Postsynthetic modification of a Zn-MOF to yield an efficient H-bond catalyst in the preparation of biologically active macromolecules

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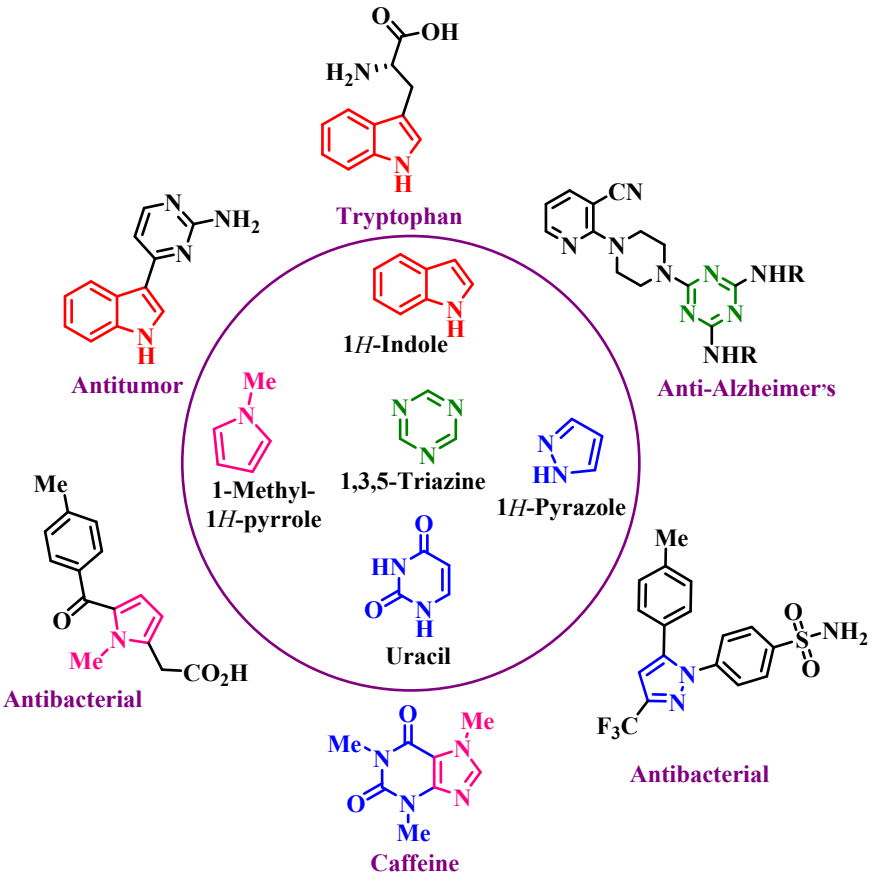
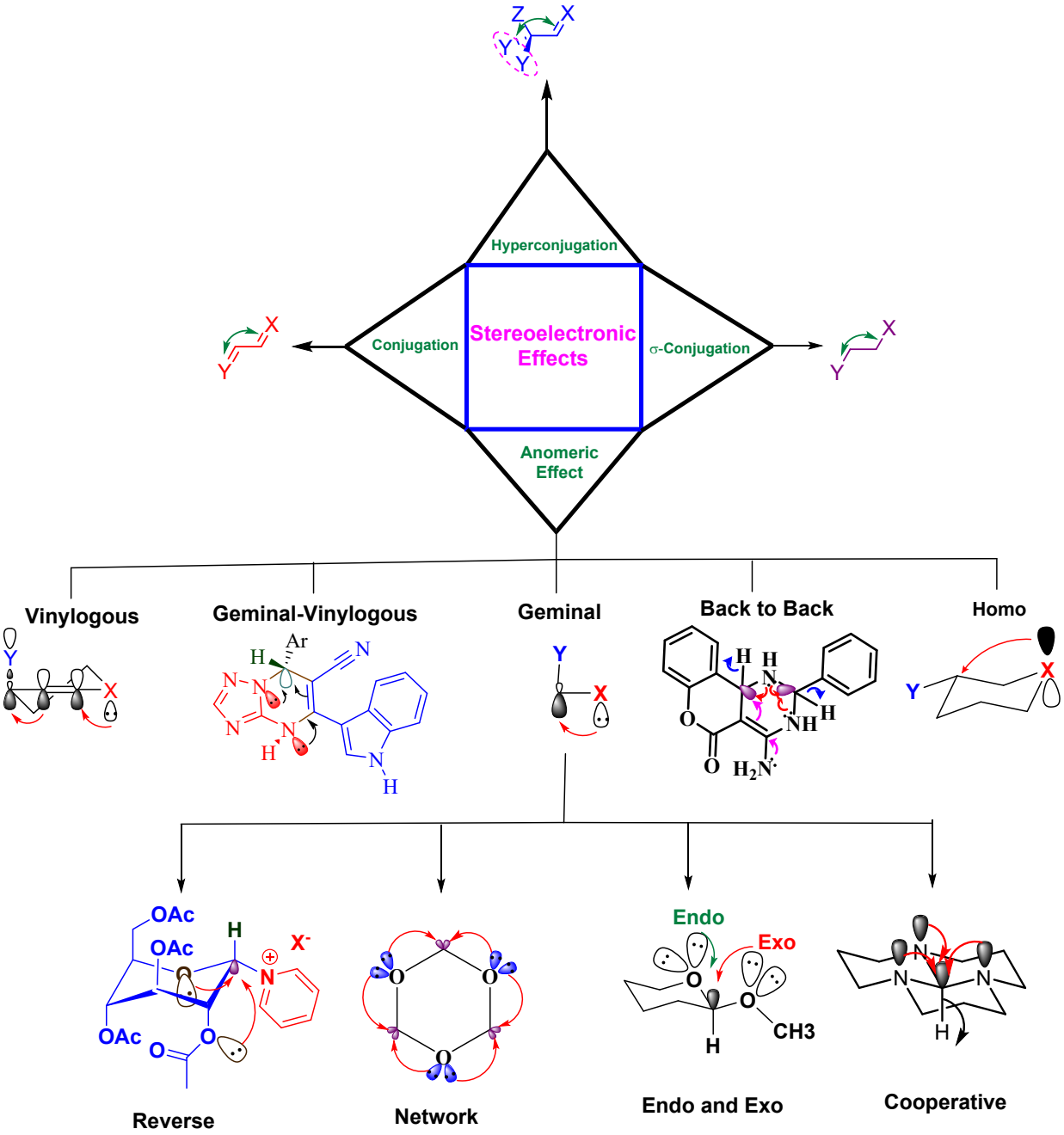
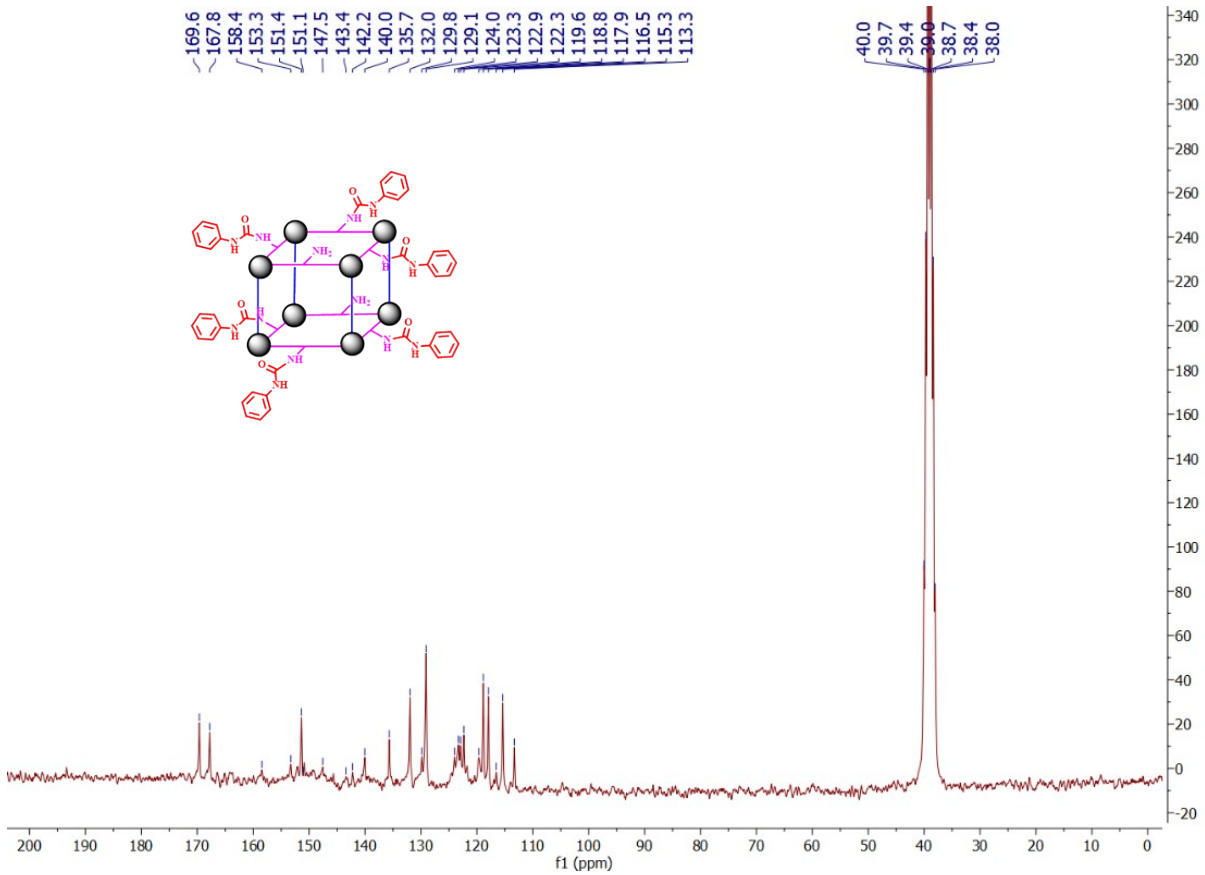


Scheme S1: Some structure of medicinal compounds containing triazine, 1*H*-indole, 1-methyl-1*H*-pyrrole, 1*H*-pyrazole, pyrimidine-2,4(1*H*,3*H*)-dione.



Scheme S2: Various kinds of stereoelectronic and anomeric effects



^{13}C-NMR spectrum of TMU-52-UR.

^{13}C NMR (63 MHz, DMSO) δ 169.6, 167.8, 158.4, 153.3, 151.4, 151.1, 147.5, 143.4, 142.2, 140.0, 135.7, 132.0, 129.8, 129.1, 124.0, 123.3, 122.3, 119.6, 118.8, 117.9, 116.5, 115.3, 113.3.

Antibacterial activity

The antibacterial activity of the synthesized compounds was investigated using a previously described Chinese Standard method [1]. Briefly, a suspension of *Staphylococcus aureus* (ATCC 25923) and *Escherichia coli* (ATCC 25922), as the representative Gram-positive and -negative bacteria was prepared in sterile normal saline, from a colony cultured on Nutrient agar medium, with a concentration equal to 0.5 McFarland (1.5×10^8 CFU/ml). Thereafter, 5 µg of the synthesized compounds was added to 1 ml of each bacterial solution. A same microtube contained no substance was also cultured as negative control. The microtubes were incubated in a shaker incubator at 37 °C (100 RPM) for 24 hours. Each solution was then serially diluted 1:10 with sterile normal saline and 100 µl of 10^{-4} dilution of the bacterial suspensions (approximately contained 30-300 CFU) with and without the examined compounds was lawn cultured on two Mueller-Hinton agar plates

followed by incubation at 37 °C for 24 hours. Colony count was performed and the average colony number was considered as the corresponding colony number. Finally, the inhibition rate for each compound was calculated using the following formula:

$$Y = \frac{Wt - Qt}{Wt} \times 100\%$$

Where:

Y = Inhibition rate of the sample

W_t = Average colony number calculated from the control bacterial suspension contained no compound (after 24 culture)

Q_t = Average colony number calculated from the bacterial suspension contained the examined compound (after 24 culture)

[1] Xie, K., Xu, S., Xu, K., Zhang, W., Yu, S., Wang, P., Han, Z., He, N. and Chen, P., 2023. Preparation and antibacterial properties of copper phthalate/polyethylene terephthalate composition fiber. *Alexandria Engineering Journal*, 75, pp.271-278.

Spectral data of target macromolecules

4,4',4'',4'''-(((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl))tetrakis(3-(4-chlorophenyl)-6-(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (1a).

White solid; M.p: 194-200 ˚C; (*n*-Hexane: Ethyl acetate 4:6), FT-IR (KBr, cm^{-1}): 3410, 3251, 3063, 2926, 2859, 2189, 1605, 1507. ^{1}H NMR (400 MHz, DMSO-d_6) δ_{ppm} 12.73 (s, 4H), 11.62 (s, 4H), 9.86 (s, 4H), 7.77 – 7.71 (m, 5H), 7.57 – 7.52 (m, 9H), 7.50 – 7.43 (m, 9H), 7.41 – 7.35 (m, 8H), 7.20 – 7.13 (m, 12H), 7.09 – 7.06 (m, 3H), 6.96 – 6.89 (m, 8H), 5.26 – 5.23 (m, 4H), 5.21 – 5.10 (m, 8H). ^{13}C NMR (101 MHz, DMSO-d_6) δ_{ppm} 156.8, 155.5, 145.0, 135.8, 132.4, 131.3, 130.9, 130.3, 128.9, 128.6, 128.3, 127.9, 127.4, 127.0, 126.1, 125.2, 122.6, 121.7, 120.6, 120.0, 119.6, 114.6, 111.9, 108.9, 79.9, 66.7, 31.4, 21.7.

