

## Supplementary materials

# Coordination chemistry of phosphate groups in systems including copper(II) ions, phosphoethanolamine and pyrimidine nucleotides

Malwina Gabryel-Skrodzka, Martyna Nowak, Anna Teubert and Renata Jastrzab

The set of EPR, UV-Vis,  $^{13}\text{C}$  NMR,  $^{31}\text{P}$  NMR spectra of the  $\text{MLH}_4\text{L}'$  type complexes as well as corresponding to the free ligand  $^{13}\text{C}$  NMR and  $^{31}\text{P}$  NMR spectra

1.  **$\text{Cu(enP)H}_4(\text{TMP})$  pH=2.5**
2.  **$\text{Cu(enP)H}_4(\text{UMP})$  pH=3.0**
3.  **$\text{Cu(enP)H}_4(\text{CMP})$  pH=2.5**

**Cu(enP)H<sub>4</sub>(TMP) pH=2.5**

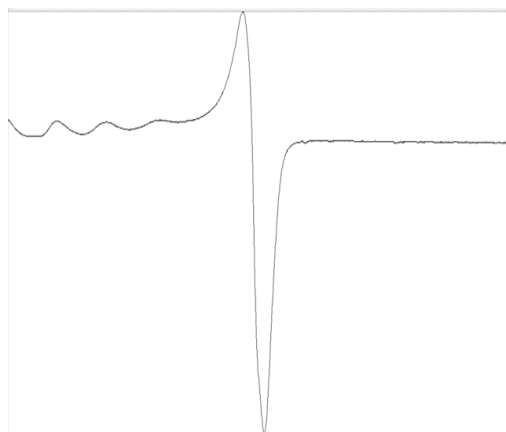


Figure S1. EPR spectrum

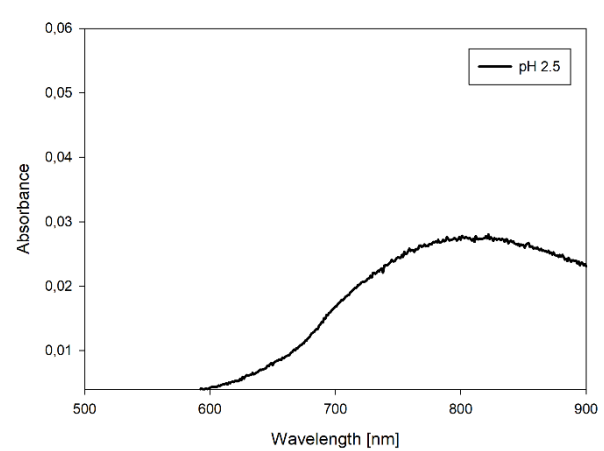


Figure S2. UV-Vis spectrum (C=0.002 M)

