Supporting Information for

Synthesis, Structure and Photophysical Properties of Near-infrared 3,5-DiarylbenzoBODIPY Fluorophores

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1. **Scheme S1.** Attempted Syntheses of BODIPY 1X.

![Scheme S1](image)

2. **Crystal Structure**

![Crystal Structure](image)

**Figure S1:** X-ray structures of 1a. C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.

**Figure S2:** Intermolecular crystal packing of 1a through H-bonding (dotted line). C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.
Figure S3: X-ray structures of 1c. C, light gray; H, gray; N, blue; B, yellow; F, light green.

Figure S4: Intermolecular crystal packing of 1c through H-bonding (dotted line). C, light gray; H, gray; N, blue; B, yellow; F, light green.
**Figure S5**: X-ray structures of 1d. C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.

**Figure S6**: Intermolecular crystal packing of 1d through H-bonding (dotted line). C, light gray; H, gray; N, blue; B, yellow; F, light green; O, red.
<table>
<thead>
<tr>
<th></th>
<th>1a</th>
<th>1c</th>
<th>1d</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Empirical formula</strong></td>
<td>C$<em>{31}$H$</em>{23}$BF$_2$N$_2$O$_2$</td>
<td>C$<em>{29}$H$</em>{17}$BF$_4$N$_2$</td>
<td>C$<em>{31}$H$</em>{23}$BF$_2$N$_2$O$_2$</td>
</tr>
<tr>
<td><strong>Formula weight</strong></td>
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<td>480.26</td>
<td>504.32</td>
</tr>
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<td>293(2)</td>
<td>293(2)</td>
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<td><strong>space group</strong></td>
<td>P-1</td>
<td>P2(1)/n</td>
<td>P-1</td>
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<td><strong>a[Å]</strong></td>
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<td><strong>b[Å]</strong></td>
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<tr>
<td><strong>c[Å]</strong></td>
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<td>12.2515(18)</td>
<td>13.064(6)</td>
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<td>90</td>
<td>85.699(6)</td>
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<td><strong>β [°]</strong></td>
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<td>97.131(2)</td>
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<td><strong>γ [°]</strong></td>
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<td><strong>V[Å$^3$]</strong></td>
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<tr>
<td><strong>Z</strong></td>
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<td><strong>Calculated density [g.cm$^{-3}$]</strong></td>
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<td>1.429</td>
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<td><strong>Absorption coefficient (mm$^{-1}$)</strong></td>
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<td><strong>F(000)</strong></td>
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<td>524</td>
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<td><strong>Crystal size (mm)</strong></td>
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<td><strong>θ max [°]</strong></td>
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<td></td>
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<td>-15 ≤ l ≤ 15</td>
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<td><strong>Reflections observed [I &gt; 2σ(I)]</strong></td>
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<td><strong>Parameters</strong></td>
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<tr>
<td><strong>R1 (on F) [I &gt; 2σ(I)]</strong></td>
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<td>0.0517</td>
<td>0.0721</td>
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<tr>
<td><strong>wR2 (on F$^2$)</strong></td>
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<td><strong>Largest diff. peak/hole (eÅ$^{-3}$)</strong></td>
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<td>0.424/-0.530</td>
<td>0.327/-0.328</td>
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Table S2. Selected Geometrical Parameters of 1a, 1c and 1d obtained from crystallography

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<th>1c</th>
<th>1d</th>
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<td>1.5521(31)</td>
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<td></td>
<td>1.5729(29)</td>
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<td>1.5809(37)</td>
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<tr>
<td>the intramolecular F-H</td>
<td>2.2466(17)</td>
<td>2.3979(15)</td>
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<tr>
<td>Hydrogen bond distances (Å)</td>
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<td>2.8012(17)</td>
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<td>dihedral angles of two pyrrole</td>
<td>6.421(70)</td>
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<td>rings in dipyrin core (deg)</td>
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<td>dihedral angles between phenyl</td>
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<td>47.329(62)</td>
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<td>ring and dipyrin core (deg)</td>
<td>56.931(63)</td>
<td>51.263(65)</td>
<td>46.090(89)</td>
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### 3. Table S3: Photophysical properties of BODIPYs 1a-e and 5, 6 in different solvents at room temperature.

