Supplementary Information

One-pot, Two-step Synthesis and Photophysical Properties of 2-(5-Phenylindol-3-yl) benzoimidazole Derivatives

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Fitted curve for the absorption spectrum of compound 3d
Figure S1 Fitted curve for the absorption spectrum of 3d in ethanol solution.
Table S1 UV-Vis absorption and fluorescence emission spectra of compounds 3b and 3d in different solvents.

<table>
<thead>
<tr>
<th>Compound(^a)</th>
<th>Solvent</th>
<th>UV-visible Absorption</th>
<th>Emission</th>
<th>Stoke’s shift(cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>( \Lambda^{1\text{max}}(\text{nm}) )</td>
<td>( \Lambda^{2\text{max}}(\text{nm}) )</td>
<td>( \Lambda^{3\text{max}}(\text{nm}) )</td>
</tr>
<tr>
<td>3b</td>
<td>Ethanol</td>
<td>262</td>
<td>325</td>
<td>375</td>
</tr>
<tr>
<td>3b</td>
<td>Dichloroethane</td>
<td>264</td>
<td>328</td>
<td>379</td>
</tr>
<tr>
<td>3b</td>
<td>n-Hexane</td>
<td>325</td>
<td></td>
<td>373</td>
</tr>
<tr>
<td>3d</td>
<td>Ethanol</td>
<td>248</td>
<td>311</td>
<td>347</td>
</tr>
<tr>
<td>3d</td>
<td>Dichloroethane</td>
<td>256</td>
<td>312</td>
<td>352</td>
</tr>
<tr>
<td>3d</td>
<td>n-Hexane</td>
<td>309</td>
<td>344</td>
<td>378</td>
</tr>
</tbody>
</table>

\( a: c = 1.0 \times 10^{-5} \text{ mol/L, at } 25^\circ\text{C}; \quad b: \) The excitation wavelength of compound 3b and 3d were 330 nm and 350 nm respectively
Spectra of selective samples of compounds 3 in ethanol solution

Figure S2. (a) UV−visible and (b) fluorescence spectra of selective samples of compounds 3 in ethanol solution.
<table>
<thead>
<tr>
<th>sample</th>
<th>Integrated emission intensity (I)</th>
<th>Abs. at 330 nm (A)</th>
<th>Refractive index of solvent</th>
<th>Quantum yield at 330 nm (Φ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quinine sulfate</td>
<td>113969.8</td>
<td>0.0147</td>
<td>1.33</td>
<td>0.54</td>
</tr>
<tr>
<td>3b</td>
<td>255398.6</td>
<td>0.0514</td>
<td>1.36</td>
<td>0.36</td>
</tr>
<tr>
<td>3i</td>
<td>198298.9</td>
<td>0.0404</td>
<td>1.36</td>
<td>0.35</td>
</tr>
<tr>
<td>3o</td>
<td>203325.1</td>
<td>0.043</td>
<td>1.36</td>
<td>0.34</td>
</tr>
<tr>
<td>3t</td>
<td>241497.8</td>
<td>0.0557</td>
<td>1.36</td>
<td>0.31</td>
</tr>
</tbody>
</table>

Quinolone sulfate (referenced dye) as a function of optical absorbance at 330 nm and relevant data
$^1$H and $^{13}$C NMR Spectra of compounds 3a - 3x

$^1$H NMR Spectra of 2-(1-ethyl-5-phenyl-$^1$H-indol-3-yl)-$^1$H-benzo[d]imidazole (3a)

$^{13}$C NMR Spectra of 2-(1-ethyl-5-phenyl-$^1$H-indol-3-yl)-$^1$H-benzo[d]imidazole (3a)
H NMR Spectra of 2-(1-ethyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3b)

13C NMR Spectra of 2-(1-ethyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3b)
$^{1}$H NMR Spectra of 2-(1-ethyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3c)

$^{13}$C NMR Spectra of 2-(1-ethyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3c)
$^1$H NMR Spectra of 4-(3-(1H-benzo[d]imidazole-2-yl)-1-ethyl-1H-indol-5-yl)-N,N-diphenylaniline (3d)

$^{13}$C NMR Spectra of 4-(3-(1H-benzo[d]imidazole-2-yl)-1-ethyl-1H-indol-5-yl)-N,N-diphenylaniline (3d)
**1H NMR Spectra of 2-(5-(4-chlorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3e)**

![1H NMR Spectra](image)

**13C NMR Spectra of 2-(5-(4-chlorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3e)**

![13C NMR Spectra](image)
$^1$H NMR Spectra of 2-(5-(4-fluorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3f)

$^{13}$C NMR Spectra of 2-(5-(4-fluorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3f)
$^1$H NMR Spectra of 2-(1-ethyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3g)

