

Deproto-metallation and computed CH acidity of 2-aryl-1,2,3-triazoles

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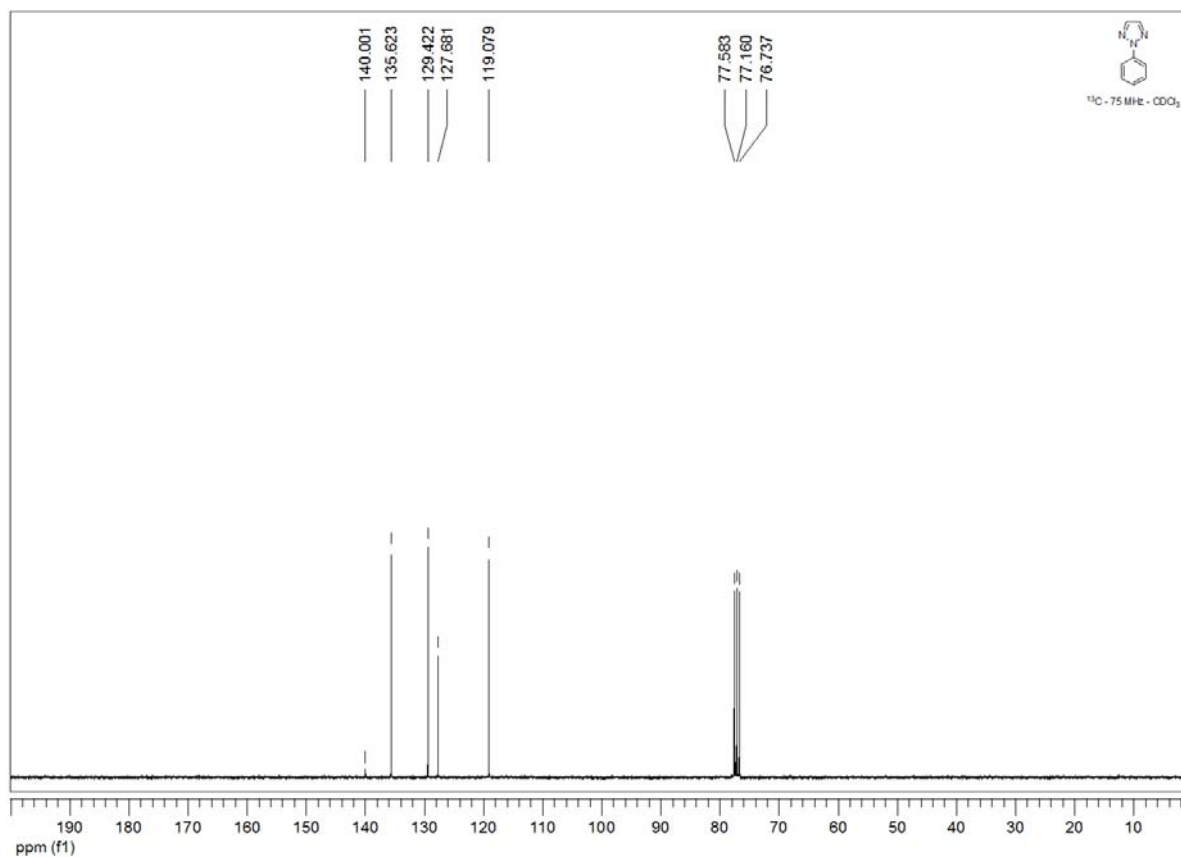
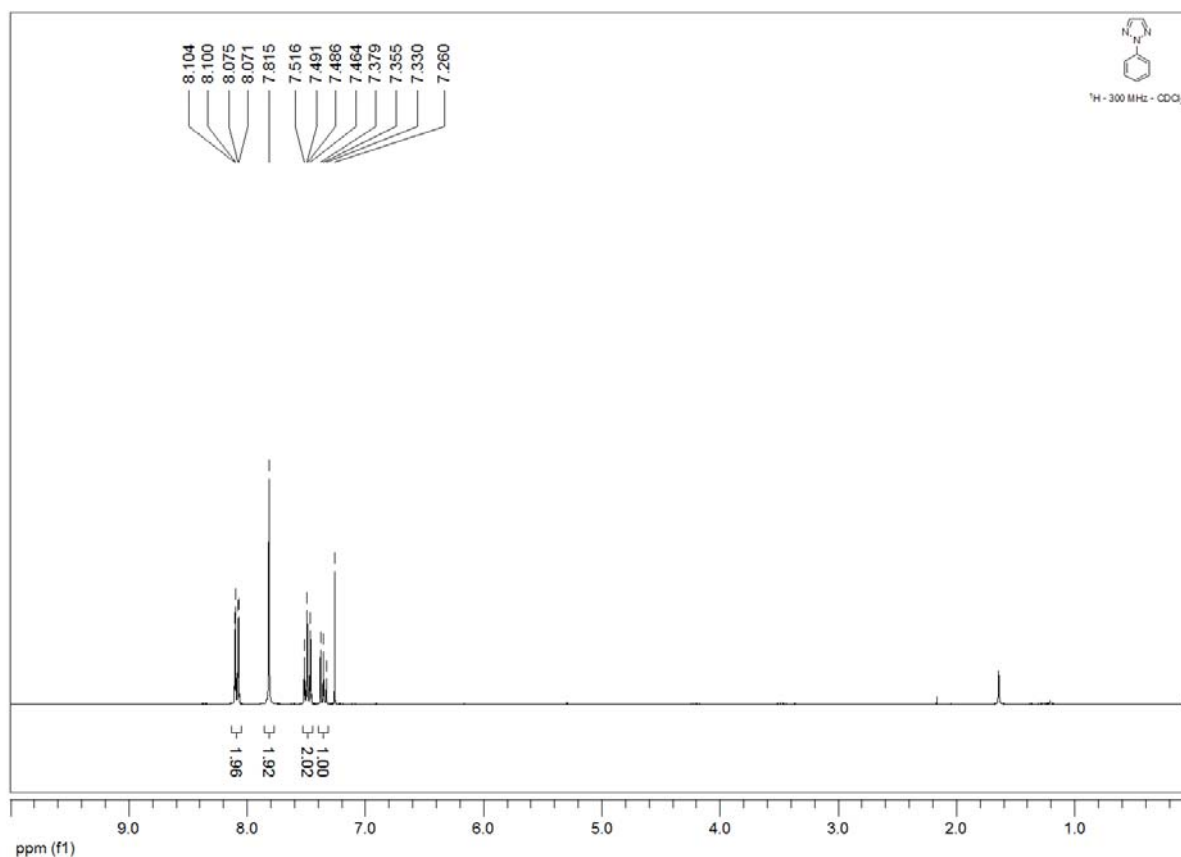
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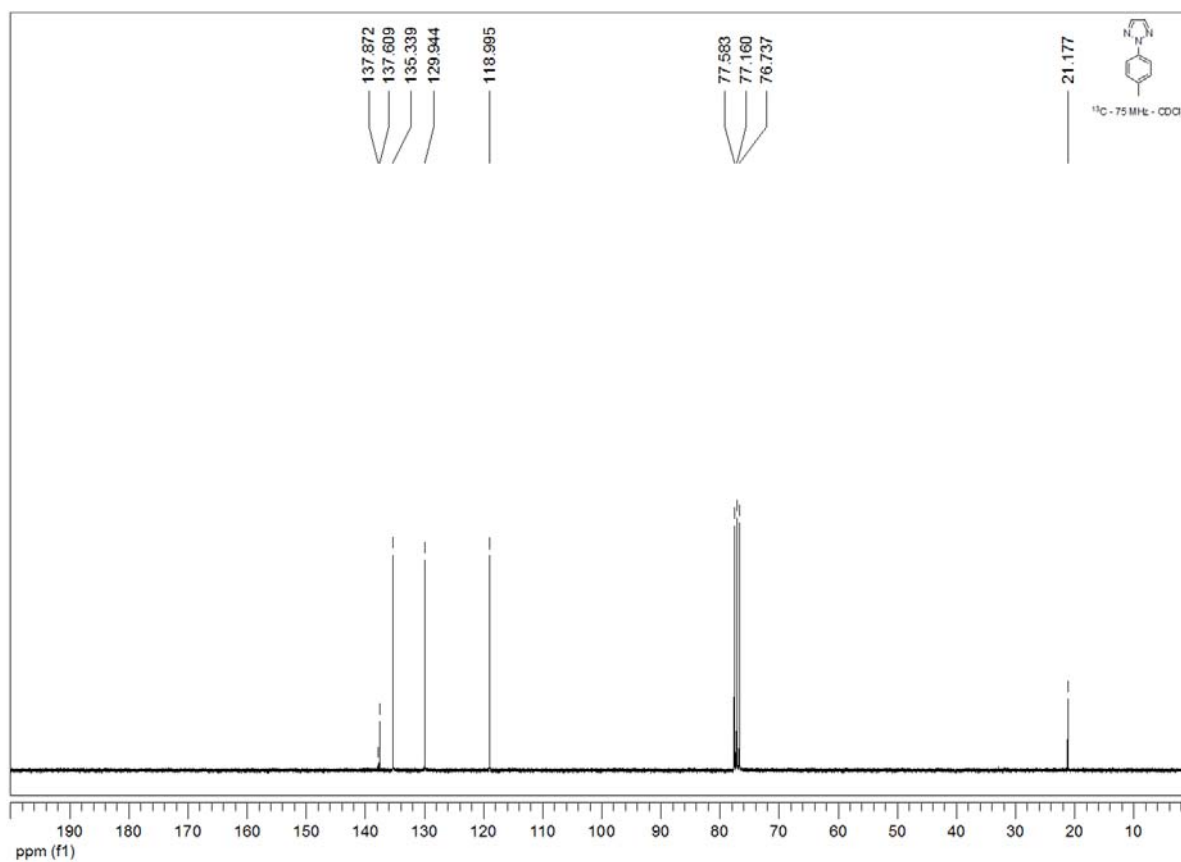
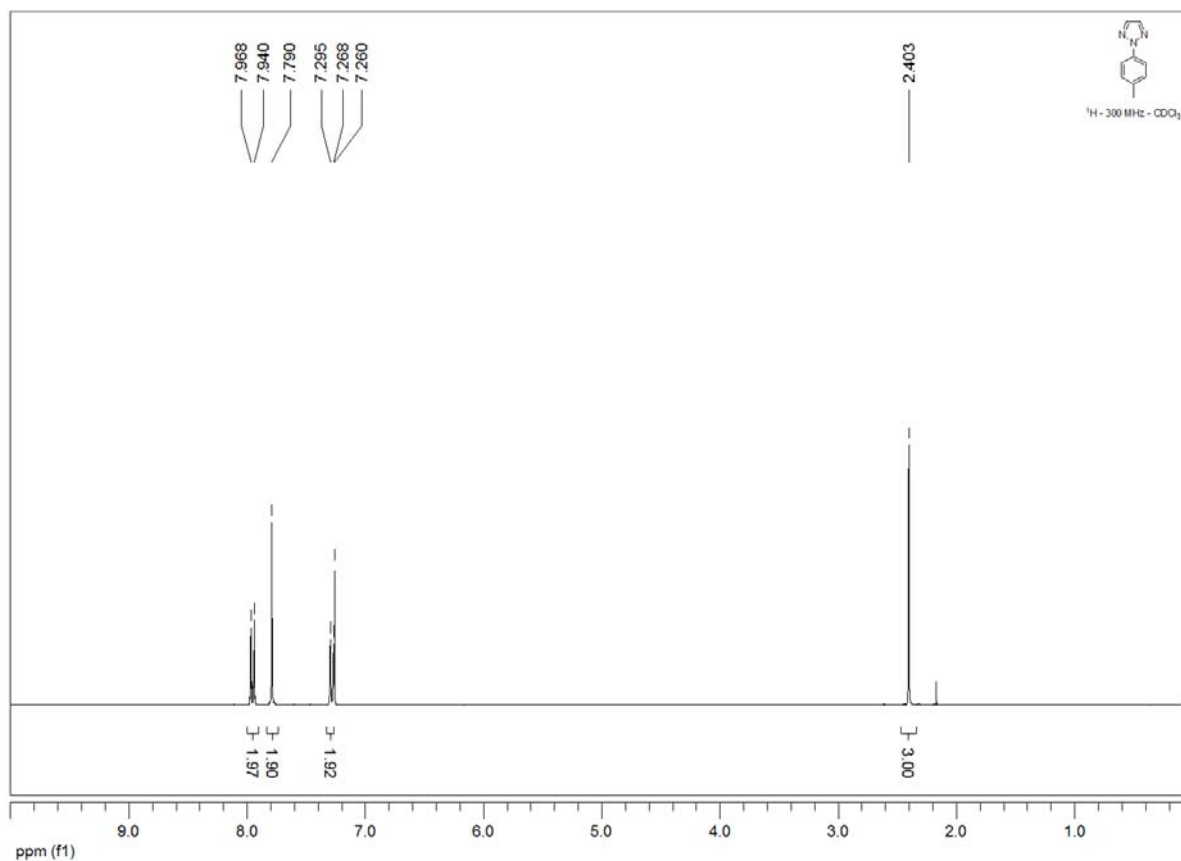
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¹H and ¹³C NMR spectra

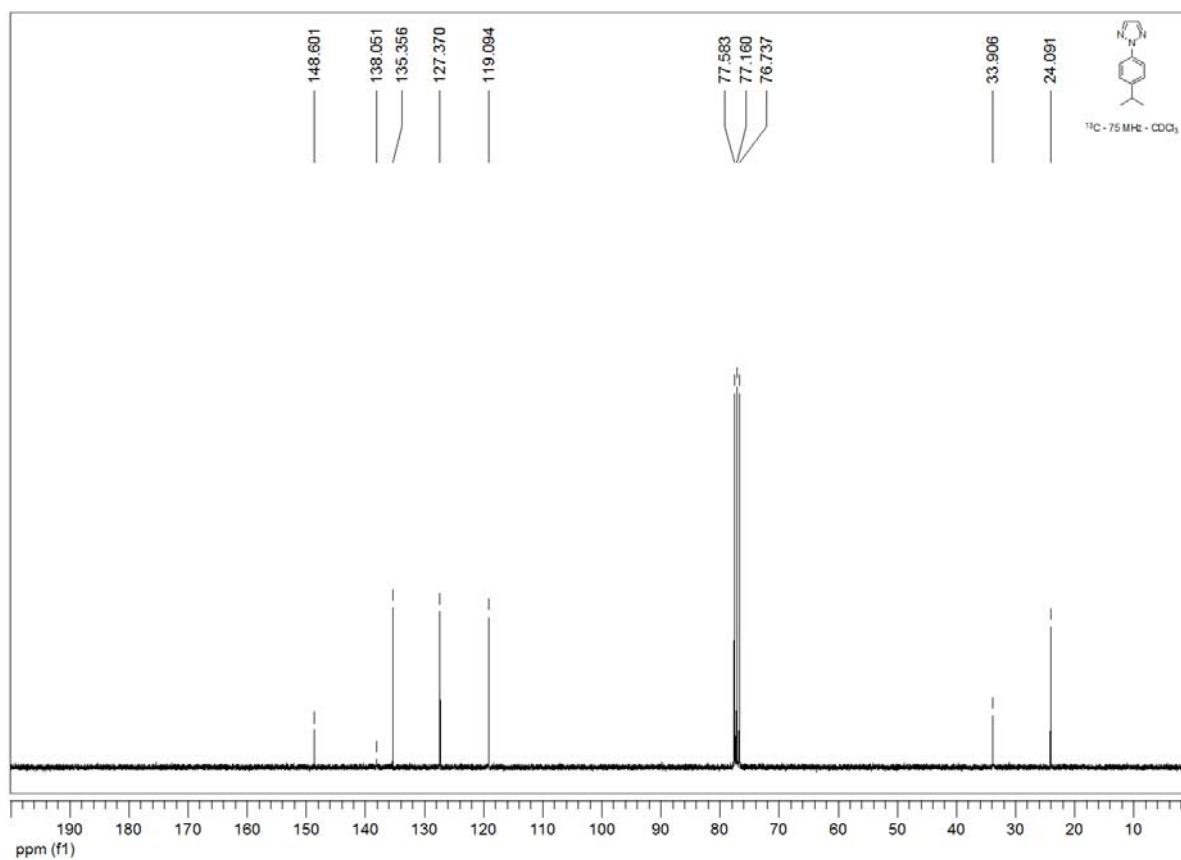
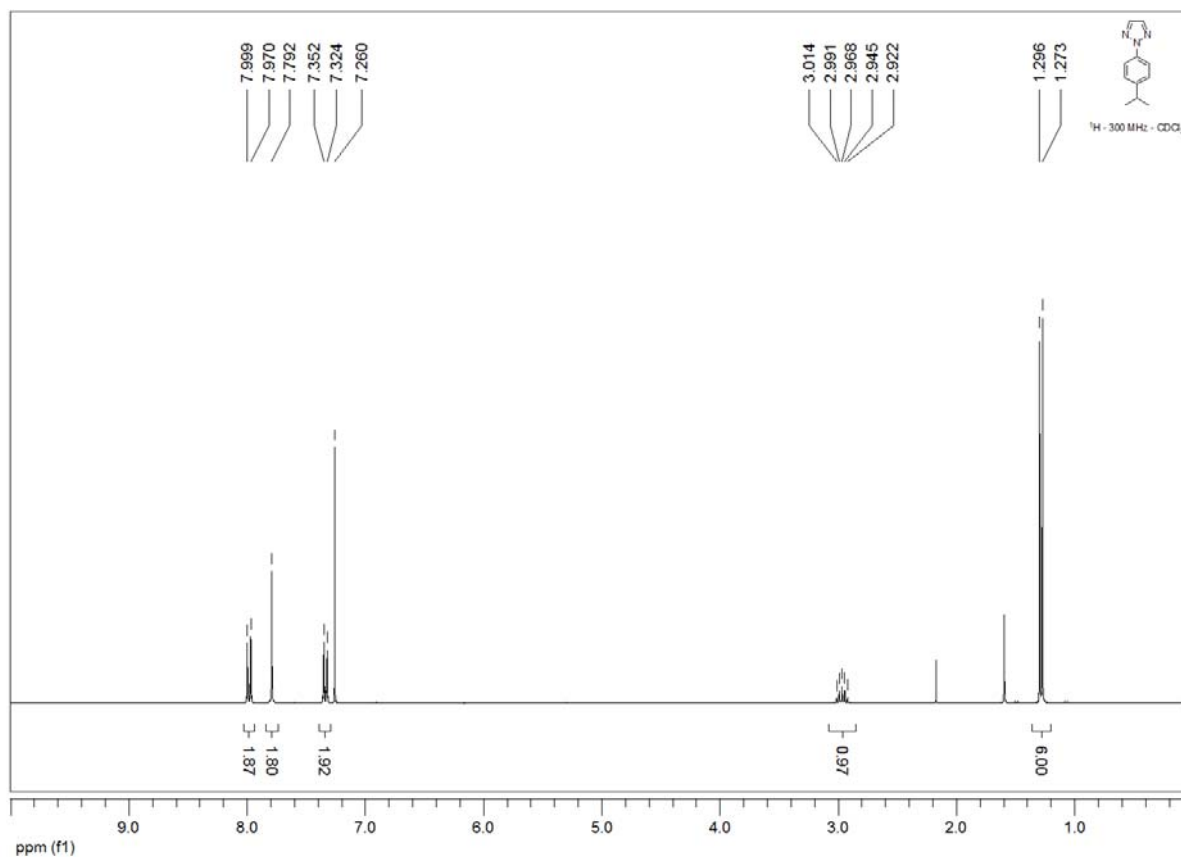
2-Phenyl-2H-[1,2,3]triazole (1a).



