

Supplementary Material

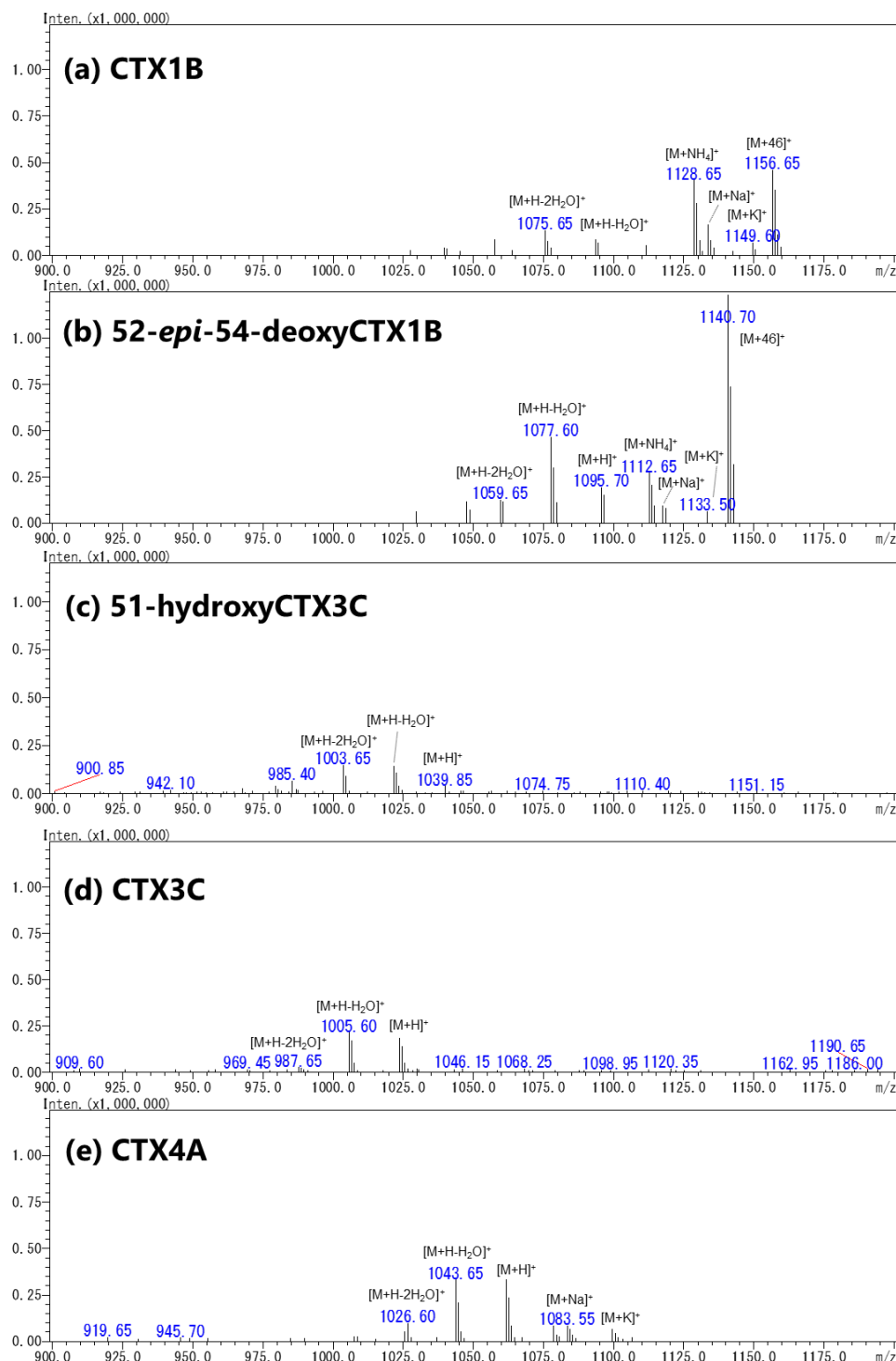


Figure S1. A. Mass spectra of CTXs observed by Scan mode under the acetonitrile mobile phase condition. (a) CTX1B, (b) 52-*epi*-54-deoxyCTX1B, (c) 51-hydroxyCTX3C, (d) CTX3C, (e) CTX4A.

