



Analysis Resource Overview

tools.iedb.org
nextgen-tools.iedb.org

Presented by: Dr. Bjoern Peters, Professor

IEDB Tools

Analysis Resource & Next-Generation Tools

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:

- T cell epitope prediction
- B cell epitope prediction
- Analysis tools

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Welcome to the Next-Generation IEDB Tools site!

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New User? Learn to use the website here!

T Cell Prediction - Class I

MHC class I binding affinity, TAP processing, and Immunogenicity predictions

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HAIHVSNGTNGTKRFDNPNVLPFNDGVYFASTEKSNIIIRGWIFGTTLDSKTQSLIVNINATNVVIVK
CEFQFCNDPFLGVVYHKNKSWMESEFRVYSSANNCTFEYVVSQPLMDLEGKQGNFKNLREF

MHC
Allele(s)

Ex: HLA-A*02:01

0



Next-Generation Tools:

- Re-implementing existing tools with a focus on improving usability and function
- Launched in 2023
- More tools to be added

nextgen-tools.iedb.org

IEDB Tools

Analysis Resource & Next-Generation Tools

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Next-Generation Tools

<https://nextgen-tools.iedb.org/>

- Launched in 2023
- Multi-year and multi-release project
- The main goals of the redesign are to:
 - simplify the user experience
 - enhance existing functionality
 - add new functionality
 - ensure consistency among the tools
 - improve the layout and aesthetics
- First release focused on:
 - T cell epitope prediction class I
 - Cluster analysis
 - PEPMatch

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The screenshot shows the 'T Cell Prediction - Class I' tool interface. At the top, a green banner reads 'New User? Learn to use the website here!'. Below this, the tool title 'T Cell Prediction - Class I' is displayed in blue, followed by a subtitle 'MHC class I binding affinity, TAP processing, and Immunogenicity predictions'. A text input area contains the instruction 'Type/paste/drag a sequence into this box or click 'Run' to use the example sequence:' and an example sequence: '> SARS2 spike glycoprotein' followed by the amino acid sequence 'MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVVYYPDKVFRSSVLHSTQDLFLPFFSNVTWFHAIHVSGTNGTKRFD NPVLPFNDGVYFASTEKSNIIIRGWIFGTTLDSTQSLIVNATNVVIKVCFCNDPFLGVVYHKNNKSWMESEFRV YSSANNCTFEYVSQPFLMDLEGKQGNFKNLREFVFKNIDGYFKIYKHTPINLVRDLPGQFSALEPLVDLPIGINITRFQT'. Below the input area, there is a field for 'MHC Allele(s)' with the example 'HLA-A*02:01' and a '0' in a black box. A blue play button is on the right. At the bottom, a yellow banner says 'More tools coming soon.'

Learn more on Day 2!

Next-Generation Tools

<https://nextgen-tools.iedb.org/>



Tools ▾ Help & Info ▾

Announcements

Next-Generation IEDB Tools
site released to public

Appearances & Events

[Virtual User Workshop](#) Nov 1-3, 2023

* Register [Here](#)

