Gibbs clustering of identified SARS-CoV-2-derived HLA-I peptides. SARS-CoV-2- and human-derived HLA-I peptides were Gibbs clustered to assign the peptides to the different HLA alleles of the patient. Logos were created to identify the HLA allele's motif using all the peptides that match this allele in the IEDB database. N - number of all peptides, V - number of viral peptides, H - number of human peptides in each cluster. The trash represents the peptides that were not assigned to any cluster. Clusters with special characteristics are marked with an asterisk.

Tandem mass spectra of the SARS-CoV-2 peptides and their corresponding synthetic peptides. (A) Fragmentation images of endogenous and synthetic peptides were extracted from MaxQuant. A head-to-tail figure was plotted to compare the fragmentation of the endogenous and synthetic peptides. The Pearson correlation and the dot product score are indicated for each comparison. (B) Stable isotopically labeled peptides were spiked into the samples and analyzed using mass spectrometry. The labeled and endogenous peptides are shown to be co-eluted. The upper image represents both the labeled and endogeneous peptides; the bottom represents the separated peptides. The synthetic peptides were also analyzed alone (marked as "synthetic peptide"), showing that the synthetic labeled peptide is not contaminated with light peptide traces. The data was analyzed using Skyline software. The m/z of each peptide is indicated in the index, "+" indicates the charge.

Correlation between peptides' experimental retention time to the predicted peptides' hydrophobicity. The peptides' RTs were plotted against the calculated hydrophobicity index for each sample. In the scatter plots, the red dots represent the viral peptides, with the human peptides marked in gray.