

**Supporting Information for**  
**A Metabolically Stable Boron-derived Tyrosine Serves as A**  
**Theranostic Agent for Positron Emission Tomography Guided**  
**Boron Neutron Capture Therapy**

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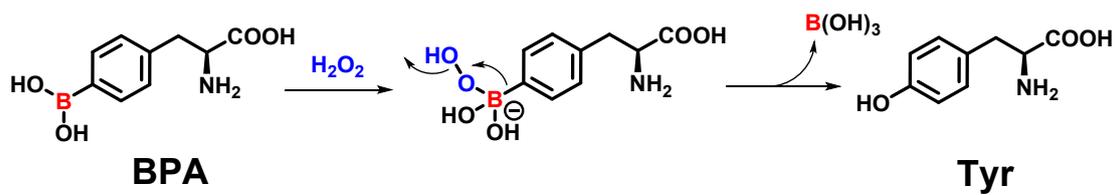
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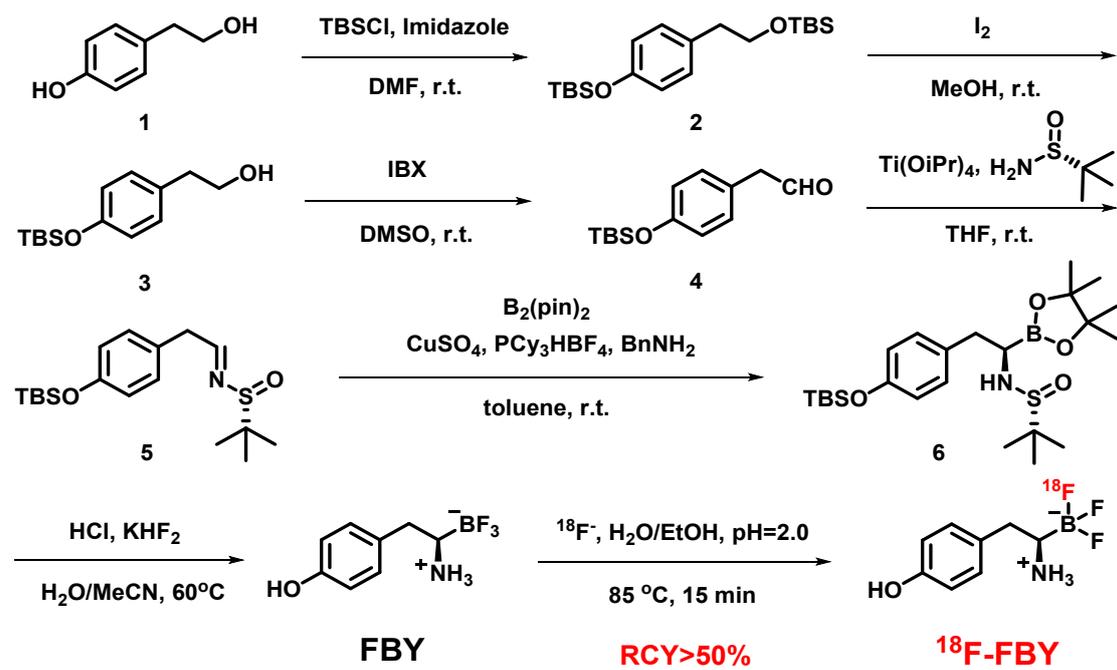
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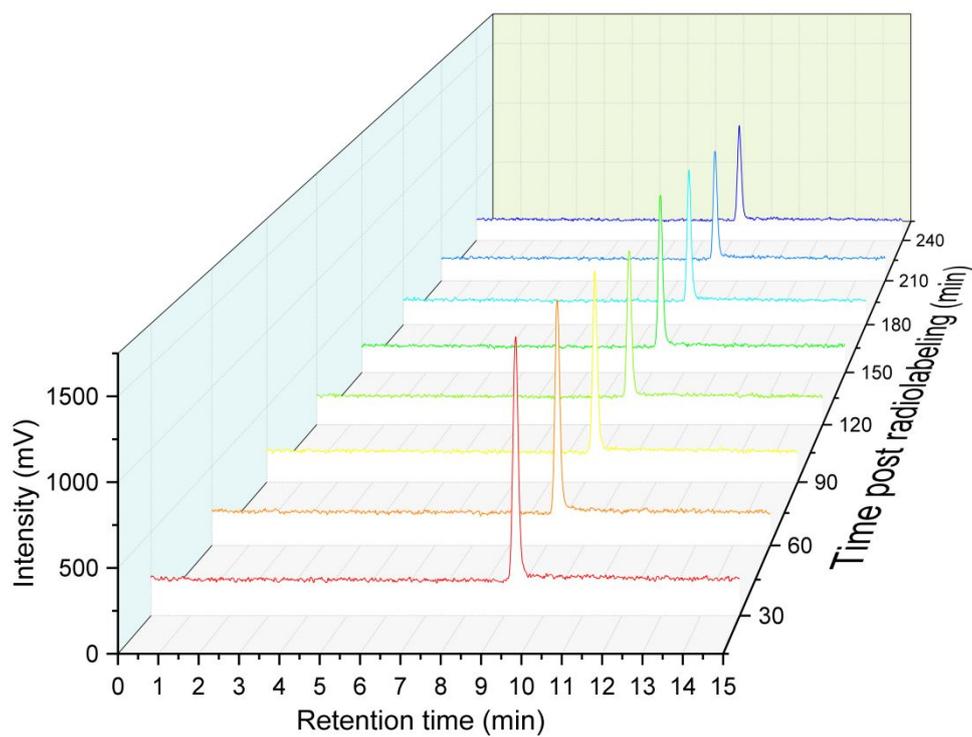
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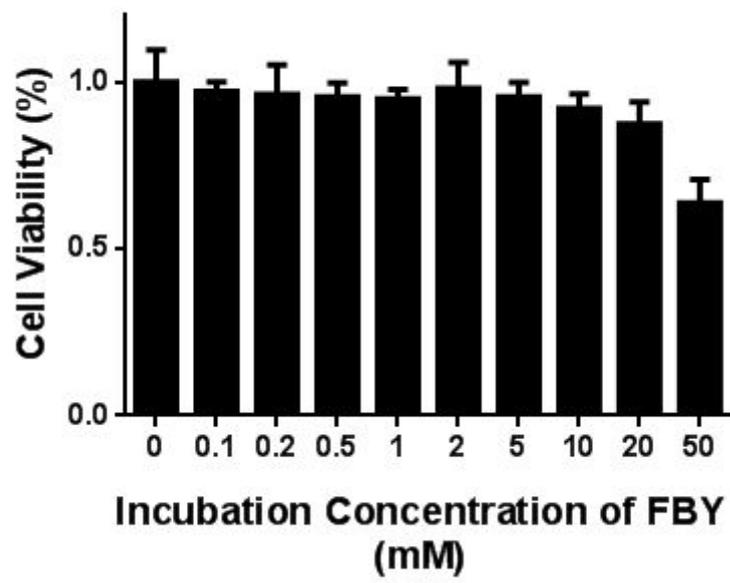
**Scheme S1:** H<sub>2</sub>O<sub>2</sub> mediated deboronation of phenylboronic acid.



