Supporting Information for Copper (II) Complexes of Bis(amino amide) Ligands: Effect of Changes in the Amino Acid Residue

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Supplementary material

S1. Species distribution curves for the different protonated forms.

S2. Species distribution curves for the different Cu (II) complexes.

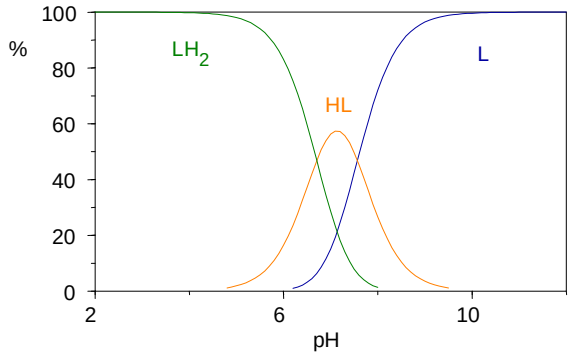
S3. UV/Vis absorption spectra in methanol for the different Cu (II) complexes for the ligands at different pH values

S4. ESI-MS spectra for the different Cu (II) complexes at several pH values.

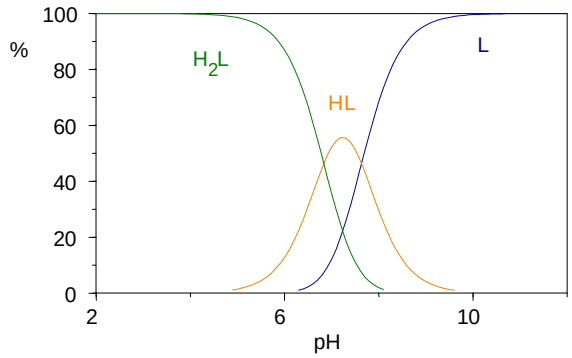
S5. Species distribution curves for the compound AlaA3 (1d, n=1) and for Cu (II) complexes. UV/Vis absorption spectra and ESI-MS spectra for the Cu (II) complexes at several pH values.

S1. Species distribution curves for the different protonated forms.

PheA2



PheA3



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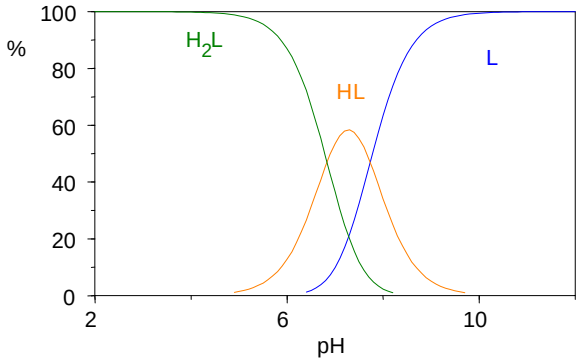

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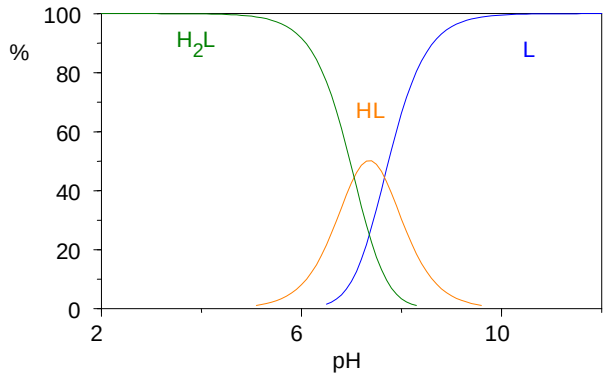

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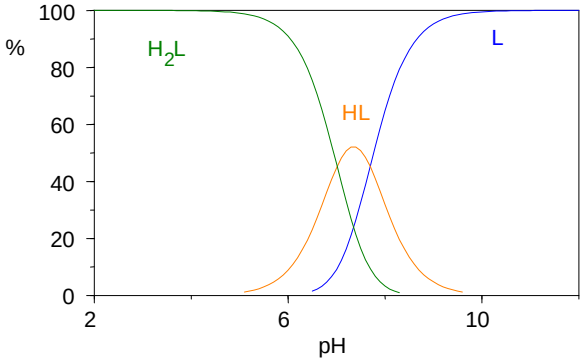

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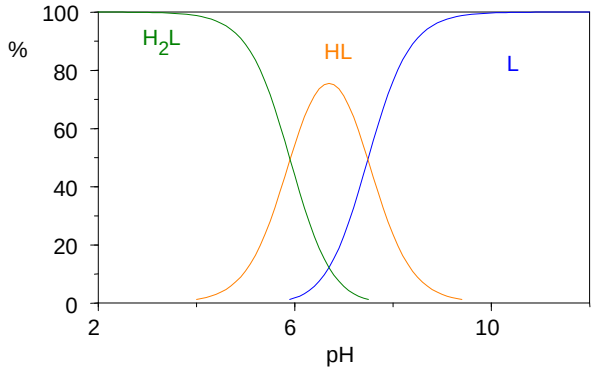

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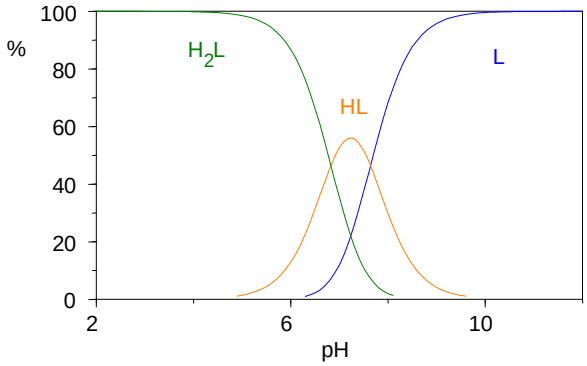
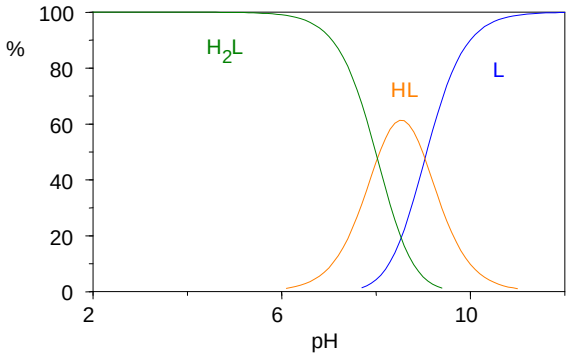


ProA2



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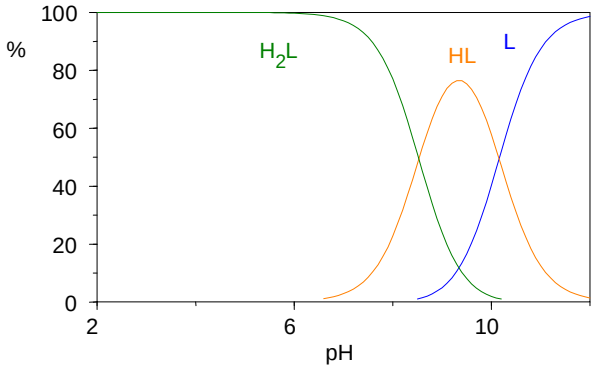
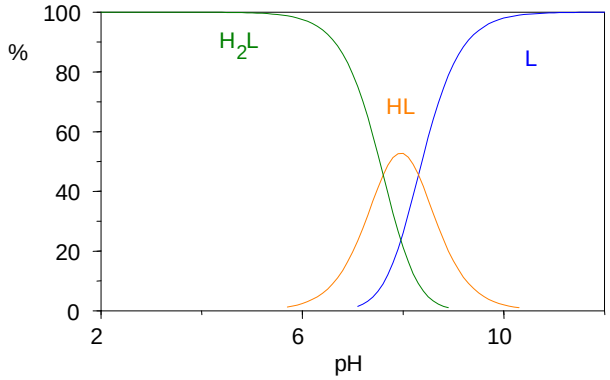


AlaA2



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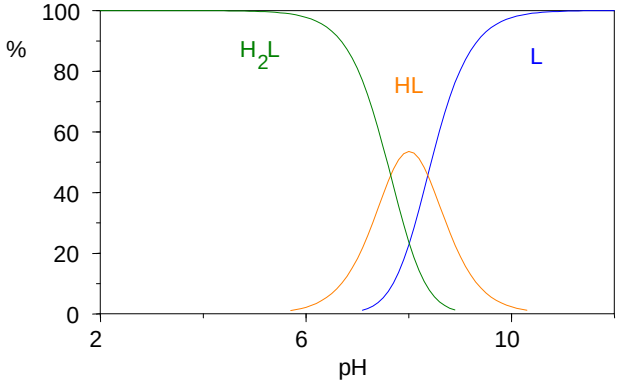

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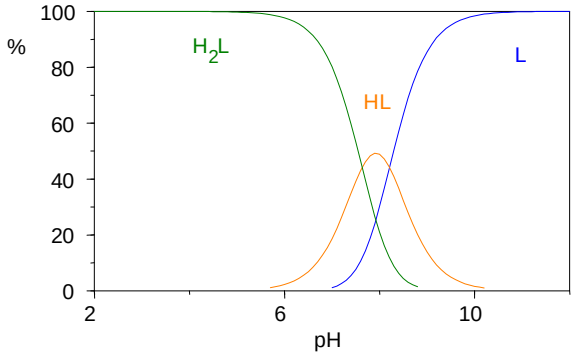

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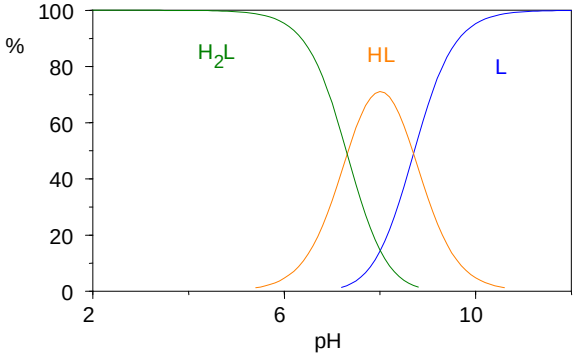
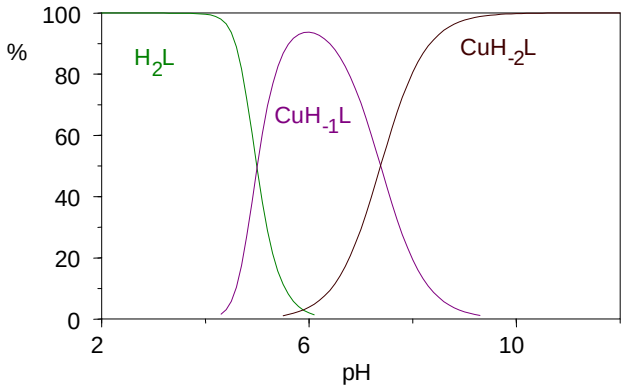


S2. Species distribution curves for the different Cu (II) complexes.

CuPheA2



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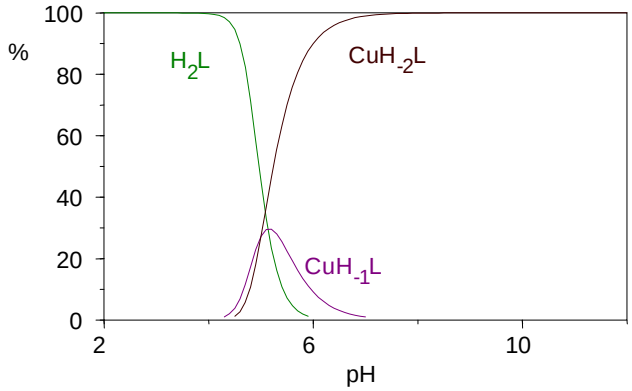
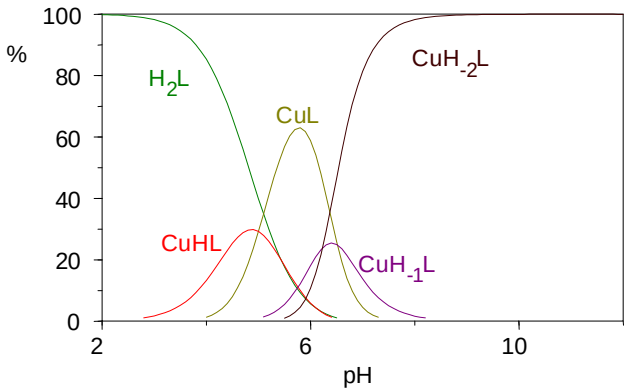
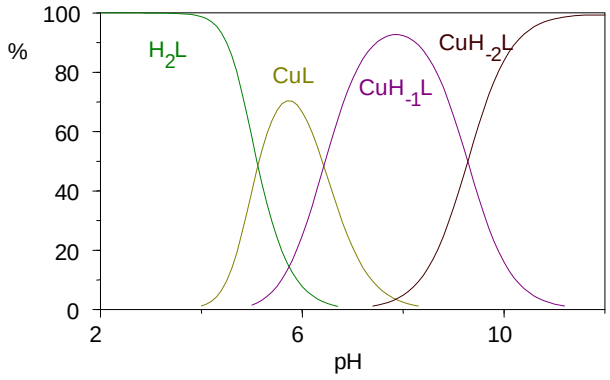


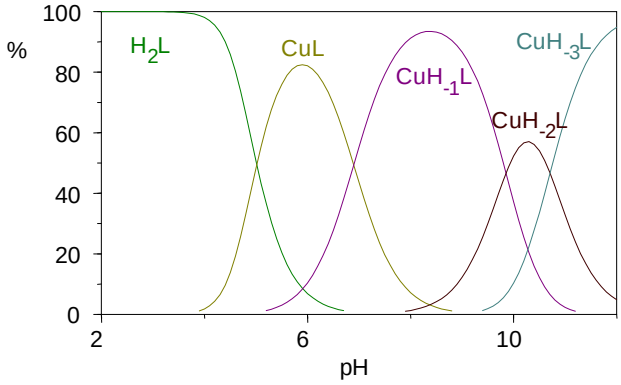
CuPheA4



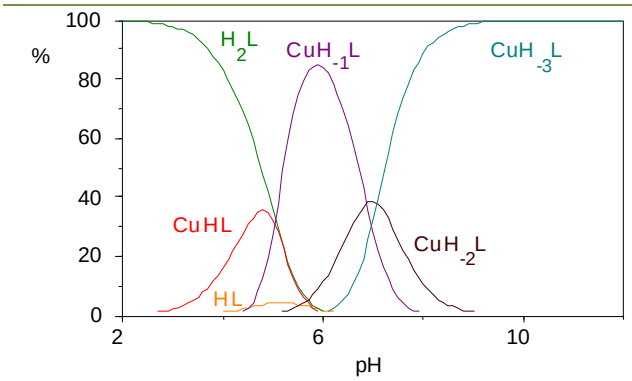
CuPheA5



CuPheA6



CuPhglyA2



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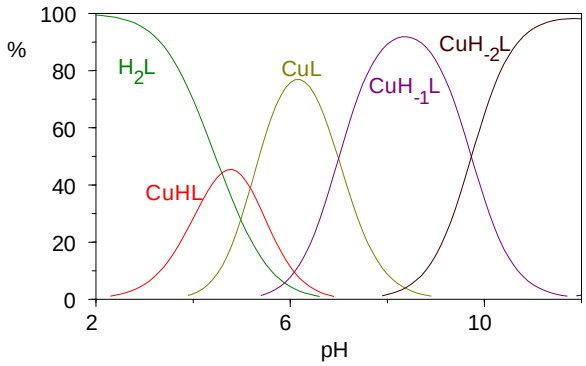
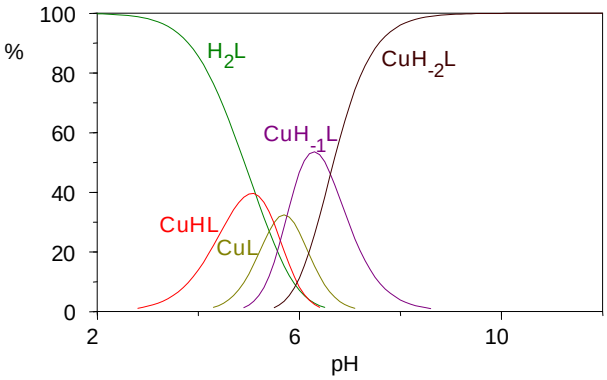


CuProA2



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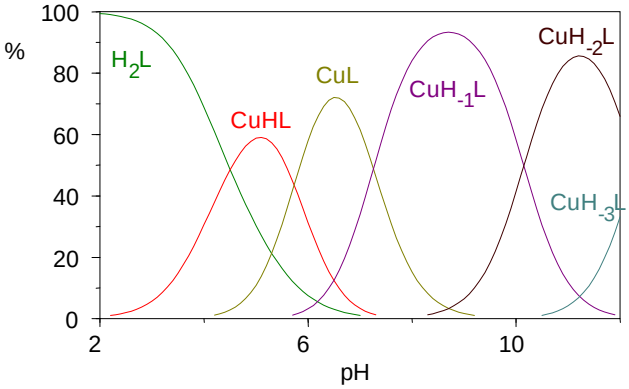
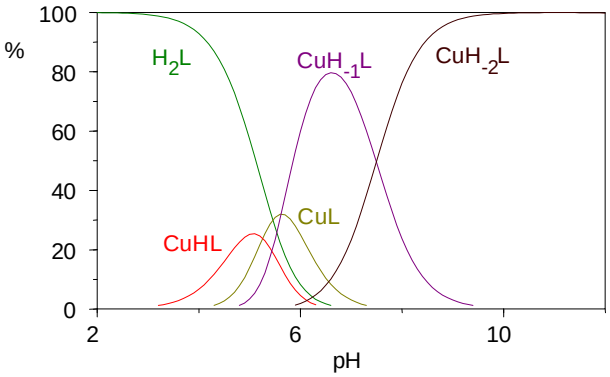


CuAlaA2



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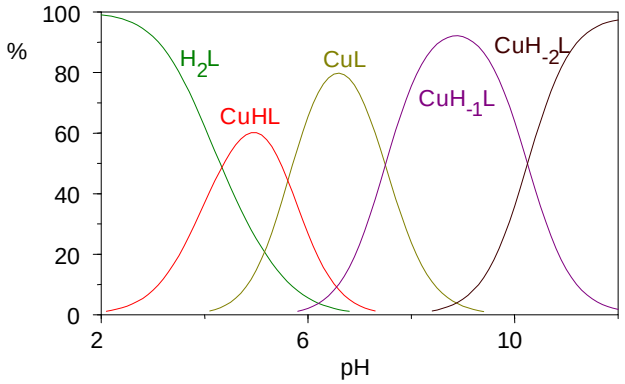
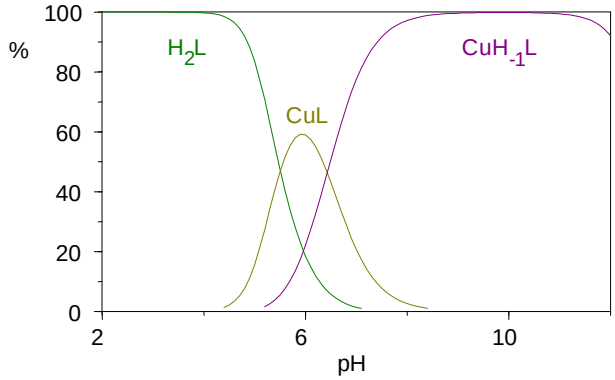
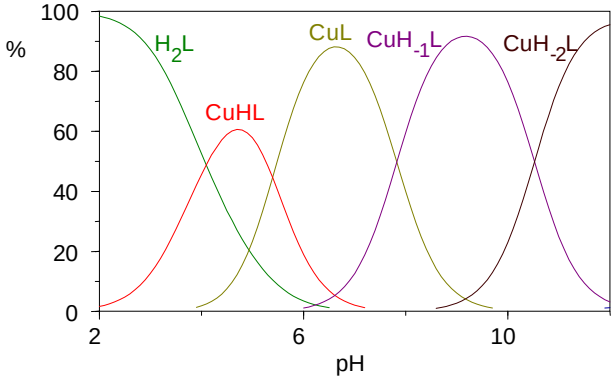


CuGlyA2

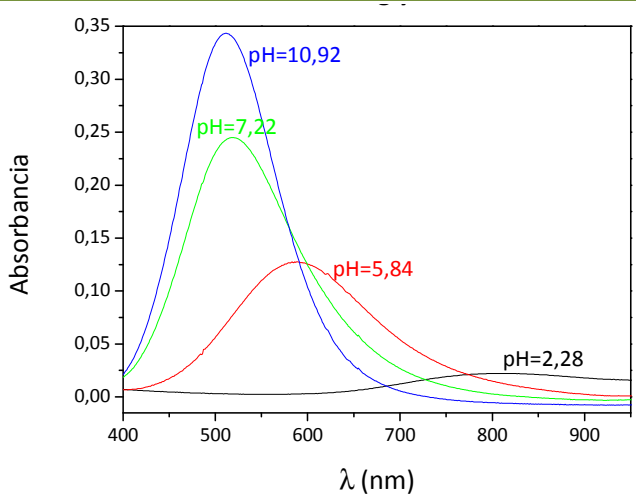


CuGlyA6

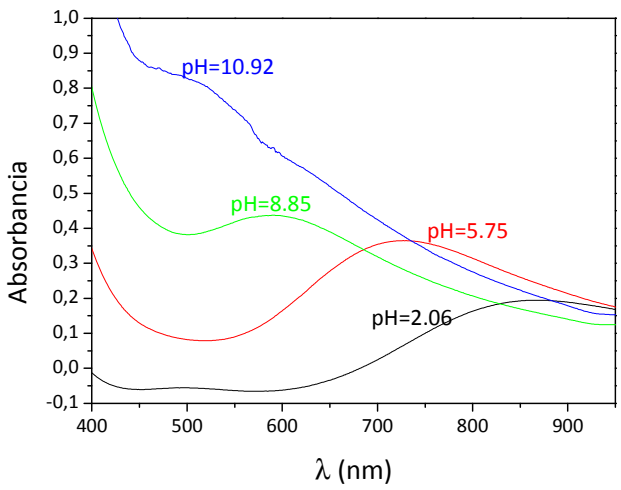


S3. UV/Vis absorption spectra in methanol for the different Cu (II) complexes for the ligands at different pH values

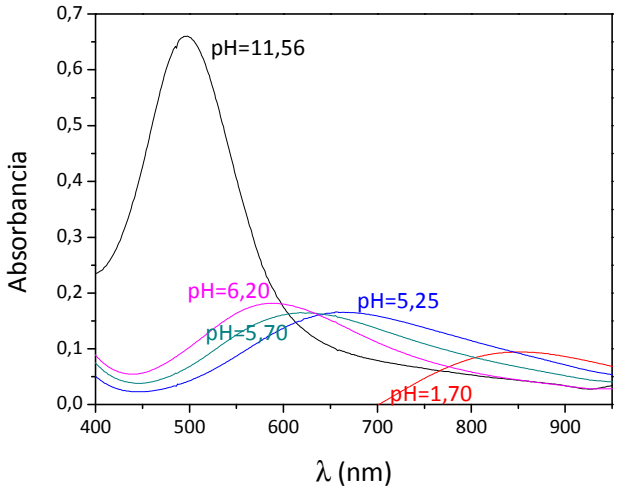
CuPhglyA2



CuPhglyA6



CuProA2



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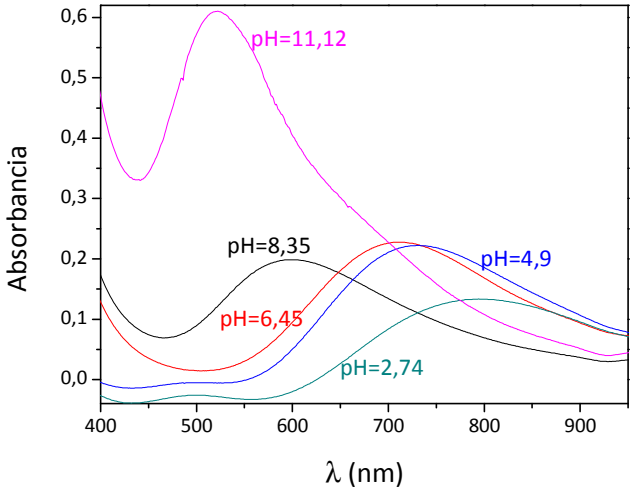
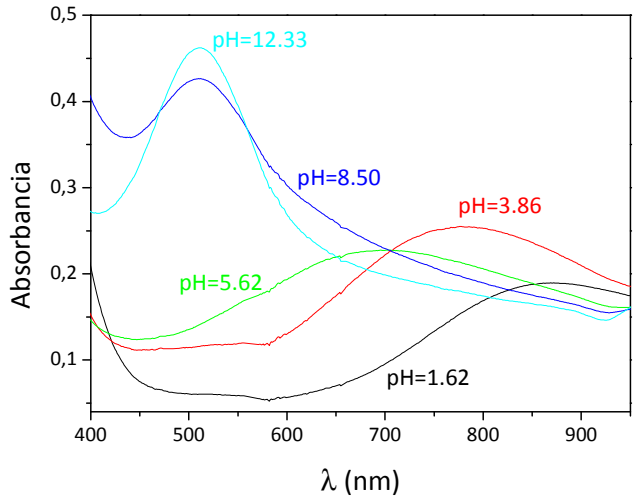
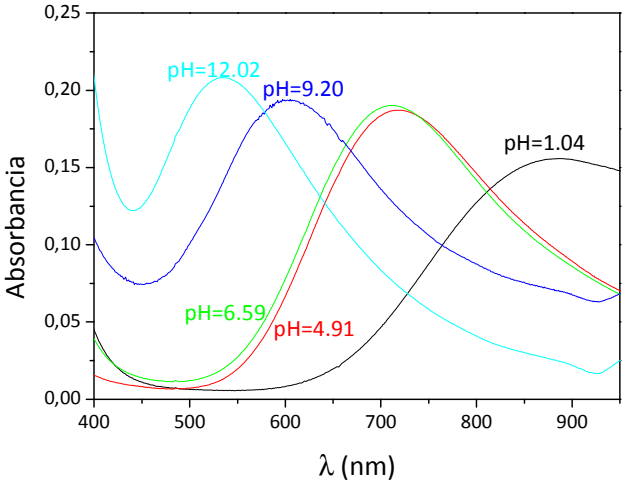
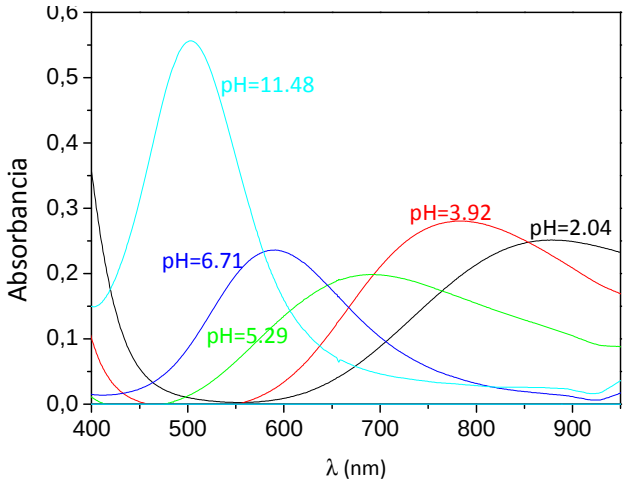
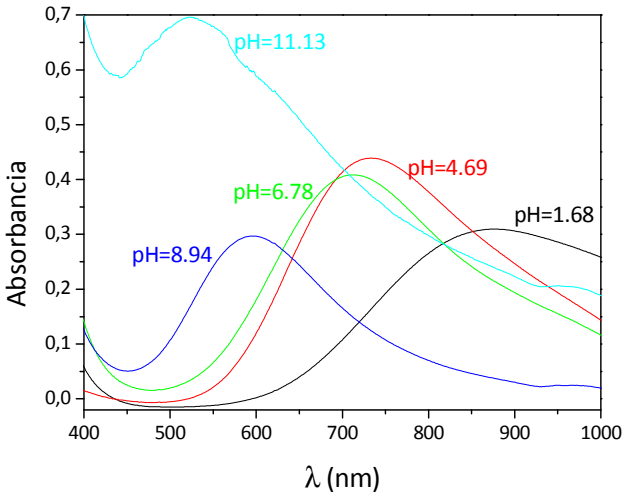


