

SUPPLEMENTARY MATERIALS

The role of the unbinding cycle on the coordination abilities of the bi-cyclopeptides toward Cu(II) ions

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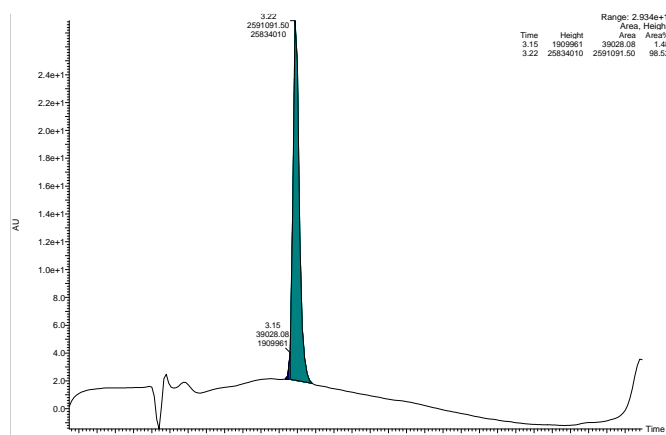


Figure S1: RP-UHPLC trace of **LNL** registered on Thermo Scientific Ultimate 3000 with a diode array detector coupled with a Thermo Scientific MSQ PLUS ESI mass spectrometer. R_t 3.22: LNL. RP-UHPLC-ESI-MS: C18 column Waters Acquity CSH™ (130 Å, 1.7 µm, 2.1 × 100 mm); temperature 45 °C; flow: 0.5 mL/min; eluent: 0.1% (v/v) TFA in H₂O (A) and 0.1% (v/v) TFA in CH₃CN (B), λ 215 nm, gradient: 25–60% B in 5 min.

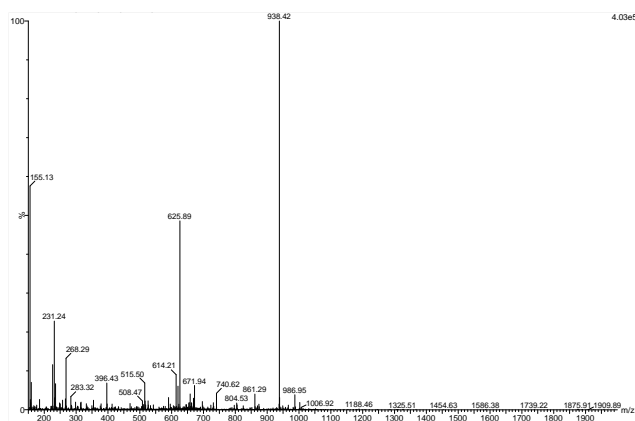


Figure S2: ESI-MS spectrum of **LNL** registered on a Thermo Scientific MSQ PLUS ESI mass spectrometer. ESI-MS (m/z): $[M+2H]^{2+}$ calcd. 938.12; $[M+2H]^{2+}$ found 938.42.

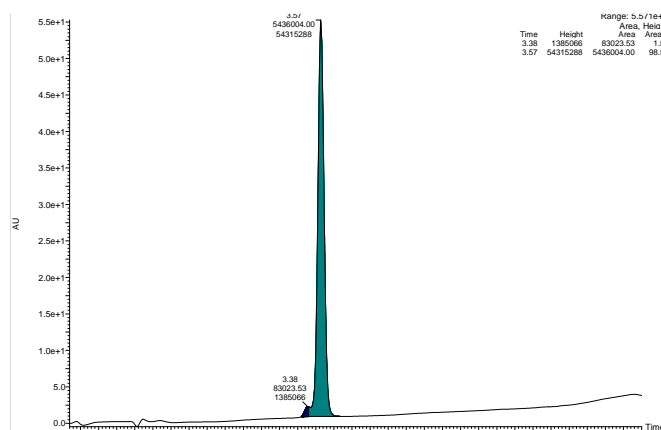


Figure S3: RP-UHPLC trace of **MCL2** registered on Thermo Scientific Ultimate 3000 with a diode array detector coupled with a Thermo Scientific MSQ PLUS ESI mass spectrometer. R_t 3.57: MCL2. RP-UHPLC-ESI-MS: C18 column Waters Acquity CSH™ (130 Å, 1.7 µm, 2.1 × 100 mm); temperature 45 °C; flow: 0.5 mL/min; eluent: 0.1% (v/v) TFA in H₂O (A) and 0.1% (v/v) TFA in CH₃CN (B), λ 215 nm, gradient: 25–60% B in 5 min.