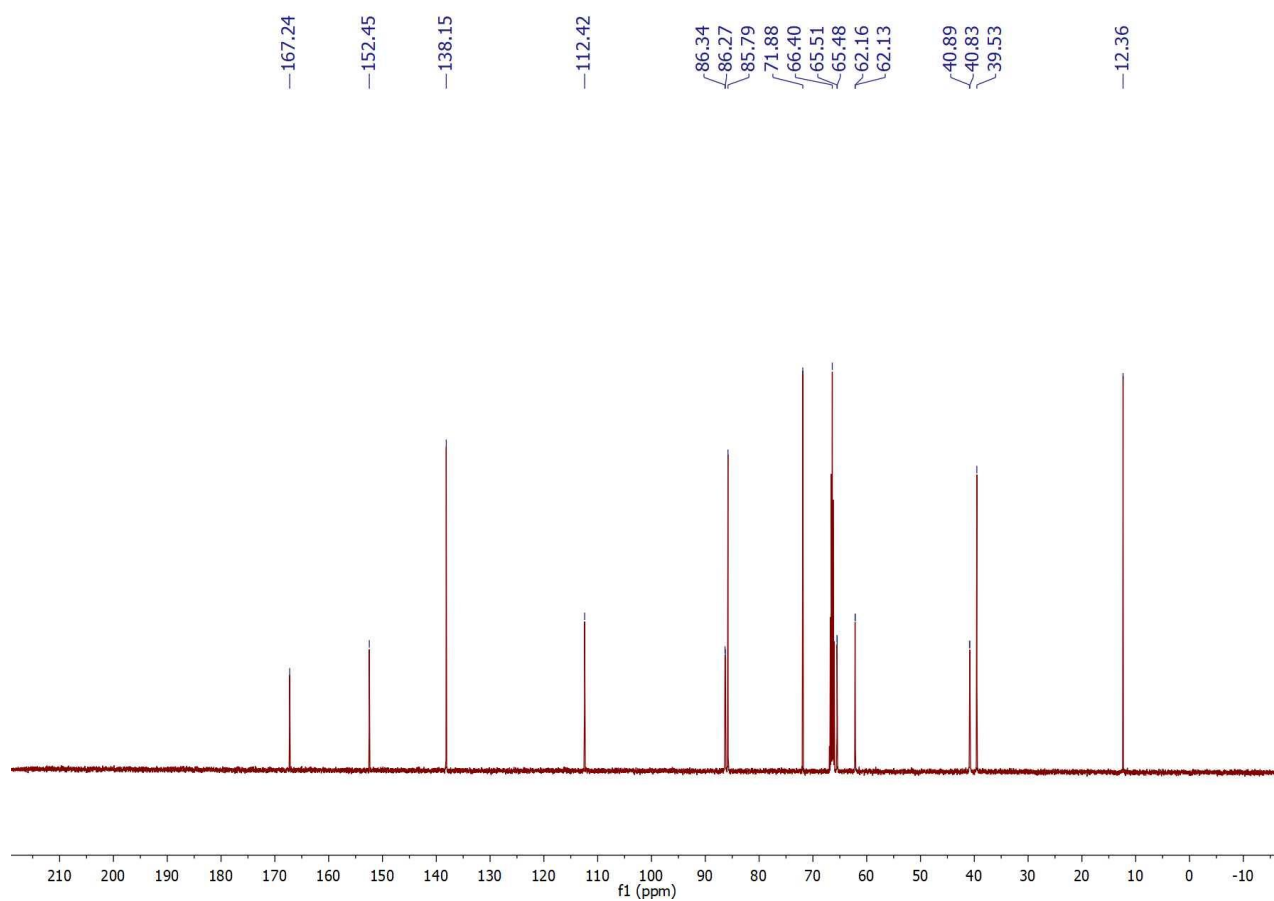


Figure S3. Cu(enP)H<sub>4</sub>(TMP) <sup>13</sup>C NMR spectrum

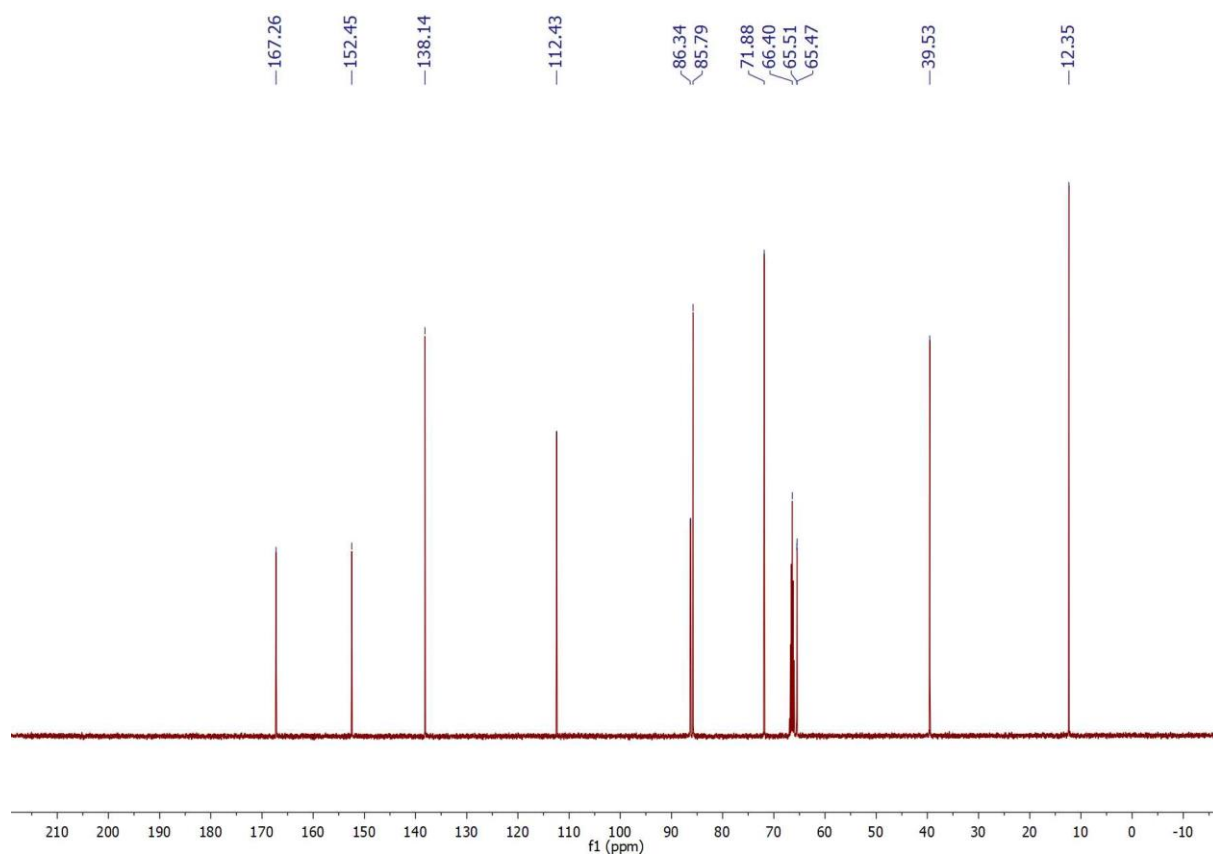


Figure S4. TMP <sup>13</sup> C NMR spectrum

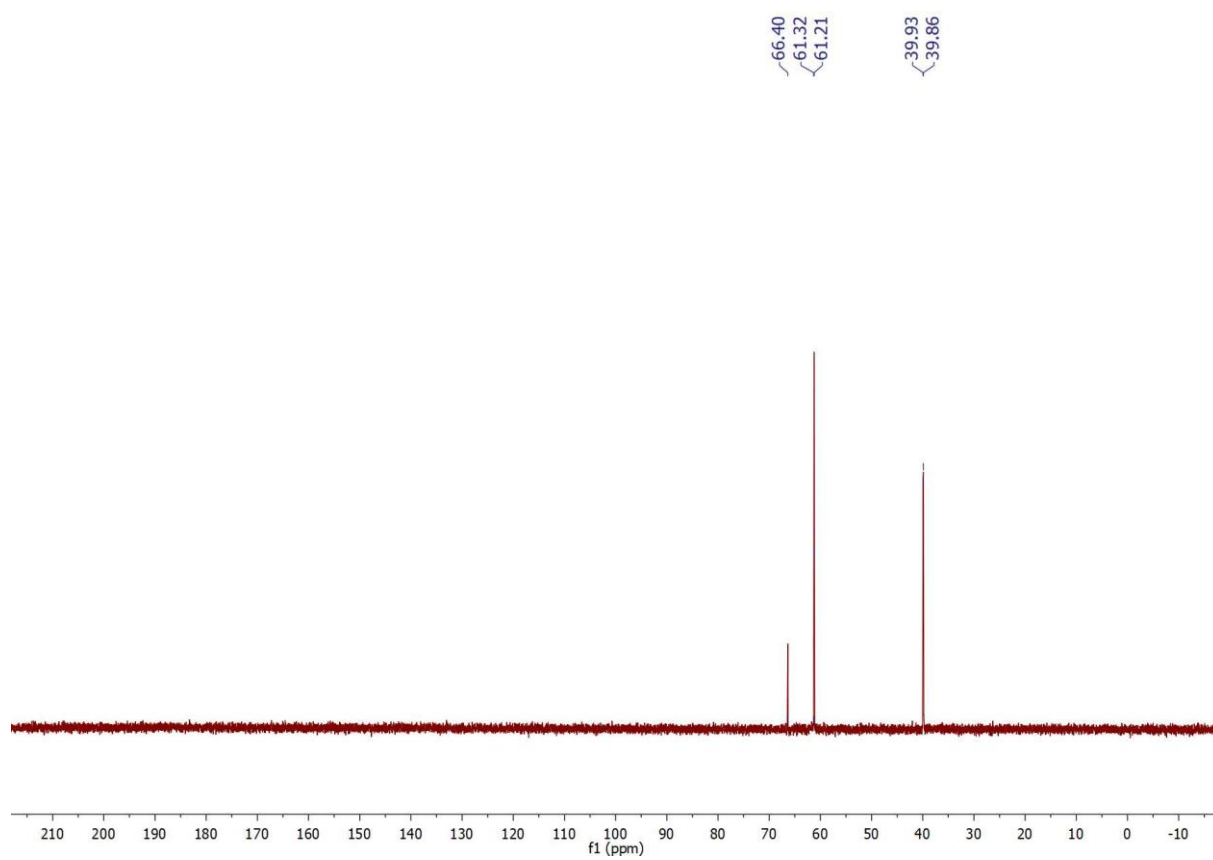


Figure S5. enP <sup>13</sup> C NMR spectrum

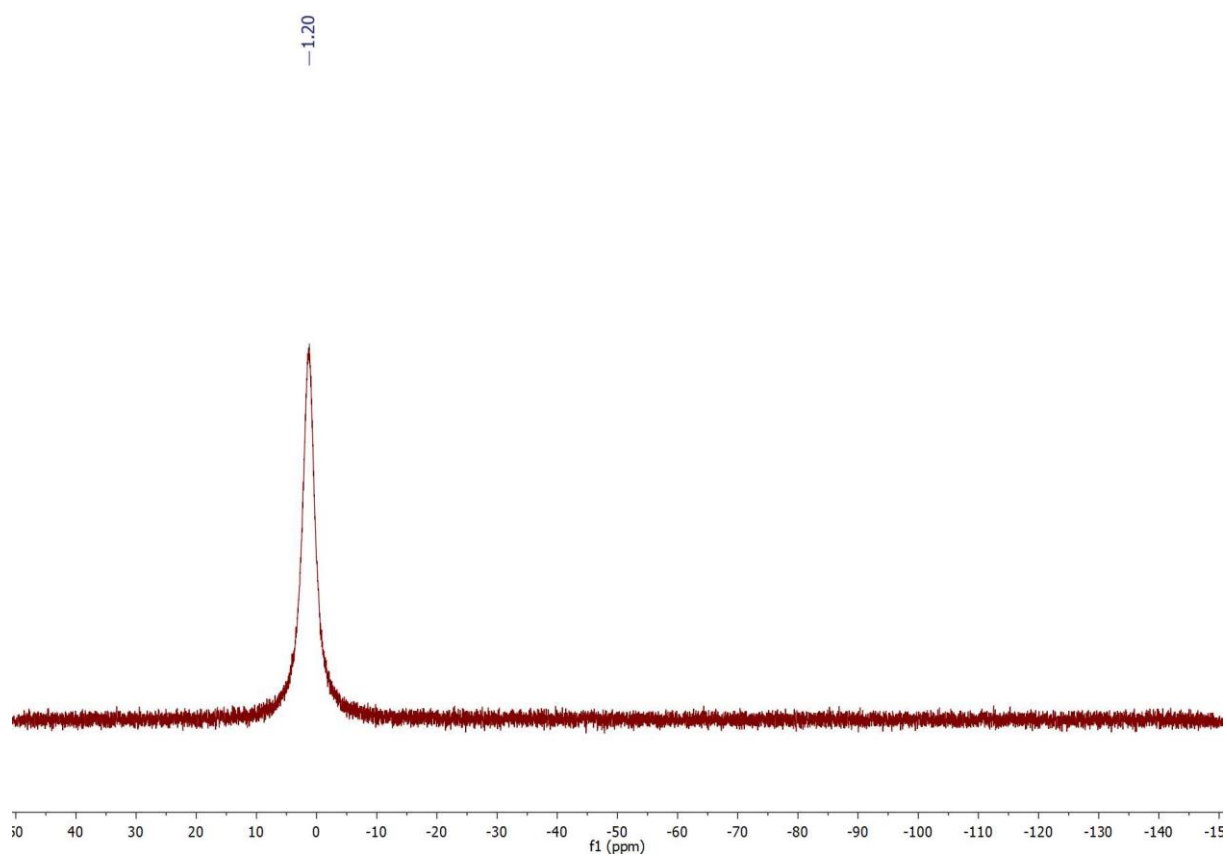


Figure S6.  $\text{Cu(enP)H}_4(\text{TMP})$   $^{31}\text{P}$  NMR spectrum

