

Single and double-stranded 1D-coordination polymers with 4'-(4-alkoxyphenyl)-3,2':6',3"-terpyridines and $\{\text{Cu}_2(\mu\text{-OAc})_4\}$ or $\{\text{Cu}_4(\mu_3\text{-OH})_2(\mu\text{-OAc})_2(\mu_3\text{-OAc})_2(\text{AcO-}\kappa\text{O})_2\}$ motifs

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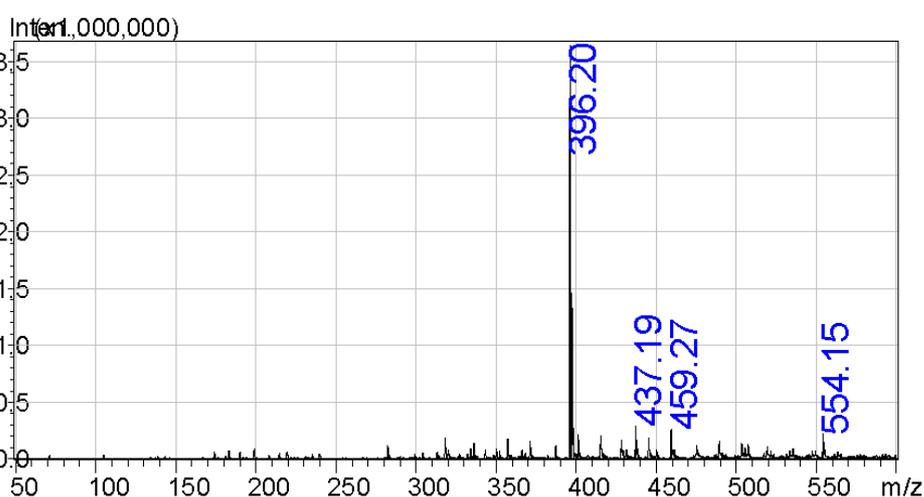


Figure S1. Electrospray mass spectrum of compound 3.

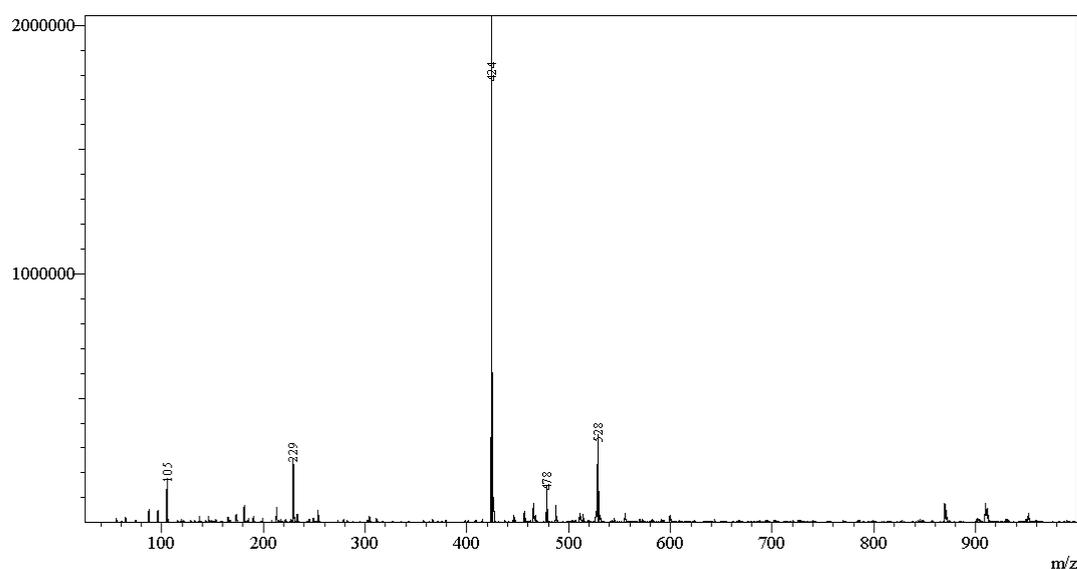


Figure S2. Electrospray mass spectrum of compound 4.

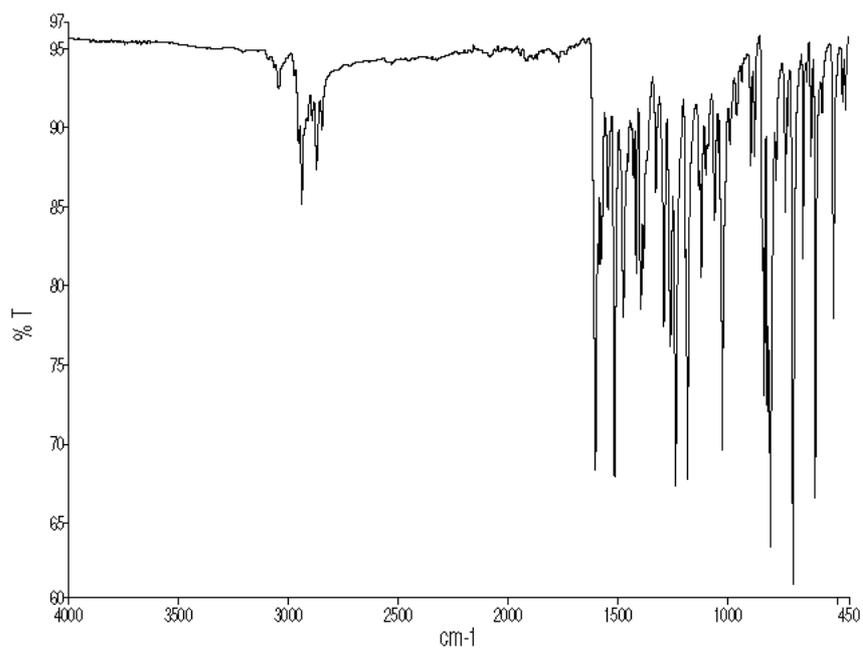


Figure S3. FT-IR spectrum of compound **3** (solid state).

