Supporting Information

3-(Propylthio)propane-1-sulfonic acid immobilized on functionalized magnetic nanoparticles as an efficient catalyst for one-pot synthesis of dihydrotetrazolo[1,5-a]pyrimidine and tetrahydrotetrazolo[5,1-b]quinazolinone derivatives

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1. **General.** The chemicals used in this work were purchased from Fluka and Merck chemical companies. Melting points were determined with a Stuart Scientific SMP2 apparatus. FT-IR spectra were recorded on a Nicolet-Impact 400D spectrophotometer. ^{1}H and ^{13}C NMR (400 and 100 MHz) spectra were recorded on a Bruker Avance 400 MHz spectrometer using DMSO-*d6* and $CDCl_3$ as solvent. Elemental analysis was performed on a LECO, CHNS-932 analyzer. Thermogravimetric analysis (TGA) was carried out on a Mettler TG50 instrument under air flow at a uniform heating rate of 20 °C min^{-1} in the range 30-700 °C. The TGA instrument was re-calibrated at frequent intervals with standards; the accuracy was always better than ±2.0%. The scanning electron microscope measurement was carried out on a Hitachi S-4700 field emission-scanning electron microscope (FE-SEM). The transmission electron microscopy (TEM) was carried out on a Philips CM10 instrument operating at 100 kV. The magnetic measurements were performed with a vibrating sample magnetometer (VSM) at Meghnatis Daghigh Kavir Co.

2. **General procedure for Preparation of [PTPSA@SiO_2-Fe_3O_4]**

Preparation of [PT@SiO_2-Fe_3O_4]:

First, silica-coated magnetite nanoparticles SiO_2-Fe_3O_4 (250 mg) were prepared according to the literature,[1a,b] and were continuously added to a solution of (3-mercaptopropyl)trimethoxysilane (MPS) (1 g) in 10 mL of ethanol and 10 mL of water and dispersed by sonication for 15 min and refluxed overnight. Finally, the precipitate (PT@SiO_2-Fe_3O_4) was separated by a permanent magnet, washed with water (3×10 mL), and dried in a vacuum oven at 50 °C. [2]

Preparation of [PTPSA@SiO_2-Fe_3O_4]

A mixture of PT@SiO_2-Fe_3O_4 (2.61 mmol, 0.196 g) and 1,3-propanesultone (2.62 mmol, 0.320 g) was intensely dispersed in 5 mL dry toluene and then, the reaction mixture was refluxed for 6 hours at 100

°C. The resulting solid was separated by a permanent magnet, washed with toluene three times and dried under vacuum to afford [PTPSA@SiO_2-Fe_3O_4].

3. **General procedure for synthesis of dihydrotetrazolo[1,5-a]pyrimidine derivatives catalyzed by [PTPSA@SiO_2-Fe_3O_4]**

A mixture of aryl aldehyde (1 mmol), 5-aminotetrazole (1 mmol), acetophenone/4-chloroacetophenone (1 mmol), and [PTPSA@SiO_2-Fe_3O_4] (5 mol%, 33 mg) was stirred at 70 °C under solvent-free conditions for the duration of suitable time mentioned in Scheme 3. The progress of the reaction was monitored by TLC (eluent: petroleum ether/EtOAc, 3:1). Upon completion of the reaction, the mixture was cooled to room temperature and EtOH (10 mL) was added. The catalyst was quickly separated by an external magnetic field and washed with EtOH (5 mL). The products were obtained by recrystallization from EtOH and dried under reduced pressure. In some cases, the organic residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate) to provide pure products in 92-98% isolated yields (Scheme 3, **4a-c**).

4. **General procedure for synthesis of dihydrotetrazolo[1,5-a]pyrimidine-6-carboxylate derivatives catalyzed by [PTPSA@SiO_2-Fe_3O_4]**

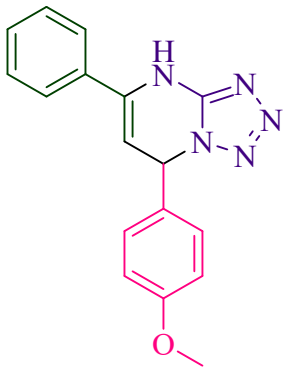
A mixture of aryl aldehyde (1 mmol), 5-aminotetrazole (1 mmol), ethyl acetoacetate (1 mmol), and [PTPSA@SiO_2-Fe_3O_4] (5 mol%, 33 mg) was stirred at 70 °C under solvent-free conditions for the appropriate time indicated in Scheme 4. Upon completion, it was monitored by TLC (eluent: petroleum ether/EtOAc, 3:1), the work-up was done as defined for synthesis of dihydrotetrazolo[1,5-a]pyrimidines and the pure product was obtained in 91-98% isolated yield (Scheme 4, **6a-f**).

5. **General procedure for synthesis of tetrahydrotetrazolo[5,1-b]quinazolinone derivatives catalyzed by [PTPSA@SiO_2-Fe_3O_4]**

A mixture of aryl aldehyde (1 mmol), 5-aminotetrazole (1 mmol), dimedone (1 mmol), and [PTPSA@SiO2-Fe3O4] (5 mol%, 33 mg) was stirred at 70 °C under solvent-free conditions for the appropriate time according to Scheme 5. The progress of the reaction was tested by TLC (eluent: petroleum ether/EtOAc, 3:1). After completion of the reaction, the work-up was done as described for the synthesis of dihydrotetrazolo[1,5-a]pyrimidines and the pure products were gained in 91-97% isolated yields (Scheme 5, **8a-f**).

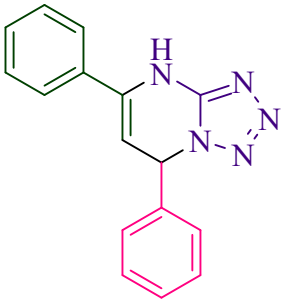
6. Spectroscopic data of the products:

7-(4-Methoxy-phenyl)-5-phenyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine (Scheme 3, 4a)



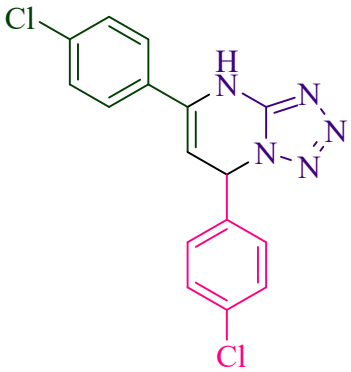
White solid, mp 237-239 °C. (Lit. [3] 226-228 °C) IR (KBr): ν_{max} = 3231, 3064, 2942, 2839, 1659, 1601, 1547, 1510, 1246, 1177, 1030, 847, 764 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ = 3.75 (s, 3H), 5.27 (dd, ^1J = 3.6 Hz, ^2J = 1.5 Hz, 1H), 6.55 (d, J = 3.6 Hz, 1H), 6.97 (d, J = 8.7 Hz, 2H), 7.30-7.32 (m, 2H), 7.44-7.47 (m, 3H), 7.64-7.67 (m, 2H), 10.50 (s, 1H). Anal. Calcd for $C_{17}H_{15}N_5O$: C, 66.87; H, 4.95; N, 22.94. Found: C, 66.70; H, 4.99; N, 22.87.

5,7-Diphenyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine (Scheme 3, 4b)



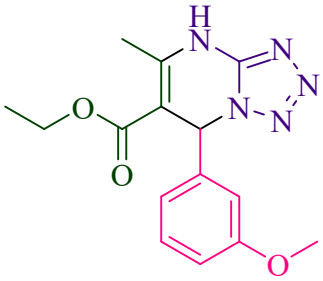
White solid, mp 236-239 °C. (Lit. [4] 244-246 °C) IR (KBr): ν_{max} = 3221, 3086, 2946, 2892, 1656, 1597, 1552, 1450, 1309, 1098, 837, 759 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 5.35 (dd, ^1J = 3.6 Hz, ^2J = 1.5 Hz, 1H), 6.65 (d, J = 3.6 Hz, 1H), 7.39-7.42 (m, 3H), 7.45-7.50 (m, 5H), 7.68-7.71 (m, 2H), 10.59 (s, 1H). Anal. Calcd for $C_{16}H_{13}N_5$: C, 69.80; H, 4.76; N, 25.44. Found: C, 69.66; H, 4.79; N, 25.37.

5,7-bis(4-chlorophenyl)-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine (Scheme 3, 4c)



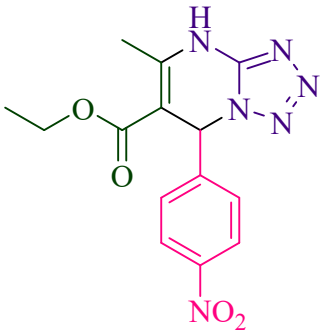
White solid, mp 235-236 °C. (Lit. [4] 233-234 °C) IR (KBr): ν_{max} = 3229, 3086, 2938, 2859, 1661, 1598, 1549, 1490 1325, 1092, 1012, 831, 806 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 5.34-5.35 (m, 1H), 6.65 (d, J = 3.5 Hz, 1H), 7.40 (d, J = 8.4 Hz, 2H), 7.48-7.53 (m, 4H), 7.68 (d, J = 8.6 Hz, 2H), 10.64 (s, 1H). Anal. Calcd for $C_{16}H_{11}Cl_2N_5$: C, 55.83; H, 3.22; N, 20.35. Found: C, 55.63; H, 3.26; N, 20.27.

Ethyl7-(3-methoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6a)



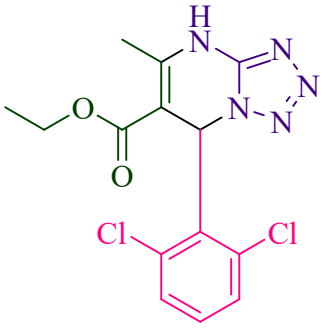
White solid, mp 168-169 °C. (Lit. [4] 164-168 °C) IR (KBr): ν_{max} = 3232, 3166, 3049, 2947, 2847, 1698, 1655, 1576, 1490, 1282, 1228, 1101, 1034, 874, 777, 707 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 0.69 (t, J = 7.1 Hz, 3H), 2.22 (s, 3H), 3.32 (s, 3H), 3.60-3.68 (m, 2H), 6.23 (s, 1H), 6.37 (dd, ^1J = 7.0 Hz, ^2J = 2.0 Hz, 1H), 6.42-6.43 (m, 1H), 6.47 (d, J = 7.7 Hz, 1H), 6.77 (d, J = 7.9 Hz, 1H), 10.32 (s, 1H). Anal. Calcd for $C_{15}H_{17}N_5O_3$: C, 57.13; H, 5.43; N, 22.21. Found: C, 57.04; H, 5.48; N, 22.14.

Ethyl 5-methyl-7-(4-nitrophenyl)-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6b)



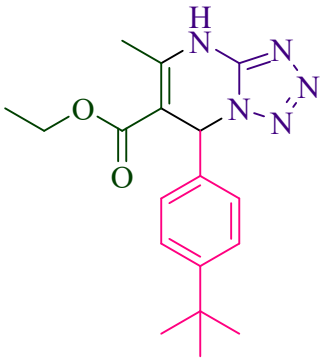
Light yellow solid, mp 220-222 °C. (Lit. [4] 218-220 °C) IR (KBr): ν_{max} = 3246, 3181, 3083, 2948, 2844, 1705, 1652, 1573, 1525, 1351, 1309, 1279, 1226, 1105, 828, 719 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ = 1.02 (t, J = 7.1 Hz, 3H), 2.47 (s, 3H), 3.91-3.99 (m, 2H), 6.84 (s, 1H), 7.64 (d, J = 8.7 Hz, 2H), 8.21 (d, J = 8.7 Hz, 2H), 11.46 (s, 1H). Anal. Calcd for $C_{14}H_{14}N_6O_4$: C, 50.91, H, 4.27; N, 25.44. Found: C, 51.05; H, 4.24; N, 25.33

Ethyl 7-(2,6-dichlorophenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6c)



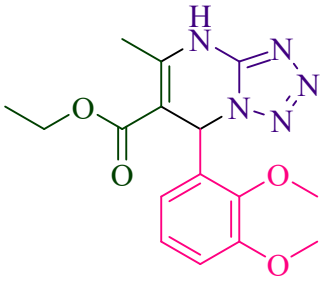
White solid, mp 248-250 °C. (Lit. [4] 249-252 °C) IR (KBr): ν_{max} = 3246, 3107, 3085, 2952, 2871, 1708, 1675, 1646, 1577, 1435, 1385, 1294, 1230, 1099, 1077, 1010, 844, 779 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.11 (t, J = 7.1 Hz, 3H), 2.65 (s, 3H), 4.04-4.13 (m, 2H), 7.21-7.27(m, 2H), 7.44 (dd, ^1J = 7.2 Hz, ^2J = 2.0 Hz, 1H), 7.58-7.59 (m, 1H), 11.16 (s, 1H). Anal. Calcd for $C_{14}H_{13}Cl_2N_5O_2$: C, 47.47, H, 3.70; N, 19.77. Found: C, 47.64; H, 3.65; N, 19.87.

