

Proposal for the Improvement of the preDQ Tool



27/05/2026



1. Insert a single sequence in one **CAPITAL** letter code. It should contain at least 9 amino acids. The result is displayed in a table.

2. Choose an allele:

HLA-DQ2.5 (A1*05:01/B1*02:01) ▼

For prediction of multiple sequences upload a file in fasta format. The result is in a .csv file.

Choose File No file chosen

References on deamidation at these positions for DQ2.8 epitope?

3. Choose deamidation position

- ☐ p1 (recommended for HLA-DQ8.1)
- ☐ p4 (recommended for HLA-DQ2.5 and HLA-DQ8.1)
- ☐ p6 (recommended for HLA-DQ2.5 and HLA-DQ8.1)
- ☐ p7 (recommended for HLA-DQ2.5)
- ☐ p9 (recommended for HLA-DQ2.5 and HLA-DQ8.1)

4. Search only peptides containing specific motif (recommended for celiac peptides and HLA-DQ2.5 allele)

- ☒ Q/E-X1-P-X2 motif
- ☒ N/D-X1-P-X2 motif

DLPY is only presented in the epitopes from bacteria. Reference on N deamidated to D via deamidation?

5. Choose the output format

- ☒ Majority voting (at least 3 models out of 5 with positive prediction)

6. Non-binders

- ☐ include
- ☒ exclude

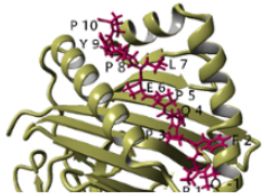
Predict

Reset form



preDQ

a tool for peptide binding prediction to HLA-DQ2 and/or HLA-DQ8



[Help](#)
[Example in plain format](#)

1. Insert a single sequence in one CAPITAL letter code. It should contain at least 9 amino acids. The result is displayed in a table.

MAAKMLALFALLALCASATSATHIPGHLPPVMPPLGTMINPCMQ
YCMNQGLASLMACPSLMLQQLLALPLQTMPVMPQMTPNM
MSPLMMPSPMSPMVLPSMMSQMMMPQCHCDVVSQIMLQQQLP
FMFNPMAMTIPPMFLQQPFVGAAF

2. Choose an allele:
HLA-DQ2.5 (A1*05:01/B1*02:01) ▼

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Choose File | No file chosen

3. Choose deamidation position
☐ p1 (recommended for HLA-DQ8.1)
☒ p4 (recommended for HLA-DQ2.5 and HLA-DQ8.1)
☒ p6 (recommended for HLA-DQ2.5 and HLA-DQ8.1)
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4. Search only peptides containing specific motif (recommended for celiac peptides and HLA-DQ2.5 allele)
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5. Choose the output format

6. Non-binders



There is a server error (500) when choosing HLA-DQ2.5 allele and corresponding deamidation position, but no motifs.