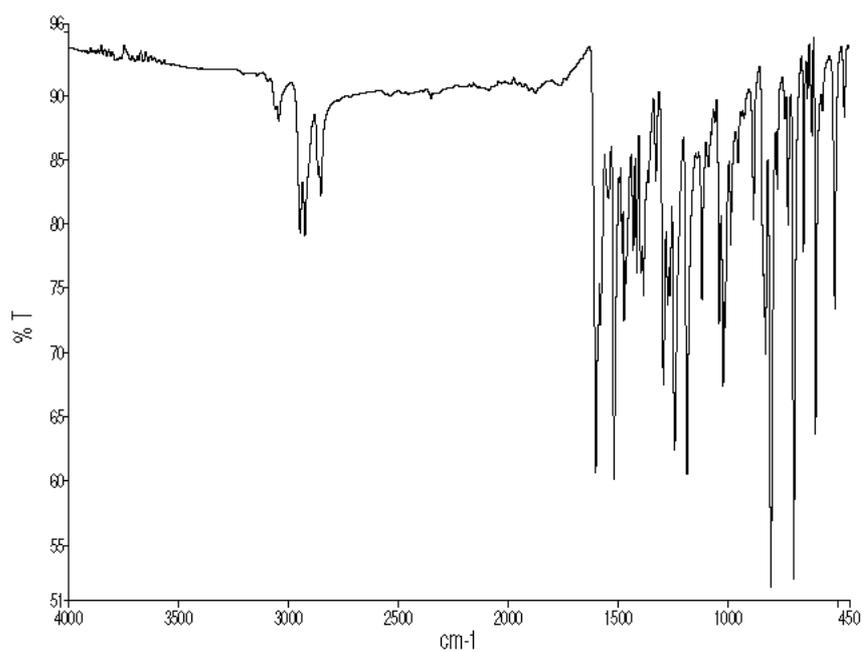


Figure S4. FT-IR spectrum of compound **4** (solid state).

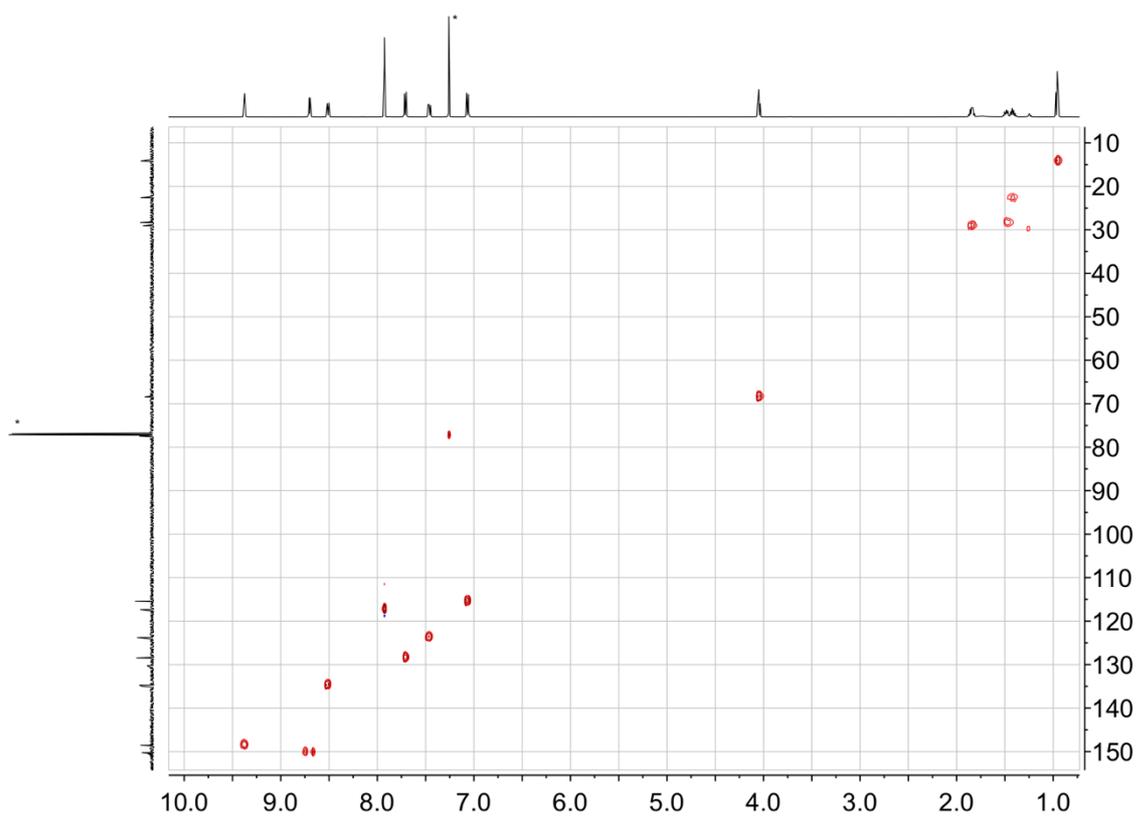


Figure S5. HMBC spectrum of **3** in CDCl₃ (500 MHz ¹H, 126 MHz ¹³C{¹H}, 298 K). * = CHCl₃/CDCl₃.

