Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supporting Information for:

Anti-Aggregation NIR-II Heptamethine-Cyanine Dye with Stereo Structure for Imaging-Guided Photothermal Therapy

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Contents

1. Experimental Procedures[1, 2]

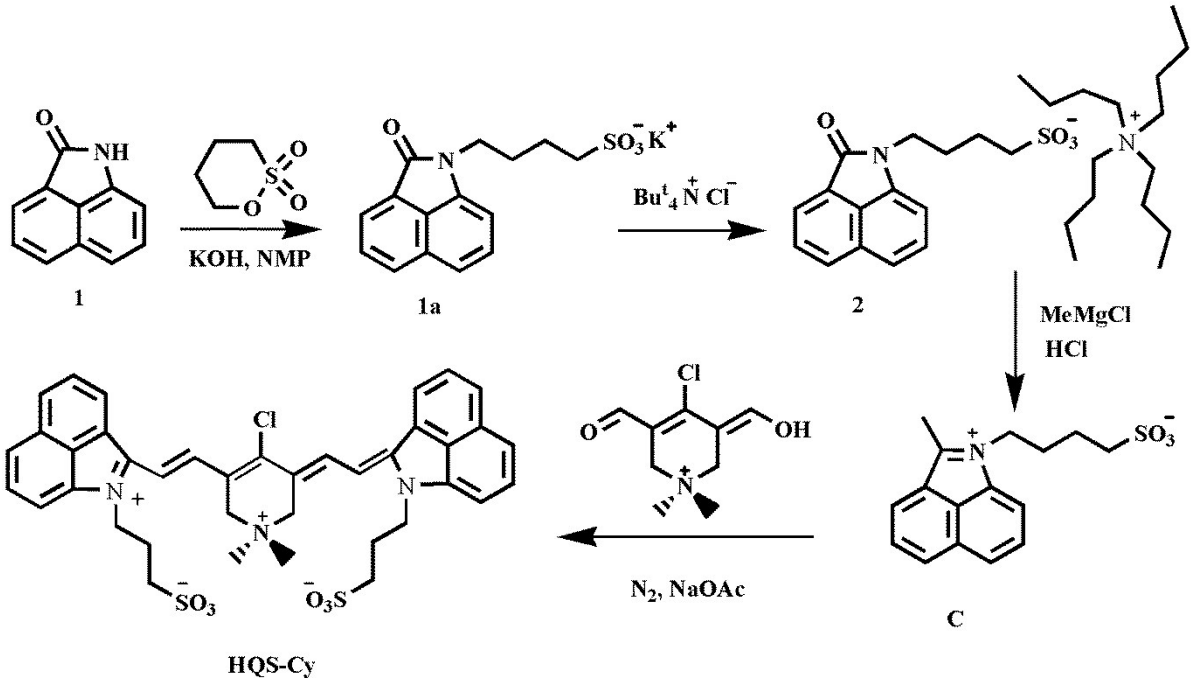

Fig. S1. Synthesis route of hydrophilic quaternary stereo-cyanine (HQS-Cy).

