Benzene-fusing bis(acenaphthoBODIPY)s as a stable near-infrared-selective dye

Hidemitsu Uno,* Takayuki Honda, Manami Kitatsuka, Shogo Hiraoka, Shigeki Mori, Tetsuo Okujima, Masayoshi Takase, and Takahiro Nakae

1 Department of Chemistry and Biology, Graduate School of Science and Engineering, Ehime University, 2-5 Bunkyo-cho, Matsuyama 790-8577, Japan
2 Division of Material Science, Advanced Research Support Center, Ehime University, 2-5 Bunkyo-cho, Matsuyama 790-8577, Japan
3 Present address: Institute of Advanced Energy, Kyoto University, Gokasyo, Uji 711-0011, Japan
Figure S1. UV-vis-NIR (solid line) and fluorescence (dotted line) spectra of 7b (red line) and 10b (blue line) in CH₂Cl₂

Figure S2. UV-vis-NIR (solid line) and fluorescence (dotted line) spectra of 8b (red line) and 11b (blue line) in CH₂Cl₂
**Figure S3.** UV-vis-NIR (solid line) and fluorescence (dotted line) spectra of 8c (red line) and 11c (blue line) in CH$_2$Cl$_2$

**Figure S4.** UV-vis-NIR (solid line) and fluorescence (dotted line) spectra of 9b (red line) and 12b (blue line) in CH$_2$Cl$_2$. Fluorescence of 12b could not be measured due to the wavelength limitation of machine.
Figure S5. Ortep drawing of 7b (top (a) and side (b) views). Solvent molecules and disordered substituents with less occupancy are omitted for clarity.
Figure S6. Ortep drawing of 10b (top (a) and side (b) views). The structure without solvent molecules (CH$_2$Cl$_2$ and acetoniteile) was refined by the Platon Squeeze technique. Disordered substituents with less occupancy are omitted for clarity.
Figure S7. Ortep drawing of top (a) and side (b) views of 11c and top view (c) of 17. Disordered substituents with less occupancies are omitted for clarity.
Figure S8. Ortep drawing of 12b (top (a) and side (b) views). Solvent molecules and disordered substituents with less occupancy are omitted for clarity.

Figure S9. UV-vis-NIR monitoring of 10a in spectroscopic-grade CH₂Cl₂
Figure S10. UV-vis-NIR monitoring of 11b in spectroscopic-grade CH₂Cl₂

Figure S11. UV-vis-NIR monitoring of 1a (CH₂Cl₂) under air in a room light.
Figure S12. UV-vis-NIR and fluorescence spectra of decomposed 1a in CH$_2$Cl$_2$.

Figure S13. UV-vis-NIR and fluorescence spectra of decomposed 11c after ca. 30 days.
**Figure S14.** MALDI-TOF MS spectrum of the decomposed sample of 11c (upper case) and simulated spectra of 18 (middle case) and 17 (lower case)
Figure S15. TD-DFT calculation spectra of 15 (blue) and the corresponding mono-(red) and di-decomplexed (green) compounds.
Figure S16. $^1$H (upper) and $^{13}$C (lower) NMR spectra of 9b
**Figure S17.** $^1$H (upper) and $^{13}$C (lower) NMR spectra of 7b
Figure S18. $^1$H (upper) and $^{13}$C (lower) NMR spectra of 8b
Figure S19. $^1$H (upper) and $^{13}$C (lower) NMR spectra of 8c
Figure S20. $^1$H (upper) and $^{13}$C (lower) NMR spectra of 10b
Figure S21. $^1$H (upper) and $^{13}$C (lower) NMR spectra of 11b
Figure S22. $^1$H (upper) and $^{13}$C (lower) NMR spectra of 11c
Figure S23. $^1$H (upper) and $^{13}$C (lower) NMR spectra of 12b