Supplementary Information for:

**Metal Induced Folding: Synthesis and Conformational Analysis of the Lanthanide Complexes of two 44-membered Hydrazone Macrocycles†**

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1. X-ray Crystallography

Fig. 1 Solid state structure of unbound ligand 1. a) tilted view; b) top view; c) side view; d) orientation of hydrazone bonds; e) important hydrogen bonds.

Fig. 2 Solid state structure of Eu²⁺ complex with CN nine. a) tilted view; b) side view.
Fig. 3 Solid state structure of Europium complex with CN ten. a) side view; b) top view; c) arrangement of N₃O₂ binding motif; d) important hydrogen bonds.
2. HRMS (High Resolution Mass Spectrometry)

Fig. 4 (-)ESI-HRMS of a) \([\text{La}^3+]\); b) \([\text{Dy}^3+]\); c) \([\text{Eu}^3+]\); d) \([2\text{La}^3+]\); e) \([2\text{Dy}^3+]\); f) \([2\text{Eu}^3+]\). All spectra were recorded in CDCl₃/MeOD (1:1).
3. UV-Vis Spectroscopy

**Fig. 5** UV-Vis spectra (left) and binding isotherms (right, ΔA_{320nm}) of titrations of 1 with a) La^{3+}, b) Eu^{3+}, c) Dy^{3+}. Increasing and decreasing bands are indicated by arrows. Binding isotherms are obtained by plotting the change in absorption at 320 nm against the guest concentration (dots) and fitting it with a model (line).
Fig. 6 UV-Vis spectra (left) and binding isotherms (right, ΔA_{320nm}) of titrations of 2 with a) La^{3+}, b) Eu^{3+}, c) Dy^{3+}. Increasing and decreasing bands are indicated by arrows. Binding isotherms are obtained by plotting the change in absorption at 320 nm against the guest concentration (dots) and fitting it with a model (line).
3. NMR

Fig. 7 NMR spectra (500 MHz, 295 K, CDCl₃/MeOD, 1:1) of 1 and its La³⁺ complex (1 mM).
Fig. 8: NOESY spectra of 1[La\textsuperscript{3+}] (1 mM in CDCl\textsubscript{3}/MeOD, 1:1, 298 K, 500 MHz, mixing time = 800 ms). The cross-peaks are indicated by dotted lines with corresponding colours in the NOESY spectrum and the structure below.
Fig. 9: NOESY spectra of 2[La³⁺] (1 mM in CDCl₃/MeOD, 1:1, 298 K, 500 MHz, mixing time = 800 ms). The cross-peaks are indicated by dotted lines with corresponding colours in the NOESY spectrum and the structure below.