

Electronic supplementary information

Radiopharmacological evaluation of caspase-3 responsive probe with optimized pharmacokinetics for PET imaging of tumor apoptosis

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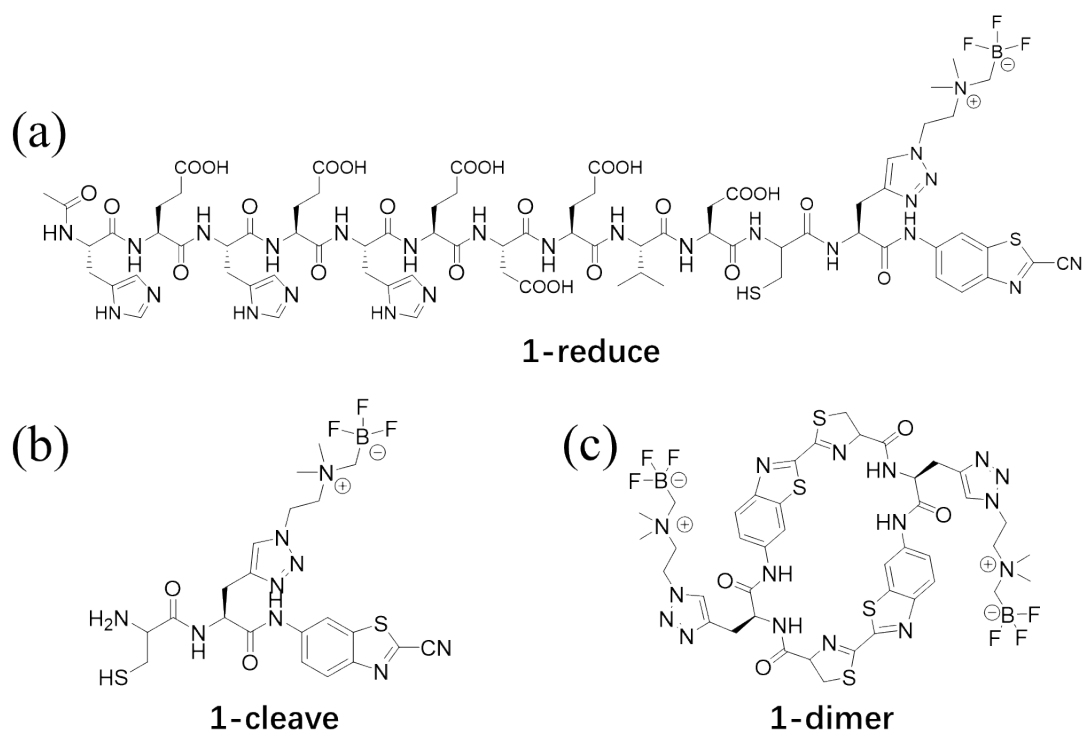


Figure S1. The structures of **1-cleave** (a), **1-cleave** (b) and **1-dimer** (c).

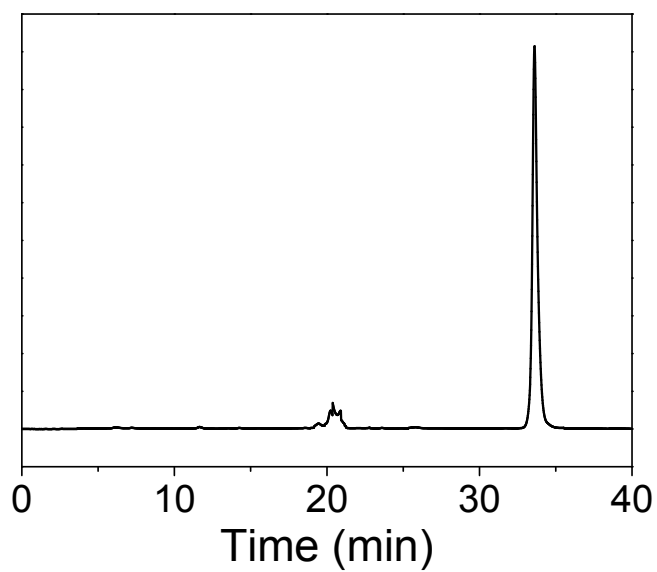


Figure S2. HPLC trace of purified Ac-HEHEHEDEV D-OH.

