Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

One-Pot Synthesis of 1,2,3-Triazoles from Boronic Acids in Water Using Cu(II)-β-Cyclodextrin Complex as a Nanocatalyst

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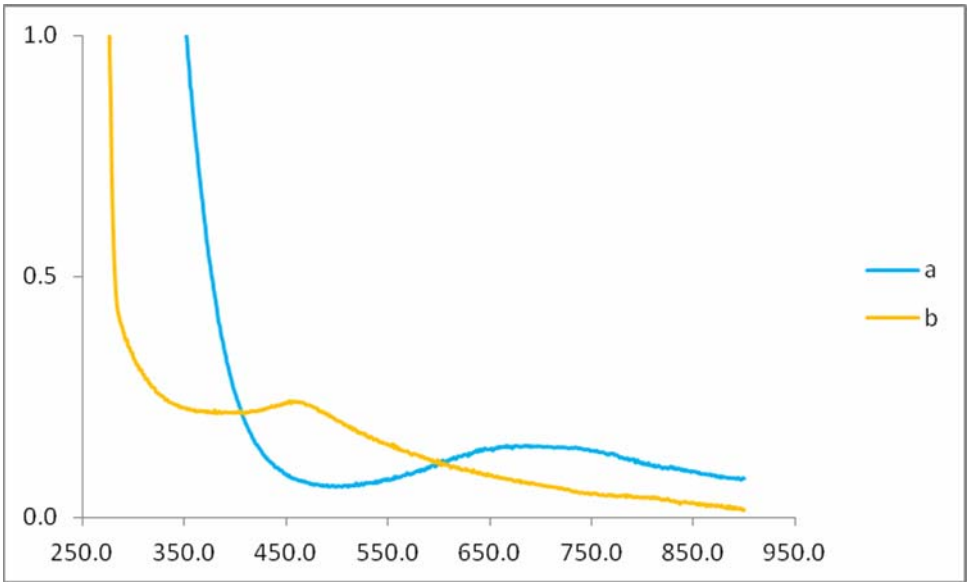
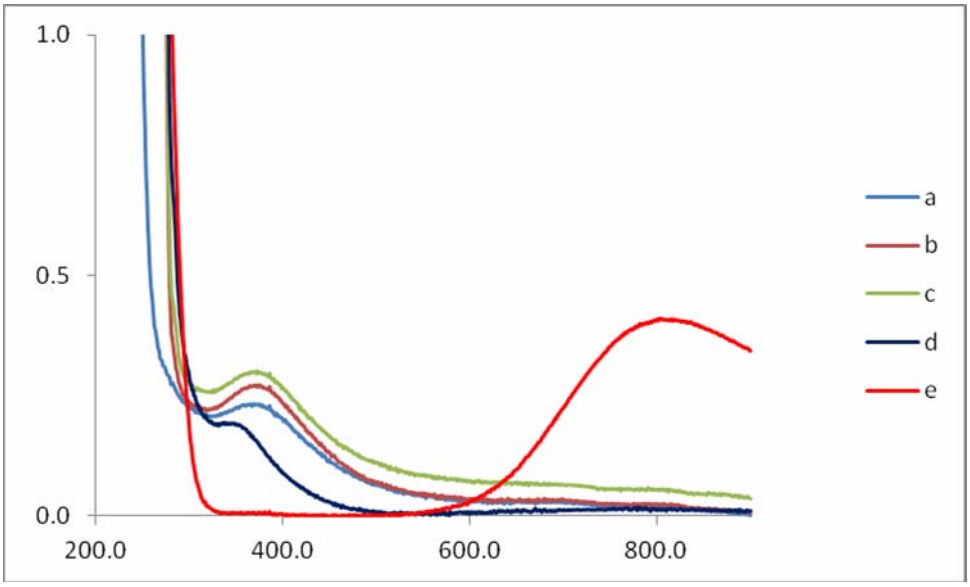
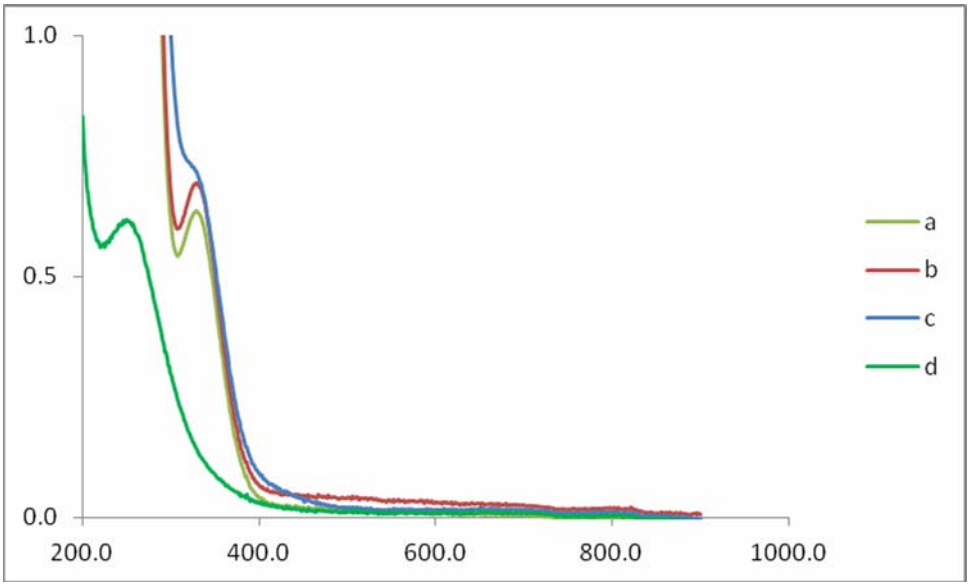


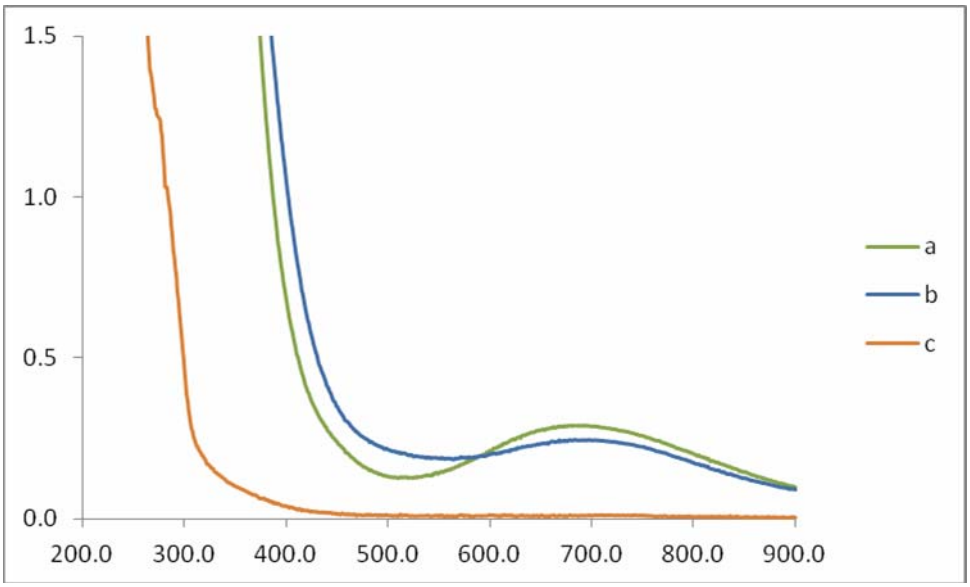
Spectral properties (UV-vis spectra in cell 1 cm) of Cu_2-β-CD in aqueous solution. a) [Cu_2-β-CD] = 0.006 M in aqueous solution. b) [Cu_2-β-CD] = 0.006 M in aqueous solution containing 0.12 M of phenylboronic acid (according to the literature, reference 18, the peak in near 450 nm is for arylcopper intermediate).



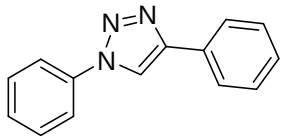
a) a) $CuSO_4$ 0.0006 M plus 60 eq NaN_3 b) $CuSO_4$ 0.0006 M, NaN_3 0.018 M and phenylboronic acid 0.0012 M c) $CuSO_4$ 0.0006 M, NaN_3 0.018 M, phenylboronic acid 0.0012 M and β-CD 0.001M d) Cu_2β-CD 0.0006 M,NaN_3 0.018 M and phenylboronic acid 0.012 M e) $CuSO_4$ 0.3 M in 0.1 cm UV cell



a) 3-Nitro phenyl azide ($3*10^{-3}$)(EtOH:H_2O 1:1). b) 3-nitro phenyl azide ($3*10^{-3}$ M) in the presence of cyclodextrin 0.003 M(H_2O: EtOH 1:1). c) 3-nitro phenyl azide ($3*10^{-3}$ M) in the presence of cyclodextrin copper complex 0.003 M (H_2O: EtOH 1:1). d) Cu_2CD 0.0006 M solution cell 0.1 cm



a) Cu_2CD 0.01 M solution b) Cu_2CD 0.01 M, NaN_3 0.6 M and phenyl boronic acid 0.2 M solution after 4 h (reaction mixture was filtrated to obtain a clear solution and its UV spectra surprisingly show Cu_2CD has retained his primer structure and almost concentration) c) 50 fold diluted solution of b in UV cell 0.1 cm



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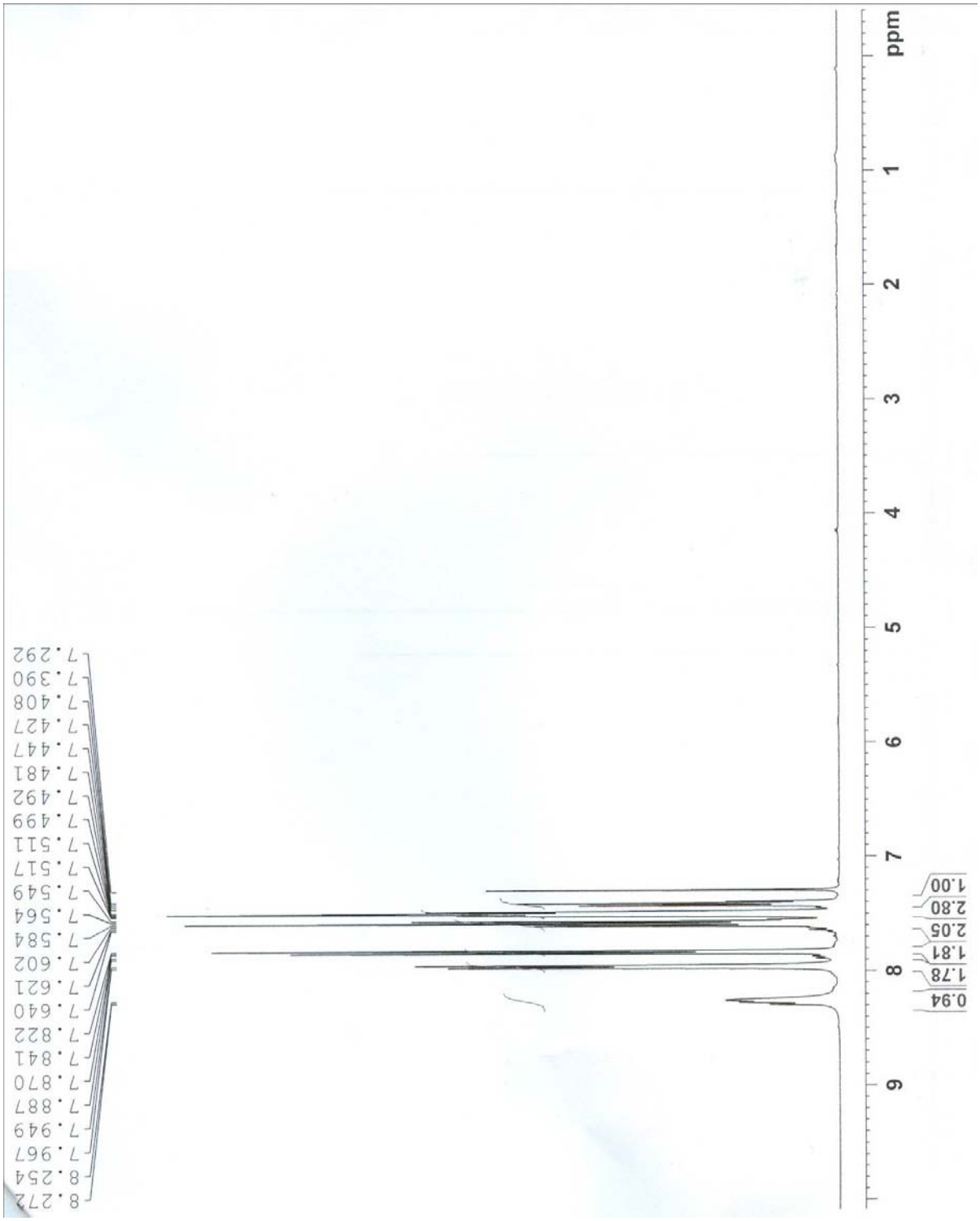

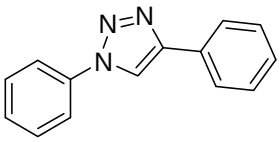

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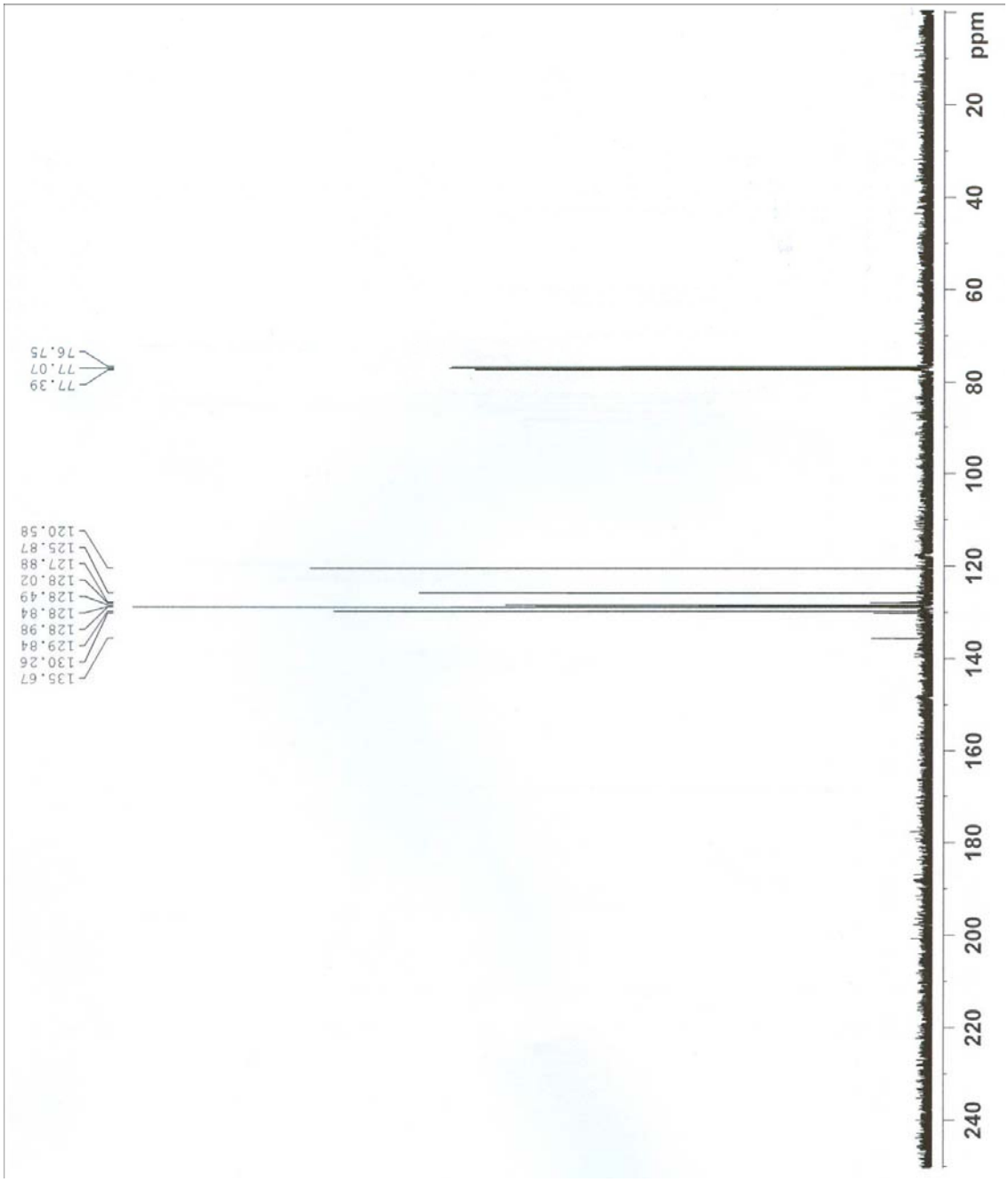

