

Supplementary Materials: Characteristic Distribution of Ciguatoxins in the Edible Parts of a Grouper, *Variola louti*

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Table S1. LC-MS/MS conditions for CTX analysis.

LC: Agilent 1290 Infinity (Agilent Technologies)	
Column: Zorbax Eclipse Plus C18	
(1.8 μ m, 2.1 $\times$ 50 mm, Agilent Technologies)	
Column Temp.: 40 $^{\circ}$ C	
Injection volume: 5 μ L	
Eluent A: 5 mM ammonium formate in 0.1% formic acid	
Eluent B: methanol	
Flow rate: 0.4 mL/min	
Gradient conditions	
1 (for general analysis):	
0 min (60%B)–0.25 min (60%B)–0.5 min (75%B)–12 min (90%B)–14 min (90%B)–14.1 min (100%B)	
2 (for less polar analogs):	
0 min (60%B)–0.25 min (60%B)–0.5 min (75%B)–23 min (90%B)–25 min (90%B)–25.1 min (100%B)	
3 (for higher polar analogs):	
0 min (50%B)–0.25 min (50%B)–0.5 min (65%B)–25 min (80%B)–27 min (80%B)–27.1 min (100%B)	
MS: 6460 Triple Quad LC/MS (Agilent Technologies)	
Ionization: ESI with Agilent Jet Stream	
Nebulizer: N ₂ , 50 psi	
Sheath gas: N ₂ , 380 $^{\circ}$ C, 11 L/min	
Dry gas: 300 $^{\circ}$ C, 10 L/min	
Capillary voltage: 5000 V	
Fragmentor voltage: 300 V	
Collision energy: 40 eV	
Monitor ions ([M+Na] ⁺ > [M+Na] ⁺)	
<i>m/z</i> 1045.6: CTX3C and 49- <i>epi</i> CTX3C	
<i>m/z</i> 1061.6: 2-hydroxyCTX3C and 51-hydroxyCTX3C	
<i>m/z</i> 1079.6: 2,3-dihydroxyCTX3C	
<i>m/z</i> 1083.6: CTX4A and CTX4B	
<i>m/z</i> 1095.6: 2,3,51-trihydroxyCTX3C	
<i>m/z</i> 1117.6: 52- <i>epi</i> -54-deoxyCTX1B and 54-deoxyCTX1B	
<i>m/z</i> 1133.5: CTX1B	