AACR 2024 Apr 5-10, 2024

Festival of Biologics Apr 15-17, 2024

AAI 2024 May 3-7, 2024

Additional Resources

API

Downloads

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```
MFVFLVLLPLVSSQCVNLTRTQLPPAYTNSFTRGVVYPDKVFRSSVLHSTQDLFLPFFSNVTWFHAIHVSGTNGTKRFDNPVLPFNDGVYFAST  
EKSNIIRGWIFGTTLDSTKQSLIVNNAATNVVIKVFCEFCNDPFLGVVYHKNNKSWMESEFRVYSSANNCTFEYVVSQPFLMDLEGKQGNFKN  
LREFVFKNIDGYFKIYSKHTPINLVRDLPQGFSALEPLVDLPIGINITRFQTLALHRSYLTGDSGSSGWTAGAAAYVGYLQPRTFLLKYNENGTIT
```

MHC Allele(s)

Ex: HLA-A*02:01

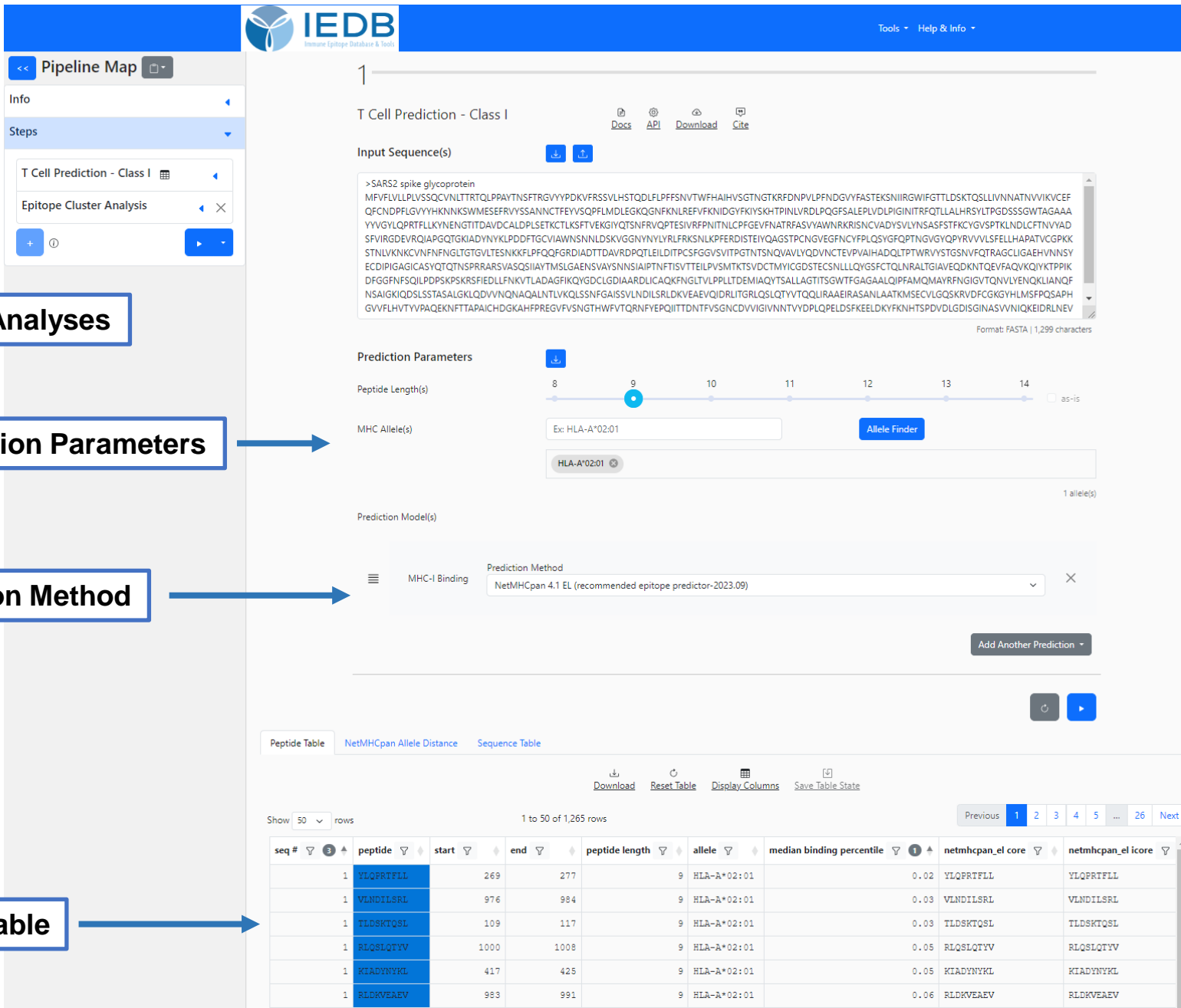
0



More tools coming soon.

Run example query from home page

Results



Build Pipeline Analyses

Change Prediction Parameters

Select Prediction Method

Results Table

T Cell Prediction - Class I

Input Sequence(s): > SARS2 spike glycoprotein
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVVYDPKVFSSVLHSTQDLFLPFSNVTFWFAIHVSGTNGTKRFDNPLPFDNGVYFASTEKSNIIIRGWIFGTLDLSDKQSLVNNATNVVVKVCFE
QFCNDPFLGVYYHKNNKSWMESEFRVYSSANNCTFEVYSQPLMDLEGKQGNFKNLREFVFNIDGVFKIVSKHTPINLVRDLPGGSALEPLVDLPIGINITRFQTLALHRSYLTGDSSSGWTAGAAA
YYVGYLQPRTFLLKYNNENGTITDAVDCALDPLSETKTLKSTVEKGIYQTSNFRVQPTESIVRFPNITNLCPFGVEVFNATRFASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPFKLNDLCFTNVYAD
SFVIRGDEVQRQIAPGQTGIADYNYKLPDDFTGCVIAWNSNLDKVGGNVNYLYRFRKSNLKPFRDSTIEIVYAGQSTPCNGVEGFNCYFPLQSYGFQPTNGVGYQPYRVVLSFELLHAPATVCGPKK
STNLVKNKCVNFNFNGLTGTGLVLTESNKKFLPFQQRDIADTTDAVRDPQTLLEILDITPCSCFGVSVITPGTNTSNQVAVLYQDVNCTEVPVAIHADQLTPWRVYVSTGSNVFQTRAGCLLGAHEVNNNSY
ECDPIGAGICASYQTQTSNRRARSVASQSIAYTMSLGAENSVAYSNNSIAIPTNFVTSVTEILPVSMTKTSVDCTMVICGDSTECNLLQLGYSFCTQLNRALTGIAVEQDKNTQVEVFAKQVKTPIIK
DFGGFNFSQLPDPSPKSRSFIEDLLFNKVTADAGFIKQYGDCLGDAARDLCAQKFNGLTVPPLITDEMIAQYTSALLAGTITSQWTFGAGAAIQPFAMQMAVRFNIGVYQNVLYENKQLIANQF
NSAIGKIQDLSSTASALGKLDVNVNQNAQALNTLVKQLSSNFGAIVSVLNDILSRLDKVEAEVQIDRLITGRQLSQTYYVTQQLIRAAEIRASANLAATKMSVCELVGQSKRVDFCGKGYHLMSPFPQSAHP
GVVFLHVTYVPAQGNFTTAPAICHGDGKAHFPREGVFNNGTHWFVTQRNFYEQIITTDNTFVSGNCDVVGIVNNTVYDPLQPELDSFKEELDKYFKNHTSPDVLGDISGINASVNIQKEIDRLNEV

Prediction Parameters

Peptide Length(s): 8 9 10 11 12 13 14

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

Prediction Model(s): MHC-I Binding

Prediction Method: NetMHCpan 4.1 EL (recommended epitope predictor-2023.09)

seq #	peptide	start	end	peptide length	allele	median binding percentile	netmhcpan_el core	netmhcpan_el icore
1	YLQPRTFLL	269	277	9	HLA-A*02:01	0.02	YLQPRTFLL	YLQPRTFLL
