

Supporting online material for

An ^{18}F -Alanine Derivative Serves as An ASCT2 Marker for Cancer Imaging

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Fig. S10. Competitive inhibition of BGC-823 cell uptake of ^{18}F -Ala-BF₃.

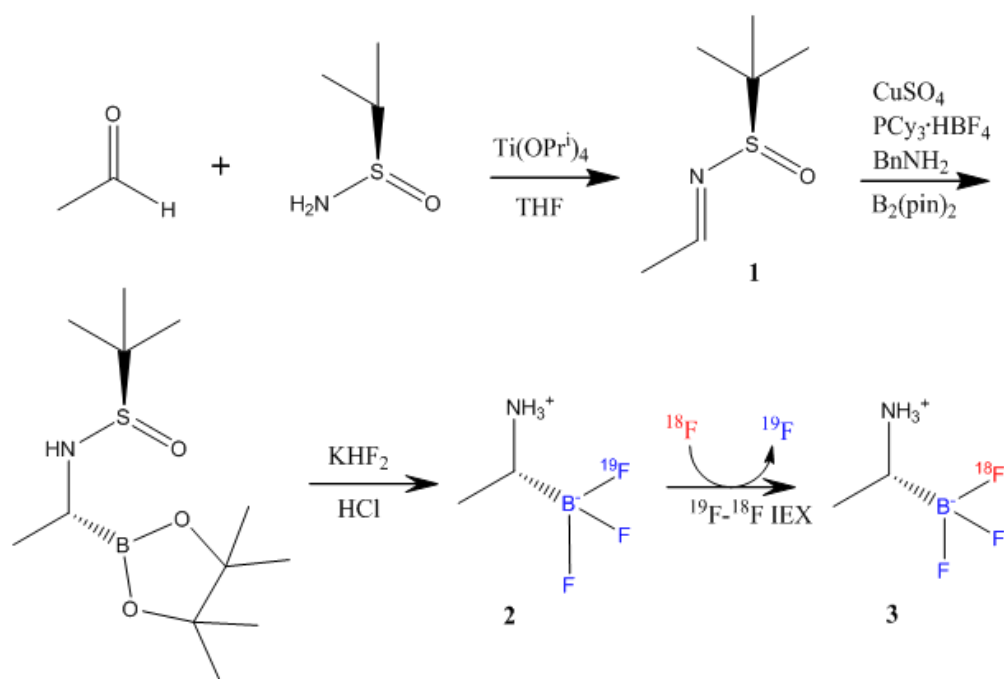


Figure S1. Synthetic route of Ala-BF₃ and radiolabeling reaction.

