

Supplemental information

Development of Glycan-3-Specific Binding Peptide using *in vivo* and *in vitro* Two-step Phage Display Screening for PET Imaging of Hepatocellular Carcinoma

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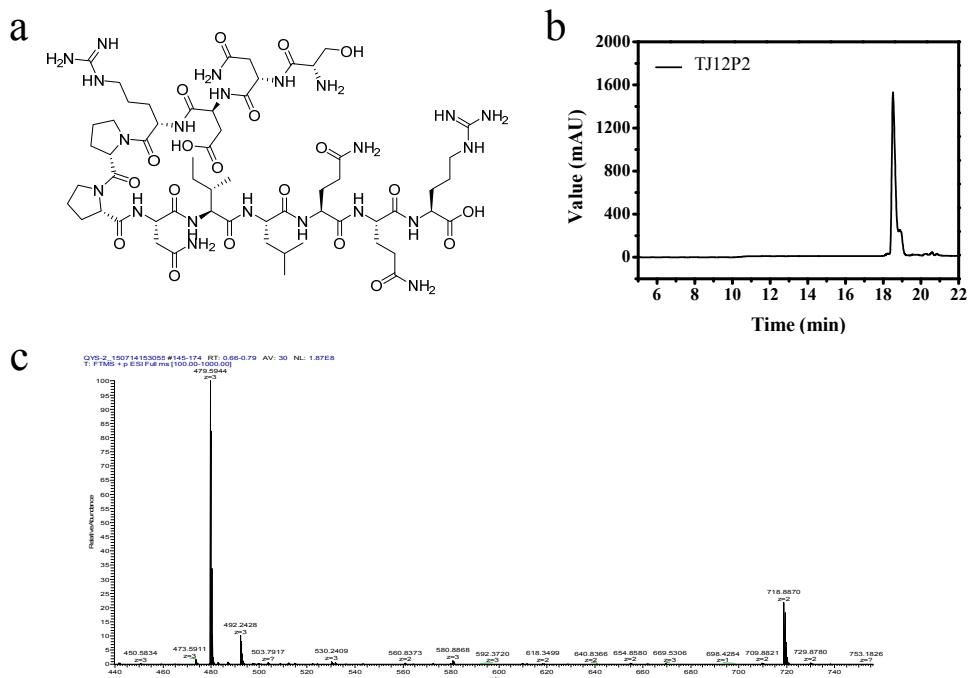


Figure S1. Synthesis of TJ12P2. (a). Chemical structure of TJ12P2 with the sequence of SNDRPPNILQKR. (b). Purity of TJ12P2 by analytical HPLC. The retention time of TJ12P2 is 18.51 min. (c). Mass spectrum analysis of molecular weight of TJ12P2, which is 1425.76 Da.