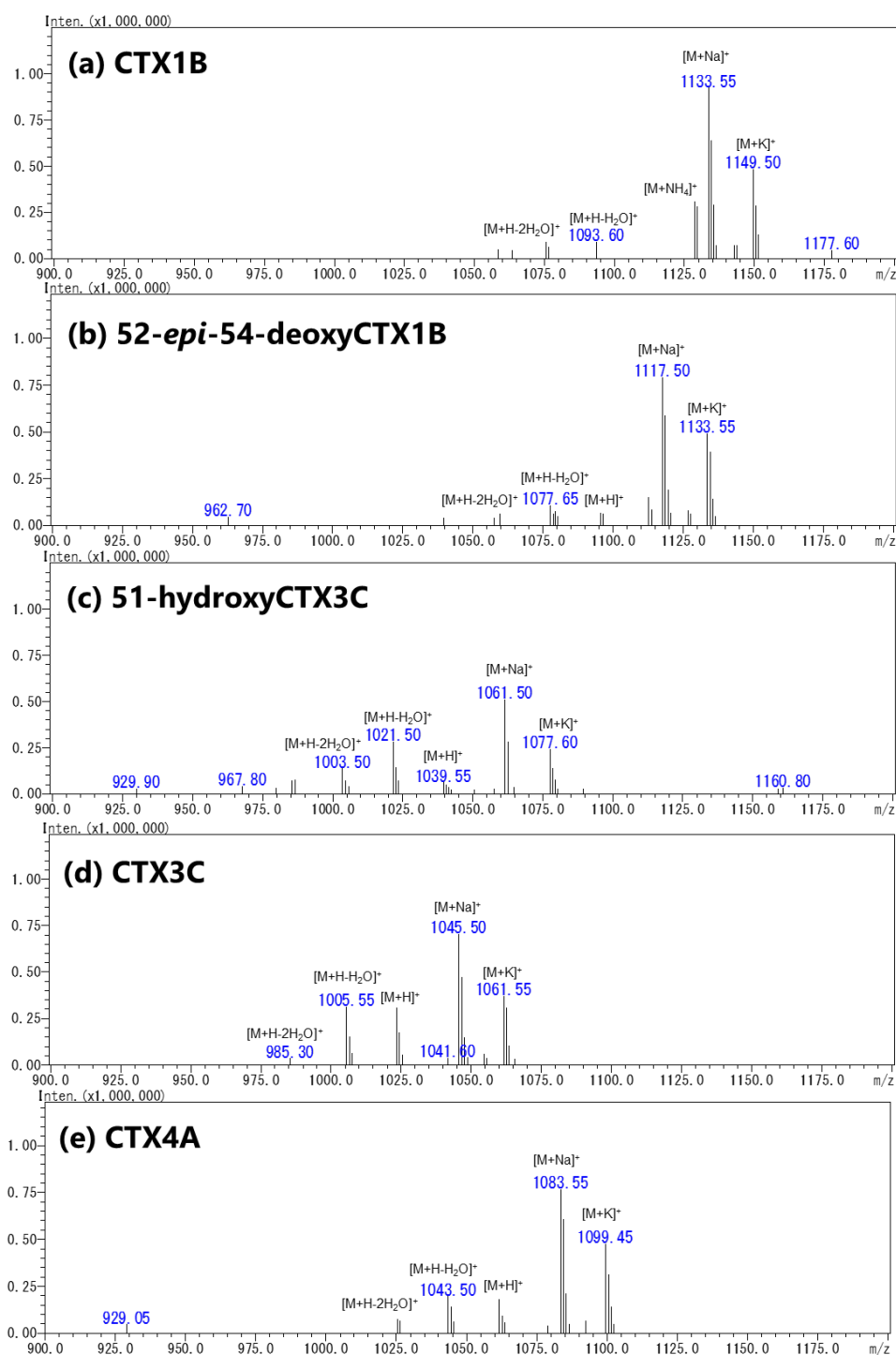


Figure S1B. Mass spectra of CTXs observed by Scan mode under the methanol mobile phase condition. (a) CTX1B, (b) 52-*epi*-54-deoxyCTX1B, (c) 51-hydroxyCTX3C, (d) CTX3C, (e) CTX4A.

