

Electronic Supplementary Information (ESI) for the article entitled:

**ICP-MS-assisted nanoHPLC-electrospray Q/time-of-flight MS/MS  
selenopeptide mapping in Brazil nuts**

by

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**Figure-ESI 1:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  2619 (detected as triply charged). **b)** Corresponding MS/MS spectra on the  $^{80}\text{Se}$  isotope, along with the sequence of the Se-peptide detected. Fragments indicated with masses in Italics were not detected.

**Figure-ESI 2:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  2505 (detected as triply charged). **b)** Corresponding MS/MS spectra on the  $^{80}\text{Se}$  isotope, along with the sequence of the Se-peptide detected. Fragments indicated with masses in Italics were not detected.

**Figure-ESI 3:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  1424 (detected as double charged). **b)** Corresponding MS/MS spectra on the  $^{80}\text{Se}$  isotope. **c)** The sequence of the Se-peptide detected.

**Figure-ESI 4:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  1224 (detected as double charged). **b)** Corresponding MS/MS spectra on the  $^{80}\text{Se}$  isotope along with the sequences of the isomers detected.

**Figure-ESI 5:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  965 (detected as double charged). **b)** Corresponding MS/MS spectrum on the  $^{80}\text{Se}$  isotope along with the sequence identified.

**Figure-ESI 6:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  1354 (detected as double charged). **b), c):** Corresponding MS/MS spectra on the  $^{80}\text{Se}$  isotope along with the sequences of the isomers detected. The analyte was fragmented two times with the difference of 0.15 min, revealing the presence of different isomers.

**Figure-ESI 7:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  1107 (detected as double charged). **b)** Corresponding MS/MS spectrum on the  $^{80}\text{Se}$  isotope along with the sequence identified.

**Figure-ESI 8:** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  1050 (detected as double charged).

**Figure-ESI 9:** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  880.

**Figure-ESI 10:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  747. **b), c):** Corresponding MS/MS spectra on the  $^{80}\text{Se}$  and  $^{82}\text{Se}$  isotopes, respectively, along with the sequences of the isomers detected. The analyte was fragmented two times with the difference of 0.21 min, revealing the presence of different isomers.

**Figure-ESI 11:** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  485. Please note that background subtraction was required because of a spectral overlap; therefore the Se-pattern is partly off the theoretical one.

**Figure-ESI 12:** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  641. This species partly co-elutes with the Se-peptide with  $m/z$  632, therefore the same ESIQTOF MS spectrum is shown. Please note the inset was background corrected.

**Figure-ESI 13:** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  632. This species partly co-elutes with the Se-peptide with  $m/z$  641, therefore the same ESIQTOF MS spectrum is shown.

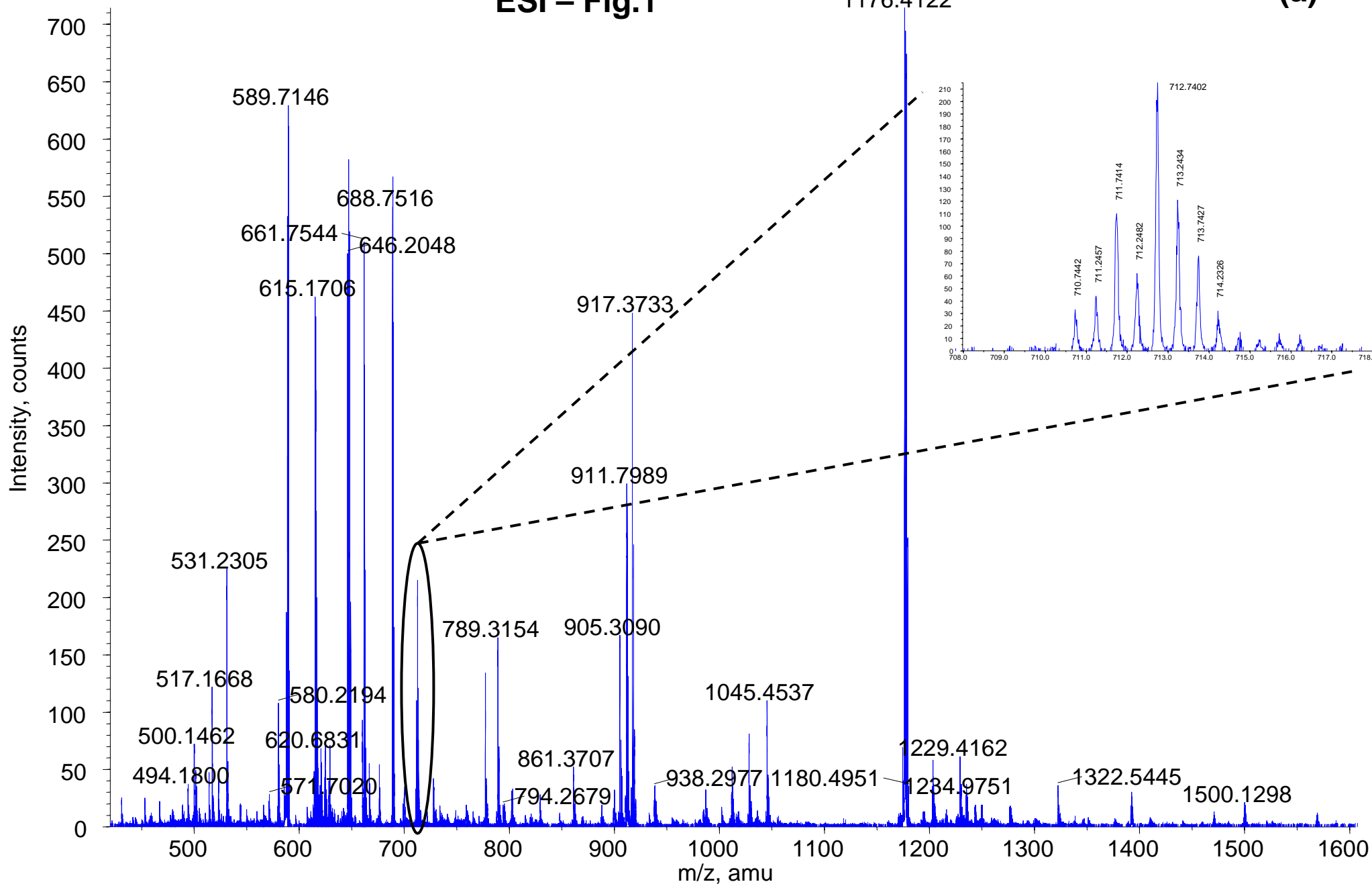
**Figure-ESI 14:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  616. **b):** Corresponding MS/MS spectrum on the  $^{78}\text{Se}$  isotope along with the sequences of the isomers detected. Please note the inset was background corrected.

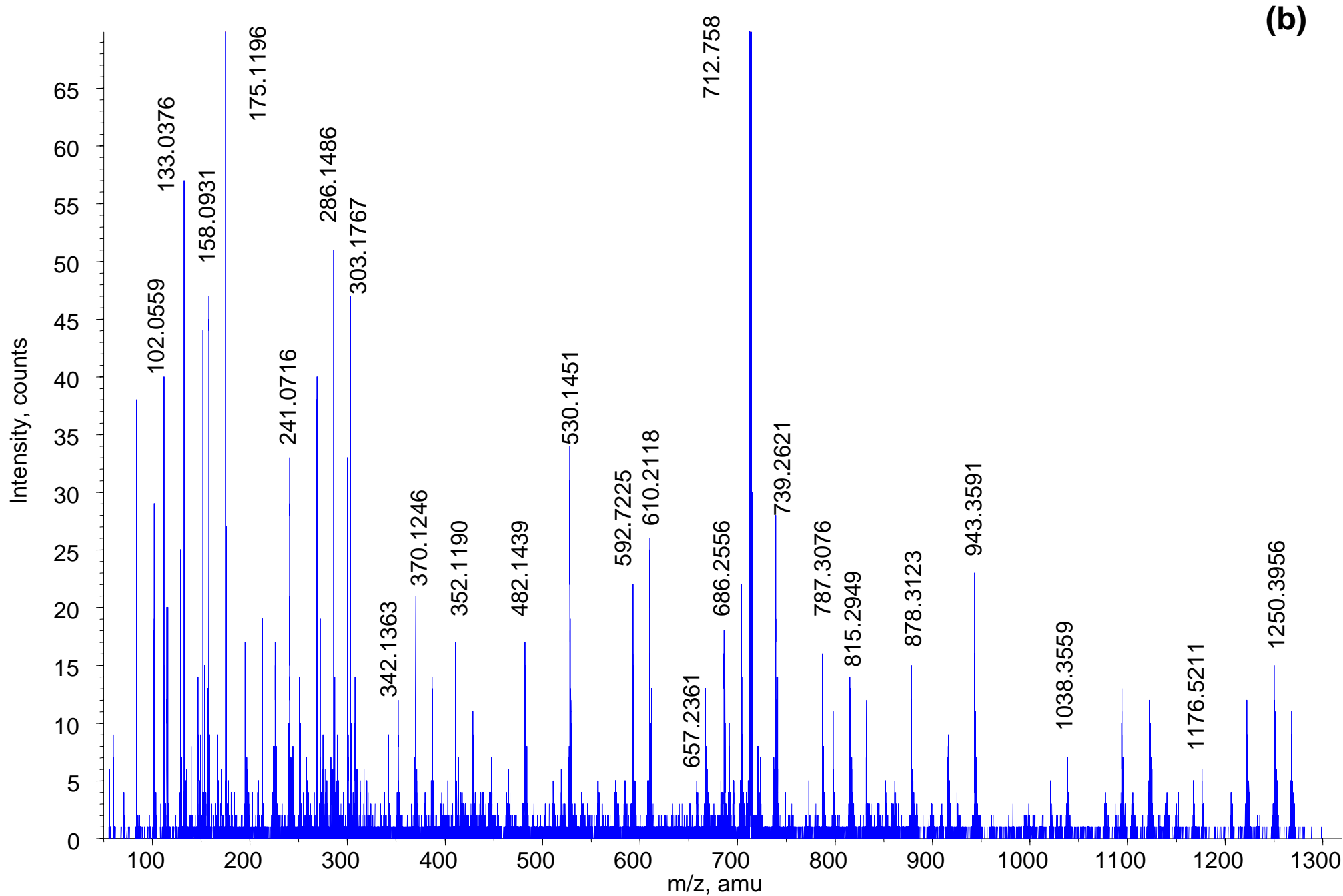
**Figure-ESI 15:** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  648. This species is partly overlapped with another peptide; therefore the correct isotopic pattern of Se can not be seen. Please note the inset was background corrected.

**Figure-ESI 16:** **a)** ESIQTOF MS spectrum of the Se-peptide with  $m/z$  795 (detected as double charged). **b):** Corresponding MS/MS spectrum on the  $^{80}\text{Se}$  isotope along with the sequences of the isomers detected.

