Electronic Supplementary Information for the article entitled:

The relationship of selenium tolerance and speciation in Lecythidaceae species

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submitted to *Metallomics*

Table 1 Chromatographic parameters applied in the multidimensional sample clean-up procedure.

	Column	Buffer A	Buffer B	Flow rate (mL min^{-1})	Gradient program	
					Time (min)	Composition
SCX	Zorbax 300 SCX 4.6 x 150 mm x 5 ?m (Agilent)	1 mM pyridine formate in water	40 mM pyridine formate in water	1.0	0-4 35 40 60	0% B 40% B 100% B 100% B
IP-RP	XTerra MS C18 4.6 x 150 mm x 5 ?m (Waters)	5% methanol with 0.1% HFBA	100% methanol with 0.1% HFBA	1.0	0-5 15 20 21 27	0% B 50% B 50% B 100% B 100% B
RP	XDB C18 4.6 x 100 mm x 1.5 ?m (Agilent)	0.1% formic acid	acetonitrile with 0.1% formic acid	0.35	0-5 15 20 25 32	5% B 50% B 100% B 100% B 5% B

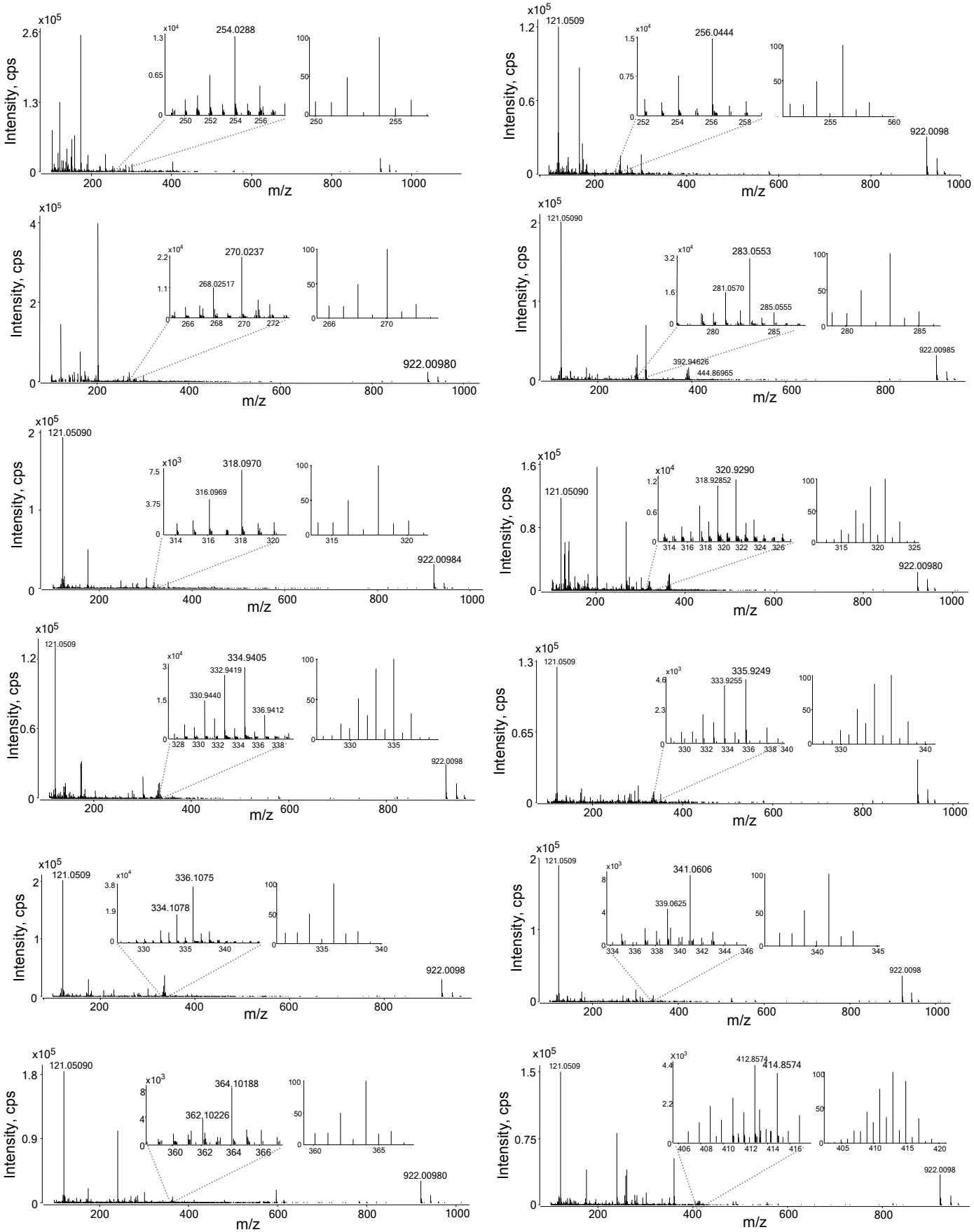
Table 2 Instrumental parameters of the HPLC-ESI-QTOF-MS set-up.

