SUPPLEMENTARY MATERIAL

Figure S1: 3D structure of R-mandelonitrile-lyase modelled in Alphafold with (A) or without (B) signal peptide.

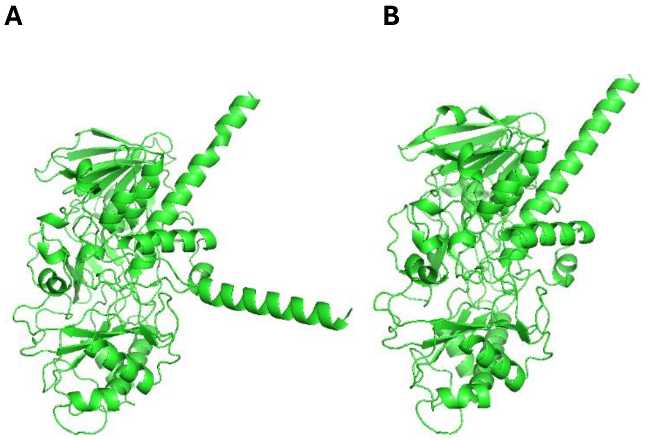

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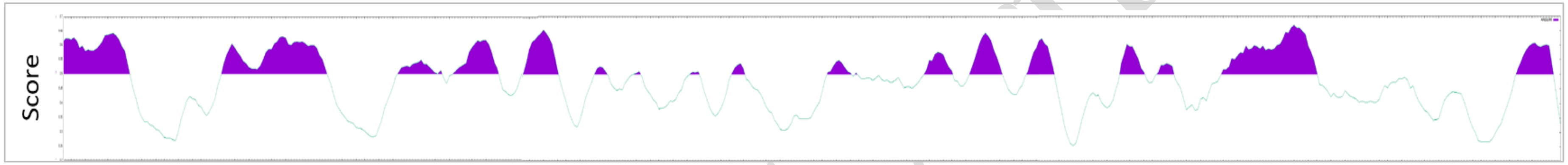
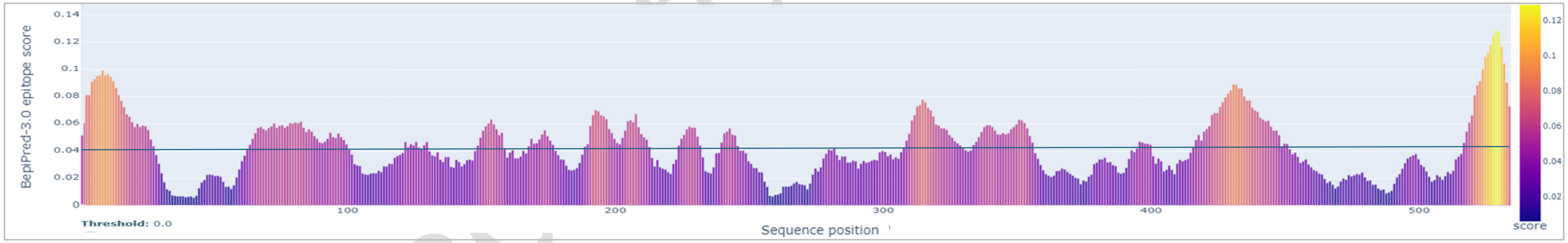
Figure S2: Epitopes identified in R-mandelonitrile-lyase. Top panel: Epitope prediction with BepiPred-2.0. Purple marked areas are those with score >0.5. Medium panel: Epitope prediction with BepiPred-3.0. The score is represented in different colors indicated on the right. Bottom panel: Optical density (O.D.) obtained by ELISA for each overlapping experimental peptide. The red line in the graphic mark the optical density of 0.1 (3x negative control values).

BepiPred-2.0



BepiPred-3.0



Experimental

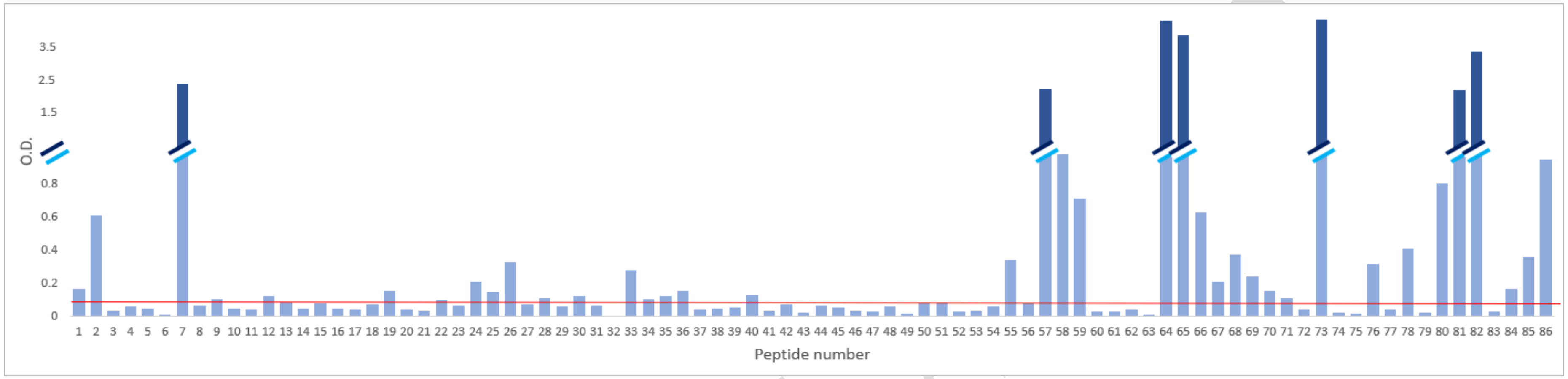


Figure S3: Location in the sequence of the epitopes identified in R-mandelonitrile-lyase. Bepipred-2.0 predicted epitopes in red, Bepipred-3.0 predicted epitopes highlighted in yellow, experimental positive peptides underlined.

