Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

The self-assembly of monosubstituted BODIPY and HFBI-RGD

Fengnan Sun,[a] Guang Yang,[a,b] Qian Zhang,[a] Zhongbo Xue,[a] Chengzhi Gu,[c] Zhuozhi Chen,[d] Boying Yan,[e] Yaqing Feng,[a,b] Zefang Wang,[d] Shuxian Meng[a*]

[a]School of Chemical Engineering and Technology, Tianjin University, Tianjin 300050, China

[b]Collaborative Innovation Center of Chemical Science and Engineering, Tianjin 300072, China

[c]School of Chemical Engineering and Technology, Shihezi University, Xinjiang 832000, China

[d]School of Life Sciences, Tianjin University, Tianjin 300072, China

[e]General hospital of Tianjin Medical University, Tianjin 300052, China

* Corresponding author: (S.M.) msxmail@tju.edu.cn.

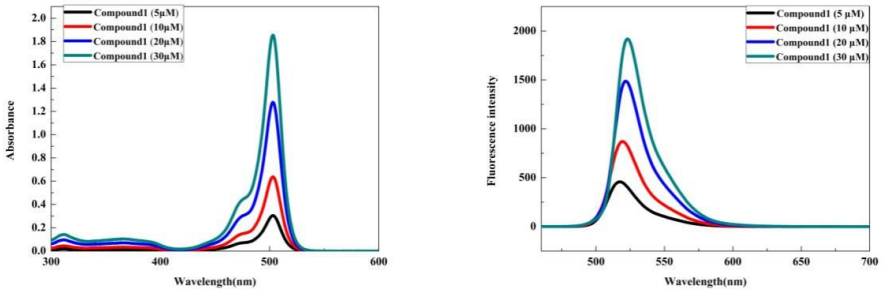
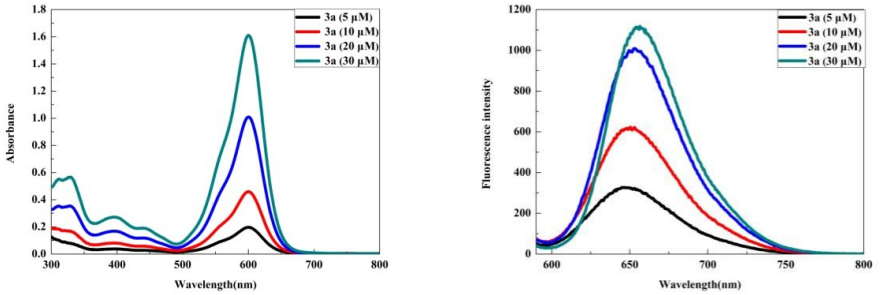
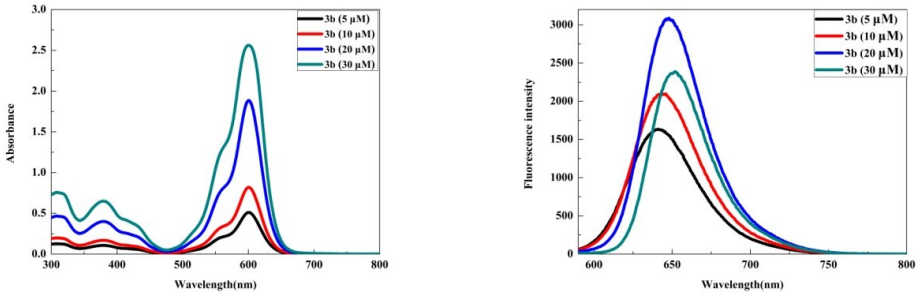


Fig. S1 The left: Ultraviolet absorption spectra of dyes **compound 1** in CH_2Cl_2 with different concentrations (5 μM, 10 μM, 20 μM, 30 μM). The right: Fluorescence spectra of dyes **compound 1** with corresponding concentration at ambient temperature.

