Electronic Supplementary Information (ESI) for:

Assessment of Time-Dependent Density Functionals for the Electronic Excitation Energies of Organic Dyes Used in DSSCs

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\[ R^2 \]
Table S3: Vertical Excitation Energies (eV) Using mGGA and GH-mGGA Functionals.

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**SD** 0.002 0.060 0.017 0.001 0.001 0.030
**R²** 0.002 0.060 0.017 0.001 0.001 0.029

Table S4: Vertical Excitation Energies (eV) Using RSH-GGA Functionals.

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**MAE** 0.424 0.198 0.563 0.476 0.398 0.499 0.499
**Max** 0.783 0.489 1.022 0.871 0.729 0.896 0.896
**Min** 0.110 -0.184 0.218 0.146 0.085 0.165 0.165
**SD** 0.227 0.134 0.266 0.248 0.229 0.251 0.251
**R²** 0.000 0.016 0.029 0.016 0.004 0.021 0.021
Table S5: Vertical Excitation Energies (eV) Using DH-GGA and RSDH-GGA Functionals.

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Table S6: Excited state properties calculated with the OLYP functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
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<td>N1</td>
<td>$S_0 \rightarrow S_3$</td>
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<td>1.621</td>
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<tr>
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<td>$S_0 \rightarrow S_3$</td>
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<td>0.711</td>
<td>H-1$\rightarrow$L (0.849)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>$\pi \rightarrow \pi^*$</td>
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Table S7: Excited state properties calculated with the BLYP functional.

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<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
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<td>N1</td>
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<tr>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>1.954</td>
<td>0.460</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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Table S8: Excited state properties calculated with the BP86 functional.

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<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
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Table S9: Excited state properties calculated with the XLYP functional.

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<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
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<td>0.846</td>
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<td>S$_0 \rightarrow$ S$_3$</td>
<td>786.7</td>
<td>1.576</td>
<td>0.118</td>
<td>H-3$\rightarrow$L (0.597)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>S$_0 \rightarrow$ S$_5$</td>
<td>571.0</td>
<td>2.171</td>
<td>0.769</td>
<td>H-1$\rightarrow$L+1 (0.547)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>S$_0 \rightarrow$ S$_7$</td>
<td>595.1</td>
<td>2.083</td>
<td>0.190</td>
<td>H-2$\rightarrow$L (0.435)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>S$_0 \rightarrow$ S$_4$</td>
<td>732.8</td>
<td>1.692</td>
<td>0.123</td>
<td>H-1$\rightarrow$L (0.870)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S10: Excited state properties calculated with the PBE functional.

<table>
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<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>S$_0 \rightarrow$ S$_3$</td>
<td>759.1</td>
<td>1.633</td>
<td>0.295</td>
<td>H-1$\rightarrow$L (0.420)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>S$_0 \rightarrow$ S$_3$</td>
<td>832.5</td>
<td>1.489</td>
<td>0.668</td>
<td>H-1$\rightarrow$L (0.853)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>S$_0 \rightarrow$ S$_2$</td>
<td>1066.4</td>
<td>1.163</td>
<td>0.024</td>
<td>H-1$\rightarrow$L (0.933)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>1093.4</td>
<td>1.134</td>
<td>0.349</td>
<td>H-1$\rightarrow$L (0.865)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>S$_0 \rightarrow$ S$_3$</td>
<td>681.3</td>
<td>1.820</td>
<td>0.097</td>
<td>H-3$\rightarrow$L (0.783)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>S$_0 \rightarrow$ S$_2$</td>
<td>627.7</td>
<td>1.975</td>
<td>0.423</td>
<td>H-1$\rightarrow$L (0.683)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>S$_0 \rightarrow$ S$_4$</td>
<td>641.8</td>
<td>1.932</td>
<td>0.825</td>
<td>H-1$\rightarrow$L (0.753)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N8</td>
<td>S$_0 \rightarrow$ S$_3$</td>
<td>924.1</td>
<td>1.342</td>
<td>0.358</td>
<td>H-1$\rightarrow$L (0.903)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>S$_0 \rightarrow$ S$_3$</td>
<td>1195.4</td>
<td>1.037</td>
<td>0.281</td>
<td>H-1$\rightarrow$L (0.902)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>S$_0 \rightarrow$ S$_3$</td>
<td>767.9</td>
<td>1.615</td>
<td>0.130</td>
<td>H-3$\rightarrow$L (0.577)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>S$_0 \rightarrow$ S$_5$</td>
<td>569.4</td>
<td>2.178</td>
<td>0.787</td>
<td>H-1$\rightarrow$L (0.563)+1</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>S$_0 \rightarrow$ S$_7$</td>
<td>588.4</td>
<td>2.107</td>
<td>0.149</td>
<td>H-2$\rightarrow$L (0.394)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>S$_0 \rightarrow$ S$_4$</td>
<td>737.5</td>
<td>1.681</td>
<td>0.121</td>
<td>H-1$\rightarrow$L (0.866)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
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Table S11: Excited state properties calculated with the mPWPW functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_3$</td>
<td>764.4</td>
<td>1.622</td>
<td>0.290</td>
<td>H-1$\rightarrow$L (0.422)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_3$</td>
<td>828.7</td>
<td>1.496</td>
<td>0.679</td>
<td>H$\rightarrow$L (0.851)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_2$</td>
<td>1065.3</td>
<td>1.164</td>
<td>0.024</td>
<td>H$\rightarrow$L (0.933)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>1101.4</td>
<td>1.126</td>
<td>0.343</td>
<td>H$\rightarrow$L (0.866)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_4$</td>
<td>683.3</td>
<td>1.814</td>
<td>0.096</td>
<td>H-3$\rightarrow$L (0.784)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>$S_0 \rightarrow S_2$</td>
<td>627.6</td>
<td>1.976</td>
<td>0.447</td>
<td>H-1$\rightarrow$L (0.733)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>$S_0 \rightarrow S_4$</td>
<td>640.2</td>
<td>1.342</td>
<td>0.358</td>
<td>H-1$\rightarrow$L (0.903)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_3$</td>
<td>923.6</td>
<td>1.432</td>
<td>0.834</td>
<td>H-2$\rightarrow$L (0.404)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_2$</td>
<td>1196.9</td>
<td>1.036</td>
<td>0.279</td>
<td>H-1$\rightarrow$L (0.901)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_3$</td>
<td>811.4</td>
<td>1.657</td>
<td>0.126</td>
<td>H-3$\rightarrow$L (0.583)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_5$</td>
<td>569.3</td>
<td>2.178</td>
<td>0.785</td>
<td>H-1$\rightarrow$L+1 (0.557)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_7$</td>
<td>587.1</td>
<td>2.112</td>
<td>0.159</td>
<td>H-2$\rightarrow$L (0.404)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>$S_0 \rightarrow S_4$</td>
<td>733.7</td>
<td>1.690</td>
<td>0.122</td>
<td>H-1$\rightarrow$L (0.867)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S12: Excited state properties calculated with the mPWLYP functional.