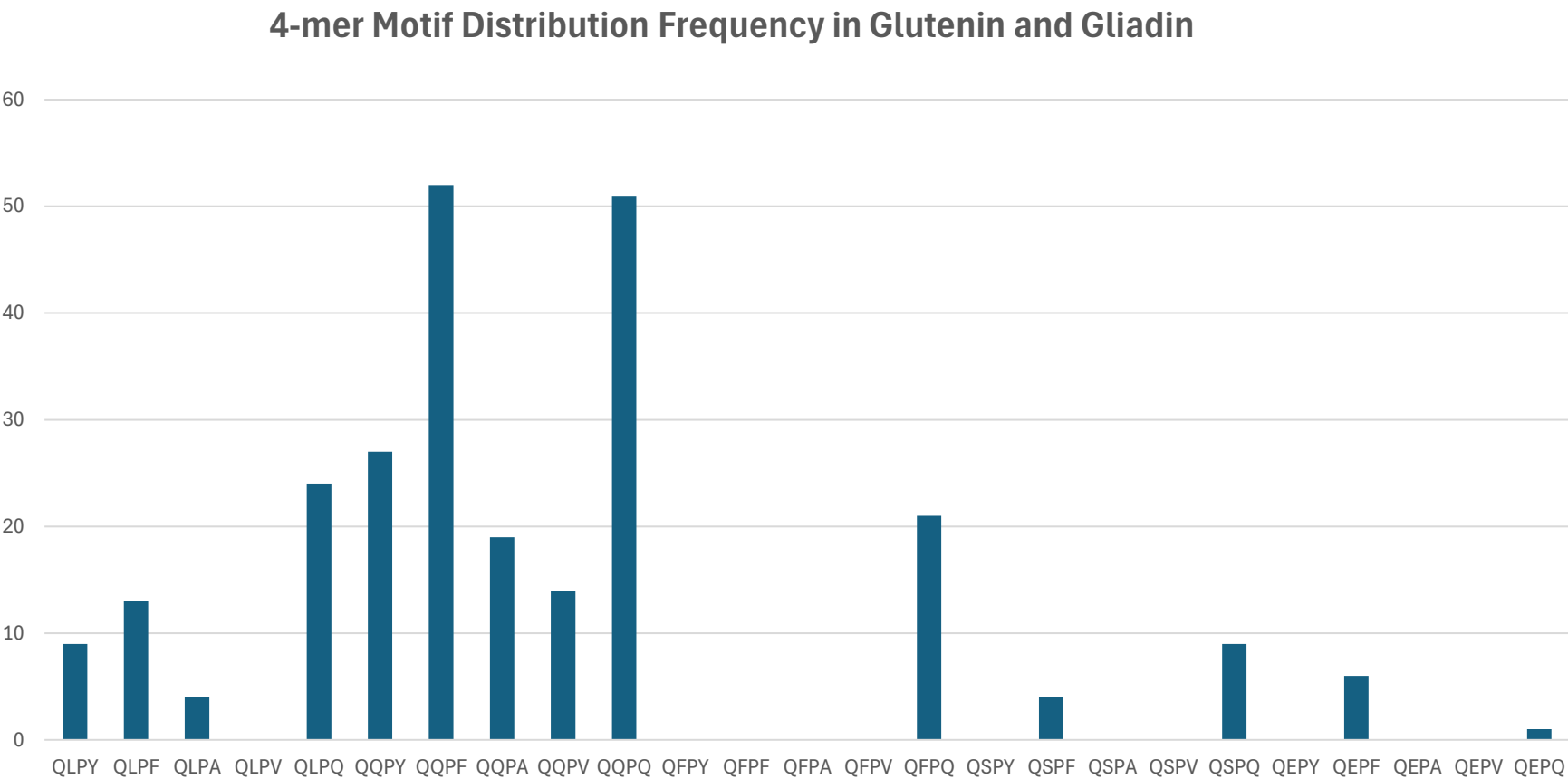
EFSA statistical models

Server Error (500)

Distribution Frequency of the 25 4-aa Motifs in 72 Known Glutenin and Gliadin from Wheat, Oats, Barley and Rye (Source AOL)

