

Supporting Information for

Amplification of Impurity upon Complex Formation: How a 2% Ligand Impurity Lowers the Corresponding Complex Purity to 50%

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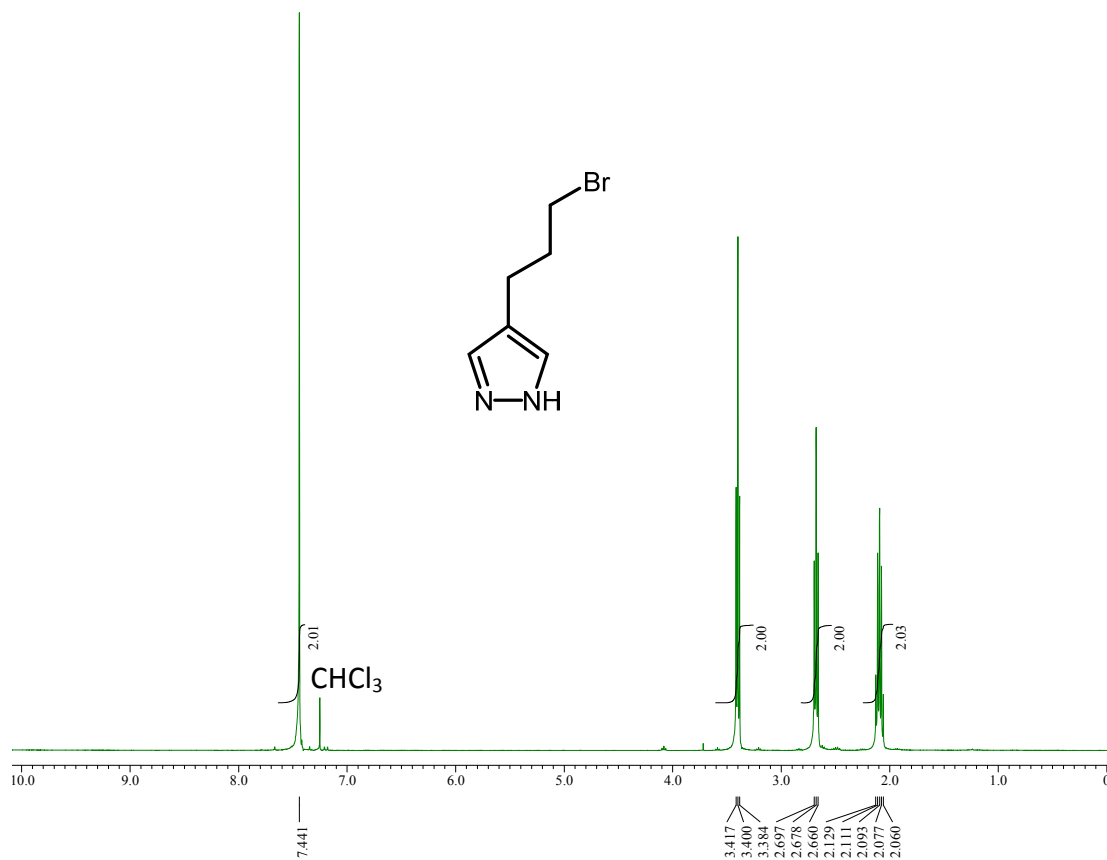


Figure S1. ¹H NMR spectrum of **2** in CDCl₃.

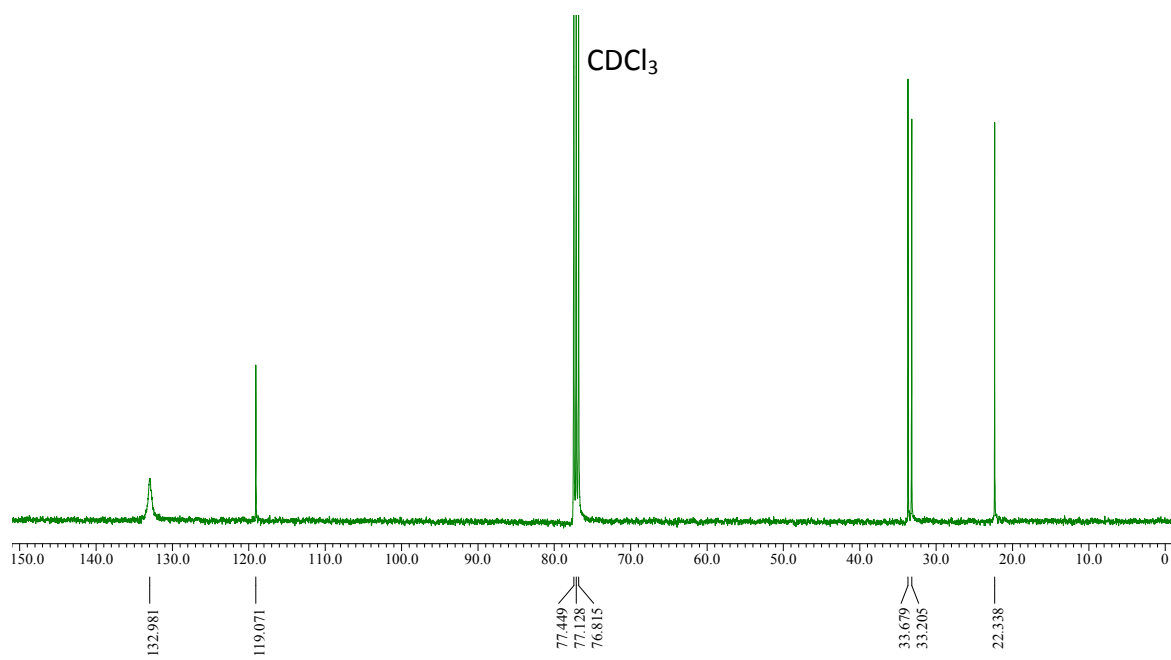


Figure S2. ¹³C NMR spectrum of **2** in CDCl₃.

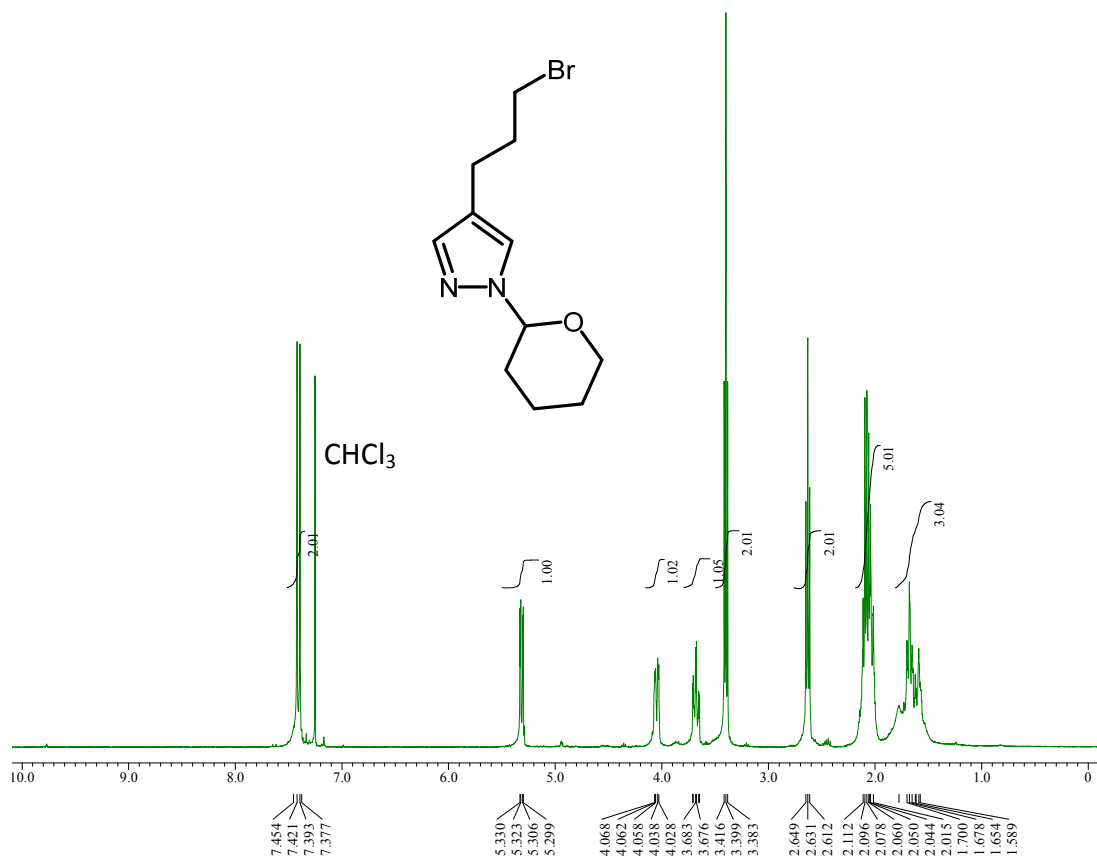


Figure S3. ^1H NMR spectrum of **3** in CDCl_3 .

