

Synthesis of 2-ureido-4-ferrocenyl pyrimidine guests. Investigation of complementary molecular recognition of 2,6-diaminopyridine

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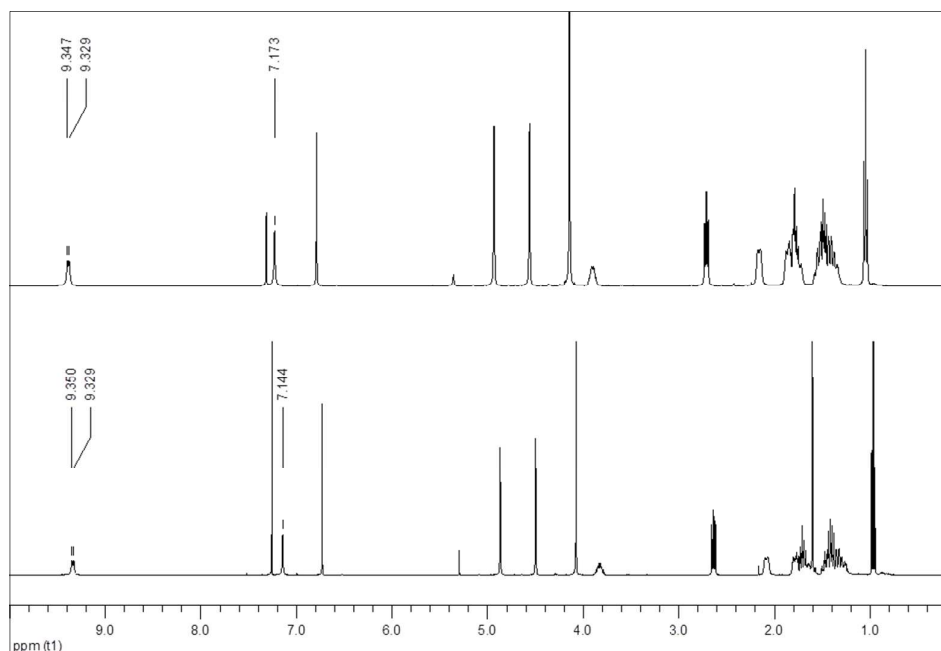


Figure S1. The change of the chemical shifts of NH protons of **5g** upon dilution (42mM (top), 7mM (bottom)) in CDCl_3

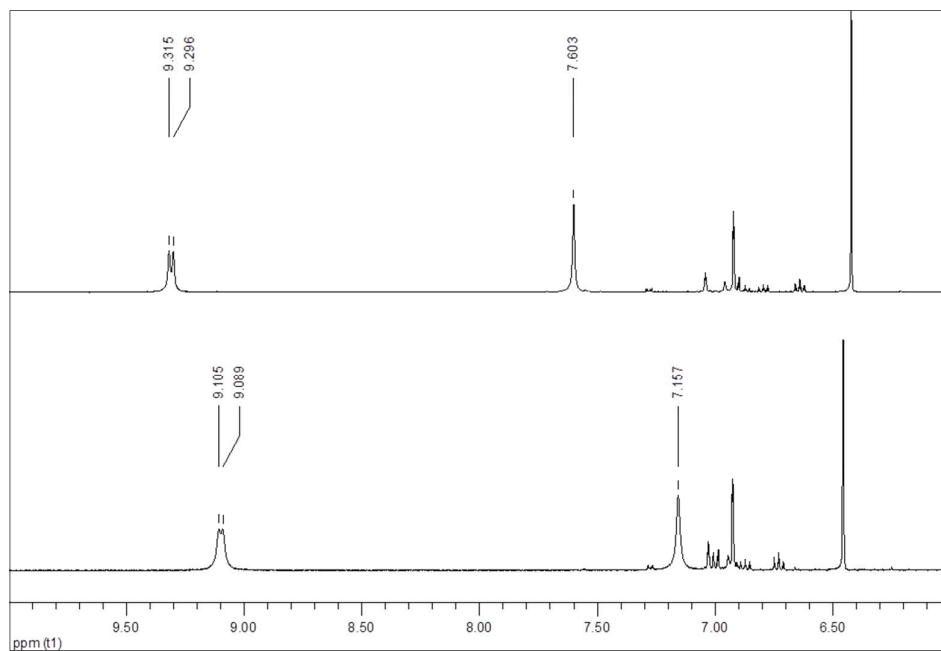


Figure S2. The change of the chemical shifts of NH protons of **5g** upon heating from 30 °C (top), to 80 °C (bottom) in toluene-d_8 .

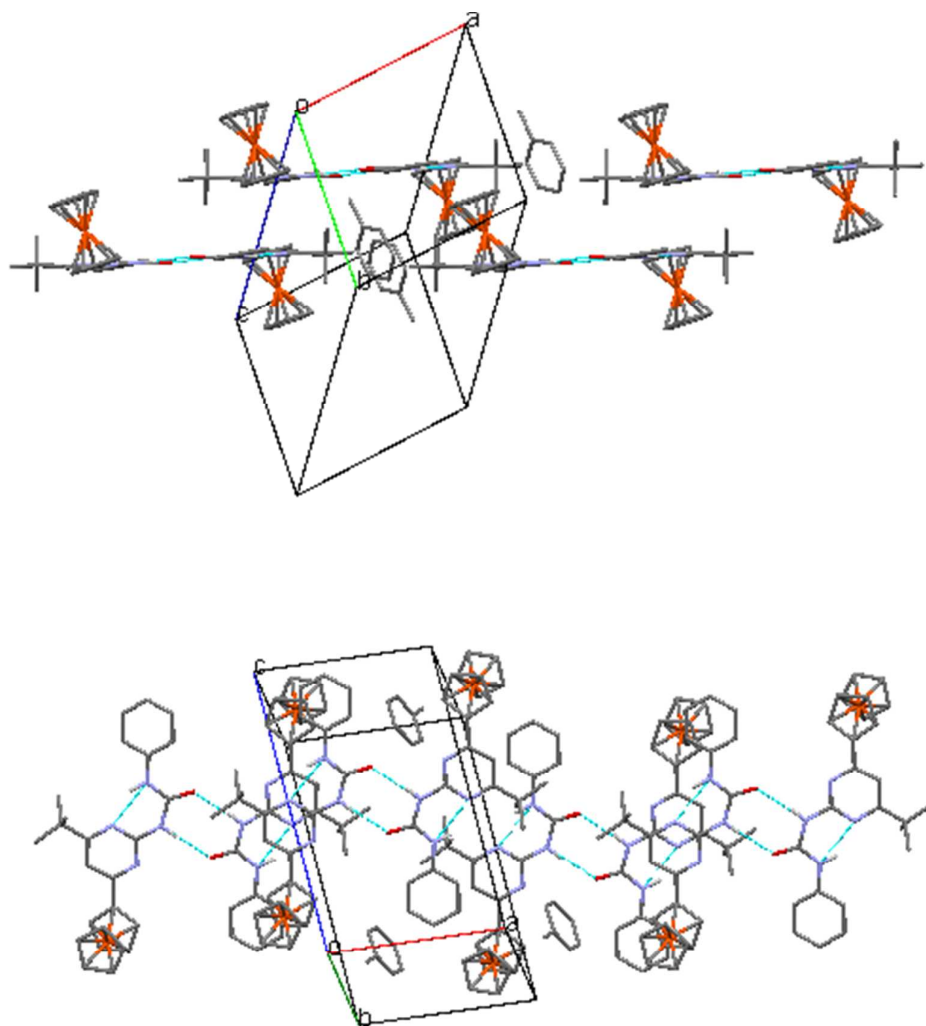


Figure S3. Two perpendicular views of the crystal packing of compound **5m**.

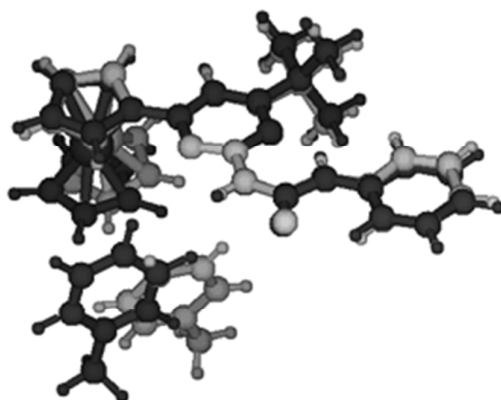


Figure S4. Comparison of the XRD structure (light grey) and the optimized structure (dark grey) of compound **5m**

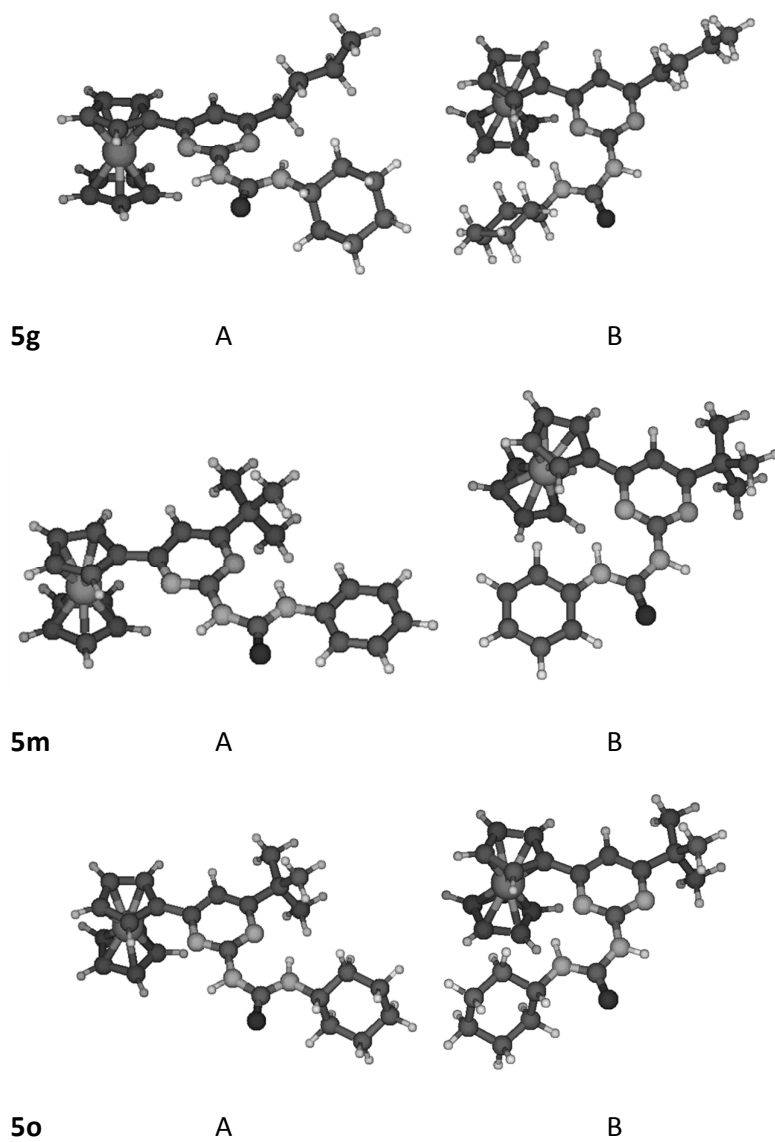


Figure S5. The optimized structures of the two possible conformers (A and B) of compounds **5g**, **5m** and **5o** using the CAM-B3LYP density functional with 6-31G* basis set

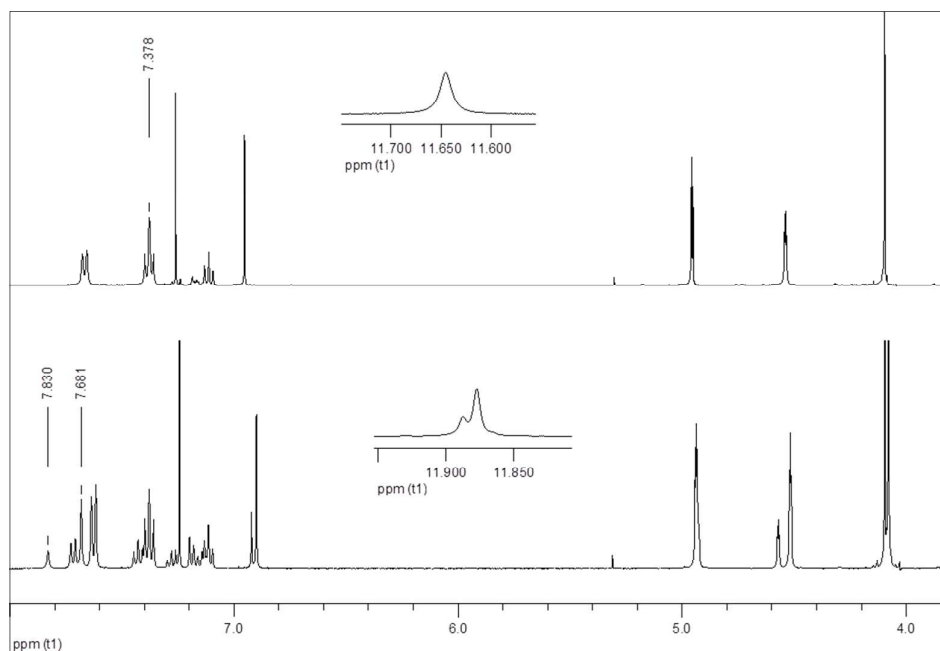


Figure S6. ^1H NMR spectra of **5m** at 25 °C (top) and -60 °C (bottom).

