## **Electronic Supplementary Information**

# **Tuning Near Infrared II Emitting Wavelength of Small Molecule Dyes by Single Atom Alteration**

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## 1. Supporting table and figures





**Figure S1.** (a) Optimized geometries (front view and top view) of FFB, FTB, and FSB at excited (S<sub>1</sub>) state and (b) corresponding values of the dihedral angles and plane angles (same as marked in **Figure 2b**)



**Figure S2.** Docking results of FFBA, FTBA, and FSBA with HSA. Upper row: Magnified view of the docking sites, and the protein is in green cartoon, small molecules are in red sticks, and polar contacts between SMDs and protein are in yellow dashes; Lower row: Overall view of the docking results, and the protein is in green surface and small molecules are in red surfaces.



**Figure S3.** (a) The concentrations of FFBA, FTBA, and FSBA were constant 1 μM and concentration of HSA was increased from 0 to 16 μM in PBS. Fluorescent intensities of these samples were recorded and the intensities of FFBA, FTBA, and FSBA with 0 μM HSA were set as 1 for each group respectively. (b) Fluorescence enhancement of FFBA@HSA, FTBA@HSA, and FSBA@HSA dispersed in PBS (1 μM, molar ratio of FXBA/HSA was 2:1) after heated at different temperatures for 10 min. Fluorescent intensities of the samples heated at 25°C were set as 1. (c) Normalized fluorescence emission spectra of FFBA@HSA, FTBA@HSA, and FSBA@HSA in PBS (1 μM, molar ratio of FXBA/HSA was 2:1, solid lines) after heated at 50°C for 10 min and FFB, FTB, and FSB in toluene (dash lines).



**Figure S4.** Optical stability of FFBA@HSA, FTBA@HSA, and FSBA@HSA under continuous 808 nm laser excitation in (a) PBS and (b) fetal bovine serum (FBS) for 120 min.



**Figure S5.** Cell viability of NIH/3T3 cells incubated with (a) FFBA@HSA, (b) FTBA@HSA, and (c) FSBA@HSA of different concentrations for 72 hours. Data are represented as mean± SEM.



**Figure S6.** Ex vivo imaging 24 h after i.v. injection of 50  $\mu$ M dye-protein complexes. Upper row from left to right: heart, liver, spleen; lower row from left to right: lung, kidneys, skin.



**Figure S7.** Hind limb vascular imaging with 1000LP filter (scale bar: 5 mm) of C57BL 5 min after i.v. injection of FFBA@HSA, FTBA@HSA and FSBA@HSA.



**Figure S8.** Signal to background ratio (SBR) of vascular imaging with different optical long pass filters after the administration of FFBA@HSA, FTBA@HSA, and FSBA@HSA complexes.



Figure S9. Schematic description of the lymphatic imaging.



Figure S10. Lymphatic images taken at 1, 4, 8, and 24 h after intradermal injection of FFBA@HSA (scale bar: 6 mm).

### 2. Materials and experiment procedures

#### Materials and general methods

All chemicals, solutions and solvents were purchased from Sigma-Aldrich (St Louis, MO) and used without further purification. The cell line NIH/3T3 were obtained from the American Type Culture Collection (Manassas, VA). High performance liquid chromatography (HPLC) were performed on a Dionex Ultimate 3000. Dissolved in deuterated solvents, nuclear magnetic resonance (NMR) spectra and matrix-assisted laser desorption/ionization time of flight mass spectra (MALDI-TOF MS) of synthesized compounds were acquired on a Bruker 400 MHz magnetic resonance spectrometer and an AB SCIEX 4700 TOF/TOF system, respectively. Absorption spectra between 600-1000 nm were records on an Agilent 8453 UV spectrophotometer (Agilent Technologies, CA). A home-built NIR-II spectrofluorometer based on NIRvana 640 (Princeton Instrument) were used to characterize the NIR-II emission spectra of prepared small molecule dyes. NIRvana 640 was also employed to obtain NIR-II imaging by coupling with a homemade small animal imaging platform. An 808 nm diode laser system was used as the excitation light source with a power density at 0.1 W/cm<sup>2</sup>, which is well below the safe laser power limit of ~329 mW/cm<sup>2</sup> at 808 nm according to the International Commission on Non-ionizing Radiation Protection.<sup>1</sup>

