

## Supporting Information

### Computational Studies and Synthesis of <sup>131</sup>Iodine-labeled Nocardiotide A analogs as a peptide-based theragnostic radiopharmaceutical ligand for cancer targeting SSTR2

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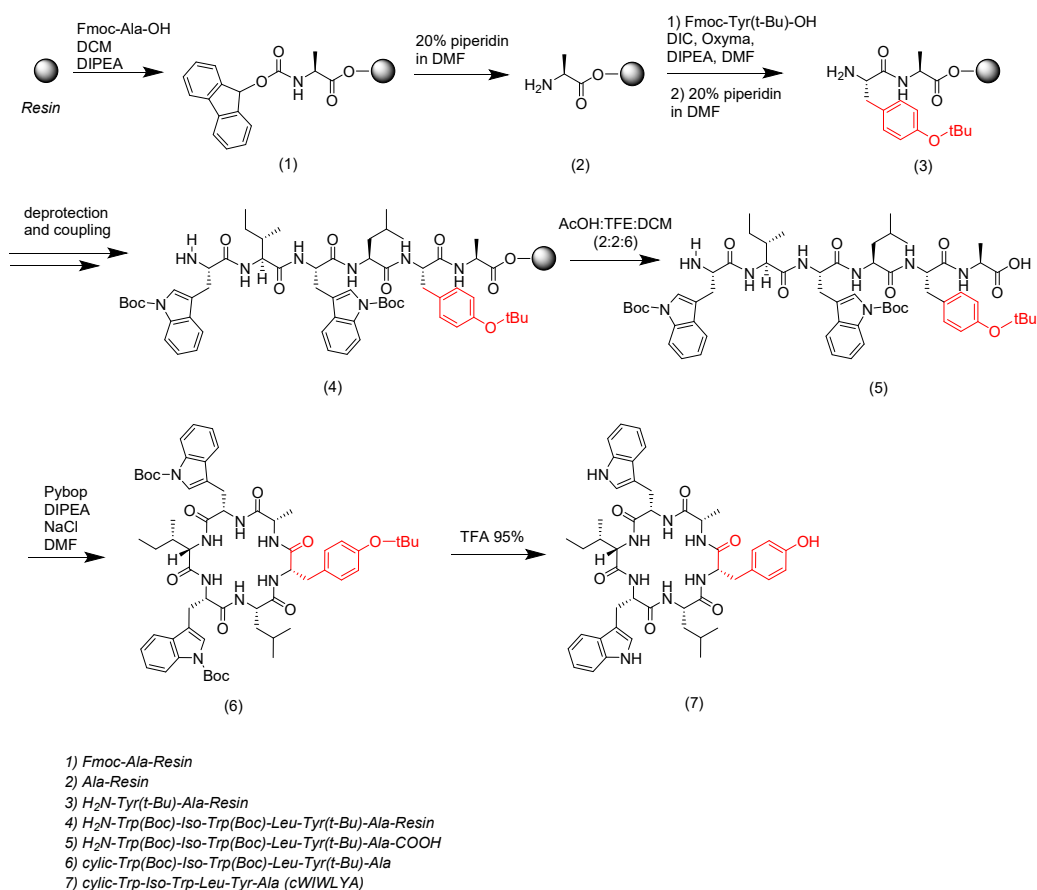


