Electronic Supplementary Information

Functional aza-boron dipyrromethenes for subcellular imaging and organelle-specific photodynamic therapy

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Contents

- Fig. S1 Electronic absorption spectra of 7 at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80.
- Fig. S2 Electronic absorption spectra of 8 at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80.
- Fig. S3 Electronic absorption spectra of 13 at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80.
- Fig. S4 Electronic absorption spectra of 14 at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80.
- Fig. S5 Visualisation of the bright-field image and intracellular fluorescence of HepG2 cells using filter sets specific for MitoTracker and 7, and the corresponding superimposed image.
- Fig. S6 Visualisation of the bright-field image and intracellular fluorescence of HepG2 cells using filter sets specific for LysoTracker and 8, and the corresponding superimposed image.
- Fig. S7 Visualisation of the bright-field image and intracellular fluorescence of MCF-7 cells using filter sets specific for MitoTracker and 7, and the corresponding superimposed image.
- Fig. S8 Visualisation of the bright-field image and intracellular fluorescence of MCF-7 cells using filter sets specific for LysoTracker and 8, and the corresponding superimposed image.
- Fig. S9 Visualisation of the bright-field image and intracellular fluorescence of HT29 cells using filter sets specific for MitoTracker and 7, and the corresponding superimposed image.

- Fig. S10 Visualisation of the bright-field image and intracellular fluorescence of HT29 cells using filter sets specific for LysoTracker and 8, and the corresponding superimposed image.
- Fig. S11 Visualisation of the bright-field image and intracellular fluorescence of HepG2 cells using filter sets specific for LysoTracker and 14, and the corresponding superimposed image.
- Fig. S12 Visualisation of the bright-field image and intracellular fluorescence of MCF-7 cells using filter sets specific for LysoTracker and 14, and the corresponding superimposed image.
- Fig. S13 Visualisation of the bright-field image and intracellular fluorescence of HT29 cells using filter sets specific for LysoTracker and 14, and the corresponding superimposed image.

¹H and ¹³C $\{$ ¹H $\}$ NMR spectra of all the new compounds



Fig. S1 Electronic absorption spectra of **7** at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80. The inset plots the Q-band absorbance versus the concentration of **7**.



Fig. S2 Electronic absorption spectra of **8** at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80. The inset plots the Q-band absorbance versus the concentration of **8**.



Fig. S3 Electronic absorption spectra of **13** at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80. The inset plots the Q-band absorbance versus the concentration of **13**.



Fig. S4 Electronic absorption spectra of **14** at various concentrations in PBS (pH = 7.4) with 0.1% (v/v) Tween 80. The inset plots the Q-band absorbance versus the concentration of **14**.



Fig. S5 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of HepG2 cells using filter sets specific for (ii) MitoTracker (1 μ M, in green) and (iii) **7** (2 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **7** (in red) and MitoTracker (in green) traced along the white lines in Figure (a).



Fig. S6 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of HepG2 cells using filter sets specific for (ii) LysoTracker (2 μ M, in green) and (iii) **8** (2 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **8** (in red) and LysoTracker (in green) traced along the white lines in Figure (a).



Fig. S7 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of MCF-7 cells using filter sets specific for (ii) MitoTracker (1 μ M, in green) and (iii) **7** (2 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **7** (in red) and MitoTracker (in green) traced along the white lines in Figure (a).



Fig. S8 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of MCF-7 cells using filter sets specific for (ii) LysoTracker (2 μ M, in green) and (iii) **8** (2 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **8** (in red) and LysoTracker (in green) traced along the white lines in Figure (a).



Fig. S9 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of HT29 cells using filter sets specific for (ii) MitoTracker (1 μ M, in green) and (iii) **7** (1 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **7** (in red) and MitoTracker (in green) traced along the white lines in Figure (a).



Fig. S10 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of HT29 cells using filter sets specific for (ii) LysoTracker (2 μ M, in green) and (iii) **8** (1 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **8** (in red) and LysoTracker (in green) traced along the white lines in Figure (a).



Fig. S11 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of HepG2 cells using filter sets specific for (ii) LysoTracker (2 μ M, in green) and (iii) **14** (4 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **14** (in red) and LysoTracker (in green) traced along the white lines in Figure (a).



Fig. S12 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of MCF-7 cells using filter sets specific for (ii) LysoTracker (2 μ M, in green) and (iii) **14** (4 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **14** (in red) and LysoTracker (in green) traced along the white lines in Figure (a).



Fig. S13 (a) Visualisation of the (i) bright-field image and intracellular fluorescence of HT29 cells using filter sets specific for (ii) LysoTracker (0.2 μ M, in green) and (iii) **14** (4 μ M, in red), and (iv) the corresponding superimposed image. Figure (b) shows the fluorescence intensity line profiles of **14** (in red) and LysoTracker (in green) traced along the white lines in Figure (a).

1H and $^{13}C\{^1H\}$ NMR spectra of ${\bf 2}$ in CDCl₃



1H and $^{13}C\{^1H\}$ NMR spectra of $\boldsymbol{3}$ in CDCl₃



1H (in CDCl₃) and $^{13}C\{^1H\}$ (in DMSO-d₆) NMR spectra of ${\bf 4}$



 ^1H (in CDCl₃) and $^{13}\text{C}\{^1\text{H}\}$ (in DMSO-d₆) NMR spectra of $\boldsymbol{5}$



¹H and ¹³C{¹H} NMR spectra of **6** in CDCl₃



 ^1H (in CD₃COCD₃) and $^{13}\text{C}\{^1\text{H}\}$ (in CDCl₃) NMR spectra of **7**



 1 H and 13 C{ 1 H} NMR spectra of 8 in CDCl₃



¹H and ¹³C{¹H} NMR spectra of **9** in CDCl₃



 1H and $^{13}C\{^1H\}$ NMR spectra of 10 in CDCl $_3$



 1H and $^{13}C\{^1H\}$ NMR spectra of 11 in CDCl3



¹H and ¹³C{¹H} NMR spectra of **12** in CDCl₃



 1H and $^{13}C\{^1H\}$ NMR spectra of $\boldsymbol{13}$ in CDCl₃



 1H and $^{13}C\{^1H\}$ NMR spectra of 14 in CDCl $_3$

