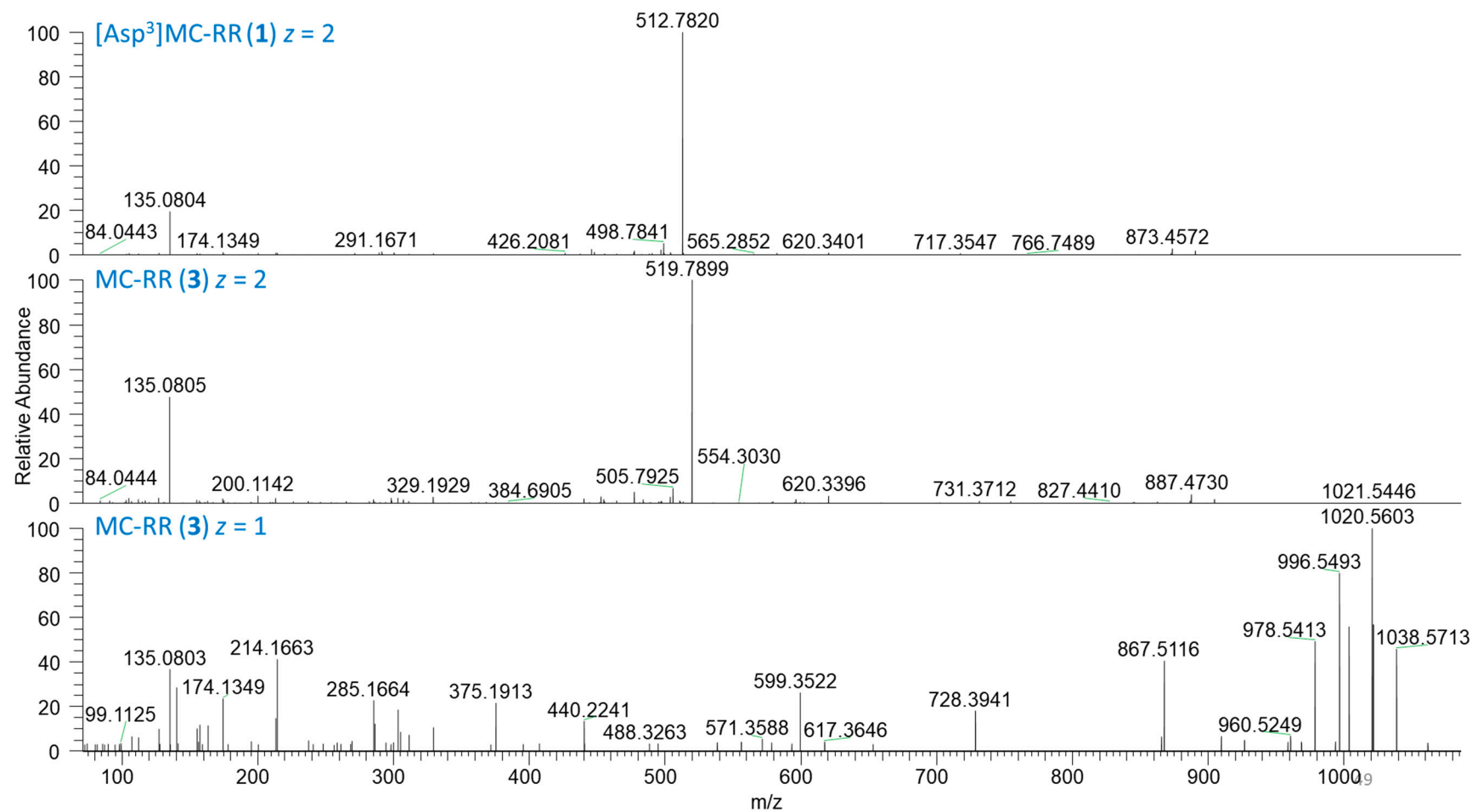


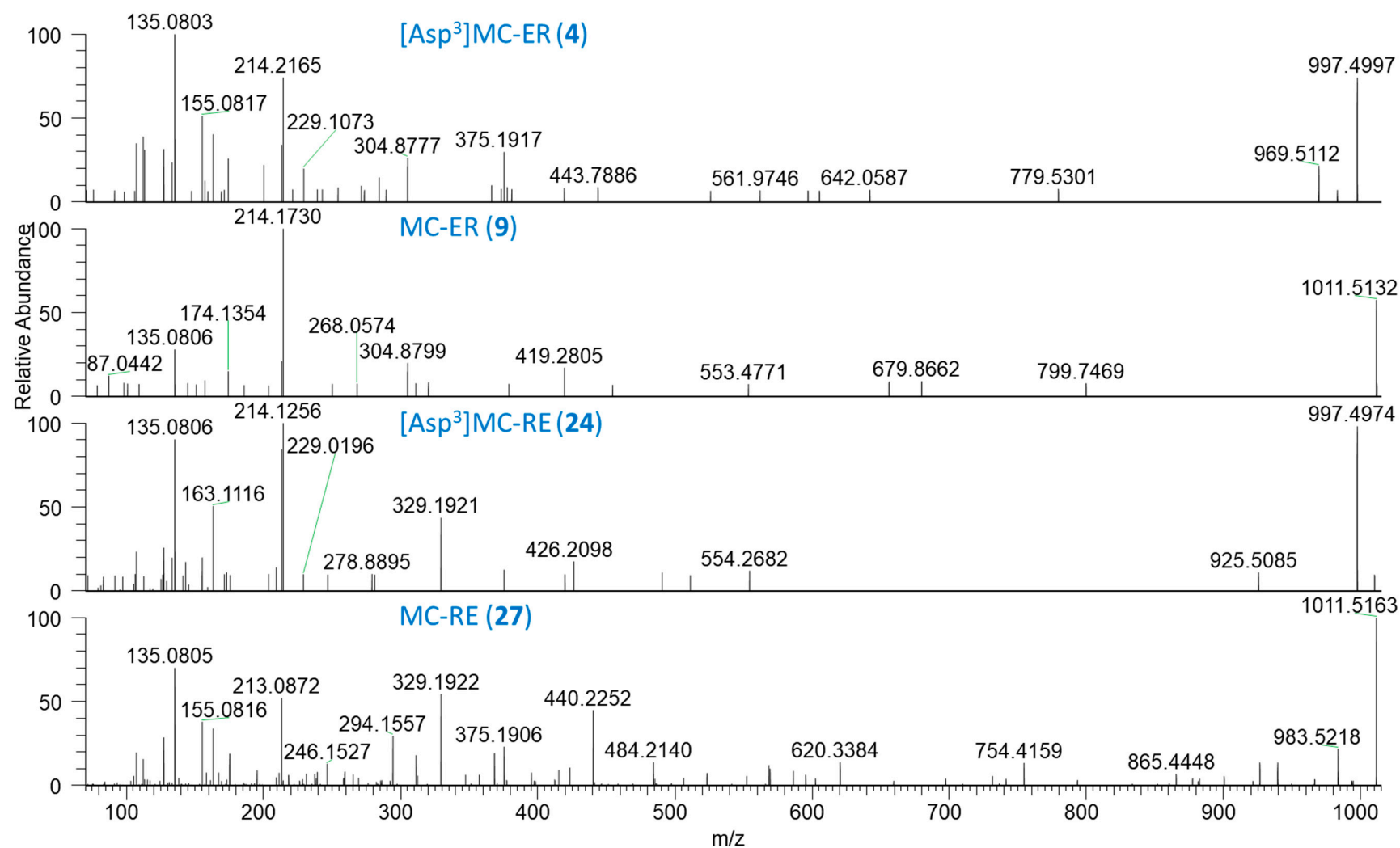
# Supplementary Materials: Cyindrospermopsin- and Deoxycyindrospermopsin-Producing *Raphidiopsis raciborskii* and Microcystin-Producing *Microcystis* spp. in Meiktila Lake, Myanmar

Andreas Ballot, Thida Swe, Marit Mjelde, Leonardo Cerasino, Vladyslava Hostyeva and Christopher O. Miles

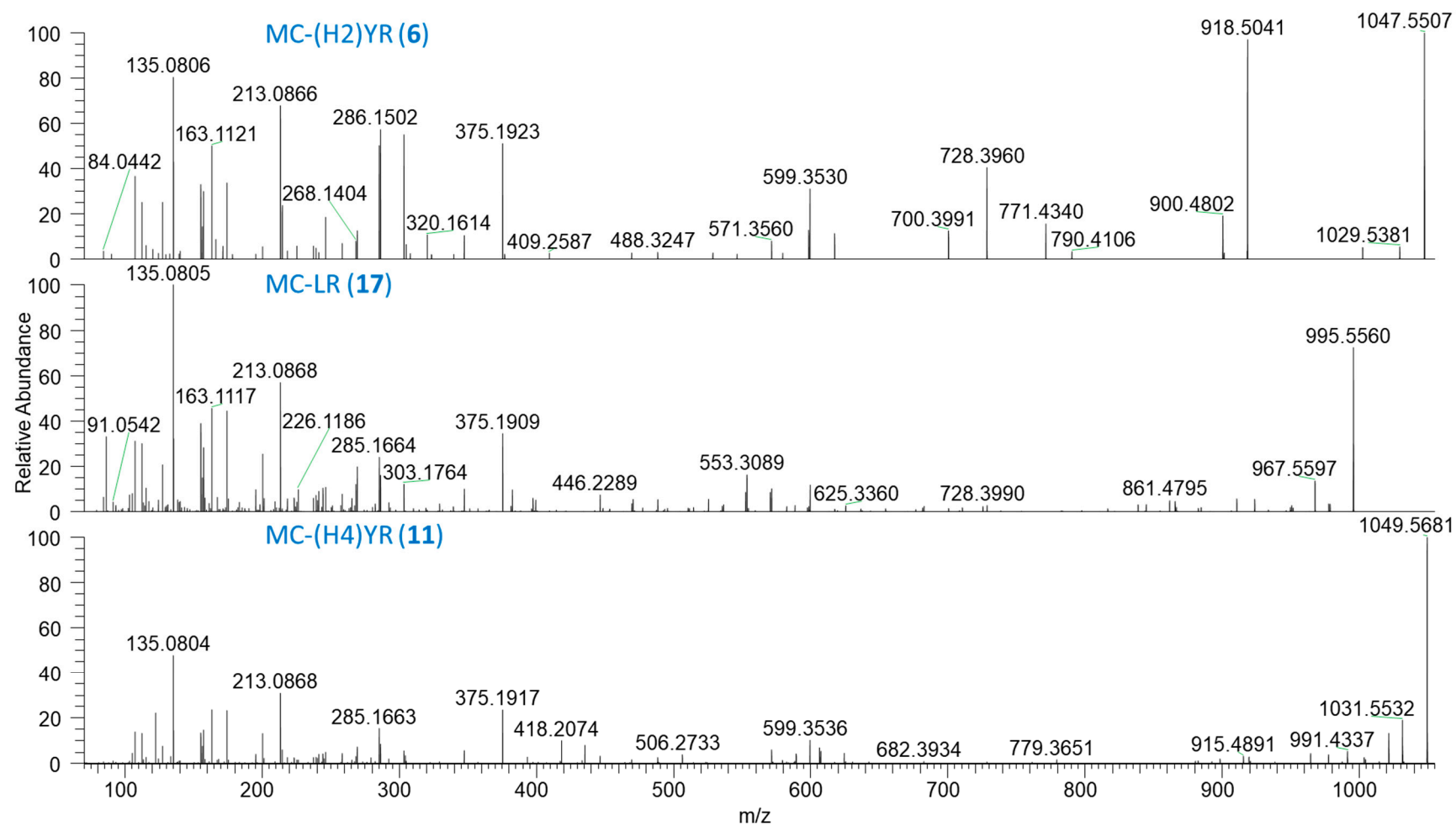
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**Figure S1.** LC-HRMS/MS spectra of  $[M+2H]^{2+}$  of [D-Asp<sup>3</sup>]MC-RR (1) and MC-RR (3), and of  $[M+H]^+$  of 3.

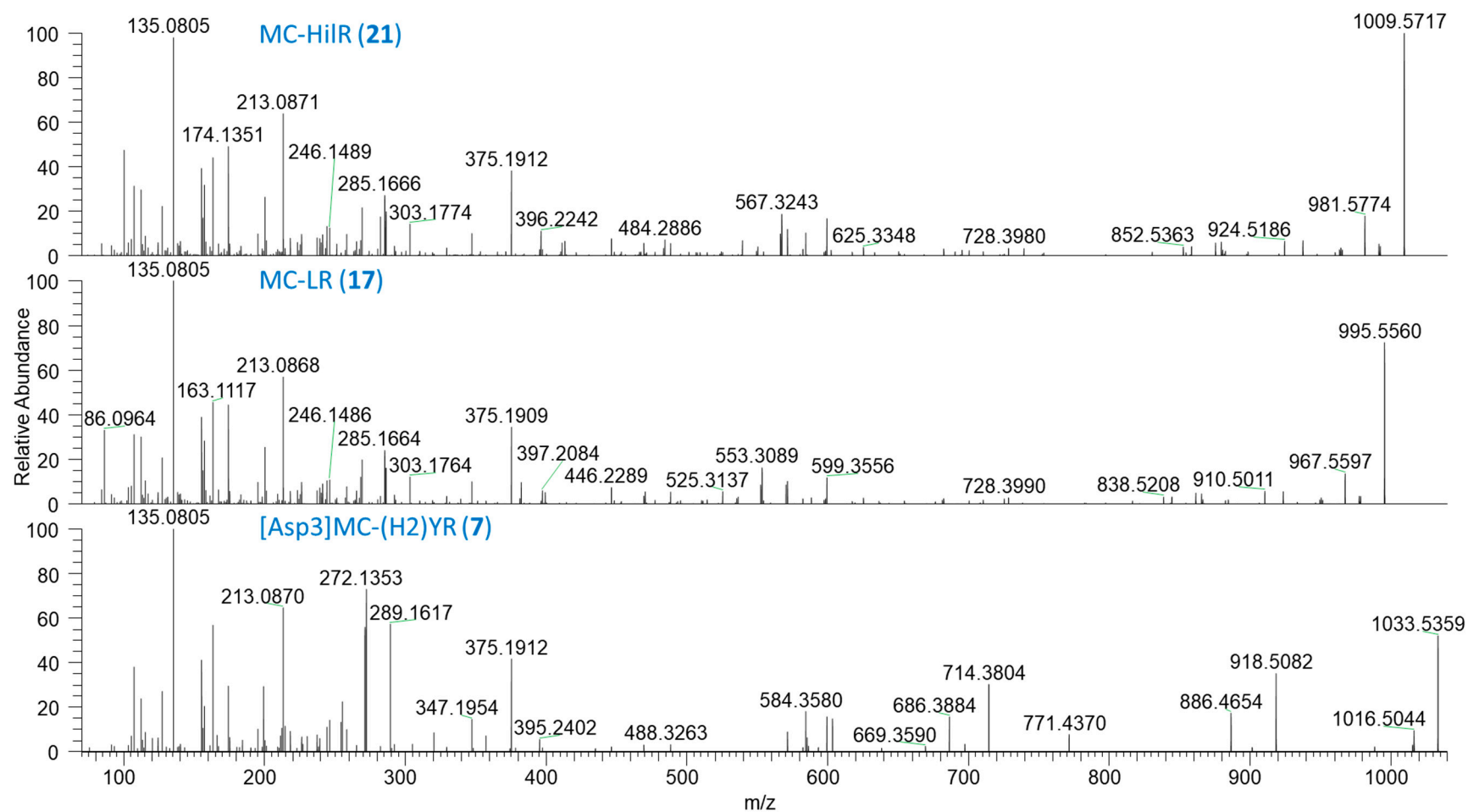


**Figure S2.** LC-HRMS/MS spectra of  $[M+H]^+$  of [D-Asp<sup>3</sup>]MC-ER (4), MC-ER (9), [D-Asp<sup>3</sup>]MC-RE (24) and MC-RE (27).



**Figure S3.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-(H2)YR (6), MC-LR (17), and MC-(H4)YR (11).





**Figure S4.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-HiLR (21), MC-LR (17), and  $[D\text{-Asp}^3]\text{MC}-(H_2)YR$  (7).

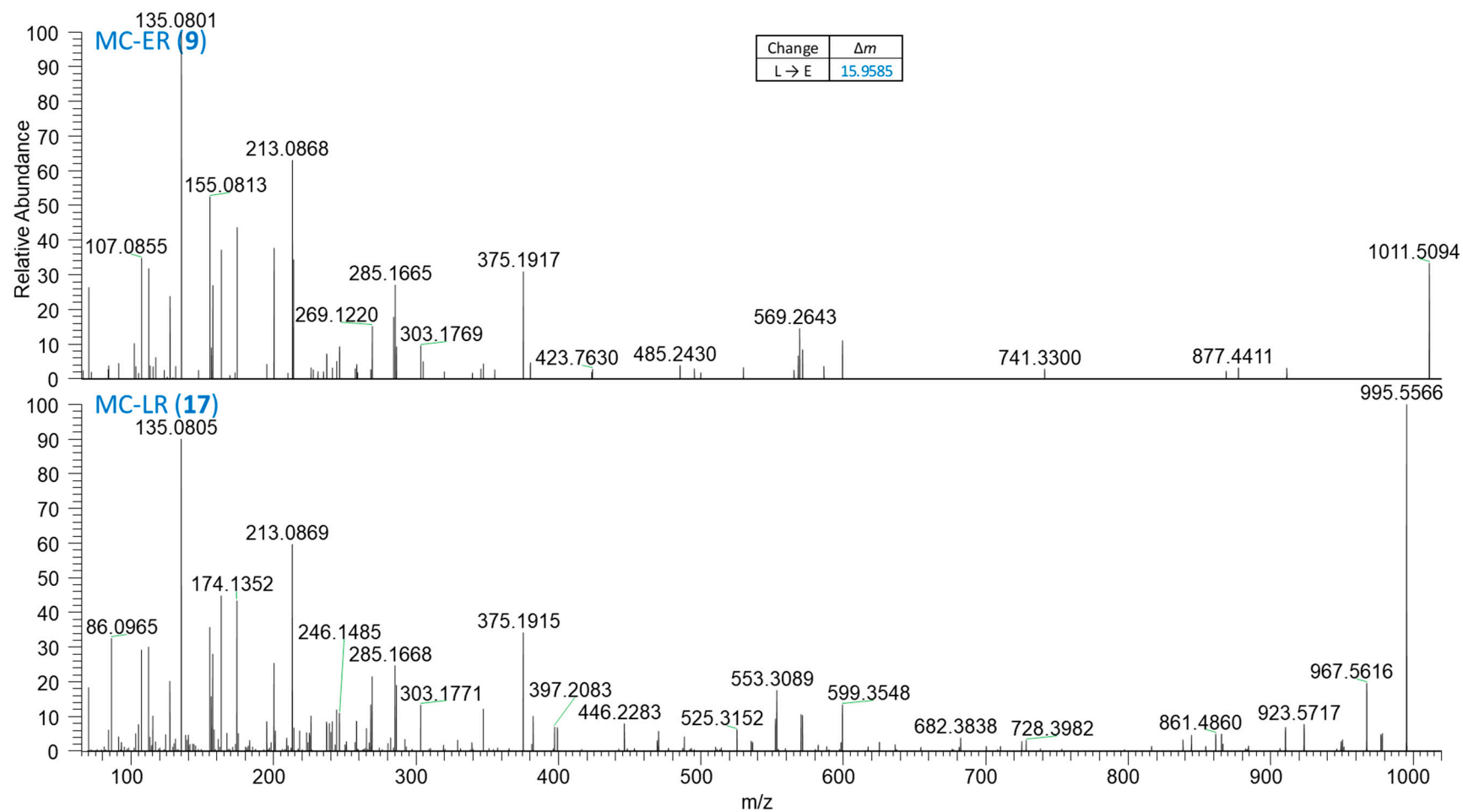
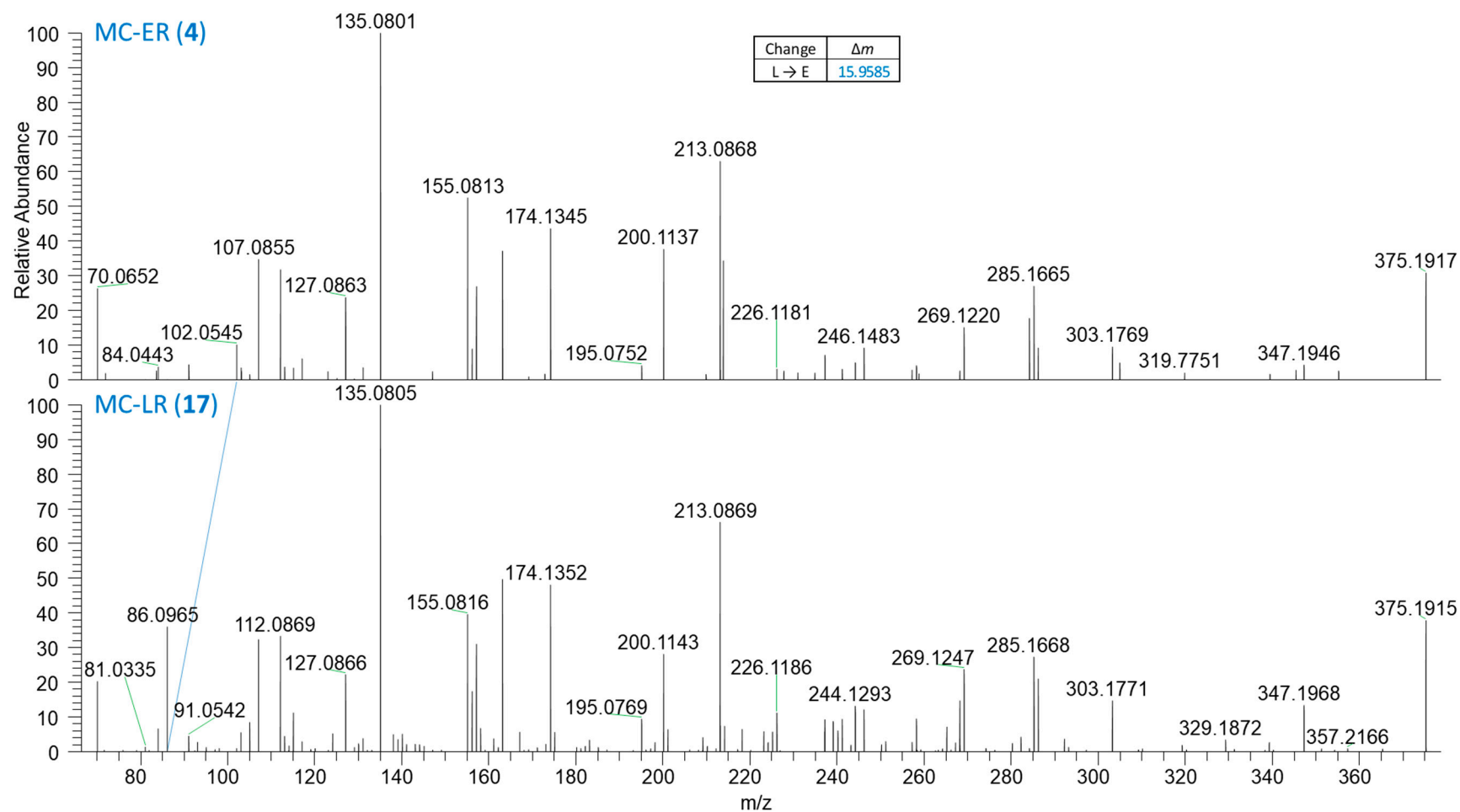
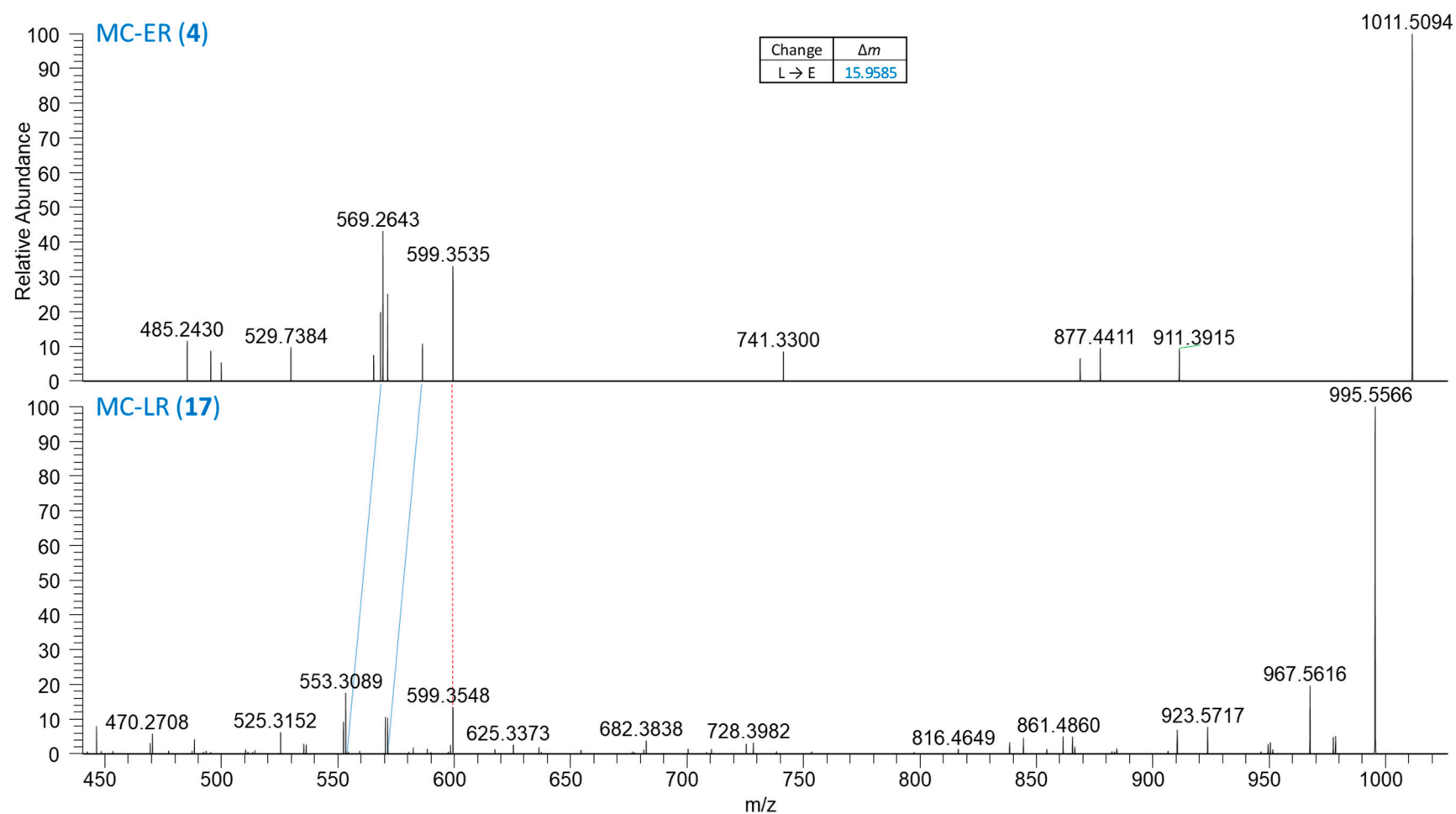


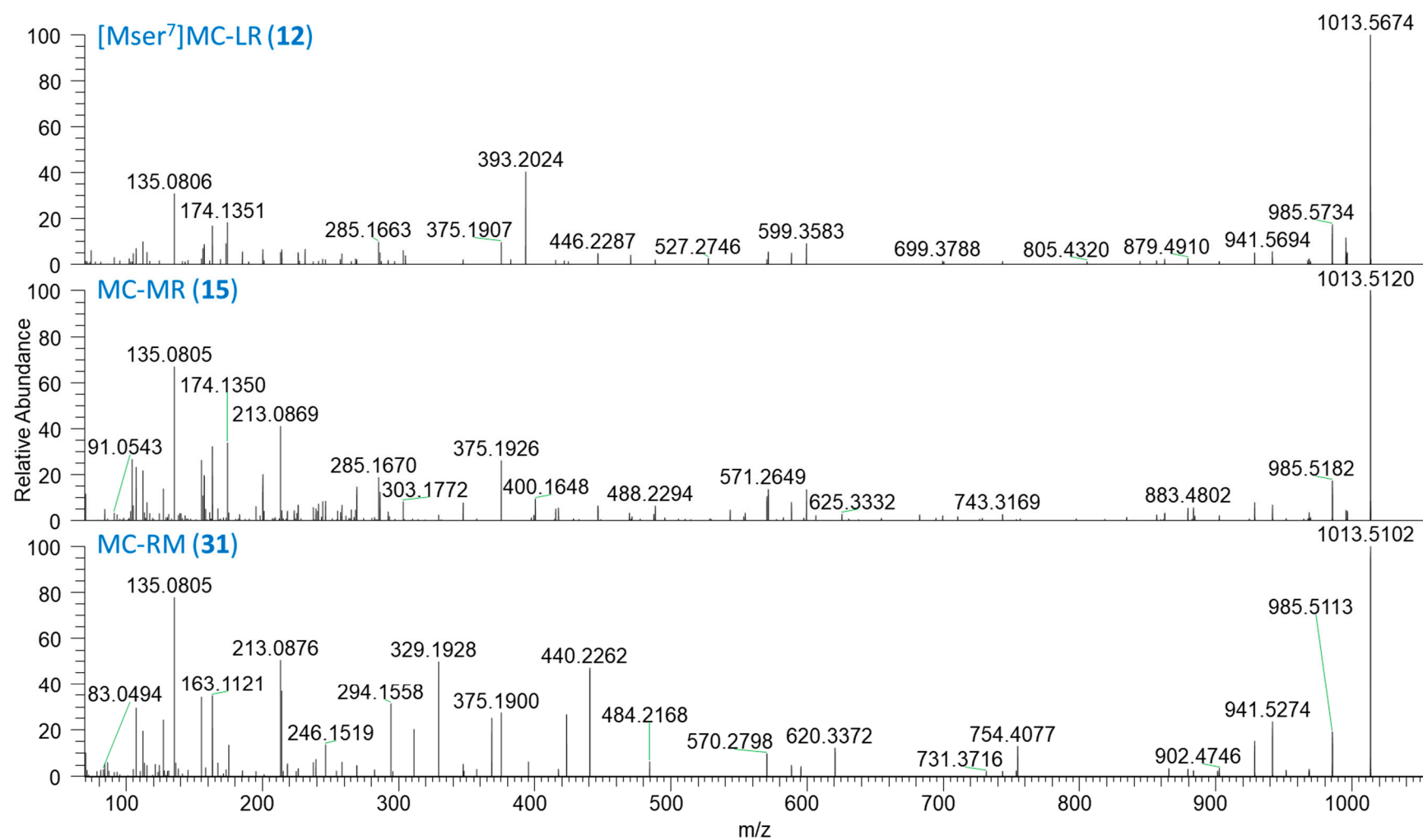
Figure S5. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-ER (9) and MC-LR (17).



