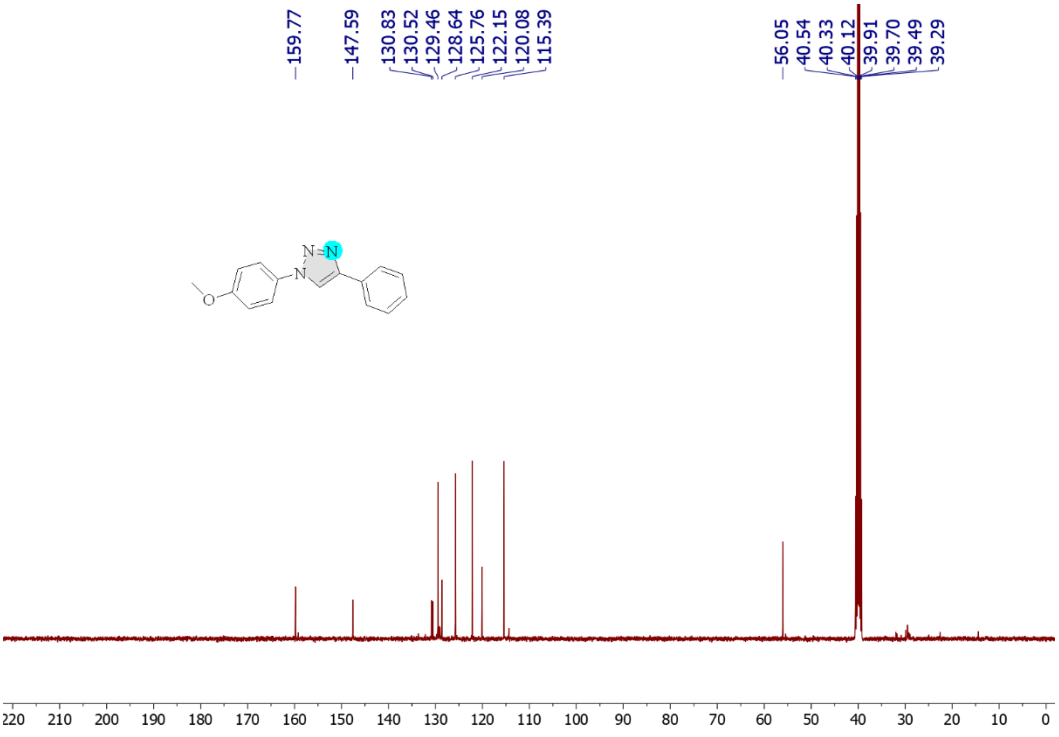


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
358.0773	358.0779	-0.6	-1.7	10.5	933.2	n/a	n/a	C16 H10 N3 F6

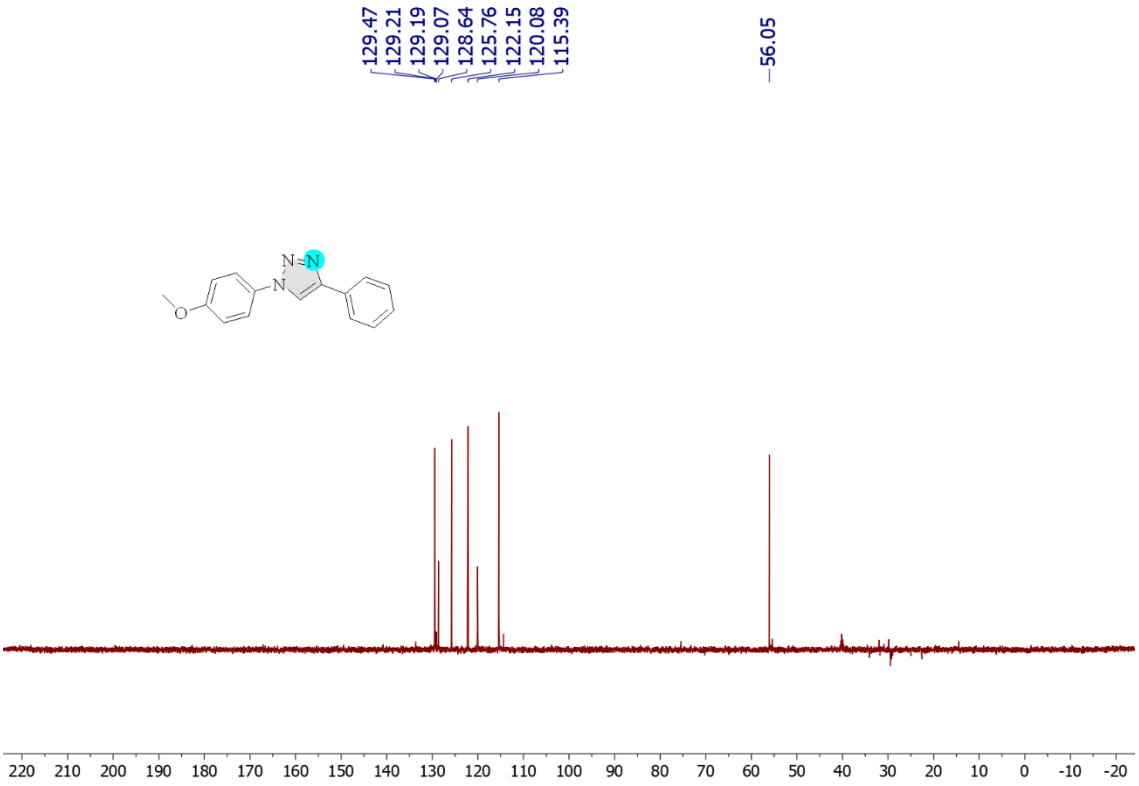
^{1}H-NMR of 1-(4-Methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (3k)



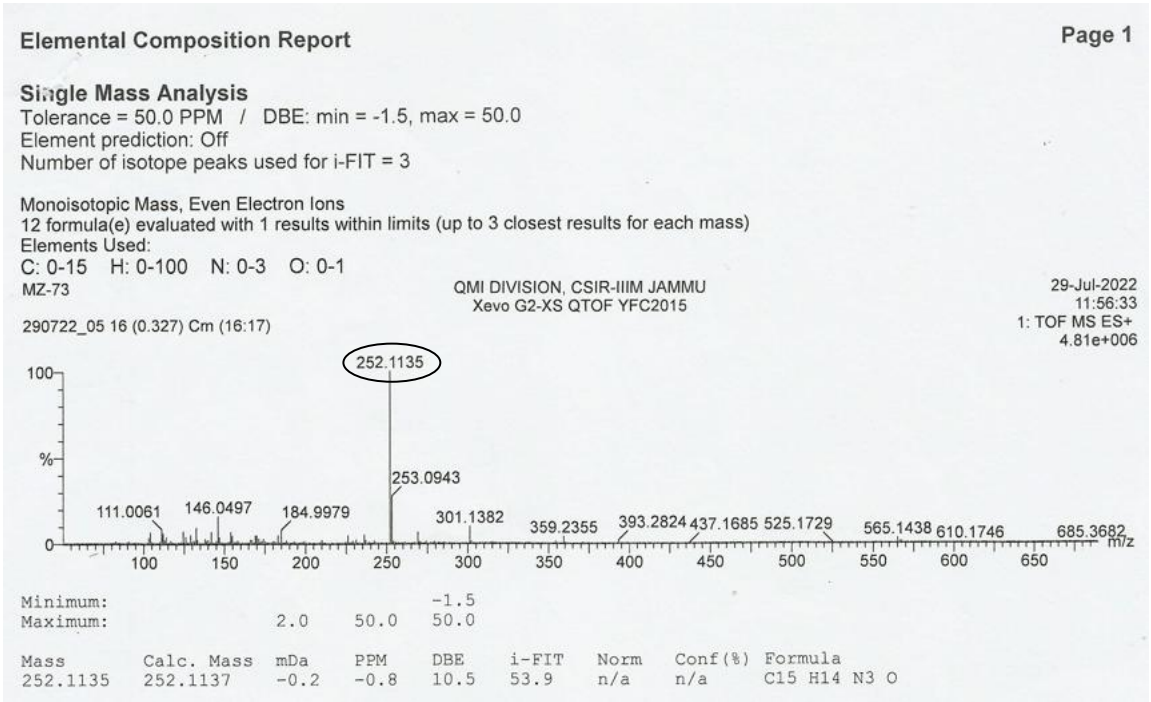
^{13}C-NMR of 1-(4-Methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (3k)



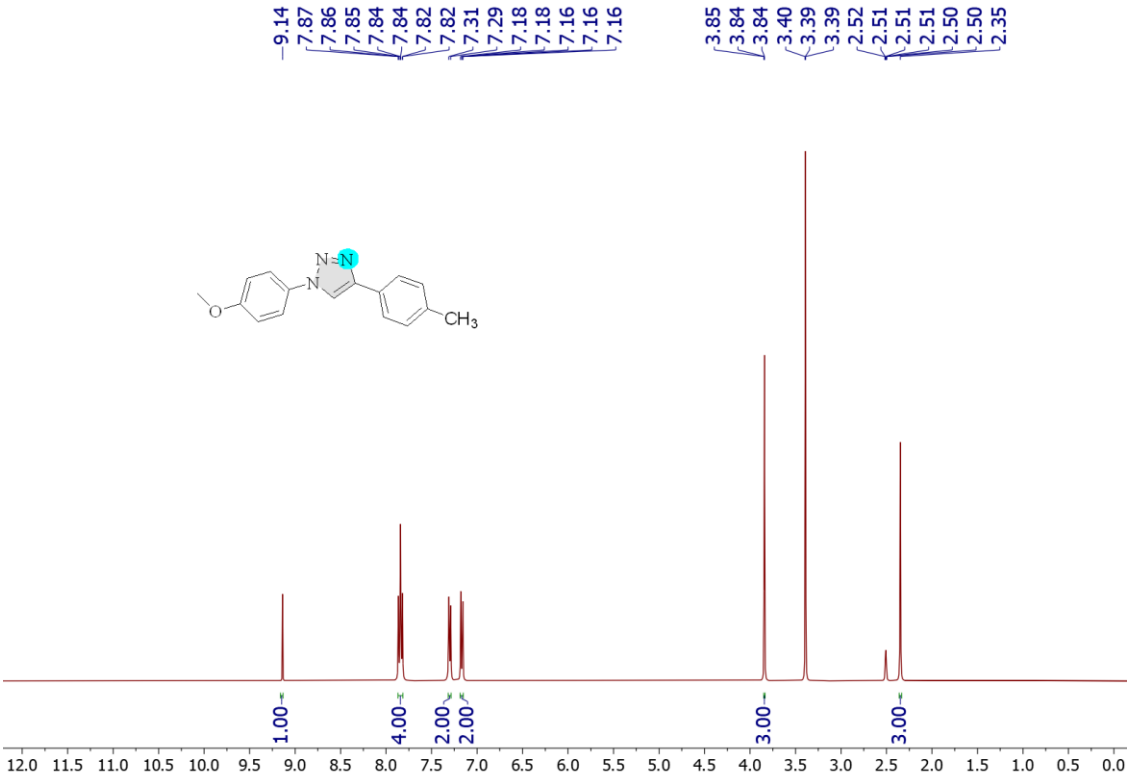
DEPT of 1-(4-Methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (3k)



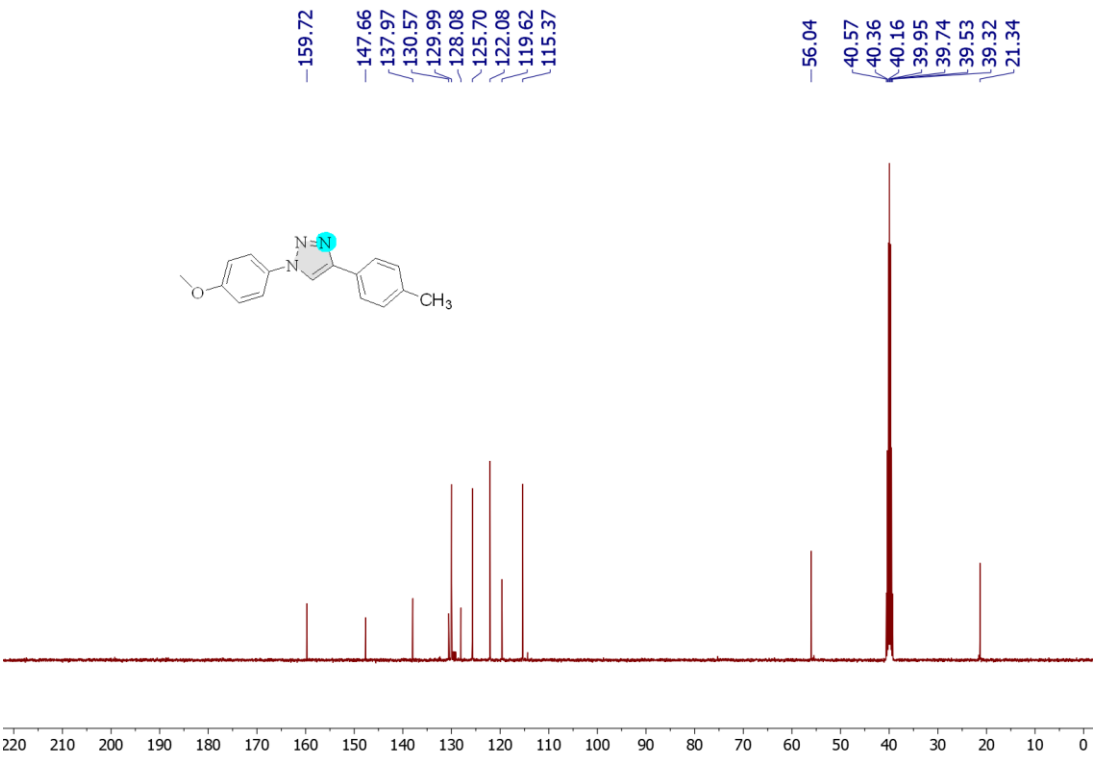
HRMS of 1-(4-Methoxyphenyl)-4-phenyl-1*H*-1,2,3-triazole (3k)



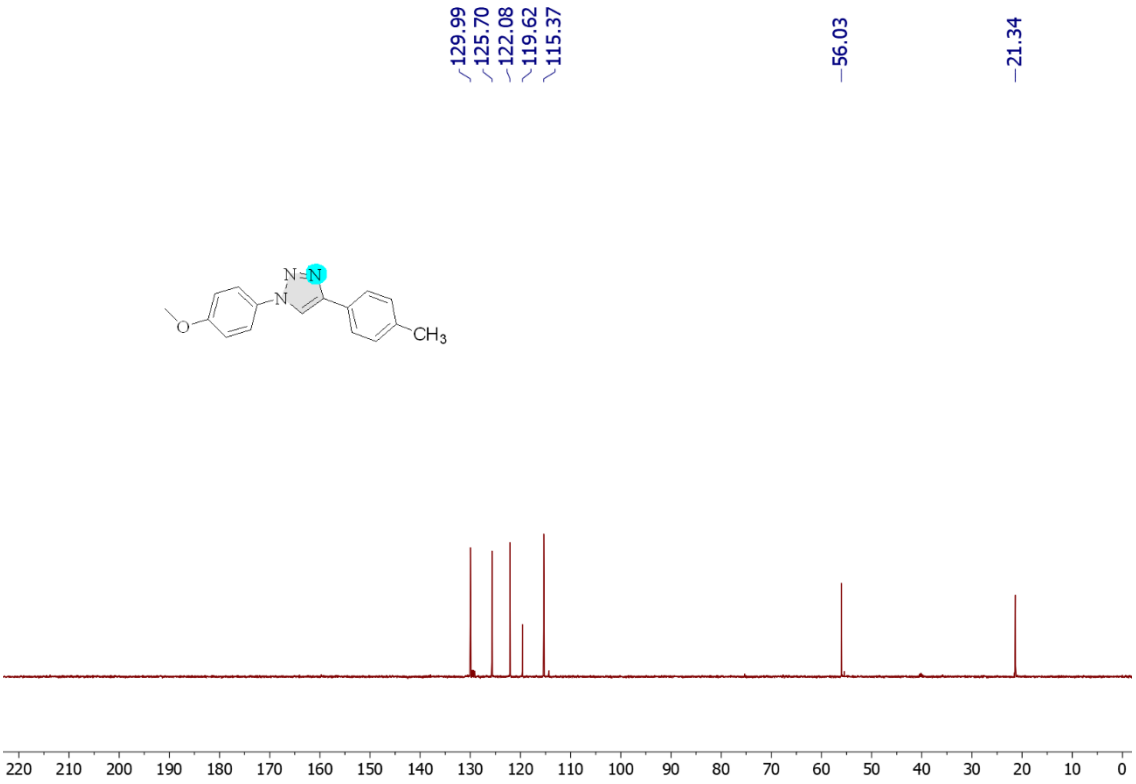
^{1}H-NMR of 1-(4-Methoxyphenyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3l)



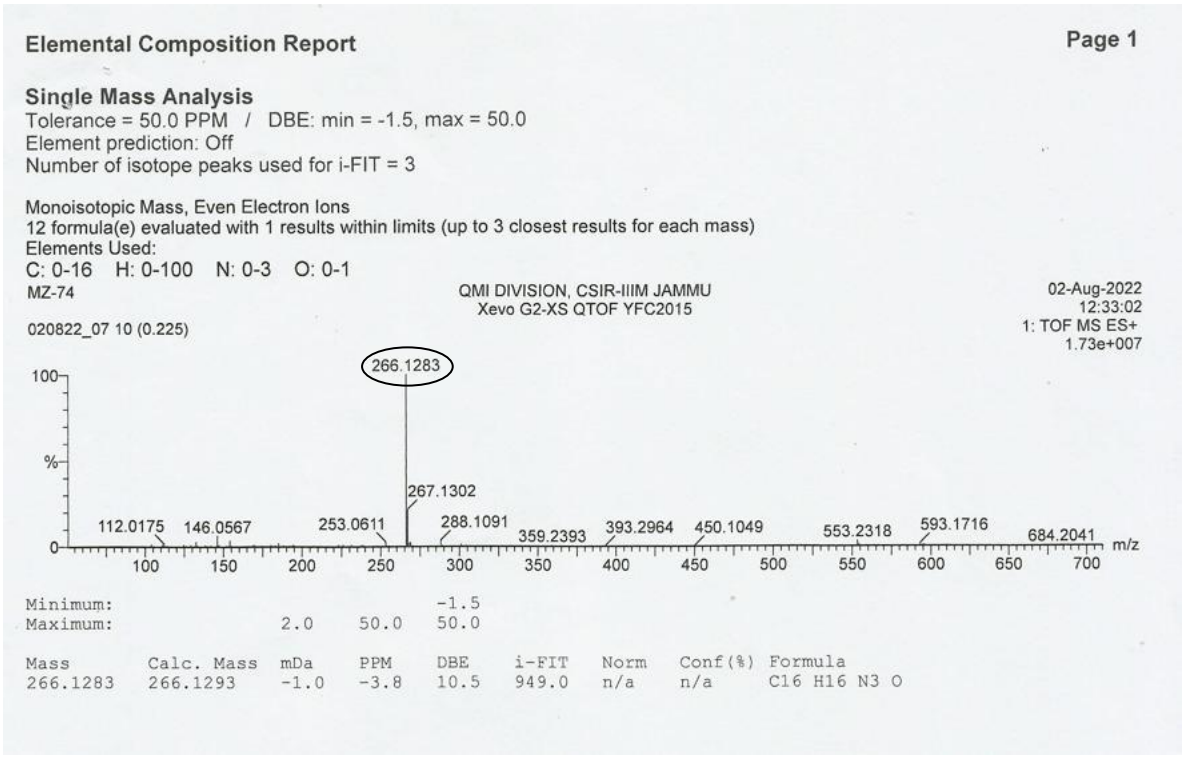
^{13}C-NMR of 1-(4-Methoxyphenyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3l)



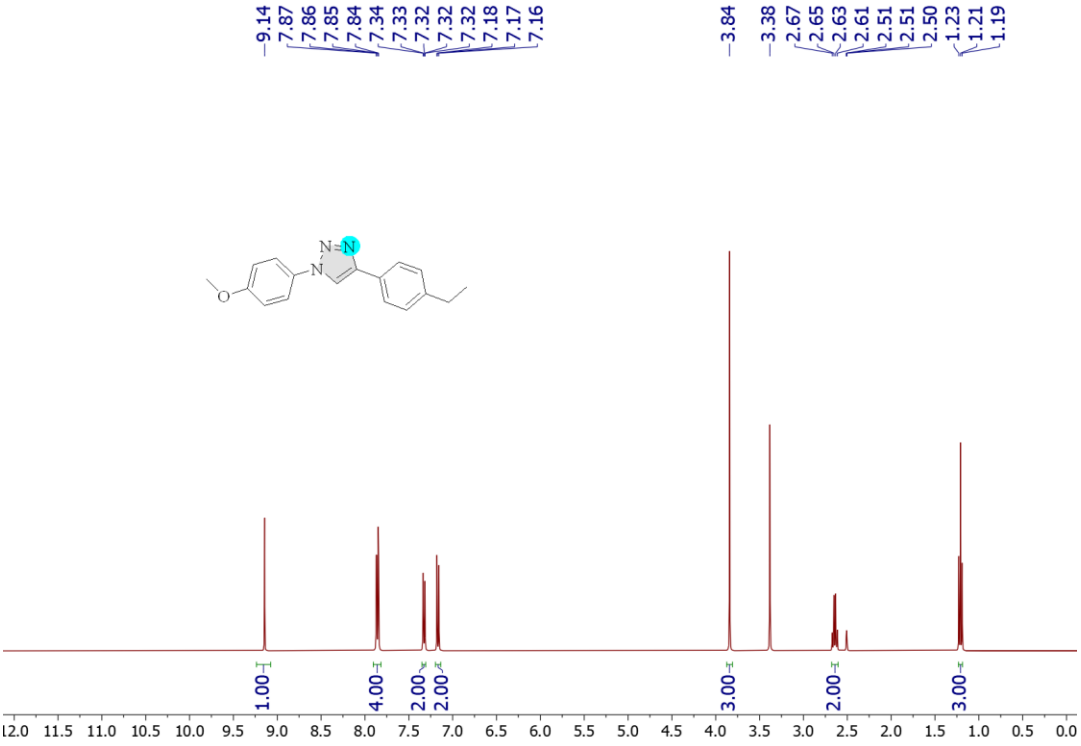
DEPT of 1-(4-Methoxyphenyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3l)



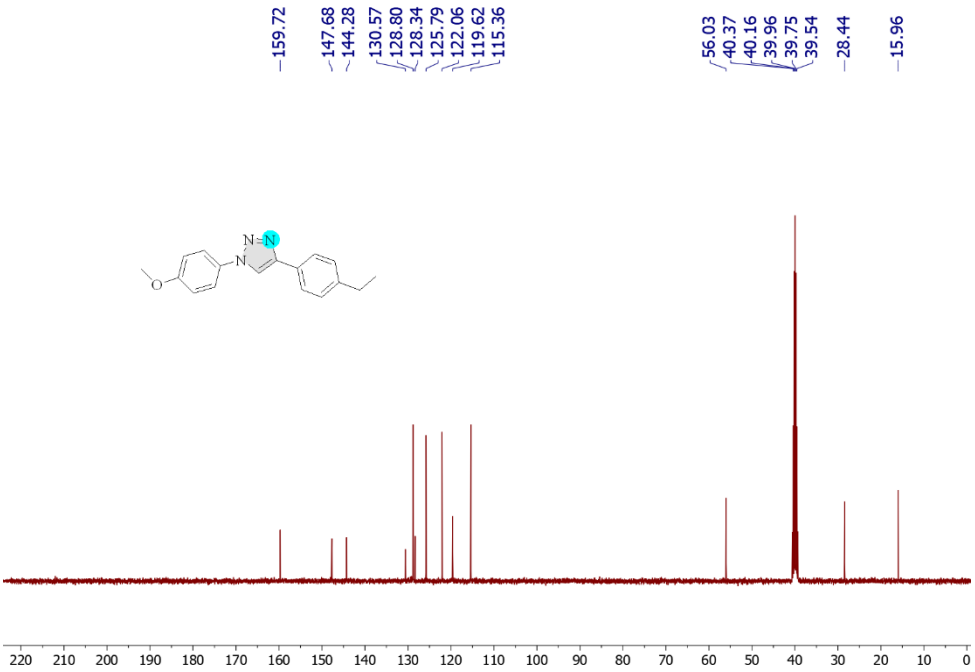
HRMS of 1-(4-Methoxyphenyl)-4-(*p*-tolyl)-1*H*-1,2,3-triazole (3l)



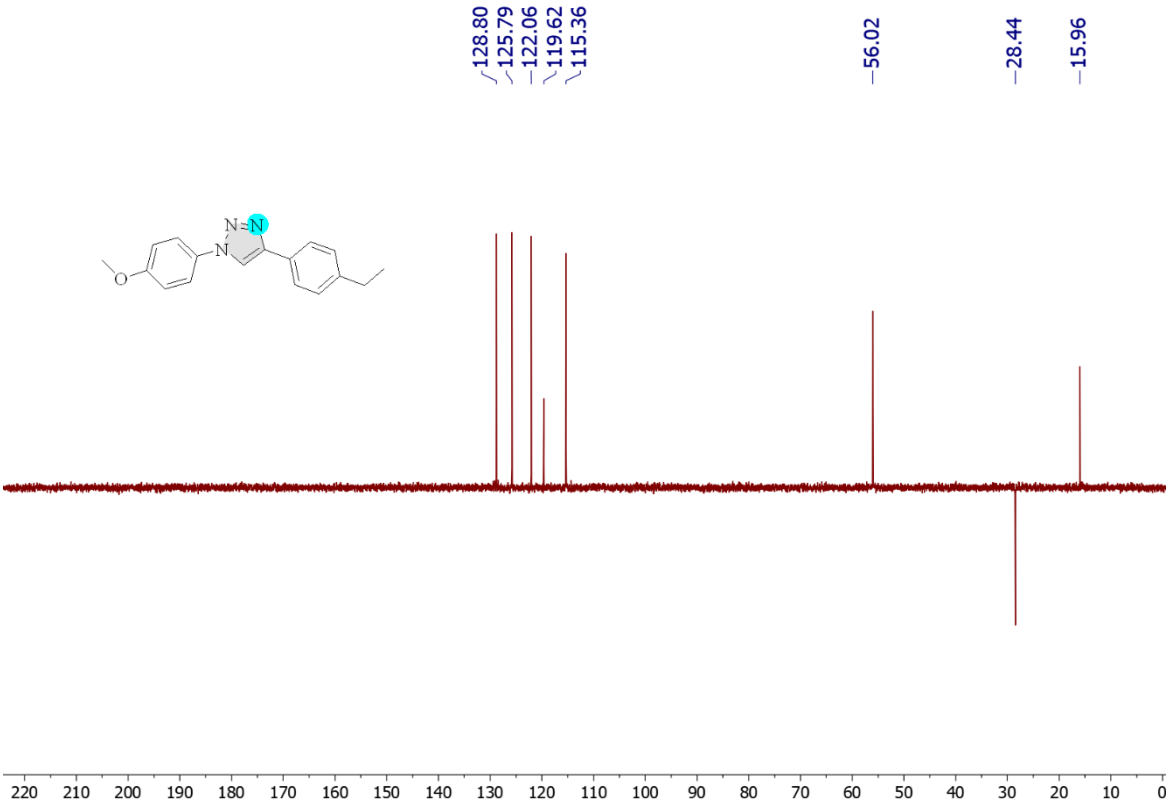
^{1}H-NMR of 4-(4-Ethylphenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3m)



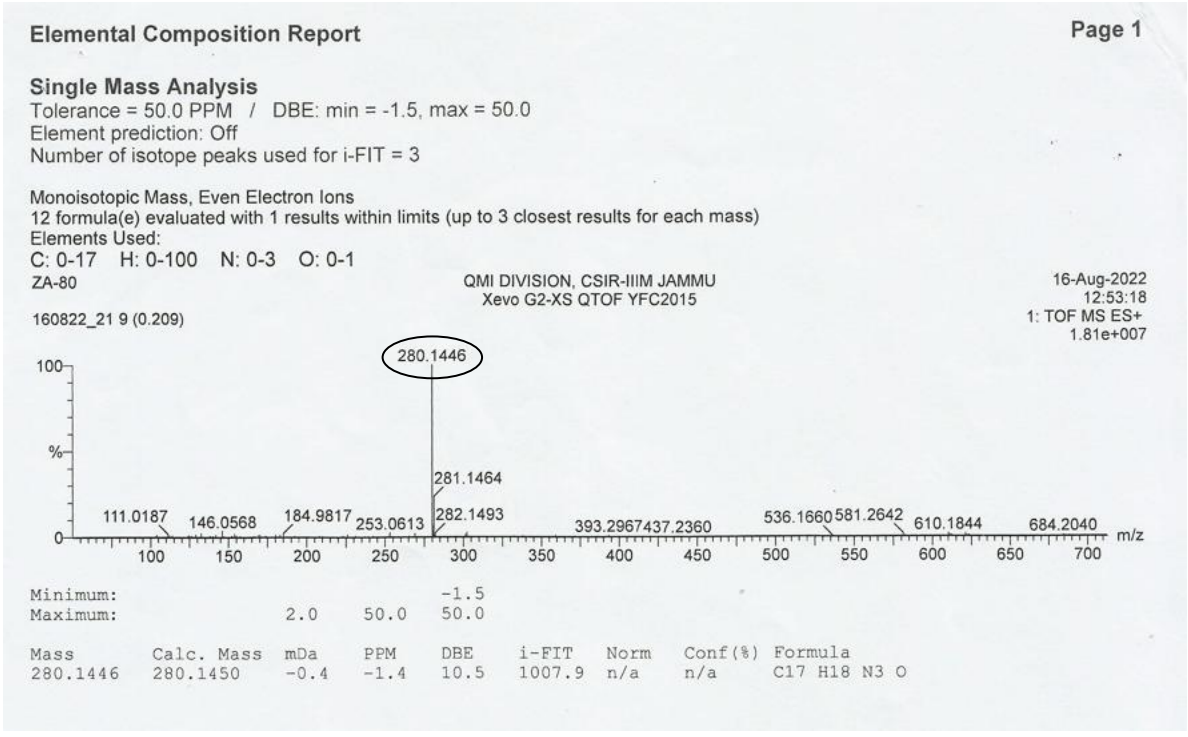
^{13}C-NMR of 4-(4-Ethylphenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3m)



DEPT of 4-(4-Ethylphenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3m)



HRMS of 4-(4-Ethylphenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3m)



Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-17 H: 0-100 N: 0-3 O: 0-1

ZA-80
160822_21 9 (0.209)

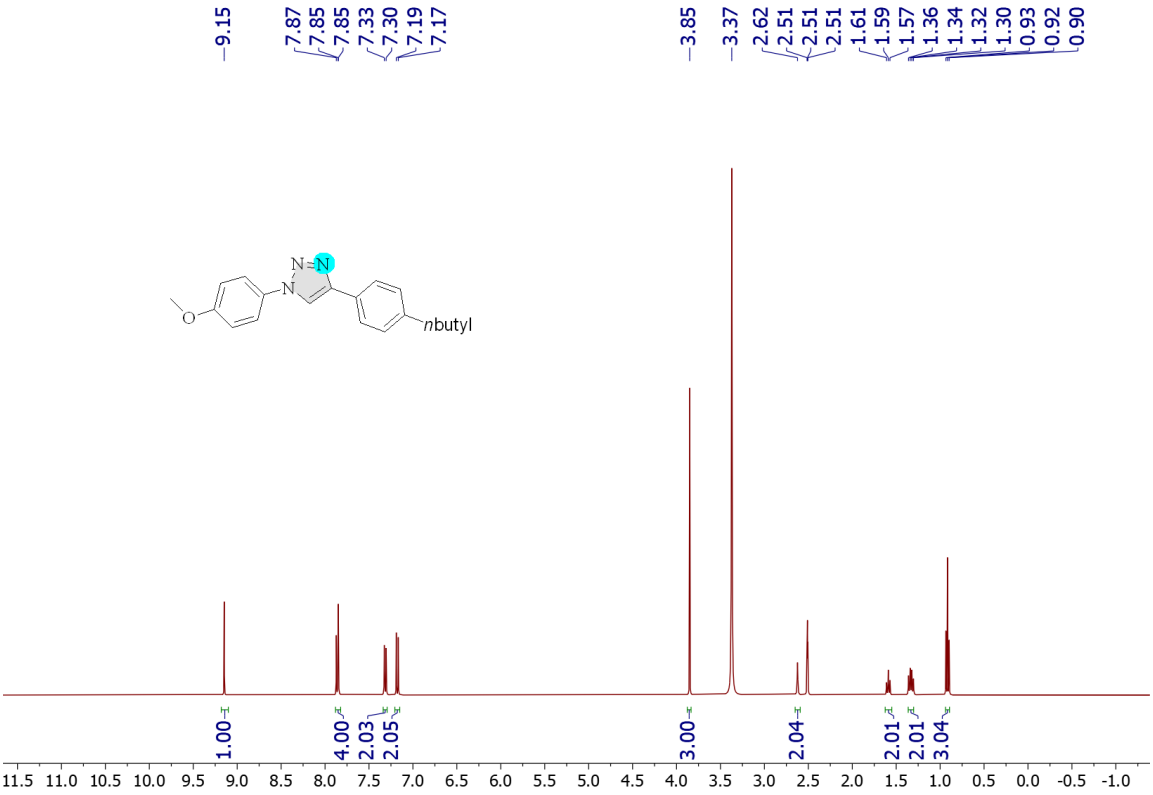
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

16-Aug-2022
12:53:18
1: TOF MS ES+
1.81e+007

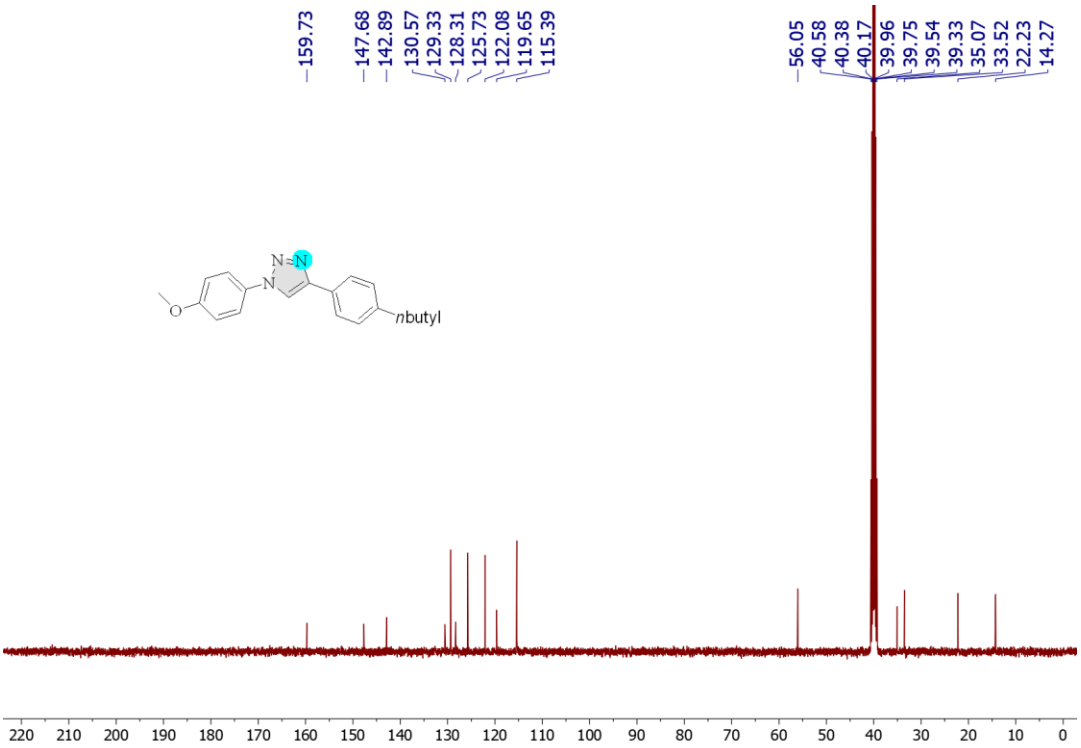
280.1446
281.1464
282.1493
111.0187
146.0568
184.9817
253.0613
393.2967
437.2360
536.1660
581.2642
610.1844
684.2040
m/z

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
280.1446	280.1450	-0.4	-1.4	10.5	1007.9	n/a	n/a	C17 H18 N3 O

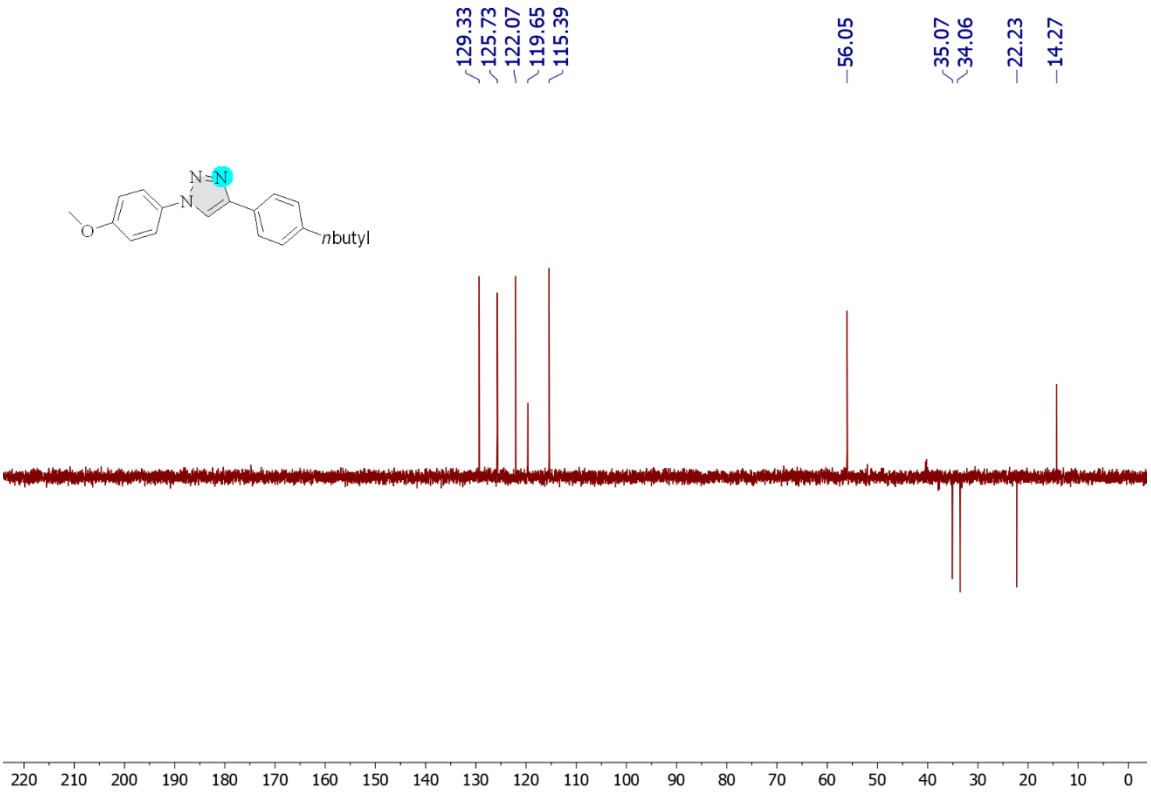
[1]H-NMR of 4-(4-Butylphenyl)-1-(4-methoxyphenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3n)



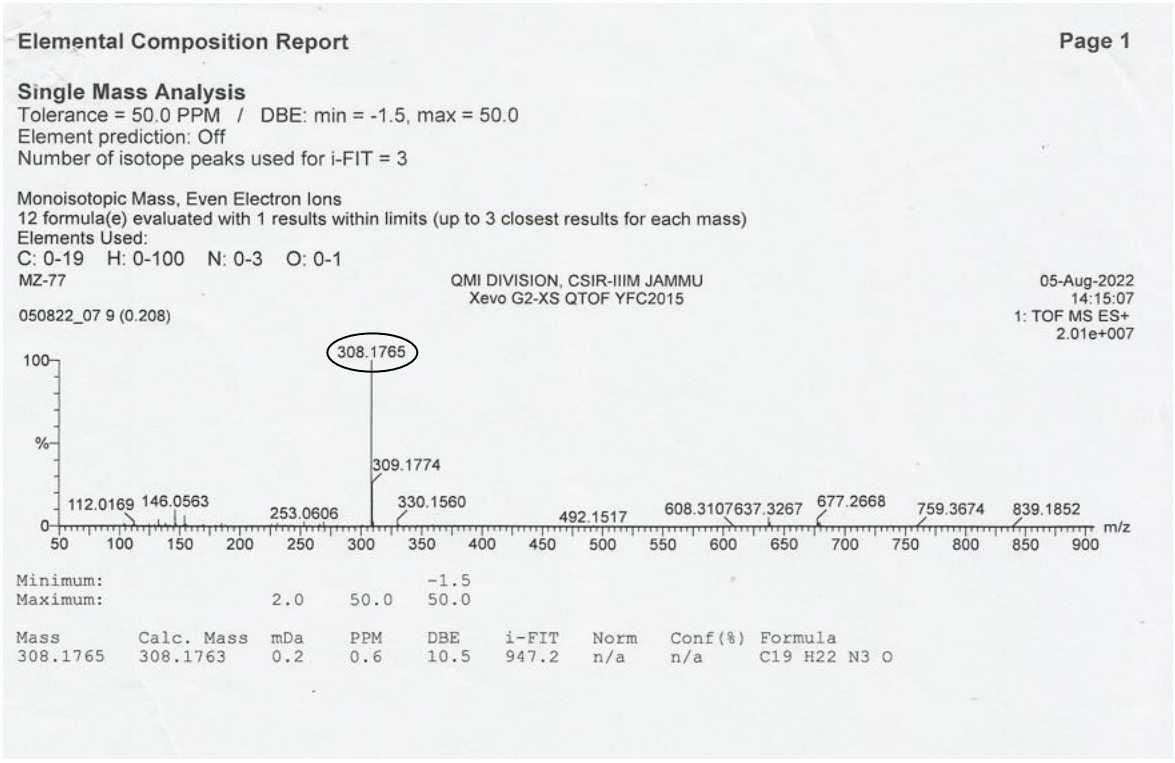
[13]C NMR of 4-(4-Butylphenyl)-1-(4-methoxyphenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3n)



DEPT of 4-(4-Butylphenyl)-1-(4-methoxyphenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3n)



HRMS of 4-(4-Butylphenyl)-1-(4-methoxyphenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3n)



Elemental Composition Report — Page 1

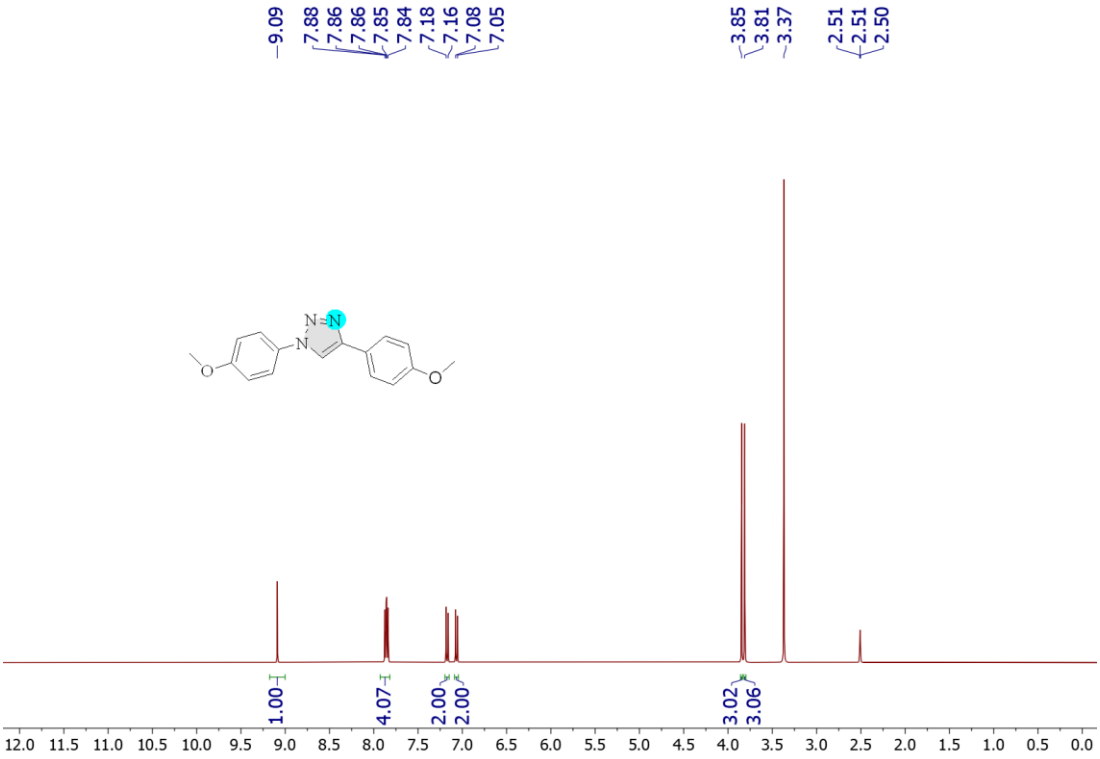
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-3 O: 0-1

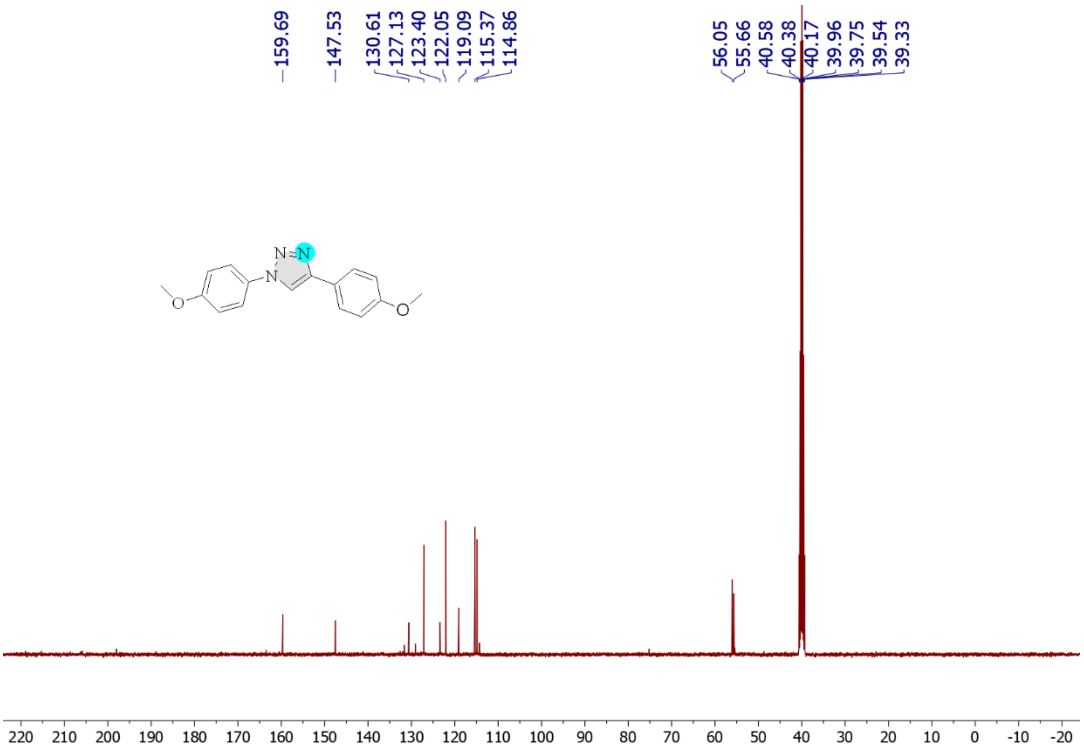
MZ-77
050822_07 9 (0.208)
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
05-Aug-2022
14:15:07
1: TOF MS ES+
2.01e+007