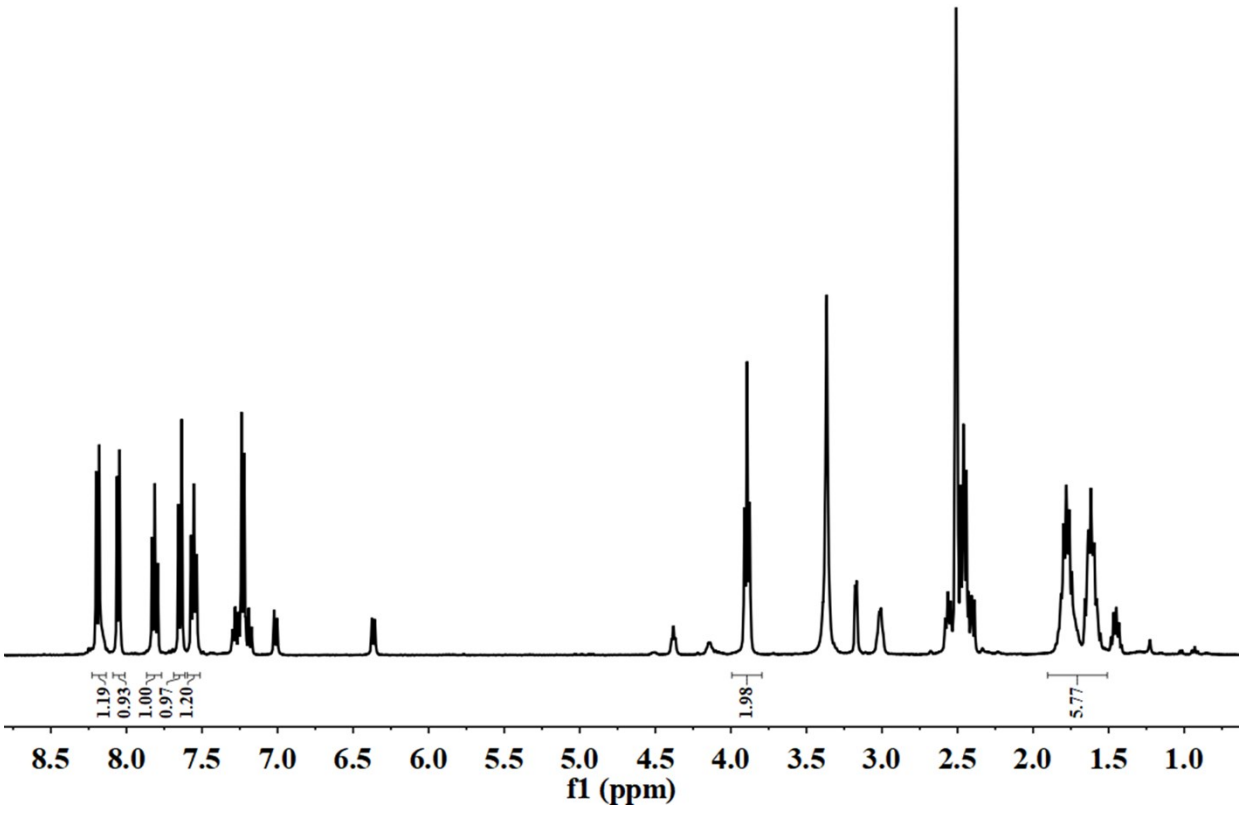

Fig. S2. 1H NMR spectra of HQS-Cy 1a.

