

Electronic supplementary information

**A Fluorine-18 Labeled Radiotracer for PET Imaging of γ -
Glutamyltranspeptidase in Living Subjects**

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Table S1. HPLC conditions for purification of compound **5**.

Time/min	Flow (mL/min)	A phase (%)	B phase (%)
0	3	80	20
3	3	80	20
6	3	47	53
30	3	35	65
35	3	10	90
40	3	80	20

A phase: 0.1% TFA of water; B phase: 0.1% TFA of MeCN.

Table S2. HPLC conditions for purification of non-radioactive probe (**GCPA**)₂.

Time/min	Flow (mL/min)	A phase (%)	B phase (%)
0	3	80	20
3	3	80	20
6	3	50	50
30	3	38	62
35	3	10	90
40	3	80	20

A phase: 0.1% TFA of water; B phase: 0.1% TFA of MeCN.

Table S3. Analytical HPLC conditions of all compounds.

Time/min	Flow (mL/min)	A phase (%)	B phase (%)
0	1	80	20
3	1	80	20
35	1	10	90
40	1	80	20

A phase: 0.1% TFA of water; B phase: 0.1% TFA of MeCN.

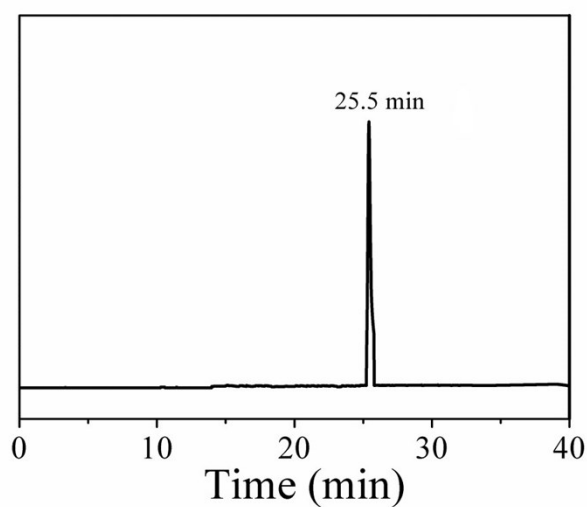


Fig. S1. HPLC trace of compound **2**.

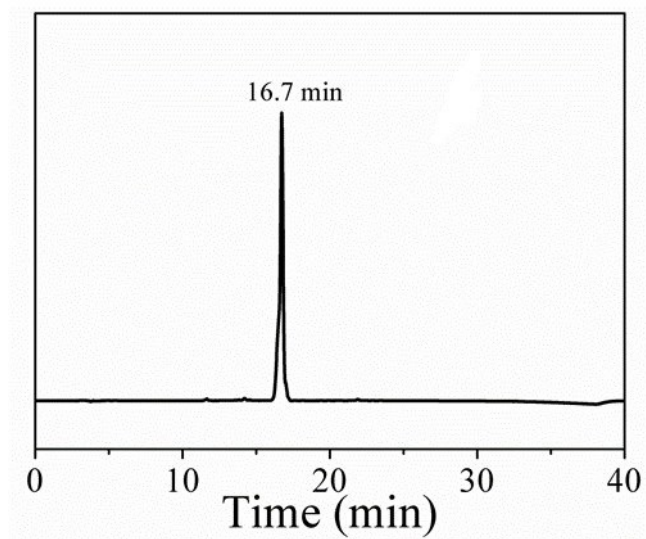


Fig. S2. HPLC trace of compound 3.

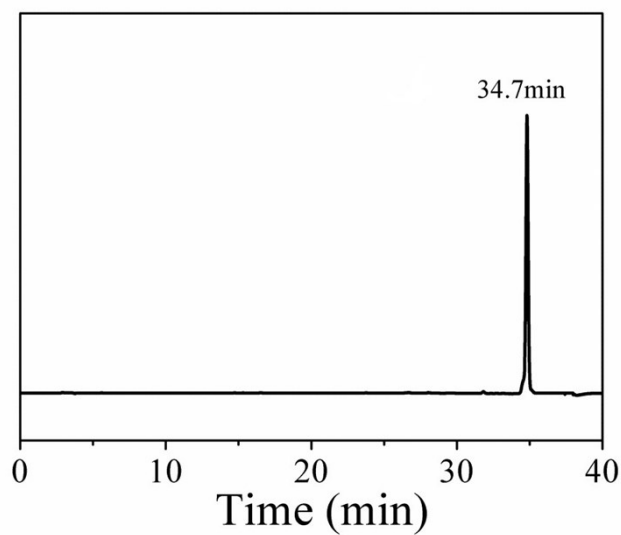


Fig. S3. HPLC trace of compound 4.

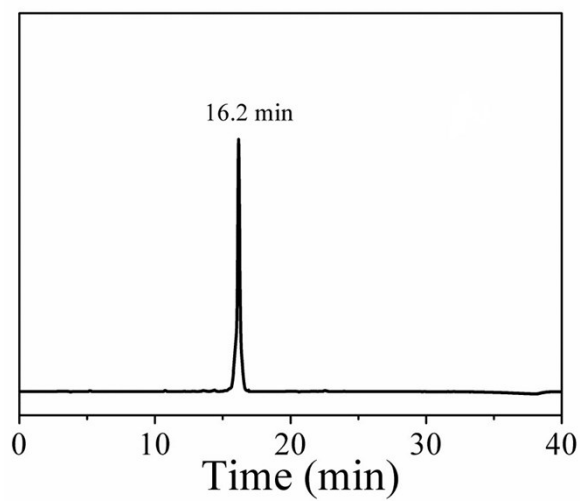


Fig. S4. HPLC trace of compound 5.

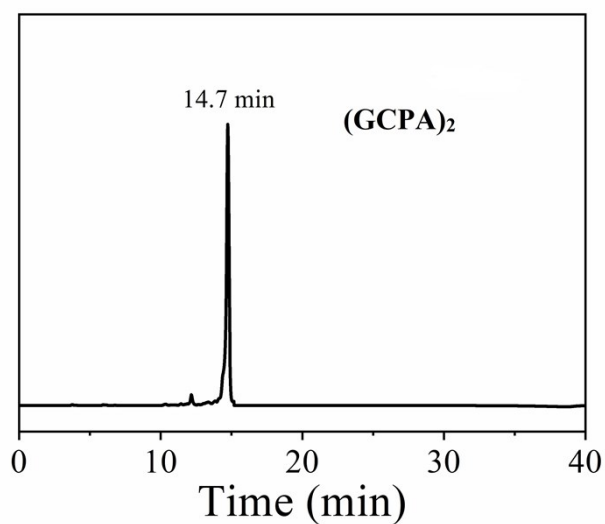


Fig. S5. HPLC trace of non-radioactive probe (GCPA)₂.