Figure S.1. Synthesis of cWIWLYA

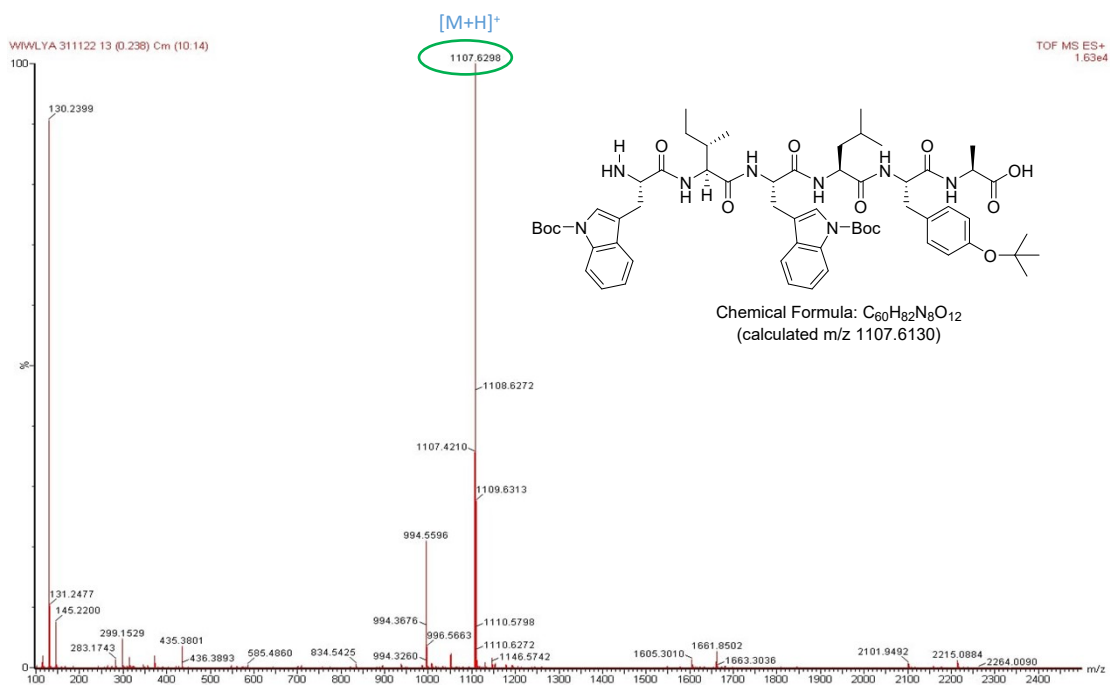


Figure S.2. Mass spectrum of protected linear WIWLYA [L-(NH<sub>2</sub>-Trp(Boc)-Ile-Trp(Boc)-Leu-Tyr(tBu)-Ala-COOH)]

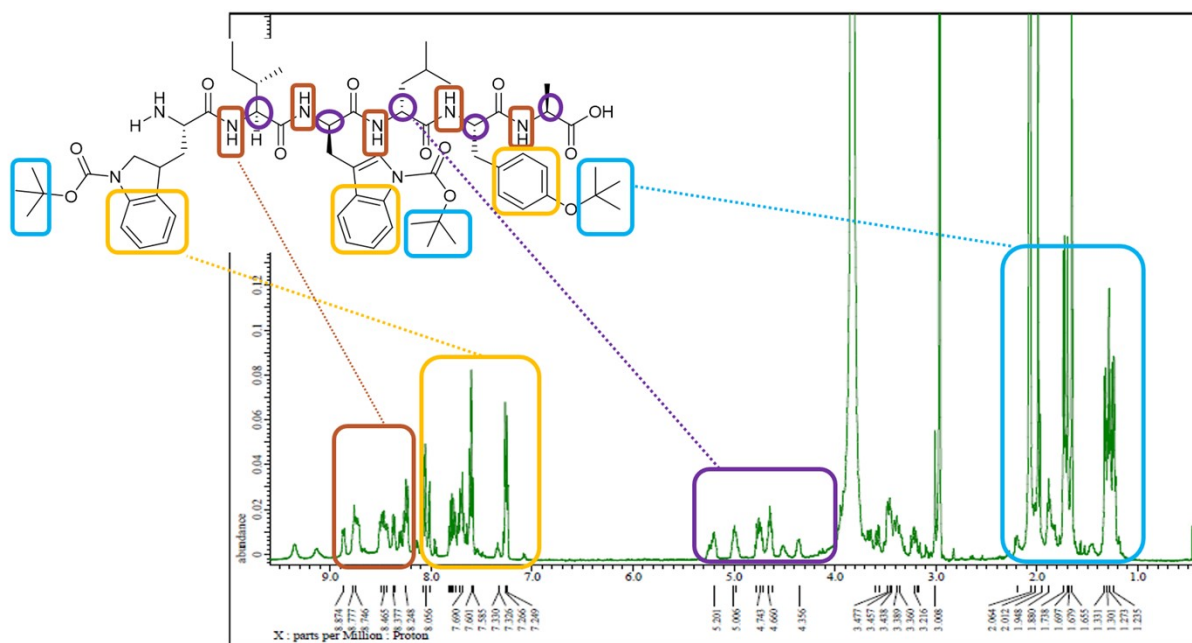


Figure S.3 <sup>1</sup>H-NMR spectrum of protected linear WIWLYA [L-(NH<sub>2</sub>-Trp(Boc)-Ile-Trp(Boc)-Leu-Tyr(tBu)-Ala-COOH)] (500 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)