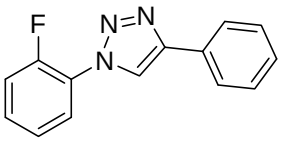

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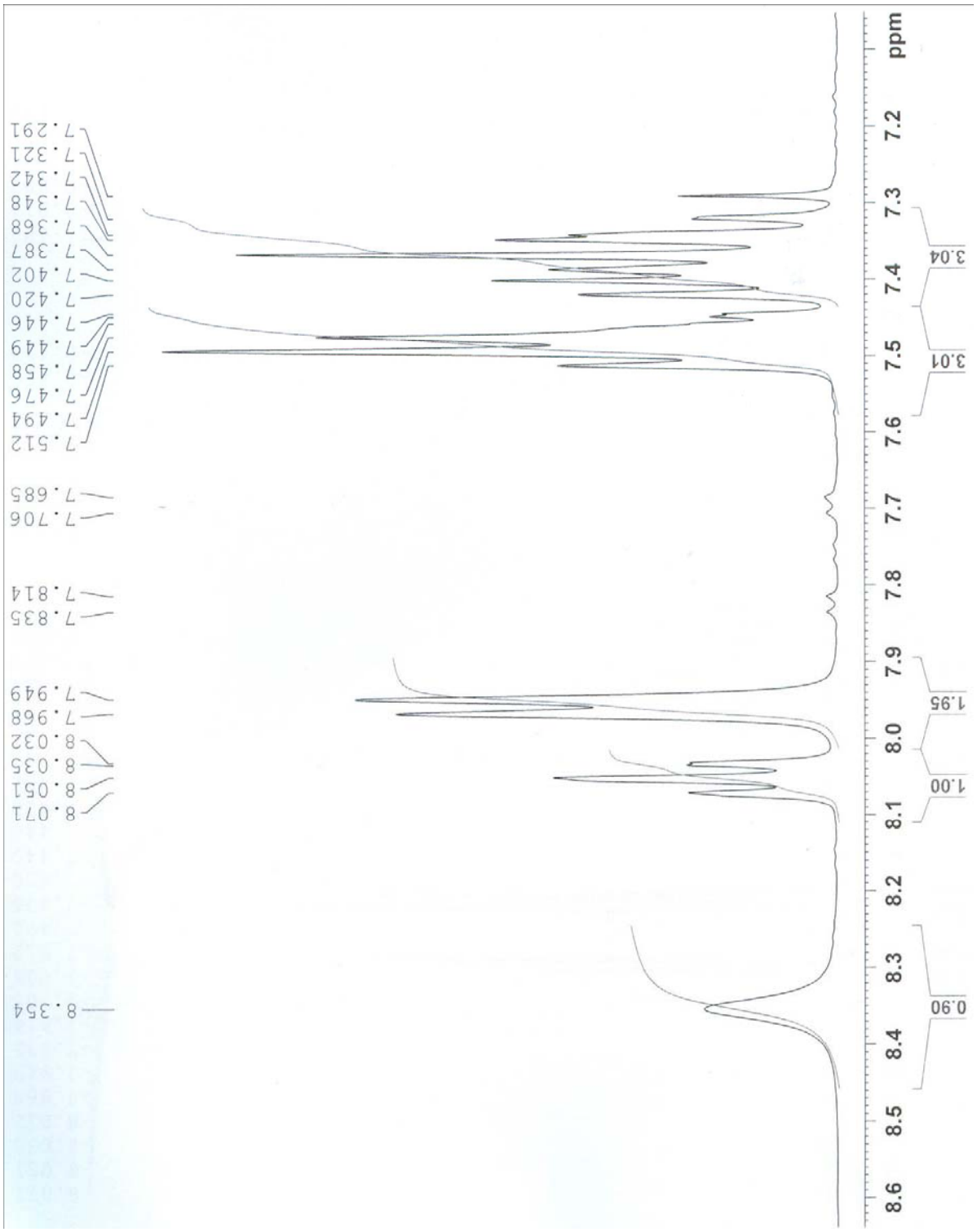

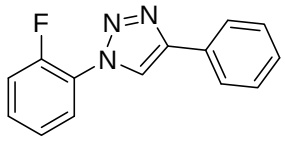
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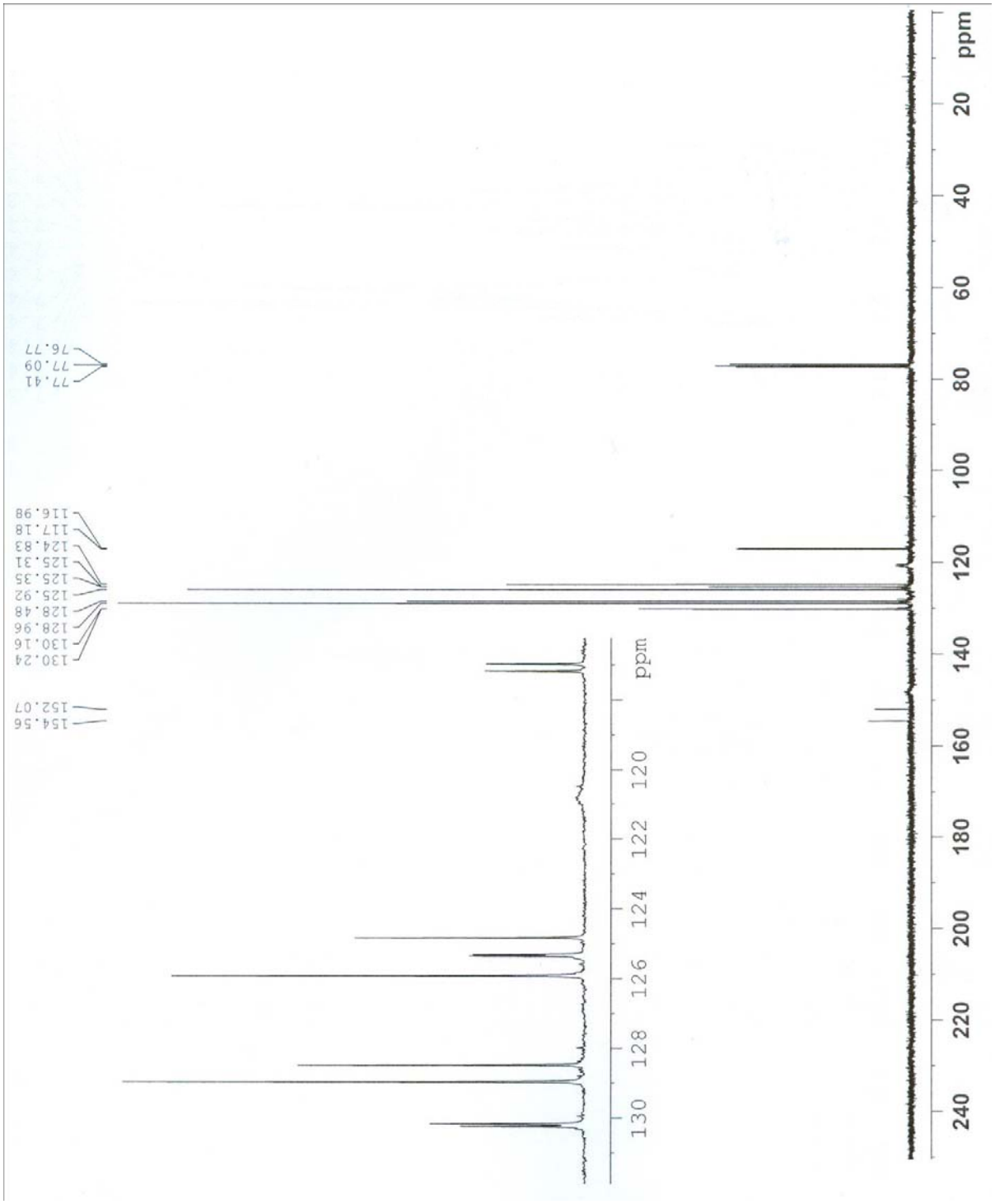
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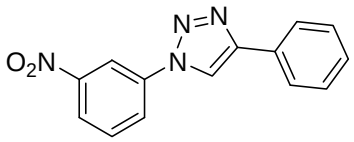

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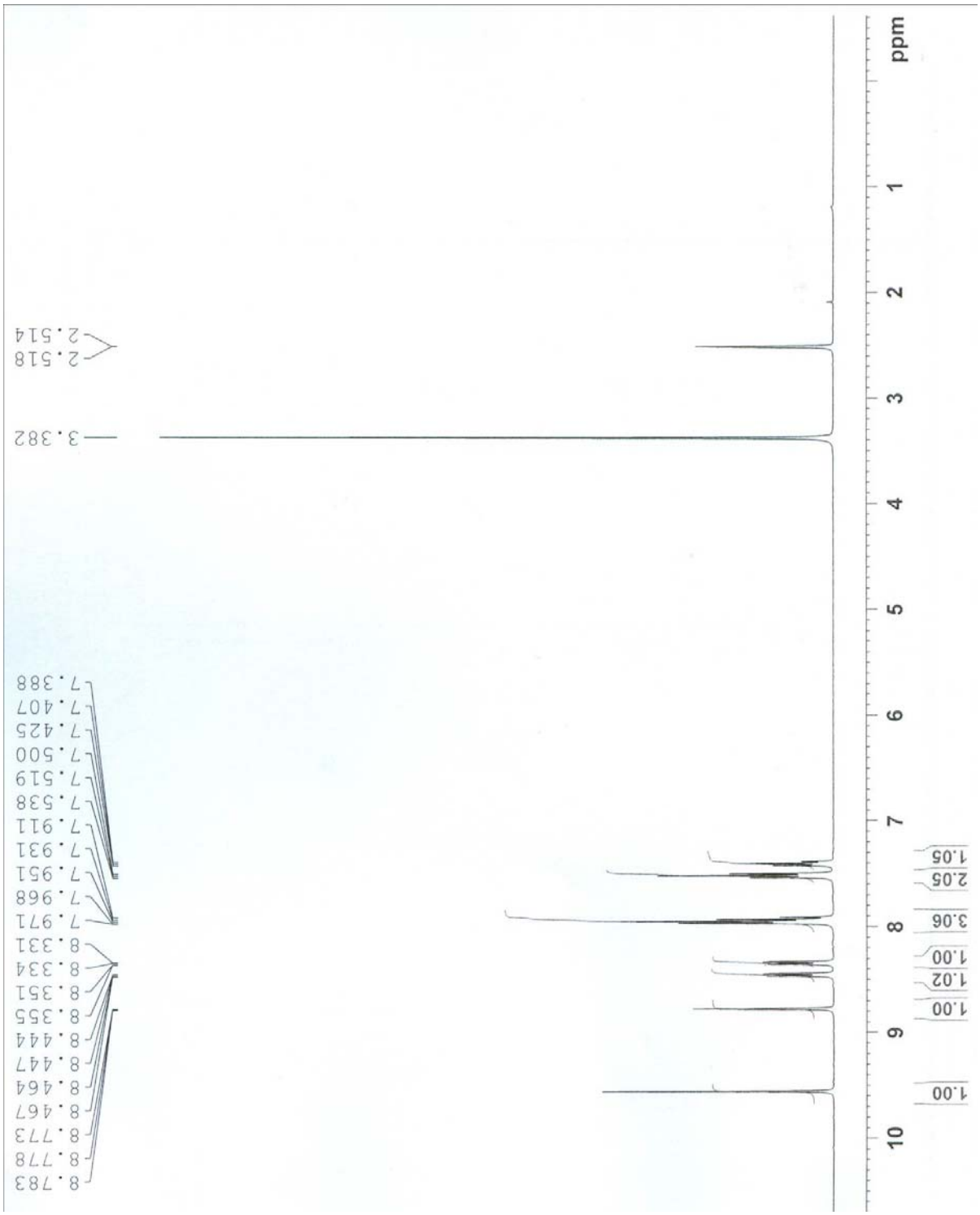

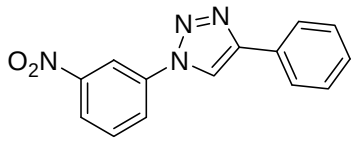

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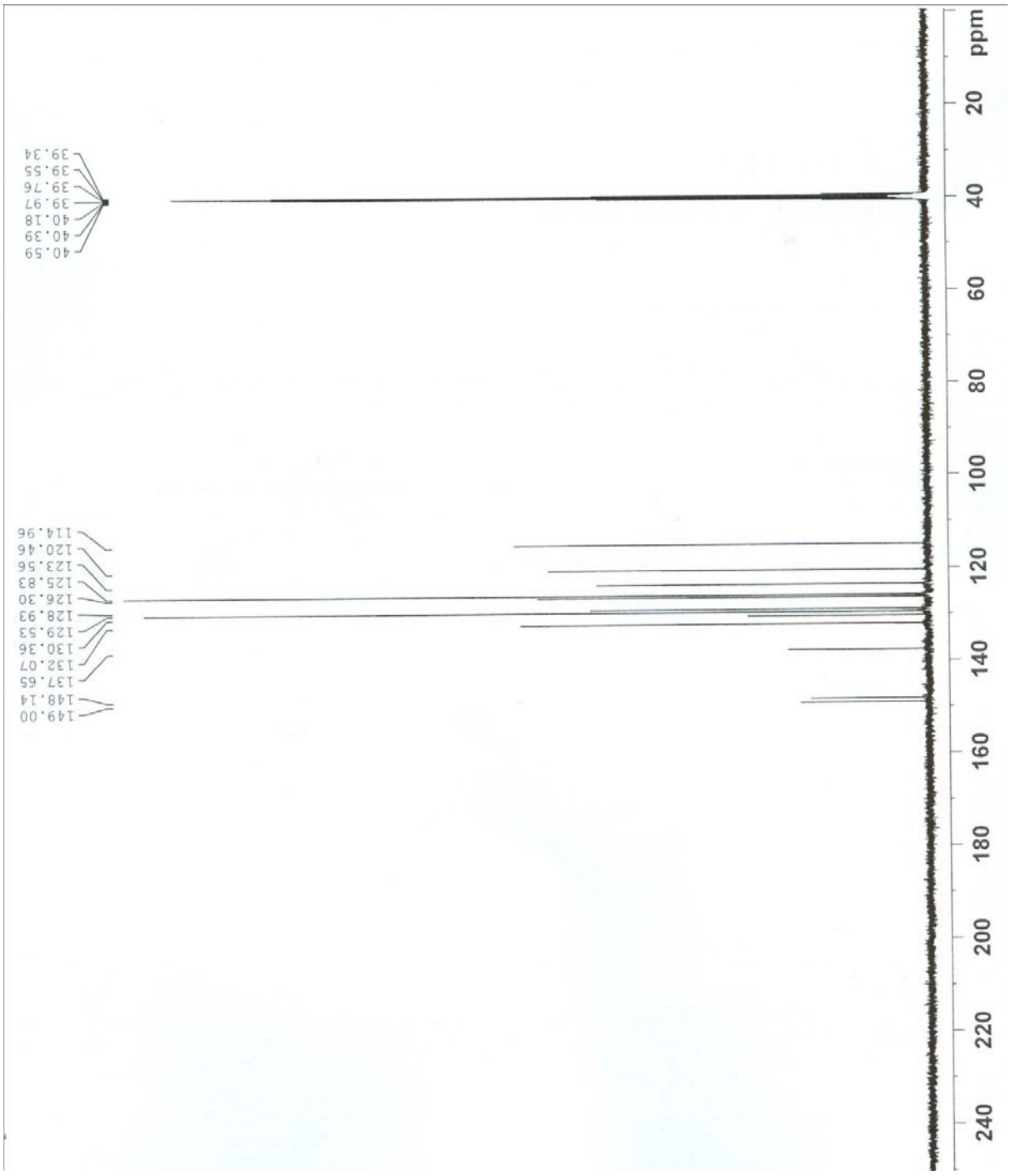
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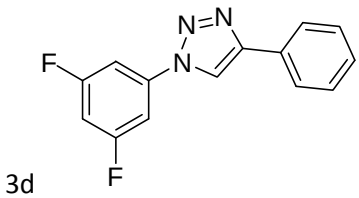
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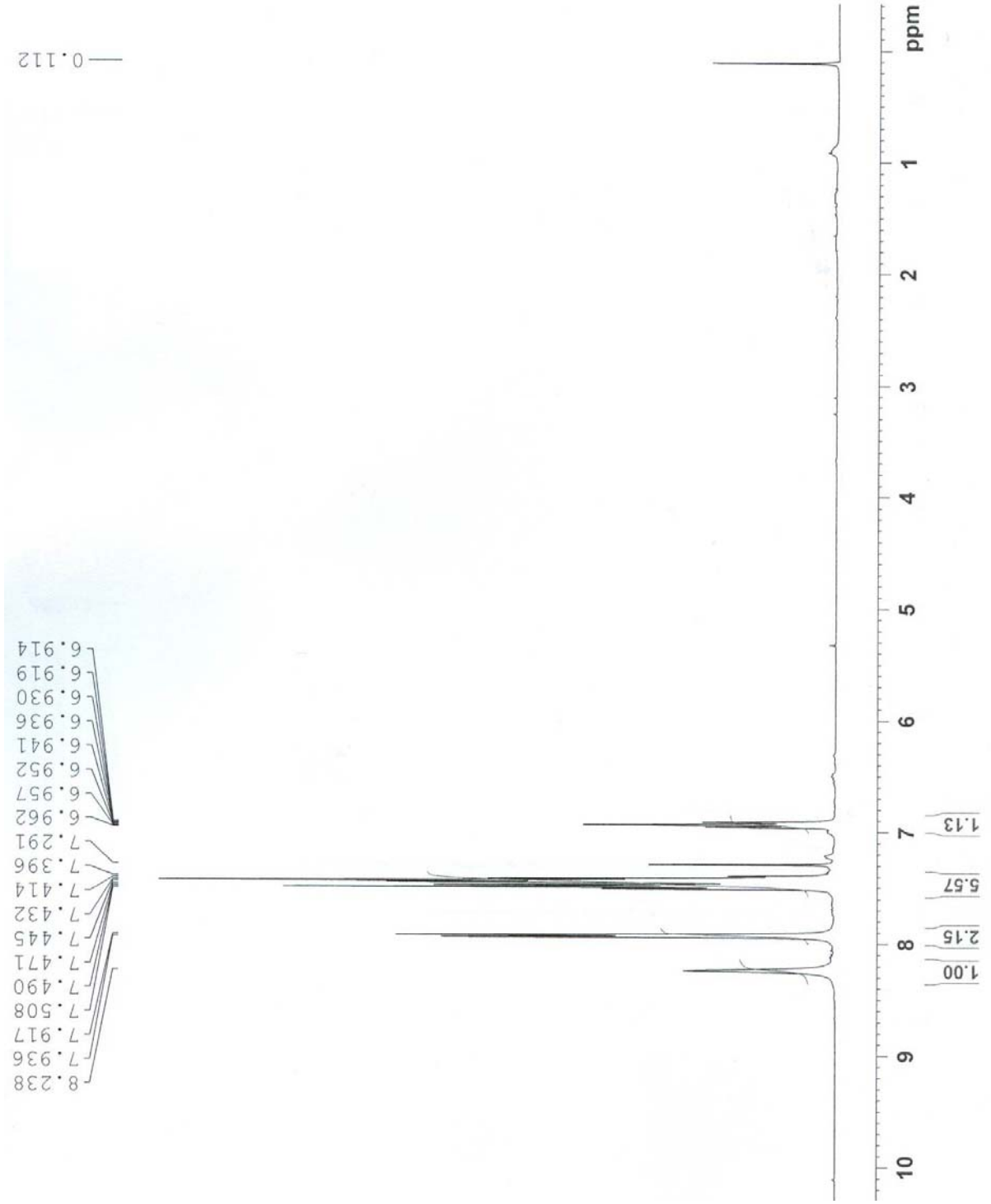
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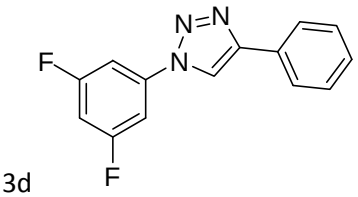

