Supporting information

Design and development of copper-manganese oxide nanocatalyst for the sustainable synthesis of 1,4-disubstituted 1,2,3-triazoles

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Electronic Supplementary Information (ESI) includes PXRD and TEM image of recycled CuO@MnO_2 nanocatalyst; Green chemistry metric calculations, ^{1}H NMR and ^{13}C NMR spectra of all compounds.

Total No of Pages: 19, Total No of Tables: 0, Total number of Figures: 2.

1. General Remarks

Chemicals and solvents were purchased from Sigma Adrich, Alfa-Aesar and Merck India Pvt. ^{1}H and ^{13}C spectra were recorded on a Jeol Spectrospin spectrometer at 400 MHz and 100 MHz respectively by keeping TMS as internal standard. Chemical shift values were recorded in terms of δ and coupling constants (J) are in hertz (Hz). FT-IR spectra were recorded on Perkin Elmer. Field Emission Scanning Electron microscopy (FESEM) measurement was performed on a ZeissGemini SEM 500 thermal field emission type with acceleration voltage 0.02 – 30kV at USIC (University Science Instrument Centre), University of Delhi, Delhi, India. Field Emission Gun -Transmission electron microscope 200 KV (HR-TEM) was obtained on a JEOL JEM 2100F at Centre for Research in Nanotechnology and Science (CRNTS), IIT Bombay, Bombay, India. X-ray diffraction (XRD) patterns were recorded on Rigaku Rotaflex spectrometer at 2θ range of 10–90° with Cu Kα radiation. The elemental composition and electronic structure analysis were obtained from X-ray photoelectron spectra (XPS) of PHI Versa Probe III instrument equipped with a monochromatic Al Kα source at ISM dhanbad. ICP-MS was measured on Agilent ICP-MS 7900 with UHMI at the ICP-MS Lab, (CRF Adopted Facility), IIT Delhi, INDIA. BET experiment was performed on BET surface area analyzer, Quantachrome Instruments, ASI-CI-11 at USIC (University Science Instrument Centre), University of Delhi, Delhi, India.

2. PXRD and TEM images of recycled $CuO@MnO_2$ nanocomposites

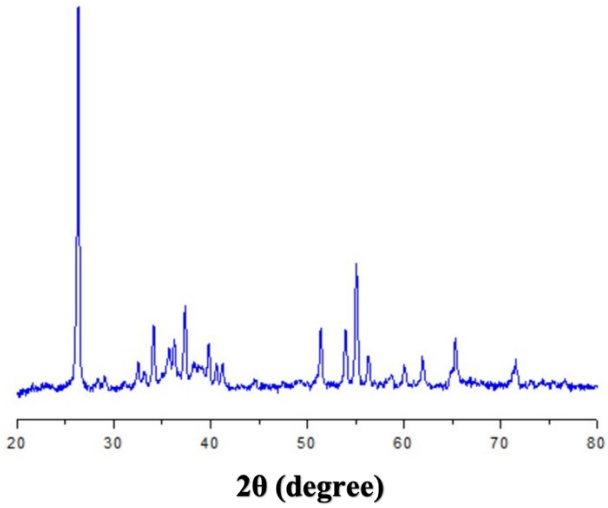


Figure S1: PXRD of recycled $CuO@MnO_2$ nanocomposites.

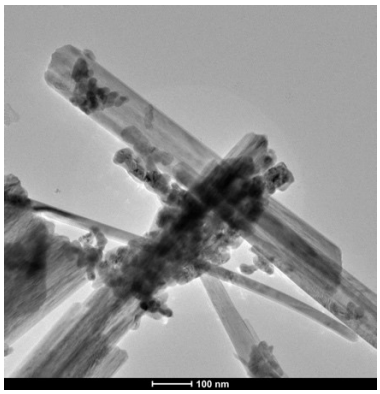
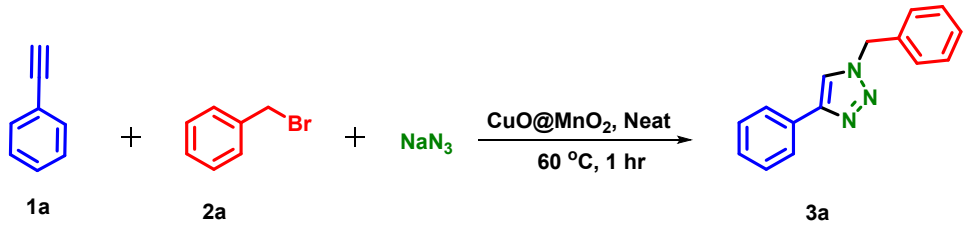


Figure S2: TEM image of recycled $CuO@MnO_2$ nanocomposites.

3. Calculation of E-factor and atom economy of compound 3a



1a 2a 3a

FW	102.13 g/mol	171.04 g/mol	65.01g/mol	235.29 g/mol
m.mol	0.50	0.50	1	0.47
amount	51 mg	86 mg	65 mg	110 mg

E-factor:

The ideal value of E-factor is zero.

E-factor = [total mass of raw materials - the total mass of product]/ mass of product.

E-factor of **3a** = [(51 + 86 + 65)-110]/110

= 0.84.

Process mass intensity (PMI):

PMI= ∑ (mass of stoichiometric reactants)/[mass of product]

= (51 + 86 + 65)/ 110

= 1.84.

Reaction mass efficiency (RME):

RME = [mass of product /∑ (mass of stoichiometric reactants)] × 100

= [110 / (51 + 86 + 65)] × 100

= 54.45%

Carbon efficiency (CE):

CE denotes the percentage of carbon in the reactants that remains in the product.

CE= [Amount of carbon in product/ Total carbon present in reactants] x 100

= [no. of moles of product x no. of carbons in product / (moles of 1a x carbons in 1a + moles of 2 x carbons in 2)] x 100

= [0.46 x 15 / (0.50 x 7 + 0.50 x 8)] x 100

= [6.9 / (3.5 + 4)] x 100

= 92%

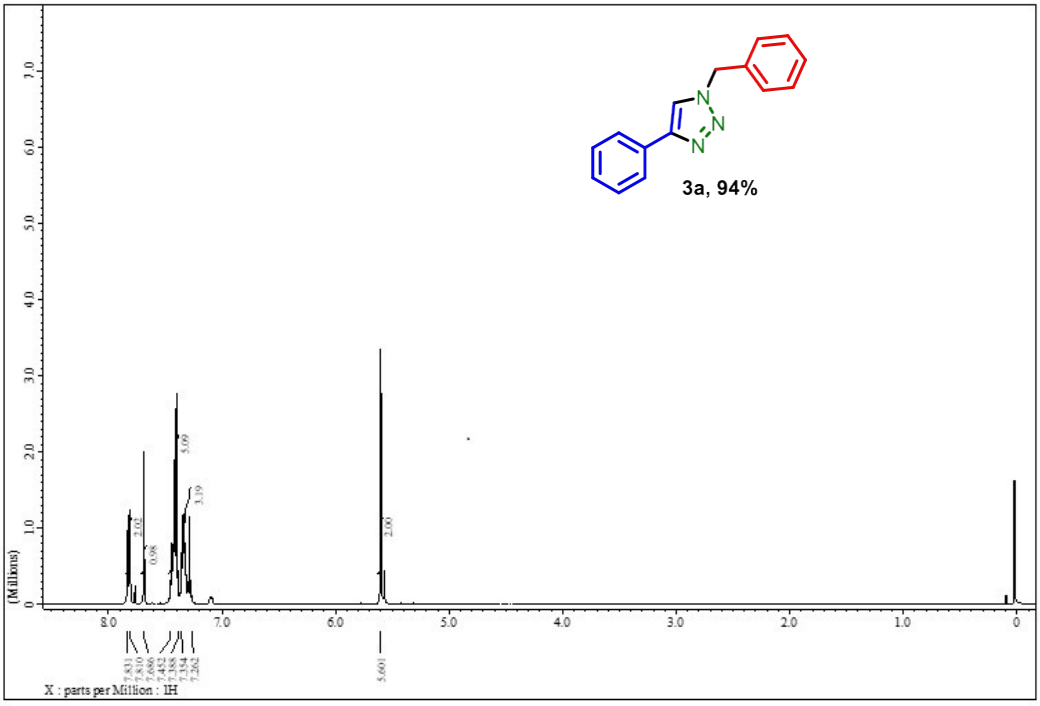
Turnover number (TON): The number of moles of substrate that converted by a mole of catalyst before its inactivation. TON is calculated for 5 cycles of the reaction with 25 mg of $CuO@MnO_2$.

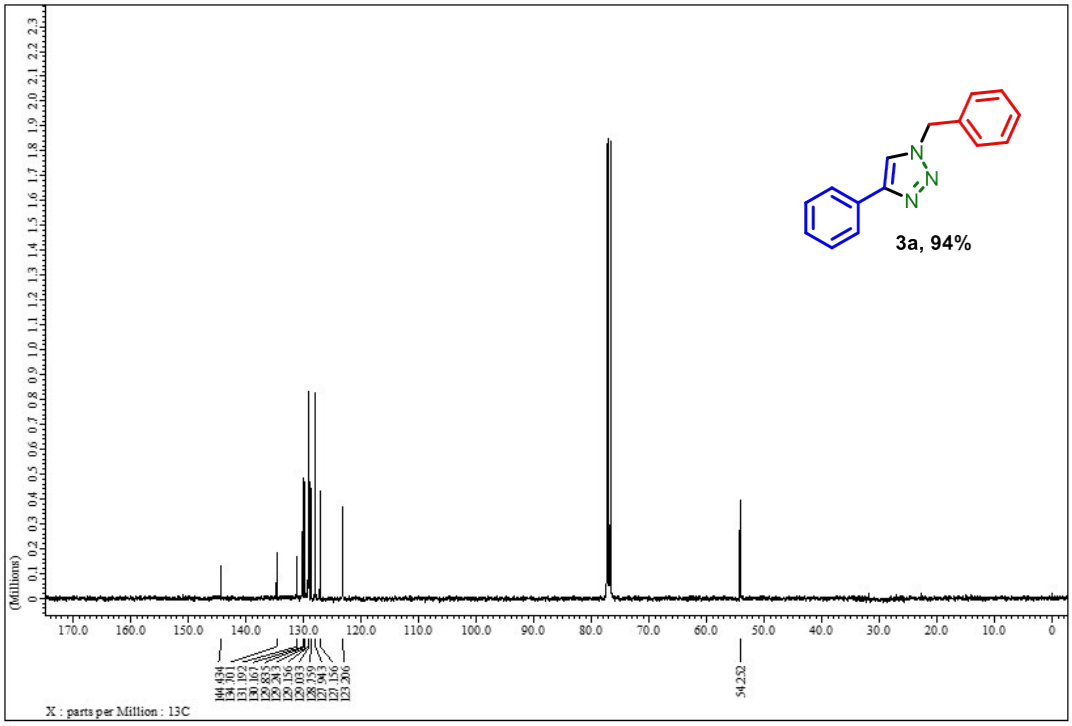
TON = [No. of moles of product] ÷ [No. of moles of catalyst]

