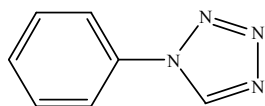


Supplementary information:

General synthesis for the preparation of 1-substituted 1*H*-tetrazoles

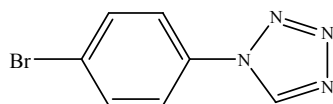
A mixture of amine (1 mmol), sodium azide (1 mmol), triethyl orthoformate (1.2 mmol) and Fe₃O₄@silica sulfonic acid (0.02 g) was taken in a round-bottomed flask and stirred at 100 °C. The progress of the reaction was monitored by thin layer chromatography (TLC). After completion of the reaction, the reaction mixture was cooled to room temperature and diluted with ethyl acetate (3×20 mL). The catalyst was removed by an external magnet, and then the resulting solution was washed with water and dried over anhydrous Na₂SO₄. After concentration, a crystallization step was performed using EtOAc-hexane (1:9). The products were characterized by ¹H NMR, ¹³C NMR, FT-IR and melting points. We have reported the spectral data of synthesized compounds.



1-(phenyl)-1*H*-tetrazole

Yellow solid; m.p=: 63-65 °C M.P_{Lit}: 65-67 °C

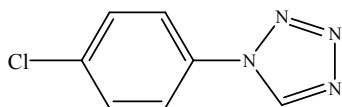
IR (KBr)/ ν (cm⁻¹): 3126 (C-H, sp² stretch Ar), 1694 (C=N), 1597, 1498 (C=C); ¹H NMR (CDCl₃, 400 MHz) δ (ppm): 7.07-7.34 (m, 5H, Ar), 8.20 (s, 1H tetrazole).



1-(4-Bromophenyl)-1*H*-tetrazole

White solid; m.p=169-170°C

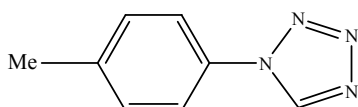
IR (KBr)/ ν (cm^{-1}): 3060 (C-H, sp^2 stretch, Ar), 1659 (C=N), 1576, 1482 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 6.92-6.94 (d, 2H), 7.40-7.42 (d, 2H), 8.09 (s, 1H tetrazole); ^{13}C NMR (CDCl_3 , 100 MHz) δ (ppm): 116.43, 120.76, 132.03, 143.99, 149.29.



1-(4-Chlorophenyl)-1H-tetrazole

White solid; m.p=153-155 °C M.P_{Lit.}:155-156 °C

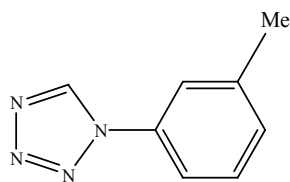
IR (KBr)/ ν (cm^{-1}): 3057 (C-H, sp^2 stretch, Ar), 1661 (C=N), 1485, 1581 (C=C) ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 6.98-7.00 (d-2H), 7.27-7.29 (d-2H), 8.09 (s-1H tetrazole); ^{13}C NMR (CDCl_3 , 100 MHz) δ (ppm): 120.35, 128.85, 129.47, 143.52, 149.50.



1-(4-Methylphenyl)-1H-tetrazole

Light yellow solid; m.p=92-99 °C

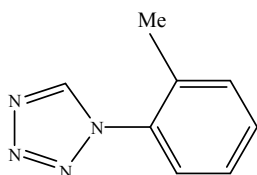
IR (KBr)/ ν (cm^{-1}): 3022 (C-H, sp^2 stretch, Ar), 2918(C-H, sp^3 stretch), 1664 (C=N), 1607, 1506 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 2.34 (s, 3H), 6.94-6.96 (d, 2H), 7.11-7.13 (d, 2H), 8.17 (s, 1H tetrazole); ^{13}C NMR (CDCl_3 , 100 MHz) δ (ppm): 20.79, 119.08, 129.63, 130.17, 142.95, 149.77.



1-(3-Methylphenyl)-1H-tetrazole

White solid; m.p=53-55 °C

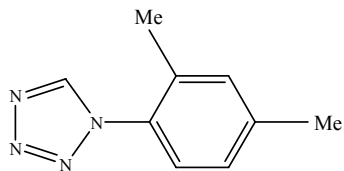
IR (KBr)/ ν (cm^{-1}): 3167 (C-H, sp^2 stretch, Ar), 2923 (C-H, sp^3 stretch), 1690 (C=N), 1594, 1483 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 2.33 (s, 3H), 6.86 (s, 1H), 6.89- 6.91 (d, 2H), 7.18-7.22(t, 1H), 8.21 (s, 1H tetrazole); ^{13}C NMR (CDCl_3 , 100 MHz) δ (ppm)): 21.43, 115.93, 119.97, 124.06, 129.19, 139.26, 145.28, 149.23



1-(2-Methylphenyl)-1H-tetrazole

White solid; m.p=152-155 °C

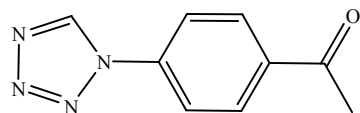
IR (KBr)/ ν (cm^{-1}): 3015 (C-H, sp^2 stretch, Ar), 2870 (C-H, sp^3 stretch), 1664(C=N), 1488, 1590 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 2.33 (s, 3H), 7.02-7.03 (d, 1H), 7.05-7.07 (d, 1H), 7.18-7.22 (t, 2H), 8.08 (s, 1HTetrazole); ^{13}C NMR (CDCl_3 , 100 MHz) δ (ppm): 17.94, 117.68, 123.43, 127, 128.71, 130.72, 144.10, 147.78.