**Scheme S2:** Chemical synthesis and radiolabeling of FBY.



**Figure S1:** An example set of Radio-HPLC chromatograms of [ $^{18}\text{F}$ ]FBY incubated in PBS from a series of time points. No peak of free fluorine anion (0-5 min) observed.



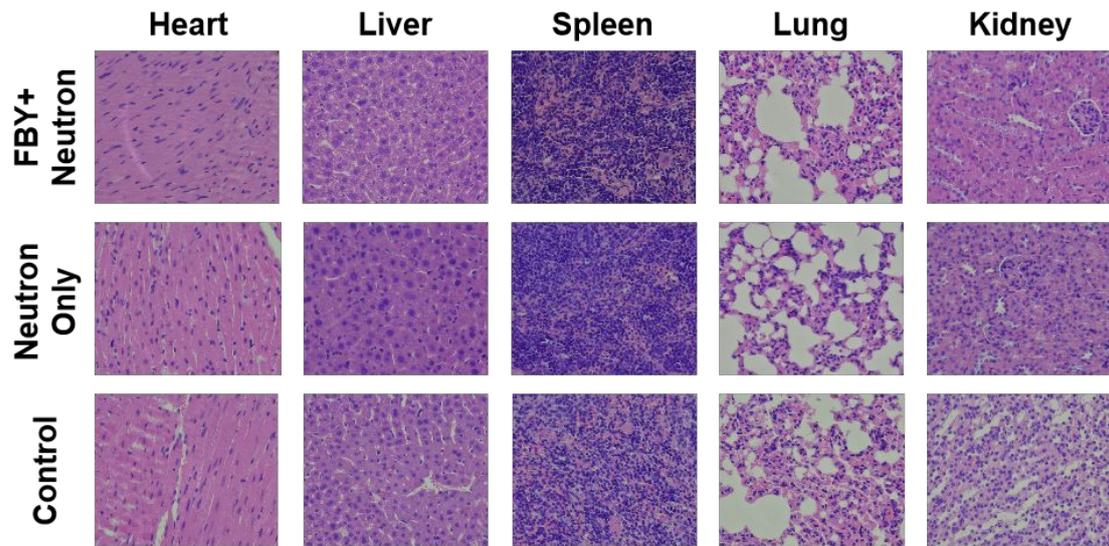
**Figure S2:** Cell viability of B16-F10 cells treated with series concentrations of FBY.



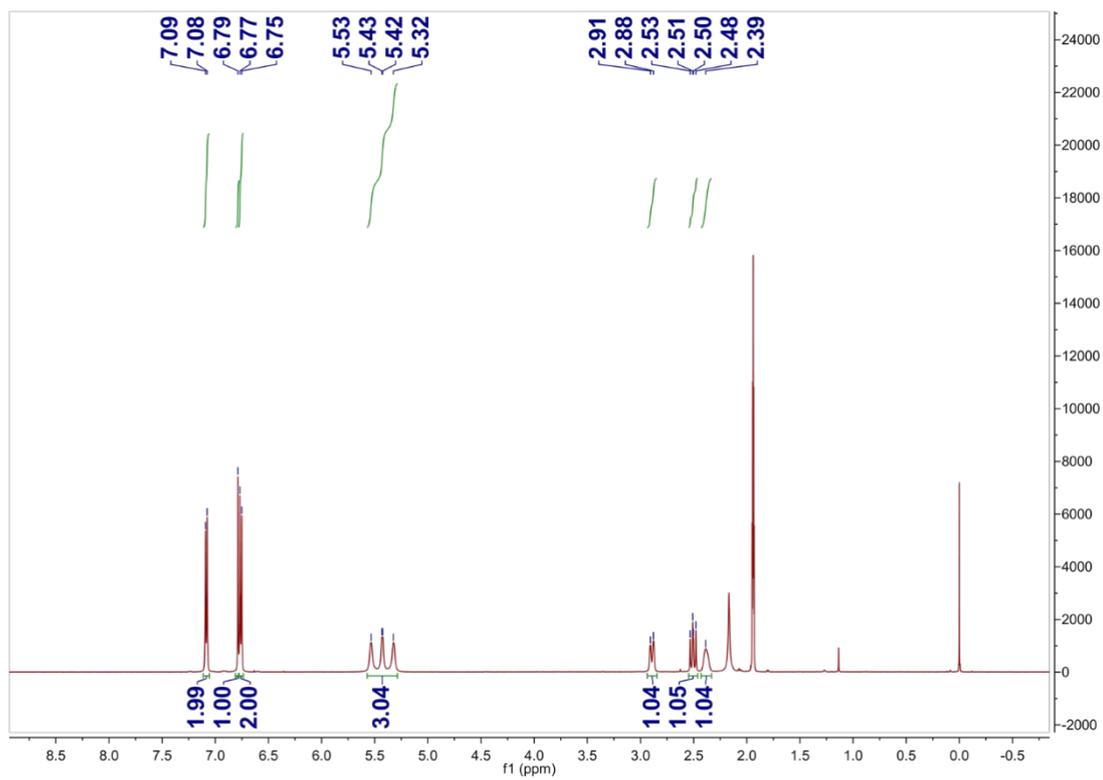
**Figure S3:** Whole-body maximum intensity projection PET images of a B16-F10 tumor-bearing mouse. Tumor (t) was indicated by white arrows.



