Supplementary data for

Molecular engineering of a high quantum yield NIR-II molecular fluorophore with aggregation-induced emission (AIE) characteristics for in vivo imaging

Pengfei Xu[#a,b], Fei Kang[#a], Weidong Yang[#a], Mingru Zhang a,Ruili Dang[b], Pei Jiang[b]* and Jing Wang[a]*

[a]Department of Nuclear Medicine, Xijing Hospital, Fourth Military Medical University. 710032. #127 West Changle Road, Xi'an, Shaanxi, China;

[b]Institute of Clinical Pharmacy & Pharmacology, Jining First People's Hospital, Jining Medical University, Jining 272000, P.R. China.

* Author of correspondence:

Dr. Pei Jiang, Institute of Clinical Pharmacy & Pharmacology, Jining First People's Hospital, Jining Medical University, Jining 272000, P.R. China. Email: jiangpeicsu@sina.com.

Prof. Jing Wang, Department of Nuclear Medicine, Xijing Hospital, Fourth Military Medical University. 710032. #127 West Changle Road, Xi'an, Shaanxi, China. Email: wangjing@fmmu.edu.cn

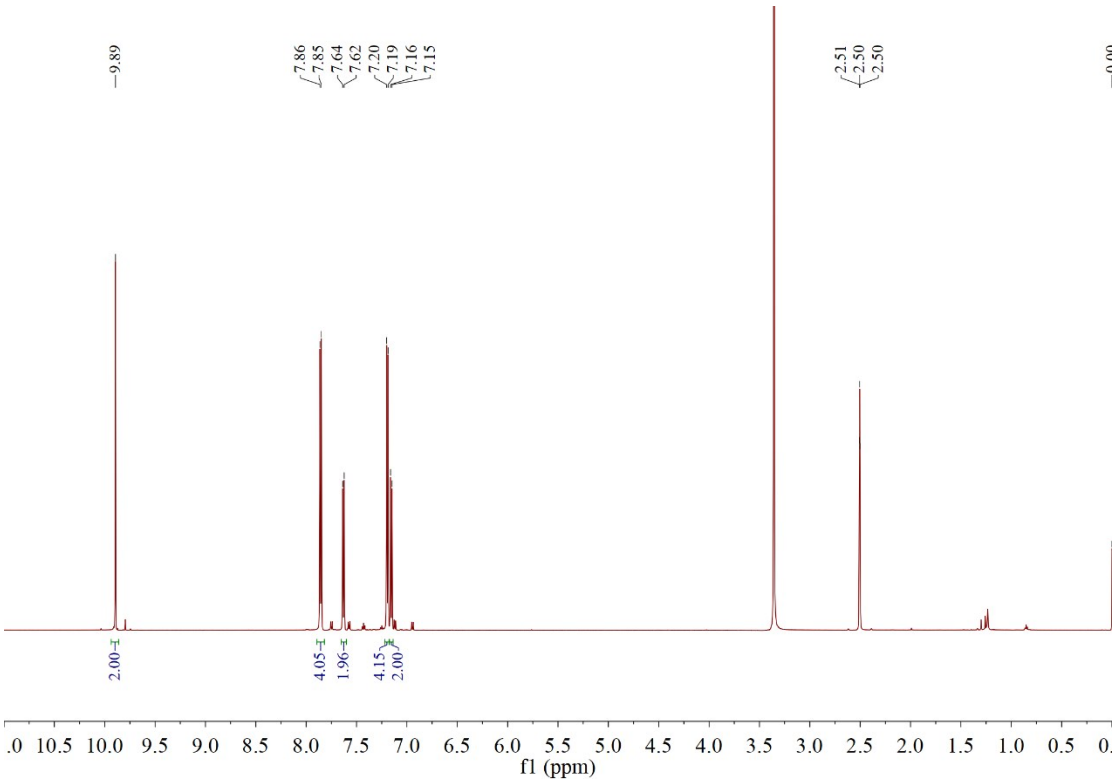

Figure S1. ^{1}H NMR spectrum of 4,4'-((4-bromophenyl)azanediyl)dibenzaldehyde in $CDCl_3$.

