

**Table S1.** Raw data used for the volcano-type graphs, where the following cut-off points were used: FC +/- 10 and *p* value ≤ 0.001.

Positive ionization mode			
Compound	FC (BL_LARGE vs RE_SMALL)	FC (BL_SMALL vs RE_SMALL)	FC (RE_LARGE vs RE_SMALL)
332.1582@12.779002	-351582.53	-351583	-351583
183.1081@8.895998	944966.1	193905.6	292198.9
332.1821@15.537998	1952130.2	1344371	1780623
394.1679@2.1199994	1346078	789117.2	796640.4
340.1479@11.869999	202920.9	347487.3	164694.1
332.188@13.166	151019	361437.9	376447
708.406@14.731998	44953.305	2016271	391480
637.1181@8.558999	49217.72	335920.8	99725.36
537.2063@9.862	65774.266	122407.1	117900.9
642.267@12.203002	89673.41	37662.87	17886.46
282.4973@11.561998	118518.72	192161	31734.24
250.1342@13.998	165751.36	69259.63	49082.79
Negative ionization mode			
Compound	FC (BL_LARGE vs RE_SMALL)	FC (BL_SMALL vs RE_SMALL)	FC (RE_LARGE vs RE_SMALL)
463.2547@10.4470005	14152.336	9173.428	-10.7329
876.1531@14.194	-1057.2604	-1057.2604	26.2196
846.1342@14.11	-1108.4723	-1108.4723	33.48628
333.0914@10.916	-1174.285	19.089523	12.55858
237.0301@11.548002	6213.2295	40793.227	-11.1154
910.5895@14.4609995	179019.19	110802.97	94966.91
298.1522@10.998998	79170.98	27540.6	1403.218
665.3774@14.526	84806.27	66009.734	140005.6
433.1104@11.046998	65116.605	57927.45	10.16416
903.4014@10.897002	5850.067	5318.0244	-10.2136
384.0724@7.732001	-4247.4536	-4247.4536	10.42428
506.2968@15.582	3396.5596	4648.3154	-11.8669
541.1014@9.895998	61347.156	48750.895	1104.502
903.4017@11.130998	4285.8647	4070.7083	-11.4437
711.2312@11.475001	63430.223	8826.391	67.52856
481.0769@11.511001	34584.086	20135.436	1139.678
664.4404@14.481002	2914.5627	-12.84924	3384.009
186.0454@12.231999	-991.906	24.399052	11.22653
341.193@11.543	32256.059	21848.102	526.2276

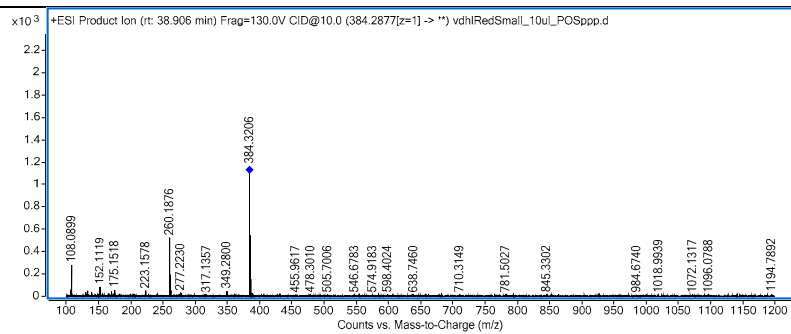
**Table S2.** The MS/MS spectra of the tentatively identified components of *Lepidium peruvianum* extracts