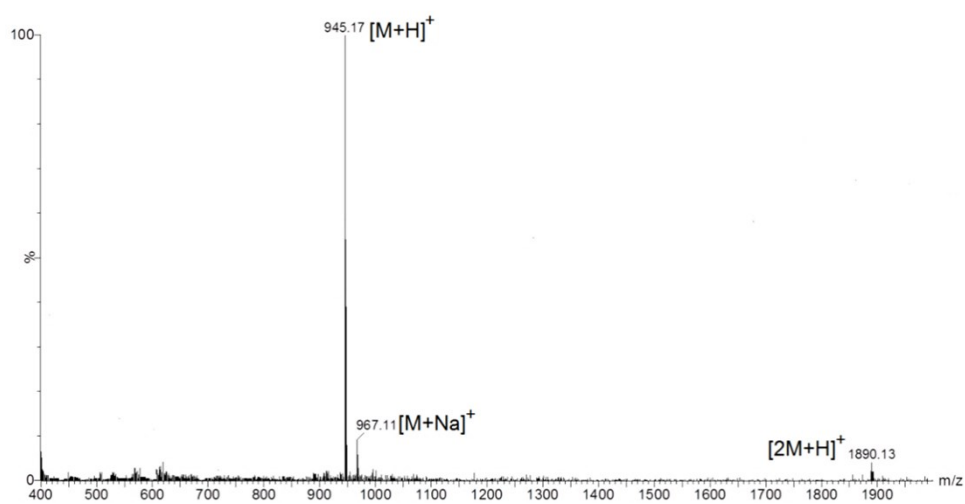


Fig. S6. ESI-MS analysis of compound 2.

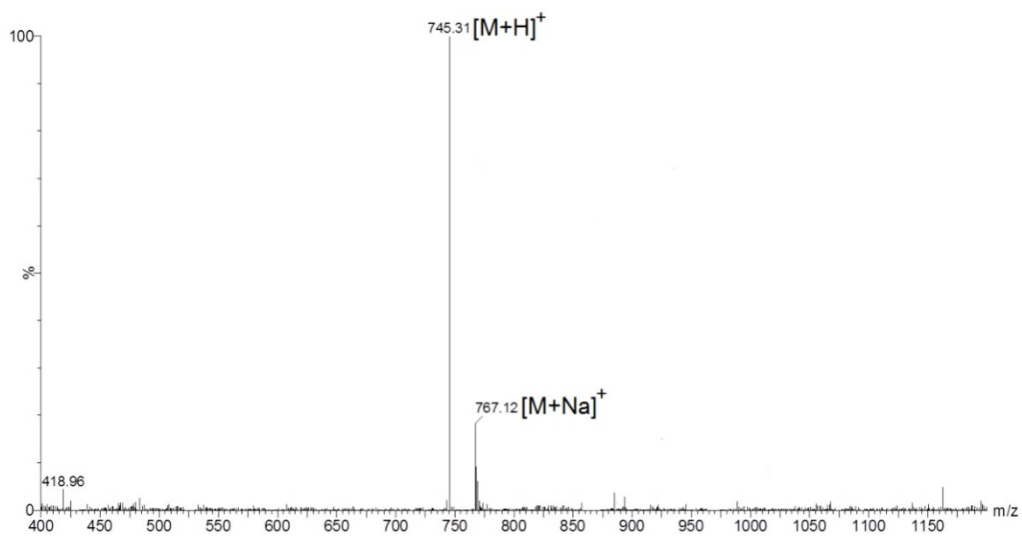


Fig. S7. ESI-MS analysis of compound 3.

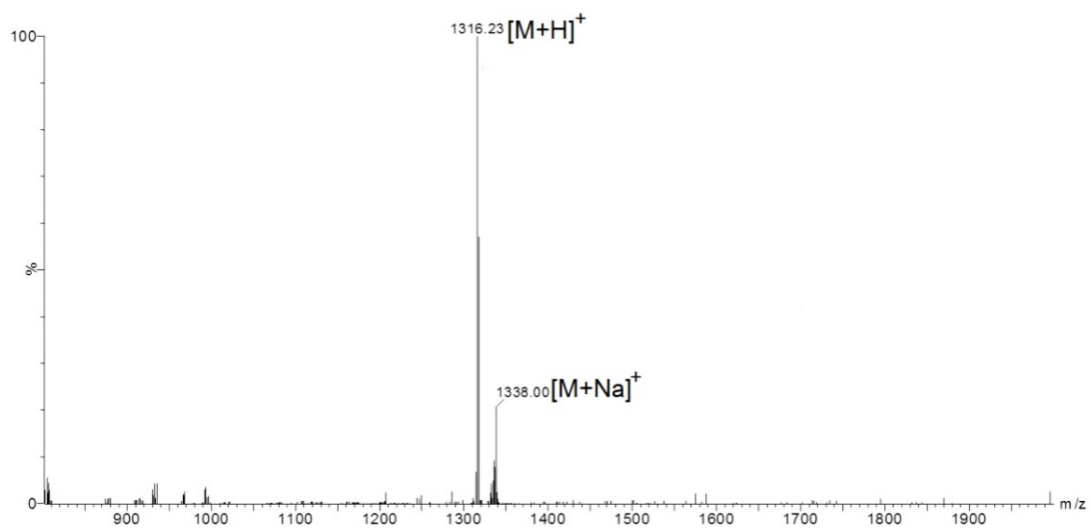


Fig. S8. ESI-MS analysis of compound 4.

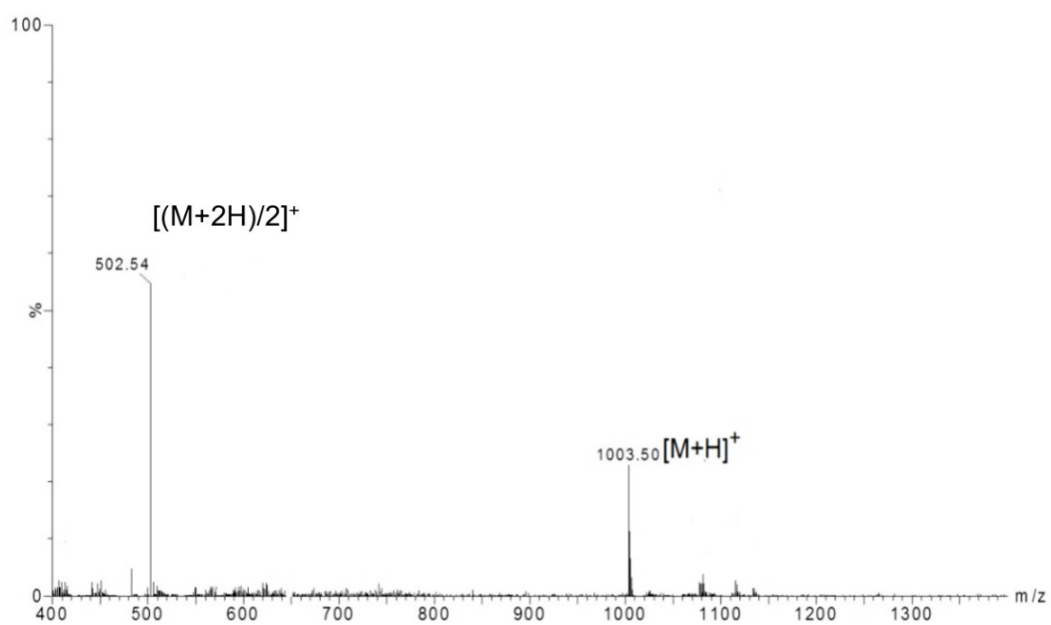


Fig. S9. ESI-MS analysis of compound 5.