5,5',5'',5'''-((Benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(benzene-4,1-diyl))tetrakis(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (2a).

White solid; M.p: 274-278 ˚C; (*n*-Hexane: Ethyl acetate 3:7), FT-IR (KBr, cm^{-1}): 3437, 3109, 2930, 2220, 1716, 1668. ^{1}H-NMR (400 MHz, DMSO-d_6) δ_{ppm} 7.31 – 7.28 (m, 6H), 7.25 – 7.22 (m, 6H), 7.19 – 7.14 (m, 8H), 7.05 – 6.97 (m, 6H), 6.25 – 6.18 (m, 4H), 5.39 – 5.27 (m, 8H), 4.01 – 3.98 (m, 9H), 3.87 – 3.82 (m, 6H), 3.65 – 3.63 (m, 9H), 3.18 – 3.14 (m, 9H), 3.09 – 3.06 (m, 3H).^{13}C NMR (101 MHz, DMSO-d_6) δ_{ppm} 18.0, 160.4, 158.6, 154.4, 151.9, 150.7, 135.1, 134.2, 130.7, 130.3, 129.4, 128.9, 127.8, 127.3, 122.0, 118.6, 117.3, 114.2, 108.8, 108.3, 105.0, 101.8, 66.8, 37.1, 37.3, 30.3, 29.3, 28.1.

5,5',5'',5'''-(((Benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl)) tetrakis(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (3a).

White solid; M.p: 248-254 ˚C; (*n*-Hexane: Ethyl acetate 5:5), FT-IR (KBr, cm^{-1}): 3422, 2925, 2226, 1720, 1675. ^{1}H NMR (400 MHz, DMSO-d_6) δ_{ppm} 7.95 – 7.90 (m, 6H), 7.44 – 7.40 (m, 6H),

7.36 – 7.32 (m, 6H), 7.21 – 7.15 (m, 6H), 7.02 – 6.96 (m, 6H), 6.91 – 6.85 (m, 4H), 5.33 – 5.21 (m, 8H), 3.70 – 3.63 (m, 9H), 3.20 – 3.13 (m, 15H), 2.46 – 2.38 (m, 12H). ^{13}C NMR (101 MHz, DMSO-d_6) δ_{ppm} 162.7, 158.7, 158.3, 155.8, 152.2, 150.6, 150.4, 145.2, 141.3, 135.1, 133.6, 131.6, 129.5, 129.3, 129.2, 128.7, 127.6, 124.0, 116.8, 114.6, 114.1, 106.8, 103.7, 66.8, 30.0, 28.2, 21.0.

5,5',5''-(((1,3,5-Triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (4a).

White solid; M.p: 296-300 ˚C; (*n*-Hexane: Ethyl acetate 7:3), FT-IR (KBr, cm^{-1}): 3426, 2931, 2854, 2219, 1722, 1673. ^{1}H NMR (400 MHz, DMSO-d_6) δ_{ppm} 7.97 – 7.94 (m, 6H), 7.45 – 7.42 (m, 6H), 7.41 – 7.36 (m, 6H), 7.28 – 7.23 (m, 6H), 3.70 – 3.69 (m, 6H), 3.21 – 3.19 (m, 12H), 2.43 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ_{ppm} 170.8, 165.2, 158.7, 158.1, 152.7, 150.7, 146.8, 141.3, 133.7, 133.0, 129.3, 129.2, 129.2, 128.6, 121.6, 116.4, 114.7, 108.0, 106.9, 103.8, 100.5, 28.1, 24.2, 18.5.

4***,4',4''-(((1,3,5-Triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(6-(1H-indol-3-yl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (5a).***

White solid; M.p: >300 ˚C; (*n*-Hexane: Ethyl acetate6:4), FT-IR (KBr, cm^{-1}): 3376, 2932, 2852, 2223, 1584. ^{1}H NMR (400 MHz, DMSO-d_6) δ_{ppm} 11.92 (s, 3H), 8.46 – 8.43 (m, 4H), 8.29 – 8.27 (m, 4H), 7.66 – 7.62 (m, 4H), 7.61 – 7.56 (m, 9H), 7.50 – 7.46 (m, 6H), 7.43 – 7.40 (m, 6H), 7.28 – 7.25 (m, 3H), 7.23 – 7.19 (m, 3H), 7.06 – 7.00 (m, 3H), 2.05 (s, 9H).^{13}C NMR (101 MHz, DMSO-d_6) δ_{ppm} 170.7, 165.2, 157.2, 155.4, 152.3, 151.7, 150.0, 143.7, 138.4, 136.4, 134.9, 129.5, 129.4, 129.2, 129.1, 128.9, 126.4, 125.8, 123.3, 122.5, 122.3, 121.5, 121.0, 120.9, 119.4, 118.4, 116.6, 115.6, 112.8, 112.2, 111.6, 99.0, 90.0, 20.0.

5,5',5''-(((1,3,5-Triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (6a).

White solid; M.p: 290-298 ˚C; (*n*-Hexane: Ethyl acetate 7:3), FT-IR (KBr, cm^{-1}): 3394, 2930, 2851, 2221, 1726, 1655. ^{1}H NMR (400 MHz, DMSO-d_6) δ_{ppm} 7.23 (t, J = 2.1 Hz, 3H), 7.18 (dd,

J = 4.2, 1.7 Hz, 3H), 7.16 – 7.12 (m, 6H), 6.86 – 6.82 (m, 6H), 6.25 (dd, J = 4.0, 2.6 Hz, 3H), 4.00 (s, 9H), 3.64 (s, 9H), 3.17 (s, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ $_{ppm}$ 165.2, 159.1, 158.6, 157.8, 154.4, 151.9, 150.7, 130.6, 129.3, 128.5, 127.3, 126.9, 121.6, 117.3, 117.2, 114.7, 108.3, 105.0, 101.9, 38.8, 37.2, 30.3, 28.1.

5,5',5''-(((1,3,5-Triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (7a).

White solid; M.p: 220-228 ˚C; (*n*-Hexane: Ethyl acetate 7:3), FT-IR (KBr, cm^{-1}): 3424, 2931, 2854, 2219, 1718, 1671. ^{1}H NMR (400 MHz, DMSO-d_6) δ $_{ppm}$ 7.96 (s, 6H), 7.51 (t, *J* = 7.9 Hz, 3H), 7.25 – 7.24 (m, 3H), 7.19 (dd, *J* = 4.1, 1.7 Hz, 3H), 7.11 (t, *J* = 1.9 Hz, 3H), 6.26 (dd, J = 4.2, 2.6 Hz, 3H), 4.01 (s, 9H), 3.65 (s, 9H), 3.16 (s, 9H).

5,5',5''-(((1,3,5-Triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(7-(1H-indol-3-yl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (8a).

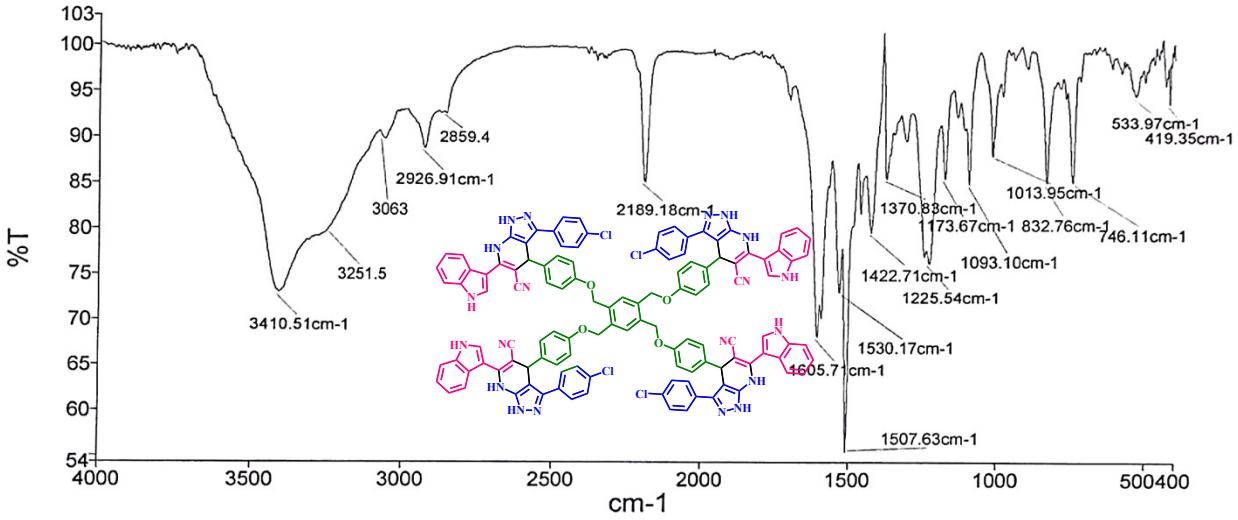
White solid; M.p: 284-287 ˚C; (*n*-Hexane: Ethyl acetate 7:3), FT-IR (KBr, cm^{-1}): 3344, 2944, 2857, 2217, 1713, 1696. 1H NMR (400 MHz, DMSO-d_6) δ $_{ppm}$ 12.06 (s, 3H), 8.59 (s, 3H), 8.49 – 8.45 (m, 4H), 7.61 – 7.57 (m, 4H), 7.39 – 7.35 (m, 6H), 7.31 – 7.29 (m, 4H), 7.27 – 7.23 (m, 6H), 3.79 (s, 9H), 3.19 (s, 9H).

4,4'-((((6-(4-(5-cyano-3,6-di(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridin-4-yl)phenoxy)-1,3,5-triazine-2,4-diyl)bis(oxy))bis(3,1-phenylene))bis(3,6-di(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (9a).

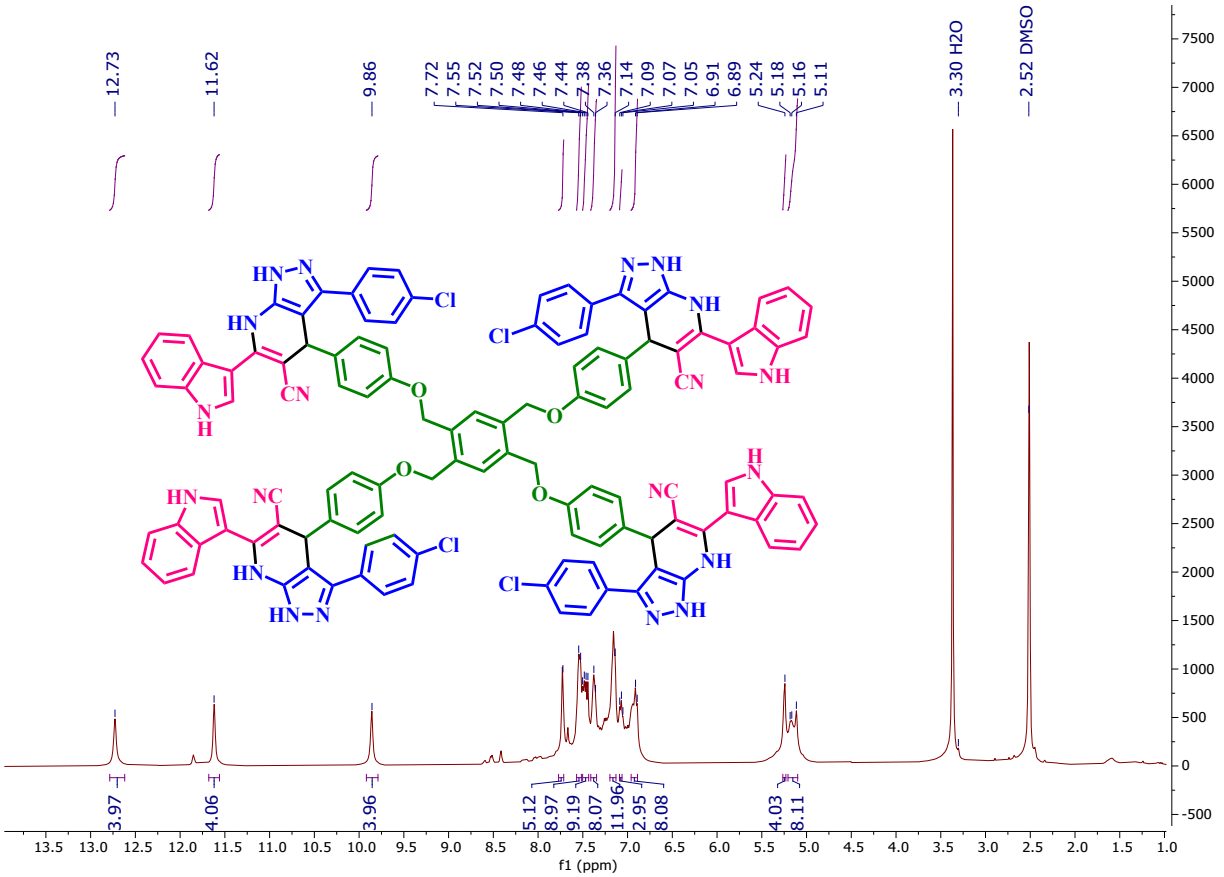
White solid; M.p: >300 ˚C; (*n*-Hexane: Ethyl acetate 5:5), FT-IR (KBr, cm^{-1}): 3395, 2190, 1598, 1563. ^{1}H NMR (400 MHz, DMSO-d_6) δ $_{ppm}$ 12.31 (s, 3H), 11.62 (s, 3H), 11.36 (s, 3H), 9.85 (s, 3H), 7.74 (s, 3H), 7.47 – 7.41 (m, 8H), 7.28 – 7.23 (m, 8H), 7.14 – 7.10 (m, 10H), 7.06 – 7.00 (m, 13H), 5.20 (s, 3H).

