Supporting Information

Trans- A₂B – Corrole Bearing 2,3-di(2-pyridyl)quinoxaline(DPQ) / Phenothiazine Moiety’s: Synthesis, Characterization, Electrochemistry and Photophysics

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<table>
<thead>
<tr>
<th>Sample</th>
<th>( \lambda_{\text{max}} )</th>
<th>( f )</th>
<th>( E ) eV</th>
<th>% of Molecular Orbital Contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>F10C-PTZ</td>
<td>306</td>
<td>0.073</td>
<td>4.04</td>
<td>H-2 ( \rightarrow ) L+2 (26%), H-1 ( \rightarrow ) L+2 (48%), H-11 ( \rightarrow ) LUMO (6%), H-1 ( \rightarrow ) L+3 (3%), HOMO ( \rightarrow ) L+5 (7%)</td>
</tr>
<tr>
<td></td>
<td>390</td>
<td>1.166</td>
<td>3.17</td>
<td>H-2 ( \rightarrow ) L+1 (61%), H-1 ( \rightarrow ) L+1 (18%), H-1 ( \rightarrow ) LUMO (4%), HOMO ( \rightarrow ) LUMO (8%)</td>
</tr>
<tr>
<td></td>
<td>399</td>
<td>0.84</td>
<td>3.10</td>
<td>H-2 ( \rightarrow ) LUMO (18%), H-1 ( \rightarrow ) L+1 (43%), HOMO ( \rightarrow ) L+1 (16%), H-1 ( \rightarrow ) LUMO (7%)</td>
</tr>
<tr>
<td></td>
<td>449</td>
<td>0.56</td>
<td>2.75</td>
<td>H-2 ( \rightarrow ) LUMO (10%), H-2 ( \rightarrow ) L+1 (13%), H-1 ( \rightarrow ) L+1 (26%), HOMO ( \rightarrow ) L+1 (44%)</td>
</tr>
<tr>
<td></td>
<td>590</td>
<td>0.279</td>
<td>2.10</td>
<td>HOMO ( \rightarrow ) LUMO (86%), H-2 ( \rightarrow ) L+1 (3%), H-1 ( \rightarrow ) LUMO (3%), H-1 ( \rightarrow ) L+1 (6%)</td>
</tr>
<tr>
<td>F10C-DPQ</td>
<td>329</td>
<td>0.063</td>
<td>3.76</td>
<td>HOMO ( \rightarrow ) L+4 (86%), H-8 ( \rightarrow ) LUMO (4%), H-6 ( \rightarrow ) LUMO (3%)</td>
</tr>
<tr>
<td></td>
<td>352</td>
<td>0.158</td>
<td>3.51</td>
<td>H-5 ( \rightarrow ) L+1 (49%), H-3 ( \rightarrow ) L+1 (14%), H-2 ( \rightarrow ) L+1 (19%), H-14 ( \rightarrow ) L+1 (4%), H-5 ( \rightarrow ) L+2 (4%)</td>
</tr>
<tr>
<td></td>
<td>393</td>
<td>1.024</td>
<td>3.15</td>
<td>H-1 ( \rightarrow ) L+2 (78%), HOMO ( \rightarrow ) LUMO (11%), H-4 ( \rightarrow ) LUMO (2%), H-2 ( \rightarrow ) LUMO (3%)</td>
</tr>
<tr>
<td></td>
<td>416</td>
<td>1.421</td>
<td>2.98</td>
<td>H-1 ( \rightarrow ) LUMO (29%), HOMO ( \rightarrow ) L+2 (58%), HOMO ( \rightarrow ) L+3 (5%)</td>
</tr>
<tr>
<td></td>
<td>569</td>
<td>0.332</td>
<td>2.17</td>
<td>H-1 ( \rightarrow ) L+2 (11%), HOMO ( \rightarrow ) LUMO (78%), H-1 ( \rightarrow ) LUMO (5%), HOMO ( \rightarrow ) L+2 (3%)</td>
</tr>
</tbody>
</table>

* Theoretical absorbance in nm, \( f \) Oscillator strength, \( E \) Excited state energy in eV.

Table S2. \( I_{(\text{dyad})} / I_{(\text{ref})} \) values for F10C-PTZ and F10C-DPQ w.r.t. reference compound “tpfc”, when excited at 420 nm.

<table>
<thead>
<tr>
<th></th>
<th>CH2Cl2</th>
<th>PhMe</th>
<th>MeCN</th>
<th>DMF</th>
</tr>
</thead>
<tbody>
<tr>
<td>F10C-PTZ</td>
<td>0.29</td>
<td>0.57</td>
<td>0.40</td>
<td>0.38</td>
</tr>
<tr>
<td>F10C-DPQ</td>
<td>0.39</td>
<td>0.55</td>
<td>0.0060</td>
<td>0.0034</td>
</tr>
</tbody>
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Fig. S21: Energy level diagram of the both the dyads in CH$_2$Cl$_2$. the singlet state energy of the F10C-DPQ was assumed to 3.04 eV, due to lack of emission of pristine DPQ, we cannot overlap the absorption and emission of the DPQ, but we have estimated the value according to previous reports reference - 22 in the main text.