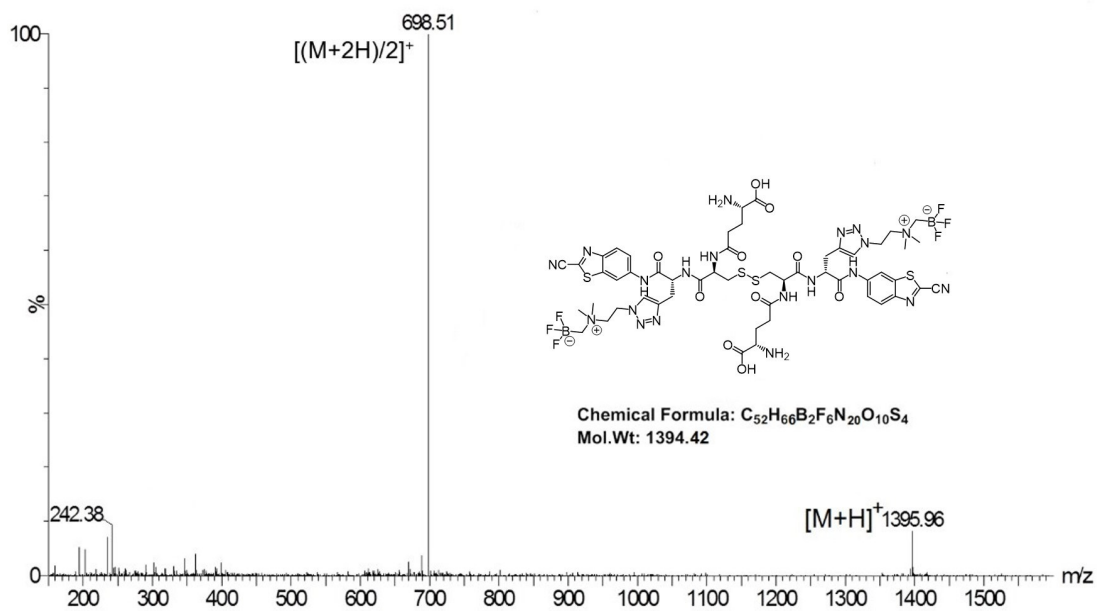


Fig. S10. ESI-MS analysis of non-radioactive probe (GCPA)₂.

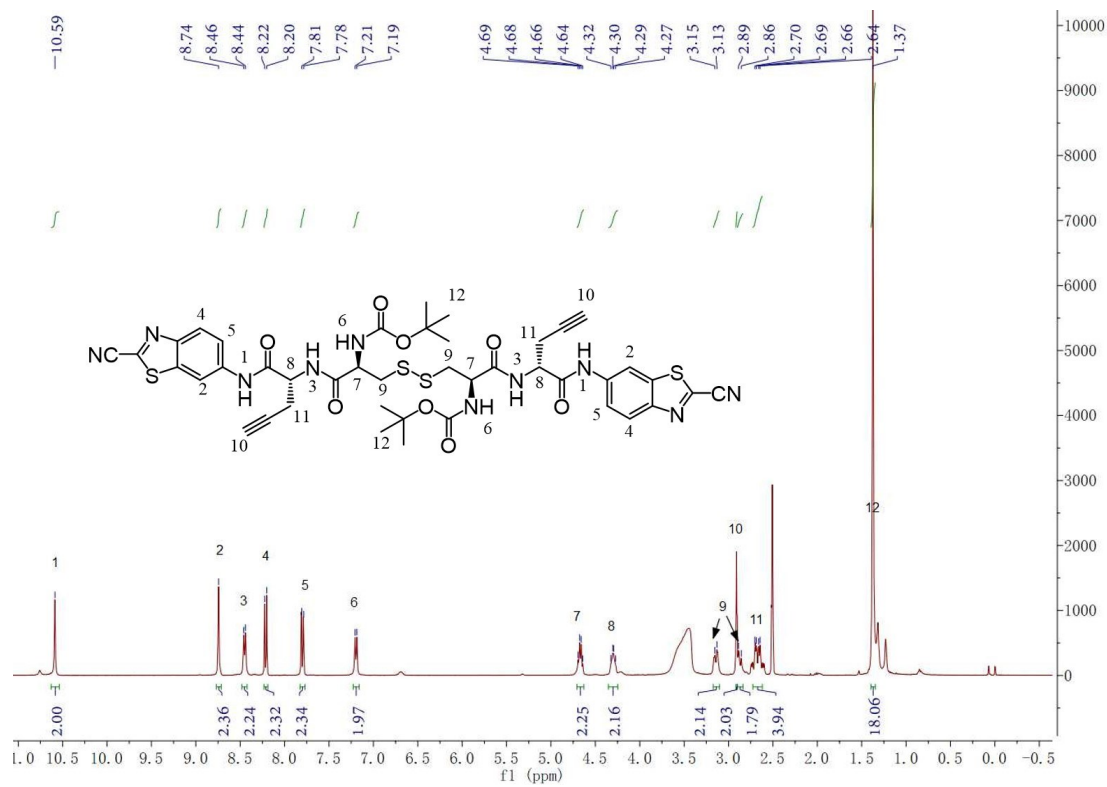


Fig. S11. ¹H NMR spectrum of compound 2.

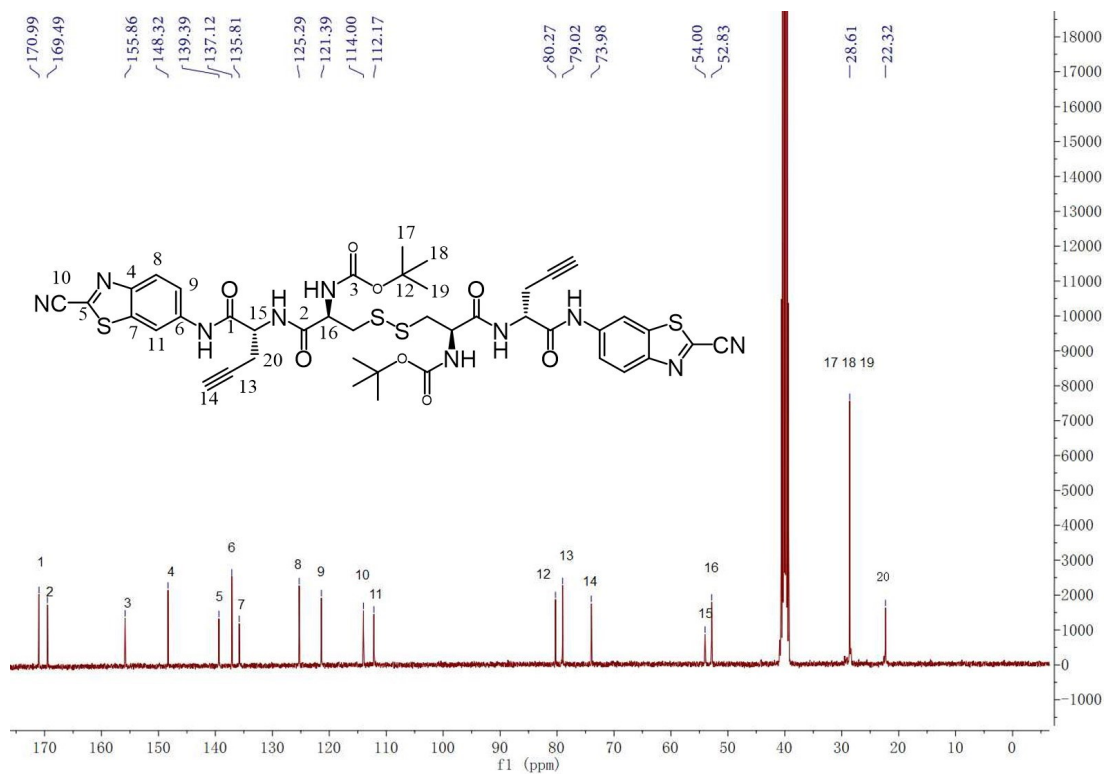


Fig. S12. ^{13}C NMR spectrum of compound 2.