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Supervisor Liuzhibo

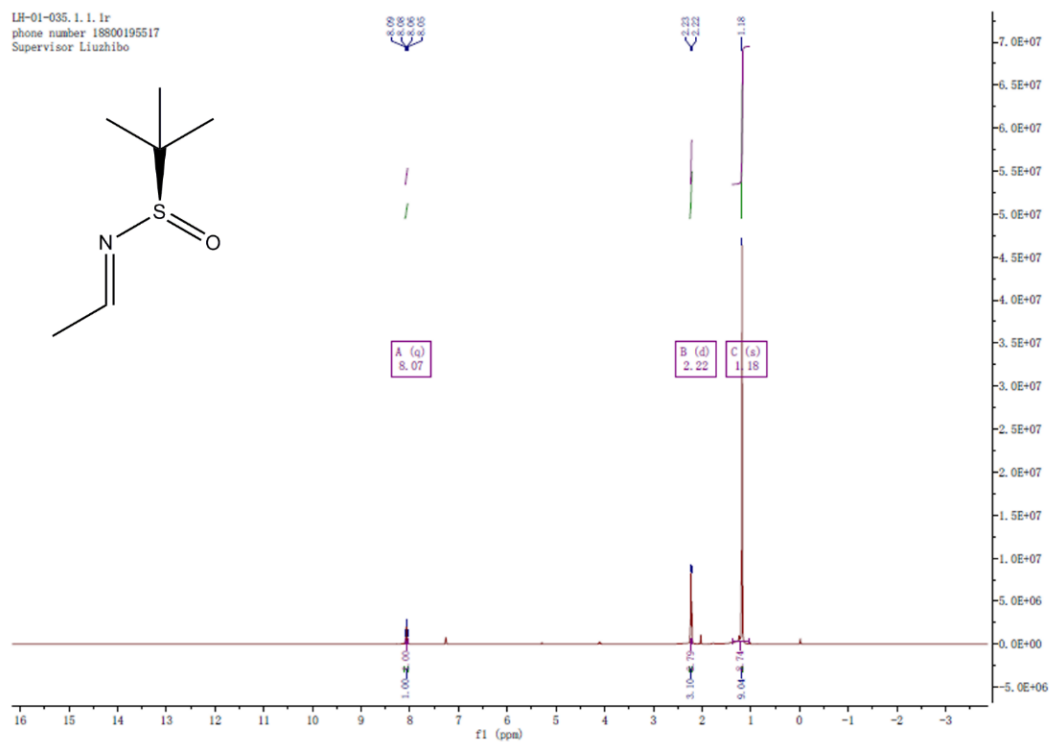


Figure S2. ¹H NMR spectrum of Ala-BF₃ precursor (compound 1).

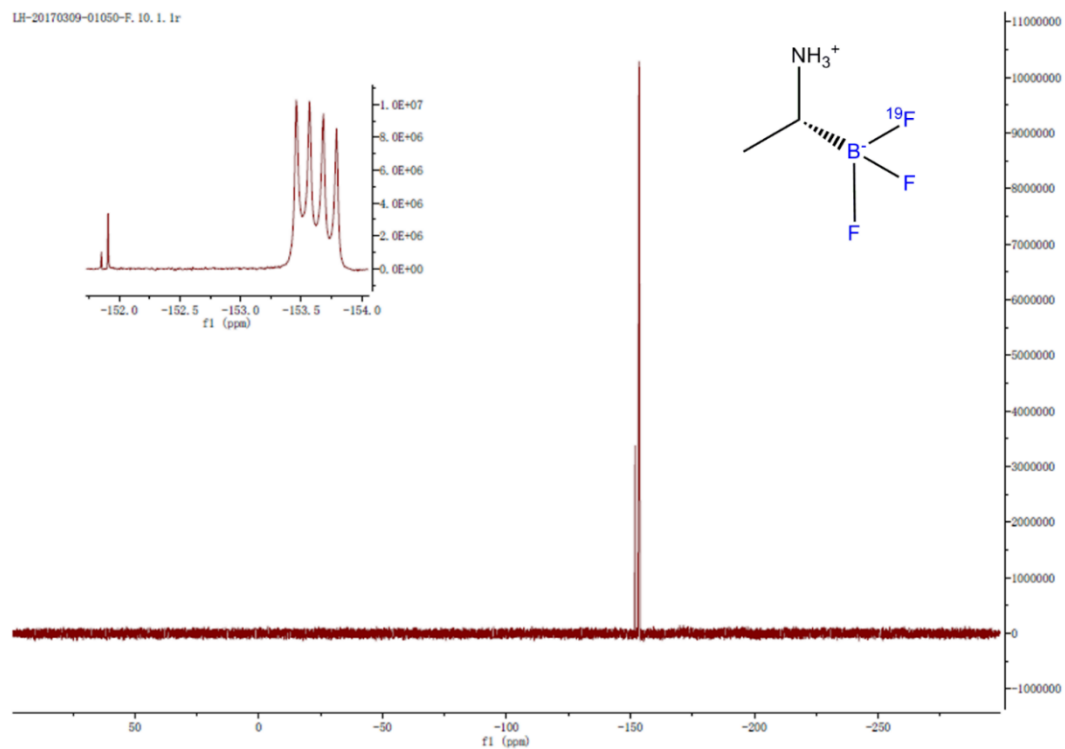


Figure S3. ^{19}F NMR spectrum of HPLC-purified Ala- BF_3 ($\delta = -153.58$ ppm).