CuGlyA2

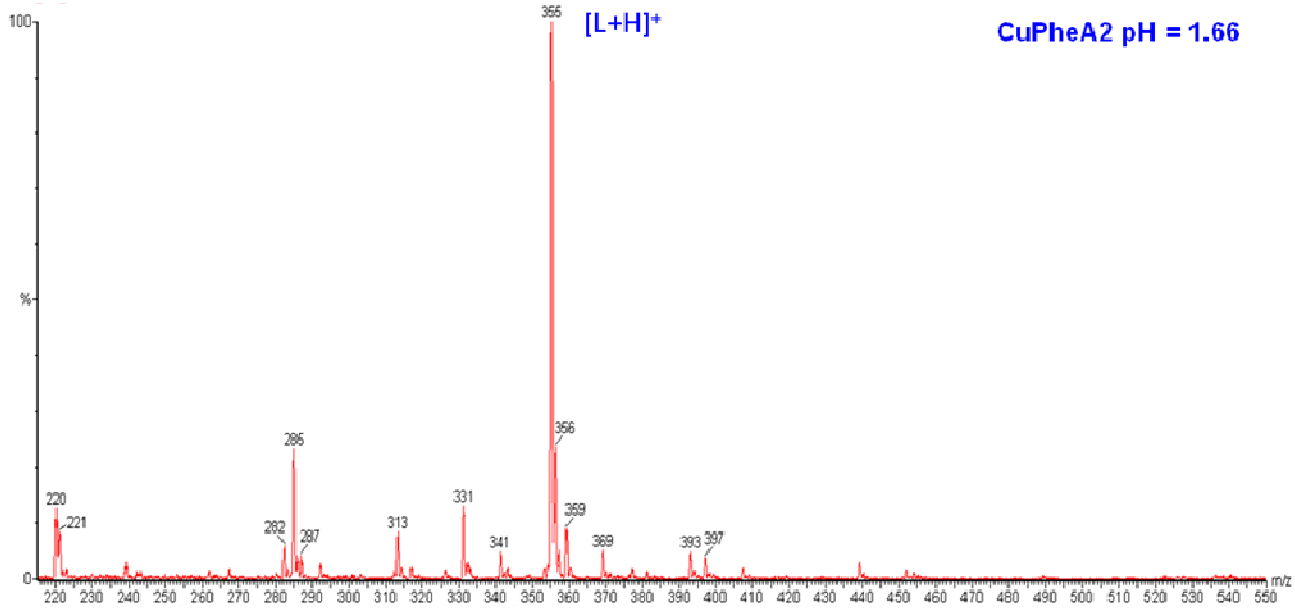


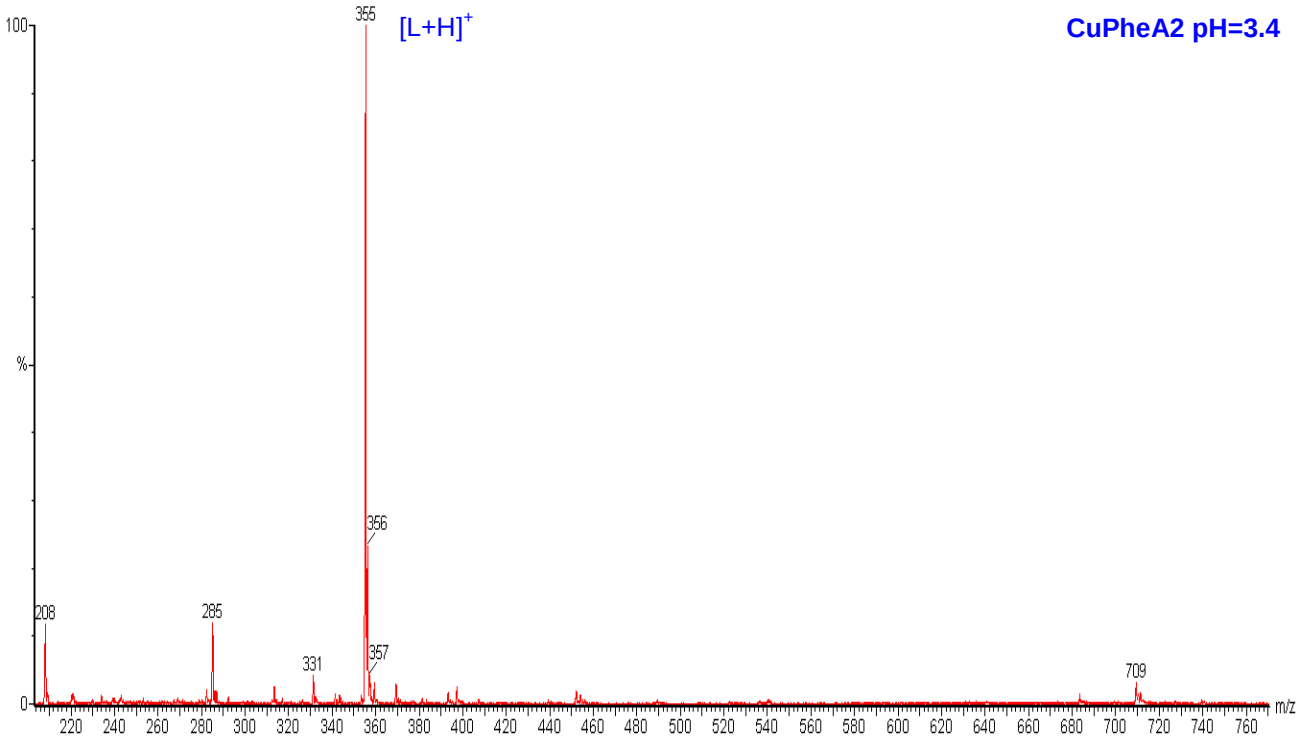
CuGlyA6

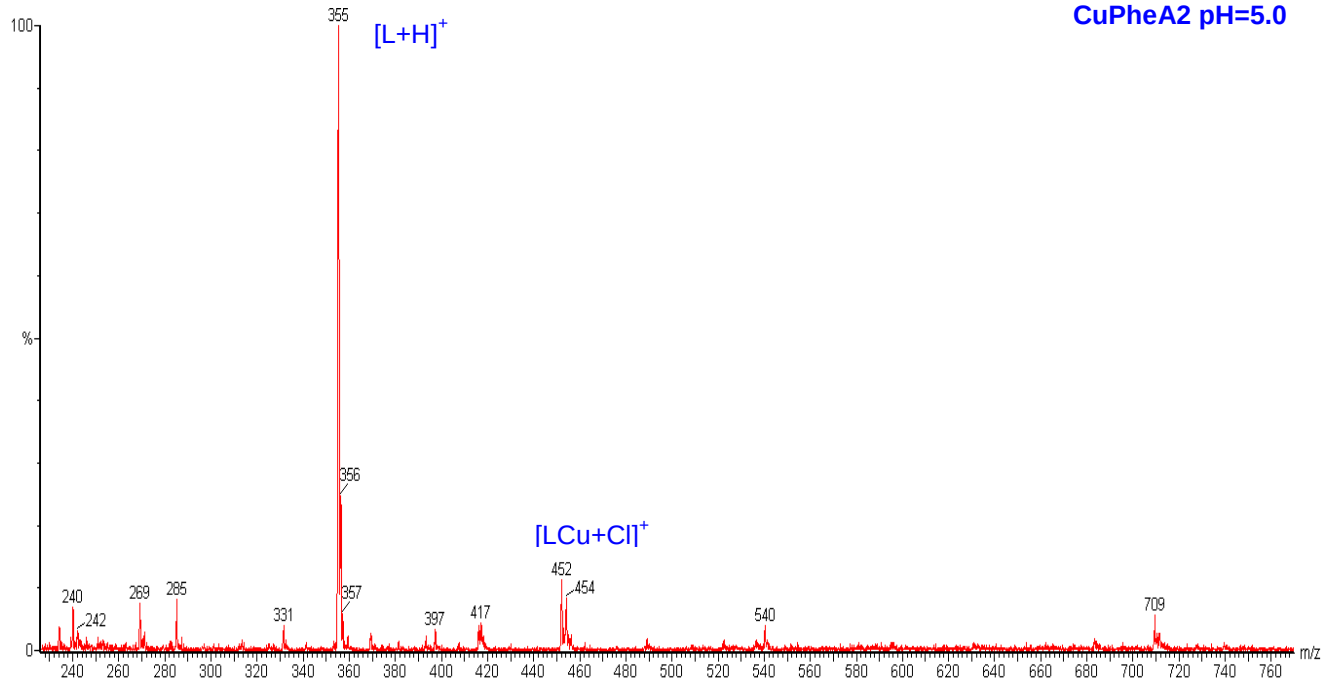


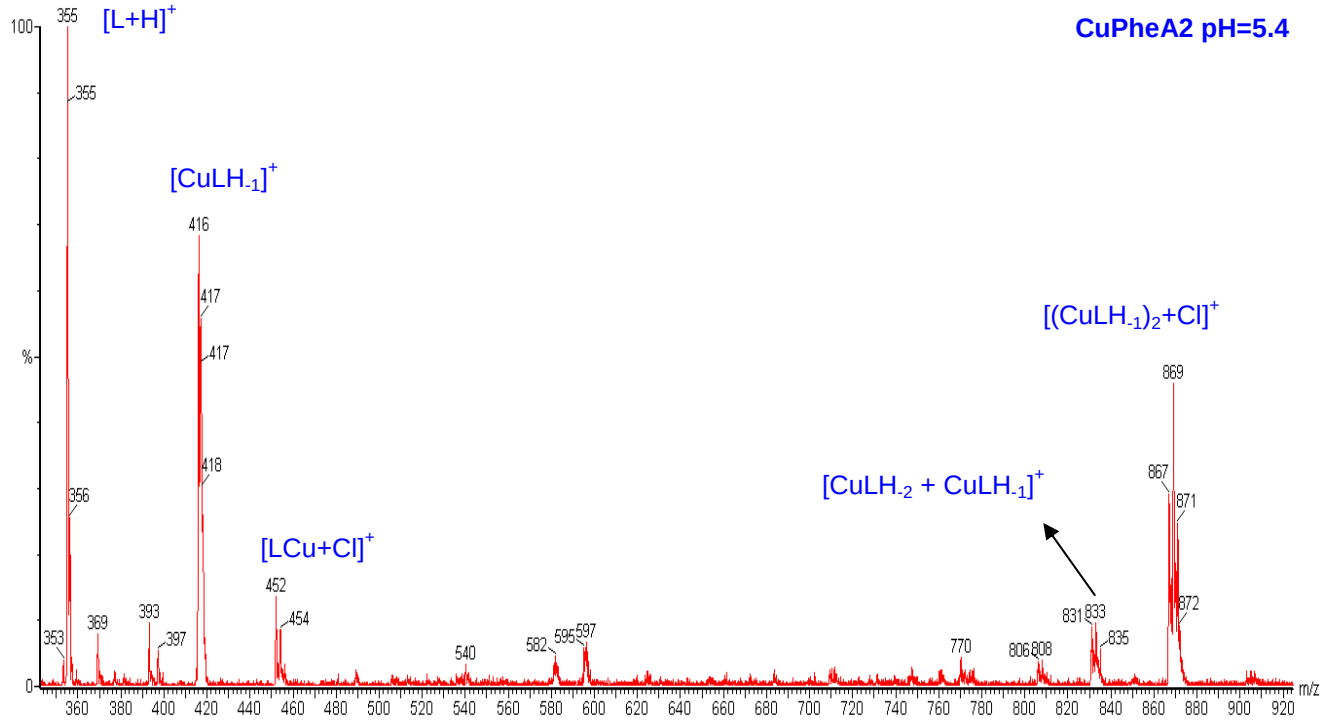
CuAlaA2	CuAlaA6
	

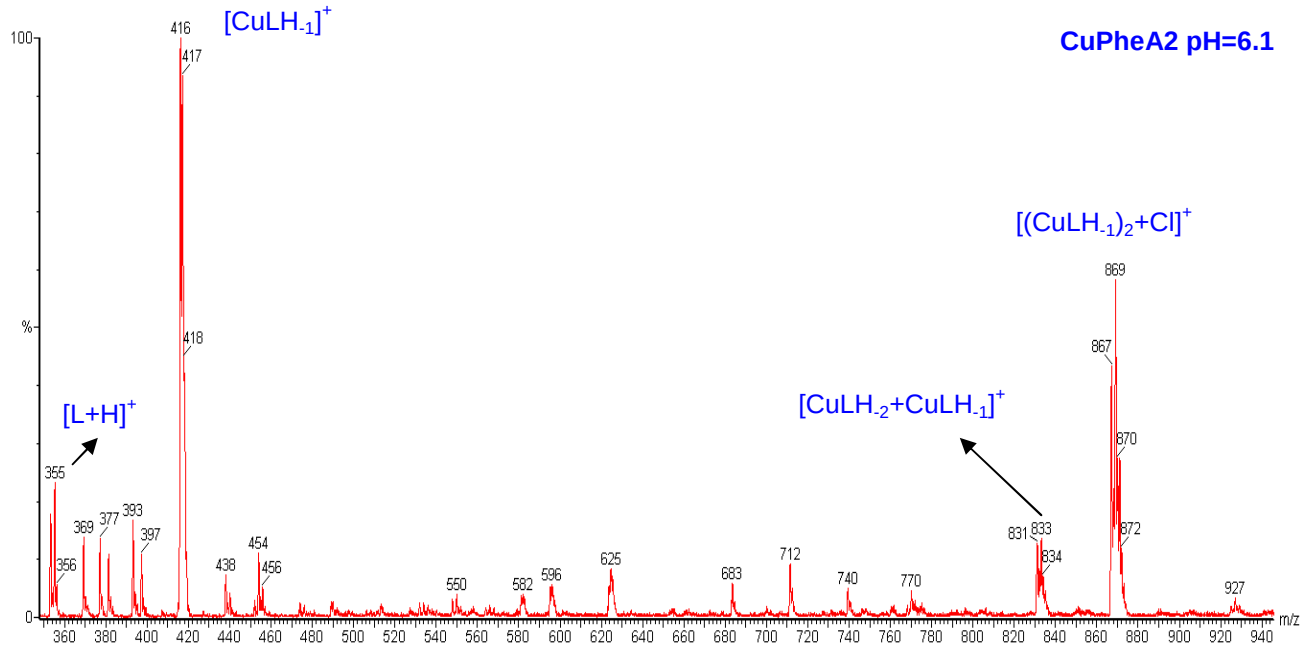
S4. ESI-MS spectra for the different Cu (II) complexes at several pH values.

