

Electronic Supplementary Information (ESI) for

**Synthesis and structure characterization of zinc and cadmium
dipeptide coordination polymers**

Andreas Puškarić*, Ivan Halasz, Matija Gredičak, Ana Palčić and Josip Bronić*

Ruder Bošković Institute (RBI), Bijenička 54, HR-10002 Zagreb, Croatia.

bronic@irb.hr

apuskar@irb.hr

Table S1. Crystallographic and Rietveld refinement parameters for Zn(GlyPhe)₂ and Cd(GlyPhe)₂

Formula	C ₂₂ H ₂₆ N ₄ O ₆ Zn	C ₂₂ H ₂₆ N ₄ O ₆ Cd
Formula weight [g mol ⁻¹]	507.86	554.87
Space group	C2	C2
<i>a</i> [Å]	29.4247(2)	30.4985(2)
<i>b</i> [Å]	5.29675(3)	5.34094(4)
<i>c</i> [Å]	7.49392(4)	7.63724(4)
β [°]	95.5986(3)	111.3718(3)
<i>V</i> [Å ³]	1162.4(2)	1158.49(1)
<i>Z</i>	2	2
Calculated density [g cm ⁻³]	1.45	1.55
Temperature [K]	293	293
Wavelength [Å]	1.54060	1.54060
Step size [°2θ]	0.02	0.02
Starting angle [°2θ]	5	5
Final angle [°2θ]	80	80
<i>R</i> _p [%]	7.64	6.46
<i>R</i> _{wp} [%]	10.76	8.68
<i>Gof</i> [%]	3.55	4.56
<i>R</i> (<i>F</i> ²) [%]	3.03	1.90
Number of variables	49	42

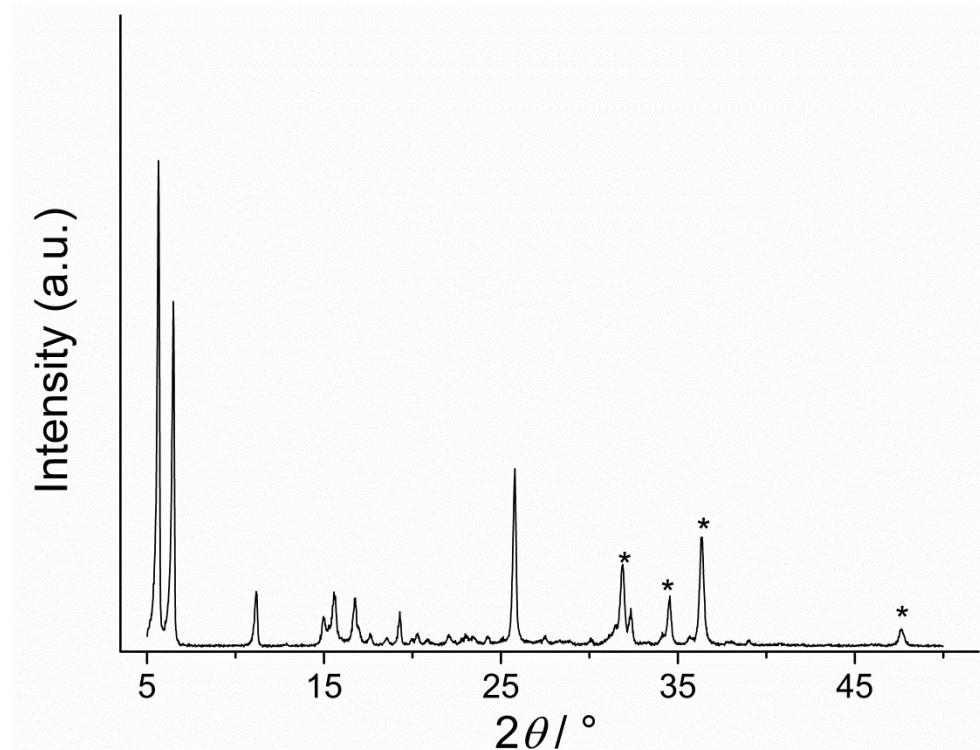


Figure S1 Powder diffraction pattern for system with molar ratio Zn²⁺:dipeptide:NaOH = 1:2:2, temperature 120 °C. Asterisks denote postions of ZnO peaks.