E L P Y
Q Q F
F A
S V
E Q

Only 28 possible motifs
are present considering
deamidation

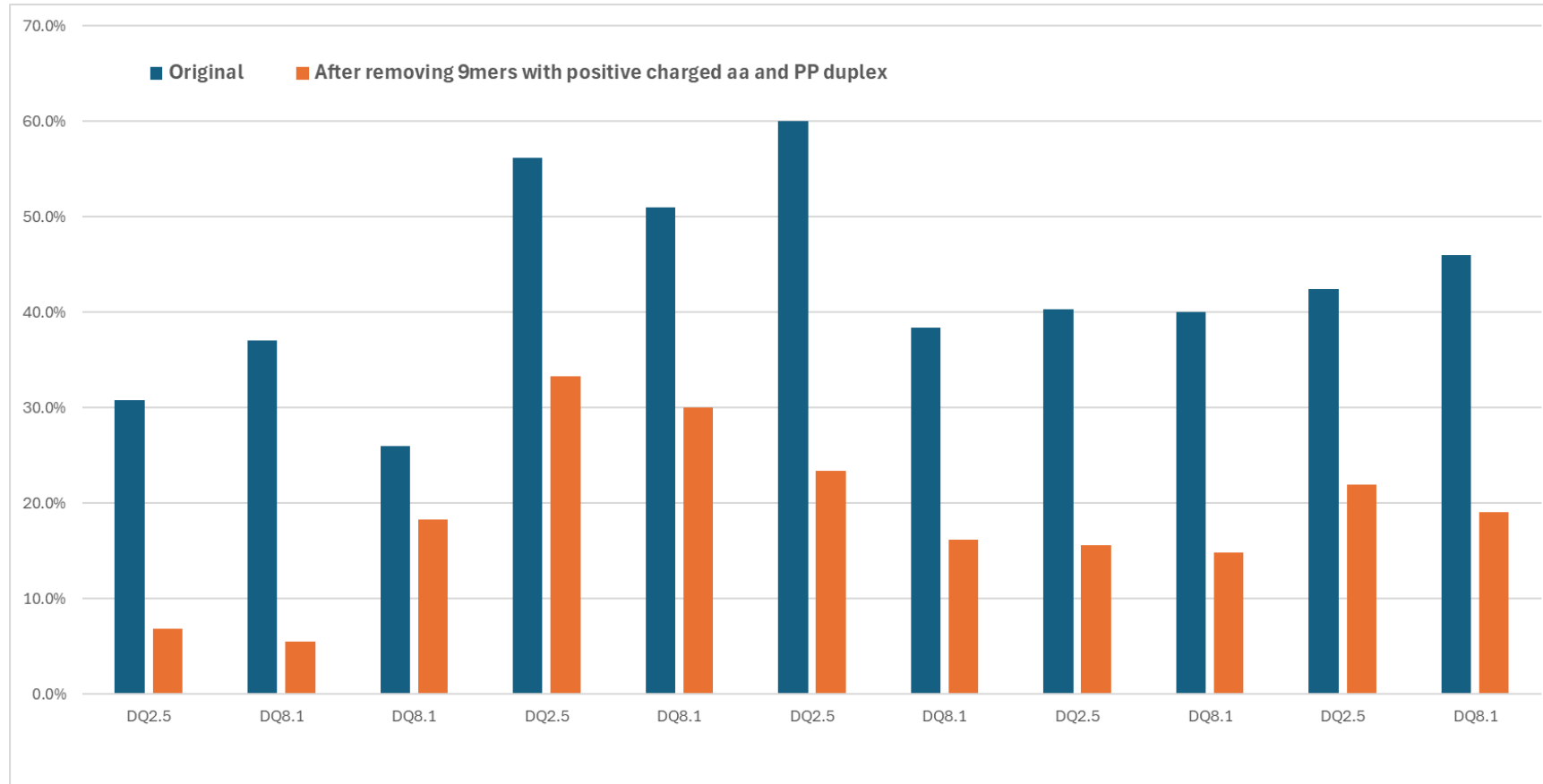


Suggestion: Only using 28 validated motifs plus “DLPY” from bacteria in the sequence identity search in Step 1

**Predicted positive 9-mer peptides include positively charged amino acids and a “PP” duplex,
both recognized for interfering with binding**