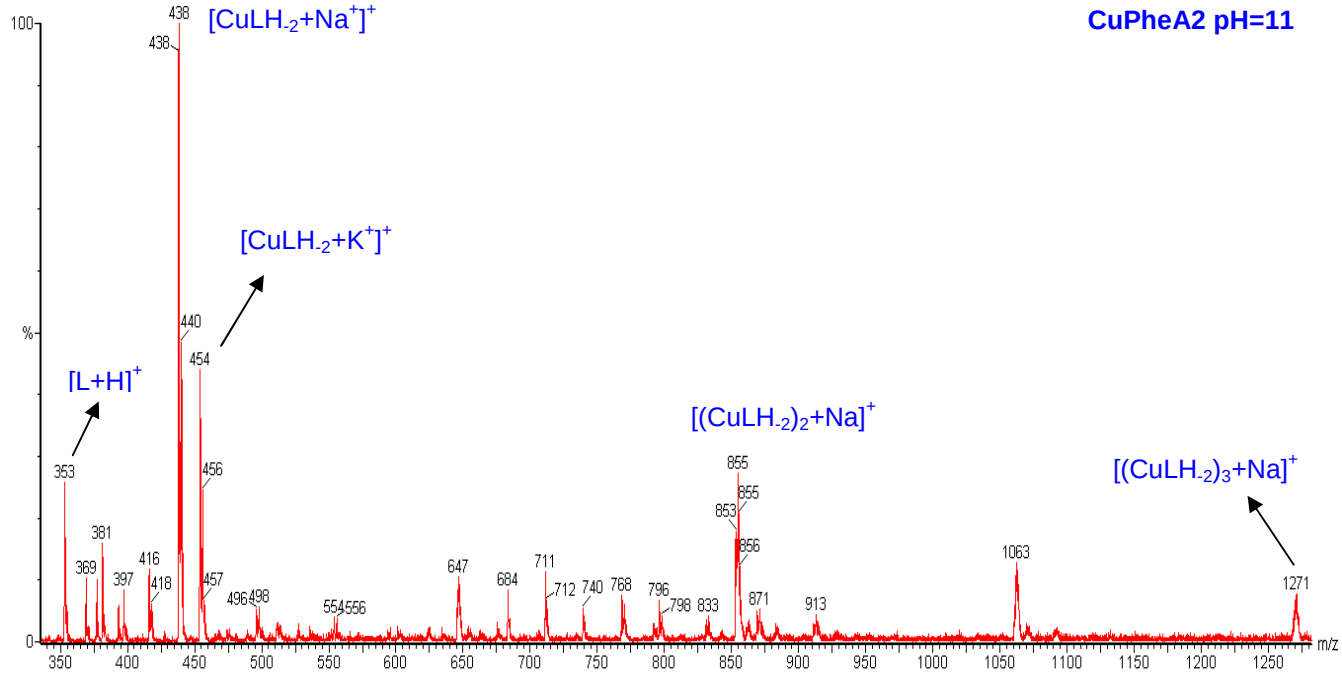


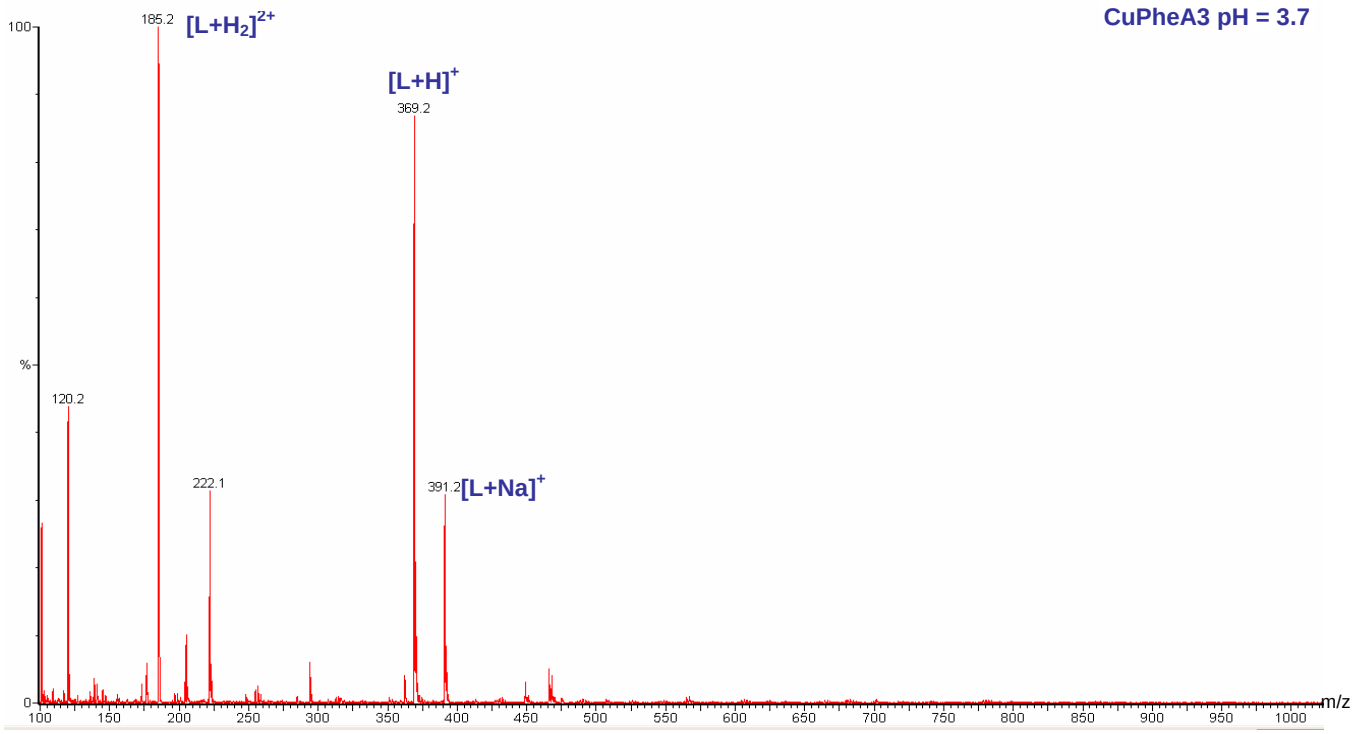


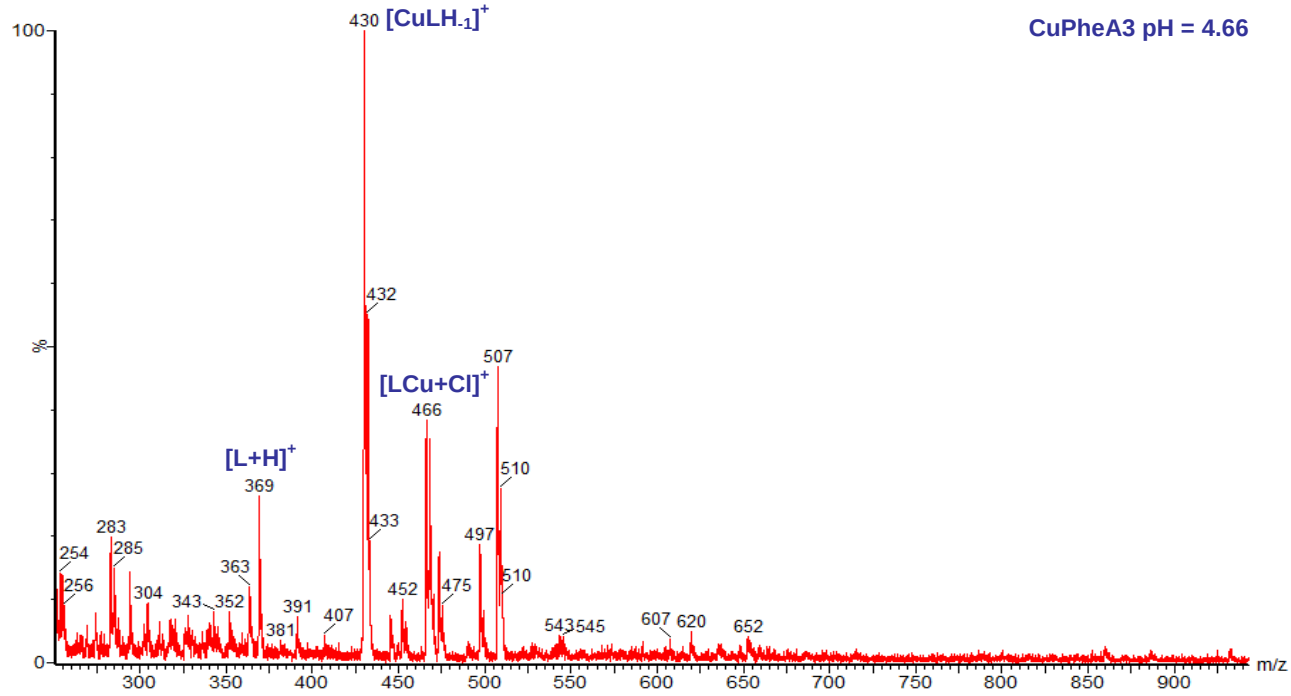


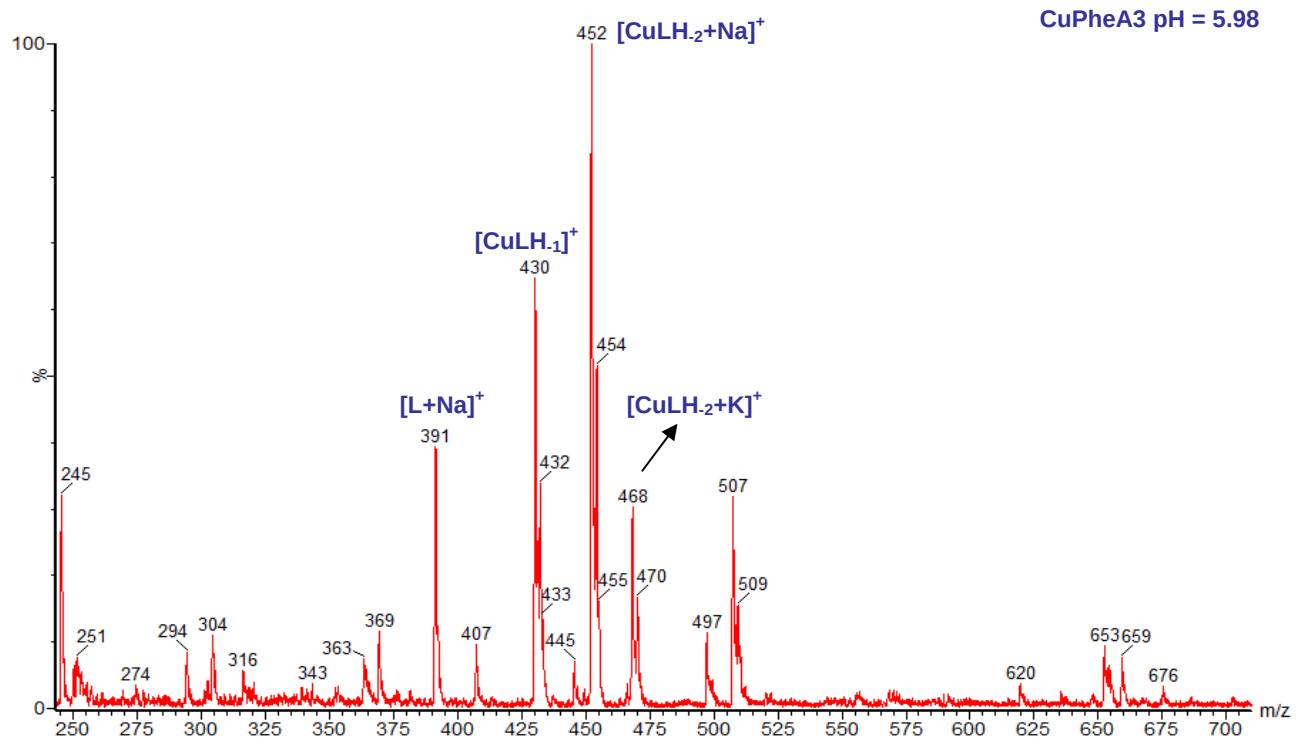


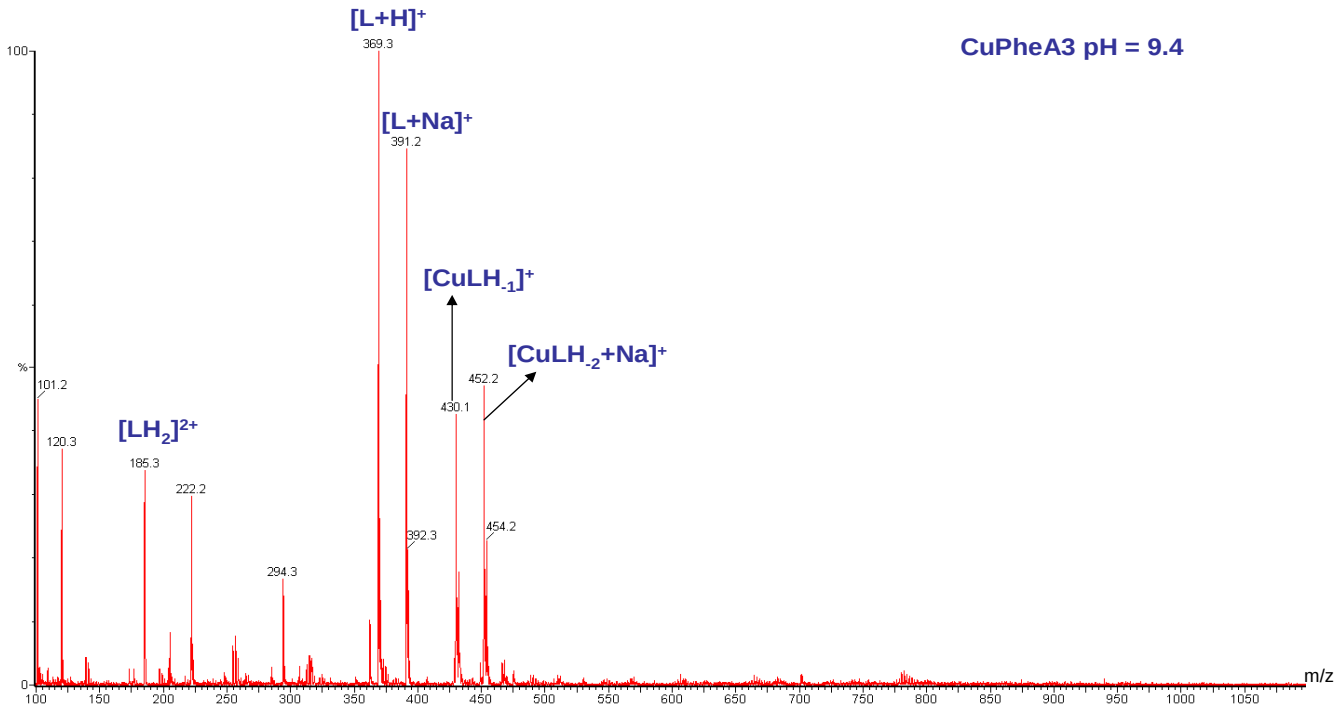


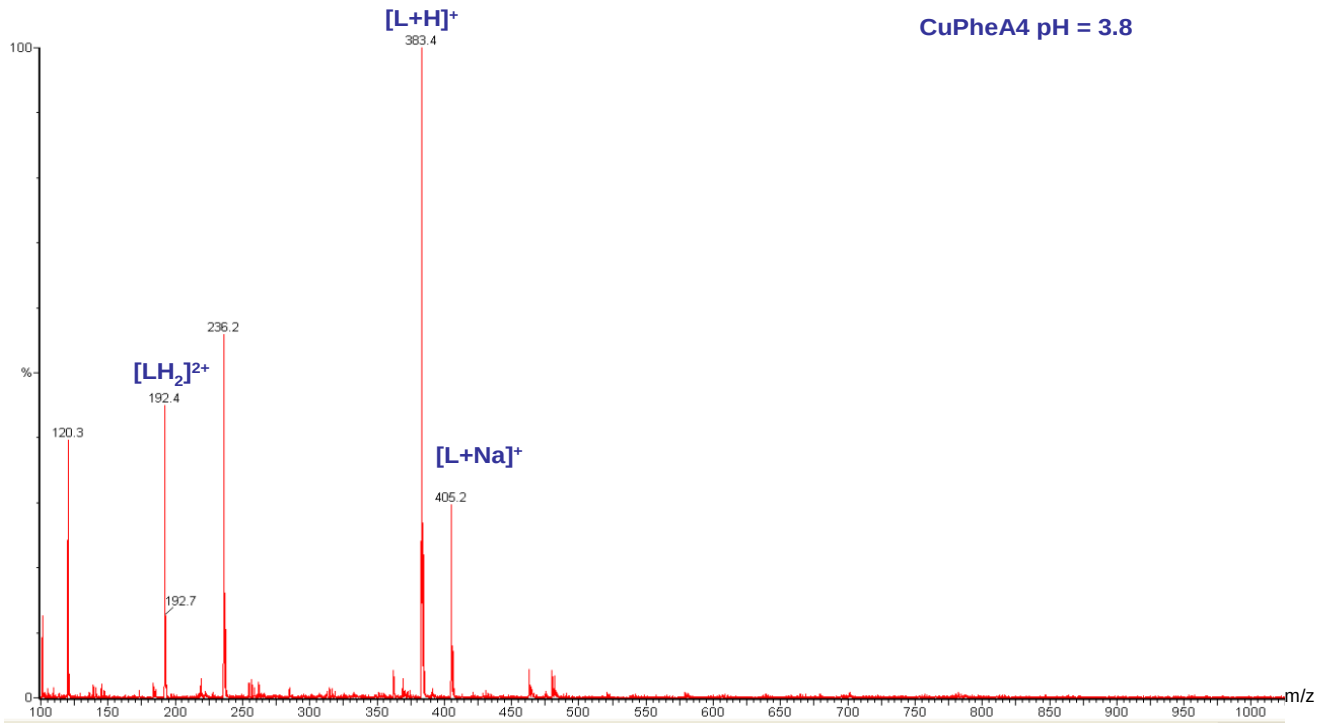


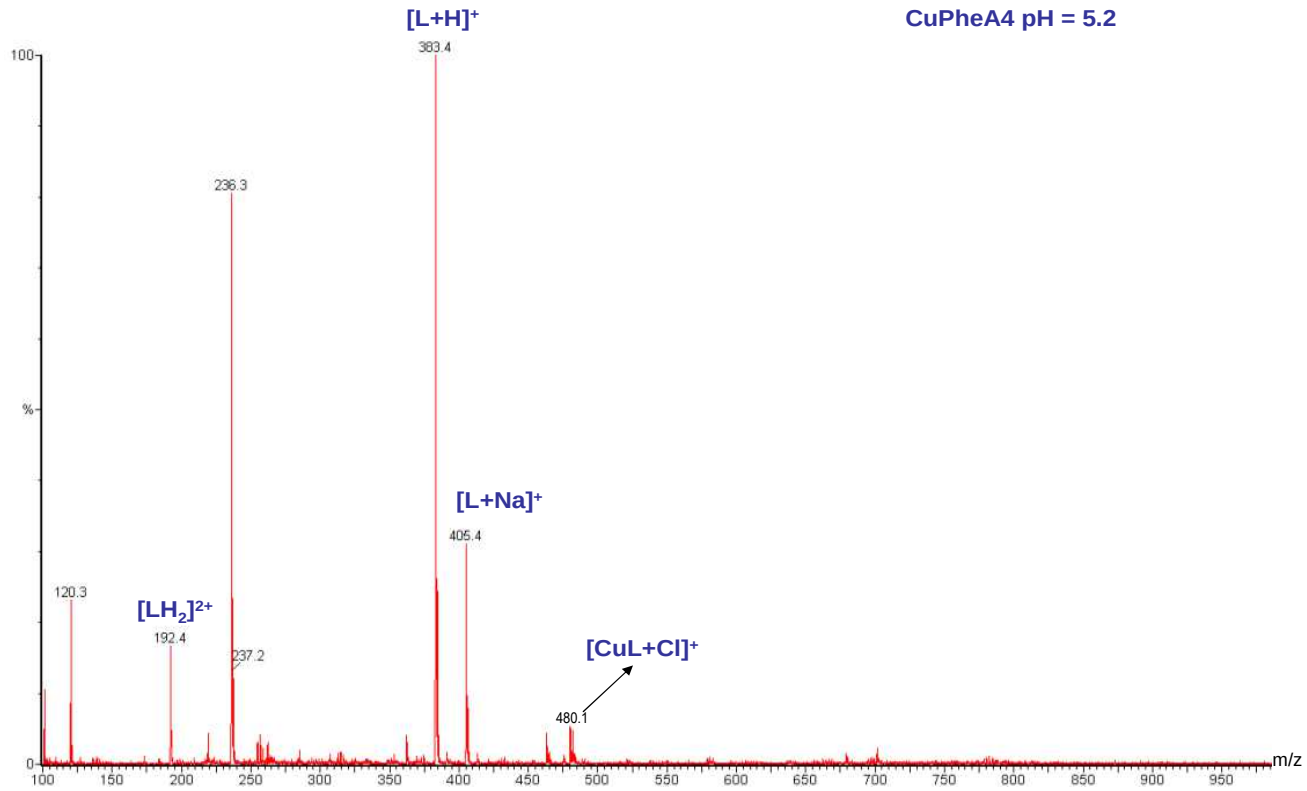


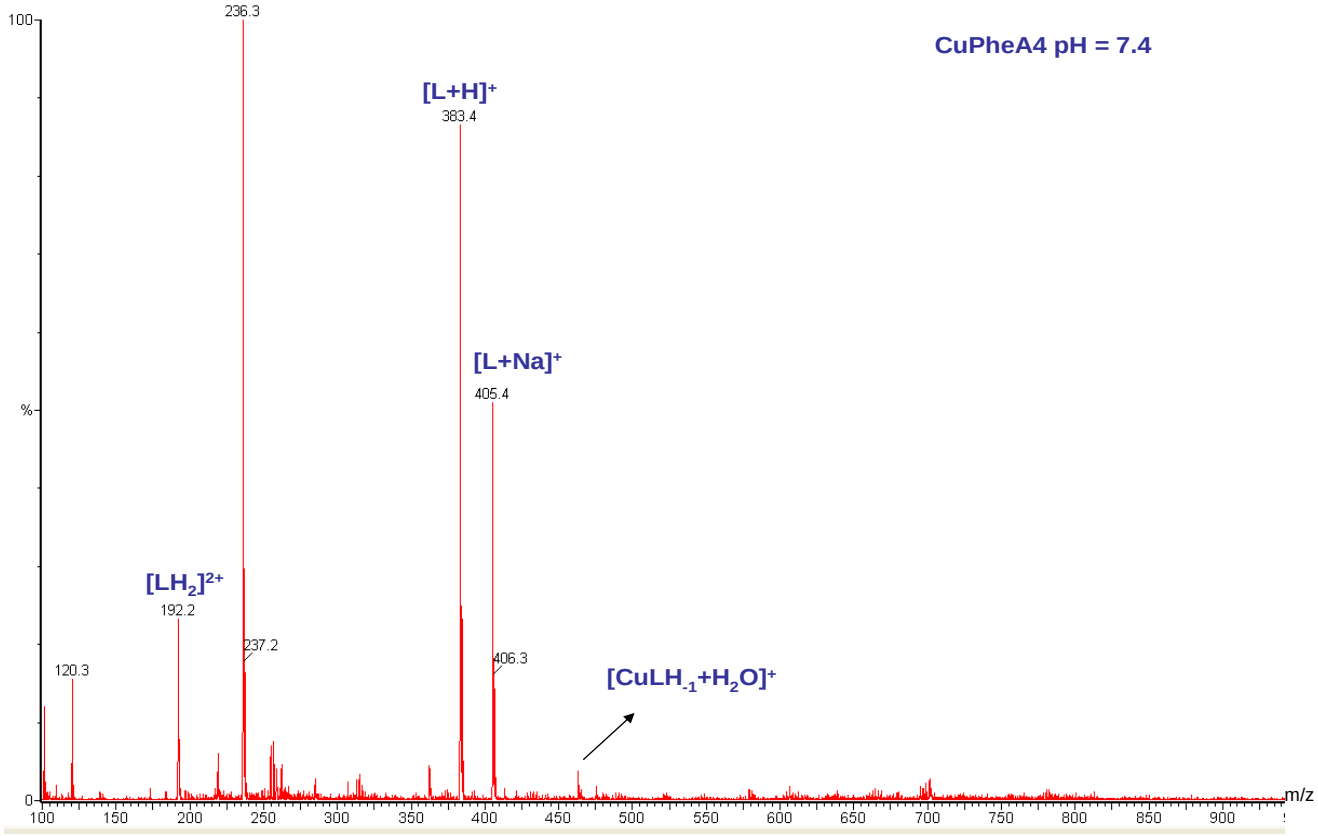


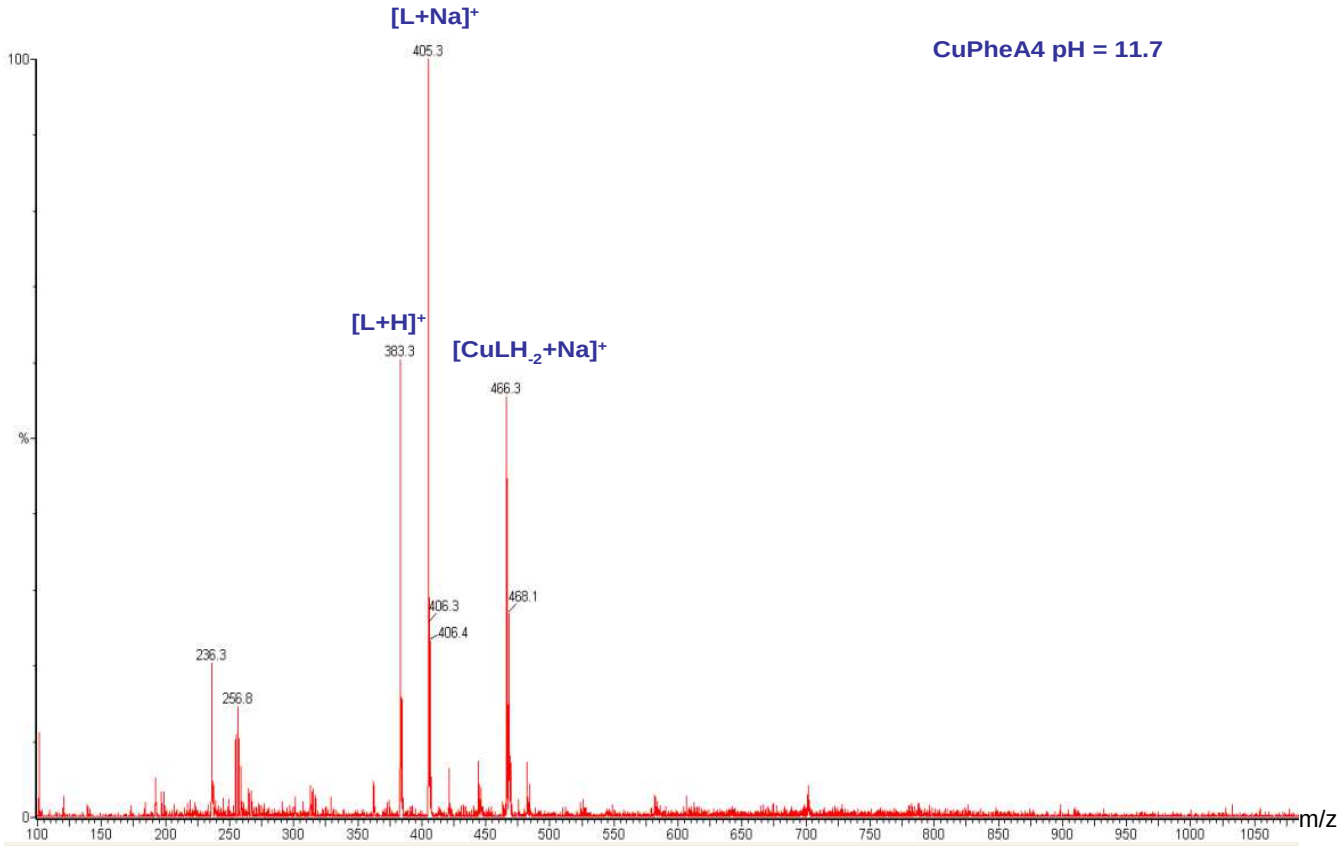


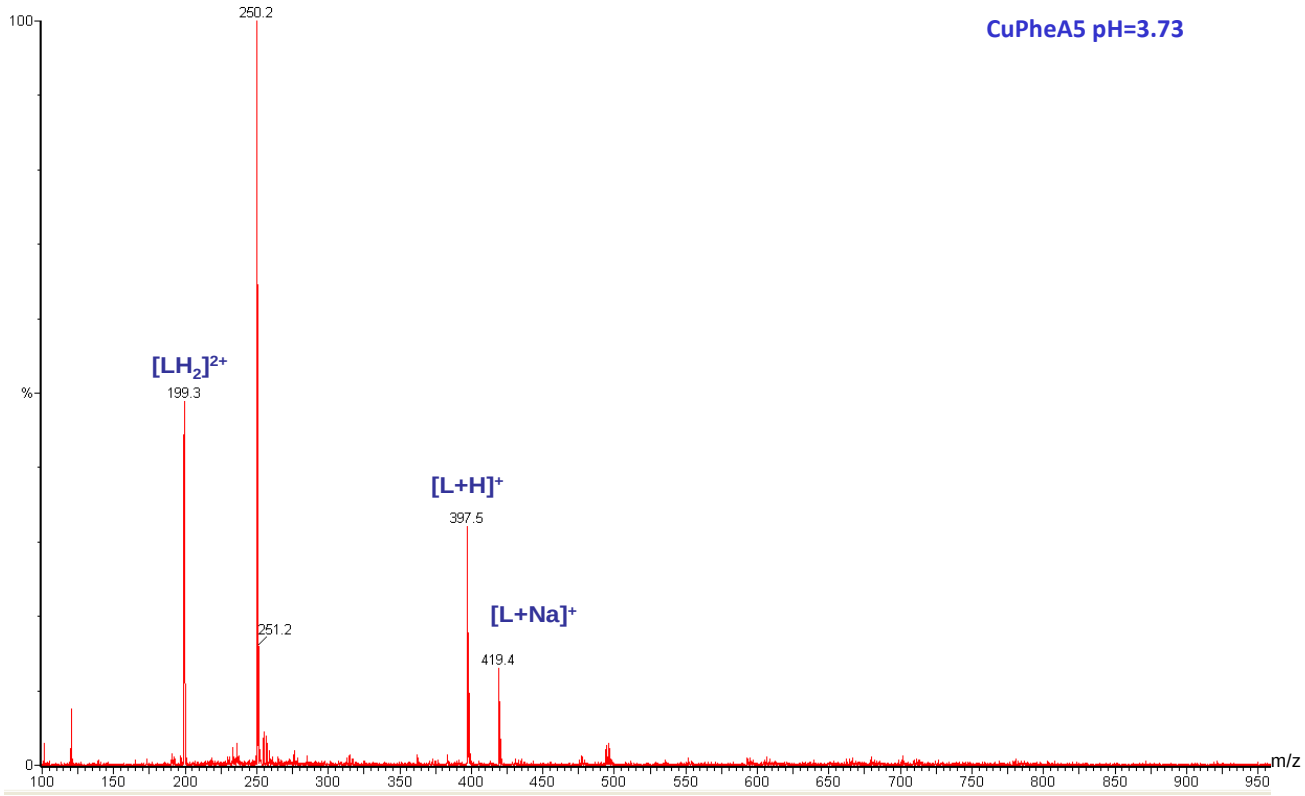


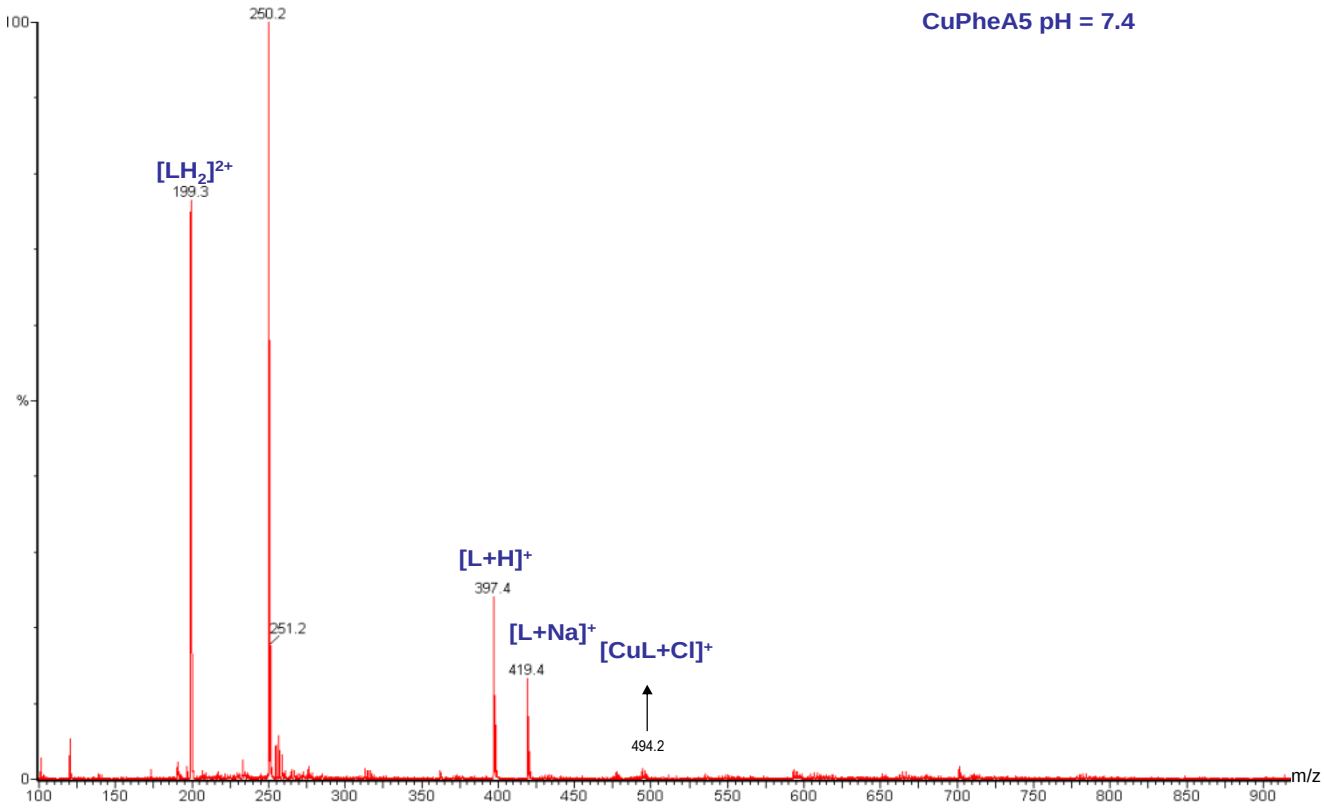