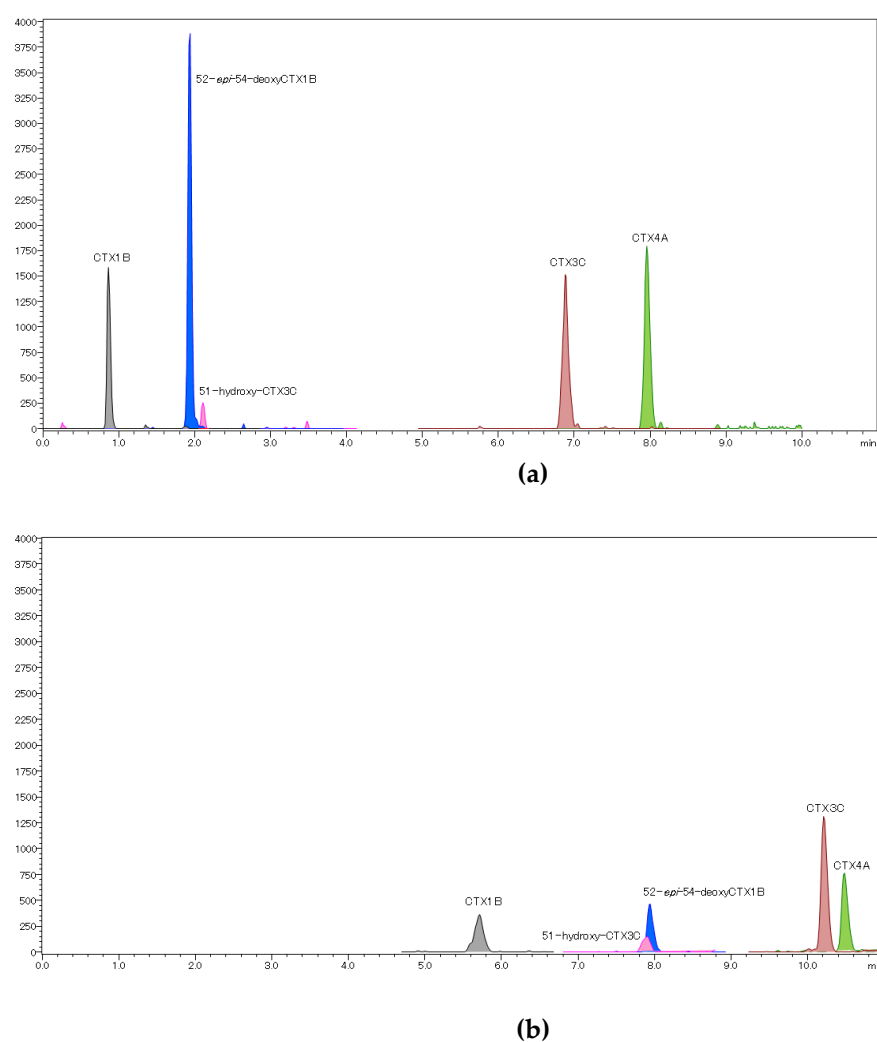


Figure S2. The LC-MS/MS (MRM) chromatograms of CTXs recording under the conditions described in previous reports (The transitions and collision energy were optimized to give best sensitivity for each analog. CTX1B: m/z 1128.60>1093.60 and CE -21.0 V, 51-hydroxy-CTX3C: m/z 1056.60>1039.60 and CE -15.0 V, 52-*epi*-54-deoxyCTX1B: m/z 1112.60>1077.60 and CE -22.0 V, CTX3C: m/z 1023.60>125.10 and CE -48.0 V, CTX4A: m/z 1078.60>1043.60 and CE; -19.0 V). (a) acetonitrile-based mobile phases [40]. (b) methanol-based mobile phases[10].

