

S2 Table. Peptides identified in each isolated rye gluten protein type. Peptide sequences, their scores, *m/z* ratios, charge states and relative molecular weights (*M_r*). For corresponding protein sequences, see S6 Table.

| Abbreviation | Gluten protein type Peptide sequence | Peptide score | <i>m/z</i> (charge state) | <i>M_r</i> |
|-----------------------|---|---------------|------------------------------|----------------------|
| HMW-secalins | | | | |
| HS.1 | QQPAQGQQGY | 58 | 634.16 (+2) | 1266.57 |
| HS.2 | KGGSFYDDETSPPQQL | 56 | 875.79 (+2) | 1749.82 |
| HS.3 | QQPGQGQQGY | 55 | 545.65 (+2) | 1089.50 |
| HS.4 | QKPGQGQQGY | 53 | 545.63 (+2) | 1089.52 |
| HS.5 | LQIGQGQQGY | 52 | 546.21 (+2) | 1090.55 |
| HS.6 | QQPGQGQQGY | 52 | 627.18 (+2) | 1252.55 |
| HS.7 | QKPGQGQQGY | 52 | 627.18 (+2) | 1252.59 |
| HS.8 | KRYYPSTSPHQGSY | 51 | 590.52 (+3) | 1768.86 |
| HS.9 | ITSPQQSGQGQQPGQW | 49 | 774.56 (+3) | 2321.09 |
| HG+HS.2 | HVSAEHQAASL | 48 | 575.11 (+2) | 1148.56 |
| HS.10 | YITSPQQSGQGQQPGQW | 47 | 828.82 (+3) | 2484.15 |
| HS.11 | YPSVTSPHQGSY | 46 | 661.74 (+2) | 1321.60 |
| HS.12 | LTSPQPGQGQQGYDSPY | 46 | 975.80 (+2) | 1949.88 |
| HS.13 | YSTSPRQPGQGQQEYPTSPQPGQW | 46 | 999.12 (+3) | 2994.36 |
| HS+D | KVAKAQQQL | 43 | 443.18 (+2) | 884.55 |
| HS.14 | YPTSPQPGQGQQGY | 41 | 818.23 (+2) | 1634.74 |
| HS.15 | QQLQQGIFW | 41 | 574.24 (+2) | 1146.59 |
| HS.16 | QQPGQGQEGY | 39 | 545.63 (+2) | 1090.48 |
| HS.17 | QQPAQGQQGY | 39 | 552.59 (+2) | 1103.51 |
| HS.18 | YLTSPQPGQGQQGY | 39 | 826.28 (+2) | 1650.77 |
| HG+HS.3 | HVSVEHQAASL | 36 | 589.18 (+2) | 1176.60 |
| HS.19 | QQPGQGQSGY | 35 | 525.14 (+2) | 1048.46 |
| HS.20 | QEPGQGQQGY | 34 | 545.61 (+2) | 1090.47 |
| HS.21 | LQIGQGQQGYPTSPQPGQGQQGY | 33 | 903.60 (+3) | 2707.27 |
| HS.22 | STSPRQPGQGQQEYPTSPQPGQW | 31 | 1416.81 (+2) | 2831.30 |
| HS.23 | KRYYPSTSPHQGSYYPGQTSL | 31 | 839.56 (+3) | 2516.22 |
| HS.24 | STSPRQPGQGQQEY | 30 | 781.66 (+2) | 1561.72 |
| HS.25 | EQTTVPPKGGSFYPSSETTPL | 29 | 712.57 (+3) | 2135.05 |
| HG+HS.1 | QQPGQGQQPGQW | 28 | 669.71 (+2) | 1337.62 |
| HS.26 | YPTSPQPGQGQQPGQGQQGY | 28 | 1199.66 (+2) | 2394.07 |
| HS.27 | LTSPQPGQGQQGY | 27 | 744.64 (+2) | 1487.71 |
| HS.28 | STSLQPGQGQQGHYPTSL | 27 | 671.92 (+3) | 2012.96 |
| HS.29 | YPSVTSPHQGSYYPGQTSL | 26 | 1034.71 (+2) | 2067.96 |
| HS.30 | KGGSFYDDETSPPQQLQRIL | 25 | 797.43 (+3) | 2389.20 |
| HS.31 | QQPGQVQPGYY | 18 | 632.69 (+2) | 1263.60 |
| γ-75k-secalins | | | | |
| γ75k.1 | QQFPQQPQQPFQQL | 68 | 968.26 (+2) | 1934.97 |
| γ75k.2 | AQVQGIHQPQQL | 61 | 661.83 (+2) | 1321.74 |
| γ75k.3 | SQLEVVRS | 59 | 515.71 (+2) | 1029.59 |
| γ75k.4 | QQHVGQGALAQQVQGIHQPQQL | 55 | 747.73 (+3) | 2240.21 |
| γ75k.5 | ASIVTGIVGH | 52 | 492.17 (+2) | 982.52 |
| γ75k.6 | ASIVTGIVGH | 50 | 477.25 (+2) | 952.54 |
| γ75k.7 | LPQSHKQHVGQGALAQQVQGIHQPQQL | 46 | 934.84 (+3) | 2802.53 |
| γ75k.8 | QQHVGQGAL | 45 | 469.21 (+2) | 936.49 |
| γ75k.9 | LPQSHKQHVGQGALAQQVQGIHQPQQL | 40 | 934.84 (+3) | 2802.50 |