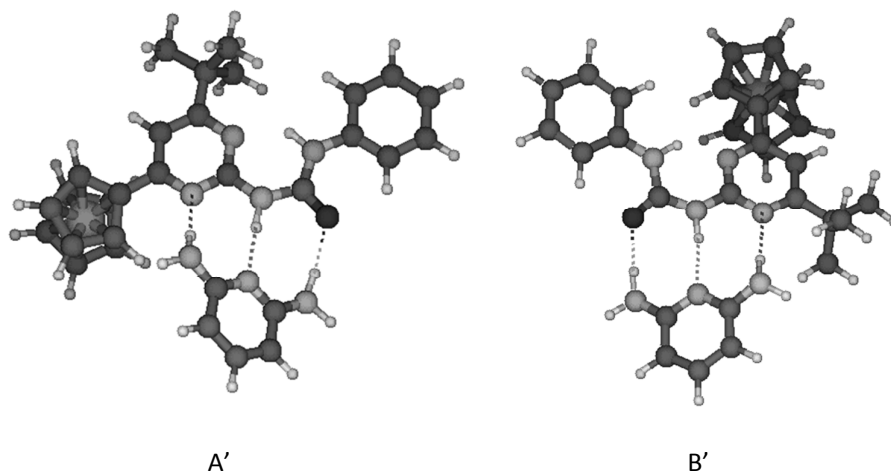


Figure S7. The optimized structures of the two possible conformers of compound **5m** with 2,6-diaminopyridine (**6**) using the CAM-B3LYP density functional and 6-31G* basis set

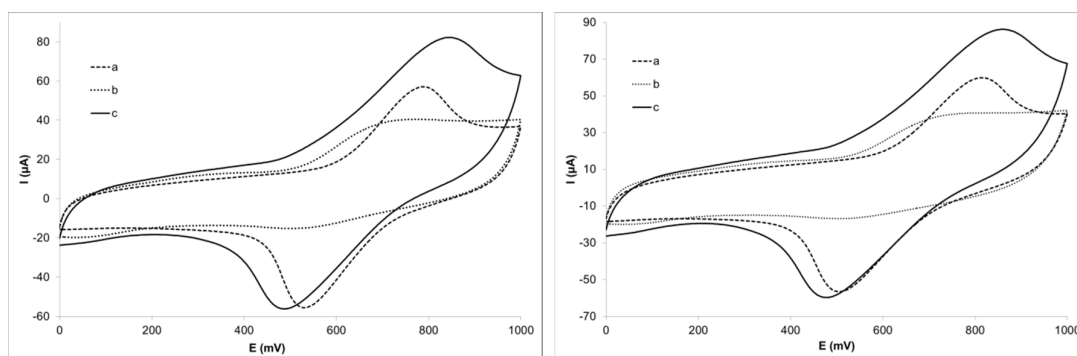


Figure S8. Cyclic voltammograms of **5g** (1 mM) (I_{5g} , a), **6** (1 mM) (I_6 , b), **5g/6=1/1** mixture (1 mM for each component) (I_{5g+6} , c) on two different spectral graphite electrodes (OD=3mm). Solvent: dichloromethane, supporting electrolyte: 0.1 M TBAClO₄.

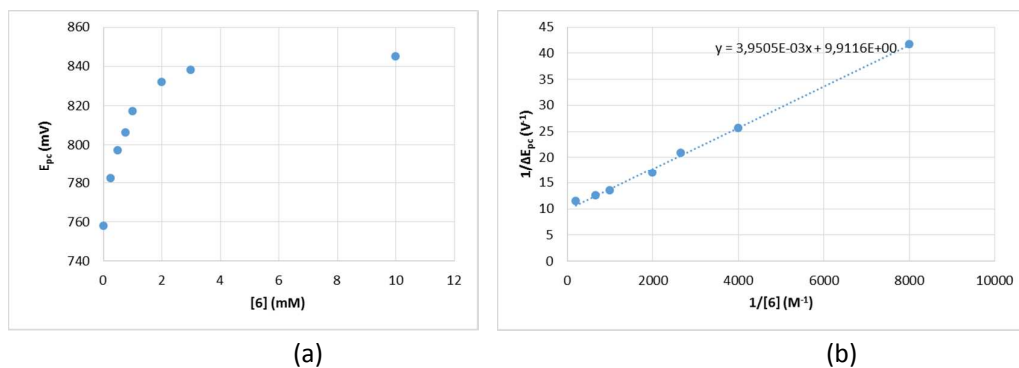


Figure S9. Titration of host **5g** (0.5 mM) with guest **6**. (a) E_{pc} values obtained by LSV. (b) Benesi-Hildebrand plot for host **5g** with guest **6** determined by LSV. Solvent: dichloromethane, supporting electrolyte: 0.1 M TBAClO₄, spectral graphite electrode (OD= 3mm).

Table S1. Change in the E_{pa} values of host **5g** and host-guest complex **5g+6** in CH₂Cl₂/CH₃CN solvent mixtures. Concentrations: 1 mM (**5g**), 1mM (**5g**)+ 1mM (**6**). Supporting electrolyte: 0.1 M TBAClO₄, spectral graphite electrode (OD= 3mm).

CH ₂ Cl ₂ /CH ₃ CN ratio	$E_{pa}(\mathbf{5g+6})$ (mV)	$E_{pa}(\mathbf{5g})$ (mV)	$\Delta E_{pa}(\text{mV})$
1/0	796	767	29
5/1	744	731	13
2/1	707	697	10
1/1	682	674	8
1/2	673	667	6
1/5	675	667	8

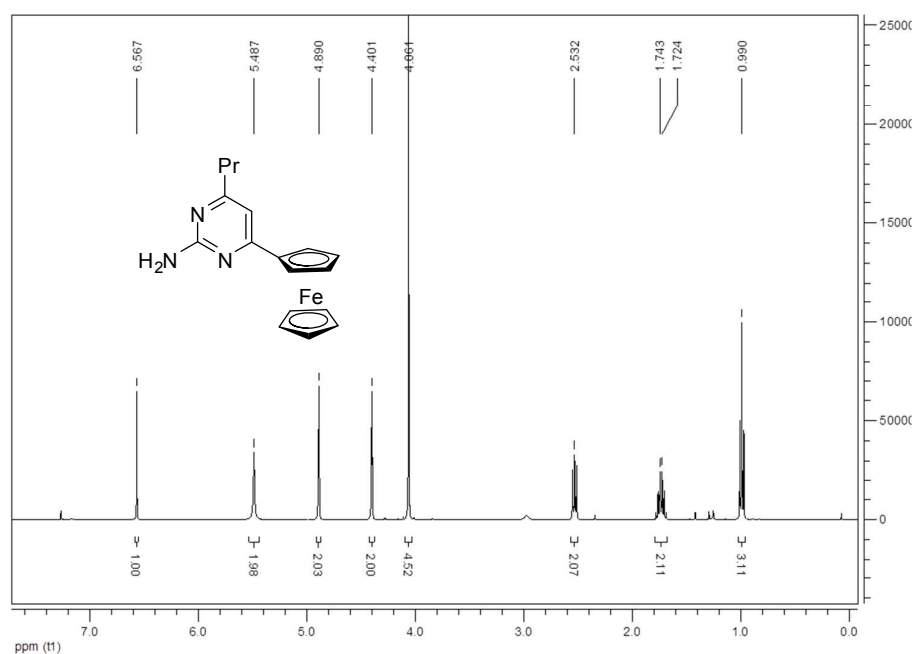


Figure S10. ¹H NMR spectrum of 2-amino-4-ferrocenyl-6-propylpyrimidine (**4c**)

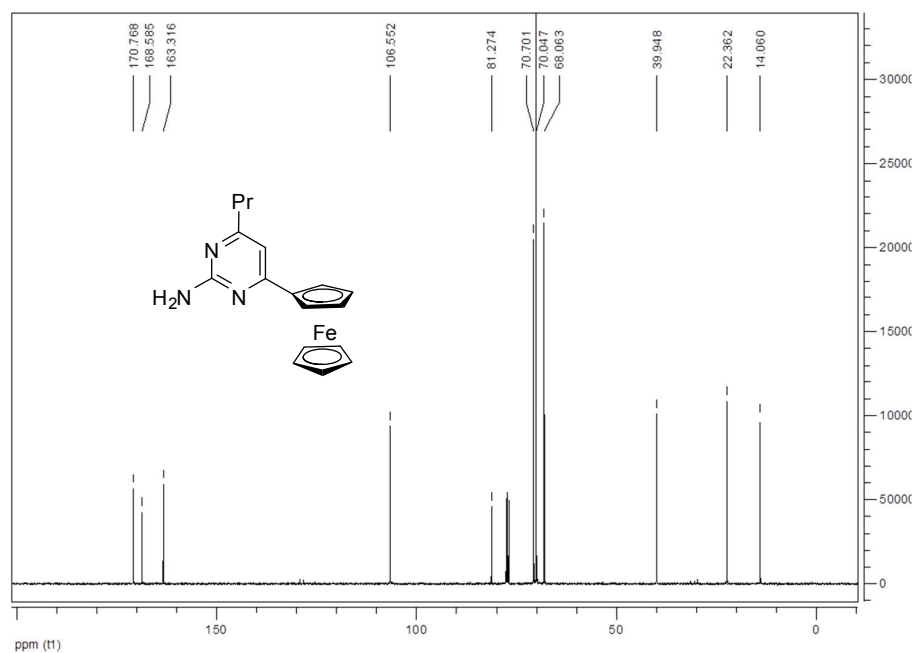


Figure S11. ¹³C NMR spectrum of 2-amino-4-ferrocenyl-6-propylpyrimidine (**4c**)

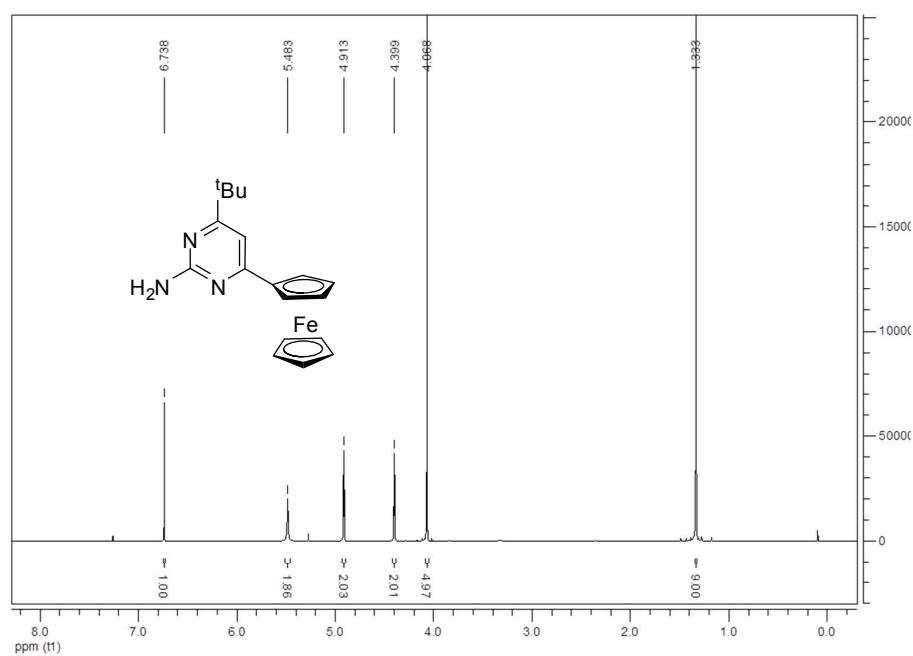


Figure S12. ¹H NMR spectrum of 2-amino-4-*tert*-butyl-6-ferrocenyl pyrimidine (**4d**)

