Design, synthesis and biological evaluation of new pyrimidine derivatives as anticancer agents

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Contents

NMR spectra for compounds **1b-g, 2a-f** and **3**

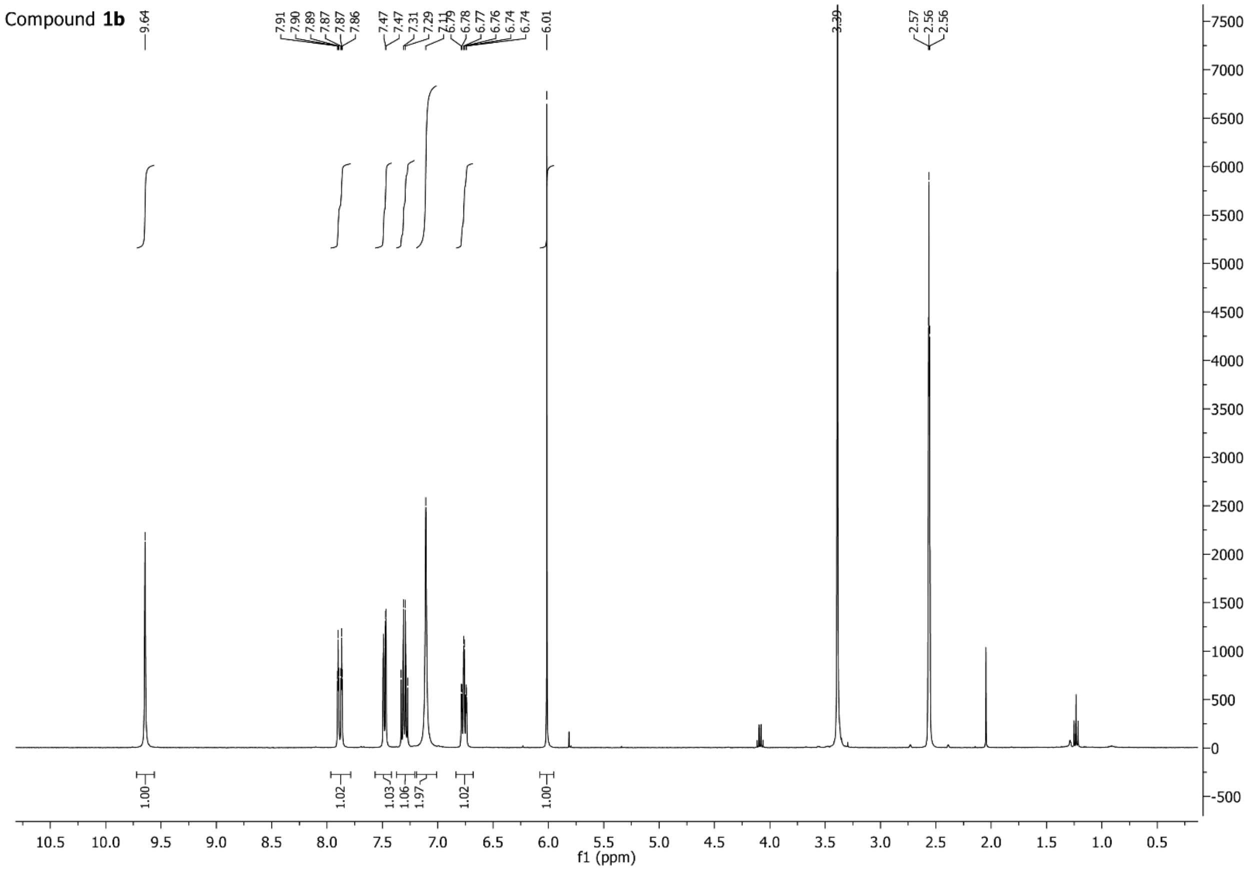

Figure S1. NMR (400 MHz, DMSO-*d*6) Spectrum for **1b**