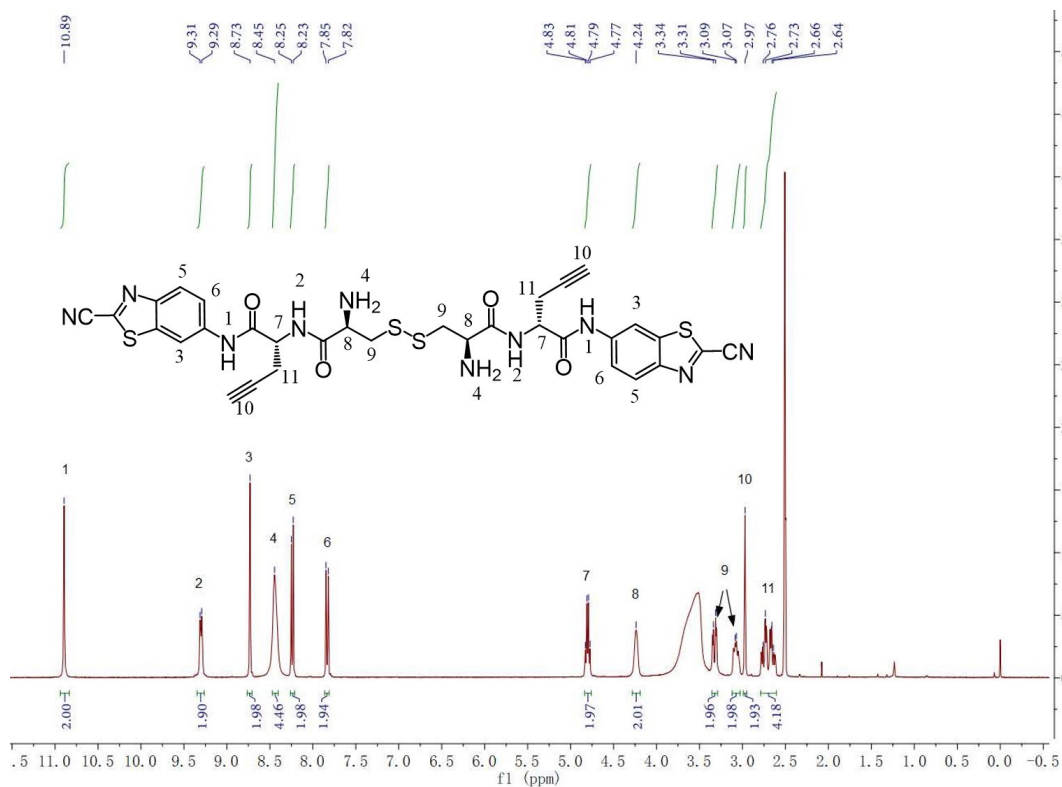


Fig. S13. ^1H NMR spectrum of compound 3.

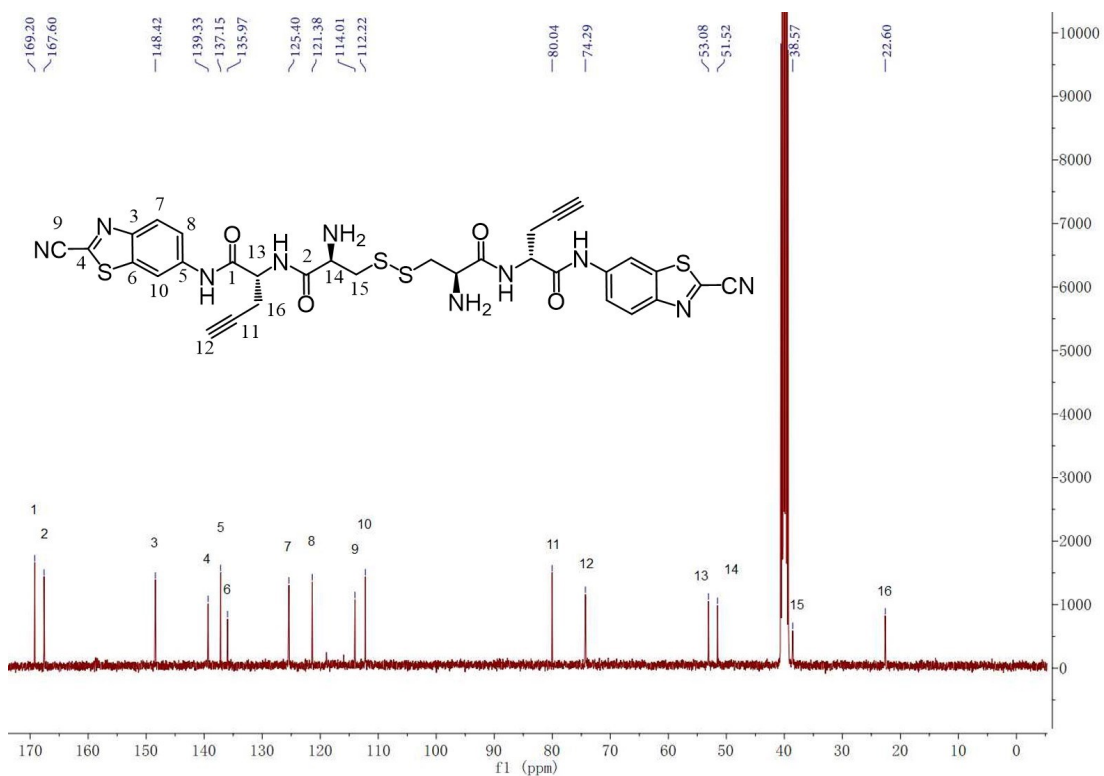


Fig. S14. ^{13}C NMR spectrum of compound 3.