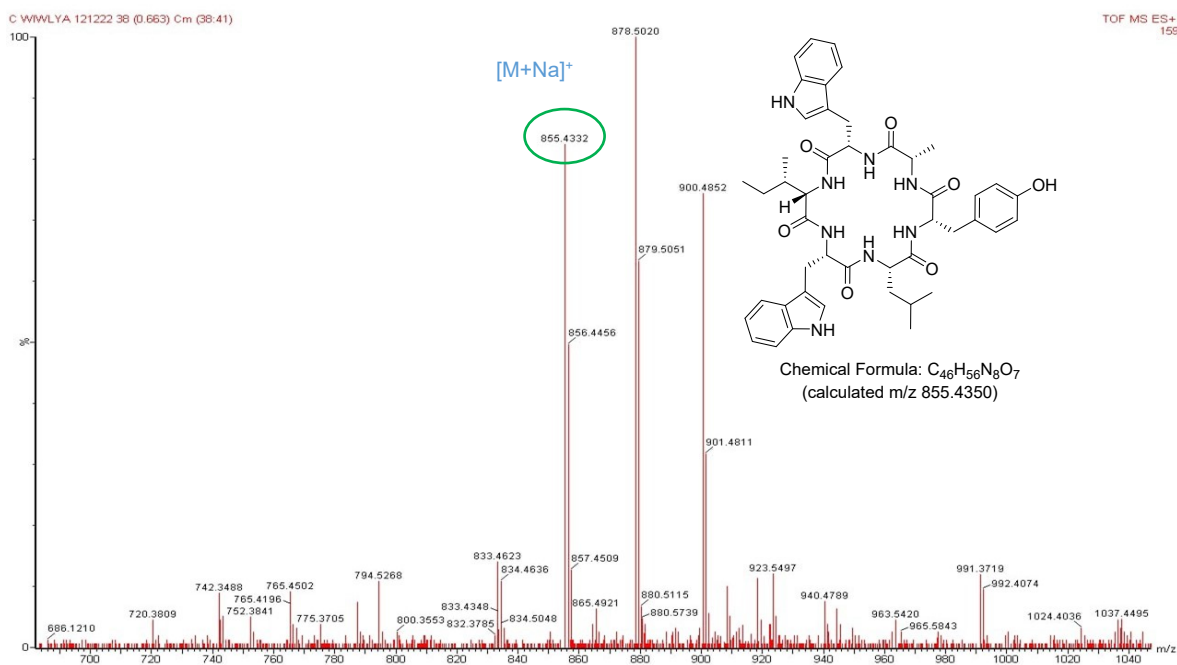


Figure S.4. Mass spectrum of cWIWLYA [cyclic-L-Trp-Ile-Trp-Leu-Tyr-Ala]