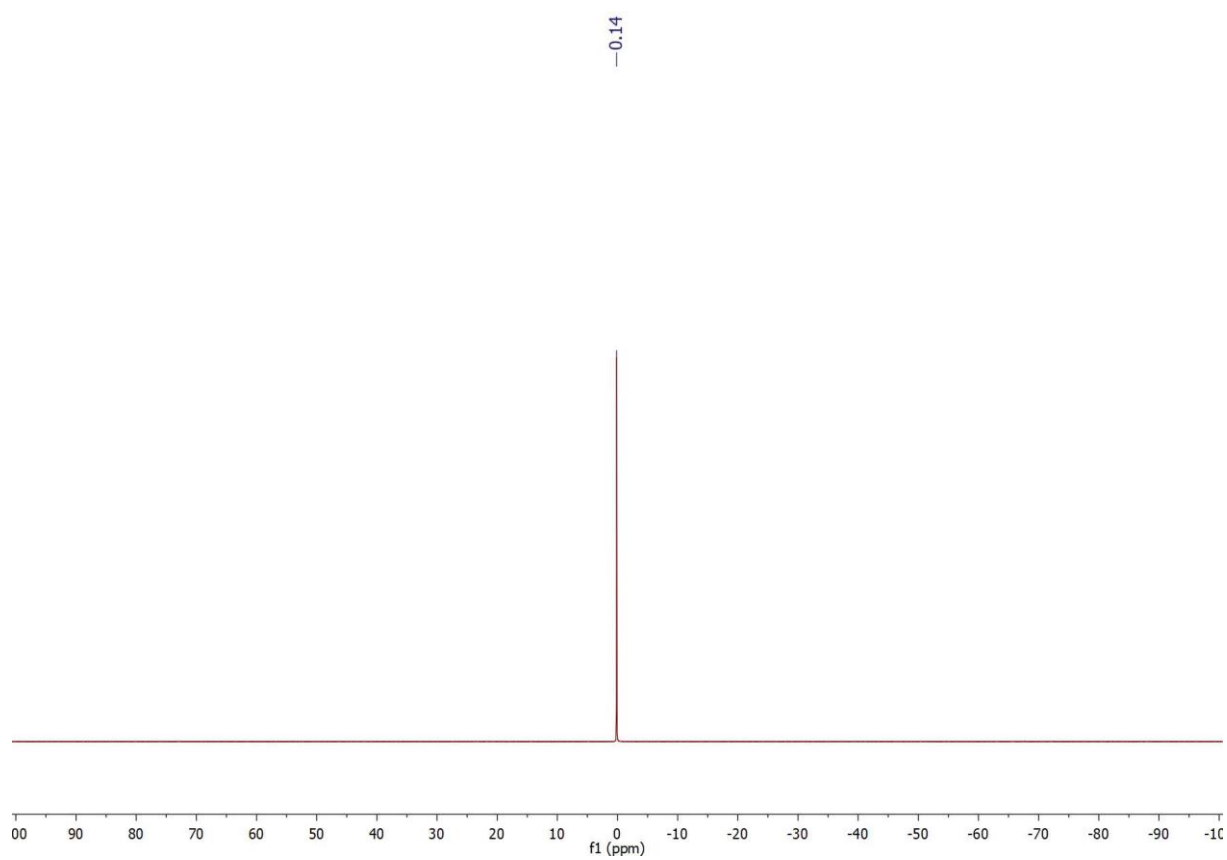


Figure S7.  $\text{TMP}$   $^{31}\text{P}$  NMR spectrum

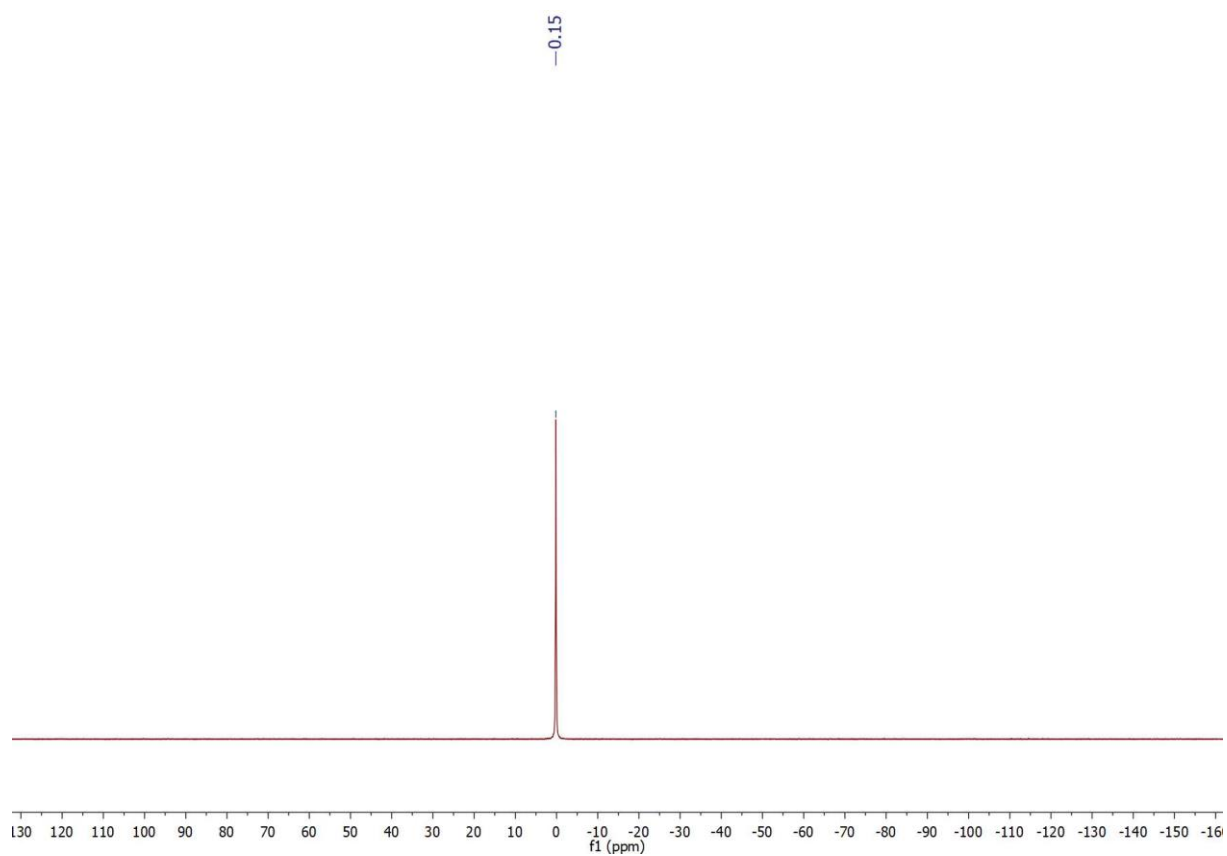


Figure S8. enP  $^{31}\text{P}$  NMR spectrum

**Cu(enP)H<sub>4</sub>(UMP) pH=3.0**

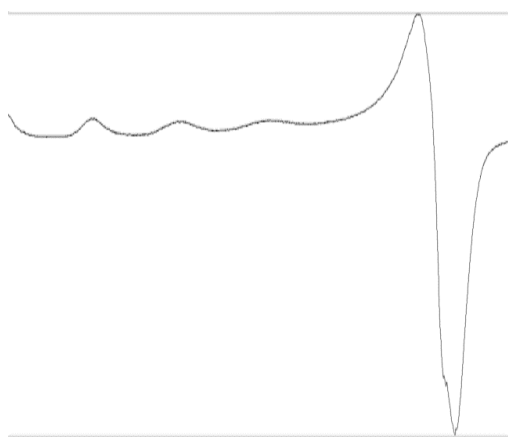


Figure S9. EPR spectrum

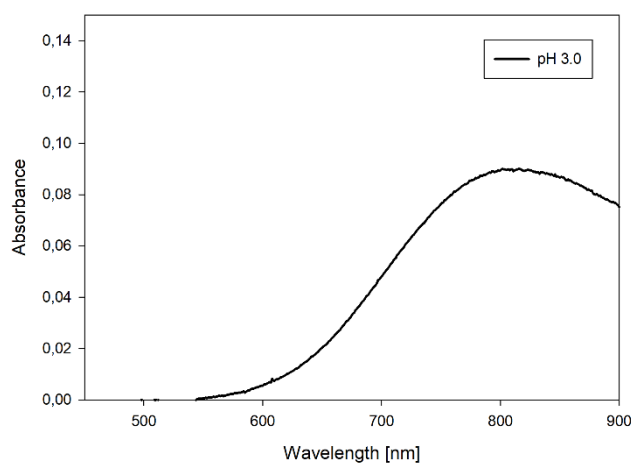


Figure S10. UV-Vis spectrum (C=0.01 M)