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
308.1765	308.1763	0.2	0.6	10.5	947.2	n/a	n/a	C19 H22 N3 O

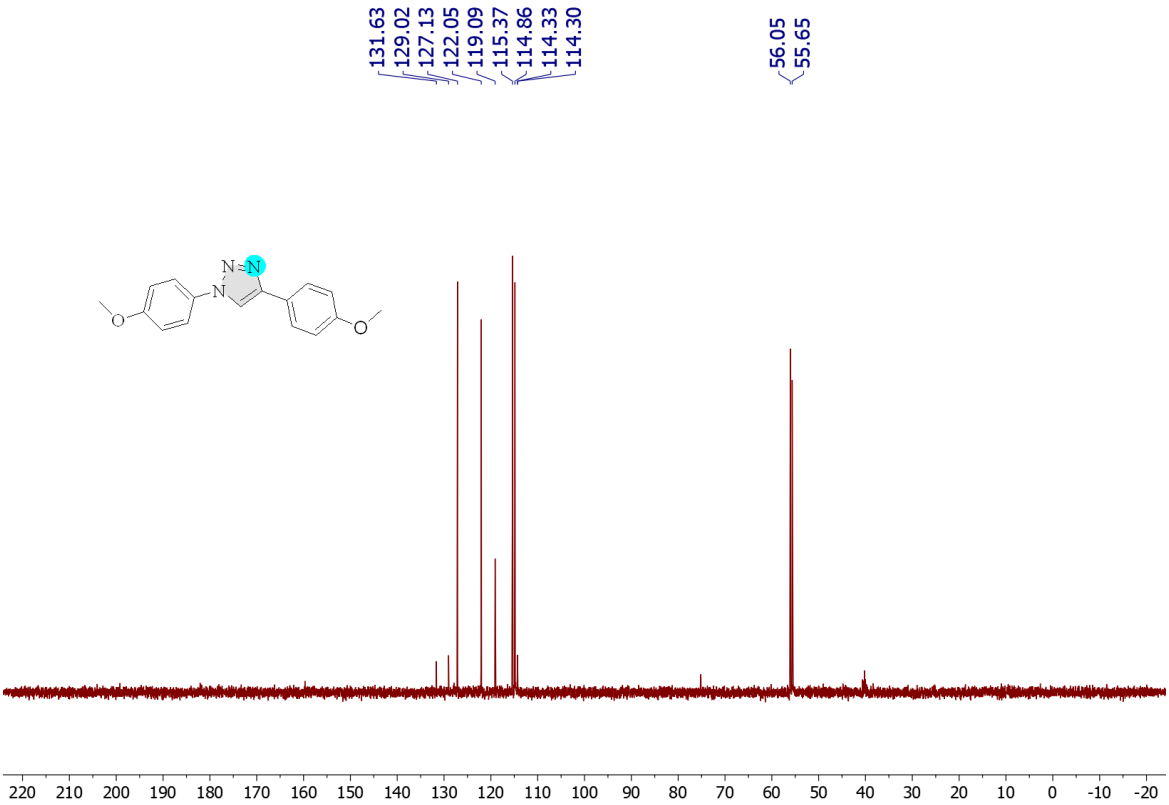
^{1}H-NMR of 1,4-Bis(4-methoxyphenyl)-1*H*-1,2,3-triazole (3o)



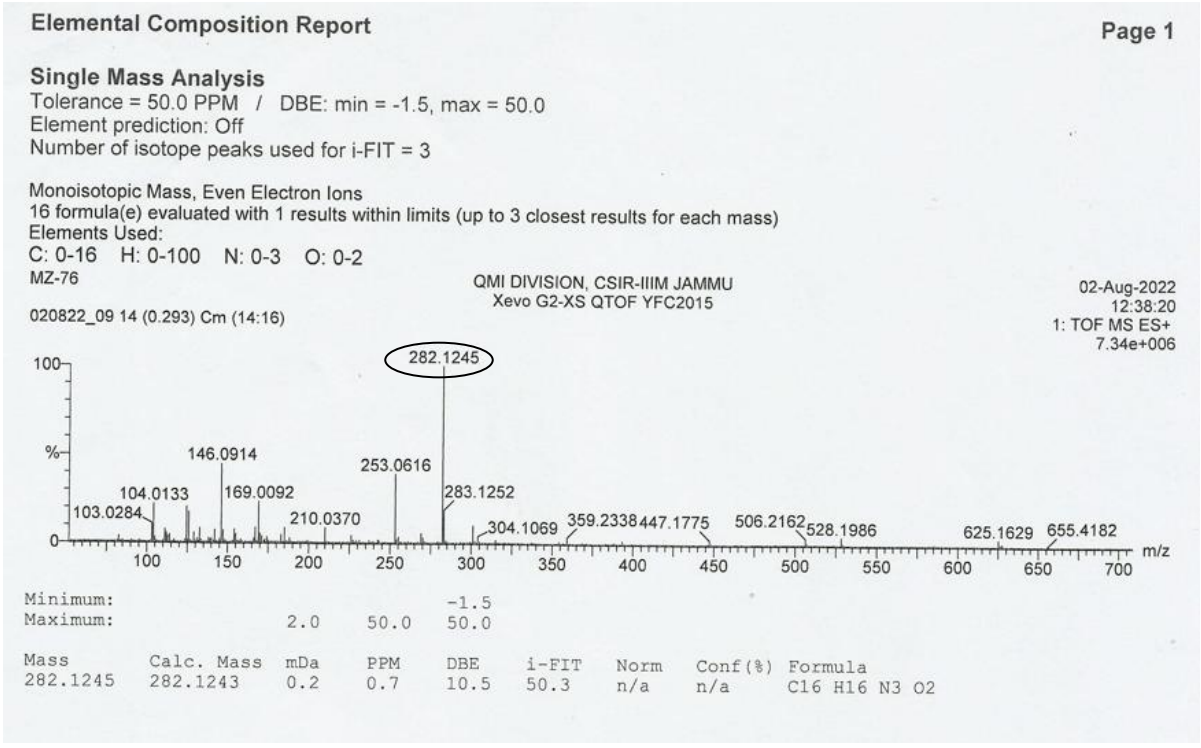
^{13}C-NMR of 1,4-Bis(4-methoxyphenyl)-1*H*-1,2,3-triazole (3o)



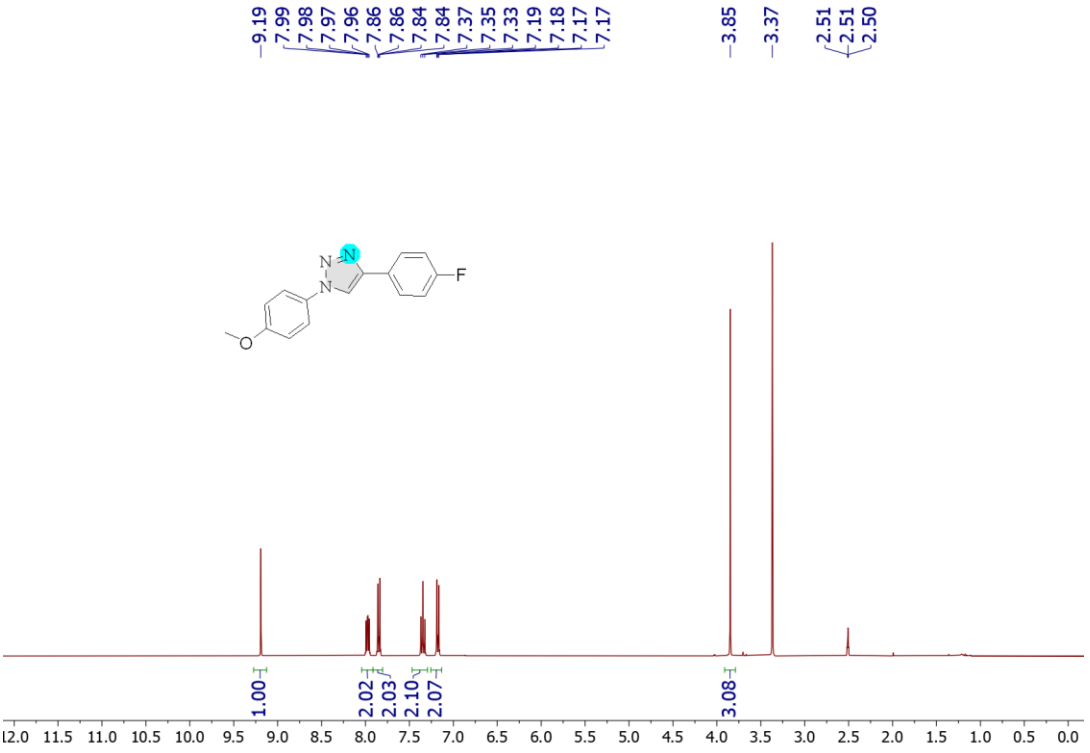
DEPT of 1,4-Bis(4-methoxyphenyl)-1*H*-1,2,3-triazole (3o)



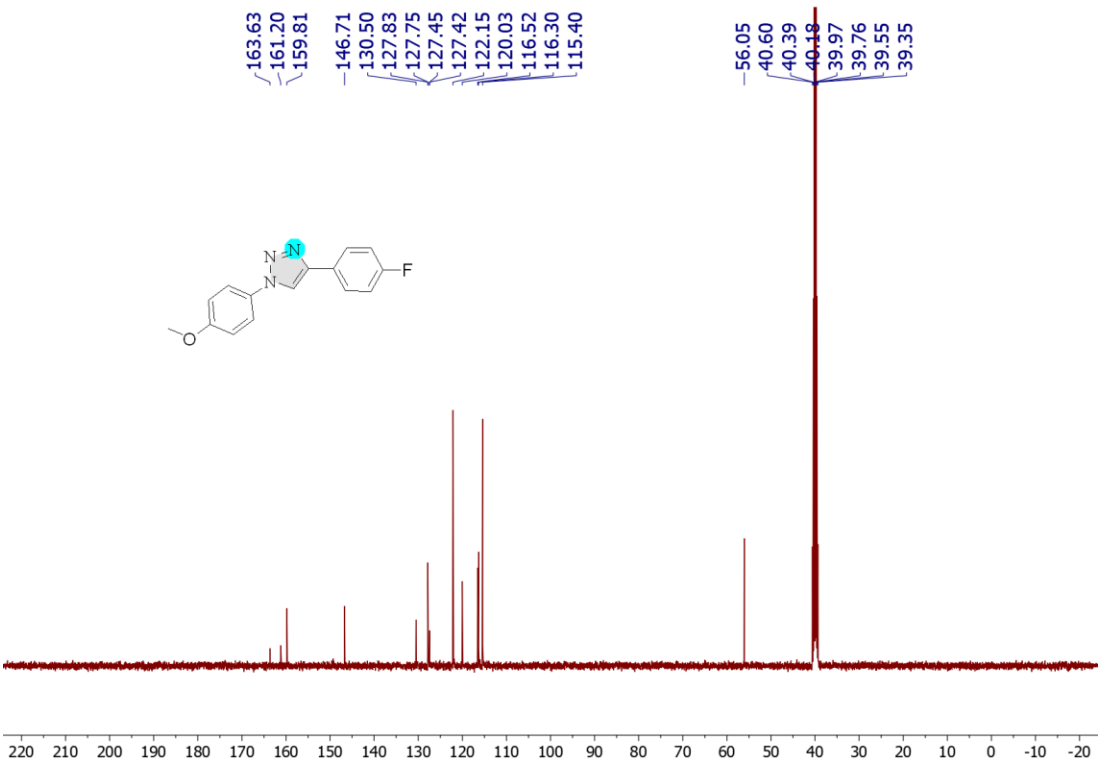
HRMS of 1,4-Bis(4-methoxyphenyl)-1*H*-1,2,3-triazole (3o)



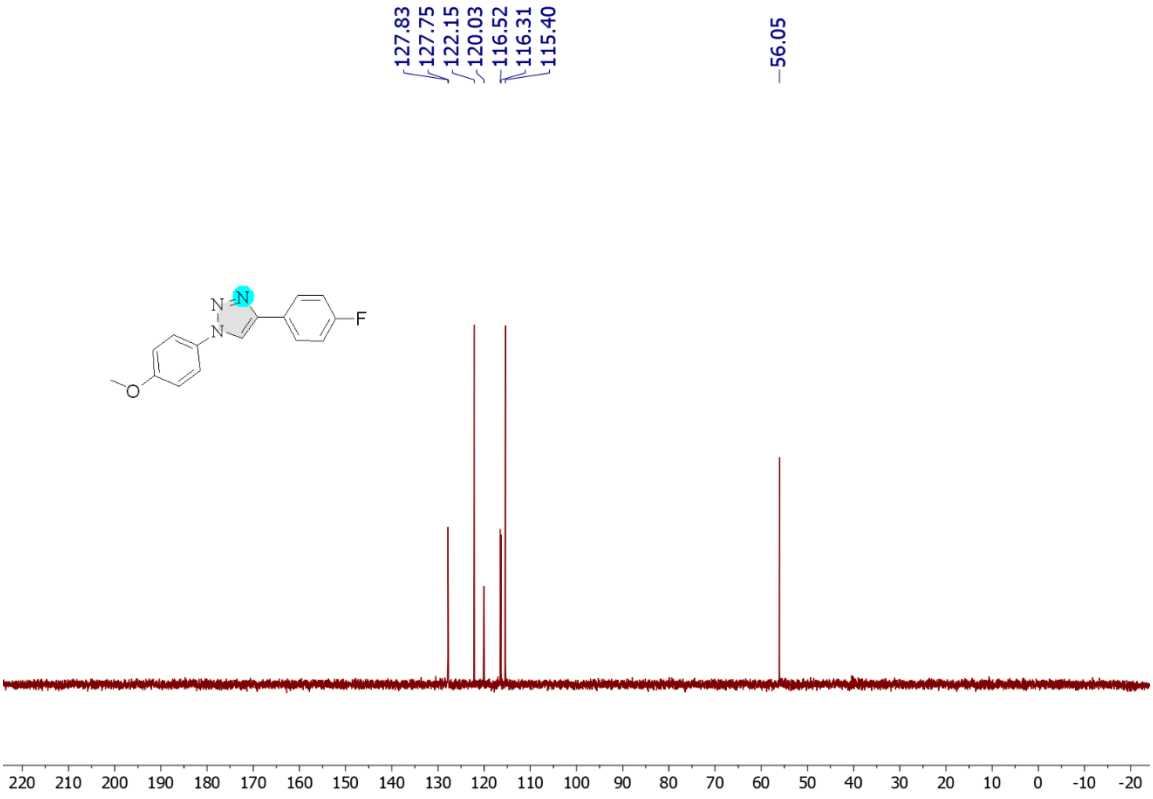
^{1}H-NMR of 4-(4-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3p)



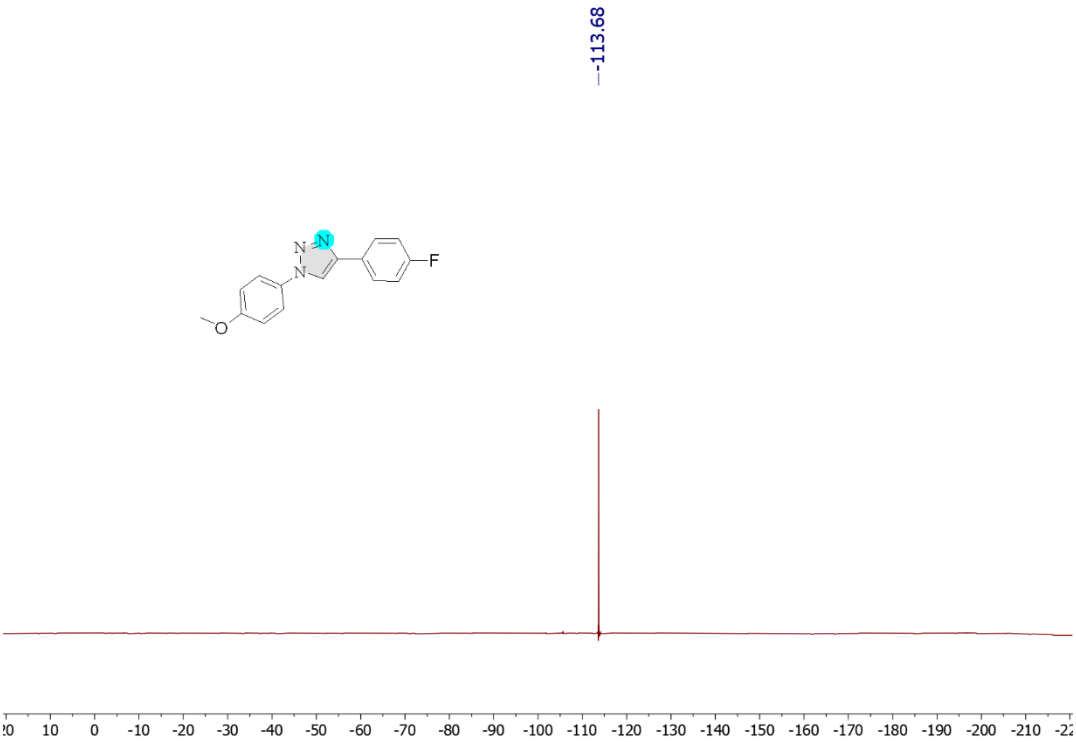
^{13}C-NMR of 4-(4-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3p)



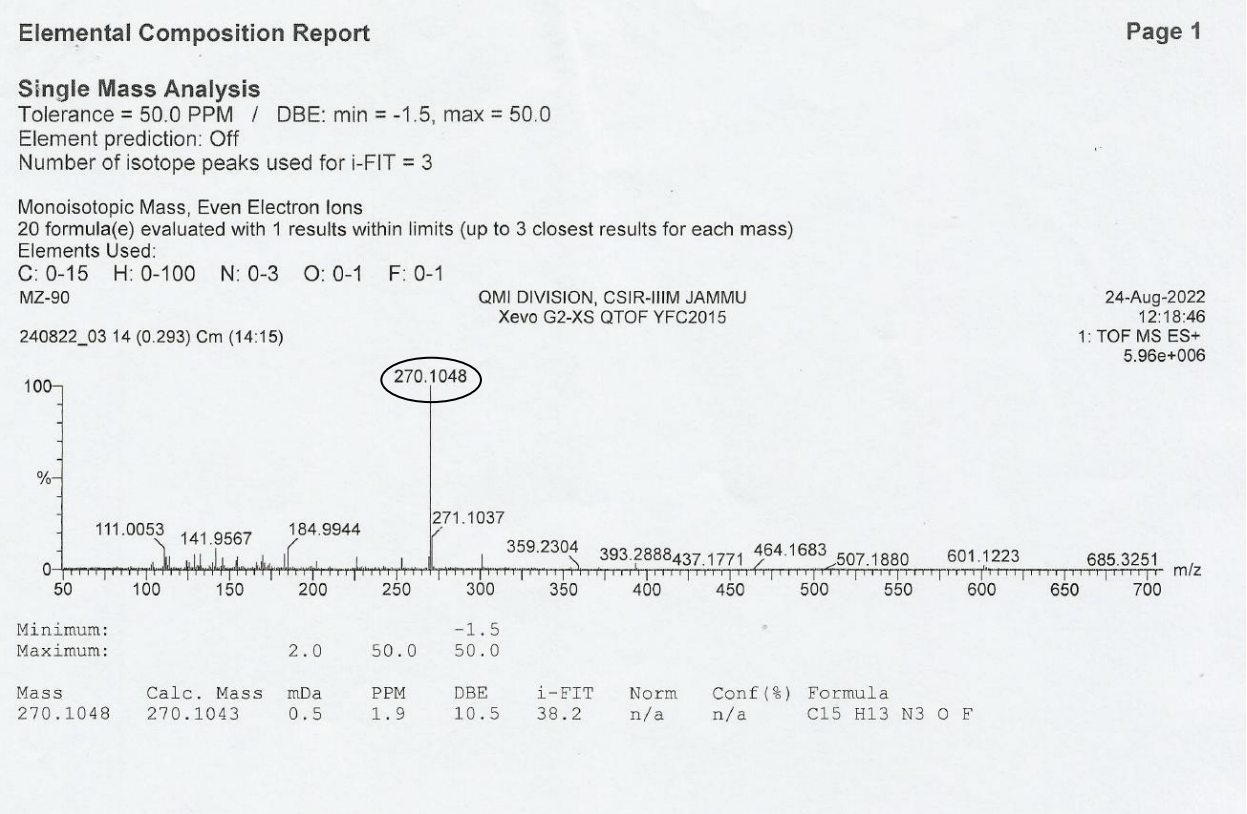
DEPT of 4-(4-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3p)



^{19}F-NMR of 4-(4-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3p)



HRMS of 4-(4-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3p)



Elemental Composition Report — Page 1

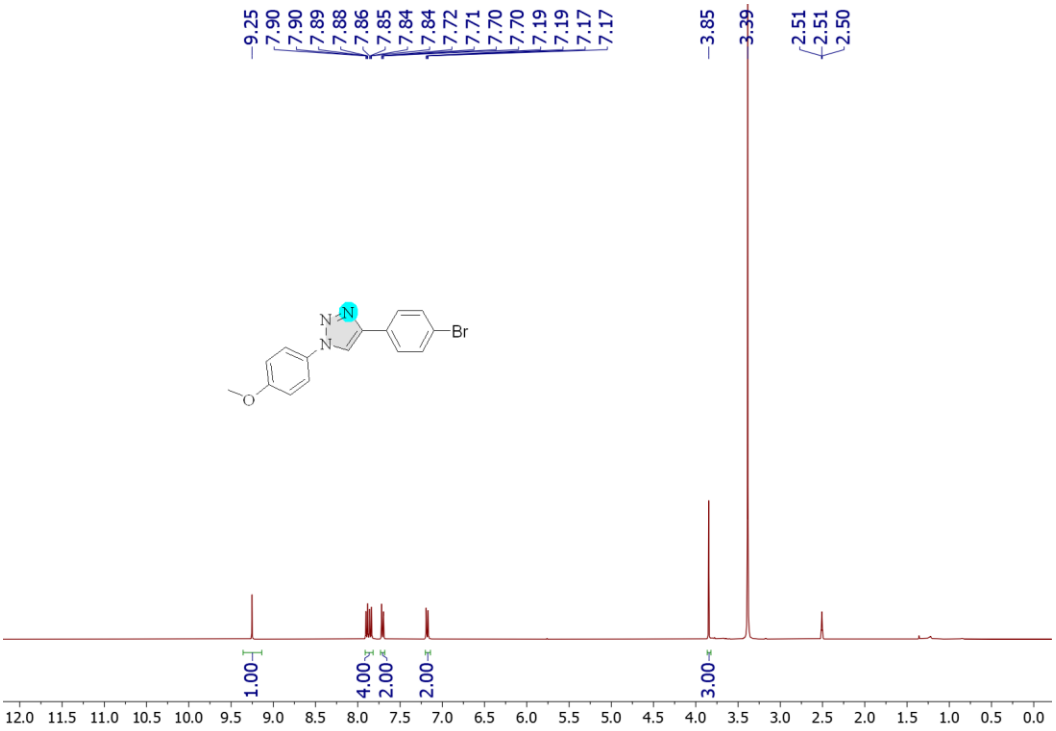
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-3 O: 0-1 F: 0-1

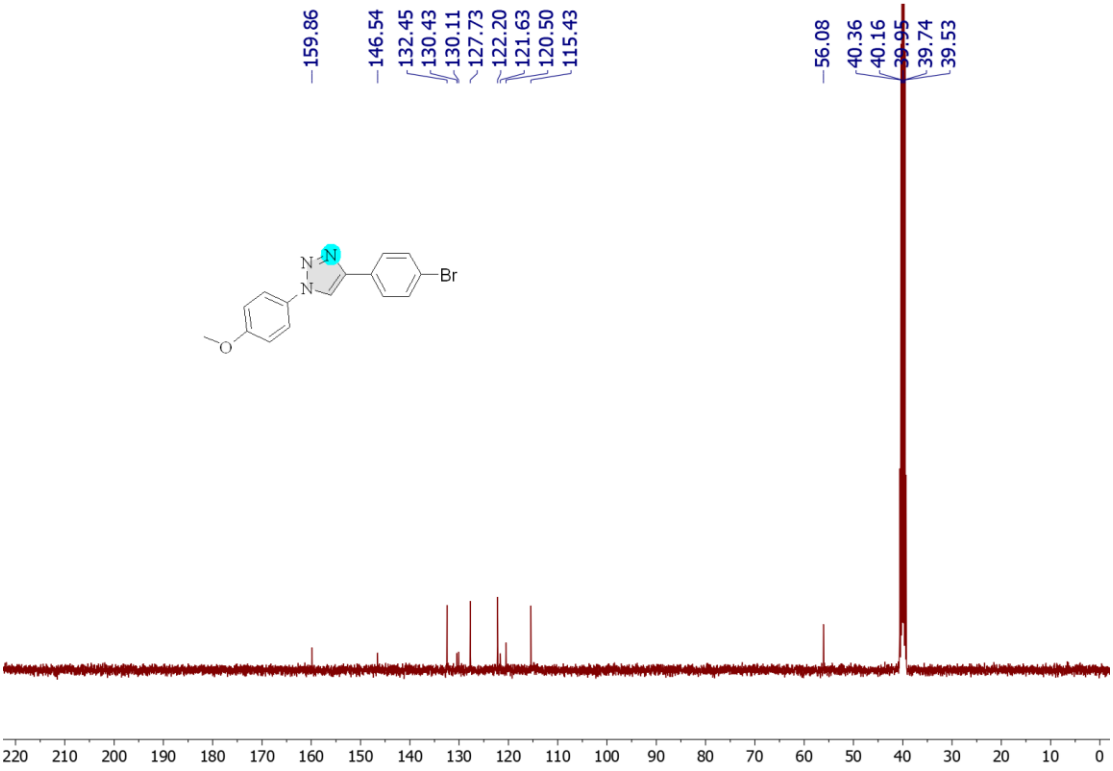
MZ-90 | QMI DIVISION, CSIR-IIIM JAMMU, Xevo G2-XS QTOF YFC2015 | 24-Aug-2022 12:18:46
240822_03 14 (0.293) Cm (14:15) | 1: TOF MS ES+ 5.96e+006

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
270.1048	270.1043	0.5	1.9	10.5	38.2	n/a	n/a	C15 H13 N3 O F

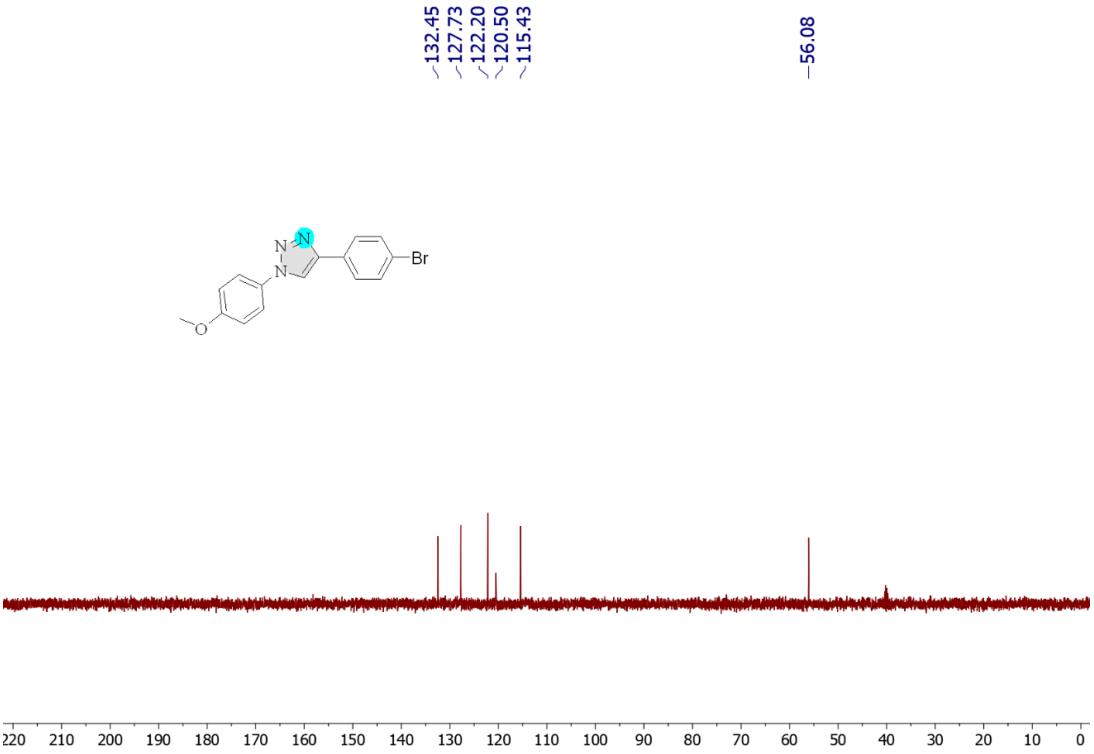
^{1}H-NMR of 4-(4-Bromophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3q)



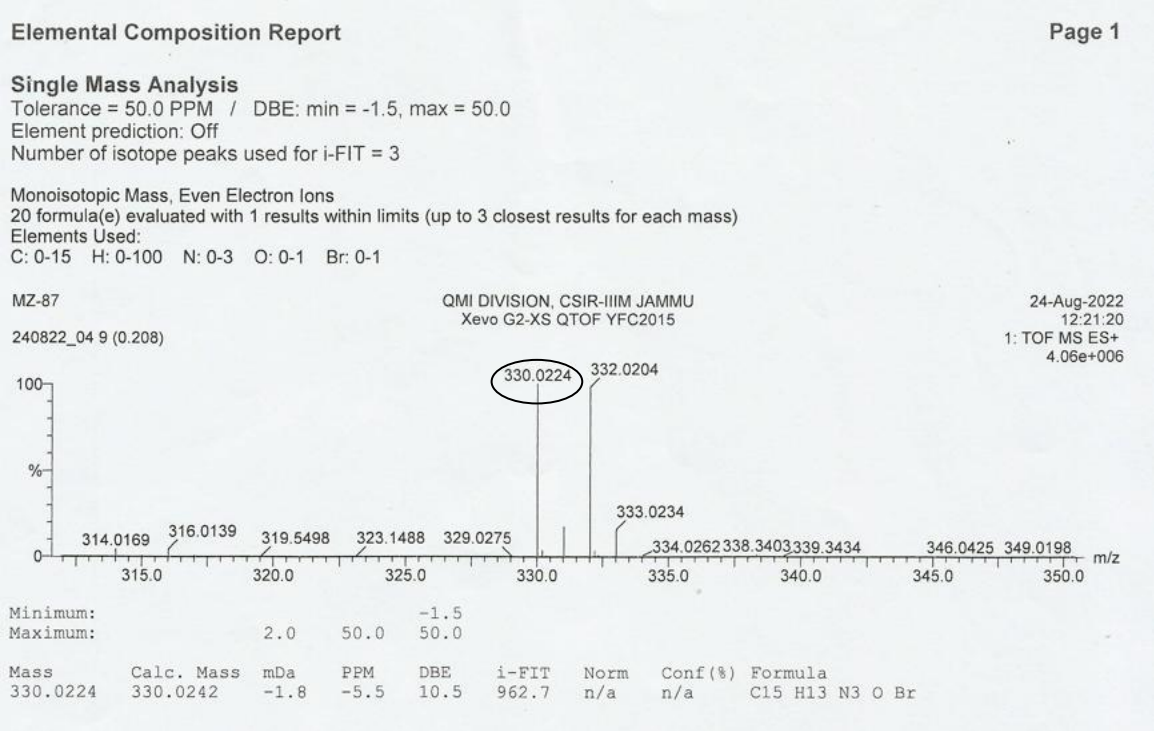
^{13}C-NMR of 4-(4-Bromophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3q)



DEPT of 4-(4-Bromophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3q)



HRMS of 4-(4-Bromophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3q)



Elemental Composition Report — Page 1

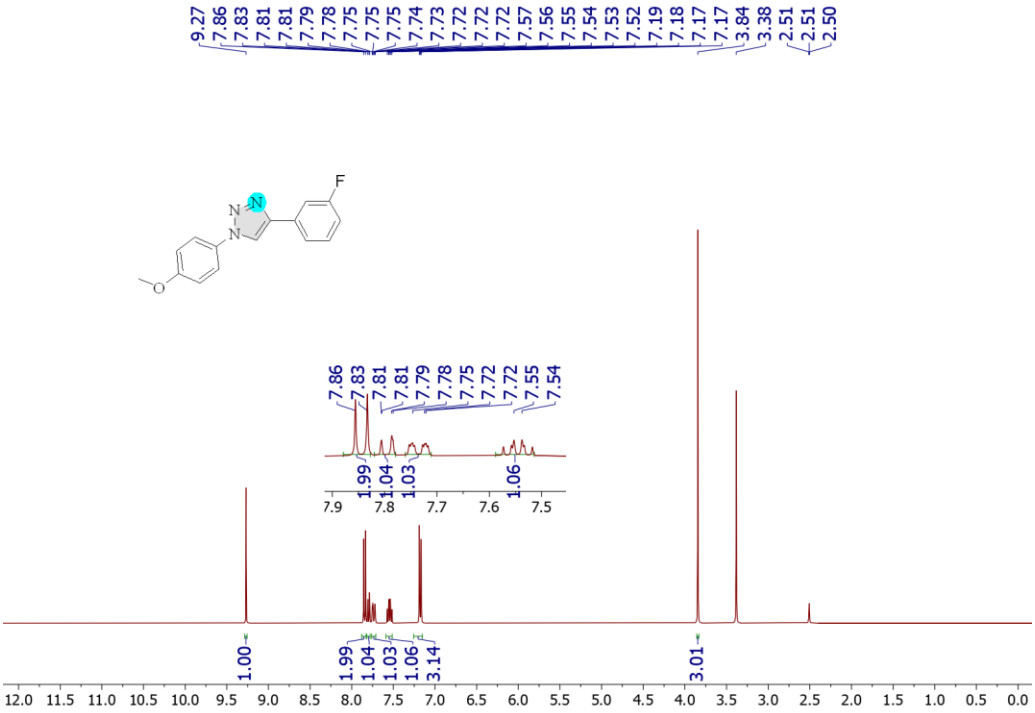
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-3 O: 0-1 Br: 0-1

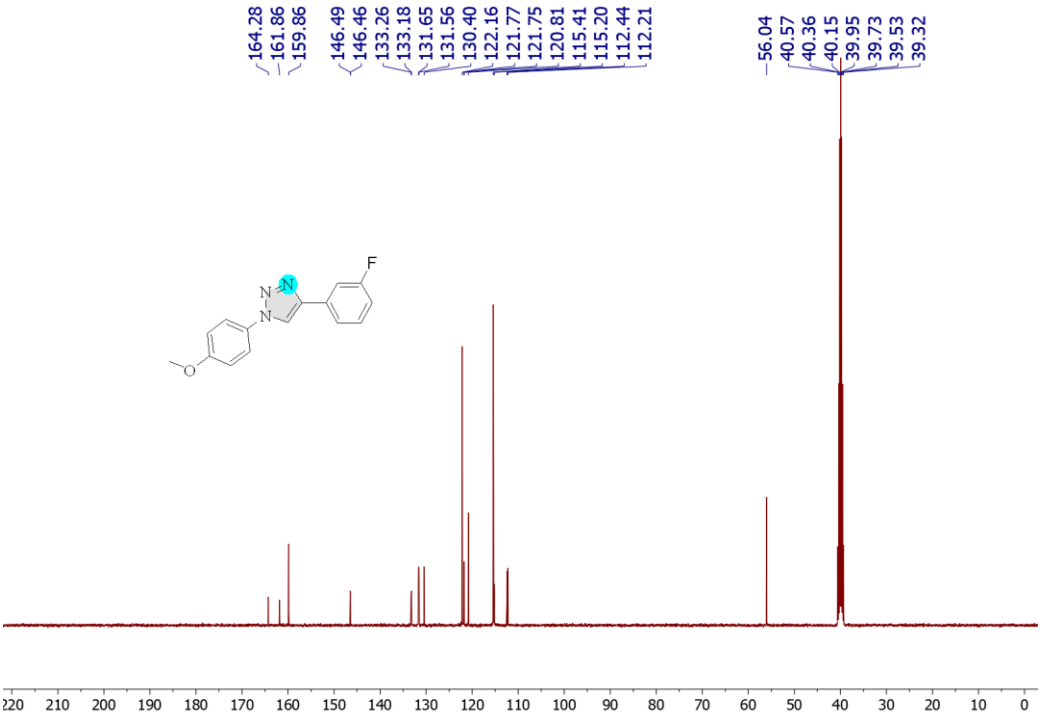
MZ-87
240822_04 9 (0.208)
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
24-Aug-2022
12:21:20
1: TOF MS ES+
4.06e+006

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
330.0224	330.0242	-1.8	-5.5	10.5	962.7	n/a	n/a	C15 H13 N3 O Br

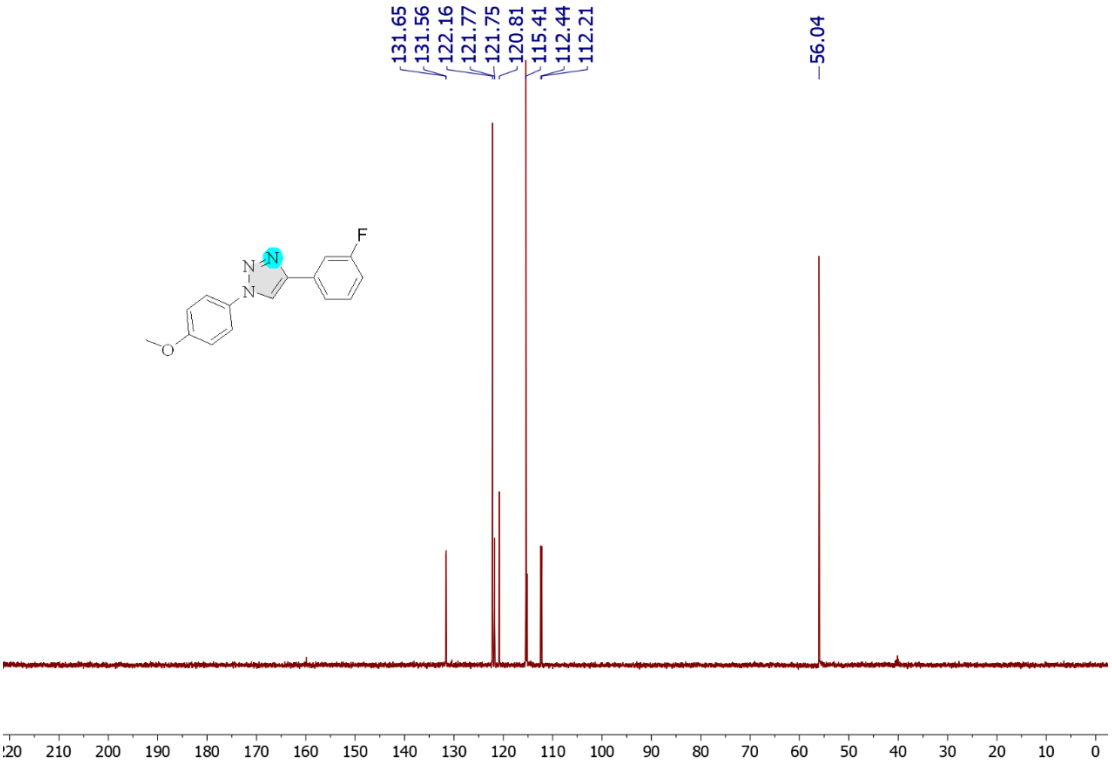
^{1}H-NMR of 4-(3-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3r)



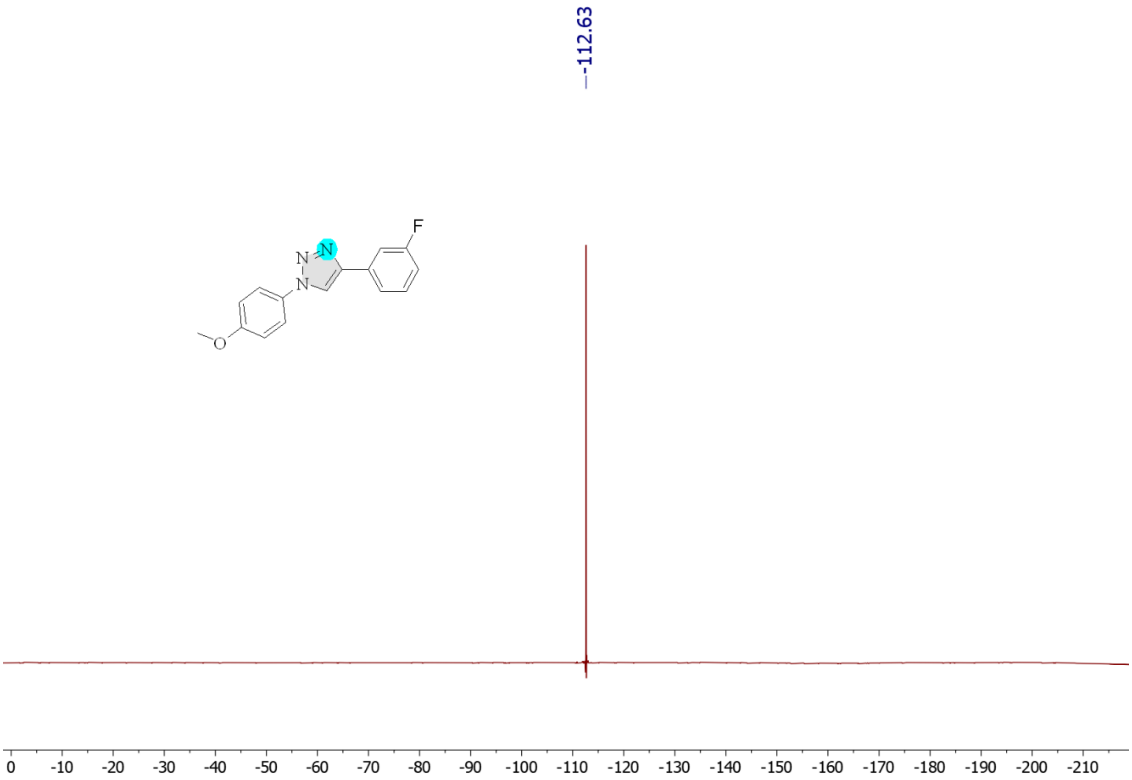
^{13}C-NMR of 4-(3-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3r)



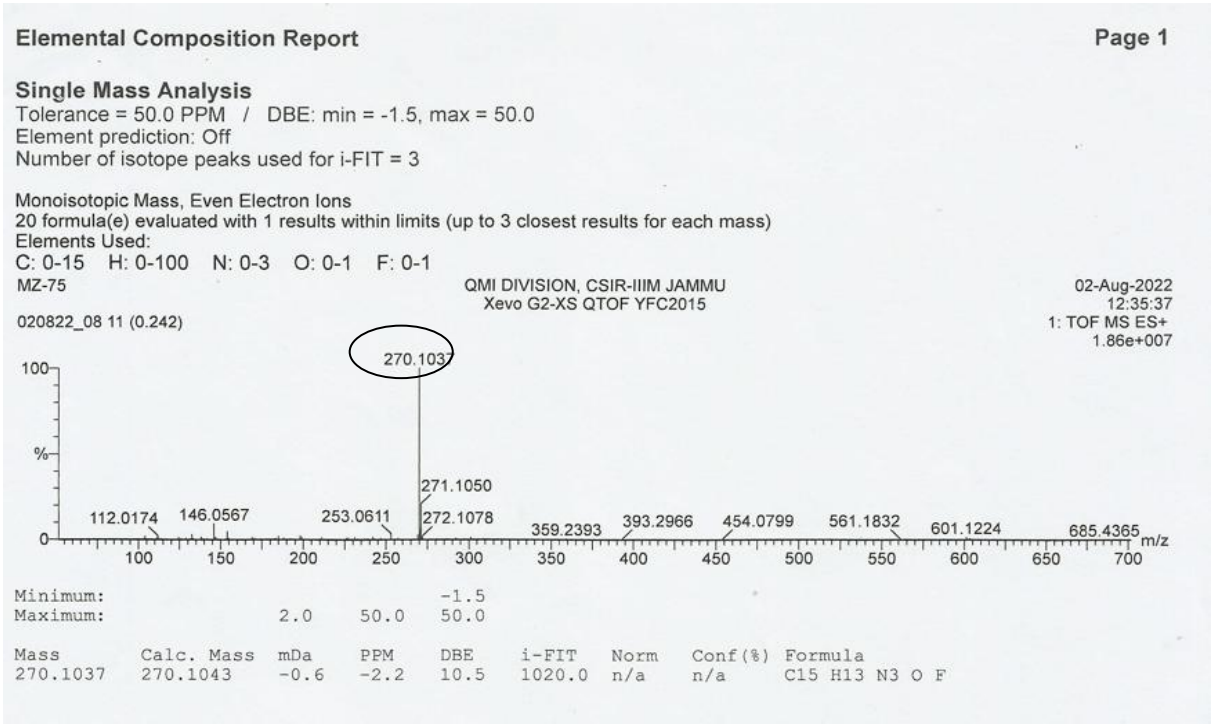
DEPT of 4-(3-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3r)



^{19}F-NMR of 4-(3-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3r)



HRMS of 4-(3-Fluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3r)



Elemental Composition Report — Page 1

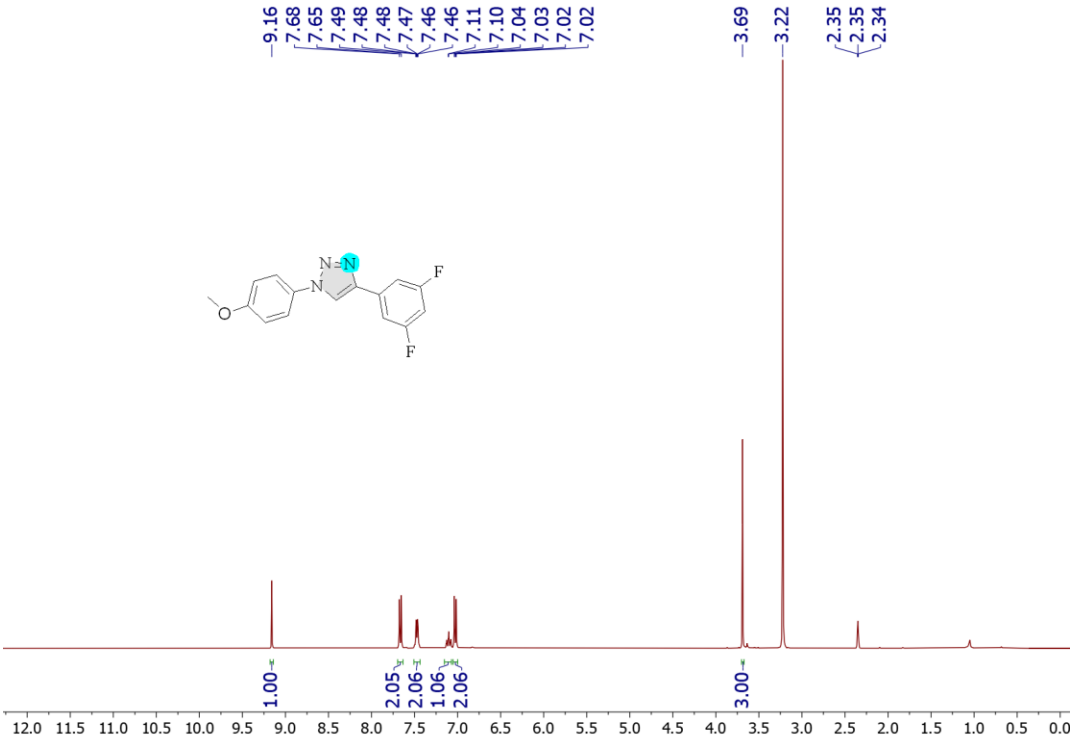
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-3 O: 0-1 F: 0-1