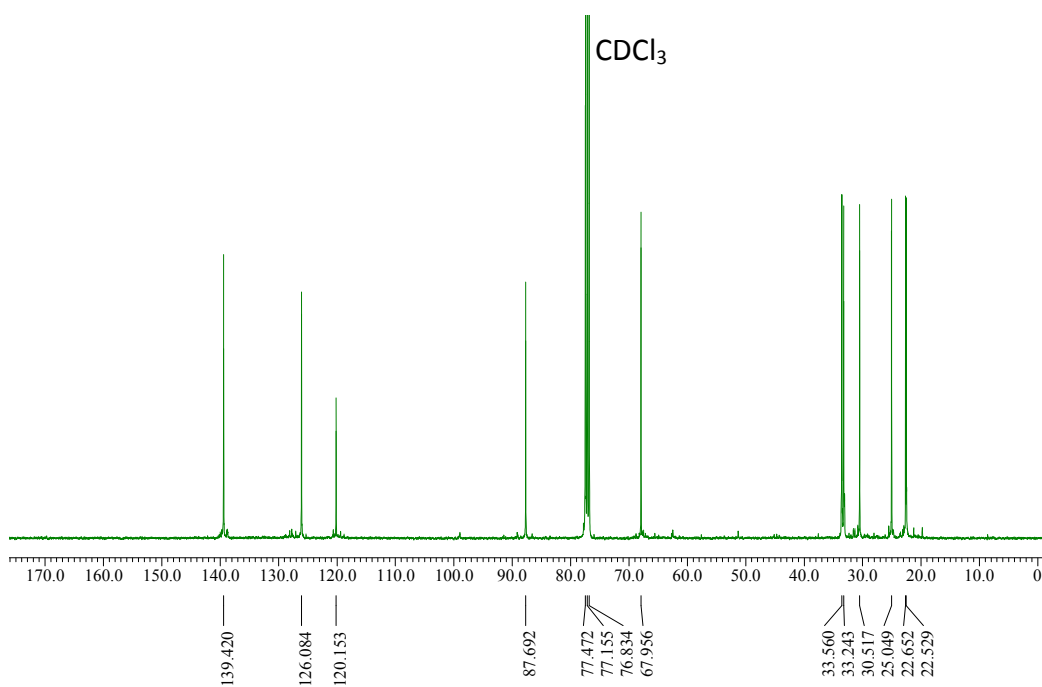


Figure S4. ^{13}C NMR spectrum of **3** in CDCl_3 .

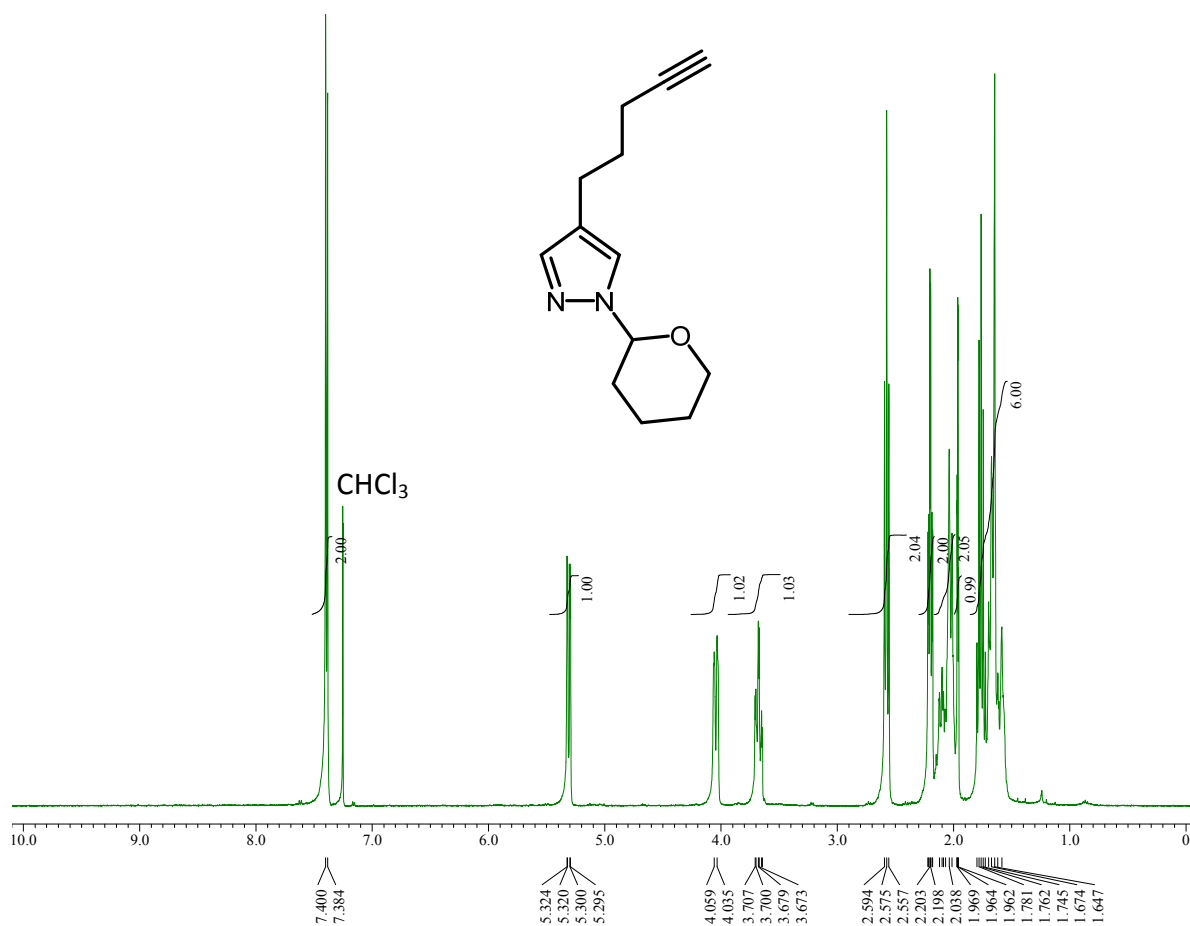


Figure S5. ¹H NMR spectrum of **4** in CDCl₃.

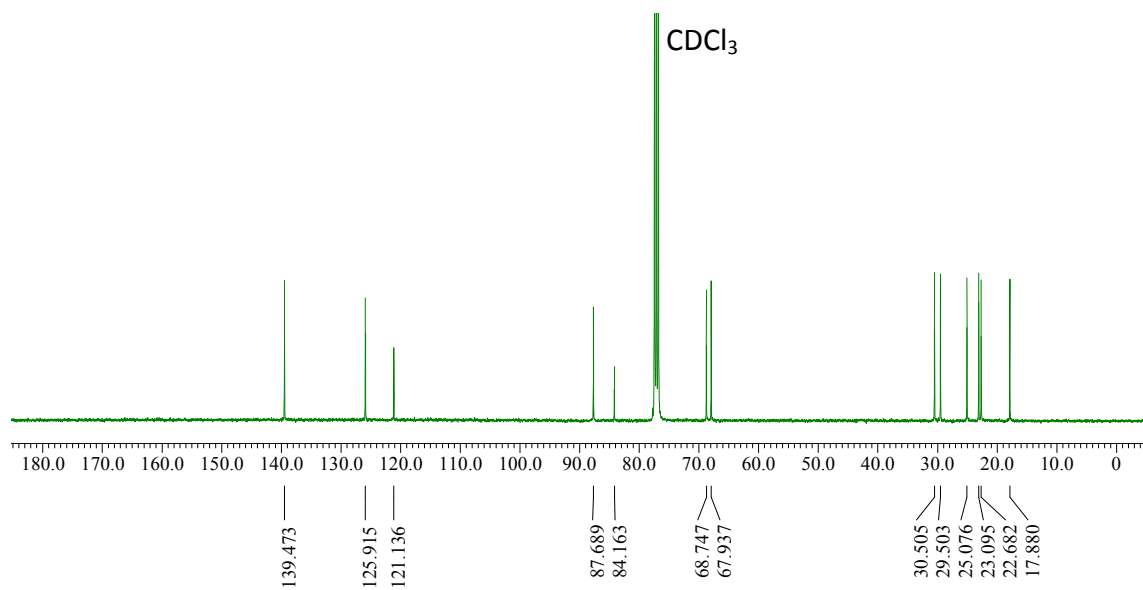


Figure S6. ¹³C NMR spectrum of **4** in CDCl₃.