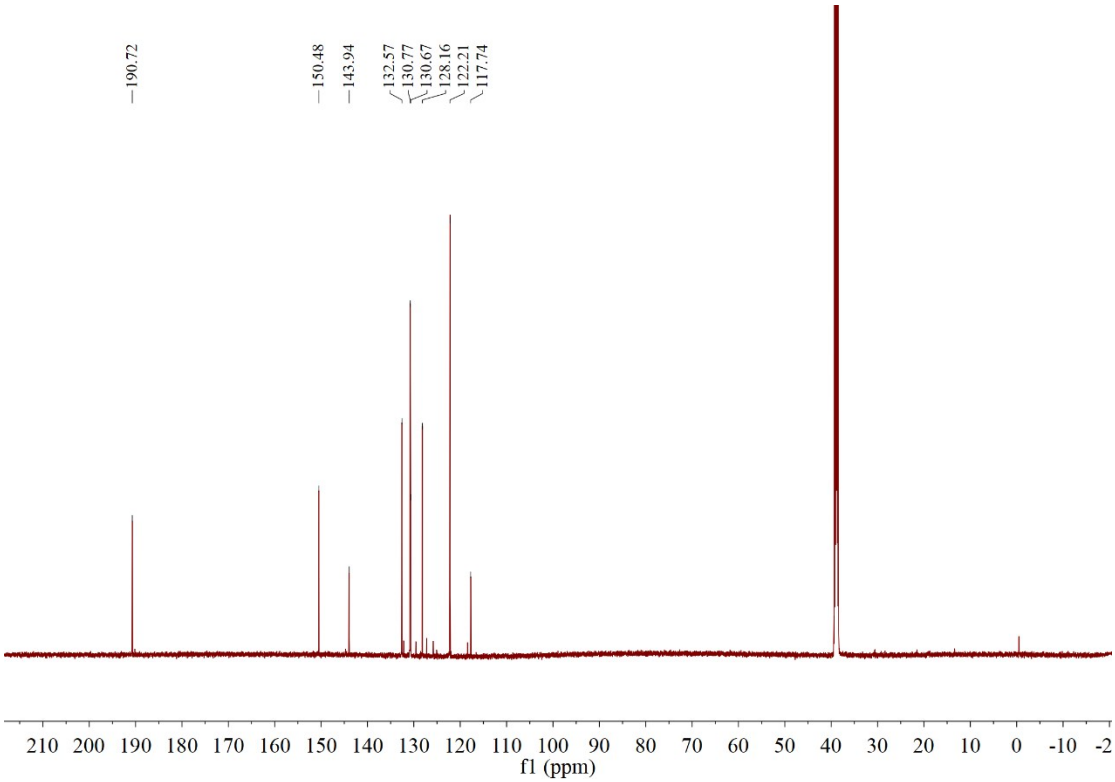

Figure S2. ^{13}C NMR spectrum of 4,4'-((4-bromophenyl)azanediyl)dibenzaldehyde in $CDCl_3$