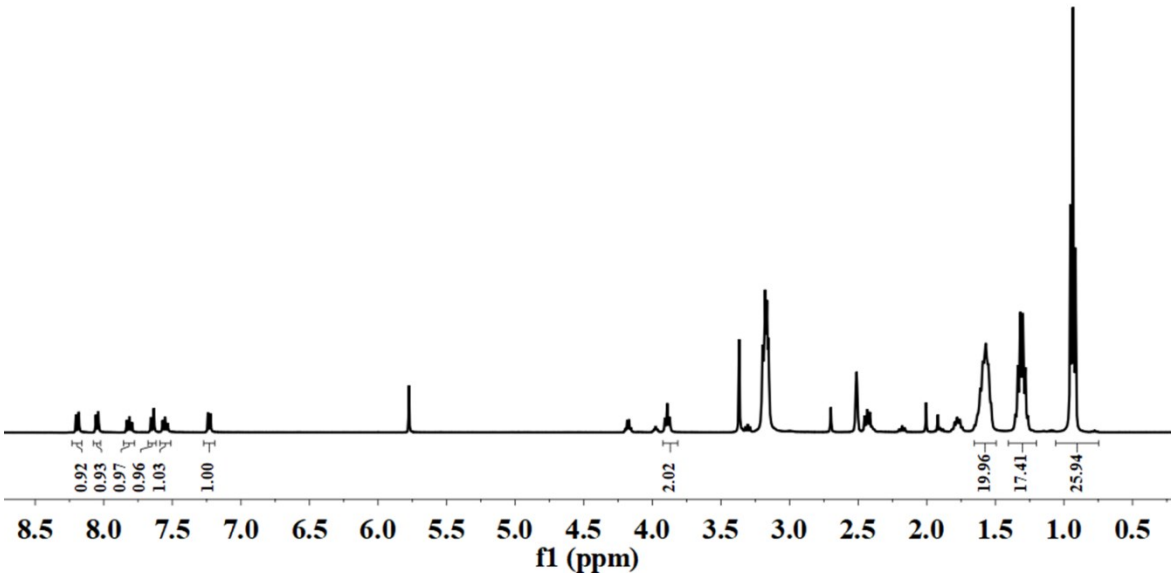

Fig. S3. 1H NMR spectra of HQS-Cy 2

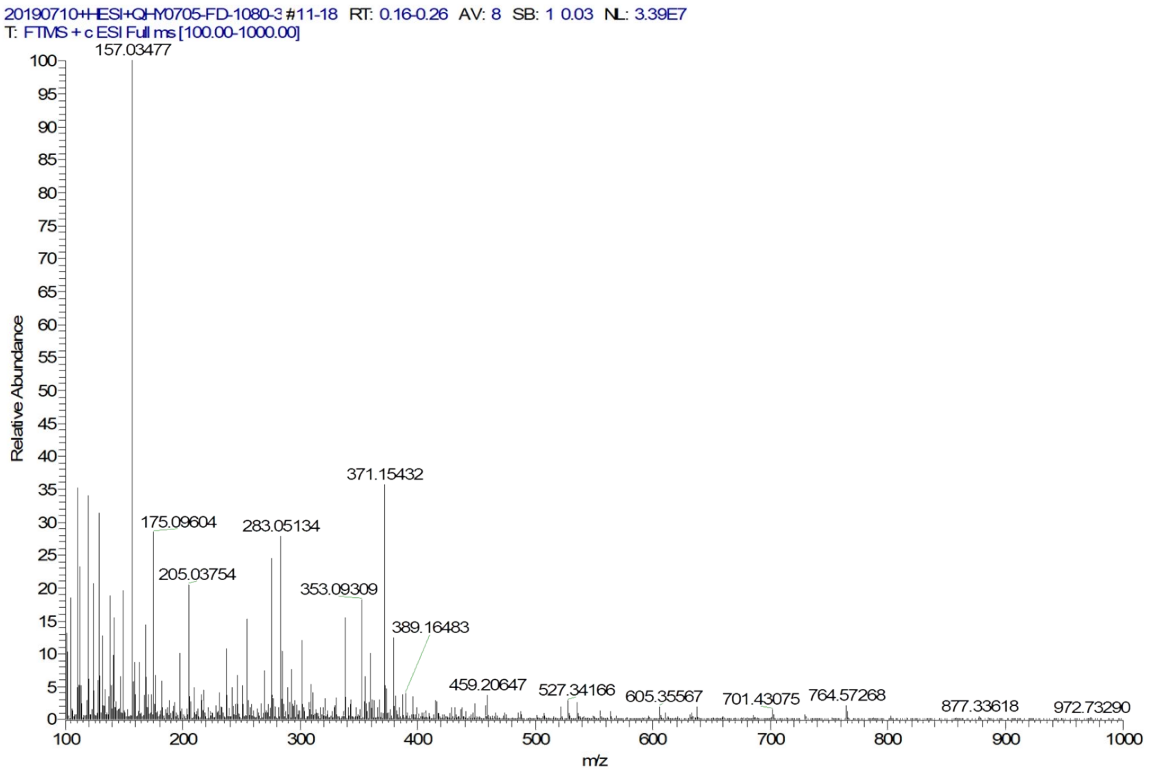

Fig. S4. ESI-MS of HQS-Cy 3

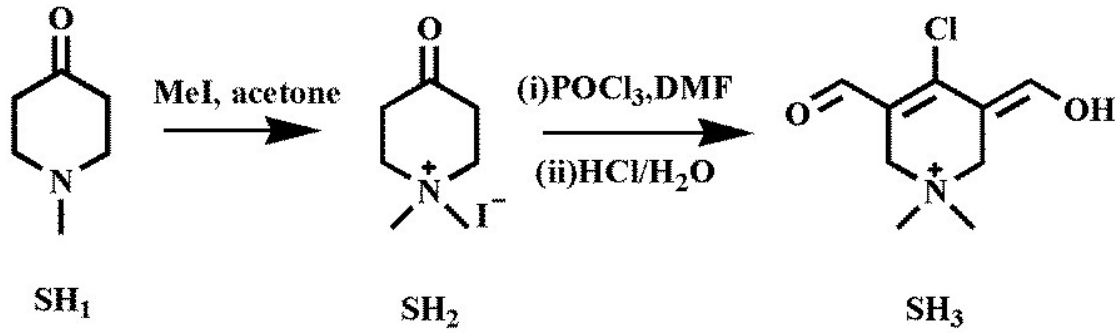

Fig. S5. Synthesis route of SH_3.

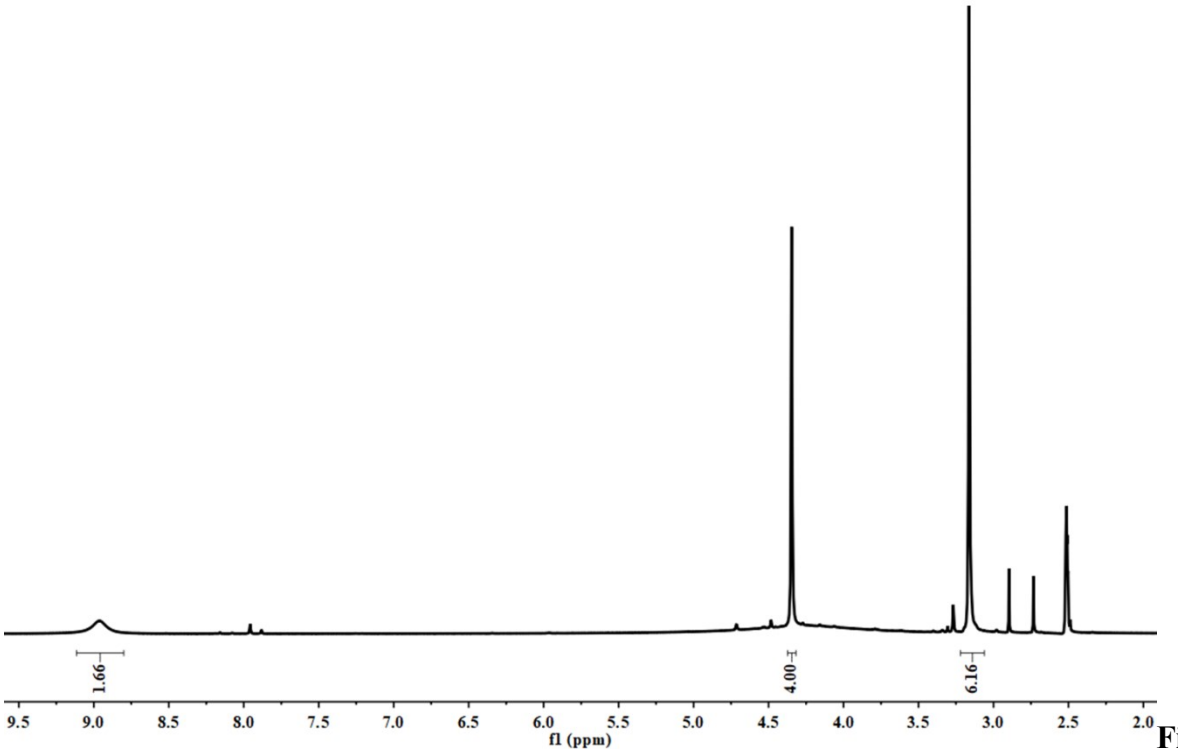

Fig. S6. 1H NMR spectra of SH_2.

