Supporting information

Structural Characterization and Absolute Quantification of Microcystin Peptides using Collision Induced- and Ultraviolet Photo-Dissociation Tandem Mass Spectrometry

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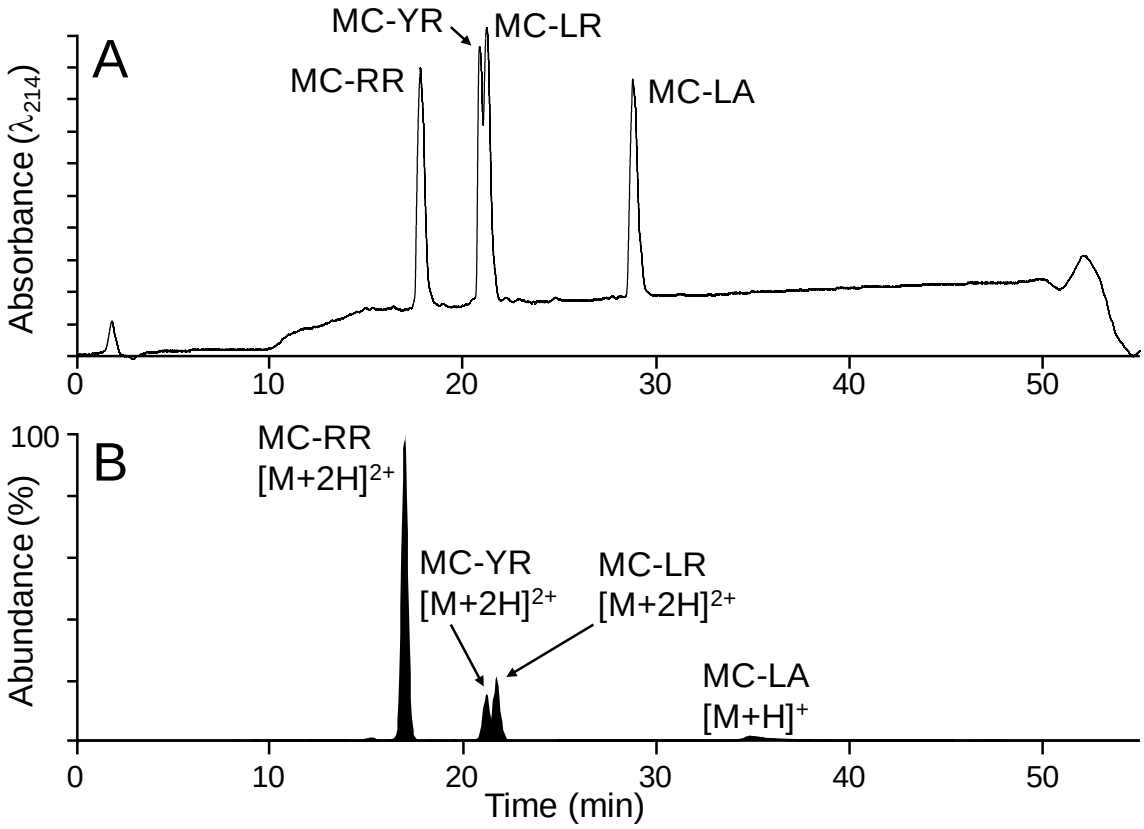

Figure S1. Equimolar mixture of Microcystin-LR, -YR, -RR and -LA showing (A) the RP-HPLC elution profile with UV detection at 214 nm (B) the capillary LC-ESI-MS base peak ion chromatograms.