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<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_3$</td>
<td>772.9</td>
<td>1.604</td>
<td>0.292</td>
<td>H-1$\rightarrow$L (0.428)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_3$</td>
<td>822.7</td>
<td>1.507</td>
<td>0.710</td>
<td>H-1$\rightarrow$L (0.844)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_2$</td>
<td>1076.7</td>
<td>1.151</td>
<td>0.025</td>
<td>H-1$\rightarrow$L (0.938)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>1125.0</td>
<td>1.102</td>
<td>0.323</td>
<td>H-1$\rightarrow$L (0.865)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_4$</td>
<td>690.3</td>
<td>1.796</td>
<td>0.095</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_2$</td>
<td>634.7</td>
<td>1.953</td>
<td>0.455</td>
<td>H-1$\rightarrow$L (0.758)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>$S_0 \rightarrow S_4$</td>
<td>941.1</td>
<td>1.317</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_3$</td>
<td>1218.0</td>
<td>1.018</td>
<td>0.269</td>
<td>H-1$\rightarrow$L (0.897)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_2$</td>
<td>786.4</td>
<td>1.577</td>
<td>0.120</td>
<td>H-3$\rightarrow$L (0.590)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_5$</td>
<td>571.5</td>
<td>2.169</td>
<td>0.769</td>
<td>H-1$\rightarrow$L+1 (0.547)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_7$</td>
<td>593.2</td>
<td>2.090</td>
<td>0.182</td>
<td>H-2$\rightarrow$L (0.425)</td>
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<tr>
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<td>738.7</td>
<td>1.678</td>
<td>0.121</td>
<td>H-1$\rightarrow$L (0.870)</td>
<td>$\pi \rightarrow \pi^*$</td>
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S9
Table S13: Excited state properties calculated with the B97-D3 functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
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<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_3$</td>
<td>770.4</td>
<td>1.609</td>
<td>0.288</td>
<td>H-1$\rightarrow$L (0.438)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_3$</td>
<td>806.7</td>
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<td>0.732</td>
<td>H-1$\rightarrow$L (0.845)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_2$</td>
<td>1045.2</td>
<td>1.186</td>
<td>0.025</td>
<td>H-1$\rightarrow$L (0.934)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>1111.7</td>
<td>1.115</td>
<td>0.323</td>
<td>H-1$\rightarrow$L (0.870)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_4$</td>
<td>680.8</td>
<td>1.821</td>
<td>0.099</td>
<td>H-3$\rightarrow$L (0.782)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_2$</td>
<td>631.6</td>
<td>1.963</td>
<td>0.479</td>
<td>H-1$\rightarrow$L (0.812)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>627.5</td>
<td>1.976</td>
<td>0.883</td>
<td>H-1$\rightarrow$L (0.767)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_3$</td>
<td>903.3</td>
<td>1.373</td>
<td>0.367</td>
<td>H-1$\rightarrow$L (0.904)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_3$</td>
<td>1185.5</td>
<td>1.046</td>
<td>0.275</td>
<td>H-1$\rightarrow$L (0.896)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_3$</td>
<td>773.2</td>
<td>1.603</td>
<td>0.113</td>
<td>H-3$\rightarrow$L (0.623)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_5$</td>
<td>565.4</td>
<td>2.193</td>
<td>0.793</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_7$</td>
<td>584.1</td>
<td>2.123</td>
<td>0.165</td>
<td>H-2$\rightarrow$L (0.404)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>715.1</td>
<td>1.734</td>
<td>0.133</td>
<td>H-1$\rightarrow$L (0.861)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S14: Excited state properties calculated with the M06-L functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_3$</td>
<td>691.8</td>
<td>1.792</td>
<td>0.338</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_2$</td>
<td>1185.5</td>
<td>1.046</td>
<td>0.332</td>
<td>H-1$\rightarrow$L (0.821)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_5$</td>
<td>513.9</td>
<td>2.413</td>
<td>0.213</td>
<td>H-2$\rightarrow$L (0.425)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>968.3</td>
<td>1.280</td>
<td>0.381</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_4$</td>
<td>595.4</td>
<td>2.082</td>
<td>0.195</td>
<td>H-3$\rightarrow$L (0.690)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
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<td>$S_0 \rightarrow S_2$</td>
<td>594.5</td>
<td>2.086</td>
<td>0.545</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_4$</td>
<td>564.8</td>
<td>2.195</td>
<td>1.057</td>
<td>H-1$\rightarrow$L (0.823)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_3$</td>
<td>773.9</td>
<td>1.602</td>
<td>0.431</td>
<td>H-1$\rightarrow$L (0.915)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_4$</td>
<td>1027.4</td>
<td>1.207</td>
<td>0.309</td>
<td>H-1$\rightarrow$L (0.896)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_3$</td>
<td>672.5</td>
<td>1.844</td>
<td>0.125</td>
<td>H-3$\rightarrow$L (0.712)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_5$</td>
<td>533.7</td>
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<td>0.857</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>$S_0 \rightarrow S_3$</td>
<td>1243.9</td>
<td>0.997</td>
<td>0.138</td>
<td>H-1$\rightarrow$L (0.849)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>2.061</td>
<td>0.179</td>
<td>H-1$\rightarrow$L (0.876)</td>
<td>$\pi \rightarrow \pi^*$</td>
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</table>
Table S15: Excited state properties calculated with the TPSS functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
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<td>$S_0 \rightarrow S_3$</td>
<td>728.7</td>
<td>1.701</td>
<td>0.322</td>
<td>H-1$\rightarrow$L (0.433)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_3$</td>
<td>797.2</td>
<td>1.555</td>
<td>0.703</td>
<td>H$\rightarrow$L (0.861)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_5$</td>
<td>544.9</td>
<td>2.275</td>
<td>0.161</td>
<td>H-2$\rightarrow$L (0.389)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>1064.0</td>
<td>1.165</td>
<td>0.345</td>
<td>H$\rightarrow$L (0.880)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_3$</td>
<td>647.0</td>
<td>1.916</td>
<td>0.122</td>
<td>H-3$\rightarrow$L (0.758)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>$S_0 \rightarrow S_2$</td>
<td>615.0</td>
<td>2.016</td>
<td>0.504</td>
<td>H-1$\rightarrow$L (0.835)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>$S_0 \rightarrow S_4$</td>
<td>595.7</td>
<td>2.081</td>
<td>0.971</td>
<td>H-1$\rightarrow$L (0.794)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_3$</td>
<td>843.2</td>
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<td>0.402</td>
<td>H-1$\rightarrow$L (0.910)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_2$</td>
<td>1118.3</td>
<td>1.109</td>
<td>0.297</td>
<td>H-1$\rightarrow$L (0.901)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_3$</td>
<td>729.1</td>
<td>1.701</td>
<td>0.120</td>
<td>H-3$\rightarrow$L (0.642)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_5$</td>
<td>553.3</td>
<td>2.241</td>
<td>0.821</td>
<td>H-1$\rightarrow$L+1 (0.590)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_4$</td>
<td>631.4</td>
<td>1.964</td>
<td>0.024</td>
<td>H-1$\rightarrow$L+1 (0.847)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>$S_0 \rightarrow S_4$</td>
<td>657.7</td>
<td>1.885</td>
<td>0.150</td>
<td>H-1$\rightarrow$L (0.863)</td>
<td>$\pi \rightarrow \pi^*$</td>
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</table>

