Supporting Information

Synthesis of 1,5-functionalized 1,2,3-triazoles using ionic liquid/iron(III) chloride as efficient and reusable homogeneous catalyst

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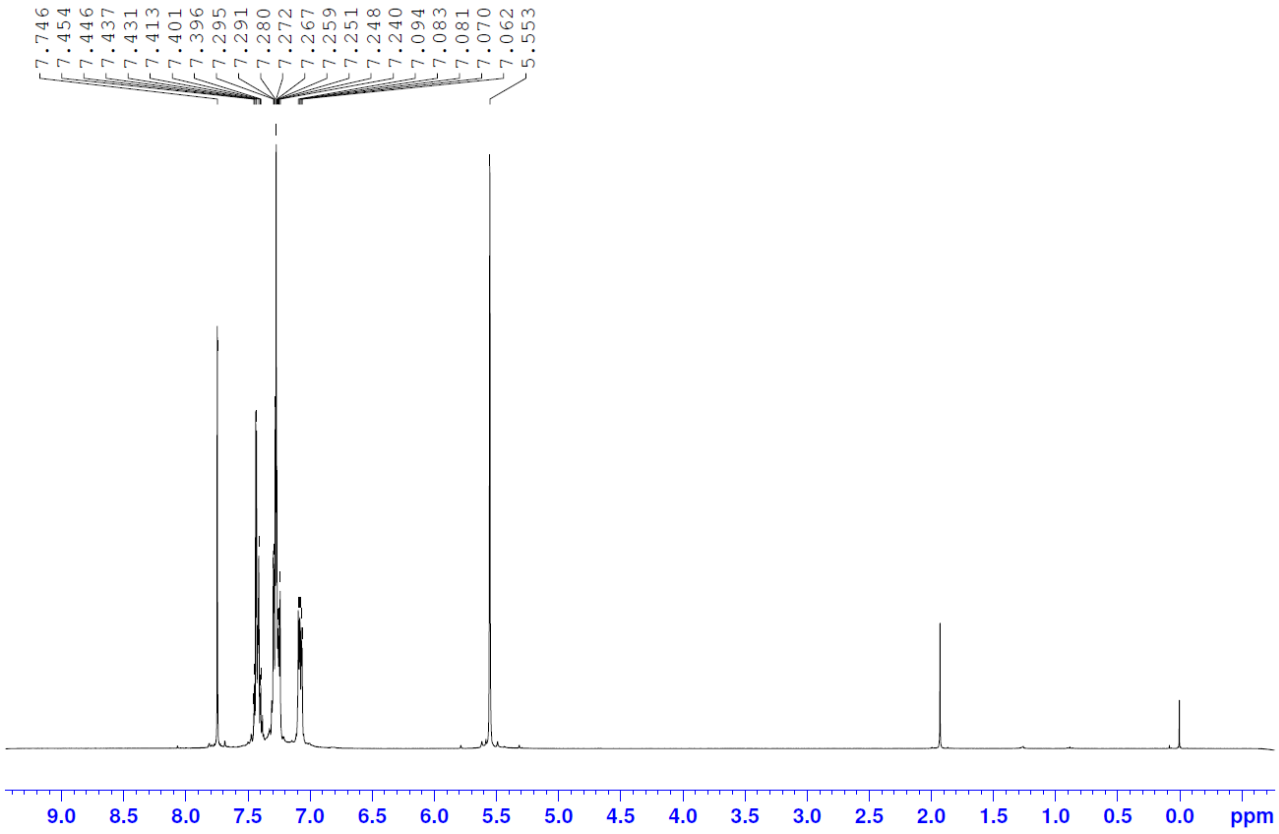
^{1}H NMR, ^{13}C NMR and ESI(+)-MS spectra…….S-2

Theoretical Calculations……S-30

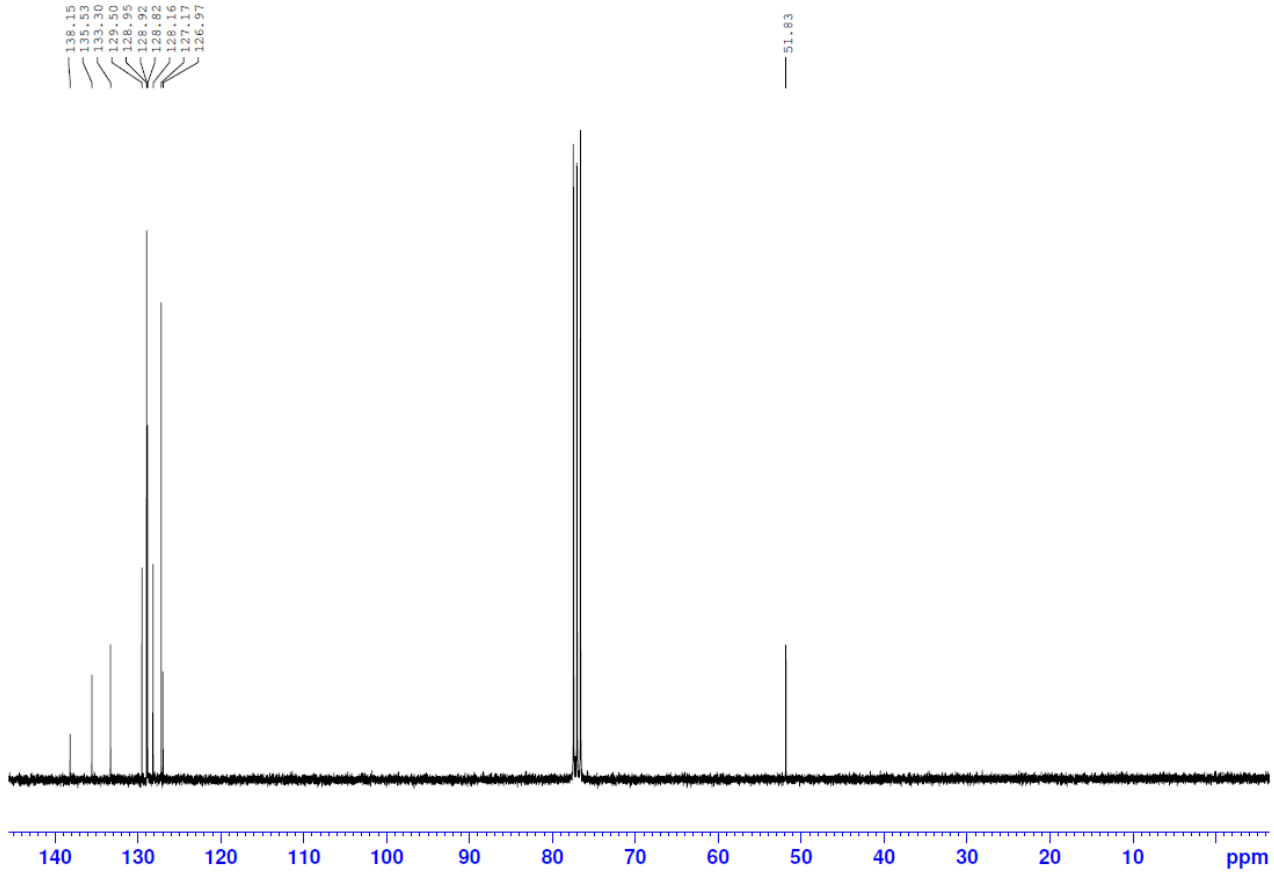
Cartesian Coordinates……...S-34

1-benzyl-5-phenyl-1,2,3-triazole (3a)

^{1}H-NMR



^{13}C-NMR



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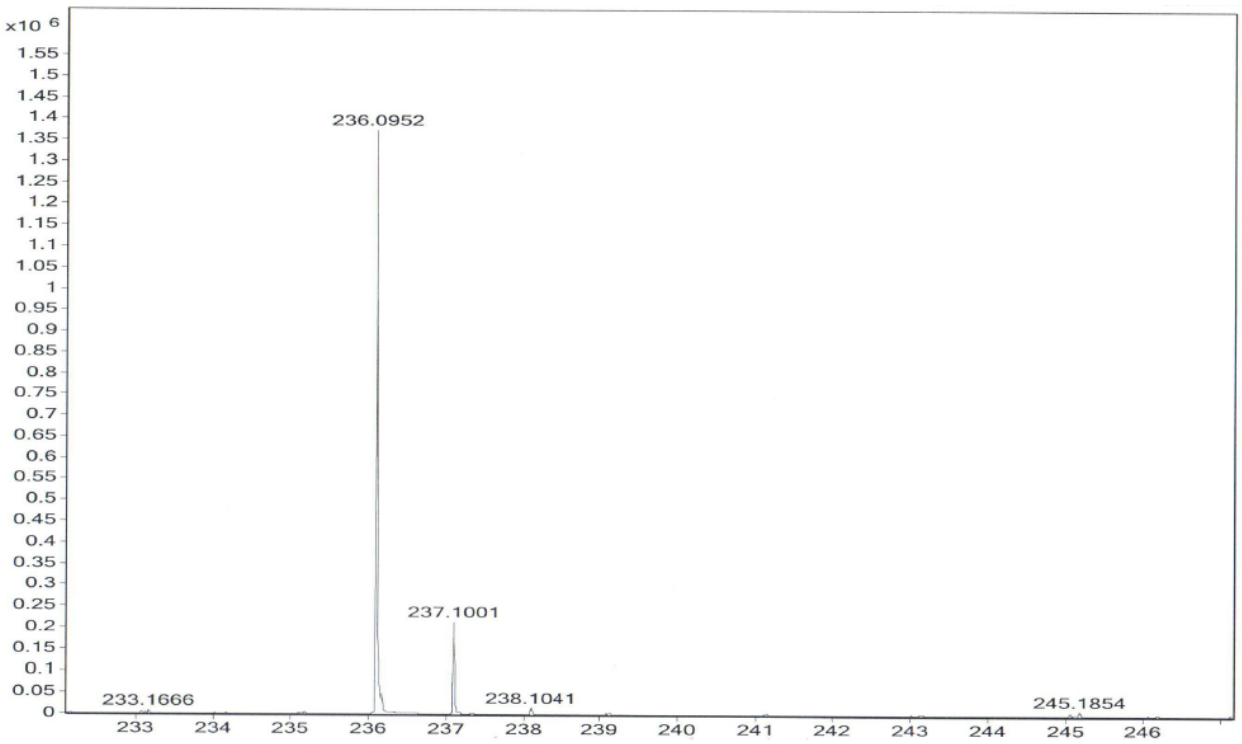
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0.05
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237.1001
233.1666
238.1041
245.1854
233
234
235
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237
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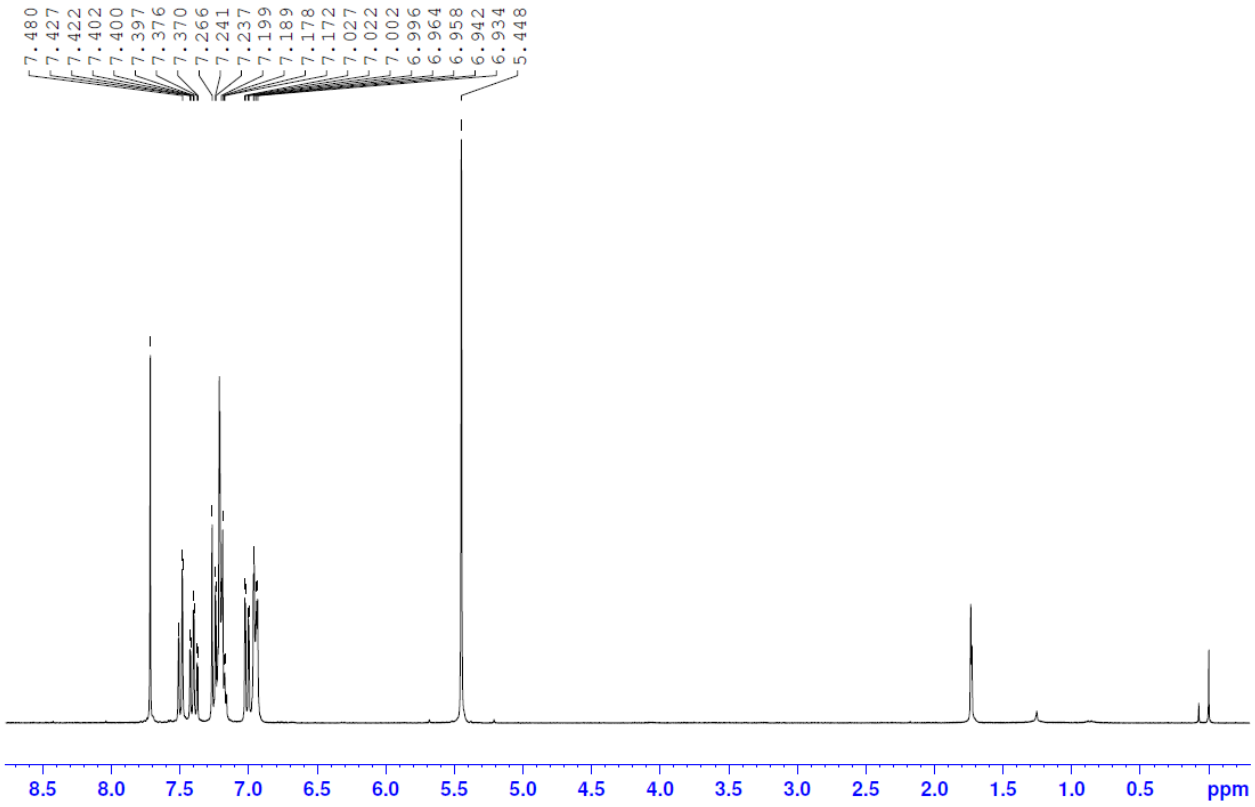
246

1-benzyl-5-(2-chlorophenyl)-1,2,3-triazole (3b)

^{1}H-NMR



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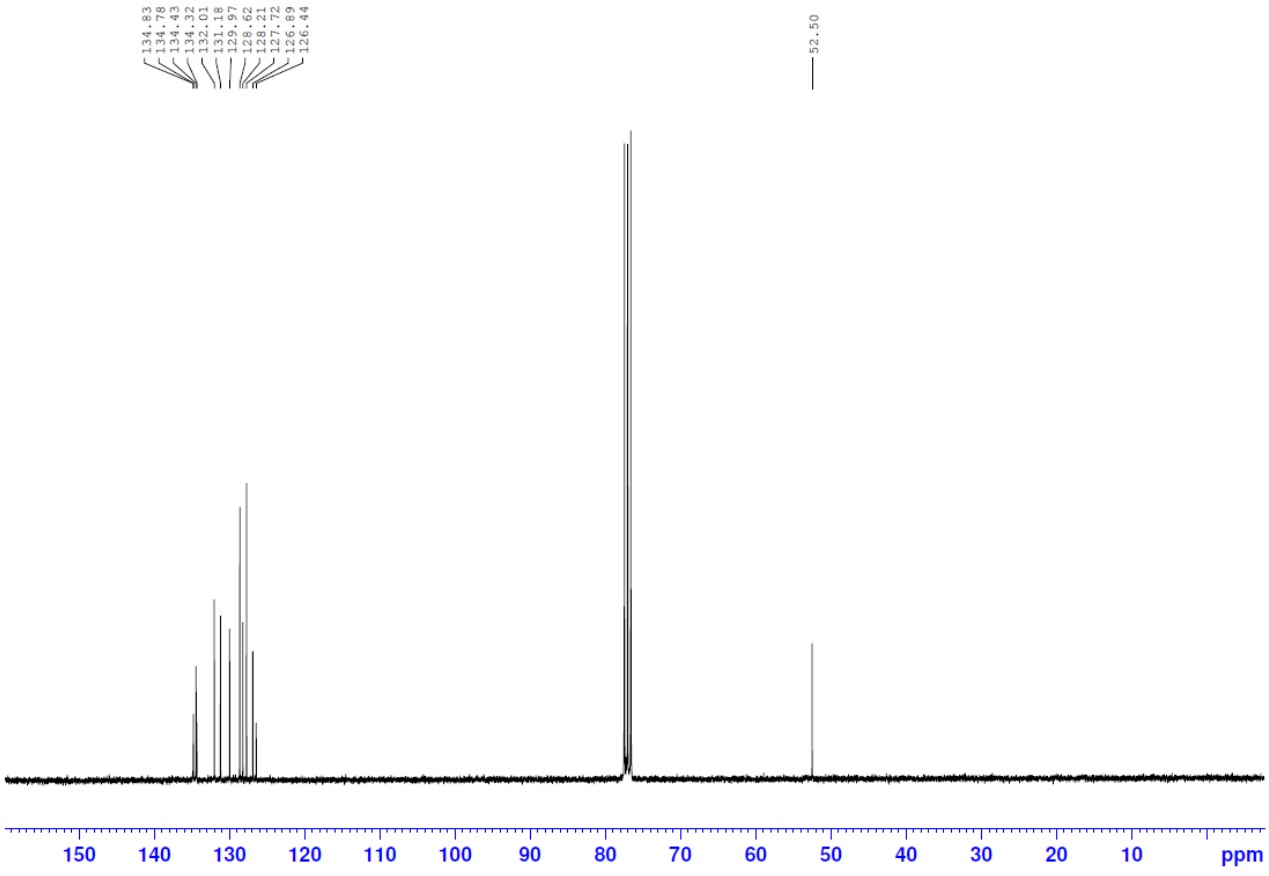

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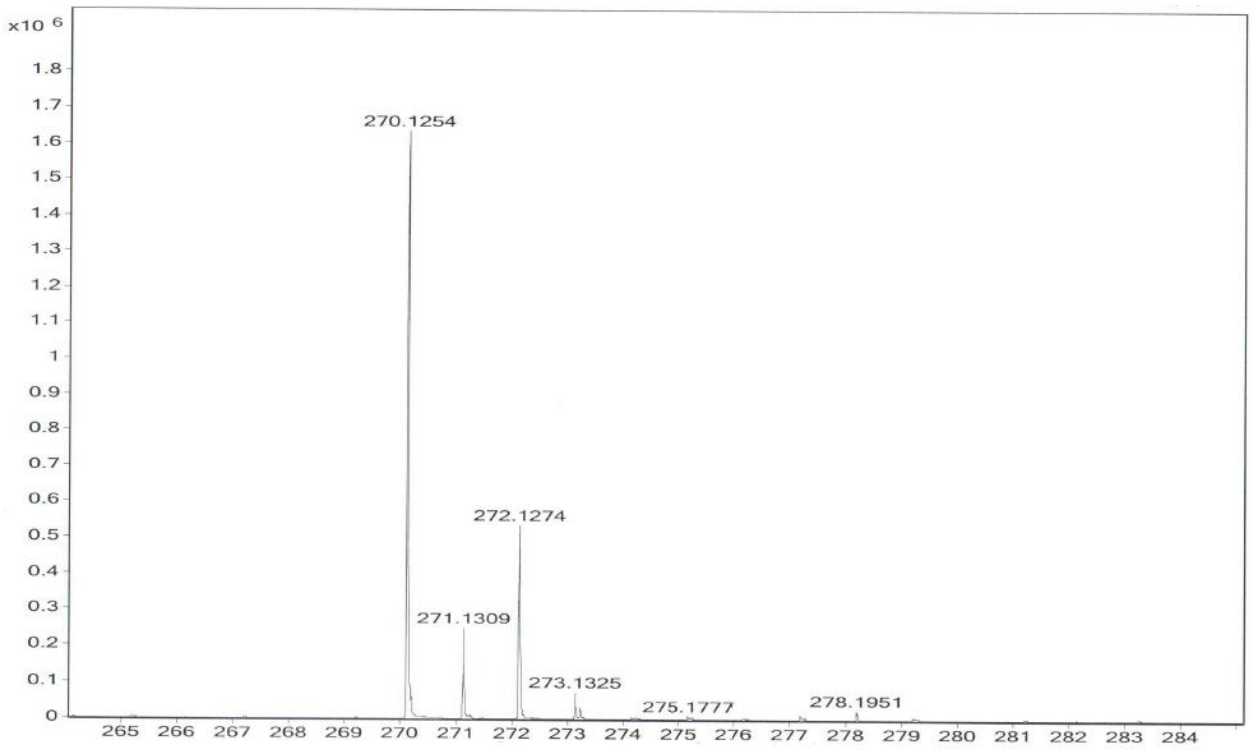
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1.4
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0.8
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0.6
0.5
0.4
0.3
0.2
0.1
0
270.1254
272.1274
271.1309
273.1325
275.1777
278.1951
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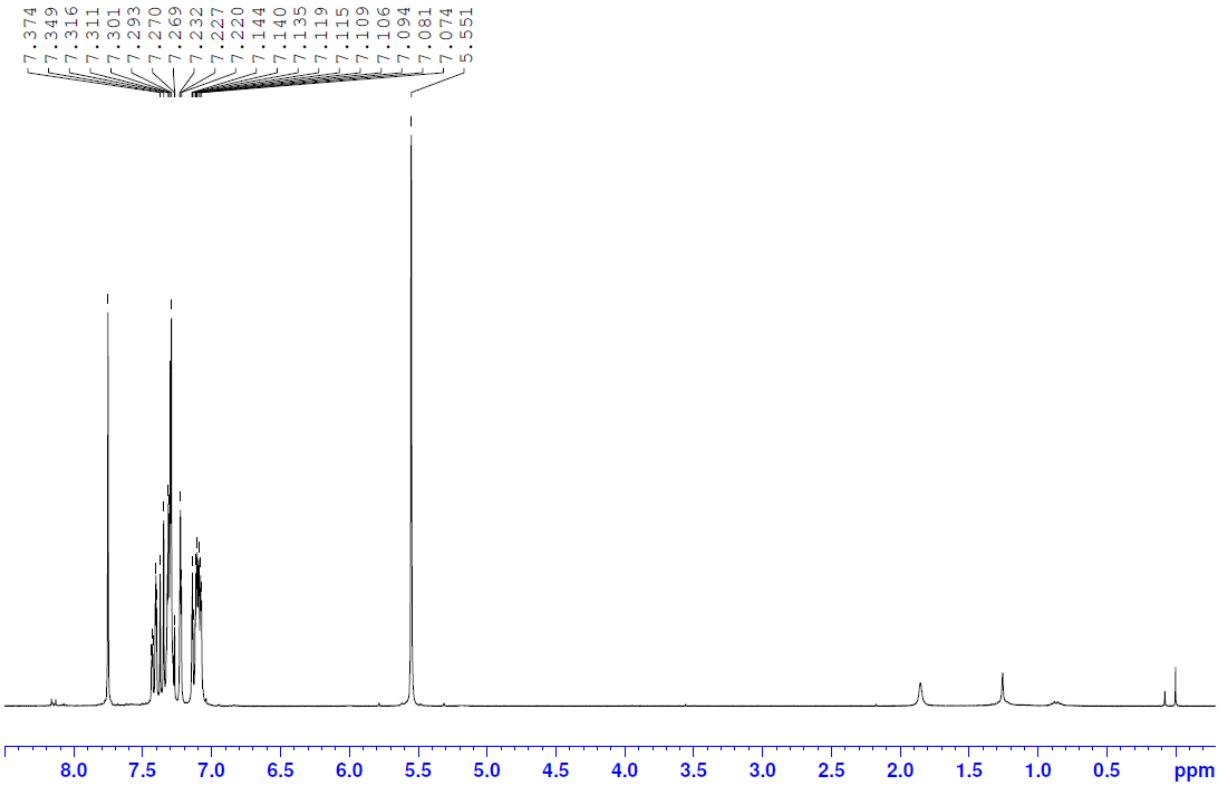
1-benzyl-5-(3-chlorophenyl)-1,2,3-triazole (3c)