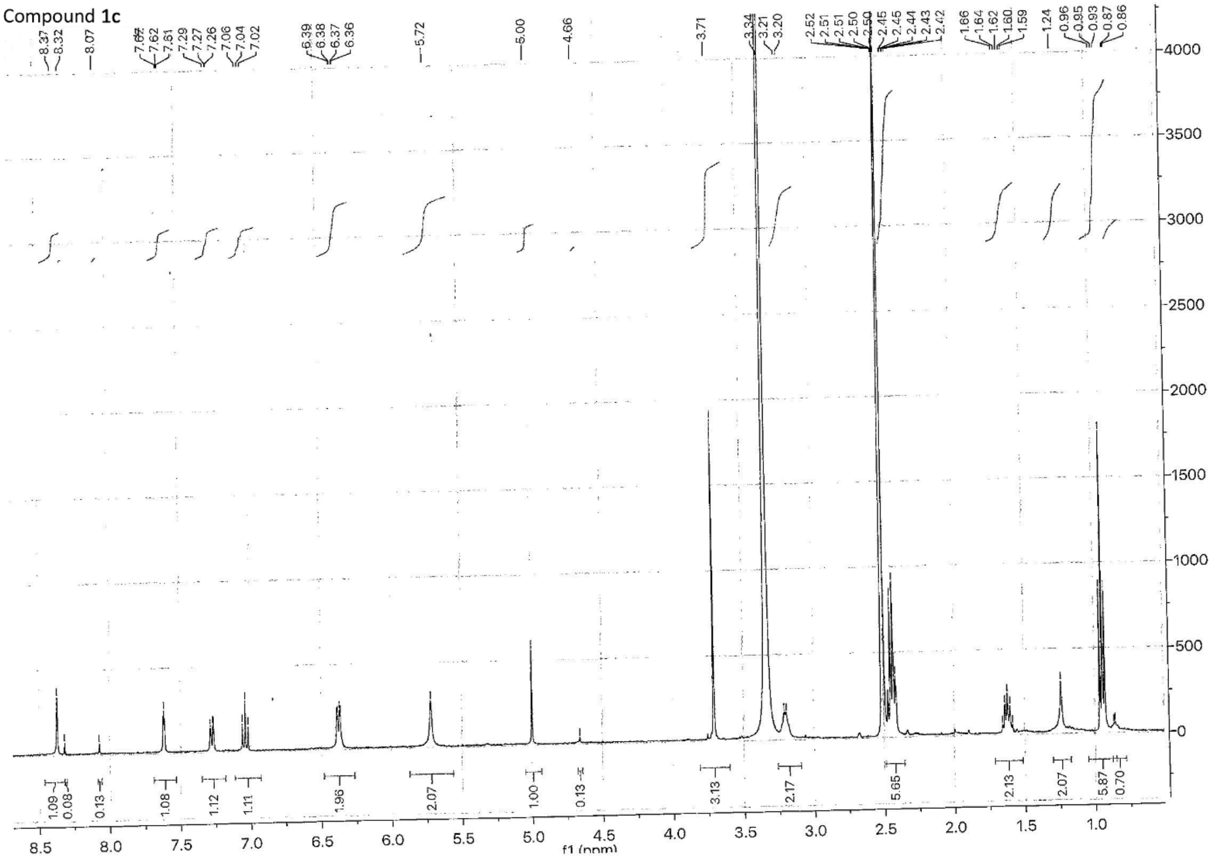

Figure S2. NMR (400 MHz, DMSO-*d6*) Spectrum for **1c**

Compound **1d**

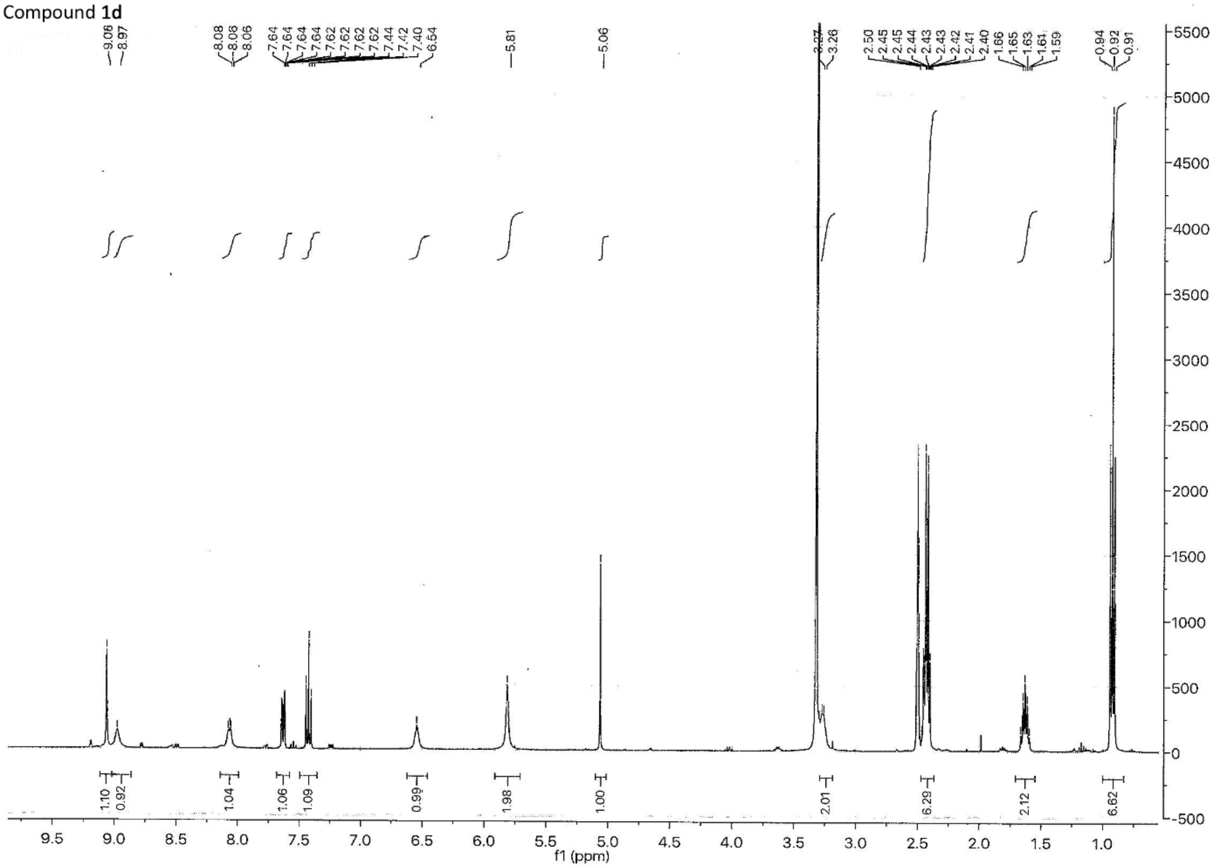

Figure S3. NMR (400 MHz, DMSO-*d*6) Spectrum for **1d**

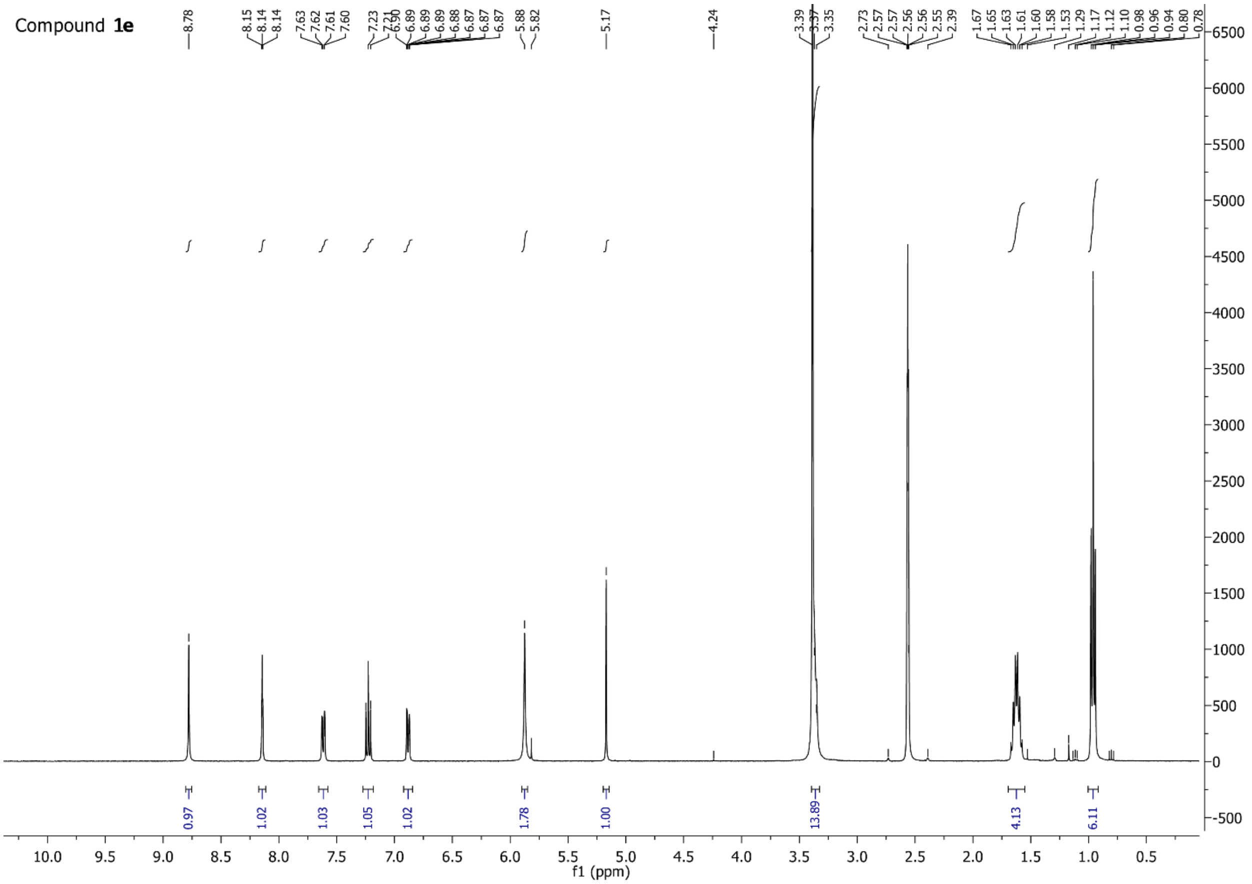

Figure S4. NMR (400 MHz, DMSO-*d*6) Spectrum for **1e**

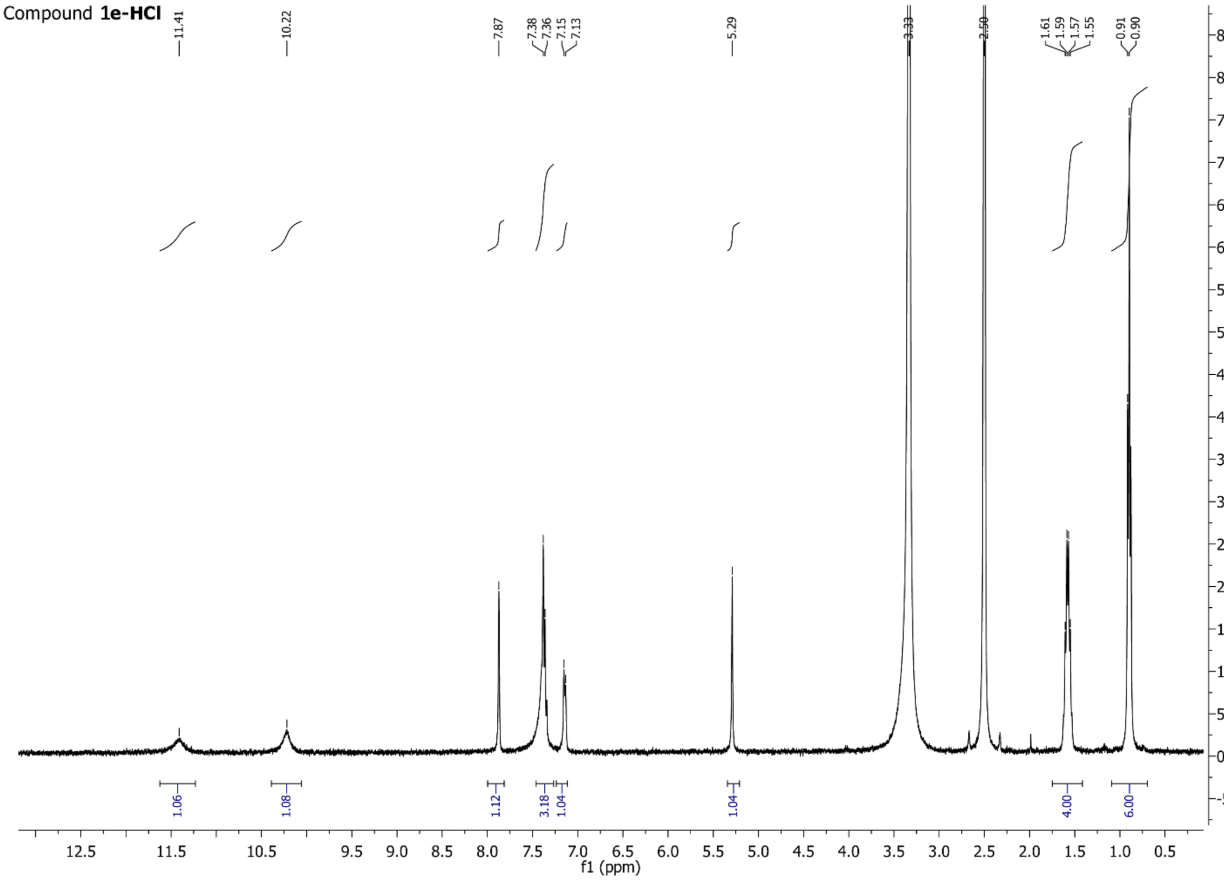