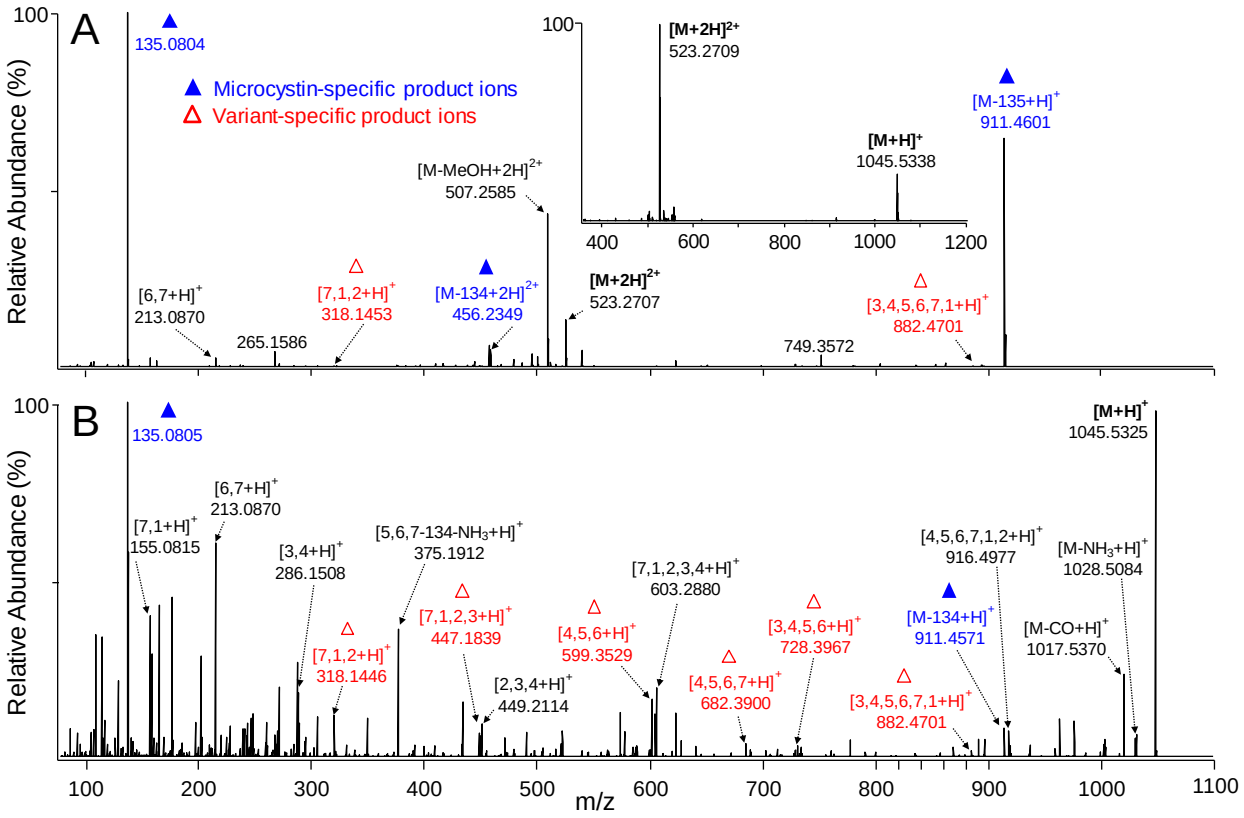

Figure S2. Representative HCD-MS/MS spectra of (A) the $[M+2H]^{2+}$ ion (12% NCE) and (B) the $[M+H]^{+}$ ion (32% NCE) of Microcystin-YR. The ESI-MS spectrum is shown in the inset to panel A. 'Global' microcystin-specific product ions are indicated by a ▲; variant-specific product ions are indicated by a △.