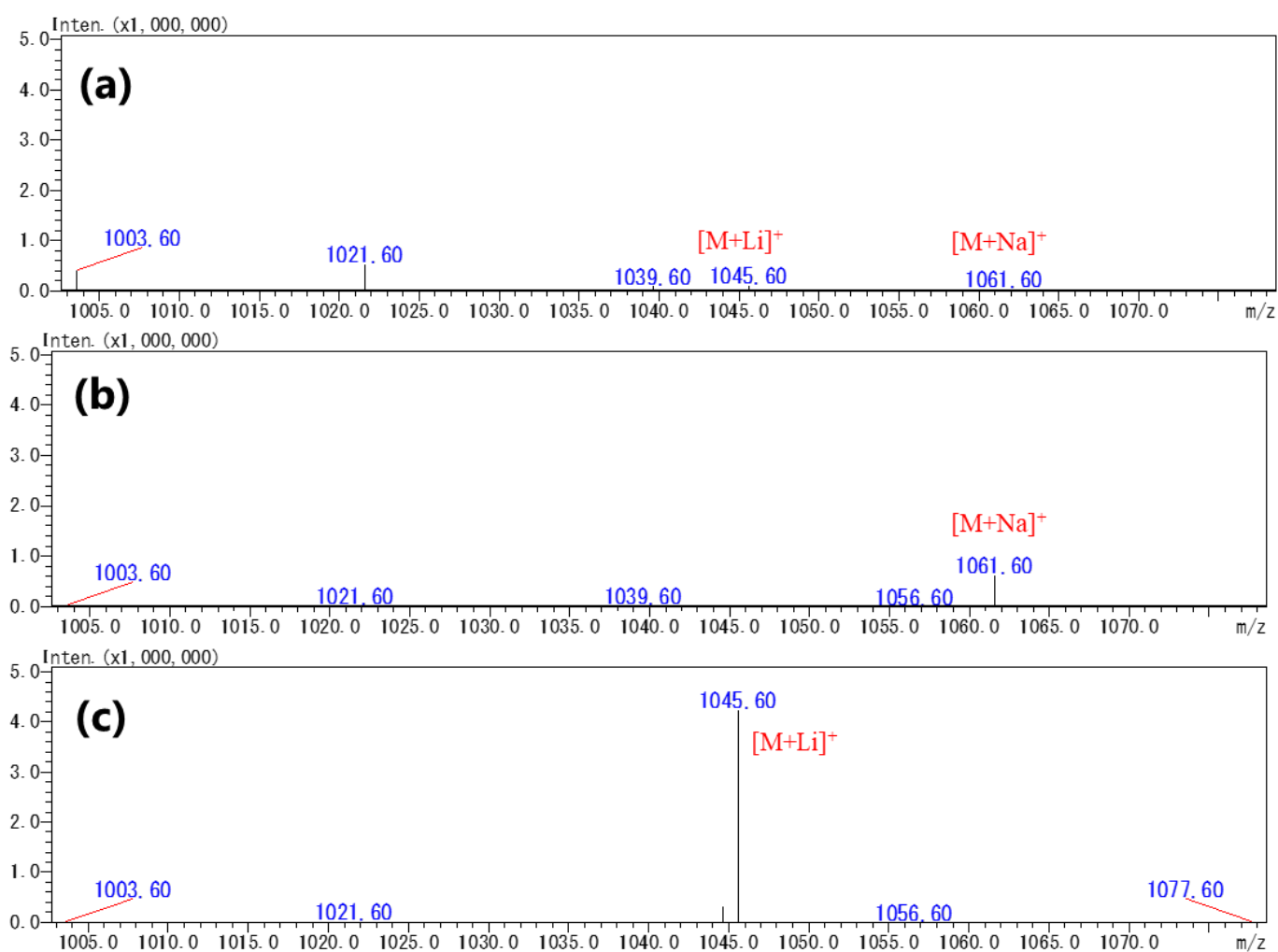


Figure S3. Mass spectra of 51-hydroxyCTX3C taken under the acetonitrile-based mobile phases (a) without any supplement, (b) supplemented with Na⁺ (NaOH), and (c) supplemented with Li⁺ (LiOH).

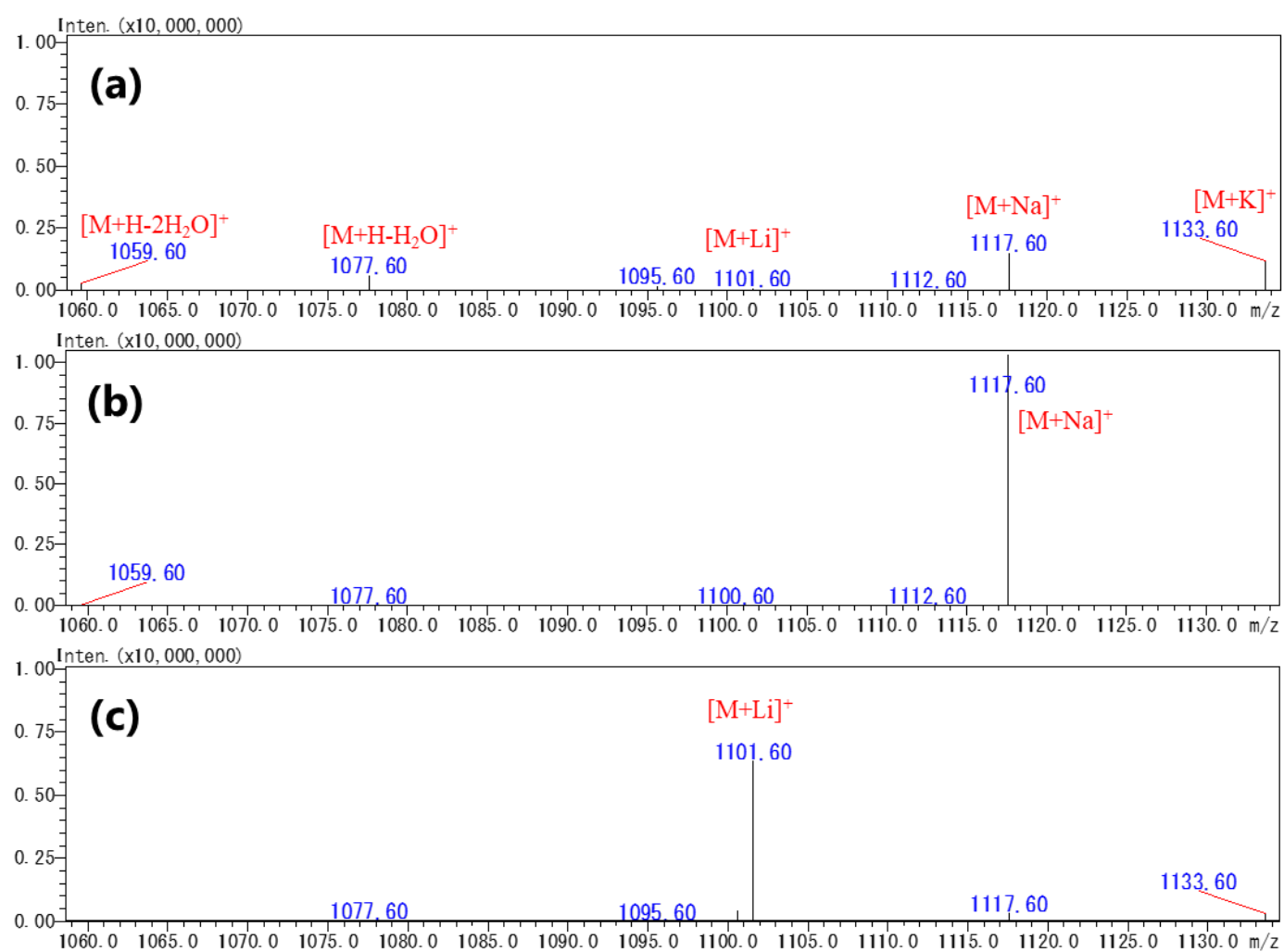


Figure S4. Mass spectra of 52-*epi*-54-deoxyCTX1B taken under the acetonitrile-based mobile phases (a) without any supplement, (b) supplemented with Na⁺ (NaOH), and (c) supplemented with Li⁺ (LiOH).