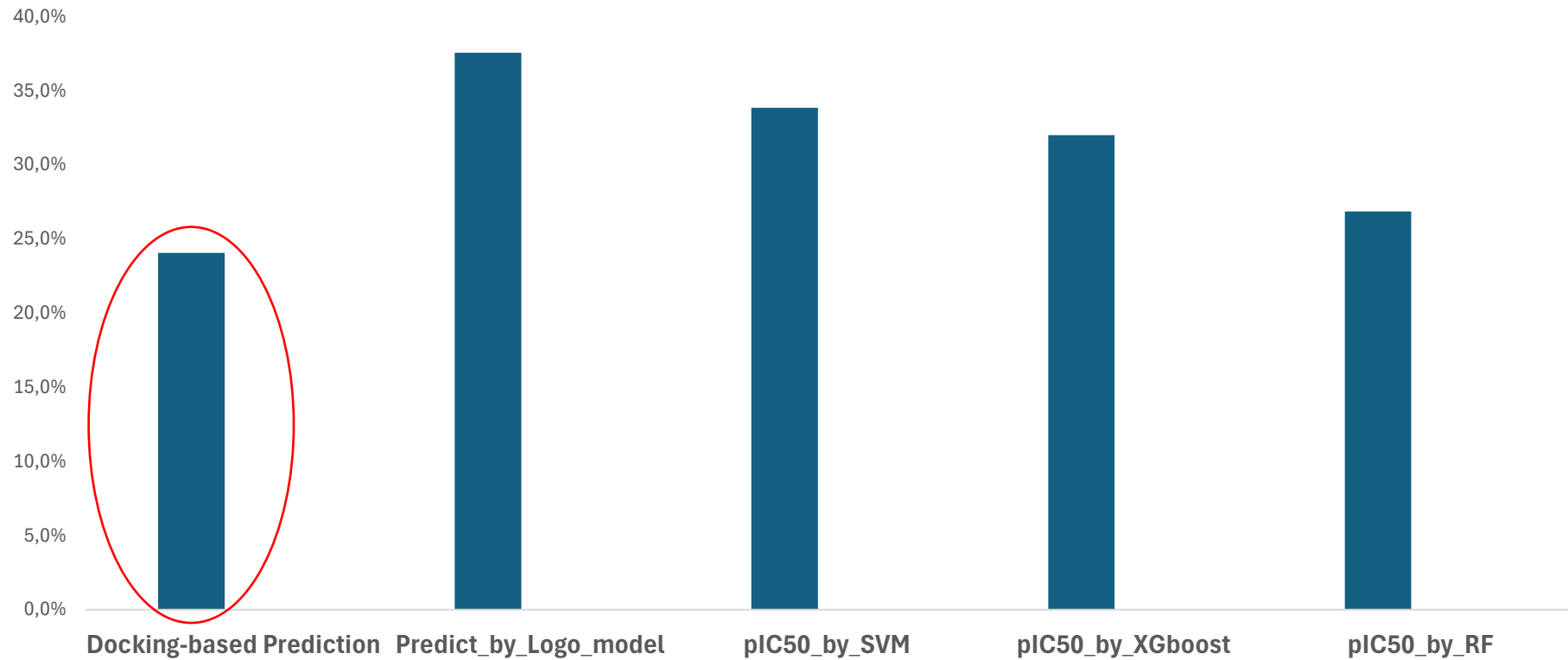
Query:	Allele:						
NP_054944.1	HLA-DQ2.5						
Position	Nonamer	Docking-based Prediction	Predict_by_Logo_model	pIC50_by_SVM	pIC50_by_XGboost	pIC50_by_RF	Positive_predictions
	cutoff	0	binding score > non-binding score	5.6	5.8	6	
1	MSPETETKA	probable non-binder (not recognized as binder by majority voting)					
2	SPQTETKAS	probable non-binder (not recognized as binder by majority voting)					
3	PQTETKASV	probable non-binder (not recognized as binder by majority voting)					
4	QTETKASVG	probable non-binder (not recognized as binder by majority voting)					
5	TETKASVGF	probable non-binder (not recognized as binder by majority voting)					
6	ETKASVGFK	probable non-binder (not recognized as binder by majority voting)					
7	TKASVGFKA	probable non-binder (not recognized as binder by majority voting)					
8	KASVGFKAG	probable non-binder (not recognized as binder by majority voting)					
→ 9	ASVGFKAGV	0.887	1	5.793	5.001	5.696	3
10	SVGFKAGVK	probable non-binder (not recognized as binder by majority voting)					
11	VGFKAGVKD	probable non-binder (not recognized as binder by majority voting)					
12	GFKAGVKDY	probable non-binder (not recognized as binder by majority voting)					
13	FKAGVKDYK	probable non-binder (not recognized as binder by majority voting)					
14	KAGVKDYKL	probable non-binder (not recognized as binder by majority voting)					
15	AGVKDYKLT	probable non-binder (not recognized as binder by majority voting)					
16	GVKDYKLTY	probable non-binder (not recognized as binder by majority voting)					
17	VKDYKLTTY	probable non-binder (not recognized as binder by majority voting)					
18	KDYKLTTYT	probable non-binder (not recognized as binder by majority voting)					
19	DYKLTTYTP	-0.148	0	5.774	6.06	6.123	3
20	YKLTTYTPE	0.02	1	5.745	5.259	7.026	4
21	KLTTYTPEY	probable non-binder (not recognized as binder by majority voting)					
22	LTYYTPEYE	0.55	1	7.021	5.912	6.884	5
23	TYTPEYET	0.05	1	6.986	5.946	5.99	4
24	YTPPEYETL	0.421	1	7.116	5.889	5.621	4
25	YTPPEYETLD	0.194	1	5.91	5.822	4.882	4
26	TPEYETLDT	probable non-binder (not recognized as binder by majority voting)					
27	PEYETLDTD	0.07	1	6.428	5.947	6.487	5
28	EYETLDTDIL	-0.94	0	5.819	7.391	6.251	3
29	YETLDTDIL	0.565	1	6.791	6.242	6.142	5
30	ETLDTDILA	probable non-binder (not recognized as binder by majority voting)					

Positive Hit Rate Reduction in Six Food Proteins after Removing 9-mer Peptides Containing Positively Charged Amino Acid and “PP” Duplex



