

Supplementary Materials

High-Performance Hybrid Phototheranostics for NIR-IIb Fluorescence Imaging and NIR-II-Excitable Photothermal Therapy

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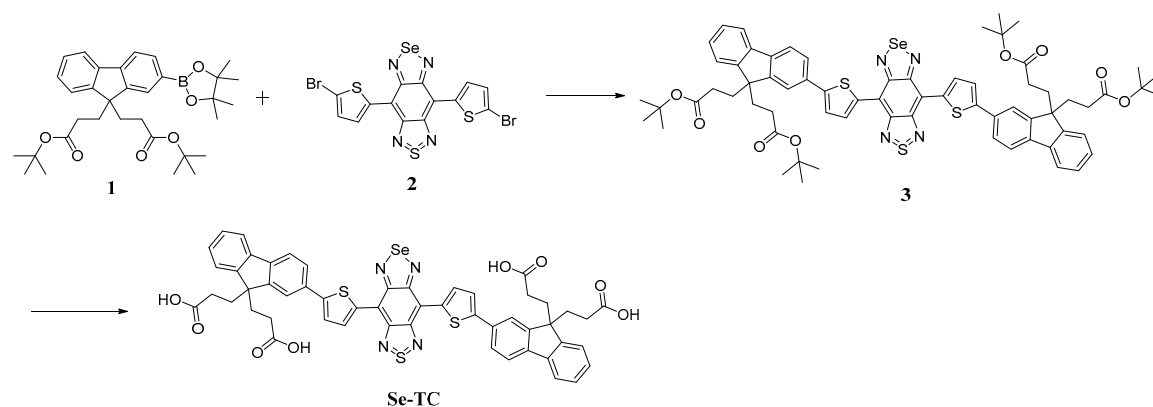
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1. Synthesis of Se-TC



Scheme S1. Synthesis of Se-TC.

Synthesis of compound 3

Compound 1^[S1] (154 mg, 0.281 mmol), compound 2^[S2] (72 mg, 0.128 mmol), Pd(PPh₃)₄ (99 mg), K₂CO₃ (100 mg) were added in toluene (15 mL)/water (3 mL). The solution was stirred for 24 h at 95°C under nitrogen, and the solvent was evaporated. Compound 3 could be obtained via column chromatography (84 mg, 52.6%). ¹H NMR (400 MHz, CDCl₃, δ): 9.11 (d, 2H), 7.85 (d, 2H), 7.80 (s, 2H), 7.74 (t, 4H), 7.64 (d, 2H), 7.43-7.36 (m, 6H), 2.47-2.42 (m, 8H), 1.43-1.33 (m, 8H), 1.31 (s, 36H). MALDI-TOF MS (m/z): [M]⁺ calcd. for C₆₈H₇₀N₄O₈S₃Se, 1246.352; found, 1246.667.

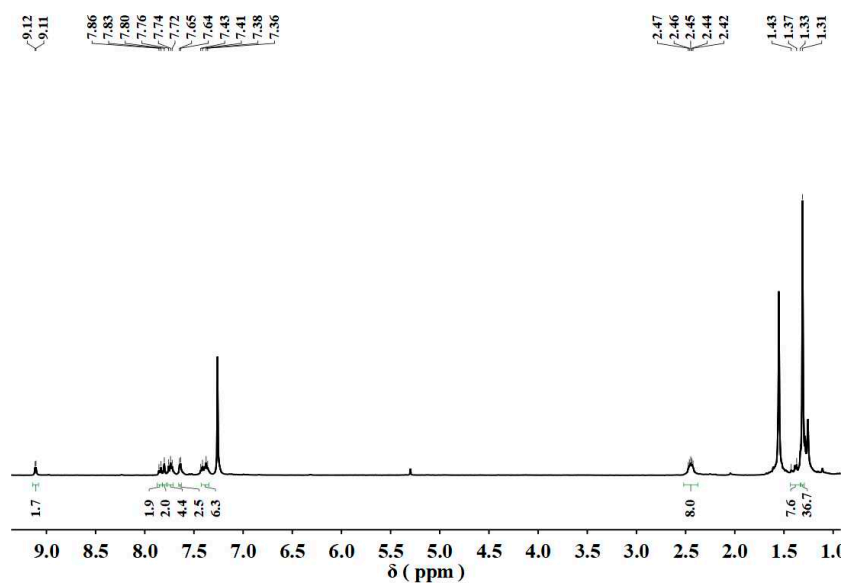


Figure S1. ¹H NMR spectrum of compound 3.

