SUPPORTING INFORMATION

Development of di-arylated 1,2,4-triazole-based derivatives as therapeutic agents against breast cancer: synthesis and biological evaluation

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1. X-ray Crystallographic Data Analysis

a. X-ray data collection, structure solution, and refinement

A single crystal suitable for data collection was obtained by slowly evaporating compound 4n from a solution of DMSO at 298 K. Diffraction intensities were collected on a single crystal with a SuperNova, Single source at offset/far, EosS2 diffractometer, with mirror-monochromated Mo-*K*α ($\lambda = 0.71073$ Å) radiation at 293(2) K. The 'CrysAlisPro 1.171.40.69a' program was used for data reduction. Data were corrected for Lorentz and polarization effects; empirical absorption correction using spherical harmonics and frame scaling, implemented in SCALE3 ABSPACK scaling algorithm. The structures were solved with SHELXT and refined with the SHELXL–2018/3 package[1-2], incorporated into the Olex2 1.5–alpha crystallographic collective package[3a]. The position of the hydrogen atoms was calculated by assuming ideal geometries and included in the last cycle of the refinement. All non–hydrogen atoms were refined with anisotropic thermal parameters by full-matrix least-squares minimization procedures on F^2.

The Perspective view of **4t** and the data collection and structure refinement details are in **Figures S1** and **Table S1** respectively.

CCDC-number 2320548 (**4t**) contains supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

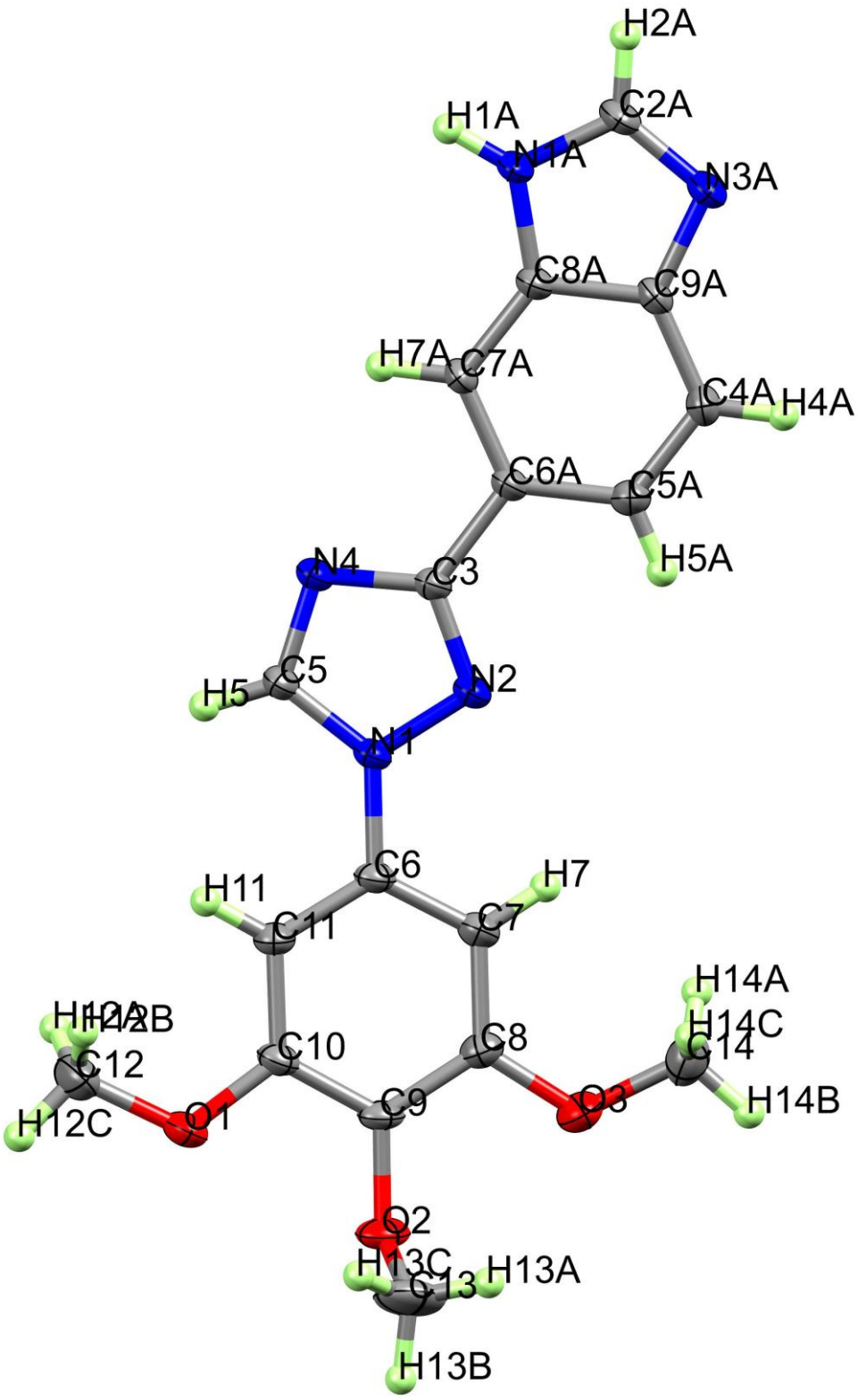


Figure S1: Perspective view of **4t** with thermal 30% ellipsoid probability

Table S1. Data collection and structure refinement parameters for compound **4t**

Parameters	4t
Empirical formula	$C_{18}H_{17}N_5O_3$
Formula weight	351.36
Crystal color, habit	White, cubic
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Crystal system	monoclinic
Space group	$P2_1/n$ (no. 14)
Crystal size (mm^3)	0.2 x 0.2 x 0.2
a (Å)	13.0154(5)
b (Å)	6.8065(2)
c (Å)	20.5824(6)
α (°)	90
β (°)	105.958(3)
γ (°)	90
V ($Å^3$)	1752.88(10)
Z	4
D_{calc} ($g\ cm^{-3}$)	1.331
μ (mm^{-1})	0.094
no. reflections collected	8558
no. unique reflection	3996 (R_{int}= 0.0258)
no. reflections used [$I > 2\sigma(I)$]	2438
R_1[a], wR_2[b] [$I > 2\sigma(I)$]	R_1 = 0.0480[a] wR_2= 0.0999[b]
R_1[a], wR_2[b] (All data)	R_1 = 0.0897[a] wR_2= 0.1128[b]
Goodness-of-fit on F^2	0.931

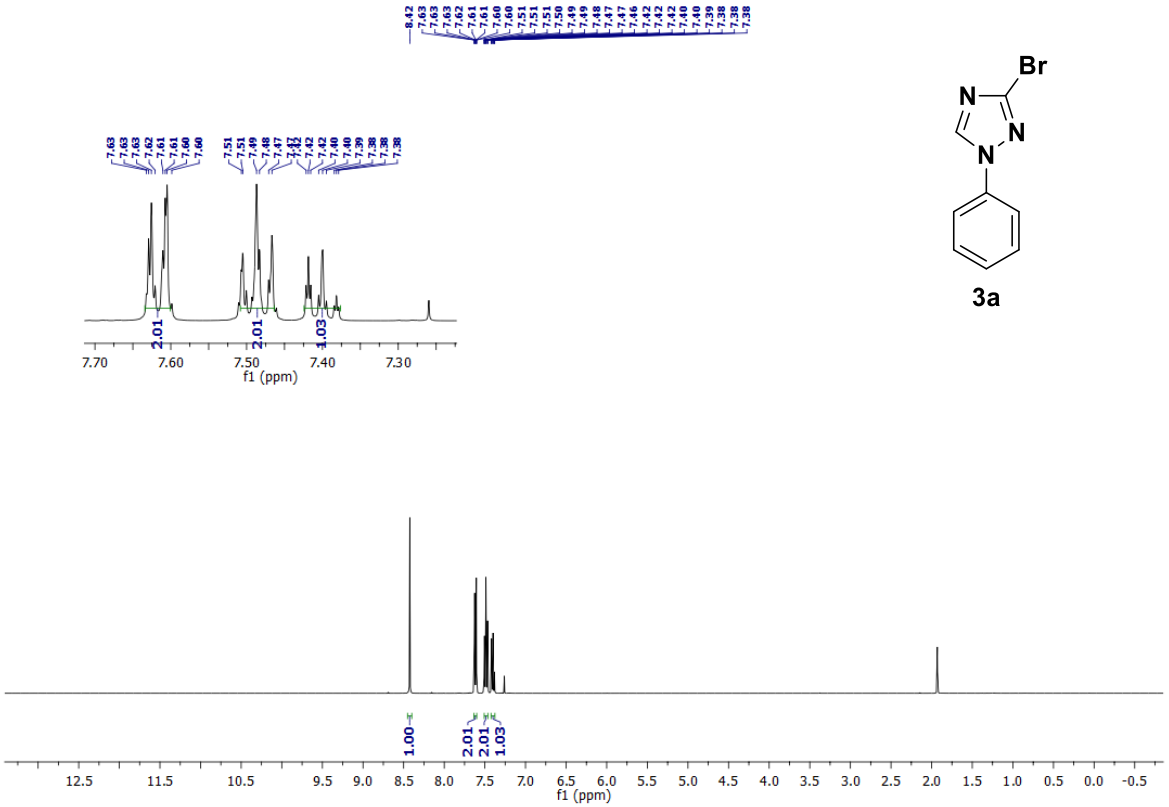
[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR_2 = \{\Sigma[w\ (|F_o|^2 - |F_c|^2)^2]/\Sigma[w(|F_o|^2)^2]\}^{1/2}$.

b. References:

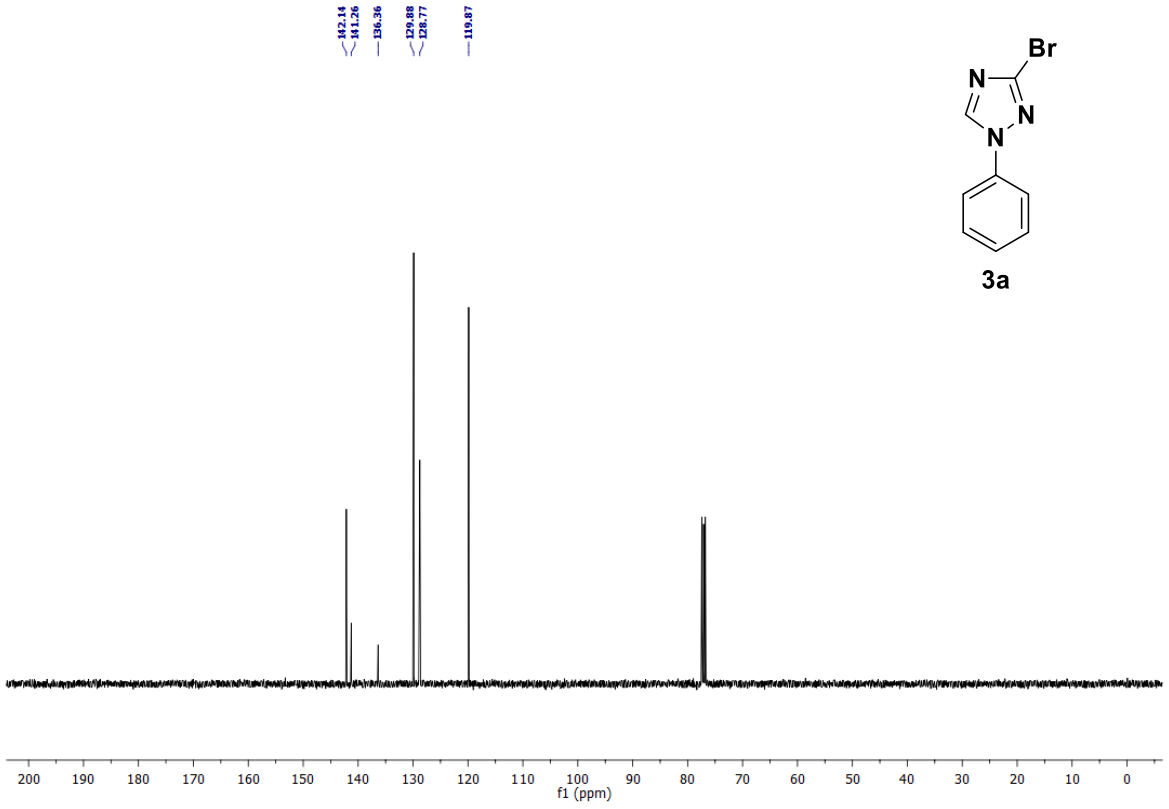
1. G.M. Sheldrick, SHELXL–2016, Program for Crystal Structure Refinement University of Göttingen, Göttingen, Germany, 2014.
2. G.M. Sheldrick, Acta Crystallogr. Sect. C: Cryst. Struct. Commun. C71 (2015) 3–8.
3. O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, J. Appl. Cryst. 42 (2009) 339–341.

2. ^{1}H, ^{13}C{1H}, ^{19}F NMR Spectra:

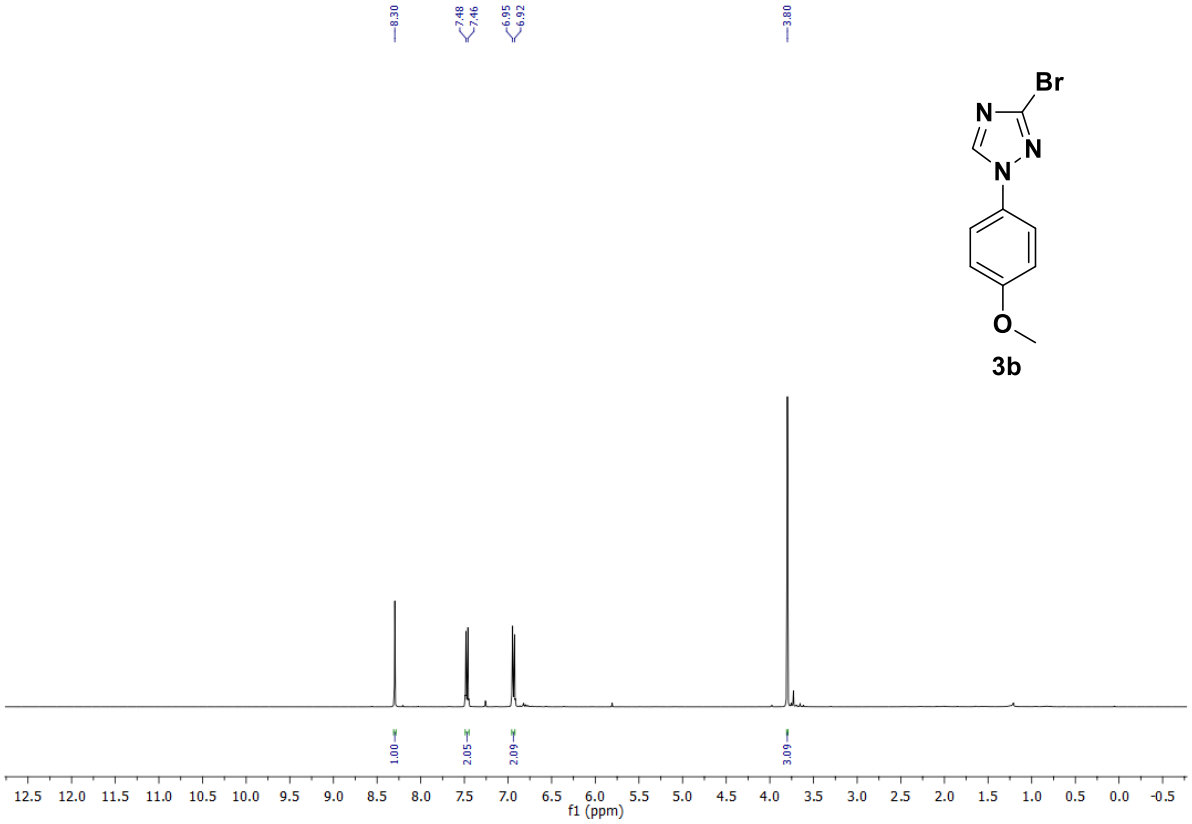
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-phenyl-1*H*-1,2,4-triazole (3a):



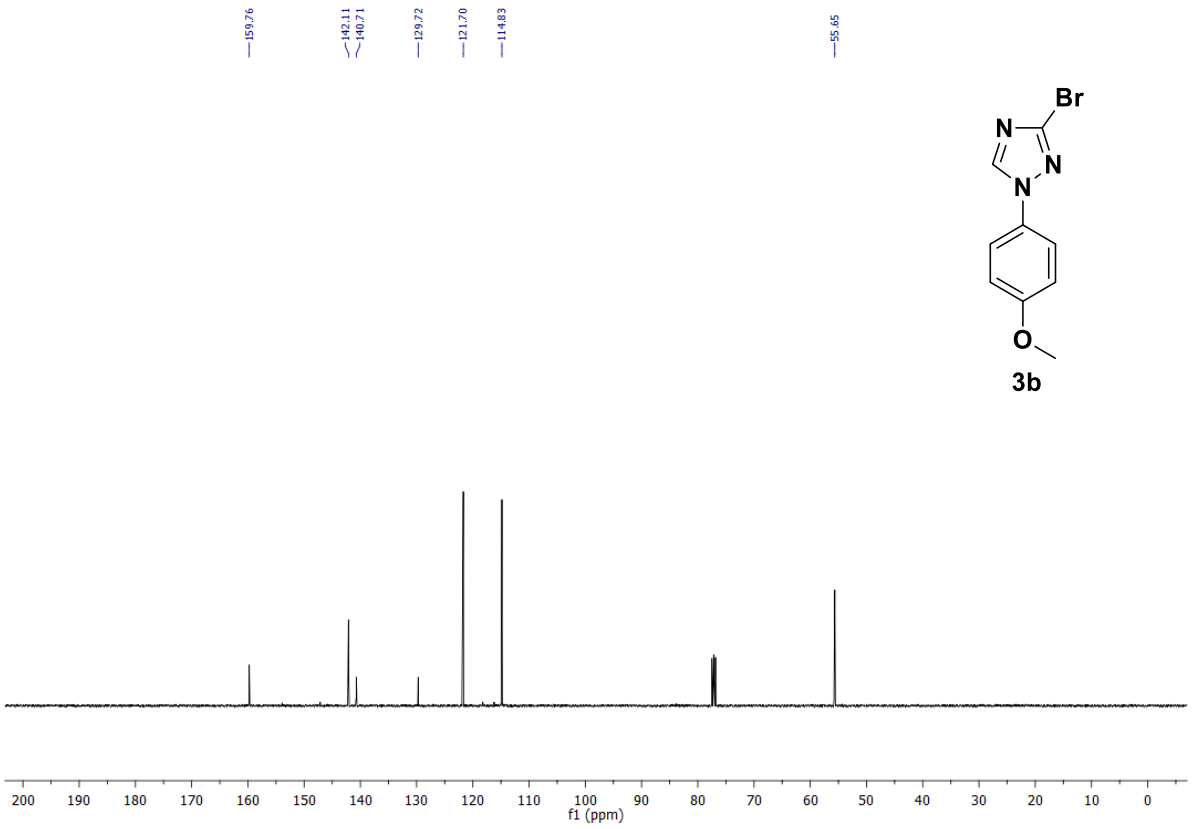
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-phenyl-1*H*-1,2,4-triazole (3a):



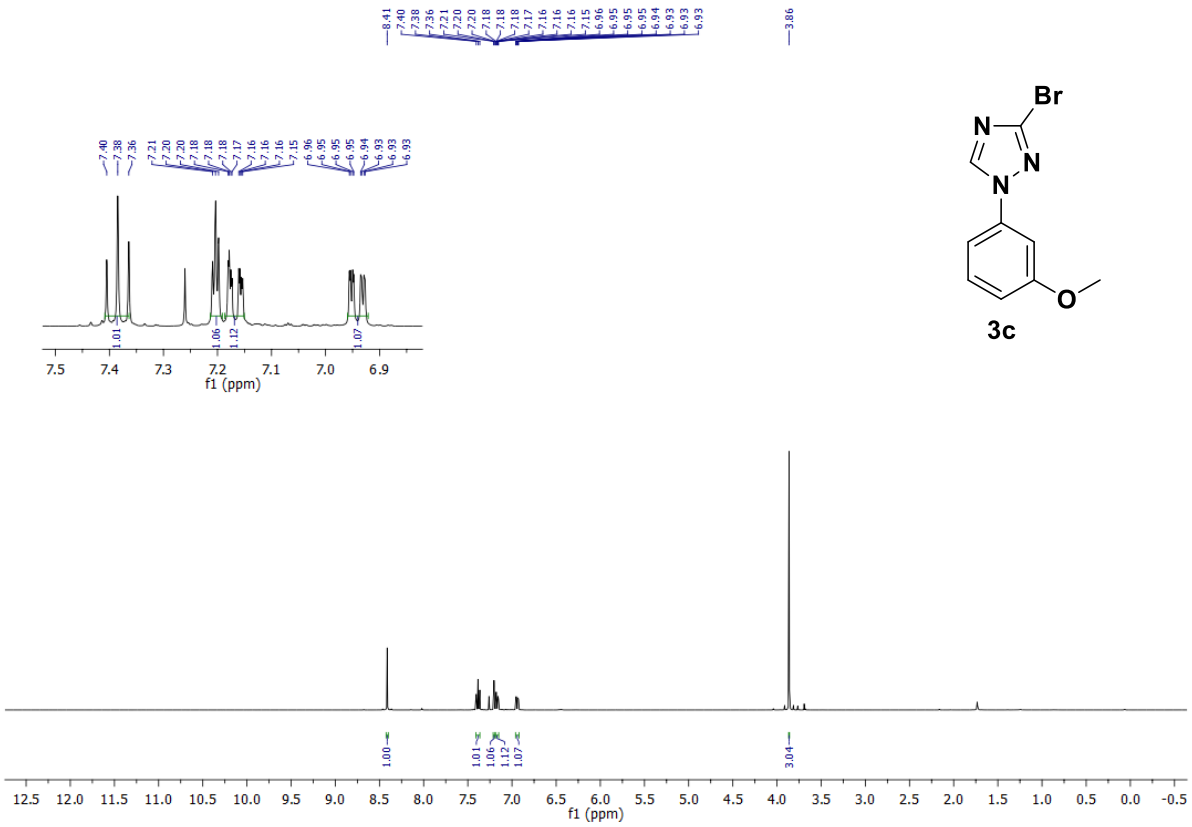
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(4-methoxyphenyl)-1*H*-1,2,4-triazole (3b):



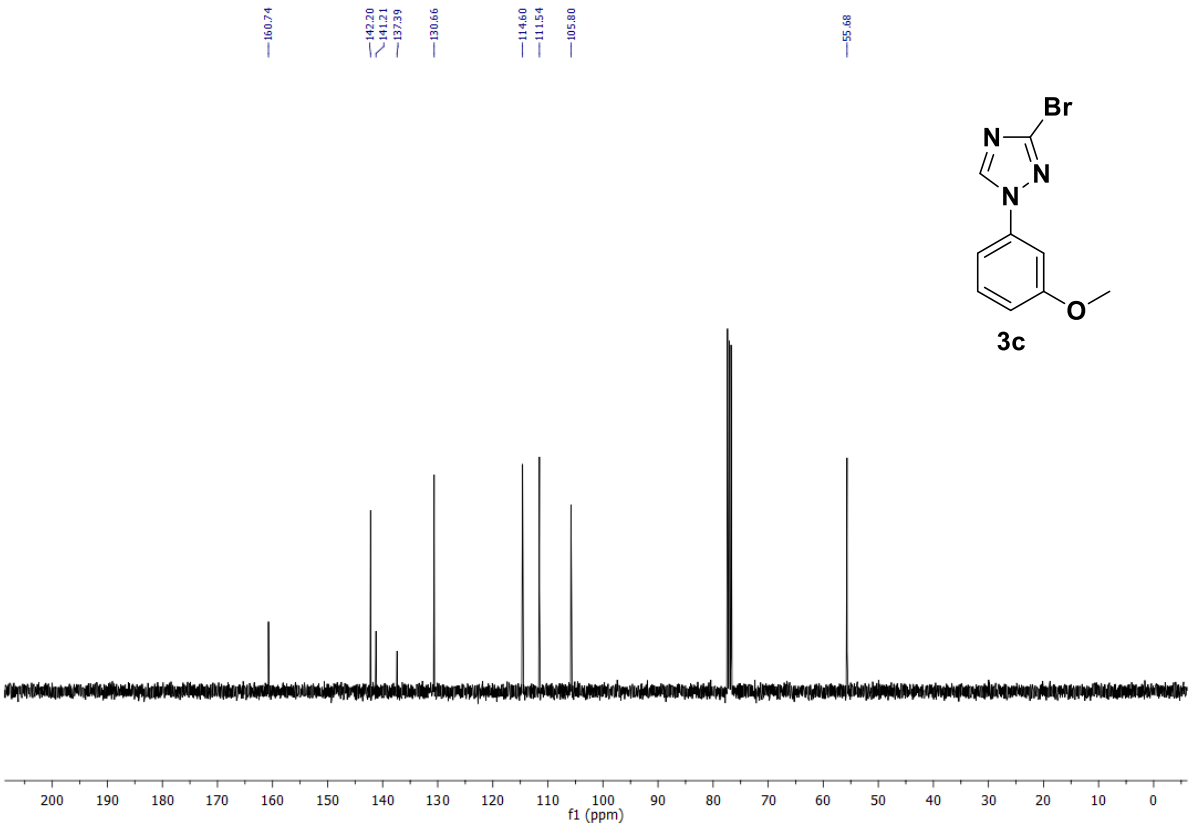
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(4-methoxyphenyl)-1*H*-1,2,4-triazole (3b):



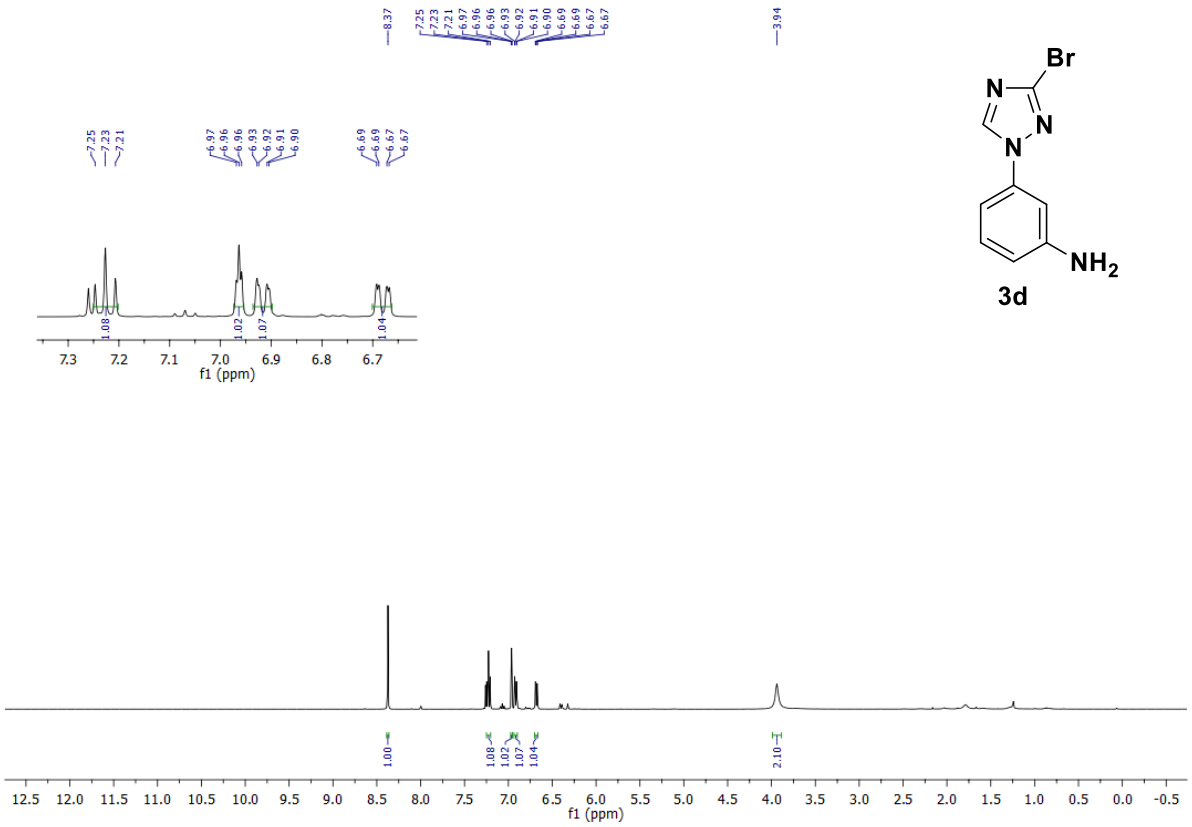
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(3-methoxyphenyl)-1*H*-1,2,4-triazole (3c):



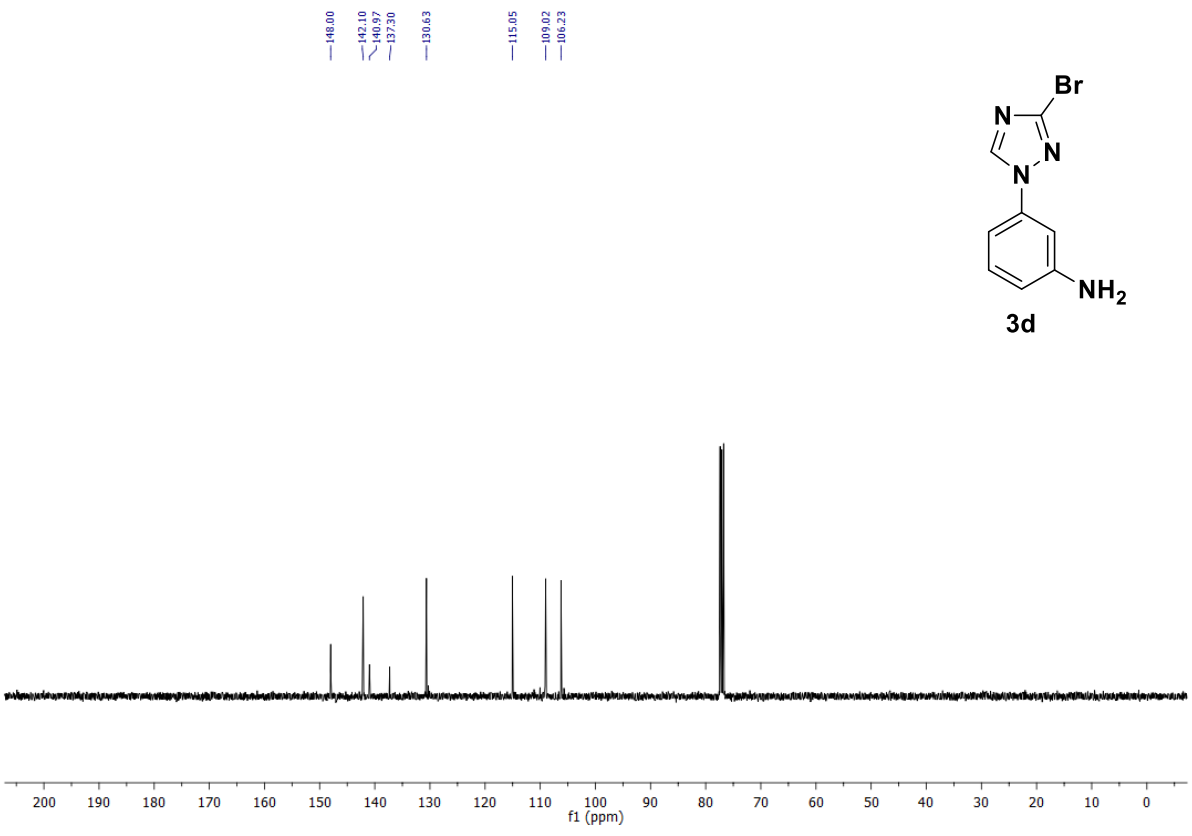
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(3-methoxyphenyl)-1*H*-1,2,4-triazole (3c):



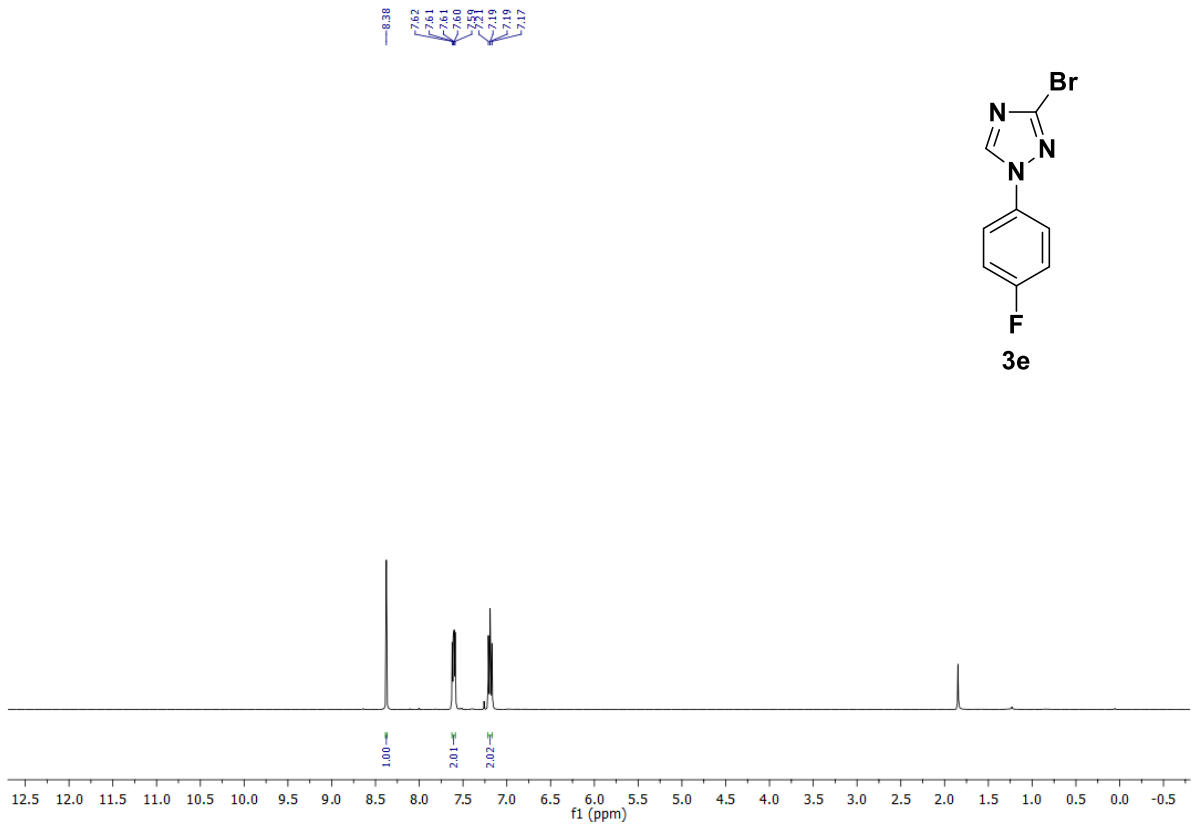
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(3-bromo-1*H*-1,2,4-triazol-1-yl)aniline (3d):



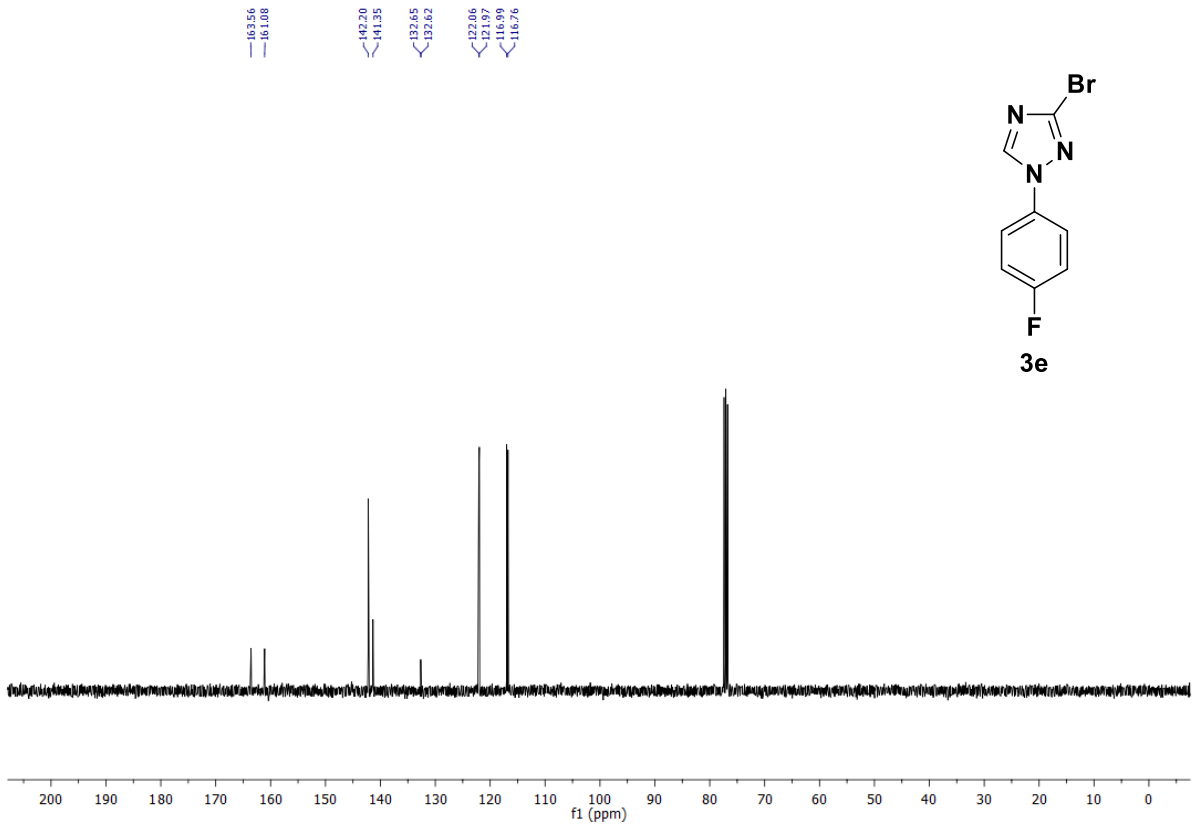
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3-bromo-1*H*-1,2,4-triazol-1-yl)aniline (3d):