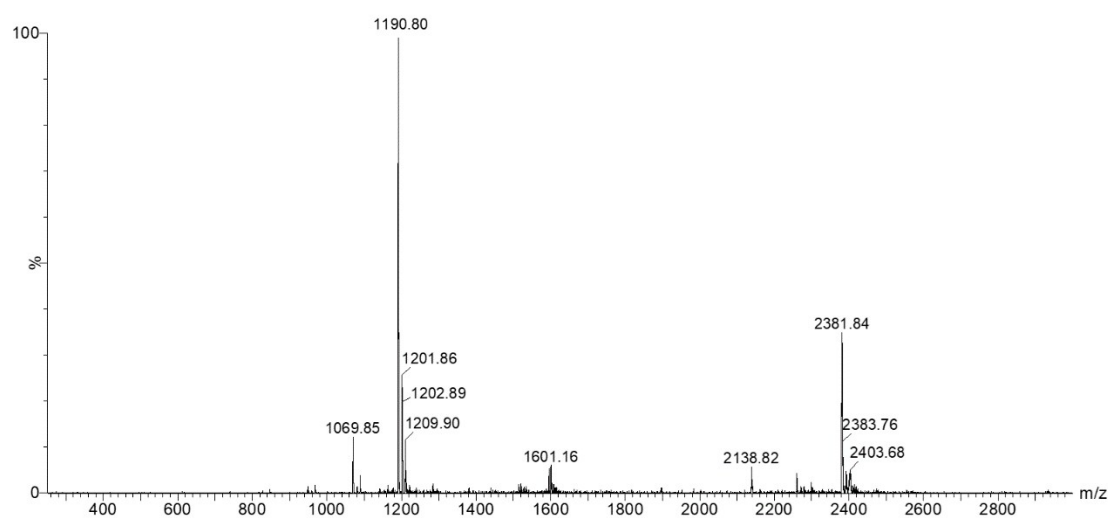


Figure S3. ESI-MS of Ac-HEHEHEDEV D-OH.

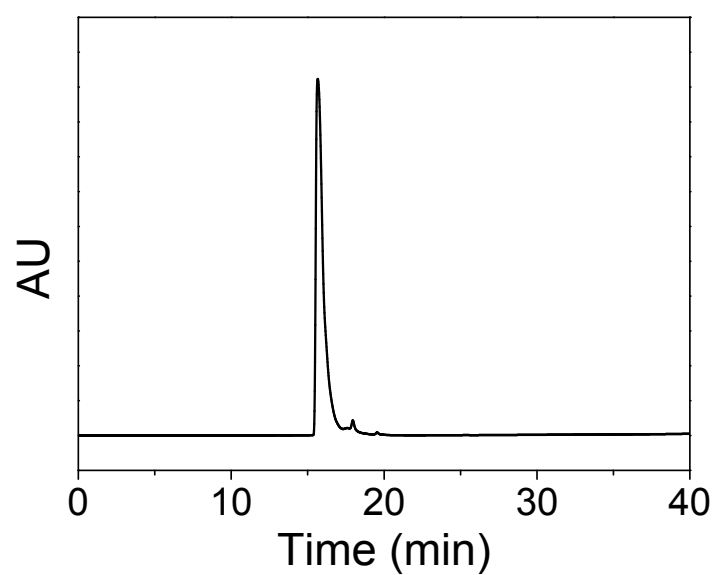


Figure S4. HPLC trace of purified compound A.

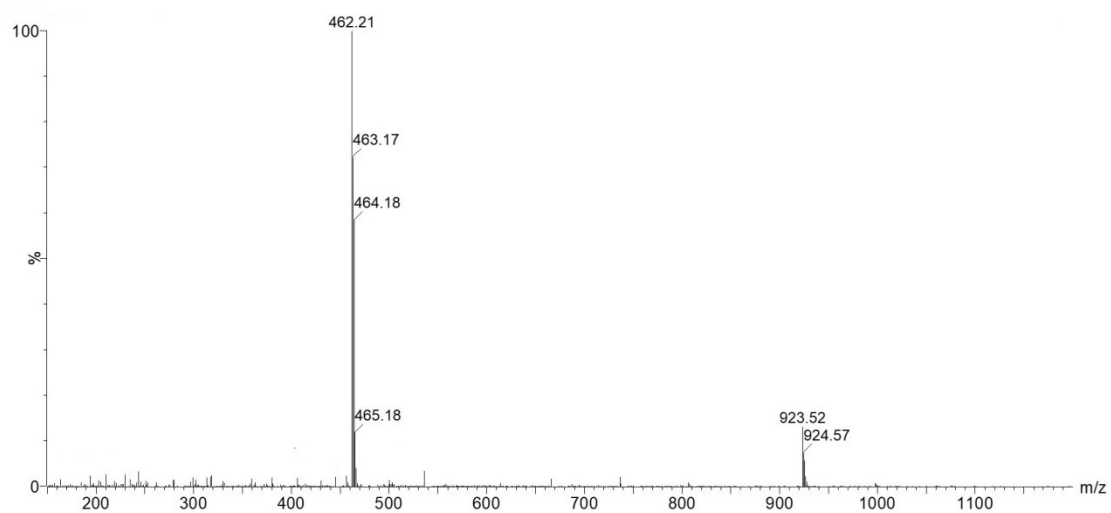


Figure S5. ESI-MS of compound A.