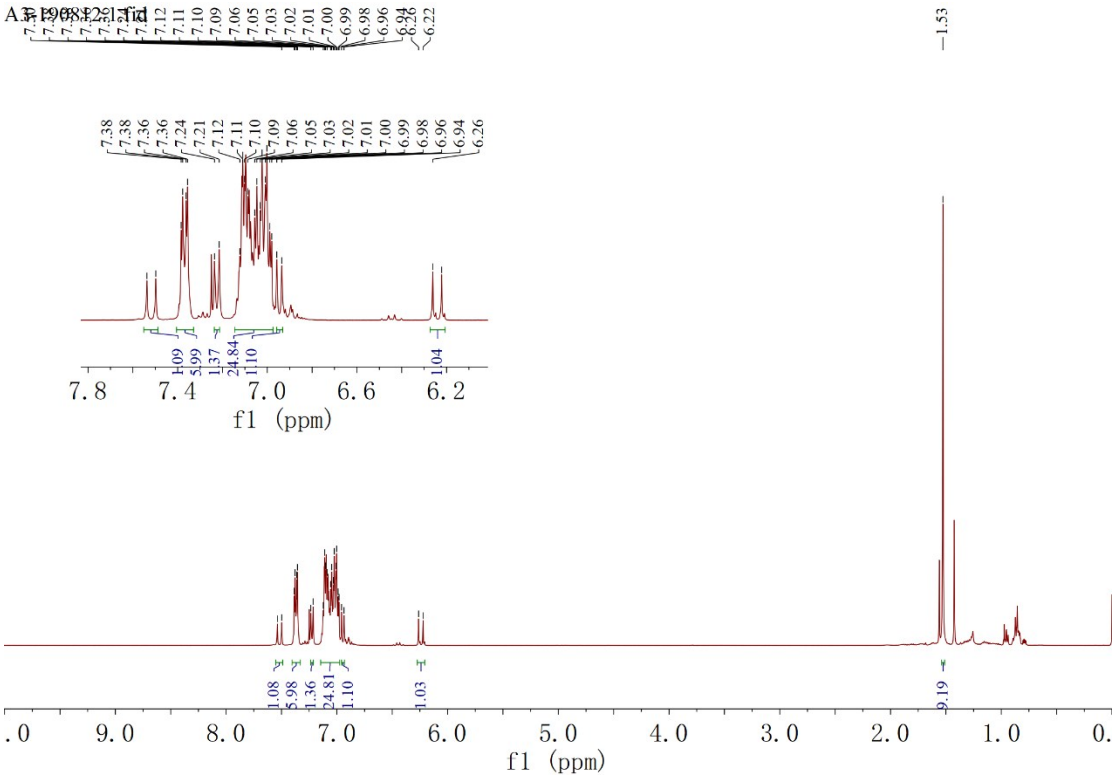

Figure S3. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

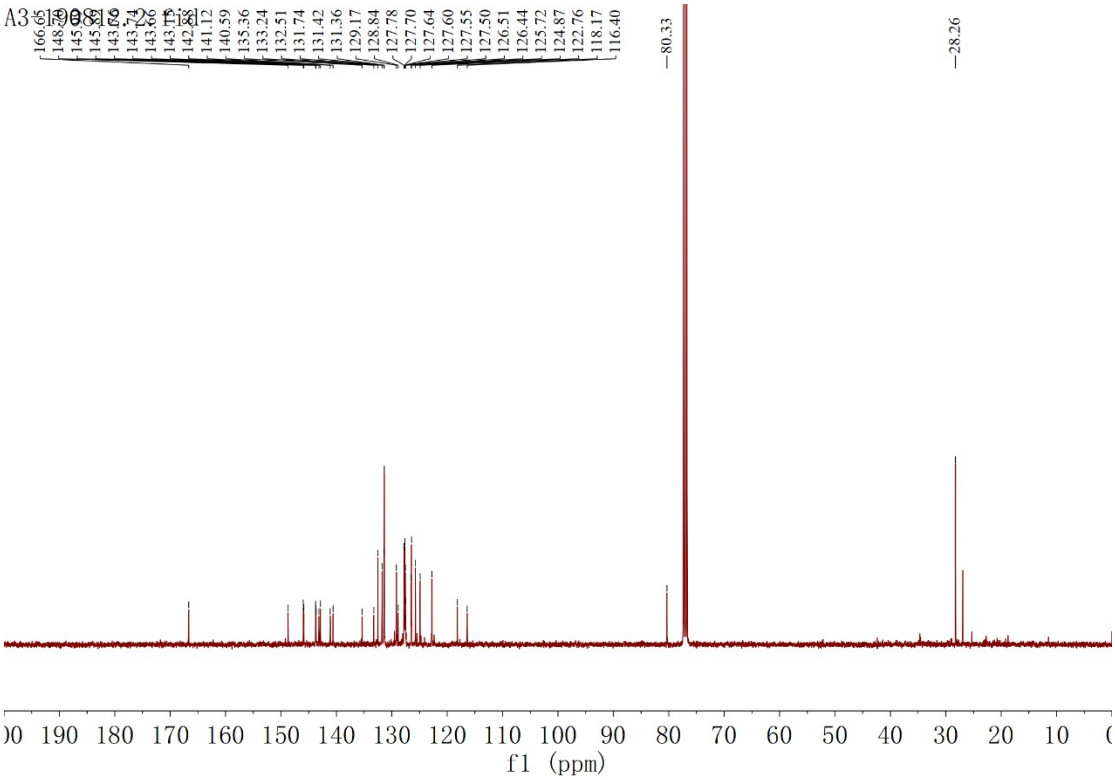

Figure S4. ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

