Supplementary Information

Chemoenzymatic synthesis of indole-containing acyloin derivatives

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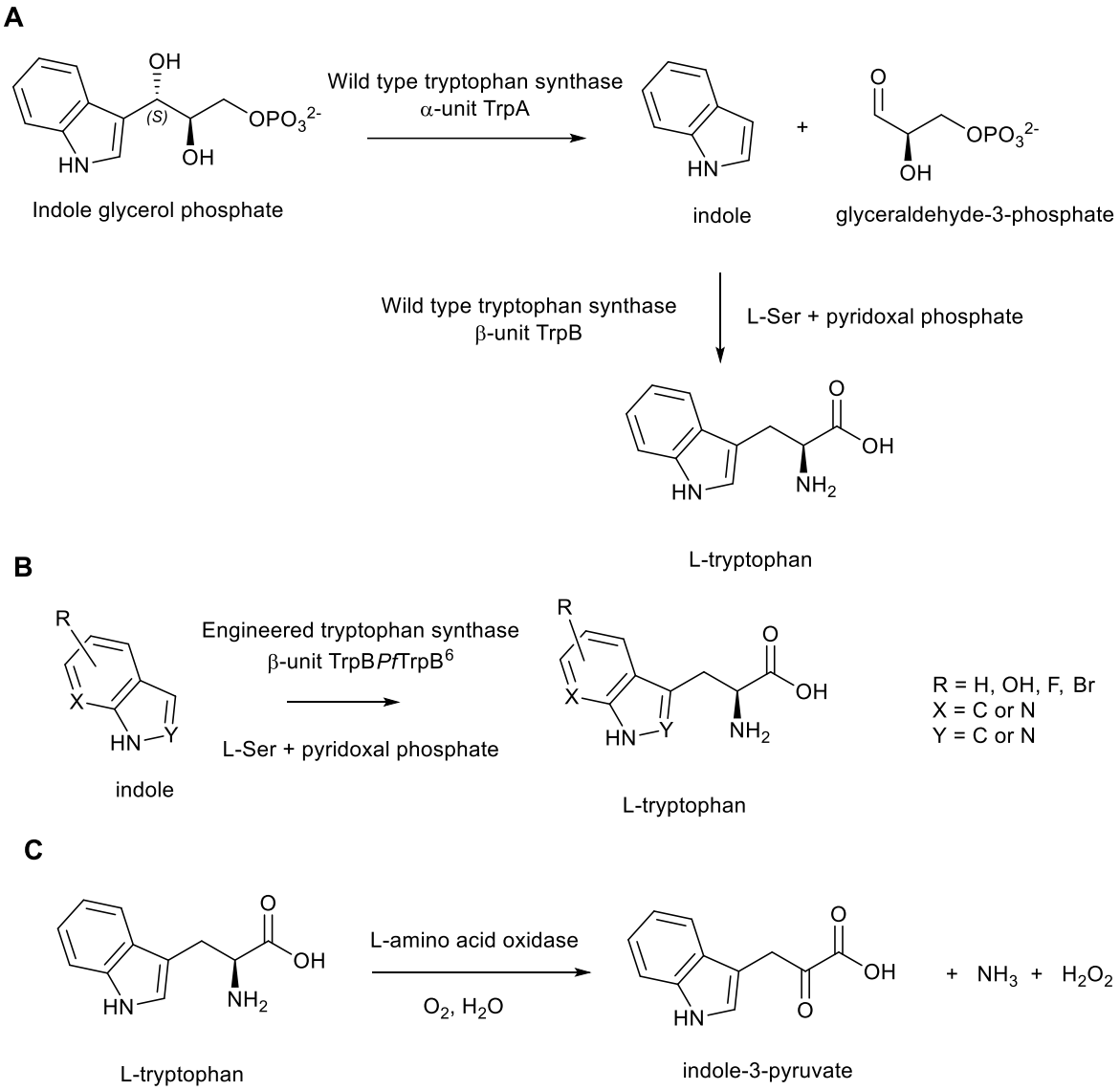


Scheme S1. The reactions of indole and L-Ser catalysed by wild type tryptophane synthase a- and b-units (**A**), the engineered tryptophan synthase b-unit *Pf*TrpB6 (**B**) and the commercially available L-amino acid oxidase (**C**).

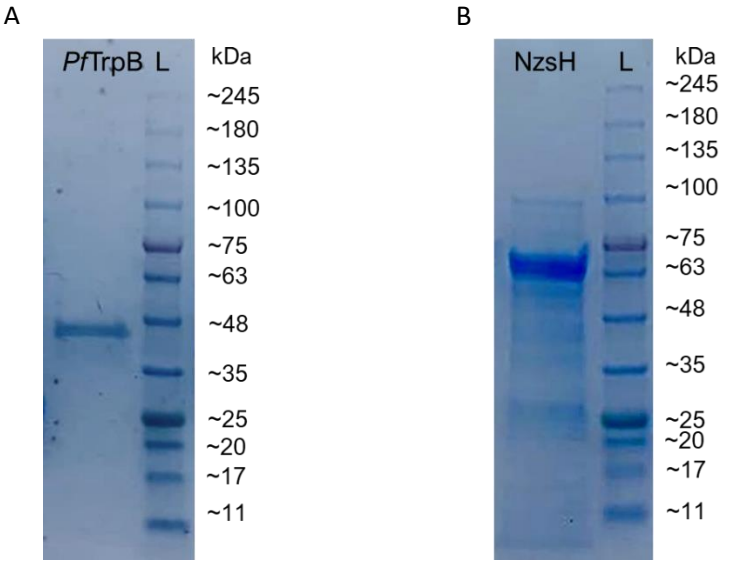


Figure S1. SDS Page electrophoresis analysis of purifies *Pf*TrpB[6](A) and NzsH(B).

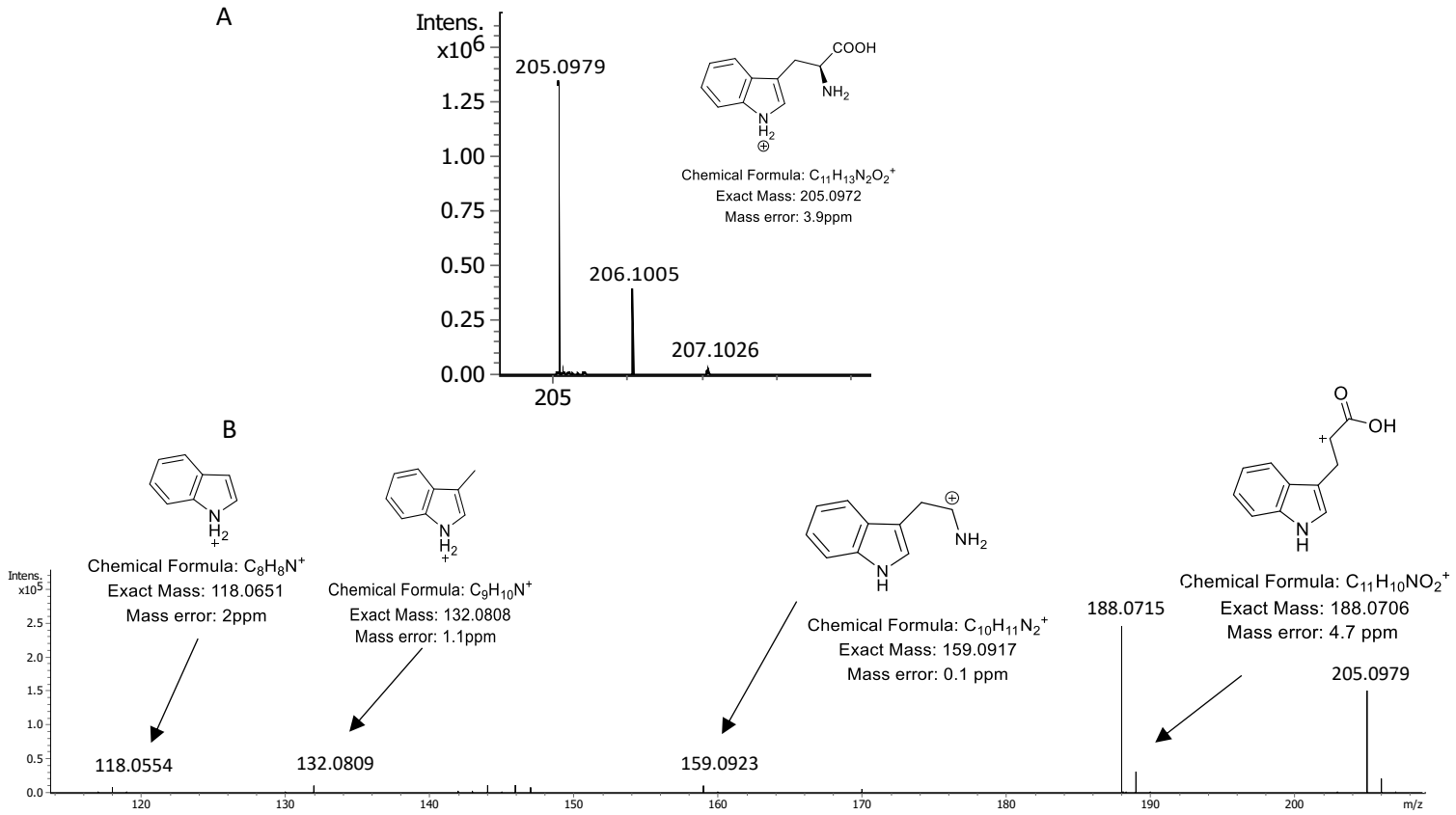


Figure S2. LC-MS (A) and MS/MS data (B) of L-tryptophan **13**.

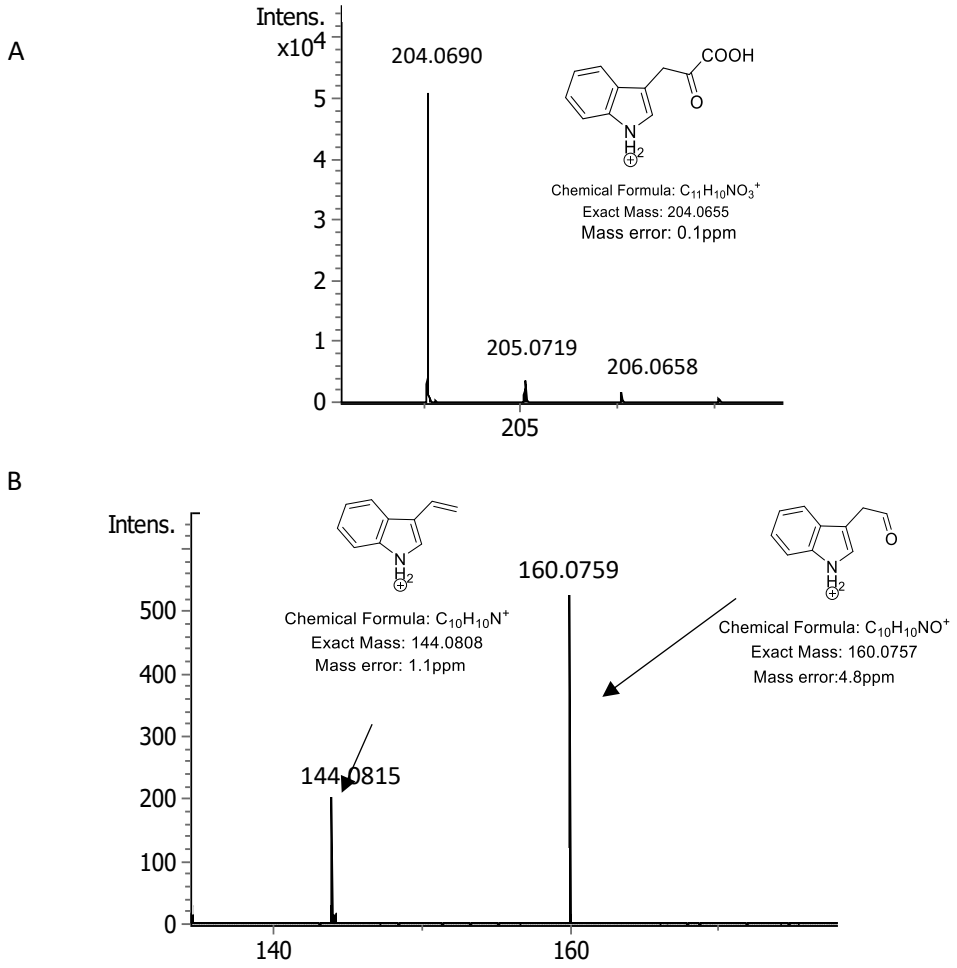


Figure S3. LC-MS (A) and MS/MS data (B) of indole-3-pyruvate **14**.