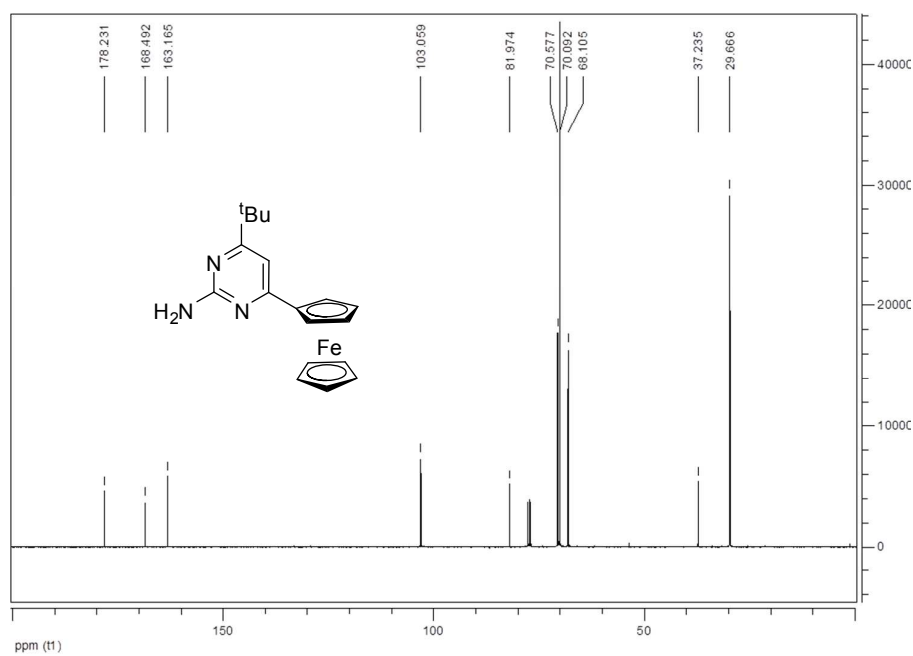


Figure S13. ¹³C NMR spectrum of 2-amino-4-*tert*-butyl-6-ferrocenyl pyrimidine (**4d**)

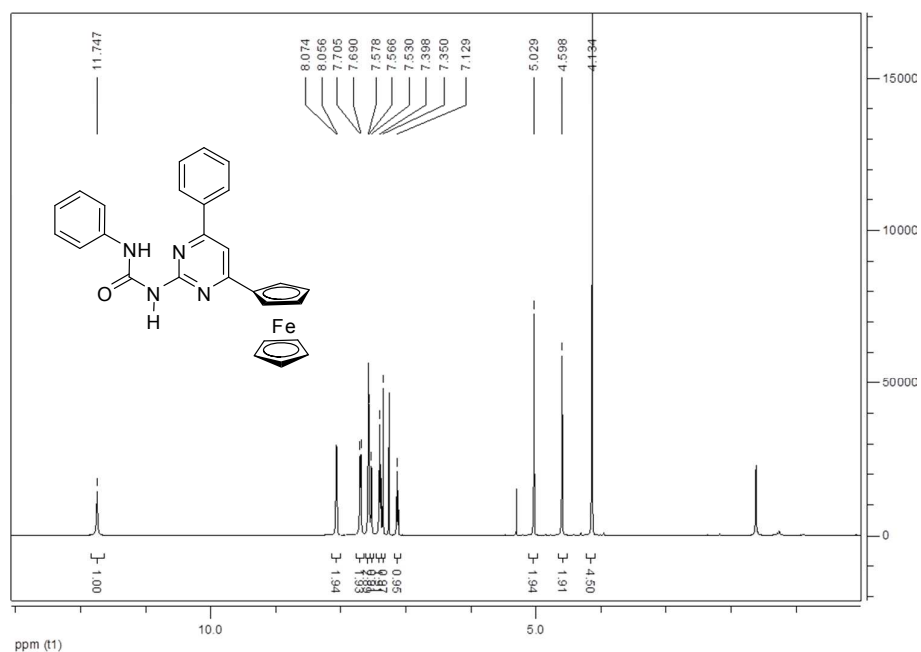


Figure S14. ¹H NMR spectrum of 1-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-3-phenylurea (**5a**)

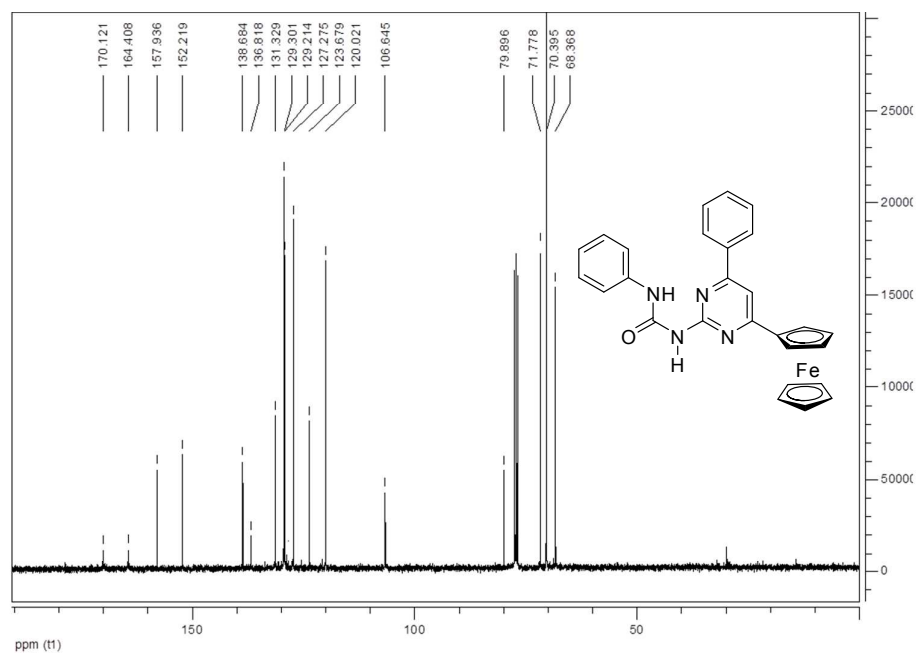


Figure S15. ¹³C NMR spectrum of 1-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-3-phenylurea (**5a**)

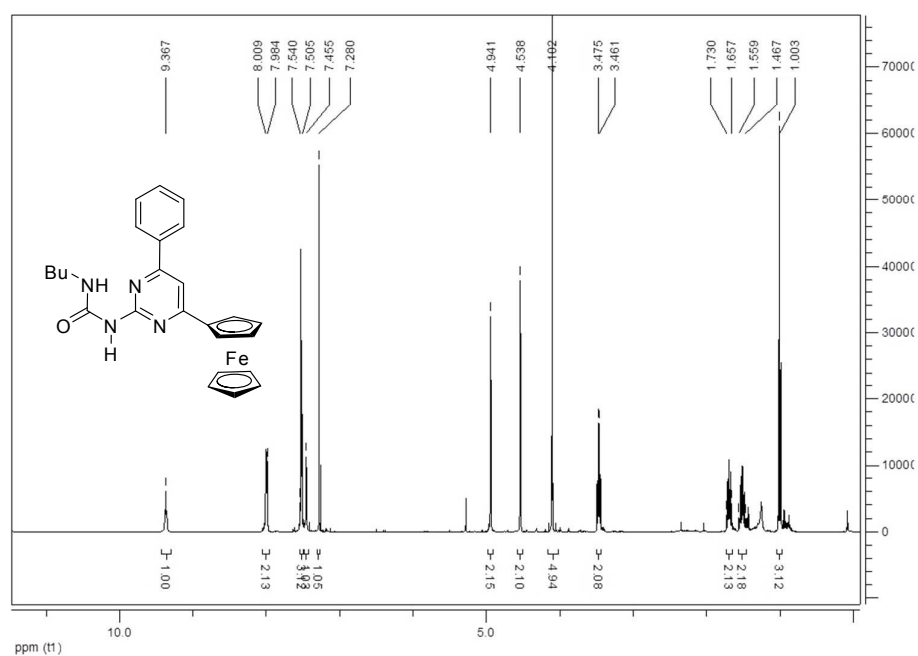


Figure S16. ¹H NMR spectrum of 1-butyl-3-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-urea (**5b**)

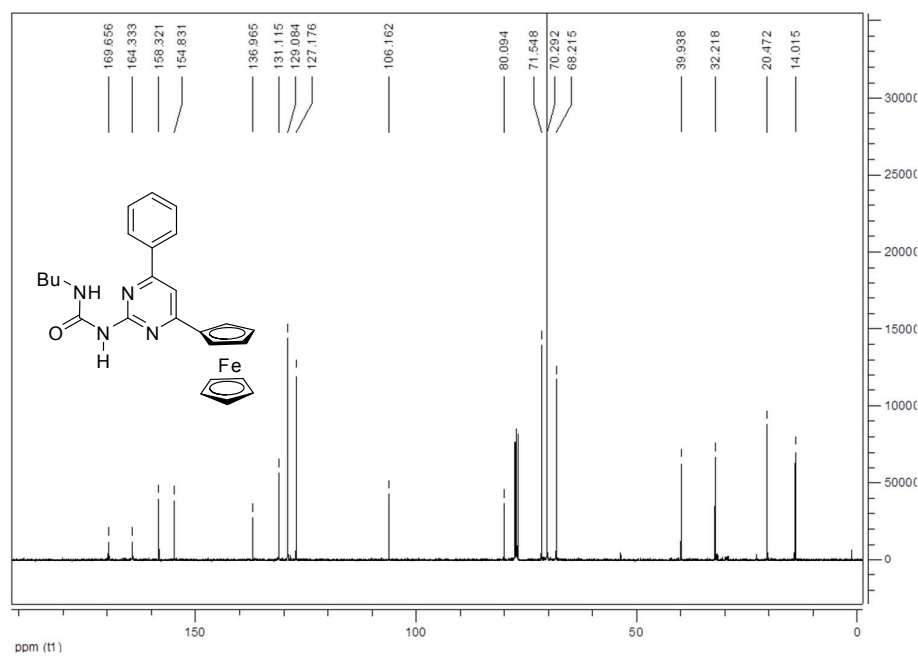


Figure S17. ¹³C NMR spectrum of 1-butyl-3-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-urea (**5b**)