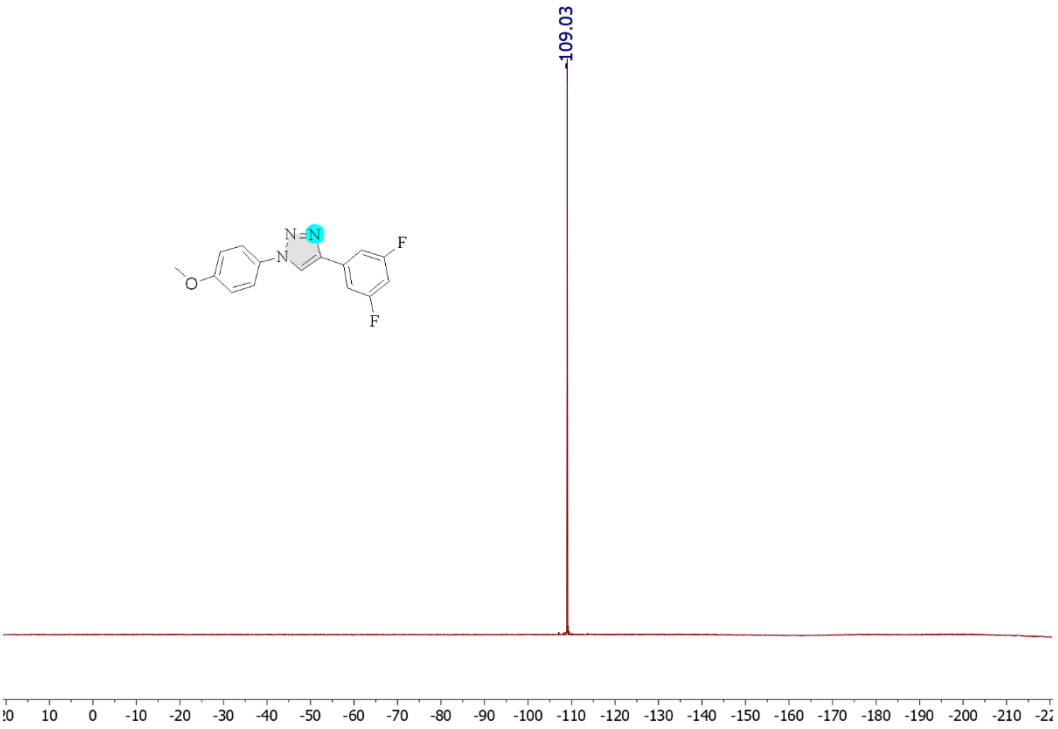
MZ-75 — QMI DIVISION, CSIR-IIIM JAMMU — Xevo G2-XS QTOF YFC2015 — 02-Aug-2022 12:35:37
020822_08 11 (0.242) — 1: TOF MS ES+ 1.86e+007

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
270.1037	270.1043	-0.6	-2.2	10.5	1020.0	n/a	n/a	C15 H13 N3 O F

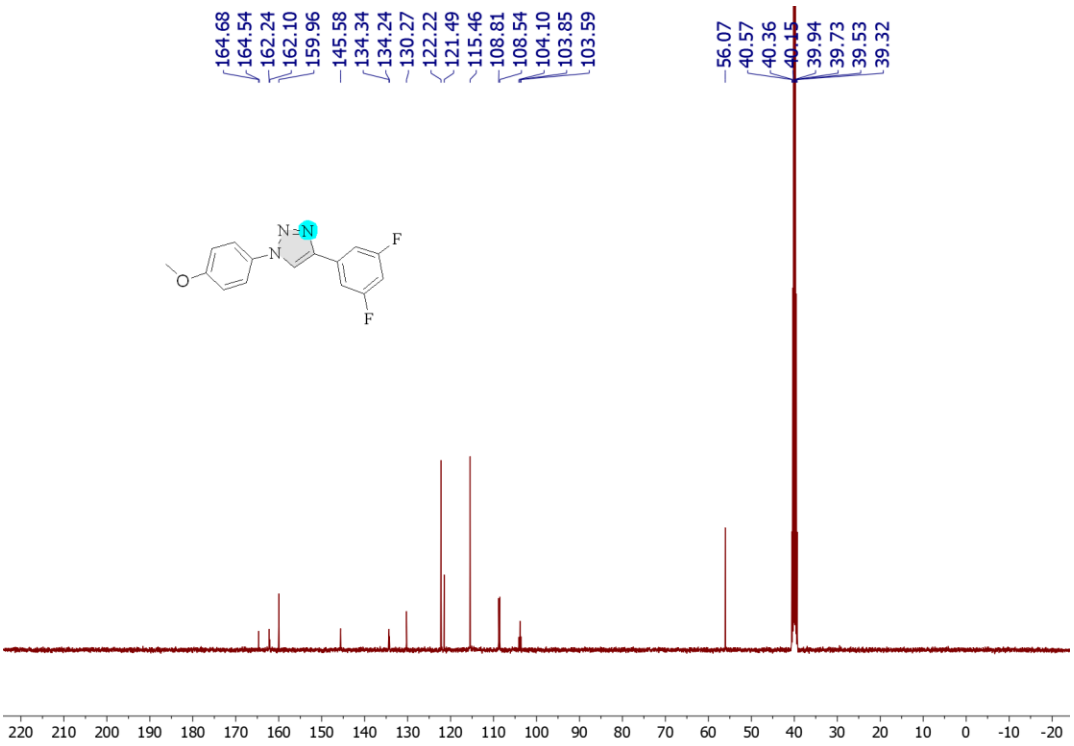
^{1}H-NMR of 4-(3,5-Difluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3s)



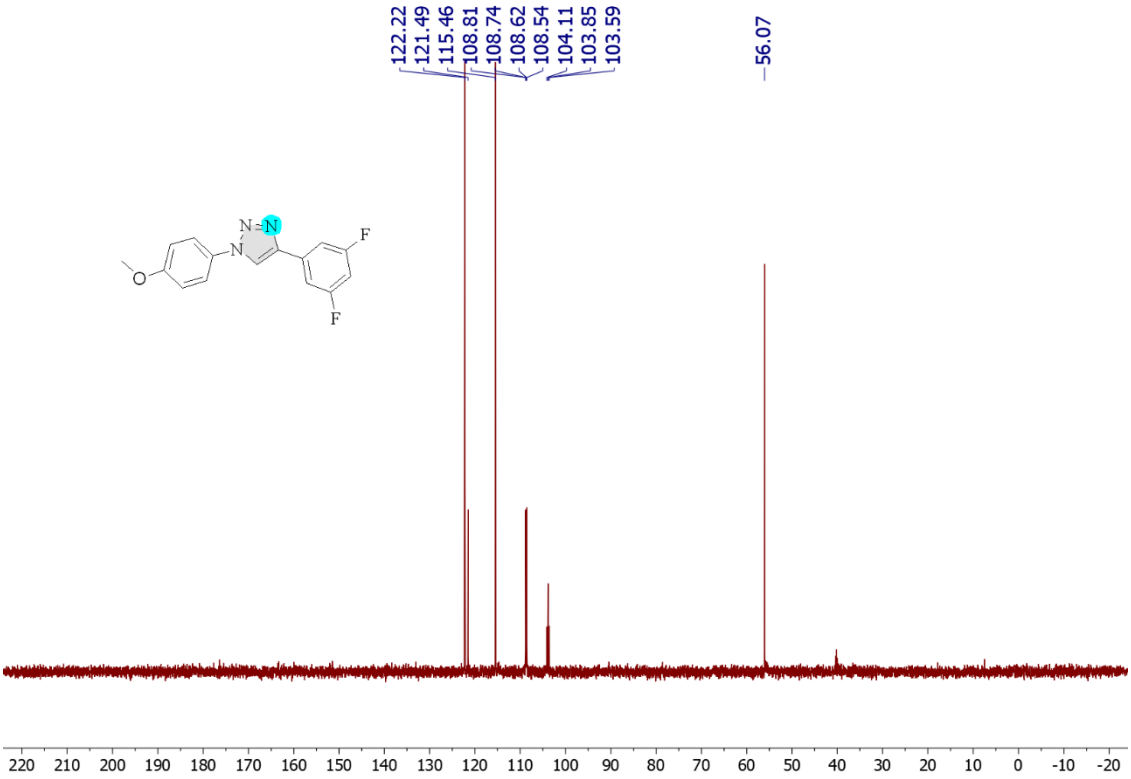
^{19}F-NMR of 4-(3,5-Difluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3s)



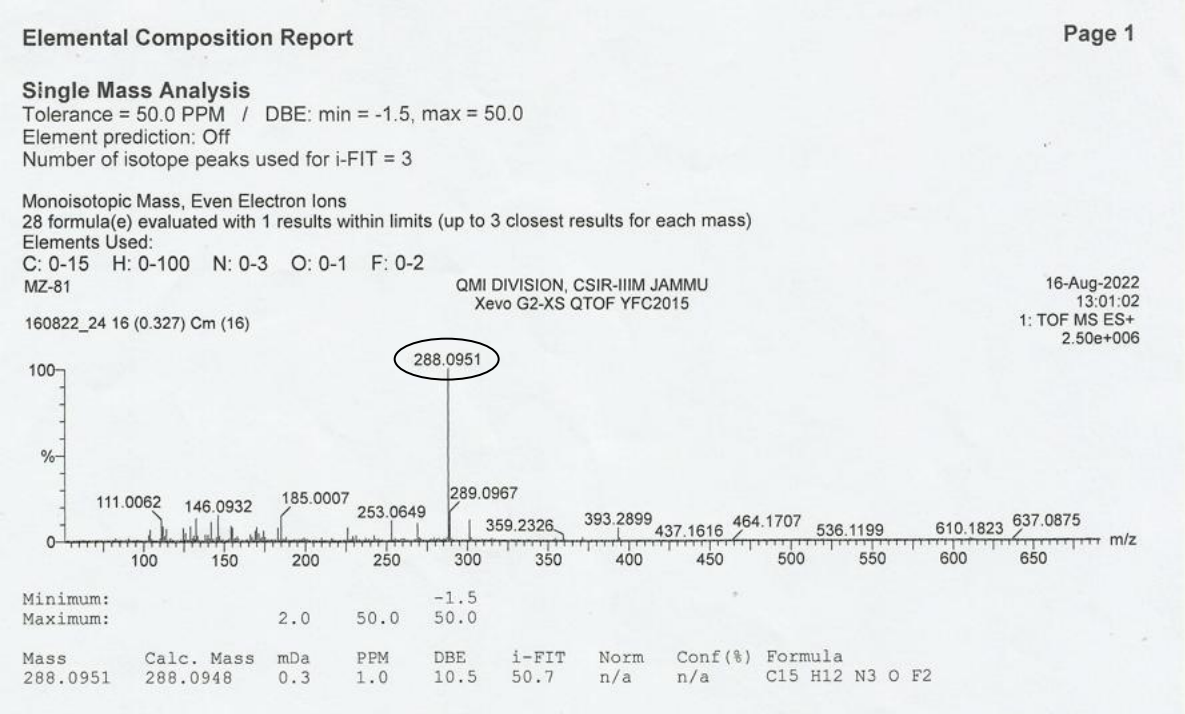
^{13}C-NMR of 4-(3,5-Difluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3s)



DEPT of 4-(3,5-Difluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3s)



HRMS of 4-(3,5-Difluorophenyl)-1-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3s)



Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-3 O: 0-1 F: 0-2

MZ-81

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

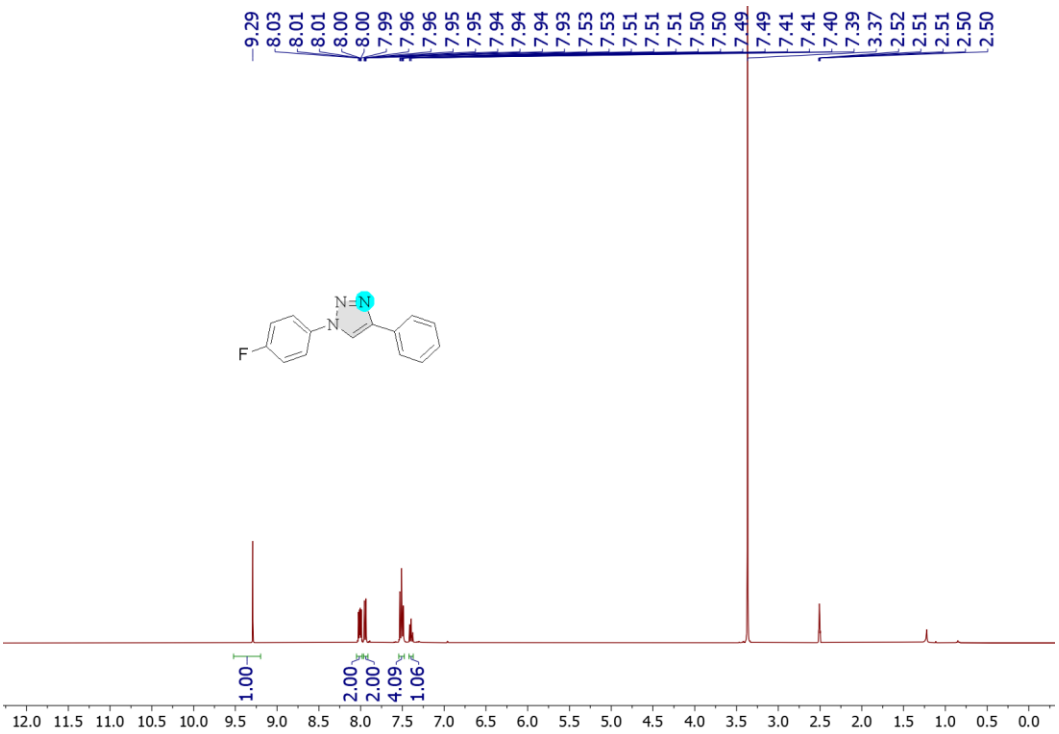
16-Aug-2022
13:01:02
1: TOF MS ES+
2.50e+006

160822_24 16 (0.327) Cm (16)

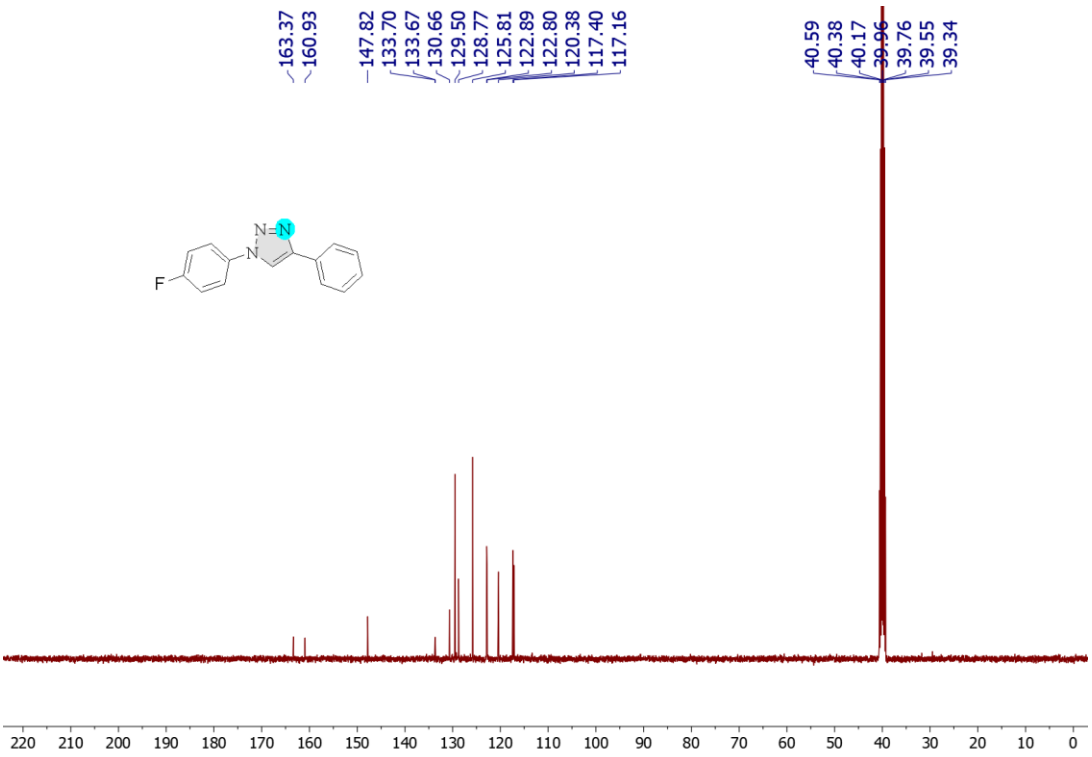
288.0951
111.0062
146.0932
185.0007
253.0649
289.0967
359.2326
393.2899
437.1616
464.1707
536.1199
610.1823
637.0875
m/z

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
288.0951	288.0948	0.3	1.0	10.5	50.7	n/a	n/a	C15 H12 N3 O F2

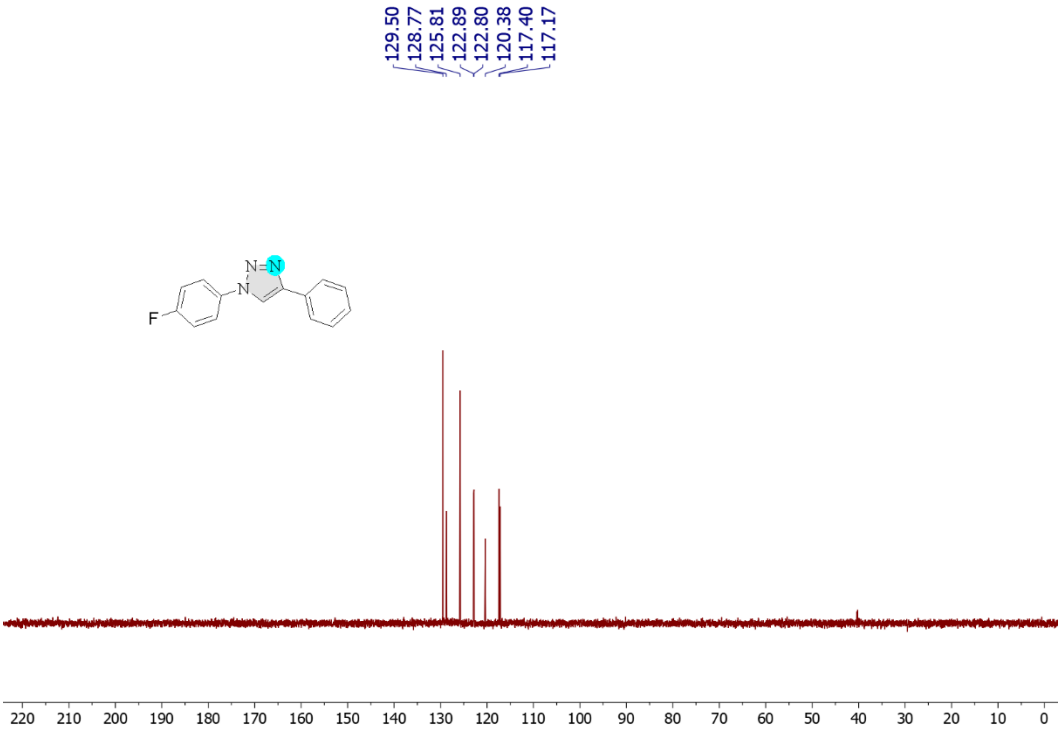
^{1}H-NMR of 1-(4-Fluorophenyl)-4-phenyl-1*H*-1,2,3-triazole (3t)



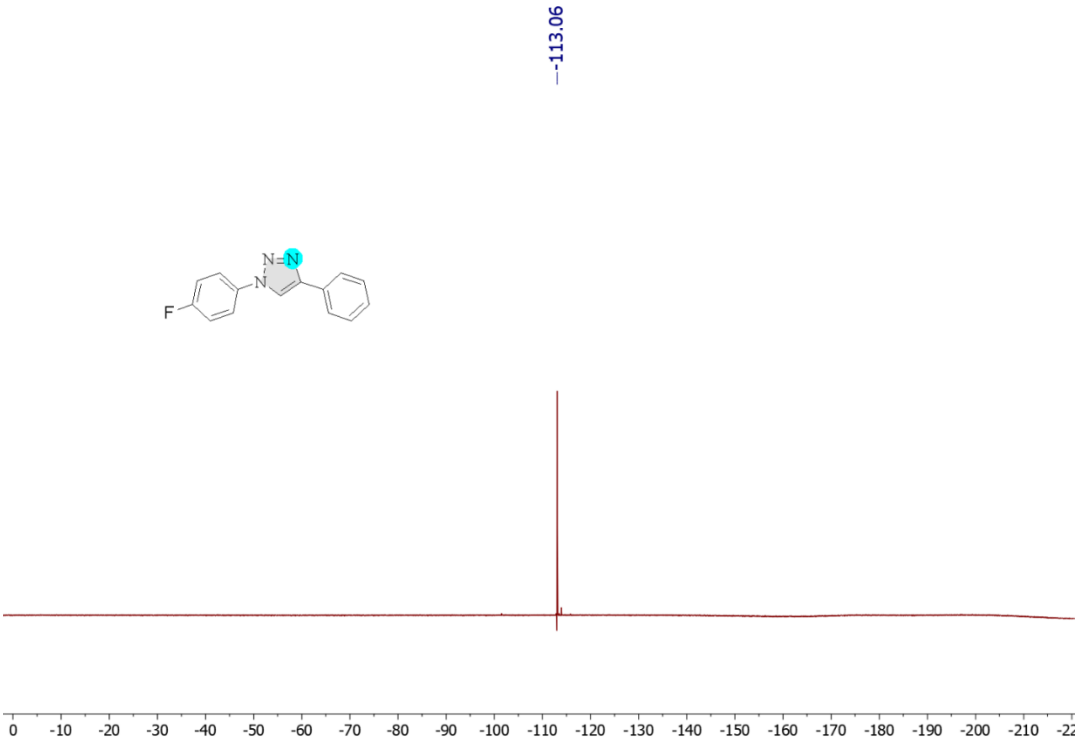
^{13}C-NMR of 1-(4-Fluorophenyl)-4-phenyl-1*H*-1,2,3-triazole (3t)



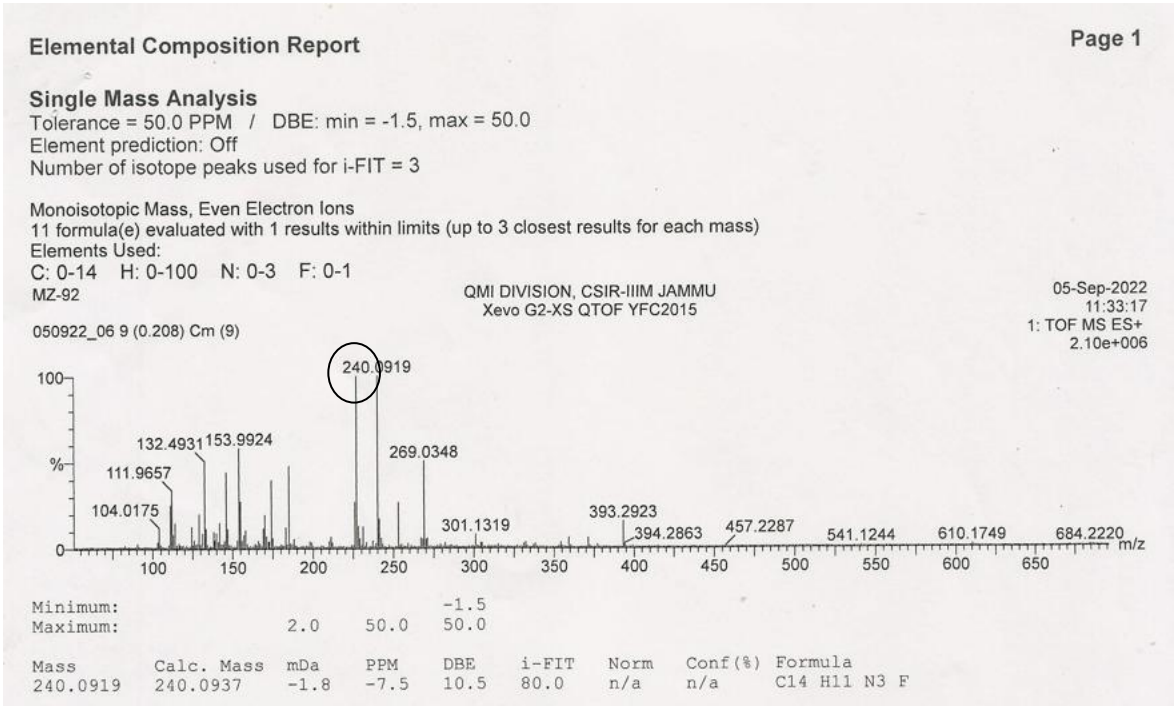
DEPT of 1-(4-Fluorophenyl)-4-phenyl-1*H*-1,2,3-triazole (3t)



^{19}F of 1-(4-Fluorophenyl)-4-phenyl-1*H*-1,2,3-triazole (3t)



HRMS of 1-(4-Fluorophenyl)-4-phenyl-1*H*-1,2,3-triazole (3t)



Elemental Composition Report Page 1

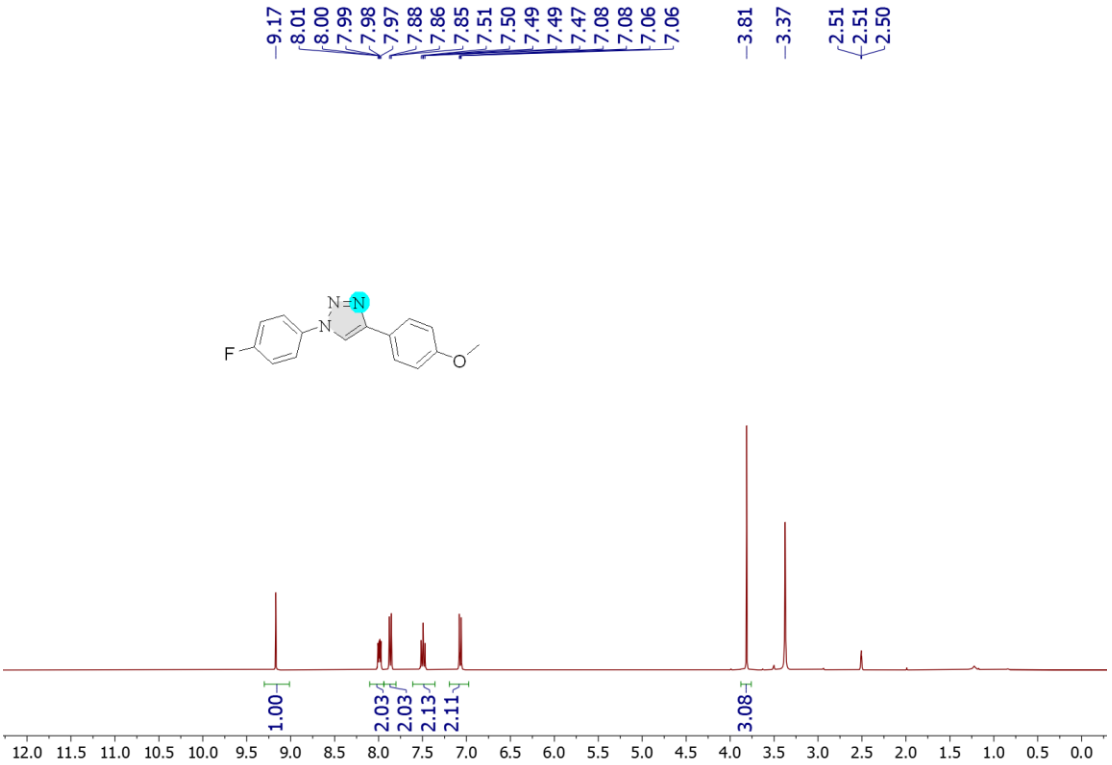
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 F: 0-1

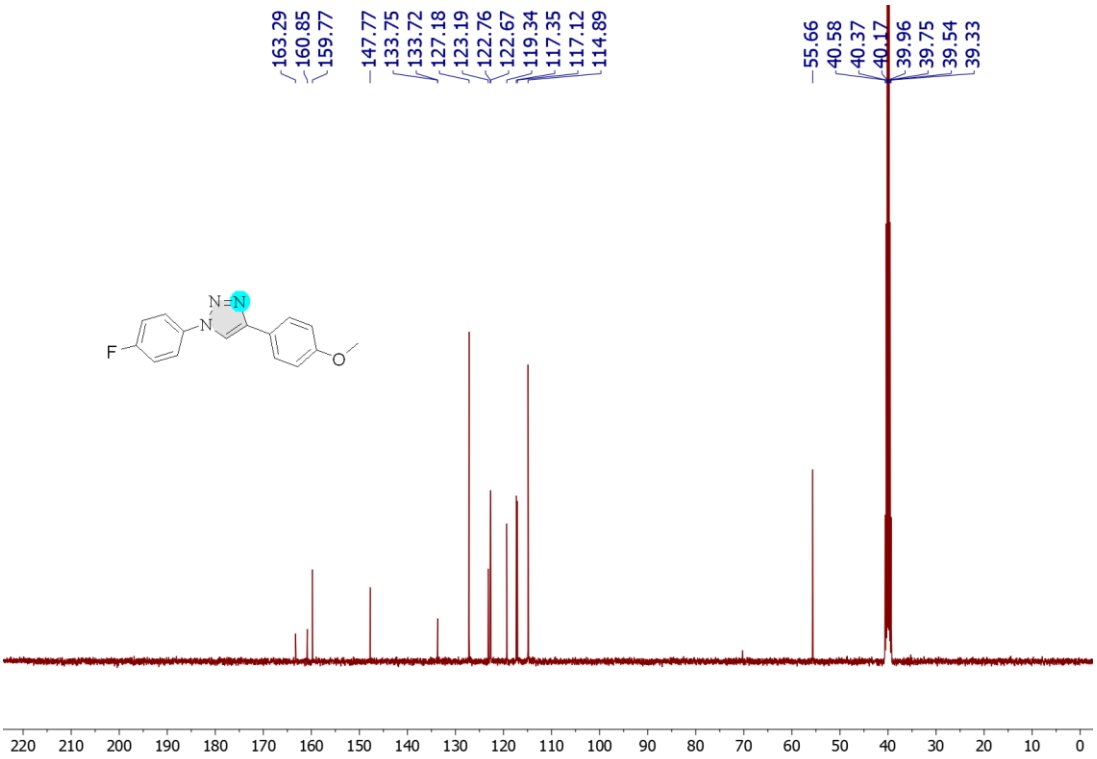
MZ-92
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
05-Sep-2022
11:33:17
1: TOF MS ES+
2.10e+006
050922_06 9 (0.208) Cm (9)

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
240.0919	240.0937	-1.8	-7.5	10.5	80.0	n/a	n/a	C14 H11 N3 F

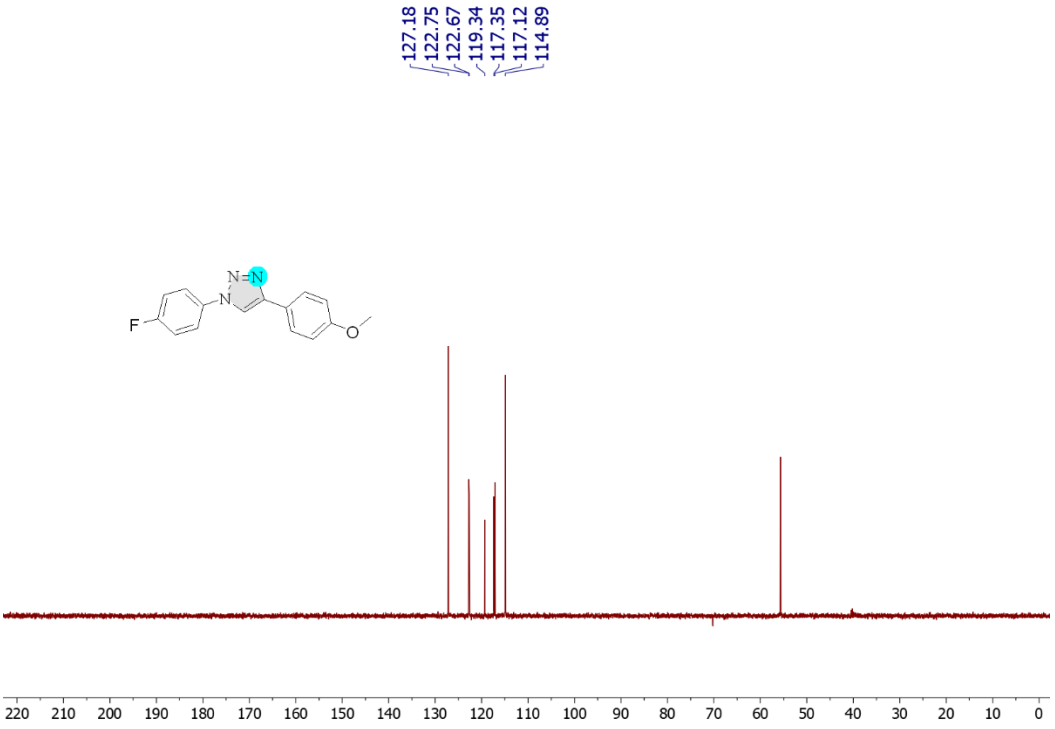
^{1}H-NMR of 1-(4-Fluorophenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3u)



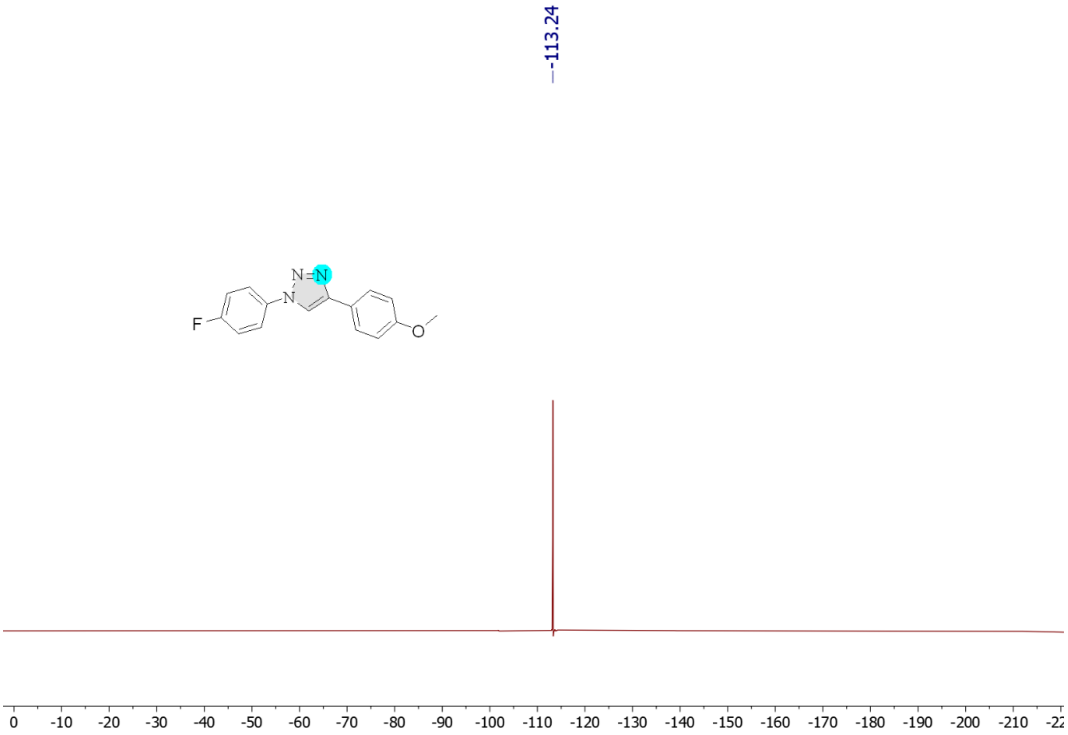
^{13}C-NMR of 1-(4-Fluorophenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3u)



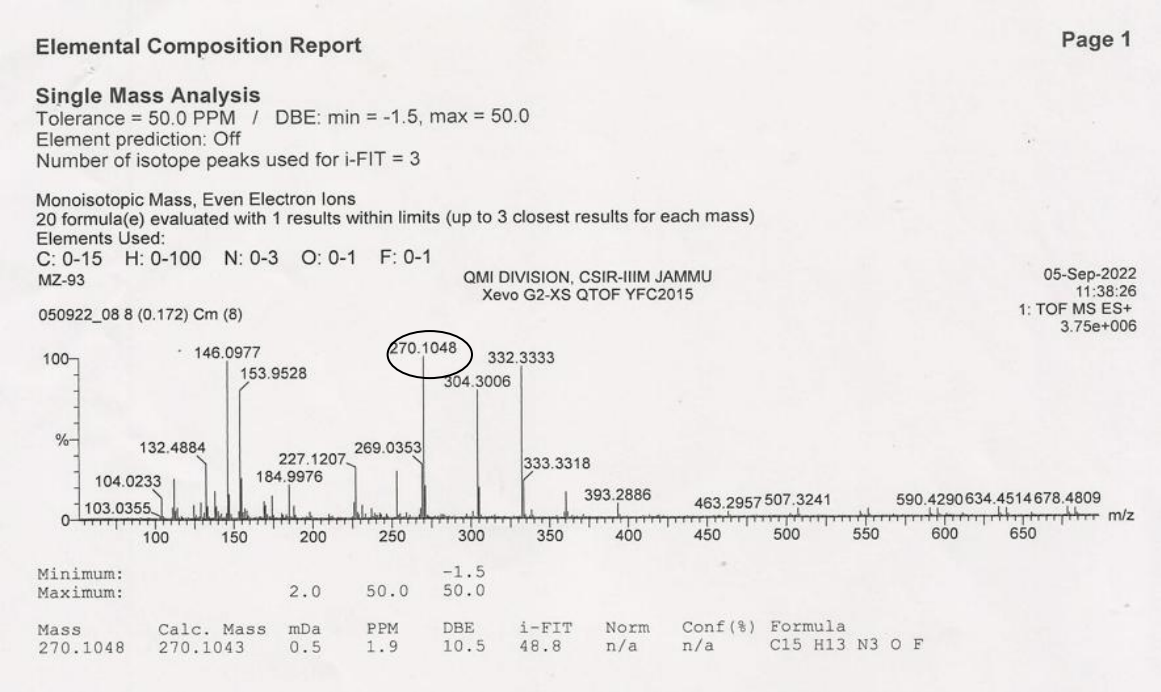
DEPT of 1-(4-Fluorophenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3u)



^{19}F of 1-(4-Fluorophenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3u)



HRMS of 1-(4-Fluorophenyl)-4-(4-methoxyphenyl)-1*H*-1,2,3-triazole (3u)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-3 O: 0-1 F: 0-1

MZ-93

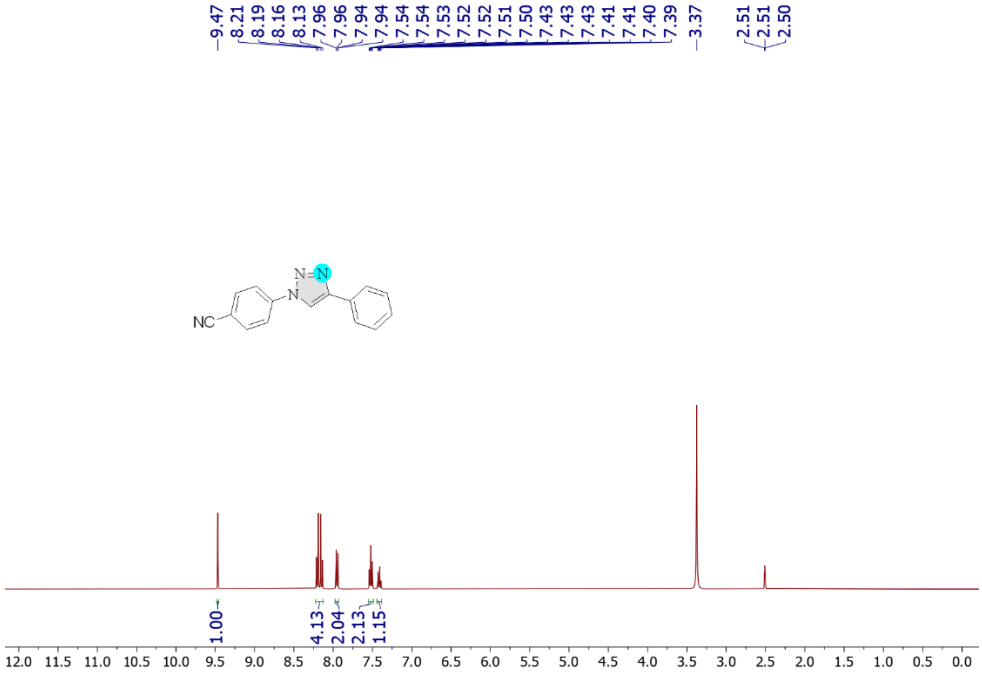
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

05-Sep-2022
11:38:26
1: TOF MS ES+
3.75e+006

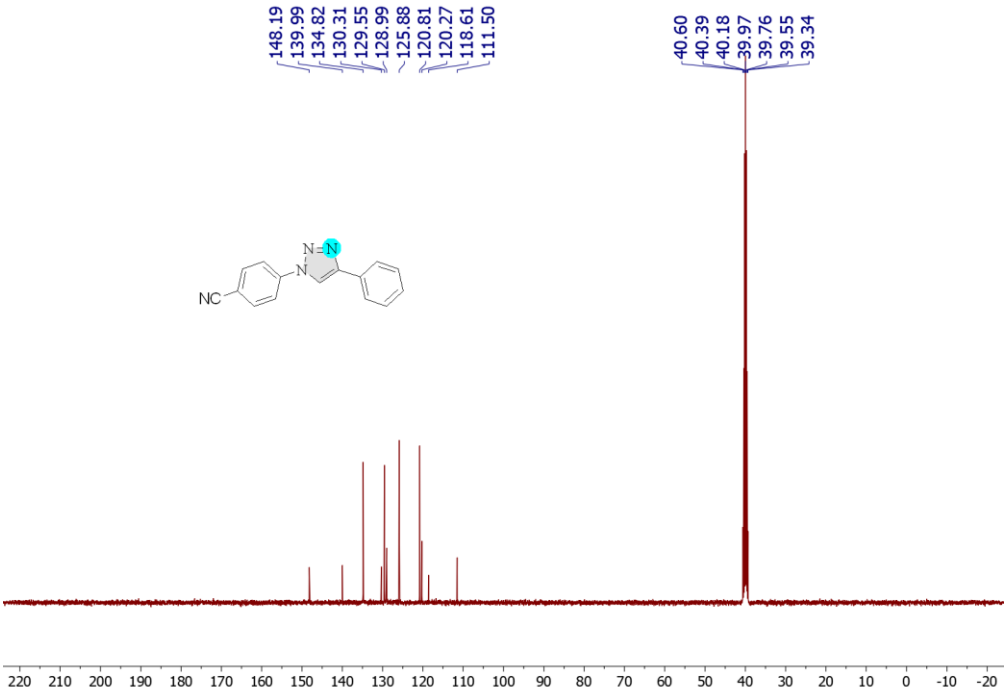
050922_08 8 (0.172) Cm (8)

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
270.1048	270.1043	0.5	1.9	10.5	48.8	n/a	n/a	C15 H13 N3 O F

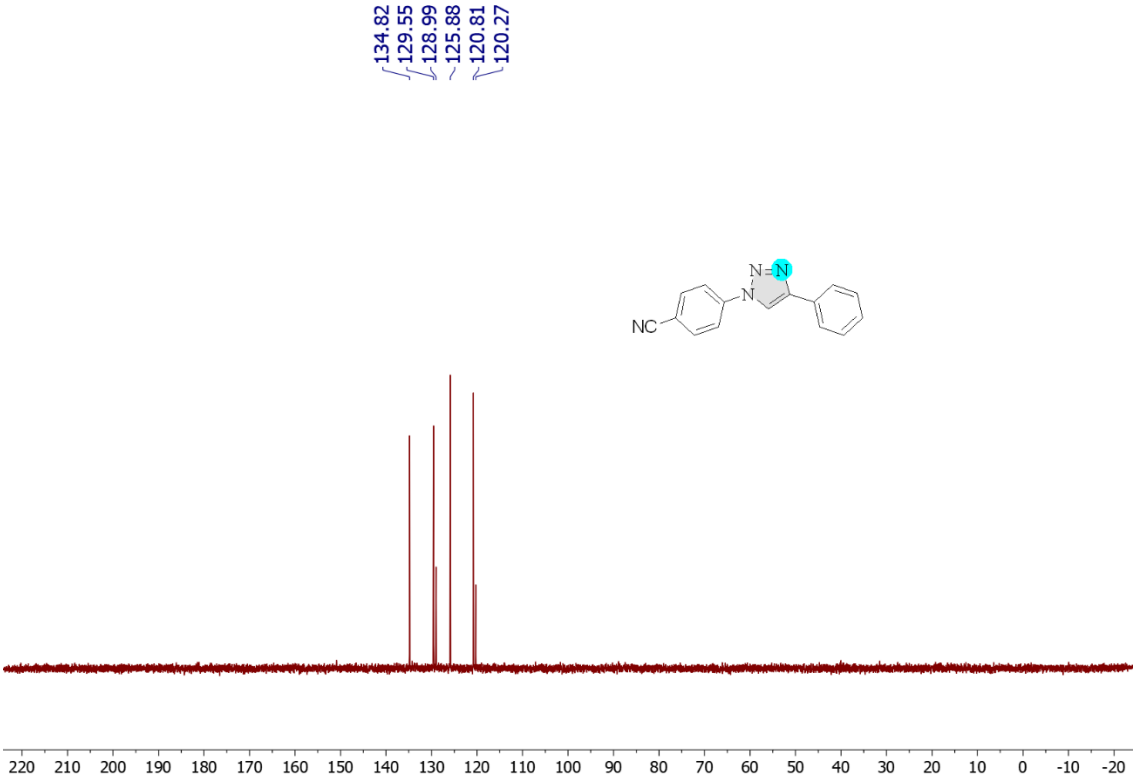
[1]H-NMR of 4-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)benzonitrile (3v)