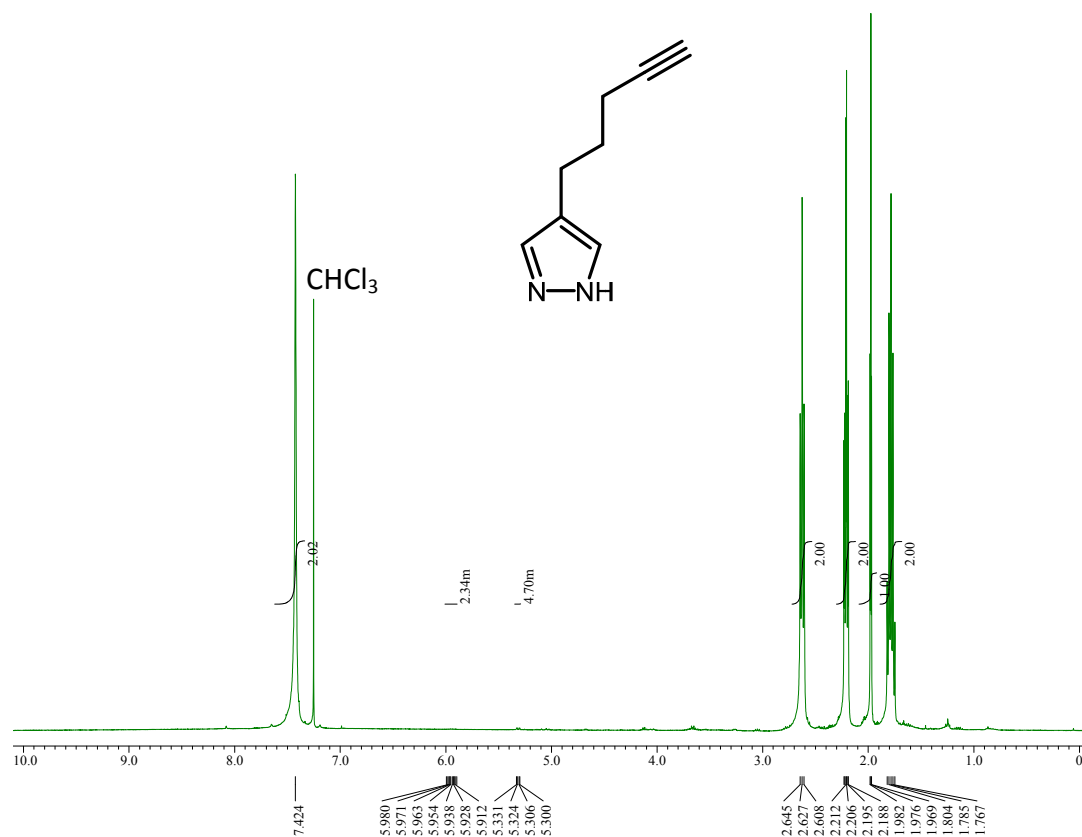


Figure S7. ¹H NMR spectrum of **5** in CDCl₃.

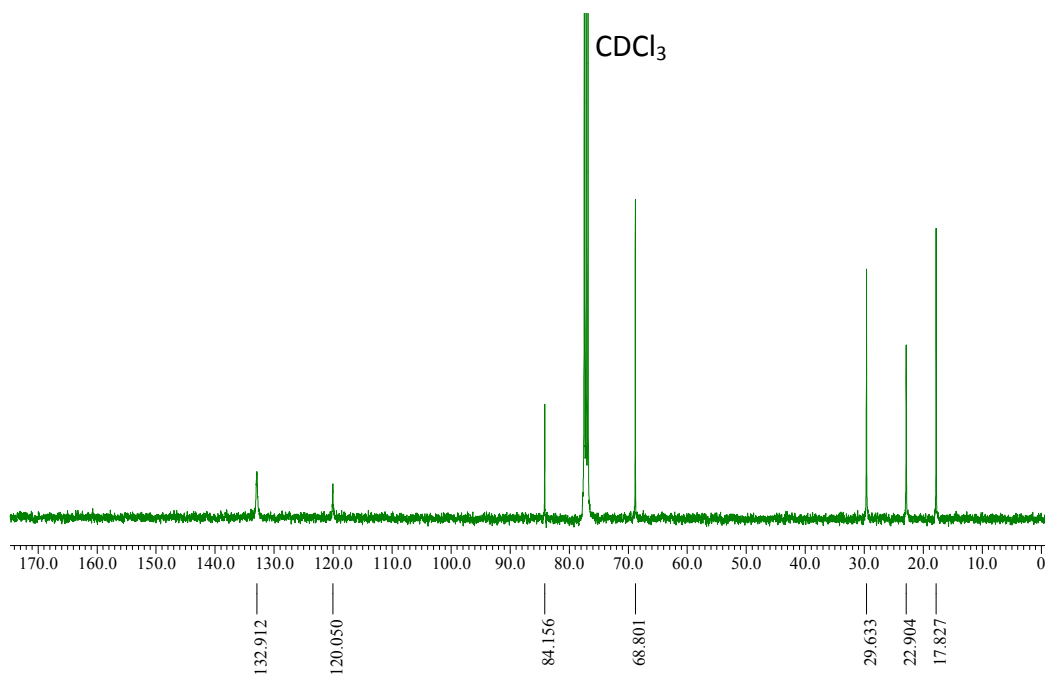


Figure S8. ¹³C NMR spectrum of **5** in CDCl₃.

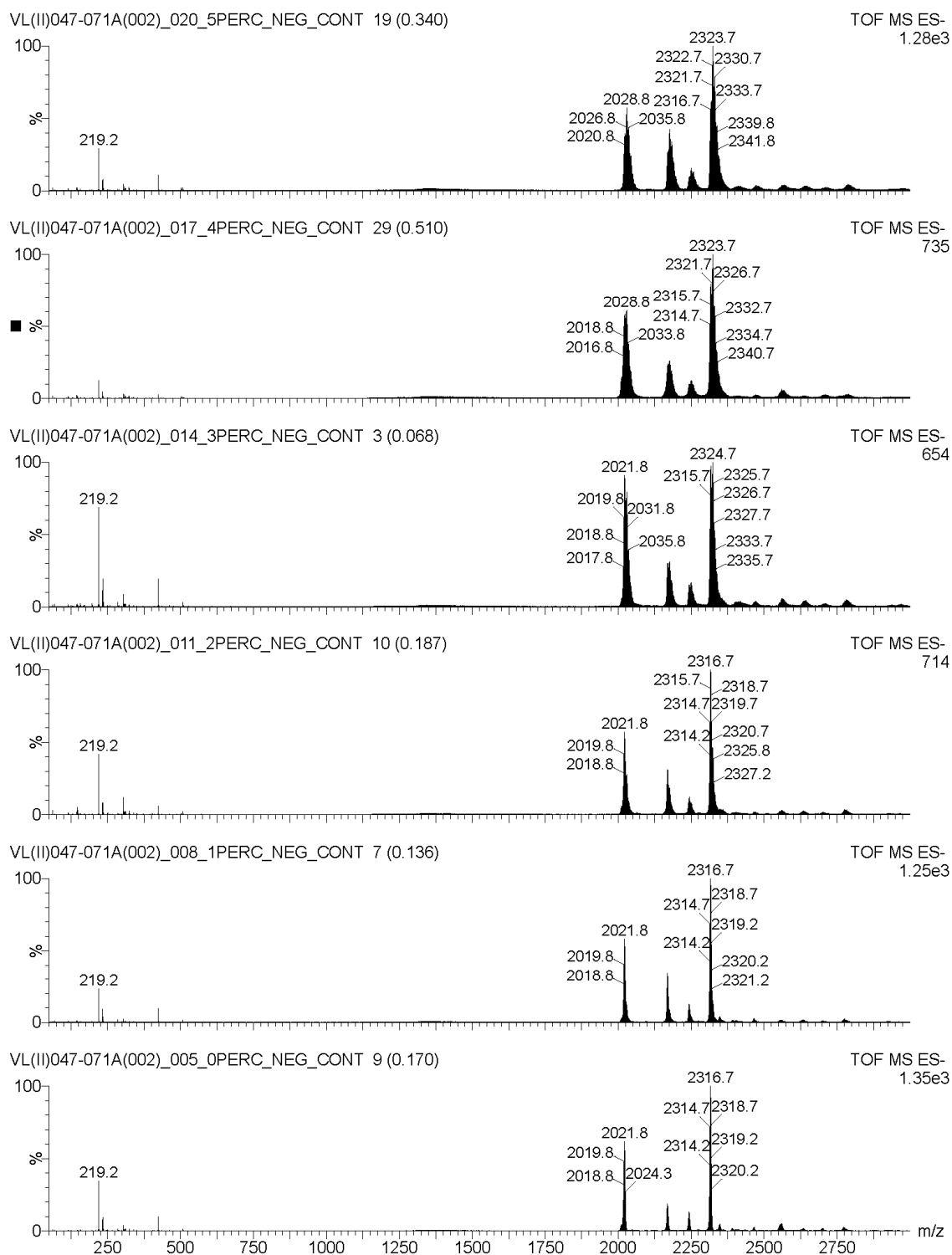


Figure S9. ESI-MS(–) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\text{C}\{\text{Cu}_n(\text{OH})_n(\text{pz})_{n-x}(4\text{-Mepz})_x\}]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 0–5 mol% 4-MepzH.

