Supporting information

for

Copper-free Sonogashira Cross-coupling Reaction Promoted by a Nitrogen-containing Chelating Ligand in Neat Water at Room Temperature

Hong Zhong, Jinyun Wang, Liuyi Li and Ruihu Wang*

Content

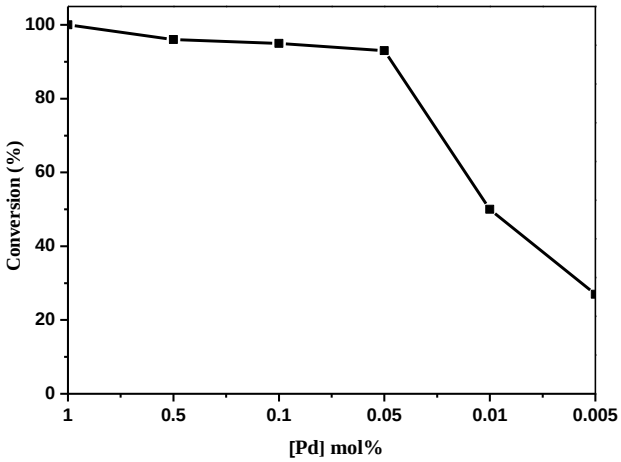


Fig. S3 The conversion of iodobenzene as a function of palladium loading. Reaction conditions: iodobenzene (0.50 mmol), phenylacetylene (0.75 mmol), $Pd(NH_3)_2Cl_2$-dpa (0.1 mol%), NEt_3 (1.50 mmol), H_2O (2.0 mL) under N_2 at 25 ^oC for 6 h.

Table S1 Charge distribution of dpa and Pd-dpa.

Atoms in dpa	Natural charge	Atoms in Pd-dpa	Natural charge
		Pd1	0.70234
		Cl2	-0.52523
		Cl3	-0.52523
N1	-0.46163	N4	-0.50062
N2	-0.64026	N5	-0.61948
N3	-0.46162	N6	-0.50064
C4	0.02331	C7	0.06497
H5	0.23314	H8	0.28089
C6	-0.31525	C9	-0.29543
H7	0.2502	H10	0.26748
C8	-0.20085	C11	-0.17679
H9	0.24898	H12	0.2604
C10	-0.30796	C13	-0.30094
H11	0.24301	H14	0.25146
C12	0.39211	C15	0.41355
C13	0.39211	C16	0.41357
C14	-0.30797	C17	-0.30094
H15	0.243	H18	0.25146
C16	-0.20085	C19	-0.17679
H17	0.24898	H20	0.2604
C18	-0.31525	C21	-0.29544
H19	0.2502	H22	0.26748
C20	0.02333	C23	0.06498
H21	0.23314	H24	0.28089
H22	0.43015	H25	0.43765

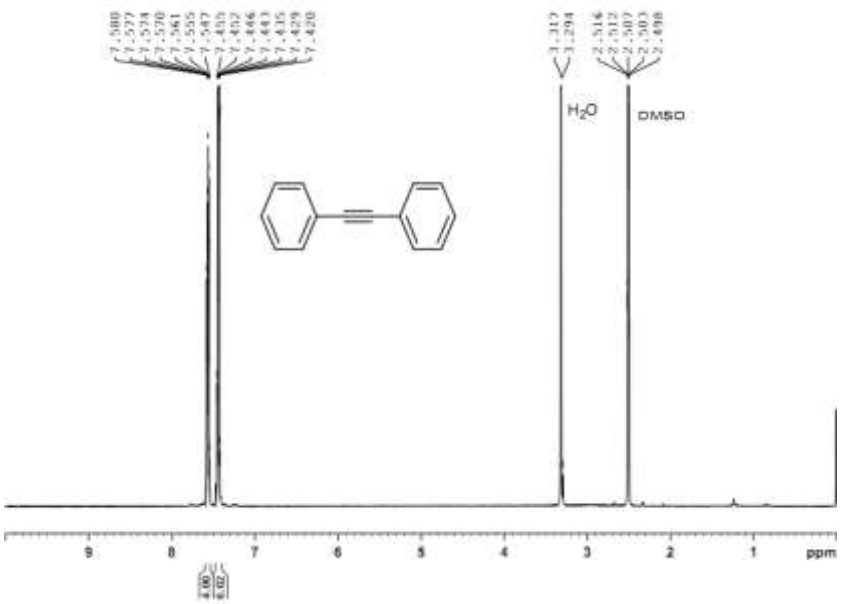
Table S2 The optimized geometry coordinates of dpa

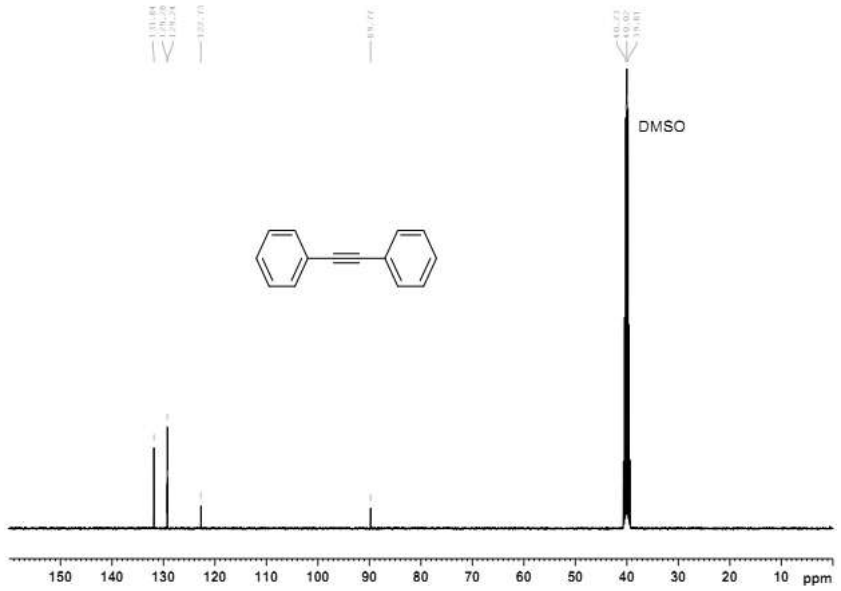
Atom	Coordinates (Angstroms)		
	X	Y	Z
N1	-1.372437	0.779776	-0.543944
N2	-0.000041	-1.050898	0.000091
N3	1.372518	0.779715	0.544135
C4	-2.590748	1.332999	-0.578148
H5	-2.638310	2.333876	-1.003080
C6	-3.750584	0.701146	-0.129785
H7	-4.712607	1.198355	-0.193990
C8	-3.624142	-0.587570	0.399577
H9	-4.493791	-1.125144	0.766798
C10	-2.365069	-1.169865	0.470606
H11	-2.227194	-2.156045	0.905024
C12	-1.259385	-0.443529	-0.018198
C13	1.259382	-0.443556	0.018283
C14	2.365002	-1.169892	-0.470568
H15	2.227186	-2.156135	-0.904871
C16	3.624103	-0.587552	-0.399757
H17	4.493695	-1.125221	-0.766974
C18	3.750601	0.701139	0.129557
H19	4.712581	1.198463	0.193509
C20	2.590796	1.332930	0.578211
H21	2.638463	2.333763	1.003253
H22	-0.000042	-2.059568	-0.000308