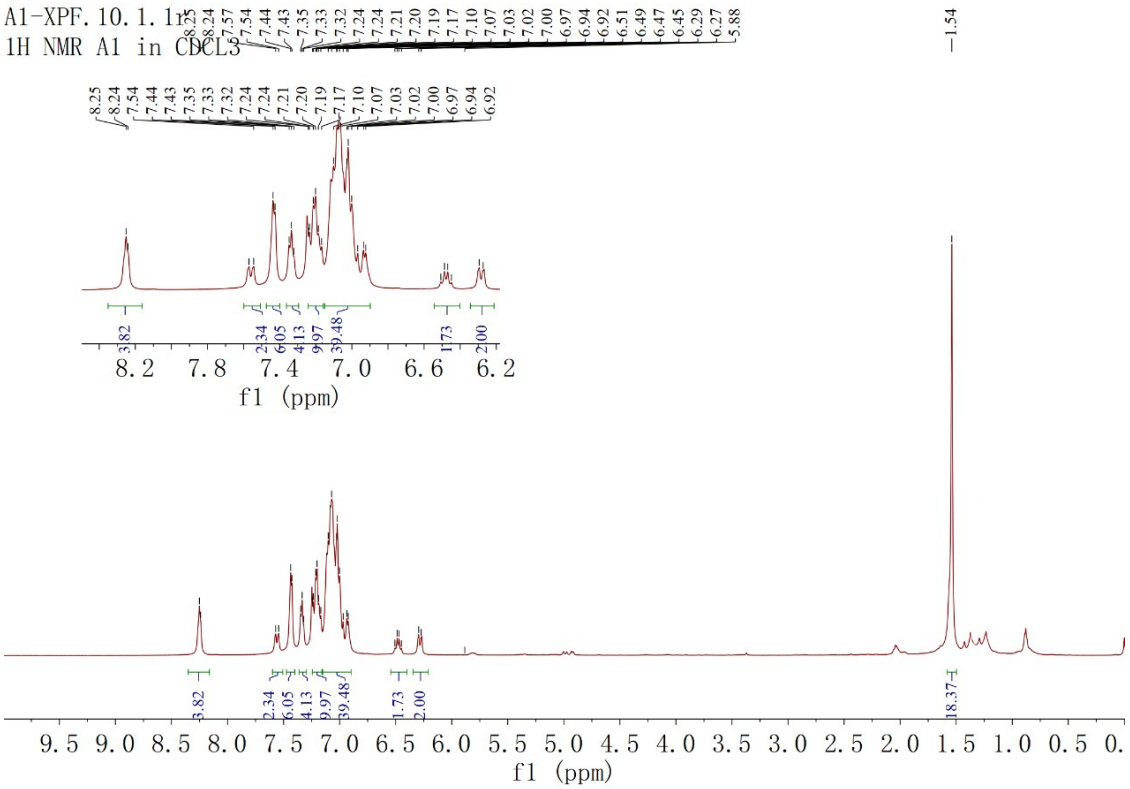

Figure S5. ^{1}H NMR spectrum of **XA1** in $CDCl_3$.

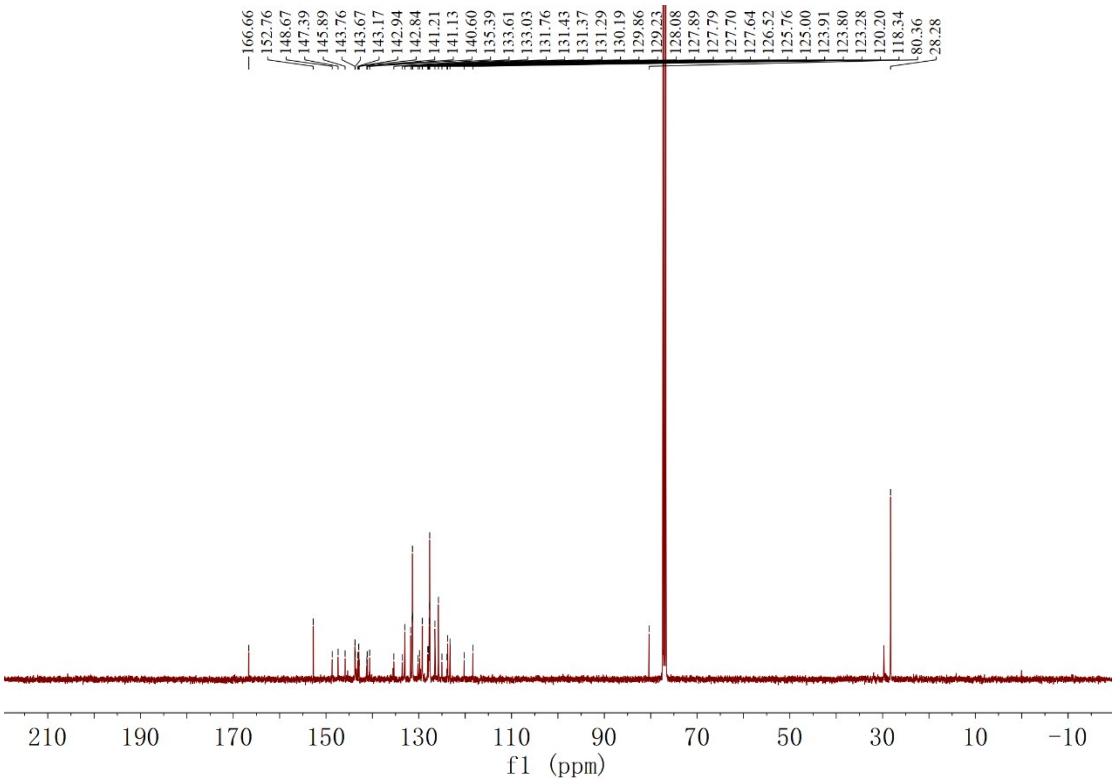

Figure S6. ^{13}C NMR spectrum of **XA1** in $CDCl_3$.