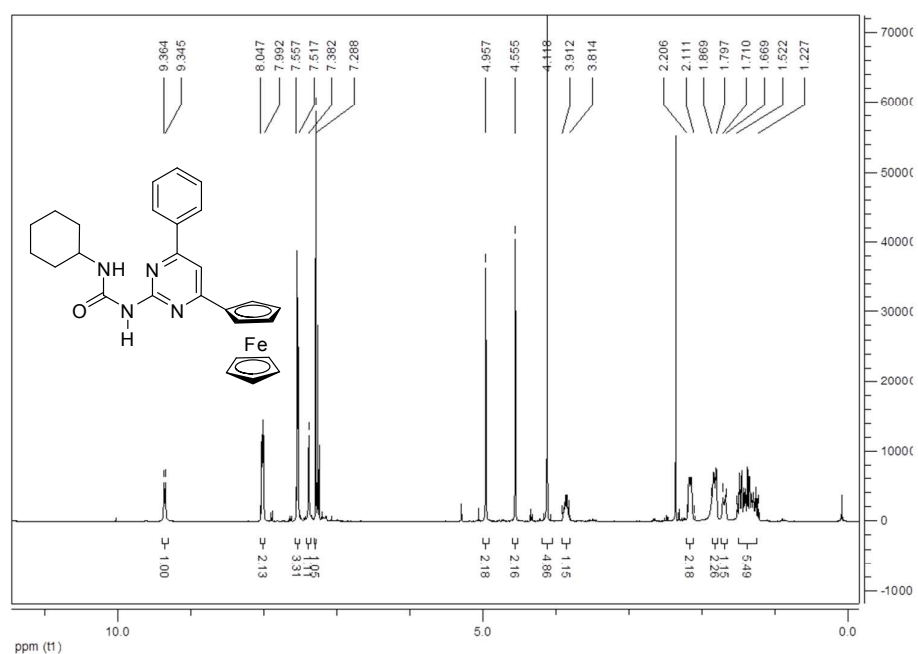


Figure S18. ¹H NMR spectrum of 1-cyclohexyl-3-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-urea (**5c**)

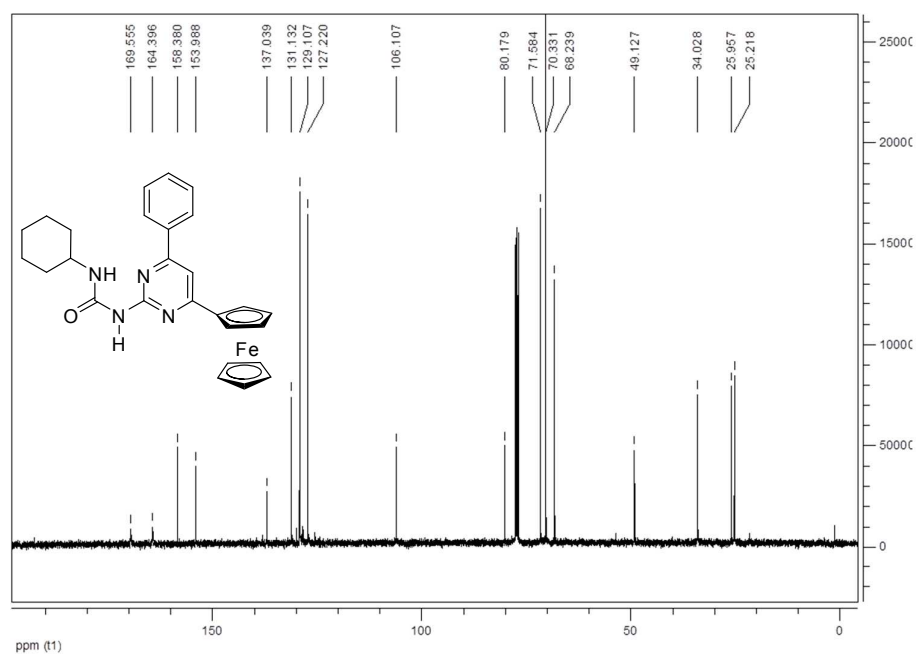


Figure S19. ¹³C NMR spectrum of 1-cyclohexyl-3-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-urea (**5c**)

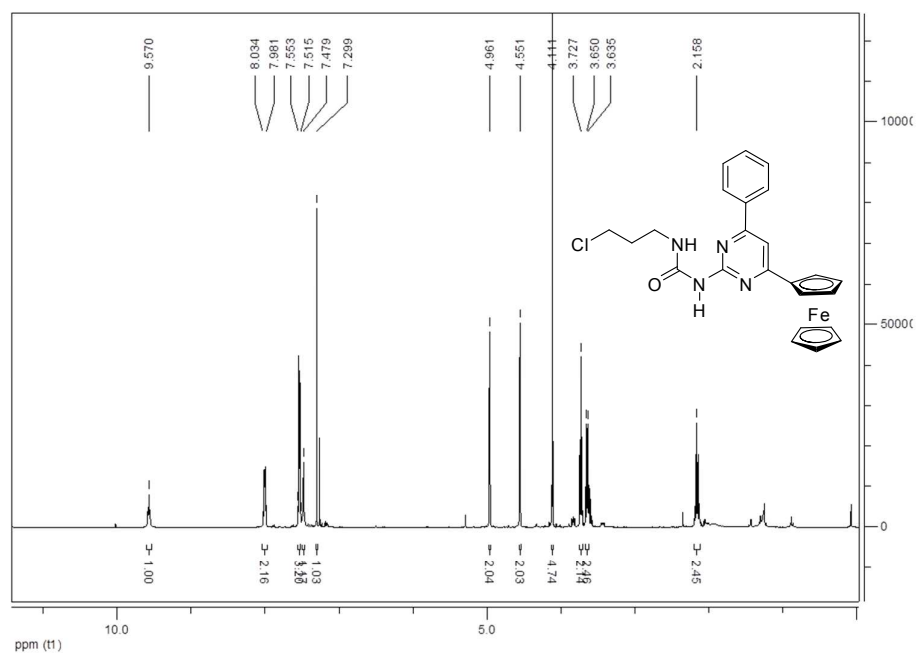


Figure S20. ¹H NMR spectrum of 1-(3-chloropropyl)-3-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-urea (**5d**)

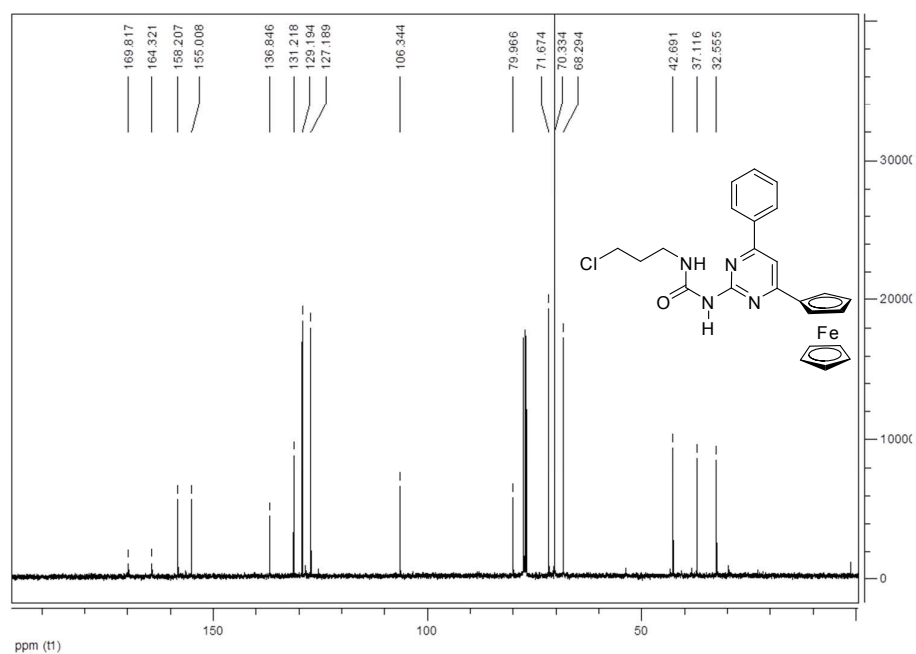


Figure S21. ¹³C NMR spectrum of 1-(3-chloropropyl)-3-(4-ferrocenyl-6-phenylpyrimidin-2-yl)-urea (**5d**)

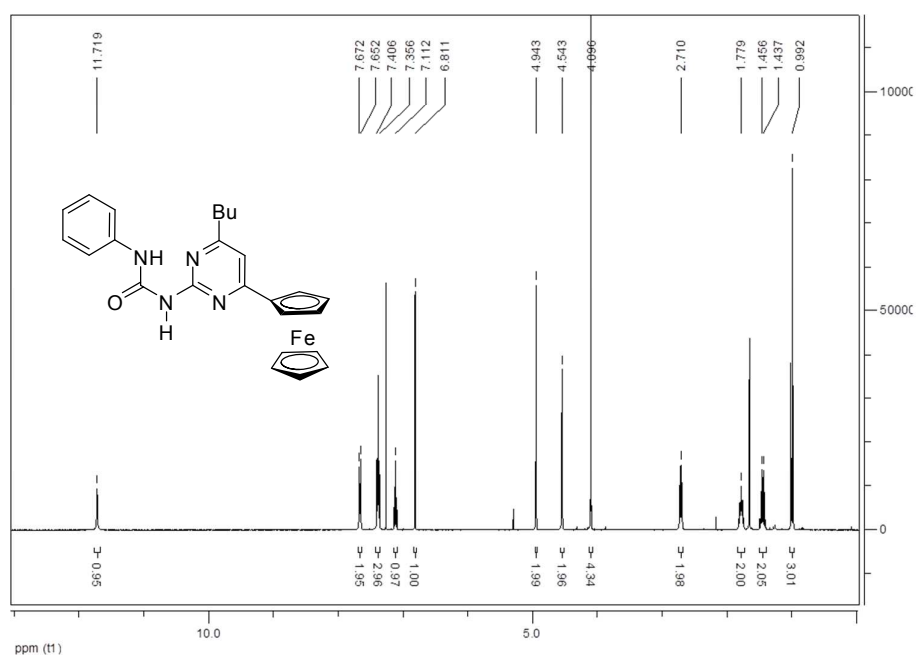


Figure S22. ¹H NMR spectrum of 1-(4-butyl-6-ferrocenylpyrimidin-2-yl)-3-phenylurea (**5e**)

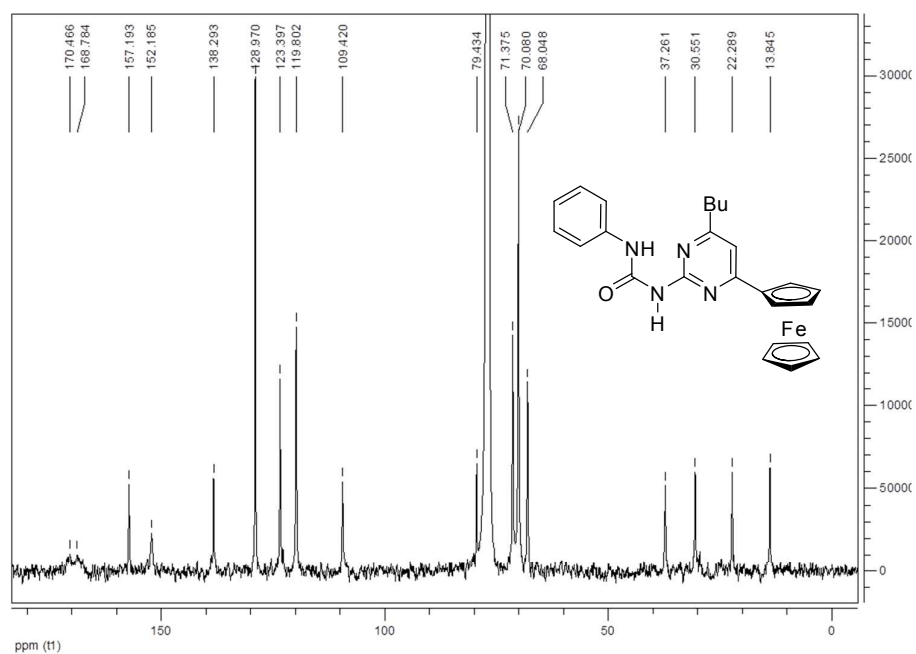


Figure S23. ¹³C NMR spectrum of 1-(4-butyl-6-ferrocenylpyrimidin-2-yl)-3-phenylurea (**5e**)

