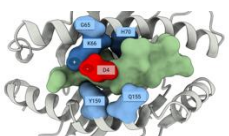


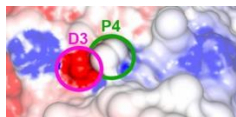


HLA-Arena 2.0

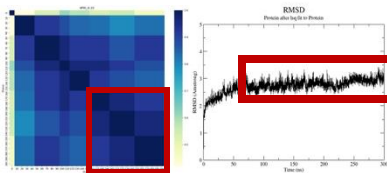
- TAA/neoantigen/epitope discovery
- APL design for peptide vaccines
- Immunogenicity prediction
- Off-target toxicity prediction
- Peptide-HLA modeling
- Dynamic binding analysis
- TCR and TCRpHLA modeling
- Molecular fingerprinting
- Data augmentation and feature extraction to accelerate AI-training



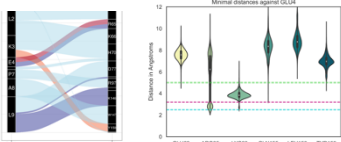
Peptide-HLA structural analysis



Surface potential TCR contacts

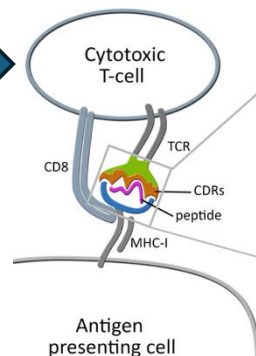


Stability analysis

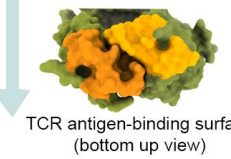
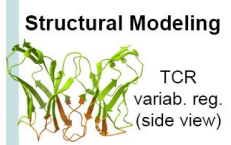
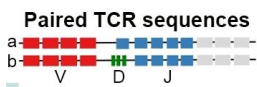


Dynamic interaction analysis

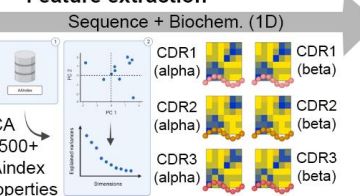
pMHC structural analysis



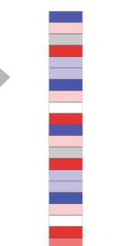
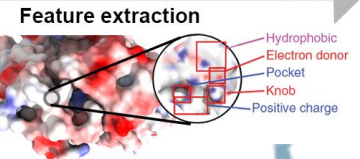
TCR structural analysis



Feature extraction



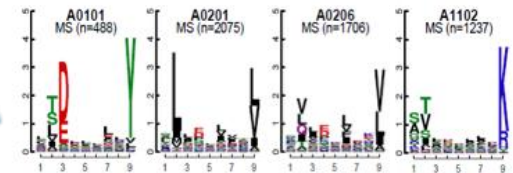
Geometry + Topology + Biochem. (3D)



Highlighted Publications (PMID)

- CrossDome and toxicity (37377956)
- TCRpHLA modeling (39104710)
- HLA-Arena environment (32667823)
- Docking and modeling (38415656, 29092940)
- Single-cell TCR analysis (37163233, 38418901)
- AI-based analysis (35365602, 38577265)
- T-cell cross-reactivity (38444853, 29046675)
- Dynamics/simulation (33184174, 37418278)

<https://dinlerantunes.com/lab>



Epitope sequence analysis

- Heterogeneity across HLAs
- Different HLAs across ethnic groups
- Incomplete and biased datasets
- **Biased AI sequence-based tools** (Gold-standard for neoantigen discovery and vaccine design)

Highlighted funded projects

- Structure-guided cancer immunotherapy design with HLA-Arena and CrossDome; NCI/NIH (1R21CA289333-01).
- Improving the design of immunotherapies for underrepresented minorities; HEALTH-RCMI pilot grant, NIMHD/NIH (U54MD015946)
- Development and optimization of mRNA vaccines using artificial intelligence methods; CNPq/Brazil
- AI-driven scoring for virtual screening of peptide-based ligands. Drug Discovery Institute (DDI) pilot funding, University of Houston.