

Supplementary Information

Raney Ni Catalyzed Azide-Alkyne Cycloaddition Reaction

H. Surya Prakash Rao* and Guravaiah Chakibanda

Department of Chemistry, Pondicherry University, Puducherry – 605 014, India.

E-mail: hspr.che@pondiuni.edu.in

Index

- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(hexyloxymethyl)-1-phenyl-1*H*-1,2,3-triazole **3e**. S3
- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-((but-1-ynyloxy)methyl)-1-phenyl-1*H*-1,2,3-triazole **3f**. S4
- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(benzyloxymethyl)-1-phenyl-1*H*-1,2,3-triazole **3g**. S5
- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(cyclohexyloxymethyl)-1-phenyl-1*H*-1,2,3-triazole **3h**. S6
- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-((4-*tert*-butylphenoxy) methyl)-1-hexyl-1*H*-1,2,3-triazole **3n**. S7
- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 1-benzyl-4-(benzyloxymethyl)-1*H*-1,2,3-triazole, 5-(benzyloxymethyl)-1-bromo-1*H*-1,2,3-triazole (1:1) **3o** and **3s**. S8
- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(benzyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole, 5-(benzyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole **3p**, **3t**. S9
- ¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of

1-benzyl-4-(cyclohexyloxymethyl)-1*H*-1,2,3-triazole, 1-benzyl-5-(cyclohexyloxymethyl)-1*H*-1,2,3-triazole **3q**, **3u**. S10

¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(cyclohexyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole, 5-(cyclohexyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole **3r** and **3v**. S11

¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(benzyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole **3t**. S12

¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 1-benzyl-4-(cyclohexyloxymethyl)-1*H*-1,2,3-triazole **3u**. S13

¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(cyclohexyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole **3v**. S14

¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of (((3-deuteroprop-2-yn-1-yl)oxy)methyl)benzene **4**. S15

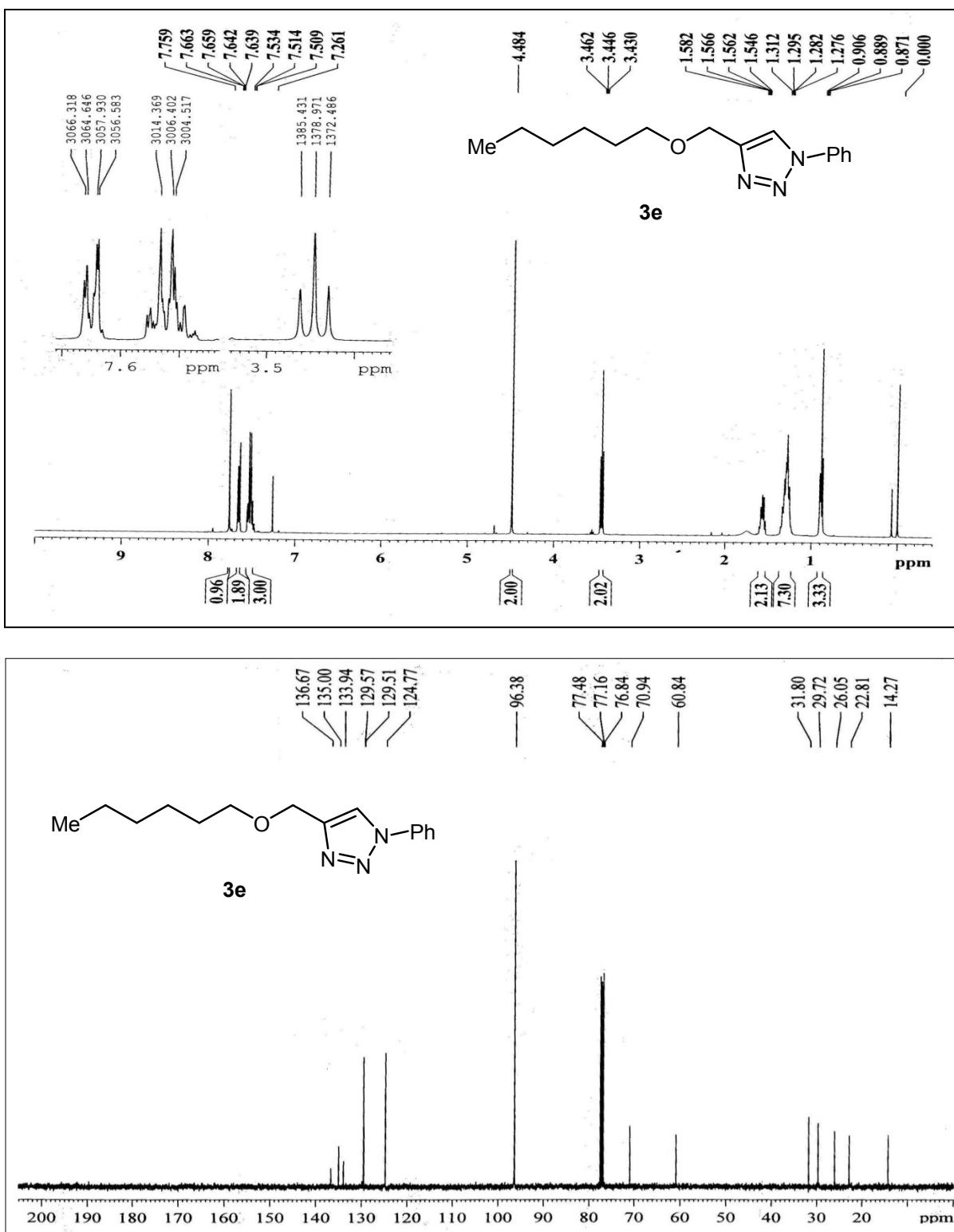
¹H (400 MHz, CCl₄:CDCl₃, 1:1) spectra of 4-(phenoxy methyl)-1-phenyl-1*D*-1,2,3-triazole **8**. S16

¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(1-(benzyloxy)cyclohexyl)-1-phenyl-1*H*-1,2,3-triazole **3x**. S17

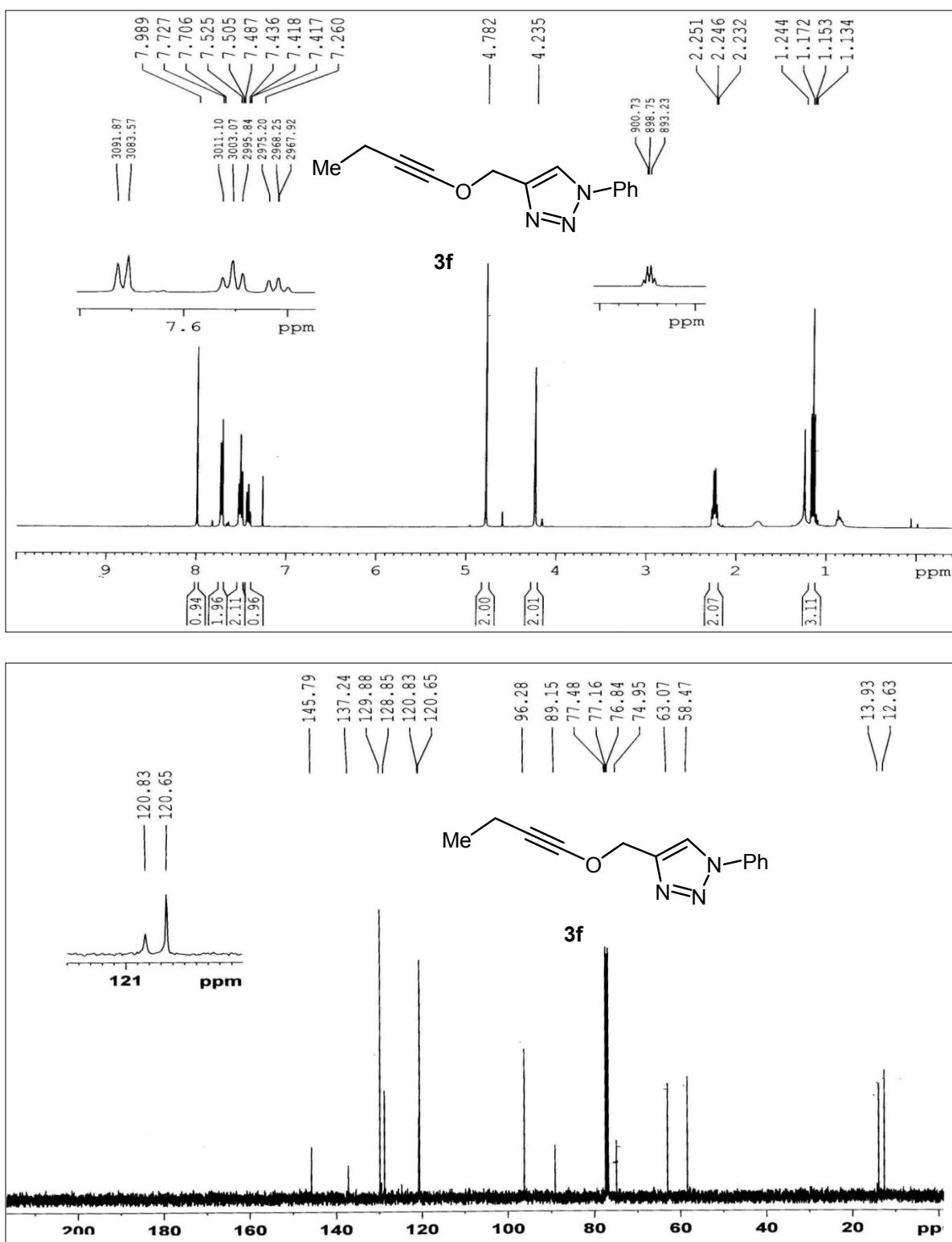
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of (1-phenyl-1*H*-1,2,3-triazol-4-yl)methanol **3y** and (1-phenyl-1*H*-1,2,3-triazol-5-yl)methanol **3z**. S18

¹H (400 MHz, CDCl₃) ¹³C (100 MHz, CDCl₃) and DEPT-135 (100 MHz, CDCl₃) NMR spectra of the crude cycloadduct from reaction of propargyl alcohol, phenyl azide and CuSO₄.5H₂O, sodium ascorbate in PEG-200 under MW irradiation (with PEG impurity). S19

