Supporting information for

Ruthenium-Catalyzed Cycloaddition of Aryl Azides and Alkynes

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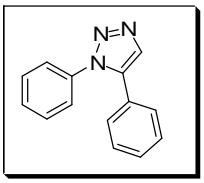
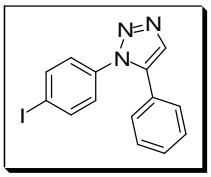
General Information:

All reactions were carried under a nitrogen atmosphere. Chemicals were obtained from commercial suppliers and used without purification unless otherwise is noted. Anhydrous DMF was obtained from EMD. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a Bruker AMX-400 or AMX-500 spectrometer. Chemical shifts (δ) are given in ppm relative to the solvent residual peak ($CHCl_3$; 7.26 ppm for ^{1}H and 77.2 for ^{13}C and DMSO; 2.50 ppm for ^{1}H and 39.5 for ^{13}C). The following abbreviations are used for multiplicity of NMR signals: s=singlet, d=doublet, t=triplet, q=quartet, qui=quintet, sex=sextet, and m=multiplet. Purification by flash chromatography was performed using Silica Gel 60 (particle size 40-63 µm, EMD) and technical grade solvents. Melting points were measured on a Bamstead Electrothermal 9300 apparatus and are uncorrected. Microwave irradiation was carried out in a Personal Chemistry Smith Synthesizer apparatus.
$(Cp^*RuCl)_4$ was prepared in two steps from commercial available $RuCl_3{\cdot}H_2O$ as previously described.[1,2]

$(Cp^*RuCl)_4$ catalyzed cycloaddition – Typical procedure.

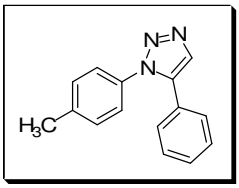


1,5-Diphenyl-1H-[1,2,3]-triazole (4):
To a solution of phenylazide (131 mg, 1.10 mmol) and phenylacetylene (102 mg, 1.0 mmol) in DMF (6 mL) was added $[Cp^*RuCl]_4$ (27 mg, 0.1 mmol). The reaction tube was flushed with nitrogen, capped and heated to 110 ºC for 20 minutes. To the reaction mixture were added ethyl acetate (20 mL) and water (20 mL). Phases were separated and the aqueous phase was extracted with ethyl acetate (2 x 20 mL). The combined organic phases were washed with brine (2 x 20 mL), dried over $MgSO_4$ and concentrated in vacuo.
Flash chromatography (ethyl acetate/hexane 1/6) yielded 87% of **4** as a brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22 (dd, J_1=7.7 Hz, J_2=1.1 Hz, 2H), 7.32-7.37 (m, 5H), 7.43 (m 3H), 7.86 (s, 1H)
^{13}C NMR (500 MHz, $CDCl_3$) δ 123.2, 125.4, 127.0 128.8, 129.0, 129.4, 129.5, 133.6, 136.8, 137.9.
MS (ESI-TOF): calcd for $C_{14}H_{12}N_3^+$ (MH^+) 222.1026 found 222.1025.
Mp.: 113-114 ºC (lit.[3] 113-112 ºC)

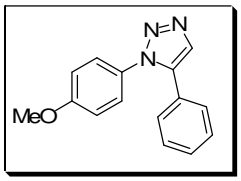


1-(4-Iodophenyl)-5-phenyl-1H-[1,2,3]-triazole (3):
Flash chromatography (ethyl acetate/hexane 1/9) yielded 72% of **3** as a brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.09 (d, J=8.4 Hz, 2H) 7.19-7.21 (m, 2H) 7.32-7.39 (m, 3H), 7.72 (d, J=8.4 Hz, 2H), 7.81 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 94.8, 126.5, 126.7, 128.7, 129.1, 129.5, 133.7, 136.3, 137.7, 138.6.

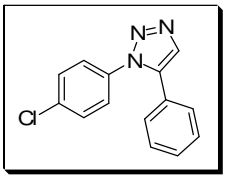
MS (ESI-TOF): calcd for $C_{14}H_{11}NI_3^+$ (MH^+) 347.9992 found 347.9993.
Mp.: 114-116 ºC (lit.[4] 112-114 ºC).



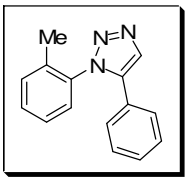
5-Phenyl-1-p-tolyl-1H-[1,2,3]-triazole (5):
Flash chromatography (ethyl acetate/hexane 1/9) yielded 51% of **5** as a light brown solid.
^{1}H NMR (500 MHz, D_6-DMSO) δ 2.36 (s, 3H) 7.27-7.39 (m, 9H), 8.11 (s, 1H)
^{13}C NMR (500 MHz, D_6-DMSO) δ 20.7, 125.4, 126.4, 128.4, 128.8, 129.1, 129.9, 133.0, 133.8, 137.5, 139.2.
MS (ESI-TOF): calcd for $C_{15}H_{14}N_3^+$ (MH^+) 236.1186 found 236.1182.
Mp.: 141-142 ºC.



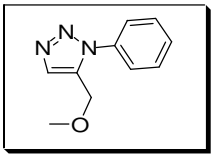
1-(4-Methoxyphenyl)-5-phenyl-1H-[1,2,3]-triazole (6):
Flash chromatography (ethyl acetate/hexane 1/5) yielded 69% of **6** as a light brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 3.91 (s, 3H), 7.00 (d, J=8.8 Hz, 2H) 7.30 (dd, J_1=7.3 Hz, J_2=1.5 Hz, 2H), 7.34 (d, J=8.8 Hz, 2H), 7.39-7.44 (m, 3H), 7.92 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 55.7, 114.7, 126.8, 127.0, 128.7, 129.0, 129.3, 129.8, 133.3, 137.9, 160.2.
MS (ESI-TOF): calcd for $C_{15}H_{14}N_3O^+$ (MH^+) 252.1131 found 252.1133.
Mp.: 84-85 ºC (lit.[4] 83-84 ºC).



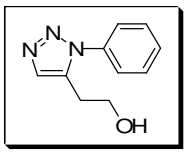
1-(4-Chlorophenyl)-5-phenyl-1H-[1,2,3]-triazole (7):
Flash chromatography (ethyl acetate/hexane 1/6) yielded 71% of **7** as a light brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (dd, J_1=7.7 Hz, J_2=1.1 Hz, 2H) 7.29 (dt, J_1=6.6 Hz, J_2=2.6 Hz, 2H), 7.33-7.39 (m, 6H), 7.82 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 126.4, 126.5, 128.7, 129.1, 129.6, 129.7, 133.6, 135.17, 135.25, 137.8.
MS (ESI-TOF): calcd for $C_{14}H_{11}NI_3^+$ (MH^+) 256.0636 found 256.0640.
Mp.: 88-89 ºC.



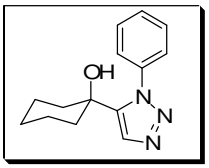
5-Phenyl-1-o-tolyl-1H-[1,2,3]-triazole (8):
Flash chromatography (ethyl acetate/hexane 1/6) yielded 43% of **8** as a brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 2.01 (s, 3H) 7.24 (dd, J_1=7.7 Hz, J_2=1.5 Hz, 2H), 7.33-7.39 (m, 6H), 7.47 (dt, J_1=7.3 Hz, J_2=1.8 Hz, 1H), 8.00 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 17.6, 126.7, 127.1, 127.69, 127.73, 129.0, 129.2, 130.3, 131.4, 132.4, 135.3, 136.0, 138.7.
MS (ESI-TOF): calcd for $C_{14}H_{11}NI_3^+$ (MH^+) 236.1182 found 236.1186.
Mp.: 82 ºC.



5-(Methoxymethyl)-1-phenyl-1H-[1,2,3]-triazole (11):[5]
Flash chromatography (ethyl acetate/hexane 1/3) yielded 78% of **11** as a yellow oil.
^{1}H NMR (500 MHz, $CDCl_3$) δ 3.34 (s, 3H), 4.43 (s, 2H), 7.26-7.51 (m, 3H), 7.59 (d, J_1=7.0 Hz, J_2=1.8 Hz, 2H), 7.78 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 58.5, 62.6, 124.9, 129.90, 129.92, 134.0, 135.4, 136.6.
MS (ESI-TOF): calcd for $C_{10}H_{12}N_3O^+$ (MH^+) 190.0975 found 190.0982.

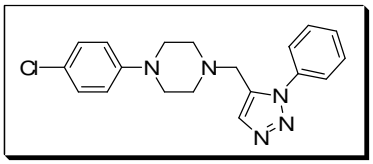


2-(1-Phenyl-1H-[1,2,3]-triazol-5-yl)ethanol (12):
Flash chromatography (ethyl acetate/hexane 3/1) yielded 73% of **12** as a brown oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.91 (m, 2H), 3.84 (t, J=6.5 Hz, 2H), 7.44-7.52 (m, 5H), 7.62 (s, 1H)
^{13}C NMR (400 MHz, $CDCl_3$) δ 27.0, 60.5, 125.6, 129.5, 129.7, 132.8, 135.6, 136.1.
MS (ESI-TOF): calcd for $C_{10}H_{12}N_3O^+$ (MH^+) 190.0975 found 190.0978.

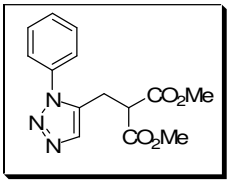


1-(1-Phenyl-1H-[1,2,3]-triazol-5-yl)cyclohexanol (13):
Flash chromatography (ethyl acetate/hexane 1/2) yielded 72% of **13** as a off white solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 1.19-1.25 (m, 1H), 1.39-1.44 (m, 2H), 1.49-1.63 (m, 3H), 1.70-1.80 (m, 4H), 2.65 (sb, 1H), 7.47-7.52 (m, 5H), 7.55 (s, 1H).

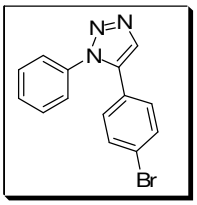
^{13}C NMR (500 MHz, $CDCl_3$) δ 21.8, 25.2, 37.4, 68.9, 127.5, 129.1, 130.0, 131.8, 138.2, 144.4.
MS (ESI-TOF): calcd for $C_{14}H_{18}N_3O^+$ (MH^+) 244.1444 found 244.1447.
Mp.: 144-145 ºC.



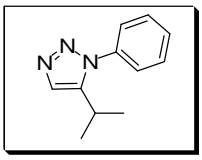
1-(4-Chlorophenyl)-4-((1-phenyl-1H-[1,2,3]-triazol-5-yl)methyl)piperazine (14):
Flash chromatography (ethyl acetate/hexane 2/3) yielded 92% of **14** as a brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 2.60 (t, *J*=5.2 Hz, 4H), 3.12 (t, *J*=4.8 Hz, 4H), 3.58 (s, 1H), 6.81 (dd, J_1=7.0 Hz, J_2=2.2 Hz, 2H), 7.19 (dd, J_1=7.0 Hz, J_2=2.2 Hz, 2H) 7.50-7.55 (m, 3H) 7.71 (dd J_1=8.1 Hz, J_2=1.5 Hz, 2H), 7.72 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 49.3, 50.6, 52.7, 117.5, 125.0, 125.2, 129.2, 129.5, 129.6, 134.1, 135.1, 136.8, 149.9.
Mp.: 152-153 ºC.
MS (ESI-TOF): calcd for $C_{19}H_{21}ClN_5^+$ (MH^+) 354.1480 found 354.1479.