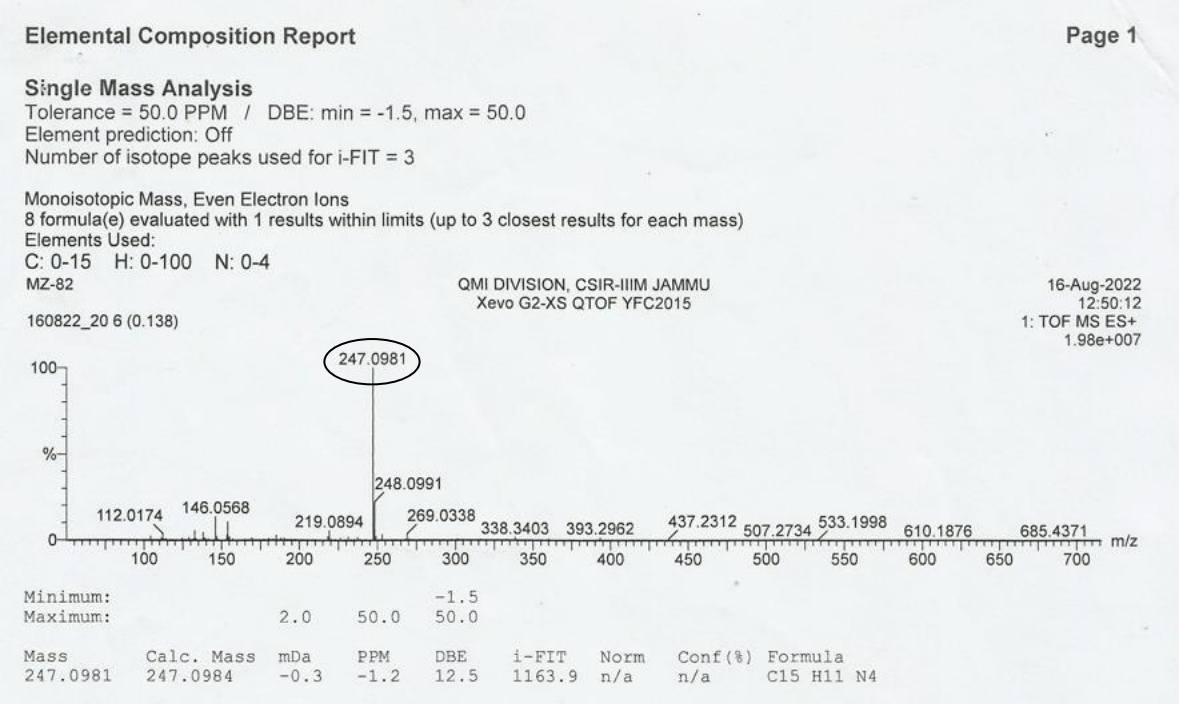
^{13}C-NMR of 4-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)benzonitrile (3v)



DEPT of 4-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)benzonitrile (3v)



HRMS of 4-(4-Phenyl-1*H*-1,2,3-triazol-1-yl)benzonitrile (3v)



Elemental Composition Report Page 1

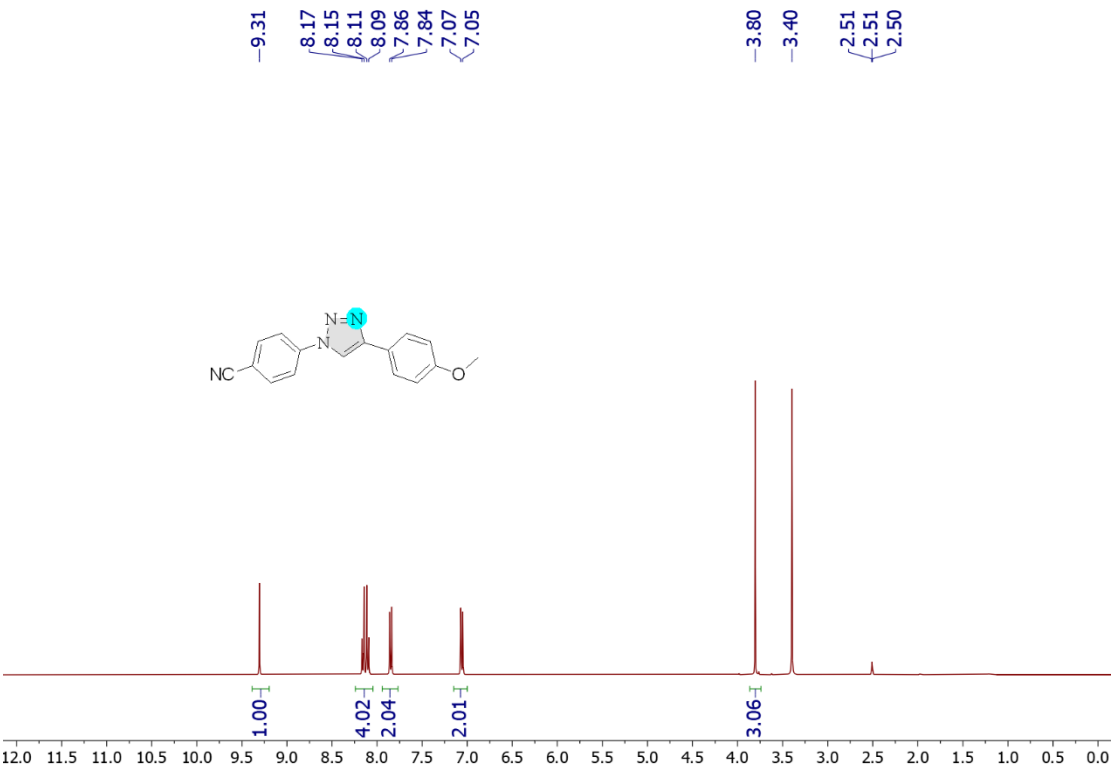
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-4

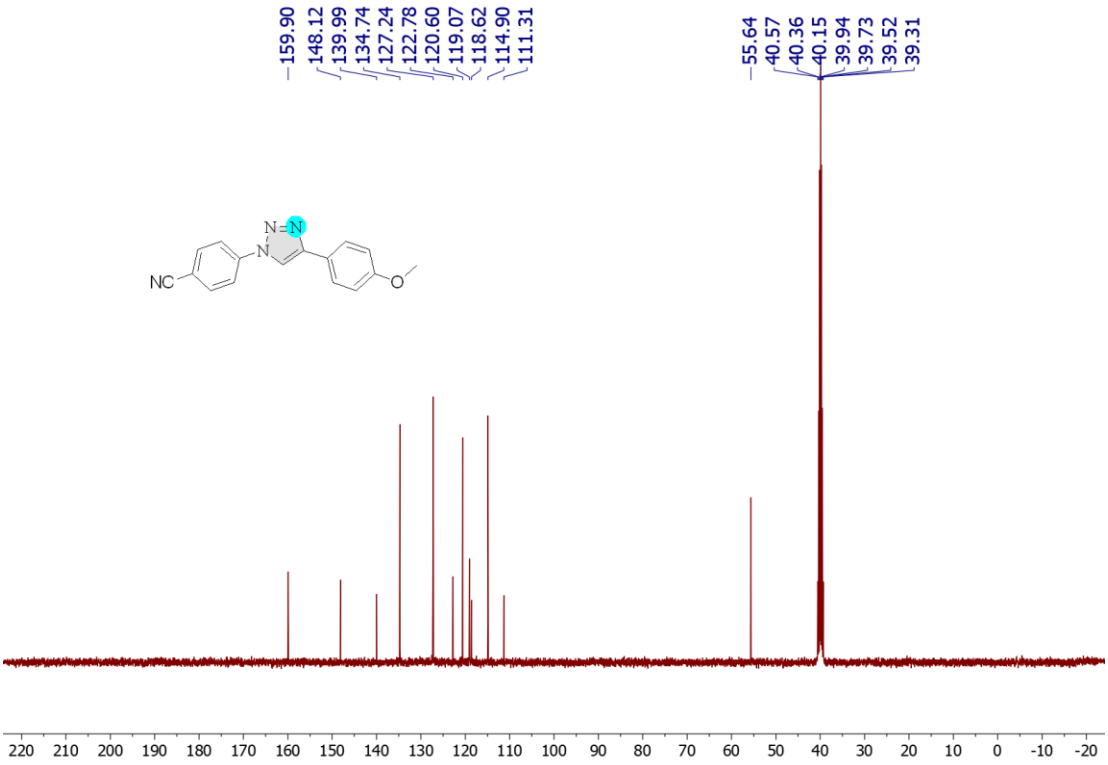
MZ-82 QMI DIVISION, CSIR-IIIM JAMMU 16-Aug-2022
Xevo G2-XS QTOF YFC2015 12:50:12
160822_20 6 (0.138) 1: TOF MS ES+
1.98e+007

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
247.0981	247.0984	-0.3	-1.2	12.5	1163.9	n/a	n/a	C15 H11 N4

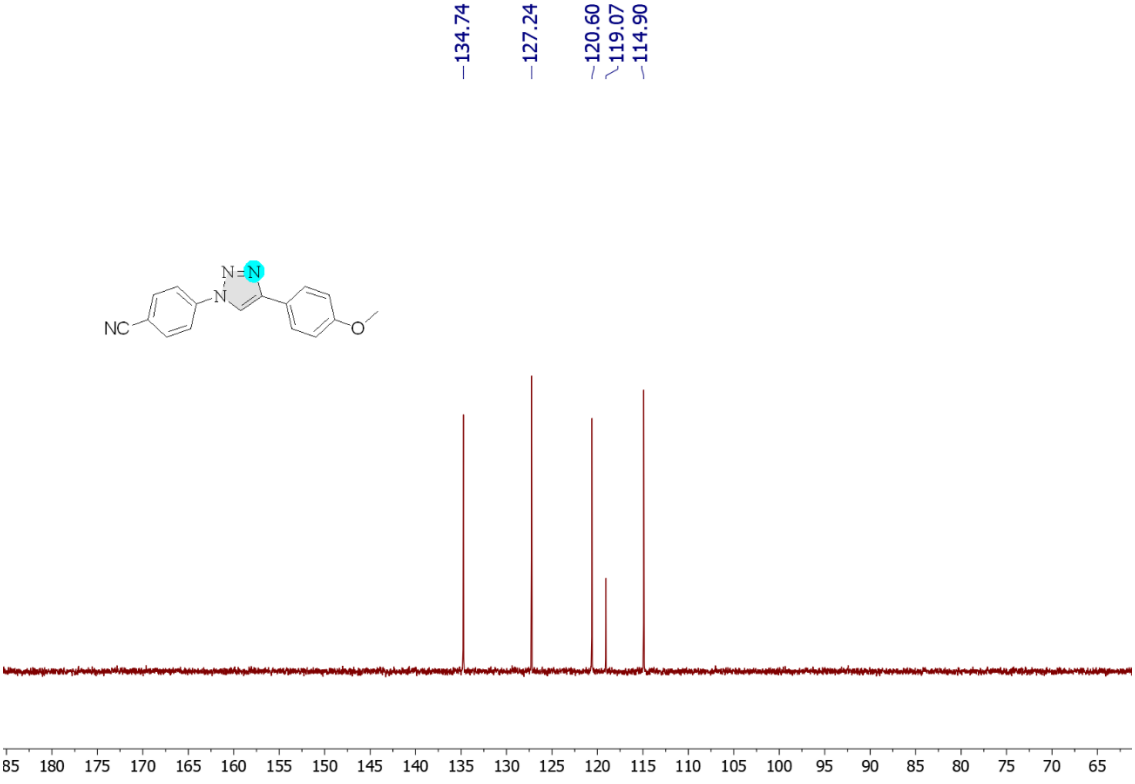
^{1}H-NMR of 4-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3w)



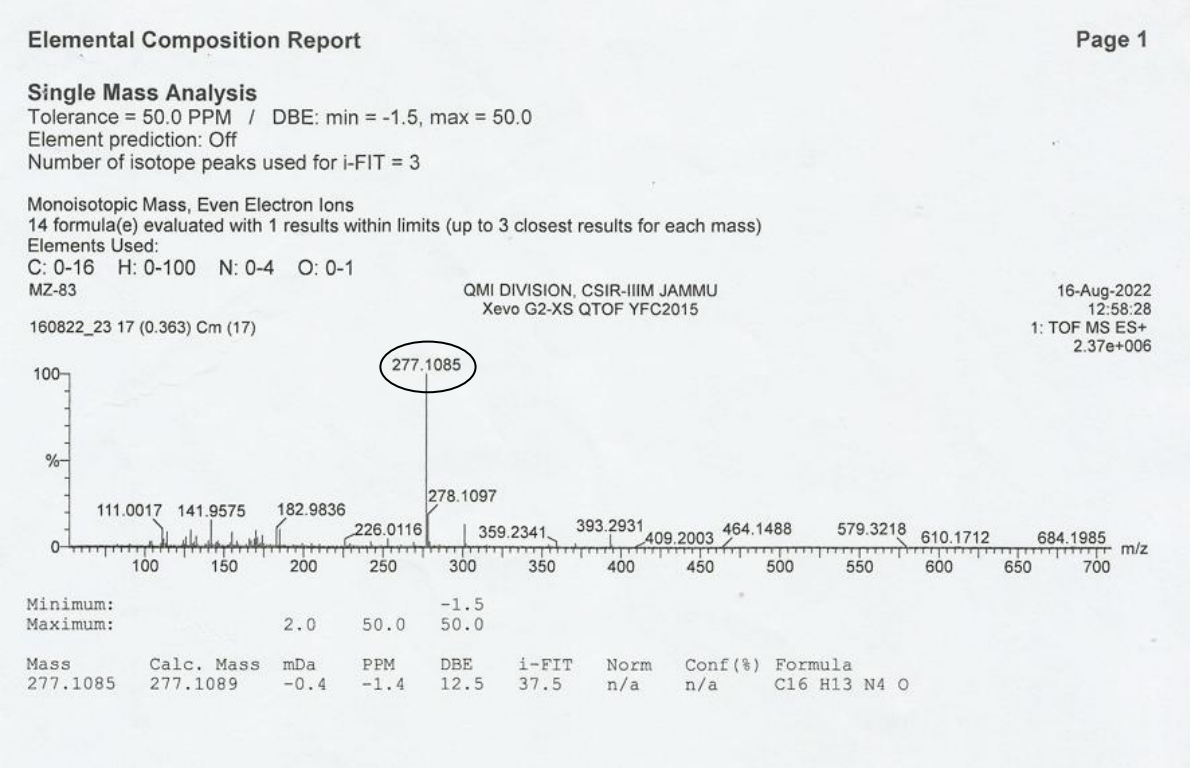
^{13}C-NMR of 4-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3w)



DEPT of 4-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3w)



HRMS of 4-(4-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3w)



Elemental Composition Report — Page 1

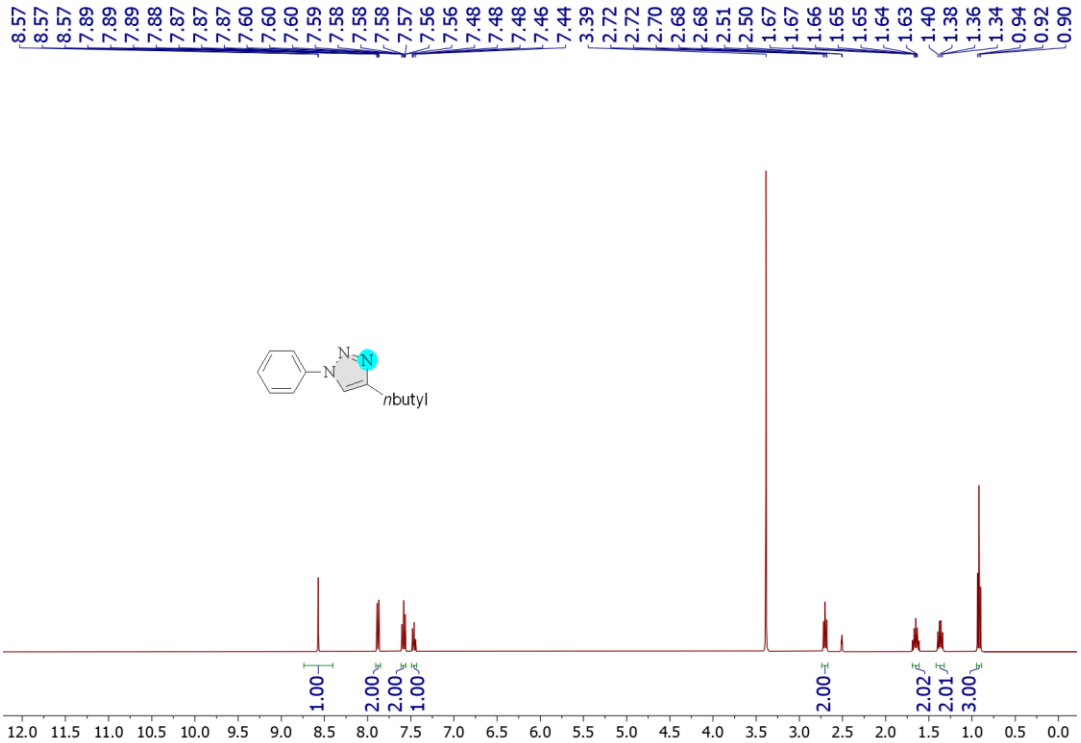
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
14 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-16 H: 0-100 N: 0-4 O: 0-1

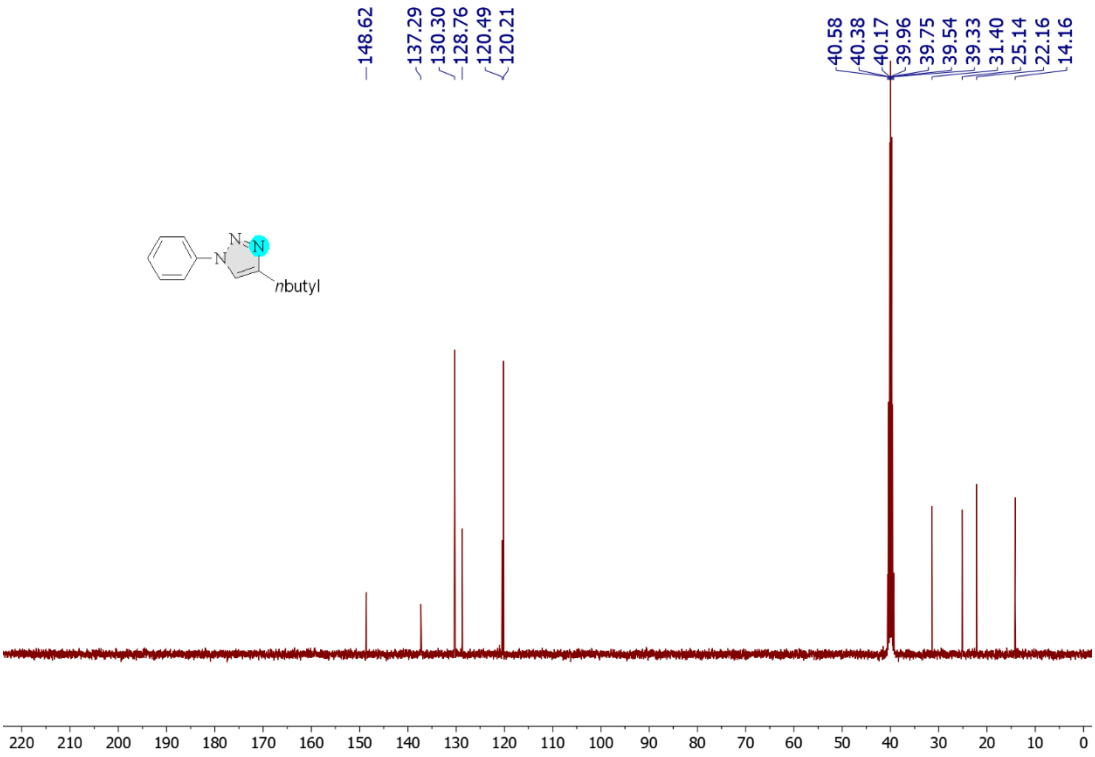
MZ-83 — QMI DIVISION, CSIR-IIIM JAMMU, Xevo G2-XS QTOF YFC2015 — 16-Aug-2022 12:58:28
160822_23 17 (0.363) Cm (17) — 1: TOF MS ES+ 2.37e+006

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
277.1085	277.1089	-0.4	-1.4	12.5	37.5	n/a	n/a	C16 H13 N4 O

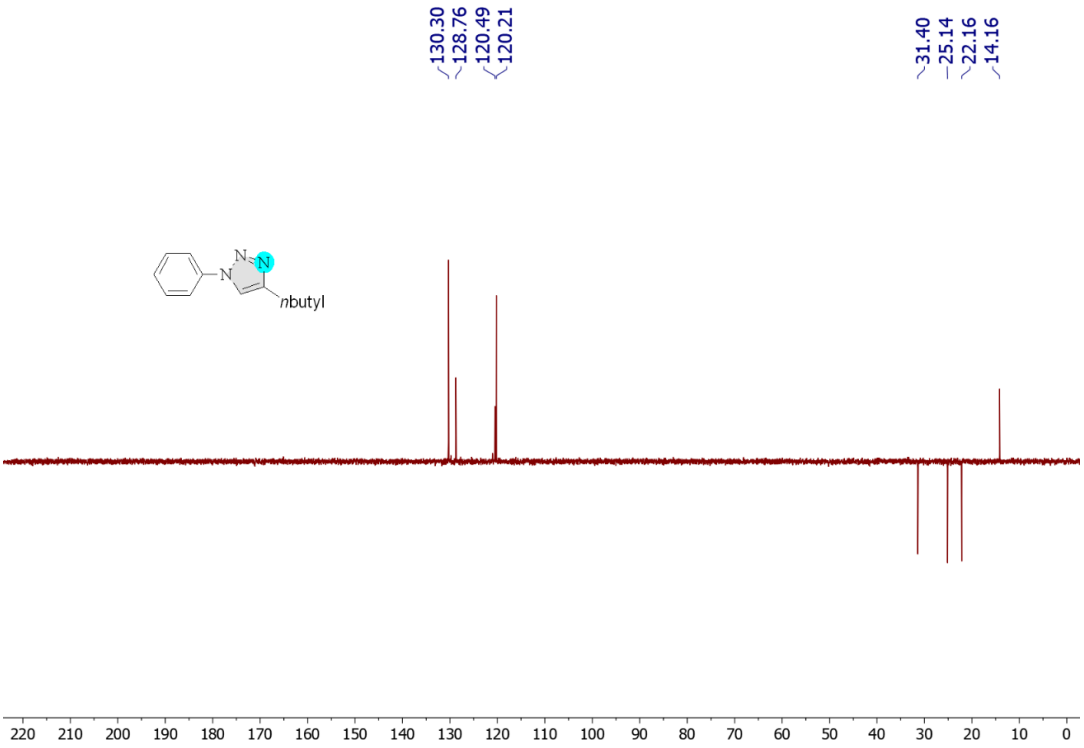
^{1}H-NMR of 4-Butyl-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3x)



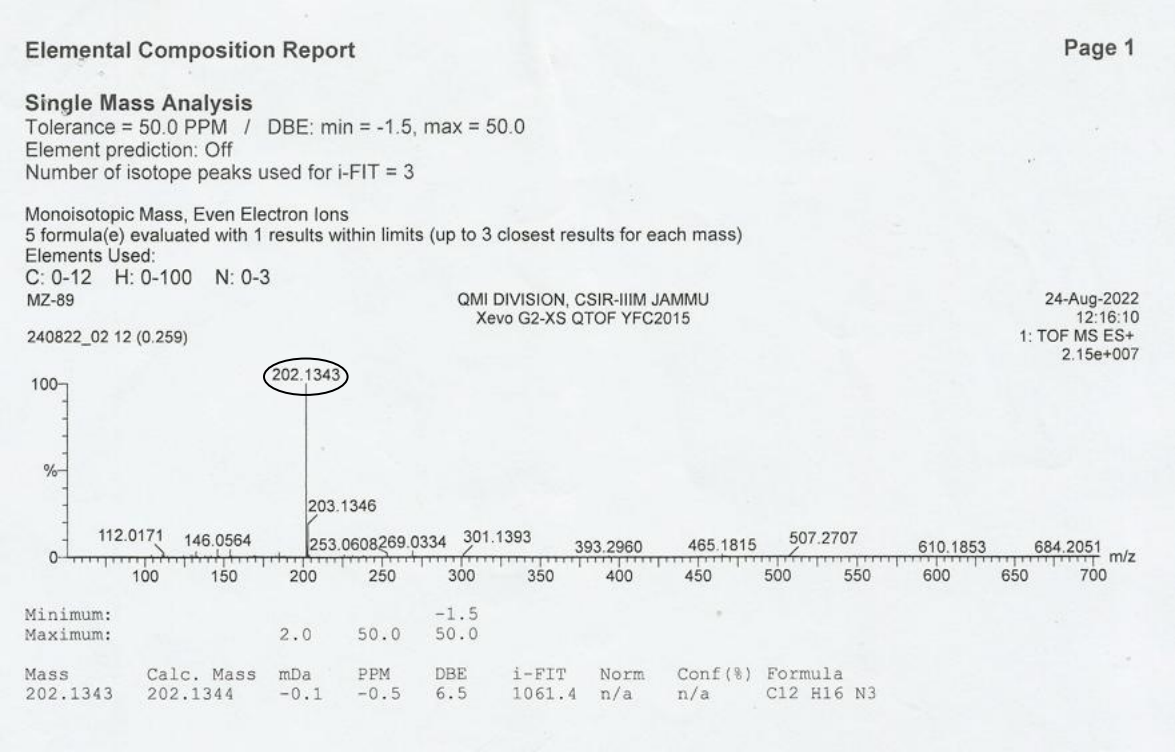
^{13}C-NMR of 4-Butyl-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3x)



DEPT of 4-Butyl-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3x)



HRMS of 4-Butyl-1-phenyl-4,5-dihydro-1*H*-1,2,3-triazole (3x)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-12 H: 0-100 N: 0-3

MZ-89

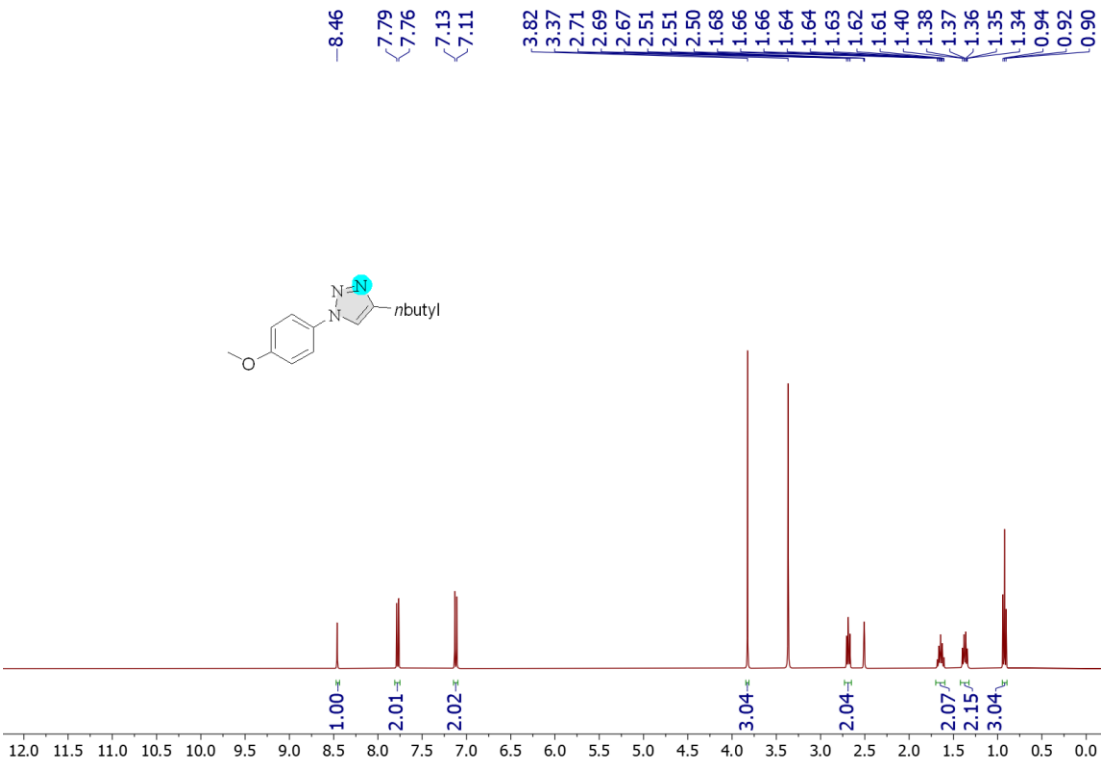
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

24-Aug-2022
12:16:10
1: TOF MS ES+
2.15e+007

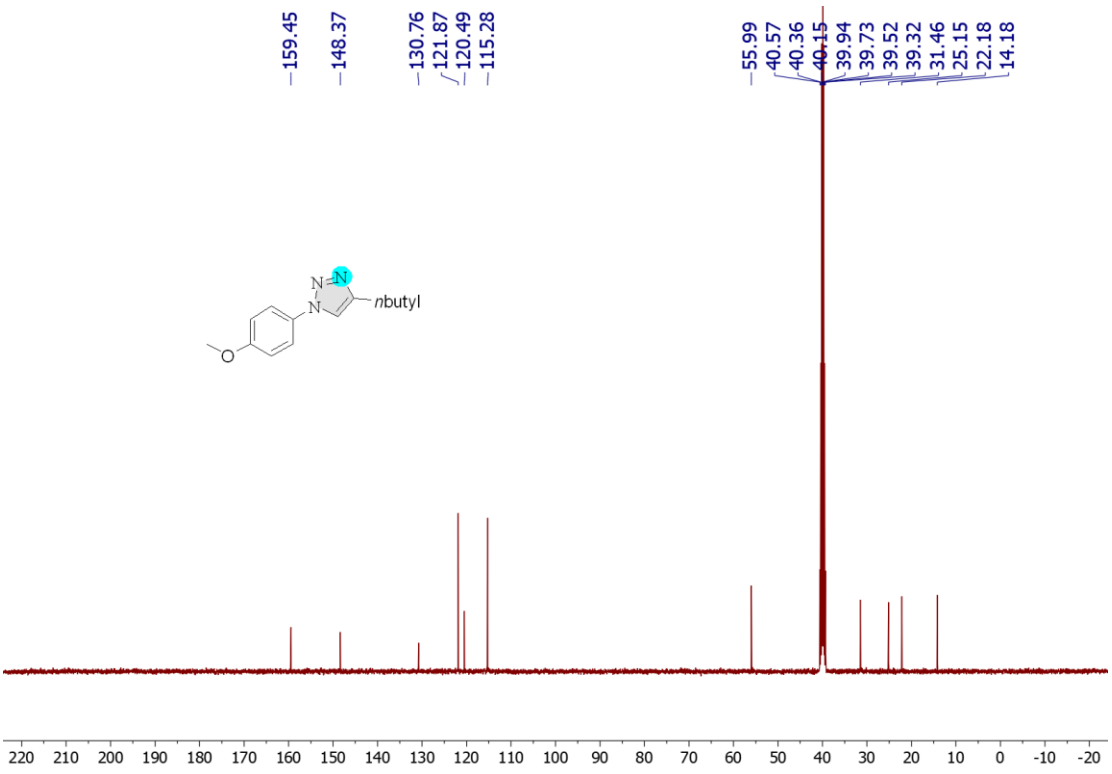
240822_02 12 (0.259)

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
202.1343	202.1344	-0.1	-0.5	6.5	1061.4	n/a	n/a	C12 H16 N3

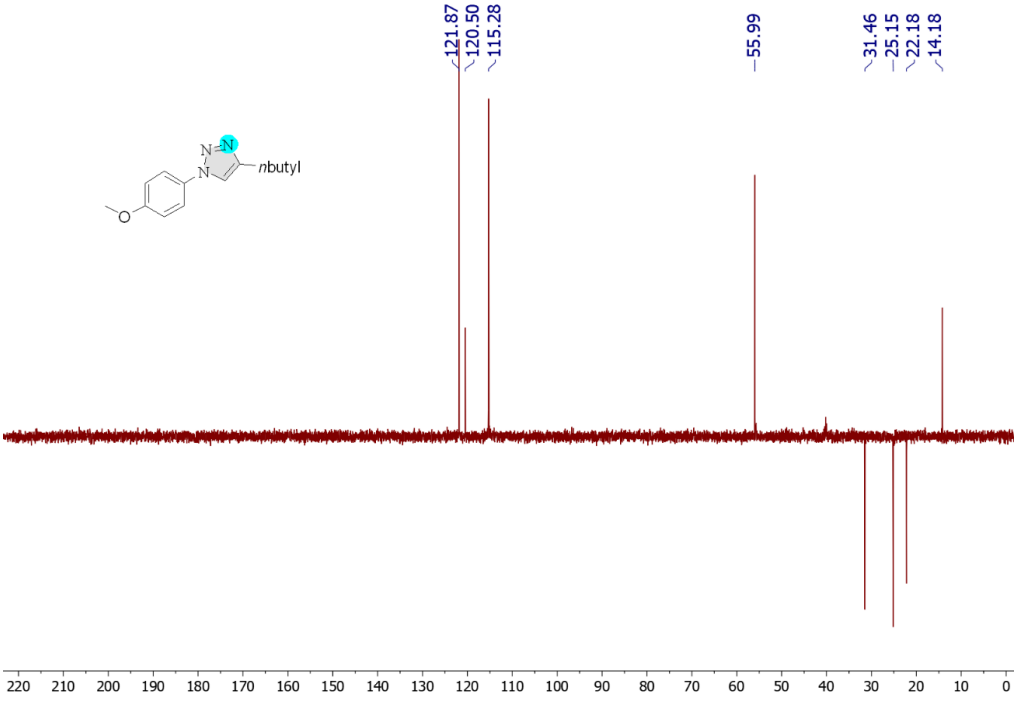
^{1}H-NMR of 4-(4-(4-Butylphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3y)



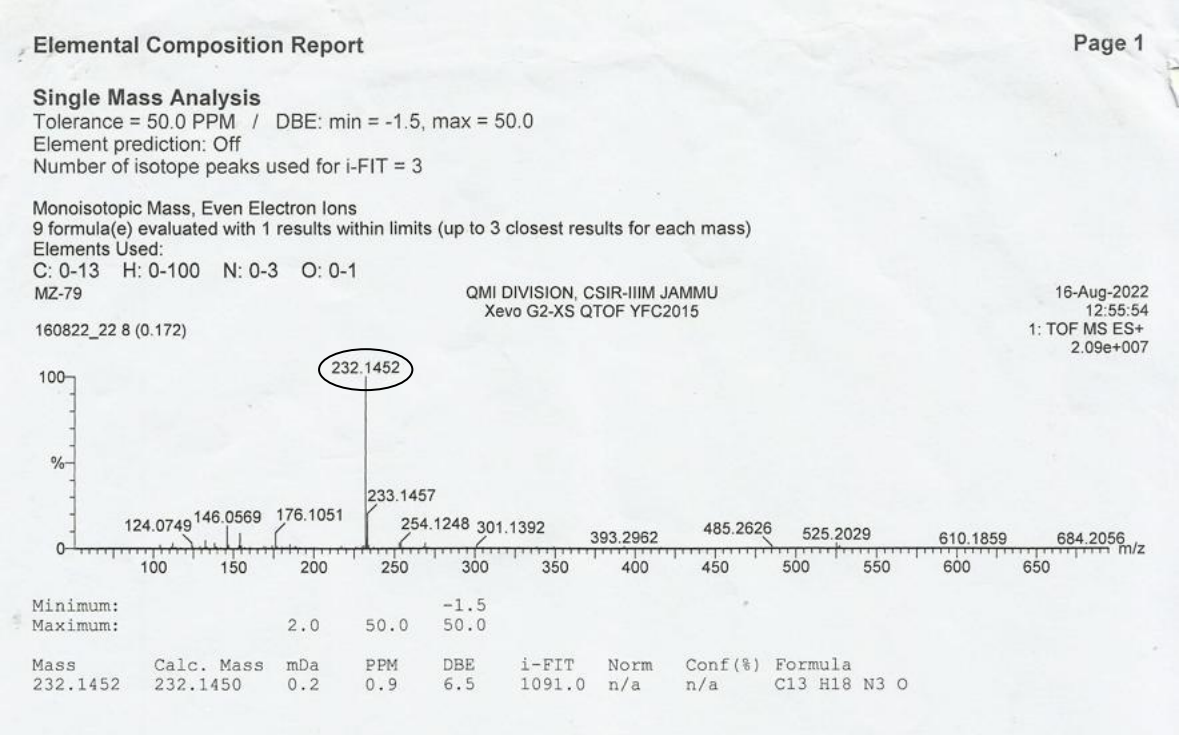
^{13}C-NMR of 4-(4-(4-Butylphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3y)



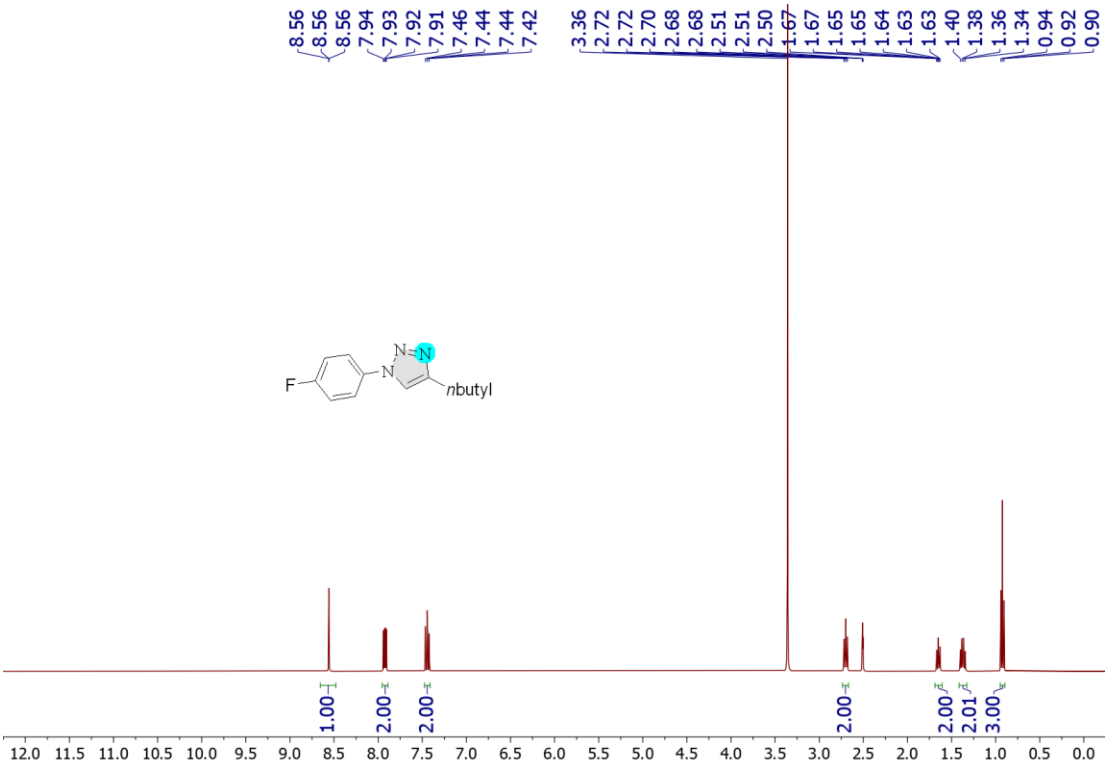
DEPT of 4-(4-(4-Butylphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3y)



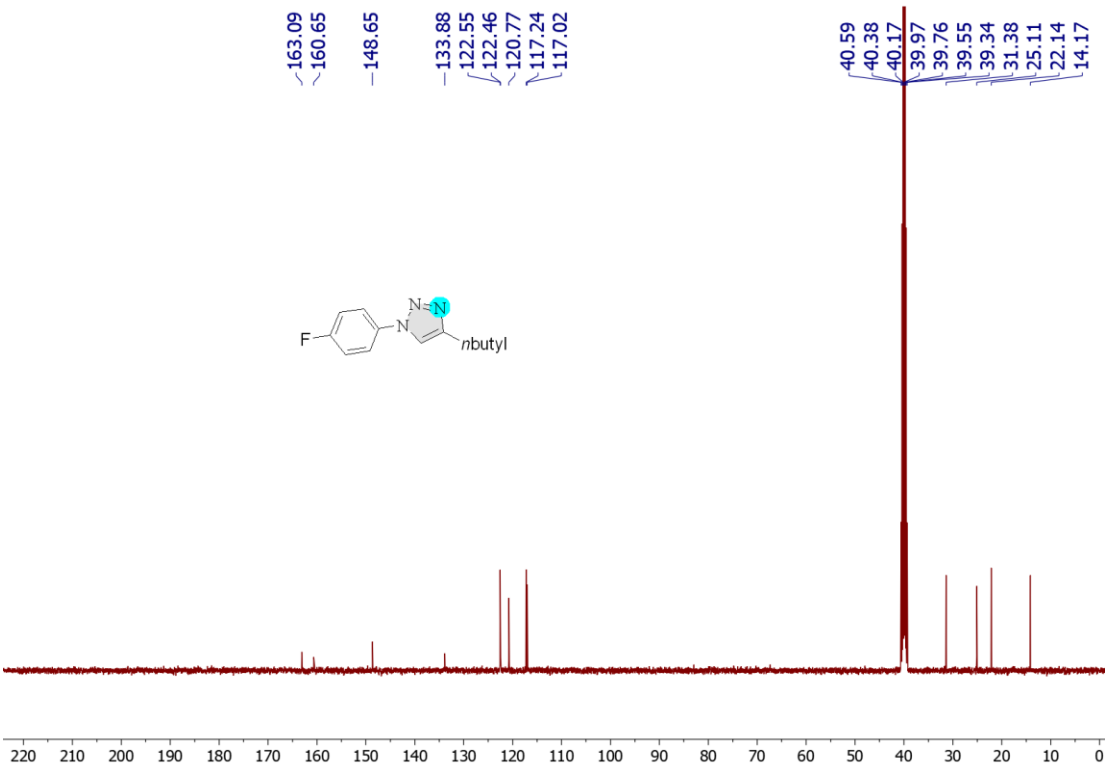
HRMS of 4-(4-(4-Butylphenyl)-1*H*-1,2,3-triazol-1-yl)benzonitrile (3y)



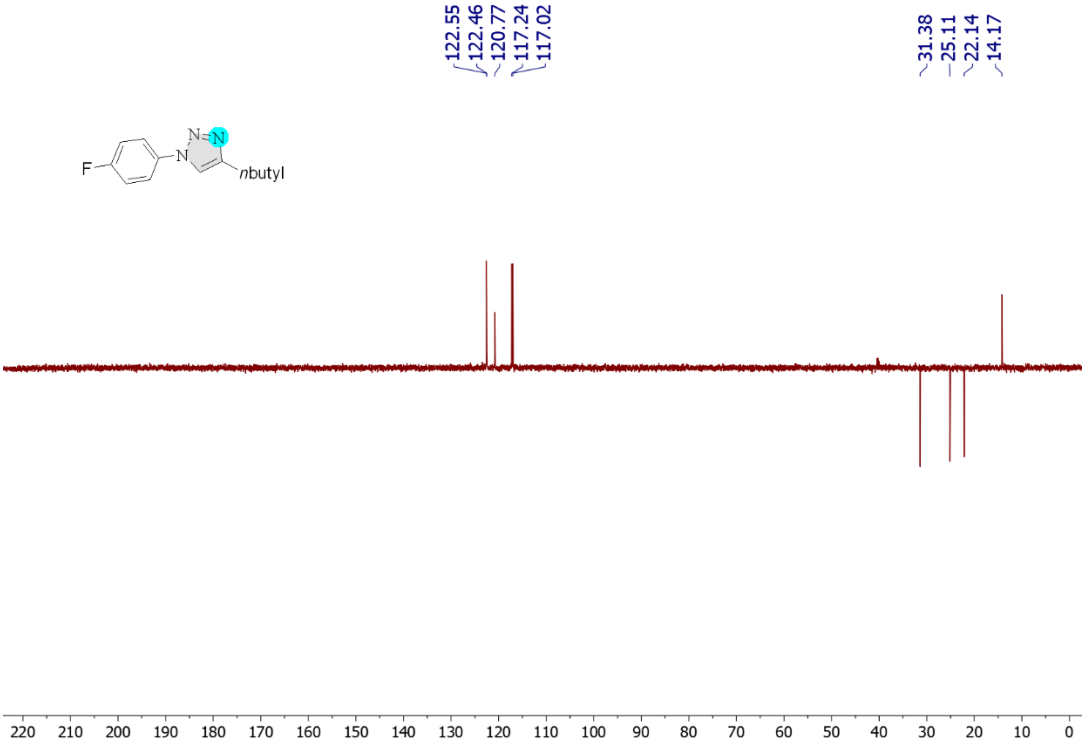
^{1}H-NMR of 4-Butyl-1-(4-fluorophenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3z)



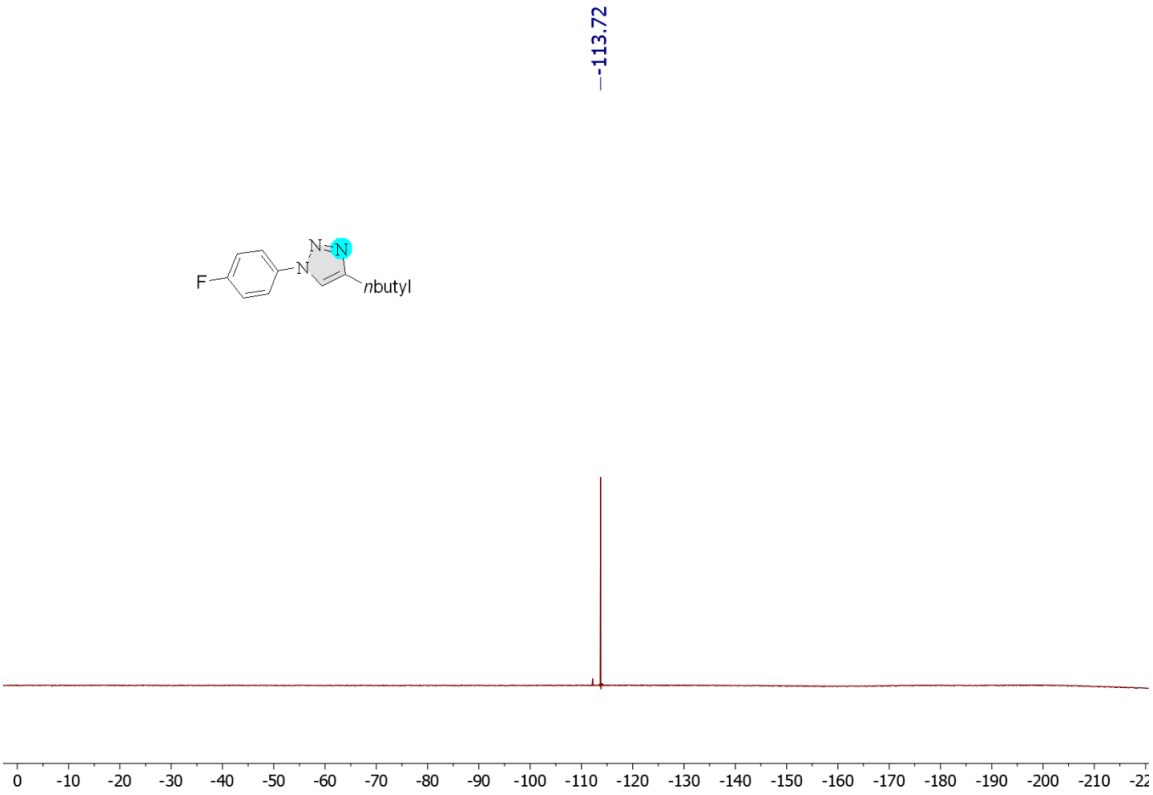
^{13}C-NMR of 4-Butyl-1-(4-fluorophenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3z)