Table S16: Excited state properties calculated with the O3LYP functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_1$</td>
<td>1376.7</td>
<td>0.901</td>
<td>0.311</td>
<td>H$\rightarrow$L (0.978)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_2$</td>
<td>867.5</td>
<td>1.429</td>
<td>0.565</td>
<td>H-1$\rightarrow$L (0.942)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>1210.5</td>
<td>1.024</td>
<td>0.324</td>
<td>H$\rightarrow$L (0.989)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>771.9</td>
<td>1.606</td>
<td>0.616</td>
<td>H-1$\rightarrow$L (0.967)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_4$</td>
<td>453.1</td>
<td>2.736</td>
<td>1.084</td>
<td>H-1$\rightarrow$L (0.704)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>$S_0 \rightarrow S_2$</td>
<td>570.6</td>
<td>2.173</td>
<td>0.516</td>
<td>H-1$\rightarrow$L (0.906)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>$S_0 \rightarrow S_3$</td>
<td>730.2</td>
<td>1.698</td>
<td>0.171</td>
<td>H-2$\rightarrow$L (0.751)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_3$</td>
<td>635.9</td>
<td>1.950</td>
<td>0.531</td>
<td>H-1$\rightarrow$L (0.979)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_2$</td>
<td>842.6</td>
<td>1.471</td>
<td>0.486</td>
<td>H-1$\rightarrow$L (0.943)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_2$</td>
<td>1081.3</td>
<td>1.147</td>
<td>0.166</td>
<td>H-1$\rightarrow$L (0.575)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_2$</td>
<td>1211.0</td>
<td>1.024</td>
<td>0.179</td>
<td>H-2$\rightarrow$L+1 (0.979)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_3$</td>
<td>785.2</td>
<td>1.579</td>
<td>0.272</td>
<td>H-1$\rightarrow$L (0.952)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>$S_0 \rightarrow S_1$</td>
<td>1263.3</td>
<td>0.981</td>
<td>0.200</td>
<td>H$\rightarrow$L (0.986)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
</tbody>
</table>
Table S17: Excited state properties calculated with the B3LYP functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>( S_0 \to S_1 )</td>
<td>982.2</td>
<td>1.262</td>
<td>0.498</td>
<td>H( \to )L (0.993)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N2</td>
<td>( S_0 \to S_1 )</td>
<td>1060.0</td>
<td>1.170</td>
<td>0.580</td>
<td>H( \to )L (0.987)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N3</td>
<td>( S_0 \to S_1 )</td>
<td>901.8</td>
<td>1.375</td>
<td>0.457</td>
<td>H( \to )L (0.984)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N4</td>
<td>( S_0 \to S_1 )</td>
<td>639.3</td>
<td>1.939</td>
<td>0.842</td>
<td>H( \to )L (0.986)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N5</td>
<td>( S_0 \to S_1 )</td>
<td>1162.9</td>
<td>1.066</td>
<td>0.017</td>
<td>H( \to )L (0.984)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N6</td>
<td>( S_0 \to S_1 )</td>
<td>794.3</td>
<td>1.561</td>
<td>0.304</td>
<td>H( \to )L (0.972)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N7</td>
<td>( S_0 \to S_1 )</td>
<td>900.2</td>
<td>1.377</td>
<td>0.020</td>
<td>H( \to )L (0.928)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N8</td>
<td>( S_0 \to S_1 )</td>
<td>959.3</td>
<td>1.292</td>
<td>0.269</td>
<td>H( \to )L (0.982)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N9</td>
<td>( S_0 \to S_1 )</td>
<td>1471.4</td>
<td>0.843</td>
<td>0.112</td>
<td>H( \to )L (0.984)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N10</td>
<td>( S_0 \to S_1 )</td>
<td>1472.8</td>
<td>0.837</td>
<td>0.110</td>
<td>H( \to )L (0.984)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N11</td>
<td>( S_0 \to S_1 )</td>
<td>1193.1</td>
<td>1.039</td>
<td>0.048</td>
<td>H( \to )L (0.825)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N12</td>
<td>( S_0 \to S_1 )</td>
<td>956.8</td>
<td>1.296</td>
<td>0.255</td>
<td>H( \to )L (0.987)</td>
<td>( \pi \to \pi^* )</td>
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Table S18: Excited state properties calculated with the B3P86 functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>( S_0 \to S_1 )</td>
<td>974.1</td>
<td>1.273</td>
<td>0.501</td>
<td>H( \to )L (0.993)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N2</td>
<td>( S_0 \to S_1 )</td>
<td>1056.8</td>
<td>1.173</td>
<td>0.572</td>
<td>H( \to )L (0.987)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N3</td>
<td>( S_0 \to S_1 )</td>
<td>901.1</td>
<td>1.376</td>
<td>0.458</td>
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<td>( \pi \to \pi^* )</td>
</tr>
<tr>
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<td>( S_0 \to S_1 )</td>
<td>637.5</td>
<td>1.945</td>
<td>0.859</td>
<td>H( \to )L (0.986)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N5</td>
<td>( S_0 \to S_1 )</td>
<td>1153.1</td>
<td>1.075</td>
<td>0.017</td>
<td>H( \to )L (0.984)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N6</td>
<td>( S_0 \to S_1 )</td>
<td>807.3</td>
<td>1.536</td>
<td>0.288</td>
<td>H( \to )L (0.974)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N7</td>
<td>( S_0 \to S_1 )</td>
<td>898.3</td>
<td>1.380</td>
<td>0.019</td>
<td>H( \to )L (0.929)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N8</td>
<td>( S_0 \to S_1 )</td>
<td>963.6</td>
<td>1.287</td>
<td>0.263</td>
<td>H( \to )L (0.983)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N9</td>
<td>( S_0 \to S_1 )</td>
<td>1480.6</td>
<td>0.837</td>
<td>0.110</td>
<td>H( \to )L (0.984)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N10</td>
<td>( S_0 \to S_1 )</td>
<td>843.3</td>
<td>1.470</td>
<td>0.370</td>
<td>H( \to )L (0.964)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N11</td>
<td>( S_0 \to S_1 )</td>
<td>1472.8</td>
<td>0.842</td>
<td>0.258</td>
<td>H( \to )L (0.990)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N12</td>
<td>( S_0 \to S_1 )</td>
<td>1162.8</td>
<td>1.066</td>
<td>0.050</td>
<td>H( \to )L (0.804)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N13</td>
<td>( S_0 \to S_1 )</td>
<td>961.9</td>
<td>1.289</td>
<td>0.260</td>
<td>H( \to )L (0.987)</td>
<td>( \pi \to \pi^* )</td>
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</table>
Table S19: Excited state properties calculated with the X3LYP functional.