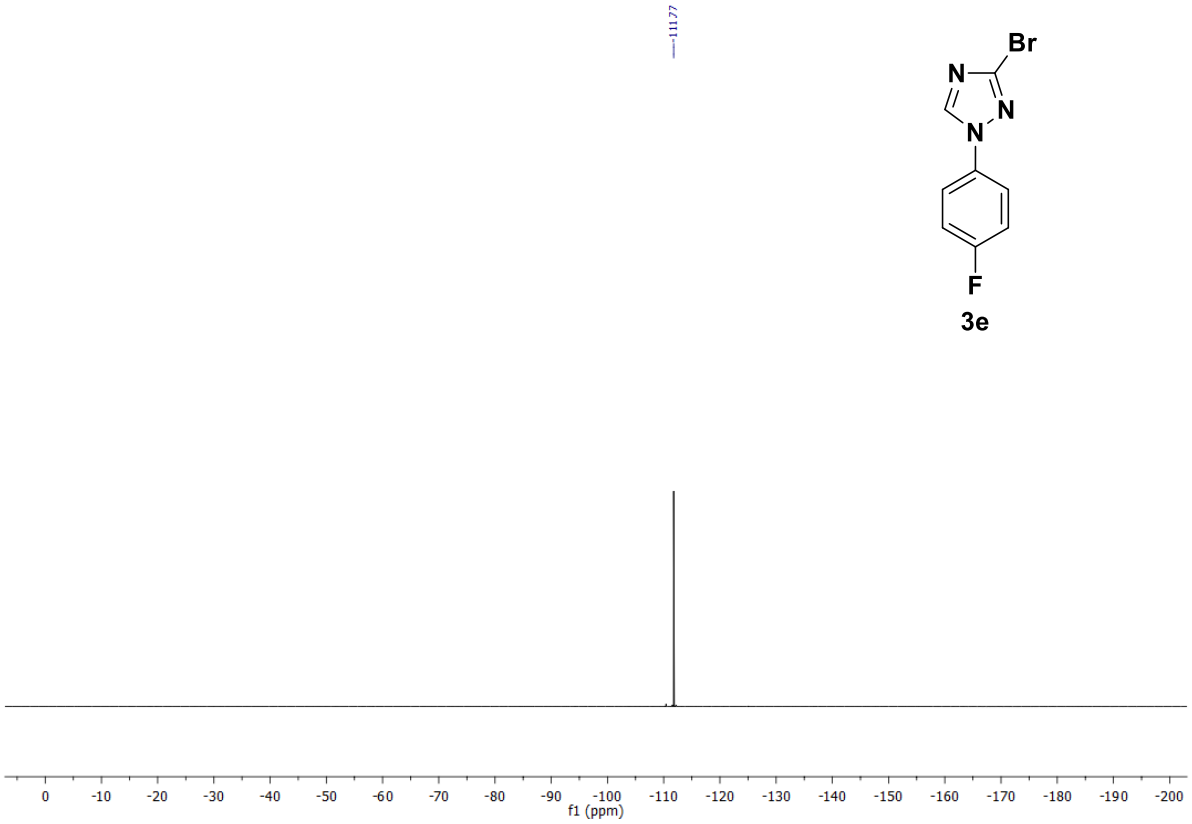
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(4-fluorophenyl)-1*H*-1,2,4-triazole (3e):



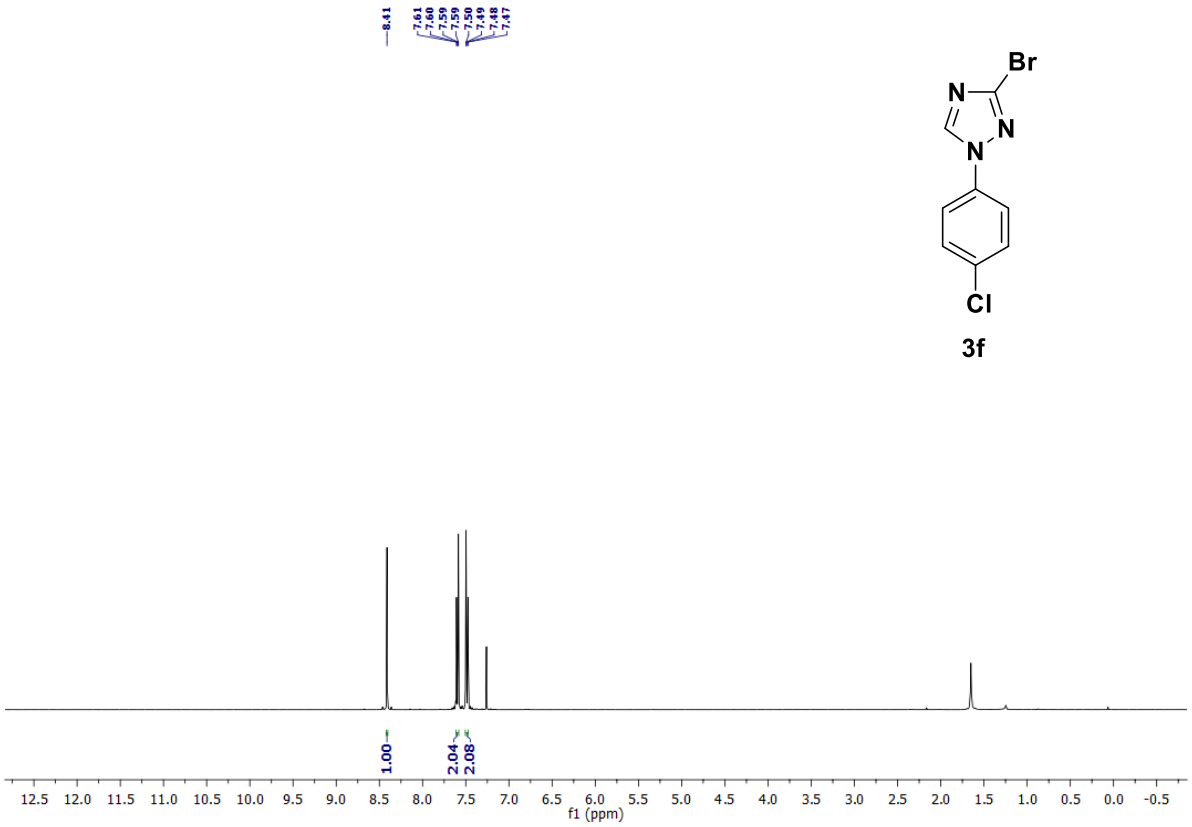
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(4-fluorophenyl)-1*H*-1,2,4-triazole (3e):



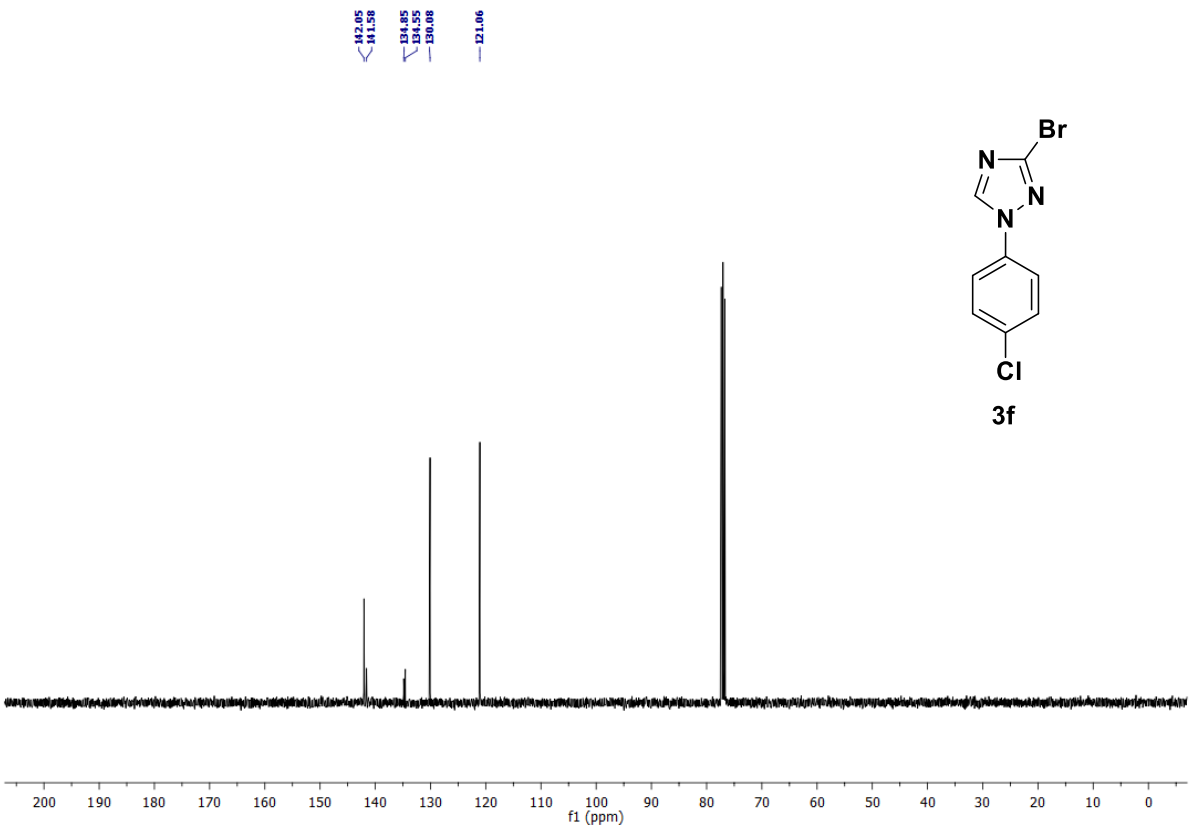
^{19}F NMR (377 MHz, $CDCl_3$) of 3-bromo-1-(4-fluorophenyl)-1*H*-1,2,4-triazole (3e):



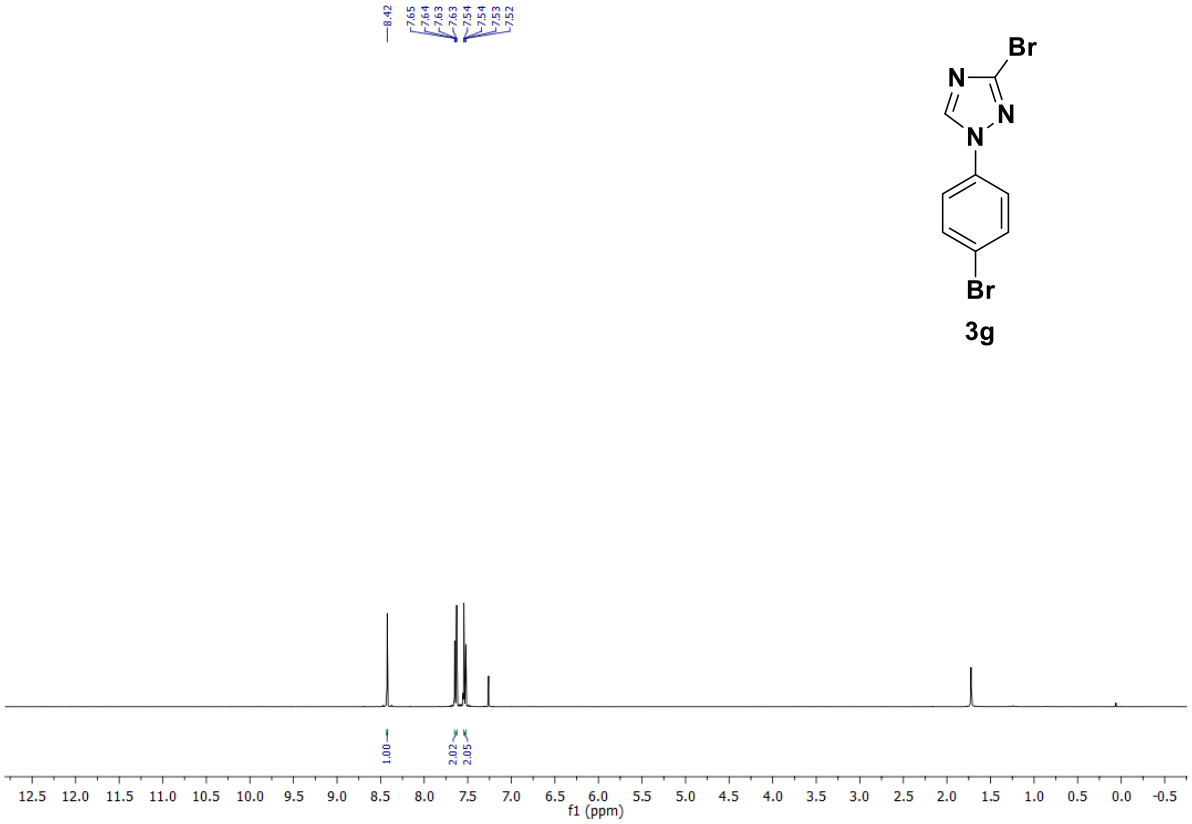
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(4-chlorophenyl)-1*H*-1,2,4-triazole (3f):



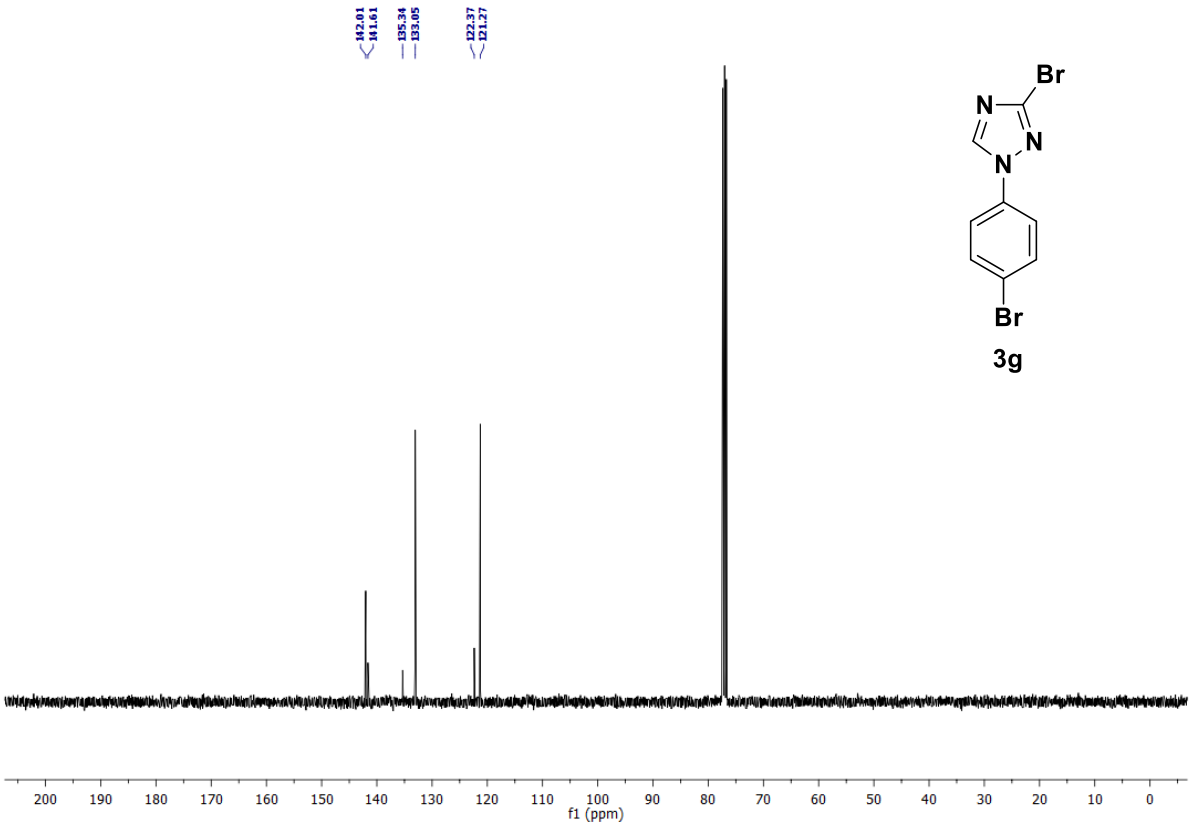
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(4-chlorophenyl)-1*H*-1,2,4-triazole (3f):



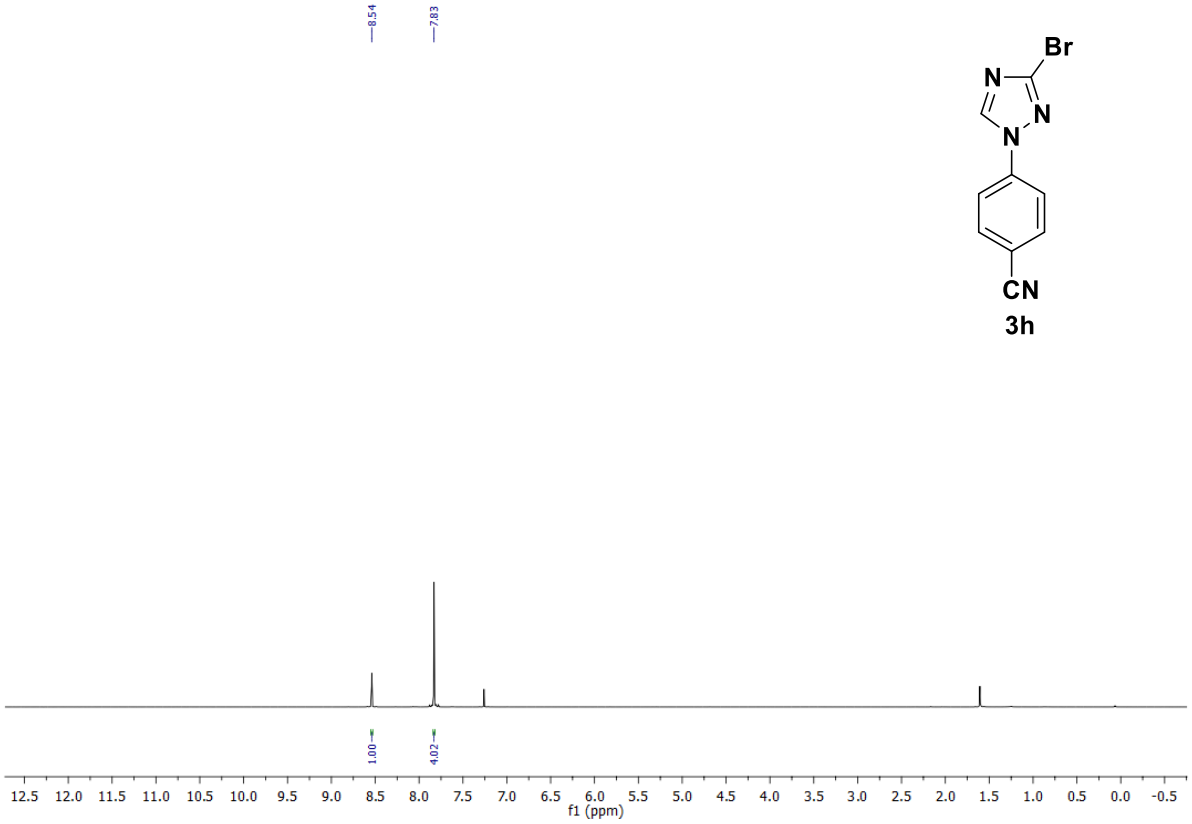
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(4-bromophenyl)-1*H*-1,2,4-triazole (3g):



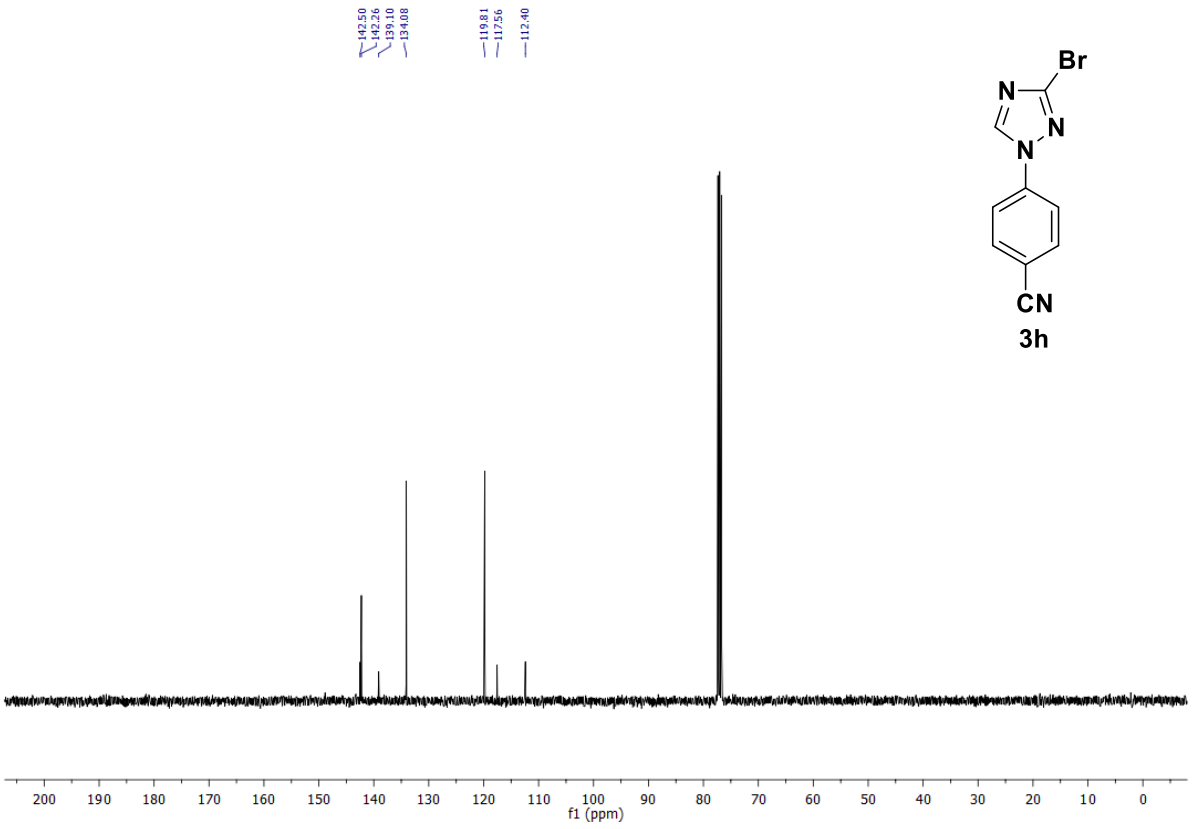
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(4-bromophenyl)-1*H*-1,2,4-triazole (3g):



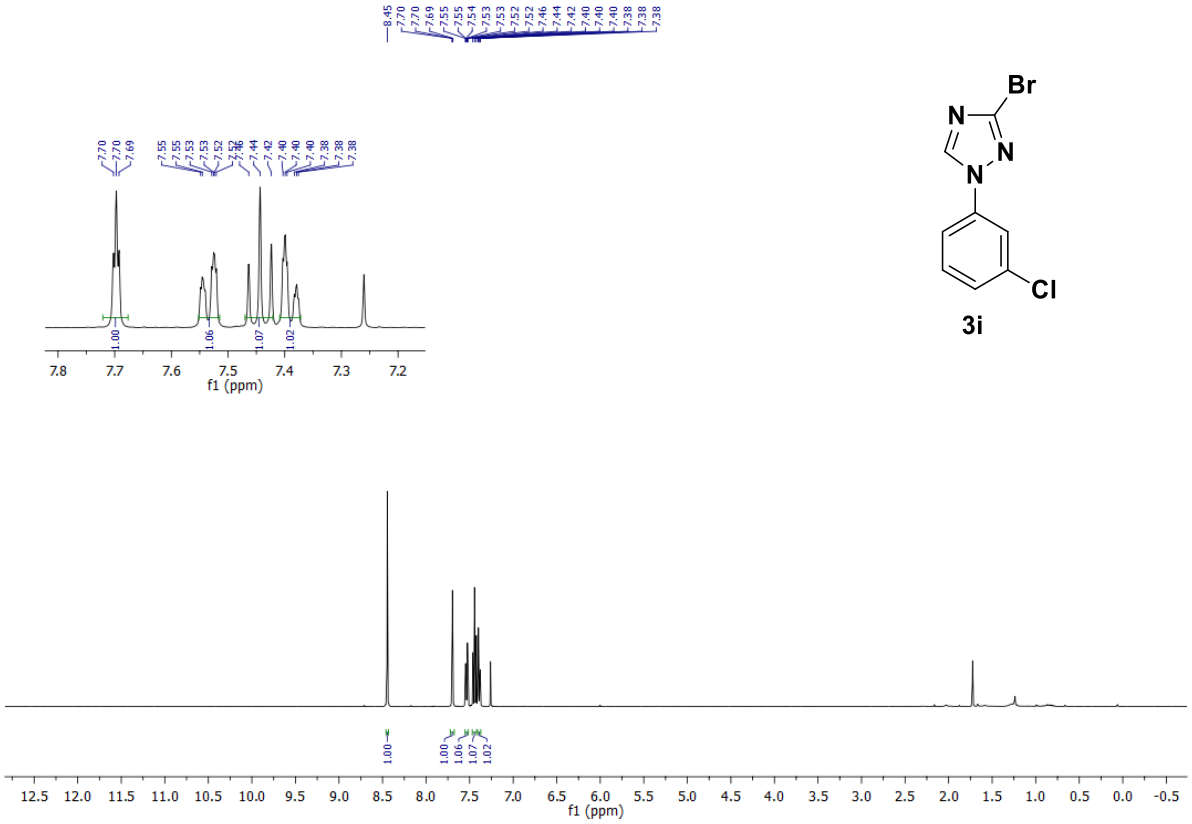
^{1}H NMR (400 MHz, $CDCl_3$) of 4-(3-bromo-1*H*-1,2,4-triazol-1-yl)benzonitrile (3h):



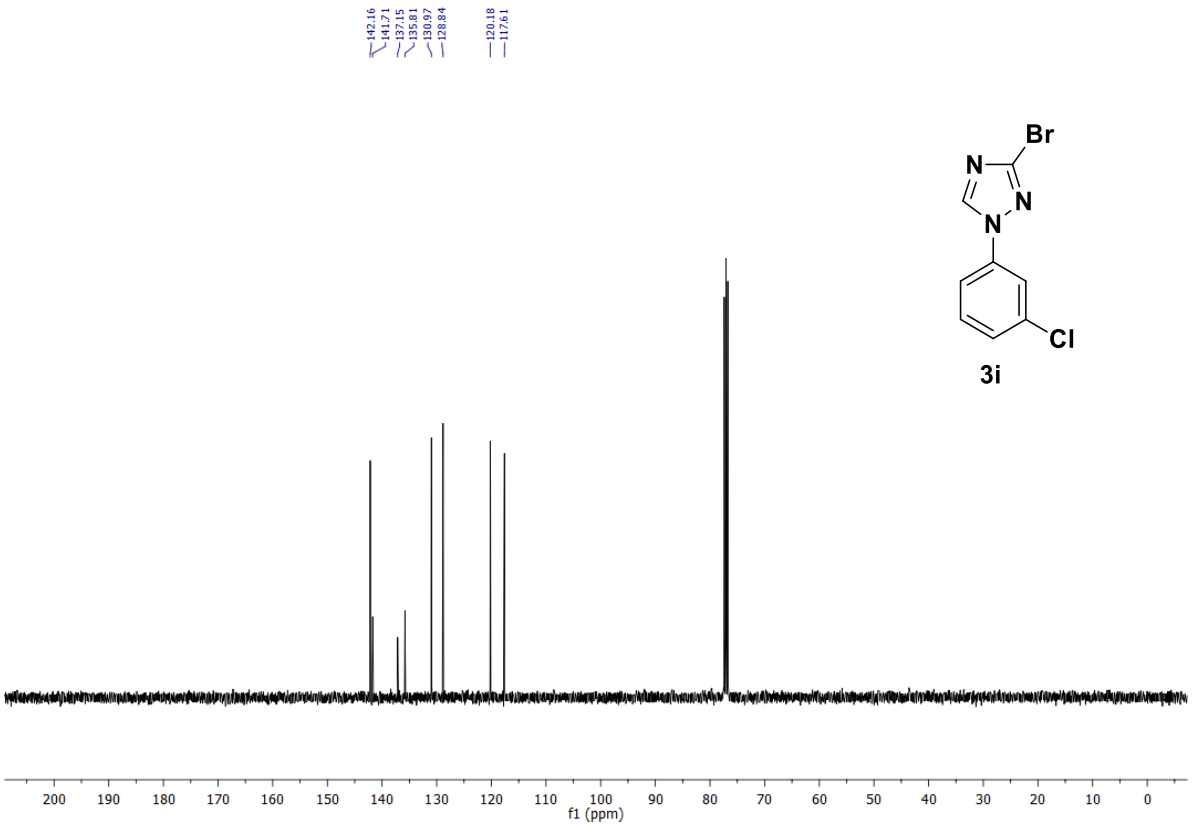
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 4-(3-bromo-1*H*-1,2,4-triazol-1-yl)benzonitrile (3h):



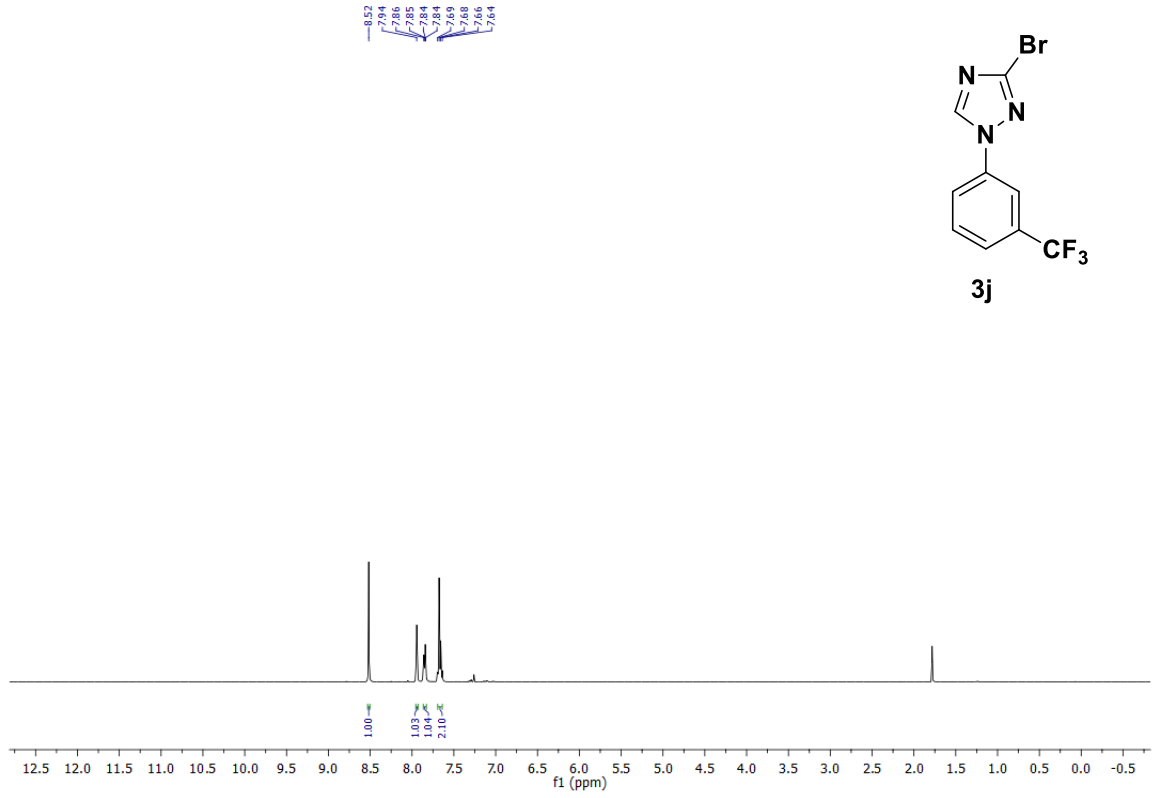
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(3-chlorophenyl)-1*H*-1,2,4-triazole (3i):



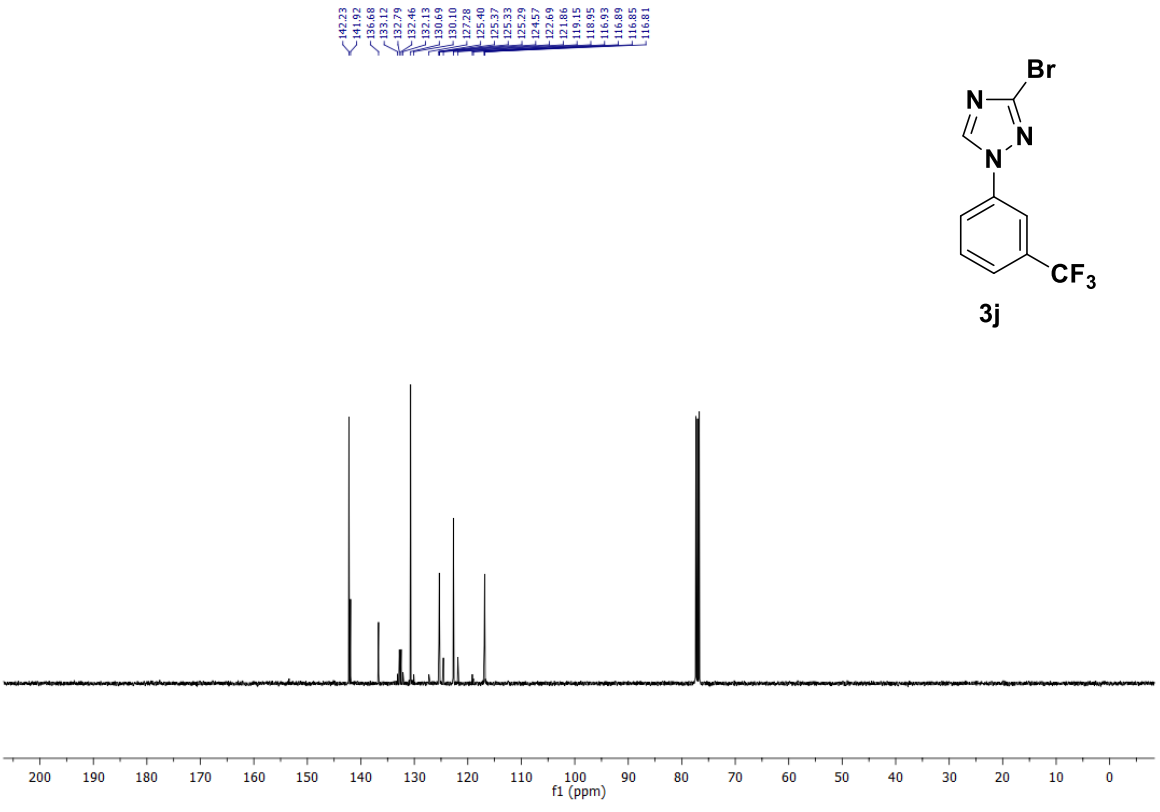
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(3-chlorophenyl)-1*H*-1,2,4-triazole (3i):



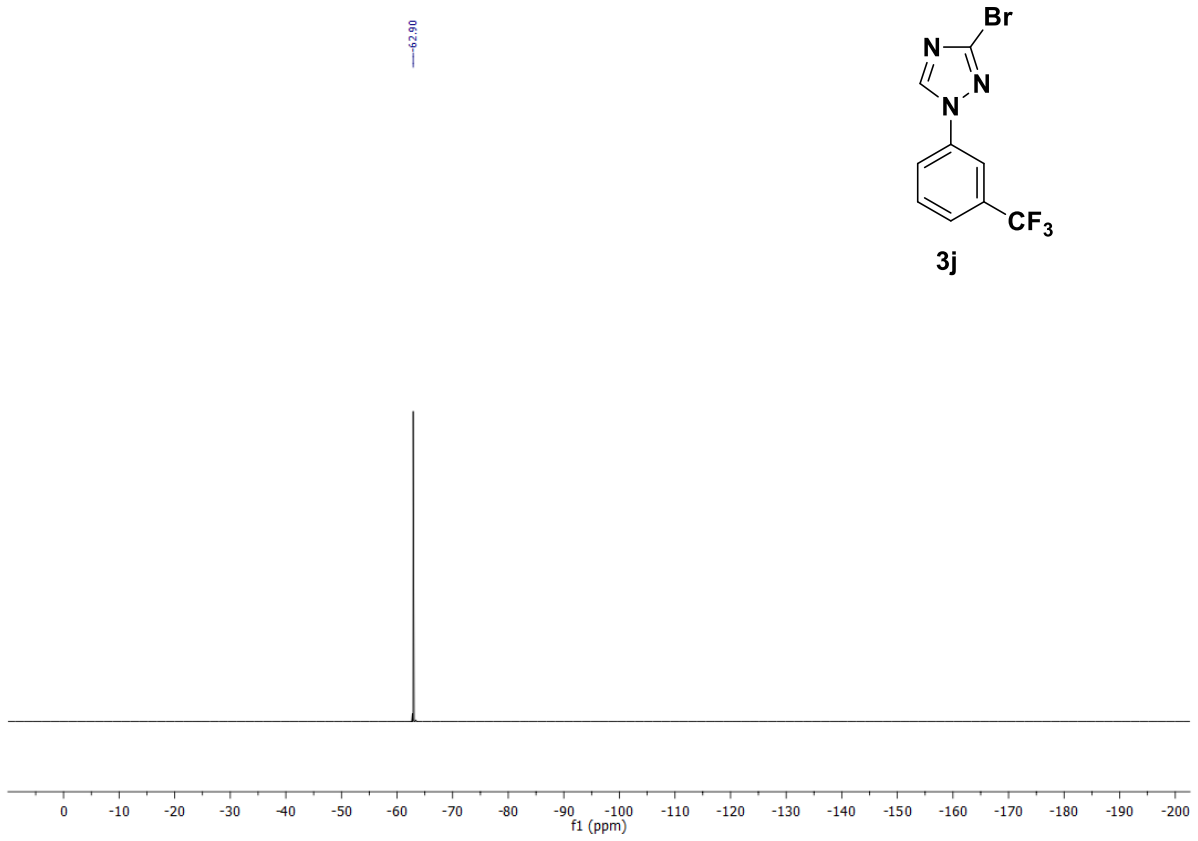
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(3-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (3j):