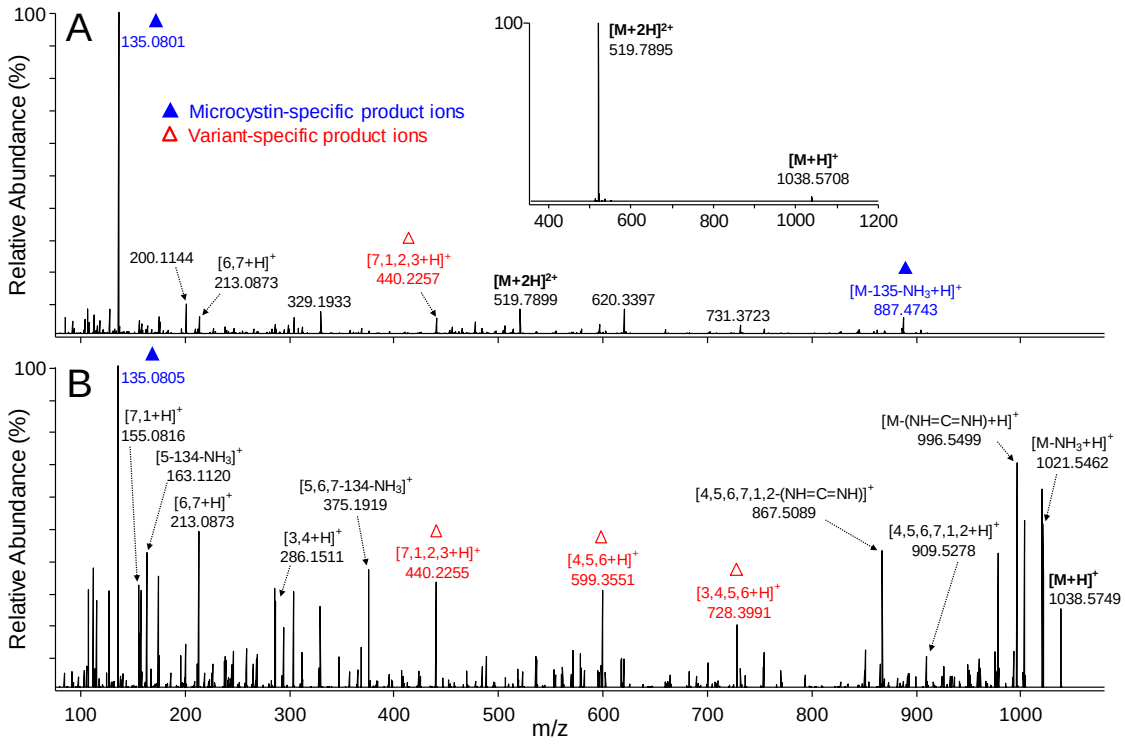

Figure S3. Representative HCD-MS/MS spectra of (A) the $[M+2H]^{2+}$ ion (34% NCE) and (B) the $[M+H]^{+}$ ion (34% NCE) of Microcystin-RR. The ESI-MS spectrum is shown in the inset to panel A. 'Global' microcystin-specific product ions are indicated by a ▲; variant-specific product ions are indicated by a △.

