ELECTRONIC SUPPLEMENTARY MATERIAL

for the paper entitled

Assignment of low molecular weight selenometabolites in the root section of white cabbage

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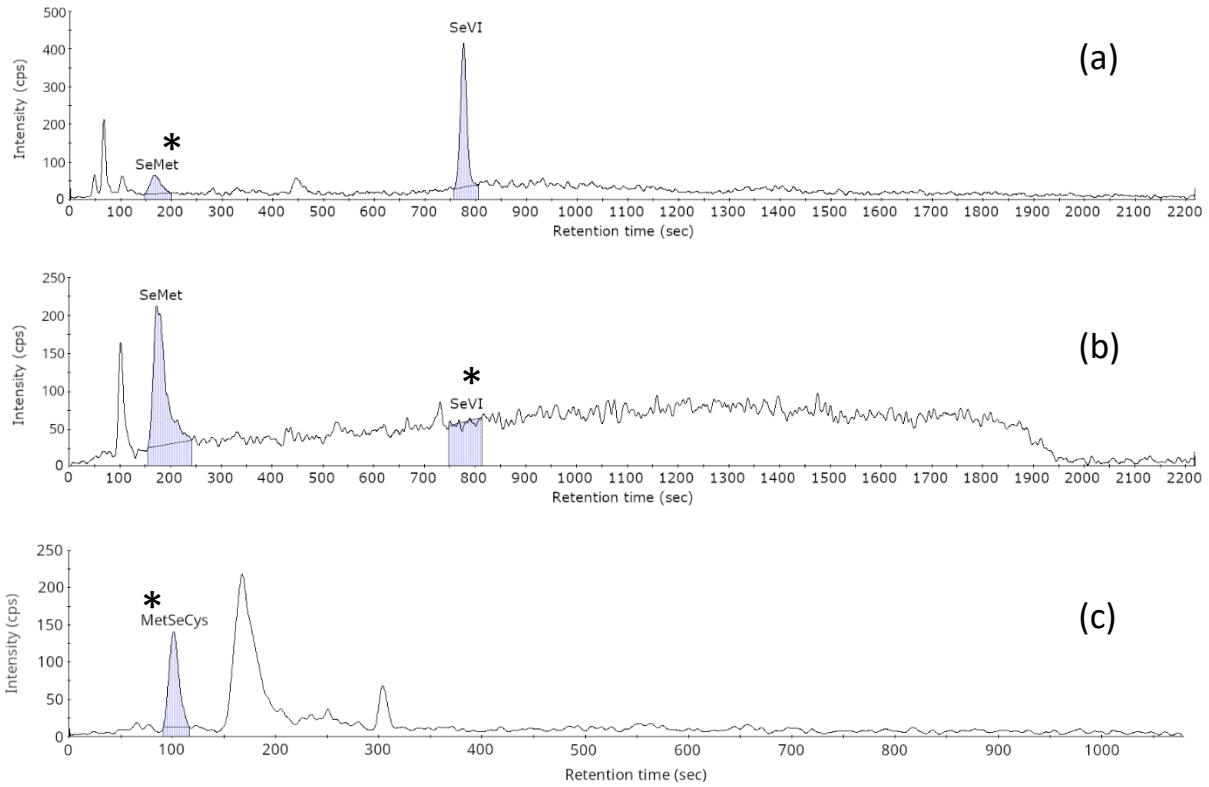
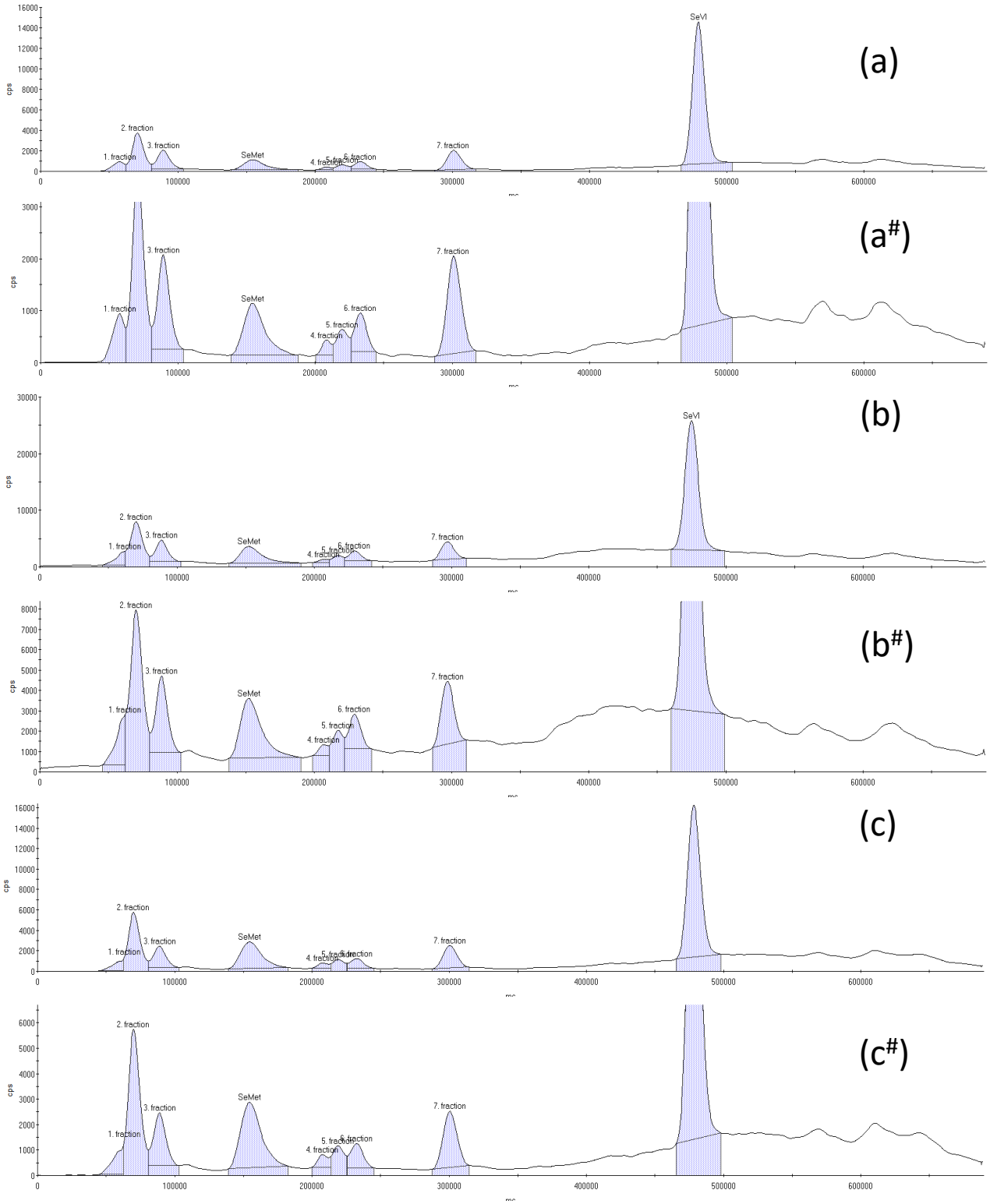
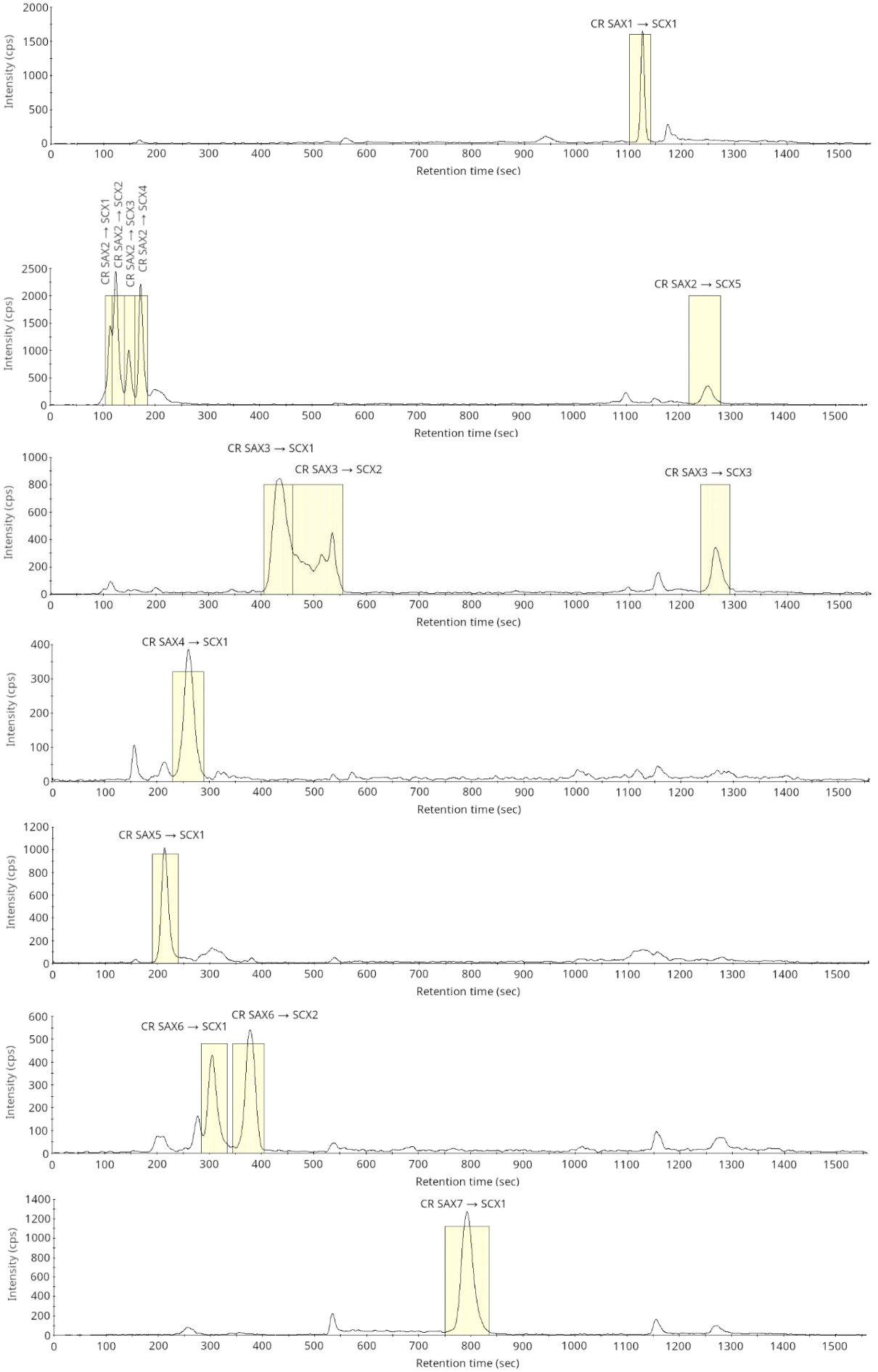