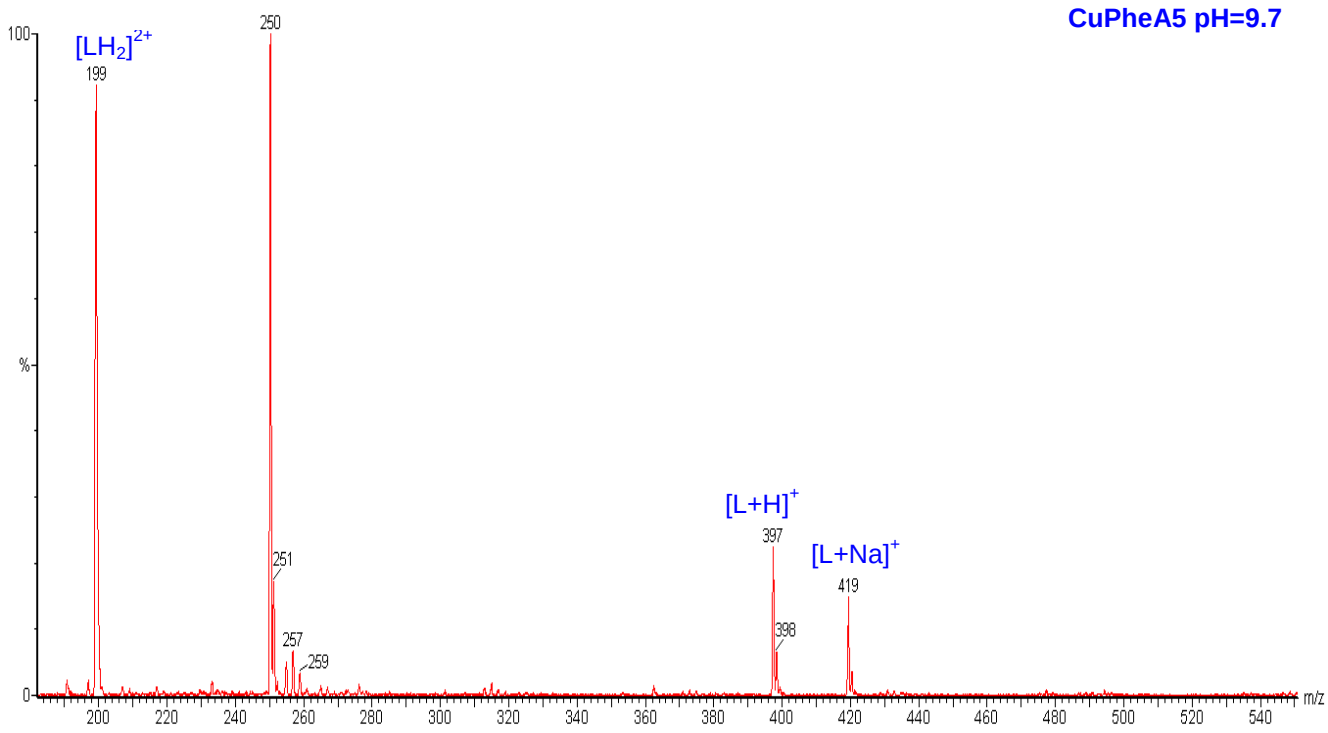


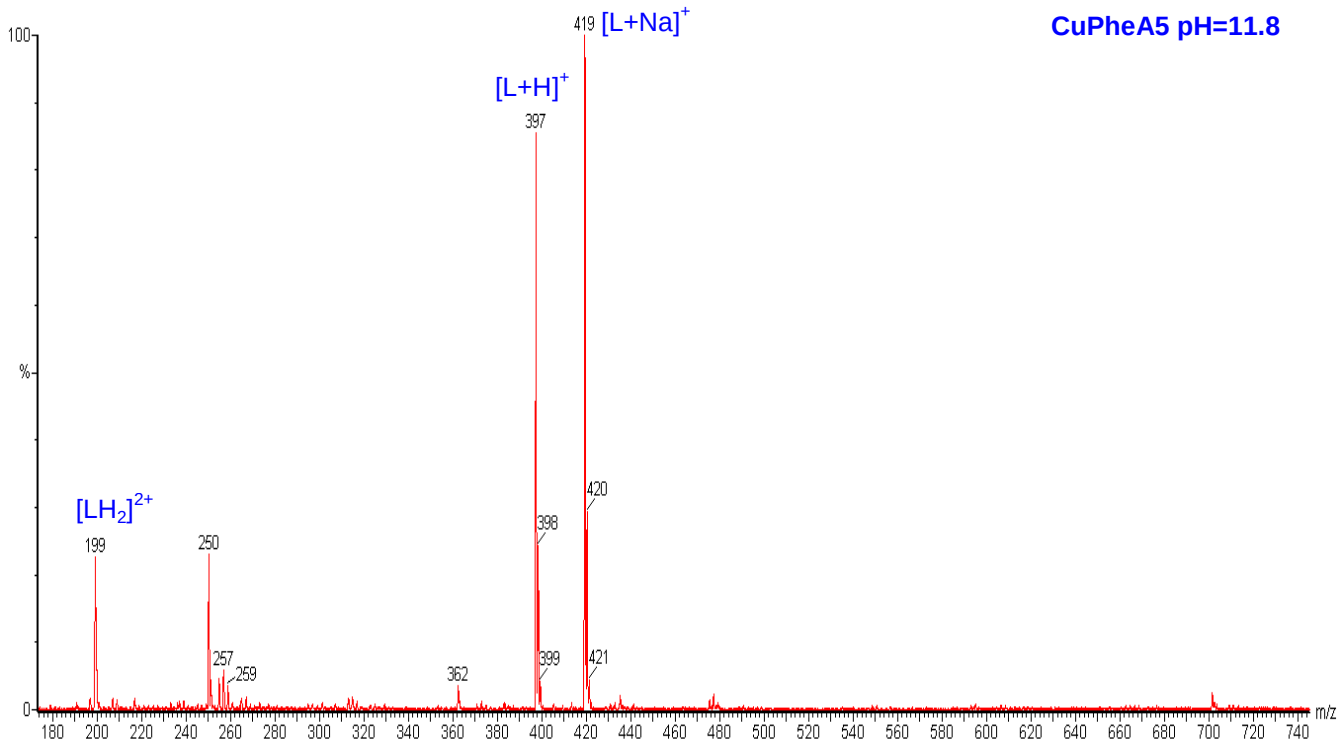


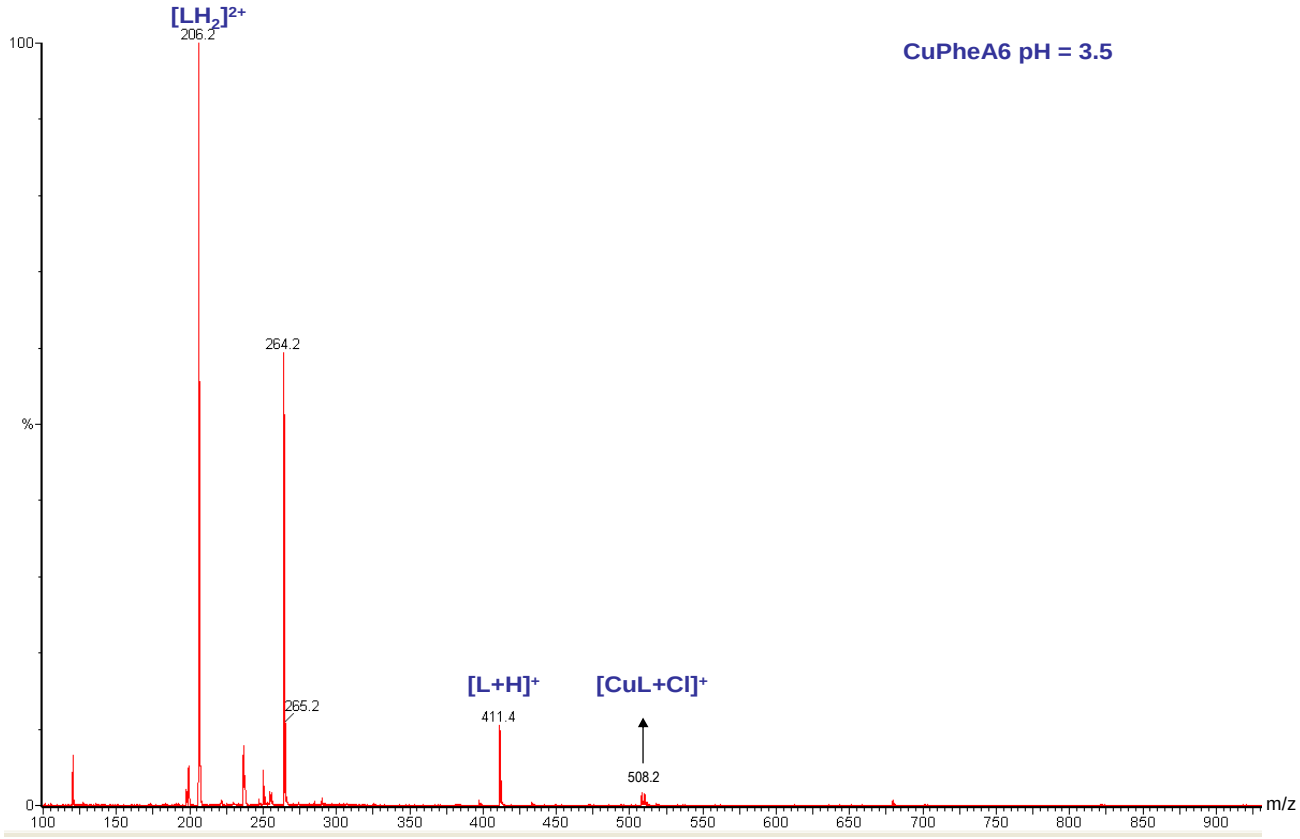


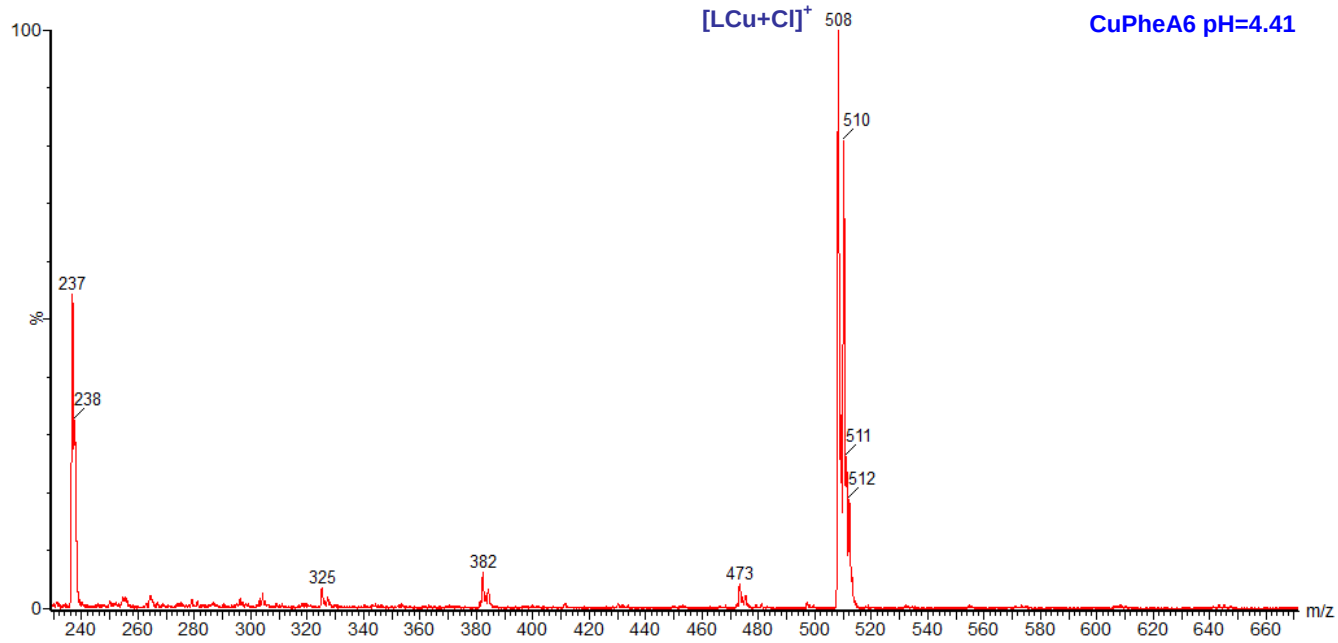


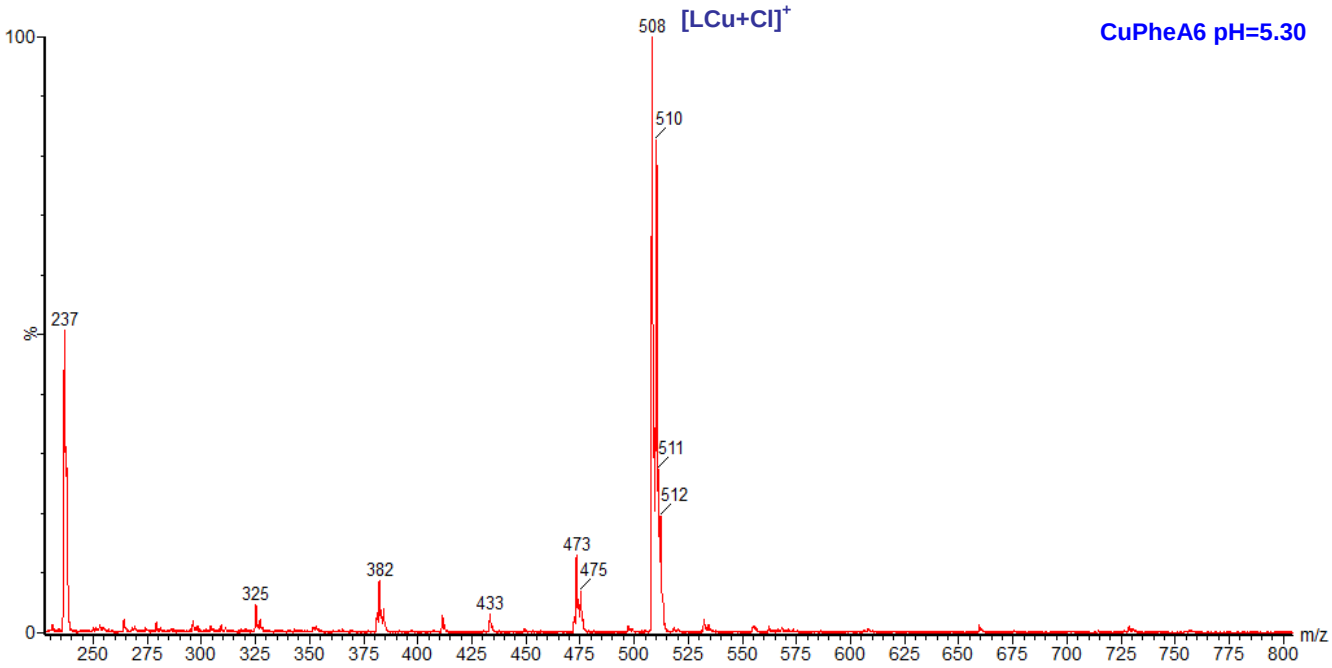


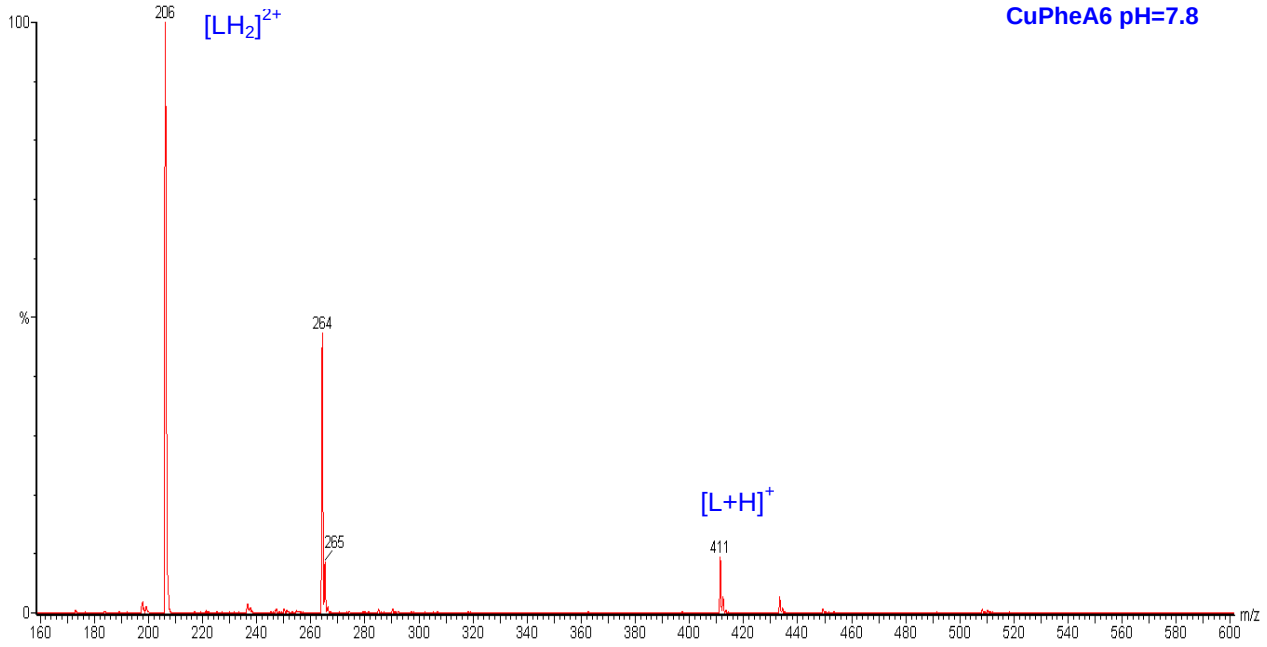


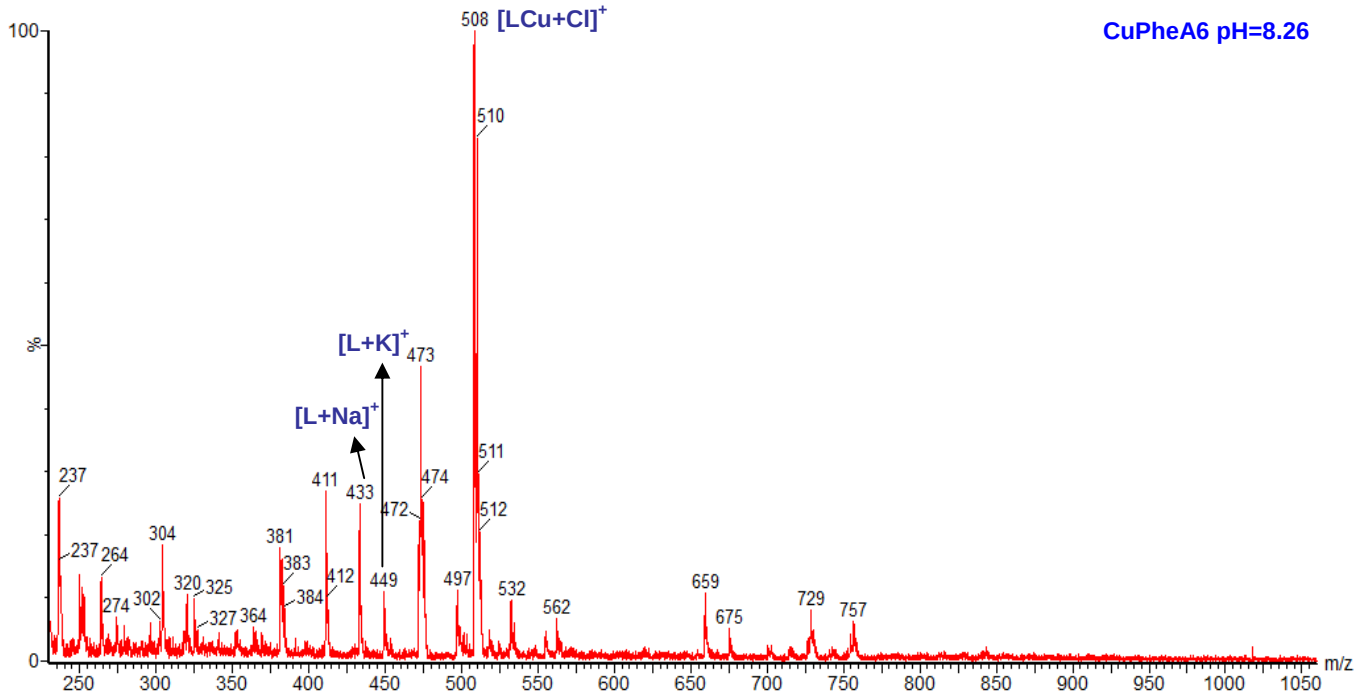


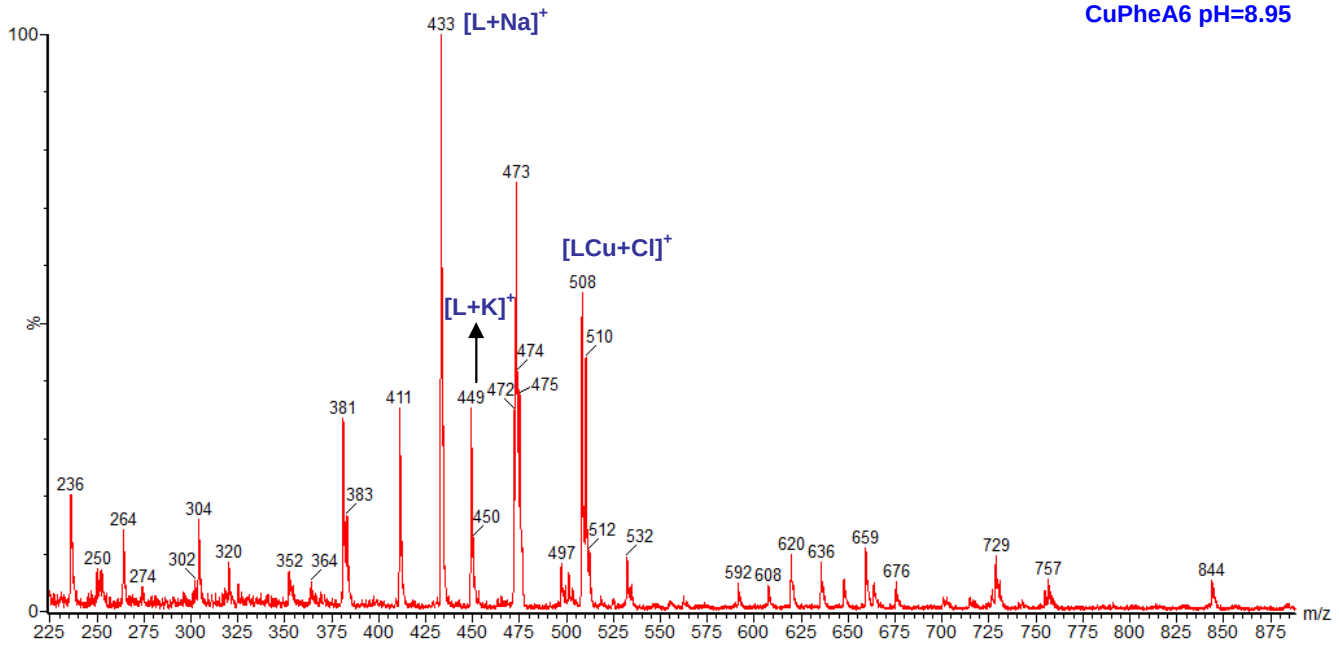


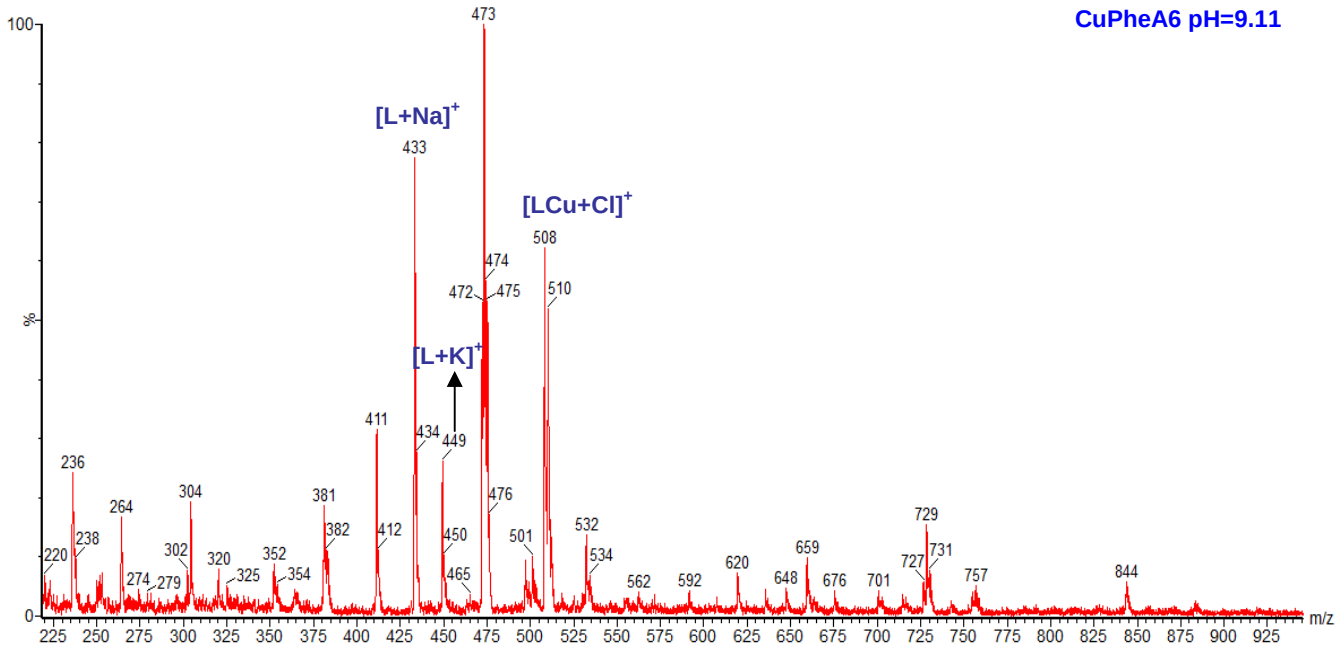


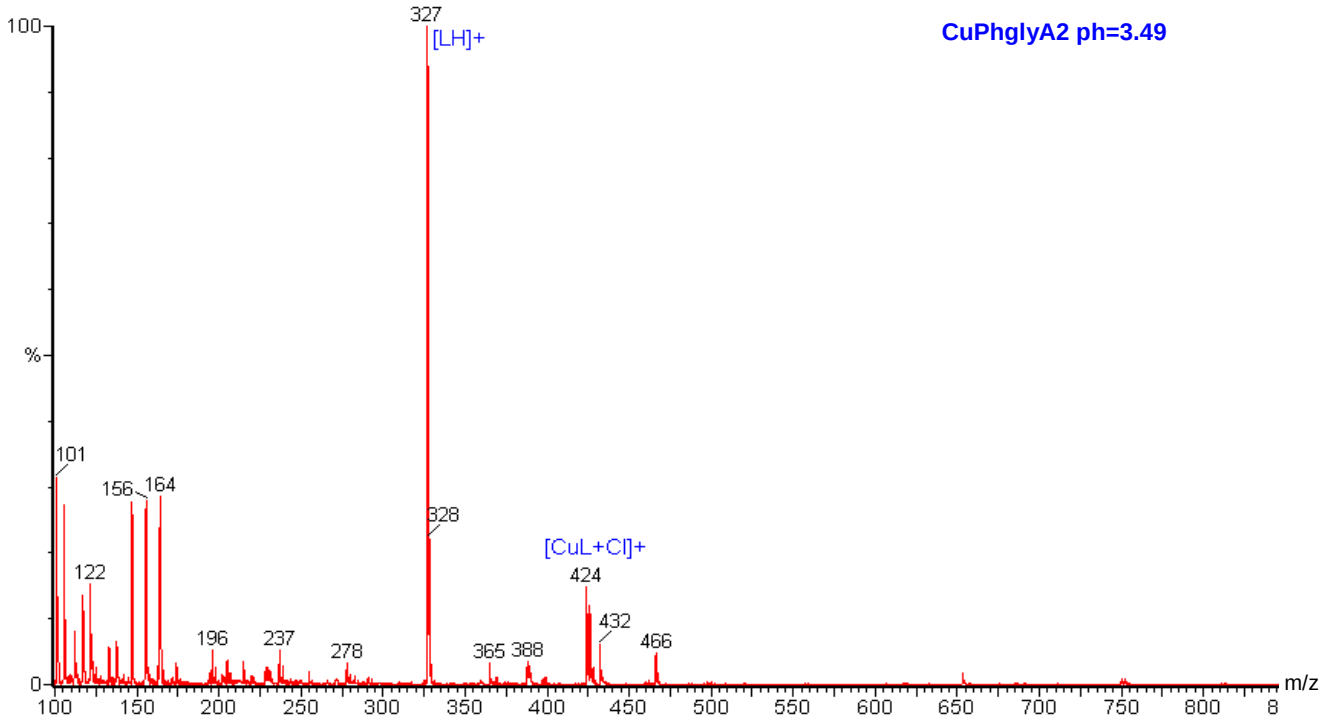


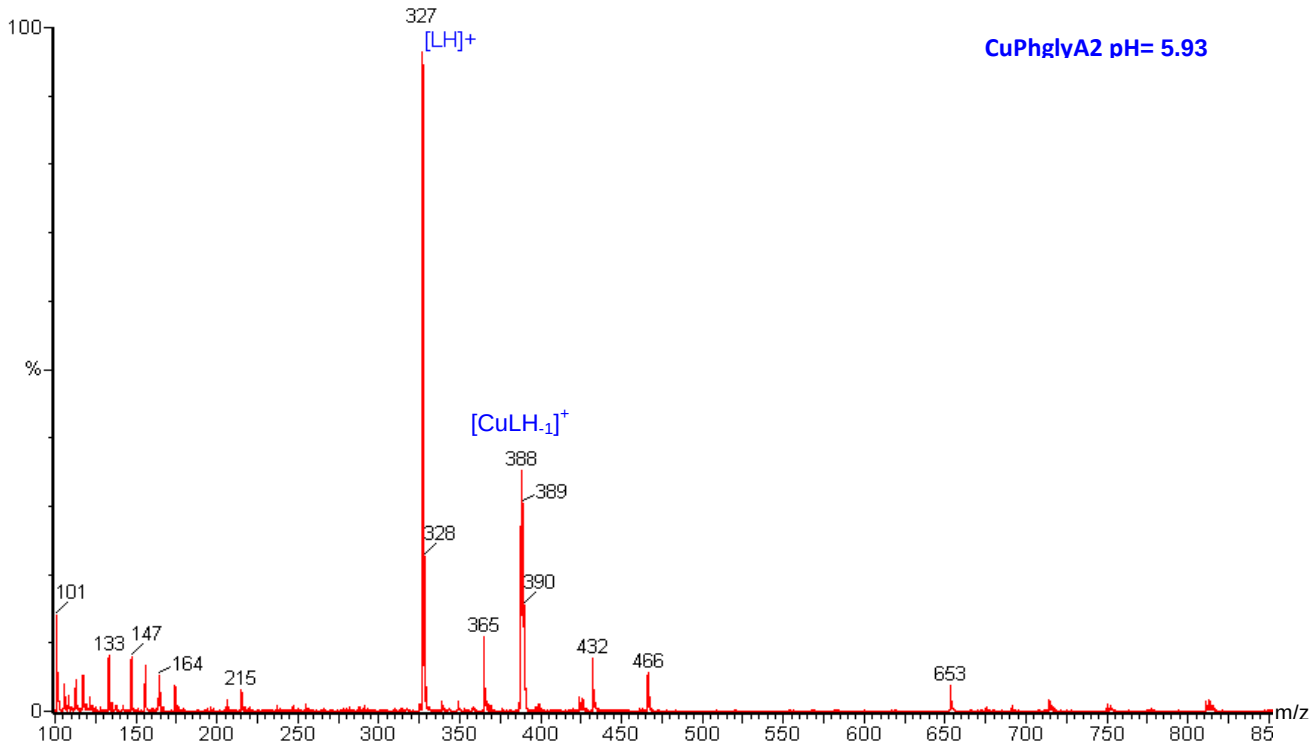


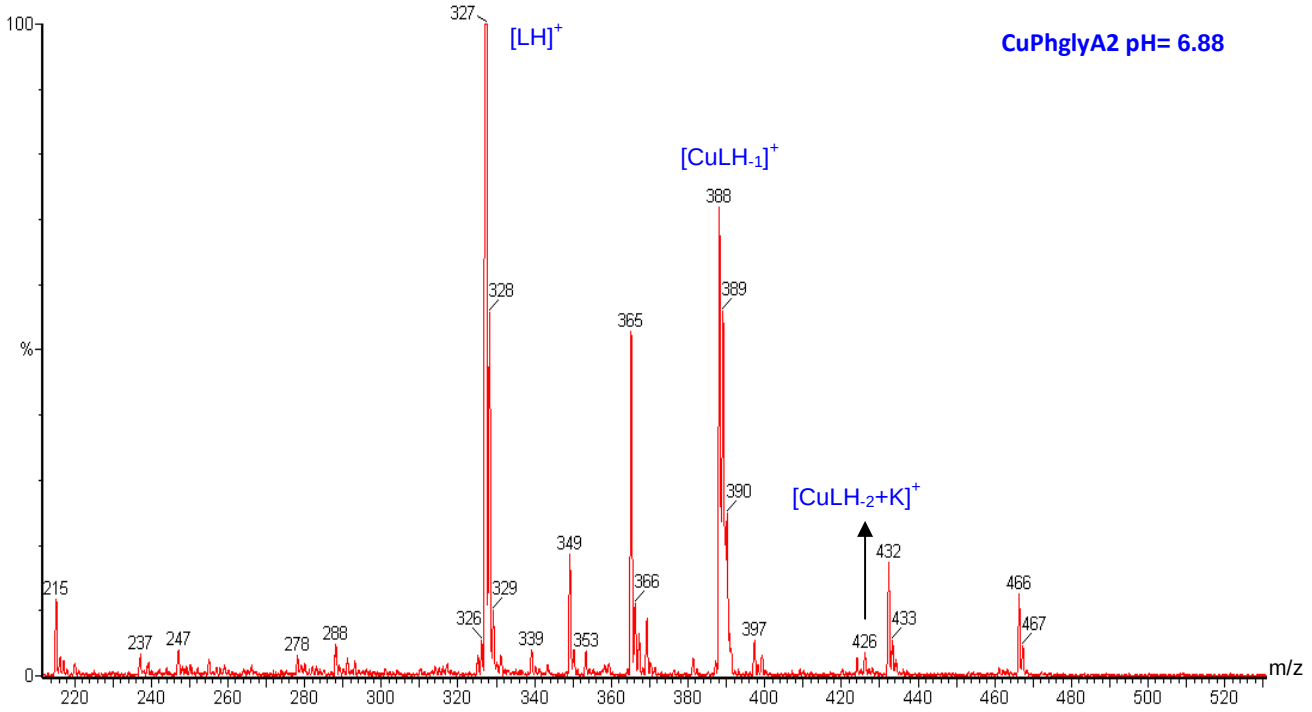