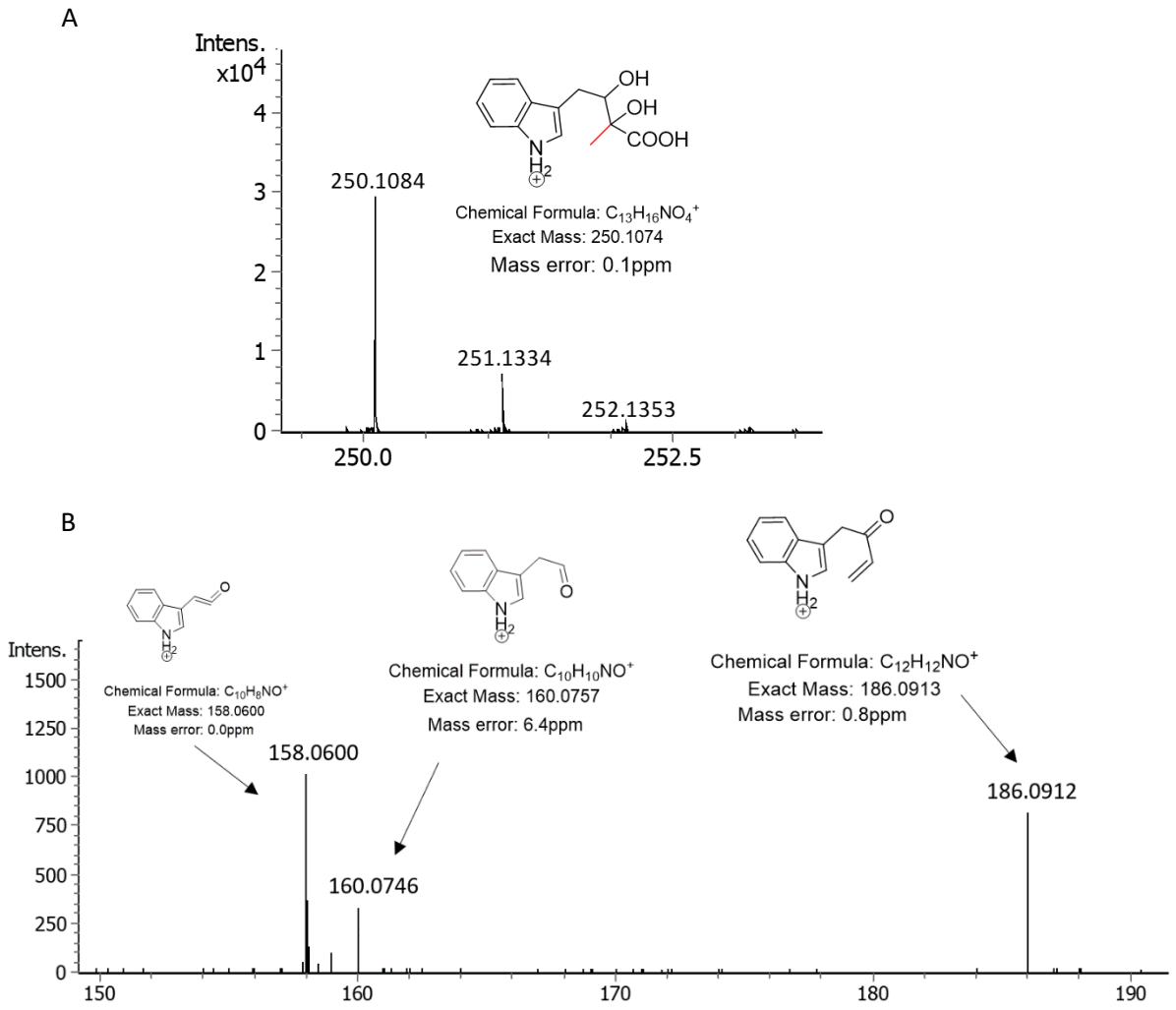


Figure S4. LC-MS (A) and MS/MS data(B) of indole-containing acyloin **15**.

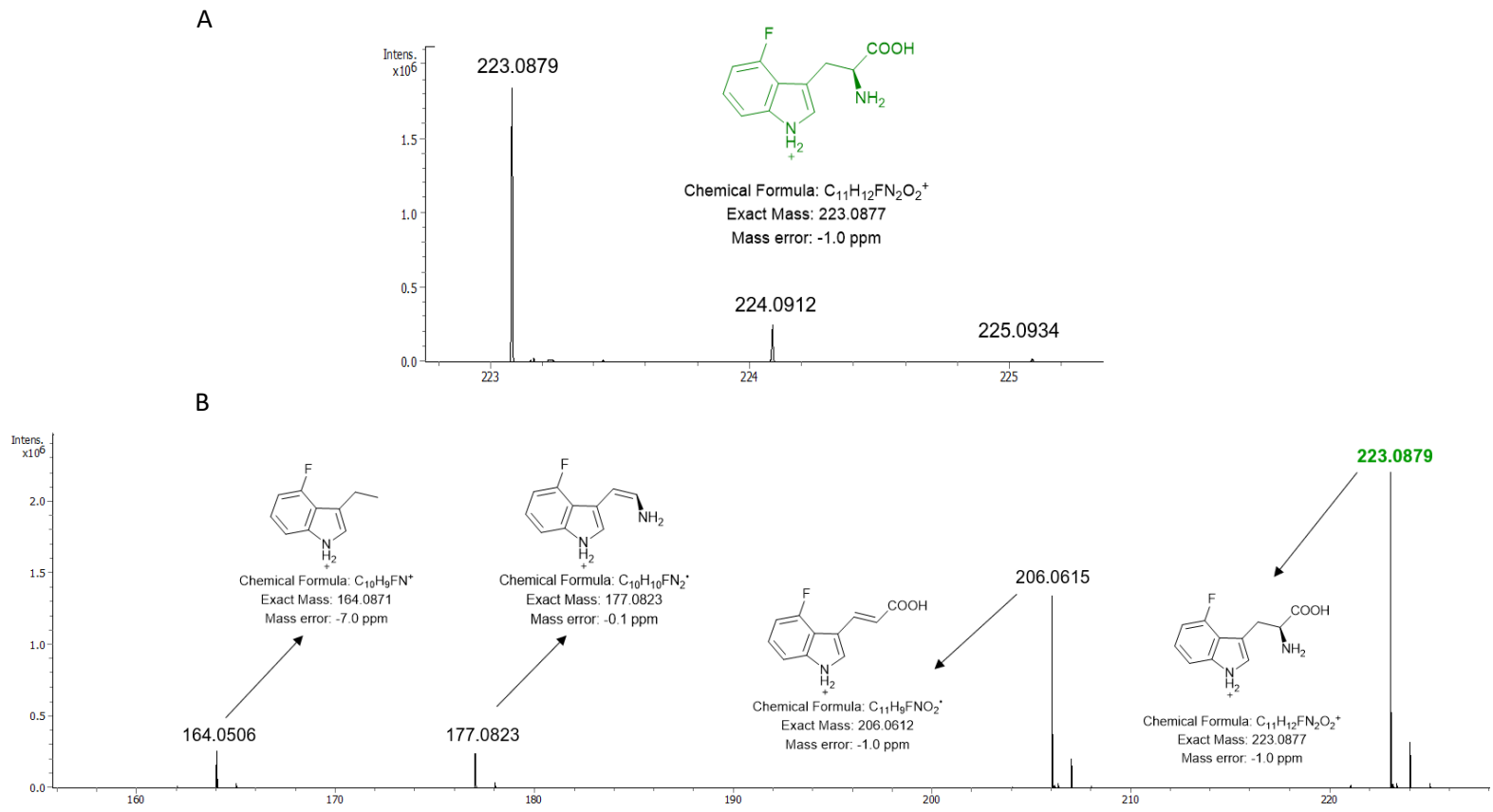


Figure S5. LC-MS (A) and MS/MS data (B) of 4-fluoro-indole-tryptophan **21**.

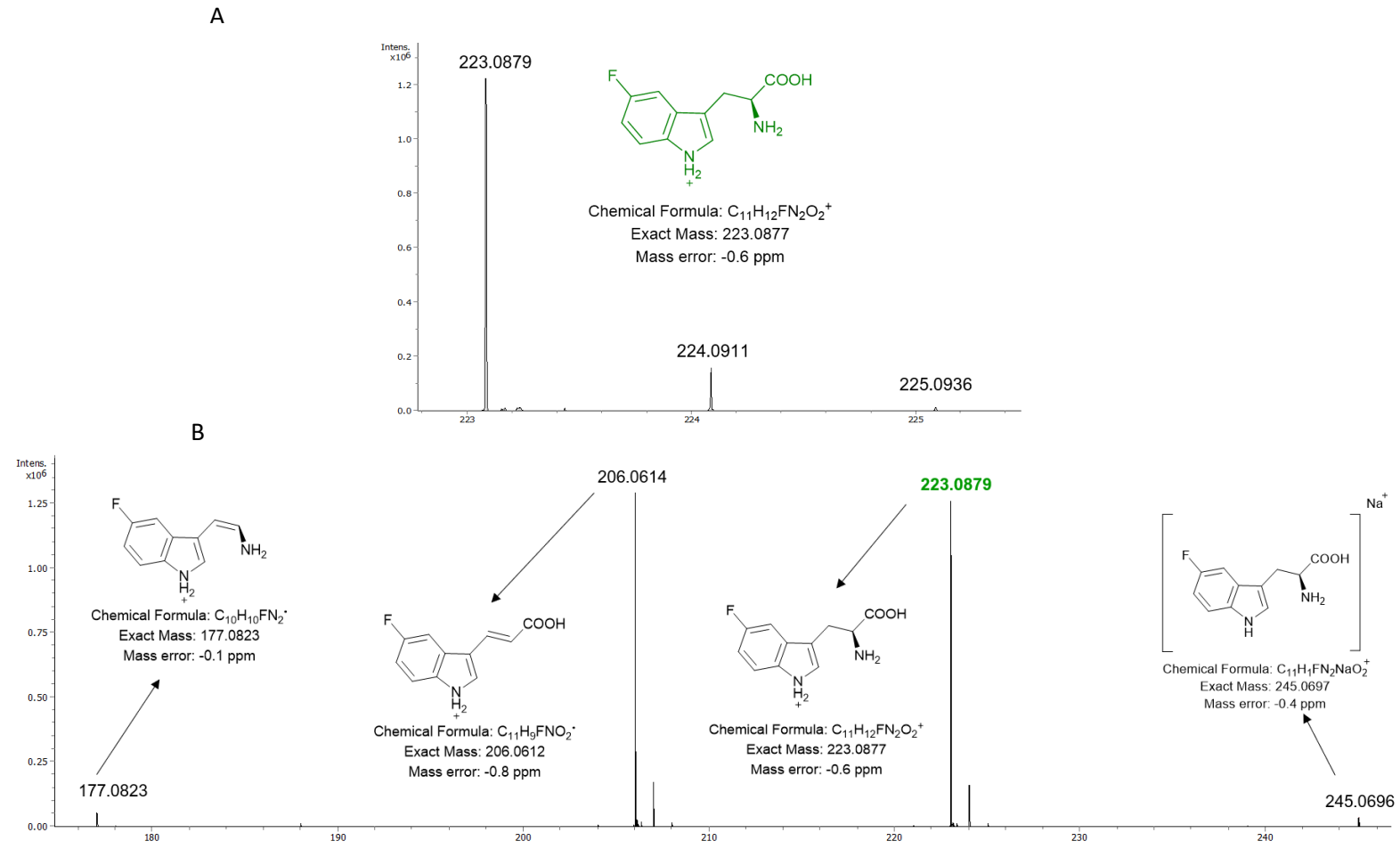


Figure S6. LC-MS (A) and MS/MS data (B) of 5-fluoro-indole-tryptophan **22**.

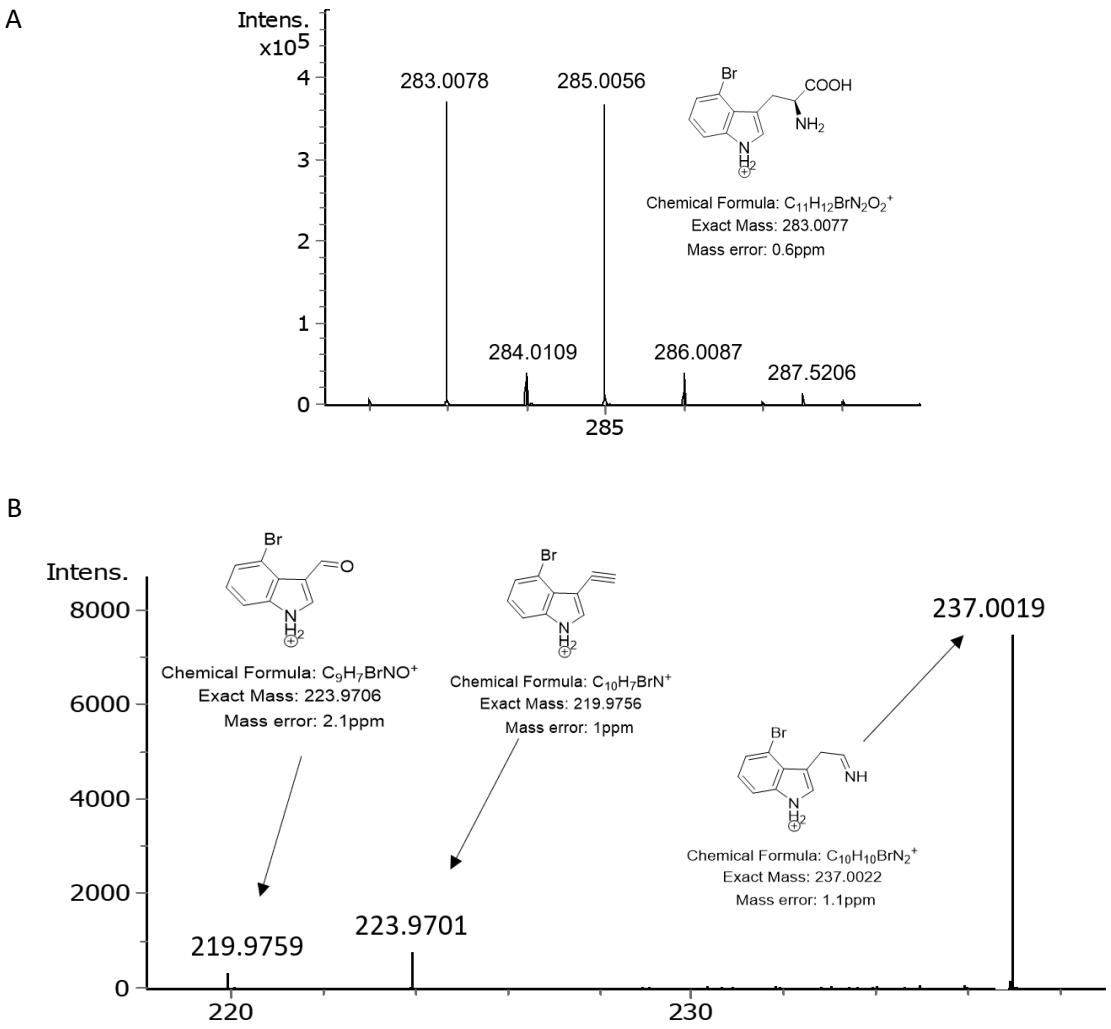


Figure S7. LC-MS (A) and MS/MS data (B) of 4-bromo-indole-tryptophan **23**.