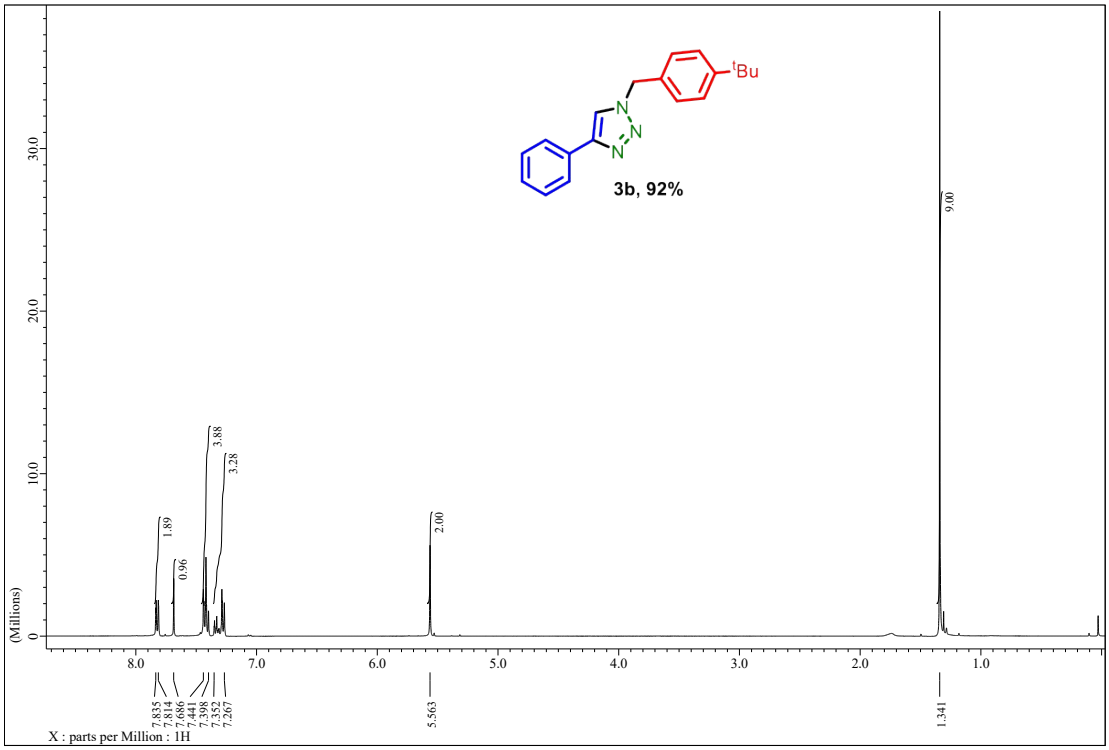
TON of compound **3a:** [0.47 (1) + 0.46 (2) + 0.46 (3) + 0.44 (4) + 0.44 (5)] / [0.00252]

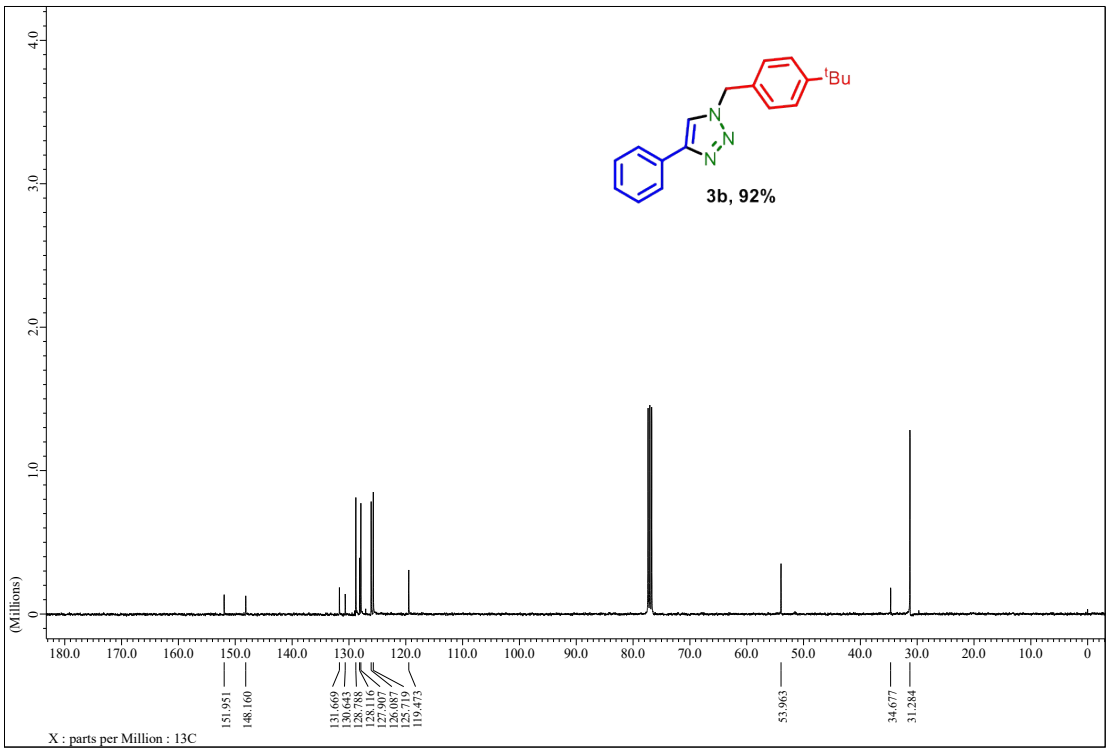
TON of compound **3a:** 901

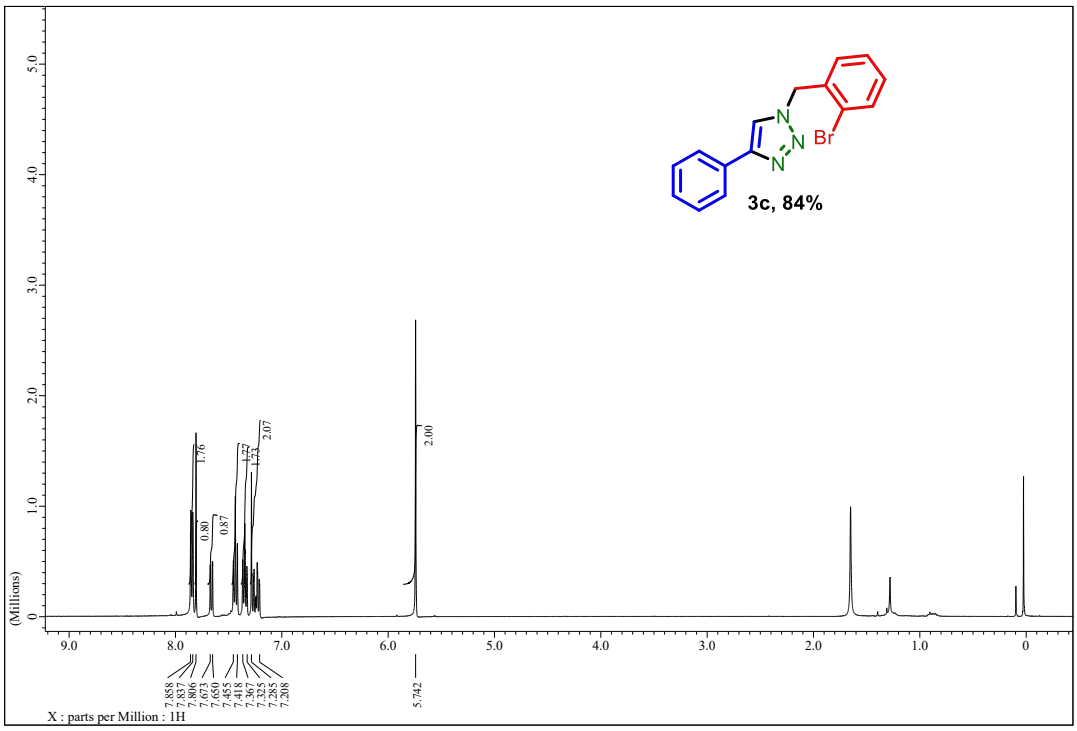
4. ^{1}H and ^{13}C Spectra of compounds