(a)



(b)



(c)

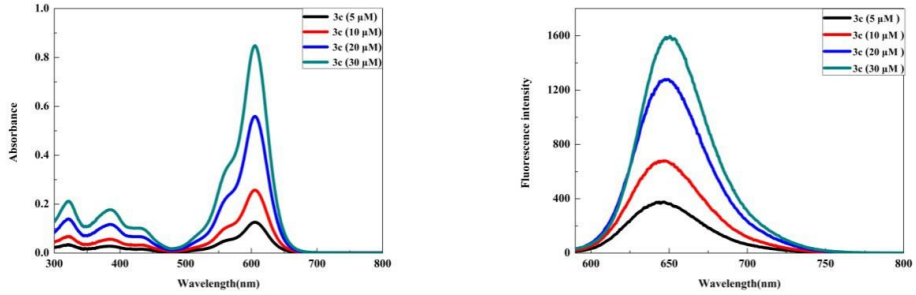
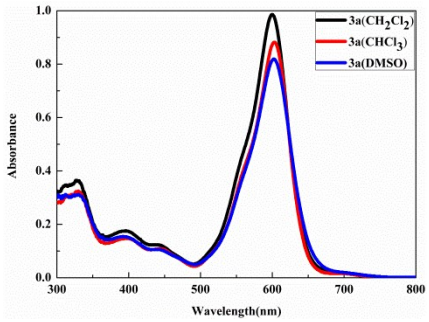
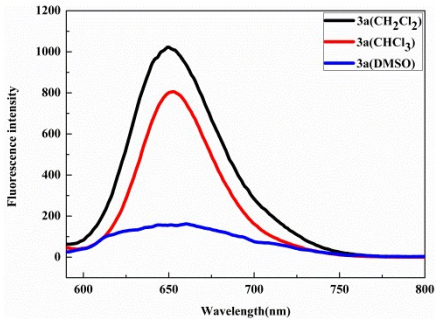


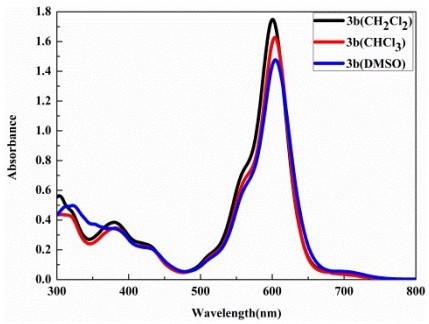
Fig. S2 (a-c) the left: Ultraviolet absorption spectra of dyes (**3a-3c**) in CH_2Cl_2 with different concentrations (5 μM, 10 μM, 20 μM, 30 μM). The right: Fluorescence spectra of dyes (**3a-3c**) with corresponding concentration at ambient temperature.

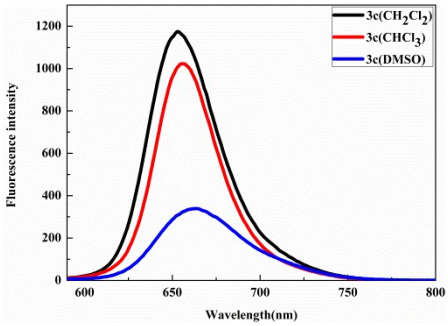
(a)



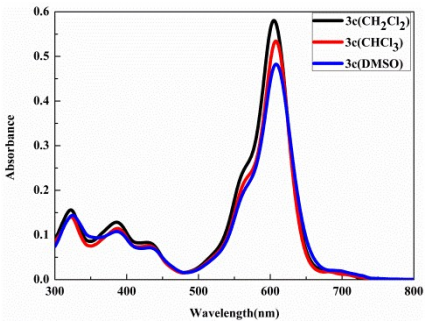


(b)





(c)