Figure S5. NMR (400 MHz, DMSO-*d*6) Spectrum for **1e-HCl**

Compound **1f**

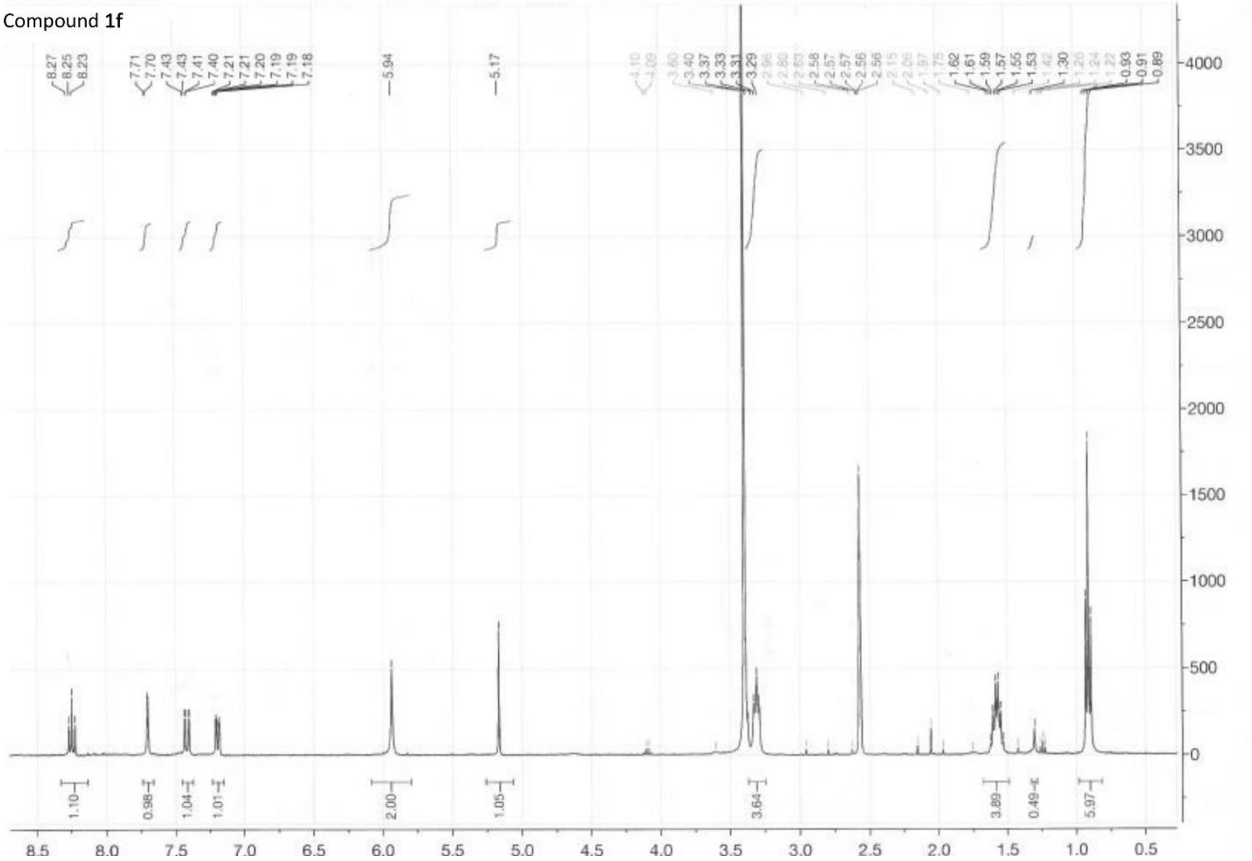

Figure S6. NMR (400 MHz, DMSO-*d*6) Spectrum for **1f**

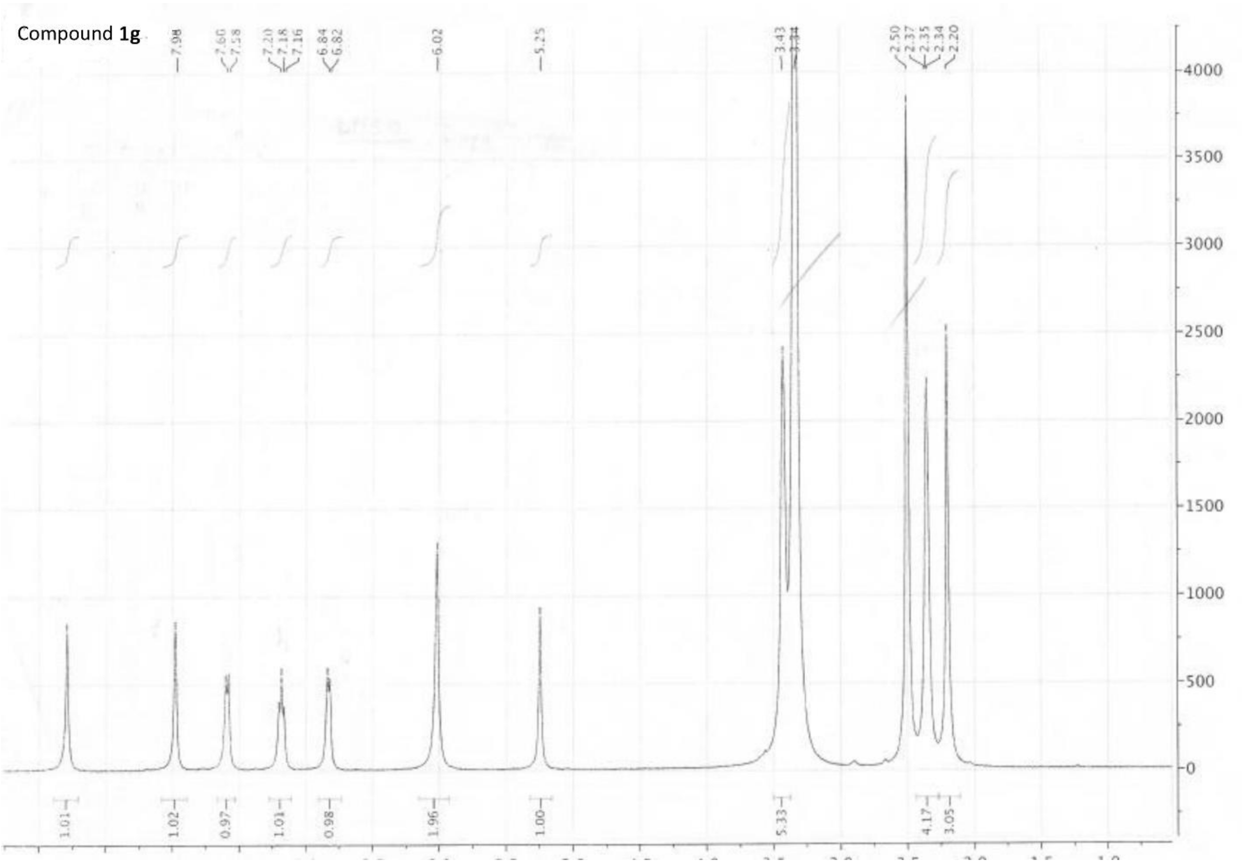
Compound **1g**

Figure S7. NMR (400 MHz, DMSO-*d*6) Spectrum for **1g**