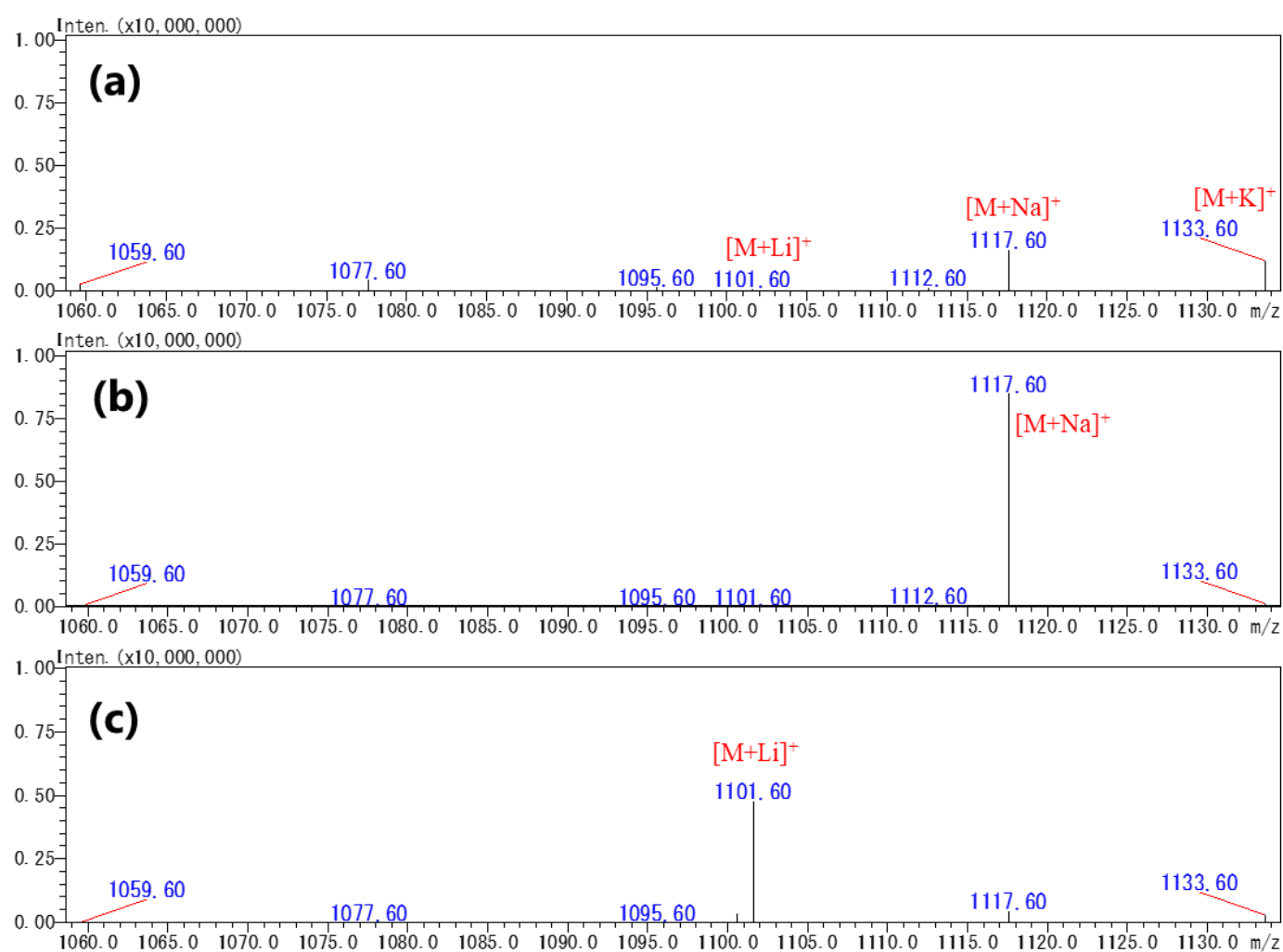


Figure S5. Mass spectra of 54-deoxyCTX1B taken under the acetonitrile-based mobile phases (a) without any supplement, (b) supplemented with Na^+ (NaOH), and (c) supplemented with Li^+ (LiOH).