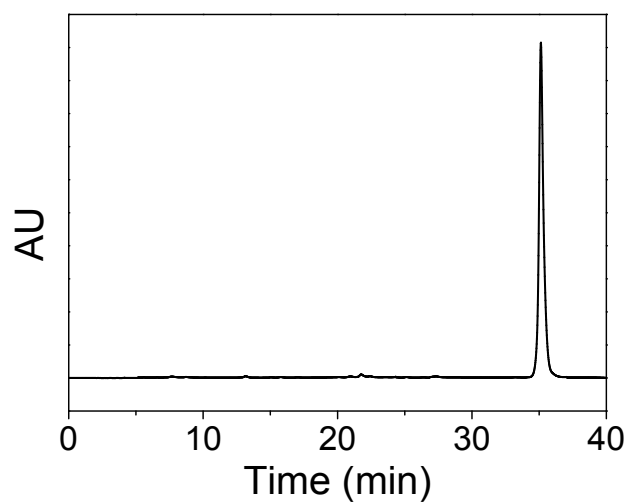


Figure S6. HPLC trace of purified compound B.

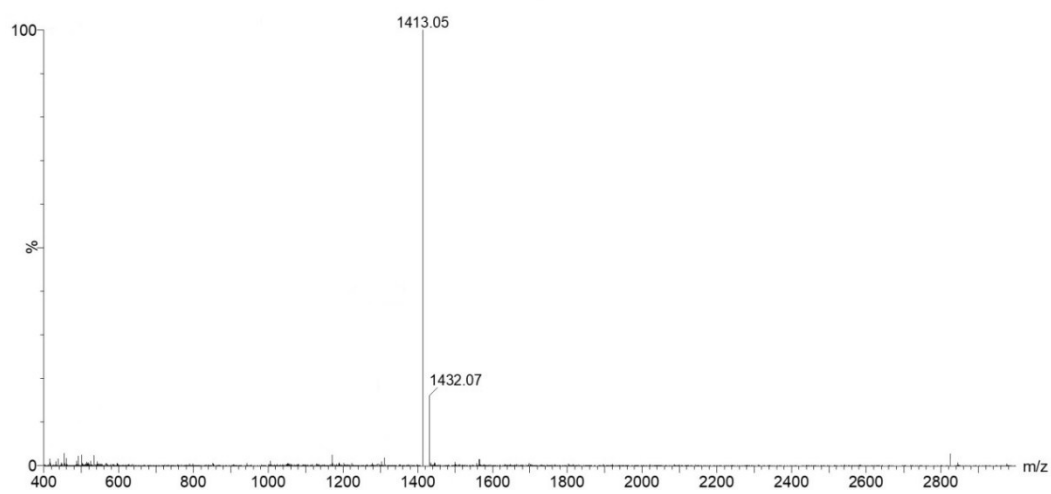


Figure S7. ESI-MS of compound B.

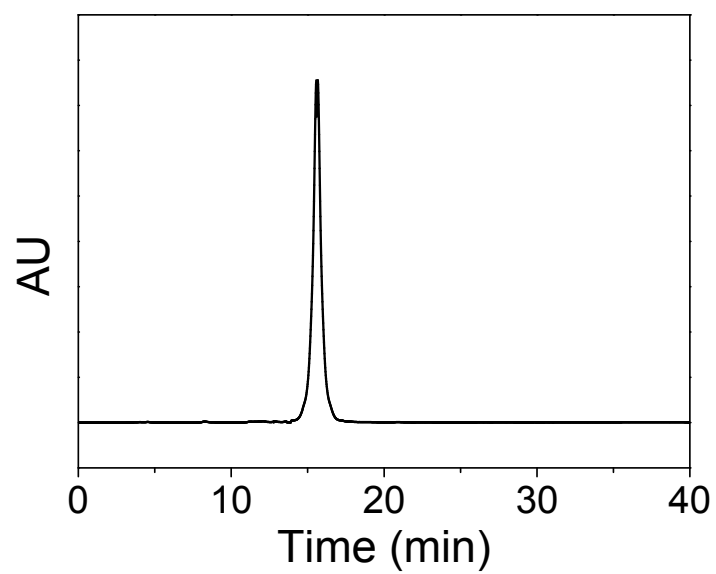


Figure S8. HPLC trace of purified compound **C**.