ESI – Fig.1

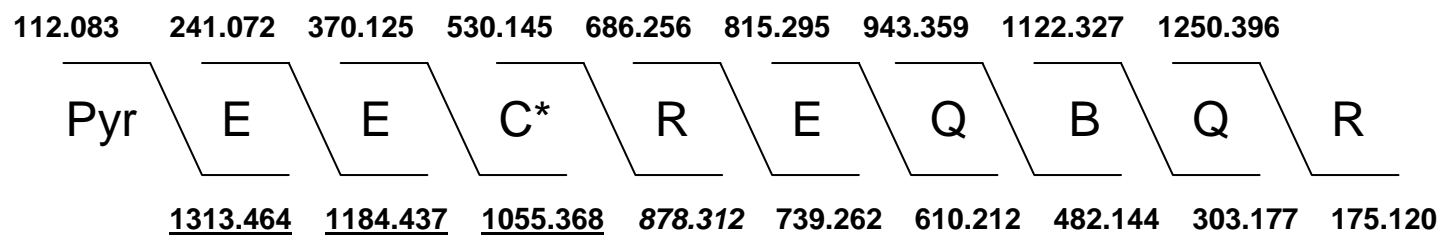
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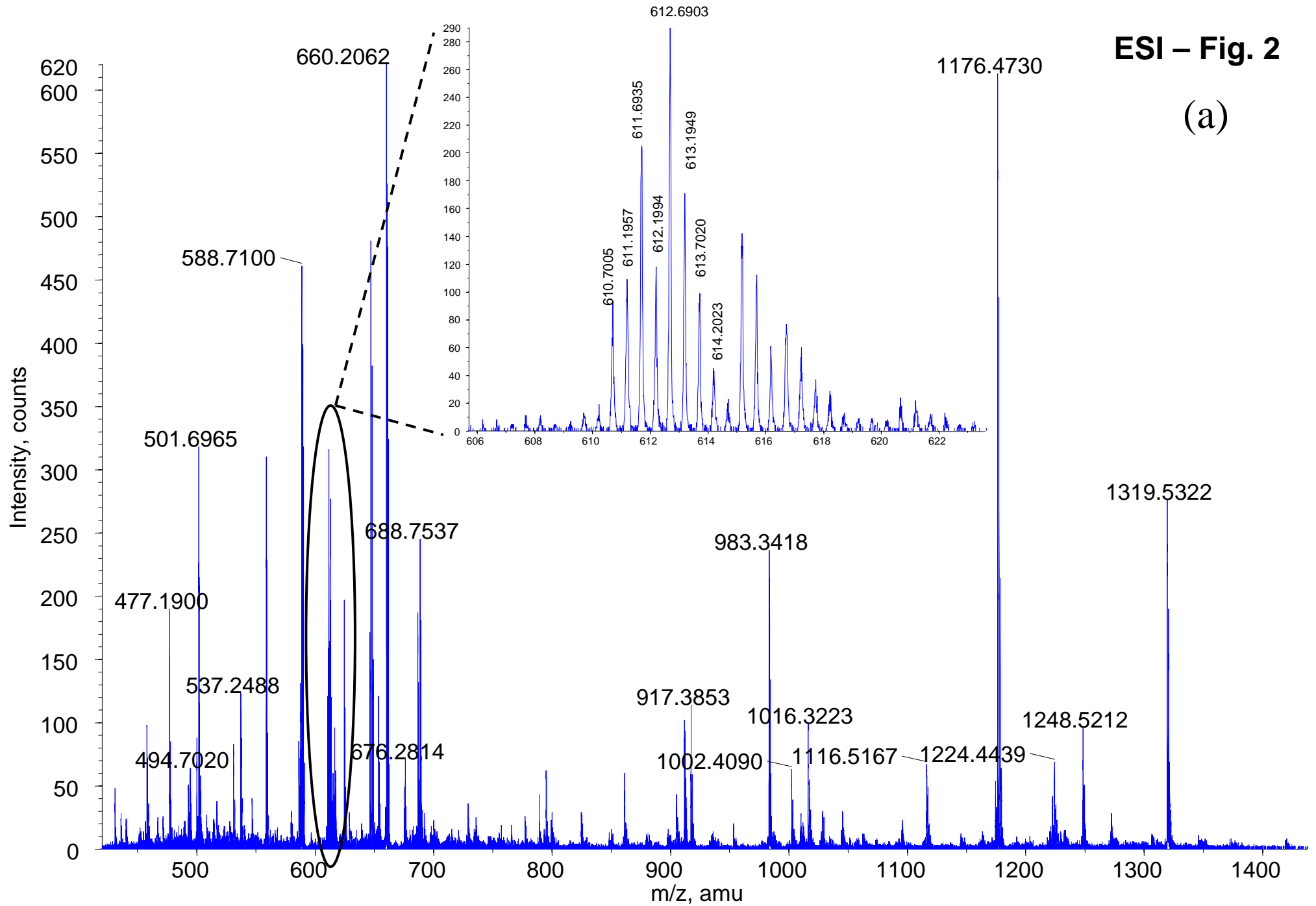
**(b)**

(c)

