

S1 Table. Peptides identified in each isolated wheat gluten protein type. Peptide sequences, their scores, *m/z* ratios, charge states and relative molecular weights (*M_r*). For corresponding protein sequences, see S5 Table.

Abbreviation	Gluten protein type Peptide sequence	Peptide score	<i>m/z</i> (charge state)	<i>M_r</i>
HMW-GS				
HG.1	YPTSLQQTGQGQSGQGQQGY	62	802.49 (+3)	2403.08
HG.2	LQPGQGQQGY	58	538.16 (+2)	1074.52
HG.3	YPGQASSQRPGQGQQPGQGQQEY	56	826.32 (+3)	2475.12
HG.4	QQTGGGQSGQGQQGY	56	921.92 (+2)	1841.80
HG.5	QPEQLQQPTQGQQRQQPGQGQQ	55	877.73 (+3)	2629.30
HG.6	WQPGQGQQGY	54	574.72 (+2)	1147.51
HG.7	YLTSPQSGQW	53	647.78 (+2)	1293.61
HG.8	YLSVTSPQVSY	51	686.69 (+2)	1370.68
HG.9	SSSLQQPGQGLQGHYPASL	51	652.60 (+3)	1953.96
HG.10	TASLQQPGQGQQGHYPASL	46	656.94 (+3)	1966.96
HG.11	YPGQASSQRPGQGQQPGQGQQEYY	46	880.43 (+3)	2638.19
HG.12	QLGQGQQGY	43	489.71 (+2)	977.46
HG+HS.1	QQPGQGQQPGQW	42	669.79 (+2)	1337.62
HG.13	LQPGQGQQGYPTSL	41	819.26 (+2)	1635.80
HG.14	YYPTSPQESGQGQQPGQW	41	1019.84 (+2)	2036.89
HG.15	STSLQQPGQGQQGHYPASL	41	992.96 (+2)	1982.95
HG.16	QQTGGGQSGQGQQGY	41	840.61 (+2)	1678.74
HG.17	SQPRQGQQGY	40	574.72 (+2)	1147.54
HG+HS.2	HVSAEHQAASL	40	575.34 (+2)	1148.56
HG.18	LSVTSPQVSY	39	604.73 (+2)	1207.62
HG.19	SSYHVSVEHQAASL	39	757.95 (+2)	1513.72
HG.20	QQPGQGQPGYY	38	611.76 (+2)	1221.55
HG.21	TTSLQQSGQGQQGY	36	741.88 (+2)	1481.68
HG.22	QQPGQGQQGHYPASL	35	798.39 (+2)	1594.76
HG.23	QQPGQGQQGHY	35	798.39 (+2)	1226.55
HG.24	HQSGQGQQGYPTSL	34	825.85 (+2)	1649.75
HG.25	KRYPSVTSPQVSY	34	902.29 (+2)	1801.91
HG+HS.3	HVSVEHQAASL	33	589.34 (+2)	1176.60
HG.26	TASLQQPGQGQQGHYPASLQQVGGQQIGQL	33	1078.65 (+3)	3231.61
HG.27	QQPGQWQQPGQGQPGYY	32	974.29 (+2)	1945.88
HG.28	QQSGQGQPGYYPTSL	30	805.97 (+2)	1609.74
HG.29	GTSSQTVQGYPSVSSPQQGPY	30	1160.03 (+2)	2317.06
HG.30	HQSGQGQQGYPSSL	29	818.88 (+2)	1635.74
HG.31	EQQPVVPSKAGSFYPSETTPSQQL	26	1303.66 (+2)	2604.28
HG.32	YPSITSPQVSY	25	686.69 (+2)	1368.66
HG.33	KACQQVMDQQLRDISPECHPVVSPVAGQY	25	1108.59 (+3)	3324.61
HG.34	QQSGGQHGYYPTSPQLSGGQQRPGQW	23	986.61 (+3)	2956.37
HG.35	YPGQASPQQPGQGQQPGKW	22	1020.20 (+2)	2037.97
