Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

The Selectivity of Water-based Pyrophosphate Recognition is Tuned by Metal Substitution in Dimetallic Receptors

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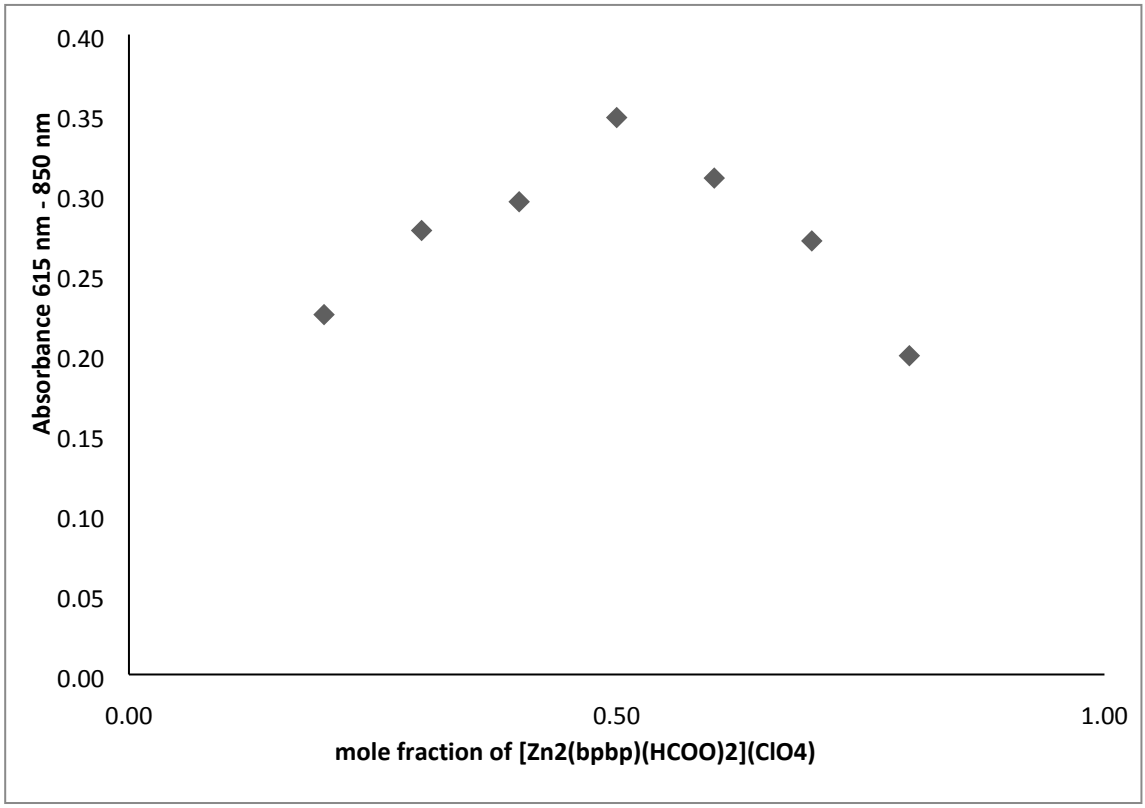

Figure S1. Job plot of 50 µM $[Zn_2(bpbp)(HCOO)_2](ClO_4)$ with pyrocatechol violet.

