

Supplementary information

Comparative Structure Activity Relationship for Heterogeneous Phosphatase-like Catalytic Activities of One-Dimensional Cu(II) Coordination Polymers

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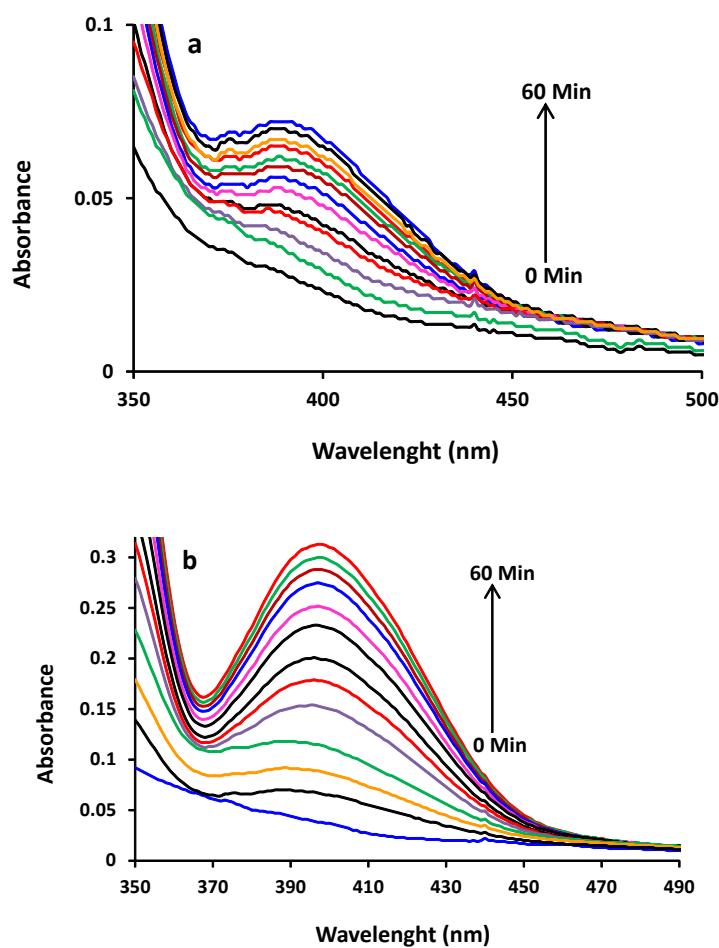


Fig. S1 Absorption spectra for the transesterification of HPNP (100 μ M) in the absence and presence of (a) complex **2** and (b) complex **3** (50 μ M) in 10% MeOH recorded at an interval of 5 minutes at 30°C.

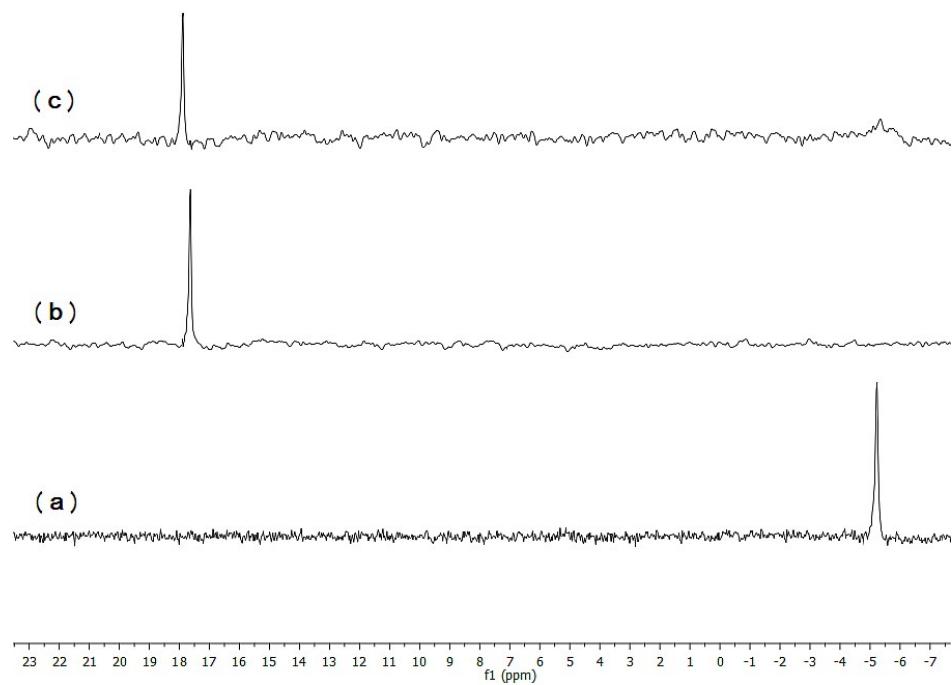


Fig. S2 ^{31}P NMR of (a) substrate (HPNP), (b) synthesised cyclic phosphate (glycero-1,2-cyclic phosphate) and (c) substrate- catalyst reaction mixture in $\text{D}_2\text{O}/\text{DMSO}-d_6$ mixture (70:30).