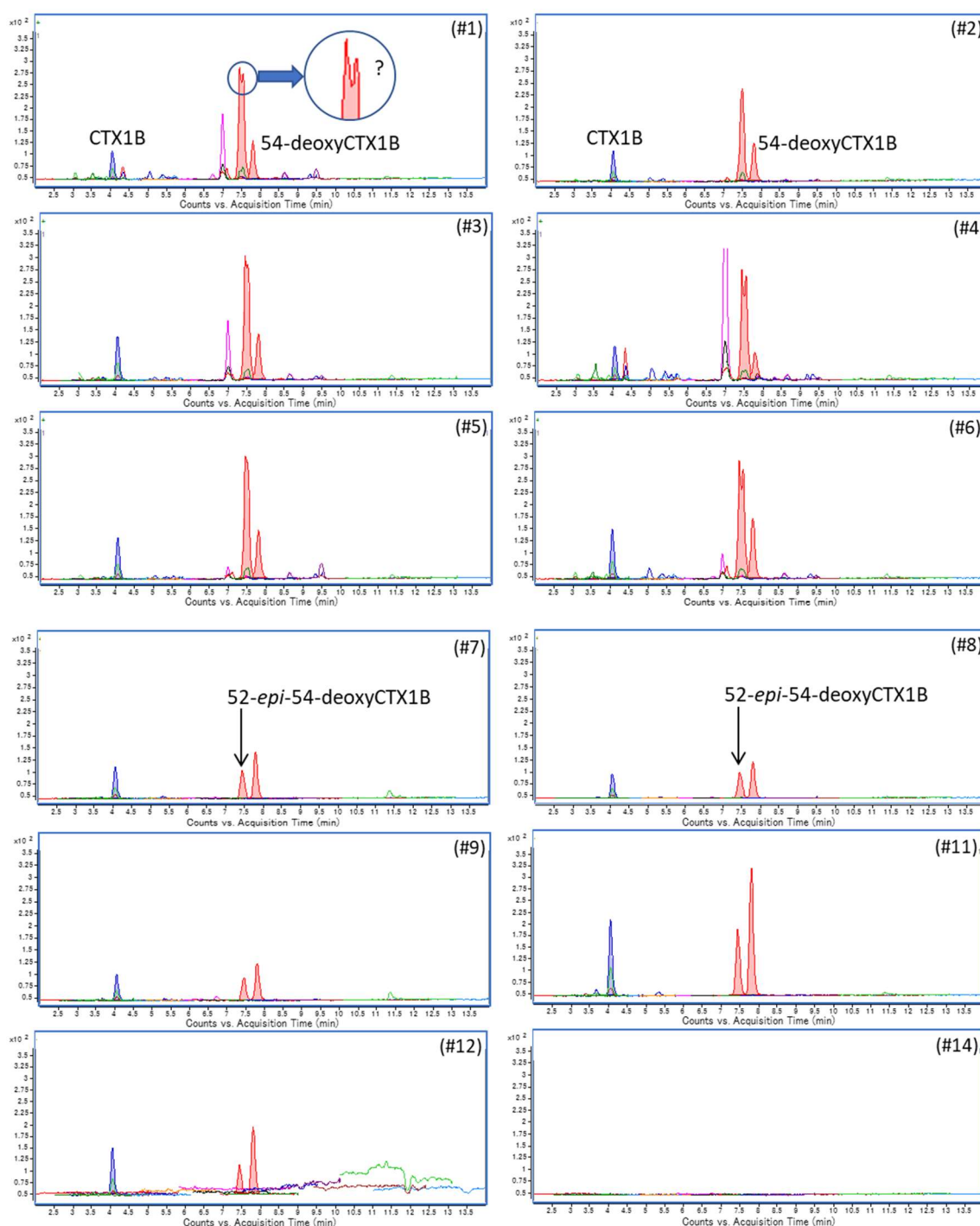


Figure S1. LC-MS/MS chromatograms in Gradient I of samples (#1–#9, #11, #12, and #14) prepared from Specimen E (ID 160136).