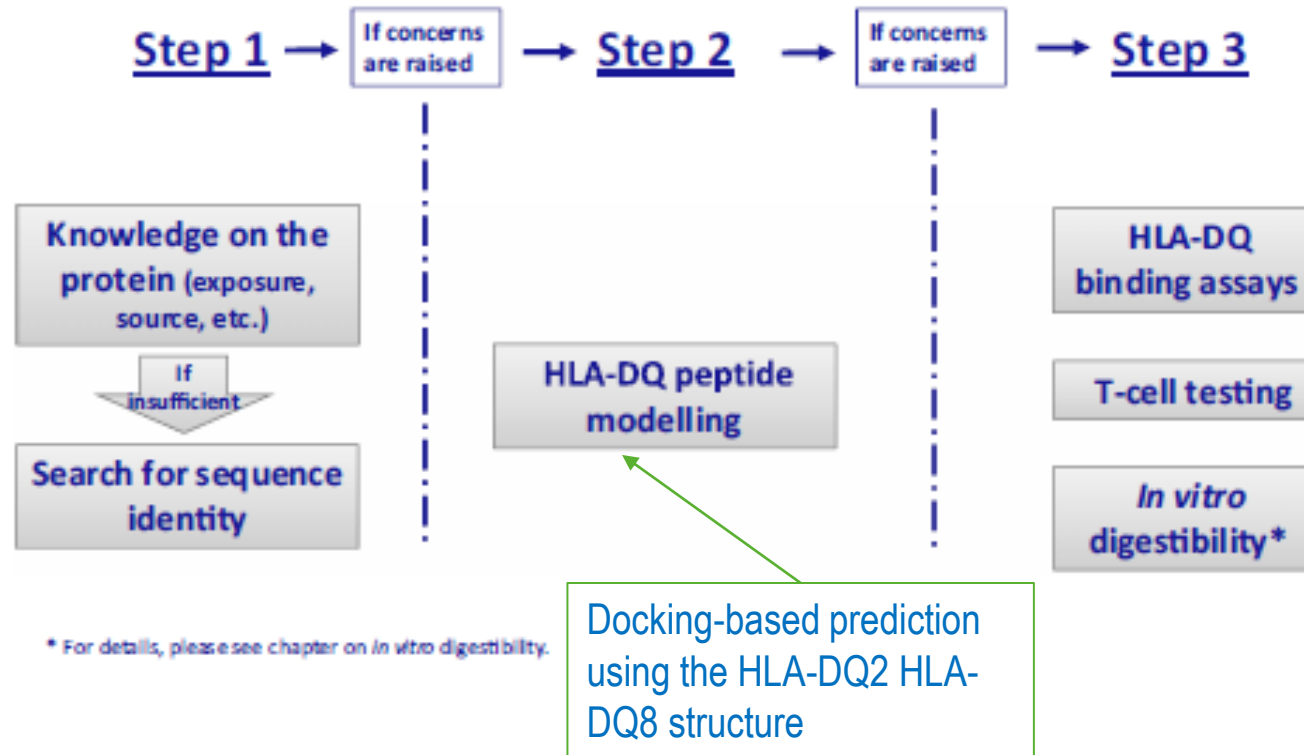
Recommendation: Exclude 9-mer peptides with positively charged amino acids at positions P1, P4, P6, P7, P9, sequences containing “PP,” and serine at position 8 prior to model analysis.

Positive Detection Rate of Six Food Proteins Across Five Algorithms in preDQ



Recommendation: Concentrate on docking-based predictions utilizing the structures of HLA-DQ2 and HLA-DQ8, consistent with Step 2.

Stepwise approach for risk assessment



EFSA journal. Naegeli, et al (2017)

Detection of Recognized Epitopes in the Food 9-mer Database (partial results)

	Epitope Name	Sequence	Food 9-mer Database	Organism
1	DQ2.5-glia- α 1a	PFPQP E LPY	PFPQP Q LPY	Wheat
2	DQ2.5-glia- α 1b	PYPQP E LPY	PYPQP Q LPY	Wheat
3	DQ2-P.fluor- α 1a	PMPMP E LPY	no	
4	DQ2-P.fluor- α 1b	PMPLP D LPY	no	
5	DQ2.5-glia- α 2	PQP E LPYPQ	PQP Q LPYPQ	Wheat
6	DQ2-P.fluor- α 2a	PMPELPYPA	no	
7	DQ2-P.fluor- α 2b	PLPELPYPA	no	
8	DQ2-B.copro- α 2a	PLPDLPYPV	no	
9	DQ2-P.aerug- α 2a	VQSELPYPE	no	
10	DQ2.5-glia- α 3var	FLPELPYPQ	no	
11	DQ2.5-glia- α 3	FRP E QYPYPQ	FRP Q QYPYPQ	Wheat
12	DQ2.5-glia- α 4	PQPEQYPYPQ	no	
13	DQ2.5-glia- α 5	PQPEYPQPQ	no	
14	DQ2.5-glia- γ 1	PQQSFP E QQ	PQQSFP Q QQ	Wheat

Recommendation: Add deamidated peptides to the Food 9-mer Database.

