

# Supplementary Material

## Discovery of Species-Specific Peptide Markers for Superseed Authentication Using Targeted LC-MS/MS Proteomics

**Sorel Tchewonpi Sagu <sup>1,\*</sup>, Beatrice Schnepf <sup>2</sup>, Peter Stenzel <sup>3</sup>, Kapil Nichani <sup>2</sup>, Alexander Erban <sup>3</sup>, Joachim Kopka <sup>3</sup>, Harshadrai M. Rawel <sup>2</sup>, Andrea Henze <sup>1</sup>**

**1** Institute of Agricultural and Nutritional Sciences, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 2, 06120 Halle (Saale), Germany; andrea.henze@landw.uni-halle.de

**2** Institute of Nutritional Science, University of Potsdam, Arthur-Scheunert-Allee 114-116, 14558 Nuthetal, Germany; bea.schnepf@gmail.com (B.S.); kapil.nichani@uni-potsdam.de (K.N.); hmrawel@yahoo.de (H.M.R.)

**3** Max-Planck-Institut of Molecular Plant Physiology, Potsdam Science Park, Am Mühlenberg 1, 14476 Potsdam, Germany; p.stenzel@uke.de (P.S.); erban@mpimp-golm.mpg.de (A.E.); kopka@mpimp-golm.mpg.de (J.K.)

**\*** Correspondence: sorel.sagu@landw.uni-halle.de; Tel.: +49-345-5522-650

## **Content**

**Figure S1.** Fat content in representative samples of eleven selected superfoods.

**Figure S2.** Distribution of fat content across all analyzed samples from (A) flaxseed, (B) sesame, (C) amaranth, (D) hemp, (E) quinoa, and (F) poppy seed, highlighting intra-species variability.

**Figure S3.** Comparison between the protein content obtained from representative samples of eleven superfoods and corresponding values reported in the literature.

**Figure S4.** Comparative analysis of protein concentration and extracted protein yield from the modified SDS extraction protocol, with and without the addition of TCEP and IAA, across flaxseed, sesame, and black cumin samples.

**Figure S5.** SDS-PAGE of flaxseed samples from the final standardized SDS extraction method.

**Figure S6.** SDS-PAGE of sesame samples from the final standardized SDS extraction method.

**Figure S7.** SDS-PAGE of (A) amaranth samples and (B) hemp samples from the final standardized SDS extraction method.

**Figure S8.** SDS-PAGE of all quinoa samples from the final standardized SDS extraction method.

**Figure S9.** SDS-PAGE of all poppy seed samples from the final standardized SDS extraction method.

**Figure S10.** Recovery of the internal standard GWGG in the S40 flaxseed, S100 amaranth, S200 hemp, S301 quinoa, S60 sesame and S510 poppy seed compared to the in blank.

**Figure S11.** Linearity of quantifier peptides of (a) amaranth, (b) flaxseed and (c) hem seeds;

**Figure S12.** Linearity of quantifier peptides of (a) poppy, (b) quinoa and (c) sesame seeds;

**Figure S13.** Visual representation of whole (upper row) and ground forms (lower row) of selected seed samples used in this study.

**Table S1.** List of the sample materials used in this study, including the different superfoods, their corresponding sample codes, color, origin, and the commercial producers.

**Table S2.** Flow gradient of the final LC-MS/MS method

**Table S3.** Overview of the final set of proteins selected for targeted HPLC-MS/MS analysis for each superfood, aiming to identify potential biomarkers

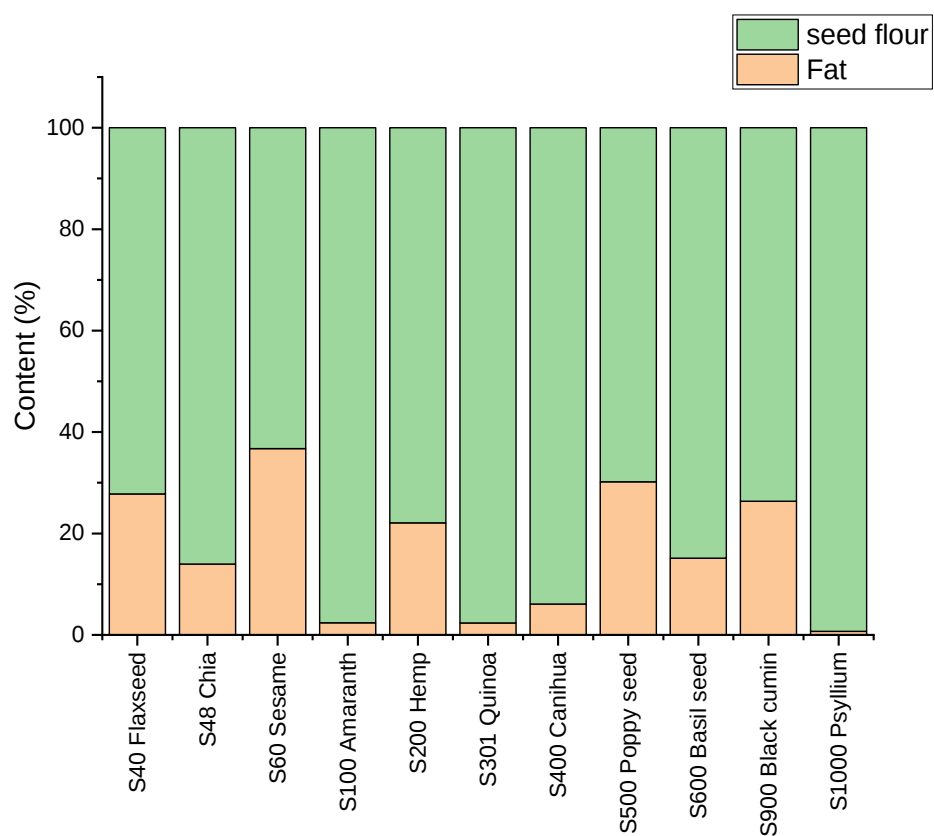
**Table S4.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected sesame proteins

**Table S5.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected amaranth proteins

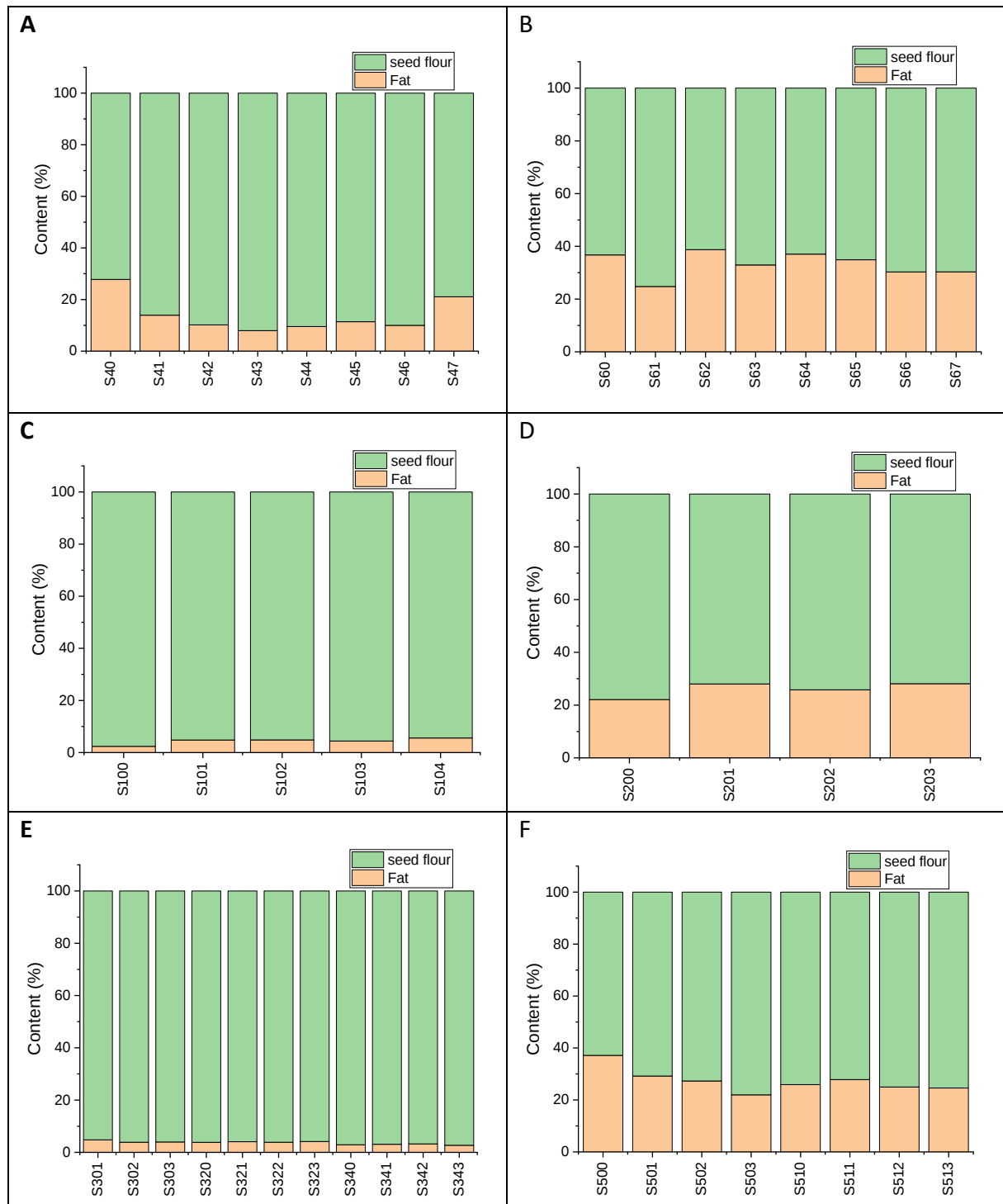
**Table S6.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected hemp proteins

