Supporting Information

Diphenylamino-substituted quinacridone derivative: red fluorescence based on intramolecular charge-transfer transition

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**Fig. S1** Absorption (solid line) and fluorescence (dashed line) spectra of NPh$_2$-QA in various solvents.

**Table S1** Photophysical data of NPh$_2$-QA in various solvents.

<table>
<thead>
<tr>
<th>Solvents</th>
<th>$\Delta f^a$</th>
<th>$\lambda_{abs}$/ nm</th>
<th>$\varepsilon$ / 10$^4$ M$^{-1}$ cm$^{-1}$</th>
<th>$\lambda_{em}$/ nm</th>
<th>Stokes shift / cm$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>0.0131</td>
<td>566</td>
<td>0.83</td>
<td>602</td>
<td>1057</td>
</tr>
<tr>
<td>CHCl$_3$</td>
<td>0.1482</td>
<td>579</td>
<td>0.73</td>
<td>649</td>
<td>1863</td>
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<tr>
<td>CH$_2$Cl$_2$</td>
<td>0.2171</td>
<td>570</td>
<td>0.71</td>
<td>644</td>
<td>2016</td>
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<tr>
<td>DMSO</td>
<td>0.2630</td>
<td>575</td>
<td>0.73</td>
<td>677</td>
<td>2620</td>
</tr>
<tr>
<td>CH$_3$CN</td>
<td>0.3046</td>
<td>564</td>
<td>0.73</td>
<td>674</td>
<td>2894</td>
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</tbody>
</table>

$^a$ orientation polarizability of the solvent.
**Lippert-Mataga plots.** Lippert-Mataga equation\(^1\) expresses the Stokes shift $\Delta \nu$ as a function of the solvent orientation polarizability $\Delta f$:

$$\Delta \nu = \frac{1}{4\pi \varepsilon_0} \frac{2(\mu_e - \mu_g)^2}{hc a^3} \Delta f + \text{constant}$$

$$= \frac{(9.05 \times 10^{34})(\mu_e - \mu_g)^2}{a^3} \Delta f \ [C^{-2}] + \text{constant}$$

where $\varepsilon_0$ represents dielectric constant of vacuum, $h$ represents Planck constant, $c$ represents light velocity, $a$ represents radius of Onsager cavity, $\mu_g$ and $\mu_e$ represent the dipole moment in ground and excited states, respectively. $C$ is the unit of quantity of electric charge. For NPh$_2$-QA, DFT-calculation at B3LYP/6-31G* level gives $a$ value of 6.65 Å. Based on the Lippert-Mataga equation, the difference of dipole moment between ground and excited states ($\mu_e - \mu_g$) is 13.4 D.

**Table S2** Fluorescence quantum yields of C$_8$-QA and NPh$_2$-QA in various solvents.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Toluene</th>
<th>CHCl$_3$</th>
<th>CH$_2$Cl$_2$</th>
<th>DMSO</th>
<th>CH$_3$CN</th>
</tr>
</thead>
<tbody>
<tr>
<td>C$_8$-QA</td>
<td>0.96</td>
<td>0.97</td>
<td>0.96</td>
<td>0.95</td>
<td>0.96</td>
</tr>
<tr>
<td>NPh$_2$-QA</td>
<td>0.56</td>
<td>0.13</td>
<td>0.09</td>
<td>0.02</td>
<td>0.02</td>
</tr>
</tbody>
</table>

**Fig. S2** Lippert–Mataga plot of NPh$_2$-QA.
**Fig. S3** Fluorescence spectra of solid thin films of C$_8$-QA (yellow line) and NPh$_2$-QA (deep red line).

**Fig. S4** Fluorescence microscopy image of the crystalline powder of NPh$_2$-QA.
**Fig. S5** TGA curves of C₈-QA and NPh₂-QA.

**Fig. S6** Two heating (solid line)-cooling (dashed line) cycles of the DSC measurements of NPh₂-QA.
**Fig. S7** Two heating (solid line)-cooling (dashed line) cycles of the DSC measurements of C₈-QA.

**Fig. S8** EL spectra of the OLED device at different driving voltages.
Fig. S9 Current density–Voltage–Brightness characteristics of the OLED device.

Fig. S10 Current efficiency and power efficiency versus brightness characteristics of the OLED device.
Fig. S11 External quantum efficiency *versus* brightness characteristics of the OLED device.

Fig. S12 $^1$H NMR spectrum of NPh$_2$-QA (400 MHz, CD$_2$Cl$_2$).
Fig. S13 $^{13}$C{$^{1}$H} NMR spectrum of NPh$_2$-QA (100 MHz, CD$_2$Cl$_2$).

**References**