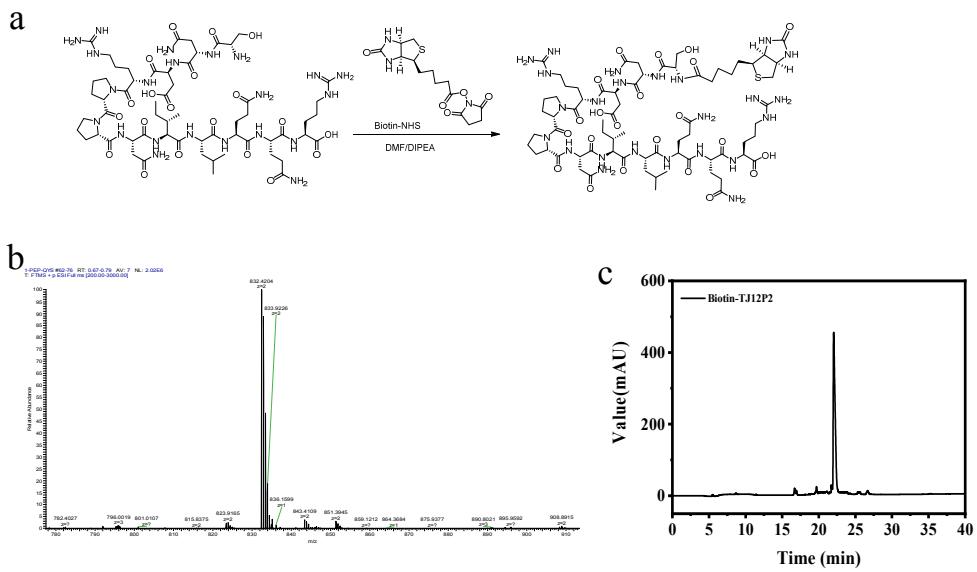


Figure S2. Synthesis of Biotin-TJ12P2. **(a)**. Chemical conjugation of Biotin onto the N-terminal of TJ12P2. **(b)**. Mass spectrum analysis of molecular weight of TJ12P2, which is 1662.8 Da. **(c)**. Purity of Biotin-TJ12P2 by analytical HPLC. The retention time of Biotin-TJ12P2 is 22 min.

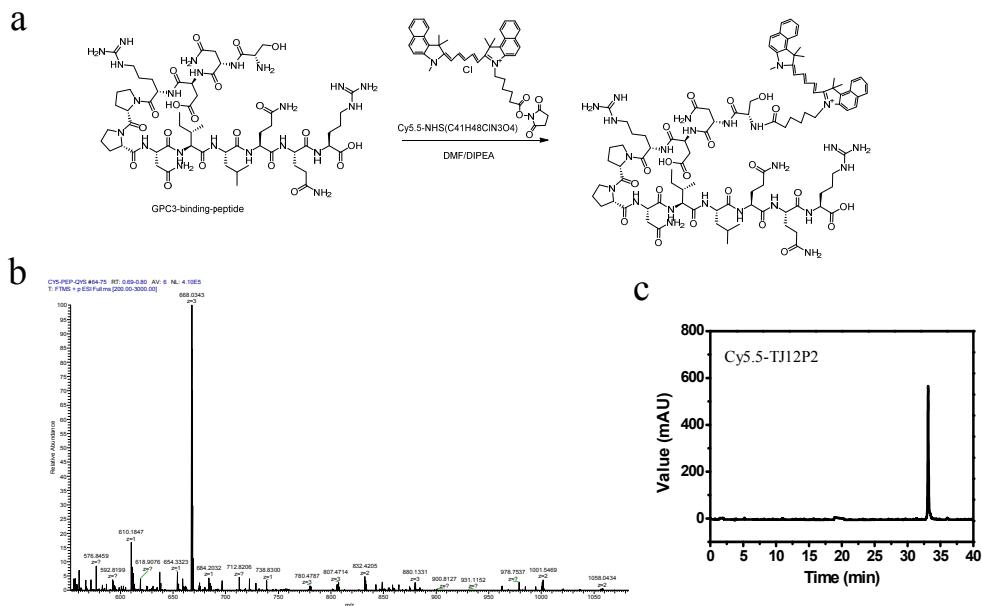


Figure S3. Synthesis of Cy5.5-TJ12P2. **(a).** Chemical conjugation of Cy5.5-NHS onto the N-terminal of TJ12P2. **(b).** Mass spectrum analysis of molecular weight of TJ12P2, which is 1662.8 Da. **(c).** Purity of Cy5.5-TJ12P2 by analytical HPLC. The retention time of Biotin-TJ12P2 is 33.12 min.