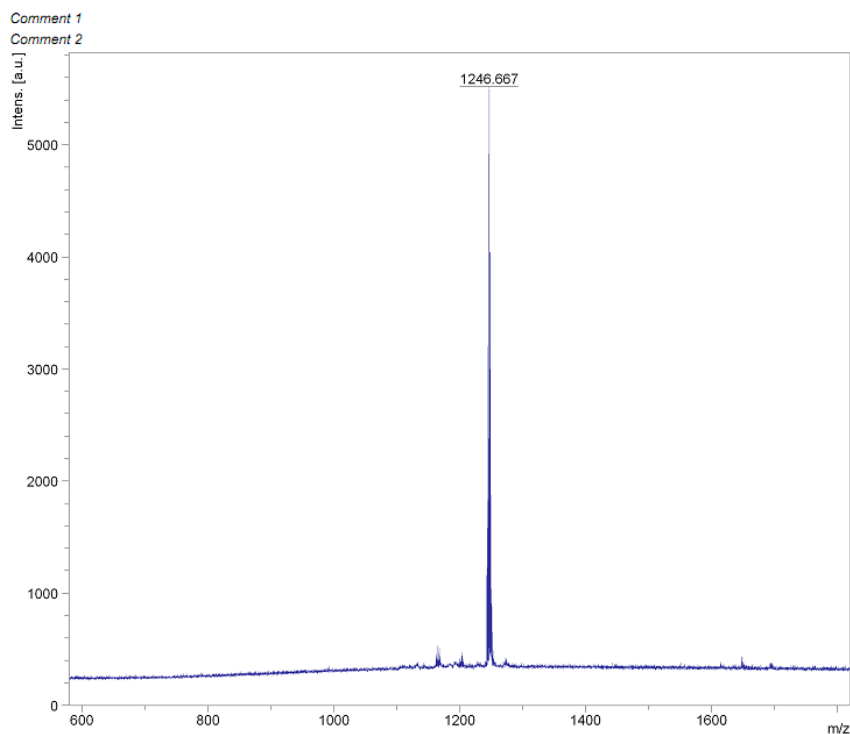


Figure S2. MALDI-TOF MS plot of compound 3.

Synthesis of Se-TC

Compound 3 (80 mg, 0.064 mmol), TFA (3 mL) were added in DCM (15 mL). The solution was stirred for 12 h at room temperature. After extraction and washing, the solvent was evaporated, and a black solid was obtained, and directly used in the following step.

2. Absorption spectrum of Se-TC in THF

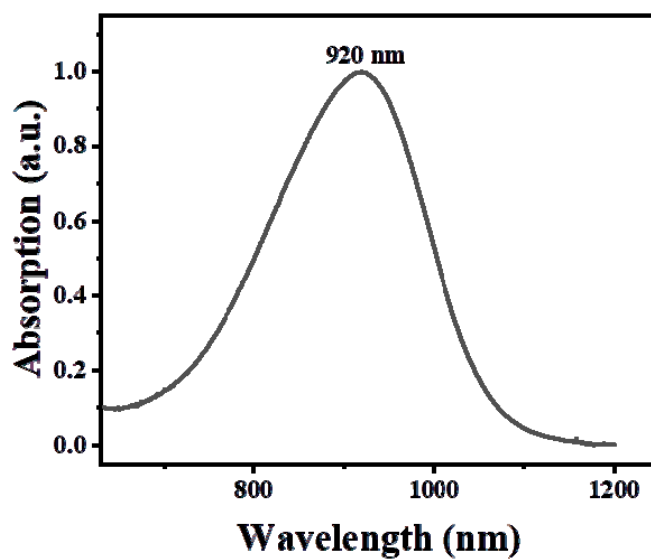


Figure S3. Absorption spectrum of Se-TC in THF.

3. NIR-II emission spectrum of RENP in chloroform

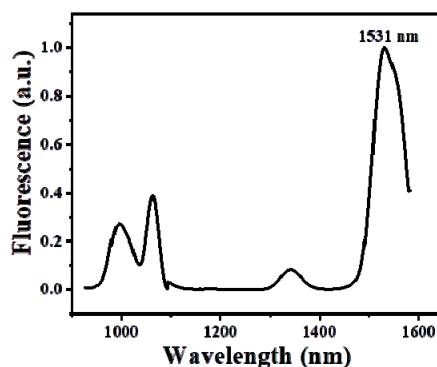


Figure S4. NIR-II emission spectrum of RENP in chloroform.

4. Extinction coefficient of Se-TC@RENP@F

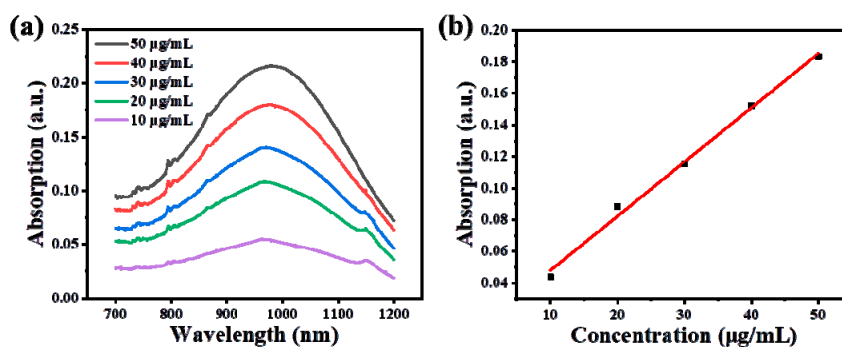


Figure S5. (a) Absorption curves of Se-TC@RENP@F at different concentrations. (b) Linear absorbance versus concentration obtained from (a).

5. The biocompatibility of Se-TC@RENP@F in vivo

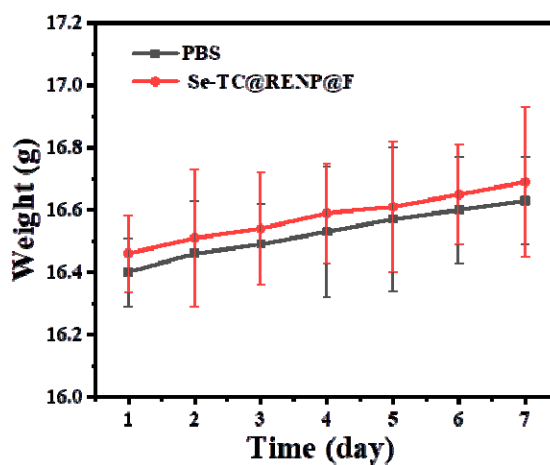


Figure S6. The body weight changes of healthy mice treated with PBS and Se-TC@RENP@F.

References:

[S1] X. Liu, R. Zhu, Y. Zhang, B. Liu, S. Ramakrishna, *Chem. Commun.* **2008**, 3789–3791, doi: 10.1039/B805060K.

[S2] Y. Cao, R. Yang, W Yang, Chinese Patent CN1389488 A, 08-01-2003.