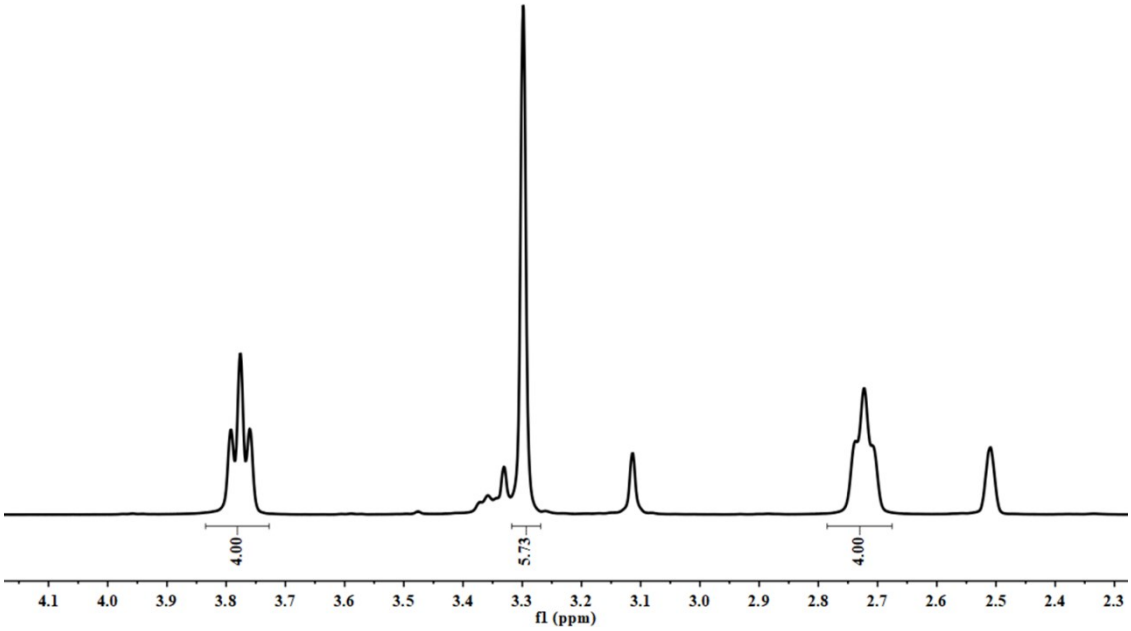

Fig. S7. 1H NMR spectra of SH_3.

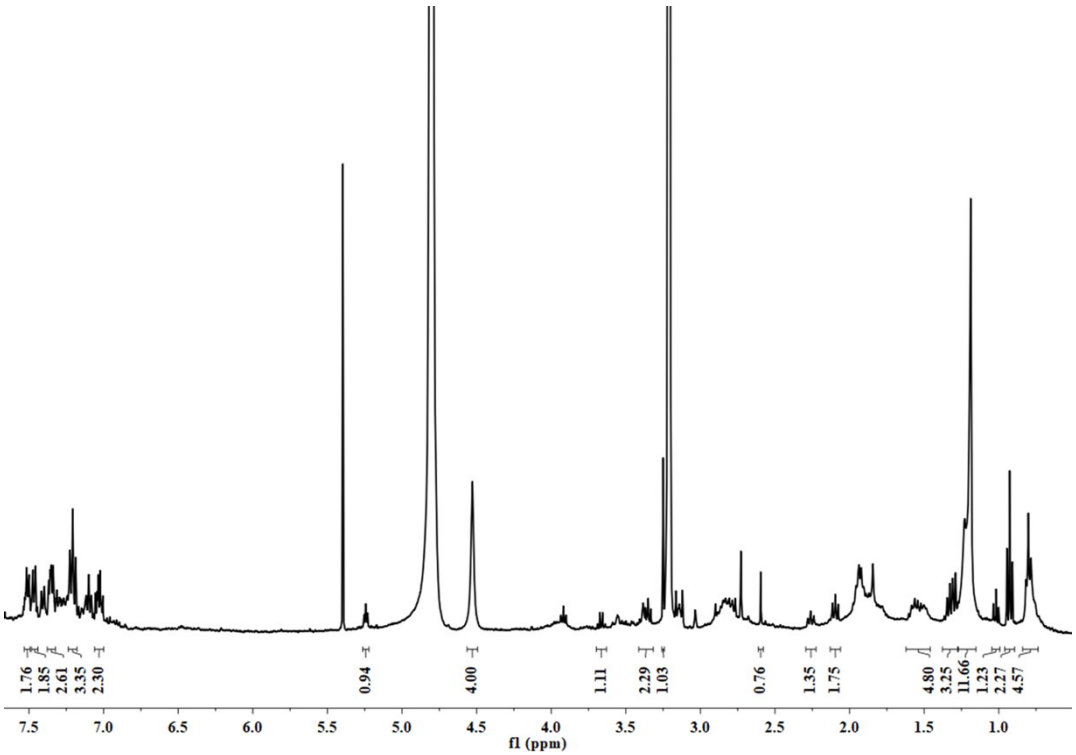

Fig. S8. 1H NMR spectra of HQS-Cy.