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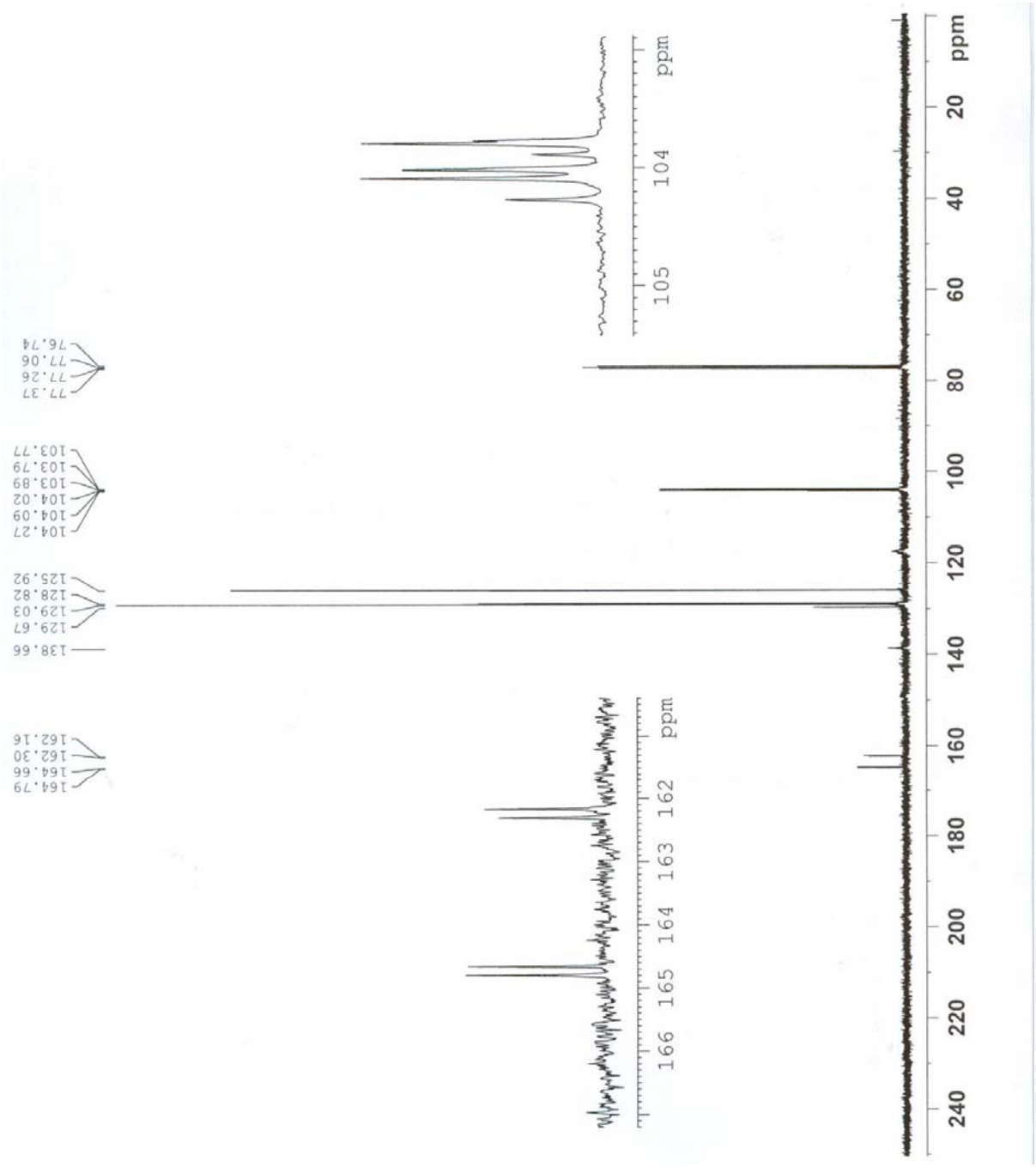

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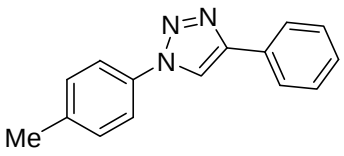

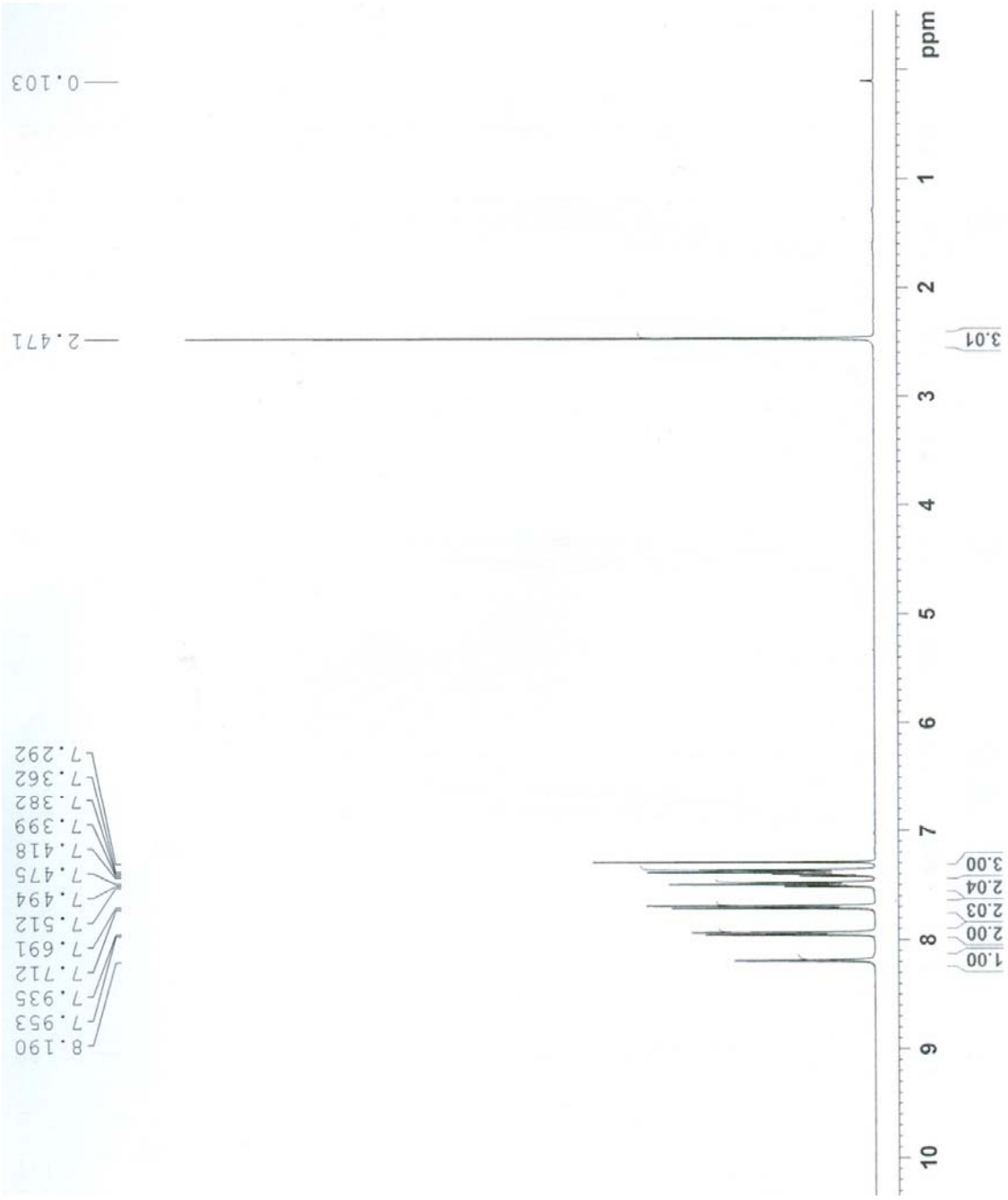

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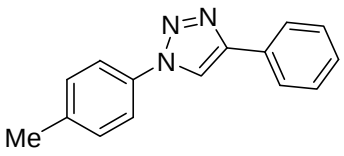

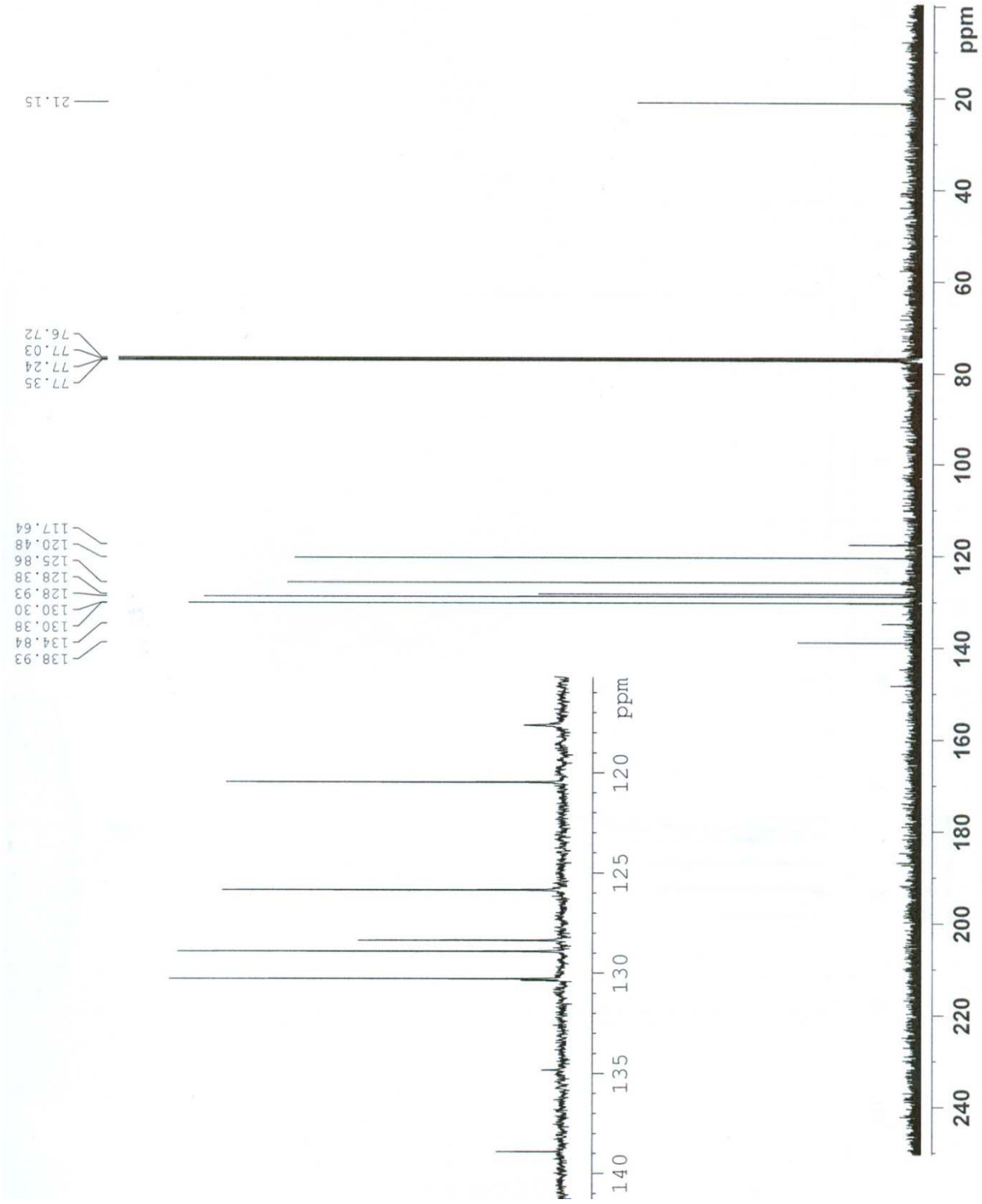

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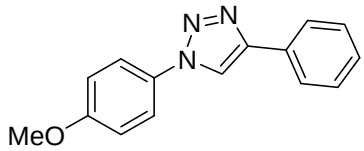
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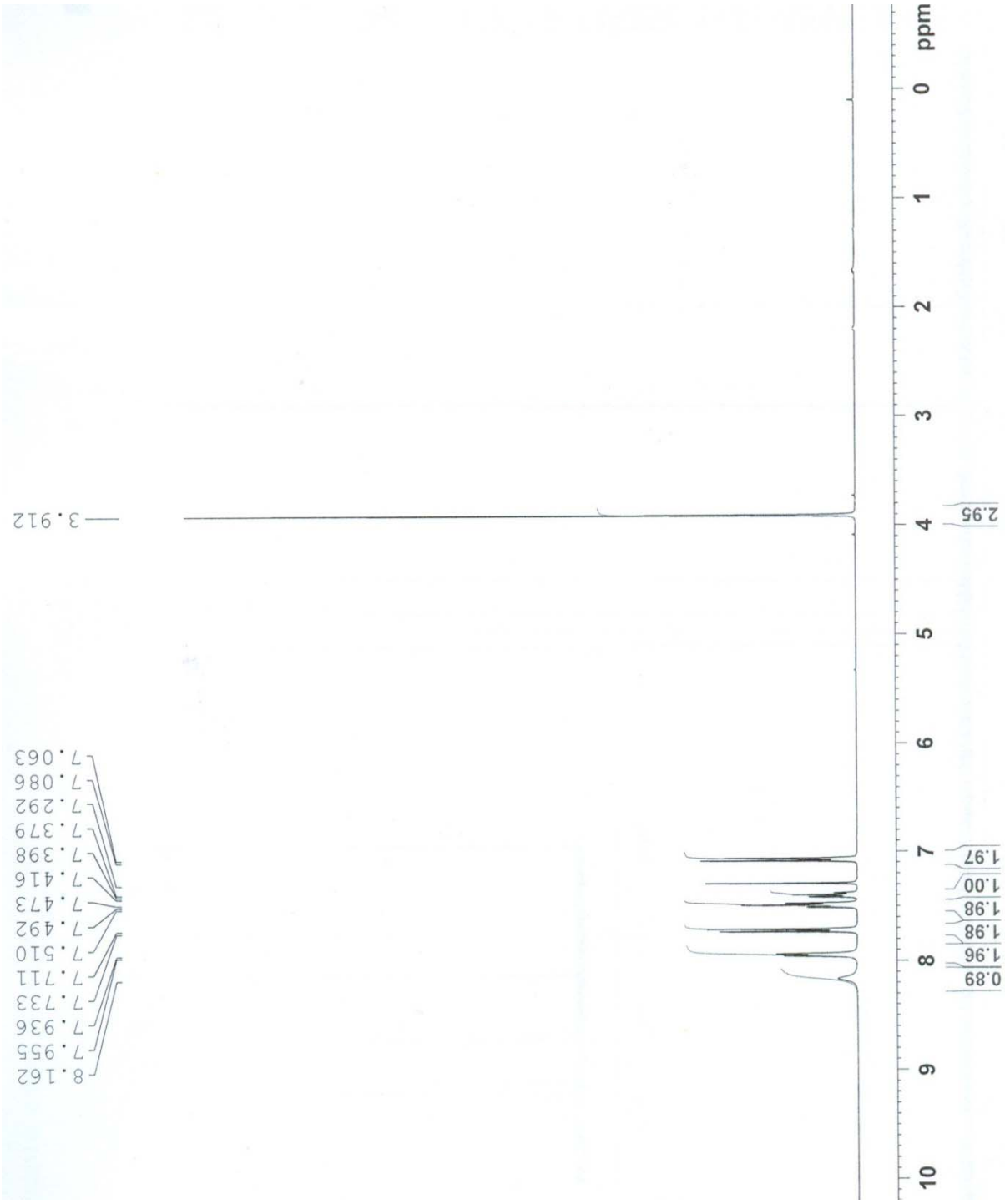
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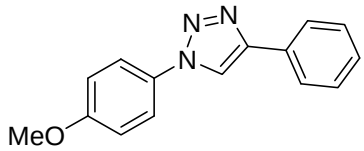
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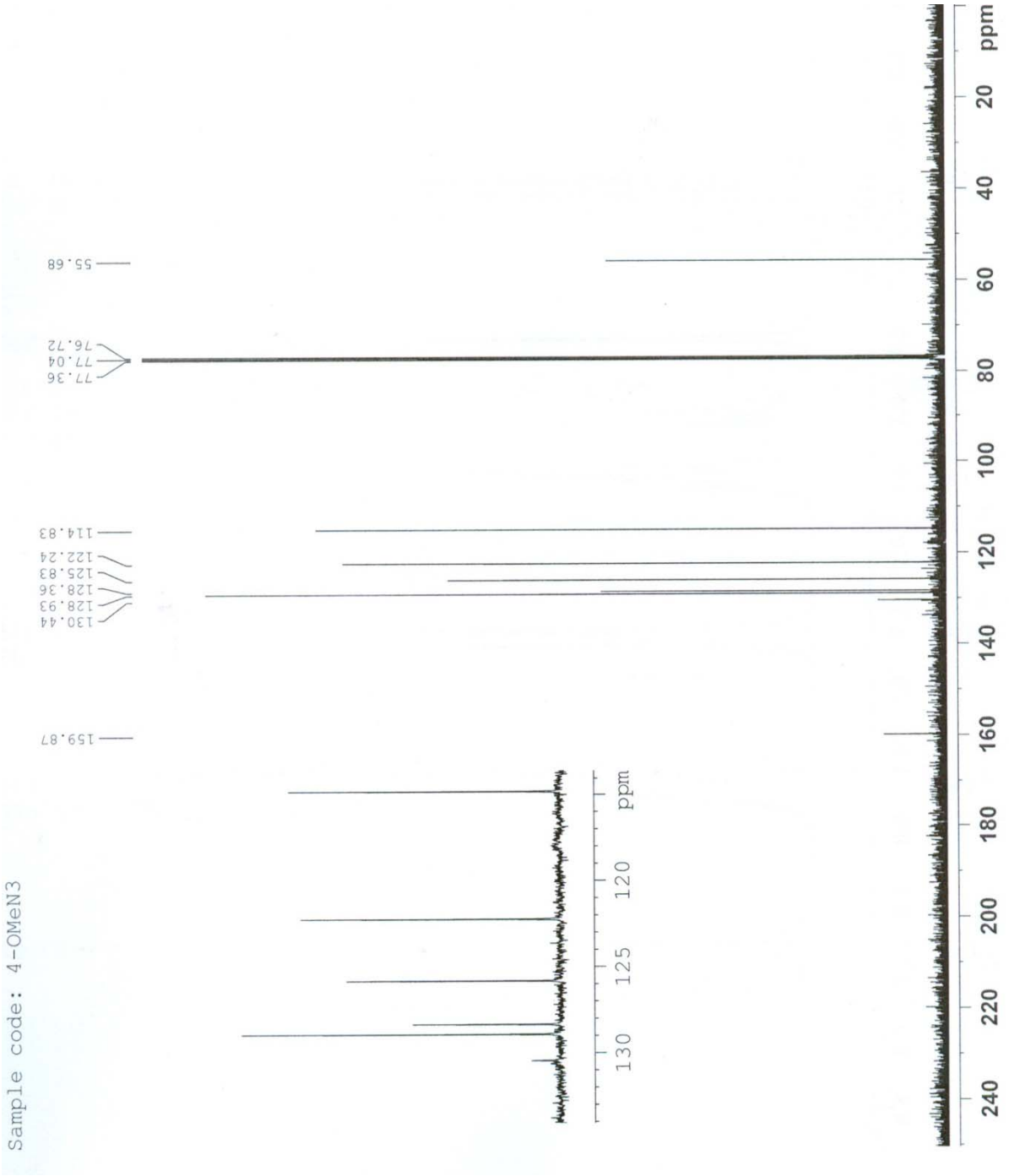
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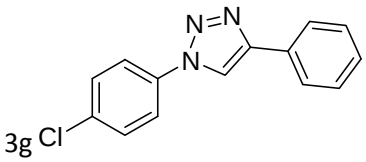

