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Supplementary Materials

The catalytic activity of carbon-supported Cu(I)-phosphine complexes for the microwave-assisted synthesis of 1,2,3-triazoles

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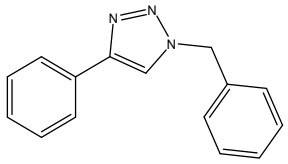
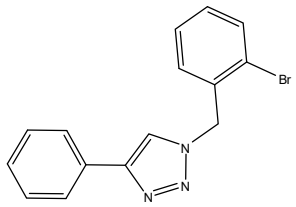
1. General remarks

Commercially available reagents were used as received and no further purification was made. ^{1}H, ^{13}C and DEPT NMR spectra were recorded on 300 or 400 MHz instruments using TMS as an internal standard. IR spectra were recorded on an FT-IR spectrometer in KBr pellets and peaks are reported in cm^{-1}. Electrospray mass (ESI-MS) spectra were obtained using the LCQ Fleet mass spectrometer with an electrospray ion source (Thermo Scientific) interfaced with an HPLC-DAD (Varian). Scanning was performed from *m/z* 100-1000. The compounds were observed and reported in the positive mode.

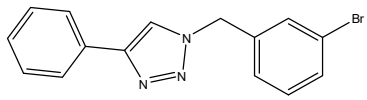
2. Spectral data of the compounds



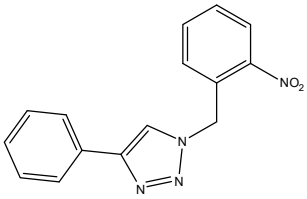
1-benzyl-4-phenyl-1H-1,2,3-triazole: ^{1}H NMR (300 MHz, DMSO-d_6): δ= 5.65 (s, 2H), 7.35-7.44 (m, 8H), 7.83-7.85 (d, *J*= 7.8 Hz, 2H), 8.64 (s, 1H). ^{13}C NMR (300 MHz, DMSO-d_6): δ= 53.49, 122.02, 125.62, 128.35, 128.63, 129.27, 129.36, 131.12, 136.48, 147.12. DEPT (300 MHz, DMSO-d_6): δ= -53.50, 122.03, 125.64, 128.36, 128.64, 129.28, 129.36.



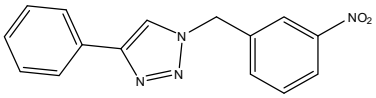
1-(2-bromobenzyl)-4-phenyl-1H-1,2,3-triazole: ^{1}H NMR (300 MHz, DMSO-d_6): δ= 5.73 (s, 2H), 7.21-7.44 (m, 6H), 7.69-7.72 (d, *J*= 7.7 Hz, 1H), 7.85-7.87 (d, *J*= 7.9 Hz, 2H), 8.60 (s, 1H). ^{13}C NMR (300 MHz, DMSO-d_6): δ= 53.41, 122.38, 123.23, 125.53, 128.42, 128.87, 129.28, 130.84, 131.44, 133.43, 135.16, 146.94. DEPT (300 MHz, DMSO-d_6): δ= -53.60, 122.43, 125.69, 128.43, 128.81, 129.37, 130.93, 130.96, 133.40.



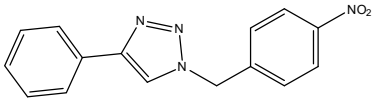
1-(3-bromobenzyl)-4-phenyl-1H-1,2,3-triazole: ^{1}H NMR (400 MHz, DMSO-d_6): δ= 5.66 (s, 2H), 7.33-7.46 (m, 5H), 7.54-7.58 (d, *J*= 7.6 Hz, 2H), 7.83-7.85 (d, *J*= 7.8 Hz, 2H), 8.65 (s, 1H). ^{13}C NMR (400 MHz, DMSO-d_6): δ= 52.66, 122.17, 122.34, 125.66, 127.52, 128.43, 129.38, 131.17, 131.50, 131.55, 139.05, 147.19. DEPT (300 MHz, DMSO-d_6): δ= -52.66, 122.17, 125.66, 127.52, 128.45, 129.39, 131.17, 131.51, 131.56.



1-(2-nitrobenzyl)-4-phenyl-1H-1,2,3-triazole: ^{1}H NMR (300 MHz, DMSO-d_6): δ=6.02 (s, 2H), 7.15-7.18 (d, *J*=7.2, 1H), 7.34-7.42 (d, *J*= 7.4 Hz, 1H), 7.45-7.47 (t, *J*=7.5 Hz, 2H), 7.65-7.68 (d, *J*=7.7 Hz, 1H), 7.74-7.77 (d, *J*= 7.8 Hz, 1H), 7.84-7.87 (d, *J*= 7.9 Hz, 2H), 8.15-8.18 (d, *J*=8.2 Hz, 1H), 8.61 (s, 1H). ^{13}C NMR (300 MHz, DMSO-d_6): δ= 50.64, 122.76, 125.60, 125.70, 127.52, 128.49, 129.40, 130.20, 130.73, 130.96, 131.13, 134.93, 147.04, 148.07. DEPT (400 MHz, DMSO-d_6): δ= -50.64, 122.75, 125.59, 125.70, 128.49, 129.40, 130.20, 130.74, 134.92.



1-(3-nitrobenzyl)-4-phenyl-1H-1,2,3-triazole: ^{1}H NMR (400 MHz, DMSO-d_6): δ=5.83 (s, 2H), 7.33-7.35 (d, *J*=7.3, 1H), 7.33-7.35 (d, *J*= 7.3 Hz, 1H), 7.42-7.46 (t, *J*=7.4 Hz, 2H), 7.71 (s, 2H), 7.83-7.85 (d, *J*= 7.8 Hz, 3H), 8.20-8.26 (d, *J*= 8.2 Hz, 3H), 8.69 (s, 1H). ^{13}C NMR (400 MHz, DMSO-d_6): δ=52.85, 122.29, 123.32, 125.67, 128.46, 129.39, 130.78, 130.95, 130.99, 135.18, 138.50, 147.23, 148.41. DEPT (400 MHz, DMSO-d_6): δ= -52.64, 122.28, 123.29, 123.64, 125.67, 128.47, 129.39, 130.95, 135.18.



1-(4-nitrobenzyl)-4-phenyl-1H-1,2,3-triazole: ^{1}H NMR (300 MHz, DMSO-d_6): δ= 5.84 (s, 2H), 7.34-7.59 (M, *J*=7.5, 6H), 7.84-7.86 (d, *J*= 7.9 Hz, 2H), 8.25-8.27 (d, *J*=8.3.4 Hz, 2H), 8.69 (s, 1H). ^{13}C NMR (300 MHz, DMSO-d_6): δ=52.59, 122.46, 124.43, 125.67, 128.48, 129.40, 129.47, 130.97, 143.87, 147.25, 147.74. DEPT (400 MHz, DMSO-d_6): δ= -52.59, 122.45, 124.43, 125.67, 128.47, 129.39.

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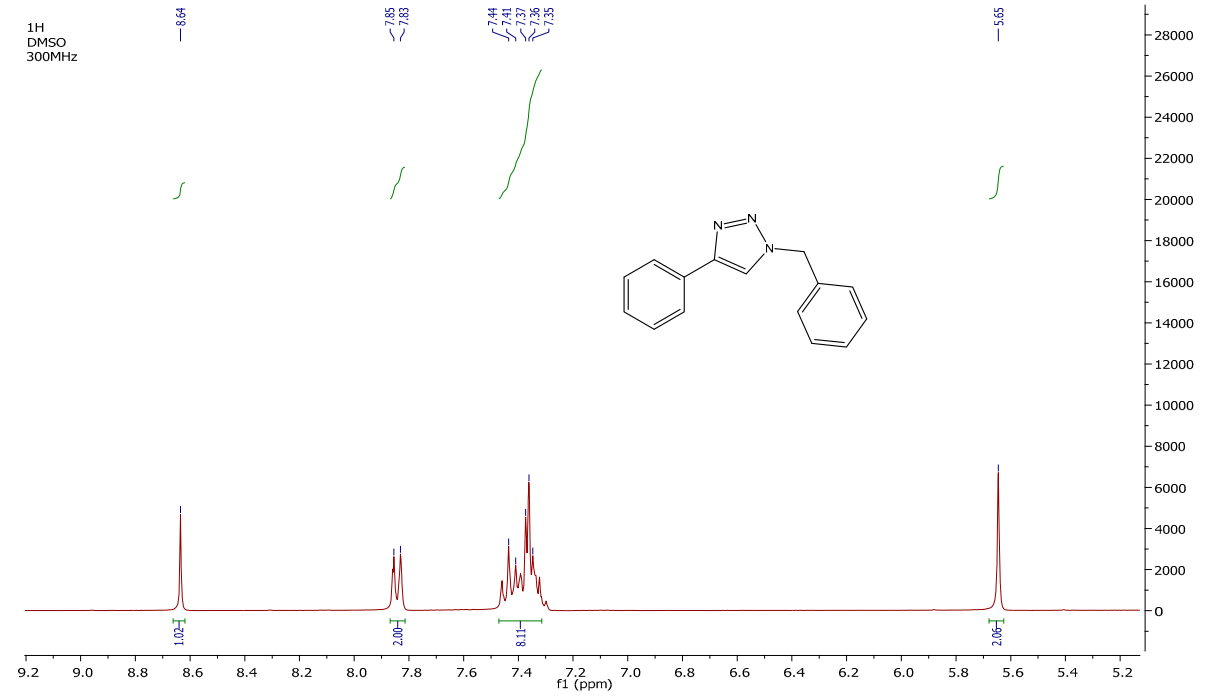
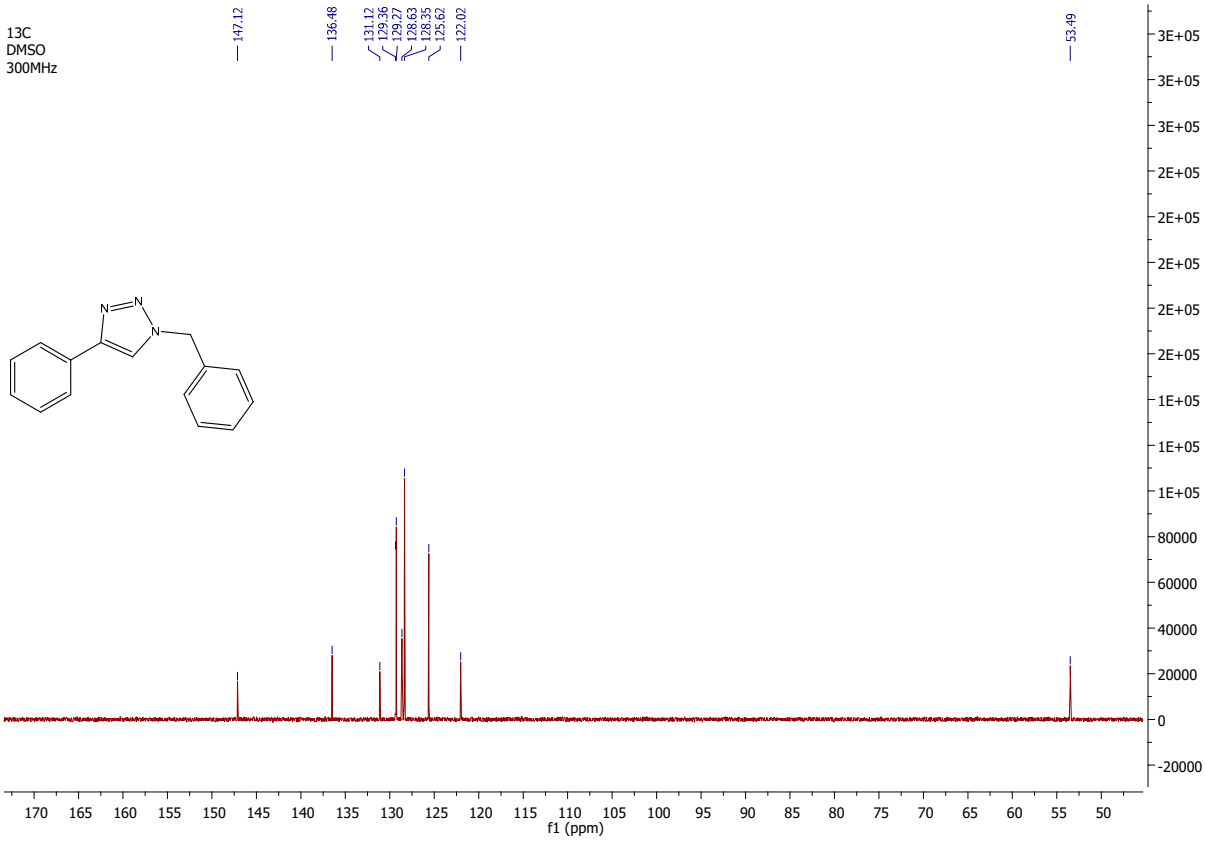
3. ^{1}H, ^{13}C and DEPT NMR spectra of 1,4-disubstituted 1,2,3-triazoles