1-(2,4-Dimethylphenyl)-1H-tetrazole

White solid; m.p=133-135 °C

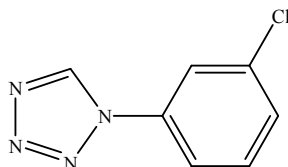
IR (KBr)/ ν (cm^{-1}): 3069 (C-H, sp^2 stretch, Ar), 2914 (C-H, sp^3 stretch), 1663 (C=N), 1495, 1607 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 2.29 (s, 3H), 2.30 (s, 3H), 6.94-6.96 (d, 1H), 6.98-7.00 (d, 1H), 7.02 (s, 1H), 8.00 (s, 1H tetrazole).



1-(4-Acetylphenyl)-1H-tetrazole

Yellow solid; m.p=175-176 °C

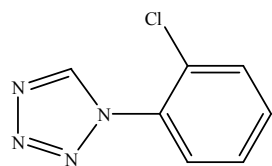
IR (KBr)/ ν (cm^{-1}): 3075 (C-H, sp^2 stretch, Ar), 2995 (C-H, sp^3 stretch), 1669 (C=N), 1499, 1585 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 2.60 (s, 3H), 7.13-7.15 (d, 2H), 7.95-7.97 (d, 2H), 8.30 (s, 1H tetrazole).



1-(3-Chlorophenyl)-1H-tetrazole

White solid; m.p=137-139 °C

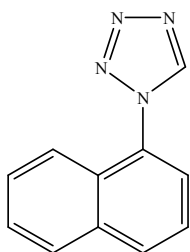
IR (KBr)/ ν (cm^{-1}): 3065 (C-H, sp^2 stretch, Ar), 1669 (C=N), 1473, 1586 (C=C). ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 6.92-6.94 (d, 1H) 7.07-7.09 (d, 2H) 7.26-7.27 (t, 1H), 8.14 (s-1H tetrazole); ^{13}C NMR (CDCl_3 , 100 MHz) δ (ppm): 117.45, 119.23, 123.73, 130.34, 135.12, 146.14, 149.72.



1-(2-Chlorophenyl)-1H-tetrazole

White solid; m.p=129-131 °C

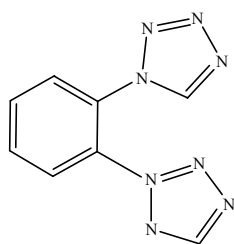
IR (KBr)/ ν (cm^{-1}): 3023 (C-H, sp^2 stretch, Ar), 1670 (C=N), 1481, 1598 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 7.03-7.50 (m-4H), 8.10 (s-1H tetrazole).



1-(naphthalene-1-yl)-1H-tetrazole

White solid; m.p=132-135 °C

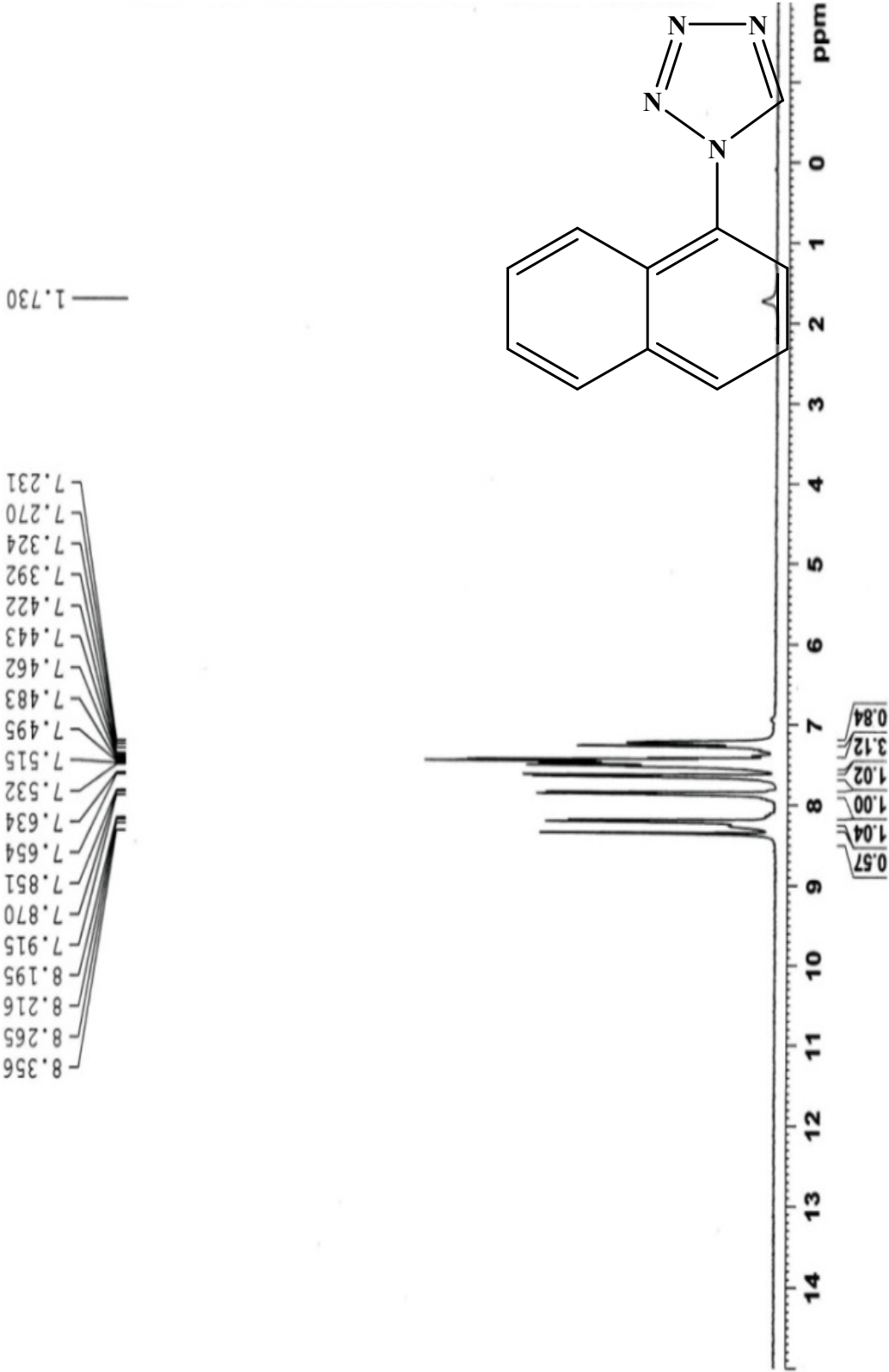
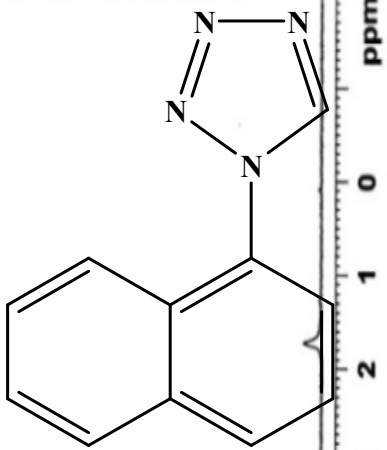
IR (KBr)/ ν (cm^{-1}): 3048 (C-H, sp^2 stretch, Ar), 1658(C=N), 1574, 1432 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 7.23-8.27 (m, 7H), 8.36 (s, 1H tetrazole).

