Closing Remarks & Survey

2021 IEDB Virtual User Workshop – Day 2

Thursday, November 4, 2021

We want to hear from you!

SurveyMonkey

Improve our resources through user feedback

Daily and post-event feedback survey

Chat

https://www.surveymonkey.com/r/QSLTPH2

SurveyMonkey

Please take some time to complete the survey now

#iedbuw2021

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Recap of Day 2

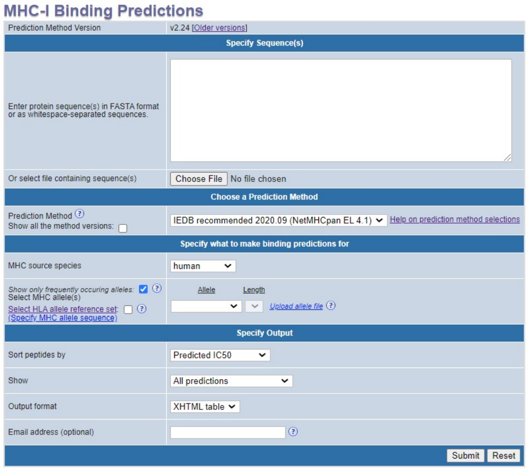
MHC Binding Predictions

Dr. Raphael Trevizani

Bioinformatics Postdoctoral Researcher

Dr. Bjoern Peters

Co-Principal Investigator



MHC-I Binding Predictions

Prediction Method Version: v2.24 [Older versions]

Specify Sequence(s)

Enter protein sequence(s) in FASTA format or as whitespace-separated sequences.

Or select file containing sequence(s): Choose File No file chosen

Choose a Prediction Method

Prediction Method: IEDB recommended 2020.09 (NetMHCpan EL 4.1) Help on prediction method selections

Show all the method versions: ☐

Specify what to make binding predictions for

MHC source species: human

Show only frequently occuring alleles: ☑

Select MHC allele(s): Allele Length Upload allele file

Select HLA allele reference set: ☐

(Specify MHC allele sequence)

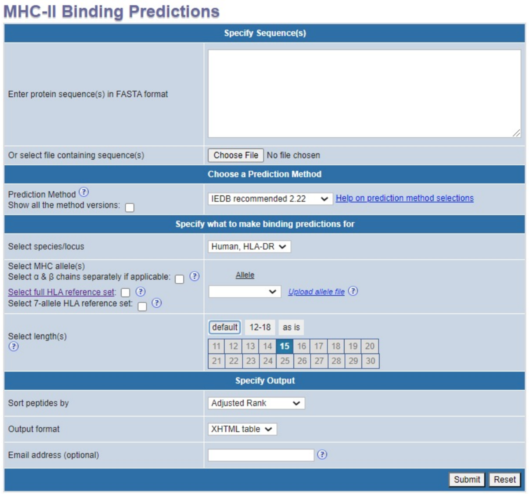
Specify Output

Sort peptides by: Predicted IC50

Show: All predictions

Output format: XHTML table

Email address (optional):



MHC-II Binding Predictions

Specify Sequence(s)