6530 Accurate Mass QTOF LC-MS (Agilent)	
ESI source	Dual ESI (Agilent)
Operational mode	Positive/negative
Precursor ion isolation in MS/MS mode	medium (4 m/z)
Mass accuracy	< 2 ppm
Mass resolution	> 10000
Detection frequency	4 GHz
Fragmentor voltage	150 V/-150 V
Curtain voltage	65 V/ -65 V
Drying gas	13 L/min
Capillary voltage	800 V
Nebulizer pressure	40 psig
Gas temperature	325 ºC
Data analysis software	Mass Hunter Acquisition B.02.01 with SP3
	Mass Hunter Qualitative Analysis B.03.01 with SP3

Table 3 List of the mass-to-charge ratios of the selenocompounds from *L. minor* and *B. excelsa* that were present in too low concentration to be identified by fragmentation. Compounds in bold are the derivatives of SeHCy (they contain the in-source fragment *m/z* 181.9715).

Positive ion mode	
Experimental m/z	
319.01876	**490.1907**
370.1117	**501.13531**
385.0508	**512.21066**
392.94684	**514.94526**
400.17601	**548.23255**
408.2374	551.16011
410.14459	557.14597
421.07289	**566.0404**
422.07166	596.19723
428.20588	629.16665
481.2540	**648.21141**
486.12433	
Negative ion mode	
Experimental m/z	
290.98243	
426.96412	
428.18383	
479.24101	

Figure 1. Fullscan spectra of the newly identified selenocompounds. The inserts show the isotopic patterns characteristic to compounds containing one or more Se atoms.