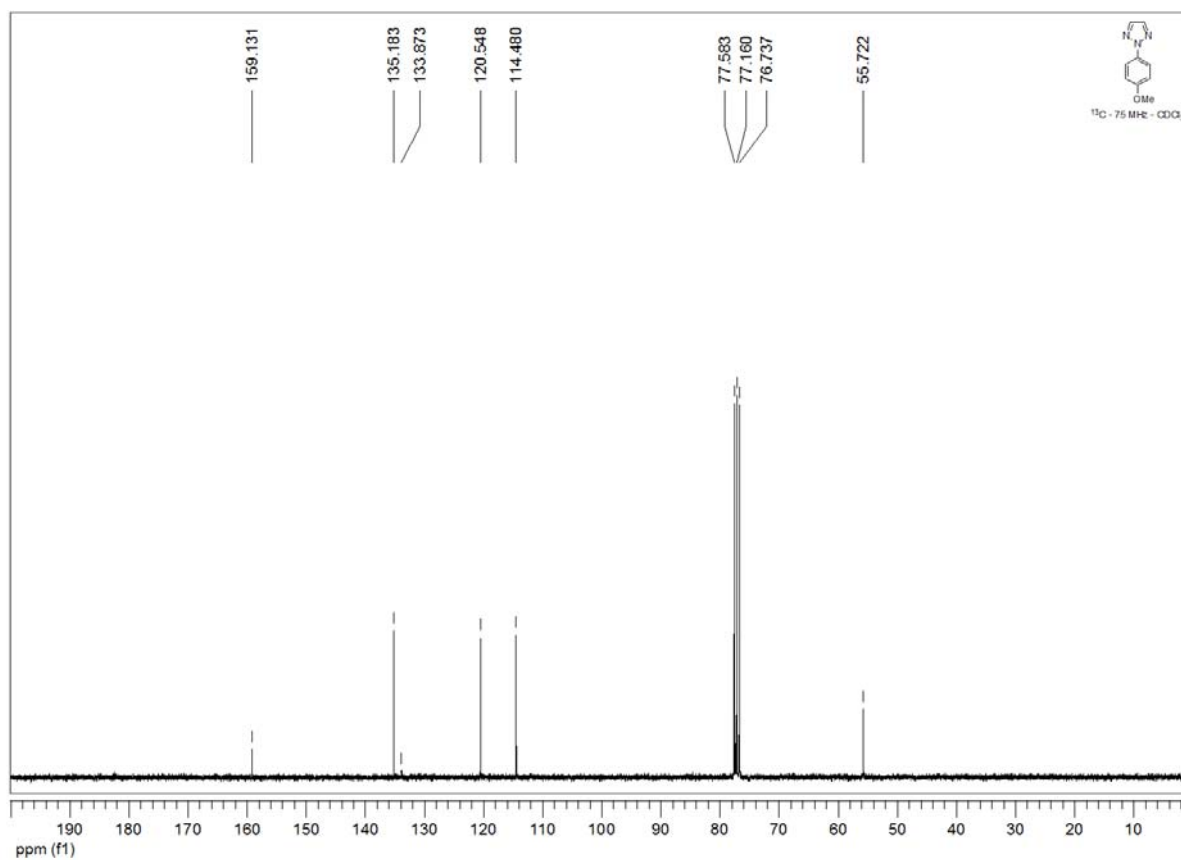
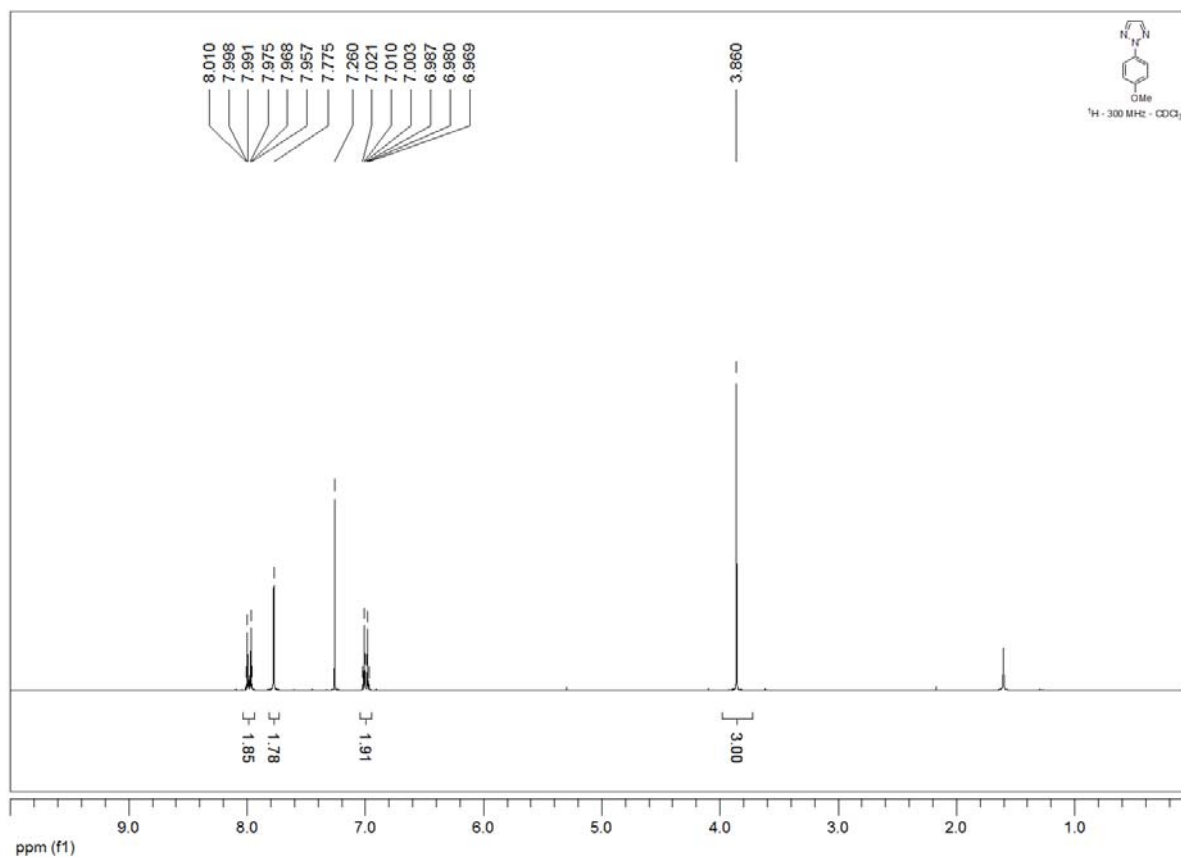
2-(4-Methylphenyl)-2H-[1,2,3]triazole (1b).



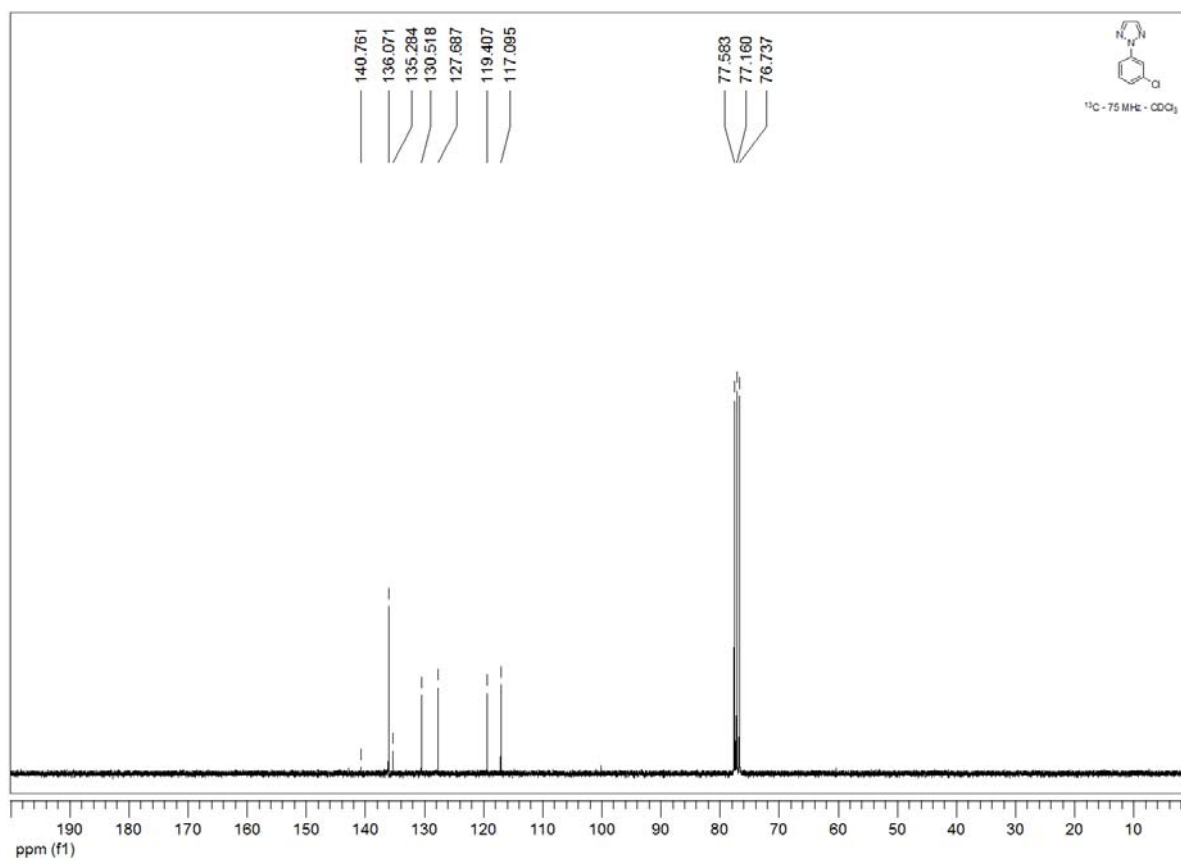
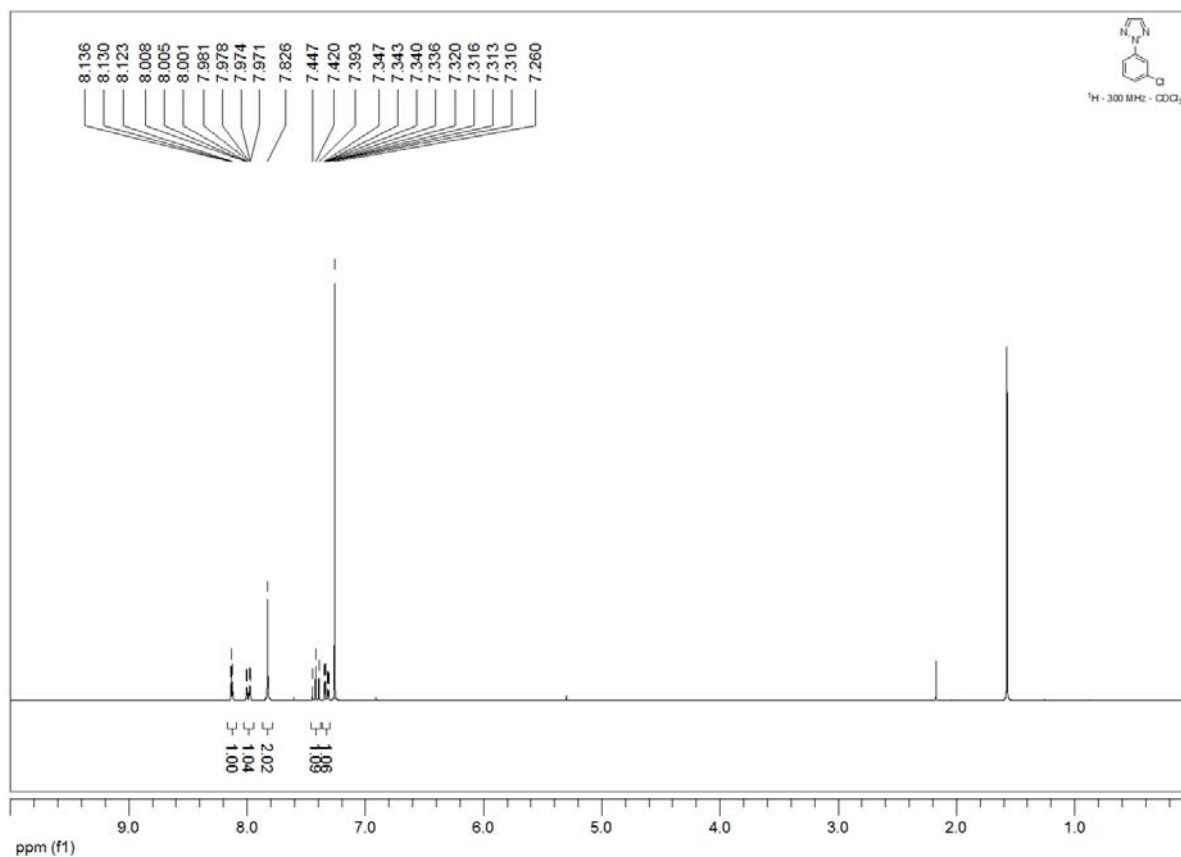
2-(4-Isopropylphenyl)-2H-[1,2,3]triazole (1c).



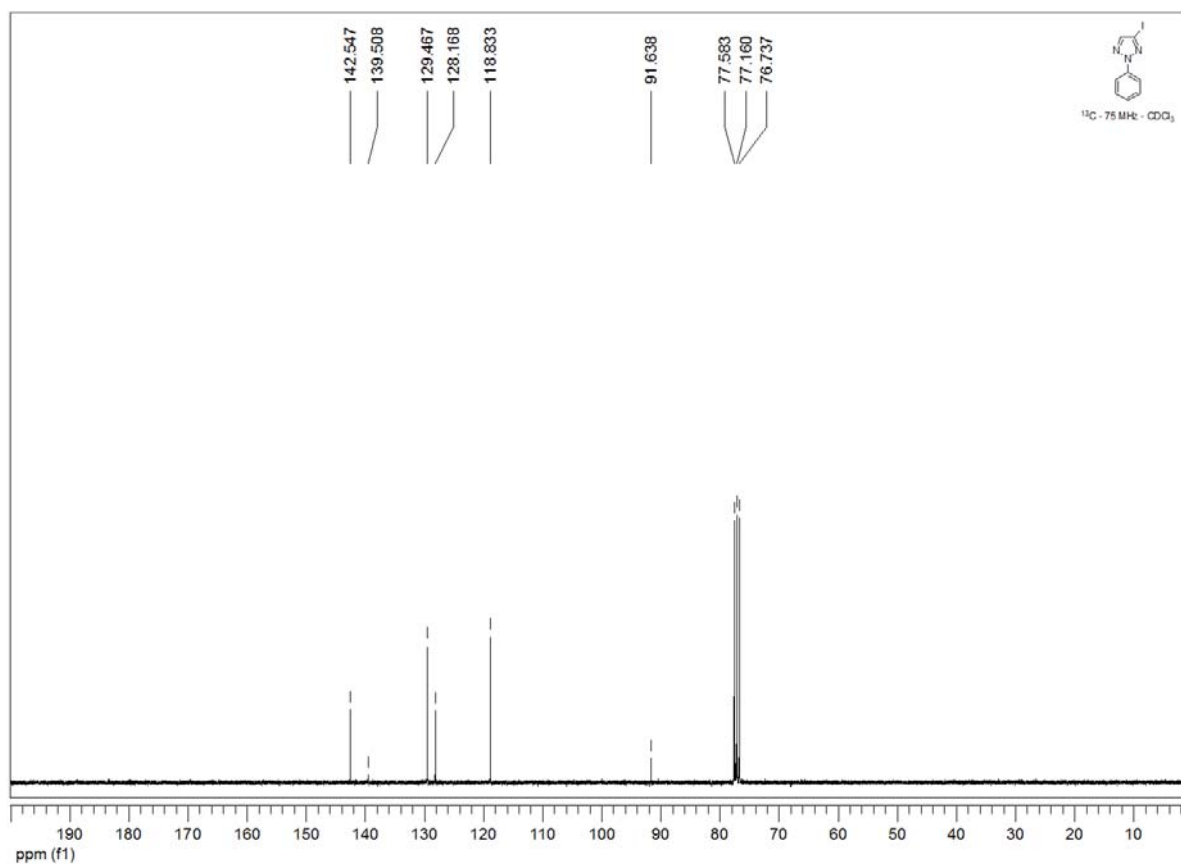
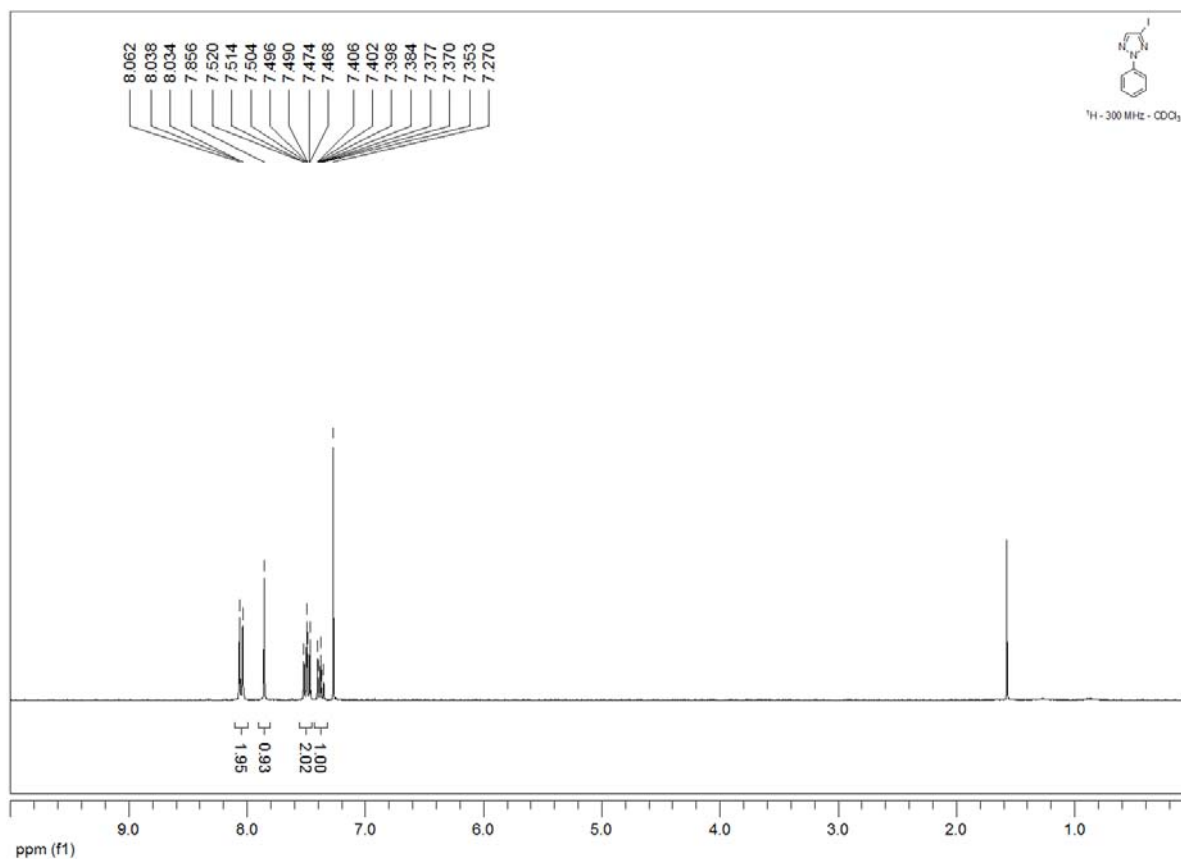
2-(4-Methoxyphenyl)-2H-[1,2,3]triazole (1d).