<table>
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<th>Compound</th>
<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>921.3</td>
<td>1.346</td>
<td>0.549</td>
<td>H( \rightarrow )L (0.993)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N2</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>959.9</td>
<td>1.292</td>
<td>0.706</td>
<td>H( \rightarrow )L (0.977)</td>
<td>( \pi \rightarrow \pi^* )</td>
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<tr>
<td>N3</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>854.0</td>
<td>1.452</td>
<td>0.491</td>
<td>H( \rightarrow )L (0.981)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N4</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>616.9</td>
<td>2.010</td>
<td>0.897</td>
<td>H( \rightarrow )L (0.984)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>1087.3</td>
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<td>0.018</td>
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<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>1297.6</td>
<td>1.289</td>
<td>0.138</td>
<td>H( \rightarrow )L (0.980)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N7</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>1008.5</td>
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<td>0.652</td>
<td>H( \rightarrow )L (0.994)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>884.8</td>
<td>1.401</td>
<td>0.311</td>
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<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N9</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>750.6</td>
<td>1.652</td>
<td>0.387</td>
<td>H( \rightarrow )L (0.954)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N10</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>867.6</td>
<td>1.429</td>
<td>0.068</td>
<td>H( \rightarrow )L (0.633)</td>
<td>( \pi \rightarrow \pi^* )</td>
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<td>( S_0 \rightarrow S_1 )</td>
<td>840.6</td>
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<td>0.307</td>
<td>H( \rightarrow )L (0.982)</td>
<td>( \pi \rightarrow \pi^* )</td>
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Table S20: Excited state properties calculated with the PBE0 functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>820.5</td>
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<td>0.652</td>
<td>H( \rightarrow )L (0.989)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N2</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>814.9</td>
<td>1.521</td>
<td>0.958</td>
<td>H( \rightarrow )L (0.946)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N3</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>778.5</td>
<td>1.593</td>
<td>0.555</td>
<td>H( \rightarrow )L (0.974)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N4</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>580.5</td>
<td>2.136</td>
<td>1.017</td>
<td>H( \rightarrow )L (0.975)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N5</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>962.1</td>
<td>1.289</td>
<td>0.023</td>
<td>H( \rightarrow )L (0.973)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N6</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>625.9</td>
<td>1.981</td>
<td>0.539</td>
<td>H( \rightarrow )L (0.979)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N7</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>750.6</td>
<td>1.652</td>
<td>0.010</td>
<td>H( \rightarrow )L (0.893)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N8</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>777.8</td>
<td>1.594</td>
<td>0.387</td>
<td>H( \rightarrow )L (0.954)</td>
<td>( \pi \rightarrow \pi^* )</td>
</tr>
<tr>
<td>N9</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>1068.5</td>
<td>1.160</td>
<td>0.189</td>
<td>H( \rightarrow )L (0.968)</td>
<td>( \pi \rightarrow \pi^* )</td>
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<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>742.2</td>
<td>1.670</td>
<td>0.452</td>
<td>H( \rightarrow )L (0.958)</td>
<td>( \pi \rightarrow \pi^* )</td>
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<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>1049.2</td>
<td>1.182</td>
<td>0.434</td>
<td>H( \rightarrow )L (0.963)</td>
<td>( \pi \rightarrow \pi^* )</td>
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<tr>
<td>N12</td>
<td>( S_0 \rightarrow S_1 )</td>
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<td>0.068</td>
<td>H( \rightarrow )L (0.633)</td>
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<tr>
<td>N13</td>
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<td>840.6</td>
<td>1.475</td>
<td>0.307</td>
<td>H( \rightarrow )L (0.982)</td>
<td>( \pi \rightarrow \pi^* )</td>
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Table S21: Excited state properties calculated with the mPW1PW functional.

<table>
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<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>819.1</td>
<td>1.514</td>
<td>0.655</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
<td>N2</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>814.1</td>
<td>1.523</td>
<td>0.966</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
<td>N3</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>776.6</td>
<td>1.596</td>
<td>0.556</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
<td>N4</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>580.4</td>
<td>2.136</td>
<td>1.011</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>961.1</td>
<td>1.290</td>
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<tr>
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<td>0.551</td>
<td>( \pi \rightarrow \pi^* )</td>
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<td>( S_0 \rightarrow S_1 )</td>
<td>750.1</td>
<td>1.653</td>
<td>0.011</td>
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</tr>
<tr>
<td>N8</td>
<td>( S_0 \rightarrow S_1 )</td>
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<td>0.392</td>
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<td>1.673</td>
<td>0.453</td>
<td>( \pi \rightarrow \pi^* )</td>
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<tr>
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<td>( S_0 \rightarrow S_1 )</td>
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<td>1.187</td>
<td>0.436</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
<td>N12</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>863.7</td>
<td>1.436</td>
<td>0.069</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
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<td>1.481</td>
<td>0.307</td>
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Table S22: Excited state properties calculated with the mPW1LYP functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>826.8</td>
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<td>0.653</td>
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<tr>
<td>N2</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>822.0</td>
<td>1.508</td>
<td>0.976</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
<td>N3</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>777.0</td>
<td>1.596</td>
<td>0.558</td>
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</tr>
<tr>
<td>N4</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>581.4</td>
<td>2.133</td>
<td>0.993</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
<td>N5</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>972.5</td>
<td>1.275</td>
<td>0.022</td>
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<tr>
<td>N6</td>
<td>( S_0 \rightarrow S_1 )</td>
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<td>2.018</td>
<td>0.581</td>
<td>( \pi \rightarrow \pi^* )</td>
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</tr>
<tr>
<td>N7</td>
<td>( S_0 \rightarrow S_1 )</td>
<td>747.9</td>
<td>1.658</td>
<td>0.017</td>
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</tr>
<tr>
<td>N8</td>
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<td>772.8</td>
<td>1.604</td>
<td>0.403</td>
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</tr>
<tr>
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<td>( S_0 \rightarrow S_1 )</td>
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<td>0.205</td>
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<tr>
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<td>1.665</td>
<td>0.450</td>
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<tr>
<td>N11</td>
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<td>N12</td>
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<td>868.7</td>
<td>1.427</td>
<td>0.070</td>
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<tr>
<td>N13</td>
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<td>833.6</td>
<td>1.487</td>
<td>0.300</td>
<td>( \pi \rightarrow \pi^* )</td>
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Table S23: Excited state properties calculated with the BH&HLYP functional.

