Lanthanide contraction for helicity fine-tuning and helix-winding control of single-helical metal complexes

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Supporting Information

Spectroscopic measurements. UV-Vis spectra were measured on a JASCO V-660 spectrophotometer in a quartz cell with an optical path length of 1.0 mm. Circular dichroic spectra (CD) were measured on a JASCO J-720 spectrophotometer in a quartz cell with an optical path length of 1.0 mm. Mass spectra (ESI-TOF, positive mode) were recorded on an Applied Biosystems QStar Pulsar *i* spectrometer. ^{1}H NMR spectra were recorded on a Bruker AVANCE600 spectrometer at 600 MHz. In NMR measurements, tetrametylsilane was used as an internal standard (0 ppm).

UV-vis absorption and CD spectra of helical complexes

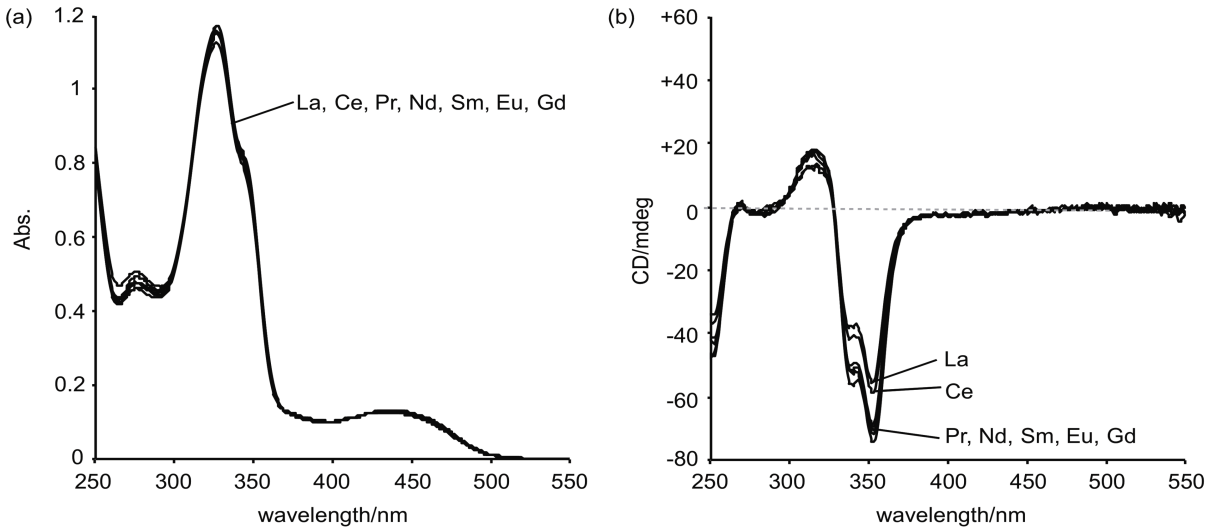

Figure S1. (a) UV-vis and (b) CD spectra (0.20 mM, chloroform/methanol, 1:1) of H_6L in the presence of zinc(II) acetate (3 equiv) and $Ln(OAc)_3$ (1 equiv, Ln = La, Ce, Pr, Nd, Sm, Eu, and Gd).

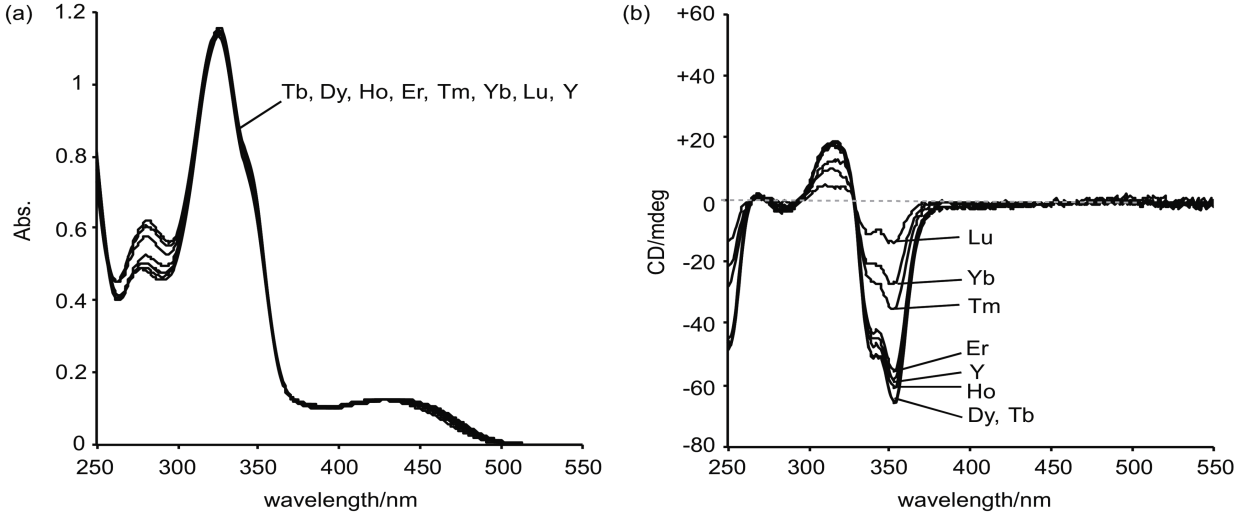

Figure S2. (a) UV-vis and (b) CD spectra (0.20 mM, chloroform/methanol, 1:1) of H_6L in the presence of zinc(II) acetate (3 equiv) and $Ln(OAc)_3$ (1 equiv, Ln = Tb, Dy, Ho, Er, Tm, Yb, Lu, and Y).