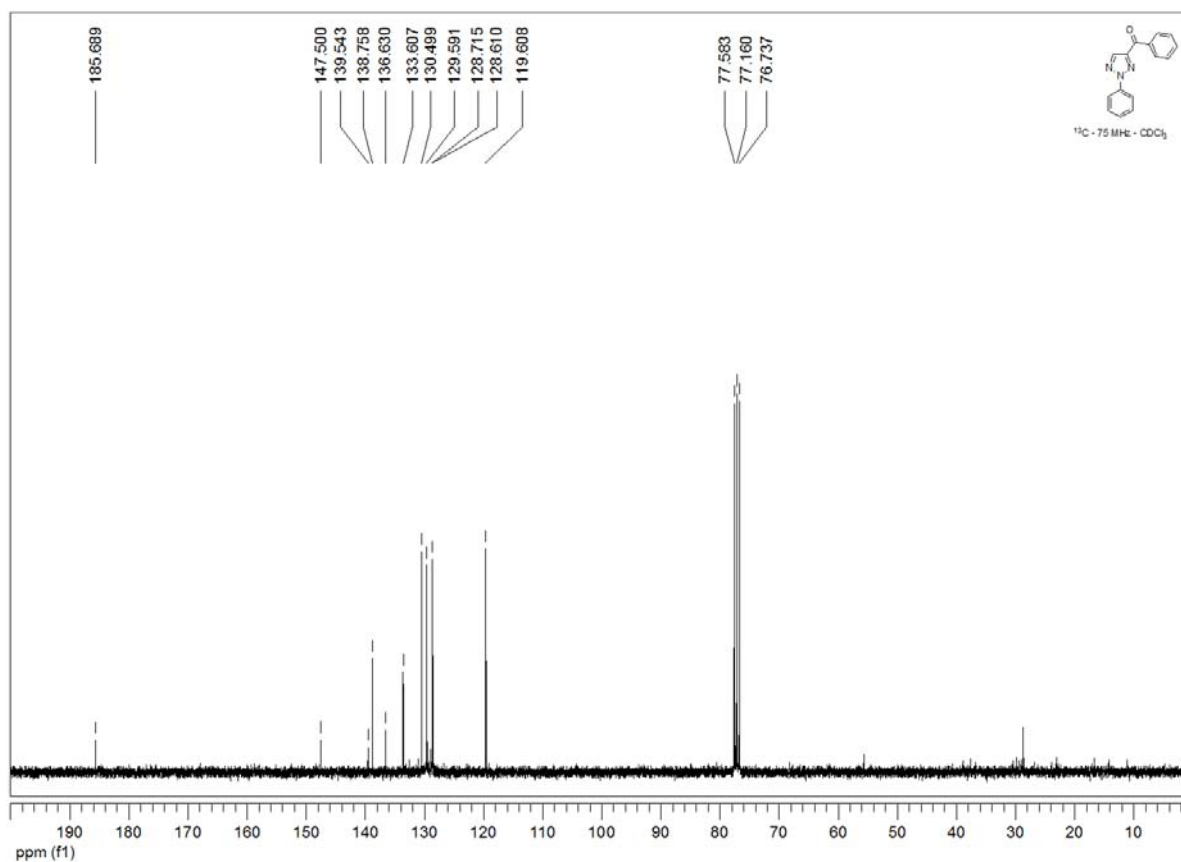
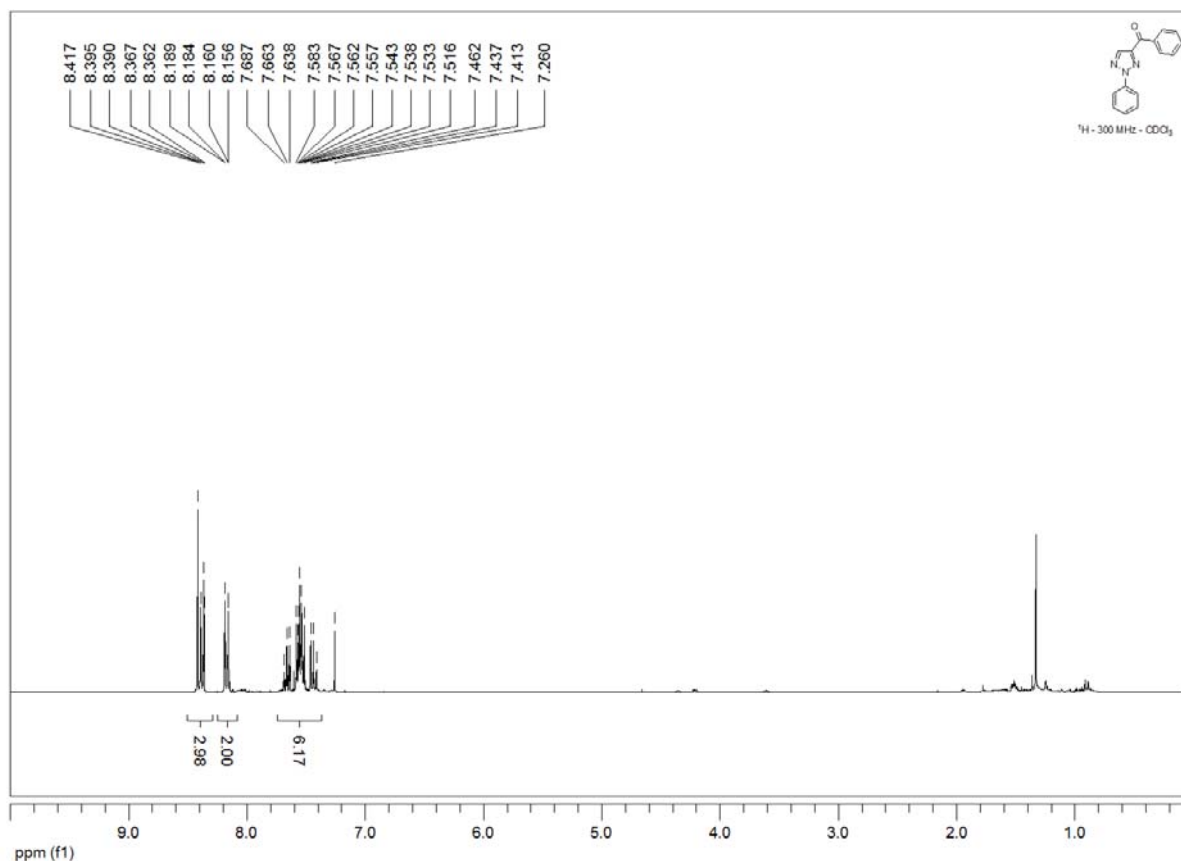
2-(3-Chlorophenyl)-2H-[1,2,3]triazole (1e).



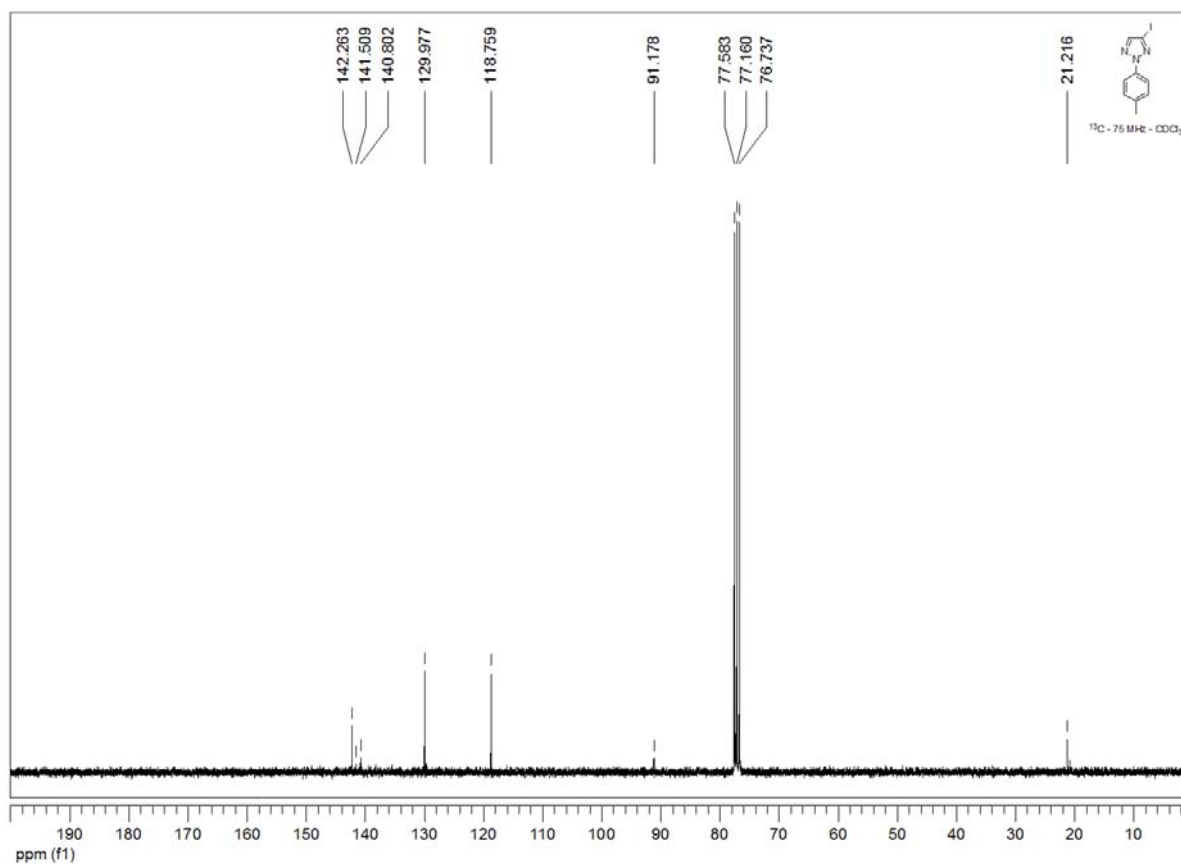
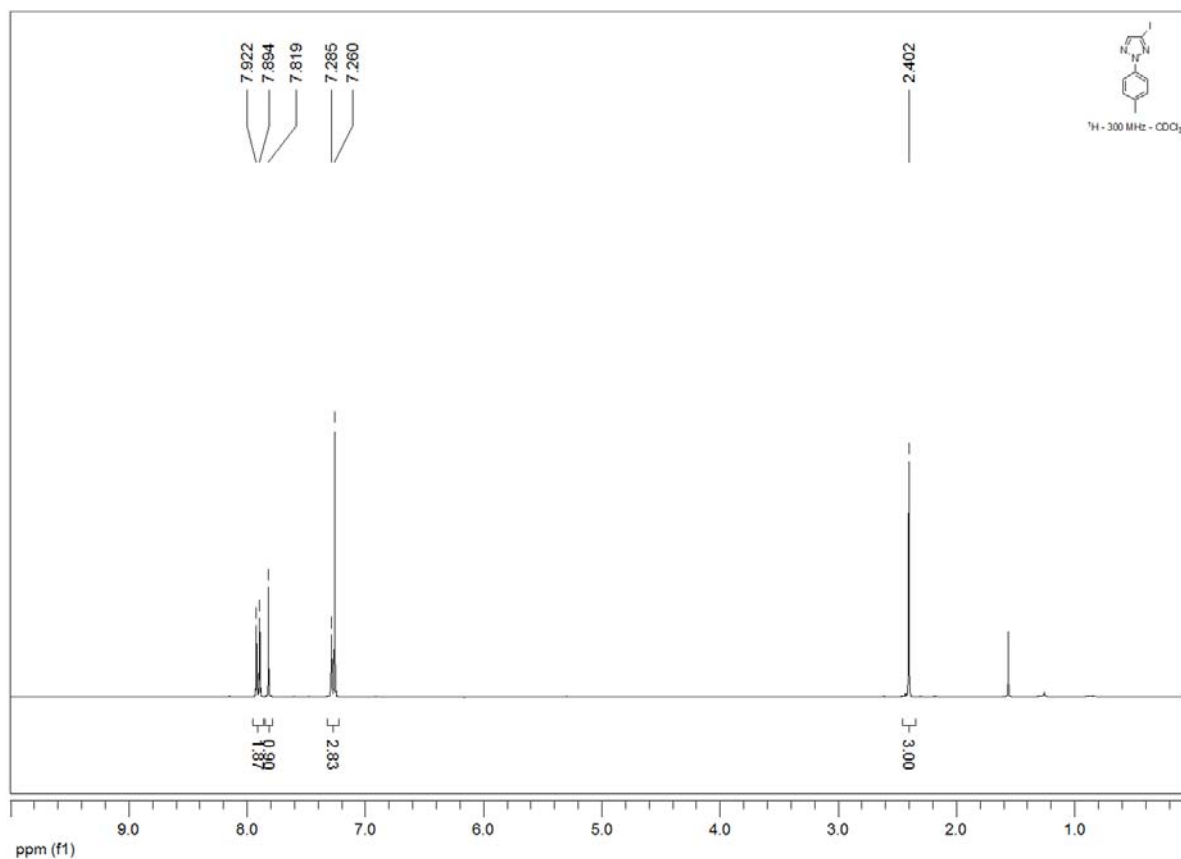
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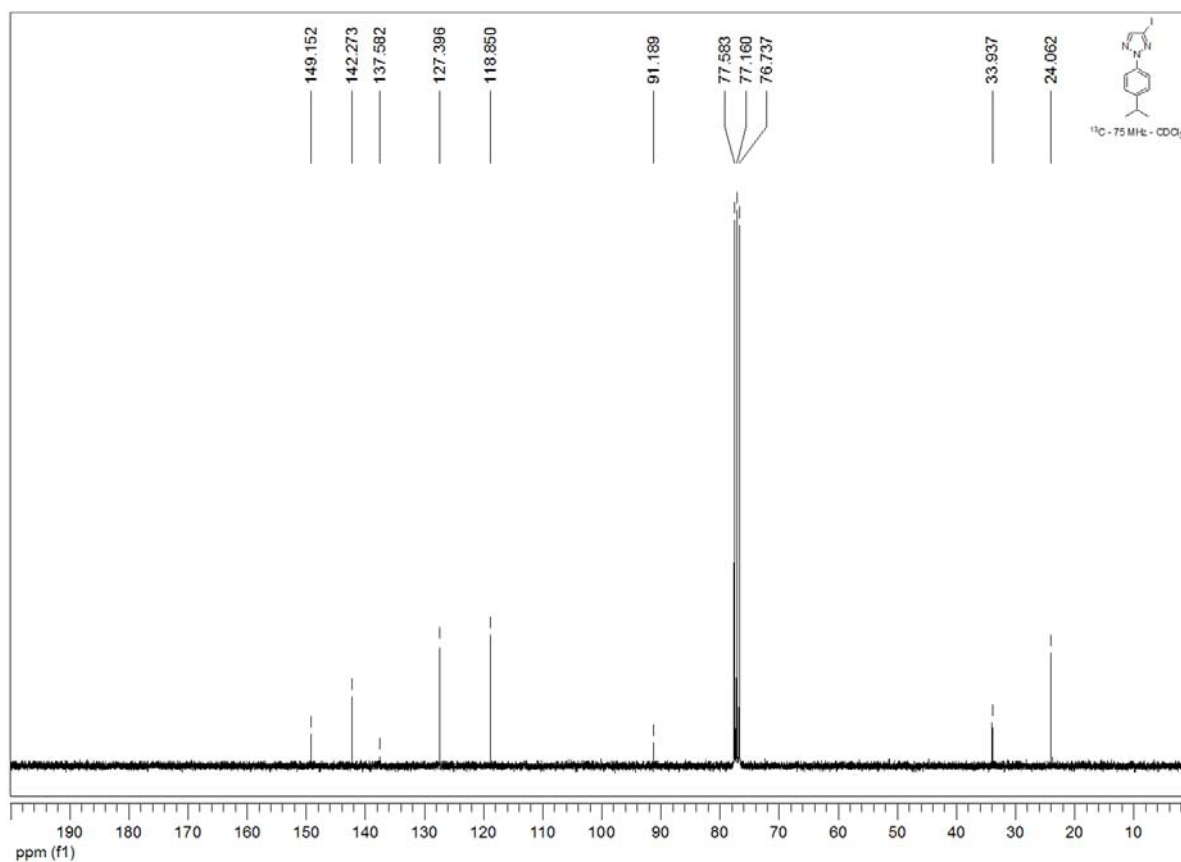
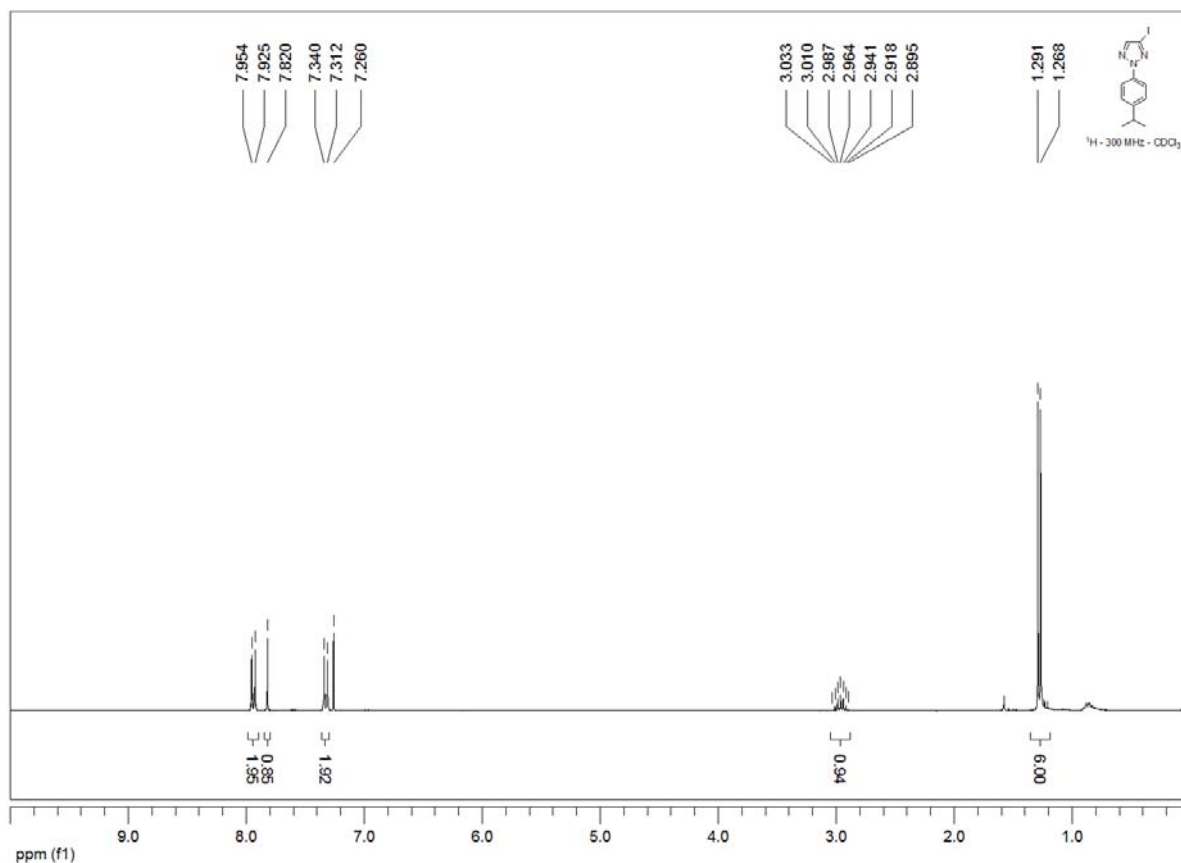
Phenyl-(2-phenyl-2*H*-[1,2,3]-triazol-4-yl)methanone (2a').