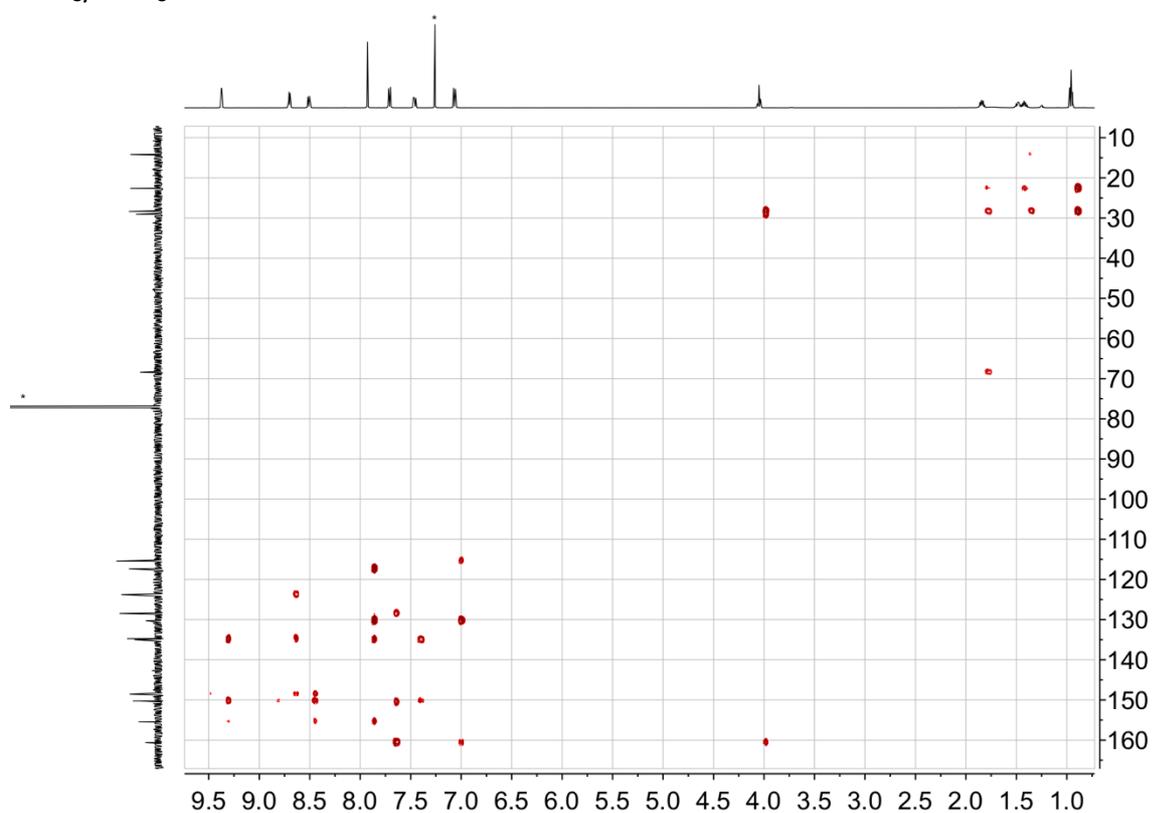


Figure S6. HMBC spectrum of **3** in CDCl₃ (500 MHz ¹H, 126 MHz ¹³C{¹H}, 298 K). * = CHCl₃/CDCl₃.

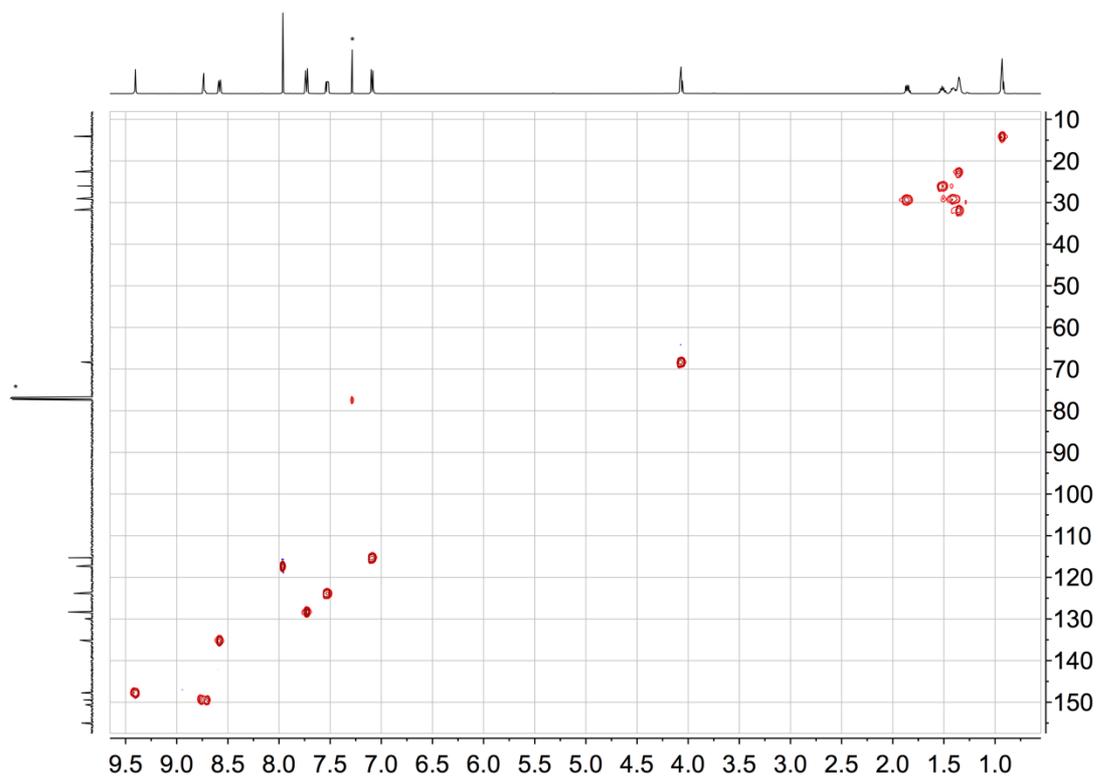


Figure S7. HMBC spectrum of **4** in CDCl₃ (500 MHz ¹H, 126 MHz ¹³C{¹H}, 298 K). * = CHCl₃/CDCl₃.