Enter protein sequence(s) in FASTA format

Or select file containing sequence(s): Choose File No file chosen

Choose a Prediction Method

Prediction Method: IEDB recommended 2.22 Help on prediction method selections

Show all the method versions: ☐

Specify what to make binding predictions for

Select species/locus: Human, HLA-DR

Select MHC allele(s): Allele Upload allele file

Select α & β chains separately if applicable: ☐

Select full HLA reference set: ☐

Select 7-allele HLA reference set: ☐

Select length(s): default 12-18 as is

11	12	13	14	**15**	16	17	18	19	20
21	22	23	24	25	26	27	28	29	30

Specify Output

Sort peptides by: Adjusted Rank

Output format: XHTML table

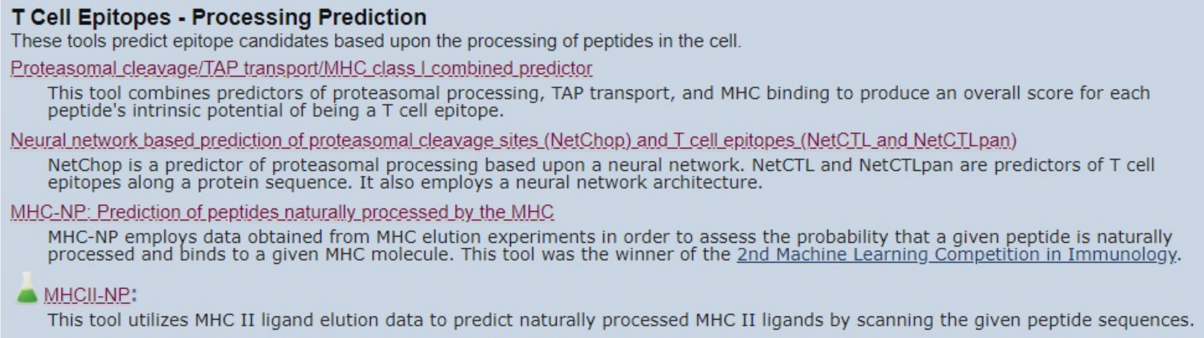
Email address (optional):

Recap of Day 2

T Cell Processing & Immunogenicity Predictions

Dr. Bjoern Peters
Co-Principal Investigator

Austin Crinklaw
Tools Research Technician



T Cell Epitopes - Processing Prediction

These tools predict epitope candidates based upon the processing of peptides in the cell.

Proteasomal cleavage/TAP transport/MHC class I combined predictor

This tool combines predictors of proteasomal processing, TAP transport, and MHC binding to produce an overall score for each peptide's intrinsic potential of being a T cell epitope.

Neural network based prediction of proteasomal cleavage sites (NetChop) and T cell epitopes (NetCTL and NetCTLpan)

NetChop is a predictor of proteasomal processing based upon a neural network. NetCTL and NetCTLpan are predictors of T cell epitopes along a protein sequence. It also employs a neural network architecture.

MHC-NP: Prediction of peptides naturally processed by the MHC

MHC-NP employs data obtained from MHC elution experiments in order to assess the probability that a given peptide is naturally processed and binds to a given MHC molecule. This tool was the winner of the 2nd Machine Learning Competition in Immunology.

MHCII-NP:

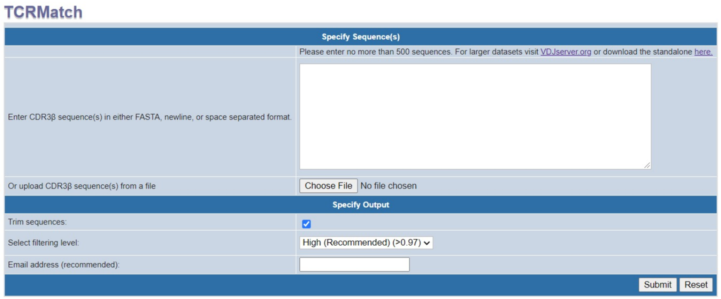
This tool utilizes MHC II ligand elution data to predict naturally processed MHC II ligands by scanning the given peptide sequences.