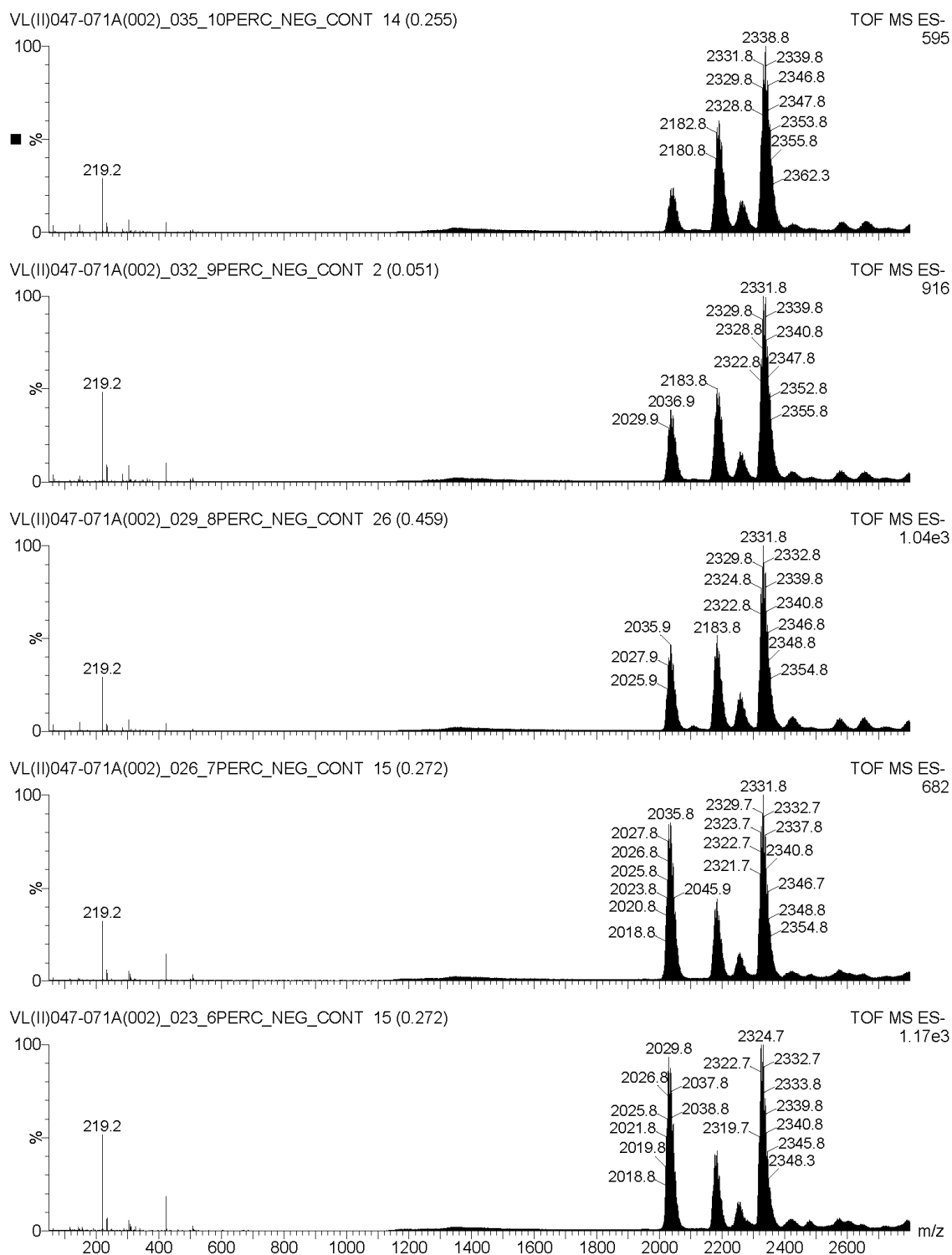


Figure S10. ESI-MS(-) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\text{C}\{\text{Cu}_n(\text{OH})_n(\text{pz})_{n-x}(4\text{-Mepz})_x\}]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 6–10 mol% 4-MepzH.

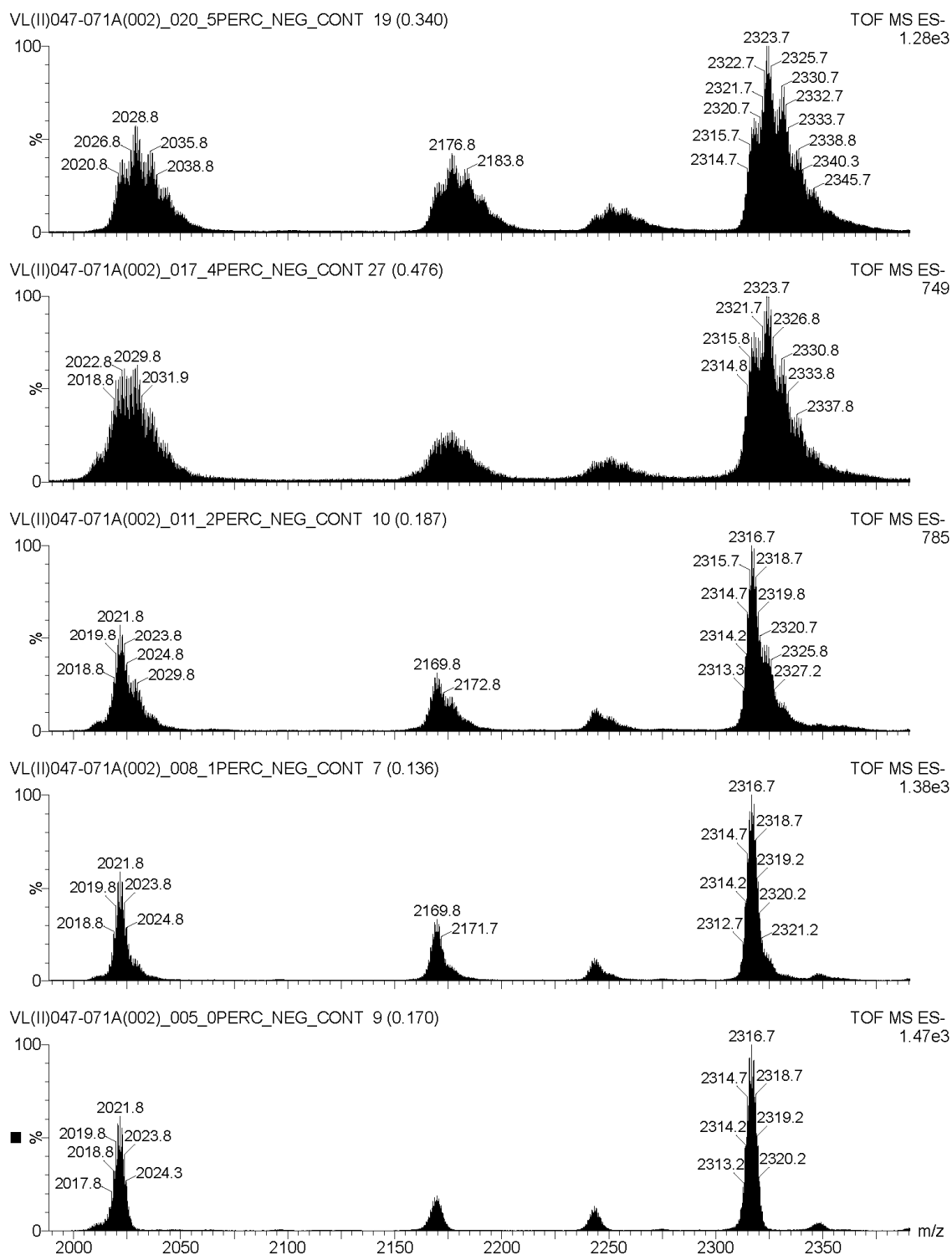


Figure S11. Zoomed portion of the ESI-MS(–) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\text{C}\{\text{Cu}_n(\text{OH})_n(\text{pz})_{n-x}(\text{4-Mepz})_x\}]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 0–5 mol% 4-MepzH.