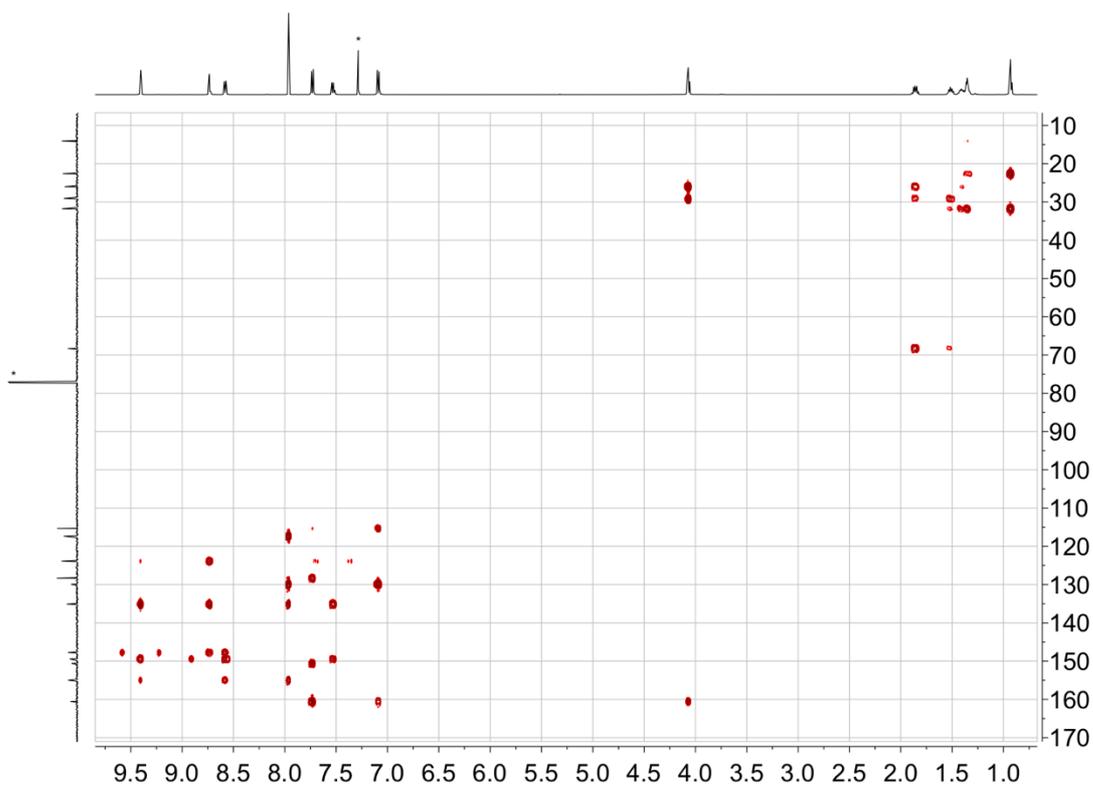


Figure S8. HMBC spectrum of **4** in CDCl₃ (500 MHz ¹H, 126 MHz ¹³C{¹H}, 298 K). * = CHCl₃/CDCl₃.

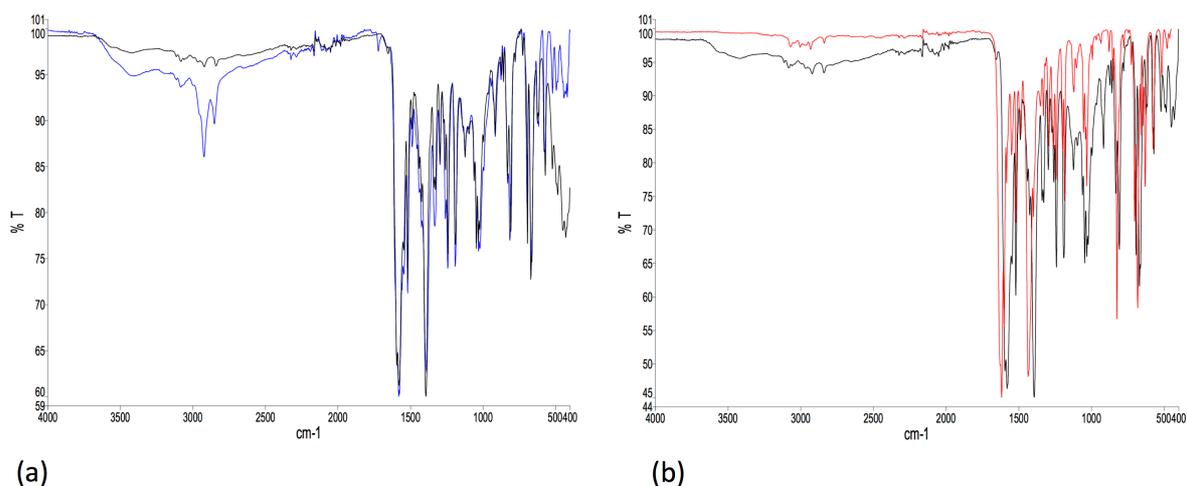


Figure S9. Normalized FT-IR spectra (solid-state) of the bulk materials from (a) experiment 1 (black line) and experiment 2 (blue line), and (b) experiment 1 (black line, $[\{\text{Cu}_4(\mu_3\text{-OH})_2(\mu\text{-OAc})_2(\mu_3\text{-OAc})_2(\text{AcO-}\kappa\text{O})_2(\mathbf{1})_2\} \cdot 2\text{MeOH}]_n$) and the preparative scale reaction (red line, $[\text{Cu}_2(\mu\text{-OAc})_4(\mathbf{1})]_n$).