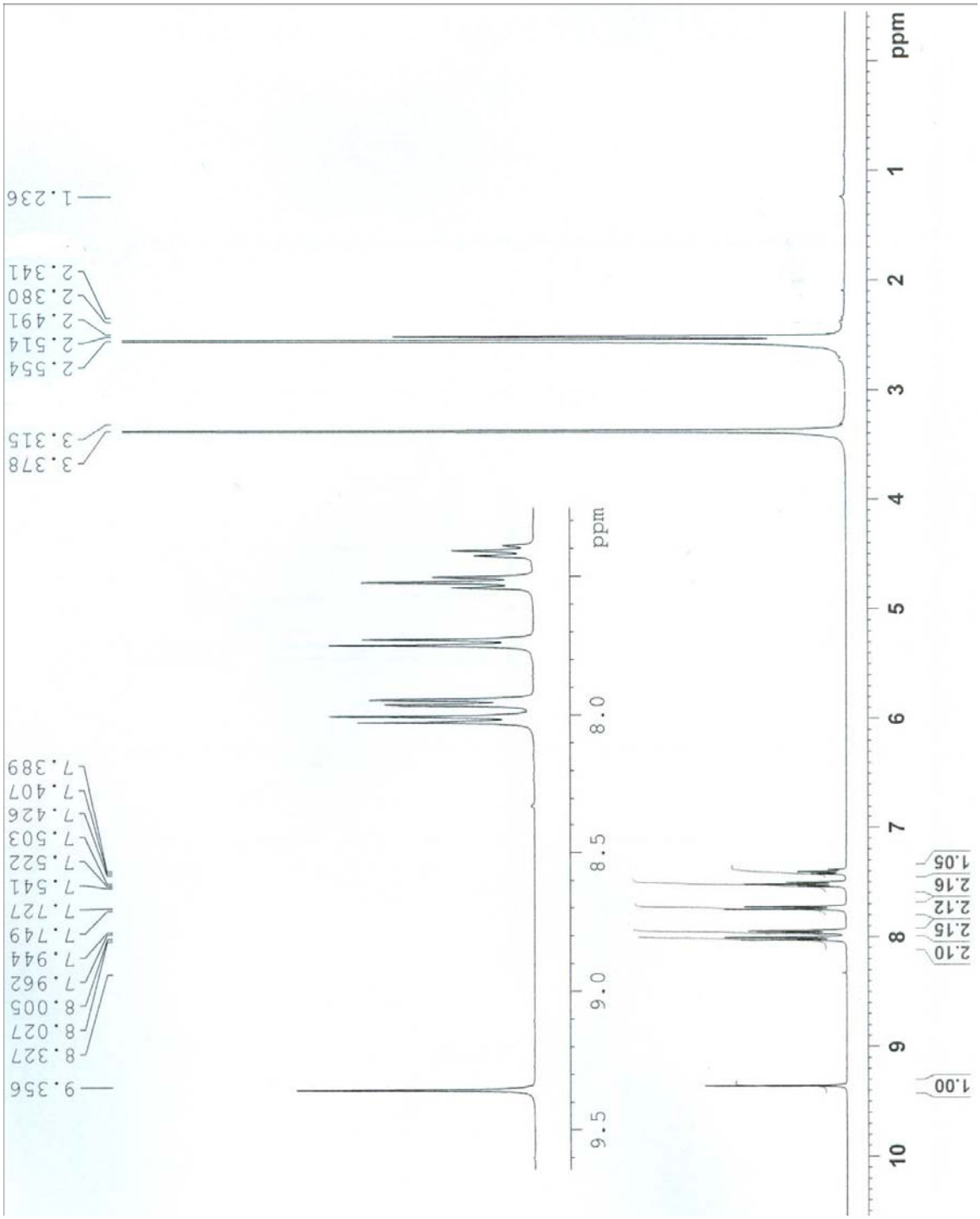

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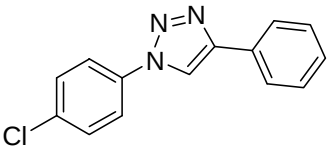
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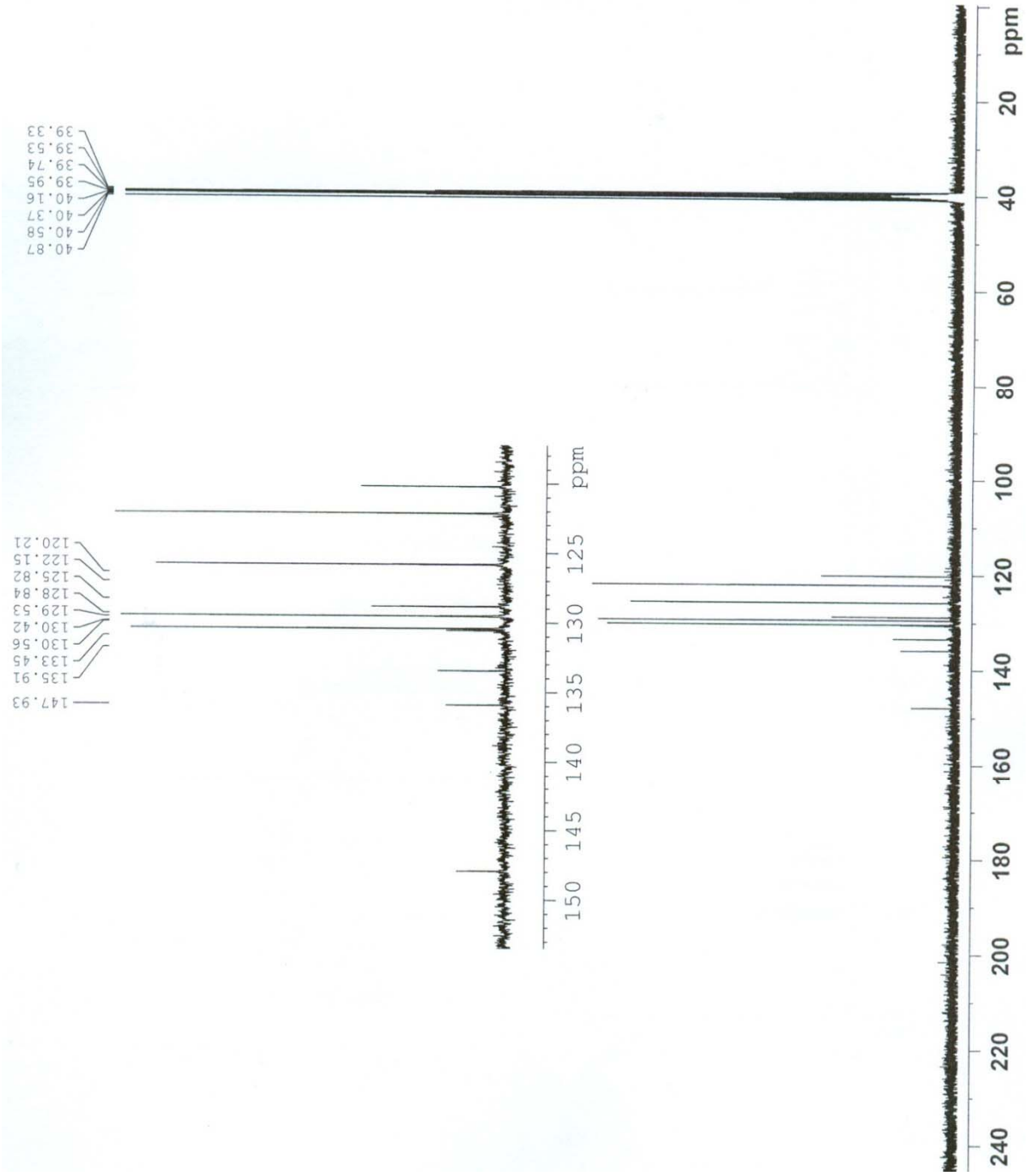
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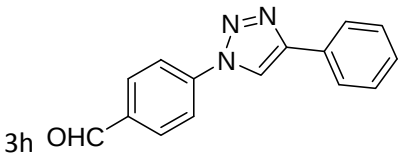

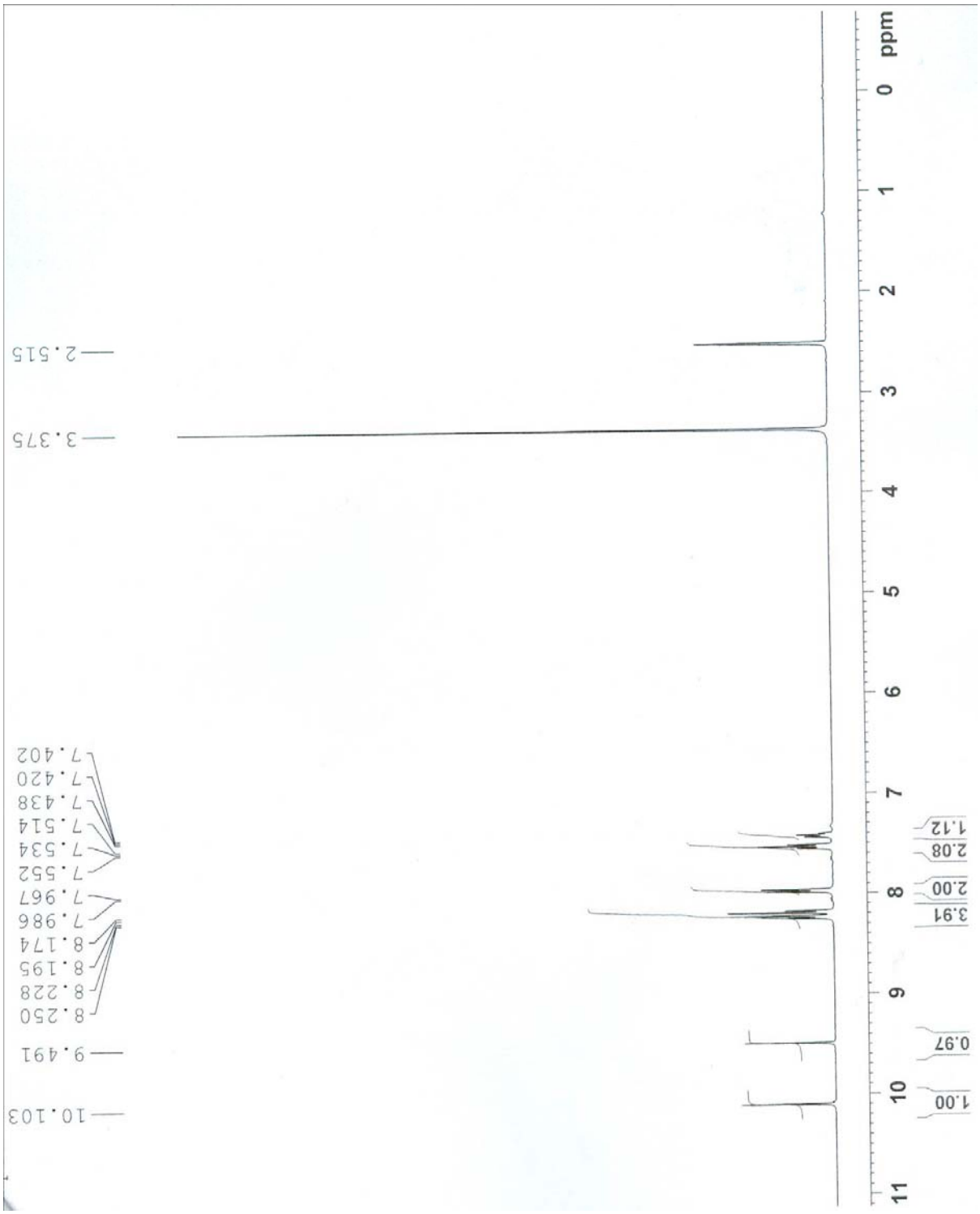

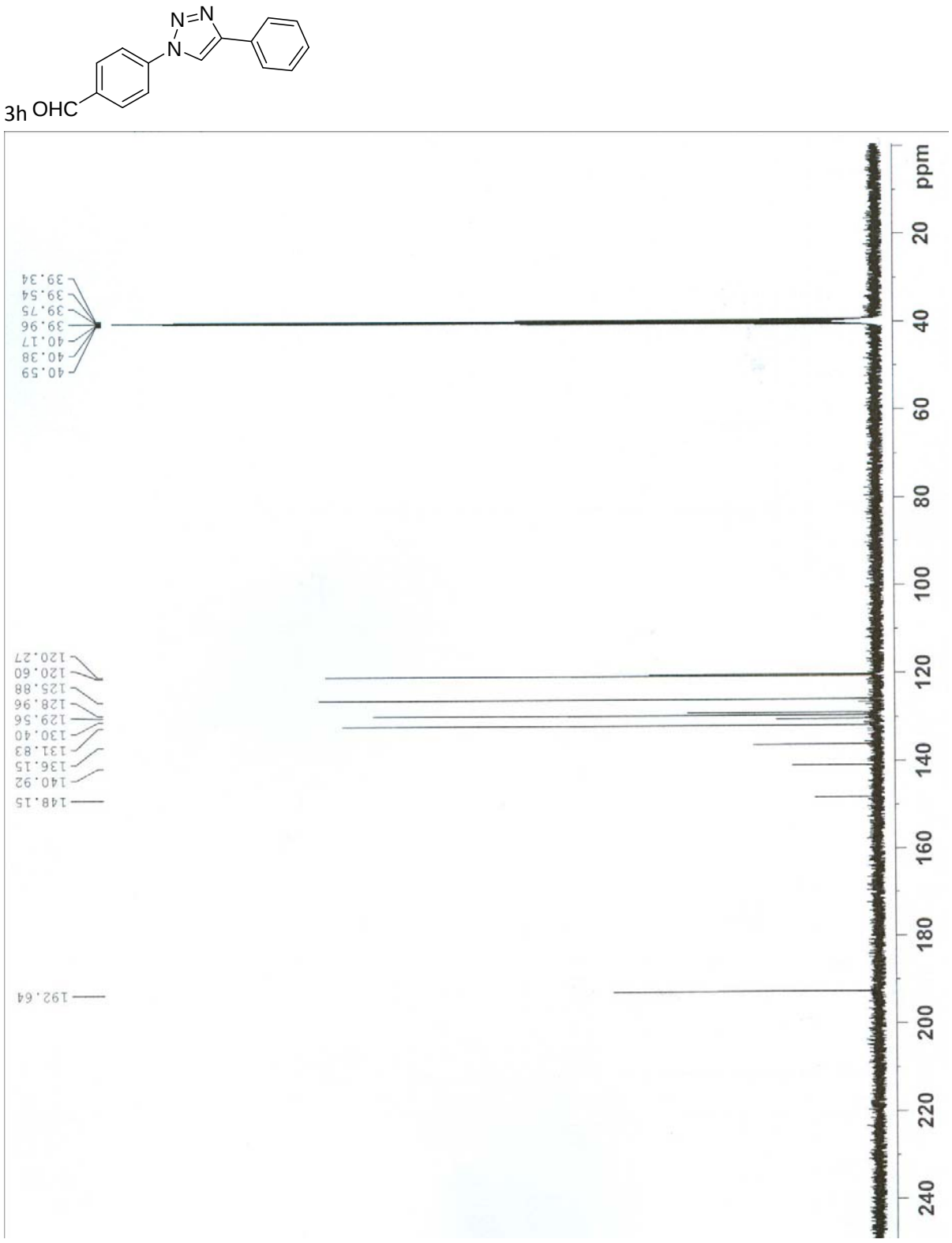
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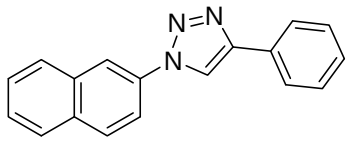