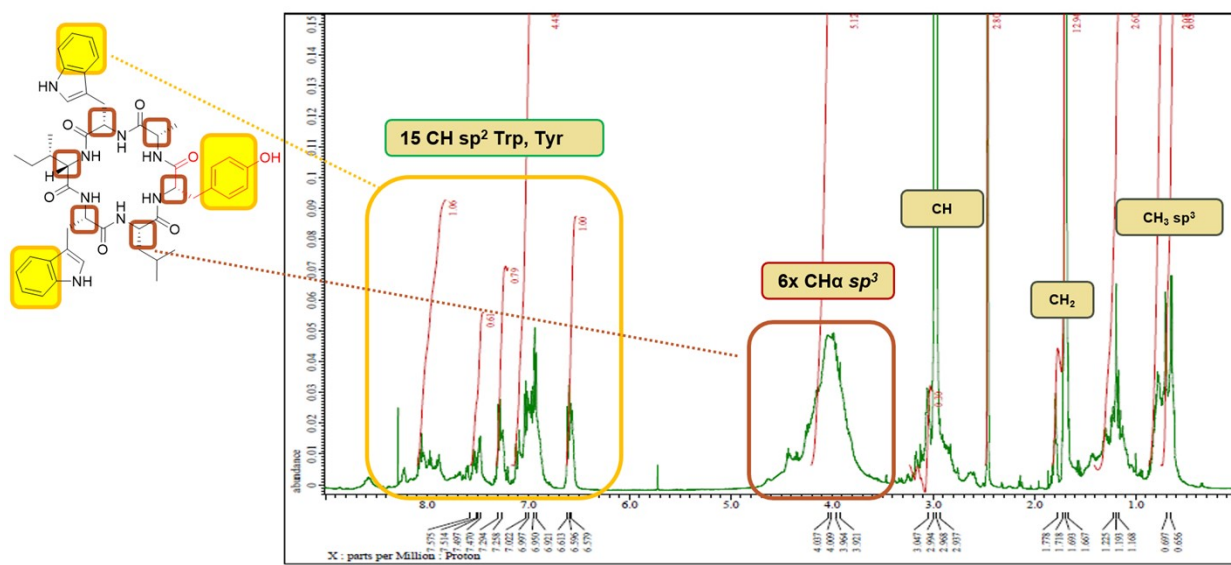


Figure S.5 <sup>1</sup>H-NMR spectrum of cWIWLYA [cyclic-L-Trp-Ile-Trp-Leu-Tyr-Ala] (500 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)

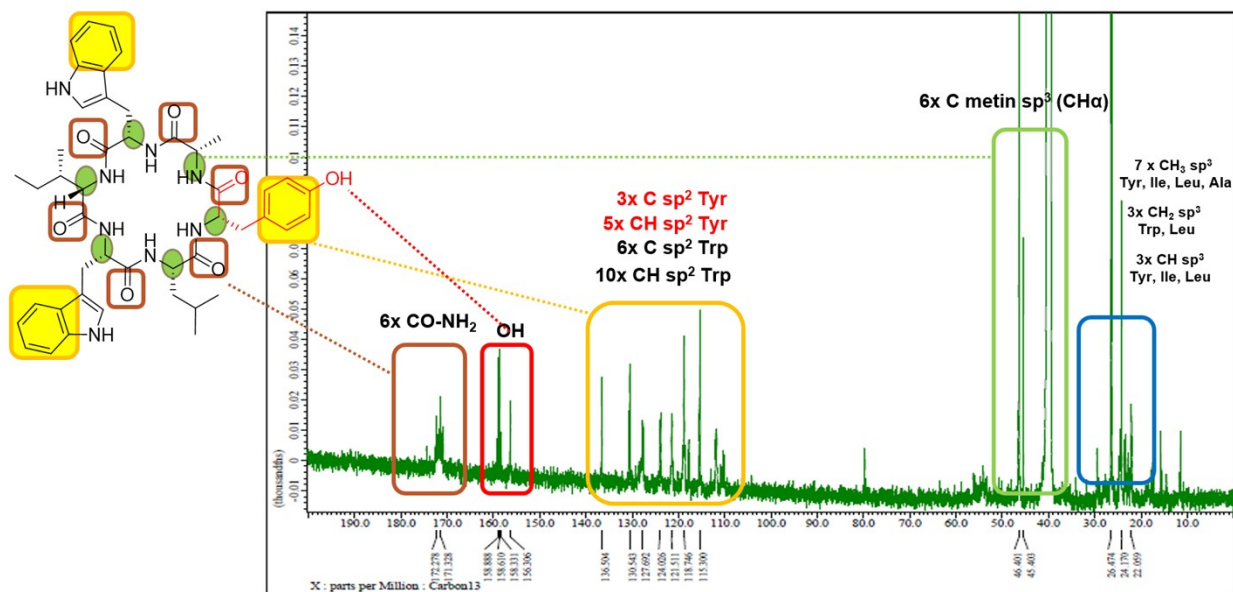


Figure S.6 <sup>13</sup>C-NMR spectrum of cWIWLVA [cyclic-L-Trp-Ile-Trp-Leu-Tyr-Ala] (125 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)

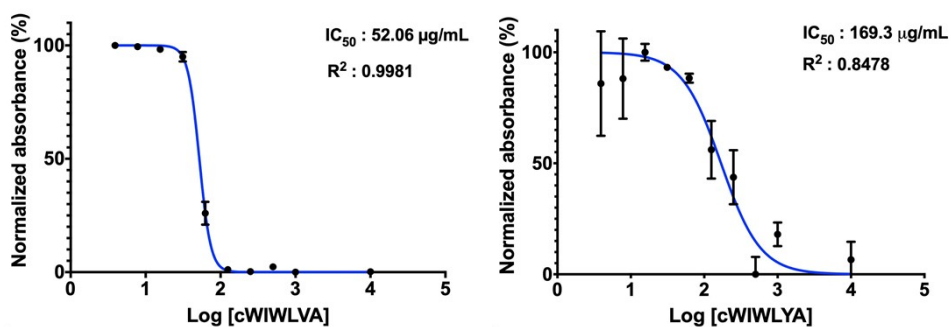


Figure S.7. The dose-response curve of nocardiotide A analog cWIWLVA and lead compound of cWIWLVA