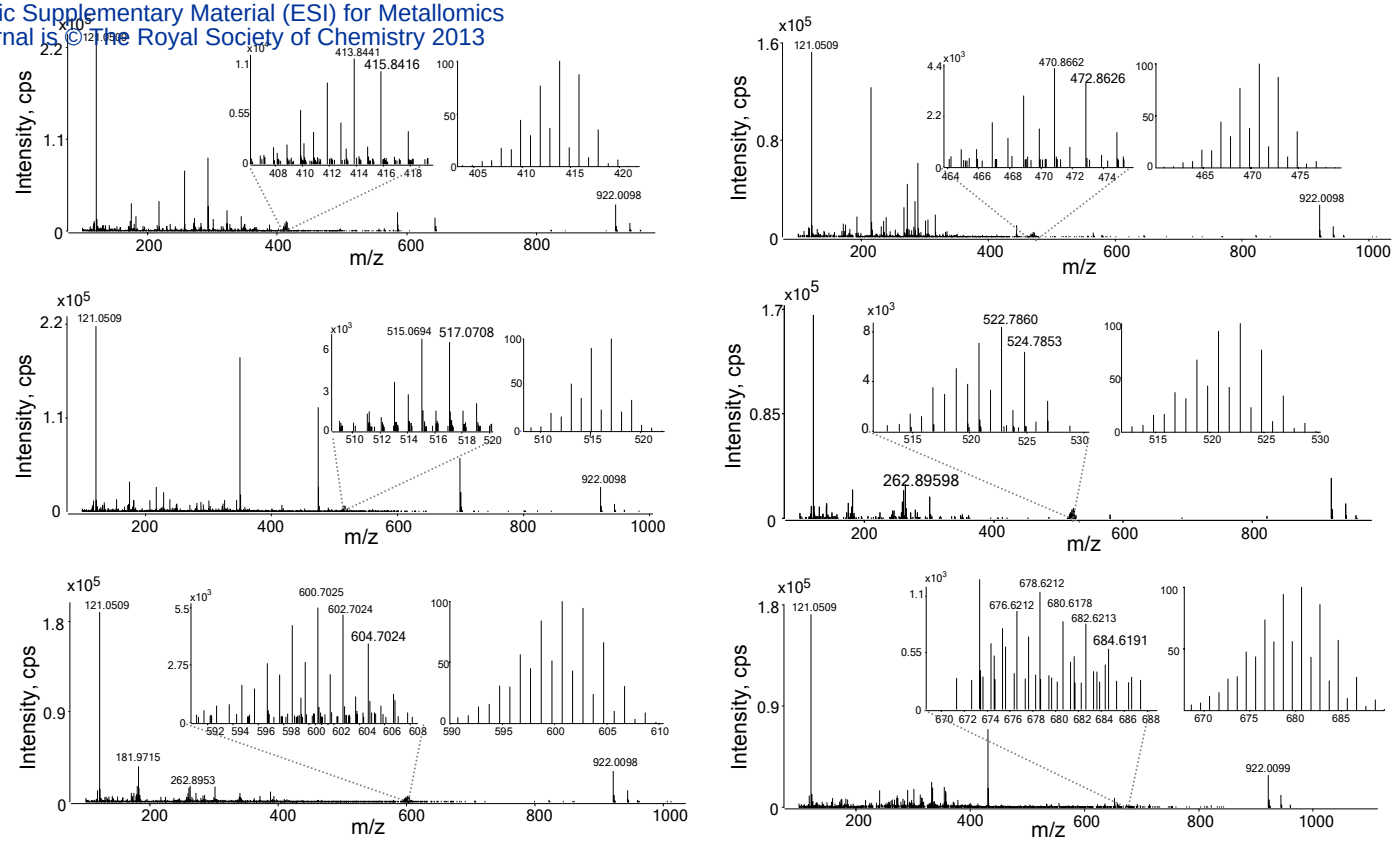
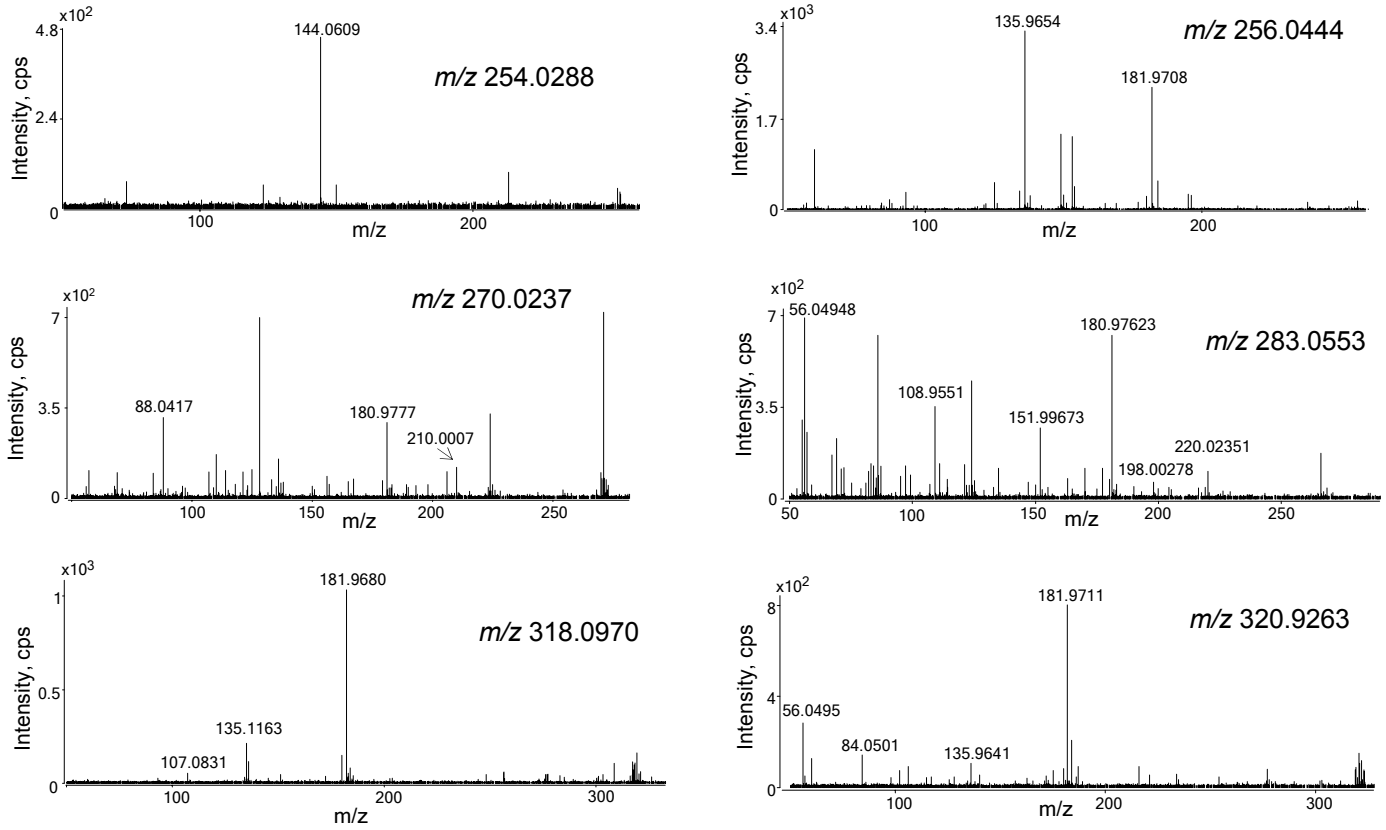
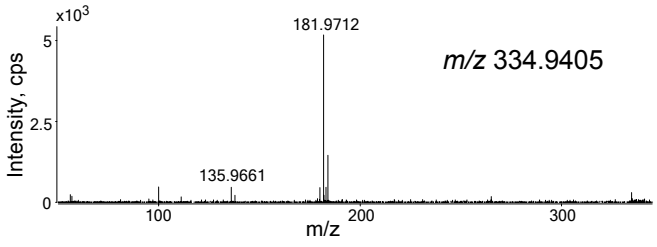
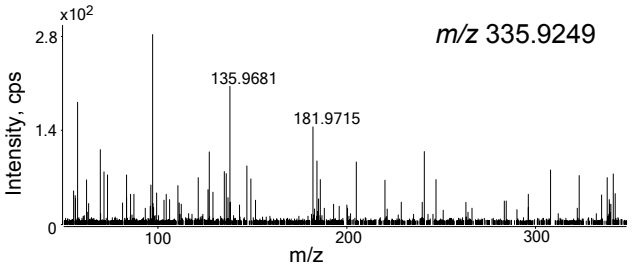
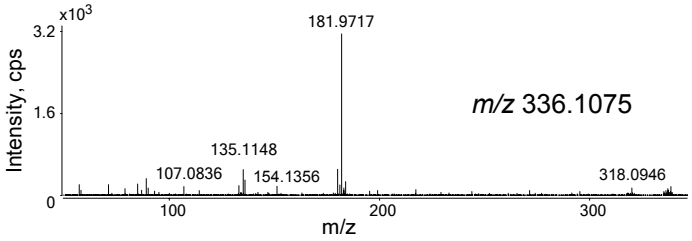