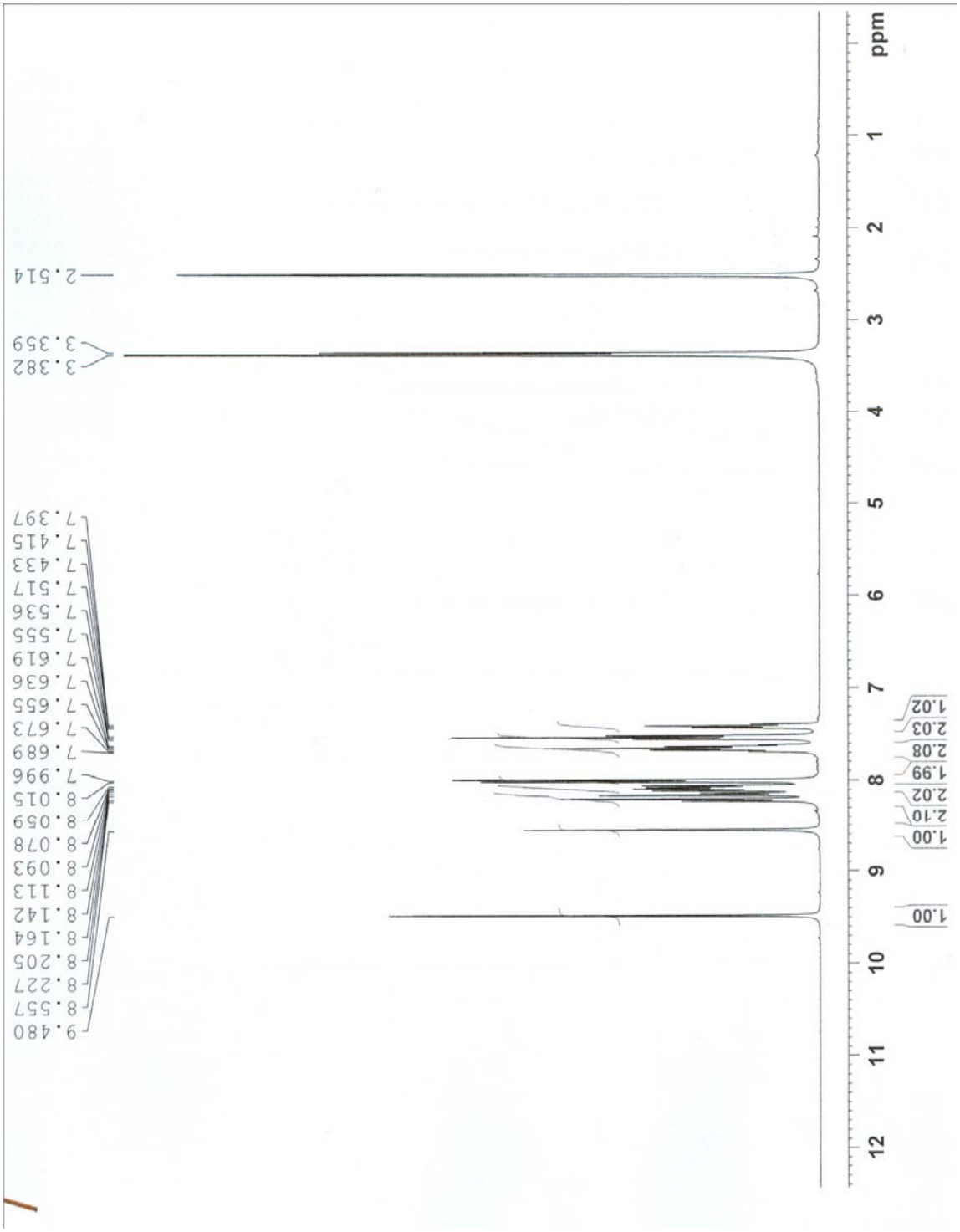

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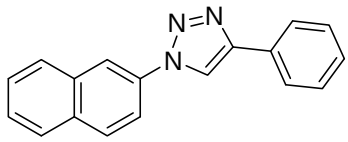

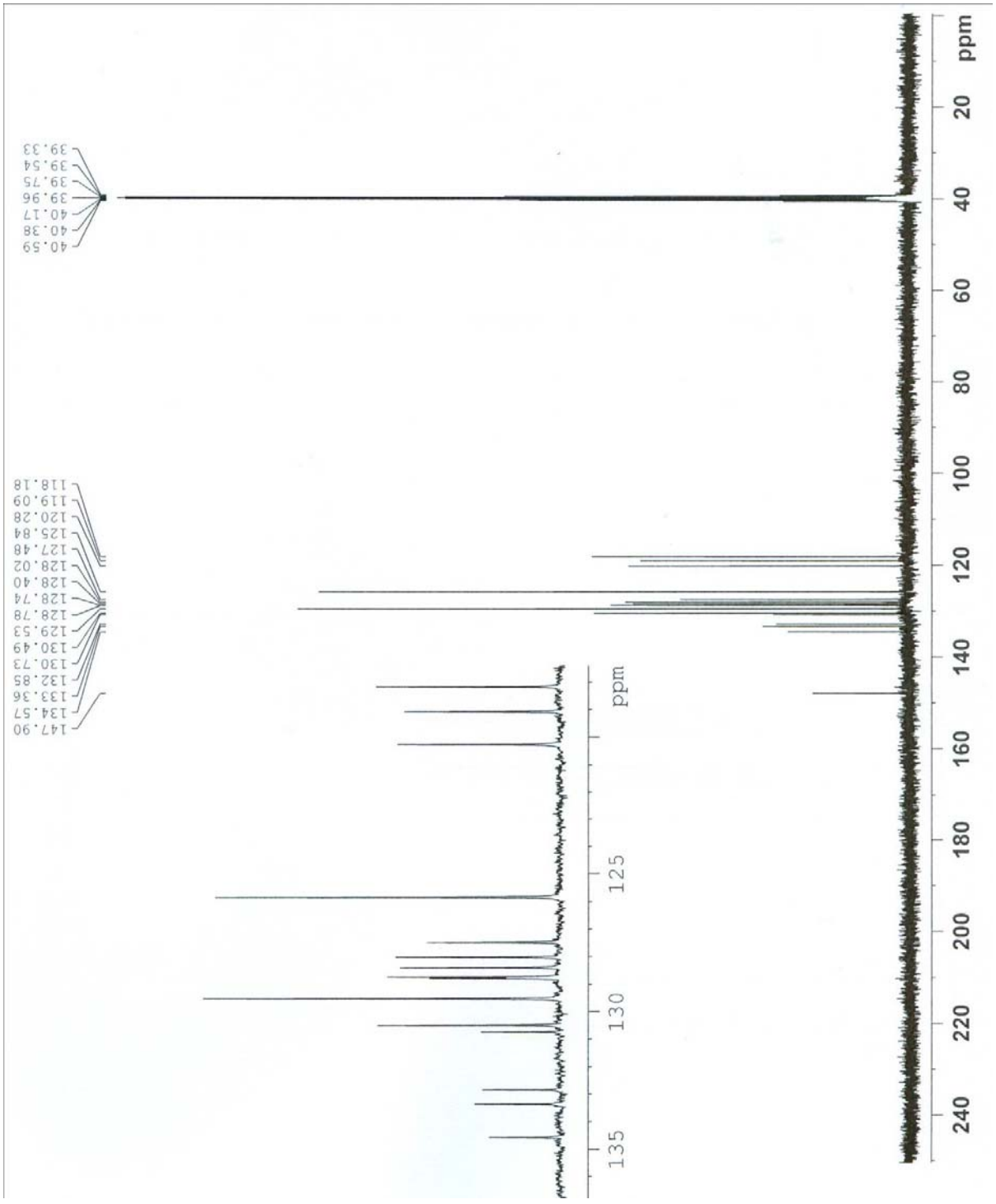

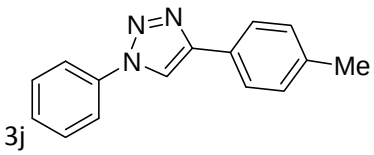

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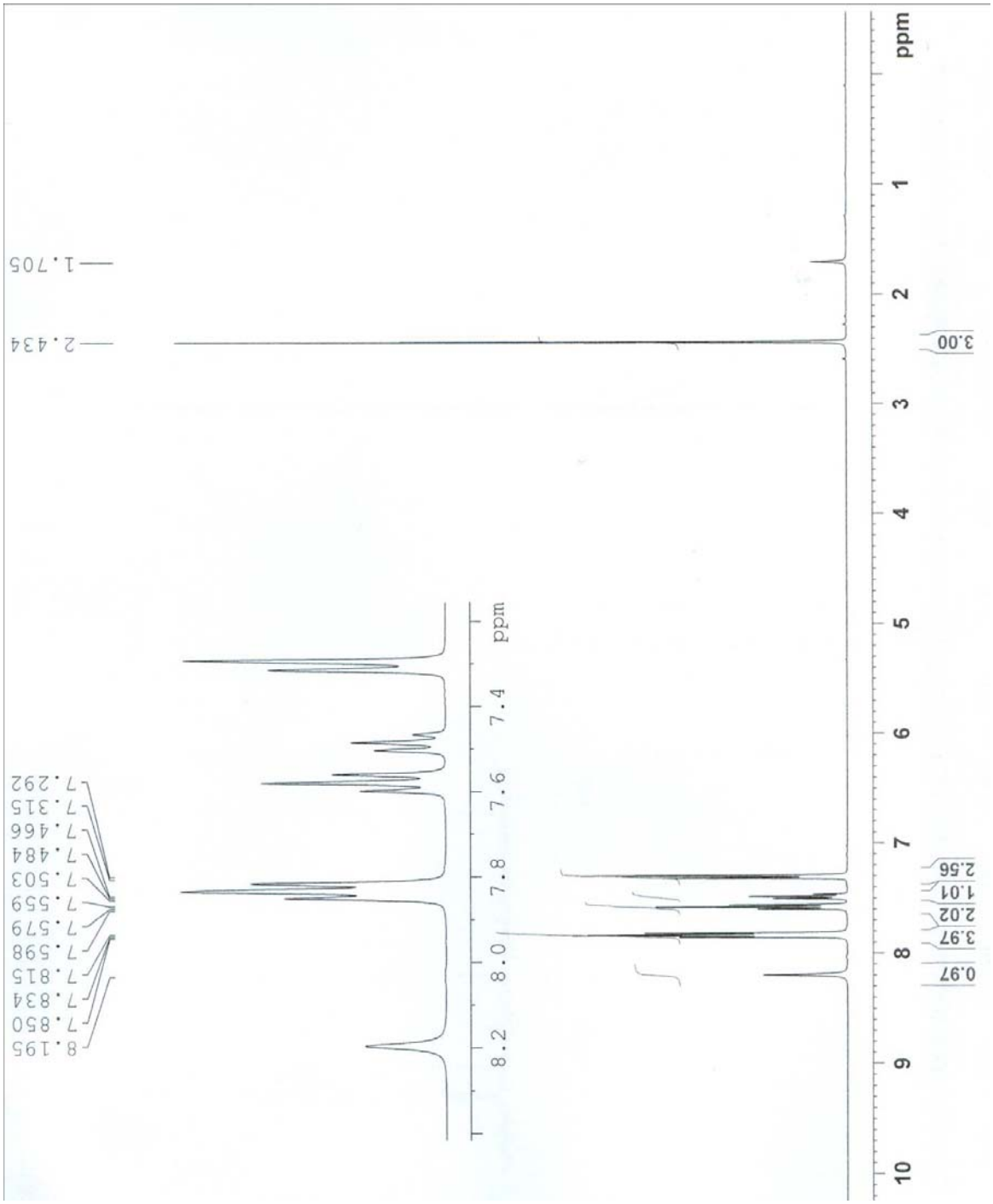

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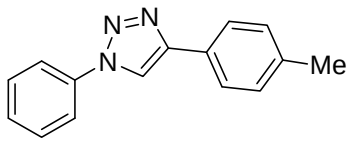
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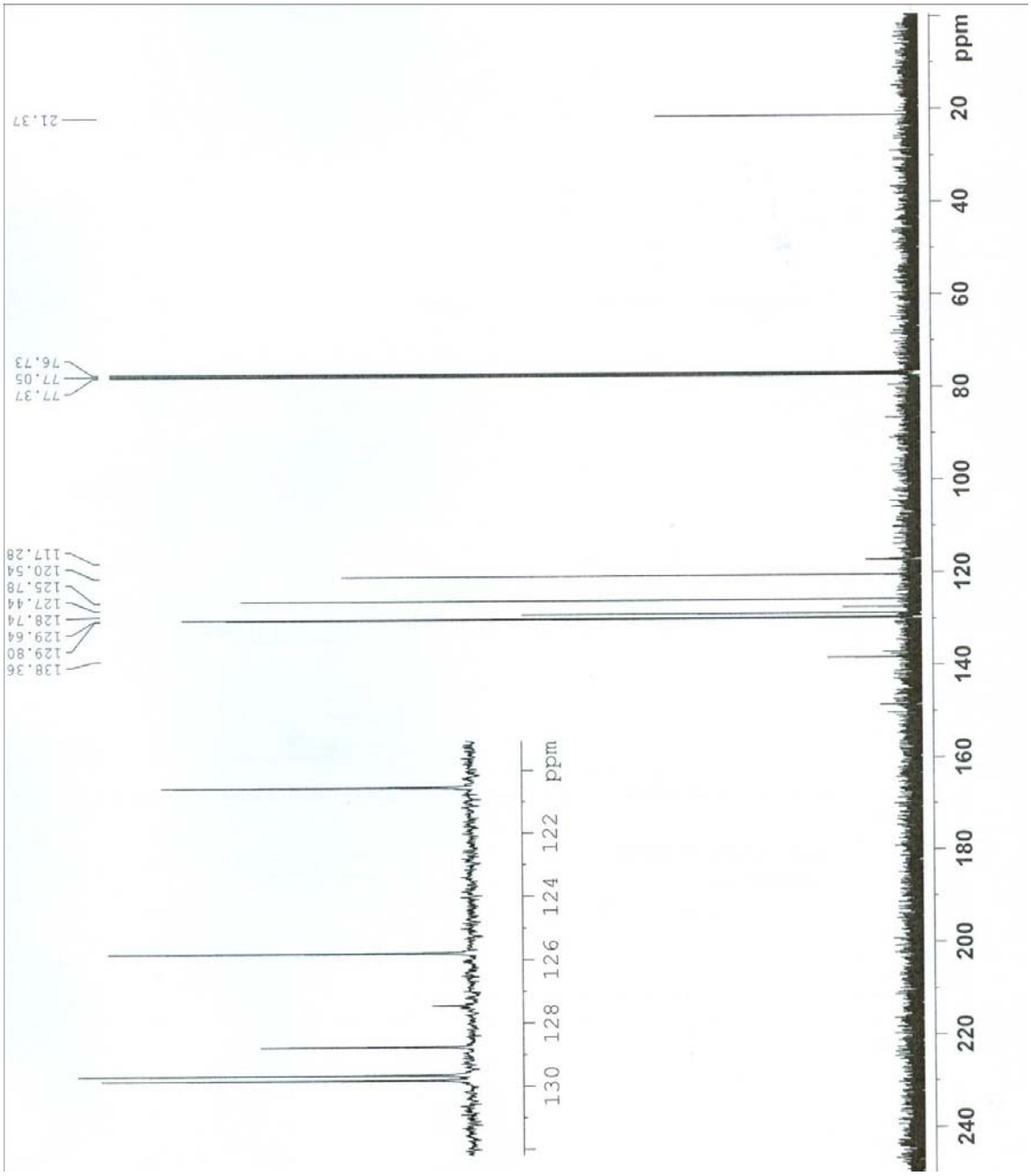
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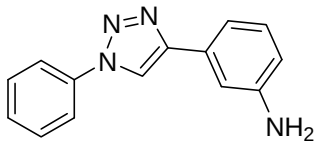

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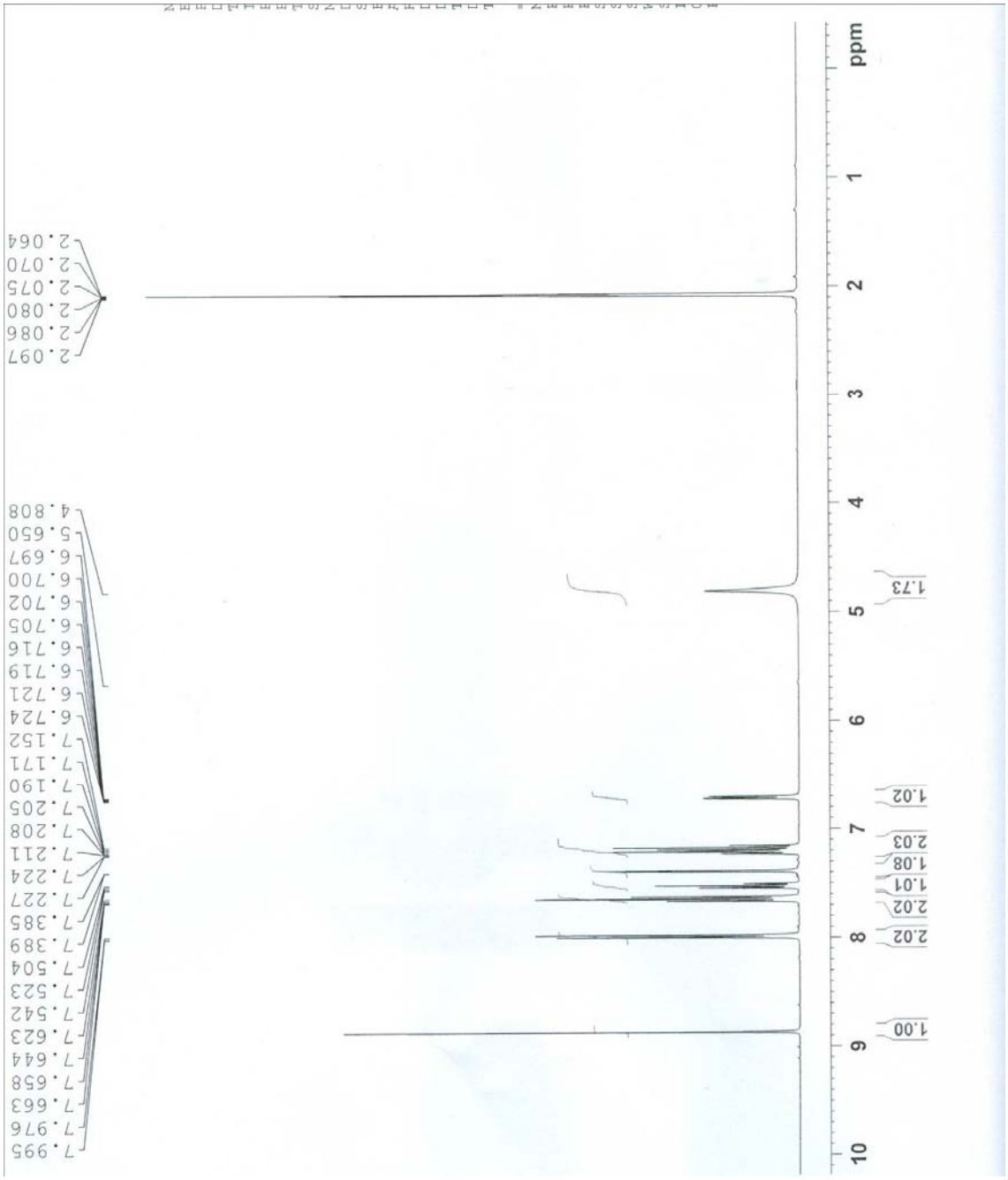