Recap of Day 2

IMMUNE EPITOPE DATABASE
AND ANALYSIS RESOURCE

T Cell Tool Spotlight: TCRMatch

Dr. William Chronister
Bioinformatics Postdoctoral Researcher

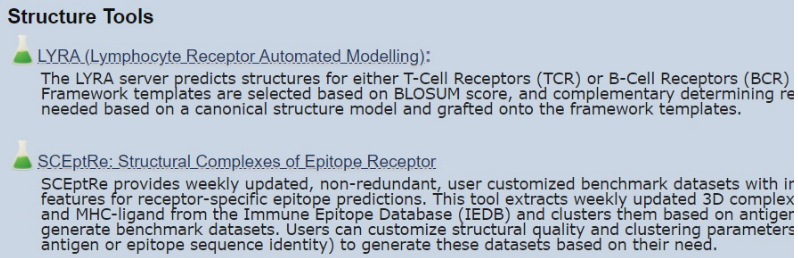


TCRMatch

Specify Sequence(s)	
	Please enter no more than 500 sequences. For larger datasets visit VDJserver.org or download the standalone here.
Enter CDR3β sequence(s) in either FASTA, newline, or space separated format.	
Or upload CDR3β sequence(s) from a file	Choose File No file chosen
Specify Output	
Trim sequences:	☑
Select filtering level:	High (Recommended) (>0.97)
Email address (recommended):	

Structure Tools: LYRA & SCEptRe

Dr. Paolo Marcatili
DTU Associate Professor



Structure Tools

LYRA (Lymphocyte Receptor Automated Modelling):
The LYRA server predicts structures for either T-Cell Receptors (TCR) or B-Cell Receptors (BCR)
Framework templates are selected based on BLOSUM score, and complementary determining re
needed based on a canonical structure model and grafted onto the framework templates.

SCEptRe: Structural Complexes of Epitope Receptor
SCEptRe provides weekly updated, non-redundant, user customized benchmark datasets with ir
features for receptor-specific epitope predictions. This tool extracts weekly updated 3D complex
and MHC-ligand from the Immune Epitope Database (IEDB) and clusters them based on antiger
generate benchmark datasets. Users can customize structural quality and clustering parameters
antigen or epitope sequence identity) to generate these datasets based on their need.

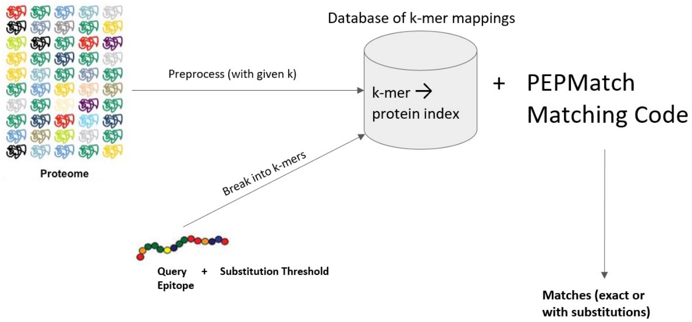
Recap of Day 2

IMMUNE EPITOPE DATABASE
AND ANALYSIS RESOURCE

PEPMatch: Homology of SARS-CoV-2 Spike Sequences to Myocarditis Antigens

Daniel Marrama
Bioinformatics Research Technician

PEPMatch Tool Overview



Proteome

Preprocess (with given k)

Database of k-mer mappings

k-mer → protein index

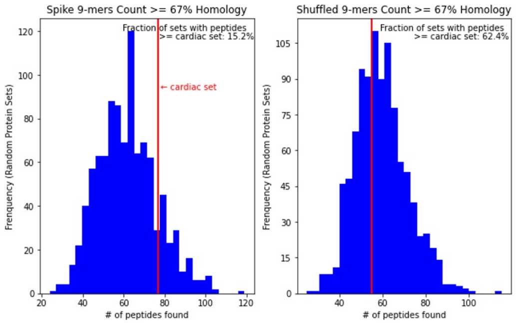
\+ PEPMatch Matching Code

Break into k-mers

Query Epitope + **Substitution Threshold**

Matches (exact or with substitutions)