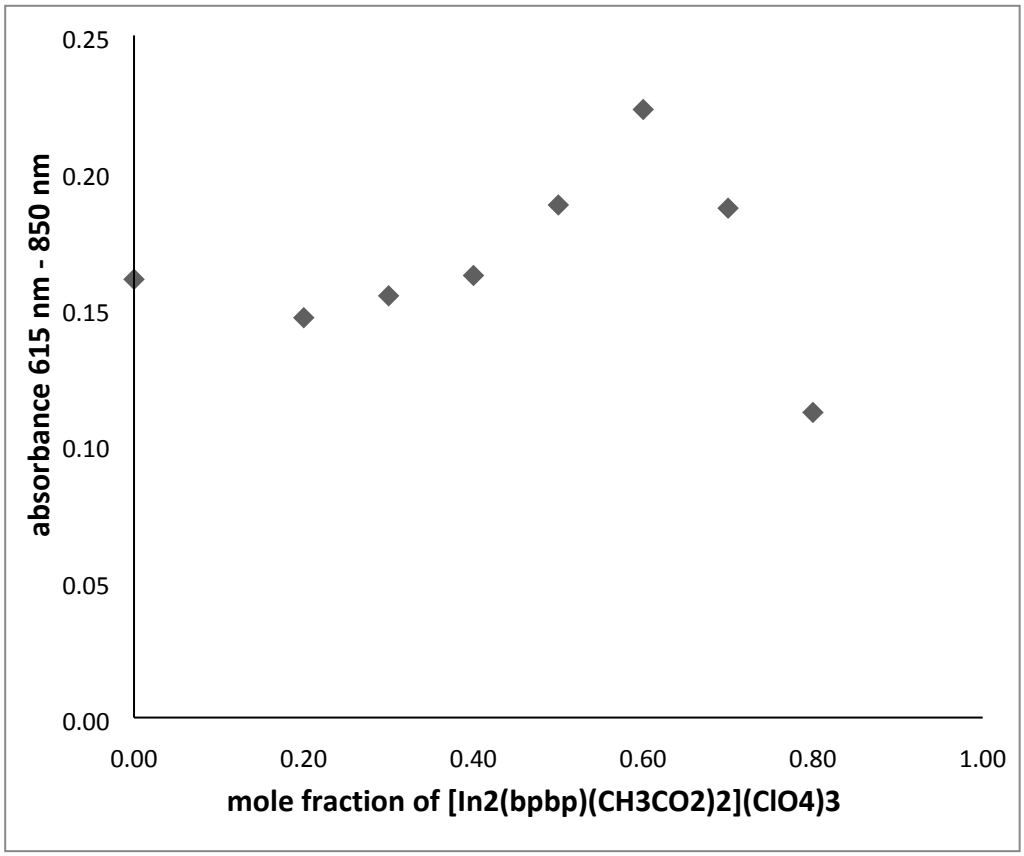

Figure S2. Job plot of 50 µM $[In_2(bpbp)(CH_3CO_2)_2](ClO_4)_3$ with pyrocatechol violet.

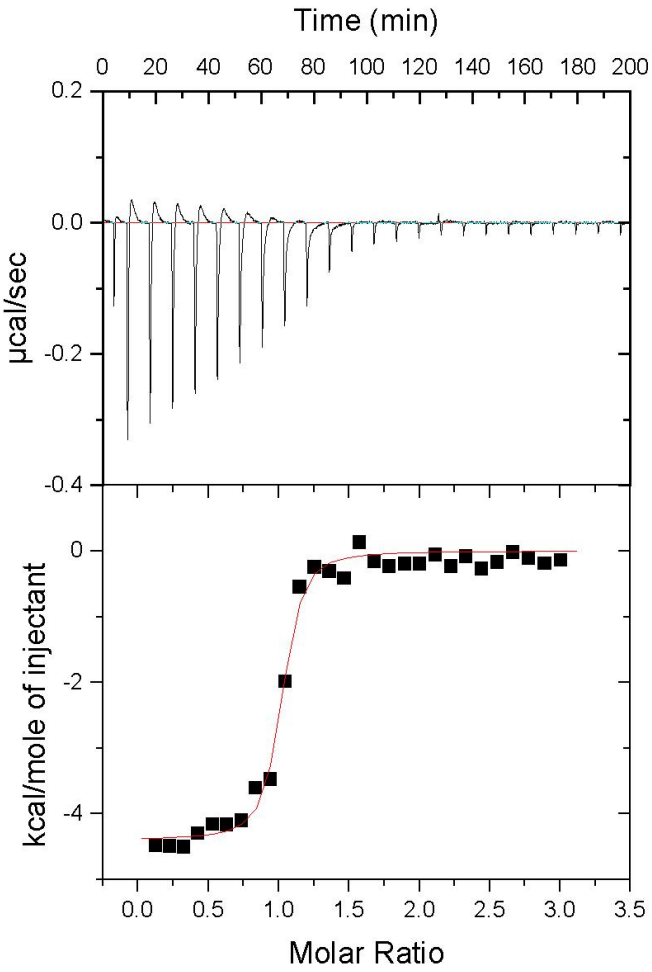

Figure S3. Binding isotherm for titration of 0.32 mM $Na_4P_2O_7$ into 0.017 mM $[Ga_2(bpbp)(OH)_2(OH_2)_2](ClO_4)_3$

