Supporting Information

Heterobimetallic Complexes Containing a N-Heterocyclic Carbene Based Multidentate Ligand and Catalyzed Tandem Click/Sonogashira Reactions

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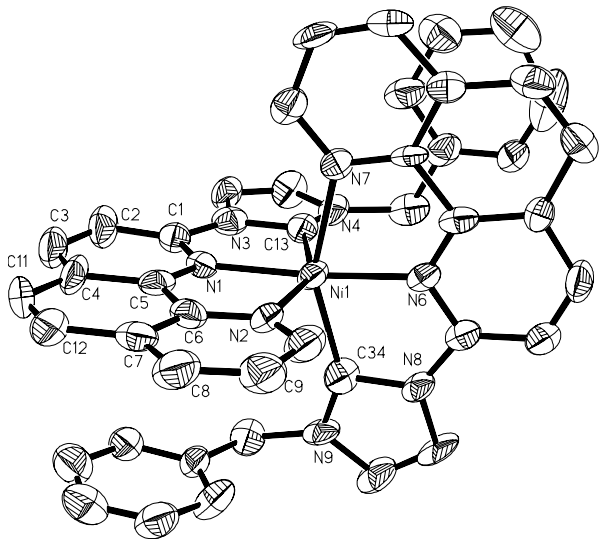


Figure S1. ORTEP drawing of the cationic section of $[Ni(L)_2](PF_6)_2$ (**2**). Thermal ellipsoids are drawn at the 30% probability level. Hydrogen atoms and anions have been removed for clarity. Selected bond distances (Å) and angles (°): Ni(1)-N(1) 1.999(8), Ni(1)-N(6) 2.022(8), Ni(1)-C(13) 2.068(12), Ni(1)-C(34) 2.075(11), Ni(1)-N(7) 2.223(8), Ni(1)-N(2) 2.233(10); N(1)-Ni(1)-N(6) 172.6(3), N(1)-Ni(1)-C(13) 77.4(4), N(6)-Ni(1)-C(13) 106.8(4), N(1)-Ni(1)-C(34) 108.4(4), N(6)-Ni(1)-C(34) 77.7(4), C(13)-Ni(1)-C(34) 93.9(4), N(1)-Ni(1)-N(7) 97.5(3), N(6)-Ni(1)-N(7) 76.2(3), C(13)-Ni(1)-N(7) 94.1(3), C(34)-Ni(1)-N(7) 153.9(4), N(1)-Ni(1)-N(2) 76.2(4), N(6)-Ni(1)-N(2) 99.2(3), C(13)-Ni(1)-N(2) 153.4(4), C(34)-Ni(1)-N(2) 97.2(4), N(7)-Ni(1)-N(2) 86.3(3).

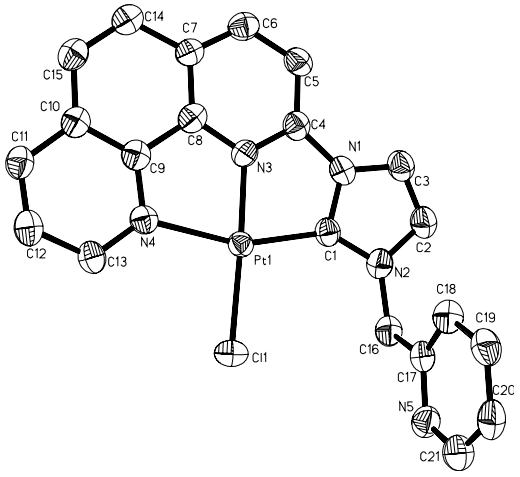
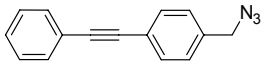


Figure S2. ORTEP drawing of the cationic section of [Pt(L)Cl](PF_6) (**4**). Thermal ellipsoids are drawn at the 30% probability level. Hydrogen atoms and one anion have been removed for clarity. Selected bond distances (Å) and angles (°): Pt(1)-N(3) 1.916(10), Pt(1)-C(1) 1.959(12), Pt(1)-N(4) 2.111(10), Pt(1)-Cl(1) 2.272(3); N(3)-Pt(1)-C(1) 78.5(5), N(3)-Pt(1)-N(4) 80.1(4), C(1)-Pt(1)-N(4) 158.6(5), N(3)-Pt(1)-Cl(1) 177.3(3), C(1)-Pt(1)-Cl(1) 104.2(4), N(4)-Pt(1)-Cl(1) 97.2(3).

