Supporting Information

for

Synthesis of novel multifunctional carbazole-based molecules and their thermal, electrochemical and optical properties

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NMR, FTIR, MS and HRMS spectra of compounds and relative quantum yield calculations
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1. $^1$H and $^{13}$C NMR spectra

**Figure S1**: $^1$H NMR spectrum of 3-bromocarbazole (2).

**Figure S2**: $^1$H NMR spectrum of 3-bromo-N-hexylcarbazole (4).
Figure S3: $^1$H NMR spectrum of $N$-hexylcarbazole-3-yl-boronic acid pincolate ester (5).

Figure S4: $^1$H NMR spectrum of compound 7a.
Figure S5: $^{13}$C NMR spectrum of compound 7a.

Figure S6: $^1$H NMR spectrum of compound 7b.

Figure S7: $^{13}$C NMR spectrum of compound 7b.
2. FTIR spectra

![FTIR spectra of compounds 7a and 7b](image)

**Figure S8:** FTIR spectrum of compounds 7a and 7b

3. Mass and HRMS spectrum

![Mass spectrum of compound 7b](image)

**Figure S9:** Mass spectrum of compound 7b.

![HRMS result of compound 7b](image)

**Figure S10:** HRMS result of compound 7b.
4. Calculations of relative fluorescence quantum yields

Relative fluorescent quantum yields of samples ($\phi_s$) were calculated from Figure S11 by using equation 1, where $y_s$ is the integrated fluorescence intensity of samples (7a/7b), $y_R$ is the integrated fluorescence intensity of reference (Rhodamine B), $n$ is the refractive index of solvents used.

$$
\phi_s = y_s \cdot \frac{\phi_R}{y_R} \cdot \frac{n_s^2}{n_r^2} \quad (1)
$$

Figure S11, plotted from Table S1, depicts absorption at 355 nm (OD, optical density) versus integrated emission (integrated fluorescence intensity of reference and samples).

For this, samples (7a and 7b) were dissolved in dichloromethane ($n = 1.435$) and reference (rhodamine B) was dissolved in absolute ethanol ($n = 1.361$). Different concentrations of reference (C1–C7) and samples (7a: C1–C5 and 7b: C1–C8) were then prepared. For each concentration absorption spectra of reference and samples were recorded as depicted in Figure S12. Both reference and samples were excited at 355 nm, then emission spectra of reference and samples were recorded as depicted in Figure S13. All of these values are summarised in Table S1.

**Figure S11:** Absorption at 355 nm-integrated emission of samples (7a and 7b) and reference (rhodamine B)
Table S1: Optical density and integrated PL intensity values of reference (rhodamine B) and samples (7a and 7b)

|           | Rhodamine B | 7a  | 7b  |
|-----------|-------------|-----|-----|
|           | \( \lambda_{\text{exc}} = 355 \text{ nm} \) | \( \lambda_{\text{exc}} = 355 \text{ nm} \) | \( \lambda_{\text{exc}} = 355 \text{ nm} \) |
| Unsorted  | OD (a.u) | Integrated PL intensity (a.u) | OD (a.u) | Integrated PL intensity | OD (a.u) | Integrated PL intensity |
|-----------|---------|-------------------------------|---------|-------------------------|---------|-------------------------|
| C1        | 0.00873 | 37591.15917                   | C1      | 0.02143                 | 14075.26276 | C1 | 0.03855                 | 312854.9439 |
| C2        | 0.00849 | 35459.07801                   | C2      | 0.03538                 | 20063.43206 | C2 | 0.03810                 | 307049.5385 |
| C3        | 0.00804 | 33547.29896                   | C3      | 0.04274                 | 28371.31840 | C3 | 0.03599                 | 297563.9041 |
| C4        | 0.00786 | 33095.41848                   | C4      | 0.06100                 | 35022.74323 | C4 | 0.03441                 | 286229.5682 |
| C5        | 0.00762 | 31942.84488                   | C5      | 0.07916                 | 41000.28228 | C5 | 0.03284                 | 256749.5341 |
| C6        | 0.00734 | 30932.30389                   | C6      | 0.02933                 | 240013.4747 | C6 | 0.02770                 | 218127.6961 |
| C7        | 0.00726 | 29668.39935                   | C7      | 0.04274                 | 28371.31840 | C7 | 0.03599                 | 297563.9041 |

Gradient = PL/OD
Refractive index of ethanol 1.361

Refraction index of dichloromethane 1.435

| | PLQY | Unit |
|----------------|------|------|
| PLQY           | 0.49 | 1.02227E-07 |
| PLQY           | 0.054| Estimated error on values ca. ± 10% RSD. |
| PLQY           | 0.974| |

Figure S12: Absorption spectra of rhodamine B, 7a and 7b.

Figure S13: Emission (PL) spectra of rhodamine B, 7a and 7b, excited at 355 nm.