## Supplementary information

**Table S1,** Peak area of LC/MS analysis on 1.00 g of pulverised and non-pulverised white Bolivian seeds extracted at 80, 100 and 120°C.

| Name of compound | [M-H]- | MSMS | PHWE at 80°C | | PHWE at 100°C | | PHWE at 120°C | |
|---|---|---|---|---|---|---|---|---|
| | m/z | m/z | Pulverised | Seed | Pulverised | Seed | Pulverised | Seed |
| Vanillic acid | 167 | 151,125,106,80, 58 | 429285 ± 26560 | 7343251 ± 312529 | 423620 ± 83732 | 61083684 ± 71992679 | 502747 ± 118151 | 9304894 ± 996688 |
| Vanillic acid glucoside | 329 | 151,133, 109 | 23529169 ± 1232595 | 26198220 ± 3361363 | 23221184 ± 1989702 | 2887539 ± 1546413 | 24488878 ± 2850139 | 4808947 ± 3752363 |
| Vanillin | 151 | 108,80,66,61 | 24054806 ± 2876132 | 14701647 ± 3895764 | 17496702 ± 2445193 | 13583596 ± 952963 | 11550842 ± 3163558 | 17884142 ± 3536010 |
| p-coumaric acid | 163 | 99,91,73,71,69,57 | 15525574 ± 891590 | 2816675 ± 401223 | 15419089 ± 615817 | 2384406 ± 255870 | 16011481 ± 1485634 | 2454211 ± 298439 |
| Ferulic acid | 193 | 147, 128, 113, 89, 77,75, 71, 67,59,57,55 | 6909818 ± 1547141 | 3321839 ± 1268691 | 9175112 ± 412082 | 3204020 ± 96495 | 12243099 ± 5204634 | 3316394 ± 543556 |
| Caffeic acid | 179 | 89, 71, 59, 57 | 71004668 ± 7488133 | 2006711 ± 188797 | 73292001 ± 3996372 | 2268681 ± 98687 | 97066891 ± 27878225 | 1993441 ± 44515 |
| Catechin | 289 | 171, 157, 145, 133,127, 111, 106 | 39767749 ± 2120859 | 855751 ± 97457 | 33305070 ± 3521007 | 1134720 ± 192802 | 32103345 ± 2451508 | 1310063 ± 375367 |
| Daidzein | 263 | 230, 166, 146, 124, 110, 107, 102 | 754375 ± 75626 | 1272921 ± 151480 | 703069 ± 28294 | 1787250 ± 183048 | 776080 ± 167326 | 1312328 ± 83216 |
| Genistein | 269 | 197, 173, 157, 143, 139, 121 | 4301403 ± 223513 | 1110627 ± 91027 | 4354205 ± 386528 | 1138212 ± 171189 | 4515149 ± 764320 | 1087311 ± 16170 |
| Quercetin | 301 | 193, 168,150, 125, 107 | 1448989 ± 65609 | 1657788 ± 649599 | 1593519 ± 136412 | 1448169 ± 140901 | 1874591 ± 196472 | 1854812 ± 914458 |
| Quercetin 3-rutinoside | 609 | 300, 285, 287, 257, 137, 114 | 17623074 ± 3972165 | 724508 ± 336429 | 16960368 ± 4479701 | 575094 ± 41257 | 14262067 ± 2046964 | 821165 ± 110140 |
| Unknown | 431 | | 47572042 ± 3440460 | 3703383 ± 796058 | 50068554 ± 262786 | 4238304 ± 96782 | 47773038 ± 6900434 | 4952239 ± 337837 |
| Unknown | 319 | 242, 206, 189, 160, 133, 125 | 9404690 ± 859827 | 2257689 ± 389281 | 9687765 ± 836753 | 2168055 ± 261909 | 8251738 ± 196762 | 2227992 ± 105674 |
| Unknown | 726 | 726,284 | 10305678 ± 1256805 | 992904 ± 452820 | 9245759 ± 1496059 | 765332 ± 39072 | 9626085 ± 561538 | 1462503 ± 398794 |
| Unkownn | 479 | 389, 318, 258, 139 | 2265209 ± 95452 | 708803 ± 288759 | 2332930 ± 215038 | 623832 ± 52634 | 2452477 ± 398245 | 821918 ± 20530 |

Results were expressed as a mean of a triplicate measurement ± SD (n=3).