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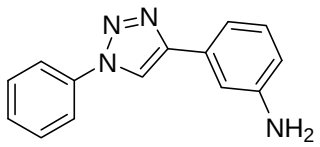
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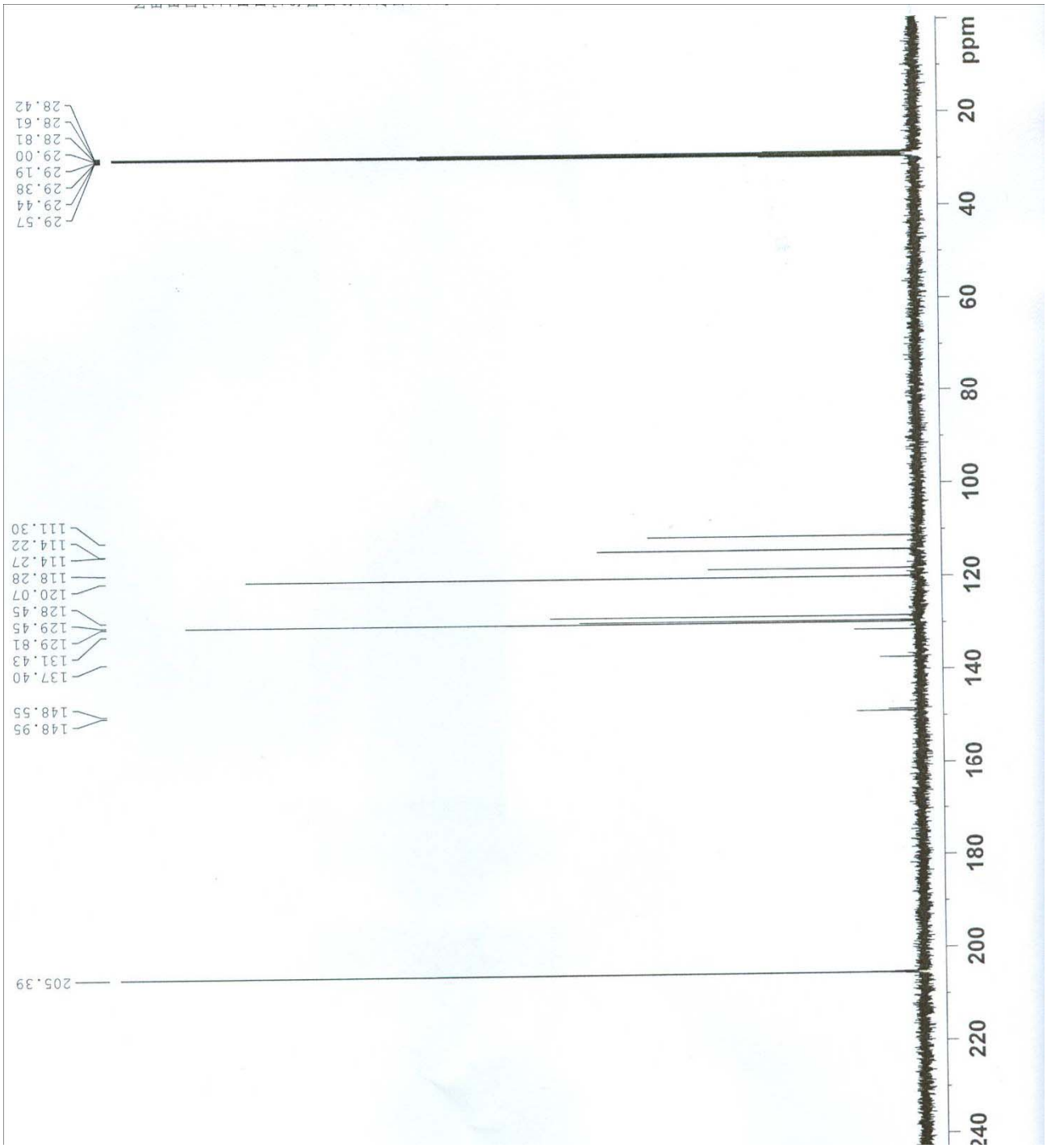
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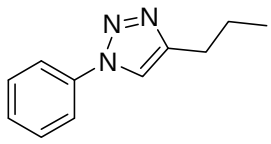
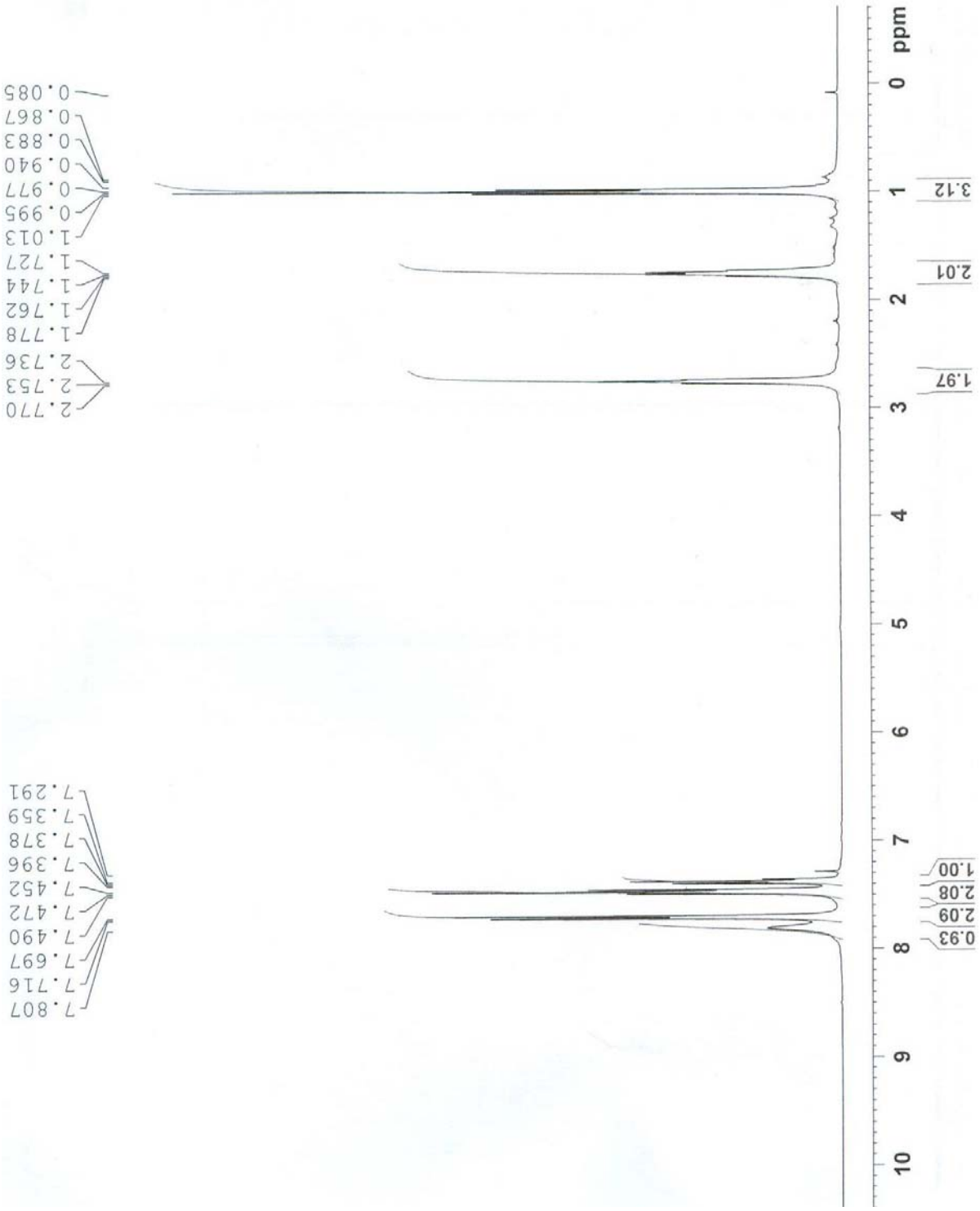
129.45
129.81
131.43
137.40
148.55
148.95
205.39
ppm
20
40
60
80
100
120
140
160
180
200
220
240

3l

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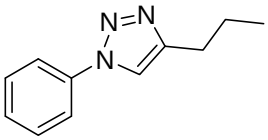
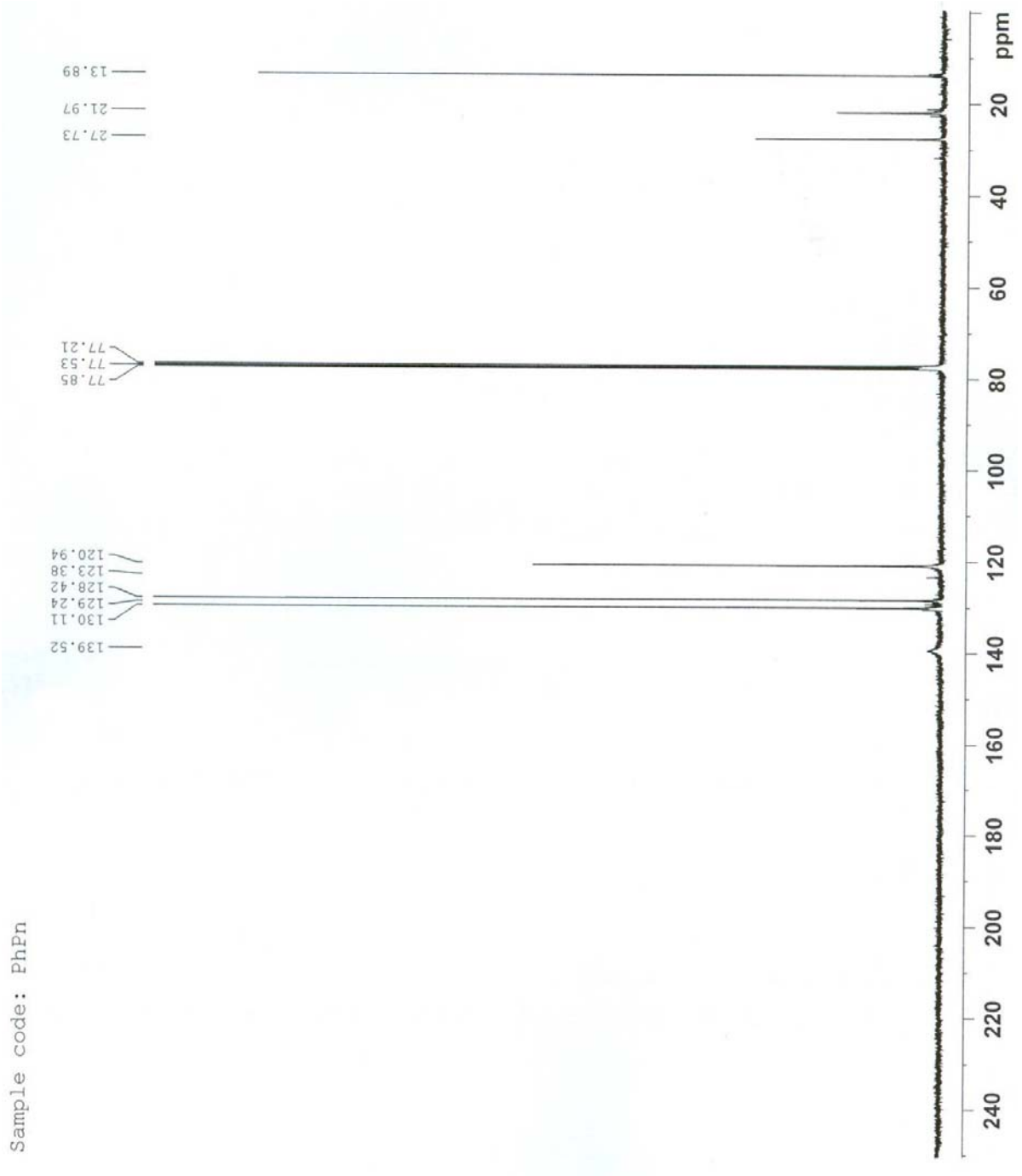
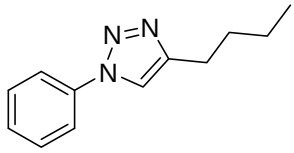
0.867
0.883
0.940
0.977
0.995
1.013
1.727
1.744
1.762
1.778
2.736
2.753
2.770
7.291
7.359
7.378
7.396
7.452
7.472
7.490
7.697
7.716
7.807
ppm
0
1
2
3
4
5
6
7
8
9
10
3.12
2.01
1.97
1.00
2.08
2.09
0.93

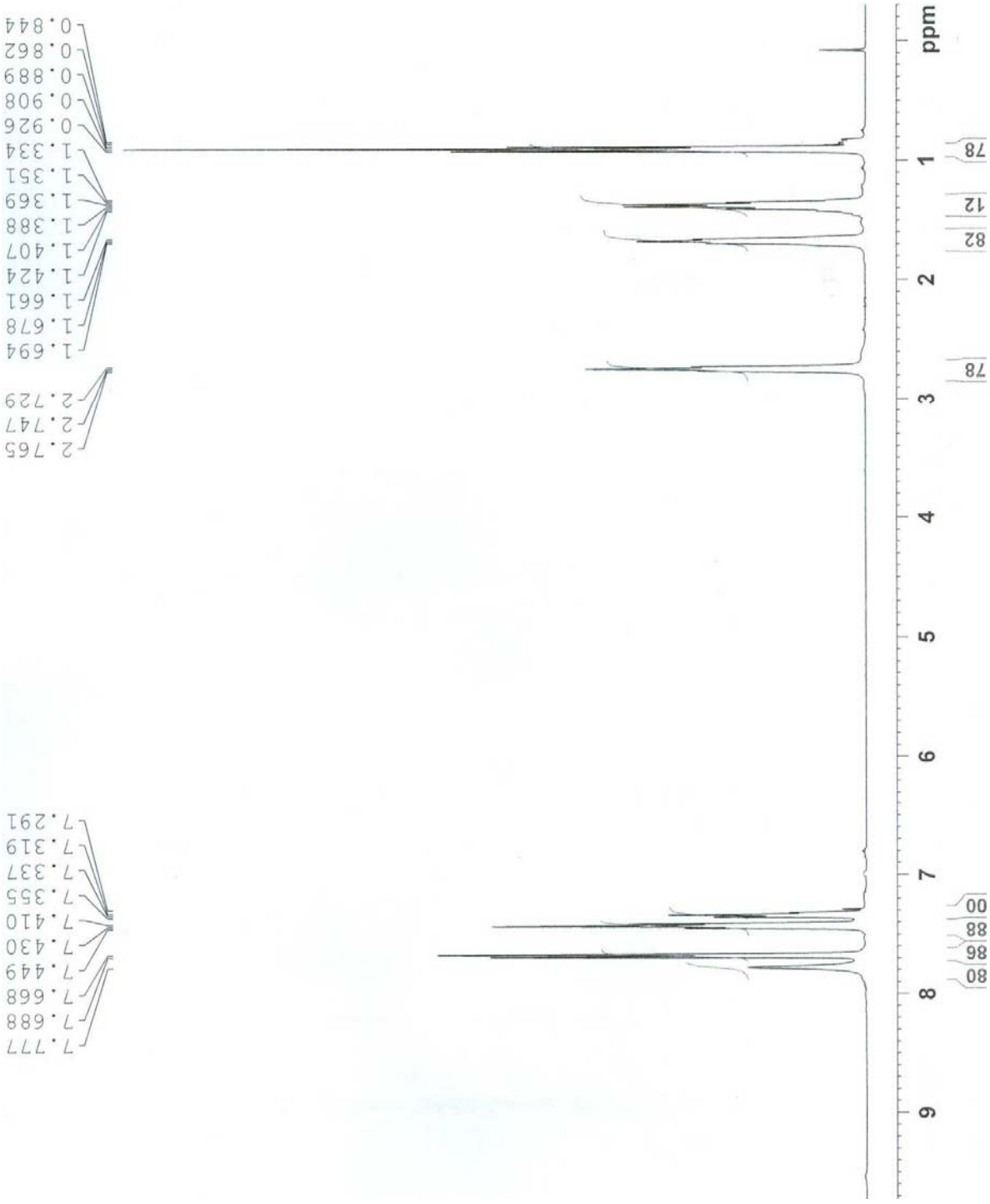
3l



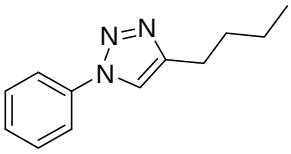

13.89
21.97
27.73
77.21
77.53
77.85
120.94
123.38
128.42
129.24
130.11
139.52
ppm
20
40
60
80
100
120
140
160
180
200
220
240
Sample code: PhPn