ESI mass spectra of H_6L in the presence of zinc(II) and metal ions

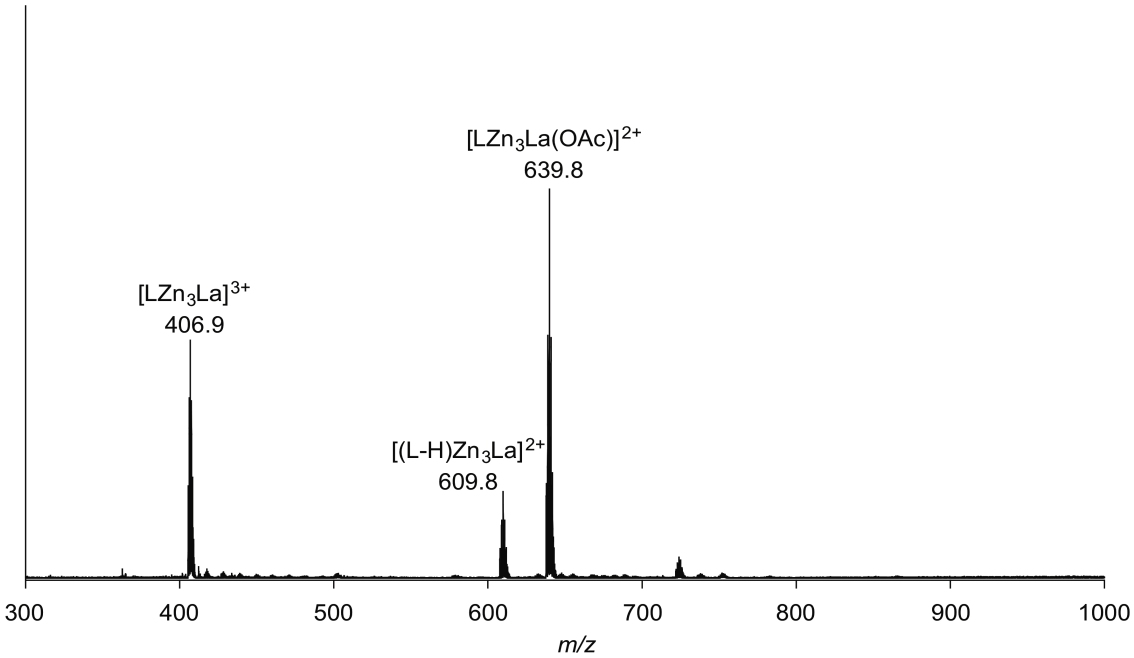

Figure S3. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $La(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

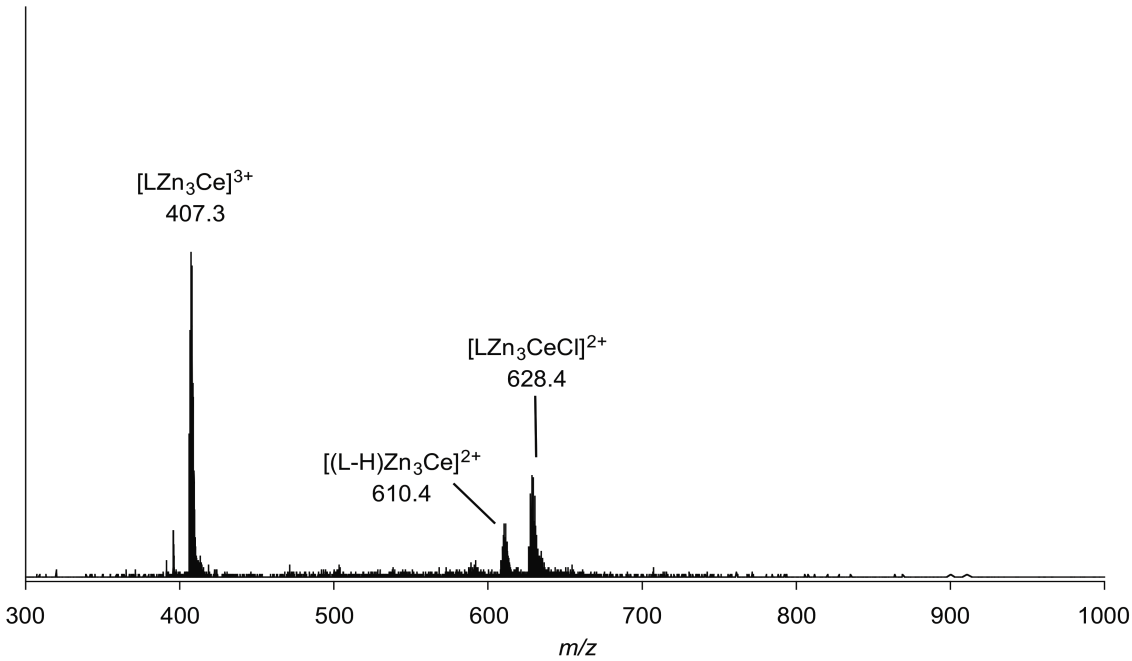

Figure S4. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Ce(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

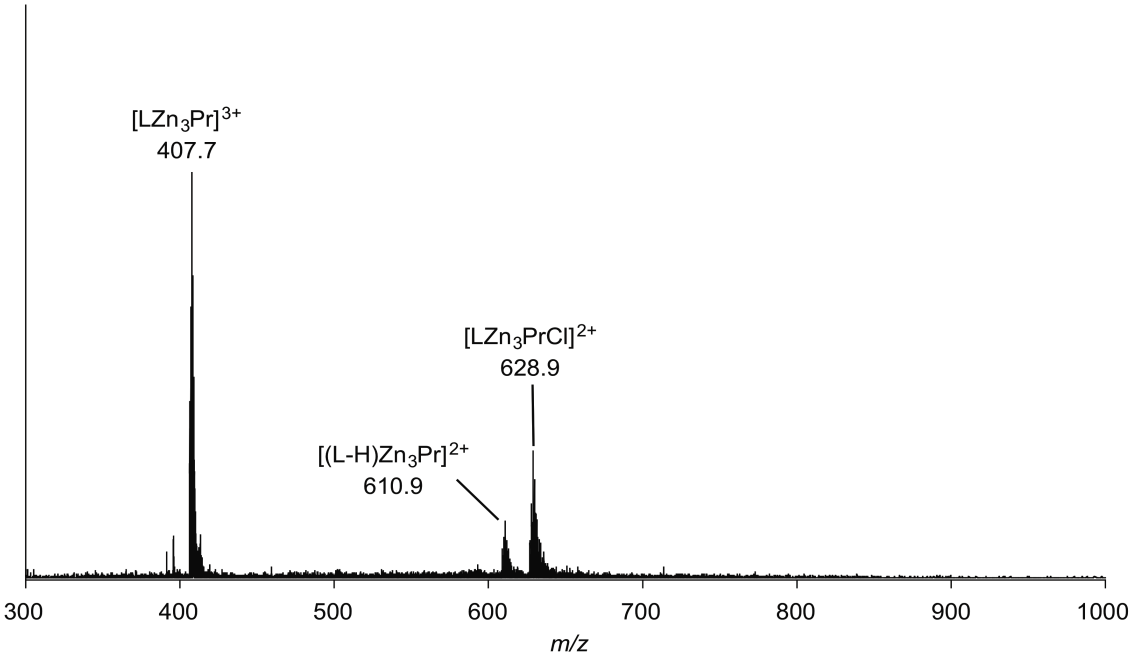

Figure S5. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Pr(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