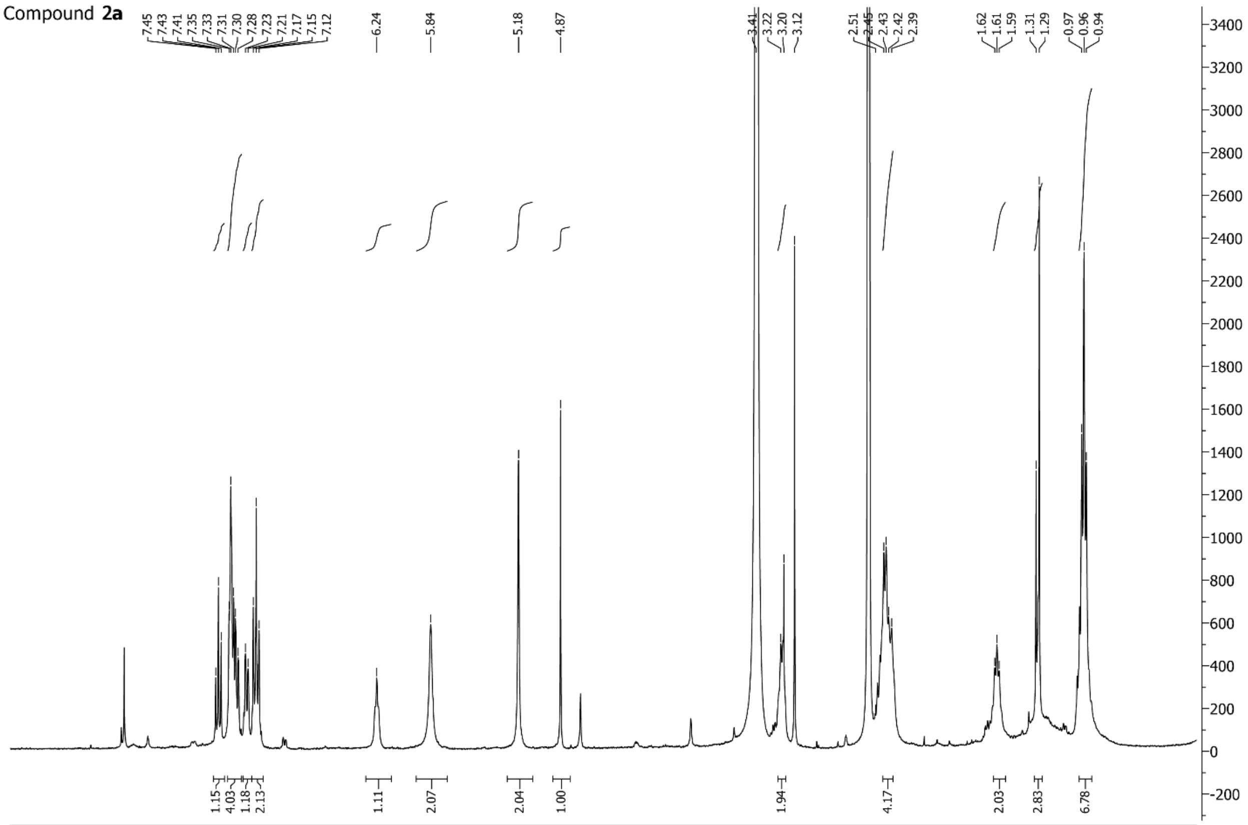

Figure S8. NMR (400 MHz, DMSO-*d*6) Spectrum for **2a**

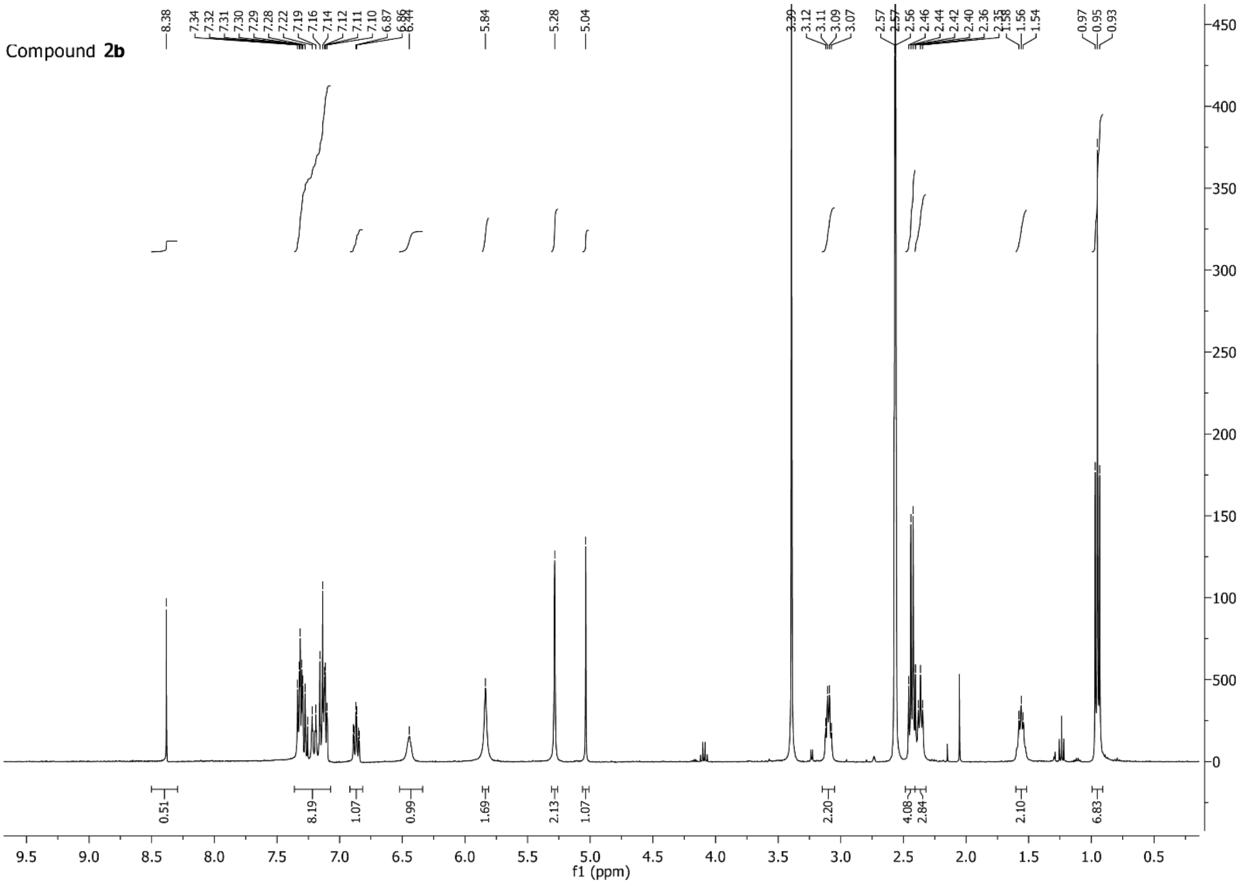

Figure S9. NMR (400 MHz, DMSO-*d*6) Spectrum for **2b**

Compound **2c**

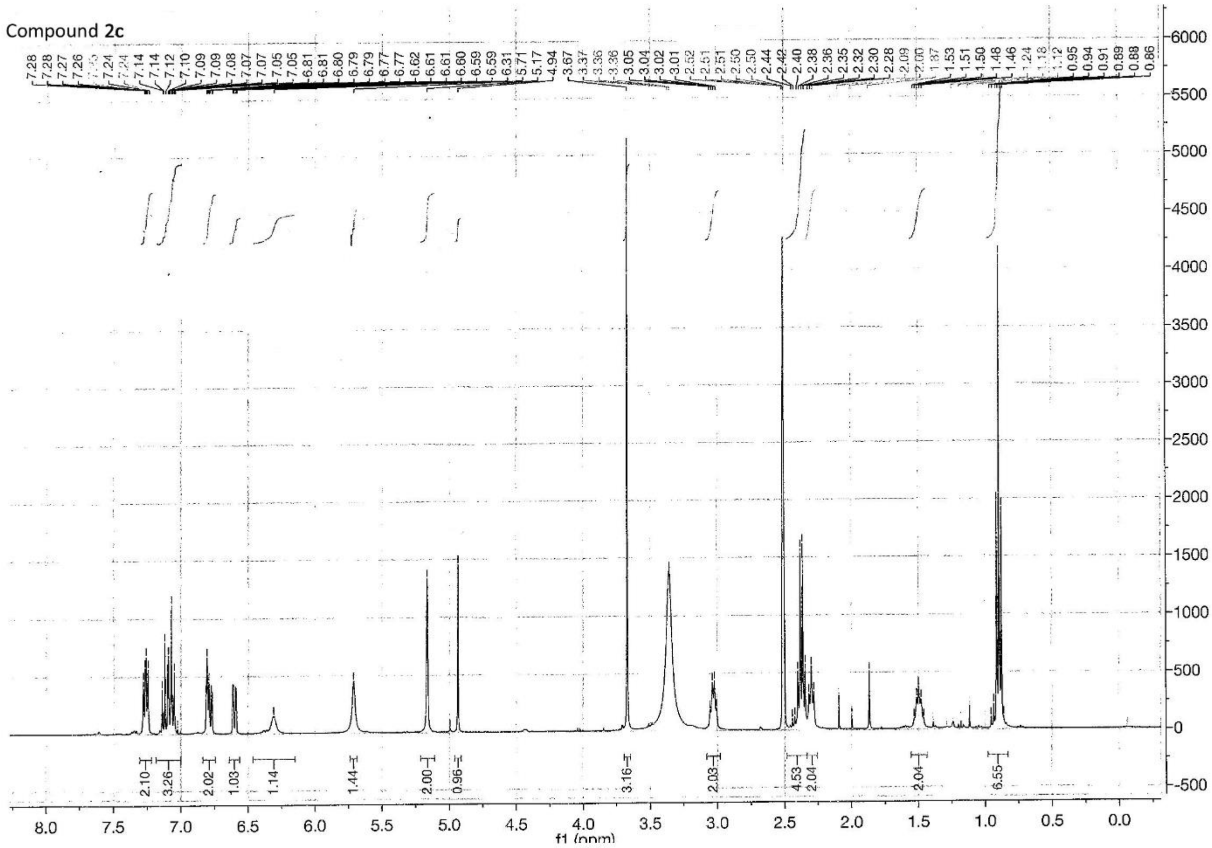

Figure S10. NMR (400 MHz, DMSO-*d6*) Spectrum for **2c**

Compound **2d**