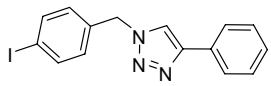
Table S1. Summary of the crystallographic data for 2 and 4.

	$[Ni(L)_2](PF_6)_2$, **2**	$[Pt(L)Cl](PF_6)$, **4**
Formula	$C_{42}H_{30}F_{12}N_{10}P_2Ni$	$C_{21}H_{15}ClF_6N_5PPt$
Fw	1023.41	712.89
Crystal system	triclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/c$
a, Å	9.664(5)	14.2205(15)
b, Å	12.003(7)	10.3577(10)
c, Å	20.703(11)	15.2229(17)
α, deg.	82.101(7)	90
β, deg.	89.724(7)	101.3910(10)
γ, deg.	78.062(7)	90
V, Å3	2327(2)	2198.0
Z	2	4
D_{calcd}, Mg/m^3	1.461	2.154
Reflections collected	11833	11070
Reflections independent, R_{int}	8017,0.0549	3864, 0.0930
Goodness-of-fit on F^2	1.048	1.055
$R1$, $wR2$ ($I > 2\sigma(I)$)	0.1932, 0.3064	0.0561, 0.1251
$R1$, $wR2$ (all data)	0.2259, 0.3393	0.0862, 0.1348

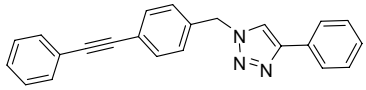
Spectroscopic data of all products



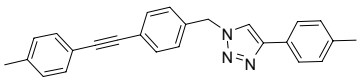
1-(azidomethyl)-4-(phenylethynyl)benzene: yellow solid; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.56 (m, 4H), 7.41-7.37 (m, 3H), 7.32 (d, 2H, *J* = 8.8 Hz), 4.38 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 135.7, 132.3, 131.9, 128.67, 128.64, 128.4, 123.6, 123.3, 90.3, 89.1, 54.8; MS (EI, *m/z*) 233 $(M)^+$.



1-(4-iodobenzyl)-4-phenyl-1H-1,2,3-triazole: light yellow solid; mp 166-168 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, 2H, *J* = 7.2 Hz), 7.72 (d, 2H, *J* = 8.8 Hz), 7.66 (s, 1H), 7.41 (t, 2H, *J* = 7.2 Hz), 7.33 (t, 1H, *J* = 7.2 Hz), 7.05 (d, 2H, *J* = 8.0 Hz), 5.52 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.4, 138.3, 134.3, 130.3, 129.8, 128.8, 128.2, 125.7, 119.4, 94.5, 53.6; MS (EI, *m/z*) 361 $(M)^+$.

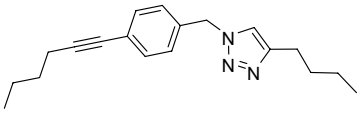


4-phenyl-1-(4-(phenylethynyl)benzyl)-1H-1,2,3-triazole: pale yellow solid; mp 182-184 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, 2H, *J* = 6.8 Hz), 7.69 (s, 1H), 7.57-7.52 (m, 4H), 7.42 (t, 2H, *J* = 8.0 Hz), 7.37-7.34 (m, 4H), 7.29 (d, 2H, *J* = 8.0 Hz), 5.61 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.3, 134.6, 132.2, 131.6, 130.4, 128.8, 128.5, 128.4, 128.2, 127.9, 125.7, 123.9, 122.9, 119.5, 90.4, 88.5, 53.9; MS (EI, *m/z*) 335 $(M)^+$.