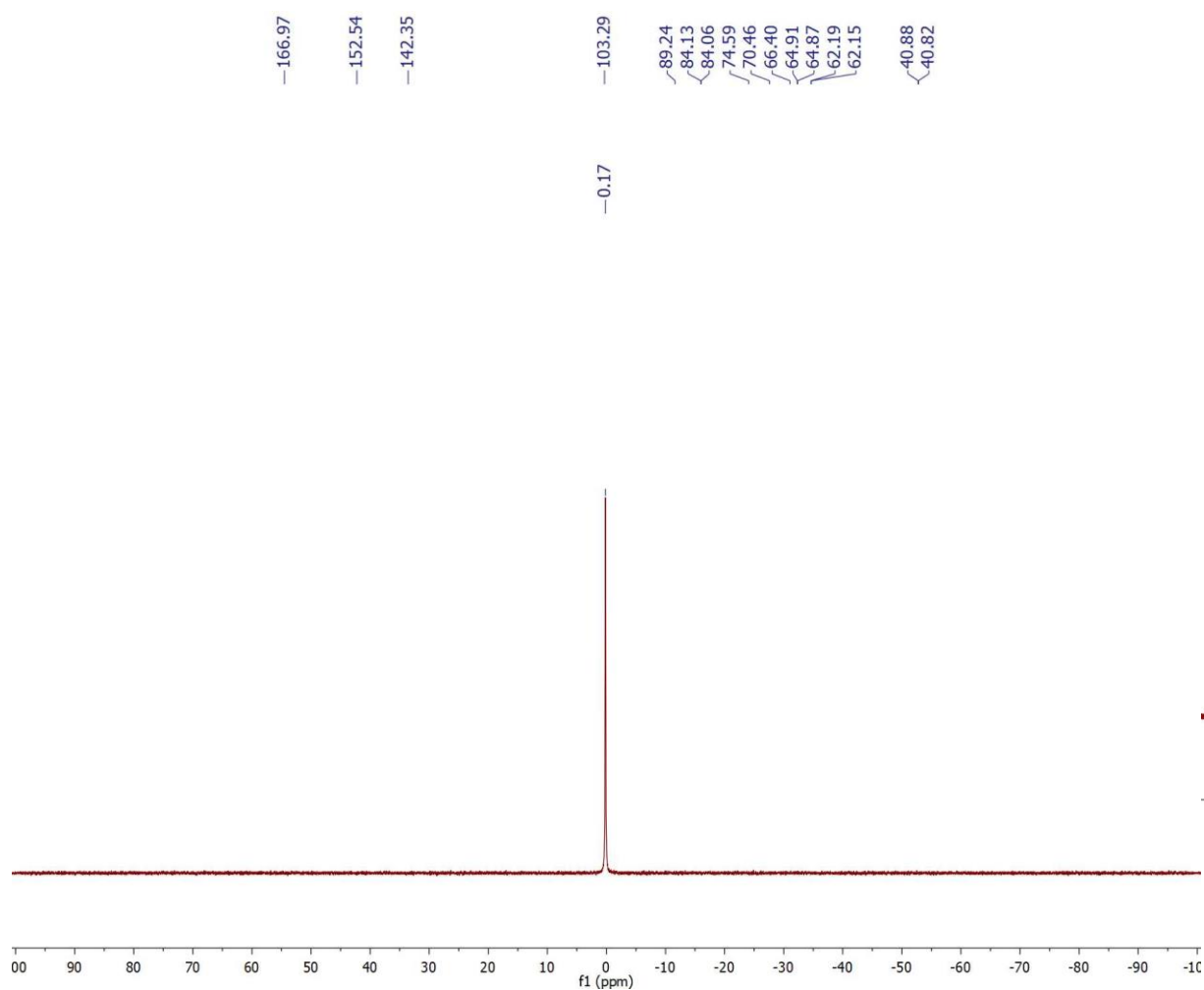


Figure S11. Cu(enP)H<sub>4</sub>(UMP) <sup>13</sup>C NMR spectrum

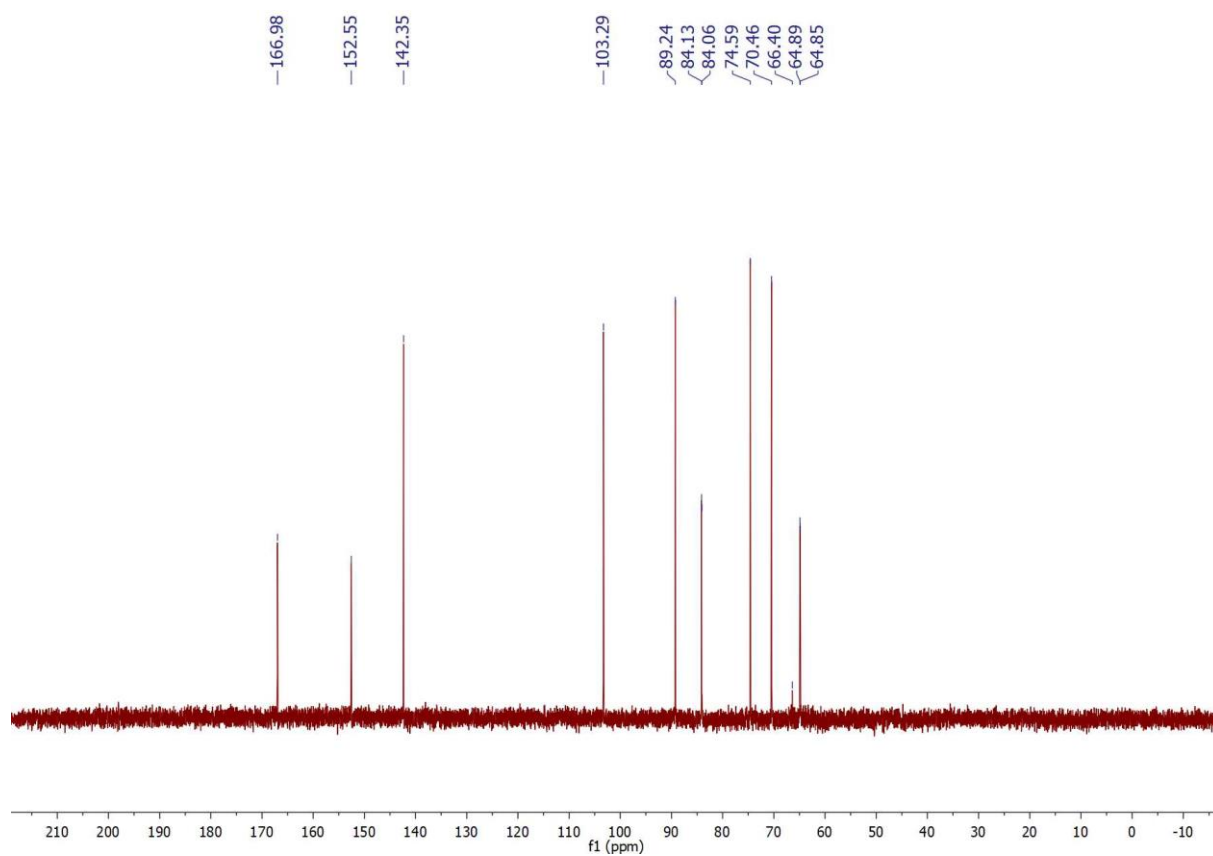


Figure S12. UMP  $^{13}\text{C}$  NMR spectrum

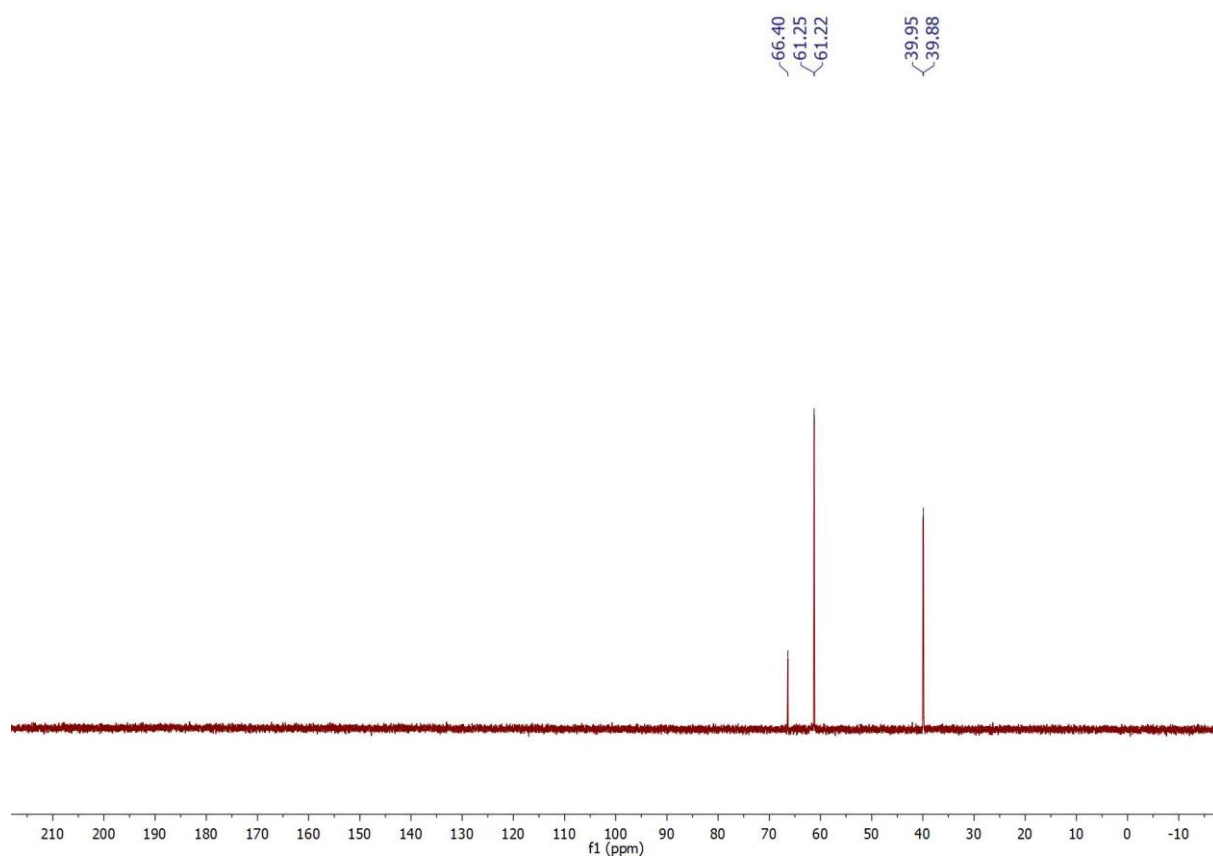