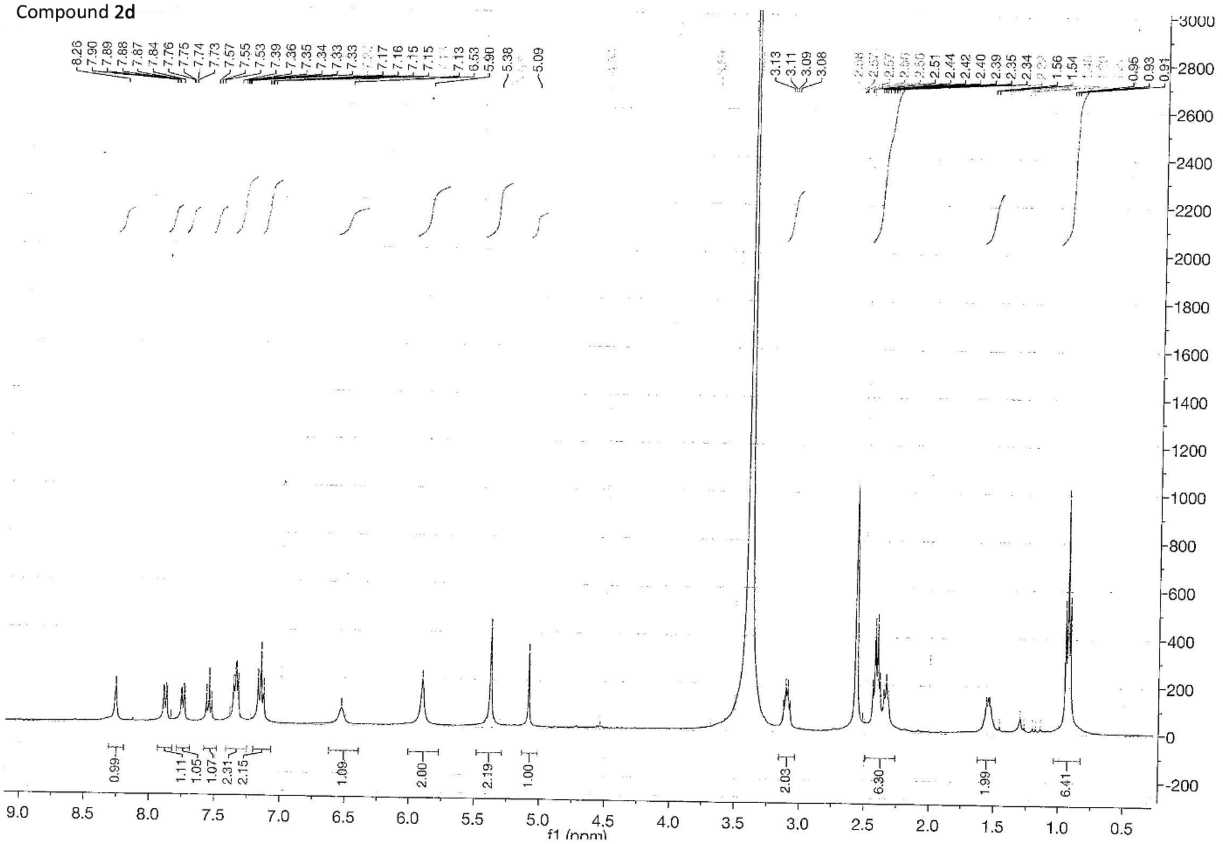

Figure S11. NMR (400 MHz, DMSO-*d*6) Spectrum for **2d**

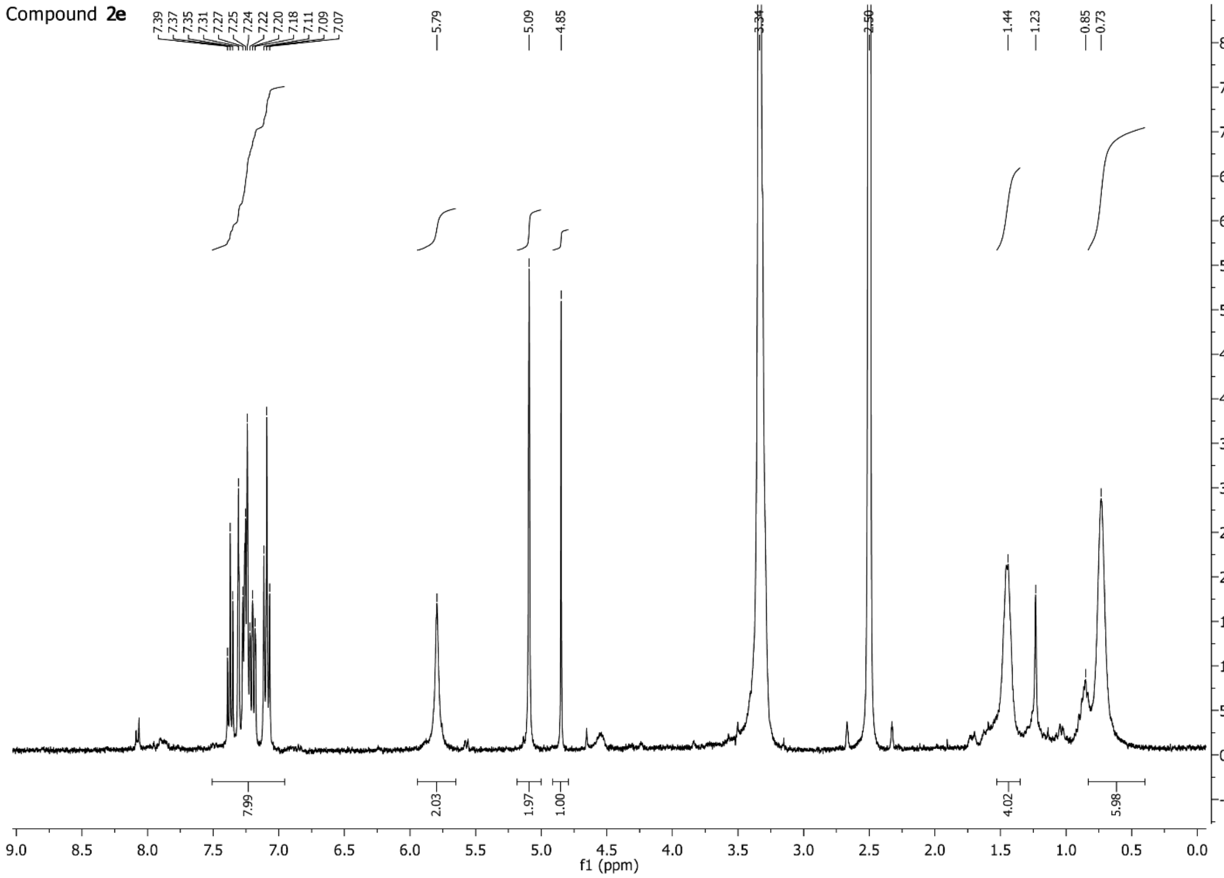

Figure S12. NMR (400 MHz, DMSO-*d*6) Spectrum for **2e**

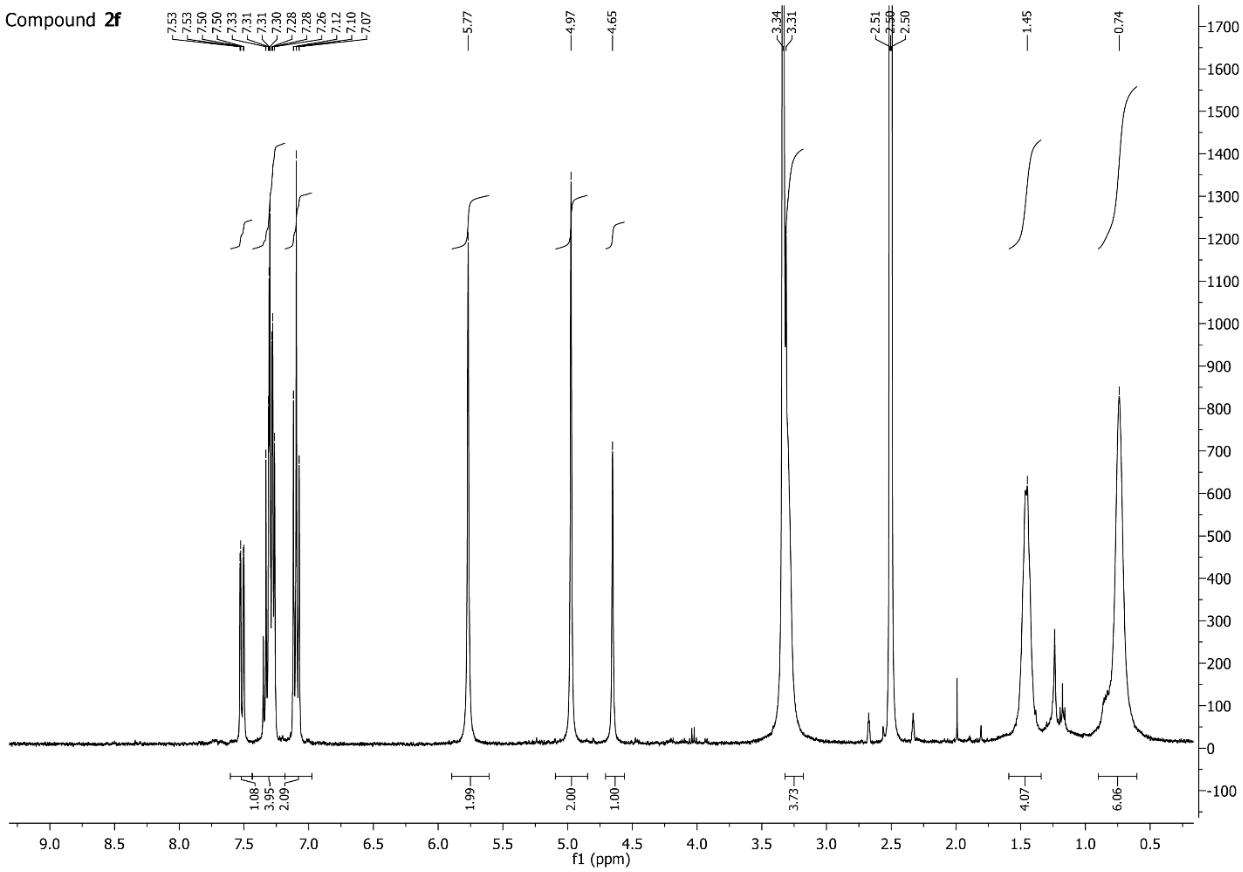

Figure S13. NMR (400 MHz, DMSO-*d*6) Spectrum for **2f**

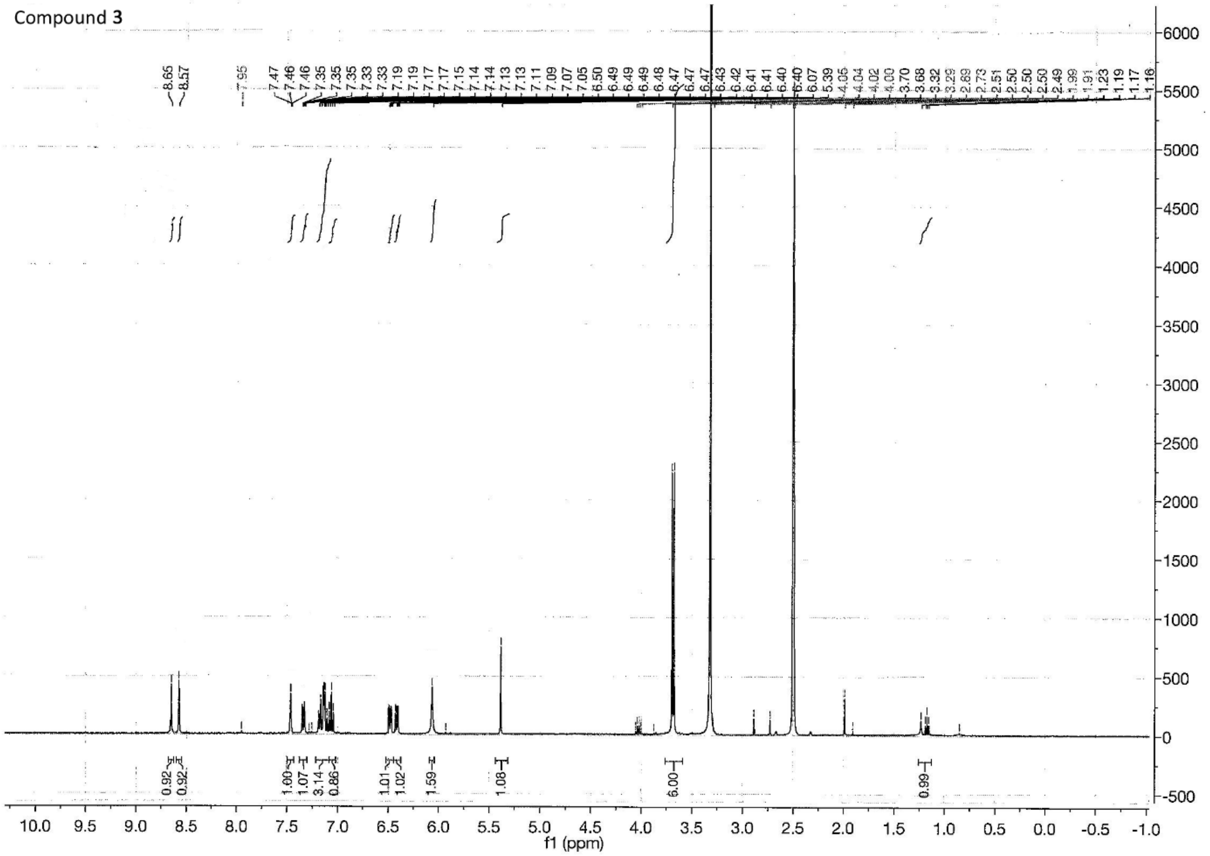