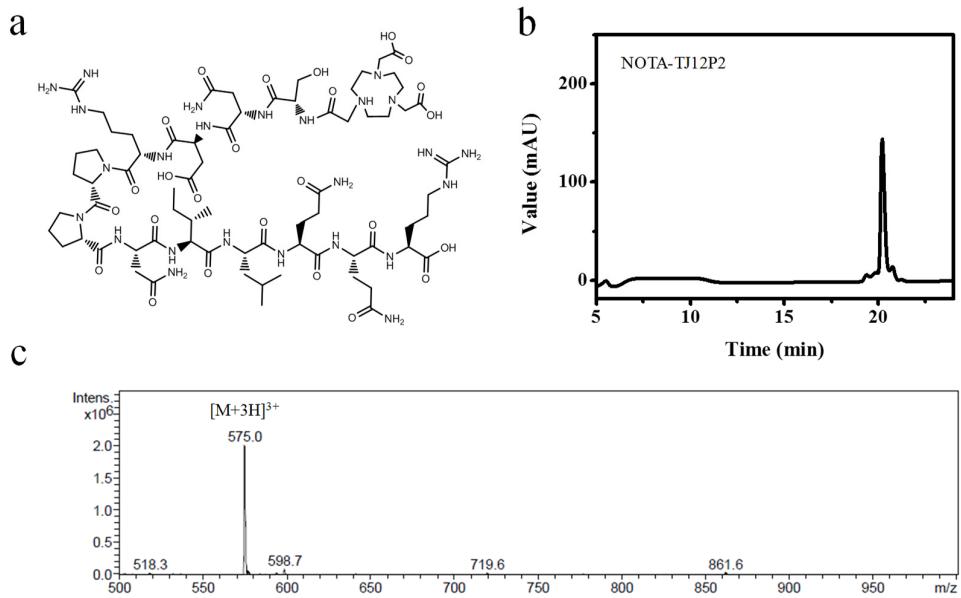


Figure S4. Synthesis of NOTA-TJ12P2. (a). Chemical structure of NOTA-TJ12P2. (b). Purity of NOTA-TJ12P2 by analytical HPLC. The retention time of Biotin-TJ12P2 is 20.20 min. (c). Mass spectrum analysis of molecular weight of TJ12P2, which is 1722 Da.

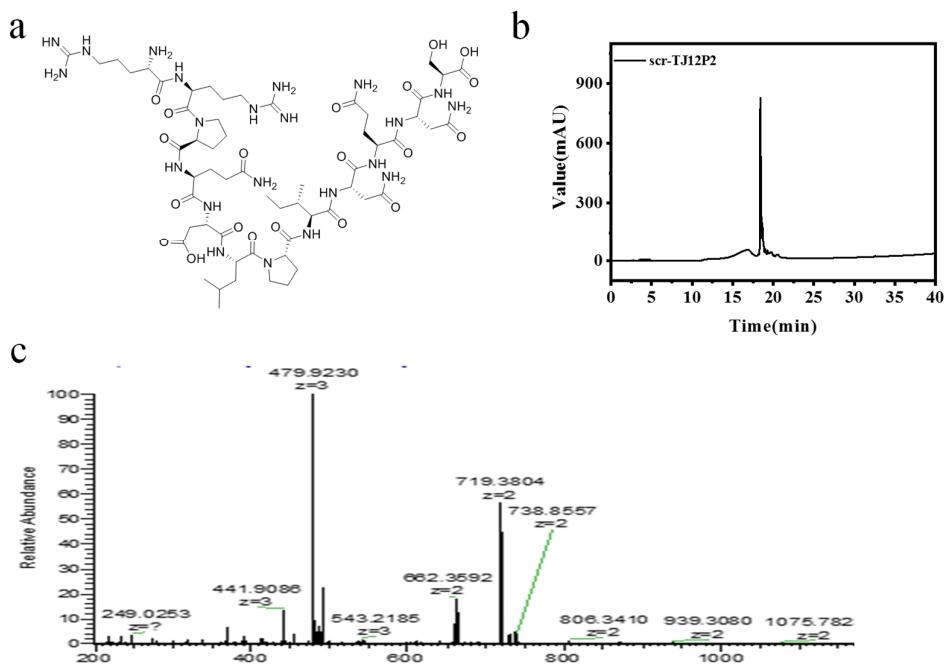


Figure S5. Synthesis of scramble TJ12P2 peptide. **(a).** Chemical structure of scramble-TJ12P2. **(b).** Purity of Cy5.5-TJ12P2 by analytical HPLC. The retention time of scramble-TJ12P2 is 18.40 min. **(c).** Mass spectrum analysis of molecular weight of scramble-TJ12P2, which is 1436.76 Da.

