# **Supporting Information**

## Pyrene-based BODIPY: Synthesis, photophysics and lasing

# properties under UV-pumping radiation

Yang Yang<sup>a,\*</sup>, Lei Zhang<sup>b</sup>, Chaoying Gao<sup>a</sup>, Liang Xu<sup>a</sup>, Suozhu Bai<sup>a</sup> and Xingyuan

Liu<sup>b</sup>

<sup>a</sup> College of Chemistry and Chemical Engineering, Inner Mongolia University for the Nationalities,

Tongliao 028000, PR China

<sup>b</sup> State Key Laboratory of Luminescence and Applications, Changchun Institute of Optics Fine

Mechanics and Physics, Chinese Academy of Sciences, Changchun 130033, PR China

Corresponding author: Yang Yang

E-mail: <u>yangyang-000@163.com</u>

Tel: +86 475 8313570

#### **1. Experimental Section**

**General:** Solvents were dried and distilled according to standard procedures prior to use. All other compounds were commercially available and used as received. All the photoluminescence (PL) spectra were measured with a Jasco FP-6500 fluorescence spectrophotometer. The UV-visible absorption spectra were recorded on a Shimadzu UV-3600 spectrophotometer. Photoluminescence quantum yield in solution were determined relative to a solution of fluorescein as the standard in 0.1 M NaOH solution ( $\Phi_F = 0.95$ ). The narrow-line width laser emission and tuning ranges of dye solutions were collected using an Ocean Optics Maya2000 Pro Fiber Optic Spectrometer. ASE investigations were performed using a Nd:YAG laser with a repetition rate of 10 Hz and pulse duration of about 10 ns. The laser power was detected by Newport 2936C laser power meter. All measurements were carried out in the air at room temperature without being specified.

#### Procedure for the Determination of Quantum yield

The fluorescence quantum yields ( $\Phi_F$ ) of the PYBDP systems were calculated according to the following method: First, the PYBDP dye to be evaluated in the various solvents was diluted at five different concentrations. The concentrations were selected, so that the absorbance of each sample was below 0.10 at the excitation wavelength and above to prevent re-absorption. Next, a graph of the absorbance (A) at a certain wavelength (496 nm) versus the integrated emission intensity (F) excited at the chosen wavelength was plotted. Then, the slope (Grad) of the fitting line to the plot of F versus A was calculated (intercept = 0). Absolute values are calculated using the standard samples which have a fixed and known fluorescence quantum yield value, according to the following relationship:

$$\Phi_{\rm X} = \Phi_{\rm ST} \left( \frac{{\rm Grad}_{\rm X}}{{\rm Grad}_{\rm ST}} \right) \left( \frac{{\rm n}_{\rm X}^2}{{\rm n}_{\rm ST}^2} \right)$$

Here, the subscripts ST and X denote standard and test respectively,  $\Phi$  is the fluorescence quantum yield, *Grad* the gradient from the plot of integrated fluorescence intensity vs absorbance, and *n* the refractive index of the solvent. The reference systems used was Fluorescein as standard [ $\Phi_{ST} = 0.95$ , in 0.1 M NaOH].

### 2. Synthesis of Reference material

The reference material Pyrene-BODIPY was prepared according to the same synthetic route shown in Scheme S1. Details can be found in *RSC Advances*, **2011**, *1*, 677–684. We took the lasing experiments as the dye PYBDP, but there was no sign of spectral narrowing or ASE phenomenon happening.



Pyrene-BODIPY

Scheme S1. Synthesis of reference material Pyrene-BODIPY

## 3. Absorbance spectra of PYBDP



Fig. S1. Overlapped Absorbance spectra of PYBDP (10µM) in different solvents.



## 4. Laser Actions of PYBDP

Fig. S2. Normalized fluorescence emission spectra for PYBDP (10  $\mu$ M) in various solvents upon excitation at 355 nm with a Q-switched pulsed Nd:YAG laser.

| Solvent           | E <sub>T</sub> (30) | $\lambda_{fl} / nm$ | FWHM | Eff <sub>max</sub> |
|-------------------|---------------------|---------------------|------|--------------------|
| Hexane            | 31.0                | 524.2               | 25.9 | 2.82%              |
| Toluene           | 33.9                | 516.7               | 37.5 | 10.86%             |
| Ether             | 34.5                | 524.8               | 33.7 | 3.91%              |
| THF               | 37.4                | 527.9               | 31   | 2.64%              |
| EtOAc             | 38.1                | 527.7               | 32.3 | 0                  |
| CHCl <sub>3</sub> | 39.1                | 536.9               | 39.4 | 0                  |
| Acetone           | 42.2                | 531.2               | 35.8 | 0                  |
| EtOH              | 51.9                | 522                 | 37   | 0                  |

Table S1. Laser parameters of PYBDP in different solvents pump at 355nm

[a] Eff: energy conversion efficiency,  $\lambda_n$ : peak wavelength of the laser emission before ASE; FWHM: full width half maximum pumped at 355 nm.



**Fig. S3.** ASE Laser output versus pump energy for PYBDP (4 mM) in toluene determined by 355 nm irradiation with a Q-switched pulsed Nd:YAG laser.



Fig. S4. Photograph of the ASE beam from PYBDP in toluene solution.



Fig. S5. Absorption and emission cross-section from PYBDP in toluene.

## 5. NMR and IR spectra copies of PYBDP



Fig. S6. The <sup>1</sup>H and <sup>13</sup>C NMR spectra of compound BYBDP in CDCl<sub>3</sub>.