**Supporting Information**

# Model peptides based on the binding loop of the copper metallochaperone Atx1: selectivity of the consensus sequence MxCxxC for metal ions Hg(II), Cu(I), Cd(II), Pb(II) and Zn(II).

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**NMR data for $P^L$.**

**$P^L$**

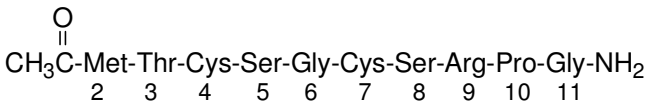


**Table S1.** $^1$H NMR (500 MHz) chemical shifts (δ ppm) for $P^L$ in $H_2O/D_2O$ 9:1 at 298 K

| Residue | HN | Hα | Hβ | others |
|---|---|---|---|---|
| Met 2 | 8.05 | 4.50 | 1.91,2.05 | $CH_2$(γ) 2.42, 2.50 $CH_3$(ε) 1.90 |
| Thr 3 | 8.21 | 4.30 | 4.15 | $CH_3$(γ)1.12 |
| Cys 4 | 8.28 | 4.42 | 2.82 | |
| Ser 5 | 8.38 | 4.42 | 3.80 | |
| Gly 6 | 8.15 | 3.82 | | |
| Cys 7 | 8.40 | 4.52 | 2.90 | |
| Ser 8 | 8.42 | 4.40 | 3.78 | |
| Arg 9 | 8.15 | 4.6 | 1.65, 1.75 | $CH_2$(γ) 1.60, $CH_2$(δ)3.31 HN(ε)7.12 |
| Pro 10 | - | 4.30 | 1.82, 2.20 | $CH_2$(γ) 1.92 , 2.10 |
| | | | | $CH_2$ (δ) 3.52, 3.70 |
| Gly 11 | 8.50 | 3.90 | | |

**Table S2.** $^3J_{HN, H\alpha}$ coupling constants (Hz) for $P^L$ in $H_2O/D_2O$ 9:1 at 298 K

| Met 2 | Thr 3 | Cys 4 | Ser 5 | Cys 7 | Ser 8 | Arg 9 |
|---|---|---|---|---|---|---|
| 7.2 | 8.0 | 7.2 | 7.2 | 7 | 6.5 | 7.2 |

**NMR data for $P^{C}_{SS}$.**

**Table S3.** $^{1}$H NMR (500 MHz) chemical shifts (δ ppm) for $P^{C}_{SS}$ in $H_2O/D_2O$ 9:1 at 298 K.

| Residue | HN | Hα | Hβ | Others |
|---|---|---|---|---|
| Gly 1 | 8.65 | 3.63, 4.09 | | |
| Met 2 | 7.75 | 4.63 | 1.96, 2.11 | $CH_2(\gamma)$: 2.36, 2.46; $CH_3(\varepsilon)$: 2.06 |
| Thr 3 | 8.55 | 4.49 | 4.28 | $CH_3(\gamma)$: 1.16 |
| Cys 4 | 7.81 | 4.62 | 3.32 | |
| Ser 5 | 8.87 | 4.29 | 3.80 | |
| Gly 6 | 9.03 | 3.73, 3.98 | | |
| Cys 7 | 7.72 | 4.38 | 3.20, 3.27 | |
| Ser 8 | 8.62 | 4.43 | 3.70, 3.84 | |
| Arg 9 | 7.59 | 4.60 | 1.65, 1.76 | $CH_2(\gamma)$: 1.56, 1.65; $CH_2(\delta)$: 3.14; HN(ε): 7.10 |
| Pro 10 | - | 4.27 | 2.23 (*pro-S*), 1.82 (*pro-R*) | $CH_2(\gamma)$: 1.94 (*pro-R*), 2.02 (*pro-S*); $CH_2(\delta)$: 3.54(*pro-S*), 3.84 (*pro-R*) |

**Table S4.** $^{3}J_{HN,H\alpha}$ coupling constants (Hz) for $P^{C}_{SS}$ in $H_2O/D_2O$ 9:1 at 298 K.

| Met 2 | Thr 3 | Cys 4 | Ser 5 | Cys 7 | Ser 8 | Arg 9 |
|---|---|---|---|---|---|---|
| 8.2 | 9.2 | 5.9 | 4.5 | 6.9 | 8.5 | 7.2 |