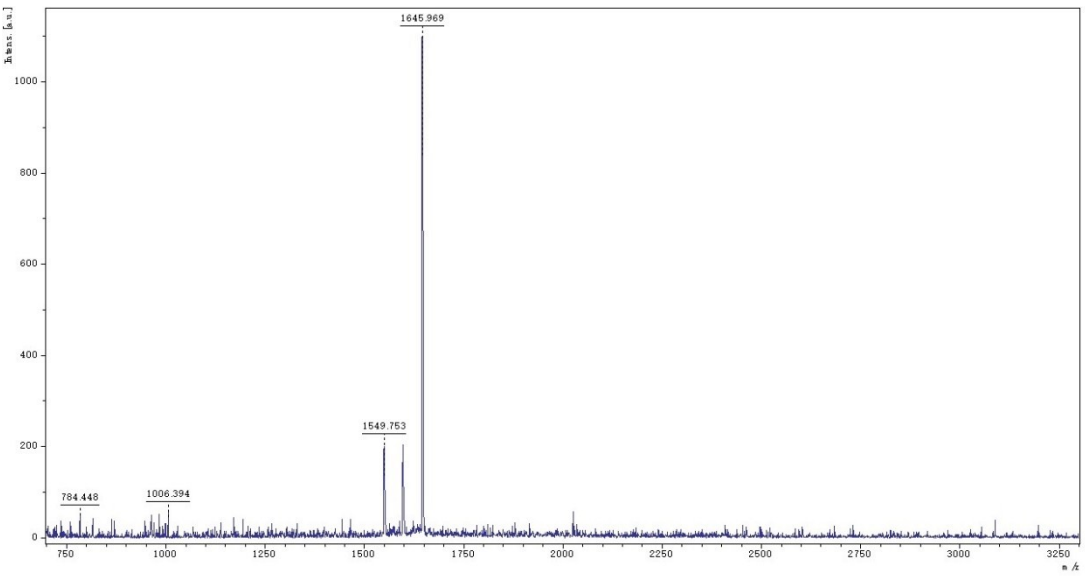

Figure S7. MALDI-TOF-MS measurement of **XA1**.

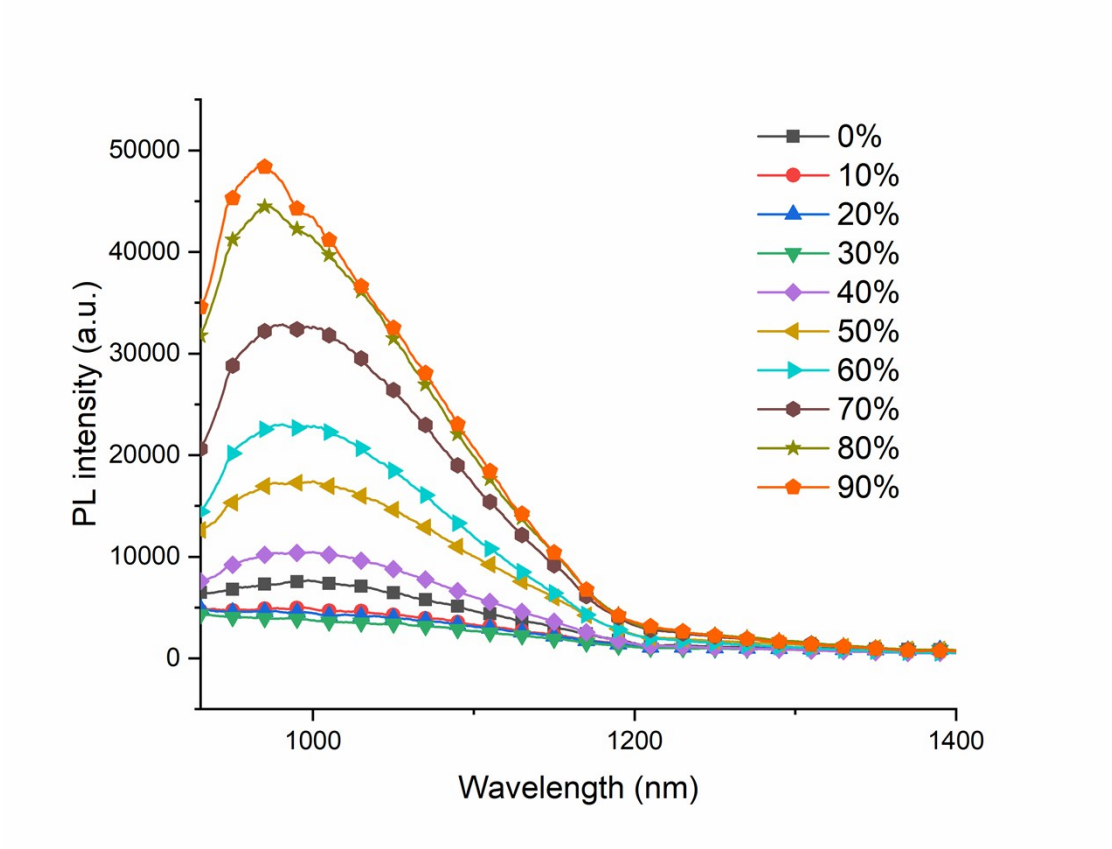

Figure S8. The emission spectra of **XA1** with different f_w.