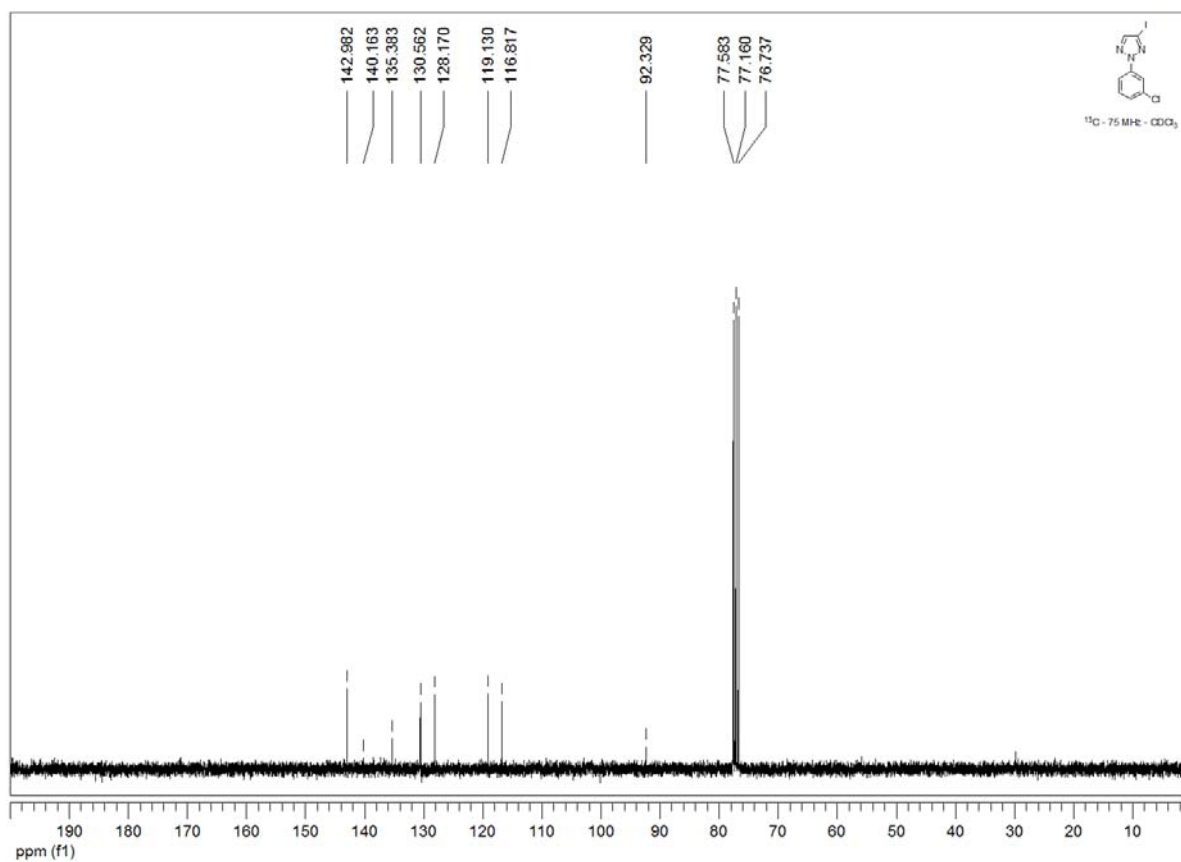
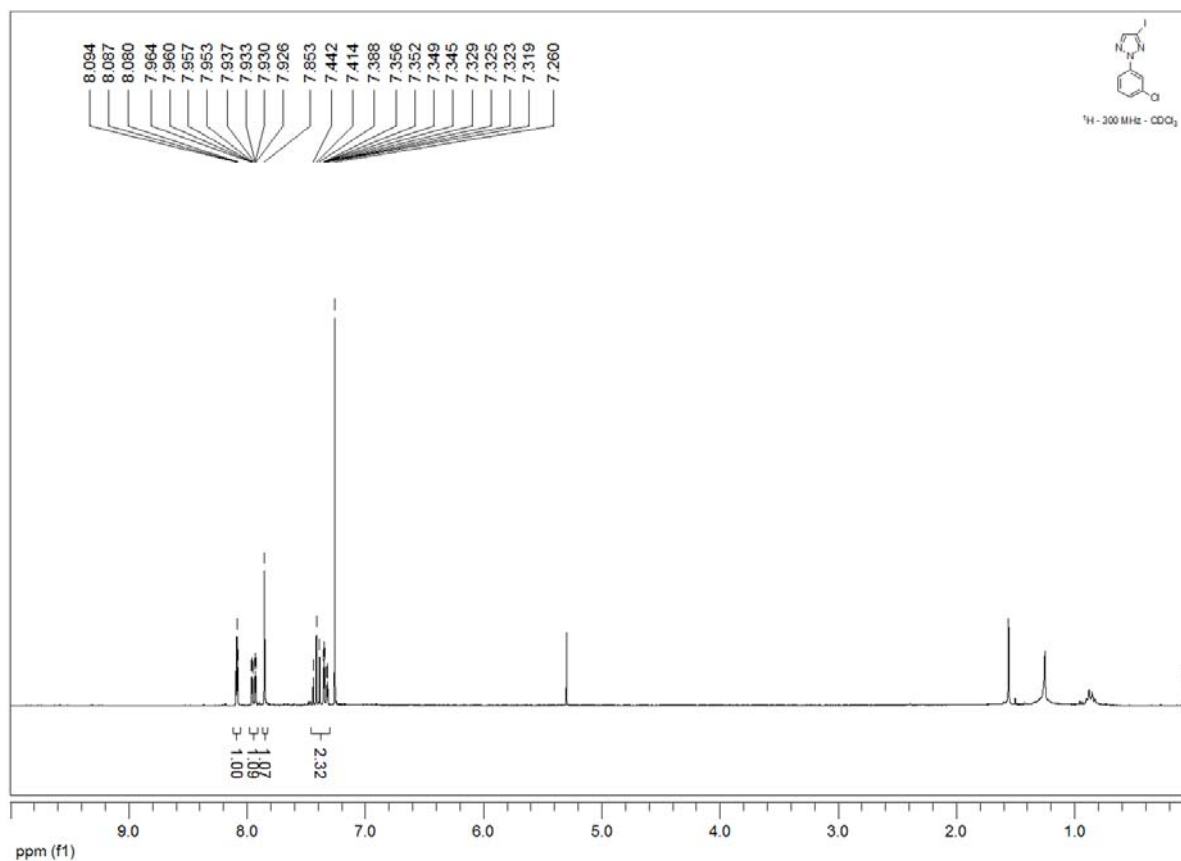
4-Iodo-2-(4-methylphenyl)-2H-[1,2,3]triazole (2b).



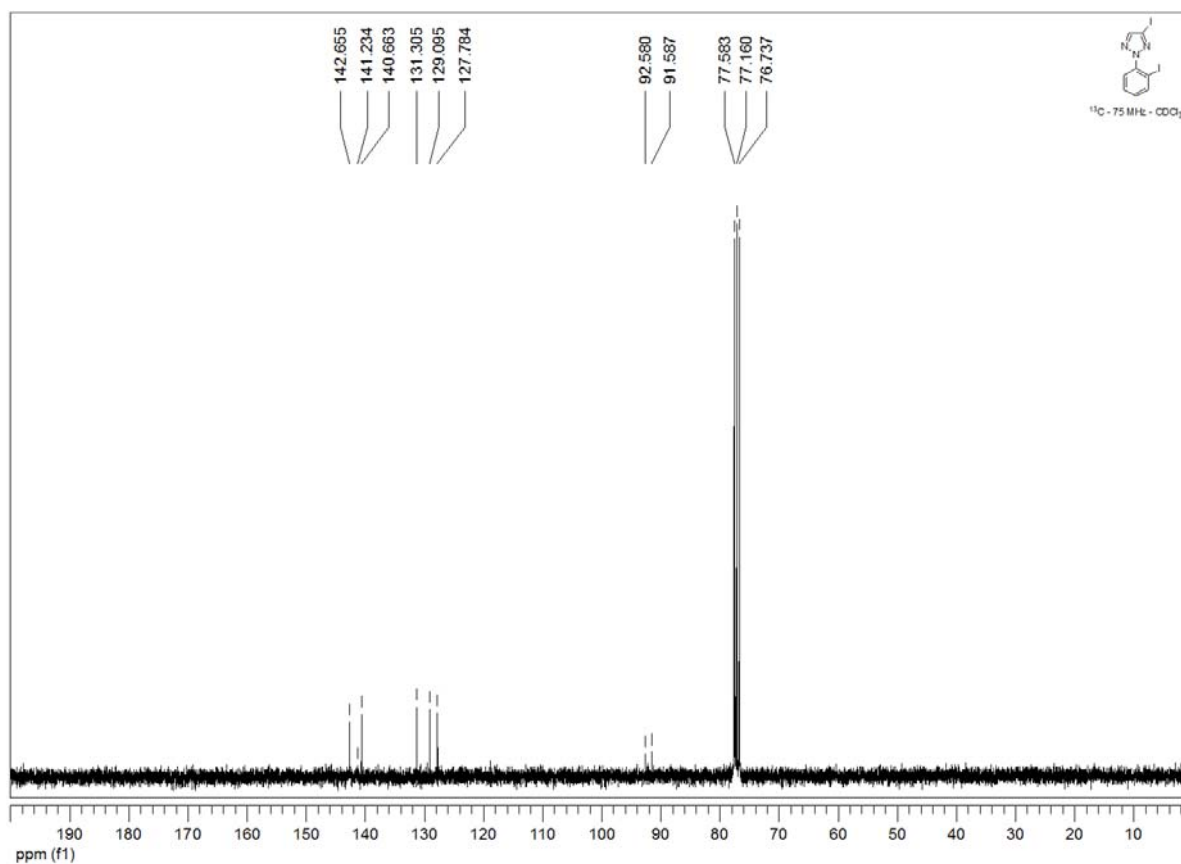
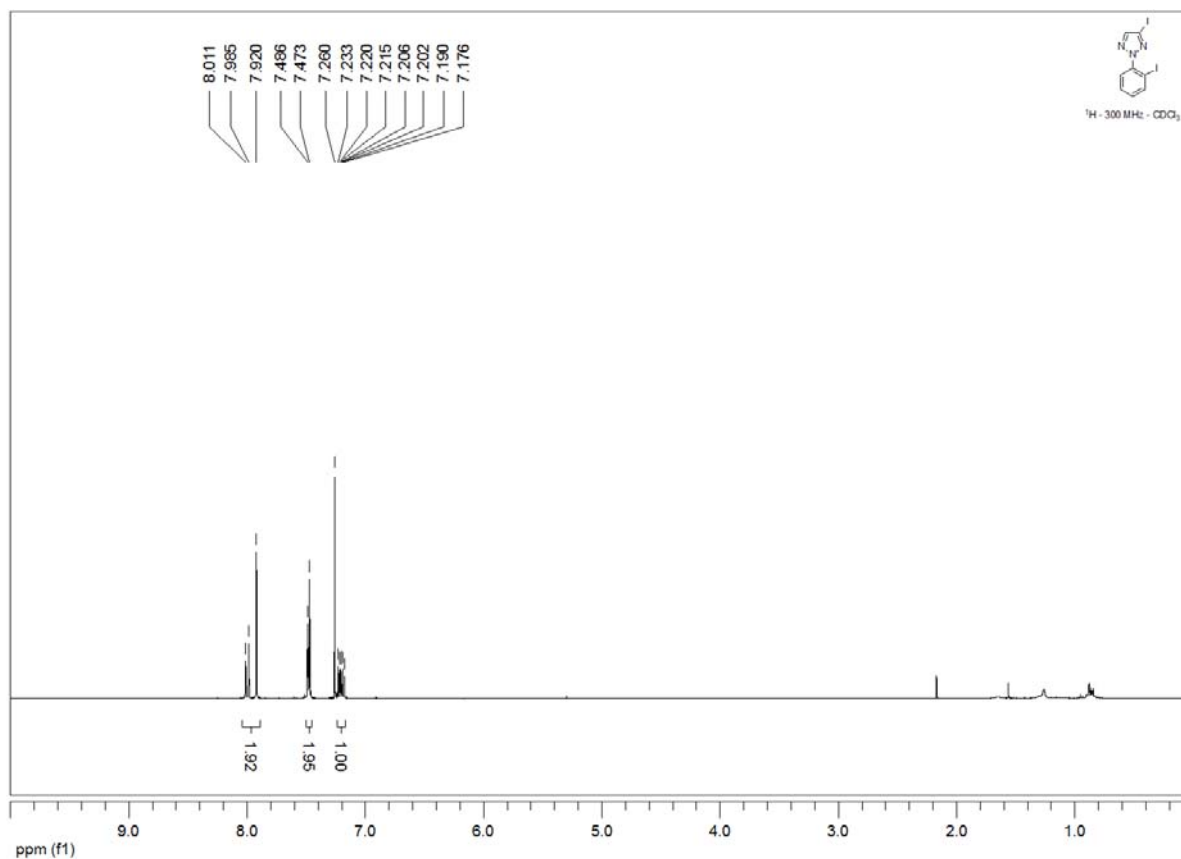
4-Iodo-2-(4-isopropylphenyl)-2H-[1,2,3]triazole (2c).