Distribution of Spike Matches in 1,000 Random Protein Sets

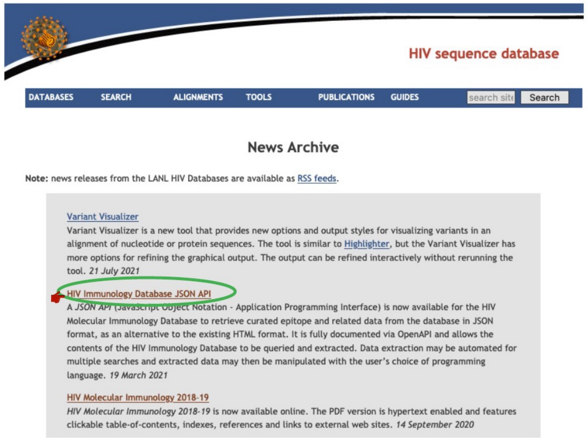


Recap of Day 2

Los Alamos
NATIONAL LABORATORY
EST. 1943

NIH Resources for Researchers:
The LANL HIV Immunology Database

Dr. Elizabeth-Sharon Fung
Annotator, Editor



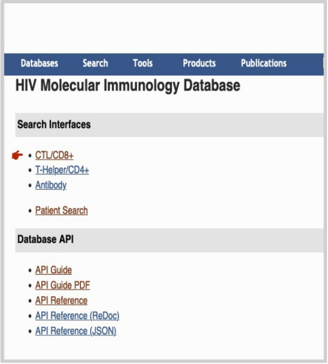
News Archive

Note: news releases from the LANL HIV Databases are available as RSS feeds.

Variant Visualizer
Variant Visualizer is a new tool that provides new options and output styles for visualizing variants in an alignment of nucleotide or protein sequences. The tool is similar to Highlighter, but the Variant Visualizer has more options for refining the graphical output. The output can be refined interactively without rerunning the tool. *21 July 2021*

HIV Immunology Database JSON API
A *JSON API* (JavaScript Object Notation - Application Programming Interface) is now available for the HIV Molecular Immunology Database to retrieve curated epitope and related data from the database in JSON format, as an alternative to the existing HTML format. It is fully documented via OpenAPI and allows the contents of the HIV Immunology Database to be queried and extracted. Data extraction may be automated for multiple searches and extracted data may then be manipulated with the user's choice of programming language. *19 March 2021*

HIV Molecular Immunology 2018-19
HIV Molecular Immunology 2018-19 is now available online. The PDF version is hypertext enabled and features clickable table-of-contents, indexes, references and links to external web sites. *14 September 2020*



HIV Molecular Immunology Database

Search Interfaces

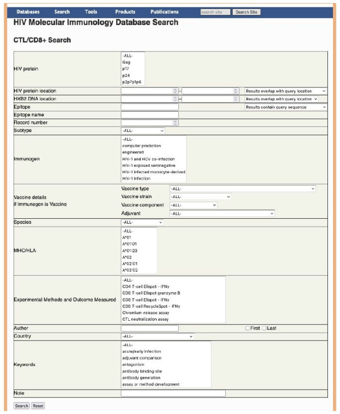
- CTL/CD8+
- T-Helper/CD4+
- Antibody

- Patient Search

Database API

- API Guide
- API Guide PDF
- API Reference
- API Reference (ReDoc)
- API Reference (JSON)

https://www.hiv.lanl.gov/mojo/immunology/index



HIV Molecular Immunology Database Search

CTL/CD8+ Search

HIV protein	-ALL- Gag p17 p24 p2p7p1p6
HIV protein location	Results overlap with query location
HXB2 DNA location	Results overlap with query location
Epitope	Results contain query sequence
Epitope name	
Record number	
Subtype	-ALL-
Immunogen	-ALL- computer prediction engineered HIV-1 and HCV co-infection HIV-1 exposed seronegative HIV-1 infected monocyte-derived HIV-1 infection
Vaccine details if Immunogen is Vaccine	Vaccine type -ALL- Vaccine strain -ALL- Vaccine component -ALL- Adjuvant -ALL-
Species	-ALL-
MHC/HLA	-ALL- A*01 A*01:01 A*01:23 A*02 A*02:01 A*02:02
Experimental Methods and Outcome Measured	-ALL- CD4 T-cell Elispot - IFNγ CD8 T-cell Elispot granzyme B CD8 T-cell Elispot - IFNγ CD8 T-cell RecycleSpot - IFNγ Chromium-release assay CTL neutralization assay
Author	☐ First ☐ Last
Country	-ALL-
Keywords	-ALL- acute/early infection adjuvant comparison antagonism antibody binding site antibody generation assay or method development
Note	