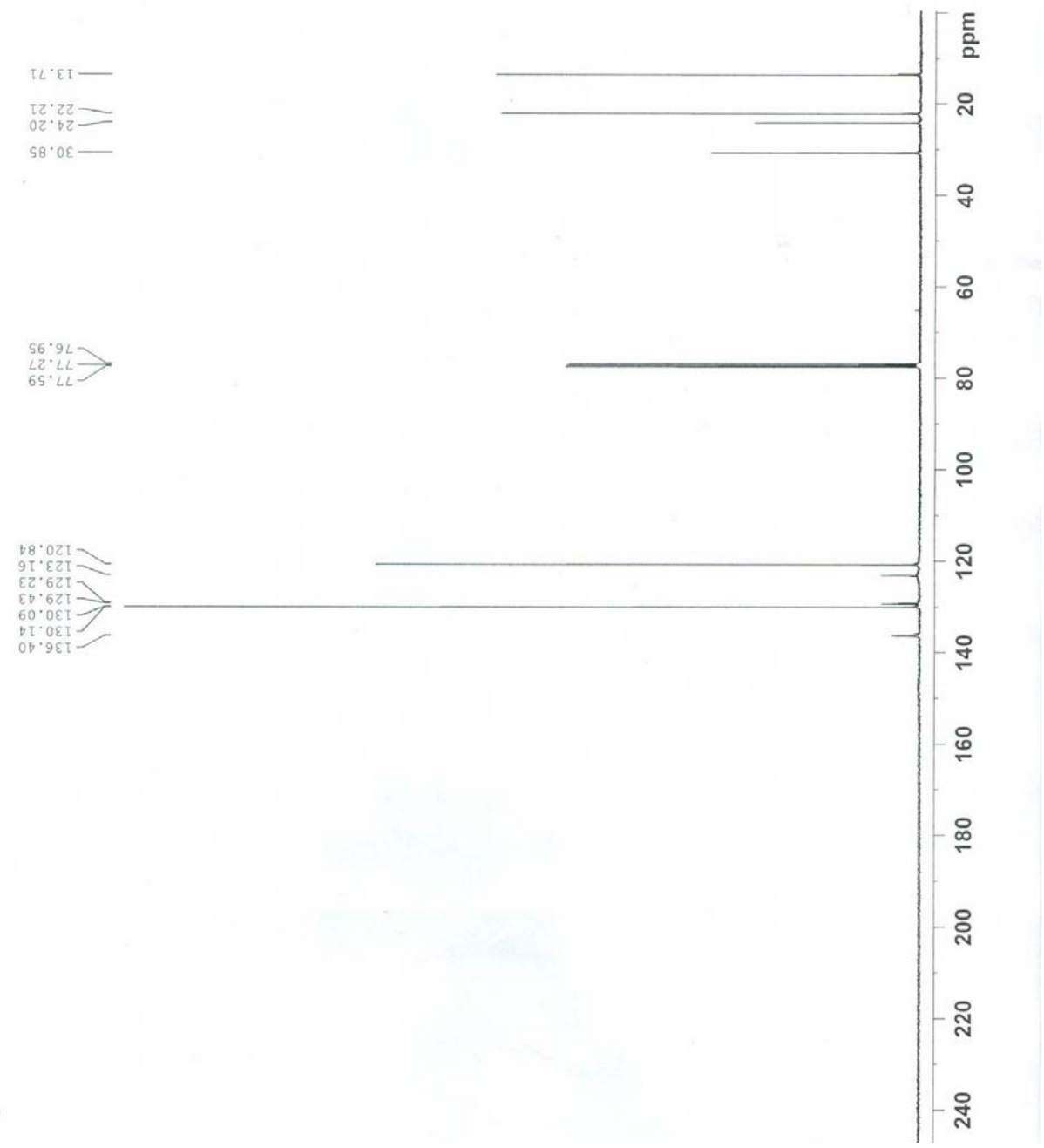
3m



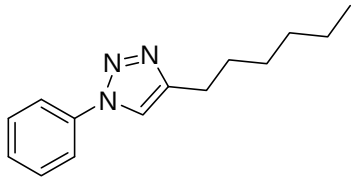


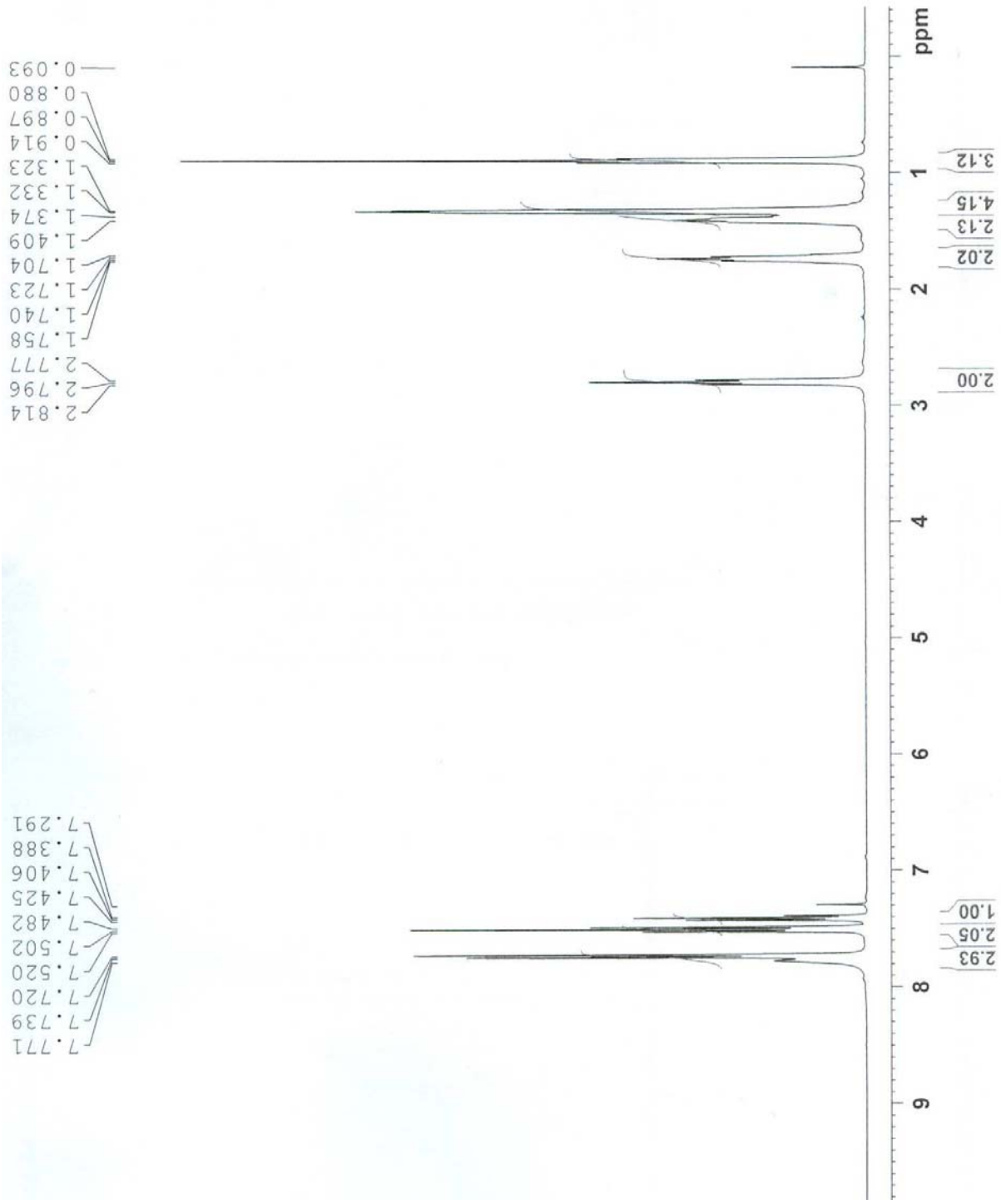
3m

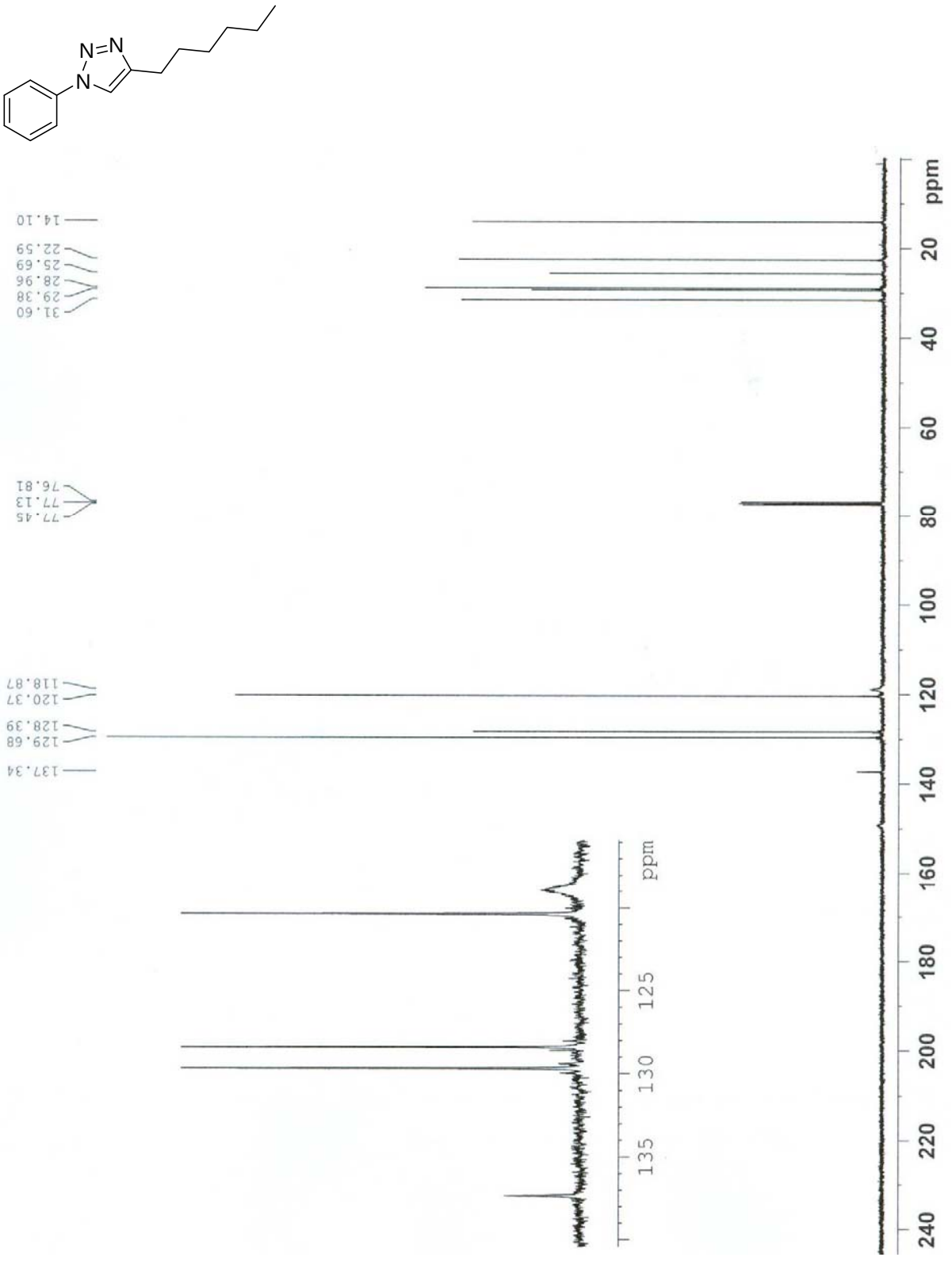




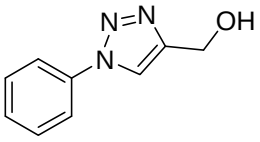
3n

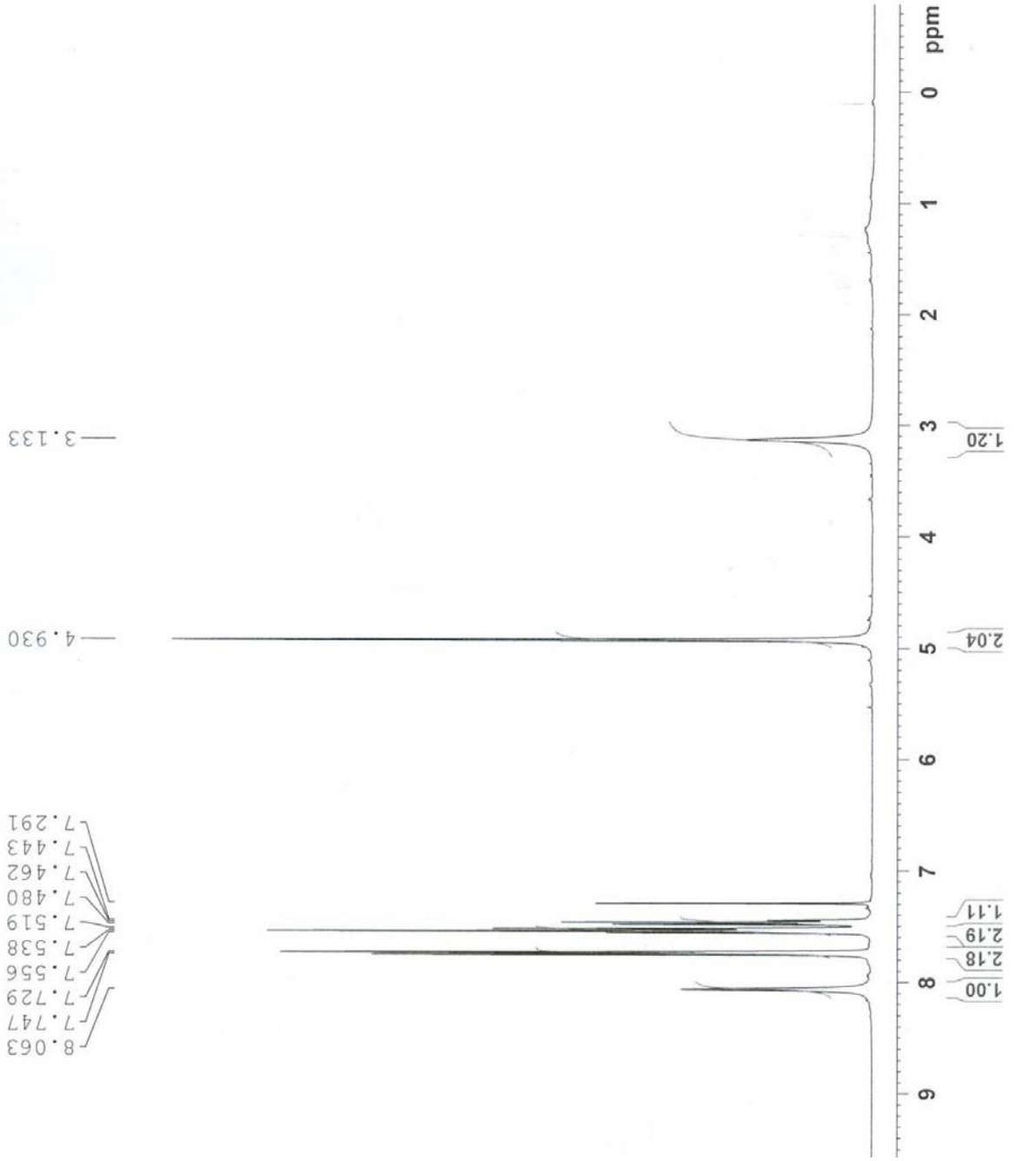



0.093
0.880
0.897
0.914
1.323
1.332
1.374
1.409
1.704
1.723
1.740
1.758
2.777
2.796
2.814
7.291
7.388
7.406
7.425
7.482
7.502
7.520
7.720
7.739
7.771
ppm
1
2
3
4
5
6
7
8
9
3.12
4.15
2.13
2.02
2.00
1.00
2.05
2.93

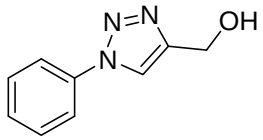


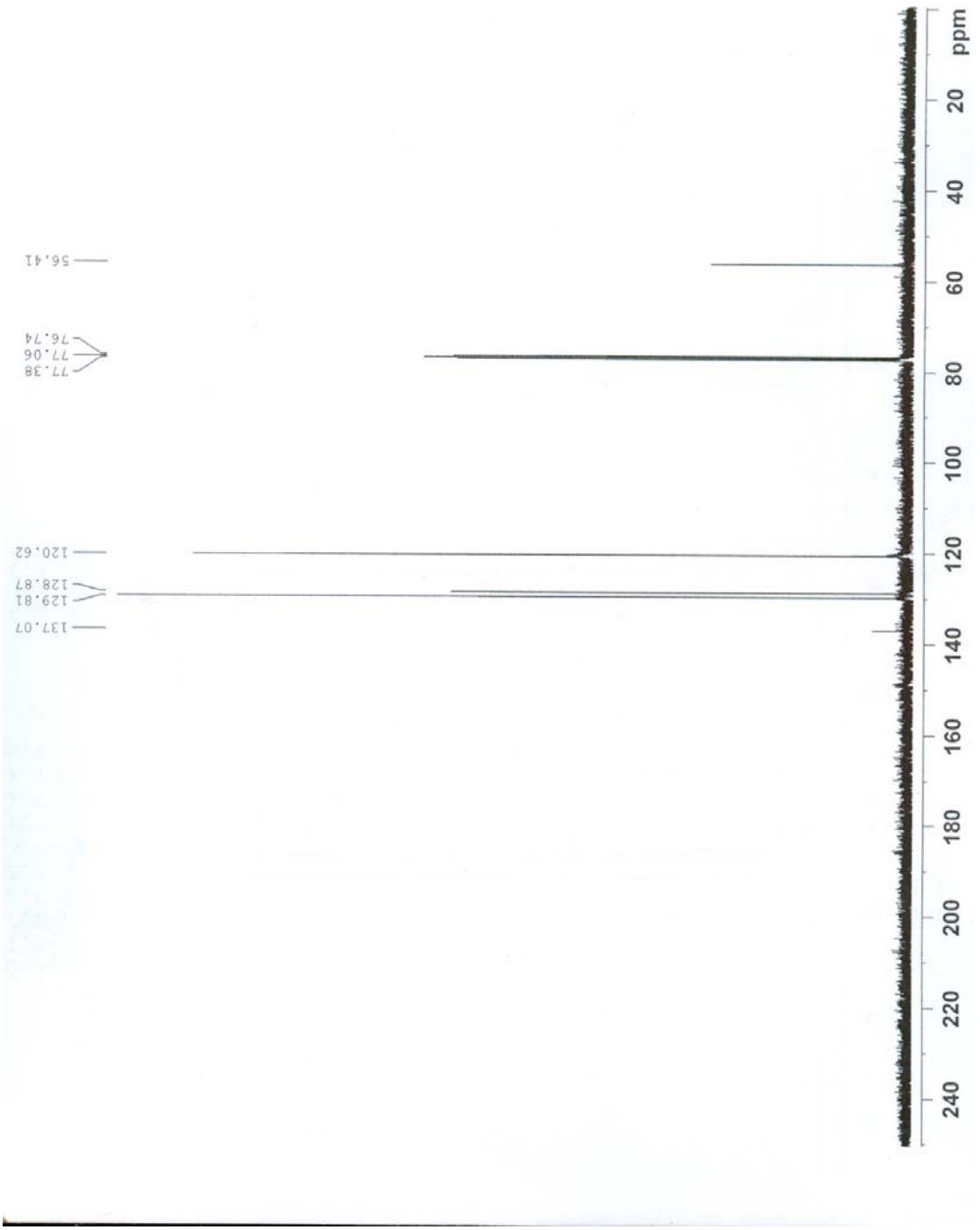
3o


N=N
N
OH

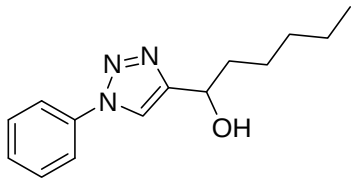

ppm
0
1
2
3
4
5
6
7
8
9
3.133
4.930
7.291
7.443
7.462
7.480
7.519
7.538
7.556
7.729
7.747
8.063
1.20
2.04
1.11
2.19
2.18
1.00