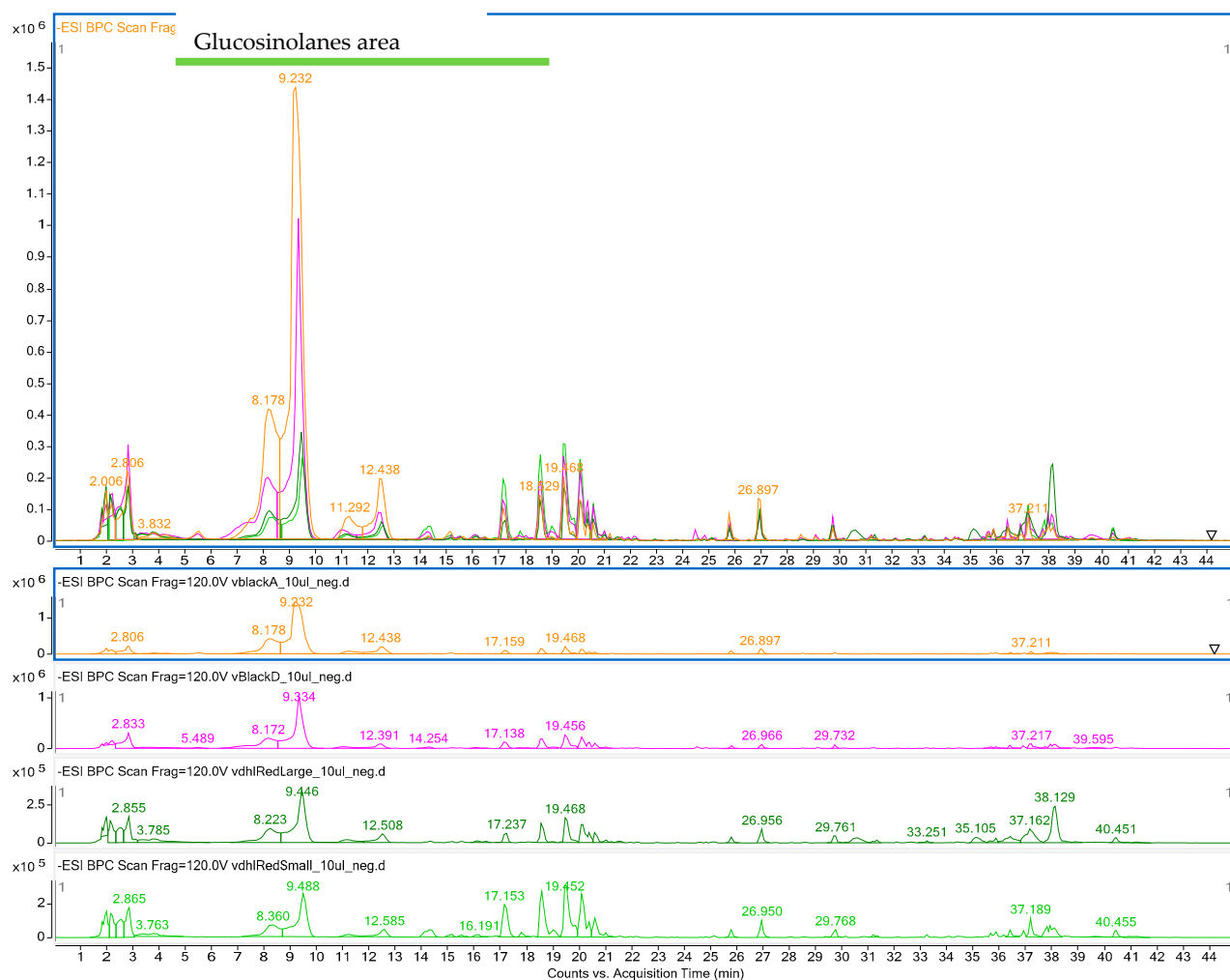
No	Name of compound	MS/MS spectrum
1	Glucosinalbin	<p>-ESI Product Ion (rt: 4.517 min) Frag=140.0V CID@20.0 (424.0397[z=1] -&gt; **) vBlackD_10ul_neg.d</p>
2	Glucotropaeolin	<p>-ESI Product Ion (rt: 9.308 min) Frag=130.0V CID@10.0 (408.0453[z=1] -&gt; **) vBlackD_10ul_neg.d</p>
3	Glucolimnanthin	<p>-ESI Product Ion (rt: 12.446 min) Frag=140.0V CID@20.0 (438.0544[z=1] -&gt; **) vdhIRedSmall_10ul_neg.d</p>
4	Pentenylglucosinolate	<p>-ESI Product Ion (rt: 16.904 min) Frag=130.0V CID@10.0 (371.1004[z=1] -&gt; **) vBlackD_10ul_neg.d</p>
5	indolyl-hexyl-methyl-cyclohexane-glucosinolate	<p>-ESI Product Ion (rt: 17.782 min) Frag=130.0V CID@10.0 (521.2051[z=1] -&gt; **) vdhIRedLarge_10ul_neg.d</p>