Figure S14. NMR (400 MHz, DMSO-*d*6) Spectrum for **3**

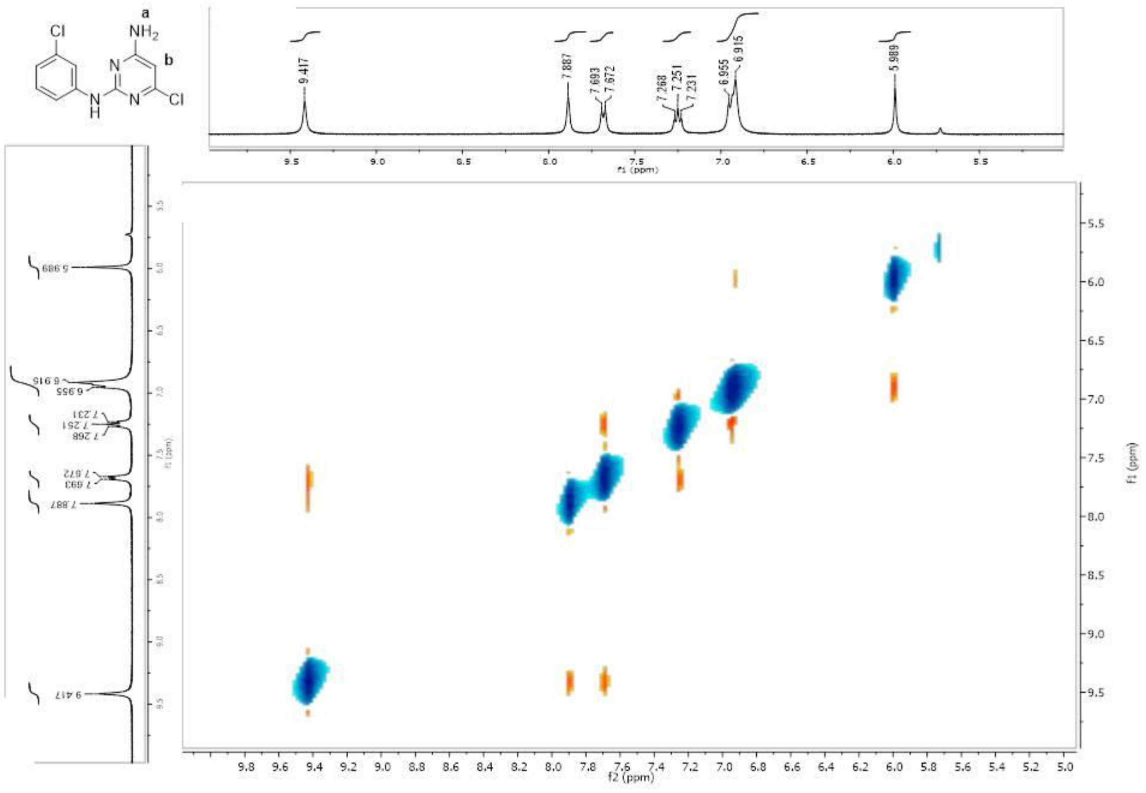

Figure S15. 2D-NMR (400 MHz, DMSO-*d*6) Spectrum for **4a**. The singlet at 5.98 ppm correlates with the broad singlet at 6.90 ppm: these signals correspond respectively to Hb and NH_2 of pyrimidine moiety. The