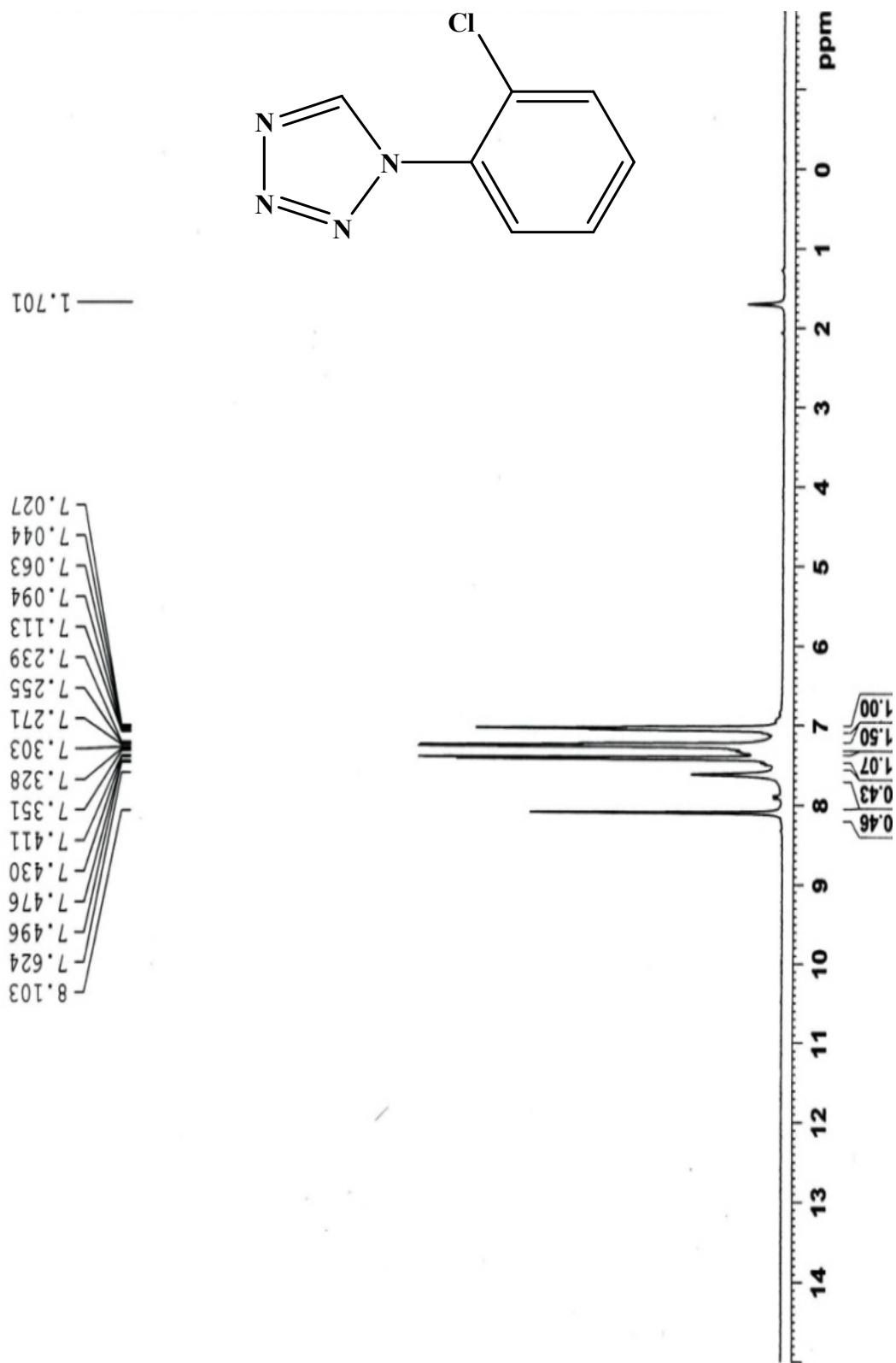
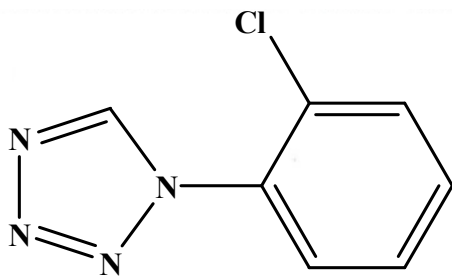