6	Lepidiline E	<p><math>\times 10^4</math></p> <p>+ESI Product Ion (rt: 17.872 min) Frag=130.0V CID@10.0 (227.1530[z=1] -&gt; **) vBlackD_10ul_POSpp.d</p> <p>Counts vs. Mass-to-Charge (m/z)</p>
7	Lepidiline A	<p><math>\times 10^4</math></p> <p>+ESI Product Ion (rt: 23.252 min) Frag=140.0V CID@20.0 (277.1681[z=1] -&gt; **) vBlackA_10ul_POSpp.d</p> <p>Counts vs. Mass-to-Charge (m/z)</p>
8	Lepidiline C	<p><math>\times 10^3</math></p> <p>+ESI Product Ion (rt: 23.587 min) Frag=130.0V CID@10.0 (307.1785[z=1] -&gt; **) vBlackA_10ul_POSpp.d</p> <p>Counts vs. Mass-to-Charge (m/z)</p>
9	Lepidiline D	<p><math>\times 10^3</math></p> <p>+ESI Product Ion (rt: 24.530 min) Frag=140.0V CID@20.0 (321.1946[z=1] -&gt; **) vdhlRedSmall_10ul_POSpp.d</p> <p>Counts vs. Mass-to-Charge (m/z)</p>
10	Macamide B	<p><math>\times 10^3</math></p> <p>+ESI Product Ion (rt: 34.955 min) Frag=140.0V CID@20.0 (346.3091[z=1] -&gt; **) vdhlRedSmall_10ul_POSpp.d</p> <p>Counts vs. Mass-to-Charge (m/z)</p>