HG.36	EQTVVPPKGGSFYPGETTPL	20	702.39 (+3)	2103.06
HG.37	EQQIVVPPKGGSFYPGETTTPPQQL	20	866.87 (+3)	2596.32
HG.38	QQSGQGQQGYPTSPQQSGQGQQPGQW	19	979.64 (+3)	2934.30
HG.39	QQSGQGQQGHYPTSLQQPGQGQQGHY	18	942.45 (+3)	2823.28
HG.40	LQPGQGQQGYPTSPQQPGQGQQ	16	863.56 (+3)	2584.24

ω5-gliadins				
ω5.1	QQYPQQQPSGSDVISISGL	53	677.95 (+3)	2031.00
ω5.2	QQYPQQQPSGSNVISISGL	33	677.95 (+3)	2030.01
ω5.3	QTPQEQQFPQEQQFPEPQQILQQQF	33	948.38 (+3)	2842.36
ω5.4	SPRGMELQTPQEQQFPQEQQFPEPQQILQQQF	32	1205.20 (+3)	3612.74
ω5.5	SPRGMELQTPQEQQFPQEQQFPEPQQIL	27	1028.40 (+3)	3081.49
ω5.6	HQQQLPQQQFPQQQFPQQQFPQQQFPQQQQL	15	1340.10 (+3)	4015.95
ω1,2-gliadins				
wg.1	ARELNPSNKEQLSPQQSF	53	1036.76 (+2)	2072.04
wg+ws.1	GQQPEQIISQRPQQPFPLQPQQQF	50	950.27 (+3)	2846.45
wg.2	GSSLTSIGGQ	48	453.58 (+2)	905.45
wg+ws.2	GEQPEQIISQRPQQPFPLQPQQPF	44	939.61 (+3)	2816.43
wg+ws.3	AQQPEQIISQQPFLQPQQPF	43	1224.98 (+2)	2448.25
wg+ws.4	AQQPEQLISQQPFLQPQQPF	43	1224.98 (+2)	2448.25
wg.3	QQPQQQL	42	435.11 (+2)	868.45
wg+ws.5	GQQPEQIISQRPQQPFPLQPKQPF	39	939.77 (+3)	2815.48
wg+ws.6	GQQPEQIISQRPQQPFPLQPQQPF	37	1408.84 (+2)	2815.45
wg.4	LRQSQQPF	36	502.16 (+2)	1002.53
wg+ws.7	GQQPMQIISQRPQQPFPLQPQQPF	34	938.83 (+3)	2817.45
wg.5	AQQPEQIISHQPFPLQPQQPF	33	820.08 (+3)	2457.25
wg+ws.8	SLQPQQPVPQQPQRPF	32	937.78 (+2)	1873.99
wg+ws.9	SQPQQPFPQQPGQIIEPQQPSPLQPQQPF	30	1173.74 (+3)	3518.77
wg.6	YQPQQPFPQQPGQIIPQQPQQPSPLQPQQPF	29	1199.47 (+3)	3593.81
wg.7	FPHQSQQPF	26	558.10 (+2)	1114.53
wg.8	SQQPQRPPQQPFPQQPQQIIPPQPQQPF	23	1064.69 (+2)	3191.63
wg.9	SQPQQPF	23	831.70 (+1)	830.40
wg.10	LQQPQQPSPQPQQVVQIIPQQPQQPFPL	22	1072.63 (+3)	3215.72
wg.11	GRQPEQIISQRPQQPFPLQPQQPF	22	950.27 (+3)	2843.49
wg+ws.10	SQPQQPFPQQPGQIIPQQPQQPSPLQPQQPF	18	1173.74 (+3)	3517.78
wg+ws.11	SQPQQPFPQQPGQIIPKQPQQPSPLQPQQPF	17	1173.95 (+3)	3517.82
wg+ws.12	GQQPEQIISRRPQQPFPLQPQQPF	17	949.97 (+3)	2843.49
wg.12	SQQPEQTISQQPQQPFPQQPHQPQQPYPQQQPY	15	1314.06 (+3)	3939.86
α-gliadins				
α.1	GSSQVLQQSTY	63	599.15 (+2)	1196.57
α.2	FQPSQQNPQAQGF	57	738.70 (+2)	1475.69
α.3	RQQQKQQQQPSSQVSF	56	644.59 (+3)	1930.97
α.4	LQLQFPQPQLPYPQPQPF	52	784.80 (+2)	2262.19
α.5	LQLQFPQPQLPY	52	784.80 (+2)	1567.85