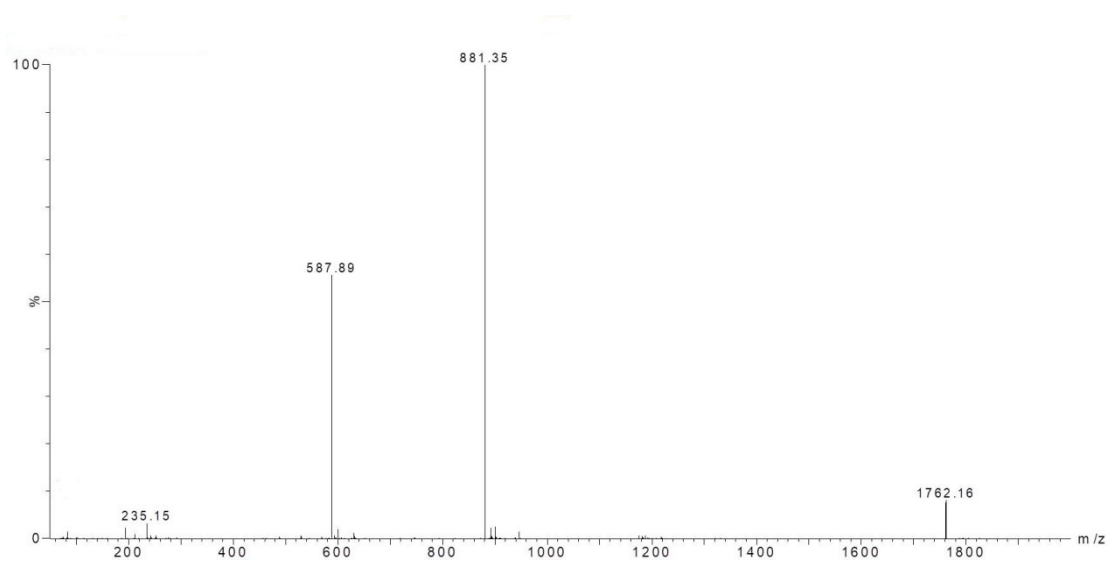


Figure S9. ESI-MS of compound **C**.

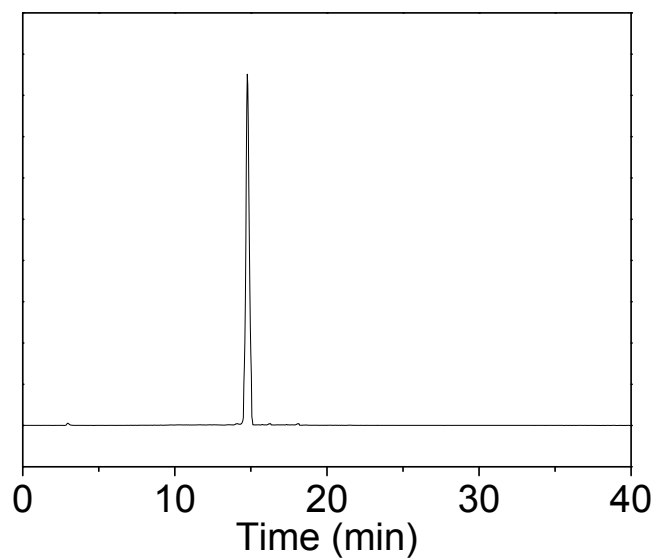


Figure S10. HPLC trace of purified probe 1.

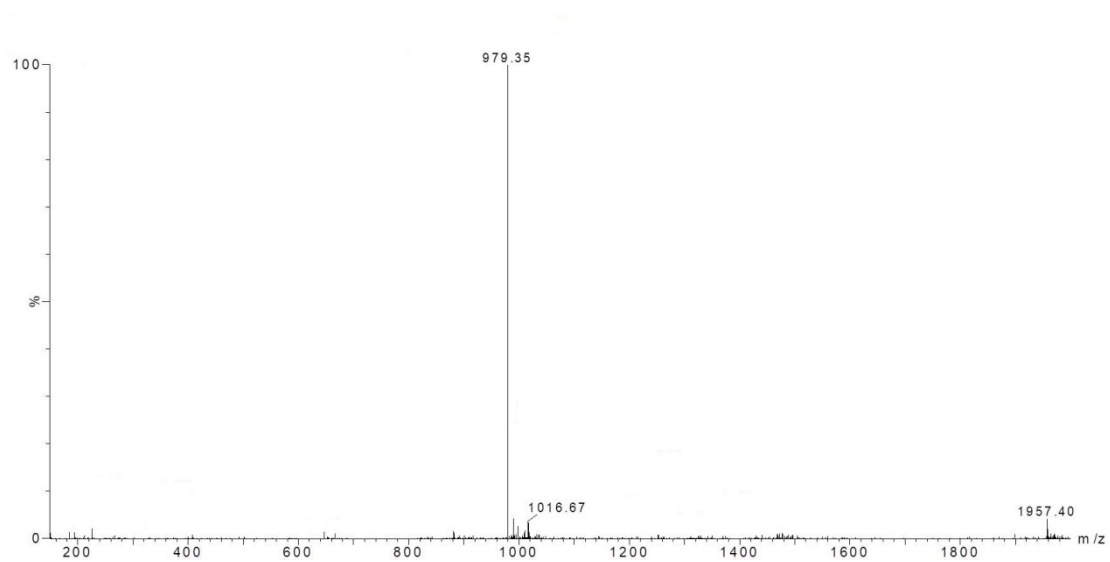


Figure S11. ESI-MS of probe 1.