**Figure S6.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-ER (9) and MC-LR (17).



**Figure S7.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-ER (9) and MC-LR (17).



**Figure S8.** LC-HRMS/MS spectra of  $[M+H]^+$  of [Mser<sup>7</sup>]MC-LR (12), MC-MR (15), and MC-RM (31).

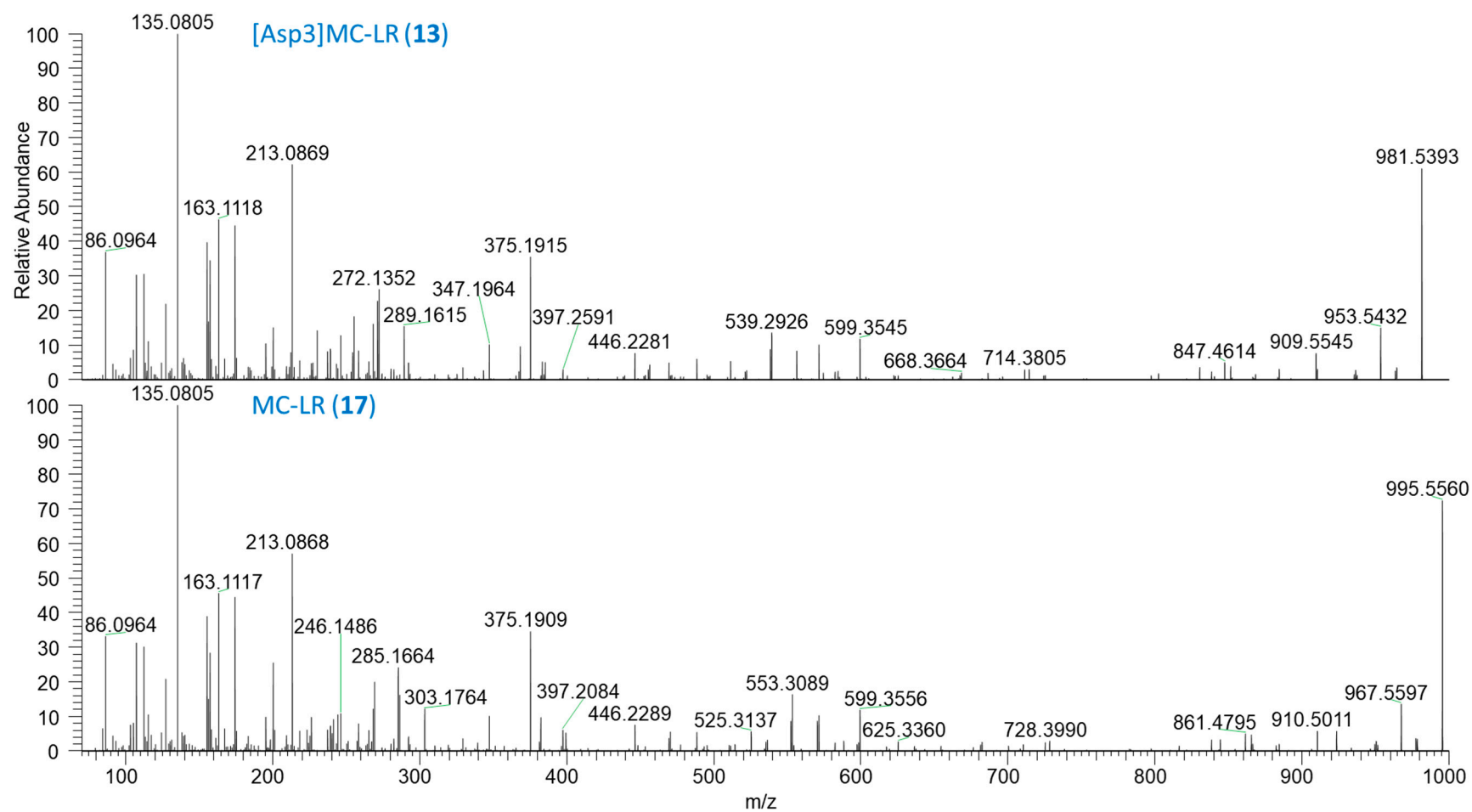


Figure S9. LC-HRMS/MS spectra of  $[M+H]^+$  of  $[D\text{-Asp}^3]\text{MC-LR}$  (13), and MC-LR (17).

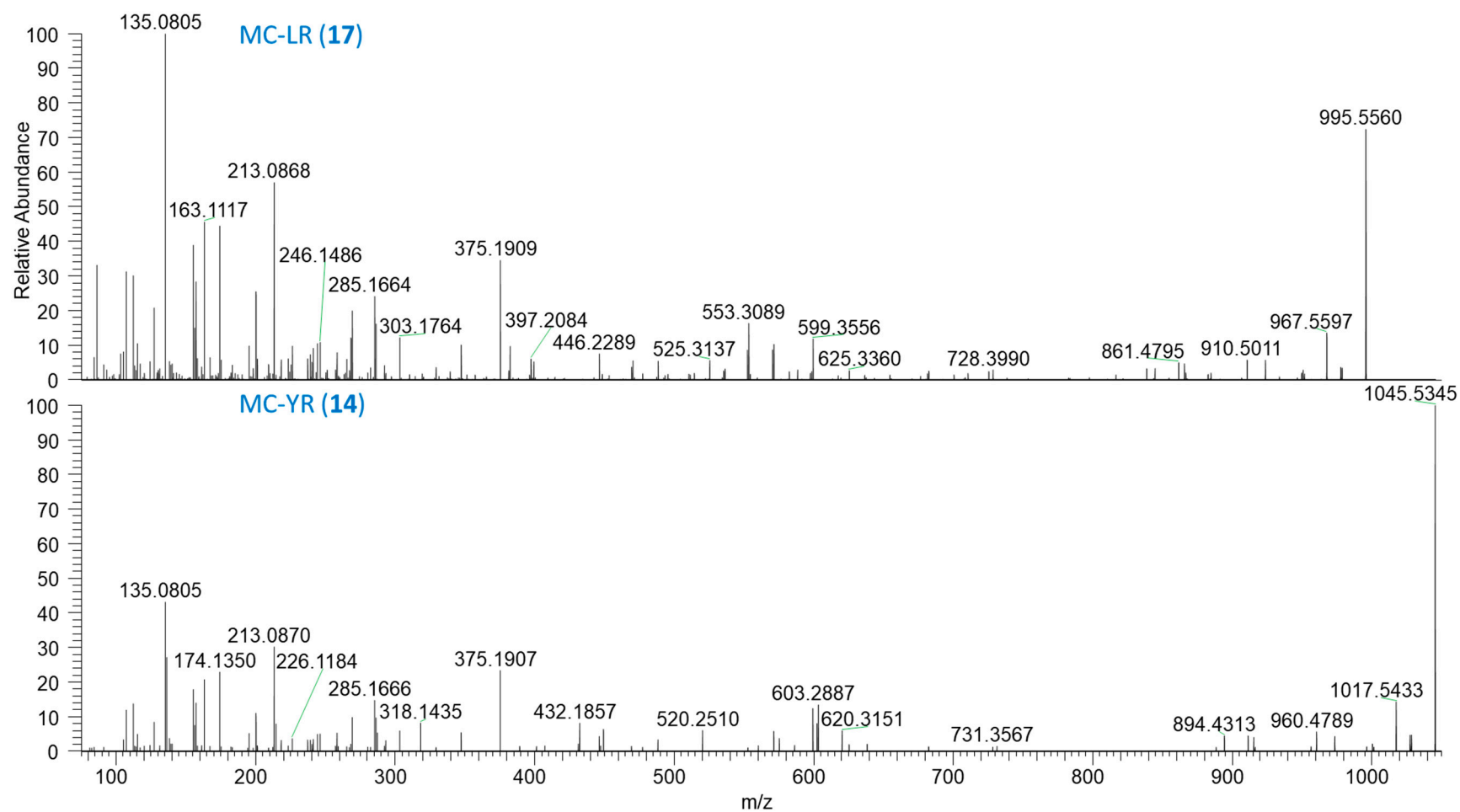
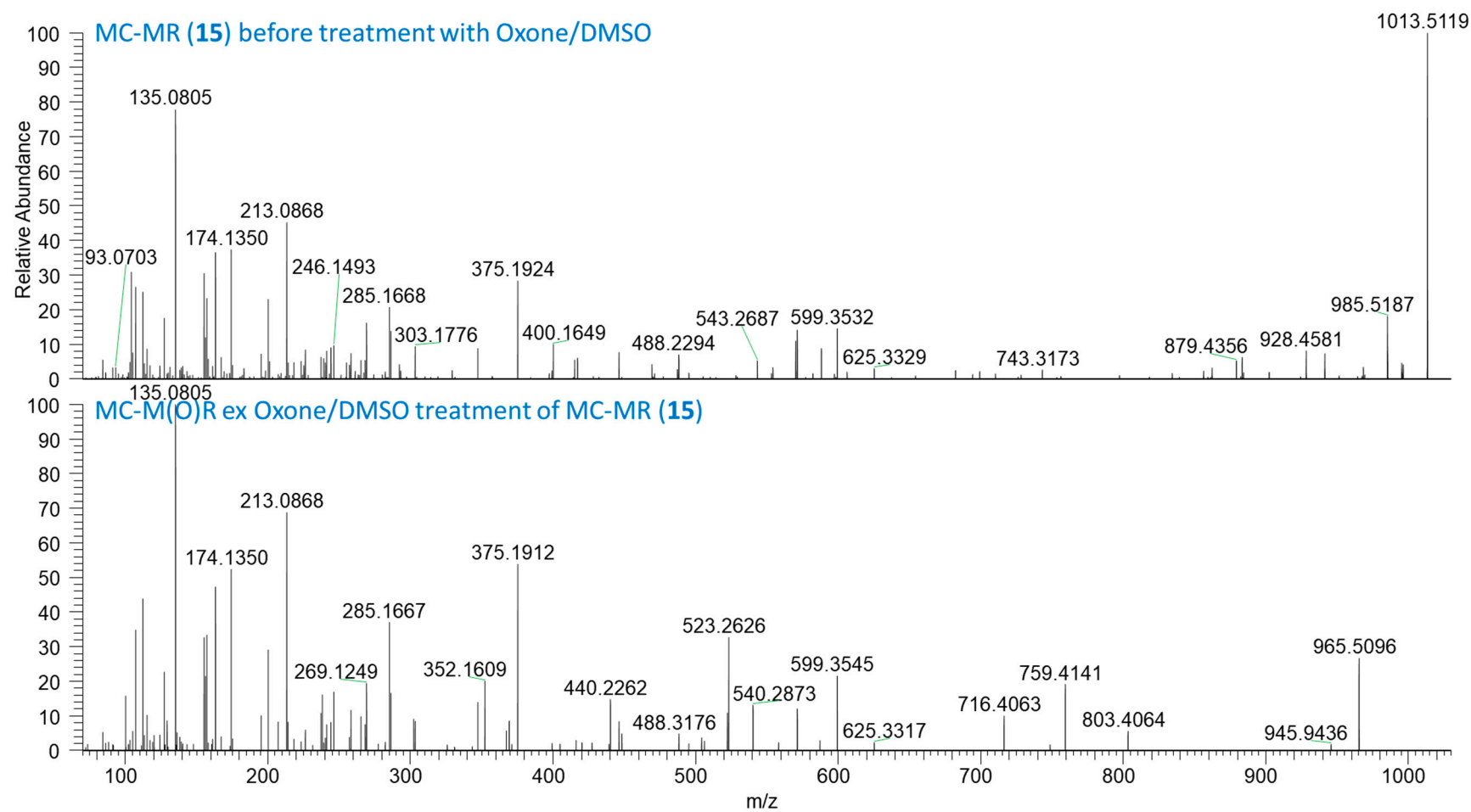
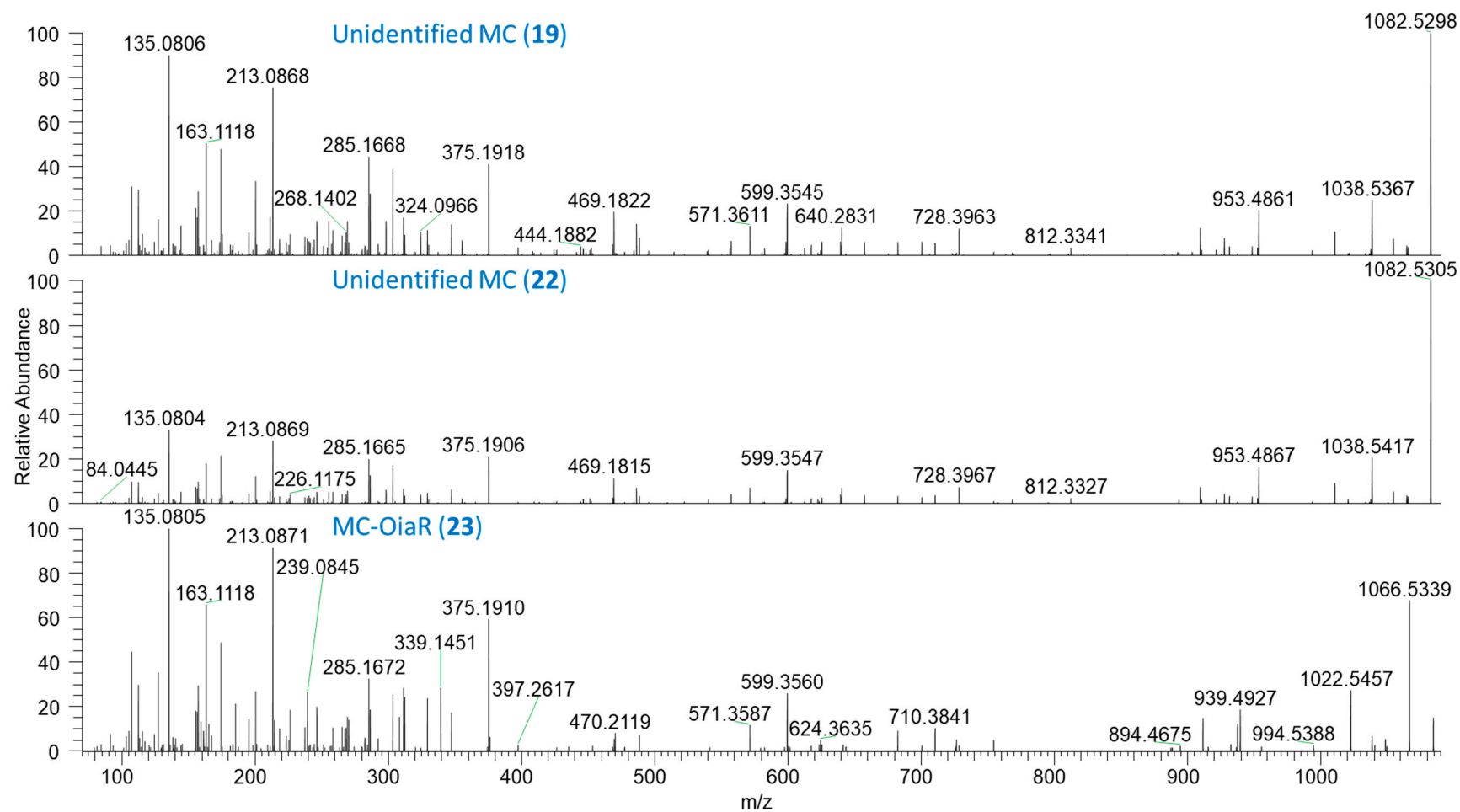


Figure S10. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-LR (17), and MC-YR (14).

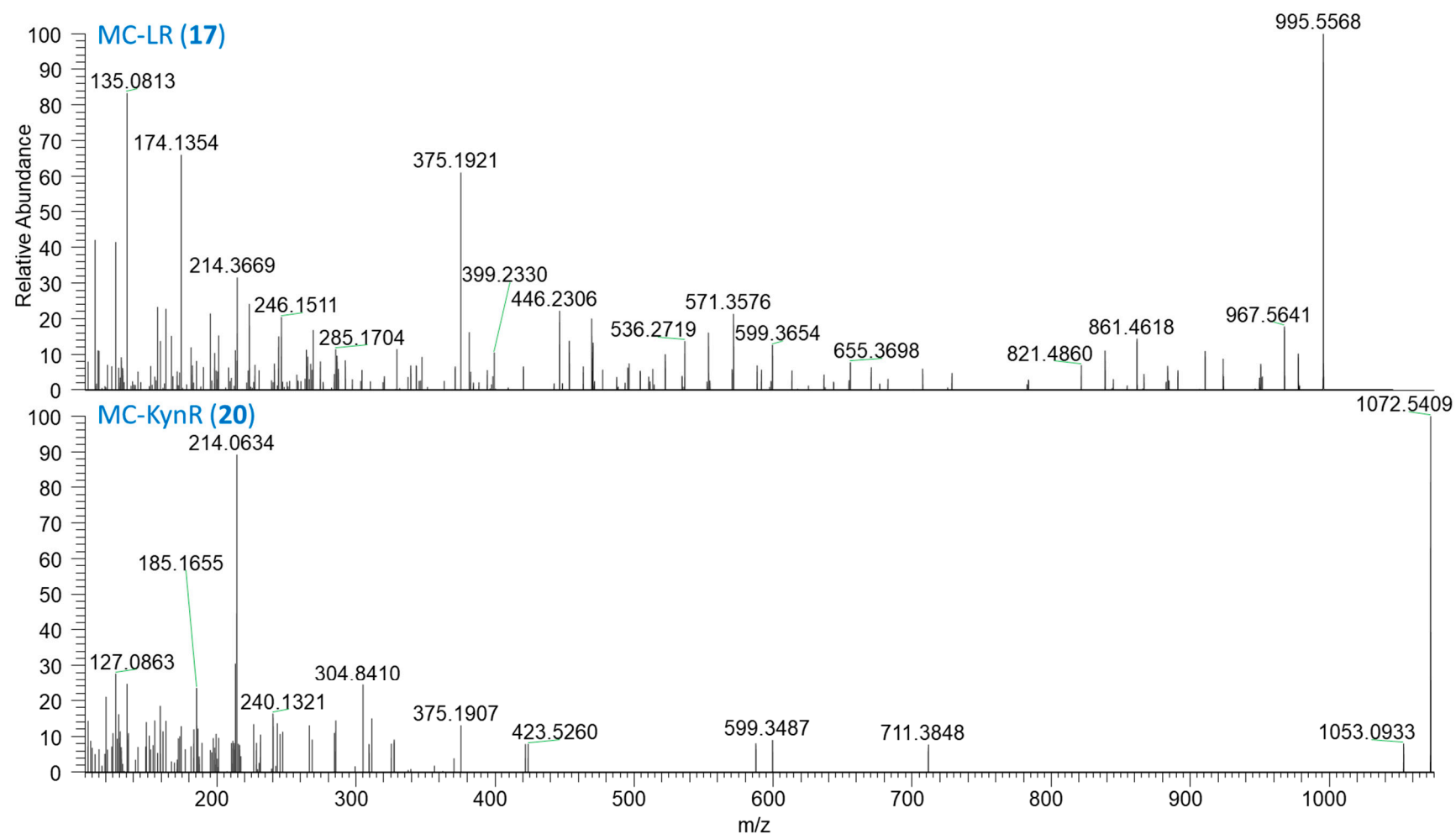


**Figure S11.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-MR (15), and MC-M(O)R produced by oxidation of 15 in the sample with Oxone and DMSO.

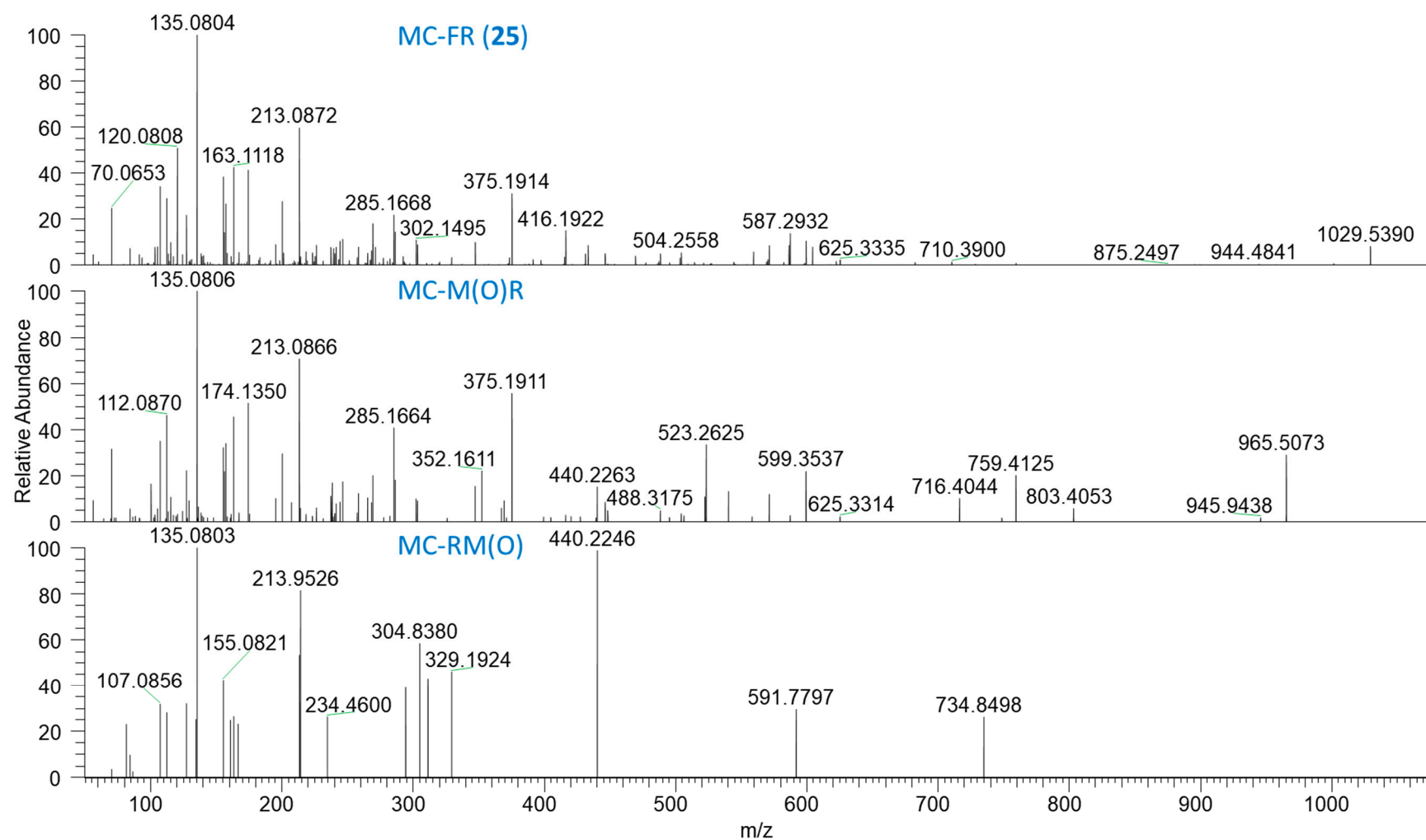




**Figure S12.** LC-HRMS/MS spectra of  $[M+H]^+$  of unidentified microcystin-19, unidentified microcystin-22, and MC-OiaR (23).



**Figure S13.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-LR (17), and MC-KynR (20).



**Figure S14.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-FR (25), and of MC-M(O)R and MC-RM(O) produced by oxidation of **15** and **31**, respectively, with Oxone/DMSO.

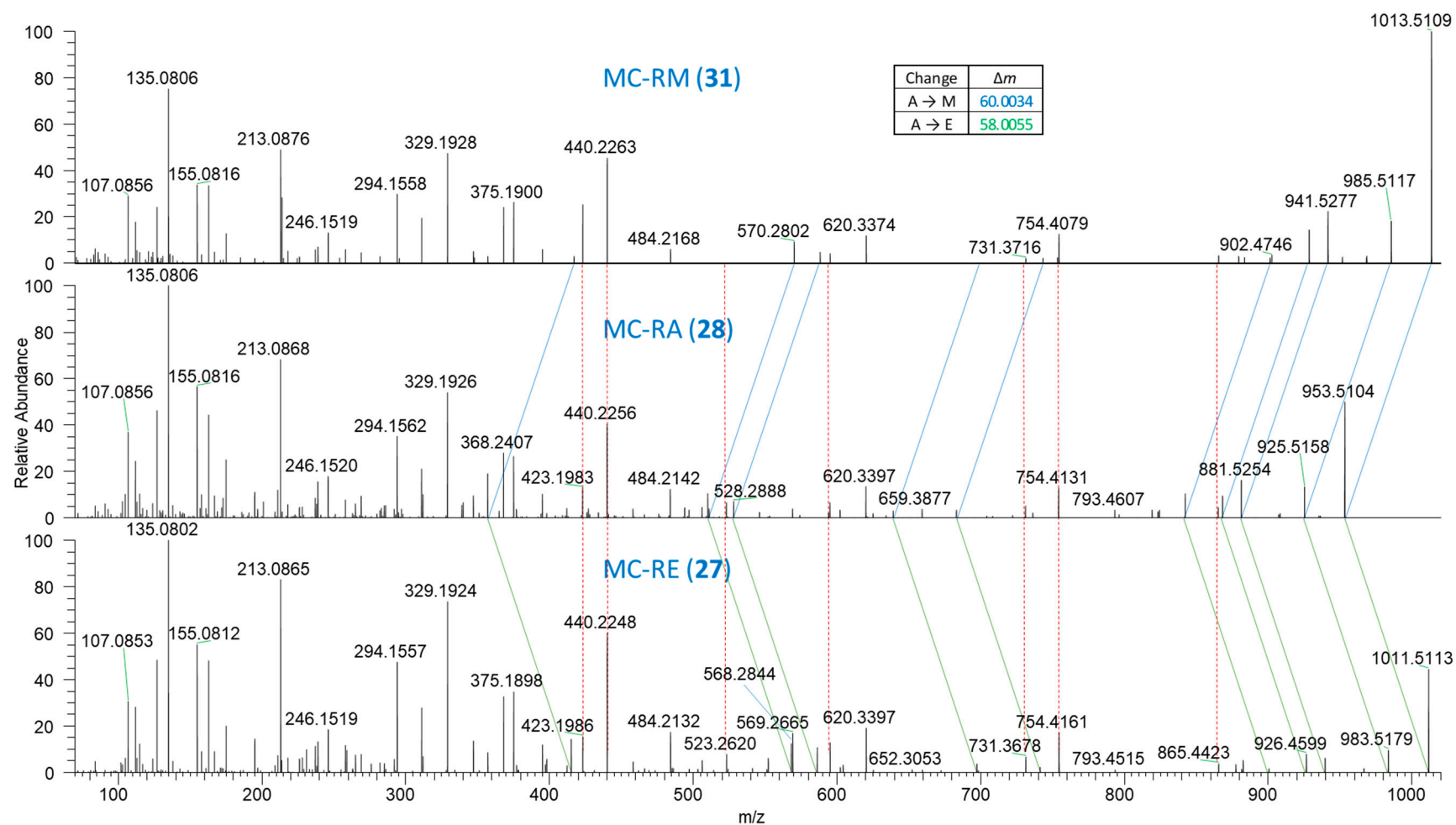


Figure S15. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-RM (31), MC-RA (28), and MC-RE (27).