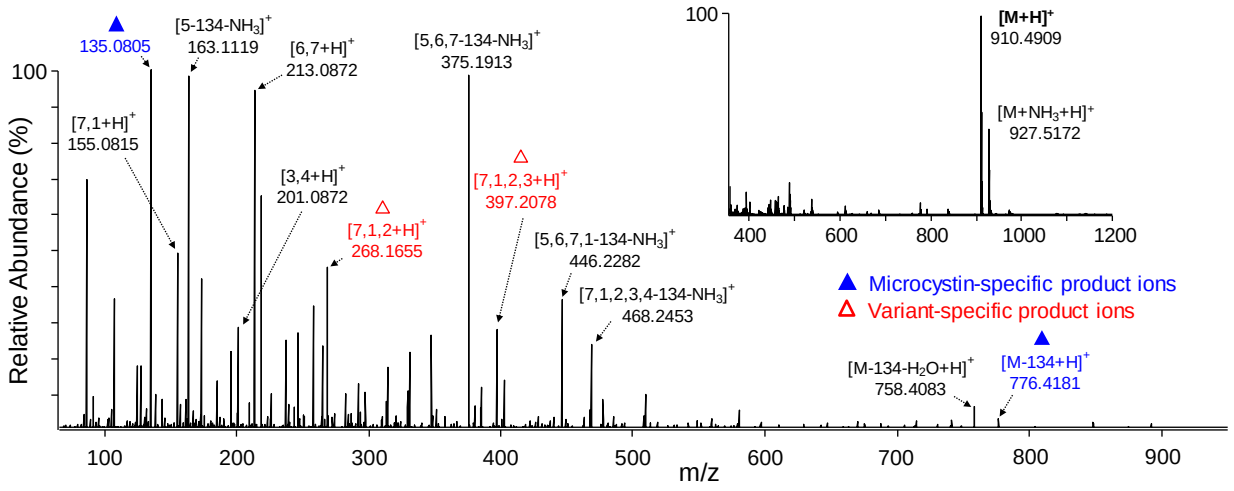

Figure S4. Representative HCD-MS/MS spectra of the $[M+H]^+$ ion (26% NCE) of Microcystin-LA. The ESI-MS spectrum is shown in the inset to panel A. Global microcystin-specific product ions are indicated by a ▲; variant-specific product ions are indicated by a △.