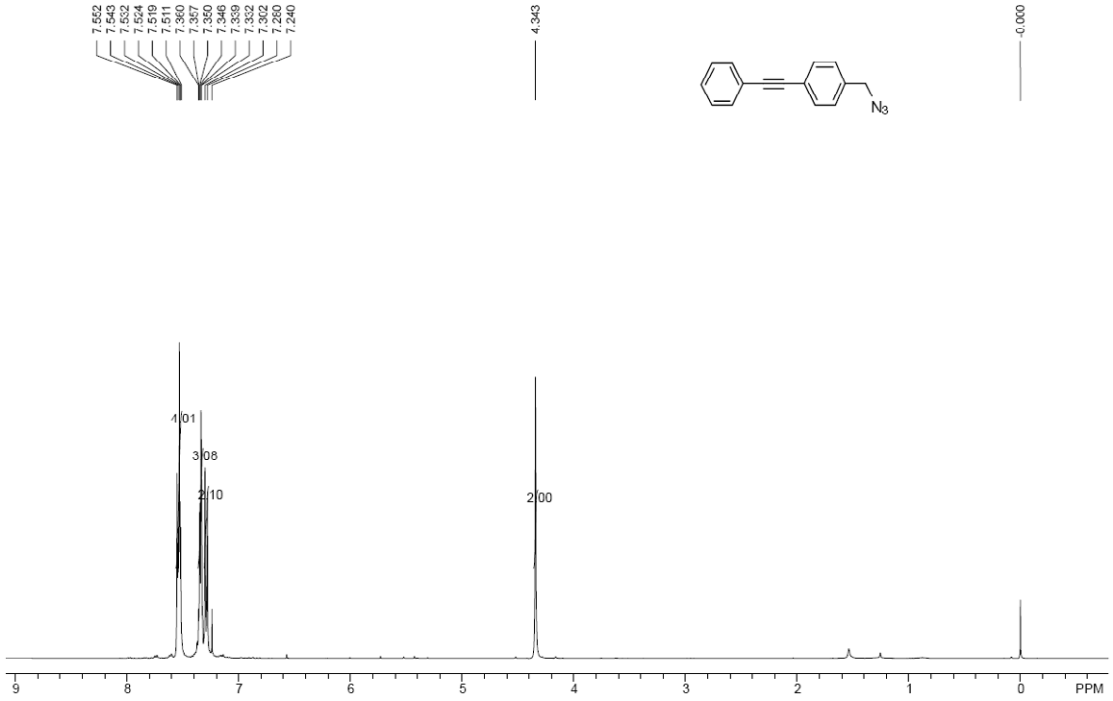
4-p-tolyl-1-(4-(p-tolylethynyl)benzyl)-1H-1,2,3-triazole: pale yellow solid; mp 179-180 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, 2H, *J* = 8.0 Hz), 7.62 (s, 1H), 7.51 (d, 2H, *J* = 8.0 Hz), 7.40 (d, 2H, *J* = 8.0 Hz), 7.25 (d, 2H, *J* = 8.0 Hz), 7.19 (d, 2H, *J* = 7.6 Hz), 7.13 (d, 2H, *J* = 7.6 Hz), 5.56 (s, 2H), 2.35 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.4, 138.7, 138.1, 134.4, 132.2, 131.5, 129.6, 129.5, 129.1, 127.9,

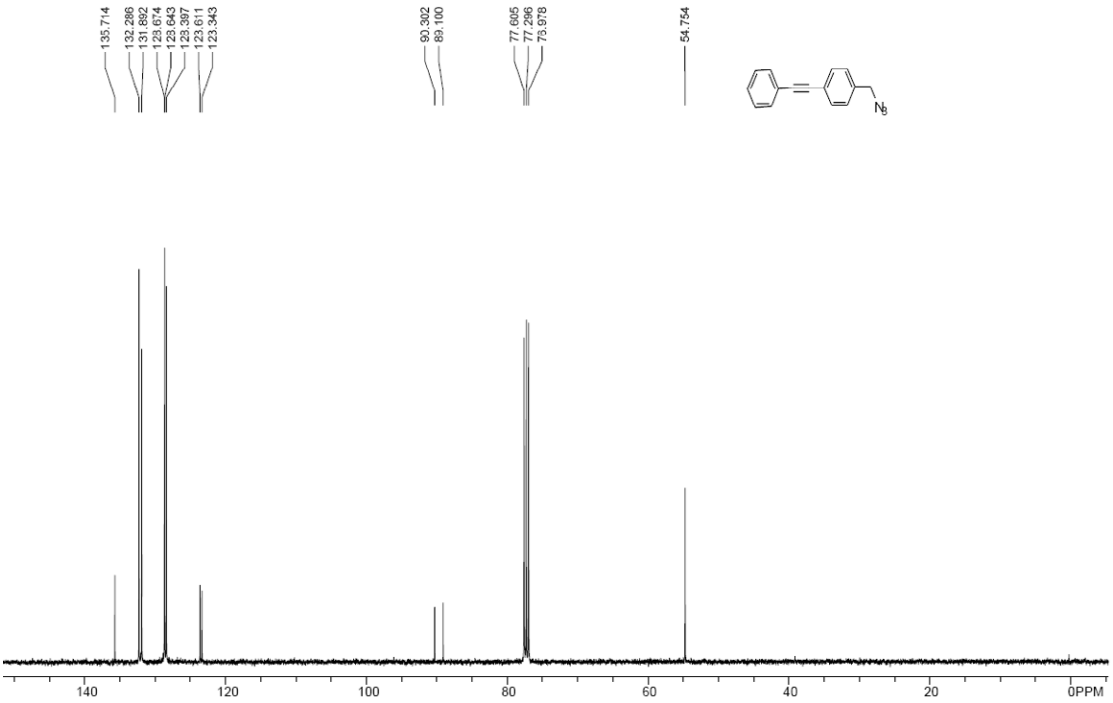
127.6, 125.9, 124.1, 119.8, 119.1, 90.6, 87.8, 53.9; MS (EI, *m/z*) 363 $(M)^+$.