**Table S2,** Normalised peak area of LC/MS analysis of pulverised and non-pulverised white Bolivian seeds based on the average peak area of the LC/MS data in Table S1.

| Name of compound | [M-H]- | MSMS | PHWE at 80°C | | PHWE at 100°C | | PHWE at 120°C | |
|---|---|---|---|---|---|---|---|---|
| | m/z | m/z | Pulverised | Seed | Pulverised | Seed | Pulverised | Seed |
| Vanillic acid | 167 | 151,125,106,80, 58 | 0.00119 ± 9.94E-05 | 0.0918 ± 0.0153 | 0.00117 ± 0.000203 | 0.363 ± 0.278 | 0.00119 ± 0.000459 | 0.141 ± 0.0324 |
| Vanillic acid glucoside | 329 | 151,133, 109 | 0.0651 ± 0.00146 | 0.0323 ± 0.0392 | 0.0642 ± 0.00576 | 0.0396 ± 0.0319 | 0.0557 ± 0.0146 | 0.0643 ± 0.0411 |
| Vanillin | 151 | 108,80,66,61 | 0.0668 ± 0.0086 | 0.176 ± 0.011 | 0.0482 ± 0.00541 | 0.169 ± 0.0767 | 0.0276 ± 0.0114 | 0.260 ± 0.0141 |
| p-coumaric acid | 163 | 99,91,73,71,69,57 | 0.0430 ± 0.00118 | 0.0345 ± 0.0019 | 0.0426 ± 0.000879 | 0.0303 ± 0.0147 | 0.0367 ± 0.0101 | 0.0360 ± 0.001 |
| Ferulic acid | 193 | 147, 128, 113, 89, 77,75, 71, 67,59,57,55 | 0.0191 ± 0.00386 | 0.0389 ± 0.00688 | 0.0254 ± 0.0017 | 0.0404 ± 0.0185 | 0.0278 ± 0.014 | 0.0487 ± 0.00565 |
| Caffeic acid | 179 | 89, 71, 59, 57 | 0.196 ± 0.0158 | 0.0248 ± 0.0031 | 0.203 ± 0.0157 | 0.0278 ± 0.118 | 0.225 ± 0.0875 | 0.0298 ± 0.00423 |
| Catechin | 289 | 171, 157, 145, 133,127, 111, 106 | 0.110 ± 0.00813 | 0.0108 ± 0.00256 | 0.0919 ± 0.00768 | 0.0150 ± 0.00786 | 0.0756 ± 0.0243 | 0.0200 ± 0.0078 |
| Daidzein | 263 | 230, 166, 146, 124, 110, 107, 102 | 0.00209 ± 0.000221 | 0.0158 ±0.00276 | 0.00194 ± 0.000101 | 0.0213 ± 0.00851 | 0.00169 ± 0.000195 | 0.0195 ± 0.0027 |
| Genistein | 269 | 197, 173, 157, 143, 139, 121 | 0.0119 ± 0.000271 | 0.0138 ± 0.00269 | 0.0121 ± 0.00124 | 0.0132 ± 0.00484 | 0.0126 ± 0.00114 | 0.0162 ± 0.00201 |
| Quercetin | 301 | 193, 168,150, 125, 107 | 0.00402 ± 0.000284 | 0.0196 ± 0.00436 | 0.00441 ± 0.000447 | 0.0175 ± 0.00742 | 0.00428 ± 0.00106 | 0.0259 ± 0.00877 |
| Quercetin 3-rutinoside | 609 | 300, 285, 287, 257, 137, 114 | 0.0488 ± 0.0108 | 0.00802 ± 0.00209 | 0.0468± 0.0121 | 0.00940 ± 0.000575 | 0.0337 ± 0.0115 | 0.0121 ± 0.00106 |
| Unknown | 431 | | 0.132 ± 0.0108 | 0.0449 ± 0.00382 | 0.138± 0.00352 | 0.0531 ± 0.0239 | 0.109 ± 0.0319 | 0.0732 ± 0.00558 |
| Unknown | 319 | 242, 206, 189, 160, 133, 125 | 0.0261 ± 0.00226 | 0.0279 ± 0.0052 | 0.0268 ± 0.00238 | 0.026 ± 0.0109 | 0.0193 ± 0.00611 | 0.033± 0.00318 |
| Unknown | 726 | 726,284 | 0.0285 ± 0.0031 | 0.0115 ± 0.003 | 0.0256 ± 0.00419 | 0.00932 ± 0.0039 | 0.0228 ± 0.00789 | 0.0210 ± 0.0025 |
| Unkownn | 479 | 389, 318, 258, 139 | 0.00628 ± 0.000324 | 0.00746± 0.00204 | 0.00646 ± 0.000708 | 0.00629 ± 0.00315 | 0.00586± 0.00249 | 0.0122± 0.00142 |