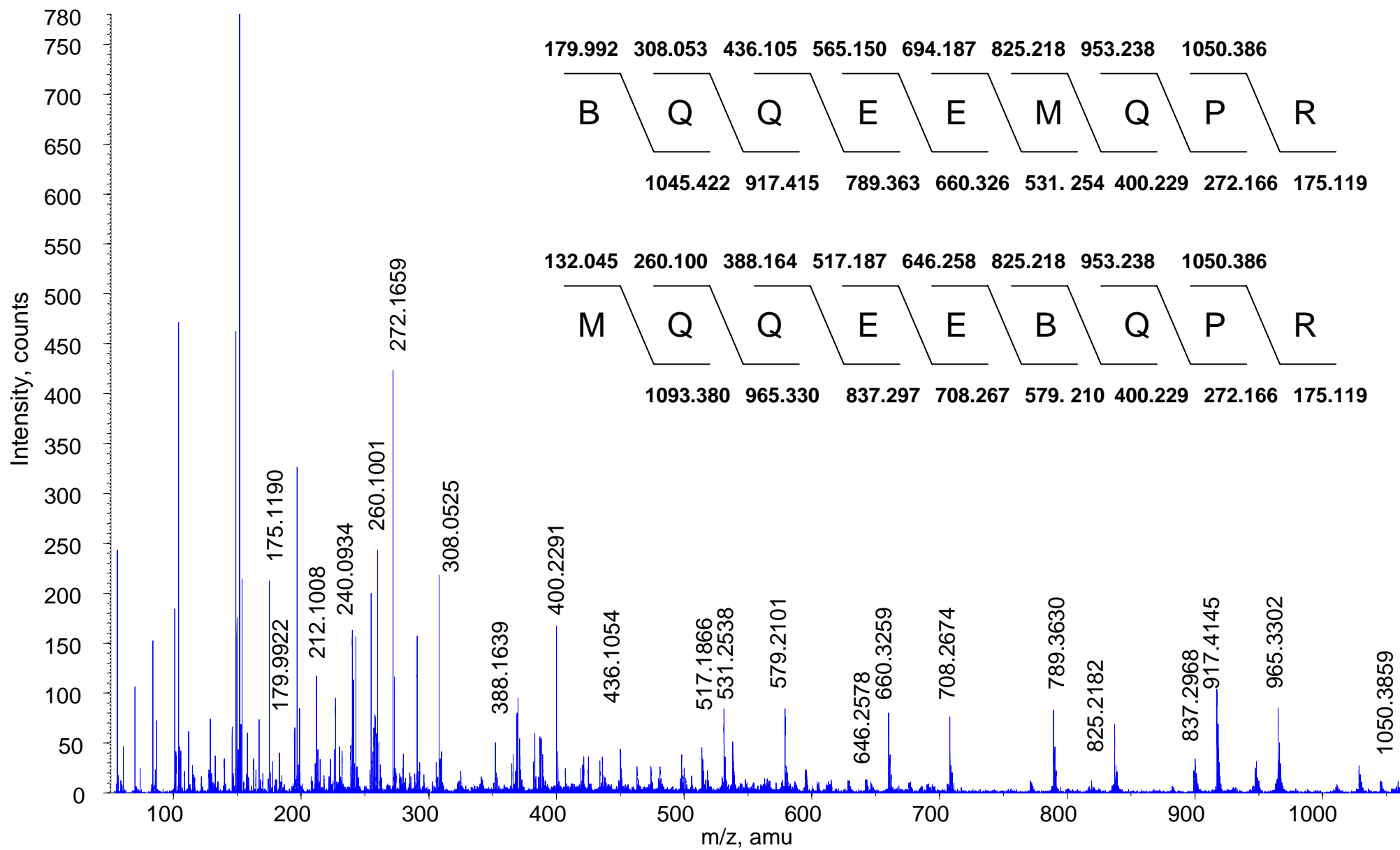


# ESI – Fig. 2

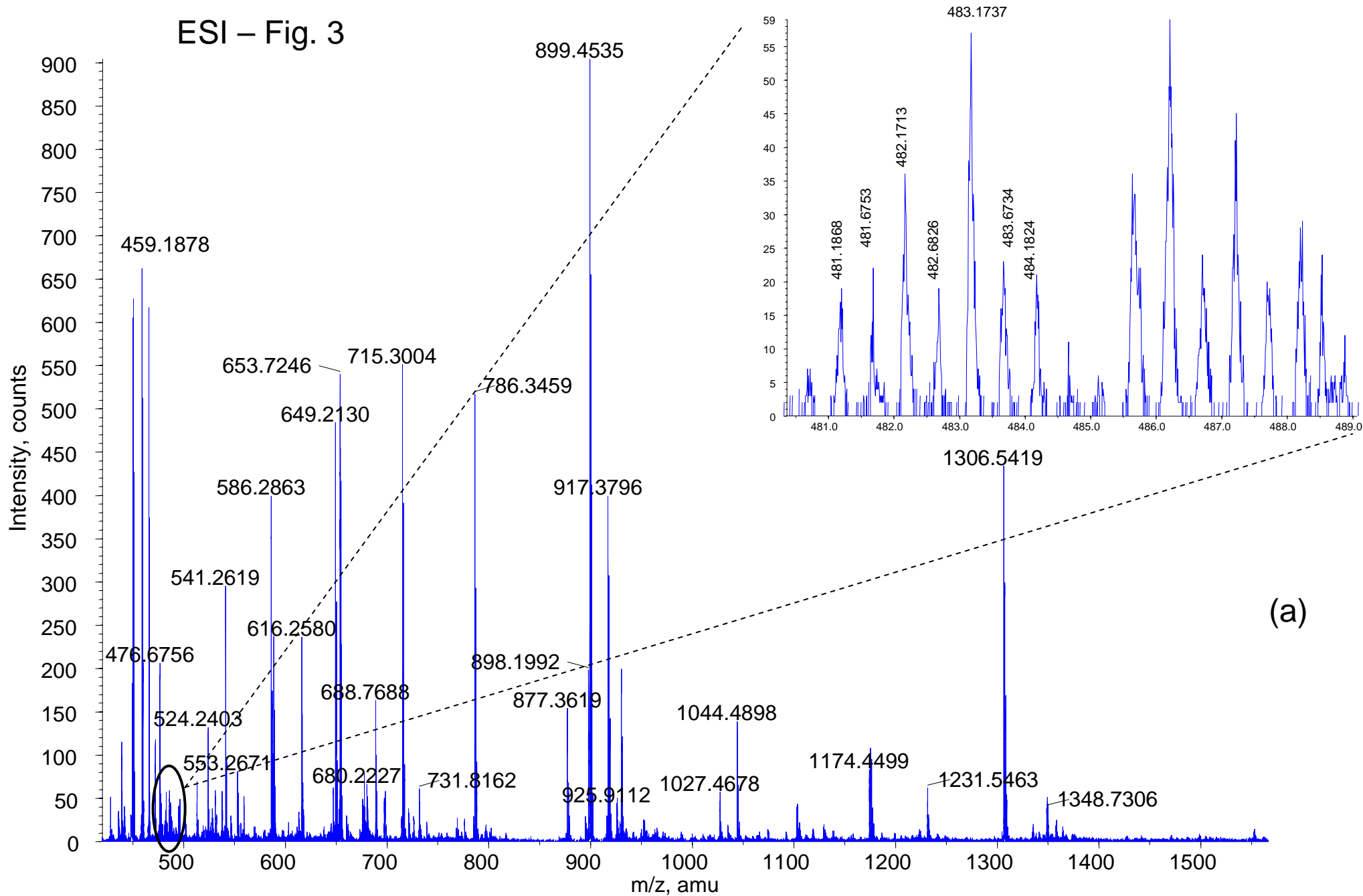
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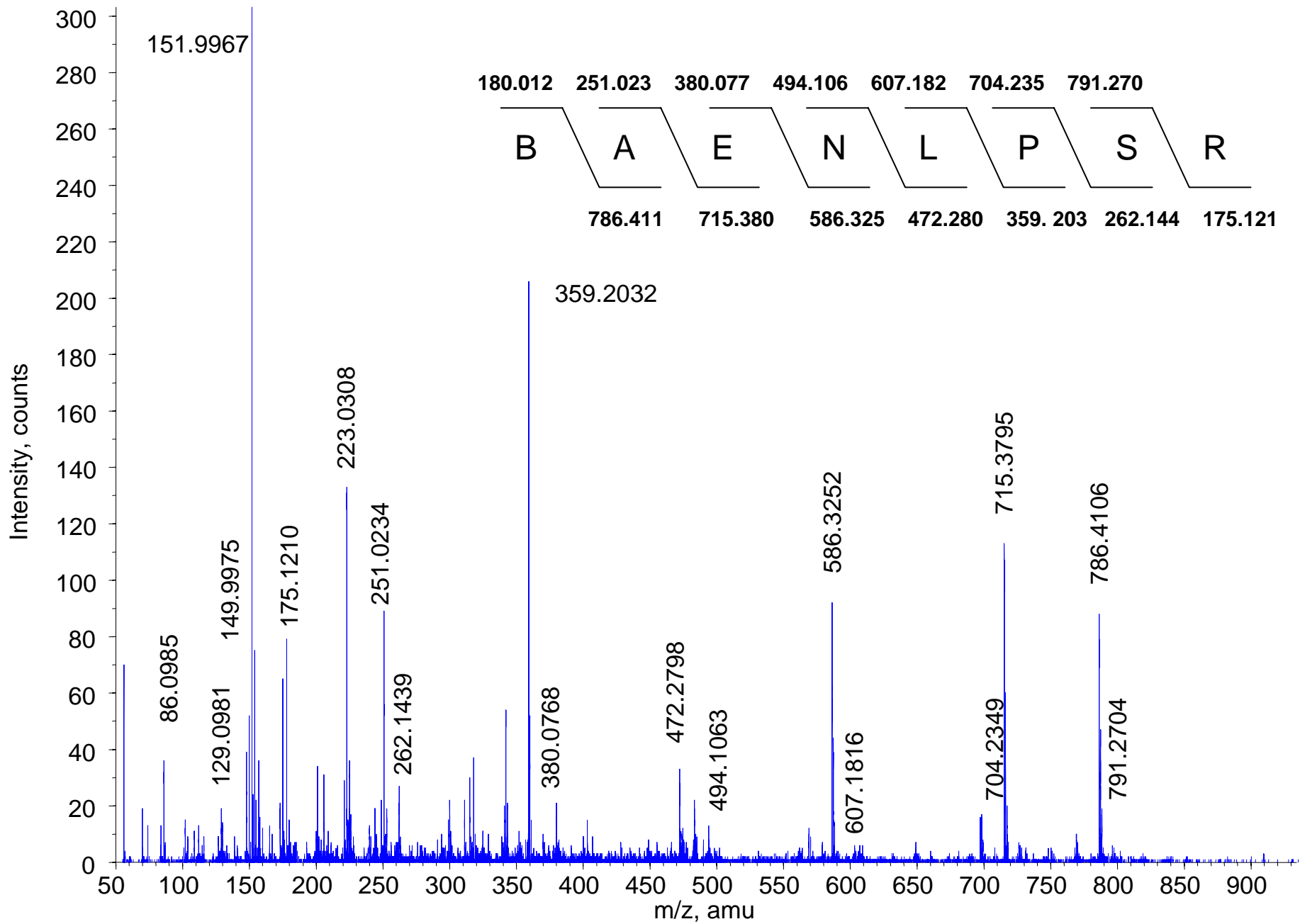
(b)



# ESI – Fig. 3



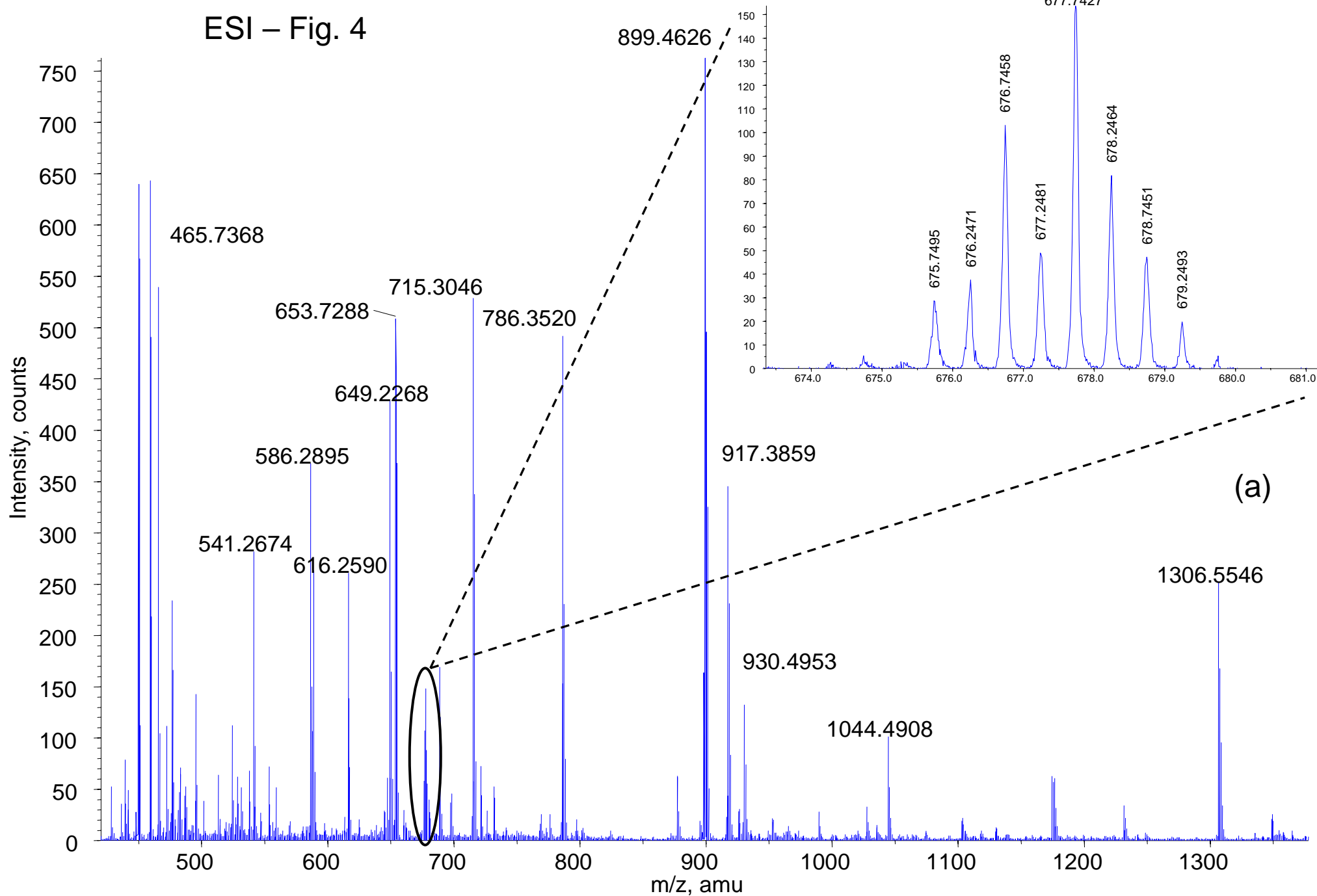
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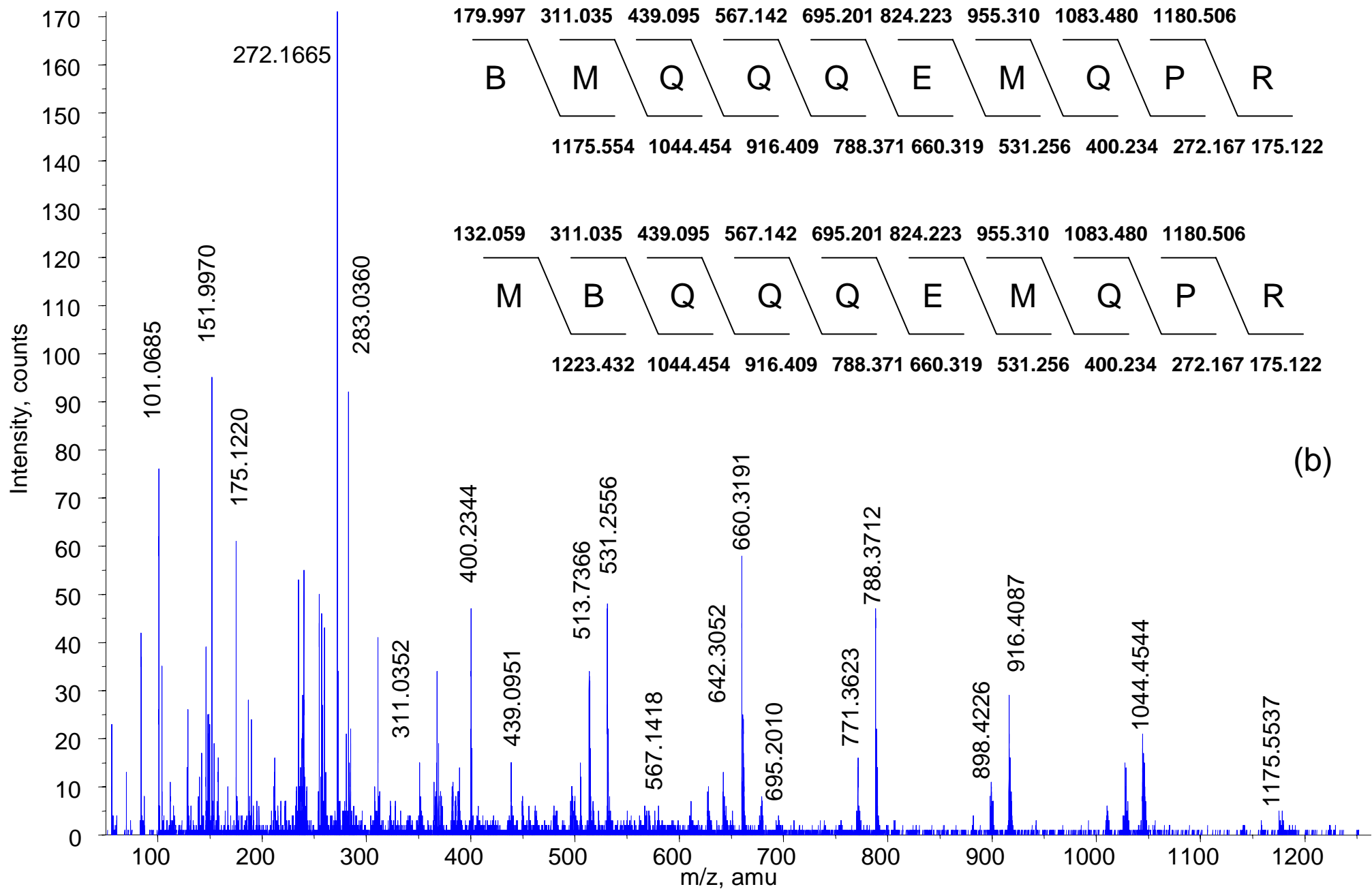