<table>
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<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_1$</td>
<td>499.2</td>
<td>2.483</td>
<td>1.569</td>
<td>H$\rightarrow$L (0.758)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
<td>500.9</td>
<td>2.475</td>
<td>2.618</td>
<td>H$\rightarrow$L (0.572)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>478.0</td>
<td>2.594</td>
<td>1.256</td>
<td>H$\rightarrow$L (0.784)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>435.6</td>
<td>2.846</td>
<td>1.568</td>
<td>H$\rightarrow$L (0.773)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_1$</td>
<td>529.9</td>
<td>2.340</td>
<td>0.129</td>
<td>H$\rightarrow$L (0.841)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>466.2</td>
<td>2.659</td>
<td>1.037</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>427.0</td>
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<td>1.816</td>
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<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>466.7</td>
<td>2.656</td>
<td>1.135</td>
<td>H$\rightarrow$L (0.565)</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>478.8</td>
<td>2.590</td>
<td>1.257</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
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<td>493.4</td>
<td>2.513</td>
<td>1.822</td>
<td>H$\rightarrow$L (0.422)</td>
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<td>$S_0 \rightarrow S_1$</td>
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<td>489.5</td>
<td>2.533</td>
<td>0.741</td>
<td>H$\rightarrow$L (0.877)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S24: Excited state properties calculated with the TPSSh functional.

<table>
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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
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<td>$S_0 \rightarrow S_2$</td>
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<td>864.5</td>
<td>1.434</td>
<td>0.588</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>$S_0 \rightarrow S_2$</td>
<td>494.6</td>
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<td>0.266</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>782.3</td>
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<td>0.577</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_2$</td>
<td>453.2</td>
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<td>H$\rightarrow$L (0.686)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_2$</td>
<td>563.4</td>
<td>2.201</td>
<td>0.534</td>
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<td>518.3</td>
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<td>H$\rightarrow$L (0.828)</td>
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<td>$S_0 \rightarrow S_2$</td>
<td>831.7</td>
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<td>0.497</td>
<td>H$\rightarrow$L (0.936)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_2$</td>
<td>1042.4</td>
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<td>$S_0 \rightarrow S_3$</td>
<td>790.5</td>
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<td>0.268</td>
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<td>1.029</td>
<td>0.201</td>
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Table S25: Excited state properties calculated with the TPSS0 functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
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<td>$S_0 \rightarrow S_1$</td>
<td>789.4</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>784.0</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>750.9</td>
<td>1.651</td>
<td>0.582</td>
<td>H$\rightarrow$L (0.973)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>567.8</td>
<td>2.183</td>
<td>1.023</td>
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<td>$S_0 \rightarrow S_3$</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>592.7</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>468.0</td>
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<td>1.605</td>
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<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>745.6</td>
<td>1.663</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>709.4</td>
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<td>0.491</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>1.261</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>789.4</td>
<td>1.571</td>
<td>0.324</td>
<td>H$\rightarrow$L (0.982)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S26: Excited state properties calculated with the M06 functional.

<table>
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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
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<td>0.761</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>716.9</td>
<td>1.729</td>
<td>1.270</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>713.8</td>
<td>1.737</td>
<td>0.610</td>
<td>H$\rightarrow$L (0.959)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>555.4</td>
<td>2.233</td>
<td>1.102</td>
<td>H$\rightarrow$L (0.954)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_2$</td>
<td>423.6</td>
<td>2.927</td>
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<td>H-1$\rightarrow$L (0.829)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>651.5</td>
<td>2.208</td>
<td>0.746</td>
<td>H$\rightarrow$L (0.939)</td>
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<tr>
<td>N7</td>
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<td>478.4</td>
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<tr>
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<td>682.1</td>
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<td>850.2</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>707.2</td>
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<tr>
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<td>0.631</td>
<td>H$\rightarrow$L (0.917)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_1$</td>
<td>747.4</td>
<td>1.659</td>
<td>0.075</td>
<td>H$\rightarrow$L (0.502)</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>820.8</td>
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<td>0.338</td>
<td>H$\rightarrow$L (0.978)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S27: Excited state properties calculated with the M06-2X functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
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<tbody>
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<td>$S_0 \rightarrow S_1$</td>
<td>497.3</td>
<td>2.493</td>
<td>1.528</td>
<td>H$\rightarrow$L (0.739)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
<td>490.7</td>
<td>2.526</td>
<td>2.548</td>
<td>H$\rightarrow$L (0.517)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>487.7</td>
<td>2.542</td>
<td>1.192</td>
<td>H$\rightarrow$L (0.776)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>454.6</td>
<td>2.727</td>
<td>1.517</td>
<td>H$\rightarrow$L (0.792)</td>
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<td>0.137</td>
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</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>469.5</td>
<td>2.641</td>
<td>1.002</td>
<td>H$\rightarrow$L (0.790)</td>
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<tr>
<td>N7</td>
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<td>1.773</td>
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<td>2.597</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>486.1</td>
<td>2.551</td>
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<td>H$\rightarrow$L (0.840)</td>
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<td>1.617</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>452.4</td>
<td>2.741</td>
<td>0.153</td>
<td>H-1$\rightarrow$L+1 (0.314)</td>
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<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>508.5</td>
<td>2.438</td>
<td>0.669</td>
<td>H$\rightarrow$L (0.867)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S28: Excited state properties calculated with the LC-BLYP functional.

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<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
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<tbody>
<tr>
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<td>2.853</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>439.4</td>
<td>2.822</td>
<td>2.699</td>
<td>H$\rightarrow$L (0.305)</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>419.3</td>
<td>2.957</td>
<td>1.481</td>
<td>H$\rightarrow$L (0.494)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>417.3</td>
<td>2.971</td>
<td>1.635</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>398.0</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>438.7</td>
<td>2.826</td>
<td>1.063</td>
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<td>1.796</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>404.6</td>
<td>3.064</td>
<td>1.349</td>
<td>H-1$\rightarrow$L (0.441)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>423.5</td>
<td>2.928</td>
<td>1.357</td>
<td>H-1$\rightarrow$L (0.399)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>2.693</td>
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<td>394.8</td>
<td>3.140</td>
<td>1.098</td>
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Table S29: Excited state properties calculated with the CAM-B3LYP functional.

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<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
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<td>484.6</td>
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<td>483.2</td>
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<td>2.655</td>
<td>H(\rightarrow)L (0.451) (\pi \rightarrow \pi^*)</td>
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<td>470.9</td>
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<td>1.268</td>
<td>H(\rightarrow)L (0.708) (\pi \rightarrow \pi^*)</td>
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<td>( S_0 \rightarrow S_1 )</td>
<td>445.0</td>
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<td>H(\rightarrow)L (0.745) (\pi \rightarrow \pi^*)</td>
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<td>501.8</td>
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<td>0.182</td>
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<td>2.654</td>
<td>1.011</td>
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<td>( S_0 \rightarrow S_1 )</td>
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<td>1.288</td>
<td>H-1(\rightarrow)L (0.401) (\pi \rightarrow \pi^*)</td>
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<tr>
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<td>( S_0 \rightarrow S_1 )</td>
<td>467.6</td>
<td>2.651</td>
<td>1.056</td>
<td>H(\rightarrow)L (0.798) (\pi \rightarrow \pi^*)</td>
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<td>489.1</td>
<td>2.535</td>
<td>1.654</td>
<td>H-1(\rightarrow)L (0.497) (\pi \rightarrow \pi^*)</td>
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<td>0.148</td>
<td>H-1(\rightarrow)L+1 (0.390) (\pi \rightarrow \pi^*)</td>
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<td>2.587</td>
<td>0.783</td>
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Table S30: Excited state properties calculated with the \(\omega\)B97 functional.