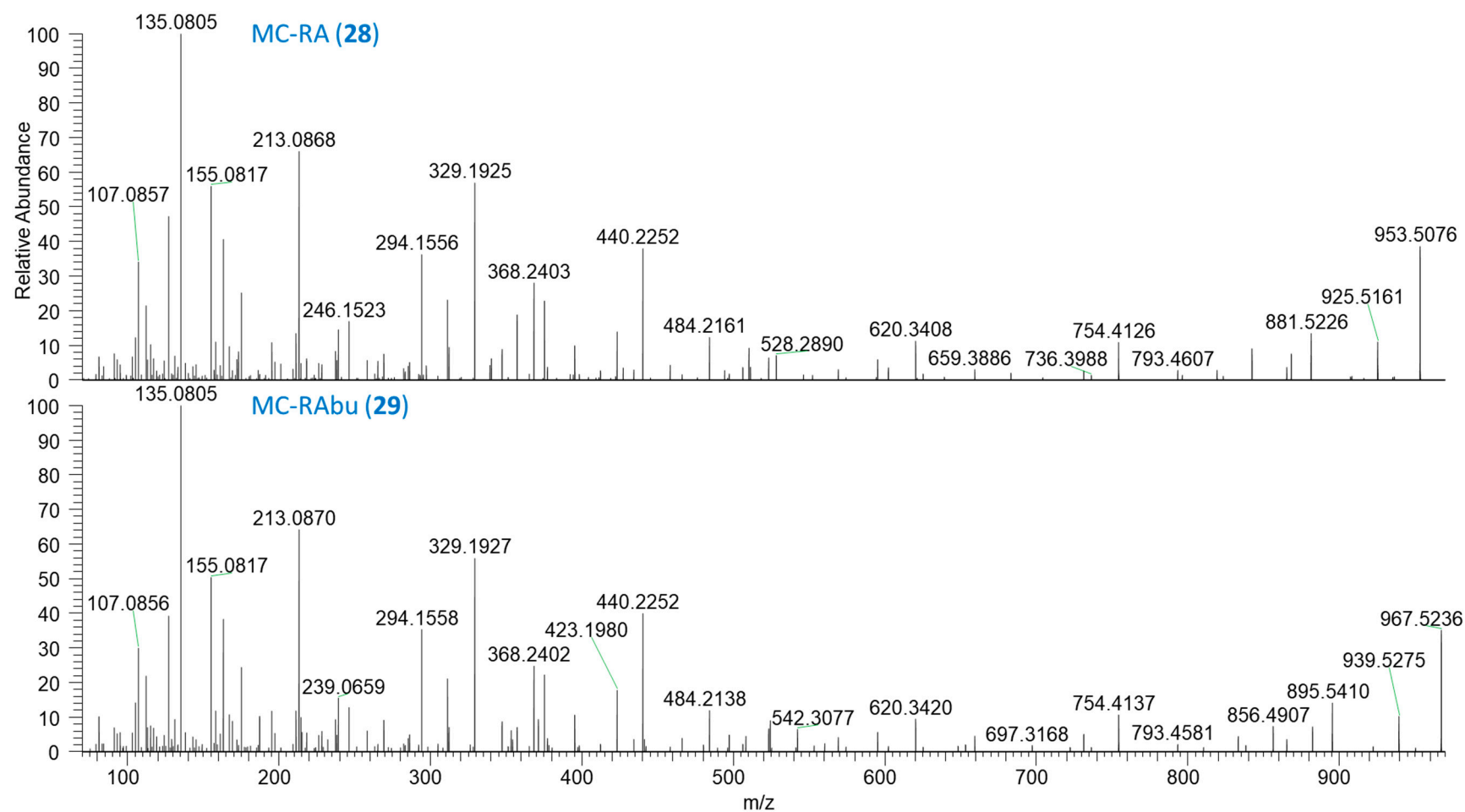


Figure S16. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-RA (28), and MC-RAbu (29).

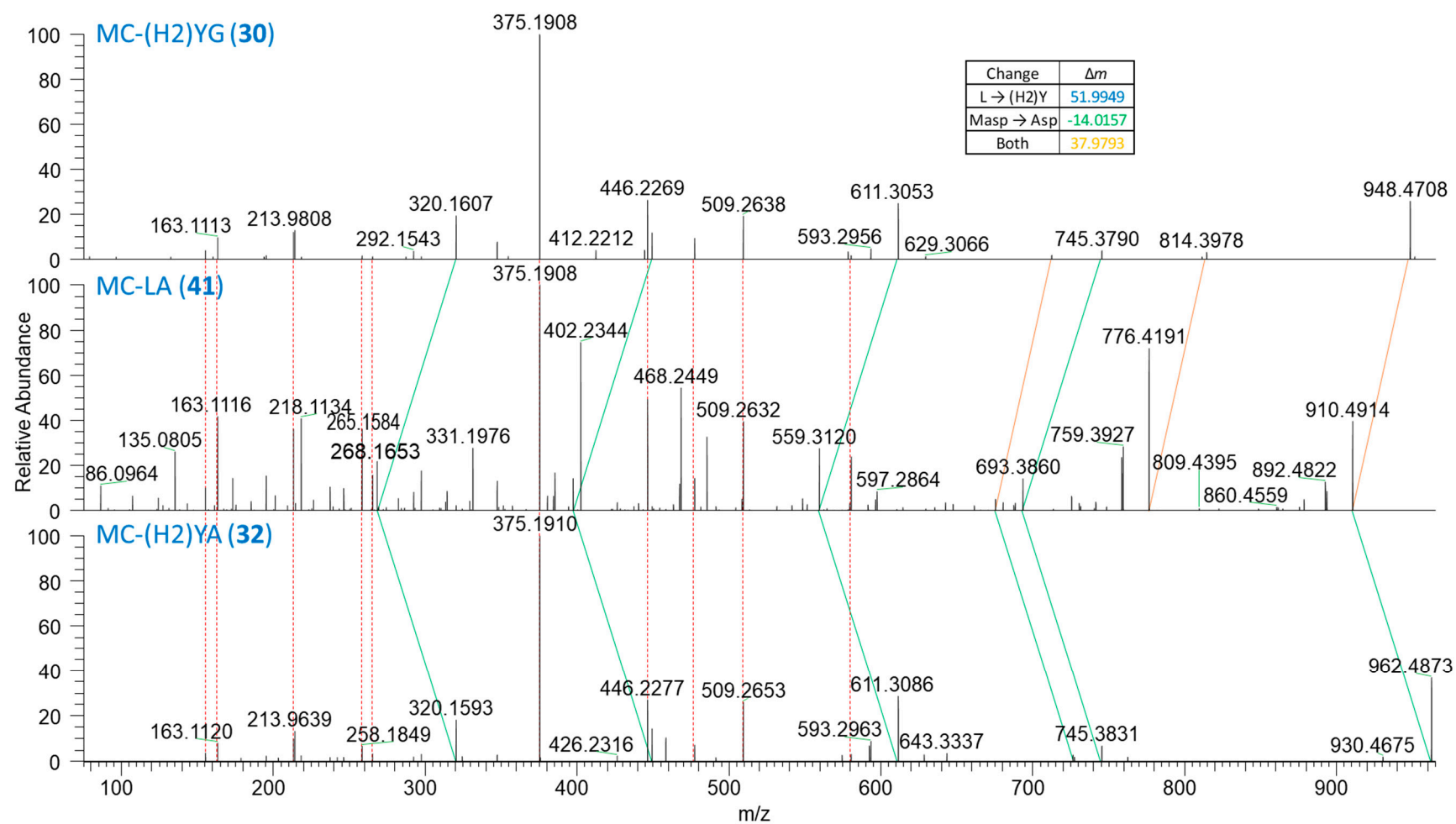


Figure S17. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-(H2)YG (30), MC-LA (41), and MC-(H2)YA (32).

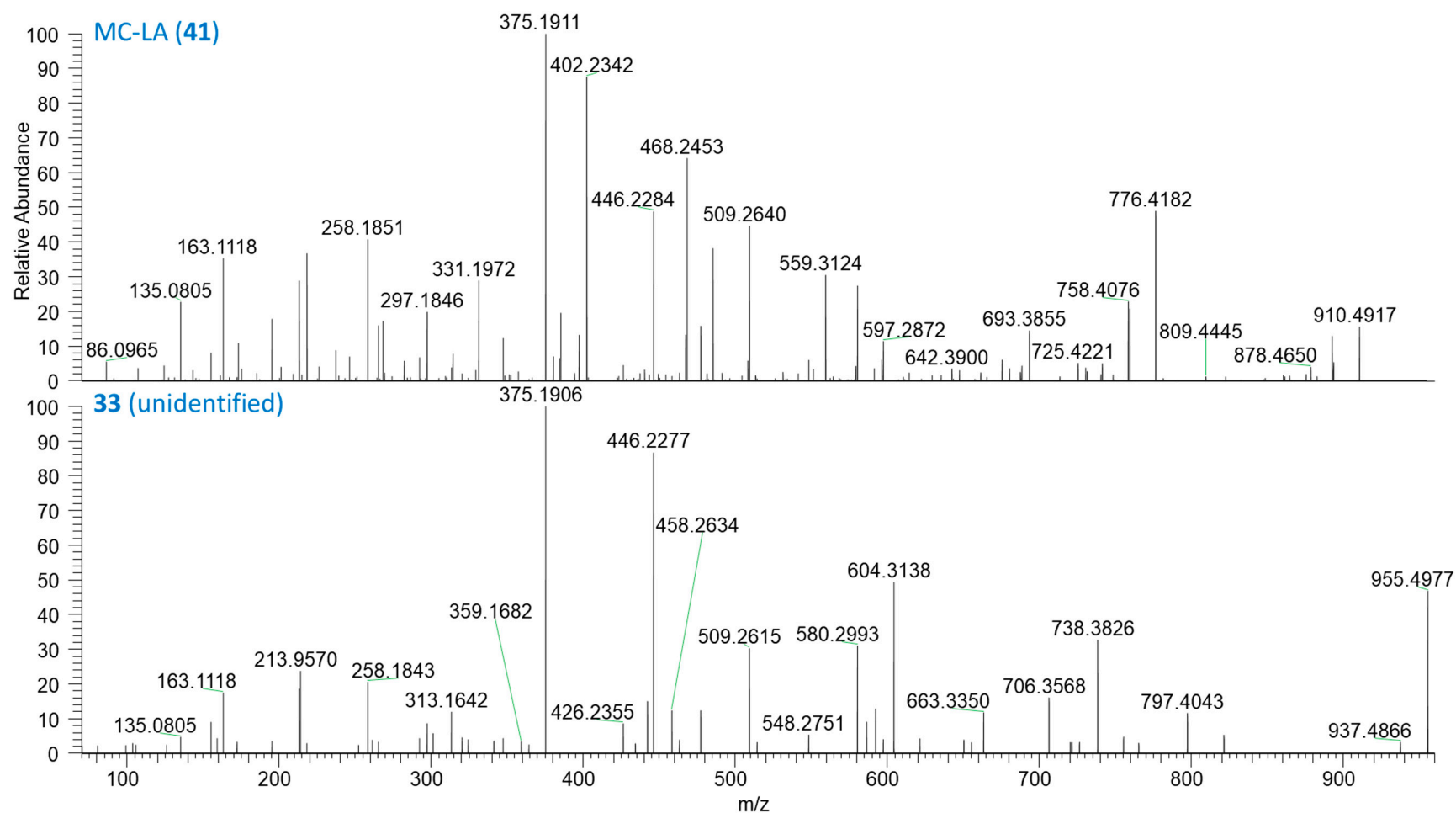
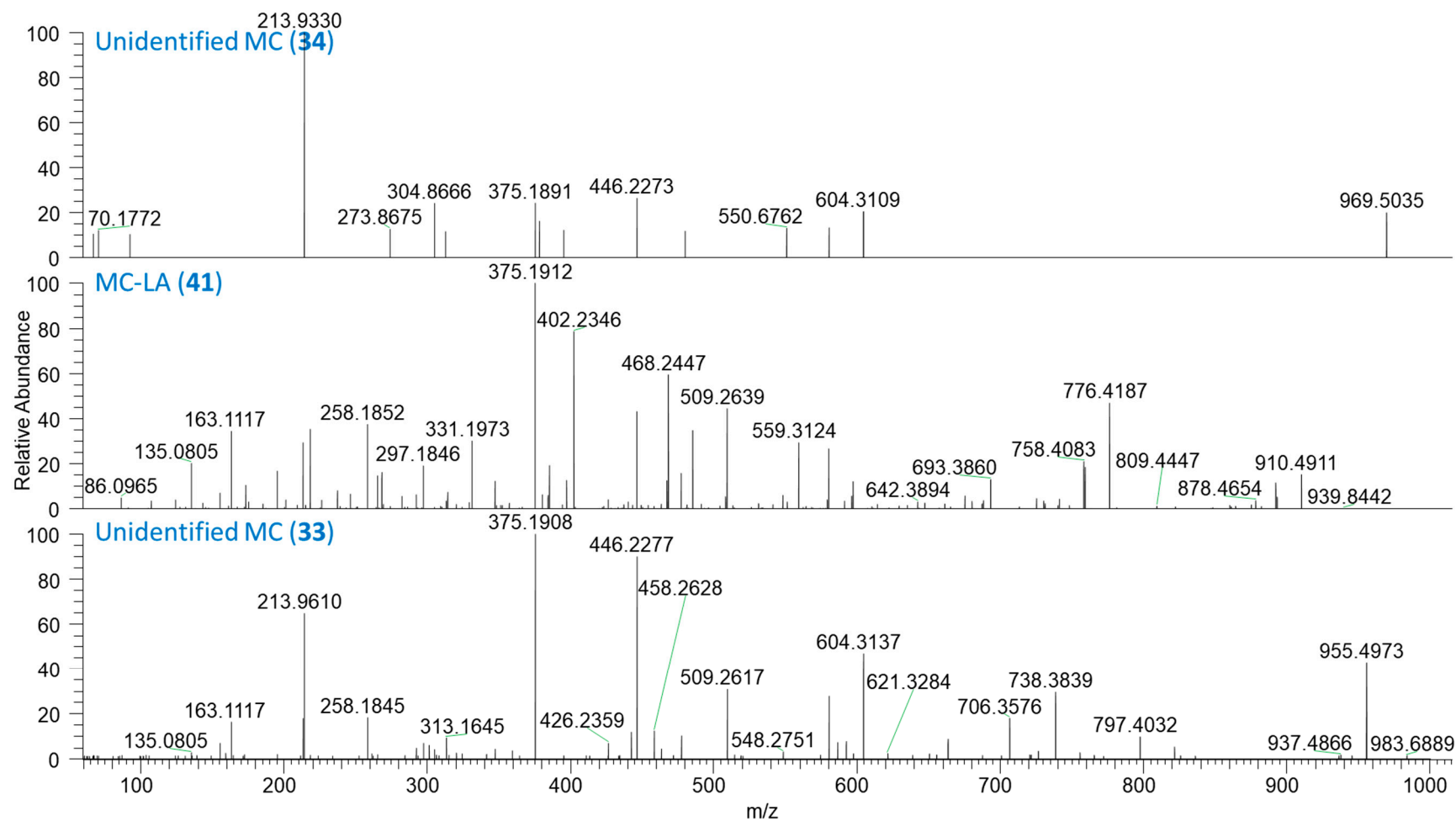
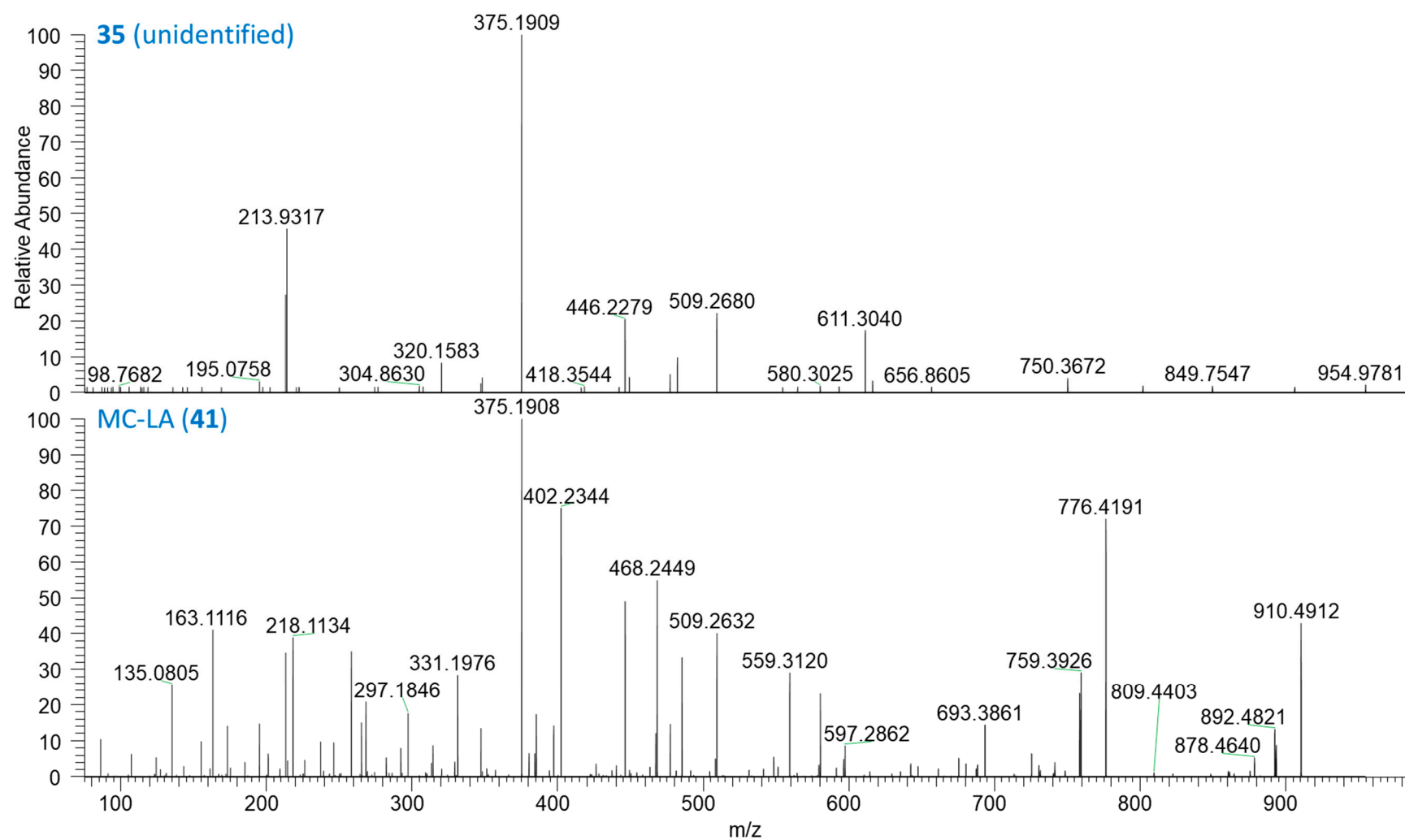


Figure S18. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-LA (41), and unidentified microcystin-33.

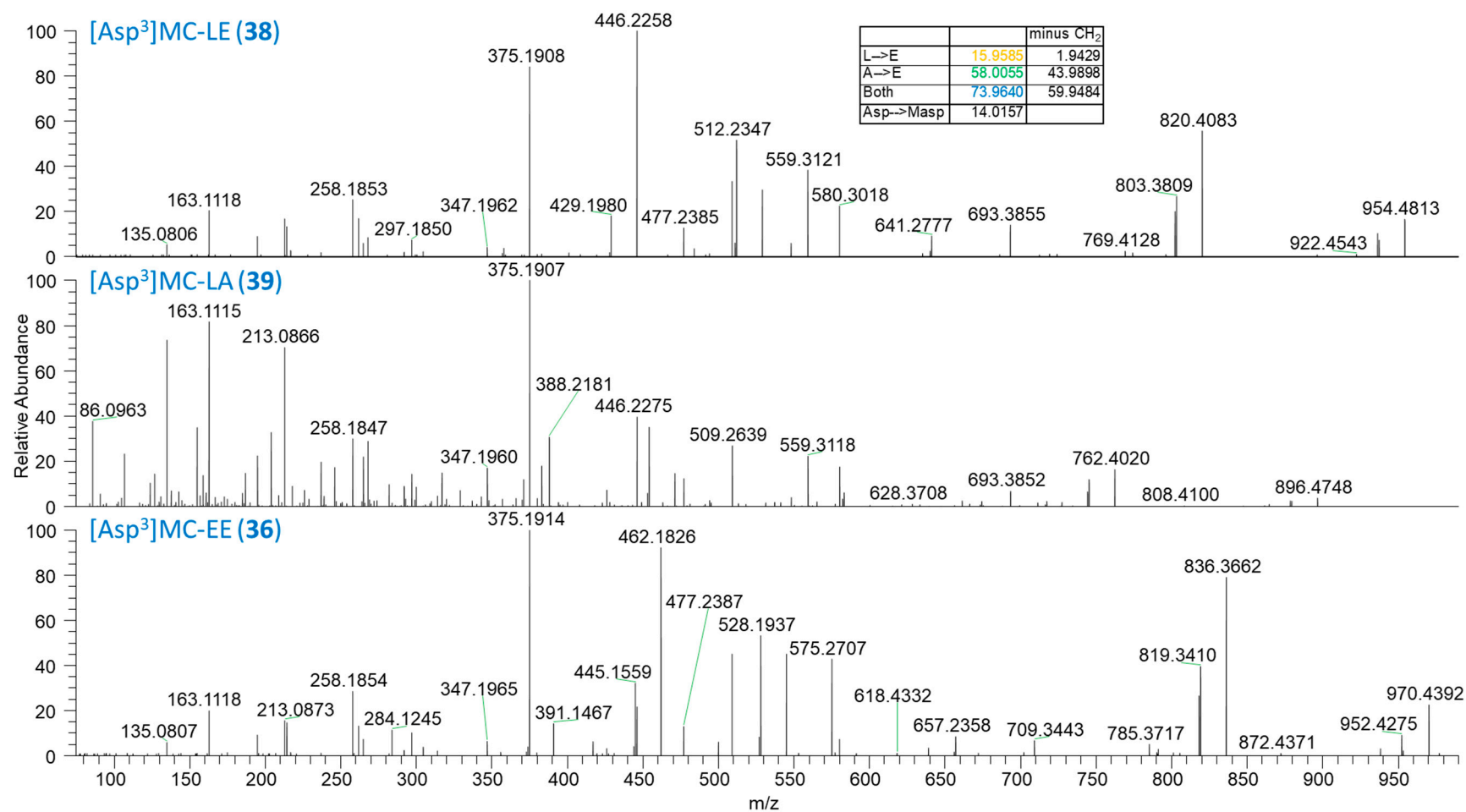


**Figure S19.** LC-HRMS/MS spectra of  $[M+H]^+$  of unidentified microcystin-34, MC-LA (41), and unidentified microcystin-33.

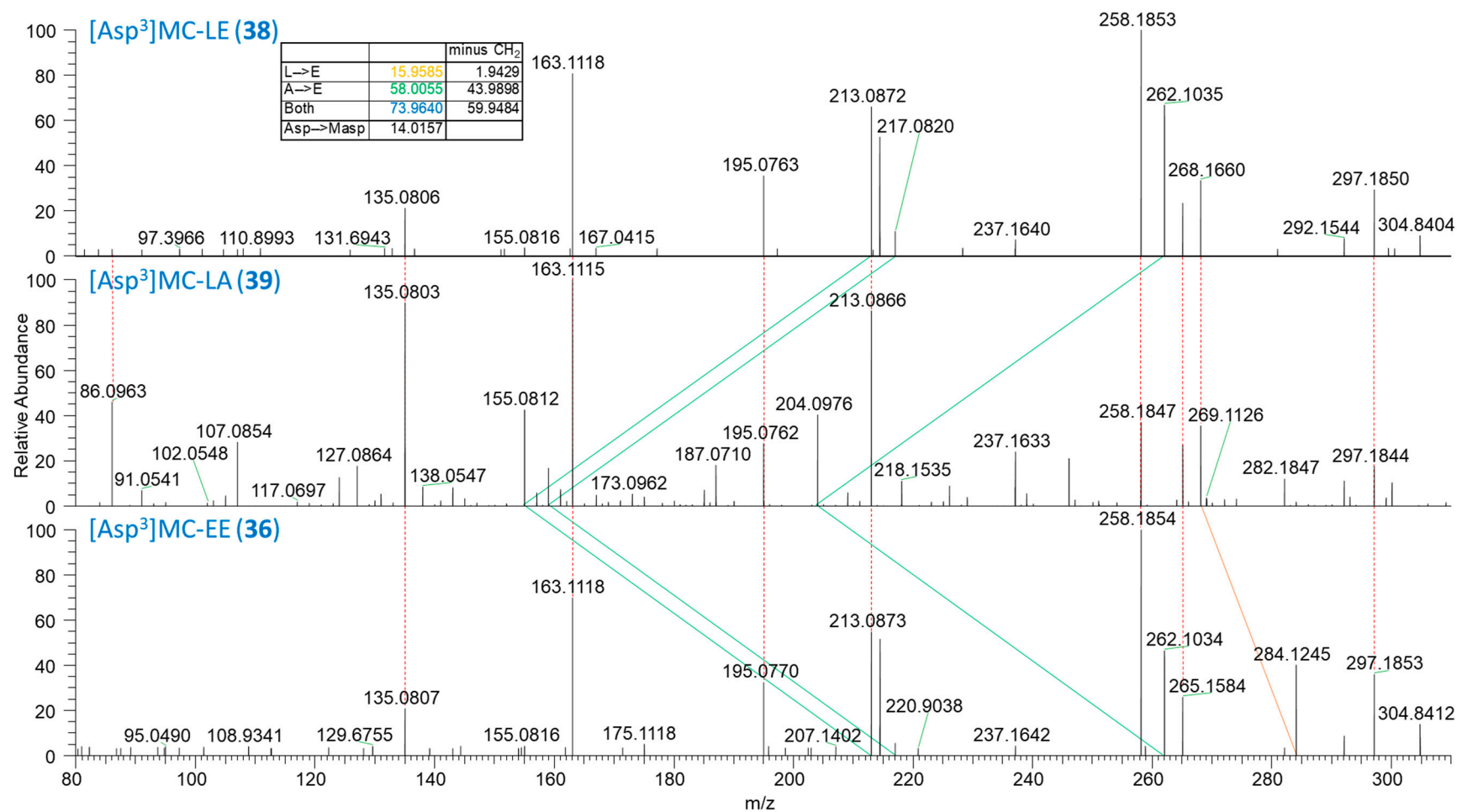




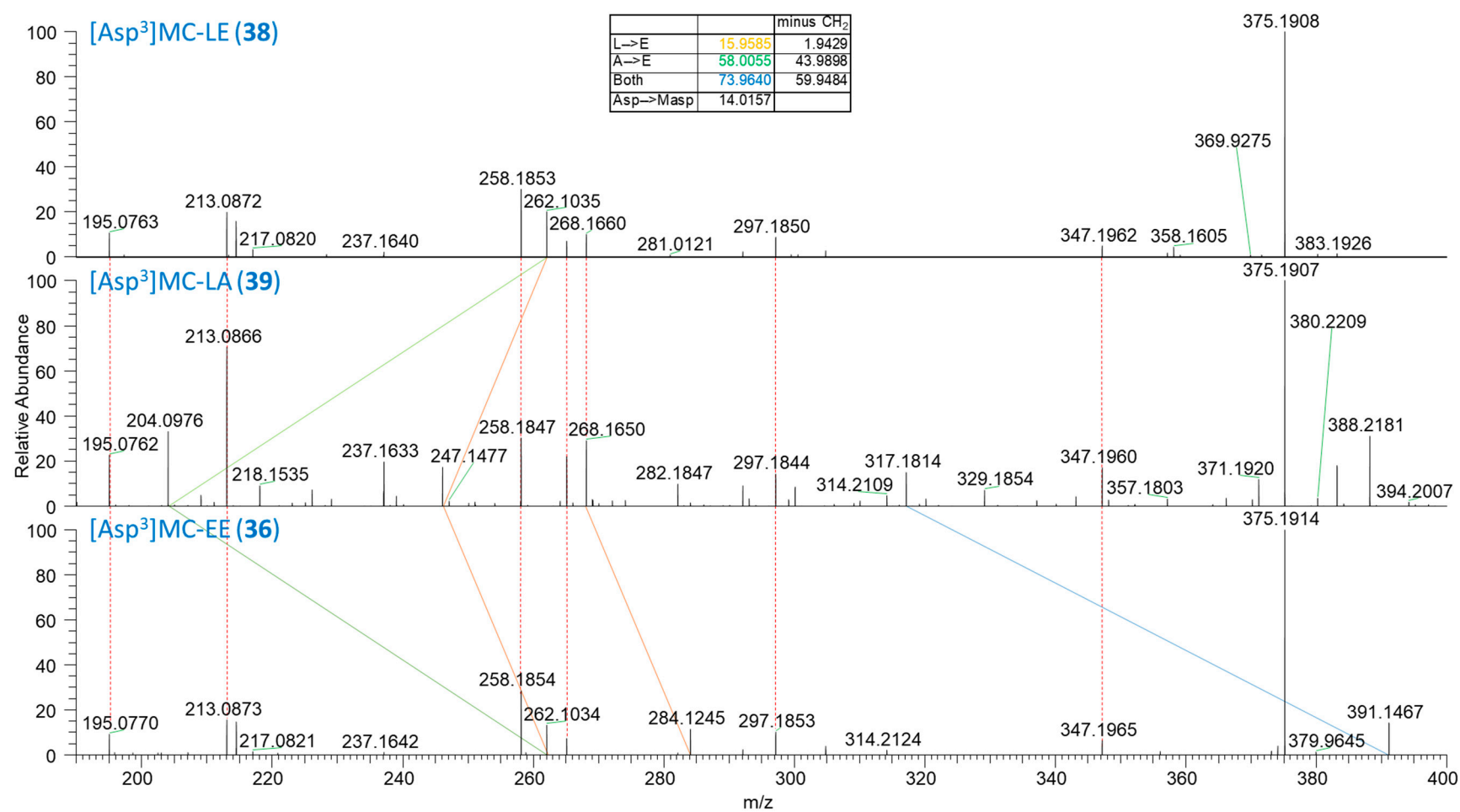
**Figure S20.** LC-HRMS/MS spectra of  $[M+H]^+$  of unidentified microcystin-35, and MC-LA (41).