(b)

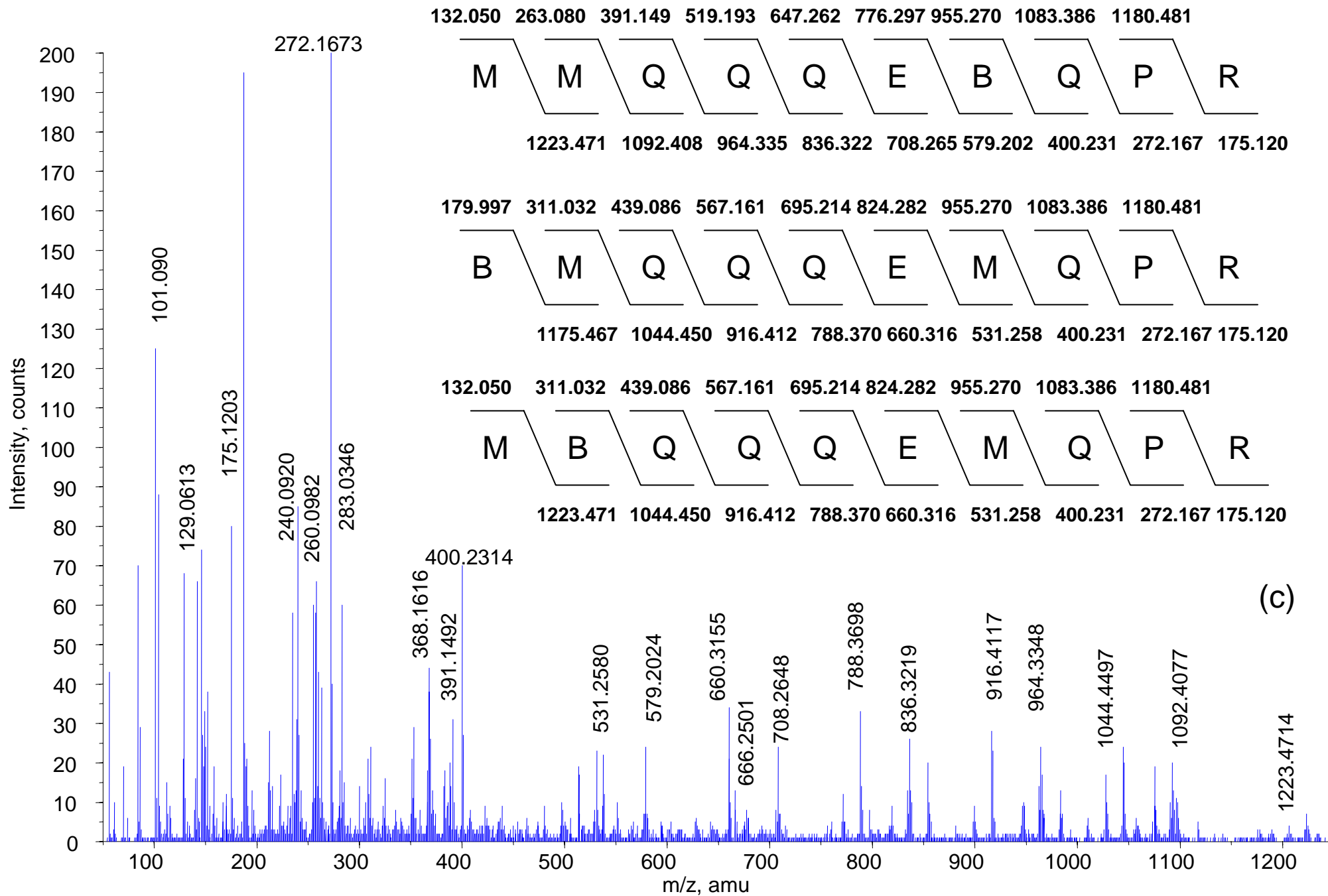


ESI – Fig. 4



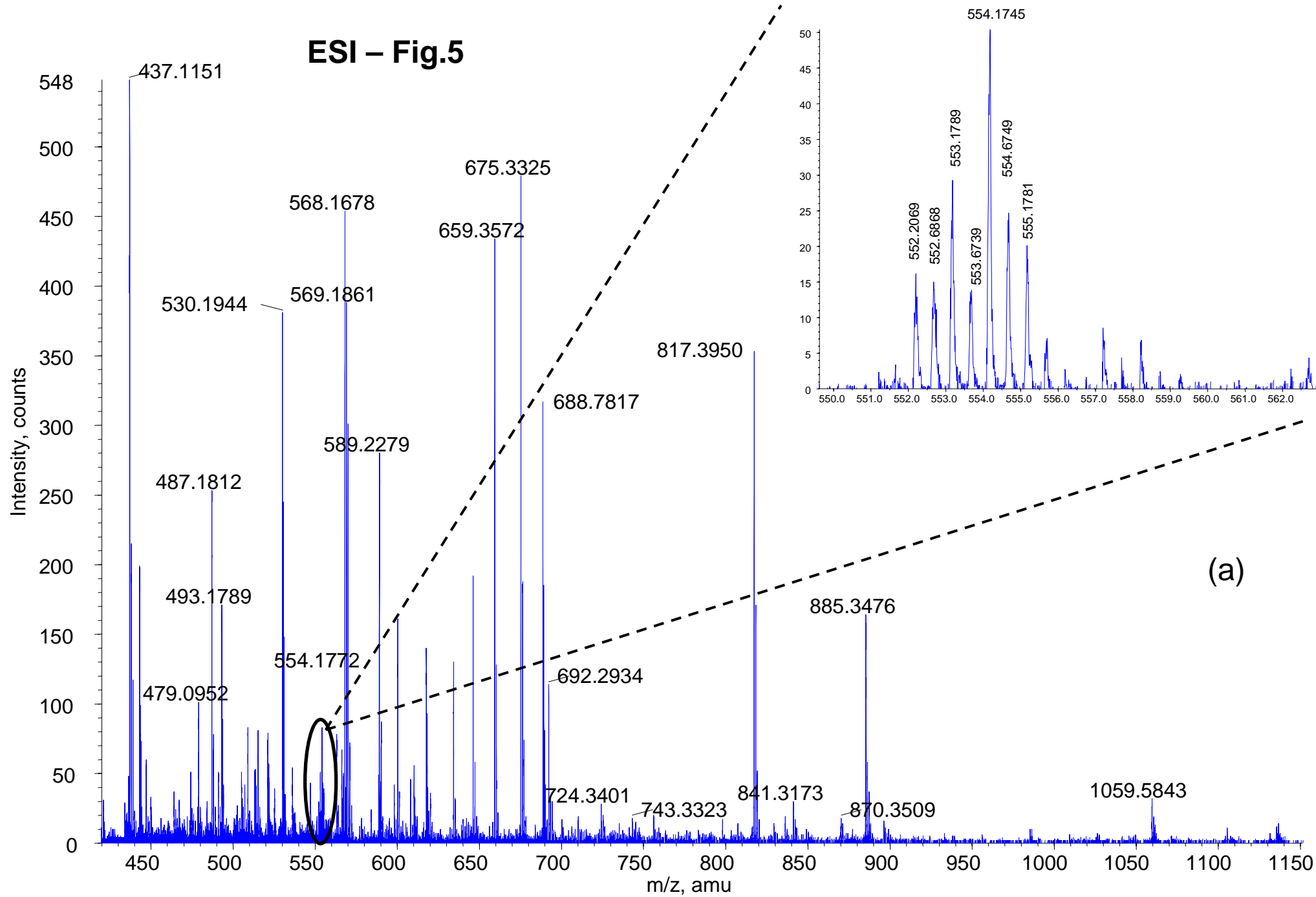


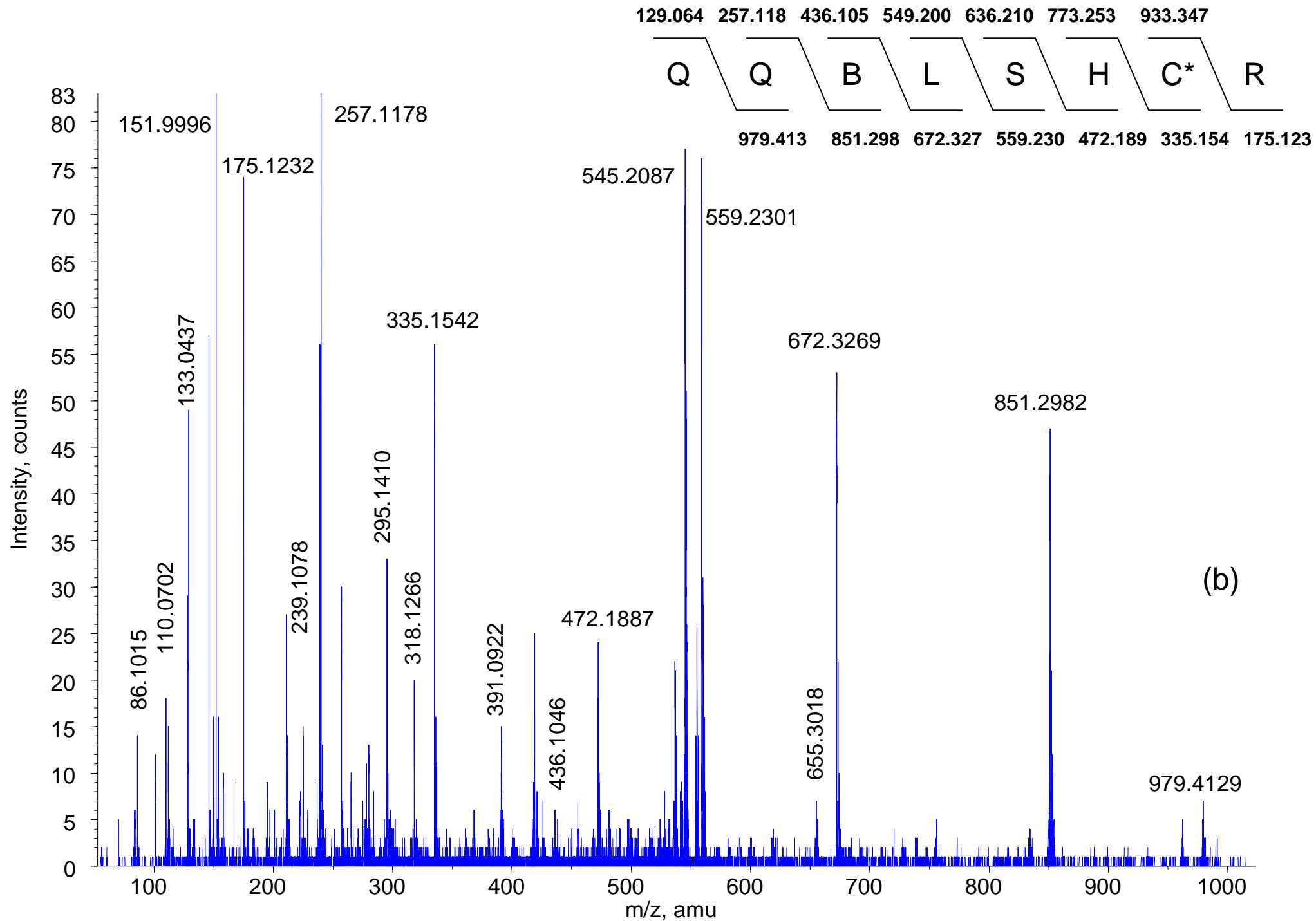
(b)