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<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
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<tbody>
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<td>( S_0 \rightarrow S_1 )</td>
<td>418.7</td>
<td>2.961</td>
<td>1.796</td>
<td>H(\rightarrow)L (0.437) (\pi \rightarrow \pi^*)</td>
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<td>( S_0 \rightarrow S_1 )</td>
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<td>401.3</td>
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<td>1.567</td>
<td>H(\rightarrow)L (0.460) (\pi \rightarrow \pi^*)</td>
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<td>( S_0 \rightarrow S_1 )</td>
<td>392.1</td>
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<td>1.735</td>
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<td>( S_0 \rightarrow S_1 )</td>
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<td>3.294</td>
<td>1.252</td>
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<td>422.3</td>
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<td>H(\rightarrow)L (0.798) (\pi \rightarrow \pi^*)</td>
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<td>393.8</td>
<td>3.148</td>
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<td>443.9</td>
<td>2.793</td>
<td>1.507</td>
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Table S31: Excited state properties calculated with the $\omega$B97X functional.

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<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
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<tr>
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<td>$S_0 \rightarrow S_1$</td>
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<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
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<td>$S_0 \rightarrow S_1$</td>
<td>404.6</td>
<td>3.065</td>
<td>1.690</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>401.2</td>
<td>3.090</td>
<td>1.356</td>
<td>H-1$\rightarrow$L (0.441)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>419.6</td>
<td>2.955</td>
<td>1.357</td>
<td>H-1$\rightarrow$L (0.377)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>$S_0 \rightarrow S_1$</td>
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<td>3.064</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<td>1.211</td>
<td>H$\rightarrow$L (0.566)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
</tbody>
</table>

Table S32: Excited state properties calculated with the $\omega$B97X-D3 functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_1$</td>
<td>438.4</td>
<td>2.828</td>
<td>1.790</td>
<td>H$\rightarrow$L (0.493)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
<td>445.6</td>
<td>2.782</td>
<td>2.776</td>
<td>H$\rightarrow$L (0.339)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>423.0</td>
<td>2.931</td>
<td>1.480</td>
<td>H$\rightarrow$L (0.526)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>415.2</td>
<td>2.986</td>
<td>1.655</td>
<td>H$\rightarrow$L (0.635)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_1$</td>
<td>404.6</td>
<td>3.064</td>
<td>0.806</td>
<td>H$\rightarrow$L (0.412)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>$S_0 \rightarrow S_1$</td>
<td>441.8</td>
<td>2.806</td>
<td>1.058</td>
<td>H$\rightarrow$L (0.781)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>$S_0 \rightarrow S_1$</td>
<td>405.5</td>
<td>3.058</td>
<td>1.305</td>
<td>H-1$\rightarrow$L (0.432)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_1$</td>
<td>429.7</td>
<td>2.885</td>
<td>1.340</td>
<td>H-1$\rightarrow$L (0.396)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_1$</td>
<td>415.6</td>
<td>2.983</td>
<td>1.302</td>
<td>H$\rightarrow$L (0.656)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_1$</td>
<td>461.3</td>
<td>2.688</td>
<td>1.532</td>
<td>H-1$\rightarrow$L (0.534)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_1$</td>
<td>415.5</td>
<td>2.984</td>
<td>0.155</td>
<td>H-1$\rightarrow$L+1 (0.413)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_1$</td>
<td>401.8</td>
<td>3.086</td>
<td>1.107</td>
<td>H$\rightarrow$L (0.613)</td>
<td>$\pi \rightarrow \pi^*$</td>
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Table S33: Excited state properties calculated with the ωB97X-D3(BJ) functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>λ_{max} (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>S_0 → S_1</td>
<td>426.4</td>
<td>2.908</td>
<td>1.803</td>
<td>H→L (0.470)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N2</td>
<td>S_0 → S_1</td>
<td>433.5</td>
<td>2.860</td>
<td>2.782</td>
<td>H→L (0.332)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N3</td>
<td>S_0 → S_1</td>
<td>408.8</td>
<td>3.033</td>
<td>1.542</td>
<td>H→L (0.497)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N4</td>
<td>S_0 → S_1</td>
<td>400.8</td>
<td>3.093</td>
<td>1.699</td>
<td>H→L (0.615)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N5</td>
<td>S_0 → S_1</td>
<td>385.4</td>
<td>3.217</td>
<td>1.076</td>
<td>H-1→L (0.494)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N6</td>
<td>S_0 → S_1</td>
<td>395.7</td>
<td>3.133</td>
<td>1.837</td>
<td>H-1→L (0.693)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N7</td>
<td>S_0 → S_1</td>
<td>398.9</td>
<td>3.108</td>
<td>1.360</td>
<td>H-1→L (0.434)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N8</td>
<td>S_0 → S_1</td>
<td>416.6</td>
<td>2.976</td>
<td>1.362</td>
<td>H-1→L (0.370)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N9</td>
<td>S_0 → S_1</td>
<td>401.6</td>
<td>3.087</td>
<td>1.370</td>
<td>H-1→L (0.630)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N10</td>
<td>S_0 → S_1</td>
<td>449.0</td>
<td>2.761</td>
<td>1.545</td>
<td>H-1→L (0.524)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N11</td>
<td>S_0 → S_1</td>
<td>401.5</td>
<td>3.088</td>
<td>0.178</td>
<td>H-1→L+1 (0.381)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N12</td>
<td>S_0 → S_1</td>
<td>381.2</td>
<td>3.253</td>
<td>1.226</td>
<td>H→L (0.573)</td>
<td>π → π*</td>
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Table S34: Excited state properties calculated with the ωB97X-V functional.