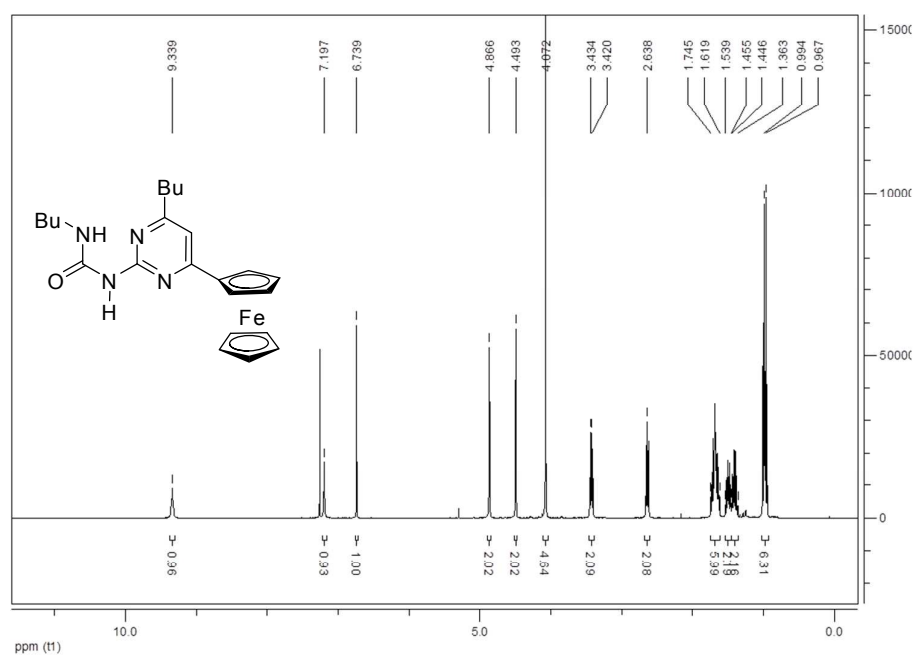


Figure S24. ¹H NMR spectrum of 1-butyl-3-(4-butyl-6-ferrocenylpyrimidin-2-yl)-urea (**5f**)

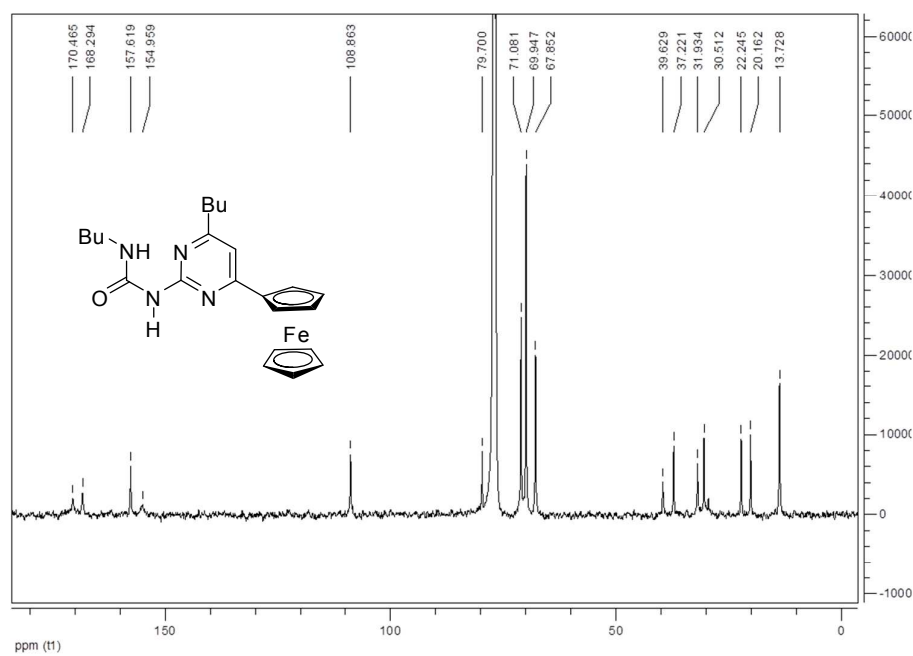


Figure S25. ¹³C NMR spectrum of 1-butyl-3-(4-butyl-6-ferrocenylpyrimidin-2-yl)-urea (**5f**)

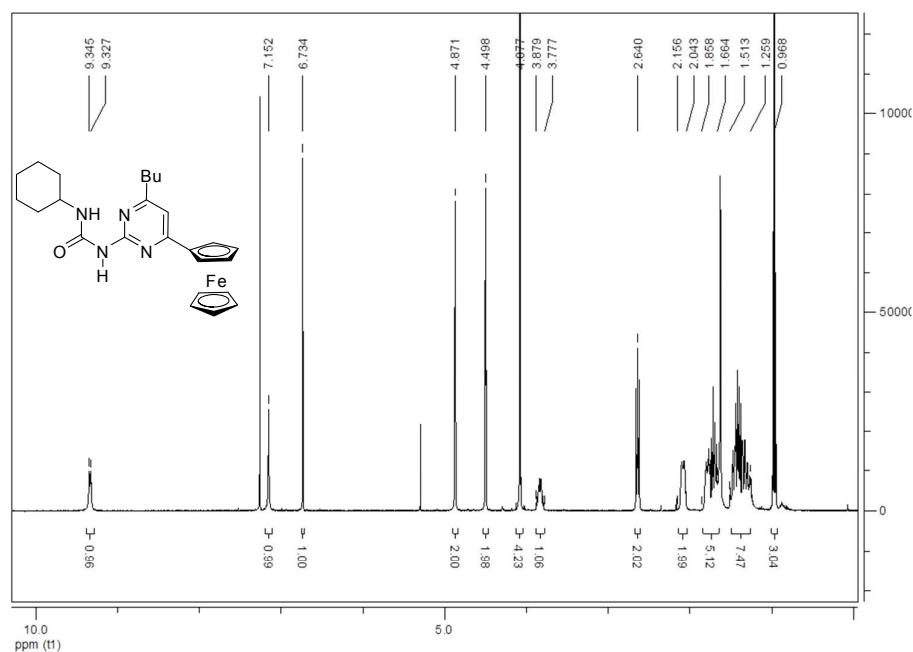


Figure S26. ¹H NMR spectrum of 1-(4-butyl-6-ferrocenylpyrimidin-2-yl)-3-cyclohexylurea (**5g**)

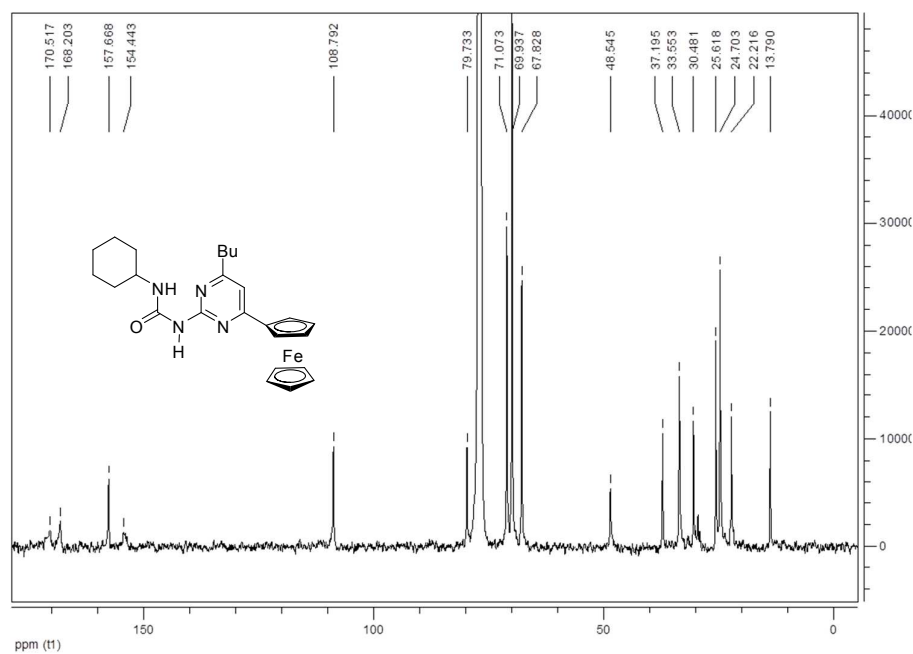


Figure S27. ¹³C NMR spectrum of 1-(4-butyl-6-ferrocenylpyrimidin-2-yl)-3-cyclohexylurea (**5g**)

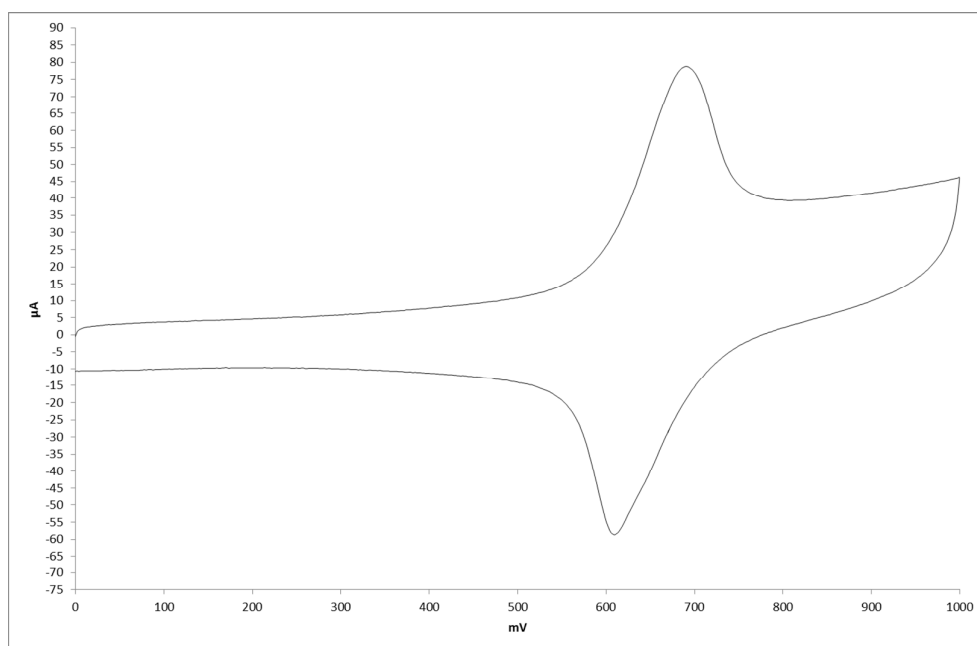


Figure S28. Cyclic voltammogram of **5g** (1 mM in acetonitrile, supporting electrolyte: 0.1 M TBAClO₄, spectral graphite electrode (OD= 3mm))

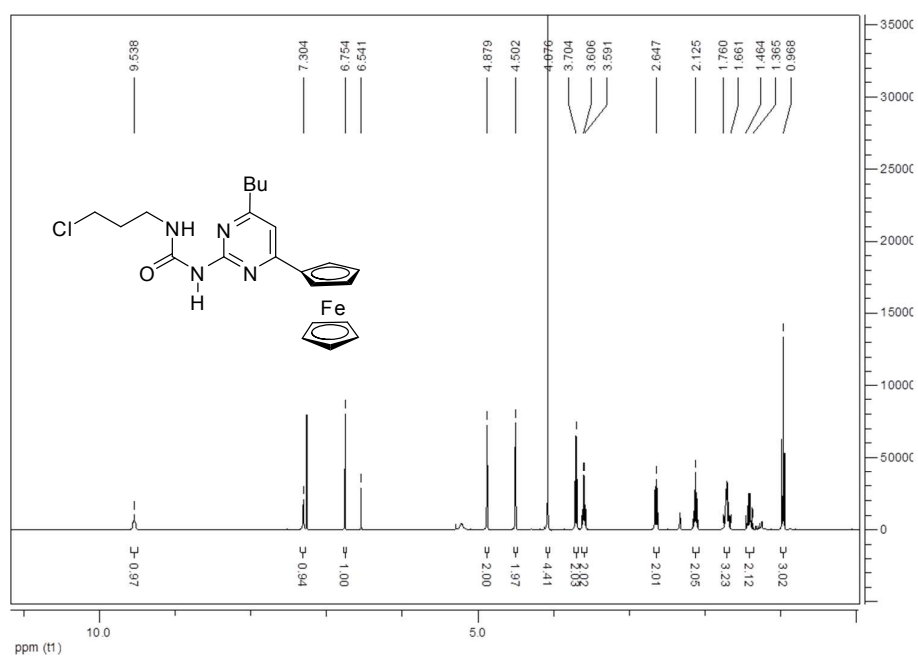


Figure S29. ¹H NMR spectrum of 1-(4-butyl-6-ferrocenylpyrimidin-2-yl)-3-(3-chloropropyl)urea (**5h**)