Results were based on the mean of a triplicate measurement ± SD (n=3).

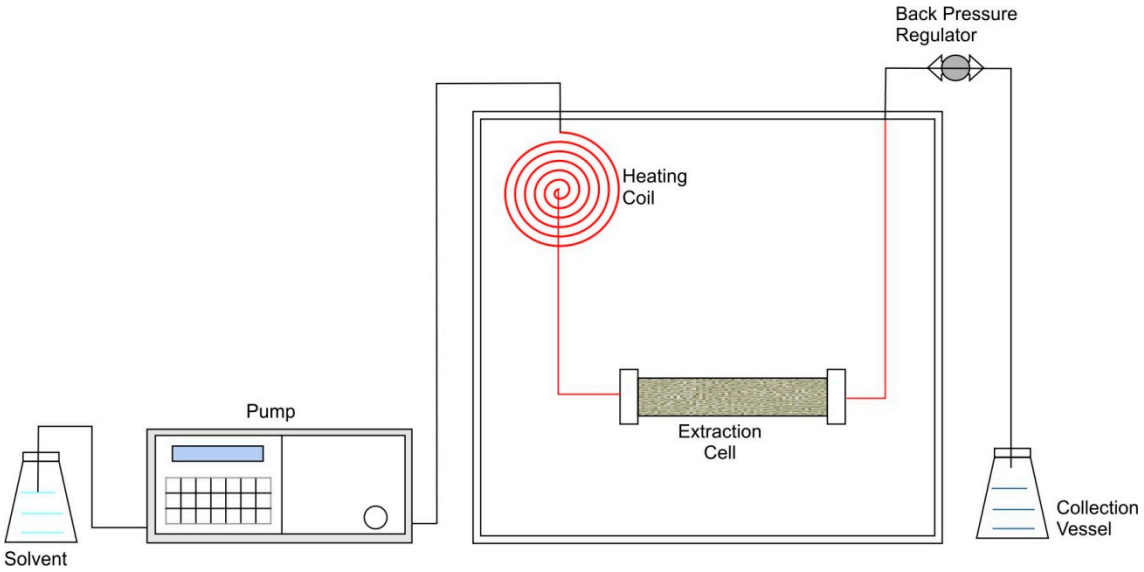



Figure S1. Instrumental setup for pressurized hot water extraction (PHWE) system.