**Table S7.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected quinoa proteins

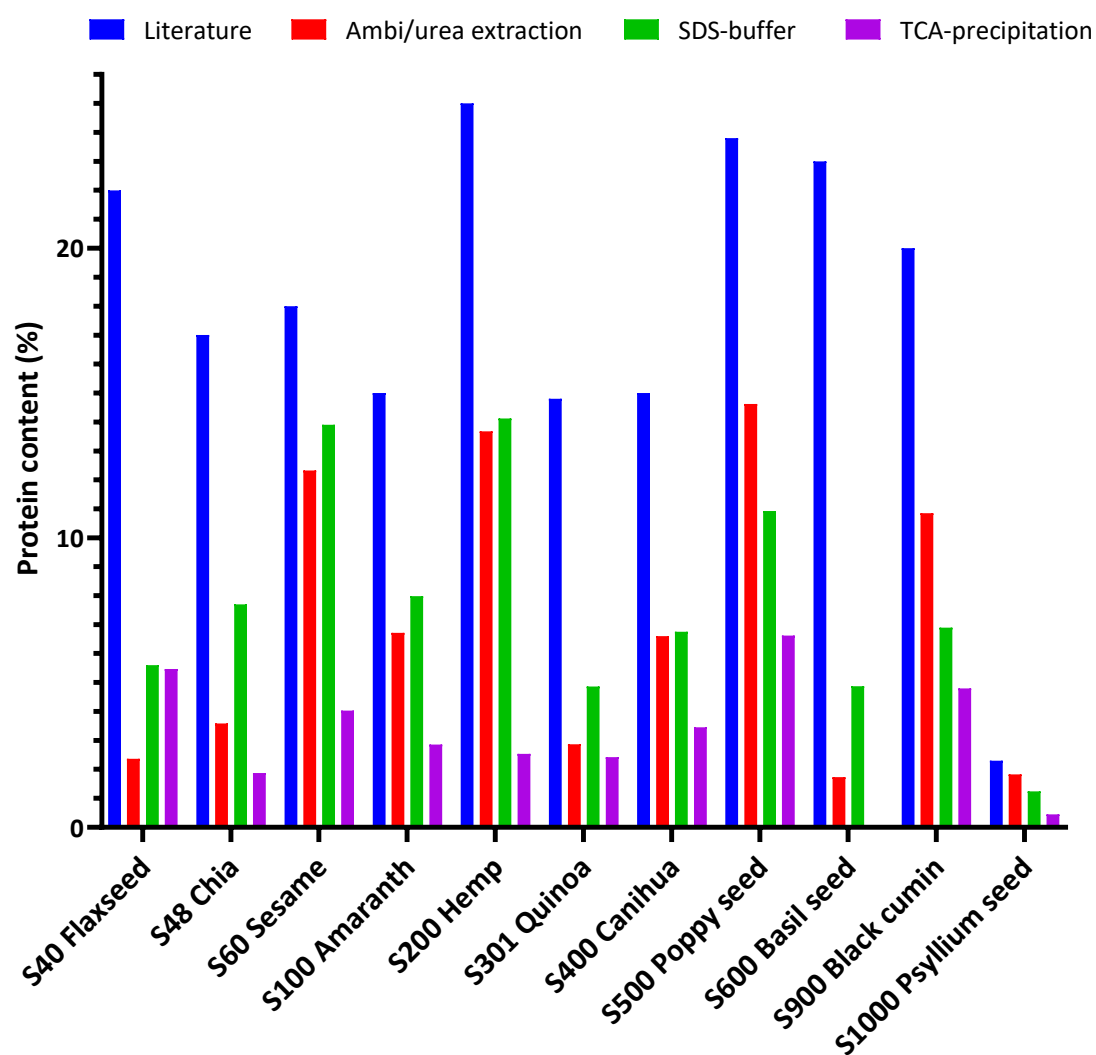
**Table S8.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected poppy seed proteins



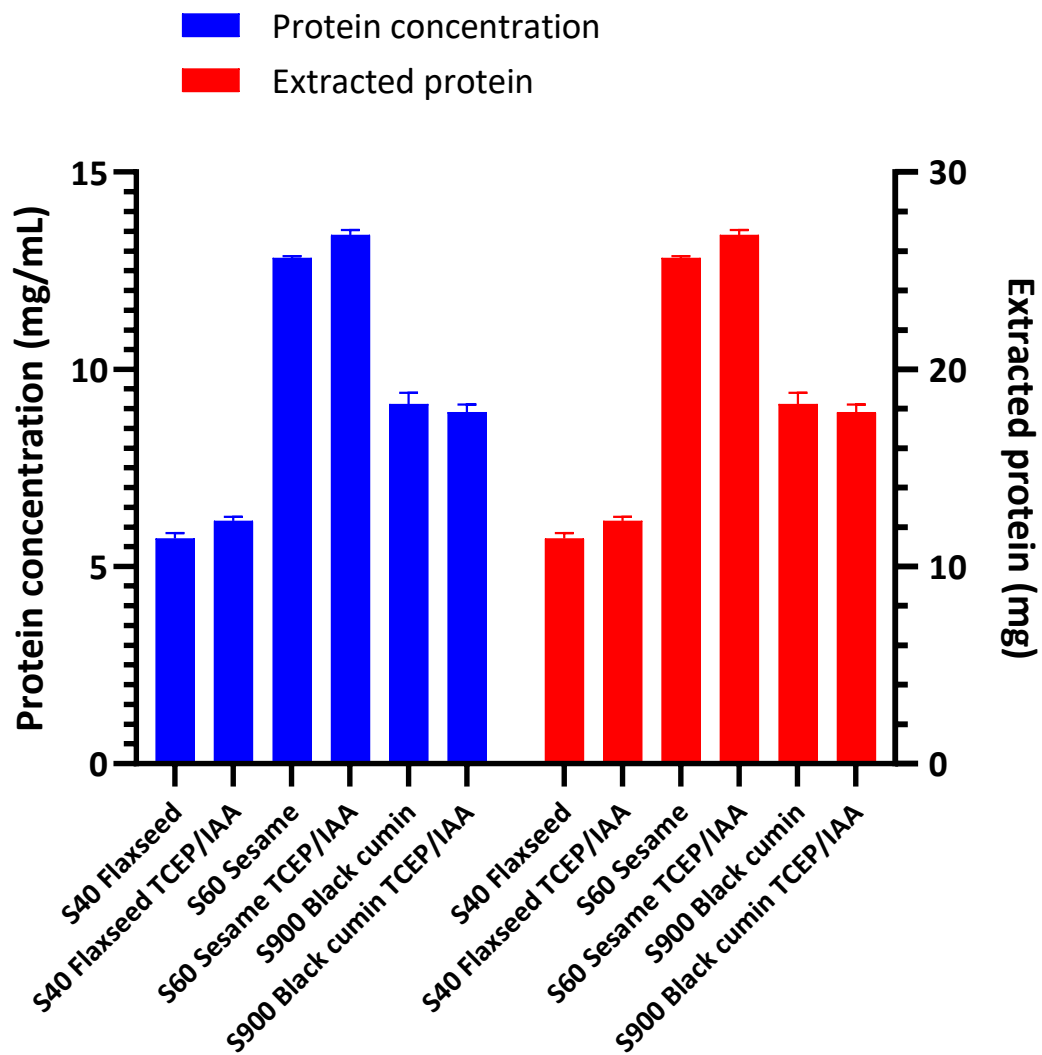
**Figure S1.** Fat content in representative samples of eleven selected superfoods.