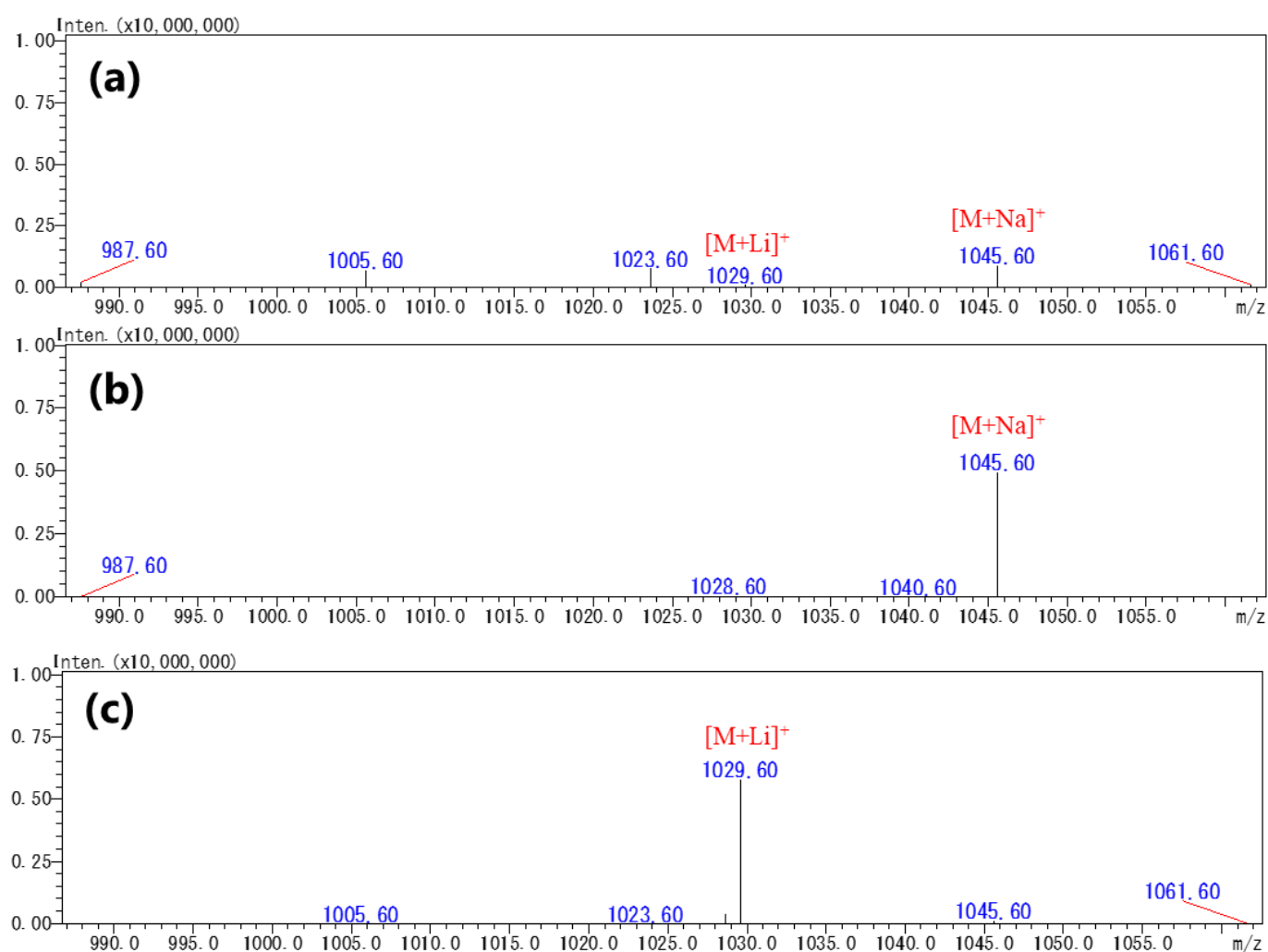


Figure S6. Mass spectra of 49-epiCTX3C taken under the acetonitrile-based mobile phases (a) without any supplement, (b) supplemented with Na^+ (NaOH), and (c) supplemented with Li^+ (LiOH).