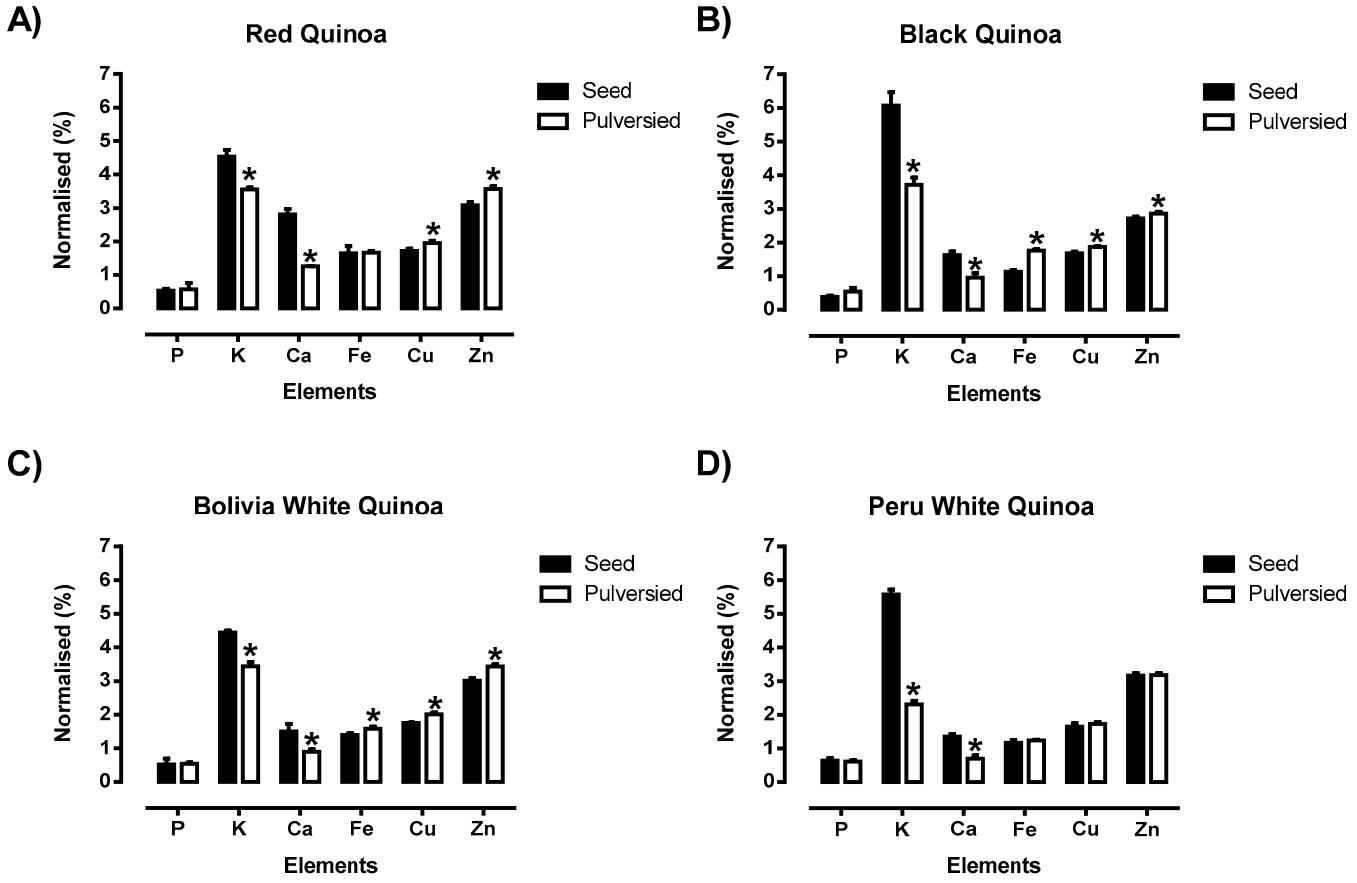



Figure S2: Normalized peak intensity by XRF from red (A), black (B), Bolivia white (C) and Peru white (D) quinoa. * Significant difference ($p \leq 0.05$) between whole seed and pulverized seeds from black, red and white quinoa. Pulverization of the quinoa significantly decreased K and Ca when compared to whole seed. However, in most cases with the exception of white quinoa (Peru), other elements such as Fe, Cu and Zn were significantly increased in the pulverized seeds when compared to whole seeds. Data are expressed as mean ± SD (n=3).