1	VLNDILSRLL	976	984	9	HLA-A*02:01	0.03	VLNDILSRLL	VLNDILSRLL
1	TLDSKTQSL	109	117	9	HLA-A*02:01	0.03	TLDSKTQSL	TLDSKTQSL
1	RLQSLQTYV	1000	1008	9	HLA-A*02:01	0.05	RLQSLQTYV	RLQSLQTYV
1	KIADYNYKL	417	425	9	HLA-A*02:01	0.05	KIADYNYKL	KIADYNYKL
1	RLDKVEAEV	983	991	9	HLA-A*02:01	0.06	RLDKVEAEV	RLDKVEAEV



Search docs

Overview

Available Tools

Pipelines

API usage

Troubleshooting

Help Documentation

Next-Generation (NXG) IEDB Tools Documentation

- Overview
 - Background & design philosophy
 - Inputs, outputs, and controls
- Available Tools
 - T cell class I
 - Cluster
 - Pepmatch
- Pipelines
 - Building a Pipeline
 - Pipeline Map
 - Saving/Sharing Pipelines
 - Notes on the Pipeline Lifecycle
 - Example pipelines
- API usage
 - Typical workflow
 - Core endpoints
 - Swagger Documentation
- Troubleshooting
 - What are the input size limits?
 - Why does PepMatch not seem to complete?
 - How do I get more personalized support?

Next ↗

IEDB Tools

Analysis Resource & Next-Generation Tools

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CEFAQCNDPFLGVVYHKNKNSWMESEFRVYSSANNCTFEYVSQPFLMDLEGKQGNFKNLREF

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IEDB Analysis Resource

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Day 2 will go into much more detail!

T Cell Tools

MHC binding prediction

- MHC I binding prediction
- MHC II binding prediction
- TepiTool

MHC ligand prediction

- NetChop/NetCTL/NetCTLpan
- MHC-NP, MHCII-NP
- AXEL-F

Immunogenicity prediction

- CD4 & CD8 T cell immunogenicity prediction tools

Other

- Deimmunization tool
- TCRMatch
- Docktope

B Cell Tools

Linear epitope prediction

- BepiPred
- Other methods

Discontinuous epitope prediction

- DiscoTope
- ElliPro

Antibody and TCR structure prediction

- LYRA
- SCEptRe

Analysis Tools

Population coverage of epitope set

- Population coverage tool

Degree of conservation

- Conservancy analysis tool

Group peptides based on sequence identity

- Epitope cluster analysis

Infer restriction in HLA typed subjects

- RATE

Aggregate heterogeneous immune response

- ImmunomeBrowser

Other

- PepSySco
- PepX

Development of Prediction Tools

- Based on machine learning techniques
 - Experimentally derived data as training input (E.g. MHC binding data, 3D crystal structures, T cell assay data) → collected in the IEDB
 - Various prediction models (e.g. Neural Networks, linear weighted models, etc.)