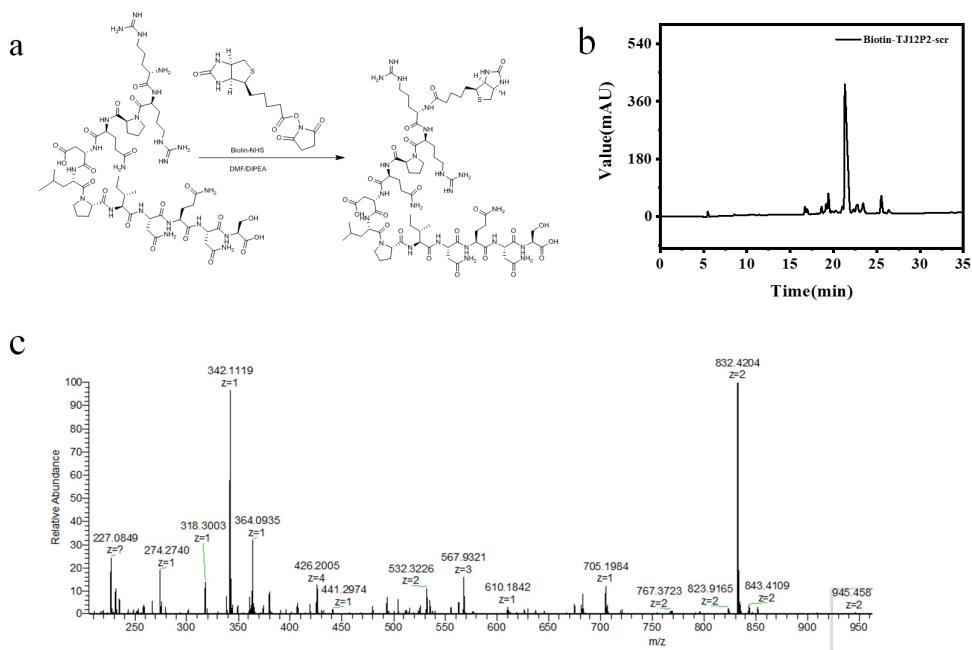


Figure S6. Synthesis of Biotin-scrambled-TJ12P2. **(a).** Chemical conjugation of Biotin onto the N-terminal of scrambled-TJ12P2. **(b).** Mass spectrum analysis of molecular weight of scrambled-TJ12P2, which is 1662.8 Da. **(c).** Purity of Biotin-scrambled-TJ12P2 by analytical HPLC. The retention time of Biotin- scrambled-TJ12P2 is 21.3 min.

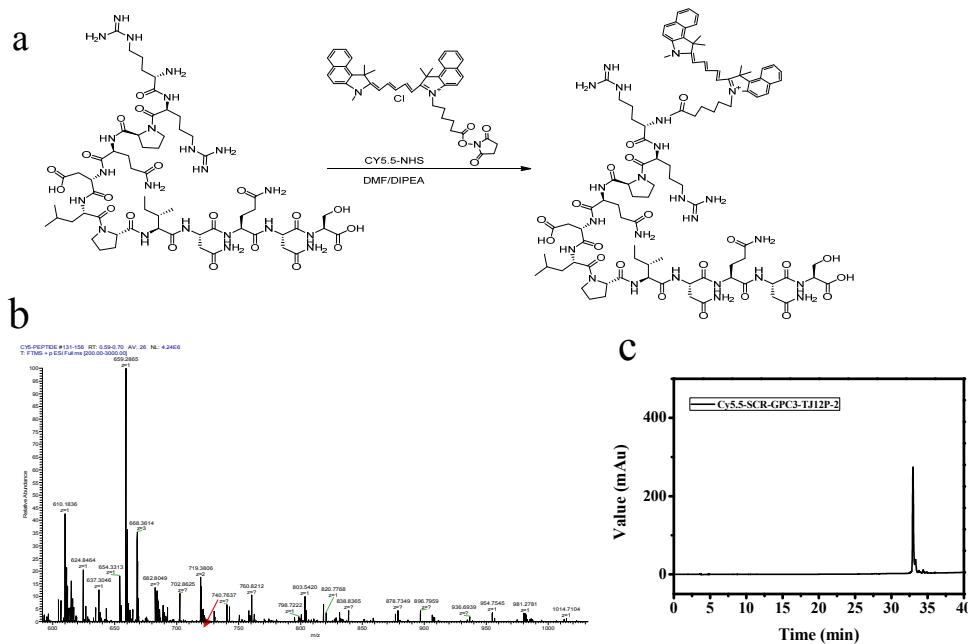


Figure S7. Synthesis of Cy5.5-scrambled-TJ12P2. **(a).** Chemical conjugation of Cy5.5-NHS onto the N-terminal of scrambled-TJ12P2. **(b).** Mass spectrum analysis of molecular weight of Cy5.5-scrambled-TJ12P2, which is 2002.09 Da. **(c).** Purity of Cy5.5-scrambled-TJ12P2 by analytical HPLC. The retention time of Biotin-TJ12P2 is 32.97 min.