A

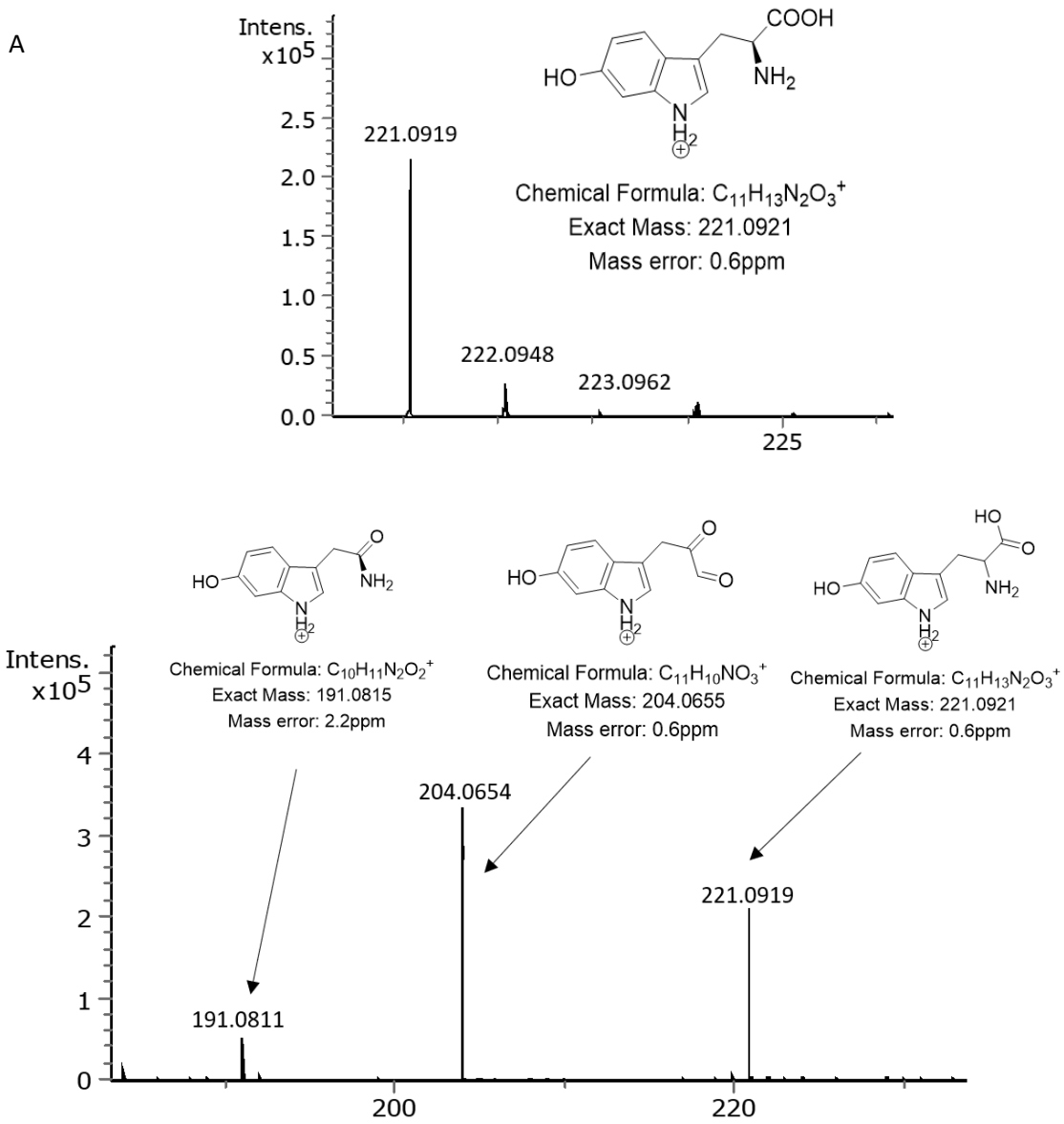


Figure S8. LC-MS (A) and MS/MS data (B) of 6-hydroxyl-tryptophan **24**.

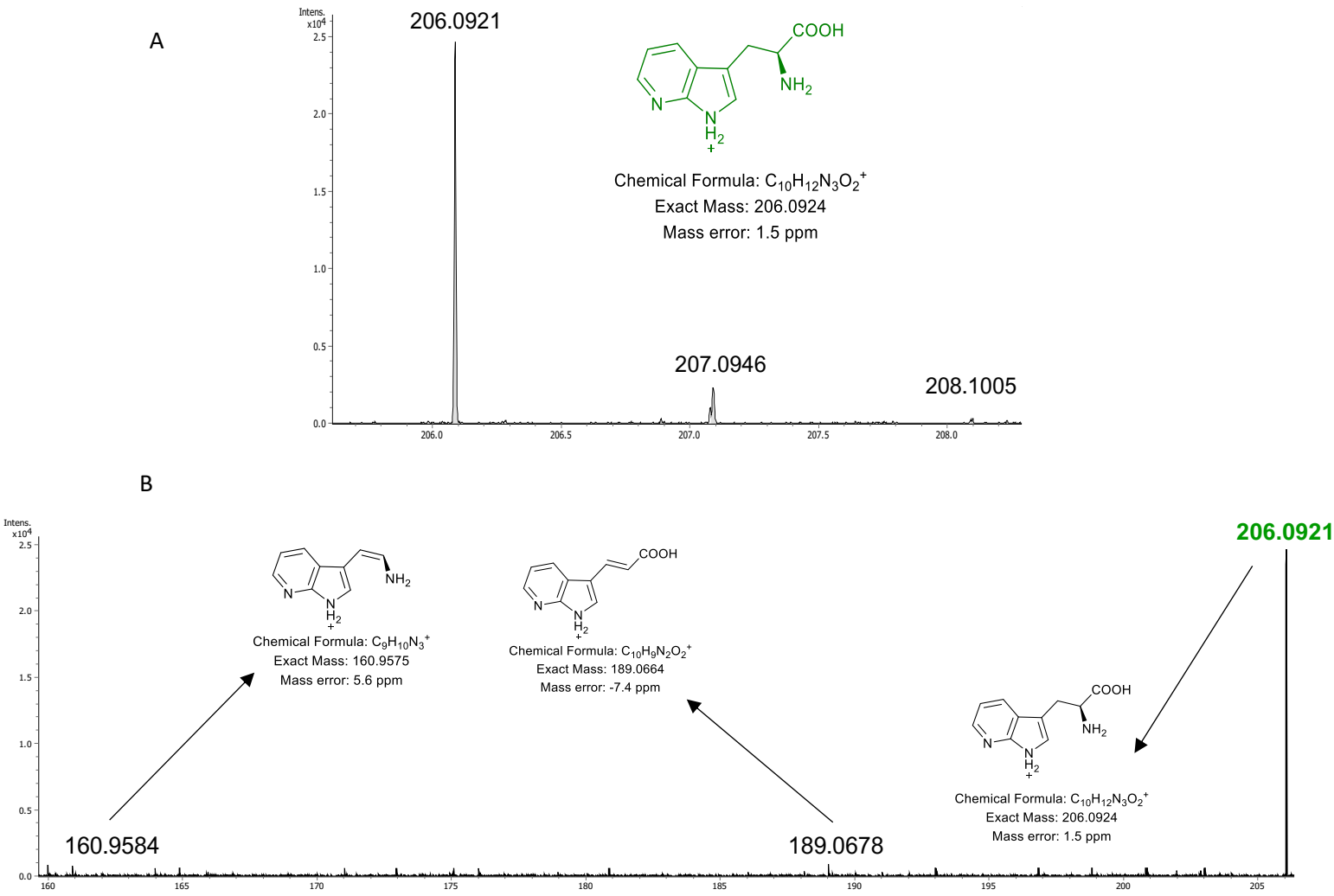


Figure S9. LC-MS (A) and MS/MS data (B) of 7-azaindole-tryptophan **25**.

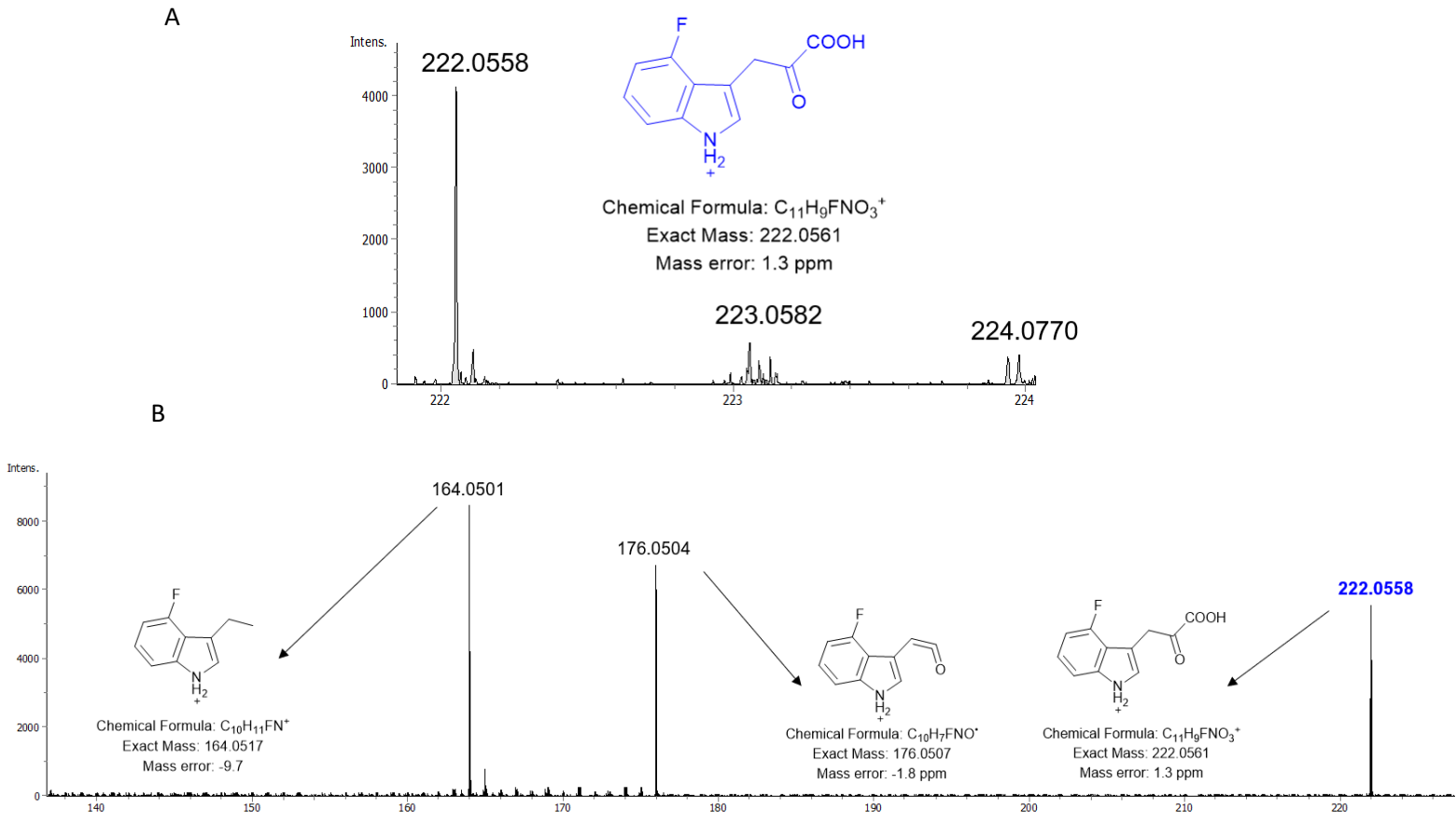


Figure S10. LC-MS (A) and MS/MS data (B) of 4-fluoro-3-indole pyruvate **26**.