Ethyl 7-(4-(tert-butyl)phenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6d)



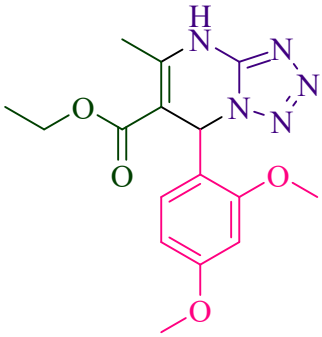
Dark white solid, mp 178-180 °C. IR (KBr): ν_{max} = 3244, 3181, 3055, 2962, 2909, 2869, 1710, 1649, 1574, 1416, 1307, 1275, 1223, 1097, 1070, 831, 705 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.16 (t, J = 7.1 Hz, 3H), 1.29 (s, 9H), 2.68 (s, 3H), 4.07-4.16 (m, 2H), 6.73 (s, 1H), 7.26 (s, 1H), 7.28 (s, 1H), 7.35 (d, J = 8.4 Hz, 2H), 10.59 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.03, 151.91, 148.83, 145.87, 136.79, 126.91, 125.78, 99.48, 60.48, 59.22, 34.62, 31.25, 19.55, 14.05. Anal. Calcd for $C_{18}H_{23}N_5O_2$: C, 63.32; H, 6.79; N, 20.51. Found: C, 62.91; H, 6.83; N, 20.40.

Ethyl 7-(2,3-dimethoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6e)



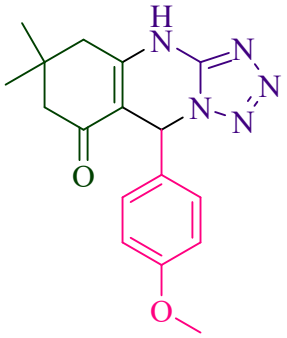
Dark white solid, mp 169-171 °C. IR (KBr): ν_{max} = 3252, 3100, 3060, 2966, 2926, 2851, 1686, 1661, 1589, 1486, 1465, 1322, 1271, 1235, 1097, 1003, 822, 783, 762 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.16 (t, J = 7.1 Hz, 3H), 2.65 (s, 3H), 3.82 (s, 3H), 3.85 (s, 3H), 4.05-4.13 (m, 2H), 6.89 (dd, ^{1}J = 8.0 Hz, ^{2}J = 1.5 Hz, 1H), 6.93-6.96 (m,2H), 7.00-7.04 (m, 1H), 10.23 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.03, 152.87, 148.92, 145.58, 132.83, 123.76, 121.28, 113.26, 98.96, 60.61, 60.37, 56.04, 55.77, 29.72, 19.75, 14.09. Anal. Calcd for $C_{16}H_{19}N_5O_4$: C, 55.64; H, 5.55; N, 20.28. Found: C 55.45; H, 5.62; N, 20.24.

Ethyl 7-(2,4-dimethoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6f)



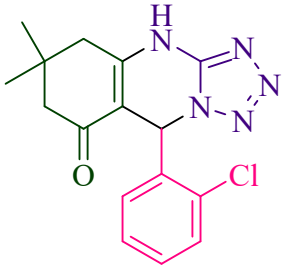
White solid, mp 225-228 °C. IR (KBr): ν_{max} = 3243, 3180, 3091, 2943, 2843, 1711, 1612, 1578, 1508, 1463, 1279, 1219, 1101, 1034, 840, 827, 778 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.19 (t, J = 7.1 Hz, 3H), 2.62 (s, 3H), 3.74 (s, 3H), 3.79 (s, 3H), 4.05-4.13 (m, 2H), 6.41 (d, J = 2.3 Hz, 1H), 6.44 (dd, ^{1}J = 8.4 Hz, ^{2}J = 2.4 Hz, 1H), 6.88 (s, 1H), 7.25 (d, J = 8.4 Hz, 1H), 9.97 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.23, 161.42, 158.46, 149.24, 145.39, 130.61, 126.00, 120.31, 104.29, 98.89, 60.29, 55.59, 55.39, 29.72, 19.62, 14.09. Anal. Calcd for $C_{16}H_{19}N_5O_4$: C, 55.64; H, 5.55; N, 20.28. Found: C, 55.53; H, 5.59; N, 20.16.

6,6-dimethyl-9-(4-methoxyphenyl)-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8a)



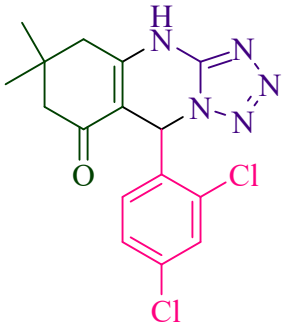
White solid, mp 238-240 °C. (Lit. [3] 226-228 °C) IR (KBr): ν_{max} = 3236, 3172, 3057, 2961, 2927, 2837, 1644, 1577, 1512, 1426, 1368, 1253, 1172, 1035, 850, 731 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 1.14 (s, 3H), 1.18 (s, 3H), 2.32 (ABq, J = 16.7 Hz, 2H), 2.73 (ABq, J = 17.2 Hz, 2H), 3.78 (s, 3H), 6.71 (s, 1H), 6.86 (d, J = 8.7 Hz, 2H), 7.27-7.28 (m, 2H), 11.31 (s, 1H). Anal. Calcd for $C_{17}H_{19}N_5O_2$: C, 62.75; H, 5.89; N, 21.52. Found: C, 62.34; H, 5.93; N, 21.41

9-(2-chlorophenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8b)



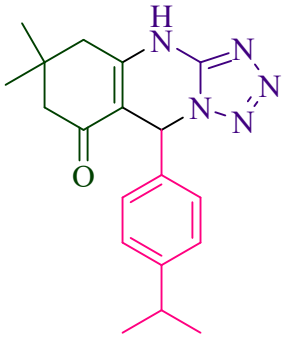
White solid, mp 272-274 °C. (Lit. [3] >270 °C) IR (KBr): ν_{max} = 3241, 3173, 3055, 2964, 2937, 2890, 1651, 1587, 1428, 1369, 1305, 1047, 987, 757, 719 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ = 1.01 (s, 3H), 1.06 (s, 3H), 2.08-2.23 (m, 2H), 2.58 (s, 2H), 6.90 (s, 1H), 7.30-7.33 (m, 2H), 7.41-7.44 (m, 2H), 11.71 (s, 1H). Anal. Calcd for $C_{16}H_{16}ClN_5O$: C, 58.27; H, 4.89; N, 21.24. Found: C, 58.10; H, 4.94; N, 21.14.

9-(2,4-dichlorophenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8c)



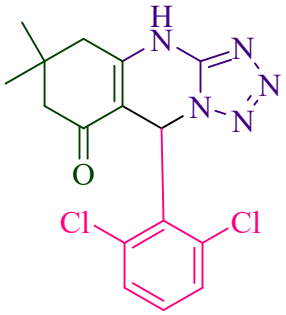
Cream solid, mp 291-294 °C. (Lit. [3] >270 °C) IR (KBr): ν_{max} = 3229, 3164, 3055, 2962, 2931, 2890, 2809, 1649, 1580, 1423, 1368, 1104, 852, 812, 775, 747 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ = 1.01 (s, 3H), 1.05 (s, 3H), 2.09-2.23 (m, 2H), 2.57 (s, 2H), 6.89 (s, 1H), 7.41 (dd, ^1J = 7.9 Hz, ^2J = 2.0 Hz, 1H) 7.48 (br s, 1H), 7.61 (d, J = 2.0 Hz, 1H), 11.75 (s, 1H). Anal. Calcd for $C_{16}H_{15}Cl_2N_5O$: C, 52.76; H, 4.15; N, 19.23. Found: C, 52.62; H, 4.18; N, 19.34.

9-(4-isopropylphenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8d)



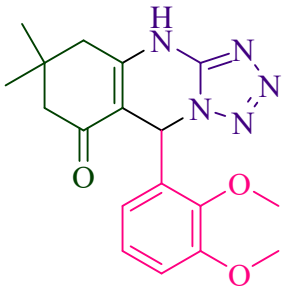
White solid, mp 284-286 °C. IR (KBr): ν_{max} = 3232, 3163, 3051, 2961, 2923, 2874, 1653, 1577, 1428, 1372, 1312, 859, 796, 739 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 1.15 (s, 3H), 1.18 (s, 3H), 1.21 (d, J = 6.9 Hz, 6H), 2.33 (s, 2H), 2.74 (ABq, J = 17.2 Hz, 2H), 2.87 (Sep, J = 6.9 Hz, 1H), 6.74 (s, 1H) 7.18 (d, J = 8.2 Hz, 2H), 7.26 (d, J =8.4 Hz, 2H), 11.35 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 192.79, 148.58, 148.06, 147.78, 135,49, 126.01, 125.99, 106.58, 56.97, 49.48, 39.81, 32.77, 31.93, 27.81, 26.64, 22.80, 22.77. Anal. Calcd for $C_{19}H_{23}N_5O$: C, 67.63; H, 6.87; N, 20.76. Found: C, 67.50; H, 6.91; N, 20.68.

9-(2,6-dichlorophenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8e)



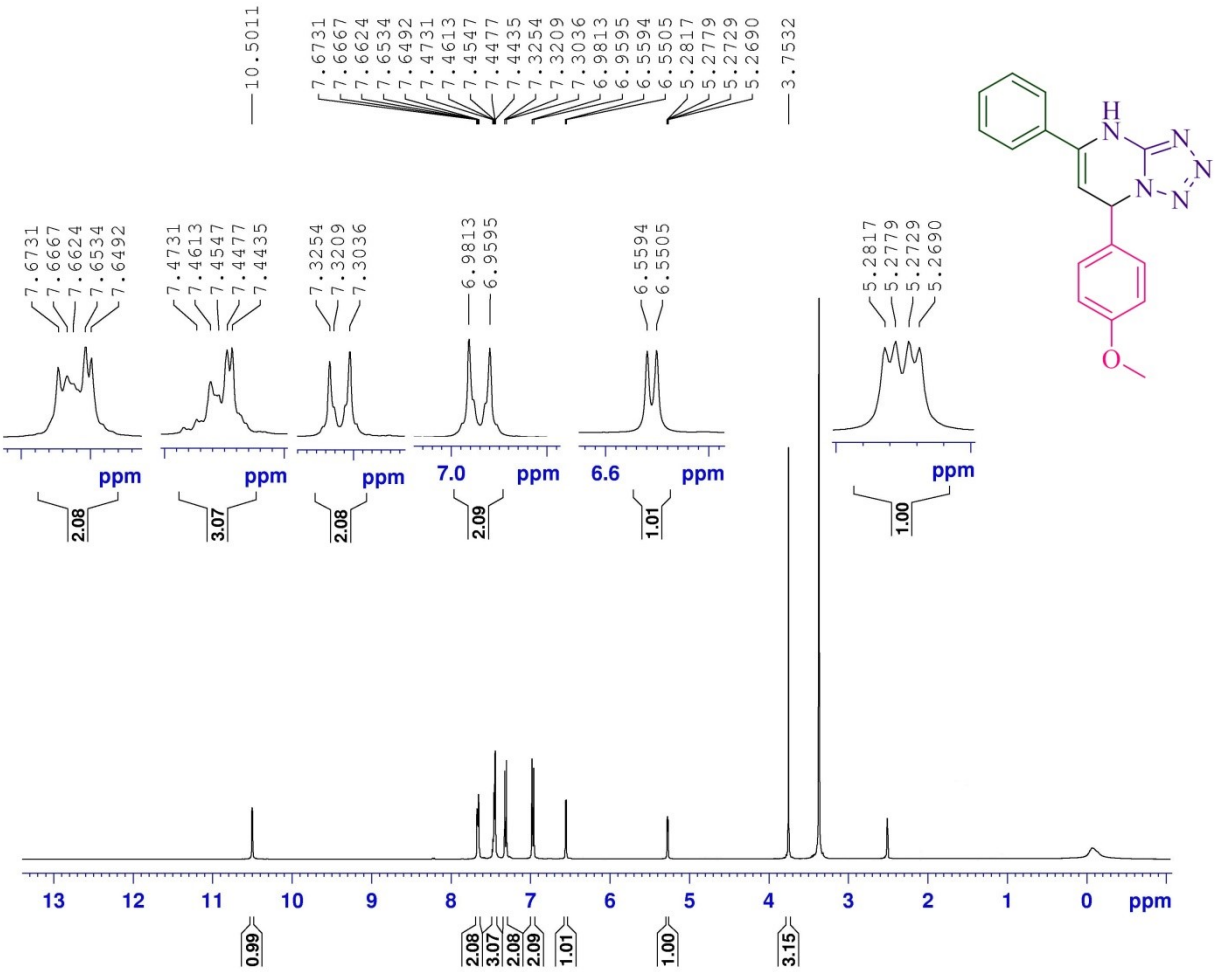
Milky solid, mp 272-274 °C. IR (KBr): ν_{max} = 3234, 3169, 3056, 2960, 2888, 2801, 1651, 1581, 1431, 1370, 1339, 1313, 1094, 987, 852, 782, 756 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 1.17 (s, 3H), 1.19 (s, 3H), 2.31 (ABq, J = 16.5 Hz, 2H), 2.70 (s, 2H), 7.20-7.25 (m, 2H), 7.49 (dd, ^1J = 6.5 Hz, ^2J = 2.8 Hz, 1H), 7.55 (s, 1H), 11.34 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 194.02, 150.84, 149.38, 137.60, 134.22, 132.19, 130.32, 129.89, 129.05, 105.09, 55.05, 50.53, 40.92, 32.73, 28.73, 27.75. Anal. Calcd for $C_{16}H_{15}Cl_2N_5O$: C, 52.76; H, 4.15; N, 19.23. Found: C, 52.61; H, 4.17; N, 19.15.