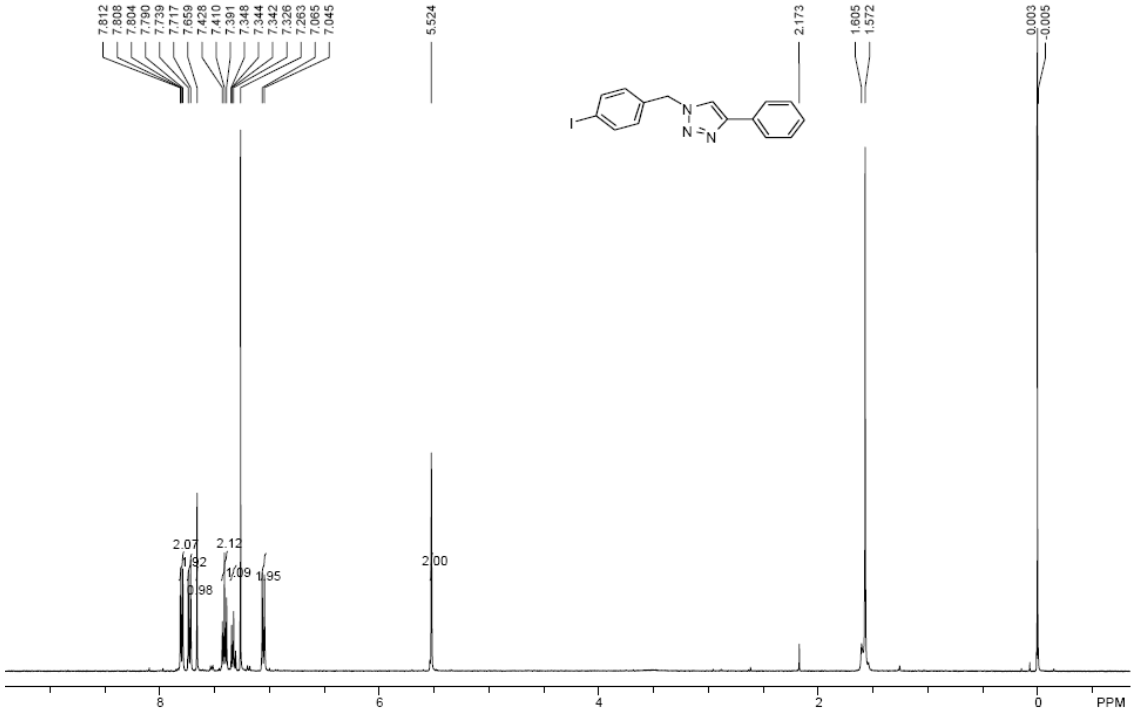


4-butyl-1-(4-(hex-1-ynyl)benzyl)-1H-1,2,3-triazole: pale yellow solid; mp: 42-44 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, 2H, *J* = 8.0 Hz), 7.17 (d, 2H, *J* = 8.0 Hz), 7.16 (s, 1H), 5.47 (s, 2H), 2.69 (t, 2H, *J* = 8.0 Hz), 2.41 (t, 2H, *J* = 7.2 Hz), 1.65-1.58 (m, 4H), 1.51-1.45 (m, 2H), 1.39-1.34 (m, 2H), 0.96 (t, 3H, *J* = 7.2 Hz), 0.92 (t, 3H, *J* = 7.2 Hz). ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.9, 134.0, 132.1, 127.7, 124.6, 120.4, 91.5, 79.8, 53.6, 31.4, 30.9, 25.3, 22.2, 21.9, 19.0, 13.7, 13.5; MS (EI, *m/z*) 295 $(M)^+$.