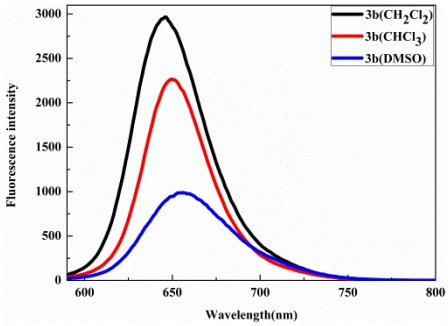


Fig. S3 (a-c) the left: Ultraviolet absorption spectra of dyes (**3a-3c**) in CH_2Cl_2,$CHCl_3$,DMSO with same concentration (20 μM). The right: Fluorescence spectra of dyes (**3a-3c**) with corresponding concentration at ambient temperature.

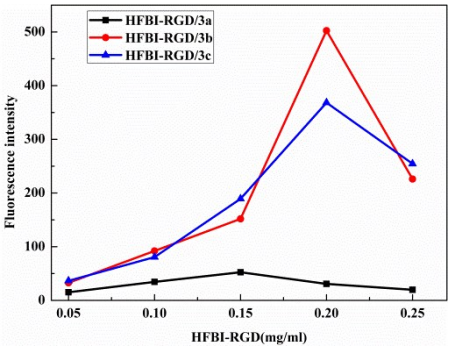
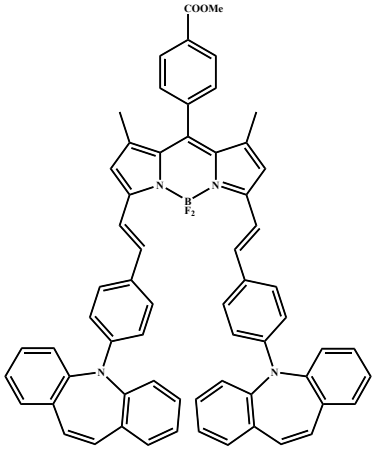


Fig. S4 Fluorescence intensity vs HFBI-RGD.

(a)



(b)

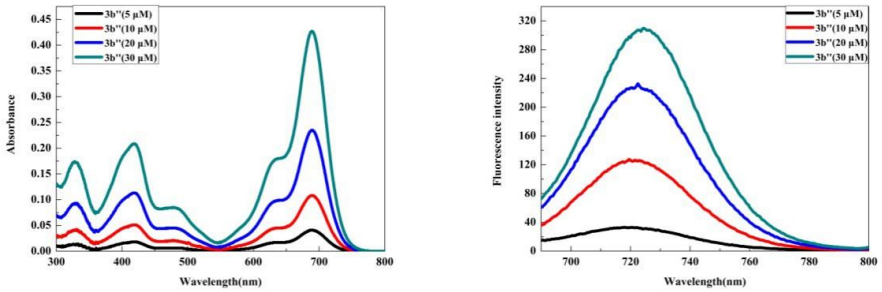


Fig. S4 (a) The structure of 3b''; (b) The left: Ultraviolet absorption spectra of dyes **3b"** in CH_2Cl_2 with different concentration (5 μM, 10 μM, 20 μM, 30 μM). The right: Fluorescence spectra of dyes **3b"** with corresponding concentration at ambient temperature.