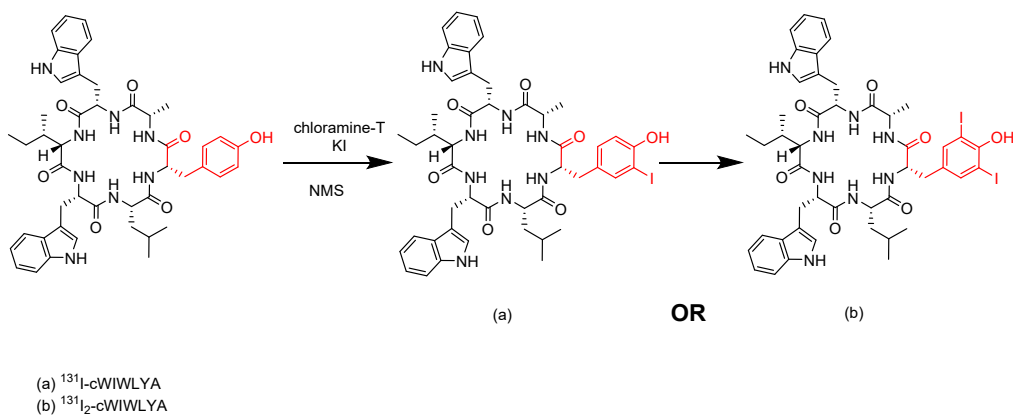


Figure S.8. Iodination of cWIWLVA

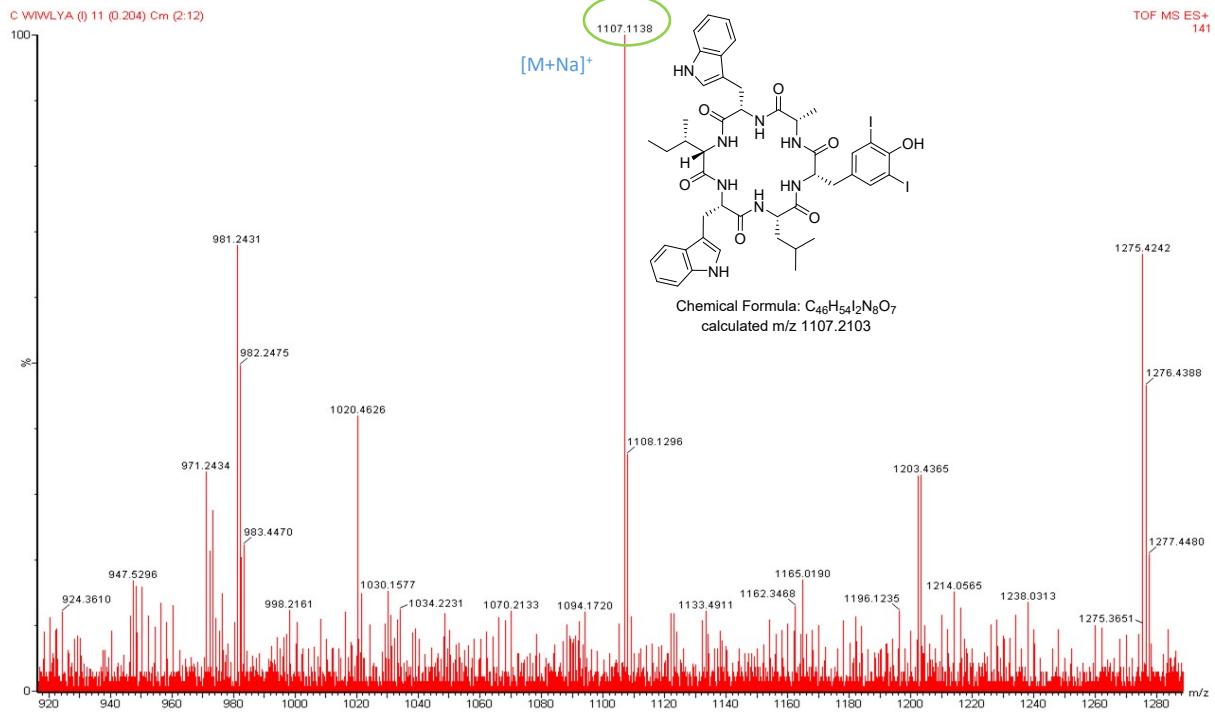


Figure S.9. Mass spectrum of I<sub>2</sub>-cWIWLYA (di-iodinated)