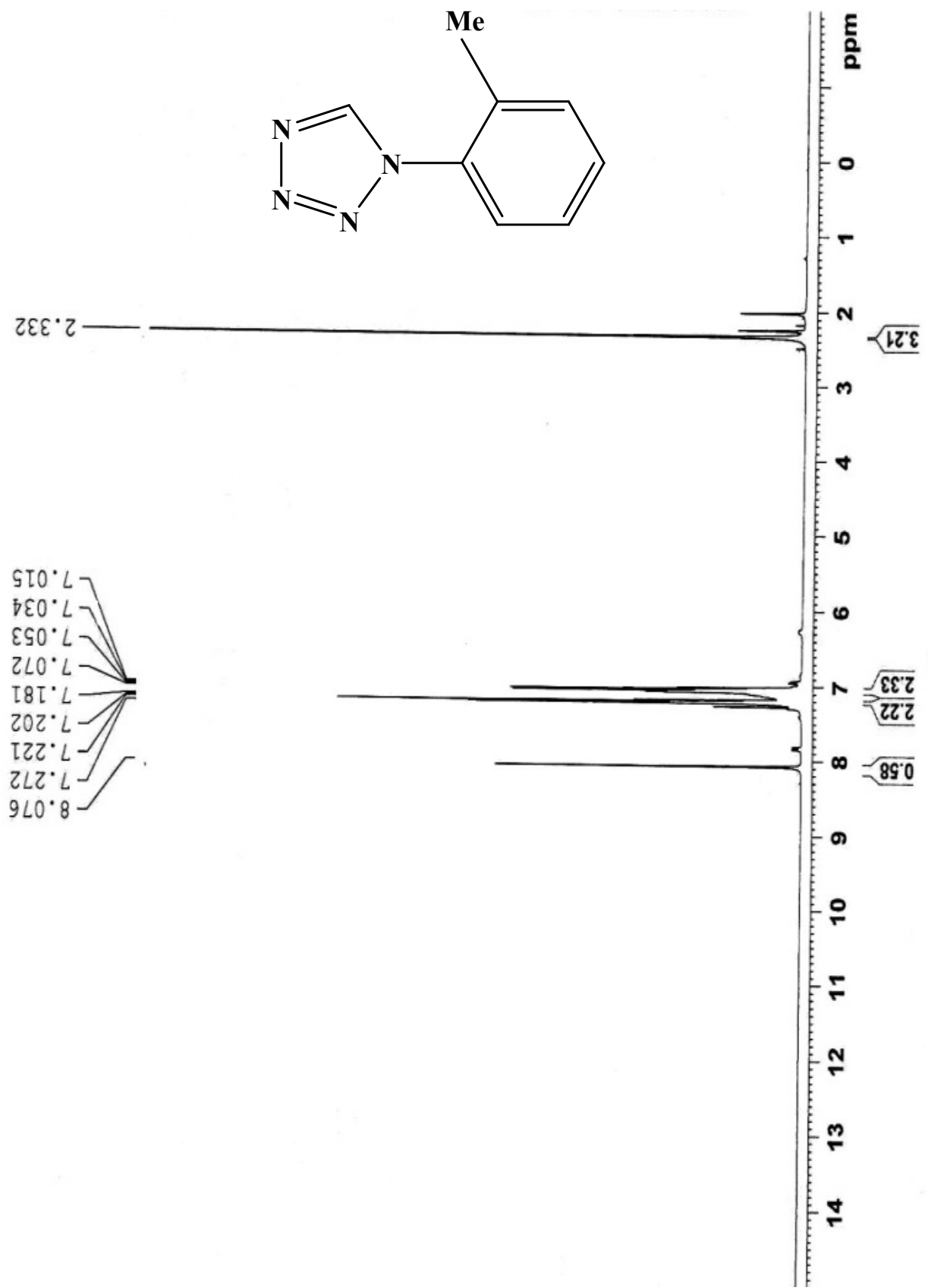
1-[2-(1H-tetrazol-1-yl) phenyl]-1H-tetrazole