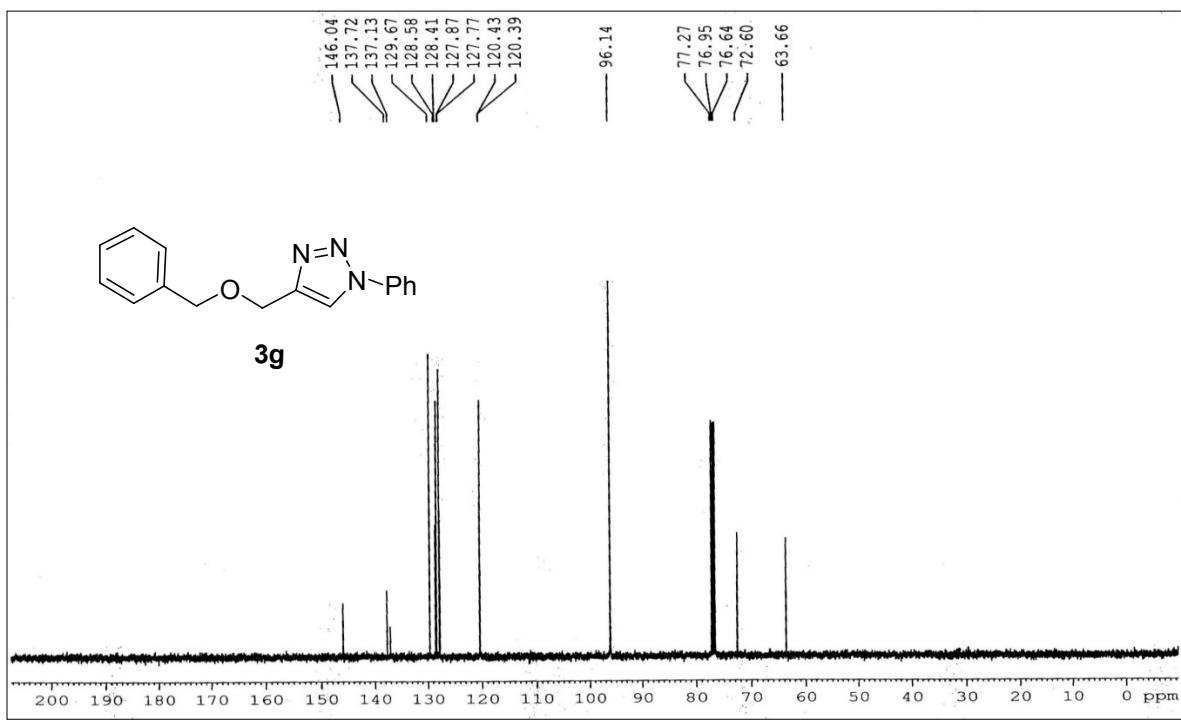
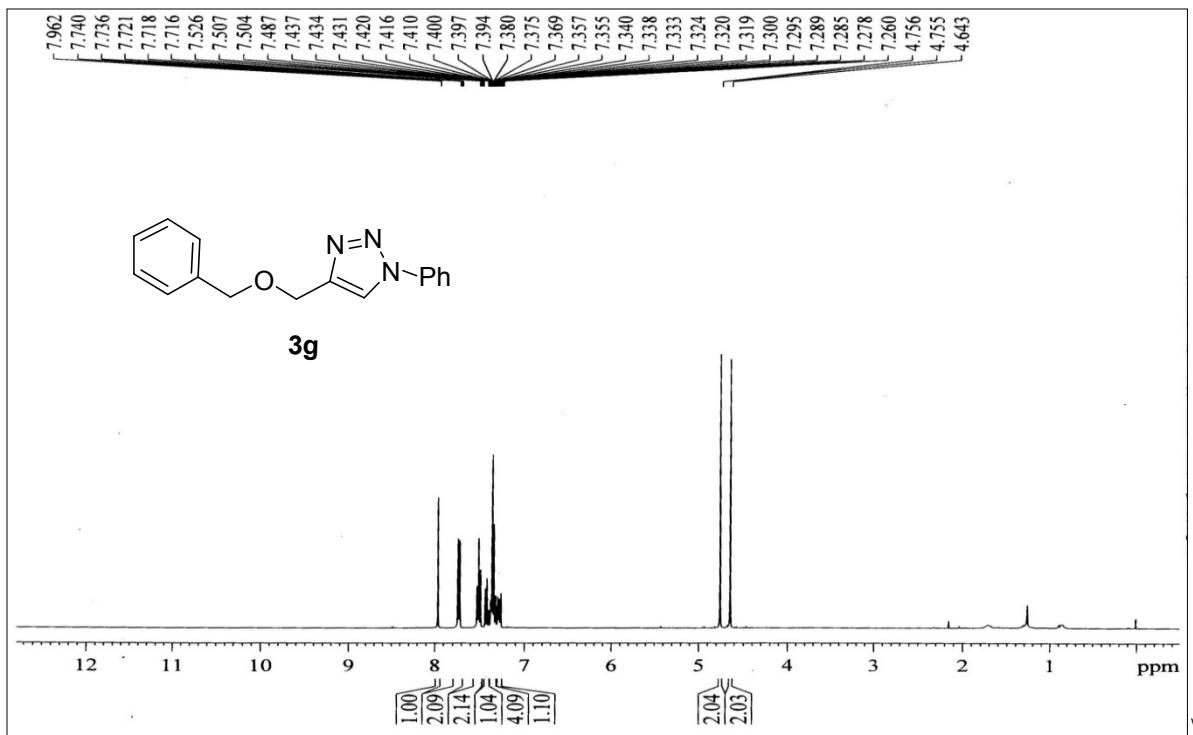
¹H (400 MHz, CDCl₃), ¹³C (100 MHz, CDCl₃) and DEPT-135 (100 MHz, CDCl₃) NMR spectra of the crude product from the reaction of propargyl alcohol, phenyl azide in PEG-200 under MW irradiation without any catalyst (with PEG impurity). S20



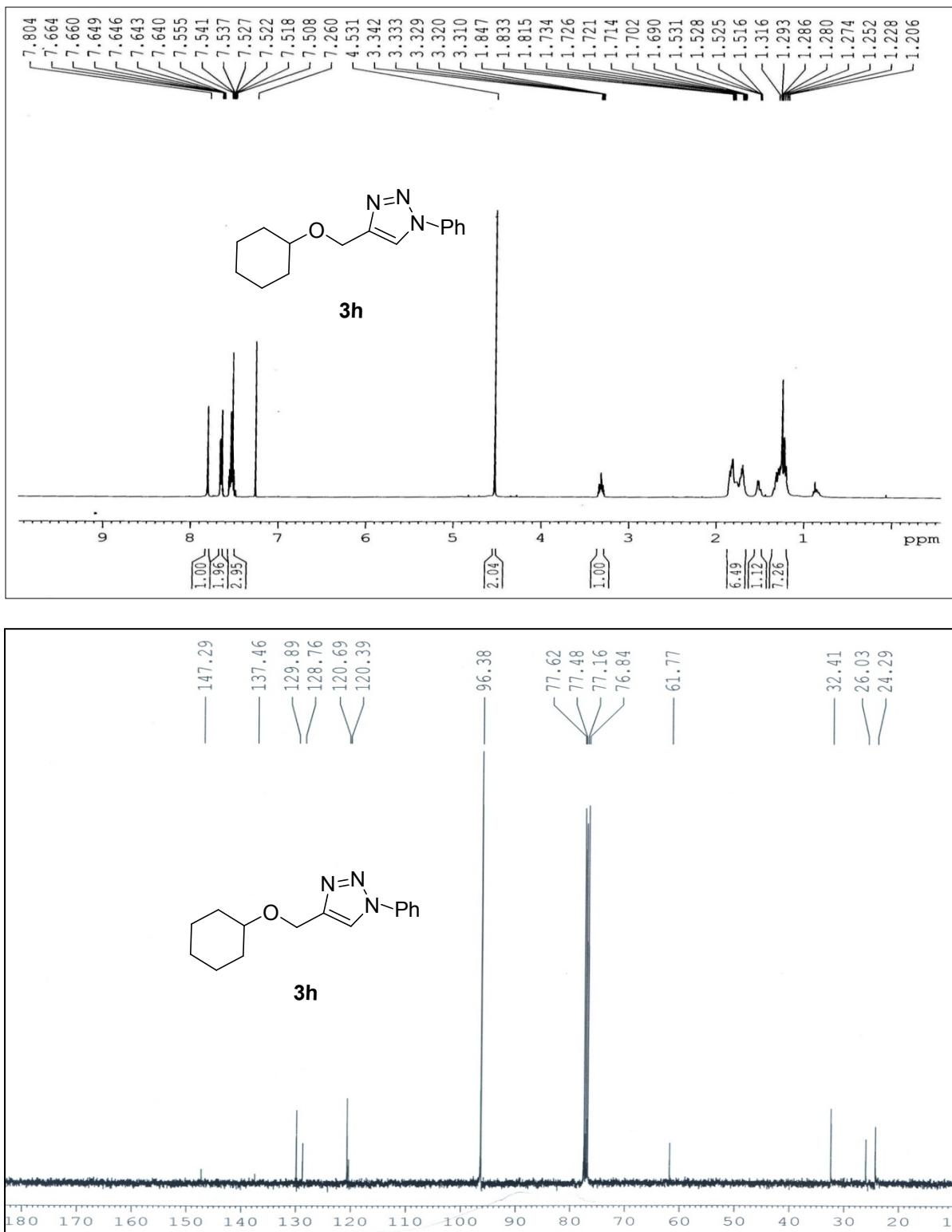
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(hexyloxymethyl)-1-phenyl-1*H*-1,2,3-triazole **3e**.