9-(2,3-dimethoxyphenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8f)

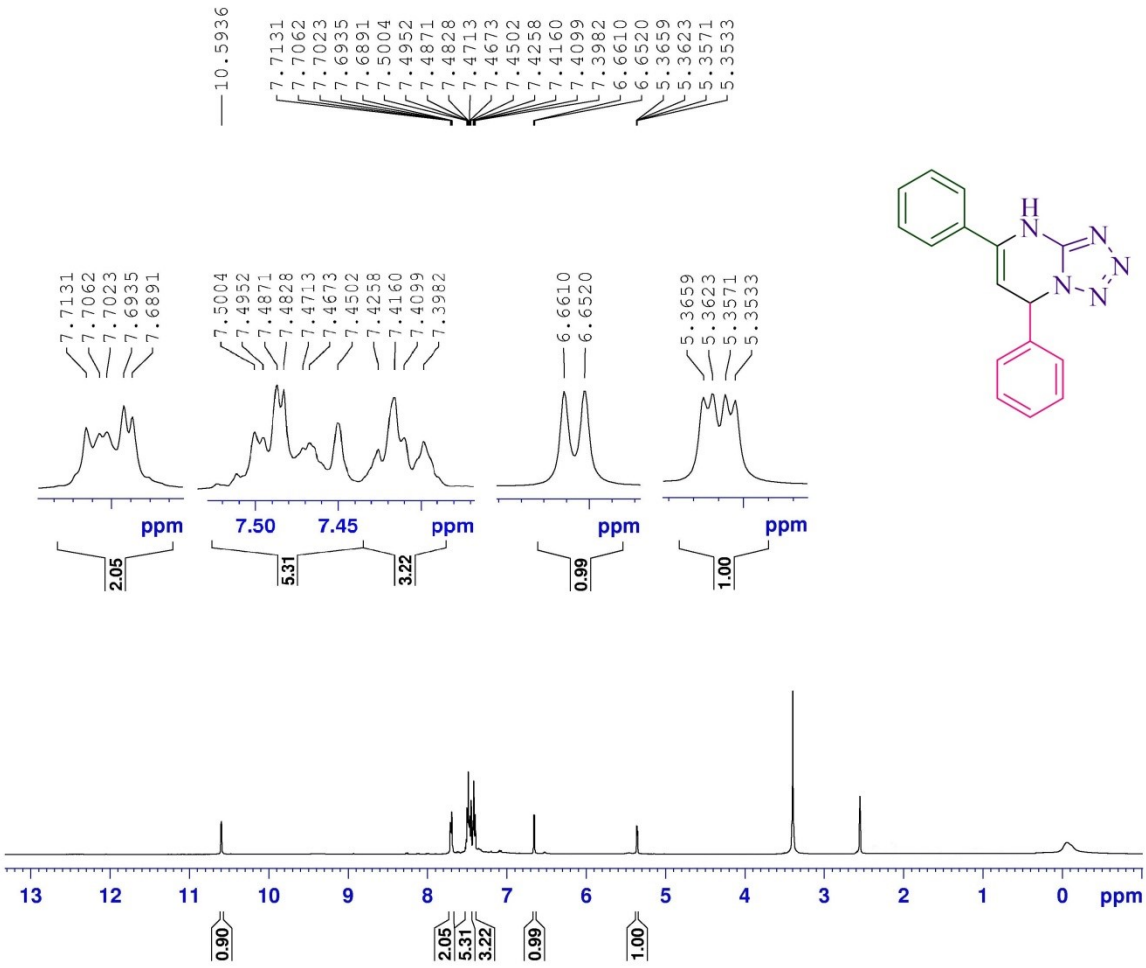


White solid, mp 256-258 °C. IR (KBr): ν_{max} = 3251, 3172, 3063, 2933, 2848, 1644, 1574, 1483, 1428, 1368, 1267, 1066, 1004, 819, 770, 739 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 1.14 (s, 3H), 1.16 (s, 3H), 2.29 (ABq, J = 16.4 Hz, 2H), 2.72 (ABq, J = 17.1 Hz, 2H), 3.78 (s, 3H), 3.84 (s, 3H), 6.89 (dd, ^1J = 7.2 Hz, ^2J = 2.5 Hz, 1H), 6.94 (s, 1H) 7.00-7.05 (m, 2H), 11.44 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ =193.86, 152.81, 149.37, 149.11, 147.17, 132.02, 123.87, 121.30, 113.36, 107.07, 60.53, 55.77, 54.93, 50.64, 40.94, 33.00, 28.50, 28.00. Anal. Calcd for $C_{18}H_{21}N_5O_3$: C, 60.83; H, 5.96; N, 19.71. Found: C, 60.96; H, 6.01; N, 19.62.

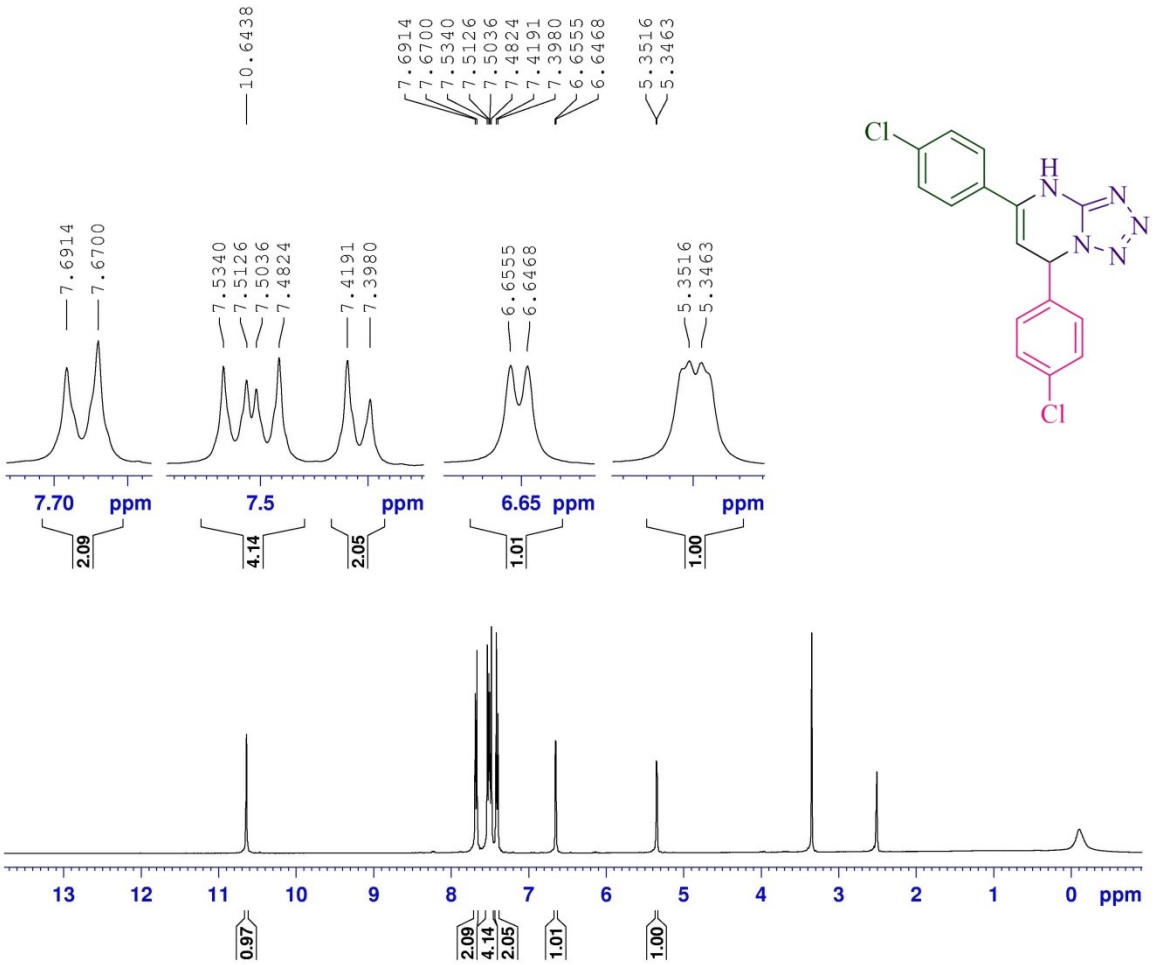
7. ^1H NMR and ^{13}C NMR Spectra of the Products:



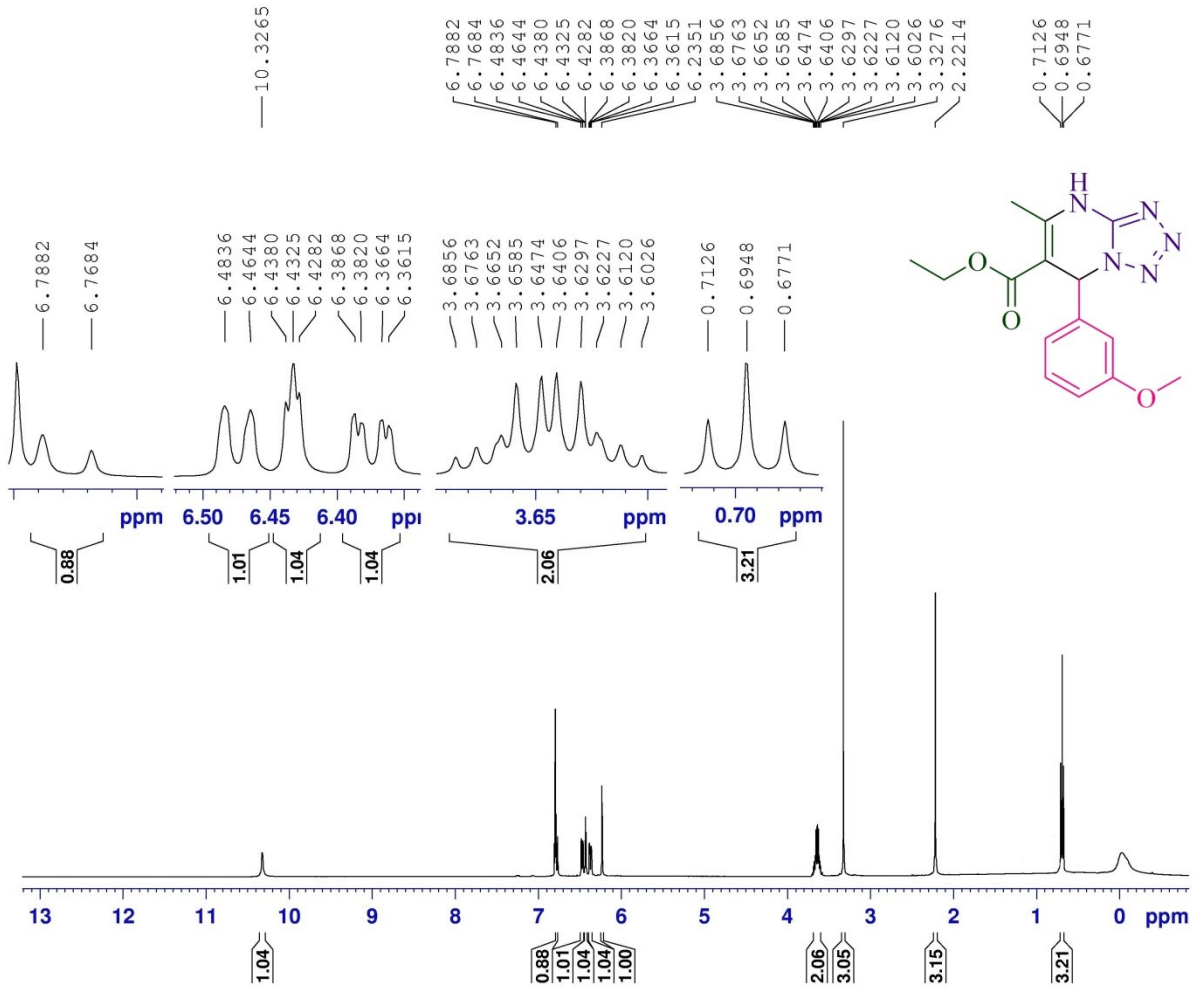
7-(4-Methoxy-phenyl)-5-phenyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine (Scheme 3, 4a);^{1}H NMR (400 MHz, DMSO-d_6)