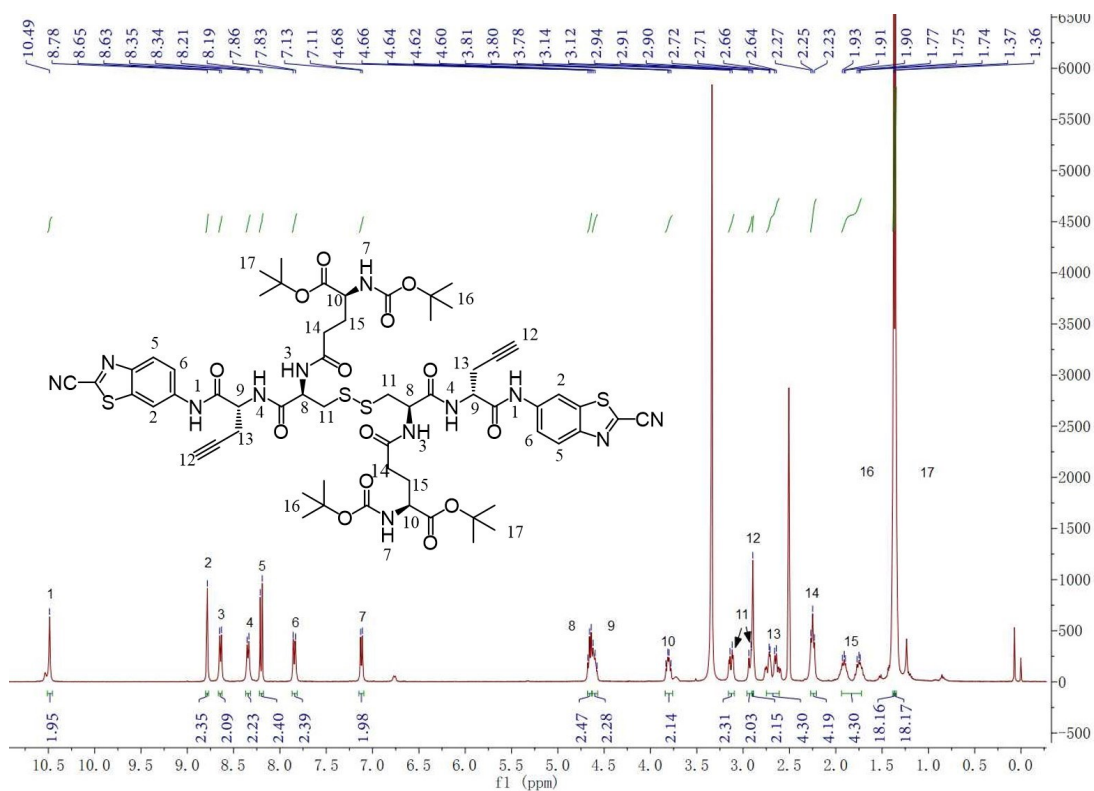


Fig. S15. ^1H NMR spectrum of compound 4.

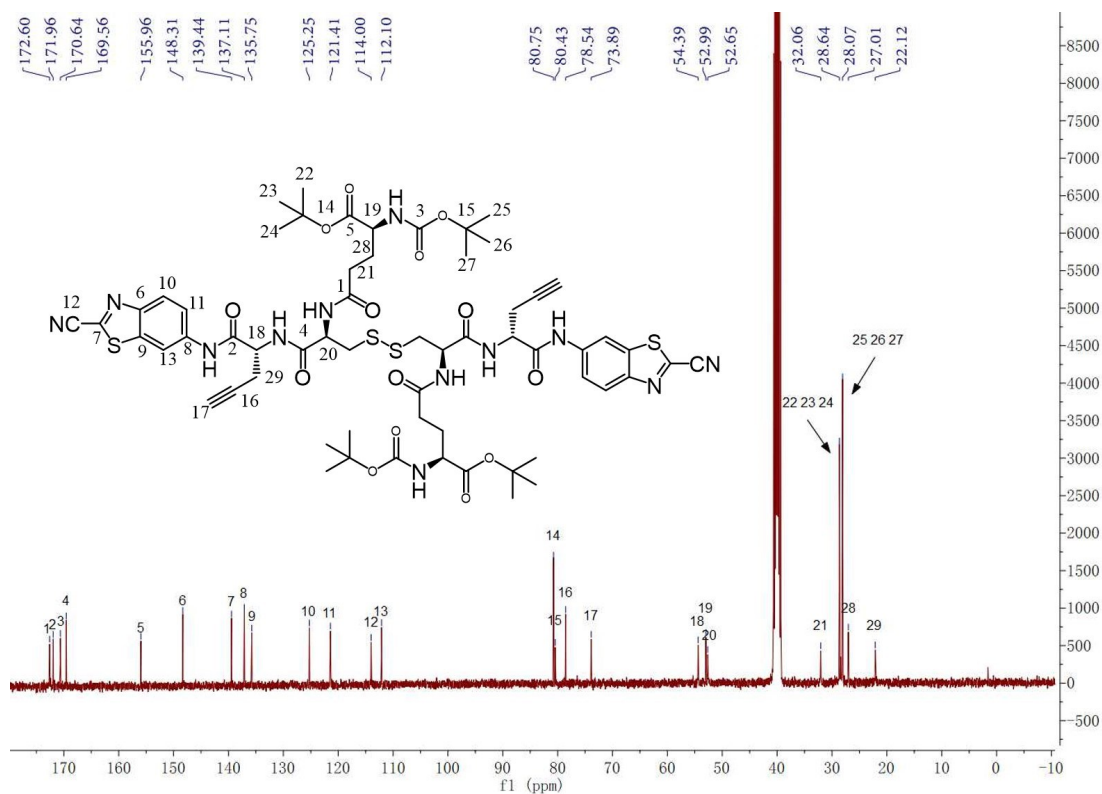


Fig. S16. ¹³C NMR spectrum of compound 4.

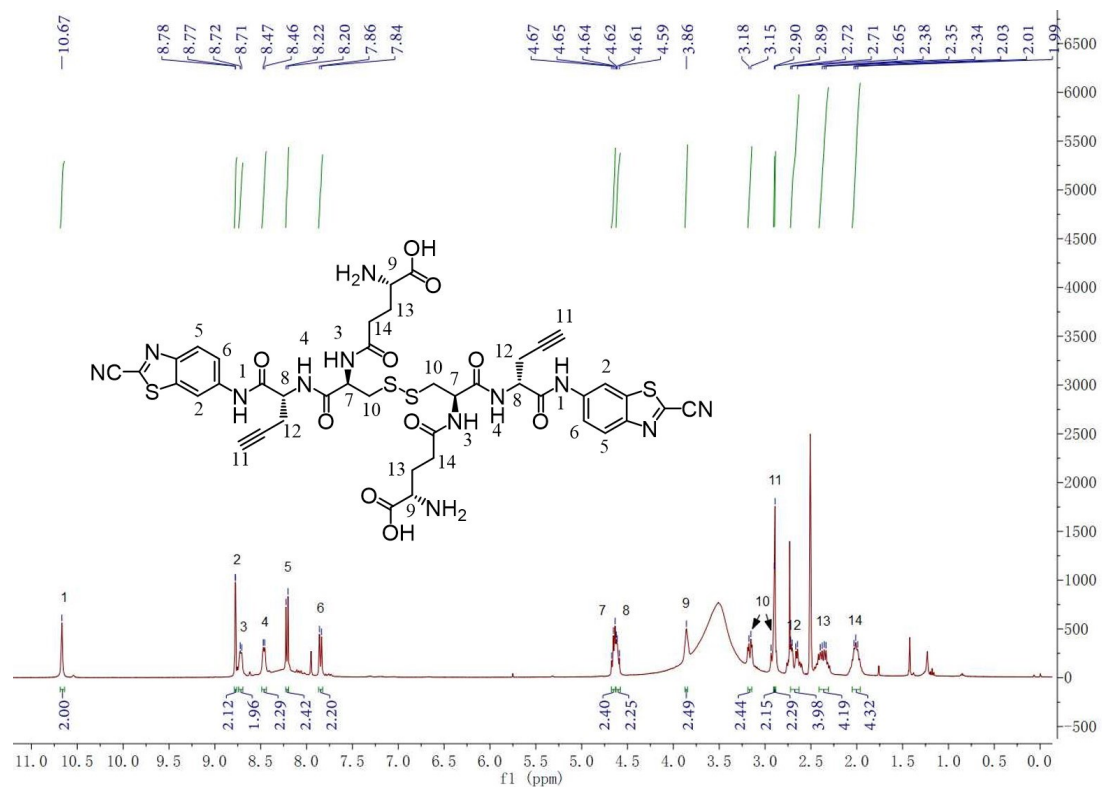


Fig. S17. ¹H NMR spectrum of compound 5.