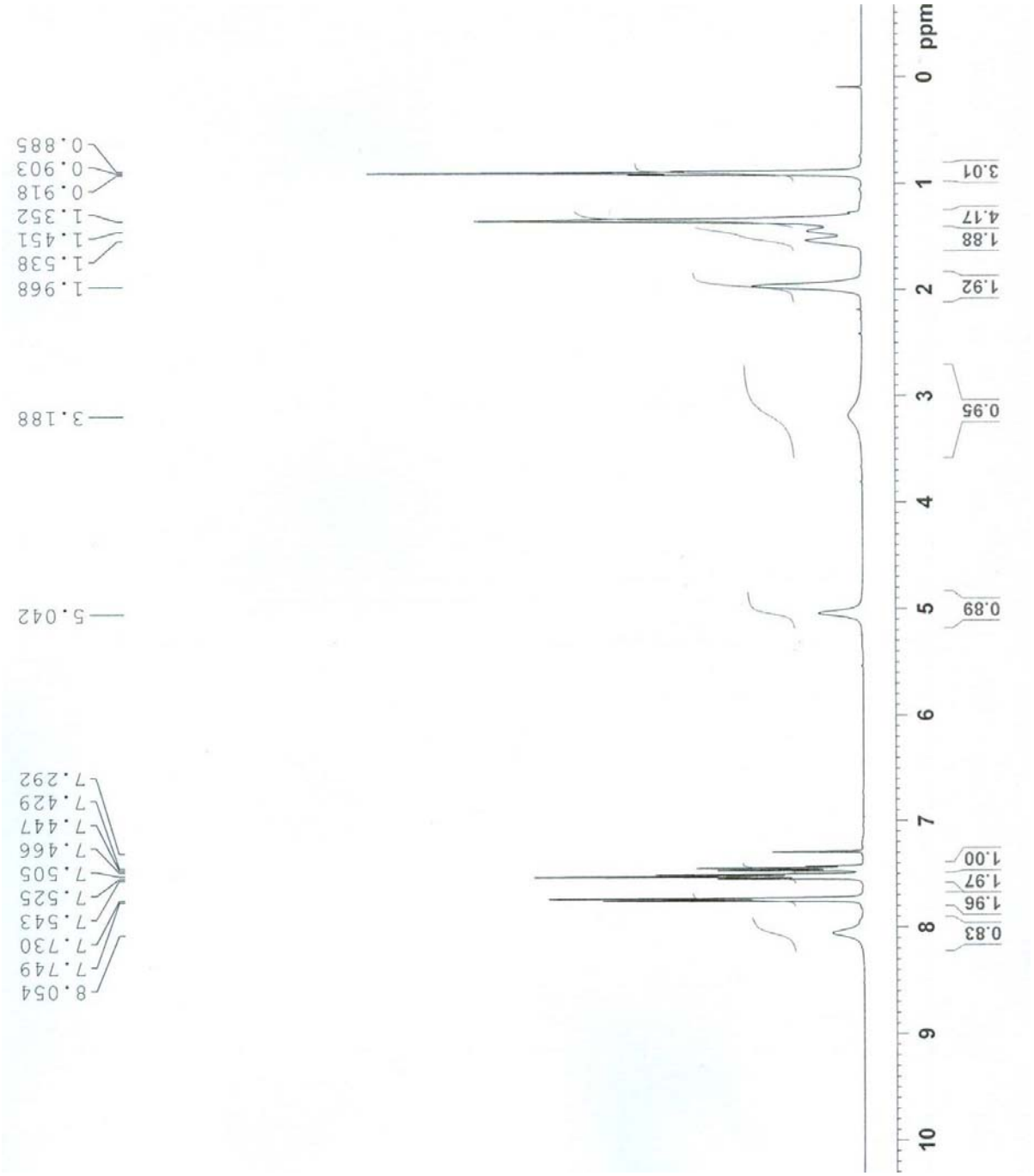
3o

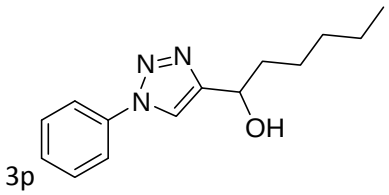

N=N
N
OH


56.41
76.74
77.06
77.38
120.62
128.87
129.81
137.07
ppm
20
40
60
80
100
120
140
160
180
200
220
240

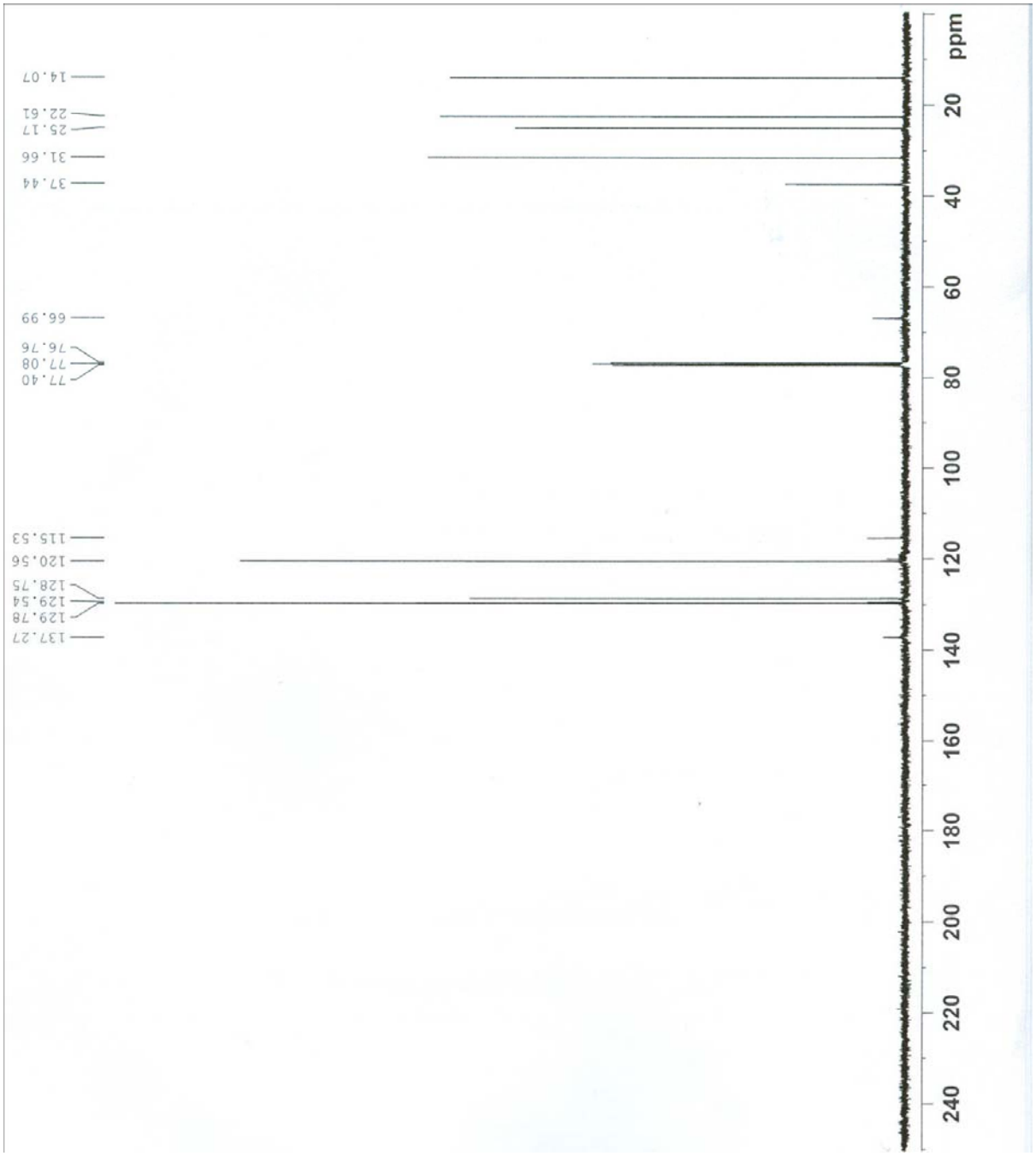
3p



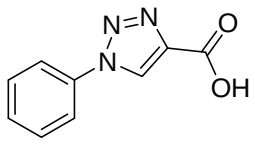


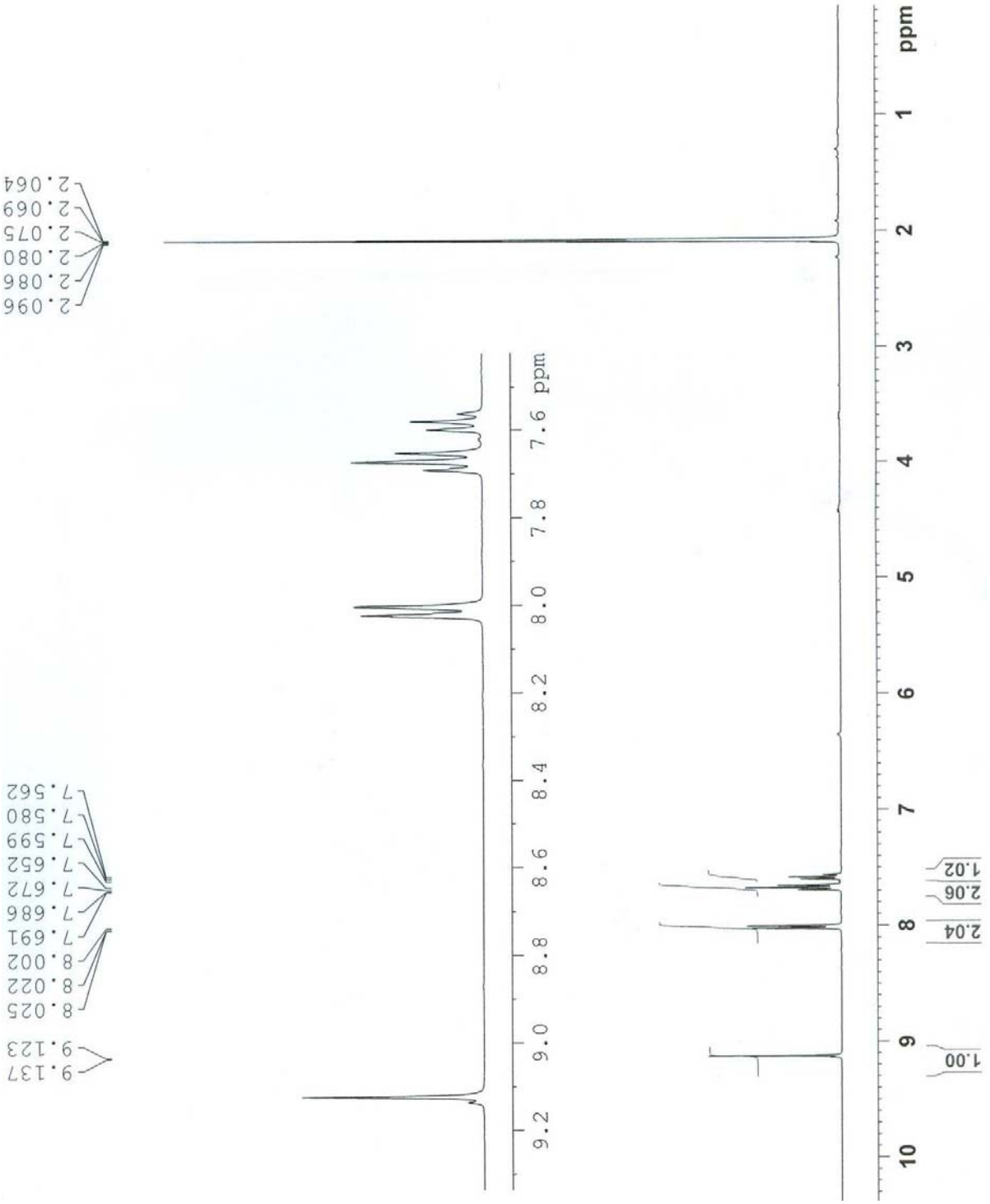

N=N
N
OH

3p

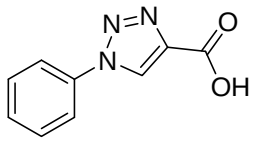

14.07
22.61
25.17
31.66
37.44
66.99
76.76
77.08
77.40
115.53
120.56
128.75
129.54
129.78
137.27
ppm
20
40
60
80
100
120
140
160
180
200
220
240

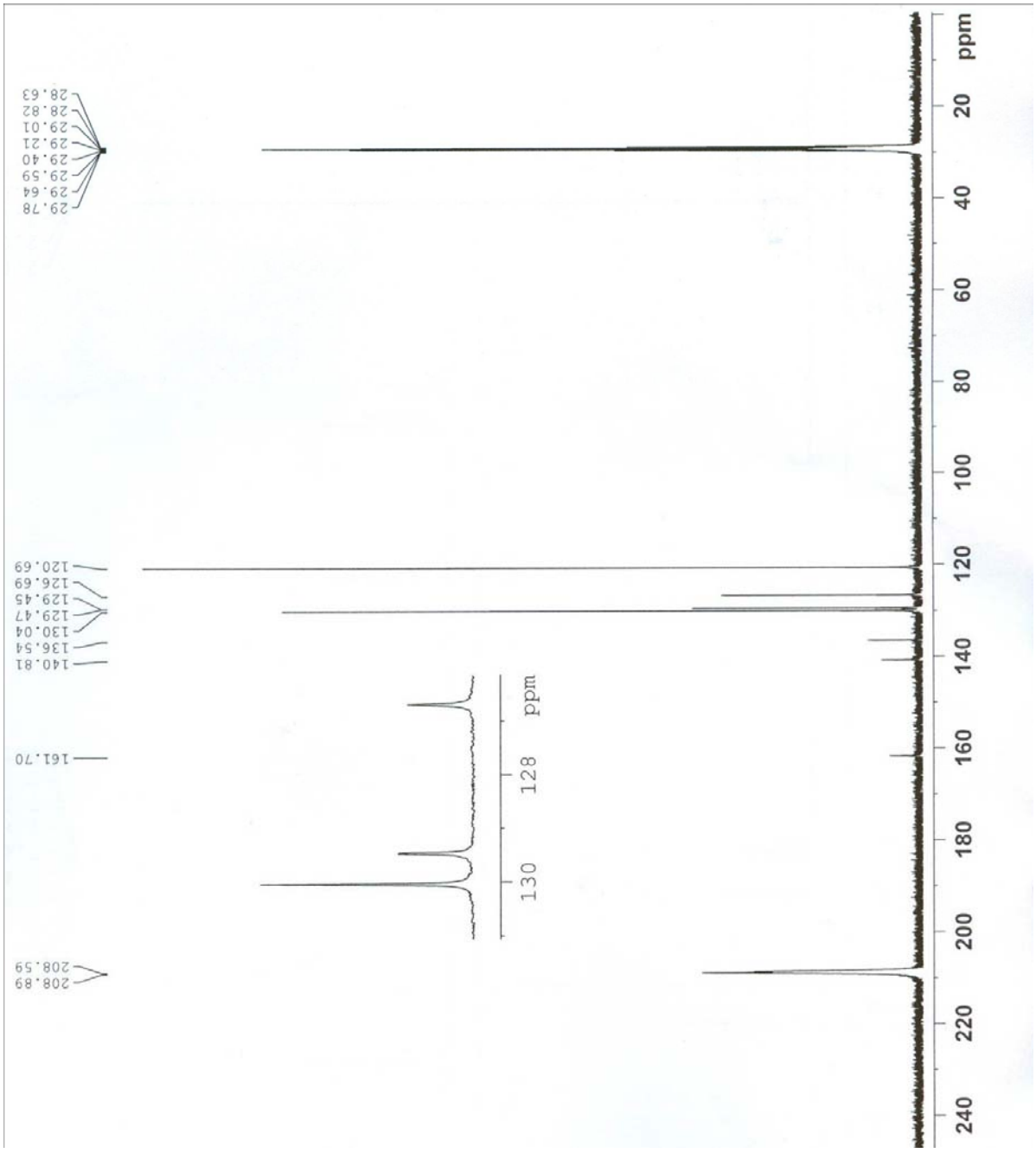
3q





3q


N=N
N
O
OH


ppm
20
40
60
80
100
120
140
160
180
200
220
240
128
130
ppm