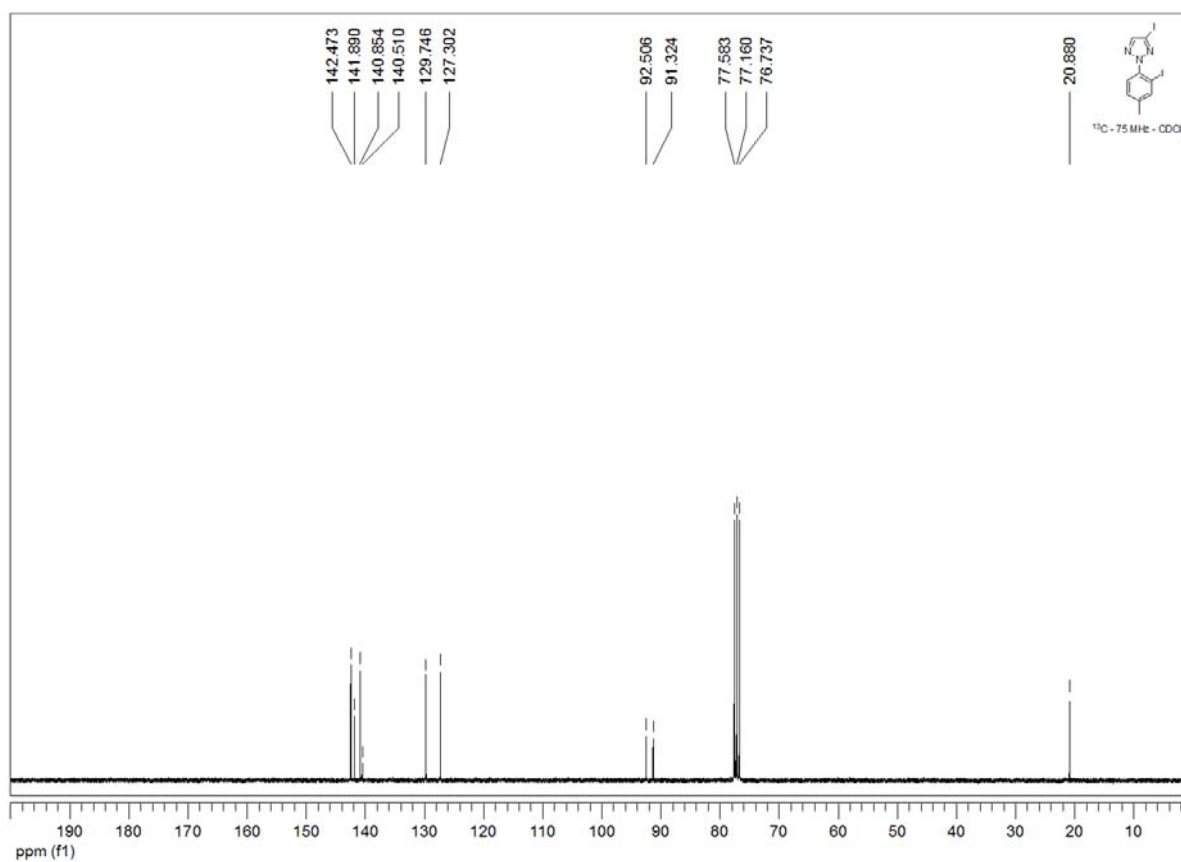
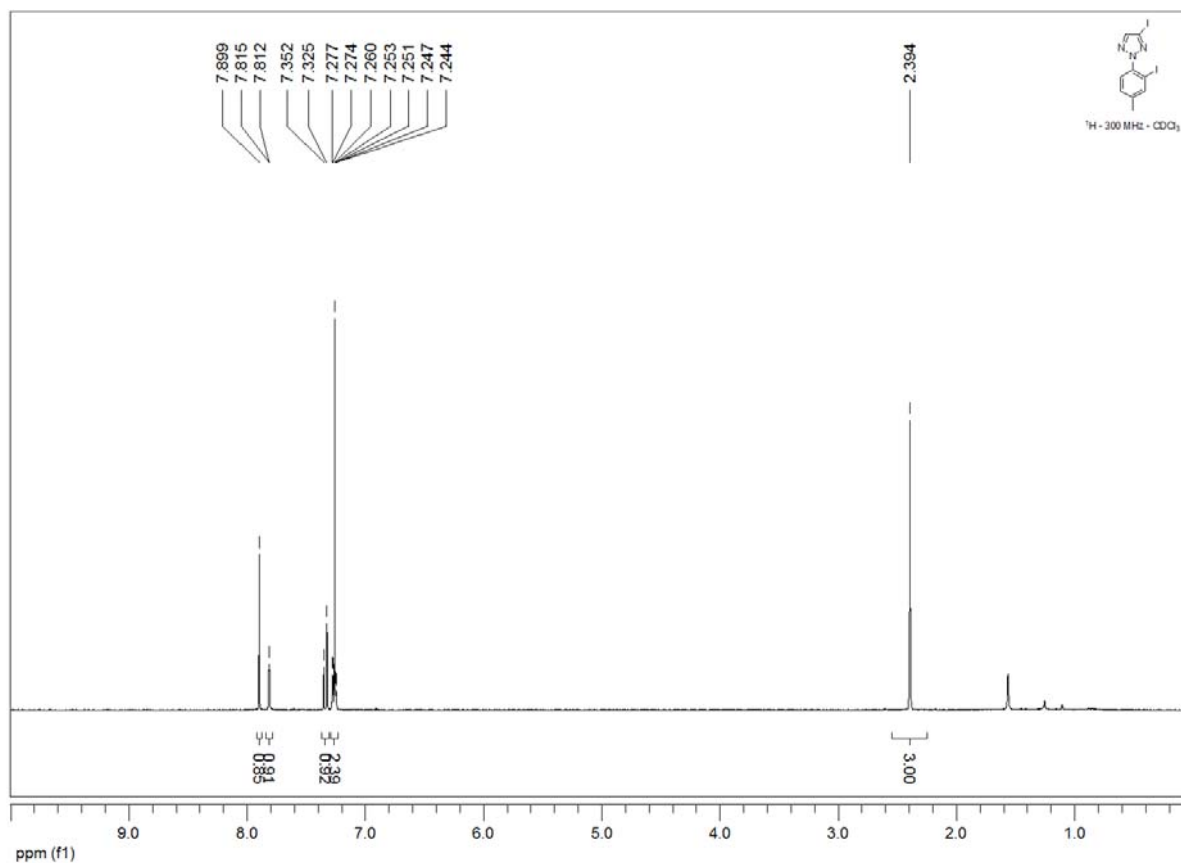
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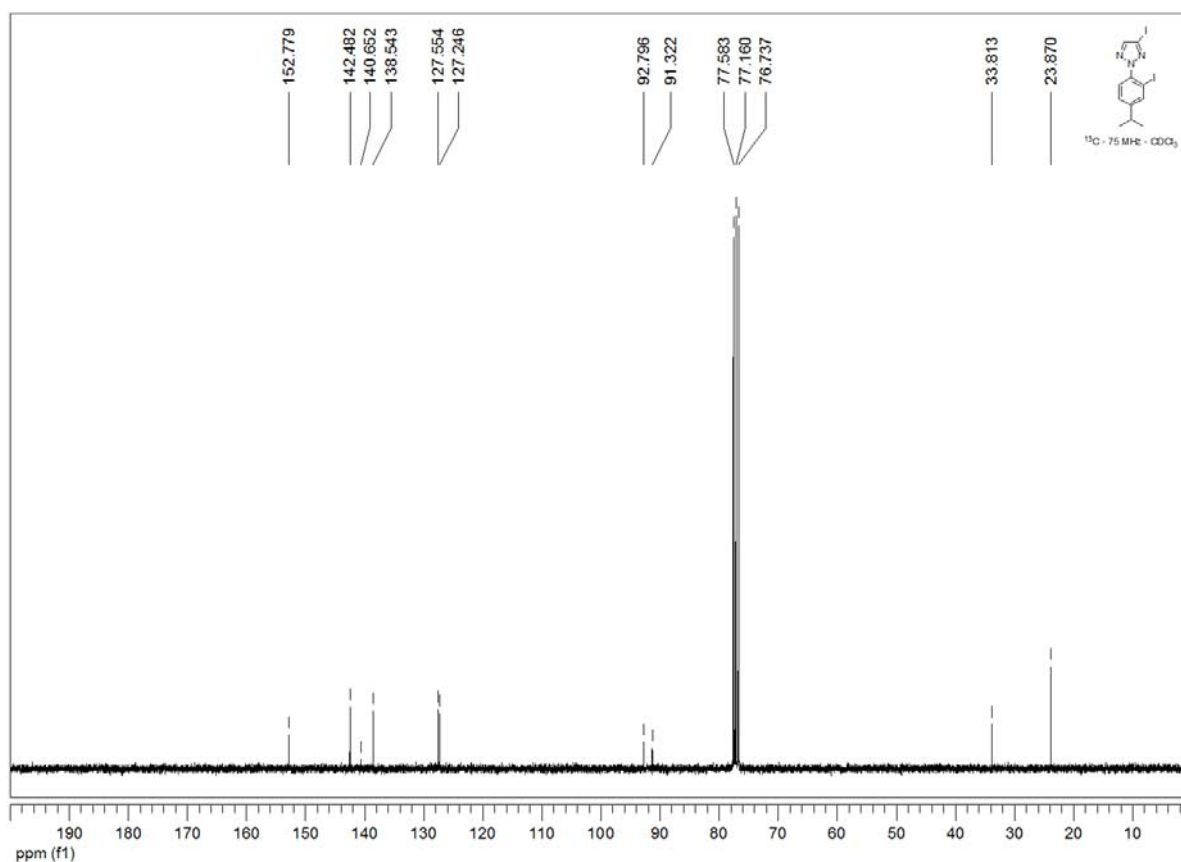
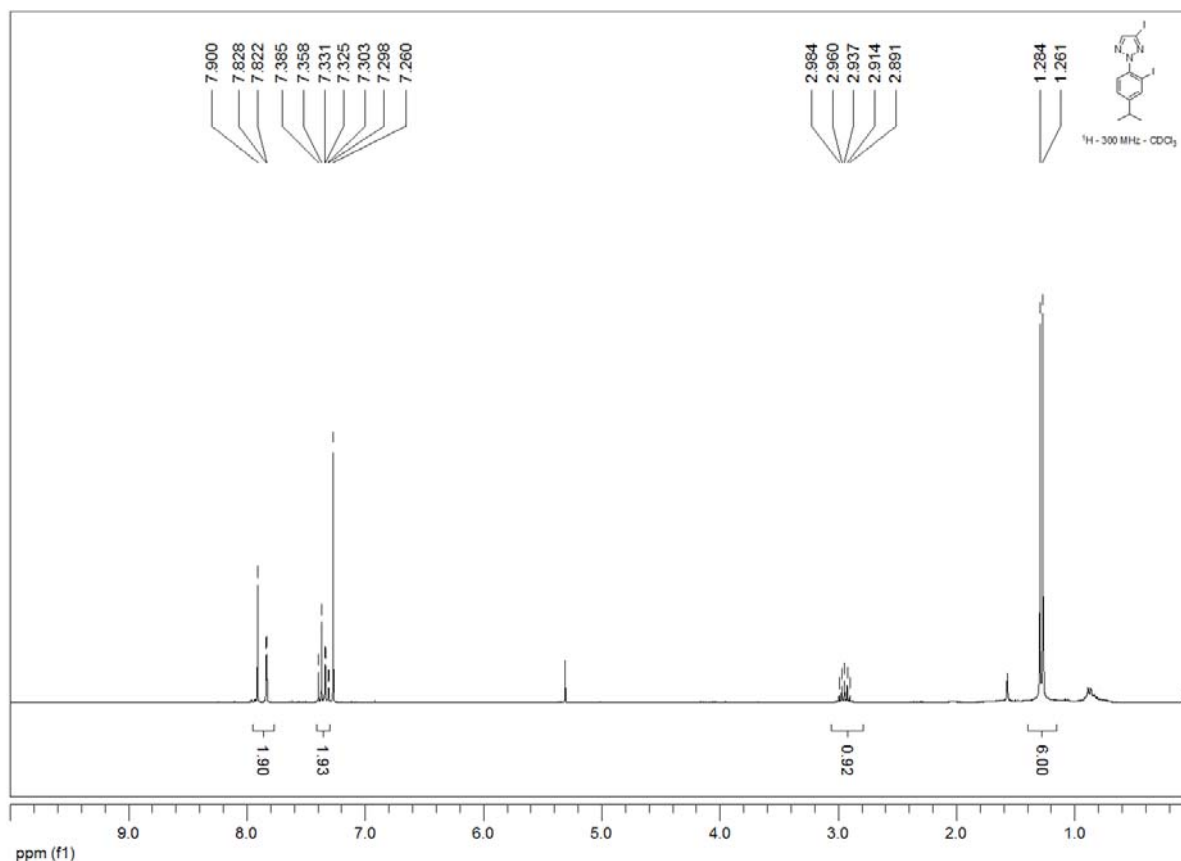
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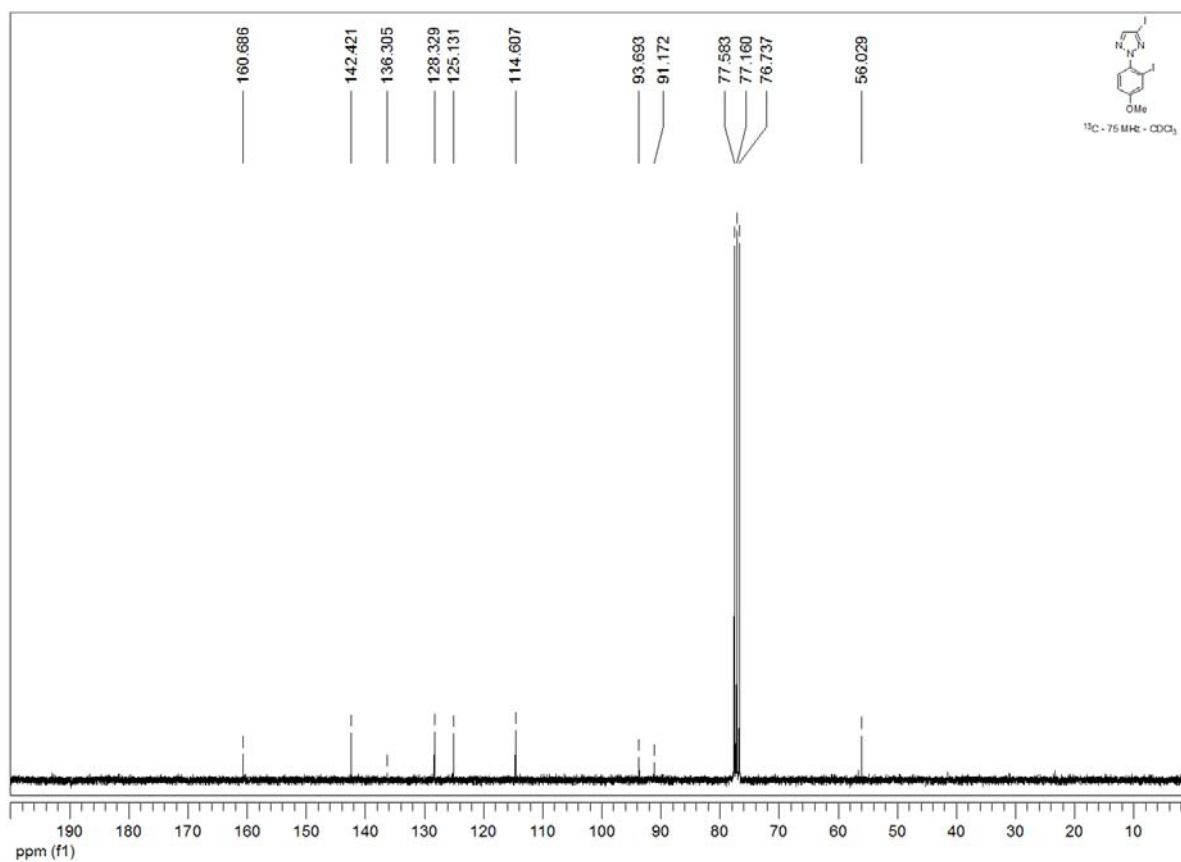
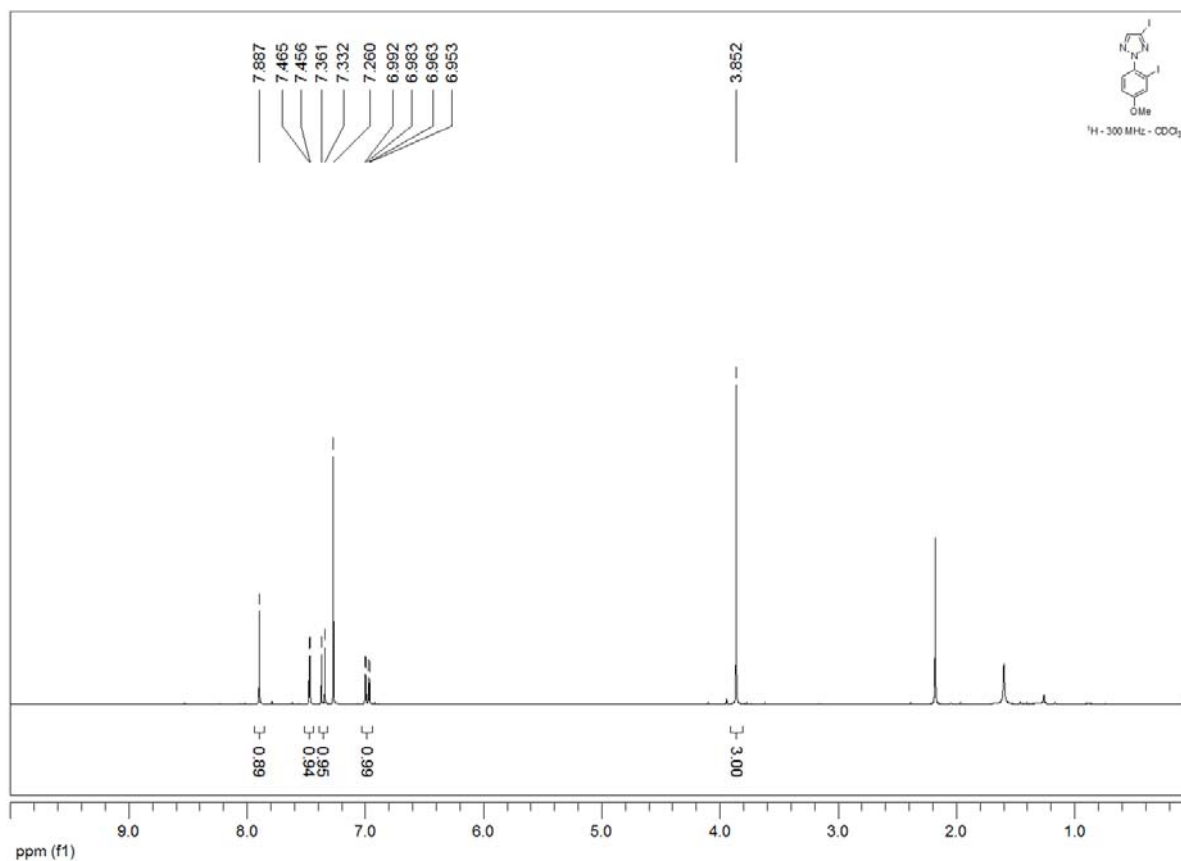
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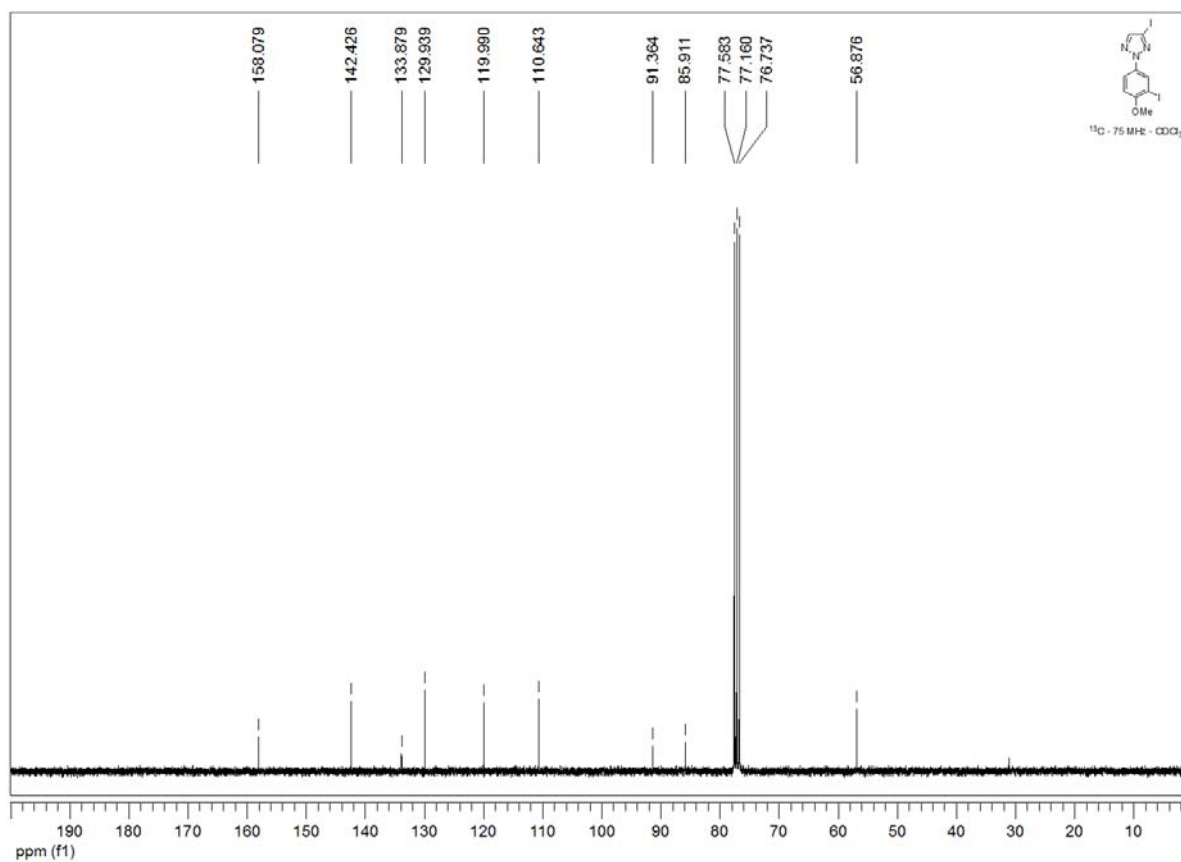
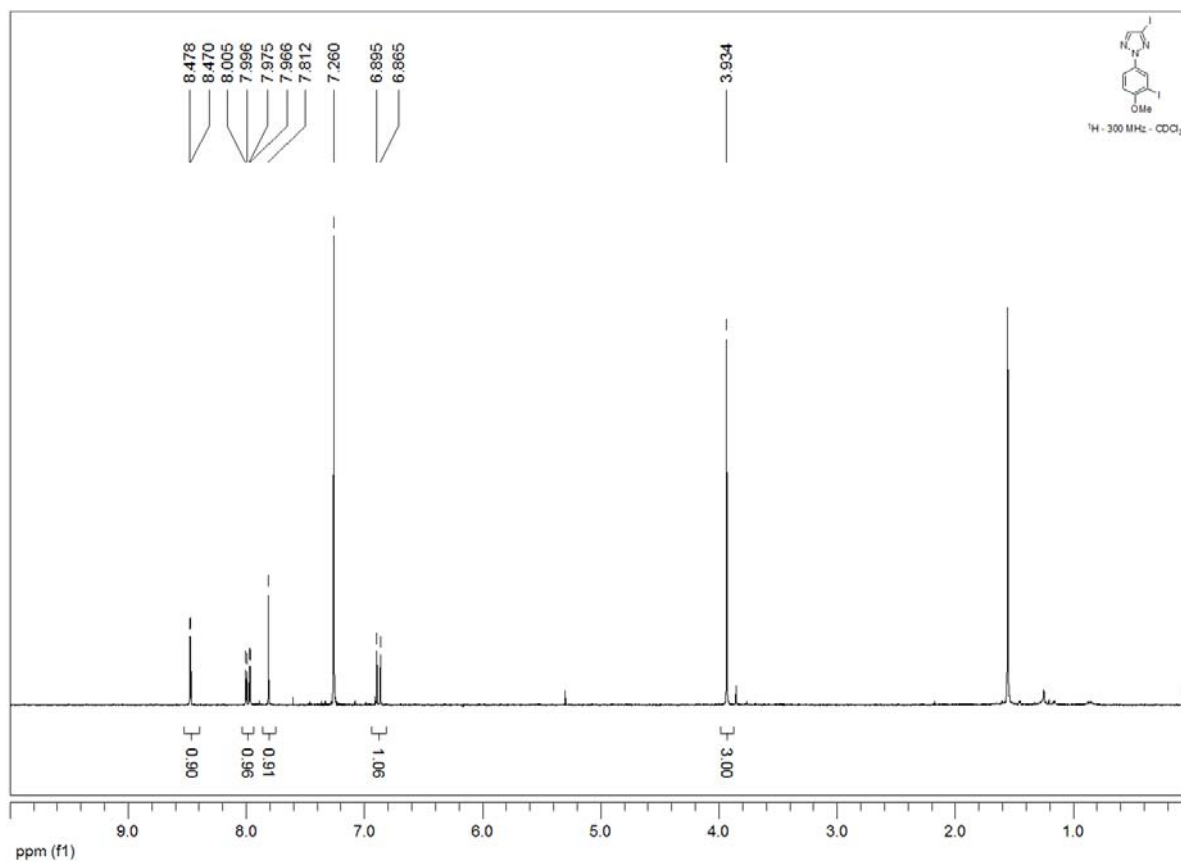
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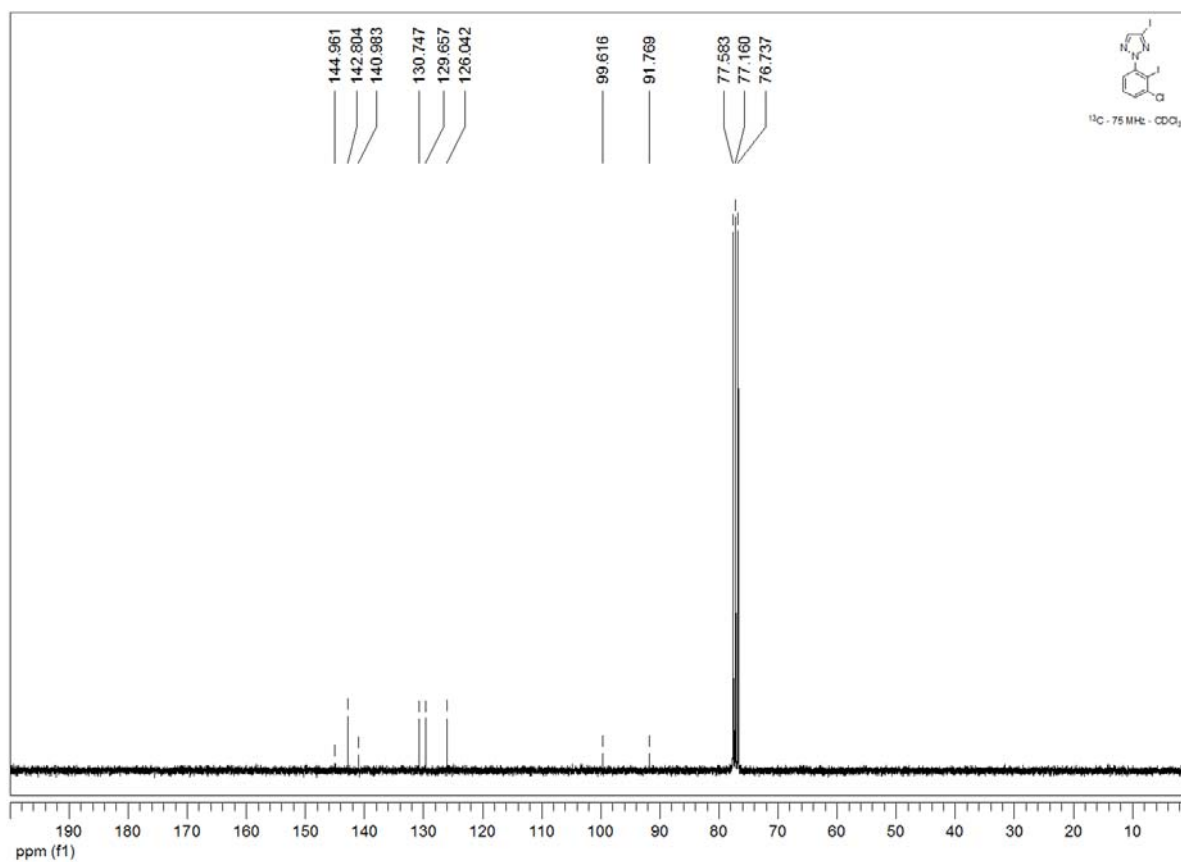
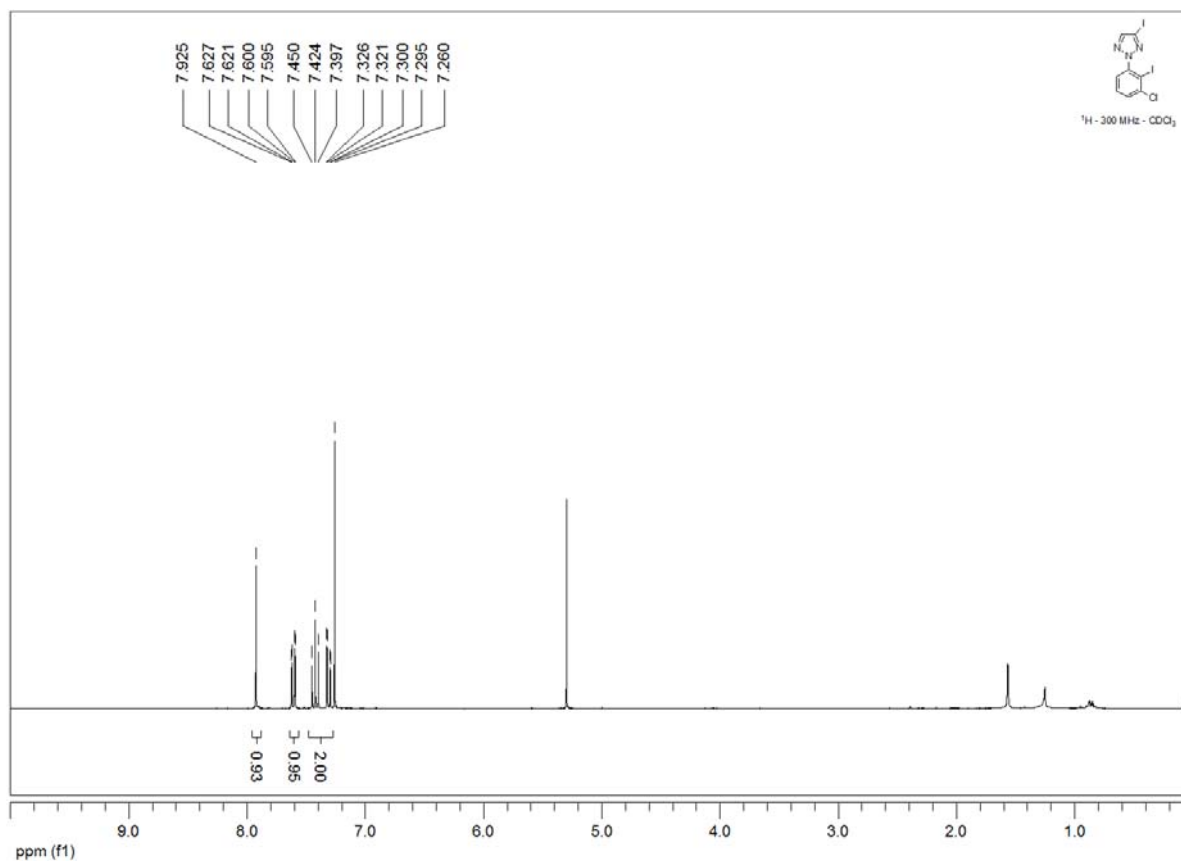
4-Iodo-2-(2-iodo-4-methoxyphenyl)-2H-[1,2,3]triazole (3d).