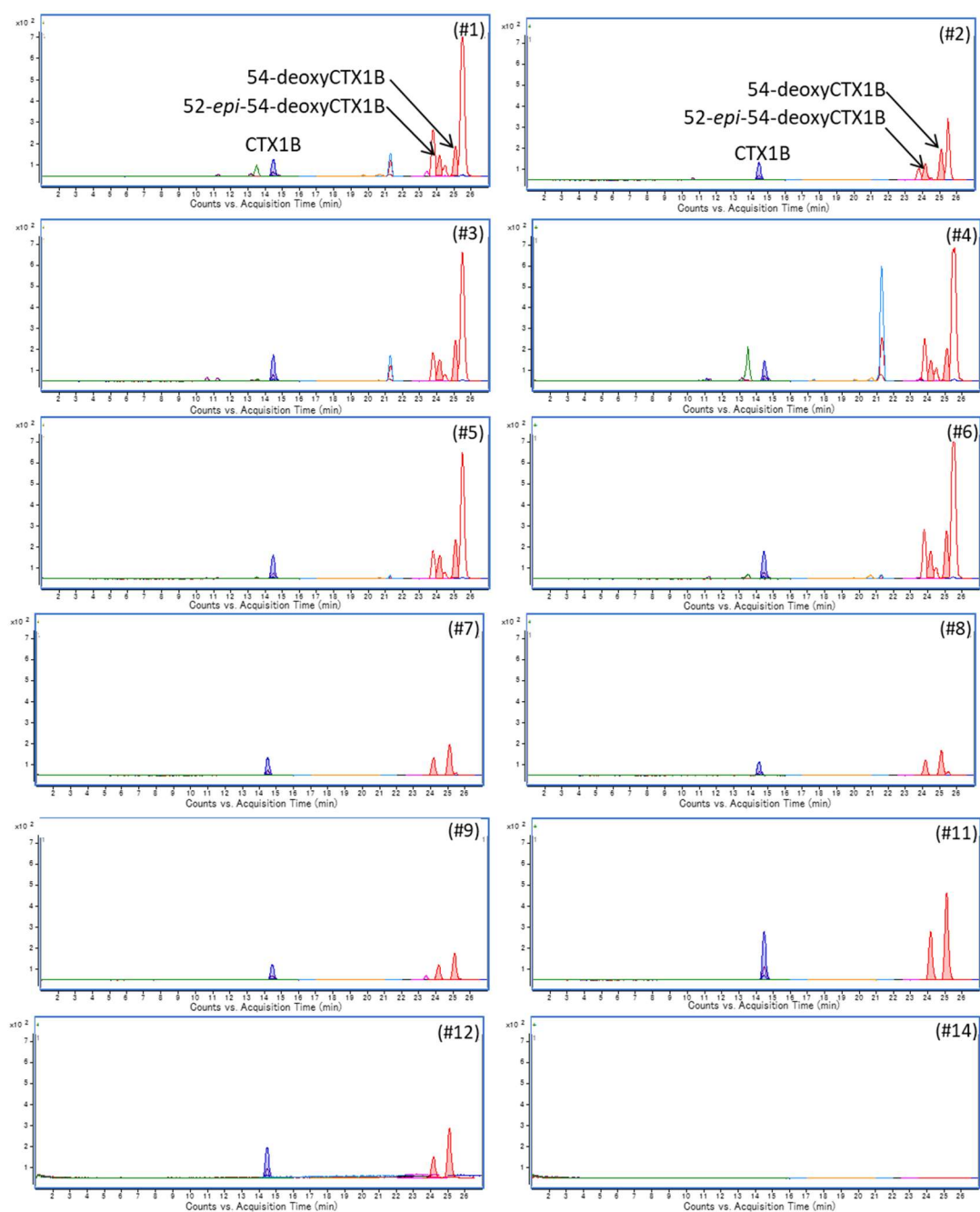


Figure S2. LC-MS/MS chromatograms in Gradient II of samples (#1–#9, #11, #12, and #14) prepared from Specimen E (ID 160136).

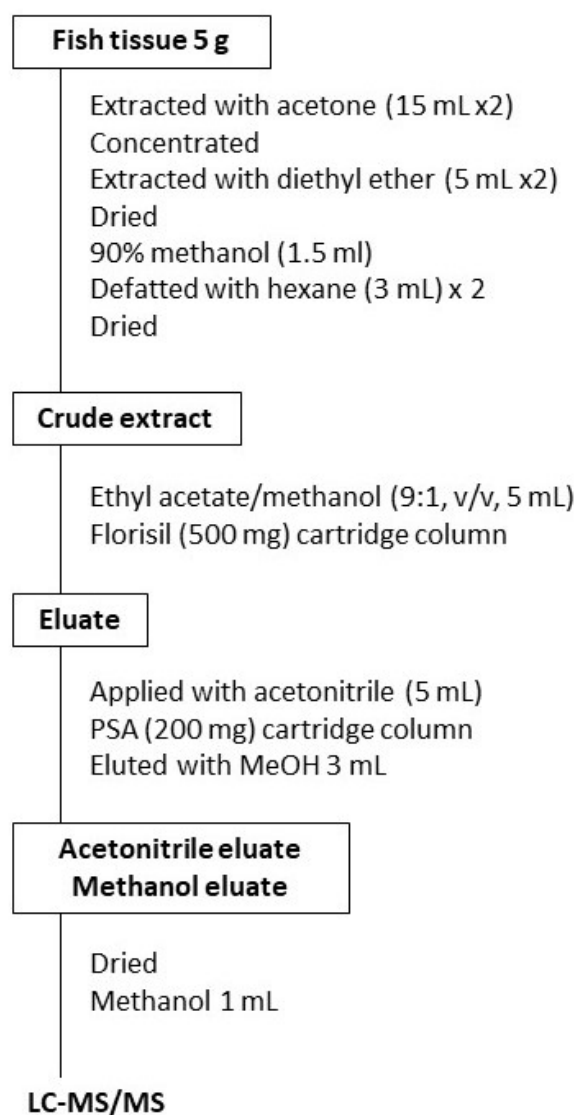


Figure S3. Sample preparation from fish flesh for LC-MS/MS.