(c)

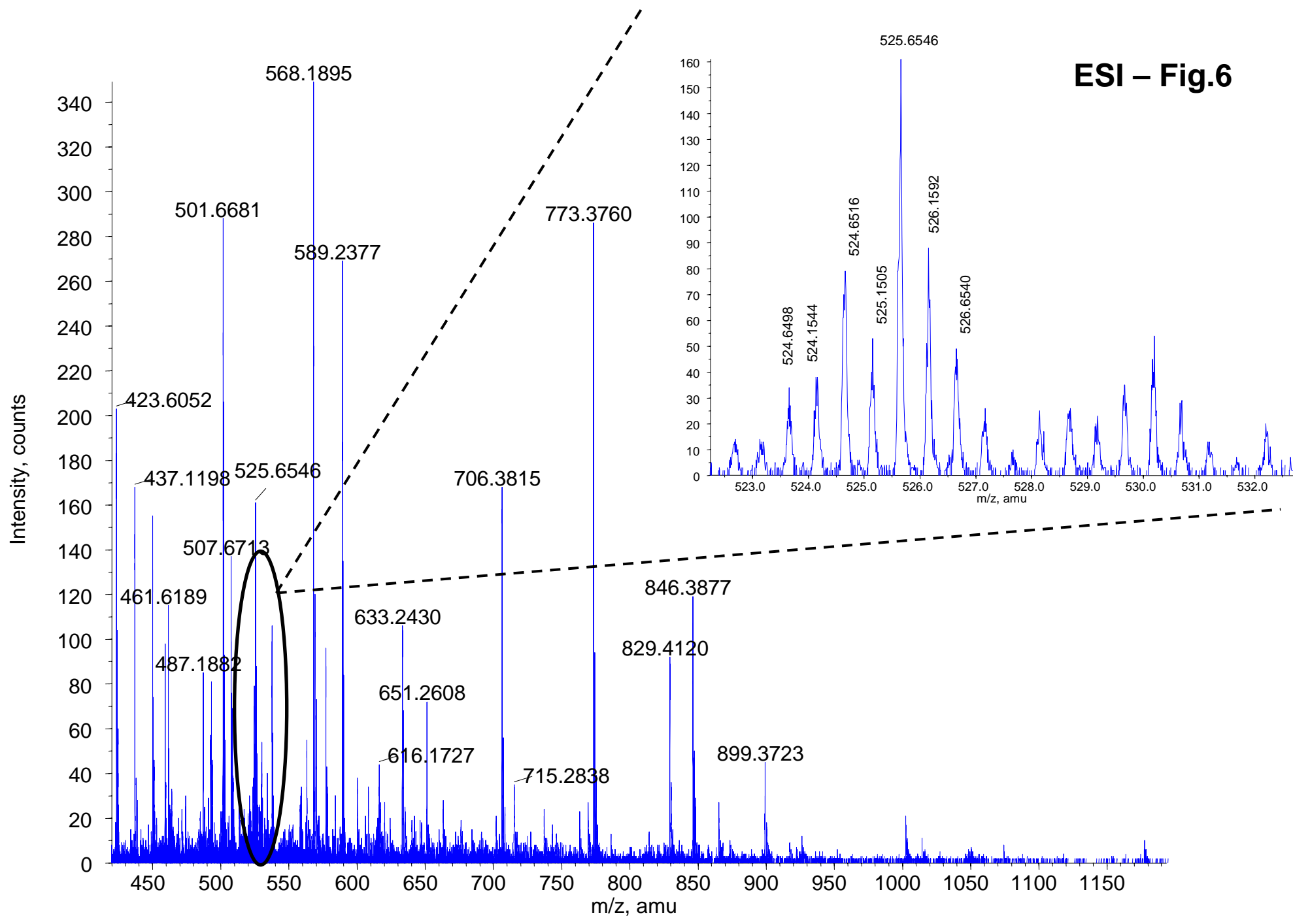
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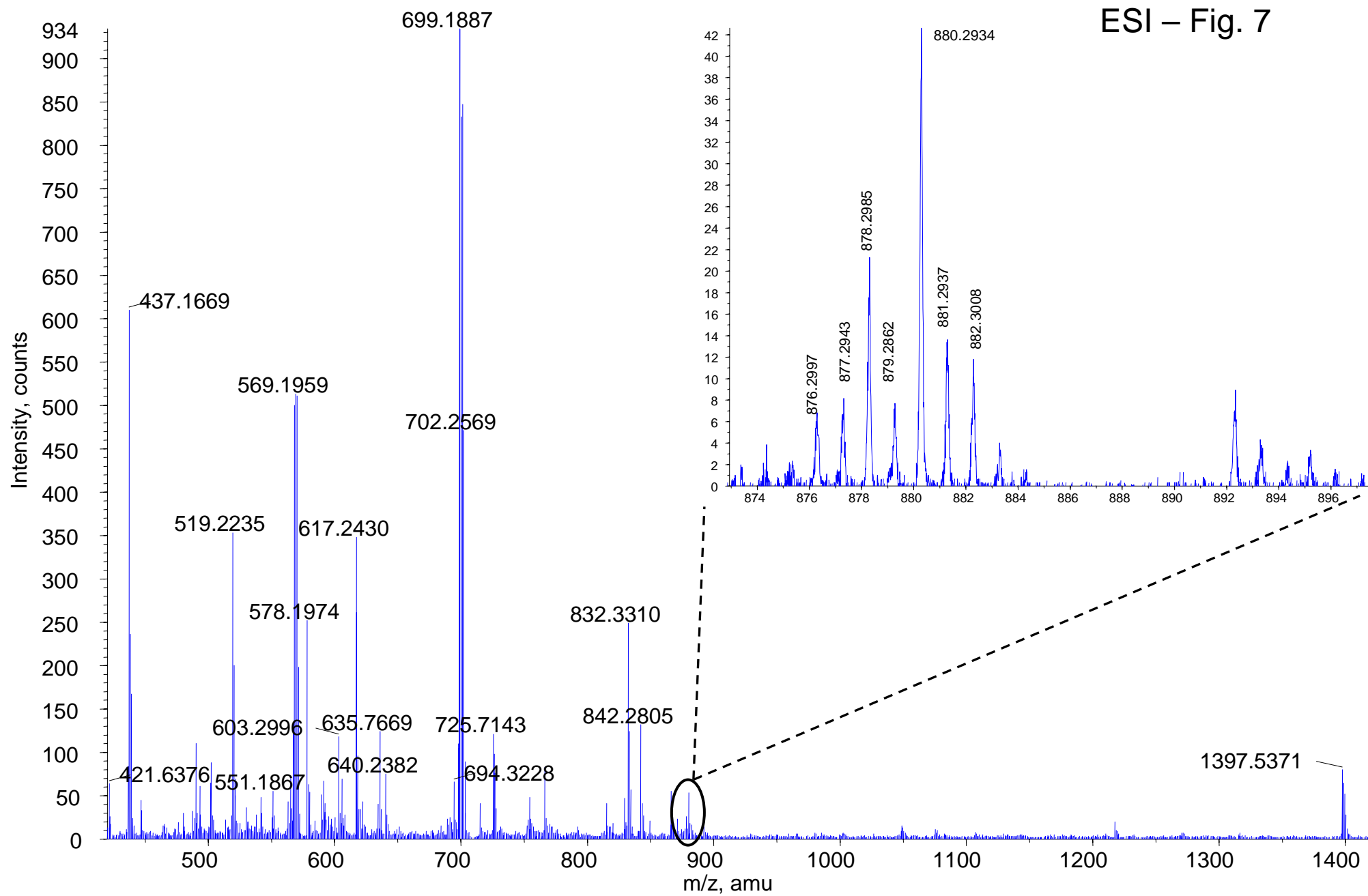


(b)