5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(8,8-dimethyl-5,8,9,10-tetrahydropyrimido[4,5-b]quinoline-2,4,6(1H,3H,7H)-trione) (10a).

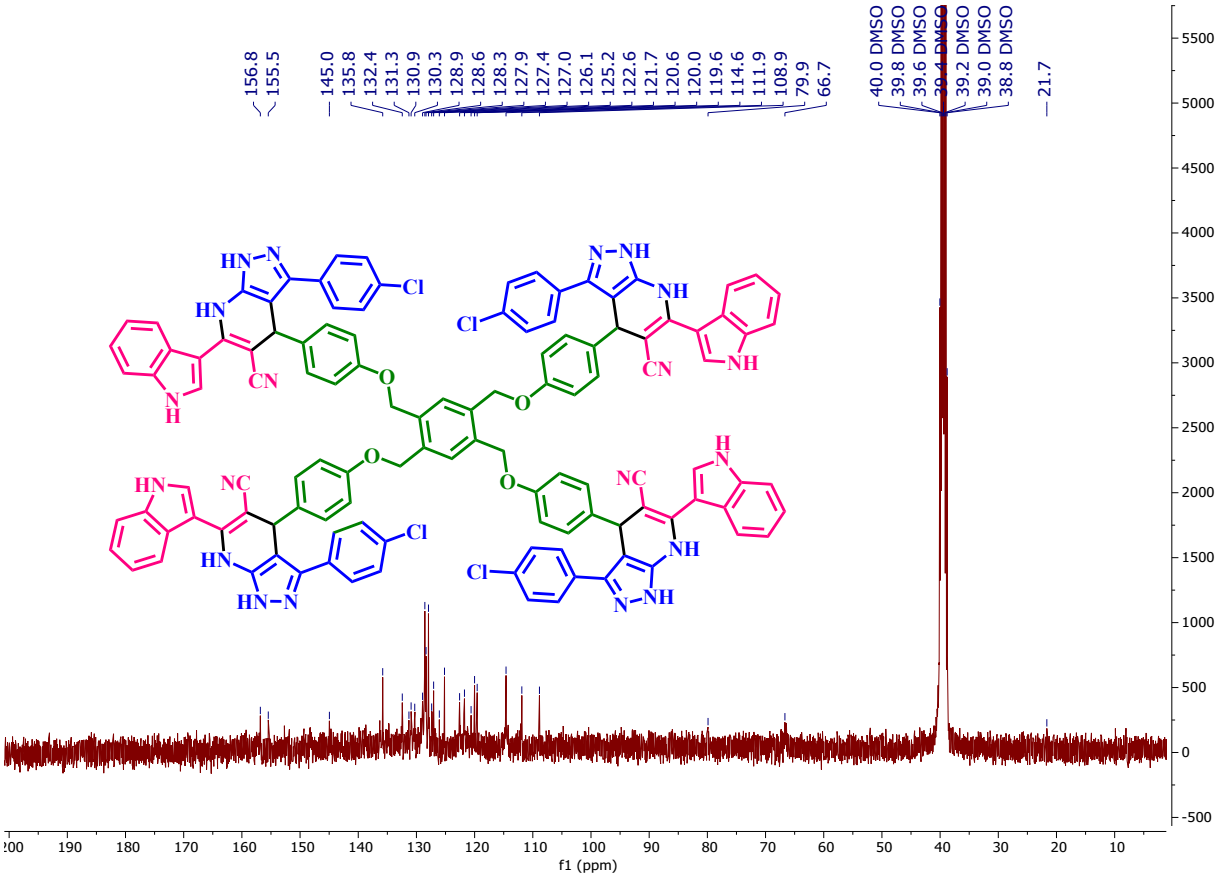
White solid; M.p: >300 ˚C; (*n*-Hexane: Ethyl acetate 6:4), FT-IR (KBr, cm^{-1}): 3370, 3172, 2961, 1715, 1628. ^{1}H NMR (400 MHz, DMSO-d_6) δ_{ppm} 10.54 (s, 3H), 10.49 (s, 3H), 10.35 (s, 3H), 7.22 (d, J = 9.6 Hz, 2H), 7.10 – 7.08 (m, 6H), 6.74 – 6.67 (m, 4H), 5.32 (s, 3H), 3.08 – 3.00 (m, 3H), 2.98 – 2.87 (m, 3H), 2.24 – 2.16 (m, 3H), 2.15 – 2.06 (m, 3H), 1.07 – 1.01 (m, 9H), 0.95 – 0.85 (m, 9H). ^{13}C NMR (101 MHz, DMSO-d_6) δ_{ppm} 194.4, 173.2, 165.7, 162.8, 156.5, 153.6, 153.1, 149.8, 149.7, 148.9, 137.3, 134.5, 131.4, 128.5, 127.6, 120.7, 120.5, 84.8, 55.6, 50.1, 32.1, 28.6, 27.7, 26.9.



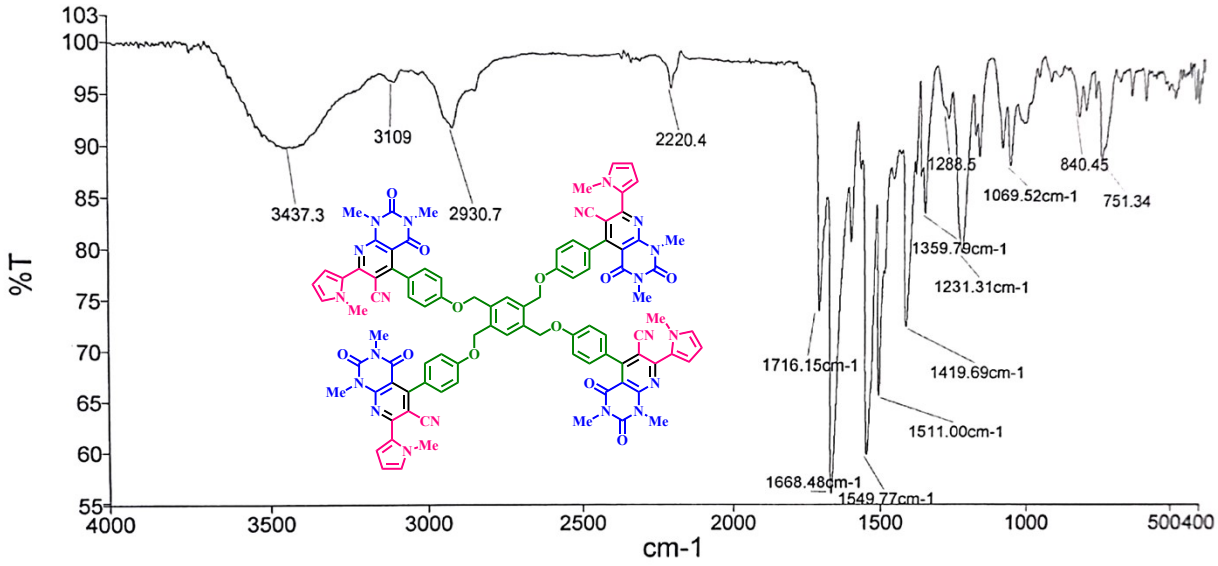
FT-IR spectrum of 4,4',4'',4'''-(((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl))tetrakis(3-(4-chlorophenyl)-6-(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (1a).



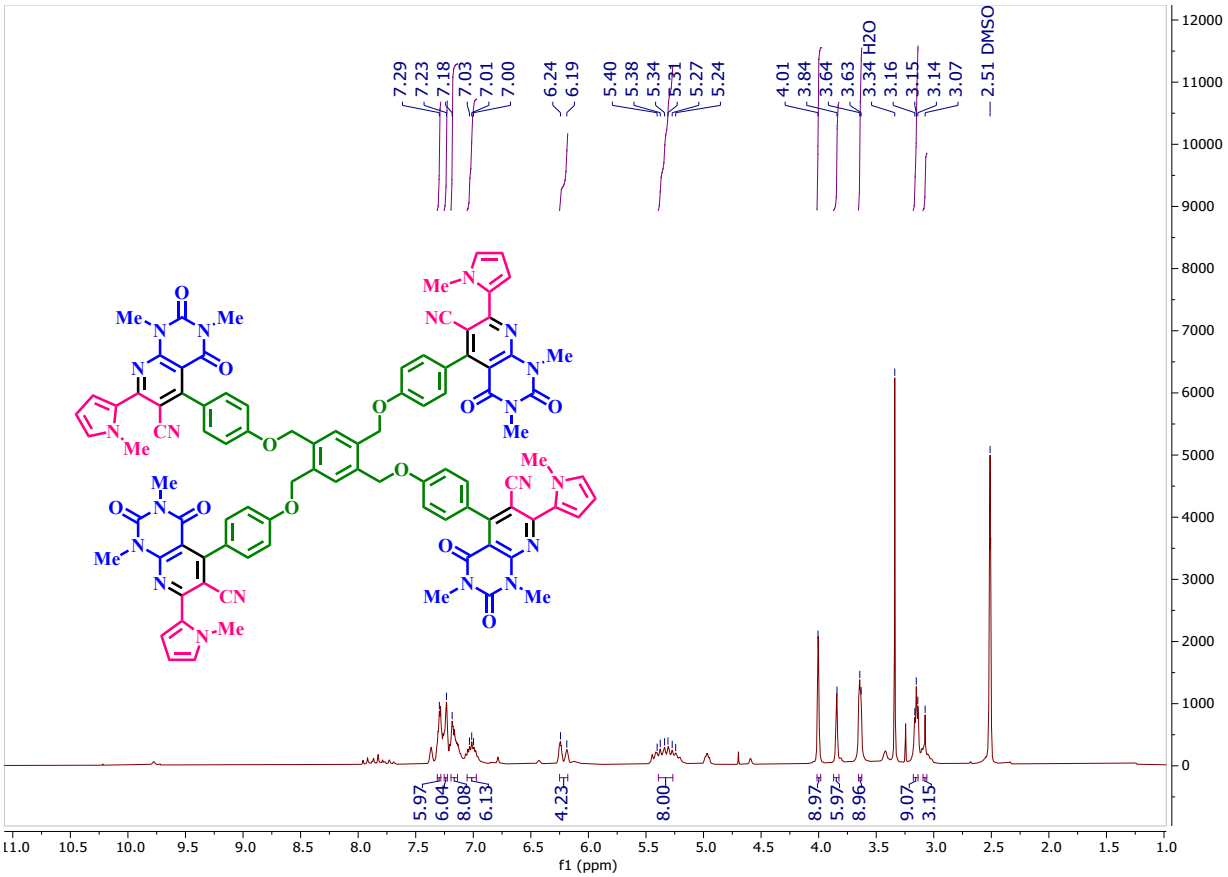
[1]H-NMR spectrum of 4,4',4'',4'''-(((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl))tetrakis(3-(4-chlorophenyl)-6-(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (1a).



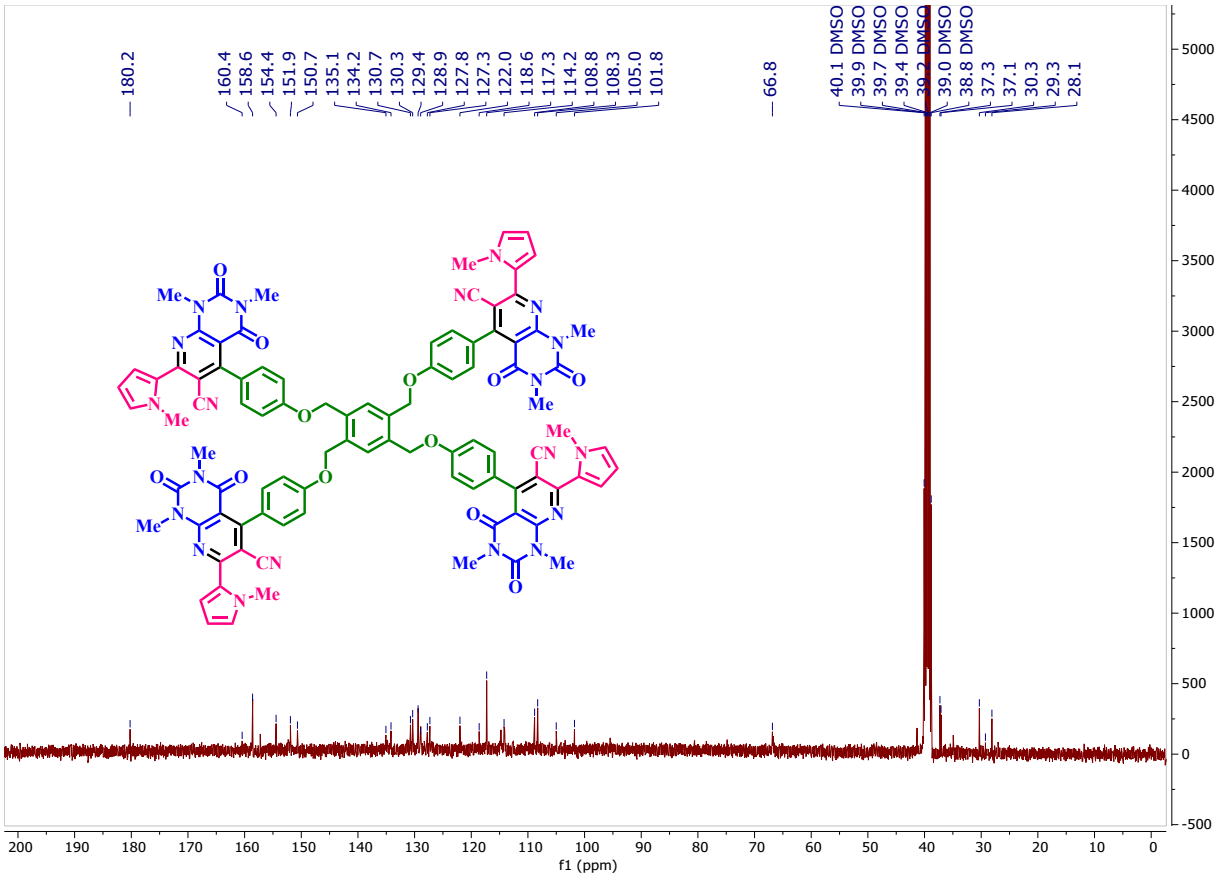
^{13}C-NMR spectrum of 4,4',4'',4'''-(((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl))tetrakis(3-(4-chlorophenyl)-6-(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (1a).