α.6	RPQQPYPQPQPY	45	813.71 (+2)	1625.80
α.7	LQLQFPQPQLPYPQPQLPYPQPQPF	45	1029.75 (+3)	3085.61
α.8	QQPQQQYPLGQGSF	39	803.16 (+2)	1604.77
α.9	MQLQFPQPQLPYPQPQLPYPQPQPF	37	1035.76 (+3)	3103.57
α.10	QQPQQQYPSGQGF	36	746.68 (+2)	1491.68
α.11	LGQQQFPFPQQPYPQPQPFPSQQPY	35	974.63 (+3)	2921.42
α.12	IGQQQFPFPQQPYPQPQPFPSQQPY	35	974.63 (+3)	2921.42
α.13	LGQEQQFPFPQQPYPQPQPFPSQQPY	33	974.63 (+3)	2922.41
α.14	VQQQQFPGRQQPFAPQQPYPQPQPFPSQQPY	31	1222.66 (+3)	3665.79
α.15	RGQQQFPFPQQPYPQPQPFPSQQPY	30	988.86 (+3)	2964.44
α.16	LGQQQFPFTPQQPYPQPQPFPSQQPY	28	974.63 (+3)	2925.42
α.17	HQQRQQPSSQVSF	27	519.53 (+3)	1555.75

α.18	LQLQFPQPQLPYQPQLPYQPQLPYQPQPF	27	1304.40 (+3)	3909.04
α.19	LGQQQTFPPQQYPQPQPFPSQQPY	26	974.63 (+3)	2925.42
α.20	VRVPVQLQPQNPSQQQPQEQVPL	26	912.53 (+3)	2733.46
α.21	VQQQQFVGQQQFPFPQQYPQPQPFPSQQPY	25	1222.27 (+3)	3665.78
α.22	QQPQQYPSGQGFQPSQQNPQAQGF	23	984.15 (+3)	2949.35
α.23	LGQQQQFPGQQQFPFPQQYPQPQPF	23	1054.99 (+3)	3162.54
α.24	VQEQQFPGQQQFPFPQQYPQPQPFPSQQPY	23	1222.33 (+3)	3664.74
α.25	QQPQQYPSGQGSFQPSQQNPQAQGF	23	964.16 (+3)	2889.31
α.26	NGQQQFPFPQQYPQPQPFPSQQPY	22	974.96 (+3)	2922.38
α.27	LGQQQFPFPQQYPQPQFPSQLPYL	21	974.63 (+3)	2922.48
α.28	VQQQQFPGQQQFPFPQQYPQPQPFPSQQPY	20	1222.27 (+3)	3663.76
α.29	LQLQFPQPQLPYPHPQLPYQPQPF	21	1032.72 (+3)	3094.61
α.30	VRVTVQLQPQNPSQQQPQEQVPL	16	912.53 (+3)	2737.46
α.31	LQLQFPQTQLPY	15	784.89 (+2)	1571.84
LMW-GS within α-gliadins				
LG.1	SHHQQQPIQQQPQPF	56	652.53 (+3)	1954.95
LG.2	SQQQQIVL	31	943.20 (+1)	942.52
LG.3	VLPQQQIPF	29	535.17 (+2)	1068.60
LG.4	GVGTGVGSY	20	796.13 (+1)	795.38
γ-gliadins				
yg.1	LQPQQPQQSFPQQQQPL	67	1010.32 (+2)	2019.02
yg.2	NIQVDPSGQVQW	54	685.74 (+2)	1369.67
yg.3	QLVQGGIIPQQAQY	48	632.75 (+3)	1895.00
yg.4	ANIDAGIGGQ	45	915.29 (+1)	914.45
yg.5	FQLVQGGIIPQQAQY	43	681.65 (+3)	2042.07
yg.6	ASIVAGIGGQ	42	436.72 (+2)	871.48
yg.7	SQQPQQAF	42	467.13 (+2)	932.44
yg.8	NIQVDPSGQVQWPQQPFPQPQPF	42	930.65 (+3)	2789.36
yg.9	SQQQQVGGSLVQGGIIPQQAQY	38	915.95 (+3)	2744.43
yg.10	QVQWPQQPFPQPQPF	29	1054.77 (+2)	2107.03
yg.11	RQPQQPF	25	450.64 (+2)	899.47
LMW-GS within γ-gliadins				
LG.1	SHHQQQPIQQQPQPF	56	652.45 (+3)	1954.95