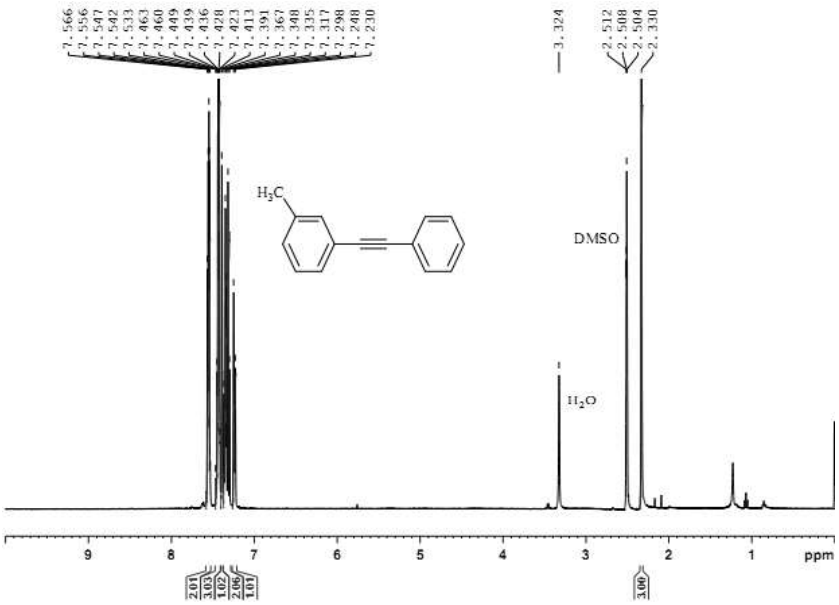
Table S3 The optimized geometry coordinates of Pd-dpa

Atom	Coordinates (Angstroms)		
	X	Y	Z
Pd1	0.061318	-1.053903	-0.003167
Cl2	-0.137091	-2.689198	-1.654150
Cl3	-0.143952	-2.700660	1.635541
N4	0.207872	0.458836	-1.465120
N5	-0.835742	2.005846	0.006084
N6	0.202743	0.448487	1.469867
C7	0.734812	0.182345	-2.681149
H8	1.143325	-0.814696	-2.787730
C9	0.702430	1.083539	-3.734236
H10	1.130084	0.806333	-4.690785
C11	0.091009	2.325289	-3.533012
H12	0.029121	3.053115	-4.336339
C13	-0.421855	2.628098	-2.280978
H14	-0.876987	3.593217	-2.080721
C15	-0.330266	1.671453	-1.252655
C16	-0.334884	1.662517	1.264202
C17	-0.430440	2.611657	2.299110
H18	-0.885243	3.578026	2.104238
C19	0.078146	2.299956	3.550680
H20	0.013196	3.021941	4.359018
C21	0.689315	1.056984	3.745075
H22	1.113801	0.773074	4.701070
C23	0.725569	0.163374	2.685674
H24	1.133972	-0.834300	2.786517
H25	-1.306441	2.899865	0.008375