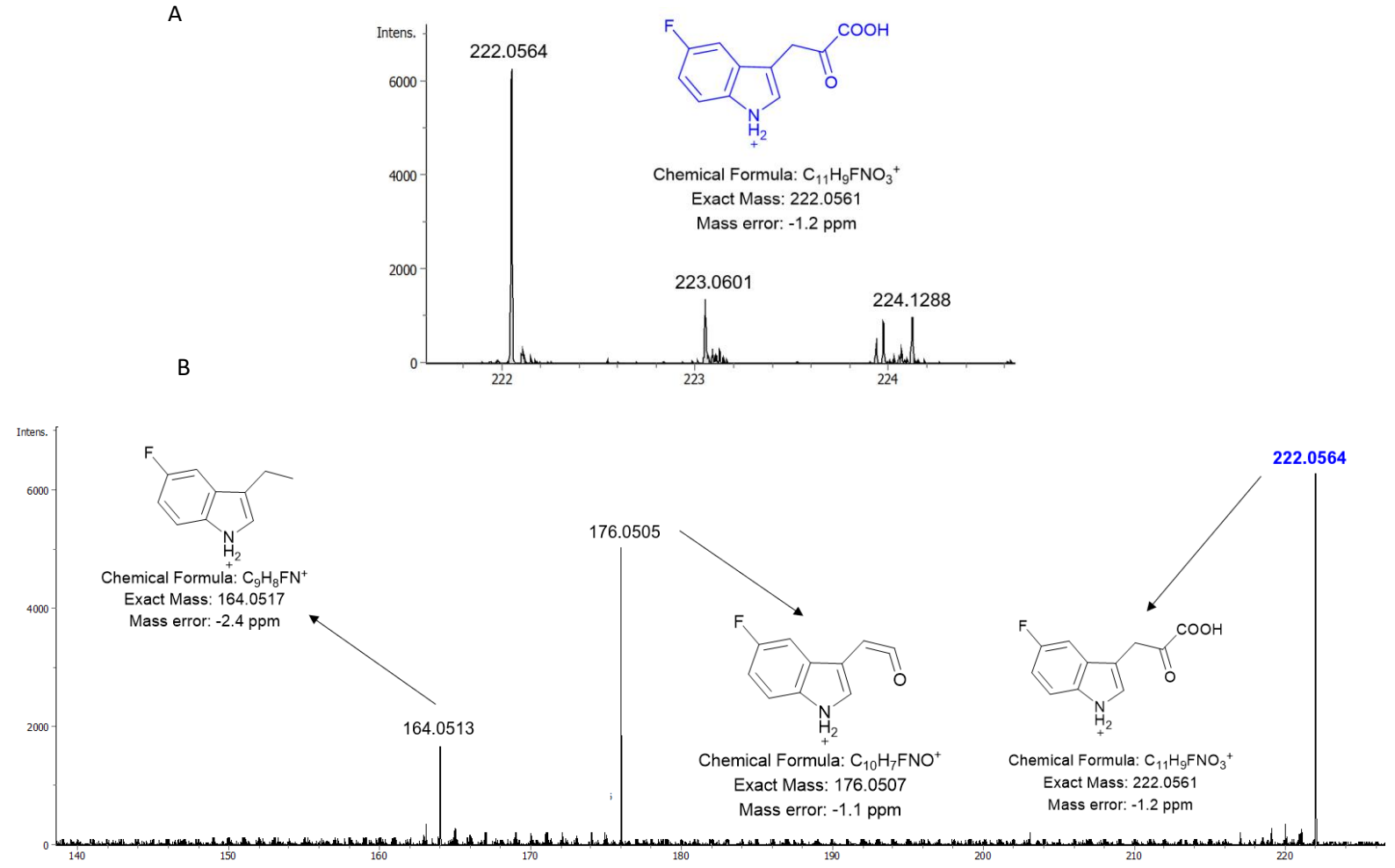
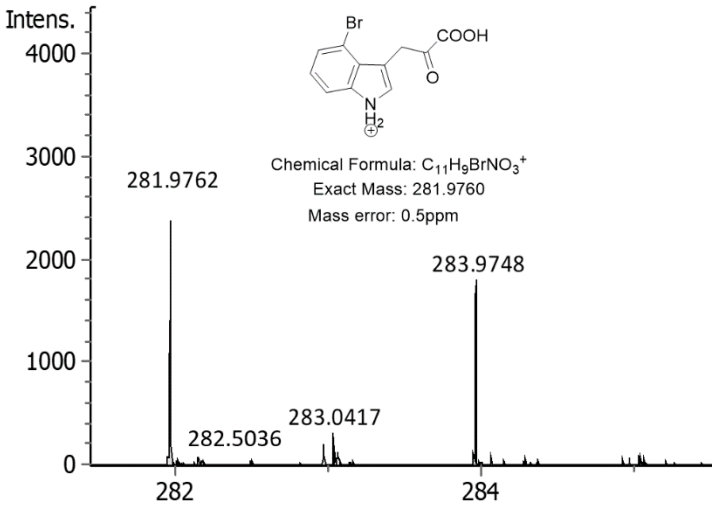


Figure S11. LC-MS (A) and MS/MS data (B) of 5-fluoro-3-indole pyruvate **27**.

A



B

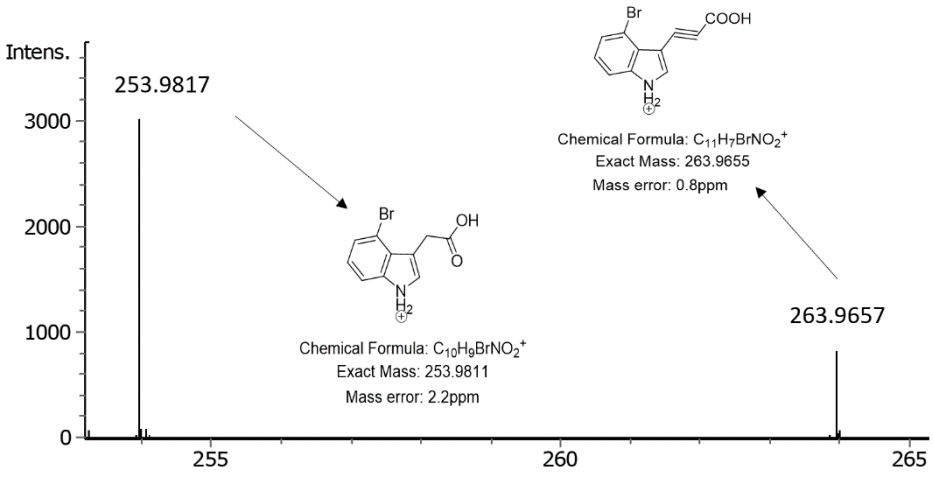


Figure S12. LC-MS (A) and MS/MS data (B) of 4-bromo-3-indole pyruvate **28**.

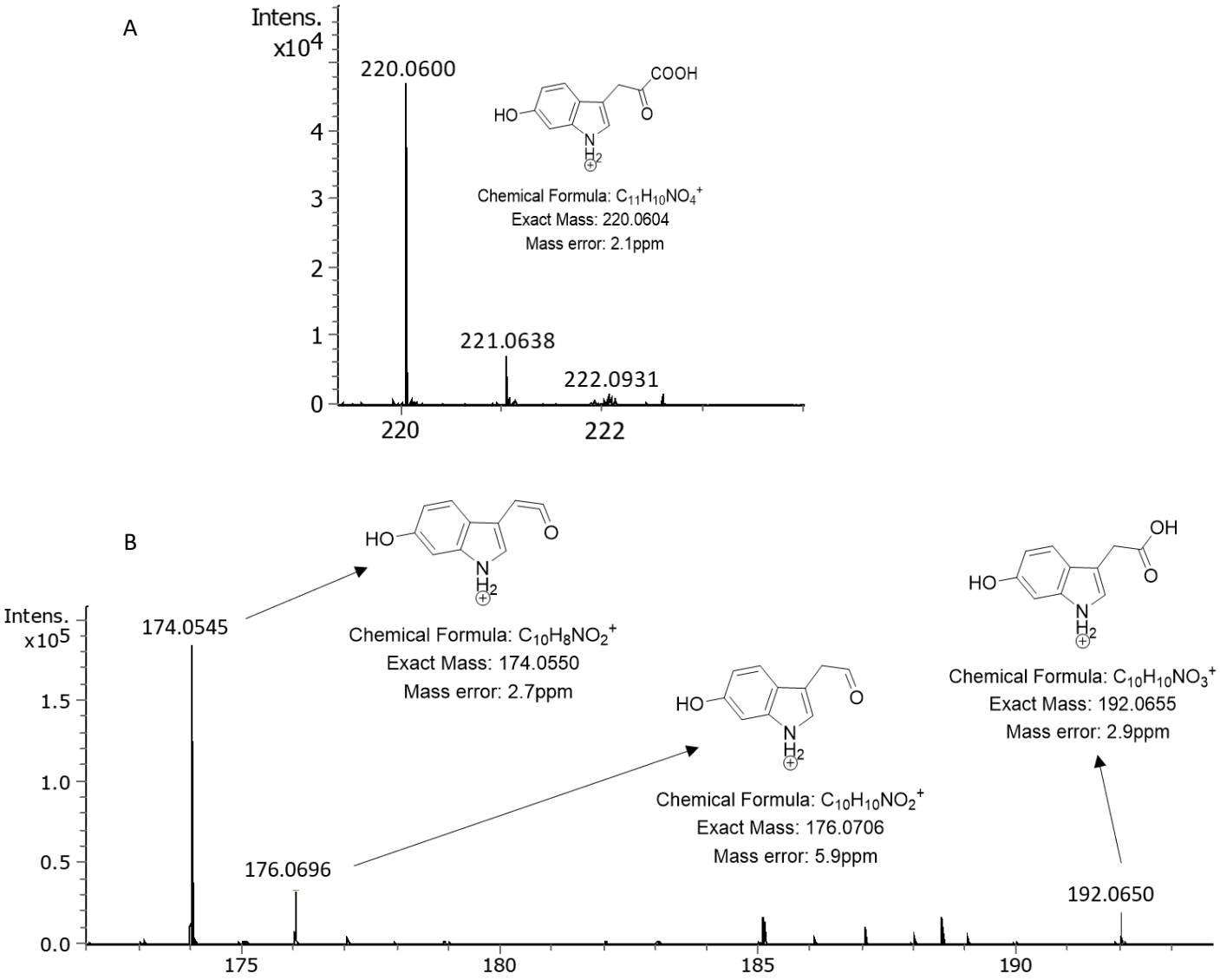


Figure S13. LC-MS (A) and MS/MS data (B) of 6-hydroxyl-3-indole pyruvate **29**.

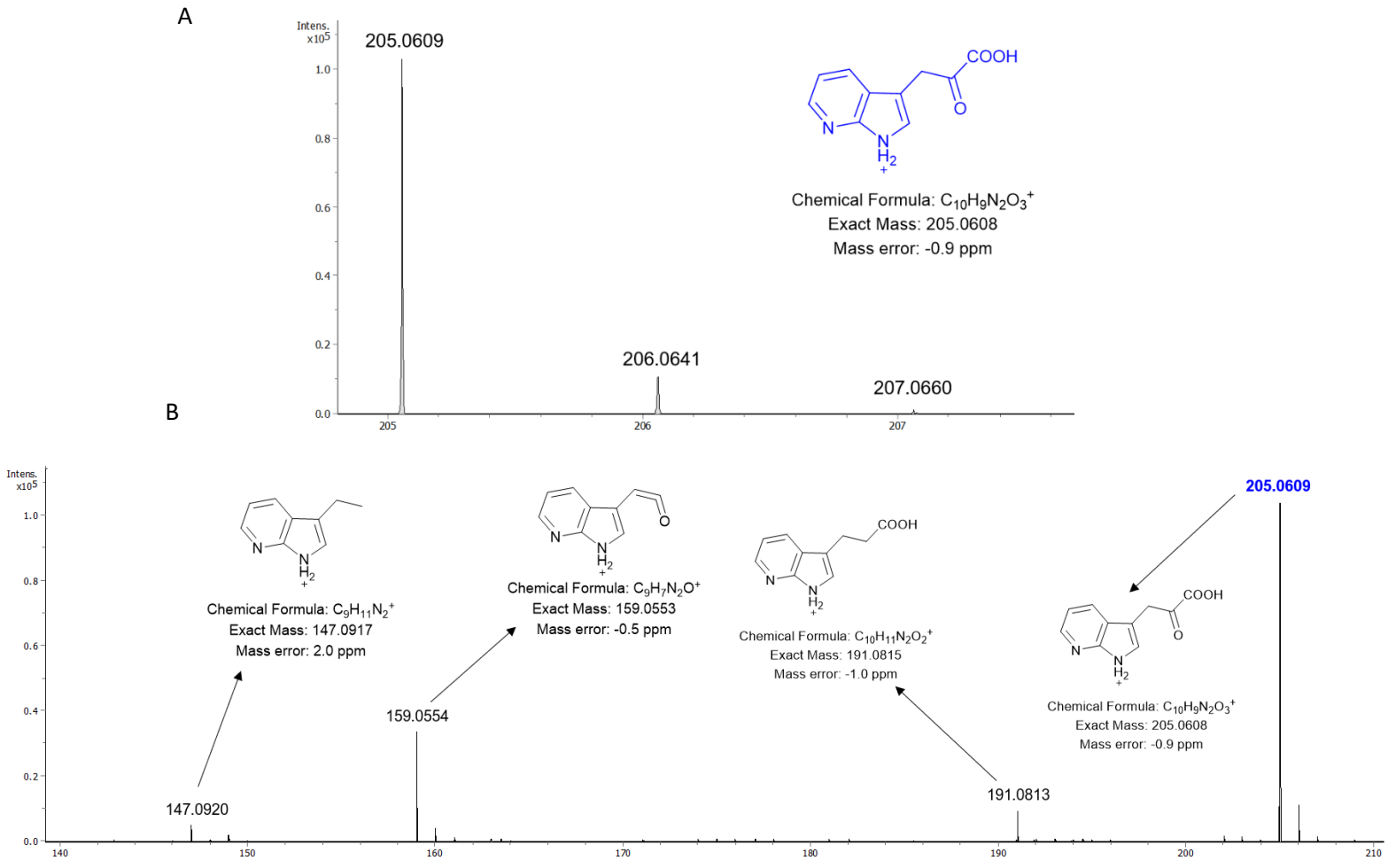


Figure S14. LC-MS (A) and MS/MS data (B) of 7-azaindole-3-pyruvate **30**.