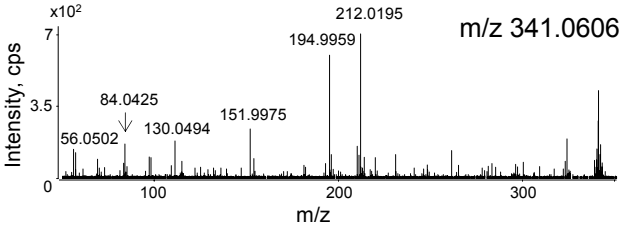
Figure 2. MS-MS spectra of the identified selenocompounds.

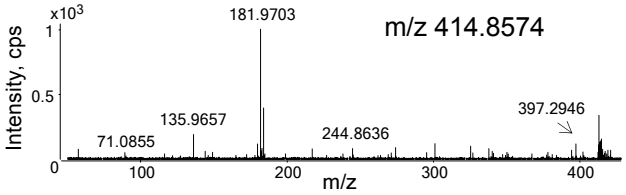


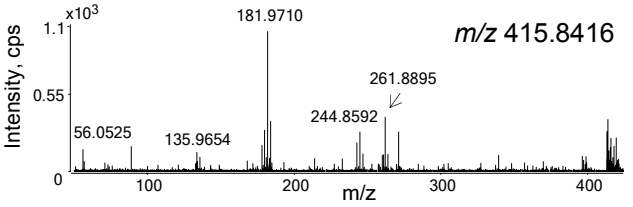


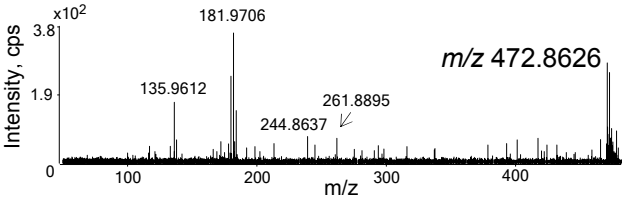


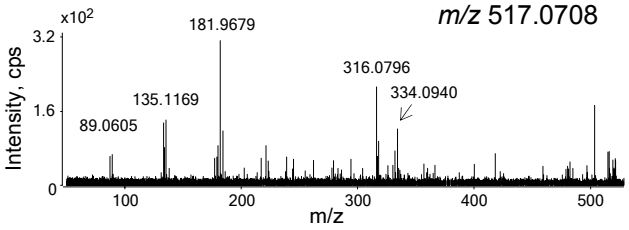


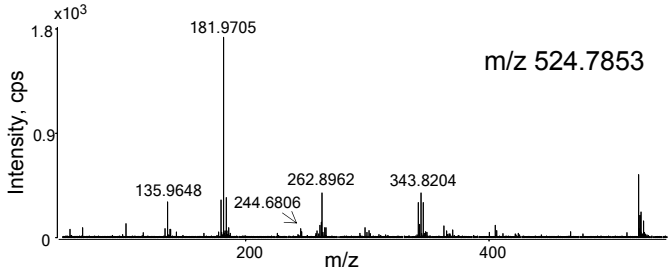












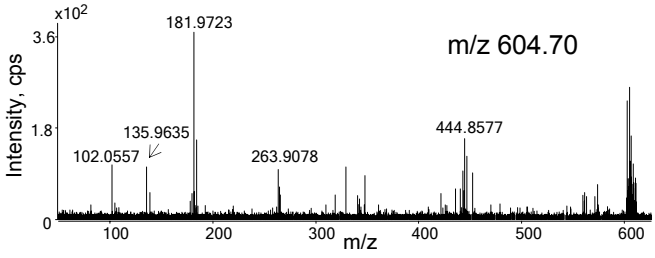


Figure 3. a) Fullscan spectra of the synthesized polychalcogenides. The inserts show the experimental and the theoretical isotopic distributions. b) The MS-MS spectrum of the compound containing two Se atoms (*m/z* 428.89573). The insert shows the structure of the molecule and its fragmentation.