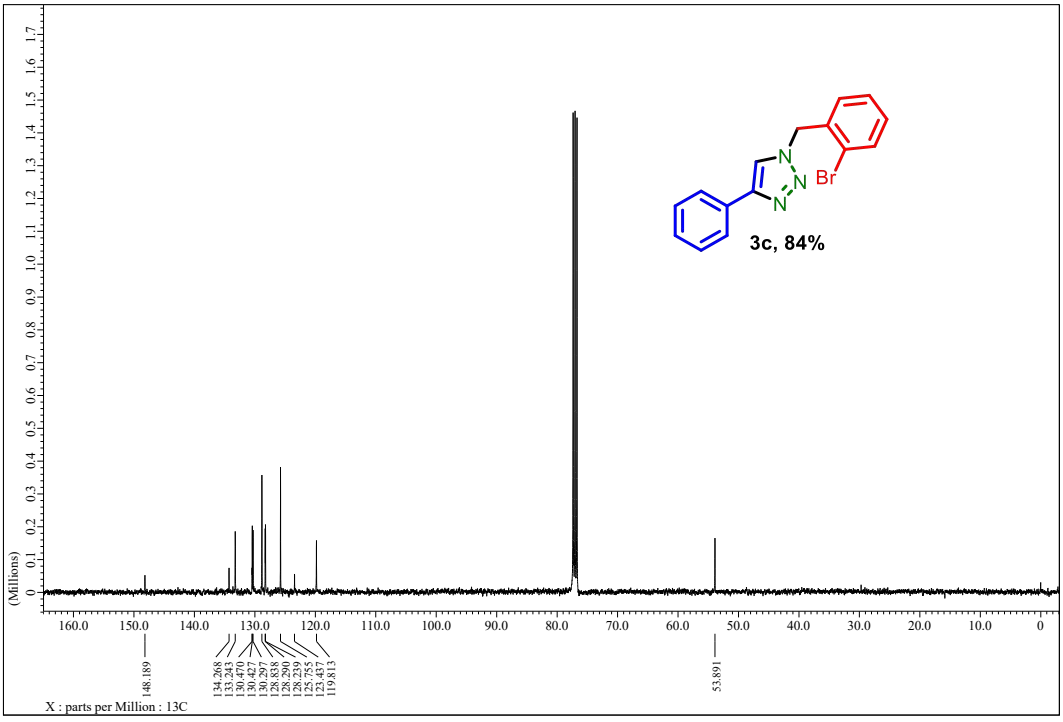


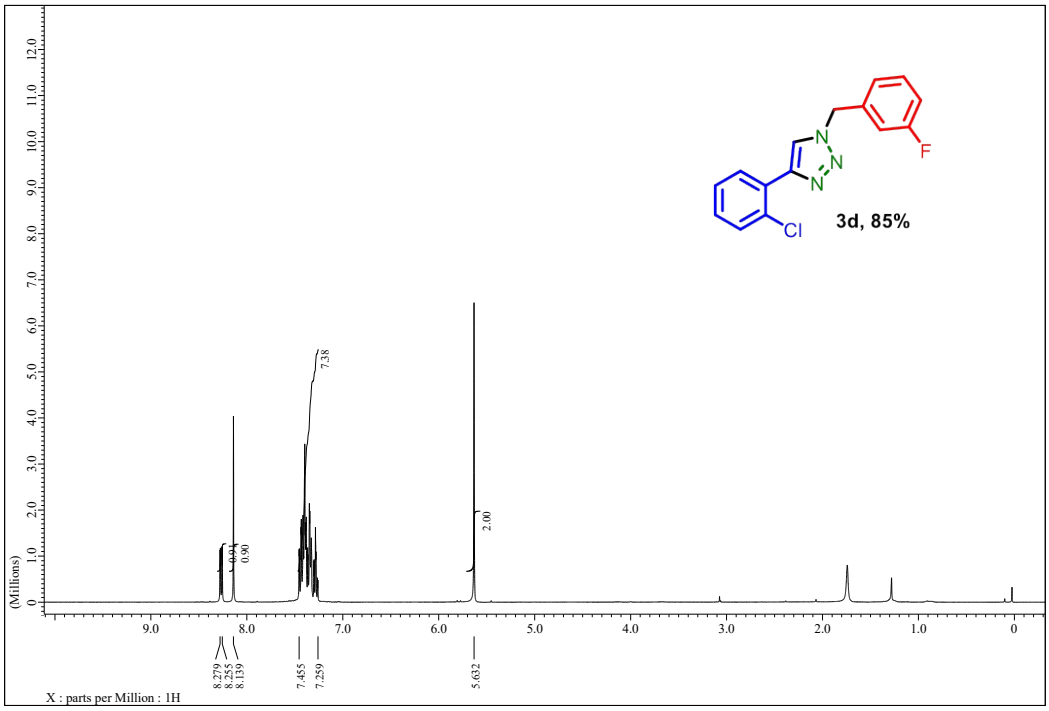


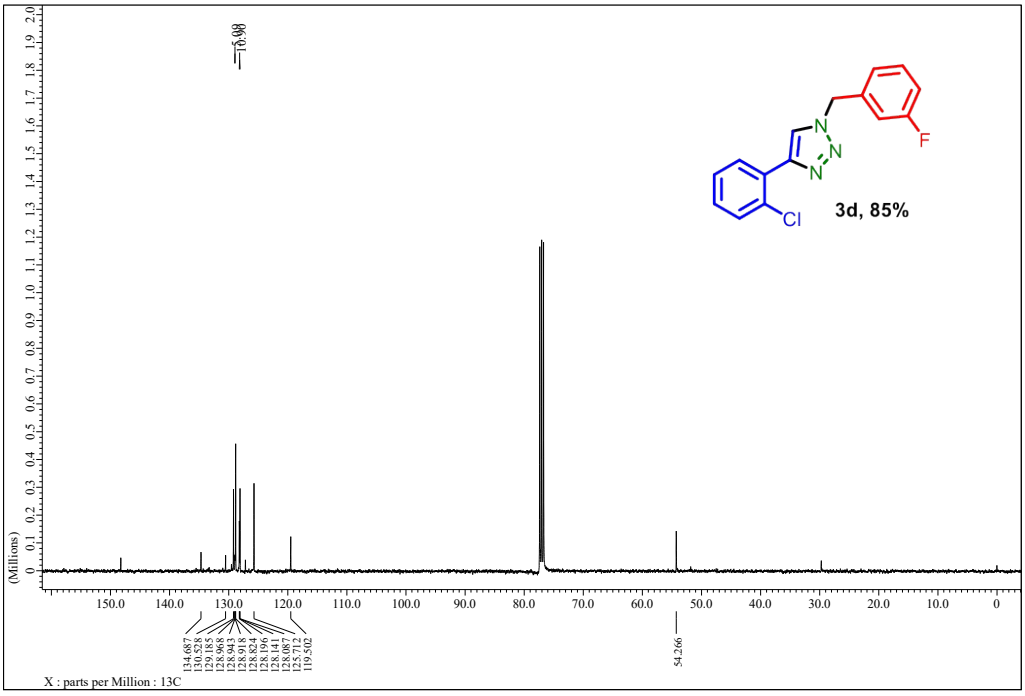

tBu
3b, 92%
(Millions)
30.0
20.0
10.0
0
1.89
0.96
3.88
3.28
2.00
9.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
7.835
7.814
7.686
7.441
7.398
7.352
7.267
5.563
1.341
X : parts per Million : 1H

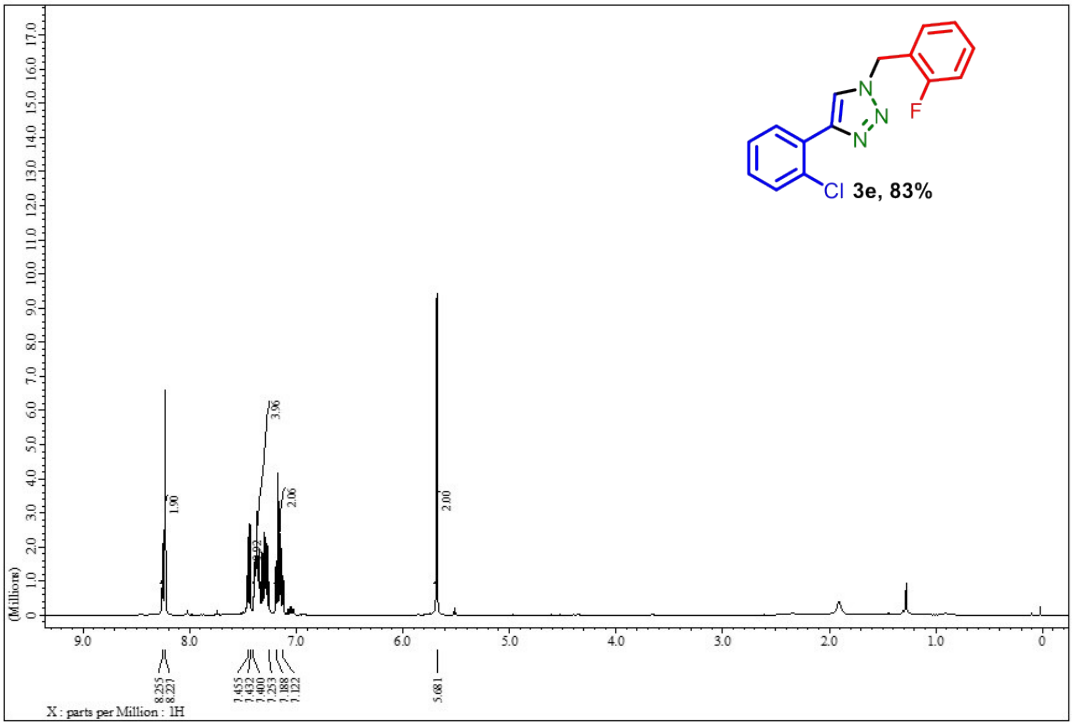

tBu
3b, 92%
(Millions)
4.0
3.0
2.0
1.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
151.951
148.160
131.669
130.643
128.788
128.116
127.907
126.087
125.710
119.473
53.963
34.677
31.284
X : parts per Million : 13C