^{1}H and ^{13}C NMR Spectra



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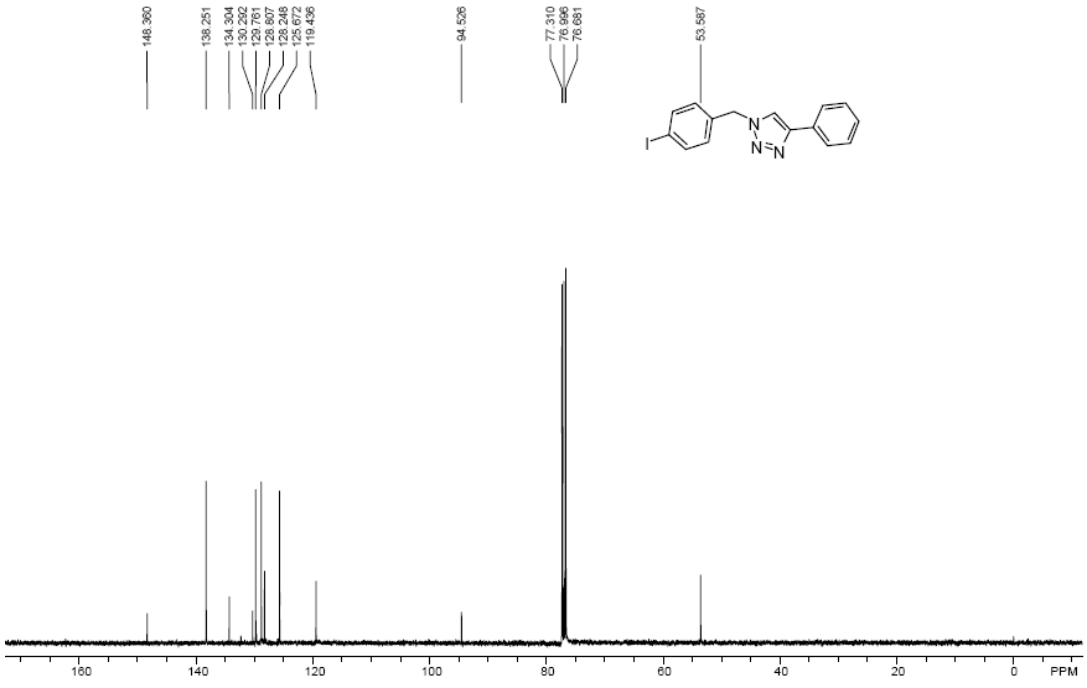
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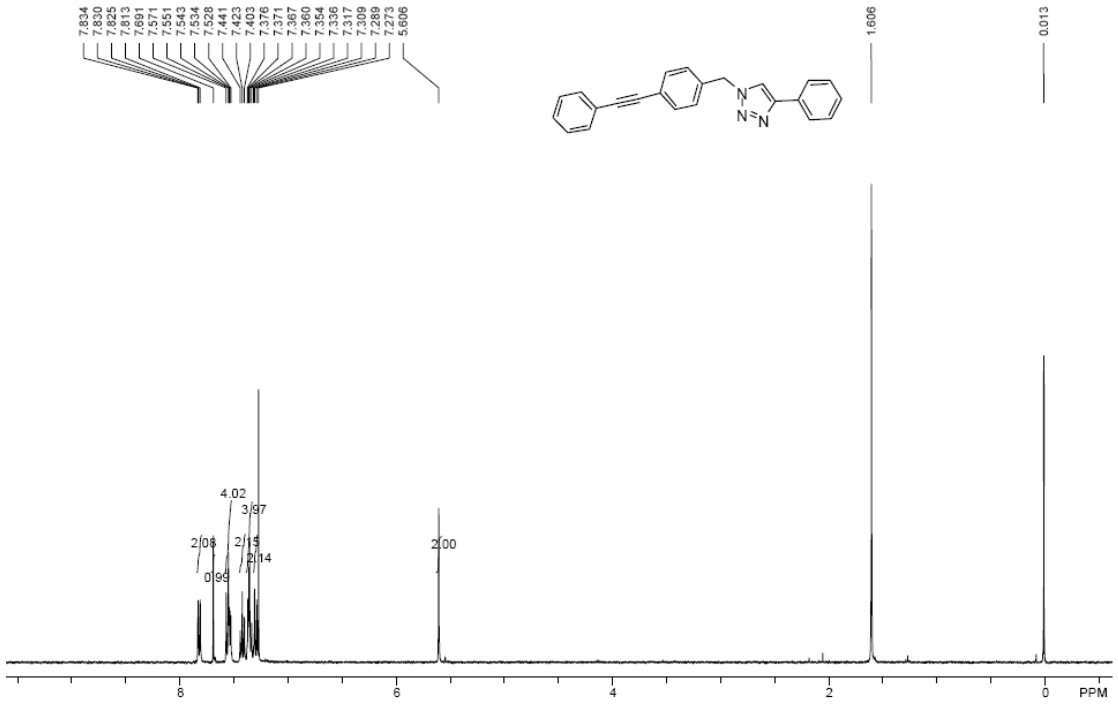