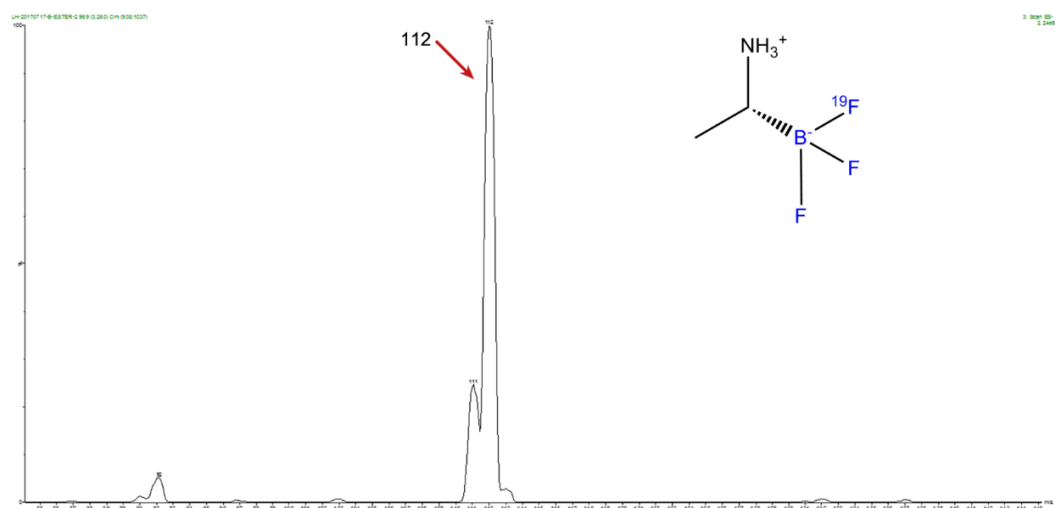


Figure S4. The LC-MS spectrum of HPLC-purified Ala-BF₃.