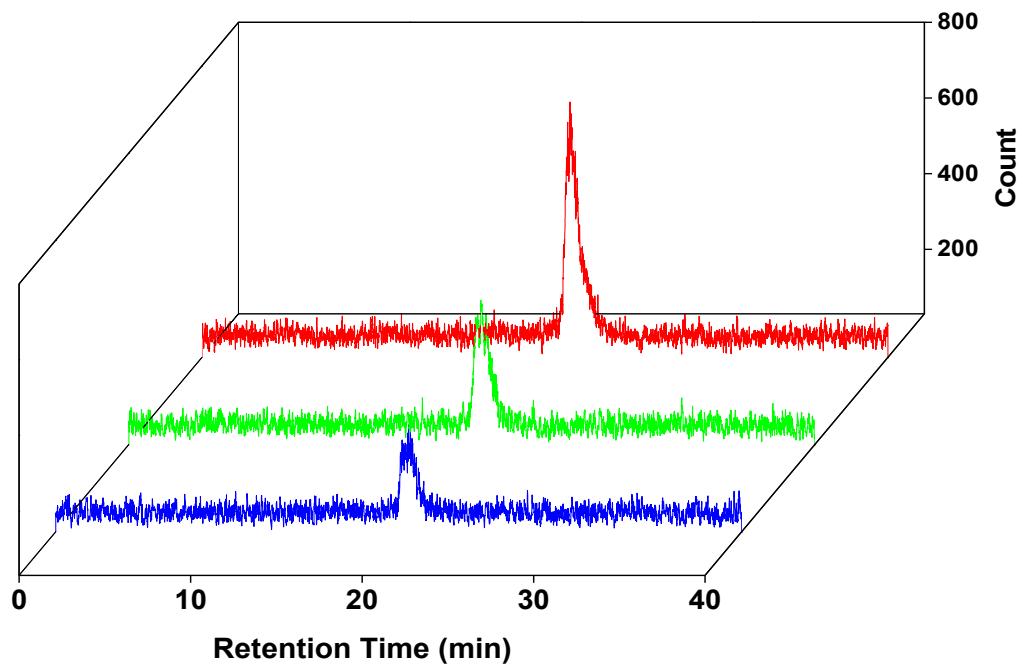


Figure S8. HPLC analysis of the stability of ^{18}F -AlF-NOTA-TJ12P2 in physiological buffer at 37°C for 4 hours.

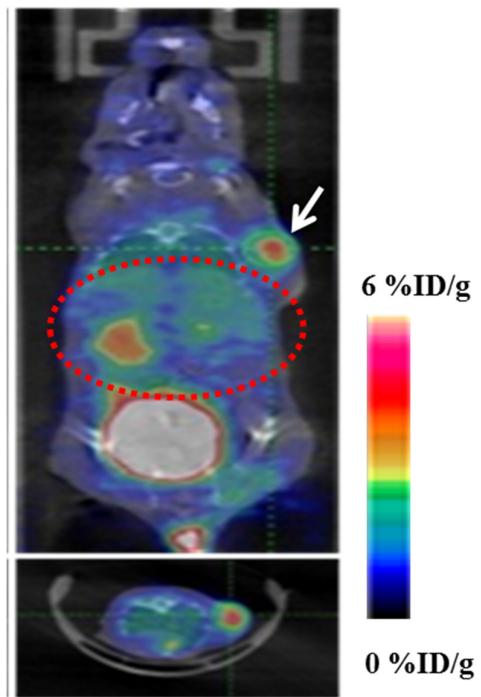


Figure S9. Micro-PET/CT imaging of 18F-AIF-NOTA-TJ12P1 targetability in HepG2 tumor bearing mouse model. White arrow points to the HepG2 tumor and red circle indicates the normal liver.