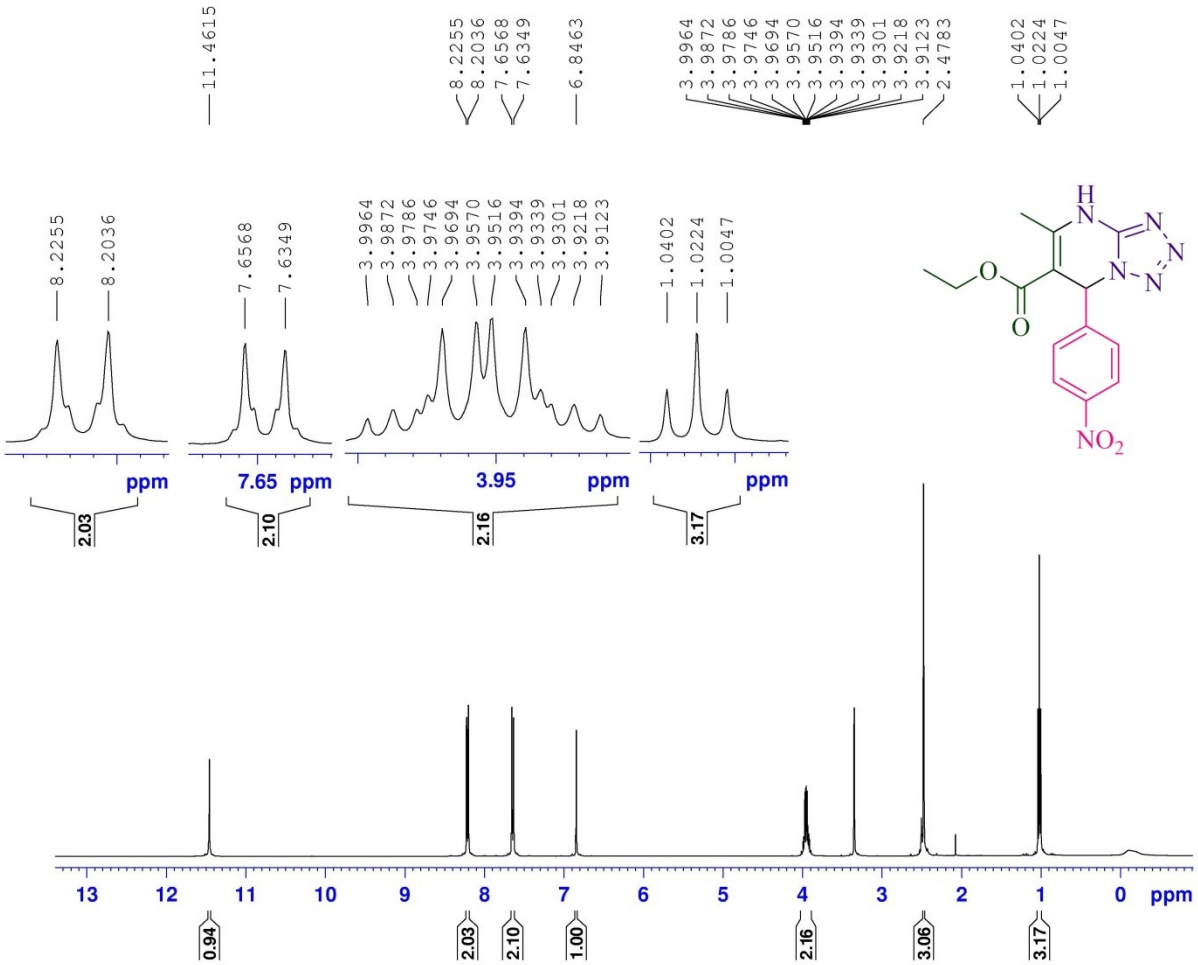
5,7-Diphenyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine (Scheme 3, 4b);^{1}H NMR (400 MHz, DMSO-d_6)



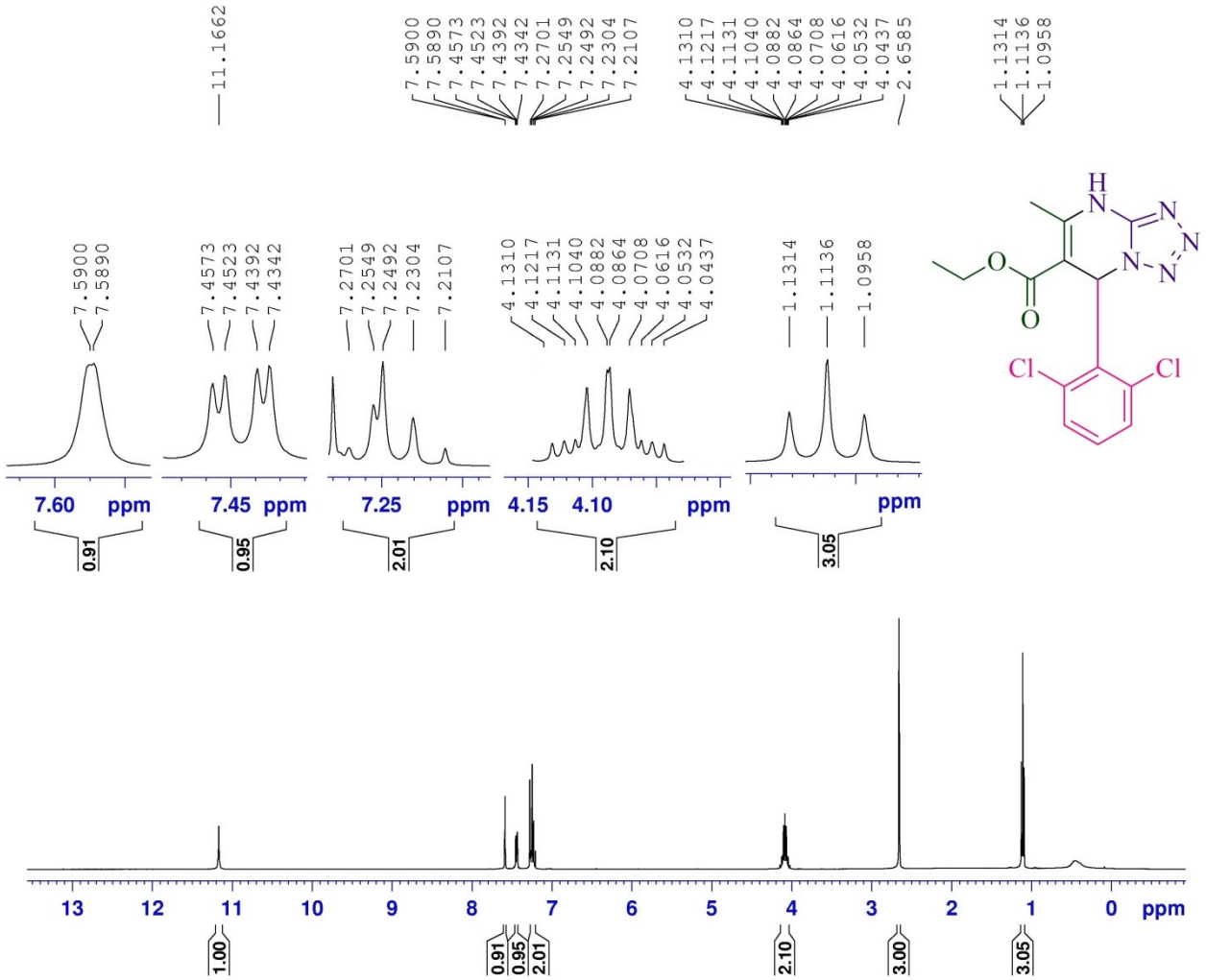
5,7-bis(4-chlorophenyl)-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine (Scheme 3, 4c);^{1}H NMR (400 MHz, DMSO-*d*$_6$)



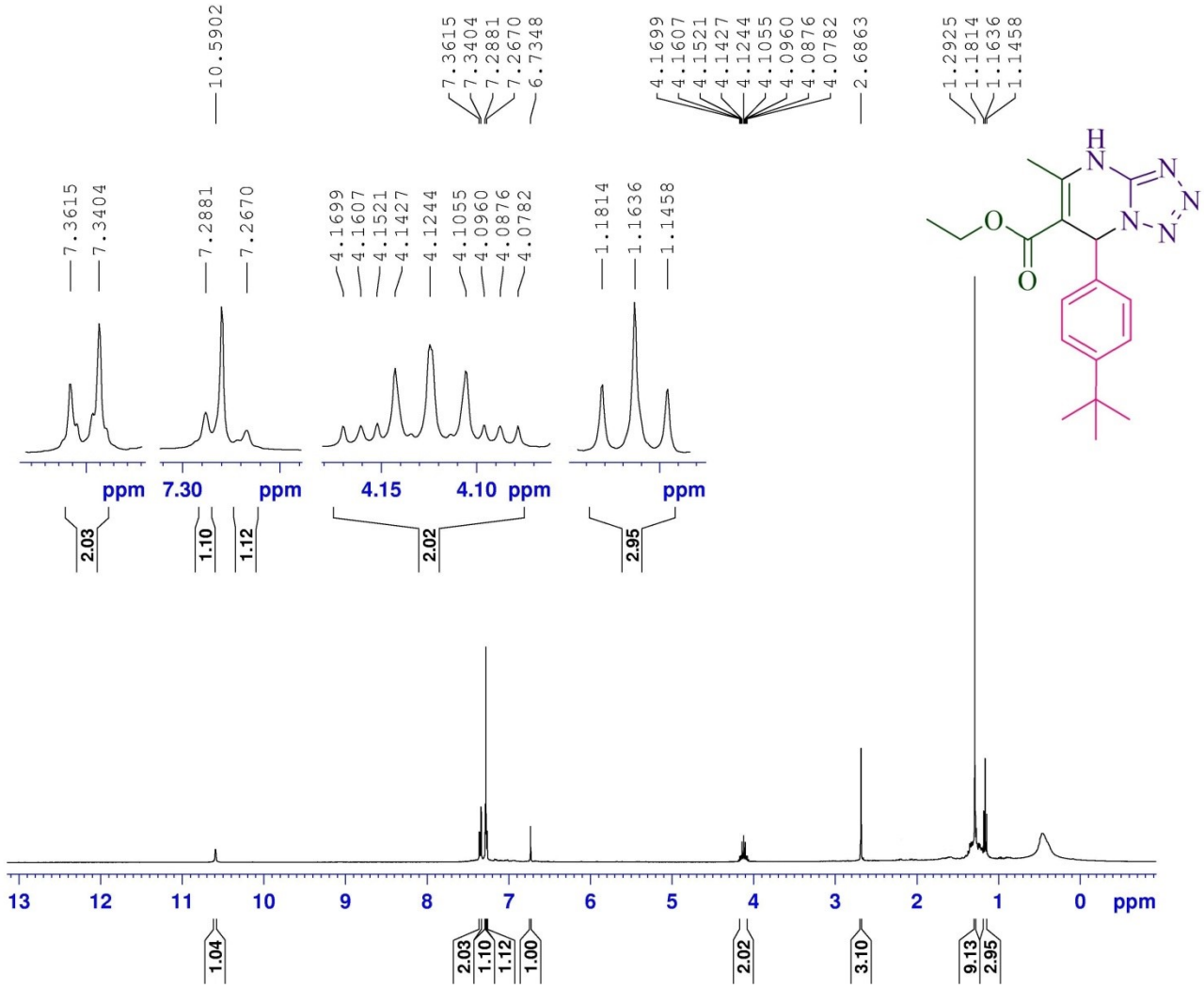
Ethyl7-(3-methoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6a);^{1}H NMR (400 MHz,$CDCl_3$)