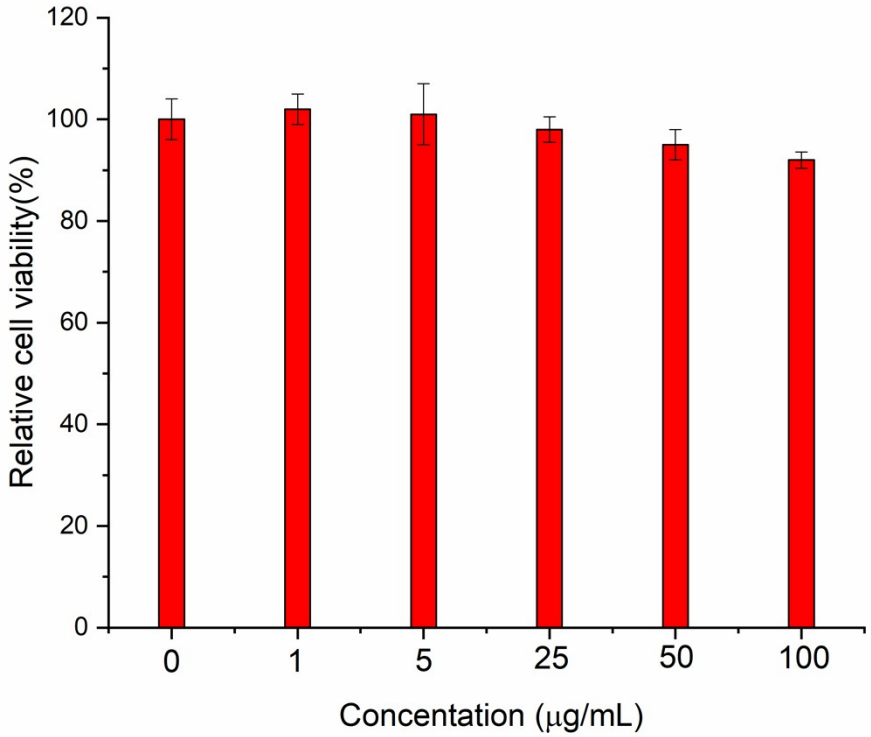

Figure S9. Cell viability of Hela cells after incubation with aqueous dispersion of **XA1** NPs with various concentrations for 48 h.

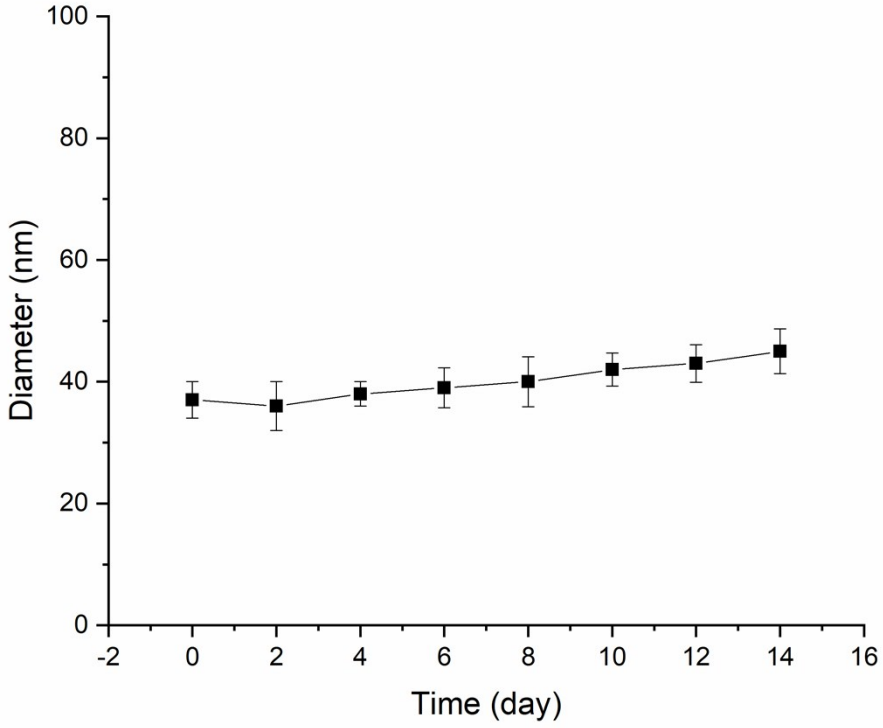

Figure S10. DLS results of **XA1** NPs in water over 14 days.