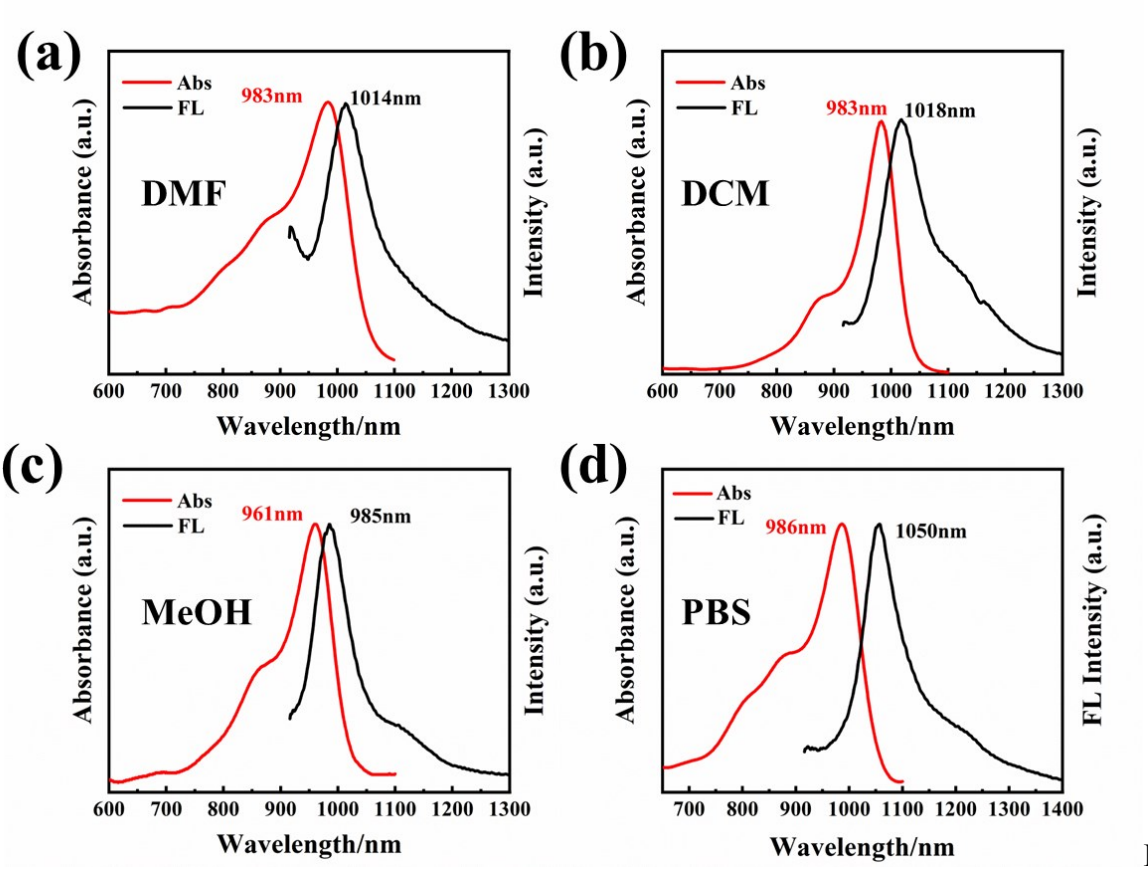

Fig. S9 (a) UV-vis-NIR absorbance spectra of HQS-Cy in DMF and (b) in DCM and (c) in MeOH and (d) HQS-Cy@P in PBS