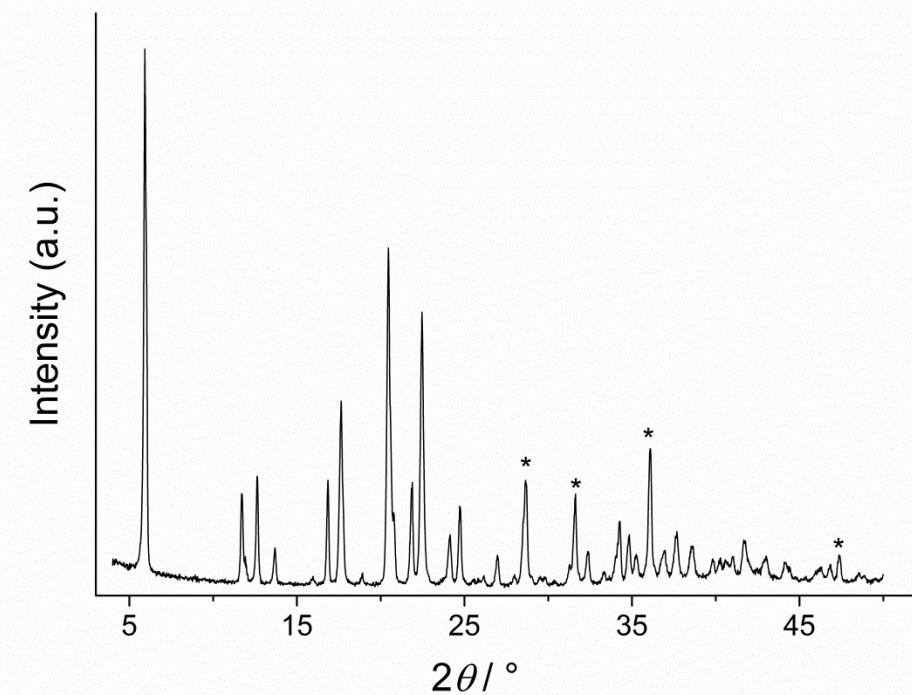


Figure S2. X-ray powder diffraction pattern for reaction system with molar ratio Zn^{2+} :dipeptide:NaOH = 1:2:2.5, temperature 85 °C. Peak positions of ZnO are denoted by asterisks.