 - Extrapolate identified patterns to new examples

Training data

species	mhc	peptide_length	sequence	inequality	meas
human	HLA-A*01:01	8	ASFCGSPY	=	51.4
human	HLA-A*01:01	8	LTDFGLSK	=	739.385479
human	HLA-A*01:01	8	FTSFFVRY	=	1285
human	HLA-A*01:01	8	KSVFNLSY	=	1466
human	HLA-A*01:01	8	RDWAHNSL	=	1804.675523
human	HLA-A*01:01	8	FSSCPVAY	=	1939.46663
human	HLA-A*01:01	8	RNWAHSSL	=	2201.794454
human	HLA-A*01:01	8	LSCAASGF	=	2830.055894
human	HLA-A*01:01	8	LASIDLKY	=	3464
human	HLA-A*01:01	8	RAFKQLL	>	5000
human	HLA-A*01:01	8	LVESGGGL	=	5886.338262
human	HLA-A*01:01	8	NIILKANF	=	8920.343726
human	HLA-A*01:01	8	RGVVFQGL	=	15645.52954
human	HLA-A*01:01	8	HHIQNLL	=	18923.65903
human	HLA-A*01:01	8	FVNRPLV	>	20000
human	HLA-A*01:01	8	RYSHWTKL	>	20000
human	HLA-A*01:01	8	STASSNSY	>	20000
human	HLA-A*01:01	8	YDPVIVK	>	20000

Input data for prediction

peptide	allele
ALPHIIDE	HLA-A*01:01
TGIKAVYN	HLA-A*01:01
VLIVITGI	HLA-A*01:01
EVINIVII	HLA-A*01:01
IVTMFEAL	HLA-A*01:01
HIIDEVIN	HLA-A*01:01
TCGIFALI	HLA-A*01:01
KAVYNFAT	HLA-A*01:01
NIVIIVLI	HLA-A*01:01
YNFATCGI	HLA-A*01:01
MGQIVTMF	HLA-A*01:01
IFALISFL	HLA-A*01:01
LLLAGRSC	HLA-A*01:01
SFLLLAGR	HLA-A*01:01



Prediction method/model

Prediction results

peptide	allele	predicted score
ALPHIIDE	HLA-A*01:01	80
TGIKAVYN	HLA-A*01:01	87
VLIVITGI	HLA-A*01:01	64
EVINIVII	HLA-A*01:01	68
IVTMFEAL	HLA-A*01:01	33
HIIDEVIN	HLA-A*01:01	85
TCGIFALI	HLA-A*01:01	32
KAVYNFAT	HLA-A*01:01	78
NIVIIVLI	HLA-A*01:01	71
YNFATCGI	HLA-A*01:01	23
MGQIVTMF	HLA-A*01:01	27
IFALISFL	HLA-A*01:01	34
LLLAGRSC	HLA-A*01:01	81
SFLLLAGR	HLA-A*01:01	70

Accessing the Analysis Resource



Check out our new IEDB updates! (1) Learn how to [customize your database exports](#) and (2) test out the new [Next-generation Tools site](#) for all your analysis and prediction needs.

Welcome

The Immune Epitope Database (IEDB) is a freely available resource funded by NIAID. It catalogs experimental data on antibody and T cell epitopes studied in humans and other animal species in the context of infectious disease, allergy, autoimmunity and transplantation. The IEDB also hosts epitope prediction and analysis tools, and has a companion site, [CEDAR](#) (funded by NCI), which houses cancer epitopes. [Learn More](#)

Upcoming Events & News

Virtual User Workshop	Nov 1-3, 2023
* register here	
AACR 2024	Apr 5-10, 2024
Festival of Biologics	Apr 15-17, 2024
AAI 2024	May 3-7, 2024

Summary Metrics

Peptidic Epitopes	1,598,102