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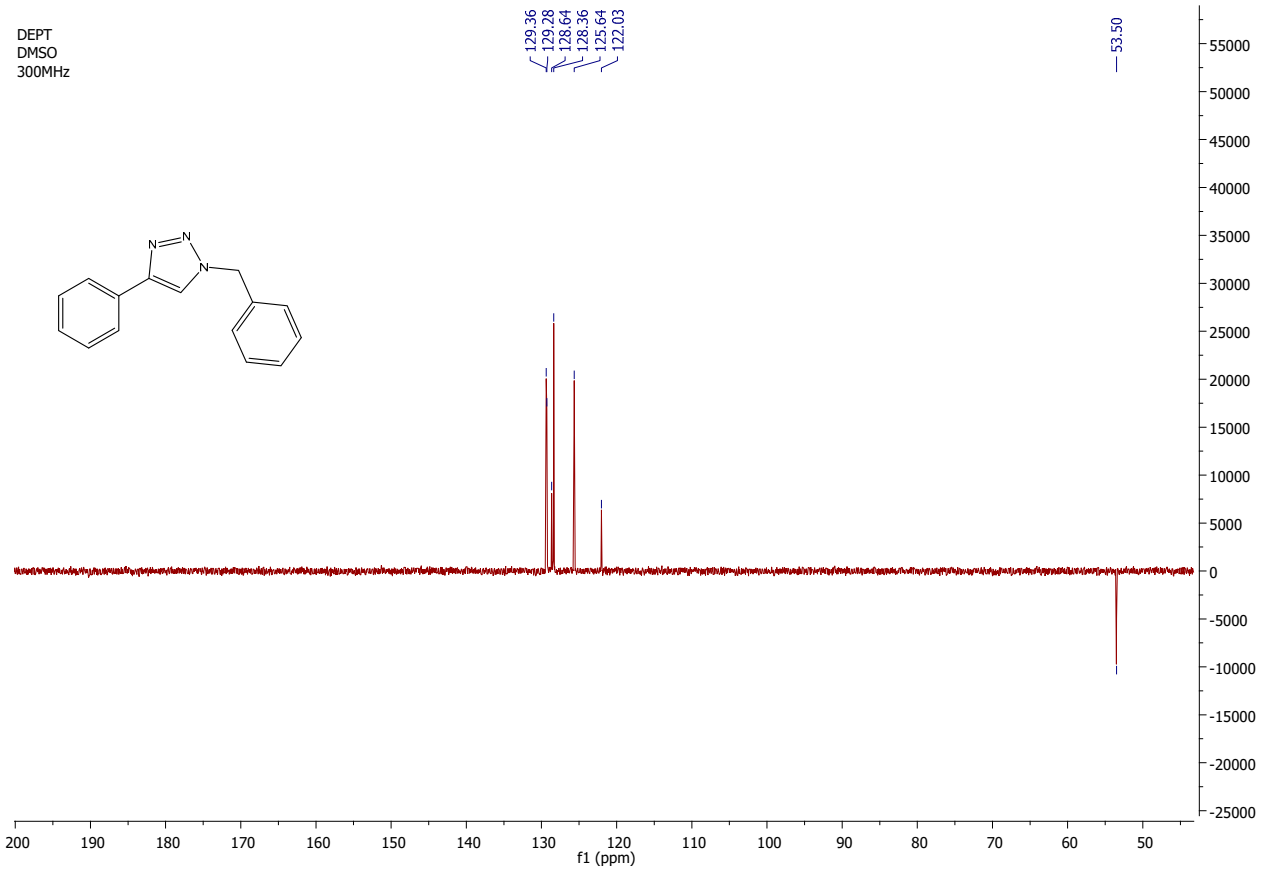

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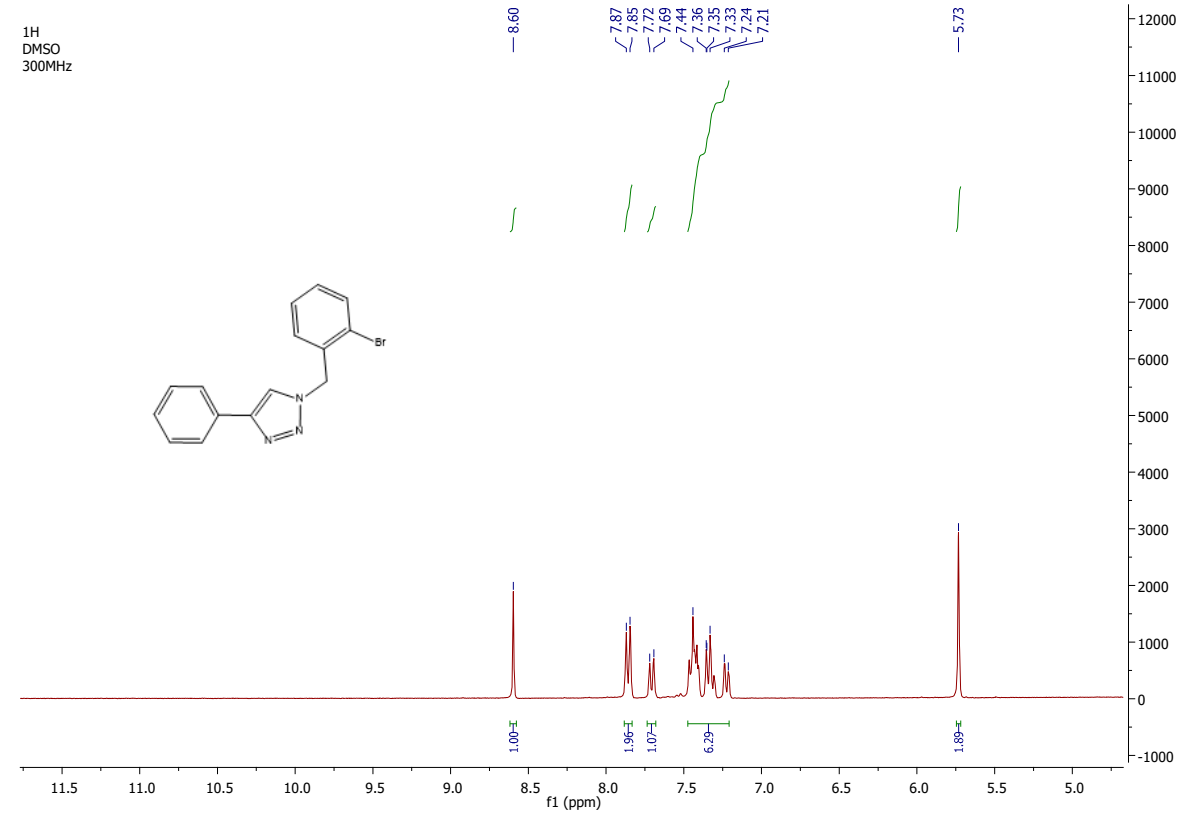