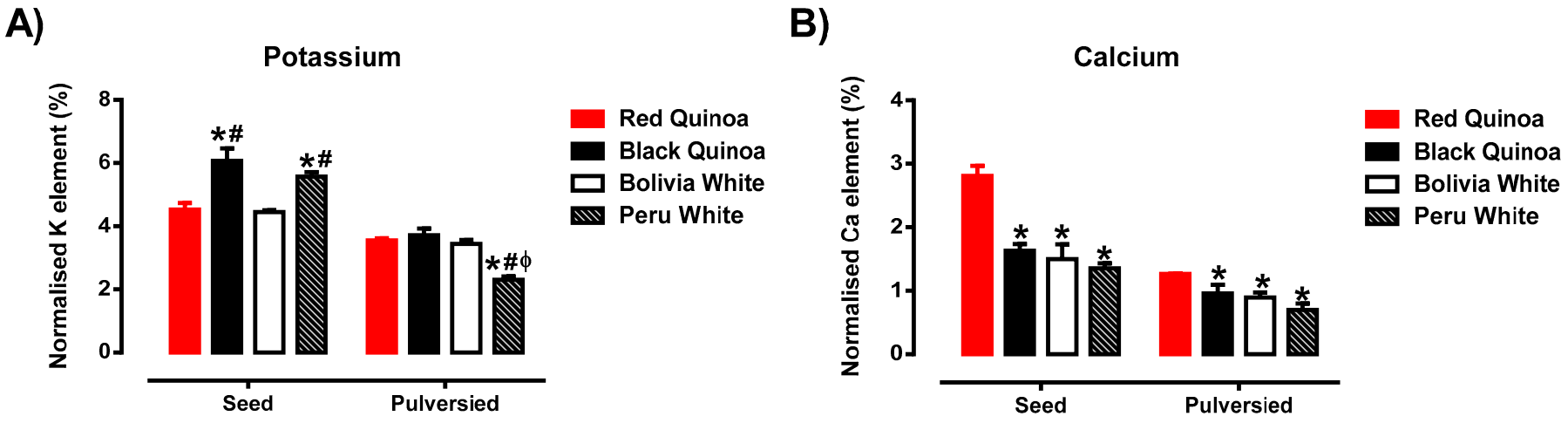
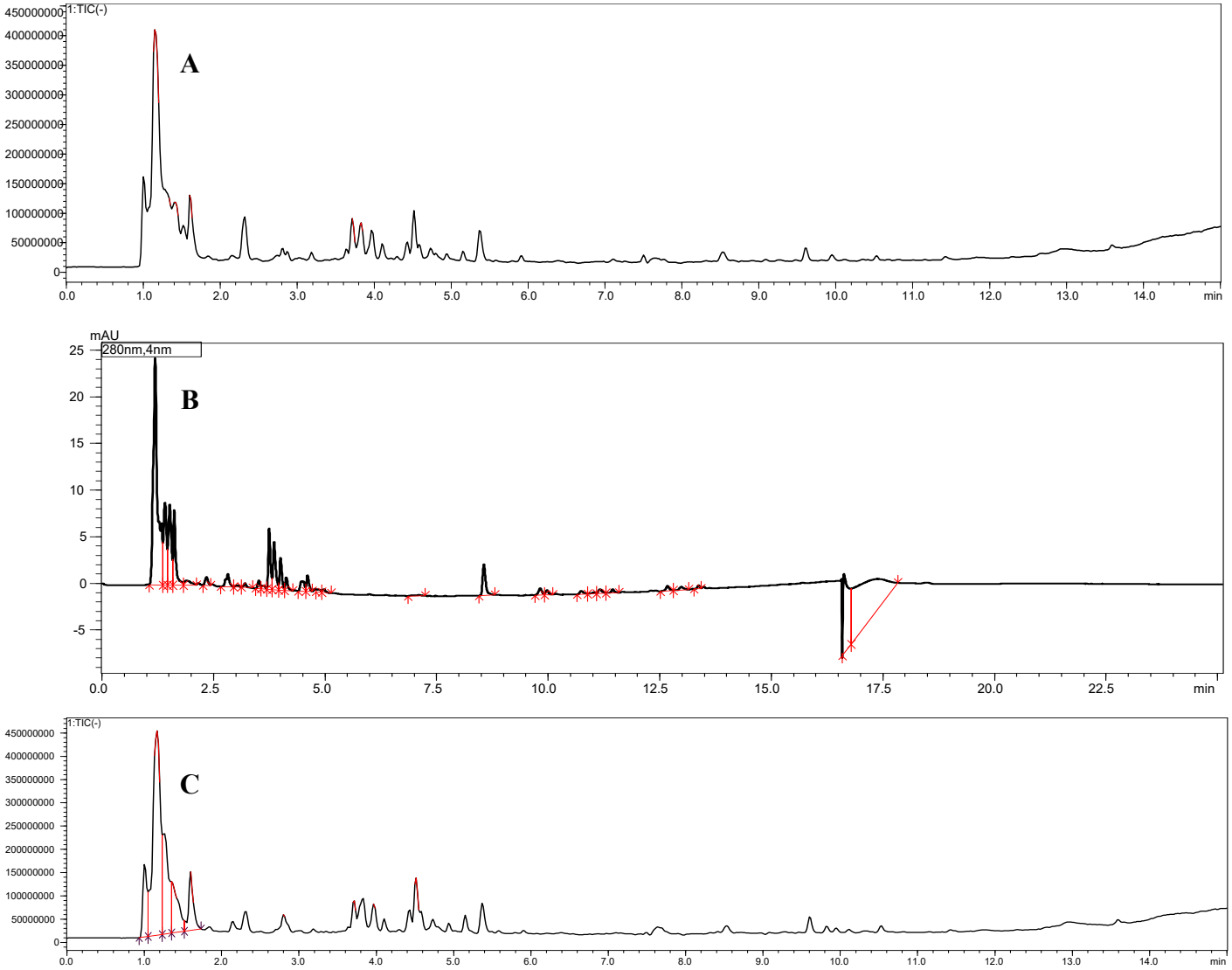