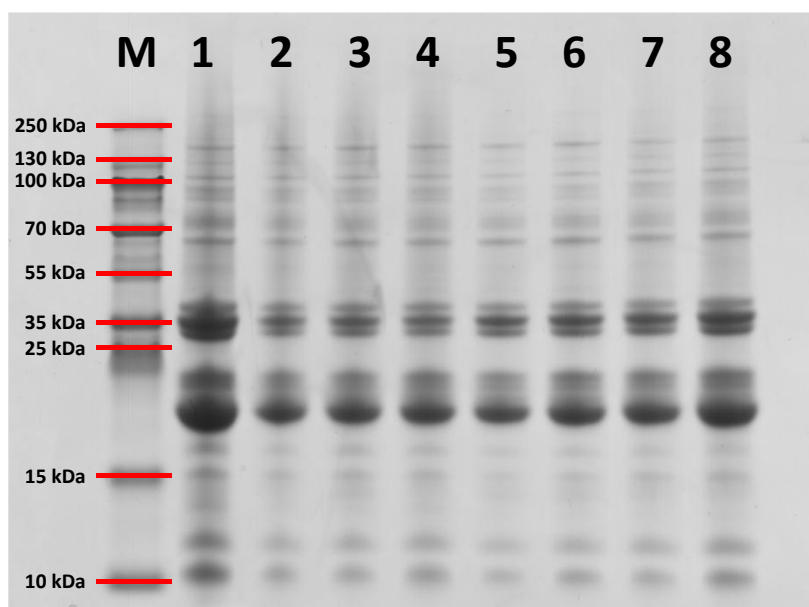
**Figure S2.** Distribution of fat content across all analyzed samples from (A) flaxseed, (B) sesame, (C) amaranth, (D) hemp, (E) quinoa, and (F) poppy seed, highlighting intra-species variability.



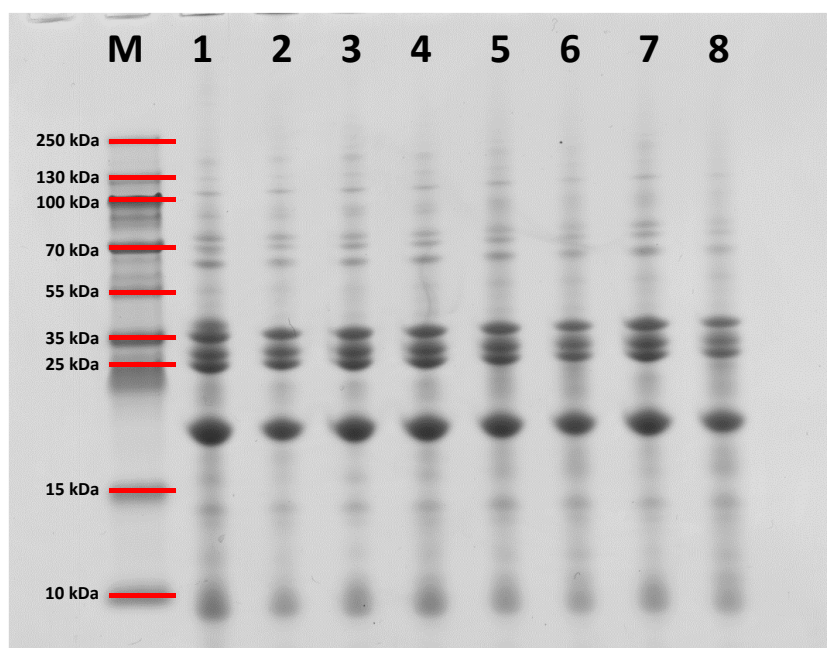
**Figure S3.** Comparison between the protein content obtained from representative samples of eleven superfoods and corresponding values reported in the literature.



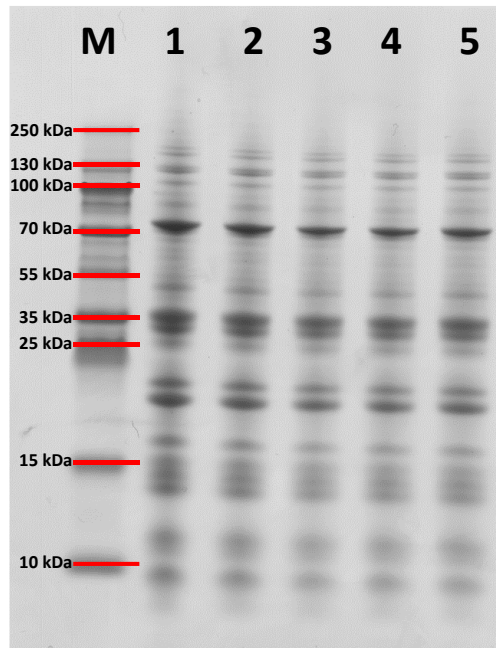
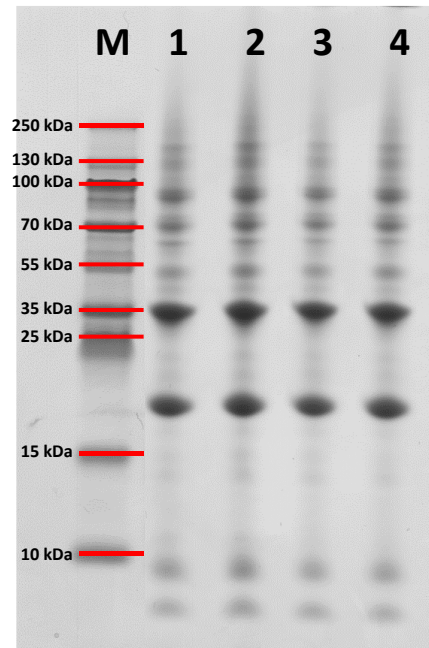
**Figure S4.** Comparative analysis of protein concentration and extracted protein yield from the modified SDS extraction protocol, with and without the addition of TCEP and IAA, across flaxseed, sesame, and black cumin samples.



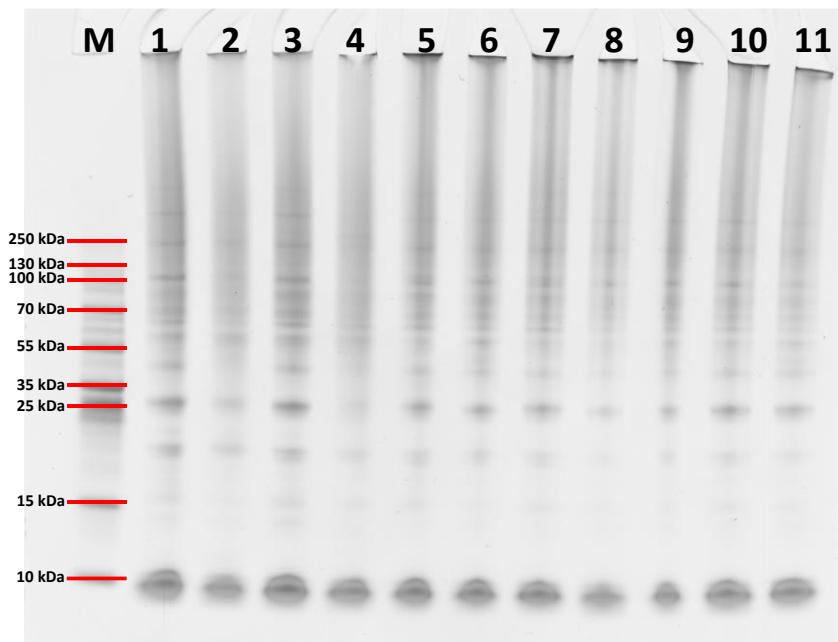
**Figure S5.** SDS-PAGE of flaxseed samples (S40–S47) from the final standardized SDS extraction method. (M) Marker, 1- S40, 2- S41, 3- S42, 4- S43, 5- S44, 6- S45, 7- S46, 8- S47 flaxseed