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<th>Compound</th>
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<th>λ_{max} (nm)</th>
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<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>S_0 → S_1</td>
<td>426.3</td>
<td>2.908</td>
<td>1.803</td>
<td>H→L (0.470)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N2</td>
<td>S_0 → S_1</td>
<td>433.5</td>
<td>2.860</td>
<td>2.782</td>
<td>H→L (0.332)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N3</td>
<td>S_0 → S_1</td>
<td>408.8</td>
<td>3.033</td>
<td>1.542</td>
<td>H→L (0.497)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N4</td>
<td>S_0 → S_1</td>
<td>400.8</td>
<td>3.093</td>
<td>1.699</td>
<td>H→L (0.615)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N5</td>
<td>S_0 → S_1</td>
<td>385.4</td>
<td>3.217</td>
<td>1.076</td>
<td>H-1→L (0.494)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N6</td>
<td>S_0 → S_1</td>
<td>395.7</td>
<td>3.133</td>
<td>1.837</td>
<td>H-1→L (0.693)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N7</td>
<td>S_0 → S_1</td>
<td>398.9</td>
<td>3.108</td>
<td>1.360</td>
<td>H-1→L (0.434)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N8</td>
<td>S_0 → S_1</td>
<td>416.6</td>
<td>2.976</td>
<td>1.362</td>
<td>H→L (0.573)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N9</td>
<td>S_0 → S_1</td>
<td>401.6</td>
<td>3.087</td>
<td>1.370</td>
<td>H→L (0.630)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N10</td>
<td>S_0 → S_1</td>
<td>449.0</td>
<td>2.761</td>
<td>1.545</td>
<td>H-1→L (0.524)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N11</td>
<td>S_0 → S_1</td>
<td>401.5</td>
<td>3.088</td>
<td>0.178</td>
<td>H-1→L+1 (0.381)</td>
<td>π → π*</td>
</tr>
<tr>
<td>N12</td>
<td>S_0 → S_1</td>
<td>381.2</td>
<td>3.253</td>
<td>1.226</td>
<td>H→L (0.573)</td>
<td>π → π*</td>
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</table>
Table S35: Excited state properties calculated with the B2PLYP functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_1$</td>
<td>565.7</td>
<td>2.192</td>
<td>1.404</td>
<td>H$\rightarrow$L (0.722)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
<td>539.7</td>
<td>2.297</td>
<td>2.449</td>
<td>H$\rightarrow$L (0.545)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>562.3</td>
<td>2.205</td>
<td>1.099</td>
<td>H$\rightarrow$L (0.749)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>523.4</td>
<td>2.369</td>
<td>1.314</td>
<td>H$\rightarrow$L (0.746)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<td>N5</td>
<td>$S_0 \rightarrow S_1$</td>
<td>713.0</td>
<td>1.739</td>
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<tr>
<td>N6</td>
<td>$S_0 \rightarrow S_1$</td>
<td>516.3</td>
<td>2.401</td>
<td>0.941</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>452.0</td>
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<td>1.710</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_1$</td>
<td>525.0</td>
<td>2.362</td>
<td>1.157</td>
<td>H$\rightarrow$L (0.491)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_1$</td>
<td>560.9</td>
<td>2.210</td>
<td>0.906</td>
<td>H$\rightarrow$L (0.819)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>553.4</td>
<td>2.240</td>
<td>1.626</td>
<td>H-1$\rightarrow$L (0.441)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_1$</td>
<td>542.1</td>
<td>2.287</td>
<td>0.184</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N13</td>
<td>$S_0 \rightarrow S_1$</td>
<td>650.5</td>
<td>1.906</td>
<td>0.594</td>
<td>H$\rightarrow$L (0.850)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
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</table>

Table S36: Excited state properties calculated with the B2GPPLYP functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_1$</td>
<td>503.4</td>
<td>2.463</td>
<td>1.596</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
<td>494.2</td>
<td>2.509</td>
<td>2.660</td>
<td>H$\rightarrow$L (0.468)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>491.2</td>
<td>2.524</td>
<td>1.324</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_1$</td>
<td>513.1</td>
<td>2.416</td>
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<td>H$\rightarrow$L (0.534)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>491.4</td>
<td>2.523</td>
<td>0.998</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N7</td>
<td>$S_0 \rightarrow S_1$</td>
<td>431.5</td>
<td>2.874</td>
<td>1.758</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_1$</td>
<td>459.9</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>472.0</td>
<td>2.627</td>
<td>1.274</td>
<td>H$\rightarrow$L (0.464)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_1$</td>
<td>489.8</td>
<td>2.531</td>
<td>1.132</td>
<td>H$\rightarrow$L (0.722)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_1$</td>
<td>513.0</td>
<td>2.417</td>
<td>1.732</td>
<td>H-1$\rightarrow$L (0.463)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_1$</td>
<td>497.9</td>
<td>2.490</td>
<td>0.338</td>
<td>H-1$\rightarrow$L (0.334)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>$S_0 \rightarrow S_1$</td>
<td>526.5</td>
<td>2.355</td>
<td>0.908</td>
<td>H$\rightarrow$L (0.726)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
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</table>
Table S37: Excited state properties calculated with the mPW2PLYP functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
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<td>S$_0 \rightarrow$ S$_1$</td>
<td>542.5</td>
<td>2.285</td>
<td>1.472</td>
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<tr>
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<td>S$_0 \rightarrow$ S$_1$</td>
<td>524.9</td>
<td>2.362</td>
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<td>S$_0 \rightarrow$ S$_1$</td>
<td>534.7</td>
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<td>1.170</td>
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</tr>
<tr>
<td>N4</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>502.4</td>
<td>2.468</td>
<td>1.373</td>
<td>H$\rightarrow$L (0.730)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>649.0</td>
<td>1.910</td>
<td>0.164</td>
<td>H$\rightarrow$L (0.781)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>502.4</td>
<td>2.468</td>
<td>1.373</td>
<td>H$\rightarrow$L (0.730)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>502.4</td>
<td>2.468</td>
<td>1.373</td>
<td>H$\rightarrow$L (0.730)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>502.4</td>
<td>2.468</td>
<td>1.373</td>
<td>H$\rightarrow$L (0.730)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>502.4</td>
<td>2.468</td>
<td>1.373</td>
<td>H$\rightarrow$L (0.730)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>502.4</td>
<td>2.468</td>
<td>1.373</td>
<td>H$\rightarrow$L (0.730)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>502.4</td>
<td>2.468</td>
<td>1.373</td>
<td>H$\rightarrow$L (0.730)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
</tbody>
</table>

