

RSC Advances:

Supporting Information

A mild process of carbon-carbon bond formation in aqueous medium: Synthesis of bis(pyrrolo[2,3-*d*]pyrimidinyl)methanes, a novel class of compounds

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General Considerations:

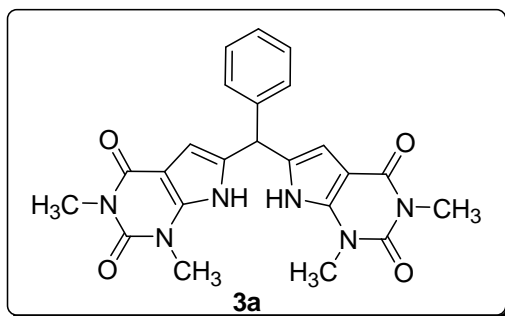
Melting Points were measured with a Buchi-540 melting point apparatus. IR spectra were recorded on a SHIMADZU FTIR-8400. ¹H NMR and ¹³C NMR Spectra were recorded on Bruker Avance-DPX 300MHz and 75MHz FT NMR in DMSO-*d*₆ using TMS as an internal standard. Chemical shifts (δ units) are given from TMS (0 ppm) and coupling constants are expressed in Hertz (Hz). Chemical shifts for DMSO-*d*₆ were reported at 3.36, 2.50 ppm respectively (δ units). Mass spectra were recorded on ESQUIRE 3000 Mass spectrometer. All experiments were monitored by Thin Layer Chromatography (TLC). TLC was performed on pre-coated silica gel plates (Merck).

General procedure for the preparation of 3a- 3t:

A mixture of 1,3-dimethylpyrrolo[2,3-*d*]pyrimidine-2,4-dione **1a** (2 mmol, 362 mg), benzaldehyde **2a** (1 mmol, 105 mg), I₂ (5 mol%, 6 mg) in water (5 mL) was taken in a round bottomed flask. To the reaction mixture SDS (sodium dodecylsulfate) (0.08 mmol, 23 mg) was added and allowed to stir at room temperature for two hour. Initially, the solid compound in the reaction mixture disappeared giving a clear brown solution which slowly changed to greenish brown in color. After completion of the reaction (monitored by TLC), the pink solid product appeared was separated by Buchner filtration, washed with water, and dried. Yield: 428 mg (96%). The compound was recrystallized from methanol. The structure of the compound was ascertained as **3a** from spectroscopic data (IR, ¹H-NMR, ¹³C-NMR, and Mass) and elemental analysis.

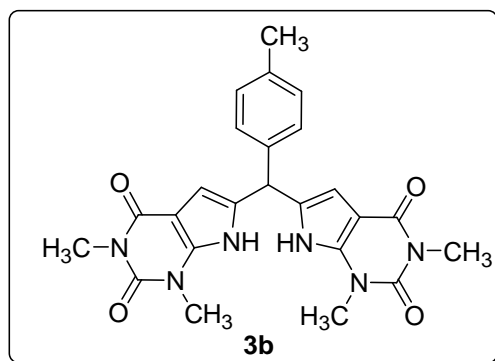
Similarly, compounds **3b-t** were synthesized and characterized.

Characterization data of the Products



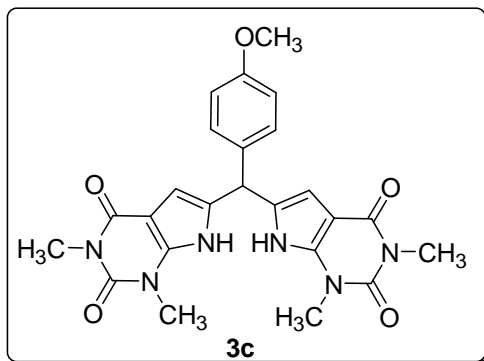
Compound 3a

Pink solid; Yield: 428 mg (96%); mp. 288- 290 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.19 (s, 6H), 3.39 (s, 6H), 5.40 (s, 1H), 5.76 (s, 2H), 7.22-7.39 (m, 5H), 11.74 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.05 (2C), 31.10 (2C), 43.25, 98.46 (2C), 103.15 (2C), 127.50, 128.76 (2C), 128.88 (2C), 132.15 (2C), 139.64 (2C), 141.07, 151.18 (2C), 158.73 (2C); IR (KBr) ν_{max} : 3373.5, 3278.5, 1687.2, 1557.6 cm^{-1} ; MS (ESI): 447.5 ($[\text{M}+\text{H}]^+$); Anal. Cald. For $\text{C}_{23}\text{H}_{23}\text{N}_6\text{O}_4$: C, 61.87; H, 4.92; N, 18.82%; Found: C, 61.88; H, 4.93; N, 18.83%.