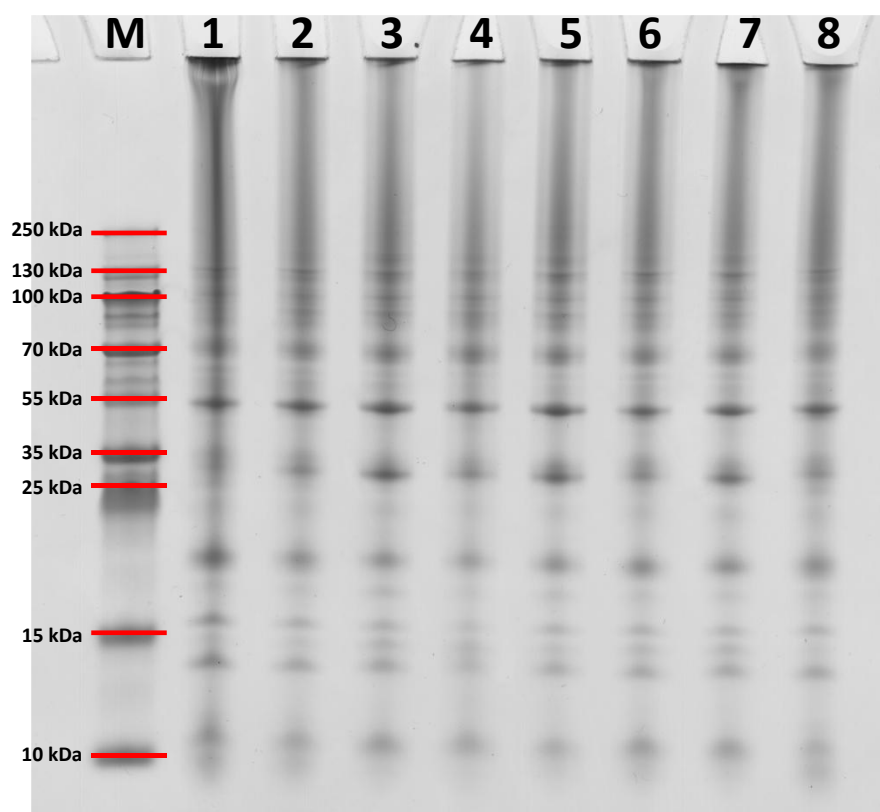
**Figure S6.** SDS-PAGE of sesame samples (S60–S67) from the final standardized SDS extraction method. (M) Marker, 1- S60, 2- S61, 3- S62, 4- S63, 5- S64, 6- S65, 7- S66, 8- S67 sesame.

**A****B**

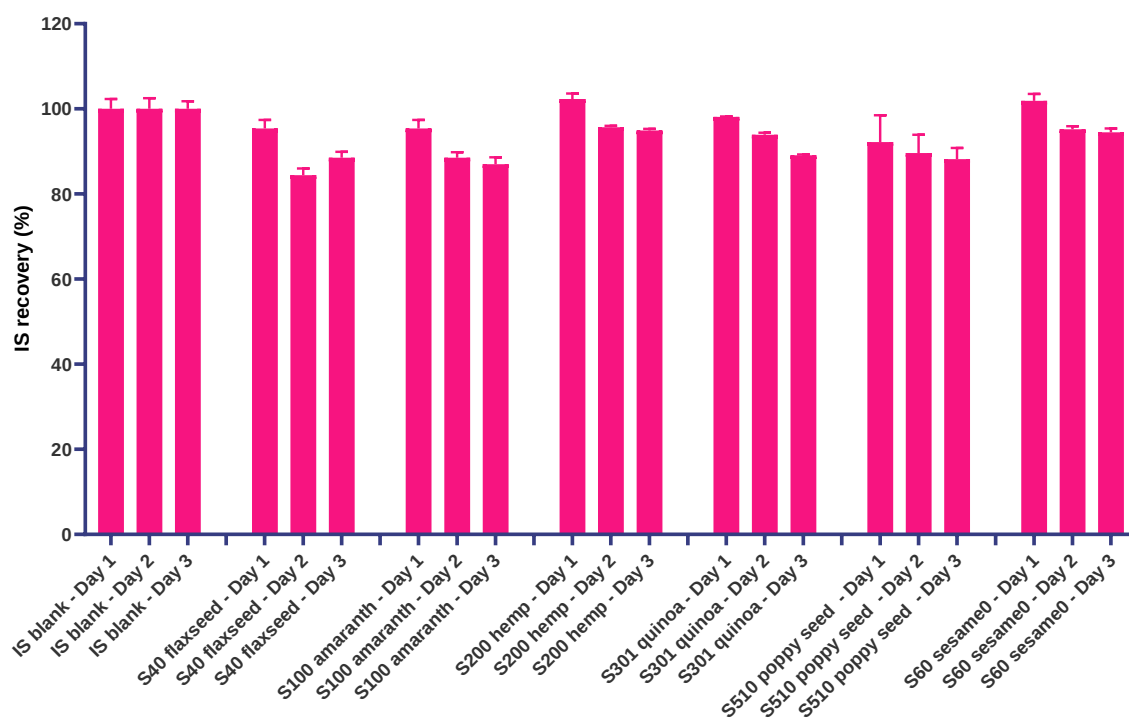
**Figure S7.** SDS-PAGE of (A) amaranth samples (S100–S104) and (B) hemp samples (S200–S203) from the final standardized SDS extraction method. A: M- Marker, 1- S100 amaranth, 2- S101 amaranth, 3- S102 amaranth, 4- S103 amaranth, 5- S104 amaranth. B: M- Marker, 1- S200 hemp (1), 2- S201 hemp (2), 3- S202 hemp (3), 4- S203 hemp (4).



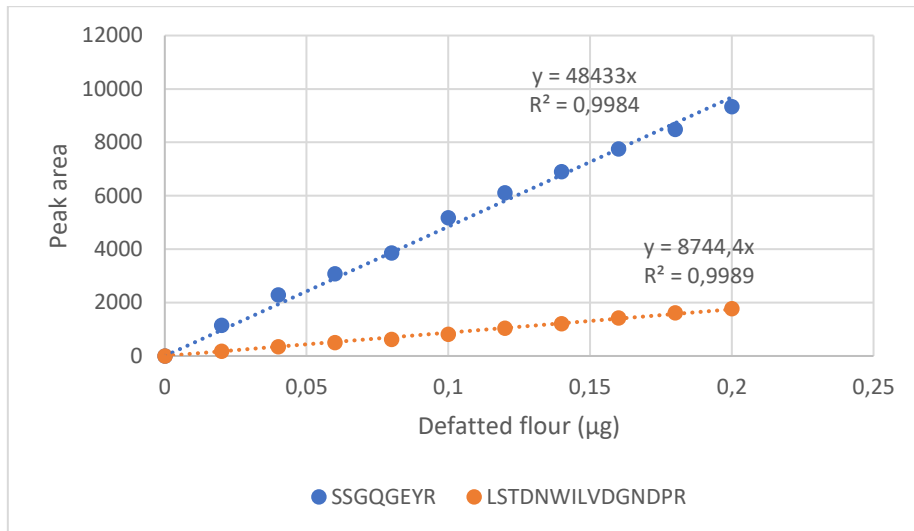
**Figure S8.** SDS-PAGE of all quinoa samples (S301–S303, S320–S323, S340–S343) from the final standardized SDS extraction method. M- Marker, 1- S301 Quinoa, 2- S302 Quinoa, 3- S303 Quinoa, 4- S320 Quinoa, 5- S321 Quinoa, 6- S322 Quinoa, 7- S323 Quinoa, 8- S340 Quinoa, 9- S341 Quinoa, 10- S342 Quinoa, 11- S343 Quinoa.