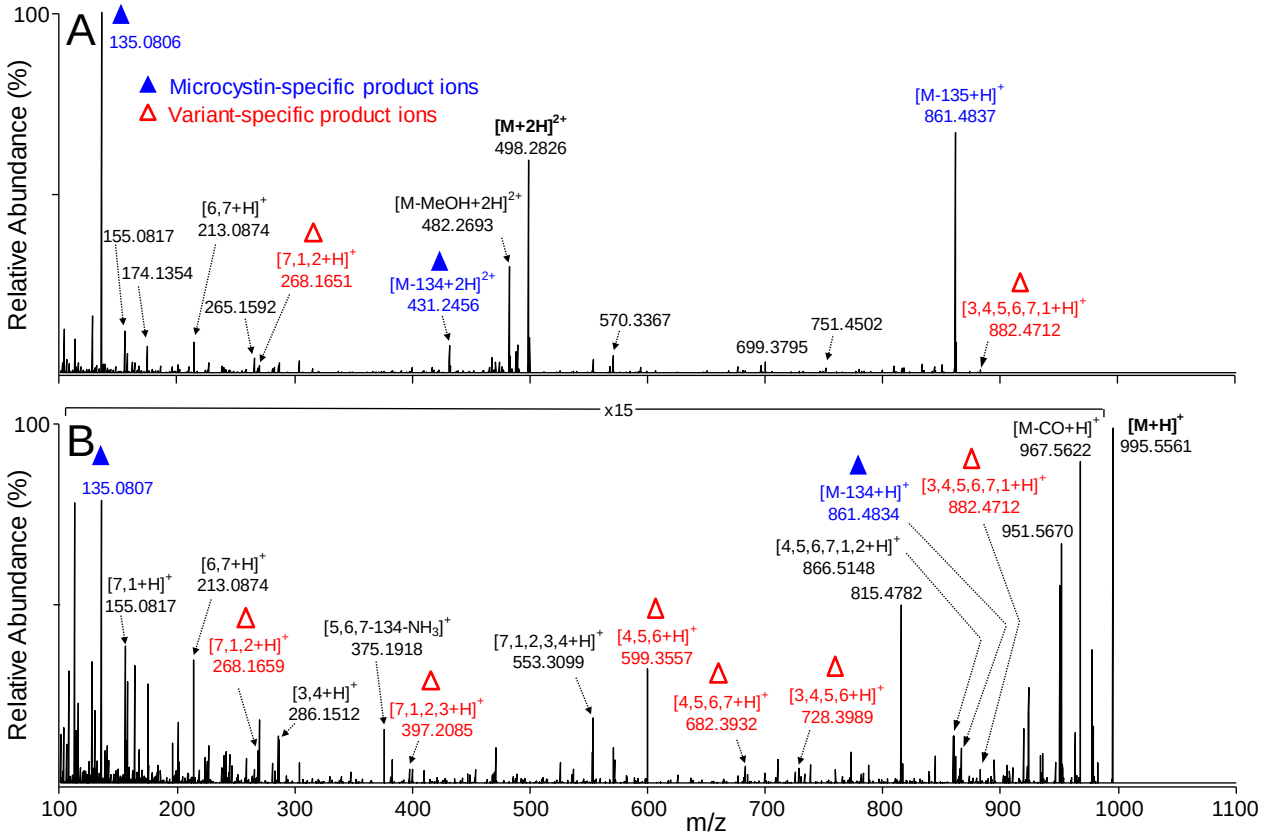

Figure S5. Optimized 193 nm UVPD-MS/MS spectra of (A) the $[M+2H]^{2+}$ ion (800V, 5 laser pulses) and (B) the $[M+H]^{+}$ ion (700V, 20 laser pulses) of Microcystin-LR. Global microcystin-specific product ions are indicated by a ▲; variant-specific product ions are indicated by a △.

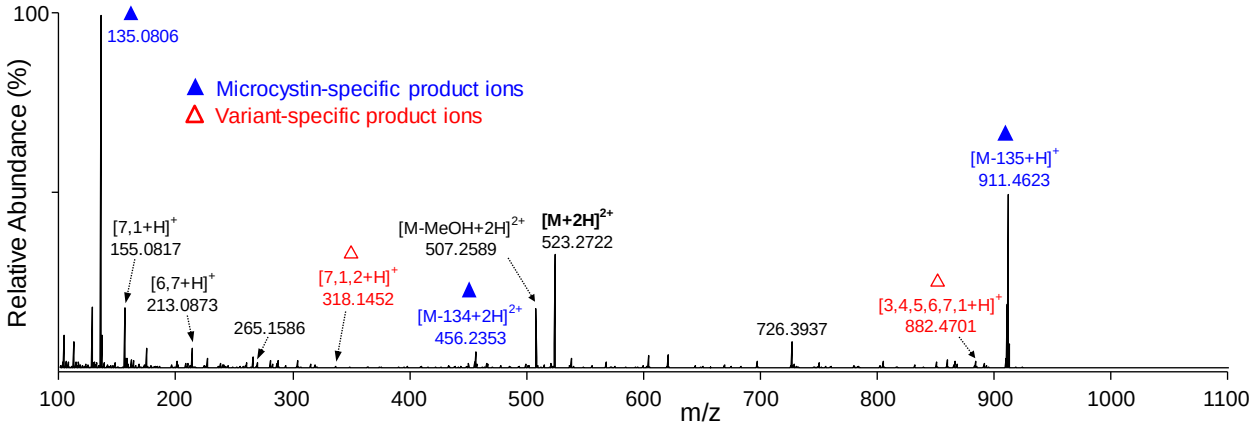

Figure S6. Optimized 193 nm UVPD-MS/MS spectra of the $[M+2H]^{2+}$ ion (700V, 10 laser pulses) of Microcystin-YR. Global microcystin-specific product ions are indicated by a ▲; variant-specific product ions are indicated by a △.