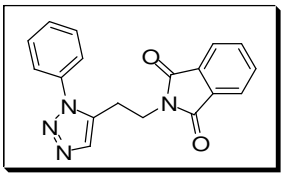
Dimethyl 2-((1-phenyl-1H-[1,2,3]-triazol-5-yl)methyl)malonate (15):
Flash chromatography (ethyl acetate/hexane 1/2) yielded 49% of **15** as a brown oil.
^{1}H NMR (500 MHz, $CDCl_3$) δ 3.26 (d, *J*=7.7 Hz, 2H), 3.63 (t, *J*=8.1 Hz, 1H), 3.67 (s,1H), 7.43 (dd, J_1=8.1 Hz, J_2=1.8 Hz, 2H), 7.51-7.56 (m, 4H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 23.1, 50.4, 53.1, 125.6, 129.8, 130.0, 132.7, 134.4, 136.0, 168.2.



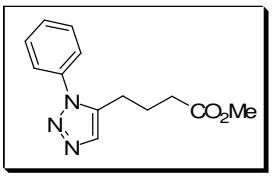
5-(4-Bromophenyl)-1-phenyl-1H-[1,2,3]-triazole (16):
Flash chromatography (ethyl acetate/hexane 1/7) yielded 79% of **16** as a yellow solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.08 (dd, J_1=6.6 Hz, J_1=1.8 Hz, 2H), 7.34 (m, 2H), 7.44-7.48 (m, 5H), 7.86 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 123.9, 125.4, 125.9, 129.6, 129.7, 130.2, 132.4, 133.6, 136.5, 136.9.
MS (ESI-TOF): calcd for $C_{14}H_{11}BrN_3^+$ (MH^+) 300.0131 found 300.0133.
Mp.: 151-152 ºC.



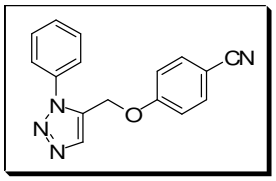
5-Isopropyl-1-phenyl-1H-[1,2,3]-triazole (17):
Flash chromatography (ethyl acetate/hexane 1/6) yielded 83% of **17** as a brown oil.
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.20 (d, *J*=7.0 Hz, 6H), 3.04 (hept, *J*=6.7 Hz, 1H), 7.39-7.46 (m, 2H), 7.52-7.54 (m, 3H), 7.59 (s, 1H).
^{13}C NMR (400 MHz, $CDCl_3$) δ 22.4, 23.9, 125.6, 129.5, 129.6, 130.5, 136.6, 144.4.
MS (ESI-TOF): calcd for $C_{11}H_{14}N_3^+$ (MH^+) 188.1182 found 188.1187.



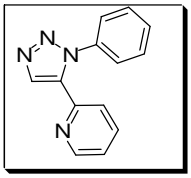
2-(2-(1-Phenyl-1H-[1,2,3]-triazol-5-yl)ethyl)isoindoline-1,3-dione (18):
Flash chromatography (ethyl acetate/hexane 1/2) yielded 55% of **18** as a brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 3.13 (t, *J*=7.0 Hz, 2H), 3.87 (t, *J*=7.0 Hz, 2H), 7.46-7.52 (m, 5H), 7.63 (s, 1H), 7.70-7.71 (m, 2H), 7.78-7.80 (m, 2H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 22.9, 36.4, 123.6, 125.6, 129.8, 129.9, 131.9, 133.3, 134.3, 134.4, 136.2, 168.0.
MS (ESI-TOF): calcd for $C_{18}H_{15}N_4O_2^+$ (MH^+) 319.1189 found 319.1187.



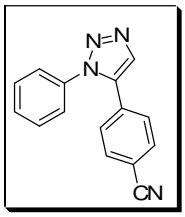
Methyl 4-(1-phenyl-1H-[1,2,3]-triazol-5-yl)butanoate (19):
Flash chromatography (ethyl acetate/hexane 1/2) yielded 74% of **19** as a brown oil.
^{1}H NMR (500 MHz, $CDCl_3$) δ 1.91 (pent, *J*=7.0 Hz, 1H), 2.31 (t, *J*=7.0 Hz, 2H), 2.72 (t, *J*=7.7 Hz, 2H), 3.61 (s, 3H), 7.42-7.44 (m, 2H), 7.49-7.52 (m, 3H), 7.53 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 23.2, 23.6, 33.1, 51.8, 125.5, 129.7, 129.8, 132.7, 136.5, 137.3, 173.1.
MS (ESI-TOF): calcd for $C_{13}H_{15}N_3O_2^+$ (MH^+) 246.1237 found 246.1241.



4-((1-Phenyl-1H-[1,2,3]-triazol-5-yl)methoxy)benzonitrile (20):
Flash chromatography (ethyl acetate/hexane 2/3) yielded 56% of **20** as a off white solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 5.12 (s, 2H), 6.95 (d, *J*=8.8 Hz, 2H), 7.52-7.54 (m, 5H), 7.60 (d, *J*=8.8 Hz, 2H), 7.92 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 58.8, 105.8, 115.6, 118.9, 125.0, 130.0, 130.3, 132.1, 134.4, 135.4, 136.0, 160.7.
MS (ESI-TOF): calcd for $C_{16}H_{13}N_4O^+$ (MH^+) 277.1084 found 277.1088.
Mp.: 140-141 ºC.



2-(1-Phenyl-1H-[1,2,3]-triazol-5-yl)pyridine (21):
Flash chromatography (ethyl acetate/hexane 1/2) yielded 56% of **21** as a brown oil.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20 (d, *J*=7.7 Hz, 1H), 7.23-7.26 (m, 1H), 7.38-7.45 (m, 5H), 7.62-7.65 (m, 1H), 8.09 (s, 1H), 8.57 (d, *J*=7.7 Hz, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 123.5, 123.7, 125.6, 129.4, 129.5, 134.6, 136.8, 137.1, 137.4, 146.8, 150.3.
MS (ESI-TOF): calcd for $C_{13}H_{11}N_4^+$ (MH^+) 223.0978 found 223.0981.
Mp.: 76-78 ºC (lit.[4] 76-78 ºC).



4-(1-Phenyl-1H-[1,2,3]-triazol-5-yl)benzonitrile (22):
Flash chromatography (ethyl acetate/hexane 1/3) yielded 74% of **22** as a brown solid.
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.35 (m, 4H), 7.47-7.51 (m, 3H), 7.64 (d, *J*=6.6 Hz, 2H), 7.95 (s, 1H).
^{13}C NMR (500 MHz, $CDCl_3$) δ 113.3, 118.2, 125.5, 129.2, 129.9, 131.5, 132.8, 134.2, 136.2, 136.3.
MS (ESI-TOF): calcd for $C_{15}H_{11}N_4^+$ (MH^+) 247.0978 found 247.0975.
Mp.: 147-148 ºC.

References

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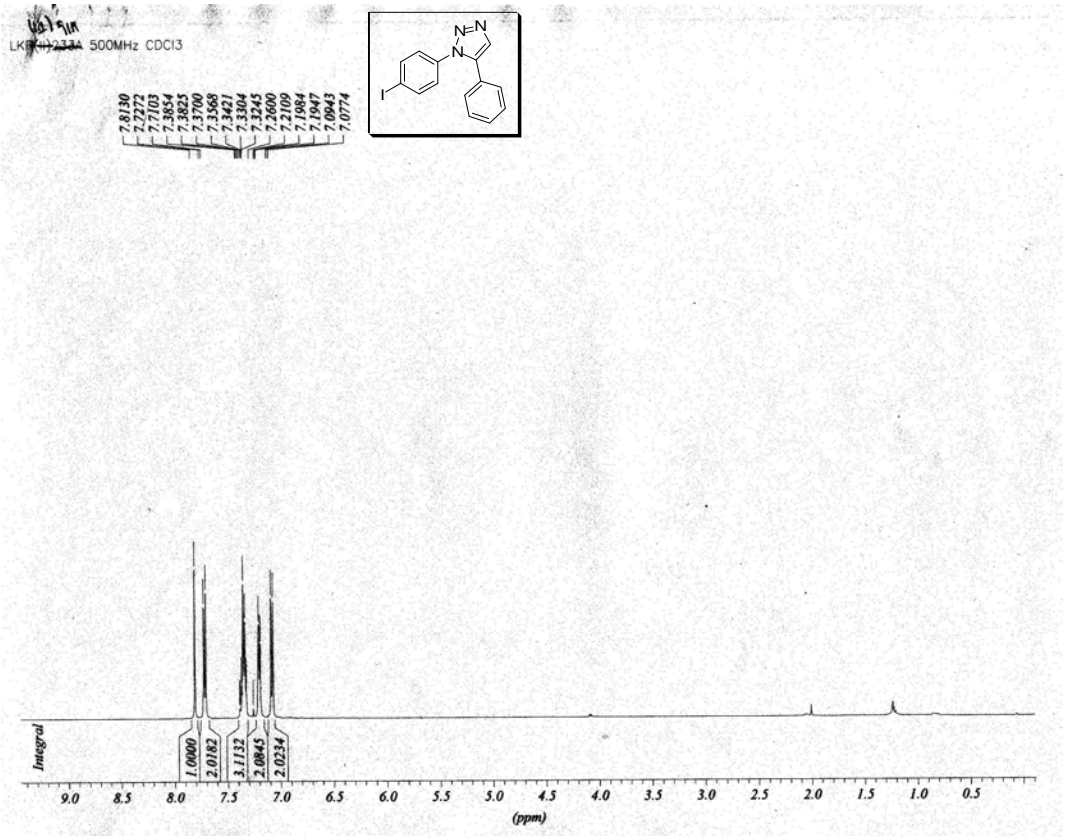
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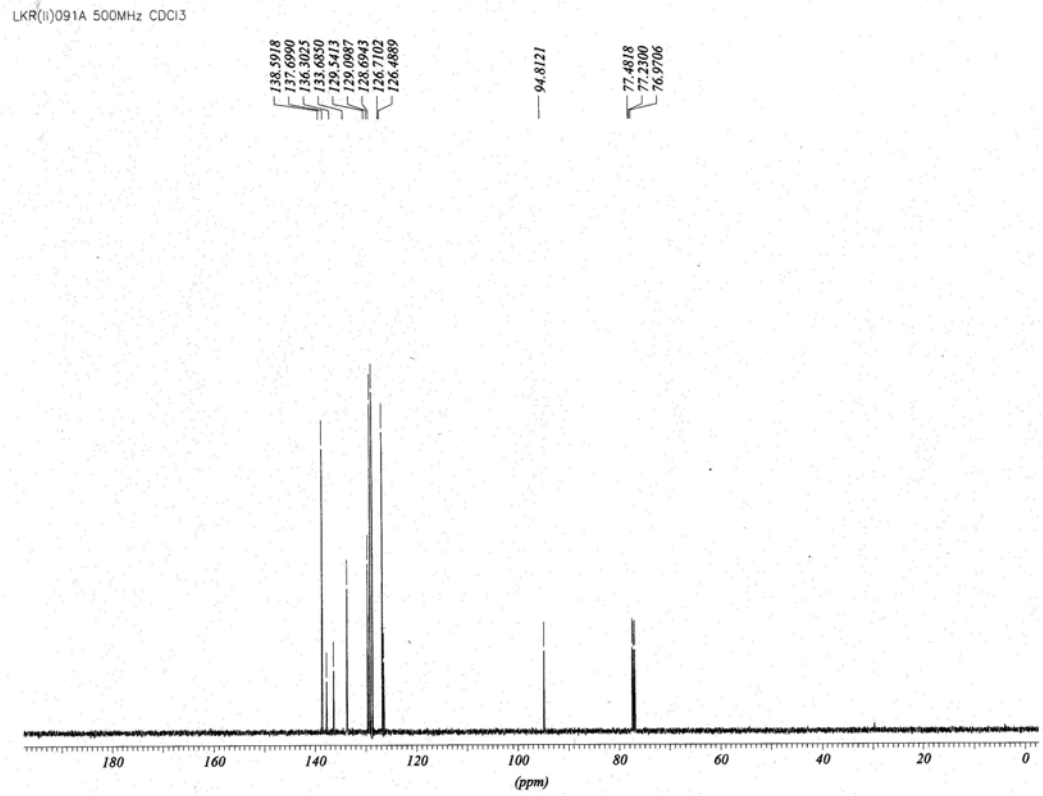
7.8130
7.7272
7.7103
7.3854
7.3825
7.3700
7.3568
7.3421
7.3304
7.3245
7.2600
7.2109
7.1984
7.1947
7.0943
7.0774
N=N
N
I
Integral
1.0000
2.0182
3.1132
2.0845
2.0234
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