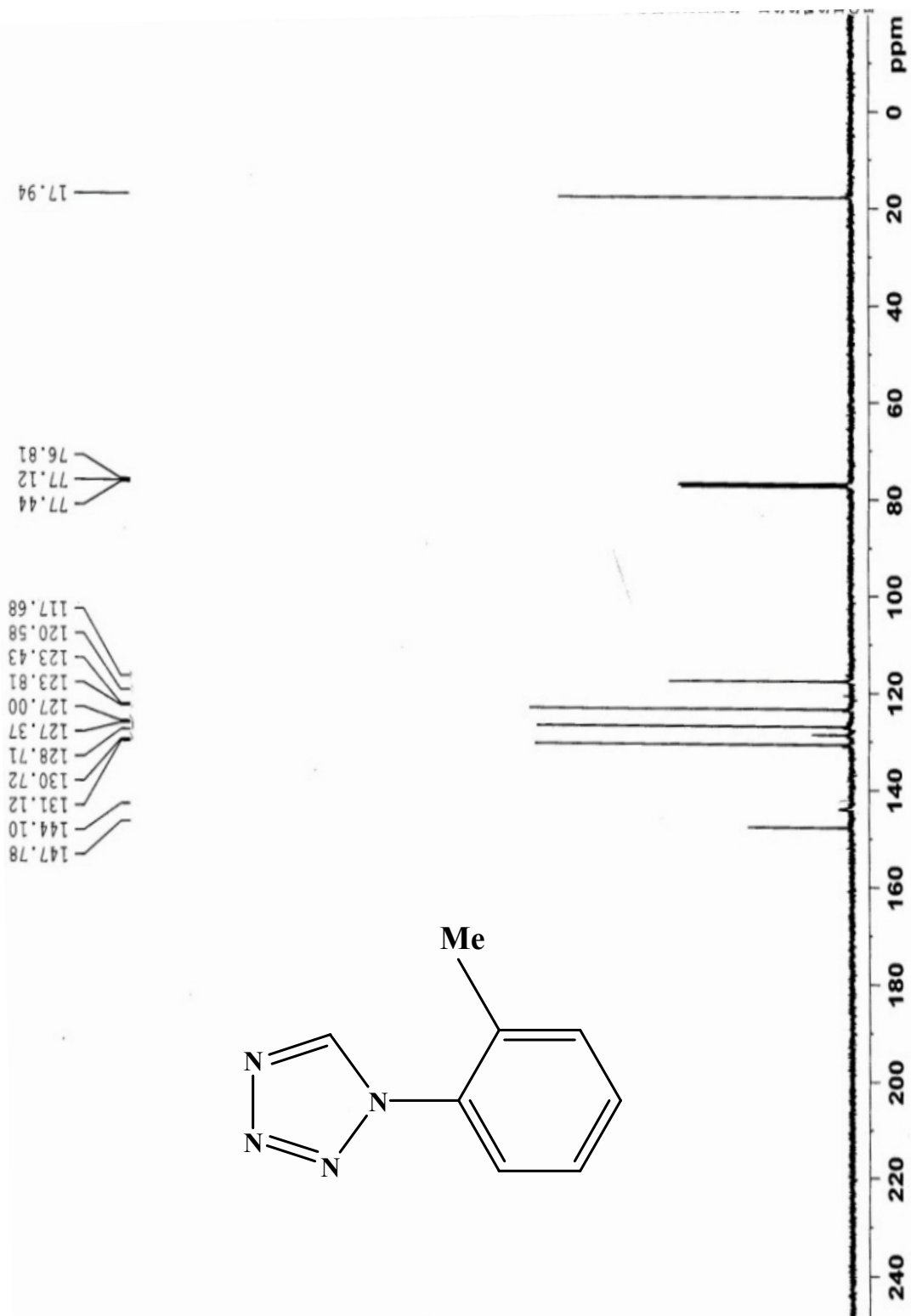
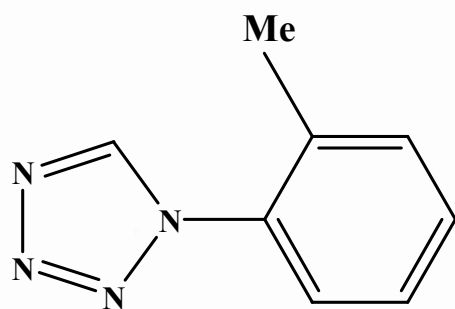
White solid; m.p=167-169 °C

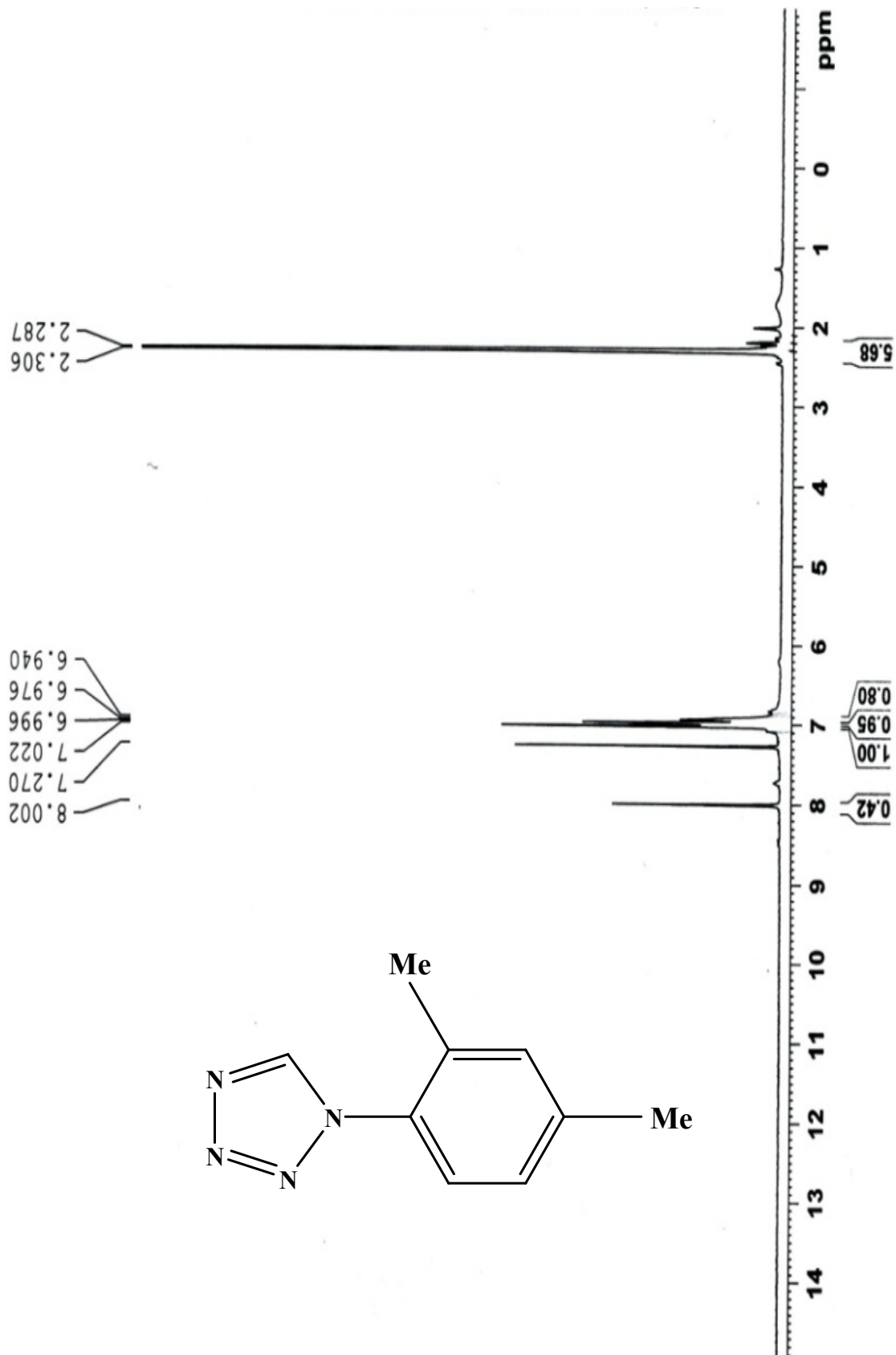
IR (KBr)/ ν (cm^{-1}): 3062 (C-H, sp^2 stretch, Ar), 1619 (C=N) 1458, 1588 (C=C); ^1H NMR (CDCl_3 , 400 MHz) δ (ppm): 7.30-7.70 (m, 4H), 8.11 (s, 1HTetrazole); ^{13}C NMR (CDCl_3 , 100 MHz) δ (ppm): 115.76, 122.37, 138.50, 142.40.