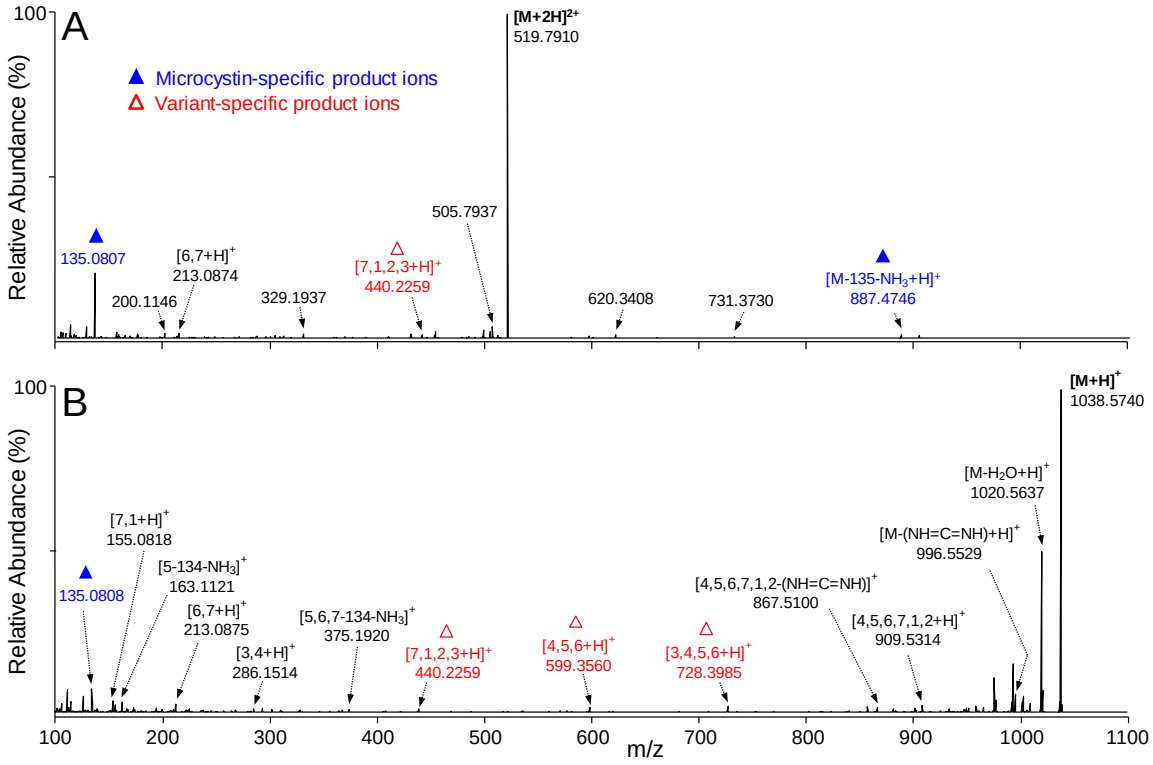

Figure S7. Optimized 193 nm UVPD-MS/MS spectra of (A) the $[M+2H]^{2+}$ ion (800V, 5 laser pulses) and (B) the $[M+H]^{+}$ ion (700V, 20 laser pulses) of Microcystin-RR. Global microcystin-specific product ions are indicated by a ▲; variant-specific product ions are indicated by a △.

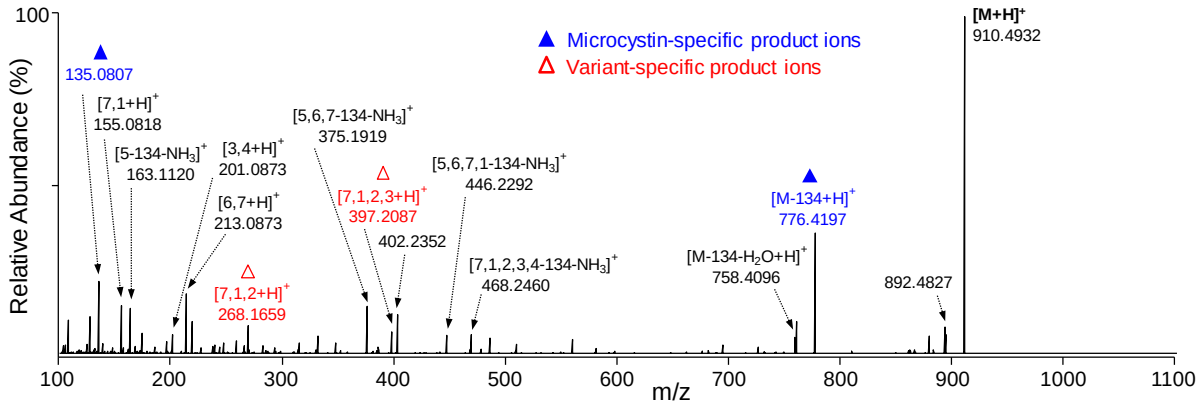

Figure S8. 193 nm UVPD-MS/MS spectra of the $[M+H]^+$ ion (800V, 5 laser pulses) of Microcystin-LA. Global microcystin-specific product ions are indicated by a ▲; variant-specific product ions are indicated by a Δ.