Supporting Information for

Investigation of rotameric conformations of substituted imidazo-[1, 2-a] pyrazine: experimental and theoretical approaches

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<td>$^{13}$C NMR spectra of Compound 2A</td>
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<td>$^1$H NMR spectra of Compound 2B</td>
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<tr>
<td>Figure S18</td>
<td>$^{13}$C NMR spectra of Compound 2B</td>
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<td>Figure S19</td>
<td>Mass spectra of compound 2B</td>
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<tr>
<td>Figure S20</td>
<td>FTIR spectra of compound 2B</td>
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<td>Figure S22</td>
<td>Frontier Molecular orbital for conformer 2B</td>
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Figure S23  Frontier Molecular orbital for conformer 2A
Figure S1: $^1$H NMR spectra of Compound 1A

Figure S2: $^{13}$C NMR spectra of Compound 1A
Figure S3: Mass spectra of compound 1A

Figure S4: FTIR Spectra of compound 1A
**Figure S5:** $^1$H NMR spectra of Compound 1B

![Figure S5](image)

**Figure S6:** $^{13}$C NMR spectra of Compound 1B

![Figure S6](image)

**Figure S7:** Mass spectra of compound 1B

![Figure S7](image)
Figure S8: FTIR Spectra of compound 1B
**Figure S9:** Experimental and theoretical $^1$H NMR (left) and $^{13}$C NMR (right) correlation for conformer 1B

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<th>H- position</th>
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<th>$^1$H NMR (IB)</th>
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<tr>
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<td>2</td>
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<td>3</td>
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<tr>
<td>4'</td>
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<tr>
<td>3'</td>
<td>7.05</td>
<td>7.34</td>
</tr>
<tr>
<td>5'</td>
<td>7.09</td>
<td>7.29</td>
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</table>
Figure S10: The absorption spectra of different compound 1A and 1B in CH$_3$CN.

Table S2: The calculated absorption value for conformer 1A and 1B in gas and CH$_3$CN solvent phase at B3LYP/6-31++G** level of theory, symmetry of frontier orbital and % contributions of Molecular orbitals

<table>
<thead>
<tr>
<th>Excited State</th>
<th>$\lambda_{ACN}$ (nm)</th>
<th>$\lambda_{Gas}$ (nm)</th>
<th>$\lambda_{Exp}$ (nm)</th>
<th>Osc. Strength</th>
<th>Symmetry</th>
<th>% Major Orbital Contribution</th>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S$_0$-S$_1$</td>
<td>370.20</td>
<td>388.50</td>
<td>380,</td>
<td>0.2567</td>
<td>Singlet-A</td>
<td>H$\rightarrow$L</td>
</tr>
<tr>
<td>S$_0$-S$_2$</td>
<td>329.15</td>
<td>326.29</td>
<td></td>
<td>0.1214</td>
<td>Singlet-A</td>
<td>H-1$\rightarrow$L</td>
</tr>
<tr>
<td>S$_0$-S$_3$</td>
<td>311.03</td>
<td>309.84</td>
<td></td>
<td>0.184</td>
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<td>H-2$\rightarrow$L</td>
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<tr>
<td>S$_0$-S$_4$</td>
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<td>281.59</td>
<td>361,</td>
<td>0.0001</td>
<td>Singlet-A</td>
<td>H-4$\rightarrow$L</td>
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<tr>
<td>S$_0$-S$_5$</td>
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<td>281.16</td>
<td>318</td>
<td>0.155</td>
<td>Singlet-A</td>
<td>H-3$\rightarrow$L</td>
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<tr>
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<td></td>
<td>0.0688</td>
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<tr>
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<td>0.2699</td>
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<tr>
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<td>0.0006</td>
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Figure S11: Frontier Molecular orbital for conformer 1B
Figure S12: $^1$H NMR spectra of Compound 2A

Figure S13: $^{13}$C NMR spectra of Compound 2A
**Figure S14:** Mass spectra of compound 2A

**Figure S15:** FTIR Spectra of compound 2A
Figure S16: Experimental and theoretical $^1$H NMR (left) and $^{13}$C NMR (right) correlation for conformer 2A.
**Figure S17:** $^1$H NMR spectra of Compound 2B

**Figure S18:** $^{13}$C NMR spectra of Compound 2B
Figure S19: Mass spectra of compound 2B

Figure S20: FTIR spectra of compound 2B
Table S3. Experimental $^1$H NMR signals for conformer 2A and 2B