^{1}H-NMR



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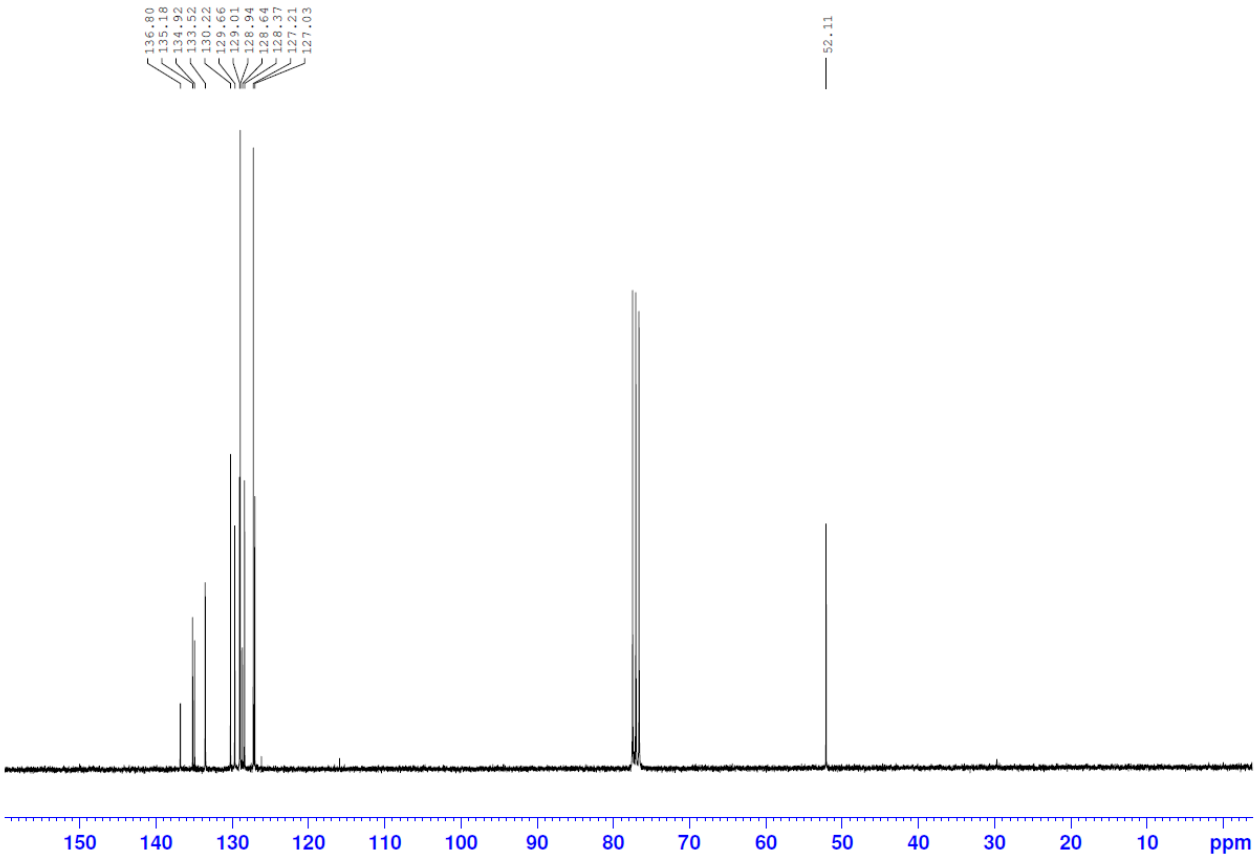

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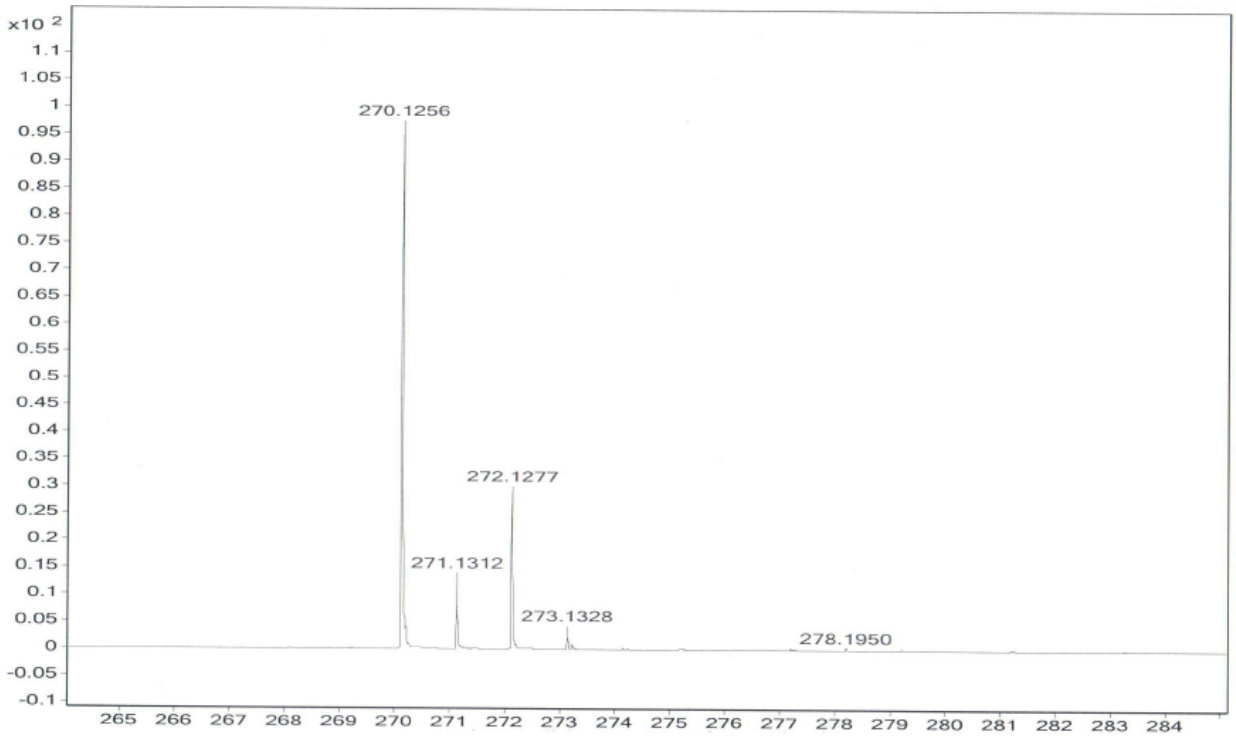
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0.9
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0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
270.1256
272.1277
271.1312
273.1328
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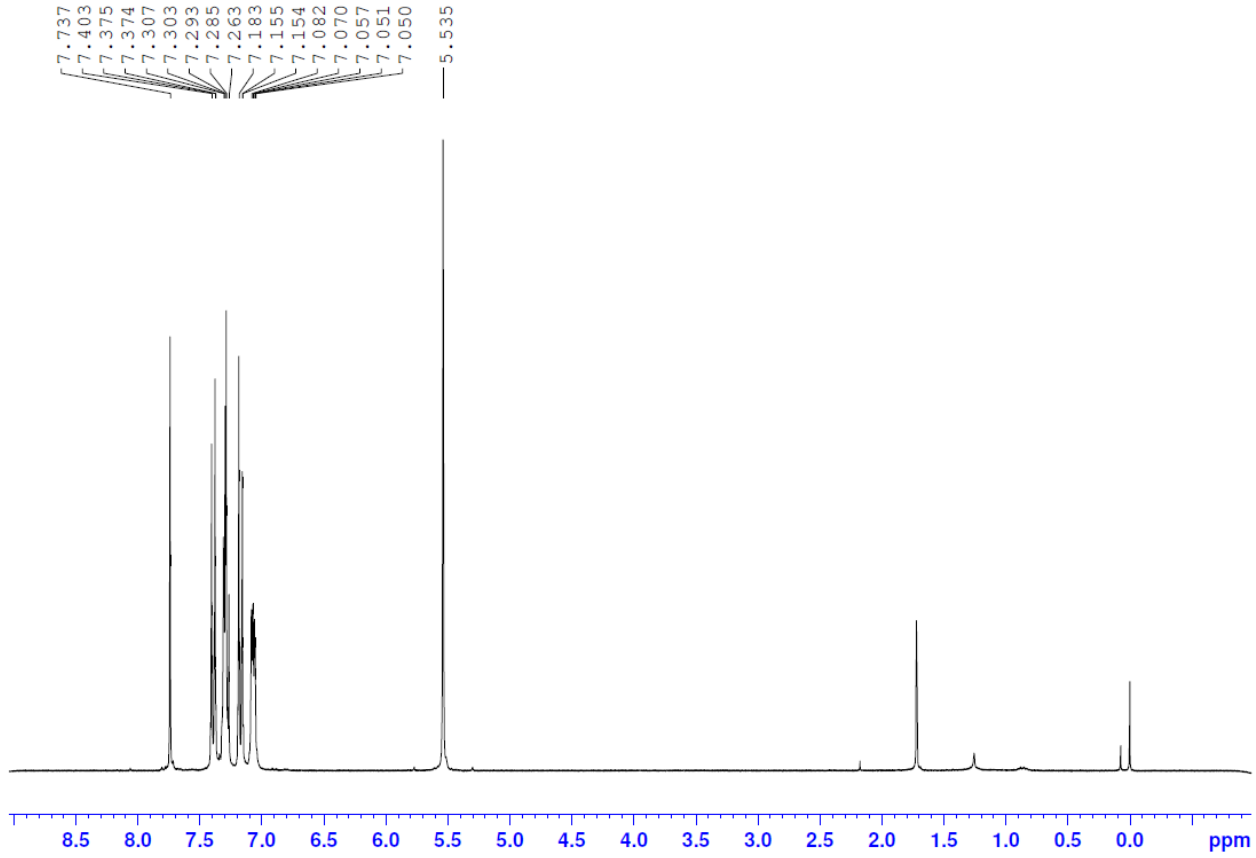
1-benzyl-5-(4-chlorophenyl)-1,2,3-triazole (3d)

^{1}H-NMR



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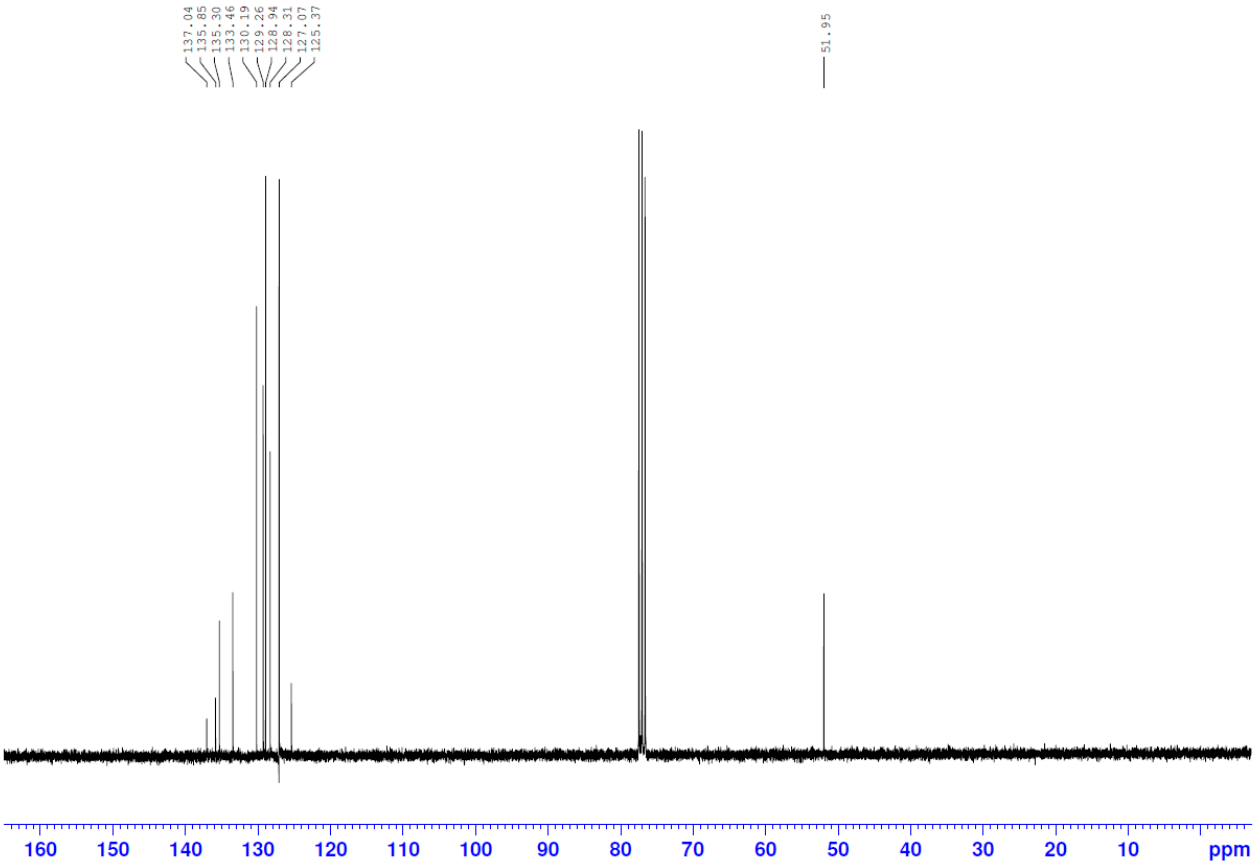

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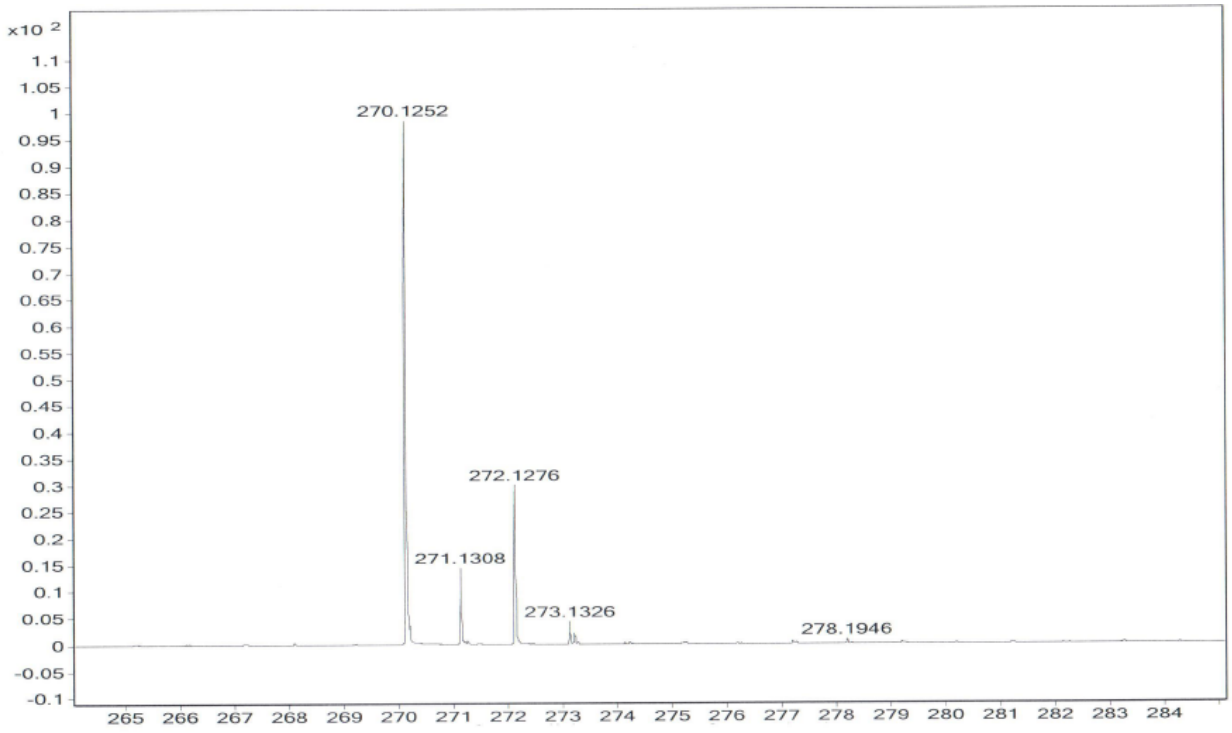
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0.9
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0.7
0.65
0.6
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0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
270.1252
272.1276
271.1308
273.1326
278.1946
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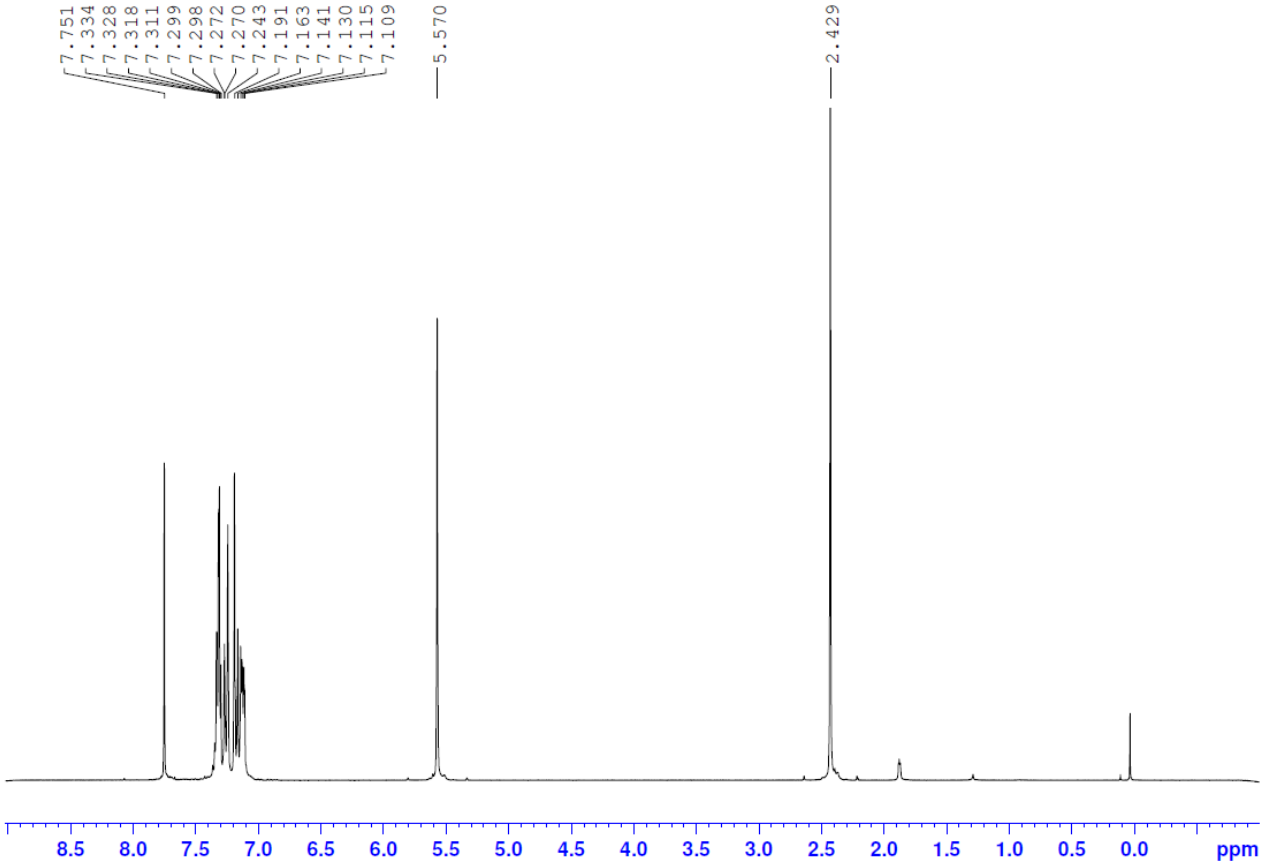
1-benzyl-5-(4-methylphenyl)-1,2,3-triazole (3e)