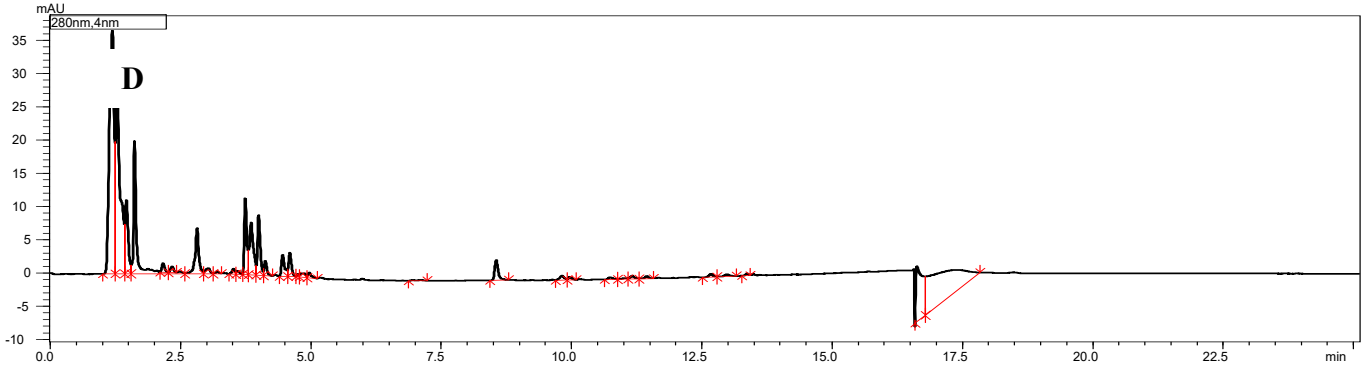
