Supplementary Information


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Figure S1. FTIR spectrum of complex 1.
Figure S2. $^1$H-NMR spectrum of ligand HL.
Figure S3. $^{13}$C-NMR spectrum of ligand HL.

Figure S4. FTIR spectrum of ligand HL.
Figure S5. UV-VIS spectrum of ligand HL in DMSO.
Figure S6. UV-VIS spectrum of Complex 1 in DMSO.
Figure S7. UV-VIS spectrum of Complex 1 in different pH at DMSO-buffer medium.
Figure S8. Spectrophotometric titration of 1 (pH value: 3.45-4.5; pKa = 4.10) Conditions: Complex = 10^{-3} [M]; [KCl] = 0.100 mol.L^{-1}; [KOH] = 0.100 mol.L^{-1}; in solution DMSO /water (75:25%v/v – 50 mL) at 25°C.

Table S1: pKa values of complex 1

<table>
<thead>
<tr>
<th>Complex</th>
<th>pKa[HL]</th>
<th>pKa[M-OH_{2}(1)]</th>
<th>pKa[M-OH_{2}(2)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.1</td>
<td>6.1</td>
<td>8.15</td>
</tr>
</tbody>
</table>
Figure S9. ESI-MS spectrum of Complex 1 in DMSO-water medium.
Figure S10. PXRD pattern of complex 1.

Table S2. $k_{\text{cat}}$ Value for Dinuclear Complex 1 for oxidation of 3,5 DTBC in DMSO.

<table>
<thead>
<tr>
<th>Complex</th>
<th>Wavelength (nm)</th>
<th>$V_{\text{max}}$ (M s$^{-1}$)</th>
<th>$K_M$ (M)</th>
<th>$k_{\text{cat}}$ (h$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>396</td>
<td>$2.11 \times 10^{-6}$</td>
<td>$2.2 \times 10^{-3}$</td>
<td>$0.762 \times 10^2$</td>
</tr>
</tbody>
</table>
Figure S11. Change of d-d band of complex 1 during catecholase activity.
Figure S12. ESI-MS spectrum of complex –DTBC adduct after 1 hour of mixing.
Figure S13. Spectral scan to detect $I^3^-$. 
Figure S14. Changes observed in UV–vis spectra of complex 1 up to 120 minutes (conc. $1 \times 10^{-4}$ M) upon addition of 100-fold 3, 5-DTBC ($1 \times 10^{-2}$ M) in 50% DMSO-water mixture.
Figure S15. Changes observed in UV–vis spectra of complex 1 up to 120 minutes (conc. $1 \times 10^{-4}$ M) upon addition of 100-fold 3, 5-DTBC ($1 \times 10^{-2}$ M) in 75% DMSO-water mixture.
Figure S16. Spectra of complex 1 in different percentage of water-DMSO medium.

Table S3. Kinetics Parameters for the Phosphatase Activity of Complex 1

<table>
<thead>
<tr>
<th>Complex</th>
<th>Wavelength (nm)</th>
<th>$V_{\text{max}}$ (M s$^{-1}$)</th>
<th>$K_M$ (M)</th>
<th>$k_{\text{cat}}$ (s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>425</td>
<td>$8.4904 \times 10^{-5}$</td>
<td>$1.06 \times 10^{-3}$</td>
<td>1.69</td>
</tr>
</tbody>
</table>
Figure S17. Wavelength scan for the hydrolysis of 4-NPP in the absence and presence of complex 1 (substrate:catalyst = 20:1) in 75% DMSO-buffer medium at pH 7.0 recorded at 25°C at an interval of 5 minutes for 90 min. [4-NPP]=1 × 10^{-3}(M), [Complex] =0.05 × 10^{-3}(M). Arrow shows the change in absorbance with reaction time.
Figure S18. Wavelength scan for the hydrolysis of 4-NPP in the absence and presence of complex 1 (substrate : catalyst = 20:1) in 75% DMSO-buffer medium at pH 7.5 recorded at 25°C at an interval of 5 minutes for 90 min. [4-NPP]=1 × 10^{-3}(M), [Complex] =0.05 × 10^{-3}(M). Arrow shows the change in absorbance with reaction time.
Figure S19. Wavelength scan for the hydrolysis of 4-NPP in the absence and presence of complex 1 (substrate: catalyst = 20:1) in 75% DMSO-buffer medium at pH 8.0 recorded at 25°C at an interval of 5 minutes for 90 min. [4-NPP]=1 × 10^{-3}(M), [Complex] =0.05 × 10^{-3}(M). Arrow shows the change in absorbance with reaction time.
Figure S20. Wavelength scan for the hydrolysis of 4-NPP in the absence and presence of complex 1 (substrate: catalyst = 20:1) in 75% DMSO-buffer medium at pH 8.5 recorded at 25°C at an interval of 5 minutes for 90 min. [4-NPP] = 1 × 10^{-3} (M), [Complex] = 0.05 × 10^{-3} (M). Arrow shows the change in absorbance with reaction time.
Figure S21. Wavelength scan for the hydrolysis of 4-NPP in the absence of complex 1 (substrate: catalyst = 20:1) in 75% DMSO-buffer medium at pH 9 recorded at 25°C at an interval of 10 minutes for 30 min. [4-NPP]=1 × 10^{-3} (M), [Complex] =0.05 × 10^{-3} (M). Arrow shows the change in absorbance with reaction time.
Figure S22. Wavelength scan for the hydrolysis of 4-NPP in the presence of Ligand HL (substrate:catalyst = 20:1) in 75% DMSO-buffer medium at pH 9 recorded at 25°C at an interval of 5 minutes for 30 mins. [4-NPP]=1 × 10⁻³(M), [Ligand]=0.05 × 10⁻³(M). Arrow shows negligible or no change in absorbance with reaction time.
Figure S23. Wavelength scan for the hydrolysis of 4-NPP in the presence of Cu(ClO$_4$)$_2$ (substrate:catalyst = 20:1) in 75% DMSO-buffer medium at pH 9 recorded at 25°C at an interval of 5 minutes for 30 mins. [4-NPP]=1 $\times$ 10$^{-3}$M), [Ligand] =0.05 $\times$ 10$^{-3}$(M). Arrow shows negligible or no change in absorbance with reaction time.
**Figure S24.** FTIR spectrum of Transformed ligand TL
Figure S25. $^1$HNMR spectrum of Transformed ligand TL
Figure S26. ESI-MS spectrum of reaction mixture in acetonitrile after 30 minutes of the addition of the ligand and Cu(ClO$_4$)$_2$. 
Figure S27. ESI-MS spectrum of deformed ligand TL after purification.
Figure S28. Cyclic voltammogram of complex 1 at the GC electrode in DMSO medium at 100 mV s$^{-1}$ scan rate.
Figure S29. Cyclic voltammogram of complex 1 at the GC electrode in Acetonitrile medium at 100 mV s$^{-1}$ scan rate.
Figure S30. Cyclic voltammogram of complex 1 at the GC electrode in acetonitrile medium at 100 mVs\(^{-1}\) scan rate.
Figure S31. ORTEP drawing (ellipsoid probability 30%) of Cu(MeCN)$_4$(ClO$_4$) (All atoms are not labeled for sake of clarity).