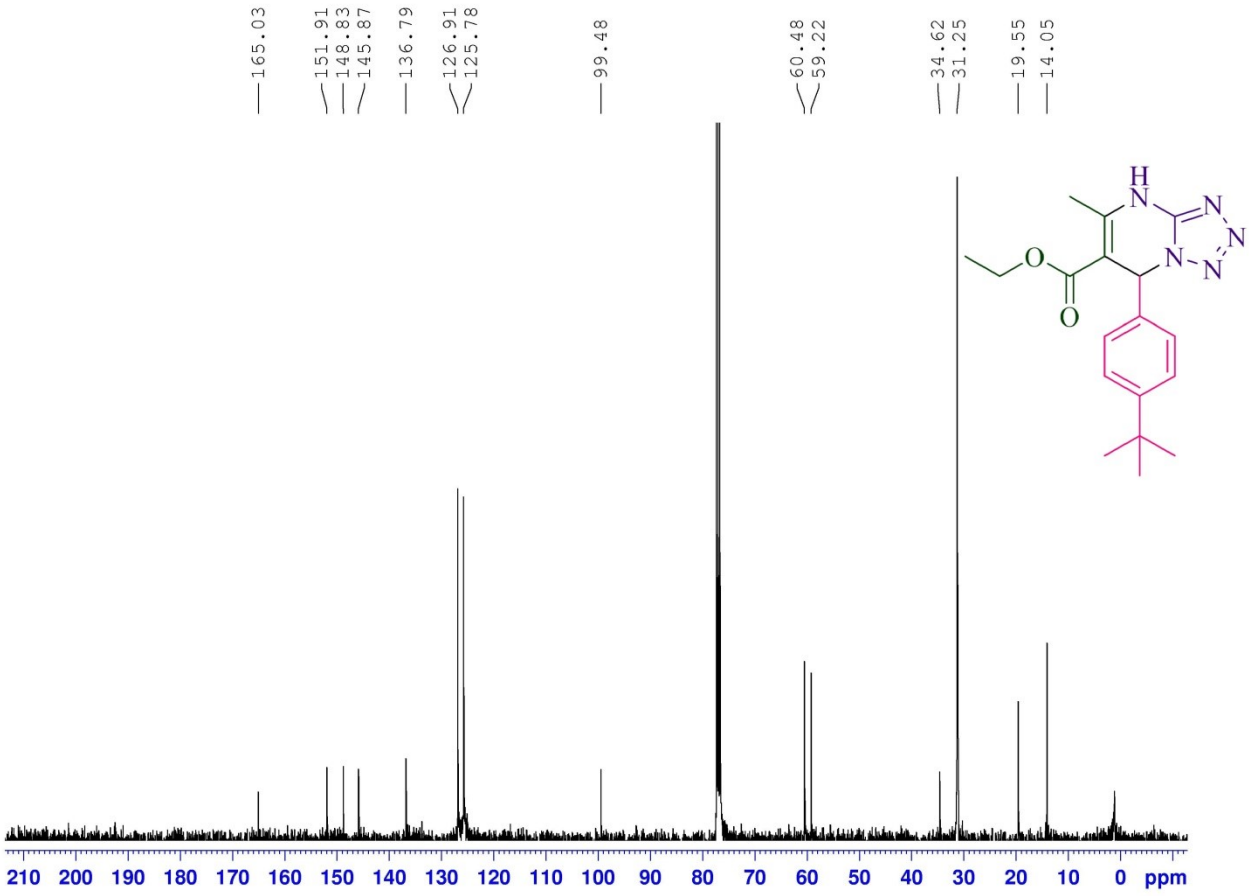
Ethyl5-methyl-7-(4-nitrophenyl)-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6b);^{1}H NMR (400 MHz, DMSO-d_6)



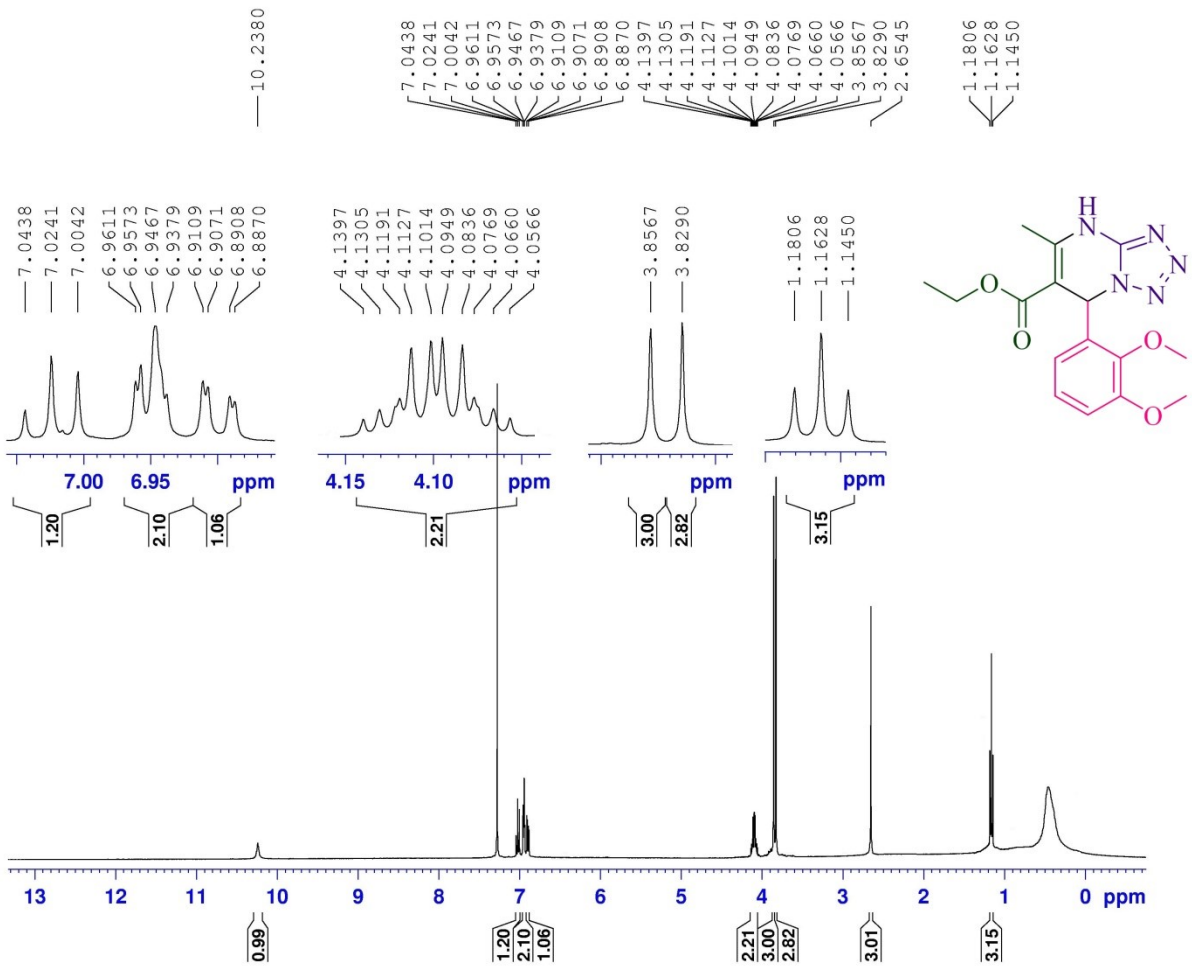
Ethyl7-(2,6-dichlorophenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6c);^{1}H NMR (400 MHz,$CDCl_3$)



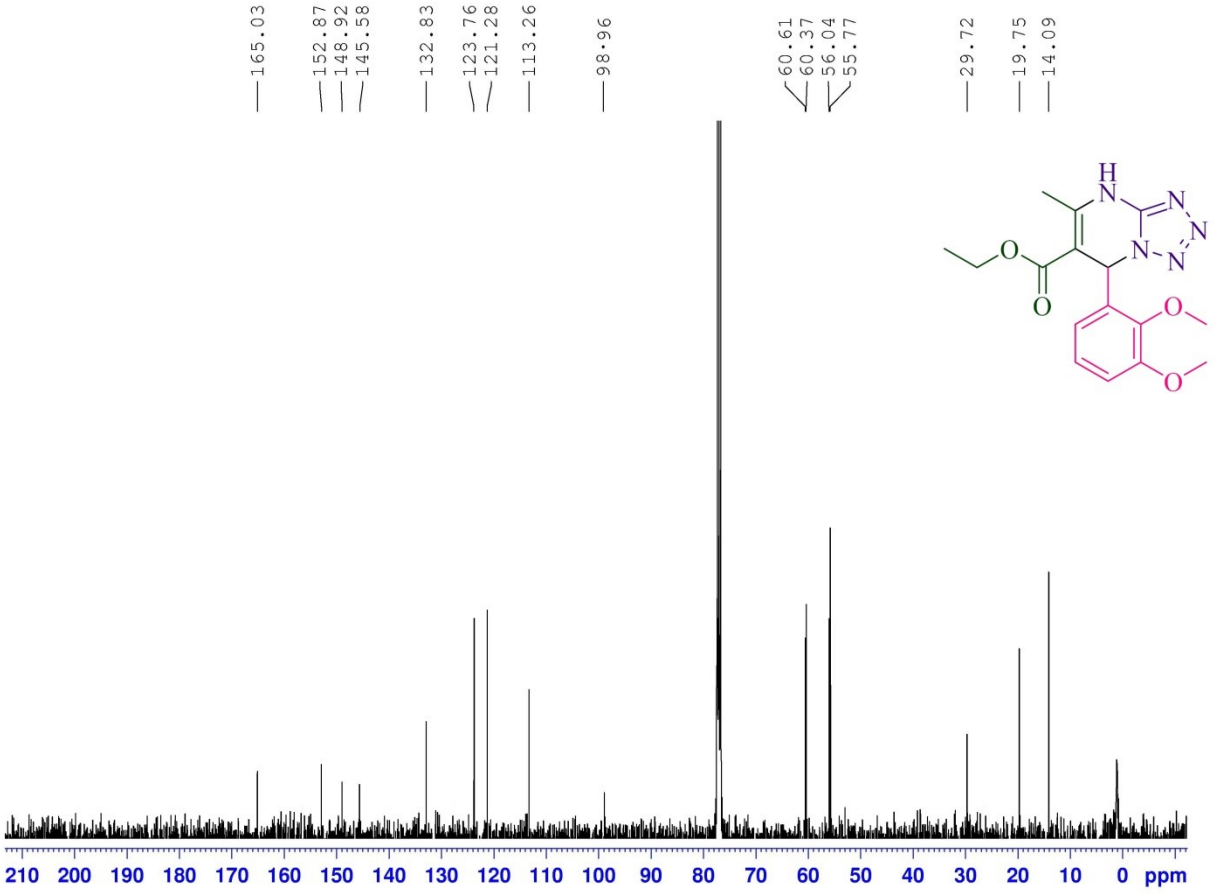
Ethyl7-(4-(tert-butyl)phenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6d); ^{1}H NMR (400 MHz,$CDCl_3$)



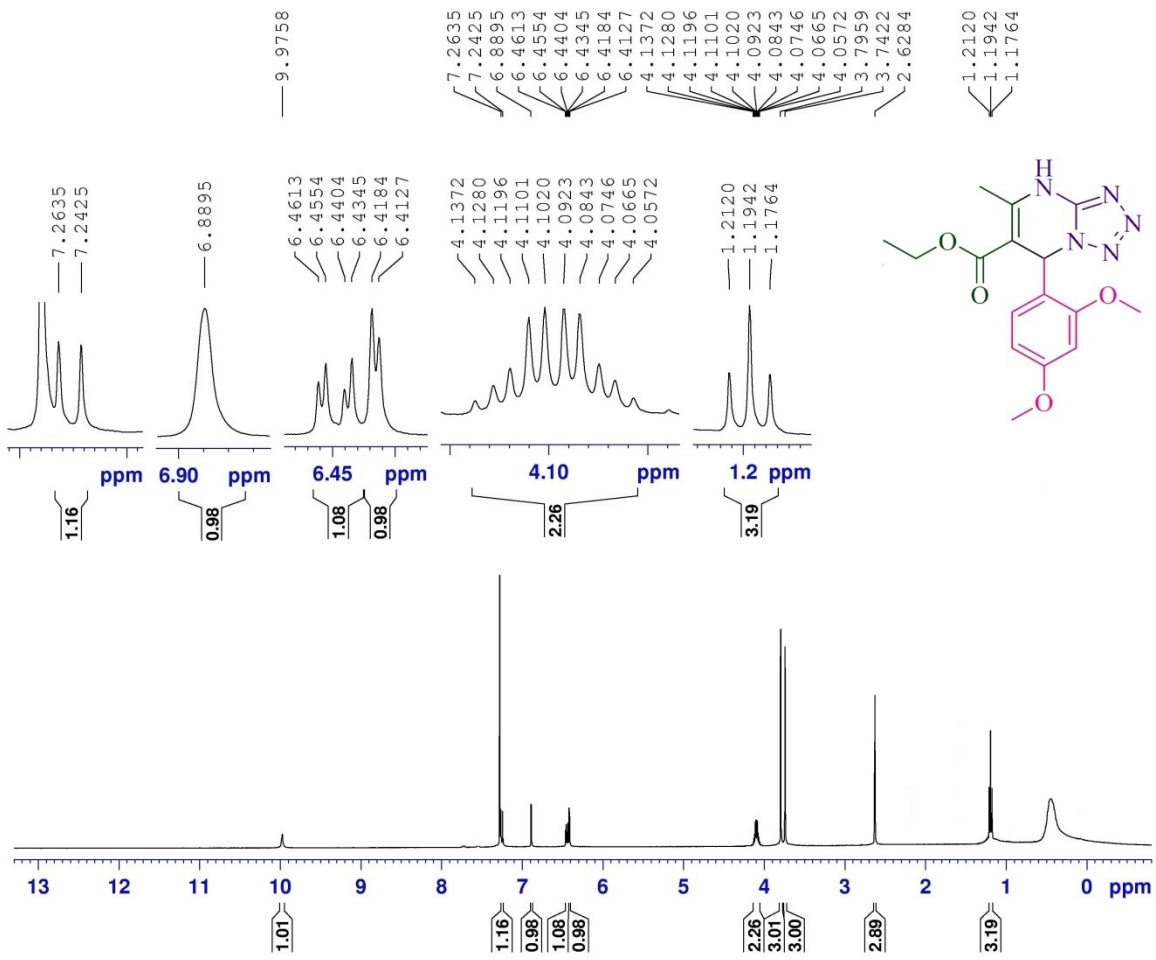
Ethyl 7-(4-(tert-butyl)phenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6d); ^{13}C NMR (100 MHz, $CDCl_3$)