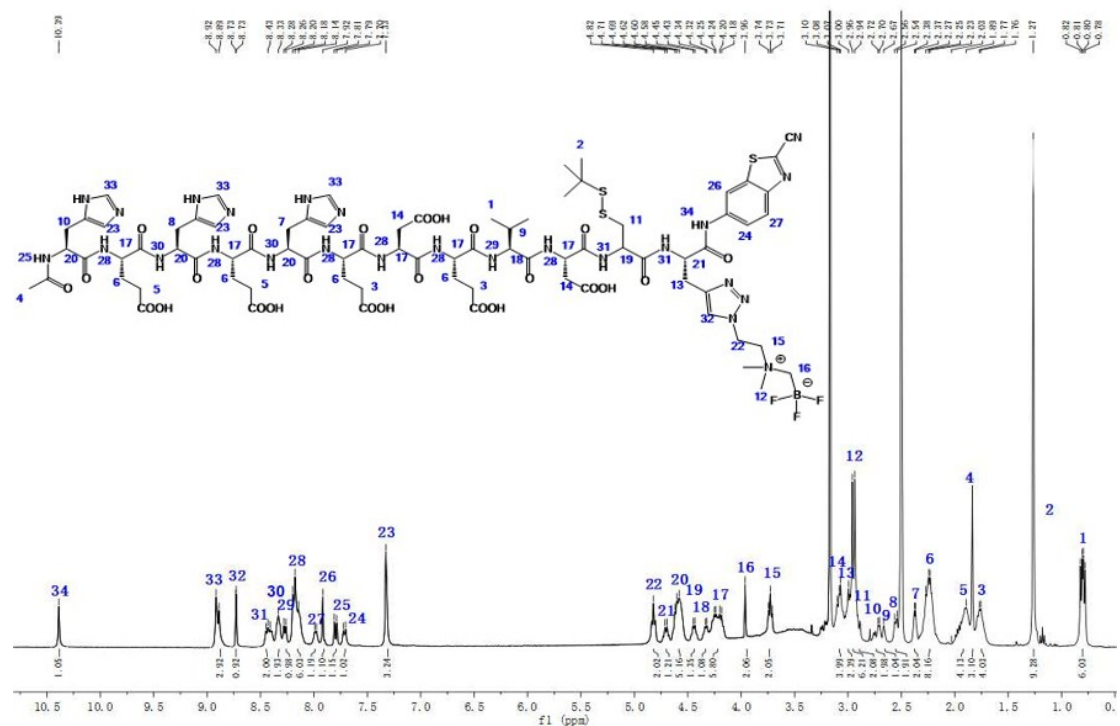


Figure S12. ^1H NMR spectrum of probe 1.