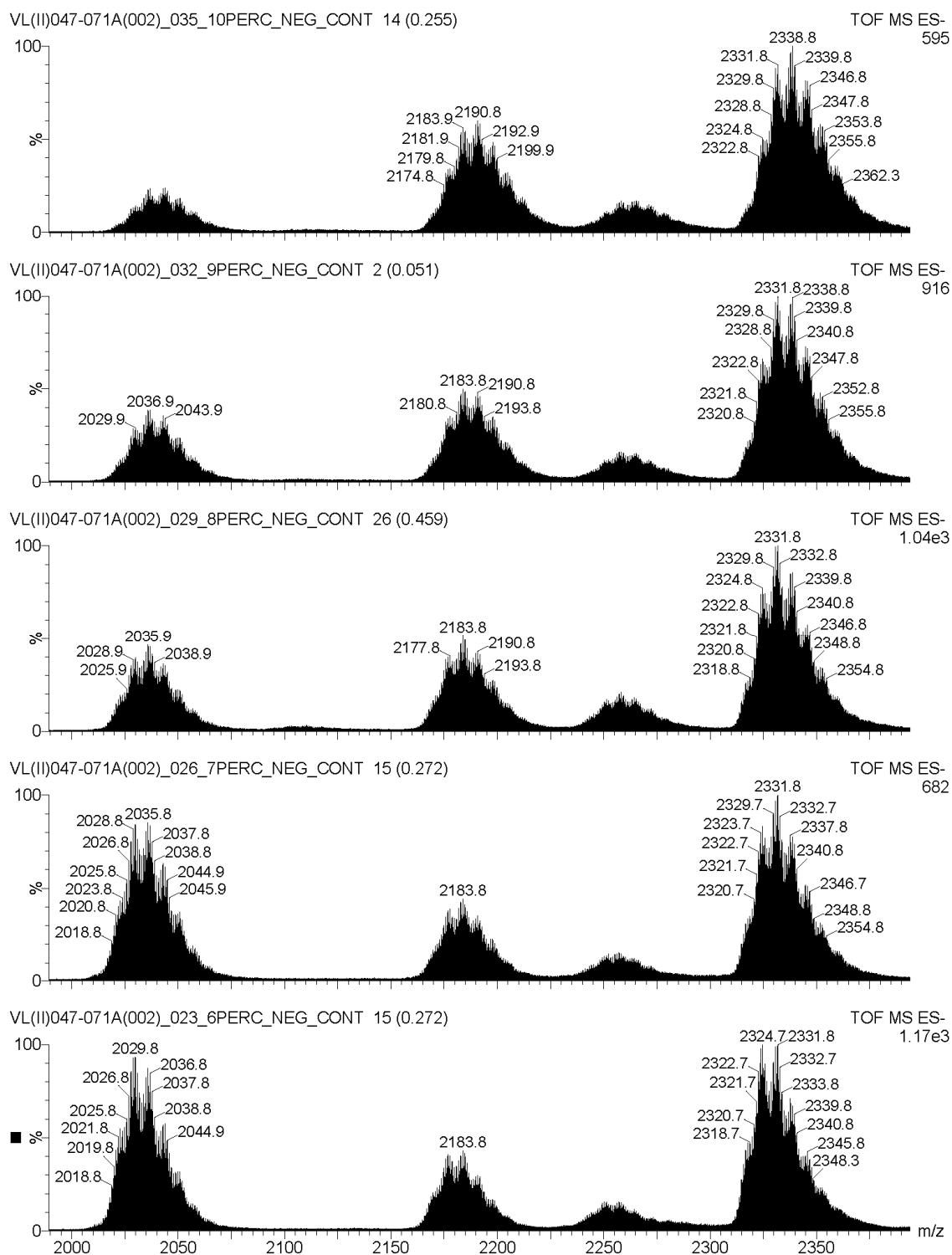


Figure S12. Zoomed portion of the ESI-MS(–) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\text{--}\{\text{Cu}_n(\text{OH})_n(\text{pz})_n\}_x(4\text{-Mepz})_x]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 6–10 mol% 4-MepzH.

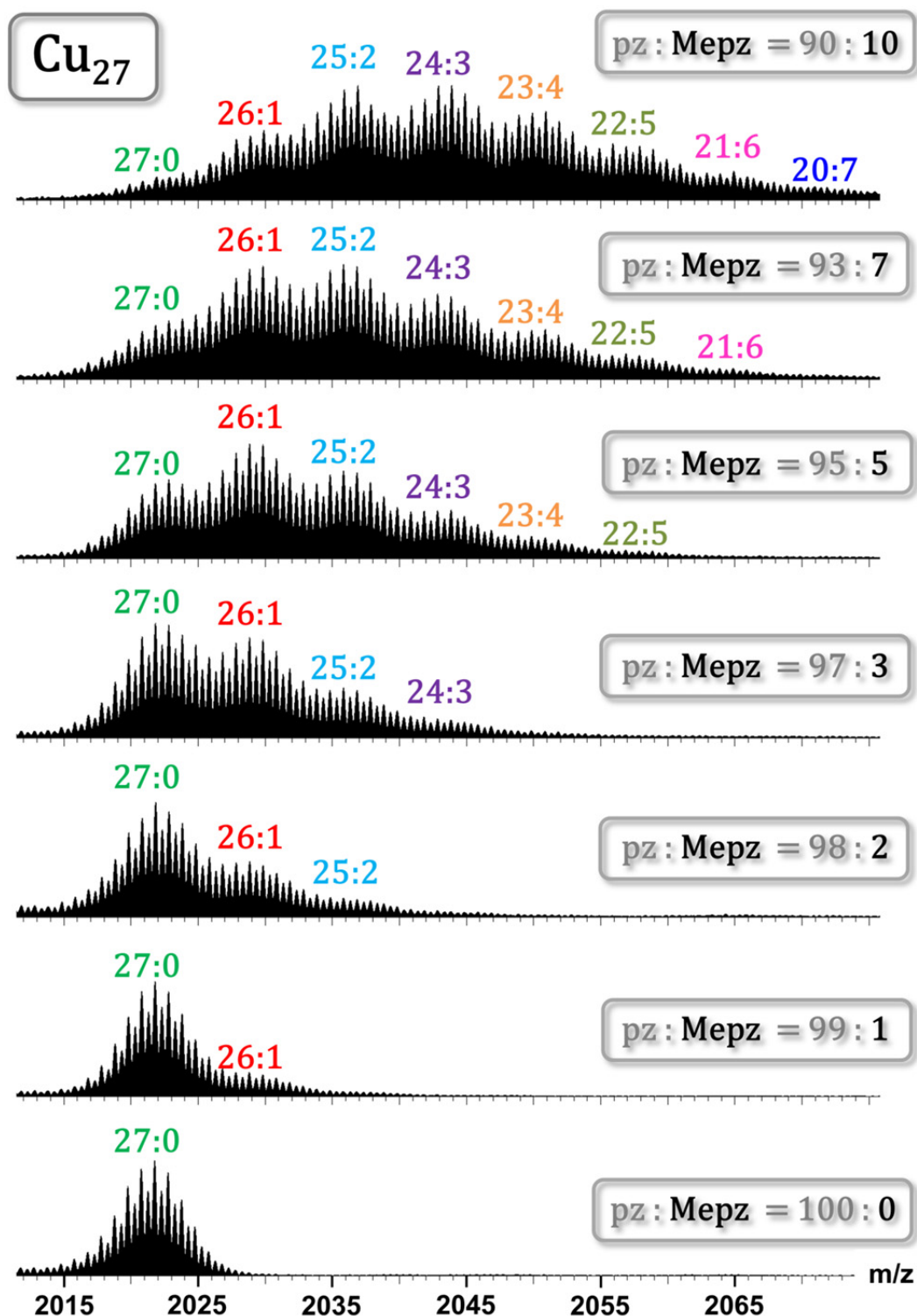


Figure S13. Zoomed portion of the ESI-MS(–) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\text{C}\{\text{Cu}_n(\text{OH})_n(\text{pz})_n\}_x(4\text{-Mepz})_x]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 0–10 mol% 4-MepzH.