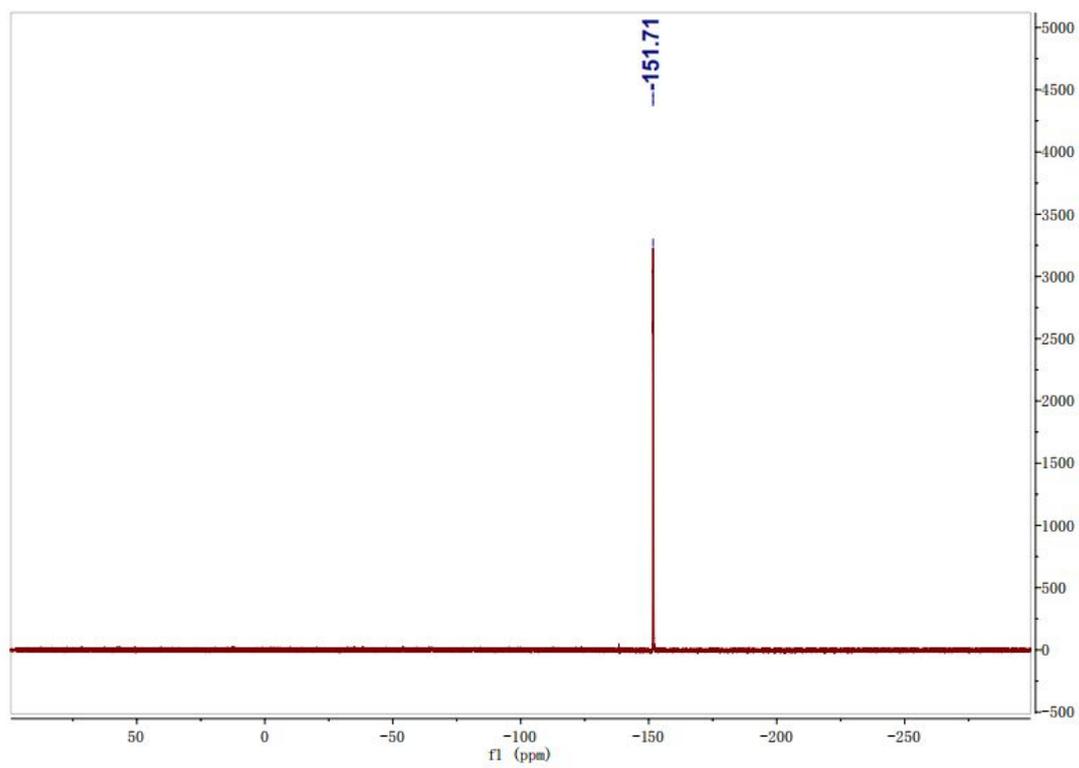
**Figure S4:** Schematic representation of the timeline of the experimental period.