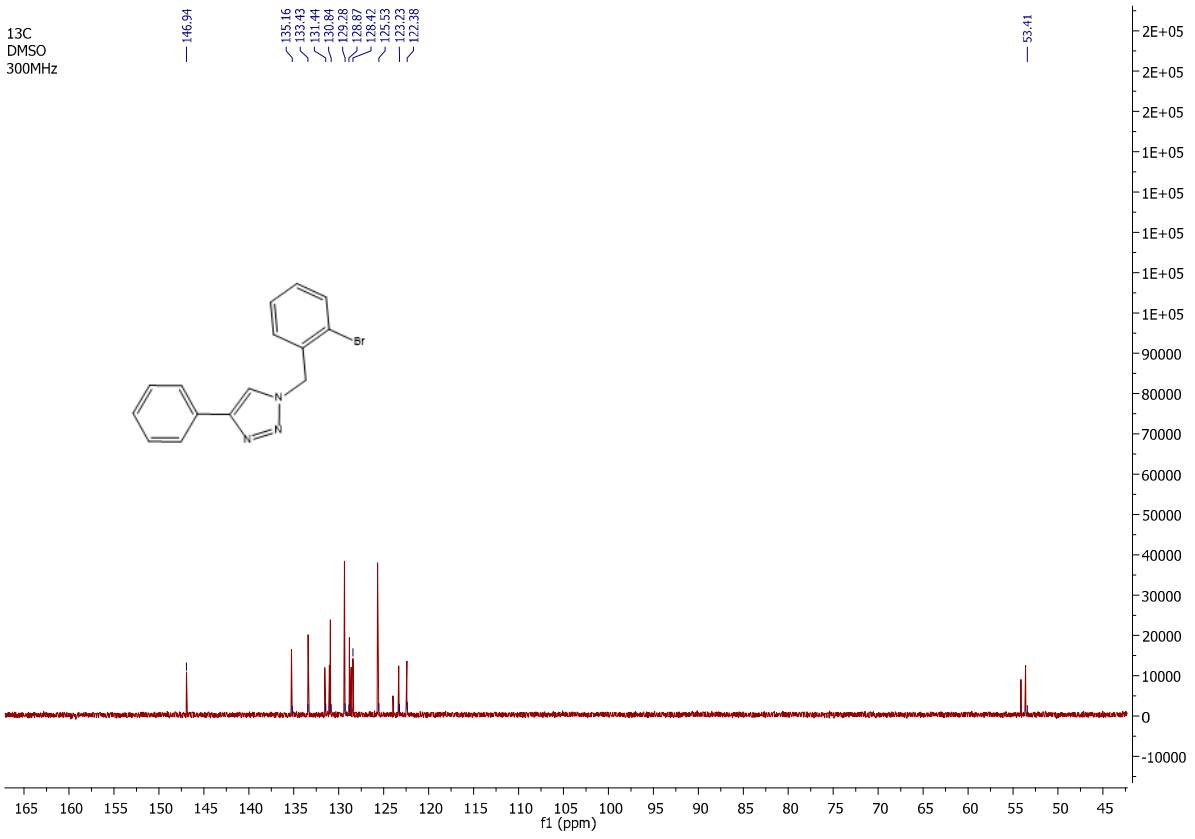

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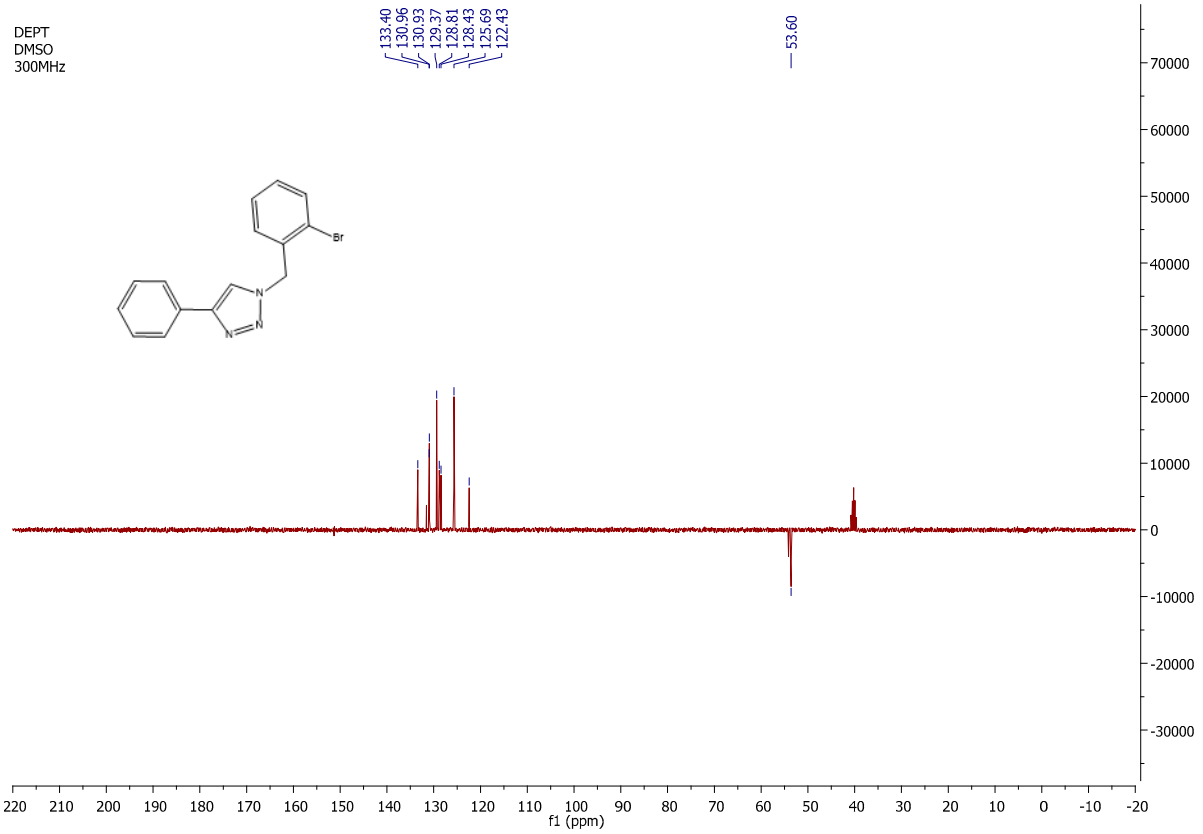

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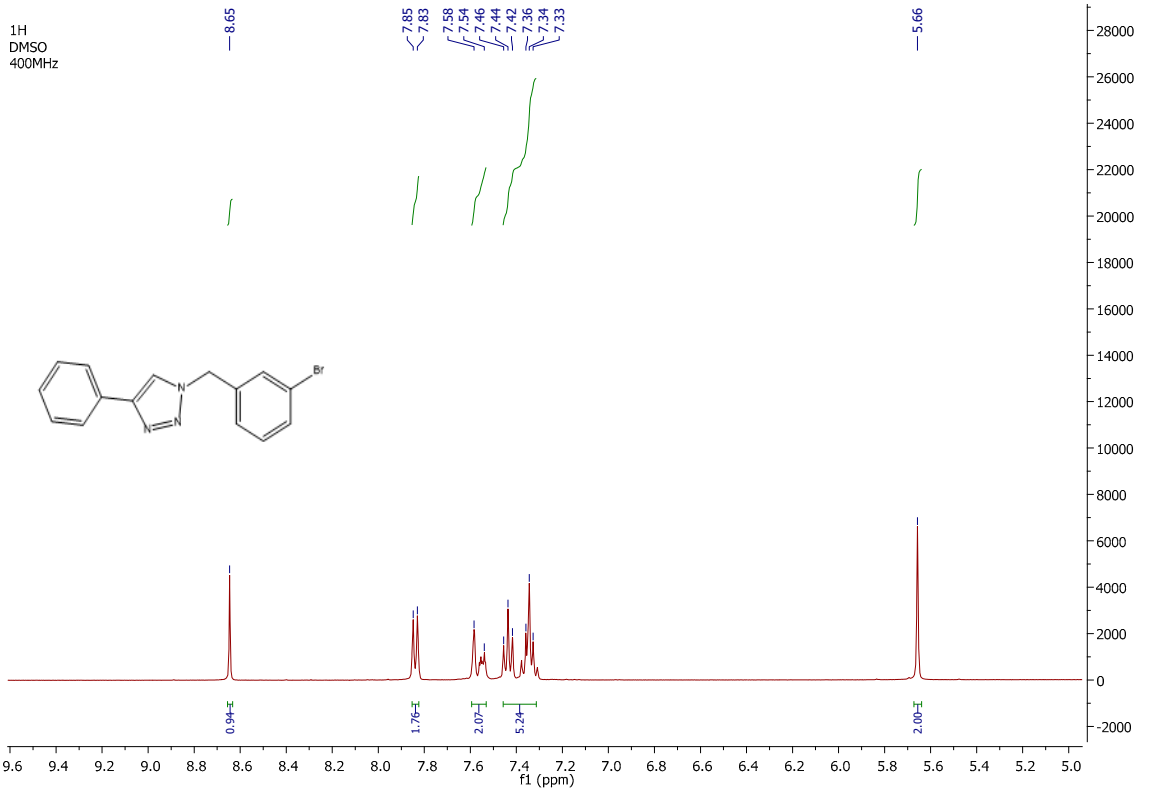