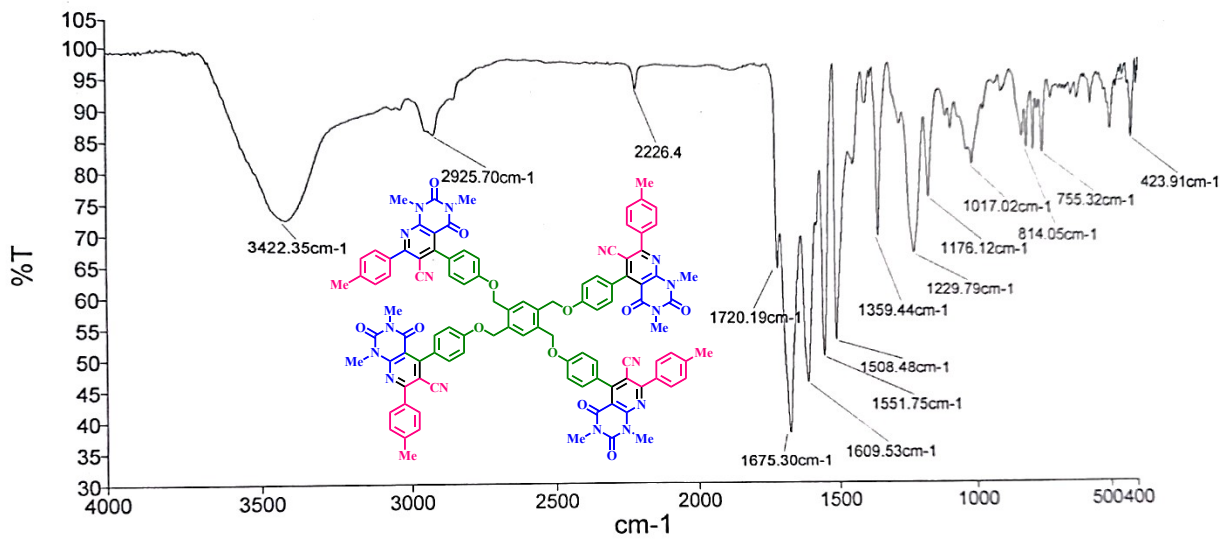
FT-IR spectrum of 5,5',5'',5'''-((benzene-1,2,4,5-tetrayltetrakis(methylene)tetrakis(benzene-4,1-diyl))tetrakis(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (2a).



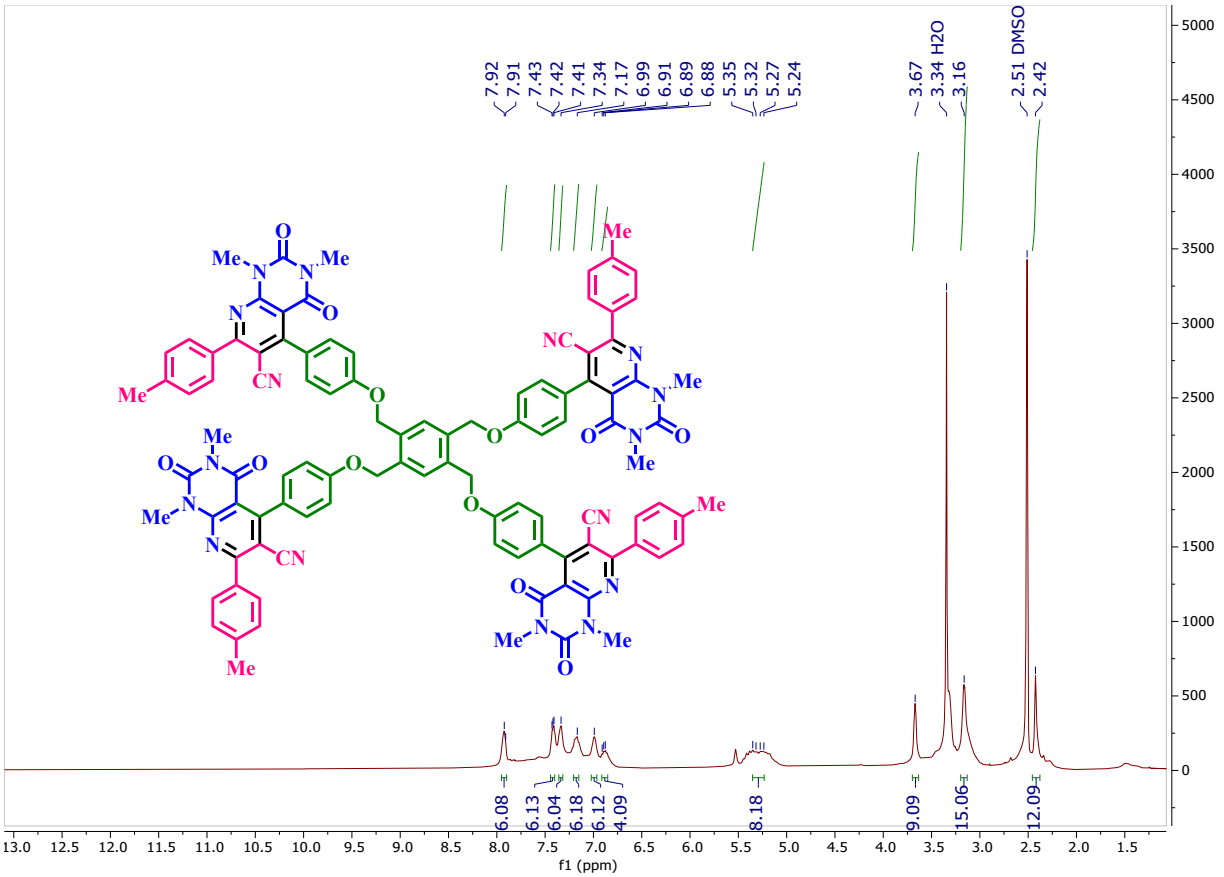
[1]H-NMR spectrum of 5,5',5'',5'''-((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(benzene-4,1-diyl))tetrakis(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (2a).



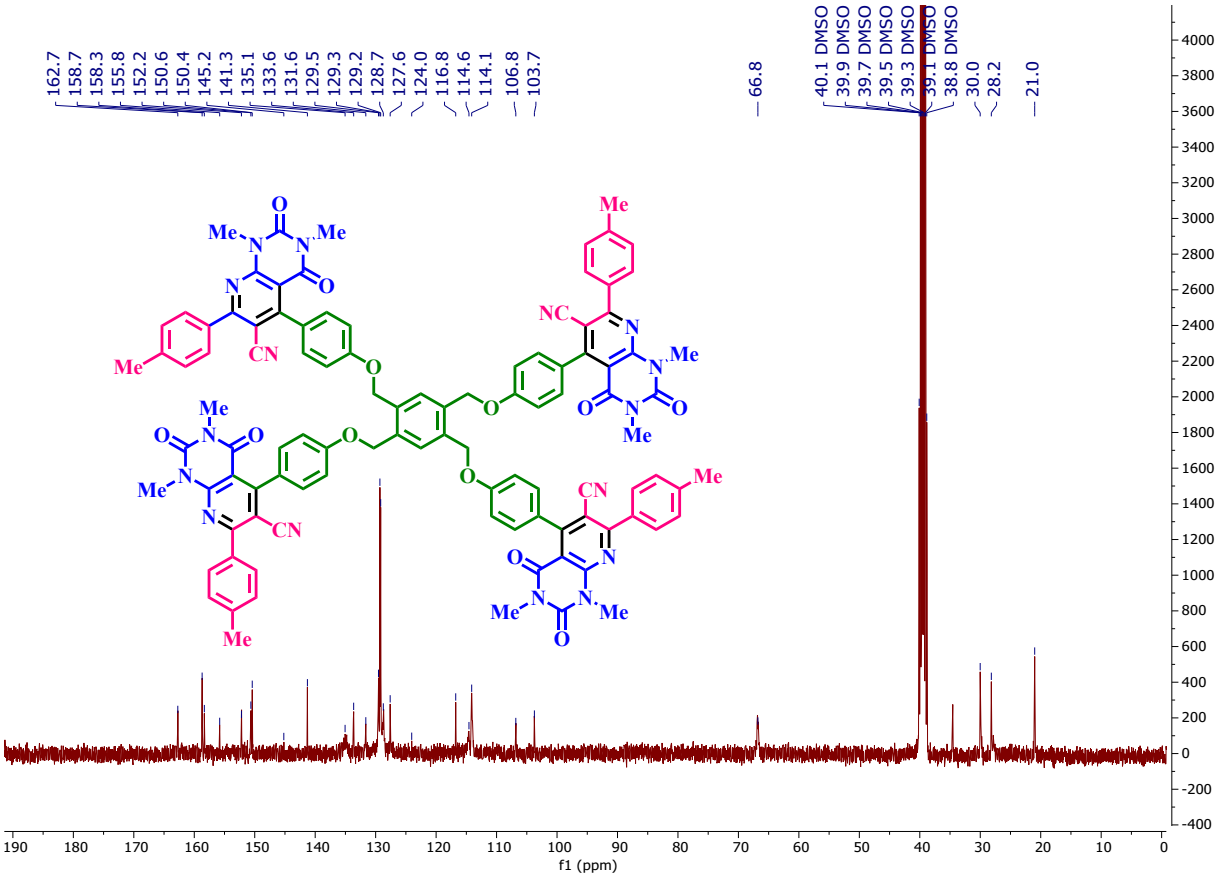
^{13}C-NMR spectrum of 5,5',5'',5'''-((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(benzene-4,1-diyl)) tetrakis(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (2a).



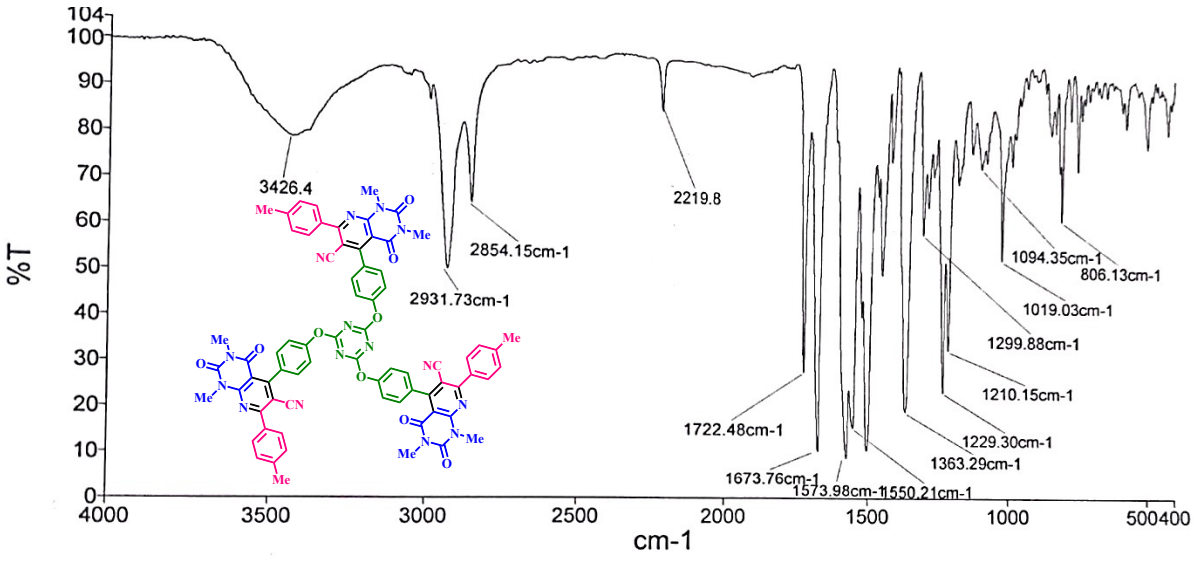
FT-IR spectrum of 5,5',5'',5'''-(((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl))tetrakis(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (3a).



