Supporting information

The self-assembly of monosubstituted BODIPY and HFBI-RGD

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**Fig. S1** The left: Ultraviolet absorption spectra of dyes **compound 1** in CH$_2$Cl$_2$ with different concentrations (5 μM, 10 μM, 20 μM, 30 μM). The right: Fluorescence spectra of dyes **compound 1** with corresponding concentration at ambient temperature.

(a)

(b)

(c)

**Fig. S2** (a-c) the left: Ultraviolet absorption spectra of dyes (3a-3c) in CH$_2$Cl$_2$ with different concentrations (5 μM, 10 μM, 20 μM, 30 μM). The right: Fluorescence spectra of dyes (3a-3c) with corresponding concentration at ambient temperature.
Fig. S3 (a-c) the left: Ultraviolet absorption spectra of dyes (3a-3c) in CH₂Cl₂, CHCl₃, DMSO with same concentration (20 μM). The right: Fluorescence spectra of dyes (3a-3c) with corresponding concentration at ambient temperature.

Fig. S4 Fluorescence intensity vs HFBI-RGD.
Fig. S4 (a) The structure of $3b''$; (b) The left: Ultraviolet absorption spectra of dyes $3b''$ in CH$_2$Cl$_2$ with different concentration (5 μM, 10 μM, 20 μM, 30 μM). The right: Fluorescence spectra of dyes $3b''$ with corresponding concentration at ambient temperature.

Fig. S5 Fluorescence spectra of compound 1 in the presence of different concentrations of HFBI-RGD aqueous solution.
| BODIPYs | Structure | Volume         |
|---------|-----------|----------------|
| compound1 | ![Structure Image](image1) | 850.0 Å³ |
| 3a      | ![Structure Image](image2) | 1417.5 Å³ |
| 3b      | ![Structure Image](image3) | 1436.5 Å³ |
| 3c      | ![Structure Image](image4) | 1497.8 Å³ |
Fig. S6 (a) Fluorescence intensity of time-dependent in vivo fluorescence images of nude mice bearing glioma cells U-87 after tail intravenous injection. (b) Fluorescence intensity of tumor at different time intervals.