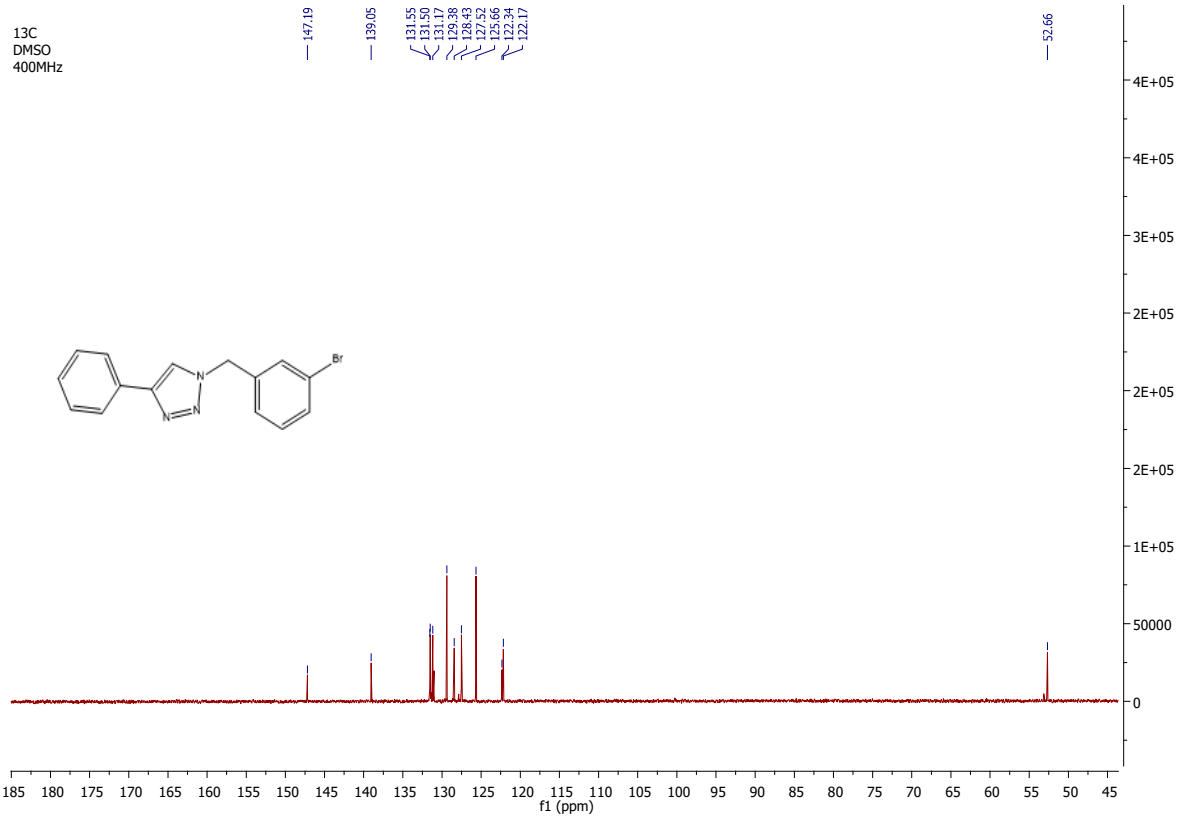

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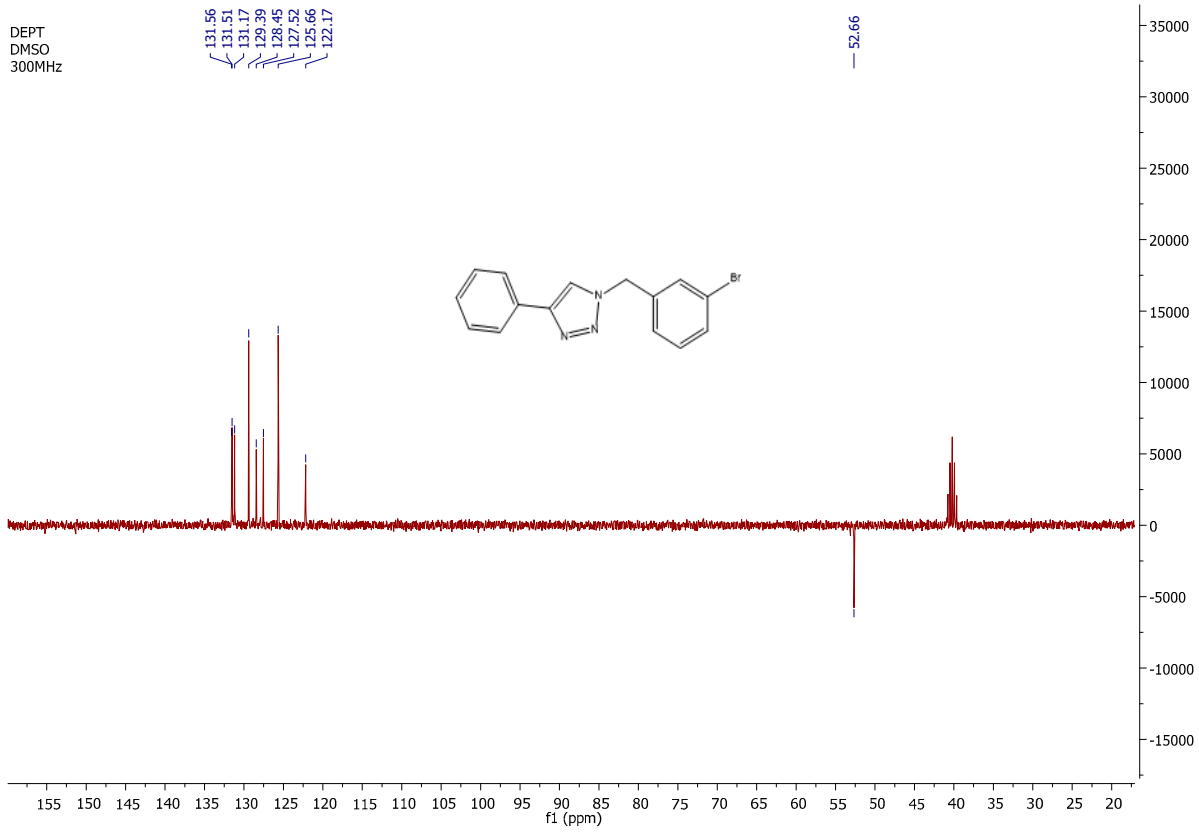

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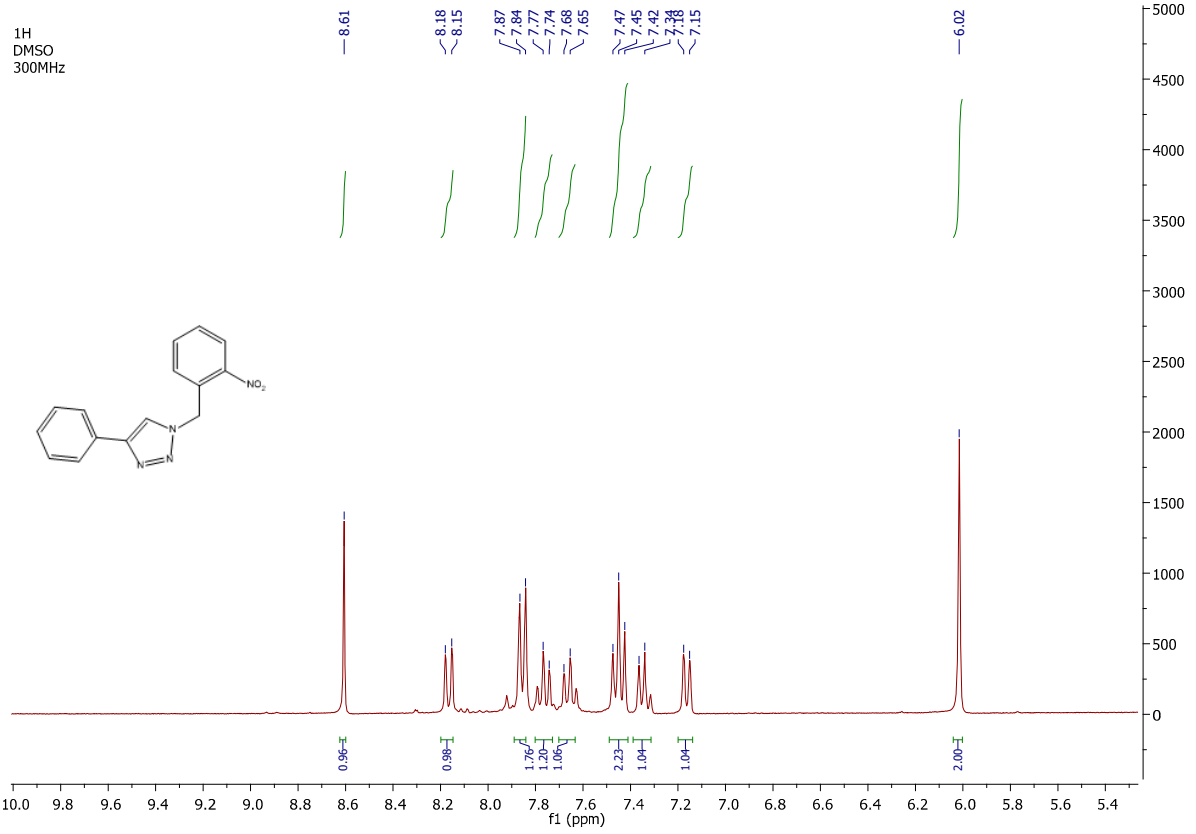

