Electronic Supplementary Information for the article entitled

Water soluble selenometabolome of *Cardamine violifolia*

by

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Table S1. UPLC-Unispray-QTOFMS instrumental setup parameters

Acquity I-Class UPLC		**Vion IMS Unispray (+/-) -QTOF-MS**	
UPLC column	Acquity BEH C_{18}, 2.1*100 mm; 1.7 µm	Source temperature	120°C
Eluent "A"	water with 0.1 v/v% formic acid	Desolvation temperature	550°C
Eluent "B"	acetonitrile with 0.1 v/v% formic acid	Capillary voltage	300 V
Flow rate	0.4 ml/min	Desolvation gas	1000 L/h
Column temperature	25°C	Cone gas	100 L/h
Gradient	0 – 1.0 min 10% „B" 1.0 – 4.0 min ↑ 80% „B" 4.0 – 4.5 min 80% „B" 4.5 – 5.0 min ↓ 10% „B" 5.0 – 7.0 min 10% „B"	IMS MS scan MS scan time Lock mass MS/MS scan	OFF 100 – 1000 m/z 0.2 s ON 50 – 1000 m/z
Injection volume	3.0 µl	Low mass ramp	20 – 30 eV
Sample temperature	8°C	High mass ramp	30 – 80 eV

Table S2. Effect of defect padding settings on the efficiency of automatic selenium pattern recognition.

Fraction	m/z	Minimally required mass padding (Da) for successful detection			
		at 20 mDa defect padding	at 40 mDa defect padding	at 60 mDa defect padding	at 80 mDa defect padding
#1	282	>1000	17	11	10
	284	89	12	11	11
	407	>1000	121	106	71
	242	27	21	21	21
	391	>1000	>1000	191	116
	391	>1000	>1000	190	116
#2	419	>1000	130	115	86
	581	>1000	>1000	>1000	437
	419	>1000	173	125	115
	401	>1000	120	103	67
	285	>1000	21	13	12
	405	106	98	85	41
	285	>1000	21	13	12
#3	441	391	138	128	100
	419	>1000	175	125	115
	446	>1000	>1000	457	180
	268	>1000	2	2	2
	197	53	52	52	52
	215	40	40	40	39
#4	254	15	12	12	12
	312	53	33	31	31
	271	1	1	1	1
	282	>1000	17	11	10
	284	89	12	11	11

Table S3. Efficiency of automatic selenium pattern recognition. It is to note that the compounds with detected theoretical selenium mass defect include false positive hits and the different isotopologues of the same compound as well.

Fraction	Number of compounds detected	Number of compounds with detected theoretical selenium mass defect	Relative amount of compounds detected with theoretical selenium mass defect	Number of compounds with detected theoretical selenium mass defect	Relative amount of compounds detected with theoretical selenium mass defect
		Settings: defect paddig, 60 mDa; mass padding, 200 Da; minimum intensity, 2000 cps		Settings: defect paddig, 80 mDa; mass padding, 200 Da; minimum intensity, 2000 cps	
#1	7293	350	4.8%	457	6.3%
#2	5062	227	4.5%	277	5.5%
#3	4838	229	4.7%	269	5.6%
#4	4572	178	3.9%	206	4.5%

Table S4. Efficiency of automatic selenium pattern recognition at optimised settings (mass padding: 200 Da; defect padding: 80 mDa). Values in bold indicate successful detection.

FR1		FR2		FR3	FR4	
m/z	background of unsuccessful automatic detection	m/z	background of unsuccessful automatic detection	m/z	m/z	background of unsuccessful automatic detection
241.99302	-	**285.05998**	-	**197.00725**	**254.02883**	-
377.07037	isobaric interference	301.09063	isobaric interference	**241.99302**	**271.02005**	-
391.08672	isobaric interference	405.06603	low intensity	**268.04482**	**282.06027**	-
407.04499	-	416.08220	low intensity	**270.02341**	**284.03997**	-
435.04004	low intensity	**419.05681**	-	**446.09233**	**312.03454**	-
447.11604	low intensity	434.09228	low intensity	**463.02100**	313.02949	low intensity
448.10670	low intensity	537.14451	low intensity		**364.95162**	-
460.10880	low intensity	581.10958	low mass padding		444.86739	low intensity + triple selenium
482.99120	low intensity				489.05794	low intensity
523.12784	low intensity					
552.06109	low intensity					
614.14680	low intensity					