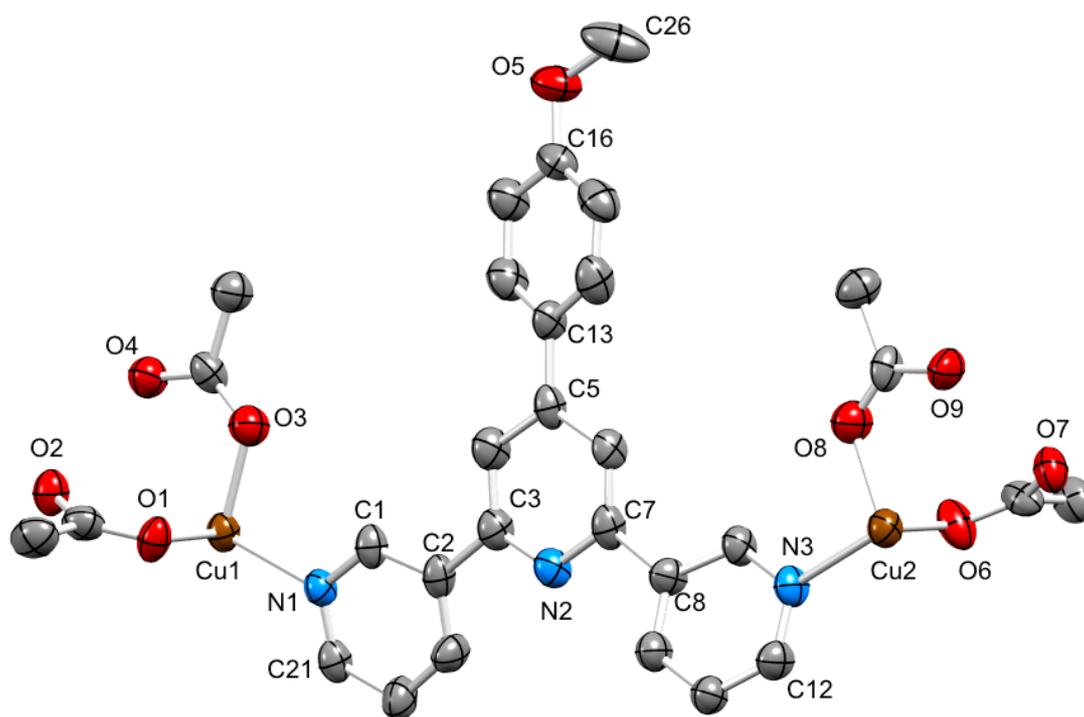


Figure S10. ORTEP-style representation of the asymmetric unit in $[\text{Cu}_2(\mu\text{-OAc})_4(\mathbf{1})]_n$ with ellipsoids plotted at 40% probability level and H atoms omitted.

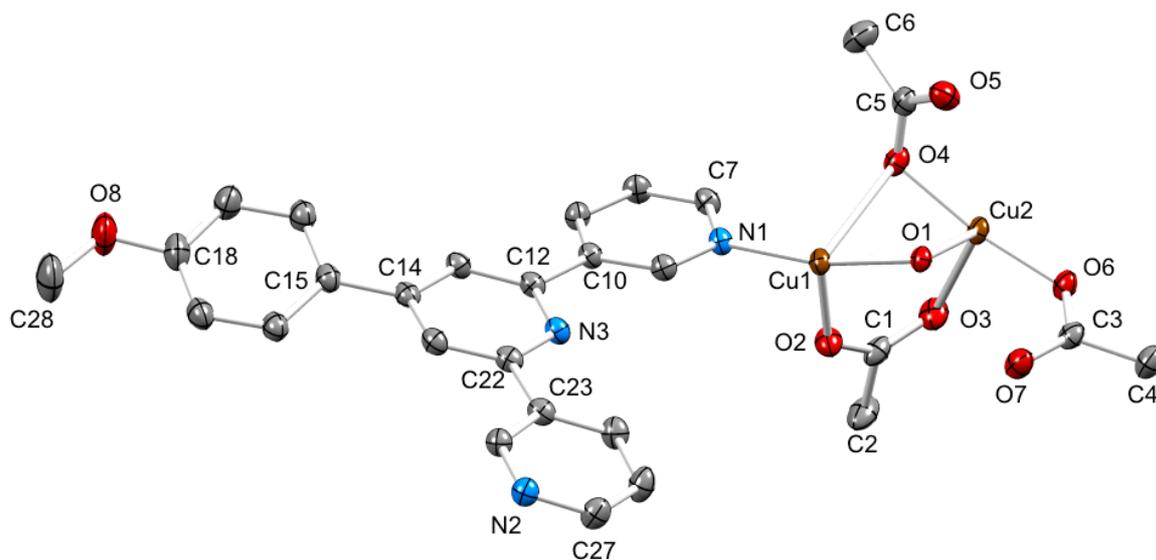


Figure S11. ORTEP-style representation of the asymmetric unit in $\{[\text{Cu}_4(\mu_3\text{-OH})_2(\mu\text{-OAc})_2(\mu_3\text{-OAc})_2(\text{AcO-}\kappa\text{O})_2(\mathbf{1})_2] \cdot 2\text{MeOH}\}_n$ with ellipsoids plotted at 40% probability level and H atoms and solvent molecules omitted.