LKR(ii)091A 500MHz CDCl3
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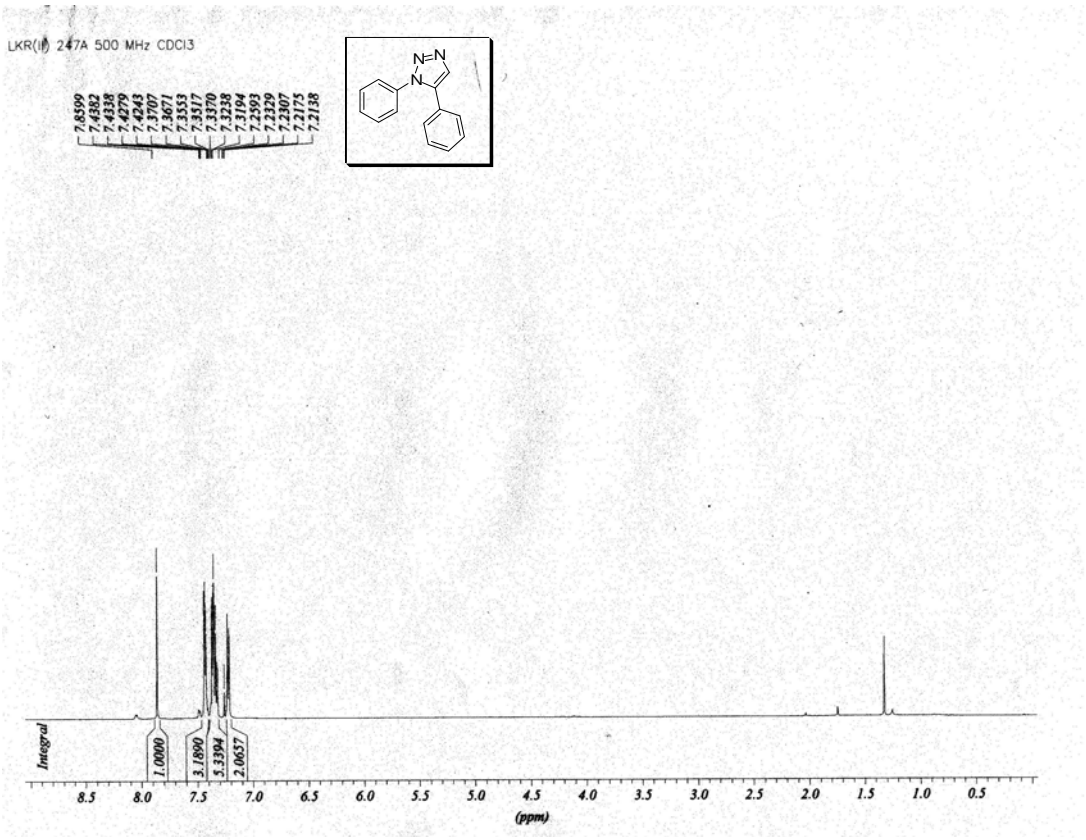
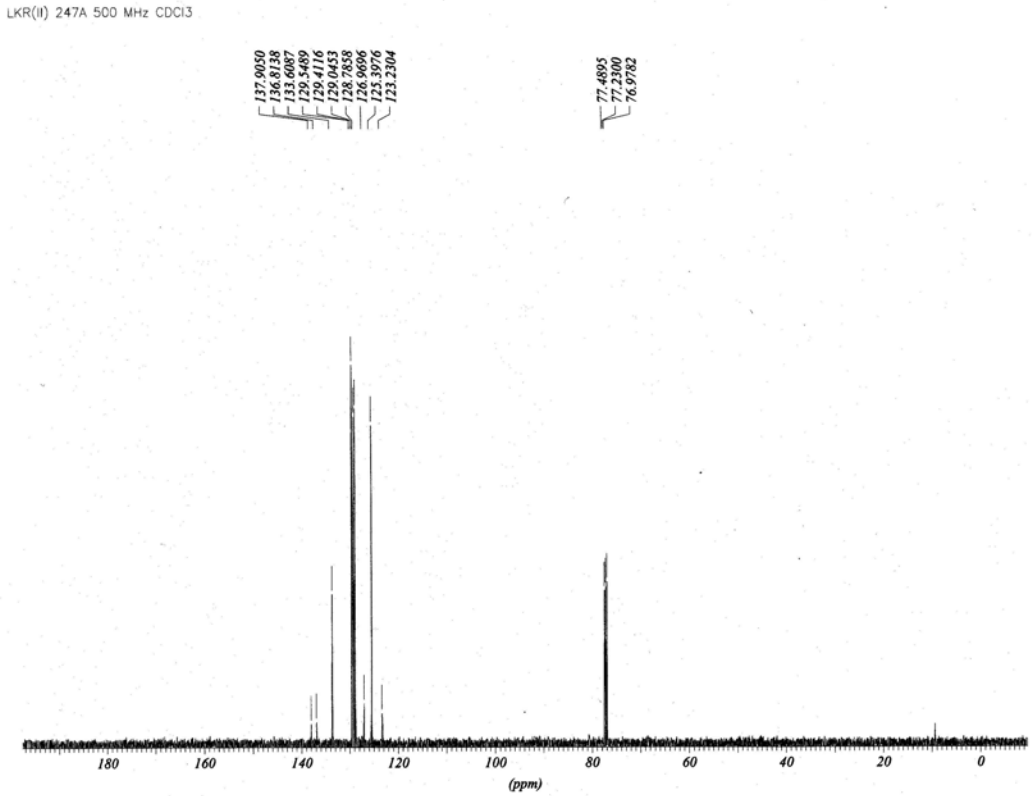
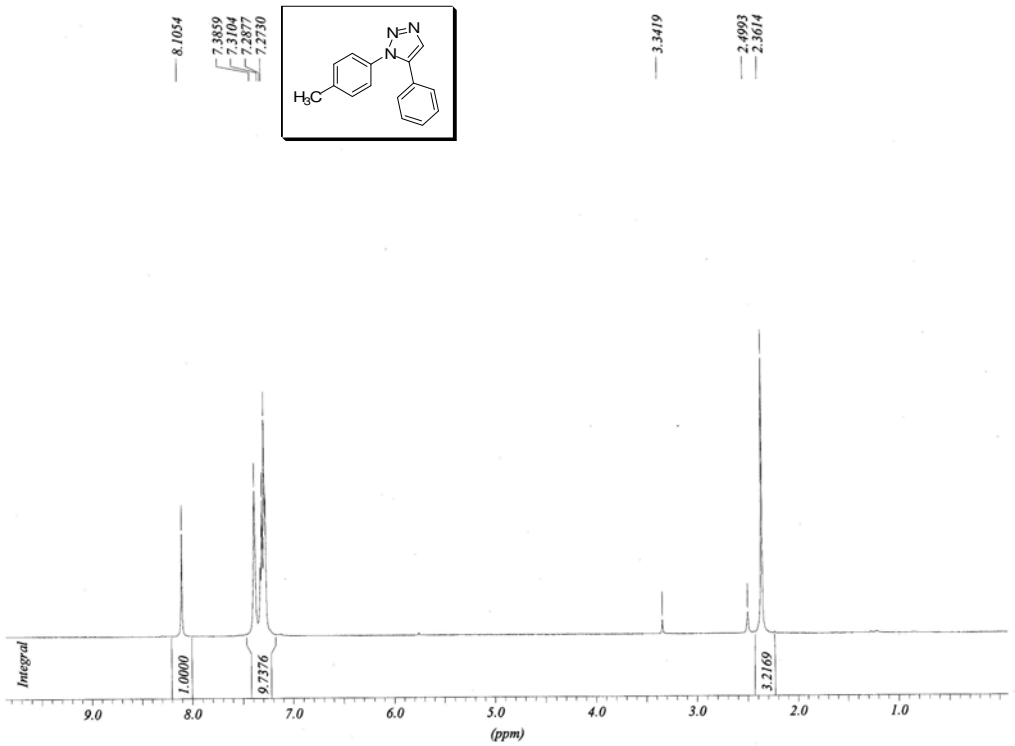
137.6990
136.3025
133.6850
129.5413
129.0987
128.6943
126.7102
126.4889
94.8121
77.4818
77.2300
76.9706
180 160 140 120 100 80 60 40 20 0
(ppm)