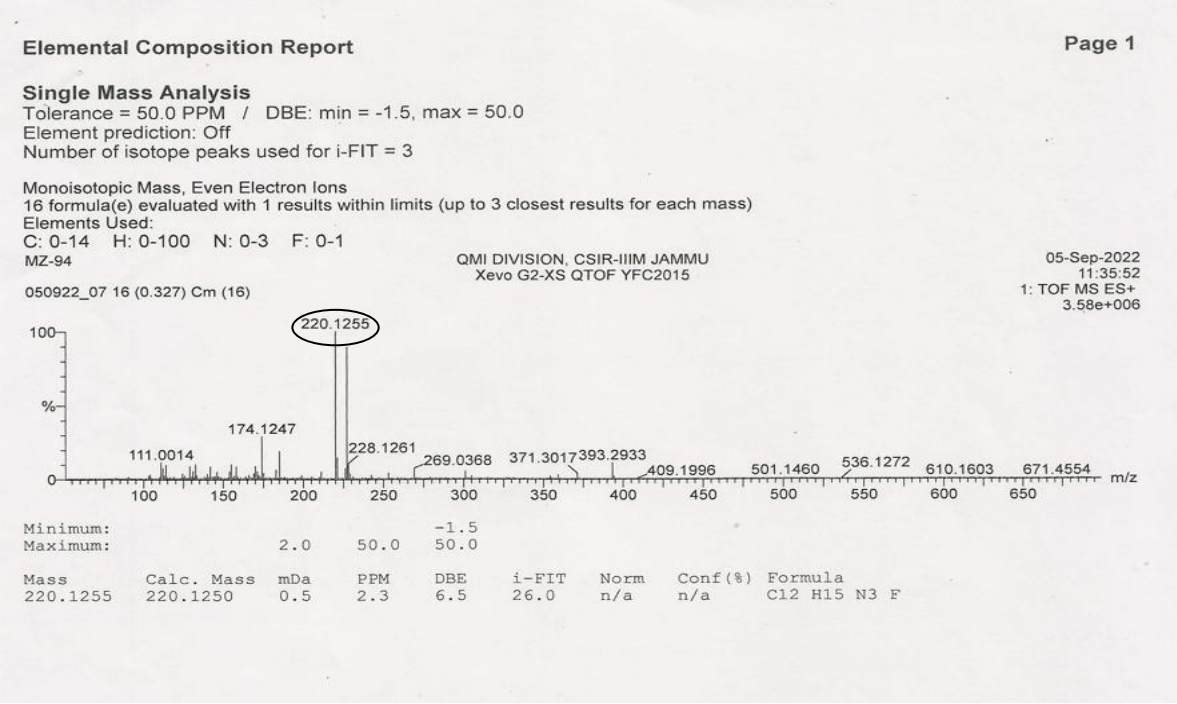
DEPT of 4-Butyl-1-(4-fluorophenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3z)



^{19}F-NMR of 4-Butyl-1-(4-fluorophenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3z)



HRMS of 4-Butyl-1-(4-fluorophenyl)-4,5-dihydro-1*H*-1,2,3-triazole (3z)



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

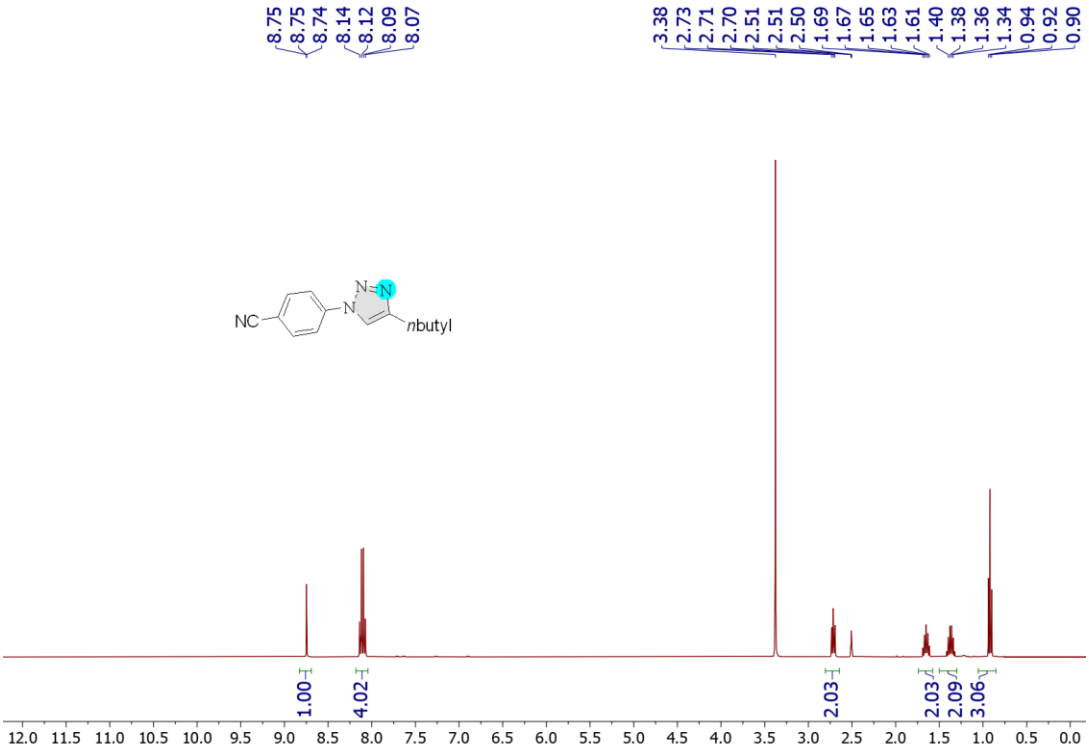
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 F: 0-1

MZ-94
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
05-Sep-2022
11:35:52
1: TOF MS ES+
3.58e+006

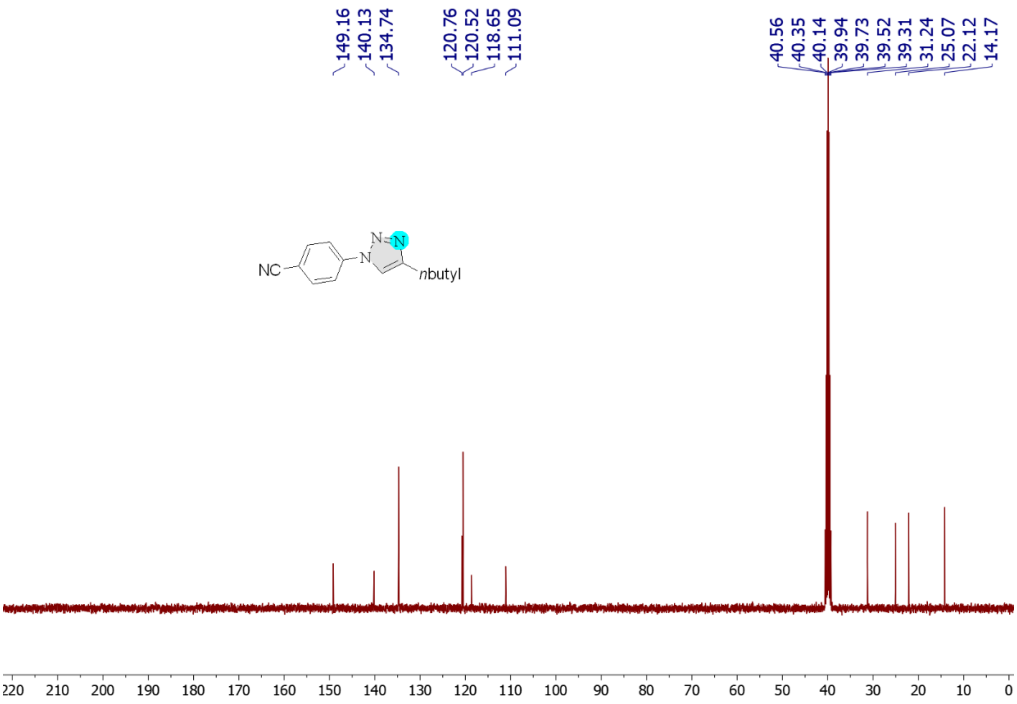
050922_07 16 (0.327) Cm (16)

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
220.1255	220.1250	0.5	2.3	6.5	26.0	n/a	n/a	C12 H15 N3 F

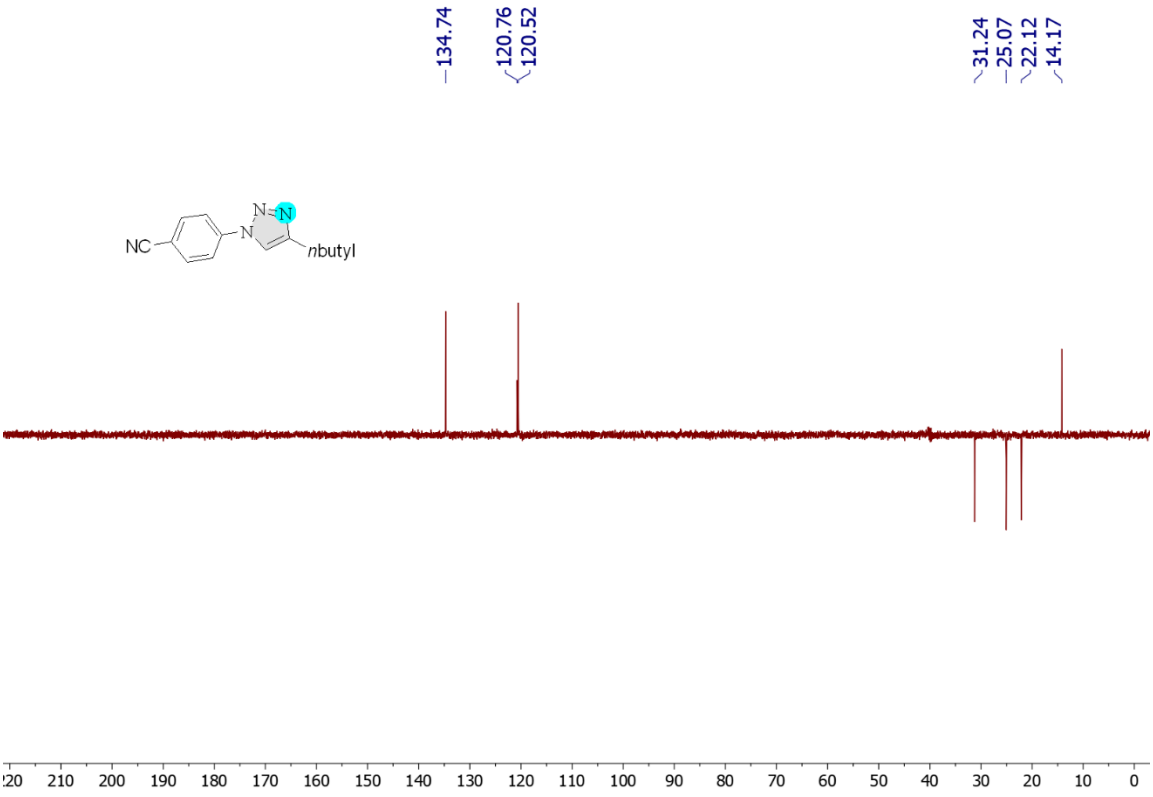
^{1}H-NMR of 4-(4-Butyl-4,5-dihydro-1*H*-1,2,3-triazol-1-yl)benzonitrile (3aa)



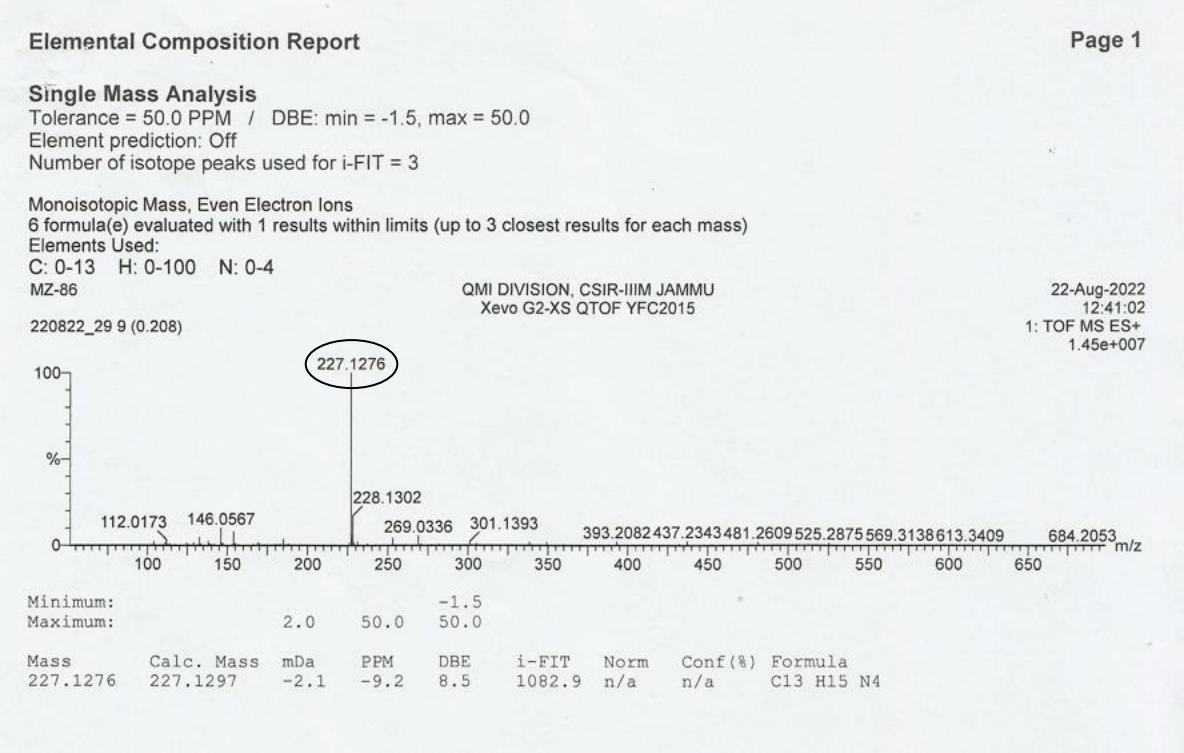
^{13}C-NMR of of 4-(4-Butyl-4,5-dihydro-1*H*-1,2,3-triazol-1-yl)benzonitrile (3aa)



DEPT of of 4-(4-Butyl-4,5-dihydro-1*H*-1,2,3-triazol-1-yl)benzonitrile (3aa)



HRMS of of 4-(4-Butyl-4,5-dihydro-1*H*-1,2,3-triazol-1-yl)benzonitrile (3aa)



Elemental Composition Report — Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

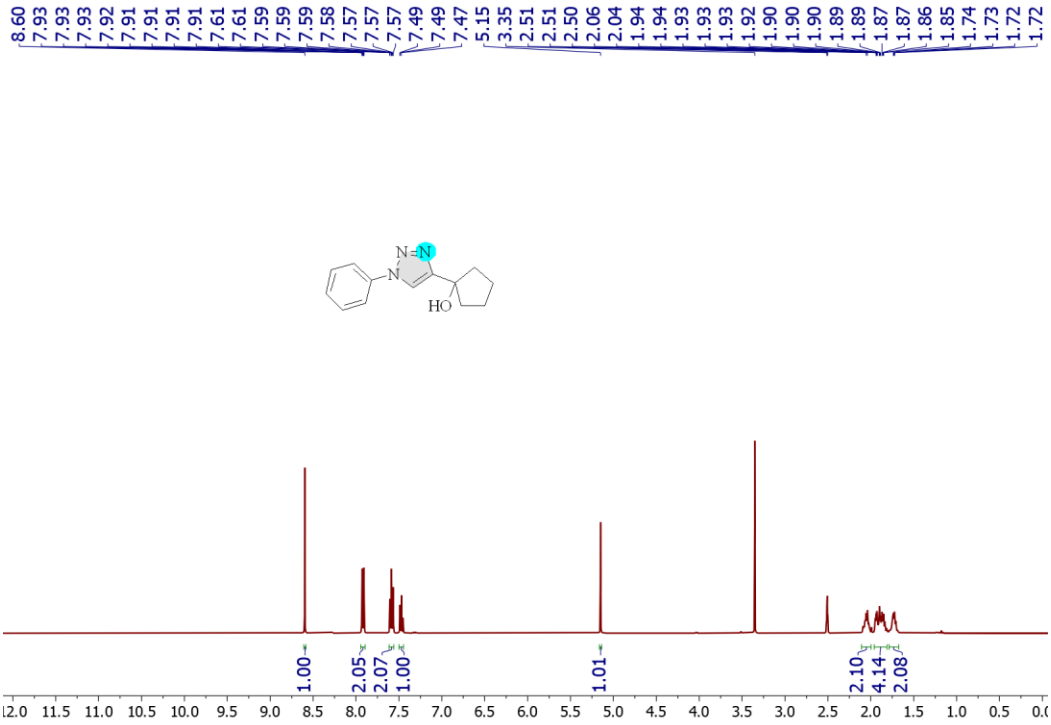
Monoisotopic Mass, Even Electron Ions
6 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-4

MZ-86 — QMI DIVISION, CSIR-IIIM JAMMU, Xevo G2-XS QTOF YFC2015 — 22-Aug-2022 12:41:02
220822_29 9 (0.208) — 1: TOF MS ES+ 1.45e+007

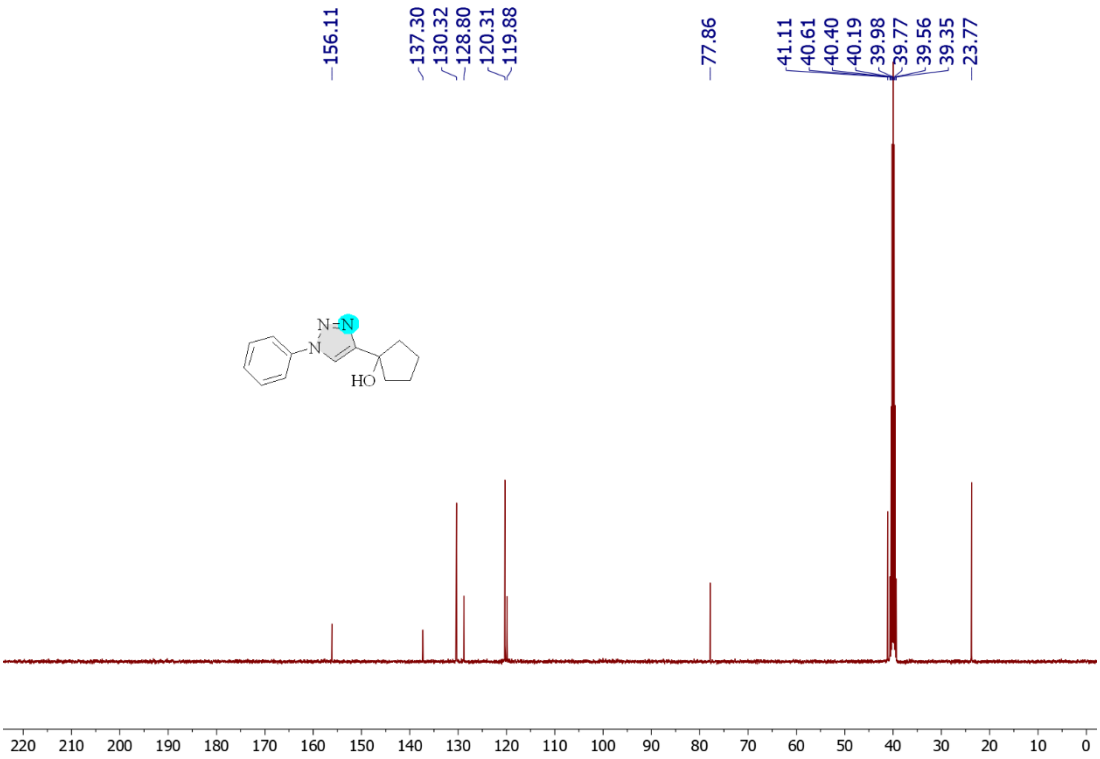
227.1276
228.1302
112.0173
146.0567
269.0336
301.1393
393.2082 437.2343 481.2609 525.2875 569.3138 613.3409 684.2053 m/z

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
227.1276	227.1297	-2.1	-9.2	8.5	1082.9	n/a	n/a	C13 H15 N4

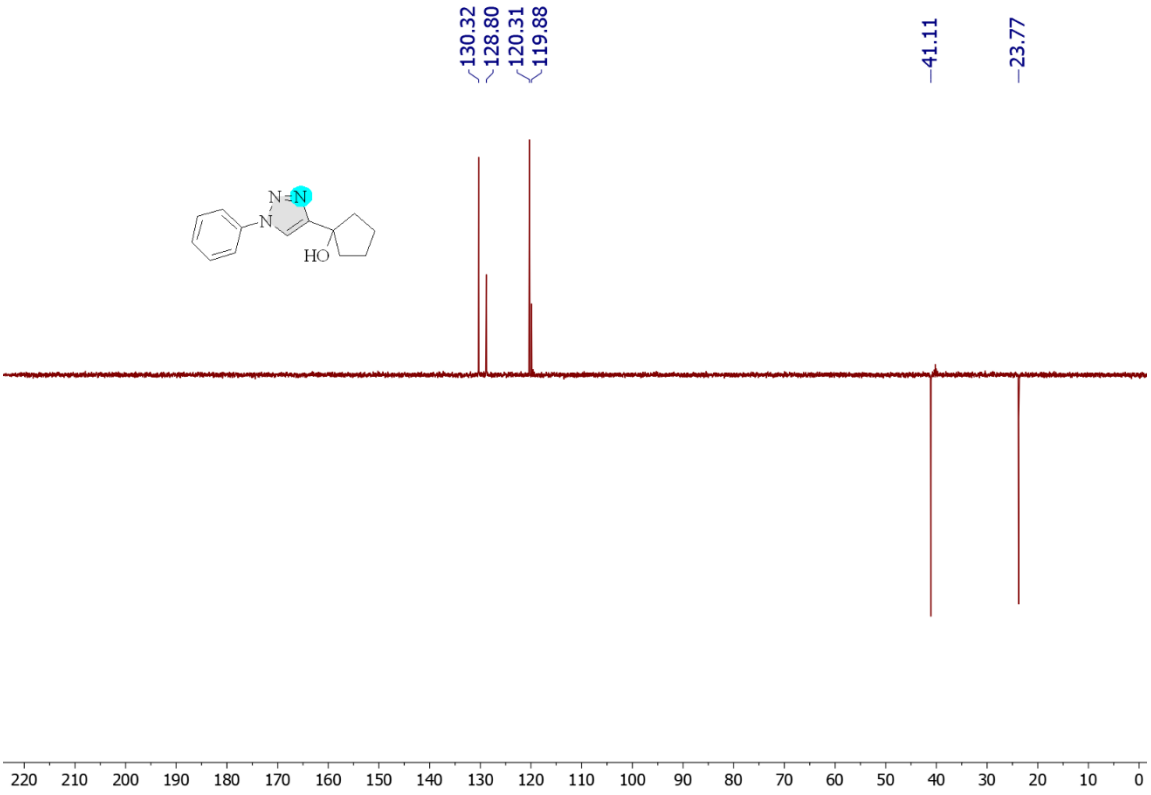
^{1}H-NMR of 1-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ab)



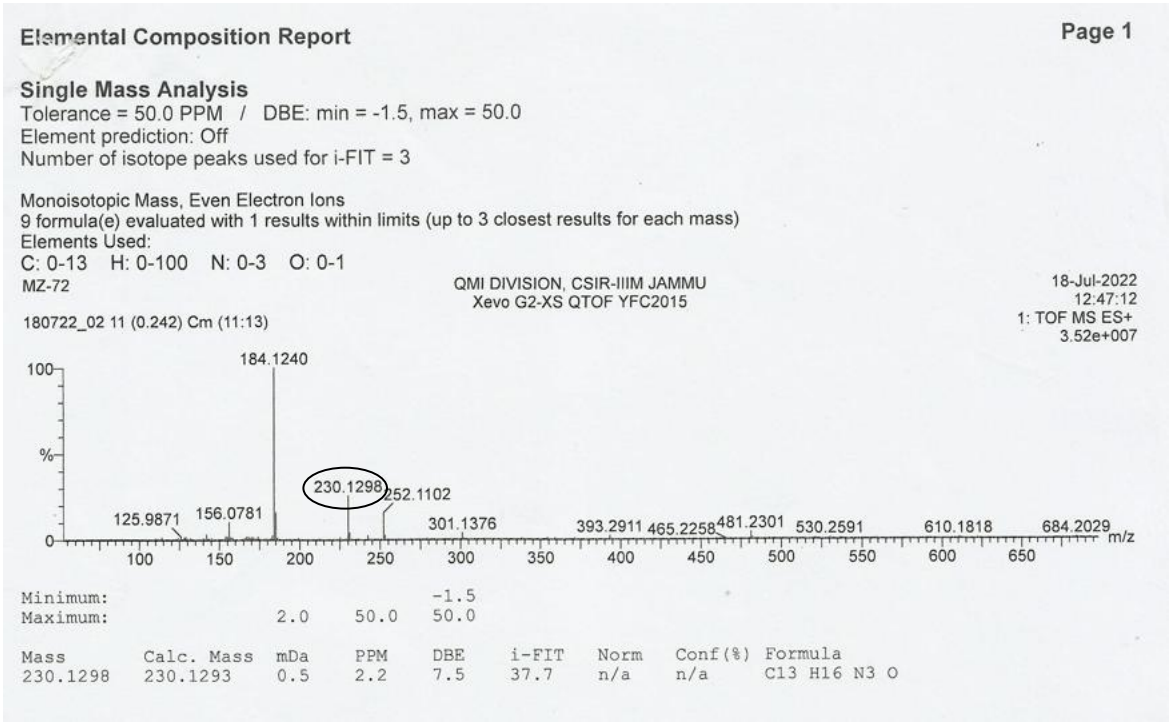
^{13}C-NMR of 1-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ab)



DEPT of 1-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ab)



HRMS of 1-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ab)



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-3 O: 0-1

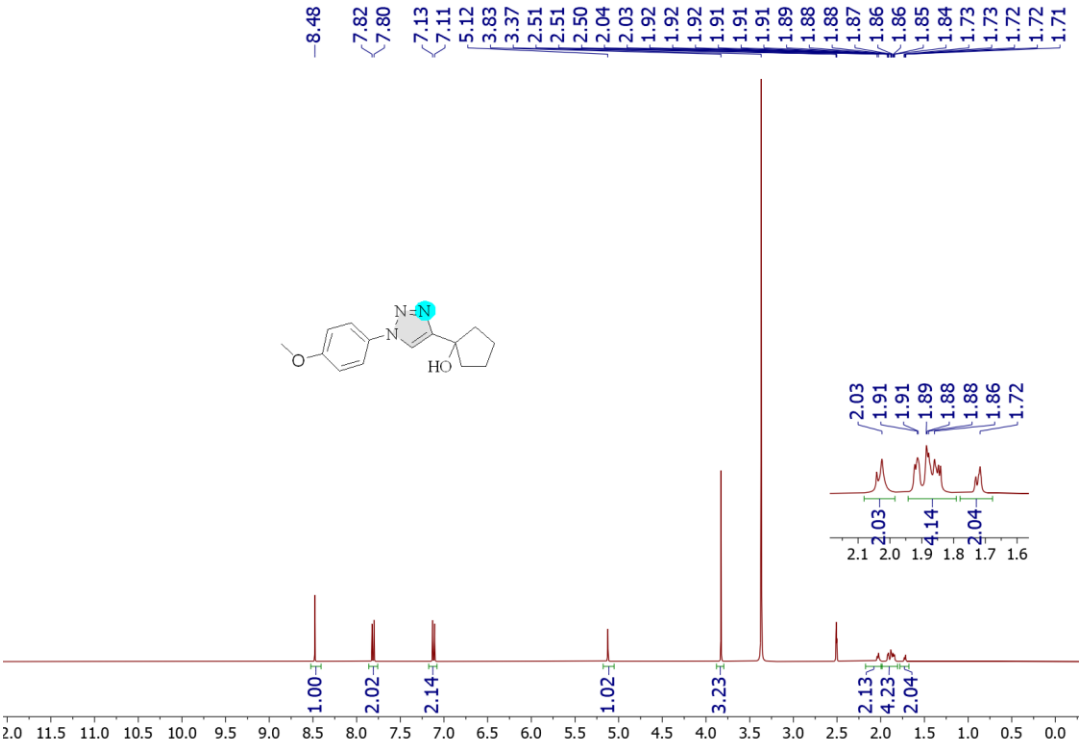
MZ-72
180722_02 11 (0.242) Cm (11:13)

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

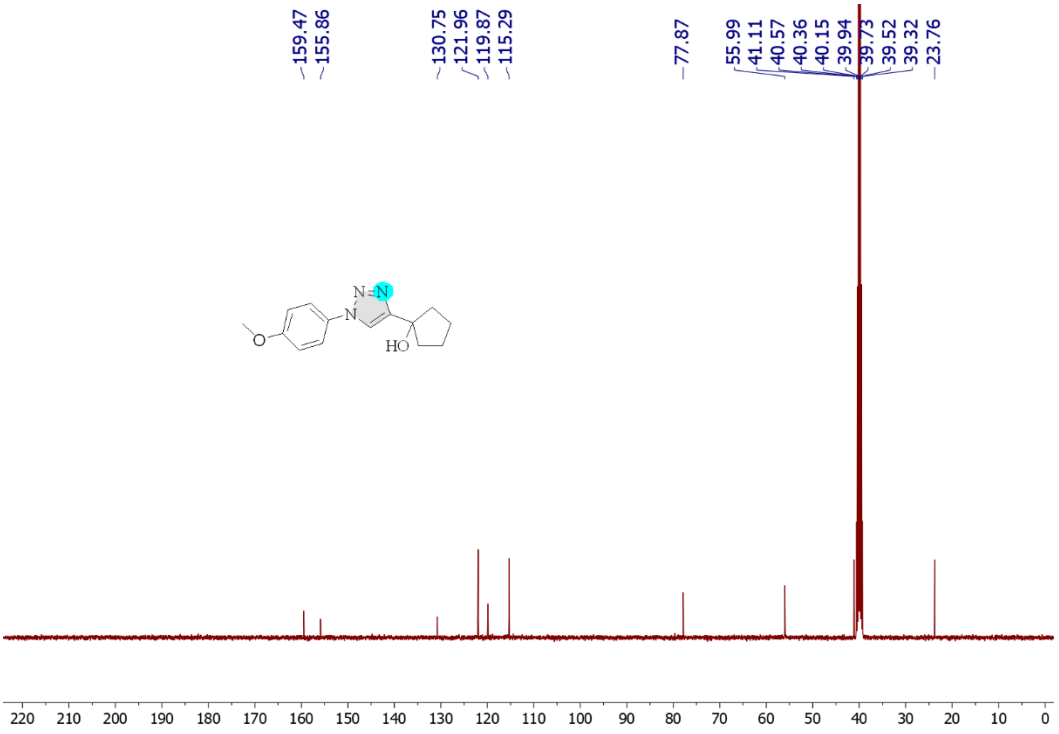
18-Jul-2022
12:47:12
1: TOF MS ES+
3.52e+007

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
230.1298	230.1293	0.5	2.2	7.5	37.7	n/a	n/a	C13 H16 N3 O

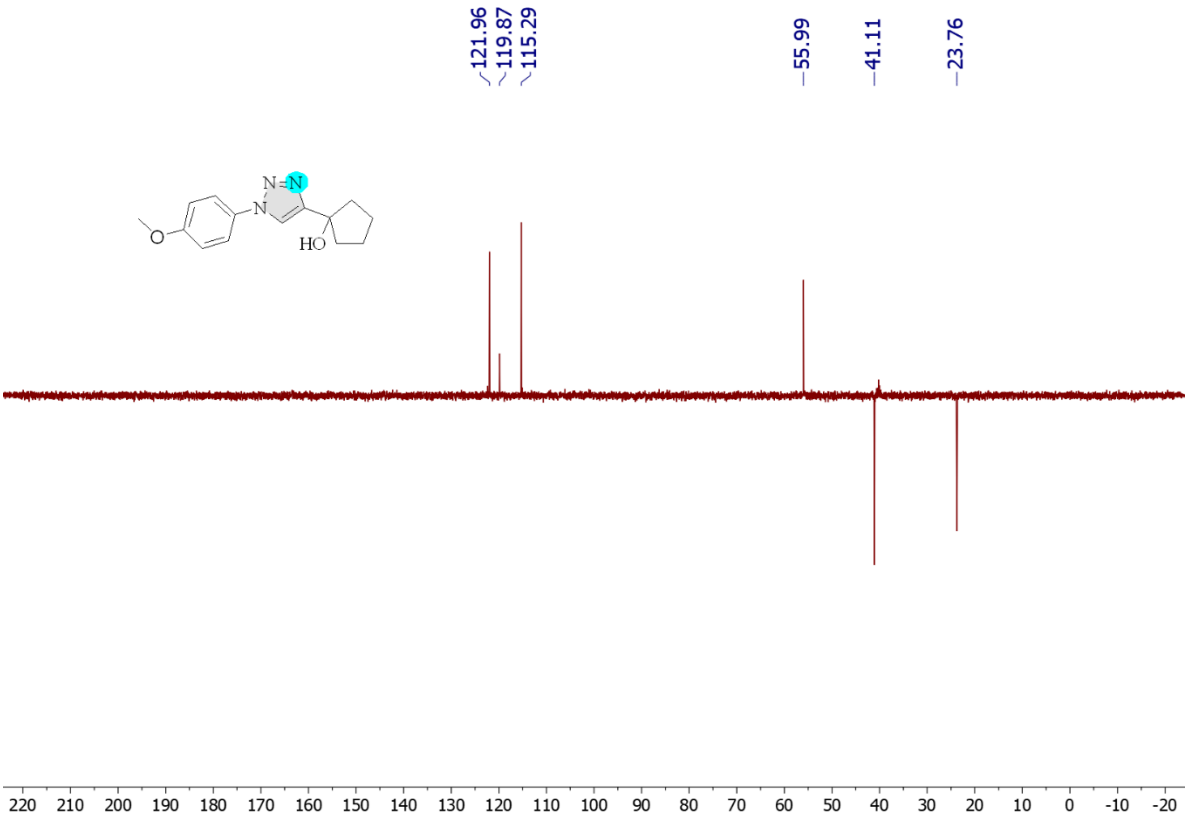
[1]H-NMR of 1-(1-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ac)



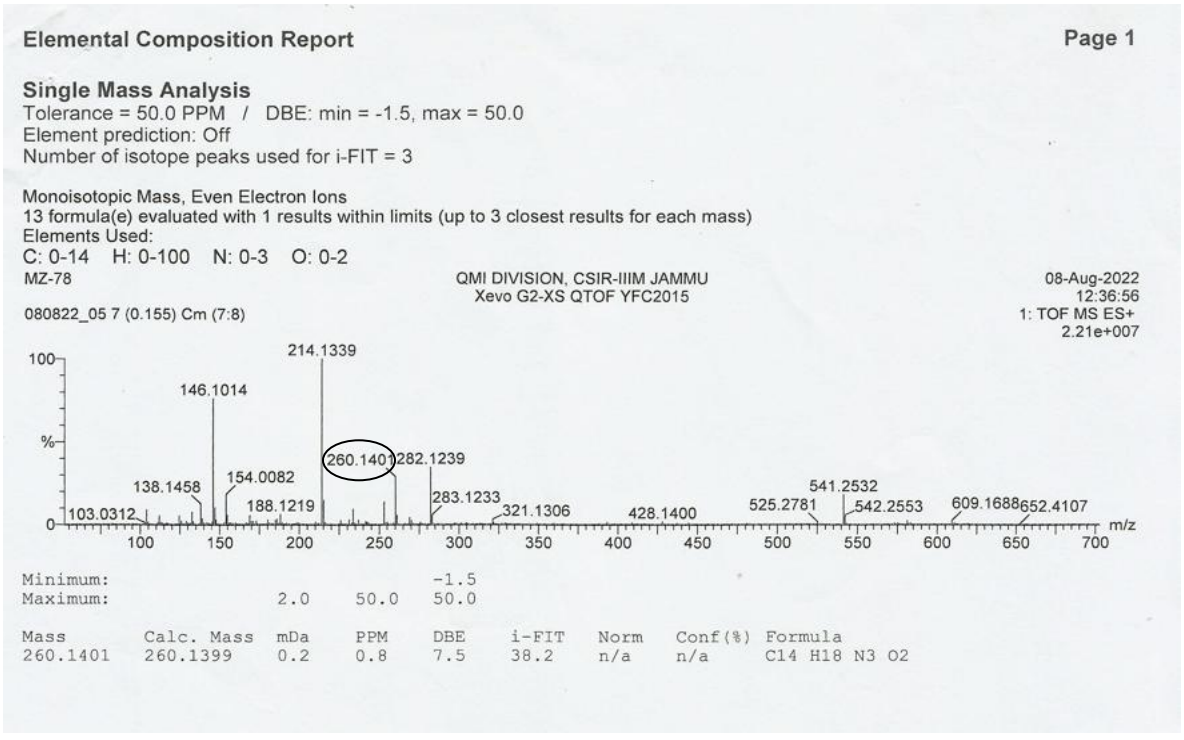
[13]C NMR of 1-(1-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ac)



DEPT of 1-(1-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ac)



HRMS of 1-(1-(4-Methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)cyclopentan-1-ol (3ac)



Elemental Composition Report Page 1

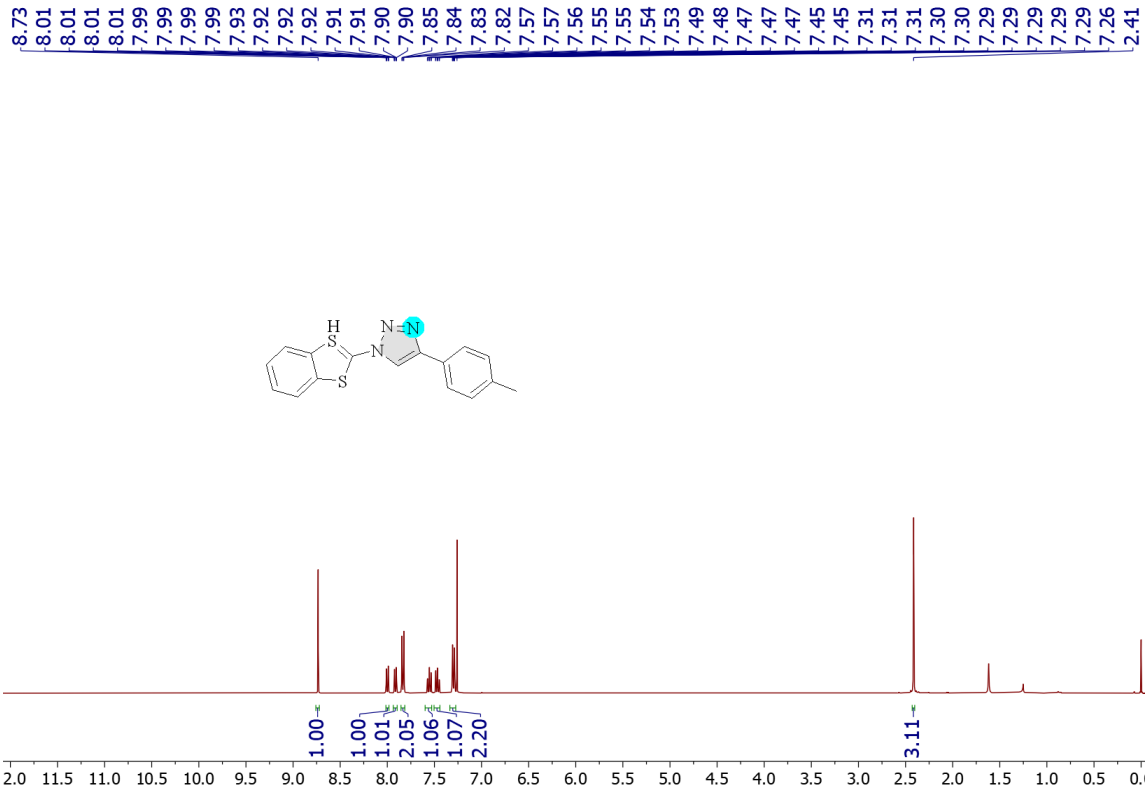
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-3 O: 0-2

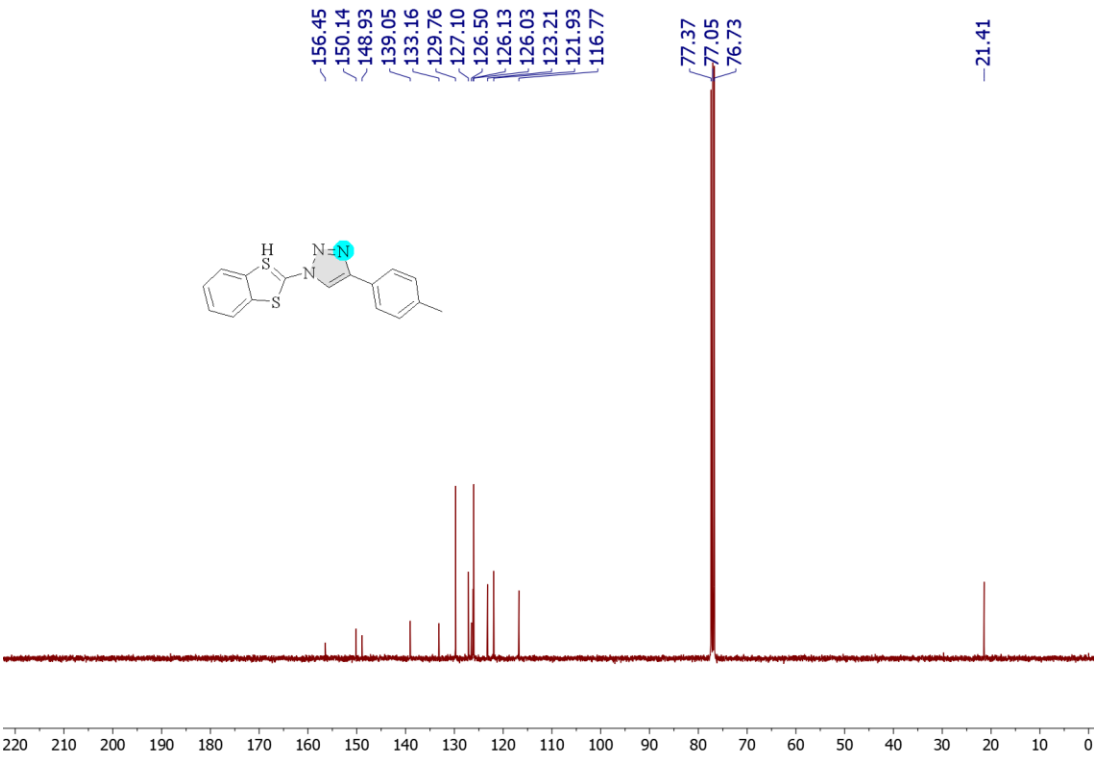
MZ-78
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
08-Aug-2022
12:36:56
080822_05 7 (0.155) Cm (7:8)
1: TOF MS ES+
2.21e+007

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
260.1401	260.1399	0.2	0.8	7.5	38.2	n/a	n/a	C14 H18 N3 O2

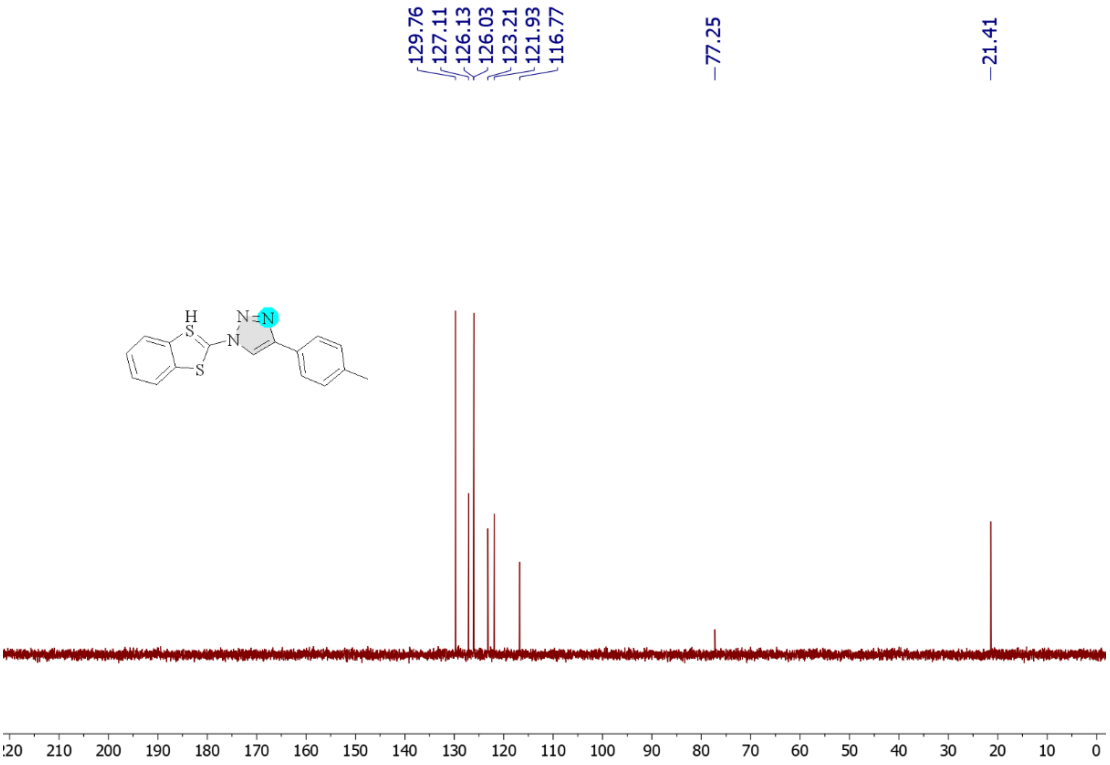
^{1}H-NMR of 2-(4-(*p*-tolyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4a)



^{13}C-NMR of 2-(4-(*p*-tolyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4a)



DEPT of 2-(4-(*p*-tolyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4a).