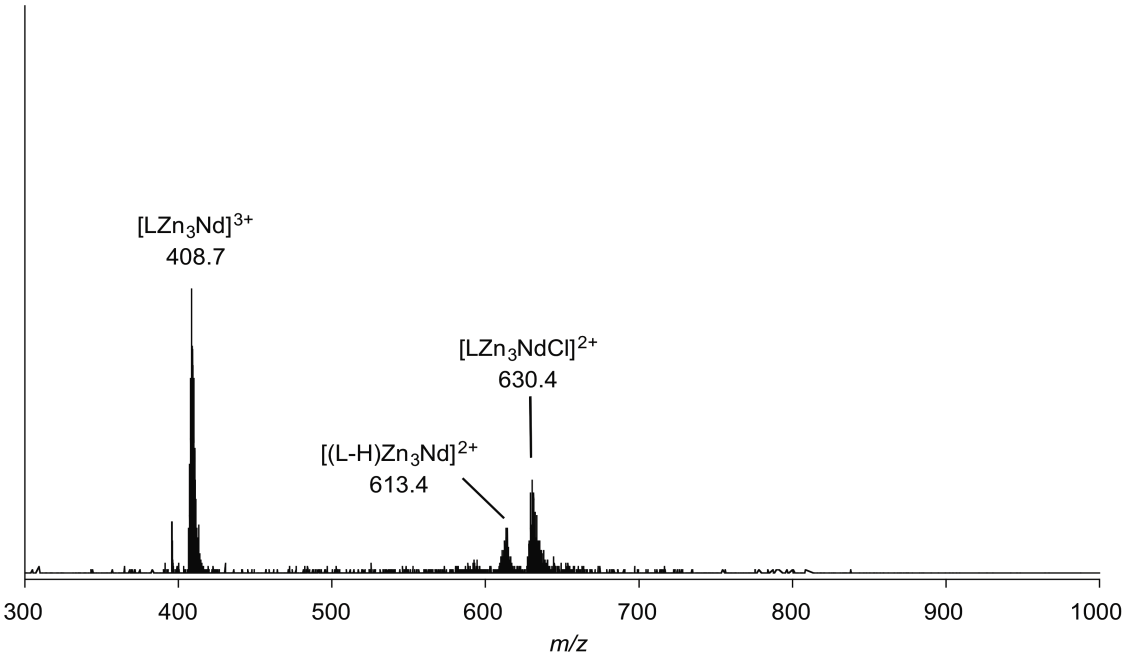

Figure S6. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Nd(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

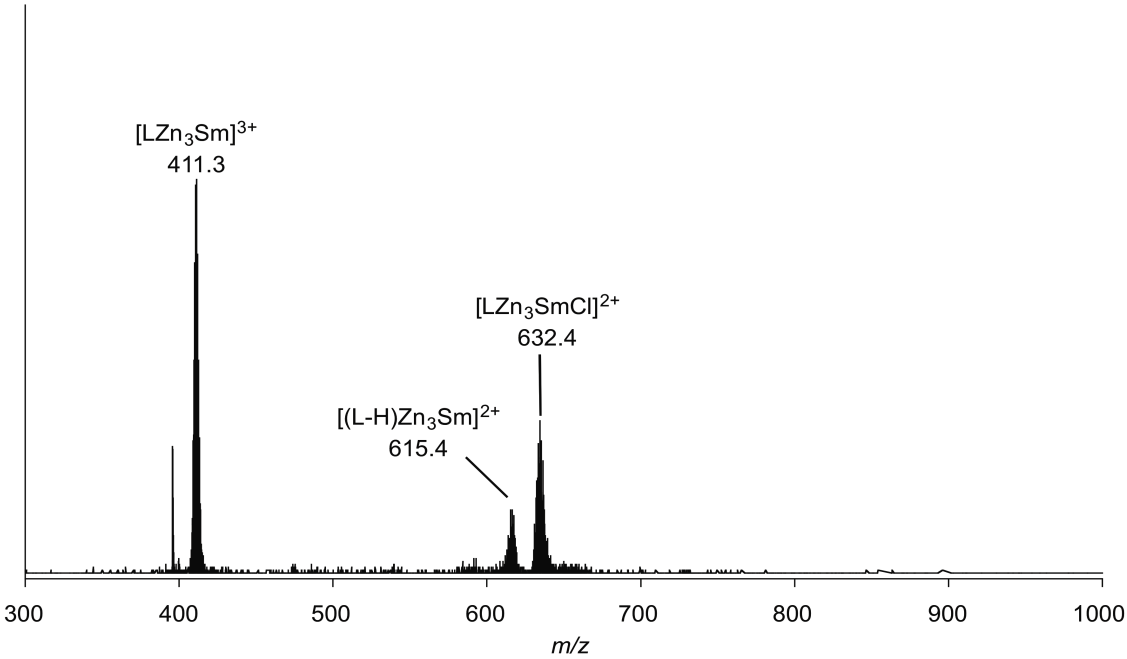

Figure S7. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Sm(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

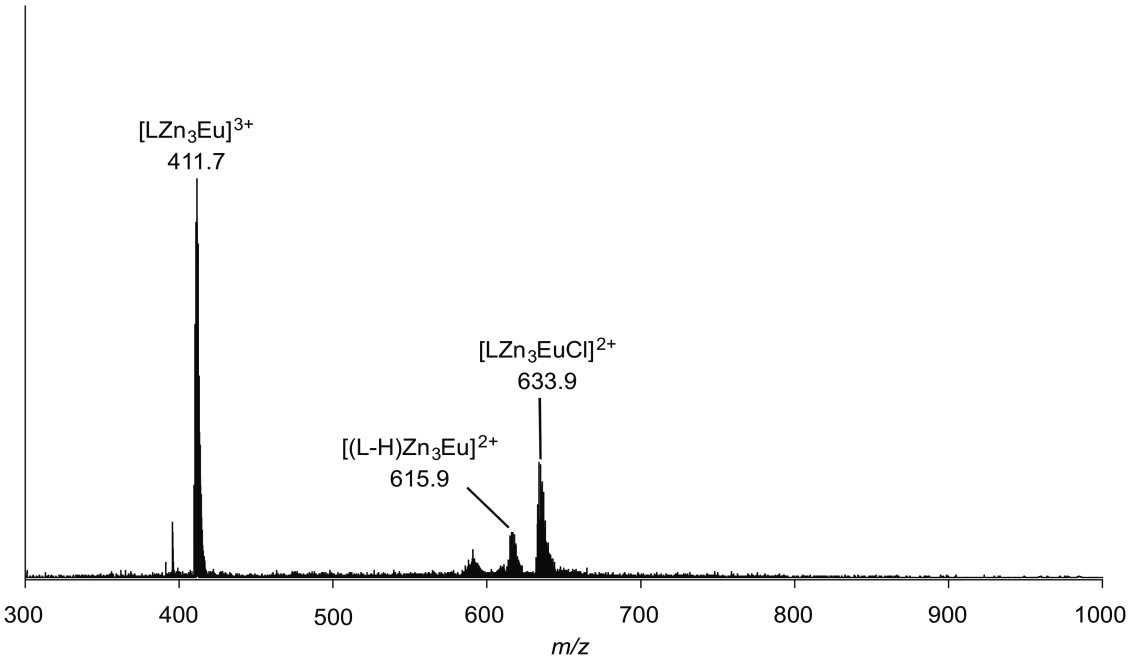

Figure S8. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Eu(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