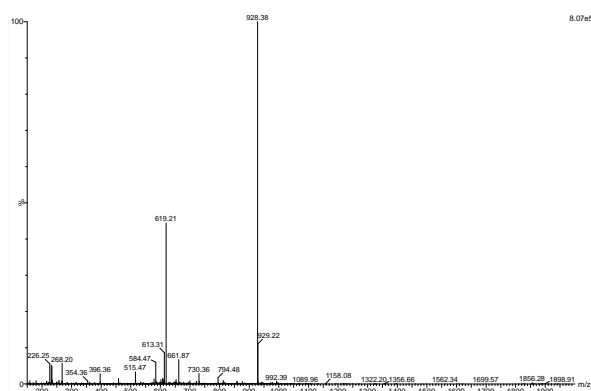


Figure S4: ESI-MS spectrum of **MCL2** registered on a Thermo Scientific MSQ PLUS ESI mass spectrometer. ESI-MS (m/z): $[M+2H]^{2+}$ calcd. 928.14; $[M+2H]^{2+}$ found 928.38.

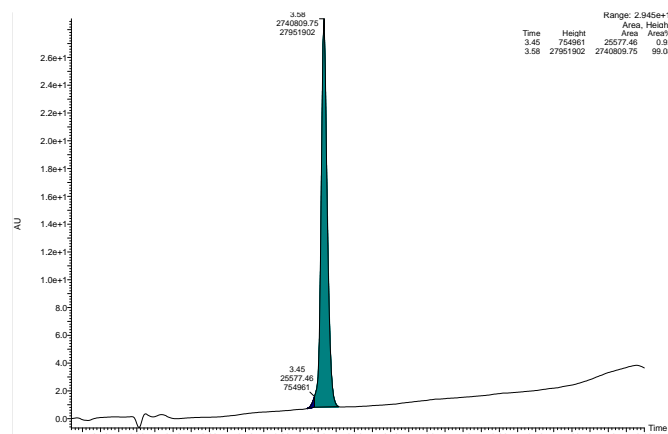


Figure S5: RP-UHPLC trace of **MCL3** registered on Thermo Scientific Ultimate 3000 with a diode array detector coupled with a Thermo Scientific MSQ PLUS ESI mass spectrometer. R_t 3.58: MCL3. RP-UHPLC-ESI-MS: C18 column Waters Acquity CSH™ (130 Å, 1.7 µm, 2.1 × 100 mm); temperature 45 °C; flow: 0.5 mL/min; eluent: 0.1% (v/v) TFA in H₂O (A) and 0.1% (v/v) TFA in CH₃CN (B), λ 215 nm, gradient: 25–60% B in 5min.

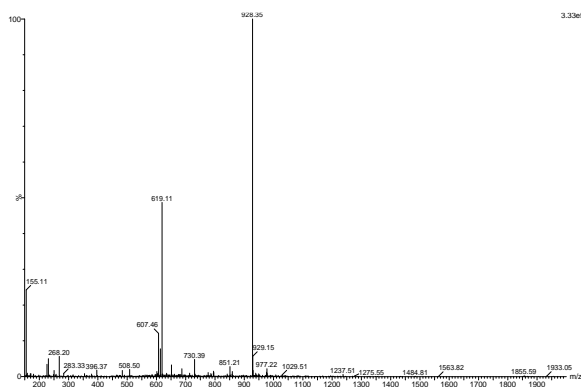


Figure S6: ESI-MS spectrum of **MCL3** registered on a Thermo Scientific MSQ PLUS ESI mass spectrometer. ESI-MS (m/z): [M+2H]²⁺ calcd. 928.14; [M+2H]²⁺ found 928.35.