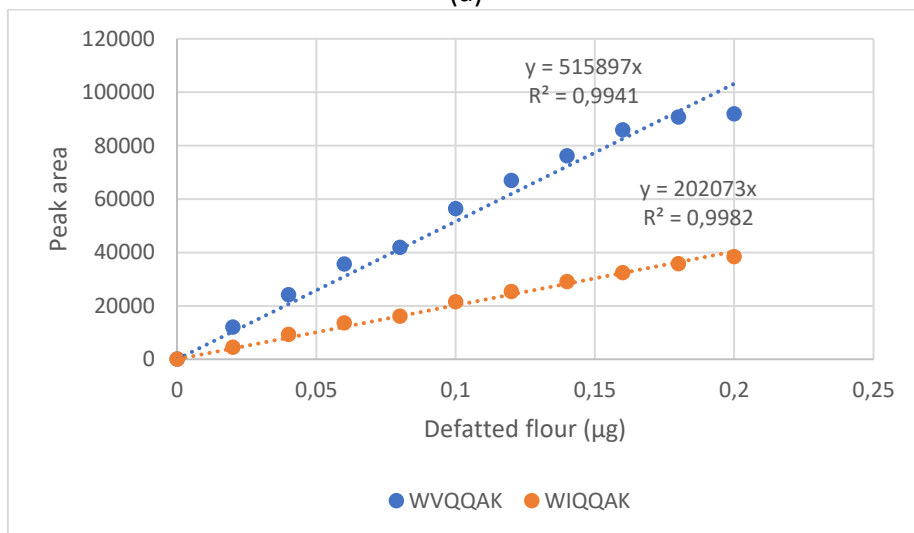
**Figure S9.** SDS-PAGE of all poppy seed samples (S500–S503, S510–S513) from the final standardized SDS extraction method. M- Marker, 1- S500 poppy, 2- S501 poppy, 3- S502 poppy, 4- S503 poppy, 5- S510 poppy, 6- S511 poppy, 7- S512 poppy, 8- S513 poppy.



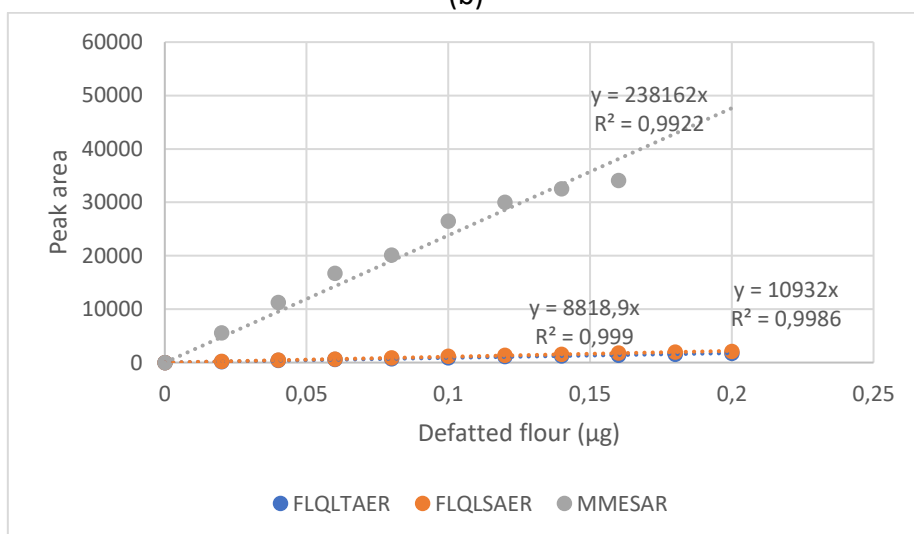
**Figure S10.** Recovery of the internal standard GWGG in the S40 flaxseed, S100 amaranth, S200 hemp, S301 quinoa, S60 sesame and S510 poppy seed compared to the in blank. Experiments were performed in three different days and each in triplicate.



(a)

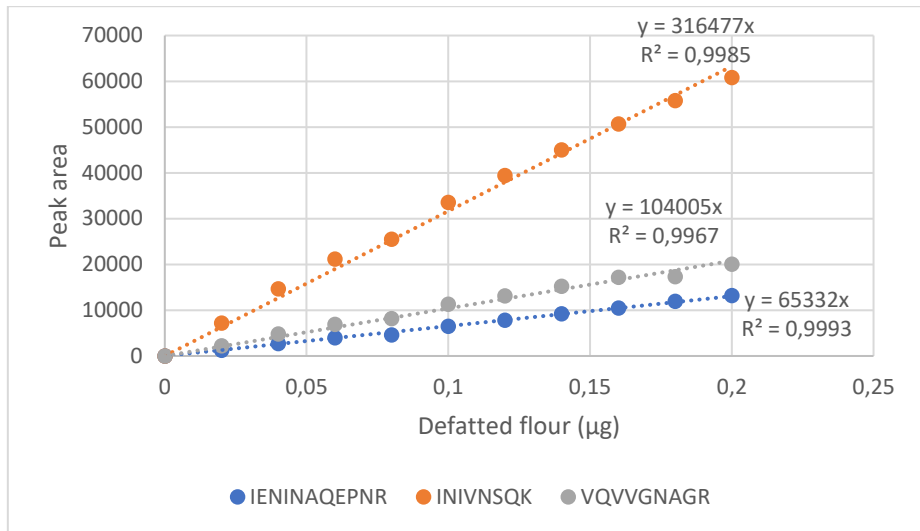


(b)

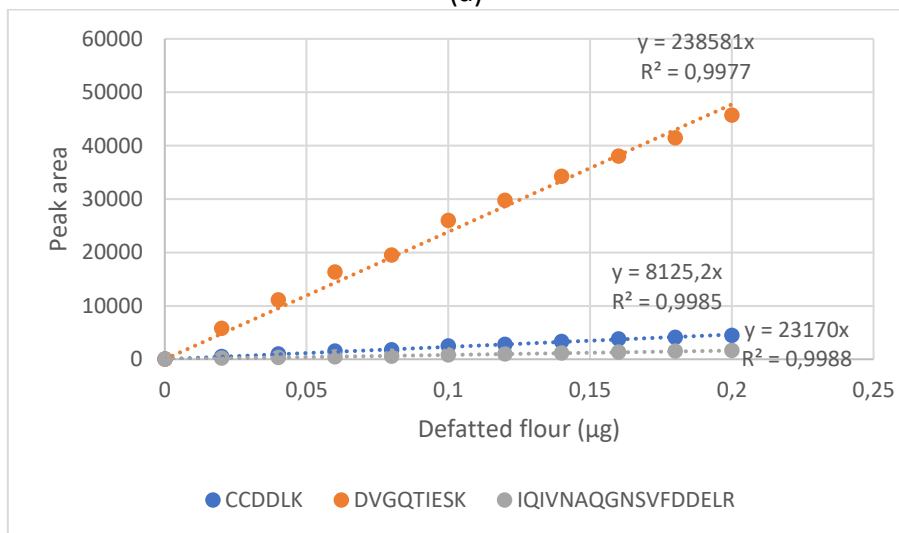


(c)

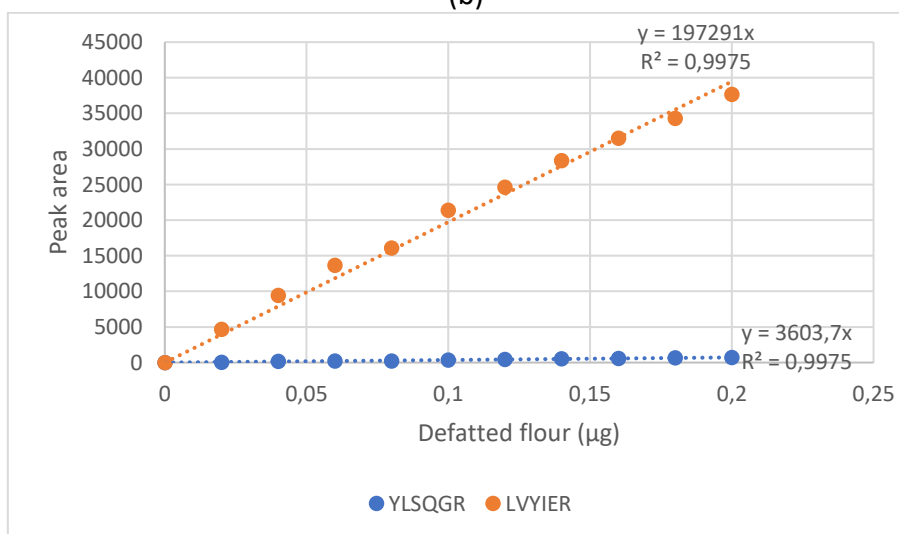
**Figure S11.** Linearity of quantifier peptides of (a) amaranth, (b) flaxseed and (c) hemp seeds