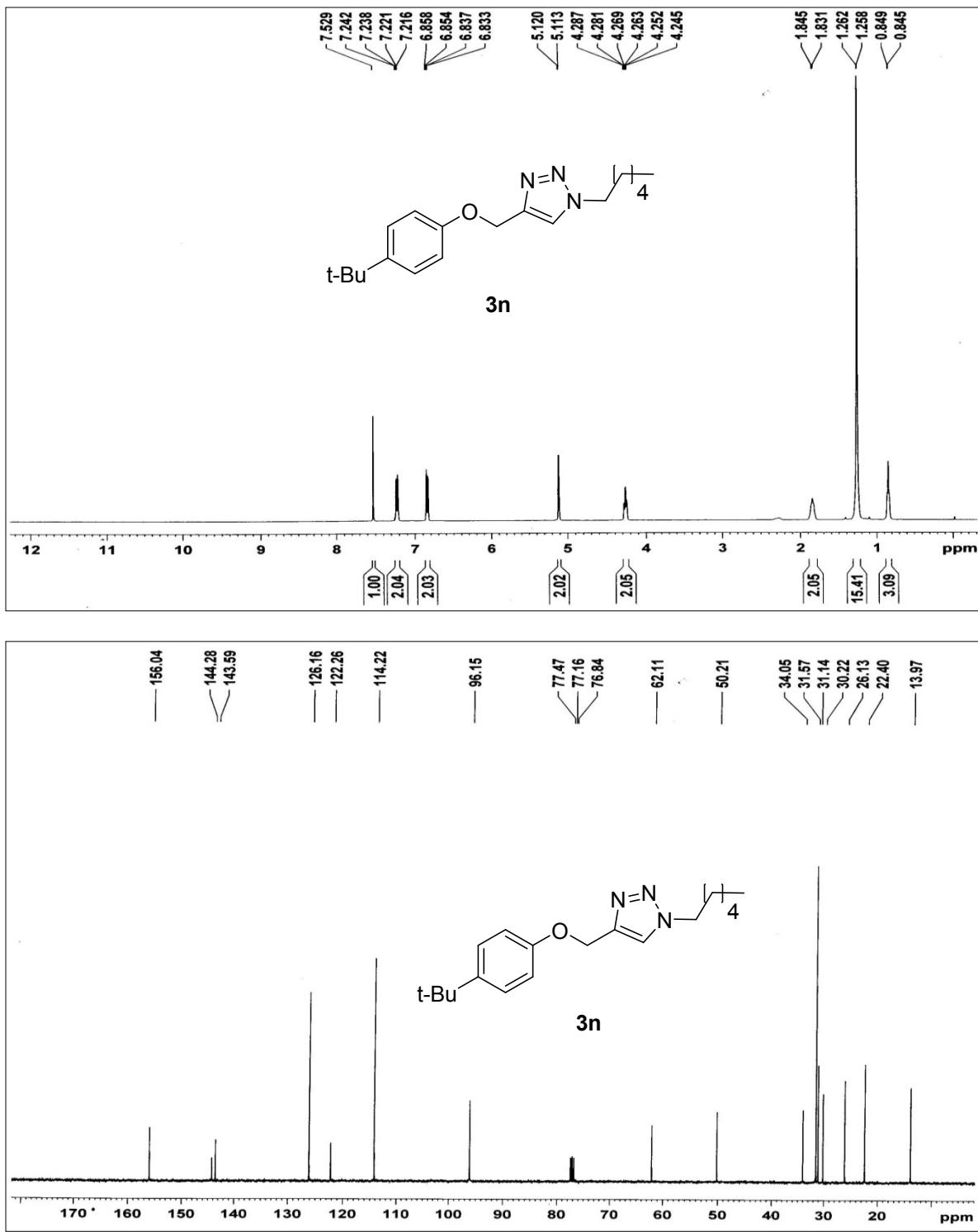
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-((but-1-ynyloxy)methyl)-1-phenyl-1*H*-1,2,3-triazole **3f**.



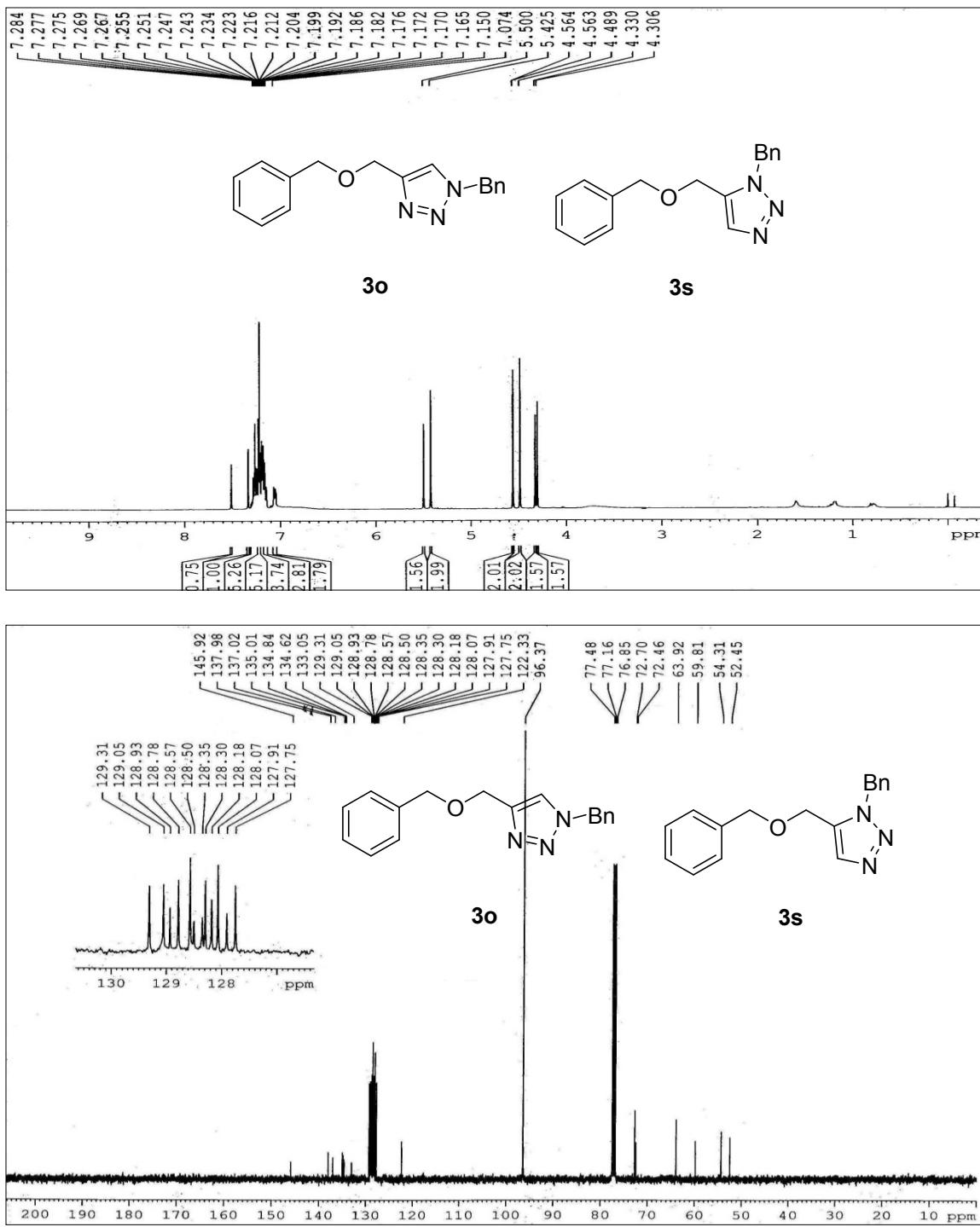
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(benzyloxymethyl)-1-phenyl-1*H*-1,2,3-triazole **3g**.



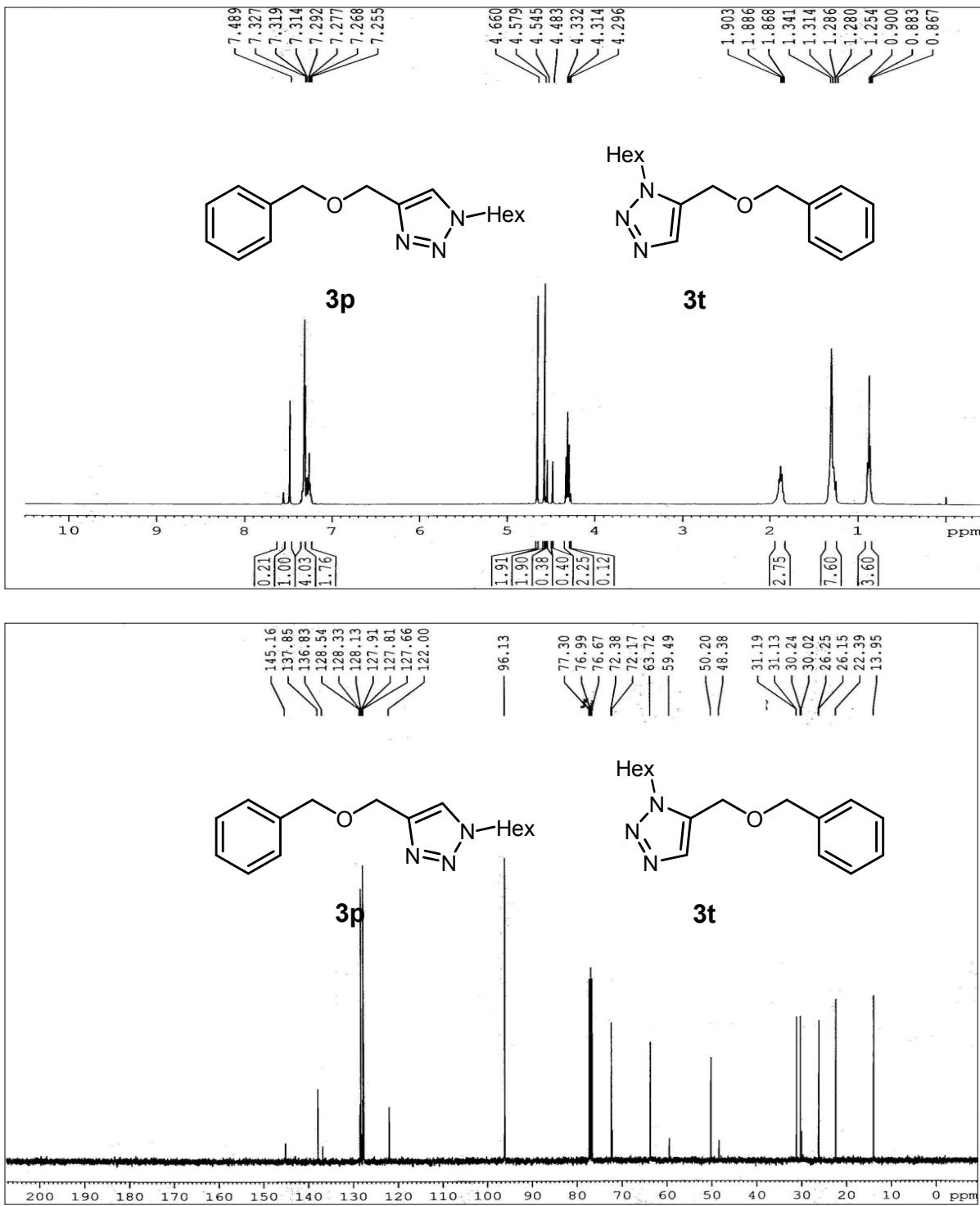
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(cyclohexyloxymethyl)-1-phenyl-1*H*-1,2,3-triazole **3h**.