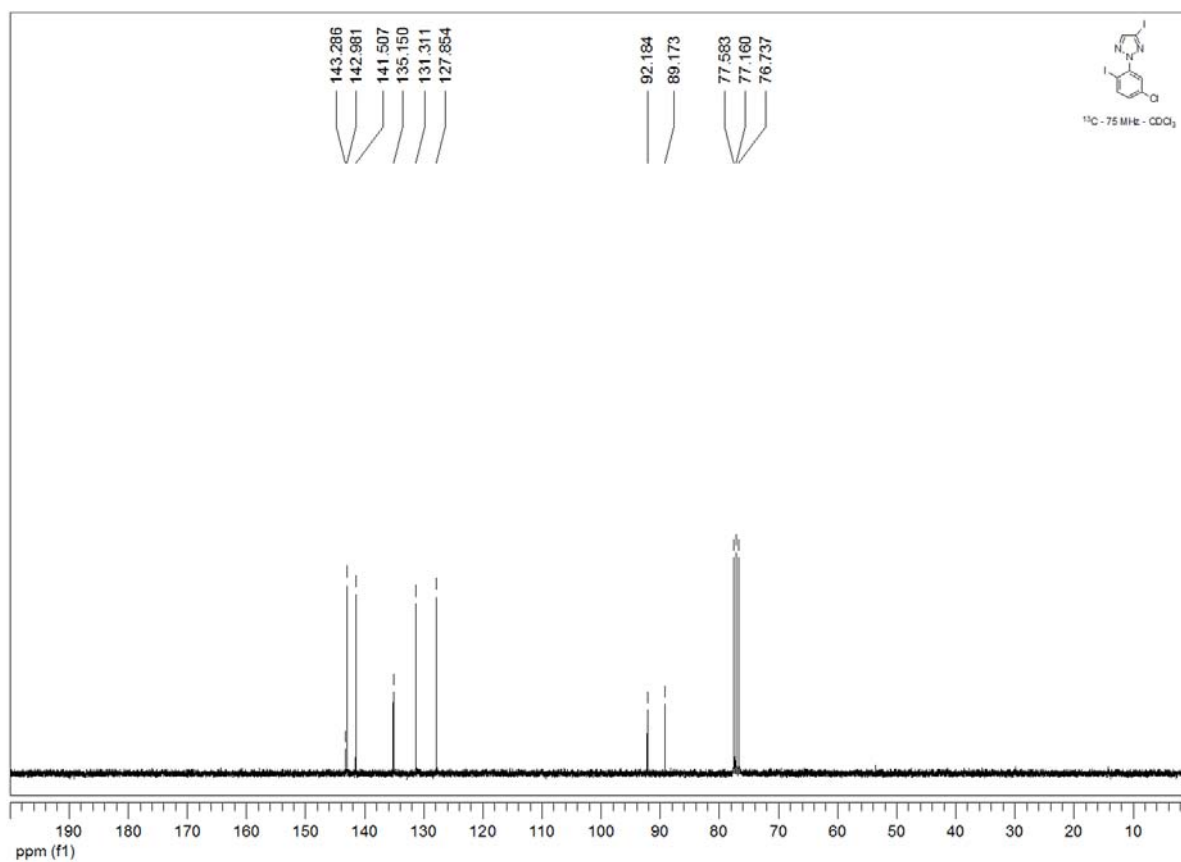
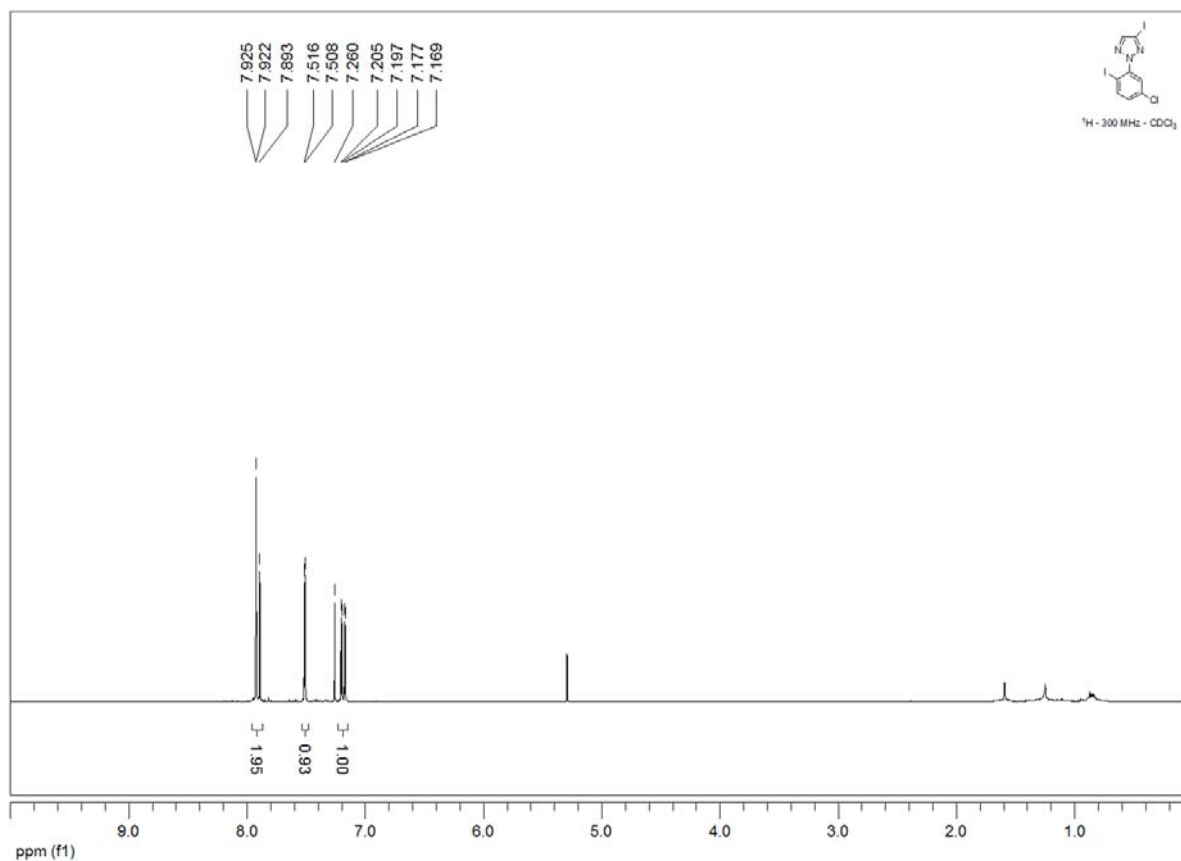
4-Iodo-2-(3-iodo-4-methoxyphenyl)-2H-[1,2,3]triazole (3'd).



