Supporting Information

SYNTHESIS OF 5-H THIAZOLES VIA THIOAMIDE DIANIONS WITH THIOFORMAMIDES: PYRIDYLMETHYL GROUP ON THE NITROGEN ATOM OF THIAZOLE PROMOTES THE FORMATION OF 5-H THIAZOLES.

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Crystal data and structure refinement S1

^{1}H NMR spectra of 5-H thiazoles S2

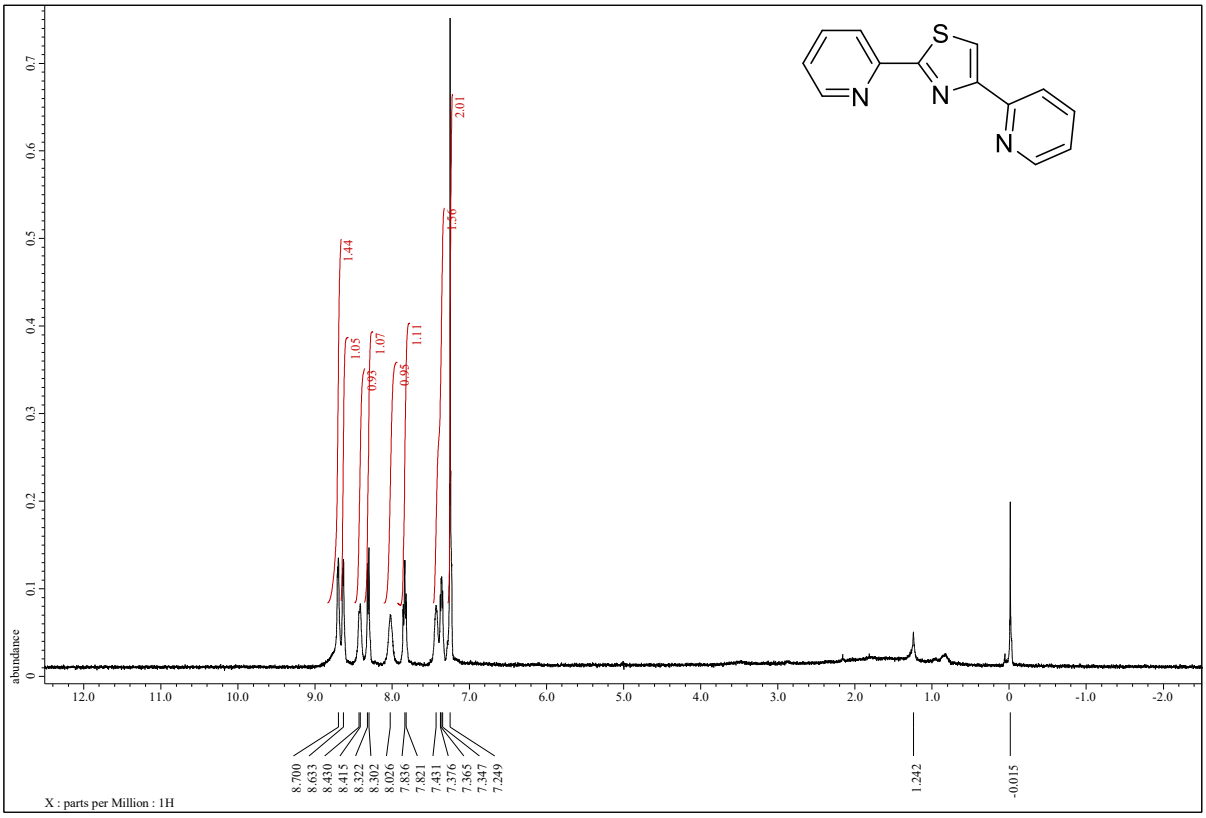
^{13}C NMR spectra of 5-H thiazoles S5

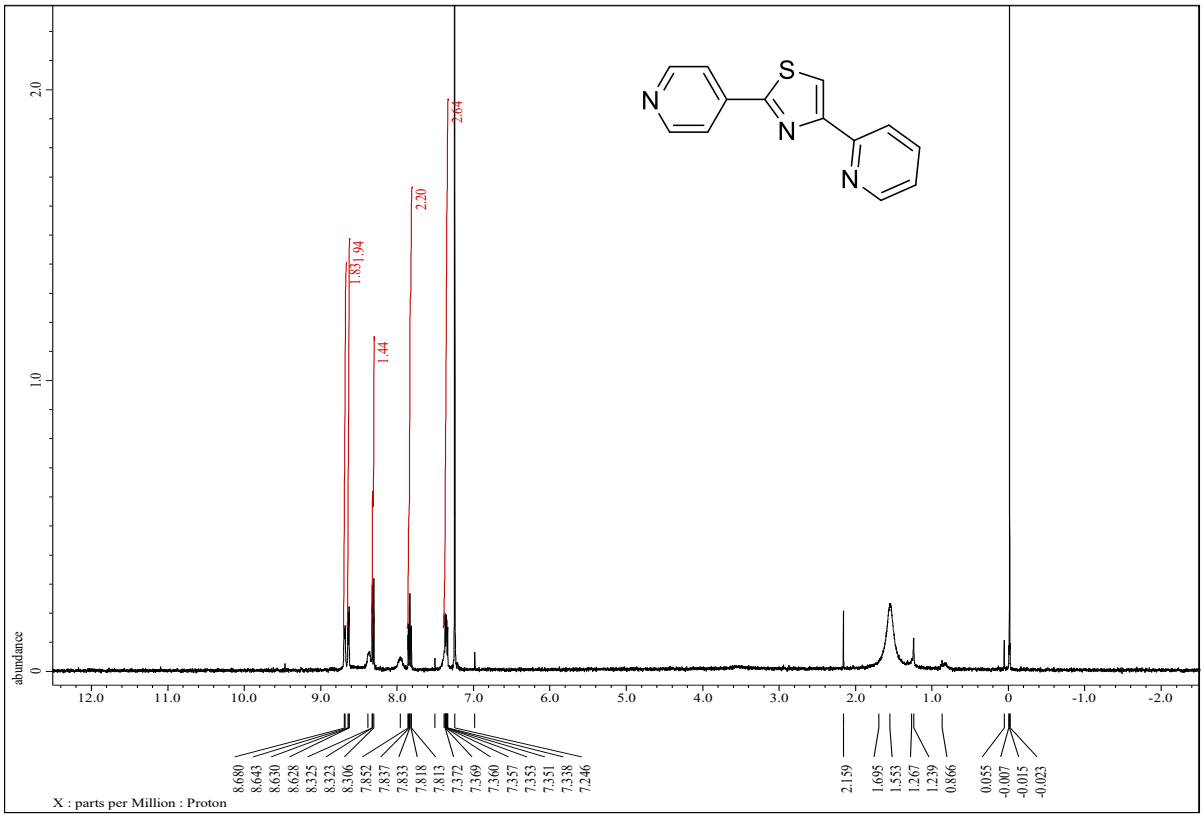
Crystal data and structure refinement

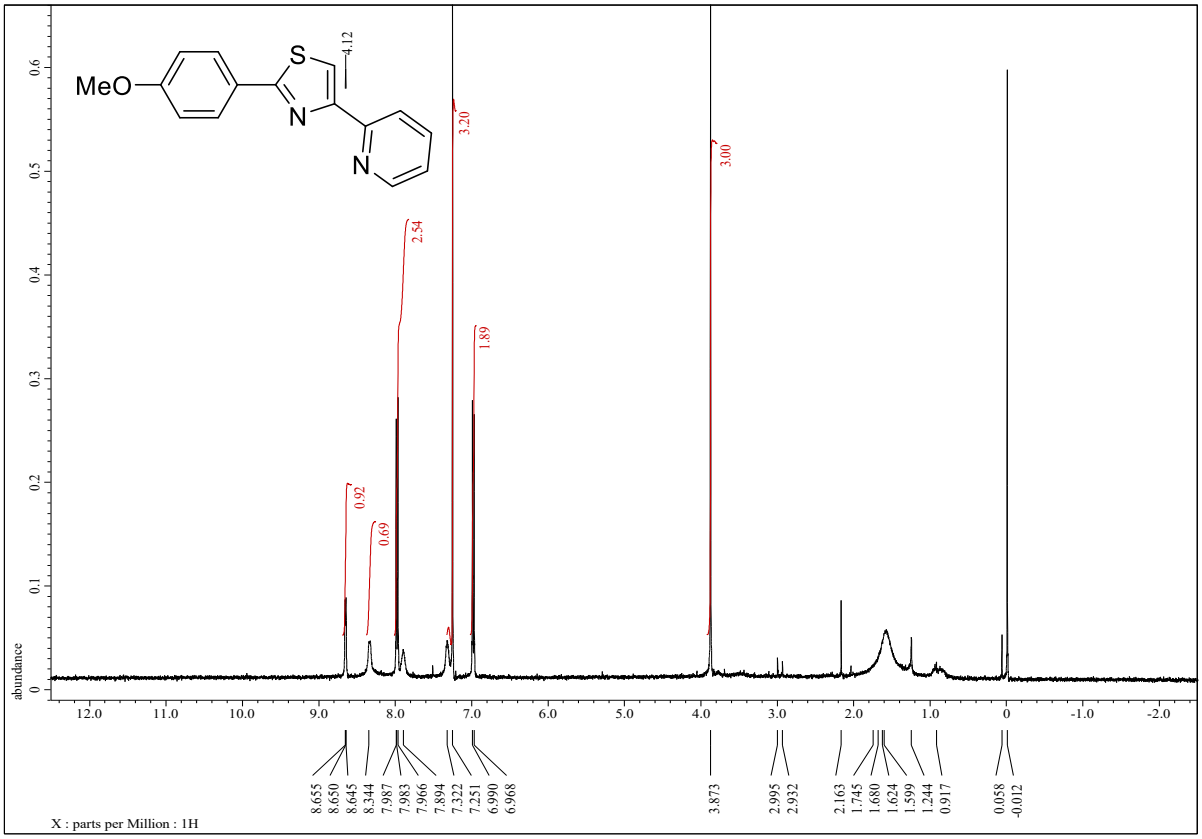
Empirical formula	$C_{13}H_9N_3S$	
Molecular weight	239.29	
Crystal system	monoclinic	
Space group	*C2/c*	
Temperature	123 (K)	
Unit cell dimension	a = 16.7618 (19) Å	α = 90
	b = 11.9433 (8) Å	β = 80.9699 (13)°
	c = 23.653 (3) Å	γ = 90
Volume	4499.5 (9) $Å^3$	
Z	16	
Density (calculated)	1.413 g cm^{-3}	
Absorption coefficient	0.265 mm^{-1}	
F(000)	1984	
Crystal size	0.20 × 0.14 × 0.11 mm^3	
The range of data collection	1.812 to 27.499°	
Index ranges	-21<=h<=21, -15<=k<=12, -30<=l<30	
Reflection collected	19766	
Independent reflection	5186 [R (int) = 0.113]	
Completeness to theta = 27.50°	99.9%	
Max. min. transmission	0.233 and 1.000	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5186 / 344 / 398	
Goodness-of-fit on F^2	1.026	
Final R indices [*I*>2sigma(*I*)]	R_1 = 0.0835, wR_2 = 0.1358	
R indices (all data)	R_1 = 1.358, wR_2 = 0.2748	
Largest diff. peak and hole	0.60 and -0.67 e $Å^{-3}$	

