

Product ion spectra of selected fragments discussed in the publication

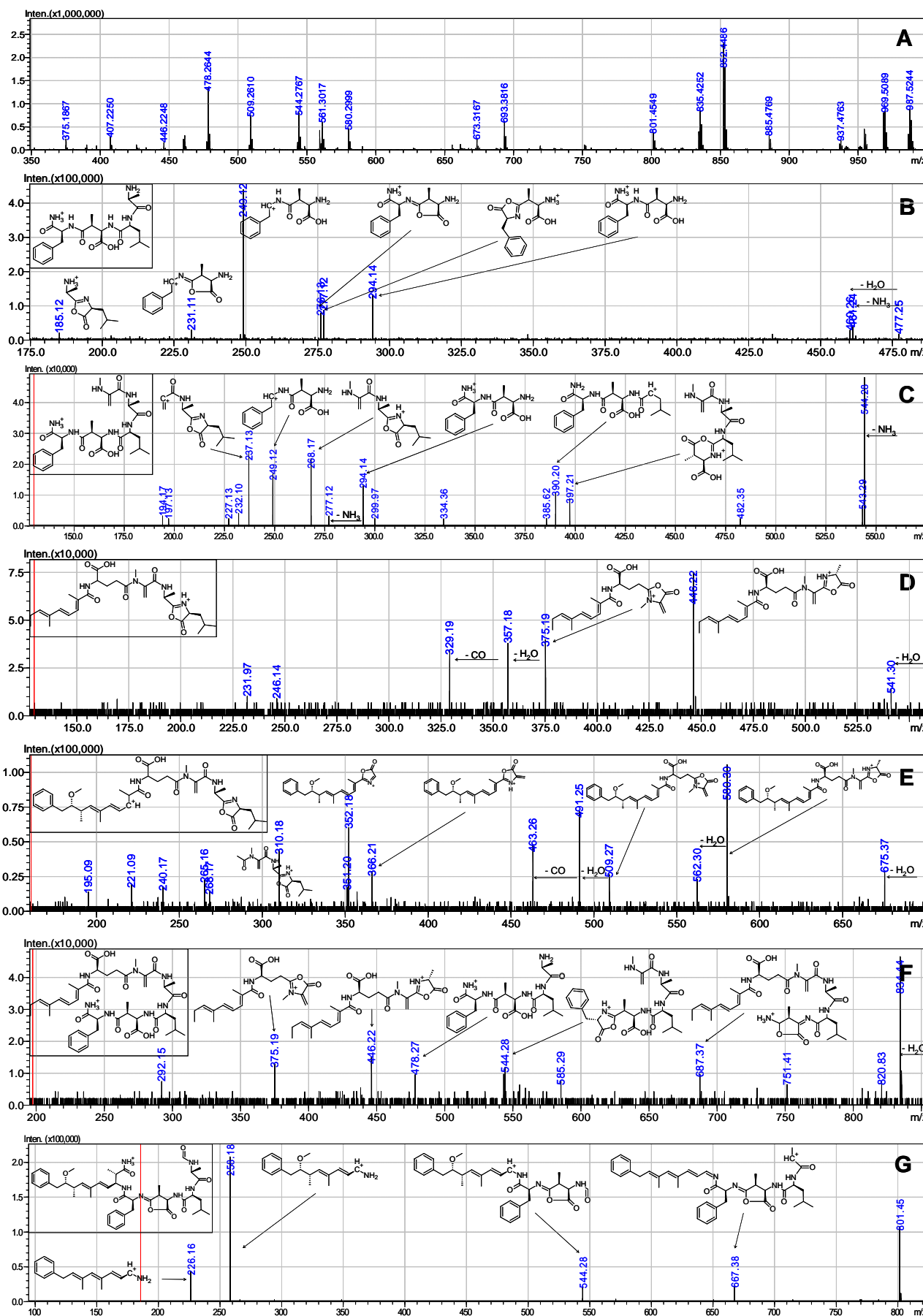


Figure S1a. MS² and MS³ spectra of microcystin LF and their interpretation. **A** Overview of MS/MS spectrum, product ion spectra of the fragments at m/z **B** 478.2644 ($C_{7[1]1[1-4]}$), **C** 561.3017 ($C_{4[5]1[1-4]}$), **D** 559.3127 ($Z_{[2]3[1]3-7]-C_9H_{10}O}$), **E** 693.3816 ($Z_{[2]3[1]3-7}$), **F** 852.4486 (M- $C_9H_{10}O$), and **G** 801.4549 ($C_{7[1]1[1-5]}-H_2O+CO$).