<table>
<thead>
<tr>
<th></th>
<th>2A</th>
<th>2B</th>
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<tr>
<td>6'</td>
<td>8.59</td>
<td>10.7</td>
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<tr>
<td>5</td>
<td>8.29</td>
<td>7.84</td>
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<td>7.8</td>
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<tr>
<td>3</td>
<td>7.65</td>
<td>7.5</td>
</tr>
<tr>
<td>4'</td>
<td>7.48</td>
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<td>4''</td>
<td>7.33</td>
<td>7.29</td>
</tr>
<tr>
<td>6''</td>
<td>7.26</td>
<td></td>
</tr>
<tr>
<td>3'</td>
<td>7.18</td>
<td></td>
</tr>
<tr>
<td>3''</td>
<td>7.12</td>
<td></td>
</tr>
<tr>
<td>5'</td>
<td>7.06</td>
<td>7.18</td>
</tr>
<tr>
<td>5''</td>
<td>6.97</td>
<td>6.82</td>
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</table>

Figure S21: The absorption spectra of different conformers 2A and 2B in CH$_3$CN.

Table S4: The calculated absorption value for conformer 2A and 2B in gas and CH$_3$CN solvent phase at B3LYP/6-31++G** level of theory, symmetry of frontier orbital and % contributions of Molecular orbitals.
### Table 2A

<table>
<thead>
<tr>
<th>Excitation $S_0$-$S_n$</th>
<th>$\lambda_{\text{Gas}}$ (nm)</th>
<th>$\lambda_{\text{ACN}}$ (nm)</th>
<th>$\lambda_{\text{Exp}}$ (nm)</th>
<th>Osc. Strength</th>
<th>Symmetry</th>
<th>Major orbital contribs.</th>
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<td>1</td>
<td>387.15</td>
<td>377.15</td>
<td>380, 360, 265</td>
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<td>Singlet-A</td>
<td>H$\rightarrow$L 96%</td>
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<tr>
<td>2</td>
<td>375.78</td>
<td>357.40</td>
<td>380, 360, 265</td>
<td>0.0624</td>
<td>Singlet-A</td>
<td>H-1$\rightarrow$L 98%</td>
</tr>
<tr>
<td>3</td>
<td>326.38</td>
<td>325.97</td>
<td>380, 360, 265</td>
<td>0.0625</td>
<td>Singlet-A</td>
<td>H-2$\rightarrow$L 89%</td>
</tr>
<tr>
<td>4</td>
<td>315.62</td>
<td>313.60</td>
<td>380, 360, 265</td>
<td>0.1080</td>
<td>Singlet-A</td>
<td>H-3$\rightarrow$L 63%</td>
</tr>
<tr>
<td>5</td>
<td>297.45</td>
<td>290.59</td>
<td>380, 360, 265</td>
<td>0.4008</td>
<td>Singlet-A</td>
<td>H$\rightarrow$L+1 55%</td>
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<tr>
<td>6</td>
<td>292.17</td>
<td>286.91</td>
<td>380, 360, 265</td>
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<td>Singlet-A</td>
<td>H-4$\rightarrow$L 81%</td>
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### Table 2B

<table>
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<tr>
<th>Excitation $S_0$-$S_n$</th>
<th>$\lambda_{\text{Gas}}$ (nm)</th>
<th>$\lambda_{\text{ACN}}$ (nm)</th>
<th>$\lambda_{\text{Exp}}$ (nm)</th>
<th>Osc. Strength</th>
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<td>315, 260</td>
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<td>H-1$\rightarrow$L 93%</td>
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<tr>
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<td>335.74</td>
<td>329.86</td>
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<td>H-2$\rightarrow$L 93%</td>
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<tr>
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<td>321.73</td>
<td>317.88</td>
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<td>H$\rightarrow$L+1 80%</td>
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<td>375, 315, 260</td>
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<td>H-1$\rightarrow$L+1 61%</td>
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<td>292.03</td>
<td>375, 315, 260</td>
<td>0.2095</td>
<td>Singlet-A</td>
<td>H-3$\rightarrow$L 59%</td>
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### Diagrams

- **2A**
  - **HOMO**
  - **LUMO**

- **2B**
  - **HOMO**
  - **LUMO**
Figure S22: Frontier Molecular orbital for conformer 2B
Figure S23: Frontier Molecular orbital for conformer 2A