$^{13}$C NMR Spectra of 2-(1-ethyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3g)
$^1$H NMR Spectra of 2-(1-ethyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3h)

$^{13}$C NMR Spectra of 2-(1-ethyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3h)
$^1$H NMR Spectra of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3i)

$^{13}$C NMR Spectra of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3i)
**1H NMR Spectra of 2-(1-butyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3j)**

![1H NMR Spectra of 2-(1-butyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3j)]

**13C NMR Spectra of 2-(1-butyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3j)**

![13C NMR Spectra of 2-(1-butyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3j)]
$^1$H NMR Spectra of 2-(1-butyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3k)

$^{13}$C NMR Spectra of 2-(1-butyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3k)
$^1$H NMR Spectra of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3m)

$^{13}$C NMR Spectra of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3m)
$^1$H NMR Spectra of 2-(1-butyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3n)

$^{13}$C NMR Spectra of 2-(1-butyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3n)
$^1$H NMR Spectra of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-1H-benzo[α]imidazole (3o)

$^{13}$C NMR Spectra of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-1H-benzo[α]imidazole (3o)
$^1$H NMR Spectra of 2-(1-allyl-5-($p$-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3p)

$^{13}$C NMR Spectra of 2-(1-allyl-5-($p$-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3p)
$^1$H NMR Spectra of 2-(1-allyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3q)

$^{13}$C NMR Spectra of 2-(1-allyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3q)
$^1$H NMR Spectra of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3r)

$^{13}$C NMR Spectra of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3r)
$^1$H NMR Spectra of 2-(1-allyl-5-(4-chlorophenyl)-1$H$-indol-3-yl)-5-methyl-1$H$-benzo[d]imidazole (3s)

$^{13}$C NMR Spectra of 2-(1-allyl-5-(4-chlorophenyl)-1$H$-indol-3-yl)-5-methyl-1$H$-benzo[d]imidazole (3s)
$^1$H NMR Spectra of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3t)

$^{13}$C NMR Spectra of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3t)
$^1$H NMR Spectra of 2-(1-benzyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3u)

$^{13}$C NMR Spectra of 2-(1-benzyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3u)
$^1$H NMR Spectra of 2-(1-benzyl-5-(4-methoxyphenyl)-1$H$-indol-3-yl)-1$H$-benzo[d]imidazole (3v)

$^{13}$C NMR Spectra of 2-(1-benzyl-5-(4-methoxyphenyl)-1$H$-indol-3-yl)-1$H$-benzo[d]imidazole (3v)
$^1$H NMR Spectra of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3w)

$^{13}$C NMR Spectra of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3w)
\(^1\)H NMR Spectra of 2-(1-benzyl-5-(\(p\)-tolyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3x)

\(^{13}\)C NMR Spectra of 2-(1-benzyl-5-(\(p\)-tolyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3x)
$^1$H NMR Spectra of 2-(1-benzyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3y)

$^{13}$C NMR Spectra of 2-(1-benzyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3y)
HR-ESI-MS Spectra of compounds 3

HR-ESI-MS spectrum of 2-(1-ethyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3a)

HR-ESI-MS spectrum of 4-(3-(1H-benzo[d]imidazole-2-yl)-1-ethyl-1H-indol-5-yl)-N,N-diphenylaniline (3d)
HR-ESI-MS spectrum of 2-(5-(4-chlorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3e)

HR-ESI-MS spectrum of 2-(5-(4-fluorophenyl)-1-ethyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3f)
HR-ESI-MS spectrum of 2-(1-ethyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3g)

HR-ESI-MS spectrum of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3i)
HR-ESI-MS spectrum of 2-(1-butyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3m)

HR-ESI-MS spectrum of 2-(1-butyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3n)
HR-ESI-MS spectrum of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3o)

HR-ESI-MS spectrum of 2-(1-allyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3p)
HR-ESI-MS spectrum of 2-(1-allyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3q)

HR-ESI-MS spectrum of 2-(1-allyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3r)
HR-ESI-MS spectrum of 2-(1-allyl-5-(4-chlorophenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3s)

HR-ESI-MS spectrum of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-1H-benzo[d]imidazole (3t)
HR-ESI-MS spectrum of 2-(1-benzyl-5-(p-tolyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3u)

HR-ESI-MS spectrum of 2-(1-benzyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-1H-benzo[d]imidazole (3v)
HR-ESI-MS spectrum of 2-(1-benzyl-5-phenyl-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3w)

HR-ESI-MS spectrum of 2-(1-benzyl-5-(p-tolyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3x)
HR-ESI-MS spectrum of 2-(1-benzyl-5-(4-methoxyphenyl)-1H-indol-3-yl)-5-methyl-1H-benzo[d]imidazole (3y)