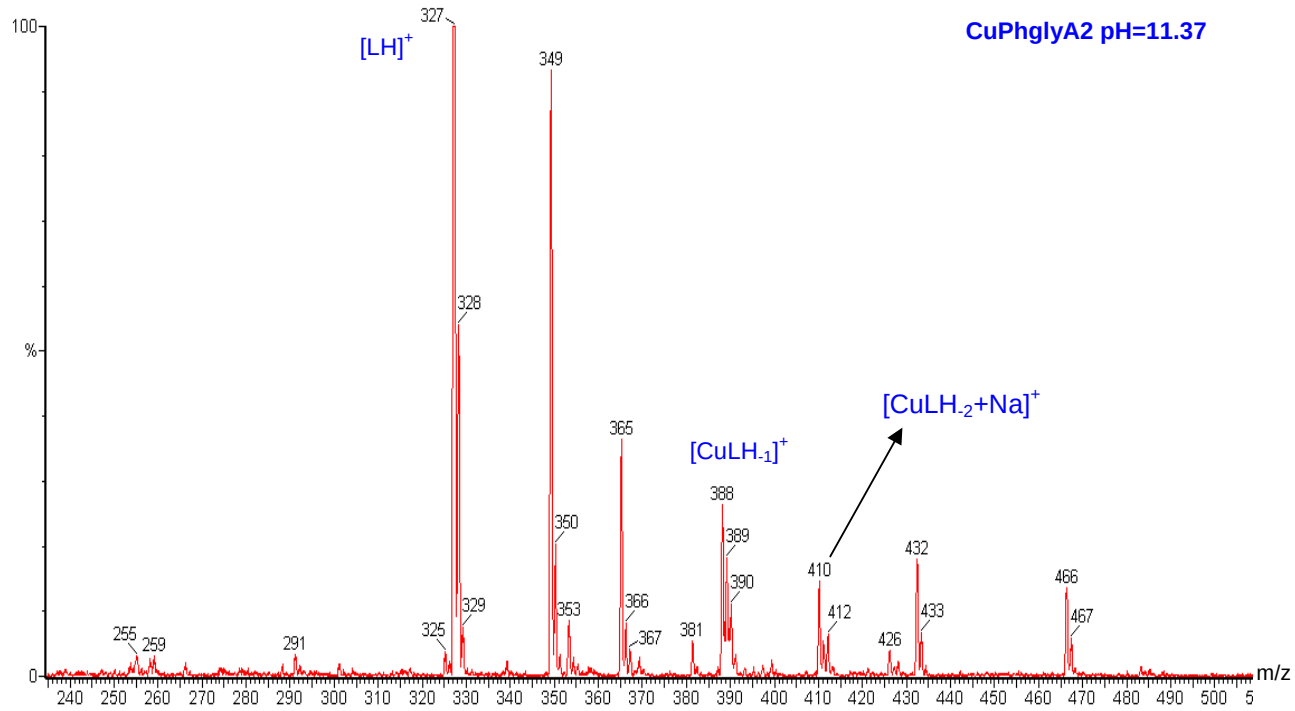


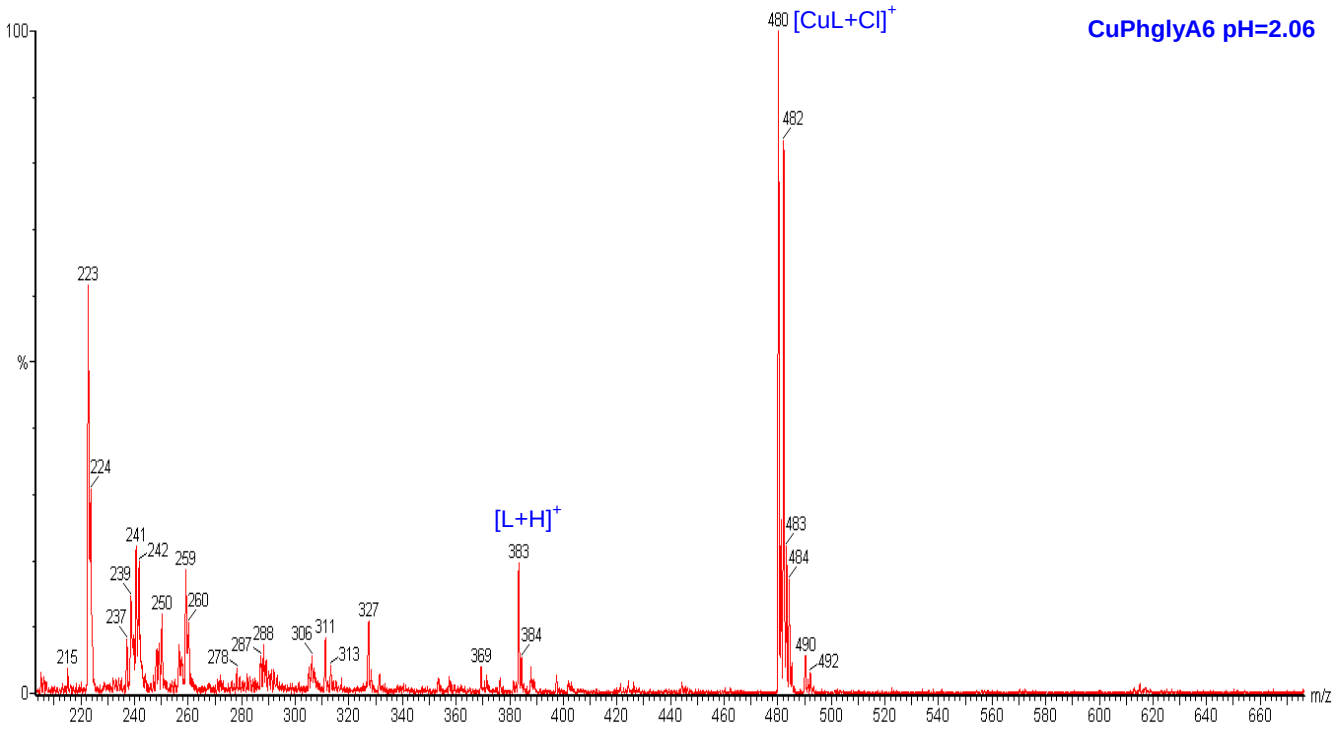












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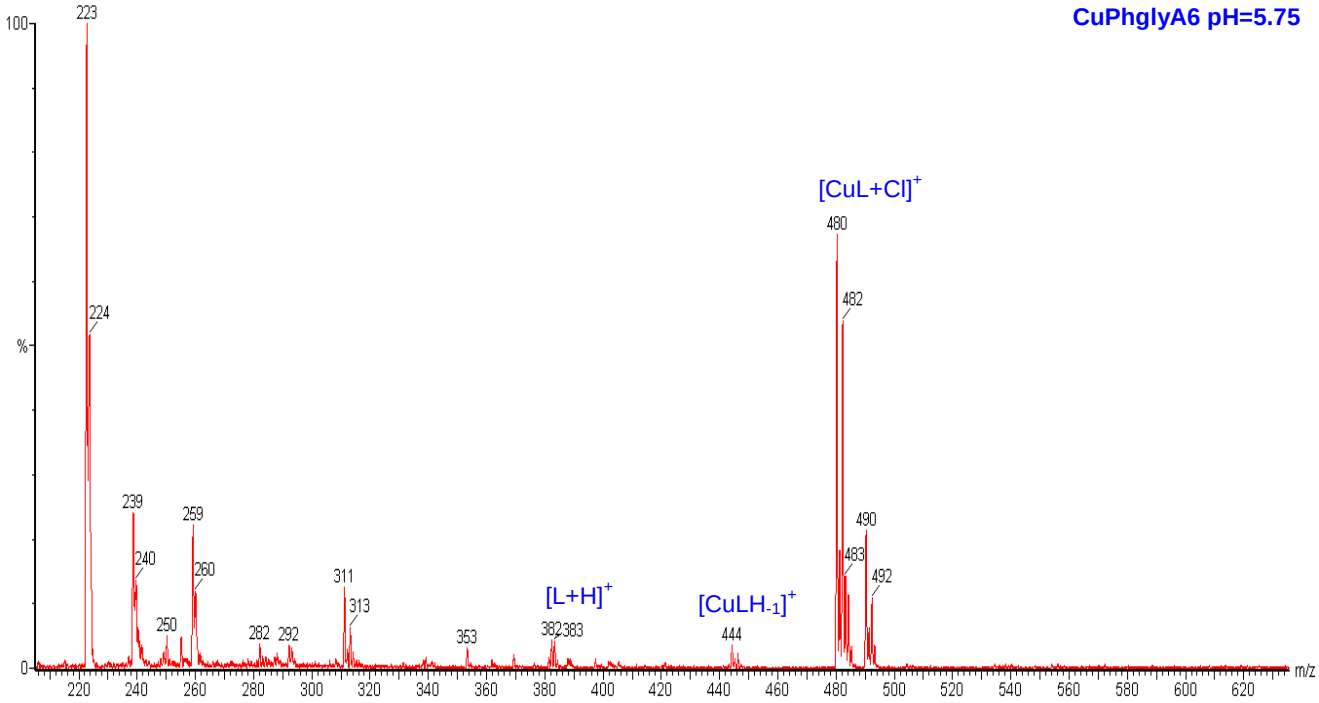

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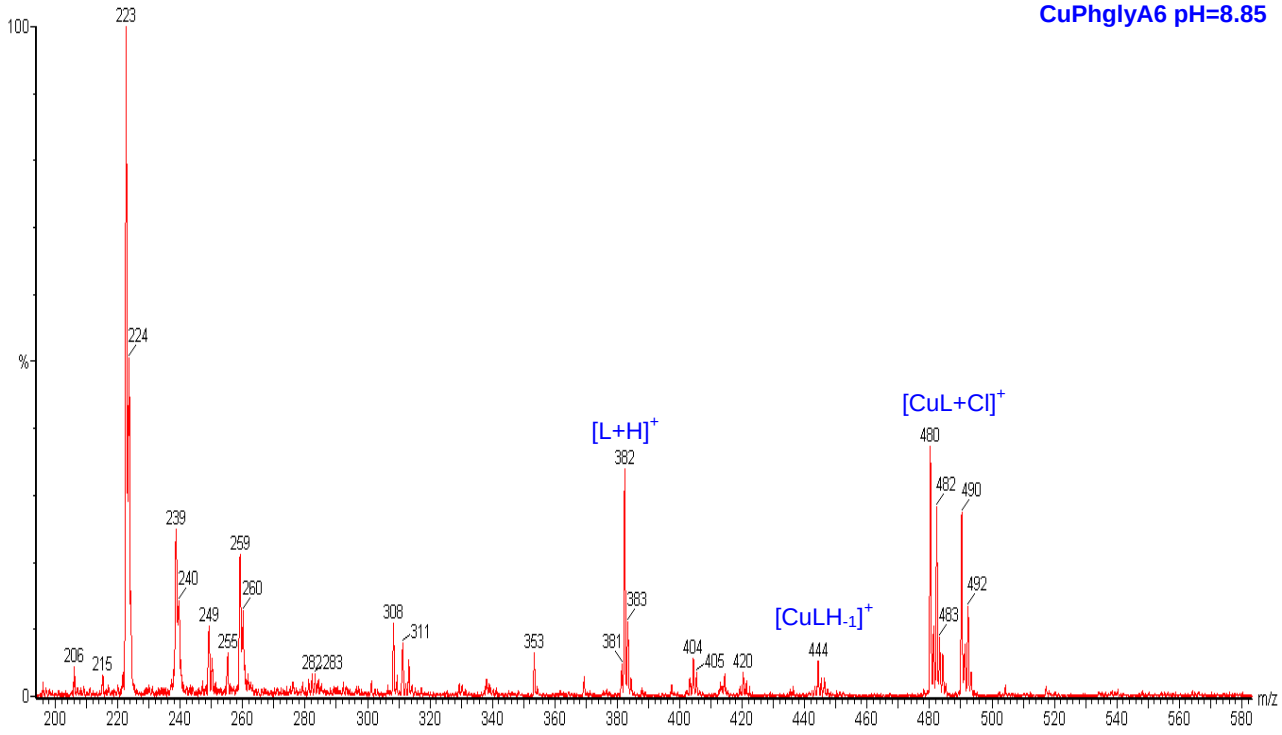
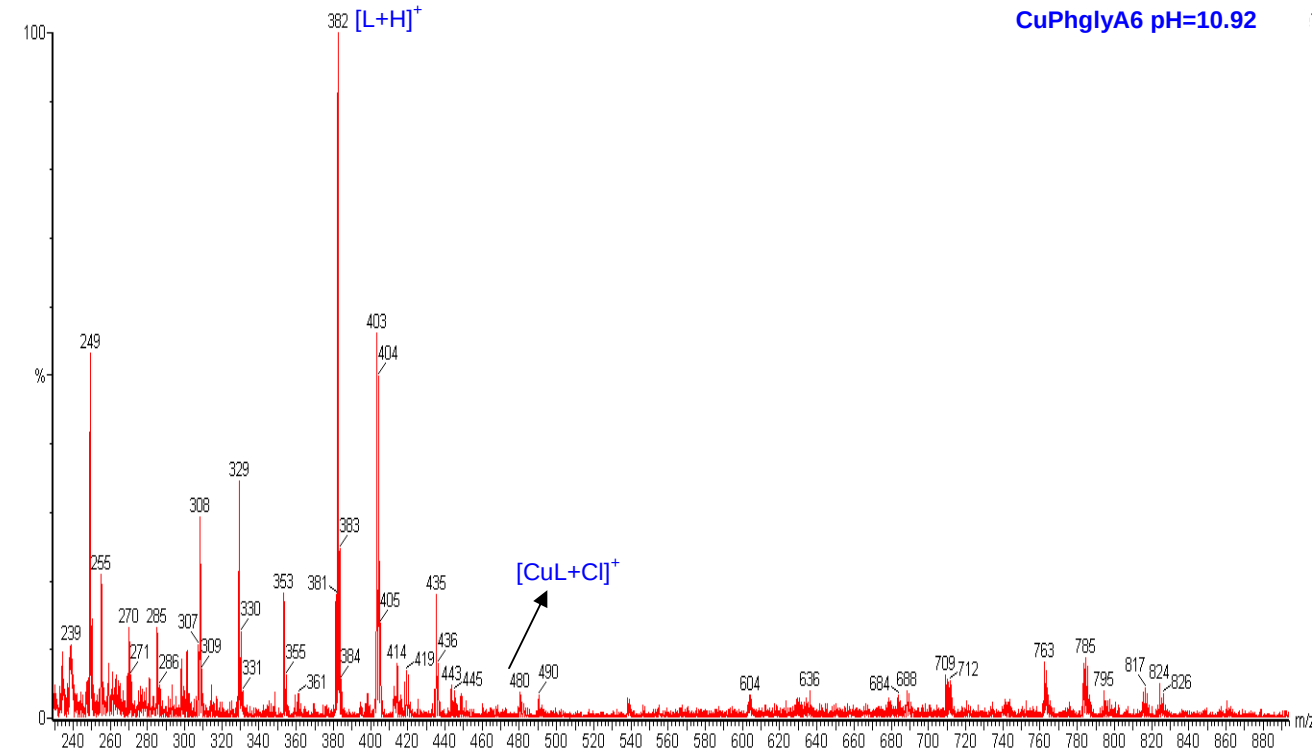
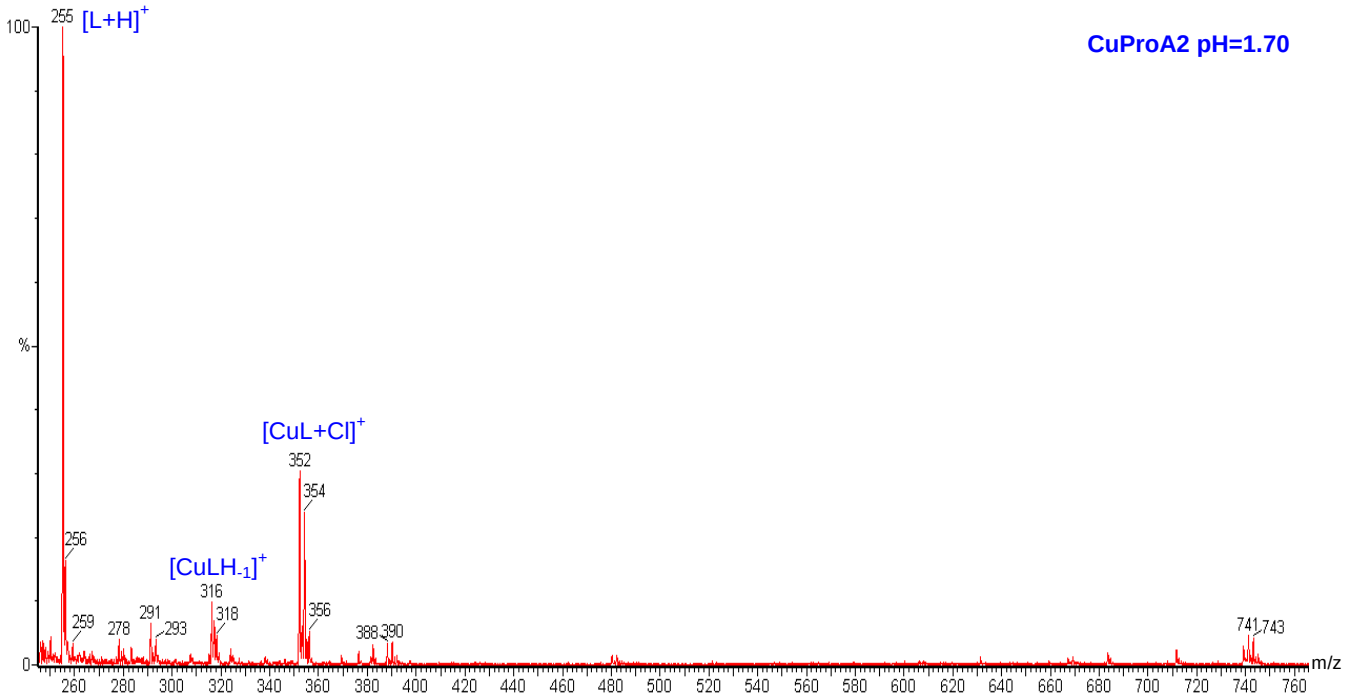
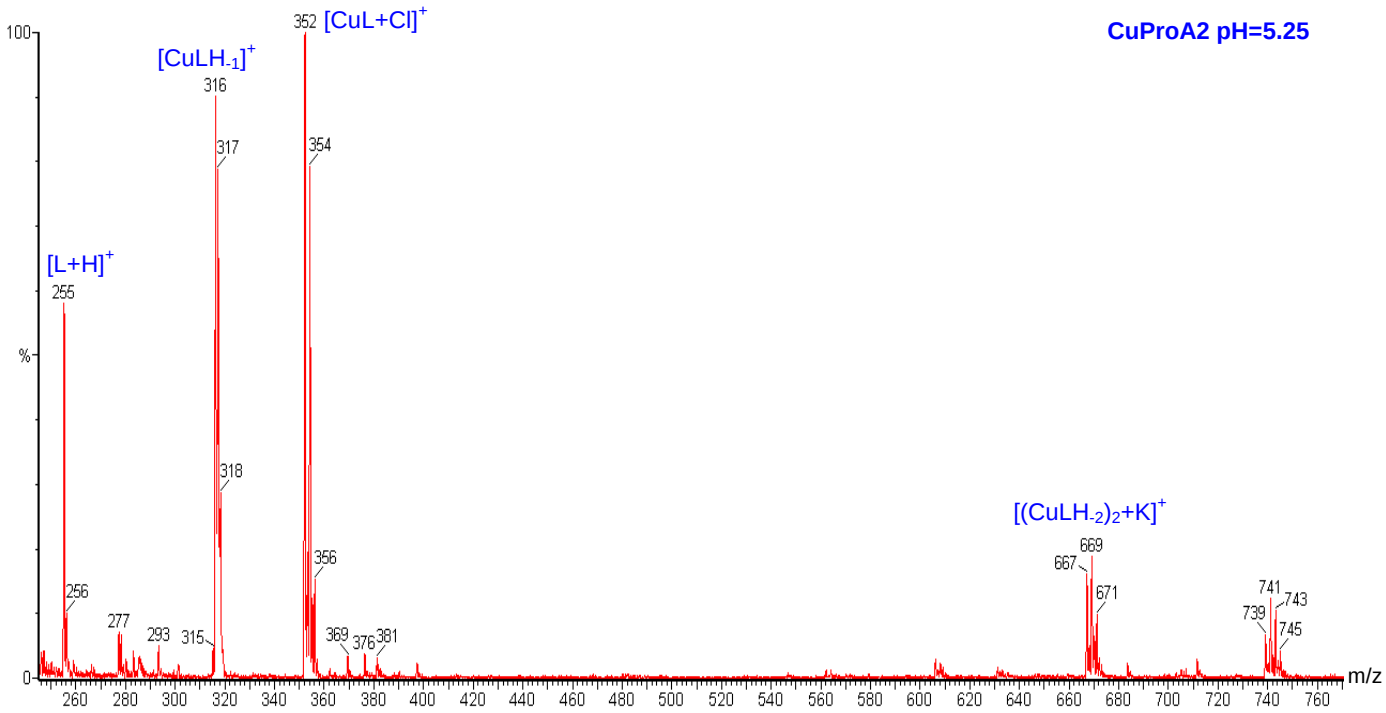
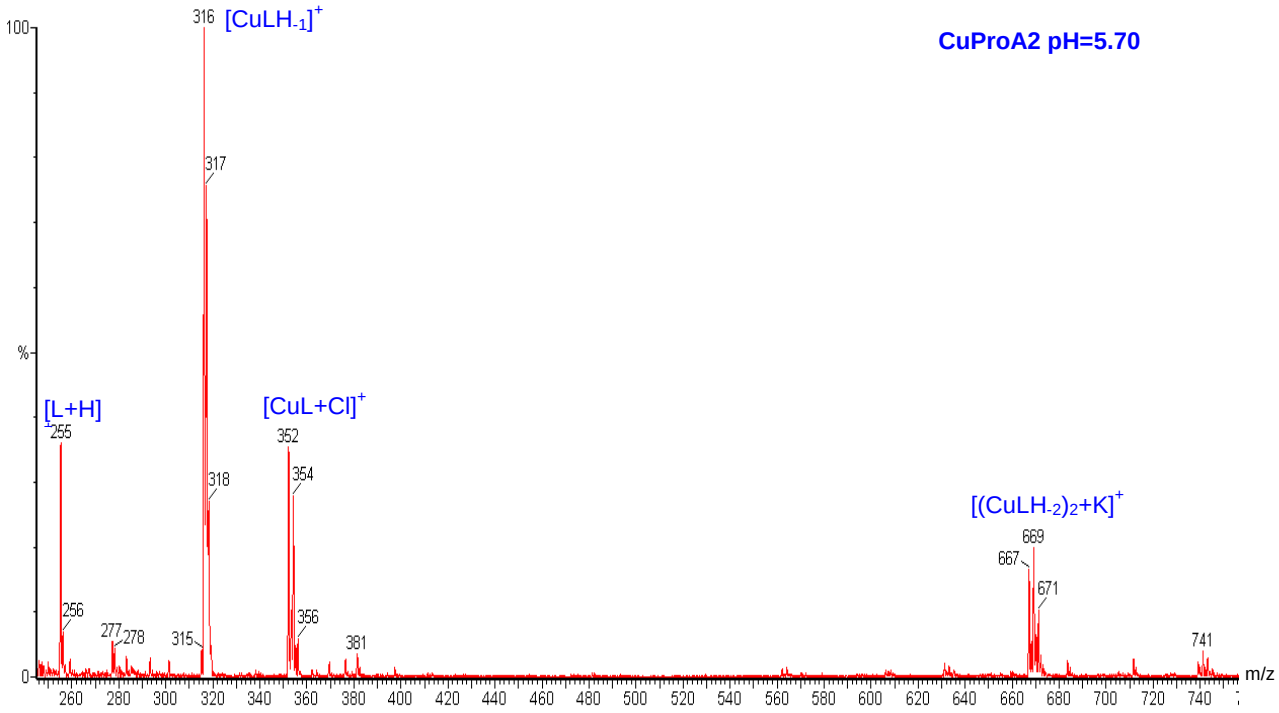
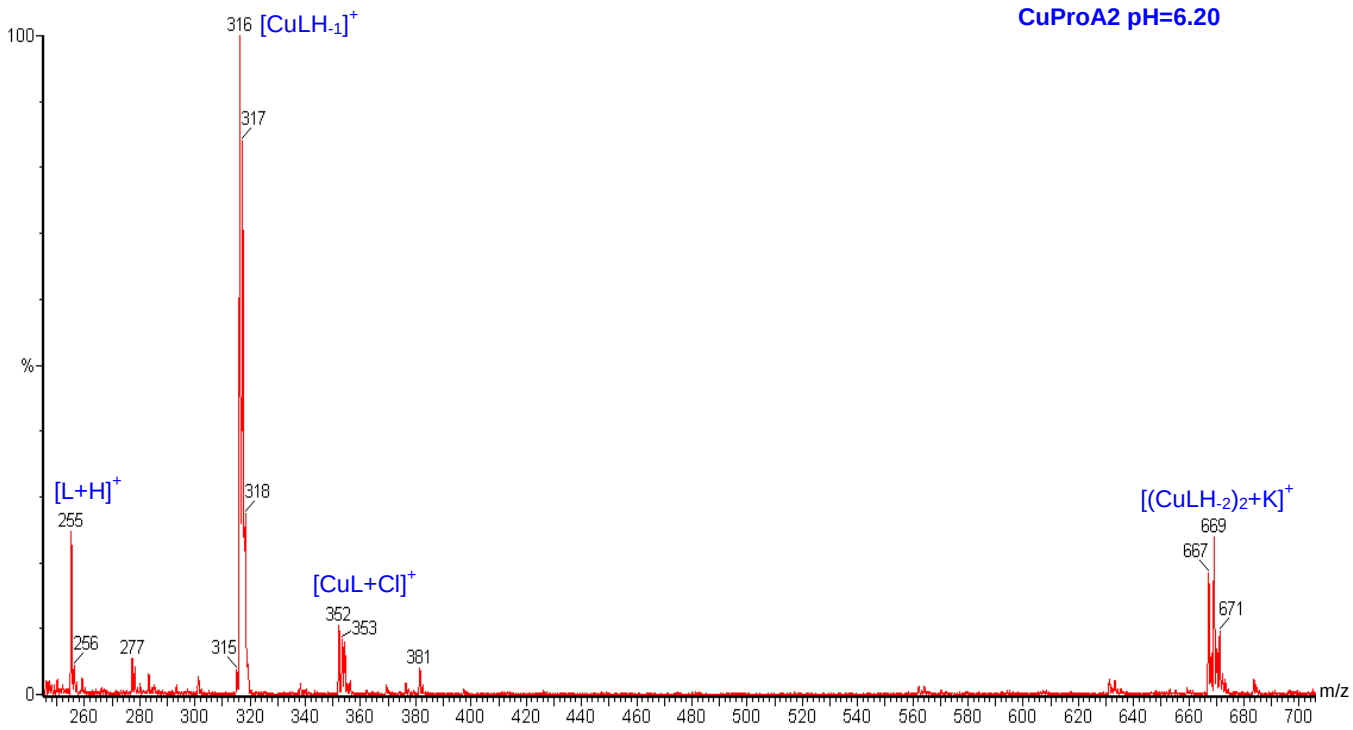