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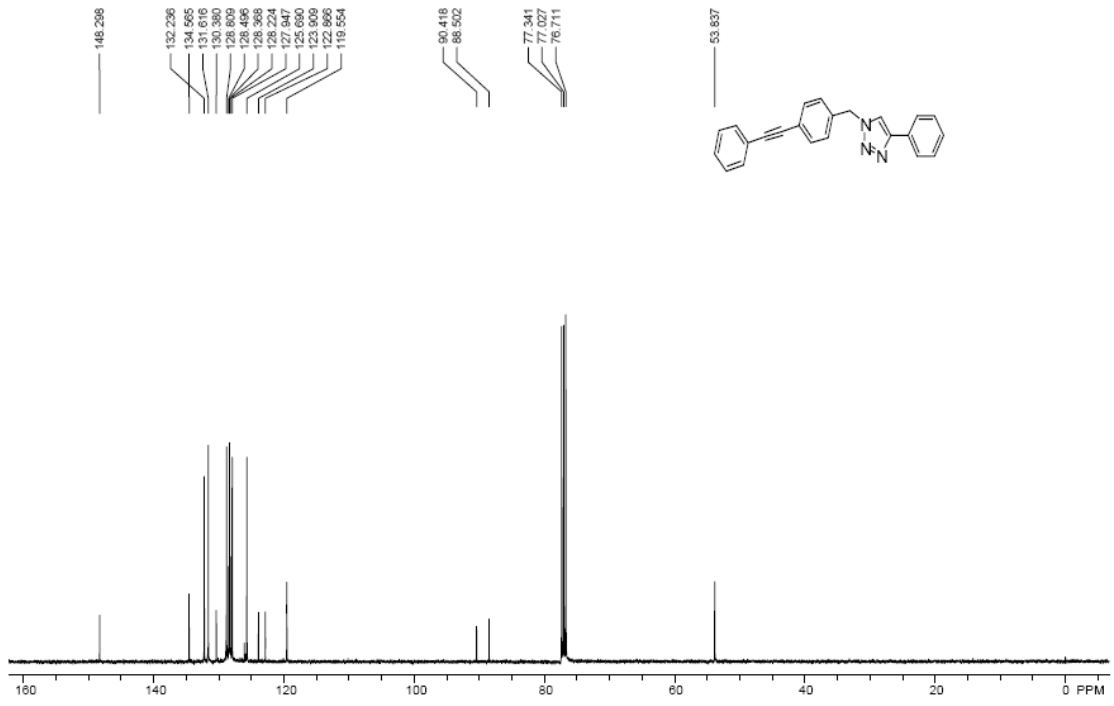
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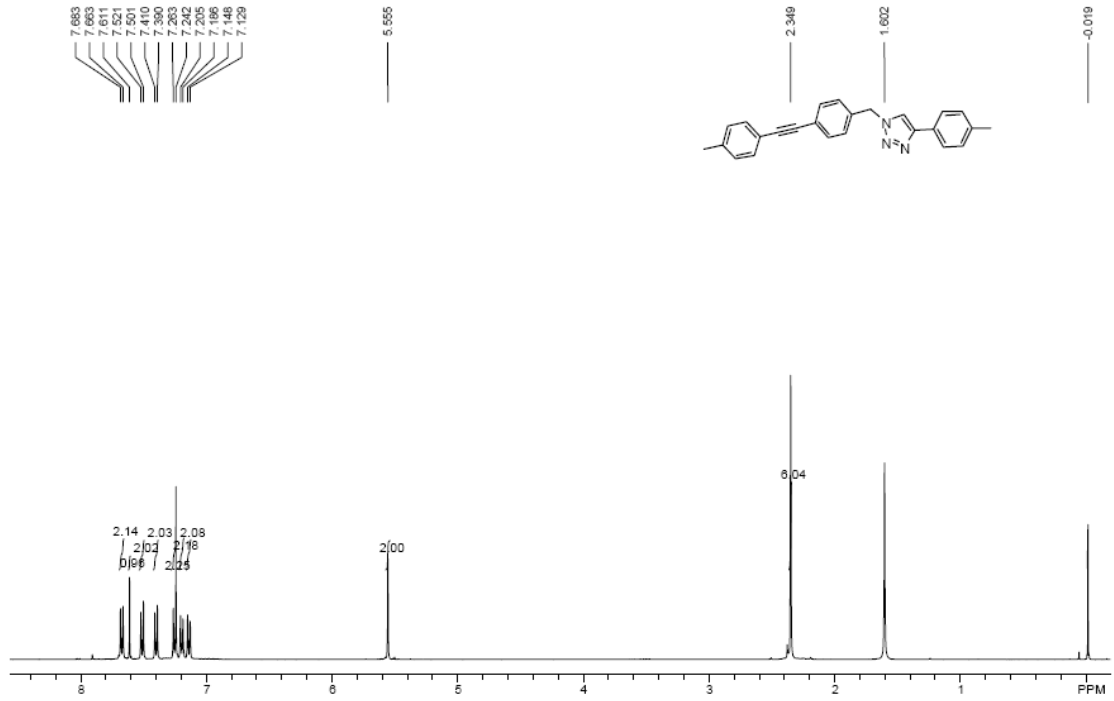