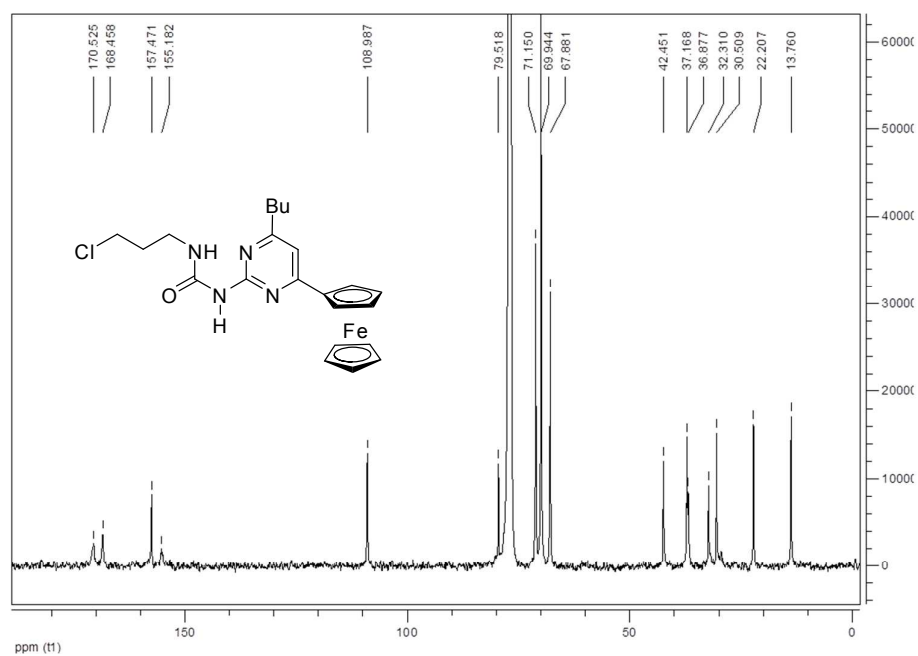


Figure S30. ¹³C NMR spectrum of 1-(4-butyl-6-ferrocenylpyrimidin-2-yl)-3-(3-chloropropyl)urea (**5h**)

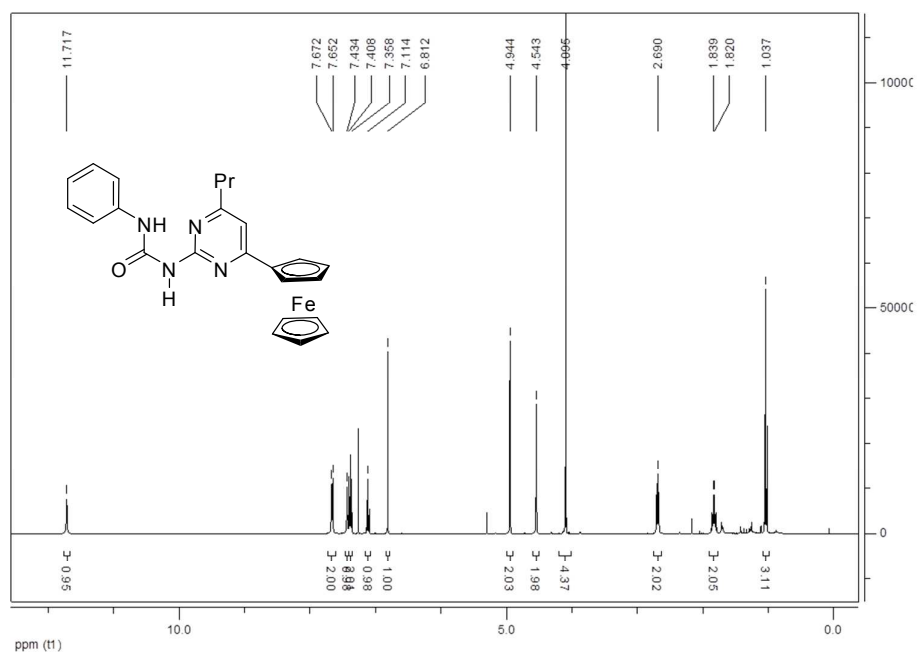


Figure S31. ¹H NMR spectrum of 1-(4-ferrocenyl-6-propylpyrimidin-2-yl)-3-phenylurea (**5i**)

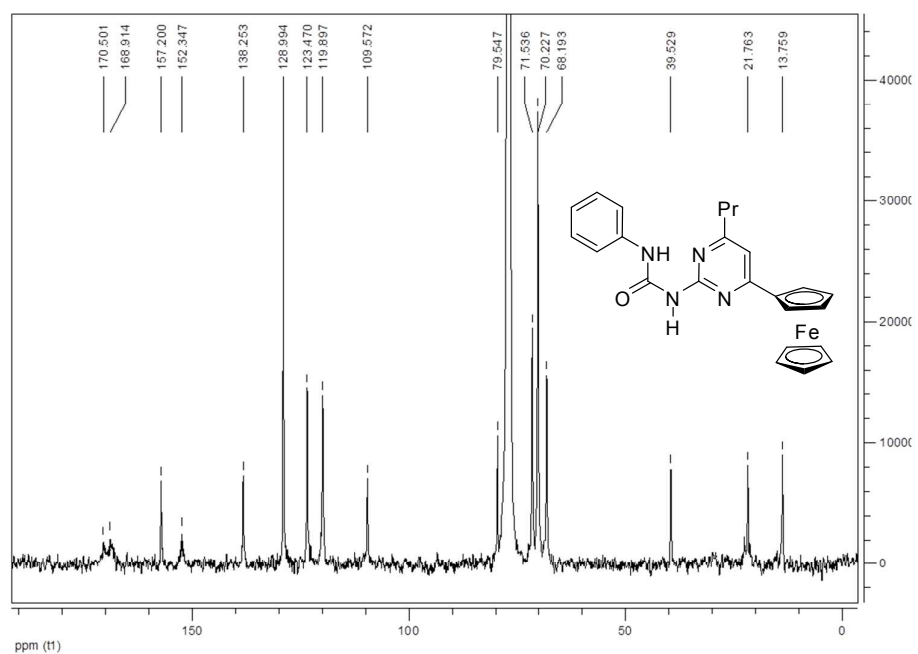


Figure S32. ¹³C NMR spectrum of 1-(4-ferrocenyl-6-propylpyrimidin-2-yl)-3-phenylurea (**5i**)

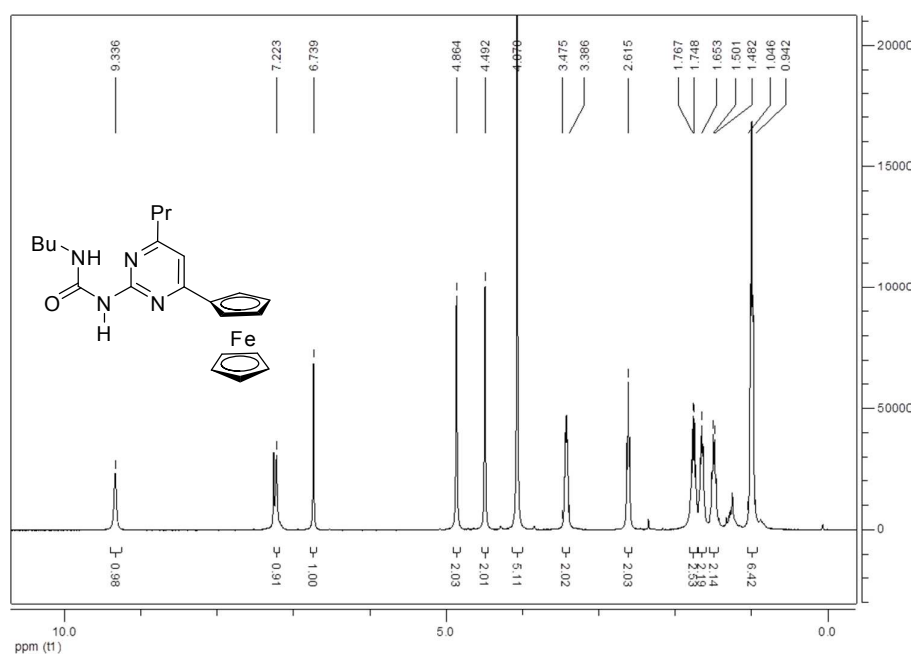


Figure S33. ¹H NMR spectrum of 1-butyl-3-(4-ferrocenyl-6-propylpyrimidin-2-yl)-urea (5j)

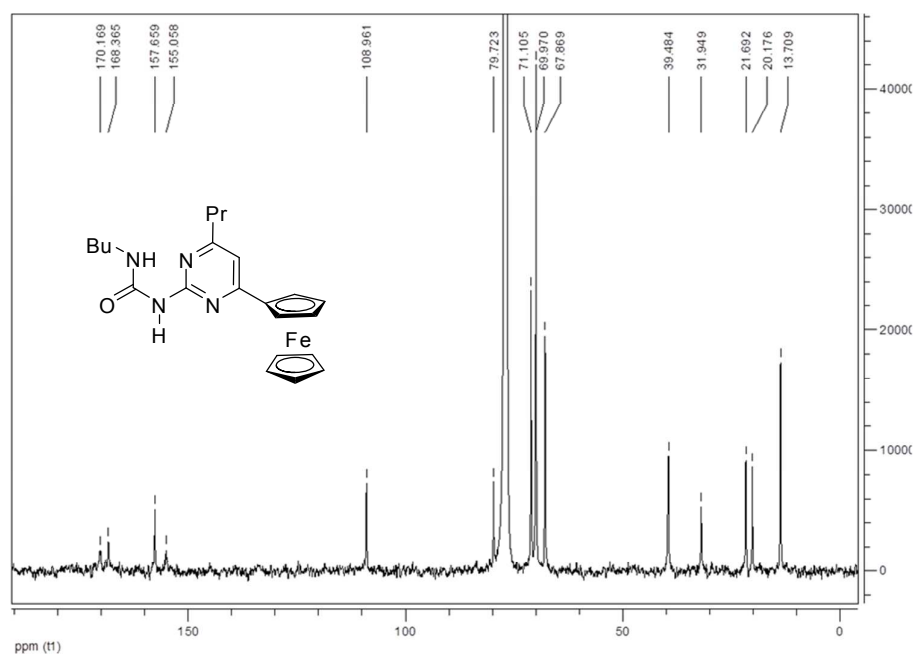


Figure S34. ¹³C NMR spectrum of 1-butyl-3-(4-ferrocenyl-6-propylpyrimidin-2-yl)-urea (5j)

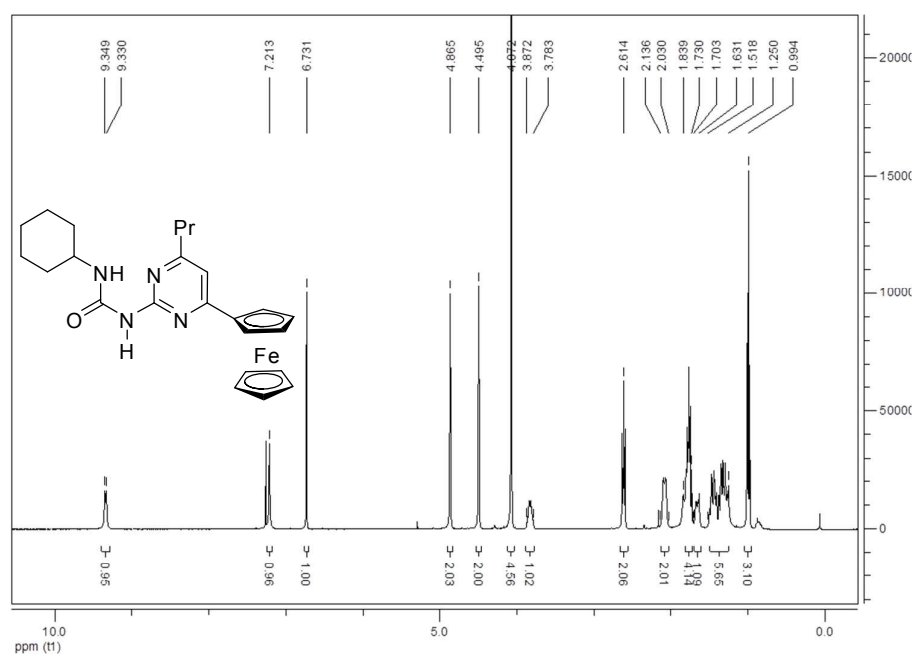


Figure S35. ¹H NMR spectrum of 1-cyclohexyl-3-(4-ferrocenyl-6-propylpyrimidin-2-yl)-urea (**5k**)