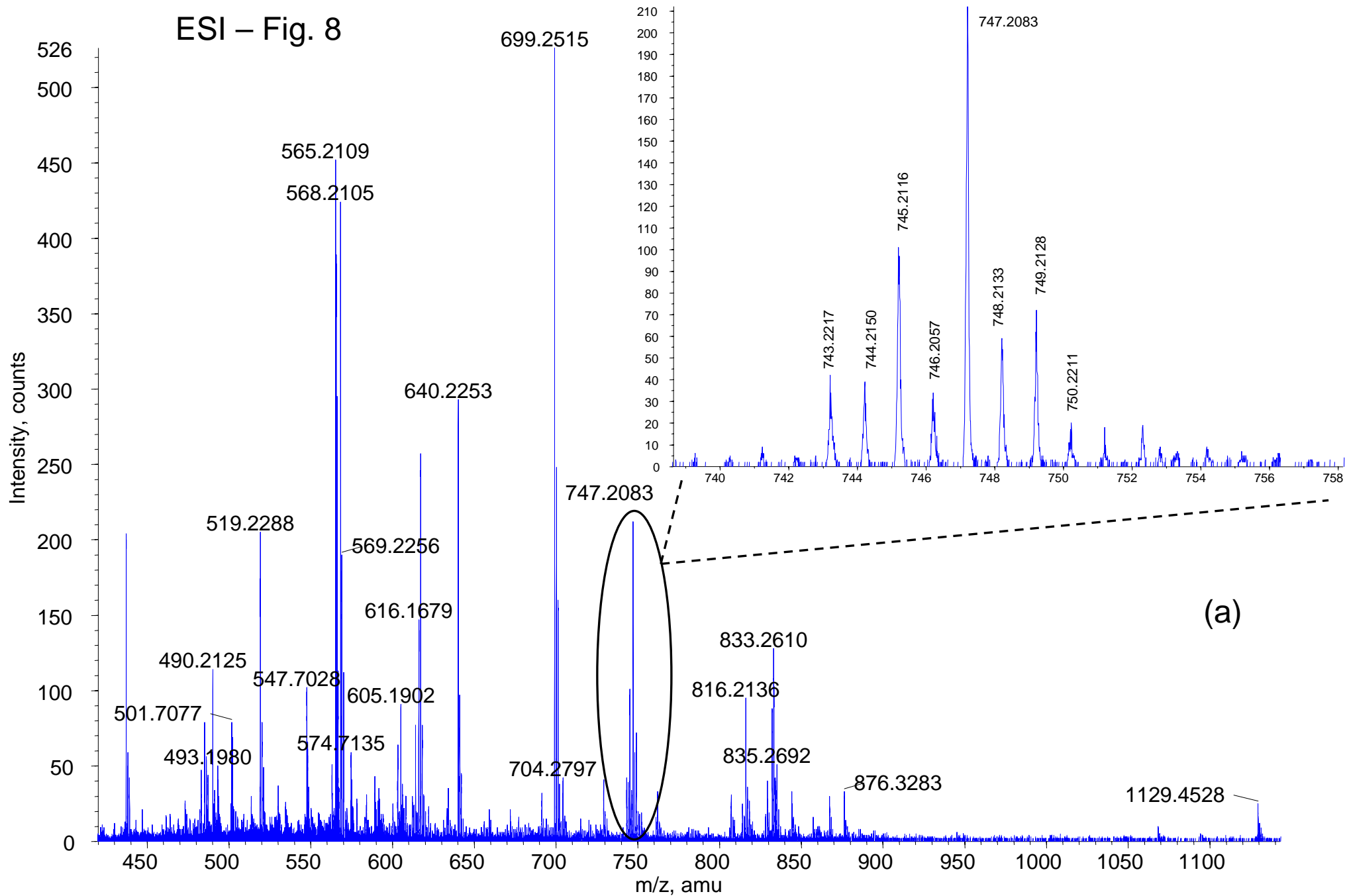
ESI – Fig.6



ESI – Fig. 7

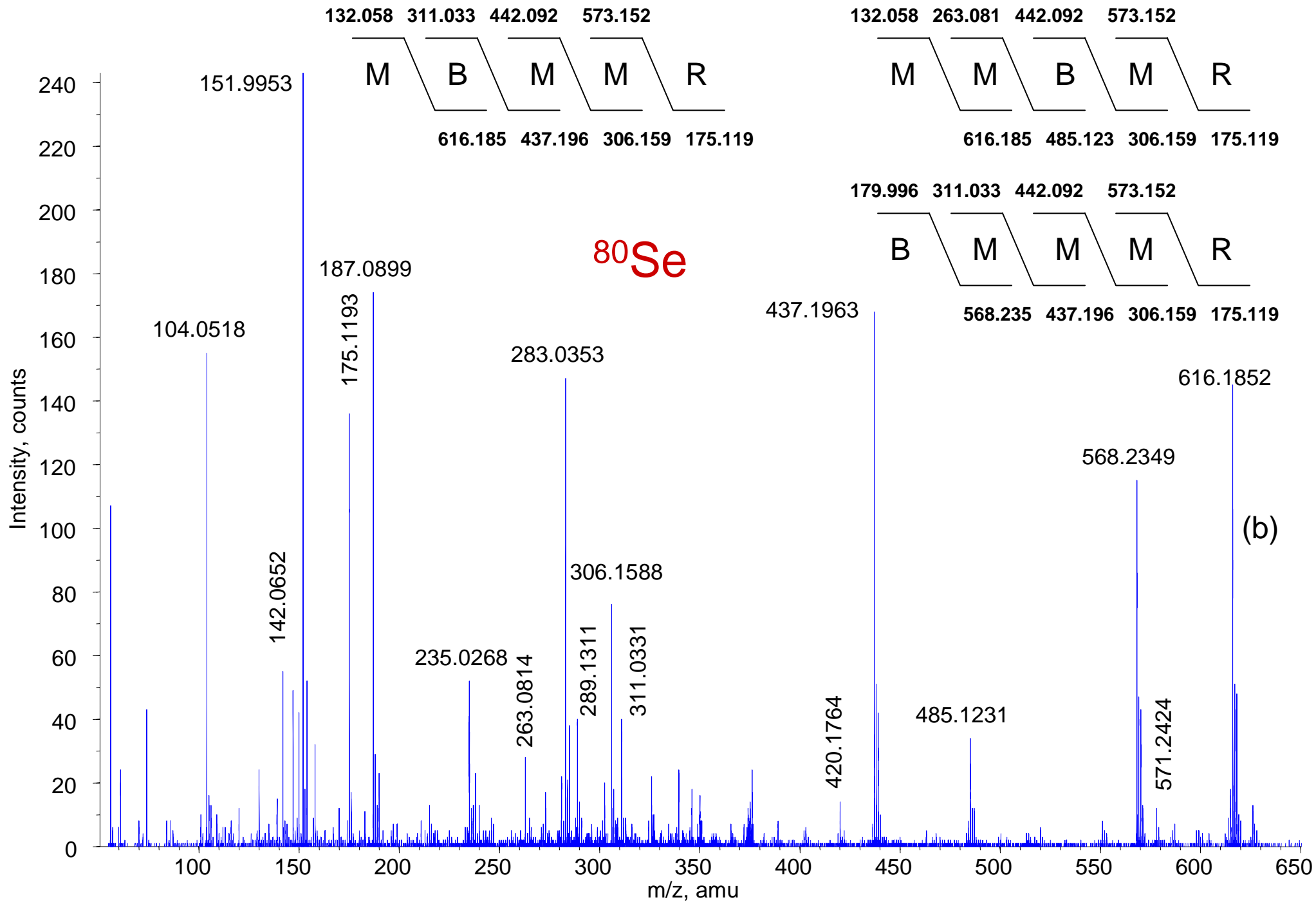


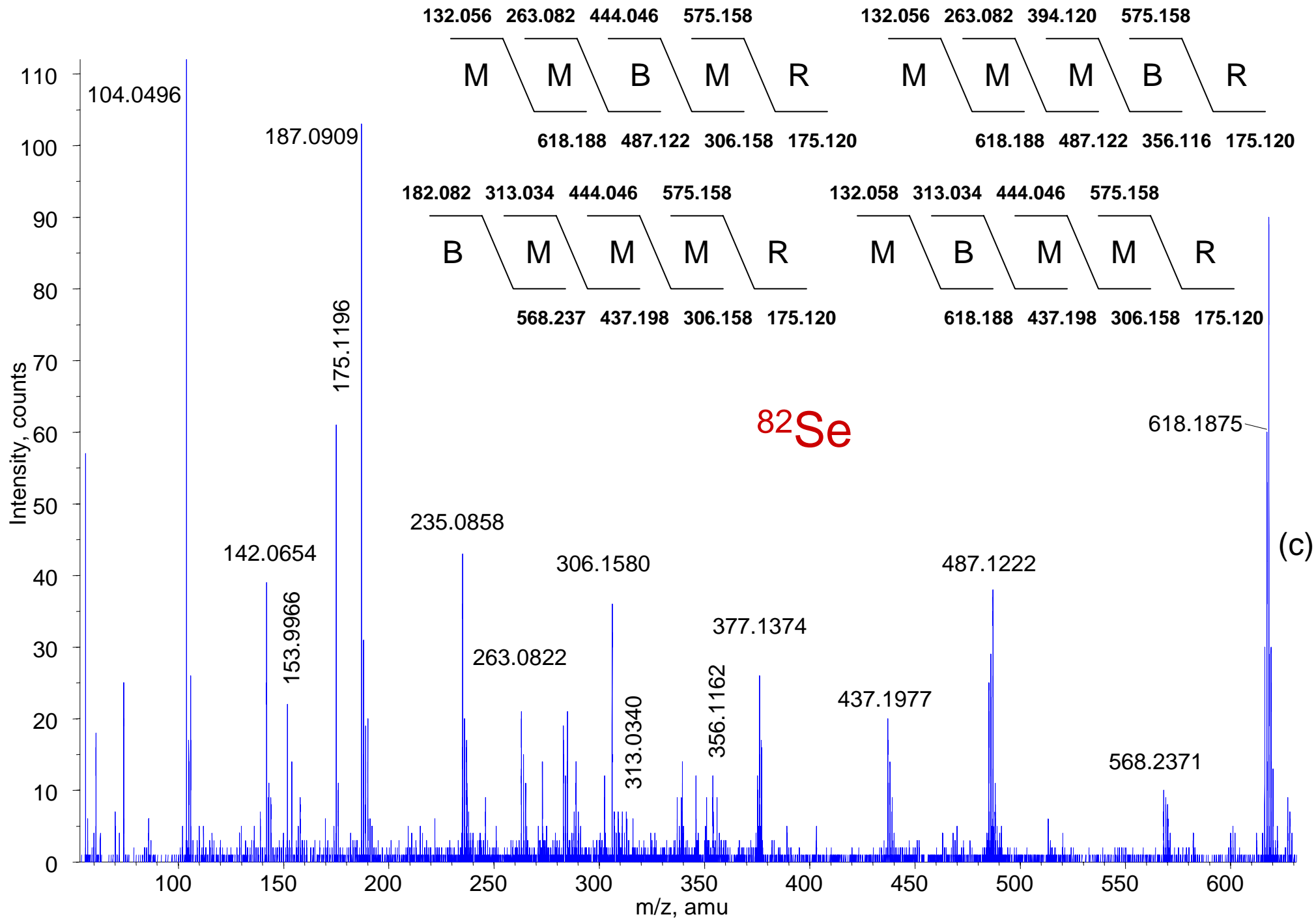
ESI – Fig. 8



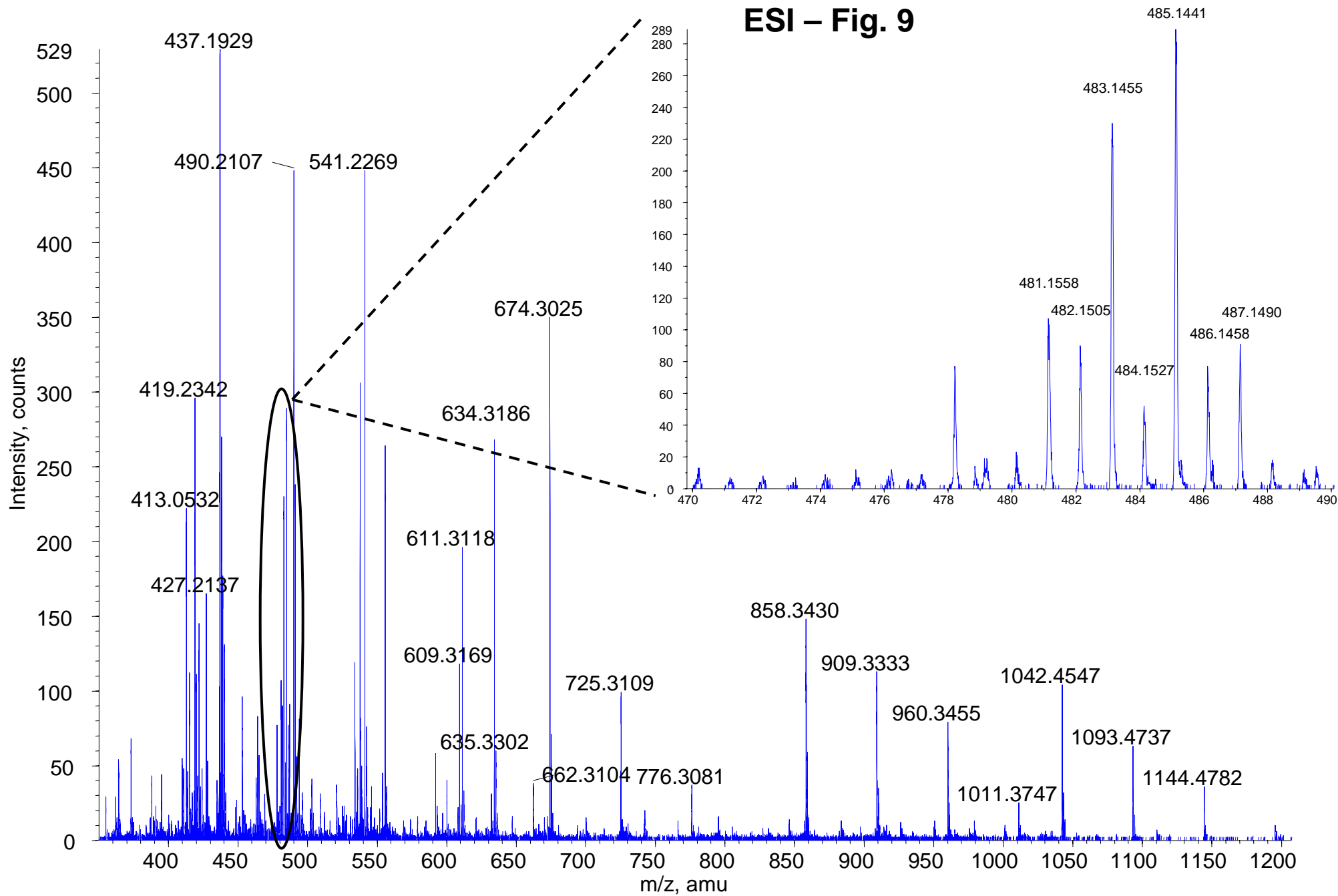
(a)