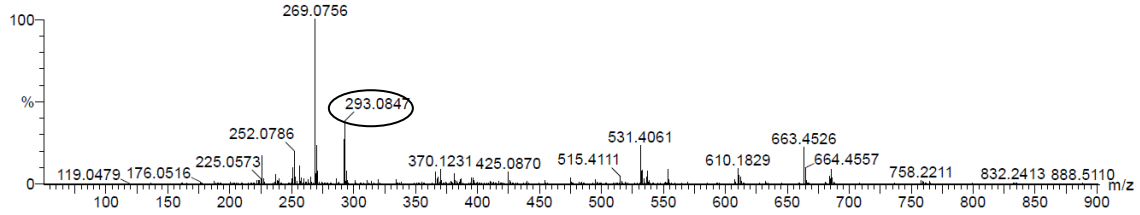
HRMS of 2-(4-(p-tolyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4a)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

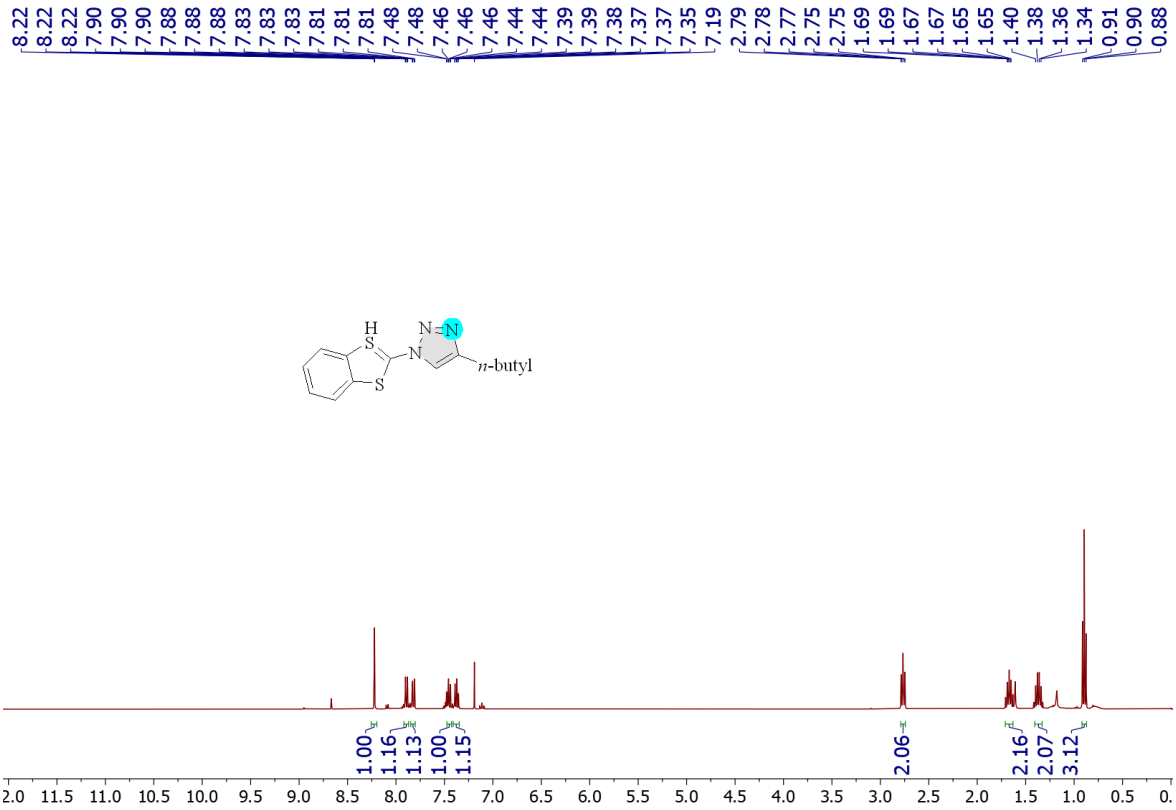
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-16 H: 0-100 N: 0-4 S: 0-1

MZ-4a
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
25-Apr-2024
13:22:18
250424_04 5 (0.121)
1: TOF MS ES+
2.00e+007

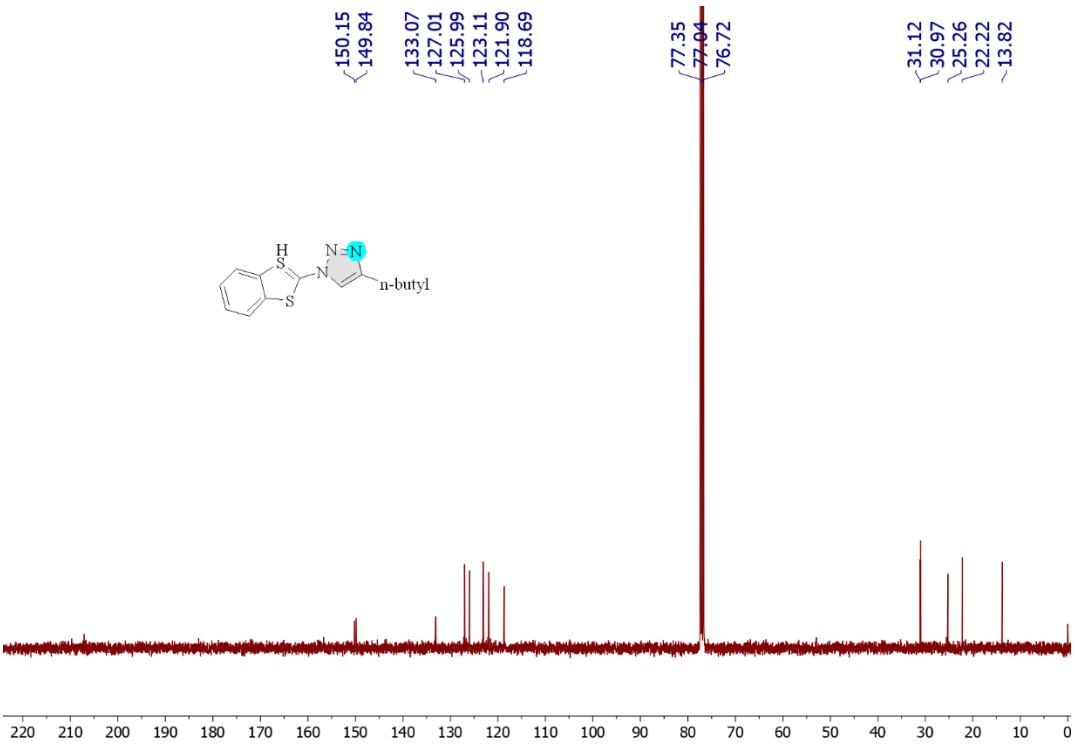


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
293.0847	293.0861	-1.4	-4.8	12.5	1307.9	n/a	n/a	C16 H13 N4 S

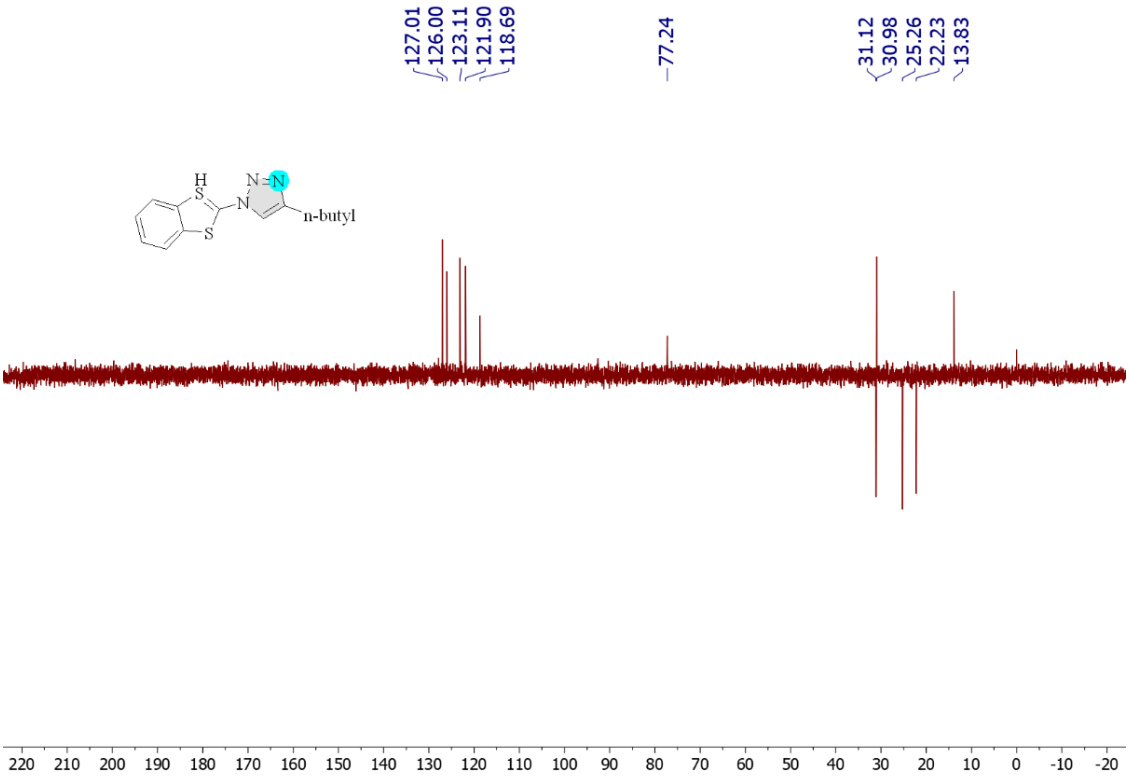
^{1}H-NMR of 2-(4-butyl-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4b)



^{13}C-NMR of 2-(4-butyl-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4b)



DEPT of 2-(4-butyl-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4b)



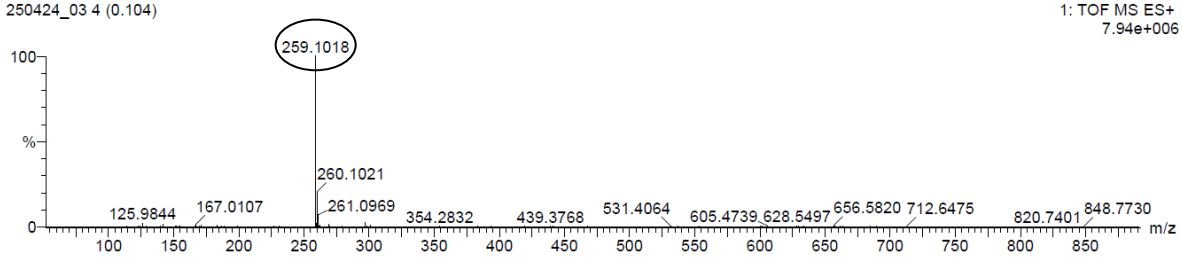
HRMS 2-(4-butyl-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4b)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

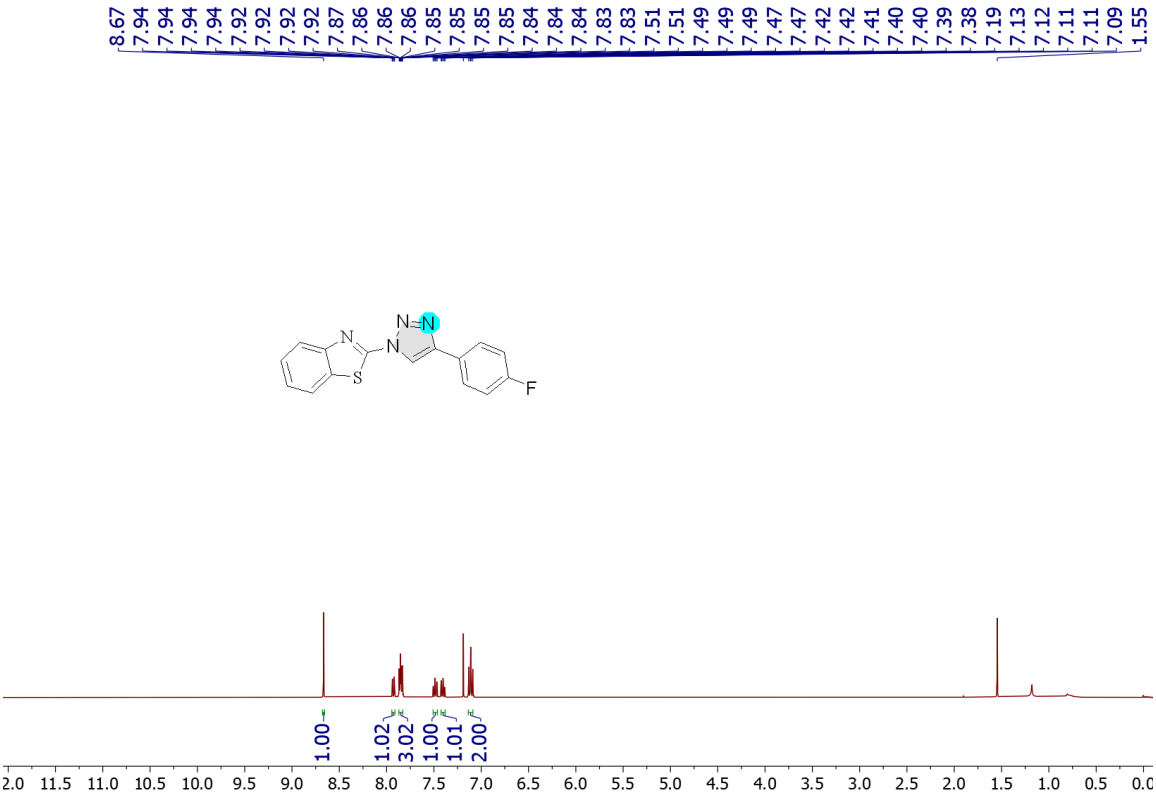
Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-4 S: 0-1

MZ-4b
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
25-Apr-2024
12:17:10
250424_03 4 (0.104)
1: TOF MS ES+
7.94e+006

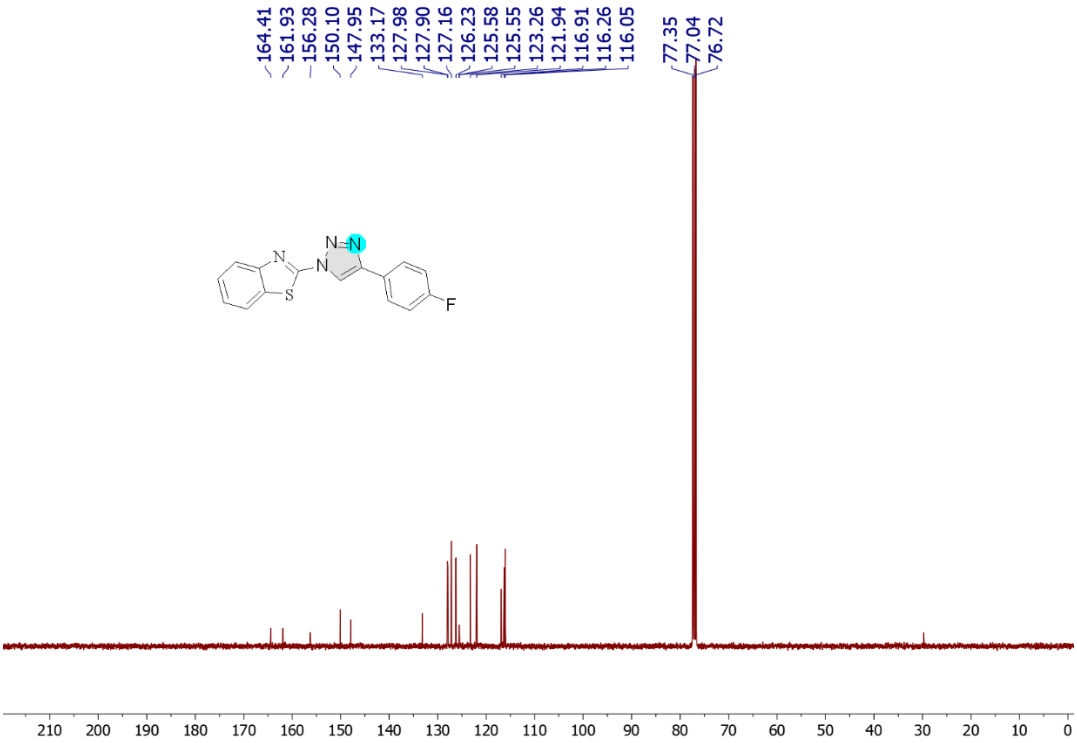


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
259.1018	259.1017	0.1	0.4	8.5	1339.2	n/a	n/a	C13 H15 N4 S

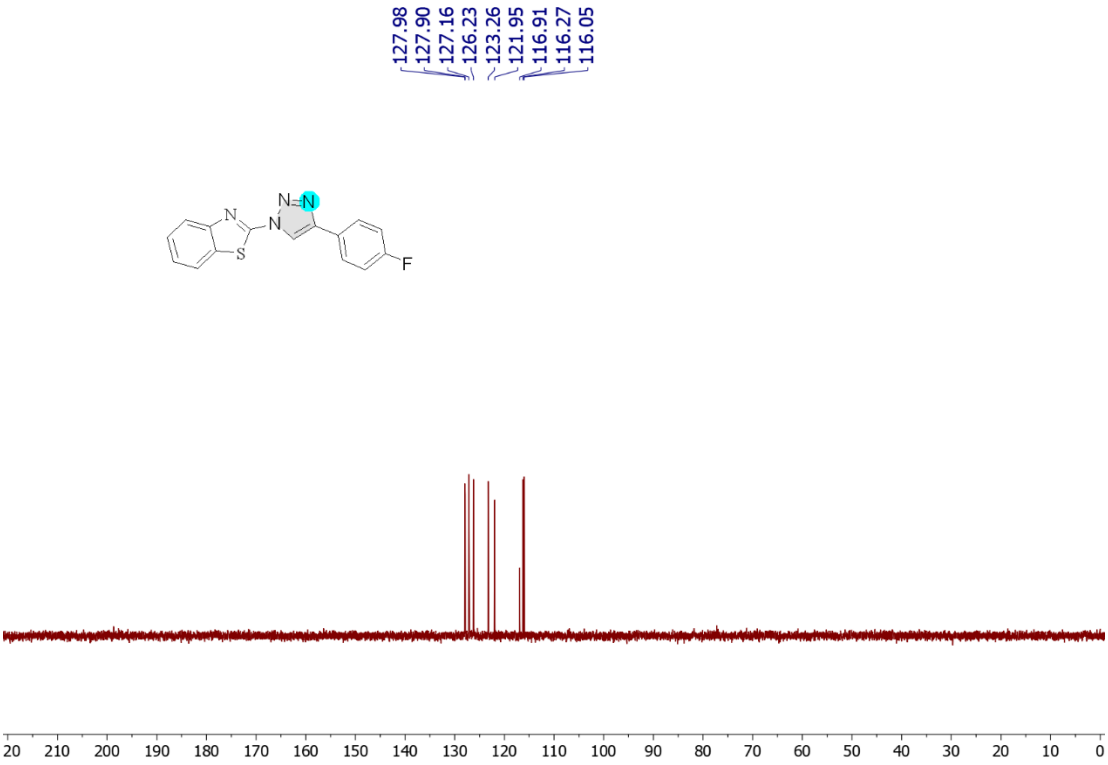
[1]H-NMR of 2-(4-(4-fluorophenyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4c)



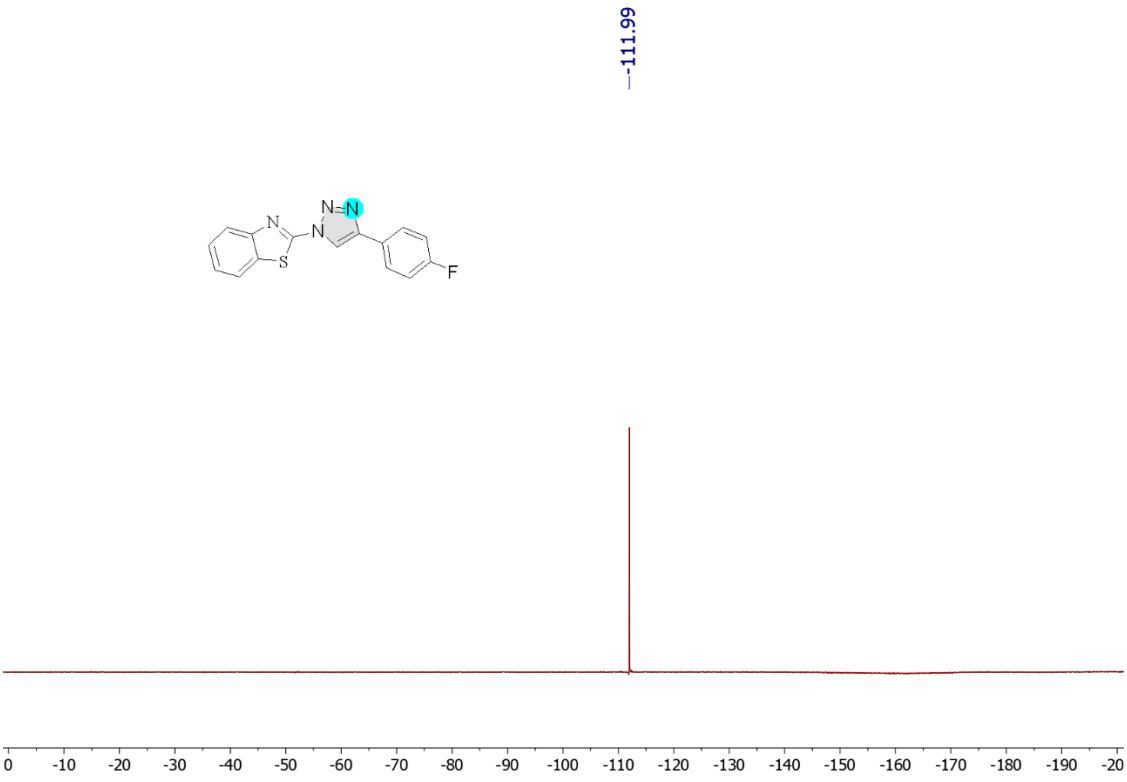
[13]C-NMR of 2-(4-(4-fluorophenyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4c)



DEPT of 2-(4-(4-fluorophenyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4c)



^{19}F-NMR of 2-(4-(4-fluorophenyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4c)



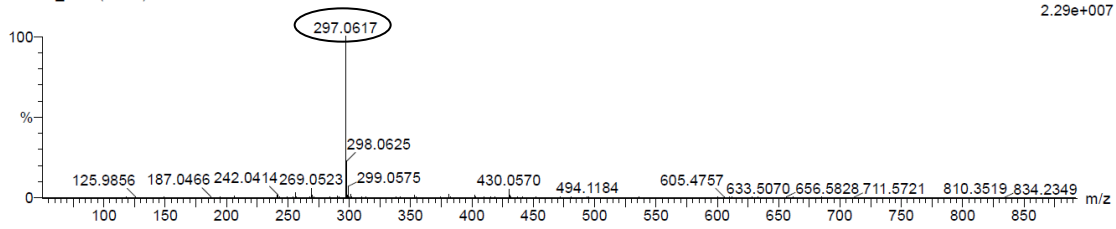
HRMS of 2-(4-(4-fluorophenyl)-*1H*-1,2,3-triazol-1-yl)benzo[*d*]thiazole (4c)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

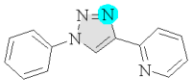
Monoisotopic Mass, Even Electron Ions
24 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-4 F: 0-1 S: 0-1

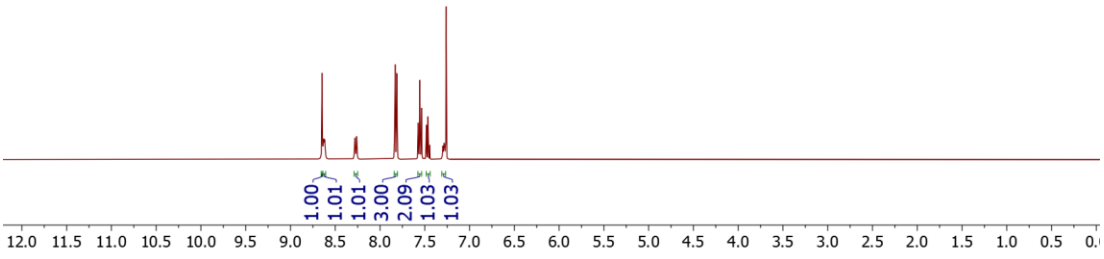
MS-Het-F(N) QMI DIVISION, CSIR-IIIM JAMMU 30-Apr-2024
Xevo G2-XS QTOF YFC2015 12:08:33
300424_13 5 (0.121) 1: TOF MS ES+
2.29e+007



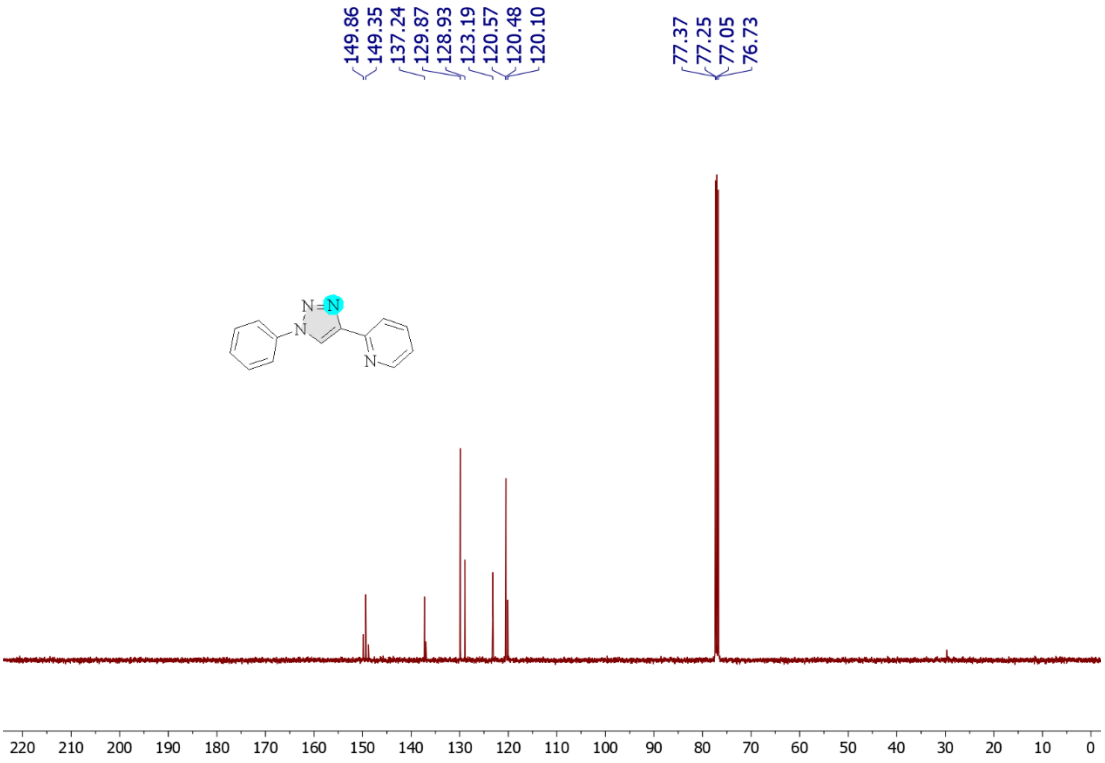
Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
297.0617	297.0610	0.7	2.4	12.5	1207.1	n/a	n/a	C15 H10 N4 F S

^{1}H-NMR of 2-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)pyridine (4d)

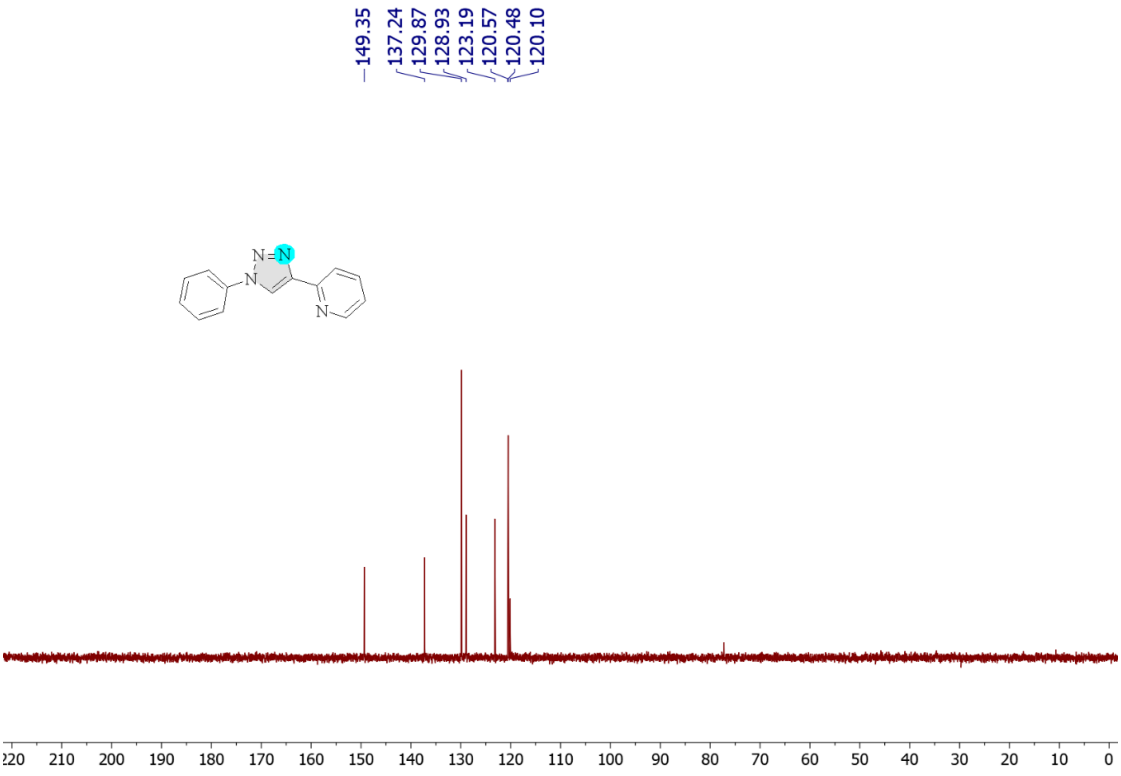




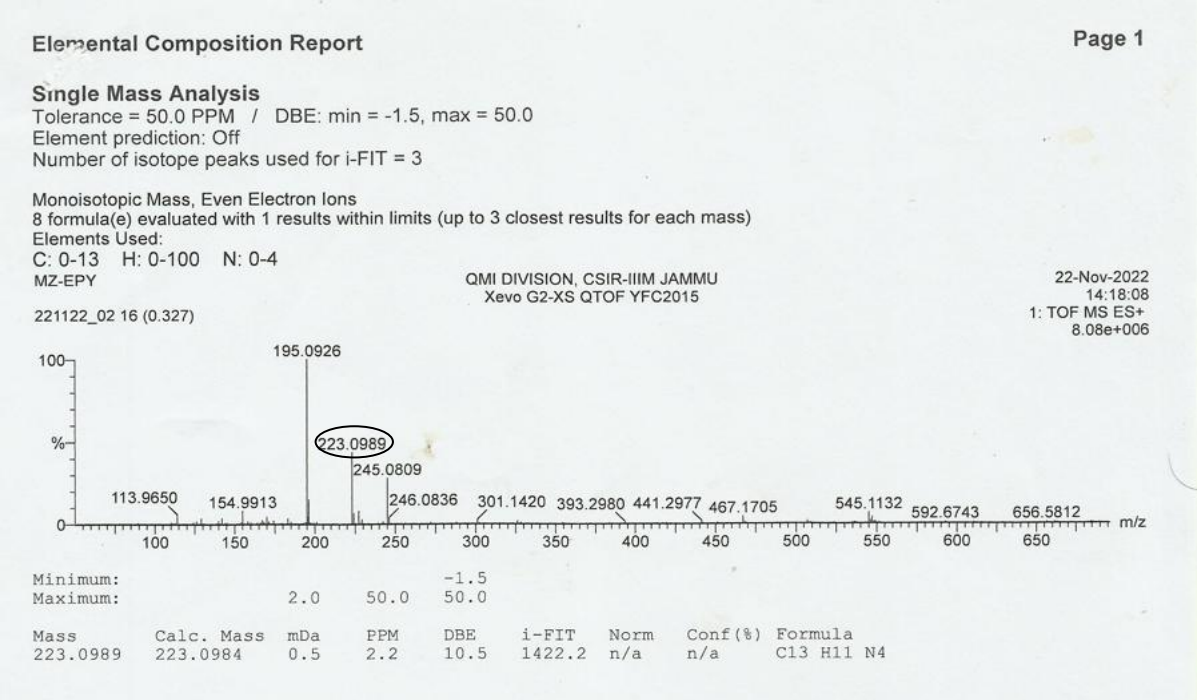
^{13}C-NMR of 2-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)pyridine (4d)



DEPT of 2-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)pyridine (4d)



HRMS of 2-(1-Phenyl-1*H*-1,2,3-triazol-4-yl)pyridine (4d)



Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-4

MZ-EPY

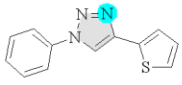
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

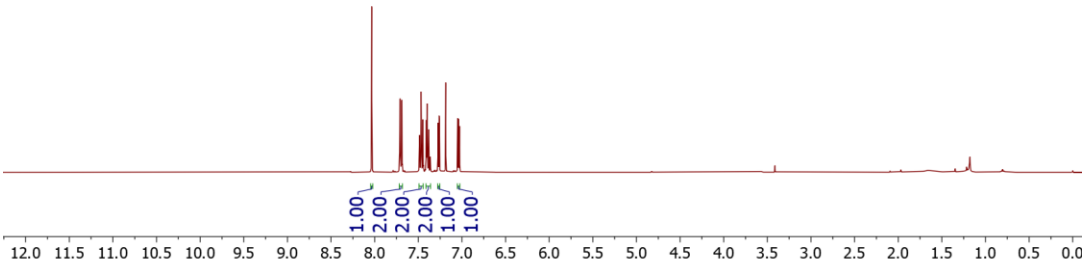
22-Nov-2022
14:18:08
1: TOF MS ES+
8.08e+006

221122_02 16 (0.327)

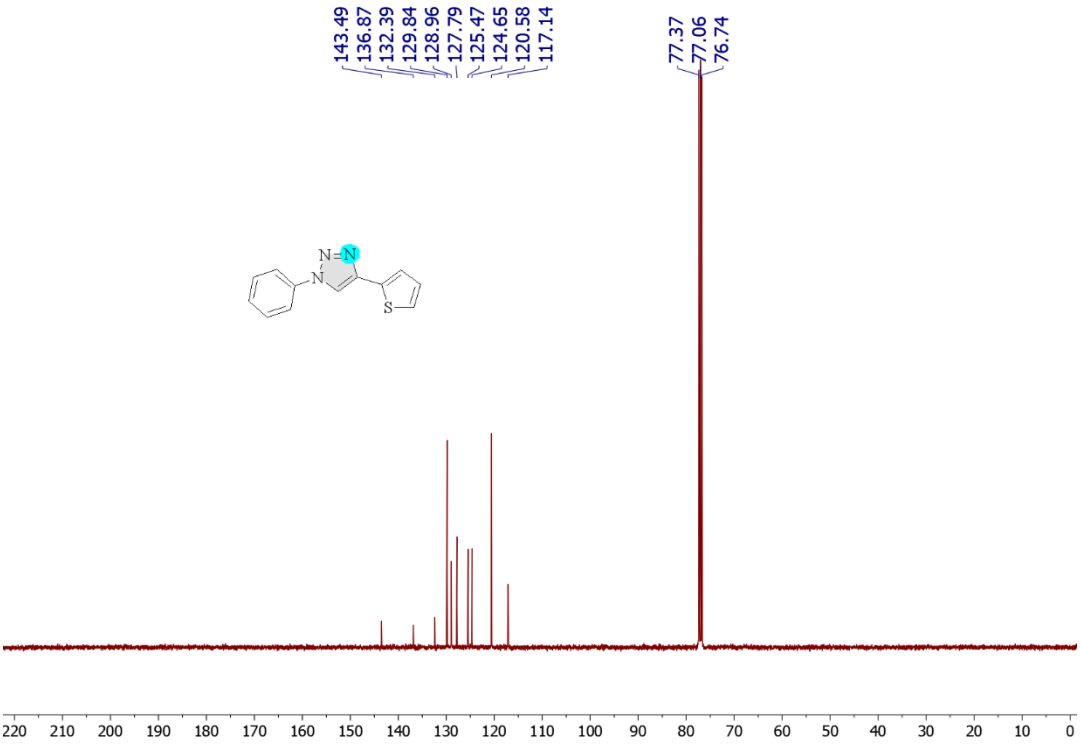
Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
223.0989	223.0984	0.5	2.2	10.5	1422.2	n/a	n/a	C13 H11 N4

^{1}H-NMR of 1-Phenyl-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4e)

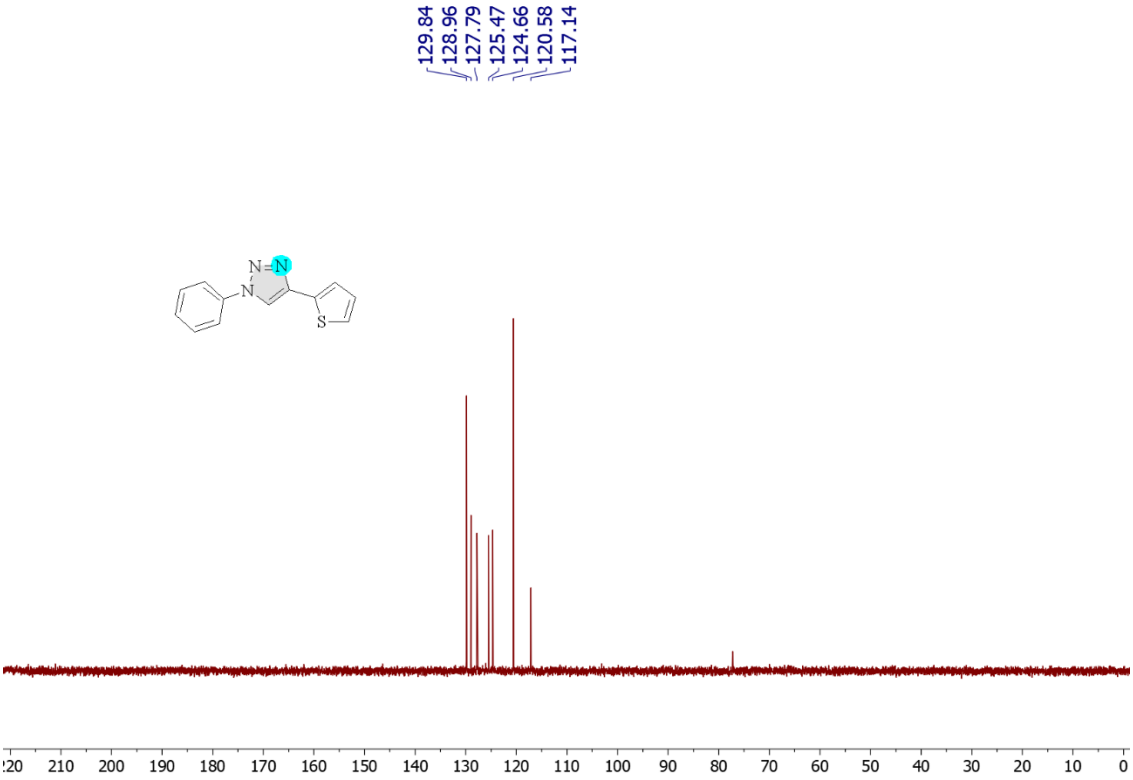




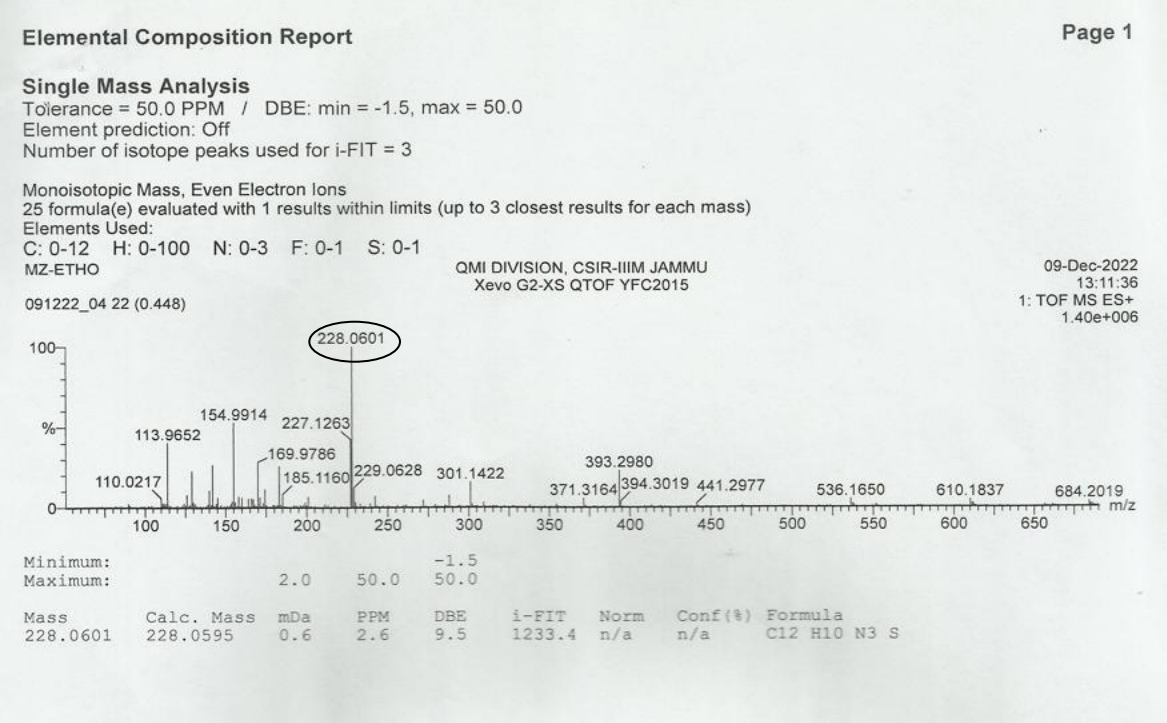
^{13}C-NMR of 1-Phenyl-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4e)



DEPT of 1-Phenyl-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4e)



HRMS of 1-Phenyl-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4e)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-12 H: 0-100 N: 0-3 F: 0-1 S: 0-1

MZ-ETHO

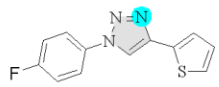
091222_04 22 (0.448)

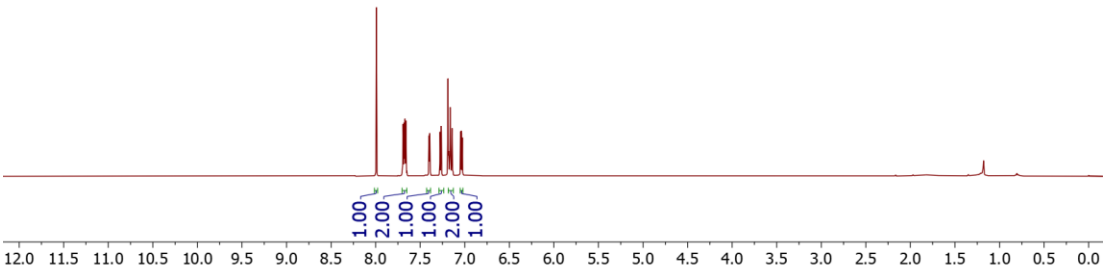
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

09-Dec-2022
13:11:36
1: TOF MS ES+
1.40e+006

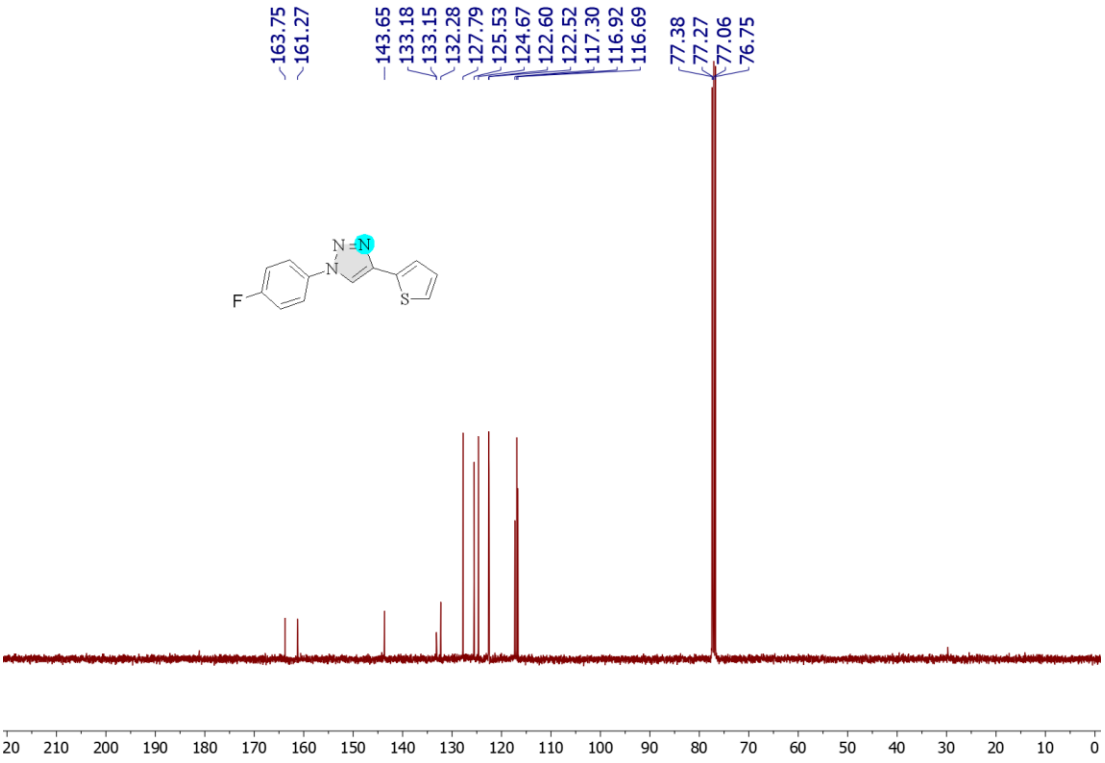
Minimum:				-1.5			
Maximum:		2.0	50.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
228.0601	228.0595	0.6	2.6	9.5	1233.4	n/a	n/a	C12 H10 N3 S

^{1}H-NMR of 1-(4-Fluorophenyl)-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4f)