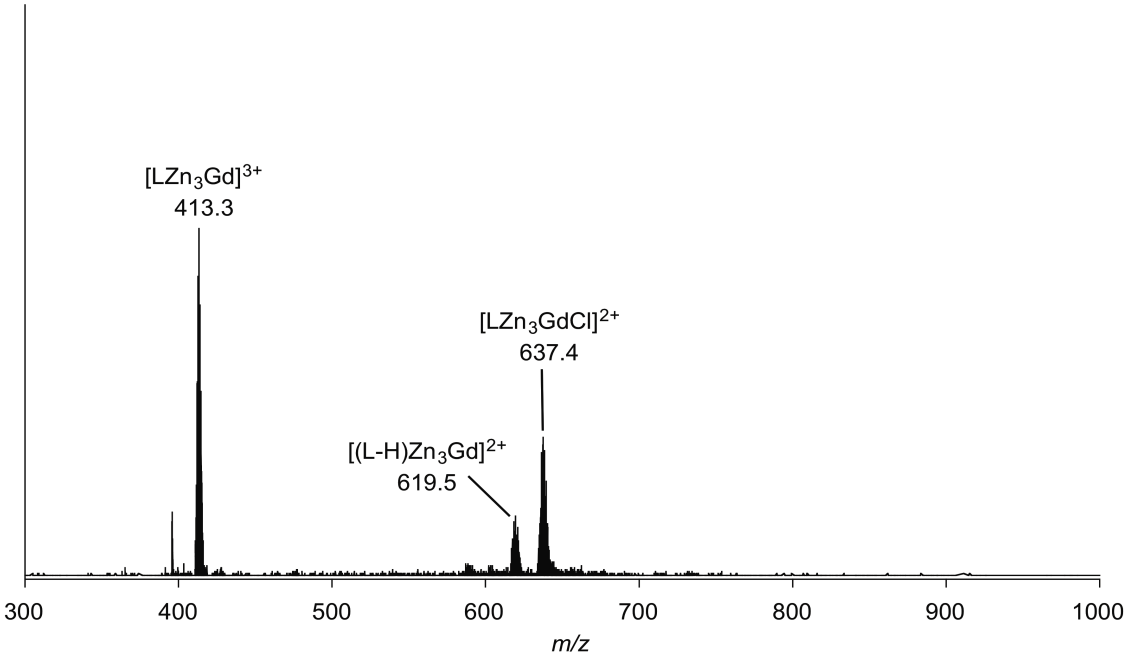

Figure S9. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Gd(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

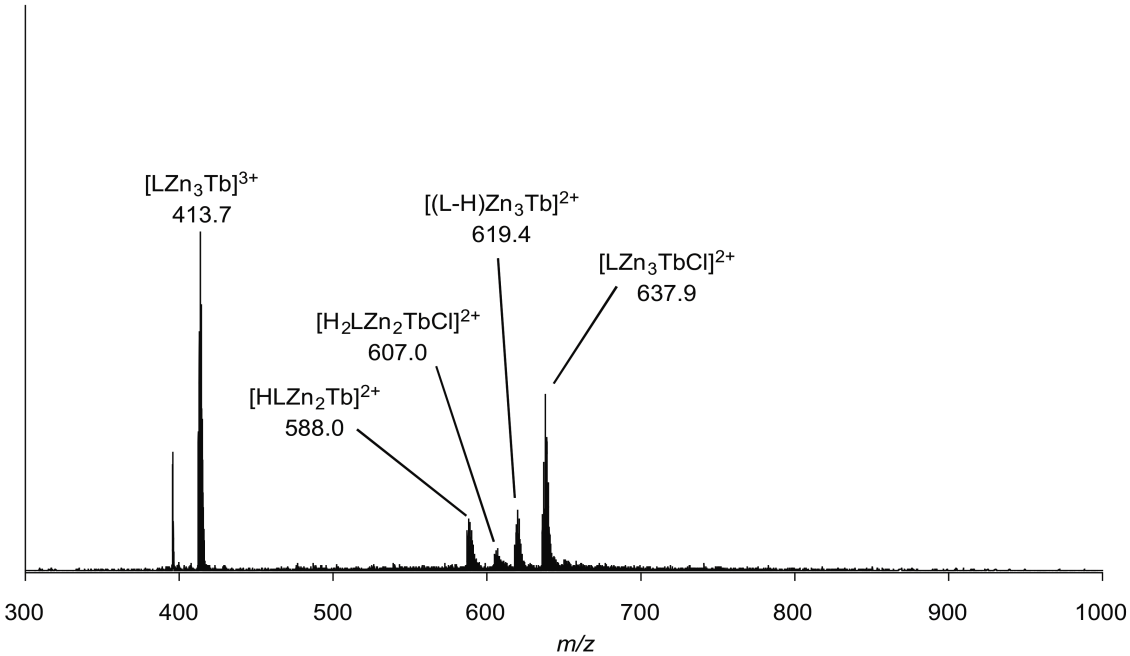

Figure S10. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Tb(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