cross peak indicates the closeness of Hb to NH_2 and confirms the structure reported for compound **4a**

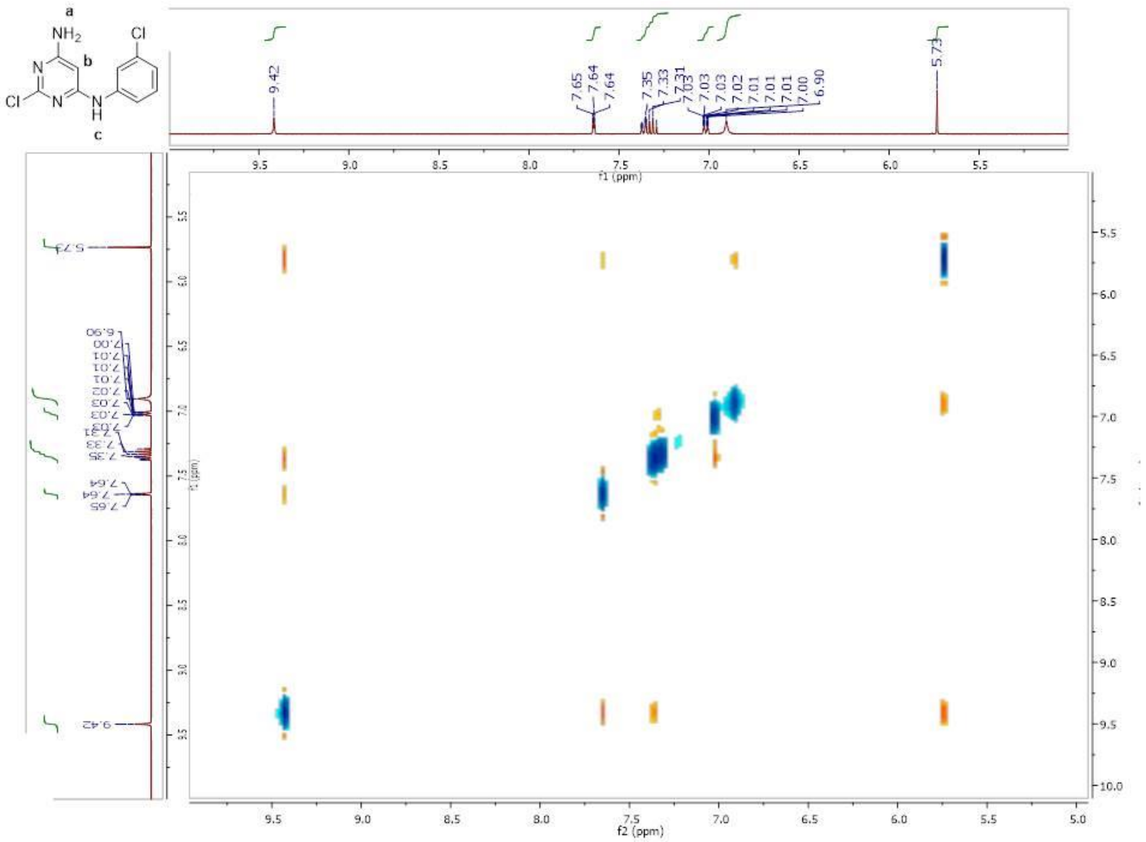

Figure S16. 2D-NMR (400 MHz, DMSO-*d*6) spectra for the regioisomer of compound **4a** (namely **4a'**). The singlet at 5.78 ppm correlates with the broad singlet at 6.90 ppm and with the singlet at 9.42 ppm: these signals correspond respectively to Hb and NH_2 of pyrimidine moiety and NH (Hc) of the aniline portion. In this spectrum there are NOE correlations between the hydrogens of pyrimidine moiety and the Hc of the aniline portion and this confirms the structure reported for compound **4a'.**