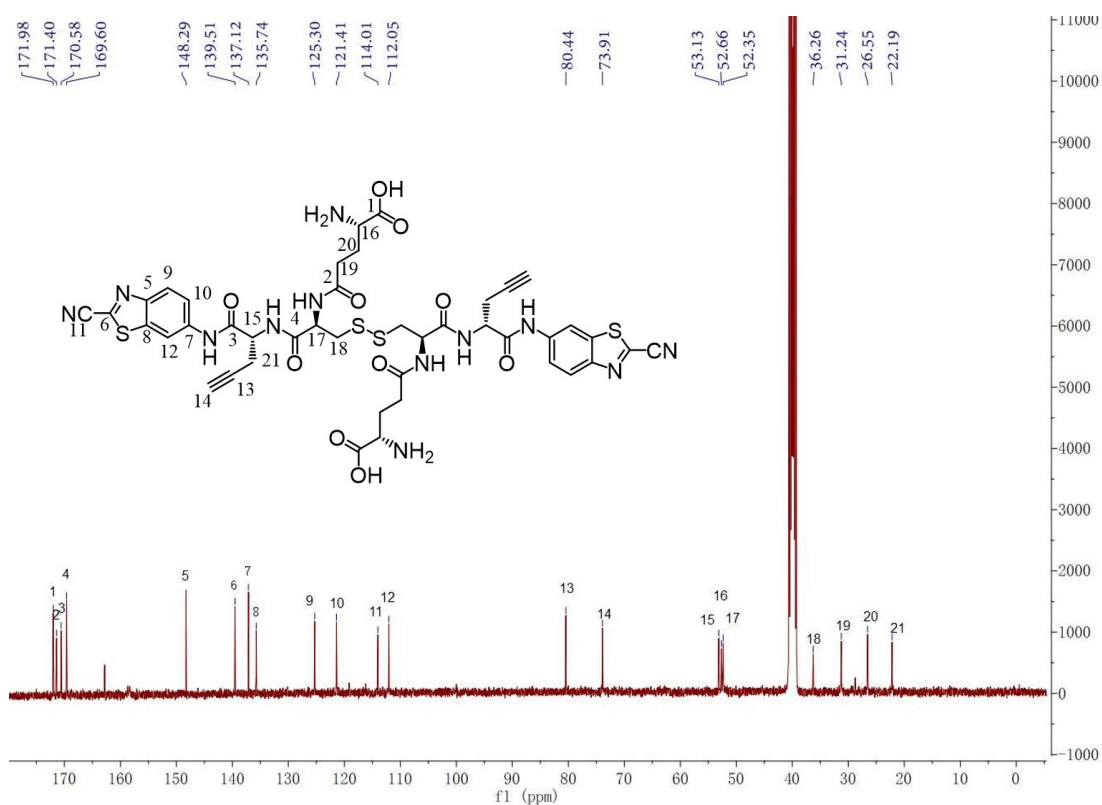


Fig. S18. ^{13}C NMR spectrum of compound 5.

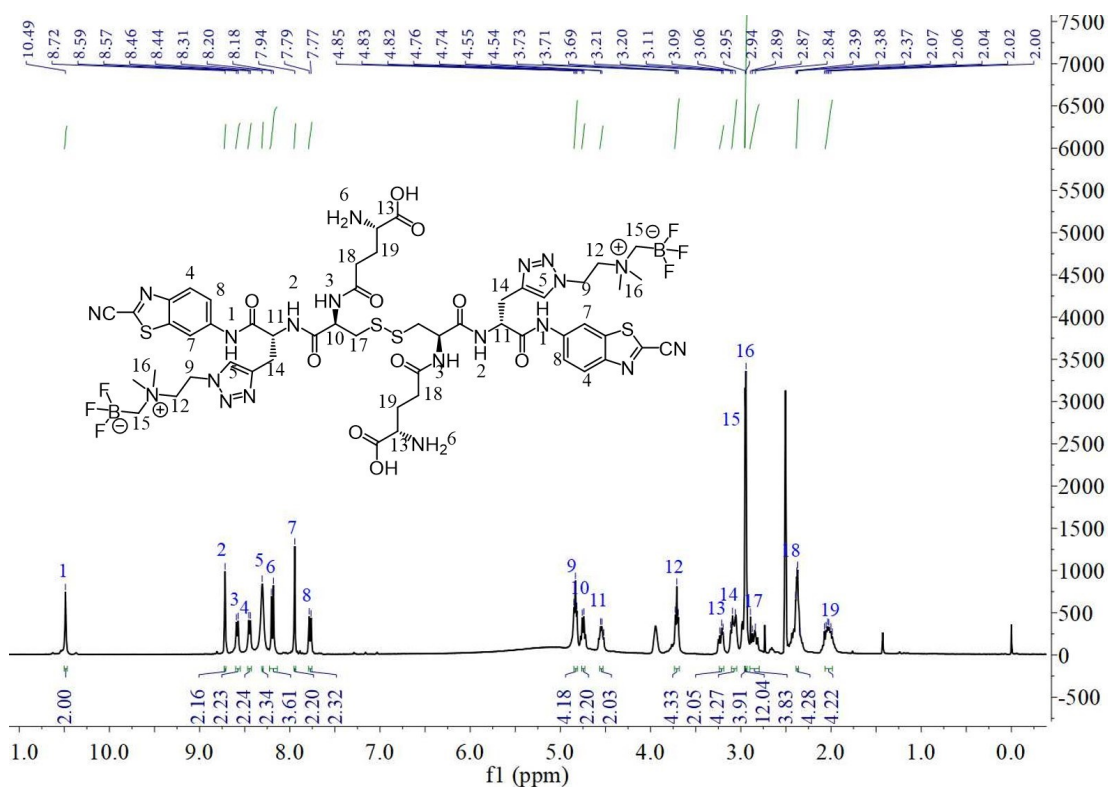


Fig. S19. ^1H NMR spectrum of non-radioactive probe $(\text{GCPA})_2$.

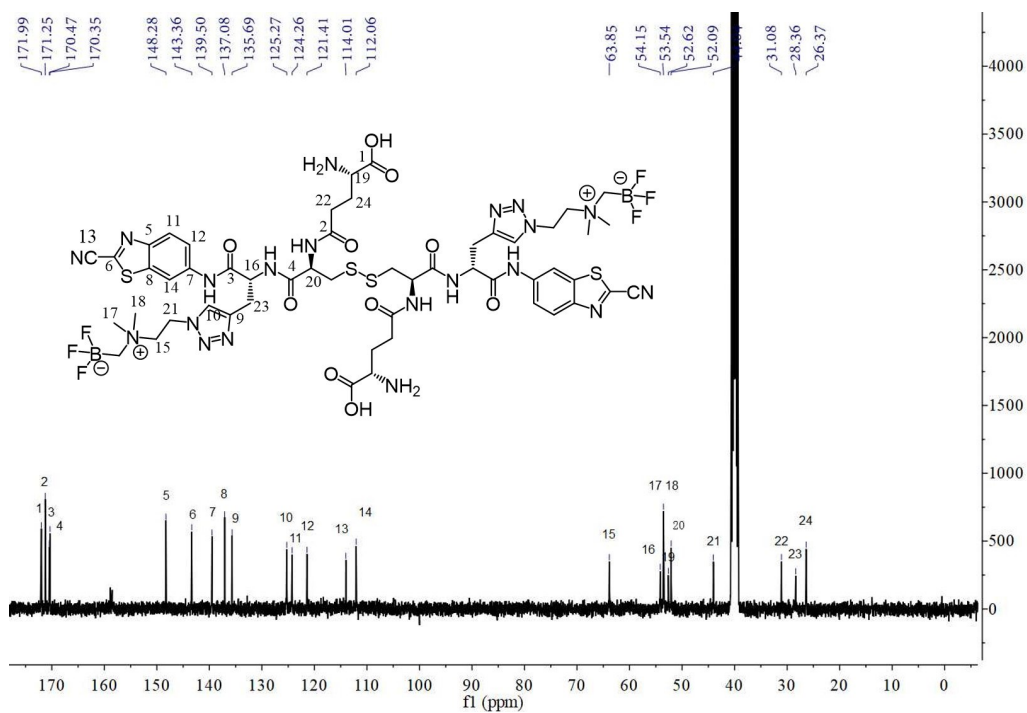


Fig. S20. ¹³C NMR spectrum of non-radioactive probe (GCPA)₂.