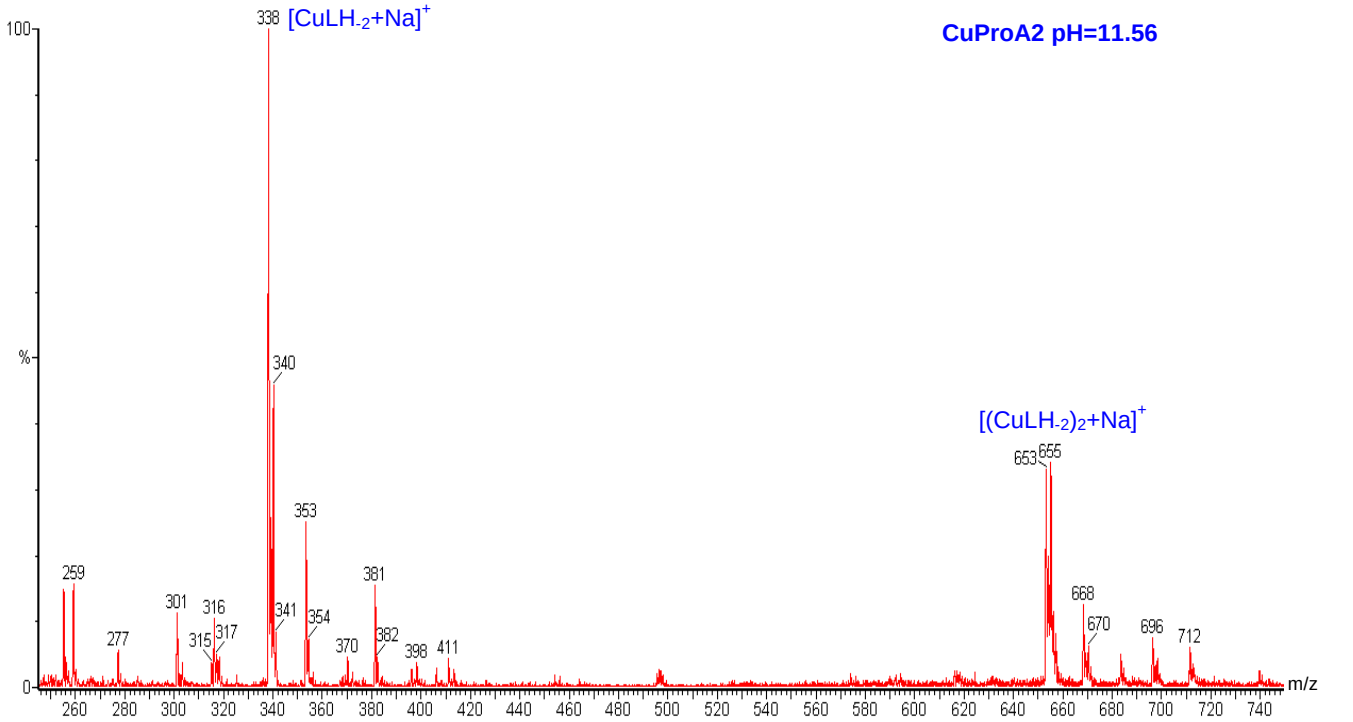


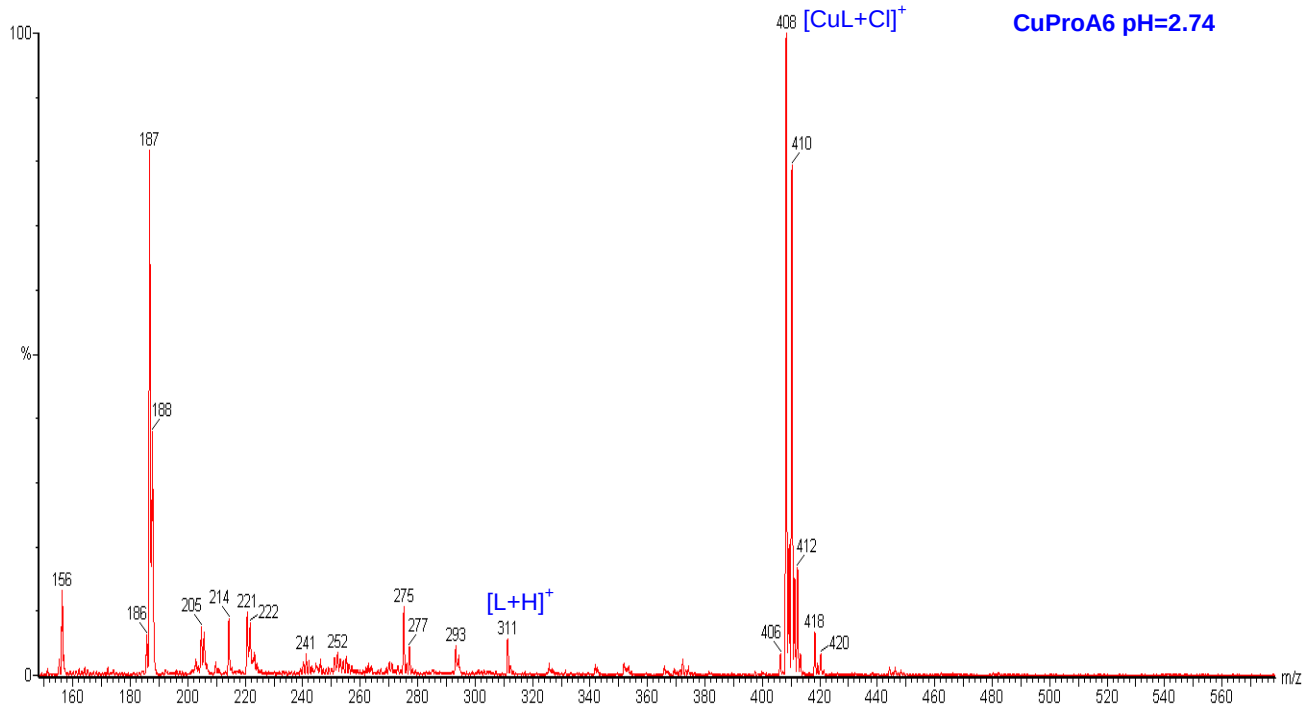


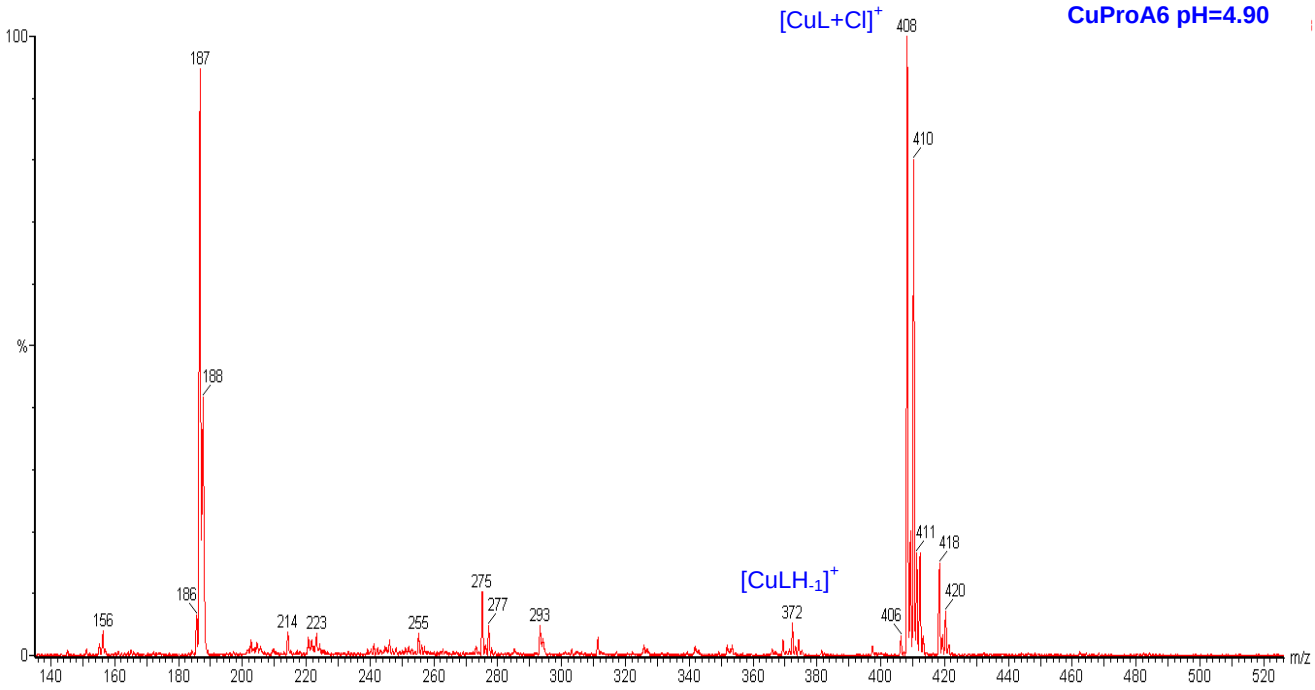


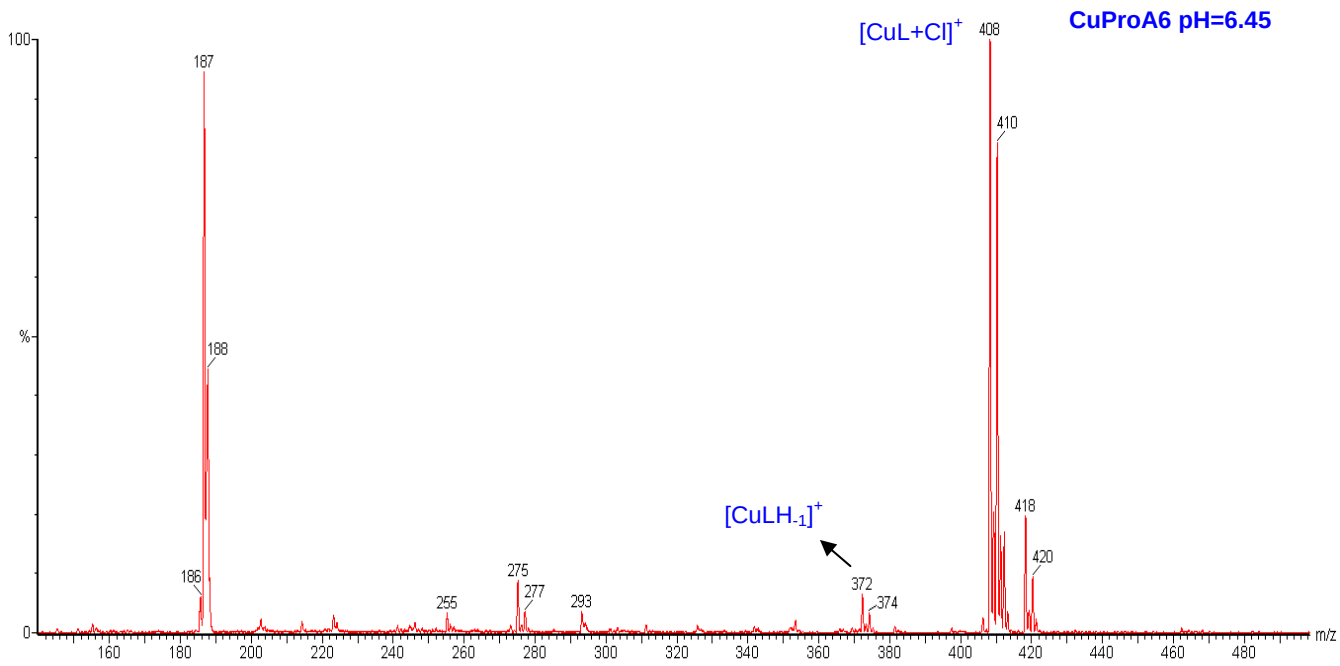


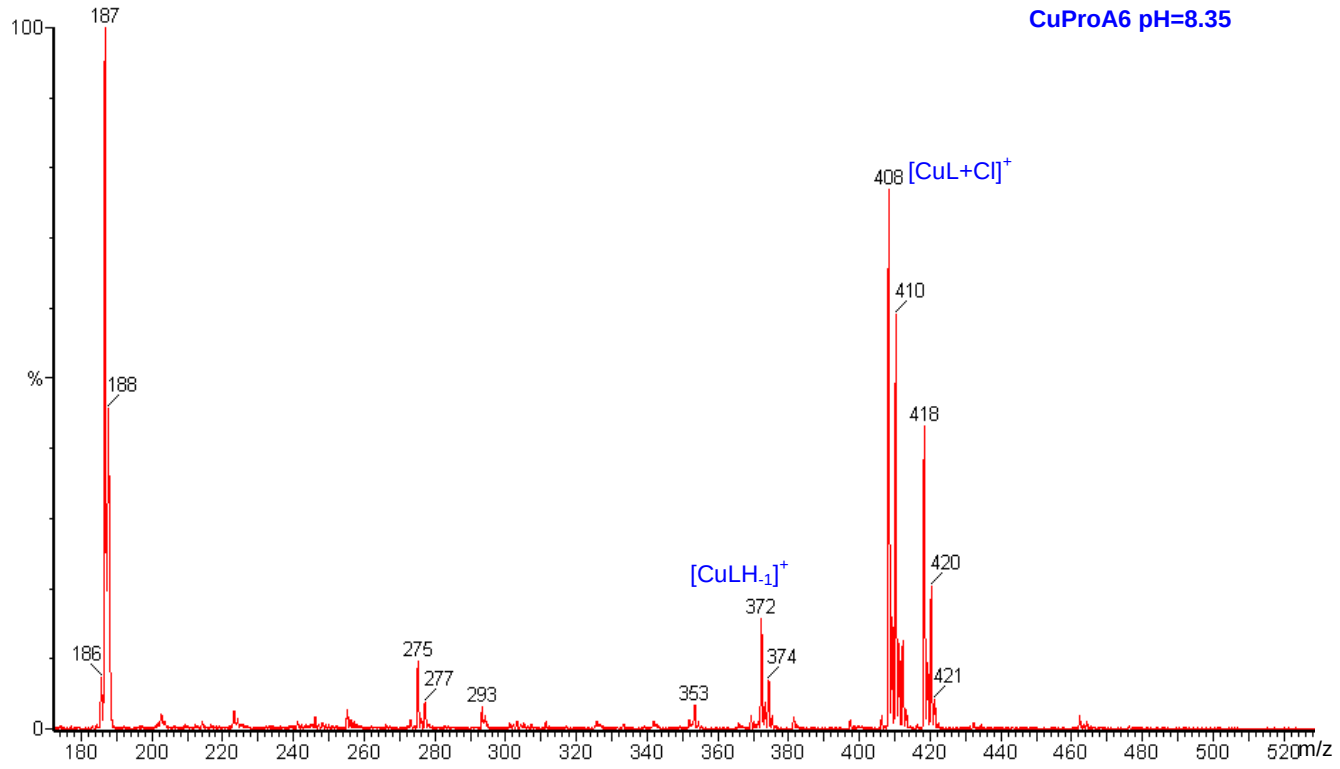


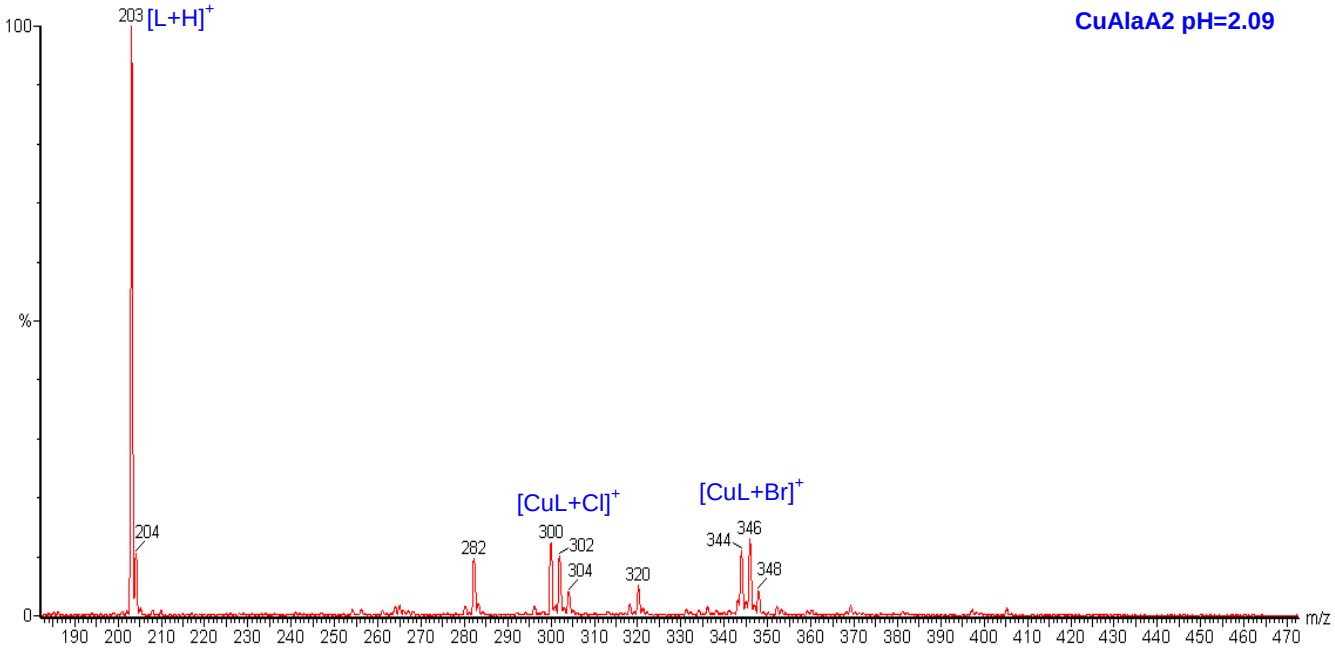


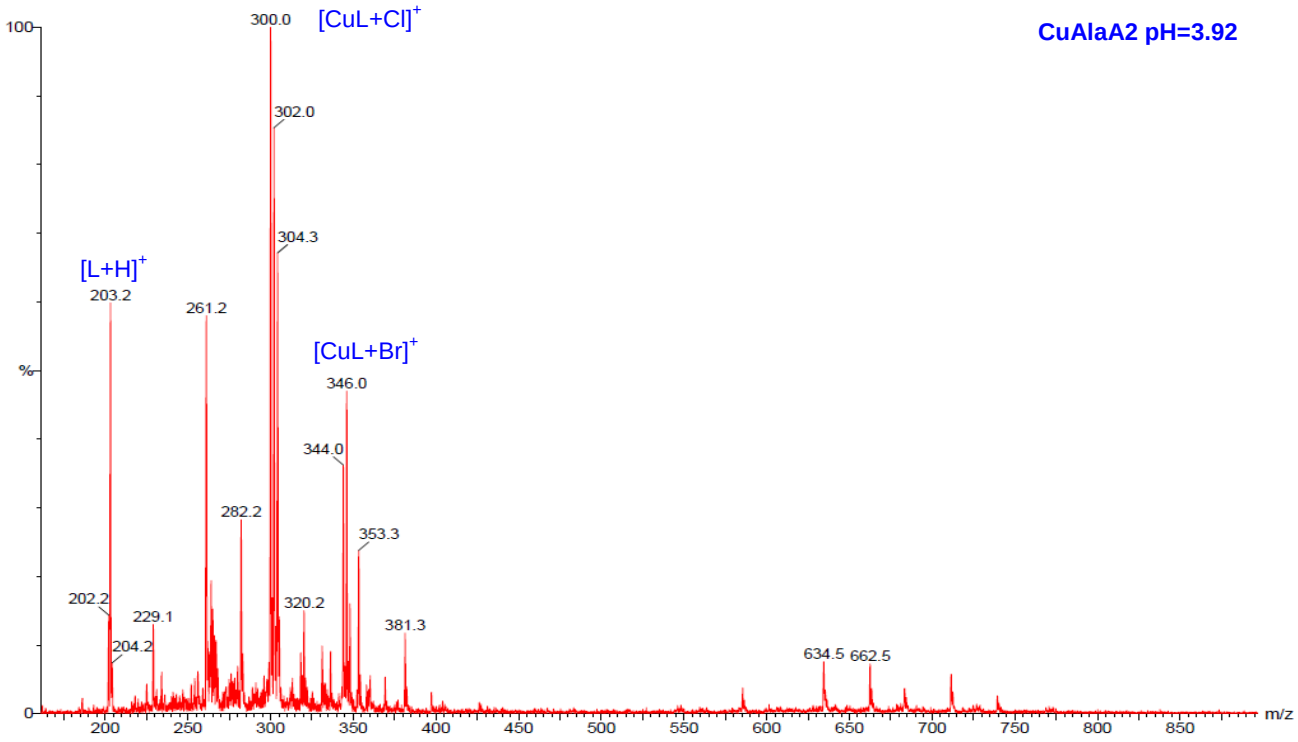


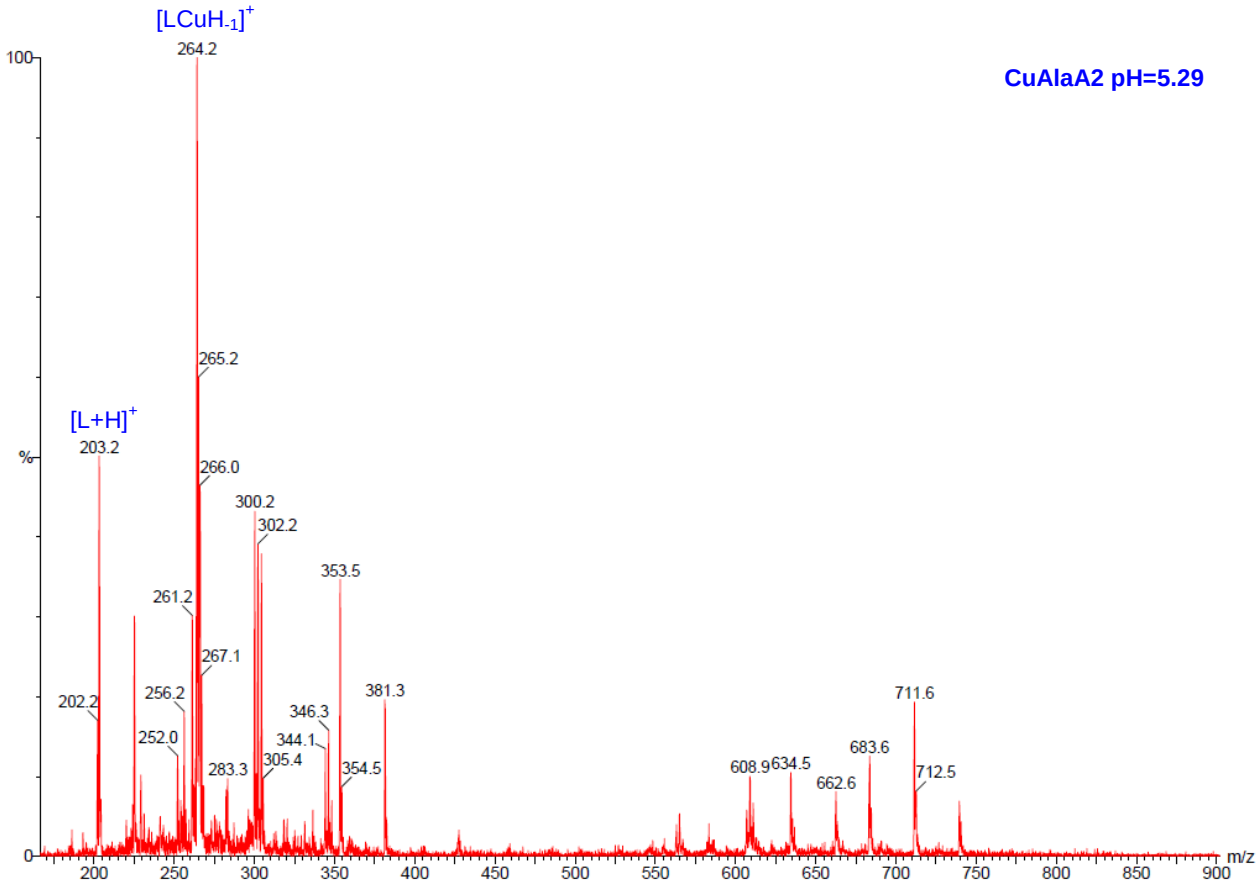


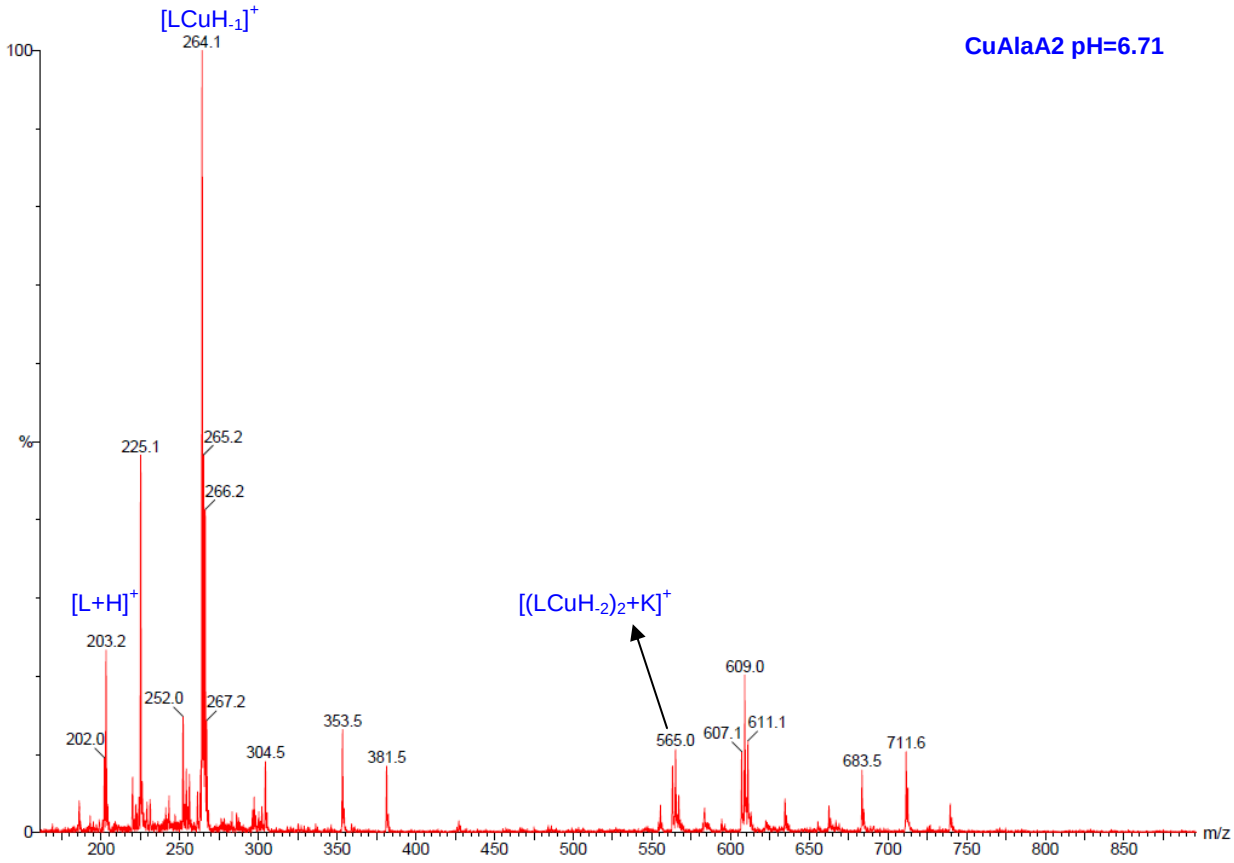


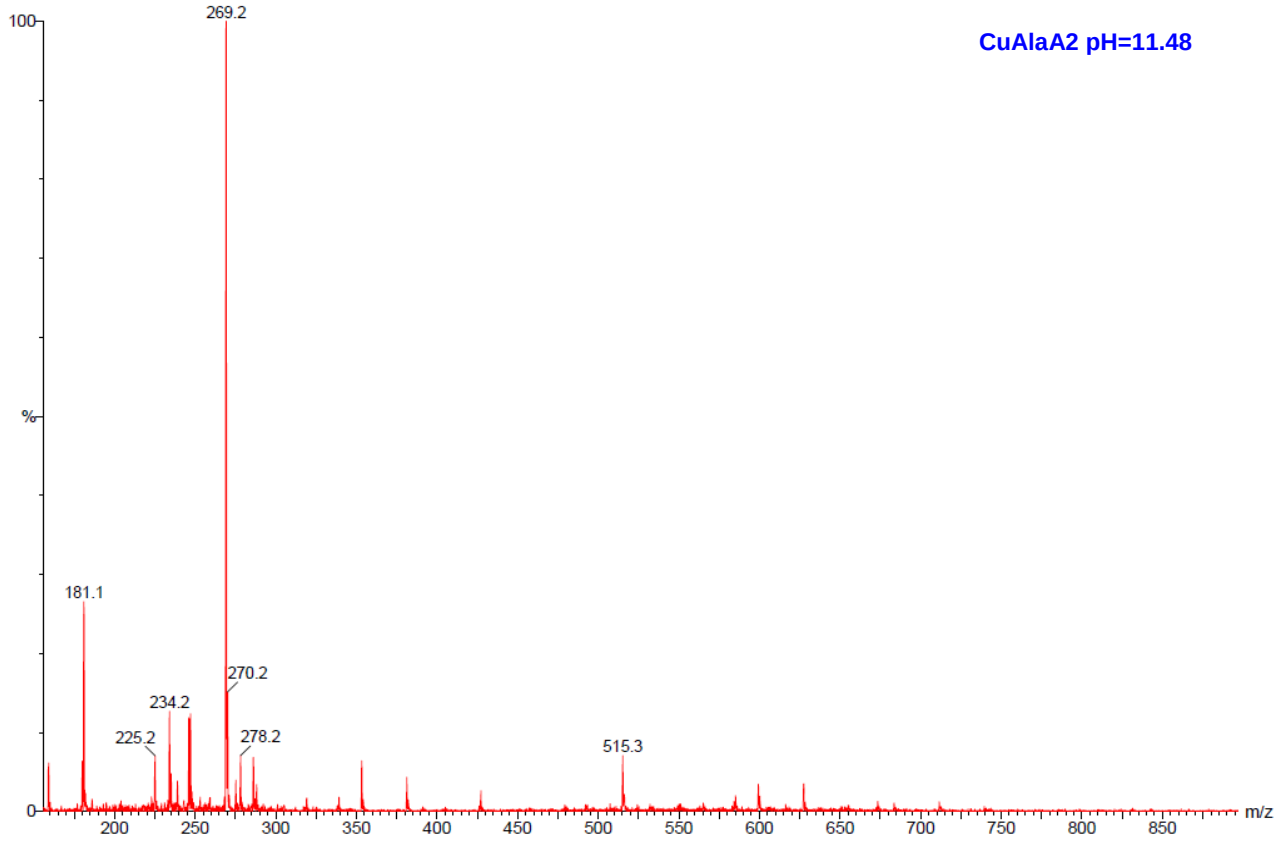


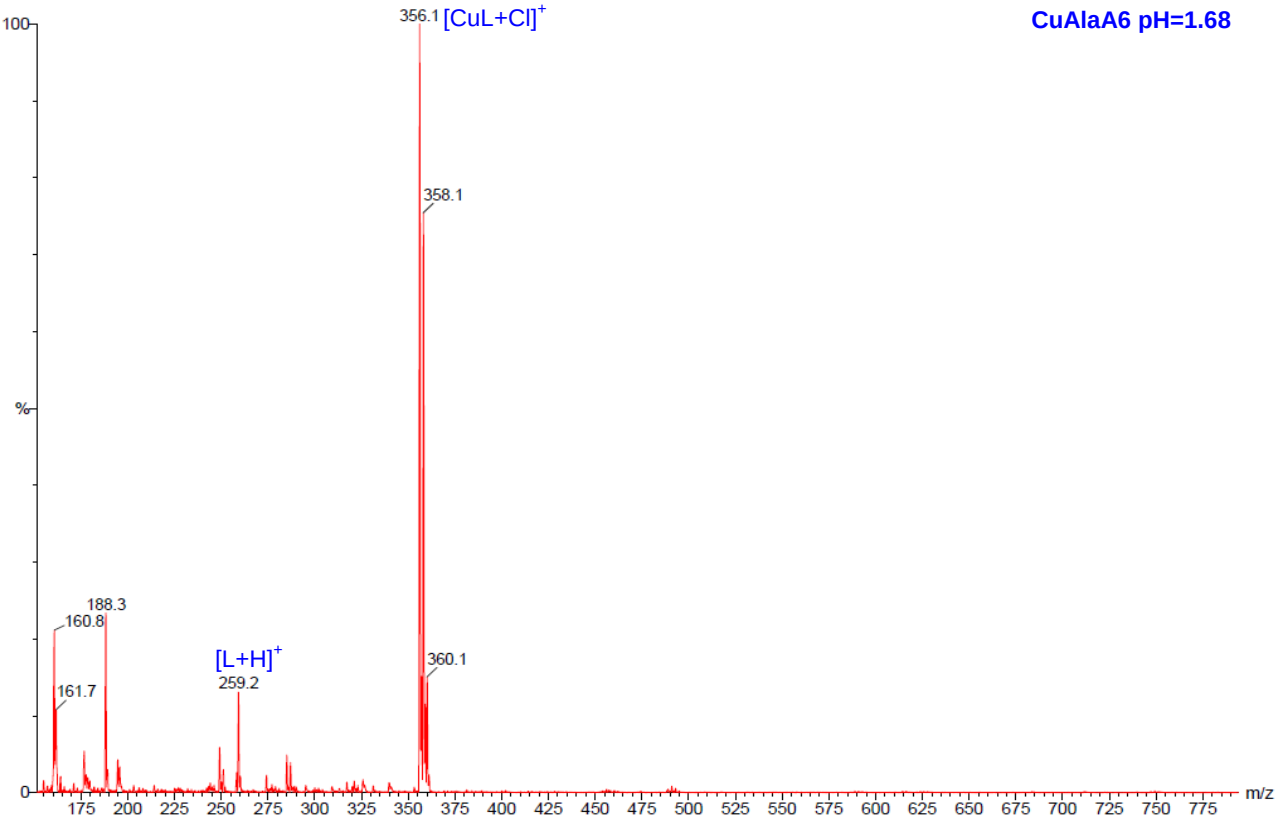


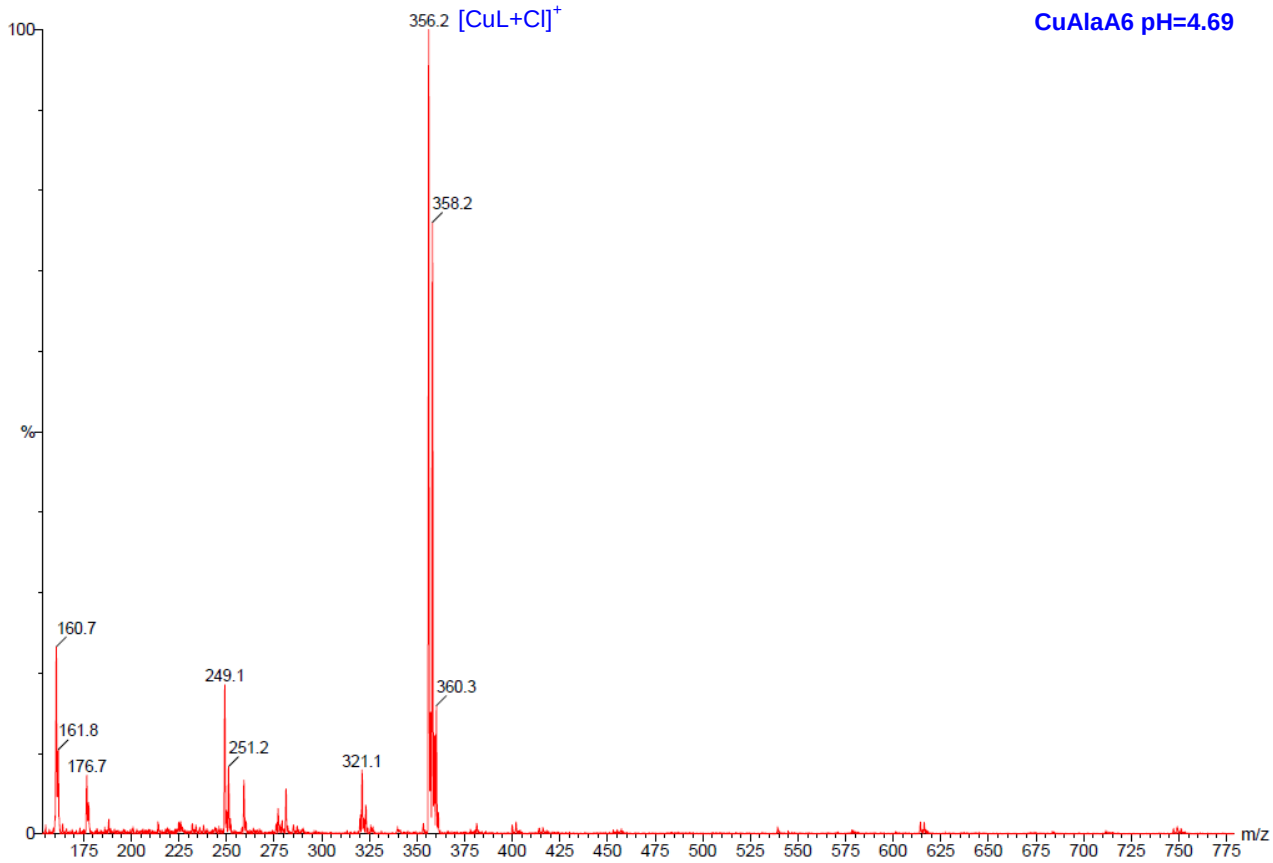


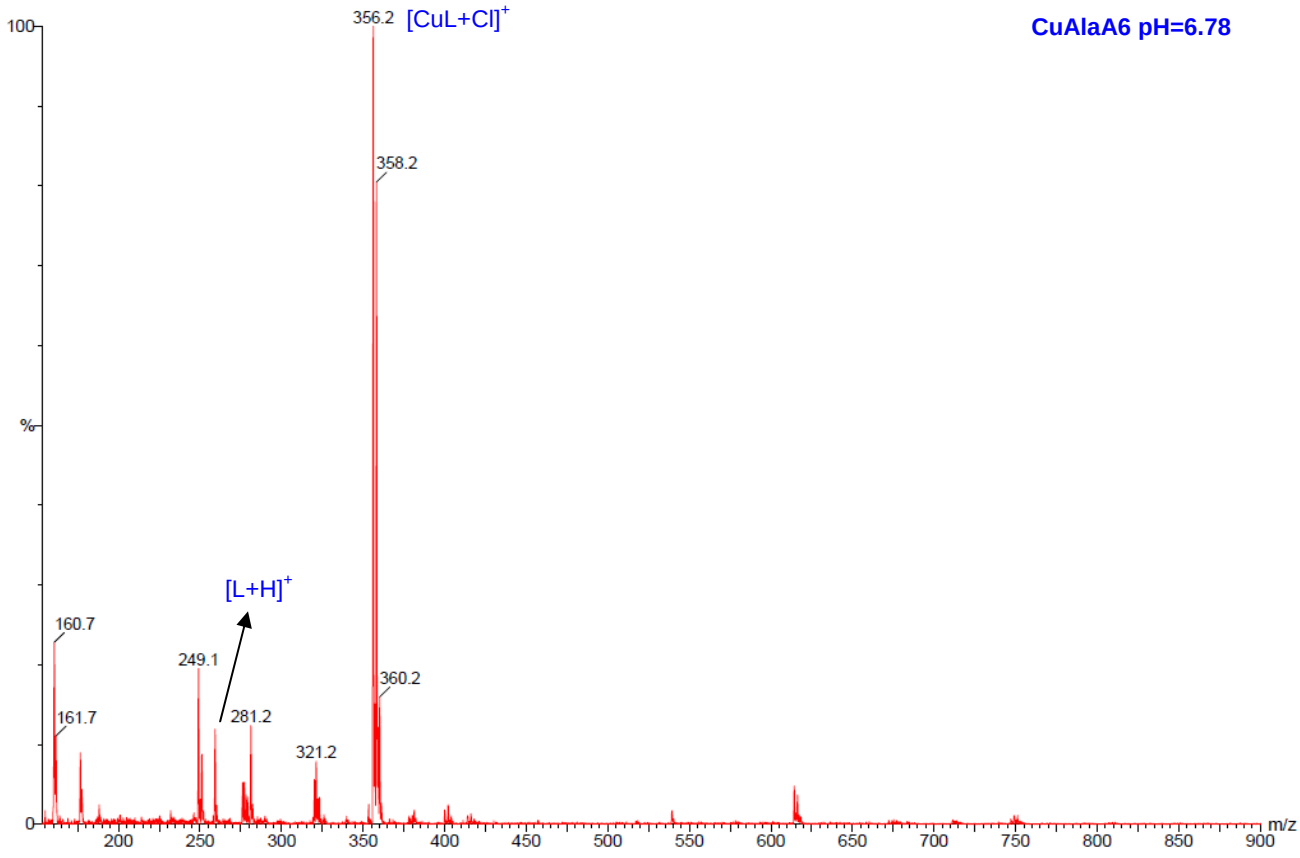


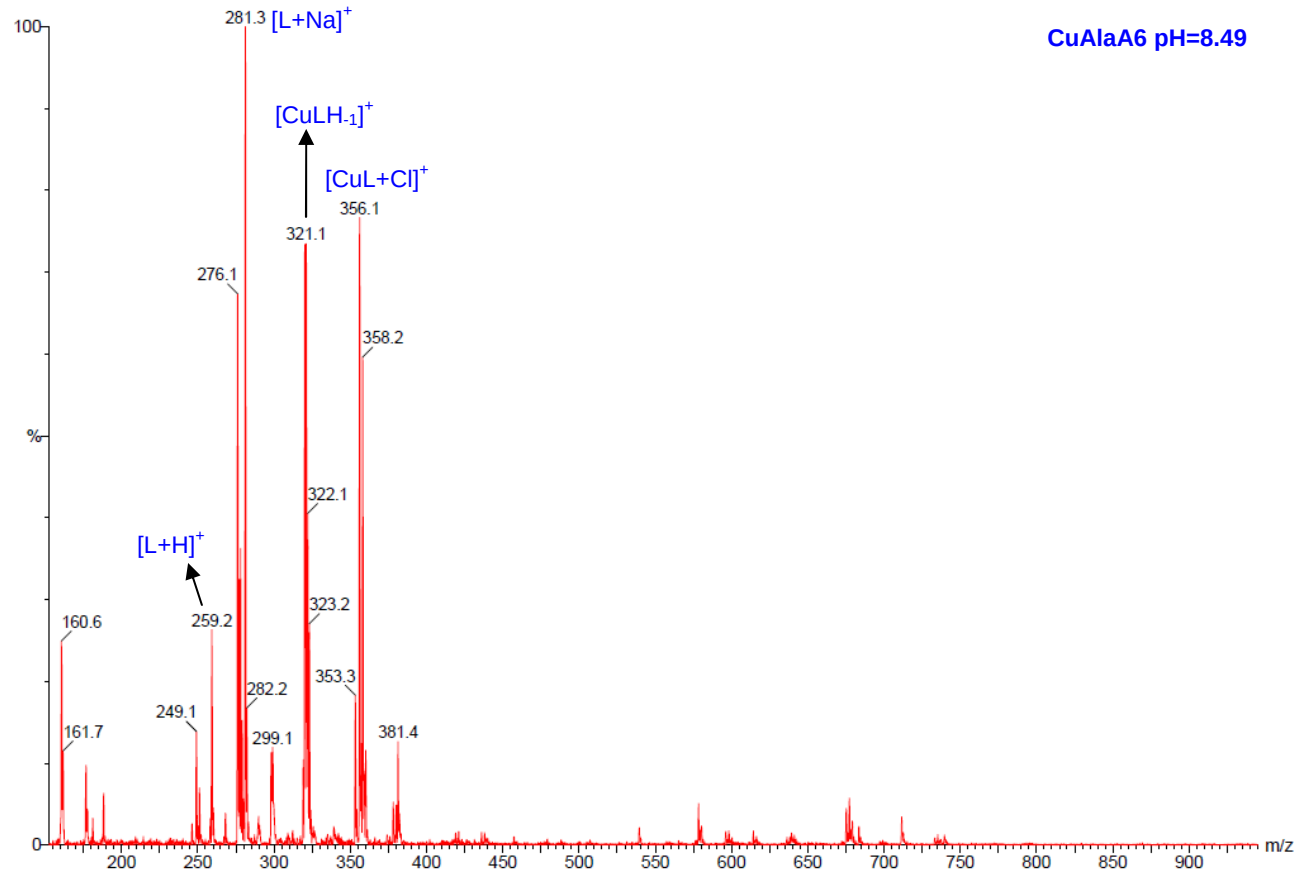


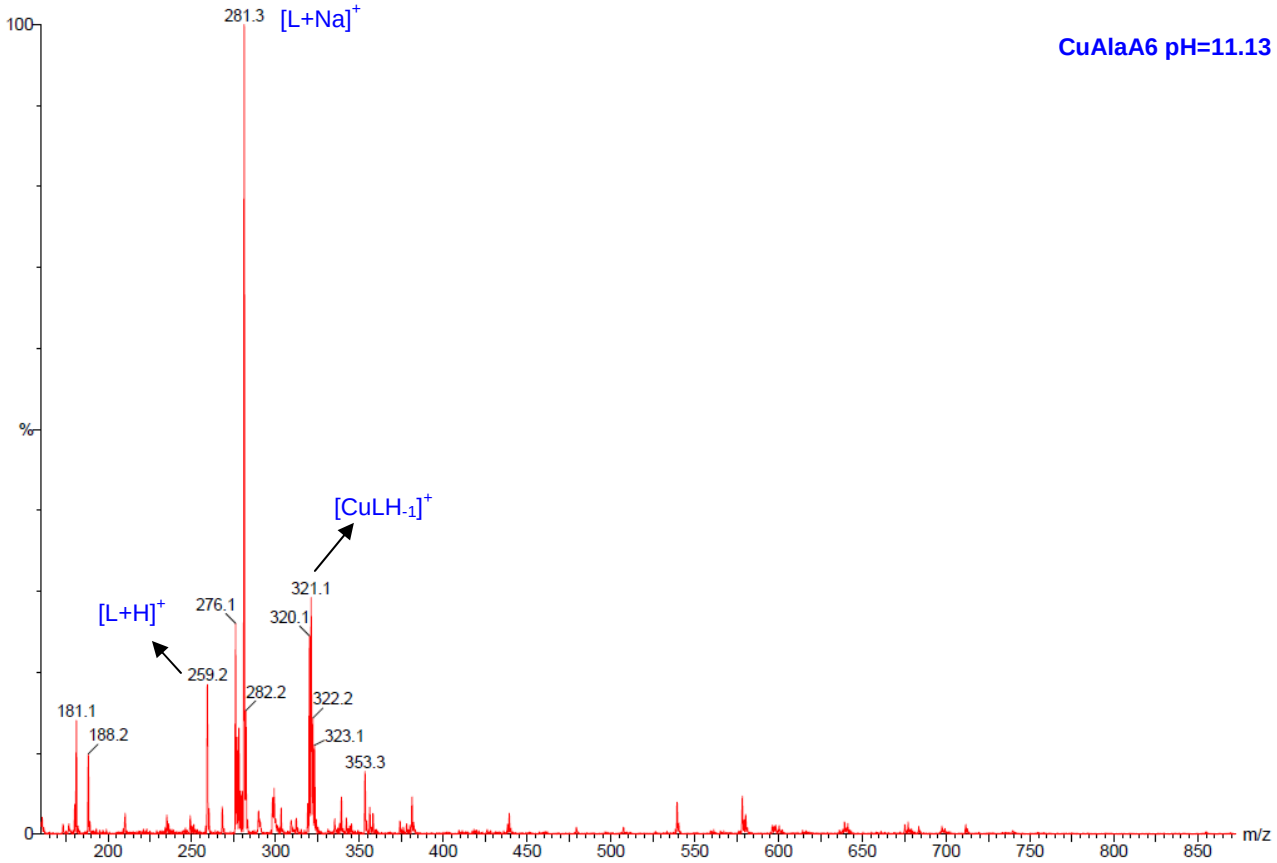


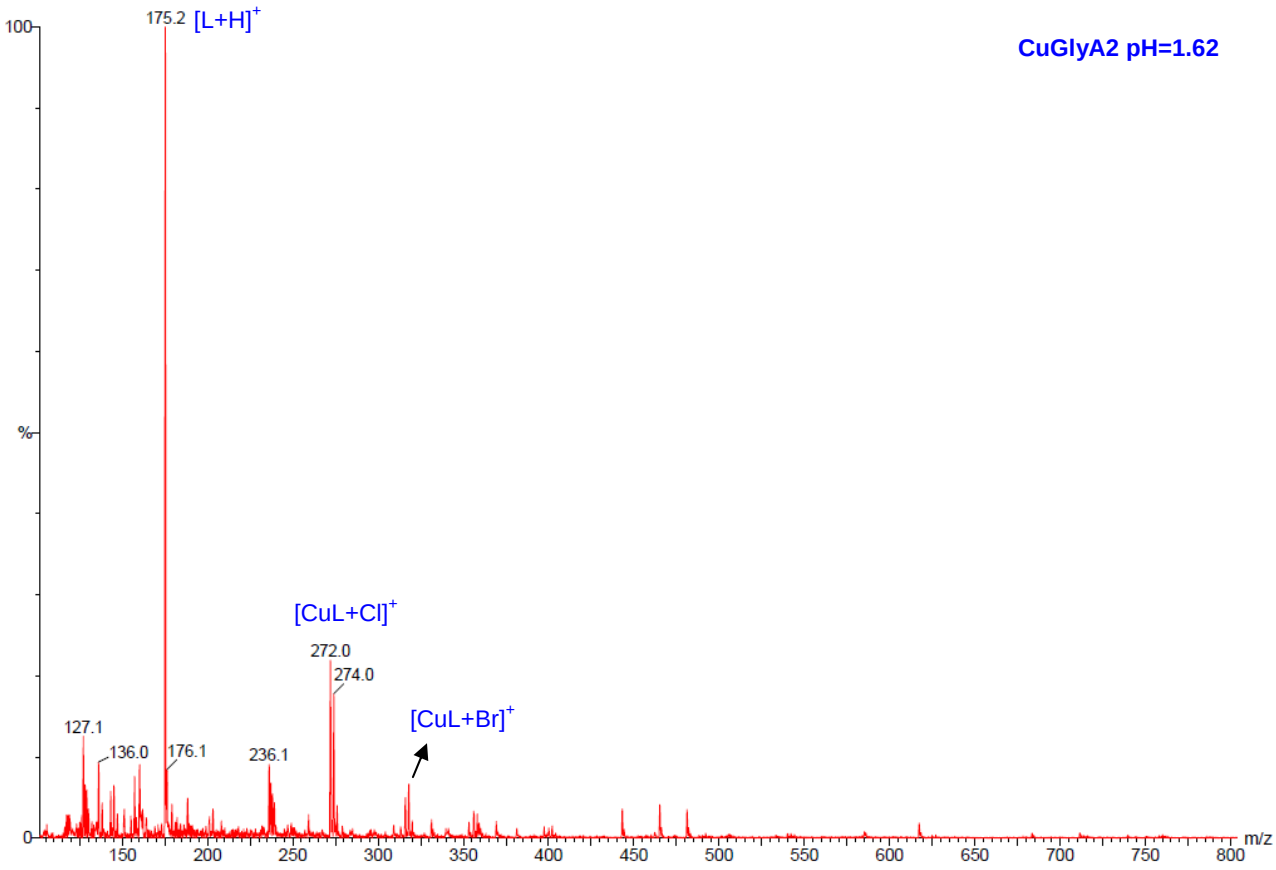


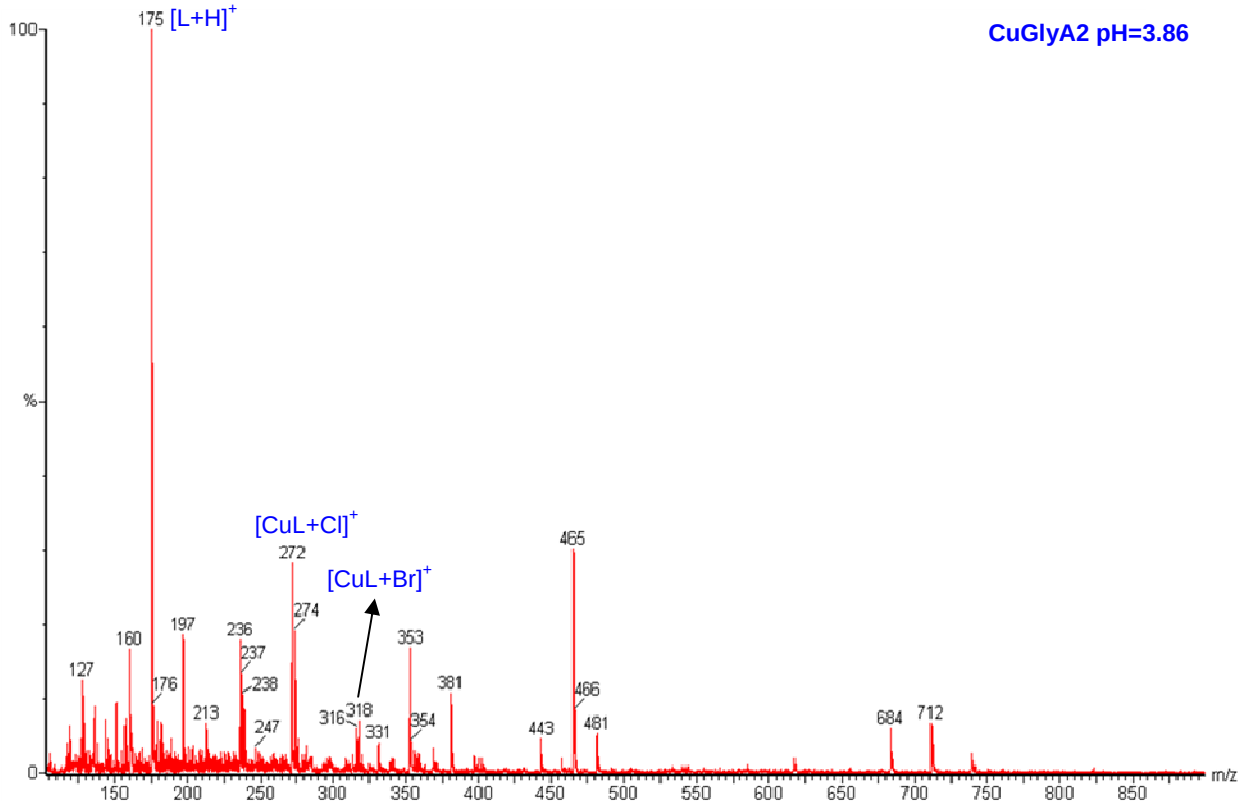


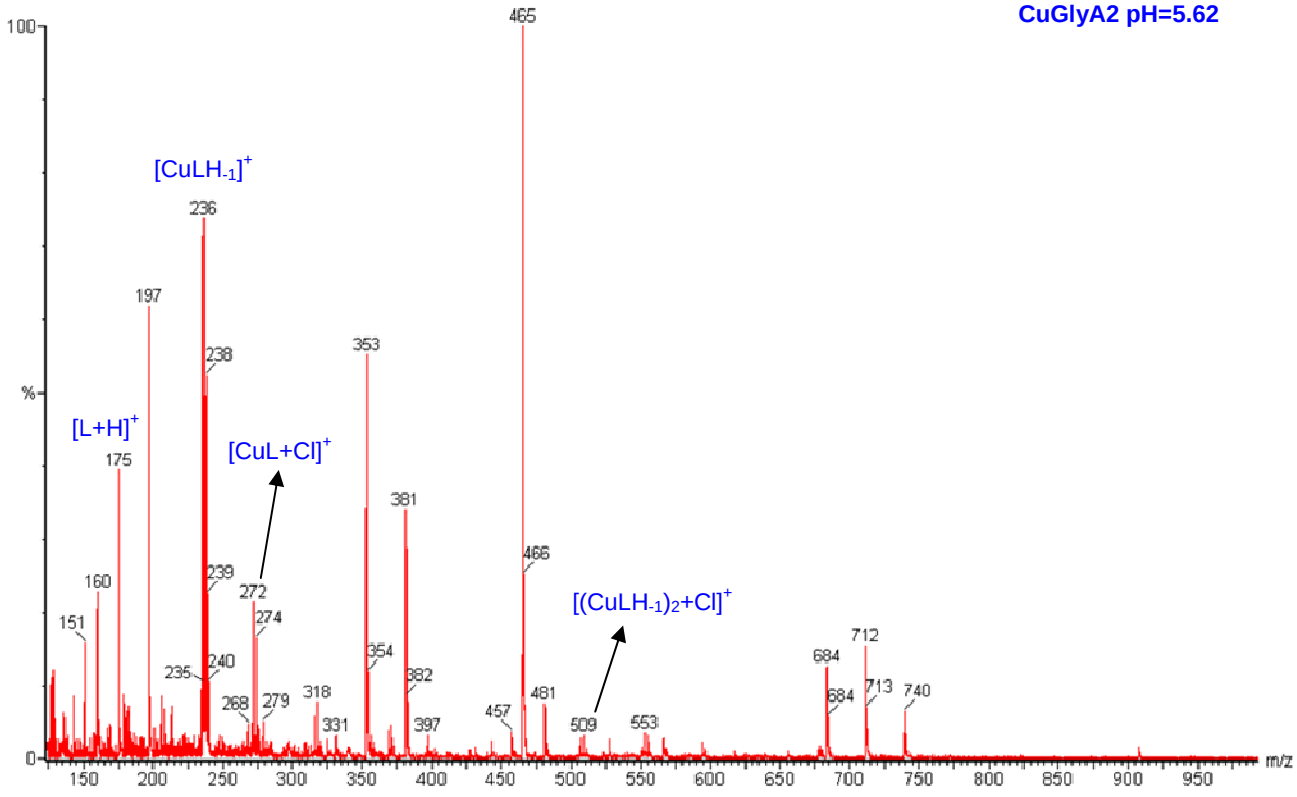


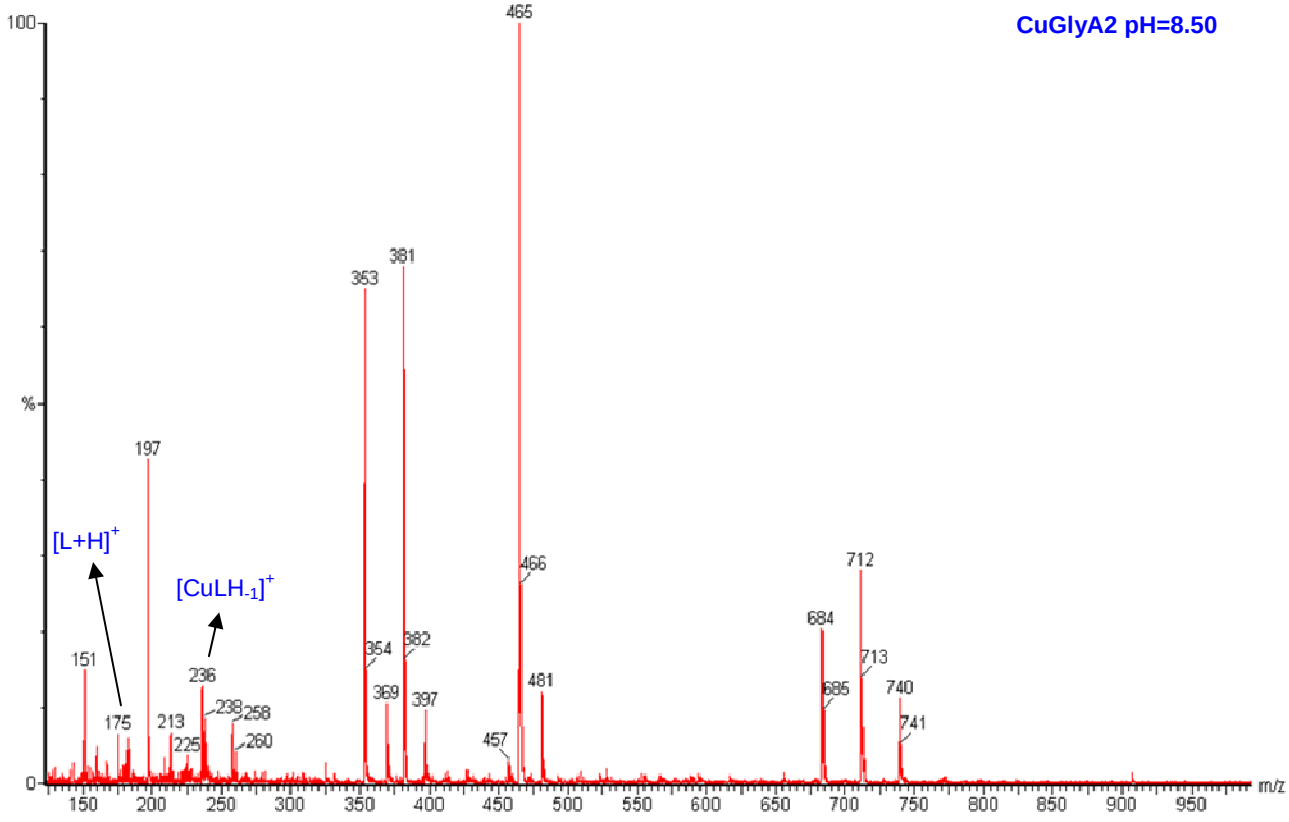


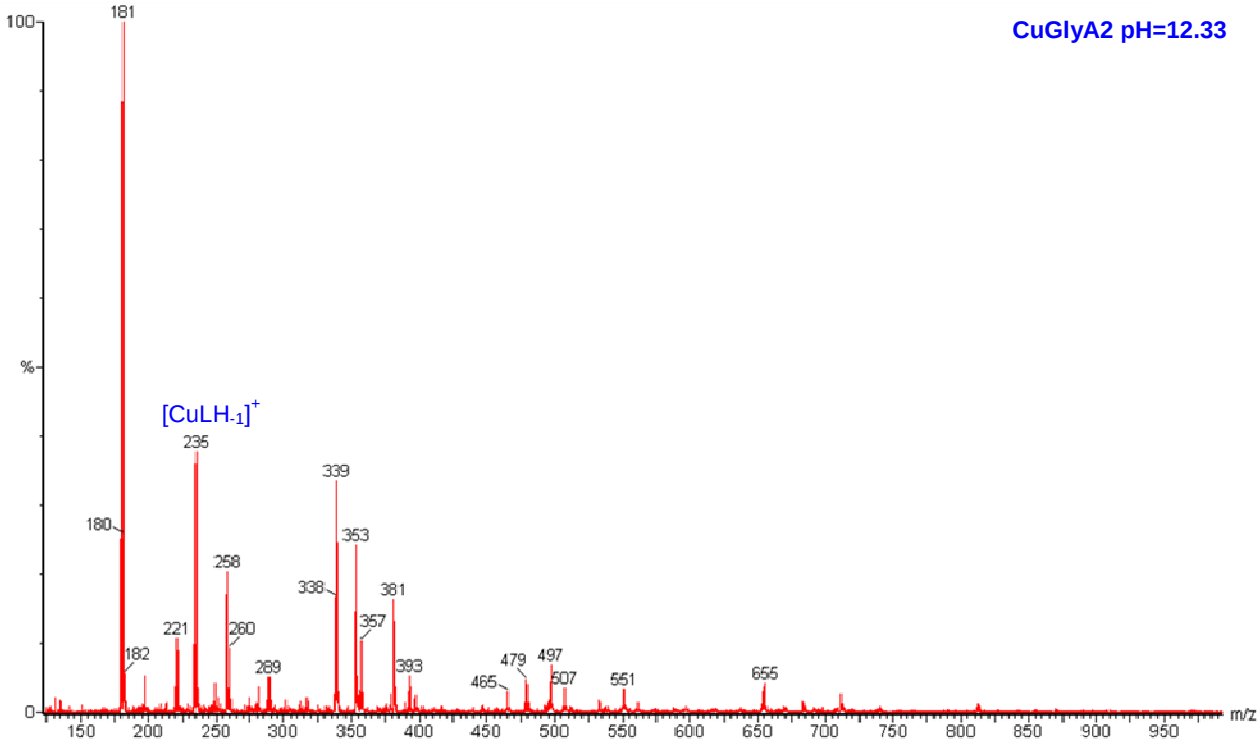


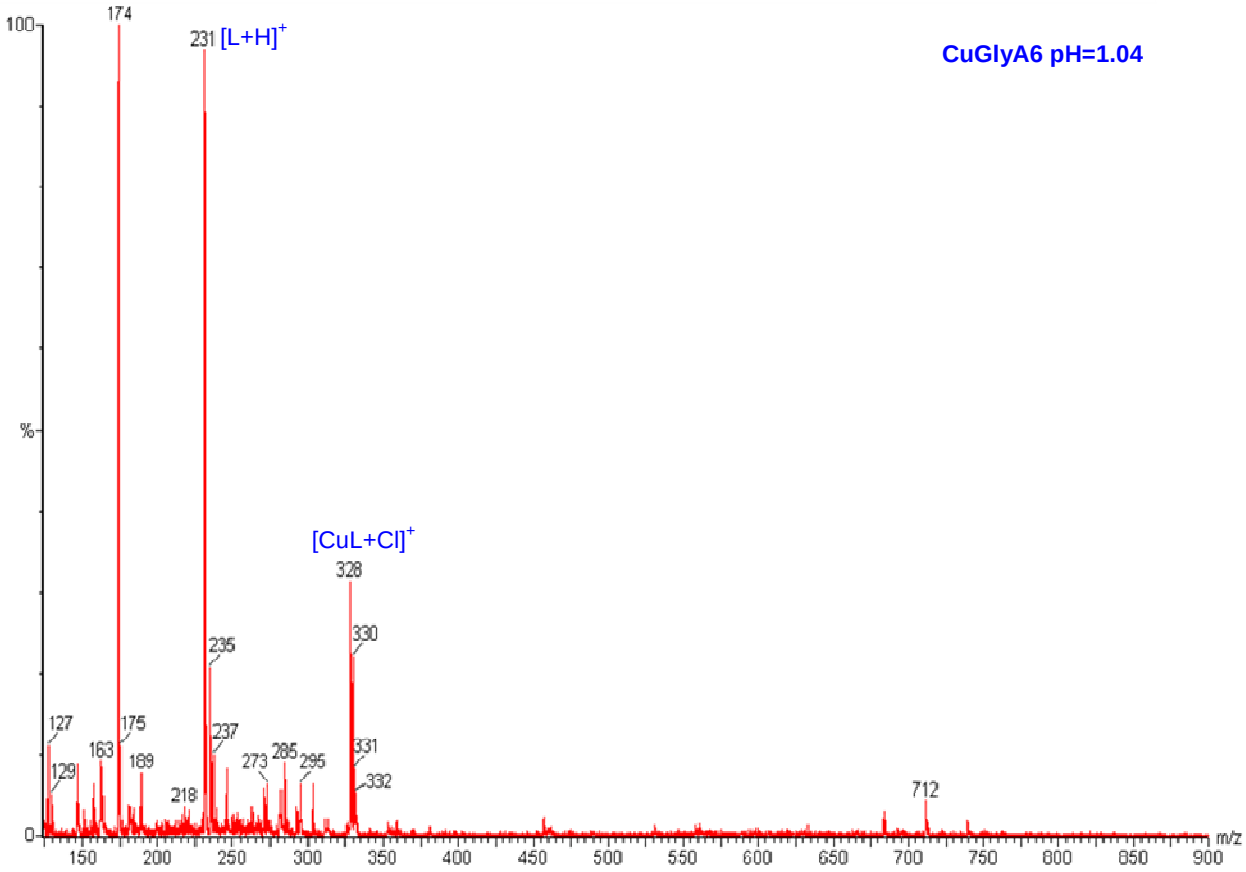


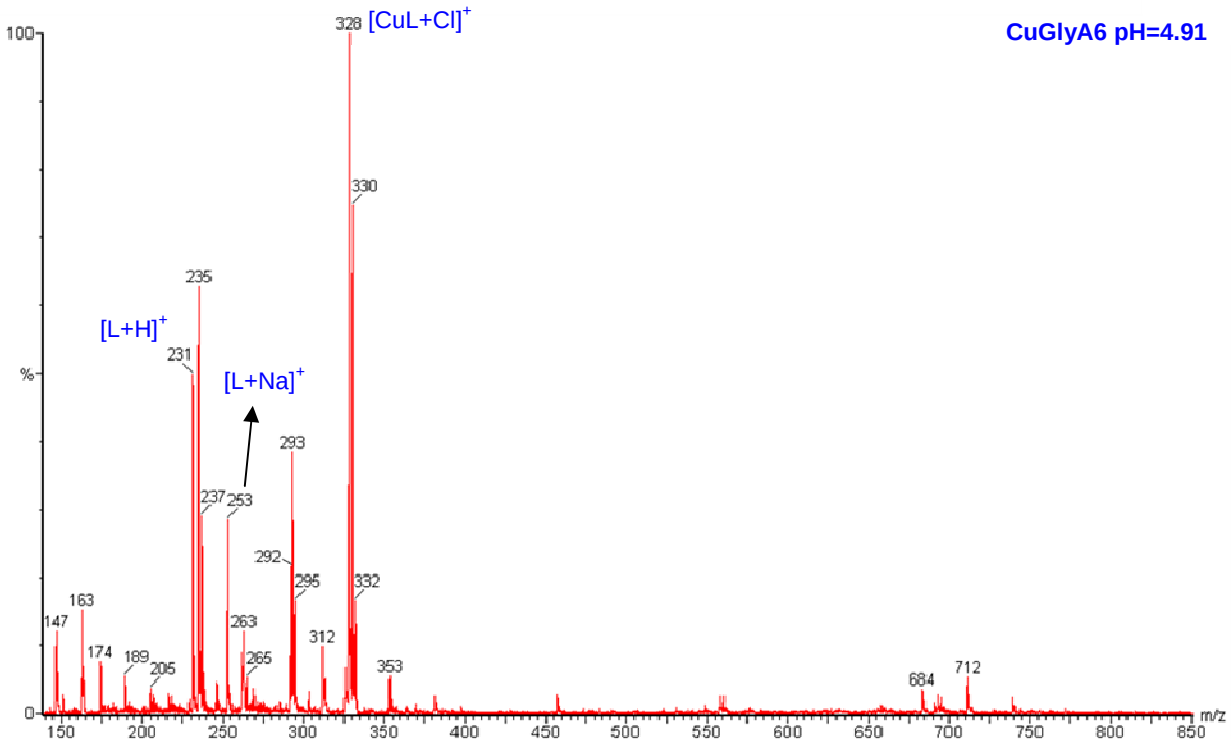