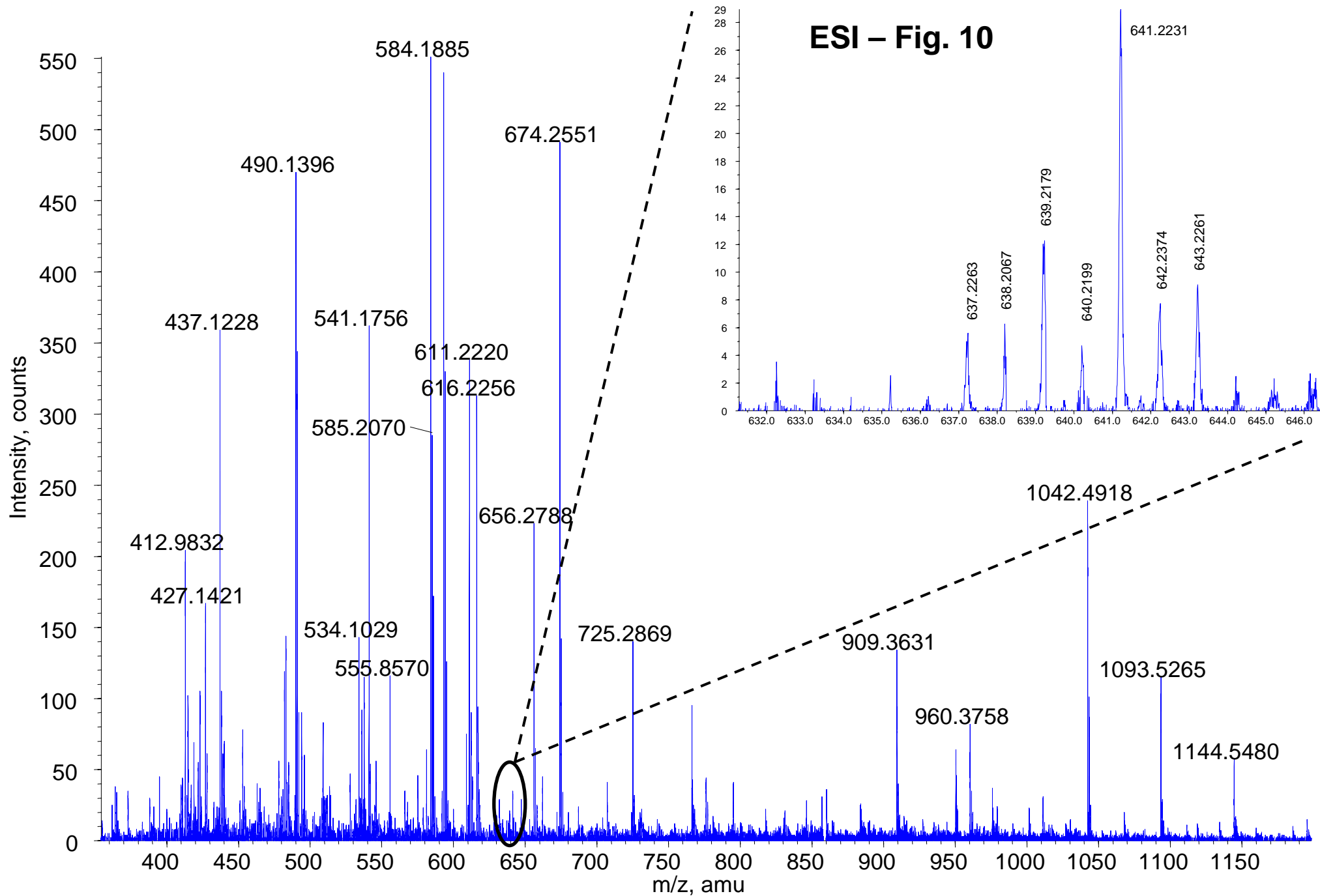


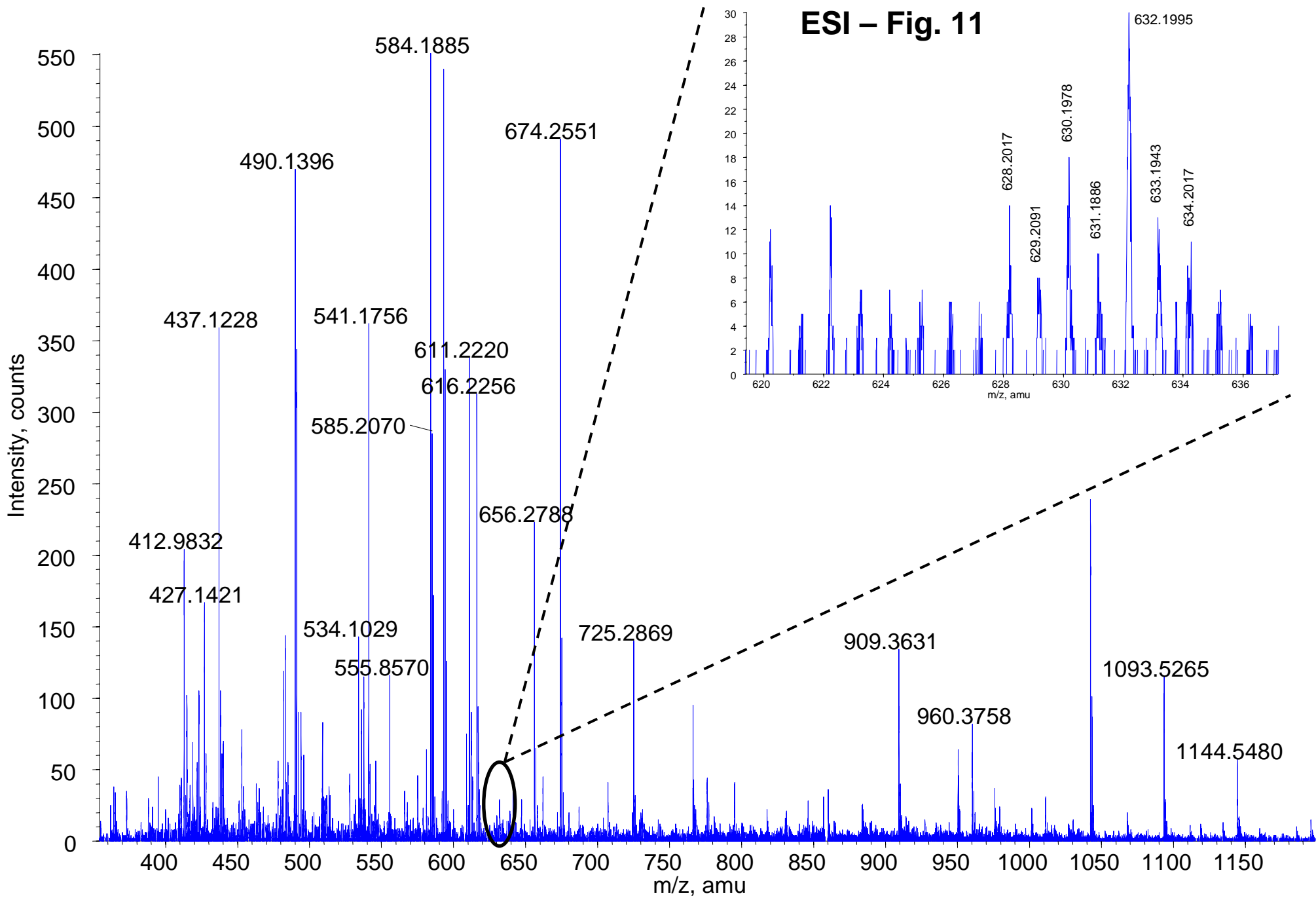




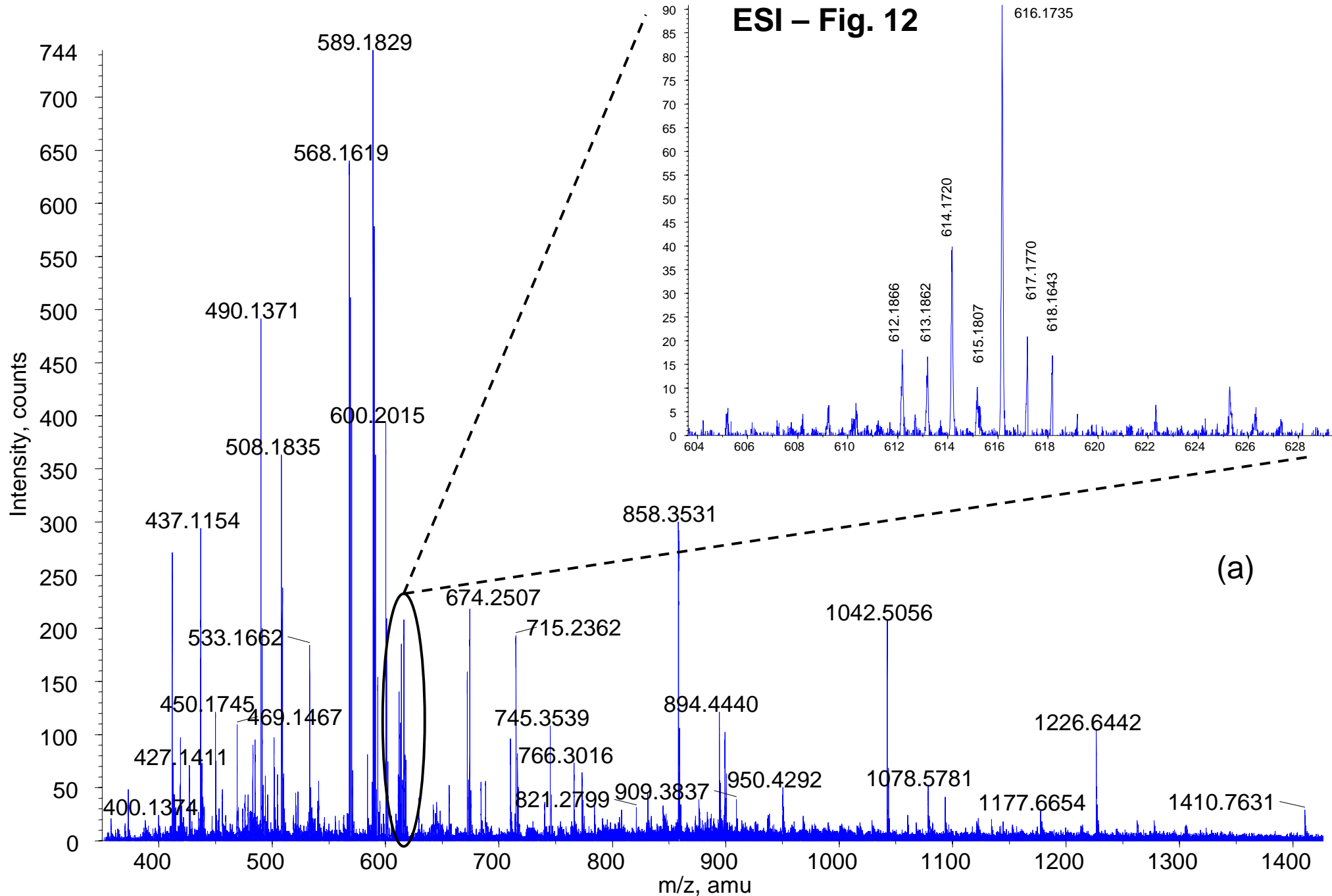
ESI – Fig. 9