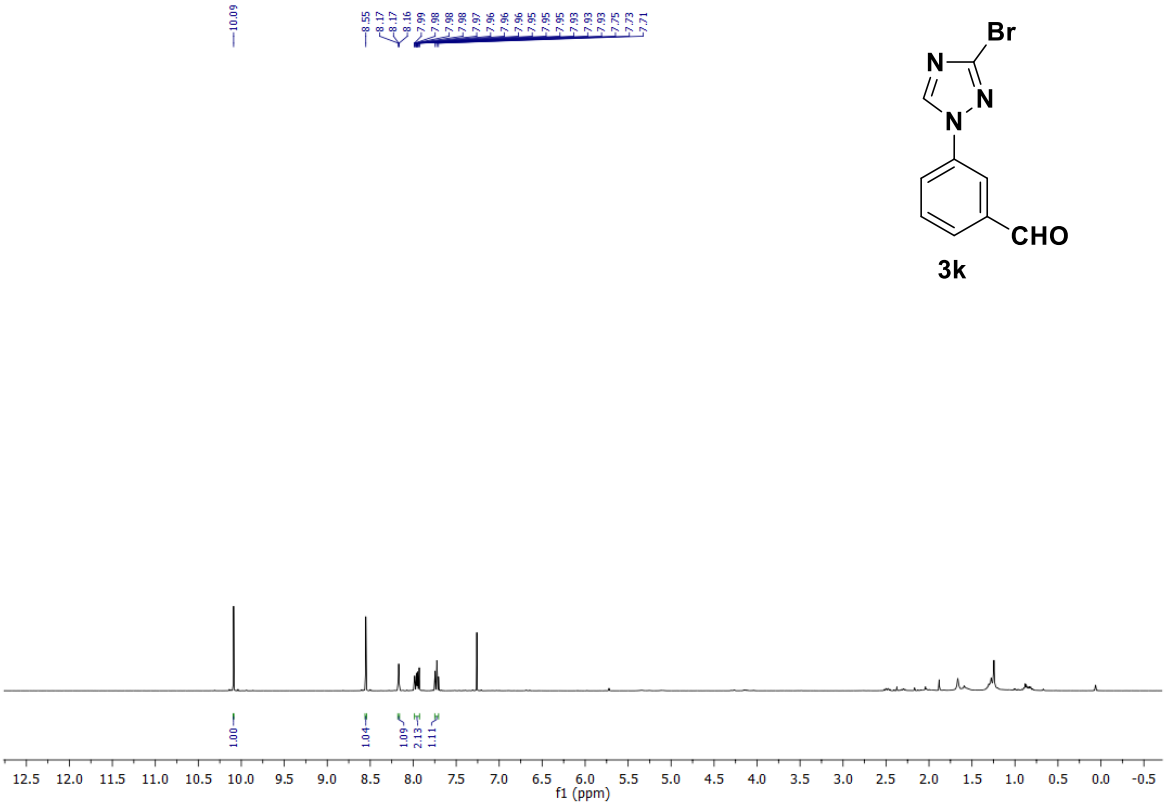
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(3-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (3j):



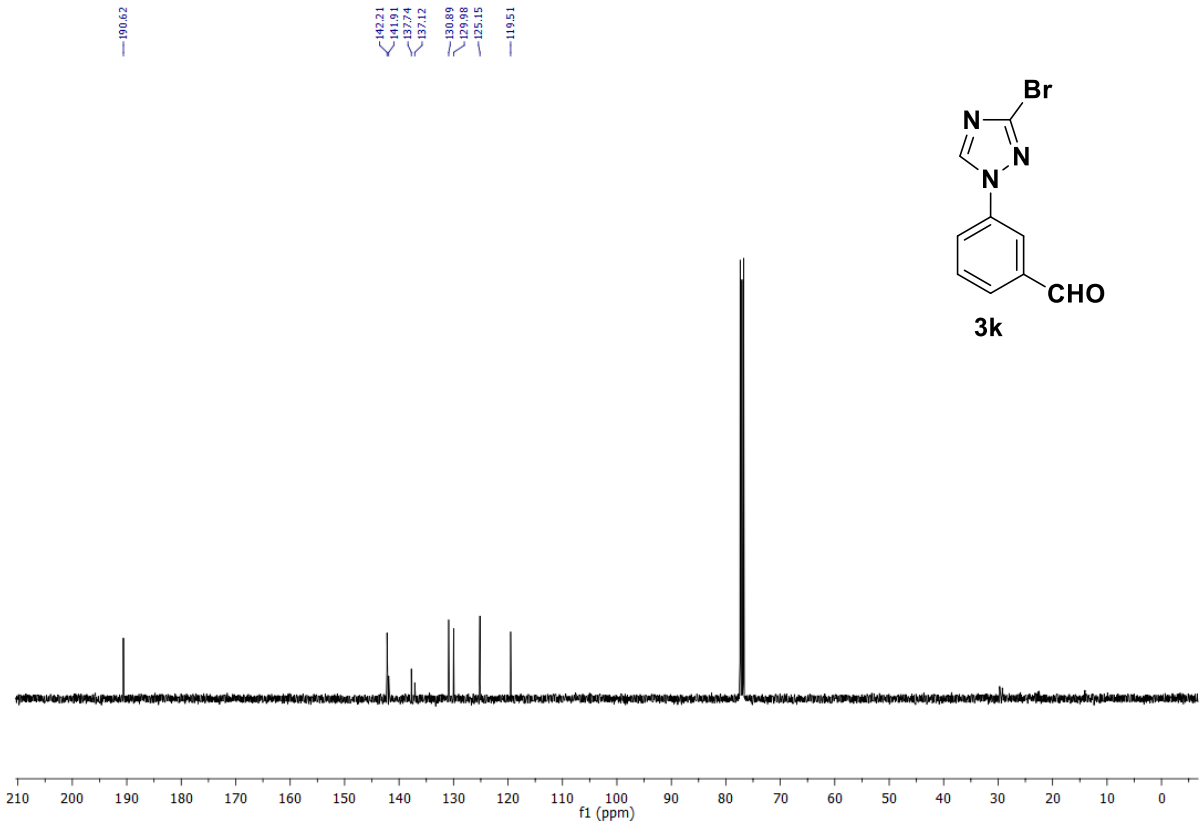
^{19}F NMR (377 MHz, $CDCl_3$) of 3-bromo-1-(3-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (3j):



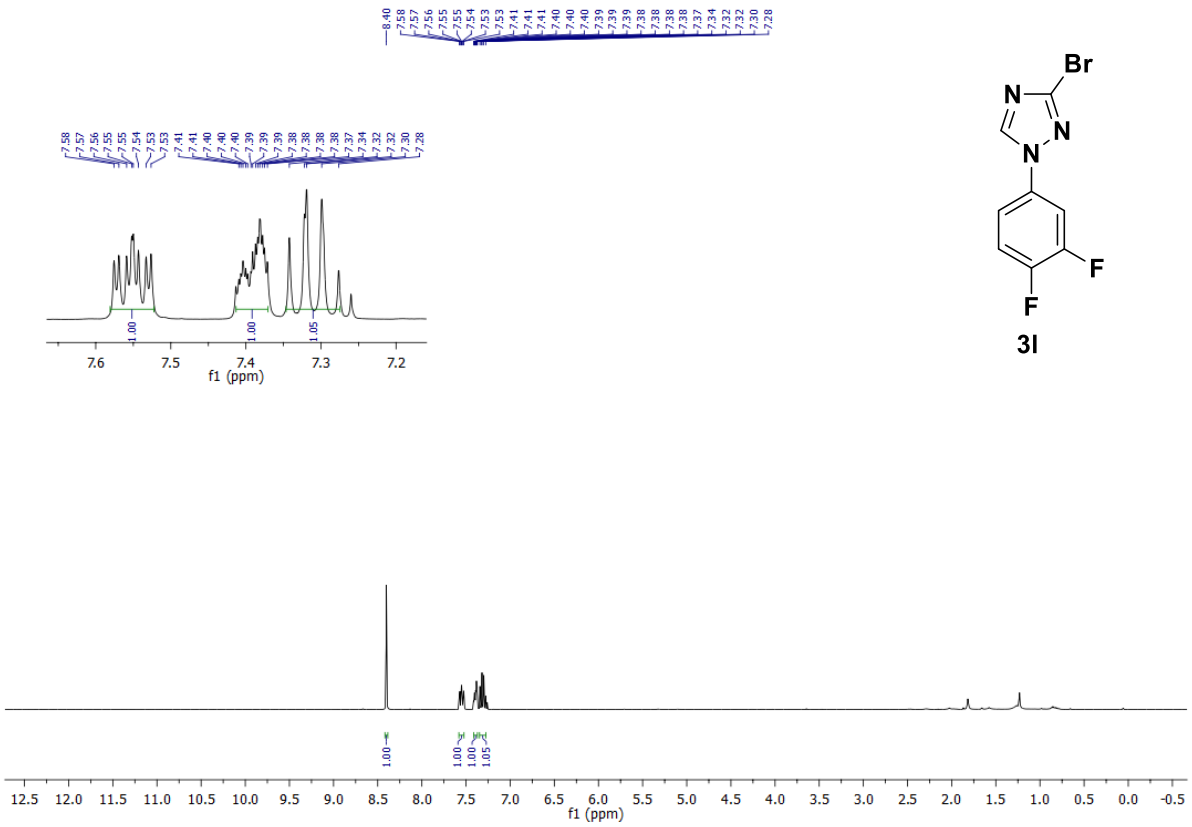
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(3-bromo-1*H*-1,2,4-triazol-1-yl)benzaldehyde (3k):



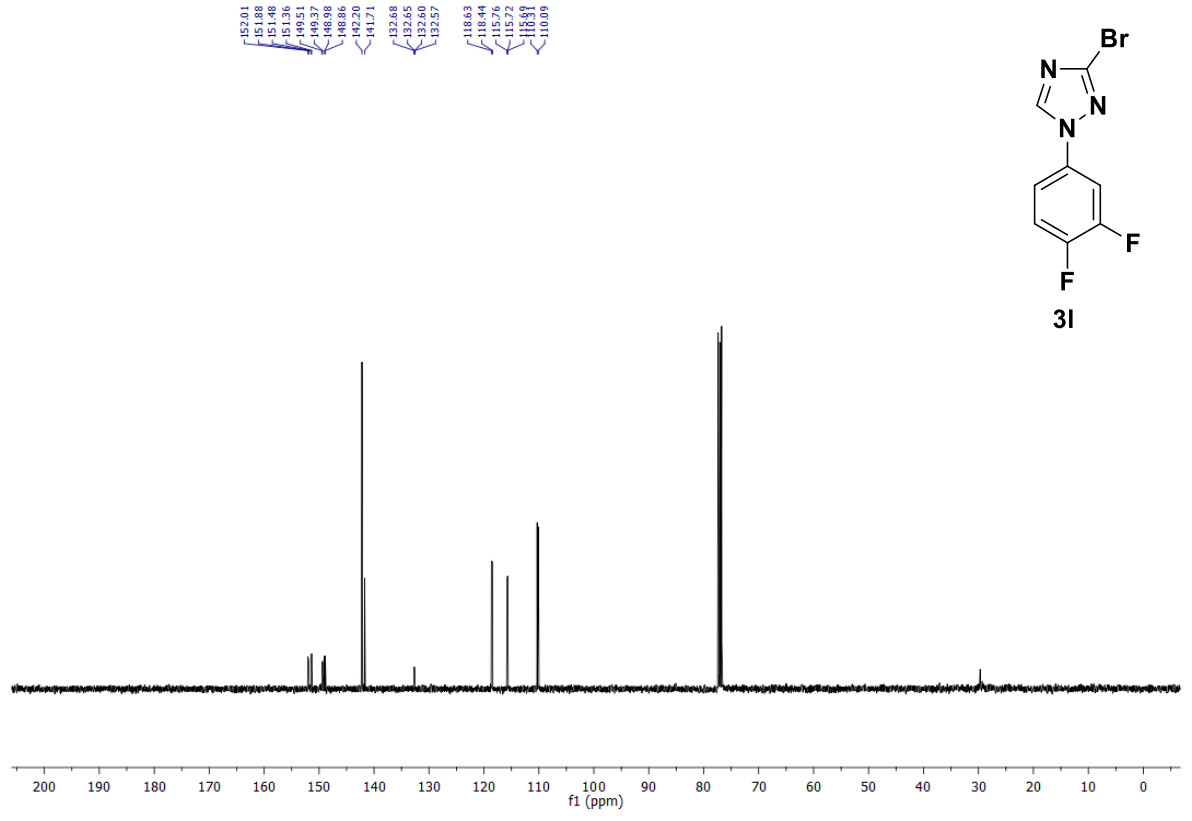
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3-bromo-1*H*-1,2,4-triazol-1-yl)benzaldehyde (3k):



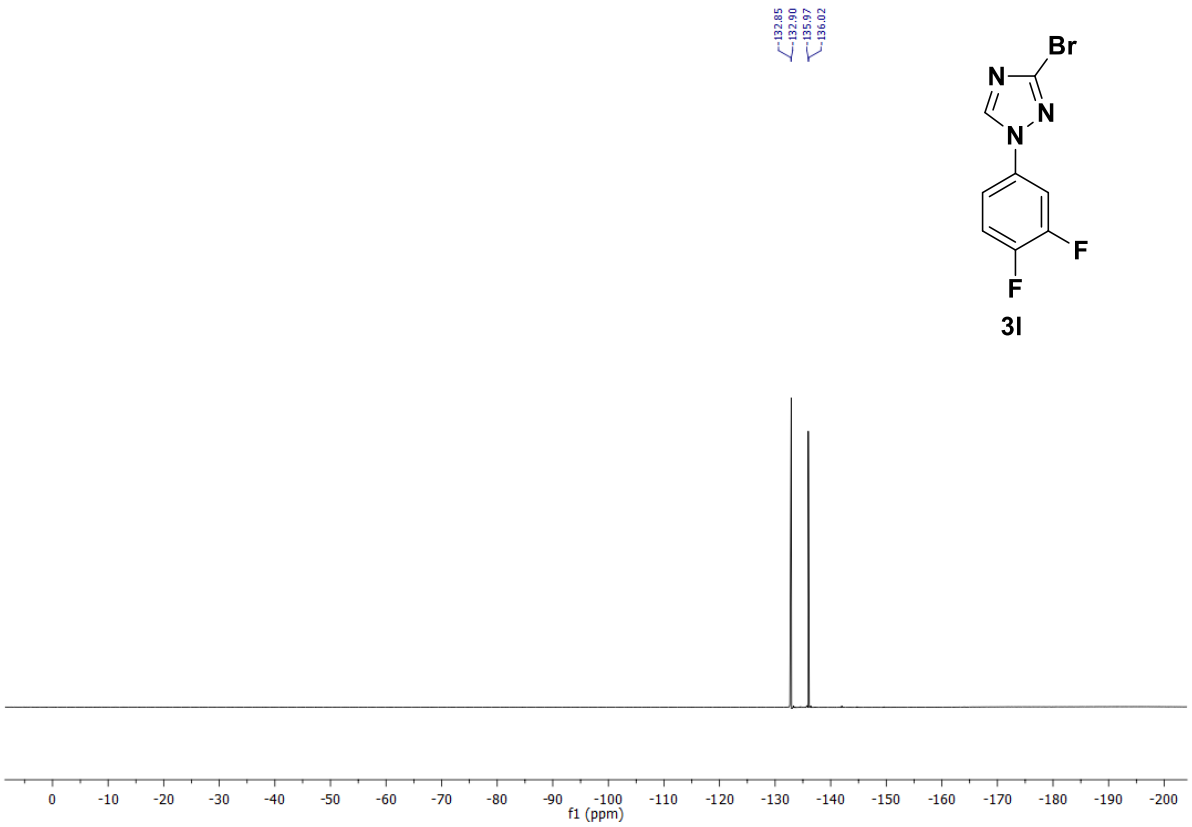
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(3,4-difluorophenyl)-1*H*-1,2,4-triazole (3l):



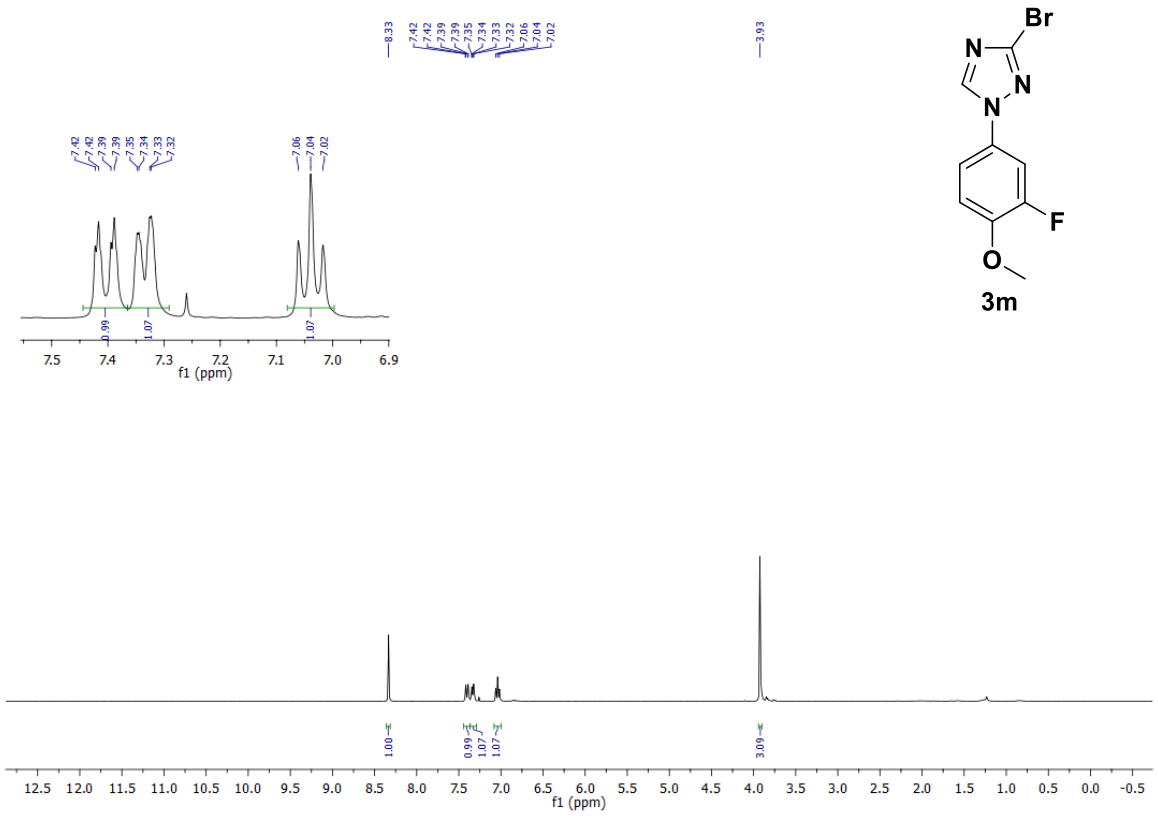
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(3,4-difluorophenyl)-1*H*-1,2,4-triazole (3l):



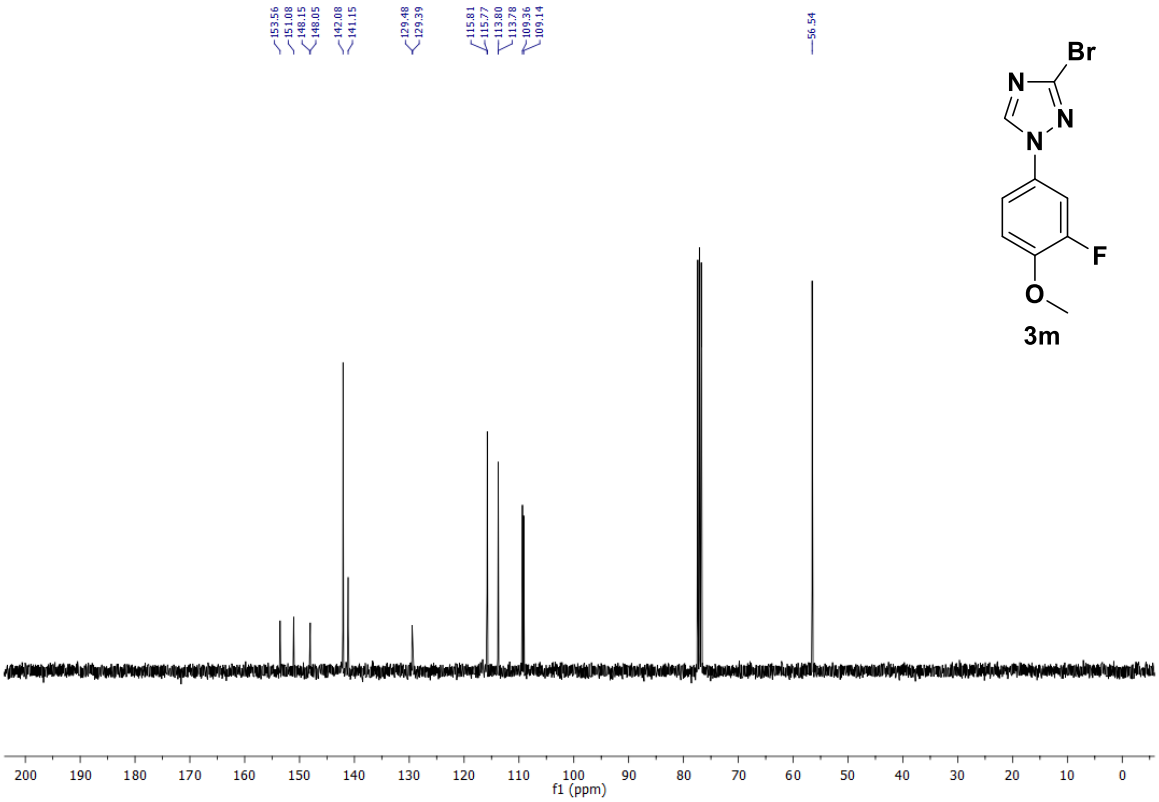
^{19}F NMR (377 MHz, $CDCl_3$) of 3-bromo-1-(3,4-difluorophenyl)-1*H*-1,2,4-triazole (3l):



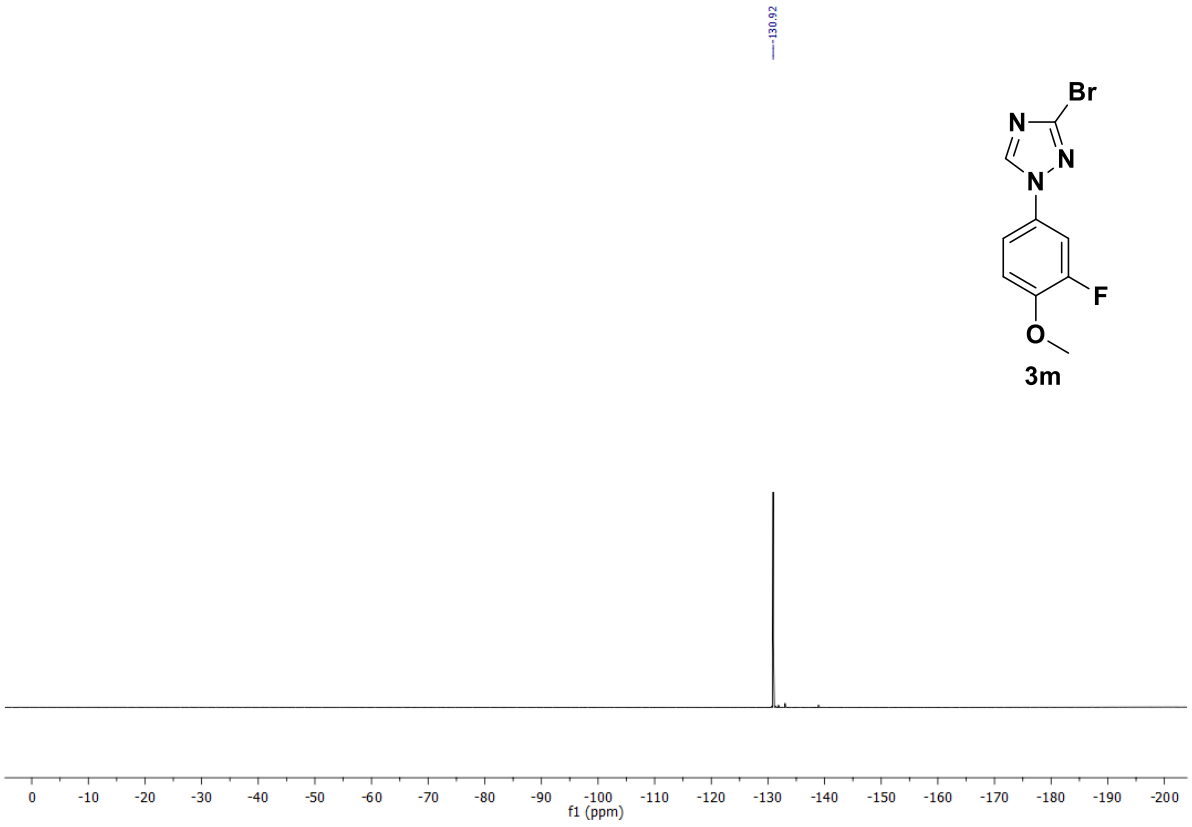
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(3-fluoro-4-methoxyphenyl)-1*H*-1,2,4-triazole (3m):



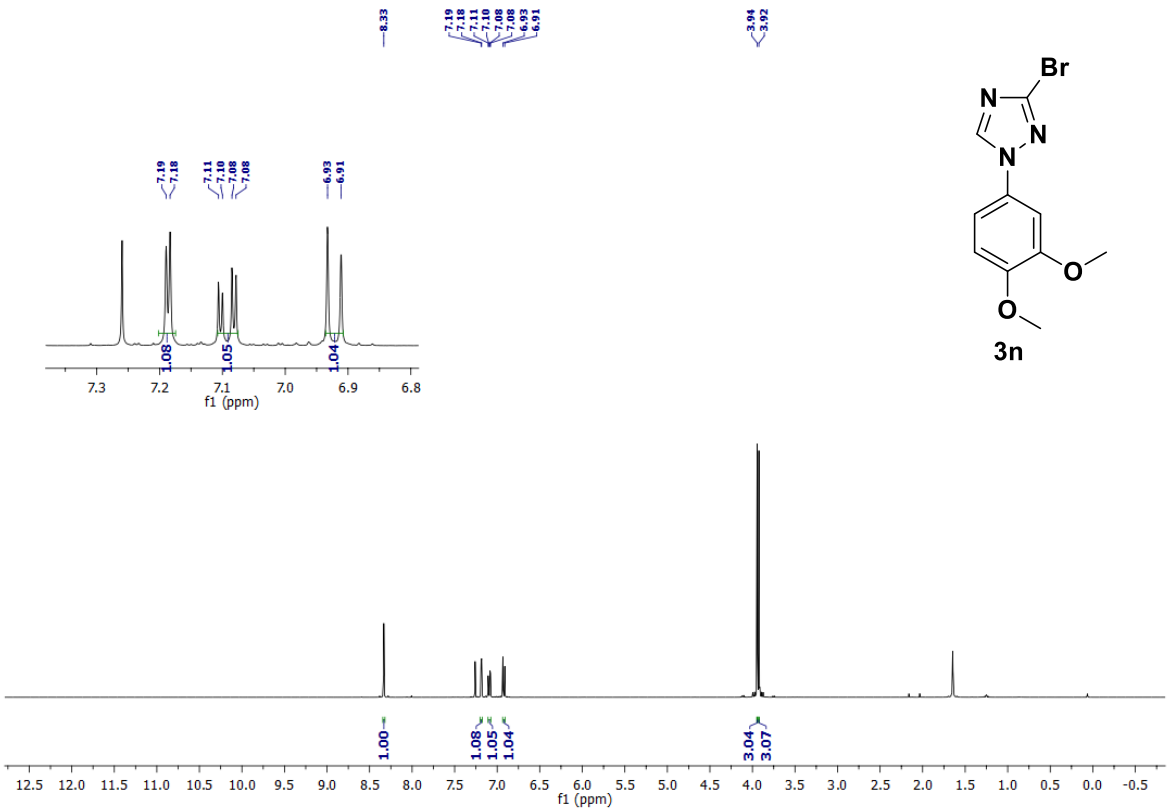
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(3-fluoro-4-methoxyphenyl)-1*H*-1,2,4-triazole (3m):



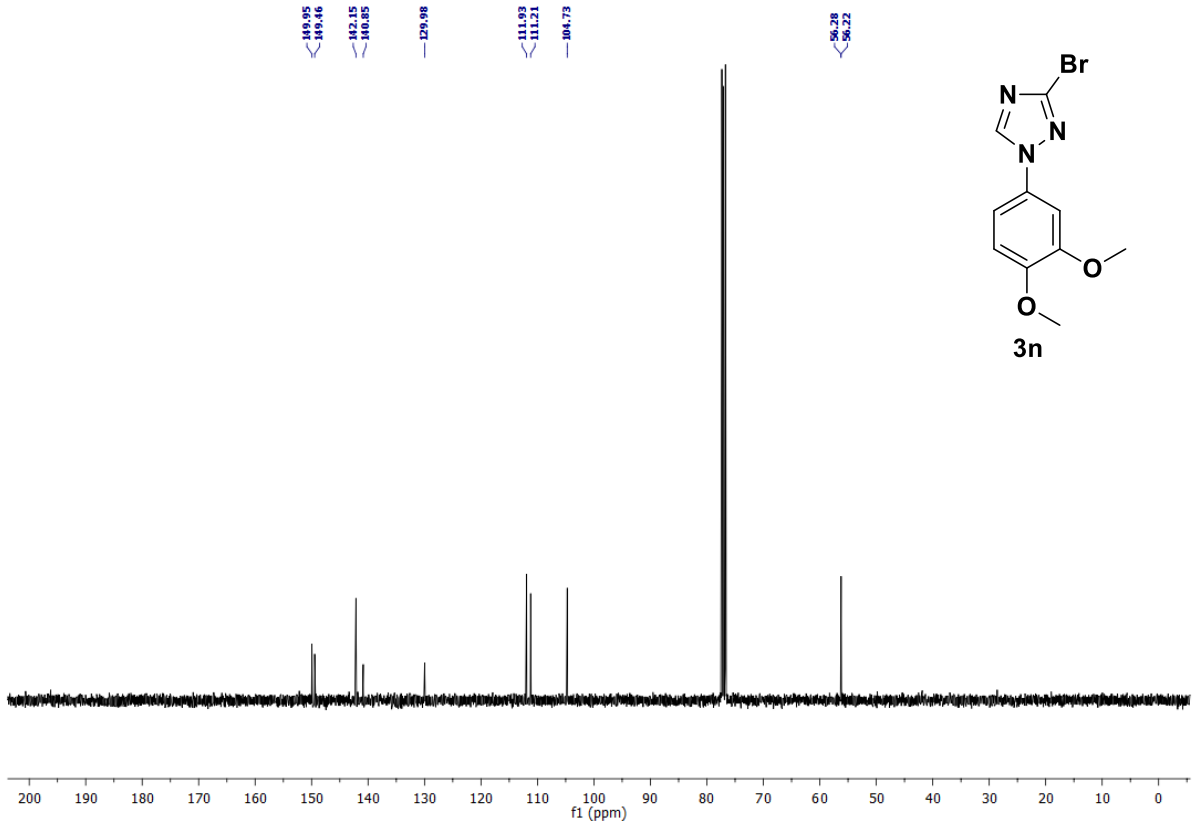
^{19}F NMR (377 MHz, $CDCl_3$) of 3-bromo-1-(3-fluoro-4-methoxyphenyl)-1*H*-1,2,4-triazole (3m):



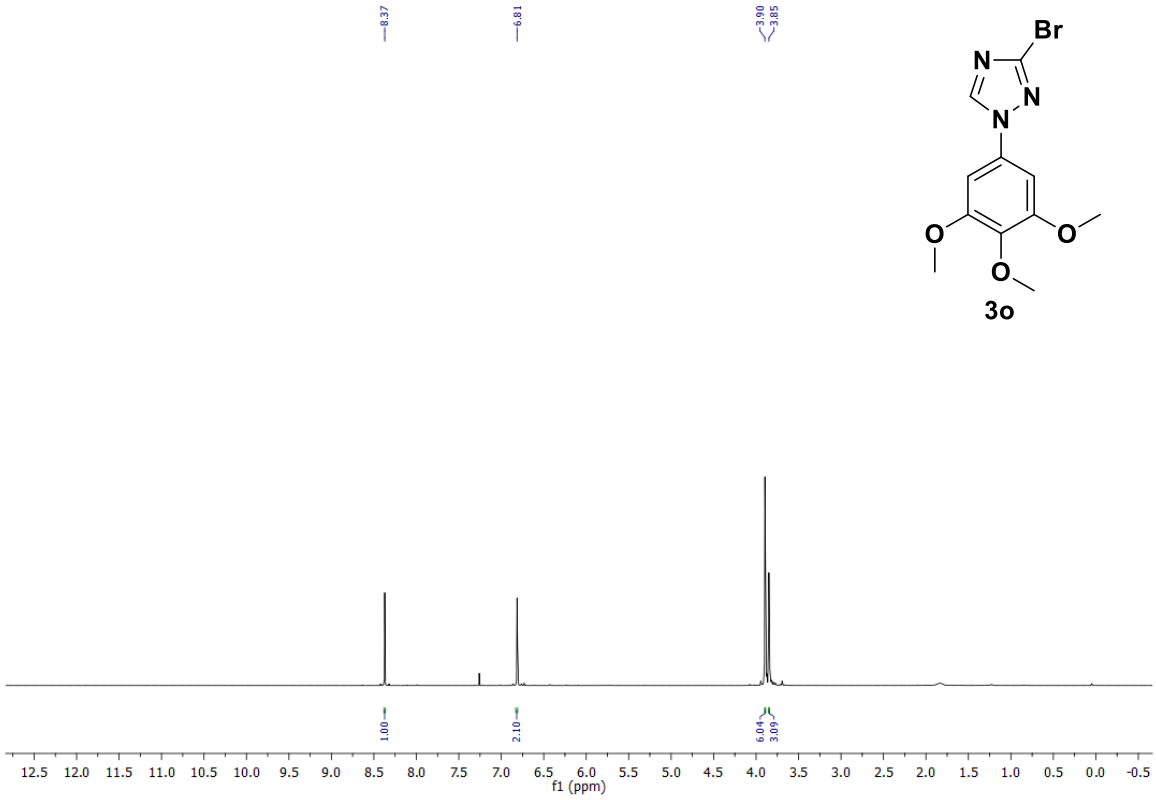
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(3,4-dimethoxyphenyl)-1*H*-1,2,4-triazole (3n):



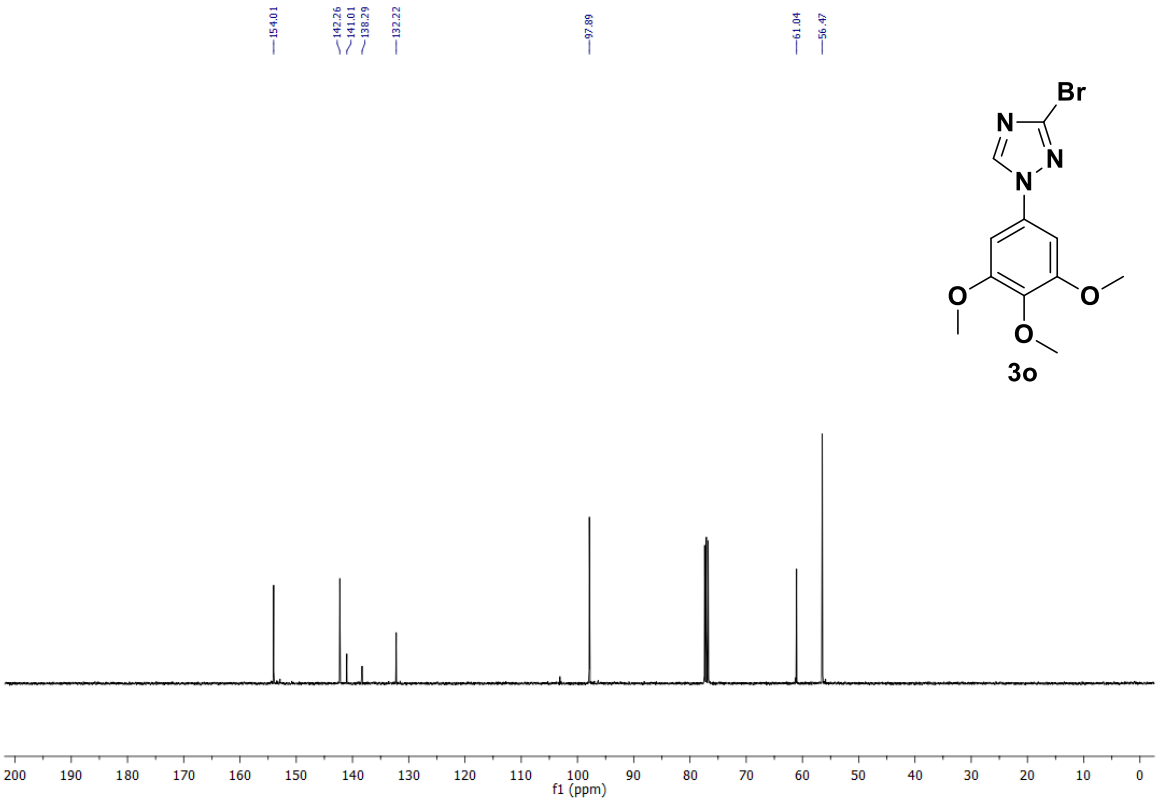
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(3,4-dimethoxyphenyl)-1*H*-1,2,4-triazole (3n):