Non-Peptidic Epitopes	3,188
T Cell Assays	508,903
B Cell Assays	1,392,337
MHC Ligand Assays	4,778,051
Epitope Source Organisms	4,403
Restricting MHC Alleles	994
References	24,243

START YOUR SEARCH HERE

Epitope

Any
 Linear peptide
Exact **N** | Ex: SIINFEKL
 Discontinuous
 Non-peptidic

Assay

T Cell
 B Cell
 MHC Ligand
Ex: neutralization | **Find**
Outcome: Positive Negative

Epitope Source

Organism
Ex: influenza, peanut | **Find**
Antigen
Ex: core, capsid, myosin | **Find**

MHC Restriction

Any
 Class I
 Class II
 Non-classical
Ex: HLA-A*02:01 | **Find**

Host

Any
 Human
 Mouse
 Non-human primate
Ex: dog, camel | **Find**

Disease

Any
 Infectious
 Allergic
 Autoimmune
Ex: asthma | **Find**

Reset **Search**

Epitope Analysis Resource

T Cell Epitope Prediction

Scan an antigen sequence for amino acid patterns indicative of:

- MHC I Binding
- MHC II Binding
- MHC I Processing (Proteasome, TAP)
- MHC I Immunogenicity

B Cell Epitope Prediction

Predict linear B cell epitopes using:

- Antigen Sequence Properties

Predict discontinuous B cell epitopes using antigen structure via:

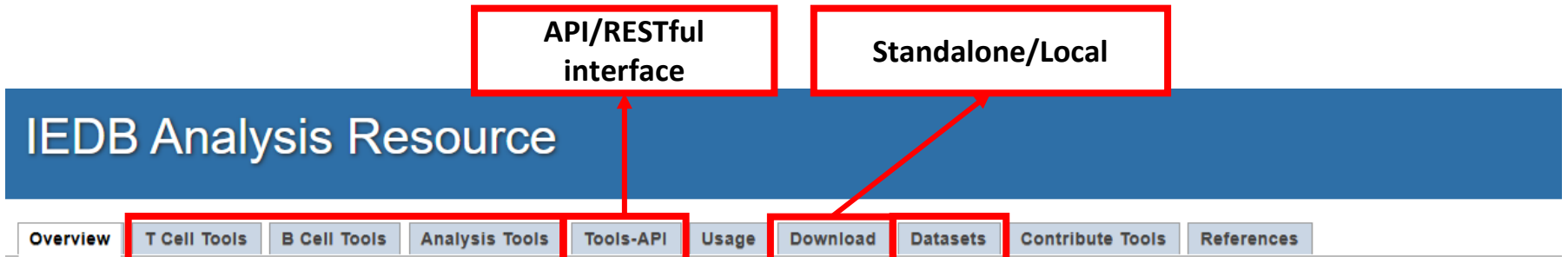
- Discotope
- ElliPro

Epitope Analysis Tools

Analyze epitope sets of:

- Population Coverage
- Conservation Across Antigens
- Clusters with Similar Sequences

Available Resources



Epitope Prediction and Analysis Tools

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IEDB-AR News

• We're Hiring

[Bioinformatician for the Immune Epitope Analysis Resource](#)

• Python 3 availability

As of 2 July 2020, all code has been ported to Python 3, including the standalone tools. Thanks for your patience and be sure to [inform us](#) of any issues that arise.

IEDB-AR Release Notes

[IEDB Analysis Resource v2.24 release notes \(1 Oct 2020\)](#)

2020-1

NEW: I

web, A

BA)...

[IEDB Analysis Resource v2.23 release notes](#)

[IEDB Analysis Resource v2.22 release notes](#)

**Solutions Center:
Tutorials, Q&A**

help@iedb.org

IEDB [Help](#) [Contact](#)

This site is best viewed with current versions of [Mozilla Firefox](#) or [Google Chrome](#).

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Supported by a contract from the [National Institute of Allergy and Infectious Diseases](#), a component of the National Institutes of Health in the Department of Health and Human Services.

IEDB Analysis Resource

