Supplementary Materials.



Figure S1. Experimental FAB spectrum (DMSO, mnba matrix) for the  $(L^{7}HCu)_{2}Zn \cdot 2CH_{3}OH$  complex.





Figure S2. Theoretical isotopic distribution for the  $[(L^7HCu)_2Zn + 1]^+$  and the  $[(L^7HCu)_2Zn + Na]^+$  monocationic species.



Figure S3. Temperature dependence of the  $\chi_M T$  product for  $(L^7 HCu)_2 VO \cdot 2CH_3 OH$  at 0.1 T applied magnetic field.



Figure S4. EPR spectrum for the NiL<sup>3</sup>VO complex at room temperature and CH<sub>2</sub>Cl<sub>2</sub> solvent.



Figure S5. EPR spectrum for the VOL<sup>3</sup>VO conformers at room temperature and  $CH_2Cl_2$  solvent.



Figure S6. Experimental FAB spectrum (DMSO, mnba matrix) (left) and theoretical spectrum (right) for the  $(L^2Cu)_2Gd(NO_3)_3 \cdot 5H_2O$  complex.



Figure S7. Temperature dependence of the  $\chi_M T$  product for  $(L^2Cu)_2Gd(NO_3)_3 \cdot 5H_2O$  at 0.1 T applied magnetic field.



Figure S8. Temperature dependence of the  $\chi_M T$  product for  $(L^5Cu)_3Gd \cdot 5H_2O$  at 0.1 T applied magnetic field.