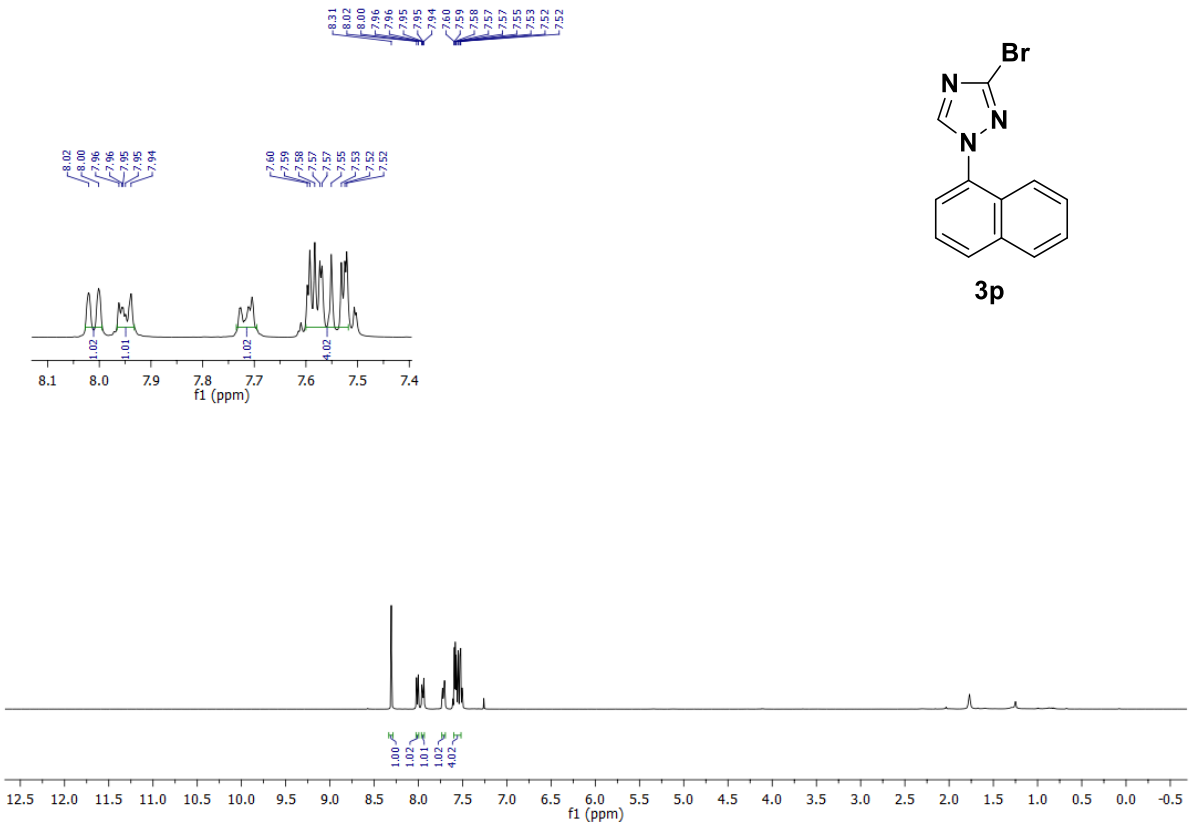
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (3o):



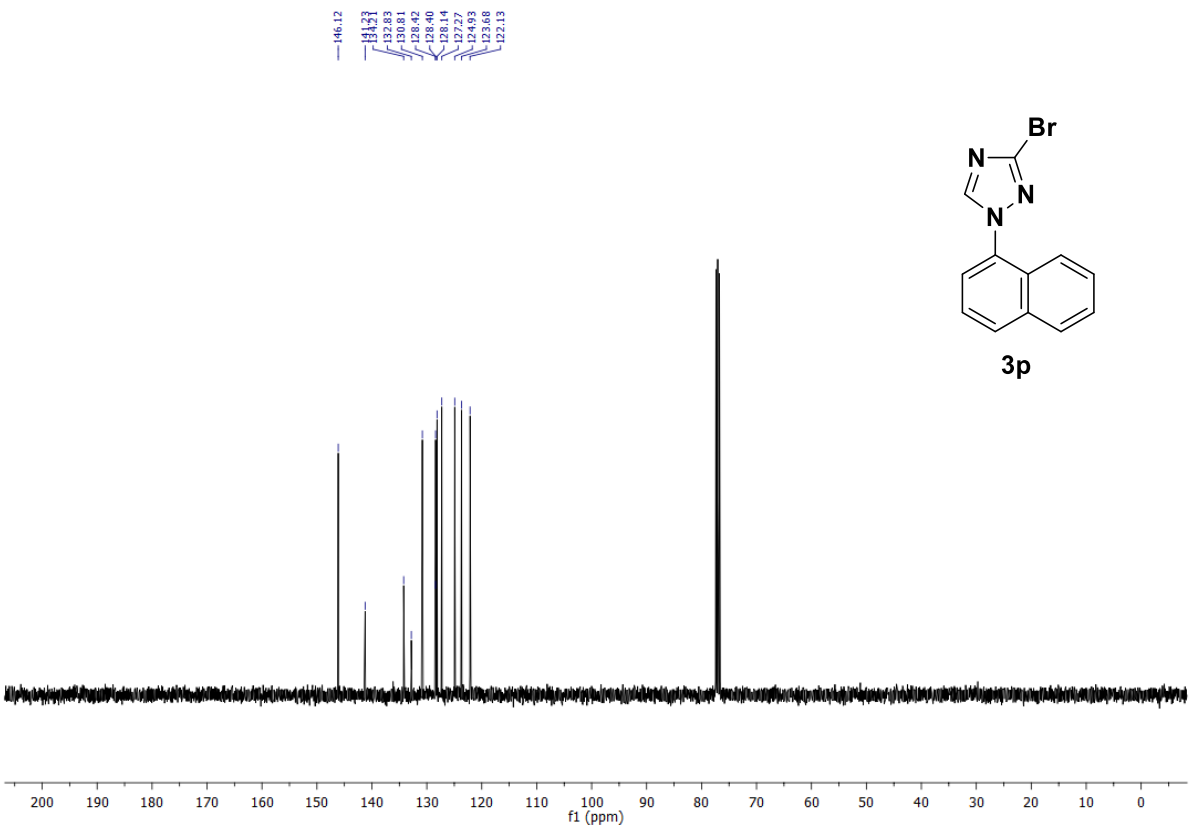
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (3o):



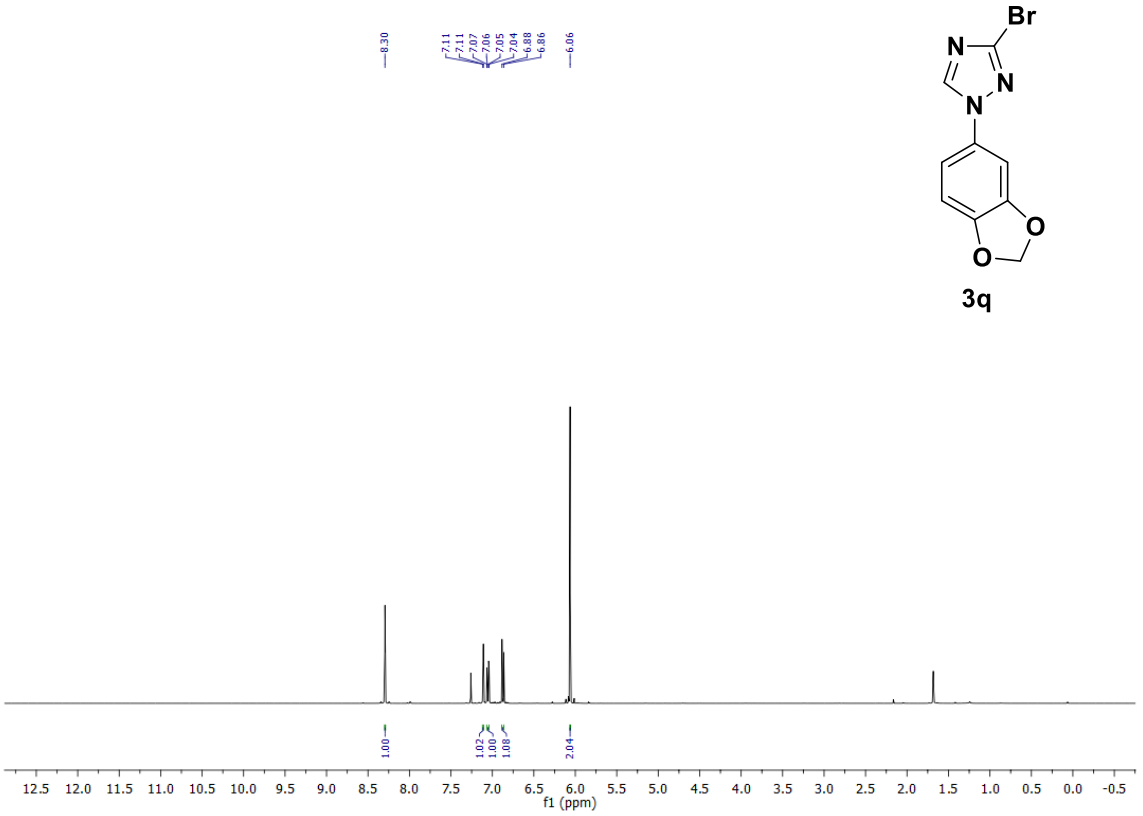
^{1}H NMR (400 MHz, $CDCl_3$) of 3-bromo-1-(naphthalen-1-yl)-1*H*-1,2,4-triazole (3p):



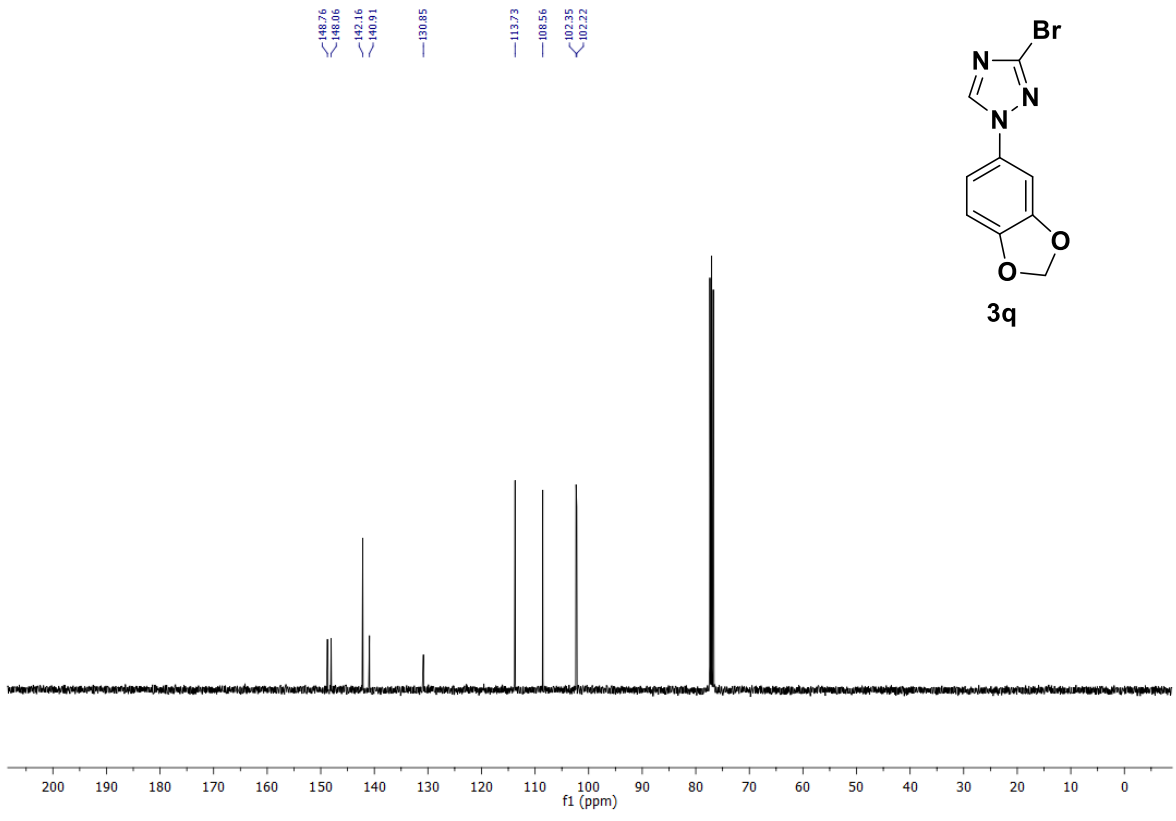
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-bromo-1-(naphthalen-1-yl)-1*H*-1,2,4-triazole (3p):



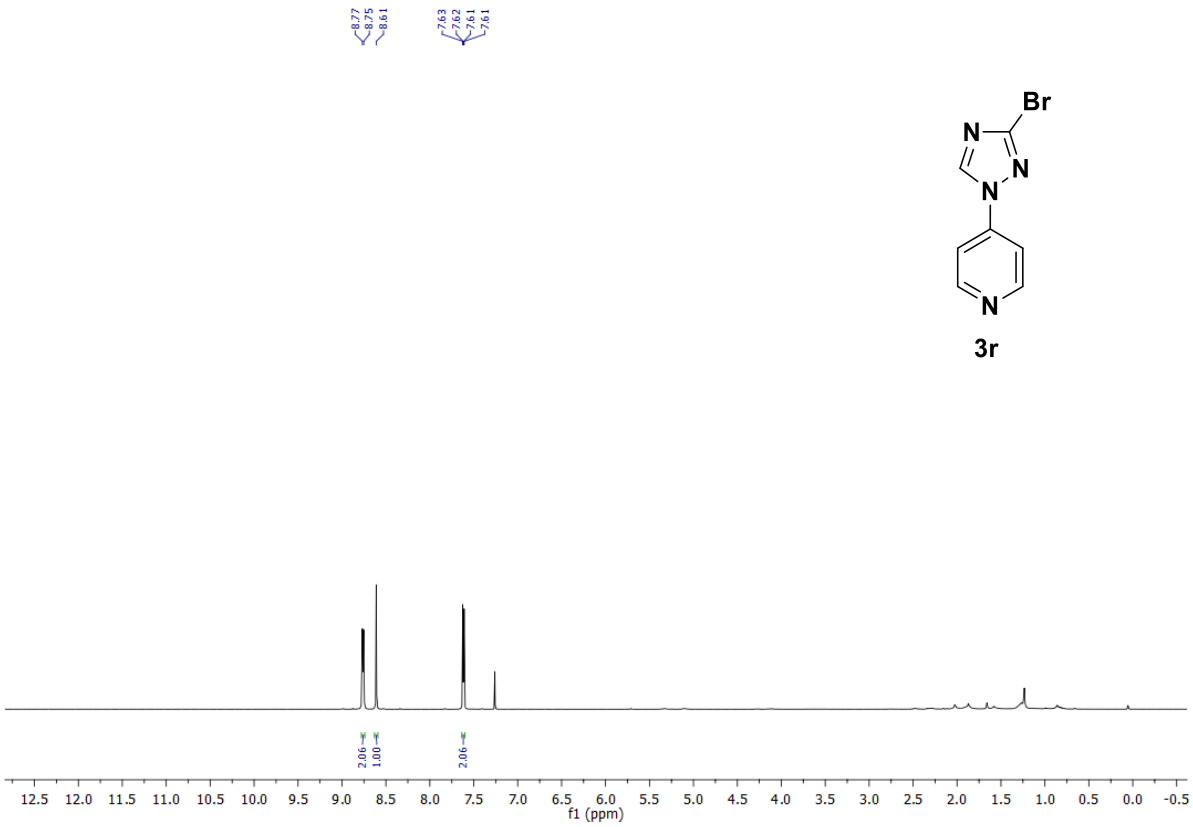
^{1}H NMR (400 MHz, $CDCl_3$) of 1-(benzo[*d*][1,3]dioxol-5-yl)-3-bromo-1*H*-1,2,4-triazole (3q):



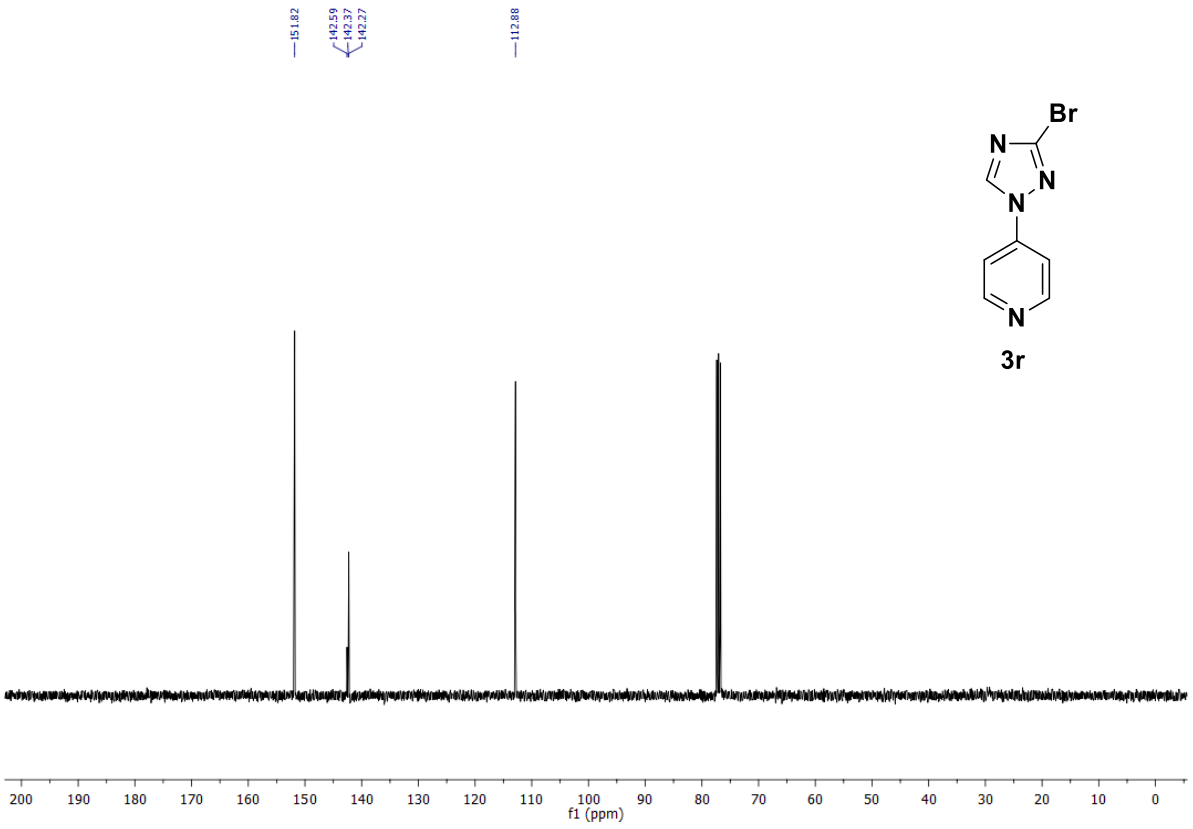
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 1-(benzo[*d*][1,3]dioxol-5-yl)-3-bromo-1*H*-1,2,4-triazole (3q):



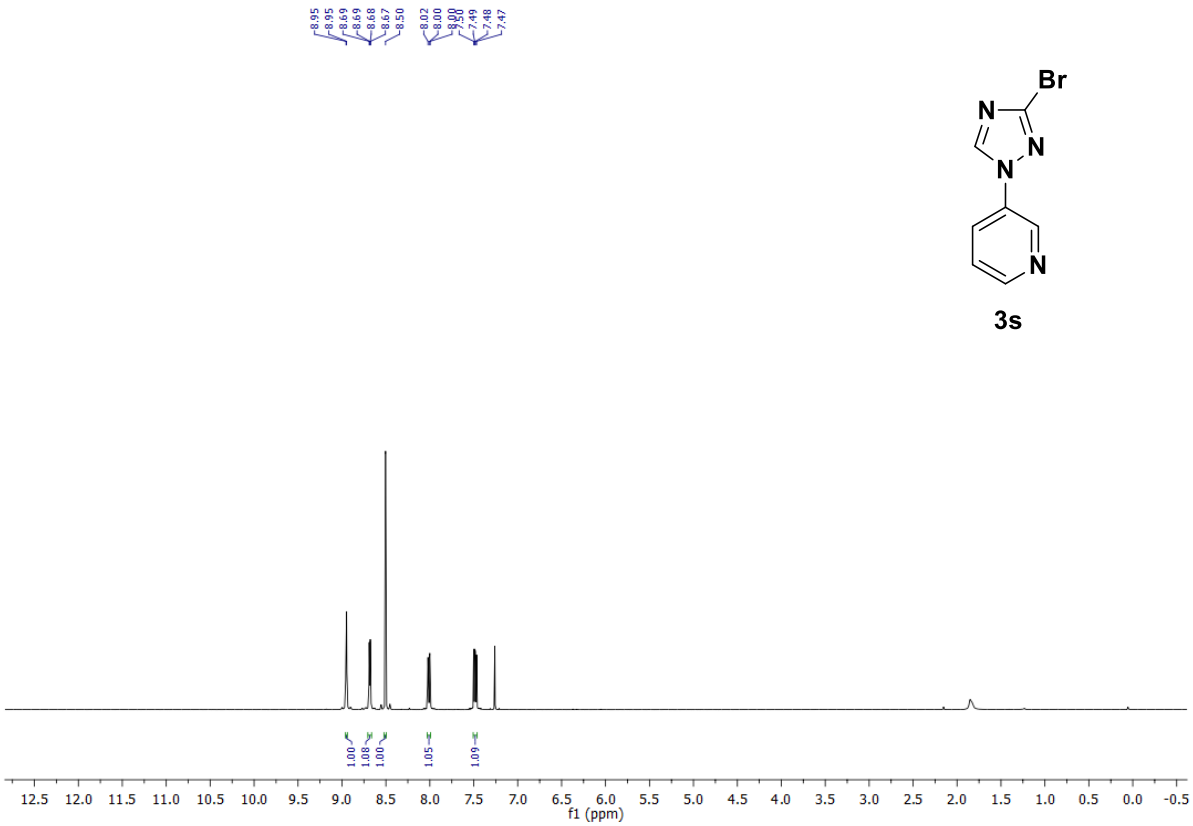
^{1}H NMR (400 MHz, $CDCl_3$) of 4-(3-bromo-1*H*-1,2,4-triazol-1-yl)pyridine (3r):



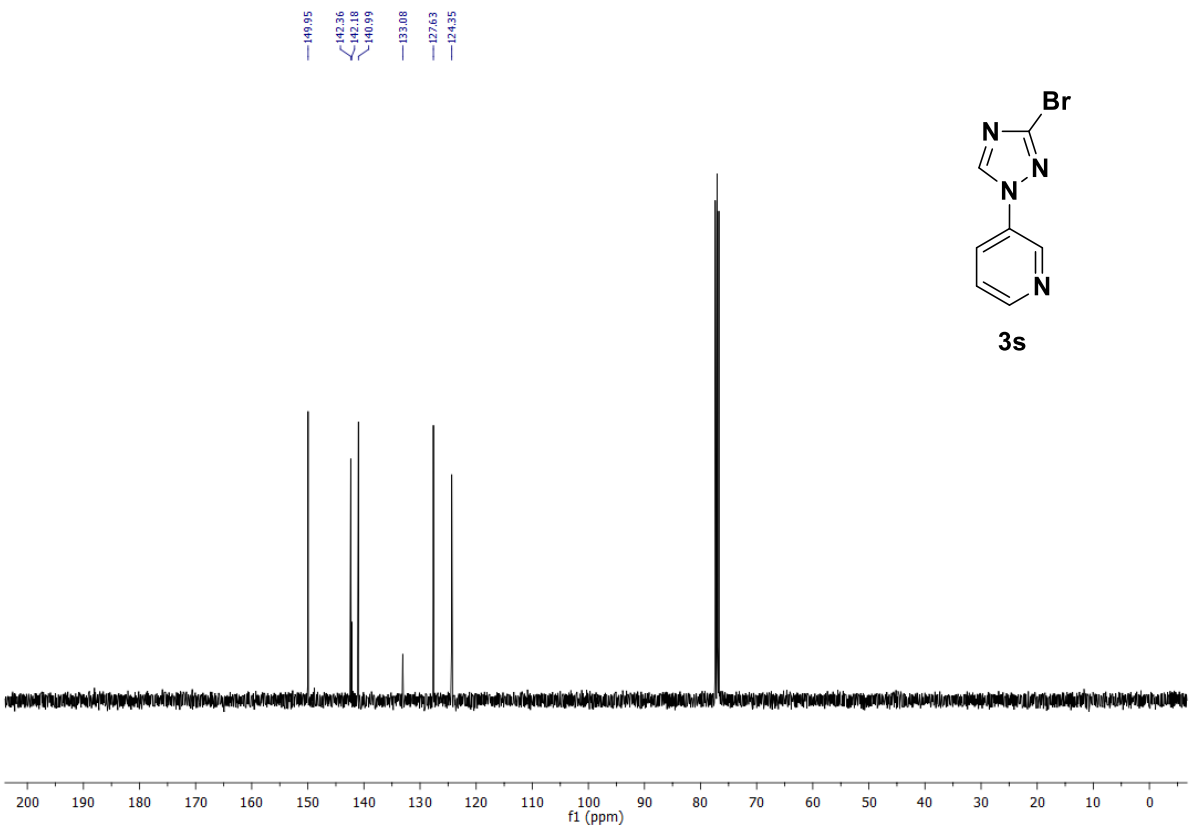
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 4-(3-bromo-1*H*-1,2,4-triazol-1-yl)pyridine (3r):



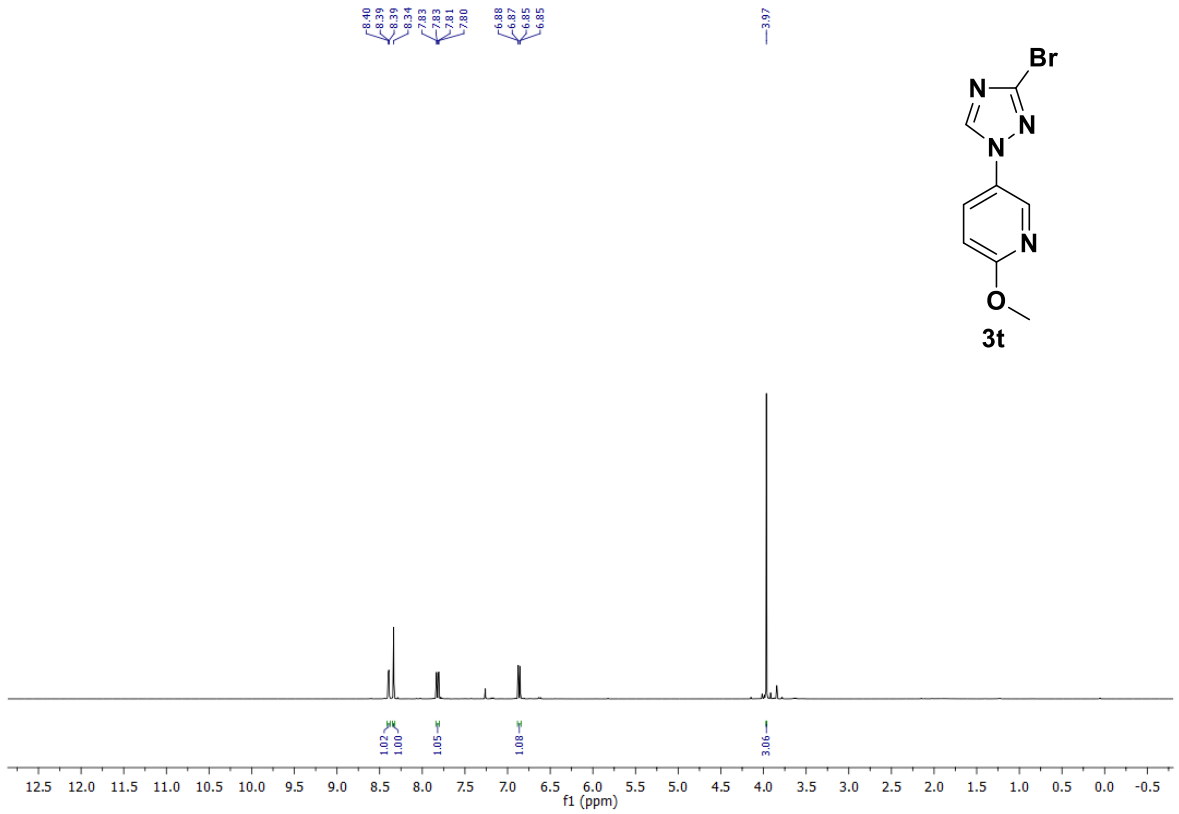
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(3-bromo-1*H*-1,2,4-triazol-1-yl)pyridine (3s):



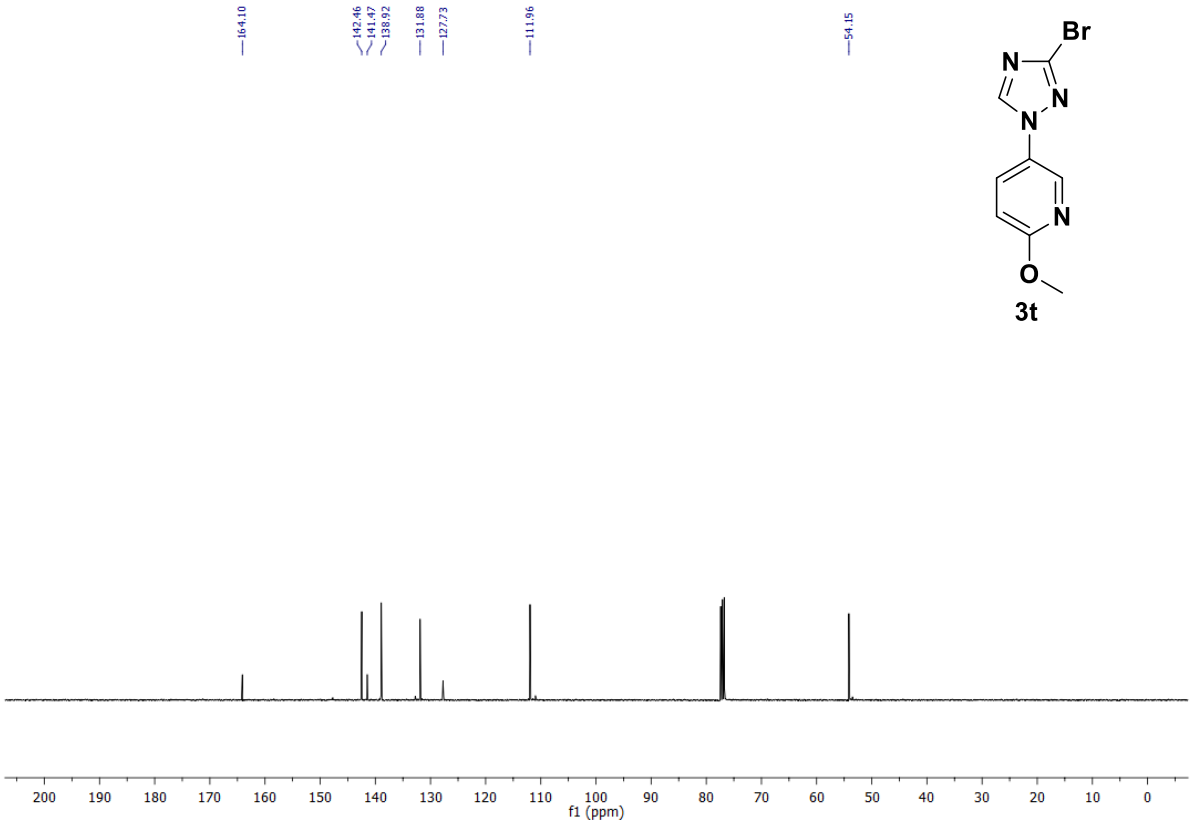
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3-bromo-1*H*-1,2,4-triazol-1-yl)pyridine (3s):



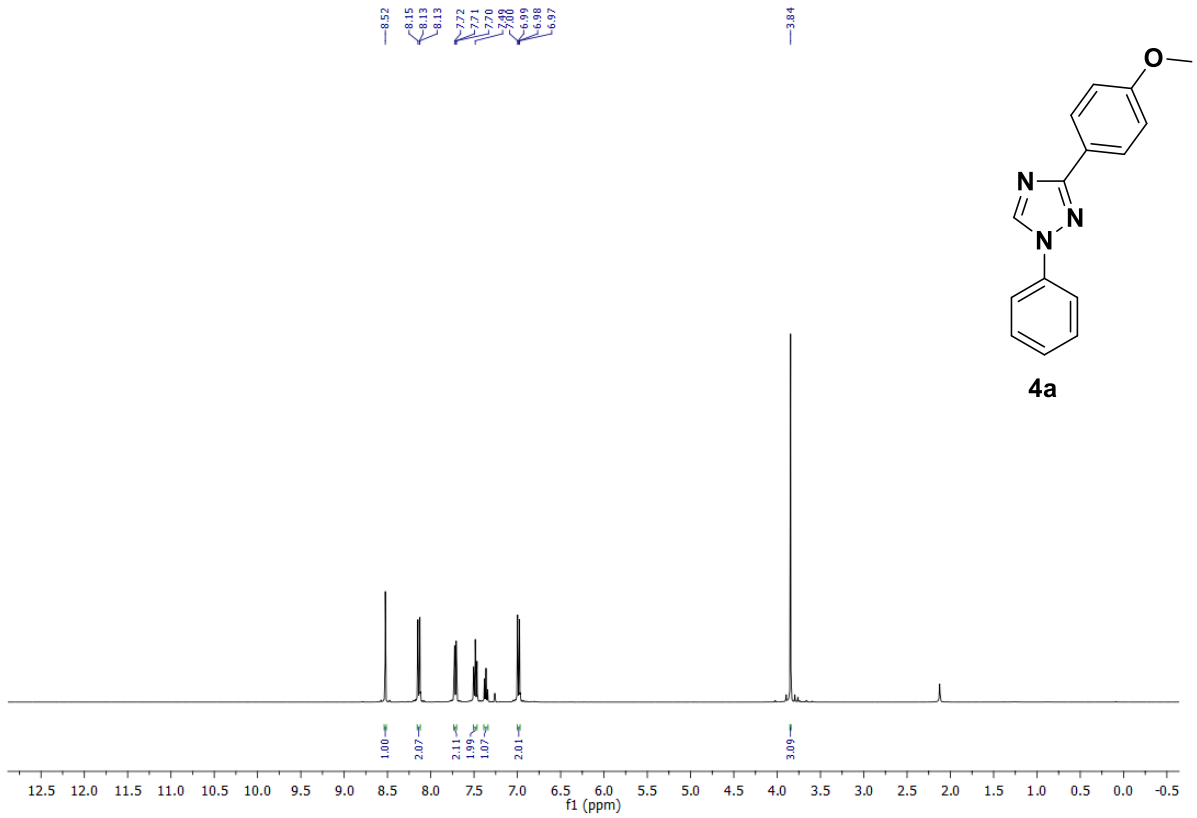
^{1}H NMR (400 MHz, $CDCl_3$) of 5-(3-bromo-1*H*-1,2,4-triazol-1-yl)-2-methoxypyridine (3t):



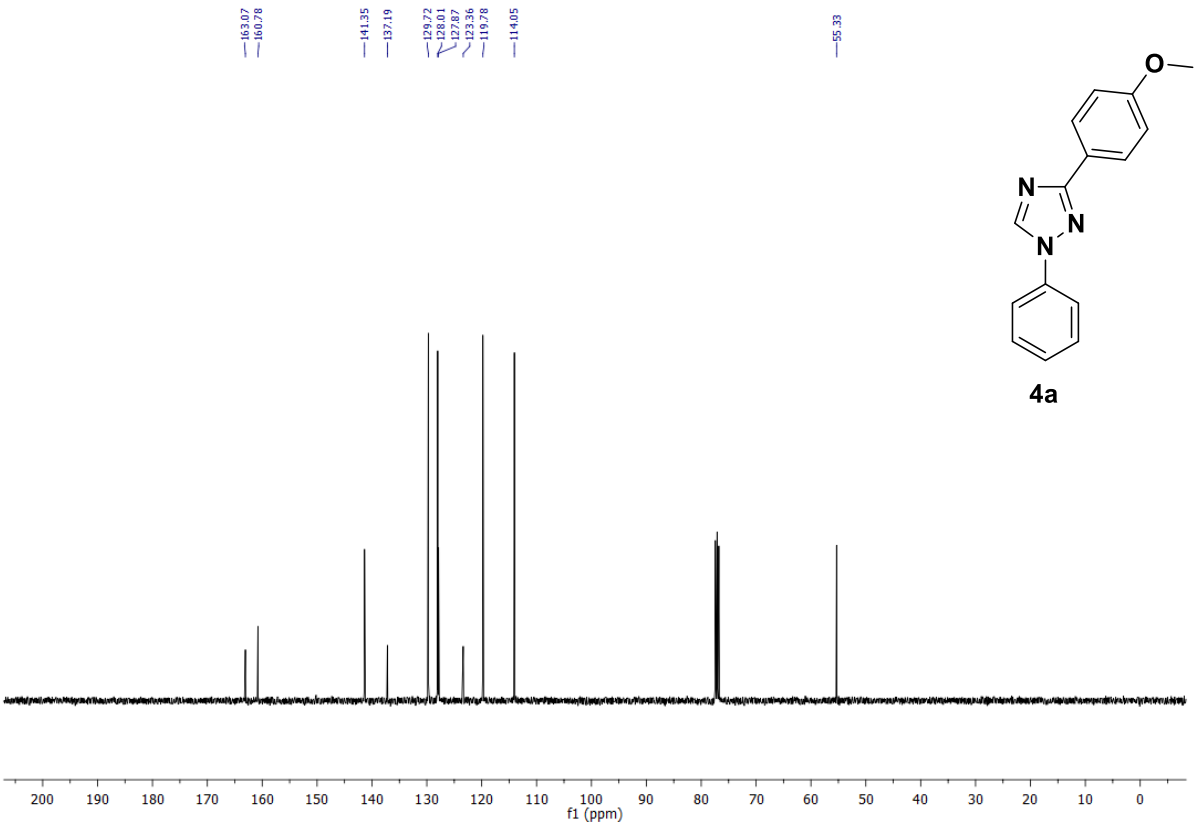
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 5-(3-bromo-1*H*-1,2,4-triazol-1-yl)-2-methoxypyridine (3t):