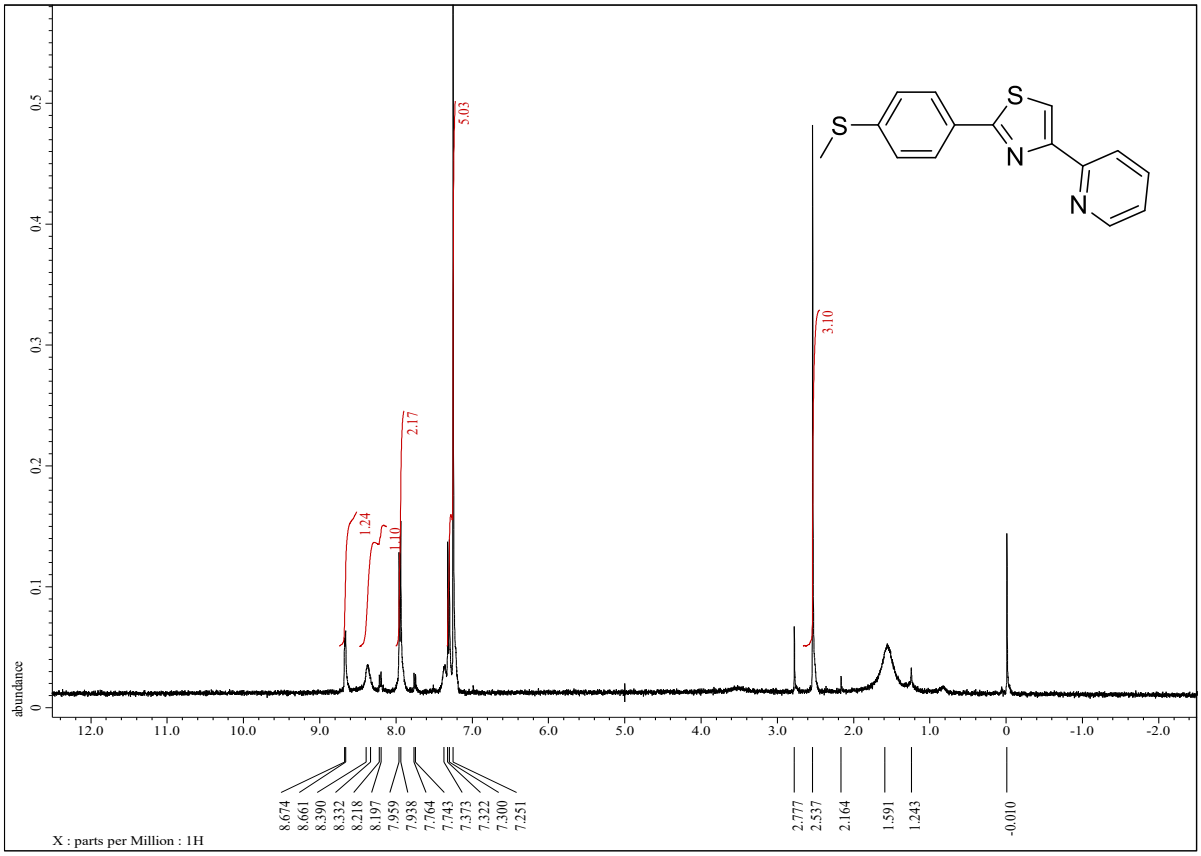
NMR spectra of 5-H thiazoles

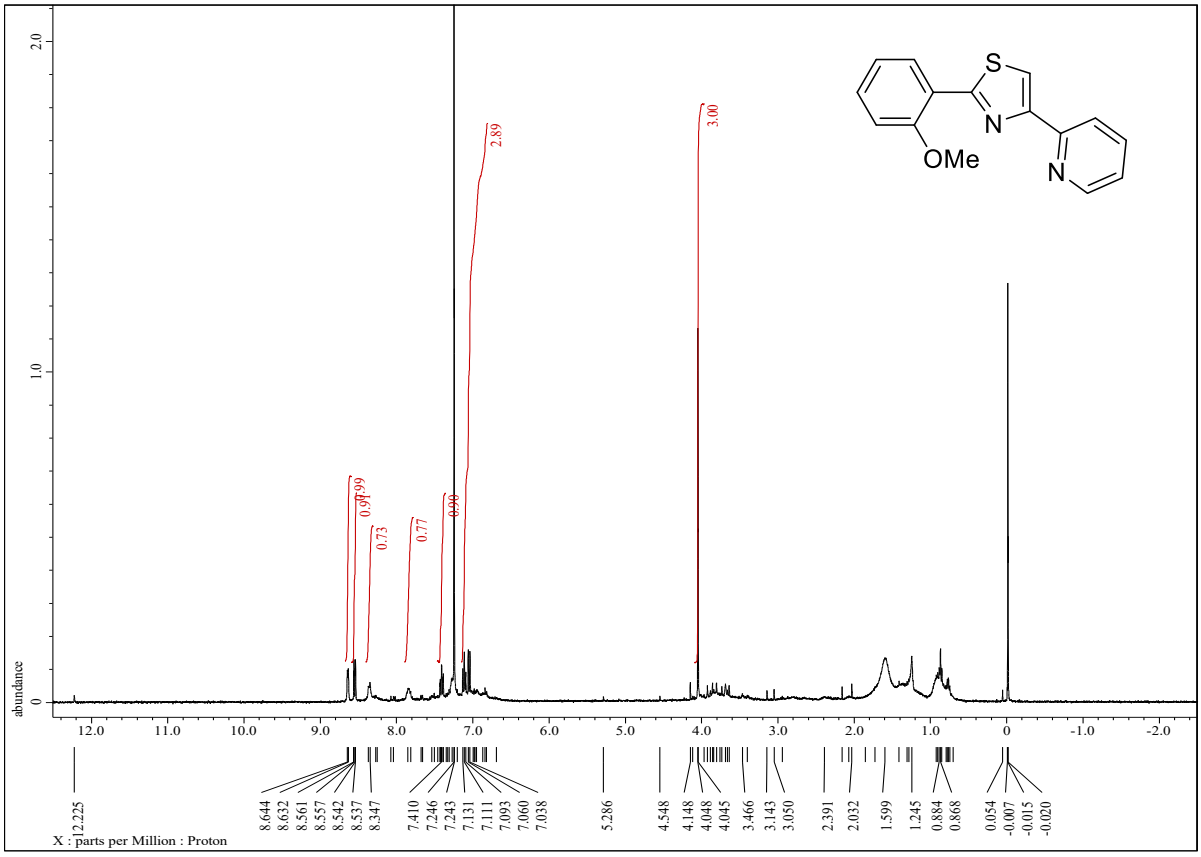
^{1}H NMR of 5-H Thiazoles

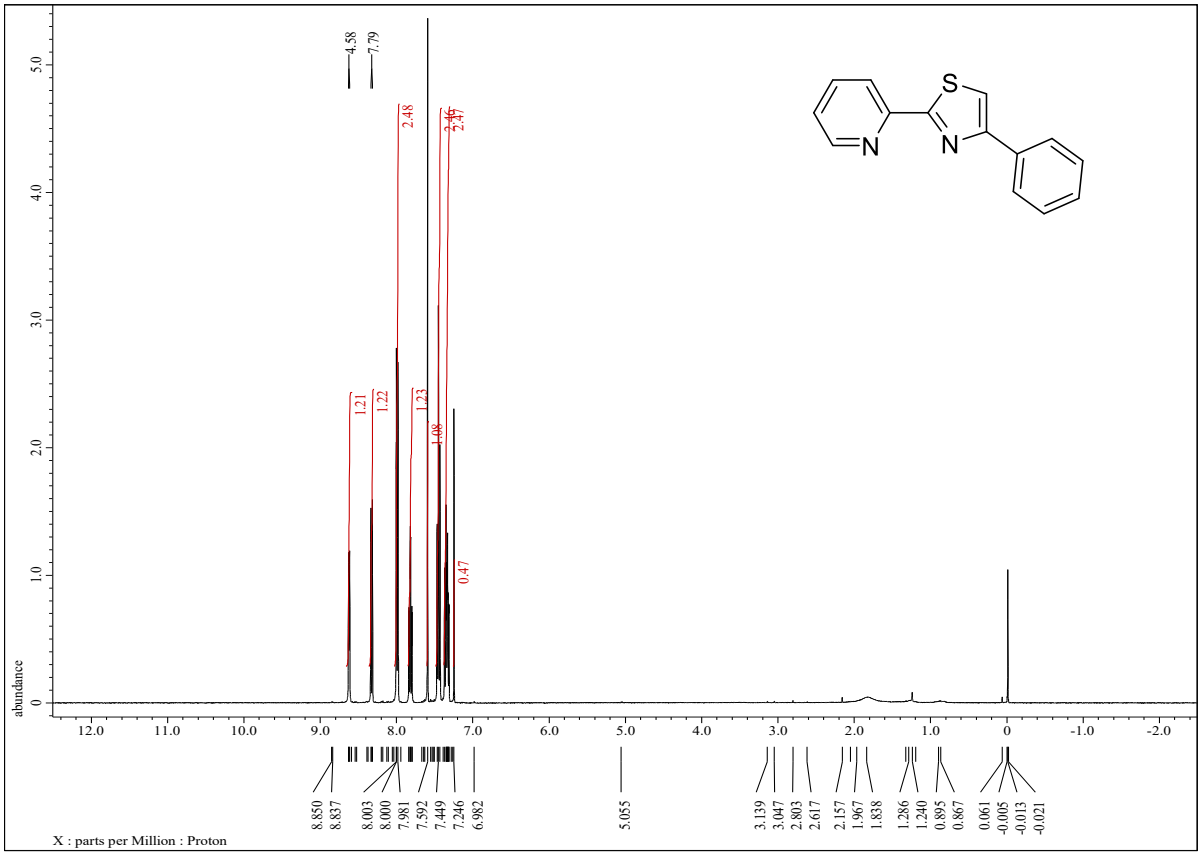




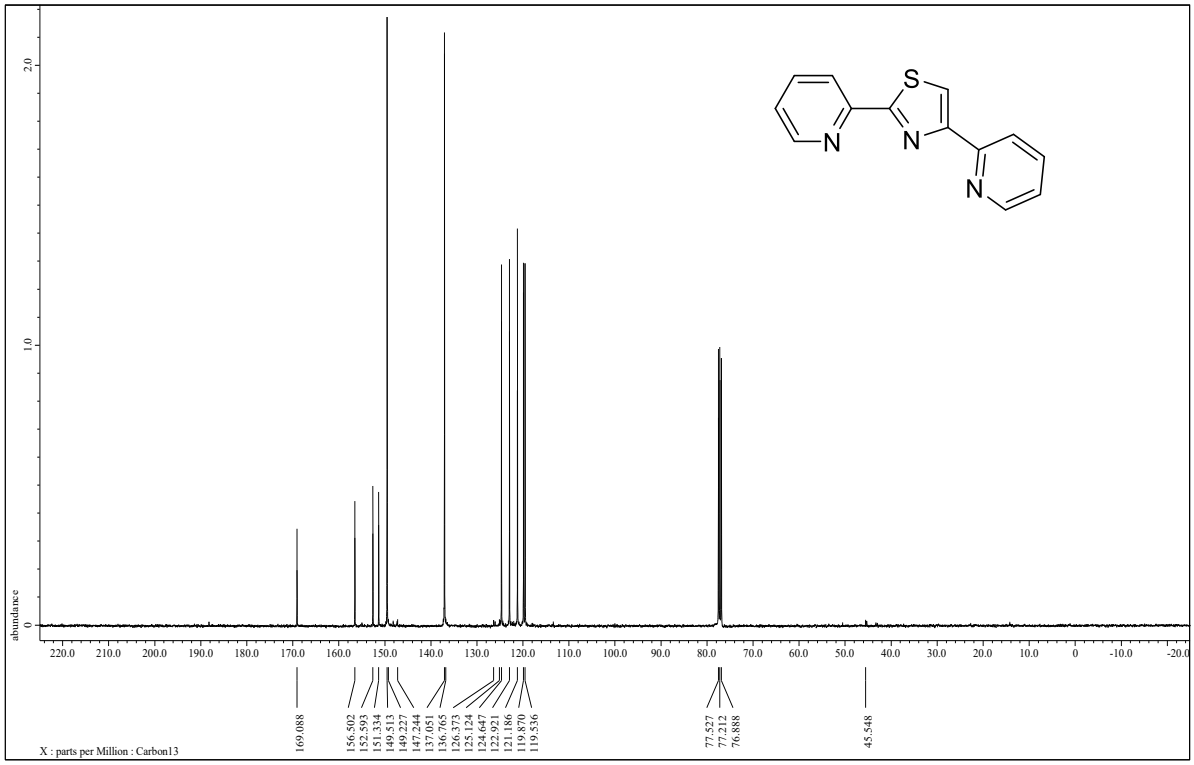

MeO
S
N
N
4.12
3.20
3.00
2.54
1.89
0.92
0.69
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.655
8.650
8.645
8.344
7.987
7.983
7.966
7.894
7.322
7.251
6.990
6.968
3.873
2.995
2.932
2.163
1.745
1.680
1.624
1.599
1.244
0.917
0.058
-0.012
X : parts per Million : 1H