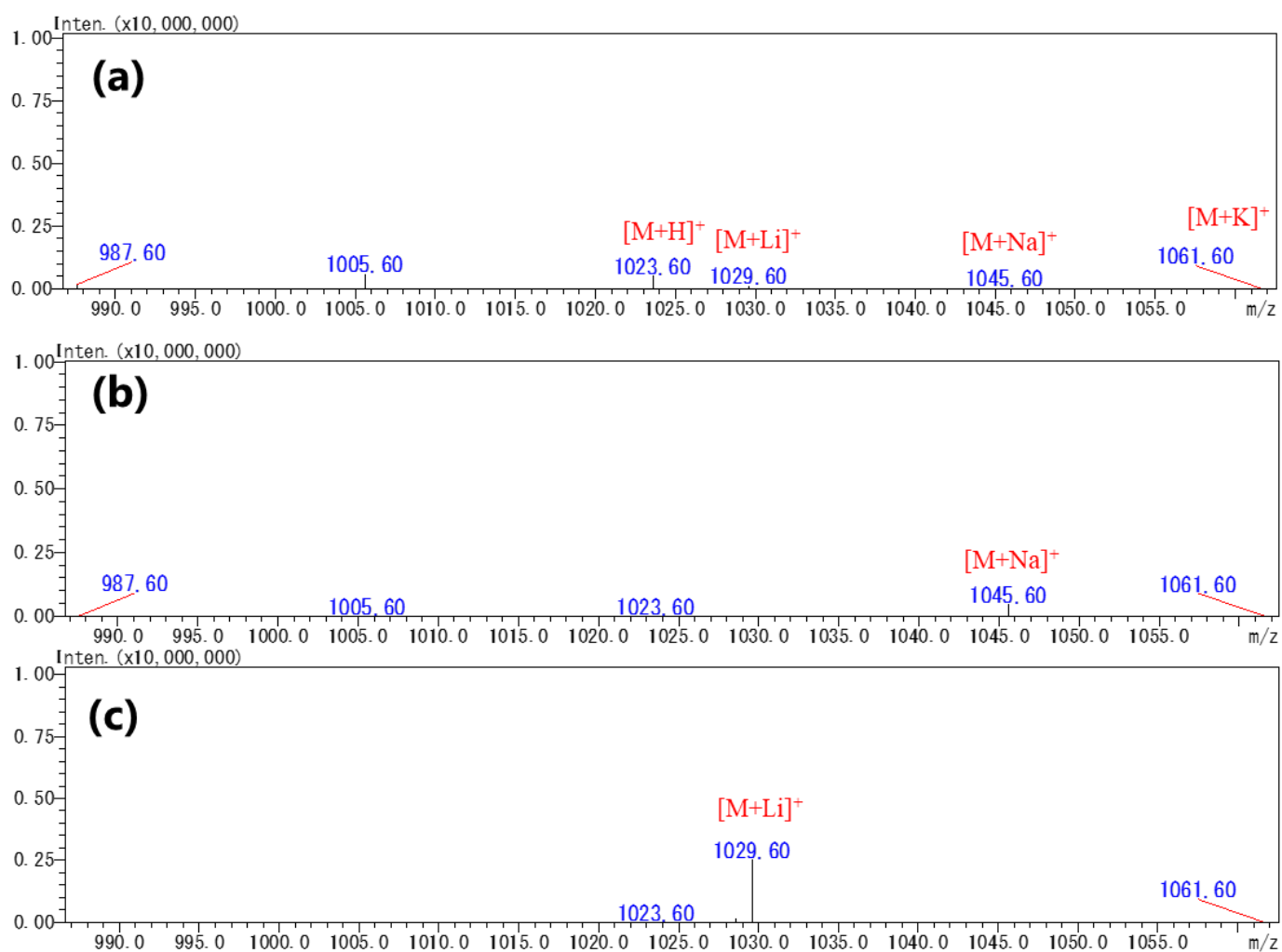


Figure S7. Mass spectra of CTX3C taken under the acetonitrile-based mobile phases (a) without any supplement, (b) supplemented with Na⁺ (NaOH), and (c) supplemented with Li⁺ (LiOH).