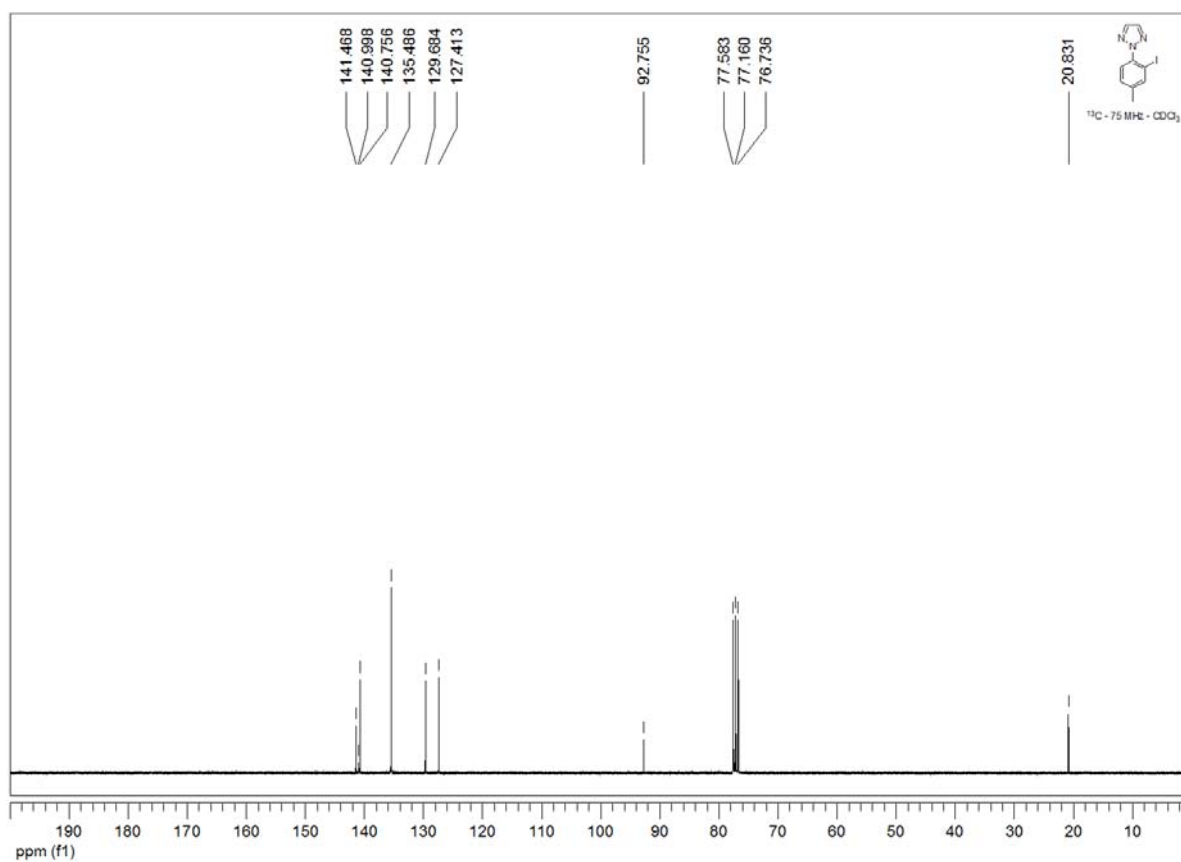
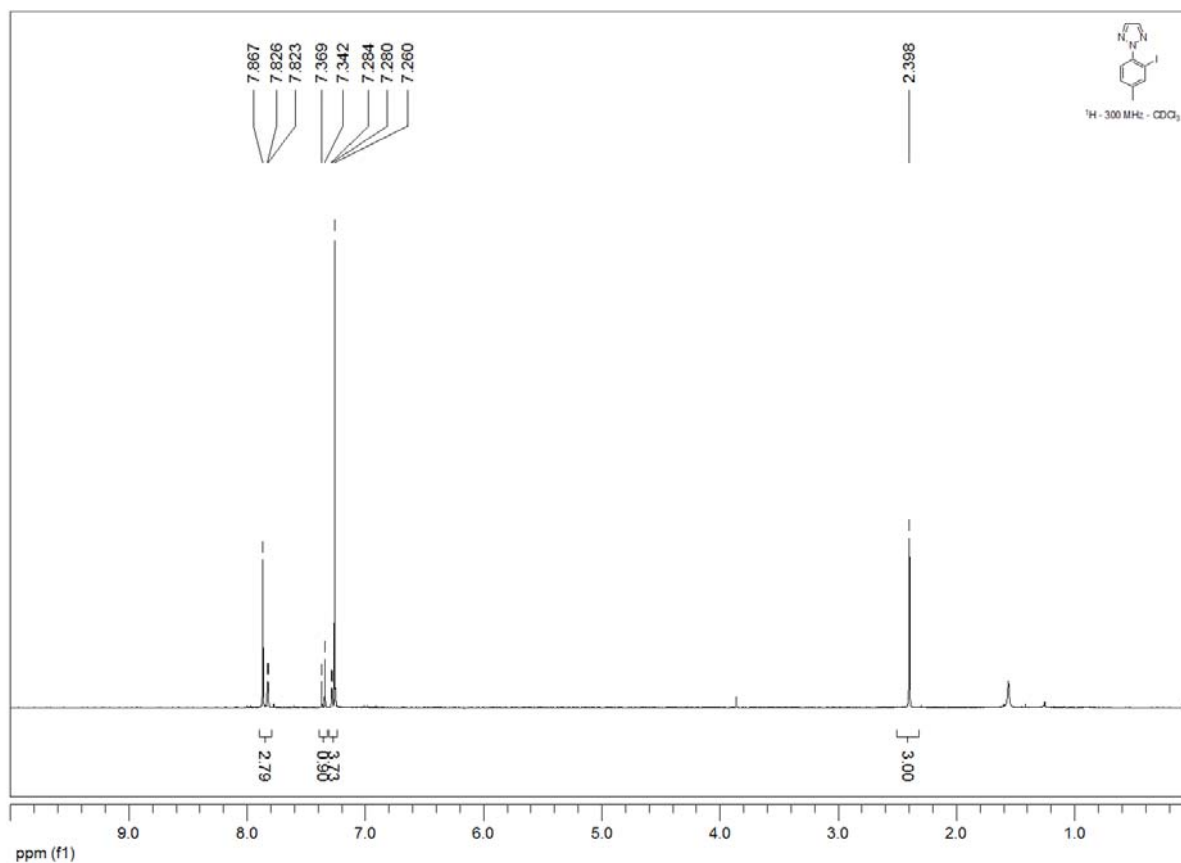
2-(3-Chloro-2-iodophenyl)-4-iodo-2*H*-[1,2,3]triazole (3e).



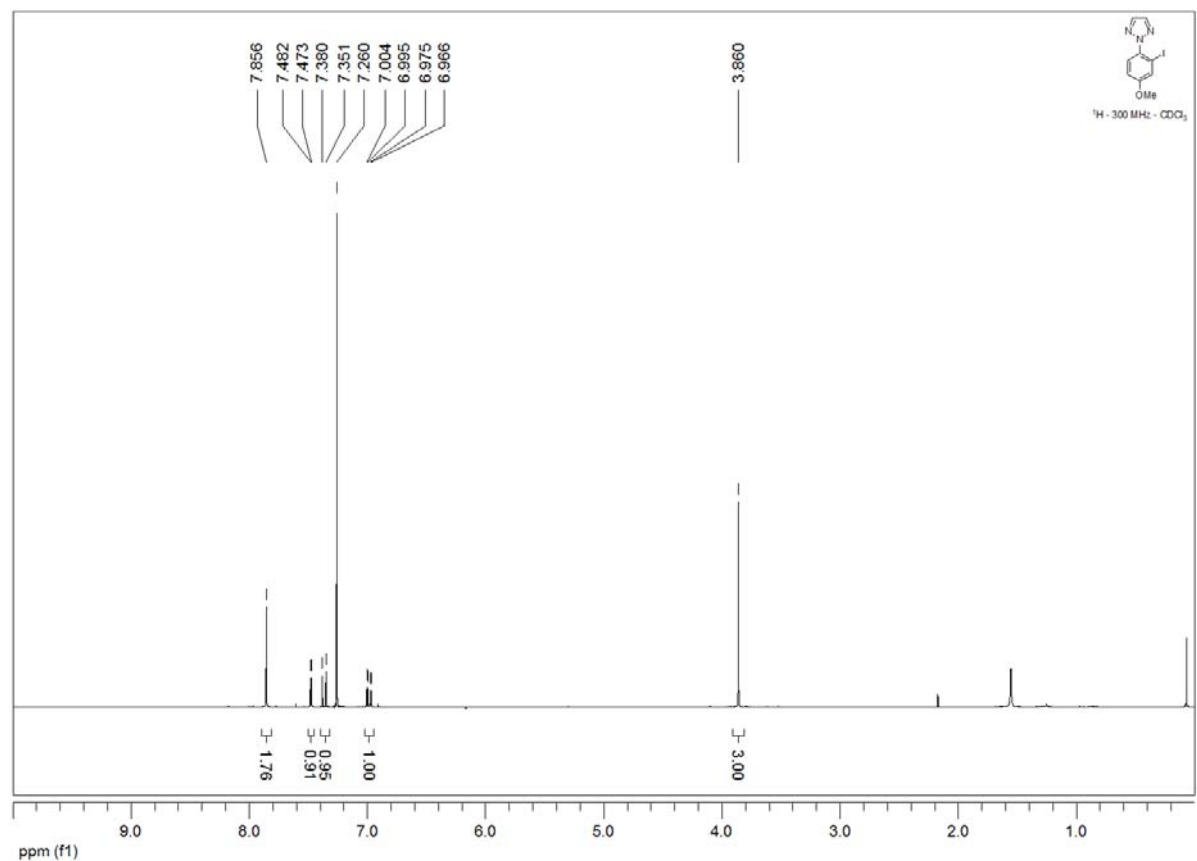
2-(5-Chloro-2-iodophenyl)-4-iodo-2*H*-[1,2,3]triazole (3'e).



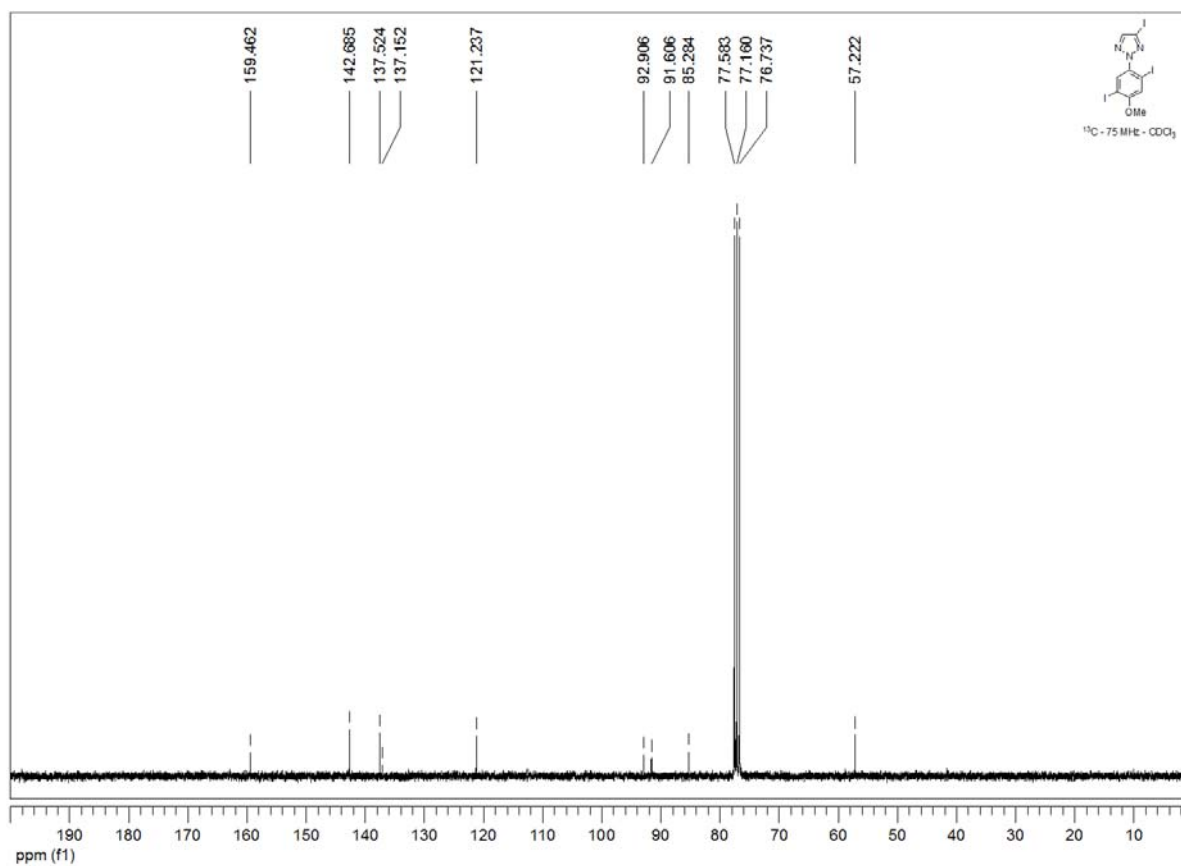
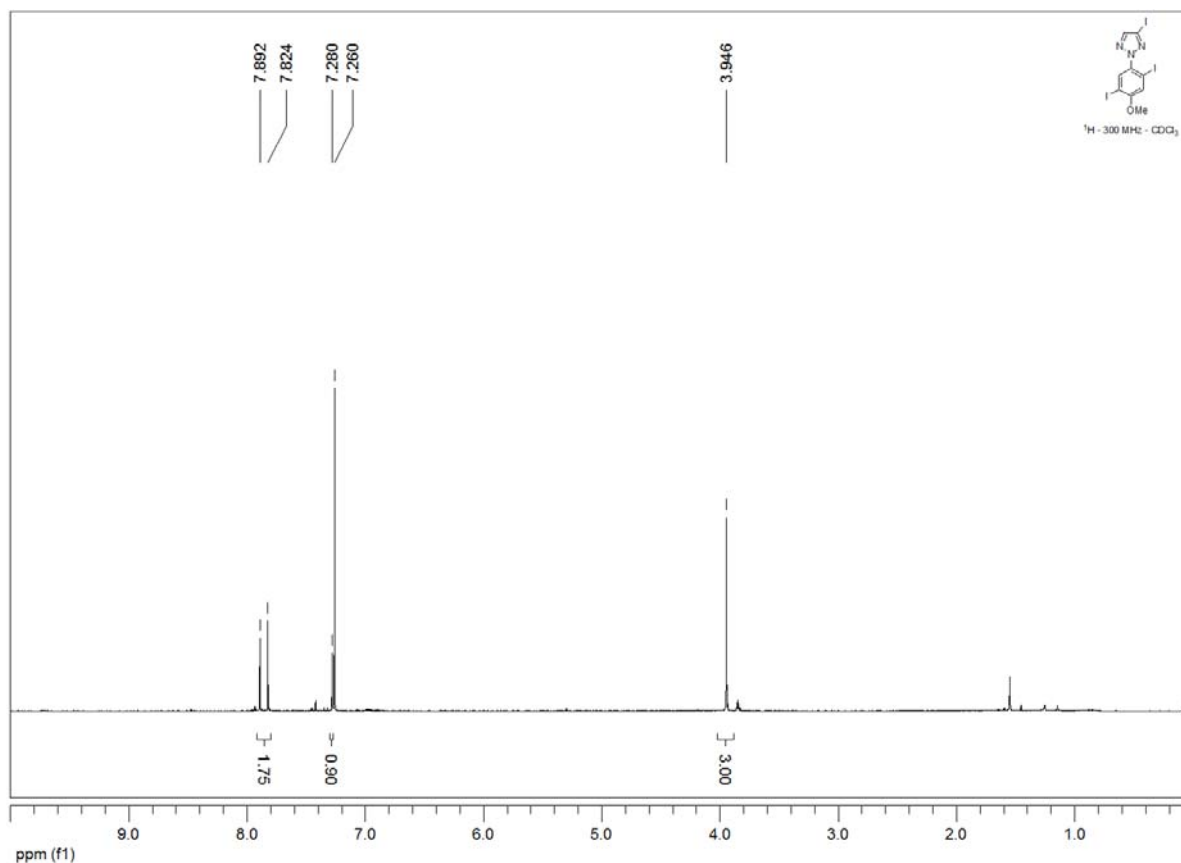
2-(2-Iodo-4-methylphenyl)-2H-[1,2,3]triazole (4b).