Overview T Cell Tools B Cell Tools Analysis Tools Tools-API Usage Download Datasets Contribute Tools References

T Cell Epitope Prediction Tools

T Cell Epitopes - MHC Binding Prediction

These tools predict IC50 values for peptides binding to specific MHC molecules. Note that binding to MHC is necessary but not sufficient for recognition by T cells.

Peptide binding to MHC class I molecules

This tool will take in an amino acid sequence, or set of sequences and determine each subsequence's ability to bind to a specific MHC class I molecule.

Peptide binding to MHC class II molecules

This tool employs different methods to predict MHC Class II epitopes, including a consensus approach which combines NN-align, SMM-align and Combinatorial library methods.

TepiTool:

The Tepitool provides prediction of peptides binding to MHC class I and class II molecules. Tool is designed as a wizard with 6 steps as described below. Each field (except sequences and alleles) is filled with default recommended settings for prediction and selection of optimum peptides. The input parameters can be adjusted as per your specific needs. You can go back to previous steps to change your selection before submission of the job. Once you submit the job (at the end of step-6), you will not be able to make any more changes and will have to start the prediction all over again with updated input parameters.

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.

T Cell Epitopes - Immunogenicity Prediction

This tool predicts the relative ability of a peptide/MHC complex to elicit an immune response.

T cell class I pMHC immunogenicity predictor

This tool uses amino acid properties as well as their position within the peptide to predict the immunogenicity of a class I peptide MHC (pMHC) complex.

Deimmunization:

The deimmunization tool is attempt to identify immunodominant regions in a given therapeutically important protein, and suggest amino-acid substitutions that create non-immunogenic versions of the proteins. So we have opted a two steps process; 1) In the first step, the deimmunization tool will list all the immunogenic regions or peptides based on selected threshold. These peptides will be generated from the protein with 15mer window size and 10mer overlap. 2) In the second step, the user can select one or more



MHC I Binding Prediction

Home Help Example Reference Download Contact

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.