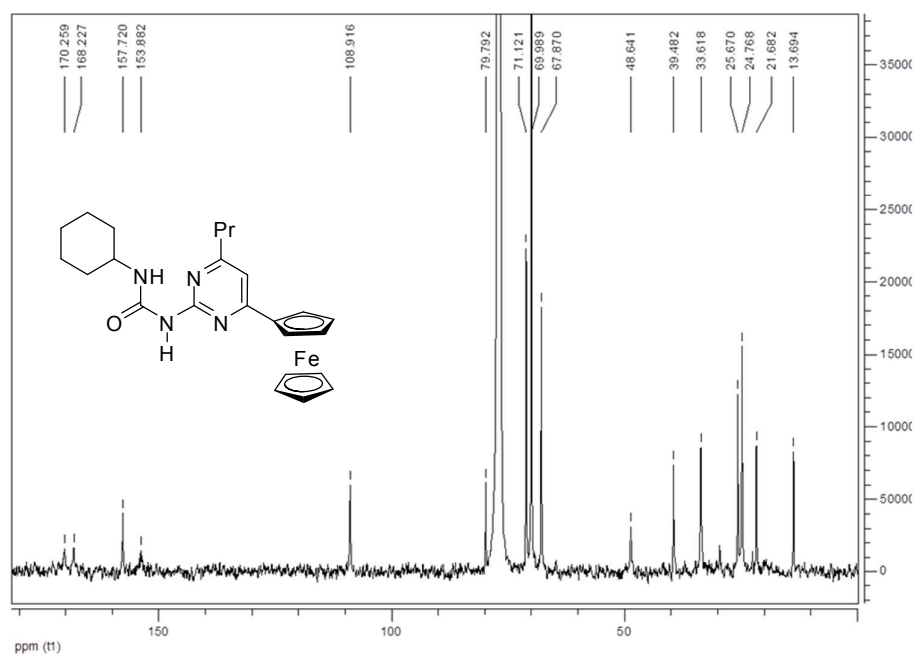


Figure S36. ¹³C NMR spectrum of 1-cyclohexyl-3-(4-ferrocenyl-6-propylpyrimidin-2-yl)-urea (**5k**)

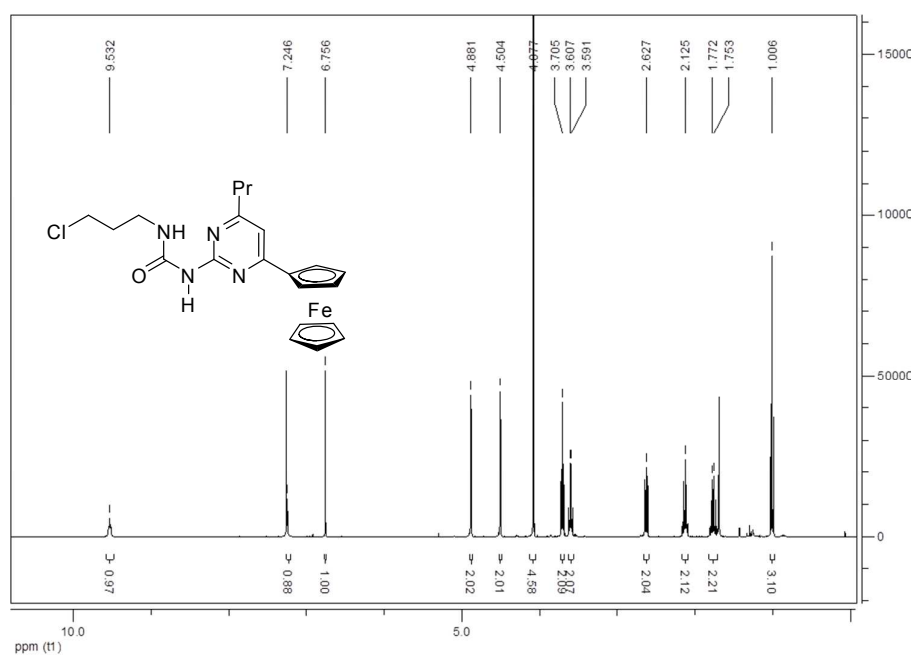


Figure S37. ¹H NMR spectrum of 1-(3-chloropropyl)-3-(4-ferrocenyl-6-propylpyrimidin-2-yl)-urea (5I)

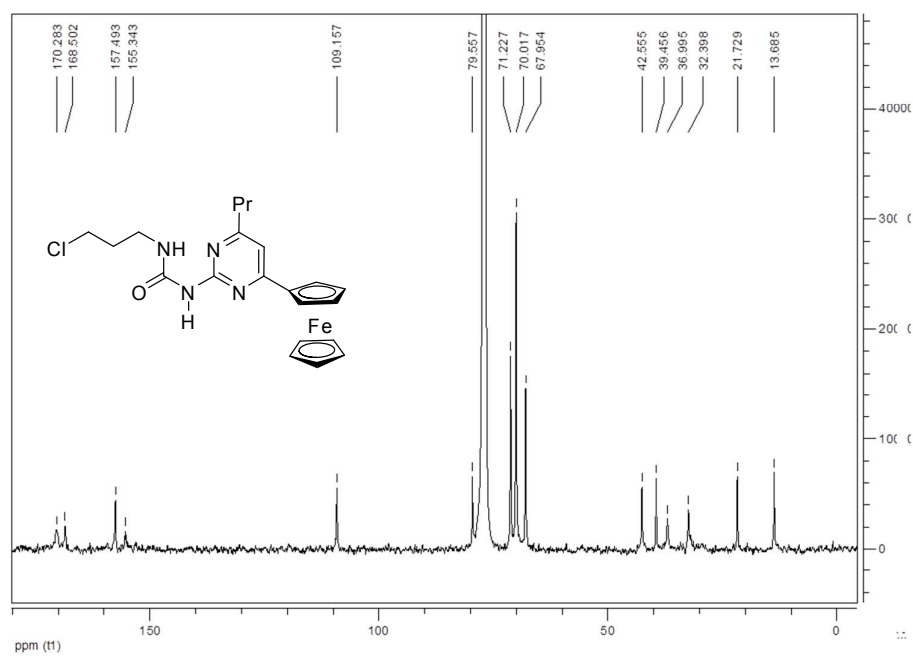


Figure S38. ¹³C NMR spectrum of 1-(3-chloropropyl)-3-(4-ferrocenyl-6-propylpyrimidin-2-yl)-urea (5I)

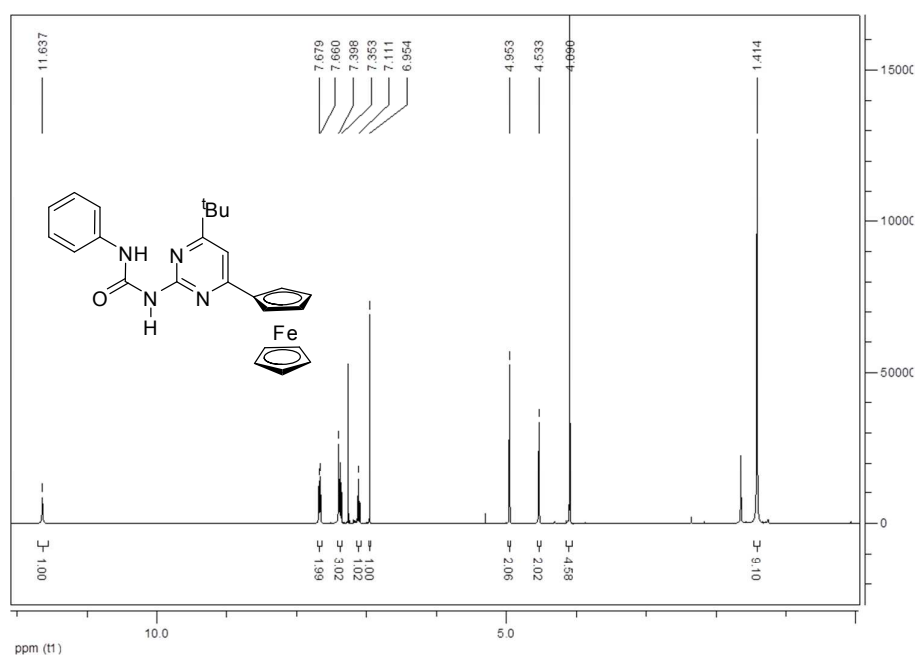


Figure S39. ¹H NMR spectrum of 1-(4-*tert*-butyl-6-ferrocenylpyrimidin-2-yl)-3-phenylurea (**5m**)

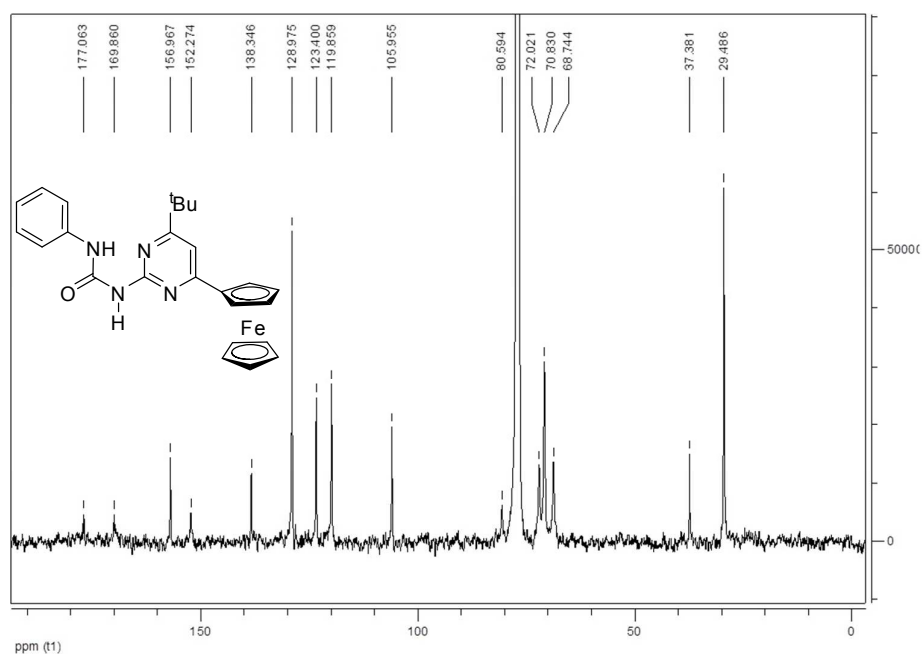


Figure S40. ¹³C NMR spectrum of 1-(4-*tert*-butyl-6-ferrocenylpyrimidin-2-yl)-3-phenylurea (**5m**)