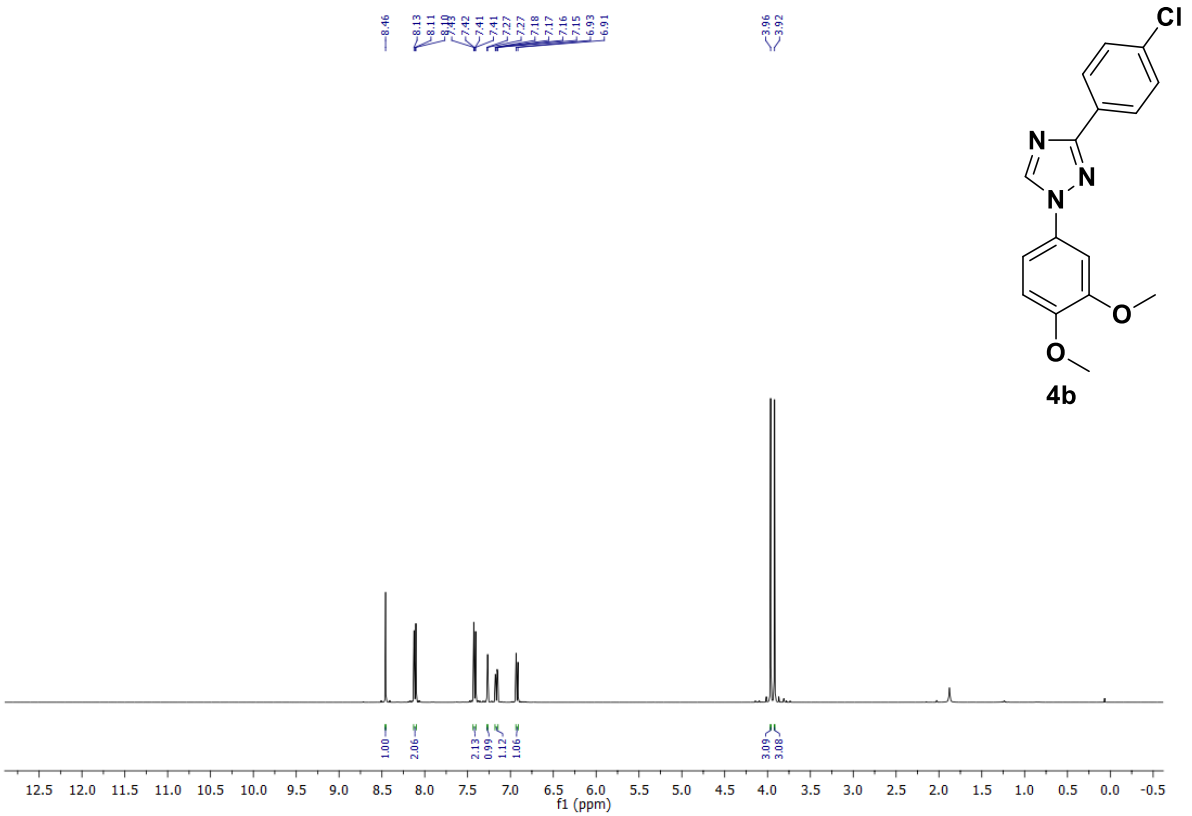
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(4-methoxyphenyl)-1-phenyl-1*H*-1,2,4-triazole (4a):



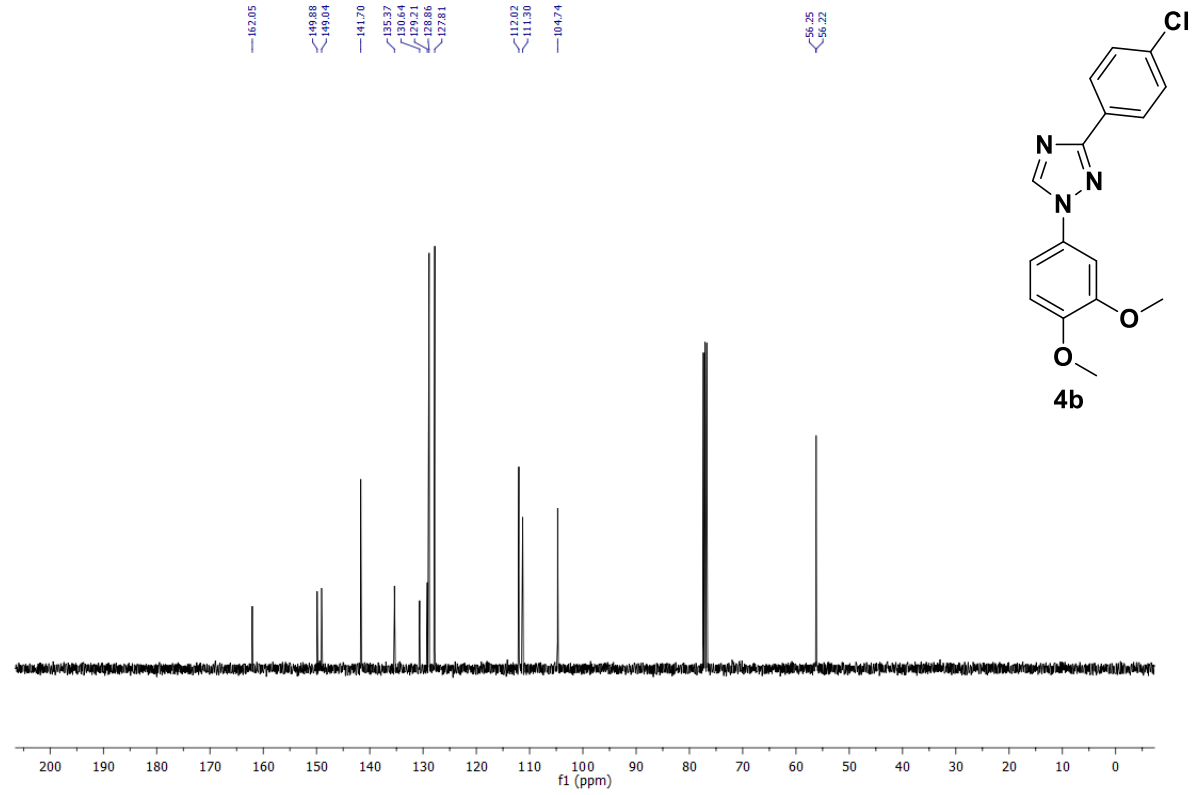
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(4-methoxyphenyl)-1-phenyl-1*H*-1,2,4-triazole (4a):



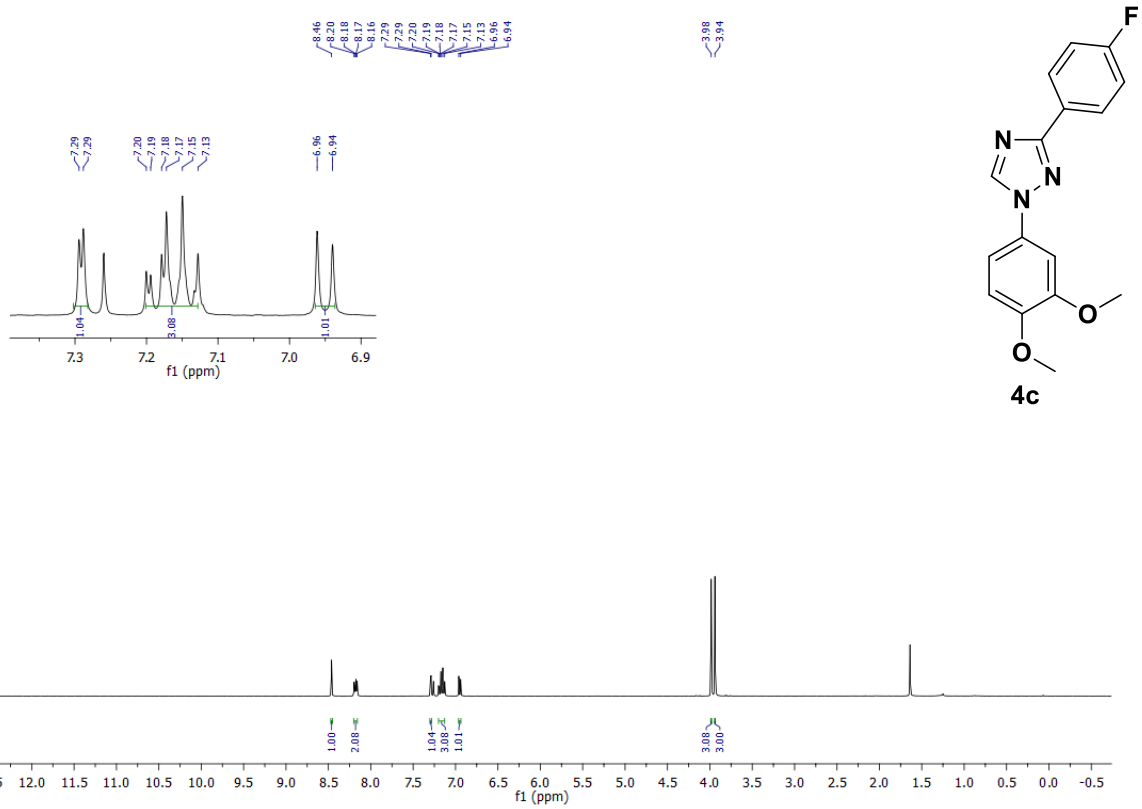
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(4-chlorophenyl)-1-(3,4-dimethoxyphenyl)-1*H*-1,2,4-triazole (4b):



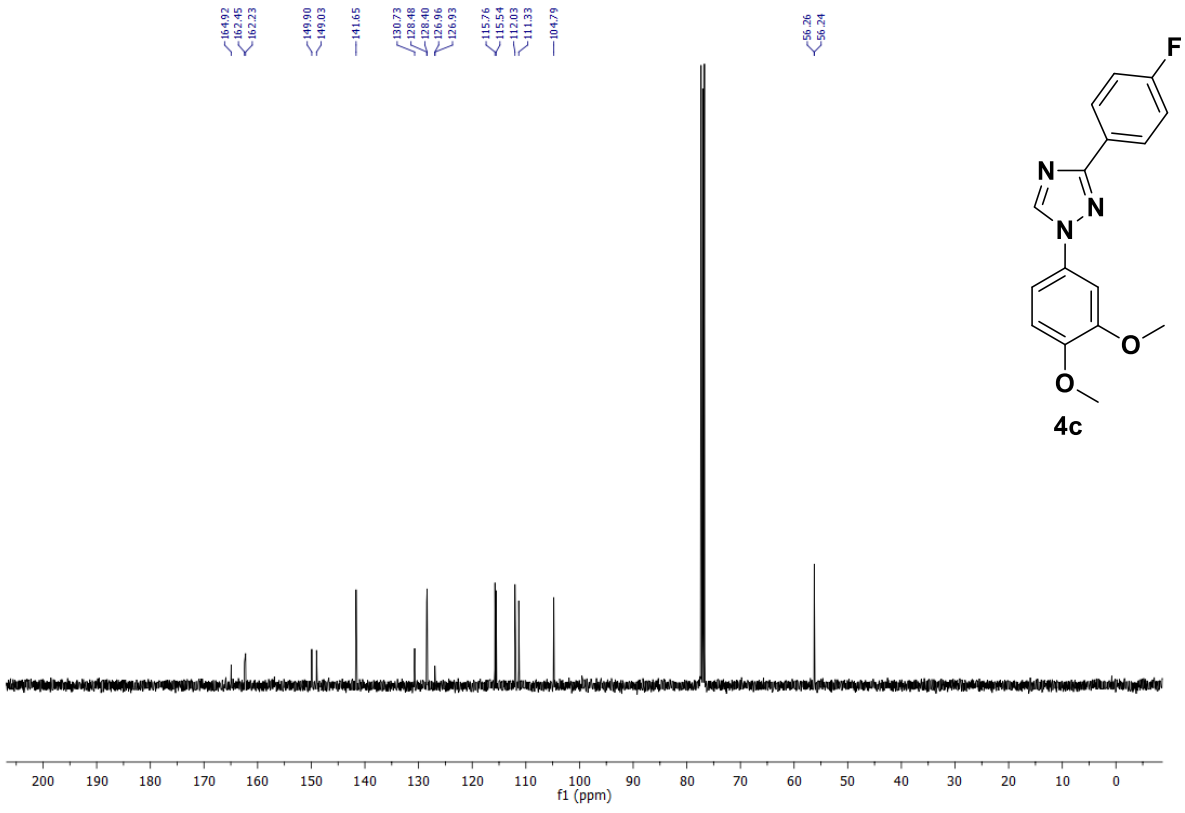
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(4-chlorophenyl)-1-(3,4-dimethoxyphenyl)-1*H*-1,2,4-triazole (4b):



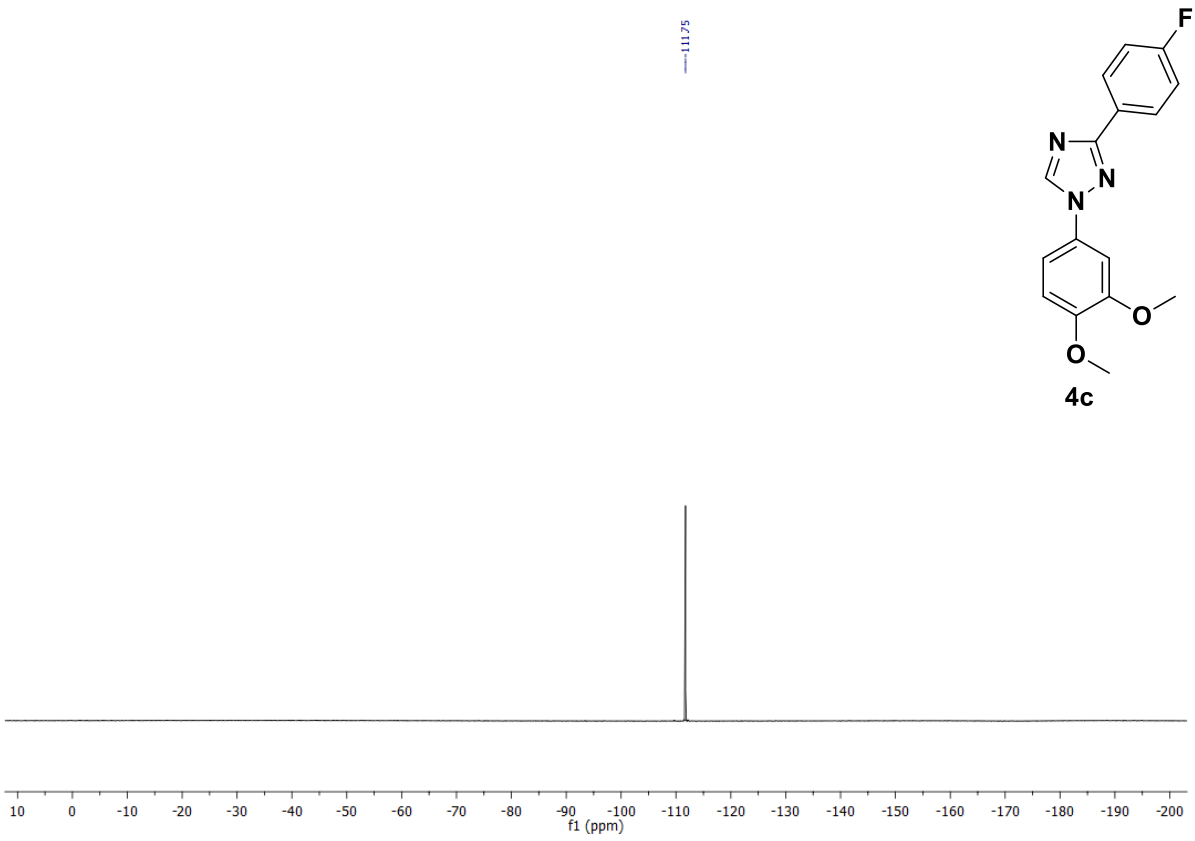
^{1}H NMR (400 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl)-1*H*-1,2,4-triazole (4c):



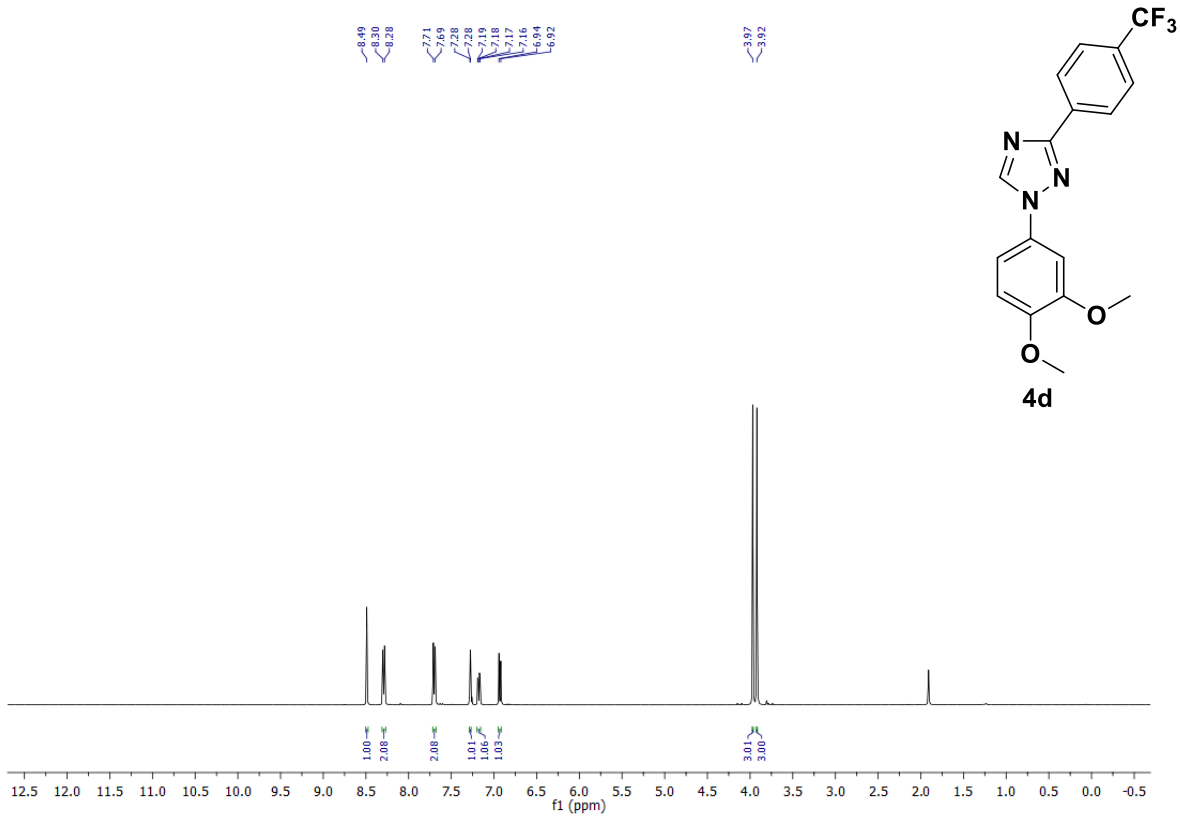
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl)-1*H*-1,2,4-triazole (4c):



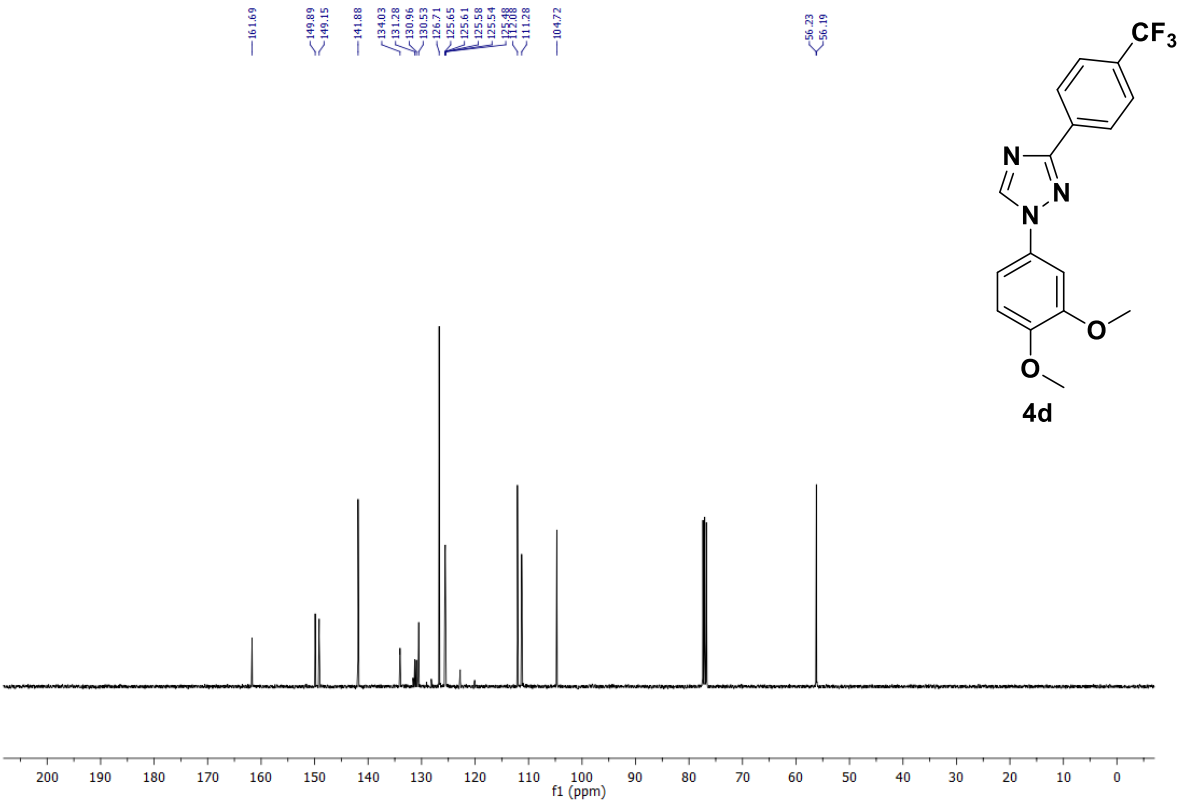
^{19}F NMR (377 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl)-1*H*-1,2,4-triazole (4c):



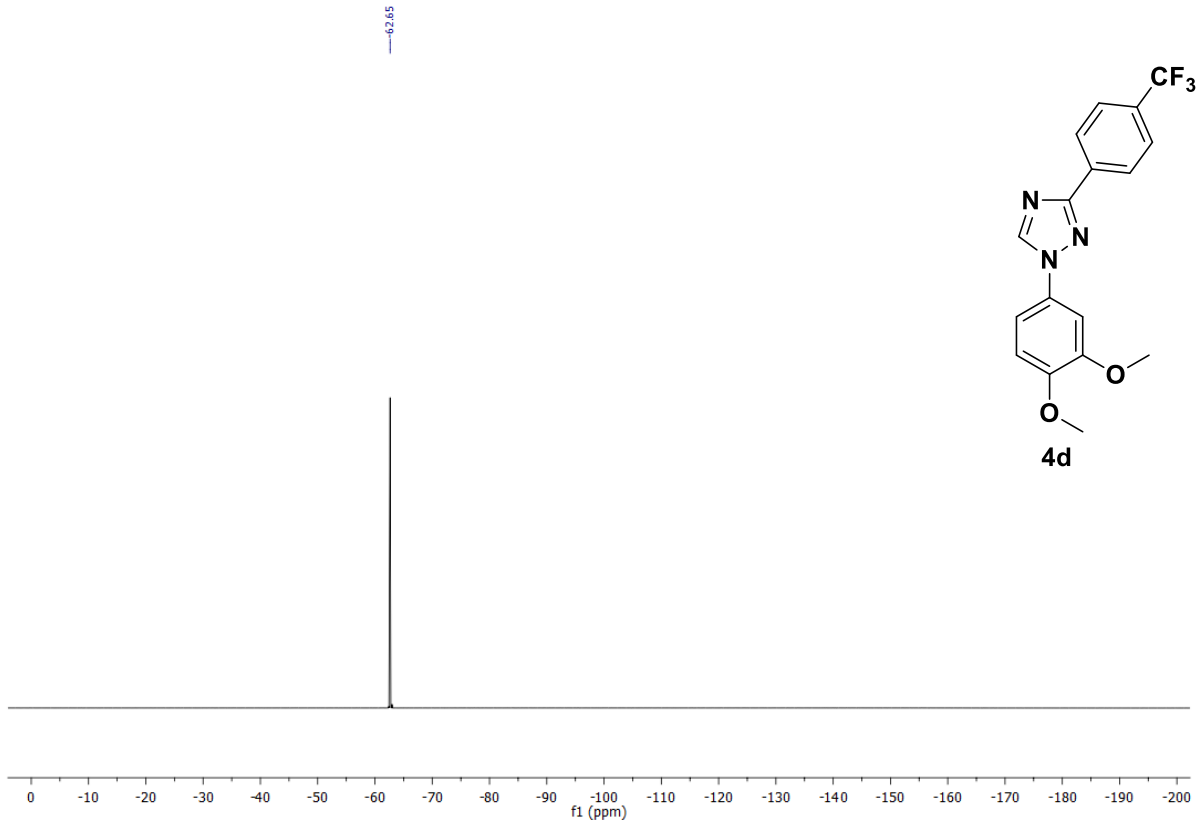
^{1}H NMR (400 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(4-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (4d):



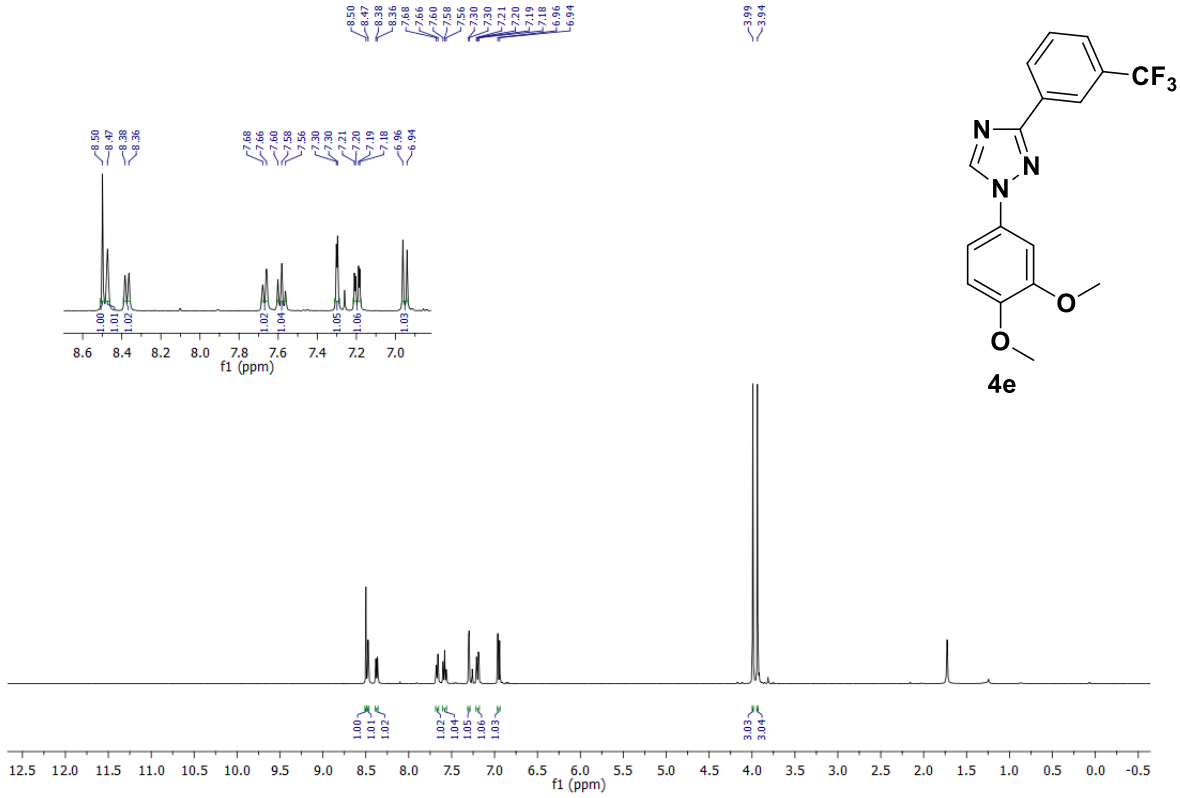
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(4-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (4d):



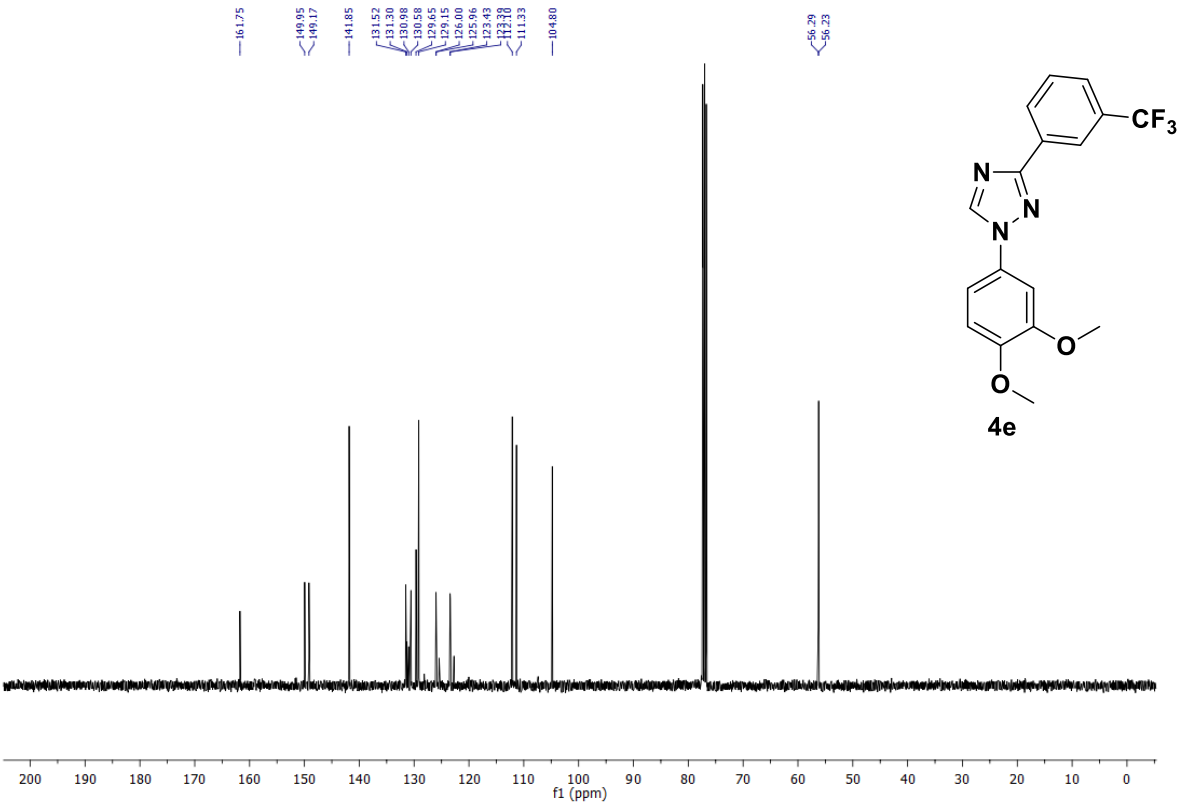
^{19}F NMR (377 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(4-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (4d):



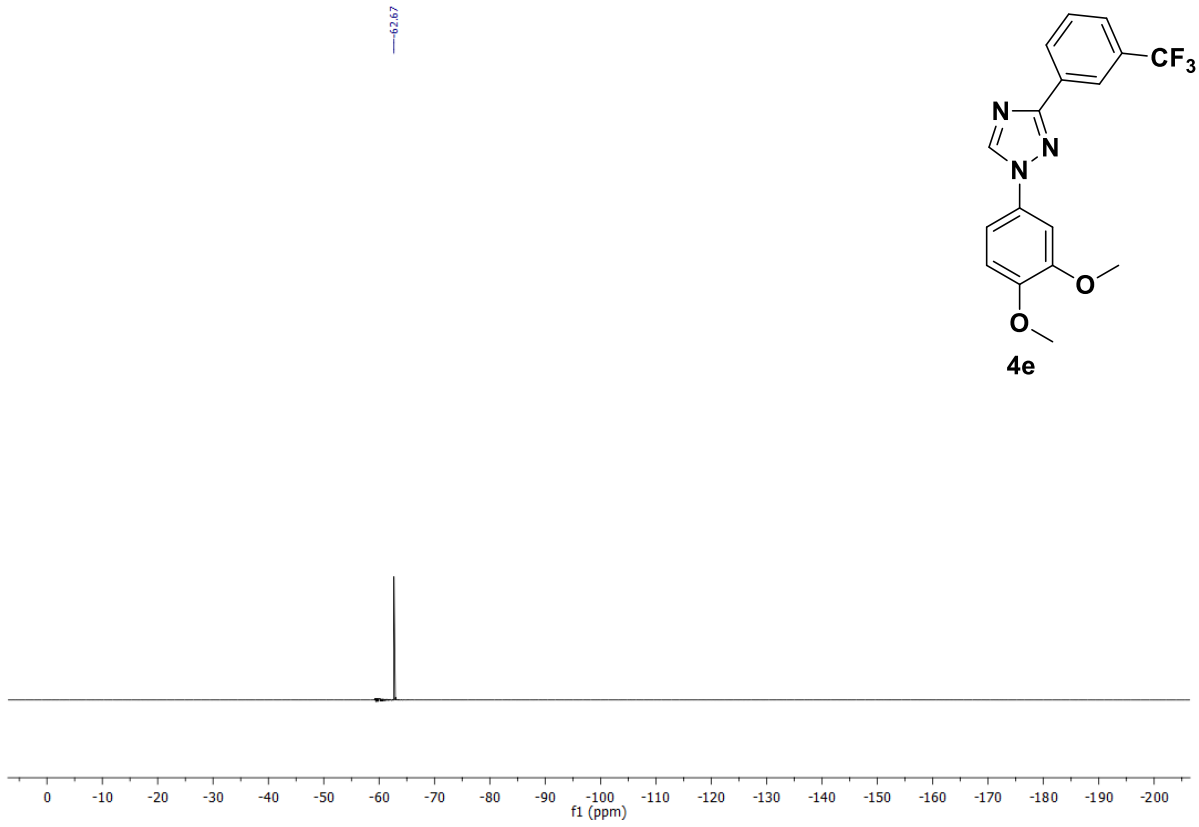
^{1}H NMR (400 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(3-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (4e):



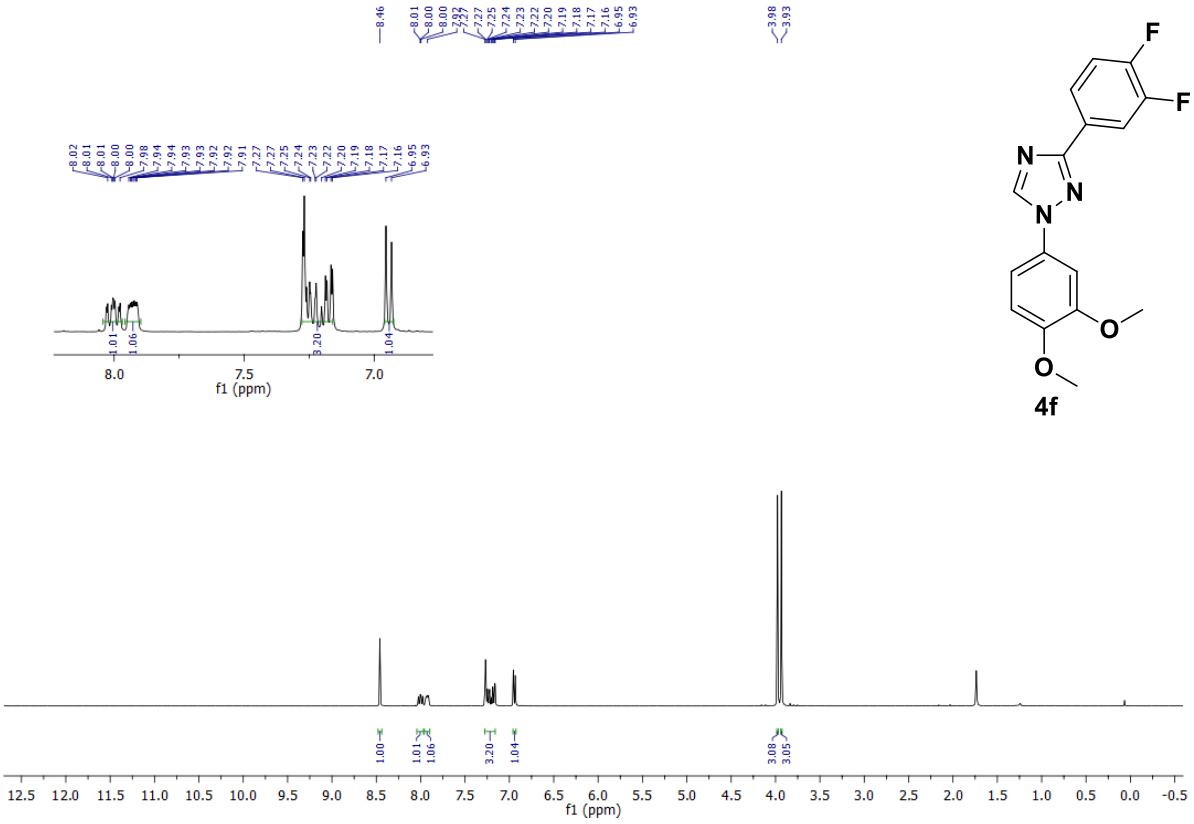
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(3-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (4e):