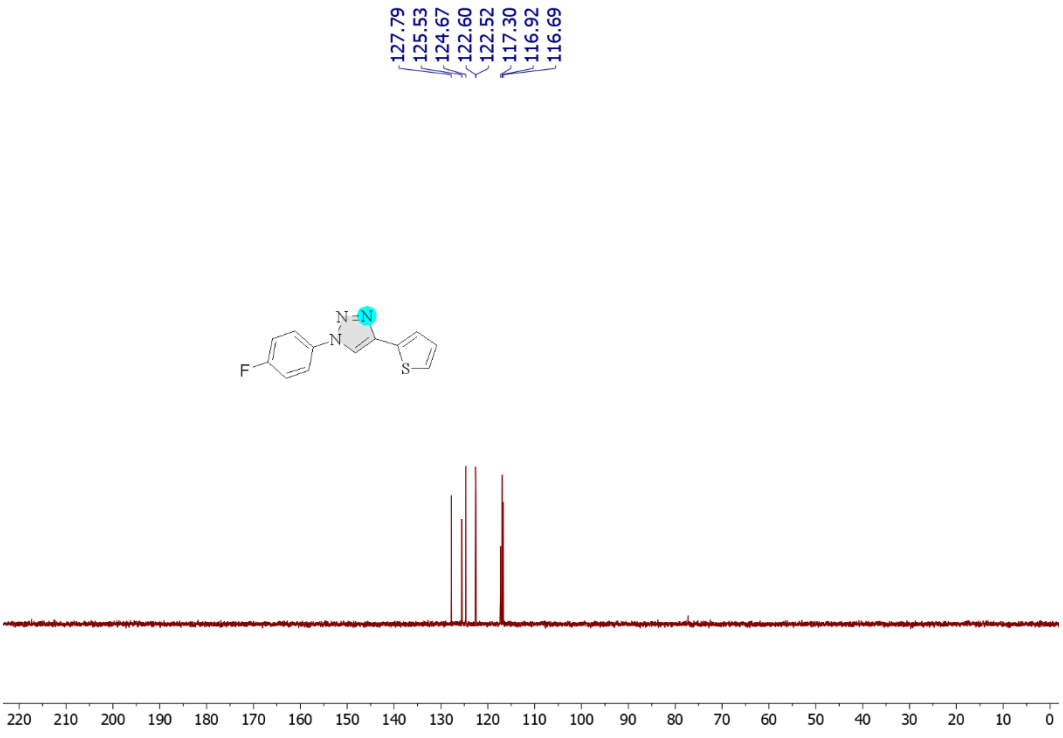




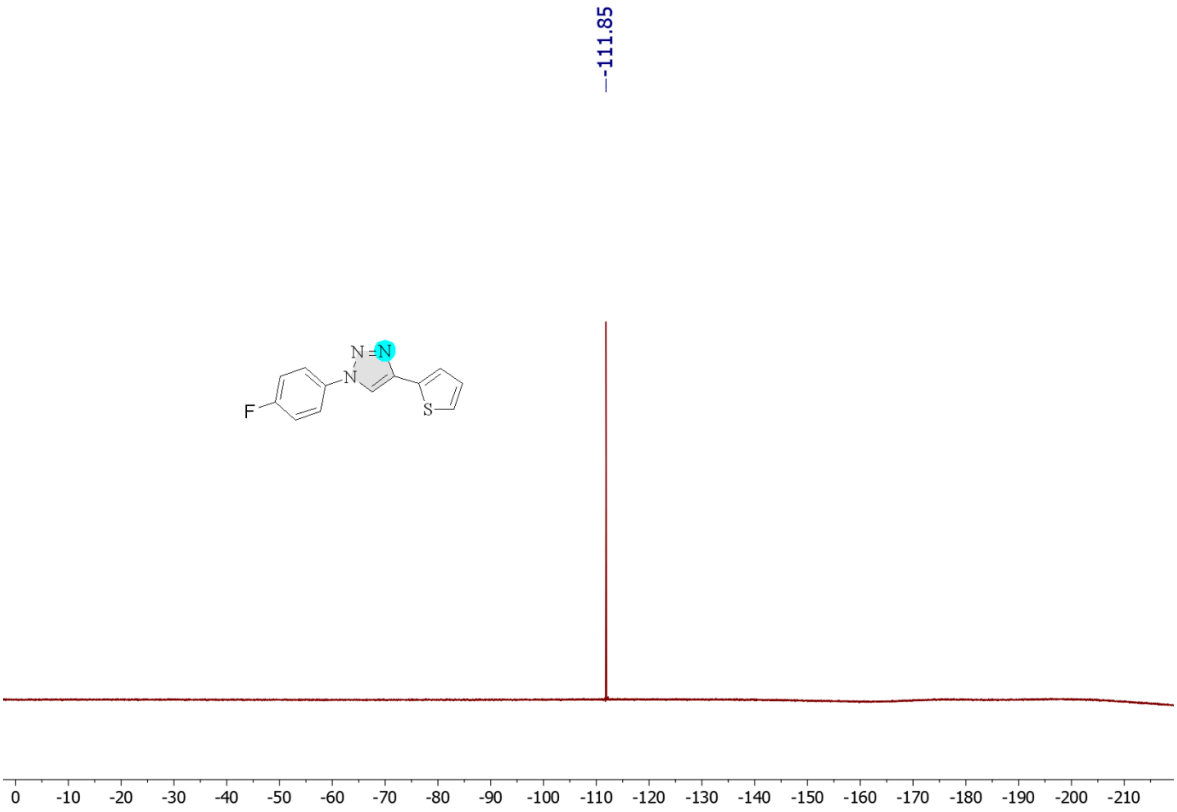
^{13}C-NMR of 1-(4-Fluorophenyl)-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4f)



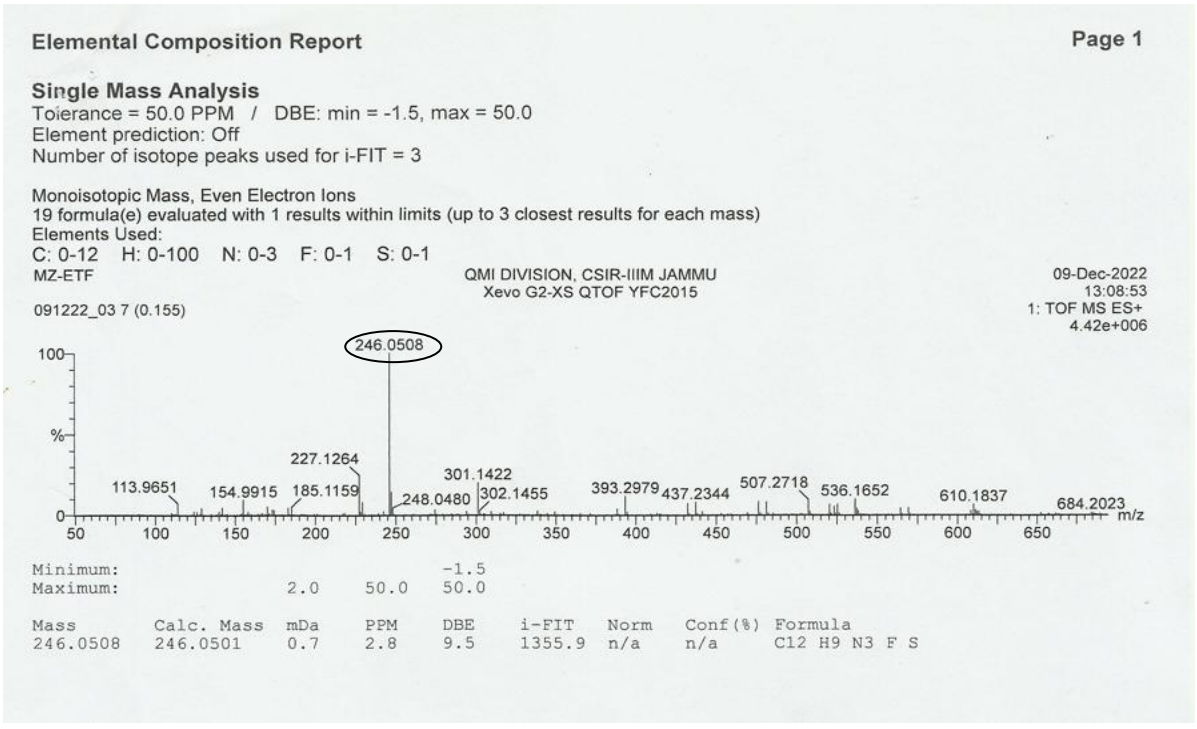
DEPT of 1-(4-Fluorophenyl)-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4f)



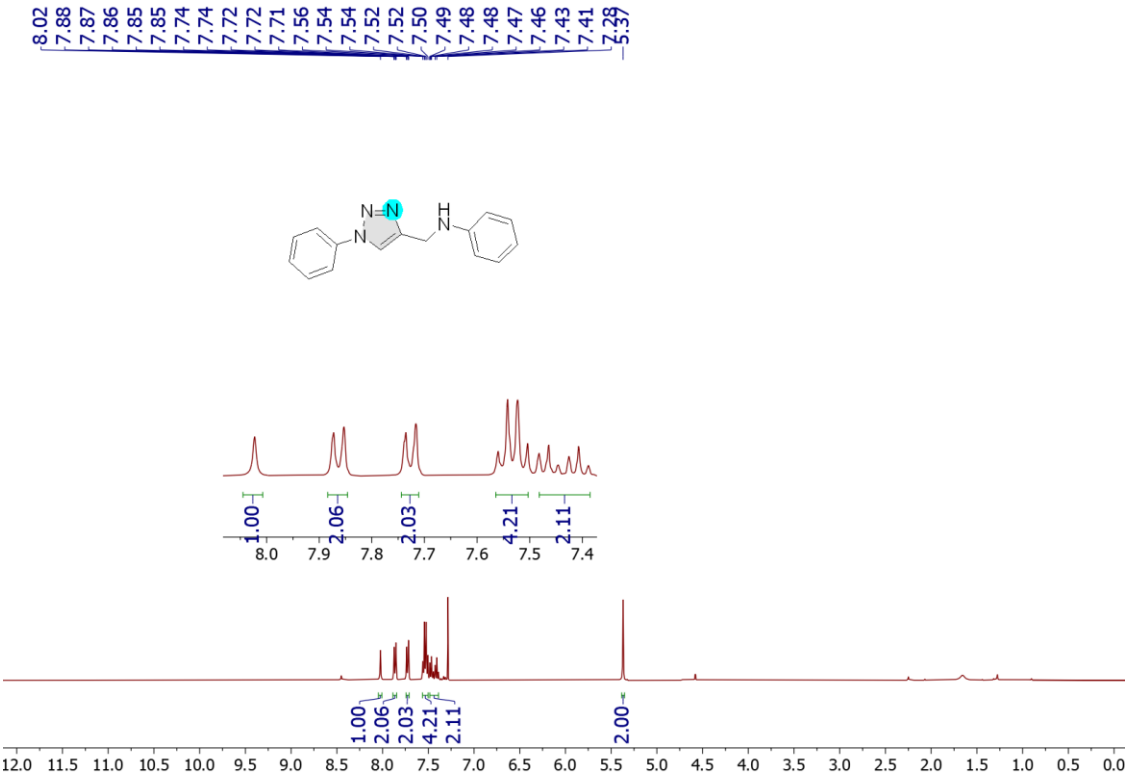
^{19}F-NMR of 1-(4-Fluorophenyl)-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4f)



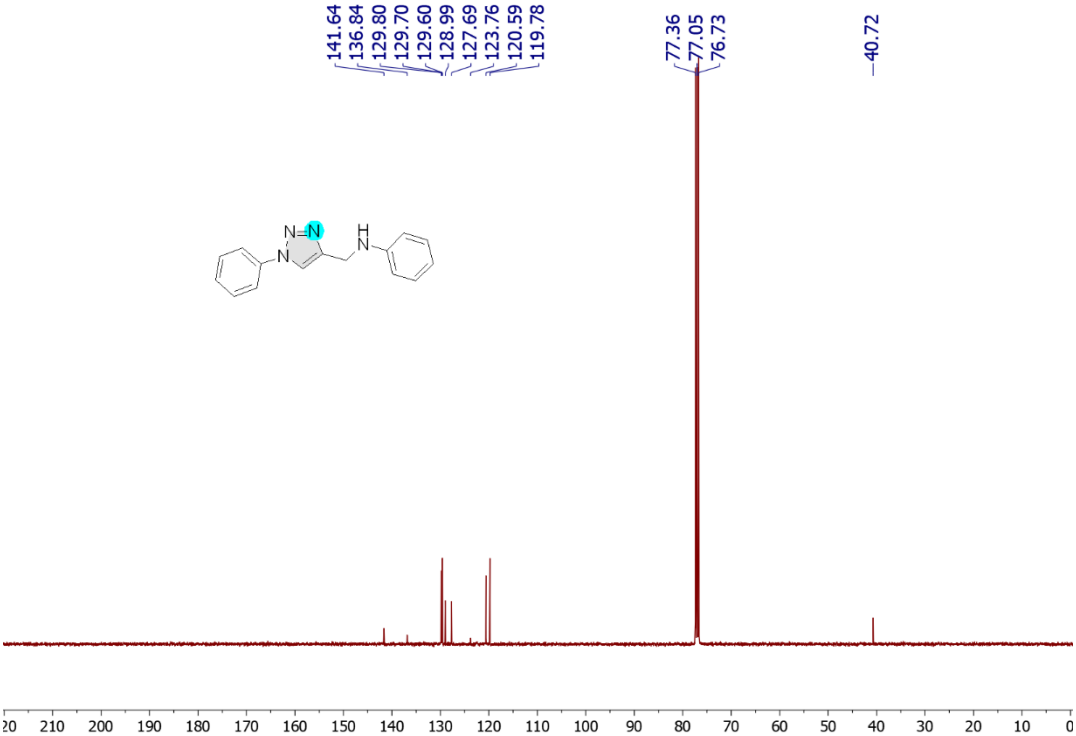
HRMS of 1-(4-Fluorophenyl)-4-(thiophen-2-yl)-1*H*-1,2,3-triazole (4f)



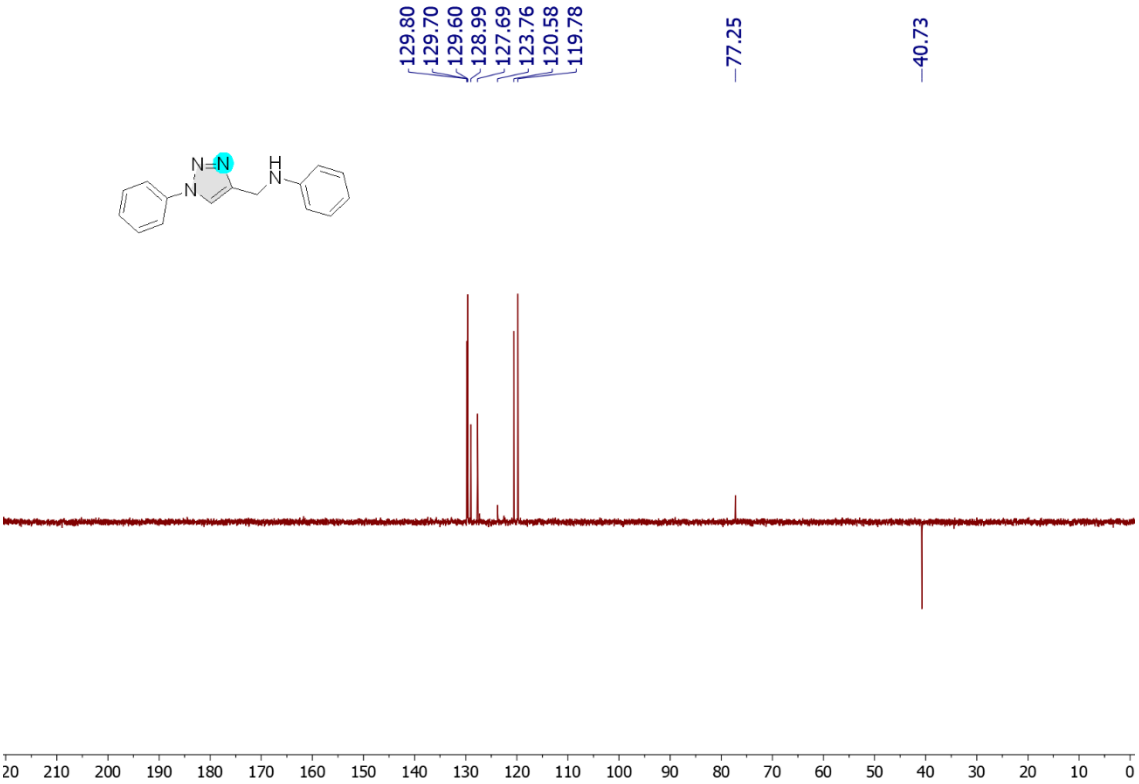
[1]H-NMR of N-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)aniline (5a)



[13]C-NMR of N-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)aniline (5a)



DEPT of N-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)aniline (5a)



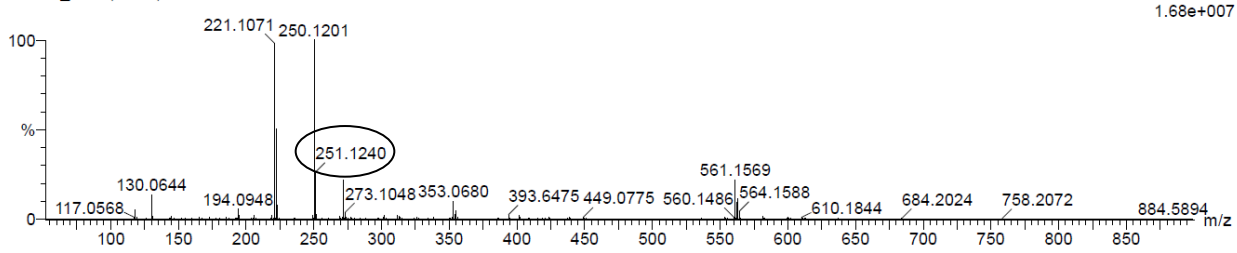
HRMS of N-((1-phenyl-1*H*-1,2,3-triazol-4-yl)methyl)aniline (5a)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

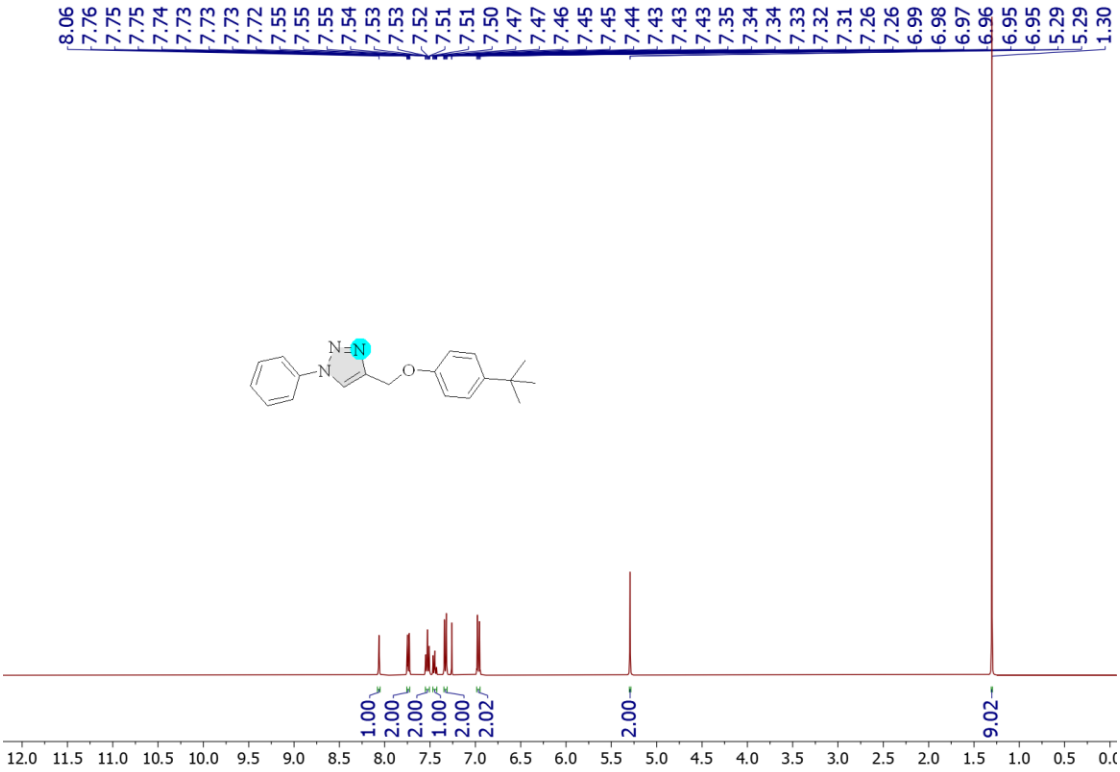
Monoisotopic Mass, Even Electron Ions
8 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-4

MS-(NHF) 2 — QMI DIVISION, CSIR-IIIM JAMMU, Xevo G2-XS QTOF YFC2015 — 30-Apr-2024 12:05:58
300424_12 5 (0.121) — 1: TOF MS ES+ 1.68e+007

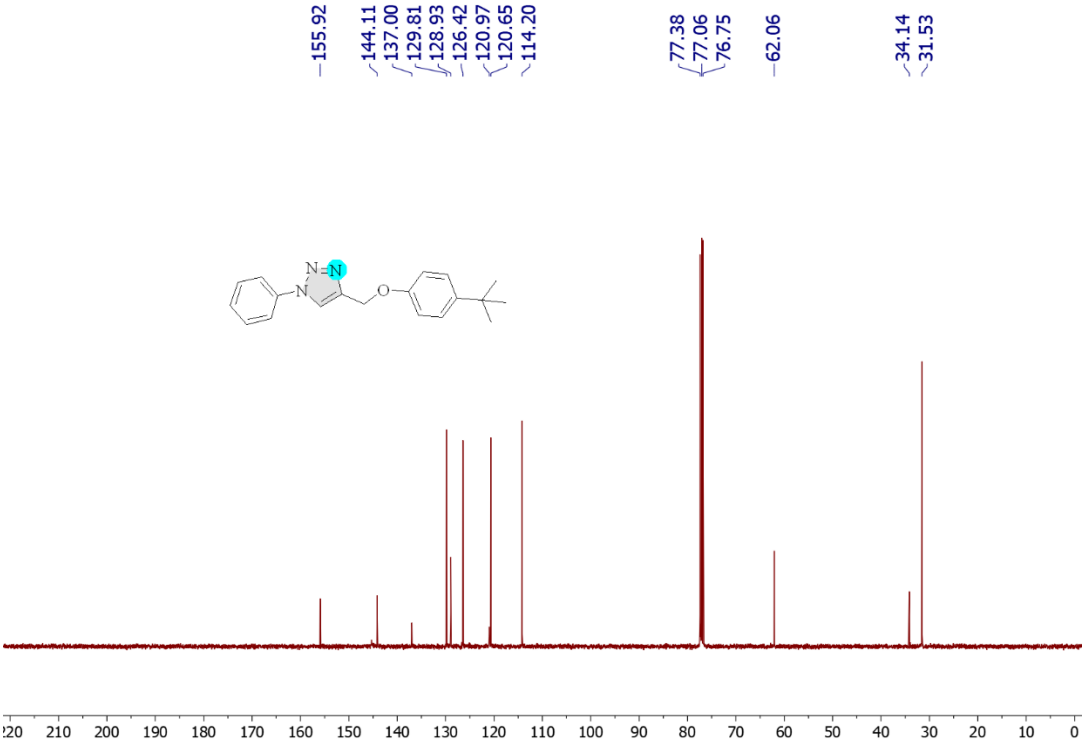


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
251.1240	251.1297	-5.7	-22.7	10.5	1427.4	n/a	n/a	C15 H15 N4

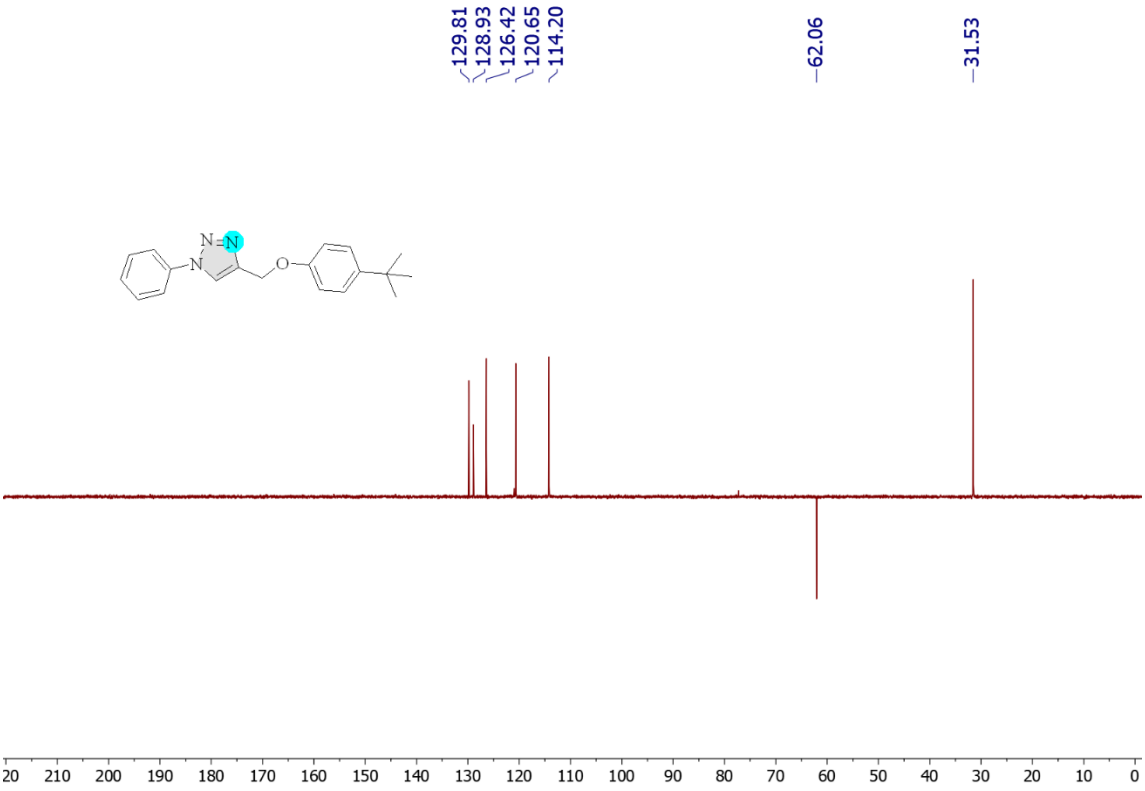
^{1}H-NMR of 4-((4-(Tert-butyl)phenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (5b)



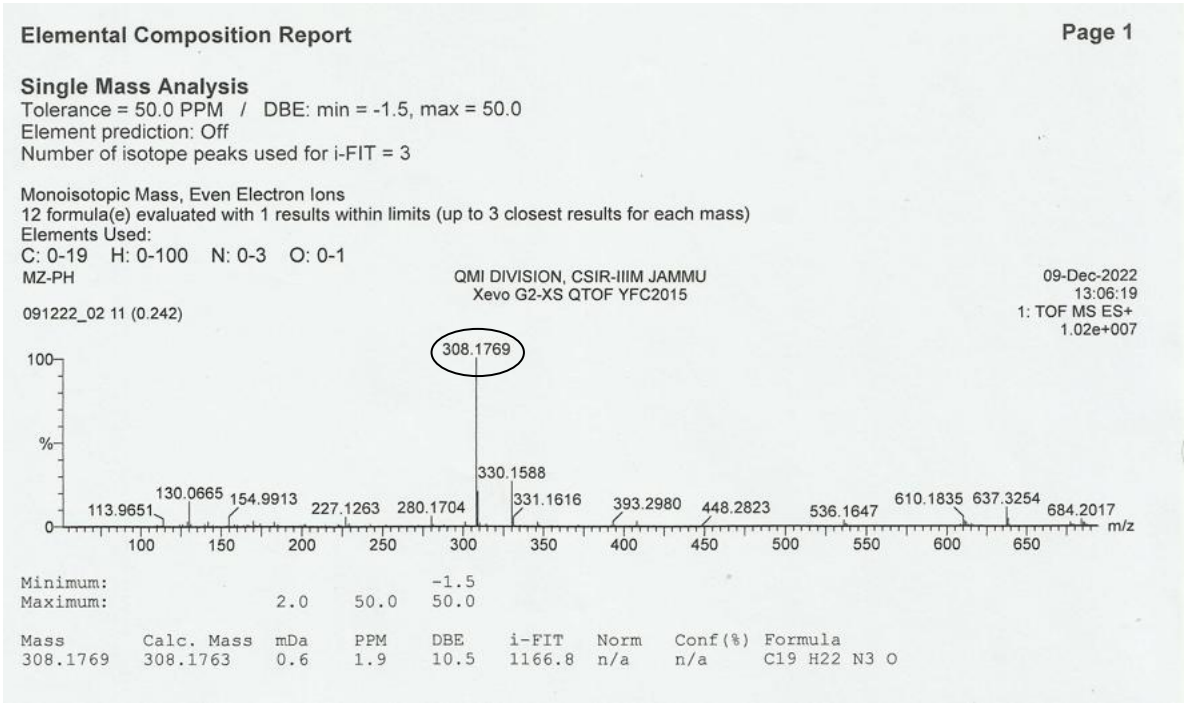
^{13}C-NMR of 4-((4-(Tert-butyl)phenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (5b)



DEPT of 4-((4-(Tert-butyl)phenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (5b)



HRMS of 4-((4-(Tert-butyl)phenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (5b)



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-3 O: 0-1

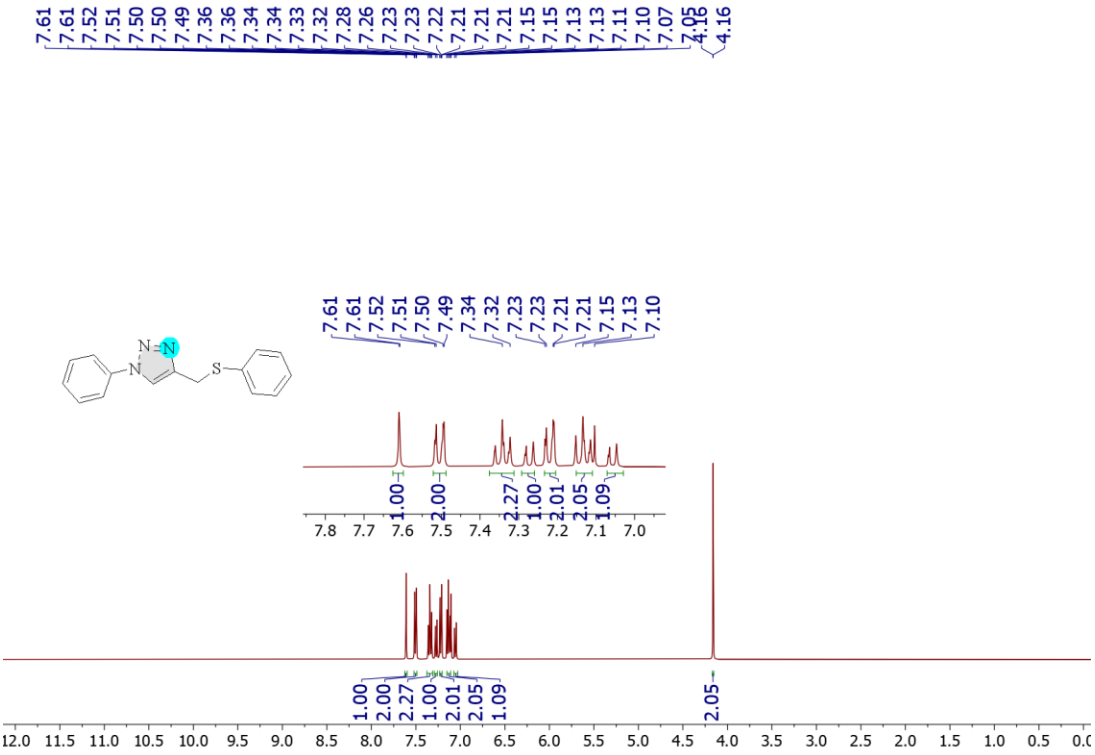
MZ-PH
091222_02 11 (0.242)

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

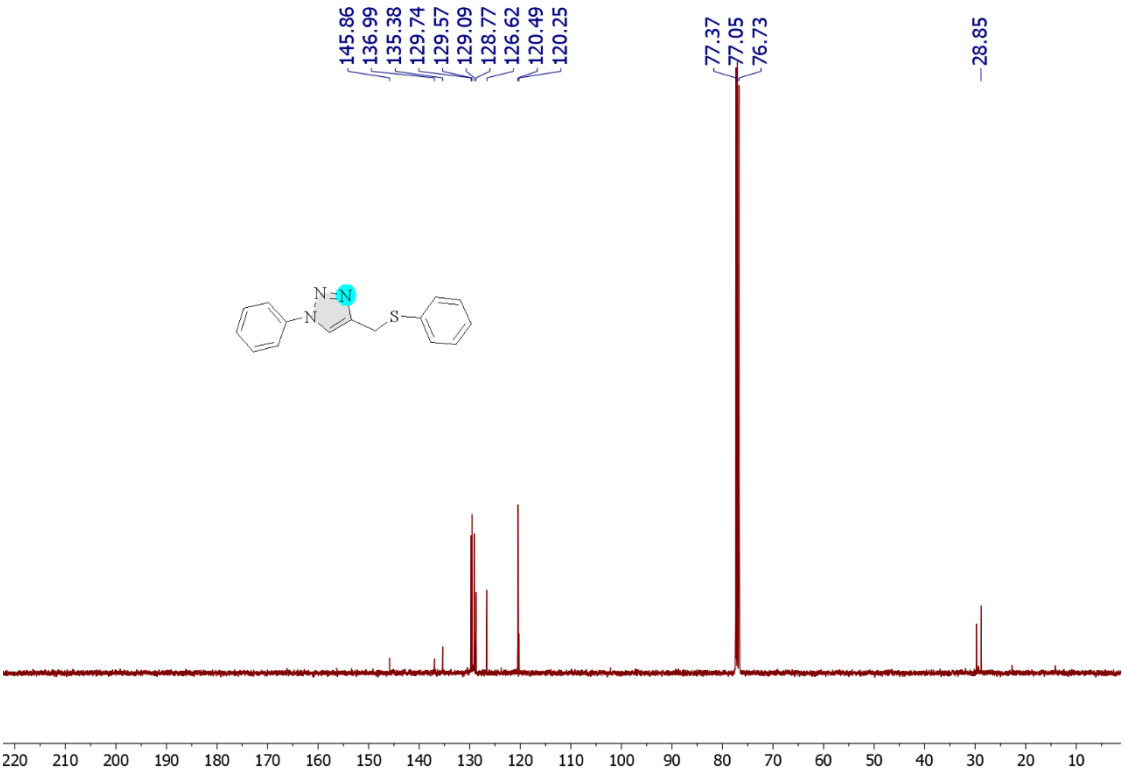
09-Dec-2022
13:06:19
1: TOF MS ES+
1.02e+007

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
308.1769	308.1763	0.6	1.9	10.5	1166.8	n/a	n/a	C19 H22 N3 O

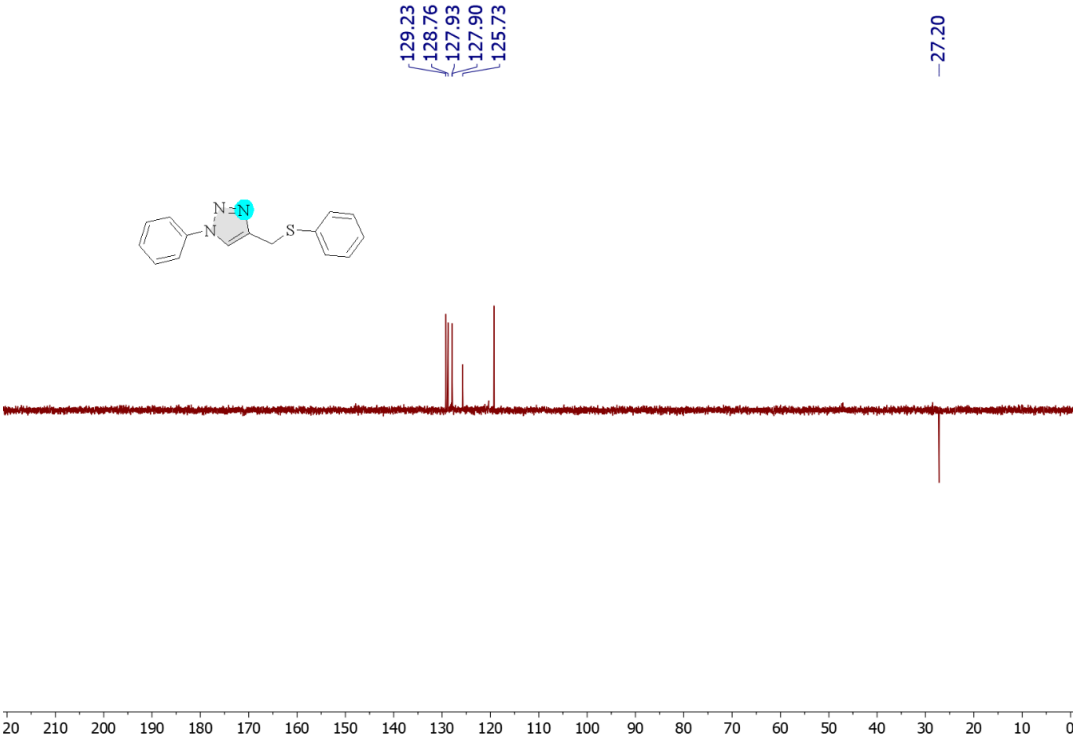
[1]H-NMR of 1-Phenyl-4-((phenylthio)methyl)-1*H*-1,2,3-triazole (5c)



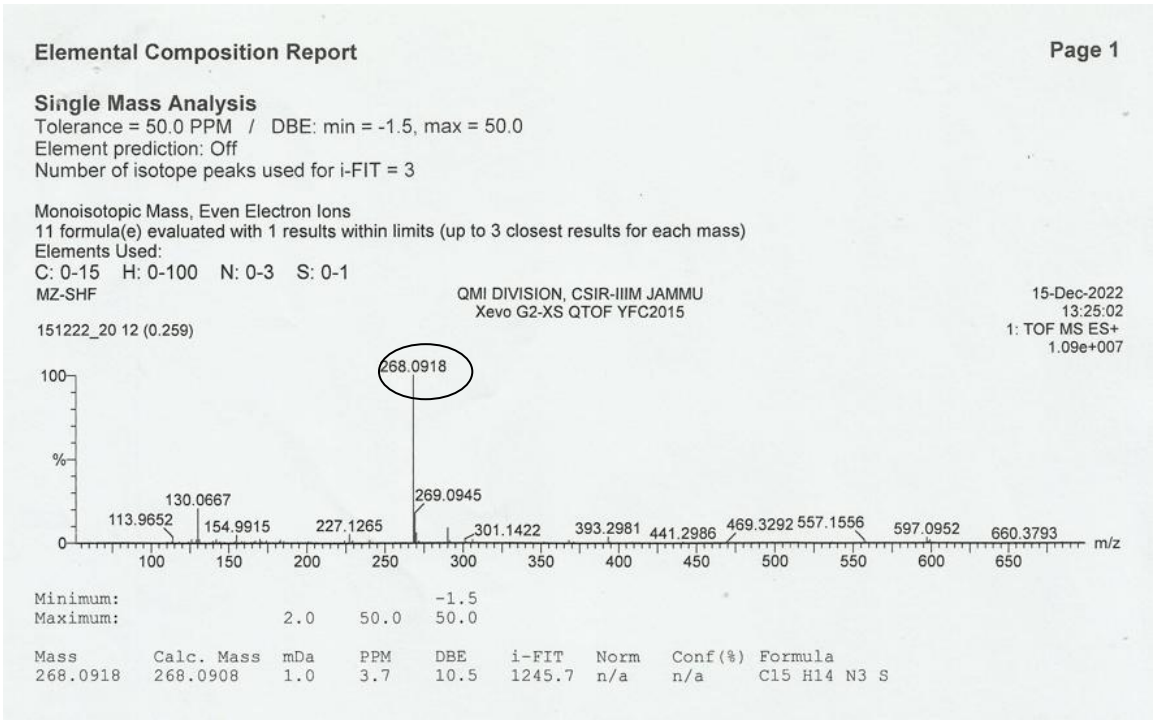
[13]C-NMR of 1-Phenyl-4-((phenylthio)methyl)-1*H*-1,2,3-triazole (5c)



DEPT of 1-Phenyl-4-((phenylthio)methyl)-1*H*-1,2,3-triazole (5c)



HRMS of 1-Phenyl-4-((phenylthio)methyl)-1*H*-1,2,3-triazole (5c)



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-3 S: 0-1

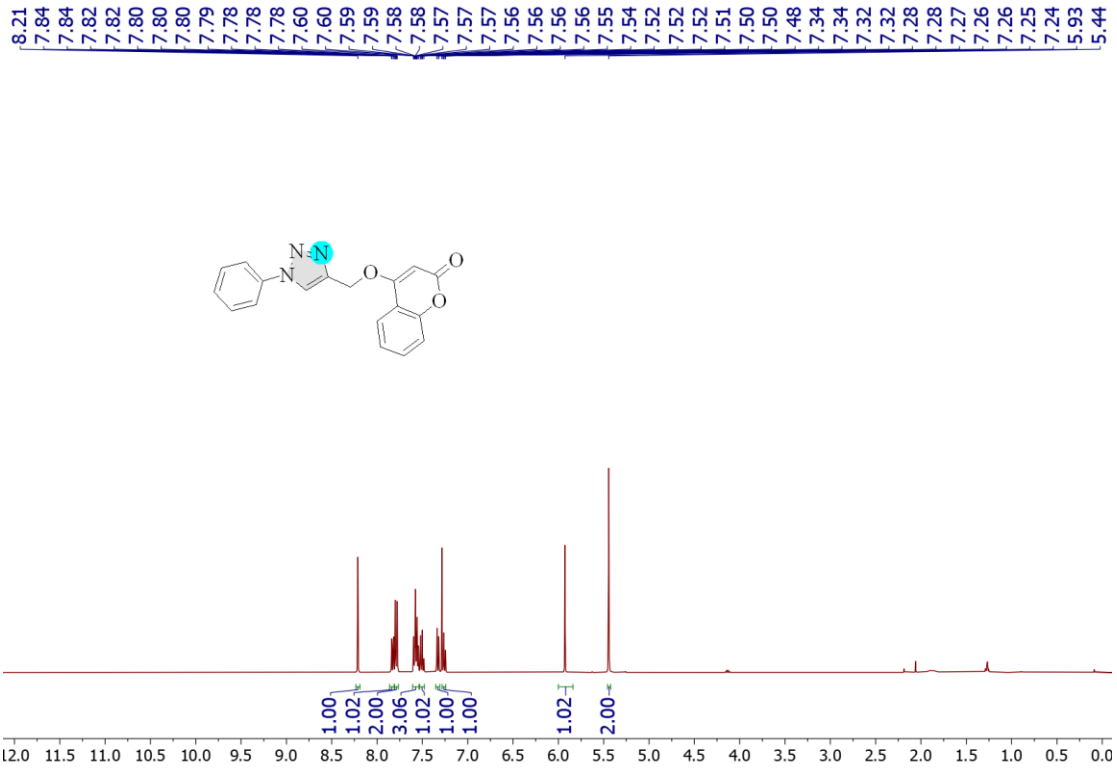
MZ-SHF
151222_20 12 (0.259)

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

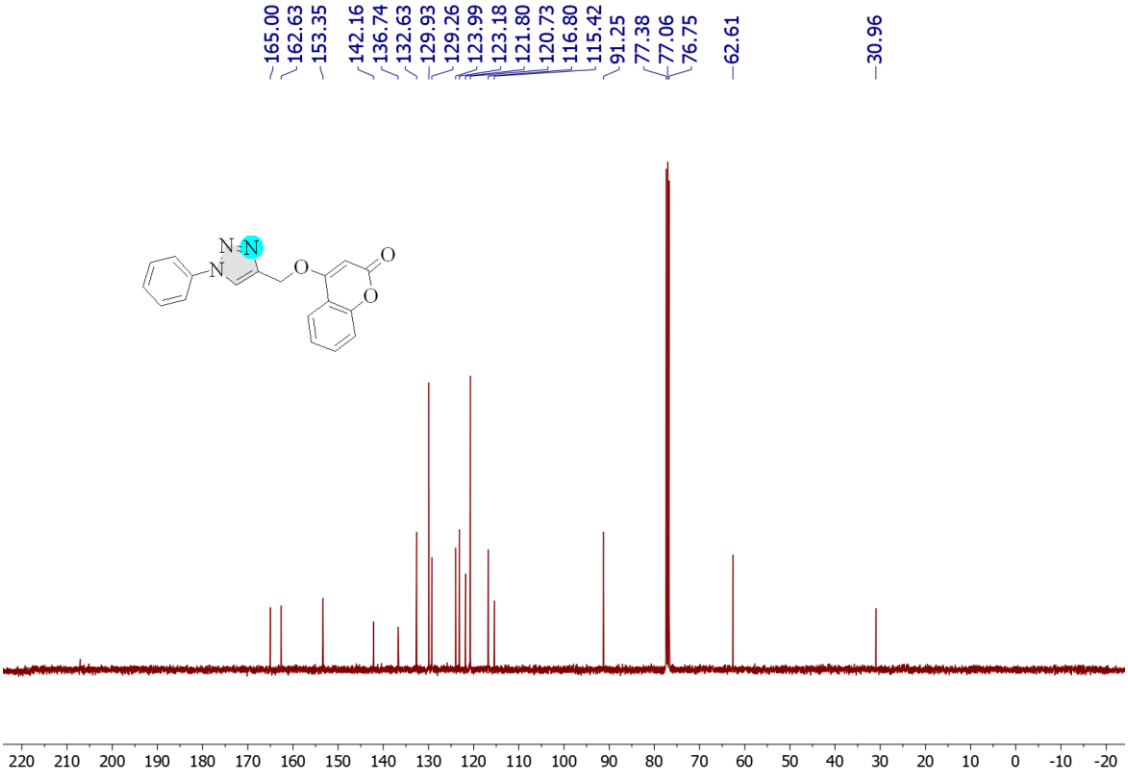
15-Dec-2022
13:25:02
1: TOF MS ES+
1.09e+007

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
268.0918	268.0908	1.0	3.7	10.5	1245.7	n/a	n/a	C15 H14 N3 S

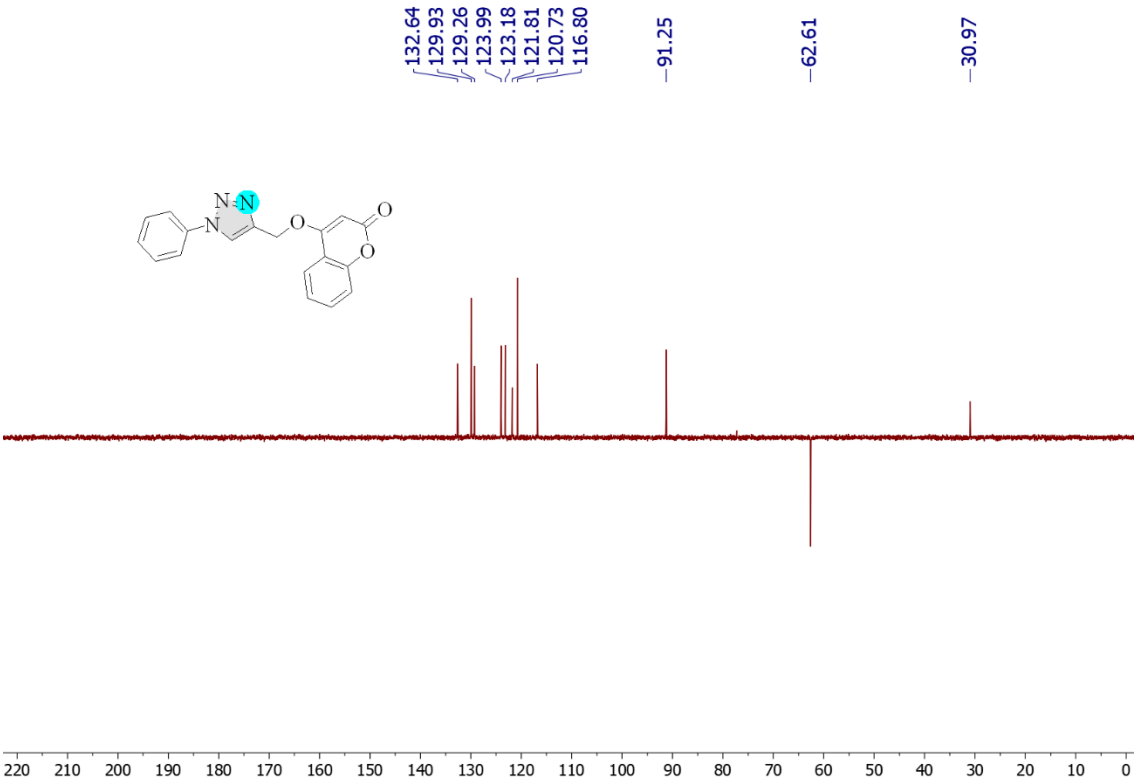
[1]H-NMR of 4-((1-Phenyl-*1H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (6a)