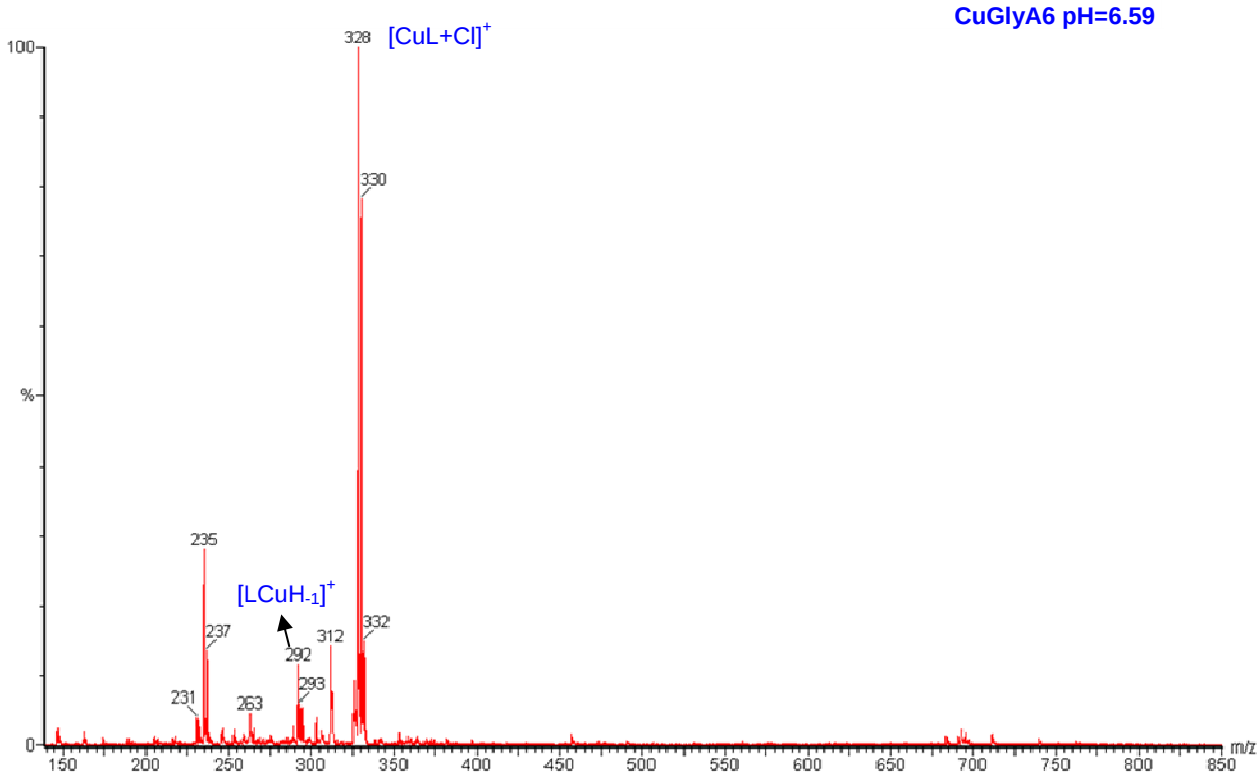


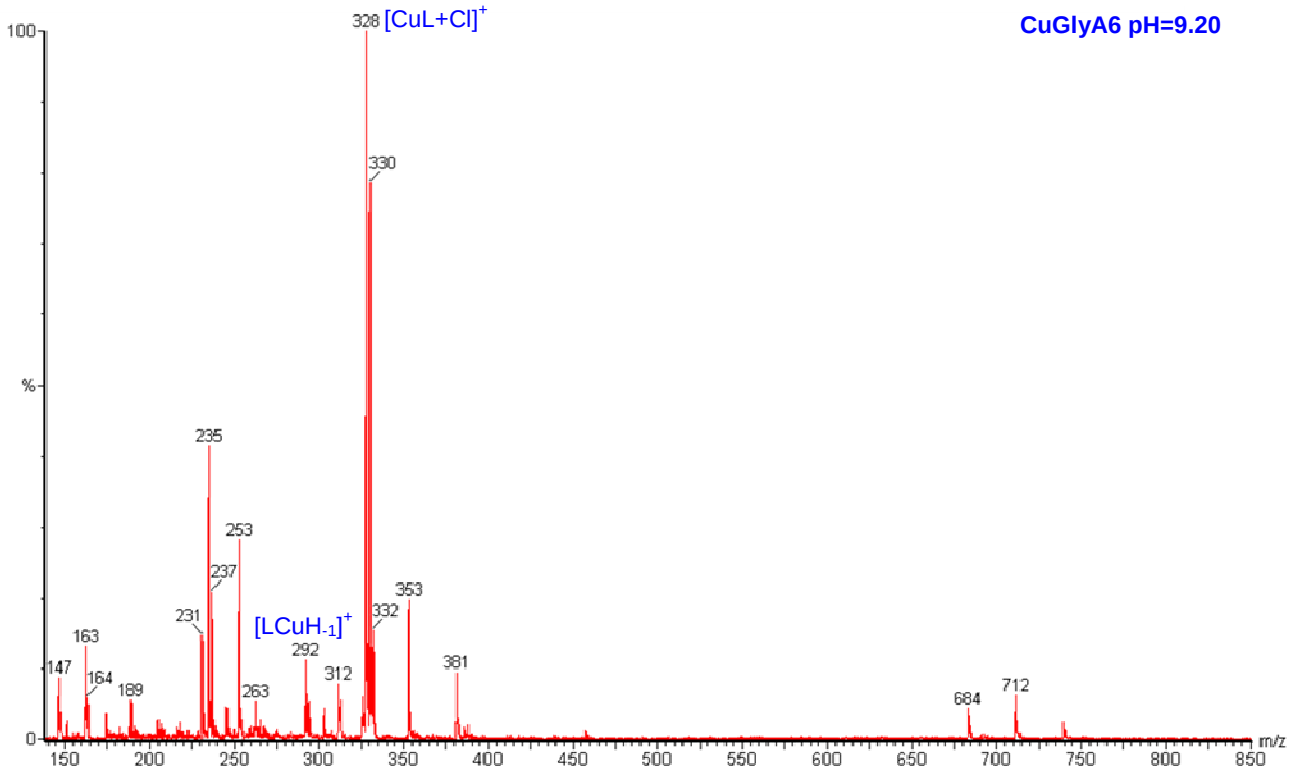


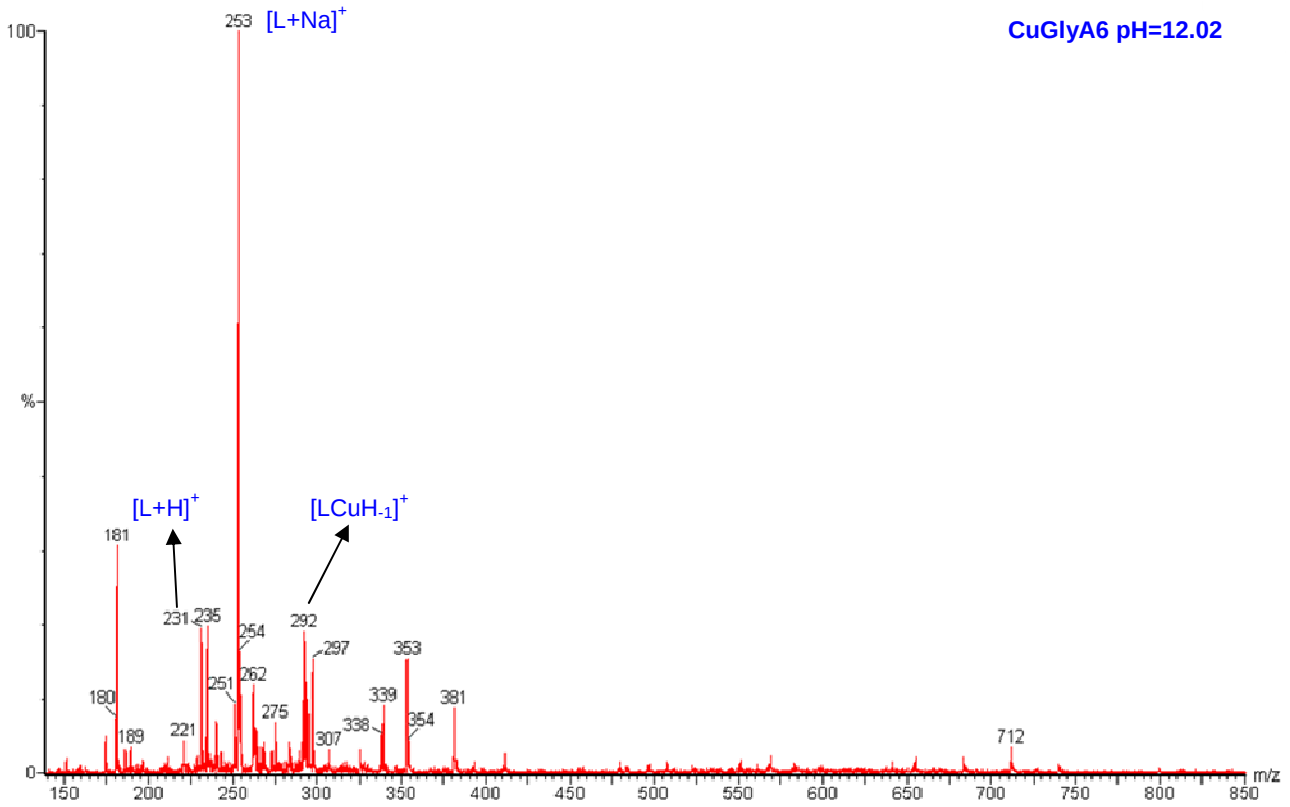












S5. Species distribution curves for the compound AlaA3 (1d, n=1) and for Cu (II) complexes. UV/Vis absorption spectra and ESI-MS spectra for the Cu (II) complexes at several pH values.

Table 1. Logarithms of the cumulative and stepwise basicity constants of AlaA3 determined in 0.1 M NaCl at 298.1 ± 0.1 K.

Reaction[a], [c]	AlaA3
$H + L \rightleftharpoons HL$	8.40(6) [b]
$2H + L \rightleftharpoons H_2L$	15.56(7)
$H + HL \rightleftharpoons H_2L$	7.16(7)

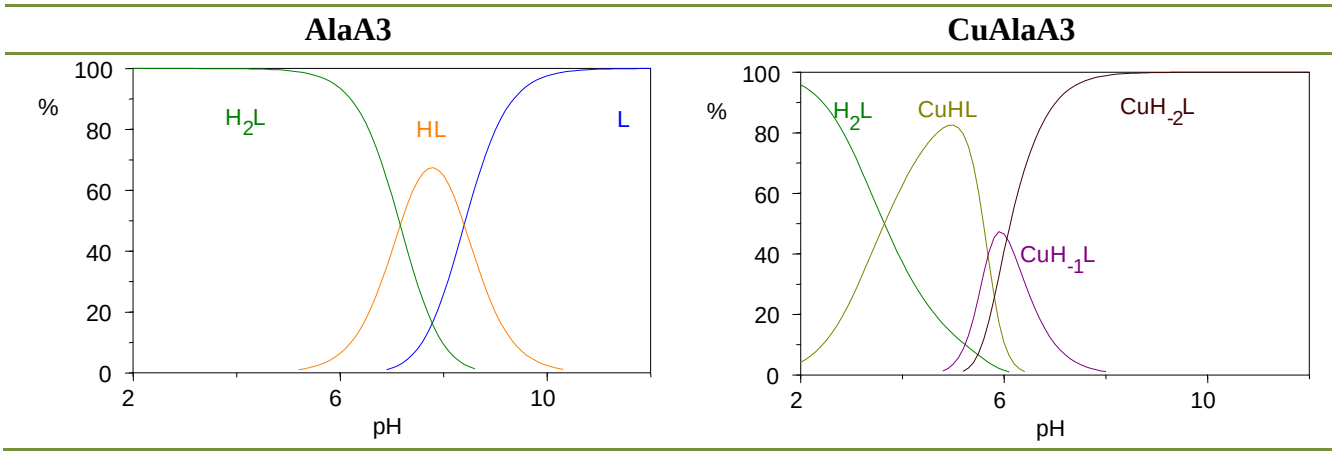
[a] Charges omitted for clarity. [b] All values in parentheses have the standard deviations in the last significant figure. [c] Determined in an aqueous solution 0.1 M NaCl using 0.1 mmol of ligand.

Table 2. Logarithms of the formation constants for the Cu^{2+} complexes of the ligand AlaA3 determined in 0.1 M NaCl at 298.1 ± 0.1 K.

