2024「中技社科技獎學金」

2024 CTCI Foundation Science and Technology Scholarship

境外生研究獎學金

Research Scholarship for International Graduate Students

Dibenzofluoran-based NIR-IIa Pdots for Deep-tissue 3D Imaging

4th year Ph.D. Student

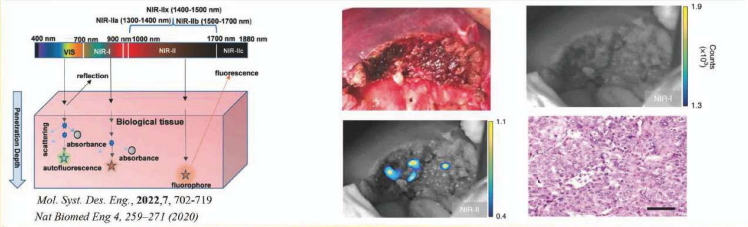
Partha Chowdhury,[a] and Yang-Hsiang Chan,[a*]

[a]Department of Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu, 30050, Taiwan, R.O.C.

Abstract

Emerging organic molecules with emissions in the second near-infrared (NIR-II) region are garnering significant attention. Unfortunately, achieving accountable organic emission intensity over the NIR-IIa (1300 nm) region faces challenges due to the intrinsic energy gap law. Up to the current stage, all reported organic NIR-IIa emitters belong to polymethine-based dyes with small Stokes shifts (<50 nm) and low quantum yield (QY; ≤0.015%). However, such polymethines have proved to cause self-absorption with constrained emission brightness, limiting advanced development in deep-tissue imaging. Here a new NIR-IIa scaffold based on rigid and highly conjugated dibenzofluoran core terminated by amino-containing moieties that reveal emission peaks of 1230–1305 nm is designed. The QY is at least 10 times higher than all synthesized or reported NIR-IIa polymethines with extraordinarily large Stokes shifts of 370–446 nm. DBF-BJ is further prepared as a polymer dot to demonstrate its in vivo 3D stereo imaging of mouse vasculature with a 1400 nm long-pass filter.

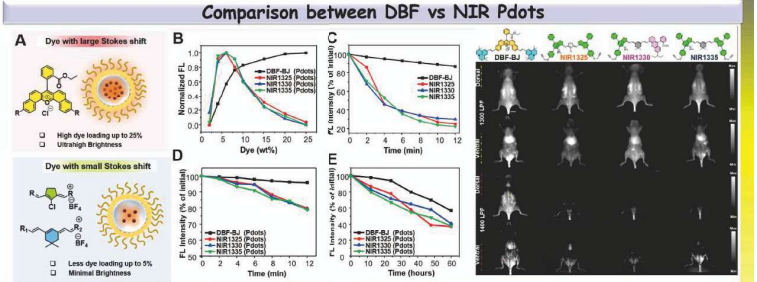
NIR-II Fluorescence-Guided Surgery



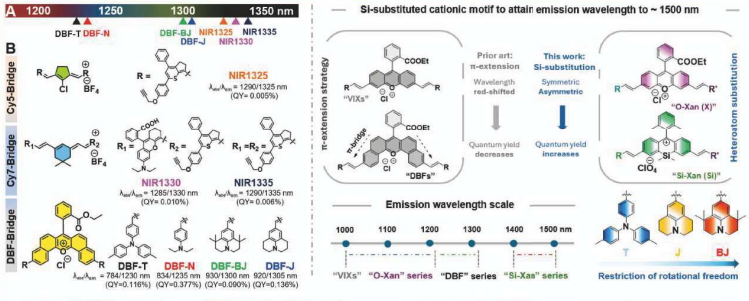
Mol. Syst. Des. Eng., **2022**,7, 702-719

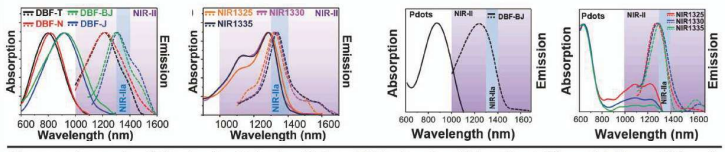
Nat Biomed Eng 4, 259–271 (2020)