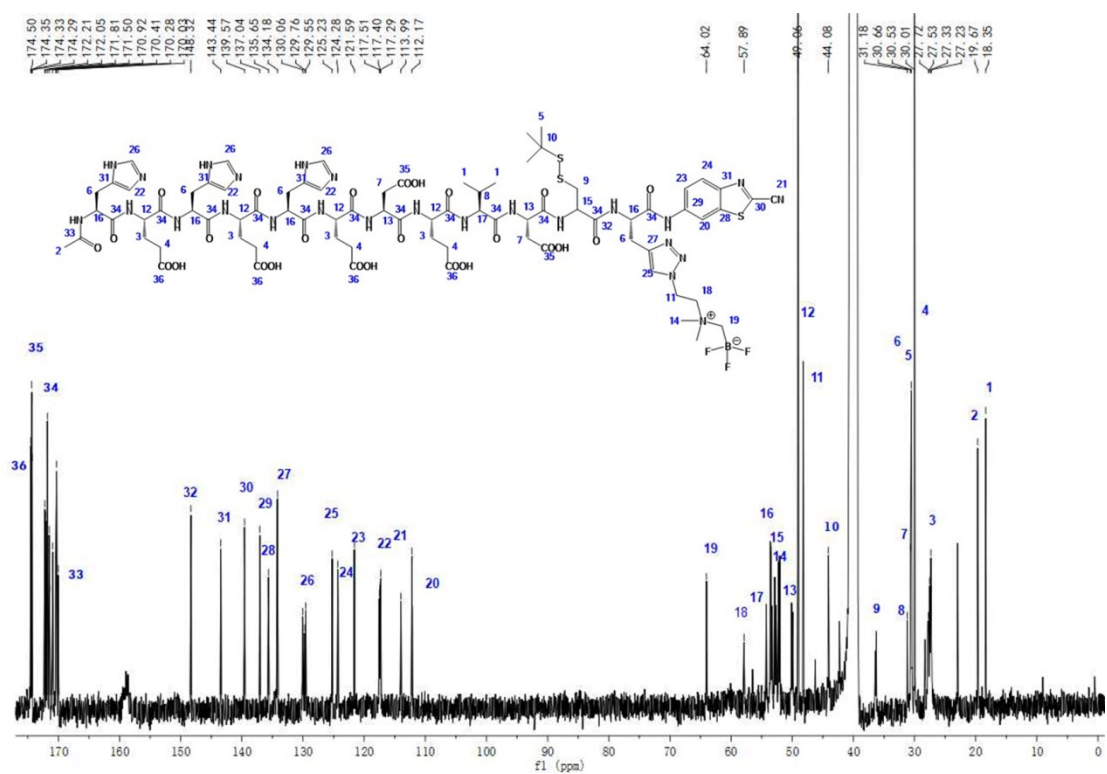


Figure S13. ^{13}C NMR spectrum of probe 1.

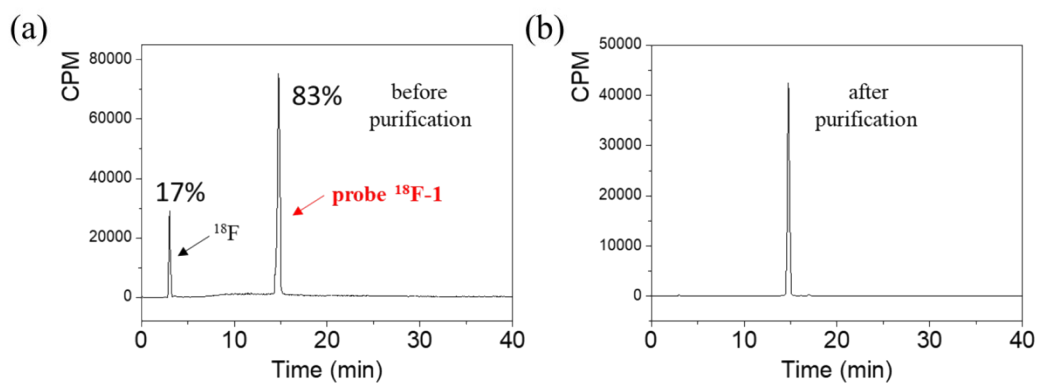


Figure S14. Radioactivity HPLC trace of ^{18}F -1 before (a) and after purification (b).

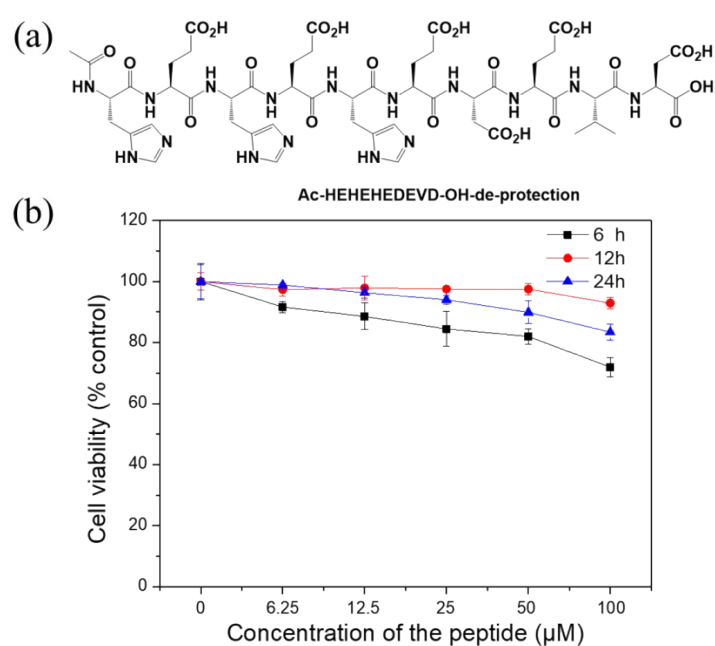


Figure S15. (a) The structure of the peptide **Ac-HEHEHE-OH-de-protection**. (b) The toxicity of the peptide **Ac-HEHEHE-OH-de-protection** against A549 cells at different concentrations.