Suppl. Fig. S1 Typical HPLC(SAX)-ICP-MS chromatograms. **a** The water extract of cabbage root. **b** The enzymatic extract of cabbage root. **c** The enzymatic extract of cabbage root with a modified gradient program. All the chromatograms are recorded on the ^{78}Se isotope. '*' indicates the given species was detected under the actual limit of quantification.

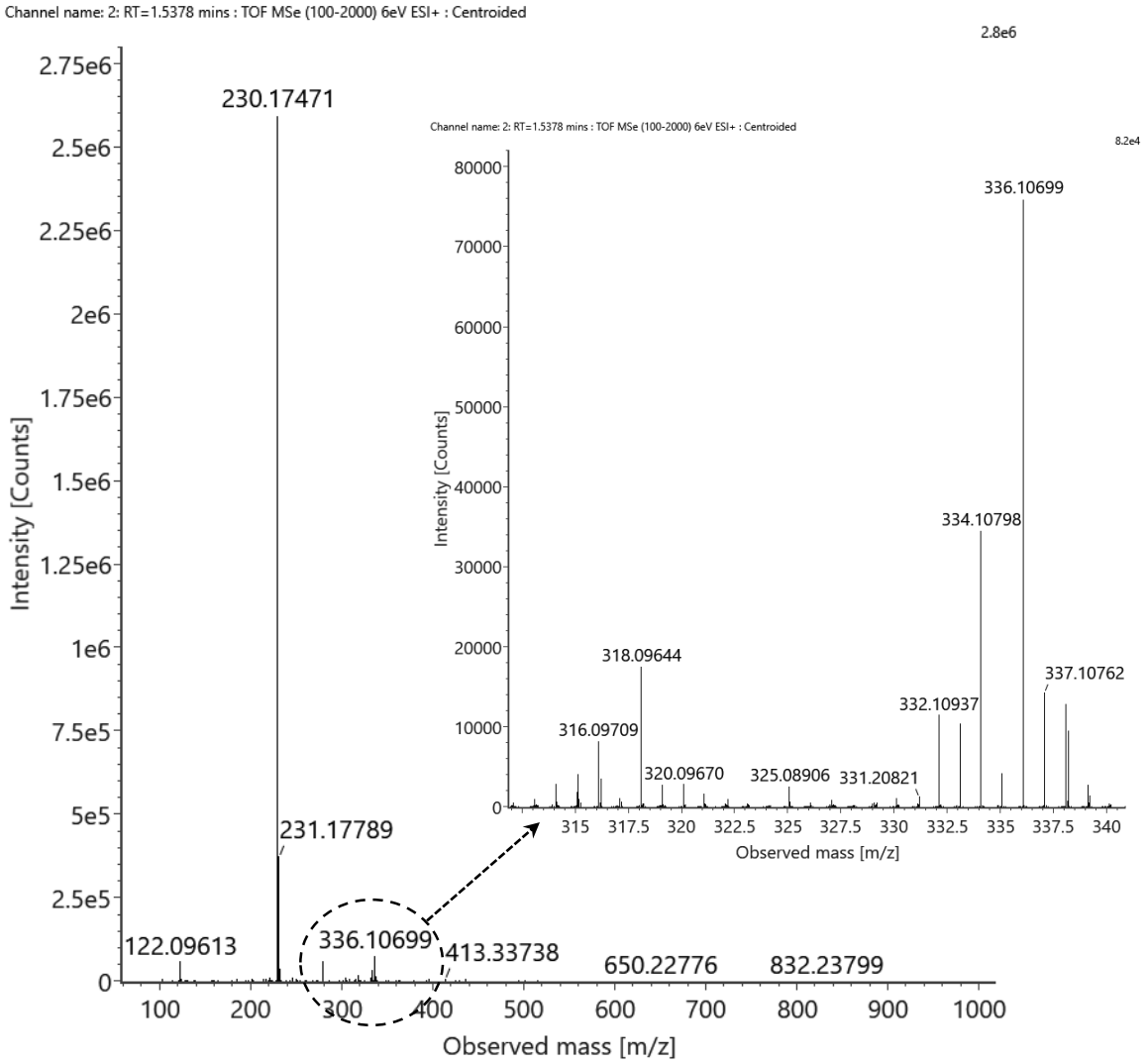


	mg kg^{-1} Se (estimated)							
Soil type/fraction No.	1	2	3	4	5	6	7	total Se
Sandy	0.19	0.77	0.37	0.05	0.14	0.15	0.45	**2.12**
Silt-Sand	0.26	1.29	0.55	0.06	0.29	0.25	0.48	**3.18**
Silty	0.20	1.17	0.43	0.09	0.23	0.20	0.51	**2.84**

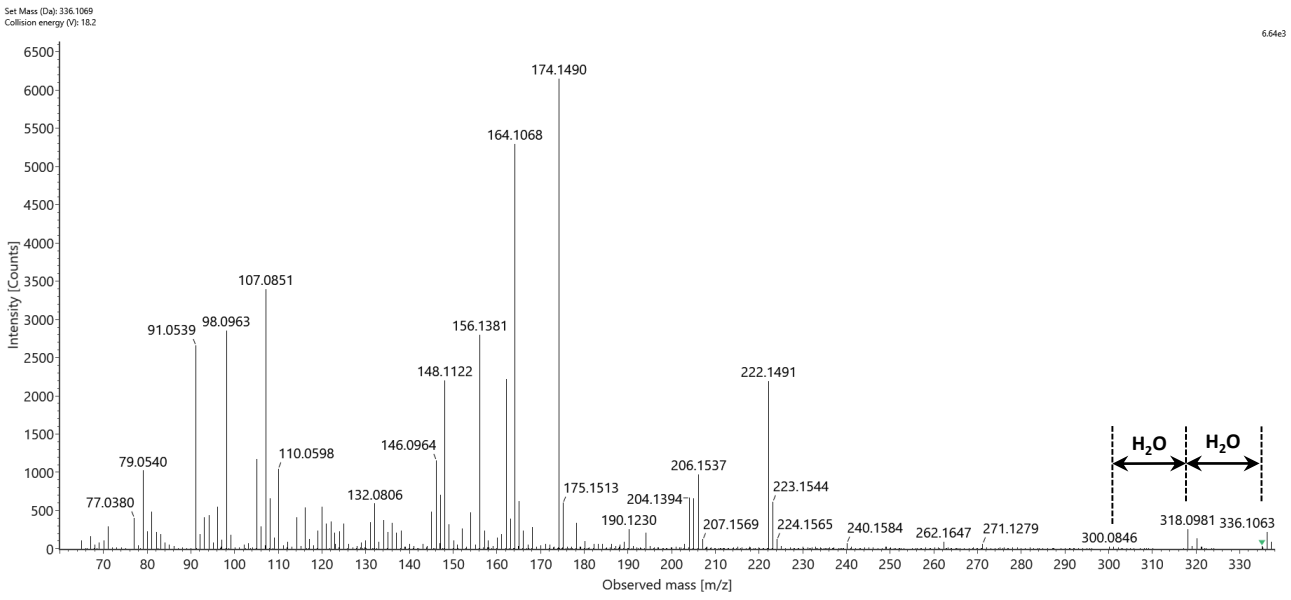
Suppl. Fig. S2 SAX-ICP-MS chromatograms of the water extracts of cabbage root. **a** From sandy soil. **b** From silt-sand soil. **c** From silty soil. All the chromatograms are recorded on the ^{78}Se isotope. Chromatograms with '#' marks are the magnified versions of the original runs. The table lists the estimated total selenium contents of each fraction.