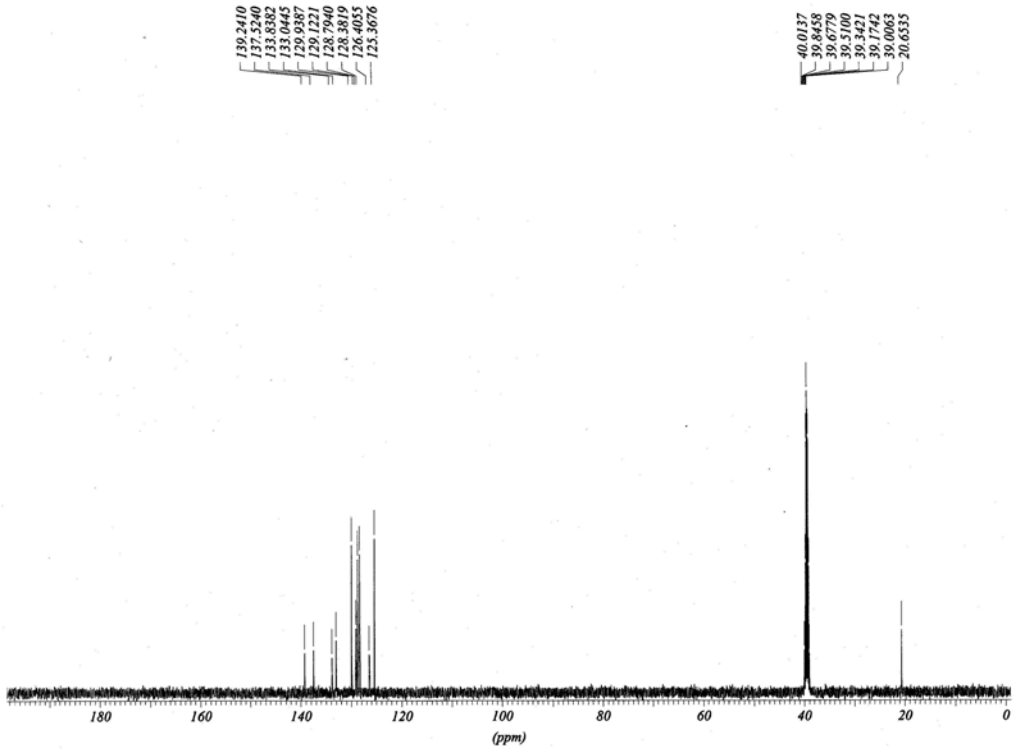

LKR(II) 247A 500 MHz CDCl3
7.8599
7.4382
7.4338
7.4279
7.4243
7.3707
7.3671
7.3553
7.3517
7.3370
7.3238
7.3194
7.2993
7.2329
7.2307
7.2175
7.2138
N=N
N
Integral
1.0000
3.1890
5.3594
2.0657
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)

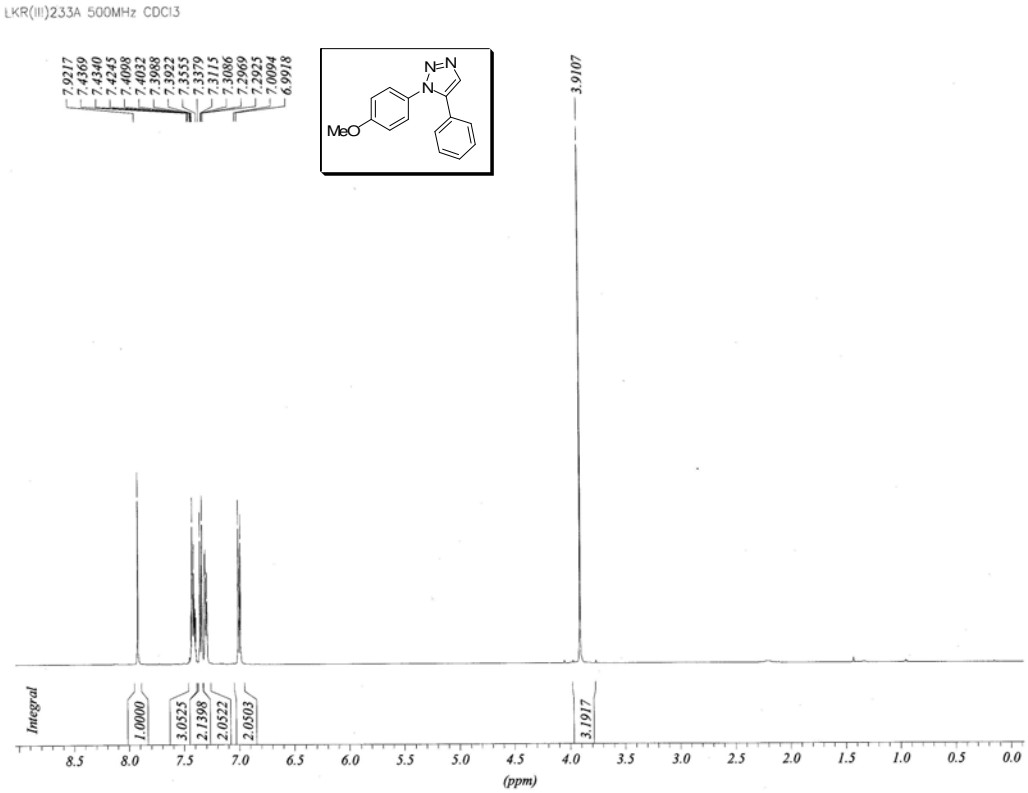

LKR(II) 247A 500 MHz CDCl3
137.9050
136.8138
133.6087
129.5489
129.4116
129.0453
128.7858
126.9696
125.3976
123.2304
77.4895
77.2300
76.9782
180
160
140
120
100
80
60
40
20
0
(ppm)

