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

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Here, we describe a software tool, named preDQ, for peptide binding prediction to HLA-DQ2 and HLA-DQ8 proteins specially designed and developed for the European Food Safety Authority. The tool is able to identify peptides binding to HLA-DQ2 and/or HLA-DQ8 proteins and to predict their binding affinities. The tool will be used to assess the risk of novel proteins to cause celiac disease.

Predictions made by preDQ are based on five robust models and the risk assessment is reported by five outputs. The models are developed using datasets of known peptides binding and non-binding to HLA-DQ2 and HLA-DQ8 proteins. The datasets are compiled from the literature and curated. Ligand-based and structure-based methods are used in the development of the computational models. The models are validated by internal cross-validation procedures and by external test sets. Only the best performing models are selected and included in preDQ.

preDQ is a comprehensive, user friendly and reliable tool for assessing the binding affinity of peptides to HLA-DQ2 and HLA-DQ8 and the capacity of the origin proteins to cause celiac disease.

Keywords: ligand-based in silico methods, structure-based in silico methods, HLA-DQ2 binding, HLA-DQ8 binding, celiac disease, machine learning