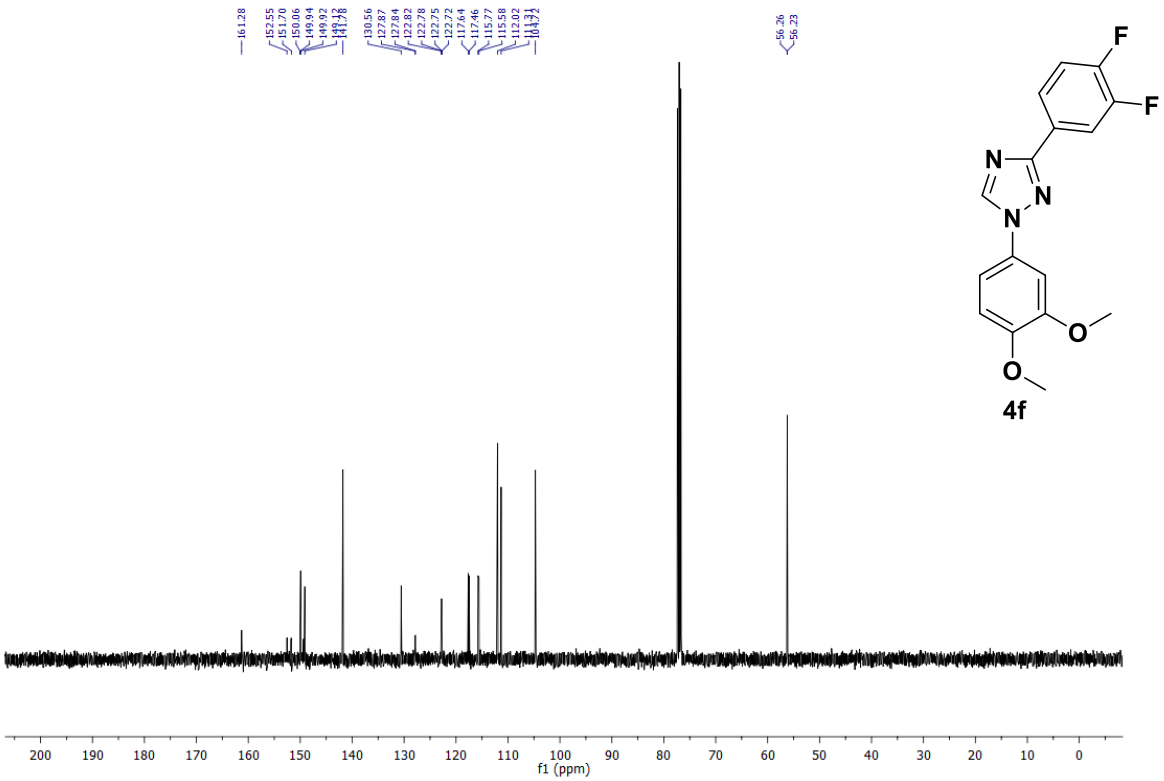
^{19}F NMR (377 MHz, $CDCl_3$) of 1-(3,4-dimethoxyphenyl)-3-(3-(trifluoromethyl)phenyl)-1*H*-1,2,4-triazole (4e):



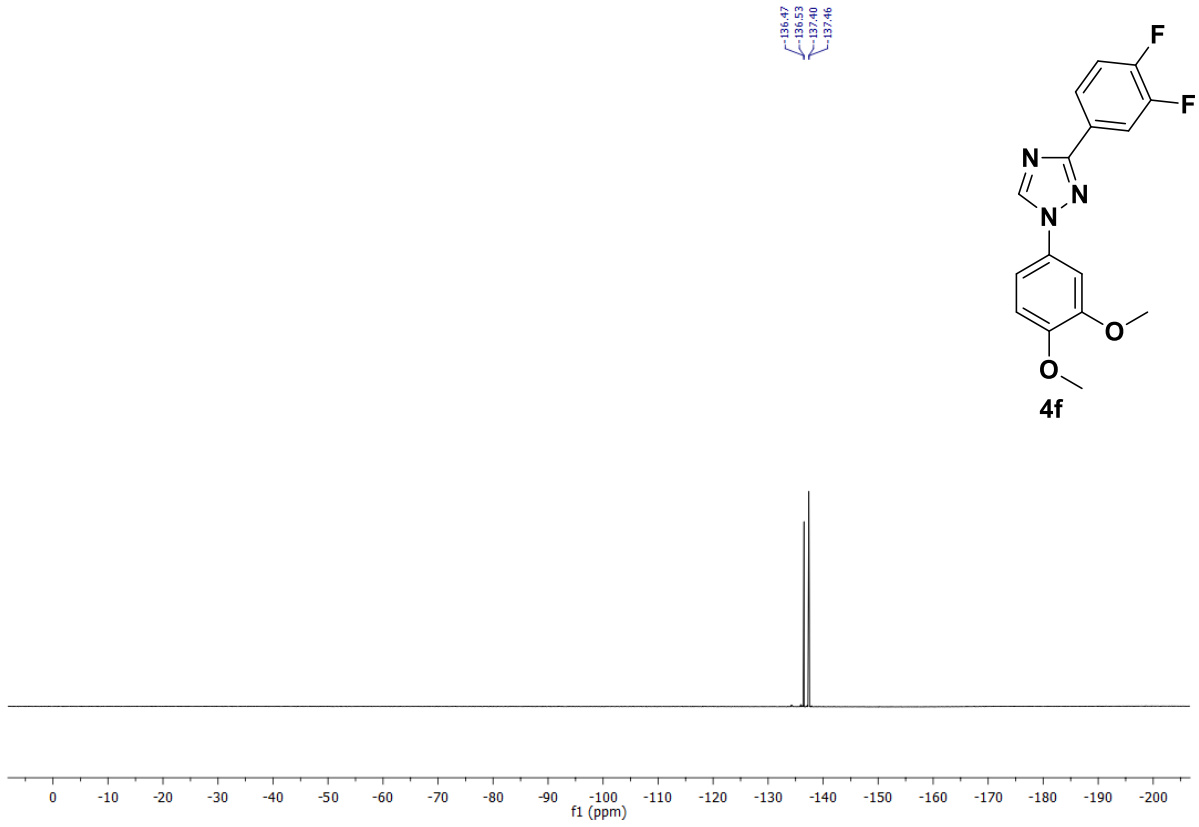
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(3,4-difluorophenyl)-1-(3,4-dimethoxyphenyl)-1*H*-1,2,4-triazole (4f):



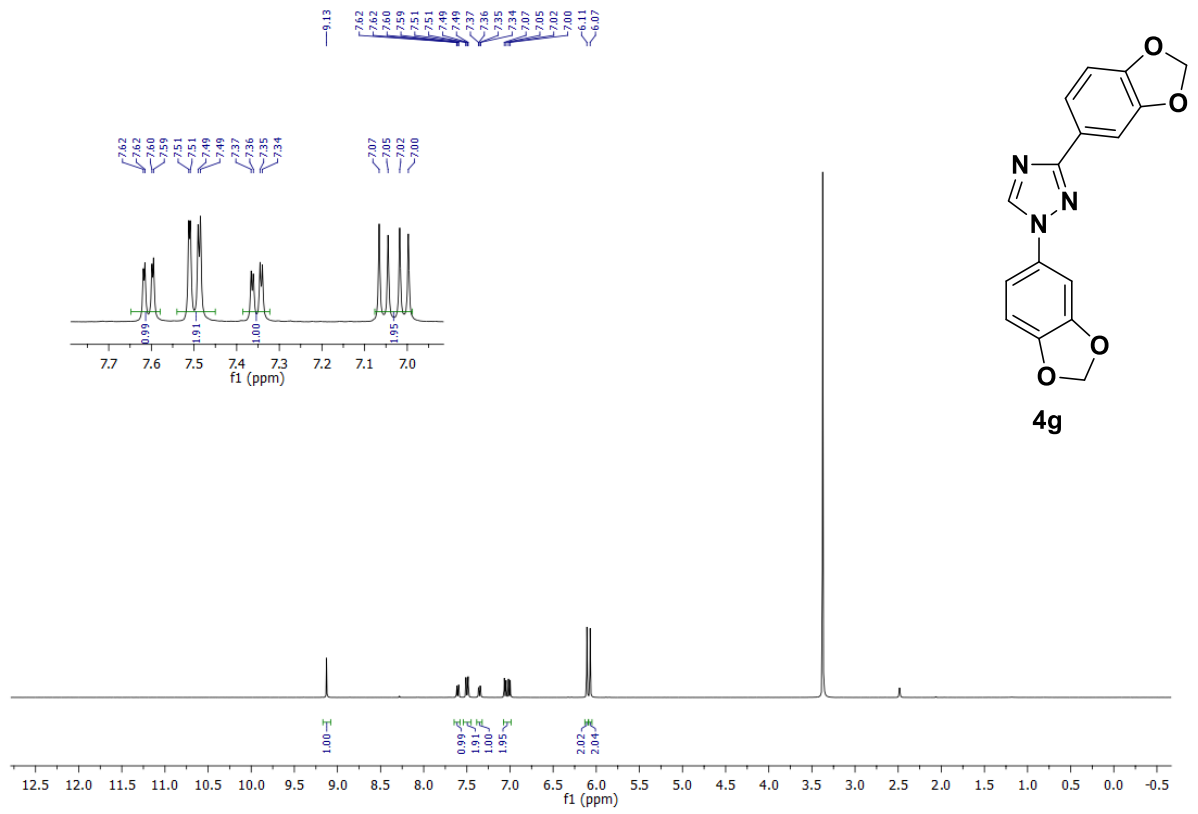
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3,4-difluorophenyl)-1-(3,4-dimethoxyphenyl)-1*H*-1,2,4-triazole (4f):



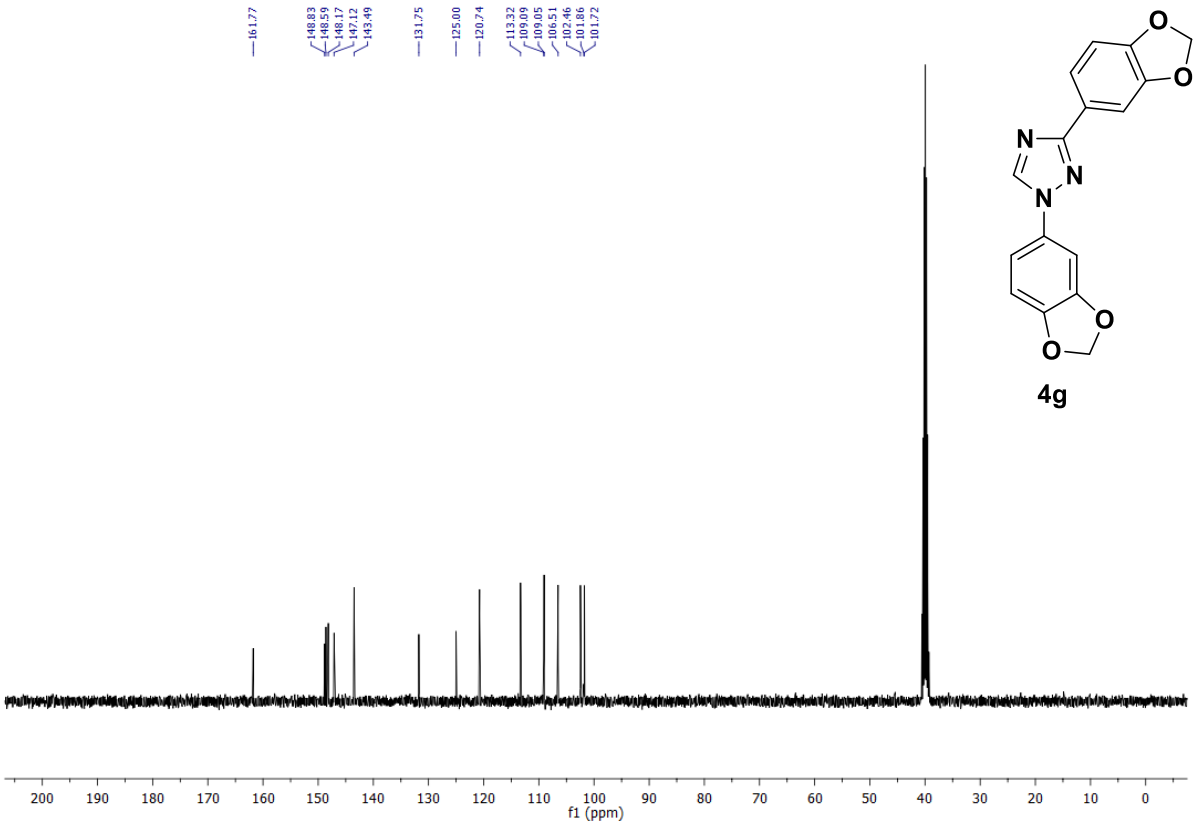
^{19}F NMR (377 MHz, $CDCl_3$) of 3-(3,4-difluorophenyl)-1-(3,4-dimethoxyphenyl)-1*H*-1,2,4-triazole (4f):



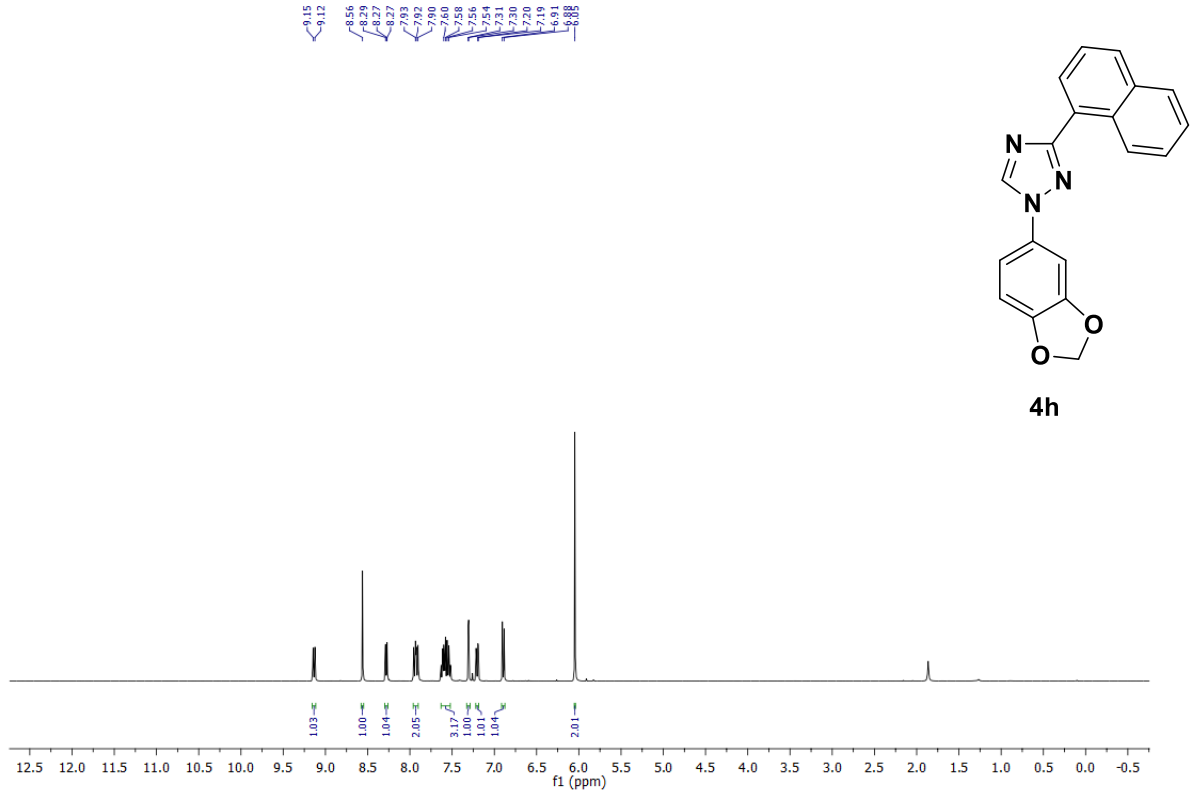
^{1}H NMR (400 MHz, DMSO-d_6) of 1,3-bis(benzo[*d*][1,3]dioxol-5-yl)-1*H*-1,2,4-triazole (4g):



^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of 1,3-bis(benzo[*d*][1,3]dioxol-5-yl)-1*H*-1,2,4-triazole (4g):

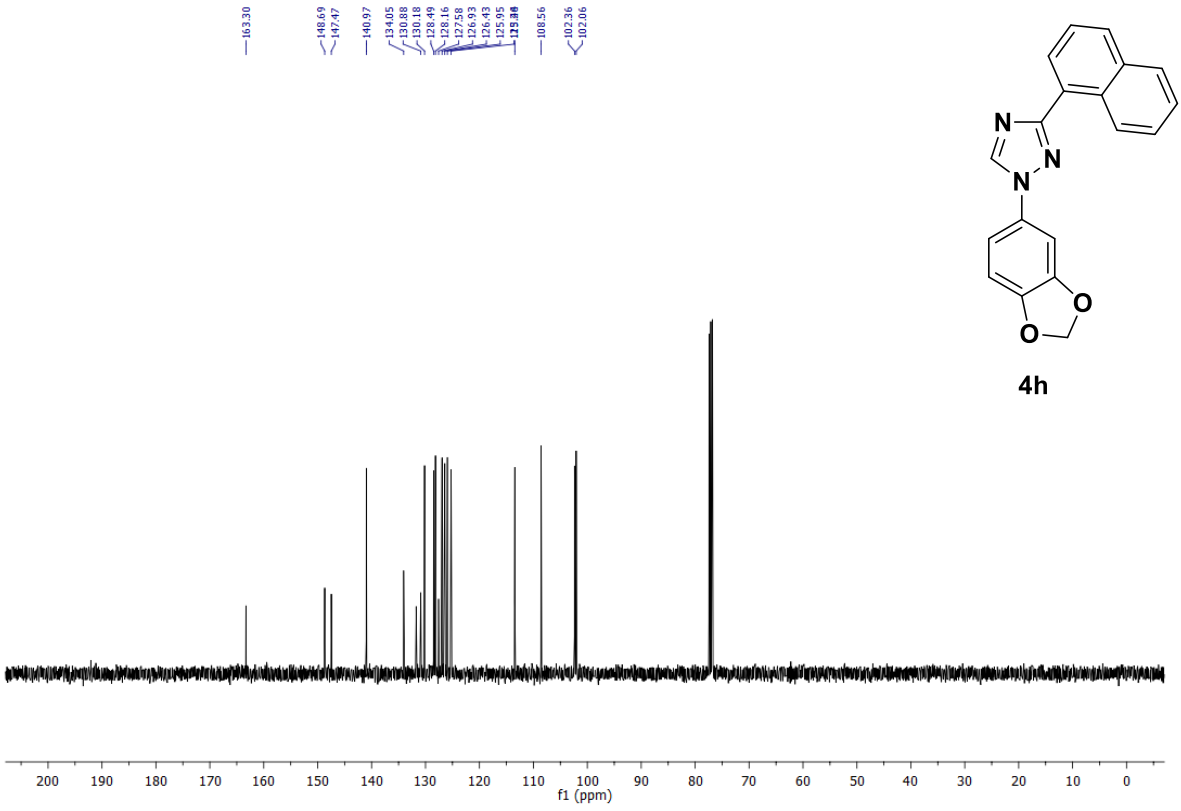


^{1}H NMR (400 MHz, $CDCl_3$) of 1-(benzo[*d*][1,3]dioxol-5-yl)-3-(naphthalen-1-yl)-1*H*-1,2,4-triazole (4h):



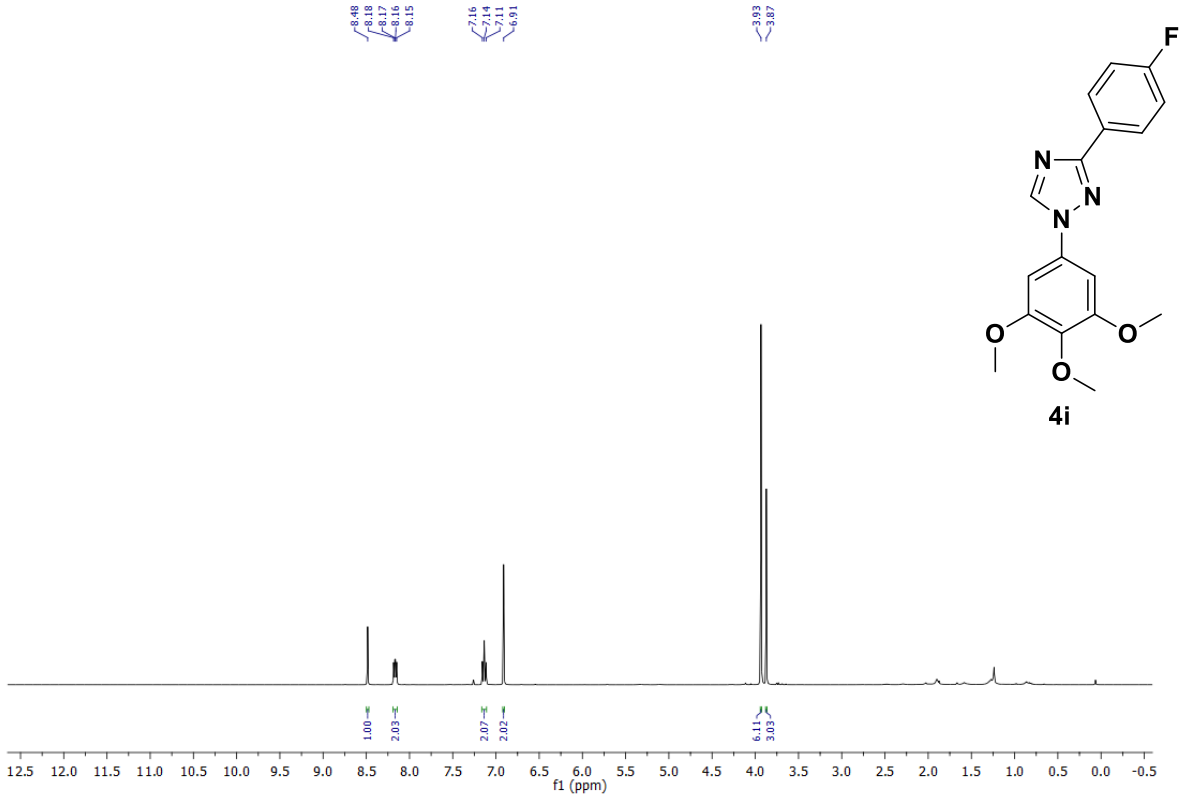
4h

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 1-(benzo[*d*][1,3]dioxol-5-yl)-3-(naphthalen-1-yl)-1*H*-1,2,4-triazole (4h):

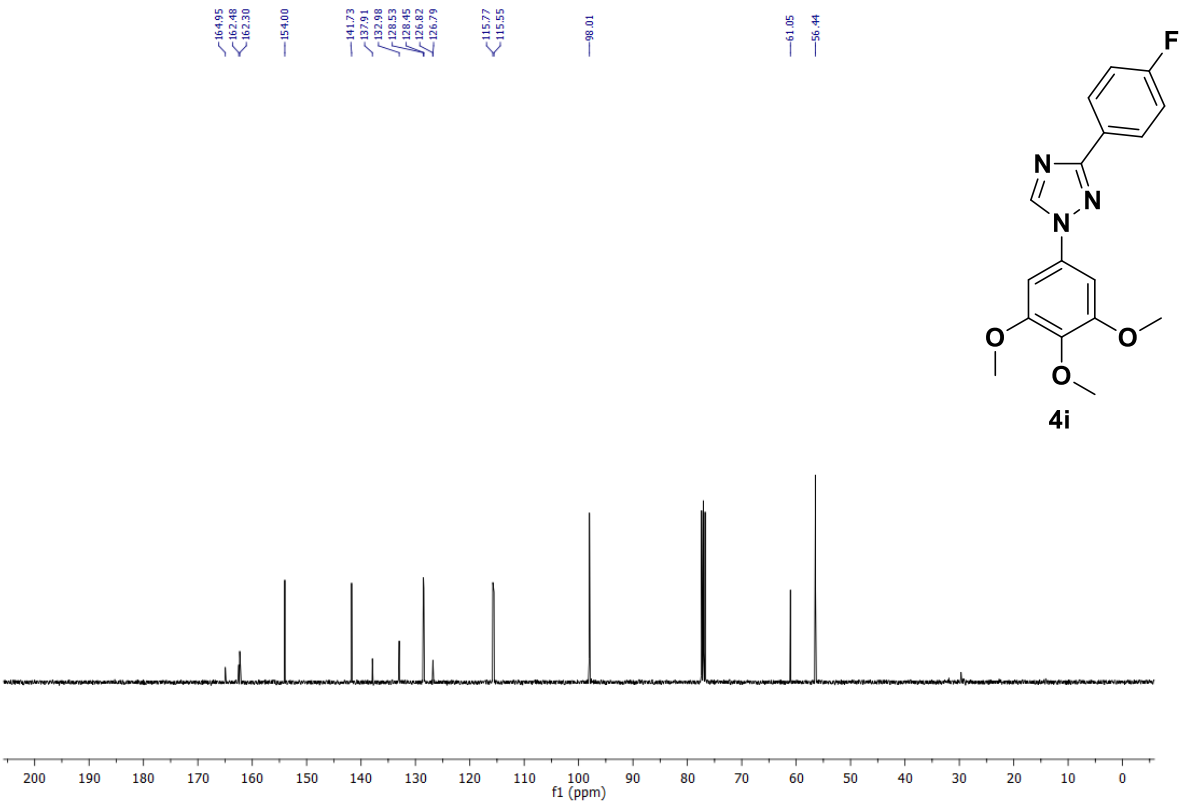


4h

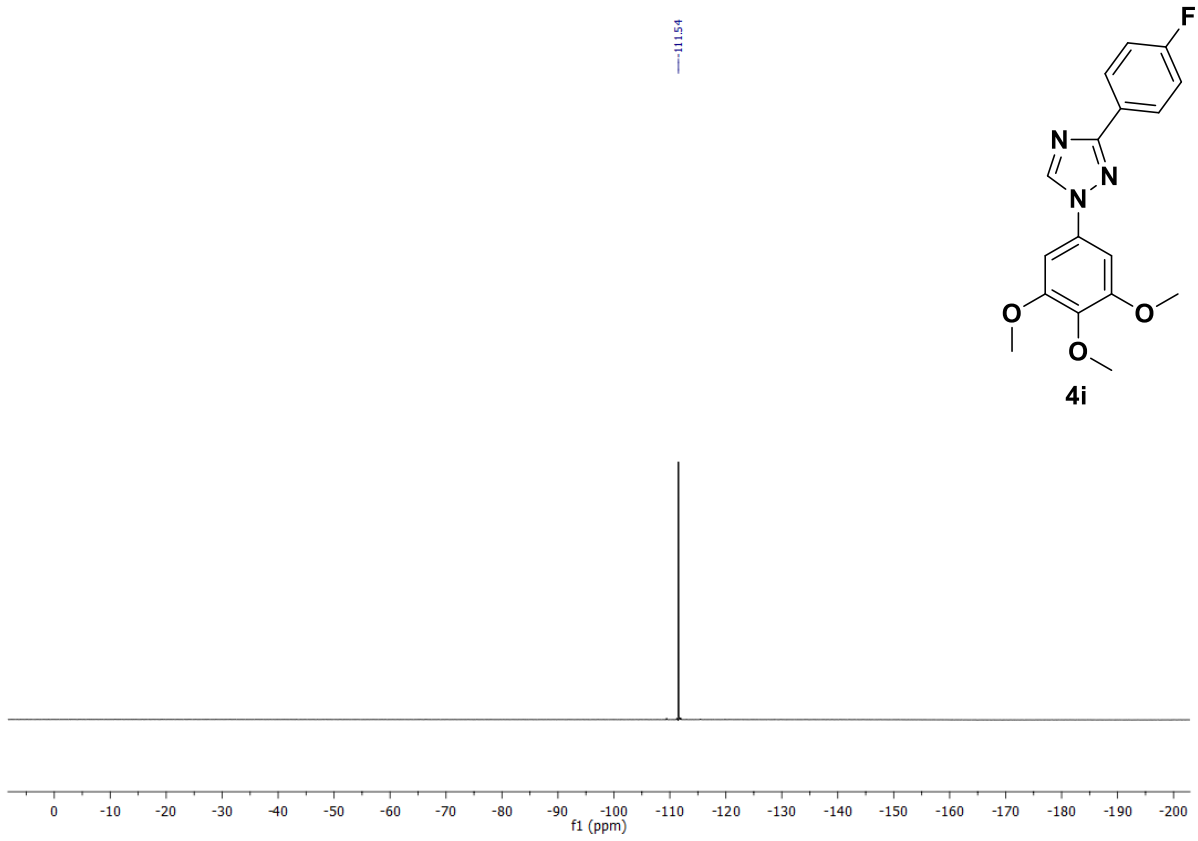
^{1}H NMR (400 MHz, $CDCl_3$) 3-(4-fluorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4i):



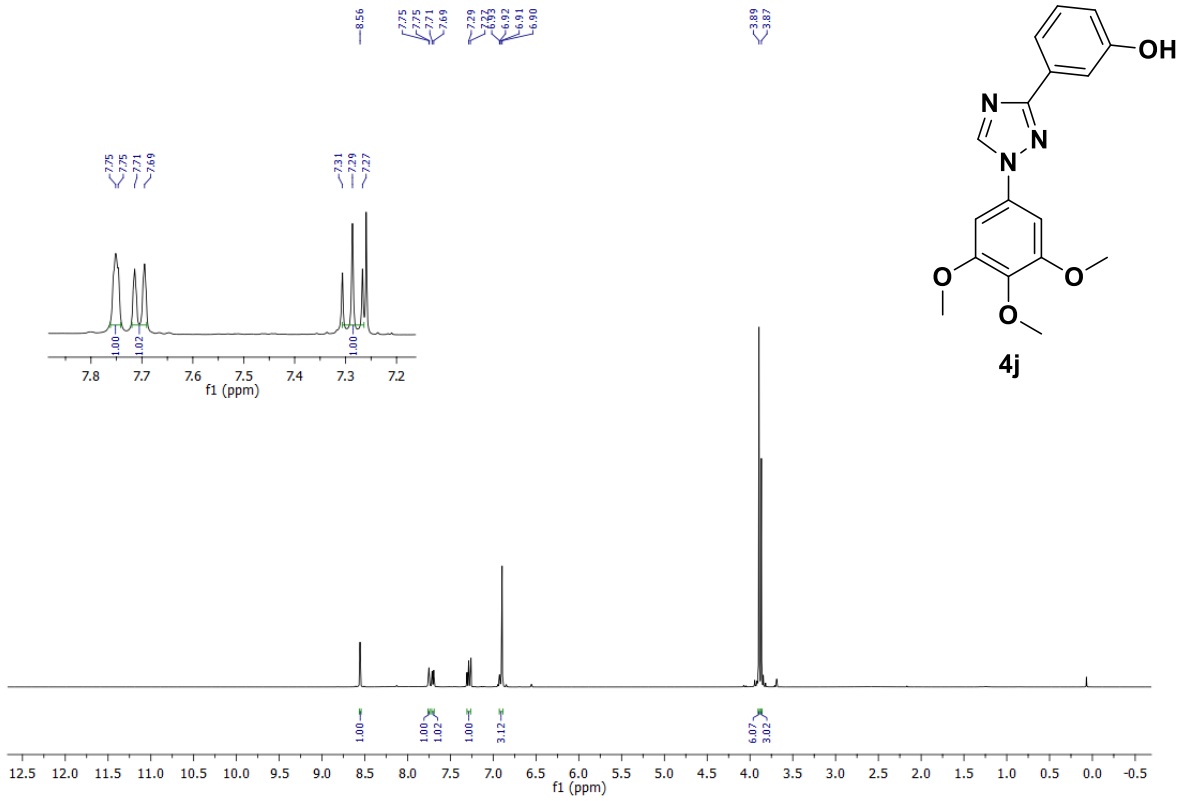
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(4-fluorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4i):



^{19}F NMR (377 MHz, $CDCl_3$) of 3-(4-fluorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4i):

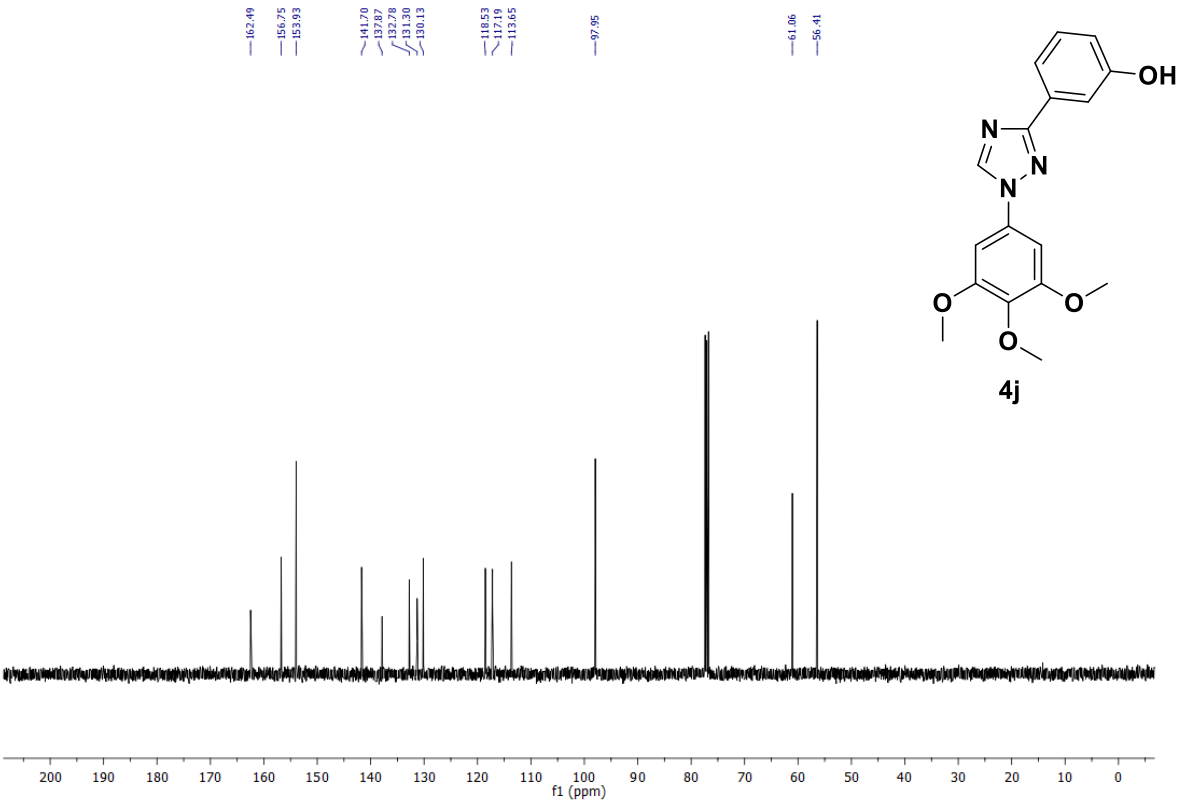


^{1}H NMR (400 MHz, $CDCl_3$) of 3-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)phenol (4j):



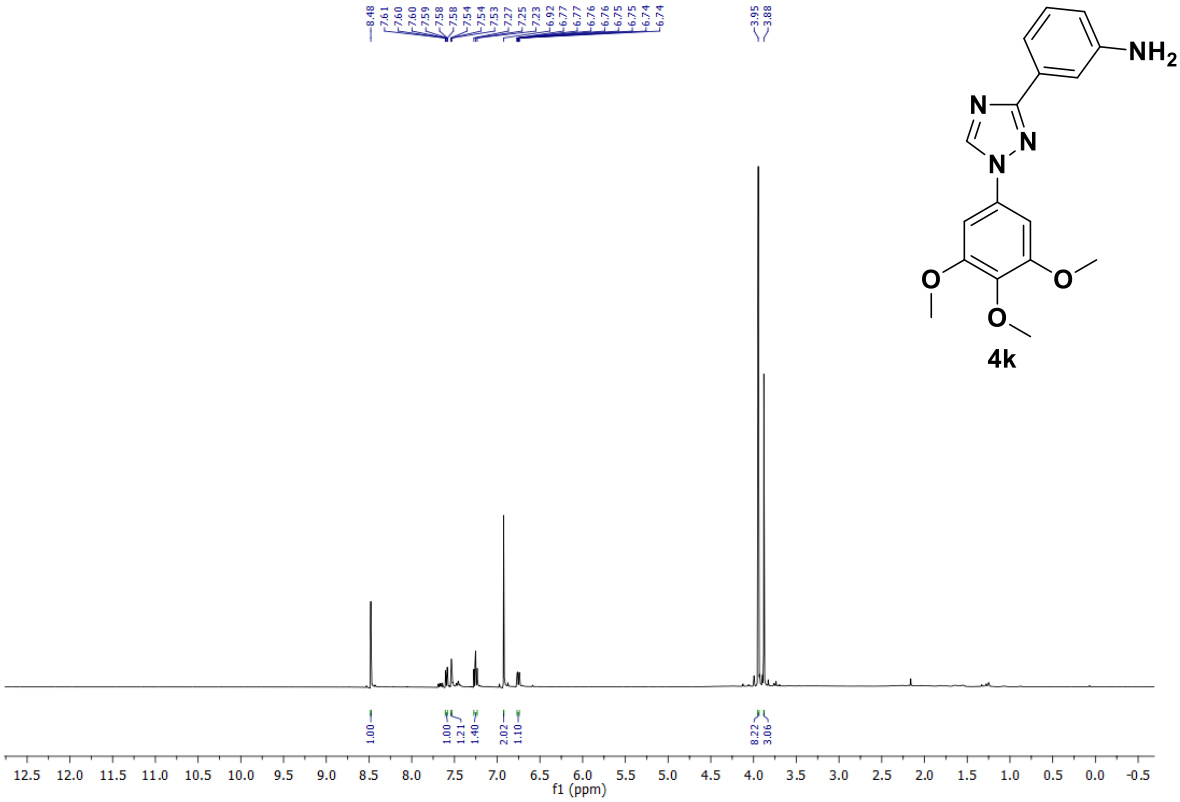
4j

^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)phenol (4j):