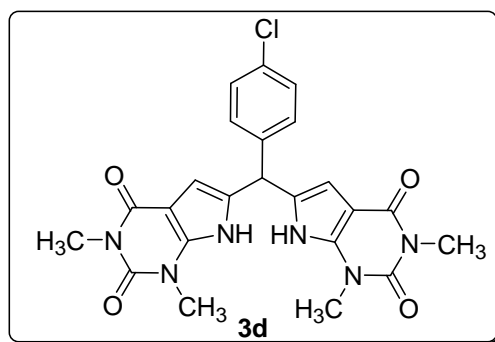
Compound 3b

Pink solid; Yield: 423 mg (92%); mp. 293- 295 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 2.30 (s, 3H), 3.19 (s, 6H), 3.39 (s, 6H), 5.35 (s, 1H), 5.75 (s, 1H), 6.17 (s, 1H), 7.09-7.18 (m, 4H), 11.71 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 21.08, 28.04 (2C), 31.07 (2C), 42.90, 98.44 (2C), 103.05 (2C), 128.63 (2C), 129.38 (2C), 132.38 (2C), 136.62, 138.03, 139.61 (2C), 151.17 (2C), 158.75 (2C); IR (KBr) ν_{max} : 3374.5, 3277.5, 1686.2, 1555.6 cm^{-1} ; MS (ESI): 461.3 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{24}\text{H}_{25}\text{N}_6\text{O}_4$: C, 62.58; H, 5.20; N, 18.25%; Found: C, 62.60; H, 5.21; N, 18.26%.



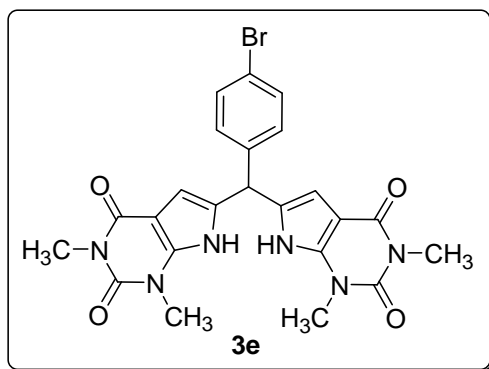
Compound 3c

Pink solid; Yield: 428 mg (90%); mp. 285- 287 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.19 (s, 6H), 3.39 (s, 6H), 3.75 (s, 3H), 5.34 (s, 1H), 5.75 (s, 2H), 6.91-6.93 (d, J = 6.65 Hz, 2H), 7.13- 7.15 (d, J = 8.40 Hz, 2H), 11.70 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.03 (2C), 31.08 (2C), 42.49, 55.56, 98.43 (2C), 102.98 (2C), 114.22 (2C), 128.53, 129.78 (2C), 132.58 (2C), 132.98, 139.61 (2C), 151.18 (2C), 158.73 (2C); IR (KBr) ν_{max} : 3375.6, 3276.8, 1684.2, 1554.5 cm^{-1} ; MS (ESI): 477.5 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{24}\text{H}_{25}\text{N}_6\text{O}_5$: C, 60.49; H, 5.02; N, 17.62%; Found: C, 60.50; H, 5.04; N, 17.64%.