#### Preparation of the designed molecules:



Compound 1 (1.15 g, 2.43 mmol) was dissolved in 10 mL of dichloromethane (DCM) with 1-ethyl-3-(3-

dimethylaminopropyl)carbodiimide hydrochloride (EDCl, 1.86 g, 9.72 mmol) and 4dimethylaminopyridine (DMAP, 59.35 mg, 0.48 mmol). The mixture was then added with 2-(trimethylsilyl) ethanol (1.15 g, 9.72 mmol) and stirred for another 2 h and loaded to a silicon chromatography column for purification when the reaction is finished. The product was oily and light yellow (929.15 mg, 56.7% yield).

Above product (0.60 g, 0.89 mmol), potassium acetate (174.78 mg, 1.78 mmol) and bis(pinacolato)diboron (339.15 mg, 1.34 mmol) were all dispersed in dimethylformamide (DMF) in argon atmosphere, followed by the addition of bis(triphenylphosphine)palladium(II) dichloride (62.49 mg, 89.04 µmol). The reaction was heated to 80°C for 2 hours before filtrated to remove catalyst. Abundant water (20 mL) was added to the mixture and washed with hexane (10 mL× 3). The organic phase was then condensed to produce white solid (compound 2, 610.01 mg, 95.0% yield). <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$ ): 7.76 (d, *J* = 7.6 Hz, 1H), 7.68-7.63 (m, 3H), 7.27-7.26 (m, 3H), 4.06 (t, *J* = 7.0 Hz, 4H), 2.02 (t, *J* = 7.2 Hz, 4H), 1.99-1.98 (m, 4H), 1.95-1.91 (m, 4H), 1.21-1.18 (m, 12H), 1.06-0.98 (m, 4H), 0.88 (t, *J* = 7.9 Hz, 4H), 0.60-0.52 (m, 4H), -0.04 (s, 18H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>,  $\delta$ ): 173.72, 170.91, 150.82, 149.35, 144.03, 140.85, 133.79, 128.67, 127.54, 126.77, 122.75, 120.08, 118.94, 83.63, 62.14, 54.85, 39.98, 34.30, 29.40, 24.96, 24.54, 23.30, 17.22, -1.56.



To a toluene solution of compound 3 (2-(tributylstannyl)furan, 232.53 mg, 0.65 mmol or 2-(tributylstannyl)selephene, 273.53 mg, 0.65 mmol), 4,7-dibromo-5,6-dinitrobenzo[c][1,2,5]thiadiazole (100 mg, 0.26 mmol) was added under inert air (N<sub>2</sub>) protection. After stirred for a few minutes, tetrakis(triphenylphosphine)palladium (Pd(PPh<sub>3</sub>)<sub>4</sub>, 30.11 mg, 0.03 mmol) was added and the mixture was then kept at 90°C overnight. Purification of the crude product by silicone gel chromatography yielded dark red powder. The resulting product were dissolved in DMF and chilled in ice bath before Nbomosuccinimide (NBS, 101.98 mg, 0.57 mmol) was added to the mixture. The reaction was stirred overnight and then warmed to ambient temperature. Orange precipitate was formed by adding 1M HCl, collected by filtration and washed by methanol. The product was dried in vacuum.

FB (71.26 mg, 53% yield): <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ,  $\delta$ ): 7.84 (d, J = 5.1 Hz, 2H), 6.97 (d, J = 5.3 Hz, 2H); <sup>13</sup>C NMR (101 MHz, DMSO- $d_6$ ,  $\delta$ ): 149.56, 147.97, 145.61, 127.79, 122.19, 116.22, 114.08. SB (83.60 mg, 50% yield): <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ,  $\delta$ ): 7.58 (d, J = 3.9 Hz, 2H), 7.36 (d, J = 3.9 Hz, 2H); <sup>13</sup>C NMR (101 MHz, DMSO- $d_6$ ,  $\delta$ ): 152.19, 140.42, 136.62, 134.41, 133.58, 123.61, 123.10.