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<th>BODIPYs</th>
<th>Solvent</th>
<th>$\lambda_{\text{abs}}$ $\text{max}$(nm)</th>
<th>$\lambda_{\text{em}}$ $\text{max}$(nm)</th>
<th>$\log \varepsilon_{\text{max}}$</th>
<th>$\Phi_a$</th>
<th>Stokes Shift (cm$^{-1}$)</th>
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<td>680</td>
<td>4.78</td>
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<tr>
<td></td>
<td>THF</td>
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<td>684</td>
<td>4.92</td>
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<td>694</td>
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<tr>
<td></td>
<td>Dichloromethane</td>
<td>654</td>
<td>687</td>
<td>4.94</td>
<td>0.76</td>
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<tr>
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<td>Toluene</td>
<td>658</td>
<td>690</td>
<td>4.84</td>
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<tr>
<td>1b</td>
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<td>671</td>
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<td>722</td>
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<td>673</td>
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<td>THF</td>
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<tr>
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<td>Dichloromethane</td>
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<td>679</td>
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<tr>
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<td>663</td>
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<tr>
<td></td>
<td>Methanol</td>
<td>635</td>
<td>664</td>
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<td></td>
<td>Dichloromethane</td>
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<td>671</td>
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<tr>
<td></td>
<td>Toluene</td>
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<td>674</td>
<td>4.94</td>
<td>0.78</td>
<td>643</td>
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<tr>
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<td>Methanol</td>
<td>637</td>
<td>671</td>
<td>4.86</td>
<td>0.96</td>
<td>795</td>
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<td>THF</td>
<td>643</td>
<td>675</td>
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<td>Dichloromethane</td>
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<td>677</td>
<td>4.98</td>
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<td>679</td>
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<td>747</td>
<td>4.86</td>
<td>0.35</td>
<td>777</td>
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</table>

The fluorescence quantum yields were calculated using ZnPc in DMF solution ($\Phi = 0.28$) as the standards for 1a-d, and 1,3,5,7-(4-methoxy)phenylazaBODIPY ($\Phi = 0.36$ in chloroform) for 1e, respectively.
4. UV-vis and Fluorescence Spectra

**Figure S7.** Absorption (top) and emission (bottom) spectra of compound 1a recorded in different solvents. Excited at 620 nm.
Figure S8. Absorption (top) and emission (bottom) spectra of compound 1b recorded in different solvents. Excited at 610 nm.
Figure S9. Absorption (top) and emission (bottom) spectra of compound 1c recorded in different solvents. Excited at 610 nm.
Figure S10. Absorption (top) and emission (bottom) spectra of compound 1d recorded in different solvents. Excited at 610 nm.
**Figure S11.** Absorption (top) and emission (bottom) spectra of compound 1e recorded in different solvents. Excited at 660 nm.
Figure S12. Excitation spectrum (dash line) and absorption spectrum (solid line) of 1a in dichloromethane.

Figure S13. Excitation spectrum (dash line) and absorption spectrum (solid line) of 1b in dichloromethane.
**Figure S14.** Excitation spectrum (dash line) and absorption spectrum (solid line) of 1c in dichloromethane.

**Figure S15.** Excitation spectrum (dash line) and absorption spectrum (solid line) of 1d in dichloromethane.
**Figure S16.** Excitation spectrum (dash line) and absorption spectrum (solid line) of 1e in dichloromethane.
5. Copies of $^1$H and $^{13}$C NMR spectra

$^1$H NMR spectrum of 2a in CDCl$_3$
$^{13}$C NMR spectrum of 2a in CDCl$_3$
$^1$H NMR spectrum of 2b in CDCl$_3$
$^{13}$C NMR spectrum of 2b in CDCl$_3$
$^{1}$H NMR spectrum of 2c in CDCl$_3$
$^{13}$C NMR spectrum of 2c in CDCl$_3$
$^1$H NMR spectrum of 2d in CDCl$_3$
$^{13}$C NMR spectrum of 2d in CDCl$_3$
\(^1\)H NMR spectrum of 2e in CDCl\(_3\)
$^{13}$C NMR spectrum of 2e in CDCl$_3$
$^1$H NMR spectrum of 1a in CDCl$_3$
$^{13}$C NMR spectrum of 1a in CDCl$_3$. 