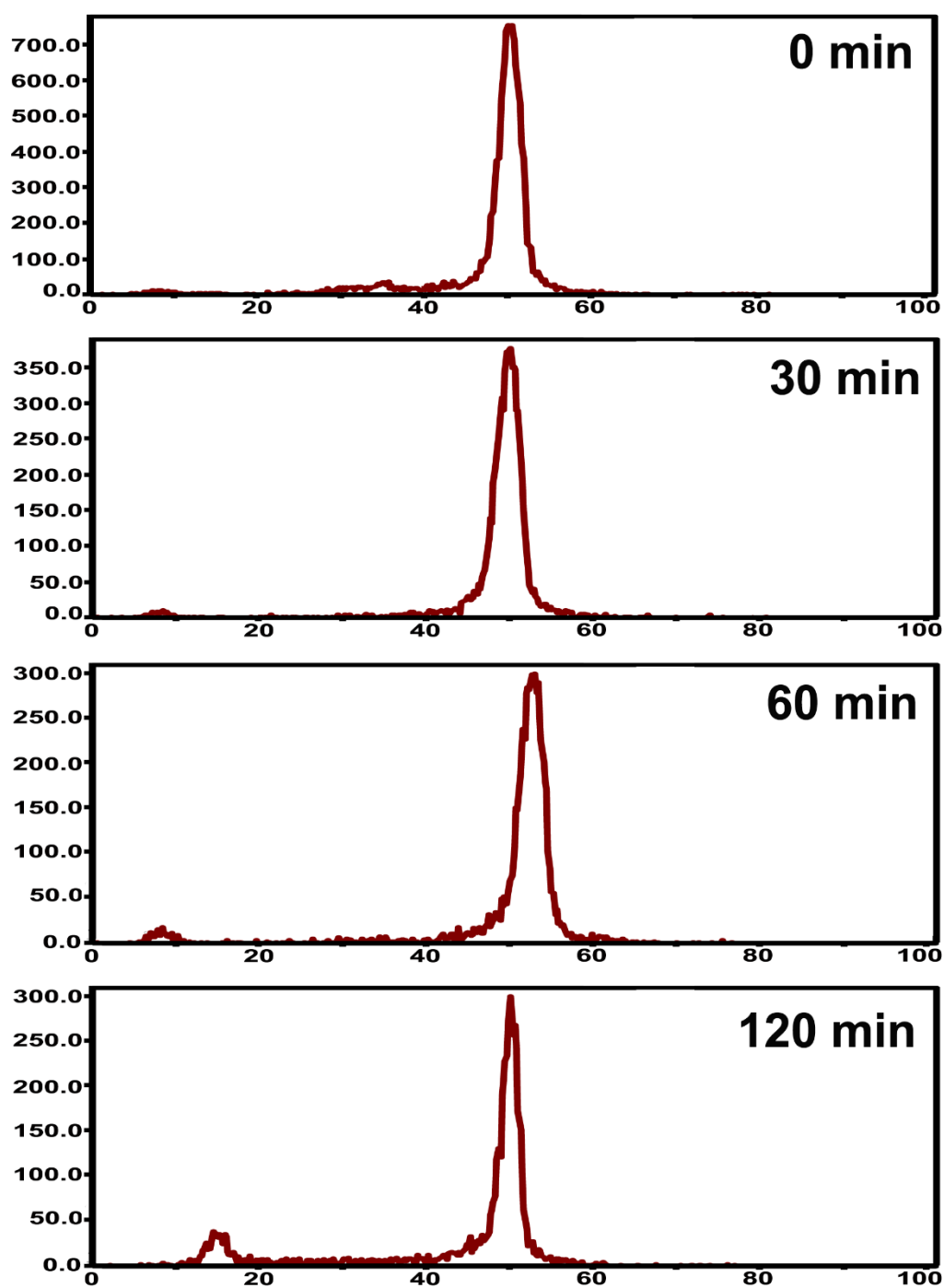


Figure S5. *In vitro* stability assay of ^{18}F -Ala- BF_3 in PBS. Radioactive TLC chromatography of Ala- BF_3 after incubation in PBS at 37 °C for 0, 30, 60 and 120 min, respectively. As presented, less than 5% of defluorination was found within 120 min, validating minor defluorination *in vitro*.