Comparison between DBF vs NIR Pdots



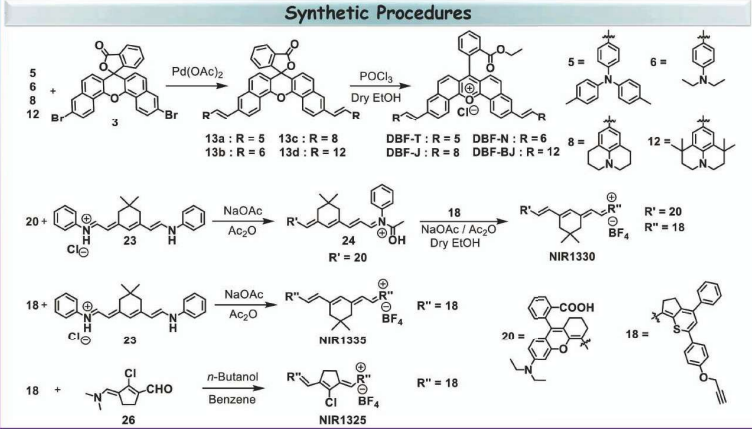
Molecular Design & Optical Properties of NIR-IIa Pdots



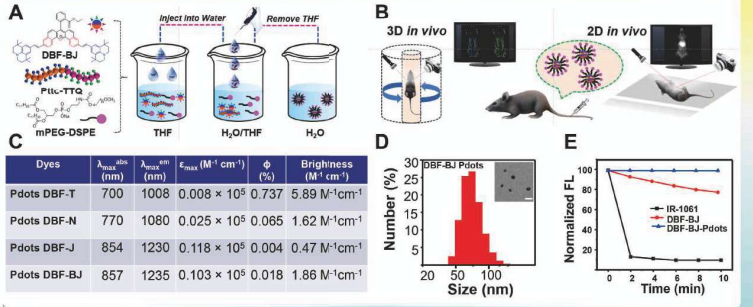


Monomer dyes	λ_{max}^{abs} (nm)	λ_{max}^{em} (nm)	Stokes shift (nm)	ε_{max} (M^{-1} cm^{-1})	Φ (%)	Brightness (M^{-1} cm^{-1})
DBF-T	784	1230	446	1.17×10^5	0.116	135.72
DBF-N	834	1235	401	1.73×10^5	0.377	652.58
DBF-J	920	1305	385	3.16×10^5	0.136	430.16
DBF-BJ	930	1300	370	2.86×10^5	0.090	257.67

Synthetic Procedures



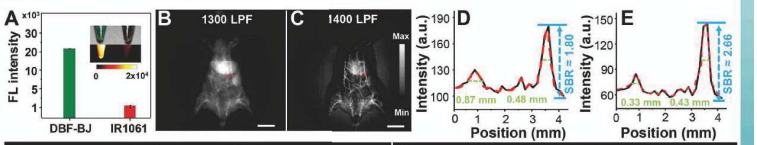
Preparation of NIR-IIa Pdots

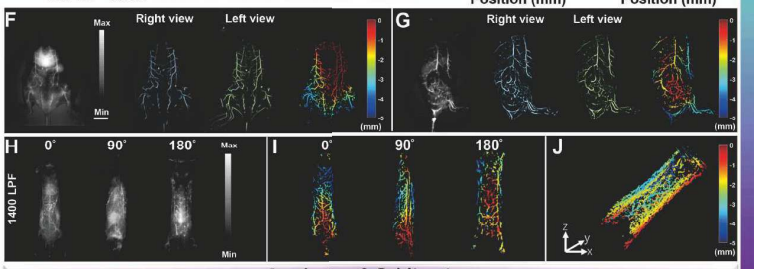


C

Dyes	λ_{max}^{abs} (nm)	λ_{max}^{em} (nm)	ε_{max} (M^{-1} cm^{-1})	Φ (%)	Brightness (M^{-1} cm^{-1})
Pdots DBF-T	700	1008	0.008×10^5	0.737	5.89 $M^{-1}cm^{-1}$
Pdots DBF-N	770	1080	0.025×10^5	0.065	1.62 $M^{-1}cm^{-1}$
Pdots DBF-J	854	1230	0.118×10^5	0.004	0.47 $M^{-1}cm^{-1}$
Pdots DBF-BJ	857	1235	0.103×10^5	0.018	1.86 $M^{-1}cm^{-1}$

3D *In Vivo* Mice Imaging





Conclusion & Publications

- We presented a novel design strategy for Organic fluorophore to attain NIR-IIa or NIR-IIb emission >1500 nm.
- We presented how an asymmetric framework offers the best trade-off between emission wavelength and quantum yield.
- Pdots were applied in high-contrast NIR-IIa vascular imaging, along with a 3D blood vessel enhancement for acquiring high-resolution 3D tumor and blood vessel images.

[1] Chowdhury, P.; Lu, Z.-Y.; Su, S.-P.; Liu, M.-H; Lin, C.-Y.; Wang, M.-W; Luo, Y.-C; Lee, Y.-J.; Chiang, H. K.; and Chan, Y.-H. "Ultrabright Dibenzofluoran-Based Polymer Dots with NIR-IIa Emission Maxima and Unusual Large Stokes Shifts for 3D Rotational Stereo Imaging". *Adv. Healthcare Mater.* 2024, 2400606.