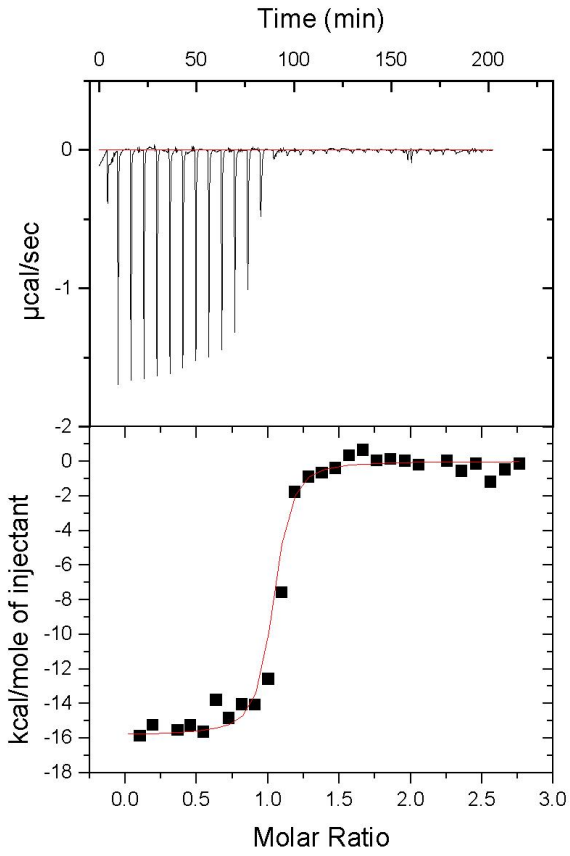

Figure S4. Binding isotherm for titration of 0.339 mM $Na_4P_2O_7$ into 0.025 mM $[Zn_2(bpbp)(HCO_2)_2](ClO_4)$

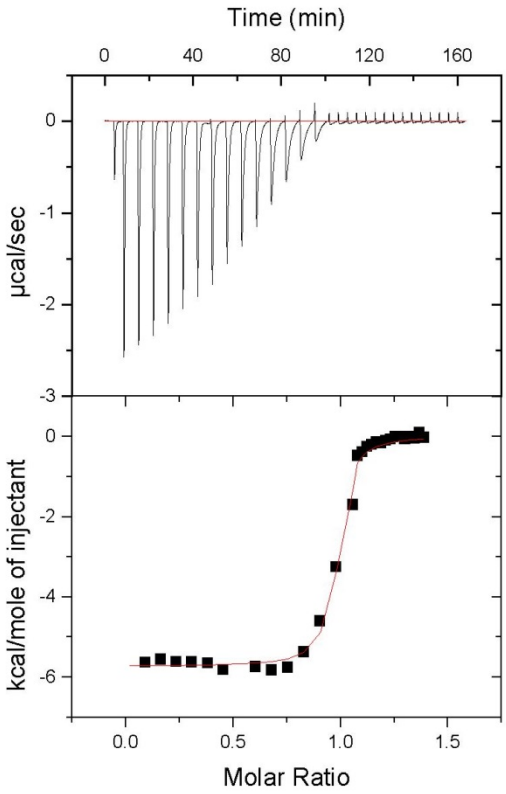

Figure S5. ITC binding isotherm for titration of 0.21 mM $[Ga_2(\mathbf{bpbp})(OH)_2(H_2O)_2](ClO_4)_3$ with 2.47 mM Na_2HPO_4 in 10 mM HEPES.