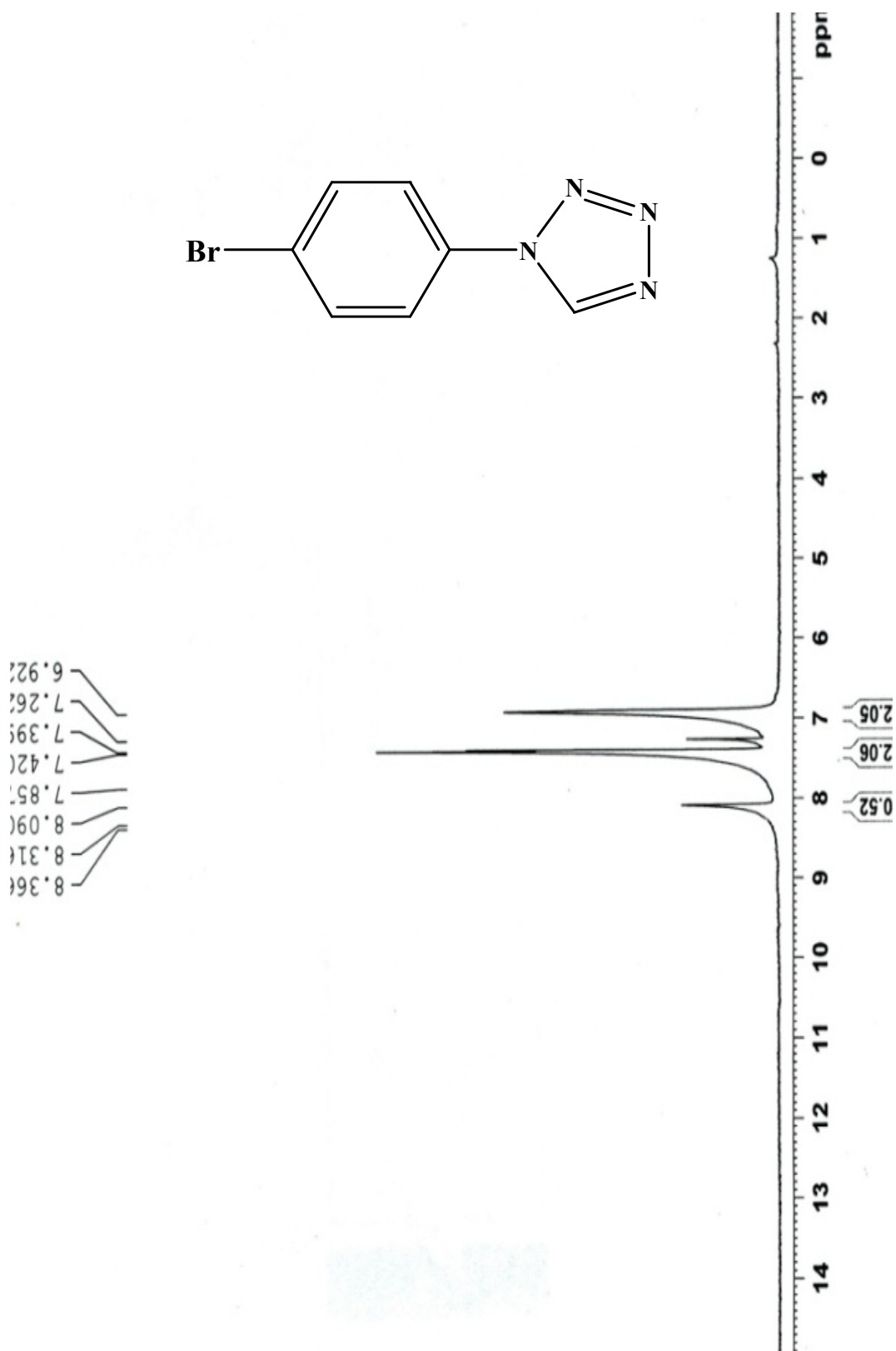
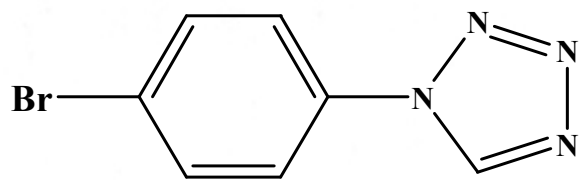