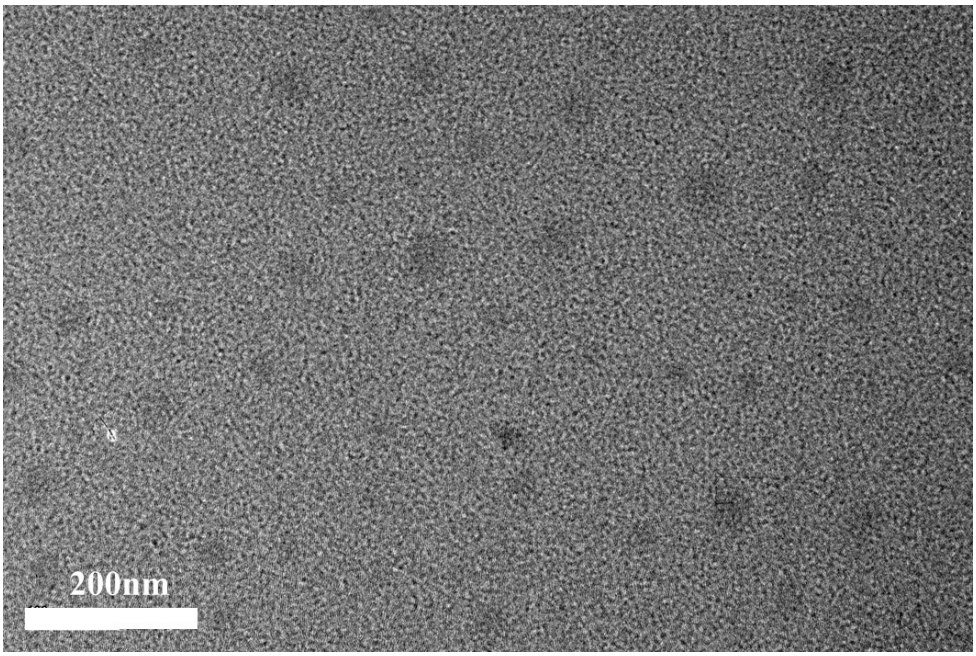

Fig. S10 TEM image of HQS-Cy@P

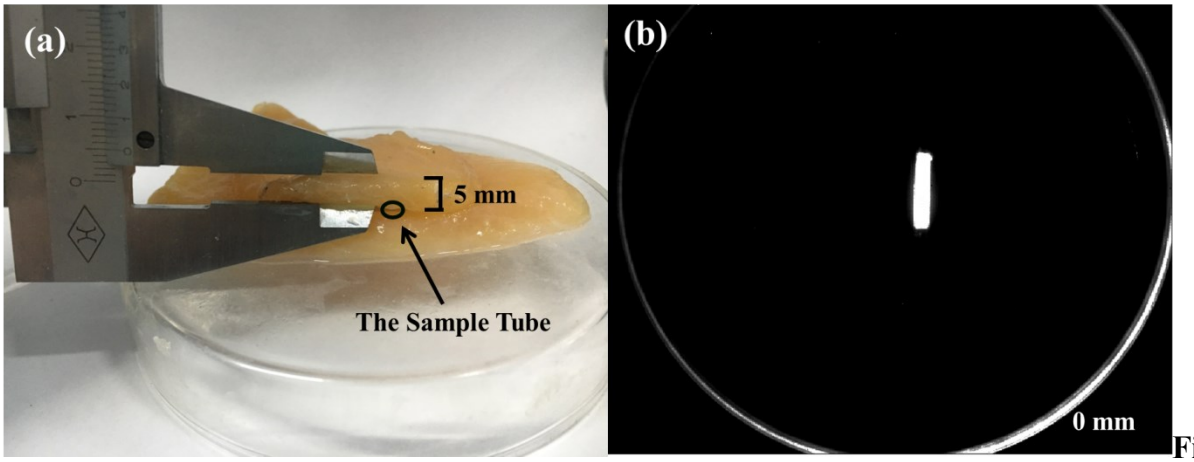

Fig. S11 Chicken penetration model assay. (a) A model for the nuggets: the sample tube was covered 5 mm thickness of chicken. (b) The fluorescence image of tube with 0 mm thickness of chicken.

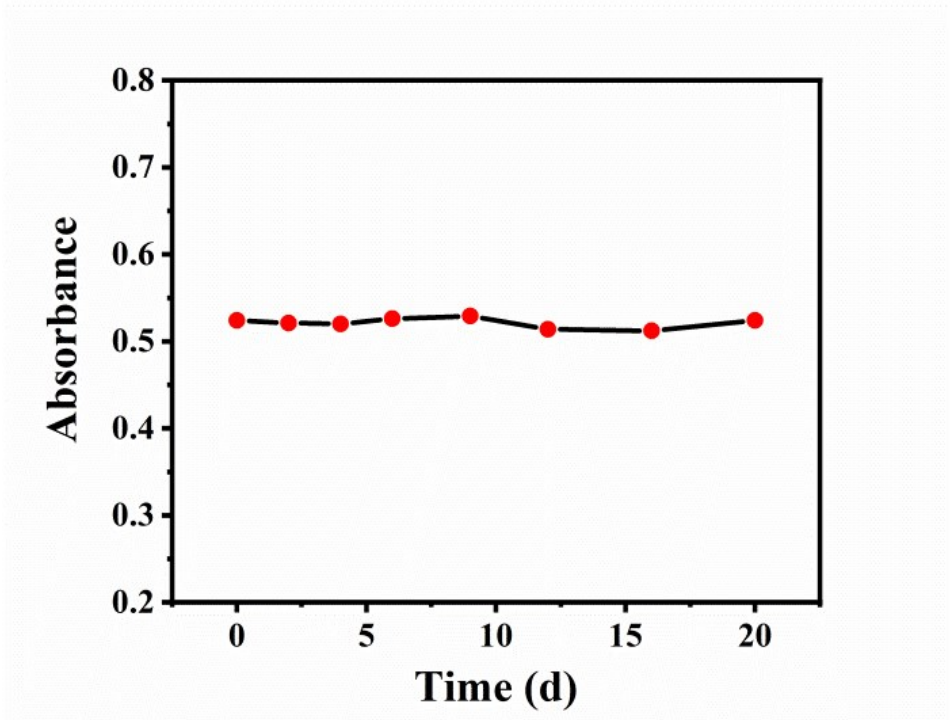

Fig. S12 The stability of HQS-Cy@P in PBS which are stored at room temperature and out of direct sunlight