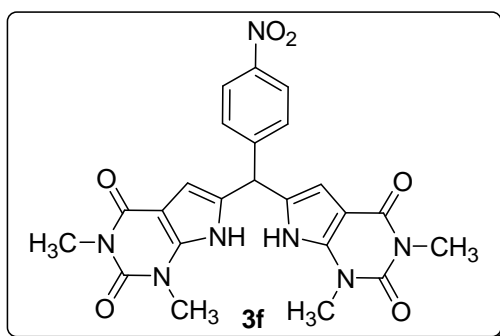
Compound 3d

Magenta solid; Yield: 446 mg (93%); mp. 297- 301 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.19 (s, 6H), 3.39 (s, 6H), 5.41 (s, 1H), 5.79 (s, 2H), 7.24 (d, J = 8.04 Hz, 2H), 7.41 (d, J = 8.10 Hz, 2H), 11.73 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.05 (2C), 31.08 (2C), 42.61, 98.49 (2C), 103.26 (2C), 128.82 (2C), 130.63 (2C), 131.67 (2C), 132.12, 139.72 (2C), 140.04, 151.16 (2C), 158.71 (2C); IR (KBr) ν_{max} : 3376.8, 3276.4, 1685.2, 1557.5 cm^{-1} ; MS (ESI): 481.1 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{23}\text{H}_{22}\text{N}_6\text{O}_4$: C, 57.44; H, 4.36; N, 17.48%; Found: C, 57.50; H, 4.37; N, 17.50%.



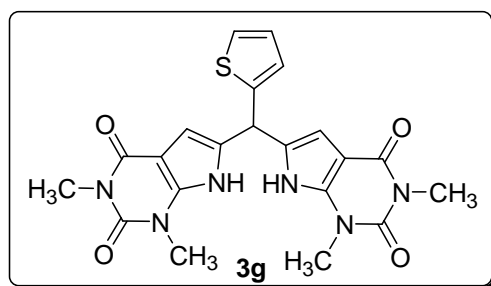
Compound 3e

Off white solid; Yield: 482 mg (92%); mp. 290- 292 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.19 (s, 6H), 3.39 (s, 6H), 5.61 (s, 1H), 5.70 (s, 2H), 7.00-7.70 (m, 4H), 11.86 (s, 2H); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.06 (2C), 31.11 (2C), 42.61, 98.45 (2C), 103.25 (2C), 128.80 (2C), 130.62 (2C), 131.65 (2C), 132.10, 139.71 (2C), 140.07, 151.15 (2C), 159.70 (2C); IR (KBr) ν_{max} : 3374.8, 3275.4, 1683.5, 1554.7 cm^{-1} ; MS (ESI): 525.7 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{23}\text{H}_{22}\text{BrN}_5\text{O}_4$: C, 54.94; H, 4.17; N, 13.32%; Found: C, 54.96; H, 4.19; N, 13.35%.



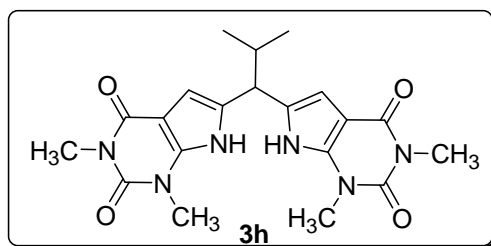
Compound 3f

Pinkish brown solid; Yield: 456 mg (93%); mp. 300- 302 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.19 (s, 6H), 3.39 (s, 6H), 5.58 (s, 1H), 5.85 (s, 2H), 7.50-8.31 (m, 4H), 11.79 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.06 (2C), 31.10 (2C), 42.98, 98.60 (2C), 103.62 (2C), 124.11 (2C), 130.13 (2C), 130.79 (2C), 139.84 (2C), 147.05, 148.66, 151.17 (2C), 158.68 (2C); IR (KBr) ν_{max} : 3374.6, 3277.8, 1685.2, 1556.5 cm^{-1} ; MS (ESI): 492.7 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{23}\text{H}_{22}\text{N}_6\text{O}_6$: C, 56.20; H, 4.25; N, 17.08%; Found: C, 56.21; H, 4.27; N, 17.10%.



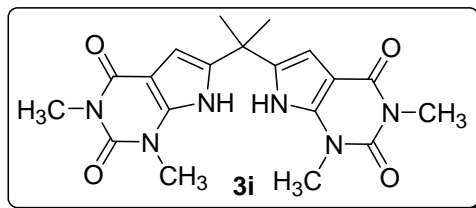
Compound 3g

Off white solid; Yield: 381 mg (90%); mp. 274- 276 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.19 (s, 6H), 3.38 (s, 6H), 5.68 (s, 1H), 5.95 (s, 2H), 6.91-7.47 (m, 3H), 11.84 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 27.95 (2C), 31.04 (2C), 38.34, 98.31 (2C), 102.60 (2C), 125.64, 126.28, 127.20, 131.79 (2C), 139.48 (2C), 144.74, 151.07 (2C), 158.63 (2C); IR (KBr) ν_{max} : 3375.8, 3275.2, 1687.2, 1554.5 cm^{-1} ; MS (ESI): 452.6 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{21}\text{H}_{21}\text{N}_5\text{O}_4\text{S}$: C, 58.52; H, 4.64; N, 15.50%; Found: C, 58.53; H, 4.65; N, 15.52%.