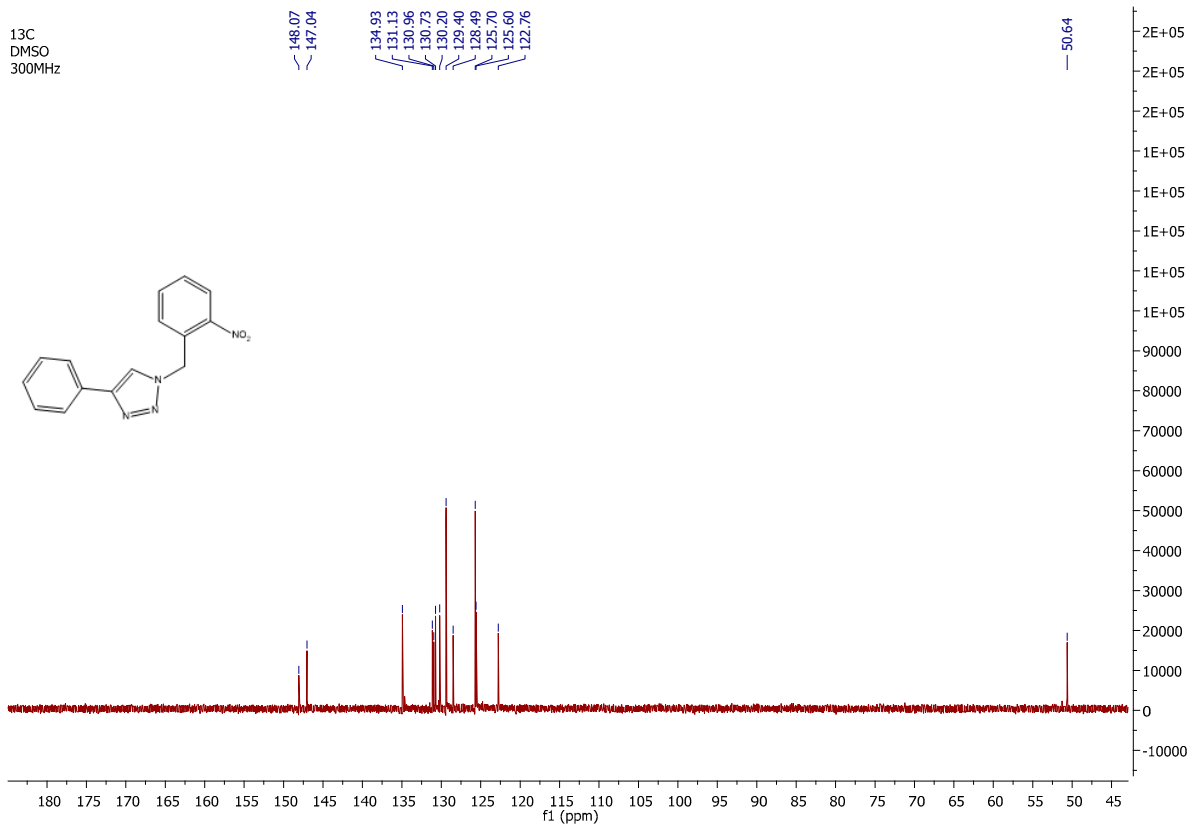

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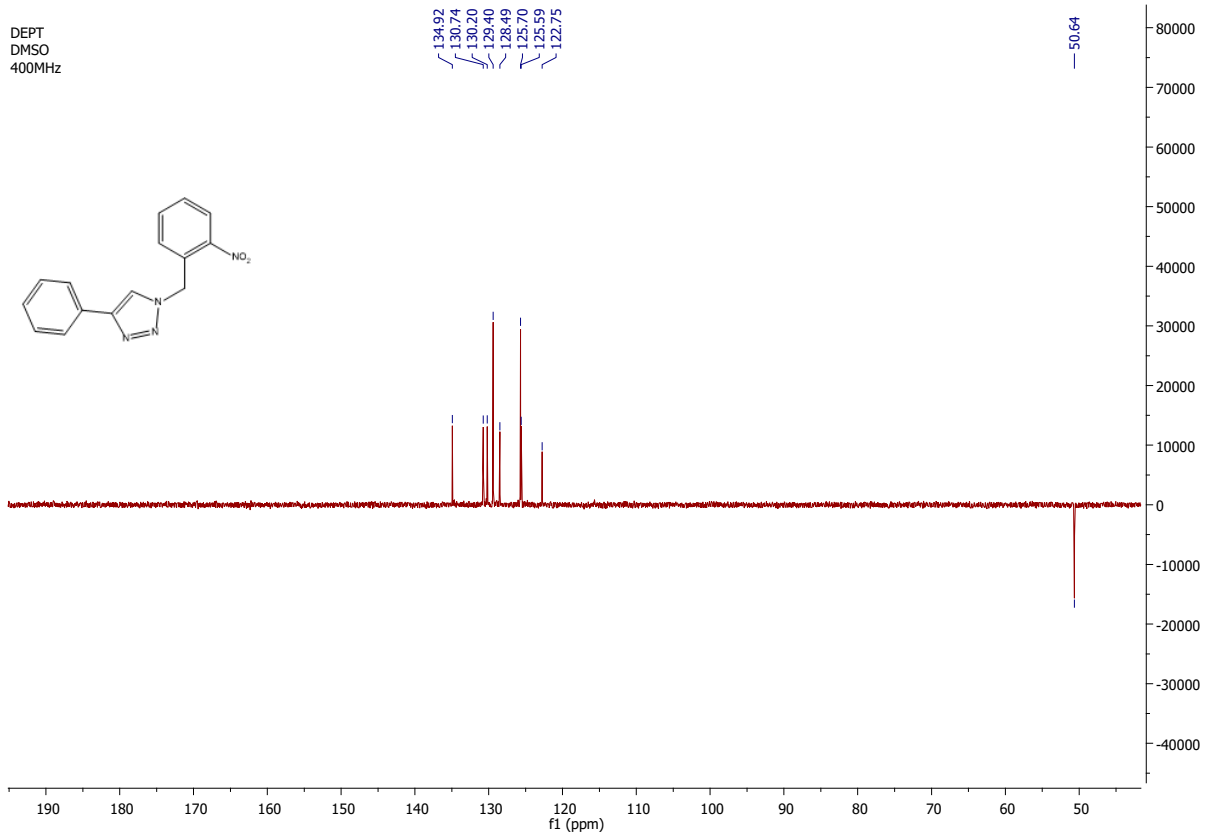

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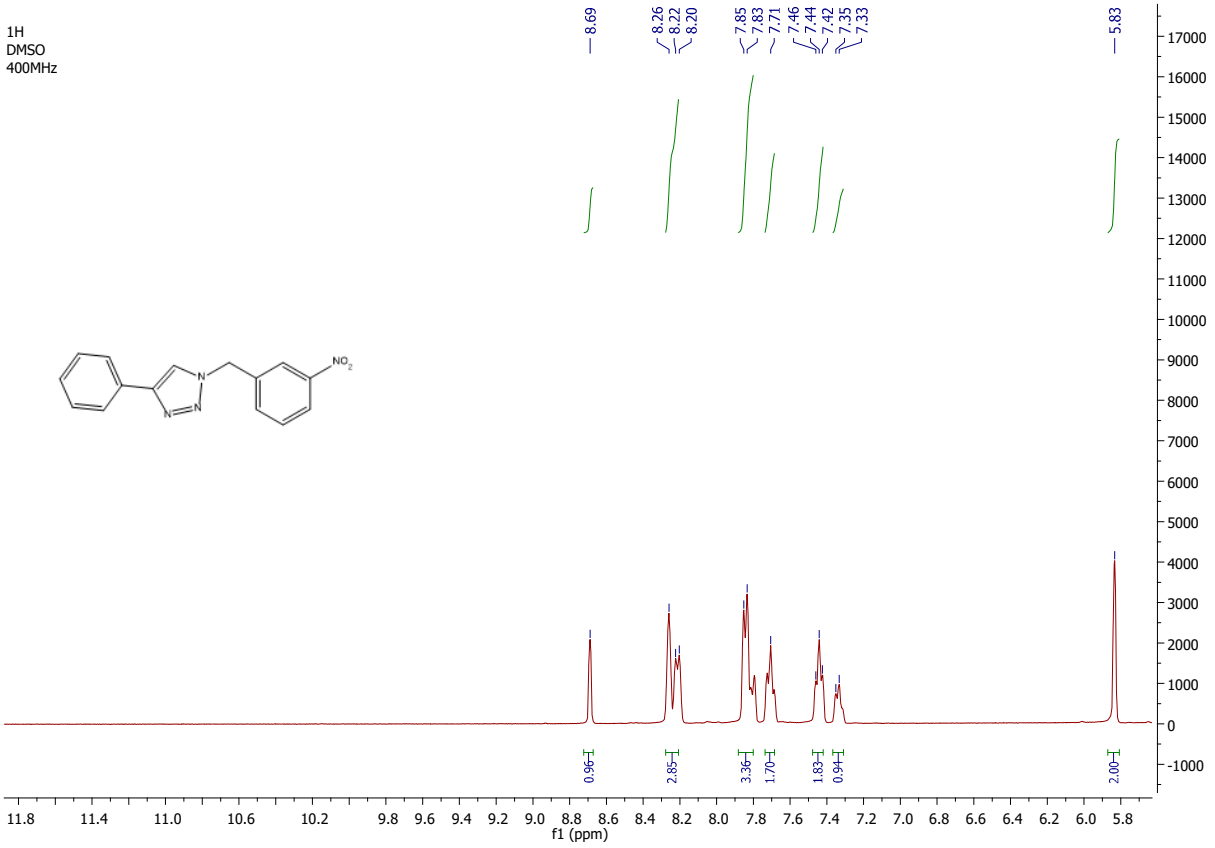