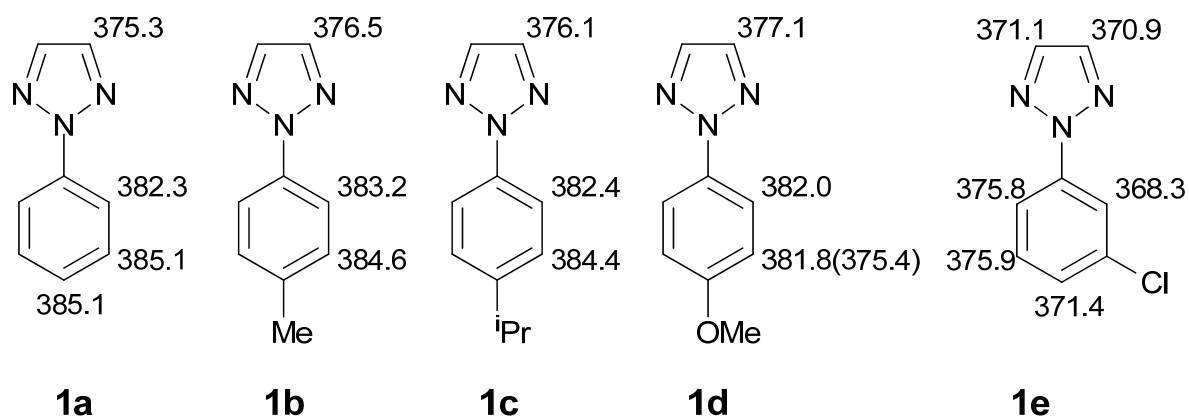
2-(2-Iodo-4-methoxyphenyl)-2H-[1,2,3]triazole (4d).



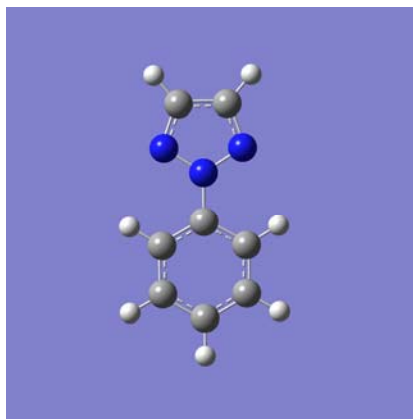
2-(2,5-Diiodo-4-methoxyphenyl)-4-iodo-2*H*-[1,2,3]triazole (5d).



Gas phase acidities ($\Delta_{\text{acid}}G$, kcal·mol⁻¹) of the investigated triazoles

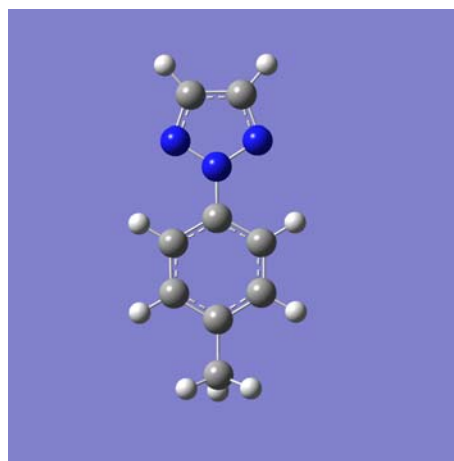


Cartesian coordinates of molecular geometry for the most stable rotamer form of the investigated aryl triazoles 1a-e (neutral molecule, gas phase) and anions obtained from 2-phenyl-2H-[1,2,3]triazole (1a) optimized at B3LYP/6-31G(d) level of theory



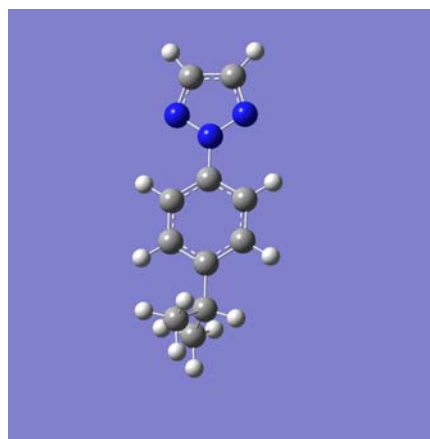
1a

C	1.2764940239	0.7163230515	-1.131567137
N	0.1108902126	1.1049173418	-0.6157295685
N	-0.6906679284	0.0530657929	-0.8188232302
C	1.1327620749	-0.5867542904	-1.6392331556
C	-2.0545240304	0.0446300716	-0.4109798031
C	-2.8380838893	-1.0872198918	-0.6527024771
C	-2.5895023867	1.1683416454	0.2250661476
C	-4.1722063607	-1.0862032619	-0.249878482
C	-3.9256349748	1.1508485785	0.6207433063
C	-4.7222355117	0.0281760806	0.3867738921
H	2.1365745915	1.3699365804	-1.114216068
H	1.8497735238	-1.2308055376	-2.1274387746
H	-1.9605316547	2.0326066604	0.4004306566
H	-2.3989037955	-1.9449056903	-1.1474789375
H	-4.7831591726	-1.9649233006	-0.4367575094
H	-4.3436054012	2.0232223253	1.1153202017
N	-0.1201952142	-0.9903312546	-1.4320679746
H	-5.7629301261	0.0217759286	0.6979834632



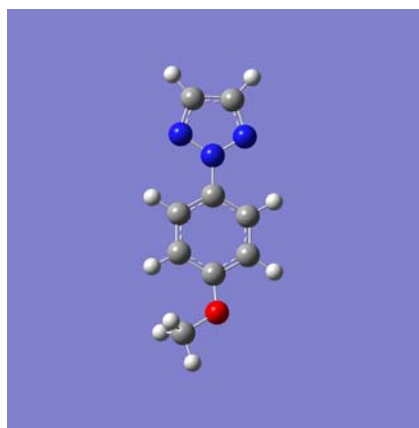
1b

C	1.2801290005	0.7073346863	-1.1302577686
N	0.1177571827	1.0994073236	-0.6083577493
N	-0.6910096643	0.0549479227	-0.8188792172
C	1.126524189	-0.589752303	-1.6488301842
C	-2.0541024878	0.0526033379	-0.409354758
C	-2.8496533869	-1.0687791248	-0.6552981096
C	-2.5845456999	1.16976111	0.2399054299
C	-4.1809132976	-1.0602739353	-0.2470347795
C	-3.9186341312	1.1542447019	0.6385528891
C	-4.7435388058	0.0464583727	0.4025129404
H	2.144384289	1.355299801	-1.1092789255
H	-1.9528501703	2.0294414851	0.4282187294
H	-4.3252616204	2.0254208499	1.1467848995
N	-0.1292485924	-0.9867333177	-1.4423442744
H	1.8377383122	-1.2343999533	-2.1446534454
H	-2.4217174292	-1.9294527799	-1.1549608965
H	-4.7946092197	-1.9374845631	-0.4379950222
C	-6.1976669399	0.0551759125	0.811488013
H	-6.361665984	0.6796703309	1.6961385535
H	-6.8346000915	0.4534605368	0.0101451288
H	-6.5563231126	-0.9543616942	1.0387925869



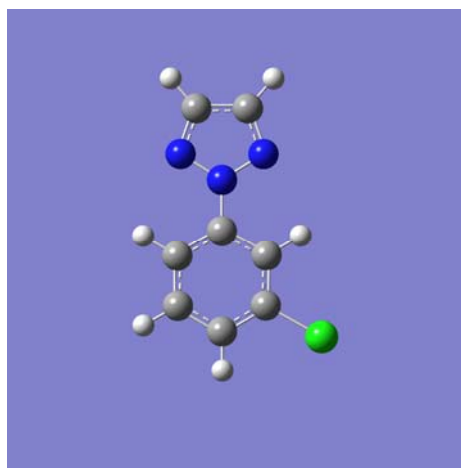
1c

C	1.3674159986	0.4472616895	-0.8250695439
N	0.2709245922	0.5561932824	-0.0747650165
N	-0.6930928692	0.0448507965	-0.8485652859
C	1.0168226639	-0.1395856074	-2.0528769459
C	-2.0491258501	-0.0337877056	-0.4237352535
C	-3.0123549143	-0.5779775707	-1.2745539838
C	-2.4065266158	0.4348599968	0.843601034
C	-4.3359144924	-0.6483041156	-0.8442677878
C	-3.7349361578	0.353444966	1.2498133594
C	-4.7277511107	-0.1879926833	0.4189373077
H	2.3260893474	0.7847911747	-0.4586490522
H	-1.646704828	0.8543932541	1.4919111643
H	-3.9981002637	0.7217129071	2.2379710549
N	-0.2929901098	-0.3876956604	-2.0495555951
C	-6.1802612898	-0.2758155112	0.8660169795
H	-6.7436291436	-0.7331860789	0.0411142049
H	1.6261919716	-0.386897849	-2.9100573982
H	-2.720816188	-0.9373314675	-2.25410445
C	-6.3475802503	-1.1859466793	2.0978191791
H	-7.406695434	-1.2829225744	2.3646039898
H	-5.949954797	-2.1886742634	1.907228294
H	-5.8214286902	-0.7780059266	2.9691122711
C	-6.7873088275	1.1170621282	1.1212214866
H	-6.7031765528	1.7550616056	0.2347983048
H	-7.8488584524	1.0329594467	1.3826720096
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H	-5.0817848066	-1.0735308994	-1.511827066



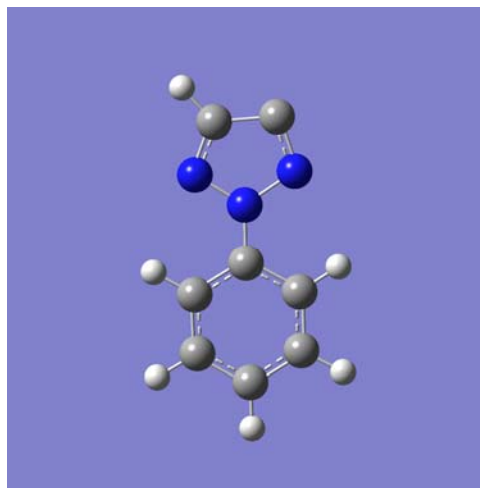
1d

C	2.9766455265	0.6608177305	-0.1946017552
N	1.7204326747	1.0018746917	-0.4875611501
N	0.9963211582	-0.0073881033	0.0070872539
C	2.9629642749	-0.5695652602	0.4817638094
C	-0.4232500455	-0.046010545	-0.0909946554
C	-1.1283907496	-1.1293438165	0.4477416537
C	-1.1046554035	0.9929887742	-0.7218467307
C	-2.5113165389	-1.1629771821	0.3500558757
C	-2.4962687158	0.9571604896	-0.8190359775
C	-3.2085130813	-0.1223913416	-0.2829348379
H	3.8036678995	1.2967380714	-0.4754126413
H	-0.5460309526	1.8246805473	-1.1340104252
H	-3.0076621645	1.7747212372	-1.3134407934
N	1.6983227908	-0.9780383828	0.6007302603
H	3.7762862625	-1.1614541666	0.8758893059
H	-0.5862039879	-1.9303620282	0.9354695699
H	-3.0776876977	-1.9927282673	0.7604616329
O	-4.5654409762	-0.2565679176	-0.3231698643
C	-5.322954881	0.765793484	-0.9510352298
H	-6.3668455515	0.4579820921	-0.8688410538
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H	-5.058258922	0.870714274	-2.0115152912



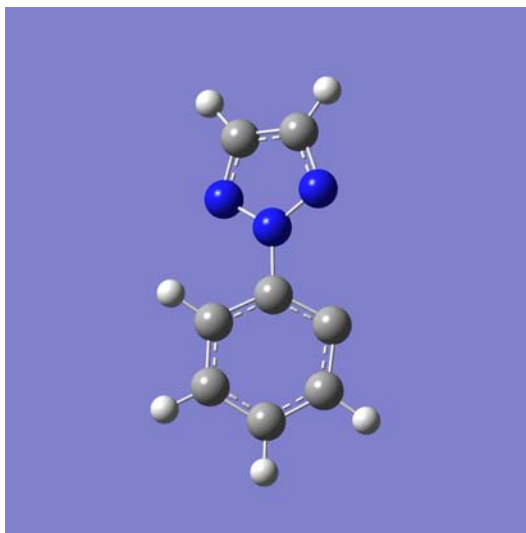
1e

C	-3.4368504593	0.699500761	-0.041867272
N	-2.172887515	1.1183023898	-0.0635482025
N	-1.4645291918	-0.0153114899	0.0084274901
C	-3.4461146642	-0.7048692257	0.0441607328
C	-0.0436527648	-0.0236908725	0.0135466411
C	0.6266104272	-1.2474964961	0.0911476021
C	0.6554319792	1.1841502563	-0.0588003001
C	2.0180602891	-1.2371889596	0.0950128712
C	2.0480844934	1.1564275243	-0.0526658262
C	2.7457608143	-0.0497324304	0.0241598026
H	-4.2555368269	1.4029255411	-0.0877494953
H	0.1083569153	2.1165698232	-0.118100168
H	2.5997987266	2.0902137467	-0.108505985
N	-2.187840595	-1.1395386005	0.0751704111
H	-4.2738686783	-1.3979385486	0.0839081263
H	0.0688103099	-2.1729264117	0.1464965379
H	3.8297559313	-0.0720975306	0.0291060106
Cl	2.875753309	-2.7685687569	0.1924285434



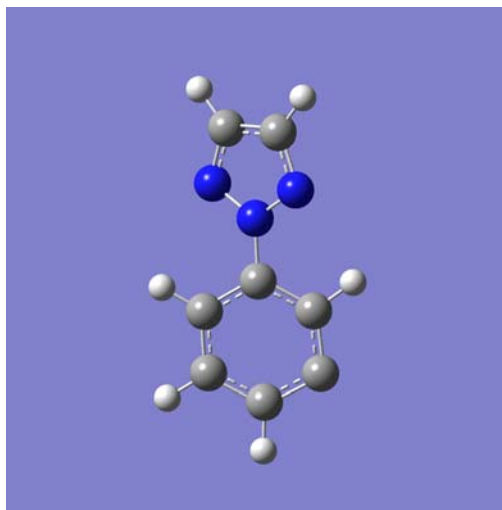
1a deprotonated at C4

C	1.2211947853	0.680328209	-1.2288966076
N	0.0988556018	1.1088547896	-0.6621333637
N	-0.7376771552	0.0680612469	-0.868525382
C	1.1373811879	-0.6549359748	-1.8187083051
C	-2.0533591004	0.068297301	-0.4385934878
C	-2.870941392	-1.0540014479	-0.6901167221
C	-2.6040508799	1.1687988163	0.2506254684
C	-4.1943068908	-1.0636731657	-0.2613878644
C	-3.931126921	1.1383537934	0.6708363078
C	-4.7432893201	0.0270287043	0.4227488828
H	2.0844932897	1.3435861576	-1.2045761698
H	-1.969783401	2.026946052	0.4397848517
H	-2.4305313338	-1.8894558407	-1.2210160082
H	-4.8086153794	-1.9397212097	-0.4653673884
H	-4.3368318572	1.9990142085	1.201378704
N	-0.1347287901	-1.0035425848	-1.5617338374
H	-5.7792738436	0.0108865949	0.7544123716



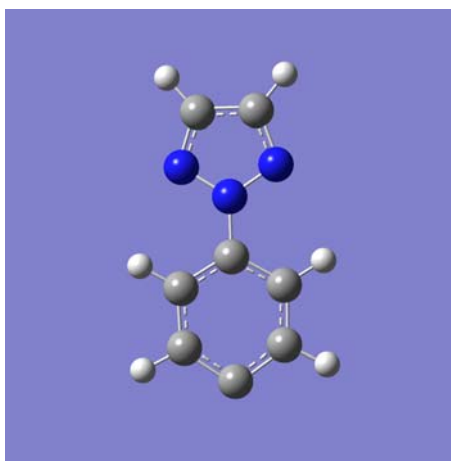
1a deprotonated at C2'

C	1.1903098069	0.8023562761	-1.3775961547
N	-0.053813126	1.1725008999	-1.0424749108
N	-0.6940937846	0.0148198659	-0.8395606886
C	1.2525827202	-0.5933059289	-1.3664422116
C	-2.1068373243	-0.037234663	-0.4323053866
C	-2.8742475608	-1.1359359688	-0.8488543223
C	-2.5264465636	1.0583851222	0.3403459017
C	-4.2080431035	-1.0142853437	-0.3757951584
C	-3.8597034466	1.1048756505	0.7448355445
C	-4.7105273513	0.0541043123	0.3784638427
H	1.945513699	1.5424067524	-1.6096945874
H	-1.8340495296	1.8519348015	0.6169209757
H	-4.9278119592	-1.8096021875	-0.6207444936
H	-4.222989885	1.9404340731	1.3430857852
N	0.0502671672	-1.074437922	-1.0182619566
H	-5.7601507764	0.078150527	0.6878692097
H	2.0758807579	-1.2633534569	-1.5775058387



1a deprotonated at C3'

C	1.2158380225	0.7677037018	-1.389058607
N	-0.0012408487	1.1864068145	-1.0134453298
N	-0.6770230114	0.0519039269	-0.792354759
C	1.2269994422	-0.6290015575	-1.3896831693
C	-2.0626392881	0.0386433498	-0.3930309627
C	-2.9028357931	-1.0233183938	-0.7673055264
C	-2.5413269466	1.1202169991	0.3537184066
C	-4.2700857282	-1.1272893986	-0.3997966354
C	-3.8859021058	1.0875843252	0.7238813929
C	-4.6899676666	-0.0079988264	0.3688629718
H	1.992549478	1.4783516758	-1.6382412584
H	-1.8802087016	1.9368062476	0.6275532779
H	-4.2925476147	1.9185335804	1.309088581
N	0.0197202015	-1.0675034123	-1.0037388594
H	-5.7284482241	0.0290571438	0.7322541083
H	2.0161402417	-1.3273727305	-1.6334988188
H	-2.4399692672	-1.7960440256	-1.3906880125



1a deprotonated at C4'

C	1.2758401675	0.7457927568	-1.2373192194
N	0.082124749	1.1530203318	-0.7789756433
N	-0.6734571304	0.0519516674	-0.8241480252
C	1.1920949844	-0.6103444953	-1.5541914006
C	-2.0482203324	0.0405225789	-0.4119500736
C	-2.8597611904	-1.0643366567	-0.6951723918
C	-2.5868183647	1.1341558634	0.2761005359
C	-4.195283865	-1.0410767084	-0.275635231
C	-3.9323228121	1.0886081363	0.6604318933
C	-4.8433077023	0.0172847845	0.4261188704
H	2.1029404993	1.438472199	-1.3133723331
H	-1.9511862679	1.9896280367	0.4979919016
H	-4.2884782911	1.9809808695	1.1969673458
N	-0.0506113996	-1.0377341324	-1.2823849895
H	1.9351547031	-1.2900425875	-1.9486008924
H	-2.4380943585	-1.9110235138	-1.2340740101
H	-4.7742121091	-1.9412270402	-0.531795787

The cartesian coordinates of the deprotonated forms of other compounds can be obtained from authors by request.