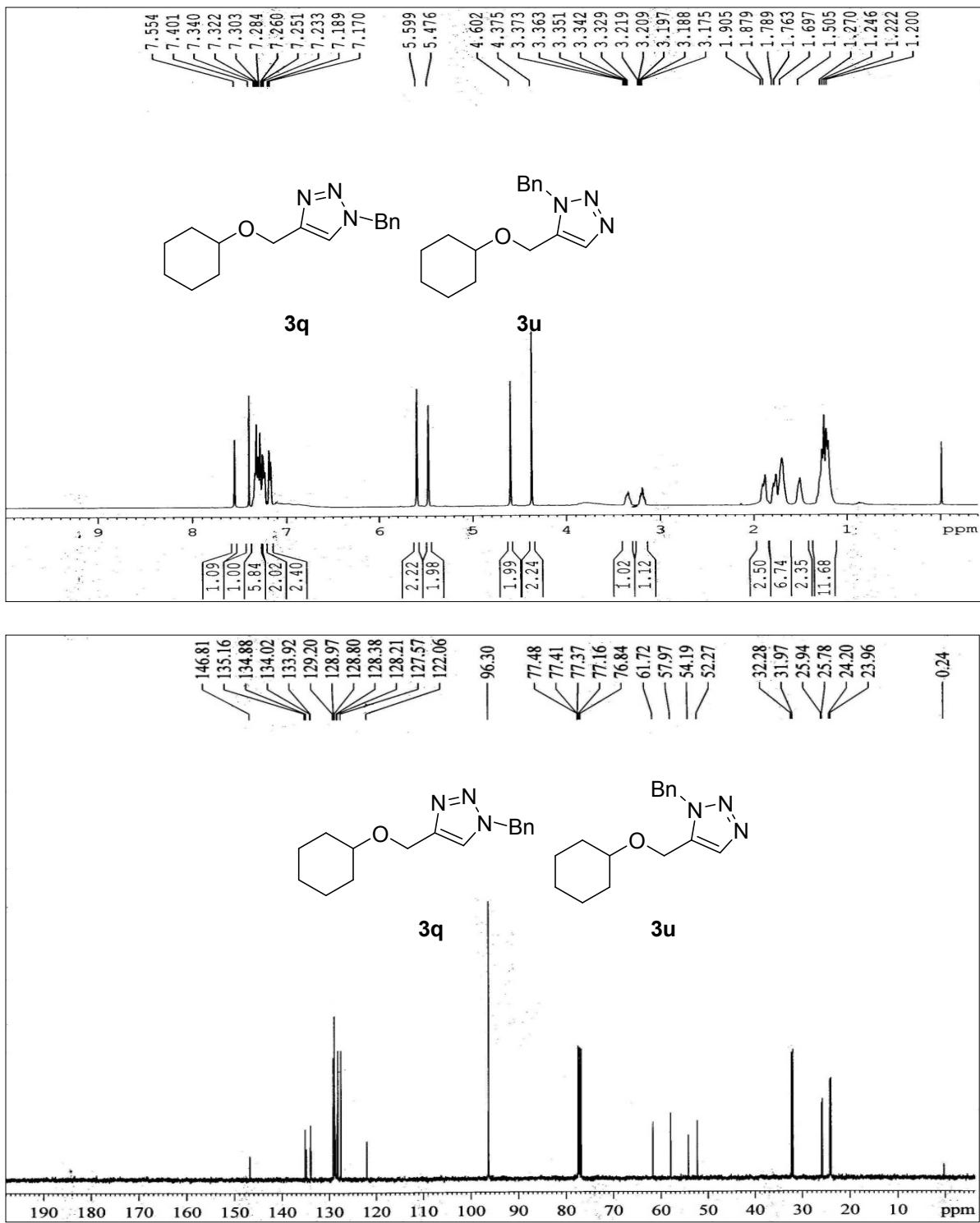
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-((4-*tert*-butylphenoxy)methyl)-1-hexyl-1*H*-1,2,3-triazole **3n**.



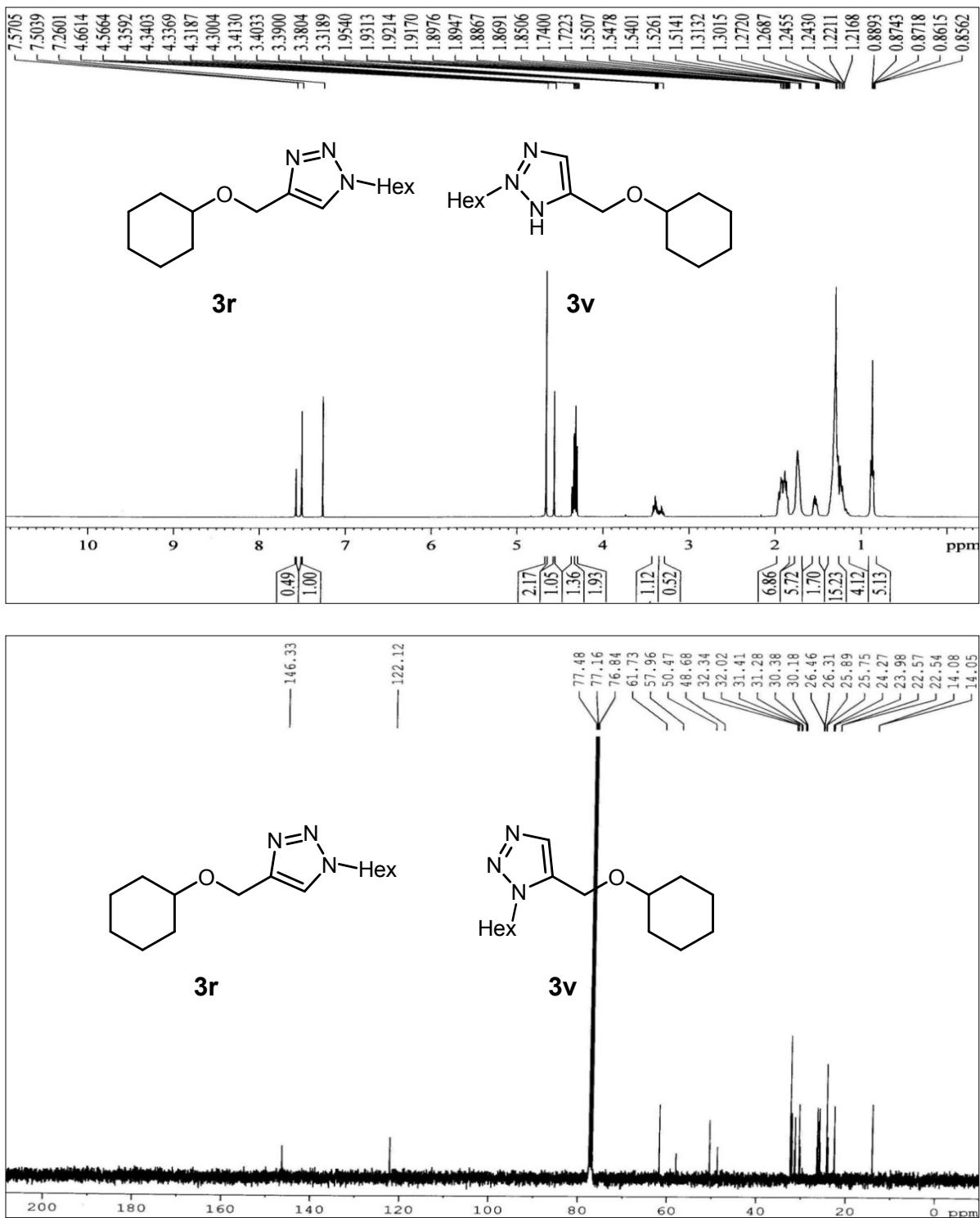
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 1-benzyl-4-(benzyloxymethyl)-1*H*-1,2,3-triazole, 5-(benzyloxymethyl)-1-bromo-1*H*-1,2,3-triazole **3o**, **3s**.

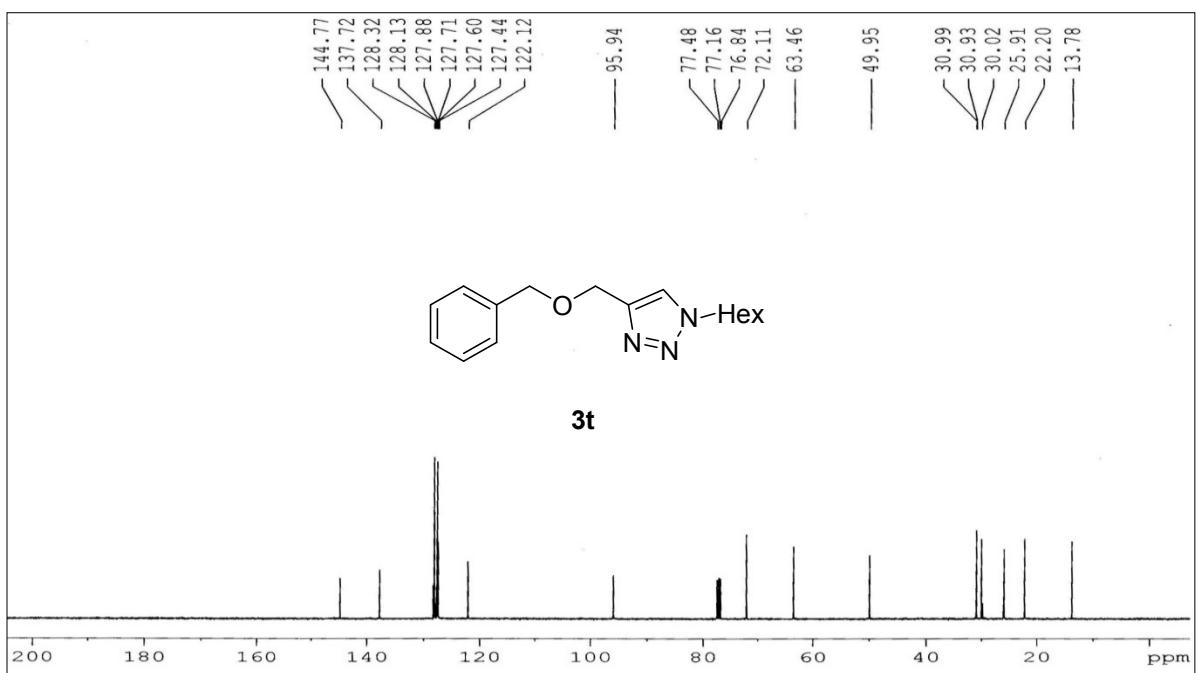
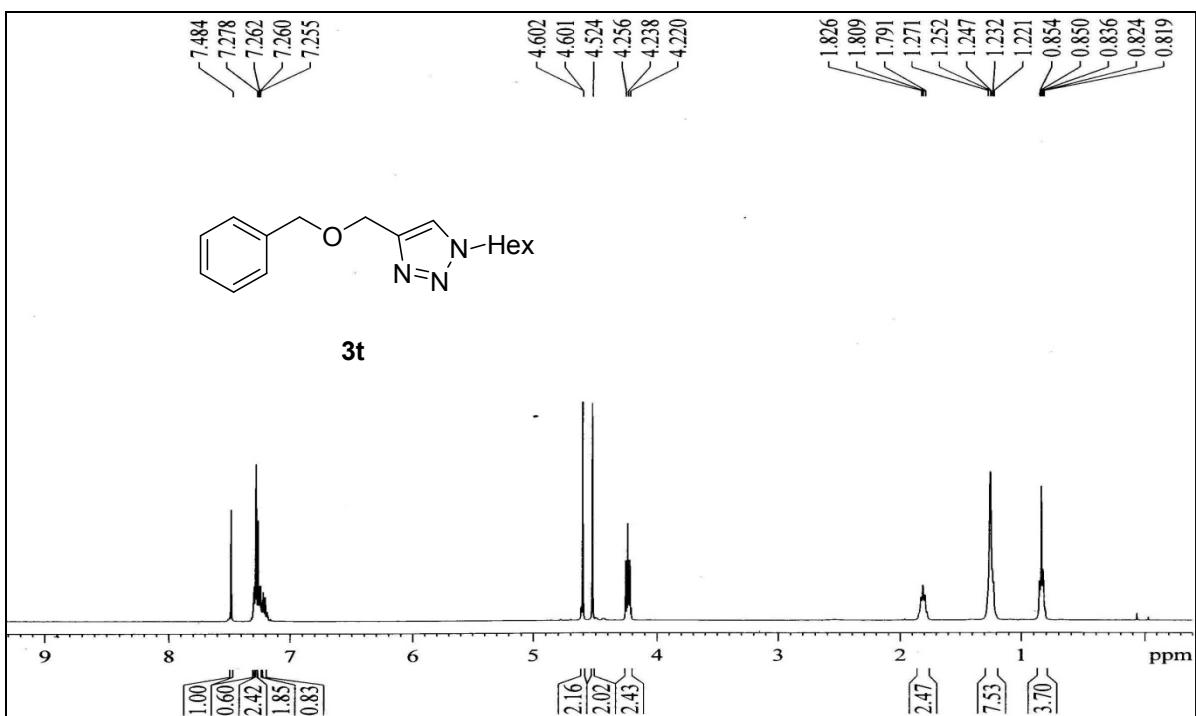


¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(benzyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole, 5-(benzyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole **3p**, **3t**.

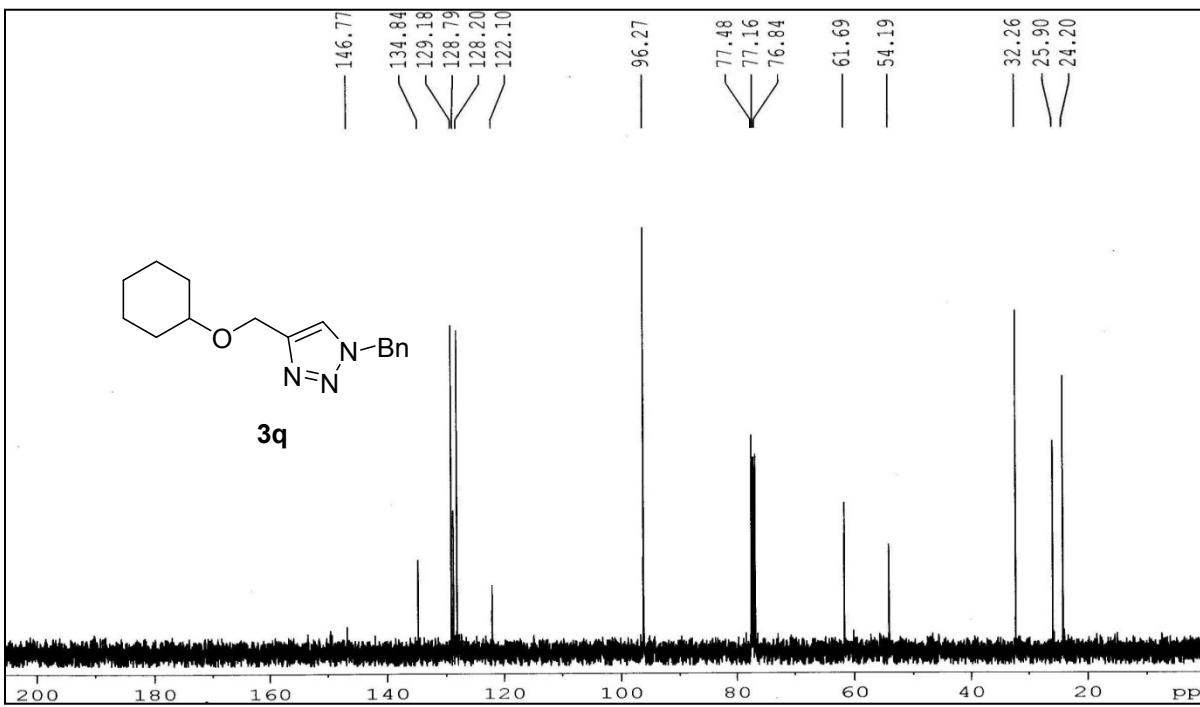
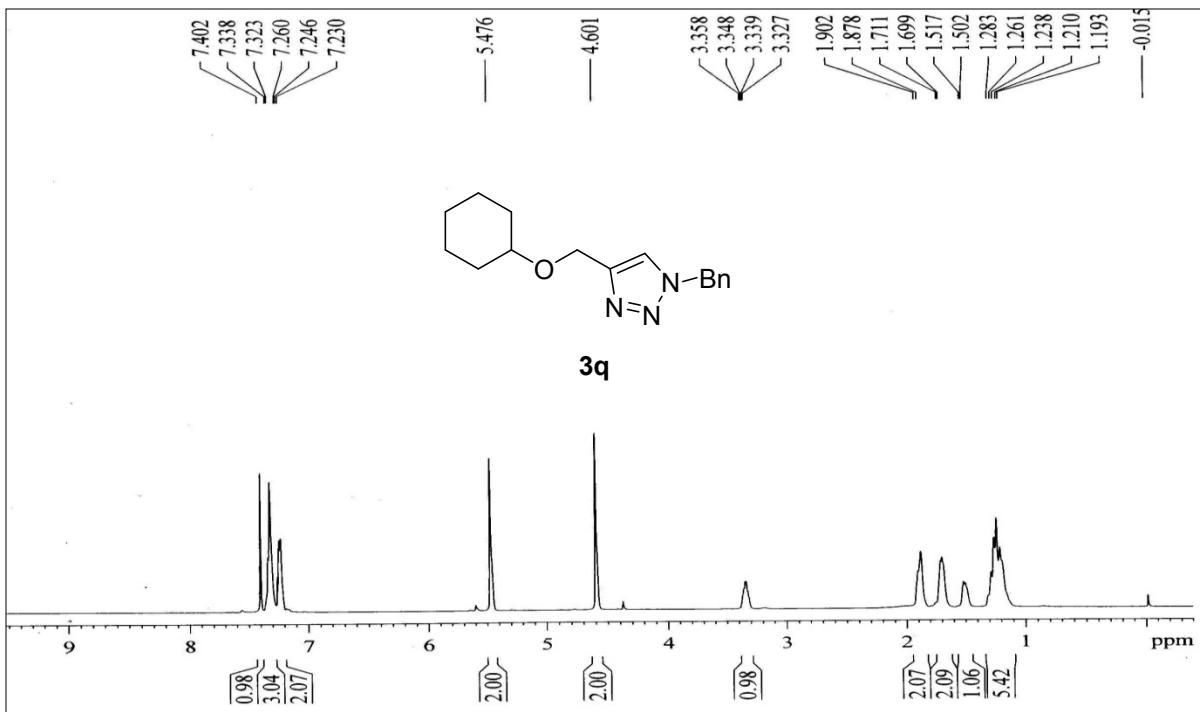


¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 1-benzyl-4-(cyclohexyloxymethyl)-1*H*-1,2,3-triazole, 1-benzyl-5-(cyclohexyloxymethyl)-1*H*-1,2,3-triazole **3q**, **3t**.

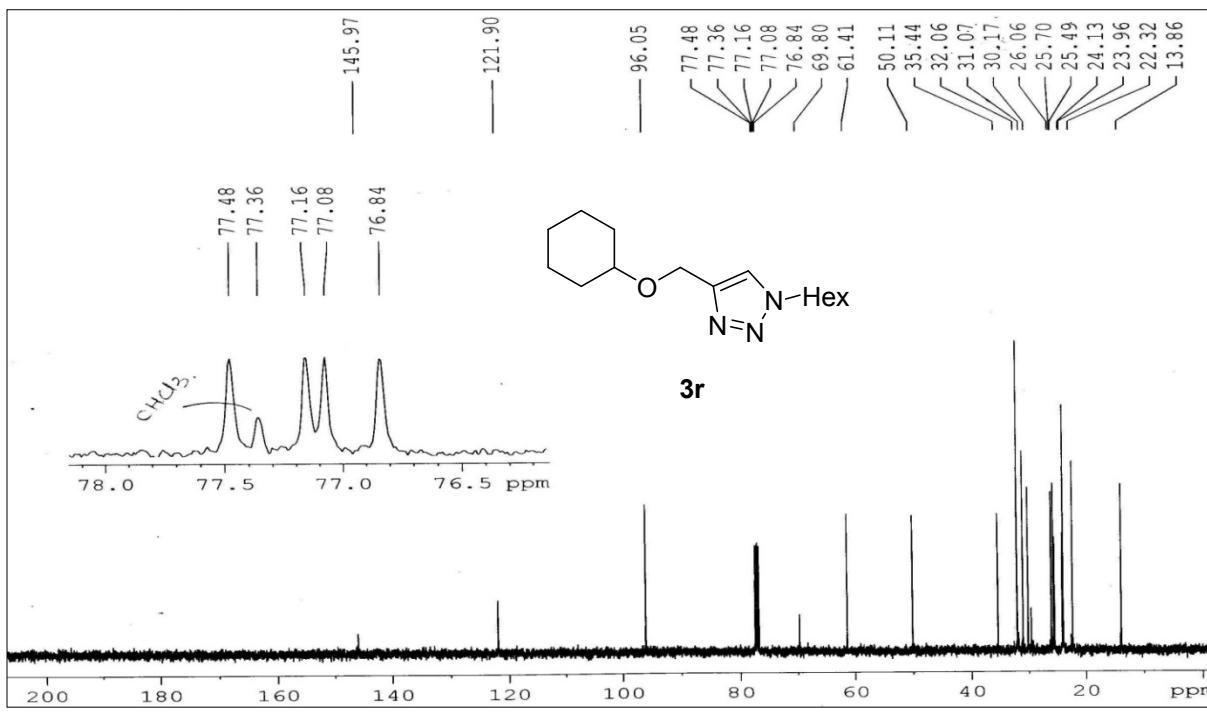
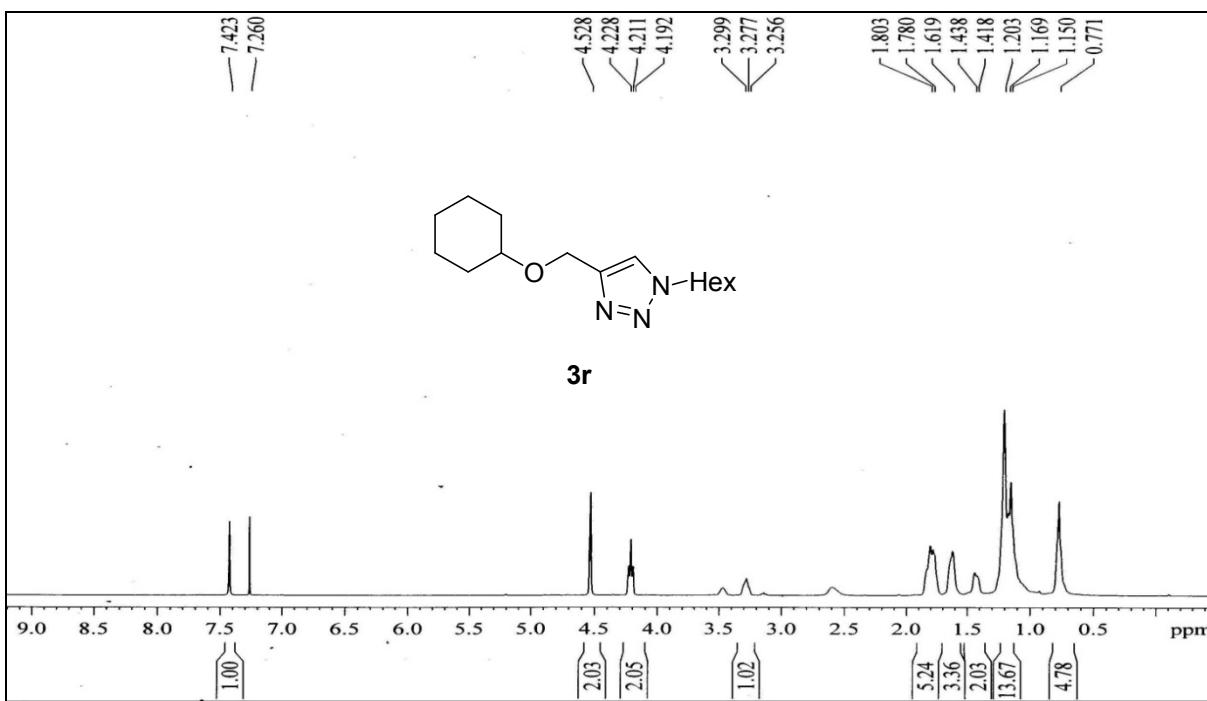