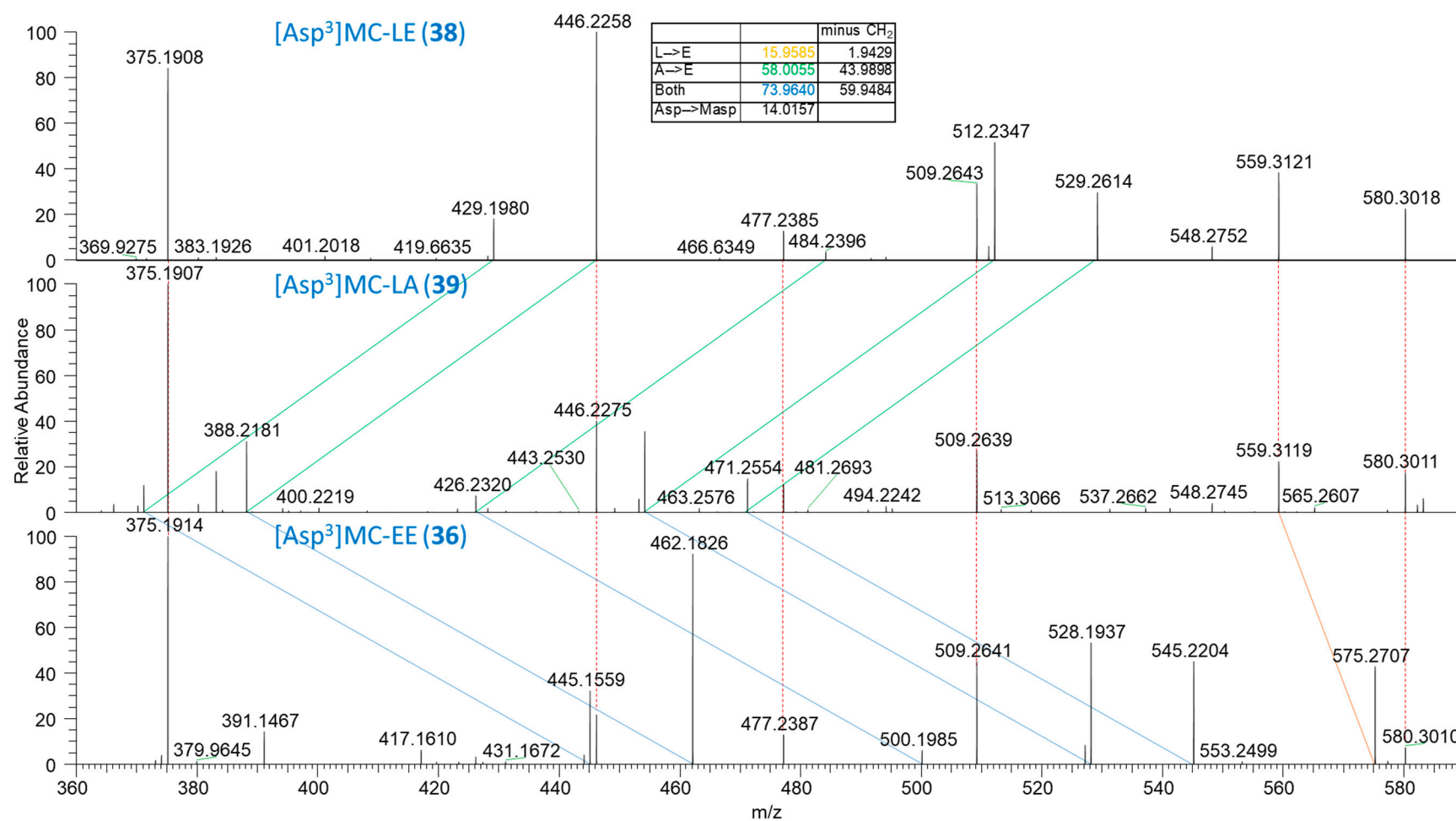
**Figure S21.** LC-HRMS/MS spectra of [M+H]<sup>+</sup> of [D-Asp<sup>3</sup>]MC-LE (38), [D-Asp<sup>3</sup>]MC-LA (39), and [D-Asp<sup>3</sup>]MC-EE (36).



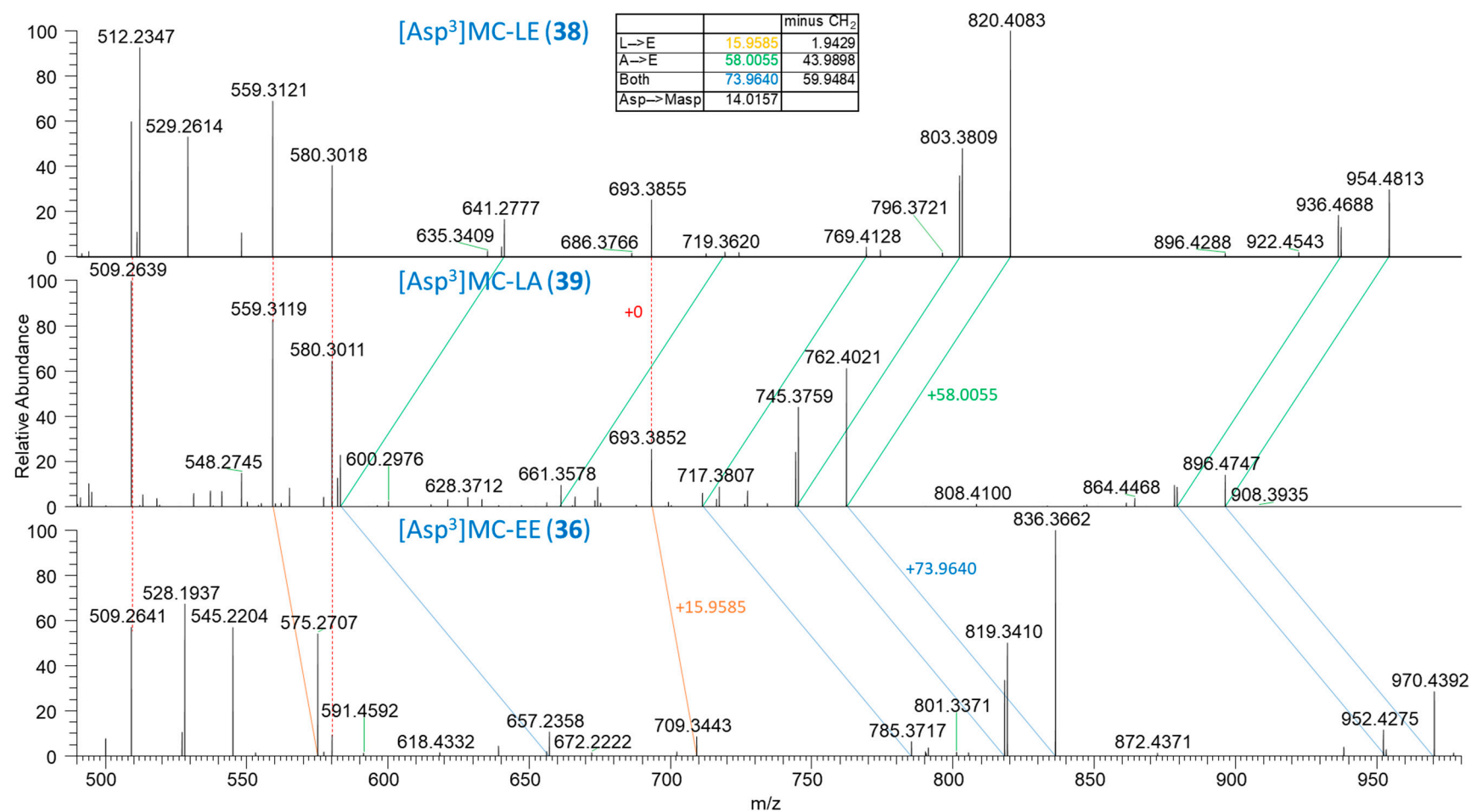
**Figure S22.** Expansion of LC–HRMS/MS spectra of [M+H]<sup>+</sup> of [D-Asp<sup>3</sup>]MC-LE (38), [D-Asp<sup>3</sup>]MC-LA (39), and [D-Asp<sup>3</sup>]MC-EE (36).



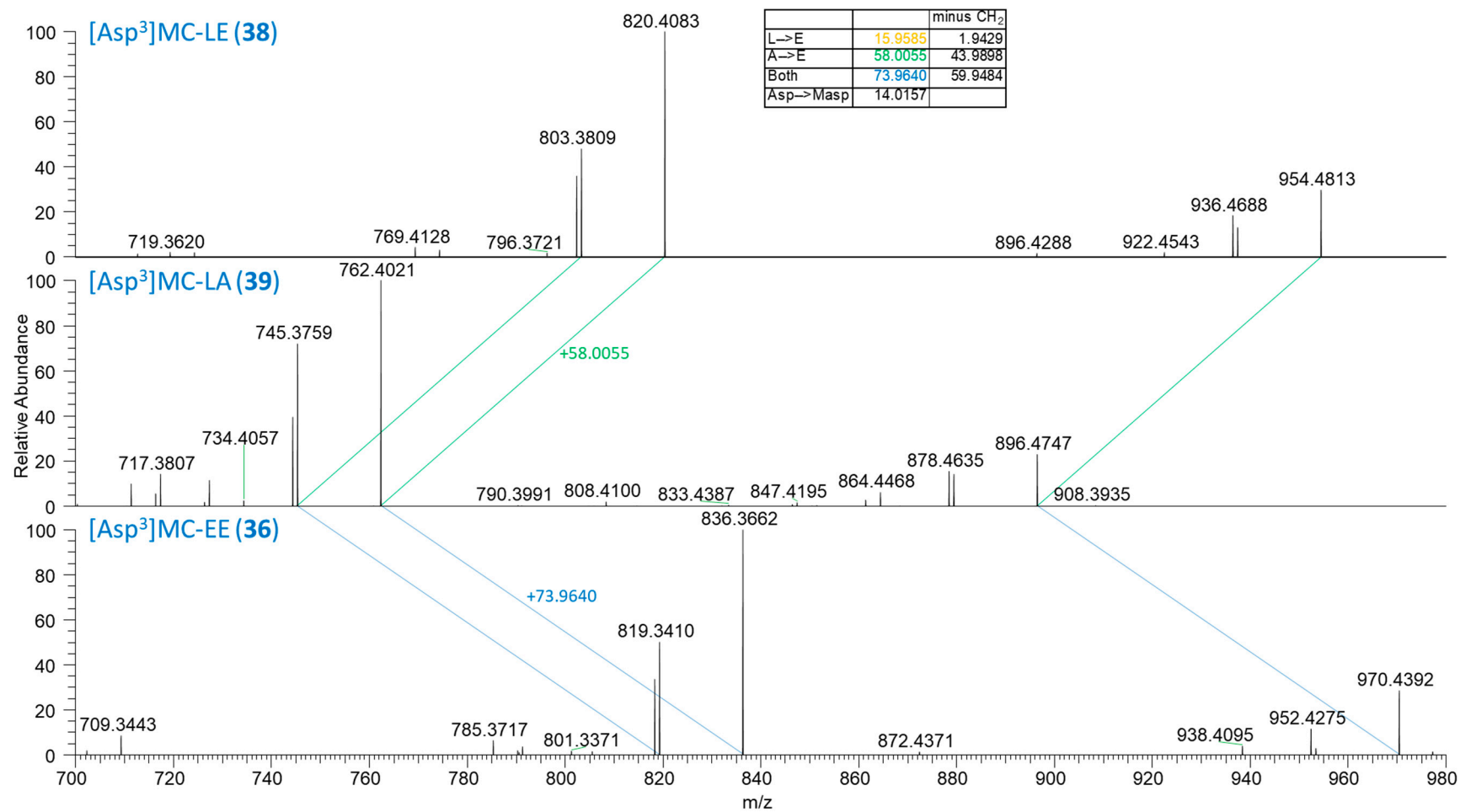
**Figure S23.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of  $[D\text{-Asp}^3]\text{MC-LE}$  (38),  $[D\text{-Asp}^3]\text{MC-LA}$  (39), and  $[D\text{-Asp}^3]\text{MC-EE}$  (36).



**Figure S24.** Expansion of LC-HRMS/MS spectra of [M+H]<sup>+</sup> of [D-Asp<sup>3</sup>]MC-LE (38), [D-Asp<sup>3</sup>]MC-LA (39), and [D-Asp<sup>3</sup>]MC-EE (36).

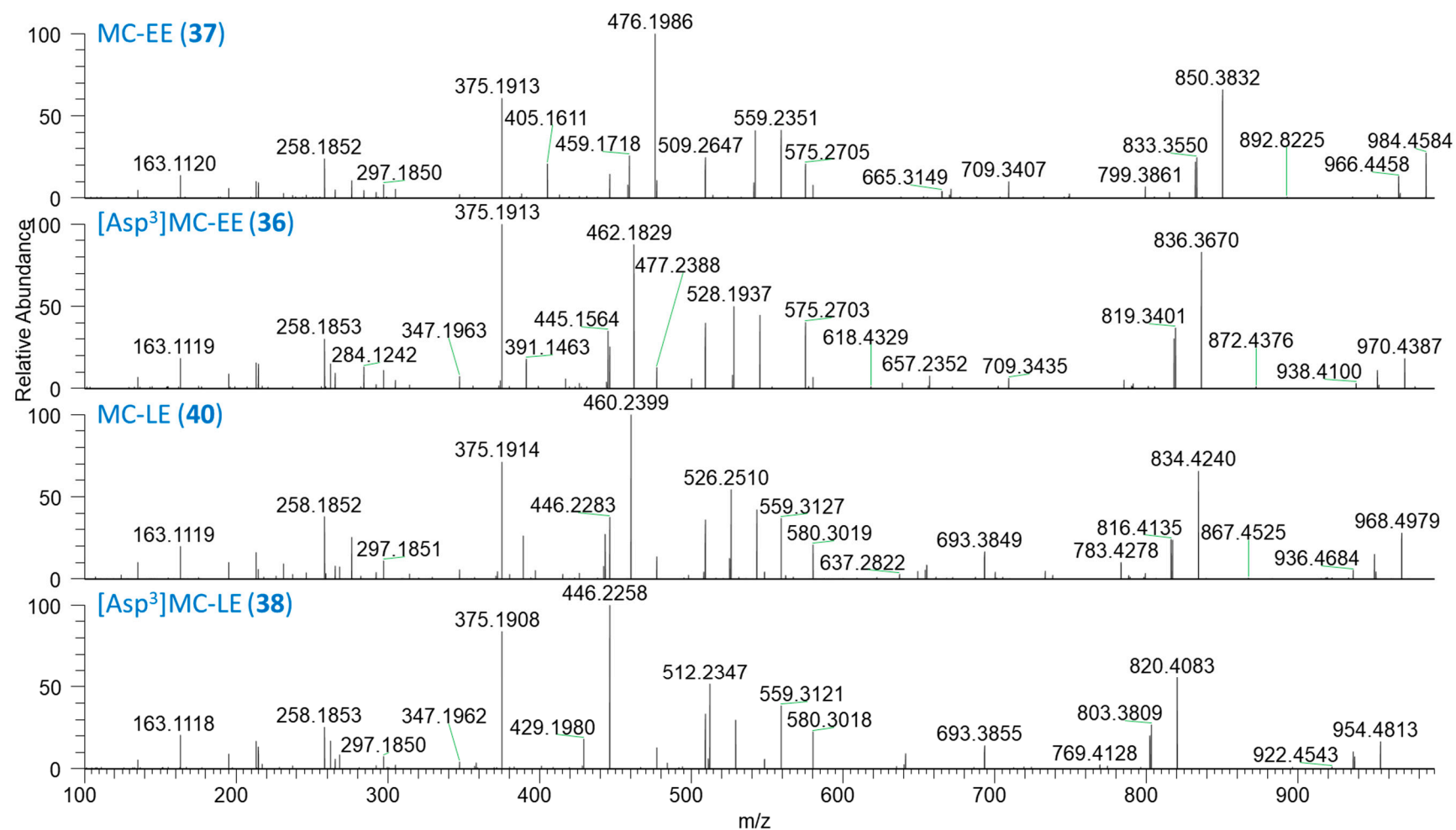


**Figure S25.** Expansion of LC-HRMS/MS spectra of [M+H]<sup>+</sup> of [D-Asp<sup>3</sup>]MC-LE (38), [D-Asp<sup>3</sup>]MC-LA (39), and [D-Asp<sup>3</sup>]MC-EE (36).



**Figure S26.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of  $[D\text{-}Asp^3]MC\text{-}LE$  (38),  $[D\text{-}Asp^3]MC\text{-}LA$  (39), and  $[D\text{-}Asp^3]MC\text{-}EE$  (36).





**Figure S27.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-EE (37),  $[D\text{-}Asp^3]MC\text{-}EE$  (36), MC-LE (40), and  $[D\text{-}Asp^3]MC\text{-}LE$  (38).



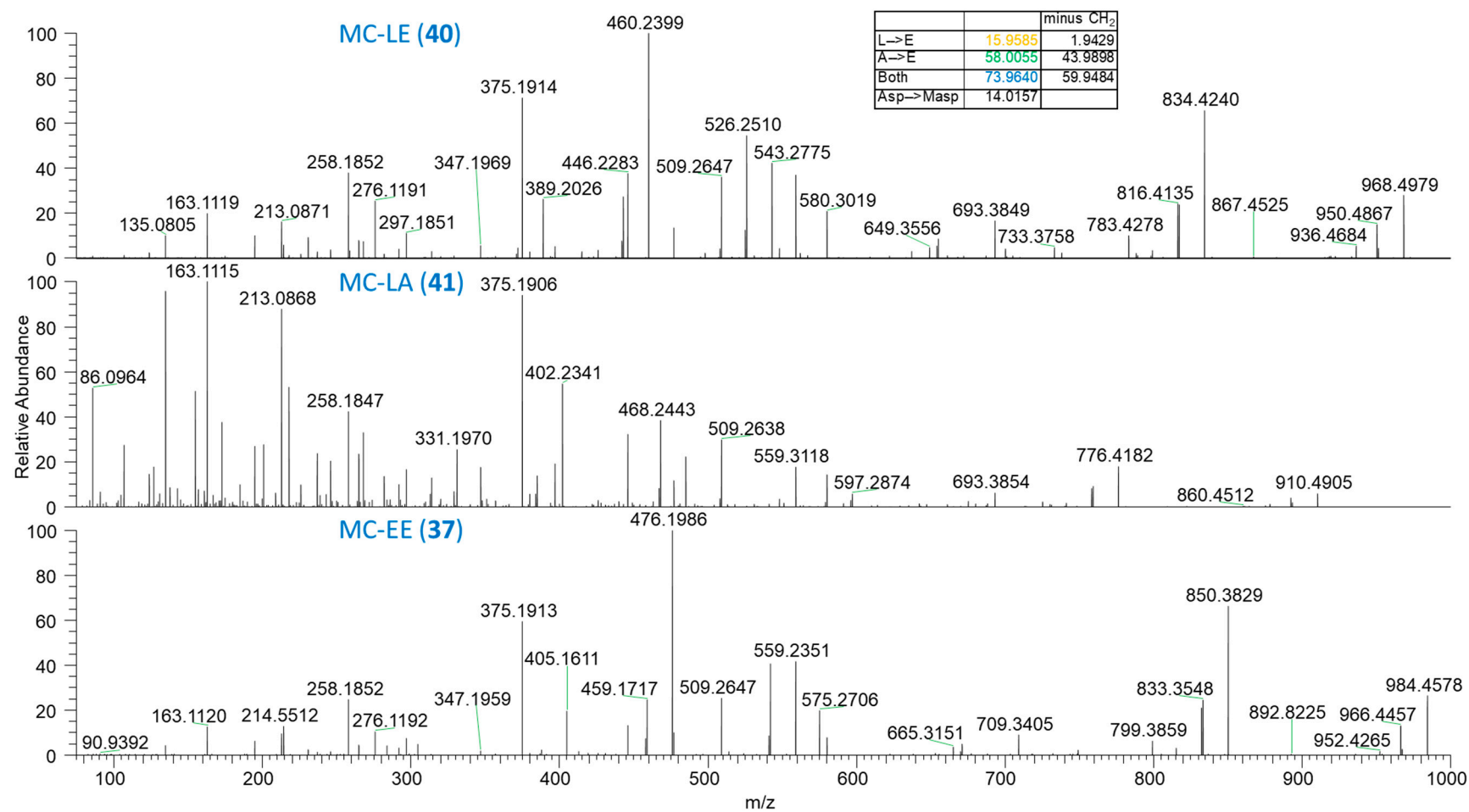
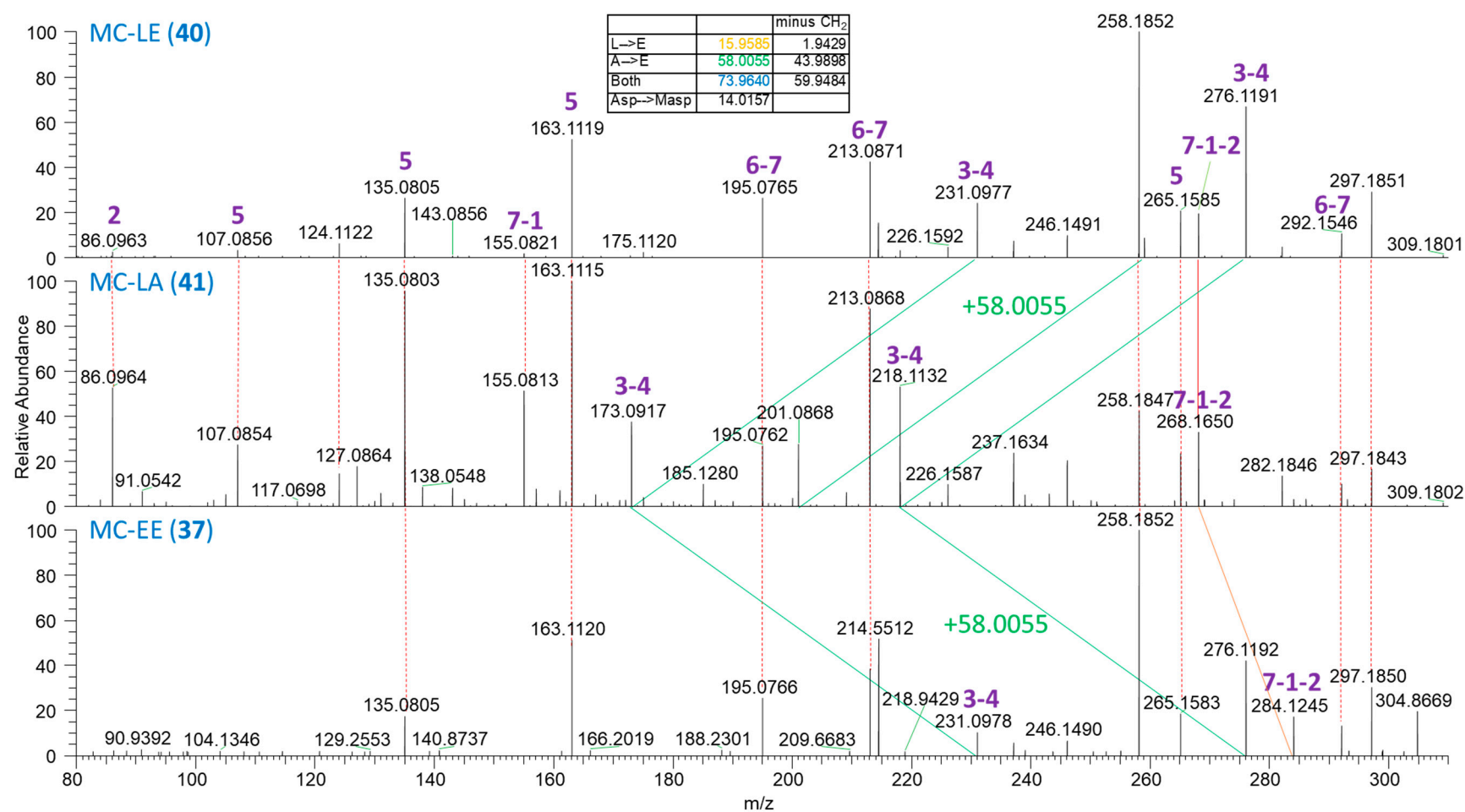
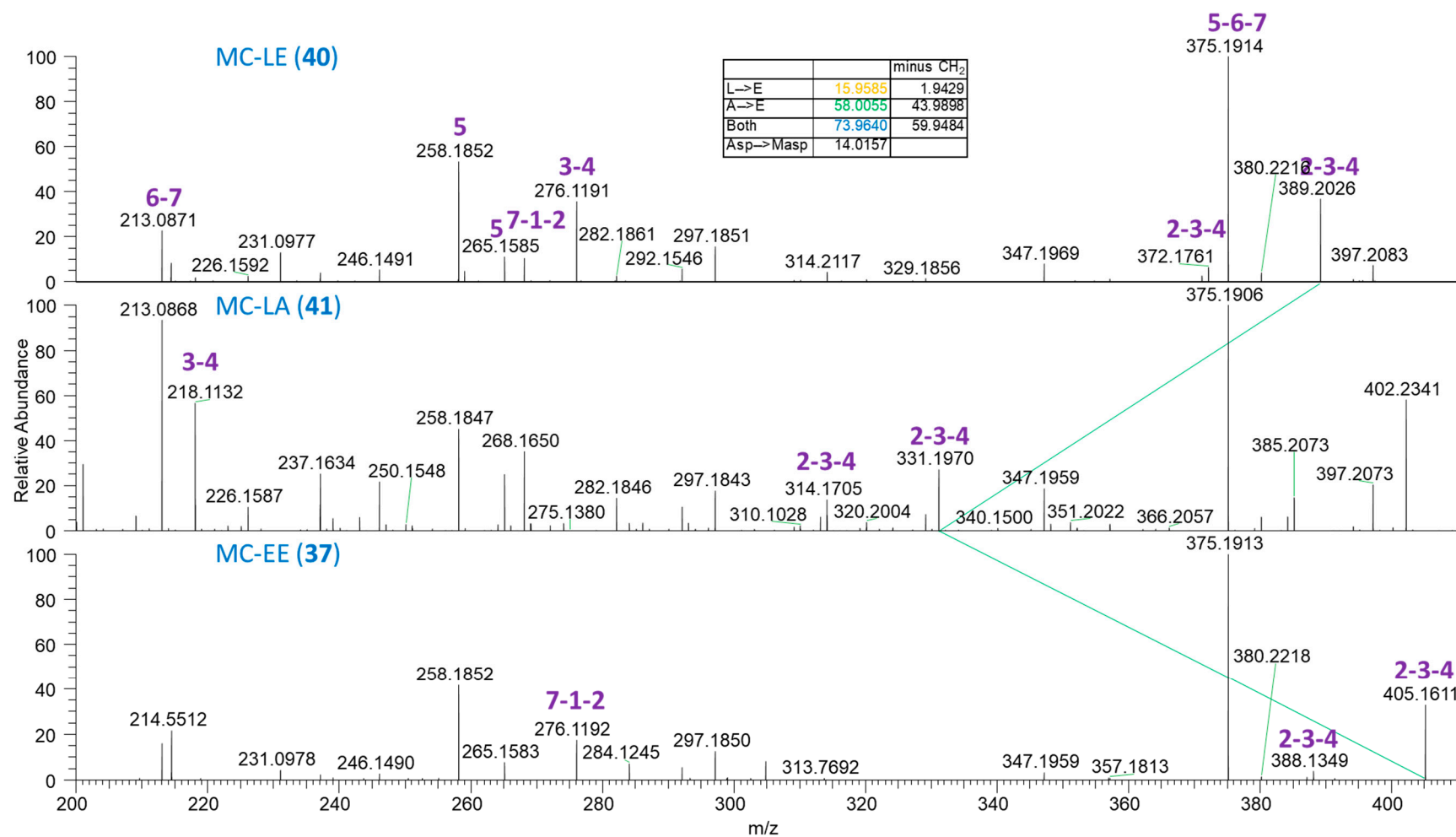


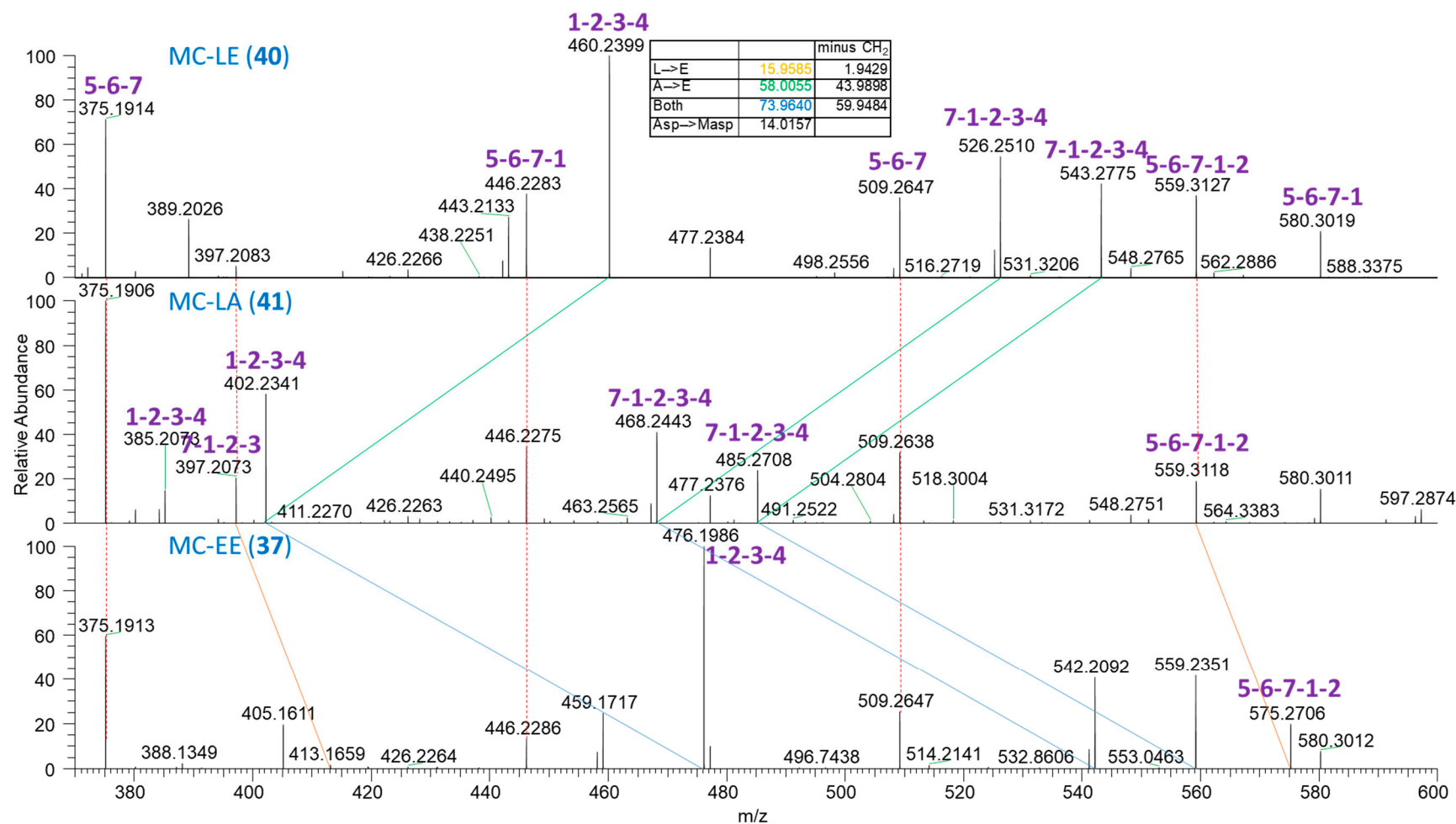
Figure S28. LC-HRMS/MS spectra of [M+H]<sup>+</sup> of MC-LE (40), MC-LA (41), and MC-EE (37).