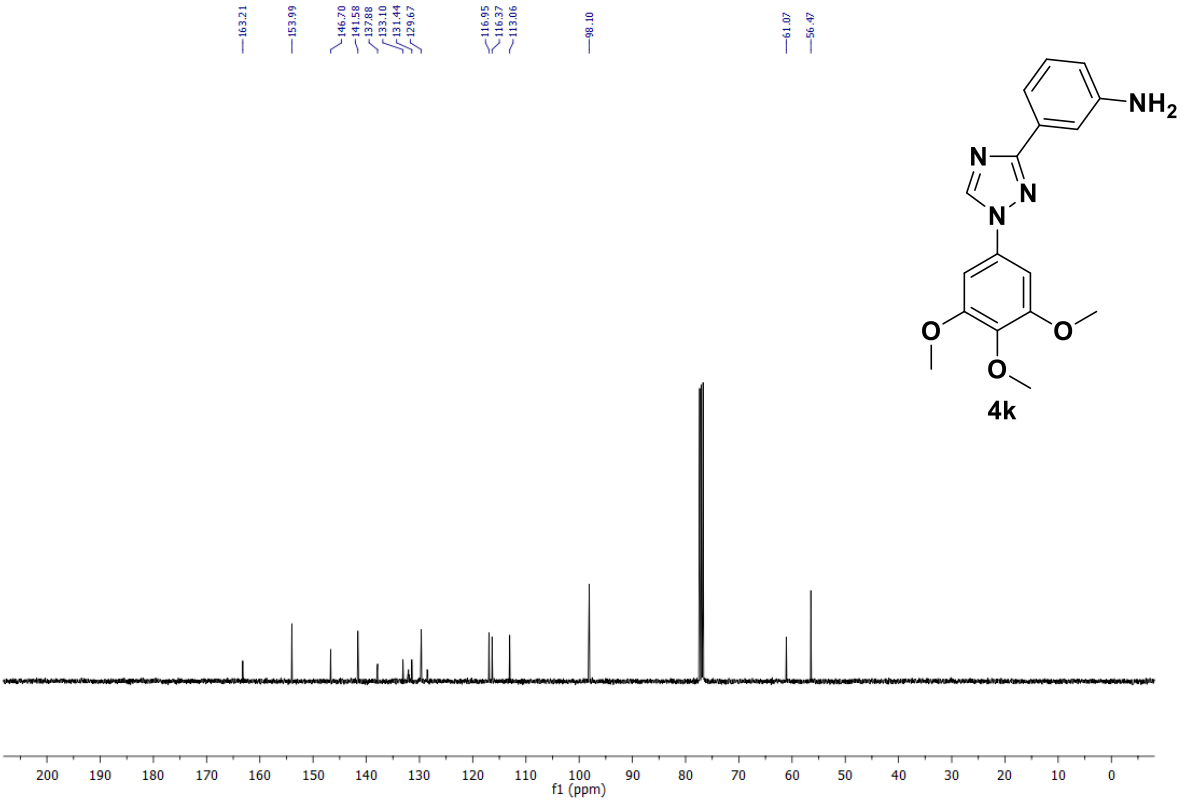


4j

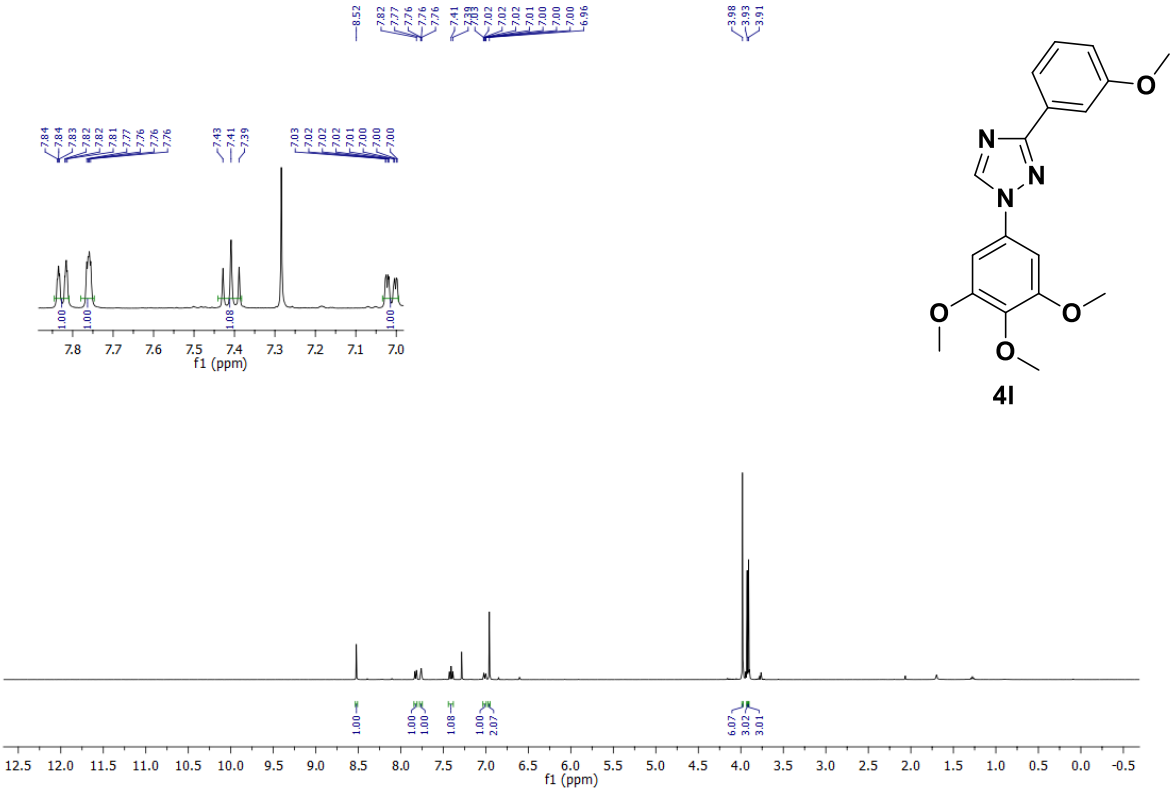
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)aniline (4k):



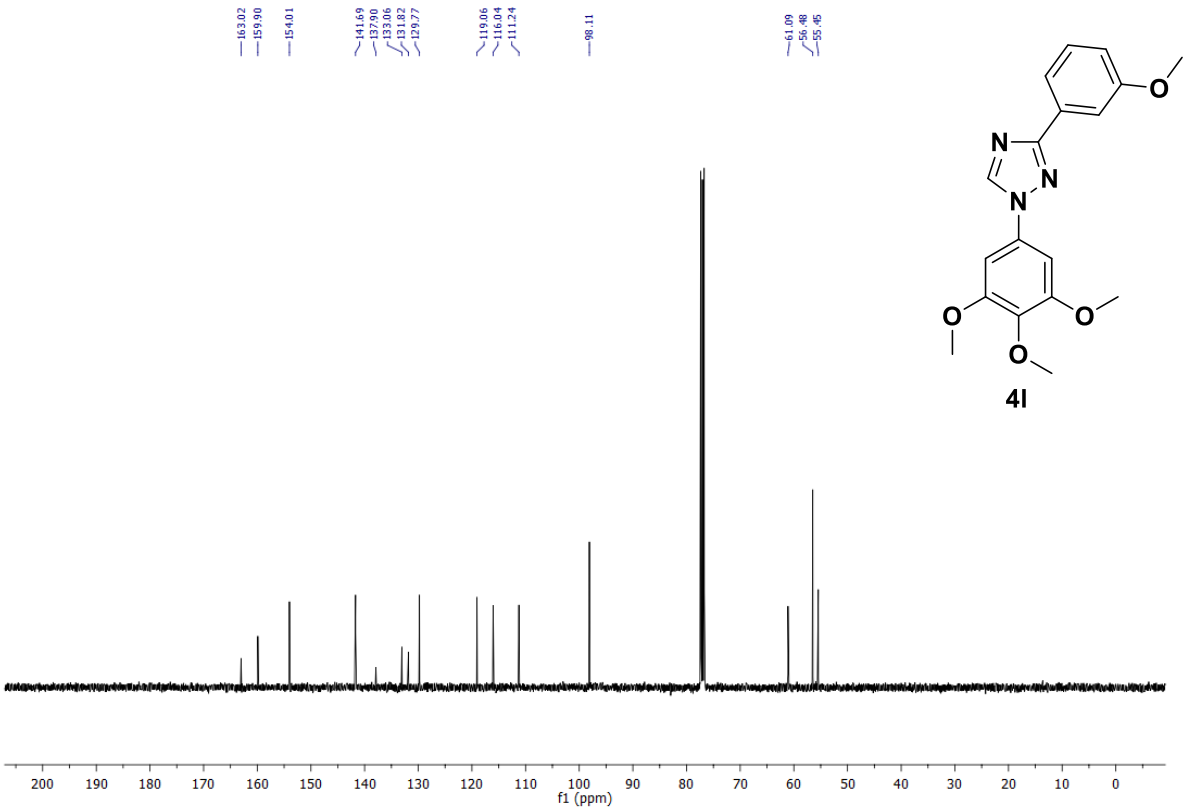
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)aniline (4k):



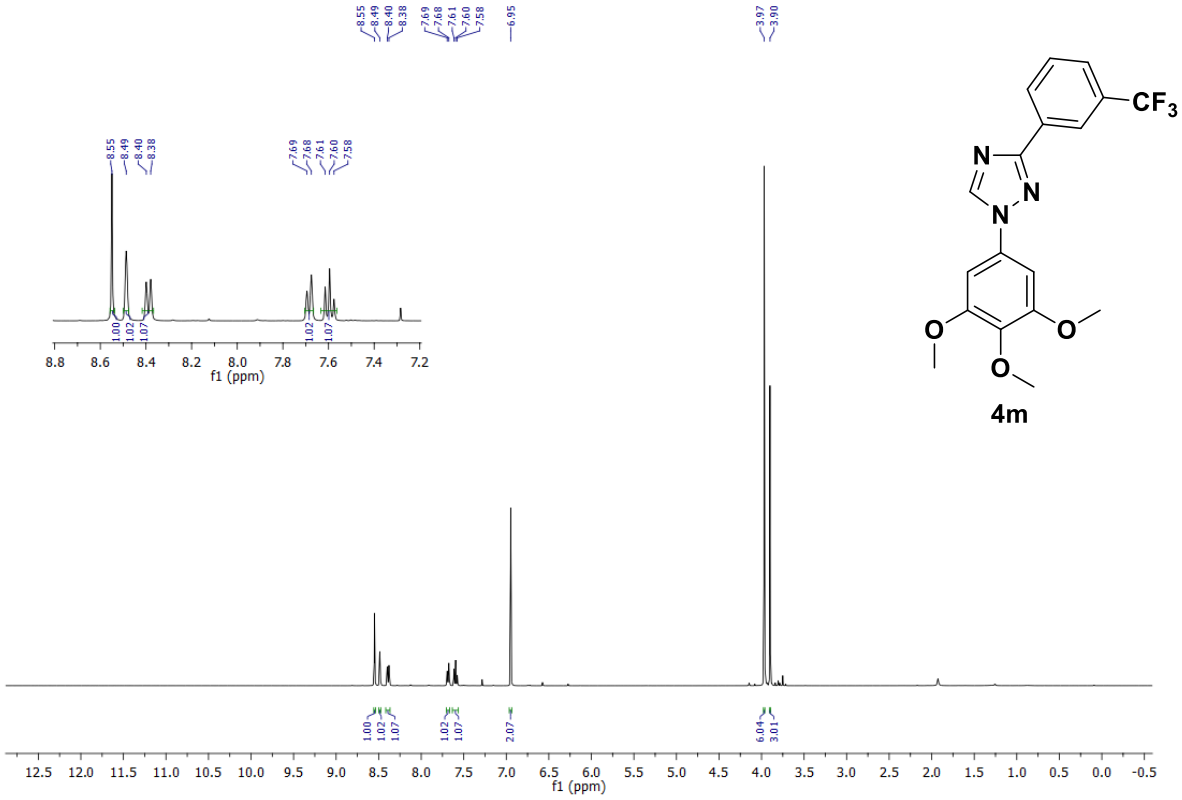
^{1}H NMR (400 MHz, $CDCl_3$) 3-(3-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4l):



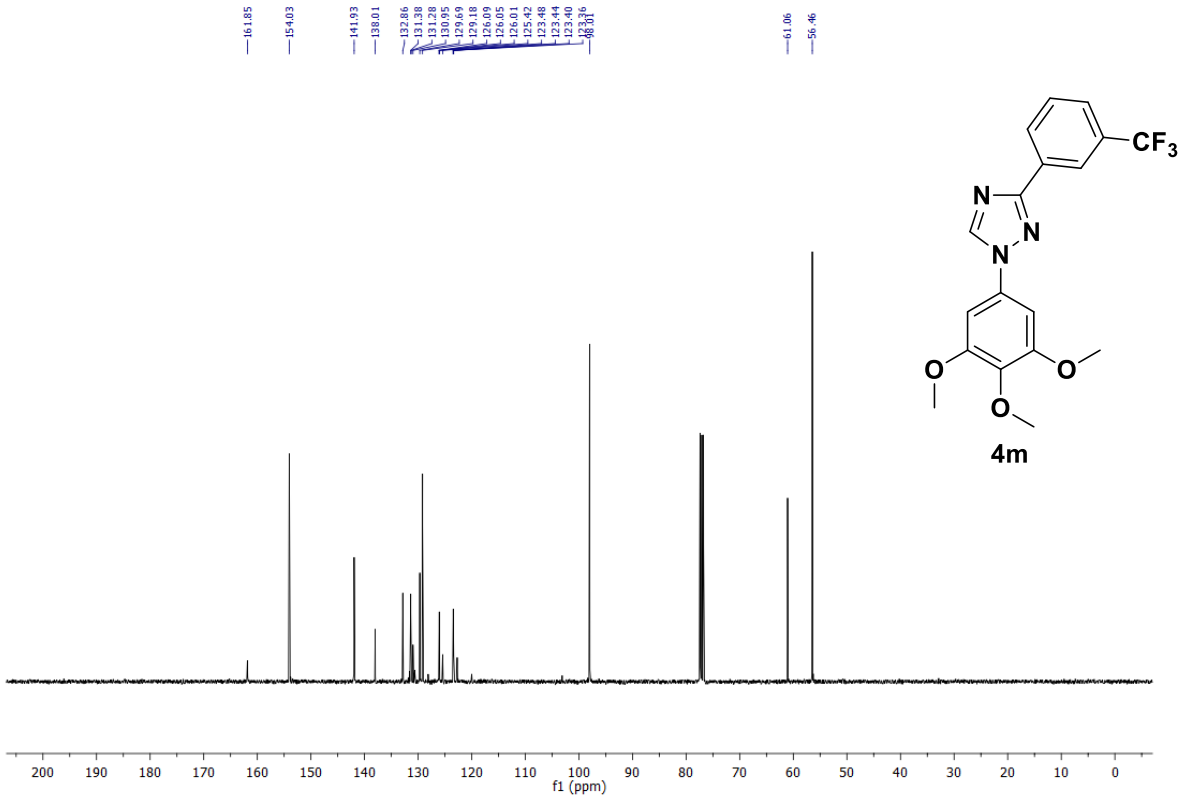
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4l):



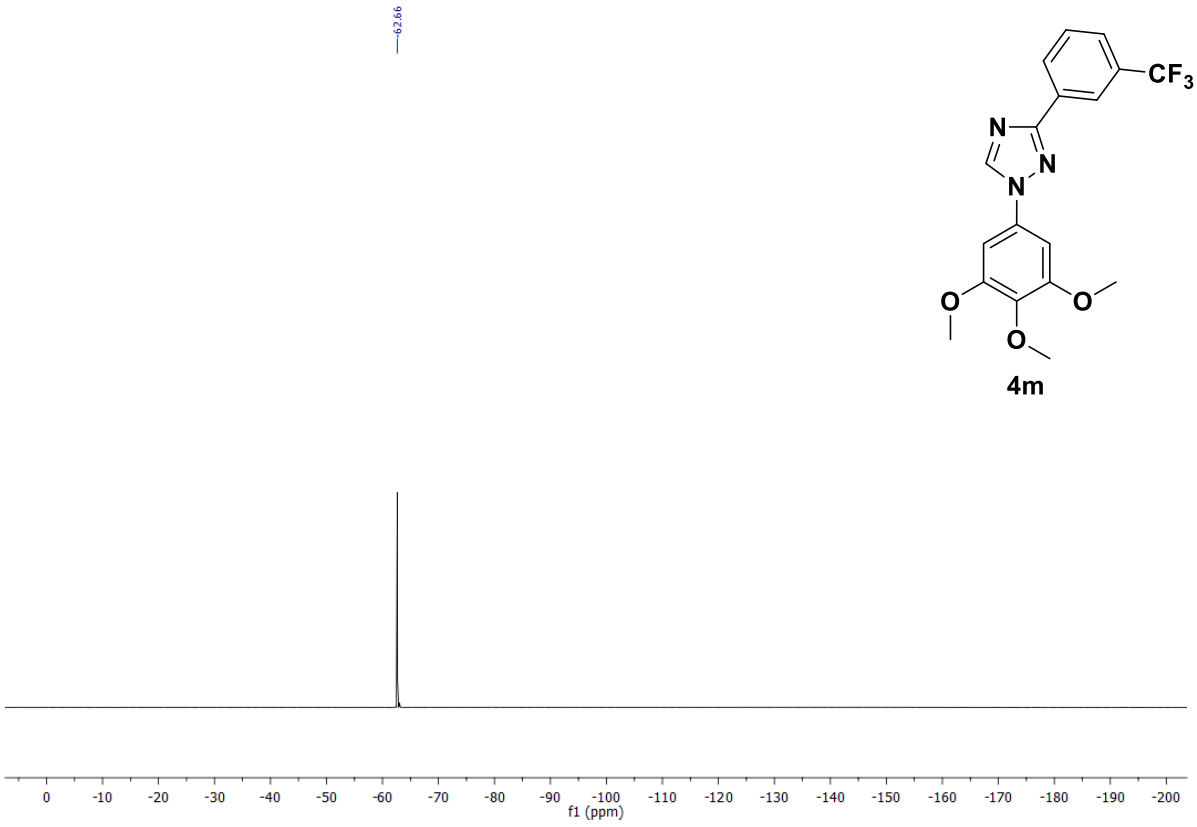
^{1}H NMR (400 MHz, $CDCl_3$) 3-(3-(trifluoromethyl)phenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4m):



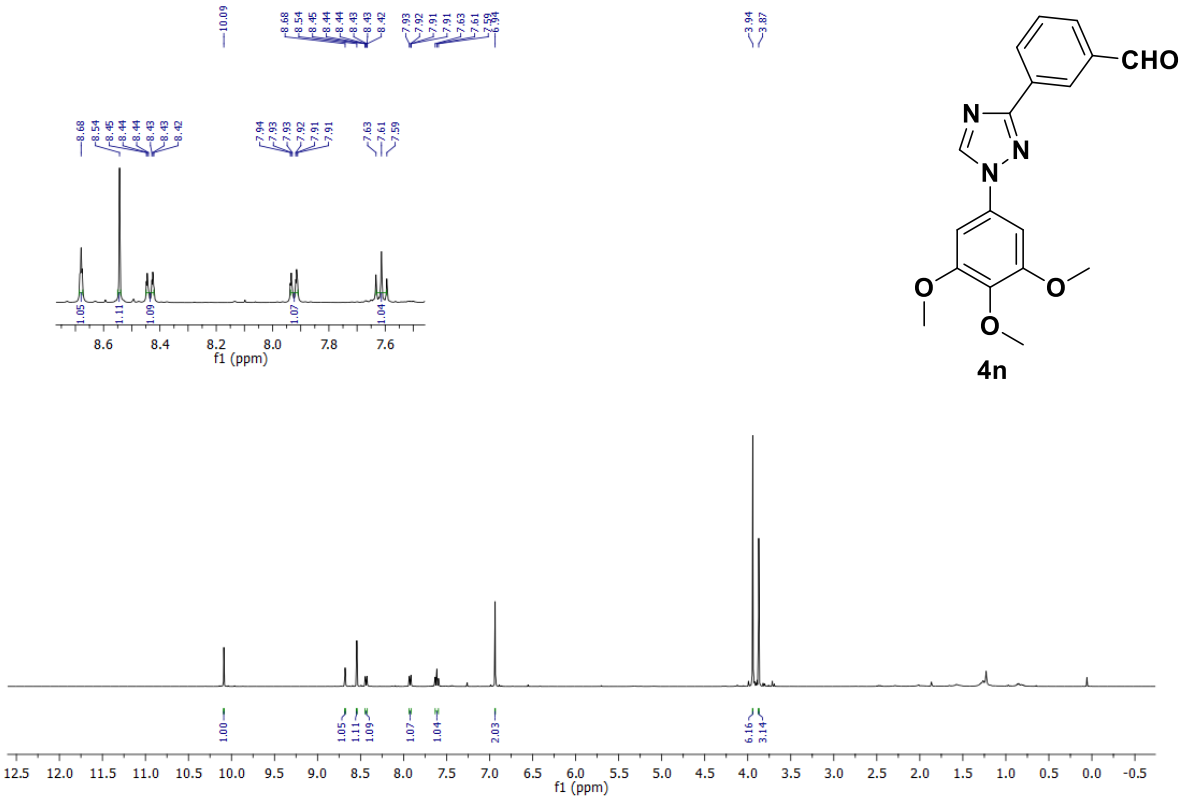
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3-(trifluoromethyl)phenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4m):



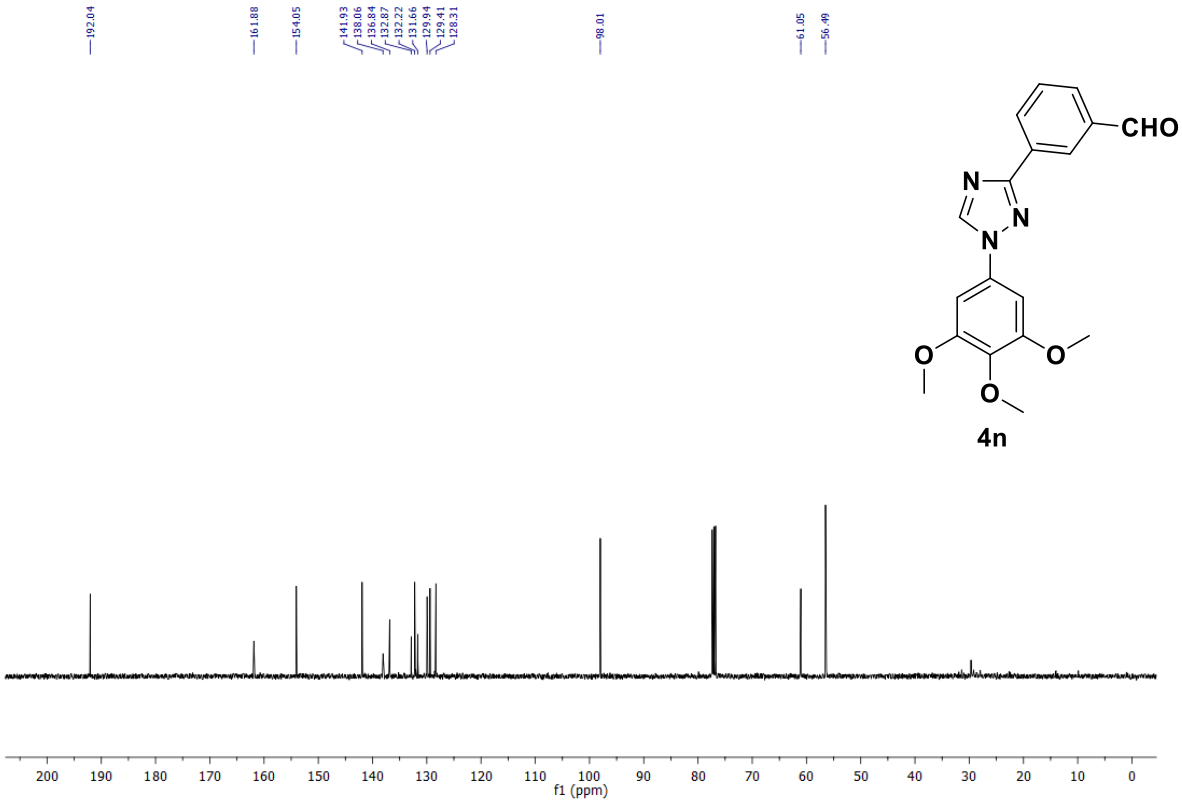
^{19}F NMR (377 MHz, $CDCl_3$) of 3-(3-(trifluoromethyl)phenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4m):



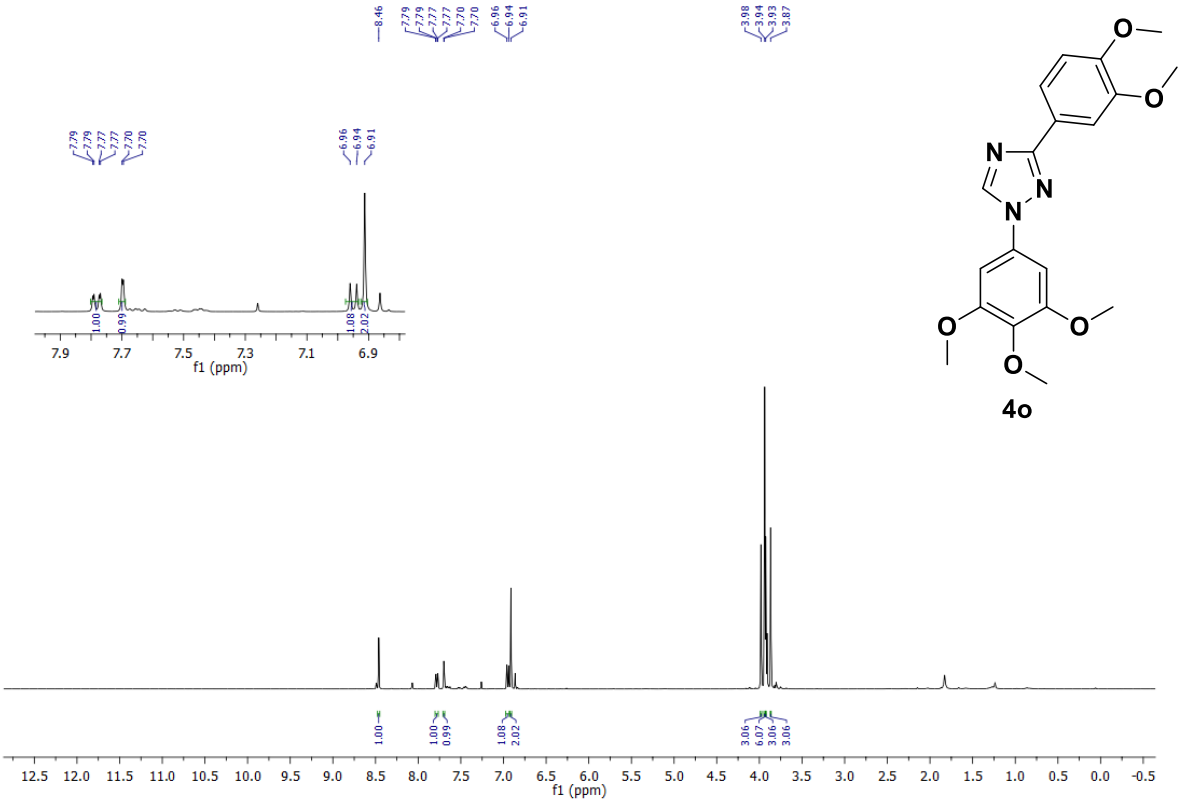
^{1}H NMR (400 MHz, $CDCl_3$) 3-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)benzaldehyde (4n):



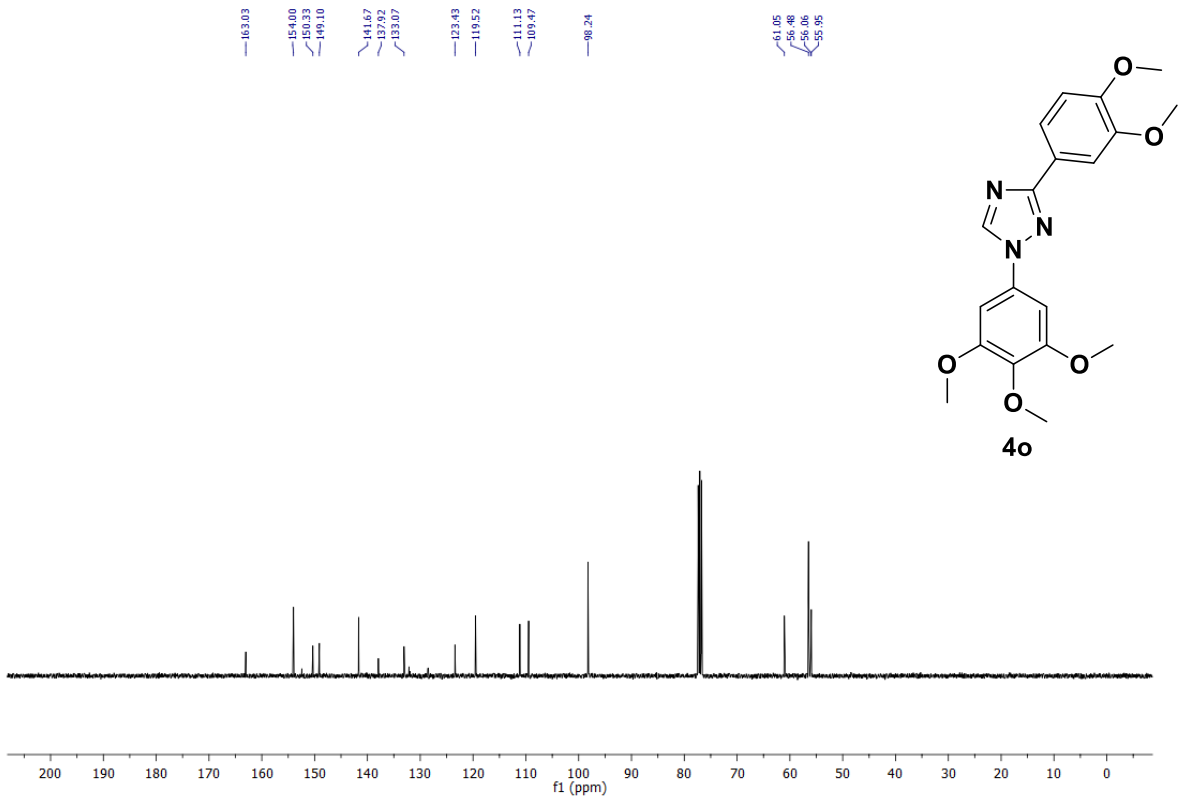
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)benzaldehyde (4n):



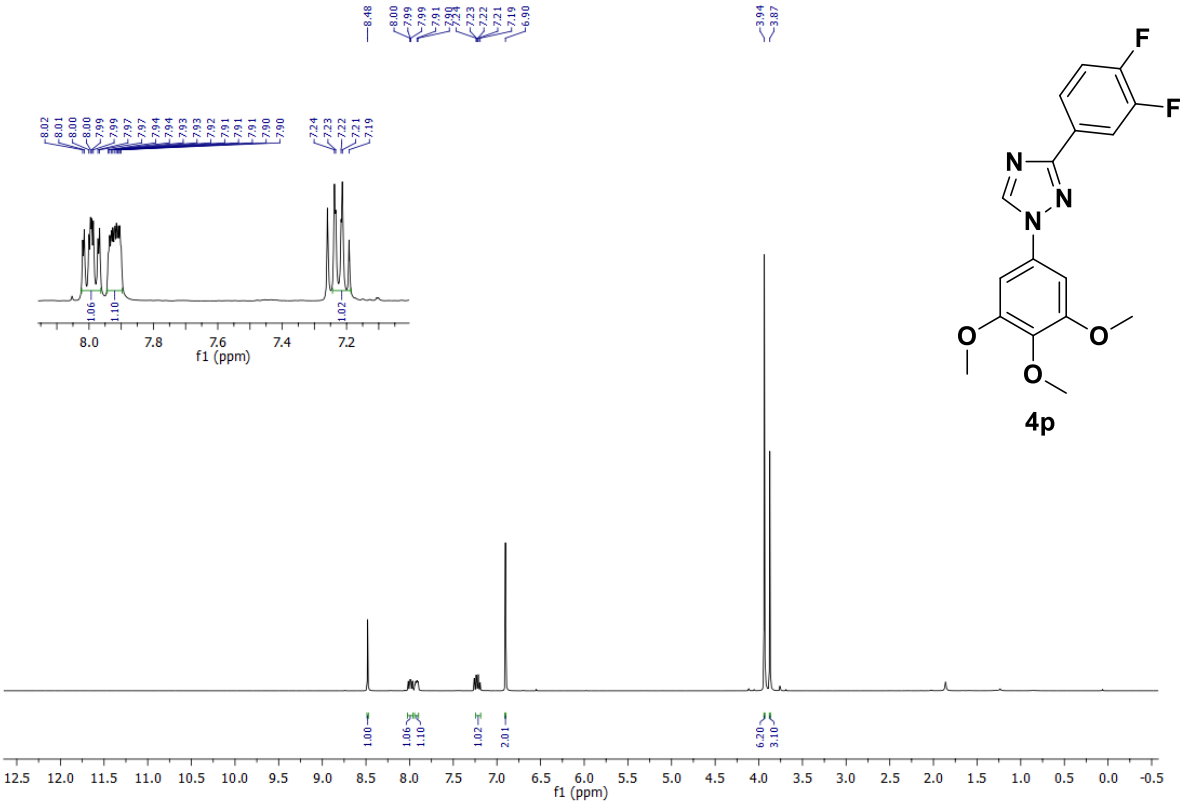
^{1}H NMR (400 MHz, $CDCl_3$) 3-(3,4-dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4o):



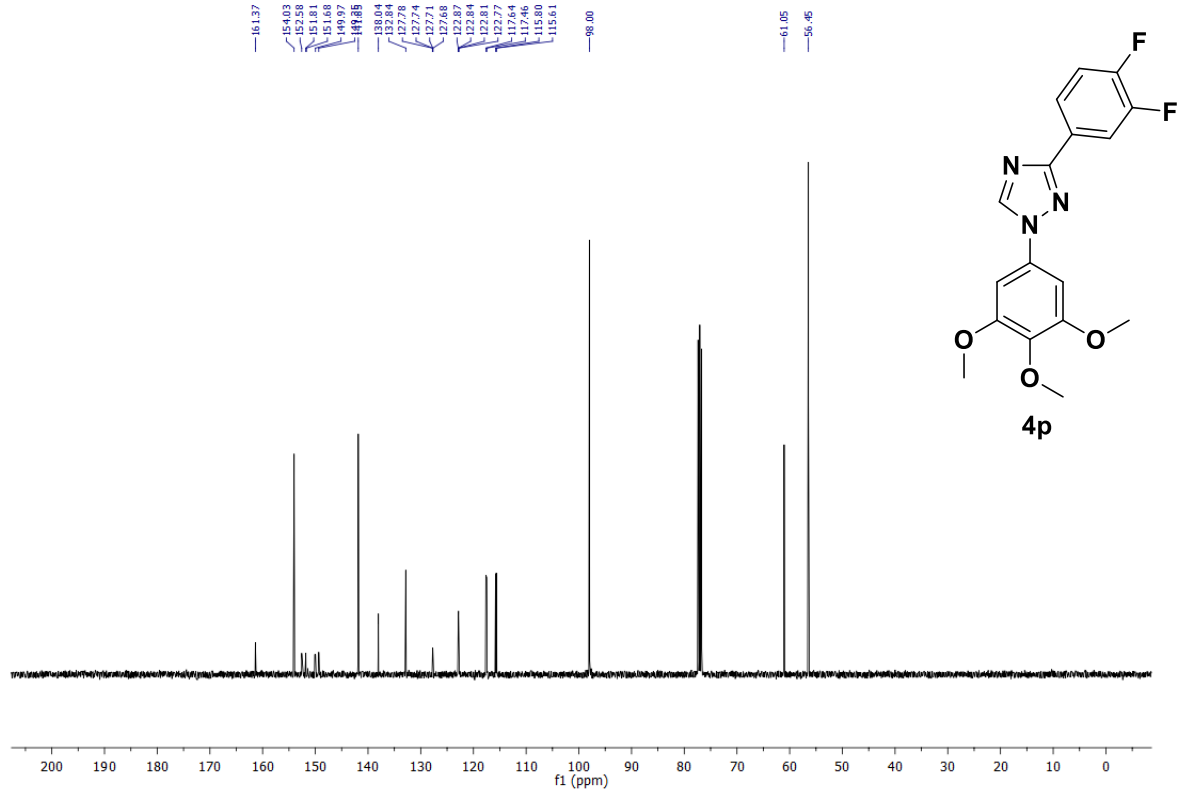
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3,4-dimethoxyphenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4o):



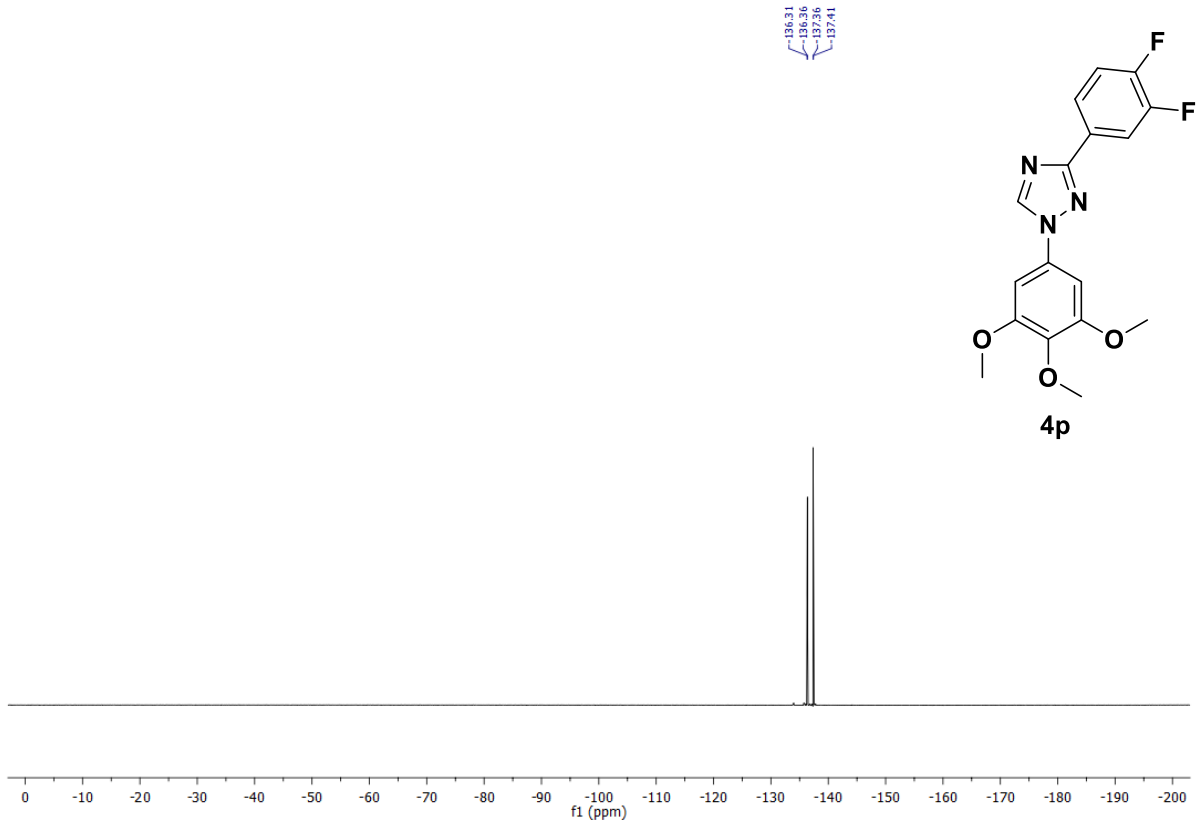
^{1}H NMR (400 MHz, $CDCl_3$) 3-(3,4-difluorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4p):



