

Identification of Isopeptides Between Human Tissue Transglutaminase and Wheat, Rye, and Barley Gluten Peptides

Supplementary Material

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Table S1. Number of identified proteins in each gluten protein type (GPT) blank sample.

GPTs wheat	Number of protein entries in database	GPTs rye	Number of protein entries in database	GPTs barley	Number of protein entries in database
HMW-GS	2233	HMW-secalins	586	D-hordeins	1673
ω 1,2-gliadins	2470	ω -secalins	777	C-hordeins	1103
ω 5-gliadins	1167				
LMW-GS	2225	γ -75k-secalins	807	B-hordeins	903
γ -gliadins	2270	γ -40k-secalins	1725	γ -hordeins	745
α -gliadins	2500				

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W1      -----WQIPEQSR-----
W12     -----WQTPEQSR-----
W2      -----AQIPQQL-----
R6      -----AQIPQHL-----
B8      -----PQQQFPQQQFHQ--QQL-----
W5      -----PQQTF--PQQPLF-----
W6      -----PQPPQQPF-----
W9      P--QQSEQVIPQQPQQPF-----
B4      IIPQQPQQPFPLQPHQPY-----
R3      -----QPQQPFPQQPQQSF-----
B7      -----PLQPQQPF PW-----
R5      -----QIPTPLQPQQPF-----
W8      -----QEQQIGQEQQPGQW-----
B3      -----PQQPGQW-----
B5      -----PQQPGQG--QQPGQR-----
B6      -----PQQPGQGQGQQGYYPGATSL
W13     -----VYYPTSPQQPGQL-----
W3      -----VQGQGI IQPQQPAQL-----
R2      -----AQVQGI IQPQQL-----
R1      I----VQGQSIIQ-QQPAQL-----
W10     -----QQQPPFWQ-QQPPF-----
B2      -----VQQQQPPF-----
W4      -----PYSQ--PQPF-----
W11     -----RPQQPYPQ--PQPQY-----
B9      -----FPQYQIPTPL-----
B1      -----QGQQGQQLGQG--QQGY-----

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Figure S1. CLUSTAL format multiple sequence alignment of all non-deamidated gluten peptides involved in isopeptide formation with human transglutaminase 2 (MAFFT online version 7.452, Jan. 16, 2020).

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W1          -----WQIPEQSR-----
W12         -----WQTPEQSR-----
W2          -----AQIPQQL-----
R6          -----AQIPQHL-----
B8          -----PEEQFPQQQFHEQQL-----
B8 '       -----PEEQFPQQQFHQEQL-----
W3          ---VQGEGIIQPQPPAQL-----
R2          ---AQVQGIIQPQQL-----
R1          I--VQGQSIIQ-EQPAQL-----
W5          -----PQQTFFPQQPL--F-----
R3          -----QPQQPFPPQQPEQSF-----
W6          -----PQPPQQPF-----
B4          -----IIPQQPQQPFPLQPHQPY-----
W9          PQQSEQVIPEQPQQPF-----
B7          -----PLQPQQPF PW-----
R5          ----QIPTPLQPQQPF-----
W8          ----EEEEIGEEQQPGQW-----
B3          -----PQQPGQW-----
W13         -----VYYPTSPQQPGQL-----
B6          -----PQQPGQEGGQQGYYPGATSL
B5          -----PEQPGQGQQPGQR-----
W10         -----EQQPPFWEQQPP-F-----
B2          -----VQQEQPPF-----
W4          -----PYSQPQP--F-----
W11        -----RPQQPYPPQPQPQ-Y-----
B9          -----FPQYEIPTPL-----
B1          -----QGQEGEQLGQGEQG--YY-----

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Figure S2. CLUSTAL format multiple sequence alignment of all gluten peptides that are involved in isopeptide formation with human transglutaminase 2 considering the detected deamidation sites (MAFFT online version 7.452, Jan. 16, 2020).