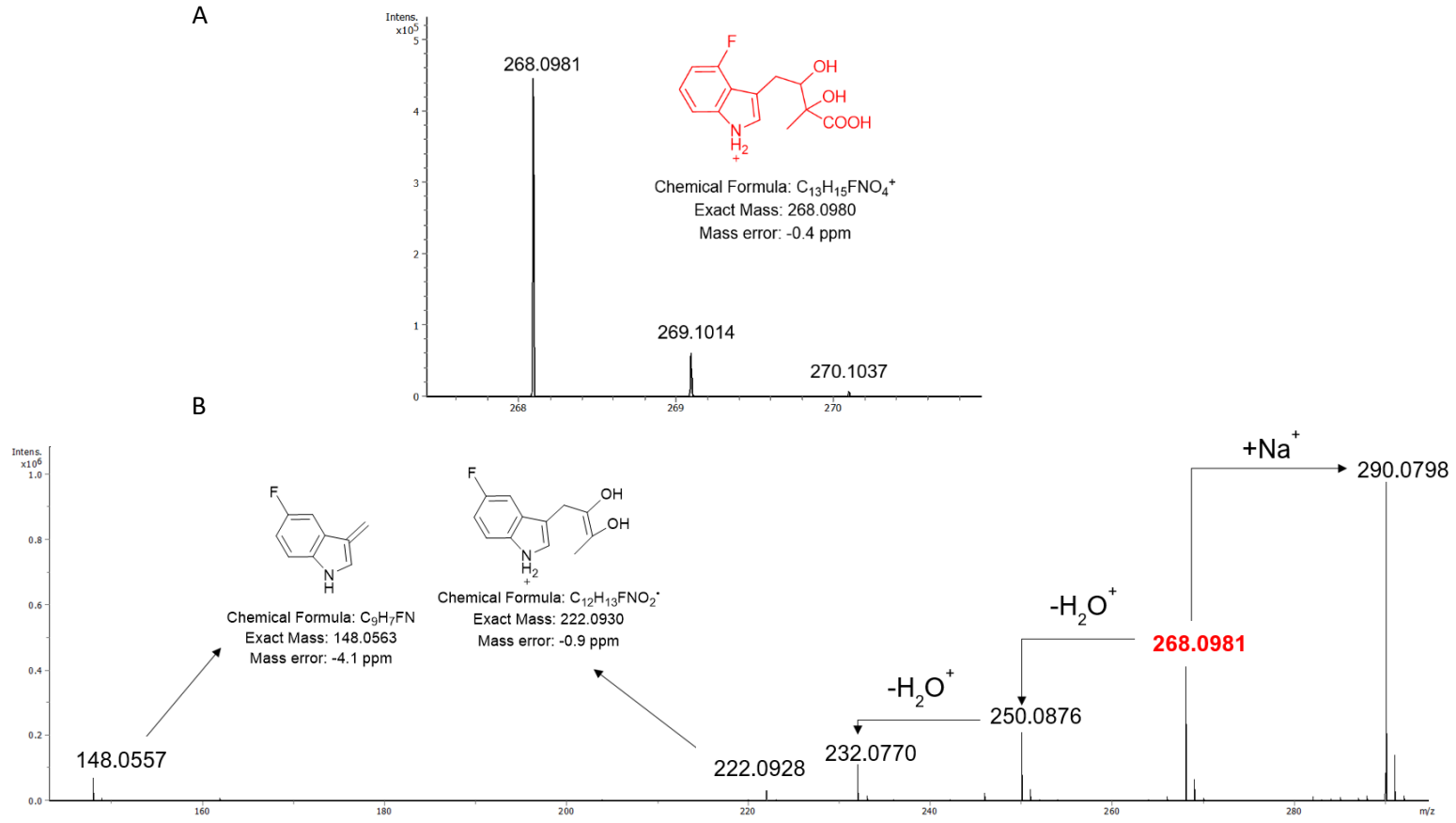


Figure S15. LC-MS (A) and MS/MS data (B) of 4-fluoro-indole-containing acyloin **31.**

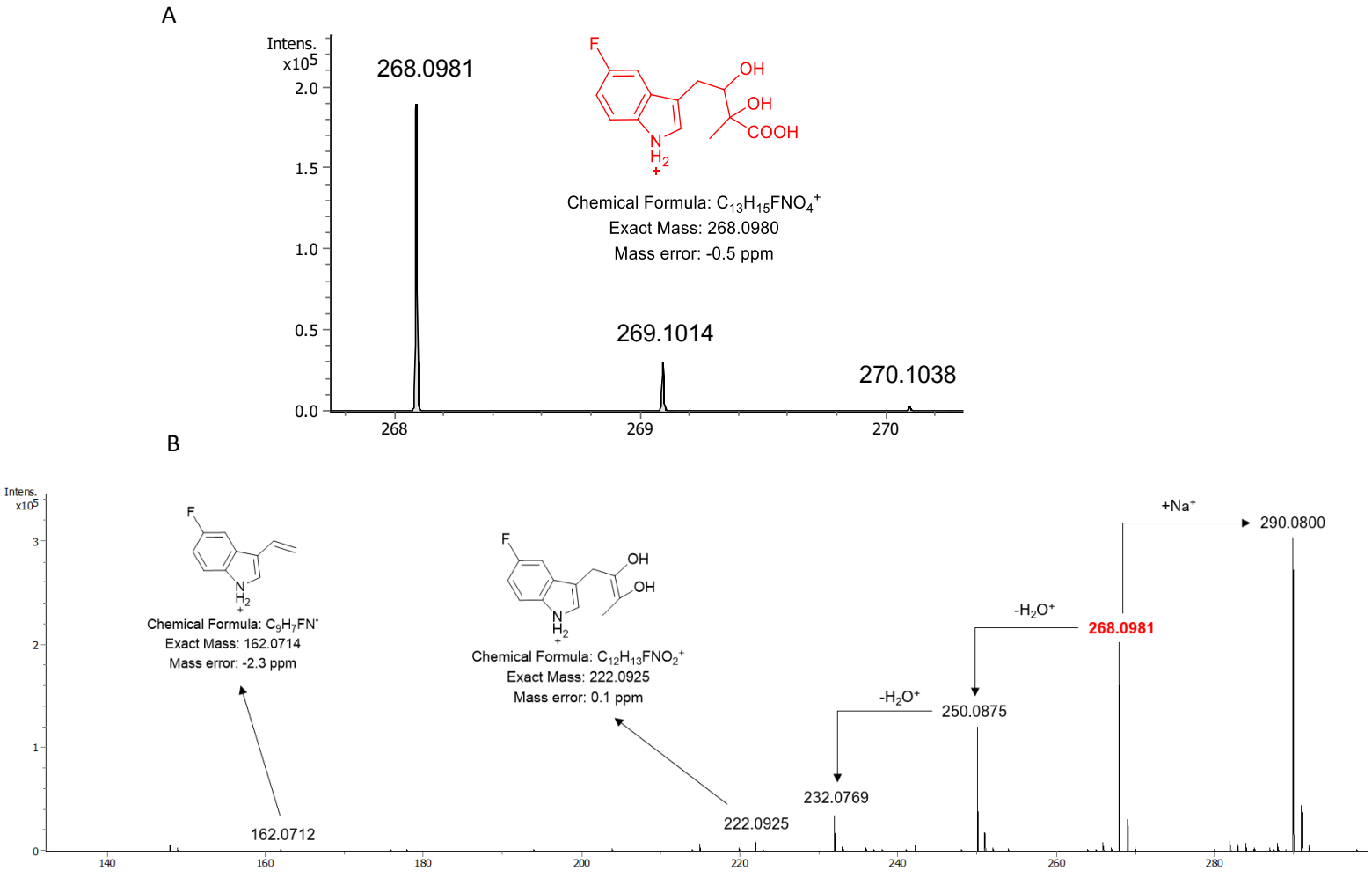


Figure S16. LC-MS (A) and MS/MS data (B) of 5-fluoro-indole-containing acyloin **32.**

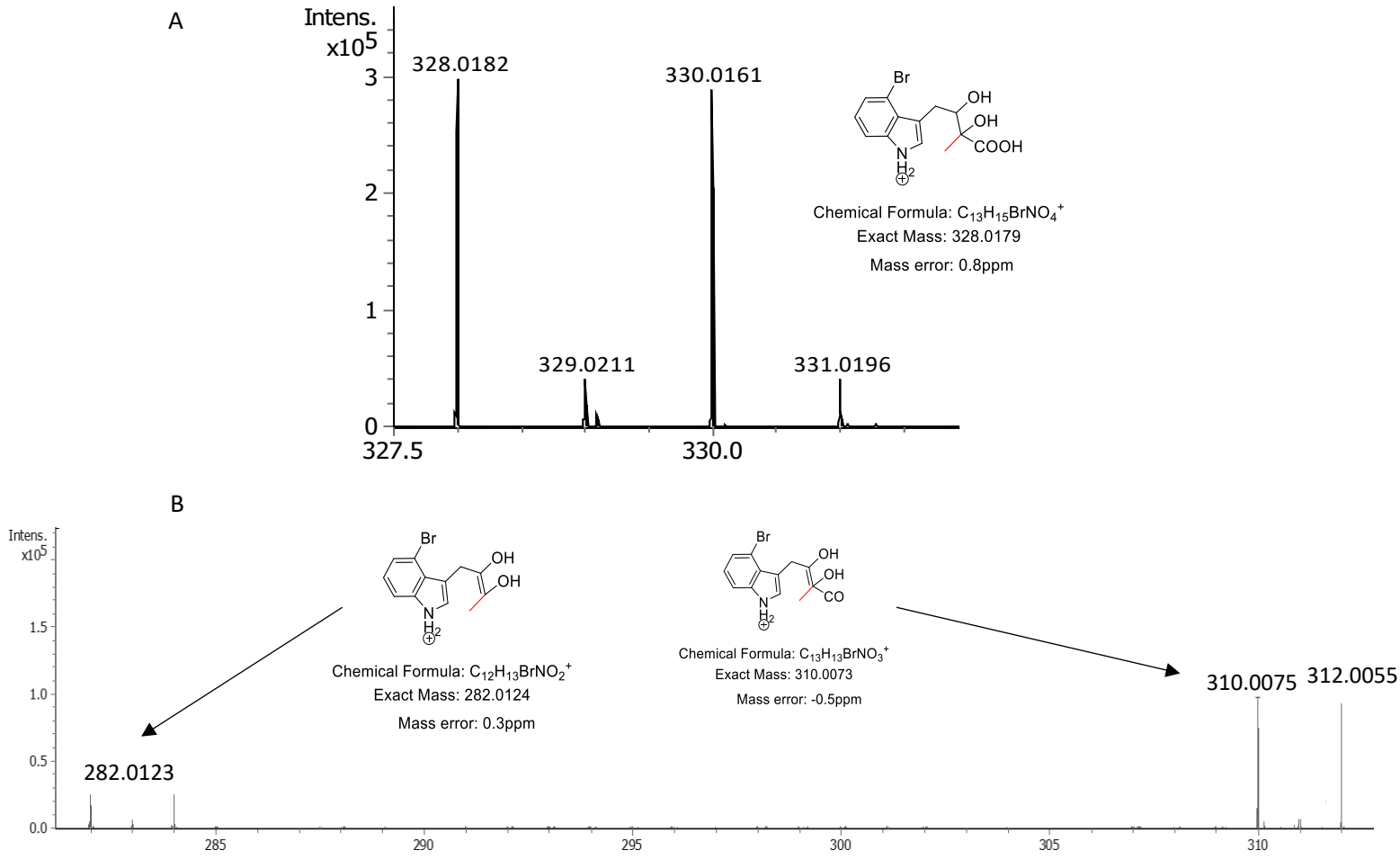


Figure S17. LC-MS (A) and MS/MS data (B) of 4-bromo-indole-containing acyloin **33**.