To a solution of compound 2 (901.19 mg, 1.25 mmol), tetrahydrofuran (THF, 2.5 mL/mmol), compound XB (FB, 258.04 mg, 0.50 mmol; TB, 274.10 mg, 0.50 mmol; SB, 321.01 mg, 0.50 mmol), and potassium

carbonate (207.30 mg, 1.50 mmol), [1, 1'-Bis(diphenylphosphino)ferrocene] dichloropalladium(II) (Pd(dppf)Cl<sub>2</sub>, 73.17 mg, 0.10 mmol) was added under N<sub>2</sub> protection and the solution was heated to 70°C and refluxed overnight. Product was purified by silicone gel chromatography (petroleum/EA = 100/10) and in the form of dark purple-red solid. Then, this product was mixed with zinc powder (653.80 mg, 10.00 mmol) and ammonium chloride (534.90 mg, 10.00 mmol) in 90% methanol (5 mL) in N<sub>2</sub> atmosphere and stirred for 4 h. Insoluble matters was then removed from the mixture by filtration and solvent was evaporated in vacuum. Water (10 mL) was added to the residue and washed by DCM (5 mL × 3). The organic phase was combined and dried over anhydrous sodium sulfate before condensed by rotary evaporator.

The left extraction was dissolved in 3 mL of pyridine and N-thionylaniline (PhNSO, 1.39 g, 10.00 mmol) along with chlorotrimethylsilane (TMSCl, 2.16 g, 20.00 mmol) was added to the reaction. After refluxing overnight, purification by chromatography (petroleum/EA = 100/20) afford the product as deep green solid.

FFB (264.65 mg, 35% yield): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ): 8.26 (d, *J* = 3.7 Hz, 2H), 8.09 (d, *J* = 7.9, 1.1 Hz, 2H), 7.90 (s, 2H), 7.84 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 7.4 Hz, 2H), 7.43 – 7.31 (m, 6H), 7.14 (d, *J* = 3.7 Hz, 2H), 4.11 – 4.01 (m, 8H), 2.21 – 1.91 (m, 16H), 1.41 (m, 8H), 1.20 – 1.01 (m, 8H), 0.96 – 0.80 (m, 8H), 0.78 – 0.64 (m, 8H), -0.02 (s, 36H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>, δ): 173.85, 157.09, 151.04, 150.72, 150.43, 141.47, 140.65, 129.19, 128.34, 127.03, 123.85, 122.83, 120.37, 119.95, 118.66, 109.17, 108.52, 77.32, 62.27, 55.04, 40.23, 34.36, 30.35, 29.48, 24.60, 23.46, 17.25, -1.54.

FTB (223.94 mg, 29% yield): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$ ): 7.82 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 0.6 Hz, 2H), 7.74 (d, *J* = 3.4 Hz, 2H), 7.72 (d, *J* = 1.6 Hz, 2H), 7.63 (d, *J* = 4.2 Hz, 2H), 7.60 – 7.51 (m, 2H), 7.39 – 7.29 (m, 6H), 4.10 – 4.05 (m, 8H), 2.12 – 1.99 (m, 16H), 1.43 – 1.36 (m, 8H), 1.16 – 1.07 (m, 8H), 0.93 – 0.88 (m, 8H), 0.74 – 0.61 (m, 8H), -0.01 (s, 36H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>,  $\delta$ ): 173.85, 151.33, 151.24, 150.58, 149.97, 141.46, 140.56, 137.33, 134.16, 133.09, 127.03, 124.37, 122.83, 119.90, 113.35, 109.77, 109.12, 99.59, 62.29, 55.15, 40.14, 34.38, 29.69, 29.48, 24.61, 23.46, 17.26, -1.53.

FSB (270.31 mg, 33% yield) : <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$ ): 7.79 (d, *J* = 4.5 Hz, 2H), 7.76 (d, *J* = 1.3 Hz, 2H), 7.74 (s, 2H), 7.72 (d, *J* = 1.6 Hz, 2H), 7.69 – 7.67 (m, 2H), 7.56 – 7.50 (m, 2H), 7.39 – 7.31 (m, 6H), 4.12 – 4.05 (m, 8H), 2.13 – 2.01 (m, 16H), 1.47 – 1.36 (m, 8H), 1.19 – 1.08 (m, 8H), 0.95 – 0.87 (m, 8H), 0.81 – 0.62 (m, 8H), -0.01 (s, 36H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>,  $\delta$ ): 173.86, 157.25, 151.29, 151.22, 150.63, 141.55, 141.26, 140.57, 136.44, 135.40, 127.46, 127.05, 126.90, 125.37, 122.86, 120.29, 120.22, 119.92, 115.02, 62.29, 55.11, 40.21, 34.39, 29.49, 24.61, 23.48, 17.26, -1.52.





