Supporting Information


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**$^{55}\text{Mn HFC Calibration}$**

Table S1: Calibration used for calculating a universal scaling factor, which has been applied to $^{55}\text{Mn HFC}$ calculations of the WOC. Here the ligand abbreviations correspond to: porph = porphyrine; SALAHE = salicylaldehydeimin-1-hydroxyethane; dtne = 1,2-bis(1,4,7-triazacyclonon-1-yl)ethane.

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Average scaling factor 1.49

Figure S1: Models used to calculate the universal scaling factor for $^{55}\text{Mn HFC}$. Colour coding: Mn$^{\text{II}}$ (dark blue), Mn$^{\text{III}}$ (green), Mn$^{\text{IV}}$ (pink), nitrogen (purple), oxygen (red) and carbon (yellow). All hydrogens have been omitted for clarity.
Figure S2: Example of the full model used for all calculations, the naming and location of residues included are also shown. Here all hydrogen atoms have been omitted for clarity. Colour coding: Mn (pink), oxygen (red), calcium (white), carbon (yellow) and nitrogen (purple). Coordinates for all models used are provided at the end of this file.
ZFS validation models

Figure S3: Models used to validate the performance of the coupled perturbed density functional theory (CP-DFT) method. Colour coding: Mn$^{IV}$ (pink), nitrogen (purple), oxygen (red) and sulphur (orange). All hydrogens have been omitted for clarity.
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