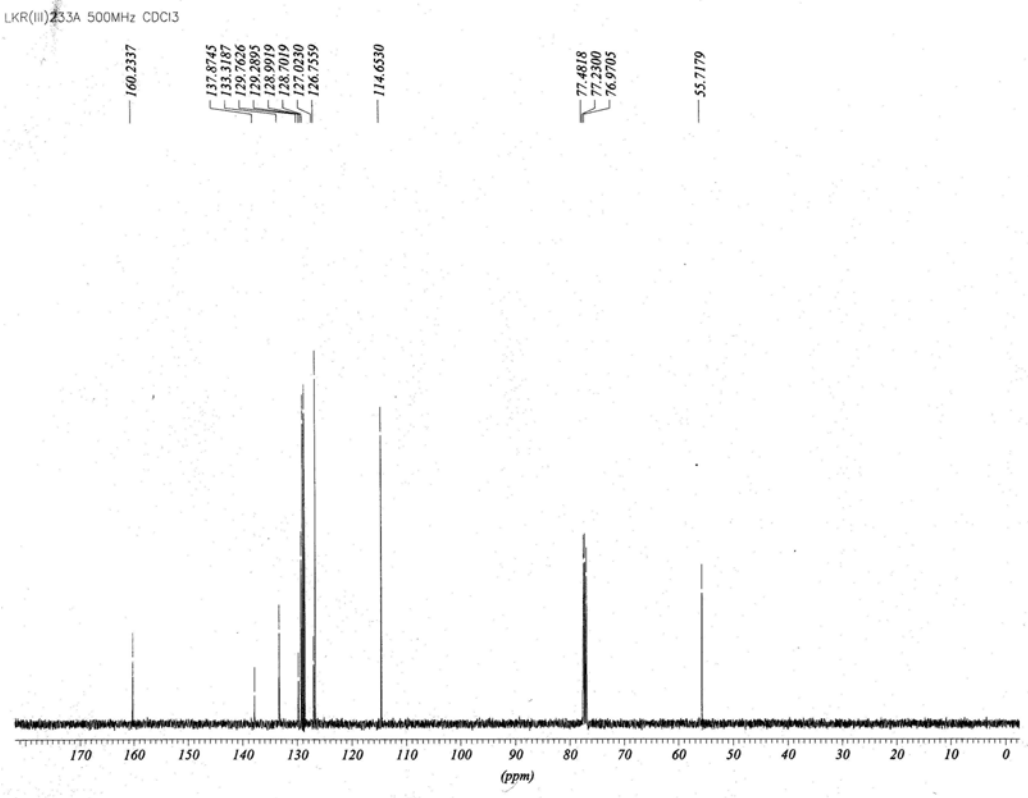
LKR(II) 265A 500 MHz CDCl3

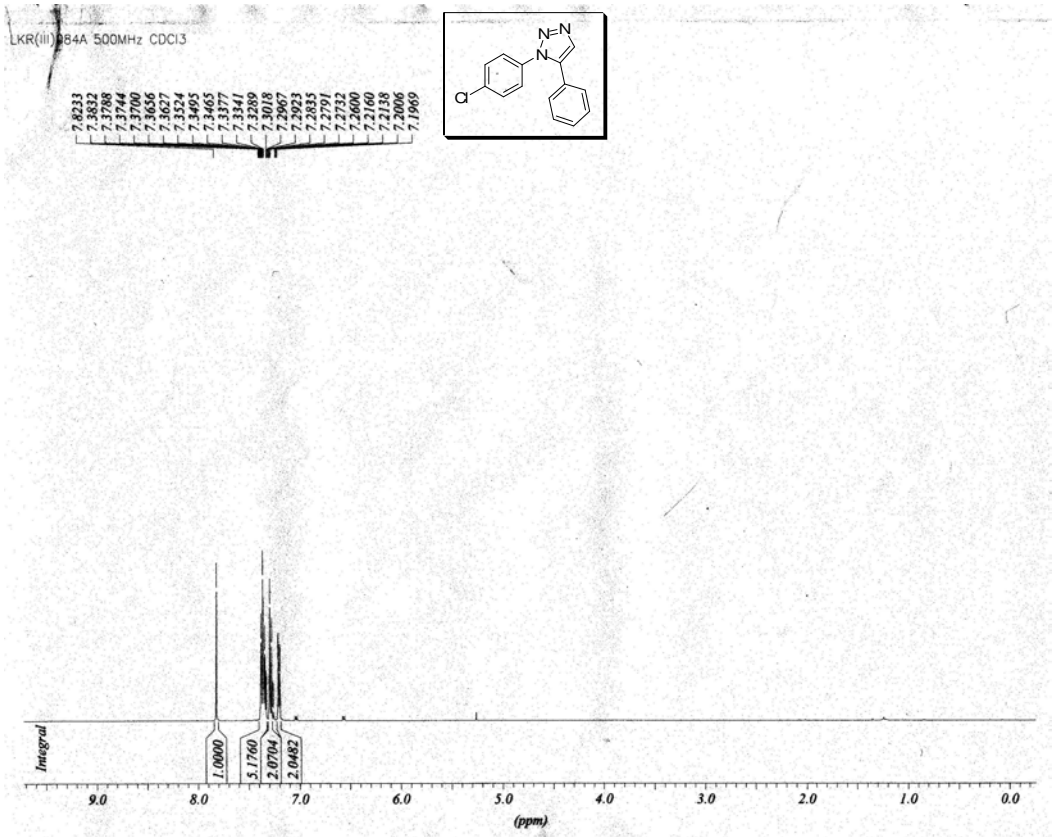


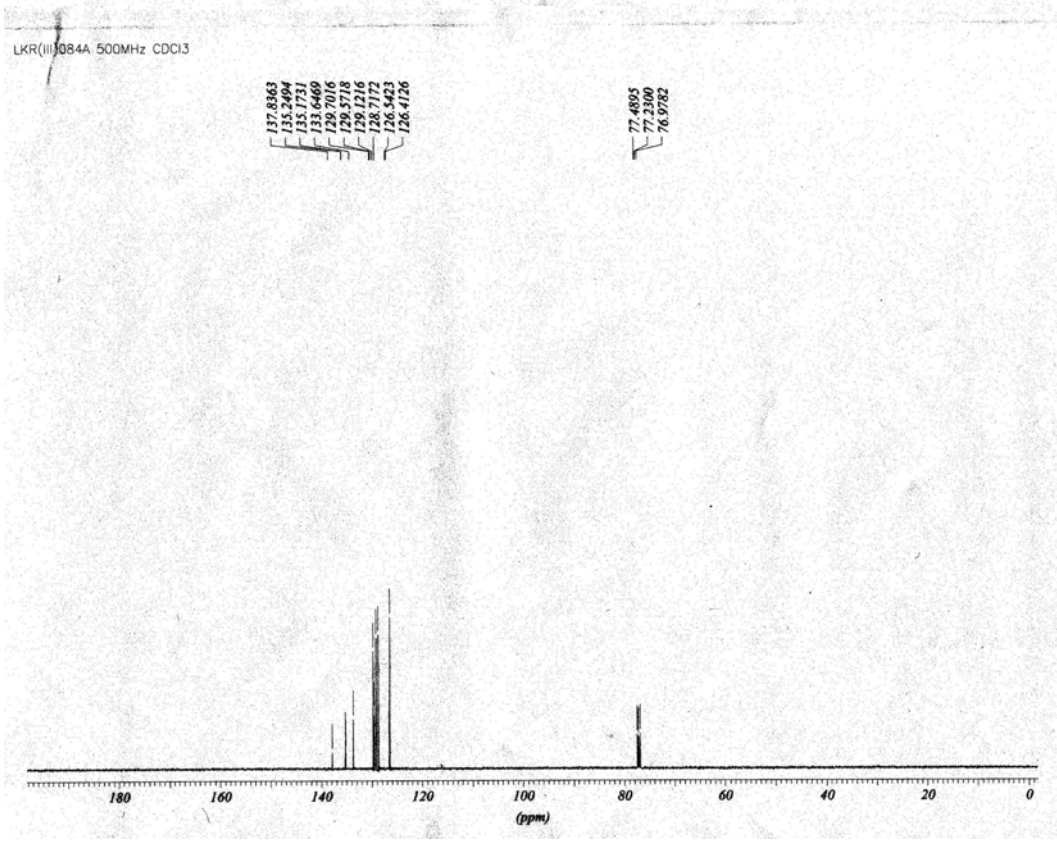
LKR(II) 265A 500 MHz DMSO

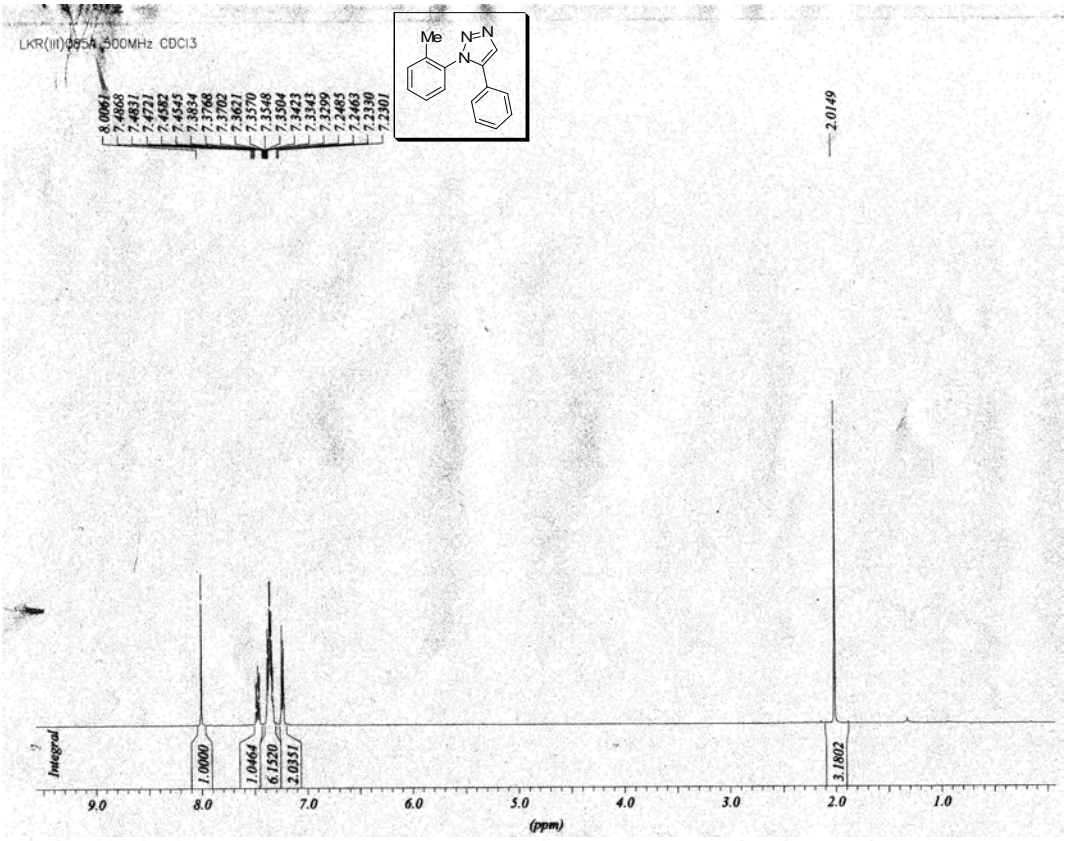



LKR(III)233A 500MHz CDCl3
7.9217
7.4369
7.4340
7.4245
7.4098
7.4032
7.3988
7.3922
7.3555
7.3379
7.3115
7.3086
7.2969
7.2925
7.0094
6.9918
3.9107
MeO
N=N
Integral
1.0000
3.0525
2.1398
2.0522
2.0503
3.1917
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)


LKR(III)233A 500MHz CDCl3
160.2337
137.8745
133.3187
129.7626
129.2895
128.9919
128.7019
127.0230
126.7559
114.6530
77.4818
77.2300
76.9705
55.7179
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)


LKR(III)084A 500MHz CDCl3
7.8233
7.3832
7.3788
7.3744
7.3700
7.3656
7.3627
7.3524
7.3495
7.3465
7.3377
7.3341
7.3289
7.3018
7.2967
7.2923
7.2835
7.2791
7.2732
7.2600
7.2160
7.2138
7.2006
7.1969
N=N
N
Cl
Integral
1.0000
5.1760
2.0704
2.0482
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
(ppm)


LKR(III)084A 500MHz CDCl3
137.8363
135.2494
135.1731
133.6469
129.7016
129.5718
129.1216
128.7172
126.5423
126.4126
77.4895
77.2300
76.9782
180
160
140
120
100
80
60
40
20
0
(ppm)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Me
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N
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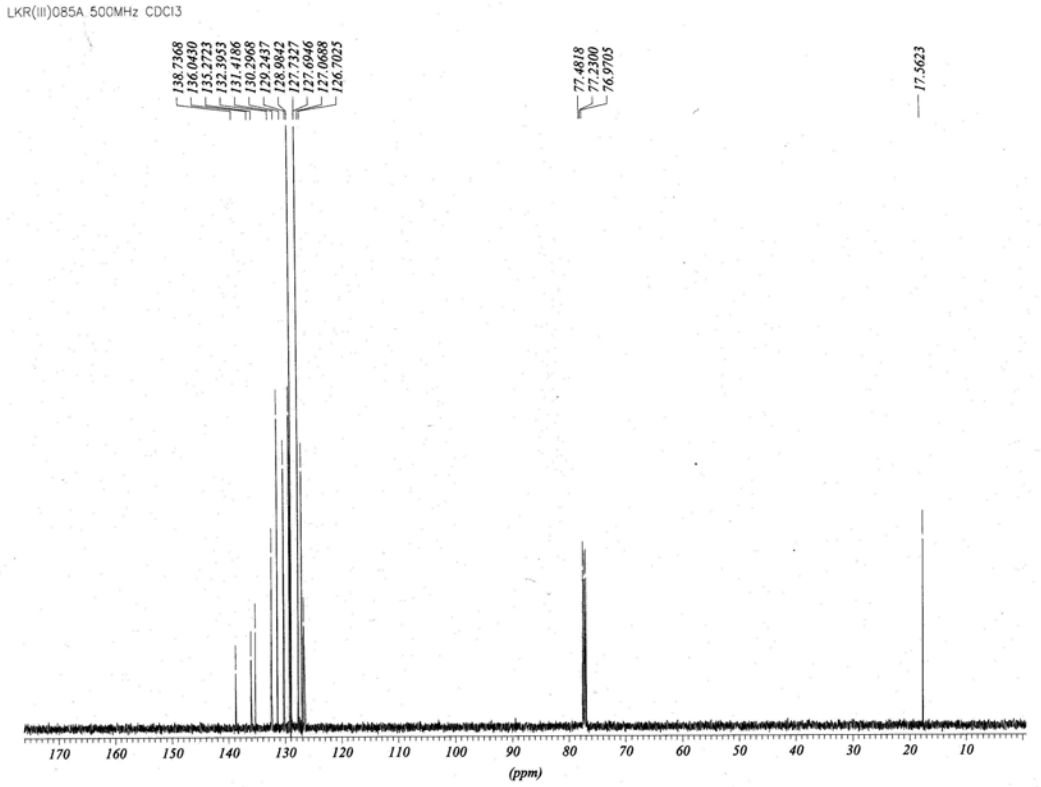
7.4668
7.4831
7.4721
7.4582
7.4545
7.3834
7.3768
7.3702
7.3621
7.3570
7.3548
7.3504
7.3423
7.3343
7.3299
7.2485
7.2463
7.2330
7.2301
2.0149
Integral
1.0000
1.0464
6.1520
2.0351
3.1802
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)


LKR(III)085A 500MHz CDCl3
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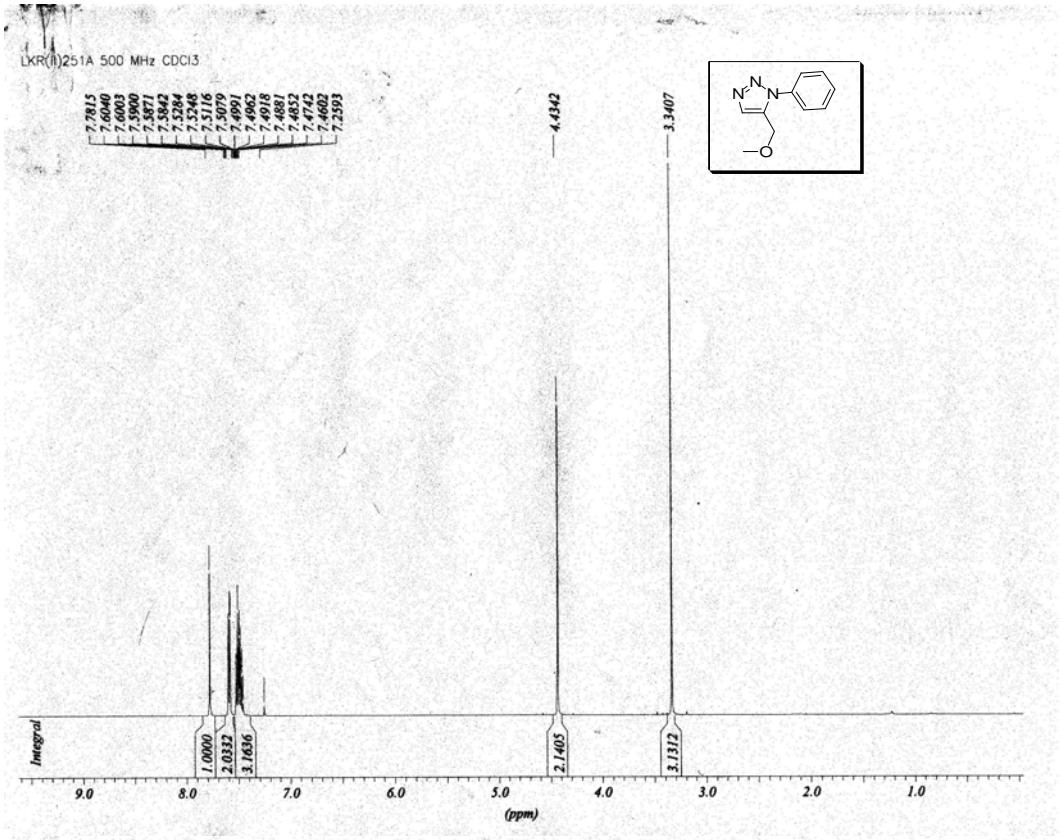
136.0430
135.2723
132.3953
131.4186
130.2968
129.2437
128.9842
127.7327
127.6946
127.0688
126.7025
77.4818
77.2300
76.9705
17.5623
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
(ppm)