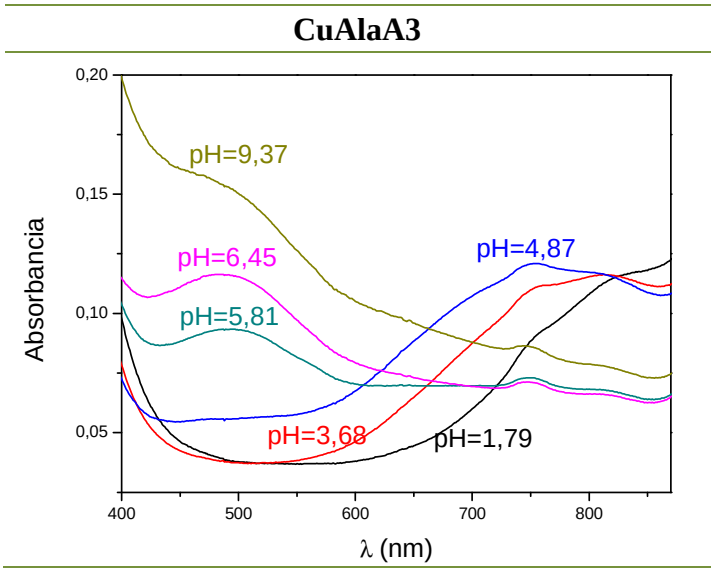
Reaction[a], [c]	AlaA3
$Cu+L \rightleftharpoons CuL$	---
$Cu + L + H \rightleftharpoons CuHL$	13.74(5) [b]
$Cu + L \rightleftharpoons CuH_{-1}L + H$	2.37(3)
$Cu + L \rightleftharpoons CuH_{-2}L + 2H$	-3.69(4)
$Cu + L \rightleftharpoons CuH_{-3} + 3H$	---
$CuL + H \rightleftharpoons CuHL$	---
$CuL \rightleftharpoons CuH_{-1}L + H$	---
$CuH_{-1}L \rightleftharpoons CuH_{-2}L + H$	-6.06(4)
$CuH_{-2}L \rightleftharpoons CuH_{-3}L + H$	----

[a] Charges omitted for clarity. [b] All values in parentheses have the standard deviations in the last significant figure. [c] Determined in an aqueous solution 0.1M NaCl using 0.1 mmol of ligand and 0.1 mmol of the cupper (II) salt

DISTRIBUTION DIAGRAMS



UV/VIS ABSORPTION SPECTRA FOR THE Cu (II) COMPLEXES AT SEVERAL pH VALUES.



ESI-MS SPECTRA FOR THE Cu (II) COMPLEXES AT SEVERAL pH VALUES.