NMR spectra of the coupling products



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H2O
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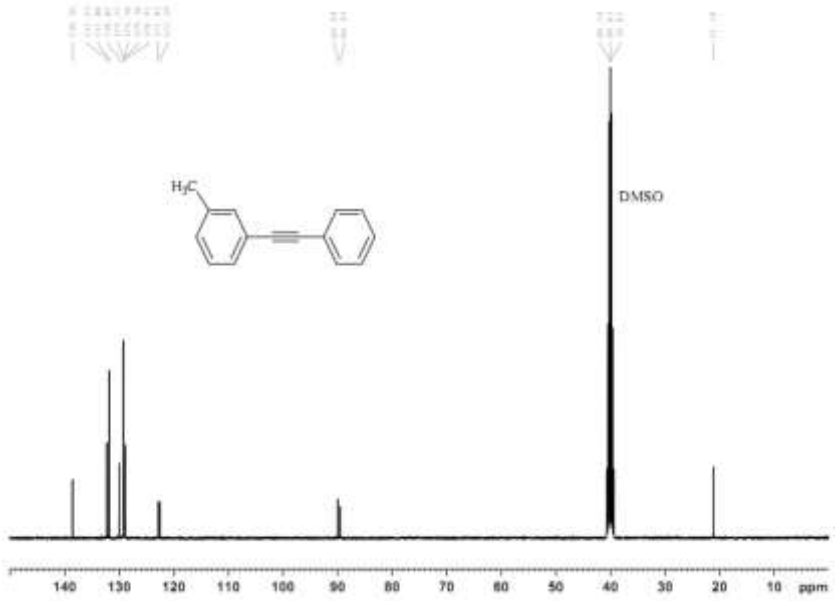
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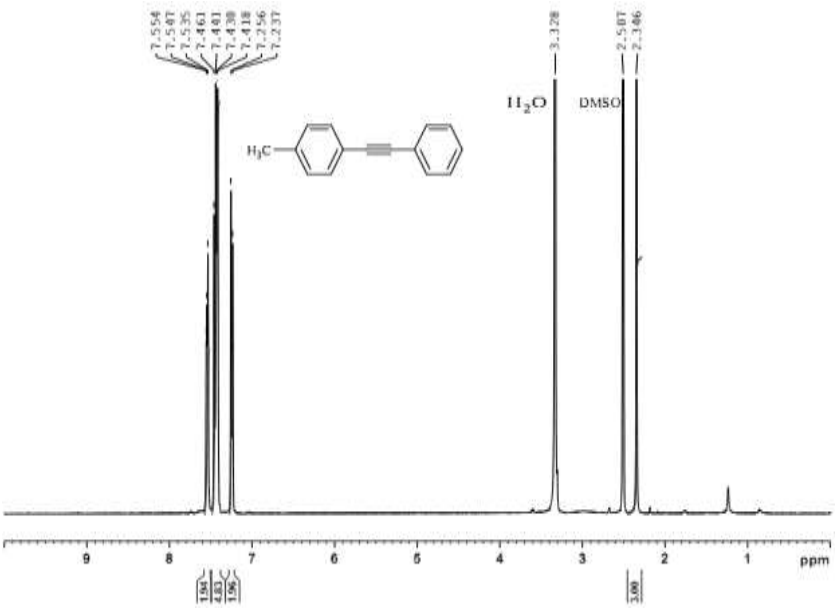
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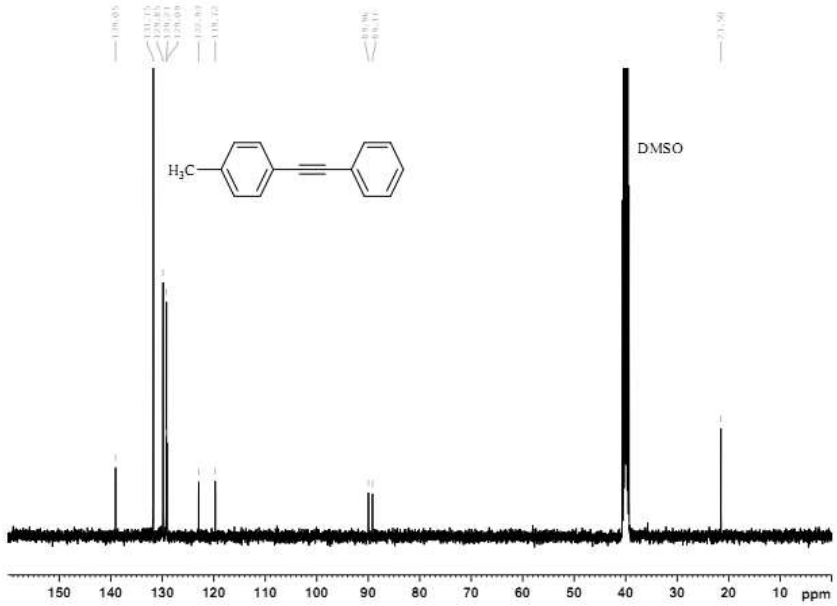
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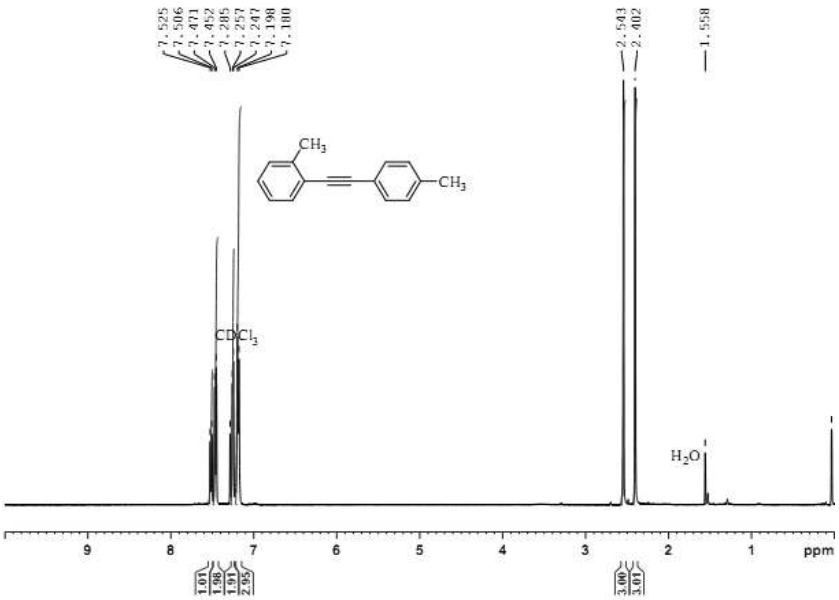