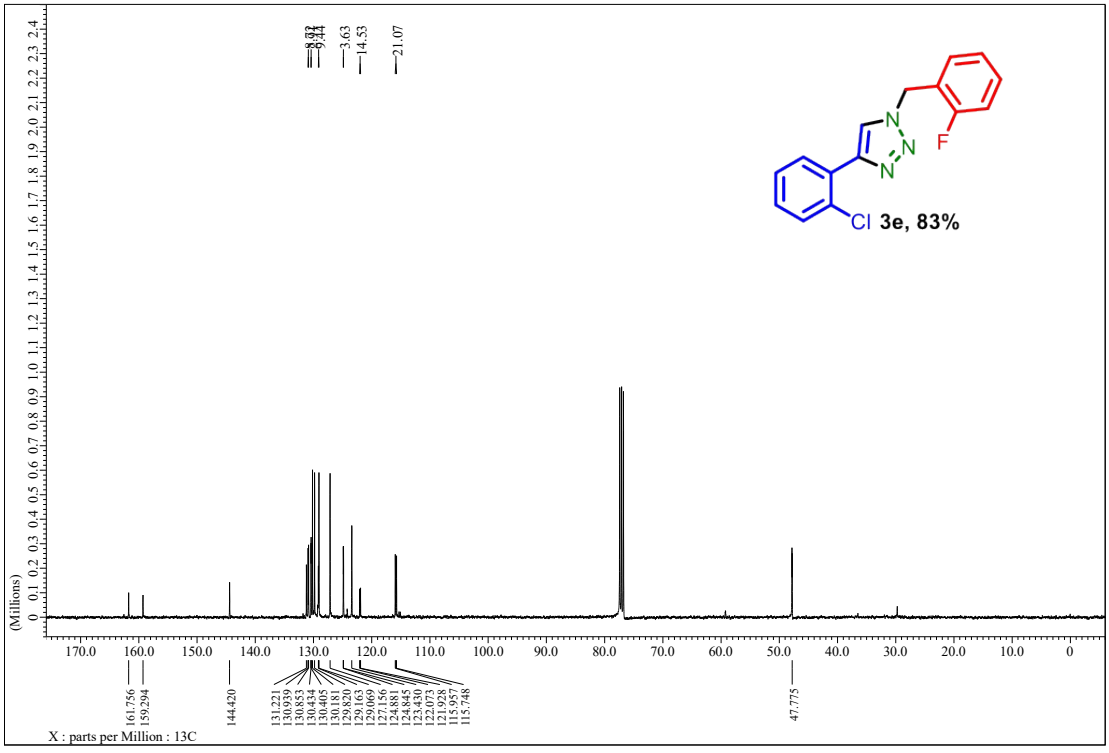

3c, 84%
(Millions)
X : parts per Million : 1H


3c, 84%
(Millions)
X : parts per Million : 13C


3d, 85%
(Millions)
X : parts per Million : 1H


3d, 85%
(Millions)
X : parts per Million : 13C


3e, 83%
(Millions)
X : parts per Million : 1H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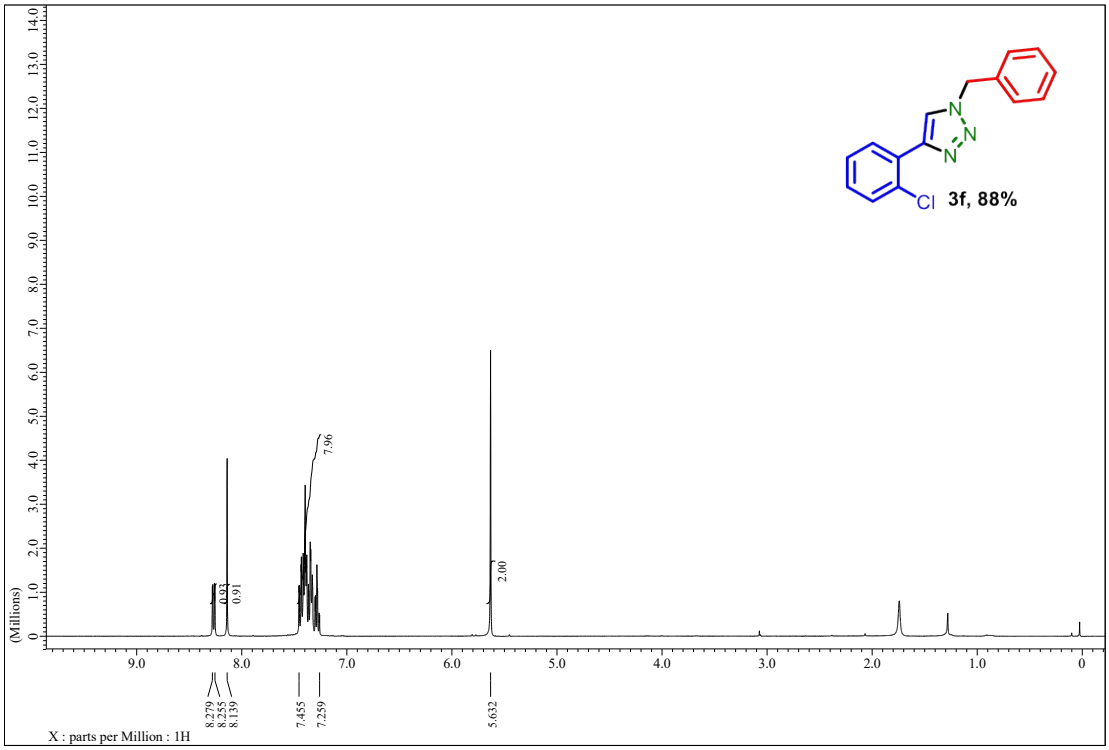
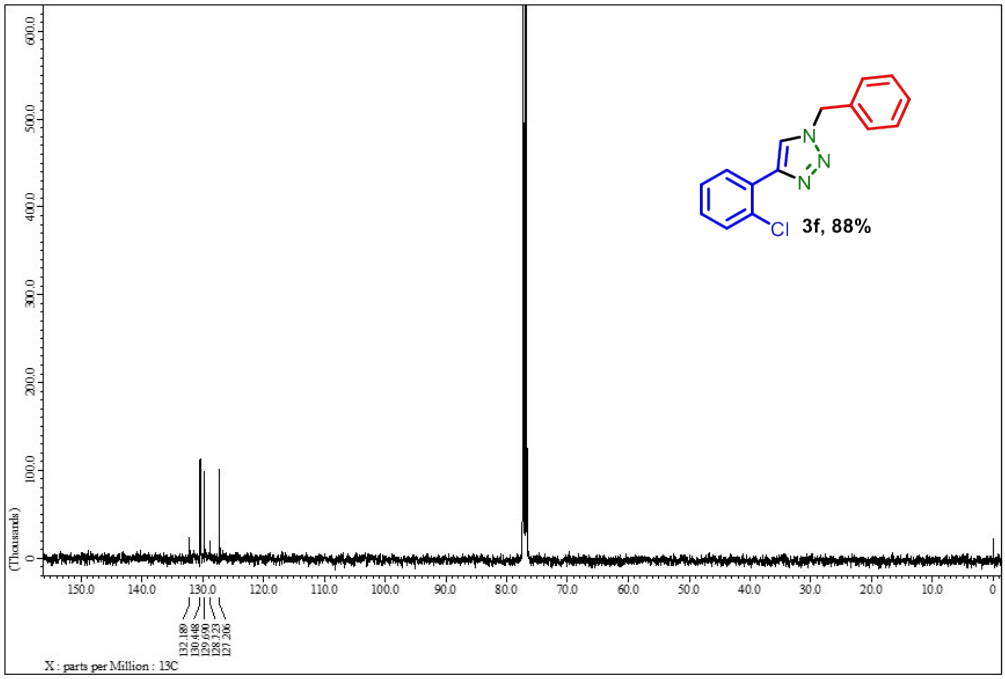
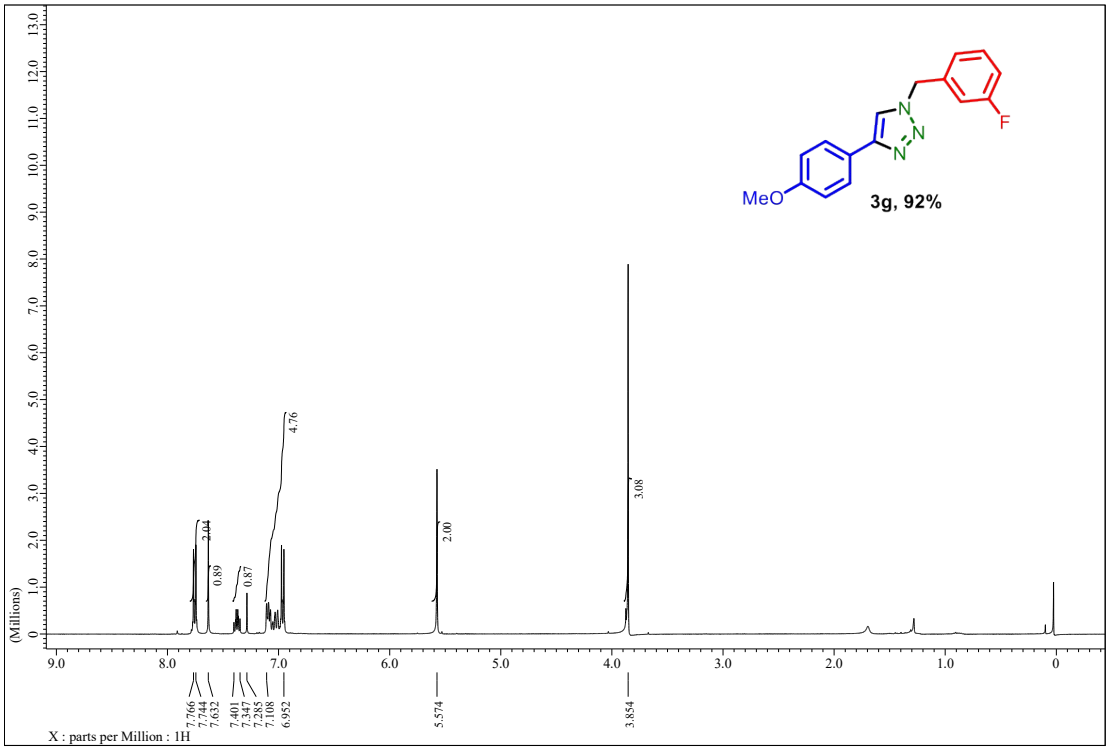
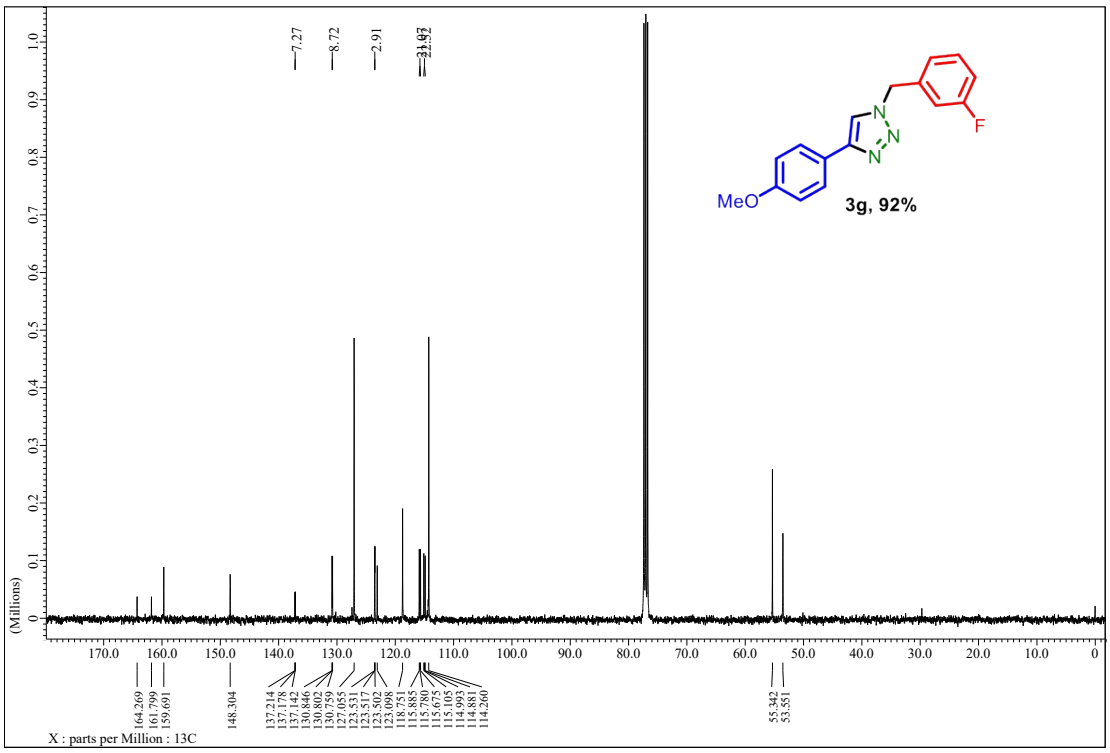
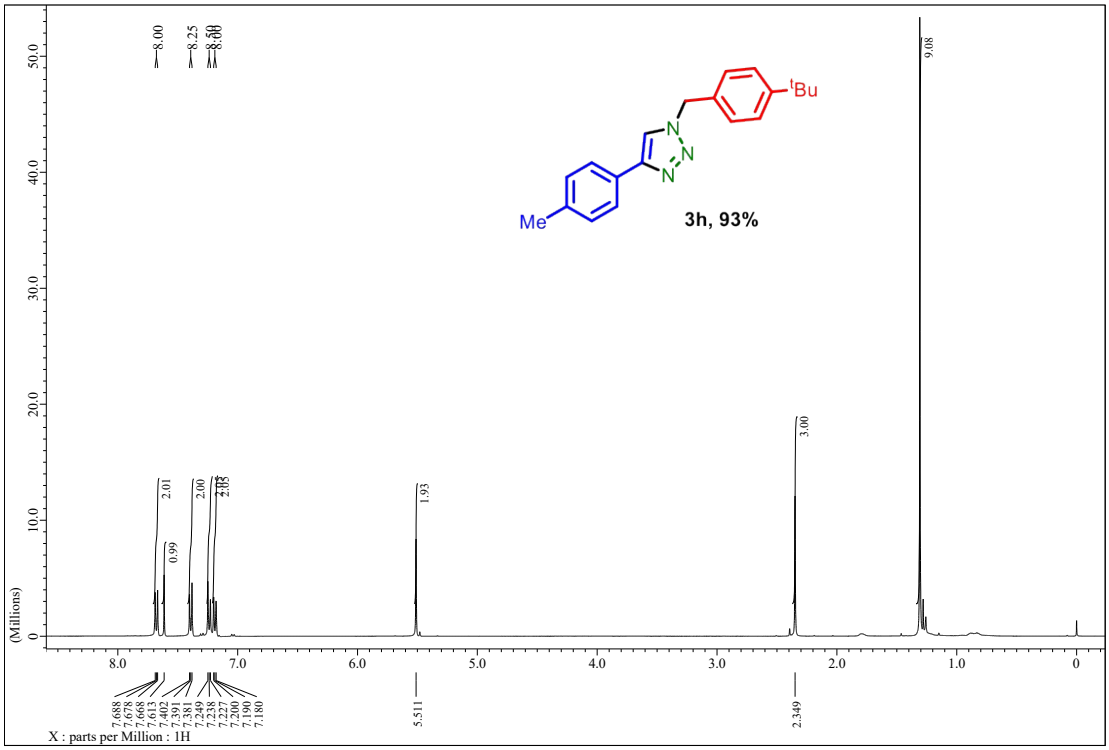
(Millions)
X : parts per Million : 13C