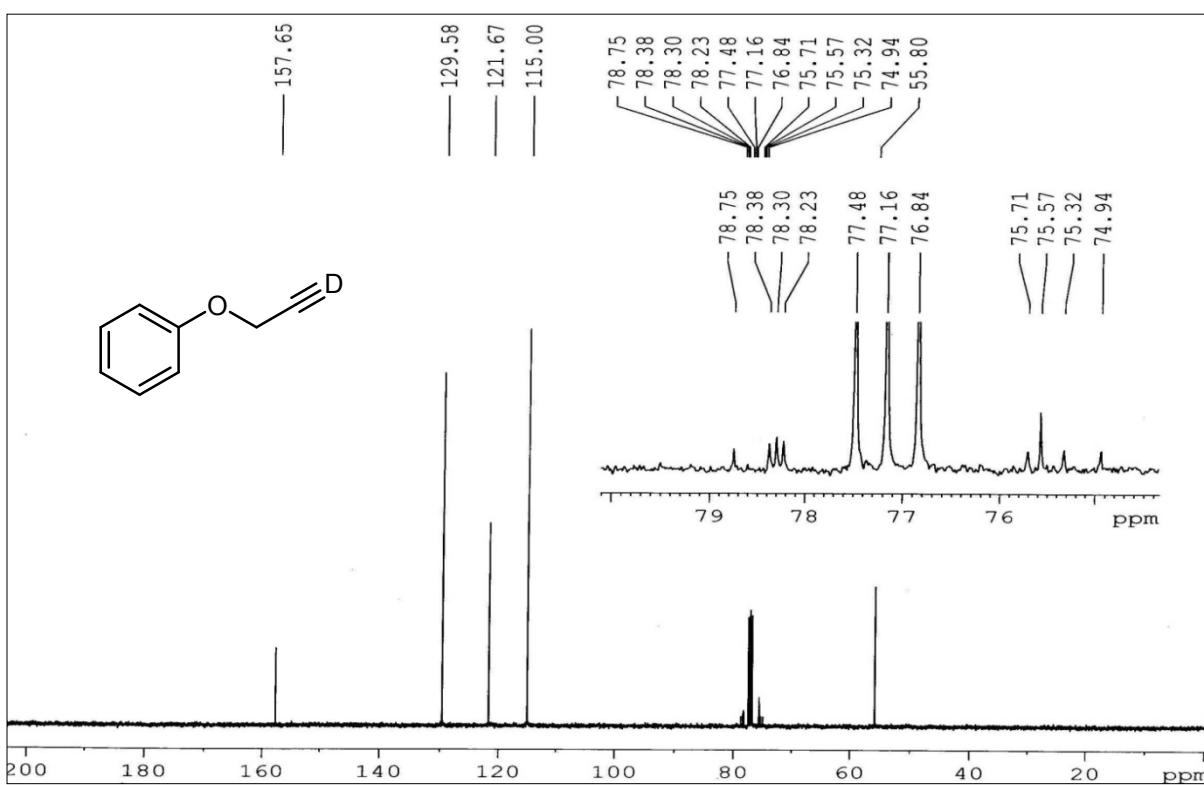
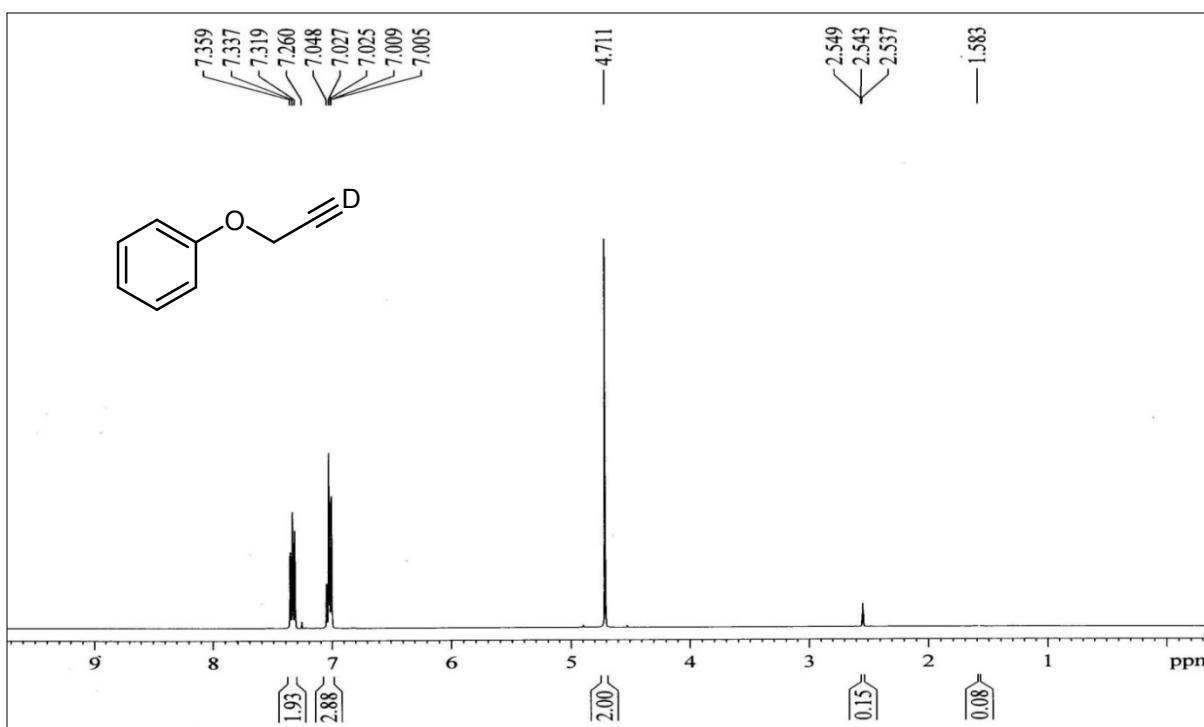
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(benzyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole **3t**.



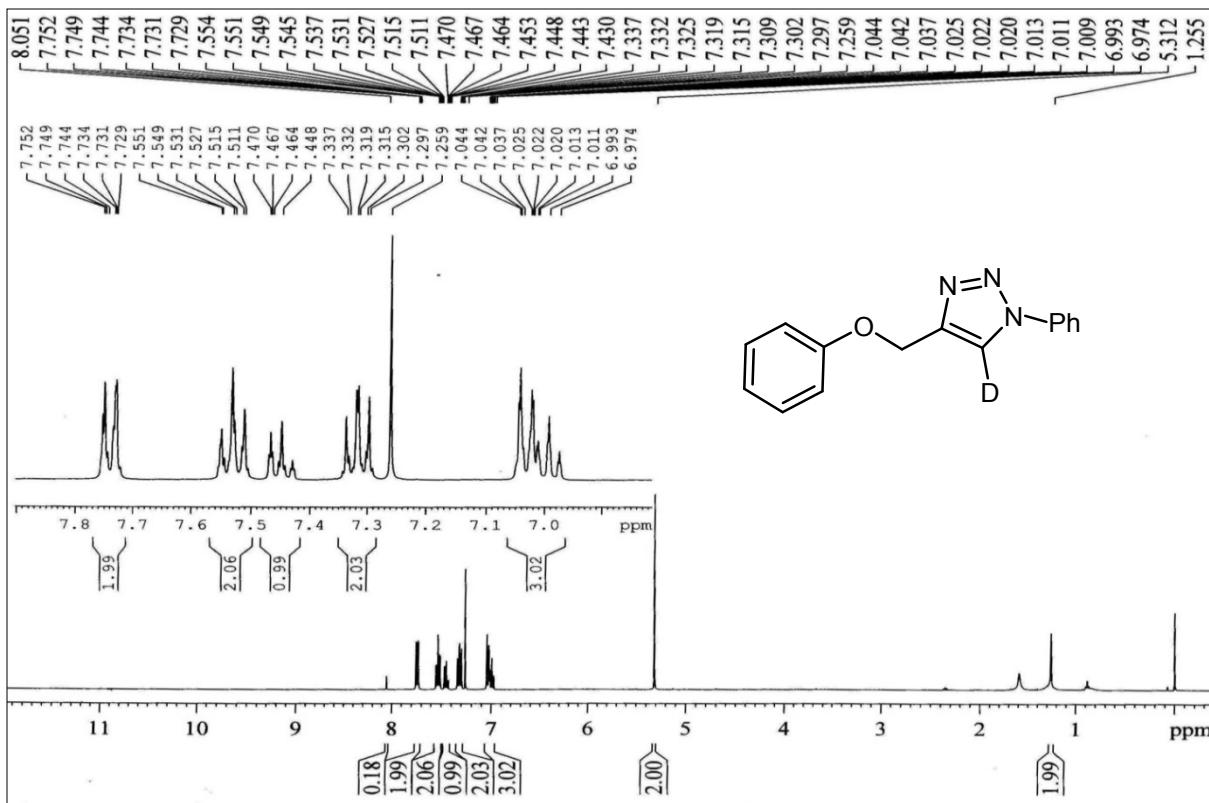
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 1-benzyl-4-(cyclohexyloxymethyl)-1*H*-1,2,3-triazole **3u**.