X=O (FFBA), S (FTBA), or Se (FSBA)

FXB (10 mg) was dissolved in 3 mL of dichloromethane with 50% trifluoroacetate (TFA) and stirred for 2 h. Solvent and TFA was removed in vacuum and FXBA was recrystallized in DCM as deep green powder. Further purification by HPLC yielded the final products.

FFBA (7.05 mg, 96% yield): <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ,  $\delta$ ): 11.81 (s, 4H), 8.16 (d, J = 3.5 Hz, 2H), 8.12 (s, 2H), 8.07 (d, J = 7.7 Hz, 2H), 7.97 (d, J = 8.1 Hz, 2H), 7.85 (d, J = 5.7 Hz, 2H), 7.65 – 7.22 (m,

8H), 2.19 – 2.02 (m, 8H), 2.02 – 1.88 (m, 8H), 1.32 – 1.15 (m, 8H), 1.15 – 0.92 (m, 8H), 0.80 – 0.41 (m, 8H); <sup>13</sup>C NMR (101 MHz, DMSO-*d*<sub>6</sub>, δ): 174.72, 157.53, 156.53, 151.40, 150.93, 150.14, 150.09, 141.37, 140.48, 129.05, 128.97, 128.16, 126.14, 123.43, 122.69, 120.66, 119.12, 108.02, 108.00, 55.12, 40.88, 33.92, 29.27, 24.62, 23.79.

FTBA (6.96 mg, 94% yield): <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ,  $\delta$ ): 11.84 (s, 4H), 7.93 (d, J = 4.8 Hz, 2H), 7.90 (d, J = 5.8 Hz, 2H), 7.87 (d, J = 4.0 Hz, 2H), 7.83 (d, J = 4.0 Hz, 2H), 7.78 ((d, J = 4.0 Hz, 2H), 7.51 – 7.33 (m, 8H), 2.19 – 2.03 (m, 8H), 1.98 (t, J = 7.4 Hz, 8H), 1.35 – 1.15 (m, 8H), 1.13 – 0.96 (m, 8H), 0.71 – 0.46 (m, 8H); <sup>13</sup>C NMR (101 MHz, DMSO- $d_6$ ,  $\delta$ ): 174.72, 151.60, 150.88, 150.82, 150.59, 149.24, 141.45, 140.45, 137.41, 136.81, 132.90, 128.38, 128.06, 127.56, 123.41, 120.58, 120.04, 112.86, 112.74, 55.28, 40.89, 33.94, 29.27, 24.63, 23.79.

FSBA (7.40 mg, 98%): <sup>1</sup>H NMR (400 MHz, DMSO- $d_6$ ,  $\delta$ ): 11.83 (s, 4H), 7.92 (d, J = 4.5 Hz, 2H), 7.86 (d, J = 4.5 Hz, 2H), 7.84 (d, J = 4.5 Hz, 2H), 7.82 (d, J = 4.5 Hz, 2H), 7.71 (d, J = 7.9 Hz, 2H), 7.54 (d, J = 8.1 Hz, 2H), 7.51 – 7.32 (m, 6H), 2.17 – 2.03 (m, 8H), 2.02 – 1.93 (m, 8H), 1.32 – 1.22 (m, 8H), 1.16 – 1.00 (m, 8H), 0.70 – 0.47 (m, 8H); <sup>13</sup>C NMR (101 MHz, DMSO- $d_6$ ,  $\delta$ ): 174.72, 151.60, 151.57, 151.49, 150.86, 150.72, 141.47, 140.90, 140.48, 130.08, 128.04, 127.73, 127.56, 127.55, 123.39, 121.11, 120.57, 120.27, 114.32, 55.25, 40.88, 33.96, 29.30, 24.65, 23.81.

Detailed NMR and MS spectra were attached to the end of this file.