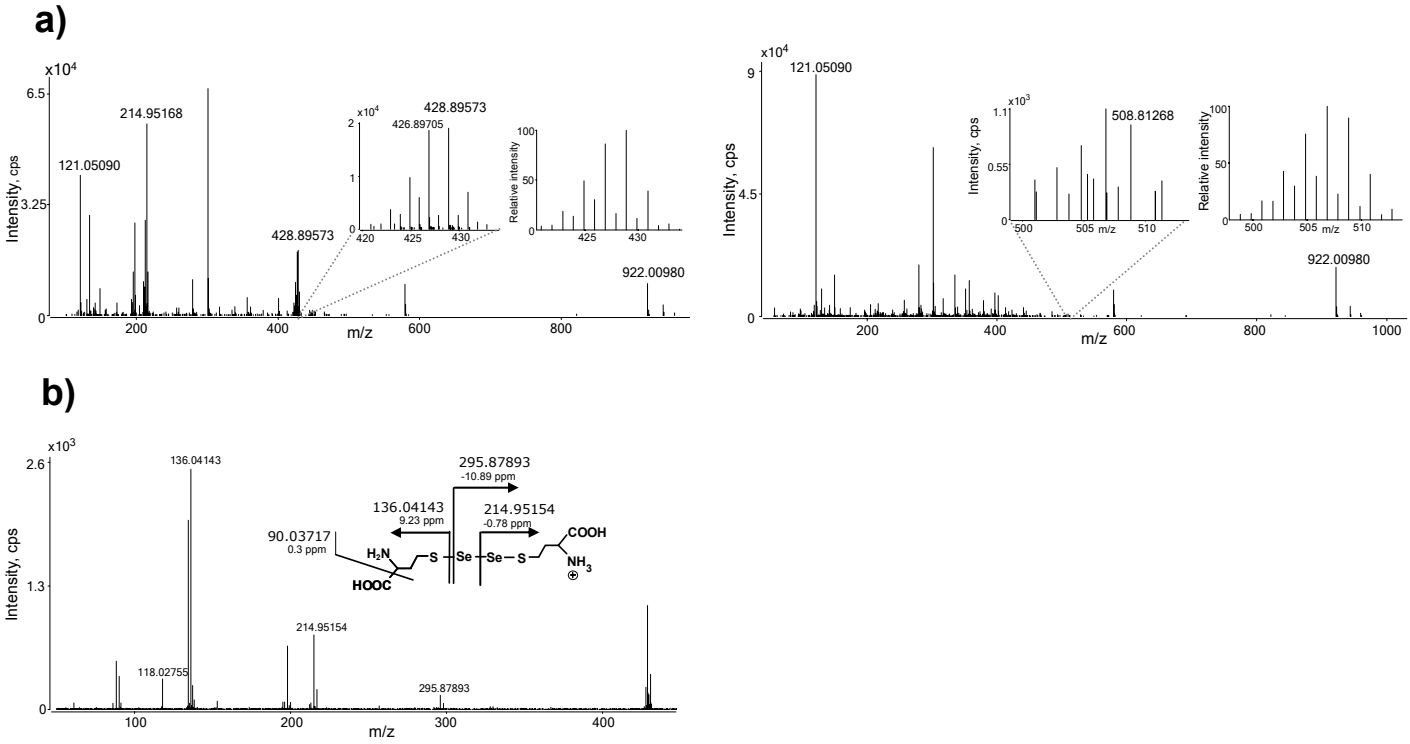


Figure 4. Fullscan spectrum of one of the compounds detected in negative ion mode (*m/z* 428.20558).