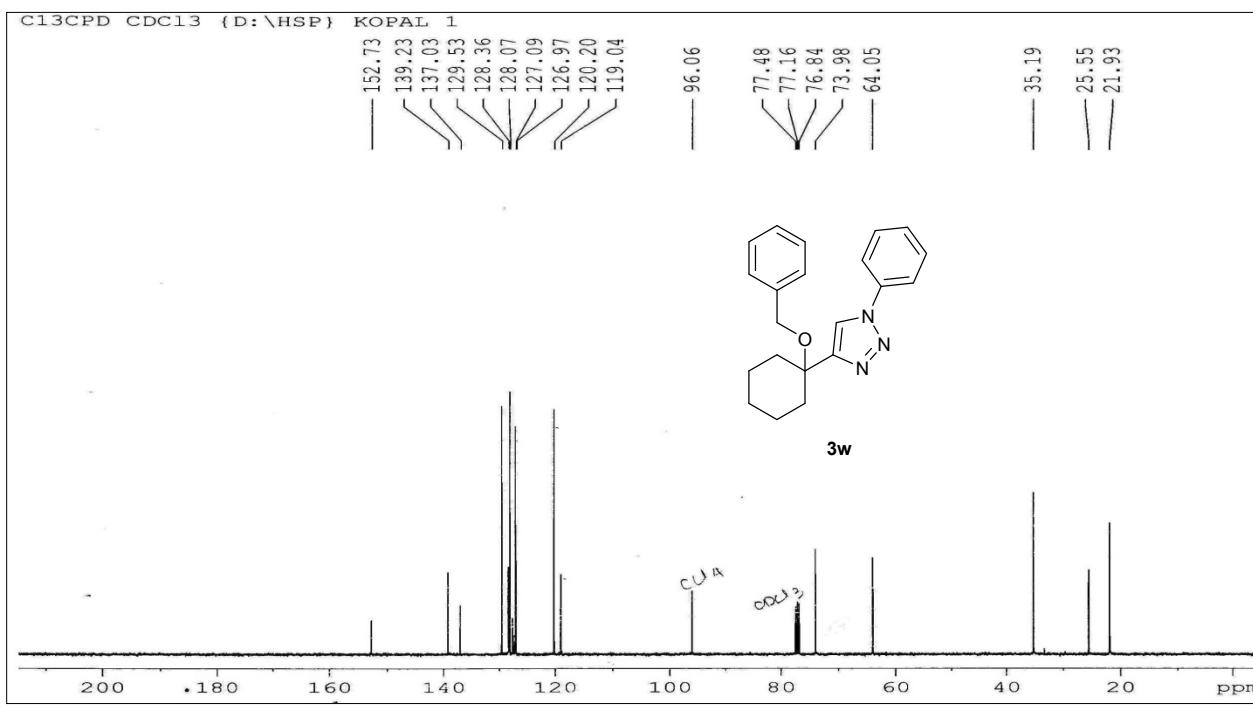
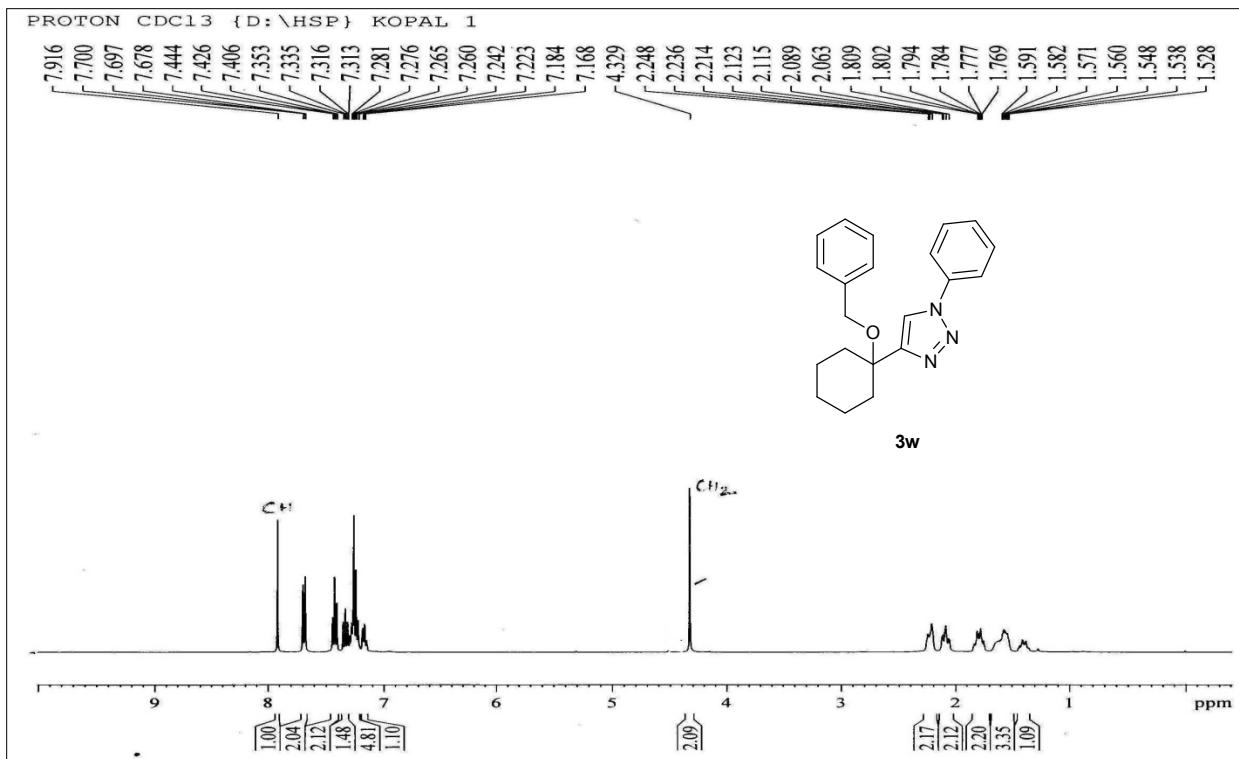
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(cyclohexyloxymethyl)-1-hexyl-1*H*-1,2,3-triazole **3v**.



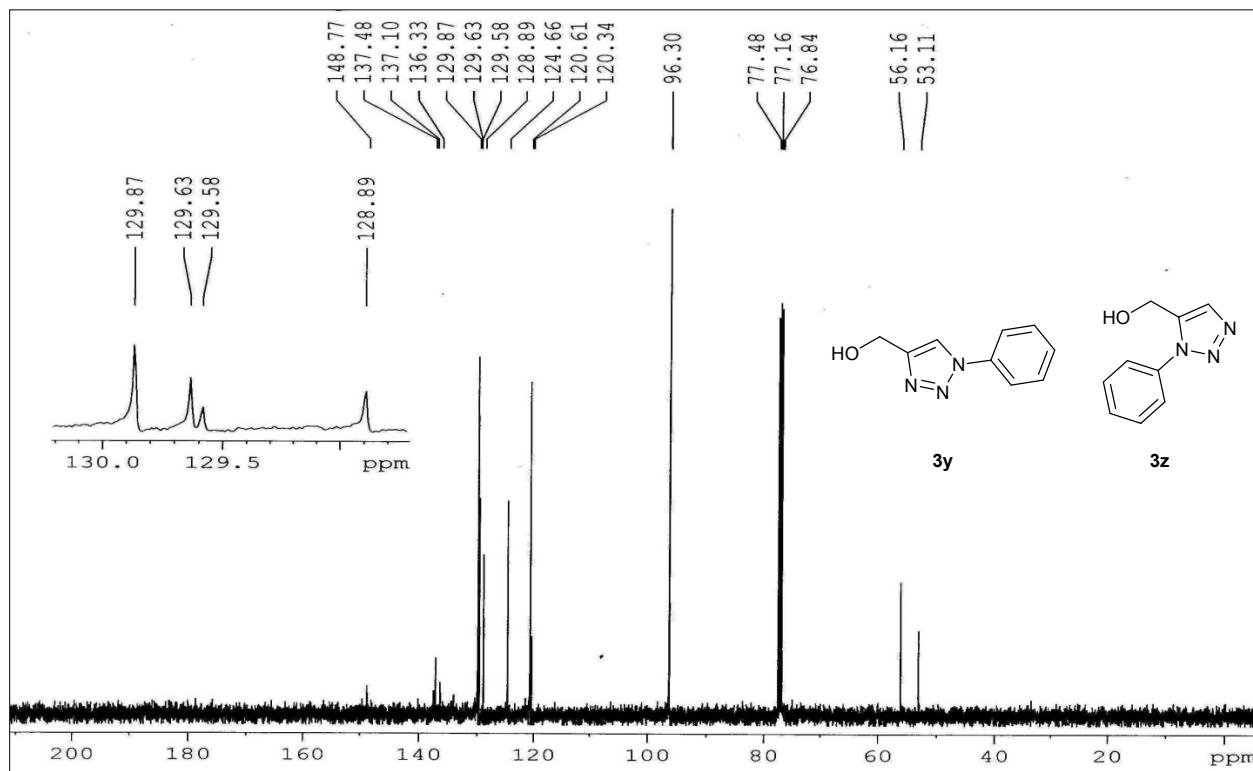
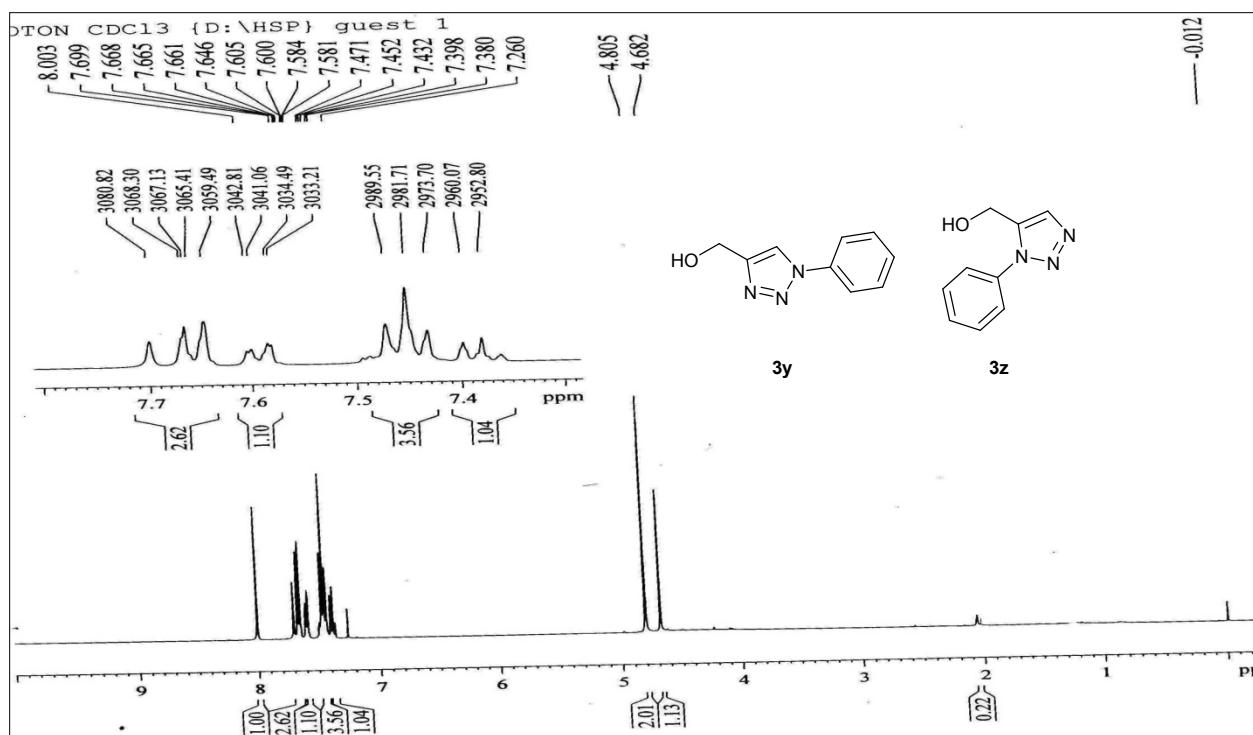
^1H (400 MHz, $\text{CCl}_4:\text{CDCl}_3$, 1:1) and ^{13}C (100 MHz, $\text{CCl}_4:\text{CDCl}_3$, 1:1) NMR spectra of (((3-deuteroprop-2-yn-1-yl)oxy)methyl)benzene **4**.