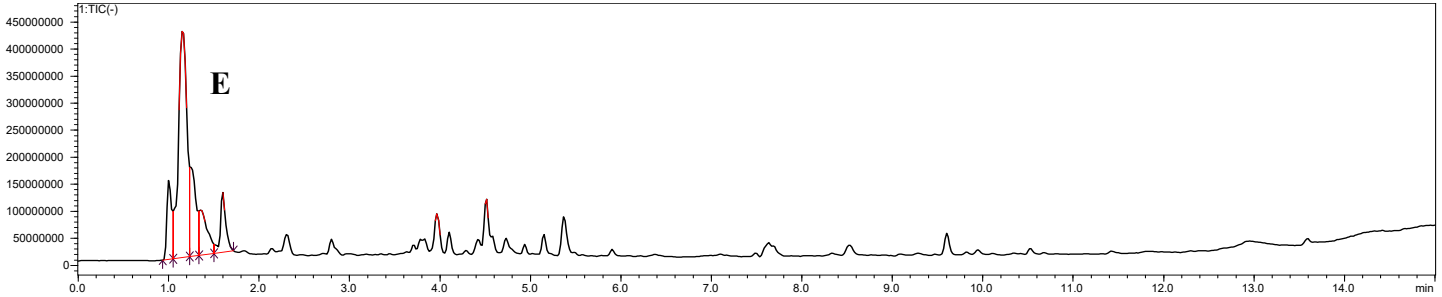
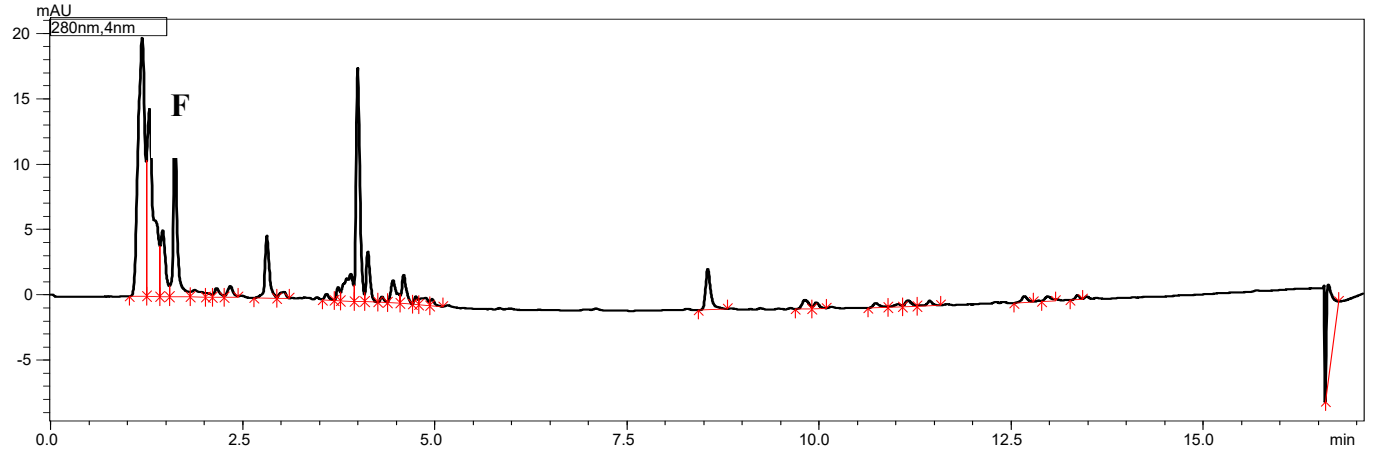