**Table S5** ROESY-derived distances (Å) and distances calculated using X-PLOR for $\mathbf{P^{C}_{SS}}$ in $H_2O/D_2O$ 9:1 at 298 K. $d(H1,H2)_{min}$ and $d(H1,H2)_{max}$ are the lower and upper distance limits used for X-PLOR calculations.

| H1 | H2 | $d$(H1,H2) | $d(H1,H2)_{min}$ | $d(H1,H2)_{max}$ |
|---|---|---|---|---|
| GLY 1 HN | MET 2 HN | 2.71 | 2.44 | 2.98 |
| GLY 1 HN | PRO 10 HA | 2.08 | 1.87 | 2.29 |
| GLY 1 HN | GLY 1 HA1 | 2.81 | 2.53 | 3.09 |
| GLY 1 HN | GLY 1 HA2 | 2.29 | 2.06 | 2.52 |
| GLY 1 HN | PRO 10 HB1 | 3.63 | 3.27 | 3.99 |
| GLY 1 HN | PRO 10 HB2 | 3.53 | 3.18 | 3.88 |
| MET 2 HN | THR 3 HN | 3.42 | 3.08 | 3.76 |
| MET 2 HN | PRO 10 HA | 3.48 | 3.13 | 3.83 |

| | | | | |
|---|---|---|---|---|
| MET 2 HN | GLY 1 HA1 | 2.91 | 2.62 | 3.20 |
| MET 2 HN | GLY 1 HA2 | 3.14 | 2.83 | 3.46 |
| MET 2 HN | MET 2 HG* | 2.91 | 2.62 | 3.90 |
| MET 2 HN | MET 2 HB* | 2.69 | 2.42 | 3.66 |
| THR 3 HN | CYS 4 HN | 2.53 | 2.27 | 2.78 |
| THR 3 HN | MET 2 HA | 2.19 | 1.97 | 2.41 |
| THR 3 HN | THR 3 HB | 2.84 | 2.56 | 3.12 |
| THR 3 HN | CYS 4 HB* | 4.73 | 4.26 | 5.91 |
| THR 3 HN | THR 3 HG2* | 3.40 | 3.06 | 4.14 |
| THR 3 HN | MET 2 HB* | 3.16 | 2.85 | 4.18 |
| THR 3 HN | MET 2 HG* | 3.98 | 3.58 | 5.08 |
| THR 3 HA | THR 3 HB | 3.08 | 2.77 | 3.38 |
| THR 3 HA | THR 3 HG2* | 2.88 | 2.59 | 3.56 |
| THR 3 HB | THR 3 HG2* | 2.45 | 2.20 | 3.09 |
| CYS 4 HN | SER 5 HN | 3.85 | 3.46 | 4.23 |
| CYS 4 HN | CYS 4 HA | 2.69 | 2.42 | 2.96 |
| CYS 4 HN | THR 3 HA | 2.46 | 2.22 | 2.71 |
| CYS 4 HN | THR 3 HB | 3.66 | 3.29 | 4.02 |
| CYS 4 HN | CYS 4 HB* | 2.99 | 2.69 | 3.99 |
| CYS 4 HN | CYS 7 HB* | 3.01 | 2.71 | 4.01 |
| CYS 4 HN | MET 2 HB* | 3.24 | 2.92 | 4.27 |
| CYS 4 HN | THR 3 HG2* | 4.41 | 3.97 | 5.25 |
| CYS 4 HA | CYS 4 HB* | 2.33 | 2.09 | 3.26 |
| SER 5 HN | CYS 4 HA | 2.18 | 1.96 | 2.40 |
| SER 5 HN | SER 5 HA | 2.70 | 2.43 | 2.97 |
| SER 5 HN | SER 5 HB* | 2.54 | 2.28 | 3.49 |
| SER 5 HN | CYS 4 HB* | 2.59 | 2.33 | 3.55 |
| SER 5 HA | SER 5 HB* | 2.37 | 2.13 | 3.30 |
| GLY 6 HN | CYS 7 HN | 2.59 | 2.33 | 2.85 |
| GLY 6 HN | SER 5 HA | 2.13 | 1.91 | 2.34 |
| GLY 6 HN | GLY 6 HA* | 2.46 | 2.22 | 3.41 |
| GLY 6 HN | SER 5 HB* | 3.93 | 3.54 | 5.02 |
| CYS 7 HN | SER 5 HA | 3.38 | 3.04 | 3.71 |
| CYS 7 HN | CYS 7 HA | 2.81 | 2.53 | 3.09 |
| CYS 7 HN | GLY 6 HA* | 3.19 | 2.87 | 4.21 |
| CYS 7 HN | CYS 7 HB* | 2.58 | 2.32 | 3.54 |
| CYS 7 HA | CYS 7 HB* | 2.66 | 2.39 | 3.62 |
| SER 8 HN | ARG 9 HN | 2.42 | 2.18 | 2.66 |
| SER 8 HN | SER 8 HA | 2.51 | 2.26 | 2.76 |
| SER 8 HN | CYS 7 HA | 2.21 | 1.99 | 2.43 |
| SER 8 HN | SER 8 HB* | 2.85 | 2.57 | 3.84 |
| SER 8 HN | CYS 7 HB* | 3.21 | 2.89 | 4.23 |
| SER 8 HA | SER 8 HB* | 2.41 | 2.17 | 3.35 |
| ARG 9 HN | ARG 9 HA | 2.70 | 2.43 | 2.97 |
| ARG 9 HN | SER 8 HA | 2.88 | 2.59 | 3.17 |
| ARG 9 HN | SER 8 HB* | 3.77 | 3.40 | 4.85 |
| ARG 9 HN | CYS 7 HB* | 3.46 | 3.12 | 3.81 |
| ARG 9 HA | PRO 10 HD1 | 2.09 | 1.88 | 2.30 |
| ARG 9 HA | PRO 10 HD2 | 2.49 | 2.24 | 2.74 |