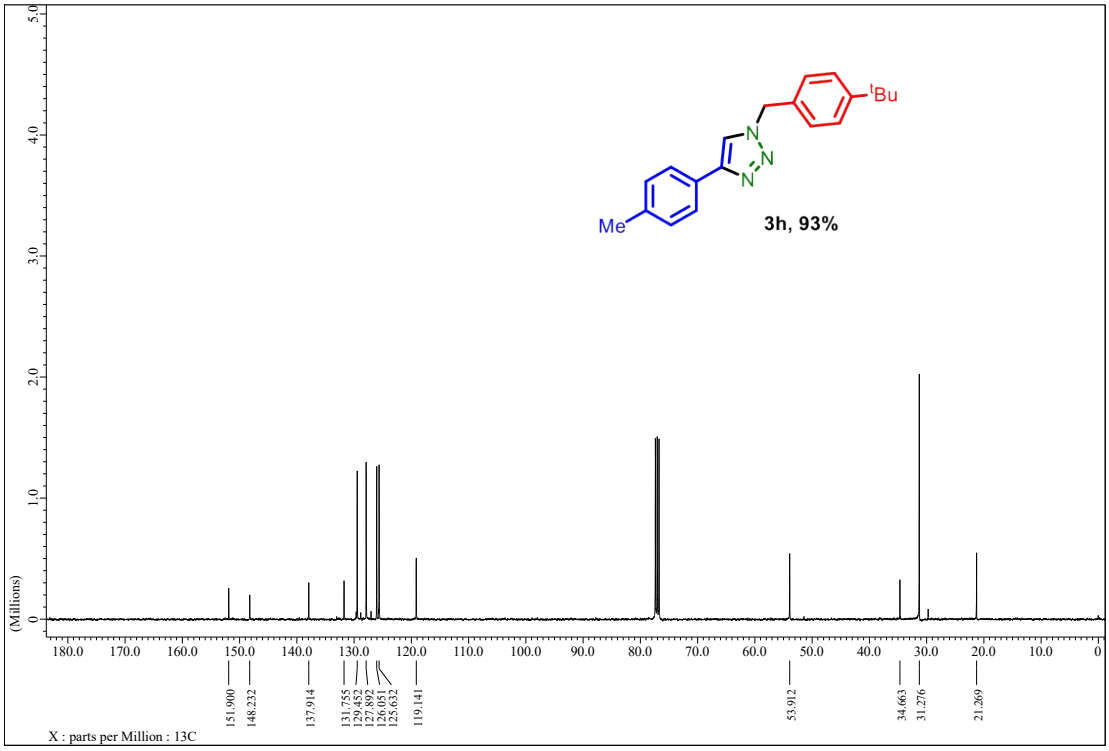

(Millions)
7.96
2.00
0.93
0.91
8.279
8.255
8.139
7.455
7.259
5.632
X : parts per Million : 1H
3f, 88%

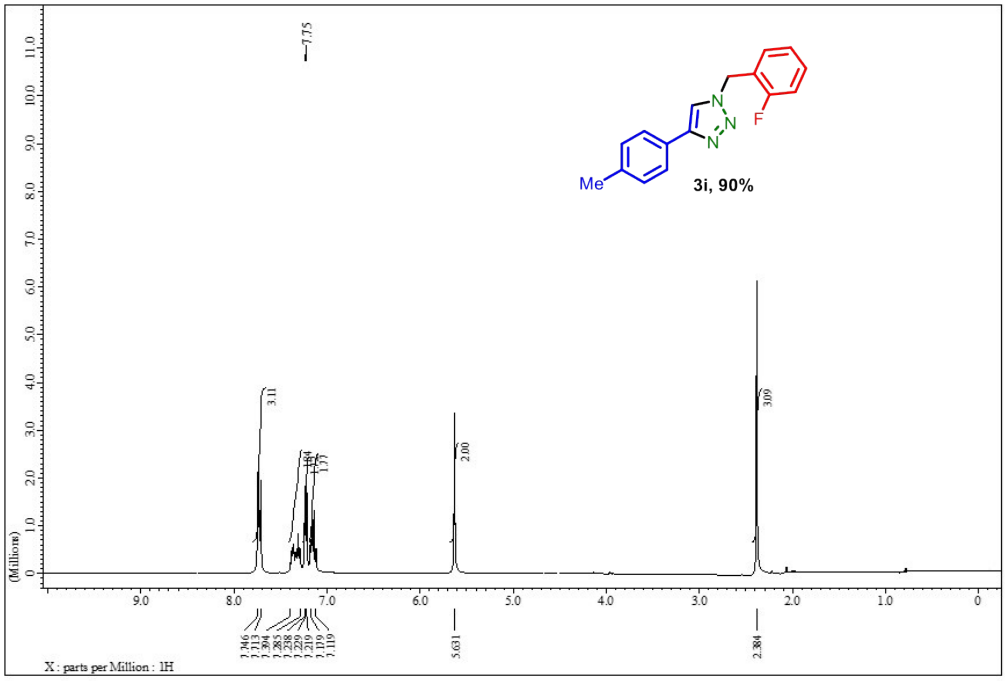

(Thousands)
132.189
130.448
129.690
128.232
127.206
X : parts per Million : 13C
3f, 88%