Table S38: Excited state properties calculated with the DSD-BLYP functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>532.3</td>
<td>2.329</td>
<td>1.485</td>
<td>H$\rightarrow$L (0.537)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>493.0</td>
<td>2.513</td>
<td>1.097</td>
<td>H$\rightarrow$L (0.521)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>506.9</td>
<td>2.446</td>
<td>1.200</td>
<td>H$\rightarrow$L (0.483)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>S$_0 \rightarrow$ S$_1$</td>
<td>504.8</td>
<td>2.456</td>
<td>0.964</td>
<td>H$\rightarrow$L (0.868)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
</tbody>
</table>
Table S39: Excited state properties calculated with the DSD-PBEP86 functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_1$</td>
<td>556.8</td>
<td>2.227</td>
<td>1.431</td>
<td>$H \rightarrow L$ (0.558)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
<td>510.3</td>
<td>2.430</td>
<td>2.546</td>
<td>$H \rightarrow L$ (0.439)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>576.1</td>
<td>2.152</td>
<td>1.134</td>
<td>$H \rightarrow L$ (0.575)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>669.0</td>
<td>1.853</td>
<td>1.045</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_1$</td>
<td>564.0</td>
<td>2.198</td>
<td>0.788</td>
<td>$H \rightarrow L$ (0.530)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>$S_0 \rightarrow S_1$</td>
<td>565.1</td>
<td>2.194</td>
<td>0.871</td>
<td>$H \rightarrow L$ (0.870)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>$S_0 \rightarrow S_1$</td>
<td>451.1</td>
<td>2.749</td>
<td>1.661</td>
<td>$H \rightarrow L$ (0.773)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_1$</td>
<td>482.6</td>
<td>2.569</td>
<td>1.161</td>
<td>$H \rightarrow L$ (0.437)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_1$</td>
<td>497.9</td>
<td>2.490</td>
<td>1.187</td>
<td>$H \rightarrow L$ (0.458)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N10</td>
<td>$S_0 \rightarrow S_1$</td>
<td>595.7</td>
<td>2.081</td>
<td>0.952</td>
<td>$H \rightarrow L$ (0.674)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N11</td>
<td>$S_0 \rightarrow S_1$</td>
<td>598.8</td>
<td>2.070</td>
<td>1.468</td>
<td>$H \rightarrow L$ (0.461)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N12</td>
<td>$S_0 \rightarrow S_1$</td>
<td>708.5</td>
<td>1.750</td>
<td>0.345</td>
<td>$H \rightarrow L$ (0.424)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N13</td>
<td>$S_0 \rightarrow S_1$</td>
<td>803.2</td>
<td>1.544</td>
<td>0.652</td>
<td>$H \rightarrow L$ (0.656)</td>
<td>$\pi \rightarrow \pi^*$</td>
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</table>

Table S40: Excited state properties calculated with the $\omega$B2PLYP functional.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>$\lambda_{\text{max}}$ (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength</th>
<th>MO designation (coefficient)</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>$S_0 \rightarrow S_1$</td>
<td>434.7</td>
<td>2.852</td>
<td>1.747</td>
<td>$H \rightarrow L$ (0.455)</td>
<td>$\pi \rightarrow \pi^*$</td>
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<tr>
<td>N2</td>
<td>$S_0 \rightarrow S_1$</td>
<td>437.7</td>
<td>2.833</td>
<td>2.762</td>
<td>$H \rightarrow L$ (0.354)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N3</td>
<td>$S_0 \rightarrow S_1$</td>
<td>417.8</td>
<td>2.968</td>
<td>1.525</td>
<td>$H \rightarrow L$ (0.466)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N4</td>
<td>$S_0 \rightarrow S_1$</td>
<td>415.0</td>
<td>2.987</td>
<td>1.658</td>
<td>$H \rightarrow L$ (0.553)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N5</td>
<td>$S_0 \rightarrow S_1$</td>
<td>386.6</td>
<td>3.207</td>
<td>1.384</td>
<td>$H \rightarrow L$ (0.715)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N6</td>
<td>$S_0 \rightarrow S_1$</td>
<td>442.3</td>
<td>2.803</td>
<td>1.093</td>
<td>$H \rightarrow L$ (0.842)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N7</td>
<td>$S_0 \rightarrow S_1$</td>
<td>399.0</td>
<td>3.107</td>
<td>1.804</td>
<td>$H \rightarrow L$ (0.767)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N8</td>
<td>$S_0 \rightarrow S_1$</td>
<td>399.9</td>
<td>3.100</td>
<td>1.383</td>
<td>$H \rightarrow L$ (0.400)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
<td>N9</td>
<td>$S_0 \rightarrow S_1$</td>
<td>417.4</td>
<td>2.970</td>
<td>1.353</td>
<td>$H \rightarrow L$ (0.401)</td>
<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
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<td>$\pi \rightarrow \pi^*$</td>
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<tr>
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<td>460.0</td>
<td>2.695</td>
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<td>418.4</td>
<td>2.963</td>
<td>0.618</td>
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<td>$\pi \rightarrow \pi^*$</td>
</tr>
<tr>
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<td>$S_0 \rightarrow S_1$</td>
<td>392.6</td>
<td>3.158</td>
<td>1.386</td>
<td>$H \rightarrow L$ (0.505)</td>
<td>$\pi \rightarrow \pi^*$</td>
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</table>
Table S41: Excited state properties calculated with the ωB2GPPLYP functional.

<table>
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<tr>
<th>Compound</th>
<th>Electronic transition</th>
<th>( \lambda_{\text{max}} ) (nm)</th>
<th>Optical gap (eV)</th>
<th>Oscillator strength (coefficient)</th>
<th>MO designation</th>
<th>Nature</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1</td>
<td>( S_0 \to S_1 )</td>
<td>436.0</td>
<td>2.844</td>
<td>1.741</td>
<td>( H\to L ) (0.457)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N2</td>
<td>( S_0 \to S_1 )</td>
<td>437.5</td>
<td>2.834</td>
<td>2.783</td>
<td>( H\to L ) (0.363)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
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<td>( S_0 \to S_1 )</td>
<td>419.4</td>
<td>2.956</td>
<td>1.517</td>
<td>( H\to L ) (0.467)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N4</td>
<td>( S_0 \to S_1 )</td>
<td>417.8</td>
<td>2.968</td>
<td>1.648</td>
<td>( H\to L ) (0.537)</td>
<td>( \pi \to \pi^* )</td>
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<tr>
<td>N5</td>
<td>( S_0 \to S_1 )</td>
<td>386.3</td>
<td>3.209</td>
<td>1.412</td>
<td>( H-1\to L ) (0.736)</td>
<td>( \pi \to \pi^* )</td>
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<tr>
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<td>( S_0 \to S_1 )</td>
<td>444.9</td>
<td>2.787</td>
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<td>( H\to L ) (0.848)</td>
<td>( \pi \to \pi^* )</td>
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<tr>
<td>N7</td>
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<td>398.9</td>
<td>3.108</td>
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<td>( H\to L ) (0.777)</td>
<td>( \pi \to \pi^* )</td>
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<td>399.7</td>
<td>3.102</td>
<td>1.385</td>
<td>( H-1\to L ) (0.388)</td>
<td>( \pi \to \pi^* )</td>
</tr>
<tr>
<td>N9</td>
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<td>2.975</td>
<td>1.350</td>
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<tr>
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<td>( S_0 \to S_1 )</td>
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<td>414.2</td>
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<tr>
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<td>1.432</td>
<td>( H\to L ) (0.497)</td>
<td>( \pi \to \pi^* )</td>
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</table>

Figure S1: Relative maximum errors (Max) of TD-DFT excitation energies.
Figure S2: Relative minimum errors (Min) of TD-DFT excitation energies.

Figure S3: Linear determination coefficients ($R^2$) of TD-DFT excitation energies.
Figure S4: Molecular orbitals (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of the dye sensitizers (N1–N13). Isosurface value = 0.02.
Figure S4: (Cont.) Molecular orbitals (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of the dye sensitizers (N1–N13). Isosurface value = 0.02.