^{1}H-NMR



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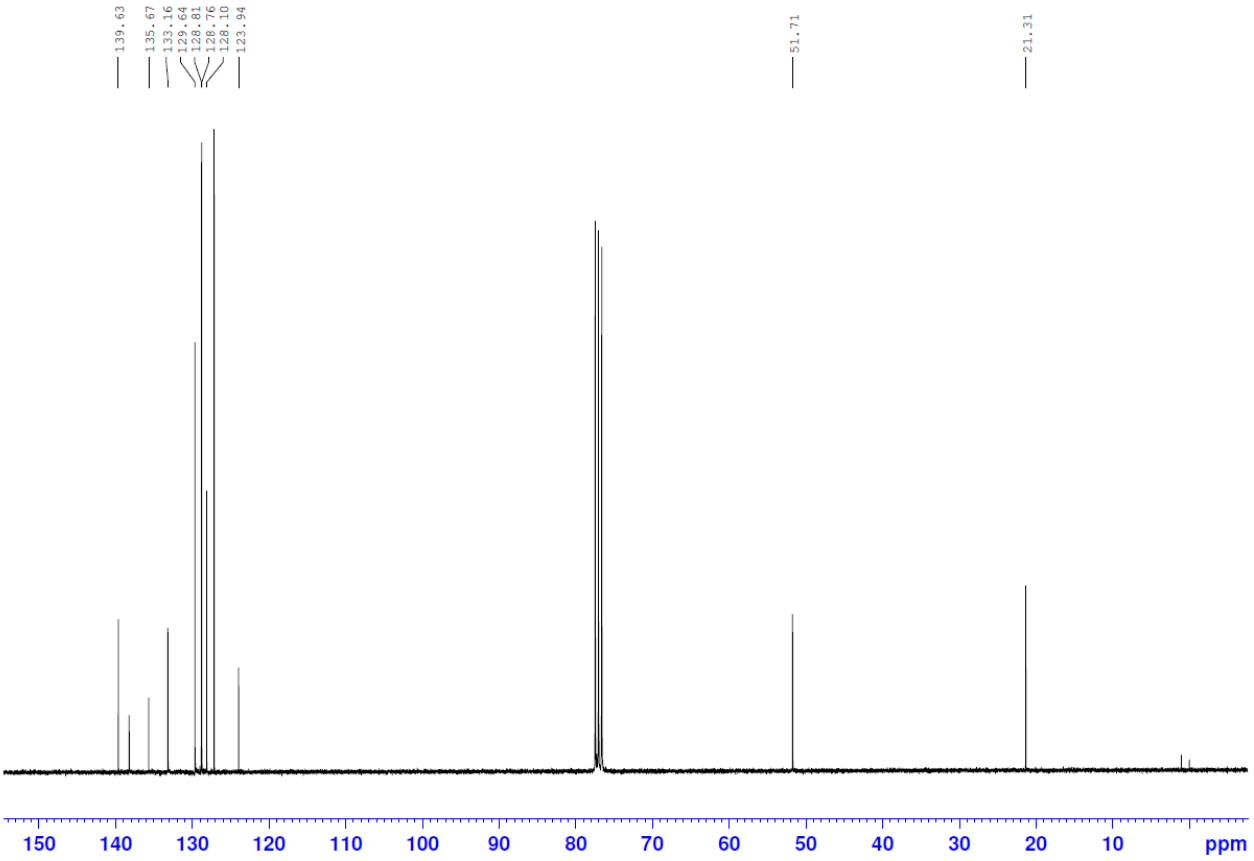

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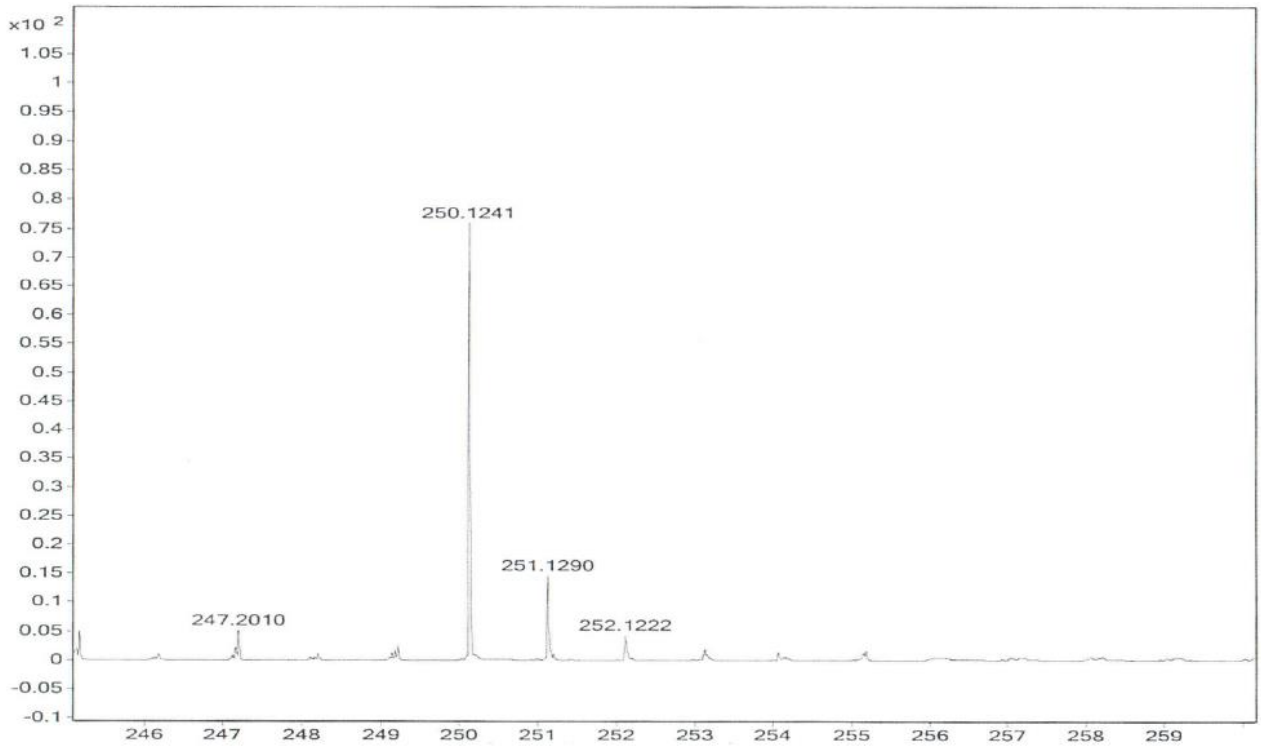
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0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
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247.2010
252.1222
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247
248
249
250
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257
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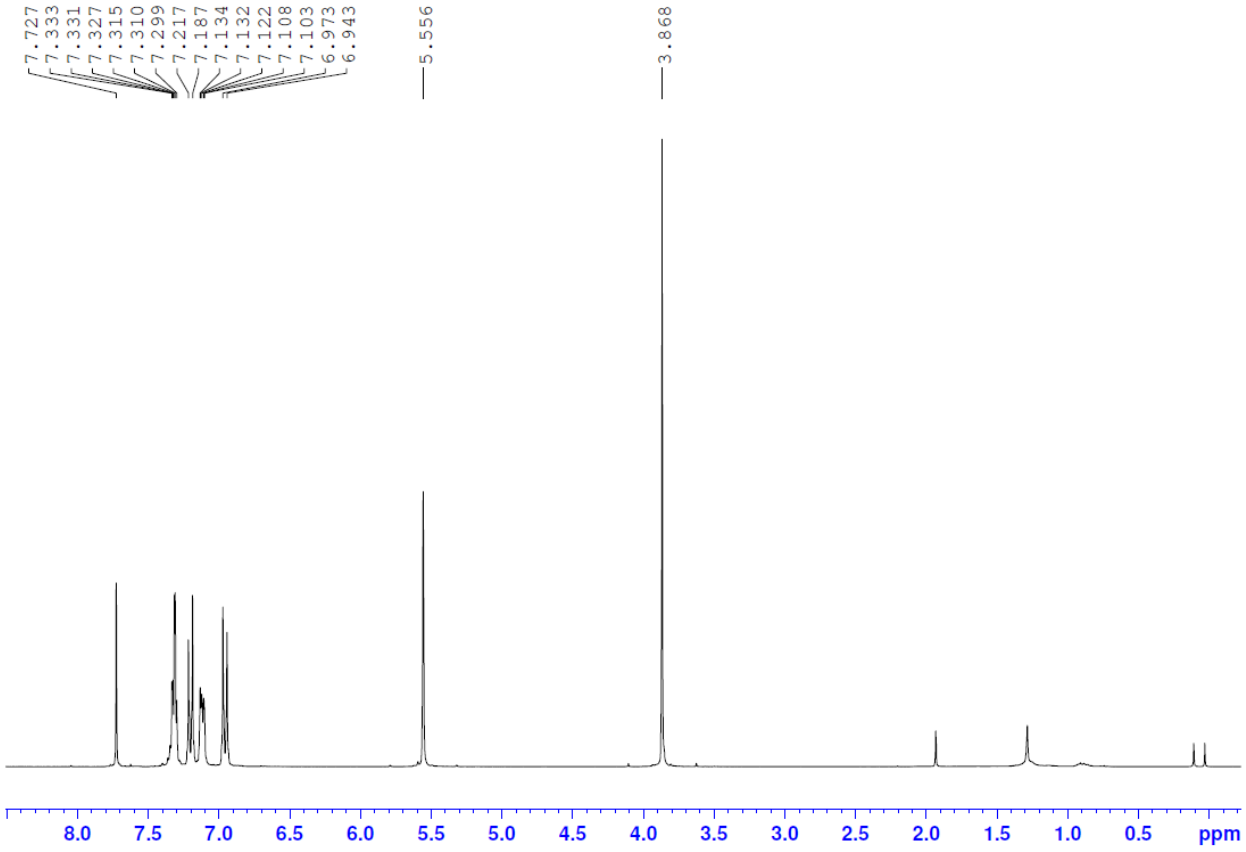
259

1-benzyl-5-(4-methoxyphenyl)-1,2,3-triazole (3f)

^{1}H-NMR



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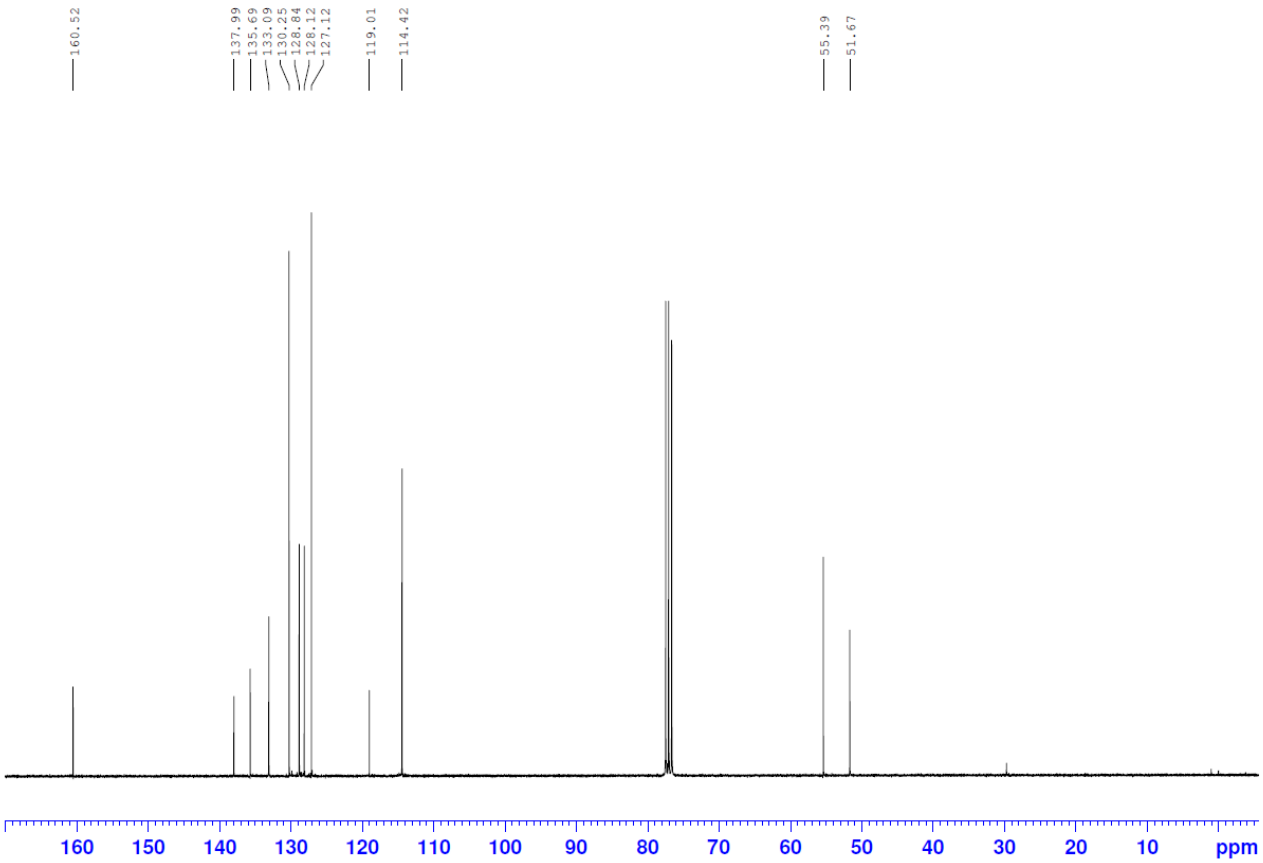

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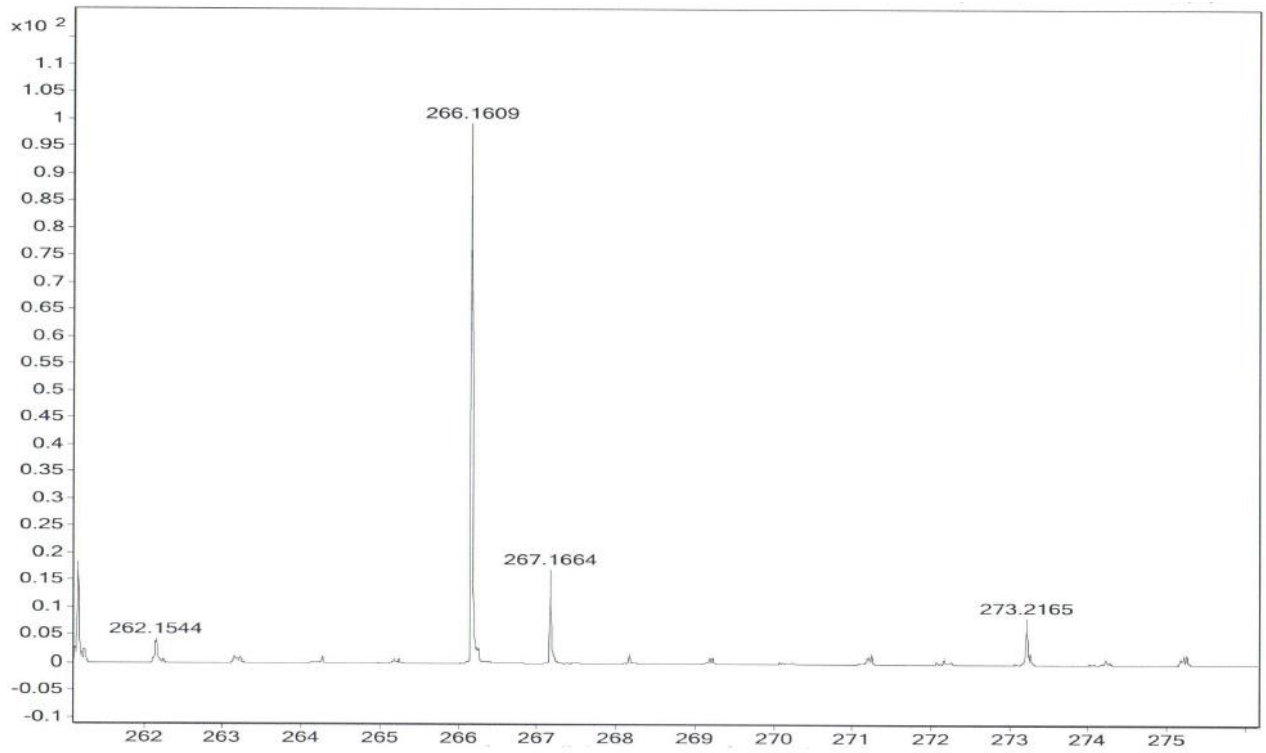
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0.05
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263
264
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266
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273
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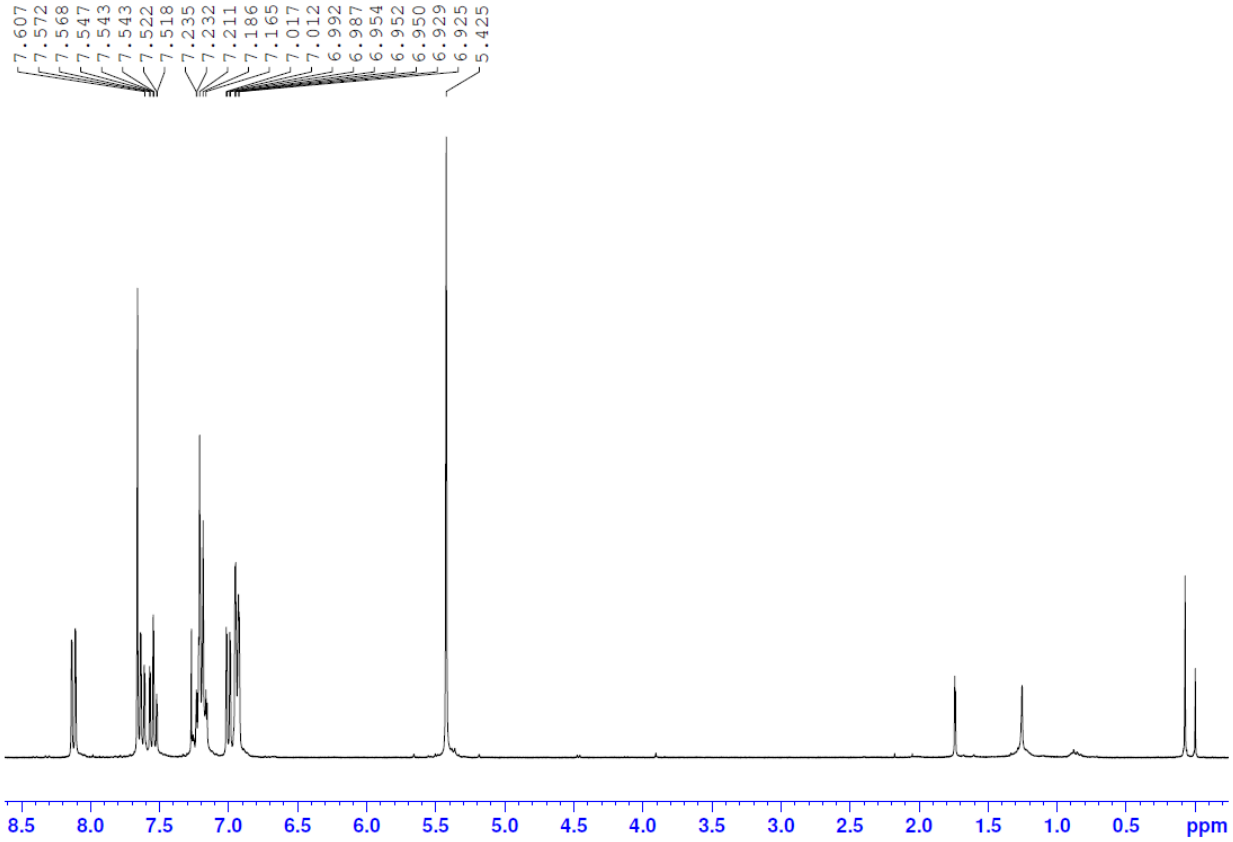
1-benzyl-5-(2-nitrophenyl)-1,2,3-triazole (3g)

^{1}H-NMR



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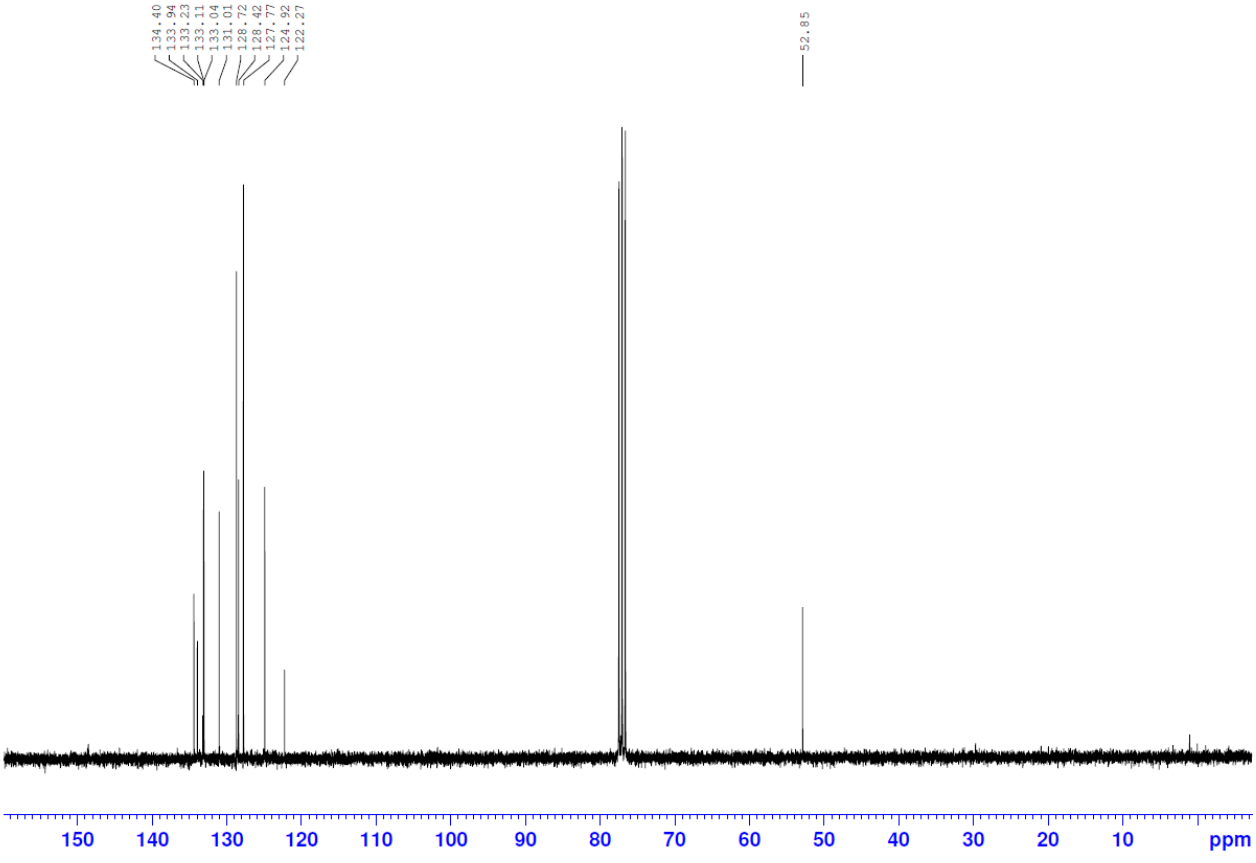