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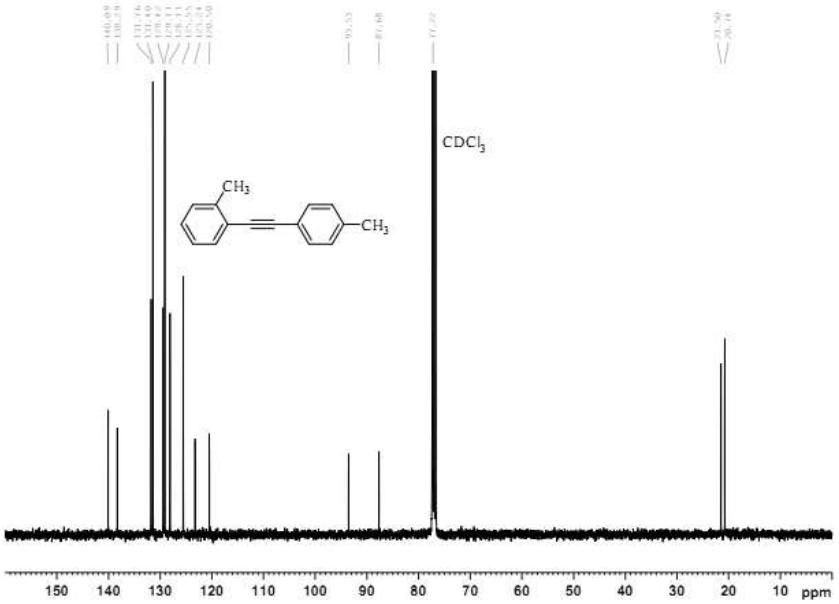
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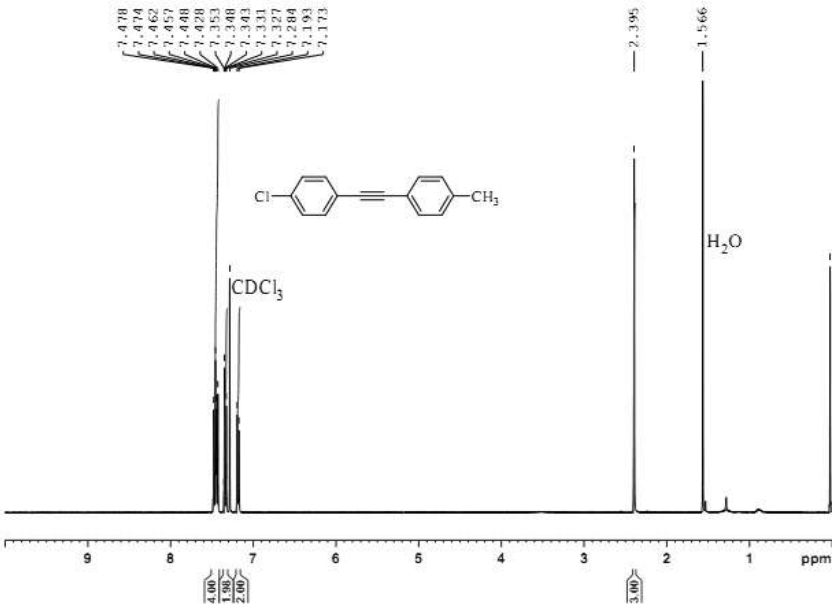
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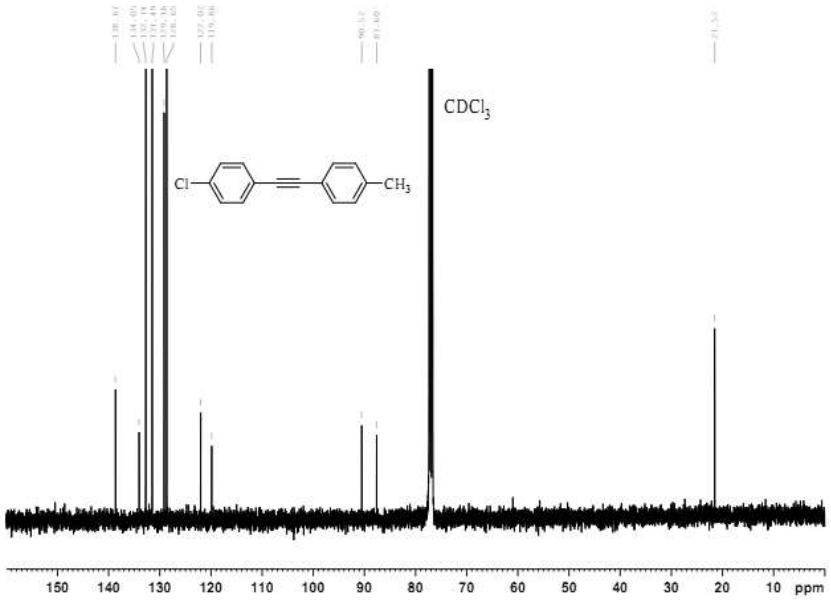
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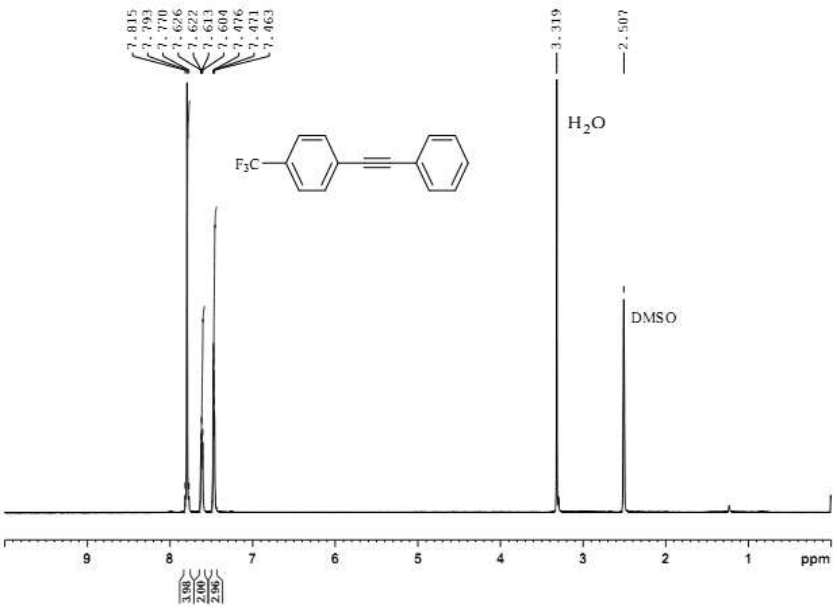