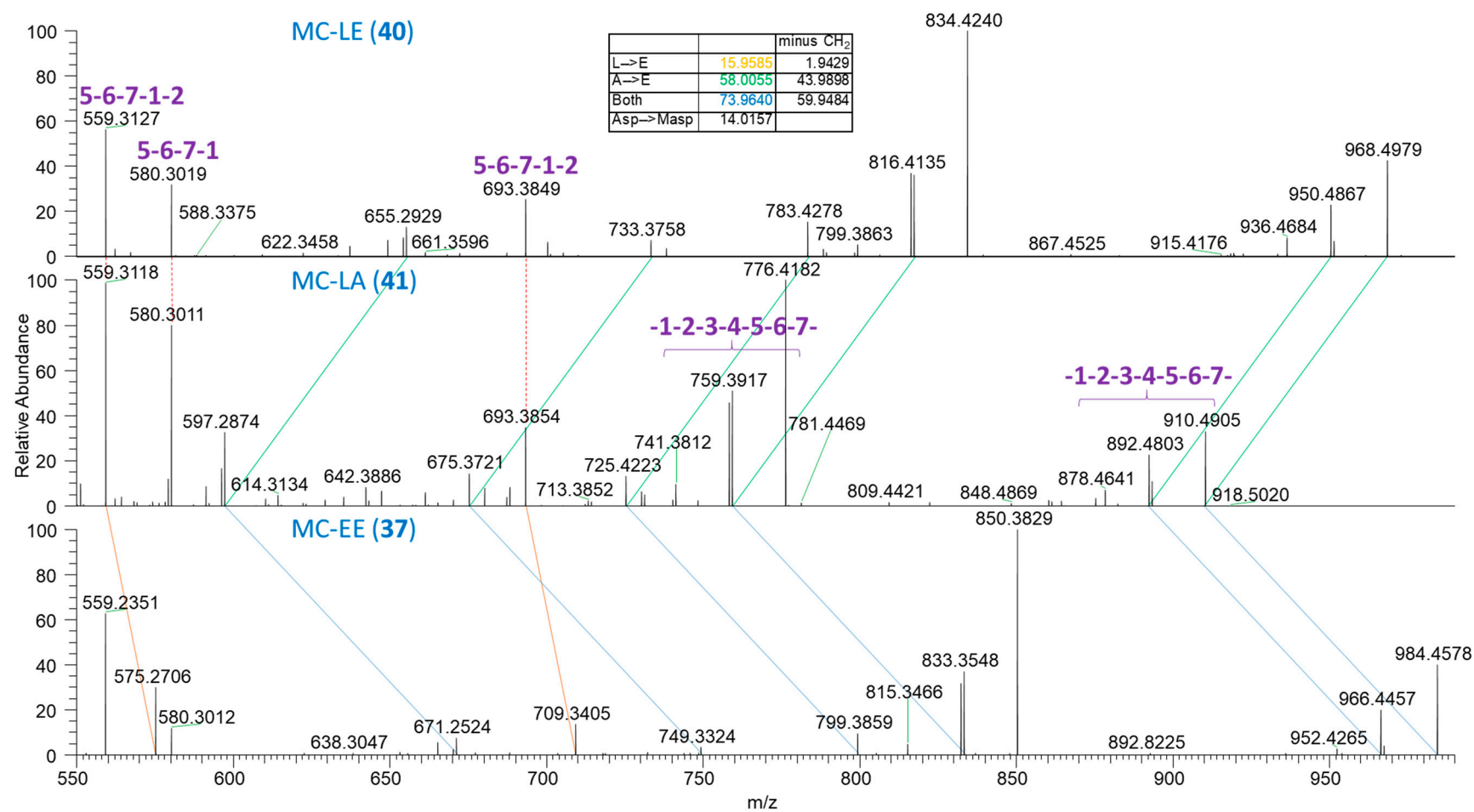
**Figure S29.** Expansion of LC-HRMS/MS spectra of [M+H]<sup>+</sup> of MC-LE (40), MC-LA (41), and MC-EE (37).



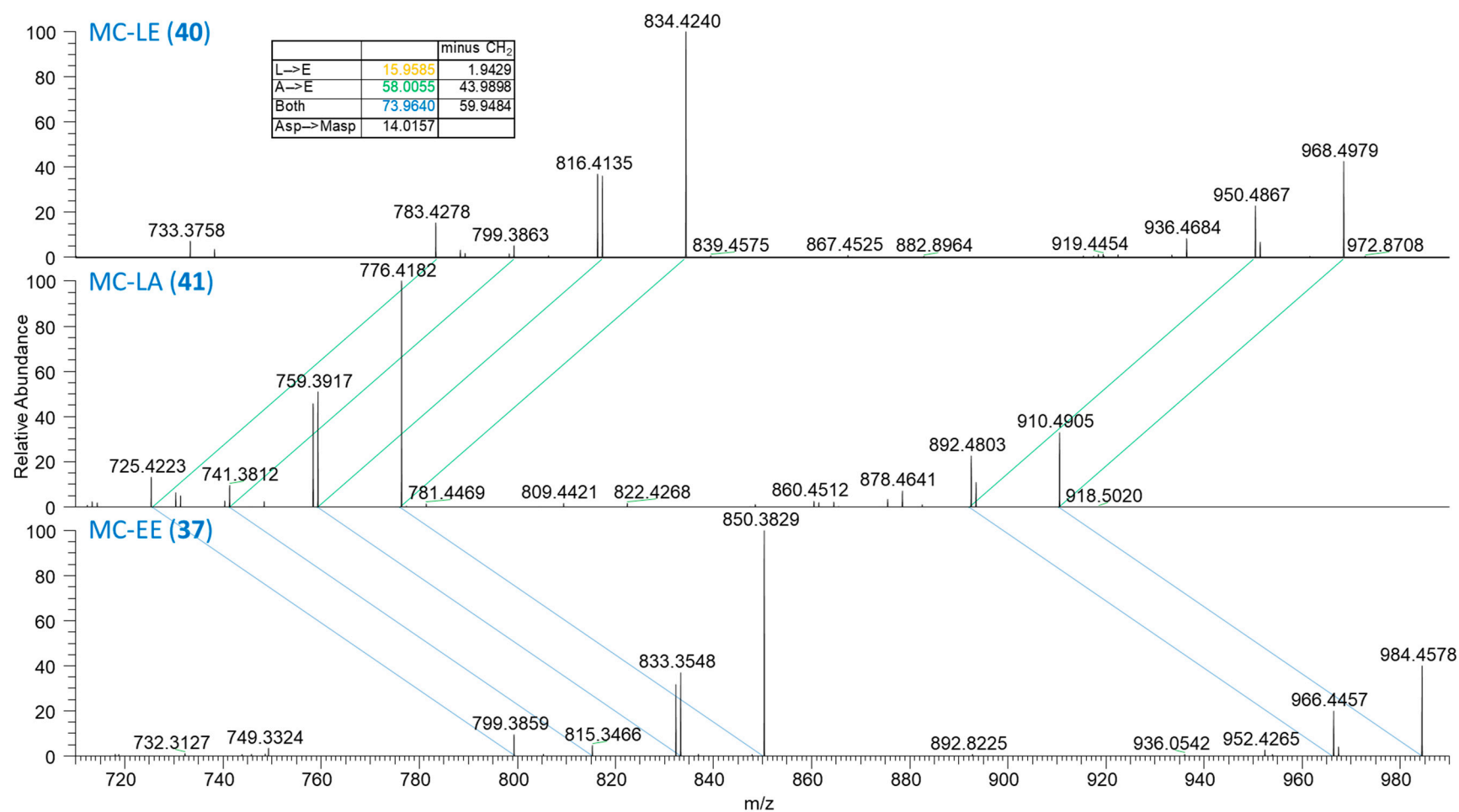
**Figure S30.** Expansion of LC-HRMS/MS spectra of [M+H]<sup>+</sup> of MC-LE (40), MC-LA (41), and MC-EE (37).



**Figure S31.** Expansion of LC-HRMS/MS spectra of [M+H]<sup>+</sup> of MC-LE (40), MC-LA (41), and MC-EE (37).



**Figure S32.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-LE (40), MC-LA (41), and MC-EE (37).



**Figure S33.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of MC-LE (40), MC-LA (41), and MC-EE (37).

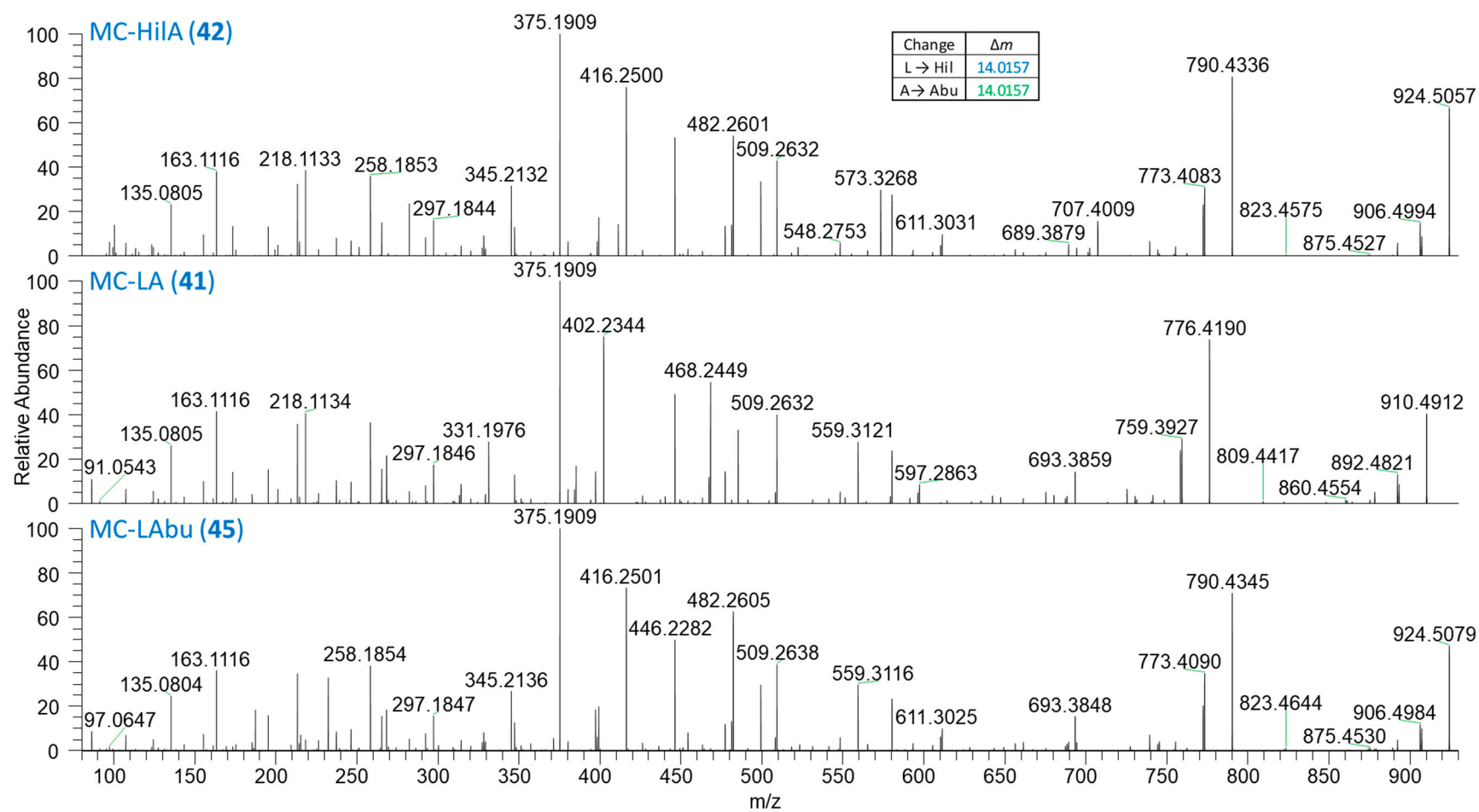


Figure S34. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-HiLA (42), MC-LA (41), and MC-LABu (45).



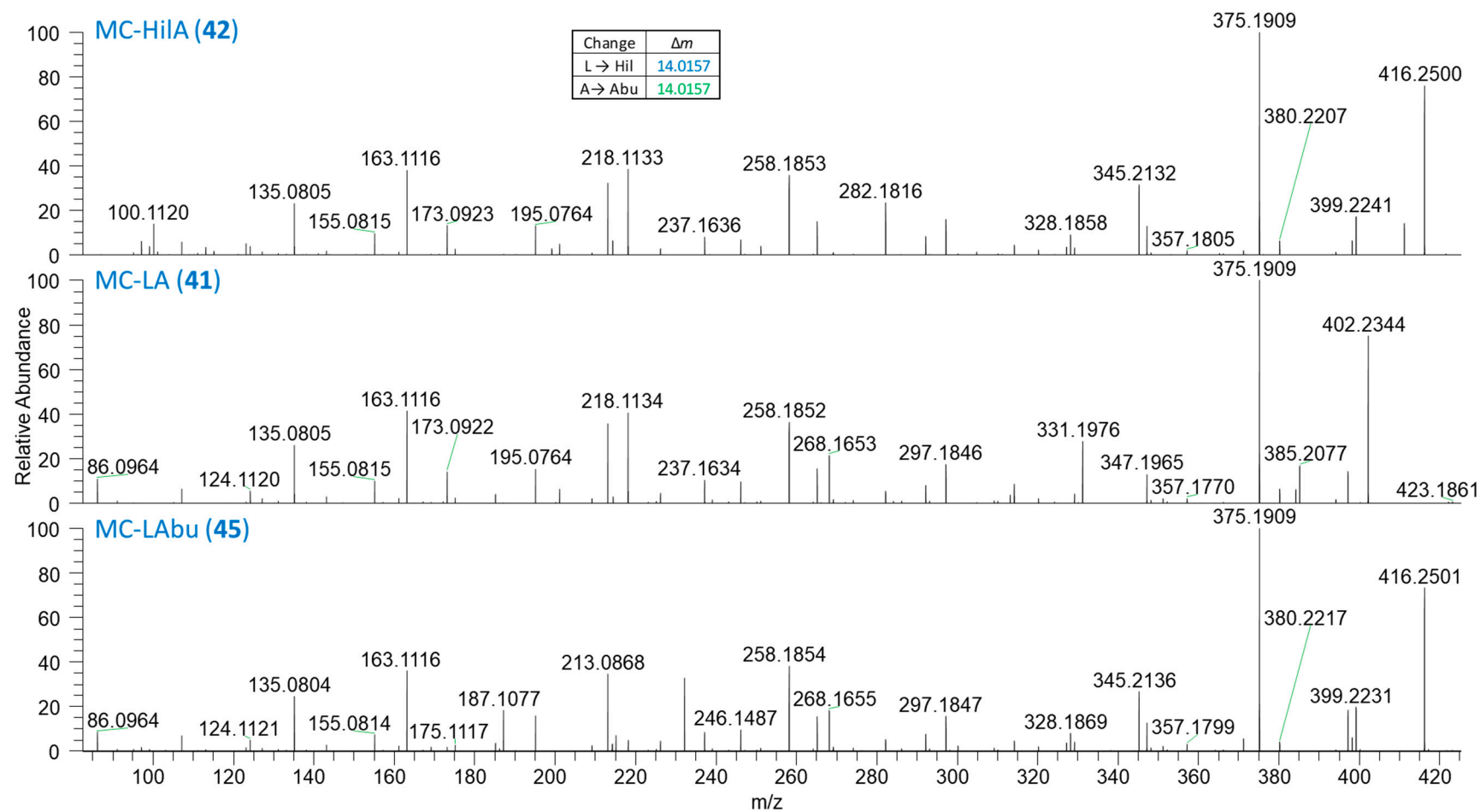
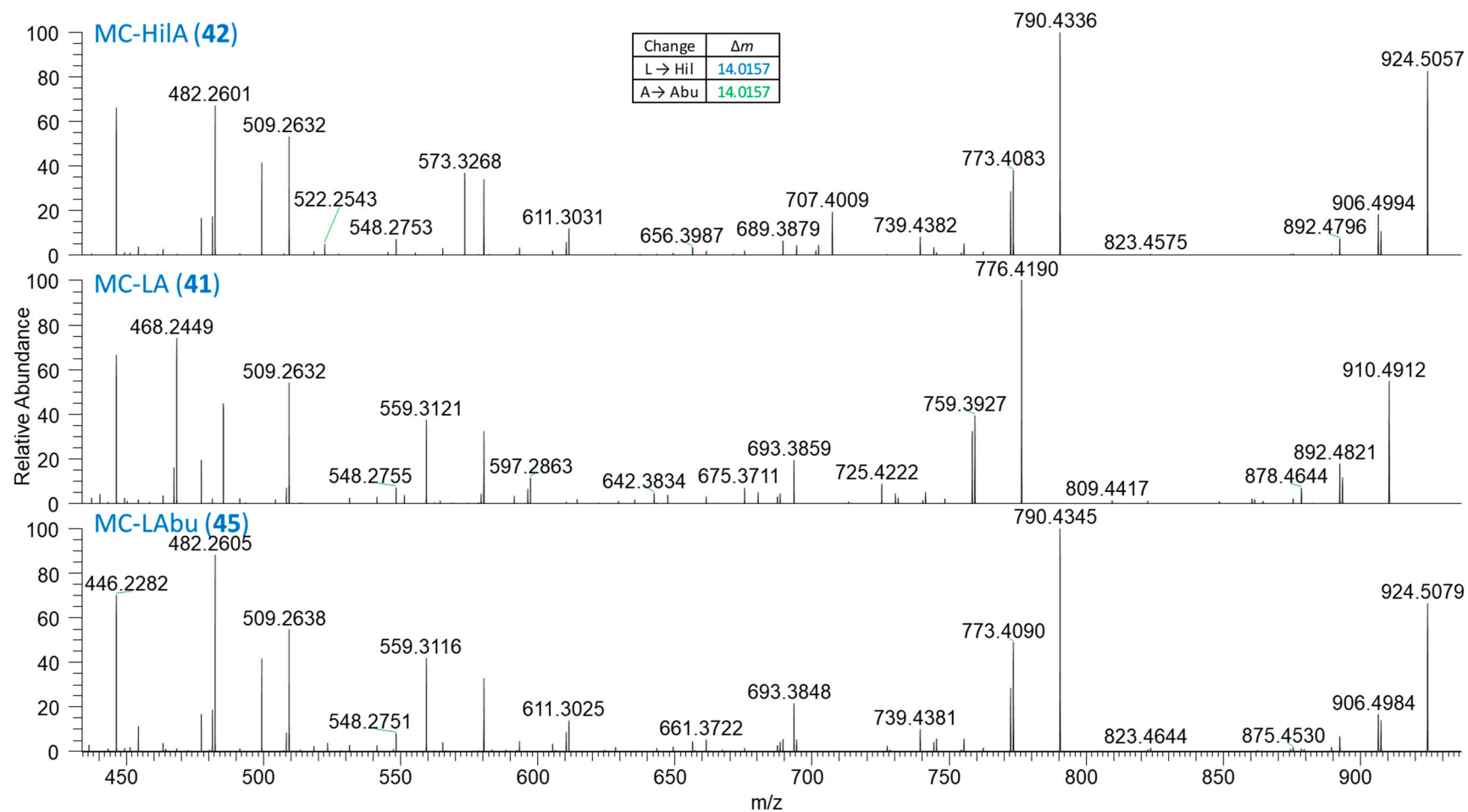
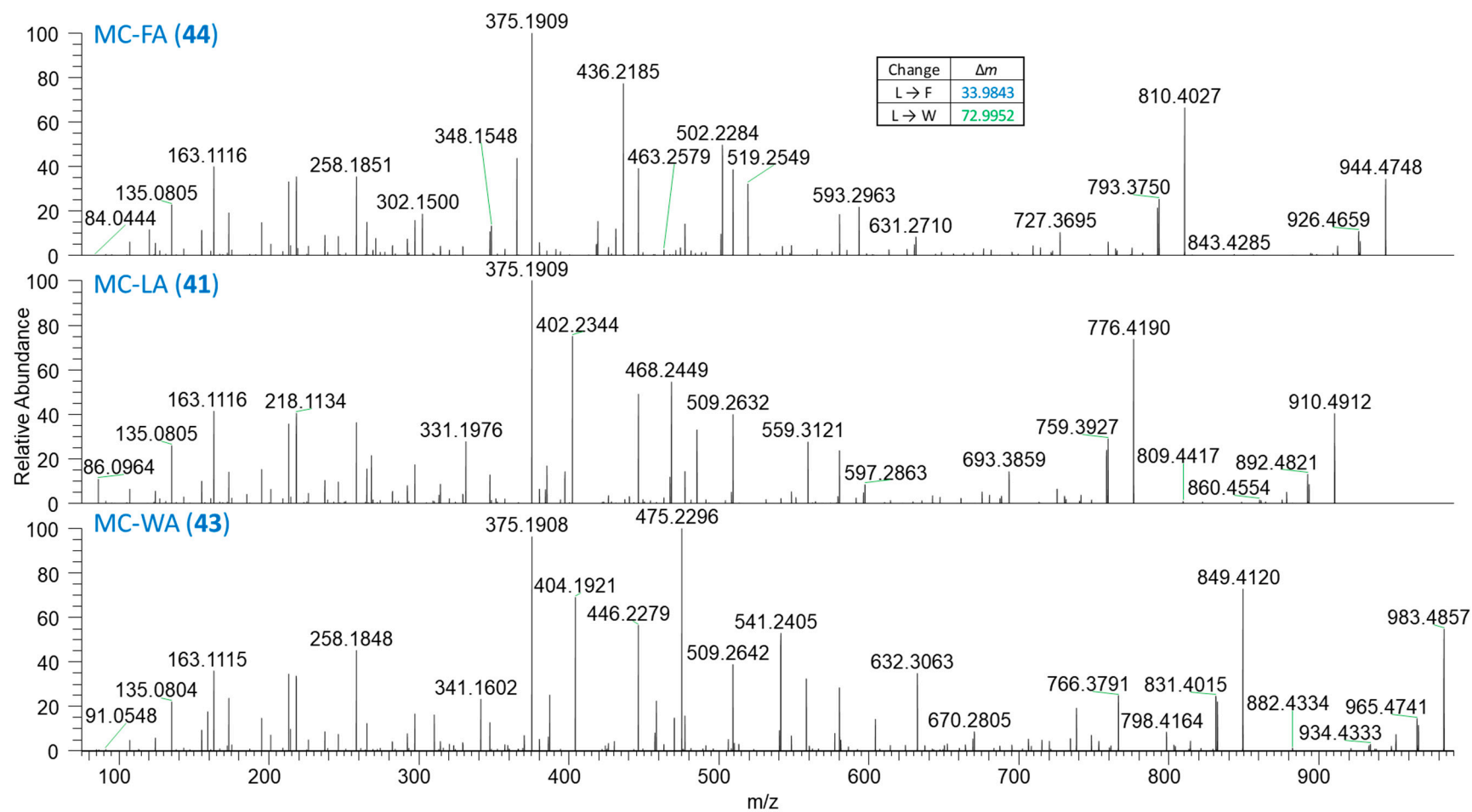


Figure S35. Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-HiLA (42), MC-LA (41), and MC-LAbu (45).