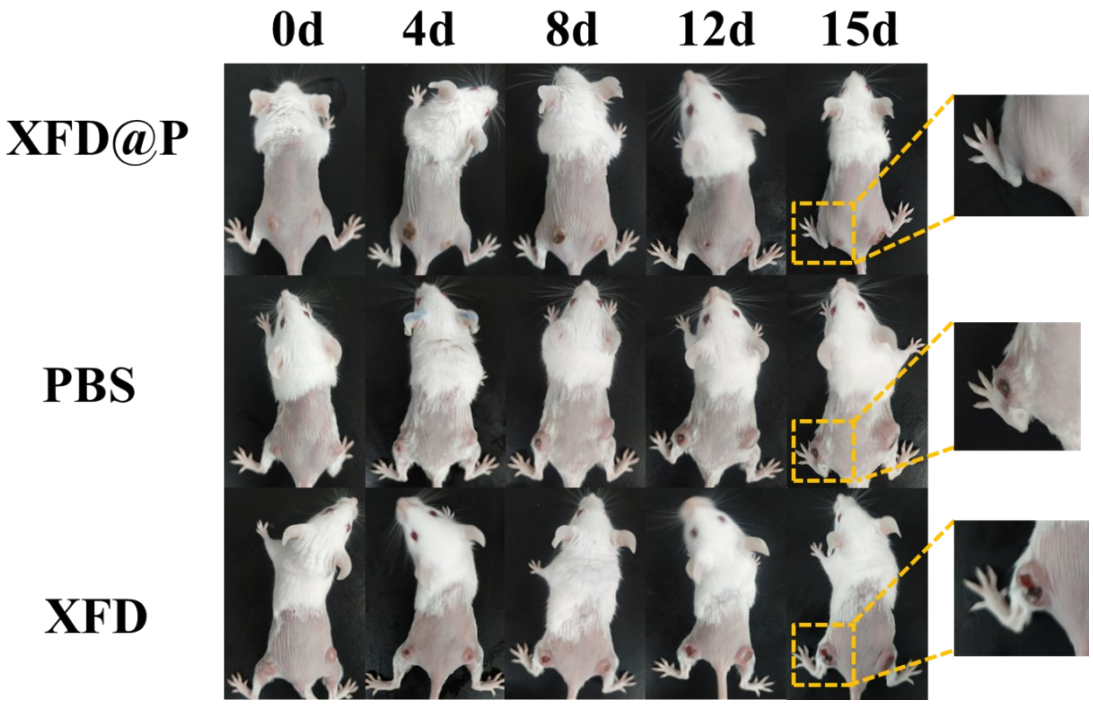

Fig. S13 Representative digital photographs of the mice during the treatment in the group of "PBS", "HQS-Cy" and "HQS-Cy@P"