LKR(II)251A 500 MHz CDCl3
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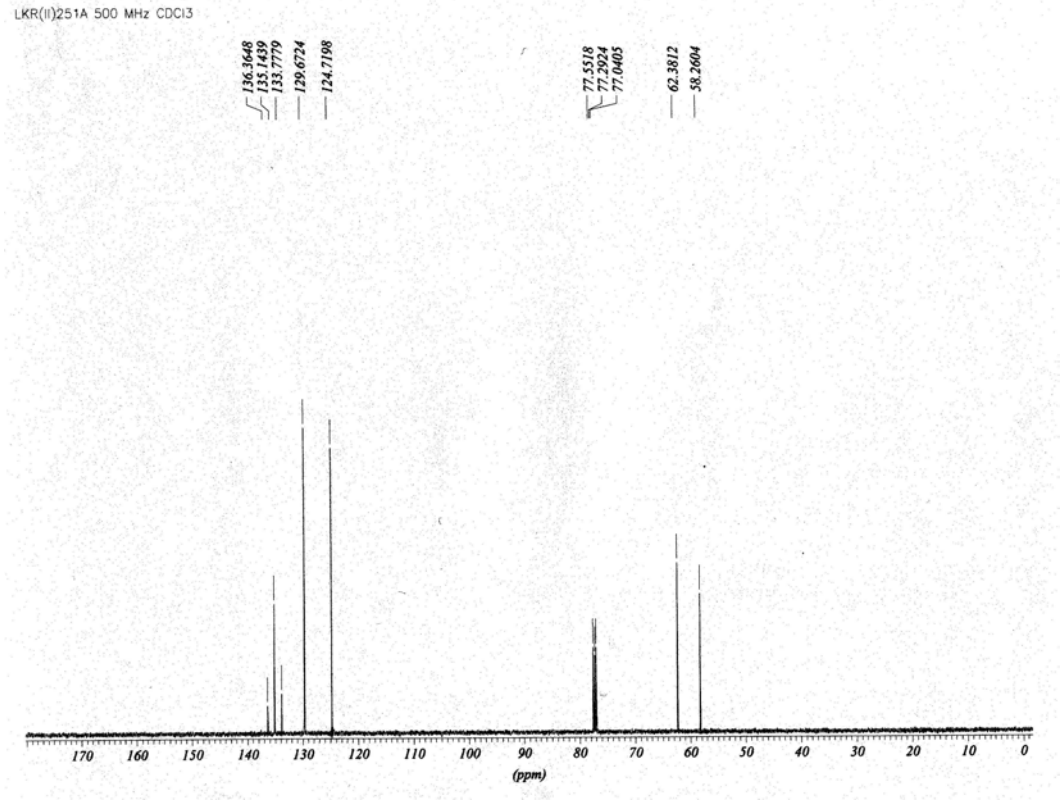
7.6040
7.6003
7.5900
7.5871
7.5842
7.5284
7.5248
7.5116
7.5079
7.4991
7.4962
7.4918
7.4881
7.4852
7.4742
7.4602
7.2593
4.4342
3.3407
Integral
1.0000
2.0332
3.1636
2.1405
3.1312
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)


LKR(II)251A 500 MHz CDCl3
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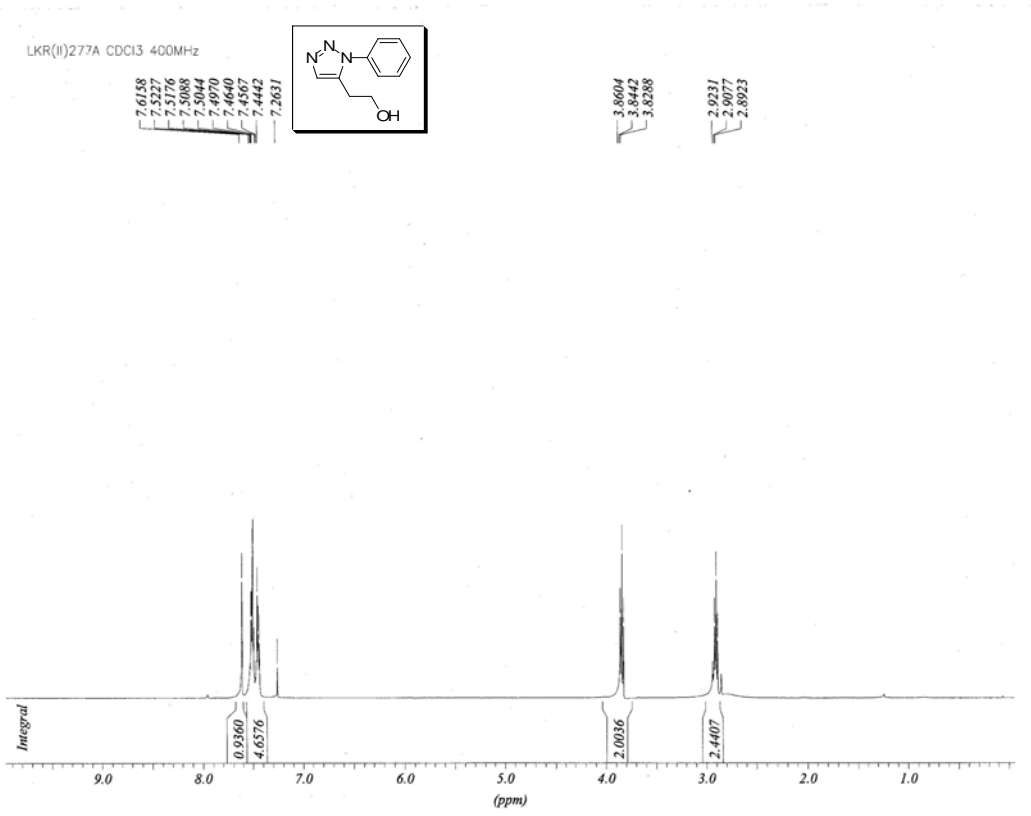
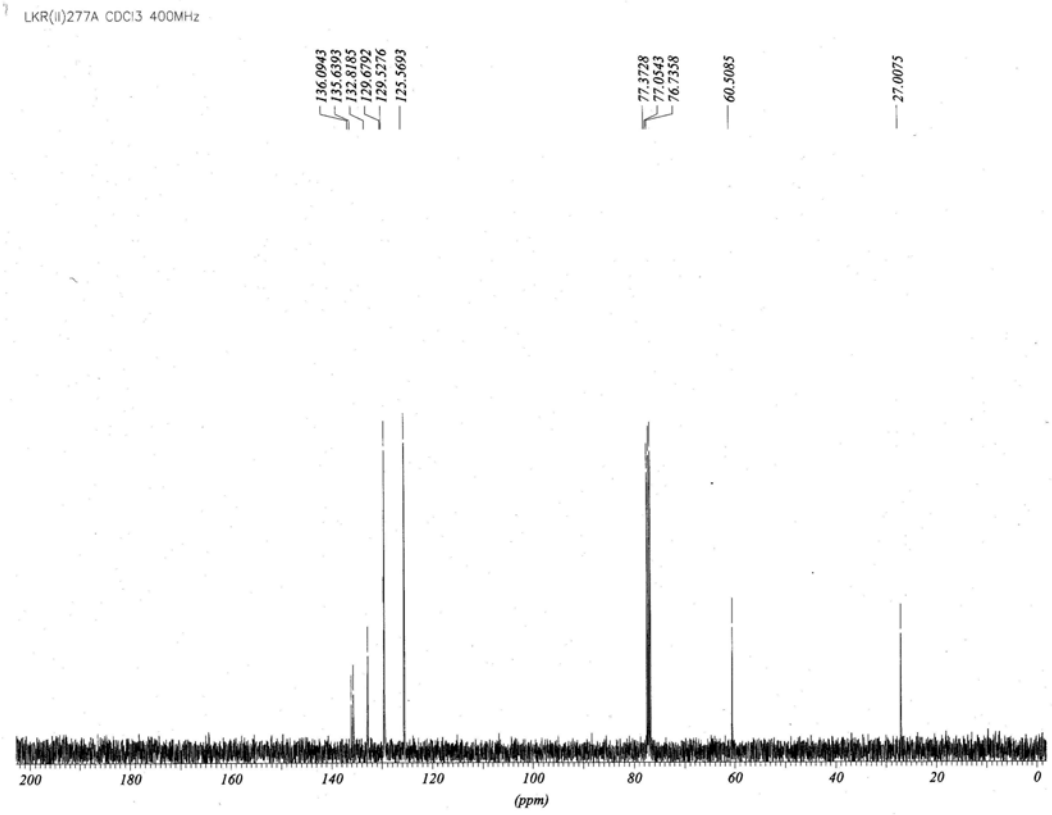
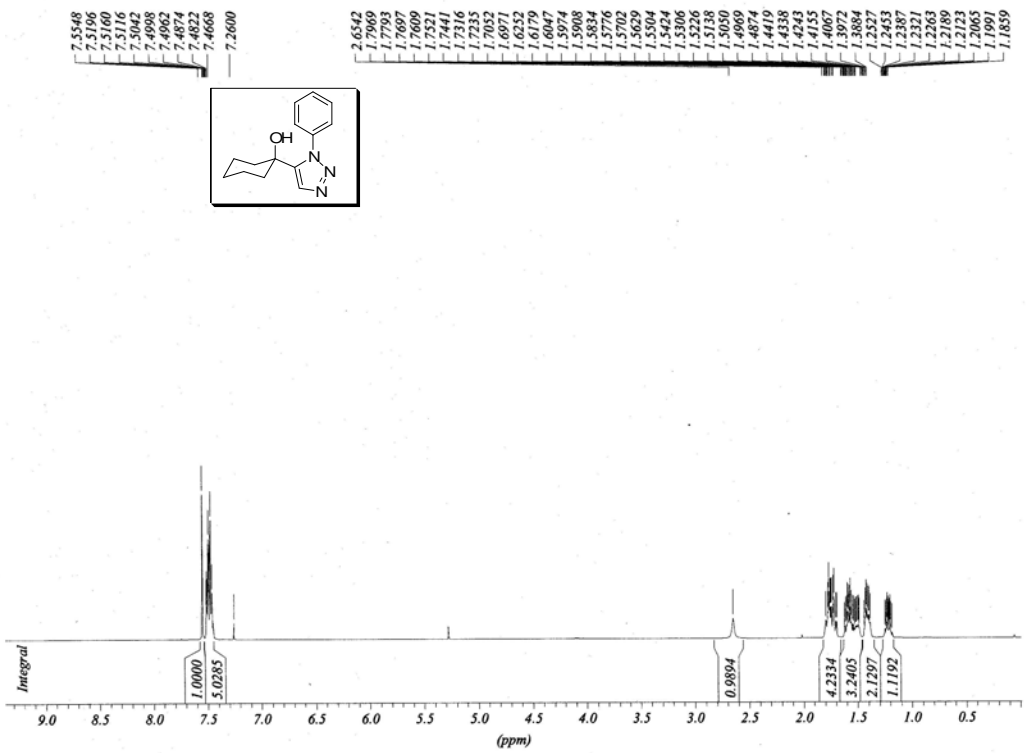
135.1439
133.7779
129.6724
124.7198
77.5518
77.2924
77.0405
62.3812
58.2604
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)