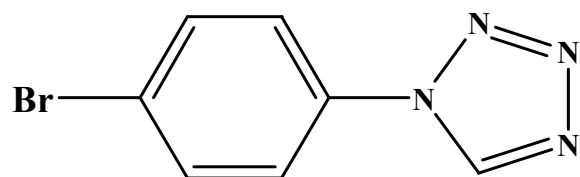


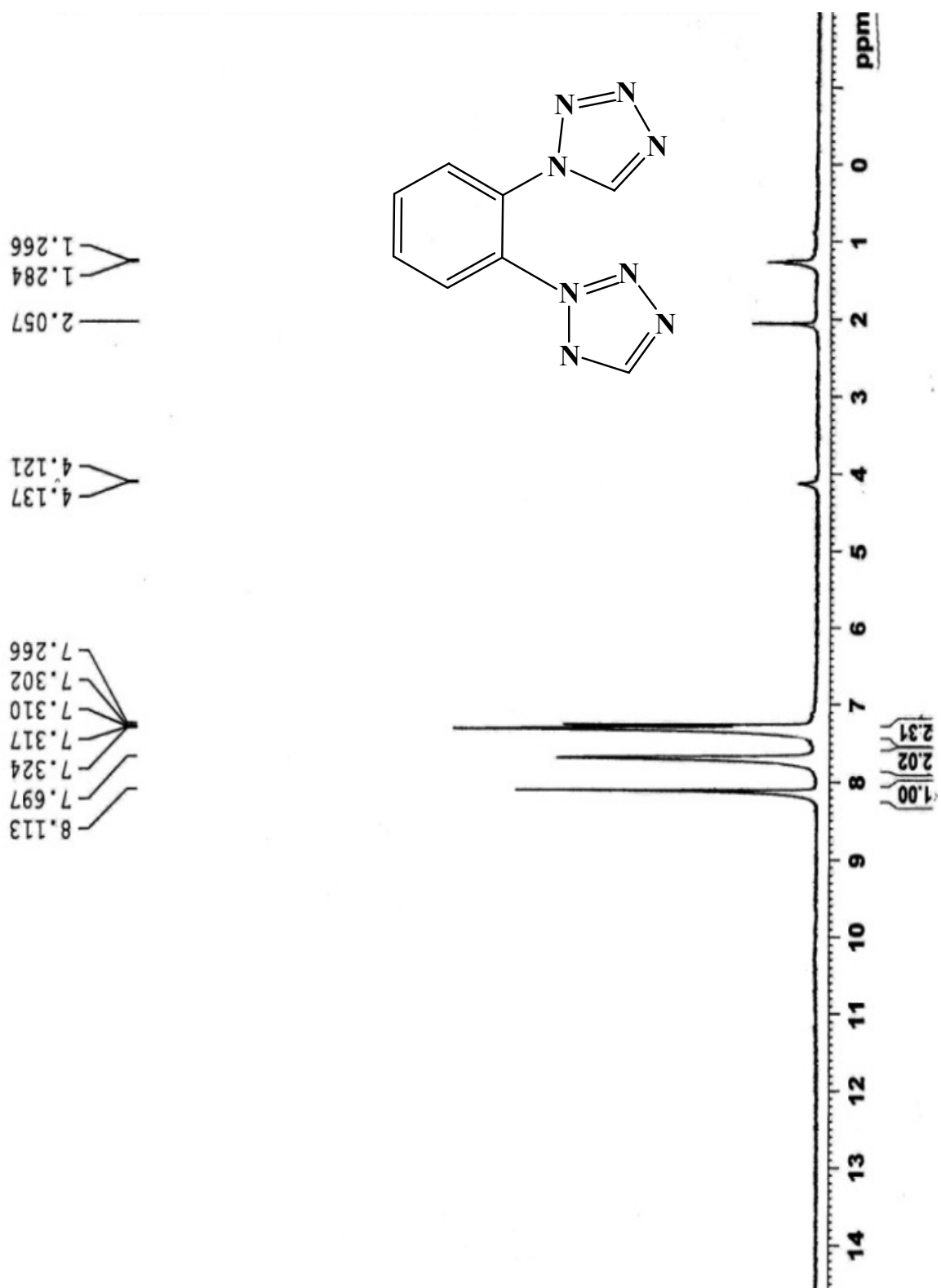


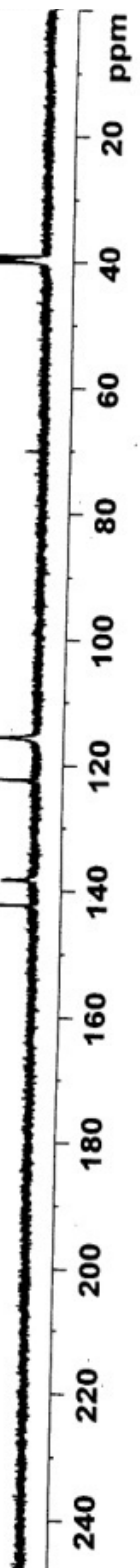
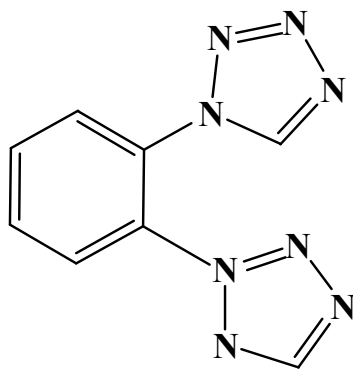




