Supplementary Information

Multi-Substituted Triazatruxene-Functionalized Pyrene Derivatives as Efficient Organic Laser Gain Media

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Figure S1. TGA thermograms of Py-nTAT.
Figure S2. DSC traces of Py-nTAT.

Figure S3. Fluorescence decay of (a) TAT and (b) Py in THF and film states.

Figure S4. Fluorescence decay of Py-nTAT in (a) THF and (b) film states.
Table S1. The PL lifetimes of Py and TAT.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$\tau_1$ (ns)$^a$</th>
<th>$\tau_2$ (ns)$^a$</th>
<th>$\tau_1$ (ns)$^b$</th>
<th>$\tau_2$ (ns)$^b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TAT</td>
<td>1.49 (22.53%)</td>
<td>4.39 (77.47%)</td>
<td>0.82 (76.52%)</td>
<td>2.23 (23.48%)</td>
</tr>
<tr>
<td>Py</td>
<td>1.11 (83.72%)</td>
<td>3.6 (16.28%)</td>
<td>0.9 (85.30%)</td>
<td>3.28 (14.70%)</td>
</tr>
</tbody>
</table>

$^a$ Measured in THF; $^b$ Measured in film states.

Table S2. The PL lifetimes of Py-2TAT and Py-4TAT films.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$\tau_1$ (ns)</th>
<th>$\tau_2$ (ns)</th>
<th>$&lt;\tau&gt;$ (ns)$^a$</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Py-2TAT</td>
<td>0.83 (69.40%)</td>
<td>2.38 (30.60%)</td>
<td>1.30</td>
<td>1.15</td>
</tr>
<tr>
<td>Py-4TAT</td>
<td>0.98 (71.71%)</td>
<td>2.55 (28.29%)</td>
<td>1.42</td>
<td>1.17</td>
</tr>
</tbody>
</table>

$^a$ the average lifetime

Figure S5. Optimized geometries and calculated frontier orbitals of Py-2TAT and Py-4TAT.
**Figure S6.** MALDI-TOF mass spectrum of TAT-Br (2).

**Figure S7.** $^1$H NMR spectrum of 2.
Figure S8. $^{13}$C NMR spectrum of 2.

Figure S9. MALDI-TOF mass spectrum of 3.
Figure S10. $^1$H NMR spectrum of 3.

Figure S11. $^{13}$C NMR spectrum of 3.
Figure S12. MALDI-TOF mass spectrum of Py-2TAT.

Figure S13. $^1$H NMR spectrum of Py-2TAT.
Figure S14. $^{13}$C NMR spectrum of Py-2TAT.

Figure S15. MALDI-TOF mass spectrum of Py-4TAT.
Figure S16. $^1$H NMR spectrum of Py-4TAT.

Figure S17. $^{13}$C NMR spectrum of Py-4TAT.