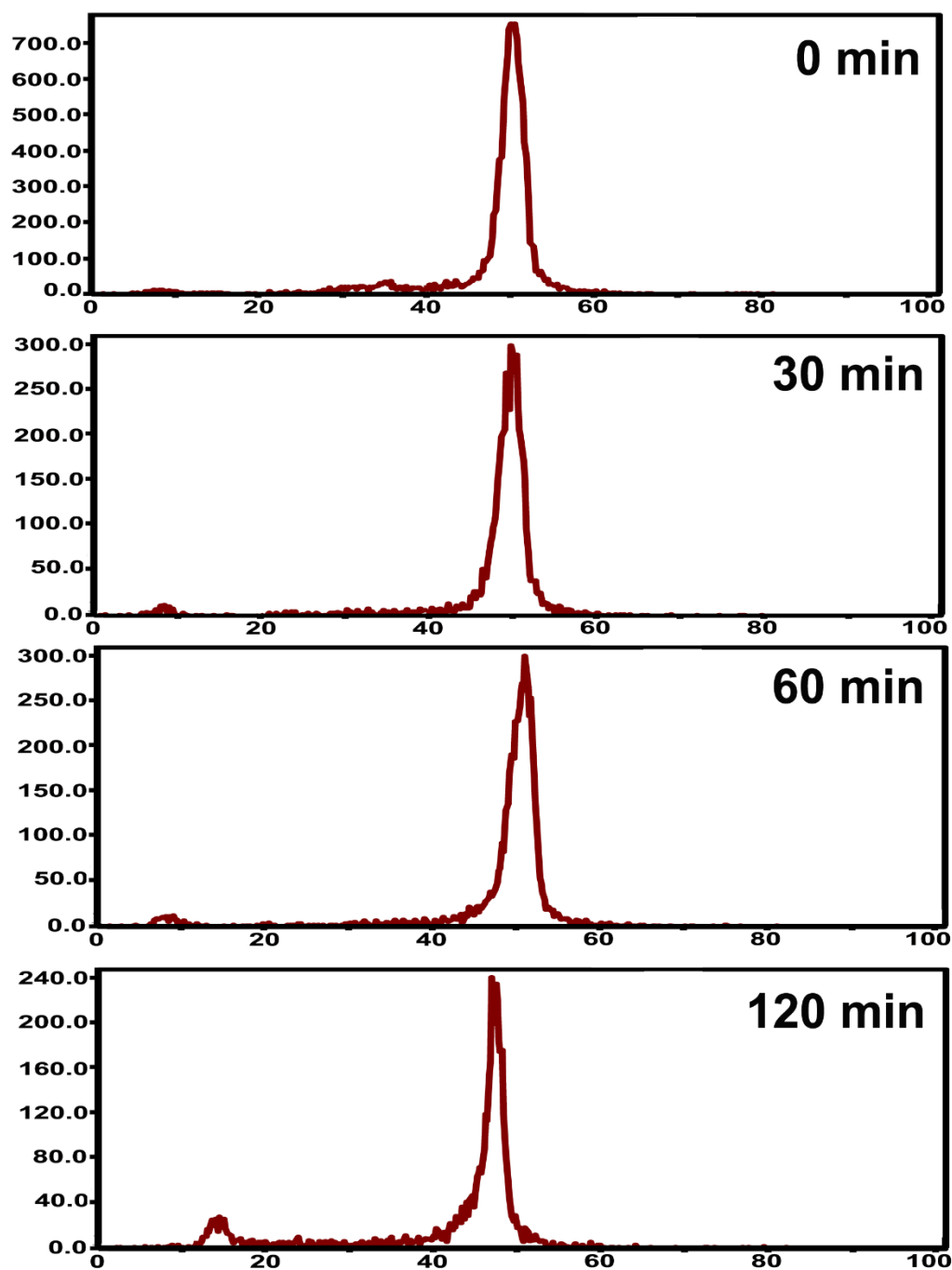


Figure S6. *In vitro* stability assay of ^{18}F -Ala- BF_3 in FBS. Radioactive TLC chromatography of Ala- BF_3 after incubation in FBS at 37 °C for 0, 30, 60 and 120 min, respectively. As presented above, no more than 5% defluorination was observed within 120 min, validating that ^{18}F -Ala- BF_3 exhibited good stability in FBS .

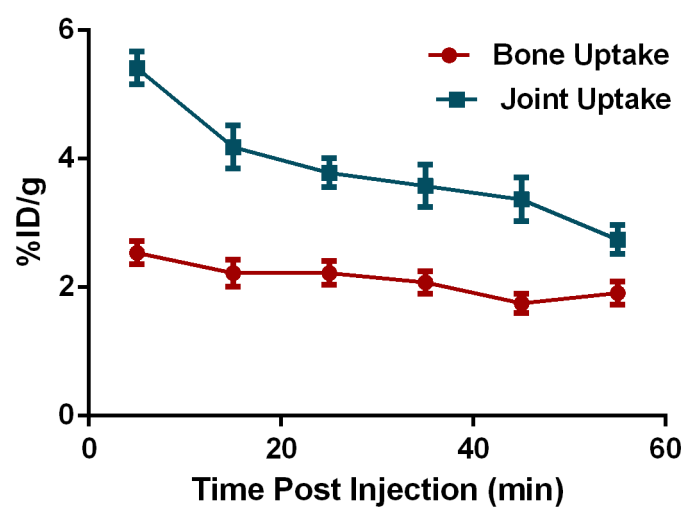


Figure S7. Time–activity curves of bone and joint from female Nu/Nu mice bearing BGC-823 xenografts. The data are from 10 min dynamic scans following intravenous injection of ^{18}F -Ala- BF_3 (200 μCi /mouse).