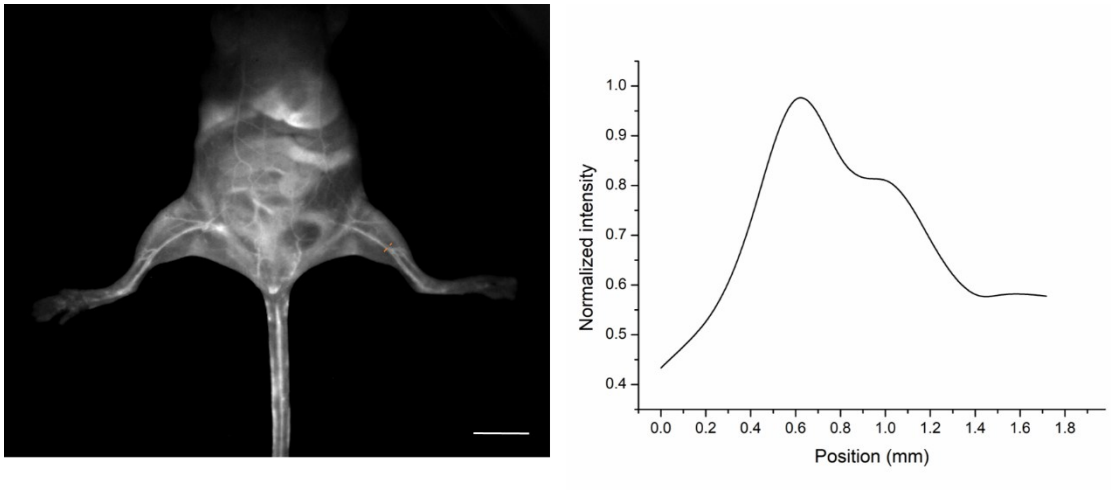

Figure S11. The line profile of the fluorescence intensity. Scale bar: 1 cm.

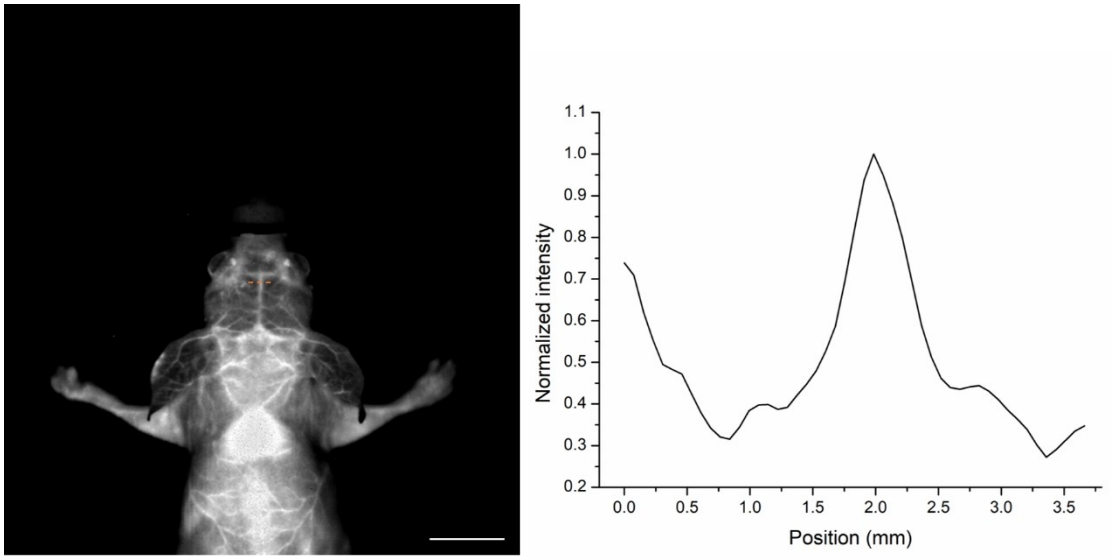

Figure S12. The line profile of the fluorescence intensity. Scale bar: 1 cm.

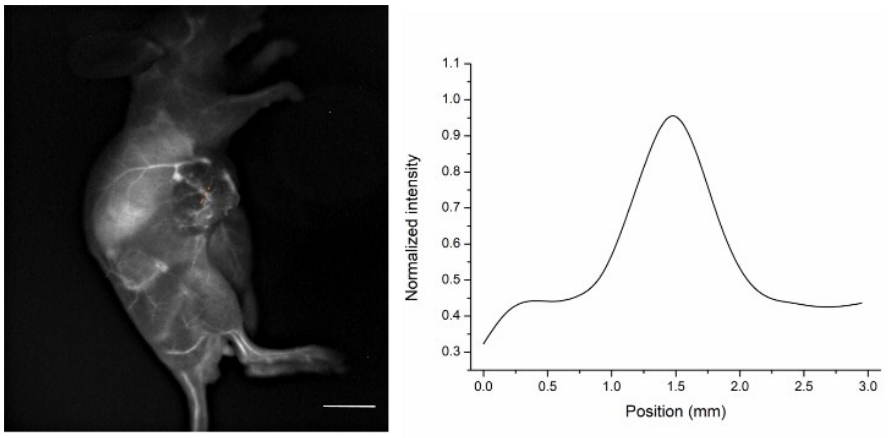

Figure S13. The line profile of the fluorescence intensity in the NIR II image of CT-

26 tumor-bearing nude mice (tumor size ≈0.75 cm^3). The image was captured at 1 min time points after a tail vein injection of **XA1** NPS. S/B=2.7± 0.2.