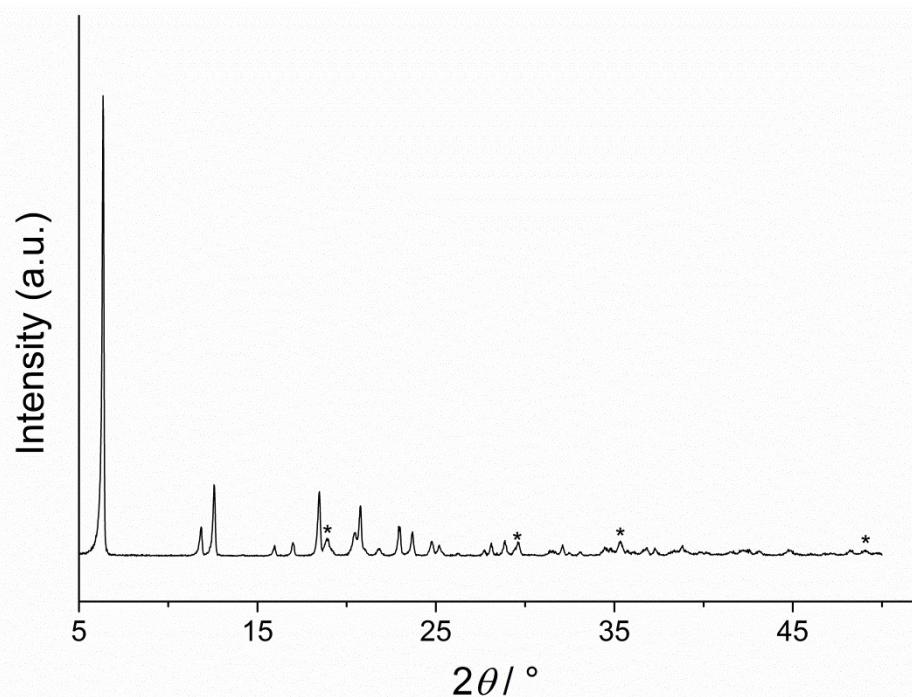


Figure S3. X-ray powder diffraction pattern of sample with molar ratio Cd^{2+} :dipeptide:NaOH = 1:2:2.5, temperature 85 °C. Peak positions of Cd(OH)₂ are denoted by asterisks.