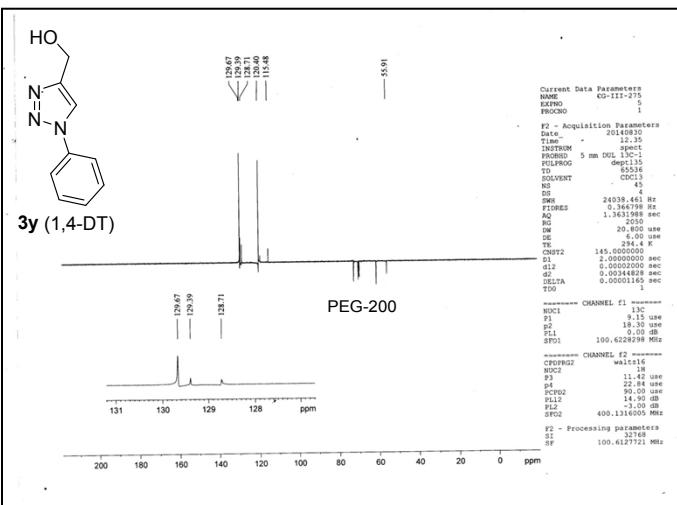
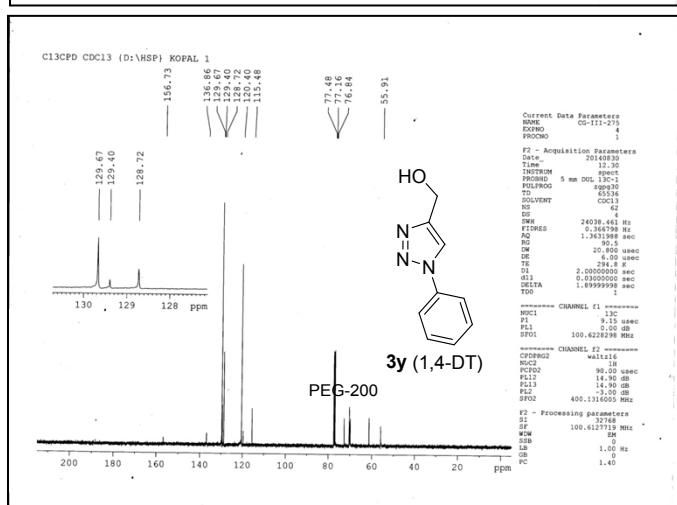
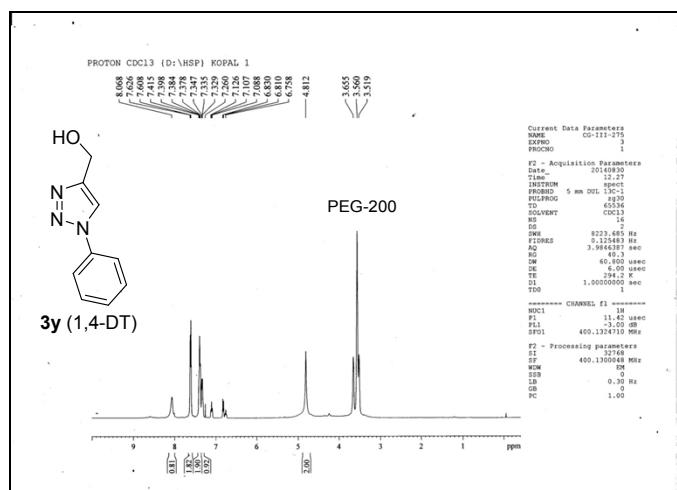
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(phenoxyethyl)-1-phenyl-1*D*-1,2,3-triazole **8**.



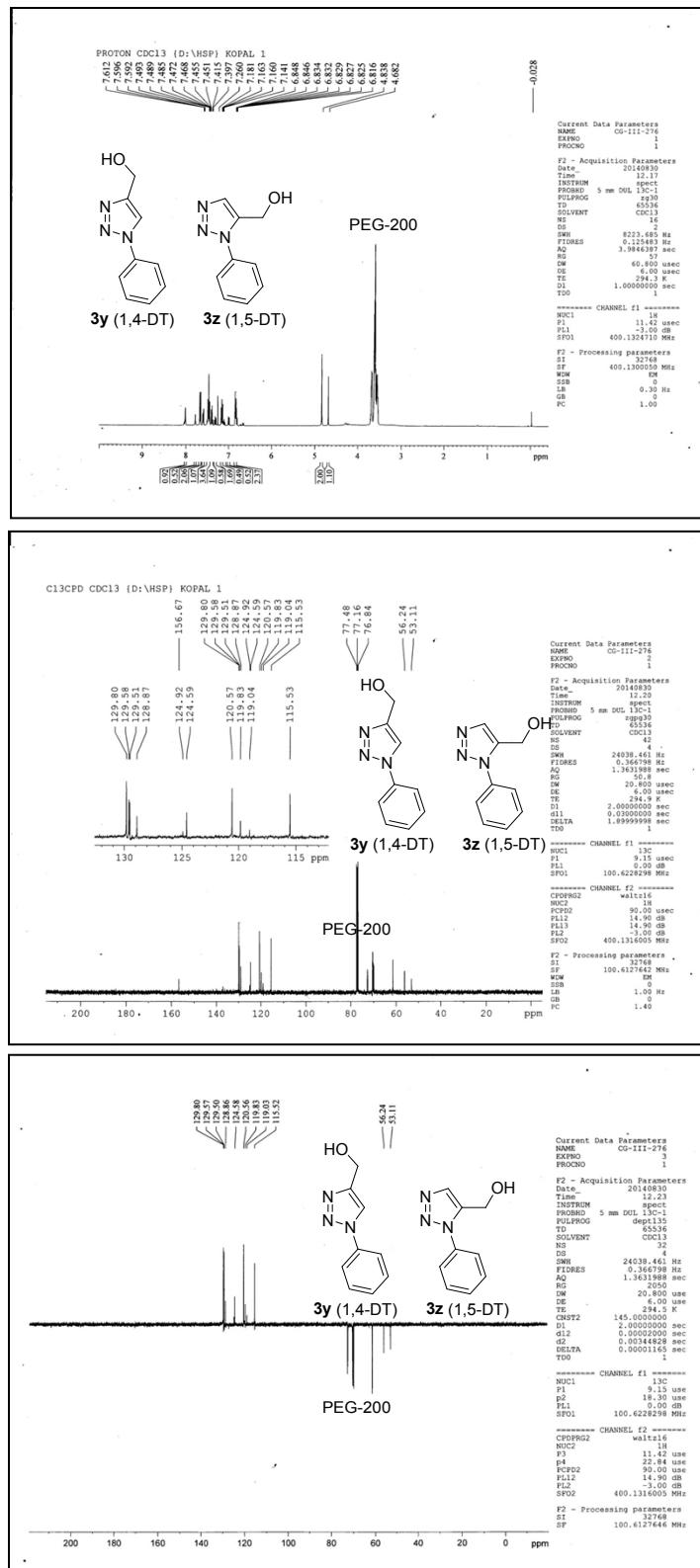
¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of 4-(1-(benzyloxy)cyclohexyl)-1-phenyl-1*H*-1,2,3-triazole **3w**.



¹H (400 MHz, CCl₄:CDCl₃, 1:1) and ¹³C (100 MHz, CCl₄:CDCl₃, 1:1) NMR spectra of (1-phenyl-1*H*-1,2,3-triazol-4-yl)methanol **3y** and (1-phenyl-1*H*-1,2,3-triazol-5-yl)methanol **3z**.



¹H (400 MHz, CDCl₃) ¹³C (100 MHz, CDCl₃) and DEPT-135 (100 MHz, CDCl₃) NMR spectra of the crude cycloadduct from reaction of propargyl alcohol, phenyl azide and CuSO₄.5H₂O, sodium ascorbate in PEG-200 under MW irradiation (with PEG impurity).



¹H (400 MHz, CDCl₃), ¹³C (100 MHz, CDCl₃) and DEPT-135 (100 MHz, CDCl₃) NMR spectra of the crude product from the reaction of propargyl alcohol, phenyl azide in PEG-200 under MW irradiation without any catalyst (with PEG impurity).