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2.03
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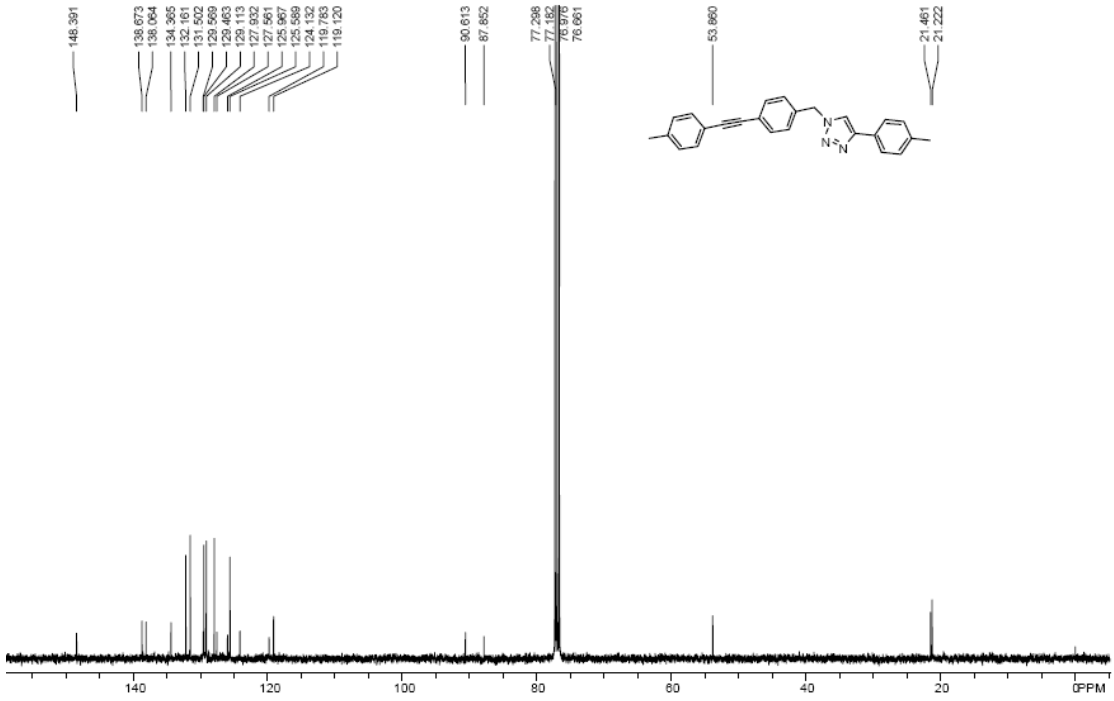
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