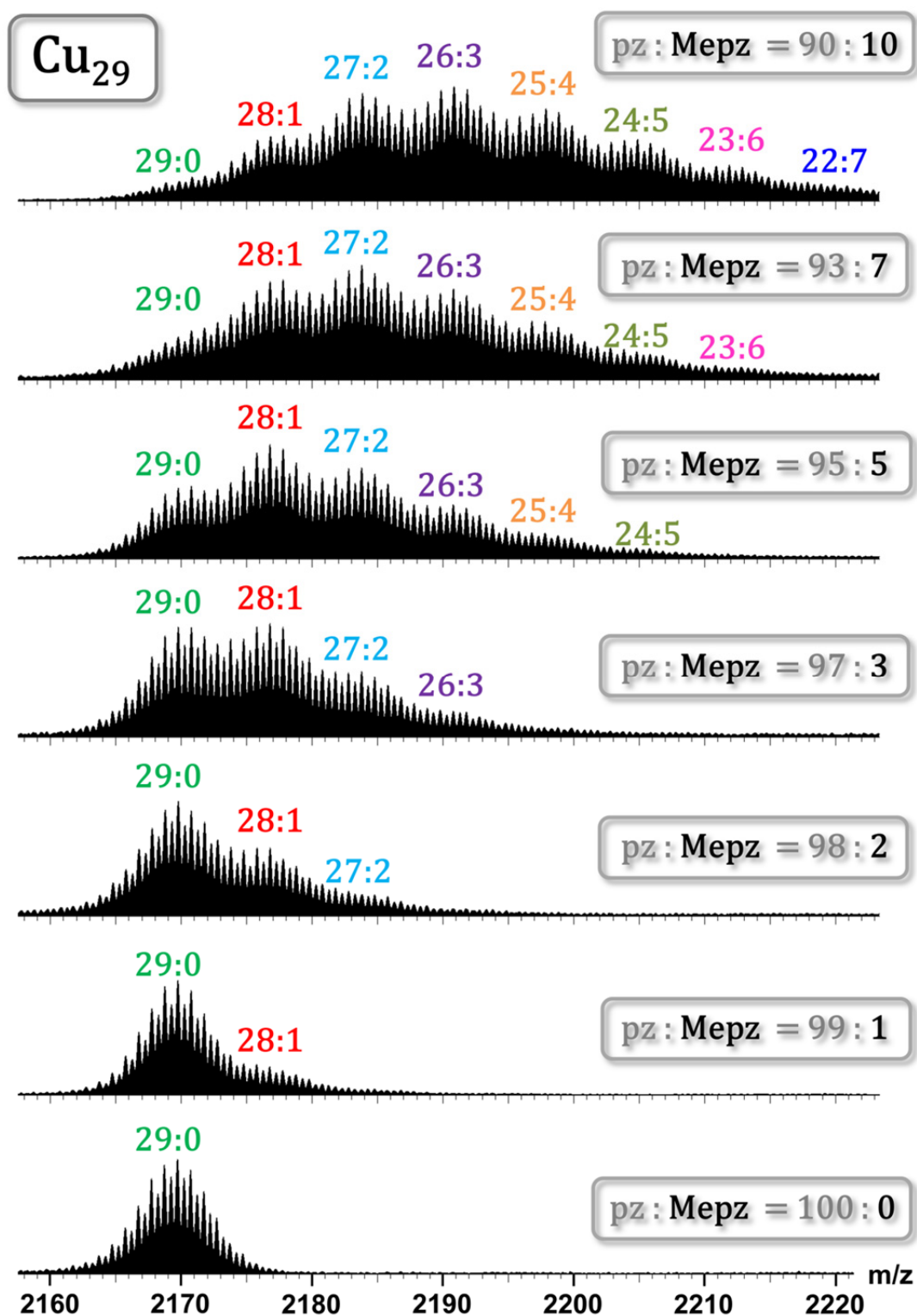


Figure S14. Zoomed portion of the ESI-MS(–) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\{\text{Cu}_n(\text{OH})_n(\text{pz})_n\}_x(4\text{-Mepz})_x]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 0–10 mol% 4-MepzH..

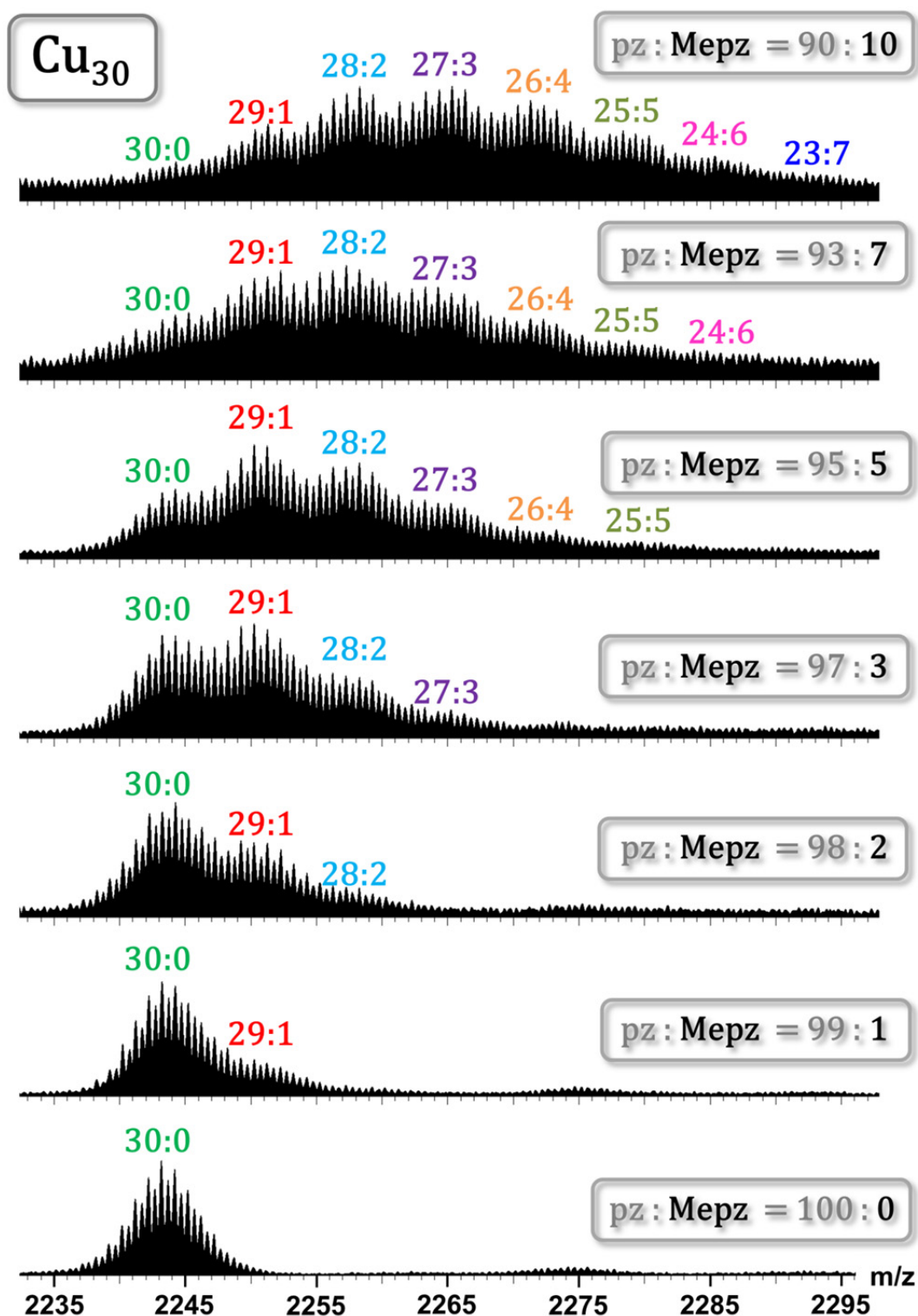


Figure S15. Zoomed portion of the ESI-MS(-) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\text{C}\{\text{Cu}_n(\text{OH})_n(\text{pz})_n\}_x(4\text{-Mepz})_x]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 0–10 mol% 4-MepzH..