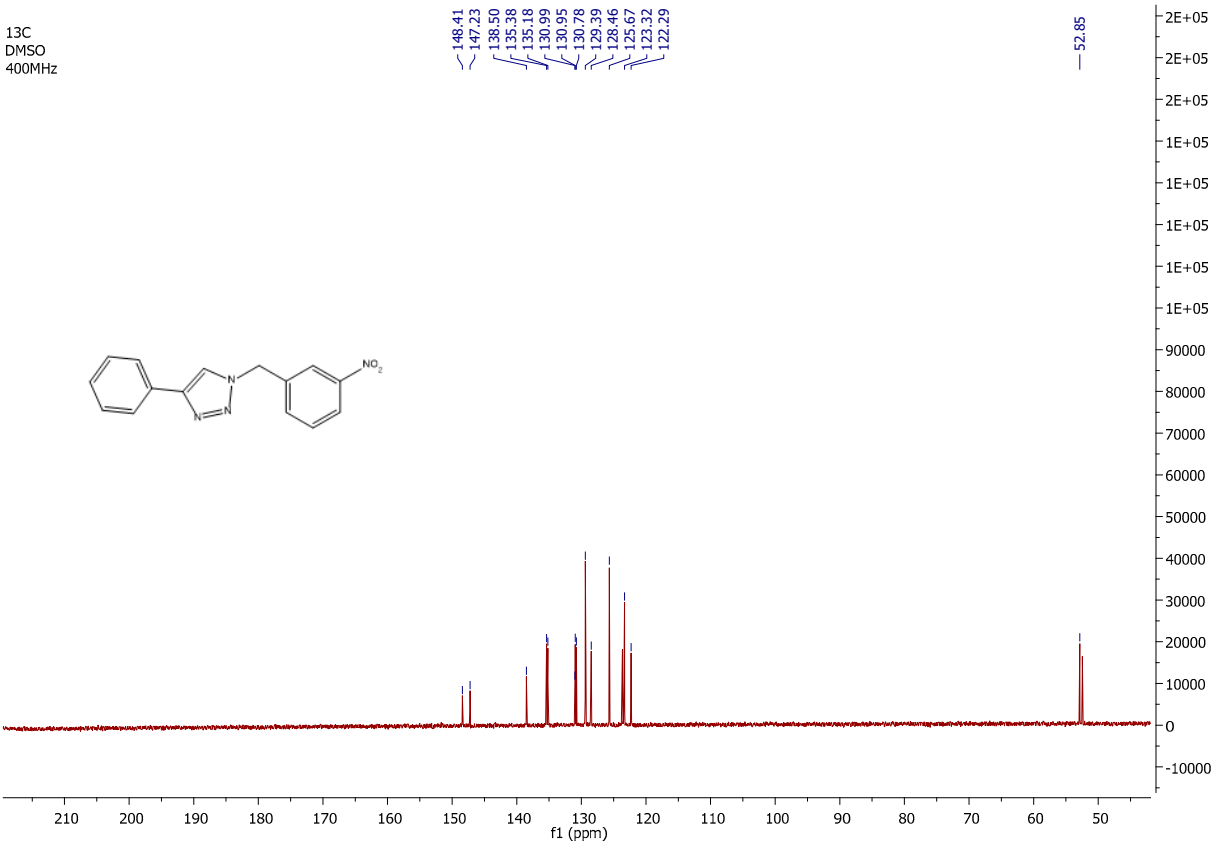

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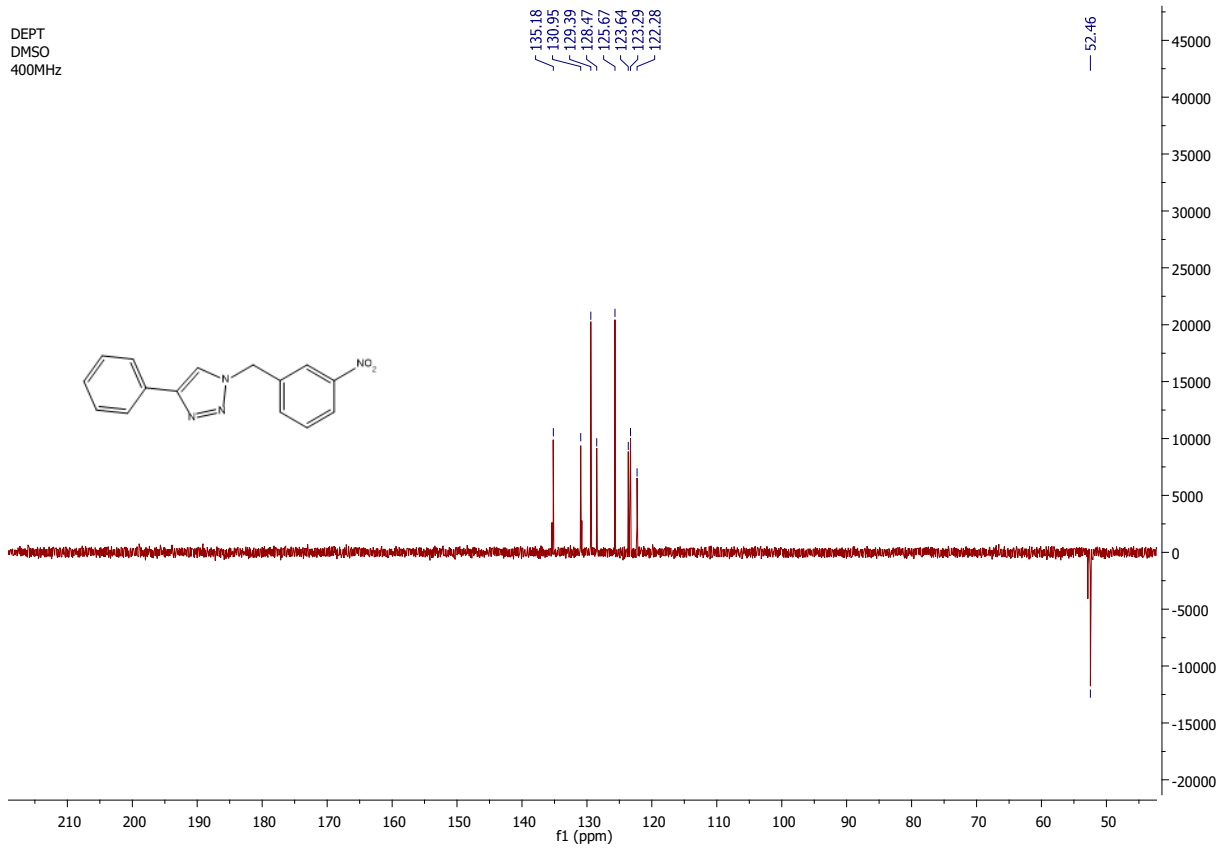

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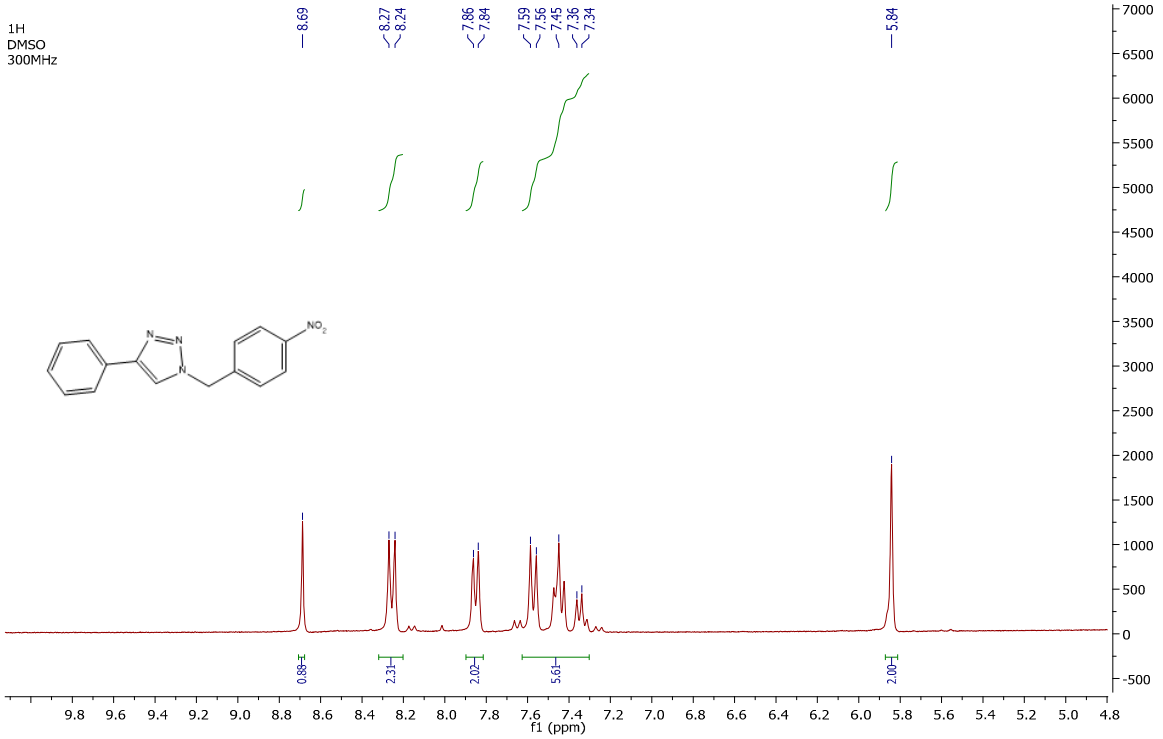

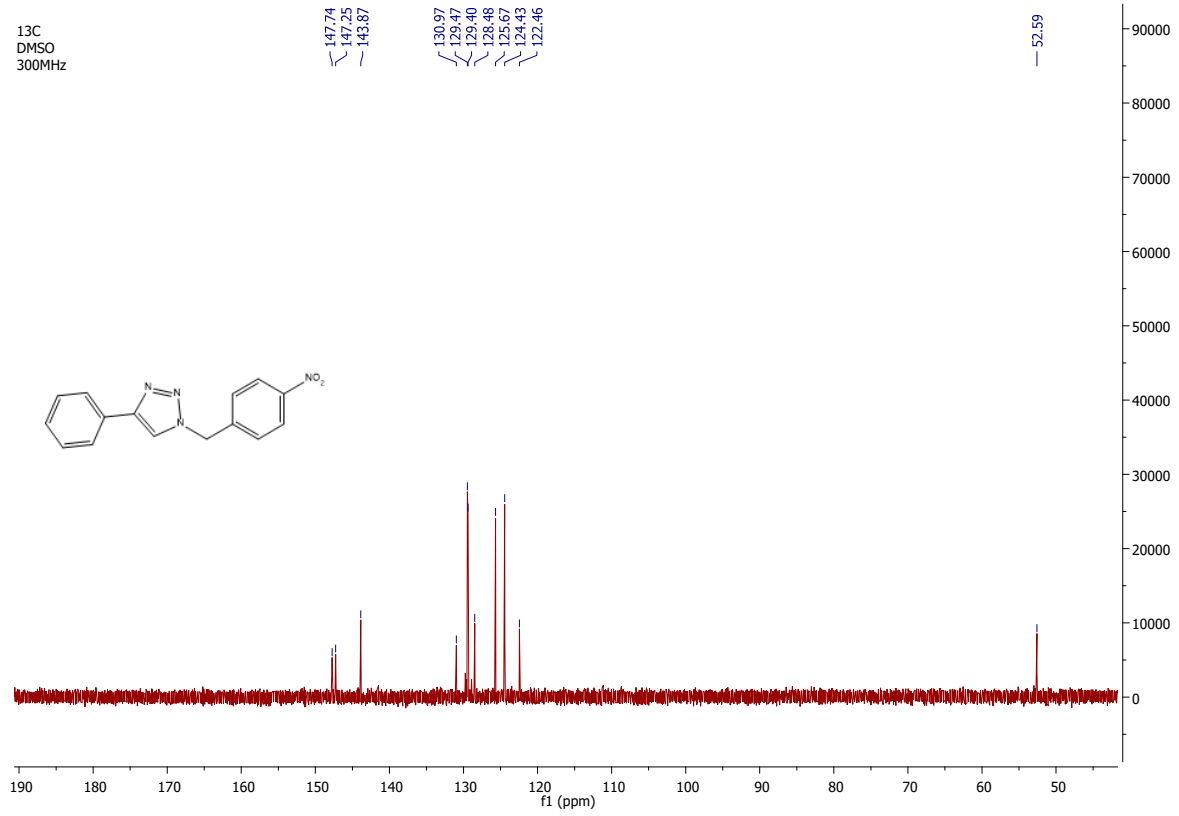

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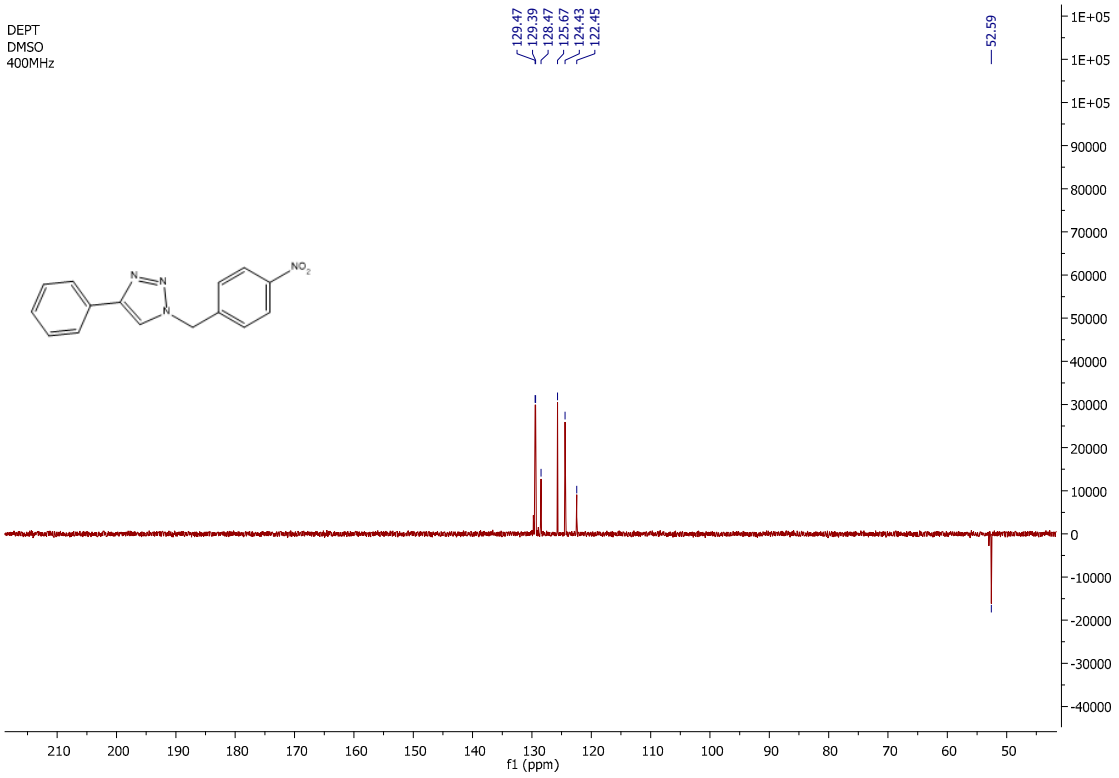