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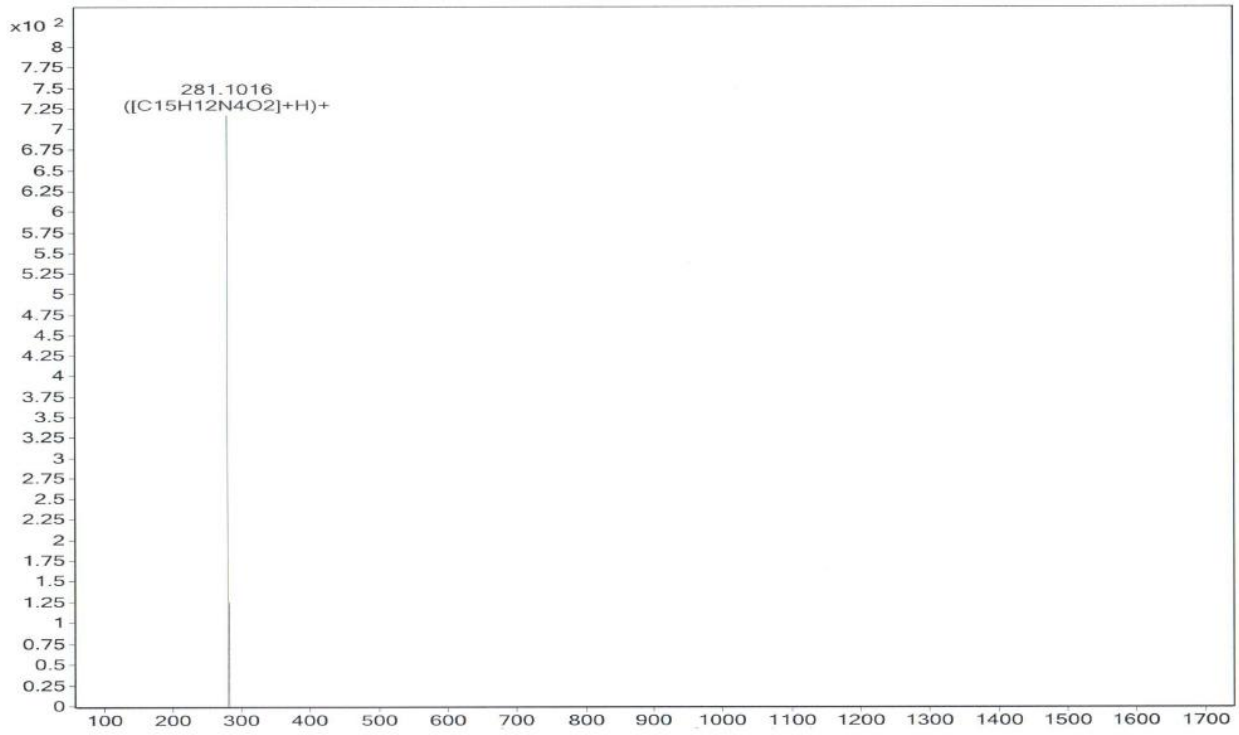
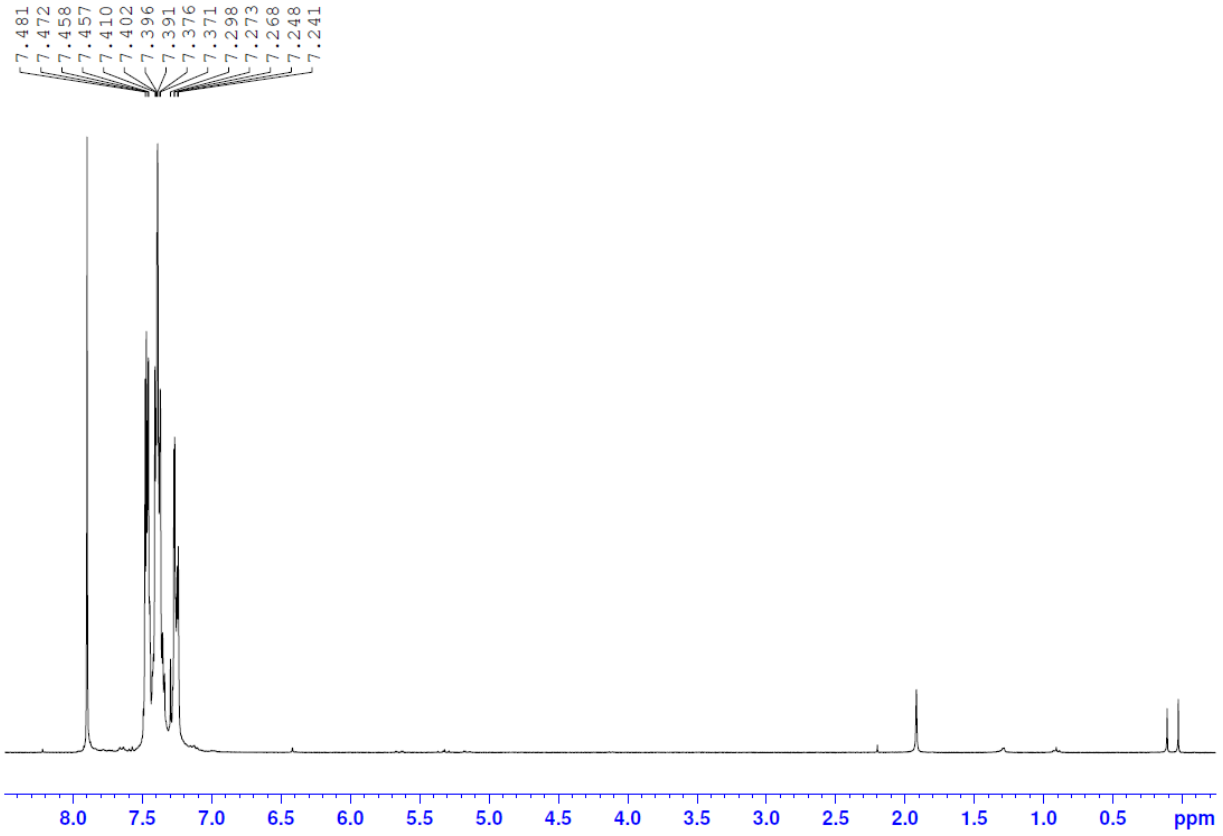


1,5-diphenyl-1,2,3-triazole (3h)

^{1}H-NMR



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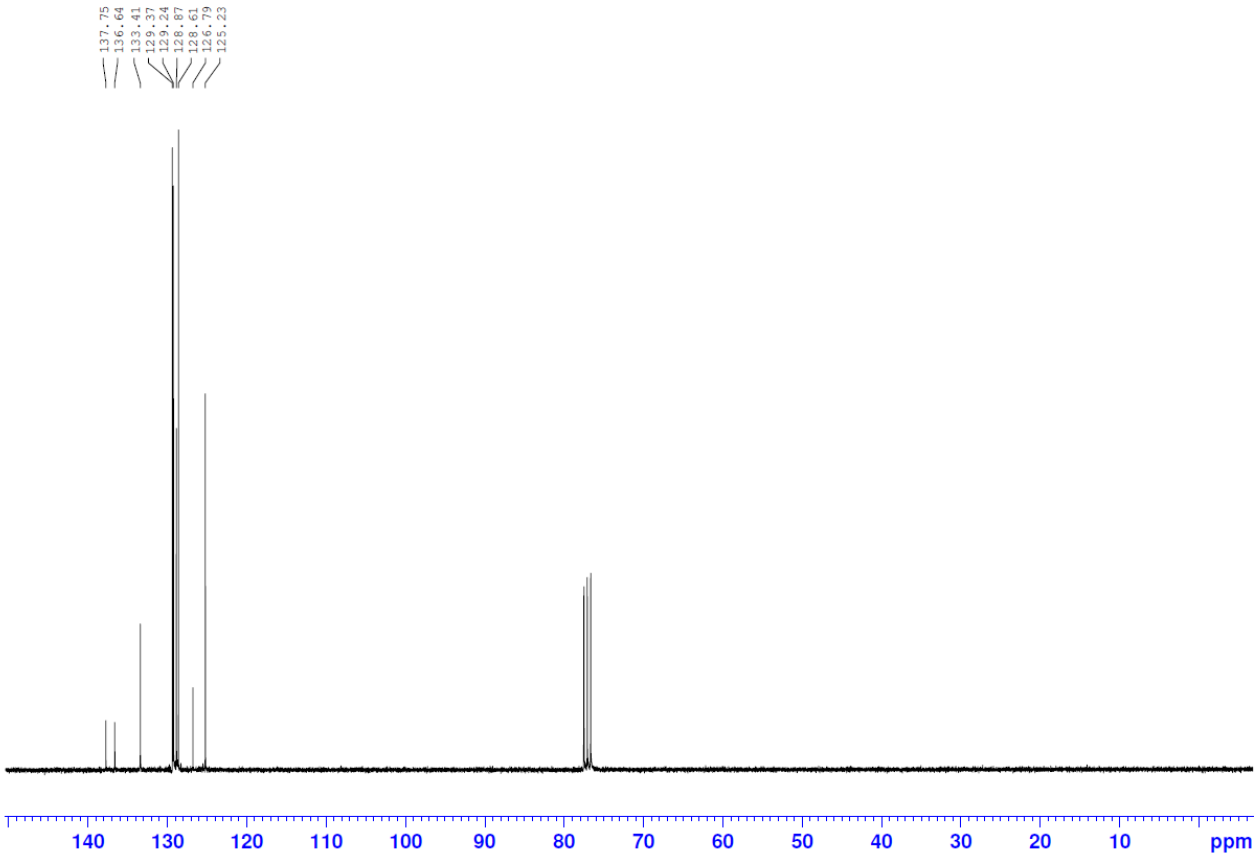

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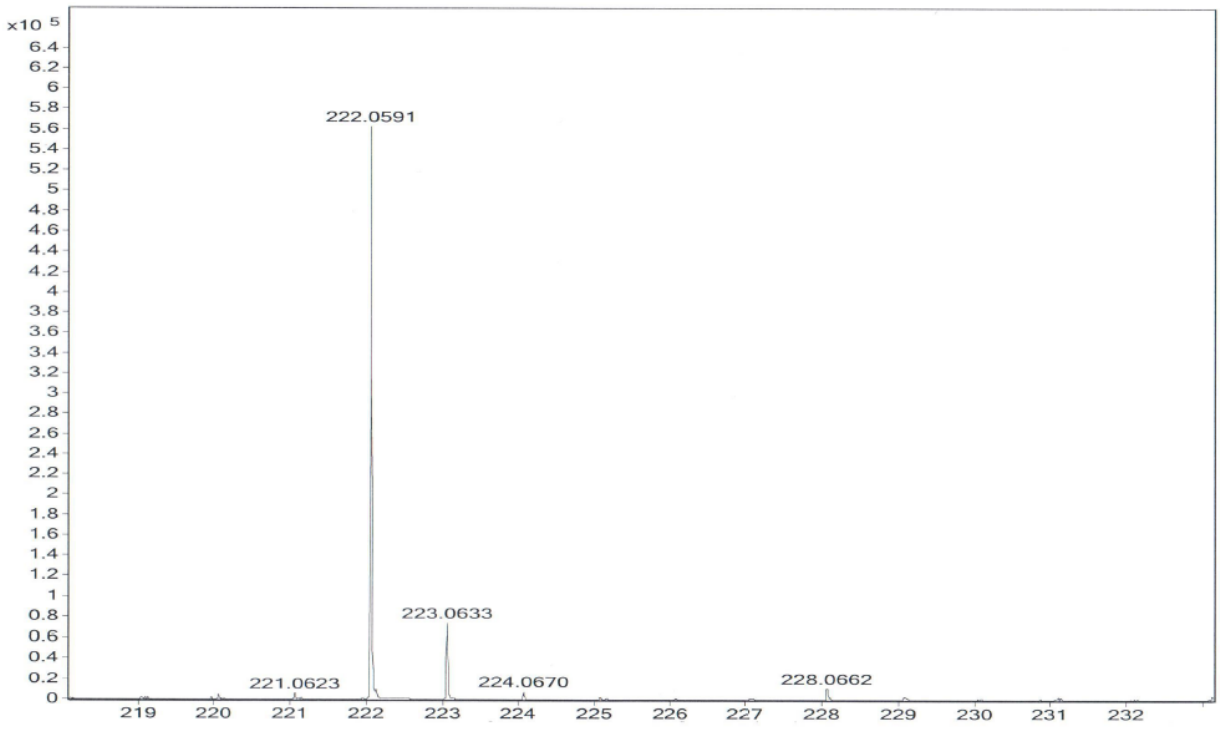
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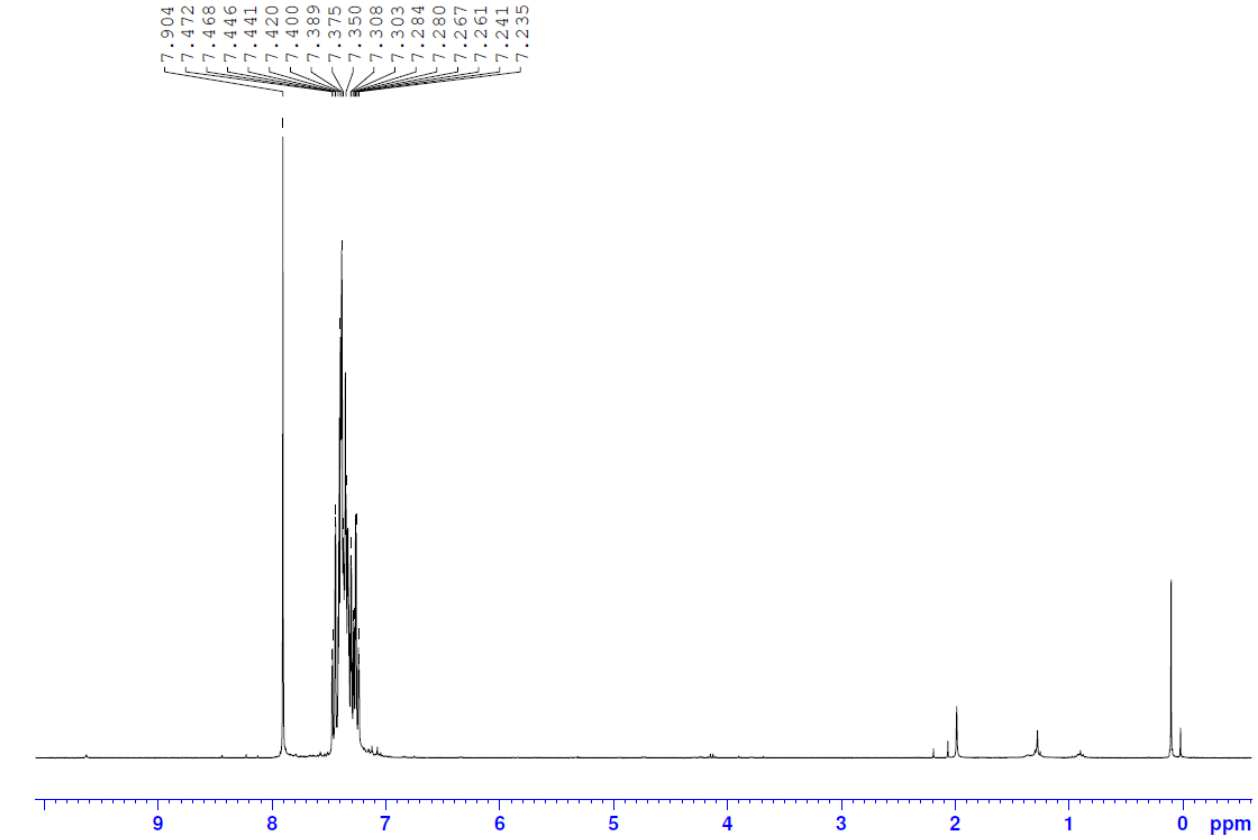
5-(2-chlorophenyl)-1-phenyl-1,2,3-triazole (3i)

^{1}H-NMR



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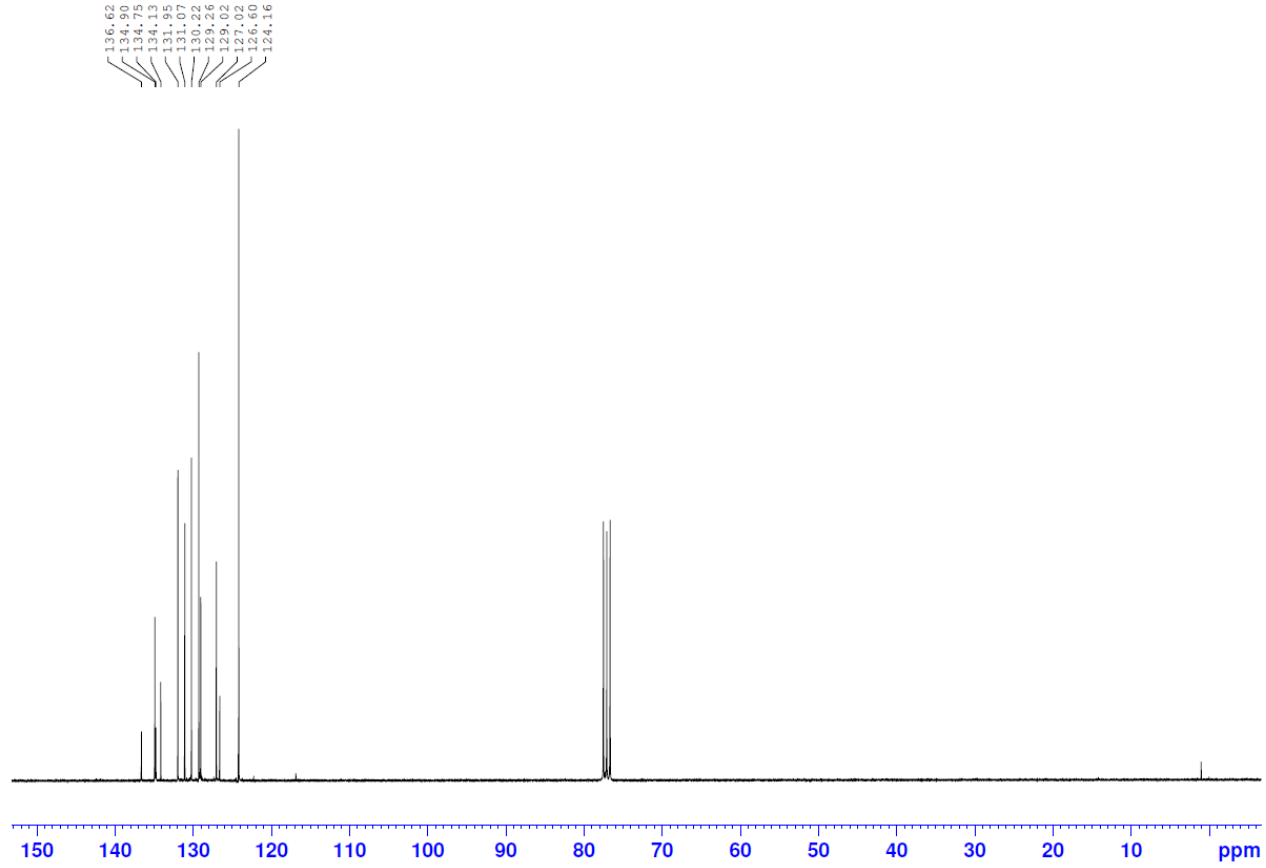