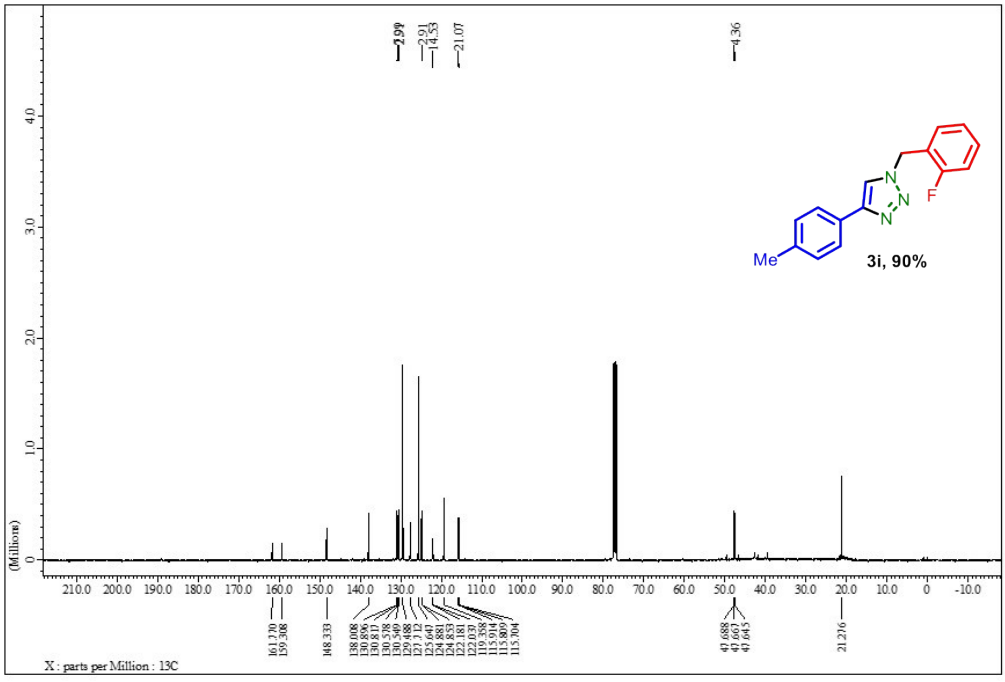

3g, 92%
MeO
F
(Millions)
4.76
3.08
2.04
2.00
0.89
0.87
7.766
7.744
7.632
7.401
7.347
7.285
7.108
6.952
5.574
3.854
X : parts per Million : 1H

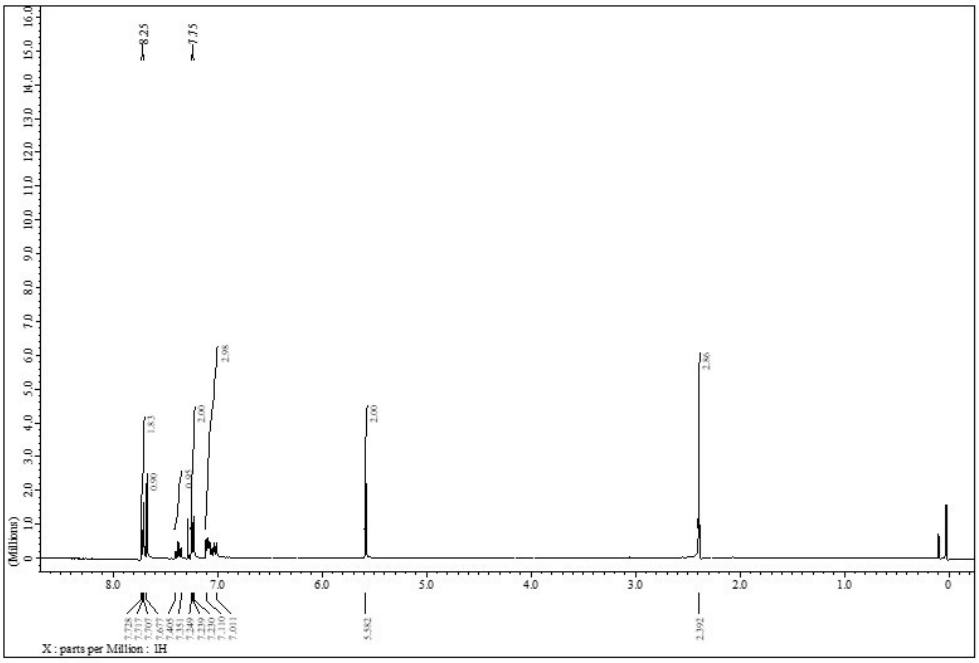

3g, 92%
MeO
F
(Millions)
7.27
8.72
2.91
164.269
161.799
159.691
148.304
137.214
137.178
137.142
130.846
130.802
130.759
127.055
123.531
123.517
123.502
123.098
118.751
115.885
115.780
115.675
115.105
114.993
114.881
114.260
55.342
53.551
X : parts per Million : 13C

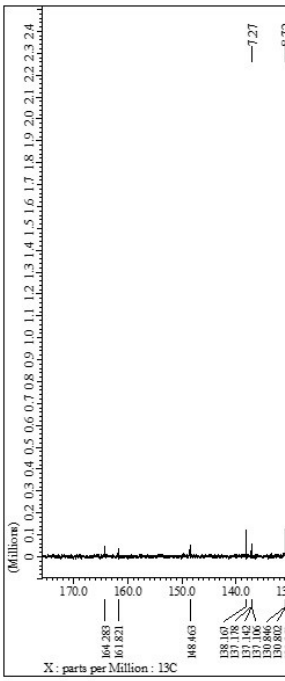

3h, 93%
Me
tBu
X : parts per Million : 1H
(Millions)

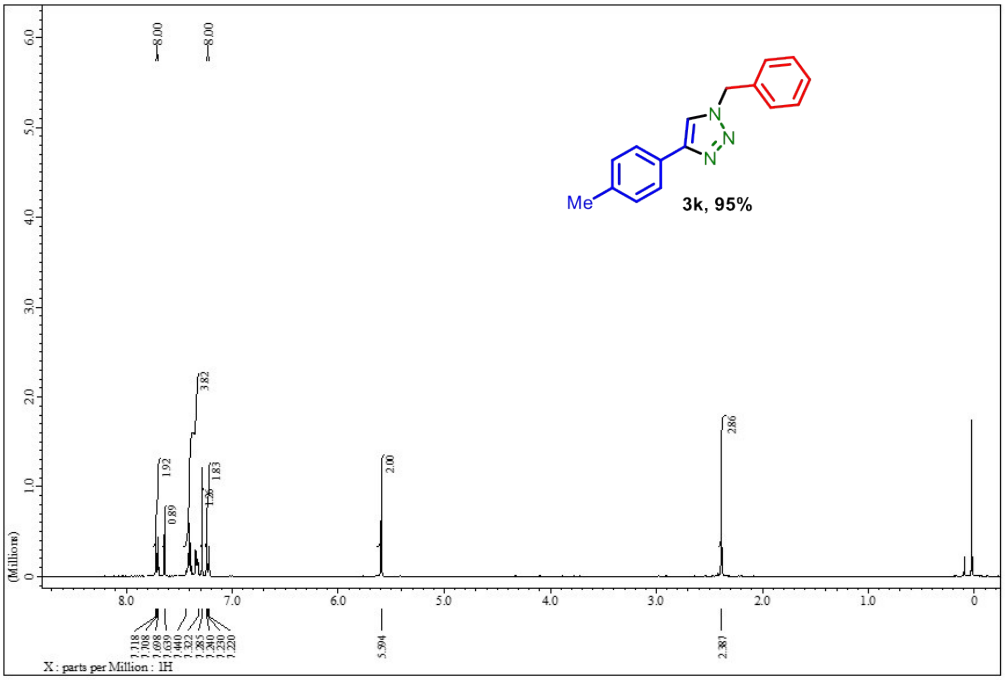

3h, 93%
Me
tBu
X : parts per Million : 13C
(Millions)