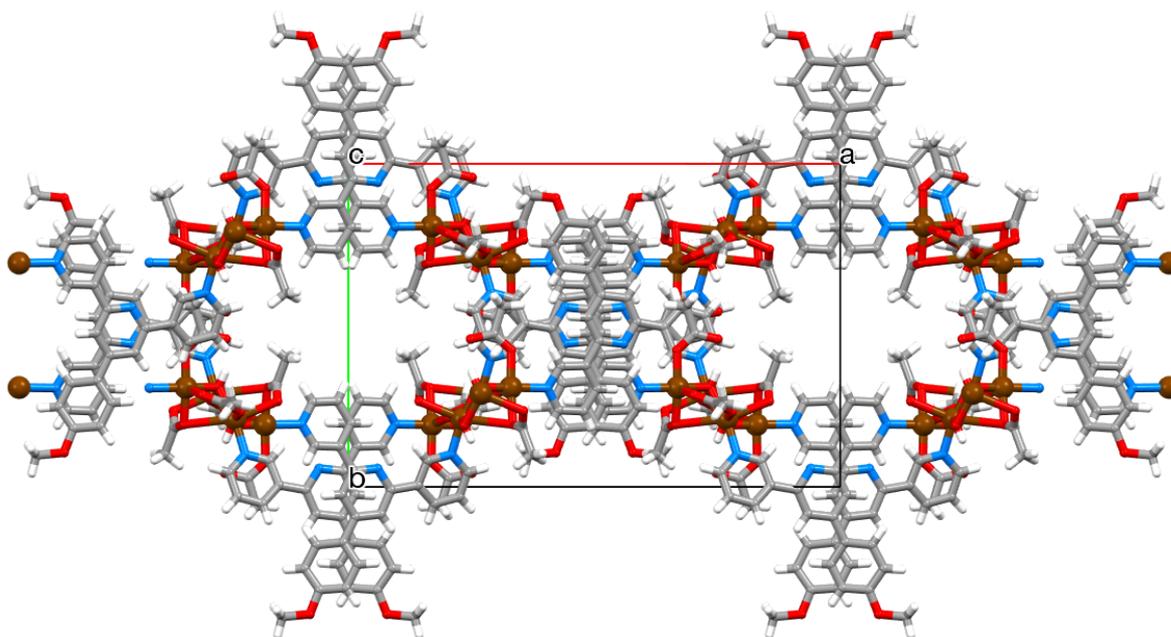


Figure S12 Packing of chains in $\{[\text{Cu}_4(\mu_3\text{-OH})_2(\mu\text{-OAc})_2(\mu_3\text{-OAc})_2(\text{AcO-}\kappa\text{O})_2(\mathbf{1})_2] \cdot 2\text{MeOH}\}_n$.

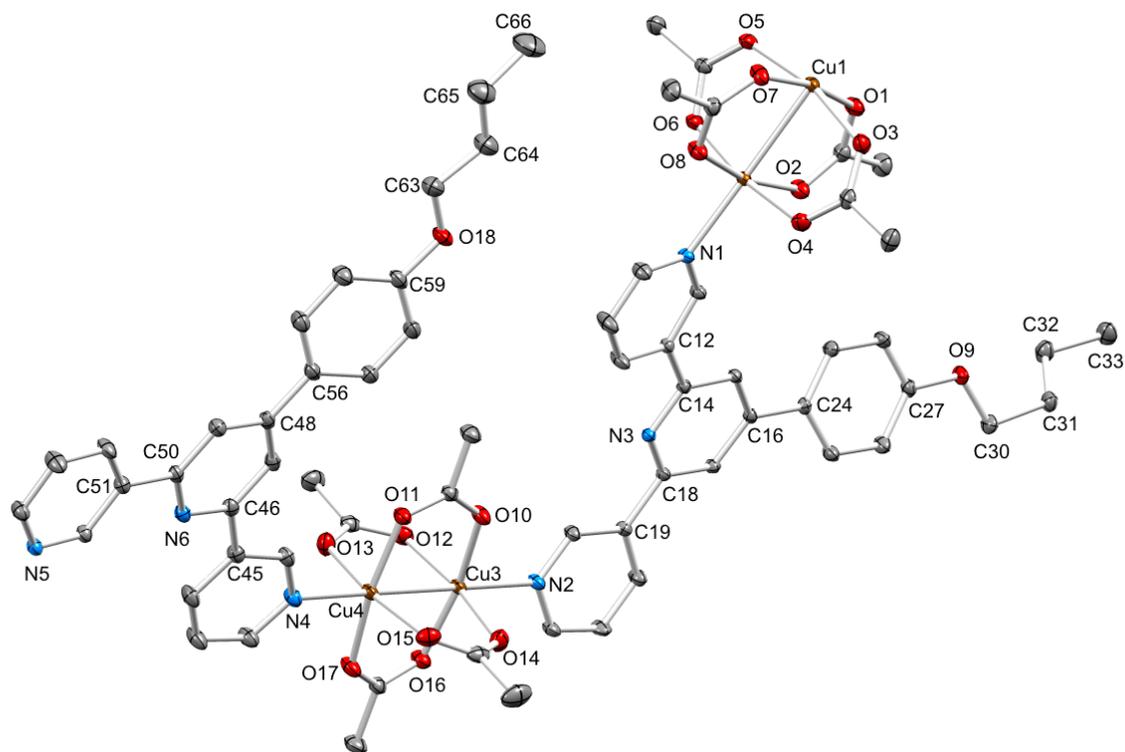


Figure S13. ORTEP-style representation of the asymmetric unit in $[2\{\text{Cu}_2(\mu\text{-OAc})_4(\mathbf{2})\}\cdot 1.25\text{MeOH}]_n$ with ellipsoids plotted at 40% probability level and H atoms and solvent molecules omitted.

