Table S1  Energy and % contribution of atomic orbitals to each molecular orbital in the frontier region for (a) [Ru(bipy)(L1)]²⁺ and (b) [Ru(bipy)(HL1)]²⁺. The contribution of both HL1 and L1⁻, the protonated and the deprotonated pyridyltriazole ligands, is divided into a pyridinetriazole component, pytrz and a contribution from the dimethoxyphenyl moiety, ph.

(a) Deprotonated

<table>
<thead>
<tr>
<th>MO</th>
<th>eV</th>
<th>Ru</th>
<th>bipy1 %</th>
<th>bipy2 %</th>
<th>pytrz %</th>
<th>ph %</th>
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</thead>
<tbody>
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(b) Protonated

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<th>eV</th>
<th>Ru</th>
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<th>bipy2 %</th>
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