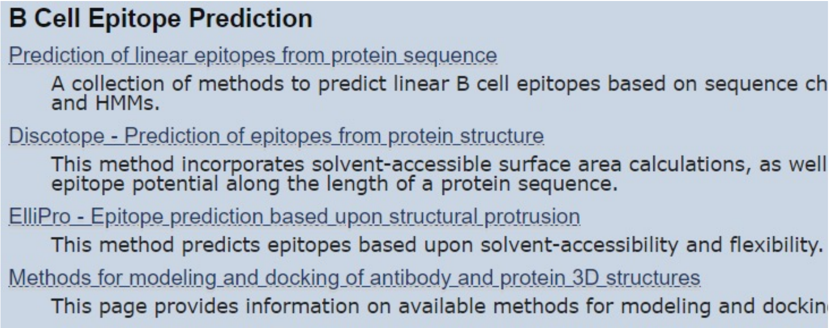
Recap of Day 2

IMMUNE EPITOPE DATABASE AND ANALYSIS RESOURCE

B Cell Epitope Prediction

Dr. Marcus Mendes

Bioinformatics Postdoctoral Researcher



B Cell Epitope Prediction

Prediction of linear epitopes from protein sequence

A collection of methods to predict linear B cell epitopes based on sequence ch
and HMMs.

Discotope - Prediction of epitopes from protein structure

This method incorporates solvent-accessible surface area calculations, as well
epitope potential along the length of a protein sequence.

ElliPro - Epitope prediction based upon structural protrusion

This method predicts epitopes based upon solvent-accessibility and flexibility.

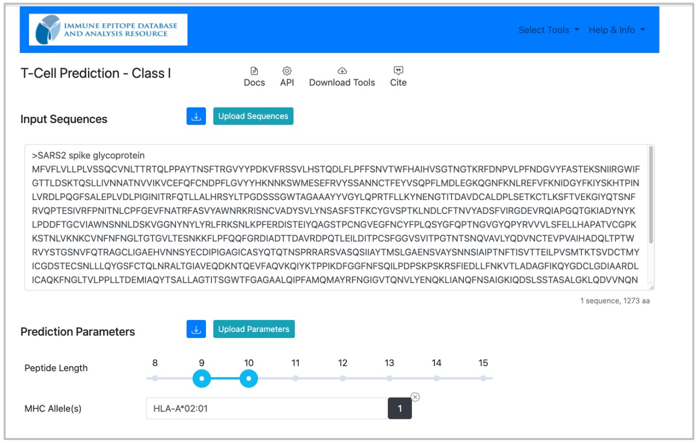
Methods for modeling and docking of antibody and protein 3D structures