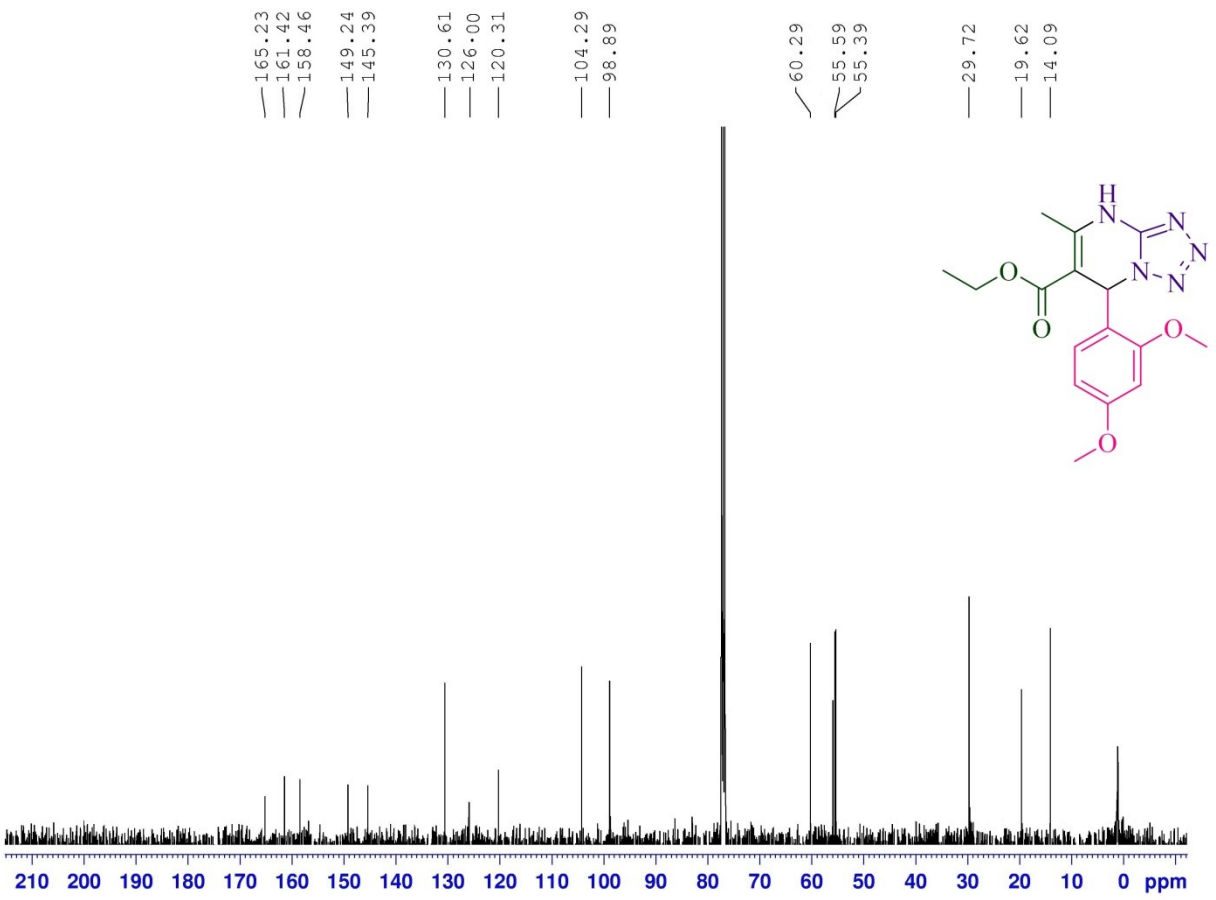
Ethyl7-(2,3-dimethoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6e); ^{1}H NMR (400 MHz,$CDCl_3$)



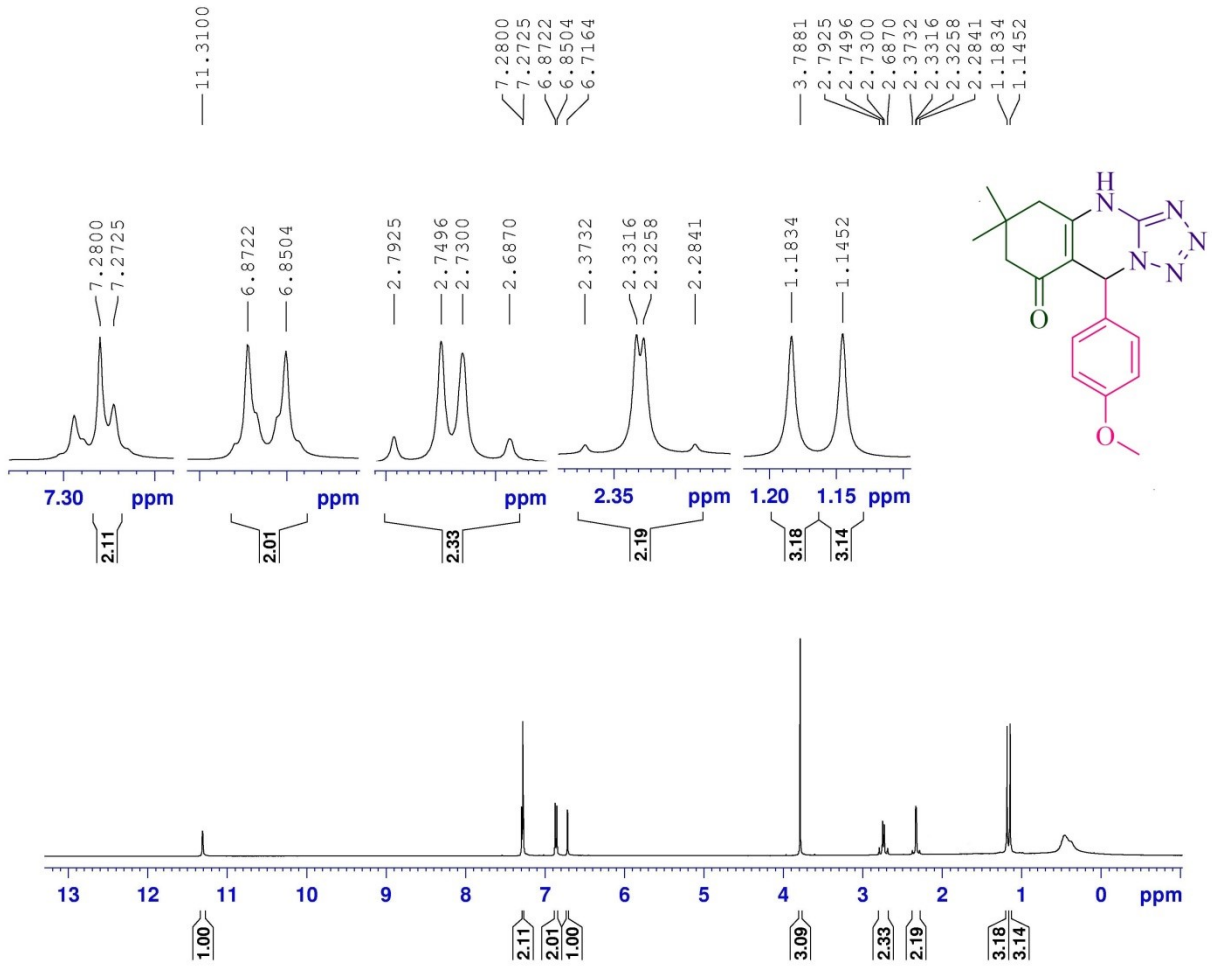
Ethyl 7-(2,3-dimethoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6e);^{13}C NMR (100 MHz, $CDCl_3$)



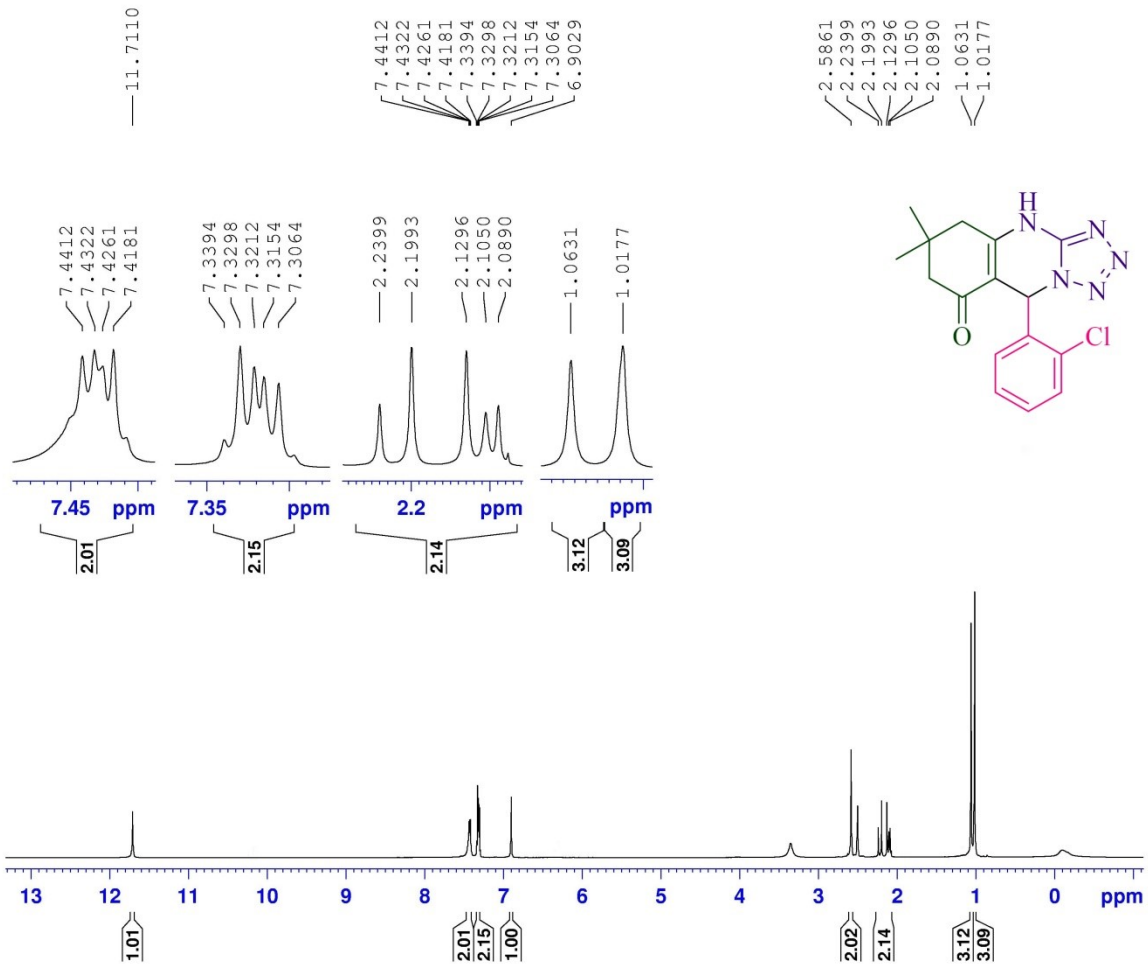
Ethyl 7-(2,4-dimethoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6f); ^{1}H NMR (400 MHz,$CDCl_3$)