(a)



(b)



(c)

**Figure S12.** Linearity of quantifier peptides of (a) poppy, (b) quinoa and (c) sesame seeds



**Figure S13.** Visual representation of whole and ground forms of selected seed samples used in this study. Seed types include: (1) blue-gray poppy, (2) white poppy, (3) black cumin, (4) brown flaxseed, (5) golden yellow flaxseed, (6) gray-brown hemp, (7) black basil, (8) dark brown chia, (9) white chia, (10) black sesame, (11) white sesame, (12) black psyllium, (13) brown psyllium, (14) black psyllium, (15) white quinoa, (16) red quinoa, (17) black quinoa, (18) red canihua, and (19) white amaranth.

**Table S1.** List of the sample materials used in this study, including the different superfoods, their corresponding sample codes, color, origin, and the commercial producers.

| Species  | Ref. Number | Seed color    | Product company                                           | Origin         |
|----------|-------------|---------------|-----------------------------------------------------------|----------------|
| Flaxseed | S40         | brown         | Rapunzel Naturkost Antersdorfer Mühle GmbH & Vertriebs KG | Italy          |
|          | S41         | brown         | Davert GmbH                                               | Poland         |
|          | S42         | brown         | Spielberger GmbH                                          | Czech Republic |
|          | S43         | brown         | Rapunzel Naturkost                                        | Origin unk     |
|          | S44         | golden yellow | Spielberger GmbH                                          | Kazakhstan     |
|          | S45         | golden yellow | dm drogerie markt GmbH                                    | Hungary        |
|          | S46         | golden yellow | Carl Wilhem Clasen GmbH                                   | China          |
|          | S47         | golden yellow |                                                           | China          |
| Chia     | S48         | dark brown    | Govinda Natur GmbH                                        | Origin unk     |
|          | S49         | dark brown    | Davert GmbH                                               | Nicaragua      |
|          | S50         | dark brown    | Rapunzel Naturkost                                        | Uganda         |
|          | S51         | dark brown    | dm drogerie markt GmbH                                    | Paraguay       |
|          | S52         | dark brown    | Märsch Importhandels GmbH                                 | Paraguay       |
|          | S53         | dark brown    | Herbert Kluth GmbH & Co. KG                               | Origin unk     |
|          | S54         | dark brown    | Midsona Germany GmbH                                      | Origin unk     |
|          | S55         | dark brown    | Govinda Natur GmbH                                        | Origin unk     |
|          | S56         | cream         | Kornwestheimer Bio-Marketing GmbH                         | Origin unk     |
|          | S57         | cream         | Tilia/Marulo                                              | Origin unk     |
|          | S58         | cream         | Davert GmbH                                               | Argentinian    |
|          | S59         | cream         | Duria Global GmbH & Co. KG                                | Origin unk     |
|          | S68         | dark brown    |                                                           | Paraguay       |
| Sesame   | S60         | white         | Bohlsener Mühle GmbH & Co. KG                             | Uganda         |
|          | S61         | white         | Davert GmbH                                               | Pakistan       |
|          | S62         | white         | Rapunzel Naturkost                                        | Egypt          |
|          | S63         | white         | Spielberger GmbH                                          | Egypt          |
|          | S64         | black         | Govinda Natur GmbH                                        | Origin unk     |
|          | S65         | black         | Arche Naturprodukte GmbH                                  | Origin unk     |
|          | S66         | black         | ReformKontor GmbH & Co. KG                                | India          |
|          | S67         | black         | TerraSana                                                 | Belarus        |
| Amaranth | S100        | white         | Bohlsener Mühle GmbH & Co. KG                             | India          |
|          | S101        | white         | Dennree GmbH                                              | India          |
|          | S102        | white         | Rapunzel Naturkost                                        | India          |
|          | S103        | white         | Carl Wilhem Clasen GmbH                                   | India          |
|          | S104        | white         | Rila Feinkost-Importe GmbH und Co. KG                     | Origin unk     |
|          | S104        | white         |                                                           | Origin unk     |
| Hemp     | S200        | brown gray    | Laia's Predeinhanf GmbH                                   | Origin unk     |
|          | S201        | brown gray    | Davert GmbH                                               | Germany        |
|          | S202        | brown gray    | Chiron W. Misslisch/L.Stury GbR                           | Origin unk     |
|          | S203        | brown gray    | ReformKontor GmbH & Co. KG                                | China          |

**Table S1. Cont.**

| <b>Species</b> | <b>Ref. Number</b> | <b>Seed color</b> | <b>Product company</b>                 | <b>Origin</b> |
|----------------|--------------------|-------------------|----------------------------------------|---------------|
| Quinoa         | S301               | white             | Antersdorfer Mühle GmbH & Vertriebs KG | Origin unk    |
|                | S302               | white             | Bohlsener Mühle GmbH & Co. KG          | Germany       |
|                | S303               | white             | Davert GmbH                            | Origin unk    |
|                | S320               | red               | Rapunzel Naturkost                     | Origin unk    |
|                | S321               | red               | Davert GmbH                            | Origin unk    |
|                | S322               | red               | EKIBIO                                 | Bolivia       |
|                | S323               | red               | Rila Feinkost-Importe GmbH und Co. KG  | Origin unk    |
|                | S340               | black             | Davert GmbH                            | Origin unk    |
|                | S341               | black             | EKIBIO                                 | Bolivia       |
|                | S342               | black             | Rila Feinkost-Importe GmbH und Co. KG  | Origin unk    |
|                | S343               | black             | Reishunger GmbH                        | Peru          |
| Canihua        | S400               | red               | Carl Wilhem Clasen GmbH                | Bolivia       |
|                | S401               | red               | Schnitzer GmbH & Co. KG                | Origin unk    |
|                | S402               | red               | Davert GmbH                            | Origin unk    |
|                | S403               | red               | Reishunger GmbH                        | Peru          |
| Poppy seeds    | S500               | Blue-gray         | Rapunzel Naturkost                     | Origin unk    |
|                | S501               | Blue-gray         | Davert GmbH                            | Turkey        |
|                | S502               | Blue-gray         | Seeberger GmbH                         | Origin unk    |
|                | S503               | Blue-gray         | Albert Ménéz                           | Origin unk    |
|                | S510               | white             | Sonnentor GmbH                         | Austria       |
|                | S511               | white             | TRS'Wholesale Co. Ltd.                 | Turkey        |
|                | S512               | white             | Jalpur Millers                         | India         |
|                | S513               | white             | Mohnhof Gressl                         | Austria       |
| Basil seeds    | S600               | black             | TRS'Wholesale Co. Ltd.                 | India         |
|                | S602               | black             | Jalpur Millers                         | India         |
|                | S603               | black             | Gesund & Leben Elke Weintraut          | Uzbekistan    |
|                | S604               | black             | Gesund & Leben Elke Weintraut          | Vietnam       |
| Black cumin    | S900               | black             | TRS'Wholesale Co. Ltd.                 | India         |
|                | S901               | black             | Wagner Gewürze GmbH                    | Egypt         |
|                | S902               | black             | Gewürzmühle Brecht GmbH                | Egypt         |
|                | S903               | black             | Bremer Gewürzhandel GmbH               | Egypt         |
| Psyllium seeds | S1000              | black             | Sonnentor GmbH                         | Austria       |
|                | S1001              | black             | Tee und Spezialitätenversand           | Origin unk    |
|                | S1002              | black             | Aleavedis Naturprodukte GmbH           | Origin unk    |
|                | S1003              | black             | Golden Peanut                          | Origin unk    |
|                | S1010              | brown             | TopFruits                              | Origin unk    |
|                | S1011              | brown             | Tee und Spezialitätenversand           | Origin unk    |
|                | S1012              | brown             | Aurica                                 | India         |
|                | S1013              | brown             | Naturprodukte Lembcke GbR              | India         |
|                | S1020              | black             | TopFruits                              | Origin unk    |
|                | S1021              | black             | Herbis Natura                          | Austria       |
|                | S1022              | black             | YouHerbit/Konstantinos Spiliadis       | Origin unk    |
|                | S1023              | black             | Edel Kraut GmbH                        | Origin unk    |