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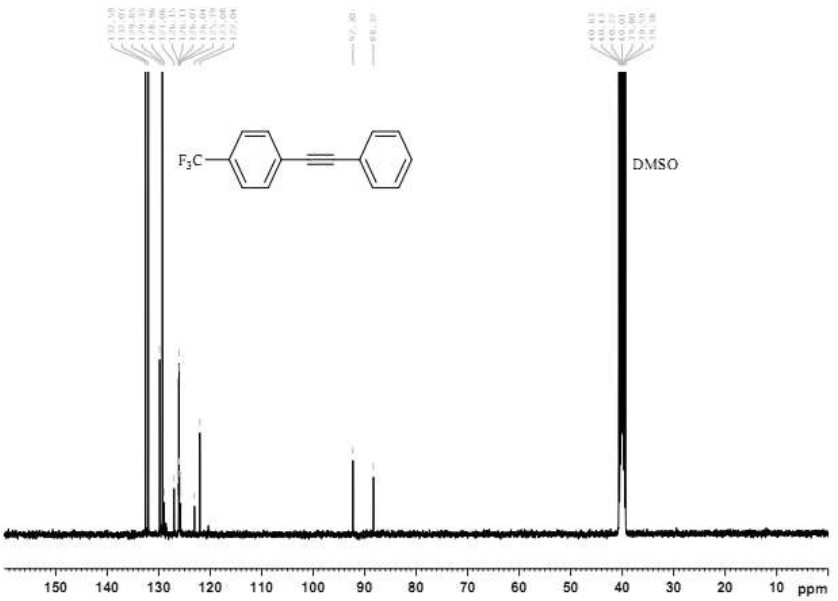
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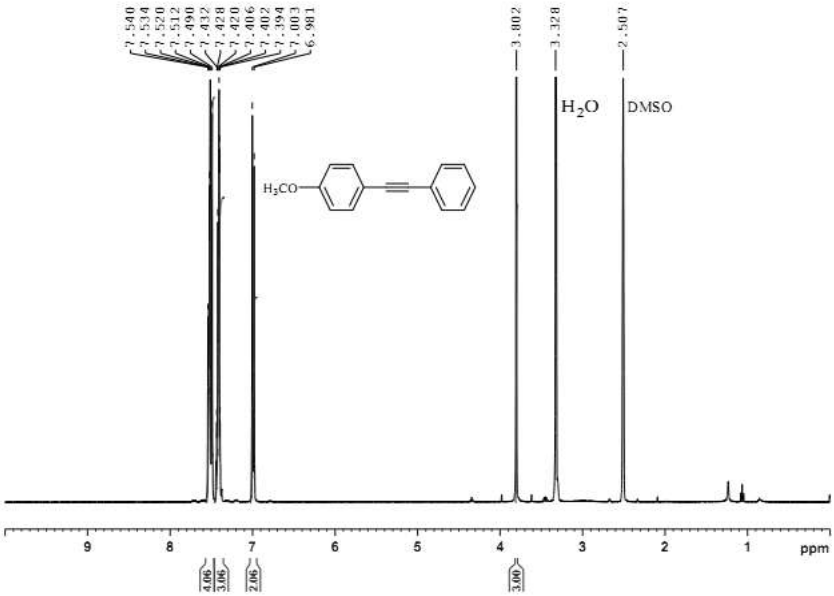
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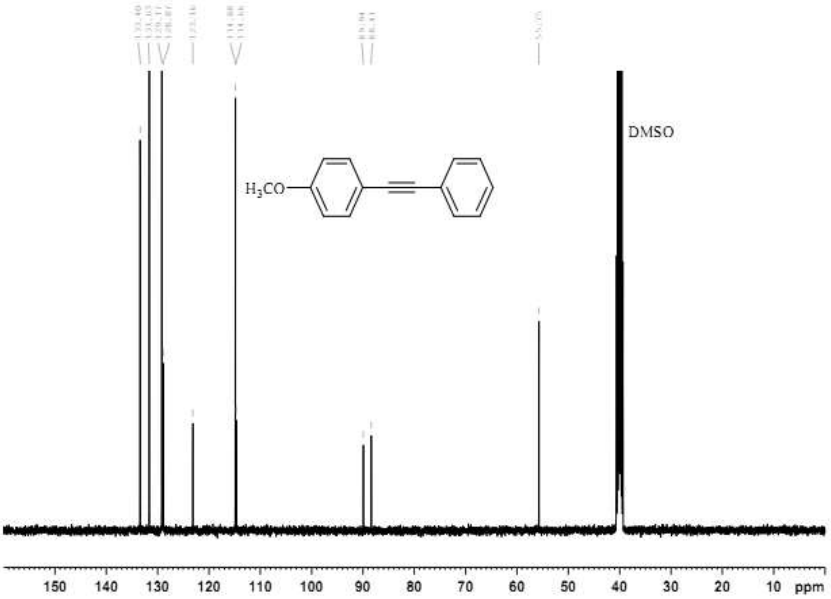
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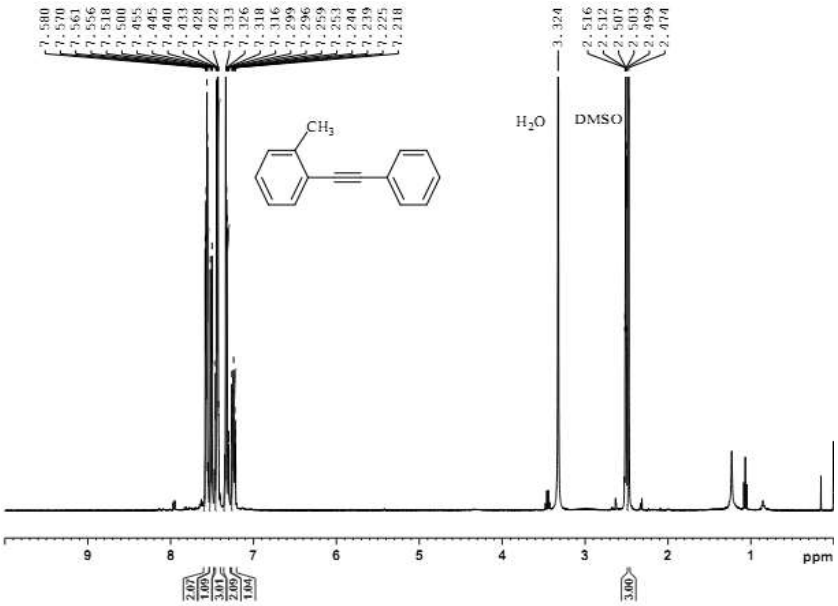
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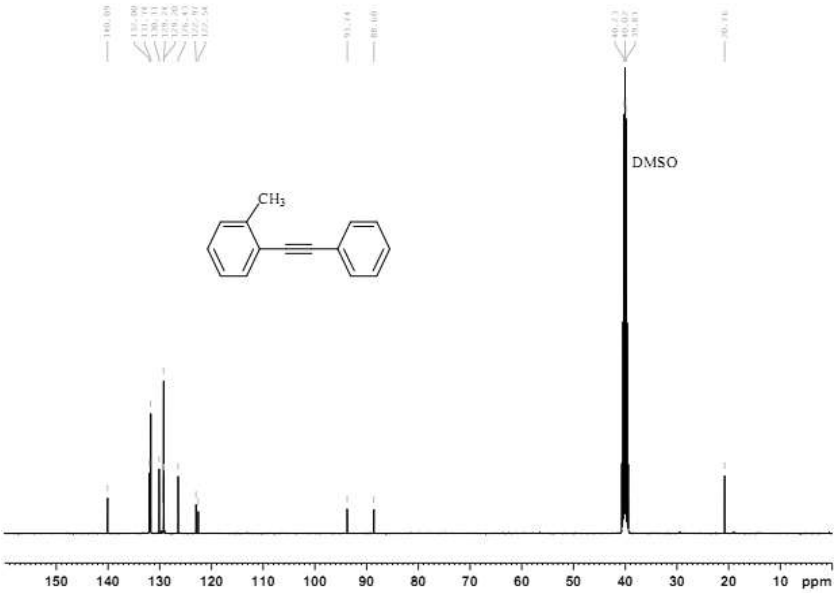