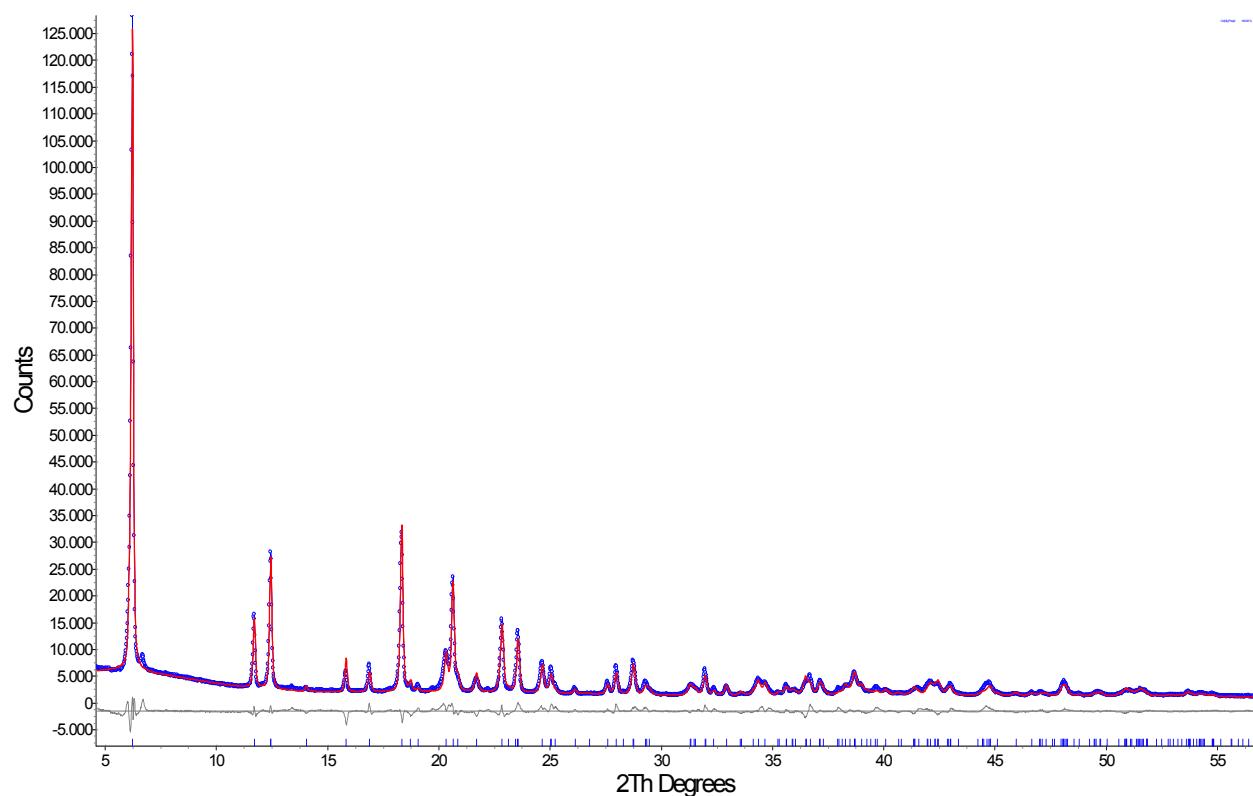


Figure S4. Rietveld refinement plot of $\text{Cd}(\text{Gly-L-Phe})_2$ to $2\theta = 50^\circ$. Experimental data are shown by blue circles, calculated values by red line, and the difference by grey line profile. Blue tick marks at bottom indicate reflection positions.

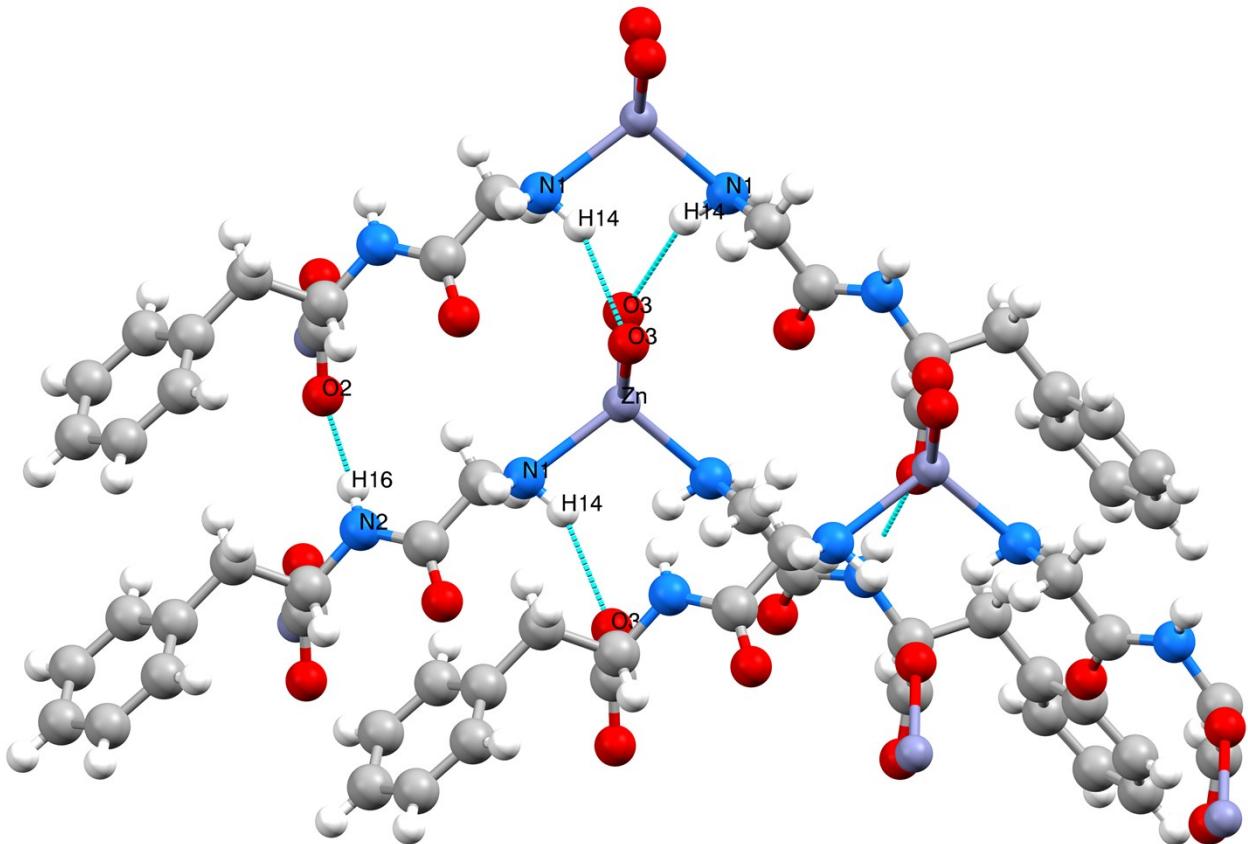


Figure S5. Characteristic hydrogen bonds in $\text{Zn}(\text{Gly-L-Phe})_2$. Some atoms are omitted for clarity. Color notation: white - H, red - O, purple - Zn, blue - N, grey - C.