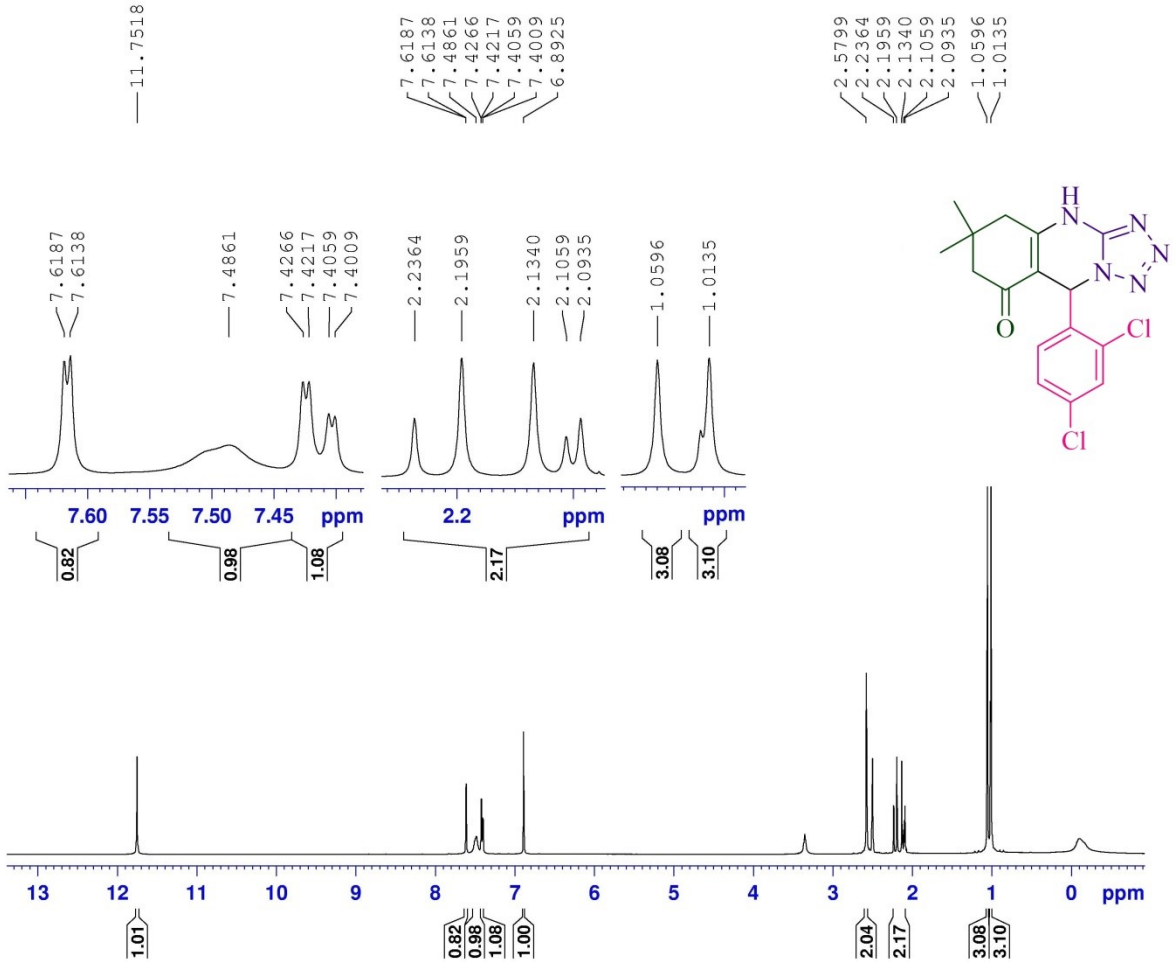
Ethyl 7-(2,4-dimethoxyphenyl)-5-methyl-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine-6-carboxylate (Scheme 3, 6f); ^{13}C NMR (100 MHz, $CDCl_3$)



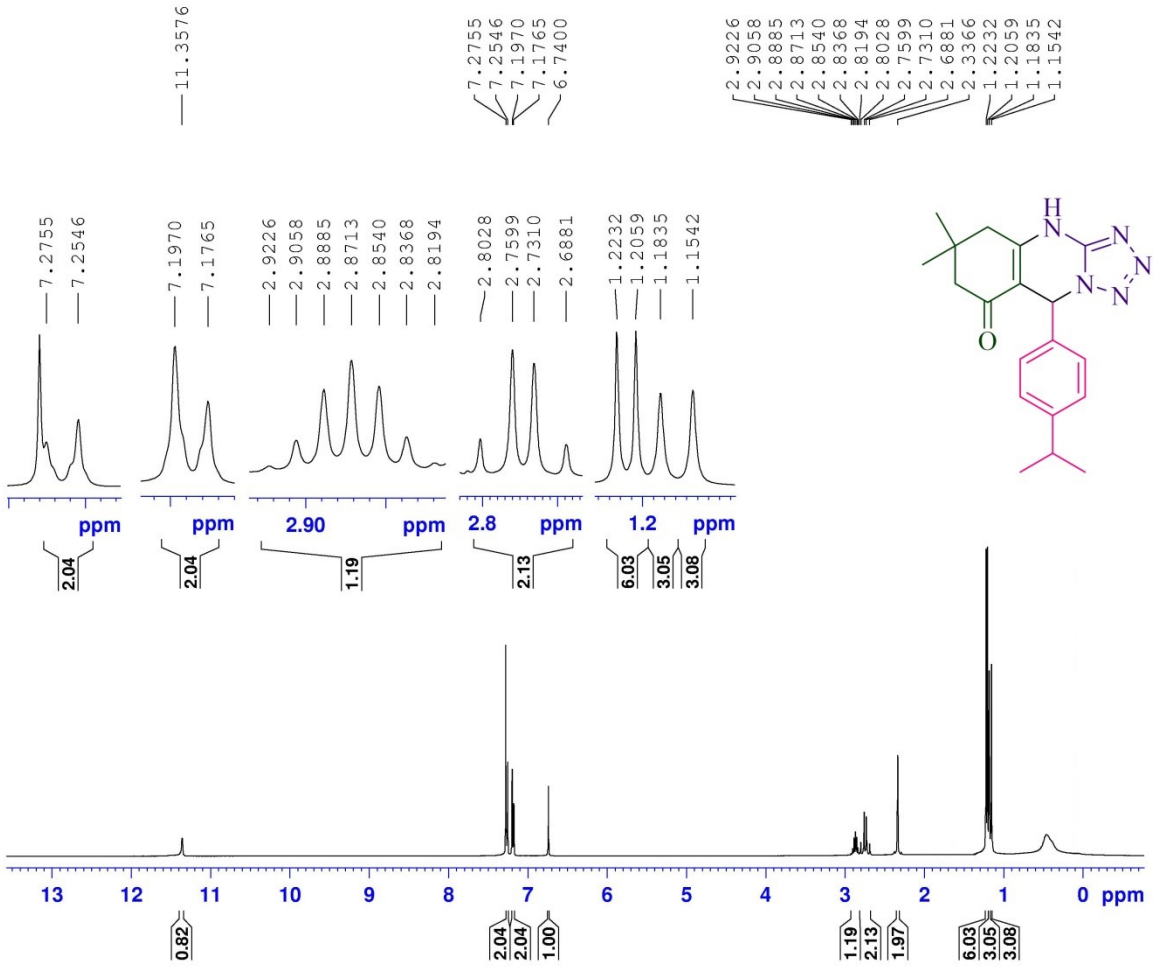
6,6-dimethyl-9-(4-methoxyphenyl)-5,6,7,9-tetrahydrotetrazolo[1,5-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8a); ^{1}H NMR (400 MHz,$CDCl_3$)



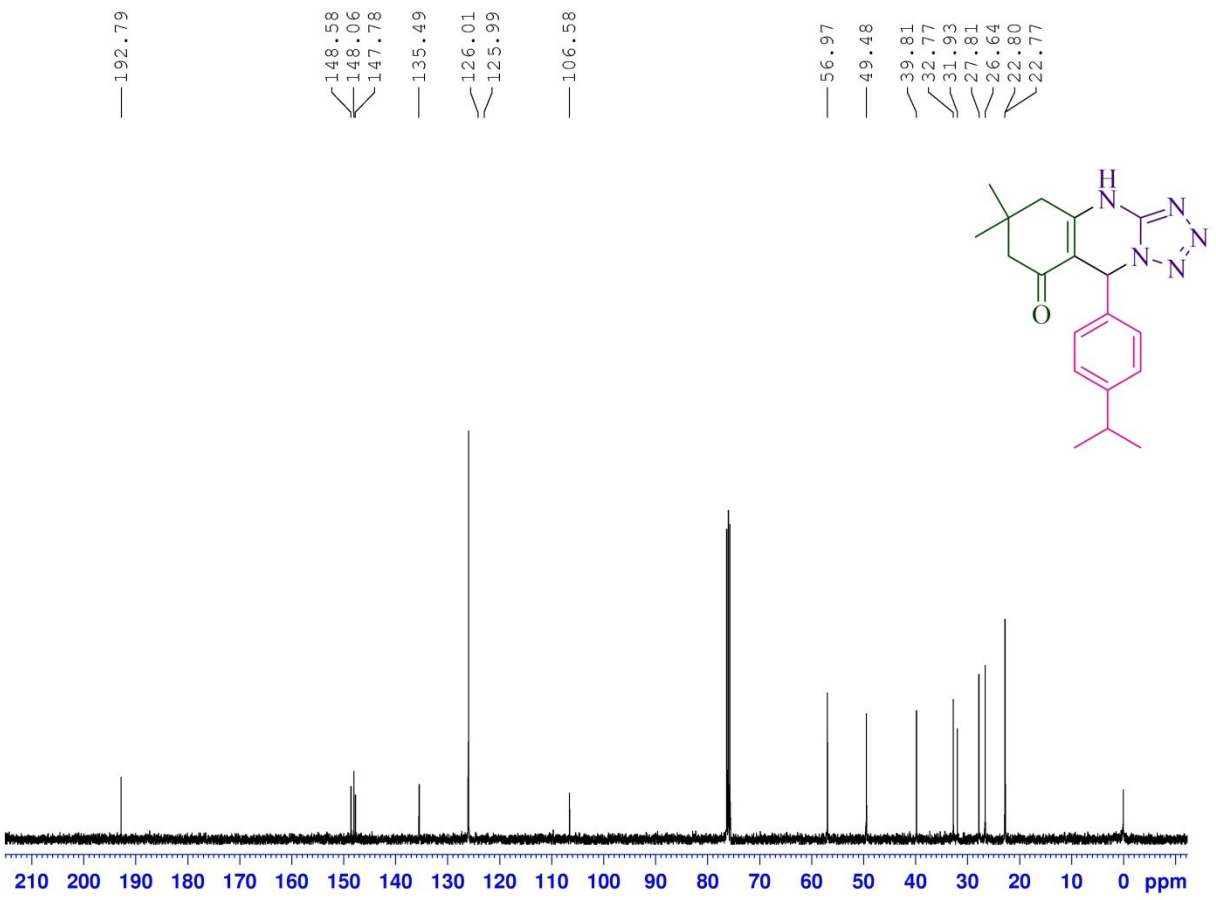
9-(2-chlorophenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8b); ^{1}H NMR (400 MHz, DMSO-d_6)



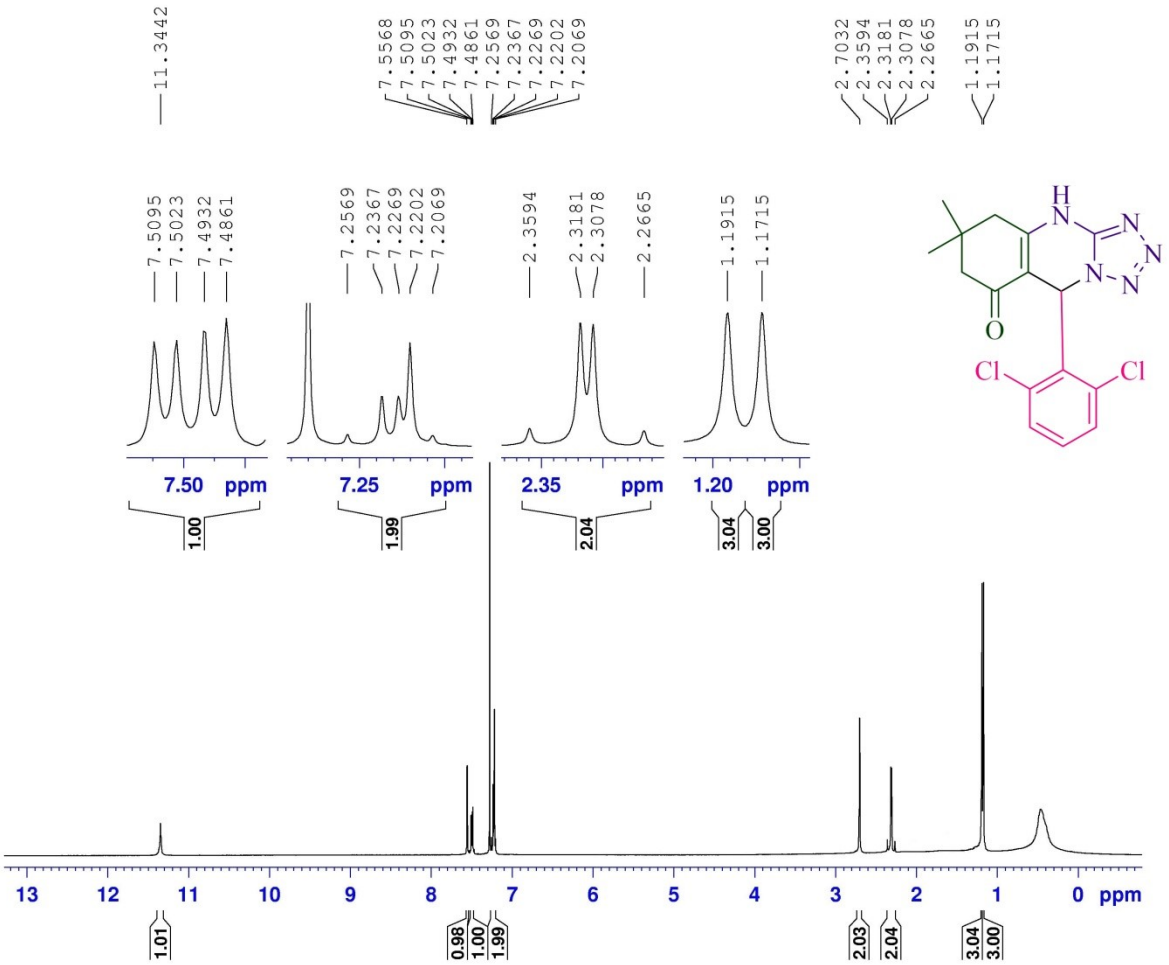
9-(2,4-dichlorophenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8c); ^{1}H NMR (400 MHz, DMSO-d_6)