Figure S13. enP  $^{13}\text{C}$  NMR spectrum

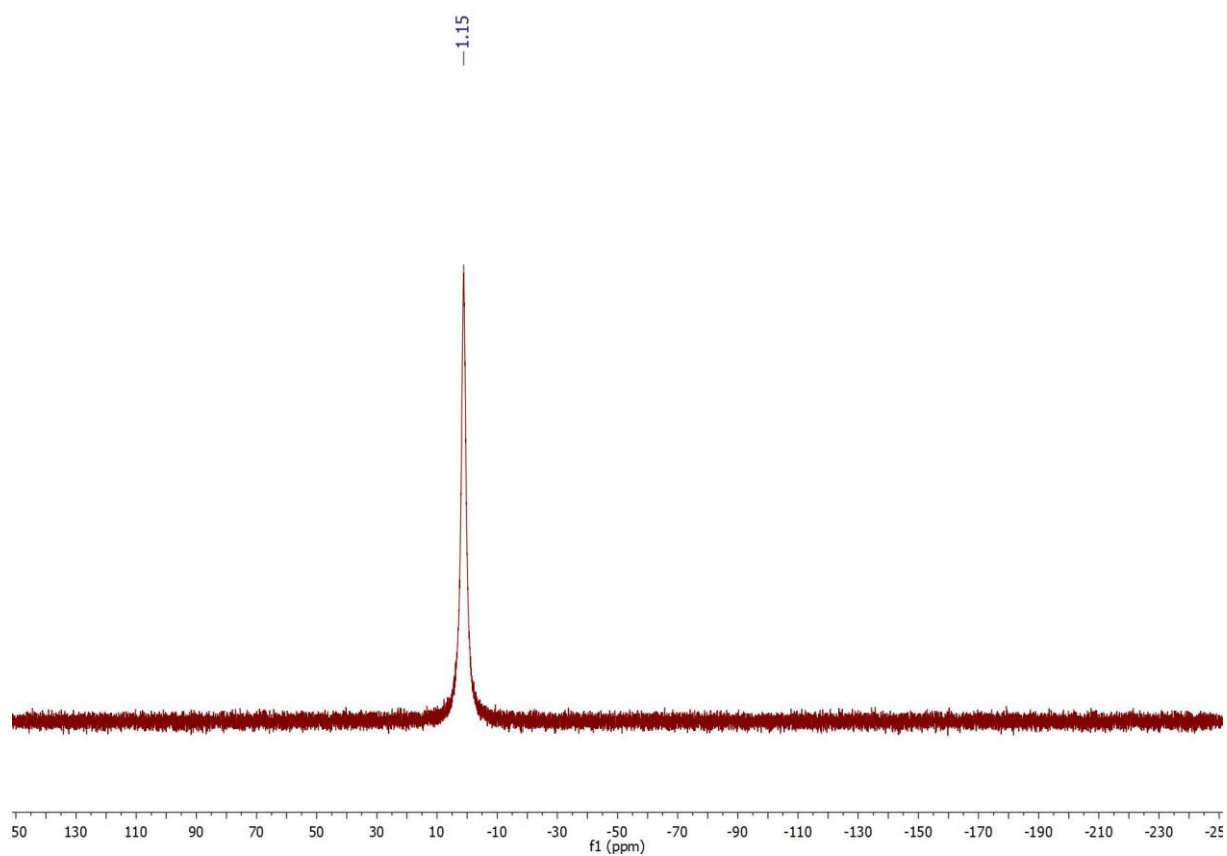


Figure S14.  $\text{Cu(enP)H}_4(\text{UMP})$   $^{31}\text{P}$  NMR spectrum

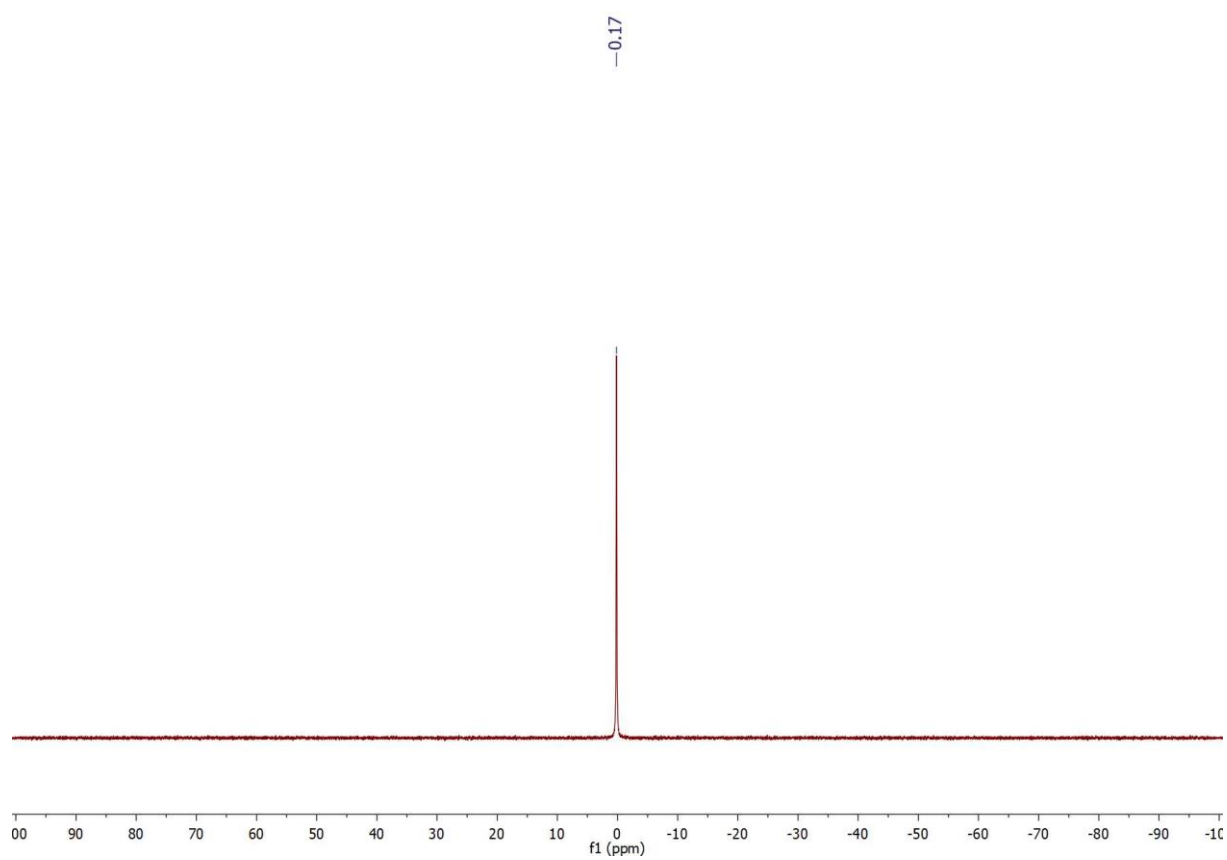


Figure S15.  $\text{UMP}$   $^{31}\text{P}$  NMR spectrum