- 160.61
- 151.32
- 134.15
- 131.91
- 130.37
- 128.83
- 127.53
- 125.07
- 123.68
- 125.55
- 118.89
- 113.87
- 113.46
- 102.84
$^1$H NMR spectrum of 1b in CDCl$_3$
$^{13}$C NMR spectrum of 1b in CDCl$_3$
$^1$H NMR spectrum of 1c in CDCl$_3$
$^{13}$C NMR spectrum of 1c in CDCl$_3$
\(^1\)H NMR spectrum of 1d in CDCl\(_3\)
$^{13}$C NMR spectrum of 1d in CDCl$_3$
$^1$H NMR spectrum of 1e in CDCl$_3$
6. Copies of HRMS

HRMS (ESI) calcd. for C_{16}H_{14}O_{2}N [M+H]^+: 252.1025, found 252.1019.

HRMS (ESI) calcd. for C_{19}H_{20}ON [M+H]^+: 278.1545, found 278.1539

HRMS (ESI) calcd. for C_{19}H_{20}ON [M+H]^+: 240.0825, found 240.0819
HRMS (ESI) calcd. for C_{16}H_{14}O_{2}N [M+H]^+: 252.1025, found 252.1019.

HRMS(ACPI) calcd. for C_{14}H_{12}NOS [M+H]^+: 242.0640, found 242.0634.
<table>
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<th>m/z</th>
<th>Intensity</th>
<th>Relative</th>
<th>Theo.</th>
<th>Delta</th>
<th>RDB</th>
<th>Composition</th>
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<td>18</td>
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<td>C31 H24 O2 N2 B F2</td>
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HRMS (ACPI) calcd. for C$_{31}$H$_{24}$O$_2$N$_2$BF$_2$ [M+H]$^+$: 505.1899, found 505.1898;
m/z  | Intensity   | Relative | Mass (mmu) | Delta (mmu) | RDB equiv. |
-----|-------------|----------|------------|-------------|------------|
509.296 | 12046101 | 48.29 | 509.295 | 0.65 | 20.5 C37 H37 N2 |
510.299 | 4770769 | 19.13 | 510.301 | -2.1 | 15.5 C33 H37 N2 B F2 |
511.303 | 900611.1 | 3.61 | 511.305 | -1.96 | 16 C35 H39 N F2 |
536.292 | 5646697 | 22.64 | 536.3 | -7.95 | 18 C36 H38 N2 F2 |
537.289 | 24943784 | 100 | 537.287 | 1.33 | 21 C37 H35 N2 B F |
538.291 | 9461482 | 37.93 | 538.295 | -3.69 | 20.5 C37 H36 N2 B F |
539.295 | 1686477 | 6.76 | 539.303 | -8.16 | 20 C37 H37 N2 B F |
556.298 | 2412247 | 9.67 | 556.286 | 11.96 | 20.5 C37 H35 N2 B F2 |
557.294 | 11010414 | 44.14 | 557.293 | 1.02 | 20 C37 H36 N2 B F2 |
558.297 | 3858148 | 15.47 | 558.301 | -4.06 | 19.5 C37 H37 N2 B F2 |

HRMS (ACPI) calcd. for C_{37}H_{36}N_{2}BF_{2} [M+H]^+: 557.2940, found 557.2944;
HRMS (ACPI) calcd. for C_{29}H_{18}N_{2}BF_4 [M+H]^+: 481.1499, found 481.1494;
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<th>Intensity</th>
<th>Relative</th>
<th>Theo. Mass (mmu)</th>
<th>Delta (mmu)</th>
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HRMS (ACPI) calcd. for C31H24O2N2BF2 [M+H]+: 505.1899, found 505.1895;
HRMS (MALDI-TOF) calcd. for C_{27}H_{20}N_{2}S_{2}BF_{2} [M+H]^+: 485.1129, found 485.1198;
7. DFT calculation

![Chemical Structure of BODIPY 7]

**Chart S1.** Chemical Structure of BODIPY 7.

**Table S4.** Selected electronic excitation energies (eV) and oscillator strengths \((f)\), configurations of the low-lying excited states of the BODIPY 1a-e calculated by TD-B3LYP/6-31+G(d,p) // B3LYP/6-31G(d) based on the optimized ground state geometries. The TDDFT of all the molecules in dichloromethane were using the Self-Consistent Reaction Field (SCRF) method and the Polarizable Continuum Model (PCM).

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\(^[a]\) Only the selected low-lying excited states are presented. \(^[b]\) Oscillator strength. \(^[c]\) Only the main configurations are presented. \(^[d]\) The CI coefficients are in absolute values.
### DFT optimized coordinates

**Compound 1a**

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|        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        | four numbers are the atomic coordinates of the molecule.
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