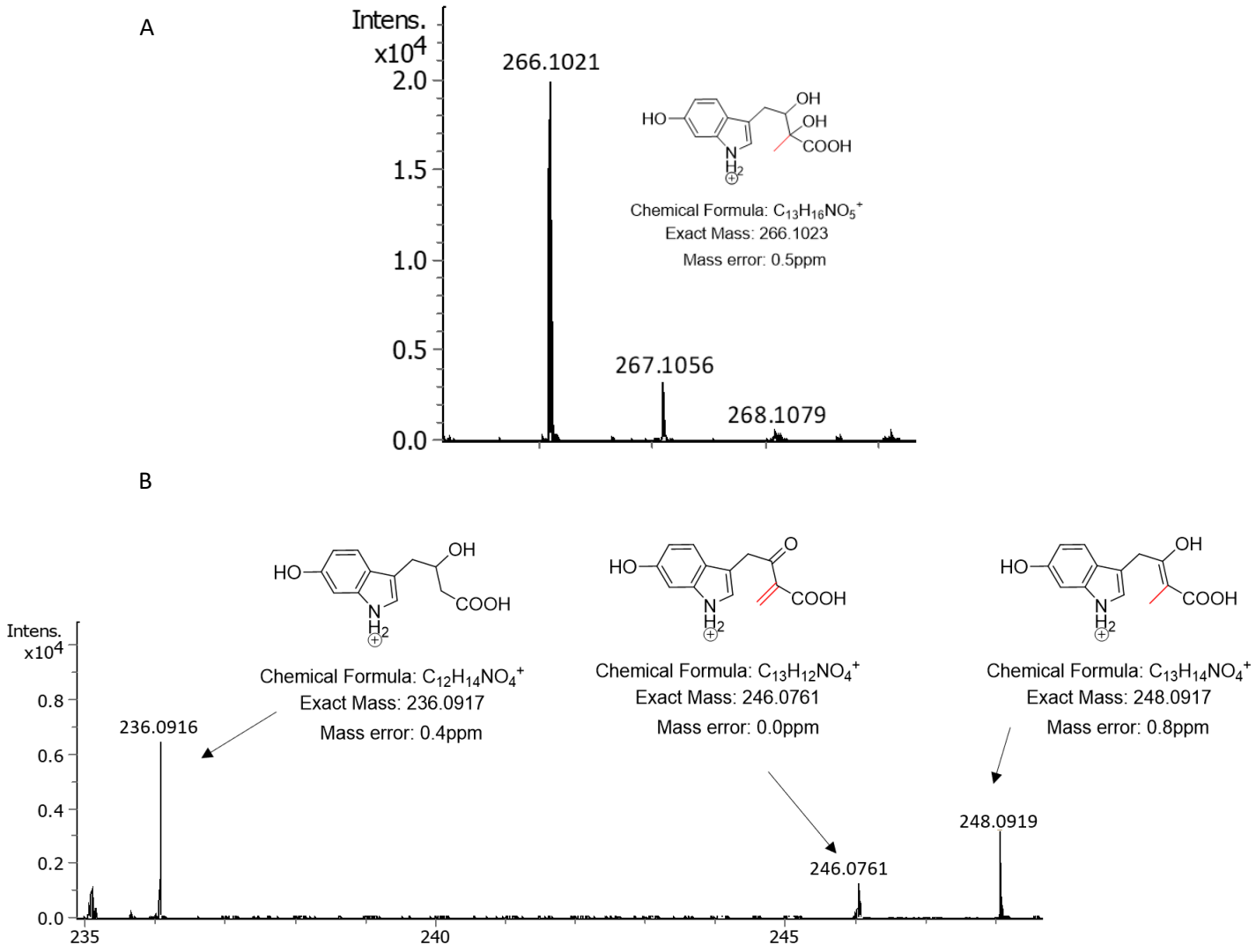


Figure S18. LC-MS (A) and MS/MS data (B) of 6-hydroxyl-indole-containing acyloin **34**.

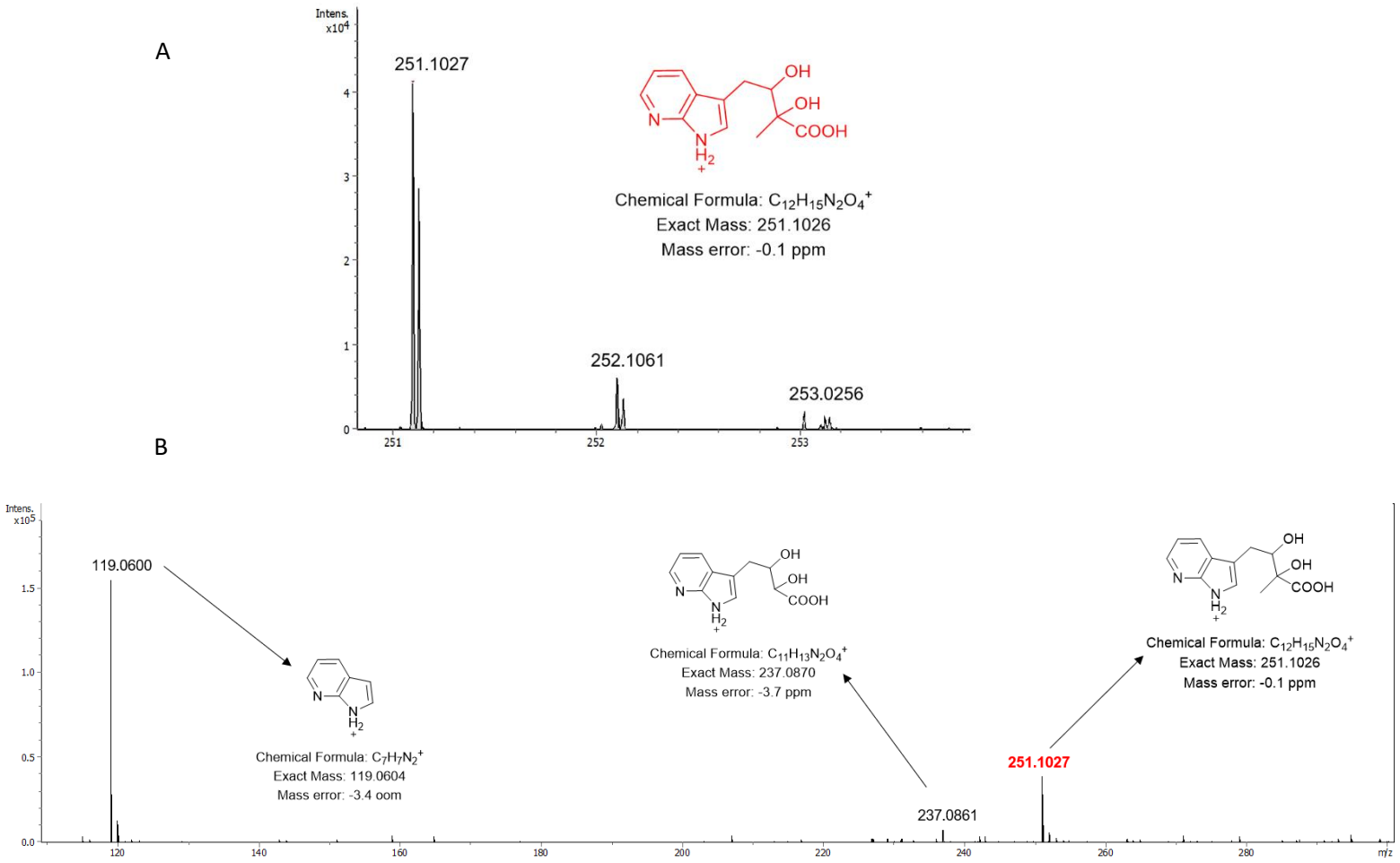


Figure S19. LC-MS (A) and MS/MS data (B) of 7-azaindole-containing-acyloin **35**.

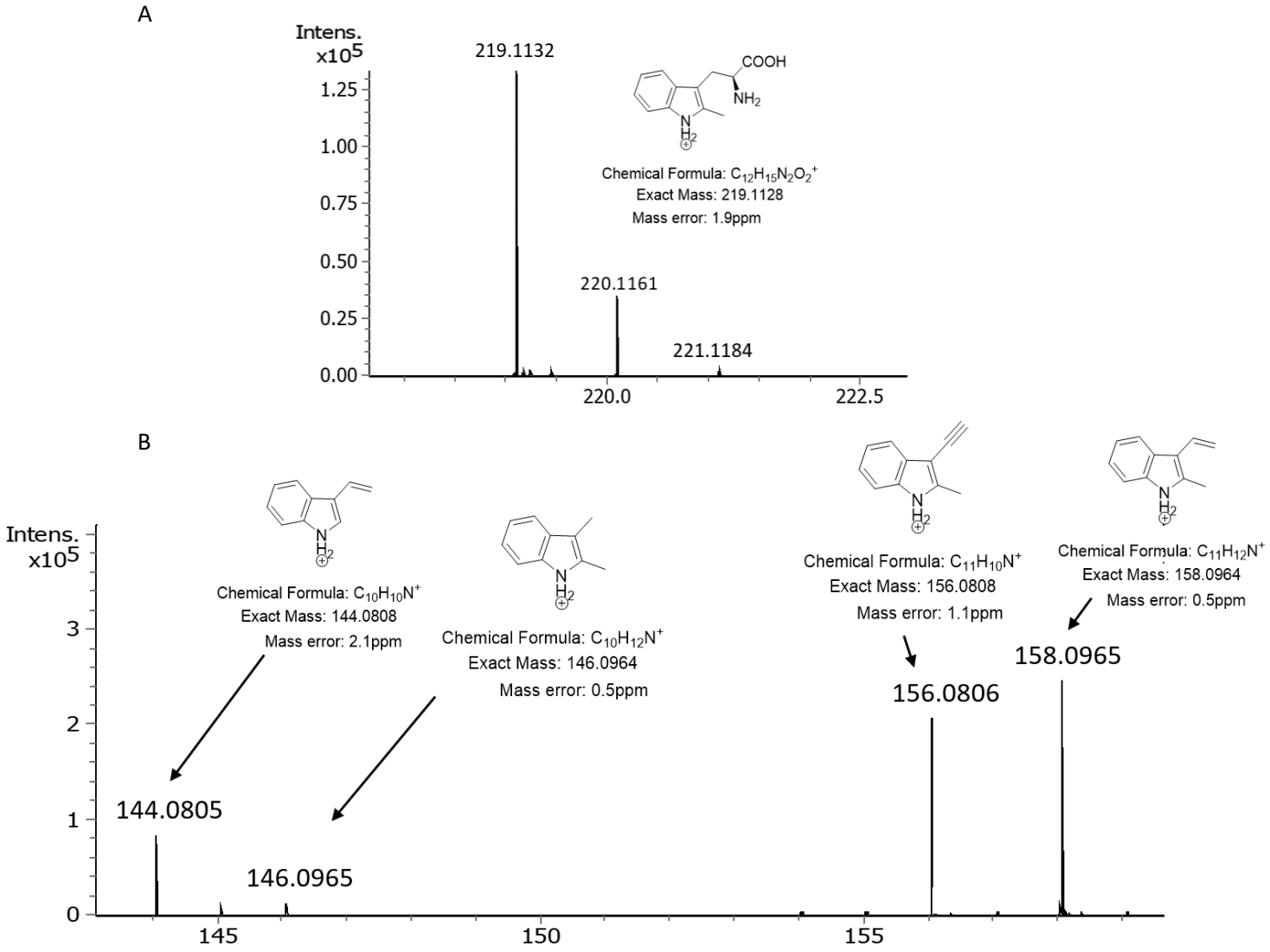


Figure S20. LC-MS (A) and MS/MS data (B) of 2-methyl-indole-tryptophan **39**.

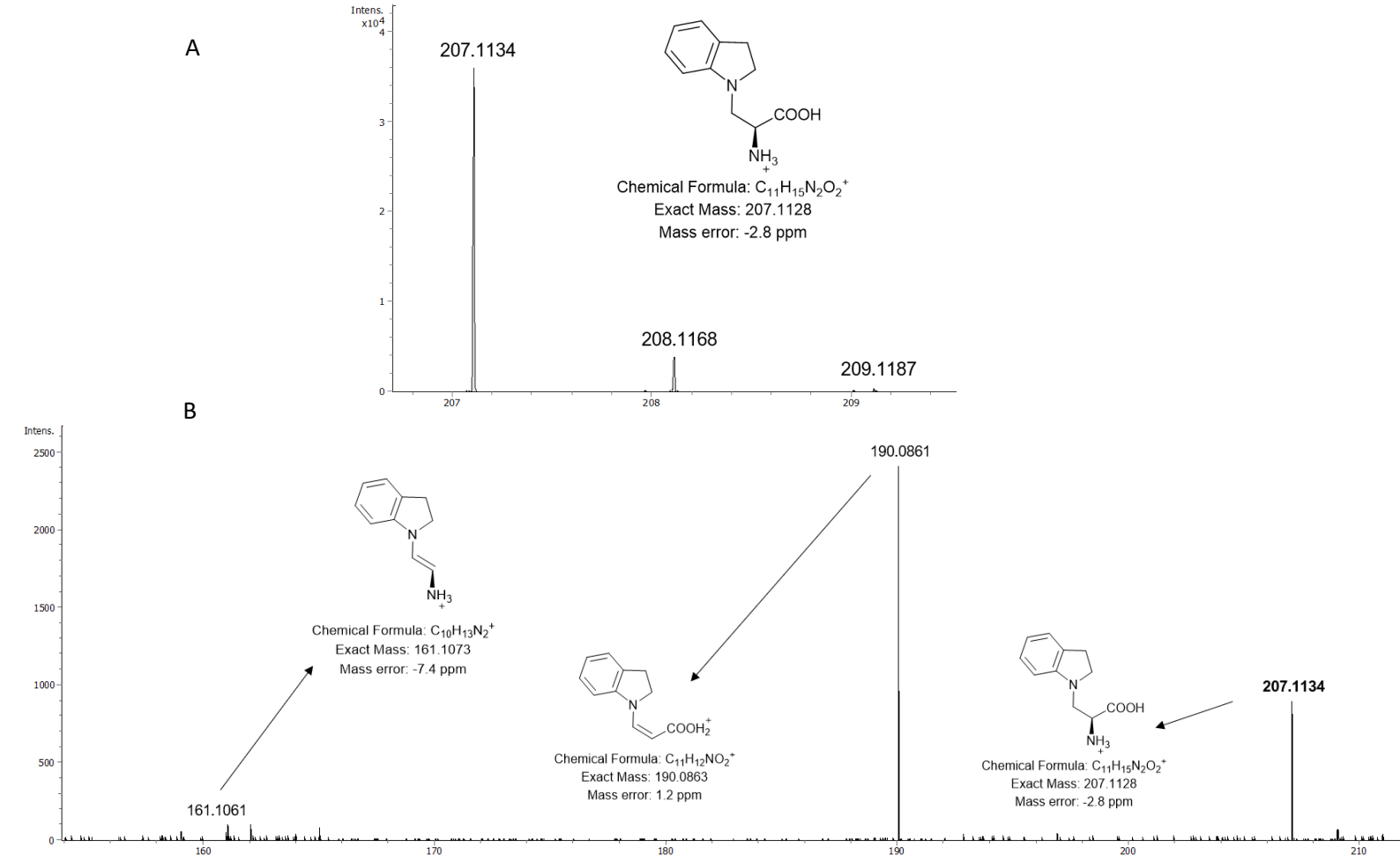


Figure S21. LC-MS (A) and MS/MS data (B) of indoline-tryptophan **40**.