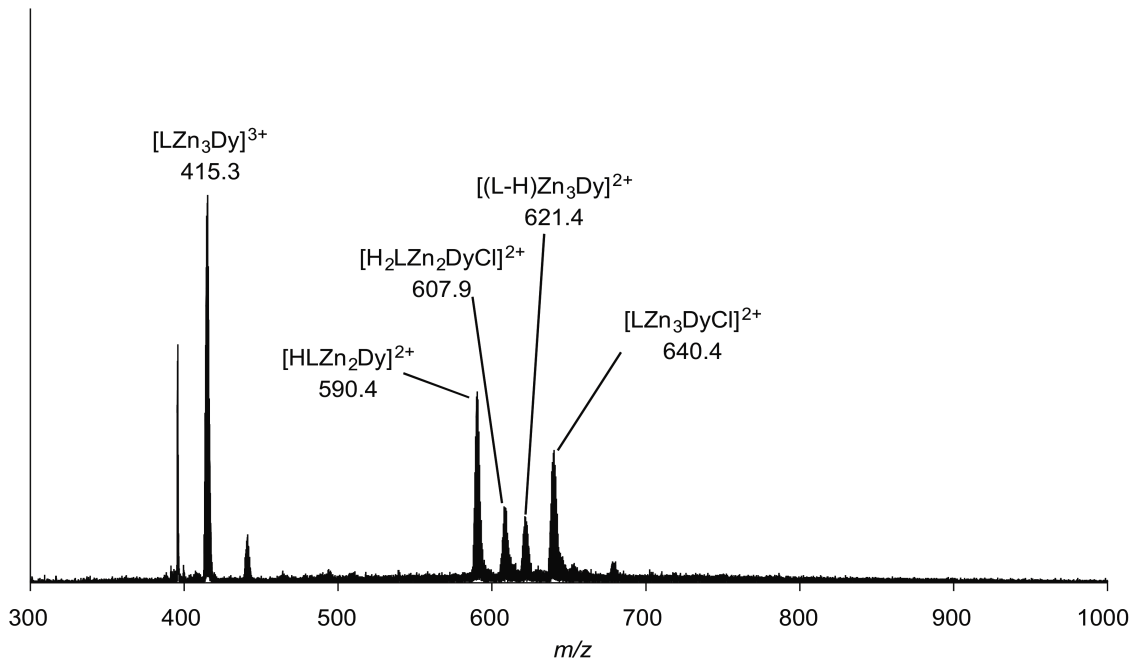

Figure S11. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Dy(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

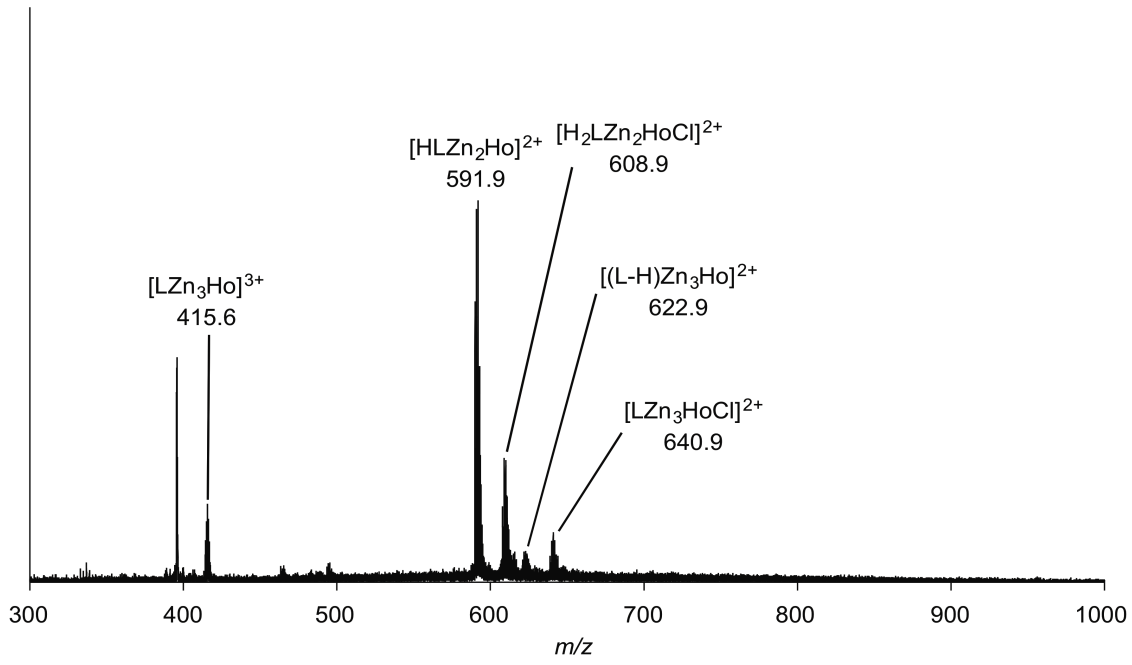

Figure S12. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Ho(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

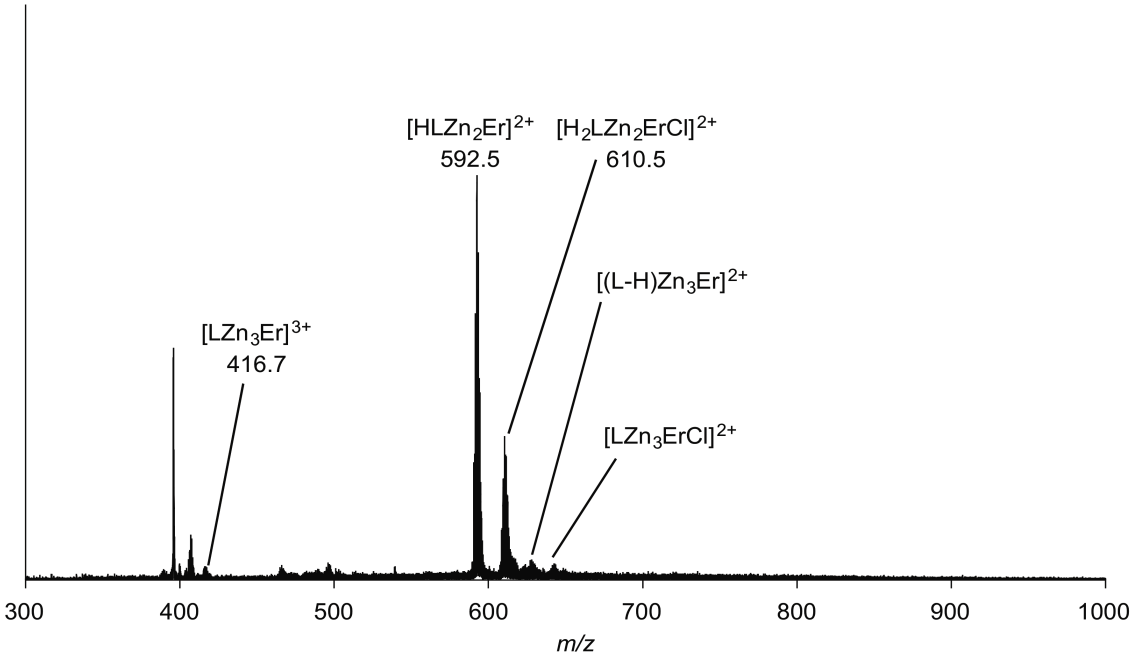

Figure S13. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Er(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