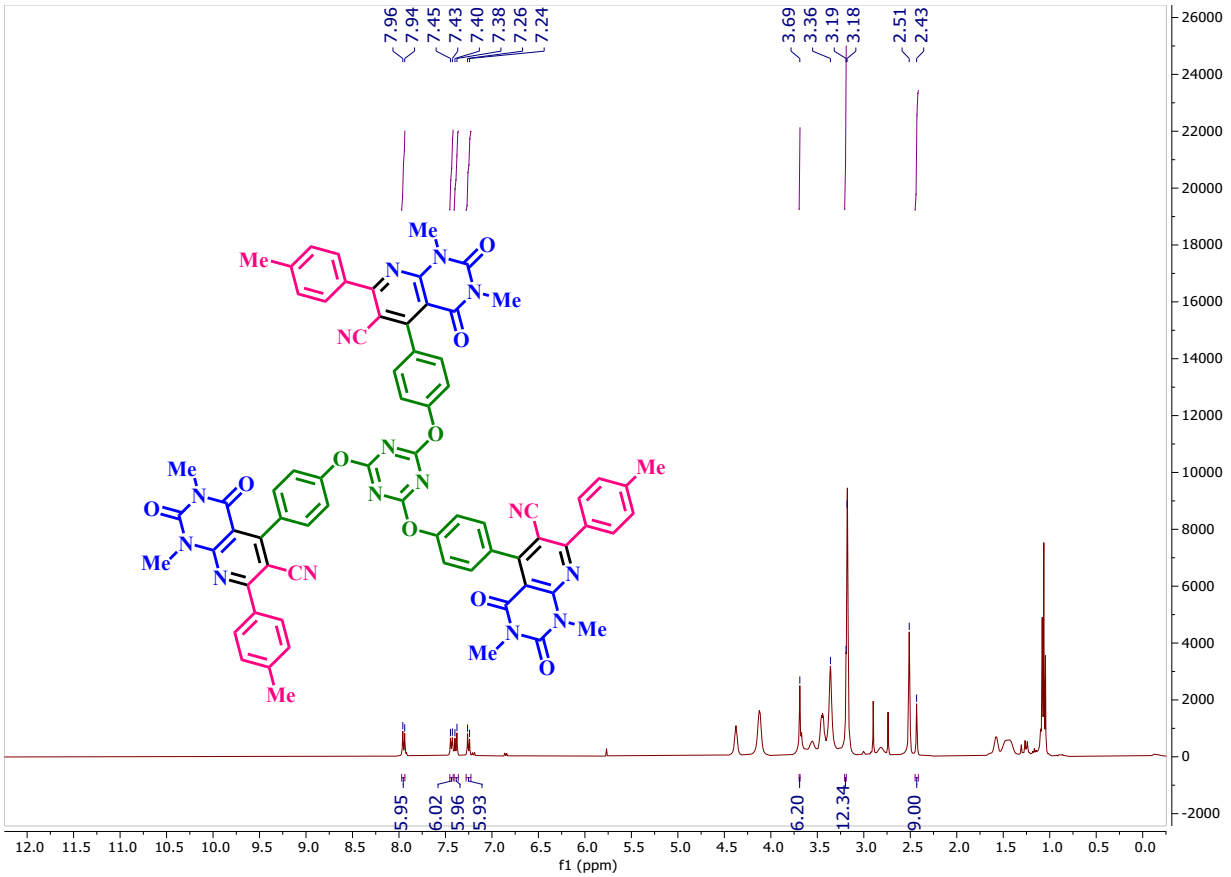
^{1}H-NMR spectrum of 5,5',5'',5'''-(((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl))tetrakis(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (3a).



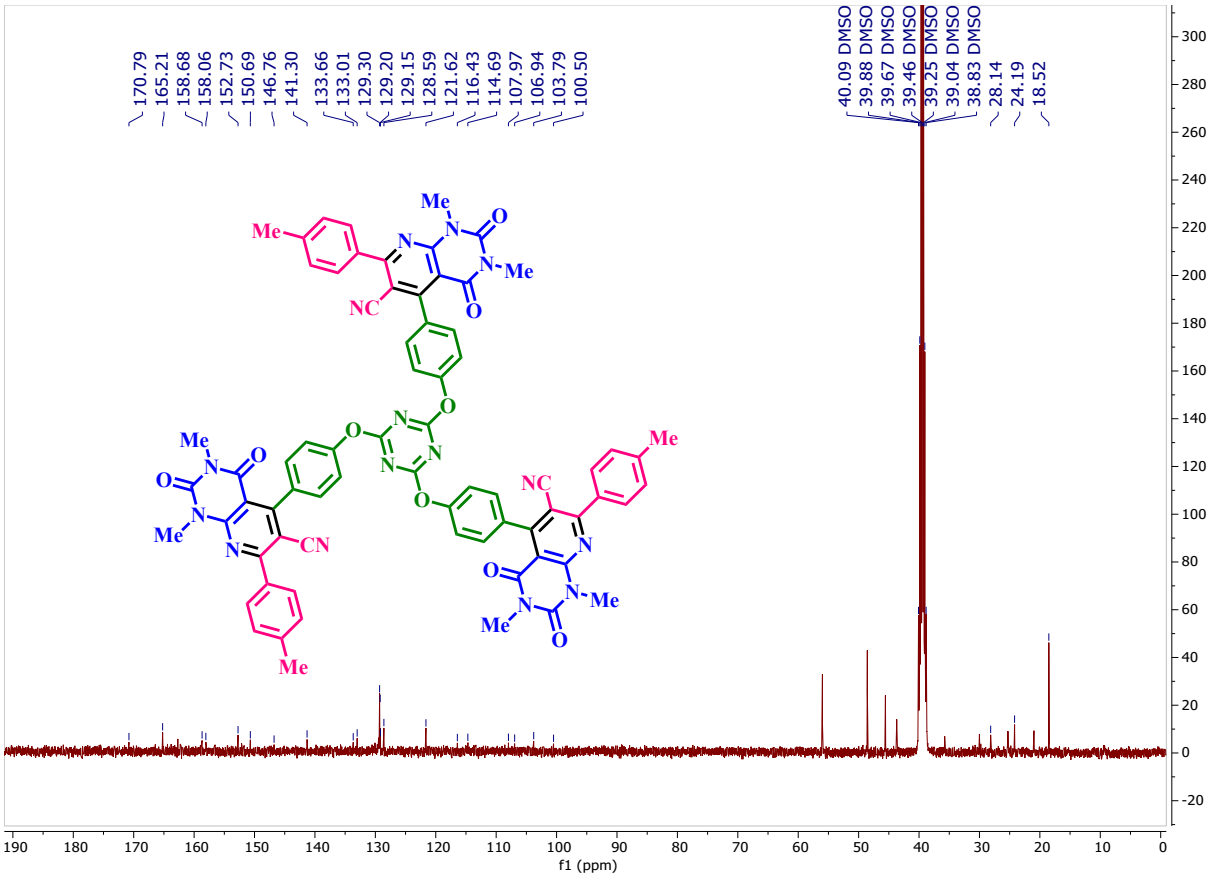
^{13}C-NMR spectrum of 5,5',5'',5'''-(((benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(oxy))tetrakis(benzene-4,1-diyl))tetrakis(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (3a).



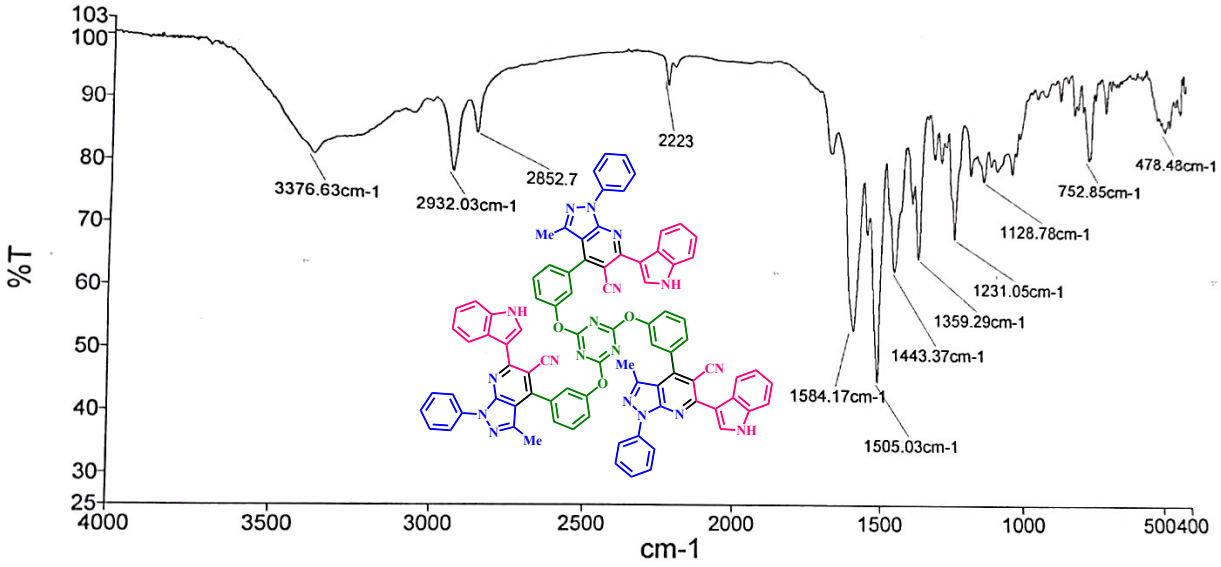
FT-IR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (4a).



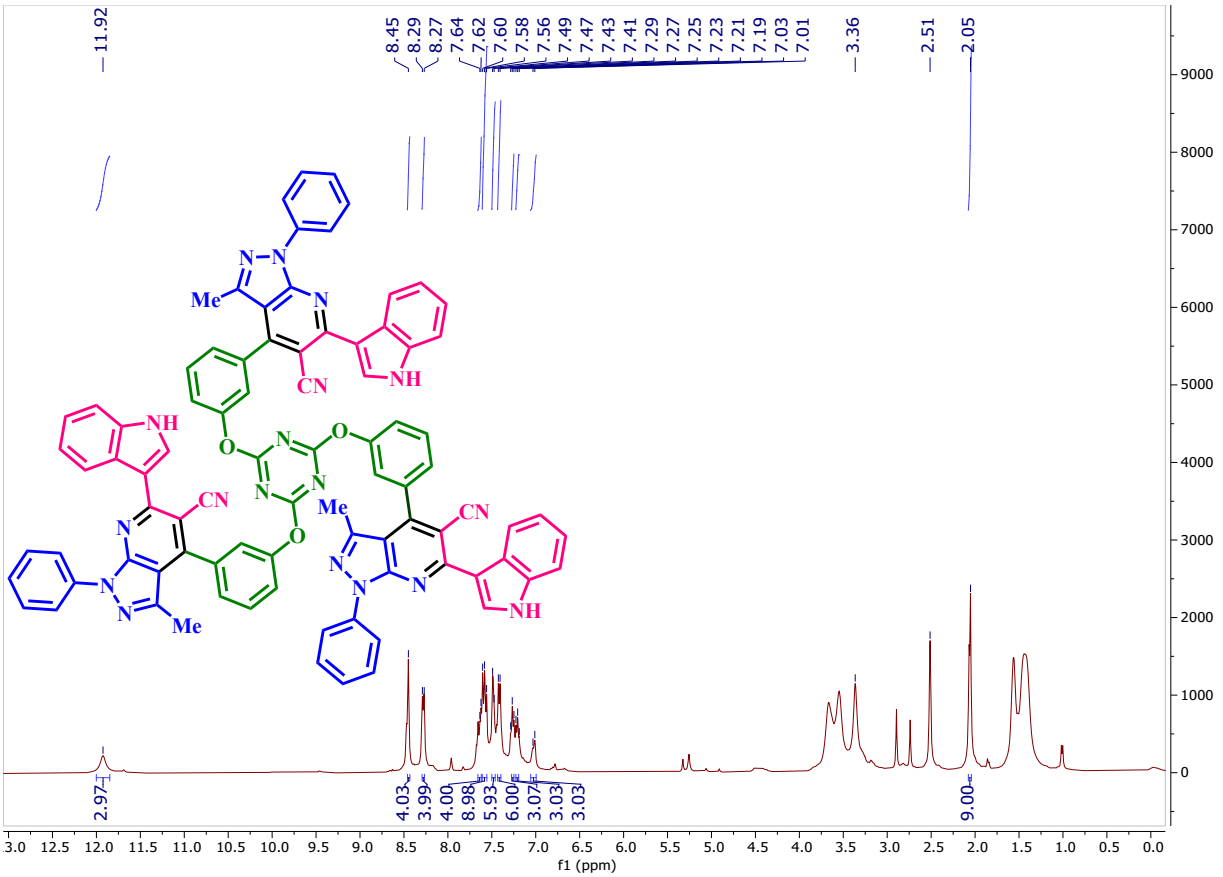
[1]H-NMR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (4a).