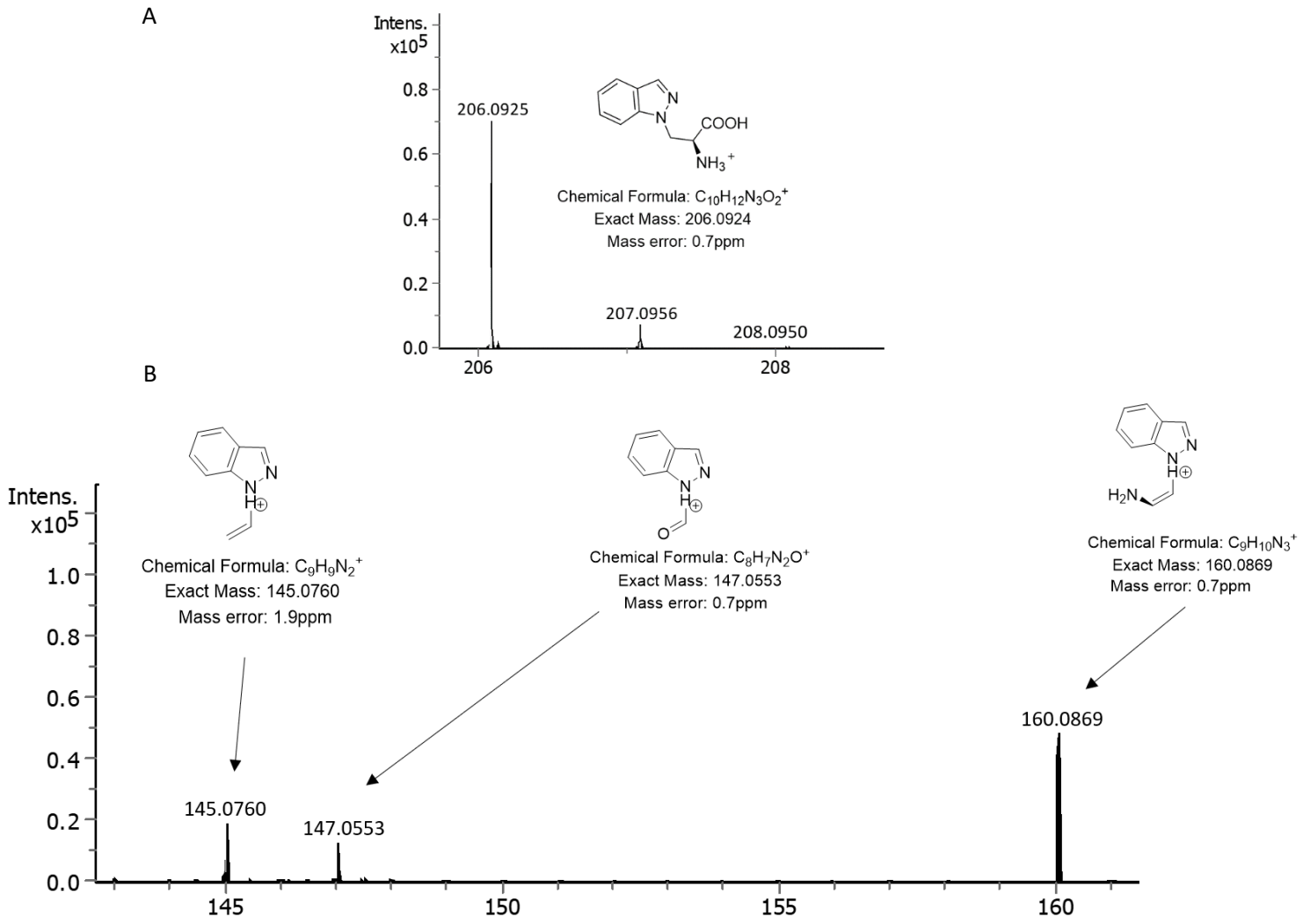


Figure S22. LC-MS (A) and MS/MS data (B) of indazole-tryptophan **41**.

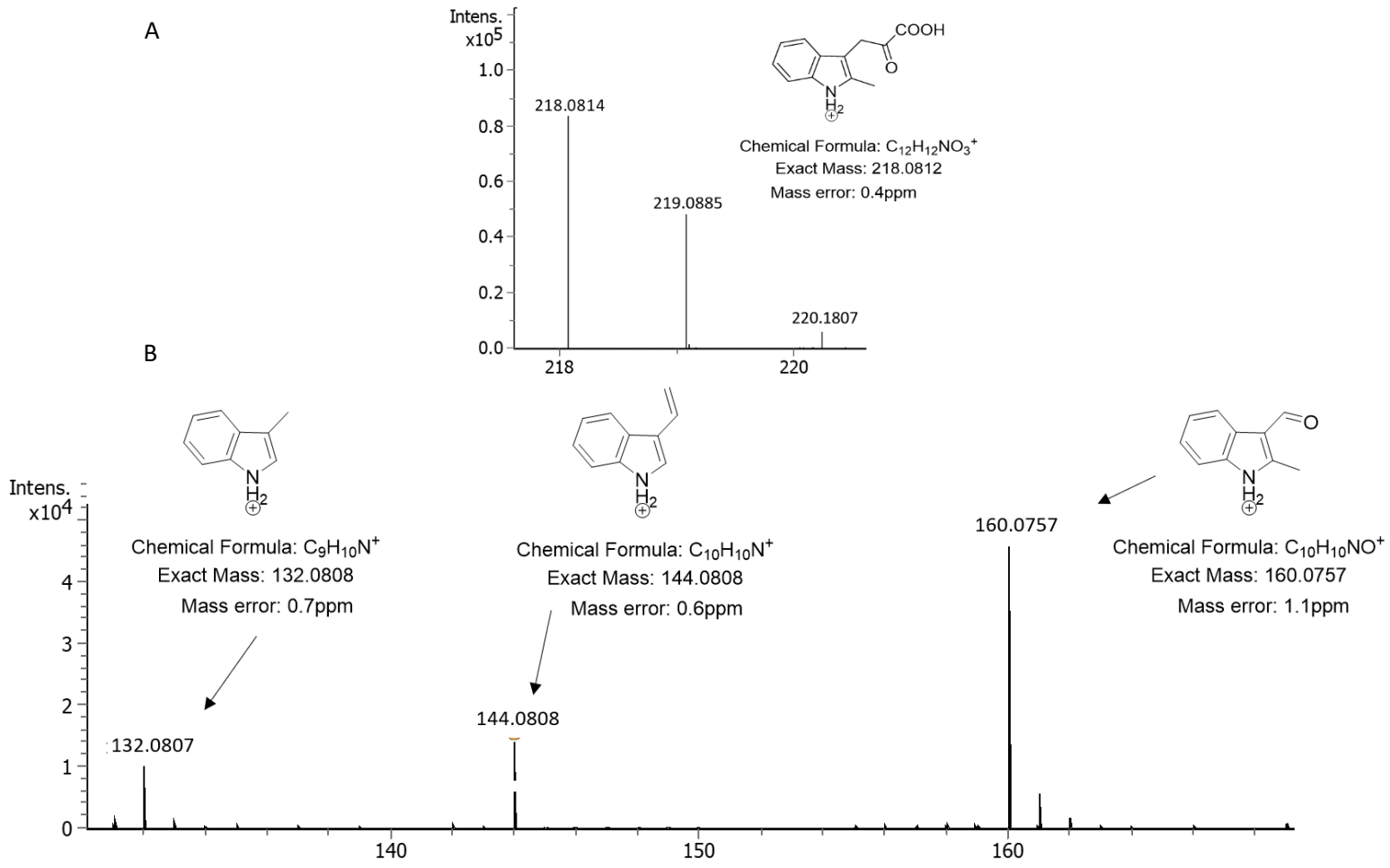


Figure S23. LC-MS (A) and MS/MS data (B) of 2-methyl-indole-3-pyruvate **42**.

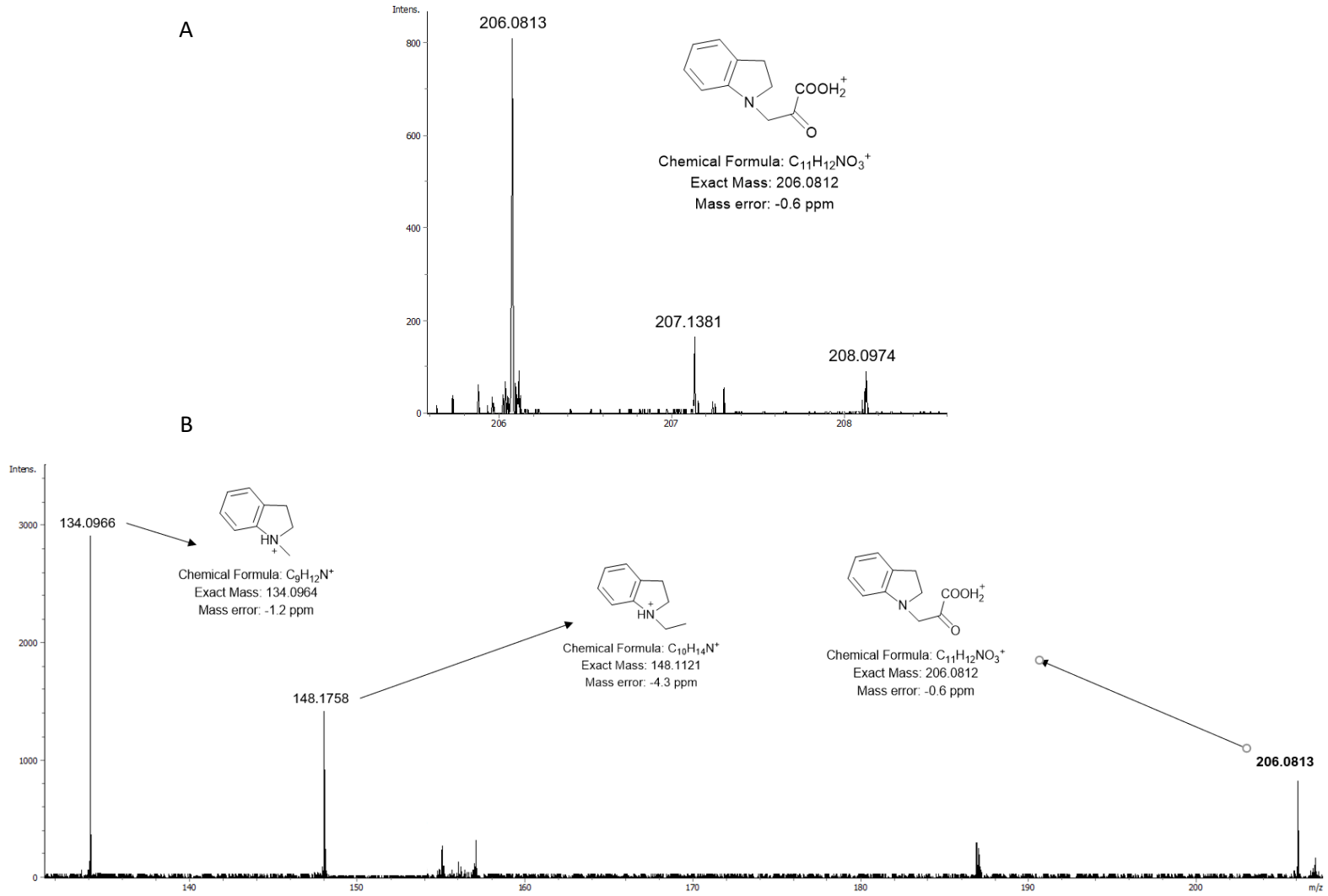


Figure S24. LC-MS (A) and MS/MS data (B) of indoline-3-pyruvate **43**.