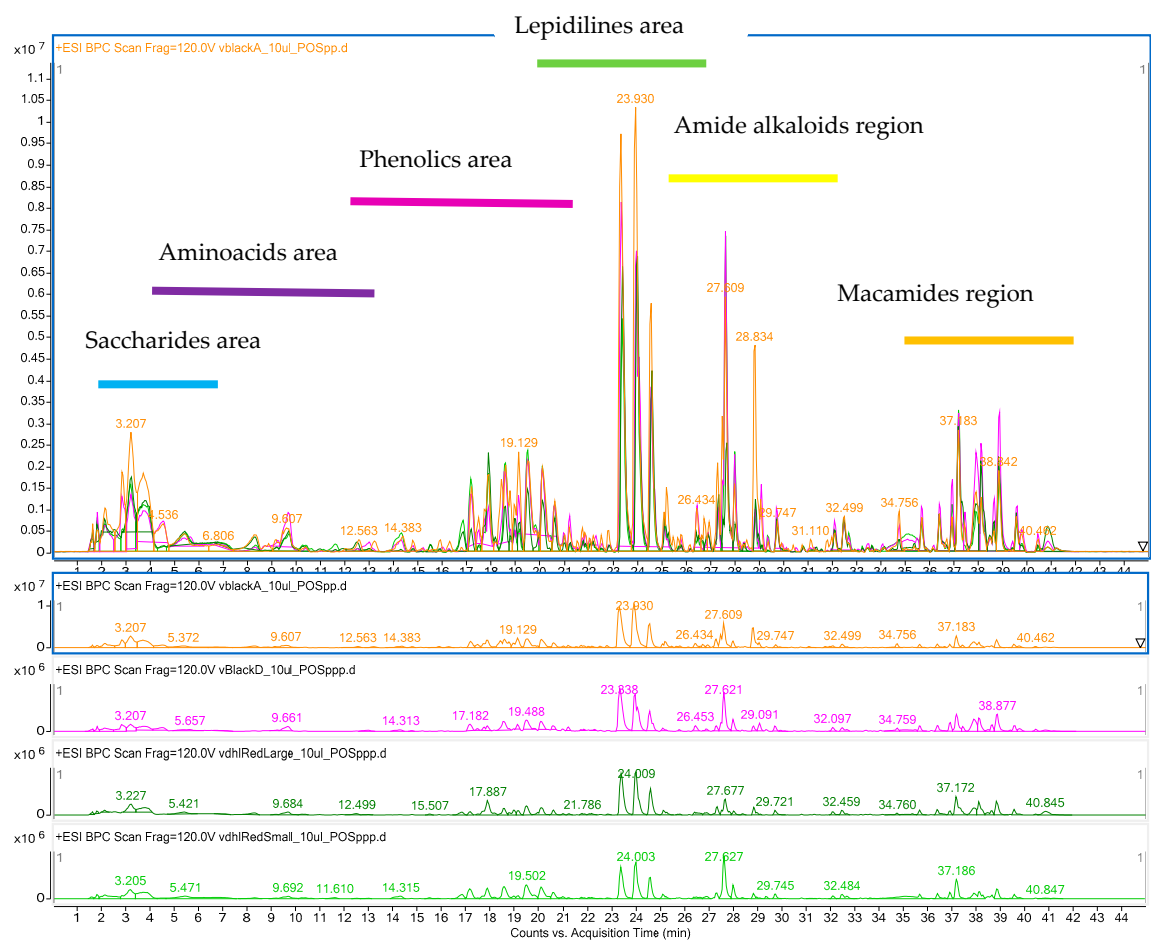
11

Benzylo-oxo-octadecadienamide





**Figure S1.** The total mass chromatograms recorded in the negative ionization mode for the tested maca samples.



**Figure S2.** The total mass chromatograms recorded in the positive ionization mode for the tested maca samples.

**Table S3.** Raw data used for the volcano-type graphs, where the following cut-off points were used: FC +/- 10 and *p* value ≤ 0.001.

Positive ionization mode			
Compound@retention time	FC (BL_LARGE vs RE_SMALL)	FC (BL_SMALL vs RE_SMALL)	FC (RE_LARGE vs RE_SMALL)
332.1582@12.779002	-351582.53	-351583	-351583
183.1081@8.895998	944966.1	193905.6	292198.9
332.1821@15.537998	1952130.2	1344371	1780623
394.1679@2.119994	1346078	789117.2	796640.4
340.1479@11.869999	202920.9	347487.3	164694.1
332.188@13.166	151019	361437.9	376447
708.406@14.731998	44953.305	2016271	391480
637.1181@8.558999	49217.72	335920.8	99725.36
537.2063@9.862	65774.266	122407.1	117900.9
642.267@12.203002	89673.41	37662.87	17886.46
282.4973@11.561998	118518.72	192161	31734.24
250.1342@13.998	165751.36	69259.63	49082.79
Negative ionization mode			
Compound@retention time	FC (BL_LARGE vs RE_SMALL)	FC (BL_SMALL vs RE_SMALL)	FC (RE_LARGE vs RE_SMALL)
463.2547@10.4470005	14152.336	9173.428	-10.7329
876.1531@14.194	-1057.2604	-1057.2604	26.2196
846.1342@14.11	-1108.4723	-1108.4723	33.48628
333.0914@10.916	-1174.285	19.089523	12.55858
237.0301@11.548002	6213.2295	40793.227	-11.1154
910.5895@14.4609995	179019.19	110802.97	94966.91
298.1522@10.998998	79170.98	27540.6	1403.218
665.3774@14.526	84806.27	66009.734	140005.6
433.1104@11.046998	65116.605	57927.45	10.16416
903.4014@10.897002	5850.067	5318.0244	-10.2136
384.0724@7.732001	-4247.4536	-4247.4536	10.42428
506.2968@15.582	3396.5596	4648.3154	-11.8669
541.1014@9.895998	61347.156	48750.895	1104.502
903.4017@11.130998	4285.8647	4070.7083	-11.4437
711.2312@11.475001	63430.223	8826.391	67.52856
481.0769@11.511001	34584.086	20135.436	1139.678
664.4404@14.481002	2914.5627	-12.84924	3384.009
186.0454@12.231999	-991.906	24.399052	11.22653
341.193@11.543	32256.059	21848.102	526.2276