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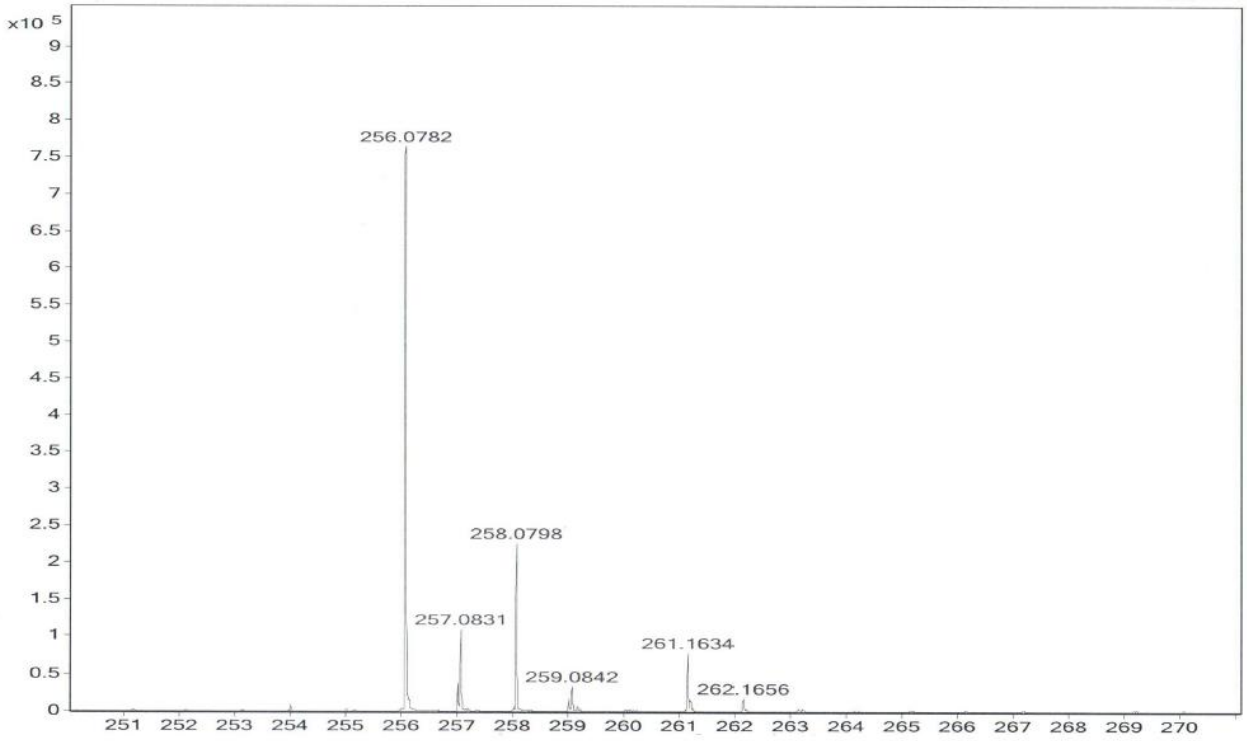
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1.5
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257.0831
261.1634
259.0842
262.1656
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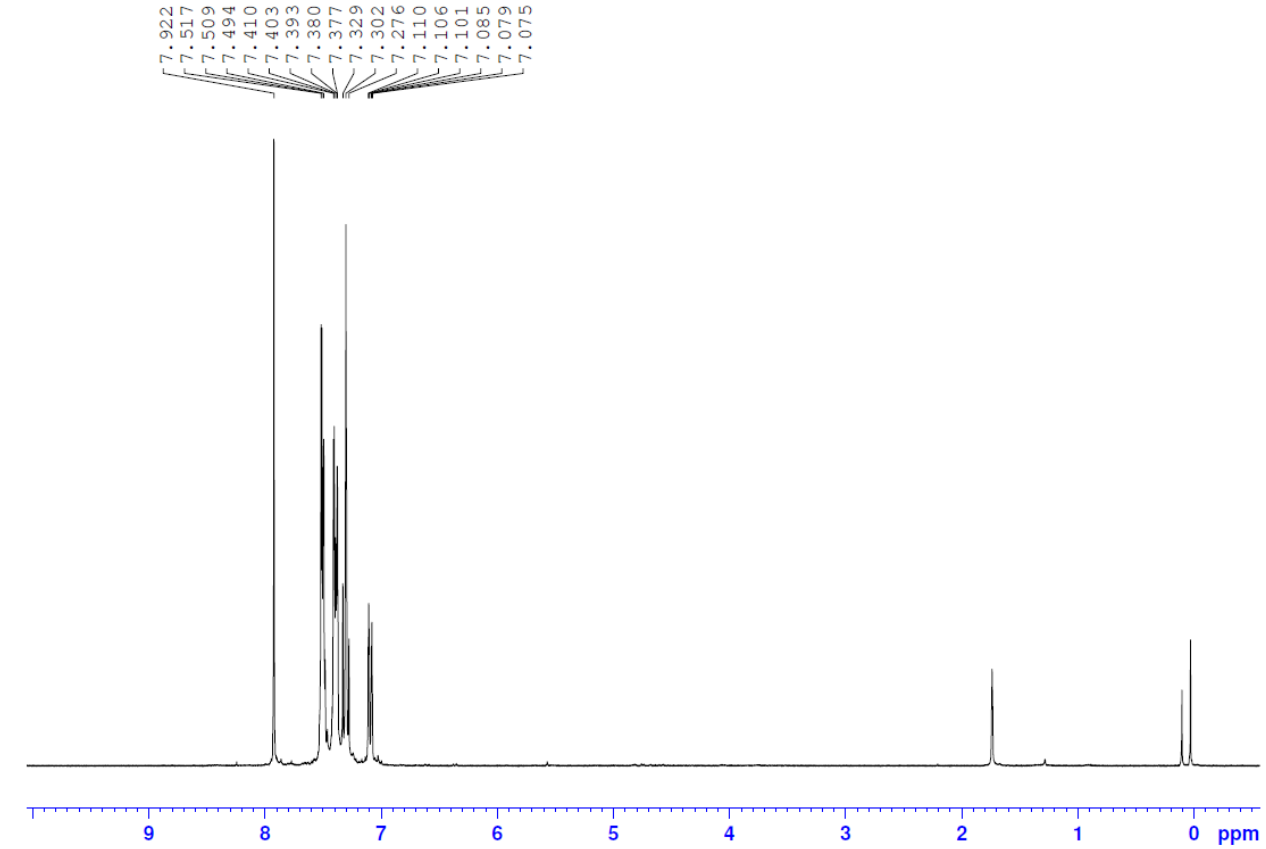
5-(3-chlorophenyl)-1-phenyl-1,2,3-triazole (3j)

^{1}H-NMR



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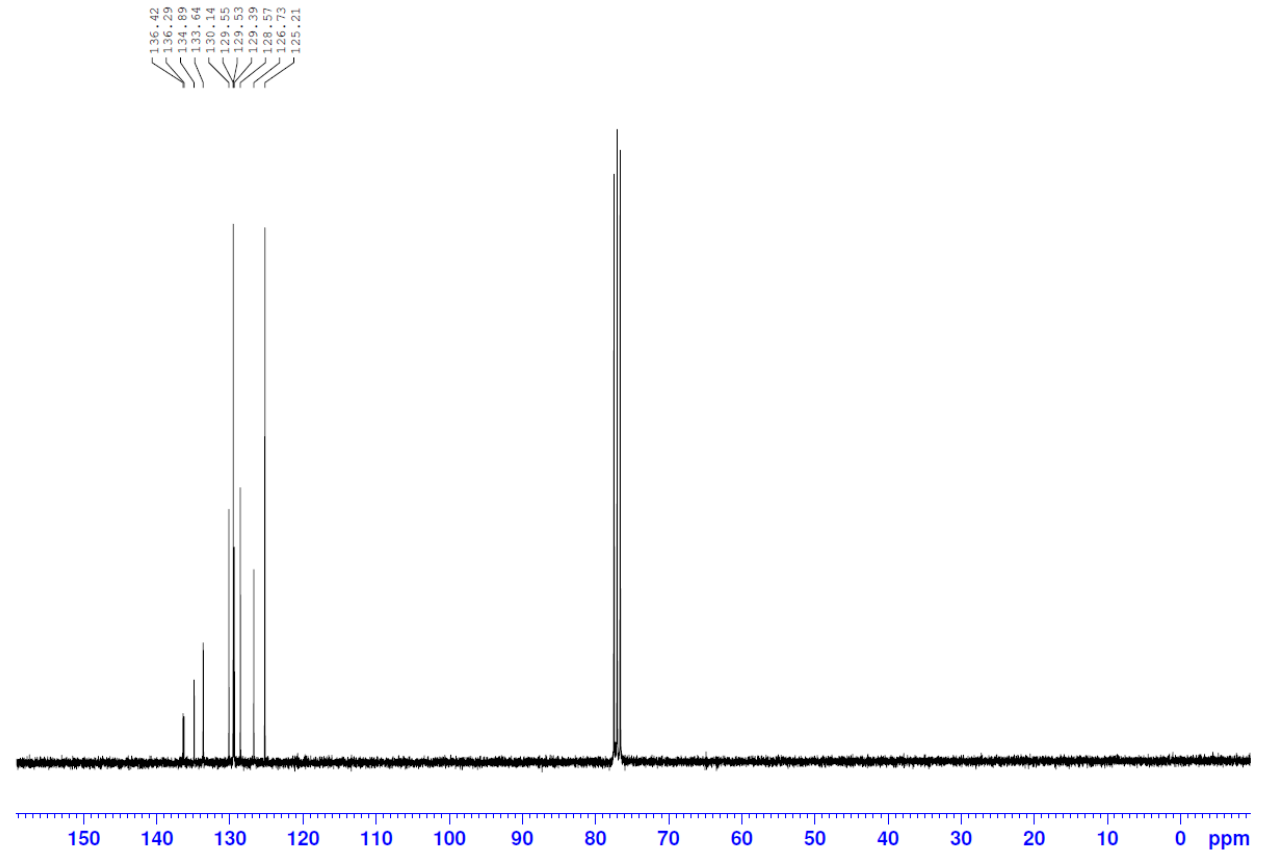

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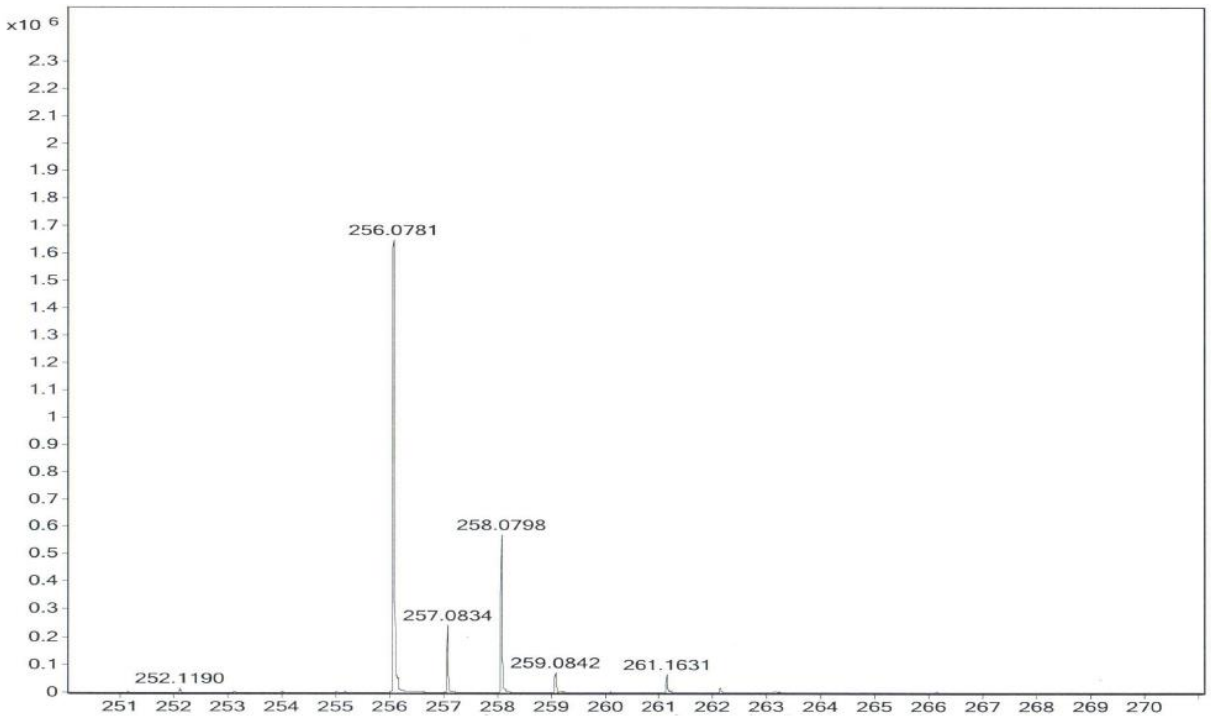
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0
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258.0798
257.0834
259.0842
261.1631
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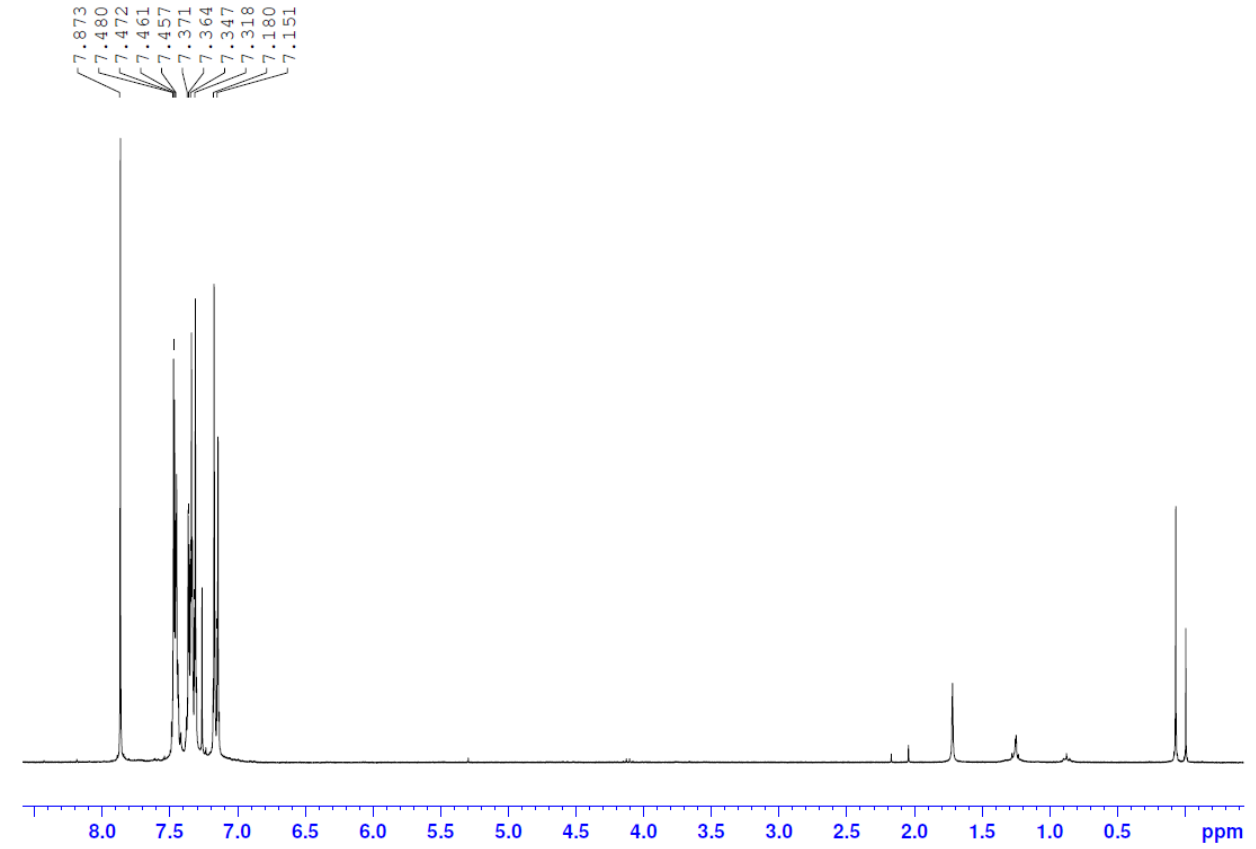
251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270

5-(4-chlorophenyl)-1-phenyl-1,2,3-triazole (3k)

^{1}H-NMR



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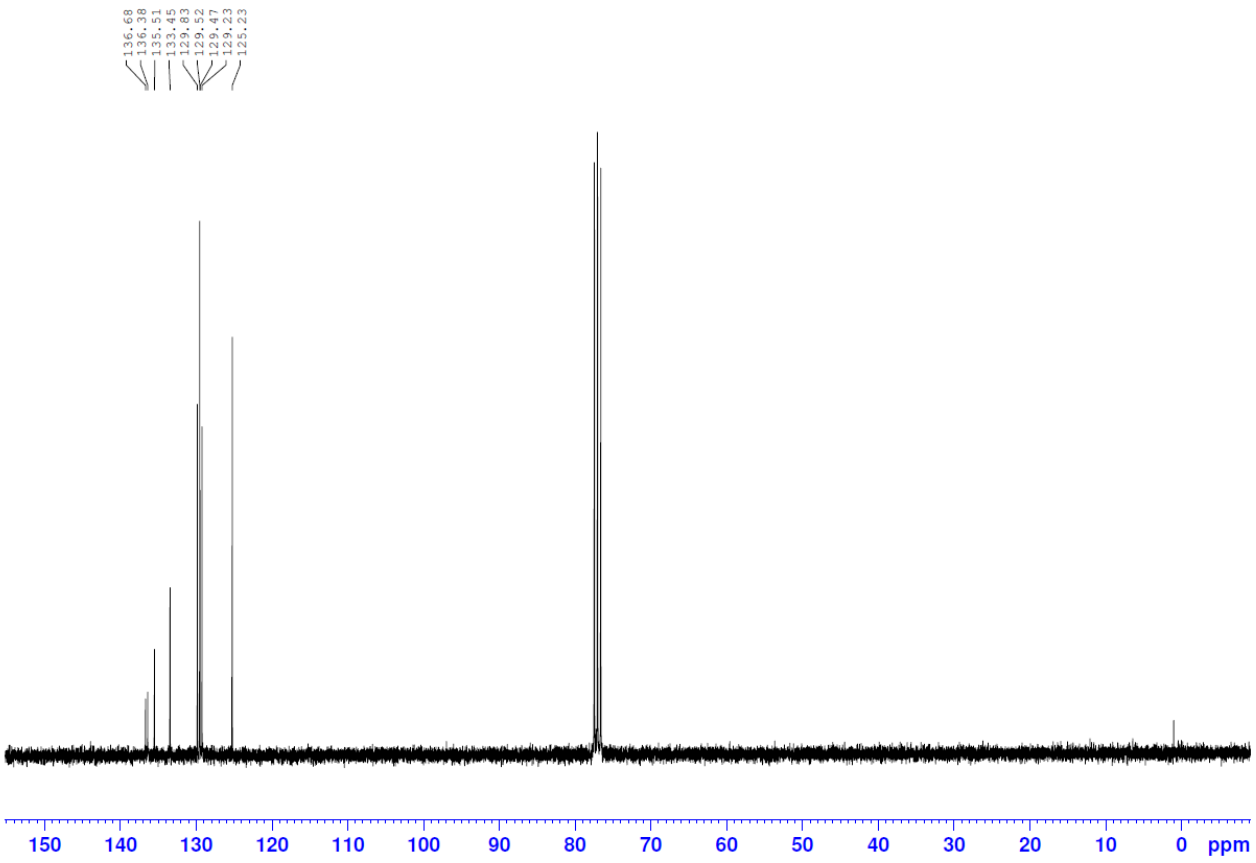