Figure S3: Comparison of normalized peak intensity of potassium (A) and Calcium (B) between red, black, Bolivia white and Peru white quinoa. * Significant difference ($p \leq 0.05$) between red quinoa within whole seed and pulverized seeds. # Significant difference ($p \leq 0.05$) between Bolivia white quinoa within whole seed and pulverized seeds. Φ Significant difference ($p \leq 0.05$) between black quinoa within whole seed and pulverized seeds. Data are expressed as mean ± SD (n=3).


1:TIC(-)
A
mAU
280nm,4nm
B
1:TIC(-)
C
min


mAU
280nm,4nm
D
35
30
25
20
15
10
5
0
-5
-10
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
22.5
min


1:TIC(-)
E
450000000
400000000
350000000
300000000
250000000
200000000
150000000
100000000
50000000
0
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
min


mAU
280nm,4nm
F
20
15
10
5
0
-5
0.0
2.5
5.0
7.5
10.0
12.5
15.0
min

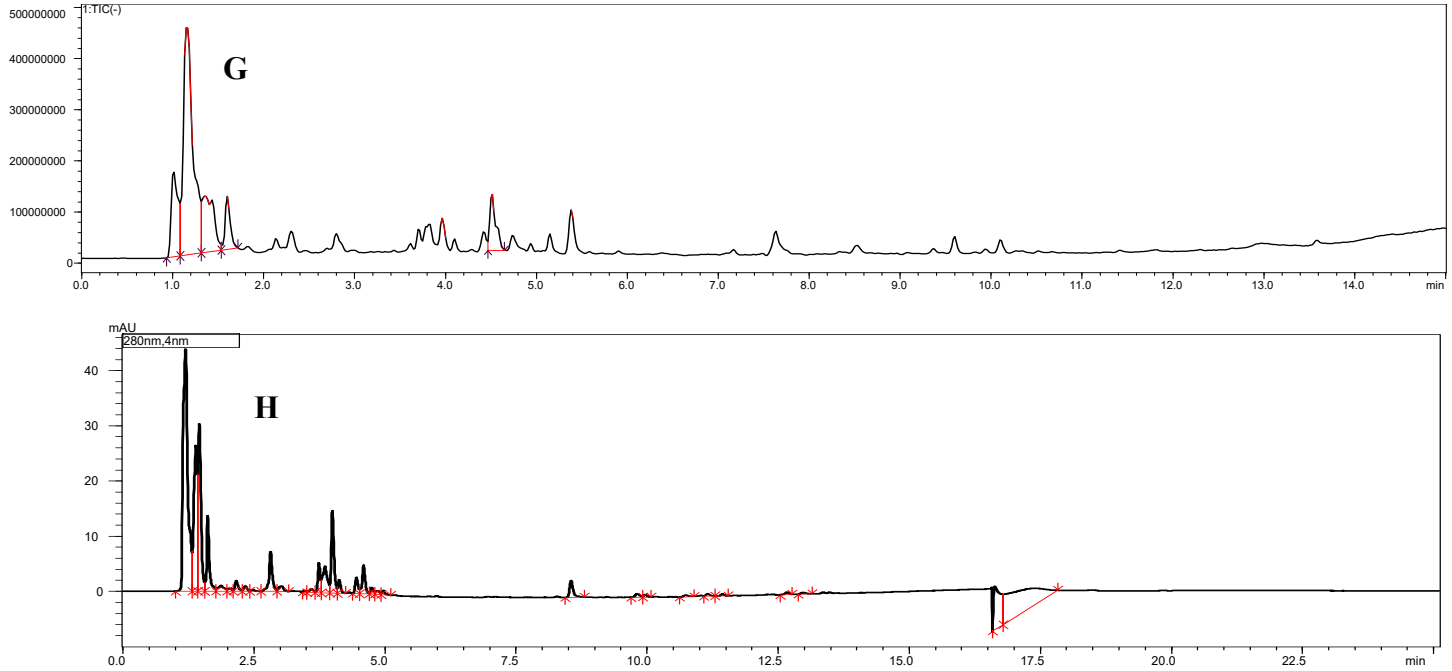



**Figure S4.** LC-UV-MS chromatograms of black, red and white quinoas. A and B: Black quinoa, C and D: Red quinoa, E and F G: White Peruvian quinoa, G and H: White Bolivian quinoa. 1: LC-MS, 2: LC-UV detected at 280nm.