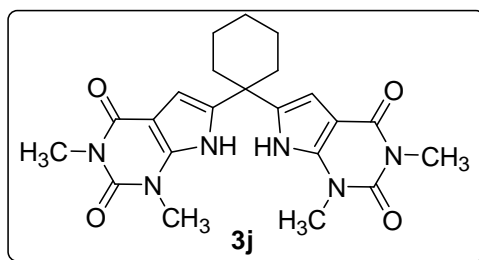
Compound 3h

Light brown solid; Yield: 374 mg (91%); mp. 352- 354 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 0.86 (m, 6H), 2.38 (m, 1H), 3.18 (s, 6H), 3.43 (s, 6H), 3.66 (d, 1H), 6.23 (s, 2H), 11.30 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 21.44 (2C), 28.02 (2C), 31.20 (2C), 31.63, 45.35, 98.56 (2C), 101.38 (2C), 132.32 (2C), 139.00 (2C), 151.14 (2C), 158.76 (2C); IR (KBr) ν_{max} : 3229.8, 3198.5, 2963.0, 1708.1 cm^{-1} ; MS (ESI): 413.1 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{20}\text{H}_{25}\text{N}_6\text{O}_4$: C, 58.24; H, 5.80; N, 20.36%; Found: C, 58.25; H, 5.82; N, 20.38%.



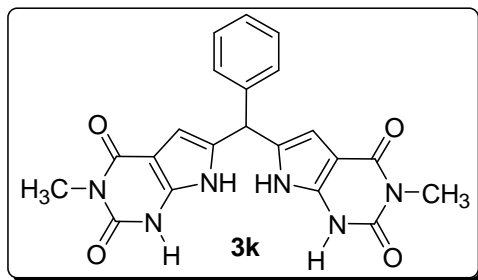
Compound 3i

Off white solid; Yield: 361 mg (91%); mp. 332-334 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 1.63 (s, 6H), 3.20 (s, 6H), 3.39 (s, 6H), 6.06 (s, 2H), 11.10 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.07 (2C), 31.43 (2C), 31.60, 35.93 (2C), 98.02 (2C), 100.44 (2C), 137.80 (2C), 139.69 (2C), 151.25 (2C), 158.80 (2C); IR (KBr) ν_{max} : 3306.9, 3265.2, 1708.2, 1695.3 cm^{-1} ; MS (ESI): 399.4 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{19}\text{H}_{23}\text{N}_5\text{O}_4$: C, 60.43; H, 5.77; N, 17.62%; Found: C, 60.45; H, 5.79; N, 17.63%.



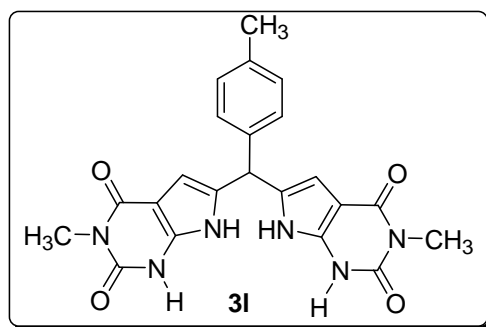
Compound 3j

Greyish solid; Yield: 402 mg (92%); mp. 319-321 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 1.47 (s, 10H), 3.19 (s, 6H), 3.45 (s, 6H), 6.06 (s, 2H), 10.93 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 22.57 (2C), 26.96, 28.06 (2C), 31.44 (2C), 35.43 (2C), 42.14, 98.05 (2C), 100.45 (2C), 137.81 (2C), 139.68 (2C), 151.25 (2C), 158.81 (2C); IR (KBr) ν_{max} : 3306.9, 3267.4, 1709.4, 1693.3 cm^{-1} ; MS (ESI): 439.4 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{22}\text{H}_{27}\text{N}_6\text{O}_4$: C, 60.26; H, 5.92; N, 19.15%; Found: C, 60.27; H, 5.93; N, 19.17%.