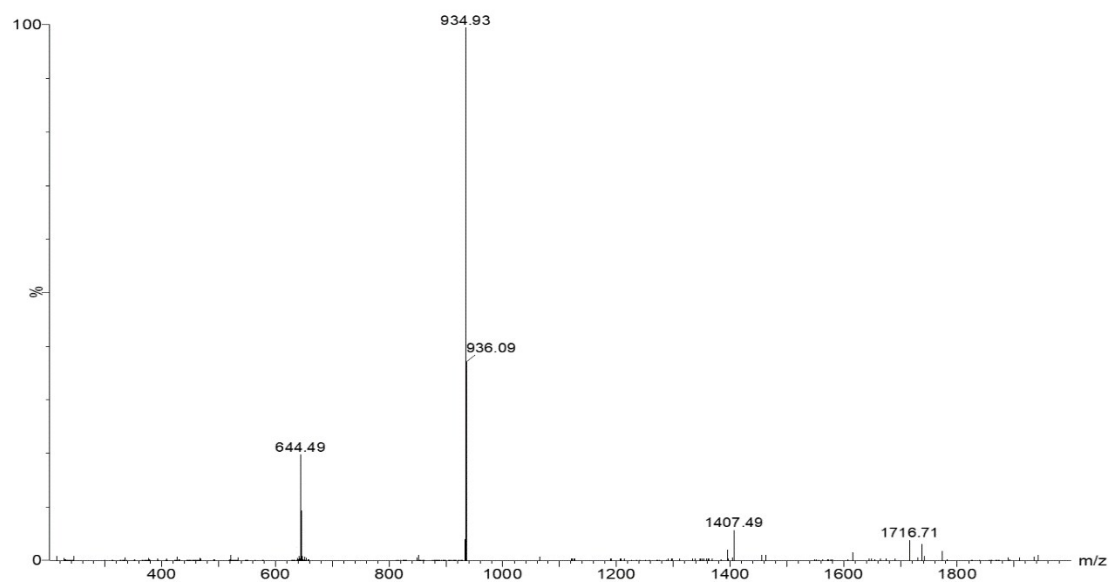


Figure S16. ESI-MS of 1-reduce.

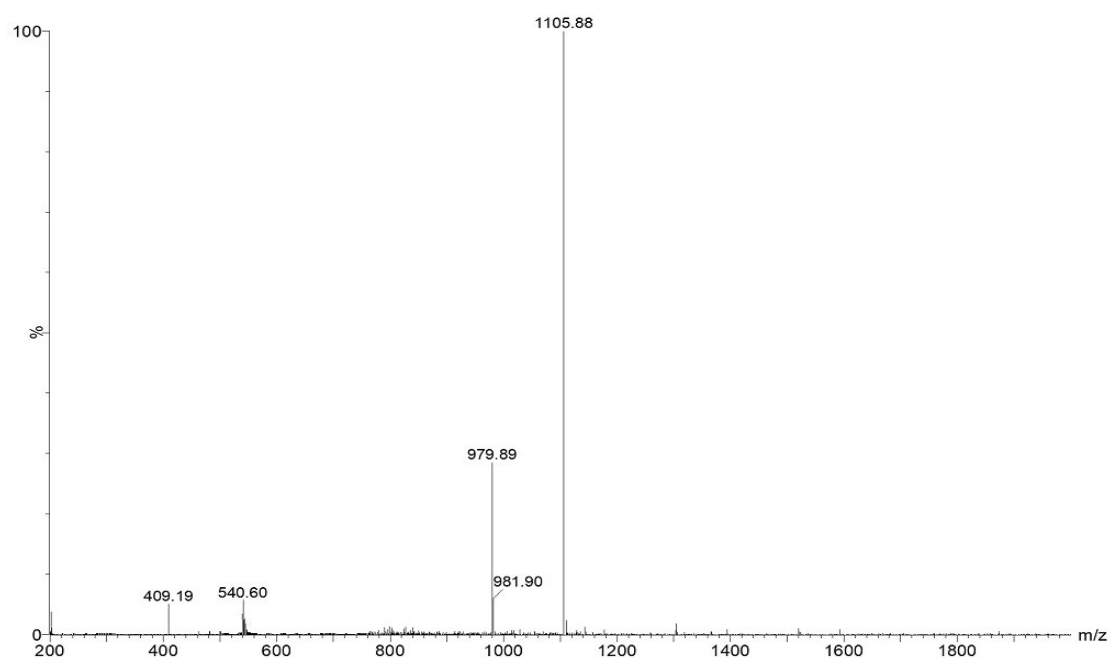


Figure S17. ESI-MS of 1-dimer.

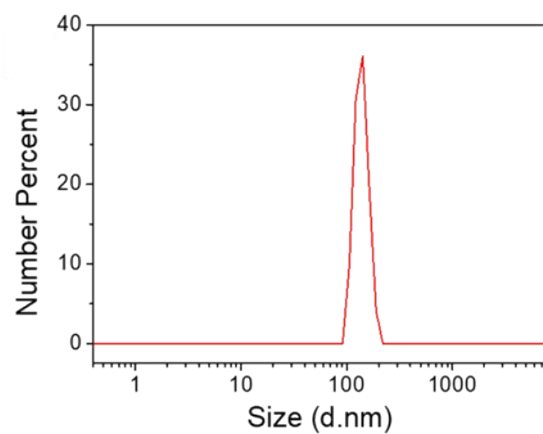


Figure S18. The size distribution of the particles formed in macrocyclization assay.