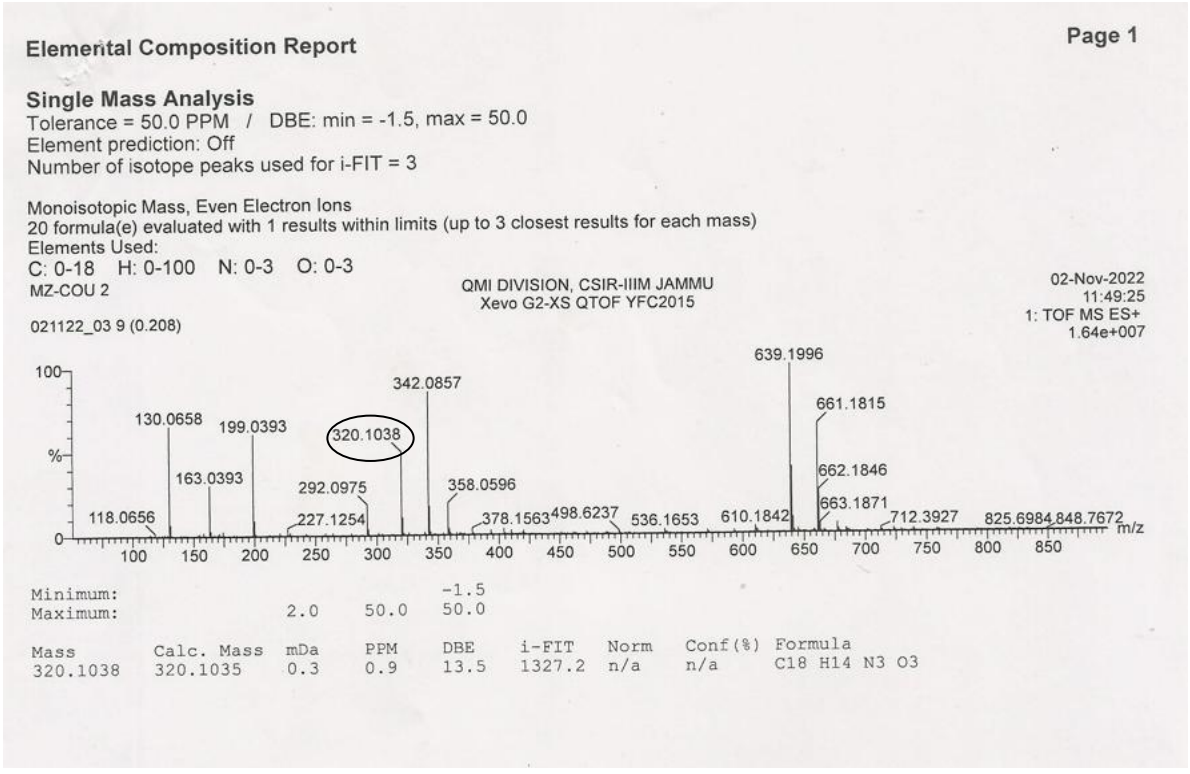
[13]C-NMR of 4-((1-Phenyl-*1H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (6a)



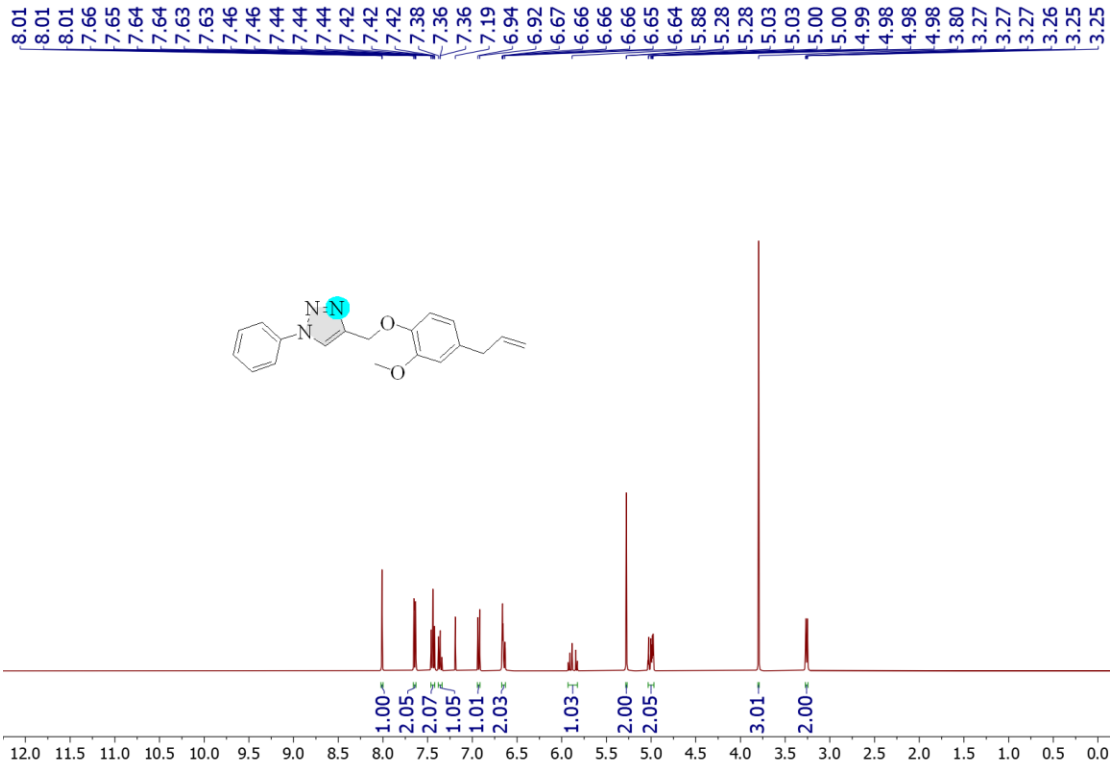
DEPT of 4-((1-Phenyl-*1H*-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (6a)



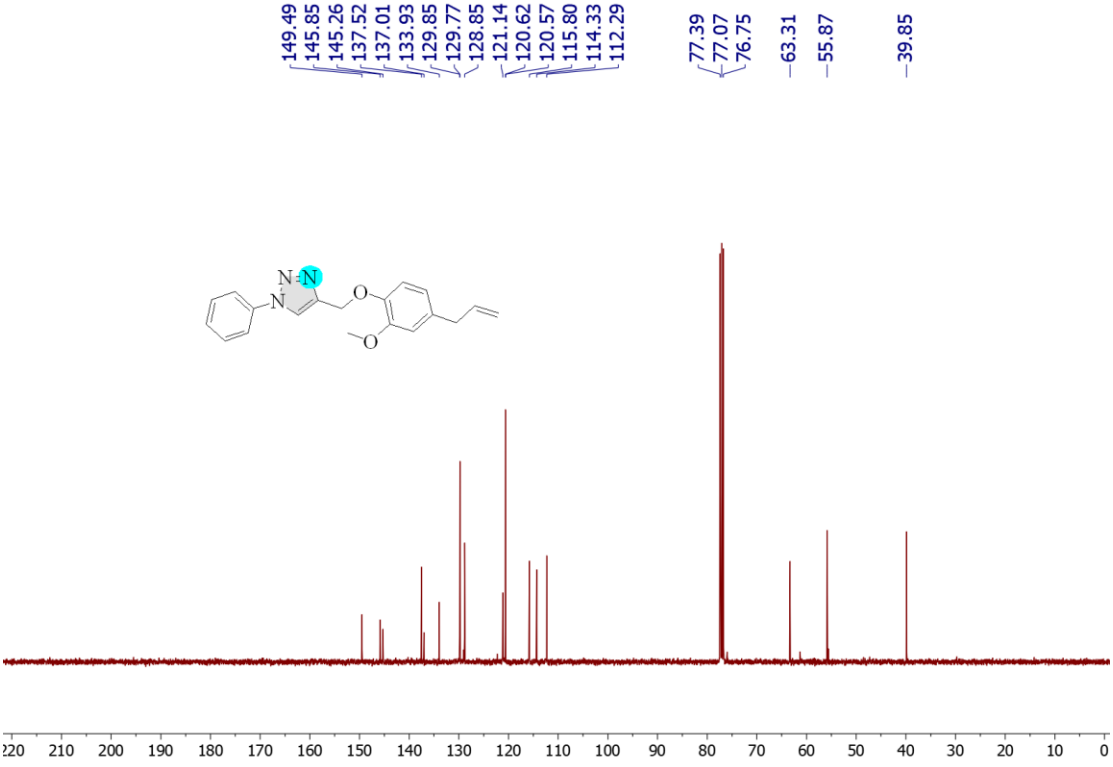
HRMS of 4-((1-Phenyl-1H-1,2,3-triazol-4-yl)methoxy)-2*H*-chromen-2-one (6a)



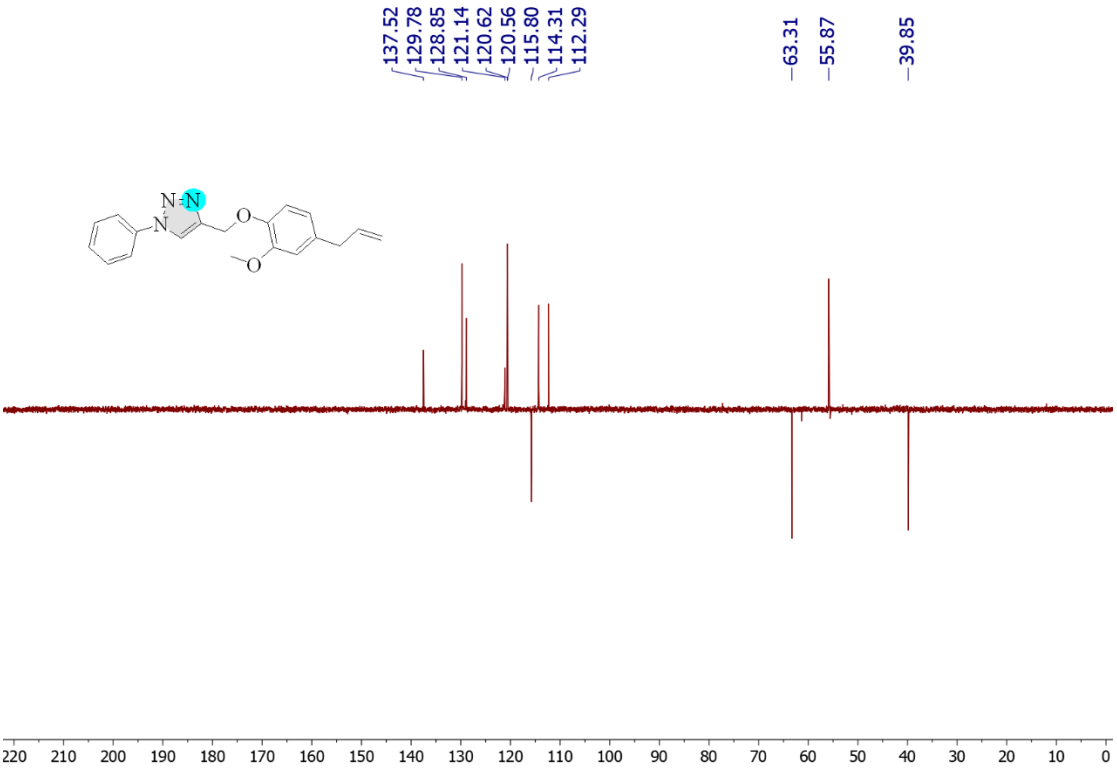
[1]H-NMR of 4-((4-Allyl-2-methoxyphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6b)



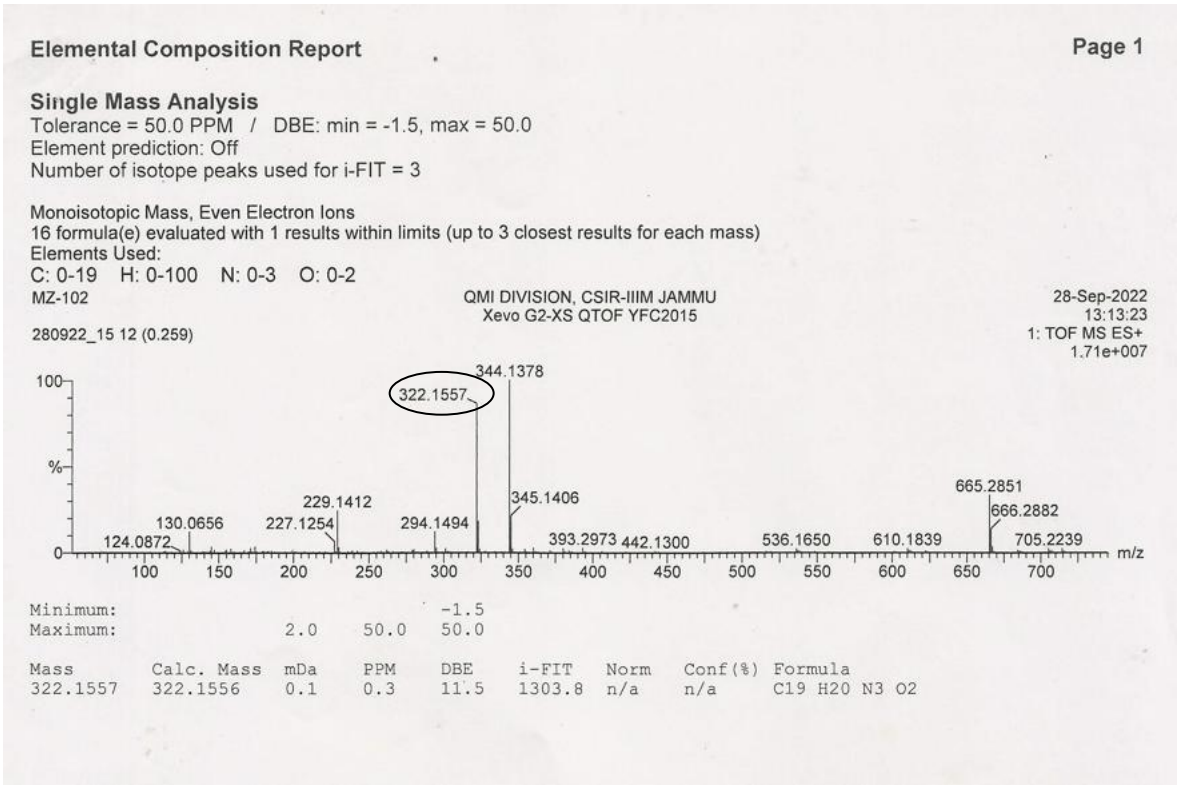
[13]C-NMR of 4-((4-Allyl-2-methoxyphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6b)



DEPT of 4-((4-Allyl-2-methoxyphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6b)



HRMS of 4-((4-Allyl-2-methoxyphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6b)



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-3 O: 0-2

MZ-102
280922_15 12 (0.259)

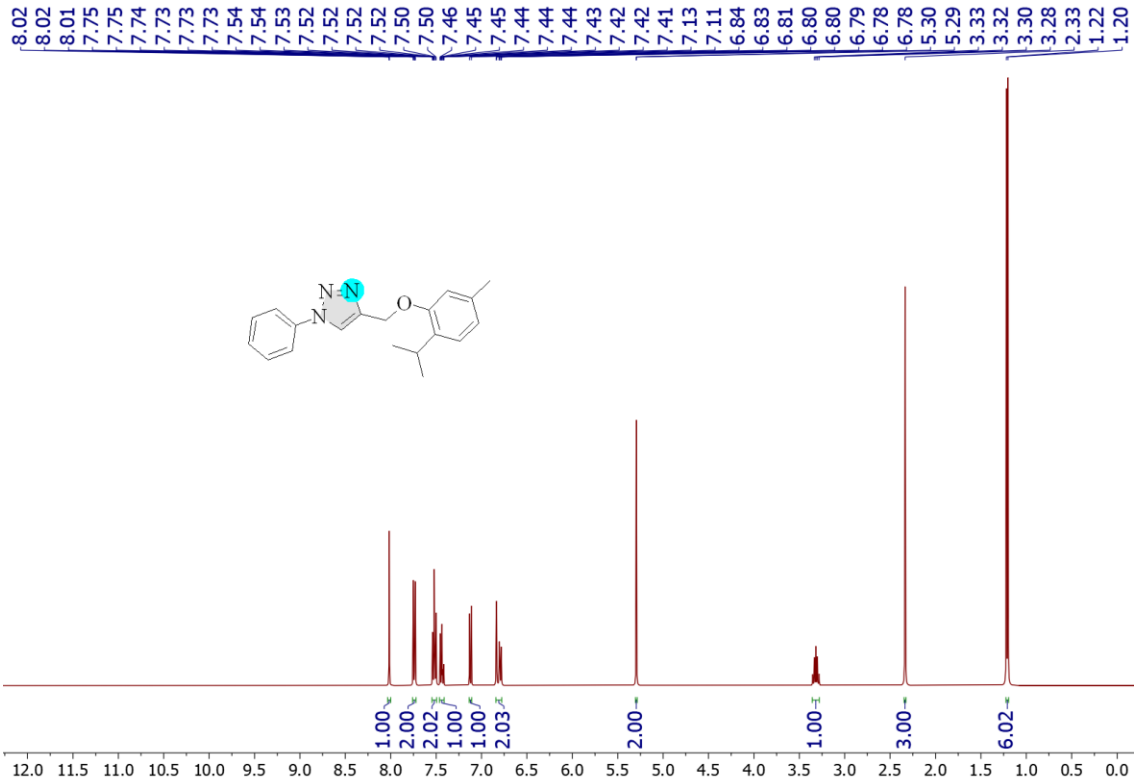
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

28-Sep-2022
13:13:23
1: TOF MS ES+
1.71e+007

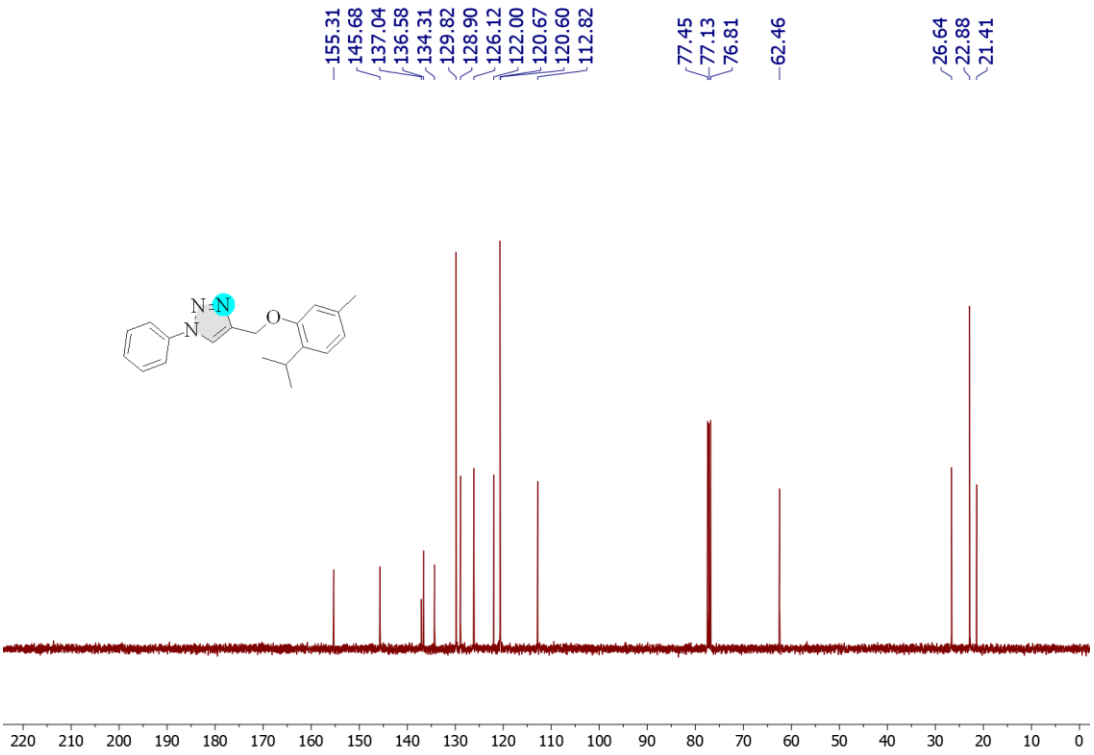
100
%
0
344.1378
322.1557
345.1406
229.1412
227.1254
294.1494
130.0656
124.0872
393.2973
442.1300
536.1650
610.1839
665.2851
666.2882
705.2239
100 150 200 250 300 350 400 450 500 550 600 650 700 m/z

Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
322.1557	322.1556	0.1	0.3	11.5	1303.8	n/a	n/a	C19 H20 N3 O2

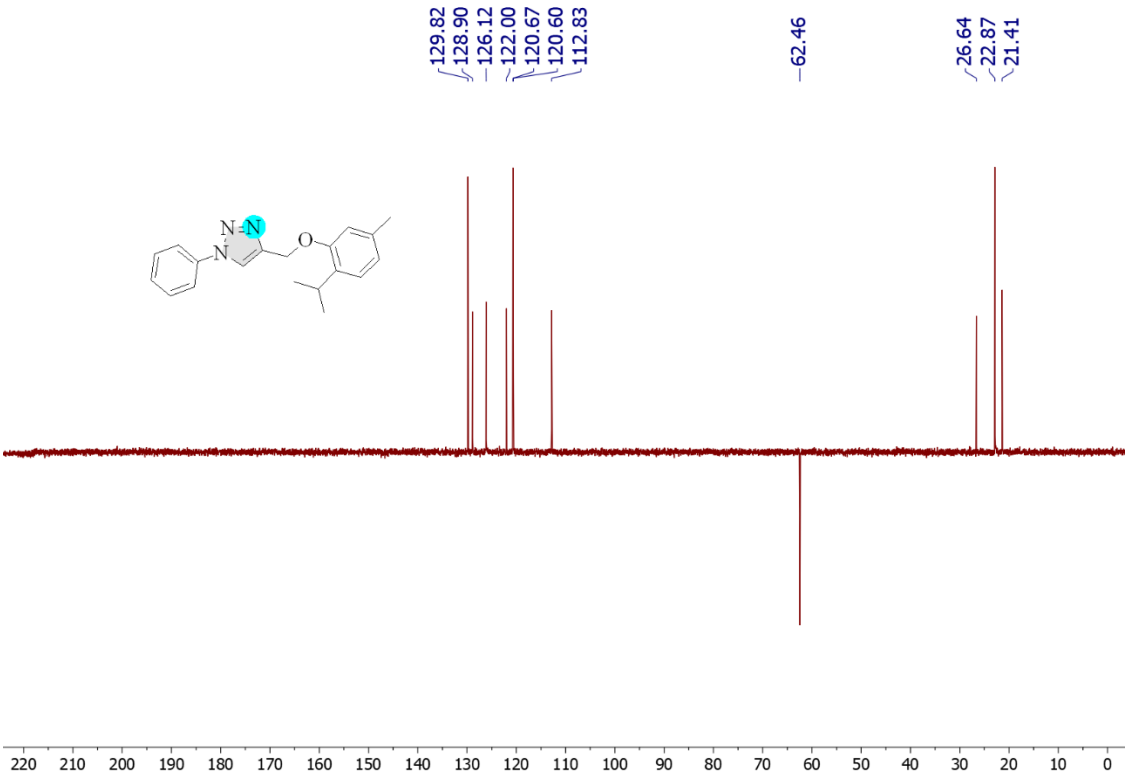
^{1}H NMR of 4-((2-Isopropyl-5-methylphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6c)



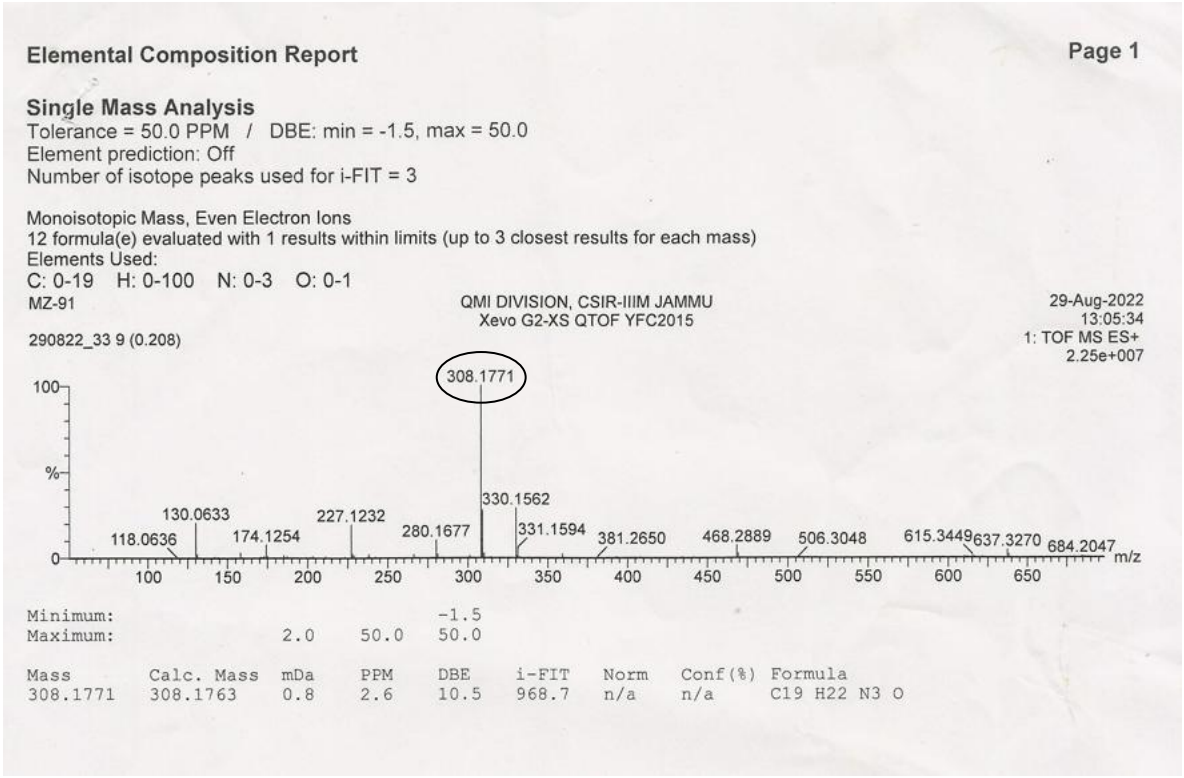
^{13}C NMR of 4-((2-Isopropyl-5-methylphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6c)



DEPT of 4-((2-Isopropyl-5-methylphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6c)



HRMS of 4-((2-Isopropyl-5-methylphenoxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6c)



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-3 O: 0-1

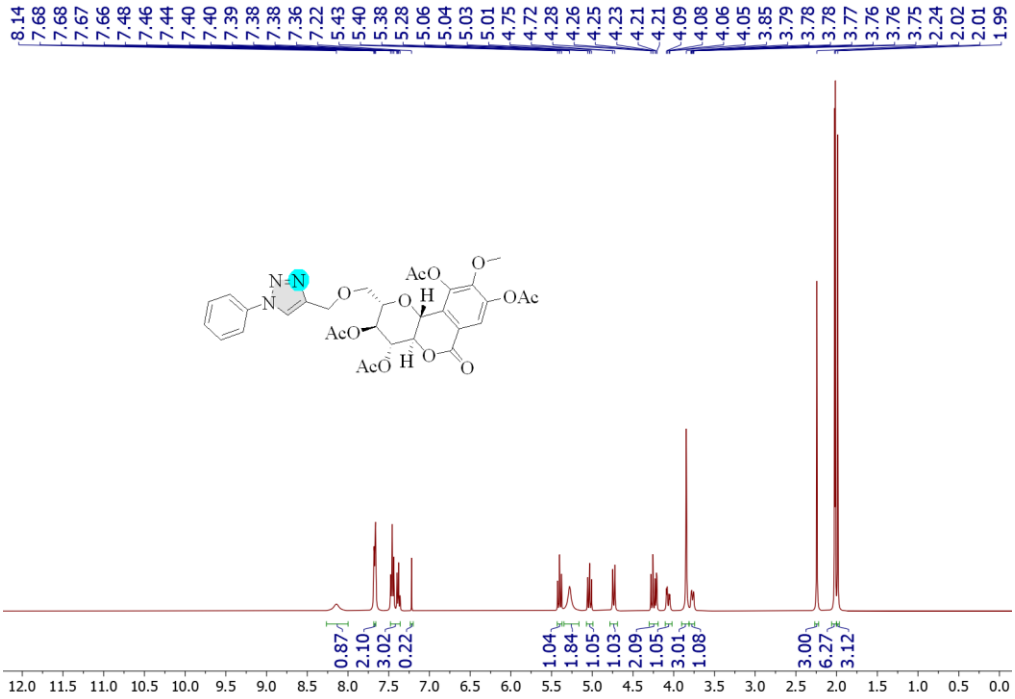
MZ-91
290822_33 9 (0.208)

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

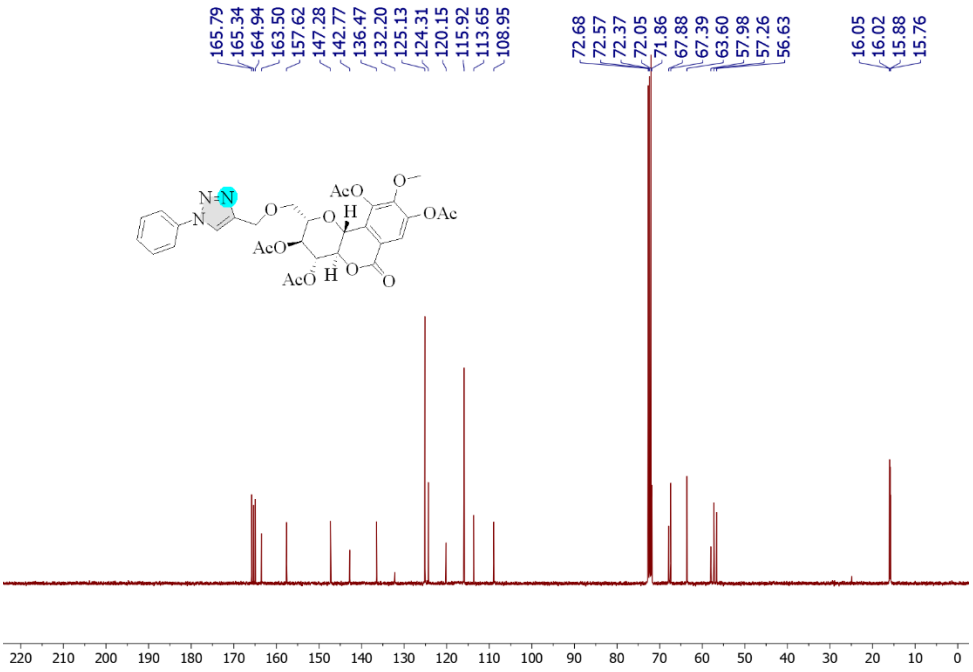
29-Aug-2022
13:05:34
1: TOF MS ES+
2.25e+007

Minimum:				-1.5			
Maximum:		2.0	50.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
308.1771	308.1763	0.8	2.6	10.5	968.7	n/a	n/a	C19 H22 N3 O

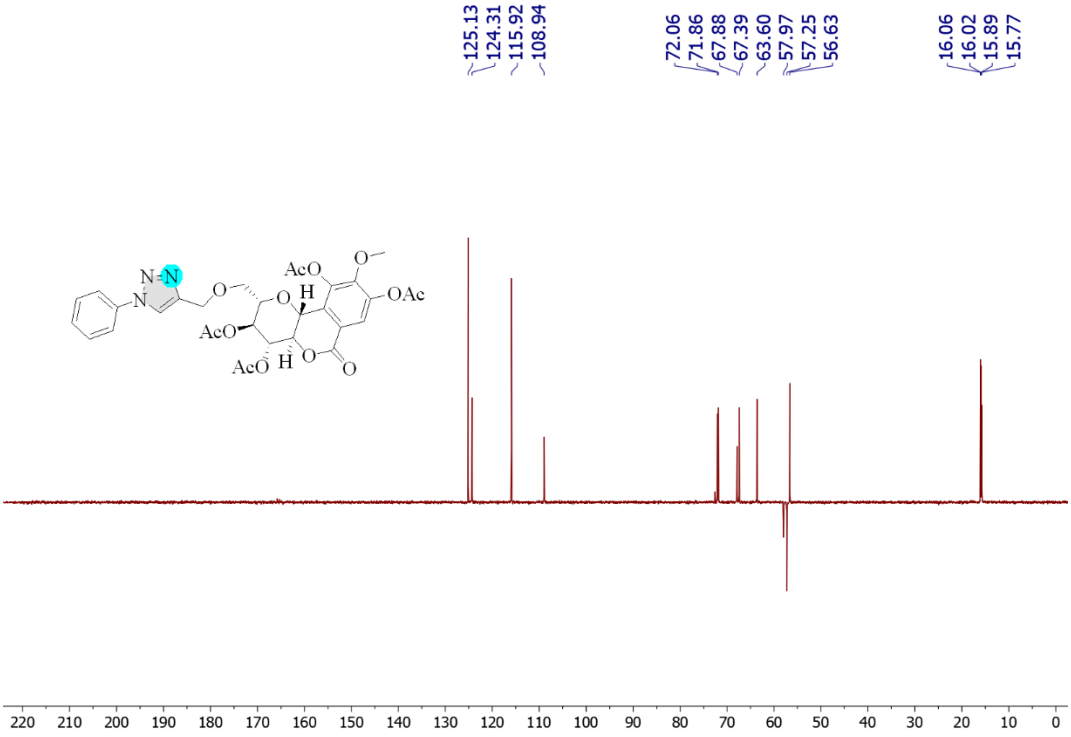
^{1}H-NMR of (2S,3S,4S,4aR,10bR)-9-Methoxy-6-oxo-2-(((1-phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)methyl)-2,3,4,4a,6,10b-hexahydropyrano[3,2-c]isochromene-3,4,8,10-tetrayl tetraacetate (6d)



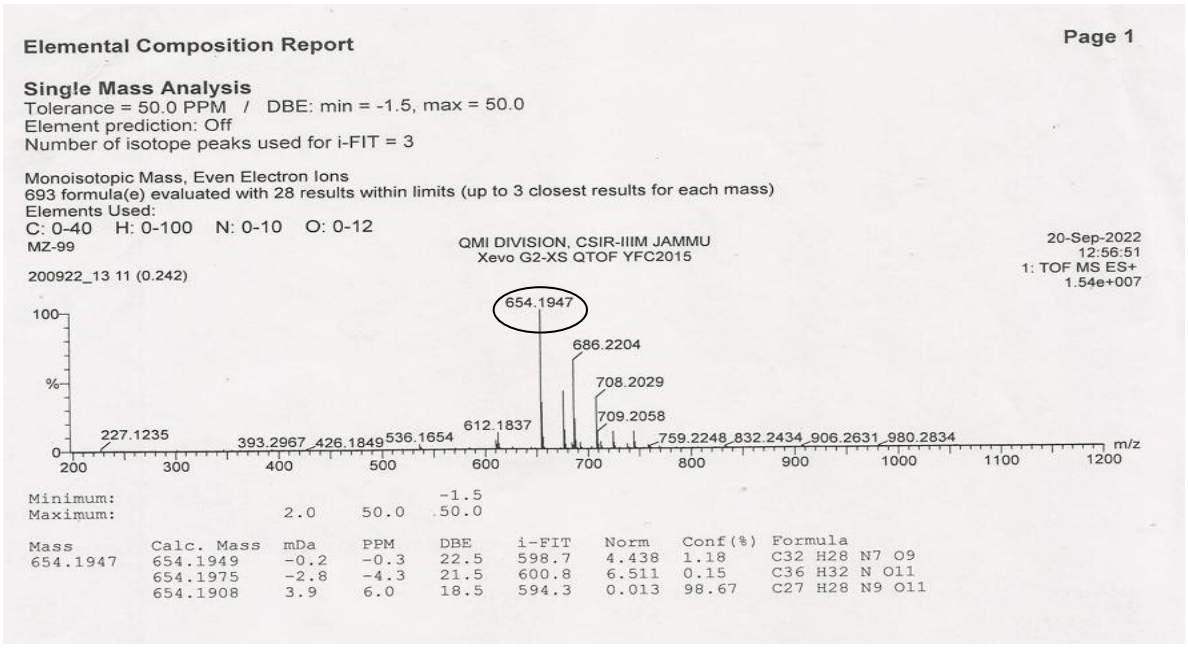
^{13}C-NMR of (2S,3S,4S,4aR,10bR)-9-Methoxy-6-oxo-2-(((1-phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)methyl)-2,3,4,4a,6,10b-hexahydropyrano[3,2-c]isochromene-3,4,8,10-tetrayl tetraacetate (6d)



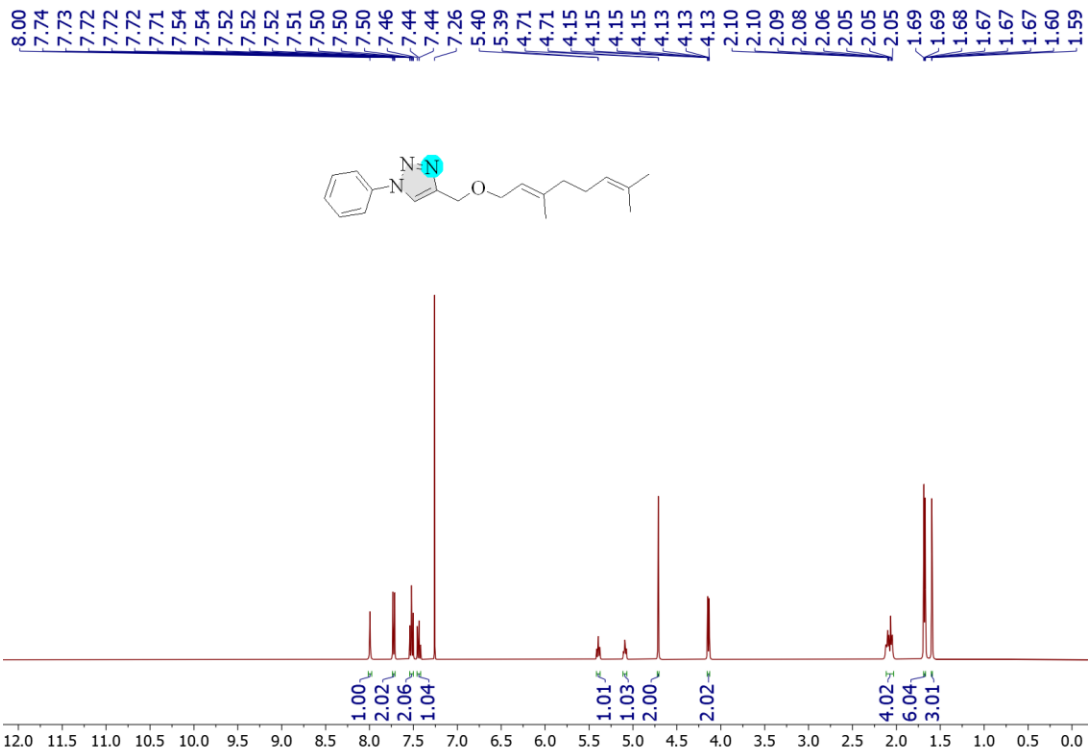
DEPT of (2S,3S,4S,4aR,10bR)-9-Methoxy-6-oxo-2-(((1-phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)methyl)-2,3,4,4a,6,10b-hexahydropyrano[3,2-c]isochromene-3,4,8,10-tetrayl tetraacetate (6d)



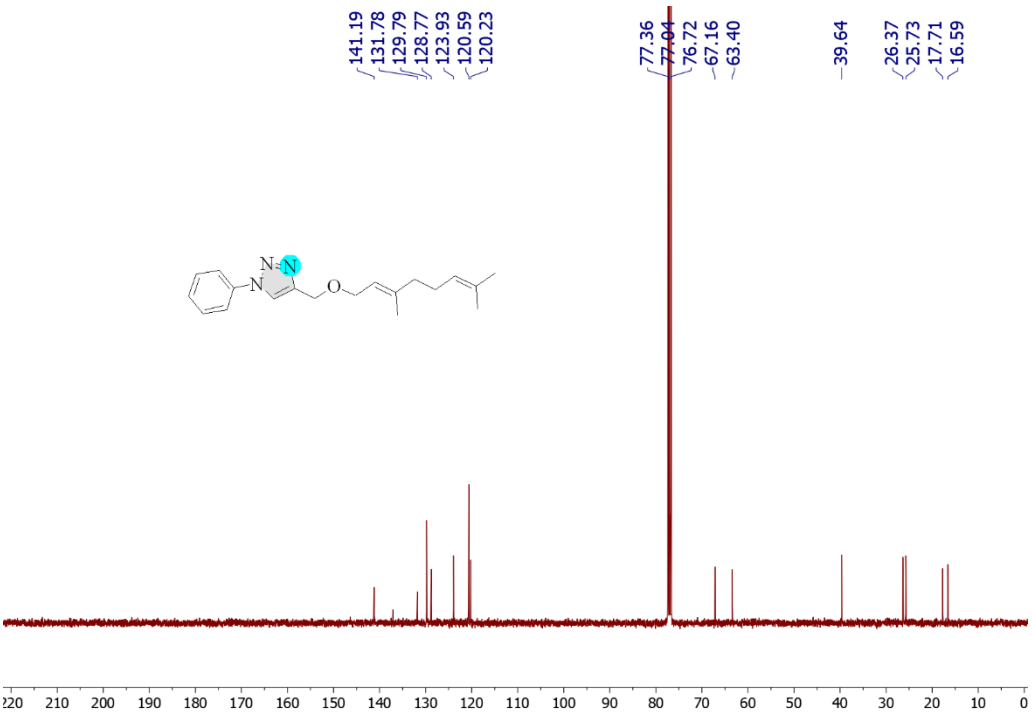
HRMS of (2S,3S,4S,4aR,10bR)-9-Methoxy-6-oxo-2-(((1-phenyl-1*H*-1,2,3-triazol-4-yl)methoxy)methyl)-2,3,4,4a,6,10b-hexahydropyrano[3,2-c]isochromene-3,4,8,10-tetrayl tetraacetate (6d)



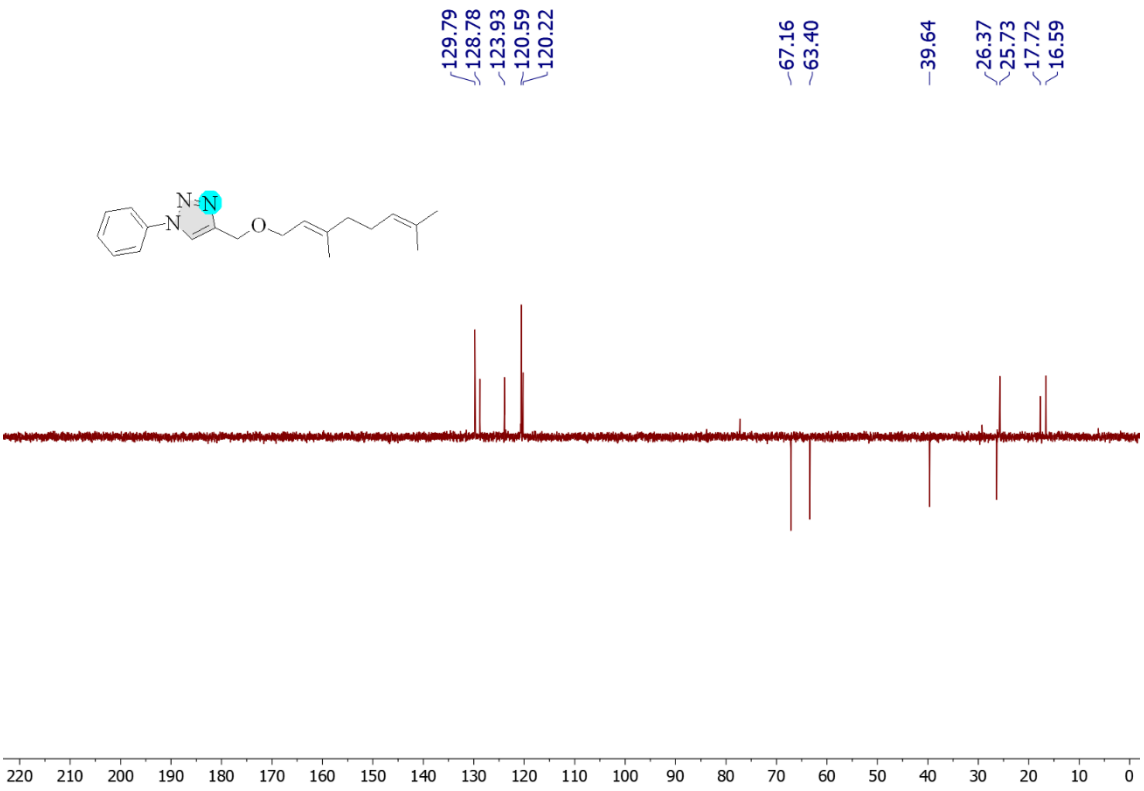
^{1}H-NMR of (E)-4-(((3,7-Dimethylocta-2,6-dien-1-yl)oxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6e)



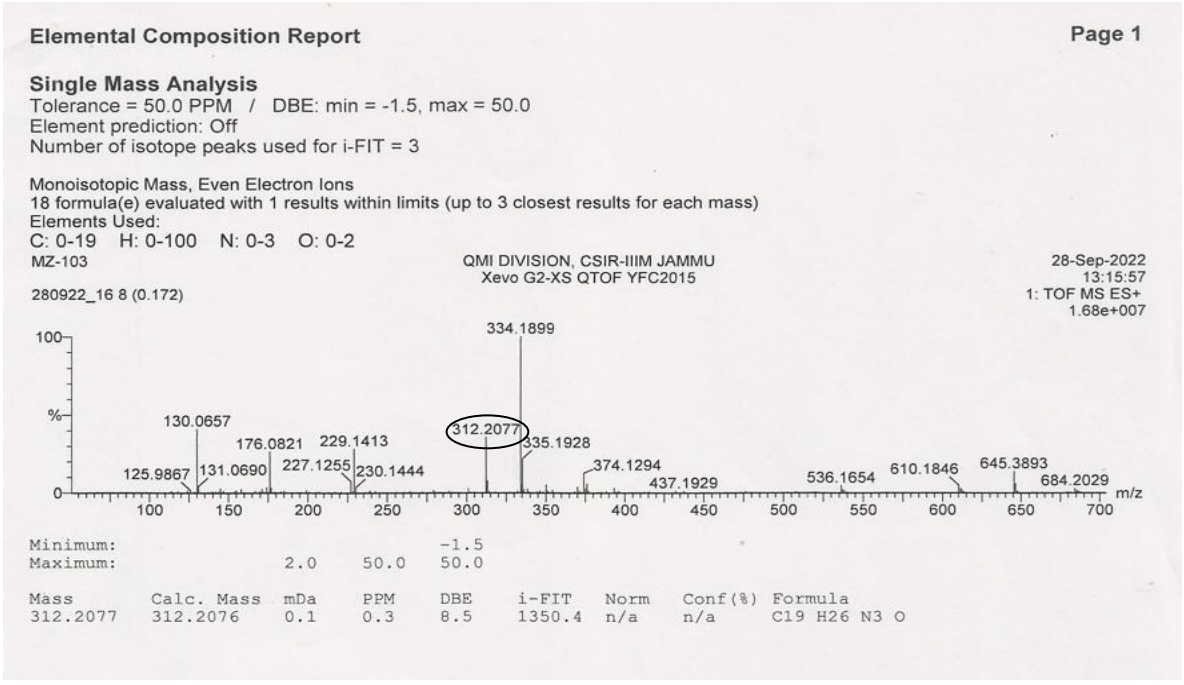
^{13}C-NMR of (E)-4-(((3,7-Dimethylocta-2,6-dien-1-yl)oxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6e)



DEPT of (E)-4-(((3,7-Dimethylocta-2,6-dien-1-yl)oxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6e)



HRMS of (E)-4-(((3,7-Dimethylocta-2,6-dien-1-yl)oxy)methyl)-1-phenyl-1*H*-1,2,3-triazole (6e)



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