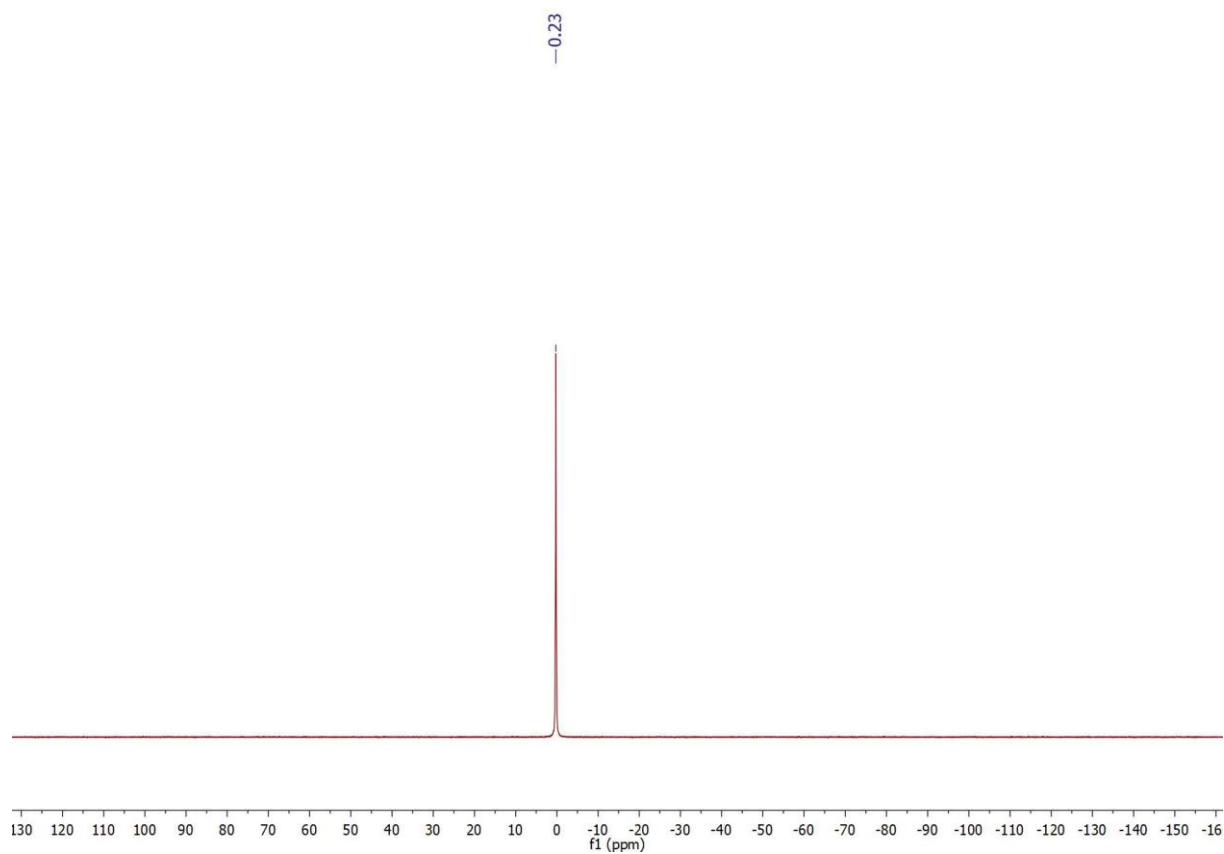


Figure S16. enP  $^{31}\text{P}$  NMR spectrum

**Cu(enP)H<sub>4</sub>(CMP) pH = 2.5**

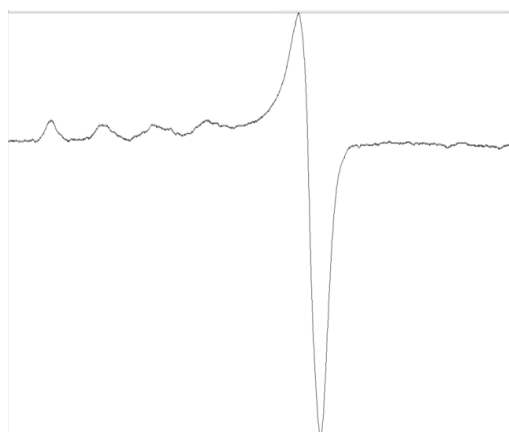


Figure S17. EPR spectrum

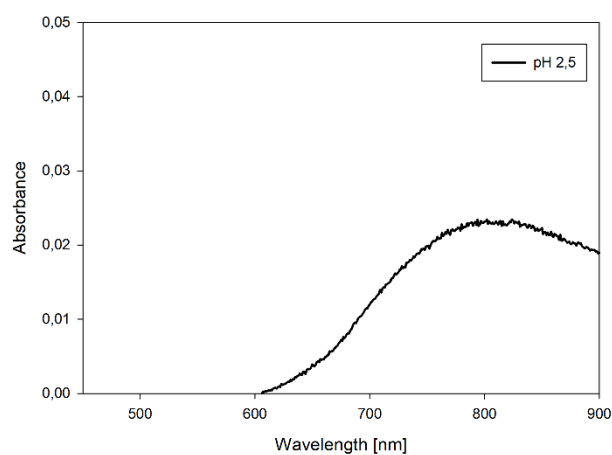


Figure S18. UV-Vis spectrum (C=0.002 M)