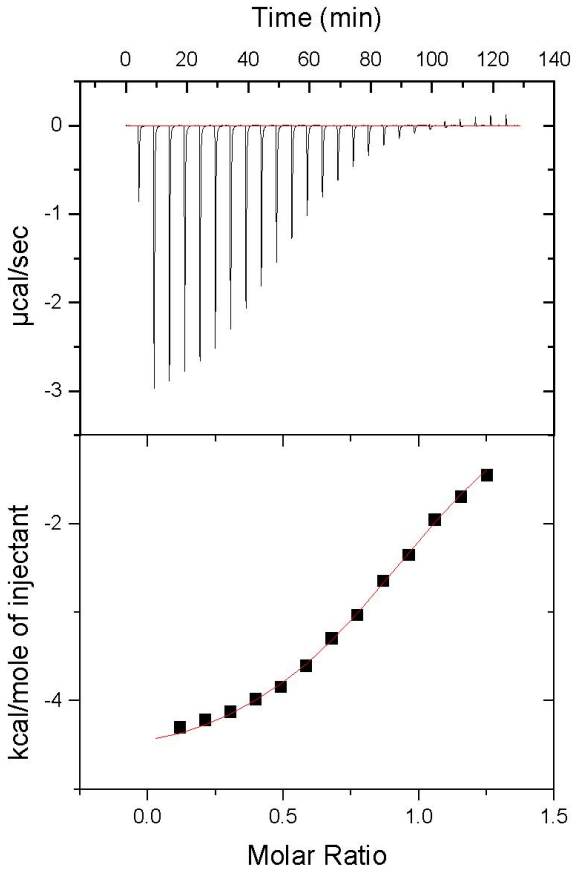

Figure S6. ITC binding isotherm for titration of 0.12 mM $[Zn_2(bpbp)(HCO_2)_2](ClO_4)$ with 2.47 mM Na_2HPO_4 in 10 mM HEPES.

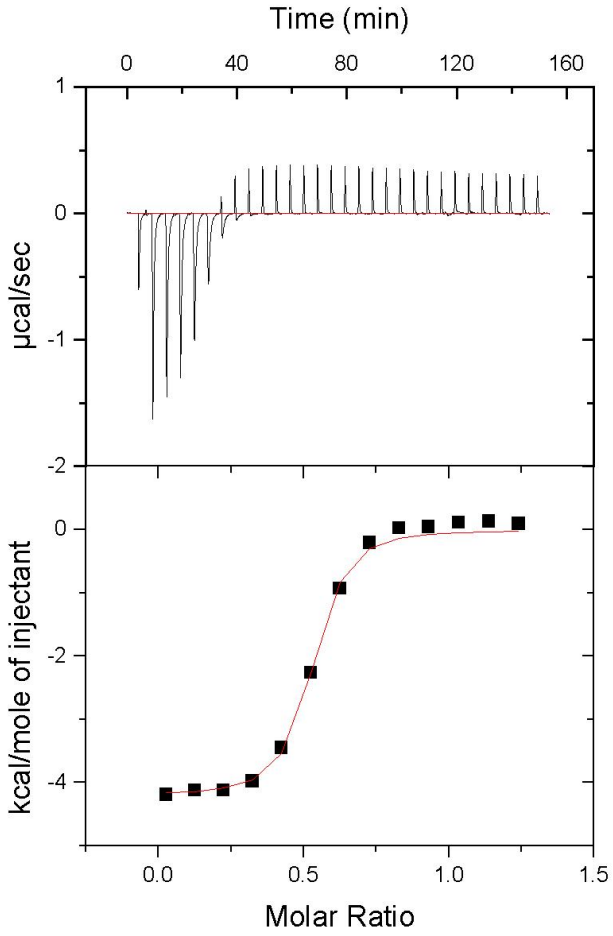

Figure S7. ITC binding isotherm for titration of 0.13 mM $[In_2(bpbp)(CH_3CO_2)_2](ClO_4)_3$ with 2.47 mM Na_2HPO_4 in 10 mM HEPES.