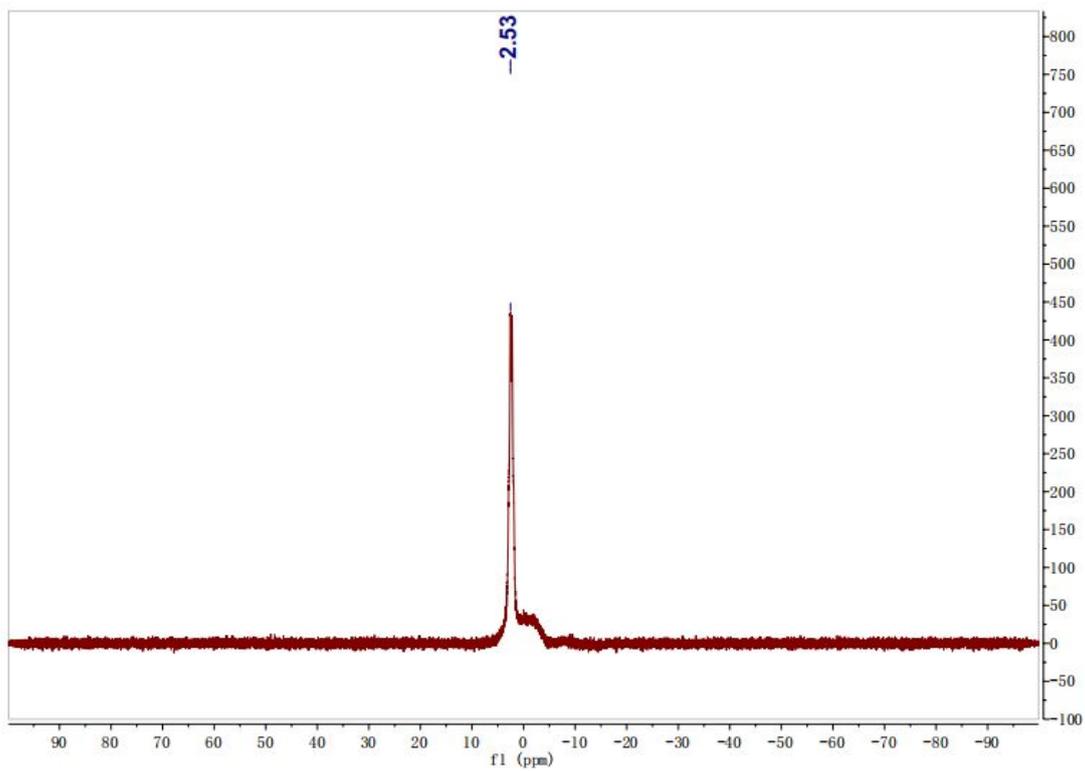
**Figure S5:** Representative histological H&E staining of major organ tissues from the FBY-BNCT group, thermal neutron irradiation only group and control group.



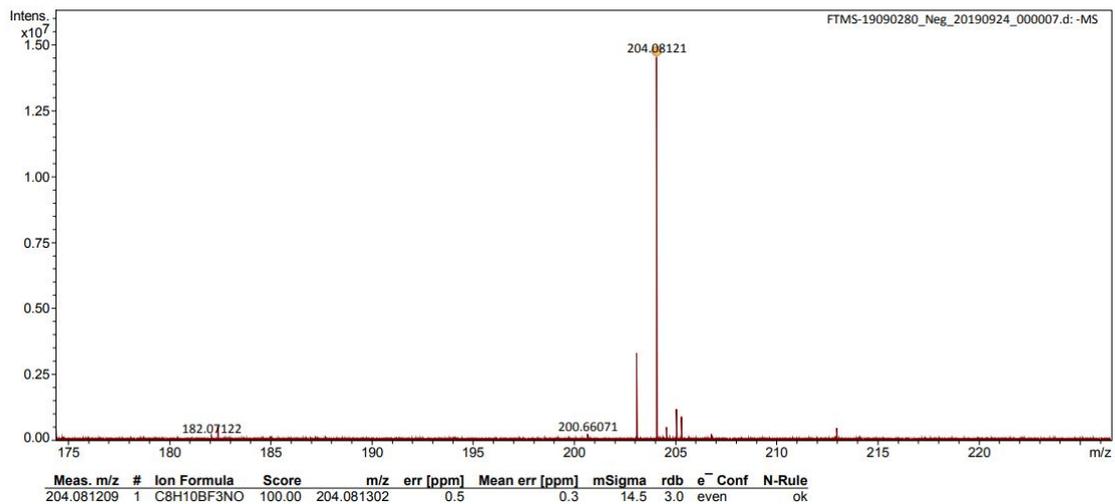
**Figure S6:** <sup>1</sup>H NMR spectrum of HPLC-purified FBY.