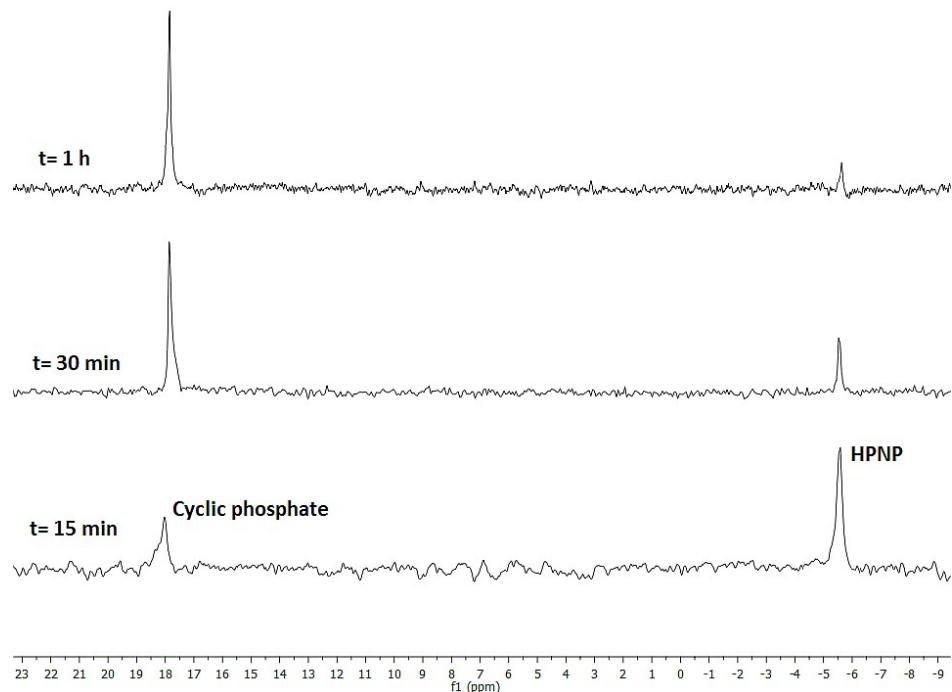


Fig. S3. Time dependent ^{31}P NMR spectra for HPNP hydrolysis by complex **1**, in $\text{D}_2\text{O}/\text{DMSO}-d_6$ mixture (70:30), $[\text{HPNP}] = 0.1 \text{ mM}$ and $[\text{Complex}] = 0.25 \text{ mM}$.

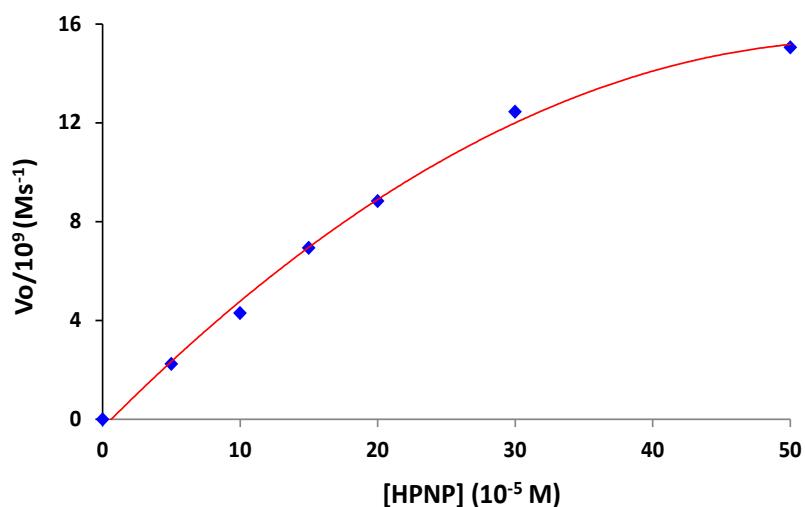


Fig. S4 Dependence of rate of reaction on substrate concentration (50-500 μ M) for complex **3** (50 μ M) at 30 °C in 10% MeOH.