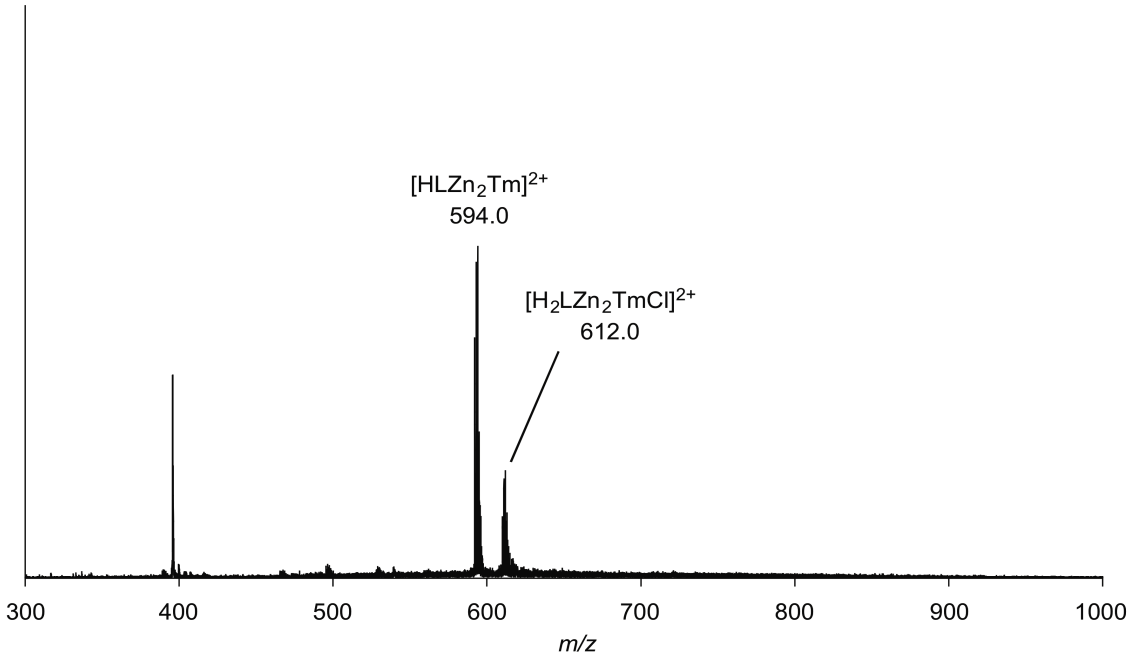

Figure S14. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Tm(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

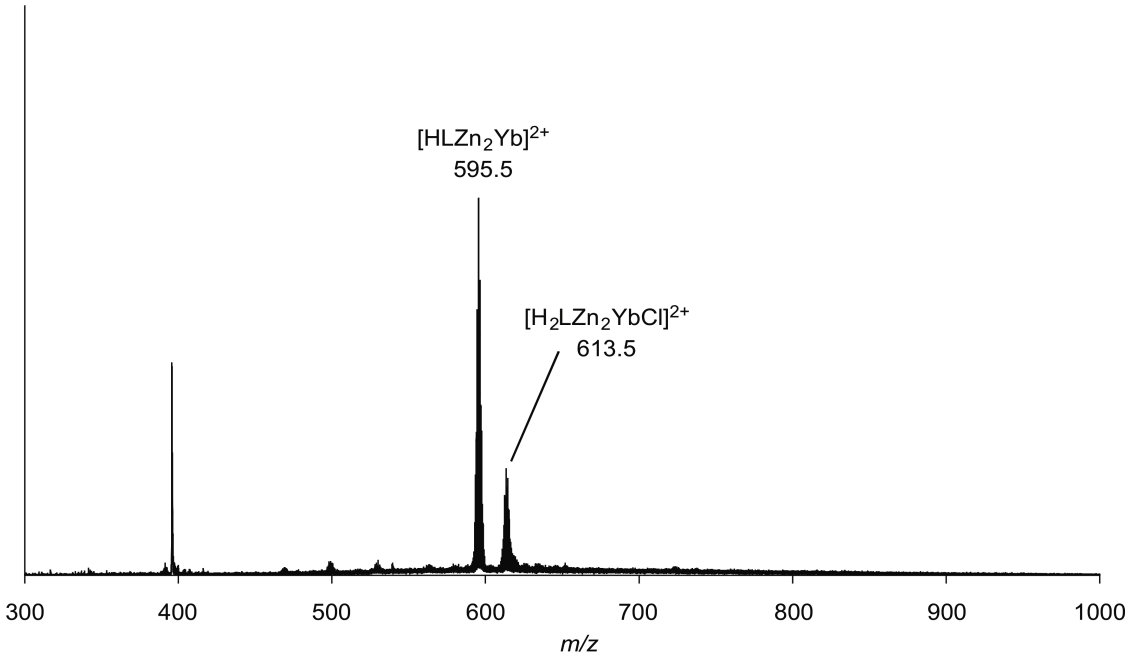

Figure S15. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Yb(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

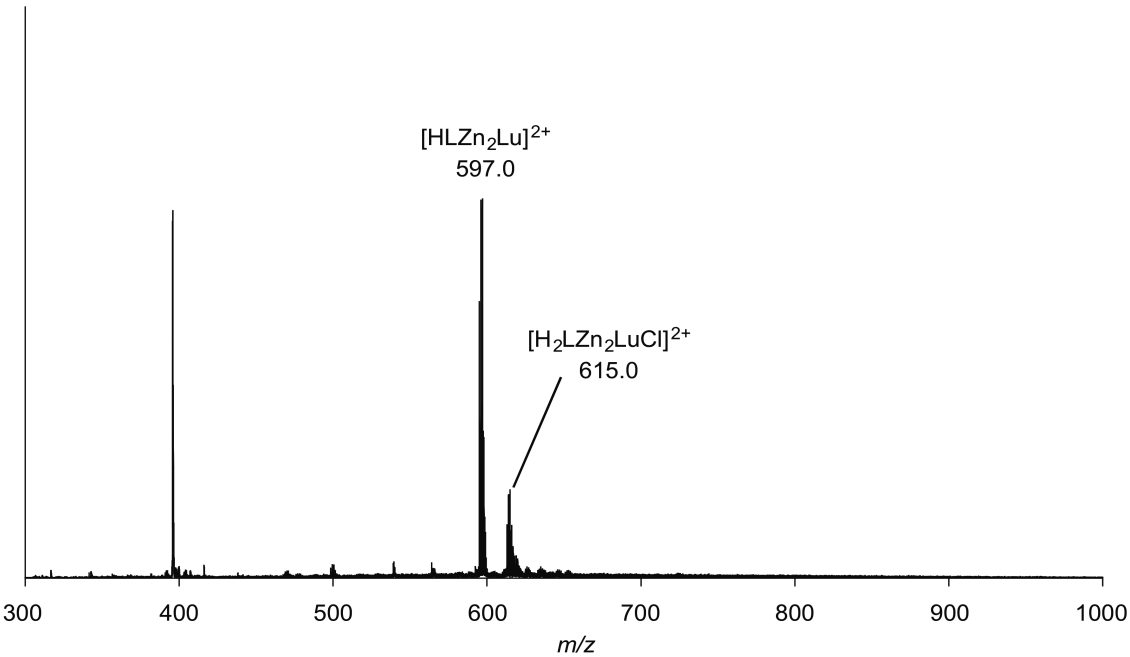

Figure S16. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Lu(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