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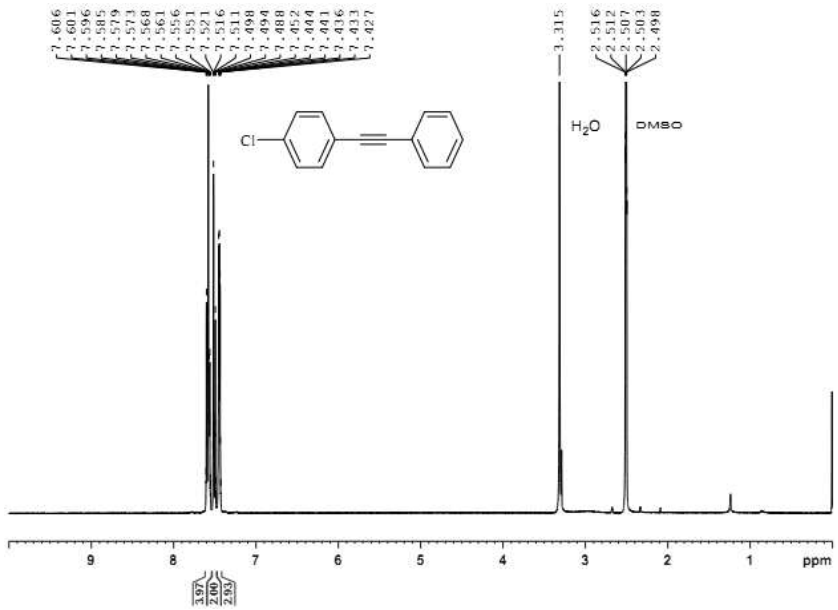
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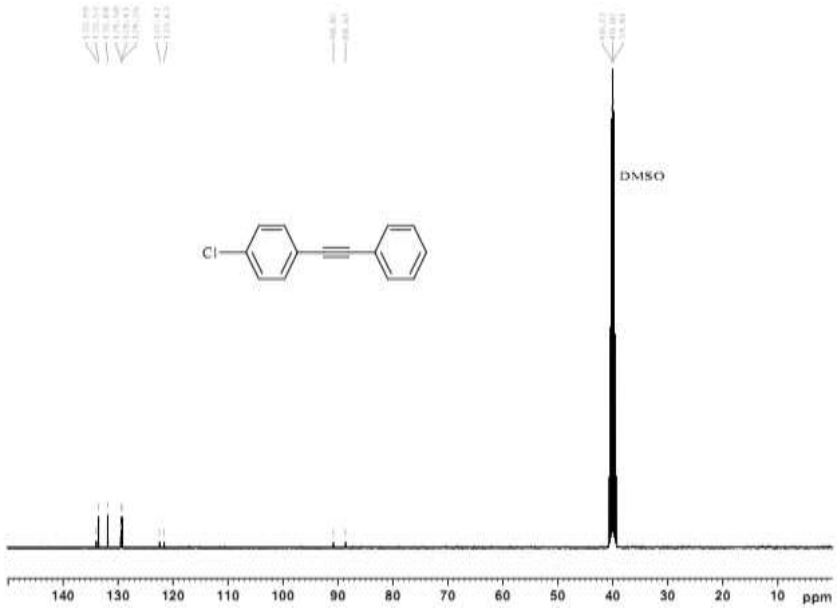
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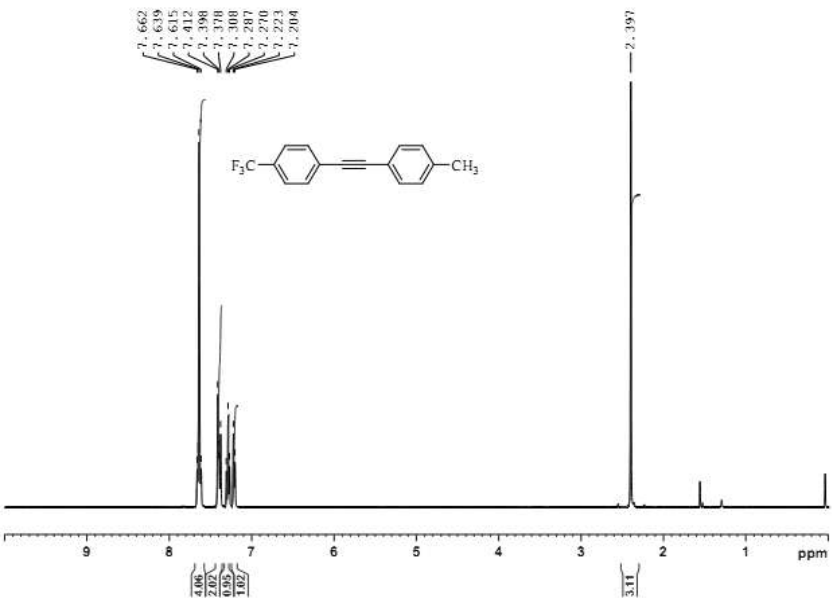
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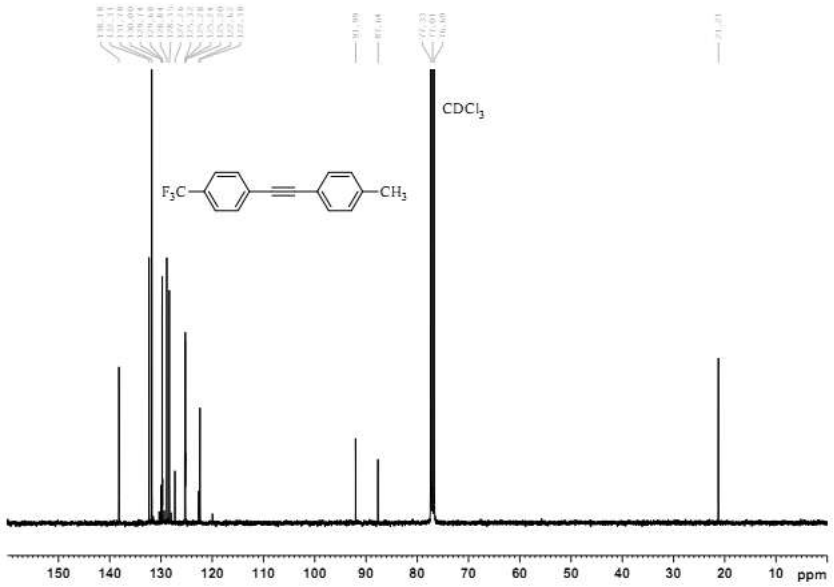