```
>LCMV Armstrong, Protein GP
MGQIVTMFEALPHIIDVINIVIVLIVITGKAVYNFATCGIFALISFLLLAGRSCGM
YGLKGPDIYKGVYQFKSVEFDMSHLNLTMPNACSAANSHHYISMGTSGLELFTNDSII
SHNFCNLTSAFNKKTFDHTLMSIVSSLHLSIRGNSNYKAVSCDFNNGITIQYNLTFSDA
QSAQSQCRTRFRGRVLDMFRTAFGGKYMRSWGWTGSDGKTTWCSTSYQYLIQNRRTWE
NHCTYAGPFGMSRILLSQEKTKFFTRRLAGFTWTLSDSSGVENPGGYCLTKWMIAAE
LKCFNGTAVAKCNVNHDAEFCDMLRLIDYNKAALSKFKEDVESALHLFKTTVNSLISDQ
LLMRNHLRDLMGVPYCNYSKFWYLEHAKTGETSVPKCWLVTNGSYLNETHFSDQIEQEA
DNMITEMLRKDYIKRQGSTPLALMDLLMFSTAYSIVLSIFLHLVKIPTRHIKGGSCP KP
HRLTNKGICSCGAFKVPGVKTVWKRR
```

Or select file containing sequence(s) No file chosen

Choose a Prediction Method

Prediction Method [Help on prediction method selections](#)

Show all the method versions:

MHC source species

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

Select MHC allele(s)

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

Sort peptides by

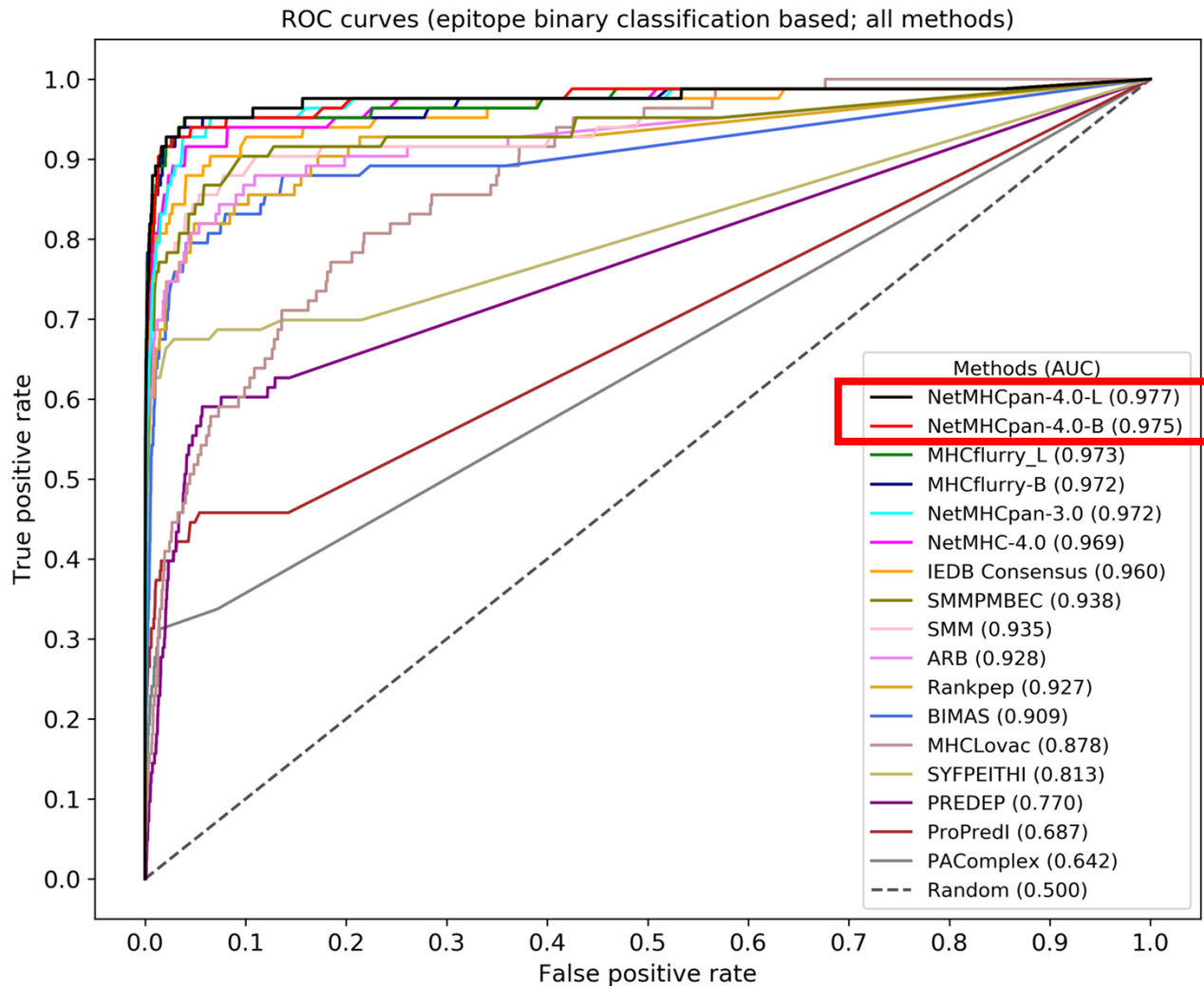
Output format

Email address (optional)

Sequence

Prediction method

MHC I Binding Prediction Methods - Benchmarking



- Comprehensive evaluation of different MHC binding prediction methods to identify T cell epitopes

MHC I Binding Prediction Methods - Benchmarking

- Automated evaluation of MHC binding predictions on newly released datasets in the IEDB
- http://tools.iedb.org/auto_bench/mhci/weekly/
- Prediction of absolute and ranked binding affinities
- Consistent scoring of the NetMHCPan 4.0+ BA methods being on top for binding predictions

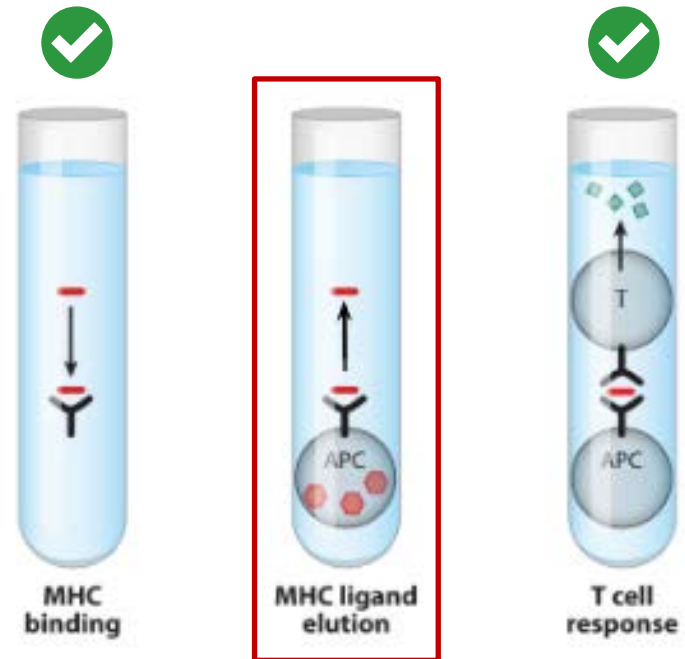
Server	2023-10-19	2023-08-10	2023-08-03	2023-06-15	2023-05-11	2023-04-20	2022-11-24	2022-10-28	2022-10-06	2022-07-22	2022-05-20	2022-04-29	2021-12-24	2021-12-10	2021-11-05	2021-10-08	2021-10-01	2021-09-03	2021-08-20	2021-08-06
NetMHCPan 4.1 BA	73	74	74	65	66	67	66	72	83	76	80	75	72	64	64	63	63	70	71	76
NetMHCons	69	70	65	64	60	57	60	56	49	61	60	69	68	57	56	49	50	52	61	71