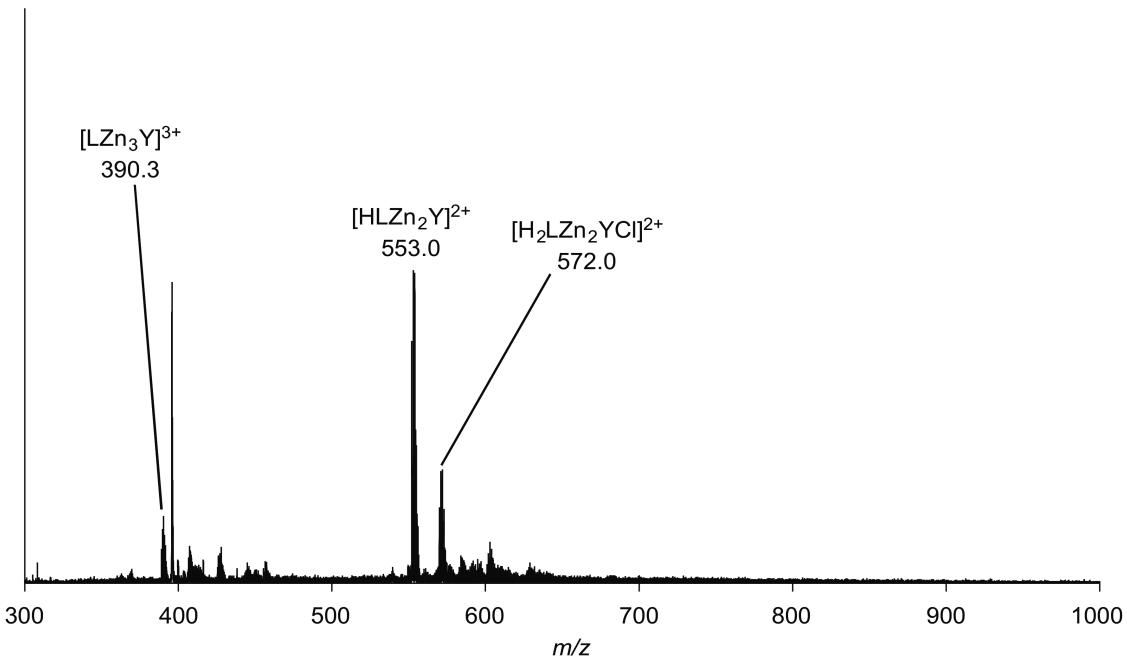

Figure S17. ESI mass spectrum of H_6L in the presence of zinc(II) acetate (3 equiv) and $Y(OAc)_3$ (1 equiv). Measurement conditions: chloroform/methanol, 1:1, ~0.01 mM.

^{1}H NMR spectra of H_6L in the presence of zinc(II) and metal ions

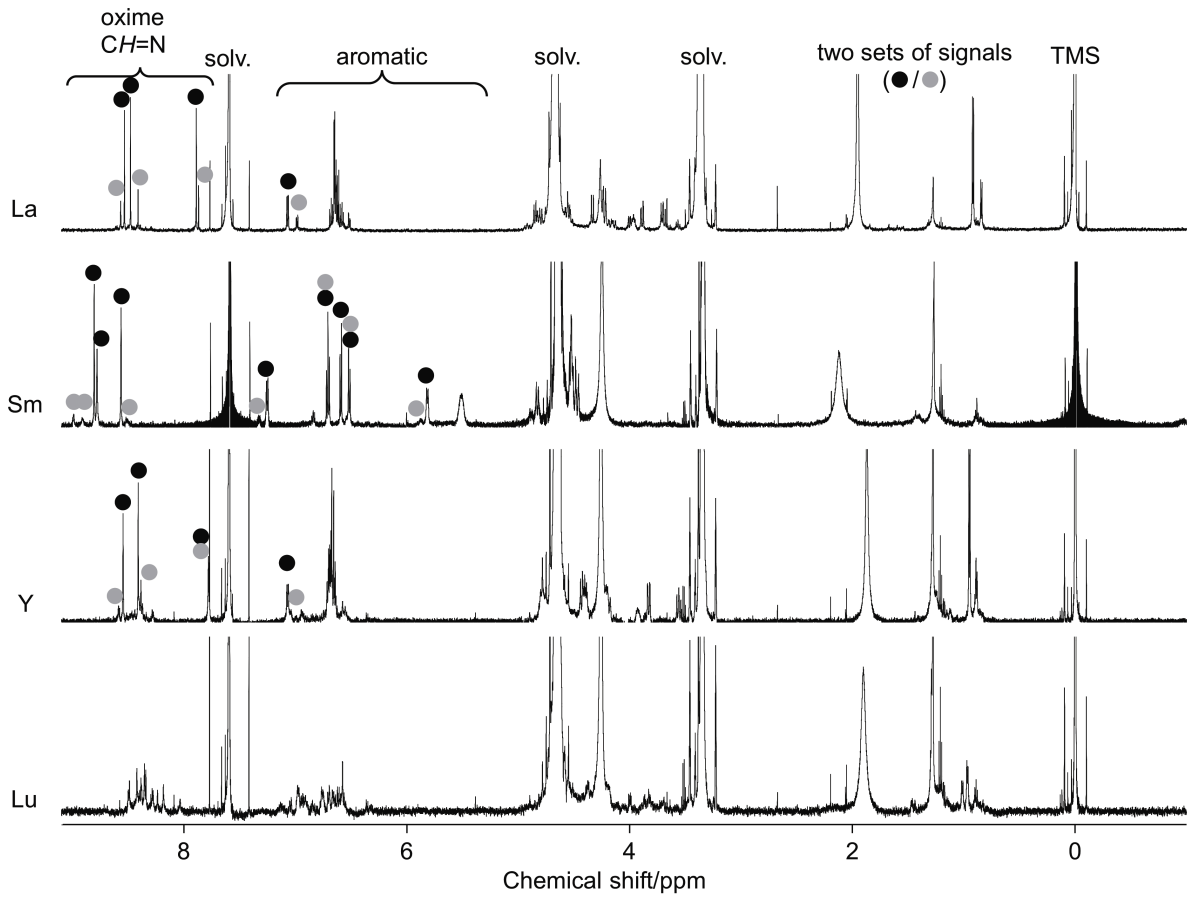

Figure S18. ^{1}H NMR spectral changes of H_6L (0.20 mM) in the presence of zinc(II) acetate (3 equiv) and $Ln(OAc)_3$ (1 equiv, Ln = La, Sm, Y, and Lu) (600 MHz, (600 MHz, $CDCl_3/CD_3OD$, 1:1).