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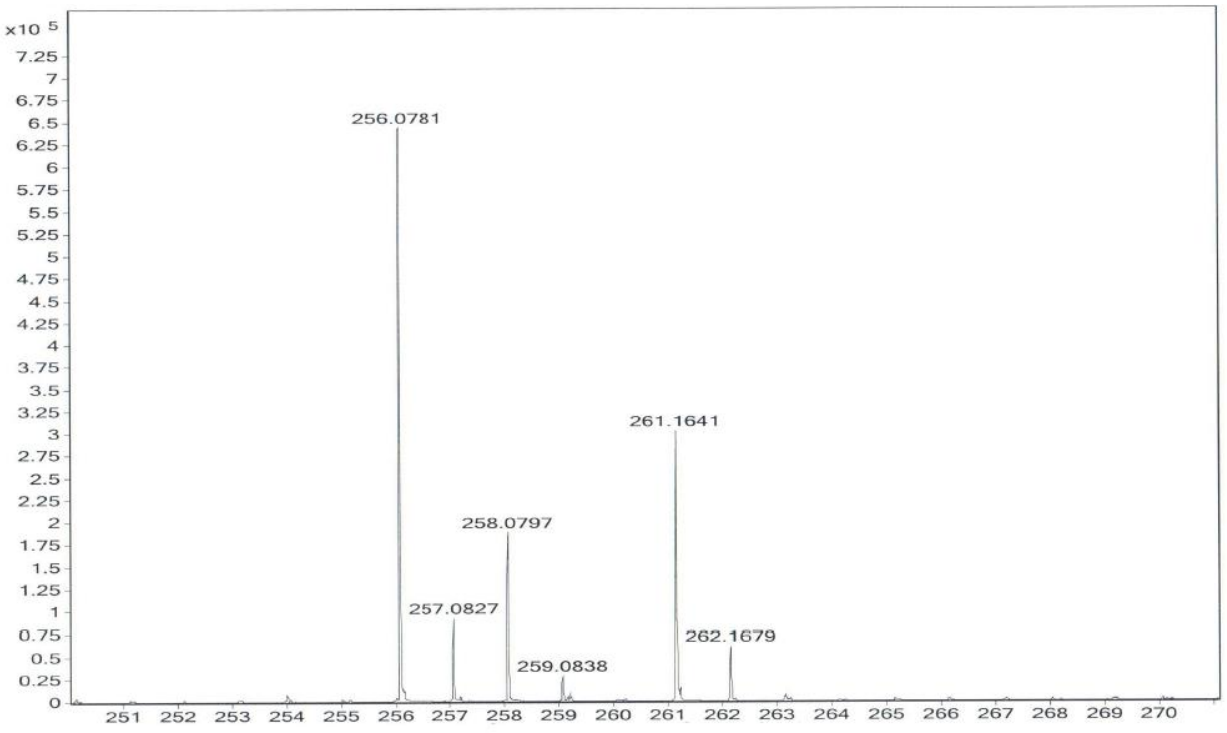
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3.75
3.5
3.25
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0.25
0
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261.1641
258.0797
257.0827
262.1679
259.0838
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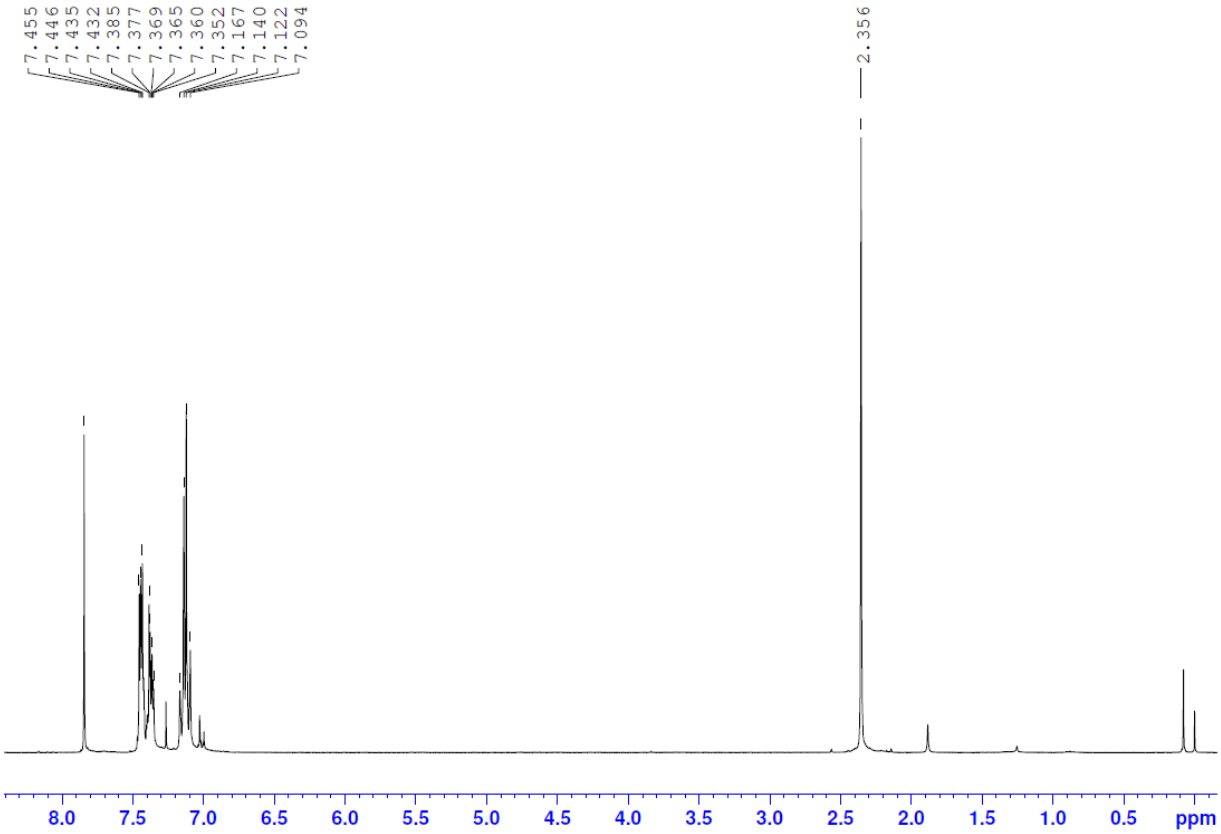
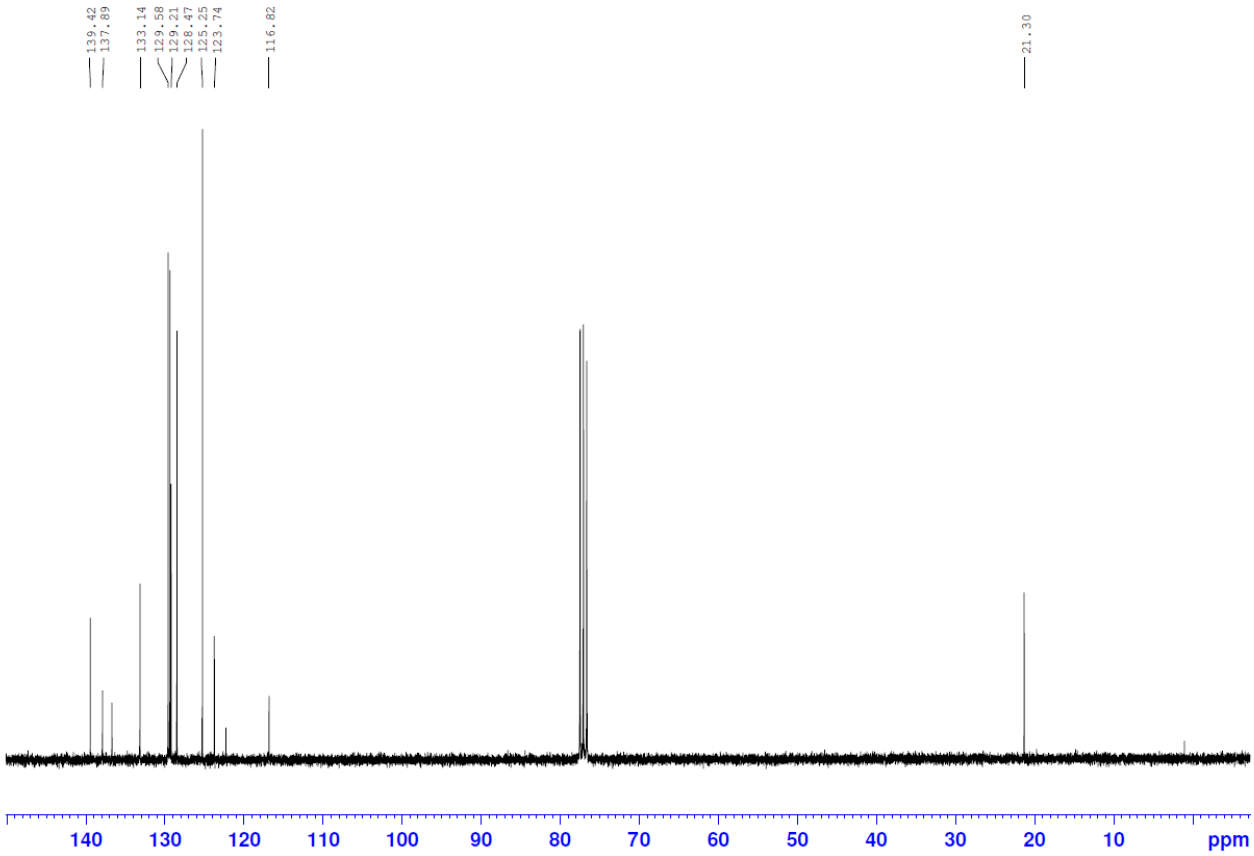
5-(4-methylphenyl)-1-phenyl-1,2,3-triazole (3l)

^{1}H-NMR



^{13}C-NMR



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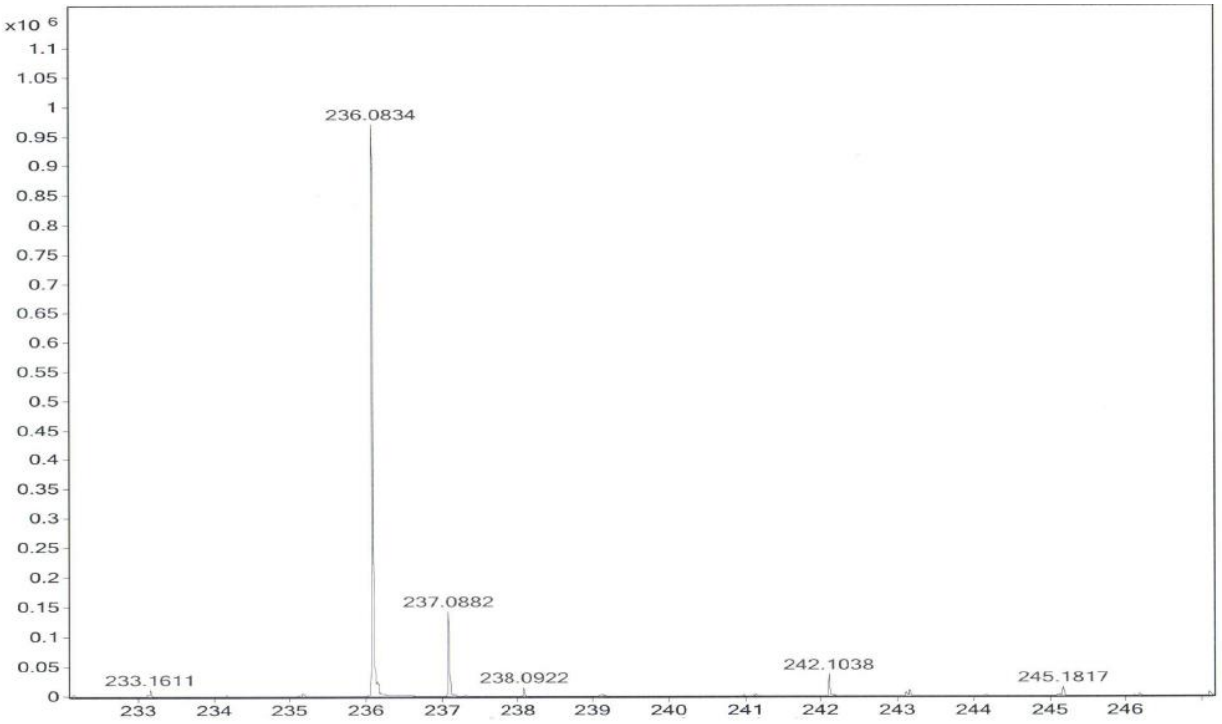
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0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
236.0834
237.0882
233.1611
238.0922
242.1038
245.1817
233
234
235
236
237
238
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242
243
244
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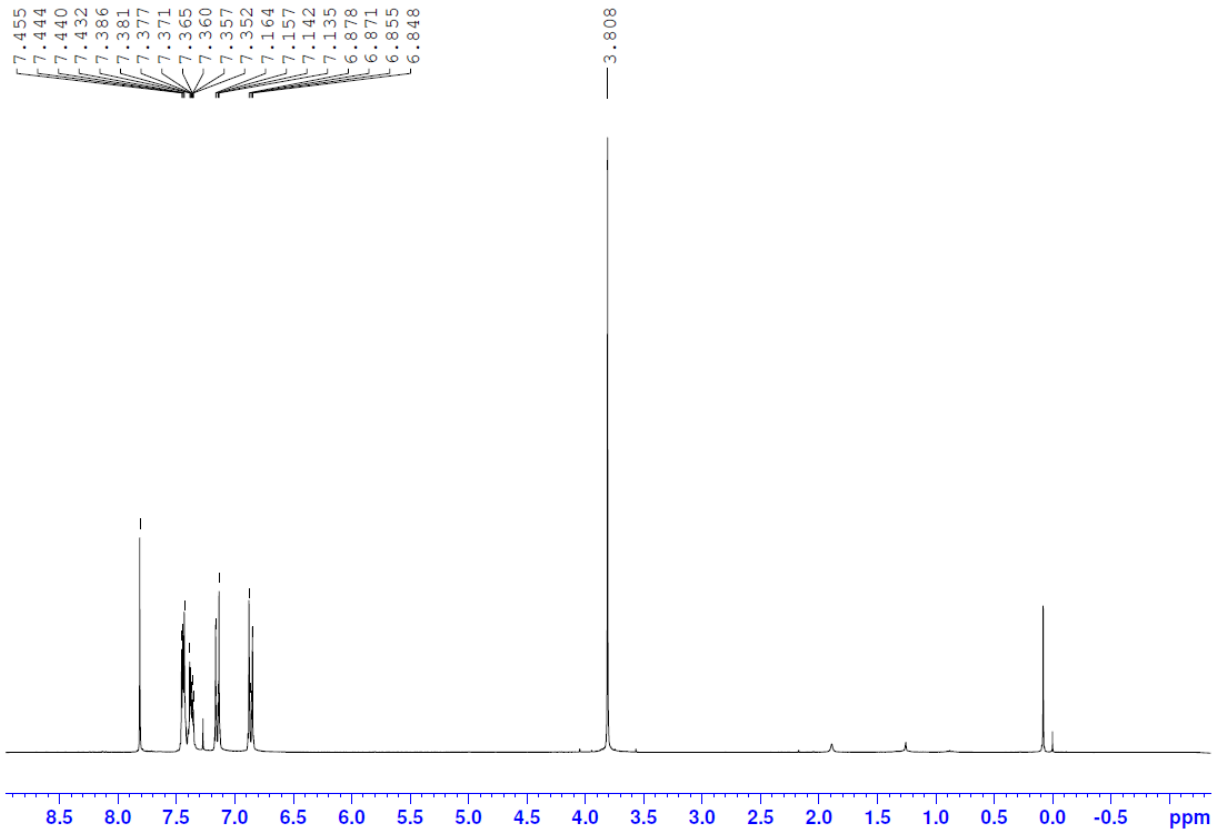
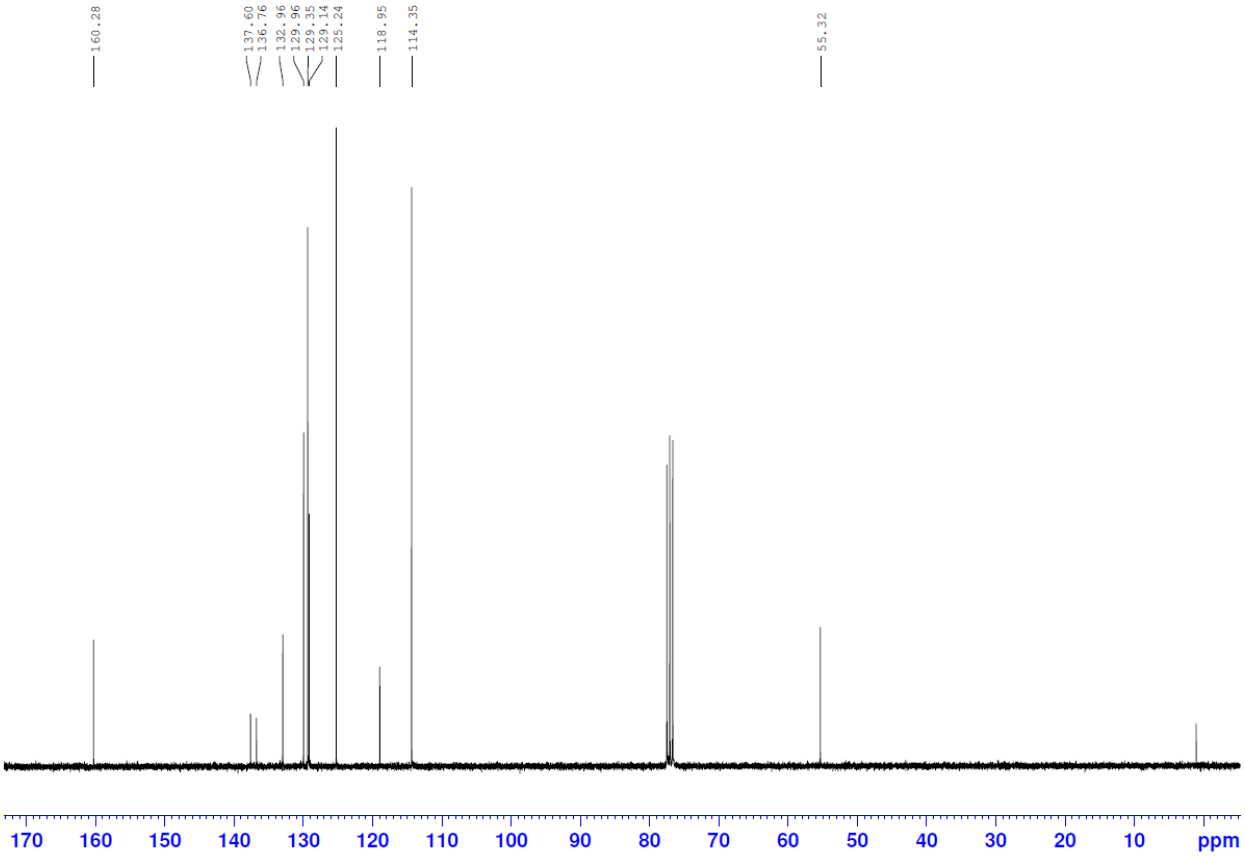
246

5-(4-methoxyphenyl)-1-phenyl-1,2,3-triazole (3m)

^{1}H-NMR



^{13}C-NMR



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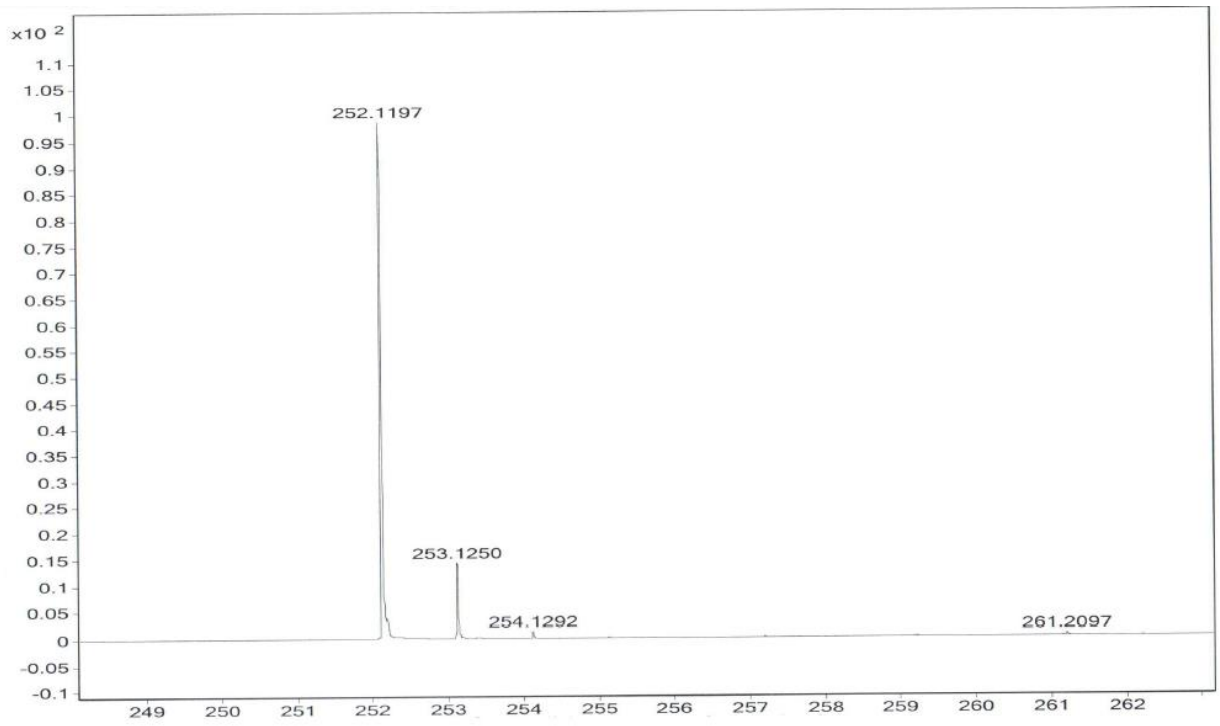
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0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
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253.1250
254.1292
261.2097
249
250
251
252
253
254
255
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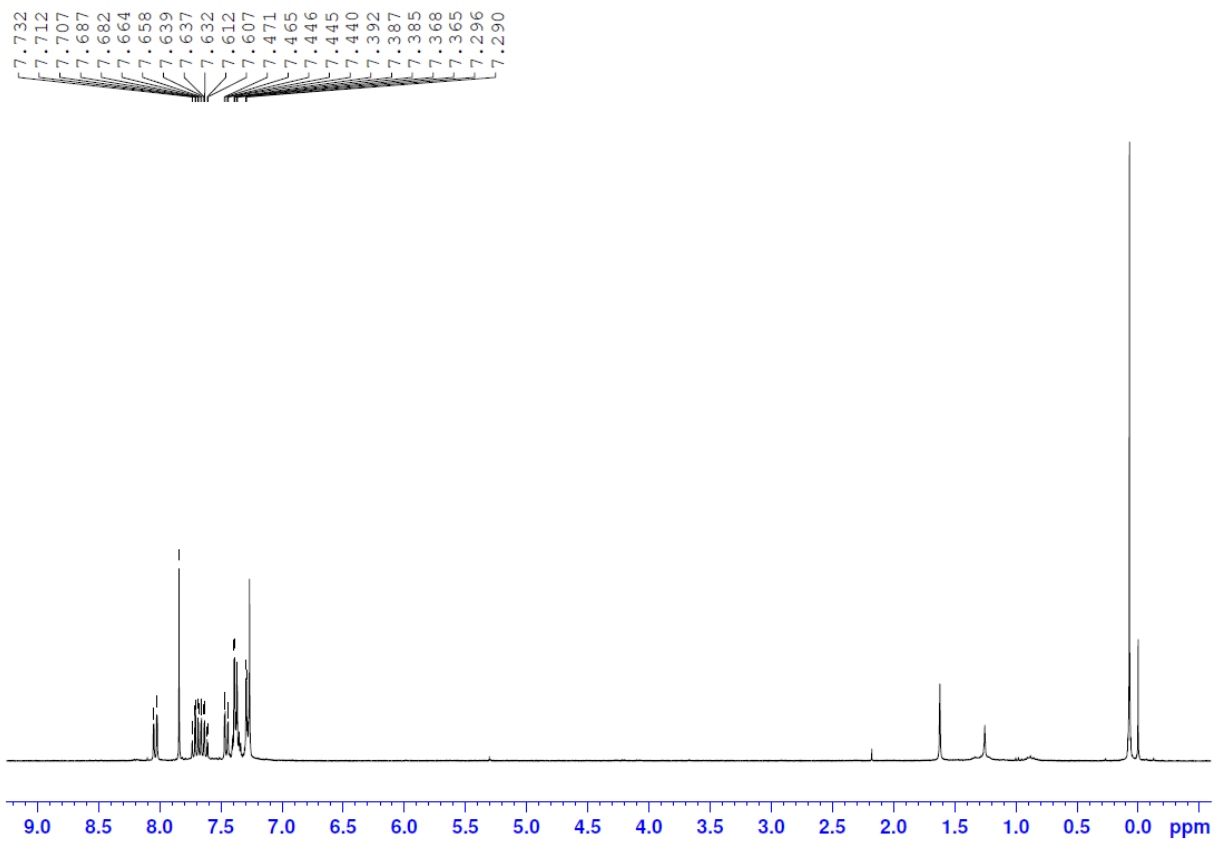
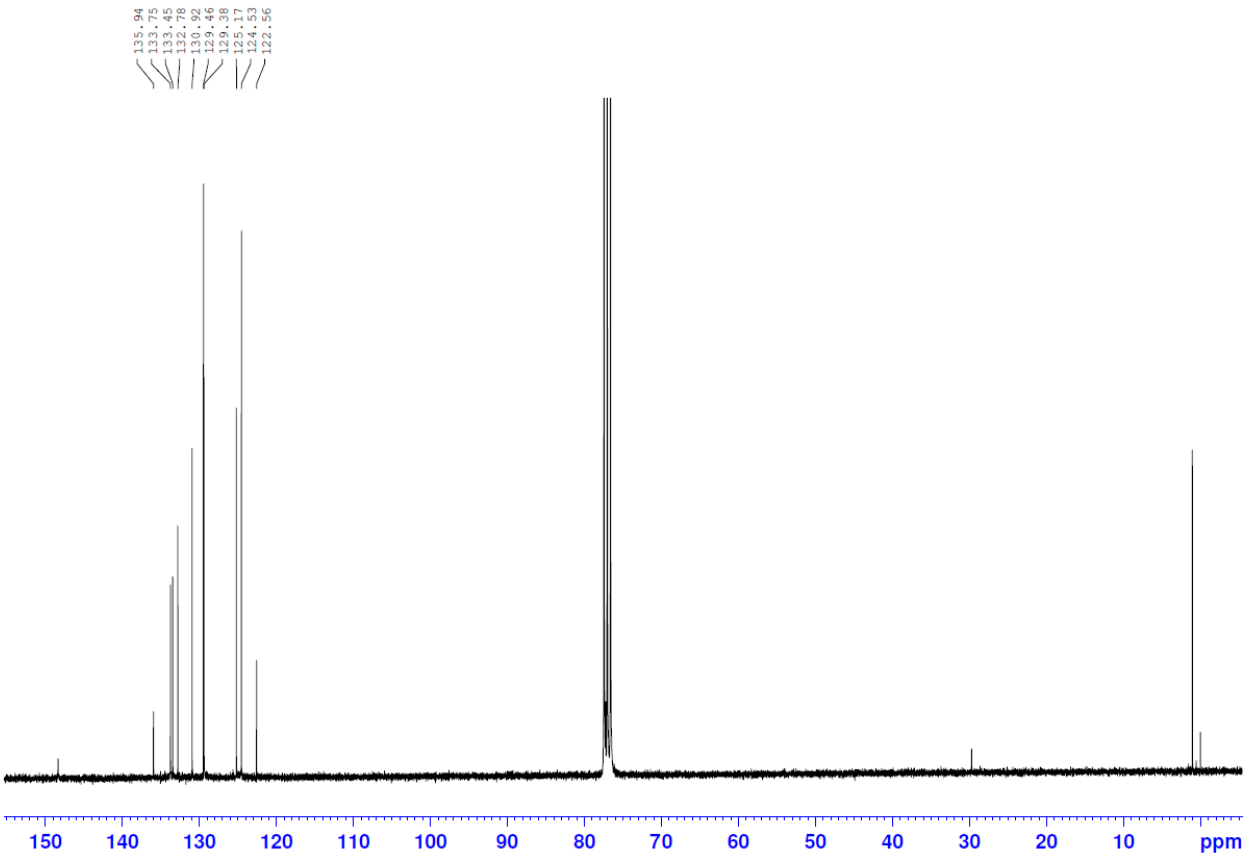
258
259
260
261
262