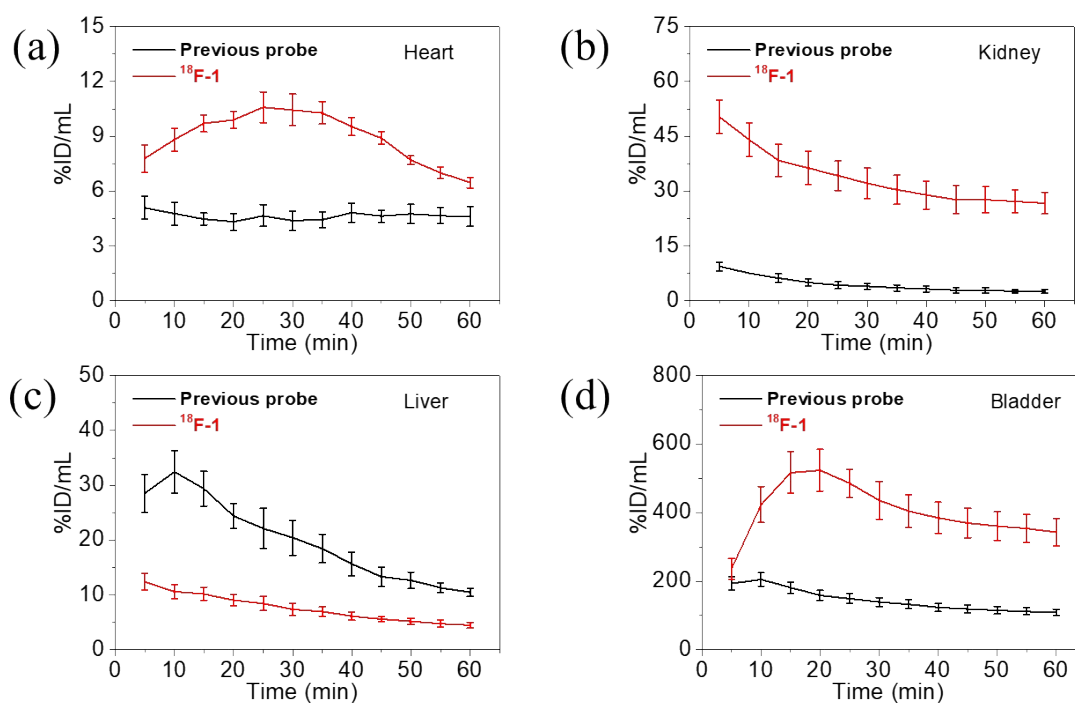


Figure S19. Heart (a), kidney (b), liver (c) and bladder (d) uptake curves of the mice injected with previous probe or $^{18}\text{F-1}$.

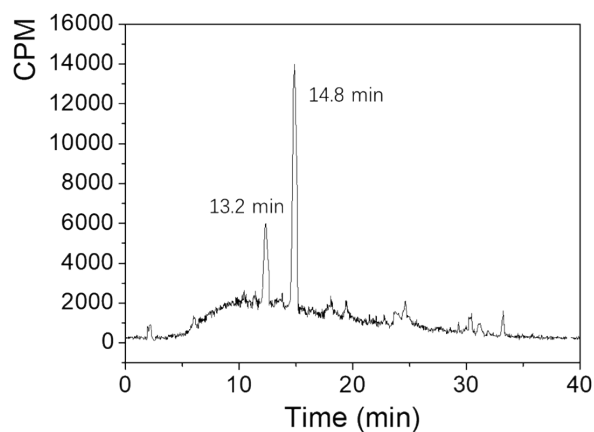


Figure S20. The radioactivity HPLC trace of the liver homogenate.

Table S1. The analytical HPLC condition for the all compounds (Method A).

Time (min)	Flow (mL/min)	(H ₂ O + 0.1 %TFA)%	(CH ₃ CN + 0.1 %TFA)%
0	1.0	80	20
3	1.0	80	20
35	1.0	10	90
40	1.0	80	20

Table S2. The HPLC condition for purification the compound **A** and probe **1** (Method B).

Time (min)	Flow (mL/min)	(H ₂ O + 0.1 %TFA)%	(CH ₃ CN + 0.1 %TFA)%
0	3.0	80	20
3	3.0	80	20
5	3.0	70	30
30	3.0	50	50
35	3.0	10	90
40	3.0	80	20