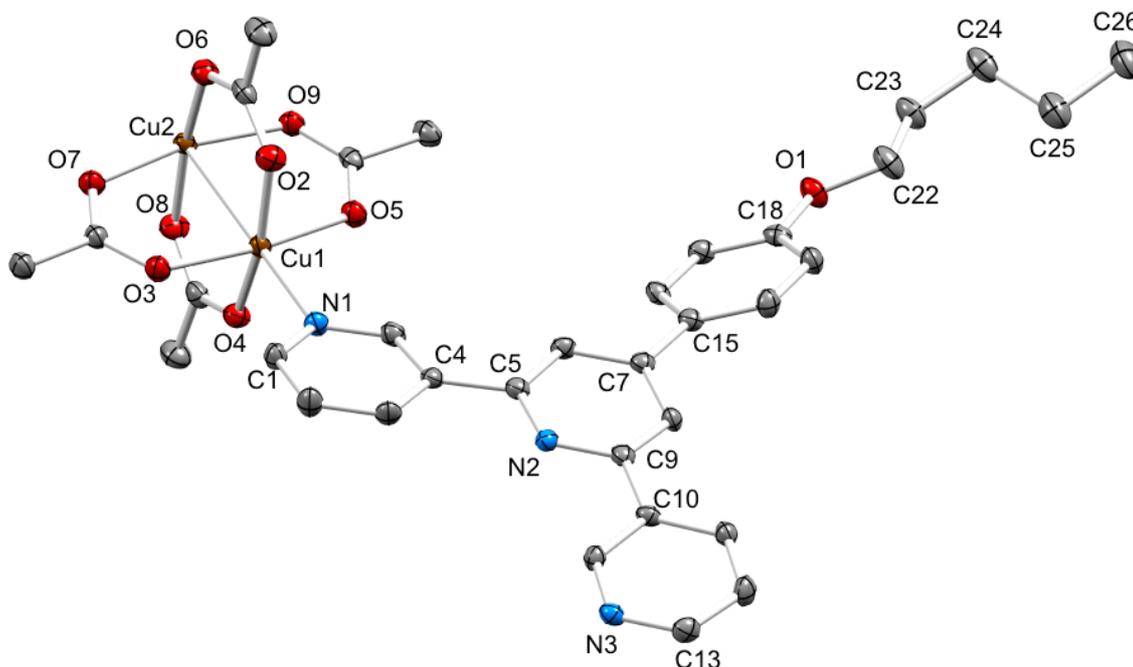


Figure S14. ORTEP-style representation of the asymmetric unit in $[\text{Cu}_2(\mu\text{-OAc})_4(\mathbf{3})]_n$ with ellipsoids plotted at 40% probability level and H atoms omitted.

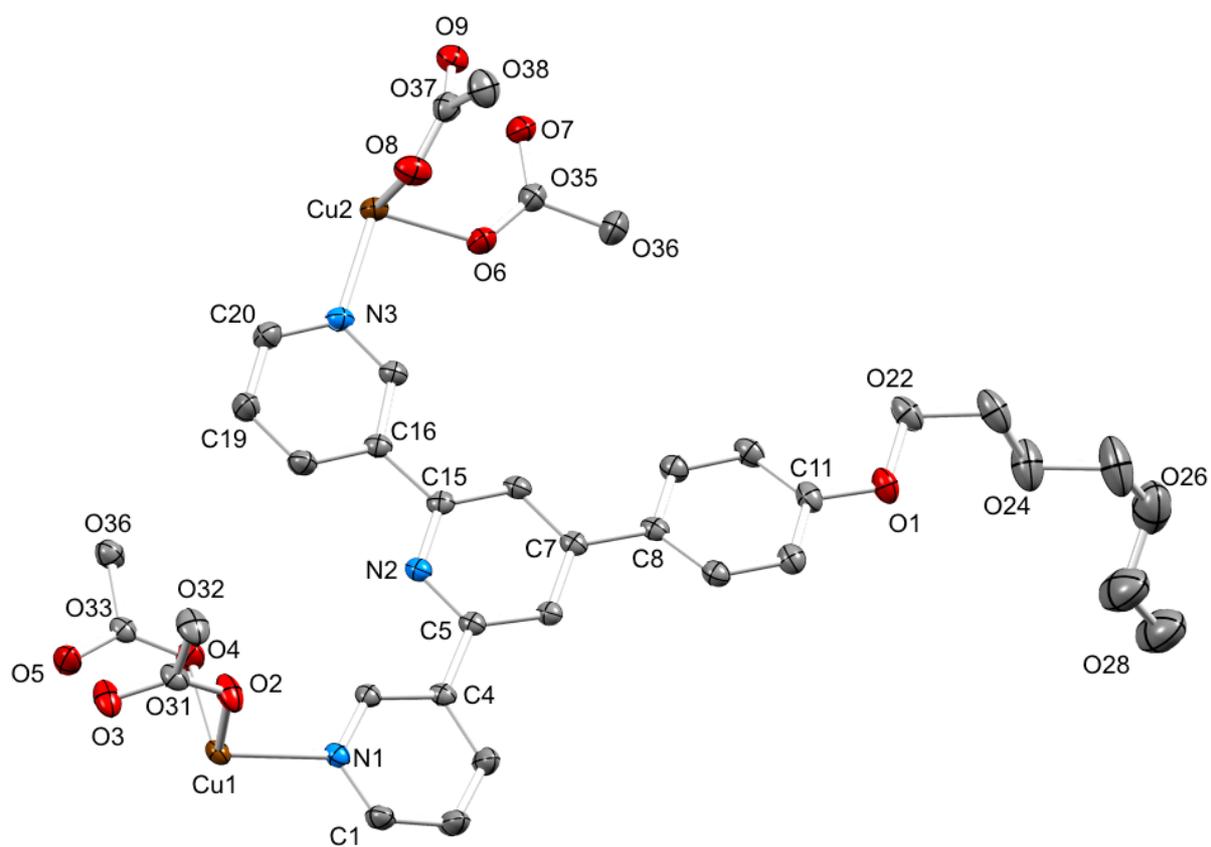


Figure S15. ORTEP-style representation of the asymmetric unit in $[\text{Cu}_2(\mu\text{-OAc})_4(\mathbf{4})] \cdot 0.2\text{CHCl}_3$ with ellipsoids plotted at 40% probability level and H atoms and solvent molecules omitted.