5-(2-nitrophenyl)-1-phenyl-1,2,3-triazole (3n)

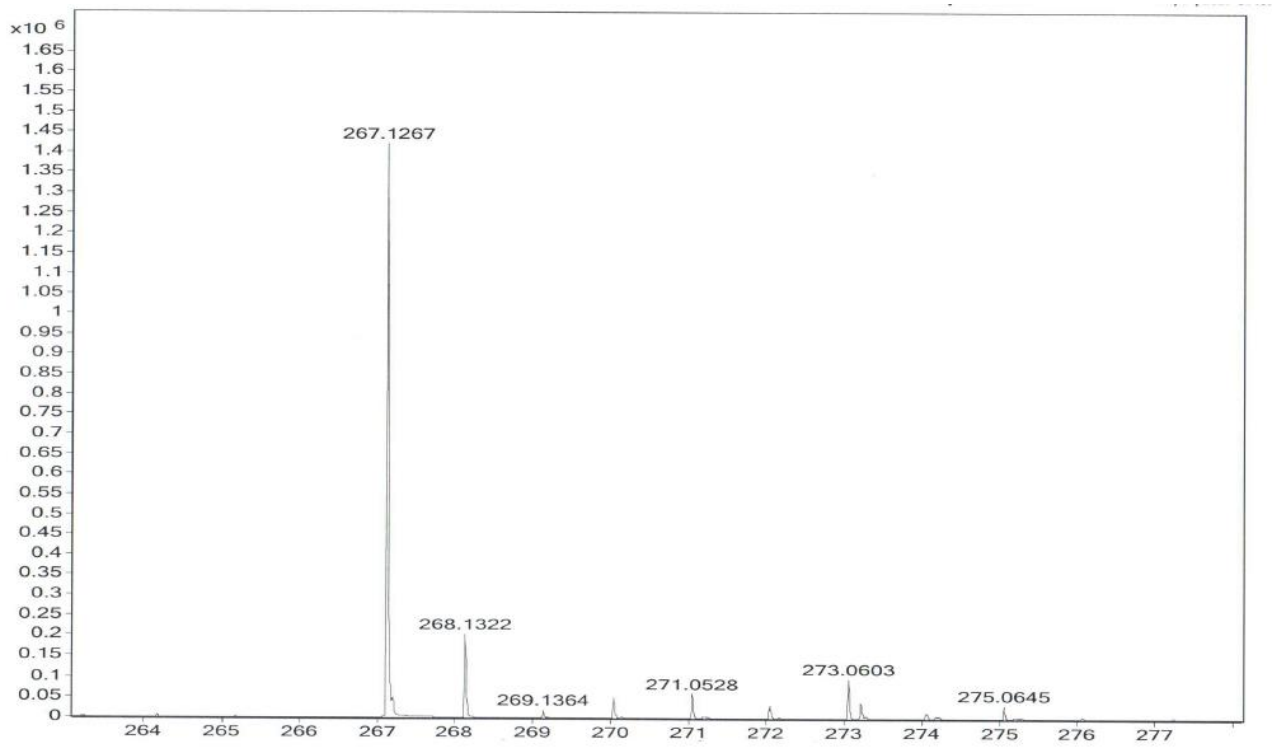
^{1}H-NMR



^{13}C-NMR



ESI(+)-MS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1.6
1.55
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1.45
1.4
1.35
1.3
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1.2
1.15
1.1
1.05
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
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268.1322
269.1364
271.0528
273.0603
275.0645
264
265
266
267
268
269
270
271
272
273
274
275
276
277

Theoretical Calculations

Computational Details

All of the calculations were performed using the Gaussian09 program.[1] Computations were done using B3LYP functional[2] in conjuction with Grimme's dispersion correction.[3] Standard basis sets def2SVP and def2TZVP were employed.[4] Geometry full optimizations were made at B3LYP-D3BJ/def2SVP level and then single point calculations at B3LYP-D3BJ/def2TZVP level were carried out in order to obtain more accurate values of the energies. The nature of stationary points was defined on the basis of calculations of normal vibrational frequencies (force constant Hessian matrix). The optimizations were carried out using the Berny analytical gradient optimization method.[5] Minimum energy pathways for the reactions studied were found by gradient descent of transition states in the forward and backward direction of the transition vector (IRC analysis),[6] using using the Hratchian-Schlegel algorithm.[7] Structural representations were generated using CYLView.[8]

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Uncatalyzed Cycloaddition

Table S1. Absolute (hartrees) and relative (kcal/mol) energies (B3LYP-D3BJ/Def2TZVP/CPCM=water// B3LYP-D3BJ/Def2SVP) corresponding to the reaction between **NS** and **PA**

	E(0)	G	im. freq	ΔE(0)[a]	ΔG[a]
NS	-514.252731	-514.288493			
PA	-395.912133	-395.943985			
TS1n	-910.135865	-910.182470	-417.7	18.2	31.4
TS1x	-910.135466	-910.182158	-413.2	18.4	31.6
TS2n	-910.139710	-910.185391	-386.2	15.8	29.5
TS2x	-910.138710	-910.185861	-393.0	16.4	29.3
P14	-910.185874	-910.233083		-13.2	-0.4
P15	-910.185728	-910.232347		-13.1	0.1

[a] Related to **PA** + **NS**.

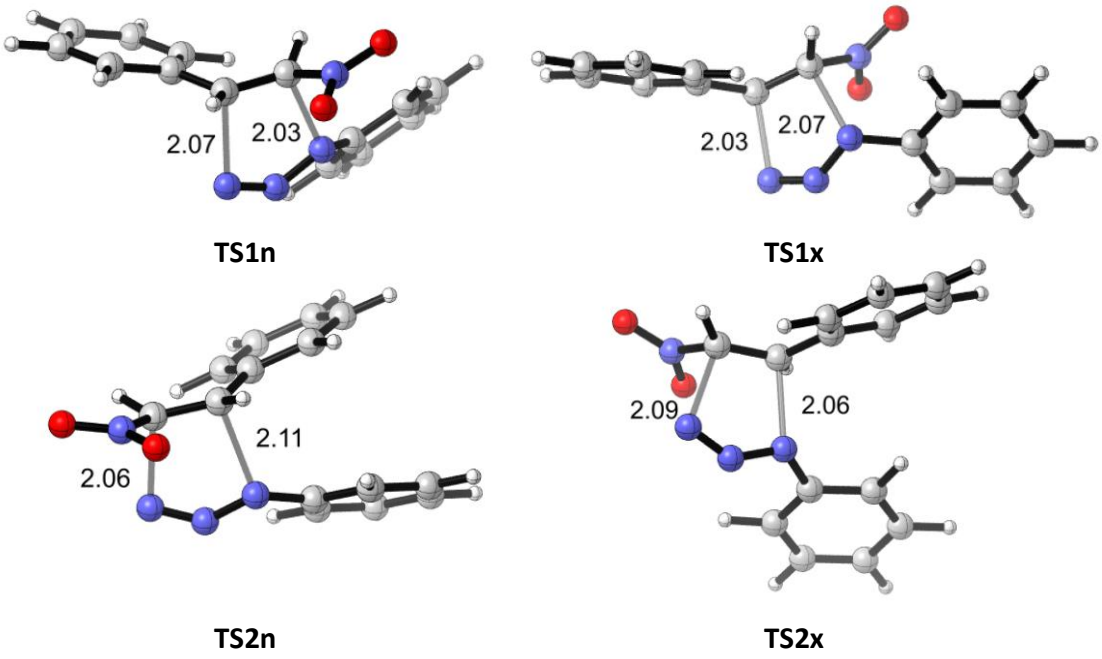

Figure S1. Optimized geometries of transition structures

Iron(III) Chloride-Catalyzed Cycloaddition

Table S2. Absolute (hartrees) and relative (kcal/mol) energies (B3LYP-D3BJ/Def2TZVP/CPCM=water// B3LYP-D3BJ/Def2SVP) corresponding to the reaction between **NS** and **PA** catalyzed by $FeCl_3$.

	E(0)	G	im. freq	ΔE(0)[a]	ΔG[a]
$FeCl_3$	-2644.511597	-2644.545020			
NS-Fe	-2644.511597	-3158.780212			
PA	-395.912133	-395.943985			
TS1n-Fe	-3554.676414	-3554.735544	-448.2	20.6	34.8
TS1x-Fe	-3554.689750	-3554.748587	-373.8	12.2	26.7
TS2n-Fe	-3554.682053	-3554.744016	-457.8	17.1	29.5
TS2x-Fe	-3554.694012	-3554.753395	-418.2	9.5	23.6
P14-Fe	-3554.720810	-3554.783938		-7.3	4.5
P15-Fe	-3554.722309	-3554.783128		-8.2	5.0

[a] Related to **PA** + **NS-Fe**.

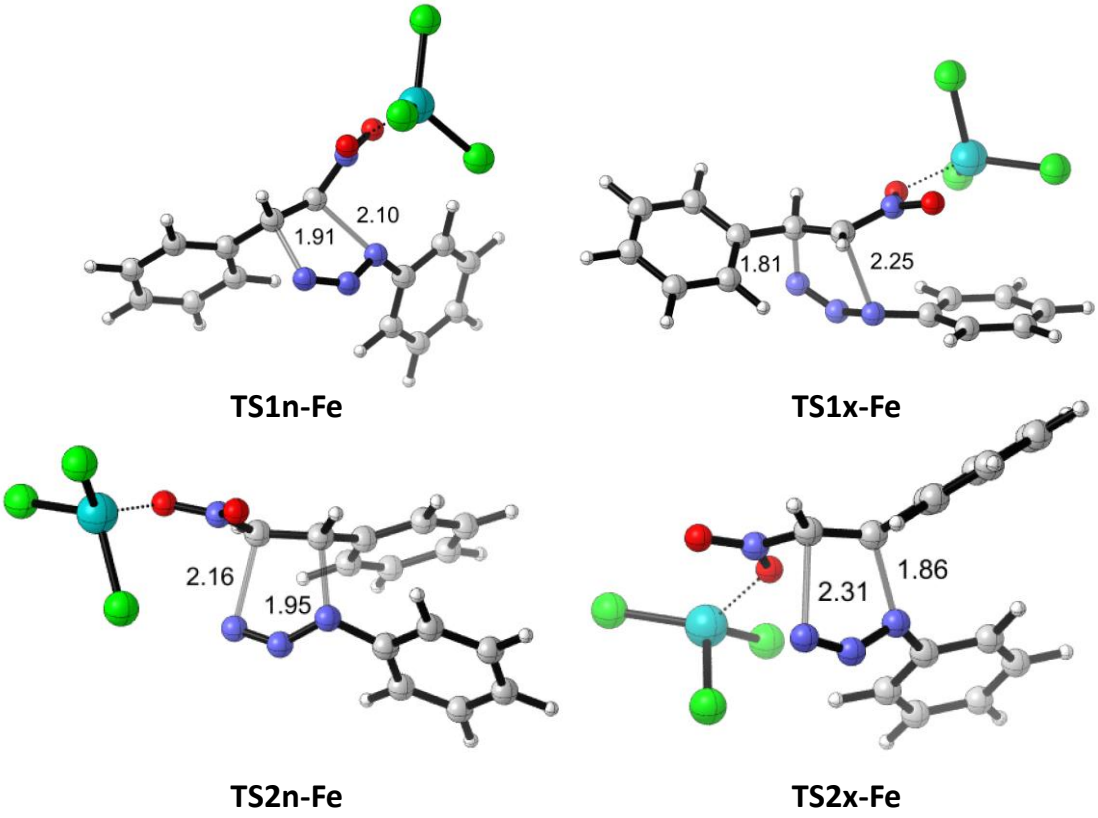

Figure S2. Optimized geometries of transition structures

Denitration Reaction

Table S3. Absolute (hartrees) and relative (kcal/mol) energies (B3LYP-D3BJ/Def2TZVP/CPCM=water// B3LYP-D3BJ/Def2SVP) corresponding to the denitration of **P15**

	E(0)	G	im. freq	ΔE(0)[a]	ΔG[a]
$FeCl_3$	-2644.511597	-2644.545020			
HNO_2	-205.777067	-205.801027			
P15	-910.185728	-910.232347			
TS3	-910.151094	-910.196560	-584.8	21.7	22.5
3h	-704.430619	-704.471295		-13.8	-25.1

[a] Related to **P15**.

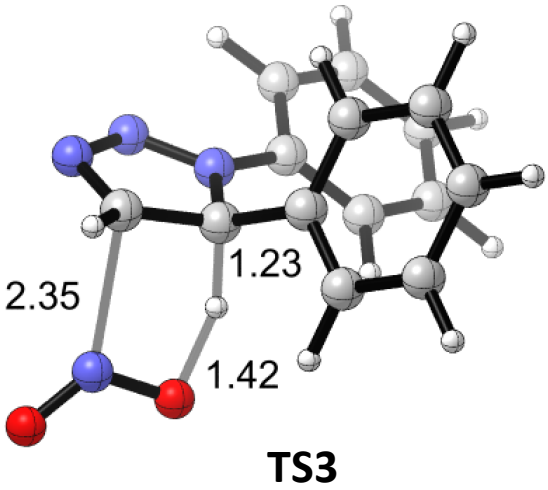

Figure S3. Optimized geometry of transition structure

Cartesian Coordinates

FeCl3
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Fe	4.9770894696	-0.5574901401	2.3293904510
Cl	4.5773932593	1.5031354156	2.6118550302
Cl	4.6360608156	-1.9173369620	3.9168686898
Cl	6.0197002956	-1.2005695448	0.6016544602

HNO2
0 1

N	3.4285475983	-1.8826535475	-0.5405215606
O	4.3040760833	-2.7258254914	0.1647044200
O	3.2474361569	-2.2692252712	-1.6302646322
H	4.3636822115	-2.2950458499	1.0344774328

NS-FeCl3
0 2

C	0.6157774704	-0.4905080346	0.0235914490
H	0.7182722320	-1.0935557023	0.9301482778
C	1.7527486831	0.0505136135	-0.4634977986
H	1.8656348771	0.6889236850	-1.3364864472
C	-0.7189070095	-0.3481654050	-0.5281930410
C	-1.7871129916	-0.9818877138	0.1402316134
C	-0.9931709558	0.3939874751	-1.6981305577
C	-3.0899357713	-0.8785531333	-0.3429289742
H	-1.5825388673	-1.5572520667	1.0462096703
C	-2.2938822357	0.4949625073	-2.1776293059
H	-0.1839621388	0.8935856303	-2.2337582651
C	-3.3451492432	-0.1403997911	-1.5018997773
H	-3.9079008302	-1.3735875881	0.1843524825
H	-2.4960657169	1.0711426807	-3.0828975817
H	-4.3655183025	-0.0575113735	-1.8829813421
N	2.9981648631	-0.1658489987	0.2000653691
O	3.9878105870	0.3964453089	-0.2133593648
O	3.0085561494	-0.9345300508	1.1935907800
Fe	4.5293078006	-0.8136414608	2.6091532474
Cl	4.3888291101	1.2900234697	3.0301884609
Cl	3.6198383447	-2.0724436962	4.0884576674
Cl	6.4683677253	-1.5451611355	2.0871290979

NS
0 1

C	0.6158600000	-0.4434960000	0.0002310000
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C	1.6062000000	0.4611900000	-0.0002710000
H	1.5181740000	1.5453130000	-0.0006020000
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C	-3.0872700000	-1.0696150000	-0.0001070000
H	-1.3006340000	-2.2829260000	-0.0000950000

C	-2.7342480000	1.3257690000	0.0000480000
H	-0.6911520000	1.9936850000	0.0003640000
C	-3.6045440000	0.2279880000	-0.0000850000
H	-3.7610240000	-1.9292530000	-0.0002040000
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H	-4.6852530000	0.3874920000	-0.0001570000
N	2.9976000000	0.0303580000	-0.0000520000
O	3.8299730000	0.9280350000	-0.0000170000
O	3.2530340000	-1.1651410000	0.0000400000

PA
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C	-0.1527110000	1.0050300000	0.0001210000
C	-1.4859060000	1.4171300000	0.0000320000
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H	0.6509040000	1.7453110000	0.0002120000
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N	1.4718110000	-0.8690780000	0.0001920000
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N	3.3772490000	0.5254850000	-0.0002070000

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C	5.5710572327	-1.0021486006	1.5626498328
C	4.3180309382	-0.5948946794	2.0303269134
C	3.2324320299	-0.5128599581	1.1575266560
H	4.7695372441	-1.4891262270	-1.7269158995
H	6.7122275609	-1.6558757865	-0.1554567777
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H	4.1792141206	-0.3488550916	3.0854239991
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C	1.2814836805	1.4851719414	-0.4999508681
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C	1.0988804115	3.9546638513	0.8333142703

H	-1.0194044363	3.5401728761	0.9757172364
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C3hi
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N	2.1157918141	-0.8291456223	-0.7069611188
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P14-Fe
0 2

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C	4.8234337030	-1.4451798426	-0.8628344061
C	3.9974722446	-0.7106945749	-1.7139544481
C	2.7482195555	-0.2605422265	-1.2793401031
H	2.8034817617	-1.5092560245	1.8977736523
H	5.0273254236	-2.3007370823	1.1137679020
H	5.8002077026	-1.7914933142	-1.2059810344
H	4.3226183832	-0.4762011561	-2.7299165695
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N	1.0592043429	-0.1028509448	0.4634829825
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O	0.3543854549	2.4889694701	-1.7119929718
O	1.1143160917	2.6552915799	0.3119664369
Fe	0.6630529398	4.7116499609	0.5552444550
Cl	-1.4785242948	4.4343674894	0.3486894502
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P14
0 1

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C	2.2175584307	2.2822163393	-0.8602391523
C	2.7336792639	2.8489290831	0.3103052912
C	2.0666455449	2.6437808748	1.5185587843
C	0.8962743522	1.8827917991	1.5663160482
H	0.6446525090	1.0800343557	-1.7417111108
H	2.7309177305	2.4328665135	-1.8128368605
H	3.6497317325	3.4421508525	0.2793782461
H	2.4579078015	3.0742767591	2.4430957496
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C	-4.1143566225	0.1671127718	1.1775689481
C	-4.5624846918	0.3797464403	2.4898563202
C	-4.9138924413	0.5636354399	0.1006743984
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H	-3.9381239834	0.0717028627	3.3336253441
C	-6.1510035692	1.1714247624	0.3364410359
H	-4.5640168263	0.3901375943	-0.9176150362
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O	-0.1226206082	-1.4674900829	2.1308853180
H	-1.8670491505	1.1822603183	2.1671261421
H	-2.7903141877	-1.5140389946	1.3773805737