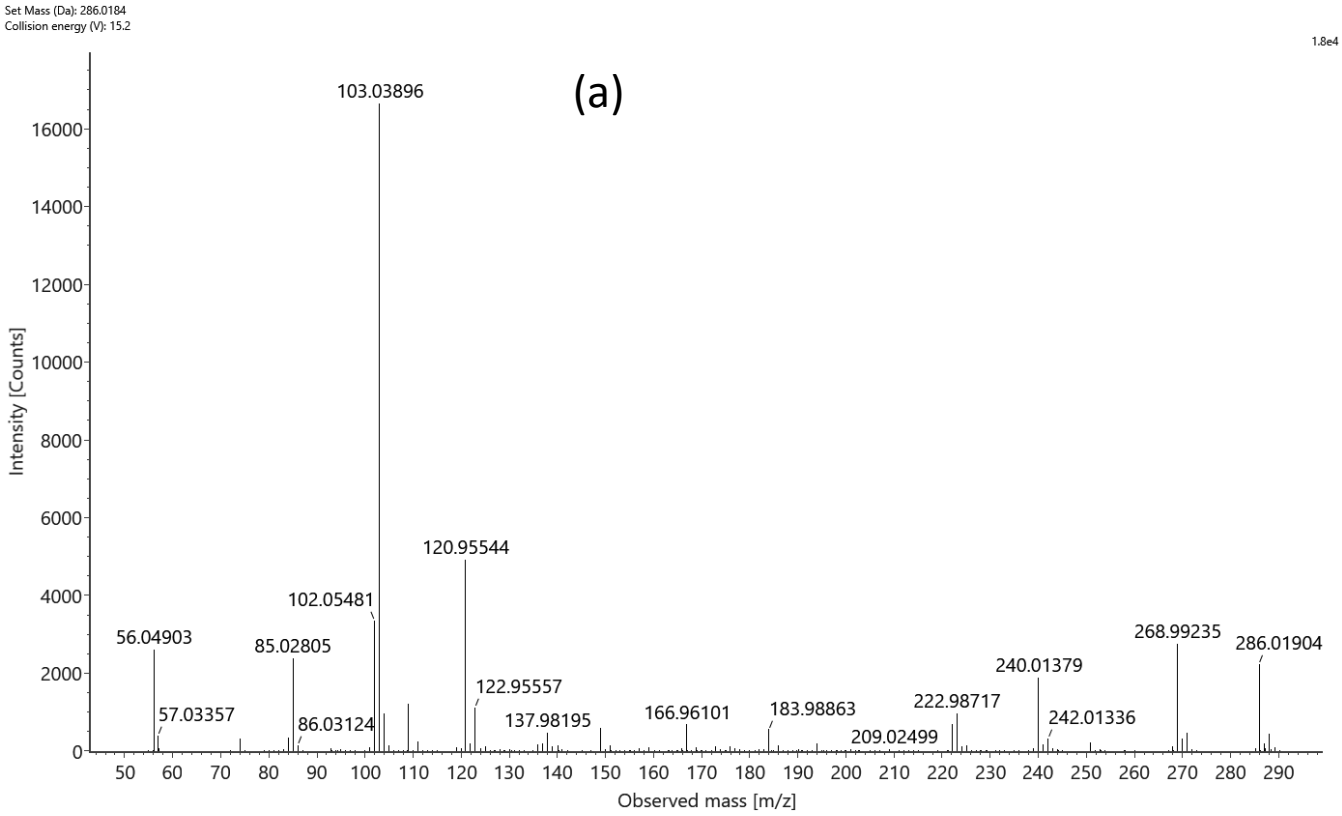
Suppl. Fig. S3 SCX-ICP-MS chromatograms of the SAX no. 1-7 fractions of cabbage root after SAX purification, recorded on the ^{78}Se isotope (see **Fig. 1** and **Suppl. Fig. S2**). Yellow squares mark the retention windows of the 14 fractions collected for the LC-ESI-HR-MS experiments.