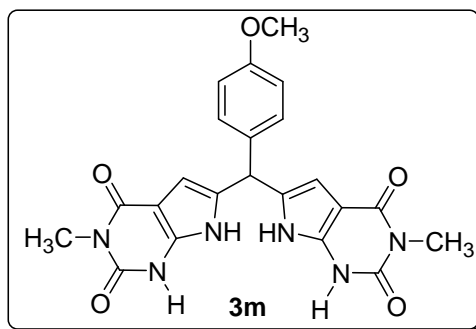
Compound 3k

Pinkish violet solid; Yield: 392 mg (94%); mp. 321- 323 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.17 (s, 3H), 3.26 (s, 3H), 5.38 (s, 1H), 5.45 (s, 1H), 5.72 (s, 1H), 7.09-7.59 (m, 5H), 10.32 (s, 2H, NH), 11.68 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.68 (2C), 42.20, 99.17 (2C), 103.07 (2C), 125.29, 127.01 (2C), 128.86 (2C), 132.15 (2C), 140.13, 141.14 (2C), 151.03 (2C), 159.28 (2C); IR (KBr) ν_{max} : 3372.5, 3279.4, 1658.7, 1615.7 cm^{-1} ; MS (ESI): 419.4 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{21}\text{H}_{19}\text{N}_6\text{O}_4$: C, 60.27; H, 4.30; N, 20.08%; Found: C, 60.28; H, 4.34; N, 20.09%.



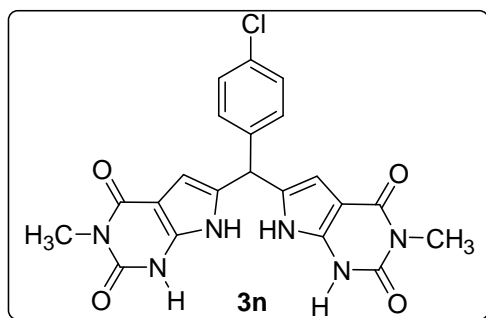
Compound 3l

Violet solid; Yield: 405 mg (94%); mp. 293- 295 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 2.31 (s, 3H), 3.19 (s, 6H), 5.34 (s, 1H), 5.77 (s, 2H), 7.10-7.21 (m, 4H), 10.65 (s, 2H, NH), 11.71 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 21.10, 28.07 (2C), 42.92, 98.45 (2C), 103.07 (2C), 128.65 (2C), 129.39 (2C), 132.39 (2C), 136.65, 138.08, 139.63 (2C), 151.15 (2C), 158.79 (2C); IR (KBr) ν_{max} : 3373.8, 3277.9, 1685.2, 1555.6 cm^{-1} ; MS (ESI): 433.6 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{22}\text{H}_{21}\text{N}_5\text{O}_4$: C, 64.02; H, 4.85; N, 16.22%; Found: C, 64.03; H, 4.87; N, 16.24%.



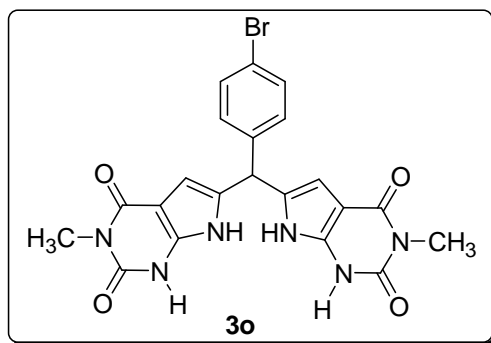
Compound 3m

Violet solid; Yield: 425 mg (95%); mp. 320- 322 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.17 (s, 6H), 3.67 (s, 3H), 5.26 (s, 1H), 5.70 (s, 2H), 6.71-7.26 (m, 4H), 10.72 (s, 2H, NH), 11.65 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.05 (2C), 42.45, 55.54, 98.42 (2C), 102.95 (2C), 114.21 (2C), 128.52 (2C), 129.76, 132.54 (2C), 132.96, 139.65 (2C), 151.17 (2C), 158.77 (2C); IR (KBr) ν_{max} : 3376.5, 3279.4, 1655.5, 1616.6 cm^{-1} ; MS (ESI): 449.5 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{22}\text{H}_{21}\text{N}_6\text{O}_5$: C, 58.90; H, 4.45; N, 18.74%; Found: C, 58.92; H, 4.46; N, 18.75%.



