Self-assembled copper(II) metallacycles derived from asymmetric Schiff base ligands: Efficient host for ADP/ATP in phosphate buffer

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Supporting Information Placeholder

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**Fig. S6** Intra-molecular hydrogen bonding interactions in $\text{H}_2\text{L}^2$.

**Fig. S7** Crystal structure of 1 showing distances from centroid of cavity to Cu(II) centre.

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Fig. S18 ESI-MS of 1 + ADP [Inset shows simulated isotopic pattern for molecular ion peak at m/z 2019.7877 \{1 + (ADP)^2^- + 3H]^+\].

Fig. S19 ESI-MS of 1+ATP [Inset shows simulated isotopic pattern for molecular ion peak at m/z 2099.2877 \{1 + (ATP)^2^- + 3H]^+\].
Fig. S20 ESI-MS of 2 + ADP [Inset showing simulated isotopic pattern for molecular ion peak at \( m/z \) 2219.7501 \( \{2^+ \text{ (ADP)}^2^- + 3\text{H}\}^+ \).]

Fig. S21 ESI-MS of 2 + ATP [Inset showing simulated isotopic pattern for molecular ion peak at \( m/z \) 2299.5135 \( \{2^+ \text{ (ATP)}^2^- + 3\text{H}\}^+ \).]
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Fig. S27 Molecular docked structures for 1 + ATP, show π–π interactions between adenine and salen core (a) and insertion of phosphate chain into the cavity shown by blue circle in (a) and space fill model (b).
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Table S1. UV/vis data of \( \text{H}_2\text{L}^1, \text{H}_2\text{L}^2, \text{1} \) and \( \text{2} \).

<table>
<thead>
<tr>
<th>Compounds</th>
<th>( \text{H}_2\text{L}^1 )</th>
<th>( \text{H}_2\text{L}^2 )</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \varepsilon ), ( 4.57 \times 10^4 ) and 262 nm ( \varepsilon ), ( 4.41 \times 10^4 )</td>
<td>( \varepsilon ), ( 2.26 \times 10^4 ) and 312 nm ( \varepsilon ), ( 4.94 \times 10^4 )</td>
<td>( \varepsilon ), ( 2.69 \times 10^4 ) and 323 nm ( \varepsilon ), ( 4.21 \times 10^4 )</td>
<td>( \varepsilon ), ( 2.14 \times 10^4 ) and 319 nm ( \varepsilon ), ( 3.94 \times 10^4 )</td>
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</table>

Table S2 Cyclic voltammetric data of \( \text{H}_2\text{L}^1, \text{H}_2\text{L}^2, \text{1} \) and \( \text{2} \).

<table>
<thead>
<tr>
<th>Compounds</th>
<th>Oxidation Potential; V (Current Density; ( \mu \text{A} ))</th>
<th>Reduction Potential; V (Current Density; ( \mu \text{A} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{H}_2\text{L}^1 )</td>
<td>0.403 (I = -4.86)</td>
<td>---</td>
</tr>
<tr>
<td>( \text{H}_2\text{L}^2 )</td>
<td>0.382 (I = -4.50)</td>
<td>---</td>
</tr>
<tr>
<td>1</td>
<td>0.564 (I = -4.15)</td>
<td>-0.306V (I = 1.671)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-0.719V (I = 1.620)</td>
</tr>
<tr>
<td>2</td>
<td>0.554 (I = -3.66)</td>
<td>-0.314V (I = 1.509)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-0.717V (I = 1.465)</td>
</tr>
</tbody>
</table>

Table S3 Cyclic voltammetric data of \( \text{1} \) and \( \text{2} \) upon addition of ATP and ADP.

<table>
<thead>
<tr>
<th>Probe</th>
<th>Probe + ATP</th>
<th>Probe + ADP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reduction Potential; V (Current Density; ( \mu \text{A} ))</td>
<td>Reduction Potential; V (Current Density; ( \mu \text{A} ))</td>
<td>Reduction Potential; V (Current Density; ( \mu \text{A} ))</td>
</tr>
<tr>
<td>( \text{1} )</td>
<td>-0.306V (I = 1.671)</td>
<td>-0.321 (I = 1.892)</td>
</tr>
<tr>
<td></td>
<td>-0.719V (I = 1.620)</td>
<td>-0.719 (I = 1.985)</td>
</tr>
<tr>
<td>( \text{2} )</td>
<td>-0.314V (I = 1.509)</td>
<td>-0.325 (I = 1.678)</td>
</tr>
<tr>
<td></td>
<td>-0.717V (I = 1.465)</td>
<td>-0.717 (I = 1.746)</td>
</tr>
</tbody>
</table>