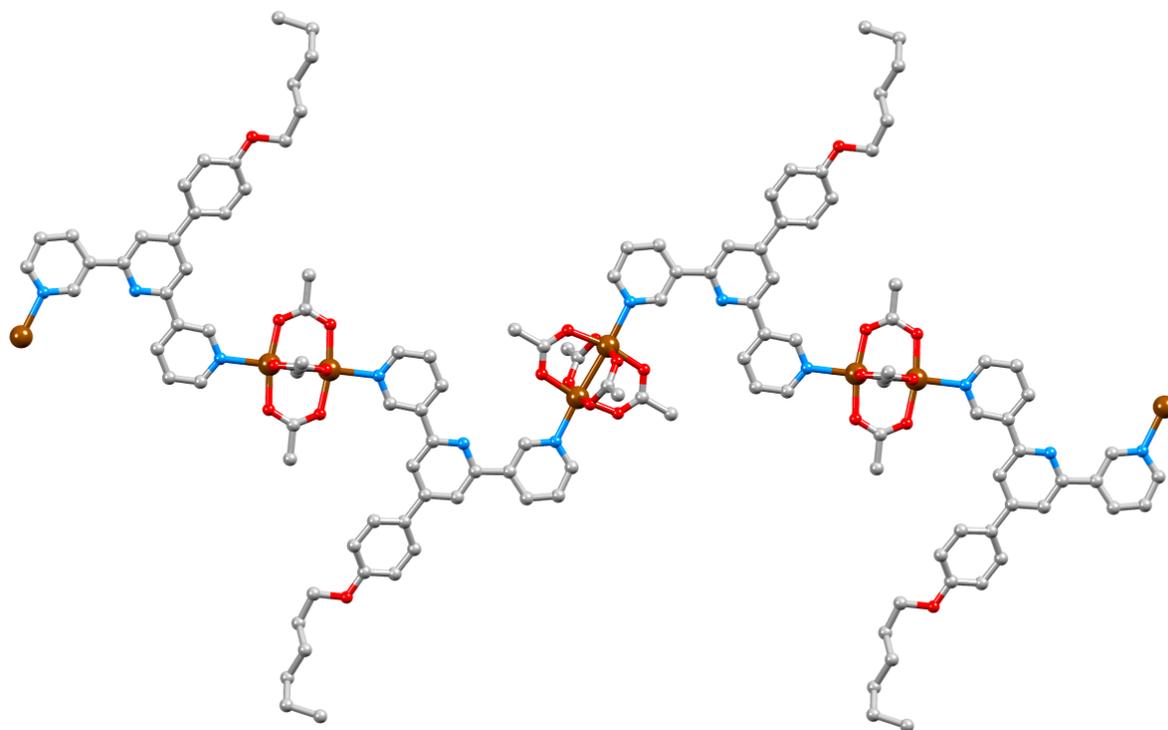


Figure S16. Part of one chain in $[\text{Cu}_2(\mu\text{-OAc})_4(\mathbf{5})] \cdot 0.2\text{CHCl}_3$, drawn using data retrieved from the CSD, refcode SADBIL [1].

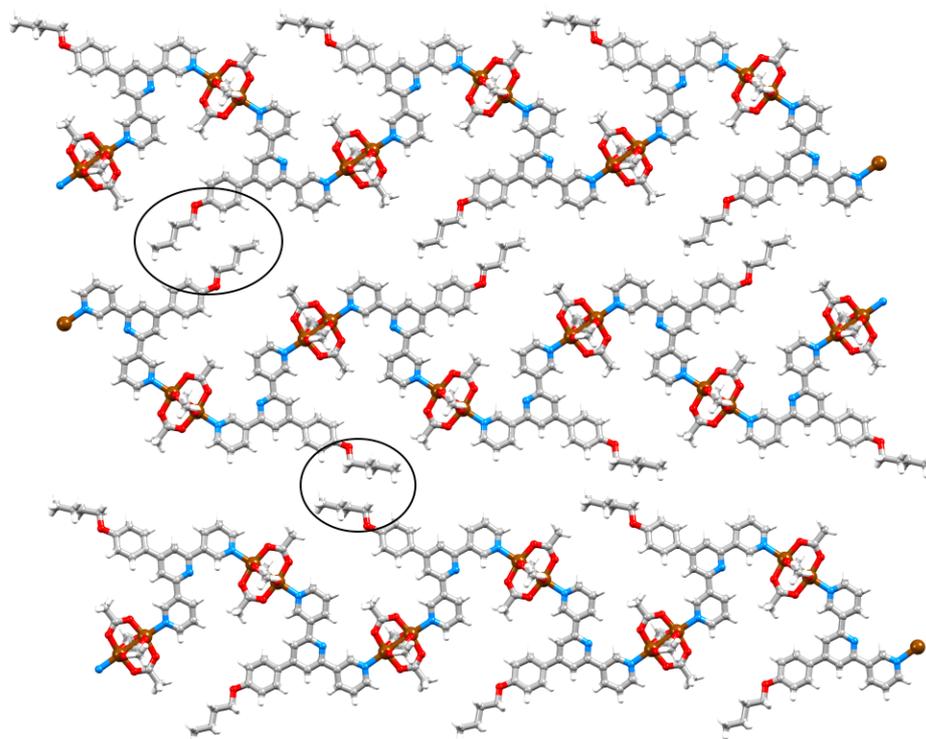


Figure S17. Packing of three adjacent chains (each runs left to right) shown in ball-and-stick representation in $[2\{\text{Cu}_2(\mu\text{-OAc})_4(\mathbf{2})\}\cdot 1.25\text{MeOH}]_n$. The two independent alkyl...alkyl van der Waals packing interactions are highlighted.

References

1. Li, L.; Zhang, Y.Z.; Yang, C.; Liu, E.; Golen, J.A.; Zhang, G. One-dimensional copper(II) coordination polymers built on 4'-substituted 4,2':6',4''- and 3,2':6',3''-terpyridines: Syntheses, structures and catalytic properties. *Polyhedron* **2016**, *105*, 115–122. DOI: 10.1016/j.poly.2015.12.042