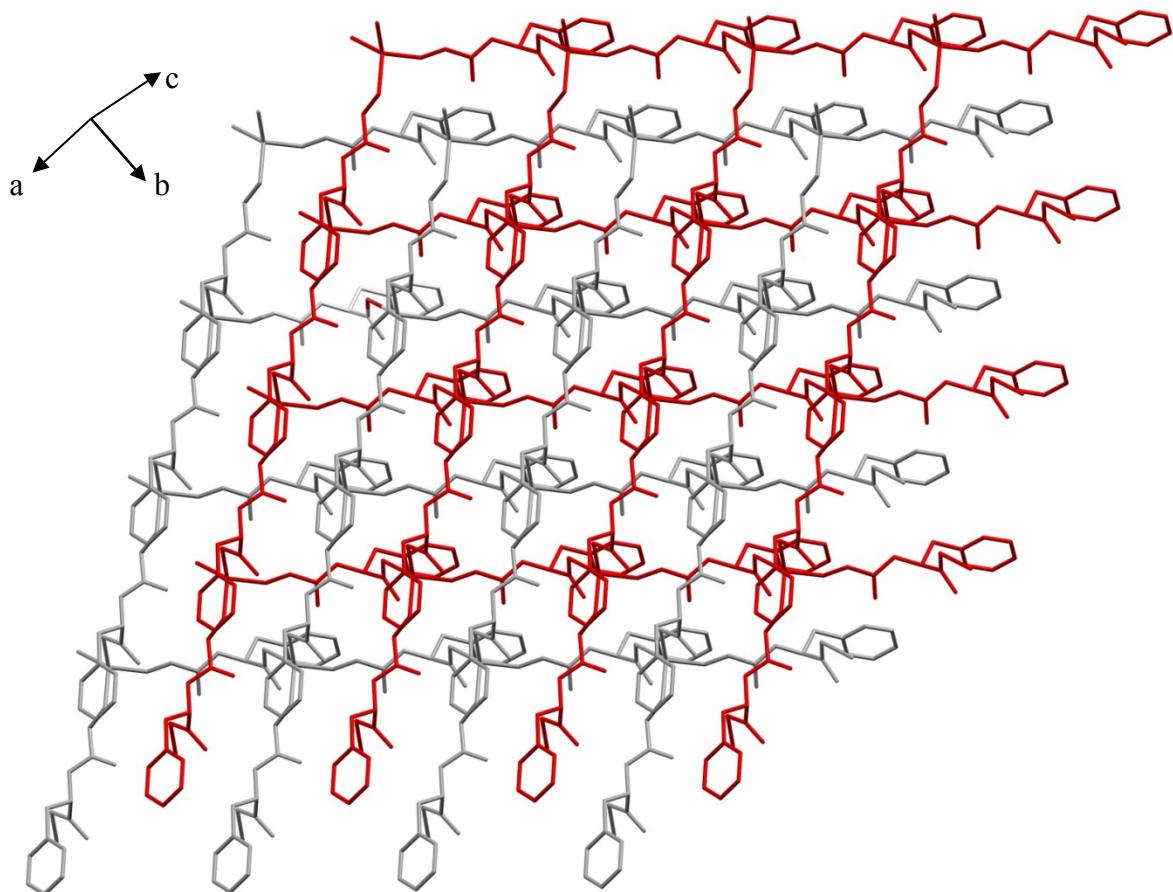


Figure S6. Interpenetrated network of $\text{Zn}(\text{Gly-L-Phe})_2$.