LG.2	SQQQQIVL	46	943.45 (+1)	942.52
LG.3	VLPQQQIPF	35	535.25 (+2)	1068.60
LMW-GS				
LG.5	SIILQEQQGF	68	645.90 (+2)	1289.67
LG.6	QQQLGKQPQQQL	65	776.36 (+2)	1550.82
LG.7	QQQLGQQPQQKL	65	776.36 (+2)	1550.82
LG.8	QQQLGQQPQQQL	65	776.36 (+2)	1550.79
LG.9	GQQPQQQQLAQGTF	63	779.94 (+2)	1557.76
LG.10	SIVLQEQQHGGQL	61	718.92 (+2)	1435.75
LG.11	SQQQPPFSQQQQQPL	56	885.31 (+2)	1767.86
LG.1	SHHQQQPIQQQPQPF	56	652.80 (+3)	1954.95
LG.12	QQPQQQLGQQPQQQQQQVL	55	754.33 (+3)	2259.14
LG.13	SIVLQEQQHGGGF	53	736.22 (+2)	1469.73
LG.14	QQPQQQLGQQPQQQVQKGTG	51	1227.1 (+2)	2451.23
LG.15	VQPQQQQPQQSVQGVY	50	921.88 (+2)	1842.91
LG.16	GKQPQQQQL	45	527.74 (+2)	1053.56
LG.17	GQQPQQQKL	45	527.74 (+2)	1053.56
LG.18	GQQPQQQQL	45	527.74 (+2)	1053.56
LG.19	LQPHQIAQLEVMNSIAL	44	953.19 (+2)	1904.03

LG.20	SILVQEQQHGGGL	44	718.92 (+2)	1435.75
LG.21	QQPQQQLGQQPQEQQVQQGTF	44	818.47 (+3)	2452.18
LG.22	QQQPLPPQQTFFQQPL	41	938.44 (+2)	1873.98
LG.23	SIILQQQQQQQQQQGQSIIQY	41	882.21 (+3)	2642.35
LG.3	VLPQQQIPF	37	535.31 (+2)	1068.60
LG.24	SHIPGLERPSQQQPLPPQQL	37	784.65 (+3)	2350.25
LG.25	SQQQQIPVIHPSVL	35	525.31 (+3)	1572.87
LG.26	LQPHQIAQLEVMTSIAL	35	946.59 (+2)	1891.03
LG.27	LQPHKIAQLEVMTSIAL	35	946.59 (+2)	1891.07
LG.28	SQQQQPPFSQQQPPF	33	886.86 (+3)	1770.84
LG.29	SQIPEQSRY	33	554.28 (+2)	1106.54
LG+B	LQPHQIAQL	32	524.31 (+2)	1046.59
LG.31	LQPHKIAQL	32	524.31 (+2)	1046.63
LG.32	DAIRAIY	31	467.77 (+2)	933.53
LG.33	EAIRAIIFSILQEQQGGF	27	735.84 (+3)	2203.21
LG.34	SQHQQPVLPQQQIPY	26	895.07 (+2)	1789.92
LG.35	IQVDPSGQVQWPQQQPPFPQQPF	25	978.39 (+3)	2931.44
LG.36	SQQQPPFSQQQPPF	23	885.31 (+2)	1770.84
LG.37	VQQQLPVVQPSIL	23	725.27 (+2)	1447.85
LG.38	VQQQIPVVQPSIL	23	725.27 (+2)	1447.85
LG.39	SIILQQQQQQQQQQGQSIIQY	23	1010.32 (+3)	3026.52
LG.40	TQQQPPFSQQPPISQQQQQQQQQPF	22	1079.74 (+3)	3234.55
LG.41	SQQQPPFSQQQPPFSQQQQQL	19	1355.76 (+2)	2708.30
α-gliadins within LMW-GS				
α.32	QQQQQQQQQQQIL	78	827.72 (+2)	1652.83
α.2	FQPSQQNPQAQGF	48	738.95 (+2)	1475.69
α.33	VQPQQLPQFEEIRNL	41	920.46 (+2)	1837.98
α.10	QQPQQQYPSGQGF	33	746.80 (+2)	1491.68
α.34	QQPNIAHASSQVSQQSY	33	937.28 (+2)	1871.88
α.35	QQPNIAHASSKVSQQSY	33	937.28 (+2)	1871.92