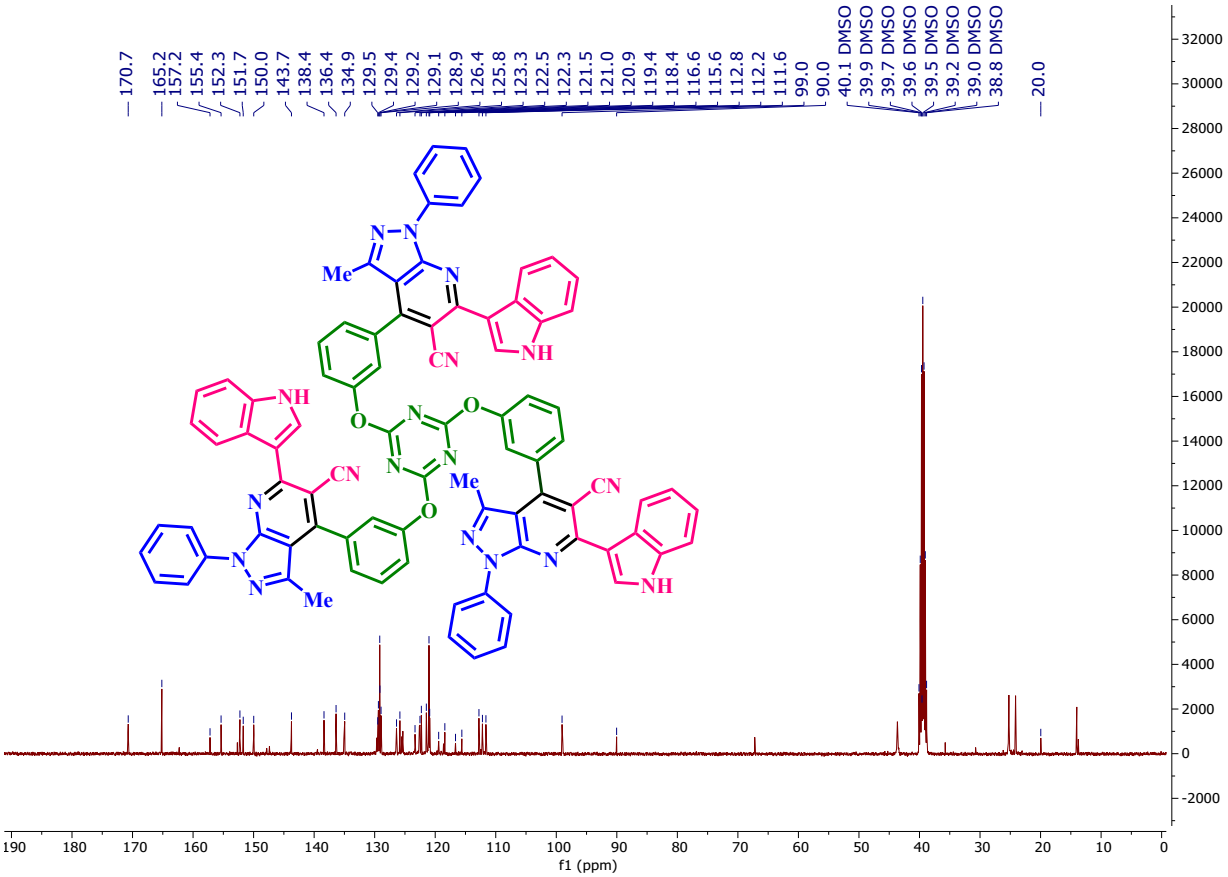
[13]C-NMR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-2,4-dioxo-7-(p-tolyl)-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (4a).



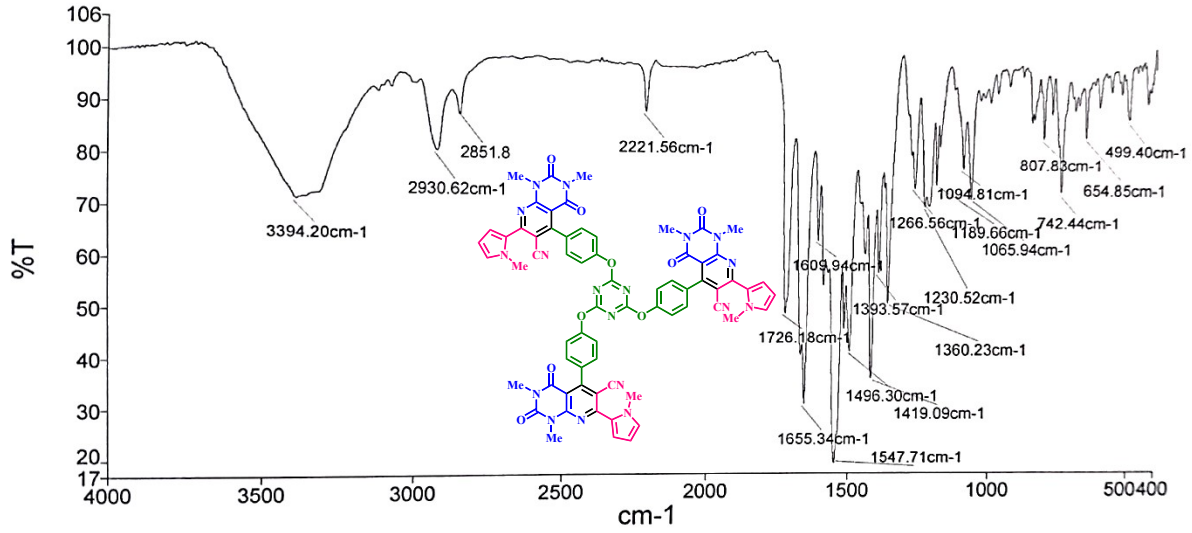
FT-IR spectrum of 4,4',4''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(6-(1H-indol-3-yl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (5a).



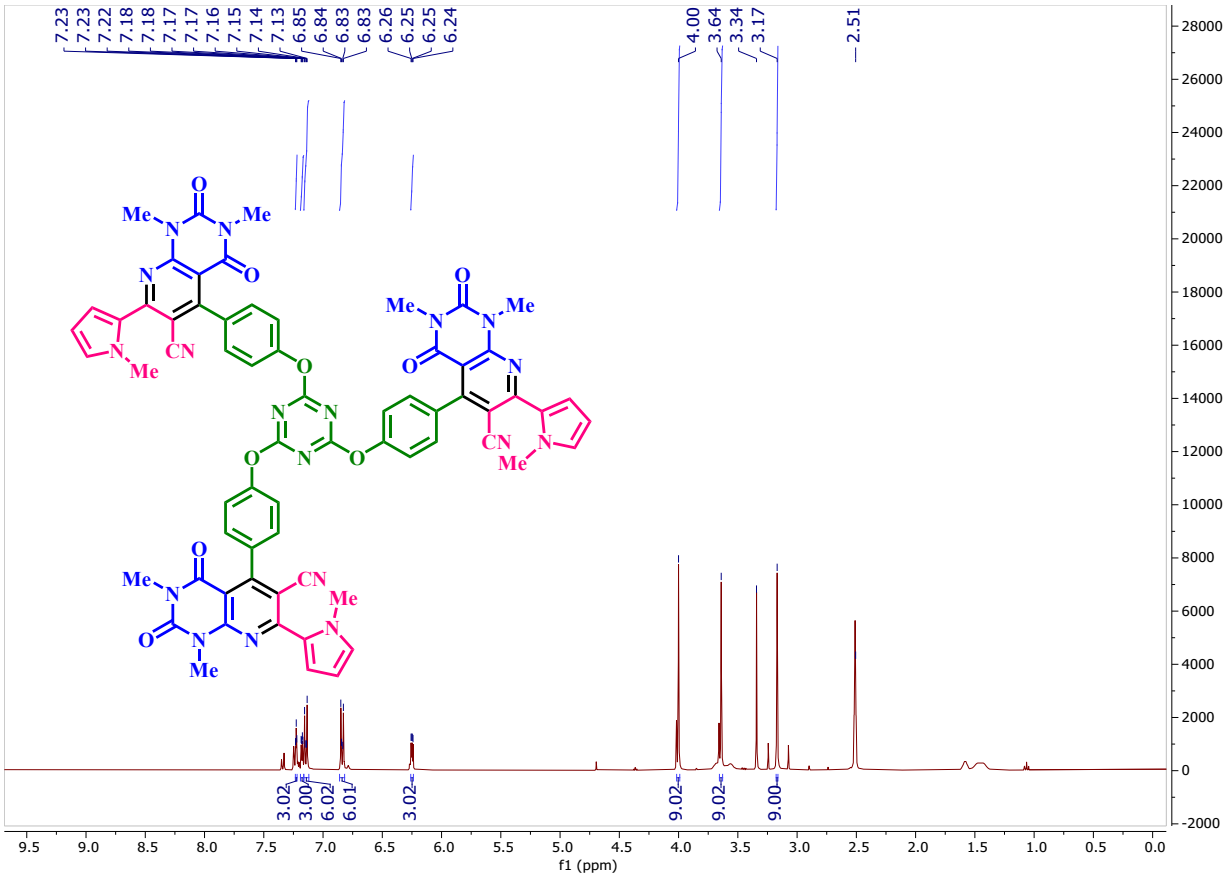
[1]H-NMR spectrum of 4,4',4''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(6-(1H-indol-3-yl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (5a).



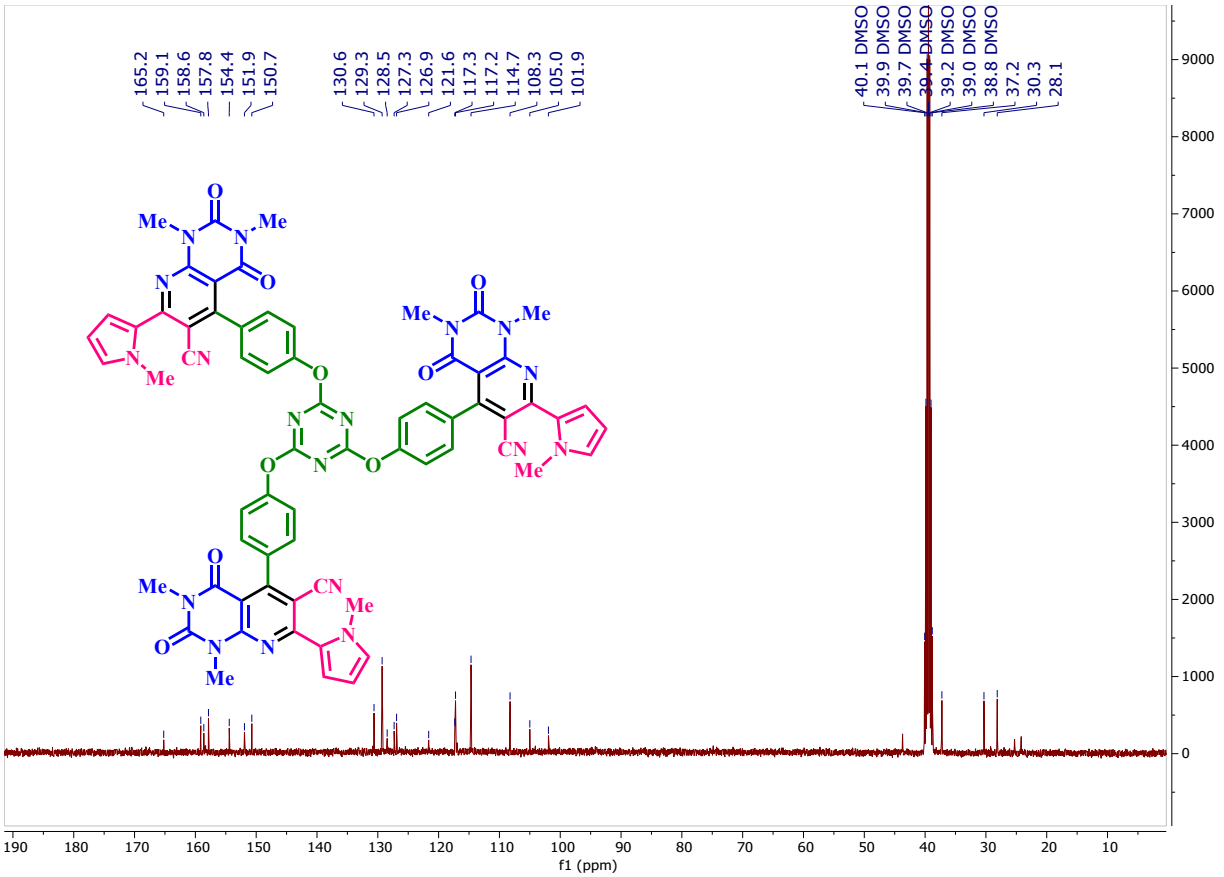
^{13}C-NMR spectrum of 4,4',4''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(6-(1H-indol-3-yl)-3-methyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (5a).



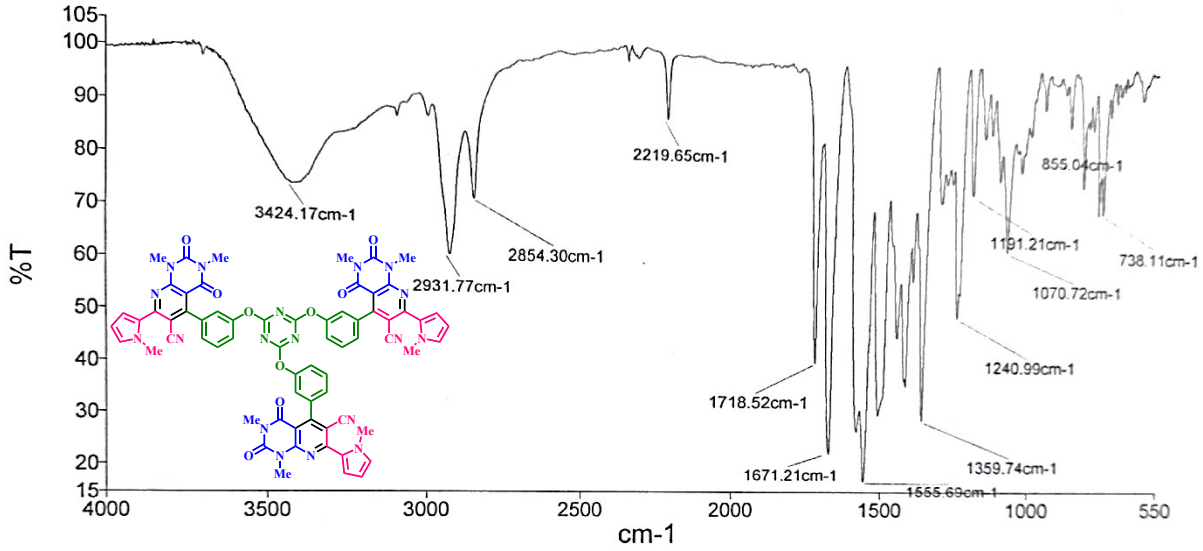
FT-IR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (6a).