This page provides information on available methods for modeling and dockin

IEDB Tools 3.0: Future of Tools

Dr. Jason Greenbaum

Bioinformatics Core Director



T-Cell Prediction - Class I

Input Sequences

```
>SARS2 spike glycoprotein
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPFFSNVTWFHAIHVSGTNGTKRFDNPVLPFNDGVYFASTEKSNIIRGWIF
GTTLDSKTQSLLIVNNATNVVIKVCEFQFCNDPFLGVYYHKNNKSWMESEFRVYSSANNCTFEYVSQPFLMDLEGKQGNFKNLREFVFKNIDGYFKIYSKHTPIN
LVRDLPQGFSALEPLVDLPIGINITRFQTLLALHRSYLTPGDSSSGWTAGAAAYYVGYLQPRTFLLKYNENGTITDAVDCALDPLSETKCTLKSFTVEKGIYQTSNF
RVQPTESIVRFPNITNLCPFGEVFNATRFASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRGDEVRQIAPGQTGKIADYNYK
LPDDFTGCVIAWNSNNLDSKVGGNYNYLYRLFRKSNLKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTNGVGYQPYRVVVLSFELLHAPATVCGPK
KSTNLVKNKCVNFNFNGLTGTGVLTESNKKFLPFQQFGRDIADTTDAVRDPQTLEILDITPCSFGGVSVITPGTNTSNQVAVLYQDVNCTEVPVAIHADQLTPTW
RVYSTGSNVFQTRAGCLIGAEHVNNSYECDIPIGAGICASYQTQTNSPRRARSVASQSIIAYTMSLGAENSVAYSNNSIAIPTNFTISVTTEILPVSMTKTSVDCTMY
ICGDSTECSNLLLQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQILPDPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDL
ICAQKFNGLTVLPPLLTDEMIAQYTSALLAGTITSGWTFGAGAALQIPFAMQMAYRFNGIGVTQNVLYENQKLIANQFNSAIGKIQDSLSSTASALGKLQDVVNQN
```

1 sequence, 1273 aa

Prediction Parameters

Peptide Length: 8 ●9 ●10 11 12 13 14 15

MHC Allele(s): HLA-A*02:01 | 1

Post-Event Details

You will receive a post-event email next week

Workshop recording will be shared with you

All presentations will be shared with you

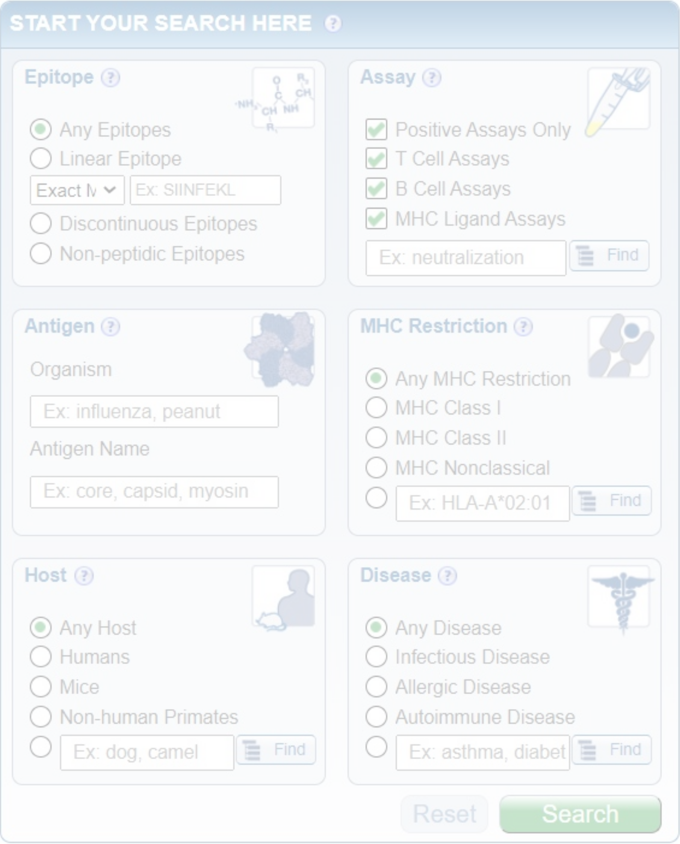
Participation certificates will be provided upon request

SurveyMonkey

Post-event feedback survey

User Workshop Structure

Day 1



START YOUR SEARCH HERE

Epitope

● Any Epitopes
○ Linear Epitope
Exact M | Ex: SIINFEKL
○ Discontinuous Epitopes
○ Non-peptidic Epitopes

Assay

☑ Positive Assays Only
☑ T Cell Assays
☑ B Cell Assays
☑ MHC Ligand Assays
Ex: neutralization | Find