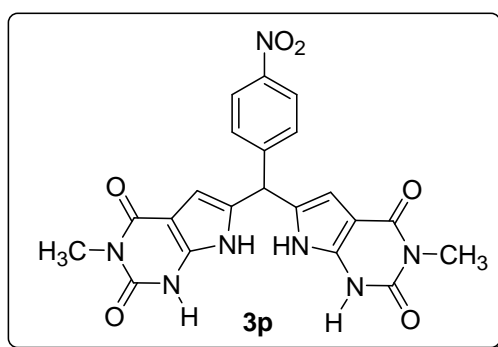
Compound 3n

Violet solid; Yield: 433 mg (96%); mp. 309- 311 °C ; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.25 (s, 6H), 4.56 (s, 1H), 5.39 (s, 1H), 5.75 (s, 1H), 7.10-7.70 (m, 4H), 10.75 (s, 2H, NH), 11.68 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 29.38, 29.85, 42.62, 99.20, 103.16, 127.93, 128.82, 129.04, 129.86, 130.63, 131.69, 132.08, 139.34, 140.12, 141.23, 150.56, 151.02, 151.69, 156.95, 159.27, 162.86; IR (KBr) ν_{max} : 3373.5, 3278.4, 1657.7, 1616.7 cm^{-1} ; MS (ESI): 453.8 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{21}\text{H}_{18}\text{ClN}_6\text{O}_4$: C, 55.70; H, 3.75; N, 18.56%; Found: C, 55.75; H, 3.76; N, 18.58%.



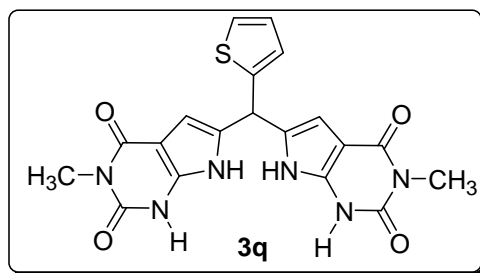
Compound 3o

Violet solid; Yield: 451 mg (91%); mp. 310-312 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.32 (s, 6H), 5.37 (s, 1H), 5.73 (s, 2H), 7.21-7.43 (m, 4H), 10.73 (s, 2H, NH), 11.68 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 29.83 (2C), 42.62, 99.25 (2C), 103.15 (2C), 129.06, 129.87 (2C), 130.67, 131.66 (2C), 140.10 (2C), 141.25 (2C), 151.68 (2C), 159.29 (2C); IR (KBr) ν_{max} : 3378.5, 3274.6, 1655.3, 1614.5 cm^{-1} ; MS (ESI): 497.4 ($[\text{M}+\text{H}]^+$).
 Anal. Cald. For $\text{C}_{21}\text{H}_{18}\text{BrN}_5\text{O}_4$: C, 53.20; H, 3.60; N, 14.09%; Found: C, 53.22; H, 3.62; N, 14.11%.



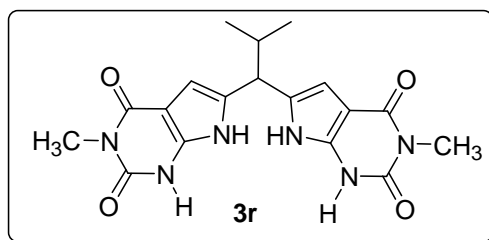
Compound 3p

Violet solid; Yield: 425 mg (92%); mp. 350- 352 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.32 (s, 6H), 5.38 (s, 1H), 5.72 (s, 2H), 7.19-7.39 (m, 4H), 10.74 (s, 2H, NH), 11.69 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.69 (2C), 42.21, 99.14 (2C), 103.02 (2C), 125.27 (2C), 127.08 (2C), 128.89 (2C), 132.13 (2C), 140.10, 141.17, 150.53 (2C), 159.25 (2C); IR (KBr) ν_{max} : 3377.5, 3275.6, 1655.8, 1616.5 cm^{-1} ; MS (ESI): 464.2 ($[\text{M}+\text{H}]^+$).
 Anal. Cald. For $\text{C}_{21}\text{H}_{18}\text{N}_7\text{O}_6$: C, 54.39; H, 3.65; N, 21.14%; Found: C, 54.42; H, 3.67; N, 21.16%.