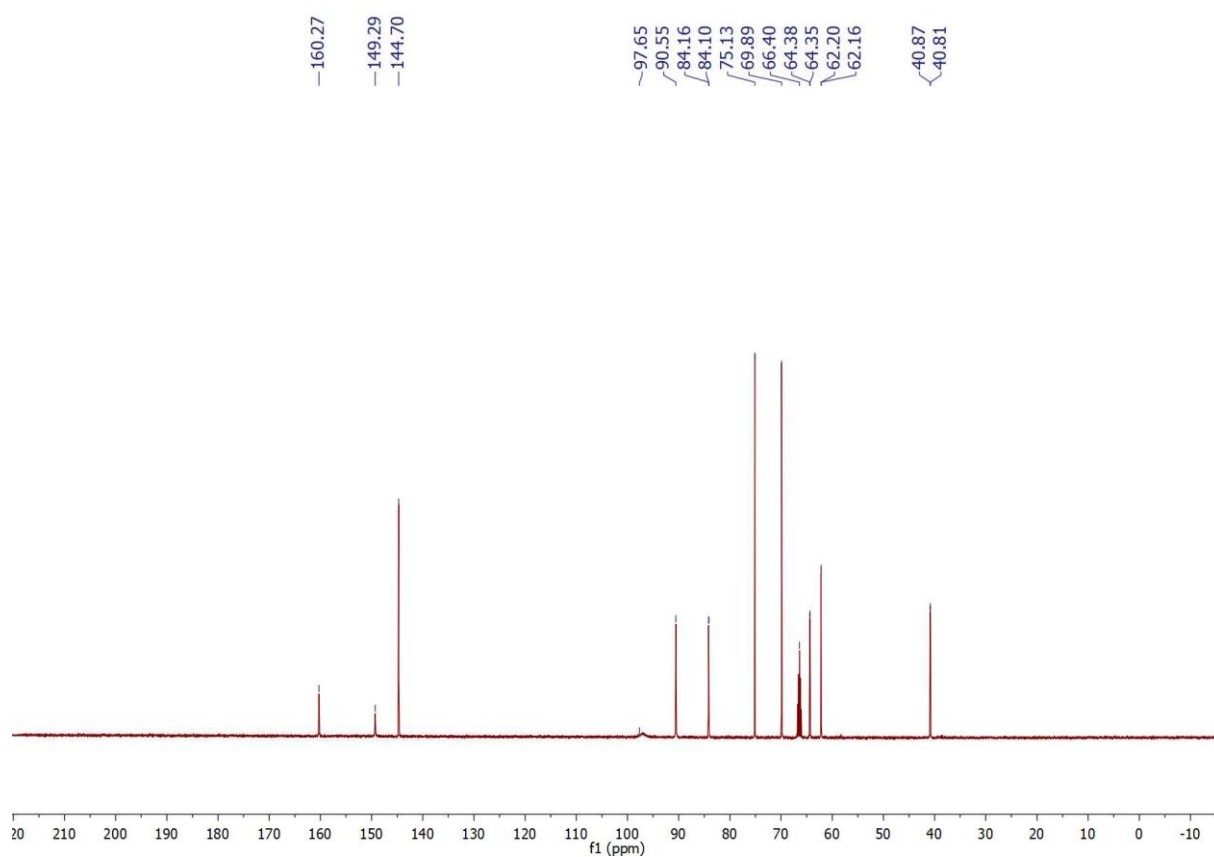


Figure S19. Cu(enP)H<sub>4</sub>(CMP) <sup>13</sup>C NMR spectrum

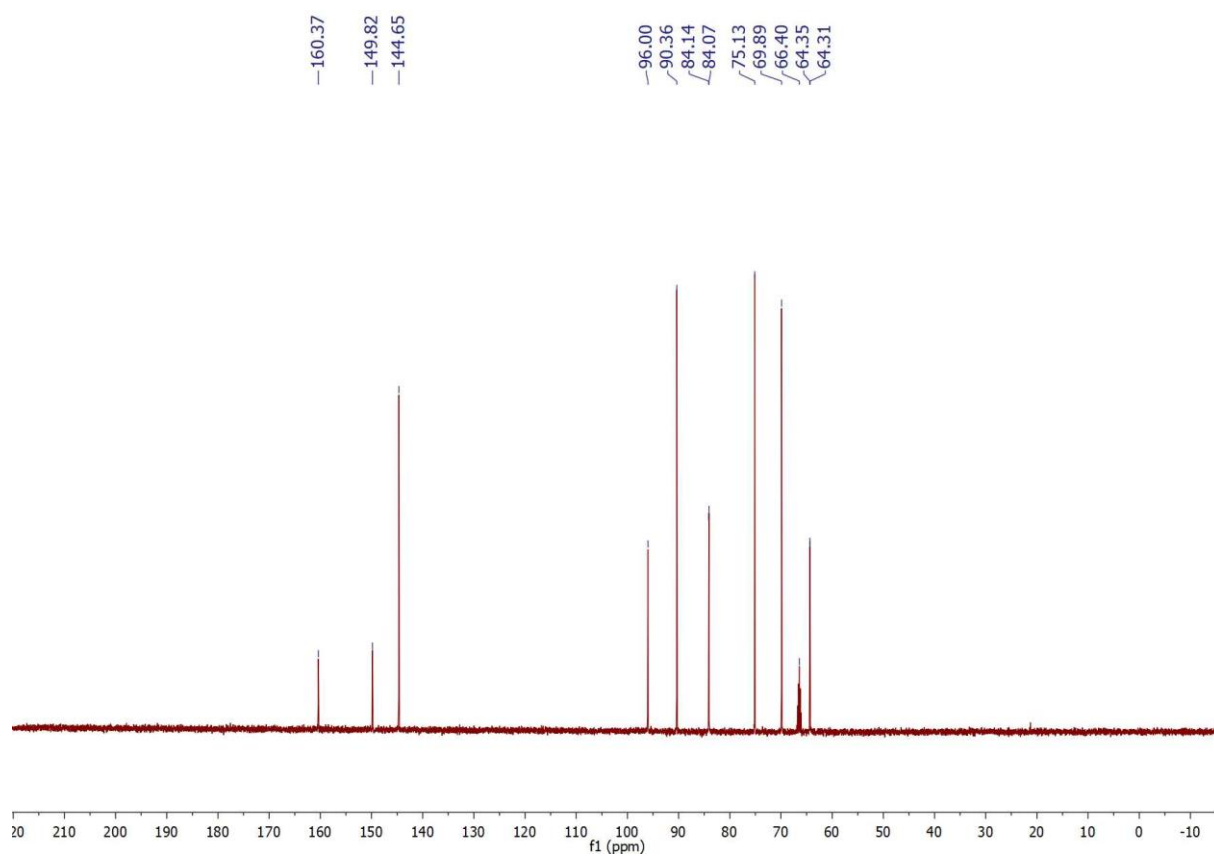


Figure S20. CMP  $^{13}\text{C}$  NMR spectrum

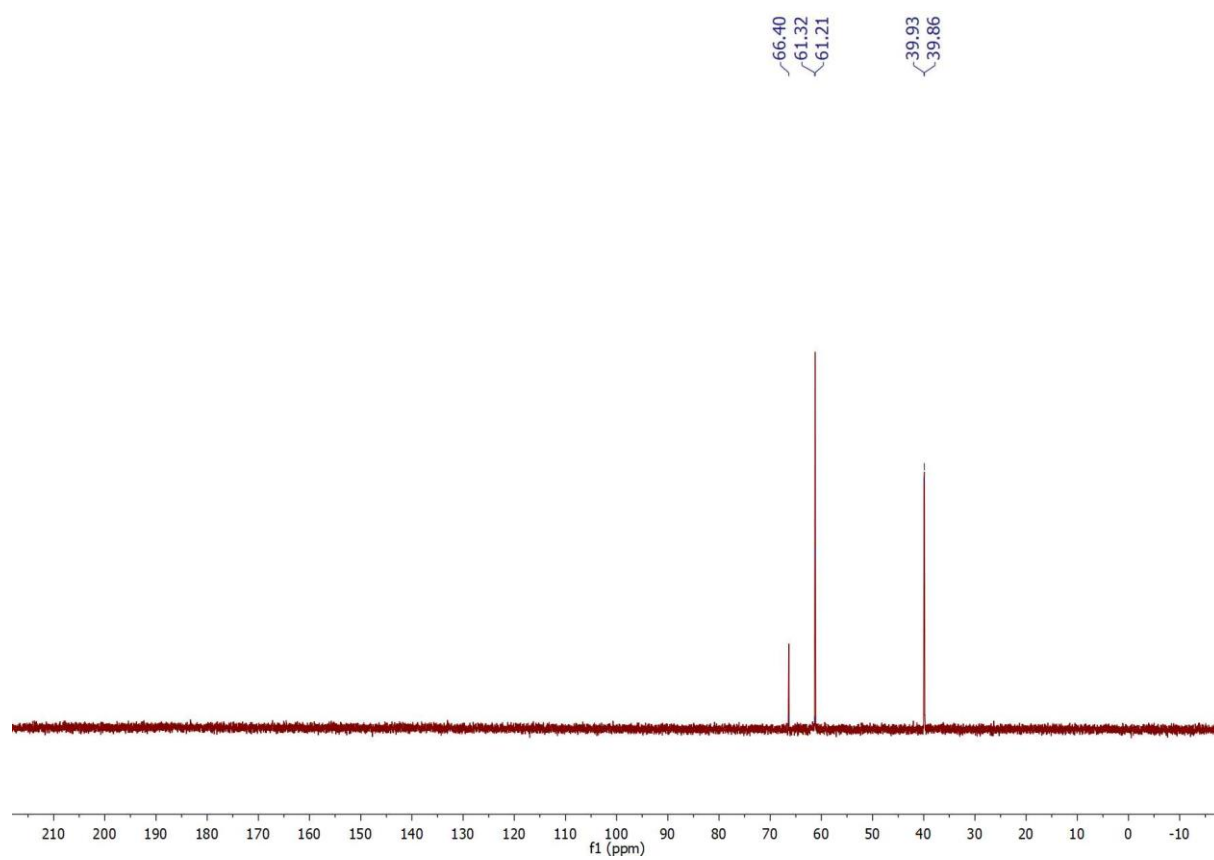


Figure S21. enP  $^{13}\text{C}$  NMR spectrum