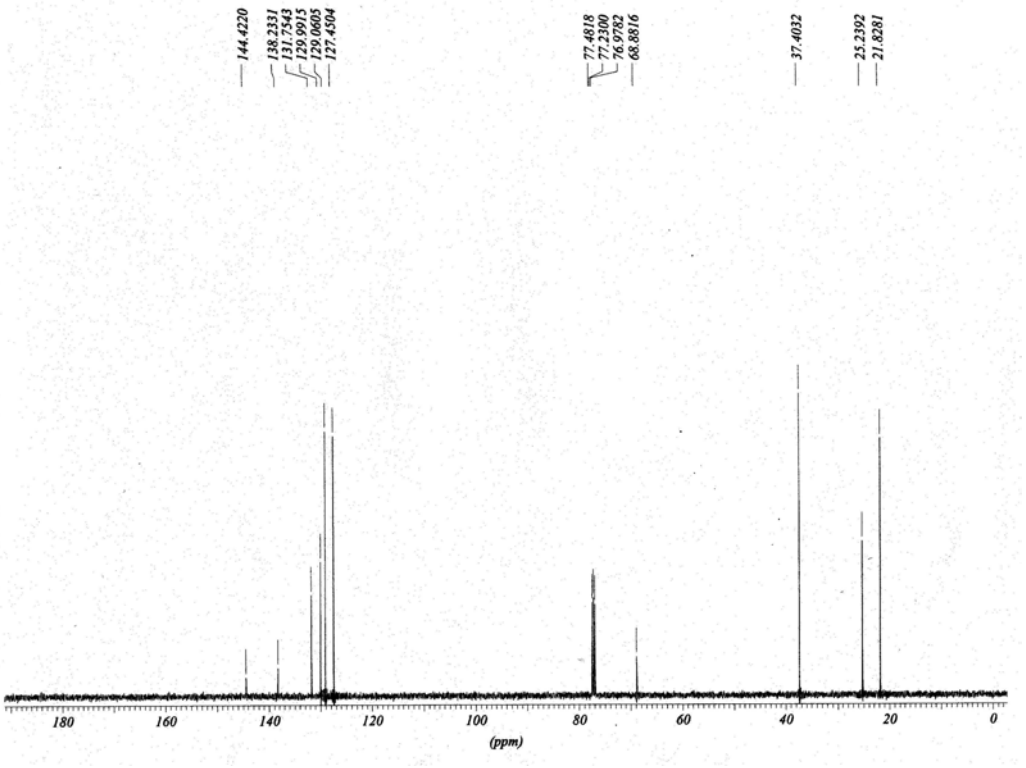

LKR(II)277A CDCl3 400MHz
7.6158
7.5227
7.5176
7.5068
7.5044
7.4970
7.4640
7.4567
7.4442
7.2631
N
N
N
OH
3.8604
3.8442
3.8288
2.9231
2.9077
2.8923
Integral
0.9360
4.6576
2.0036
2.4407
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
(ppm)

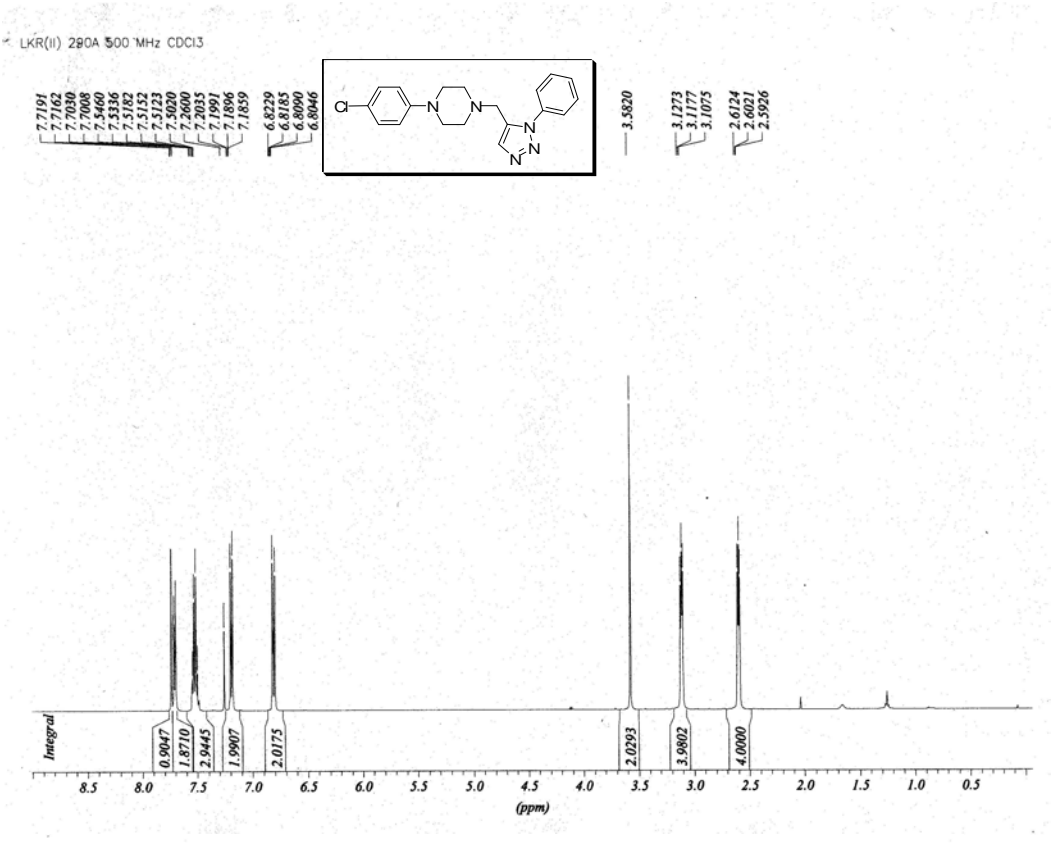

LKR(II)277A CDCl3 400MHz
136.0943
135.6393
132.8185
129.6792
129.5276
125.5693
77.3728
77.0543
76.7358
60.5085
27.0075
200
180
160
140
120
100
80
60
40
20
0
(ppm)