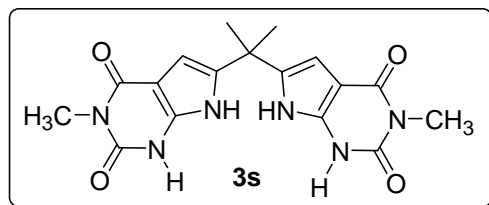
Compound 3q

Off white solid; Yield: 380 mg (90%); mp. 304- 306 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 3.19 (s, 6H), 5.67 (s, 1H), 5.95 (s, 2H), 6.90-7.47 (m, 3H), 10.40 (s, 2H, NH), 11.84 (s, 2H, NH) ; ^{13}C NMR (DMSO- d_6 , 75MHz) δ 31.05 (2C), 38.33, 98.30 (2C), 102.62 (2C), 125.65, 126.27, 127.21, 131.77 (2C), 139.47 (2C), 144.73, 151.06 (2C), 158.62 (2C); IR (KBr) ν_{max} : 3375.8, 3275.2, 1687.2, 1554.5 cm^{-1} ; MS (ESI): 425.5 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{19}\text{H}_{17}\text{N}_5\text{O}_4\text{S}$: C, 56.72; H, 4.00; N, 16.50%; Found: C, 56.73; H, 4.01; N, 16.54%.



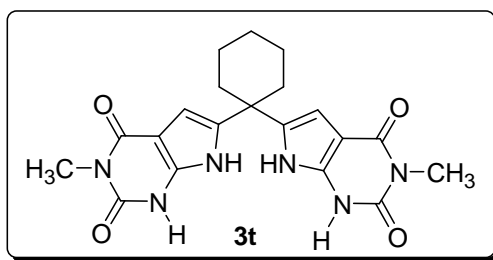
Compound 3r

Light brown solid; Yield: 344 mg (90%); mp. 360-362 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 0.86 (m, 6H), 2.35 (m, 1H), 3.18 (s, 3H), 3.43 (s, 3H), 3.60 (d, 1H), 6.21 (s, 2H), 10.55 (s, 2H, NH), 11.45 (s, 2H, NH) ; ^{13}C NMR (DMSO- d_6 , 75MHz) δ 21.44 (2C), 28.03 (2C), 31.25, 45.33, 98.57 (2C), 101.39 (2C), 132.30 (2C), 139.10 (2C), 151.18 (2C), 158.77 (2C); IR (KBr, cm^{-1}) ν_{max} : 3228.8, 3197.5, 2965.0, 1709.1 cm^{-1} ; MS (ESI): 385.1 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{18}\text{H}_{21}\text{N}_5\text{O}_4$: C, 59.52; H, 5.46; N, 18.26%; Found: C, 59.53; H, 5.48; N, 18.27%.



Compound 3s

Off white solid; Yield: 335 mg (91%); mp. 332-334 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 1.63 (s, 6H), 3.24 (s, 6H), 6.06 (s, 2H), 10.77 (s, 2H, NH), 11.11 (s, 2H, NH); ^{13}C NMR (DMSO- d_6 , 75MHz) δ 28.05 (2C), 31.42 (2C), 35.94, 98.04 (2C), 100.43 (2C), 137.81 (2C), 139.67 (2C), 151.26 (2C), 158.83 (2C) ; IR (KBr) ν_{max} : 3305.9, 3267.2, 1704.2, 1696.3 cm^{-1} ; MS (ESI): 370.3 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{17}\text{H}_{19}\text{N}_5\text{O}_4$: C, 58.52; H, 5.13; N, 18.96%; Found: C, 58.53; H, 5.14; N, 18.97%.



Compound 3t

White solid; Yield: 372 mg (91%); mp. 320-322 °C; ^1H NMR (DMSO- d_6 , 300 MHz) δ 1.46 (s, 10H), 3.19 (s, 6H), 6.06 (s, 2H), 10.95 (s, 2H, NH), 11.65 (s, 2H, NH) ; ^{13}C NMR (DMSO- d_6 , 75MHz) δ 22.56 (2C), 26.95, 28.08 (2C), 31.45 (2C), 42.12, 98.03 (2C), 100.44 (2C), 137.82 (2C), 139.69 (2C), 151.27 (2C), 158.82 (2C); IR (KBr, cm^{-1}) ν_{max} : 3305.9, 3267.8, 1707.5, 1693.8 cm^{-1} ; MS (ESI): 411.1 ($[\text{M}+\text{H}]^+$). Anal. Cald. For $\text{C}_{20}\text{H}_{23}\text{N}_5\text{O}_4$: C, 61.60; H, 5.61; N, 17.10%; Found: C, 61.61; H, 5.62; N, 17.11%.