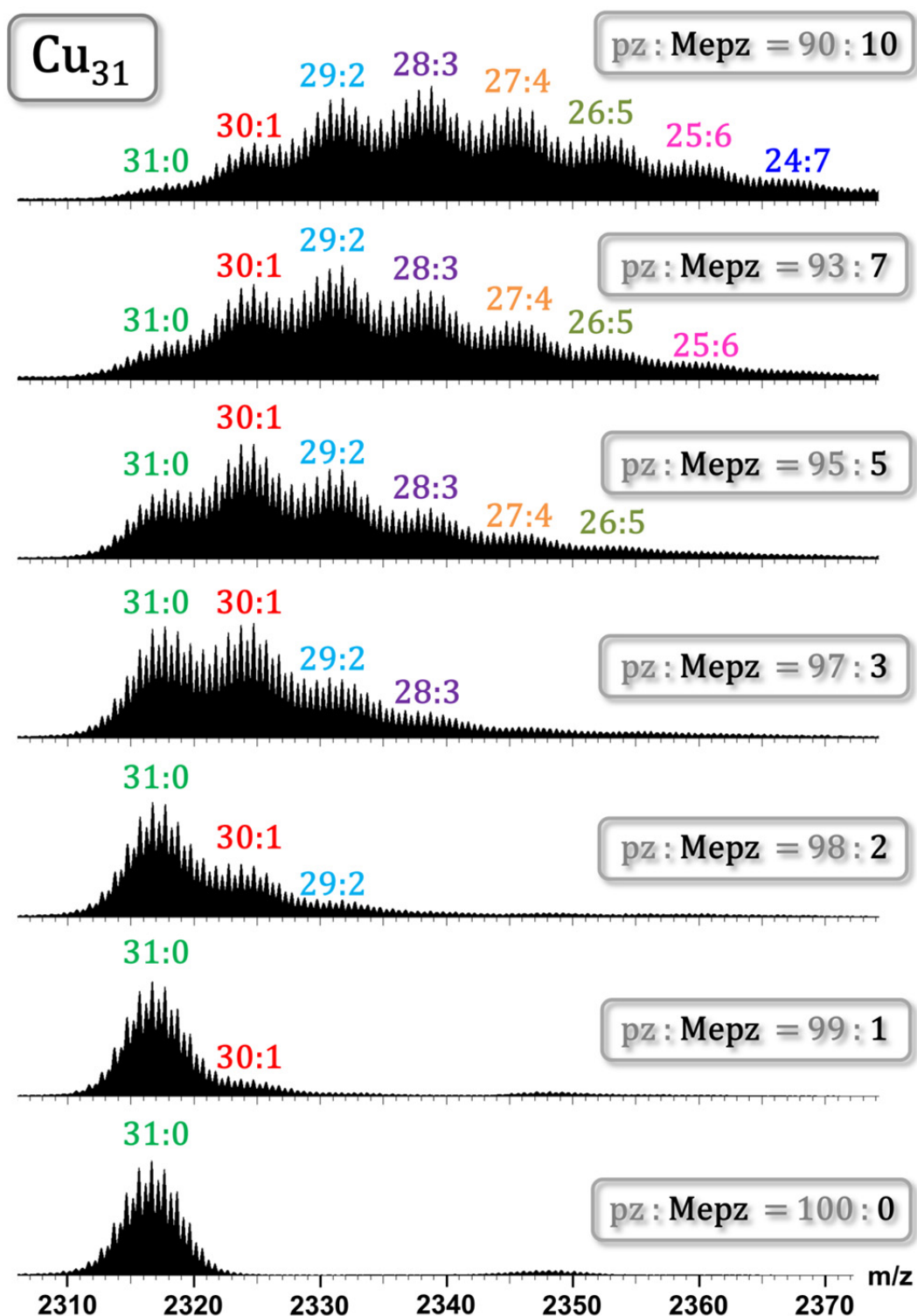


Figure S16. Zoomed portion of the ESI-MS(–) spectra of the $(\text{Bu}_4\text{N})_2[\text{CO}_3\text{--}\{\text{Cu}_n(\text{OH})_n(\text{pz})_n\}_x(4\text{-Mepz})_x]$ ($n = 27, 29, 30, 31$) nanojar mixtures obtained using 0–10 mol% 4-MepzH.

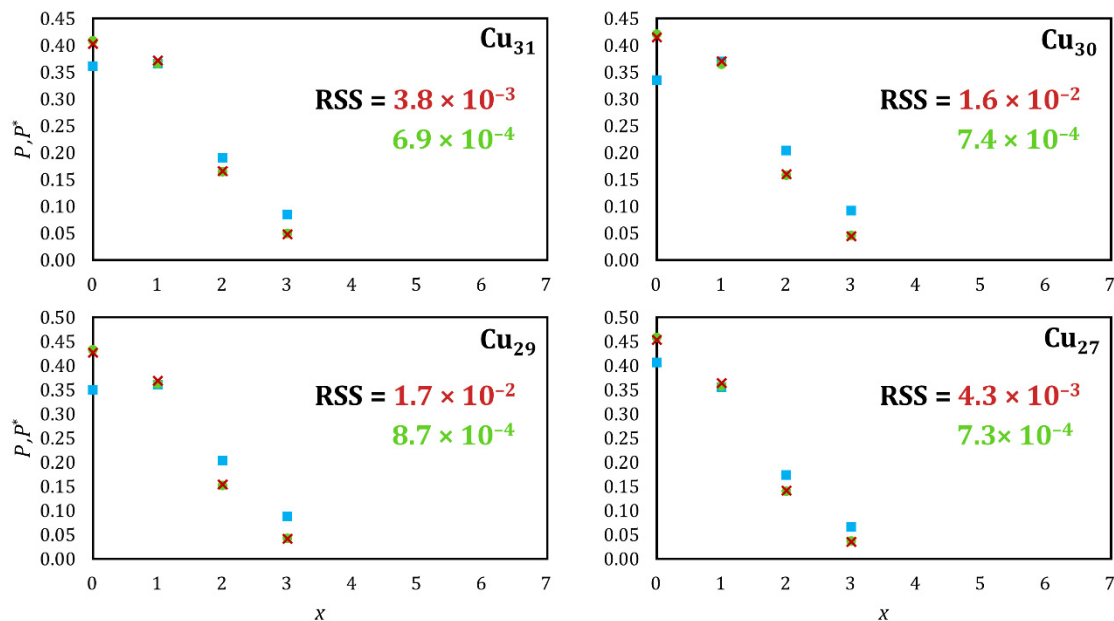


Figure S17. Plots of binomial (red), Poisson (green) and experimental (blue) distributions for different sized nanojars with 97:3 pz:4-Mepz ligand mixture.

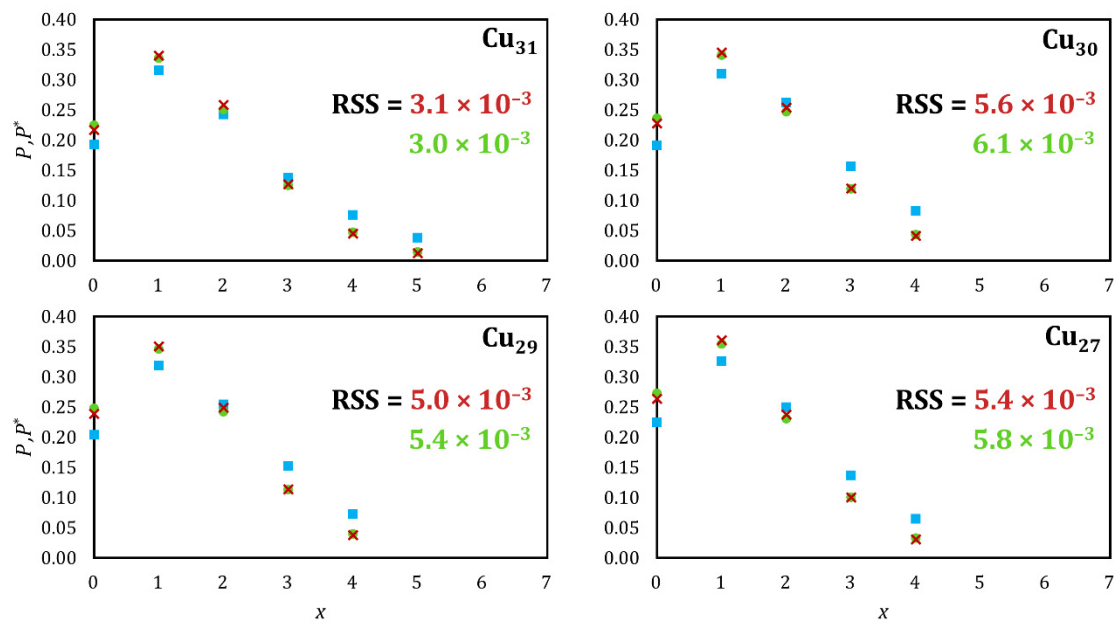


Figure S18. Plots of binomial (red), Poisson (green) and experimental (blue) distributions for different sized nanojars with 95:5 pz:4-Mepz ligand mixture.