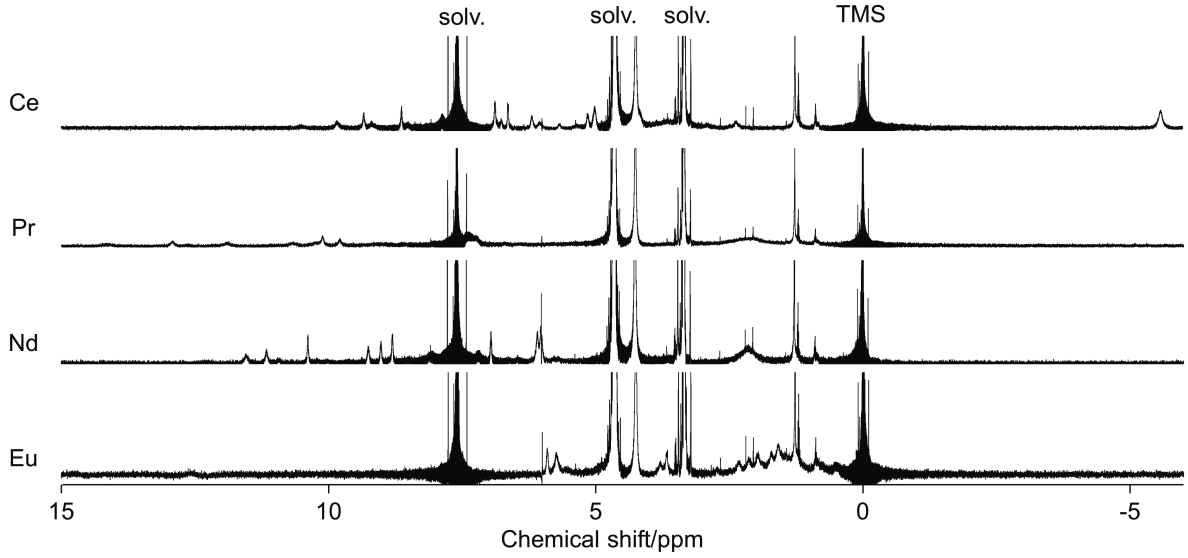

Figure S19. ^{1}H NMR spectral changes of H_6L (0.20 mM) in the presence of zinc(II) acetate (3 equiv) and $Ln(OAc)_3$ (1 equiv, Ln = Ce, Pr, Nd, and Eu) (600 MHz, $CDCl_3/CD_3OD$, 1:1).

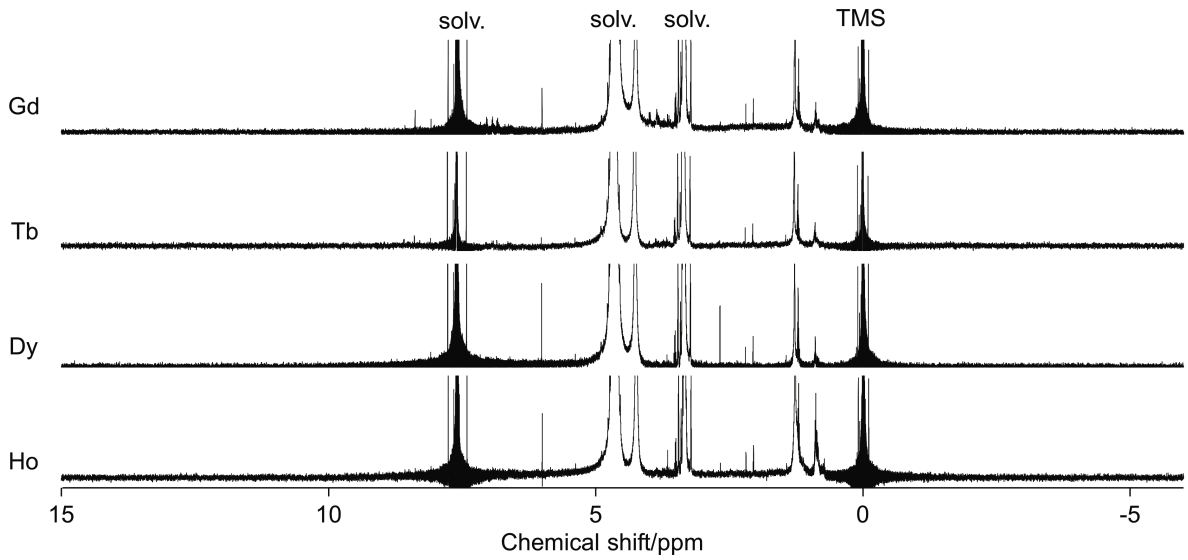

Figure S20. ^{1}H NMR spectral changes of H_6L (0.20 mM) in the presence of zinc(II) acetate (3 equiv) and $Ln(OAc)_3$ (1 equiv, Ln = Gd, Tb, Dy, and Ho) (600 MHz, $CDCl_3/CD_3OD$, 1:1).

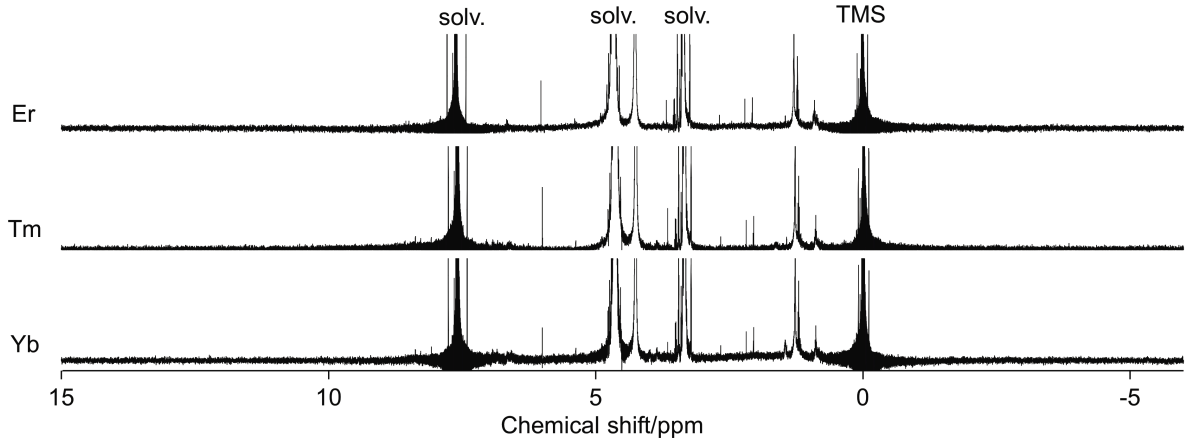

Figure S21. ^{1}H NMR spectral changes of H_6L (0.20 mM) in the presence of zinc(II) acetate (3 equiv) and $Ln(OAc)_3$ (1 equiv, Ln = Er, Tm and Yb) (600 MHz, $CDCl_3/CD_3OD$, 1:1).