Antigen

Organism
Ex: influenza, peanut
Antigen Name
Ex: core, capsid, myosin

MHC Restriction

● Any MHC Restriction
○ MHC Class I
○ MHC Class II
○ MHC Nonclassical
○ Ex: HLA-A*02:01 | Find

Host

● Any Host
○ Humans
○ Mice
○ Non-human Primates
○ Ex: dog, camel | Find

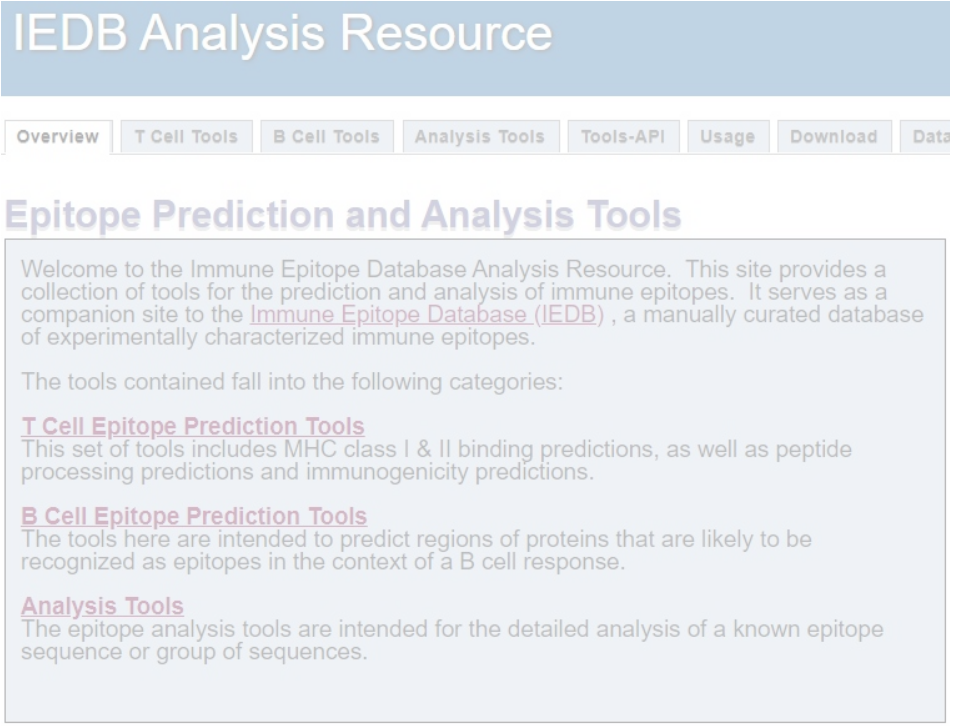
Disease

● Any Disease
○ Infectious Disease
○ Allergic Disease
○ Autoimmune Disease
○ Ex: asthma, diabet | Find

Reset | Search

Process Overview and Database

Day 2



IEDB Analysis Resource

Overview | T Cell Tools | B Cell Tools | Analysis Tools | Tools-API | Usage | Download | Data

Epitope Prediction and Analysis Tools

Welcome to the Immune Epitope Database Analysis Resource. This site provides a collection of tools for the prediction and analysis of immune epitopes. It serves as a companion site to the Immune Epitope Database (IEDB) , a manually curated database of experimentally characterized immune epitopes.

The tools contained fall into the following categories:

T Cell Epitope Prediction Tools
This set of tools includes MHC class I & II binding predictions, as well as peptide processing predictions and immunogenicity predictions.

B Cell Epitope Prediction Tools
The tools here are intended to predict regions of proteins that are likely to be recognized as epitopes in the context of a B cell response.

Analysis Tools
The epitope analysis tools are intended for the detailed analysis of a known epitope sequence or group of sequences.

Analysis Resource

Thank you!

We appreciate your time and interest in the IEDB!

Optional Q&A

This will be to answer any remaining questions from the day