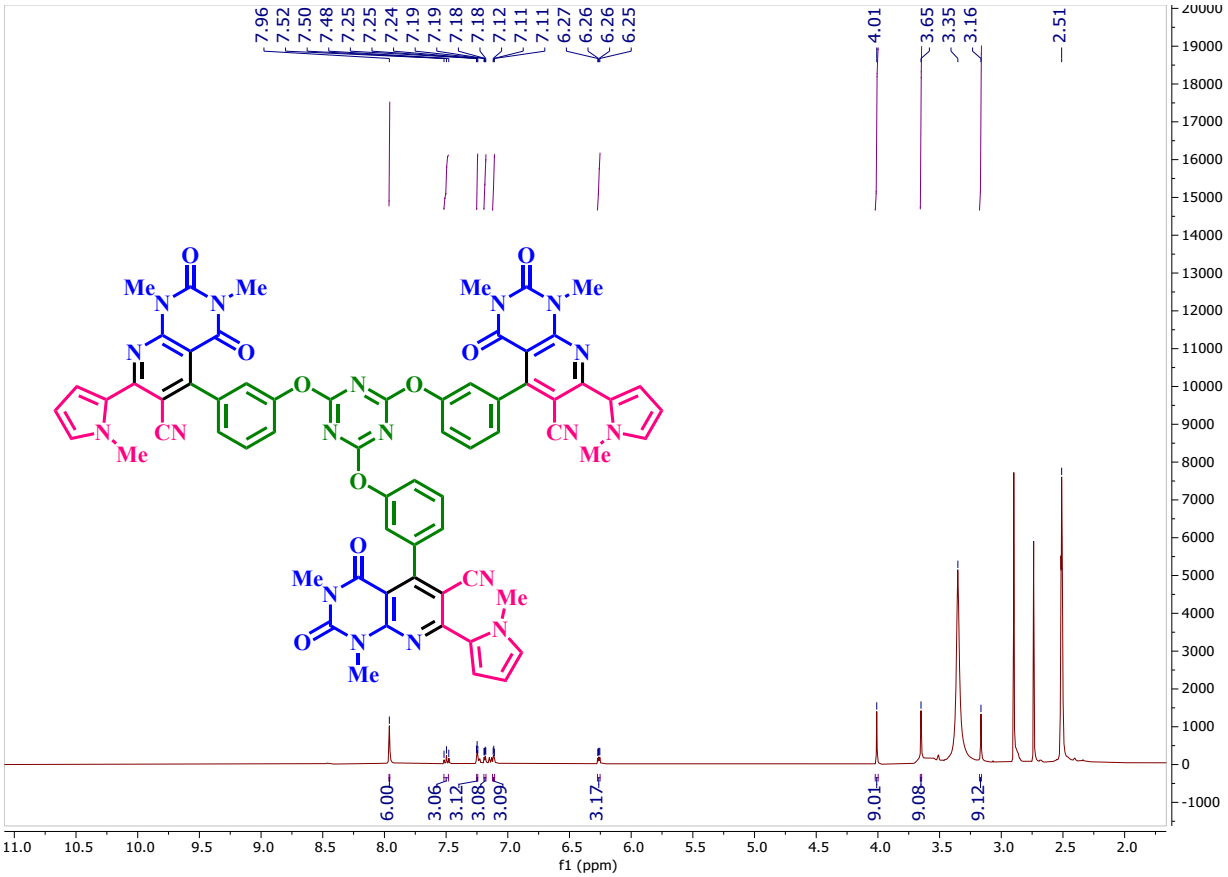
[1]H-NMR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (6a).



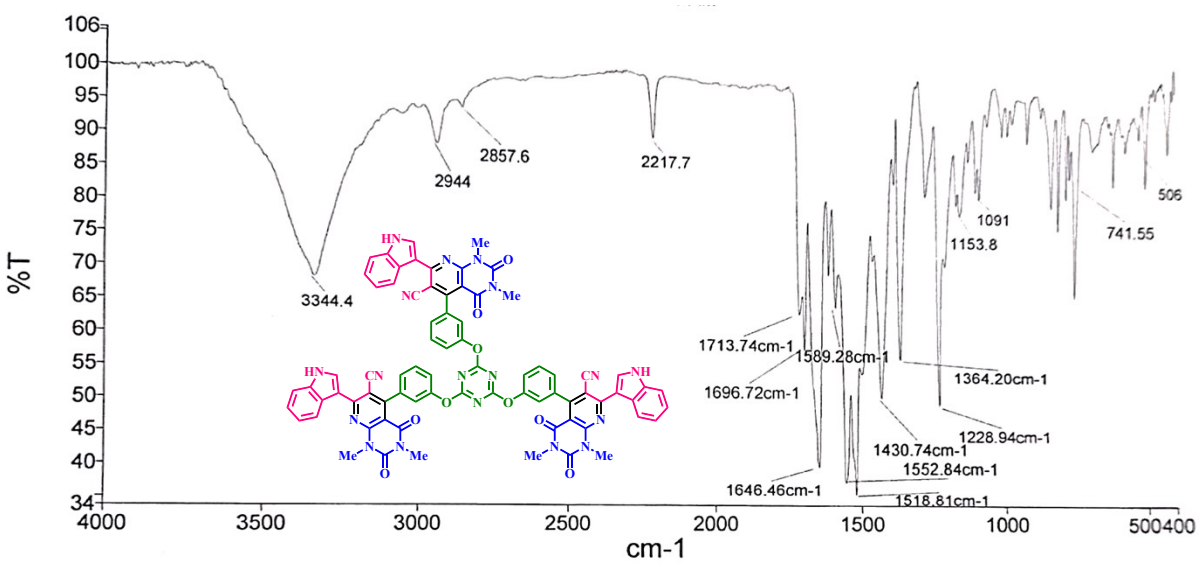
^{13}C-NMR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (6a).



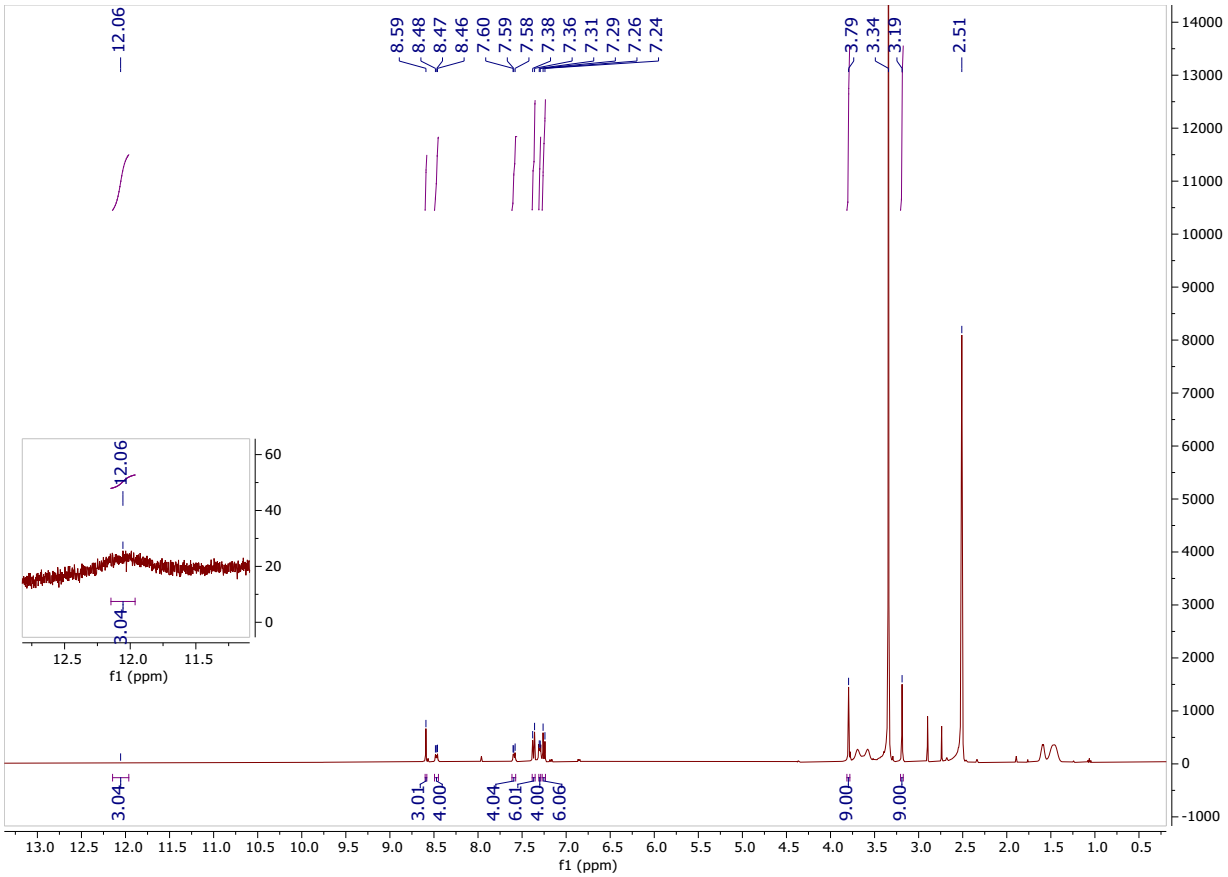
[1]H-NMR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (7a).



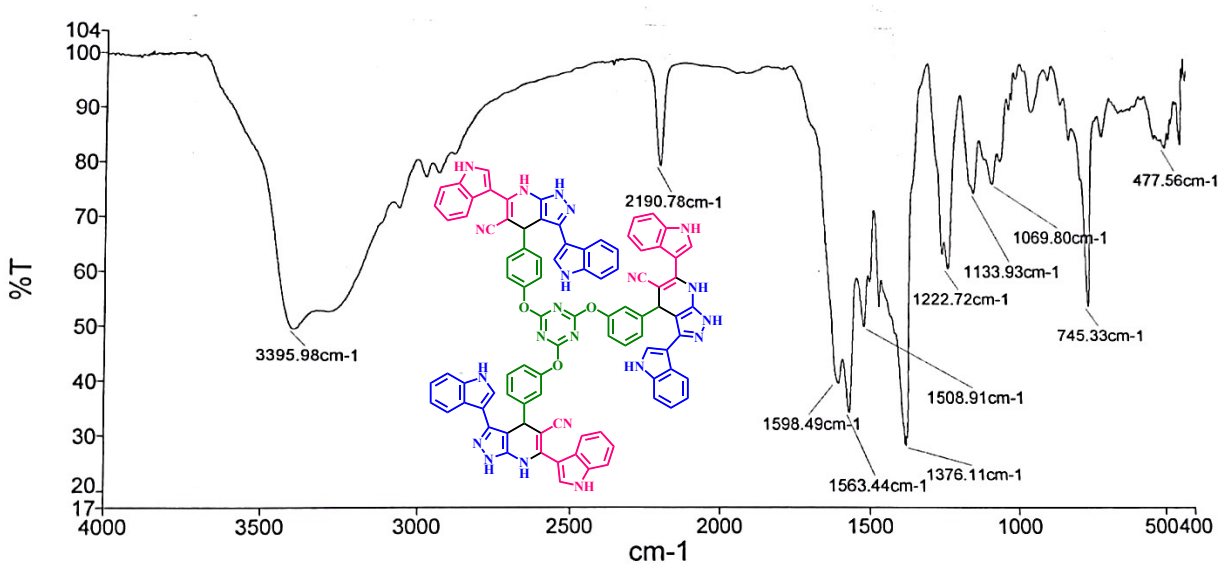
[1]H-NMR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(1,3-dimethyl-7-(1-methyl-1H-pyrrol-2-yl)-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (7a).