P15-Fe
0 2

C	-1.8888050498	-0.6672036669	0.2479774828
C	-3.0218451063	-0.9554327630	1.0256298324
C	-4.2865323976	-0.6354515658	0.5367305444
C	-4.4388307755	-0.0302755933	-0.7156814883
C	-3.3066328712	0.2522206315	-1.4813388876
C	-2.0305690869	-0.0616410121	-1.0087916226
H	-2.8973270141	-1.4298314950	1.9980563263
H	-5.1649963997	-0.8633452577	1.1448340513
H	-5.4337891501	0.2180284059	-1.0904673909
H	-3.4088950105	0.7228236506	-2.4616293277
H	-1.1579490305	0.1700306829	-1.6185259344
N	-0.6003070714	-0.9833717249	0.7263298357
N	-0.4137920580	-1.7031414735	1.8284739557
N	0.7935672796	-1.9709496615	2.0671246611
C	0.6624624903	-0.6615208581	0.0512588843
C	1.6232692370	-1.4149104398	1.0120375786
C	0.9760117117	0.8099791560	-0.0619452926
C	1.8172557726	1.2384982894	-1.0975071349
C	0.4964397624	1.7317979750	0.8761377896
C	2.1794612345	2.5836840172	-1.1888863069
H	2.1973167251	0.5229973654	-1.8290616633
C	0.8546317828	3.0776858312	0.7759003006
H	-0.1666090906	1.3985043151	1.6776649126
C	1.6976492684	3.5051210704	-0.2546474108
H	2.8401677426	2.9082470425	-1.9956812374
H	0.4727682112	3.7956889914	1.5051720286
H	1.9774884766	4.5583643862	-0.3301612260
H	2.4498104298	-0.8017124996	1.3885978146
H	0.6754028645	-1.1227384507	-0.9481461282
N	2.2880309965	-2.5183771894	0.2146212254
O	3.3278780834	-2.1538320267	-0.3744695843
O	1.7651402448	-3.5847538552	0.0907865830
Fe	3.6723773796	-2.3845033521	-2.4150267715
Cl	4.6640621453	-0.5634857532	-2.9429141562
Cl	4.7994135170	-4.0953974138	-2.9778917400
Cl	1.5999232767	-2.2986014085	-3.0463815034

P15
0 1

C	1.1298225558	-1.4391481881	-0.5262040891
C	1.5760899869	-2.2860134969	-1.5553196462
C	2.8231229654	-2.8975234384	-1.4500083015
C	3.6381847363	-2.6793326734	-0.3336176397
C	3.1880570113	-1.8377693627	0.6845635140

C	1.9404624461	-1.2163921716	0.5971235171
H	0.9371043073	-2.4565444480	-2.4204898672
H	3.1614743942	-3.5556417605	-2.2538181358
H	4.6146593118	-3.1622476529	-0.2599404356
H	3.8113175432	-1.6562214592	1.5631680493
H	1.6107875576	-0.5554152015	1.3973545512
N	-0.1268246585	-0.8147981243	-0.6155015798
N	-0.9677003942	-1.0679734889	-1.6218233757
N	-2.0649654383	-0.4677961762	-1.5307483050
C	-0.6944627217	0.1392046689	0.3460468769
C	-2.0891243527	0.3070352820	-0.2771839334
C	0.0826703605	1.4323815608	0.4437379562
C	0.1842492210	2.0926809893	1.6739721088
C	0.6704034021	2.0007707348	-0.6936583439
C	0.8615802443	3.3110218806	1.7671032546
H	-0.2669134777	1.6487229483	2.5657057987
C	1.3495101865	3.2166039949	-0.6000979062
H	0.6057962003	1.4824191844	-1.6531824210
C	1.4456788652	3.8748321770	0.6298292863
H	0.9373887384	3.8180464218	2.7317255624
H	1.8086453801	3.6508013305	-1.4911067126
H	1.9795163721	4.8251042989	0.7021839843
N	-3.1962631741	-0.2944874705	0.5877468334
O	-4.2930272040	0.2091105341	0.4727972193
O	-2.9057118542	-1.2491538836	1.2850282081
H	-2.4034377431	1.3409493277	-0.4576253078
H	-0.7906167381	-0.3411923273	1.3306962801

TS1n-Fe
0 2

C	1.2370610623	2.2777229878	0.4709096561
C	2.5036052548	2.7391885526	0.8719242591
C	2.9209340613	4.0088414038	0.4796953941
C	2.0954620614	4.8061355935	-0.3235860257
C	0.8405678589	4.3365627178	-0.7240828764
C	0.3981347624	3.0767156118	-0.3217021254
H	3.1391225682	2.1070649960	1.4959600776
H	3.8970768204	4.3797942393	0.8000011559
H	2.4309629058	5.7989238762	-0.6311348268
H	0.1927072452	4.9617766500	-1.3419667817
H	-0.5872019655	2.6980459682	-0.5964760992
N	0.7732327087	0.9870746243	0.7753929910
N	1.2504557722	0.2883427886	1.7166594209
N	1.5612183203	-0.8476712826	1.8297795151
C	0.9600736229	-0.4833989069	-0.7098465918
C	1.5375974784	-1.5320203947	0.0465235132
C	2.9641301156	-1.8744209751	-0.1557167396
C	3.3854839816	-3.2043130067	-0.0026682062
C	3.9189573810	-0.8902738054	-0.4680751484
C	4.7273907855	-3.5475978569	-0.1741582710
H	2.6524079680	-3.9739727719	0.2504411738
C	5.2589614922	-1.2344001168	-0.6390432814

H	3.6195092775	0.1566937359	-0.5640352128
C	5.6672109806	-2.5647292033	-0.4949715400
H	5.0401149432	-4.5874568932	-0.0560580187
H	5.9905671072	-0.4602265217	-0.8811927130
H	6.7176880485	-2.8327136699	-0.6281851265
H	1.4984909239	0.0906360927	-1.4608919782
H	0.8665390616	-2.3598827179	0.2866448037
N	-0.4423804229	-0.4811984986	-0.9688271022
O	-0.8802496591	0.1980480543	-1.8723200840
O	-1.1750066294	-1.1484459136	-0.1971442949
Fe	-3.1626652120	-0.5453289694	-0.0298728257
Cl	-4.4862946531	-0.9028898115	-1.6675496681
Cl	-3.7387758728	-1.7581172222	1.6358303130
Cl	-2.8522361549	1.5286936451	0.4950562645

TS1n
0 1

C	2.0875301191	-0.3296066772	0.4672039275
C	2.1399335427	-1.6334226816	0.9884328208
C	3.1008755657	-2.5245094992	0.5118750025
C	3.9929876121	-2.1356183682	-0.4929563298
C	3.9260518679	-0.8403063796	-1.0163212768
C	2.9858511614	0.0700988704	-0.5350127099
H	1.4372442425	-1.9328353422	1.7683558765
H	3.1487416480	-3.5341324791	0.9265450912
H	4.7395077250	-2.8403517557	-0.8652375221
H	4.6198750078	-0.5296886167	-1.8006762418
H	2.9215996666	1.0853327490	-0.9297823814
N	1.1237344447	0.6144202258	0.8718621263
N	0.3402874092	0.3886133915	1.8500804589
N	-0.7976698502	0.5995190374	2.0587714312
C	-0.2168851268	1.3310111337	-0.4759094086
C	-1.4445364013	1.1523696006	0.1751935814
C	-2.3054579336	-0.0072248625	-0.1189489313
C	-3.6908007945	0.0849364794	0.0970754280
C	-1.7764399930	-1.2248837690	-0.5873116842
C	-4.5272405549	-1.0010924183	-0.1628475877
H	-4.1114019133	1.0216086981	0.4708913023
C	-2.6132646170	-2.3092643332	-0.8463500498
H	-0.6992971979	-1.3348439715	-0.7354485876
C	-3.9923227941	-2.2015840962	-0.6378748162
H	-5.6025718879	-0.9096951889	0.0071055827
H	-2.1859820045	-3.2473283891	-1.2084738789
H	-4.6462308237	-3.0528687846	-0.8403423300
N	0.3474857855	2.6847248189	-0.5436708715
O	1.2023279579	2.8707318771	-1.3994472674
O	-0.0457499882	3.5192043709	0.2525466747
H	0.1158330166	0.7258472856	-1.3169699559
H	-1.9193228919	2.0573220746	0.5577265272

TS1x-Fe
0 2

C	-0.2981981524	2.3801256924	-0.2477187678
C	-1.2308599683	1.9399694356	-1.2109744234
C	-2.5784264455	2.2255931890	-1.0330704600
C	-3.0065782680	2.9282920903	0.1007244529
C	-2.0833986541	3.3524777179	1.0606527006
C	-0.7277515920	3.0832797909	0.8925340603
H	-0.8964315873	1.3625462180	-2.0737387472
H	-3.3030004200	1.8561207232	-1.7594861778
H	-4.0705081243	3.1240389588	0.2436474729
H	-2.4235042851	3.8858370076	1.9502187669
H	0.0122445506	3.3946429831	1.6310598483
N	1.0561261537	2.0470937774	-0.3100981832
N	1.5792167091	1.6173815897	-1.3813095274
N	2.2657108825	0.6992532689	-1.6843577290
C	1.6072603273	0.1573119321	0.7739253229
C	2.4194595809	-0.4037379720	-0.2532833062
H	1.9916512805	-1.2874424121	-0.7331499990
H	1.9857469050	0.6166878819	1.6826386006
C	3.8916656926	-0.4398775155	-0.0450064390
C	4.6237330222	-1.5631072586	-0.4561453191
C	4.5699558519	0.6457929445	0.5344591527
C	6.0063474643	-1.6113602664	-0.2709316687
H	4.1034822997	-2.4051855245	-0.9188207431
C	5.9514546168	0.5972854911	0.7163697081
H	4.0170800253	1.5410218747	0.8304049610
C	6.6726214501	-0.5329294874	0.3172004802
H	6.5654659347	-2.4942383523	-0.5885138159
H	6.4696880262	1.4469507625	1.1664309159
H	7.7549305526	-0.5697341979	0.4599757202
N	0.2589653440	-0.1919267186	0.8664566076
O	-0.4011143020	0.1118027926	1.8462134113
O	-0.2771067769	-0.7173508436	-0.1585092142
Fe	-2.2489685256	-1.1432810517	0.0418163805
Cl	-3.9534593770	-0.2507697442	0.9893716167
Cl	-2.6146879992	-1.2049159602	-2.0909504941
Cl	-1.9712801921	-3.0091428177	1.0665738354

TS1x
0 1

C	-2.1943366459	-0.6958485642	0.3693715031
C	-3.0061086350	0.0409966117	1.2477679884
C	-4.3831701059	0.0772630364	1.0413110081
C	-4.9529341271	-0.5911470135	-0.0480057639
C	-4.1385473575	-1.3043492235	-0.9325061236
C	-2.7615577539	-1.3641271453	-0.7249881462
H	-2.5498796268	0.5749032426	2.0831048183
H	-5.0160667960	0.6415917268	1.7297820120
H	-6.0323965238	-0.5516700168	-0.2090717876
H	-4.5787438868	-1.8213557282	-1.7878057008
H	-2.1110116476	-1.9187845488	-1.4028144173
N	-0.7900767231	-0.7224701587	0.4856262113
N	-0.2215399527	-0.4264515338	1.5901293724

N	0.7465412262	0.1765247954	1.8818367669
C	0.2946648128	0.5396418538	-0.7385624075
C	1.3665842938	0.9016382912	0.0954760555
H	1.3559051214	1.9301623077	0.4589689002
H	0.3860267867	-0.1454520792	-1.5773745353
N	-0.7781471708	1.5026166619	-0.9479501110
O	-1.4546189899	1.3525255195	-1.9555949556
O	-0.9686942495	2.3538155276	-0.0882252222
C	2.6794732849	0.2355796797	-0.0203065455
C	3.8472730496	0.9380746875	0.3197992827
C	2.7947495411	-1.1024322738	-0.4401699562
C	5.0989271659	0.3287757218	0.2234422028
H	3.7680954680	1.9736138771	0.6596922698
C	4.0457819121	-1.7104240839	-0.5350861010
H	1.8961379810	-1.6779042714	-0.6749591778
C	5.2031770201	-0.9965947902	-0.2071530673
H	5.9974678785	0.8915730157	0.4870671052
H	4.1186103119	-2.7507539190	-0.8608283088
H	6.1824693380	-1.4749542060	-0.2812471692

TS2n-Fe
0 2

C	2.9561297603	-1.4448016679	-0.2427010394
C	3.8365394629	-1.2112394601	-1.3089634940
C	5.1660749047	-1.6146011724	-1.2005640900
C	5.6246184384	-2.2281907754	-0.0295314902
C	4.7439430040	-2.4516807838	1.0326921478
C	3.4068446209	-2.0671904242	0.9278318711
H	3.4742629961	-0.7139459733	-2.2106475471
H	5.8519245267	-1.4397851021	-2.0323632938
H	6.6692973602	-2.5356593348	0.0522957559
H	5.0967022768	-2.9380000887	1.9446921019
H	2.7008972701	-2.2445726664	1.7412043812
N	1.6267370935	-0.9699093853	-0.2503588941
N	0.9603434003	-0.8370034075	-1.3286116209
N	0.1005757717	-0.1382983188	-1.6975207751
C	1.2645476226	0.6964130624	0.6908795859
C	0.0610197017	1.1116913023	0.0653524571
C	2.5178616975	1.4414971121	0.4807518191
C	3.5452467371	1.3370539771	1.4332599591
C	2.7515740998	2.1789715835	-0.6950009191
C	4.7742134465	1.9618375140	1.2233952471
H	3.3769463029	0.7548600778	2.3415411585
C	3.9799308789	2.8035786180	-0.9023176437
H	1.9770085740	2.2508454032	-1.4613193106
C	4.9943211712	2.6962941156	0.0554346475
H	5.5637959638	1.8718587356	1.9723683493
H	4.1497811060	3.3738839596	-1.8181543012
H	5.9572072386	3.1842624729	-0.1113630061
H	-0.0719406231	2.0372414119	-0.4861750178
H	1.1436216451	0.1993040850	1.6550213577
N	-1.1533725447	0.5908265949	0.5758163976

O	-1.1694602257	-0.3447724085	1.3491898394
O	-2.2070632723	1.1276380059	0.1350735078
Fe	-3.8906721885	-0.0178102141	0.1326642549
Cl	-5.0153392163	-0.8747770159	1.7386356449
Cl	-5.1306554466	1.3541508732	-0.9592531361
Cl	-3.0185025552	-1.6303927057	-1.0085569046

TS2n
0 1

C	0.9391741544	-1.4767206791	-0.1862753968
C	1.7363571777	-1.1102803160	-1.2831564117
C	3.1243622712	-1.1468475050	-1.1696791272
C	3.7265855628	-1.5308154729	0.0338390834
C	2.9309796015	-1.8914728935	1.1251875660
C	1.5407134867	-1.8699315776	1.0180700424
H	1.2590000613	-0.7943848989	-2.2126128322
H	3.7423239848	-0.8635491086	-2.0248011874
H	4.8152523822	-1.5510241313	0.1184958215
H	3.3960295046	-2.1972870283	2.0650894727
H	0.9022673517	-2.1506220131	1.8576333746
N	-0.4586019526	-1.3505483560	-0.1918597446
N	-1.1280758129	-1.3718841745	-1.2720108024
N	-2.0958392087	-0.8273572542	-1.6618023969
C	-1.2530999450	0.4127372501	0.6399826628
C	-2.4289070570	0.4943916681	-0.1231306672
C	-0.1080163903	1.3023971982	0.4191282685
C	0.8880925219	1.3984146069	1.4070967076
C	0.0787693855	1.9925571341	-0.7944139978
C	2.0338016759	2.1639470532	1.1942887889
H	0.7605706898	0.8567308014	2.3465058924
C	1.2225249513	2.7601231138	-1.0042999184
H	-0.6666558035	1.9127789875	-1.5881183426
C	2.2050335939	2.8474169089	-0.0121031000
H	2.7990558190	2.2224315195	1.9713684324
H	1.3531769127	3.2885487779	-1.9514485669
H	3.1036355672	3.4448713083	-0.1817801988
N	-3.6367298625	-0.1240818548	0.4216805960
O	-4.6991683302	0.2690139093	-0.0334845159
O	-3.5083772151	-1.0003587283	1.2662496213
H	-2.6734351222	1.3348880347	-0.7674077289
H	-1.3433259561	-0.0720482799	1.6122256053

TS2x-Fe
0 2

C	-1.2123005136	1.7455930594	0.7480139567
C	0.0911171460	2.2533259412	0.8065904485
C	0.3201489997	3.5714912122	0.4154174211
C	-0.7362421860	4.3660124152	-0.0415965772
C	-2.0330365404	3.8449846553	-0.1038961584
C	-2.2798268907	2.5309268744	0.2959229038
H	0.9144069312	1.6179697419	1.1356465937
H	1.3383234510	3.9632685890	0.4437536499

H	-0.5471711340	5.3947379366	-0.3561449142
H	-2.8580483884	4.4667054831	-0.4583978315
H	-3.2843132407	2.1063306001	0.2655887570
N	-1.4829451441	0.3837409203	1.0543629193
N	-0.8609223896	-0.2391841907	1.9689655369
N	-0.4840179324	-1.3079865303	2.2035609965
C	-1.7003874296	-0.8253135531	-0.3406710121
H	-1.2316859716	-0.1754405724	-1.0830989203
C	-0.9203306580	-1.9541210411	0.0281072193
H	-1.3070051282	-2.9405447455	0.2679181753
C	-3.1716731869	-0.9626760965	-0.4541836349
C	-3.8480170415	-0.2708465245	-1.4707822703
C	-3.9091473189	-1.7459296878	0.4498806276
C	-5.2353696610	-0.3706779006	-1.5919153683
H	-3.2794466570	0.3461007614	-2.1706885197
C	-5.2945141959	-1.8416165510	0.3297184334
H	-3.3993051340	-2.2698739167	1.2617429075
C	-5.9607764630	-1.1561468017	-0.6924777911
H	-5.7509061619	0.1666461579	-2.3909651017
H	-5.8596570372	-2.4507387836	1.0386171261
H	-7.0464395645	-1.2332852209	-0.7847913257
N	0.4523232836	-1.9435087756	-0.2486306813
O	0.9380346139	-0.8368788930	-0.6674881860
O	1.1446435760	-2.9233879398	-0.0758651189
Fe	2.8690330299	-0.4056603305	-0.3459934505
Cl	2.7433536701	-0.2928599085	1.8127037716
Cl	4.6541778289	-1.4615868324	-0.8458760878
Cl	2.8129874386	1.5316104480	-1.2989034943

TS2x
0 1

C	-1.6933635822	-0.6907007713	0.5571111380
C	-2.9494735228	-0.1023810119	0.3382271961
C	-4.0048757959	-0.8909159147	-0.1158598901
C	-3.8093269858	-2.2520300372	-0.3786882663
C	-2.5507207300	-2.8275493648	-0.1799040892
C	-1.4912104767	-2.0534773407	0.2951042074
H	-3.0780432933	0.9681177113	0.5084172048
H	-4.9848283742	-0.4369383524	-0.2796868624
H	-4.6390446658	-2.8625514999	-0.7416679416
H	-2.3952724985	-3.8892570049	-0.3845665051
H	-0.5044457977	-2.4846565773	0.4709597009
N	-0.5726412089	0.0644559912	0.9522386258
N	-0.6825638968	1.1213471919	1.6449960756
N	-0.1451142695	2.1643412538	1.6777160265
C	0.7541601589	0.6825356520	-0.4927183237
H	0.0274777719	0.4890876325	-1.2840300094
C	0.9037663410	2.0289534321	-0.1295168793
H	1.8390565157	2.4729842749	0.2028908208
C	1.8257229648	-0.3128366537	-0.3176474884
C	1.8658983984	-1.4315287044	-1.1670372611
C	2.7955803780	-0.1955052952	0.6941095208

C	2.8574720845	-2.4029600959	-1.0188780111
H	1.1114823118	-1.5342204915	-1.9507914393
C	3.7843407390	-1.1663069426	0.8415852525
H	2.7641102483	0.6522484954	1.3820975362
C	3.8203029360	-2.2727235243	-0.0149255425
H	2.8786181498	-3.2641588258	-1.6907570373
H	4.5300114513	-1.0637705778	1.6333599787
H	4.5963493600	-3.0323494675	0.1035308975
N	0.0386095112	2.9999138174	-0.7880423994
O	0.4381931504	4.1514467024	-0.8362262593
O	-1.0405683728	2.6072972988	-1.2208879763

TS3
0 1

C	3.3949515791	-1.2942476227	-0.1073251141
C	4.3911990439	-2.1485933397	-0.6008629581
C	5.4188128155	-2.5568693824	0.2471157352
C	5.4637118428	-2.1148848255	1.5738485143
C	4.4655080898	-1.2636279354	2.0544327899
C	3.4250579152	-0.8513357105	1.2213066726
H	4.3435179669	-2.4813325435	-1.6371999559
H	6.1951441682	-3.2233146427	-0.1350513568
H	6.2744294781	-2.4353114339	2.2314994263
H	4.4883400190	-0.9195328079	3.0905626040
H	2.6420898102	-0.1980806895	1.6044926641
N	2.3502772462	-0.8729635556	-0.9641294319
N	2.0306821396	-1.5559029141	-2.0443852337
N	1.0336759020	-0.9852827092	-2.6672668700
C	1.4622802626	0.2385086406	-0.7687354250
C	0.6242881832	0.0832615470	-1.9519568091
C	2.0374512550	1.5677432325	-0.3648924006
C	1.3052013707	2.4079514487	0.4845492630
C	3.2841718828	1.9875536608	-0.8491131612
C	1.8133940040	3.6599800617	0.8393024216
H	0.3385686967	2.0746811394	0.8686197482
C	3.7937134368	3.2340214230	-0.4828447558
H	3.8577990439	1.3341733592	-1.5101737260
C	3.0589310418	4.0737967282	0.3600038233
H	1.2360379341	4.3107129357	1.4999948662
H	4.7675752495	3.5531404008	-0.8613228479
H	3.4584856060	5.0501102207	0.6436735372
H	-0.0682441064	0.8116256557	-2.3652303390
H	0.6399264799	-0.0845198466	0.0903929564
N	-1.1499844496	-0.5754189788	-0.5657610487
O	-2.2914219406	-0.9170326632	-0.7091274834
O	-0.6388489669	-0.4428908530	0.5822608949