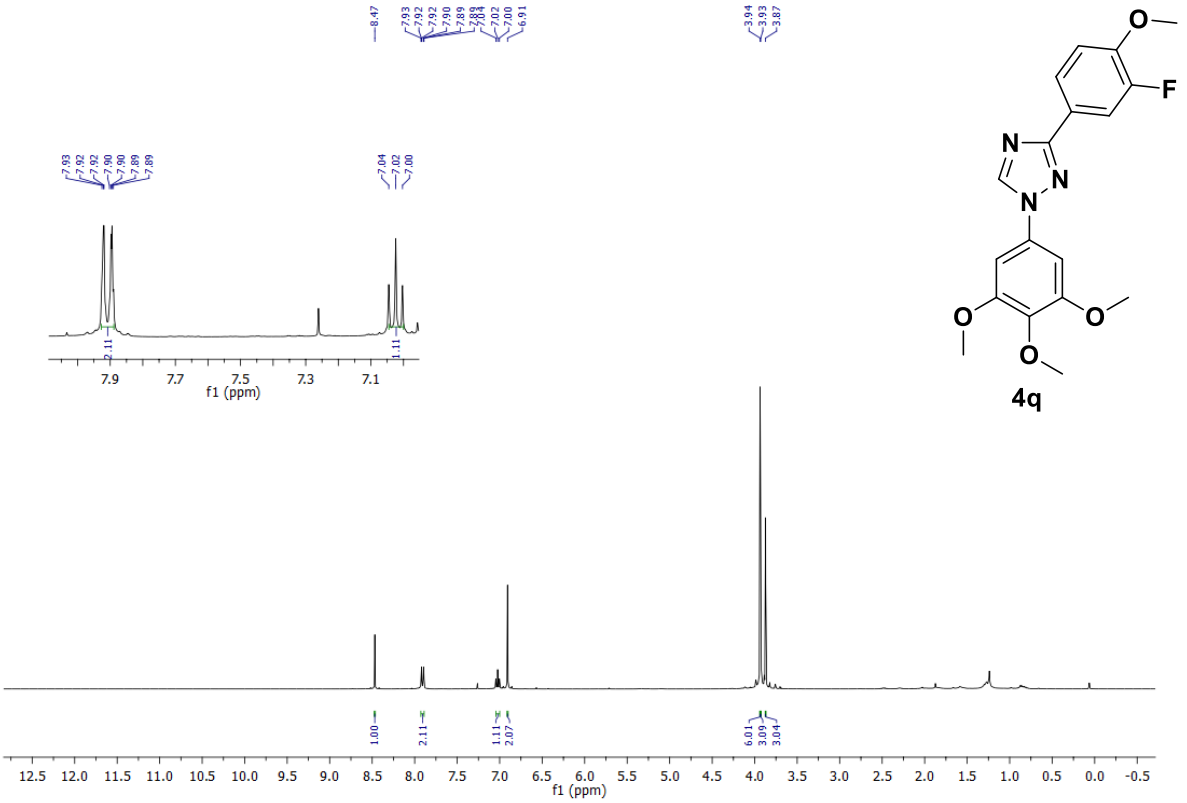
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3,4-difluorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4p):



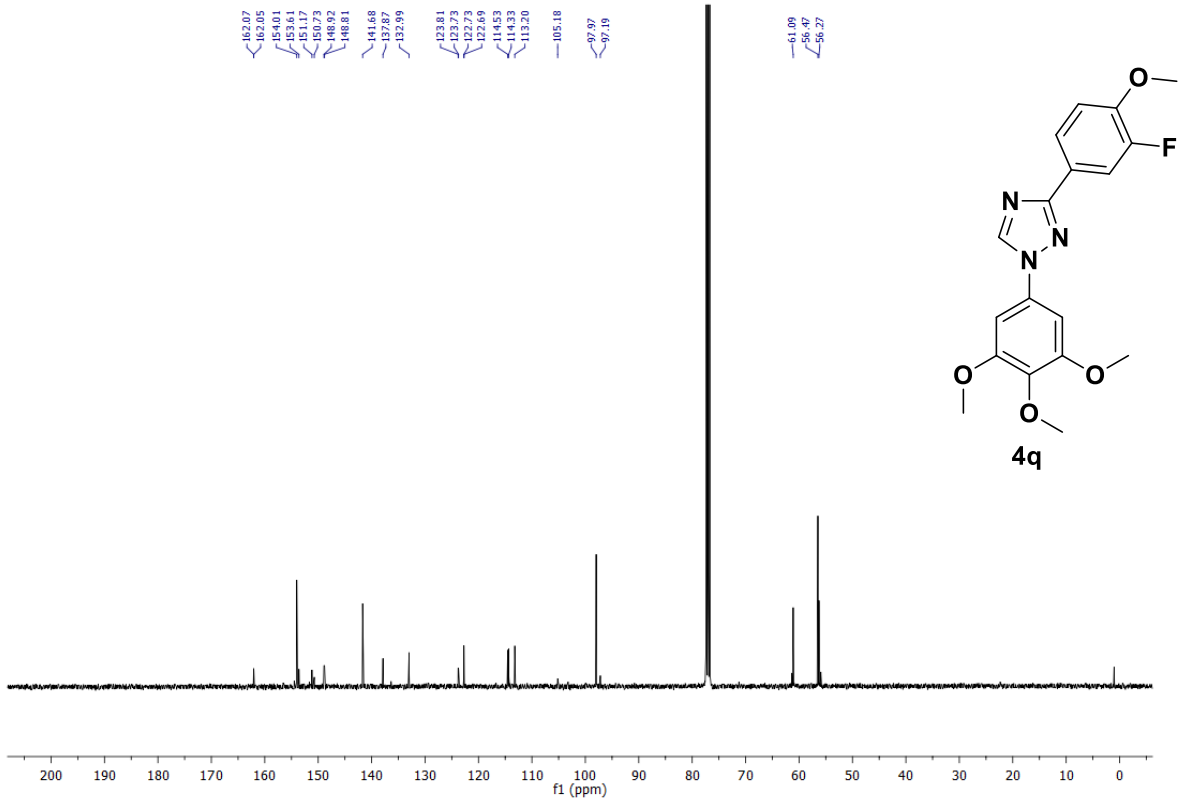
^{19}F NMR (377 MHz, $CDCl_3$) of 3-(3,4-difluorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4p):



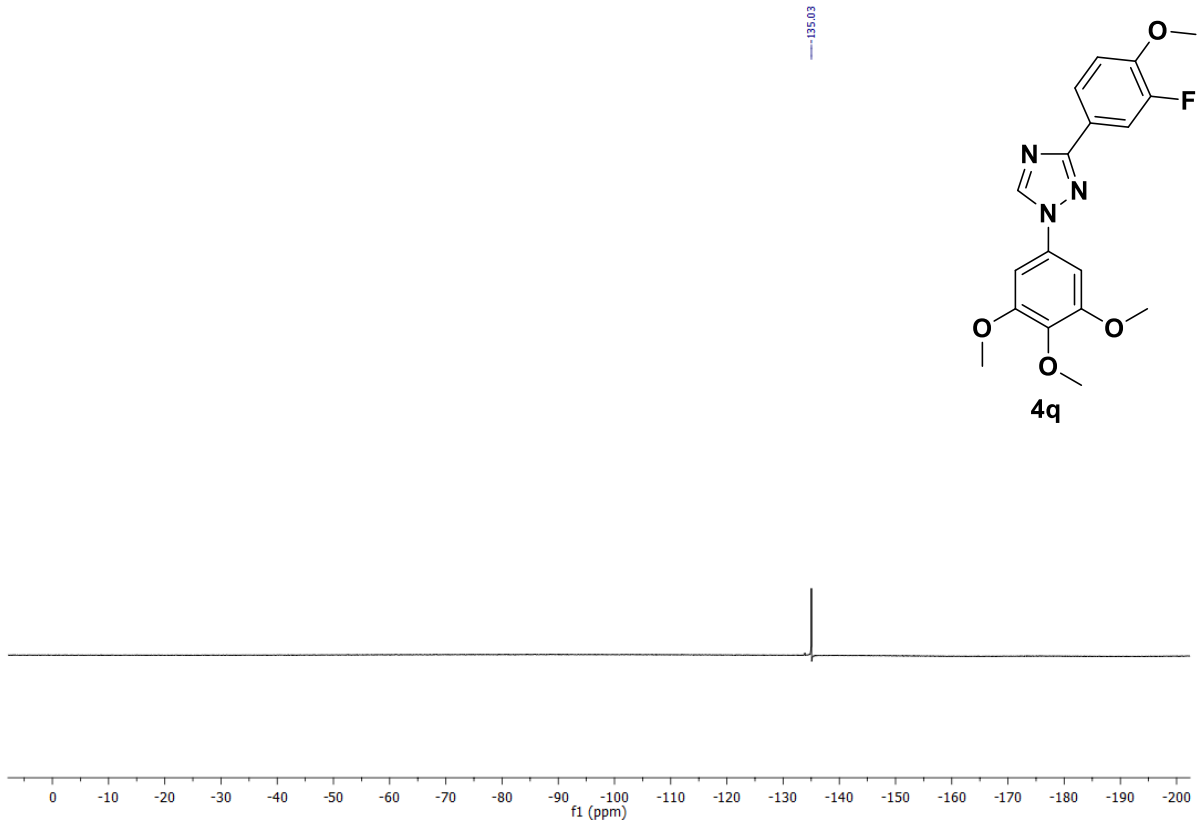
^{1}H NMR (400 MHz, $CDCl_3$) of 3-(3-fluoro-4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4q):



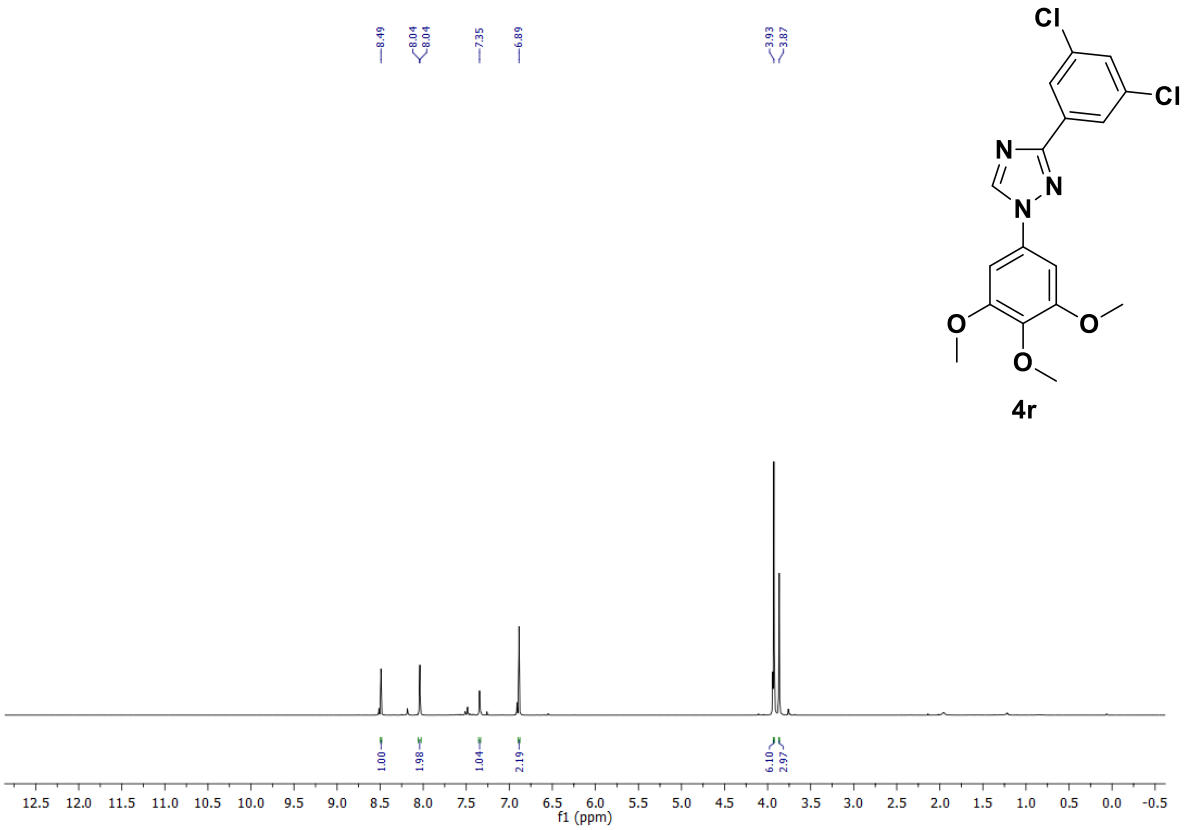
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3-fluoro-4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4q):



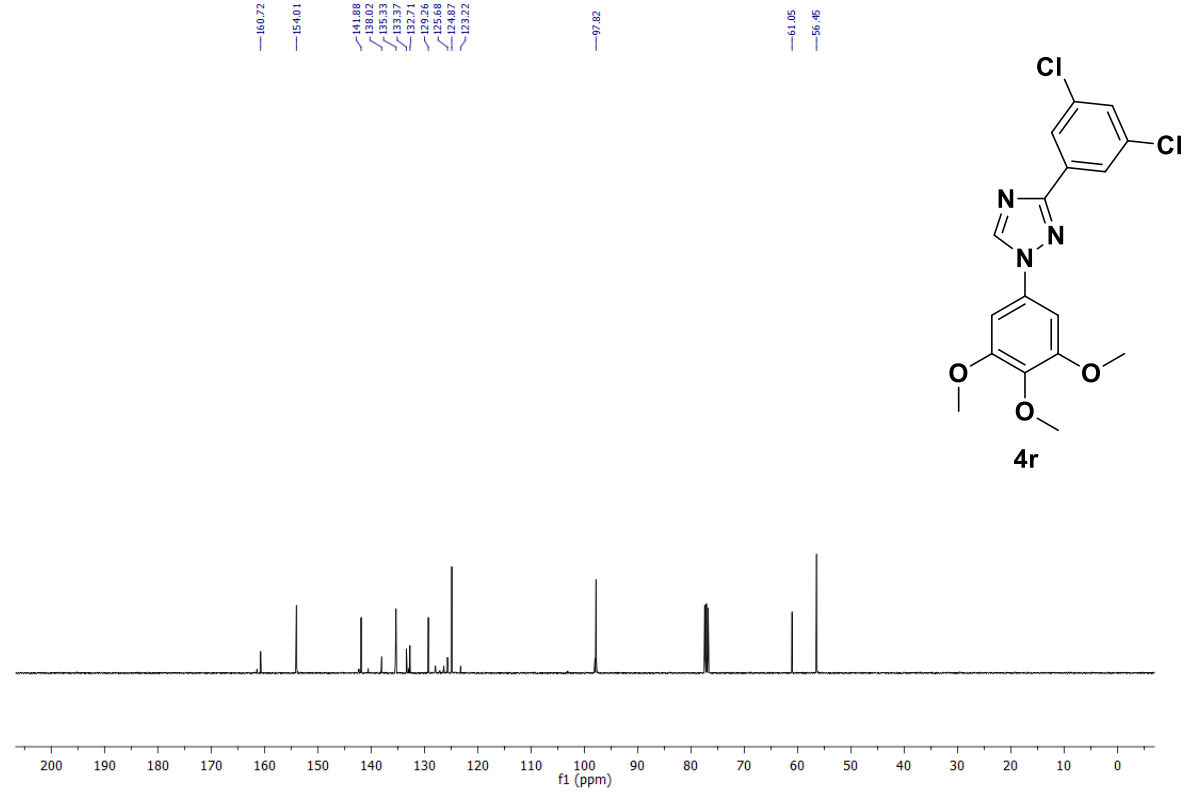
^{19}F NMR (377 MHz, $CDCl_3$) of 3-(3-fluoro-4-methoxyphenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4q):



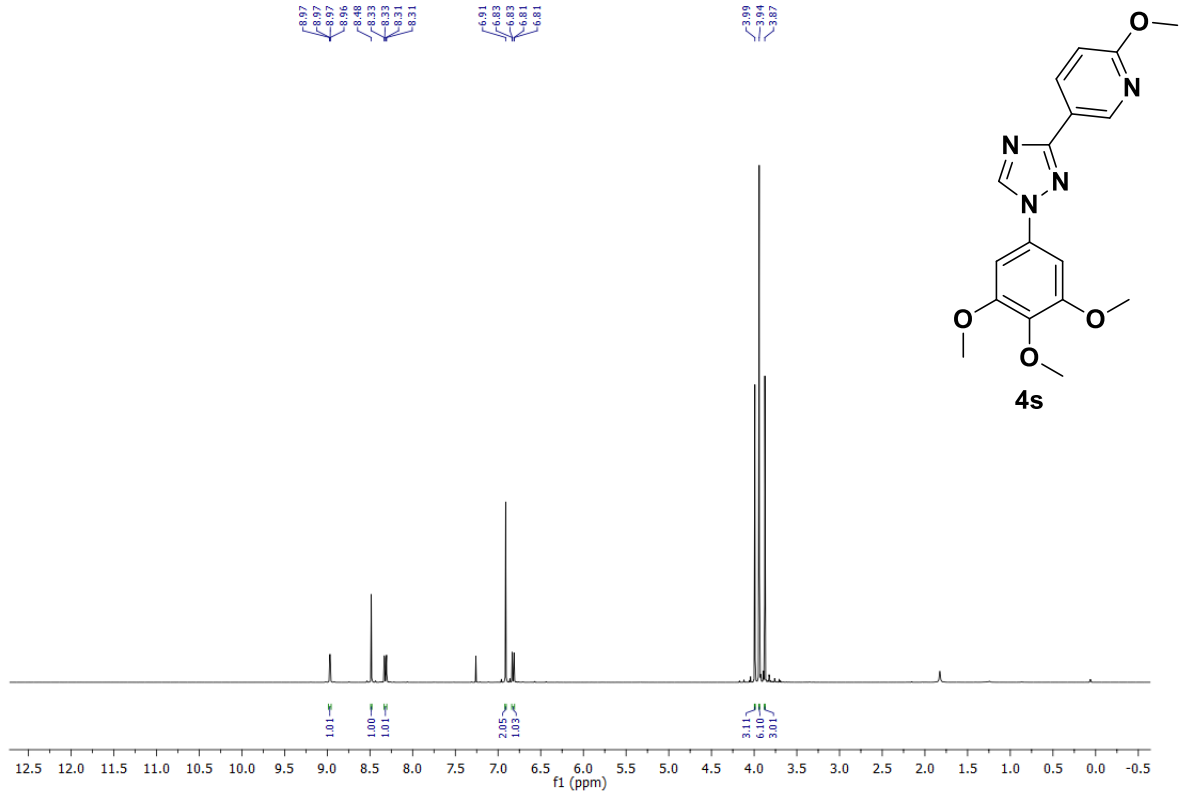
^{1}H NMR (400 MHz, $CDCl_3$) 3-(3,5-dichlorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4r):



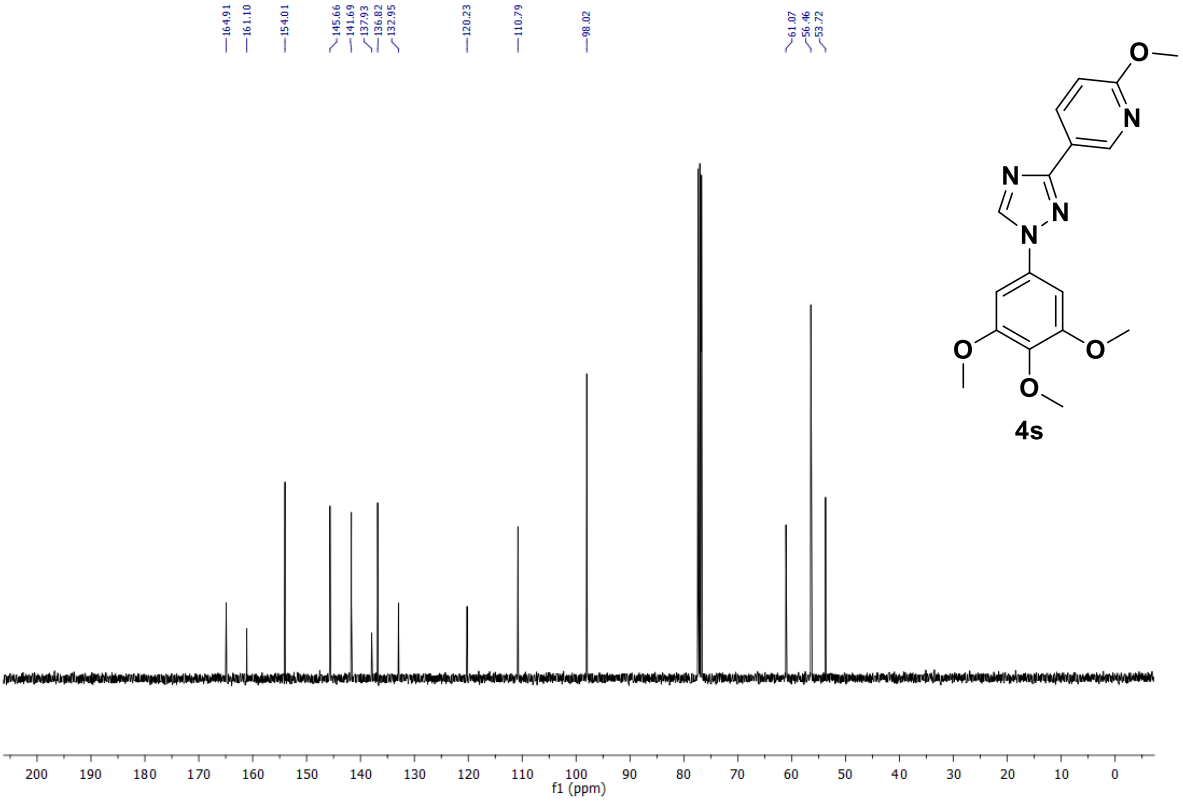
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(3,5-dichlorophenyl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4r):



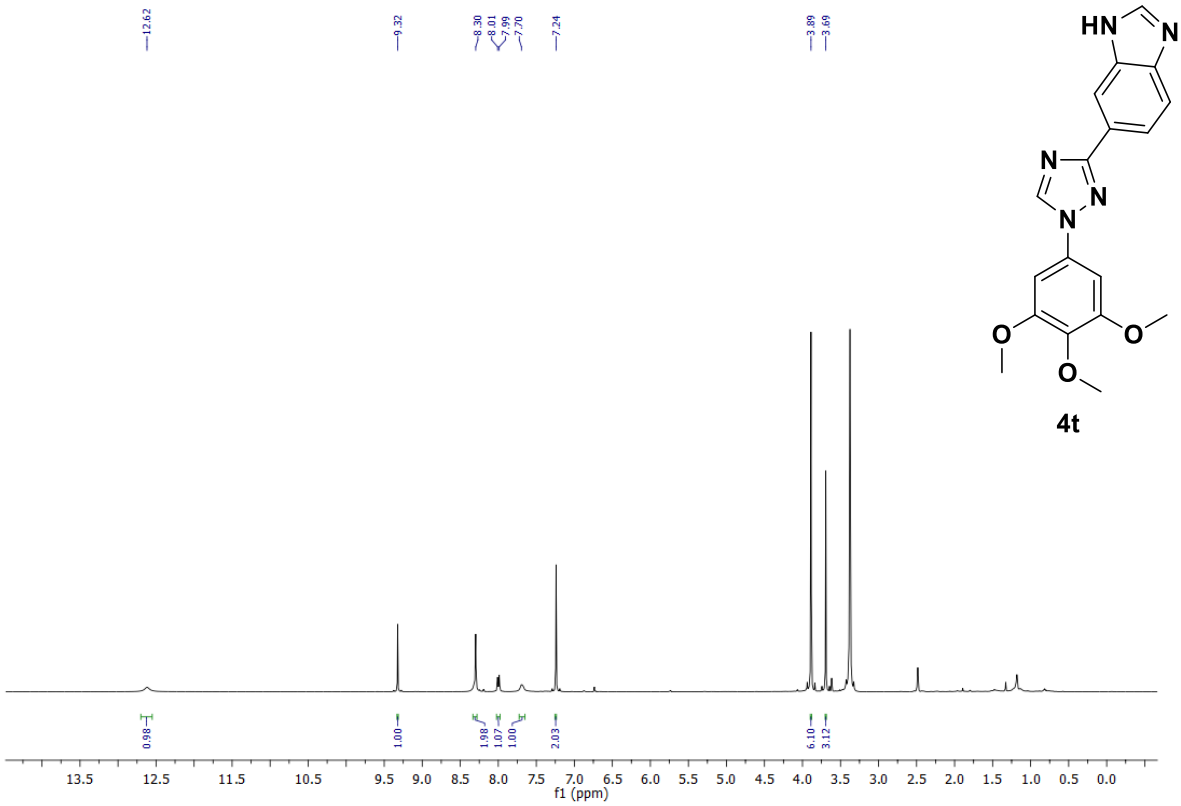
^{1}H NMR (400 MHz, $CDCl_3$) of 2-methoxy-5-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)pyridine (4s):



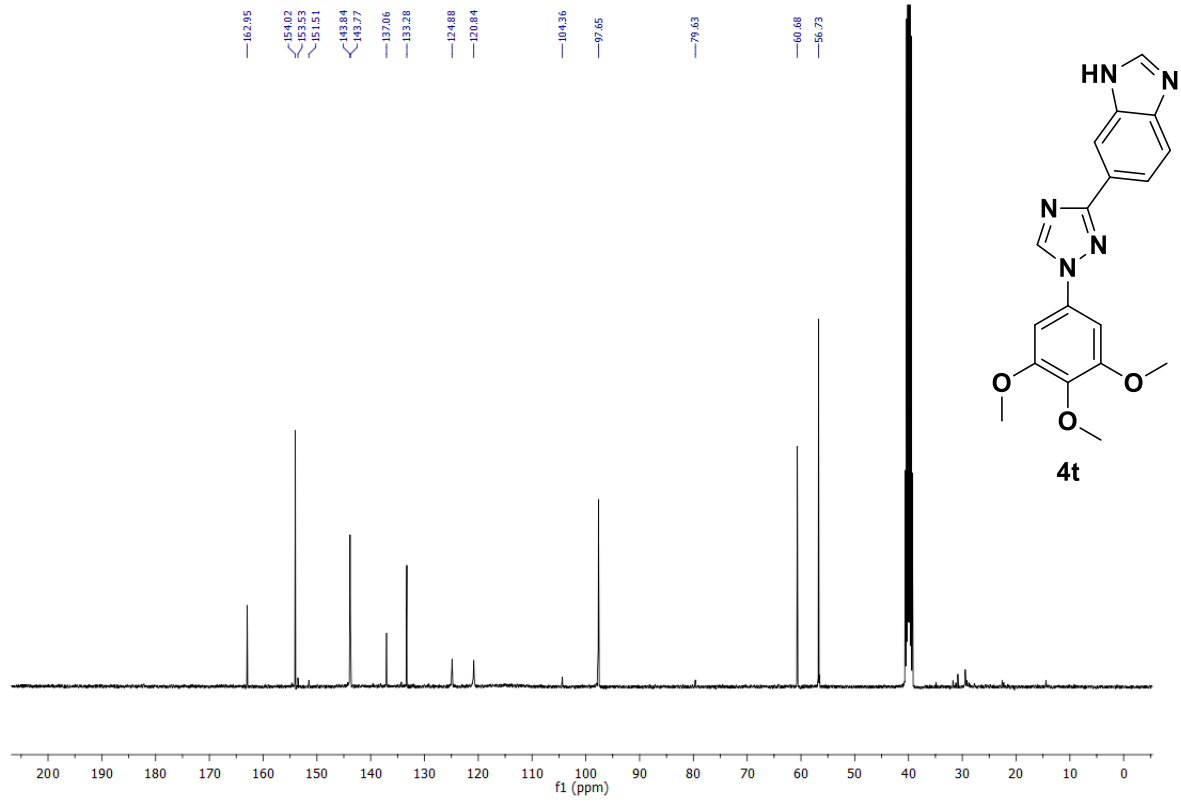
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 2-methoxy-5-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)pyridine (4s):



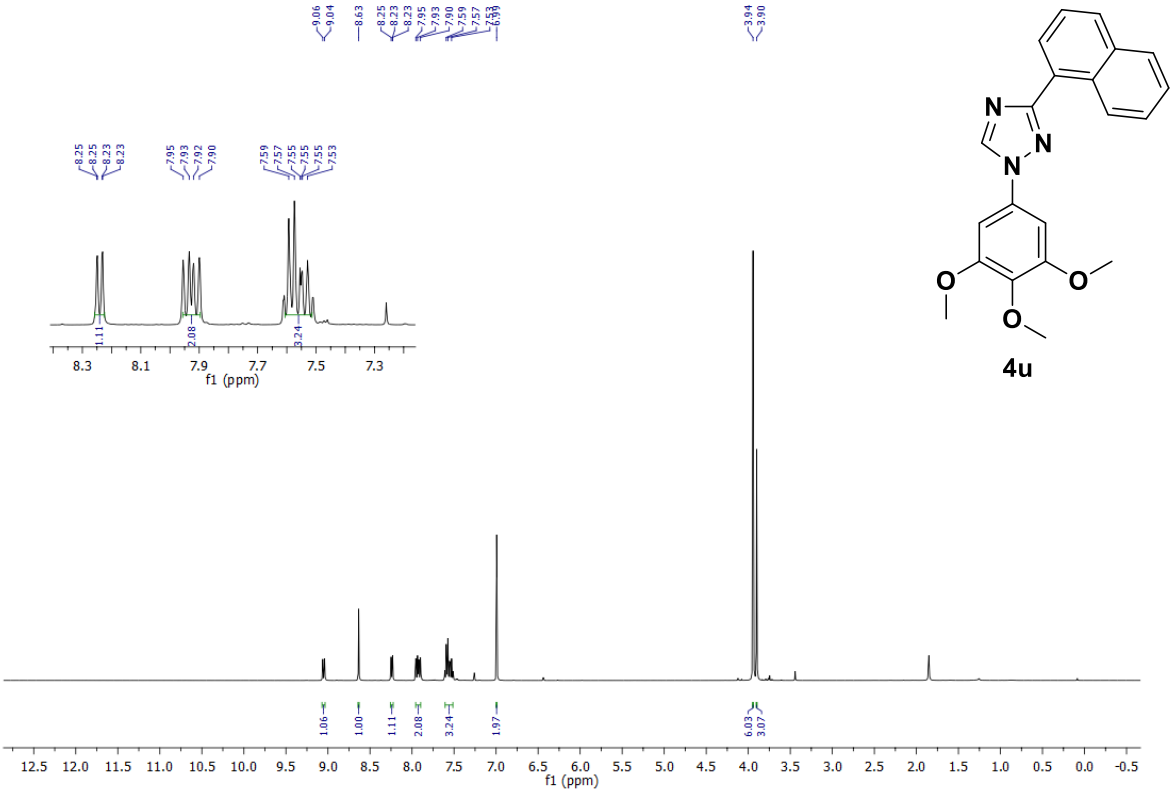
^{1}H NMR (400 MHz, DMSO-d_6) 6-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)-1*H*-benzo[*d*]imidazole (4t):



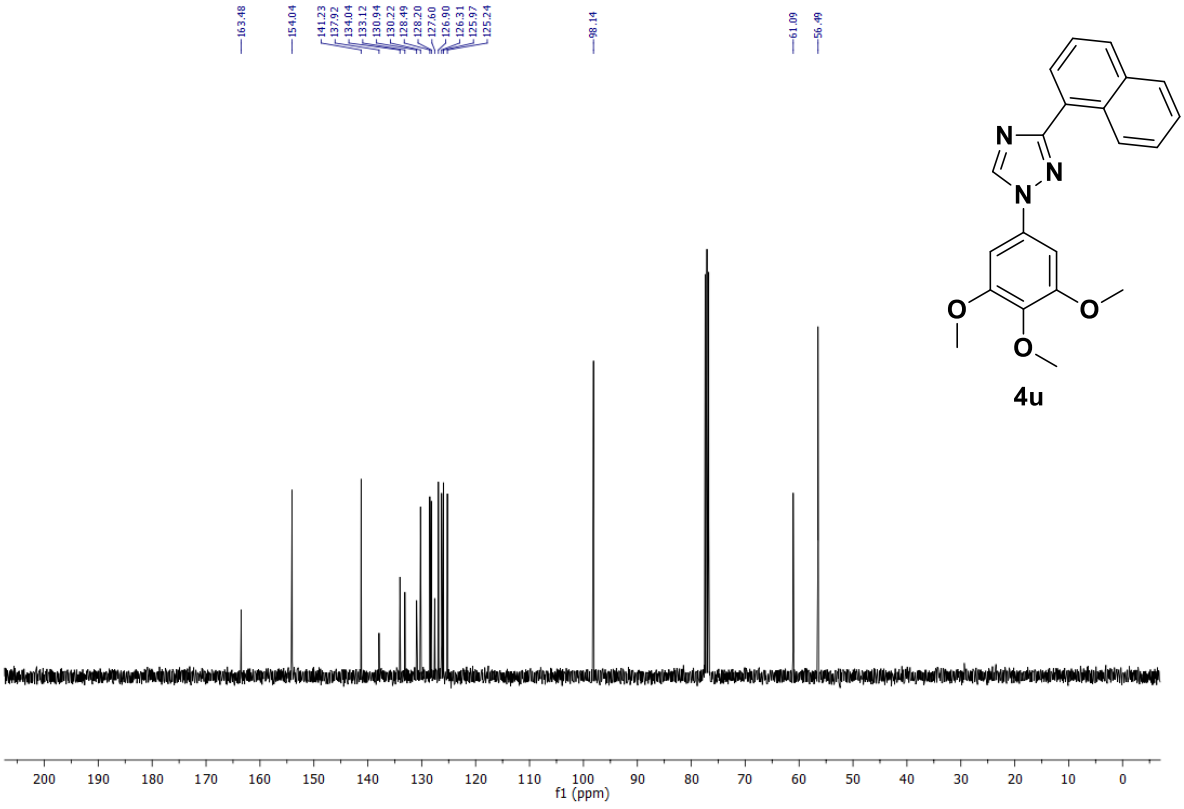
^{13}C{^{1}H} NMR (101 MHz, DMSO-d_6) of 6-(1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazol-3-yl)-1*H*-benzo[*d*]imidazole (4t):



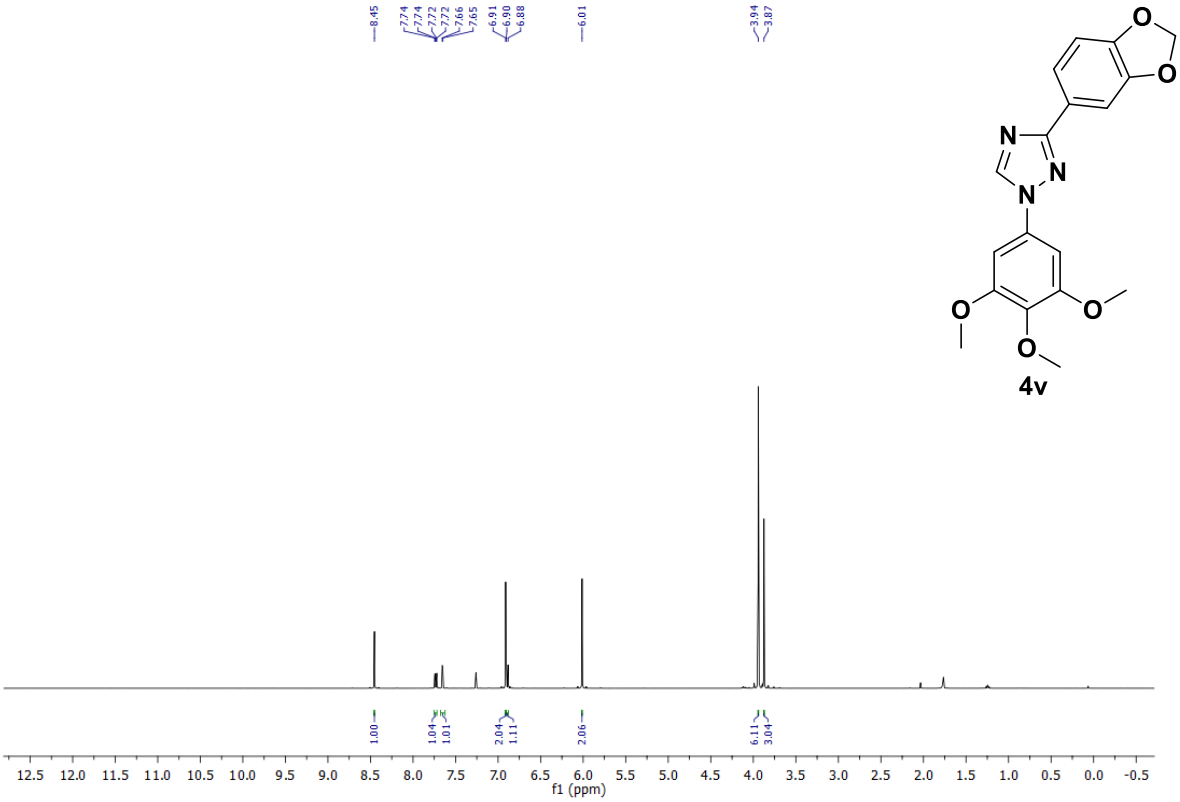
^{1}H NMR (400 MHz, $CDCl_3$) 3-(naphthalen-1-yl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4u):



^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(naphthalen-1-yl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4u):



^{1}H NMR (400 MHz, $CDCl_3$) of 3-(benzo[*d*][1,3]dioxol-5-yl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4v):



^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) of 3-(benzo[*d*][1,3]dioxol-5-yl)-1-(3,4,5-trimethoxyphenyl)-1*H*-1,2,4-triazole (4v):