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LANTSAHDFSYLKFVYNATDTSLEGSYDYIVIGGGTSGCPLAATLSEKFKVLLLERGTIATEYPNTLTADGFAYNLQQQDDGKTPVERFVSEDGIDNVRARILGGTTIINAGVYARANISFYSETGIEW
DLDLVNKTYEWVEDAIVVKPNNQSWQSVIGEGFLEAGILPDNGFSLDHEAGTRLTGSTFDNNGTRHAADELLNKGDPNNLLVAVQASVEKILFSSNTSNLSAIGVIYTDSDGNSHQAFVRGYGEVIVSA
GTIGTPQLLLLSGVGPESYLSSLNITVIQPNPYVGQFVYDNPRNFINILPPNPIEASVVTVLGITSDYYQVSLSSLPFSTPPFSLFPTTSYPLPNSTFAHIVSQVPGPLSHGSVTLNSSSDVRIAPNIK
FNYYSNSTDLANCVSGTKKLGDLLRTKALEPYKARDVPGIDGFNYLGVPLPENQTDDASFETFCLDNVASYWHYHGGSLVGKVLDDSFRVMGIKALRVVDASTFPDEPNSHPQGFYLMLGRYVGLQILQ
ERSIRLEAIHNIHESK
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Figure S4: T-cell epitome of peach R-mandelonitrile-lyase. Predicted epitopes for MHC-II alleles were mapped corresponding from top to bottom to: HLA-DPA1*01:03/DPB1*02:01, HLA-DPA1*01:03/DPB1*04:01, HLA-DPA1*02:01/DPB1*01:01, HLA-DPA1*02:01/DPB1*05:01, HLA-DPA1*02:01/DPB1*14:01, HLA-DPA1*03:01/DPB1*04:02, HLA-DQA1*01:01/DQB1*05:01, HLA-DQA1*01:02/DQB1*06:02, HLA-DQA1*03:01/DQB1*03:02, HLA-DQA1*04:01/DQB1*04:02, HLA-DQA1*05:01/DQB1*02:01, HLA-DQA1*05:01/DQB1*03:01, HLA-DRB1*01:01, HLA-DRB1*03:01, HLA-DRB1*04:01, HLA-DRB1*04:05, HLA-DRB1*07:01, HLA-DRB1*08:02, HLA-DRB1*09:01, HLA-DRB1*11:01, HLA-DRB1*12:01, HLA-DRB1*13:02, HLA-DRB1*15:01, HLA-DRB3*01:01, HLA-DRB3*02:02, HLA-DRB4*01:01 and HLA-DRB5*01:01. Only regions with the highest T-cell prediction are represented residues 36-49, 86-98, 172-195, 249-262, 310-346, 371-385, 402-427 and 443-458. Highest recognition corresponds to Rank = 0 (red color).

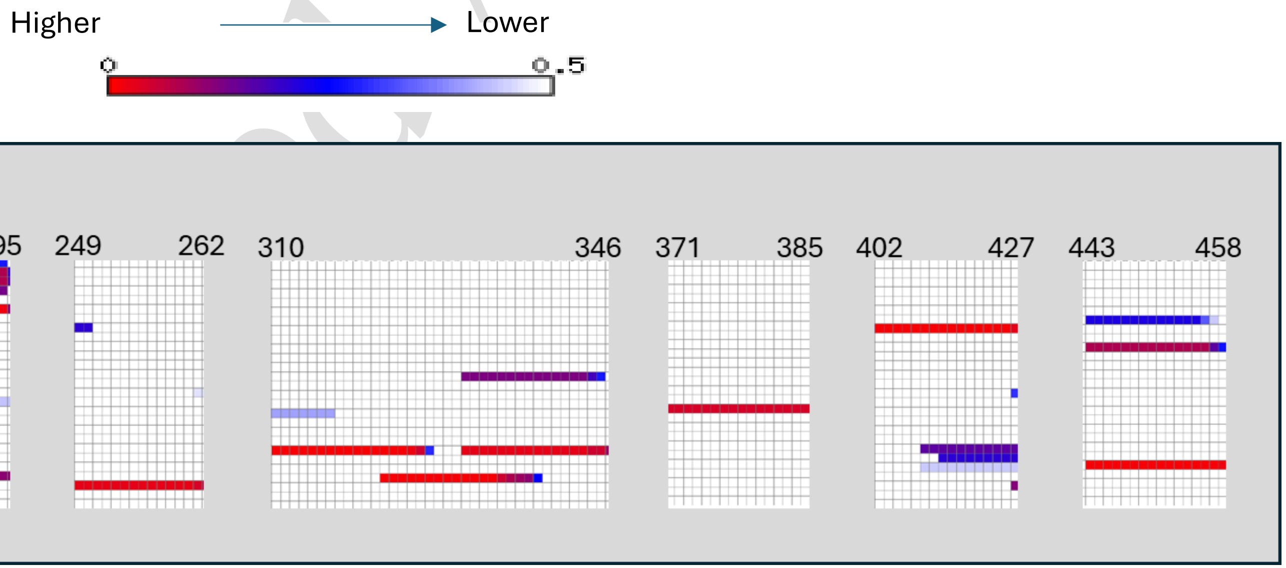

Figure S5: Location on the 3D structure of the B- and T-predicted epitopes common areas (in blue in the figure). These areas correspond to the amino acid position: 36-44, 88-92, 172-180, 189-194, 251-256, 336-345, 371-380, 404-412 and 417-422 of A0A251QUN8 protein.