Electronic Supplementary Information for:

Control of molecular packing of chloroboron(III) and fluoroboron(III) subnaphthalocyanines by designing peripheral substituents

Akuto Takagi and Tadashi Mizutani

Department of Molecular Chemistry and Biochemistry, Faculty of Science and Engineering, Doshisha University, Kyotanabe, Kyoto 610-0321 Japan

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Figure S1. H NMR of 1a (Low-field region).
Figure S1. 1H NMR of 1a (up-field region).
**Figure S1.** $^1$H NMR of 1a (Low-field region 2).

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**Notes:**
- All $^1$H NMR spectra were recorded at 298 K.
- Samples were dissolved in DMSO-d$_6$.
- Spectra were acquired using a JEOL spectrometer.
Figure S2. 13C NMR of 1a.
Figure S.3. $^1$H NMR of 1b (Low-field region)
Figure S.3. $^1$H NMR of 1b (Up-field region).
Figure S3: $^1$H NMR of 1b (Up-field region 2).
Figure S4. 13C NMR of 1b (Up-field region).
Figure S7. $^1$H NMR of 1e.
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**HNMR of 1e (Up-field region)**
Figure S10. H NMR of 2b.
Figure S11. H NMR of 2d.
Figure S1. 1H NMR of 2d (Low-field region).
Figure S1. H NMR of 2d (Up-field region).
Figure S14. $^1$H NMR of 2g.
Figure S15. 13C NMR of 2g.

[Image of 13C NMR spectrum with chemical shifts and peak assignments.]

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*Figure S15* 13C NMR of 2g.
Figure S15. 13C NMR of 2g (up-field region).
Figure S16: 1H NMR of 13.
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Figure S25. MALDI-TOF mass spectrum of 2a (Molecular ion peaks).
Figure S26. MALDI-TOF mass spectrum of 2b.
Figure S26. MALDI-TOF mass spectrum of 2b (Molecular ion peaks).
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Figure S27. MALDI-TOF mass spectrum of 2c (Molecular ion peaks).
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Figure S29. MALDI-TOF mass spectrum of 2e.
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Figure S30. MALDI-TOF mass spectrum of 2f.
Figure S30. MALDI-TOF mass spectrum of 2f (Molecular ion peaks).
Figure S31. MALDI-TOF mass spectrum of 2g.
Figure S31. MALDI-TOF mass spectrum of 2g (Molecular ion peaks).
Figure S32. MALDI-TOF mass spectrum of 13.
Figure S32. MALDI-TOF mass spectrum of 13 (Molecular ion peaks).
Figure S33. MALDI-TOF mass spectrum of 14.
Figure S33. MALDI-TOF mass spectrum of 14 (Molecular ion peaks).
Figure S34. MALDI-TOF mass spectrum of 15.
Figure S34. MALDI-TOF mass spectrum of 15 (Molecular ion peaks).
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Figure S36. HPLC chart of 1b.
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Figure S39. HPLC chart of 1e.
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Figure S40. HPLC chart of 1f.
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Figure S41. HPLC chart of 2a.
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Figure S42. HPLC chart of 2b.
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Figure S43. HPLC chart of 2c.
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Figure S44. HPLC chart of 2d.
Figure S45. HPLC chart of 2e.
Figure S46. HPLC chart of 2f.
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Figure S47. HPLC chart of 2g.
Figure S48 Powder X-ray diffraction patterns of 1d.
Figure S49 Powder X-ray diffraction patterns of 1e.
Figure S50 Powder X-ray diffraction patterns of 1f.
Figure S51. Fluorescence spectra of 2b, 2e, 2f and 2g in CH$_2$Cl$_2$-DMSO (1:1. v/v).

Figure S52. Excitation spectra of 2b in CH$_2$Cl$_2$-DMSO (1:1. v/v).
Figure S52. Excitation spectra of 2e in CH₂Cl₂-DMSO (1:1. v/v).