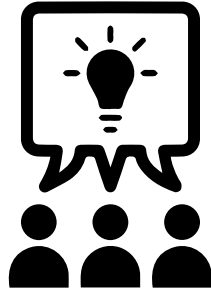


Closing Remarks & Survey

2020 IEDB Virtual User Workshop – Day 2

Friday, November 6, 2020

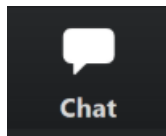
We want to hear from you!



Improve our resources
through user feedback



Daily and post-event
feedback survey



<https://www.surveymonkey.com/r/MLB9YFY>



**Please take some time to
complete the survey now**

Recap of Day 2

MHC Binding Predictions



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): 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:

Show only frequently occurring alleles: [?](#)
Select MHC alleles:

Select HLA allele reference set: [?](#)
[\[Specify MHC allele sequence\]](#)

Specify Output

Sort peptides by:

Show:

Output format:

Email address (optional):

MHC-II Binding Predictions

Specify Sequence(s)

Enter protein sequence(s) in FASTA format

Or select file containing sequence(s): 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/focus:

Select MHC allele(s):

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:

Output format:

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.

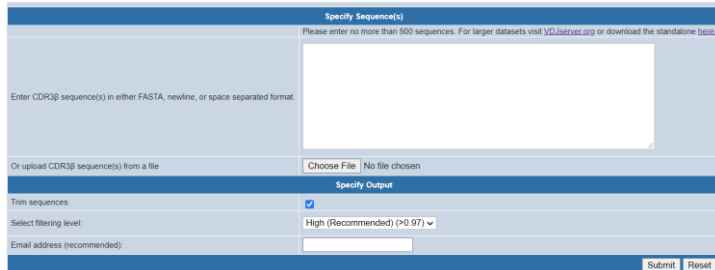
Recap of Day 2

T Cell Tool Spotlight: TCRMatch



Dr. William Chronister
*Bioinformatics Postdoctoral
Researcher*

TCRMatch



The screenshot shows the TCRMatch web interface. At the top, there is a section titled "Specify Sequence(s)" with a text input field and a "Choose File" button. Below this, there are several checkboxes and dropdown menus for "Specify Output", including "Trim sequences", "Select filtering level" (set to "High (Recommended) (>0.97)"), and "Email address (recommended)". At the bottom right, there are "Submit" and "Reset" buttons.

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 regions are 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 information 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 antigen and MHC-ligand. 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

HIV Sequence & Immunology Databases



Dr. Brian Foley
Research Scientist



Dr. Elizabeth-Sharon Fung
Annotator, Editor

Recap of Day 2

B Cell Epitope Prediction



Dr. Bjoern Peters
Co-Principal Investigator

IEDB Tools 3.0: Future of Tools



Dr. Jason Greenbaum
Bioinformatics Core Director

B Cell Epitope Prediction

[Prediction of linear epitopes from protein sequence](#)

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

[Discotope - Prediction of epitopes from protein structure](#)

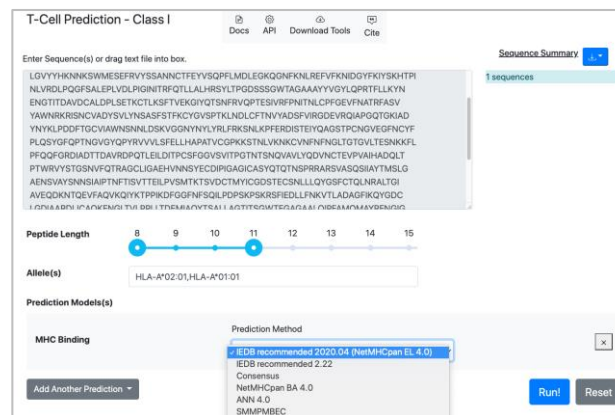
This method incorporates solvent-accessible surface area calculations, as well as epitope potential along the length of a protein sequence.

[ElliPro - Epitope prediction based upon structural protrusion](#)

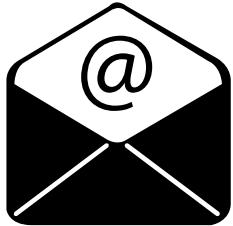
This method predicts epitopes based upon solvent-accessibility and flexibility.

[Methods for modeling and docking of antibody and protein 3D structures](#)

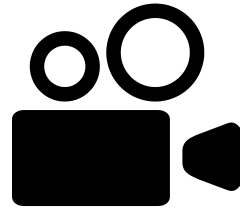
This page provides information on available methods for modeling and docking



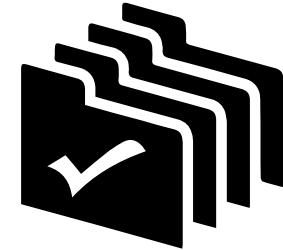
Post-Event Details



You will receive a post-event email next week



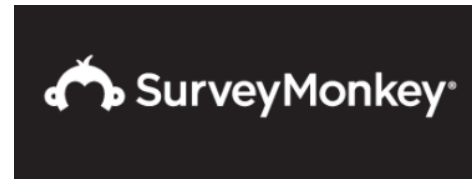
Workshop recording will be shared with you



All presentations will be shared with you



Participation certificates will be provided



Post-event feedback survey

User Workshop Structure

Day 1

START YOUR SEARCH HERE ?

Epitope ?

- Any Epitopes
- Linear Epitope

Exact Iv Ex: SIINFEKL

- Discontinuous Epitopes
- Non-peptidic Epitopes



Assay ?

- Positive Assays Only
- T Cell Assays
- B Cell Assays
- MHC Ligand Assays

Ex: neutralization



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



Host ?

- Any Host
- Humans
- Mice
- Non-human Primates
- Ex: dog, camel



Disease ?

- Any Disease
- Infectious Disease
- Allergic Disease
- Autoimmune Disease
- Ex: asthma, diabet



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