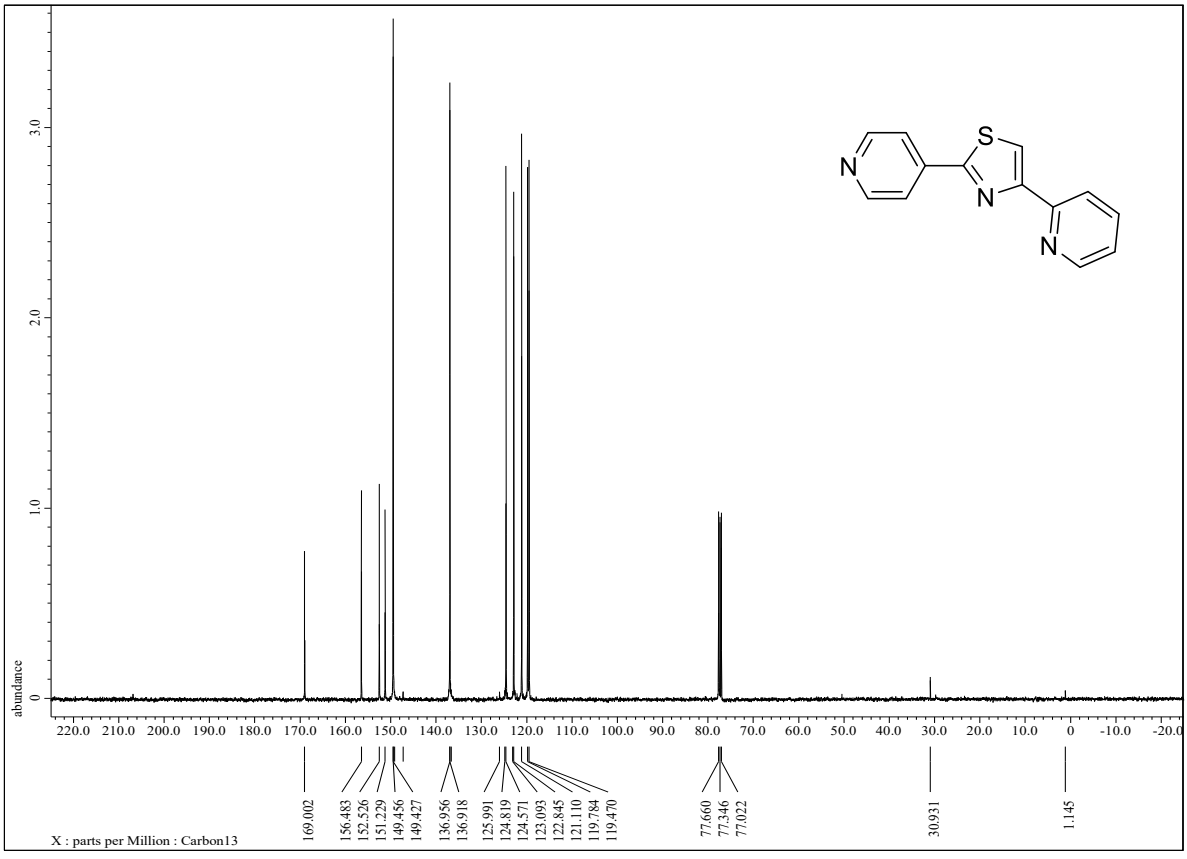

S
S
N
N
5.03
3.10
2.17
1.24
1.10
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.674
8.661
8.390
8.332
8.218
8.197
7.959
7.938
7.764
7.743
7.373
7.322
7.300
7.251
2.777
2.537
2.164
1.591
1.243
-0.010
X : parts per Million : 1H