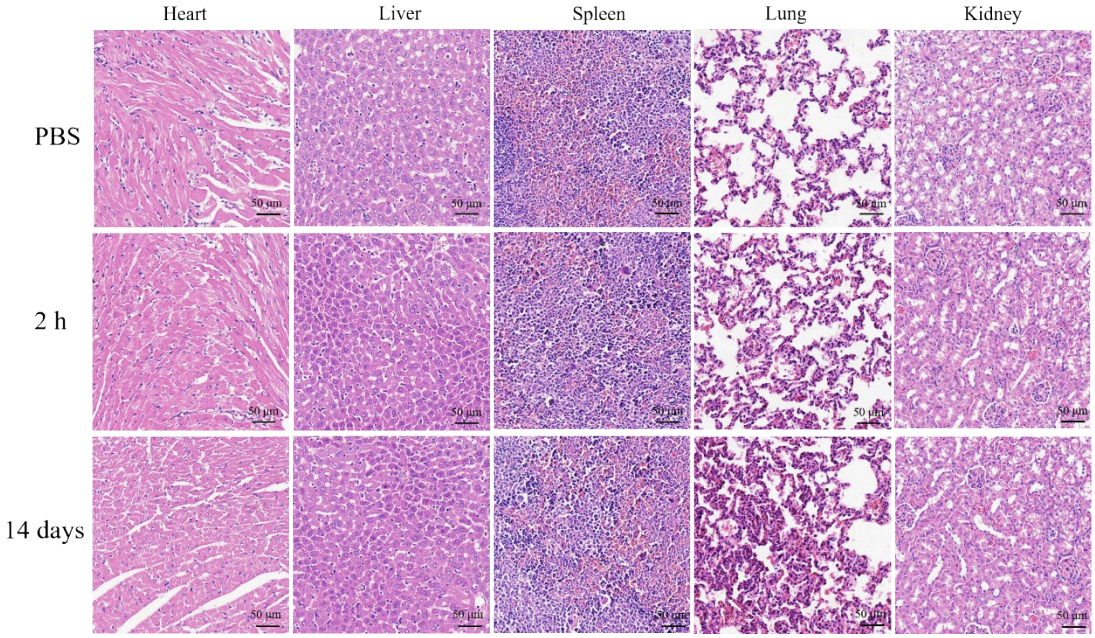

Figure S14. Histological H&E staining for main organs (heart, liver, spleen, lung and kidney) of the mice intravenously administrated with PBS and **XA1** NPs(10 times than the imaging doses, 5 mg of XA1 per kg mouse) for 2 h and 14 days.

The QY of XA1 was calculated according the previous reported calculation method.[1-3]

$$QY_{sample} = QY_{ref} \frac{slope_{sample}}{slope_{ref}} \left(\frac{n_{sample}}{n_{ref}} \right)^2$$

The QYs were measured by the linear-regression plot of integrated fluorescent intensities at different concentrations on a molar basis. Where QY_{ref} of IR-26 in dichloroethane is 0.5%, and n_{sample} and n_{ref} are the refractive index of water and dichloroethane, respectively.

$$QY=0.5\% \times \frac{29179925.14}{835364.08} \times \left(\frac{1.33}{1.4448} \right)^2 = 14.8\%$$

1. K. Cheng, H. Chen, C. H. Jenkins, G. Zhang, W. Zhao, Z. Zhang, F. Han, J. Fung, M. Yang, Y. Jiang, L. Xing and Z. Cheng, *ACS Nano*, 2017, **11**, 12276-12291.

2. Z. Sheng, B. Guo, D. Hu, S. Xu, W. Wu, W. H. Liew, K. Yao, J. Jiang, C. Liu, H. Zheng and B. Liu, *Adv Mater*,

2018, **29**, 1800766-1800774.

3. H. Wan, J. Yue, S. Zhu, T. Uno, X. Zhang, Q. Yang, K. Yu, G. Hong, J. Wang, L. Li, Z. Ma, H. Gao, Y. Zhong, J. Su, A. L. Antaris, Y. Xia, J. Luo, Y. Liang and H. Dai, *Nat Commun*, 2018, **9**, 1171.