**Figure S36.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-HiLA (42), MC-LA (41), and MC-LAbu (45).



**Figure S37.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-FA (44), MC-LA (41), and MC-WA (43).

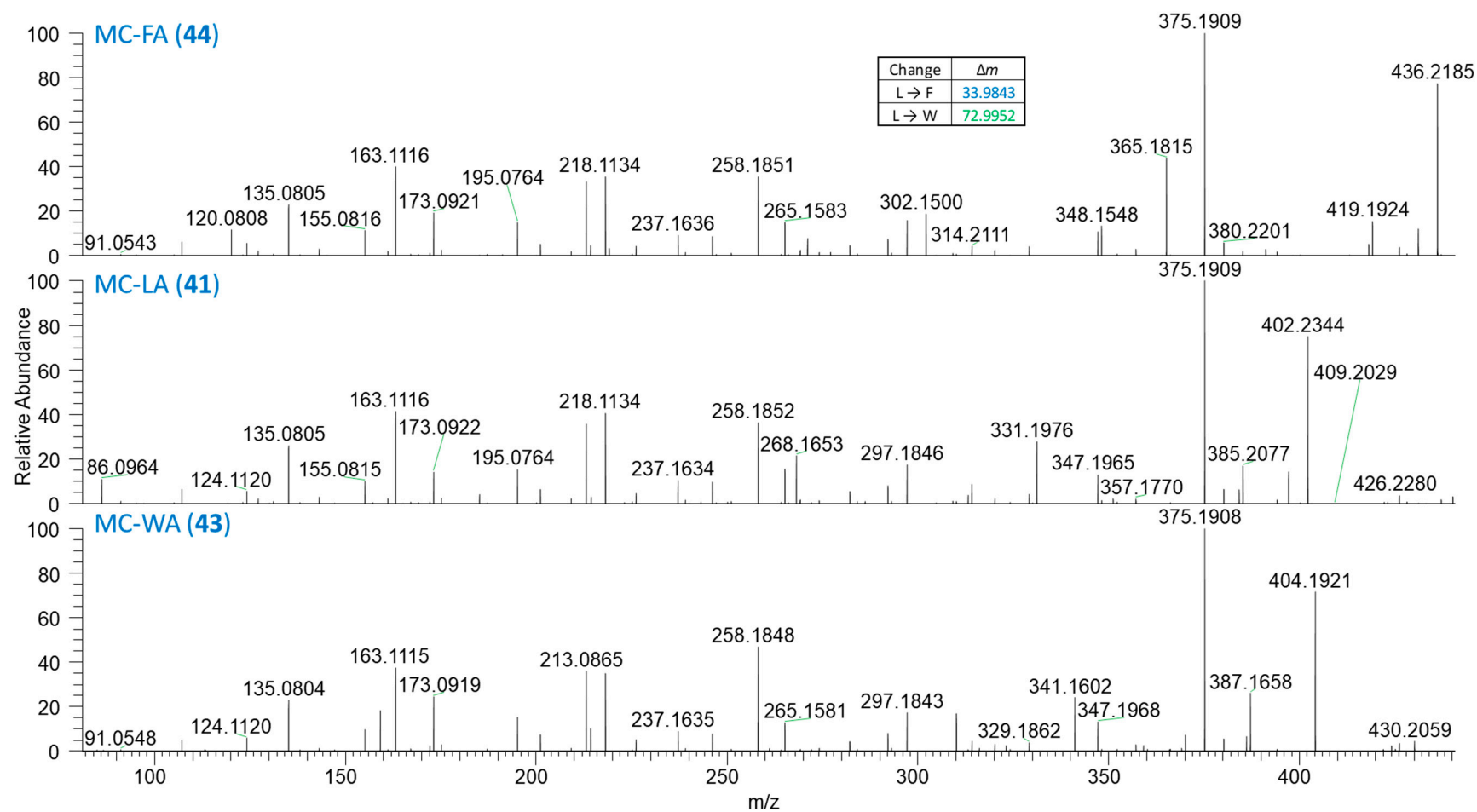
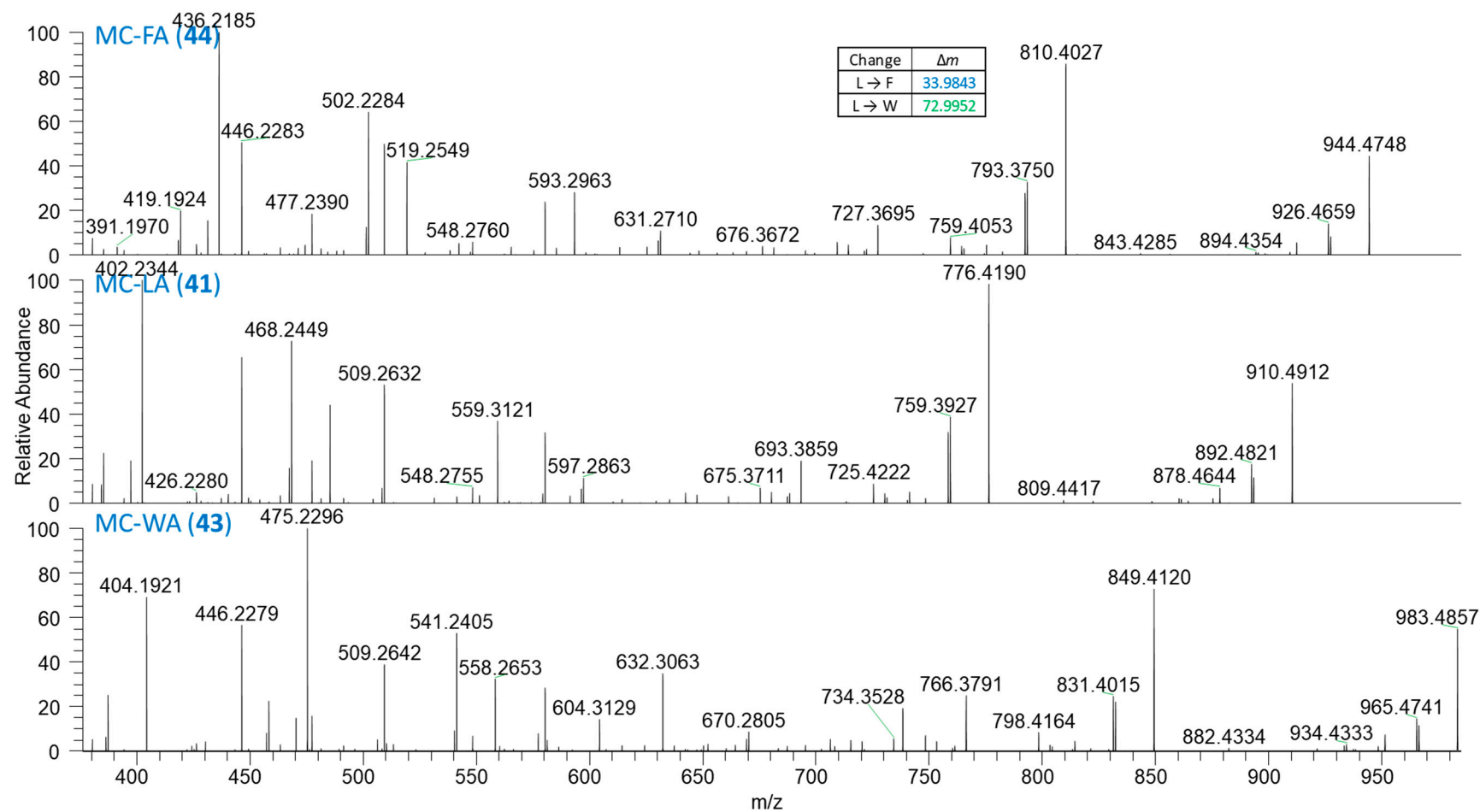


Figure S38. Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of MC-FA (44), MC-LA (41), and MC-WA (43).



**Figure S39.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of MC-FA (44), MC-LA (41), and MC-WA (43).

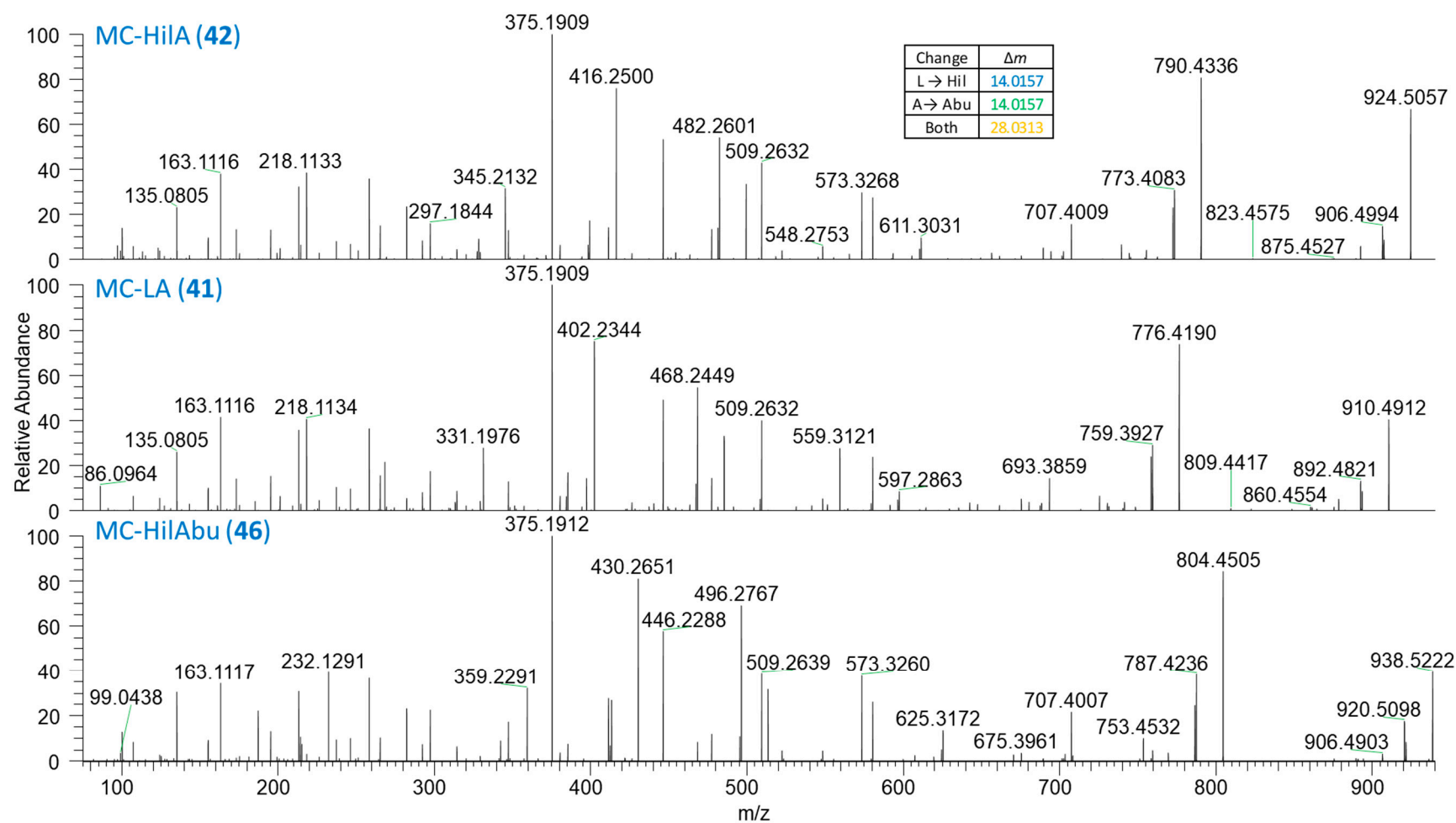
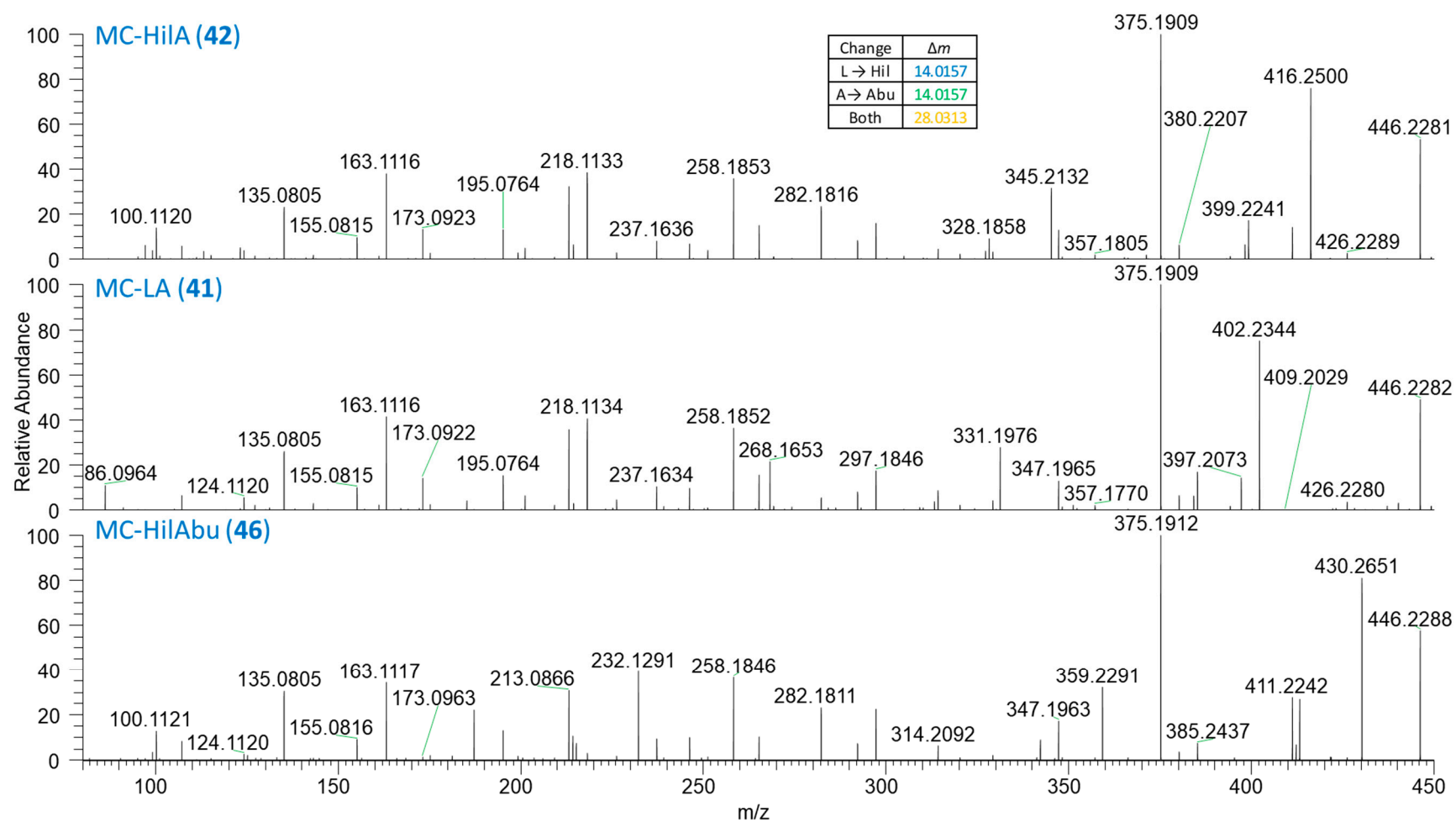
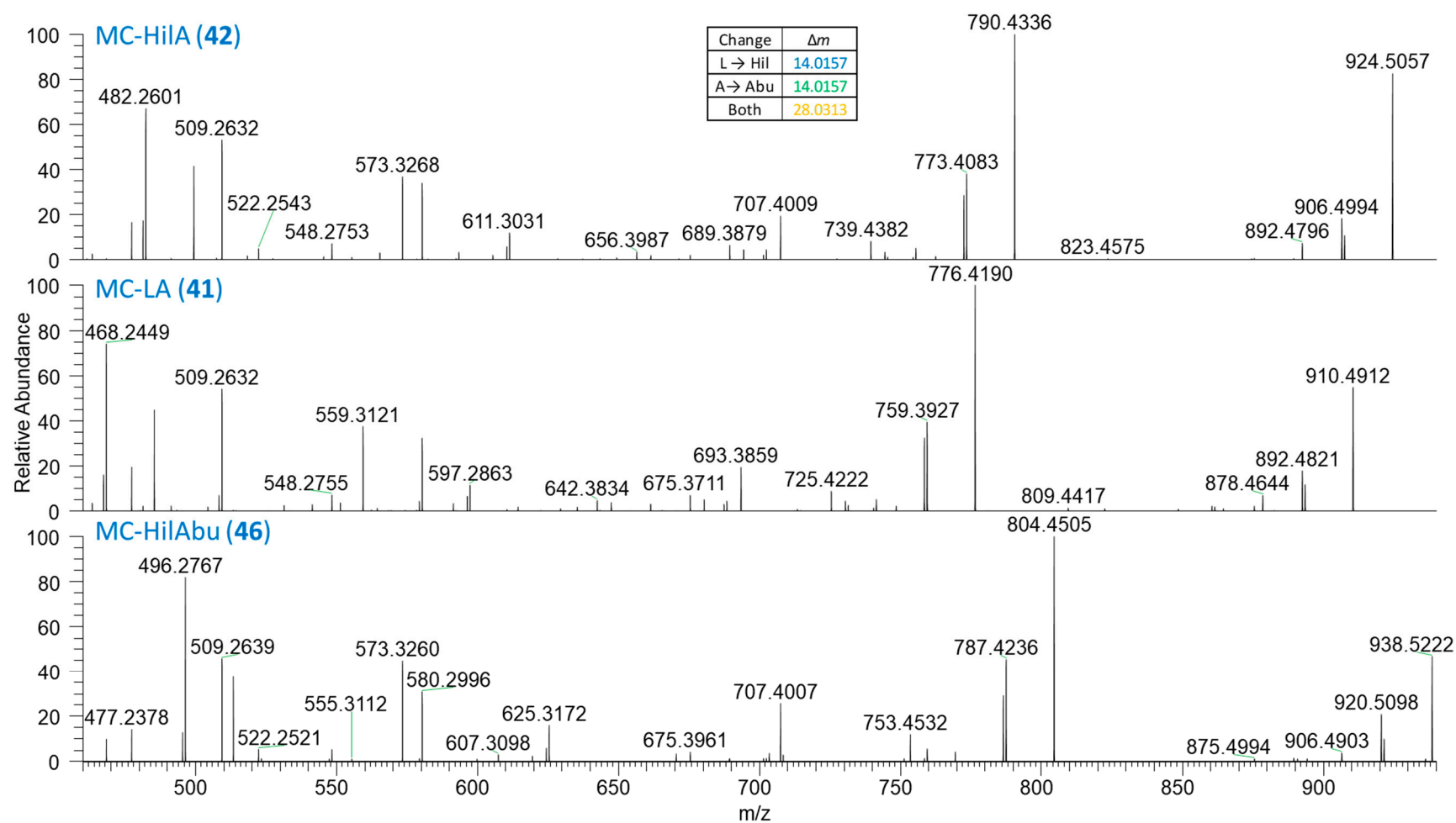


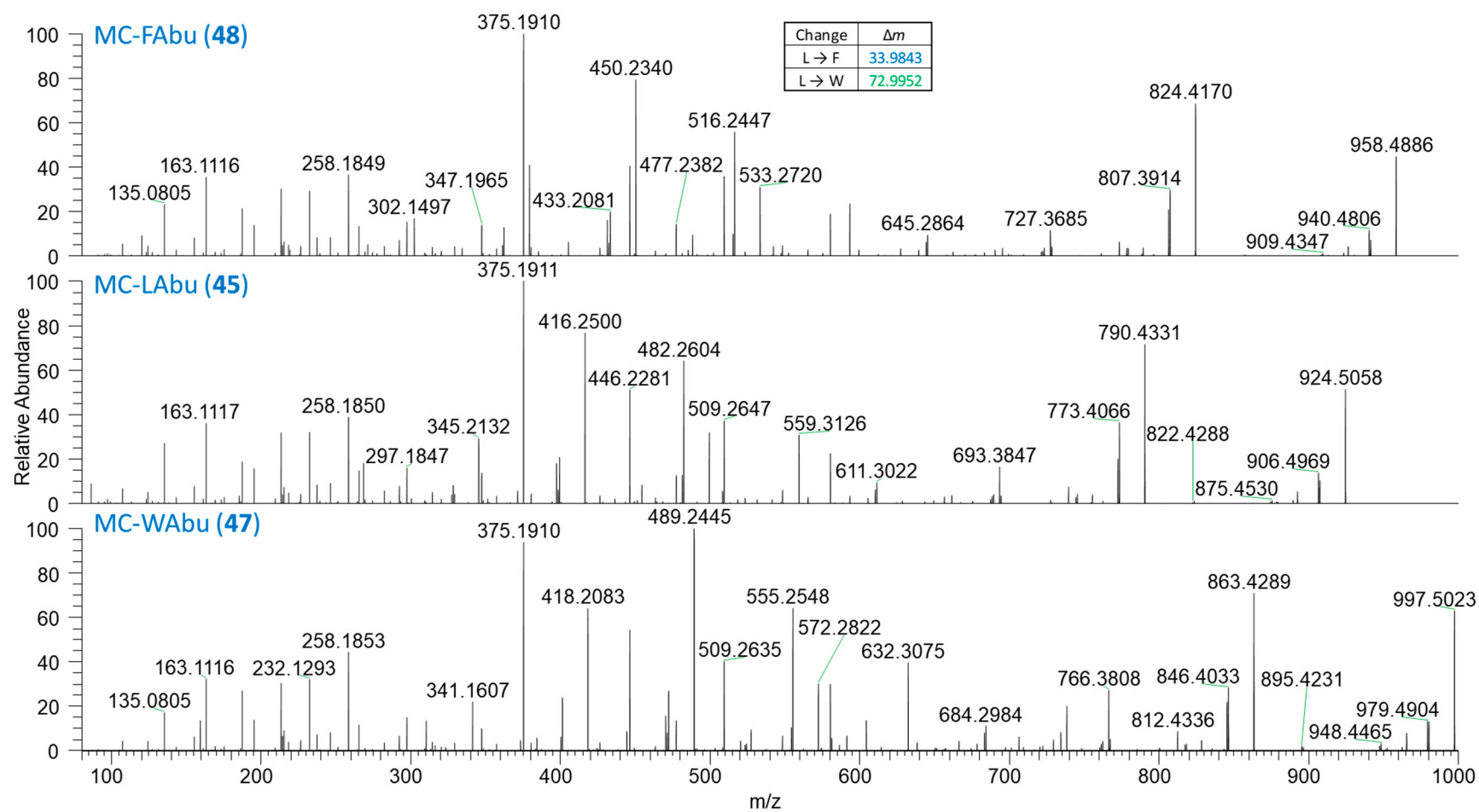
Figure S40. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-HilA (42), MC-LA (41), and MC-HilAbu (46).