**Table S2.** Flow gradient of the final LC-MS/MS method

| <b>Time (min)</b> | <b>Eluent A (%)</b> | <b>Eluent B (%)</b> |
|-------------------|---------------------|---------------------|
| 0                 | 100                 | 0                   |
| 2                 | 100                 | 0                   |
| 18                | 50                  | 50                  |
| 18.1              | 5                   | 95                  |
| 22                | 5                   | 95                  |
| 22.1              | 100                 | 0                   |
| 28                | 100                 | 0                   |

**Table S3.** Overview of the final set of proteins selected for targeted HPLC-MS/MS analysis for each superfood, aiming to identify potential biomarkers

|                   | UniProt entry number | Name                                   | Organisms                                            | Gen          | Length (AA) | Mass (Da) | Status     |
|-------------------|----------------------|----------------------------------------|------------------------------------------------------|--------------|-------------|-----------|------------|
| <b>Flaxseed</b>   | Q8LPD3               | Conlinin 2                             | Linum usitatissimum (Flax)                           | cnl2         | 168         | 19,012    | unreviewed |
|                   | Q8LPD4               | Conlinin 1                             | Linum usitatissimum (Flax)                           | cnl1         | 169         | 19,063    | unreviewed |
| <b>Sesame</b>     | Q9XHP0               | 11S globulin seed storage protein 2    | Sesamum indicum (Oriental sesame)                    | n.a.         | 459         | 51,830    | Reviewed   |
|                   | Q9AUD1               | 2S albumin                             | Sesamum indicum (Oriental sesame)                    | LOC105174067 | 153         | 17,504    | unreviewed |
|                   | Q9AUD0               | 7S globulin                            | Sesamum indicum (Oriental sesame)                    | n.a.         | 585         | 67,069    | unreviewed |
| <b>Amaranth</b>   | Q38712               | 11S globulin seed storage protein      | Amaranthus hypochondriacus (Prince-of-Wales feather) | n.a.         | 501         | 56,672    | unreviewed |
|                   | Q38719               | Agglutinin                             | Amaranthus hypochondriacus (Prince-of-Wales feather) | AHA          | 304         | 34,958    | unreviewed |
| <b>Hemp</b>       | A0A090DLH8           | Edestin 1                              | Cannabis sativa (Hemp) (Marijuana)                   | ede1A        | 511         | 58,504    | unreviewed |
|                   | A0A090CXP8           | Edestin 2                              | Cannabis sativa (Hemp) (Marijuana)                   | ede2C        | 491         | 55,986    | unreviewed |
|                   | A0A219D1L6           | Albumin                                | Cannabis sativa (Hemp) (Marijuana)                   | Cs2S-1       | 142         | 16,742    | unreviewed |
|                   | A0A219D3H6           | Edestin 3                              | Cannabis sativa (Hemp) (Marijuana)                   | CsEde3B      | 491         | 55,938    | unreviewed |
| <b>Quinoa</b>     | Q6Q385               | 11S seed storage                       | Chenopodium quinoa (Quinoa)                          | 11S          | 480         | 53,641    | unreviewed |
|                   | A0A803M3Q4           | Oleosin                                | Chenopodium quinoa (Quinoa)                          | n.a.         | 185         | 19,083    | unreviewed |
|                   | A0A803LYI9           | AAI domain-containing protein          | Chenopodium quinoa (Quinoa)                          | n.a.         | 129         | 15,358    | unreviewed |
| <b>Poppy seed</b> | A0A4Y7J814           | Protein-serine/threonine phosphatase   | Papaver somniferum (Opium poppy)                     | C5167_014922 | 853         | 95,547    | unreviewed |
|                   | A0A4Y7K3R5           | Cupin type-1 domain-containing protein | Papaver somniferum (Opium poppy)                     | C5167_011661 | 468         | 53,356    | unreviewed |
|                   | A0A4Y7KLU8           | Cupin type-1 domain-containing protein | Papaver somniferum (Opium poppy)                     | C5167_048617 | 514         | 57,714    | unreviewed |

n.a: not available

**Table S4.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected sesame proteins

| Entry number | Peptide sequence | Q1-Mass  | Q3-Mass   | Retention time (min) |
|--------------|------------------|----------|-----------|----------------------|
| Q9XHP0       | R.LVYIER.G       | 396.7343 | 679.3774  | 10.0                 |
|              |                  |          | 580.3089  |                      |
|              | R.VHVVD.R.N      | 362.7087 | 417.2456  | 6.7                  |
|              |                  |          | 213.1598  |                      |
|              |                  |          | 488.2827  |                      |
| Q9AUD1       | K.YMDLSAEK.G     | 478.7233 | 389.2143  | 9.7                  |
|              |                  |          | 237.1346  |                      |
|              | R.YLSQGR.S       | 362.1928 | 336.2030  | 7.2                  |
|              |                  |          | 793.3760  |                      |
|              |                  |          | 662.3355  |                      |
| Q9AUD0       | R.DCCQQLR.N      | 490.2078 | 547.3086  | 7.4                  |
|              |                  |          | 295.1111  |                      |
|              | R.NVMNQLER.E     | 502.2531 | 560.3151  | 10.0                 |
|              |                  |          | 447.2310  |                      |
|              |                  |          | 232.1404  |                      |
| Q9AUD0       | K.EACIQACK.E     | 490.2204 | 277.1547  | 7.4                  |
|              |                  |          | 704.3508  |                      |
|              | R.ESLNIK.Q       | 352.2029 | 544.3202  | 9.0                  |
|              |                  |          | 288.2030  |                      |
|              |                  |          | 276.0649  |                      |
| Q9AUD0       | K.EACIQACK.E     | 490.2204 | M790.3876 | 7.4                  |
|              |                  |          | 659.3471  |                      |
|              | R.ESLNIK.Q       | 352.2029 | 545.3042  | 9.0                  |
|              |                  |          | 345.1591  |                      |
|              |                  |          | 619.3232  |                      |
| Q9AUD0       | K.EACIQACK.E     | 490.2204 | 506.2391  | 7.4                  |
|              |                  |          | 378.1806  |                      |
|              | R.ESLNIK.Q       | 352.2029 | 307.1435  | 9.0                  |
|              |                  |          | 487.3239  |                      |
|              |                  |          | 374.2398  |                      |
| Q9AUD0       | K.EACIQACK.E     | 490.2204 | 260.1969  | 7.4                  |
|              |                  |          | 217.0819  |                      |
|              | R.ESLNIK.Q       | 352.2029 |           |                      |

**Table S5.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected amaranth proteins

| Entry number | Peptide sequence    | Q1-Mass  | Q3-Mass  | Retention time (min) |
|--------------|---------------------|----------|----------|----------------------|
| Q38712       | R.LTALEPTNR.I       | 507.7826 | 800.4261 | 10.8                 |
|              |                     |          | 729.3890 |                      |
|              |                     |          | 616.3049 |                      |
|              |                     |          | 487.2623 |                      |
|              | R.CAGVSVIR.R        | 431.2342 | 630.3933 | 10.8                 |
|              |                     |          | 573.3719 |                      |
|              |                     |          | 474.3035 |                      |
|              |                     |          | 387.2714 |                      |
|              | R.SSGQGEYR.R        | 442.1989 | 796.3584 | 9.1                  |
|              |                     |          | 709.3264 |                      |
|              |                     |          | 652.3049 |                      |
|              |                     |          | 709.2788 |                      |
| Q38719       | R.LSTDNWILVDGNDPR.E | 857.9234 | 998.5265 | 13.8                 |
|              |                     |          | 885.4425 |                      |
|              |                     |          | 772.3584 |                      |
|              |                     |          | 673.2900 |                      |
|              | K.ILDPLAQFEVEPSK.T  | 793.4272 | 963.4782 | 14.9                 |
|              |                     |          | 460.2402 |                      |
|              |                     |          | 331.1976 |                      |
|              |                     |          | 342.2023 |                      |
|              | K.TYDGLVHIK.S       | 523.2875 | 781.4567 | 11.4                 |
|              |                     |          | 666.4297 |                      |
|              |                     |          | 496.3242 |                      |
|              |                     |          | 397.2558 |                      |