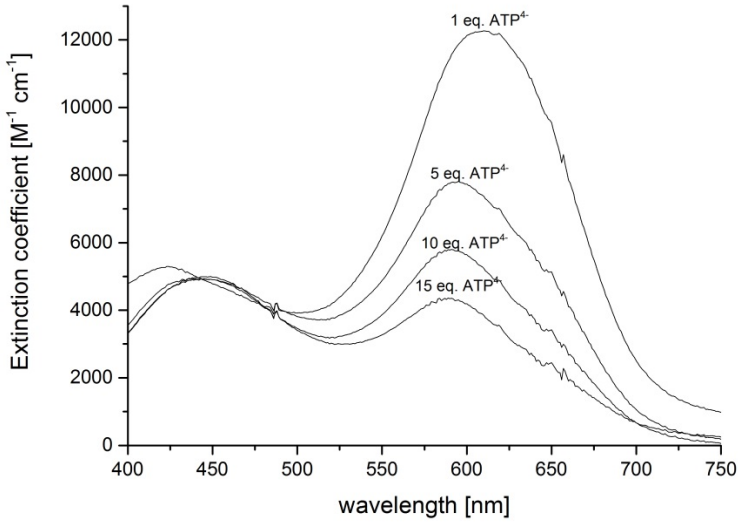

Figure S8. Uv-vis of 25 µM $\{Ga_2(bpbp)(H_nPV)\}^{1+n+}$ in 10 mM HEPES, pH 7.2 with 1 eq., 5 eq., 10 eq. or 15 eq. ATP^{4-} after 8 h at 25°C.

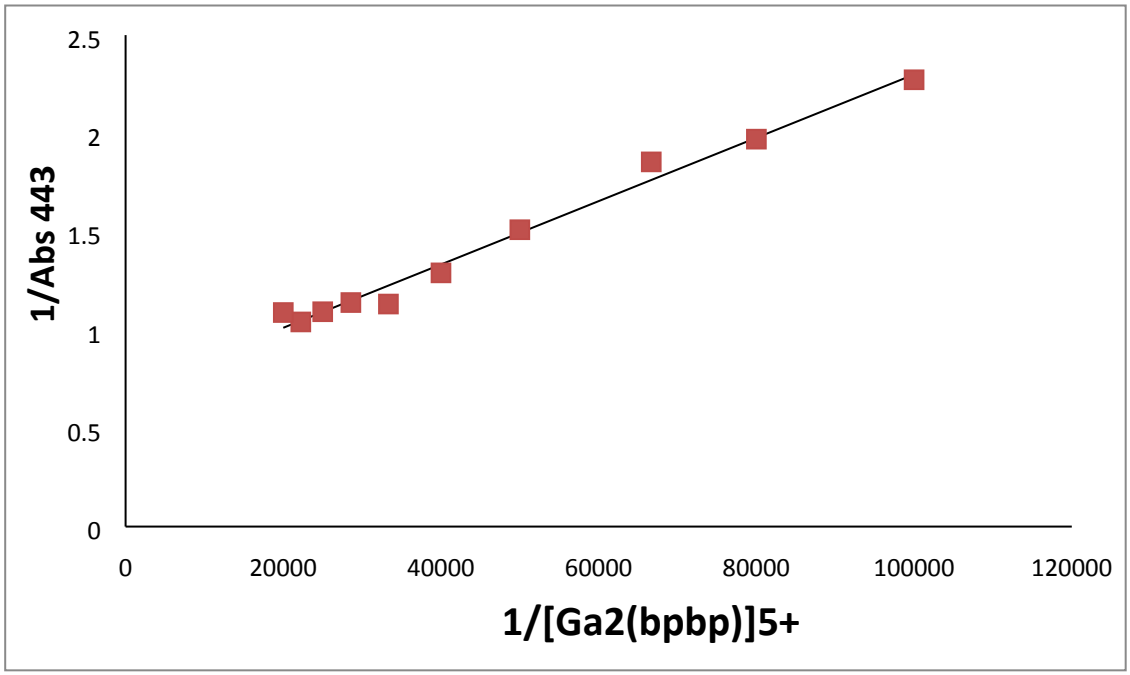

Figure S9. Benesi-Hildebrand plot of $[Ga_2(bpbp)(OH)_2(H_2O)_2](ClO_4)_3$ titrated into 50 µM PV and linear fit for calculation K_a. Equation and R^2 value is displayed in plot.