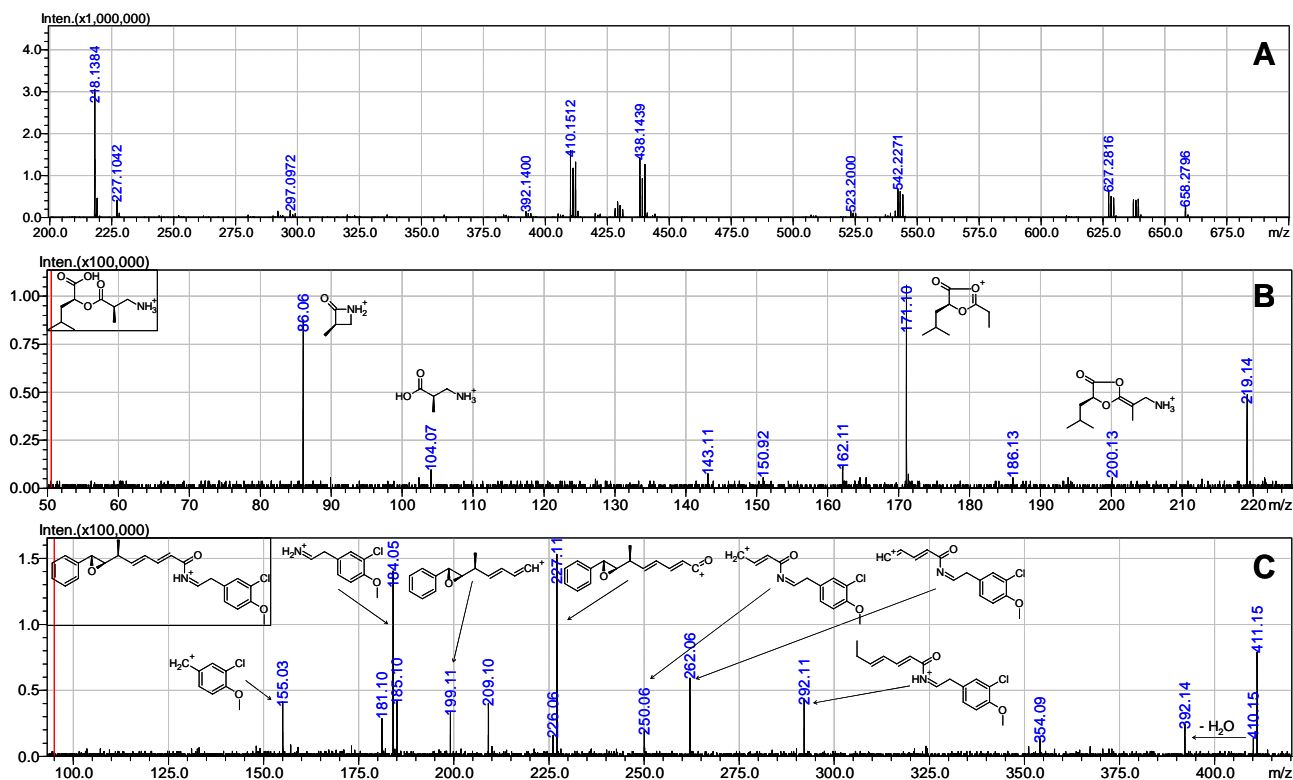


Figure S1b. MS² and MS³ spectra of cryptophycin-1 and their interpretation. **A** Overview of MS/MS spectrum, product ion spectra of the fragments at m/z **B** 218.1384 ($b_{[2][3][1-2]}+H_2O$) and **C** 410.1512 ($a_{[4][1][1-2]}-H_2O$).