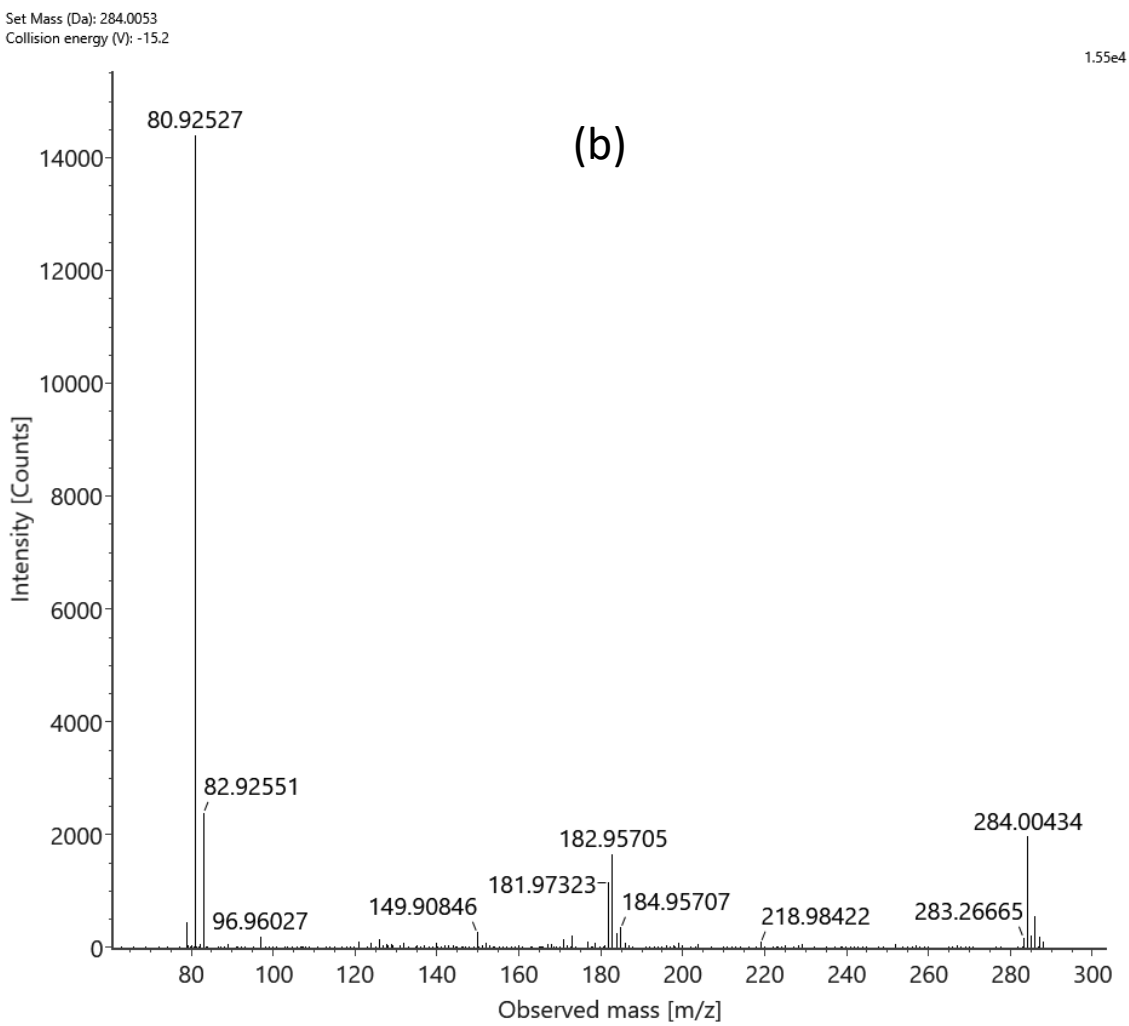


Suppl. Fig. S4 Full scan spectrum of the $C_{14}H_{25}NO_3Se$ selenocompound (neutral composition), detected in the ESI '+' mode at RT=1.55 min (Table 2). The inset shows the magnified spectrum of the monoselenized species, together with its ion source fragment (-18 Da; water loss).

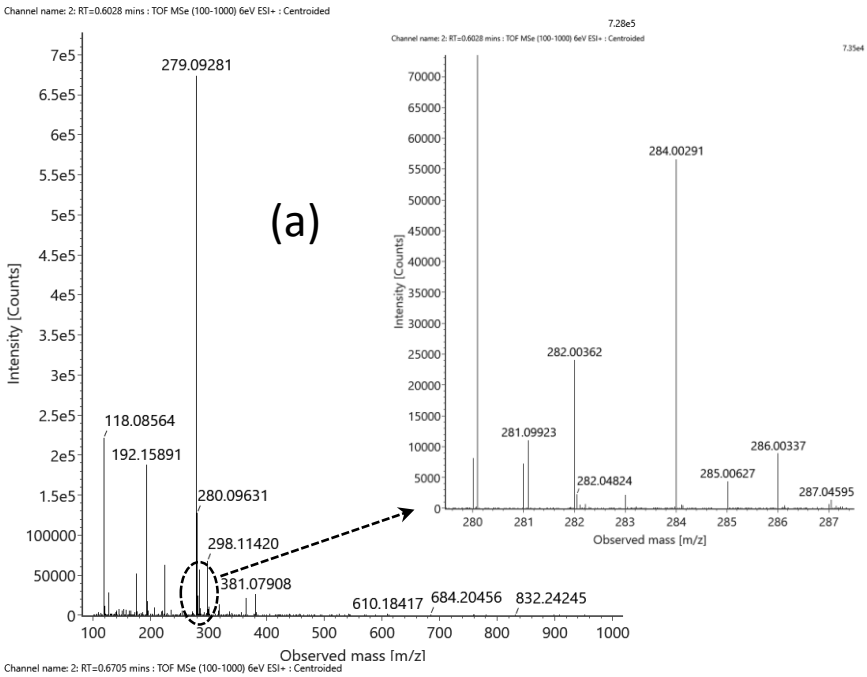


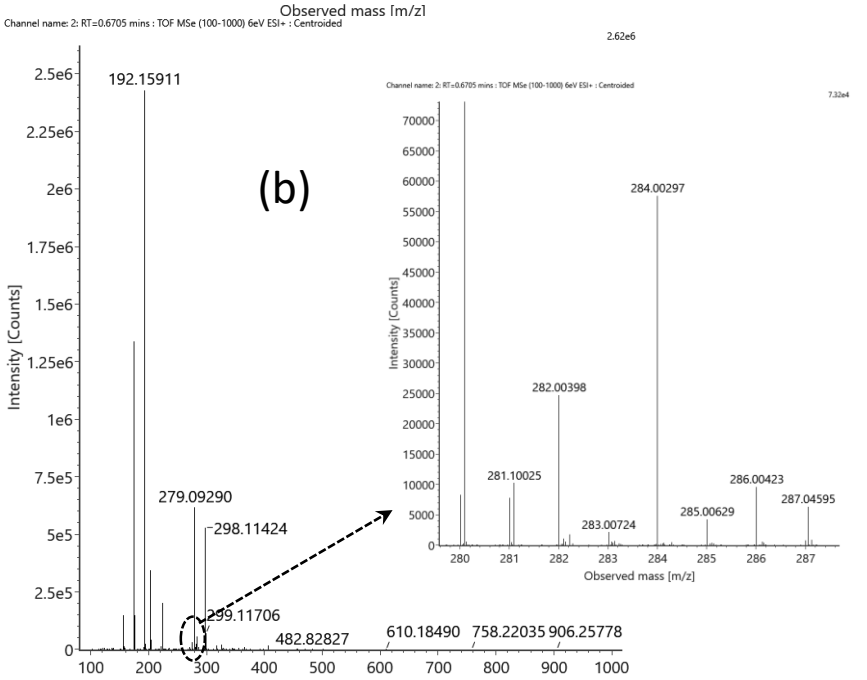
Suppl. Fig. S5 MS/MS spectrum of the $C_{14}H_{25}NO_3Se$ selenocompound (neutral composition), detected in the ESI '+' mode (collision energy: 18.2 eV).