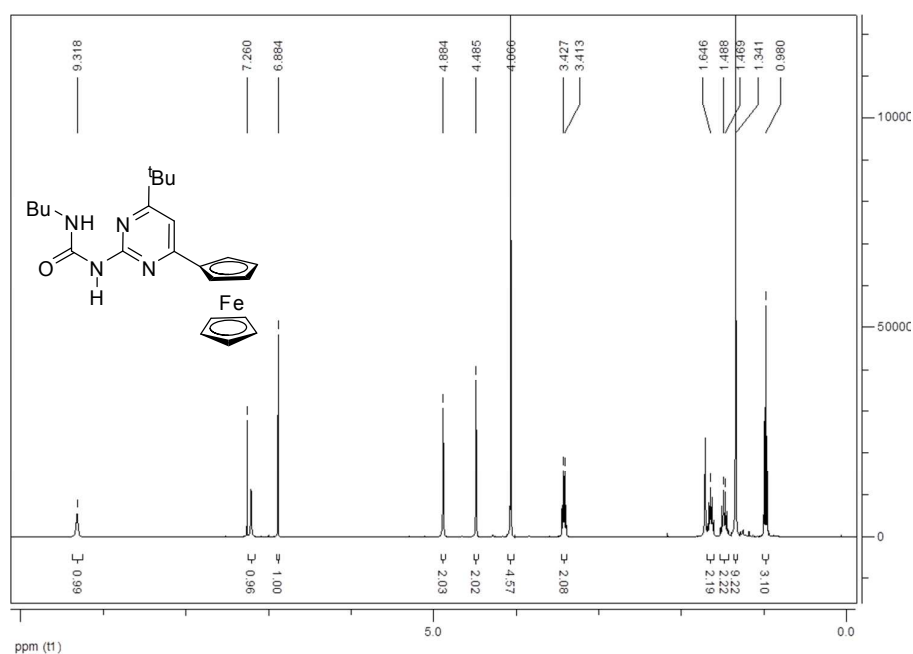


Figure S41. ¹H NMR spectrum of 1-butyl-3-(4-tert-butyl-6-ferrocenylpyrimidin-2-yl)-urea (**5n**)

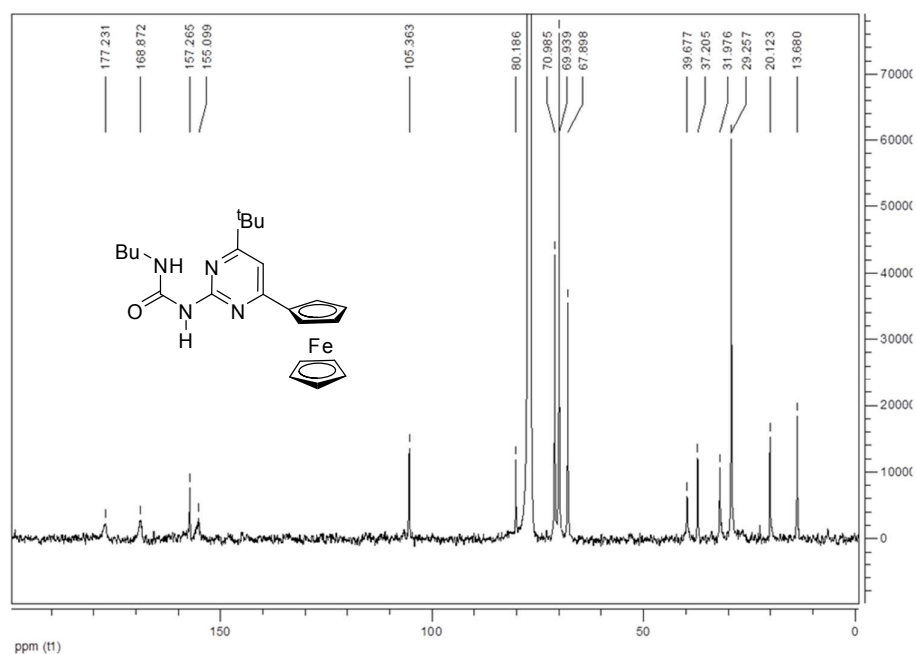


Figure S42. ¹³C NMR spectrum of 1-butyl-3-(4-tert-butyl-6-ferrocenylpyrimidin-2-yl)-urea (**5n**)

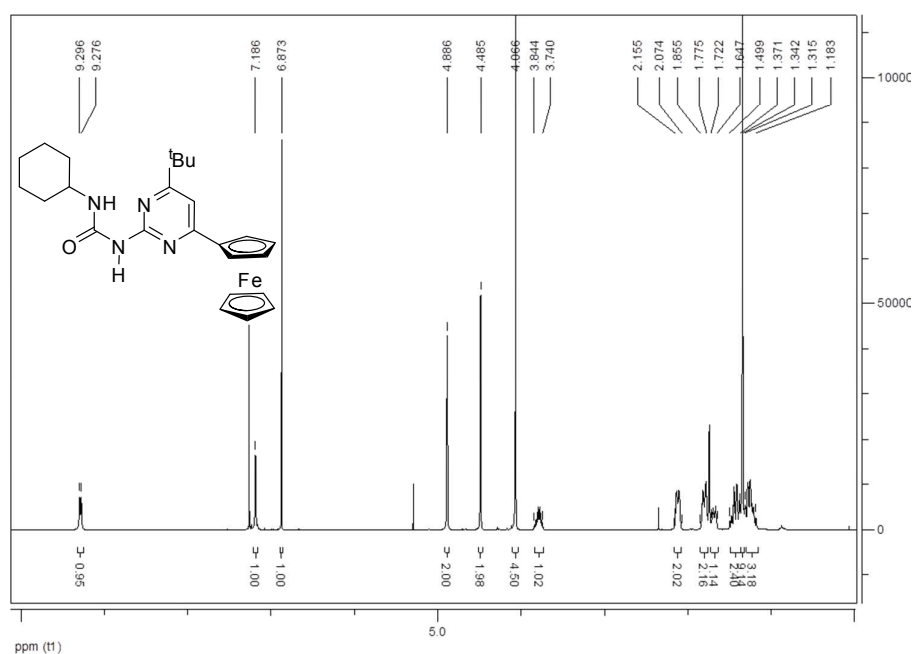


Figure S43. ¹H NMR spectrum of 1-(4-tert-butyl-6-ferrocenylpyrimidin-2-yl)-3-cyclohexylurea (**5o**)

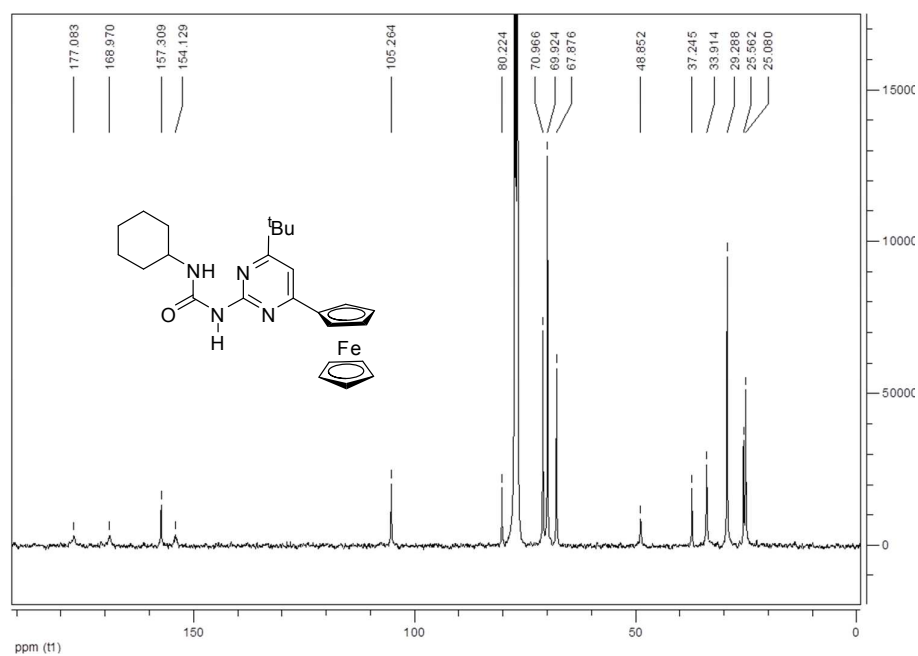


Figure S44. ¹³C NMR spectrum of 1-(4-tert-butyl-6-ferrocenylpyrimidin-2-yl)-3-cyclohexylurea (**5o**)

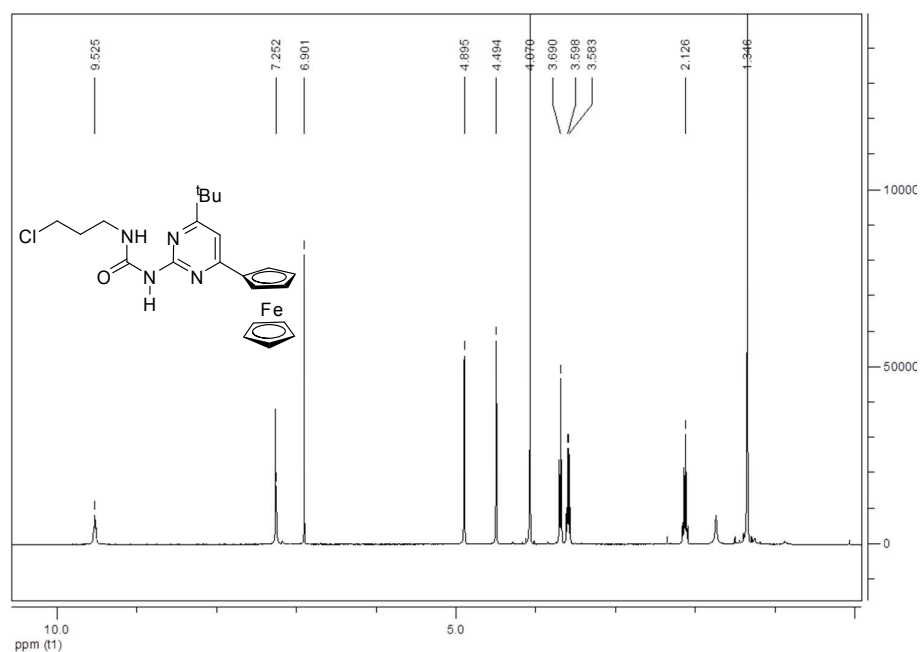


Figure S45. ¹H NMR spectrum of 1-(4-tert-butyl-6-ferrocenylpyrimidin-2-yl)-3-(3-chloropropyl)urea (5p)

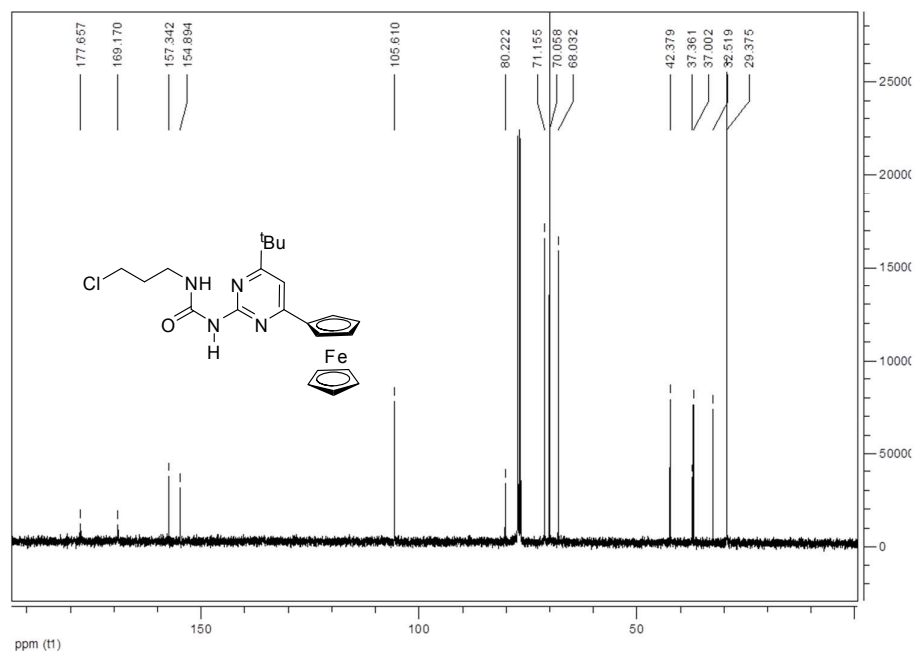


Figure S46. ¹³C NMR spectrum of 1-(4-tert-butyl-6-ferrocenylpyrimidin-2-yl)-3-(3-chloropropyl)urea (5p)