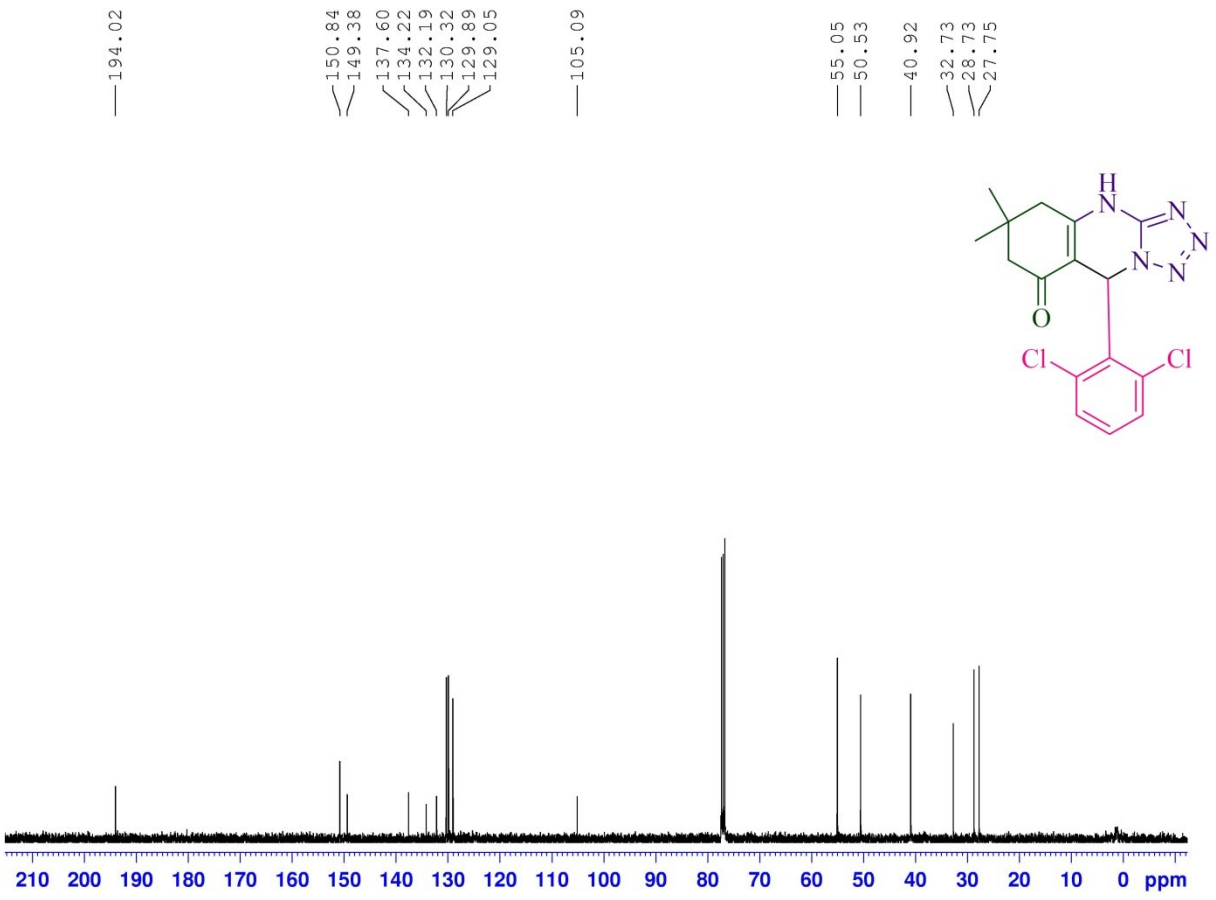
9-(4-isopropylphenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8d); ^{1}H NMR (400 MHz,$CDCl_3$)



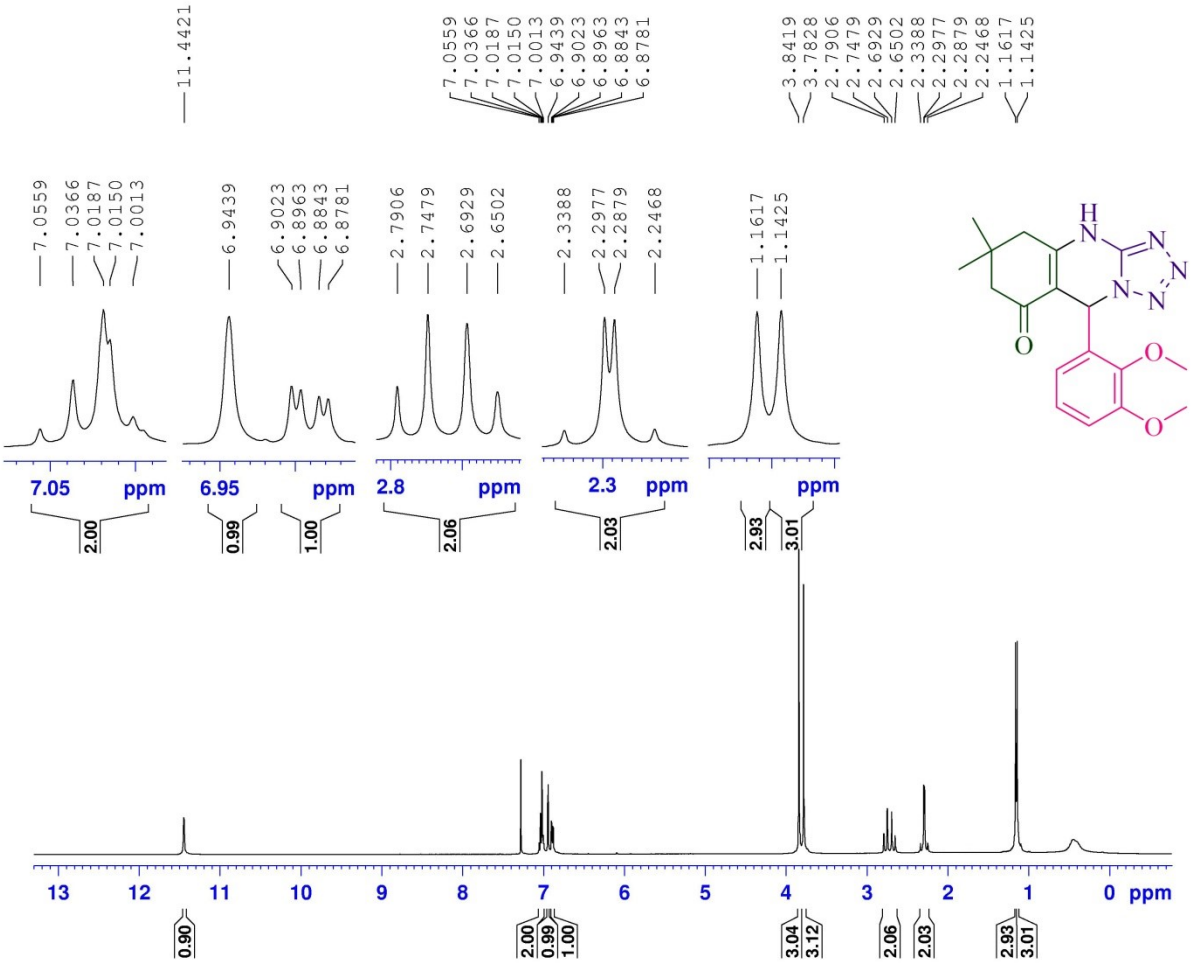
9-(4-isopropylphenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8d); ^{13}C NMR (100 MHz, $CDCl_3$)



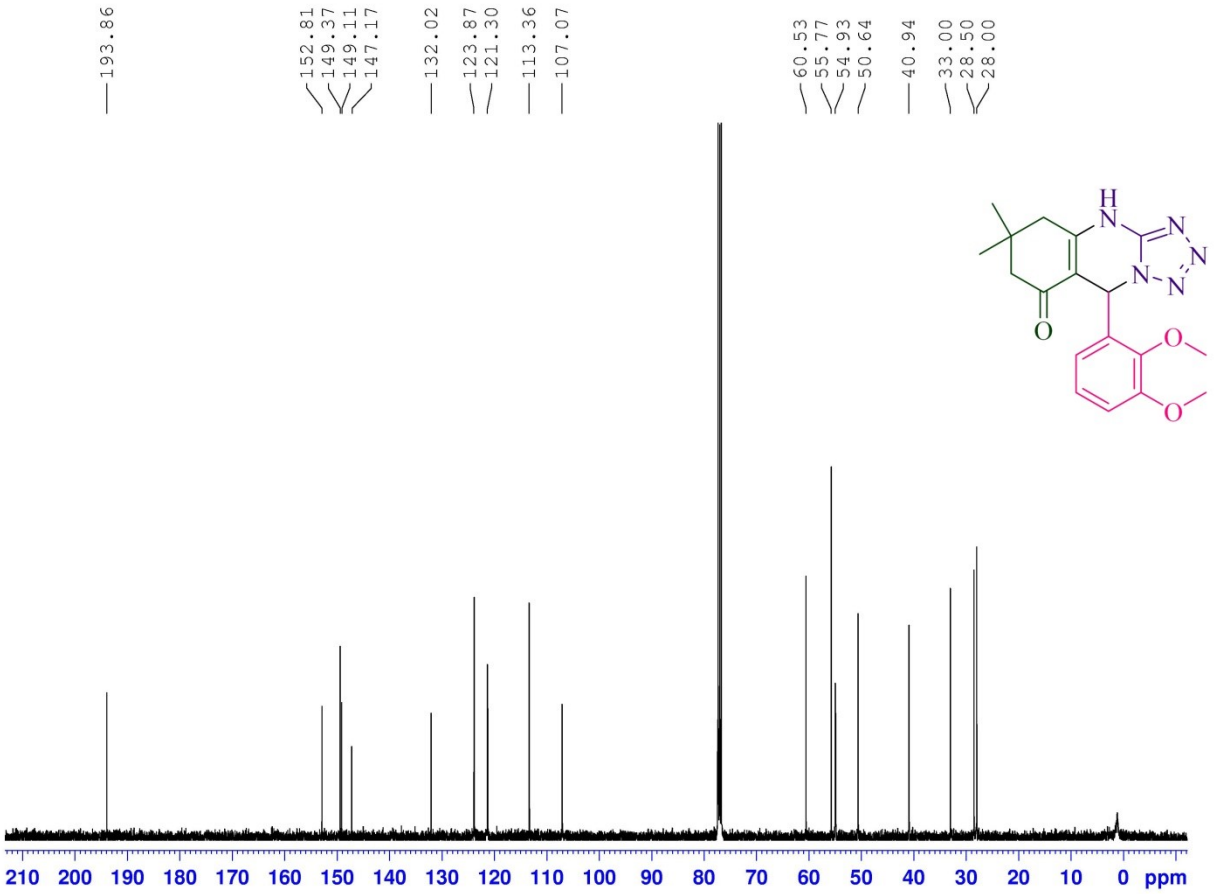
9-(2,6-dichlorophenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8e); ^{1}H NMR (400 MHz,$CDCl_3$)



9-(2,6-dichlorophenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8e); ^{13}C NMR (100 MHz, $CDCl_3$)



9-(2,3-dimethoxyphenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8f); ^{1}H NMR (400 MHz,$CDCl_3$)



9-(2,3-dimethoxyphenyl)-6,6-dimethyl-5,6,7,9-tetrahydrotetrazolo[5,1-*b*]quinazolin-8(4*H*)-one (Scheme 3, 8f); ^{13}C NMR (100 MHz, $CDCl_3$)

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