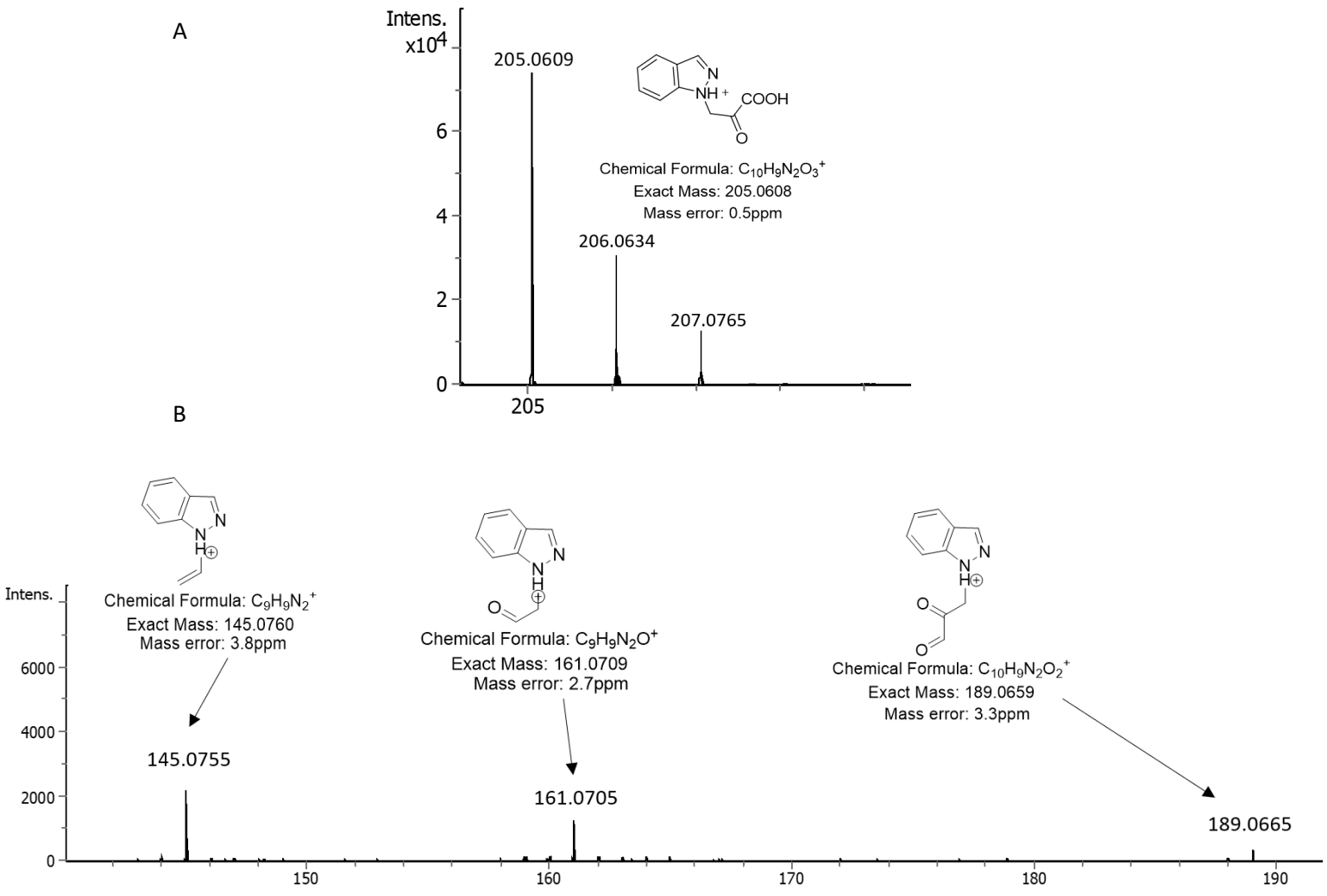


Figure S25. LC-MS (A) and MS/MS data (B) of indazole-3-pyruvate **44**.

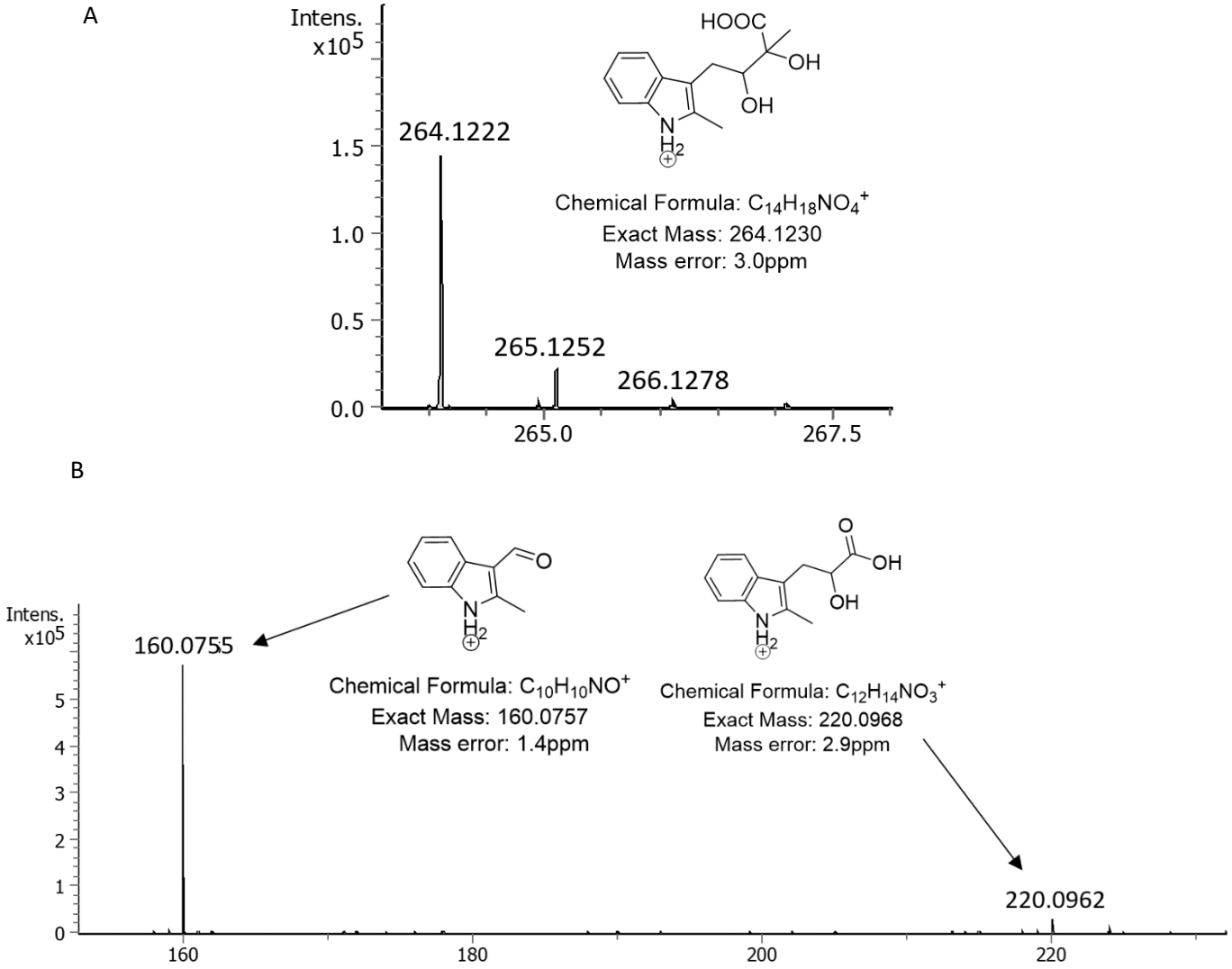
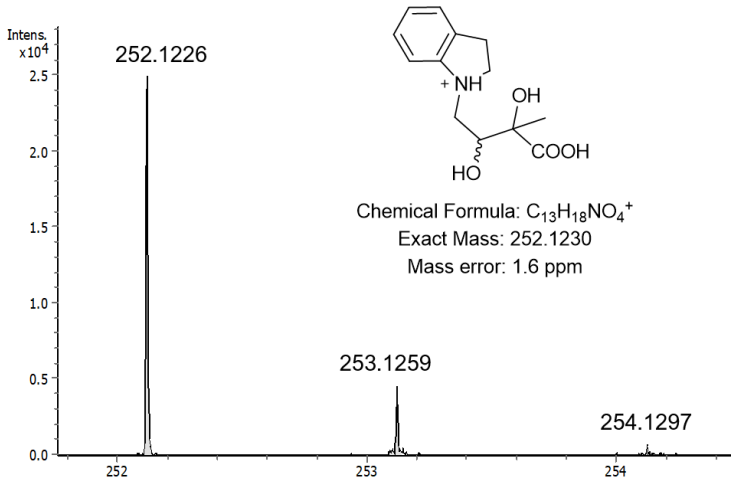


Figure S26. LC-MS (A) and MS/MS data (B) of 2-methyl-indole-containing-acyloin **45**.

A



B

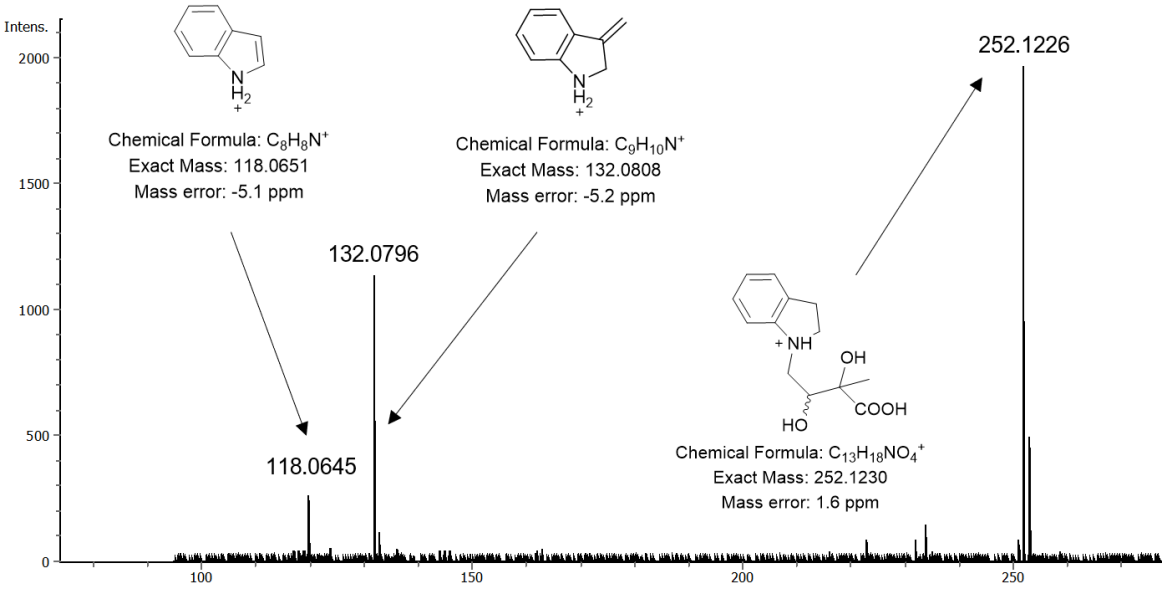
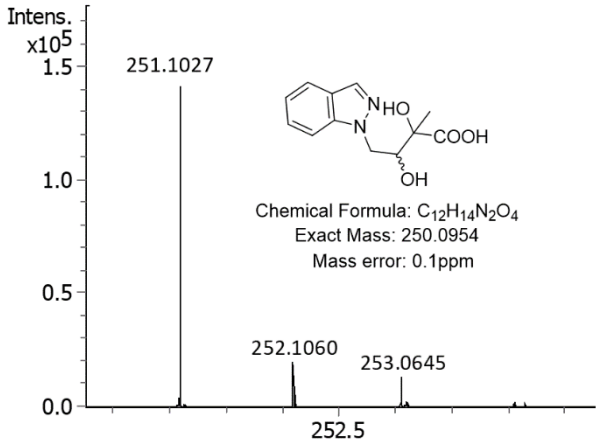


Figure S27. LC-MS (A) and MS/MS data (B) of indoline-containing-acyloin **46**.

A



B

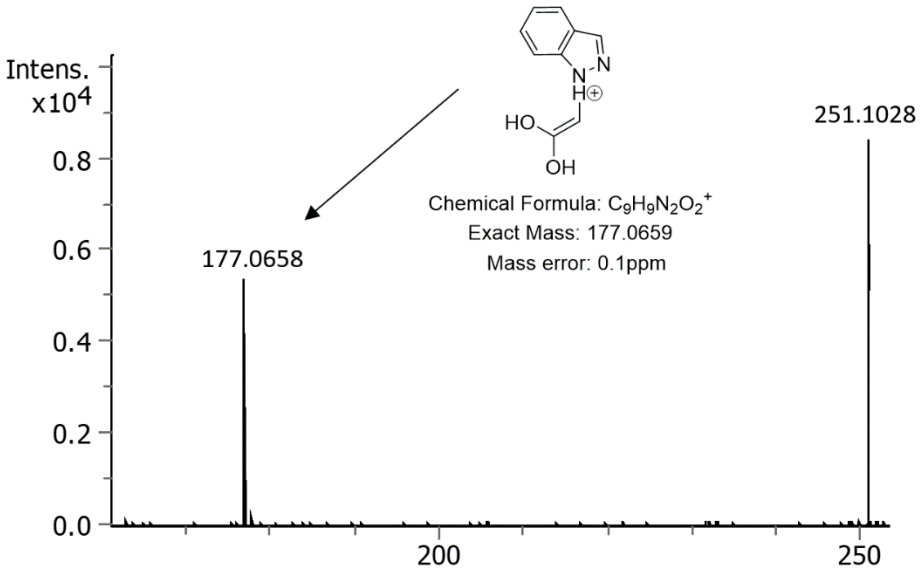


Figure S28. LC-MS (A) and MS/MS data (B) of indazole-containing-acyloin **47**.