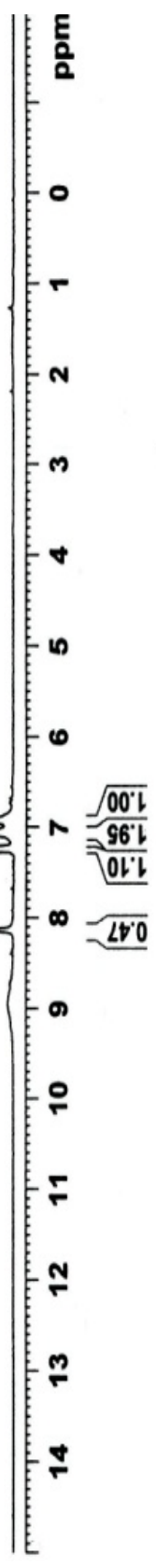
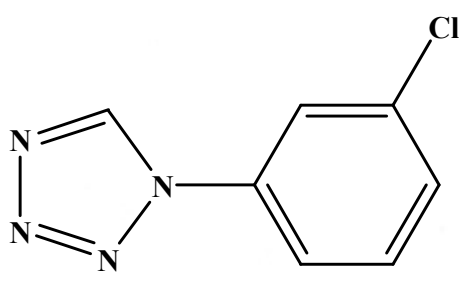


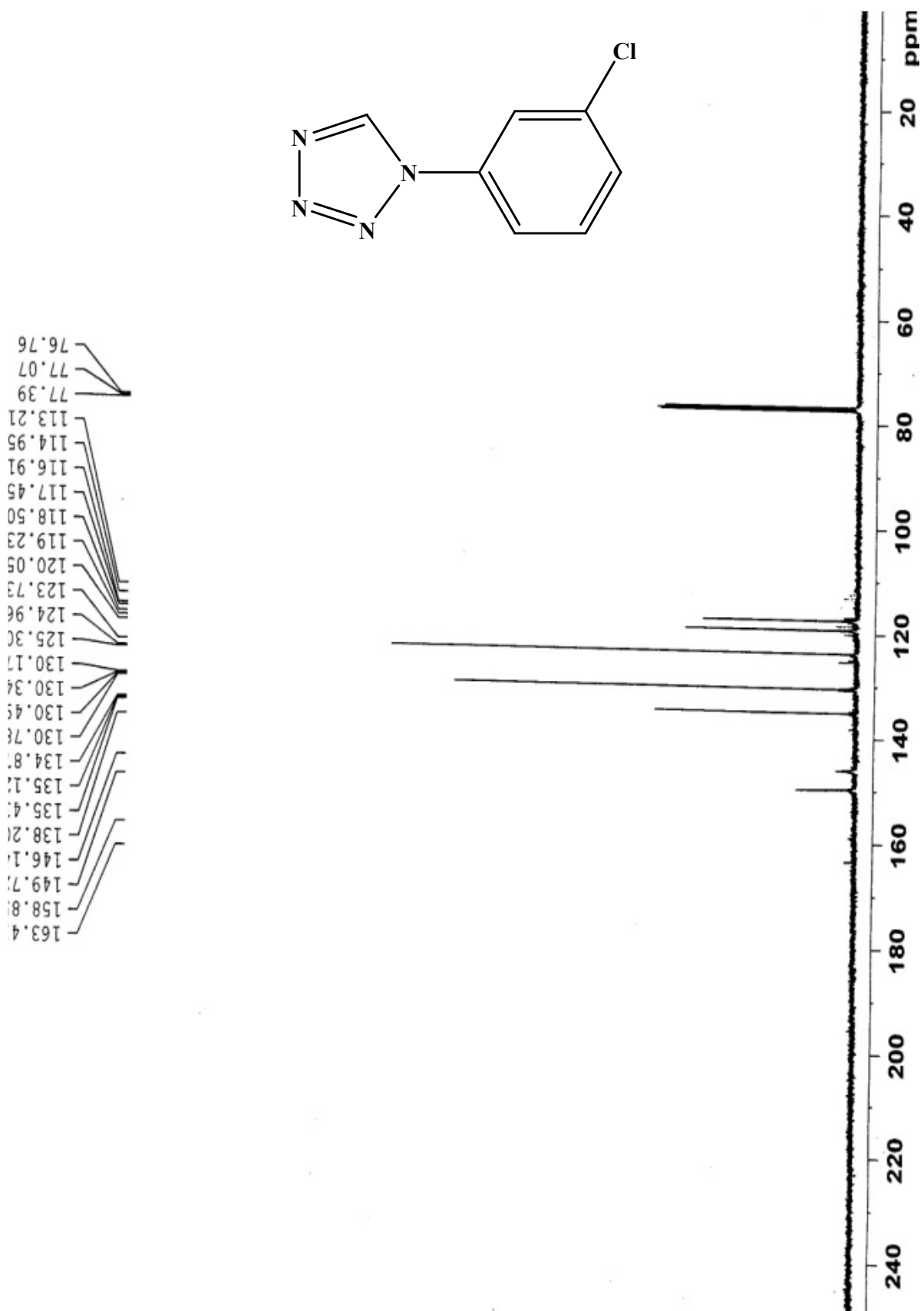
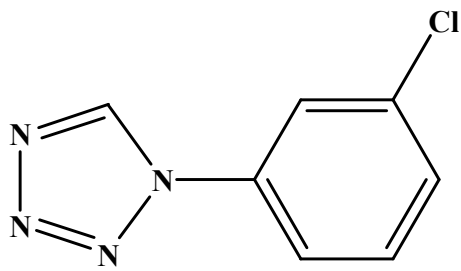


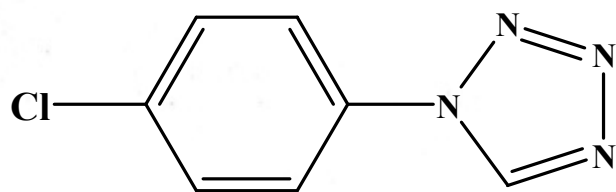




6.919
6.938
7.071
7.092
7.225
7.245
7.270
8.141







2.186

6.982
7.000
7.271
7.290
8.086

3.13
1.49
1.00

ppm
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