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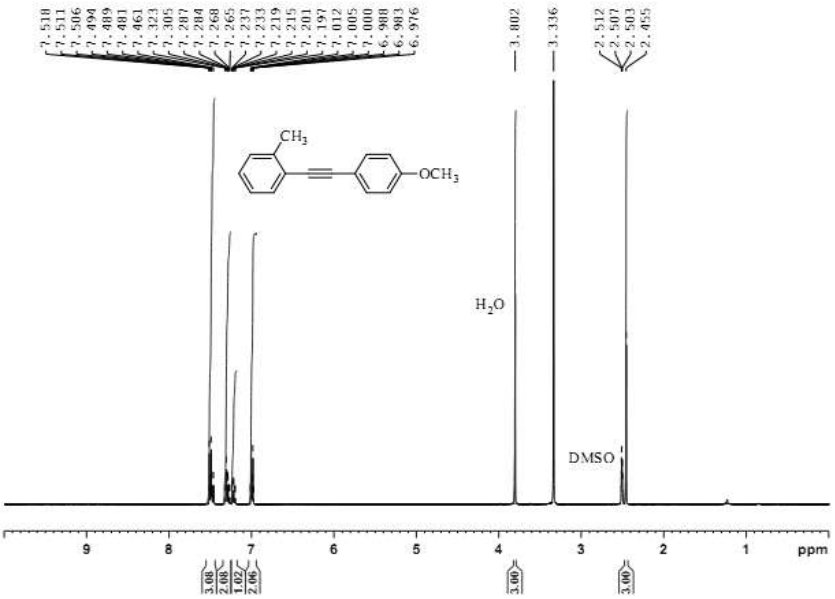
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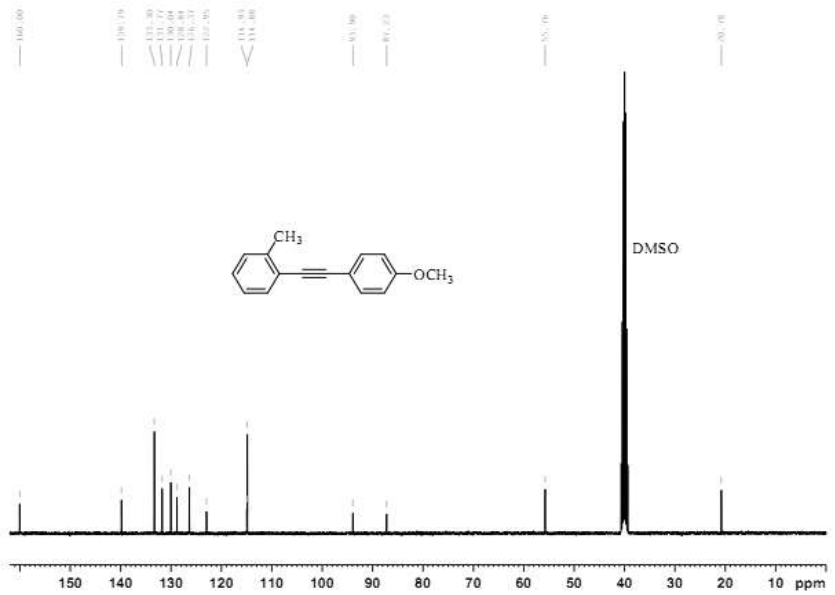
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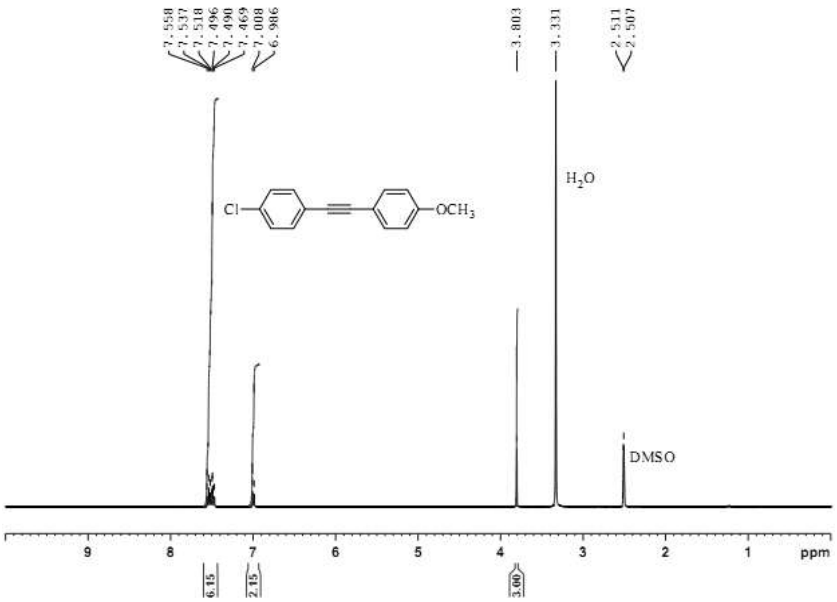
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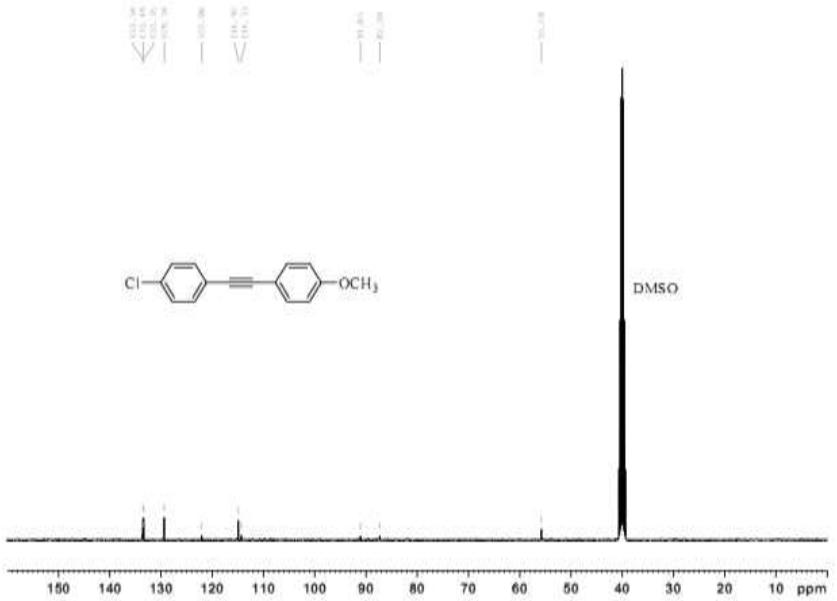
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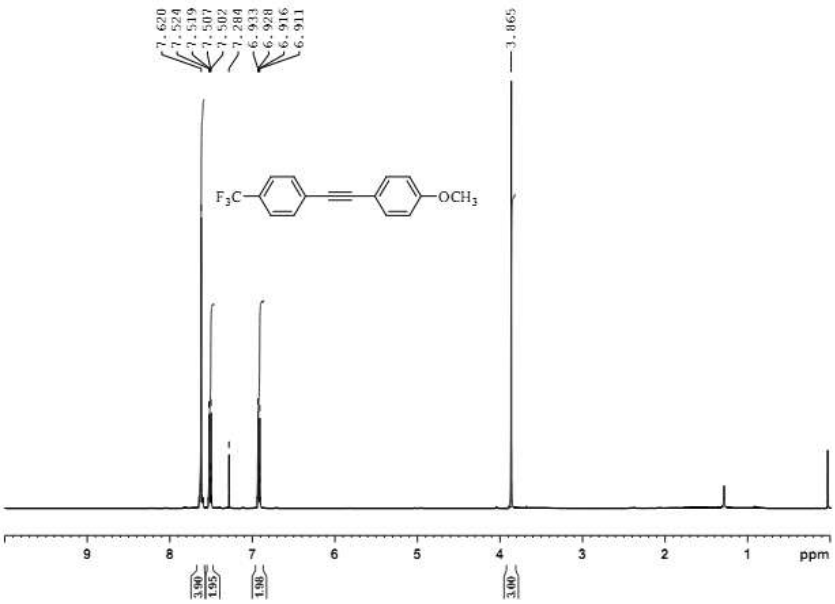