**Figure S41.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of MC-HiLA (42), MC-LA (41), and MC-HiABu (46).

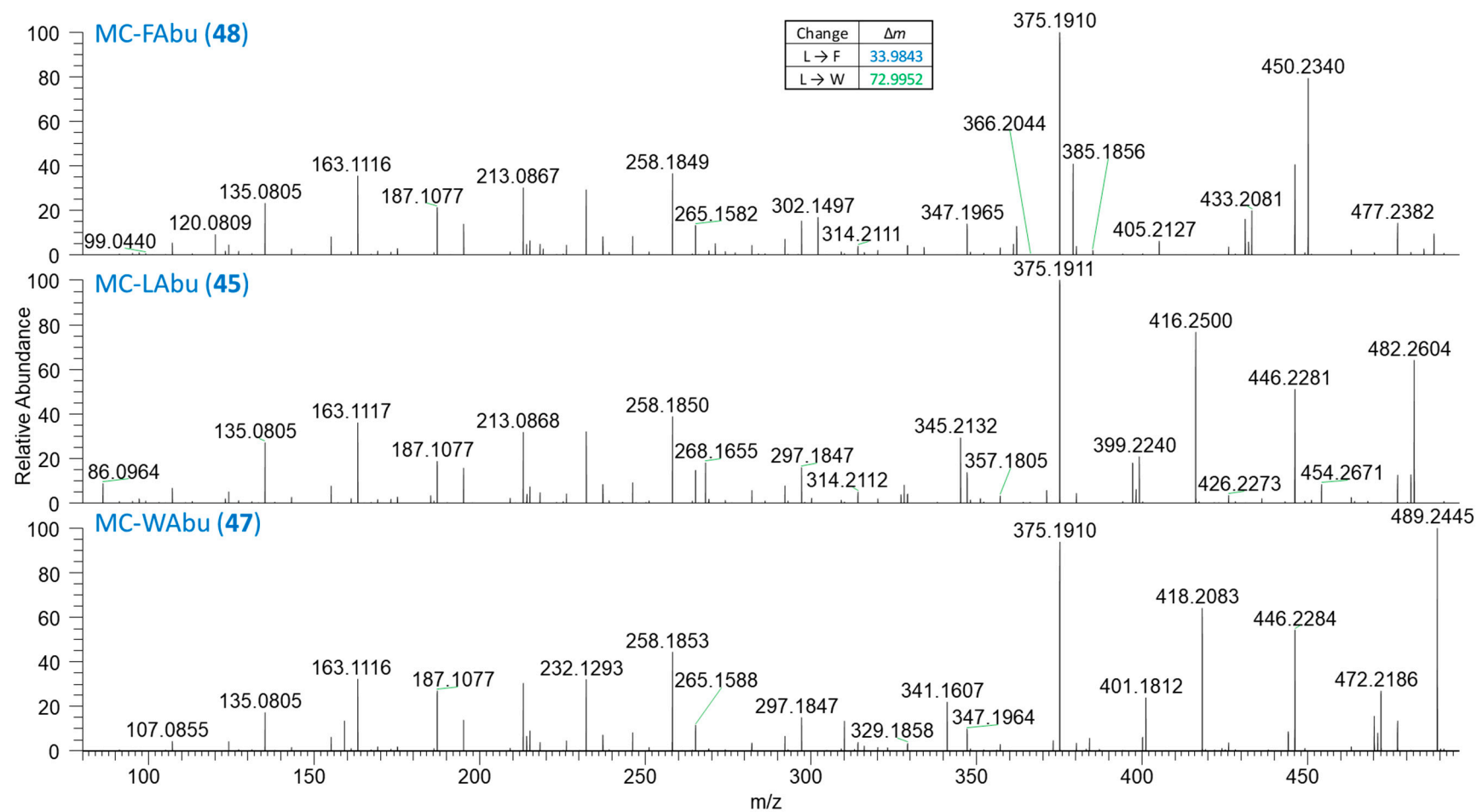


**Figure S42.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of MC-HilA (42), MC-LA (41), and MC-HilAbu (46).

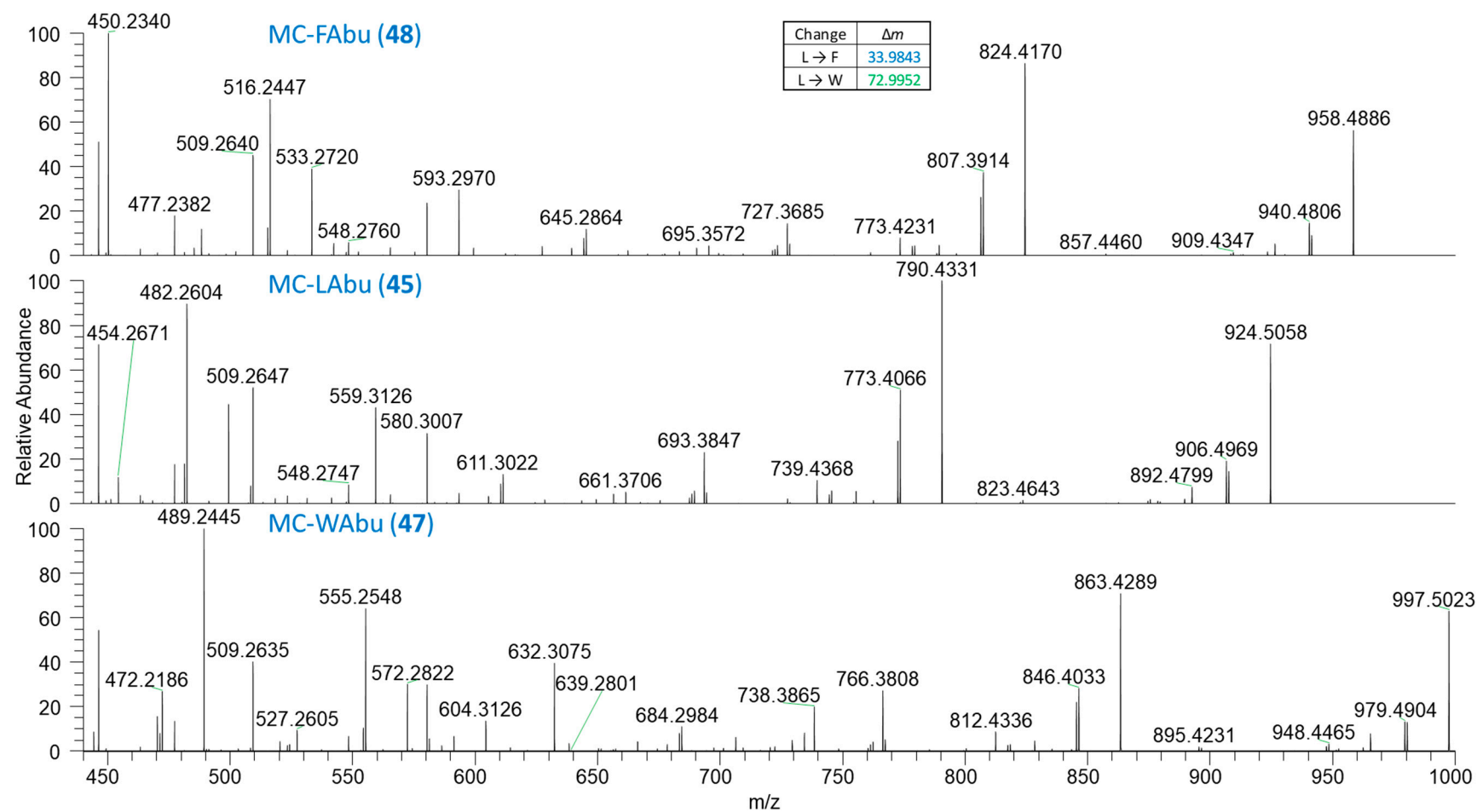


**Figure S43.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-FAbu (48), MC-LAbu (45), and MC-WAbu (47).





**Figure S44.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of MC-FAbu (48), MC-LAbu (45), and MC-WAbu (47).



**Figure S45.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-FABu (48), MC-LABu (45), and MC-WABu (47).

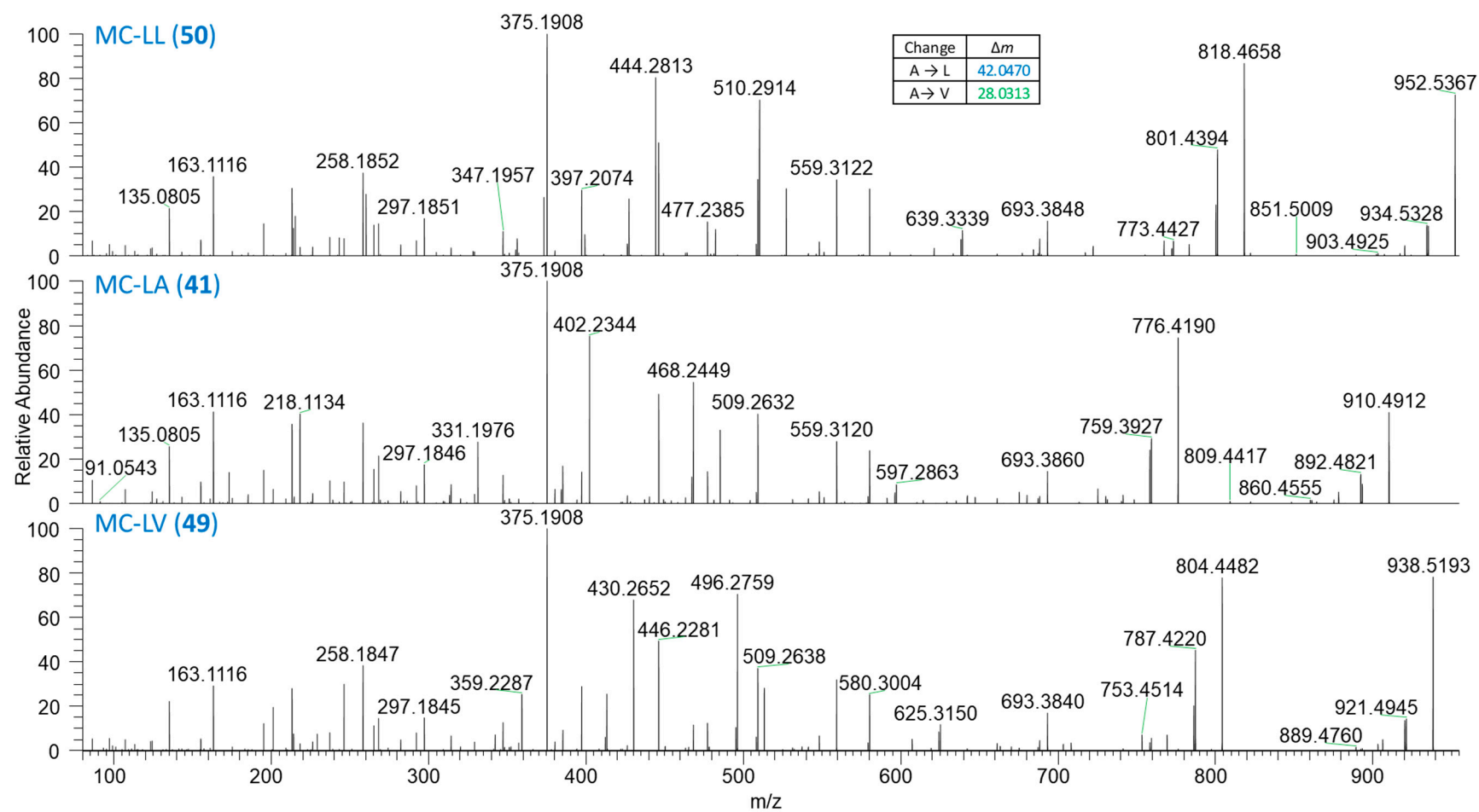
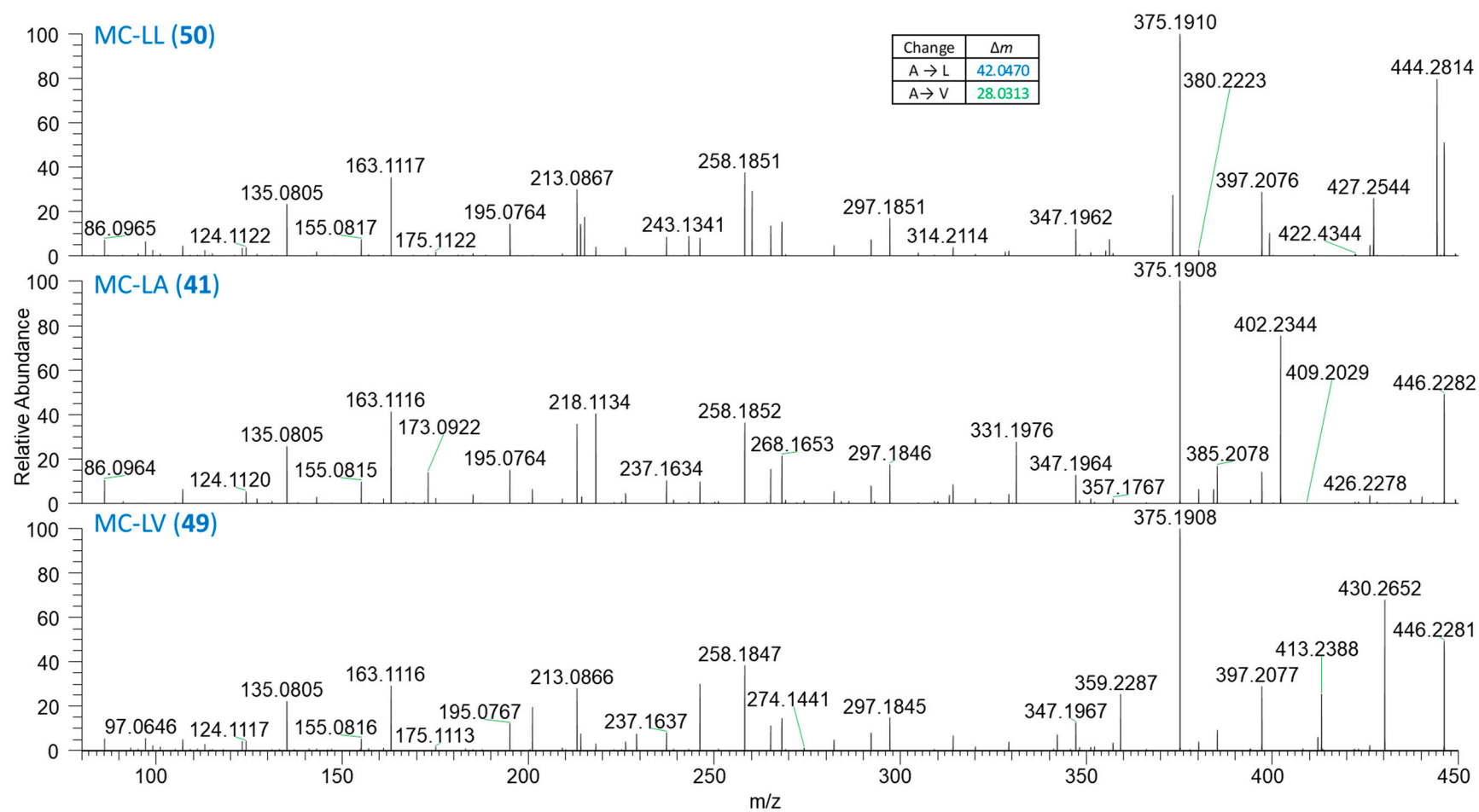
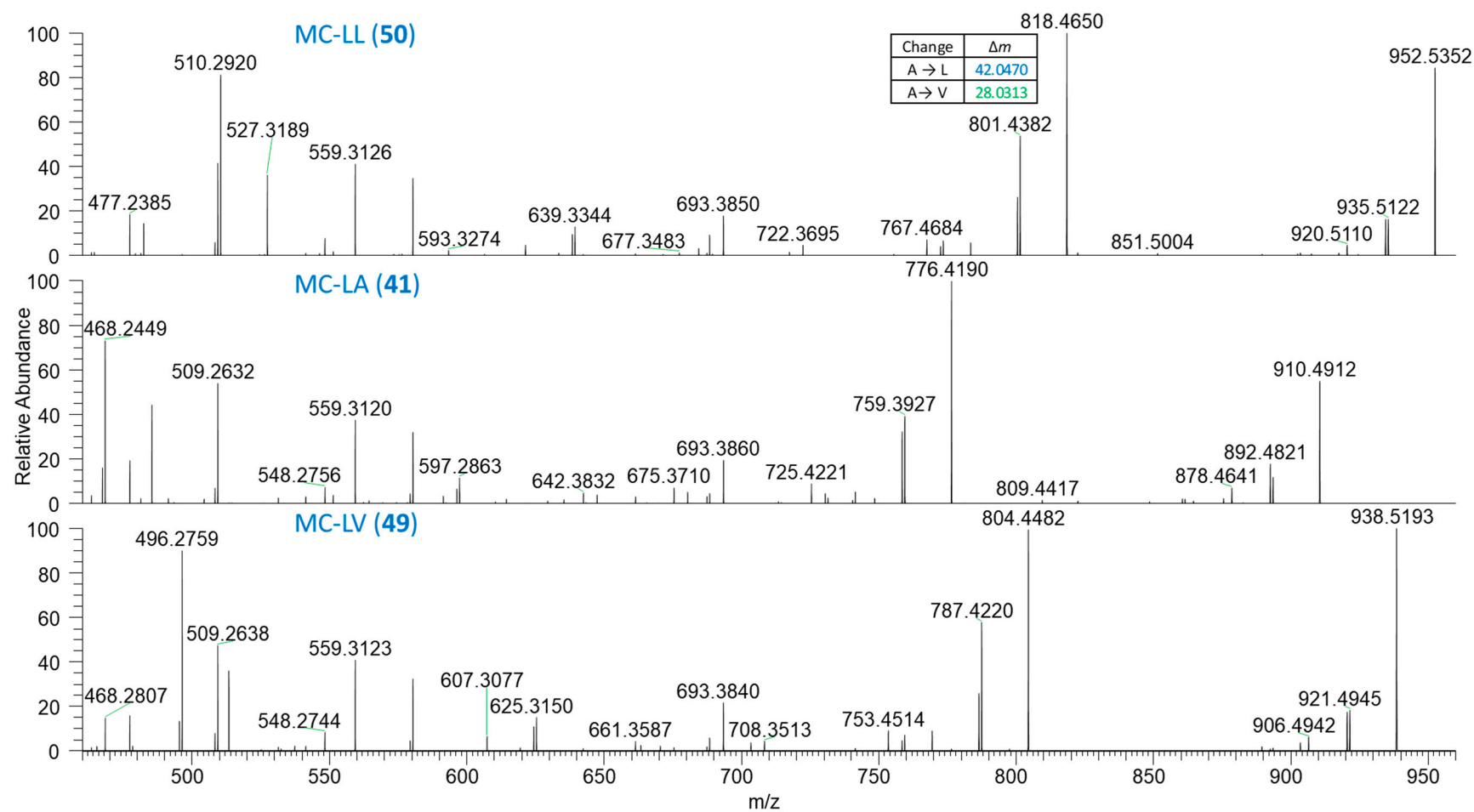


Figure S46. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-LL (50), MC-LA (41), and MC-LV (49).



**Figure S47.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-LL (50), MC-LA (41), and MC-LV (49).



**Figure S48.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of MC-LL (50), MC-LA (41), and MC-LV (49).

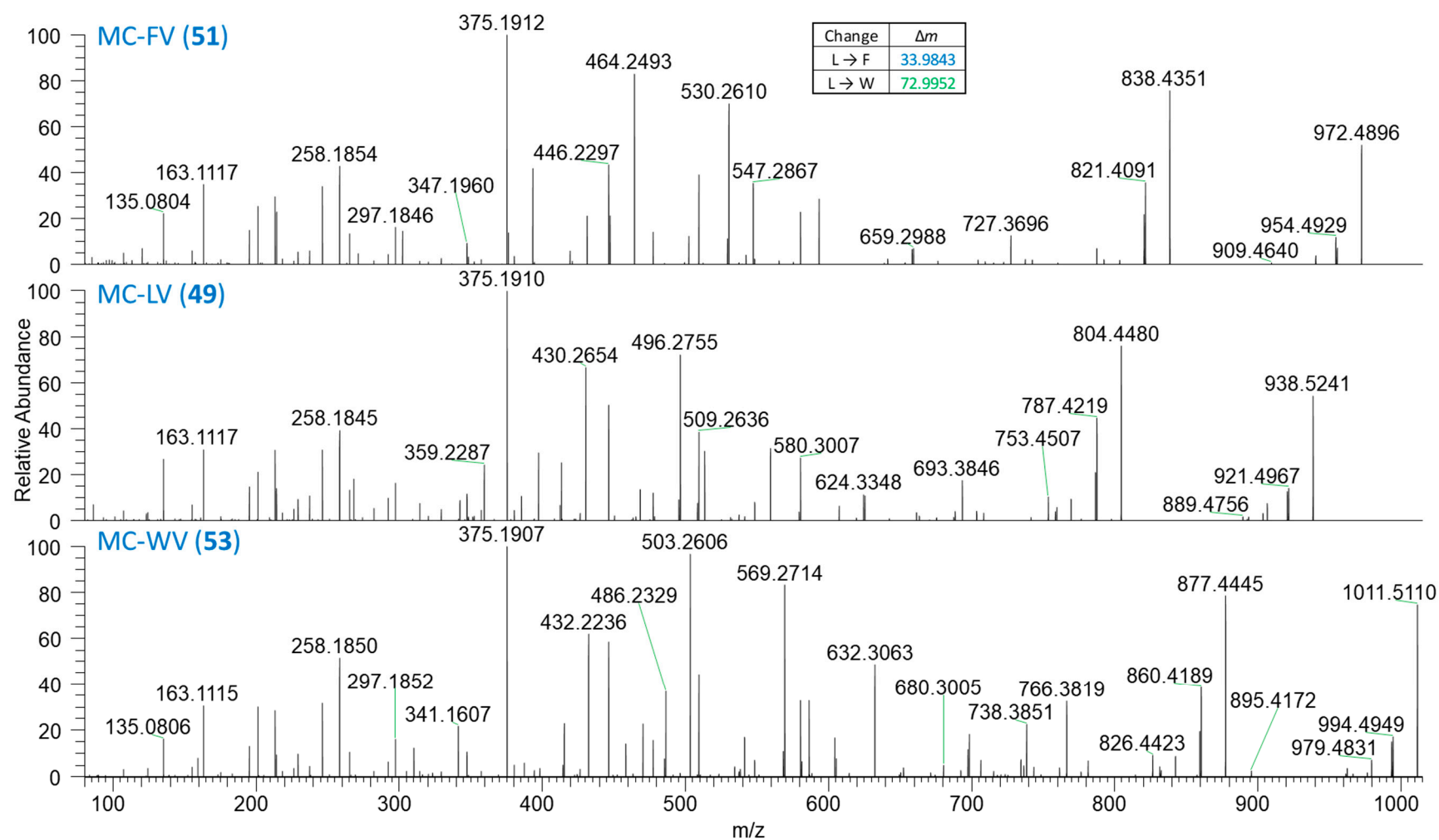


Figure S49. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-FV (51), MC-LV (49), and MC-WV (53).

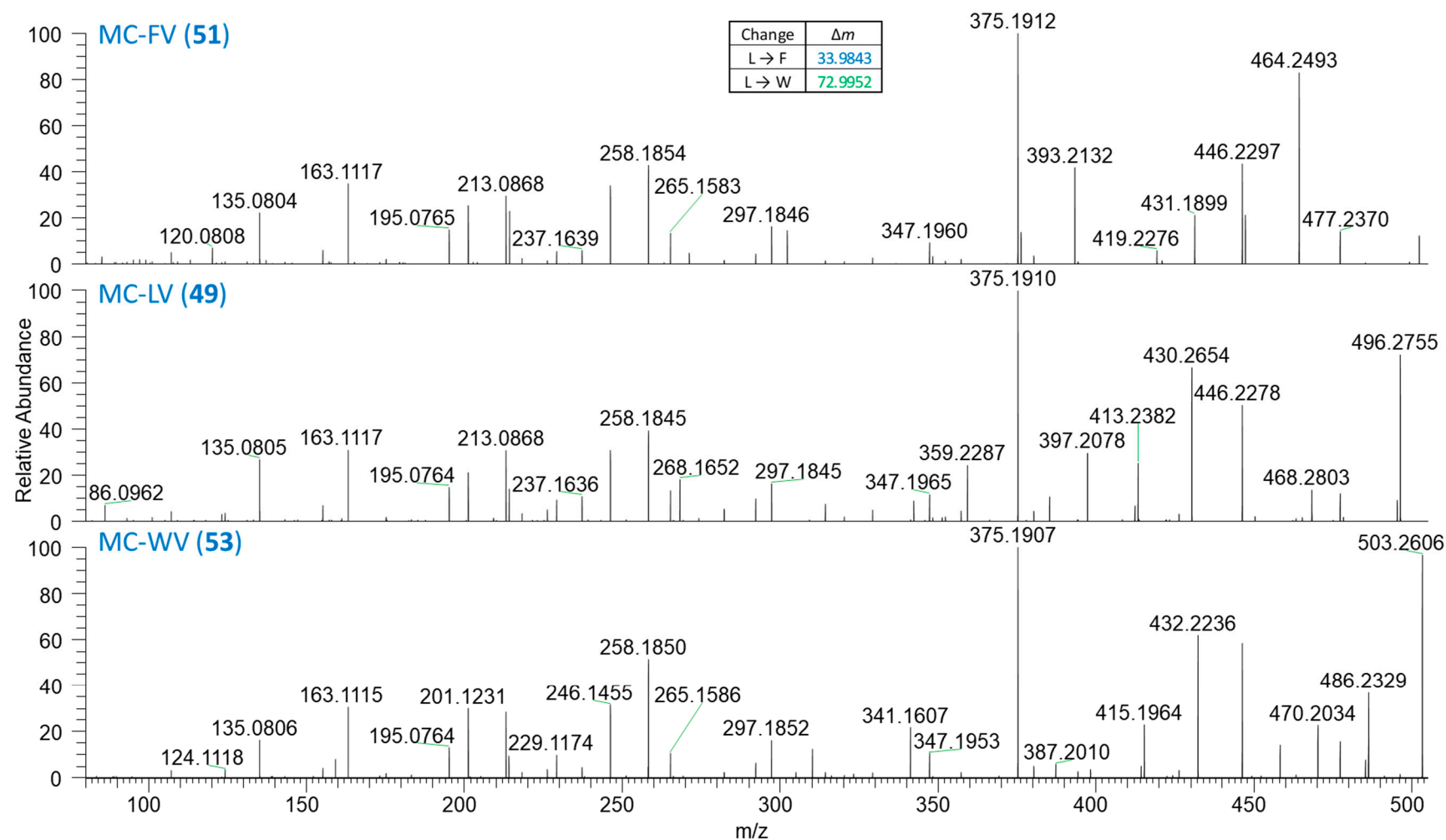
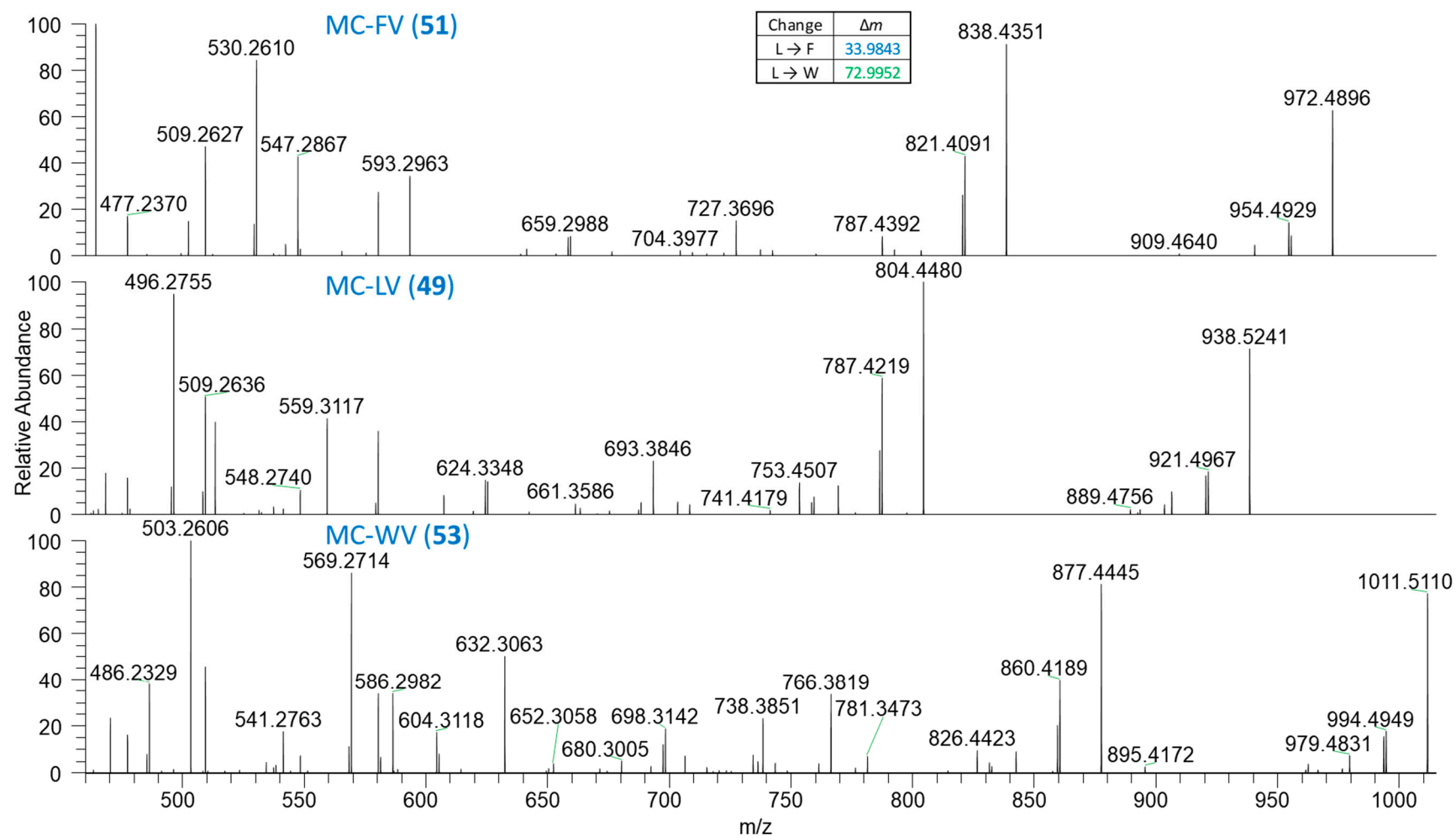


Figure S50. Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-FV (51), MC-LV (49), and MC-WV (53).



**Figure S51.** Expansion of LC-HRMS/MS spectra of  $[M+H]^+$  of MC-FV (51), MC-LV (49), and MC-WV (53).



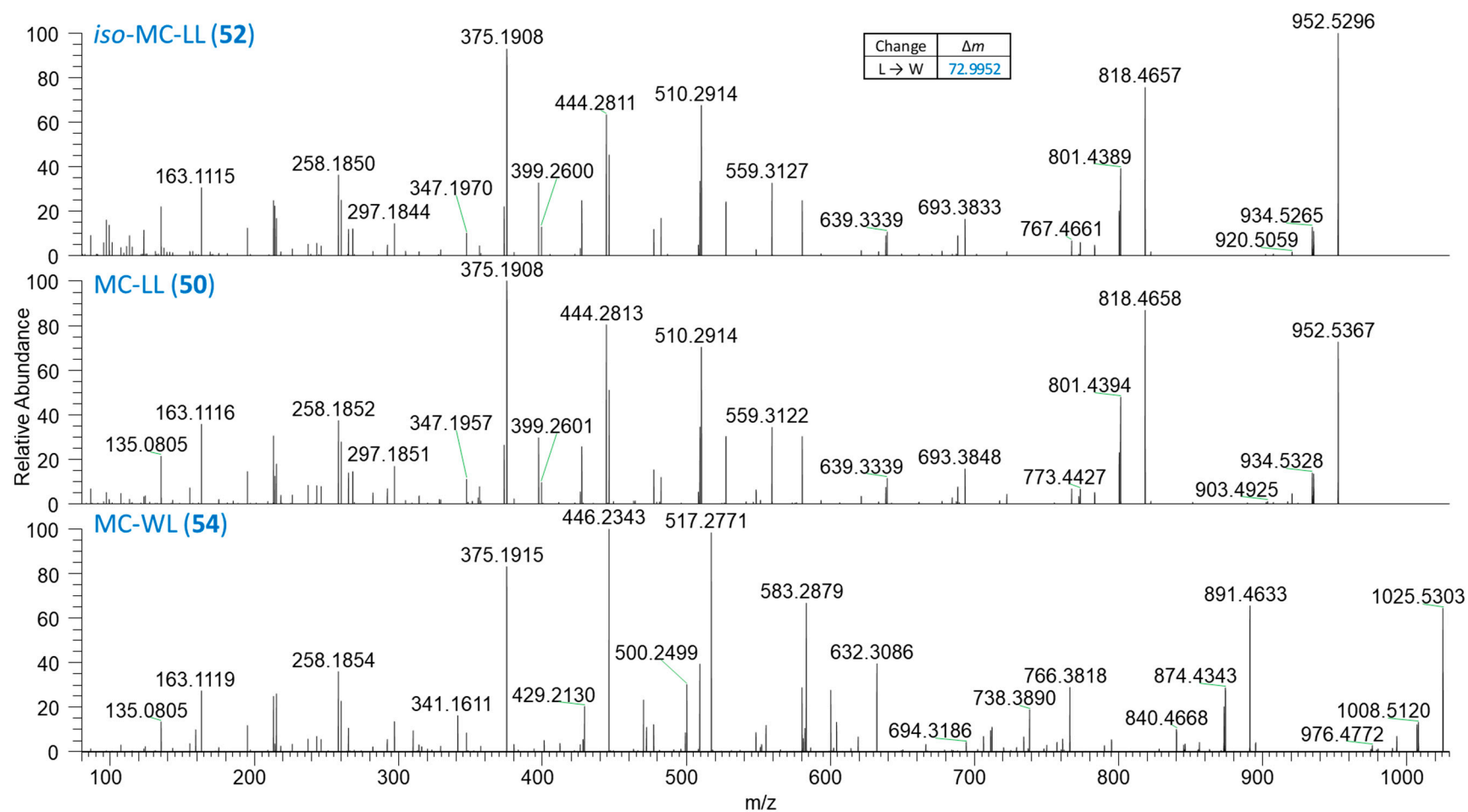
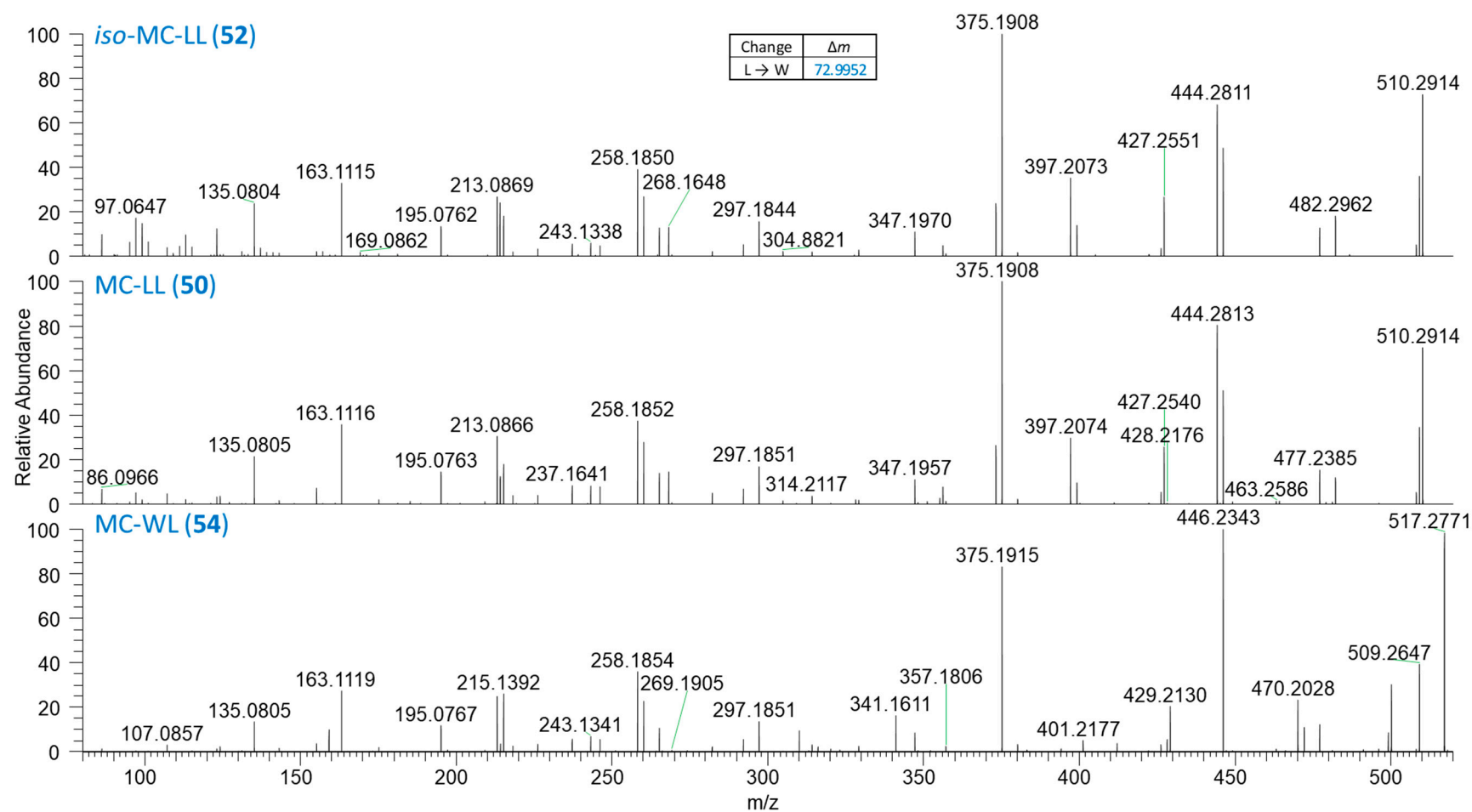
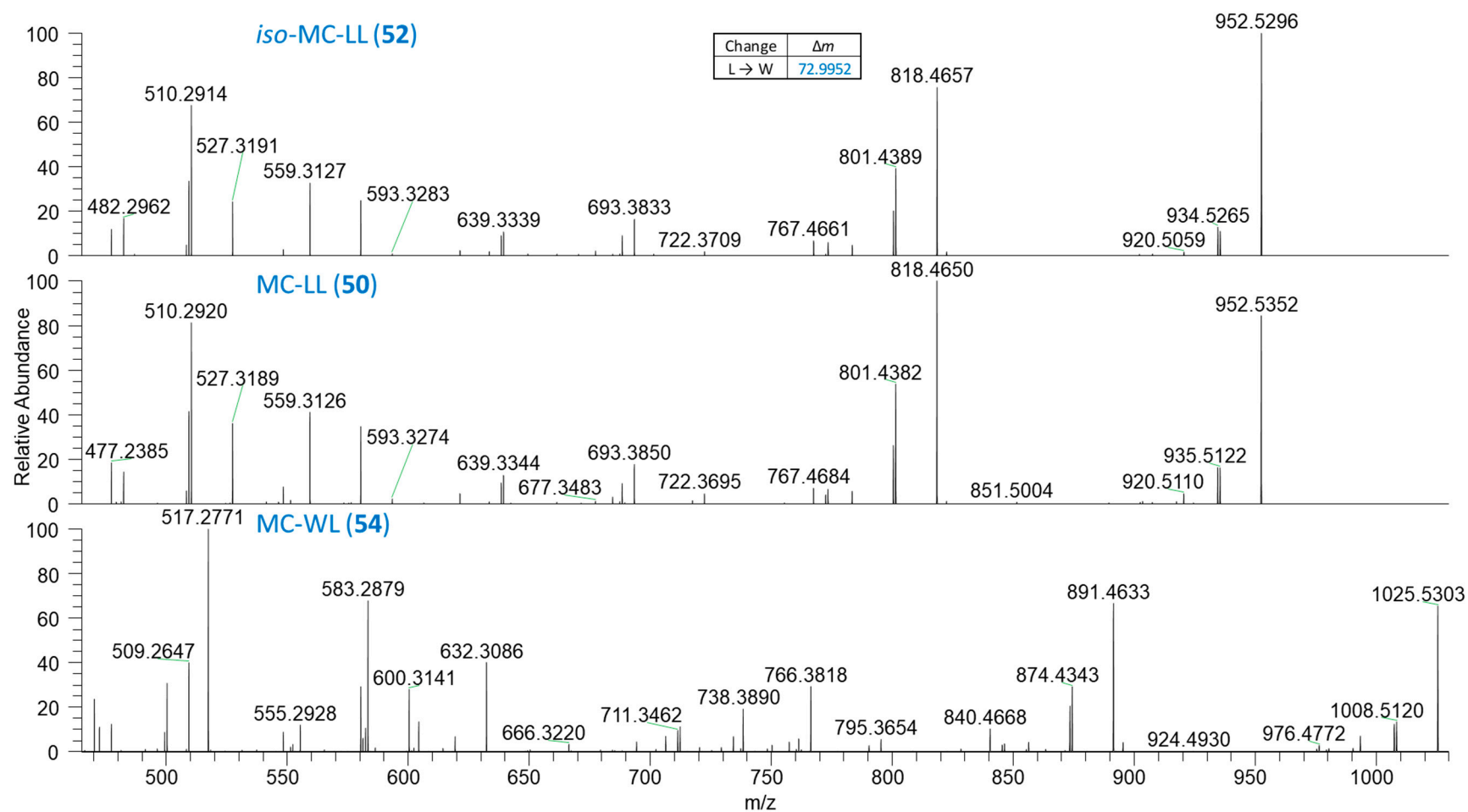