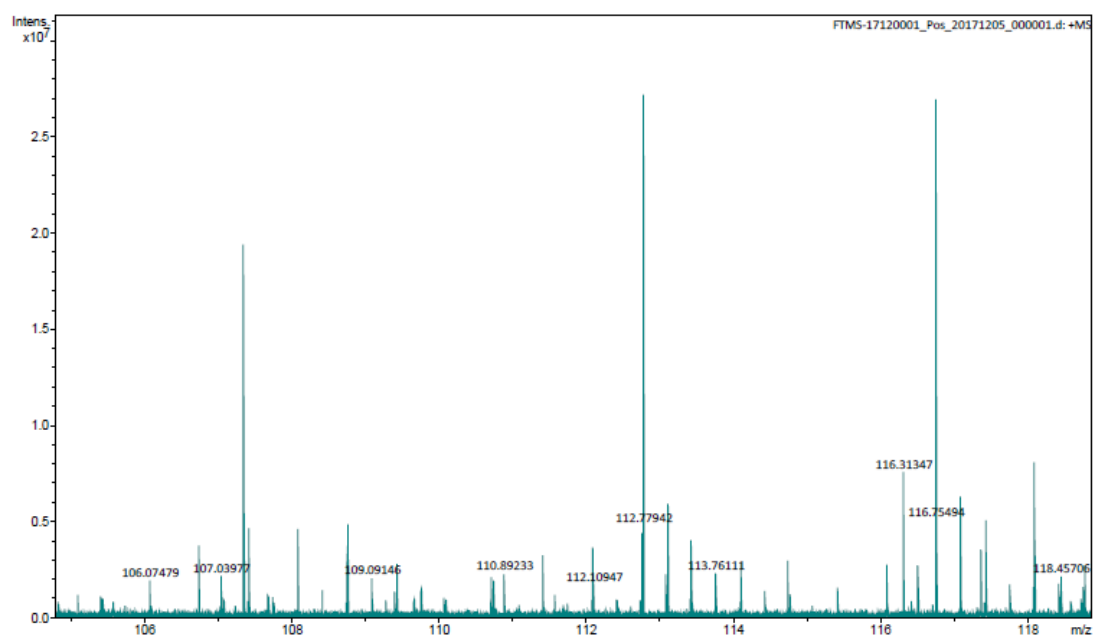


Figure S8. High-resolution mass spectrum (HRMS) of Ala-BF₃.