**Table S6.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected hemp proteins

| Entry number | Peptide sequence | Q1-Mass  | Q3-Mass  | Retention time (min) |
|--------------|------------------|----------|----------|----------------------|
| A0A090DLH8   | R.FLQLSAER.G     | 482.27   | 816.4574 | 11                   |
|              |                  |          | 703.3733 |                      |
|              |                  |          | 575.3148 |                      |
| A0A090DLH8   | K.GTLDLVSP.LR.S  | 535.8139 | 462.2307 | 12.6                 |
|              |                  |          | 799.4672 |                      |
|              |                  |          | 684.4403 |                      |
| A0A090DLH8   | R.SQDESYR.Q      | 442.69   | 571.3562 | 6.6                  |
|              |                  |          | 385.2558 |                      |
|              |                  |          | 669.2838 |                      |
| A0A090CXP8   | R.FLQLTAER.G     | 489.27   | 554.2569 | 11.3                 |
|              |                  |          | 425.2143 |                      |
|              |                  |          | 460.1674 |                      |
| A0A090CXP8   | R.GEDLQIAPSR.I   | 599.8250 | 717.3890 | 11                   |
|              |                  |          | 589.3304 |                      |
|              |                  |          | 375.1987 |                      |
| A0A090CXP8   | K.ASAQGFEWIAVK.T | 653.84   | 784.4676 | 12.9                 |
|              |                  |          | 656.4090 |                      |
|              |                  |          | 359.2037 |                      |
| A0A219D1L6   | R.MMESAR.N       | 362.66   | 656.3250 | 7                    |
|              |                  |          | 949.5142 |                      |
|              |                  |          | 745.4243 |                      |
| A0A219D1L6   | R.CPALEMEIQK.E   | 609.7965 | 990.4680 | 10.9                 |
|              |                  |          | 593.2712 |                      |
|              |                  |          | 333.1881 |                      |
| A0A219D1L6   | R.NIPSMCGMQPR.T  | 645.79   | 392.1308 | 10.4                 |
|              |                  |          | 961.5023 |                      |
|              |                  |          | 890.4652 |                      |
| A0A219D3H6   | K.LDLVKPQR.S     | 484.7980 | 777.3811 | 9.1                  |
|              |                  |          | 648.3385 |                      |
|              |                  |          | 400.2303 |                      |
| A0A219D3H6   | K.IQSQDDFR.G     | 504.74   | 895.3904 | 8.5                  |
|              |                  |          | 767.3319 |                      |
|              |                  |          | 680.2998 |                      |
| A0A219D3H6   | R.ENMGDPA.R.A    | 445.20   | 646.2977 | 7.4                  |
|              |                  |          | 515.2572 |                      |
|              |                  |          | 458.2358 |                      |
|              |                  |          | 343.2088 |                      |

**Table S7.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected quinoa proteins

| Entry number | Peptide sequence       | Q1-Mass  | Q3-Mass   | Retention time (min) |
|--------------|------------------------|----------|-----------|----------------------|
| Q6Q385       | R.LTALEPTNR.I          | 507.7826 | 800.4261  | 10.7                 |
|              |                        |          | 729.3890  |                      |
|              |                        |          | 616.3049  |                      |
| Q6Q385       | K.LQAEQDER.G           | 494.7383 | 487.2623  | 8.4                  |
|              |                        |          | 747.3268  |                      |
|              |                        |          | 676.2897  |                      |
| Q6Q385       | R.IQIVNAQGNSVFDDEL.R.Q | 959.4869 | 547.2471  | 13.8                 |
|              |                        |          | 304.1615  |                      |
|              |                        |          | 1151.5327 |                      |
| A0A803M3Q4   | K.DVGQTIESK.A          | 488.7509 | 980.4684  | 9.7                  |
|              |                        |          | 794.3679  |                      |
|              |                        |          | 647.2995  |                      |
| A0A803LYI9   | K.CCDDLK.M             | 405.6597 | 762.3992  | 8.6                  |
|              |                        |          | 705.3777  |                      |
|              |                        |          | 577.3192  |                      |
| A0A803LYI9   | R.MCGTMQR.K            | 442.1828 | 363.1874  | 8.8                  |
|              |                        |          | 650.2814  |                      |
|              |                        |          | 260.1969  |                      |
| A0A803LYI9   | K.GMMHEQR.M            | 444.6944 | 321.0686  | 8.6                  |
|              |                        |          | 551.1225  |                      |
|              |                        |          | 752.3178  |                      |
| A0A803LYI9   | K.GMMHEQR.M            | 444.6944 | 592.2872  | 8.6                  |
|              |                        |          | 535.2657  |                      |
|              |                        |          | 434.2180  |                      |
| A0A803LYI9   | K.GMMHEQR.M            | 444.6944 | 700.3195  | 8.6                  |
|              |                        |          | 569.2790  |                      |
|              |                        |          | 432.2201  |                      |
| A0A803LYI9   | K.GMMHEQR.M            | 444.6944 | 303.1775  | 8.6                  |
|              |                        |          | 303.1775  |                      |
|              |                        |          | 303.1775  |                      |

**Table S8.** Parameters of the applied MRM method for identifying and quantifying potential biomarker peptides derived from tryptic digestion of selected poppy seed proteins

| Entry number | Peptide sequence | Q1-Mass  | Q3-Mass   | Retention time (min) |
|--------------|------------------|----------|-----------|----------------------|
| A0A4Y7J814   | R.CQIVGNQGR.Q    | 516.2562 | 743.4159  | 9.1                  |
|              |                  |          | 630.3318  |                      |
|              |                  |          | 531.2634  |                      |
|              |                  |          | 402.1806  |                      |
| A0A4Y7J814   | R.IENINAQEPNR.R  | 649.3284 | 1055.5228 | 9.8                  |
|              |                  |          | 828.3959  |                      |
|              |                  |          | 643.3158  |                      |
|              |                  |          | 386.2146  |                      |
| A0A4Y7J814   | R.QSVQLR.G       | 365.7139 | 602.3620  | 9.5                  |
|              |                  |          | 515.3300  |                      |
|              |                  |          | 416.2616  |                      |
|              |                  |          | 288.2030  |                      |
| A0A4Y7K3R5   | R.INIVNSQK.L     | 458.2665 | 802.4417  | 10.1                 |
|              |                  |          | 688.3988  |                      |
|              |                  |          | 575.3148  |                      |
|              |                  |          | 476.2463  |                      |
| A0A4Y7K3R5   | R.ETFQNVFR.A     | 520.7616 | 911.4734  | 12.5                 |
|              |                  |          | 810.4257  |                      |
|              |                  |          | 663.3573  |                      |
|              |                  |          | 535.2987  |                      |
| A0A4Y7K3R5   | R.QYLDNPR.E      | 453.2274 | 614.3257  | 9.7                  |
|              |                  |          | 501.2416  |                      |
|              |                  |          | 386.2146  |                      |
|              |                  |          | 292.1292  |                      |
| A0A4Y7KLU8   | R.VQVVGNAQR.Q    | 450.2565 | 672.3787  | 9.3                  |
|              |                  |          | 573.3103  |                      |
|              |                  |          | 474.2419  |                      |
|              |                  |          | 327.2027  |                      |
| A0A4Y7KLU8   | R.EETLILTPGLR.S  | 621.3586 | 769.4930  | 13.5                 |
|              |                  |          | 656.4090  |                      |
|              |                  |          | 543.3249  |                      |
|              |                  |          | 442.2772  |                      |
| A0A4Y7KLU8   | R.HIIQPR.G       | 382.2323 | 626.3984  | 8.7                  |
|              |                  |          | 513.3144  |                      |
|              |                  |          | 400.2303  |                      |
|              |                  |          | 492.2929  |                      |