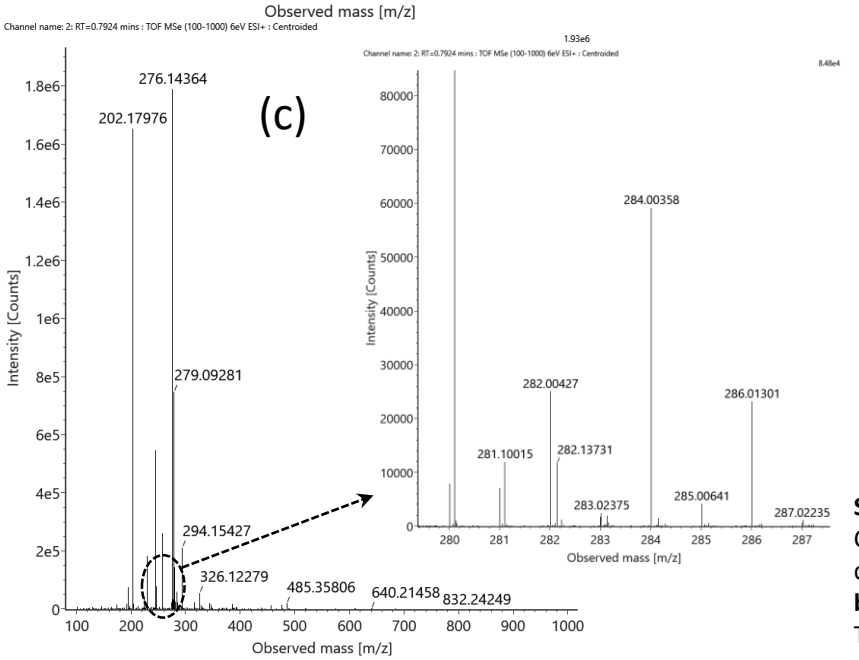




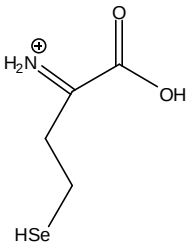
Suppl. Fig. S6 MS/MS spectra of mono-deaminated hydroxy-selenohomolanthionine. **a** Detected in the ESI ’+’ mode. **b** Detected in the ESI ’-’ mode.



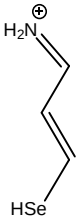




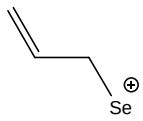
Suppl. Fig. S7 Full scan spectra of the $C_8H_{13}NO_5Se$ selenocompounds (neutral state) detected in the ESI '+' mode. **a** At RT=0.60 min. **b** At RT=0.67 min. **c** At RT=0.79 min (Table 2). The insets show the magnified spectra of the monoselenized species.



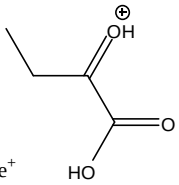
Chemical Formula: $C_4H_8NO_2Se^+$
Exact Mass: 181.9715

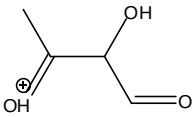


Chemical Formula: $C_3H_6NSe^+$
Exact Mass: 135.9660

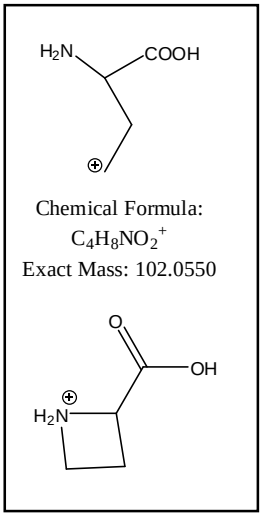


Chemical Formula: $C_3H_5Se^+$
Exact Mass: 120.9551

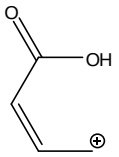




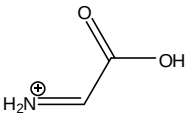
Chemical Formula: $C_4H_7O_3^+$
Exact Mass: 103.0390



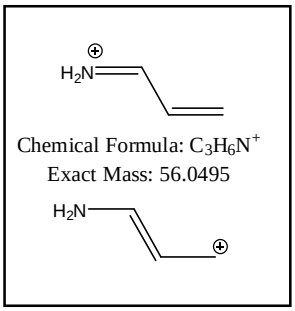
Chemical Formula:
$C_4H_8NO_2^+$
Exact Mass: 102.0550



