Electronic Supporting Information for:

A comparison of optical, electrochemical and self-assembling properties of two structural isomers based on 1,6- and 1,8-pyrenedione chromophores

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Figure 1. $^1$H and $^{13}$C NMR of 3

$R_1^1 - R_2^2 - R_3^3 - R_4^4$

$3 \ R_1^1 = \text{OTIPS}, \ R_2^4 = \text{H}$

$\begin{array}{c}
\text{Chemical Shift (ppm)}
\end{array}$

$\begin{array}{c}
0 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6 \ 7
\end{array}$

$\begin{array}{c}
1.91 \ 2.10 \ 2.09 \ 2.08
\end{array}$

$\begin{array}{c}
6.35 \ 37.34
\end{array}$

$\begin{array}{c}
\text{Chemical Shift (ppm)}
\end{array}$

$\begin{array}{c}
190 \ 180 \ 170 \ 160 \ 150 \ 140 \ 130 \ 120 \ 110 \ 100 \ 90 \ 80 \ 70 \ 60 \ 50 \ 40 \ 30 \ 20 \ 10
\end{array}$

$\begin{array}{c}
126.7 \ 125.1 \ 124.7 \ 123.0 \ 121.0 \ 116.2
\end{array}$

$\begin{array}{c}
150.0
\end{array}$

$\begin{array}{c}
18.3 \ 13.4
\end{array}$
Figure 2. $^1$H and $^{13}$C NMR of 4
Figure 3. $^1$H and $^{13}$C NMR of 5
Figure 4. \(^1\)H and \(^{13}\)C NMR of 6

\[ \text{R}^1 \quad \text{R}^2 \]
\[ \text{R}^3 \quad \text{R}^4 \]

\(6 \text{ R}^1,4 = \text{OTIPS}; \text{R}^2,3 = \text{Br}\)
Figure 5 \(^1\)H and \(^{13}\)C NMR of 7

7 \(R^{1,3}\) = OTIPS; \(R^{2,4}\) = donor

Chemical Shift (ppm)

Chemical Shift (ppm)
Figure 6. $^1$H and $^{13}$C NMR of 8

$^a$ $R^{1,4} =$ OTIPS, $R^{3,3} =$ donor

$^8$ $R^{1,4} =$ OTIPS, $R^{3,3} =$ donor
Figure 7. $^1$H and $^{13}$C NMR of 16ketPyr
Figure 8. $^1$H and $^{13}$C NMR of 18ketPyr
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Table 1. Allowed transitions calculated with TD-DFT for compounds \textbf{16ketPyr} and \textbf{18ketPyr}.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Major Transition</th>
<th>Wavelength (nm)</th>
<th>Energy (eV)</th>
<th>Oscillator Strength</th>
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<tbody>
<tr>
<td>\textbf{16ketPyr}</td>
<td>HOMO - LUMO (100%)</td>
<td>788</td>
<td>1.57</td>
<td>0.6615</td>
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<tr>
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<td>HOMO-2 - LUMO (91%)</td>
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<td>HOMO-3 - LUMO+1 (9%)</td>
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<td>\textbf{18ketPyr}</td>
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