4. ESI(+) MS Spectra of 1,2,3-triazoles

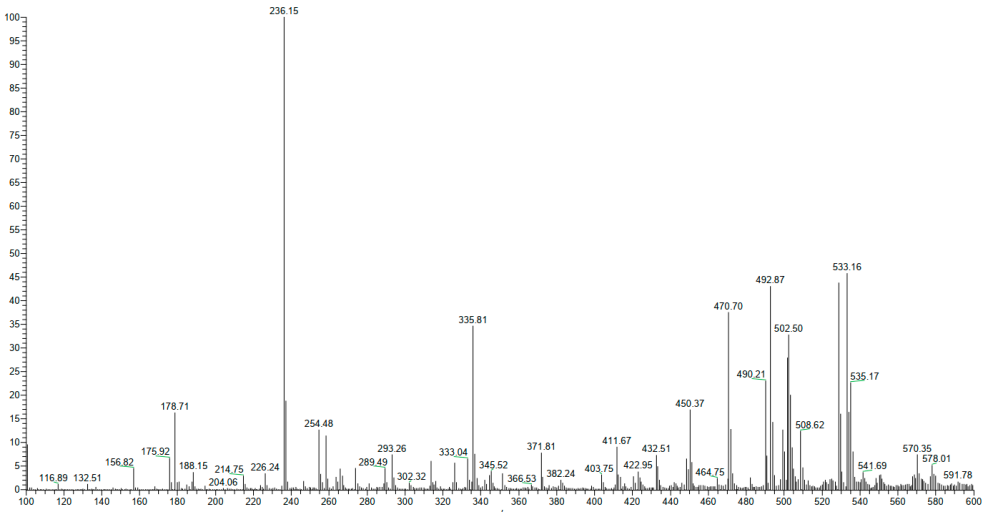

Figure S1: ESI-MS$^+$ spectrum of 1-benzyl-4-phenyl-1H-1,2,3-triazole.

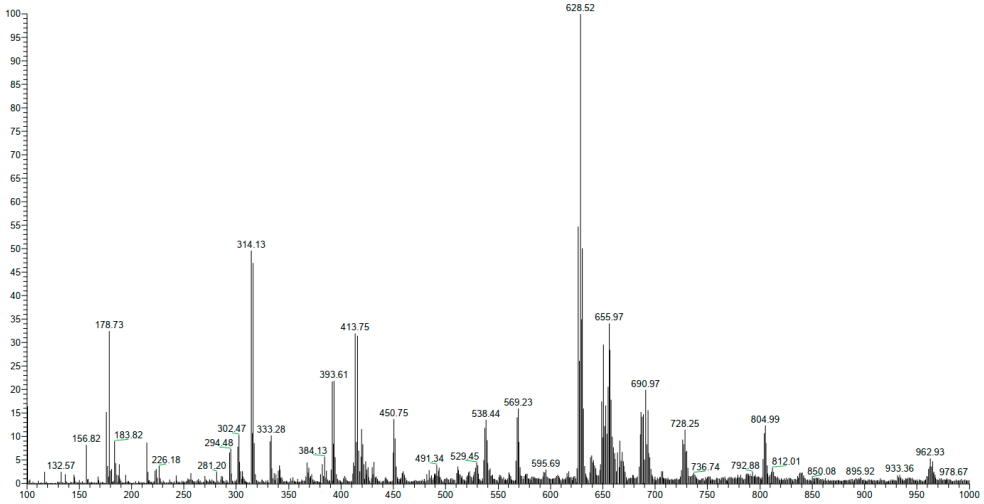

Figure S2: ESI-MS$^+$ spectrum of bromobenzyl-4-phenyl-1H-1,2,3-triazole.

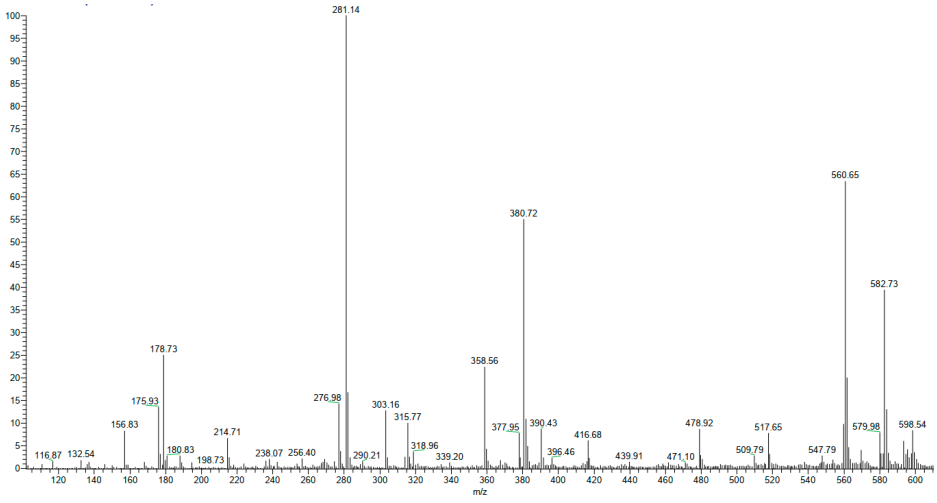

Figure S3: ESI-MS$^+$ spectrum of nitrobenzyl-4-phenyl-1H-1,2,3-triazole.

5. FTIR Spectra of 1,2,3-triazoles

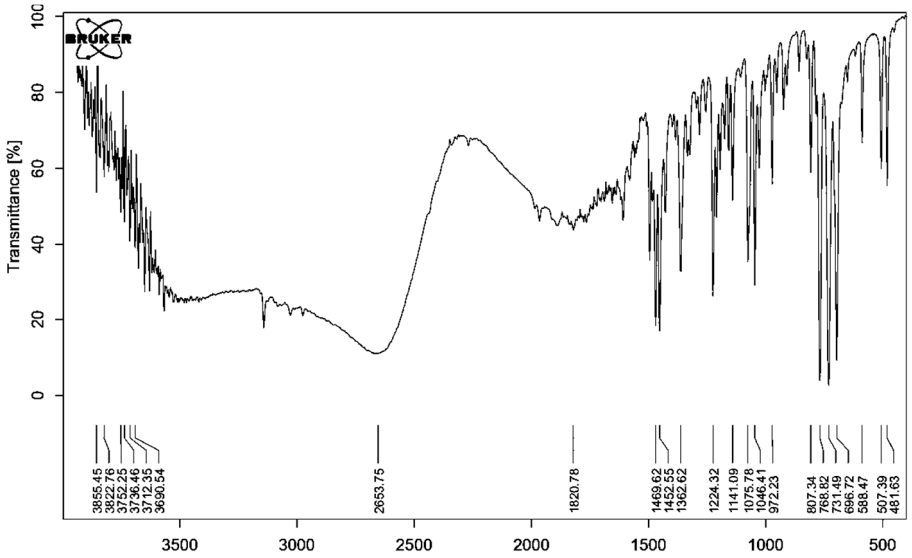

Figure S4: FTIR spectrum of 1-benzyl-4-phenyl-1H-1,2,3-triazole.

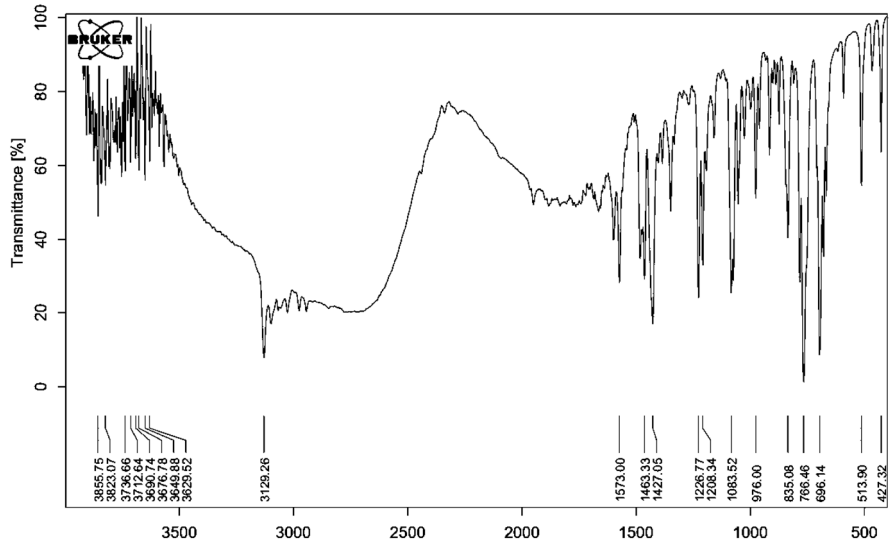

Figure S5: FTIR spectrum of bromobenzyl-4-phenyl-1H-1,2,3-triazole.