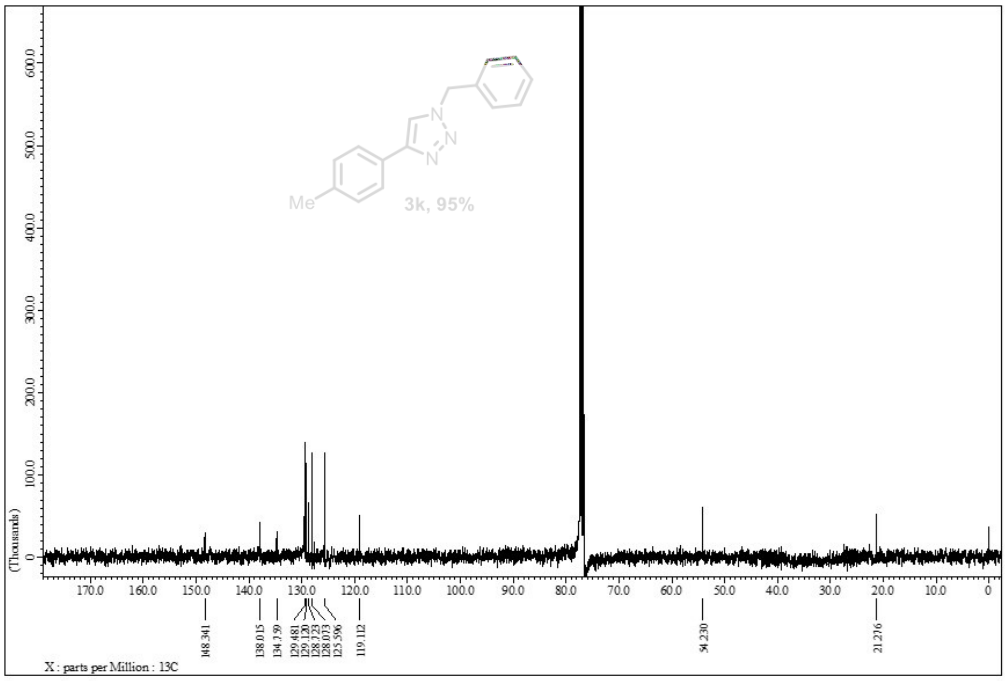

7.75
3.11
2.00
3.09
Me
F
3i, 90%
X : parts per Million : 1H

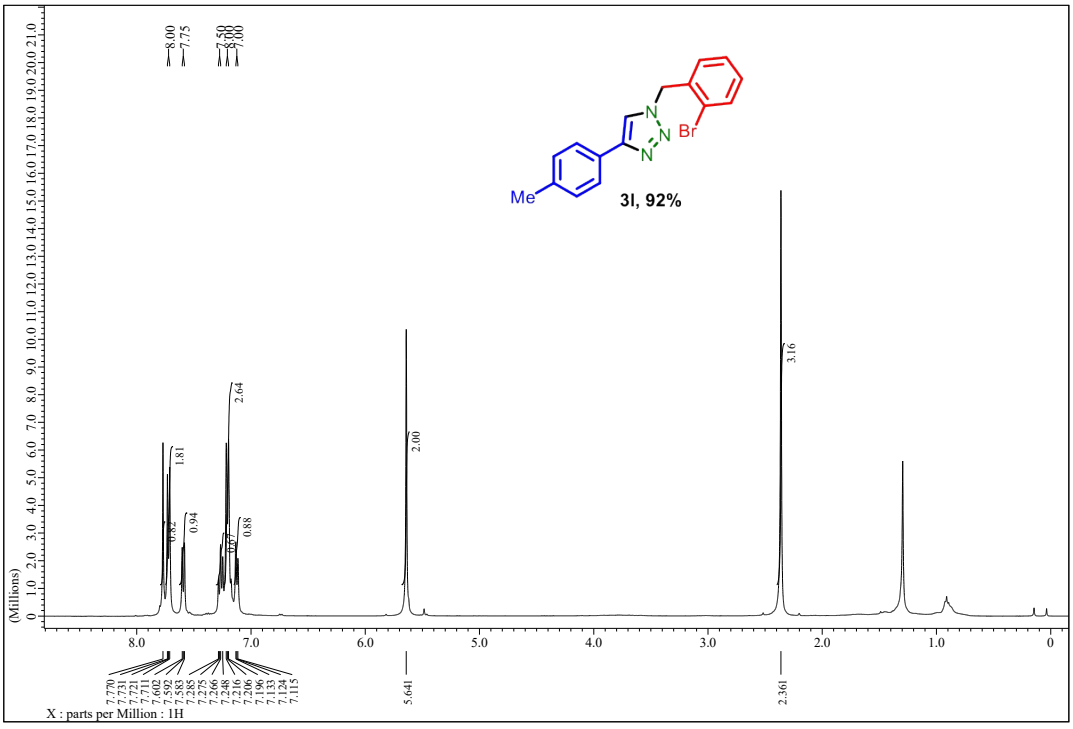

14.53
21.07
41.36
Me
F
3i, 90%
X : parts per Million : 13C

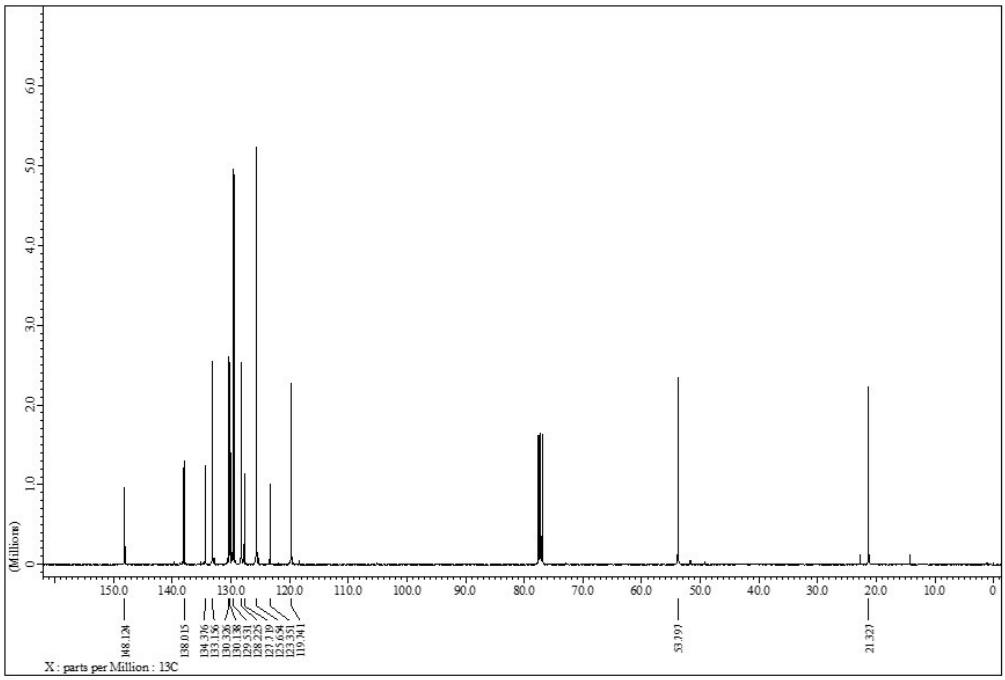

8.25
7.75
(Million)
X : parts per Million : 1H

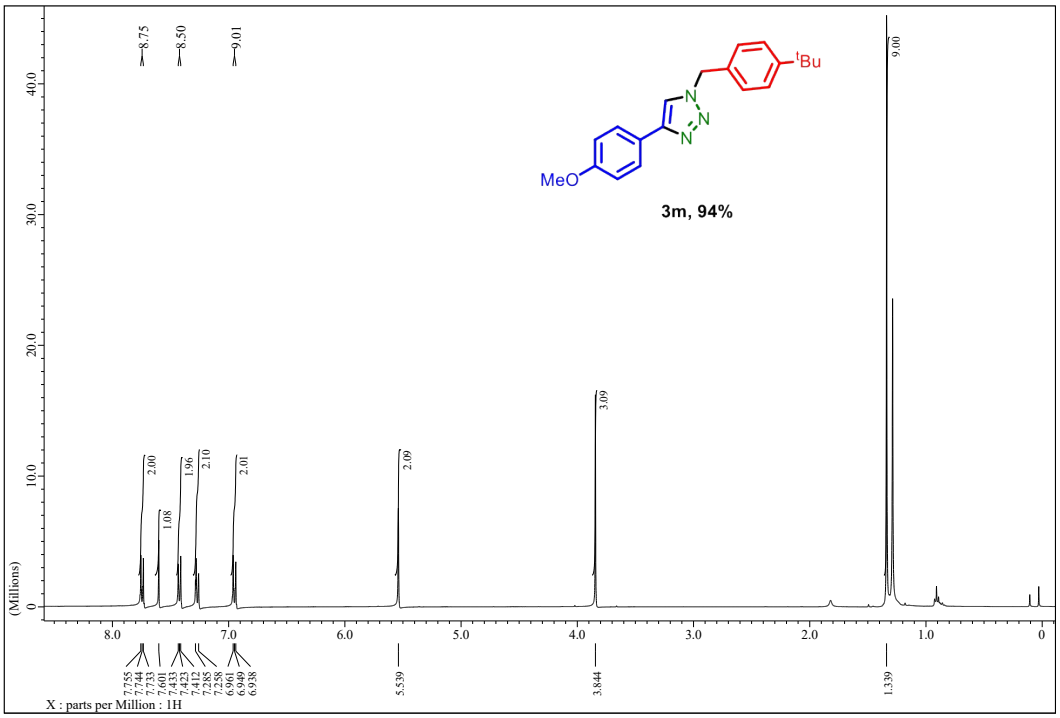

7.27
(Million)
X : parts per Million : 13C

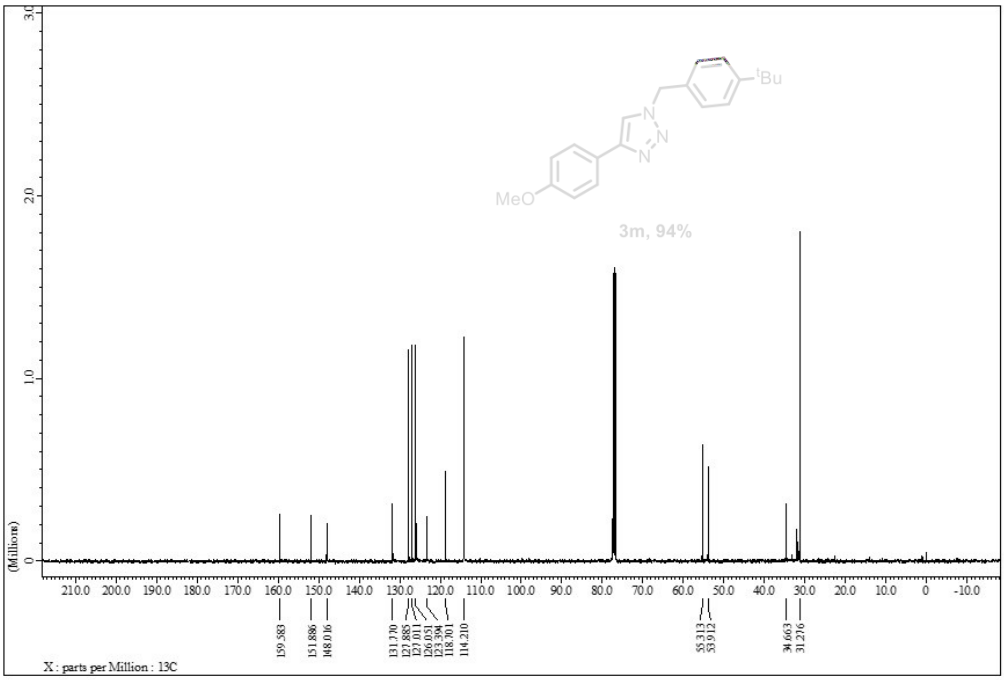

8.00
8.00
Me
3k, 95%
(Million)
X : parts per Million : 1H

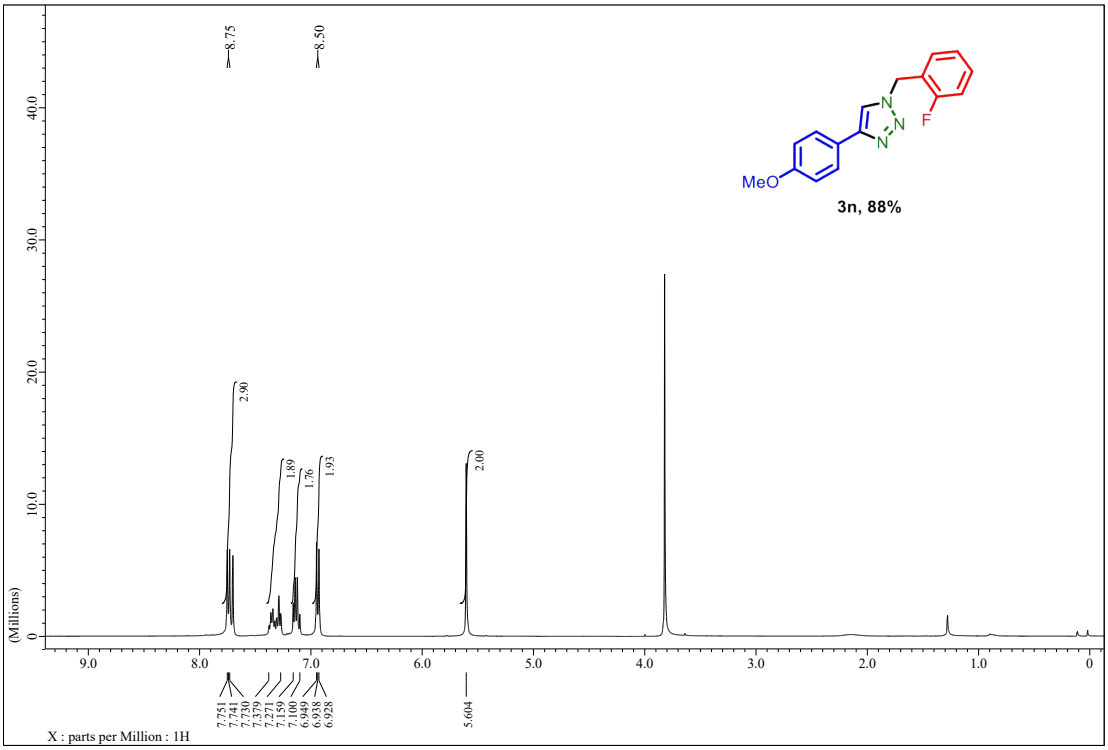

Me
3k, 95%
(Thousands)
X : parts per Million : 13C

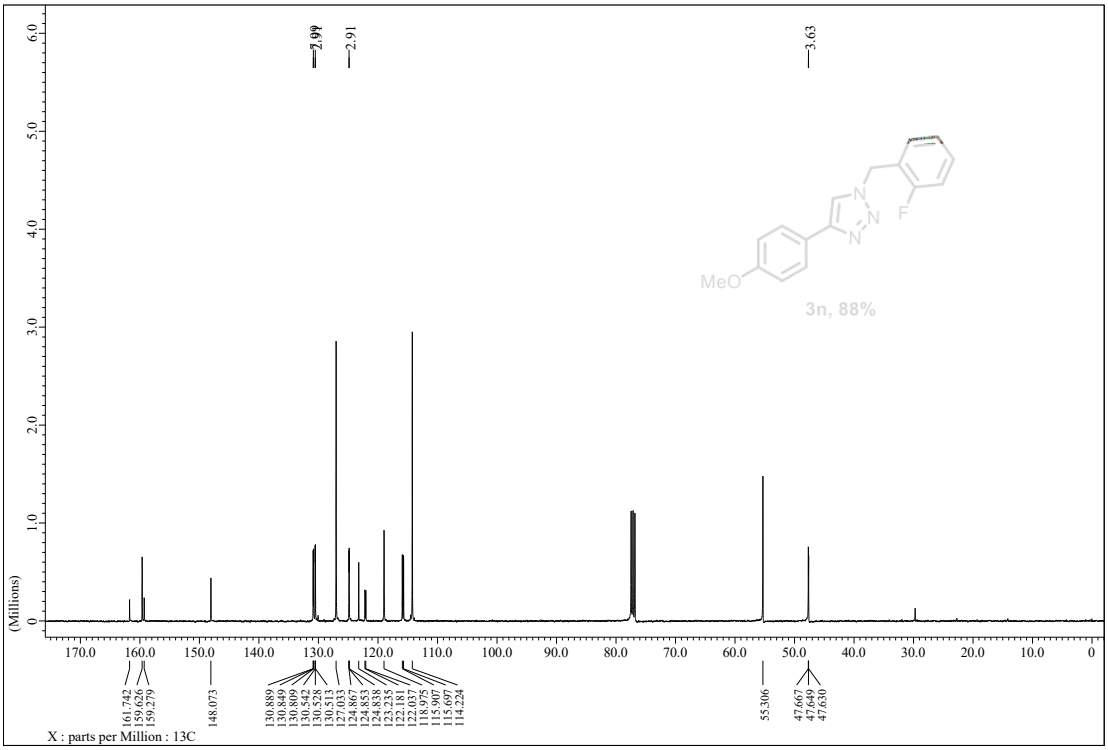

Br
Me
3l, 92%
(Millions)
X : parts per Million : 1H

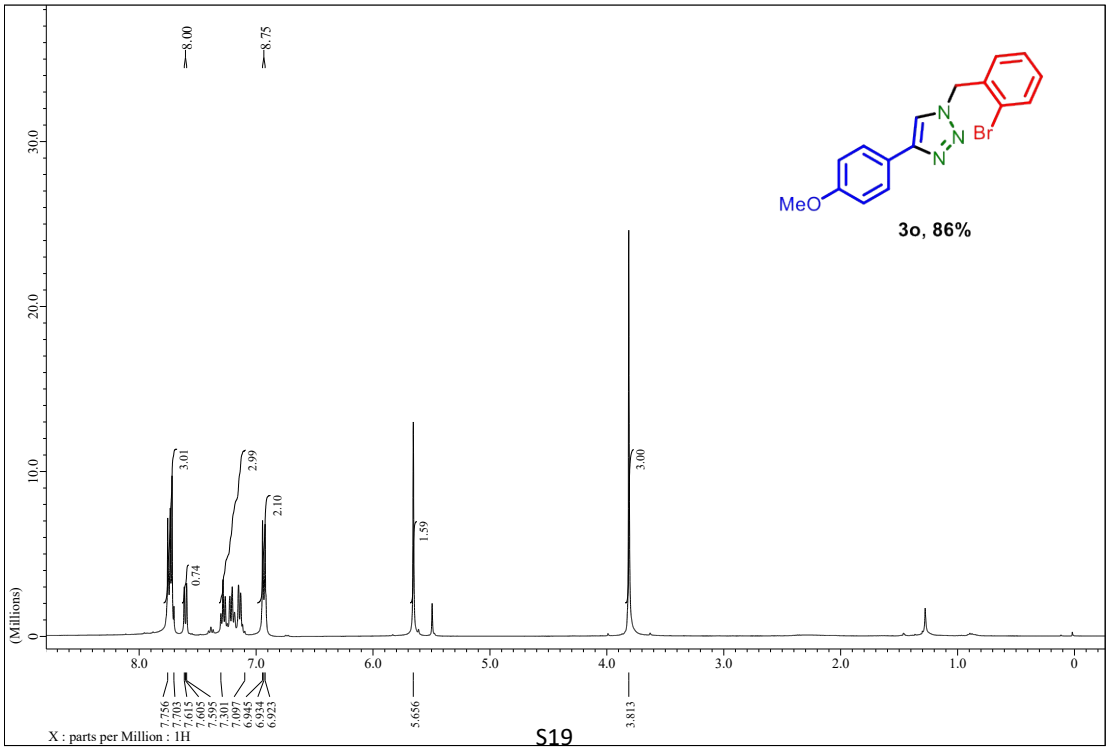

(Millions)
X : parts per Million : 13C

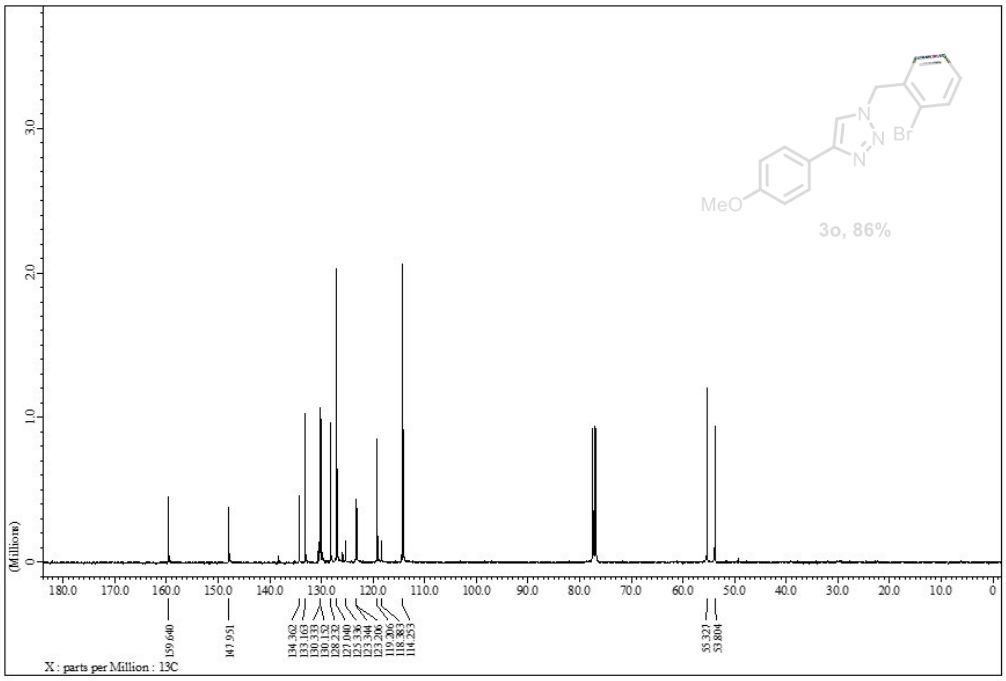

8.75
8.50
9.01
9.00
tBu
N
N
N
MeO
3m, 94%
(Millions)
X : parts per Million : 1H


3m, 94%
(Millions)
X : parts per Million : 13C


3n, 88%
(Millions)
X : parts per Million : 1H


2.99
2.91
3.63
MeO
F
3n, 88%
(Millions)
161.742
159.626
159.279
148.073
130.889
130.849
130.809
130.542
130.528
130.513
127.033
124.867
124.853
124.838
123.235
122.181
122.037
118.975
115.907
115.697
114.224
55.306
47.667
47.649
47.630
X : parts per Million : 13C


8.00
8.75
Br
MeO
3o, 86%
(Millions)
3.01
2.99
2.10
1.59
0.74
3.00
7.756
7.703
7.615
7.605
7.595
7.301
7.097
6.945
6.934
6.923
5.656
3.813
X : parts per Million : 1H


3o, 86%
(Million)
X : parts per Million : 13C
159.640
147.951
134.362
133.163
130.153
130.133
128.232
127.040
123.336
123.344
123.206
119.206
118.883
114.253
55.327
55.804