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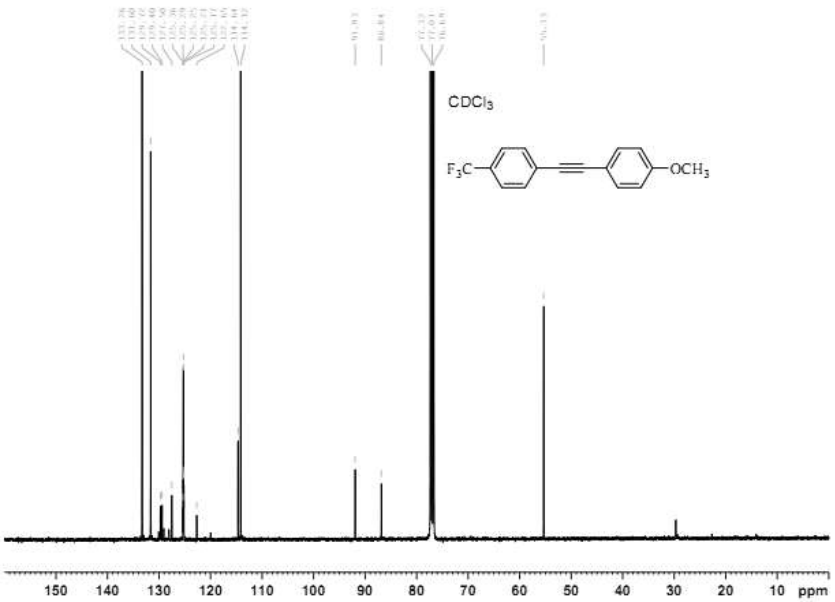
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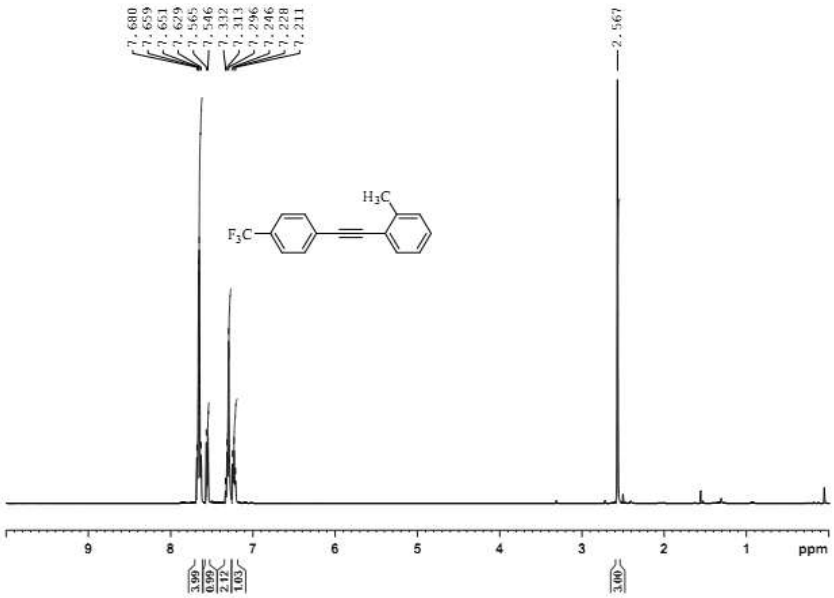
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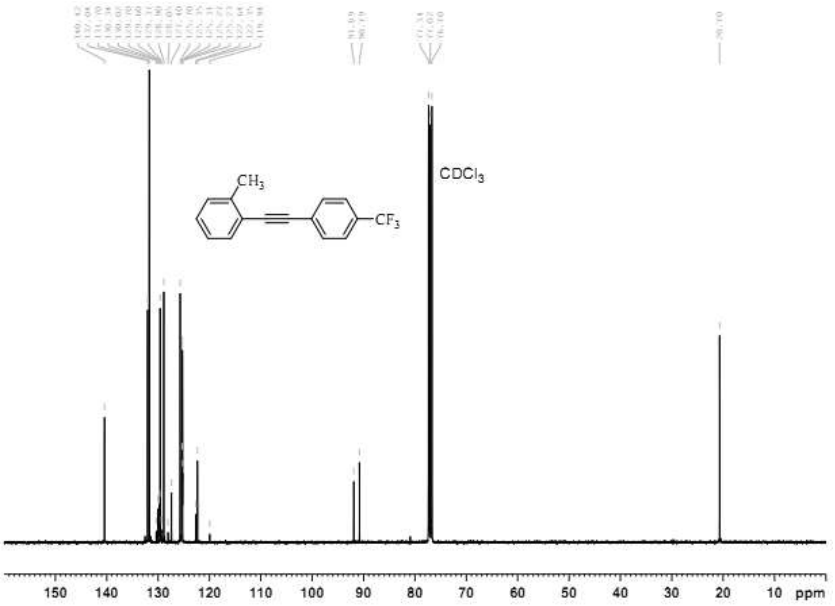
1.03
3.00


CH3
CF3
CDCl3
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140
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20
10
ppm