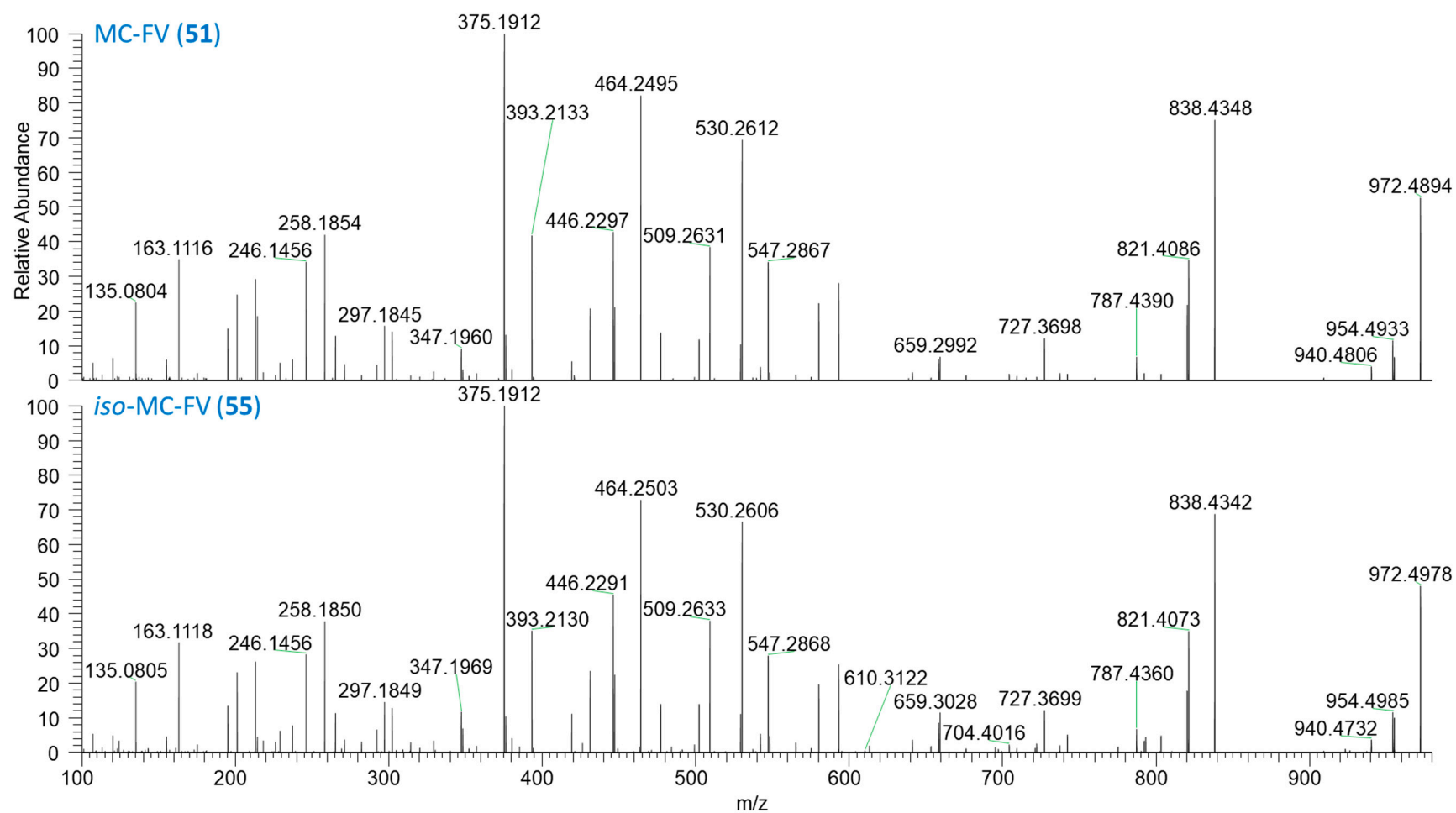
Figure S52. LC-HRMS/MS spectra of  $[M+H]^+$  of *iso*-MC-LL (52), MC-LL (50), and MC-WL (54).



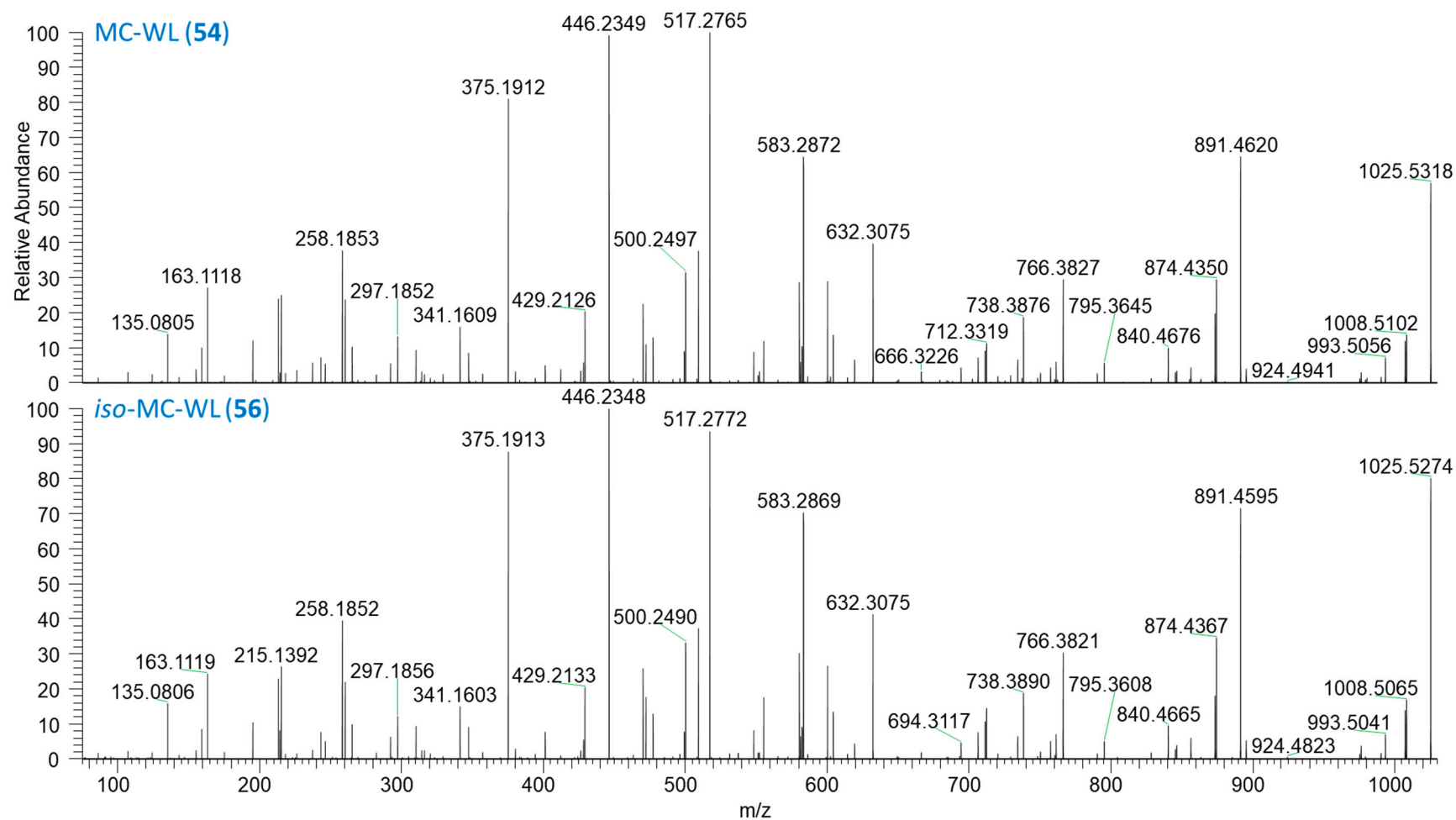
**Figure S53.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of *iso*-MC-LL (52), MC-LL (50), and MC-WL (54).



**Figure S54.** Expansion of LC–HRMS/MS spectra of  $[M+H]^+$  of *iso*-MC-LL (52), MC-LL (50), and MC-WL (54).



**Figure S55.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-LL (51), and *iso*-MC-FV (55).



**Figure S56.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-WL (54), and *iso*-MC-WL (56).

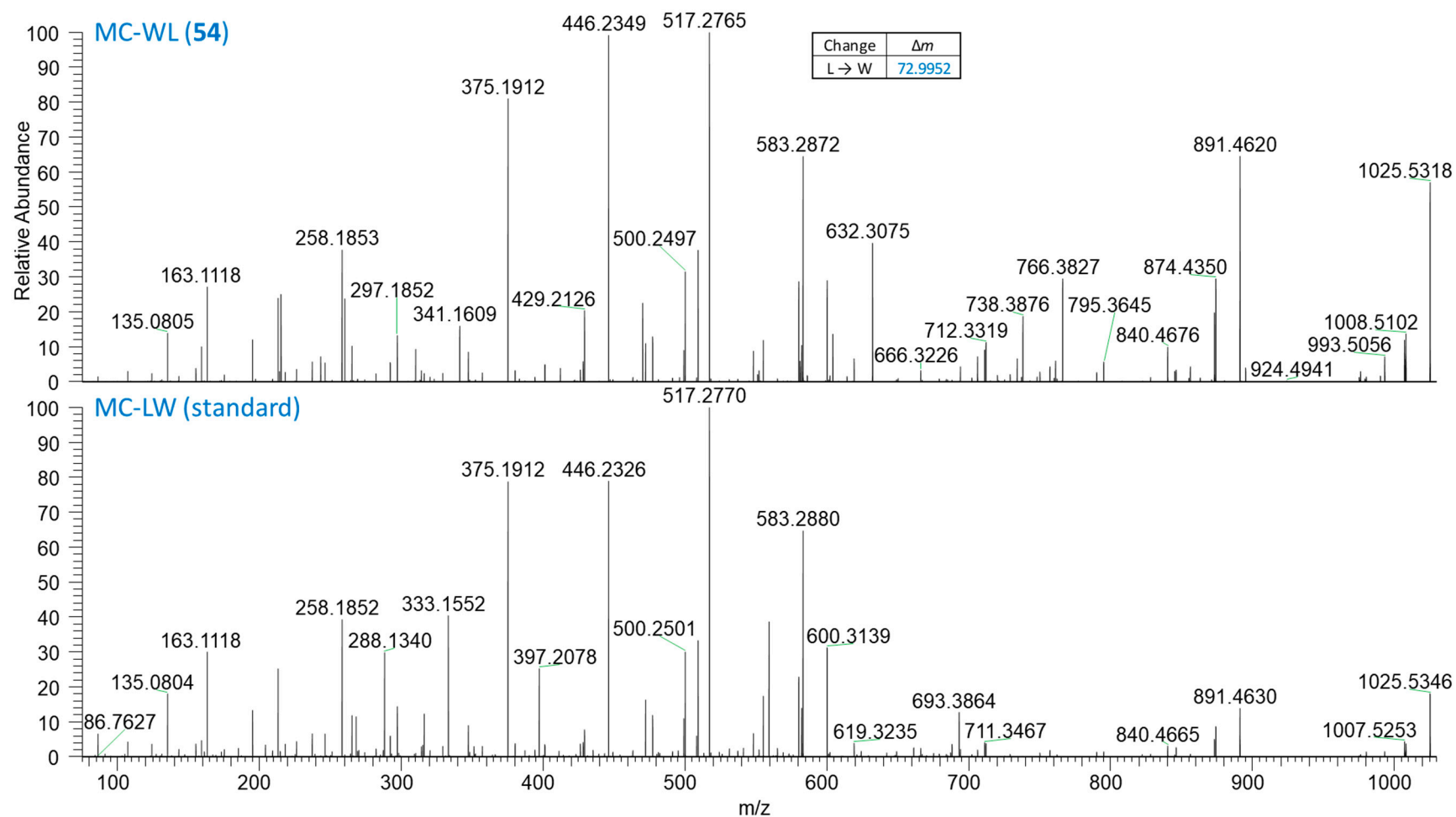


Figure S57. LC–HRMS/MS spectra of  $[M+H]^+$  of MC-WL (54), and a standard of MC-LW.

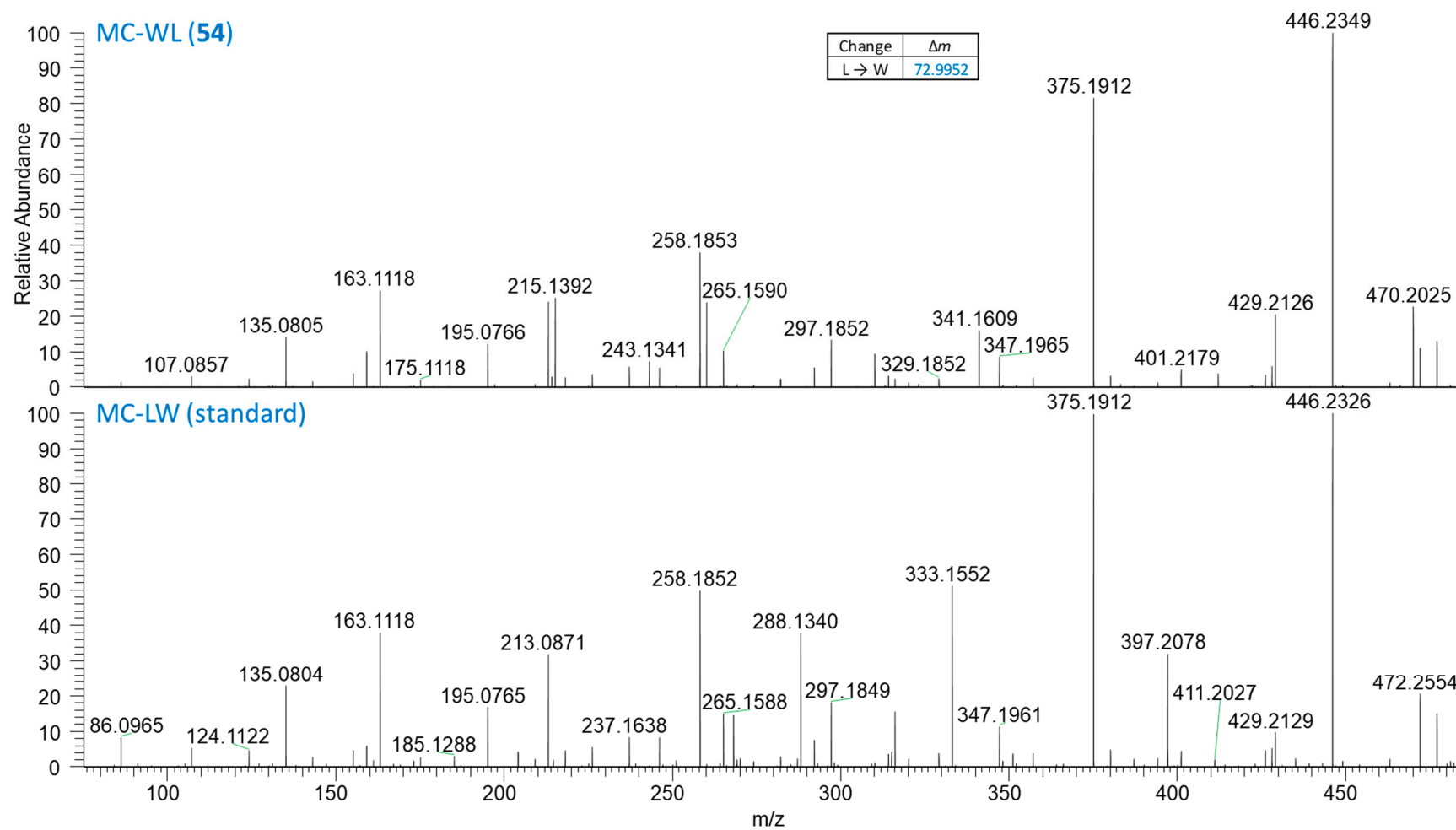
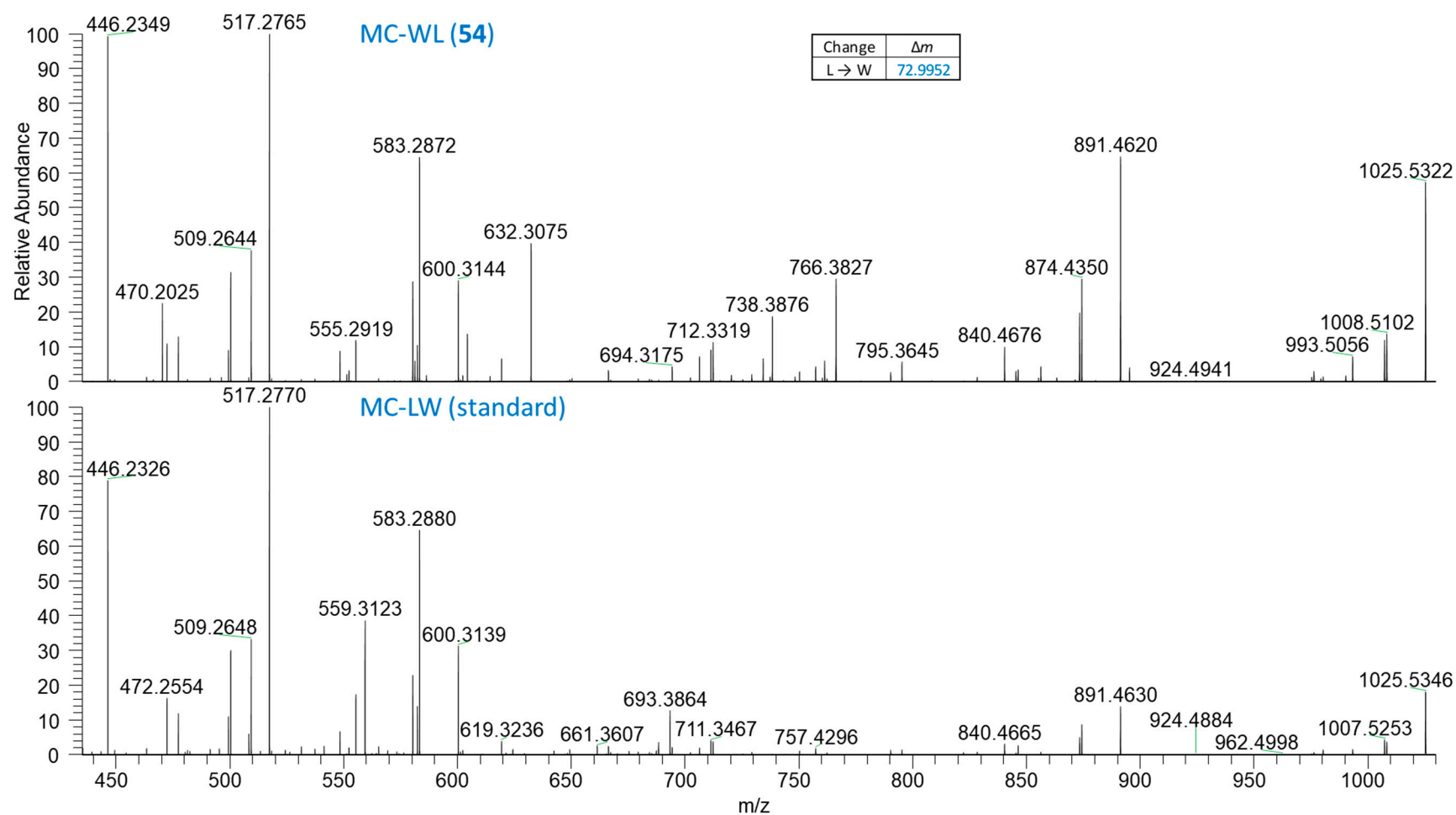
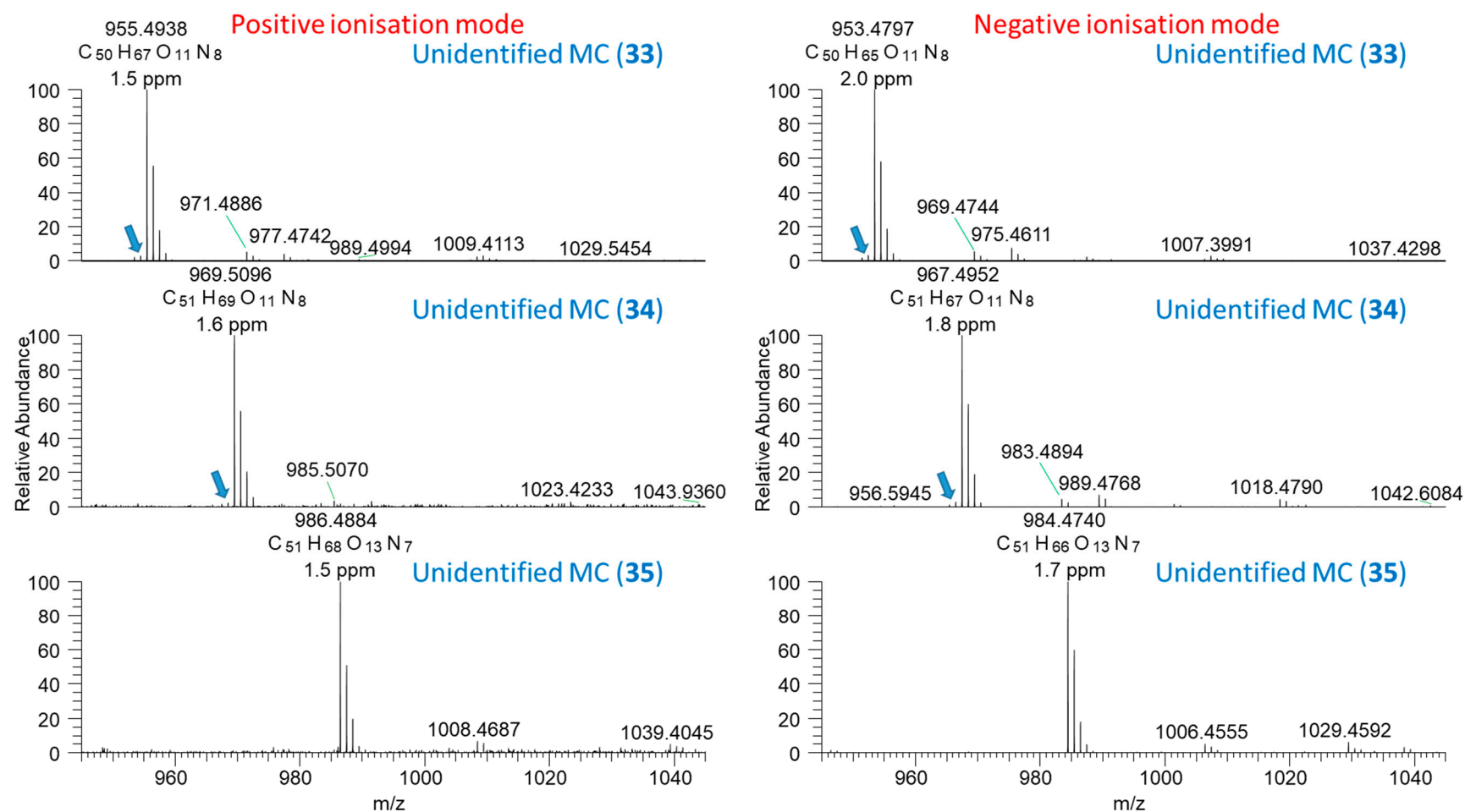


Figure S58. LC-HRMS/MS spectra of  $[M+H]^+$  of MC-WL (54), and a standard of MC-LW.



**Figure S59.** LC-HRMS/MS spectra of  $[M+H]^+$  of MC-WL (54), and a standard of MC-LW.





**Figure S60.** LC-HRMS full scan spectra of  $[M+H]^+$  of unidentified microcystins 33–35 in positive (left) and negative (right) ionisation modes. Note the peaks to the low-mass side of the main peaks for 33 and 34, as well as the apparent presence of  $[M+15.9949]$ , in both ionisation modes.