**Figure S1.** Calibration curve and experimental results for the determination of molecular weights of the peptides by size exclusion chromatography in aqueous buffer at pH 7.

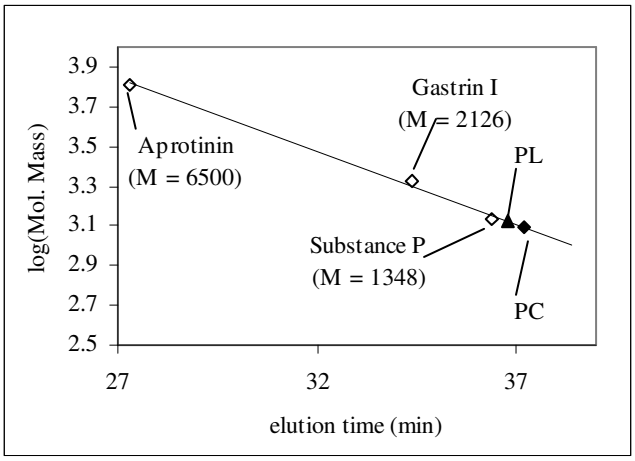


**Figure S2.** UV titration of $P^L$ (54 μM) with mercury chloride at pH 7 (20 mM phosphate buffer). Spectra shown are difference spectra ($\Delta\varepsilon = \varepsilon HgP^L - \varepsilon P^L$) and correspond to samples with 0-1.3 equiv of Hg (II) per $P^L$. The insert shows the Δε at 220 and 250 nm *vs* equiv of Hg(II) per $P^L$.

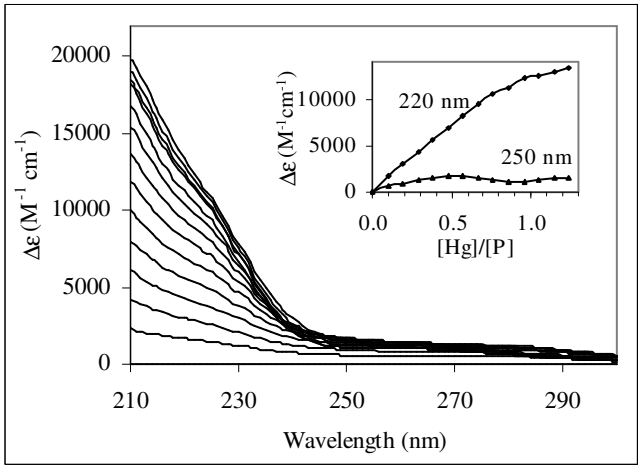

**Figure S3.** UV titration of $P^L$ (54 μM) with cadmium chloride at pH 7 (20 mM phosphate buffer). Spectra shown are difference spectra ($\Delta\varepsilon = \varepsilon CdP^L - \varepsilon P^L$) and correspond to samples with 0-1.4 equiv of Cd (II) per $P^L$. The insert shows the absorbance at 225 and 240 nm *vs* equiv of Cd(II) per $P^L$.