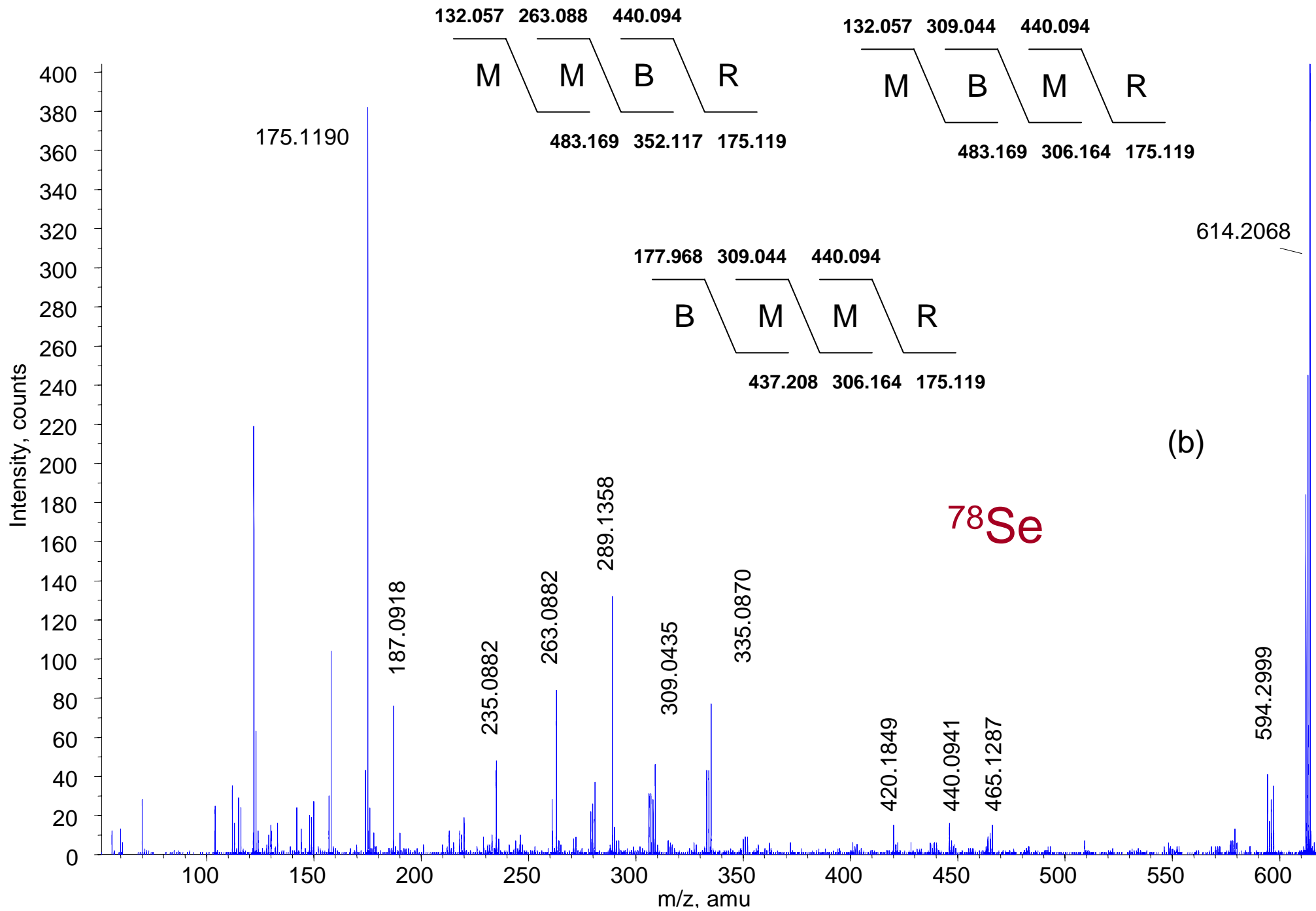


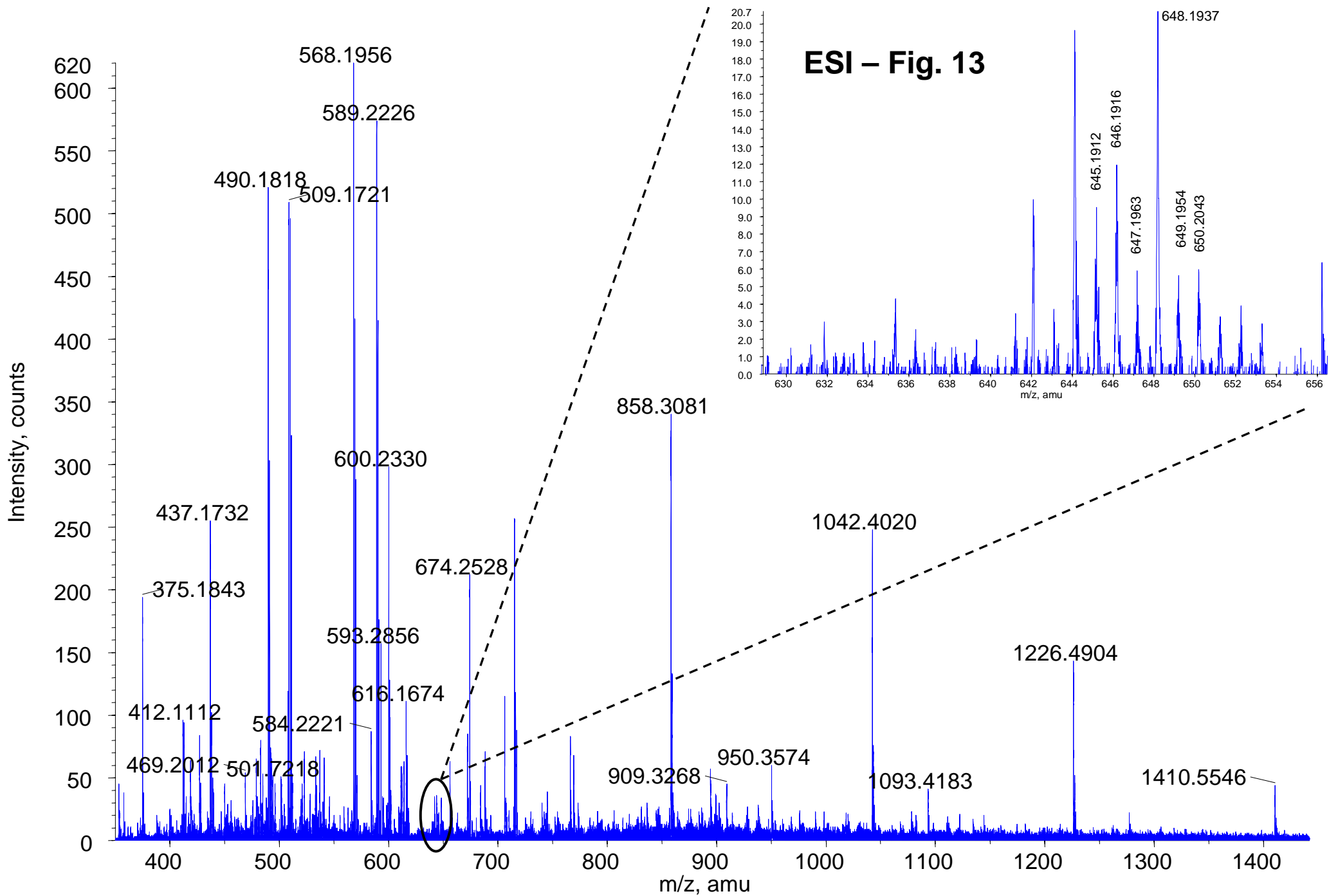




# ESI – Fig. 12

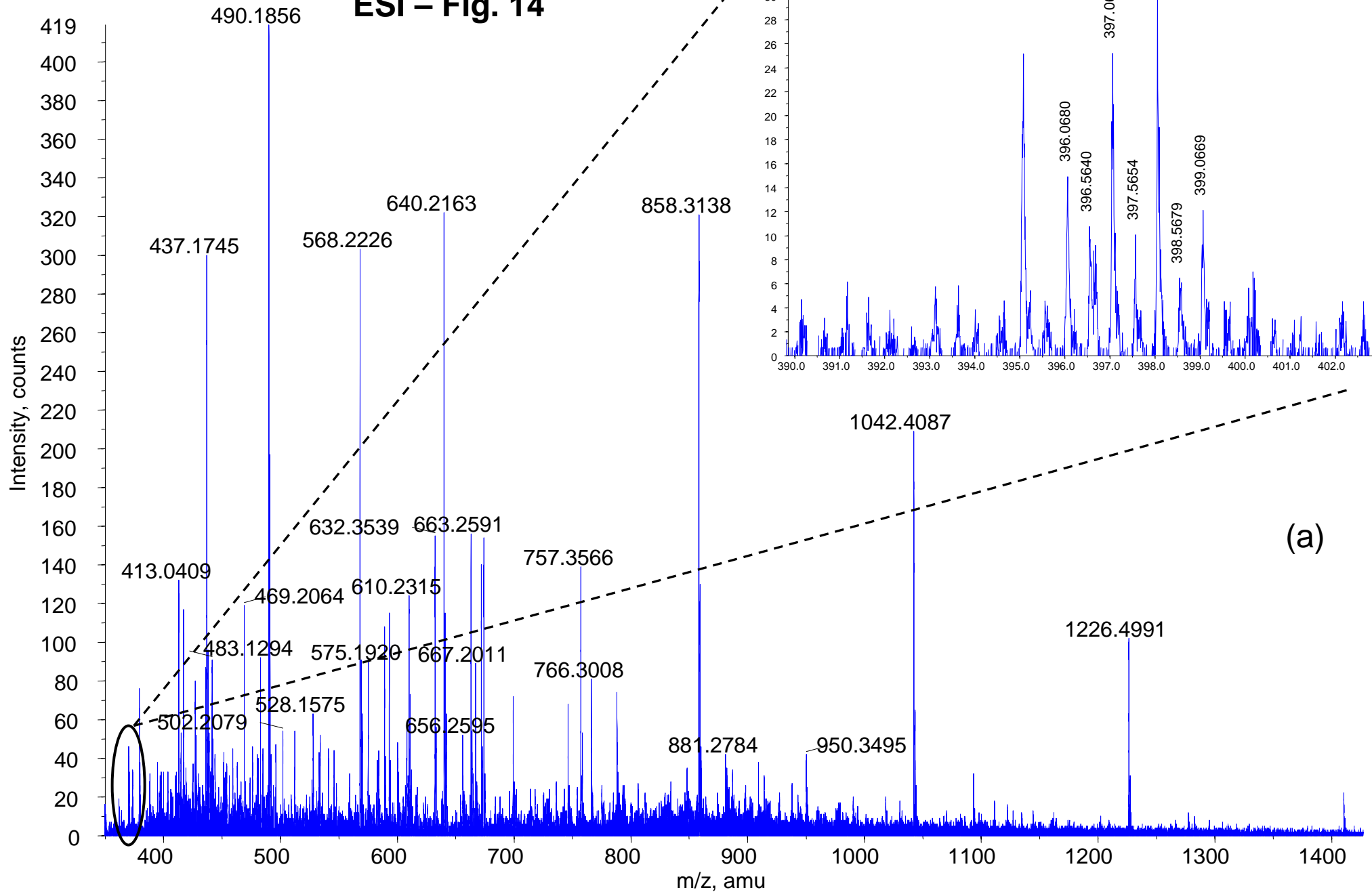








# ESI – Fig. 14



(a)