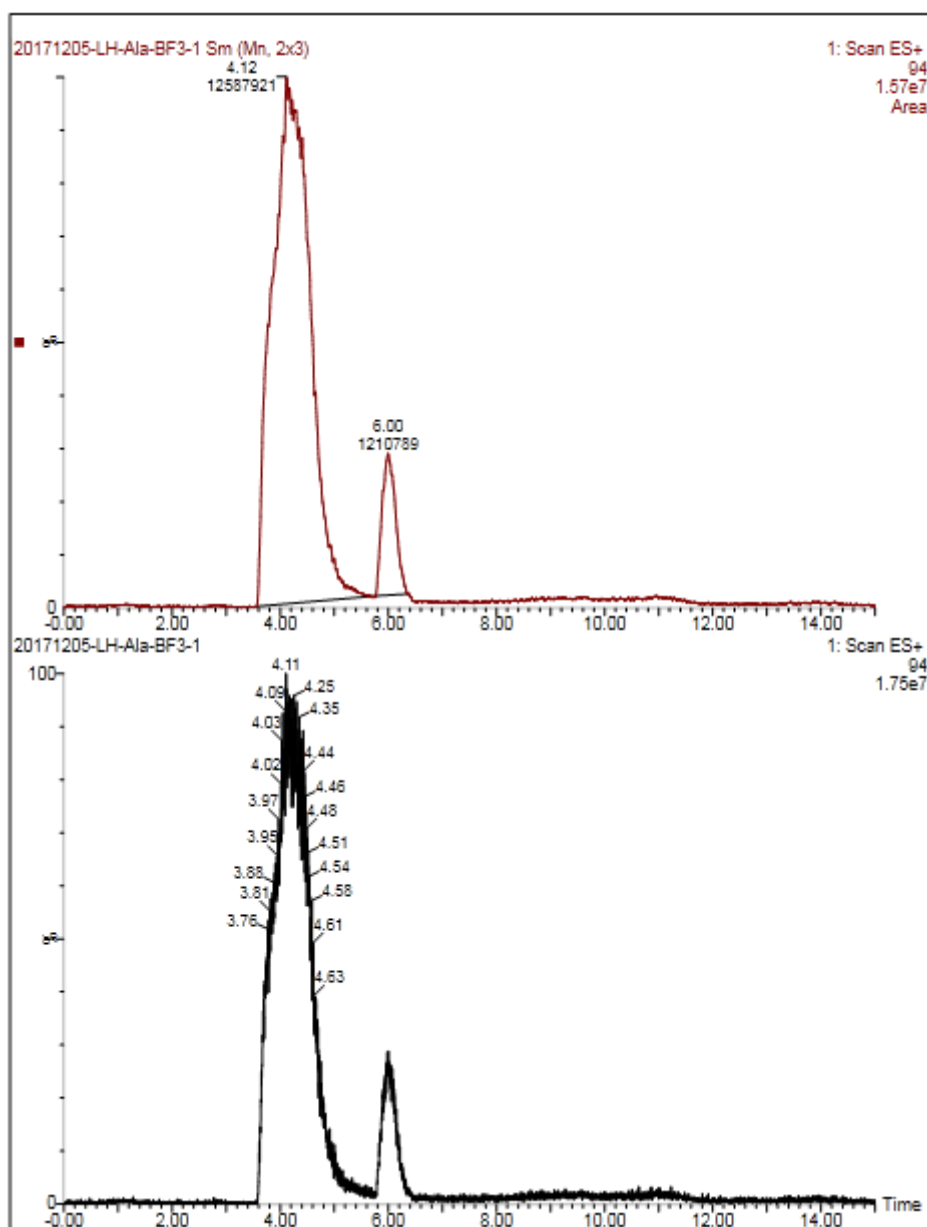


Figure S9. HPLC analysis of enantiomeric purity of L-isomer of Ala-BF₃. Enantiomeric purity of each compound was analyzed on a CROWNPAK column using an elution solution of Acetonitrile:water = 95:5 at a flow rate of 0.2 ml/min.

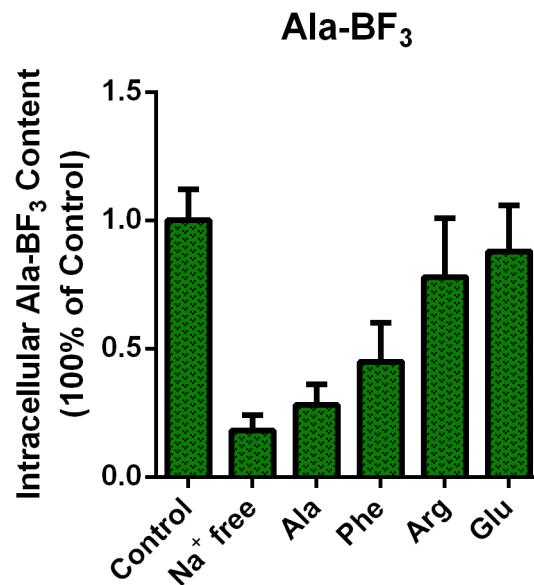


Figure S10. Competitive inhibition of BGC-823 cell uptake of ¹⁸F- Ala-BF₃. Cells are incubated in sodium-free phosphate-buffered saline (PBS) buffer or co-incubated with other AAs at 25 mM for 50 min. As shown, the entry of ¹⁸F- Ala-BF₃ is channel-specific and can be inhibited efficiently by the natural Alanine .