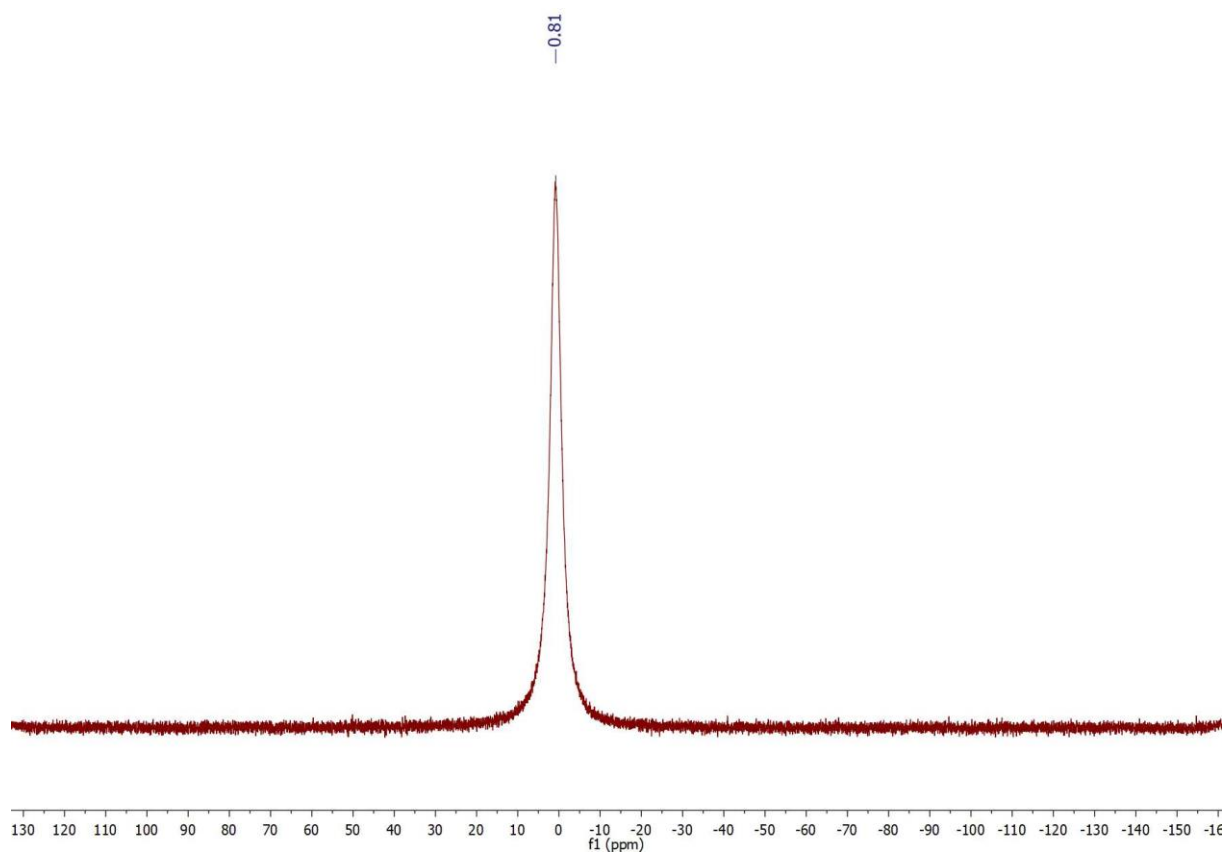


Figure S22.  $\text{Cu}(\text{enP})\text{H}_4(\text{CMP})$   $^{31}\text{P}$  NMR spectrum

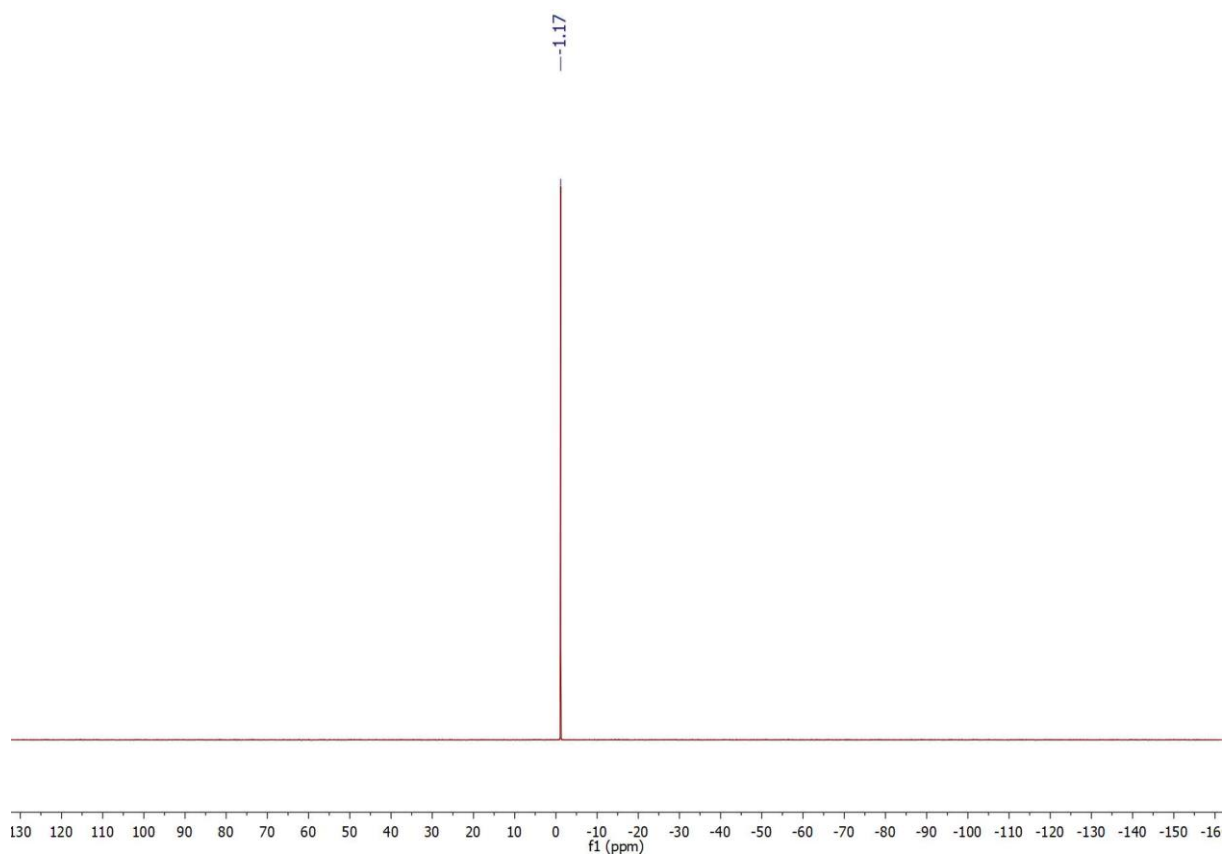


Figure S23.  $\text{CMP}$   $^{31}\text{P}$  NMR spectrum

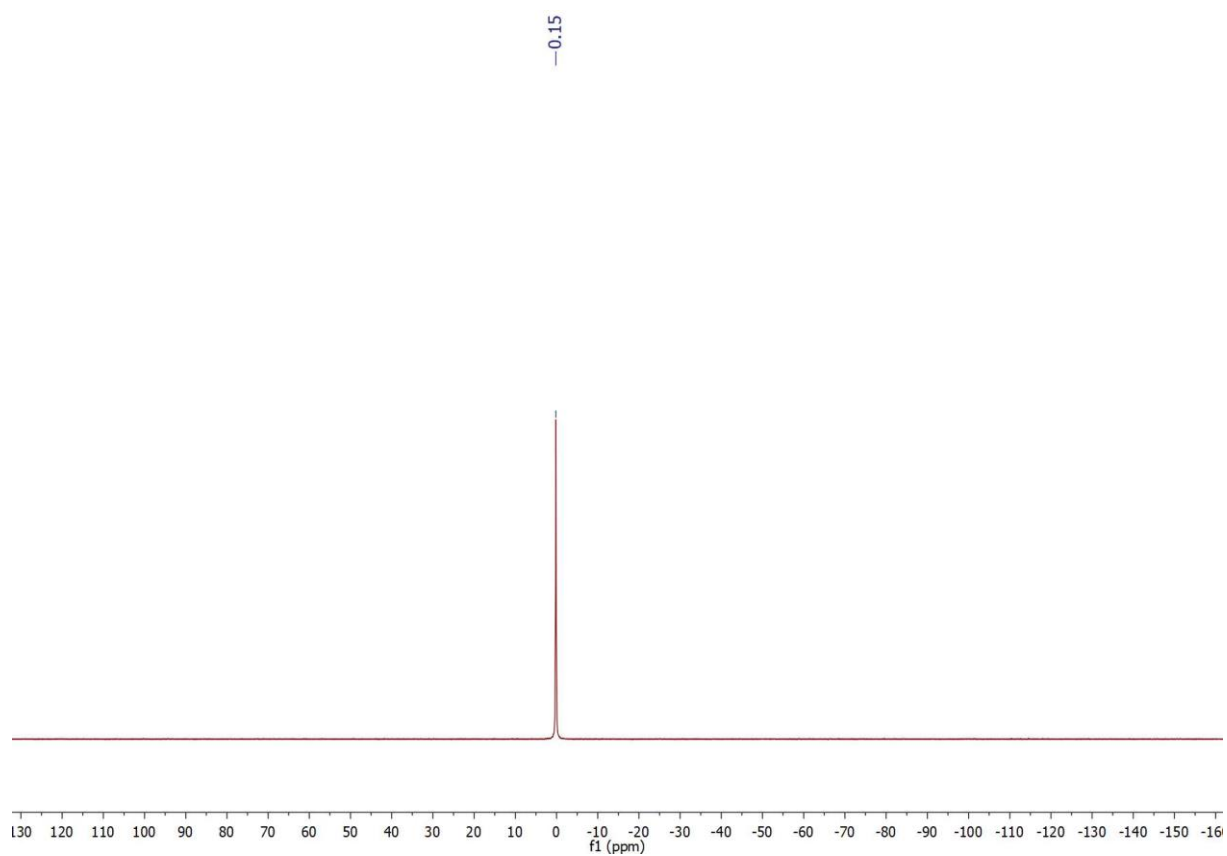


Figure S24. enP  $^{31}\text{P}$  NMR spectrum