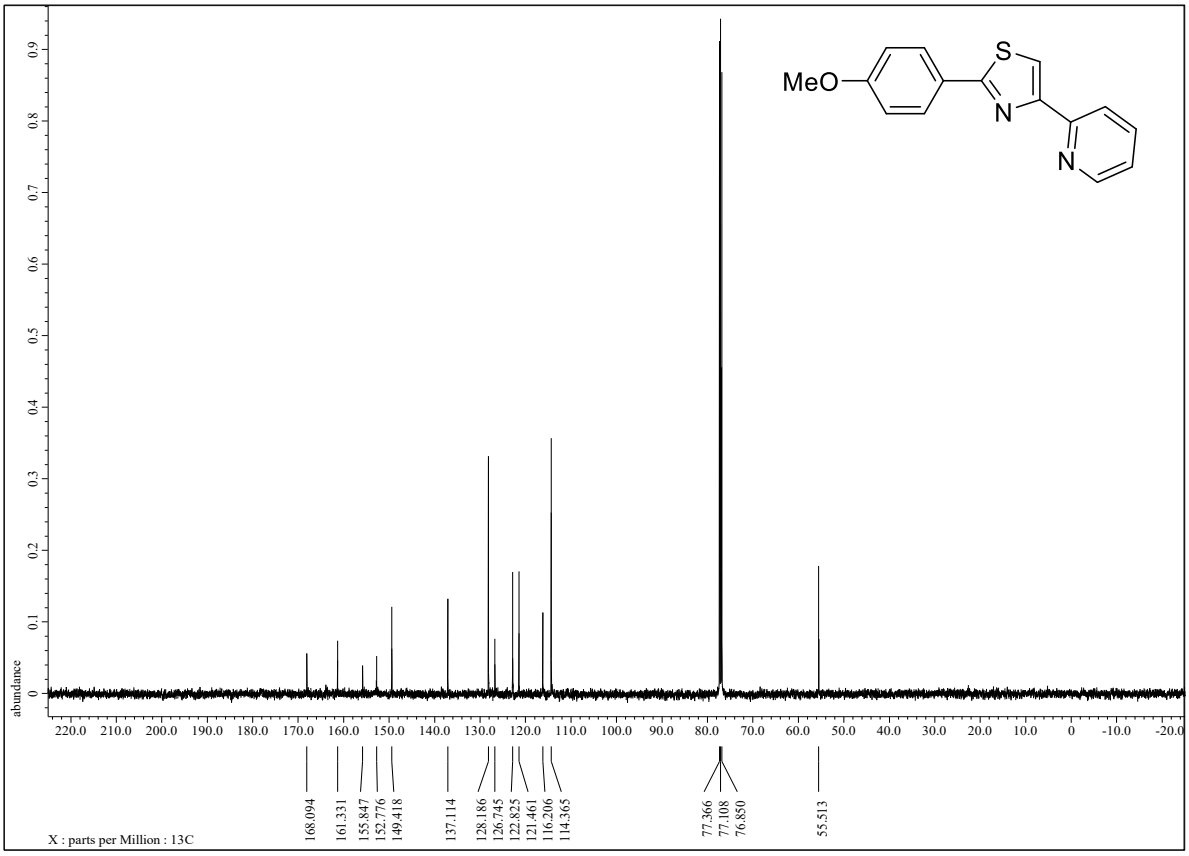

S
N
OMe
N
abundance
X : parts per Million : Proton

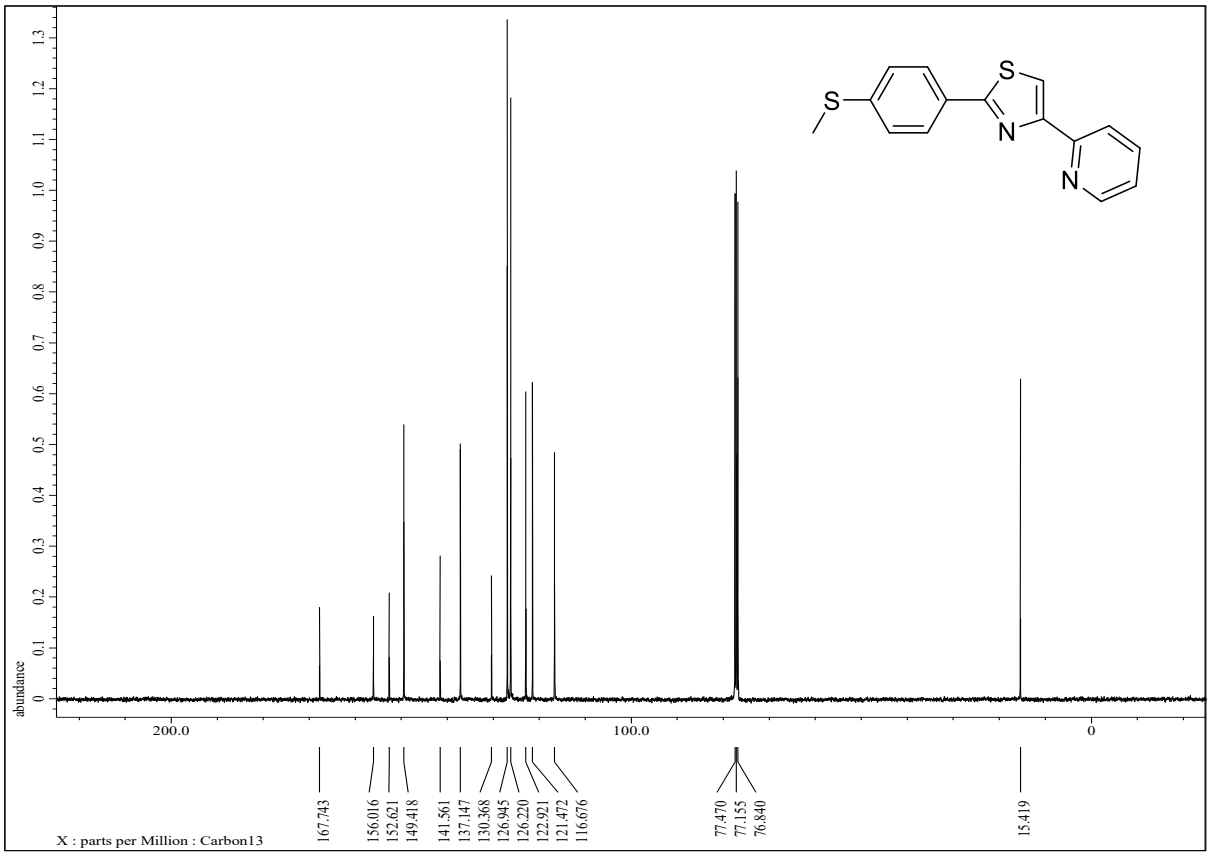

S
N
N
abundance
X : parts per Million : Proton

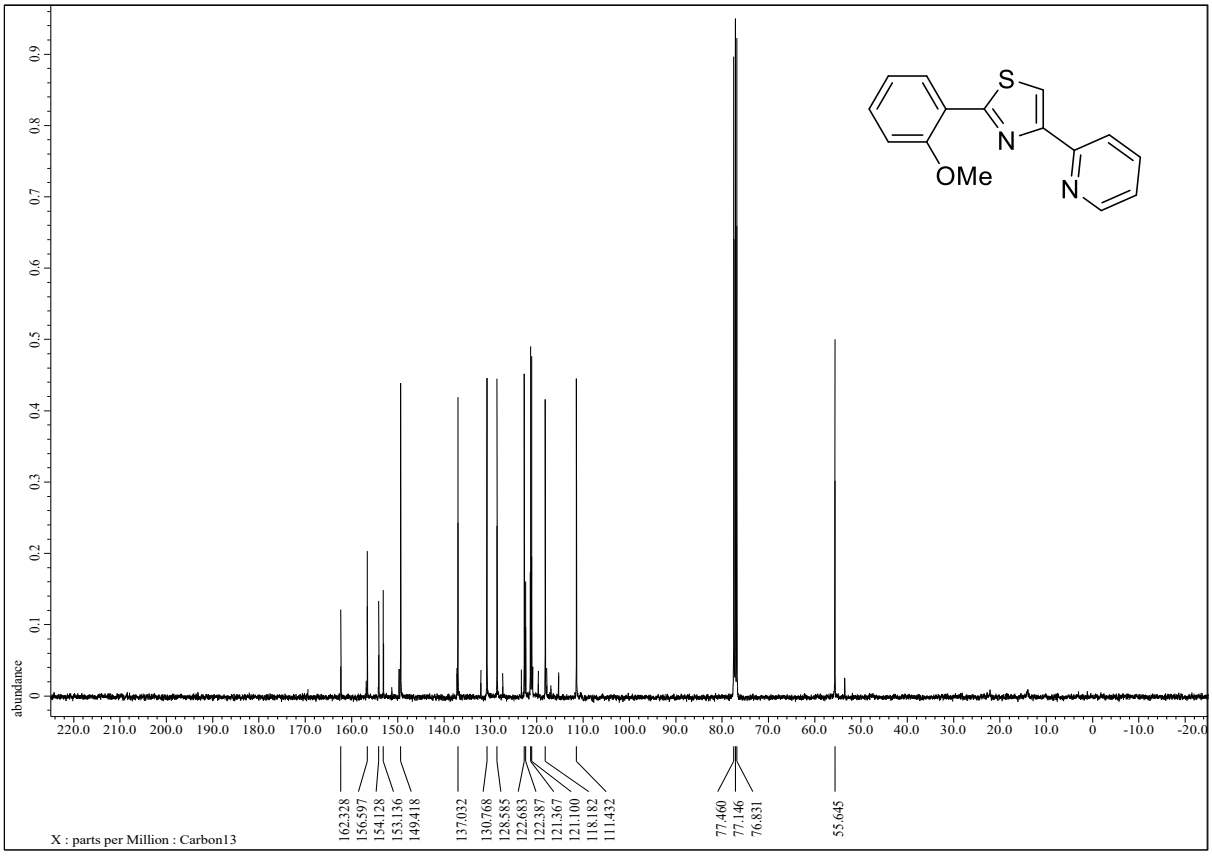
^{13}C NMR of 5-H Thiazoles

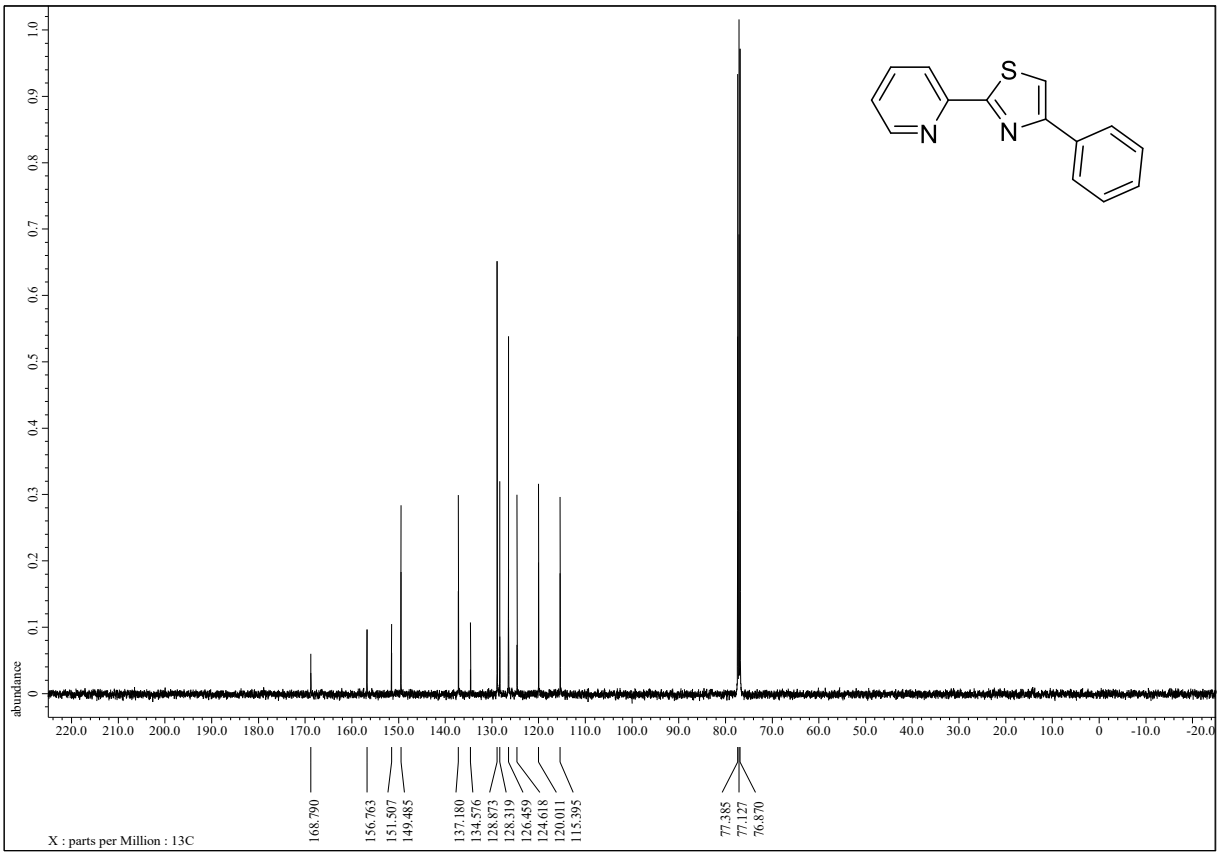





MeO
S
N
N
abundance
X : parts per Million : 13C
168.094
161.331
155.847
152.776
149.418
137.114
128.186
126.745
122.825
121.461
116.206
114.365
77.366
77.108
76.850
55.513


S
S
N
N
abundance
X : parts per Million : Carbon13
167.743
156.016
152.621
149.418
141.561
137.147
130.368
126.945
126.220
122.921
121.472
116.676
77.470
77.155
76.840
15.419


S
N
OMe
N
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
162.328
156.597
154.128
153.136
149.418
137.032
130.768
128.585
122.683
122.387
121.367
121.100
118.182
111.432
77.460
77.146
76.831
55.645
X : parts per Million : Carbon13


S
N
N
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
168.790
156.763
151.507
149.485
137.180
134.576
128.873
128.319
126.459
124.618
120.011
115.395
77.385
77.127
76.870
X : parts per Million : 13C