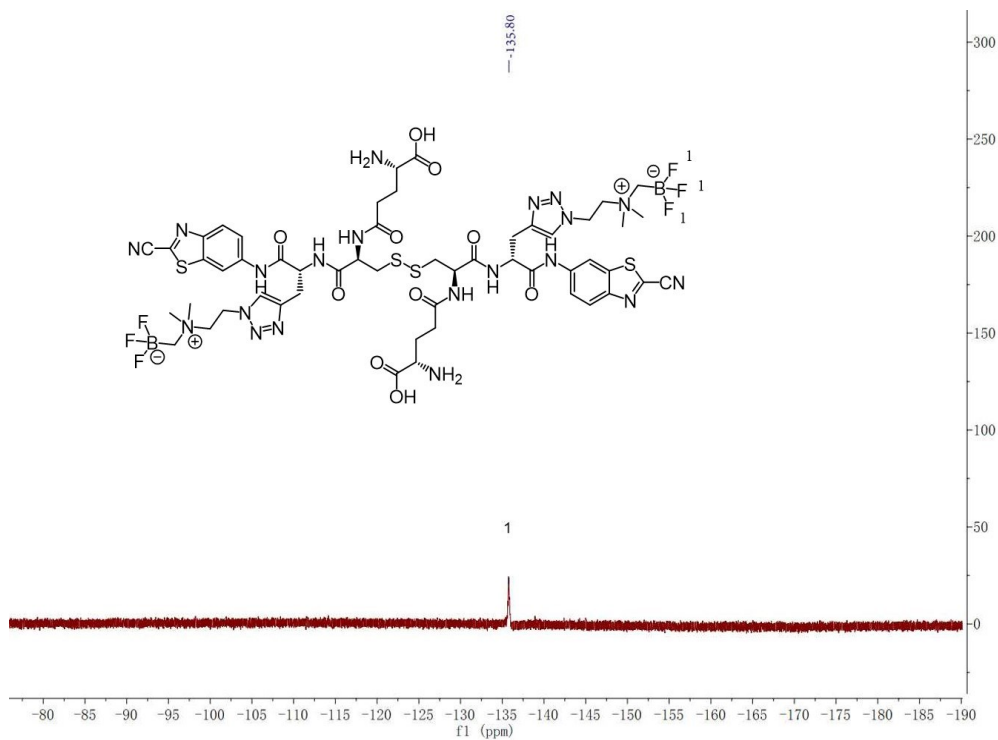


Fig. S21. ¹⁹F NMR spectrum of non-radioactive probe (GCPA)₂.

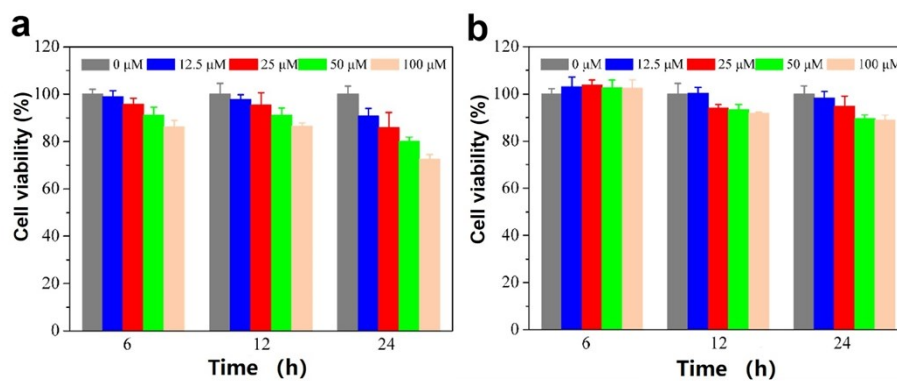


Fig. S22. Cytotoxicity assay of non-radioactive probe (GCPA)₂ against (a) L929 and (b) HCT116 at different concentrations (0.0, 12.5, 25.0, 50.0 and 100.0 μM) after incubated for 6, 12, and 24 h.

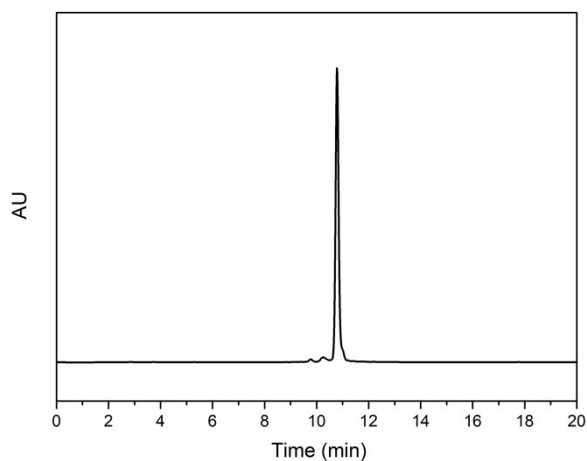


Fig. S23. HPLC trace of GGT cleavage product C1.

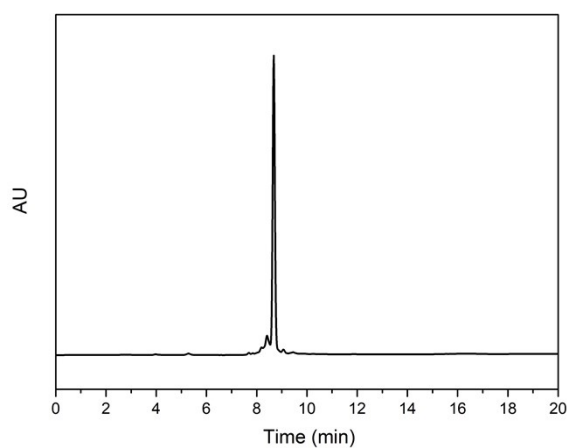


Fig. S24. HPLC trace of GGT cleavage product C2.