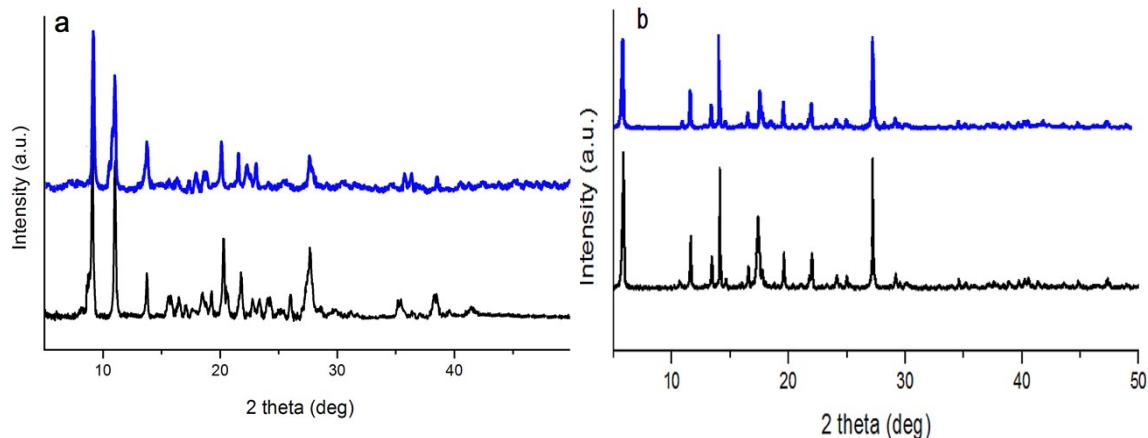


Fig. S5 PXD patterns of (a) **1** and (b) **3** before catalytic experiments (black coloured) and after third cycle of catalytic experiments (blue coloured)

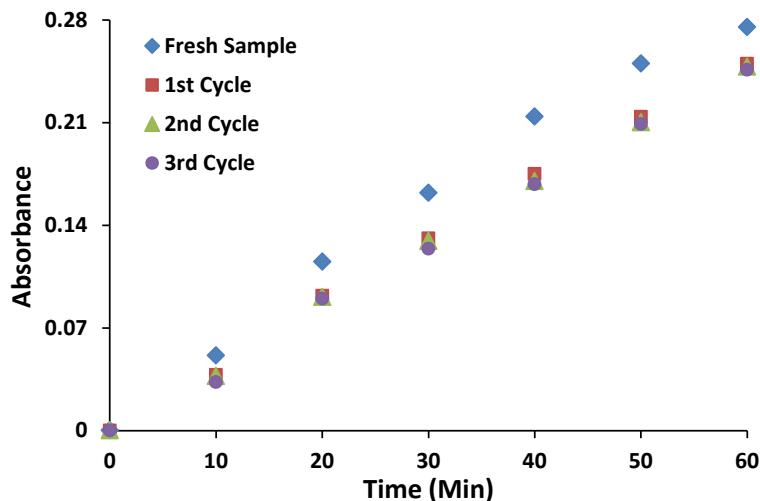


Fig. S6 Reusability of complex **3** for repeated HPNP phosphate ester bond cleavage experiments.

Table S1 Phosphotase like activities from reported complexes

Complex	Substrate	Conditions	$K_{cat} (s^{-1})$	Reference
$[\text{Ni}_2\text{L}(\text{H}_2\text{O})_4]4\text{H}_2\text{O}\cdot 2\text{ClO}_4$	4-NPP	acetonitrile–water (2.5% (v/v), 25 °C)	3.5×10^{-4}	S1
$[\text{Zn}(\text{bpy})\text{Cl}_2]$	BNPP	water, 25 °C	5.7×10^{-7}	S2
$[\text{Zn}_2(\text{L}_2)\text{-}(\mu\text{-O}_2\text{CMe})_2(\text{MeCN})_2]\text{[PF}_6]$	HPNP	MeOH-H ₂ O (33%, v/v), 30 °C	3.44×10^{-4}	S3
$[\text{Zn}_2(\text{L})(\text{H}_2\text{O})_2]$	3',5'-UpU	water, 25 °C	2.8×10^{-5}	S4
$[\text{Cu}_2(\text{H}_2\text{pat}^1)\text{-}(\mu\text{-OH})(\text{H}_2\text{O})_2]$	BDNPP	$\text{H}_2\text{O} : \text{MeCN} : \text{MeOH} = 50 : 45 : 5$, 25 °C	3.95×10^{-3}	S5
$\text{Zn}_2(\text{bpmp})(\mu\text{-OH})(\text{ClO}_4)_2$	HPNP	DMSO-H ₂ O (30%, v/v), 25 °C	6.4×10^{-4}	S6
$\{[\text{Cu}_3(\text{L}^1)(\text{NO}_3)_2(\text{DMF})(\text{H}_2\text{O})]\cdot 3(\text{DMF})\}_n$ (1)	HPNP	MeOH-H ₂ O (10%, v/v), 30 °C	9.6×10^{-3}	Present work

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