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| γ75k.10 | AQIPQQ | 33 | 399.18 (+2) | 796.45 |
| γ75k.11 | QQFPQQPQQSFPQQPQQPVPQQPL | 24 | 943.73 (+3) | 2827.41 |
| ω-secalins | | | | |
| ωg+ωs.1 | GQQPEQIISQRPQQPFPLQPQQQF | 53 | 949.89 (+3) | 2846.45 |
| ωg+ωs.5 | GQQPEQIISQRPQQPFPLQPKQPF | 50 | 939.57 (+3) | 2815.48 |
| ωg+ωs.2 | GEQPEQIISQRPQQPFPLQPQQPF | 48 | 939.69 (+3) | 2816.43 |
| ωg+ωs.6 | GQQPEQIISQRPQQPFPLQPQQPF | 46 | 939.64 (+3) | 2815.45 |
| ωg+ωs.8 | SLQPQQPVPQQPQRPF | 44 | 625.60 (+3) | 1873.99 |
| ωg+ωs.7 | GQQPMQIISQRPQQPFPLQPQQPF | 43 | 939.58 (+3) | 2817.45 |
| ωg+ωs.3 | AQQPEQIISQQPFPLQPQQPF | 37 | 817.49 (+3) | 2448.25 |
| ωg+ωs.4 | AQQPEQLISQQPFPLQPQQPF | 35 | 1224.84 (+2) | 2448.25 |
| ωs.1 | GQQPWQIISQRPQQPFPLQPQQPF | 36 | 959.80 (+3) | 2873.48 |
| ωs.2 | AQQPEQLISQQPFPL | 36 | 862.85 (+2) | 1722.90 |
| ωs.3 | RQLNPSEQEL | 32 | 607.22 (+2) | 1212.62 |
| ωg+ωs.9 | SQPQQPFPQQPGQIIEQPQQPSPLQPQQPF | 31 | 1173.89 (+3) | 3518.77 |
| ωs.4 | ISQQPFPLQPQQPF | 25 | 828.36 (+2) | 1653.86 |
| ωg+ωs.10 | SQPQQPFPQQPGQIIPQQPQQPSPLQPQQPF | 25 | 1173.97 (+3) | 3517.78 |
| ωg+ωs.12 | GQQPEQIISRRPQQPFPLQPQQPF | 21 | 949.89 (+3) | 2843.49 |
| ωg+ωs.11 | SQPQQPFPQQPGQIIPKQPQQPSPLQPQQPF | 17 | 1173.95 (+3) | 3517.82 |
| ωs.5 | AQQPKQIISQQPFPLQPQQPF | 17 | 1225.33 (+2) | 2447.30 |
| ωs.6 | QSPQQPVPKEQSYPPQQPYPSHQPFPTPQQY | 17 | 1180.05 (+3) | 3535.69 |
| HMW-secalins within ω-secalins | | | | |
| HS.5 | LQIGQGQQGY | 56 | 546.21 (+2) | 1090.55 |
| HG+HS.2 | HVSAEHQAASL | 40 | 575.28 (+2) | 1148.56 |
| HS.12 | LTSPQQPGQGQQGYDSPY | 39 | 975.77 (+2) | 1949.88 |
| γ-40k-secalins | | | | |
| γ40k.1 | FQIVQGQSIIQQQPAQLEVIRSL | 75 | 1312.48 (+2) | 2622.46 |
| γ40k.2 | FQIVQGQSIIQQQPAQL | 70 | 963.82 (+2) | 1925.08 |
| γ40k.3 | FKIVQGQSIIQQQPAQL | 70 | 642.67 (+3) | 1925.08 |
| γ40k.4 | FQIVQGKSIIQQQPAQL | 70 | 642.67 (+3) | 1925.08 |
| γ40k.5 | RPLFQIVQGQSIIQQQPAQL | 66 | 765.32 (+3) | 2291.28 |
| γ40k.6 | RPLFKIVQGQSIIQQQPAQL | 66 | 1146.90 (+2) | 2291.32 |
| γ40k.7 | RPLFQIVQGKSIIQQQPAQL | 66 | 1146.90 (+2) | 2291.32 |
| γ40k.8 | KIVQGQSIIQQQPAQL | 60 | 889.82 (+2) | 1778.01 |
| γ40k.9 | QIVQGQSIIQQQPAQL | 60 | 889.83 (+2) | 1777.98 |
| γ40k.10 | QIVQGKSIIQQQPAQL | 60 | 889.82 (+2) | 1778.01 |
| γ40k.11 | QIVQGQSIIQQQPAQLEVIRSL | 52 | 826.31 (+3) | 2475.39 |
| γ40k.12 | QIVQGQSIIQQQL | 42 | 741.79 (+2) | 1481.83 |
| γ40k.13 | VRPDCSNIRTPF | 41 | 468.83 (+3) | 1403.71 |
| γ40k.14 | IESSLQQQMNPKNF | 36 | 883.29 (+2) | 1765.82 |
| γ40k.15 | IQSSLQQQMNPKNF | 23 | 883.23 (+2) | 1764.84 |
| γ40k.16 | IKSSLQQQMNPKNF | 23 | 883.23 (+2) | 1764.87 |
| γ-75k-secalins within γ-40k- secalins | | | | |
| γ75k.3 | SQLEVVRSL | 51 | 515.71 (+2) | 1029.59 |
| γ75k.6 | ASIVTGIVGH | 45 | 477.17 (+2) | 952.54 |