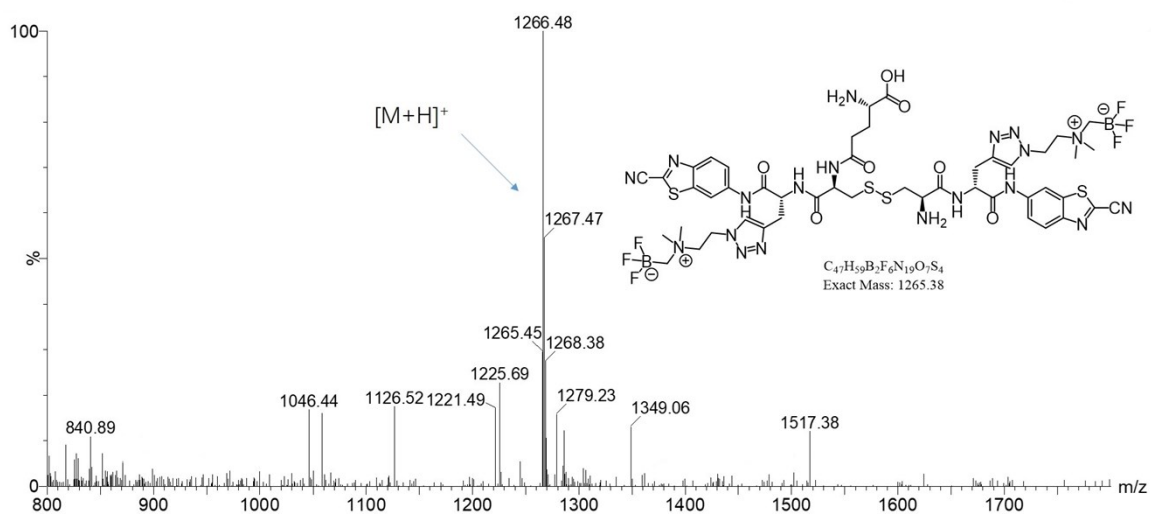


Fig. S25. ESI-MS analysis of GGT cleavage product C1.

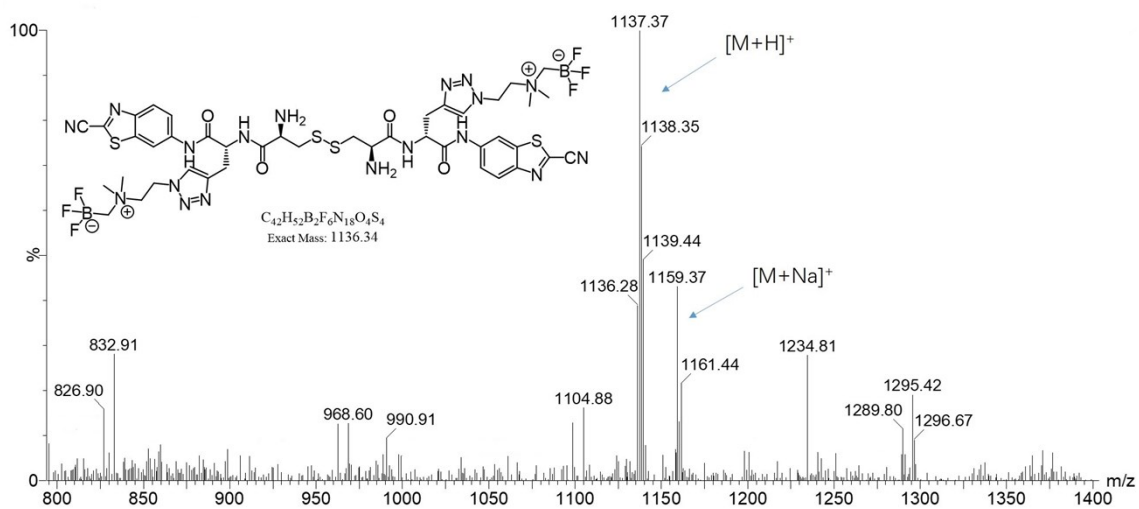


Fig. S26. ESI-MS analysis of GGT cleavage product C2.

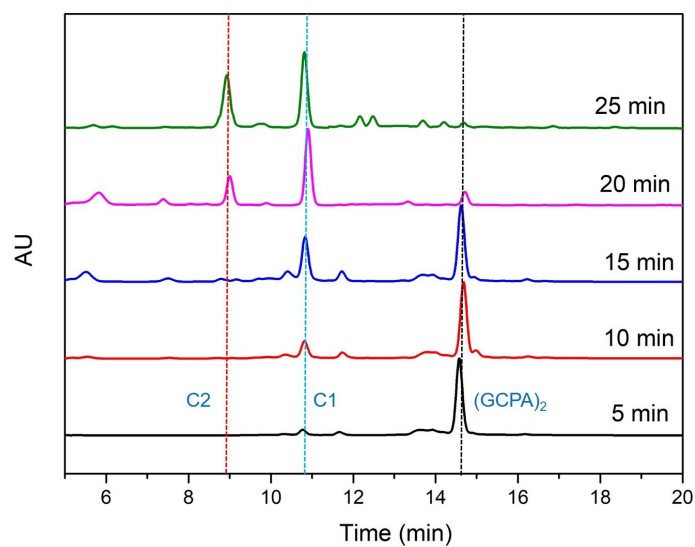


Fig. S27. Time-course of $(CGPA)_2$, C1 and C2 signal as $(GCPA)_2$ incubated with GGT from 5 to 25 min.

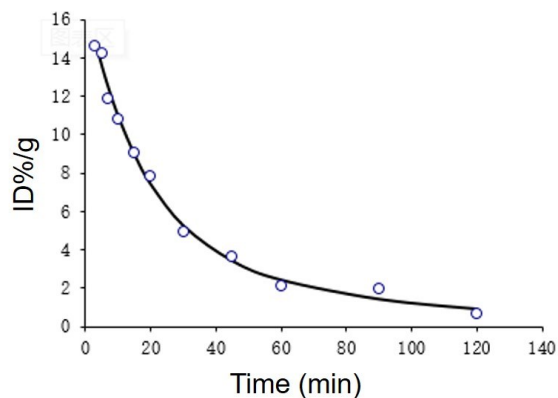


Fig. S28. Correlation between the blood radioactivity and time for the probe ($[^{18}\text{F}]\text{GCPA}$)₂.

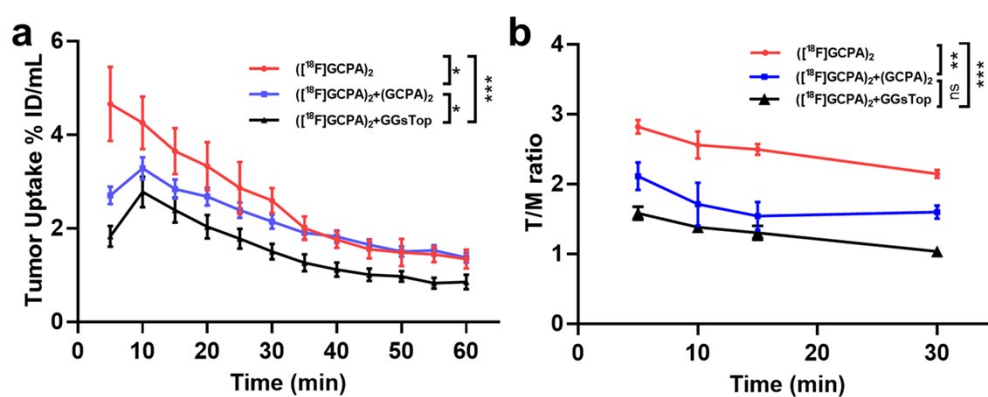


Fig. S29. Statistical analysis of tumor uptake (a) and T/M ratios (b) between different treatment groups. (* $P < 0.05$, ** $P < 0.01$, *** $P < 0.001$)