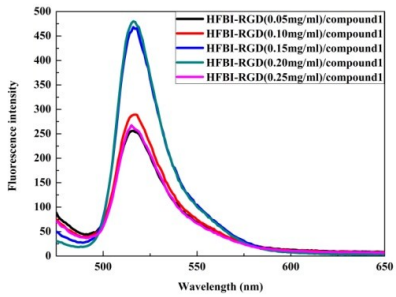
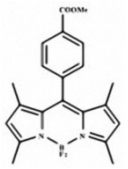
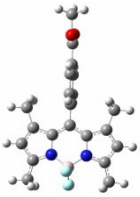
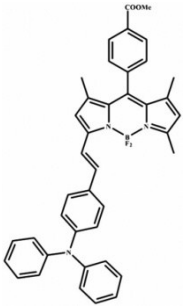
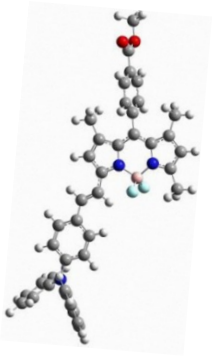
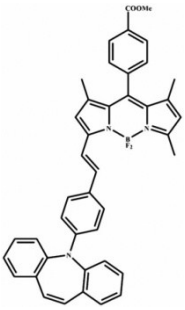
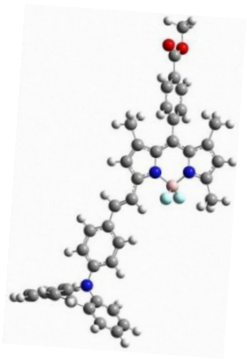
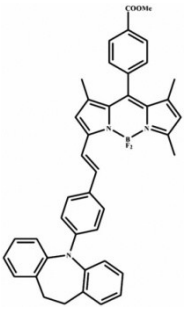
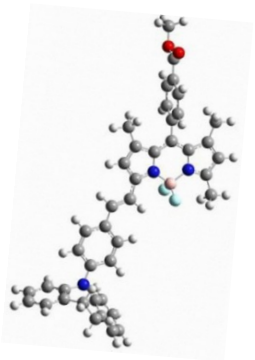
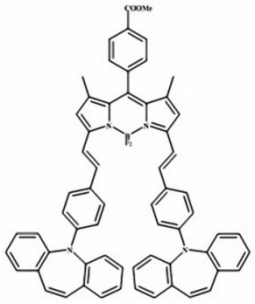


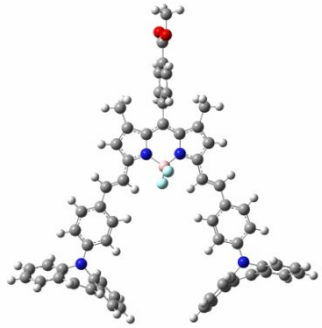
Fig. S5 Fluorescence spectra of **compound 1** in the presence of different concentrations of HFBI-RGD aqueous solution.

Table S1. Computational Data of BODIPYs

BODIPYs	Structure	Volume
 **compound1**		850.0 Angstrom^3
 **3a**		1417.5 Angstrom^3
 **3b**		1436.5 Angstrom^3
 **3c**		1497.8 Angstrom^3



3b”



2119.2 Angstrom^3

(a) (b)

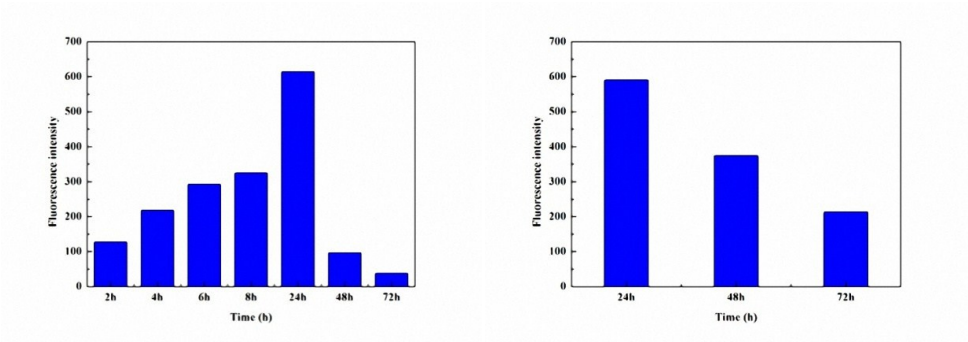


Fig. S6 (a) Fluorescence intensity of time-dependent *in vivo* fluorescence images of nude mice bearing glioma cells U-87 after tail intravenous injection. (b) Fluorescence intensity of tumor at different time intervals.