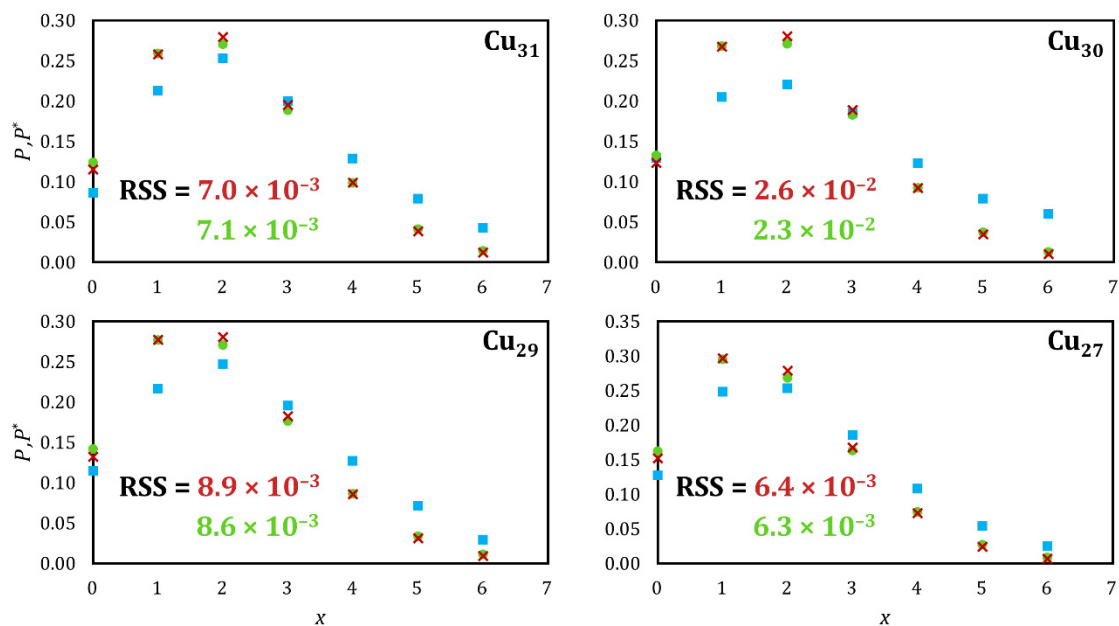


Figure S19. Plots of binomial (red), Poisson (green) and experimental (blue) distributions for different sized nanojars with 93:7 pz:4-Mepz ligand mixture.

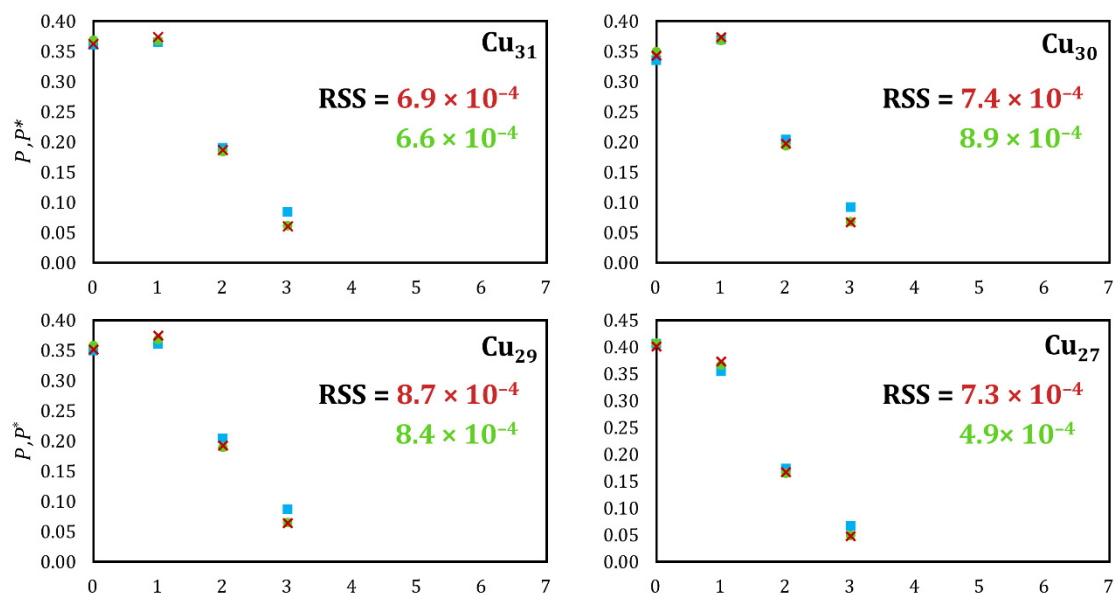


Figure S20. Plots of binomial (red), Poisson (green) and experimental (blue) distributions using j_{ad} for different sized nanojars with 97:3 pz:4-Mepz ligand mixture.

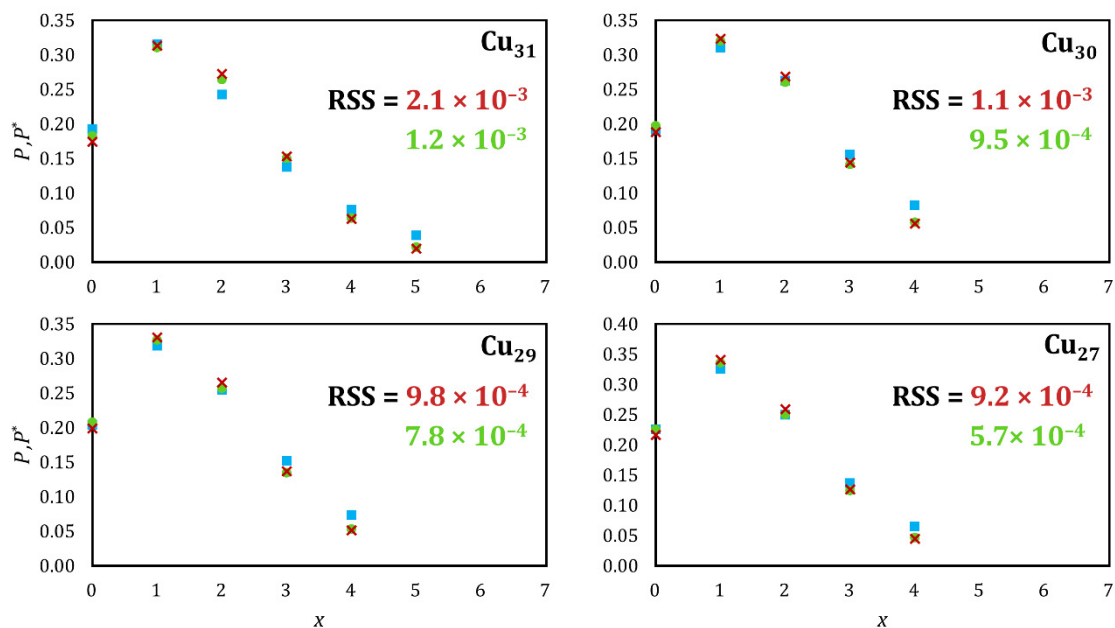


Figure S21. Plots of binomial (red), Poisson (green) and experimental (blue) distributions using j_{ad} for different sized nanojars with 95:5 pz:4-Mepz ligand mixture.

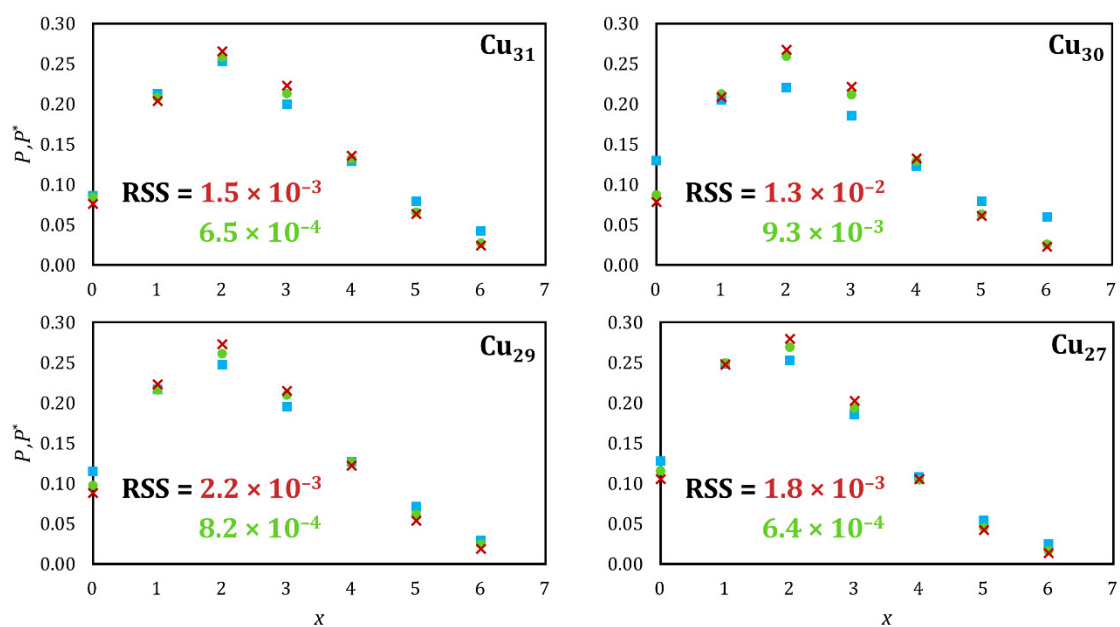


Figure S22. Plots of binomial (red), Poisson (green) and experimental (blue) distributions using j_{ad} for different sized nanojars with 93:7 pz:4-Mepz ligand mixture.