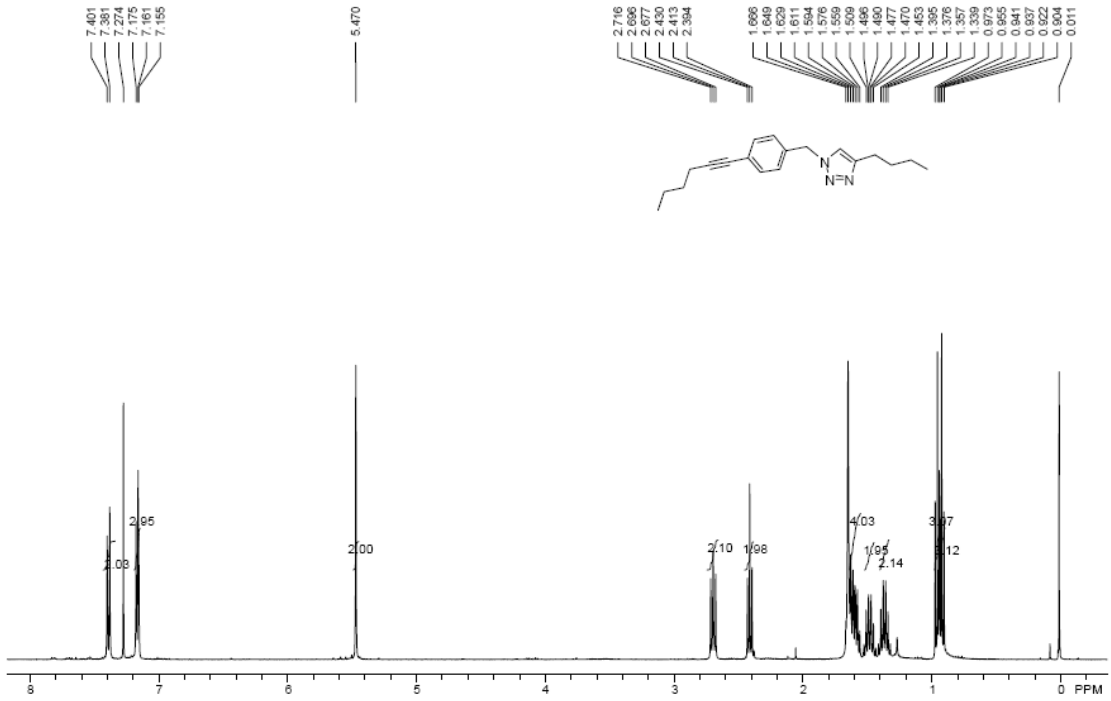
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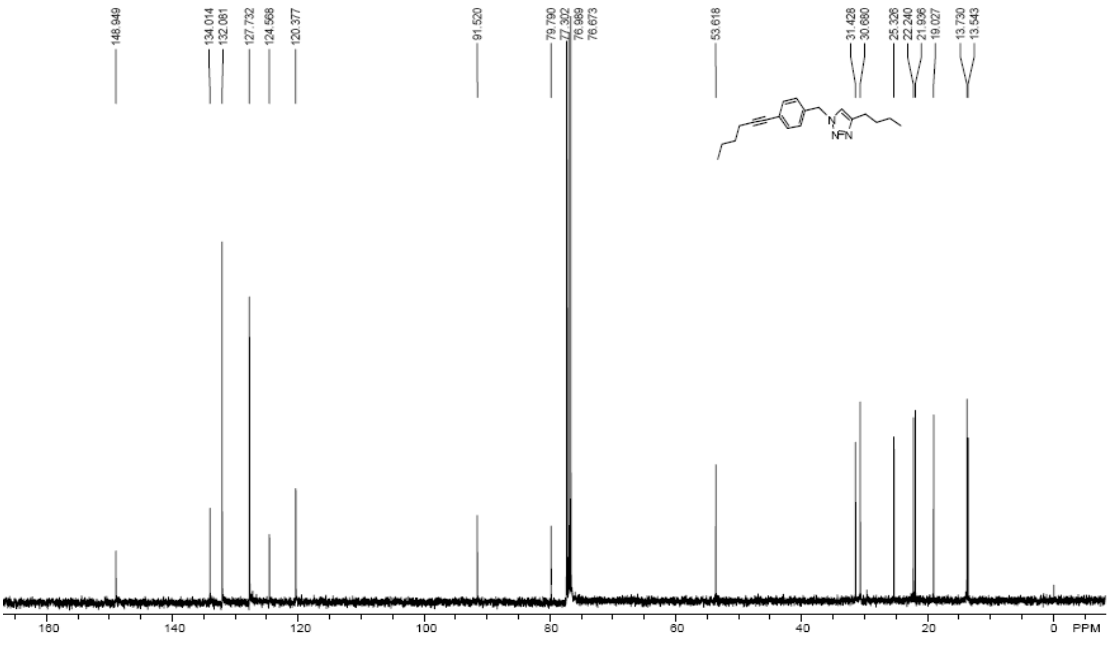
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