Chemical Formula:
$C_4H_5O_2^+$
Exact Mass: 85.0284

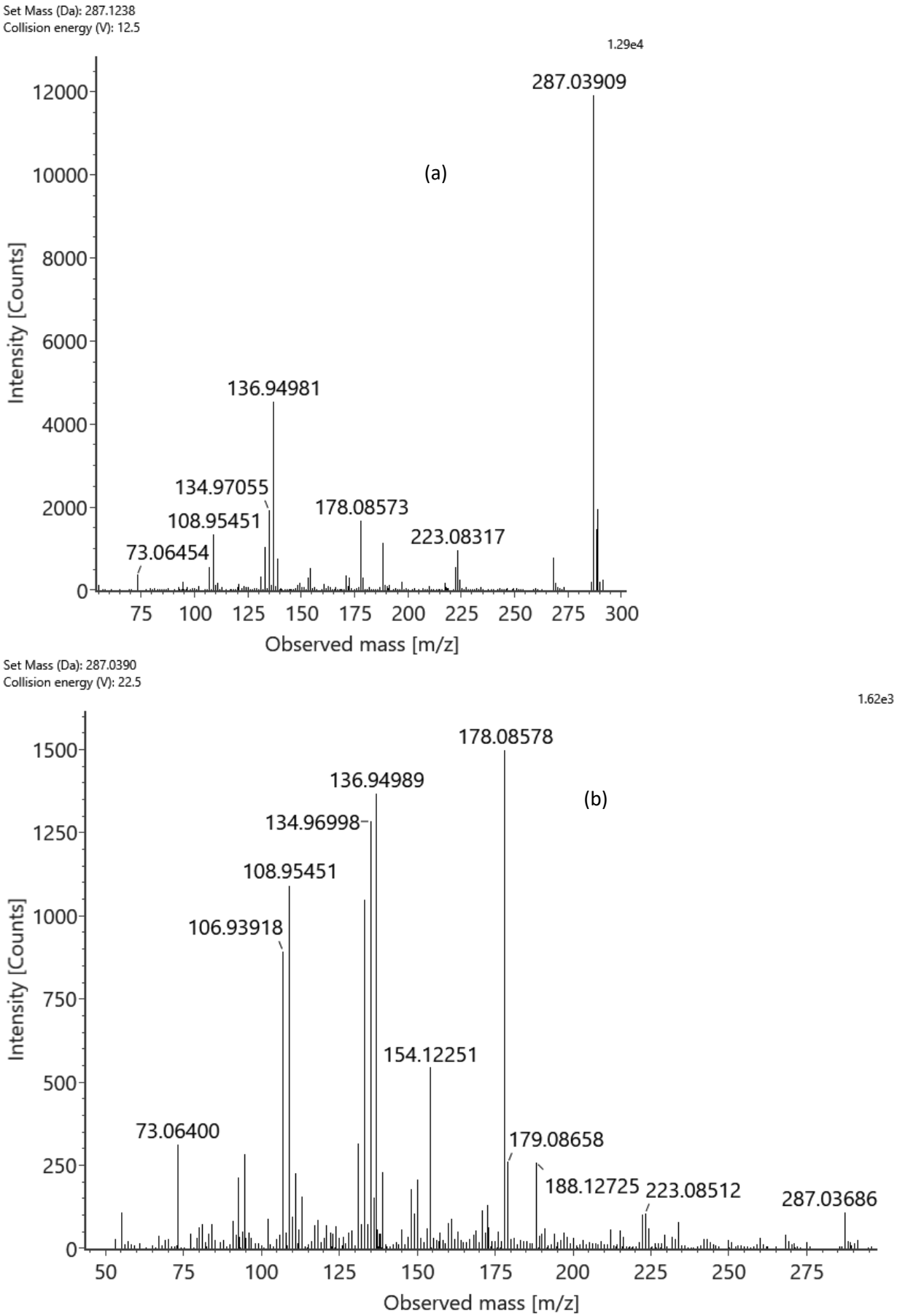


Chemical Formula: $C_2H_4NO_2^+$
Exact Mass: 74.0237

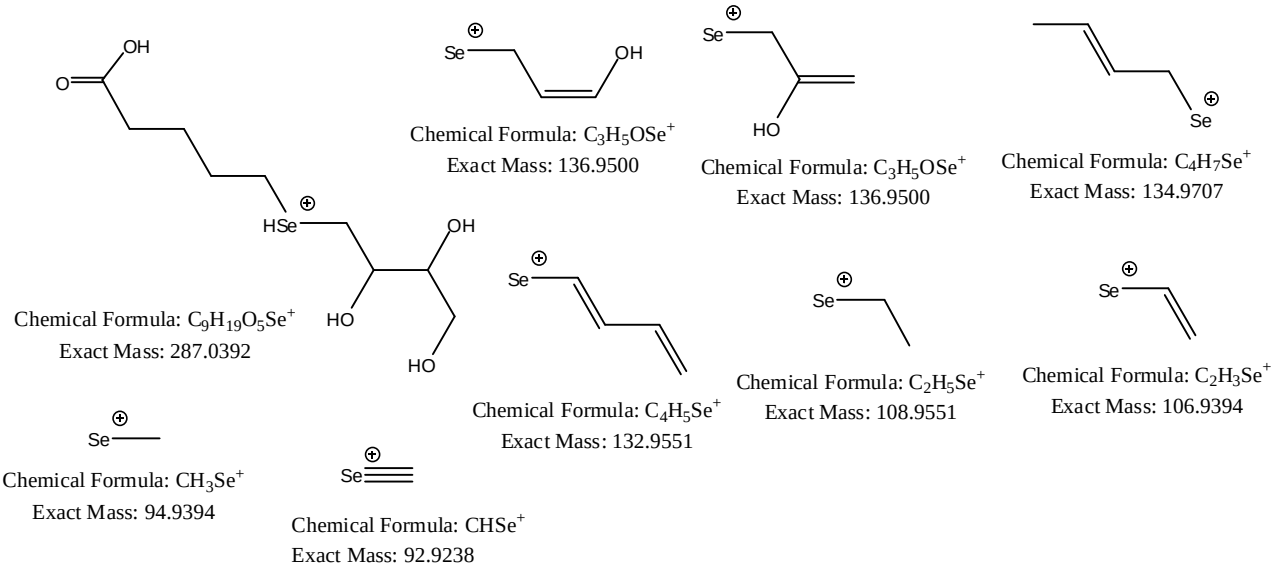


Chemical Formula: $C_3H_6N^+$
Exact Mass: 56.0495

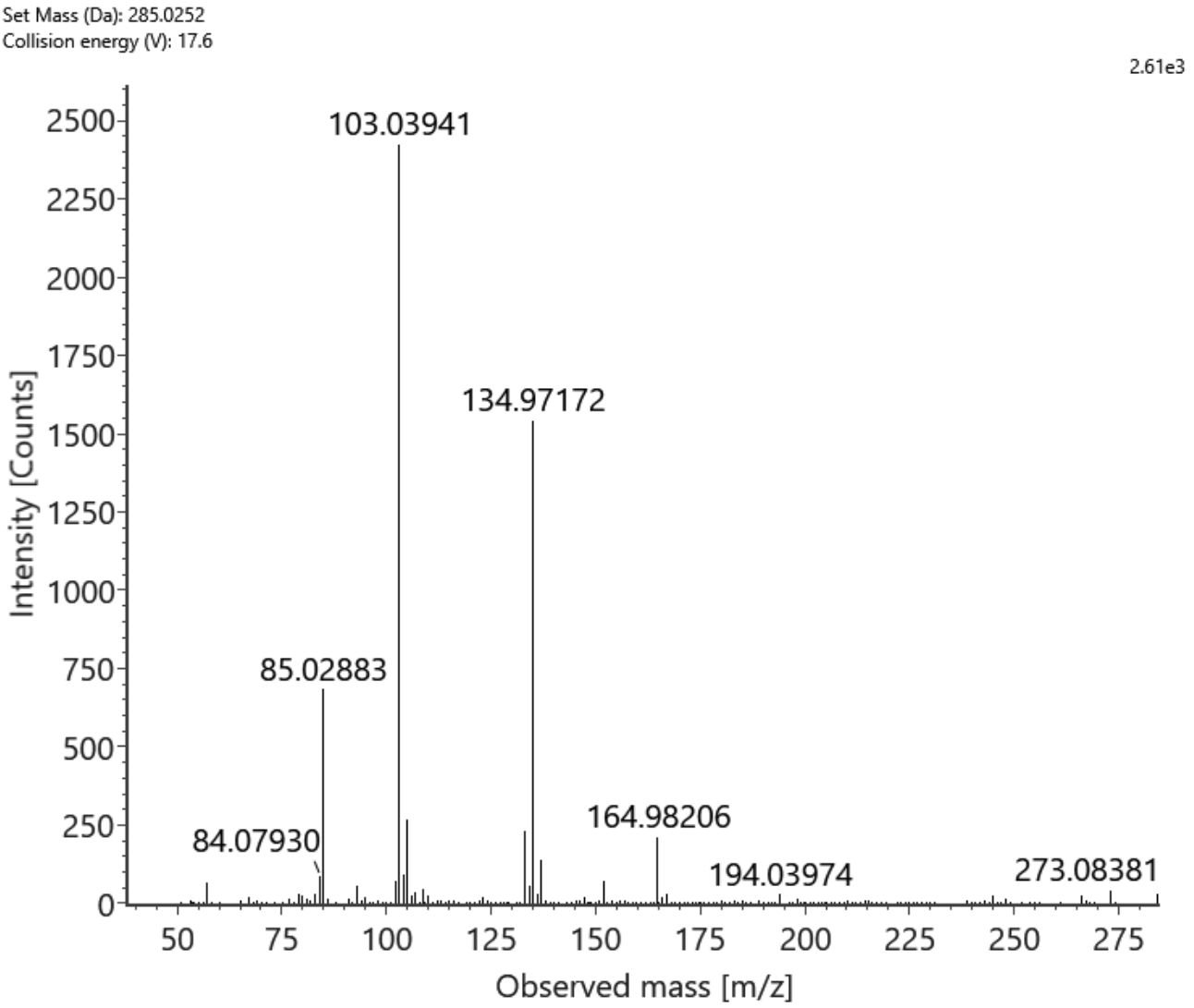
Suppl. Fig. S8 Tentative structures suggested for the fragments obtained from the MS/MS analysis of the isomers of the $C_8H_{14}NO_5Se^+$ selenospecies. Please note that the structures are subject to change, e.g., ionization and neutral losses can occur at different moieties, therefore the structures are intended for demonstrative purposes only.



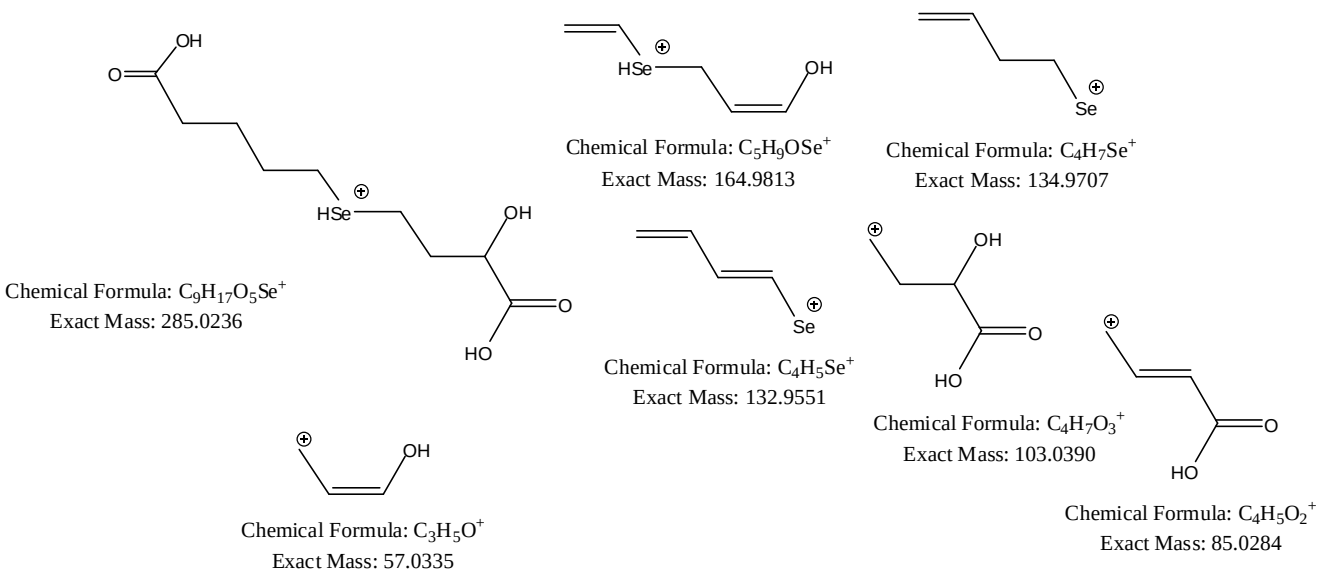
Suppl. Fig. S9 MS/MS spectra of the $C_9H_{18}O_5Se$ (neutral state; theoretical *m/z* 287.03922 for $C_9H_{19}O_5Se^+$) selenocompound recorded in the ESI '+' mode. **a** At 12.5 eV collision energy setting. **b** At 22.5 eV collision energy setting.



Suppl. Fig. S10 Tentative structures suggested for the $C_9H_{19}O_5Se^+$ selenospecies and its fragments obtained from the MS/MS analysis.



Suppl. Fig. S11 MS/MS spectrum of the $C_9H_{16}O_5Se$ (neutral state; theoretical *m/z* 285.02357 for $C_9H_{17}O_5Se^+$) selenocompound recorded in the ESI '+' mode at 17.6 eV collision energy setting.



Suppl. Fig. S12 Tentative structures suggested for the $C_9H_{17}O_5Se^+$ selenospecies and its fragments obtained from the MS/MS analysis.