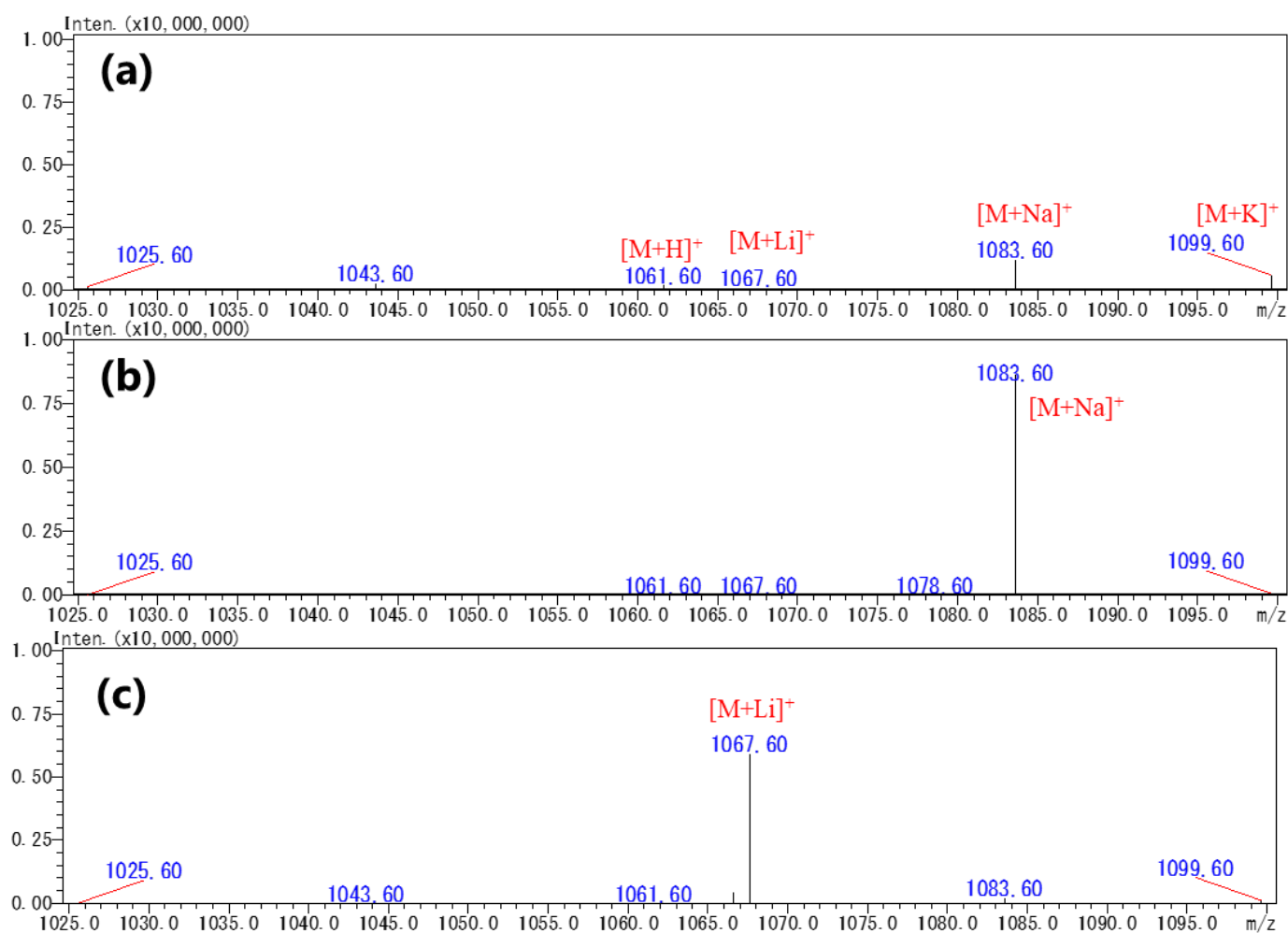


Figure S8. Mass spectra of CTX4A taken under the acetonitrile-based mobile phases (a) without any supplement, (b) supplemented with Na⁺ (NaOH), and (c) supplemented with Li⁺ (LiOH).

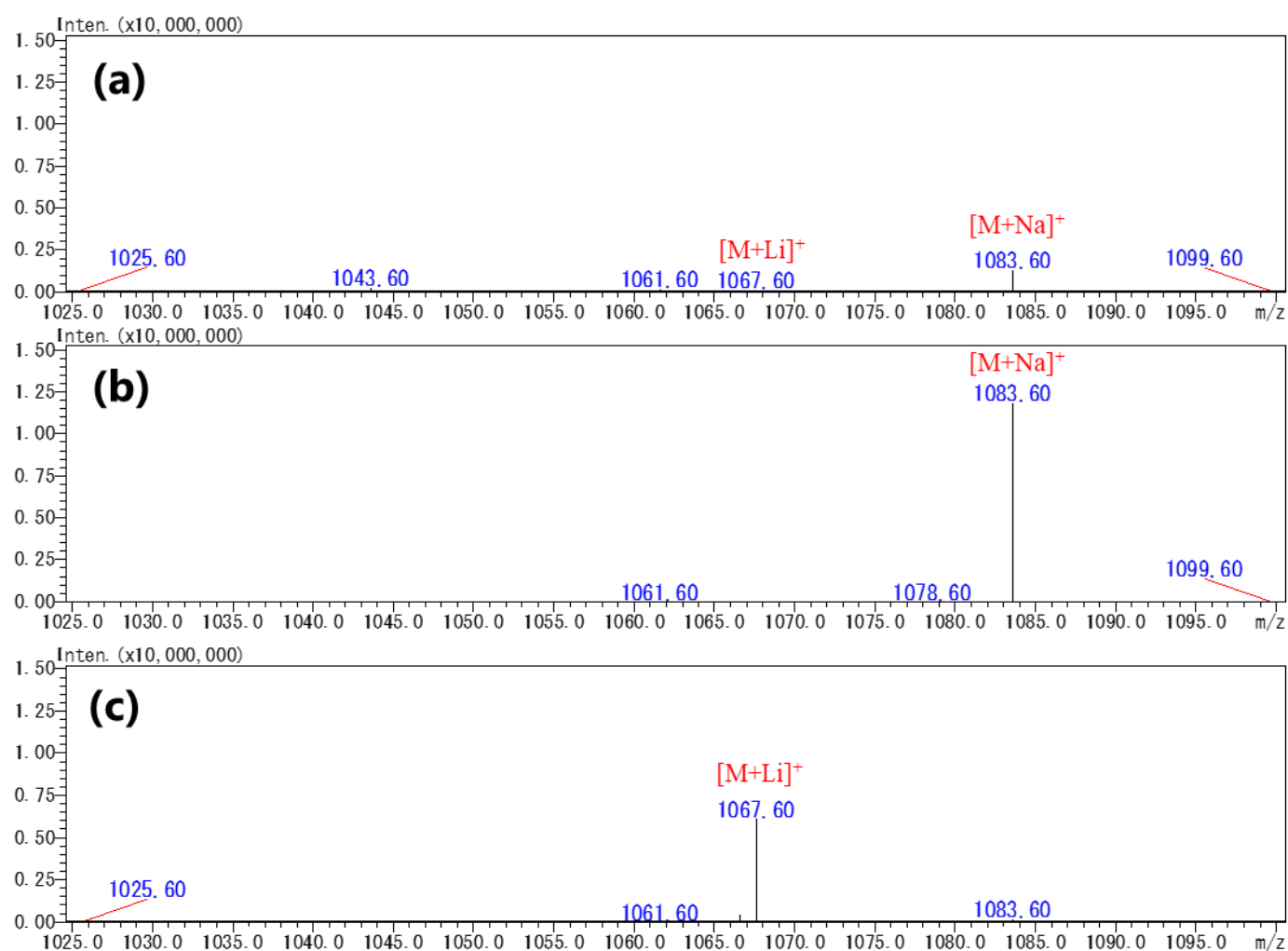


Figure S9. Mass spectra of CTX4B taken under the acetonitrile-based mobile phases (a) without any supplement, (b) supplemented with Na^+ (NaOH), and (c) supplemented with Li^+ (LiOH).