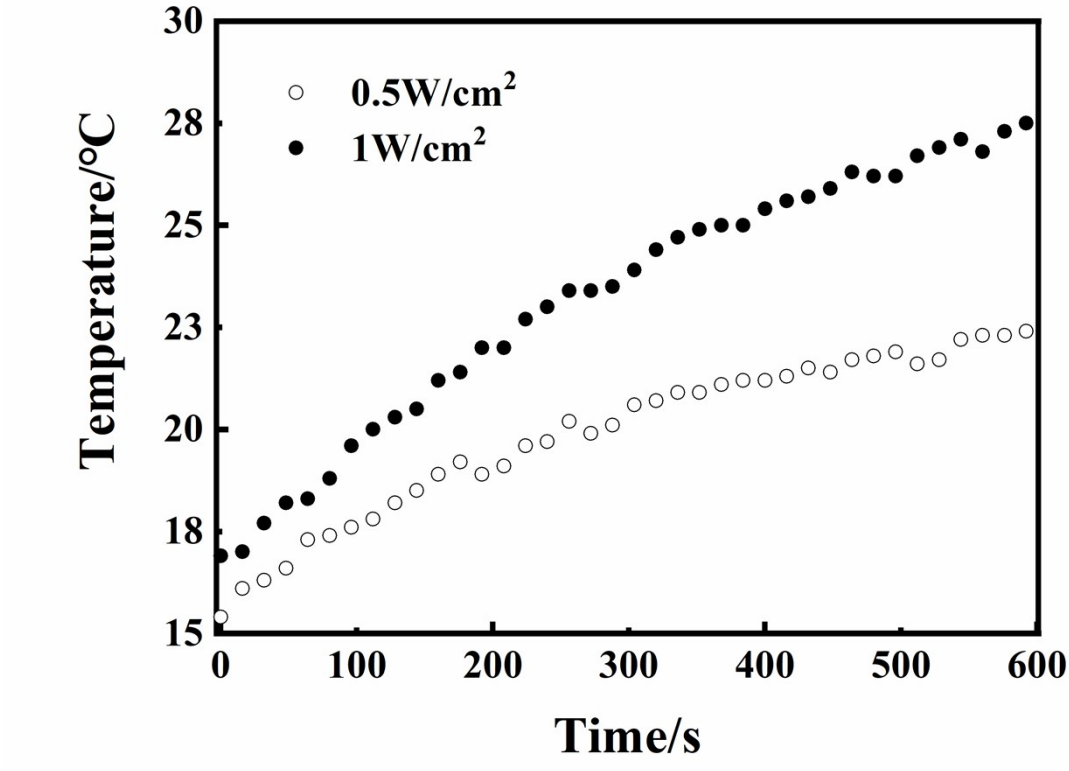

Fig. S14 The heating curve of water under the 980nm laser irradiation

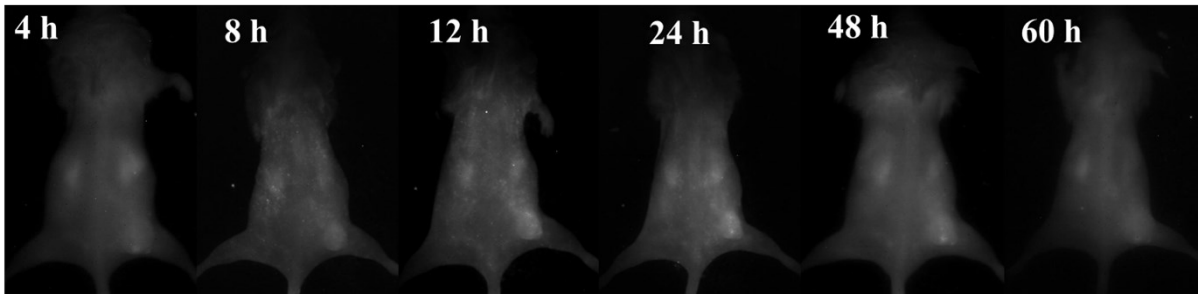

Figure S15. NIR-II fluorescence imaging of HQS-Cy@P in vivo at the selected time.

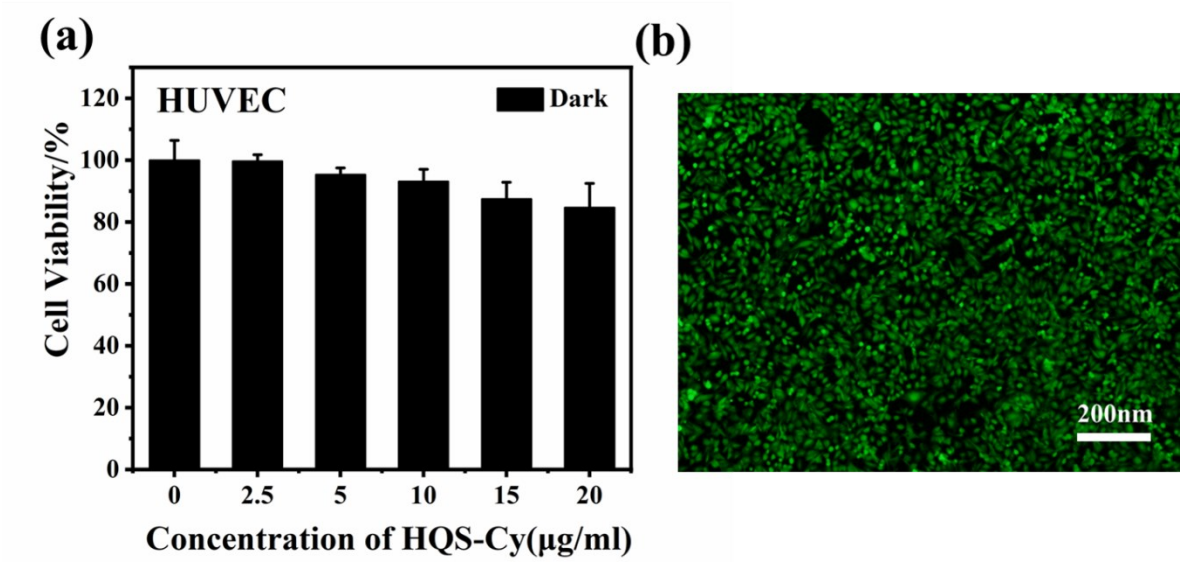

Figure S16. (a) Cytotoxicity assays of HQS-Cy@P against human umbilical vein endothelial cells (HEVUC) under dark conditions and (b) Fluorescence imaging of HUVEC cells treated with 20μg/mL HQS-Cy@P for live/dead assays.

3. References

[1] B. Li, L. Lu, M. Zhao, Z. Lei, F. Zhang, An Efficient 1064 nm NIR-II Excitation Fluorescent Molecular Dye for Deep-Tissue High-Resolution Dynamic Bioimaging, Angew Chem Int Ed Engl 57(25) (2018) 7483-7487.

[2] S. Thavornpradit, S.M. Usama, G.K. Park, J.P. Shrestha, S. Nomura, Y. Baek, H.S. Choi, K. Burgess, QuatCy: A Heptamethine Cyanine Modification With Improved Characteristics, Theranostics 9(10) (2019) 2856-2867.