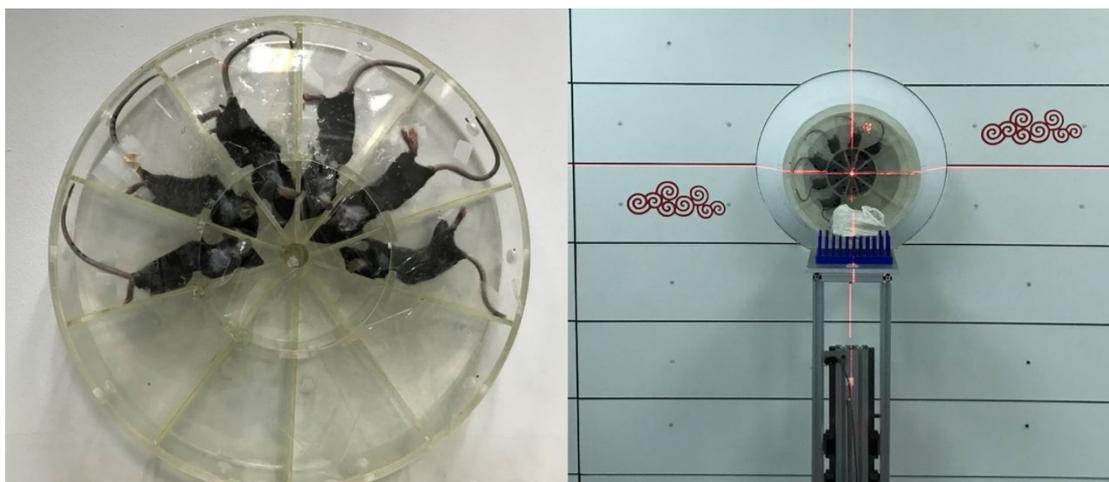
**Figure S7:**  $^{19}\text{F}$ NMR spectrum of HPLC-purified FBY.



**Figure S8:**  $^{11}\text{B}$ NMR spectrum of HPLC-purified FBY.



**Figure S9:** High resolution MS spectrum of HPLC-purified FBY.



**Figure S10:** Photos of the special-made model to fix the mice during irradiation.

<b>Organs</b>	<b>Mean(%ID/g)</b>	<b>SD(%ID/g)</b>
<b>Blood</b>	<b>0.98</b>	<b>0.14</b>
<b>Pancreas</b>	<b>2.28</b>	<b>0.25</b>
<b>Spleen</b>	<b>1.36</b>	<b>0.13</b>
<b>Intestine/s</b>	<b>1.32</b>	<b>0.11</b>
<b>Intestine/l</b>	<b>1.38</b>	<b>0.24</b>
<b>Fat</b>	<b>0.36</b>	<b>0.13</b>
<b>Liver</b>	<b>1.44</b>	<b>0.15</b>
<b>Stomach</b>	<b>0.90</b>	<b>0.11</b>
<b>Heart</b>	<b>0.94</b>	<b>0.16</b>
<b>Lung</b>	<b>0.74</b>	<b>0.08</b>
<b>Muscle</b>	<b>0.97</b>	<b>0.07</b>
<b>Bone</b>	<b>0.48</b>	<b>0.09</b>
<b>Brain</b>	<b>0.21</b>	<b>0.01</b>
<b>Tumor</b>	<b>3.04</b>	<b>0.35</b>

**Table S1:** Biodistribution of [<sup>18</sup>F]FBY in B16-F10 tumor bearing mice at 75 minutes post injection (n= 4).

<b>Organs</b>	<b>Mean(%ID/g)</b>	<b>SD(%ID/g)</b>
<b>Muscle</b>	<b>2.57</b>	<b>0.28</b>
<b>Brain</b>	<b>0.50</b>	<b>0.04</b>
<b>Tumor</b>	<b>6.11</b>	<b>0.47</b>

**Table S2:** SUV profile of [<sup>18</sup>F]FBY (coinjection with 20 mg of FBY) in B16-F10 tumor bearing mice at 75 minutes post injection (n= 4).

<b>Organs</b>	<b>Mean(ppm)</b>	<b>SD(ppm)</b>
<b>Blood</b>	<b>9.03</b>	<b>1.21</b>
<b>Liver</b>	<b>14.87</b>	<b>1.62</b>
<b>Muscle</b>	<b>8.17</b>	<b>0.50</b>
<b>Brain</b>	<b>1.64</b>	<b>0.24</b>
<b>Tumor</b>	<b>19.59</b>	<b>0.47</b>

**Table S3:** Boron concentration of main organs of FBY (20 mg) in B16-F10 tumor bearing mice at 75 minutes post injection (n= 4).