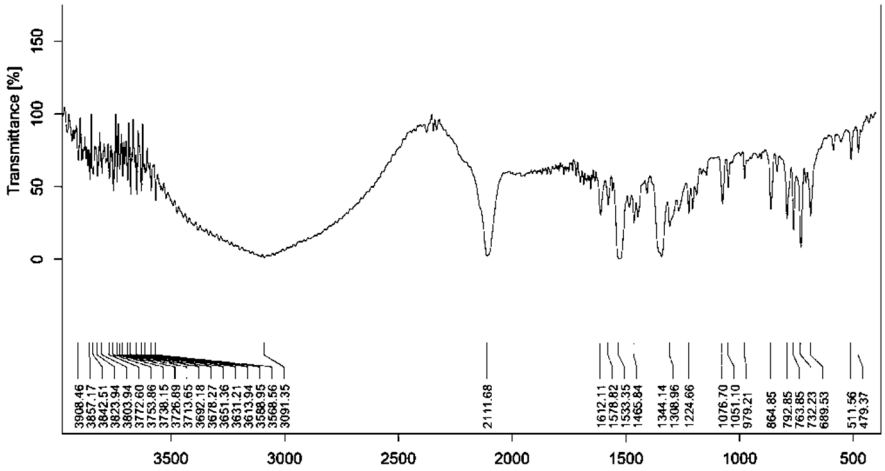

Figure S6: FTIR spectrum of nitrobenzyl-4-phenyl-1H-1,2,3-triazole.

6. FTIR Spectra of CNT-ox-Na materials (note: Based on Ref. 41-44, the 2000-400 cm^{-1} spectral range is commonly reported since this region contains absorption bands which are associated with oxygen surface groups)

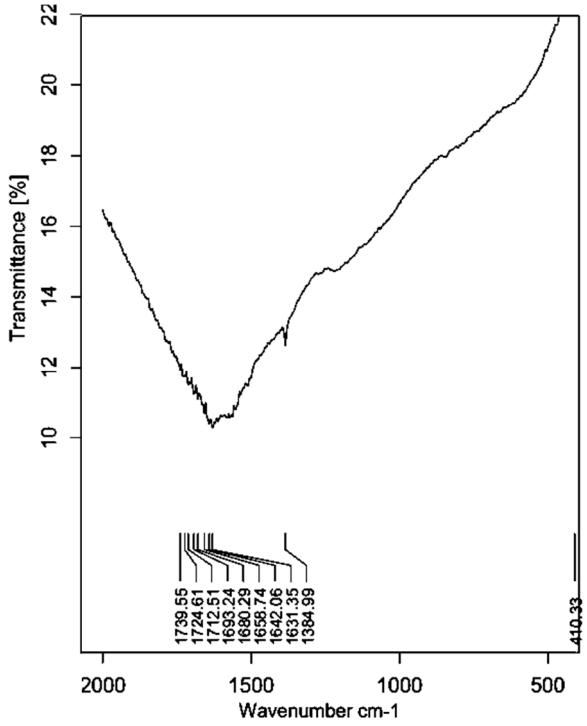

Figure S7: FTIR spectrum of CNT-ox-Na support (2000-400 cm^{-1}).

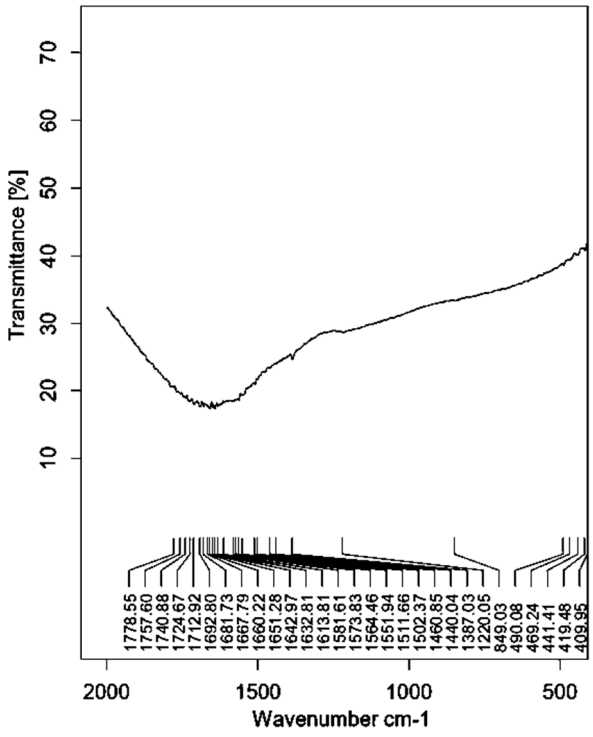

Figure S8: FTIR spectrum of **2**_CNT-ox-Na (2000-400 cm^{-1}).

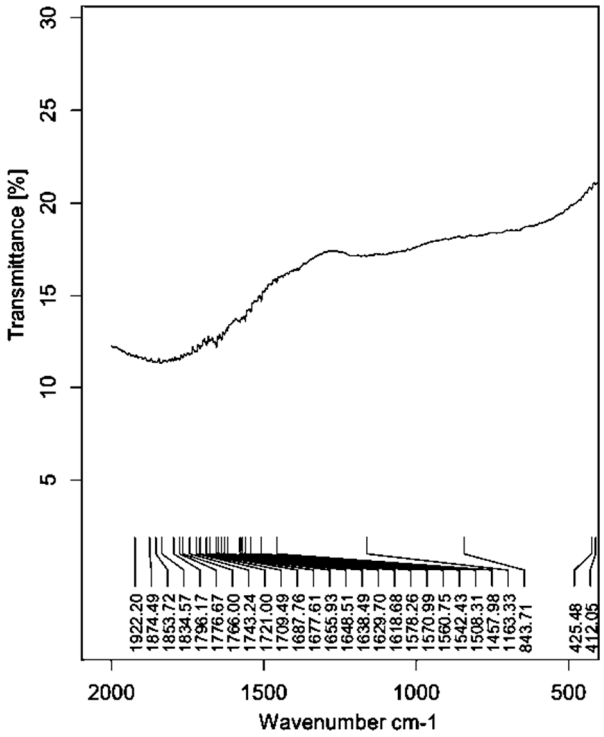

Figure S9: FTIR spectrum of **4**_CNT-ox-Na (2000-400 cm^{-1}).

7. Plausible anchorage of Cu(I)-phosphine complexes on carbon materials (Complex **2** as model for illustrative purposes)

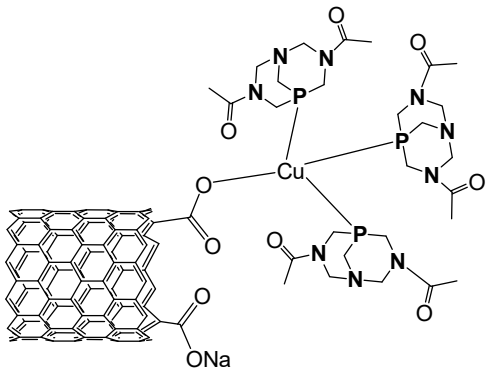

Figure S10: Coordination at the Cu centre through a carboxylate group upon replacement of an iodo ligand.

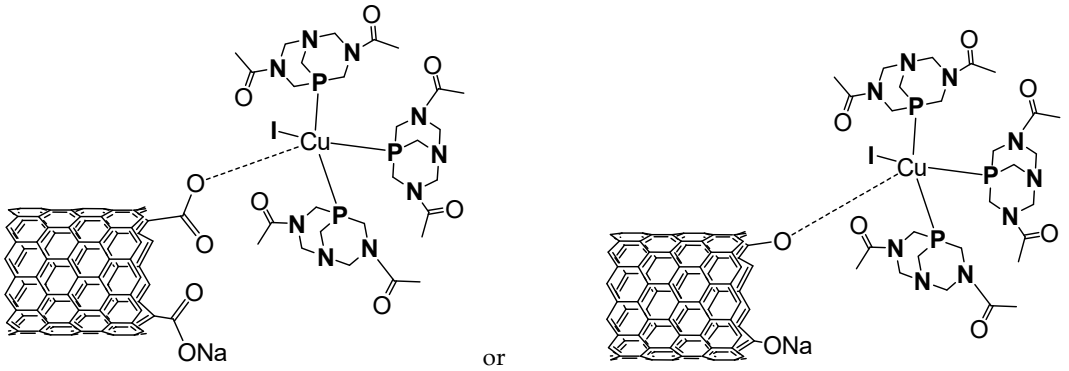

Figure S11: Coordination at the Cu centre through a carboxylate or a phenolate group.

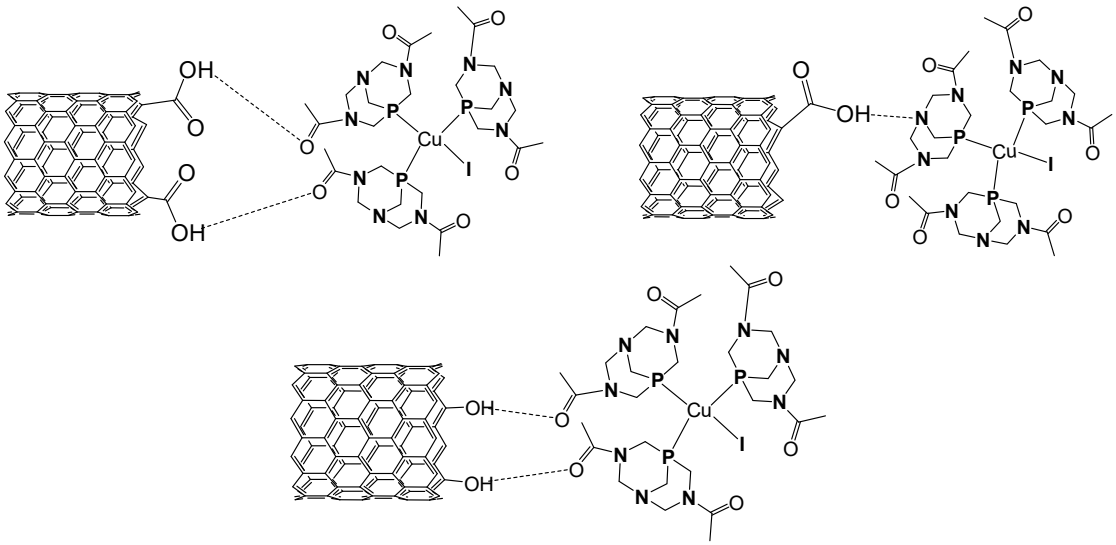

Figure S12: Via hydrogen bonding from a carboxylic or a phenolic group.

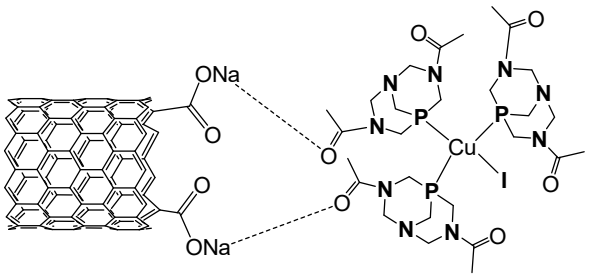

Figure S13: Via ionic interactions.