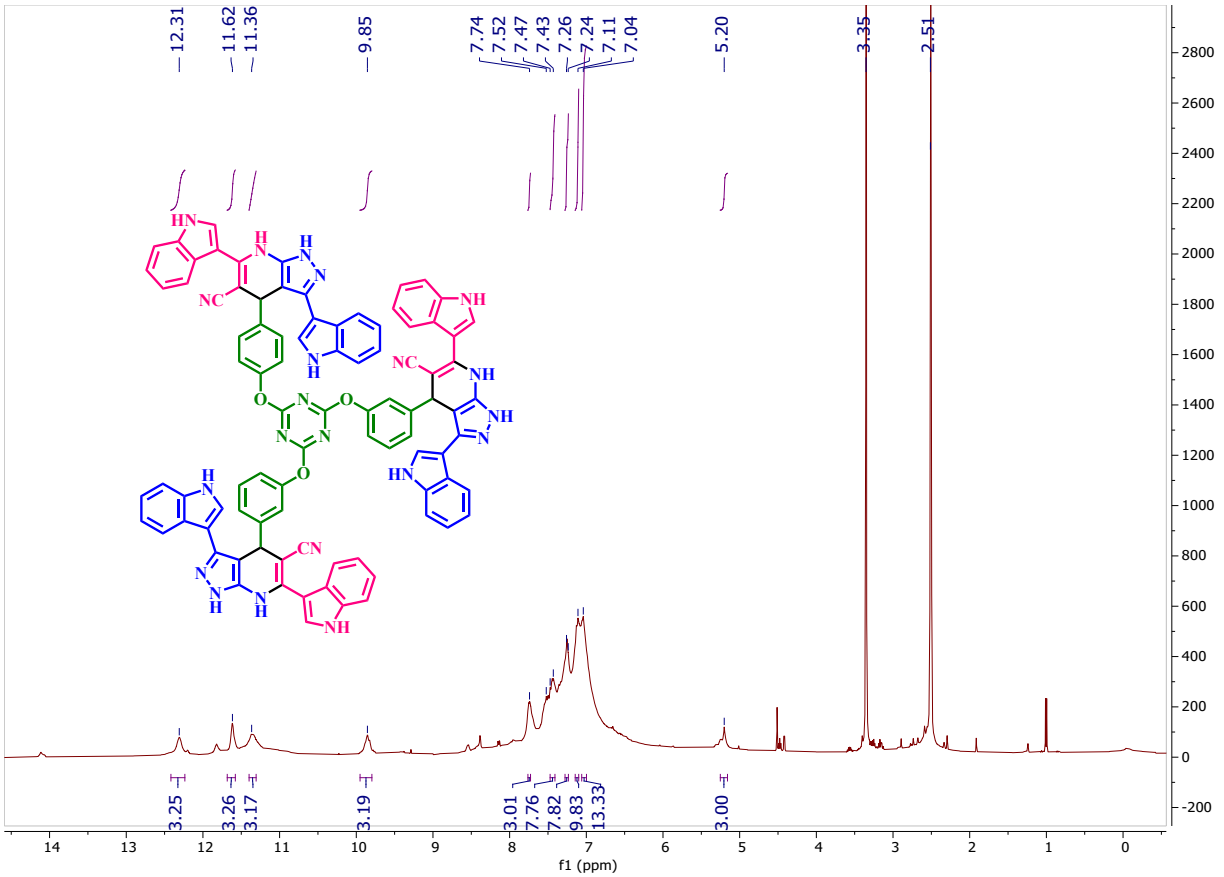
FT-IR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(7-(1H-indol-3-yl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (8a).



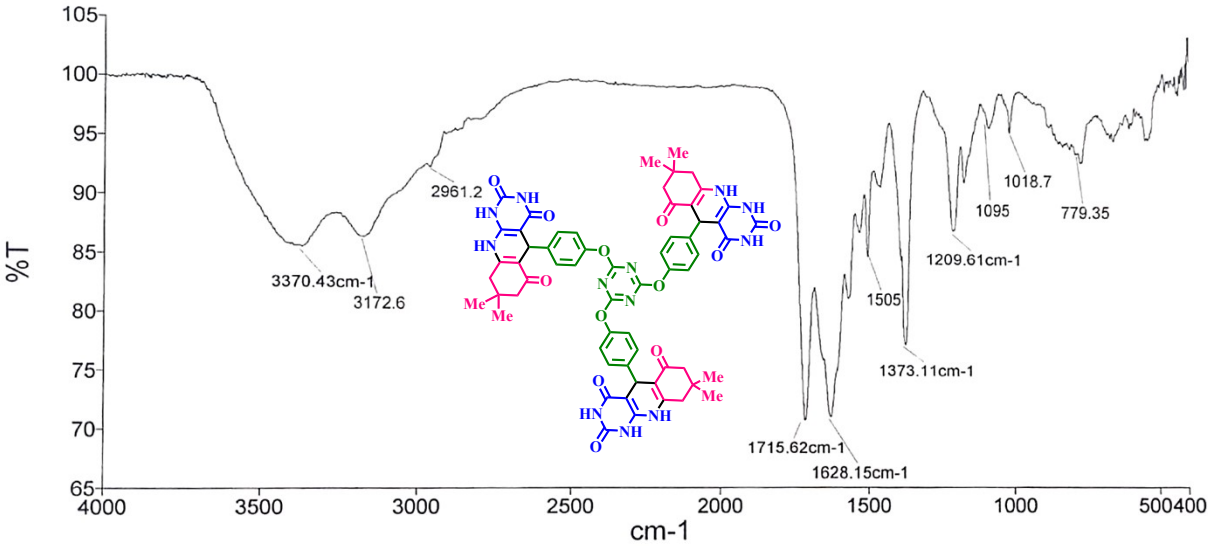
[1]H-NMR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-3,1-diyl))tris(7-(1H-indol-3-yl)-1,3-dimethyl-2,4-dioxo-1,2,3,4-tetrahydropyrido[2,3-d]pyrimidine-6-carbonitrile) (8a).



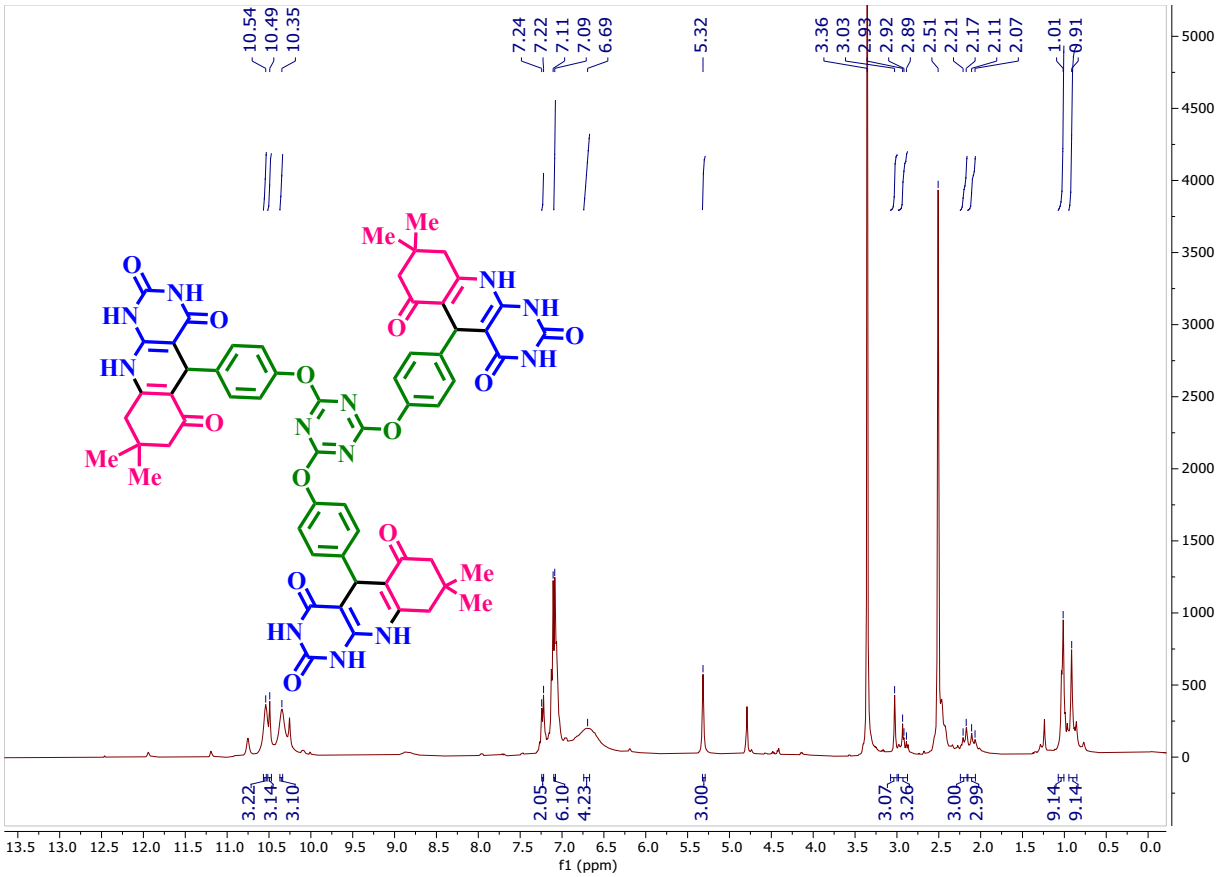
FT-IR spectrum of 4,4'-(((6-(4-(5-cyano-3,6-di(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridin-4-yl)phenoxy)-1,3,5-triazine-2,4-diyl)bis(oxy))bis(3,1-phenylene))bis(3,6-di(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (9a).



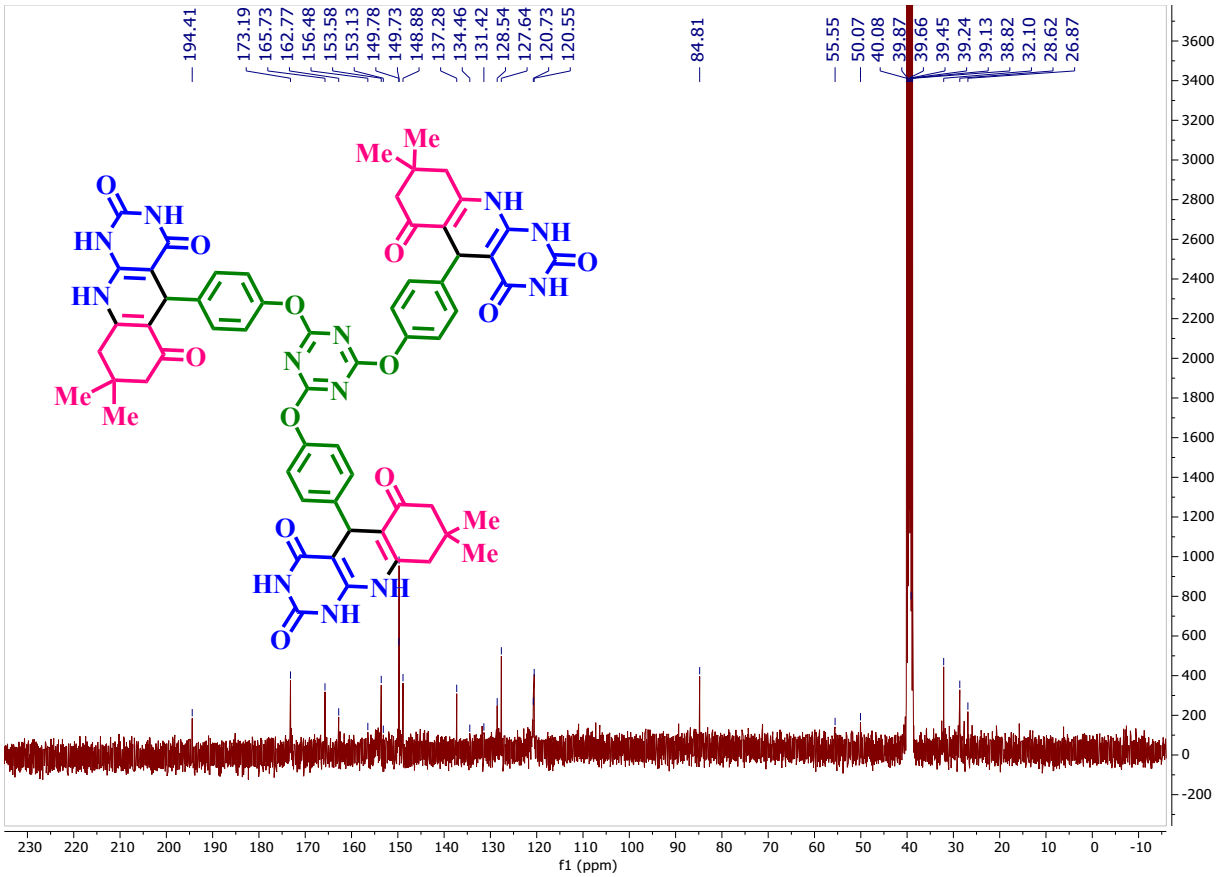
[1]H-NMR spectrum of 4,4'-((((6-(4-(5-cyano-3,6-di(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridin-4-yl)phenoxy)-1,3,5-triazine-2,4-diyl)bis(oxy))bis(3,1-phenylene))bis(3,6-di(1H-indol-3-yl)-4,7-dihydro-1H-pyrazolo[3,4-b]pyridine-5-carbonitrile) (9a).



FT-IR spectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(8,8-dimethyl-5,8,9,10-tetrahydropyrimido[4,5-b]quinoline-2,4,6(1H,3H,7H)-trione)) (10a)



[1]H-NMRspectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(8,8-dimethyl-5,8,9,10-tetrahydropyrimido[4,5-b]quinoline-2,4,6(1H,3H,7H)-trione) (10a)



[13]C-NMRspectrum of 5,5',5''-(((1,3,5-triazine-2,4,6-triyl)tris(oxy))tris(benzene-4,1-diyl))tris(8,8-dimethyl-5,8,9,10-tetrahydropyrimido[4,5-b]quinoline-2,4,6(1H,3H,7H)-trione) (10a)