LKR(II) 262A 500 MHz CDCl3



LKR(II) 262A 500 MHz CDCl3

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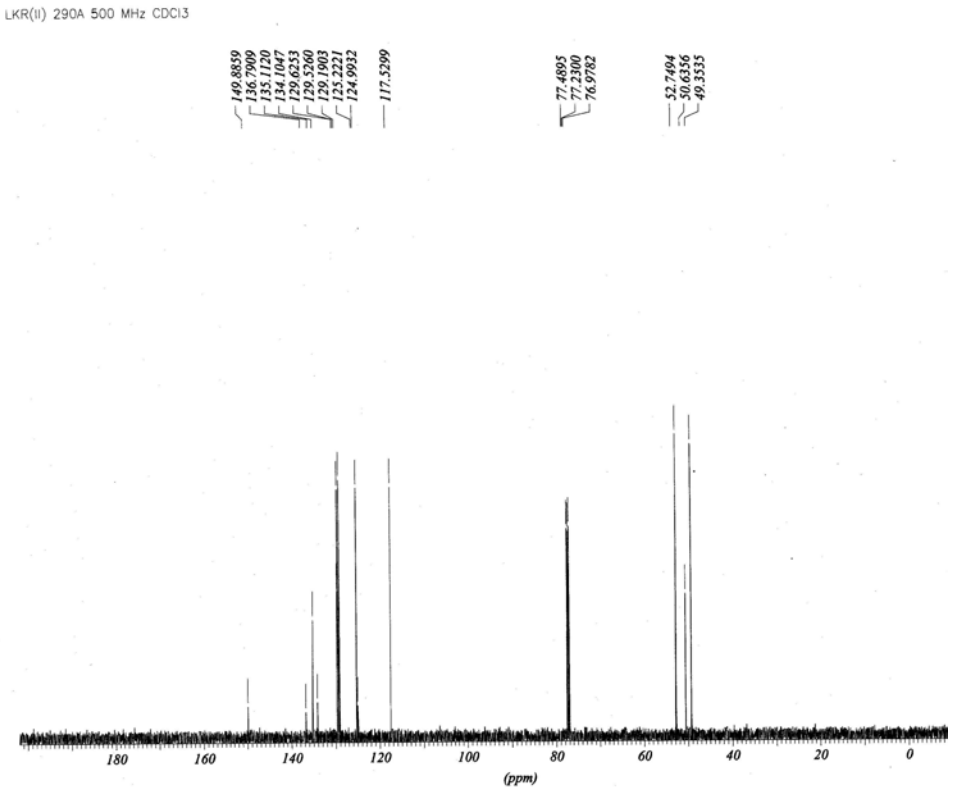
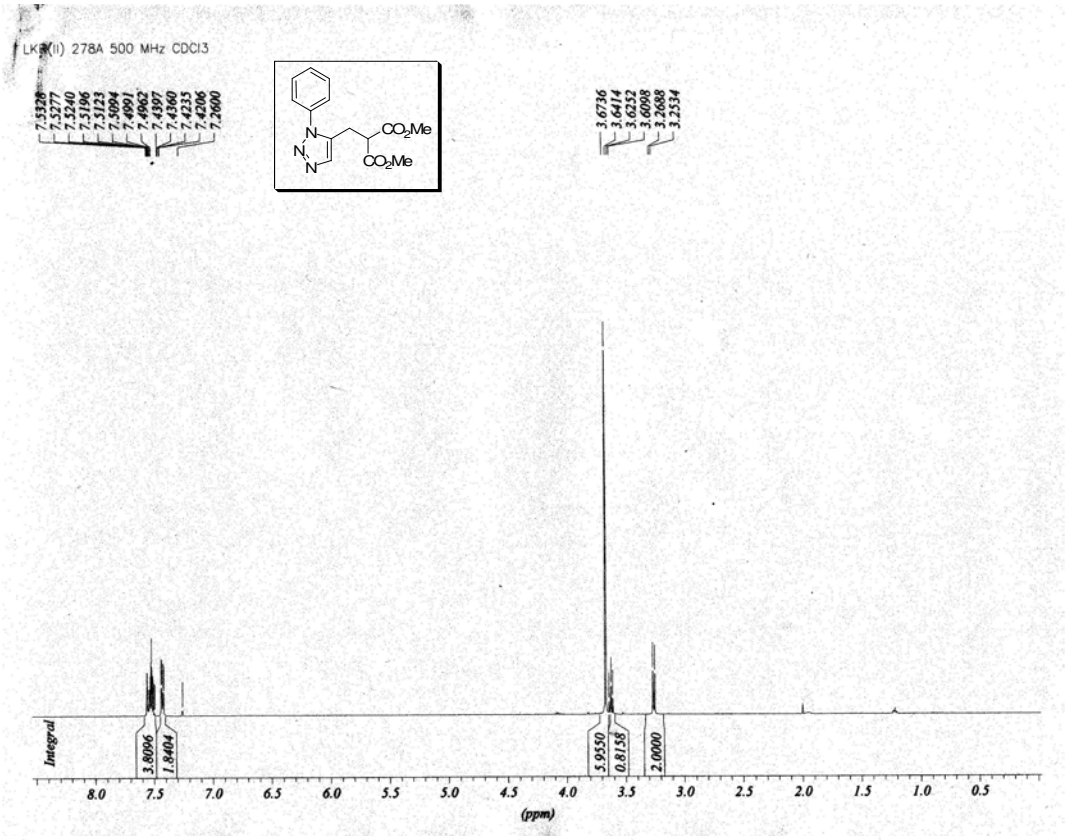
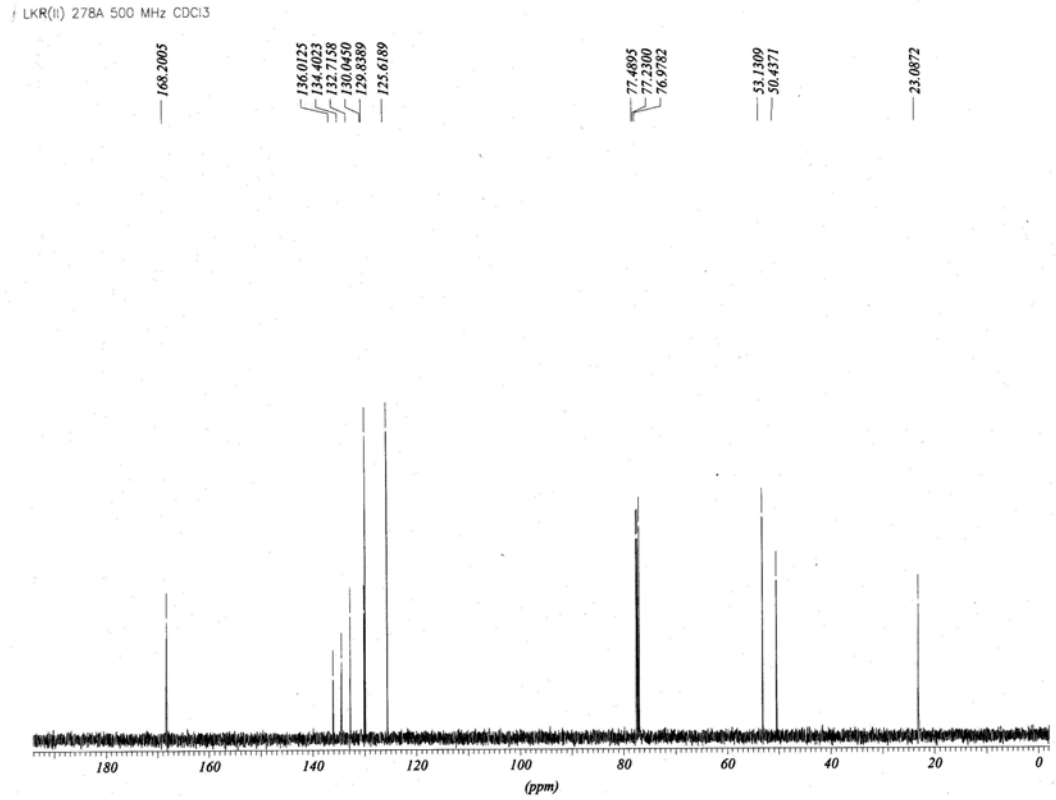
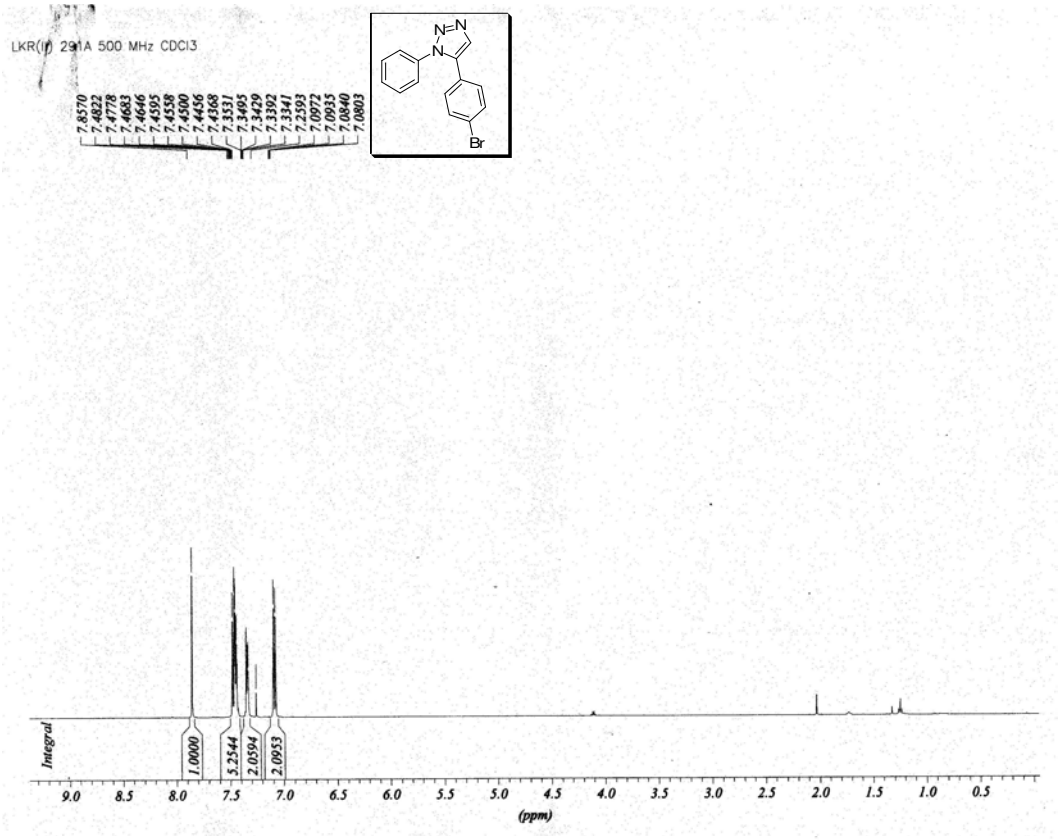
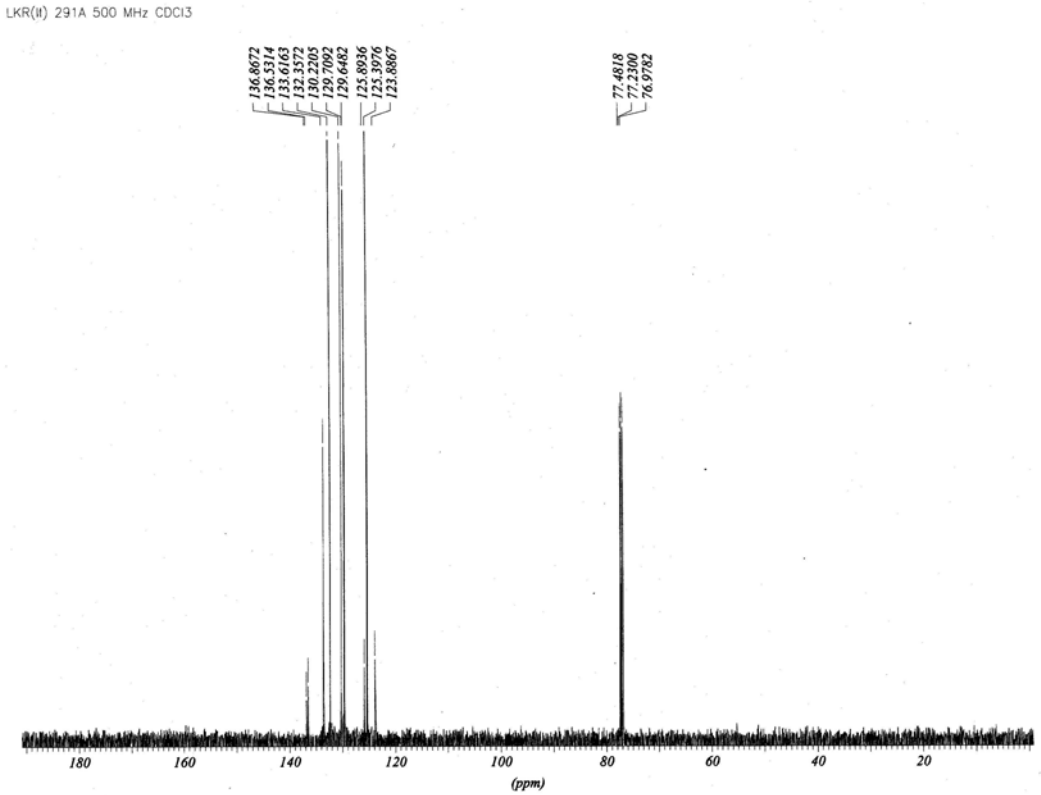
7.7191
7.7162
7.7030
7.7008
7.5460
7.5336
7.5182
7.5152
7.5123
7.5020
7.2600
7.2035
7.1991
7.1896
7.1859
6.8229
6.8185
6.8090
6.8046
3.5820
3.1273
3.1177
3.1075
2.6124
2.6021
2.5926
Integral
0.9047
1.8710
2.9445
1.9907
2.0175
2.0293
3.9802
4.0000
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


LKR(II) 290A 500 MHz CDCl3
149.8859
136.7909
135.1120
134.1047
129.6253
129.5260
129.1903
125.2221
124.9932
117.5299
77.4895
77.2300
76.9782
52.7494
50.6356
49.3535
180
160
140
120
100
80
60
40
20
0
(ppm)


LKR(II) 278A 500 MHz CDCl3
7.5328
7.5277
7.5240
7.5196
7.5123
7.5094
7.4991
7.4962
7.4397
7.4360
7.4233
7.4206
7.2600
3.6736
3.6414
3.6252
3.6098
3.2688
3.2534
CO2Me
CO2Me
Integral
3.8096
1.8404
5.9550
0.8158
2.0000
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)


LKR(II) 278A 500 MHz CDCl3
168.2005
136.0125
134.4023
132.7158
130.0450
129.8389
125.6189
77.4895
77.2300
76.9782
53.1309
50.4371
23.0872
180
160
140
120
100
80
60
40
20
0
(ppm)


LKR(II) 291A 500 MHz CDCl3
7.8570
7.4822
7.4778
7.4683
7.4646
7.4595
7.4558
7.4500
7.4456
7.4368
7.3531
7.3491
7.3429
7.3392
7.3341
7.2593
7.0972
7.0935
7.0840
7.0803
N=N
N
Br
Integral
1.0000
3.2544
2.0594
2.0953
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
(ppm)


LKR(II) 291A 500 MHz CDCl3
136.8672
136.5314
133.6163
132.3572
130.2205
129.7092
129.6482
125.8936
125.3976
123.8867
77.4818
77.2300
76.9782
180 160 140 120 100 80 60 40 20
(ppm)