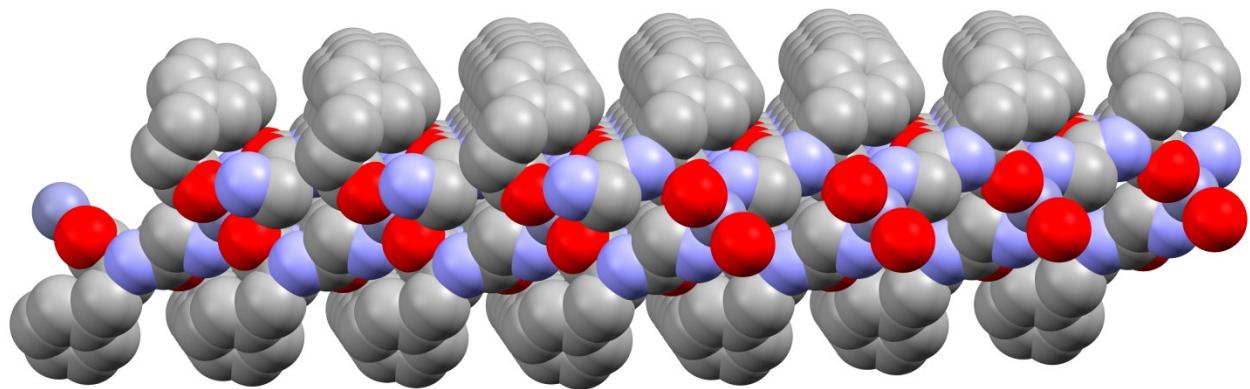


Figure S7. Spacefill representation of layered structure of $\text{Zn}(\text{GlyPhe})_2$ emphasizing position and orientation of phenyl rings. View down crystallographic axis b with slight offset.

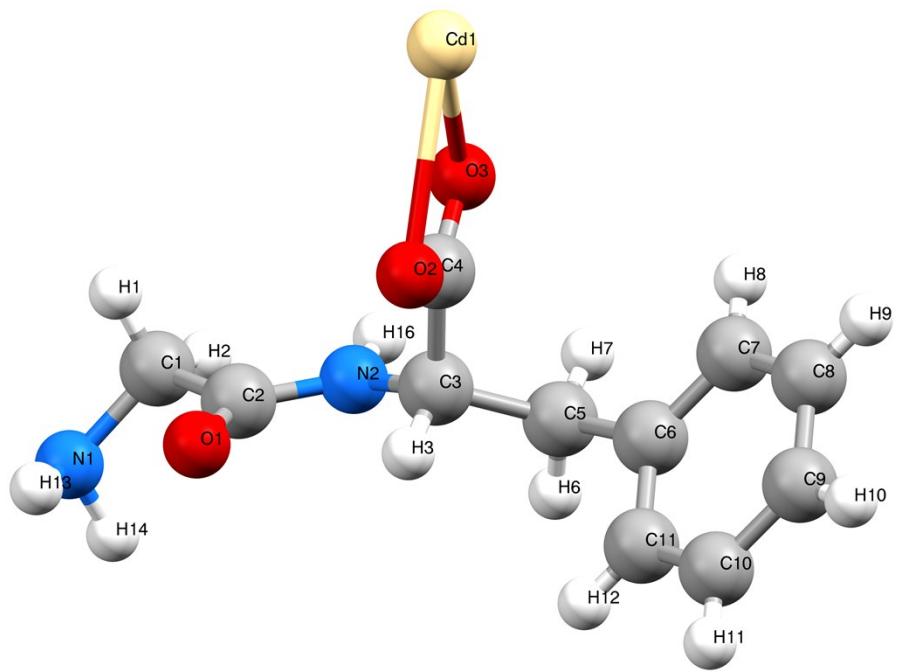


Figure S8. Asymmetric unit of $\text{Cd}(\text{Gly-L-Phe})_2$. Color notation: white - H, red - O, gold - Cd, blue - N, grey - C.