#### Quantum yield calculation

Quantum yields of these molecules were calculated as described before.<sup>2</sup> Briefly, several concentrations ( $n\geq 5$ ) of tested molecules were dissolved in solvents with an optical density below 0.1. Then, the absorbance at 808 nm and emission spectra between 900-1500 nm of each sample were measured and integrated fluorescence was plotted against corresponding absorbance to find the linear fitting slope *K*. And QY was calculated by the following equation:

$$QY_x = QY_{ref} \times \frac{n_x^2}{n_{ref}^2} \times \frac{K_x}{K_{ref}}$$

where x stands for the tested sample, and *ref* stands for reference compound IR-26. Index of refraction of corresponding solvents were designated as n.

#### Density function theory calculation

Gaussian 09 software<sup>3</sup> was used to perform the theoretic calculations. Ground state ( $S_0$ ) optimization was calculated using opt B3LYP/6-31G(d) method and excited state ( $S_1$ ) geometries were further optimized using  $S_0$  results with opt TD B3LYP/6-31G(d) method. Side chains of fluorenes were replaced by methyl groups to reduce calculation burden.

#### **Molecular modeling**

The structures of FFBA, FTBA, and FSBA were generated and optimized by Sybyl-X software (Tripos Inc., MO). The crystal structure of HSA (PDB ID: 1h9z) was obtained from RCSB Protein Data Bank and prepared by Sybyl-X software. Molecular docking was carried out in a Surflex Dock program with the following parameters: additional starting conformation per molecule, 20; Angstroms to expand search grid, 6; max conformation per fragment, 20; max number of rotatable bonds per molecule, 100.

#### Cytotoxicity assay

Mouse embryonic fibroblasts NIH/3T3 cells were cultured in the Dulbecco's Modified-Eagle's Medium

supplemented with 10% fetal bovine serum (FBS). The cells were incubated at 37°C in an atmosphere with 5% CO<sub>2</sub>. When cells reach logarithmic growth phase, about 3000 cells per well were seeded on a 96-well plate and incubated overnight. The culture medium was then replaced by 200  $\mu$ L/well of medium containing different concentration of tested structures (0-60  $\mu$ M, at least 3 wells for each concentration). After incubated for 72 h, 20  $\mu$ L of 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) solution (5 mg/mL in PBS) was added to each well with tested substances and the plates was incubated in dark for 4 h before the medium was removed and cells were washed by PBS for 3 times. Then DMSO (150  $\mu$ L/well) was added to dissolve the formed purple precipitation. The absorption at 490 nm of each well was tested and used to calculate the viability of cells.

#### Vascular and lymphatic imaging

All animal experiments were performed in compliance with the Guidelines for the Care and Use of Research Animals as established by the Stanford University Animal Studies Committee.

For vascular imaging, each tested SMD@HSA complex (heated) was dissolved in 150  $\mu$ L of PBS with a concentration of 50  $\mu$ M and injected to C57BL/6J mice intravenously. Five minutes later, NIR-II imaging of mouse in supine position was obtained on our homemade in vivo imaging system.

For lymphatic imaging, 20  $\mu$ L of previously prepared FFBA@HSA (50  $\mu$ M, heated) was intradermally injected to the hind paw of nude mice, and NIR-II imaging was performed at 20 min, 1 h, 4 h, 8 h, and 24 h post injection. All animals were in prone position. The exposure time was 0.5 s, 2 s for 1000LP and 1150LP filters, respectively, and excited by 808 nm laser.

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## 3. NMR and MS spectra of synthesized compounds

## <sup>1</sup>H NMR spectrum of Compound 2



<sup>1</sup>H NMR spectrum of Compound FB





### <sup>13</sup>C NMR spectrum of Compound SB





<sup>13</sup>C NMR spectrum of Compound FFB







## MS spectrum of Compound FTB







### <sup>13</sup>C NMR spectrum of Compound FSB



## MS spectrum of Compound FSB



<sup>1</sup>H NMR spectrum of Compound FFBA



## MS spectrum of Compound FFBA



<sup>1</sup>H NMR spectrum of Compound FTBA



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## MS spectrum of Compound FTBA



### <sup>1</sup>H NMR spectrum of Compound FSBA



## MS spectrum of Compound FSBA