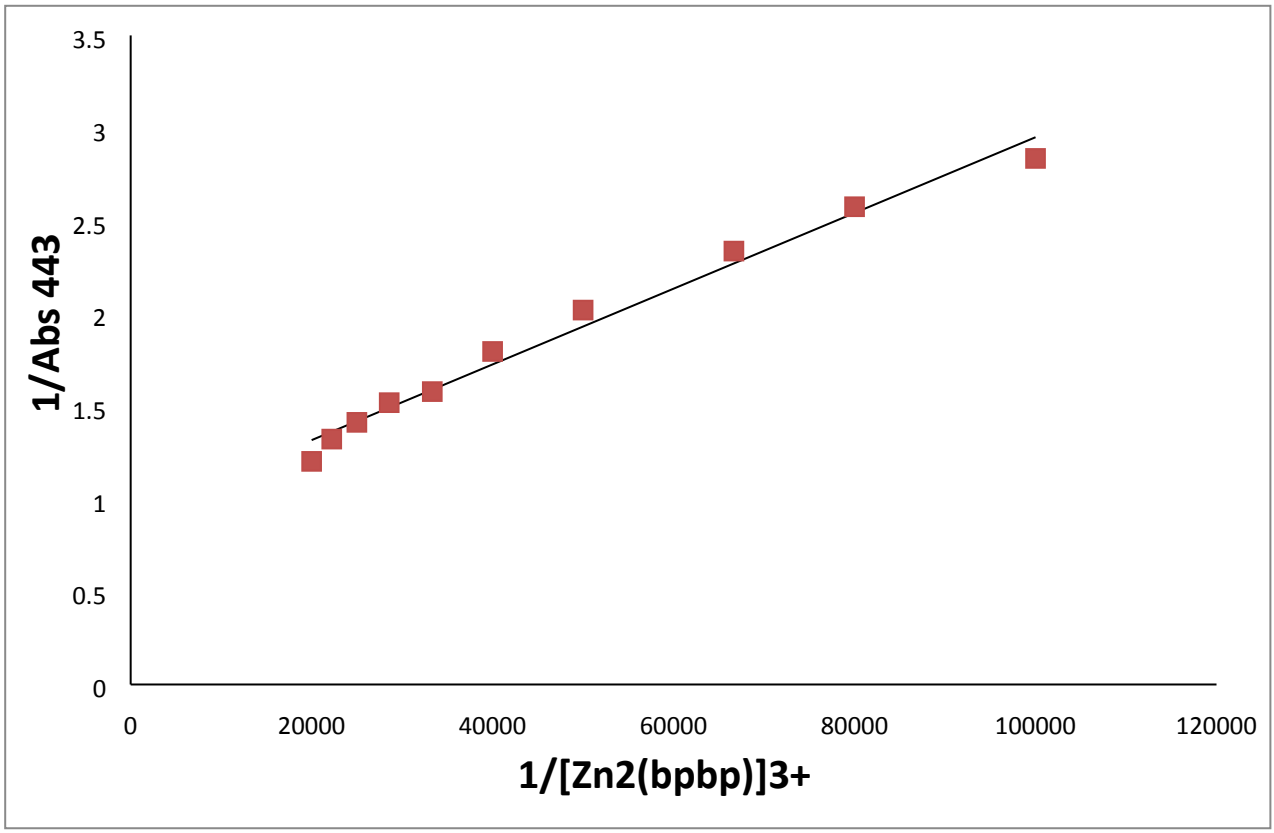

Figure S10. Benesi-Hildebrand plot of $[Zn_2(bpbp)(HCO_2)_2](ClO_4)$ titrated into 50 µM PV and linear fit for calculation K_a. Equation and R^2 value is displayed in plot.