NetMHCPan 4.0 BA	68	66	61	48	60	60	60	68	76	76	80	80	80	71	70	62	61	66	58	69
NetMHCPan 3.0	65	65	64	58	68	65	70	73	72	74	74	73	72	68	64	58	57	56	49	64
ANN 3.4	64	66	62	73	64	63	61	50	44	48	45	47	45	46	50	53	53	51	63	69
mhcfurry 1.2.0	63	56	51	56	58	61	56	59	42	33	49	54	60	61	59	68	70	74	72	50
NetMHCPan 2.6	60	65	59	41	60	57	63	69	46	54	48	65	65	63	60	48	49	50	51	64
ANN 4.0	56	55	60	53	64	65	67	73	76	64	57	56	51	54	52	50	53	46	54	67
SMPMBEC	50	56	73	75	57	60	61	61	73	62	50	43	46	53	53	64	61	67	67	54
IEDB Consensus	48	52	58	65	71	72	69	71	69	58	60	52	54	58	57	62	59	60	63	62
SMM	46	51	54	55	56	57	56	61	58	52	54	39	43	50	49	63	62	65	68	60
NetMHCPan 4.0 EL	45	42	37	51	46	43	46	37	25	36	34	44	42	50	47	42	44	28	40	60
NetMHCPan 4.1 EL	34	32	32	56	51	48	42	36	25	26	39	50	49	57	52	44	46	39	26	38
PickPocket	34	40	46	54	57	57	68	68	55	41	40	34	38	52	54	56	55	59	49	60
ARB	31	34	48	52	48	49	53	41	37	42	34	27	24	26	27	34	37	44	28	29

Trolle et al, *Bioinformatics*, 2015

Trevizani et al, *Briefings in Bioinformatics*, 2022

New Tools Benchmarks *with Ligand Elution Data*

- MHC ligand experiments generate massive amounts of data
- MHC ligands incorporate features of T cell epitopes beyond MHC binding
- Generation of negative datasets is not trivial
- Best results so far using peptides from UniProt (significantly differs from random)



MHC I Binding Prediction

Home Help Example Reference Download Contact

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.

```
>LCMV Armstrong, Protein GP
MGQIVTMFEALPHIIDVINIIVLIVITGIKAVYNFATCGIFALISFLLLAGRSCGM
YGLKGPDIYKGVYQFKSVEFDMSHLNLTPNACSAANSHHYISMGTSGLELFTNDSII
SHNFCNLTSAFNKKTFDHTLMSIVSSLHLSIRGNSNYKAVSCDFNNGITIQYNLTFSDA
QSAQSQCRTRFRGRVLDMPRTAFGGKYMRSQGWGTGSDGKTTWCSTSYQYLIQNRWTE
NHCTYAGPFGMSRILLSQEKTKFFTRRLAGFTTWLSDSSGVENPGGYCLTKWMILAAE
LKCFGNTAVAKCNVNHDAEFCDMLRLIDYNKAALSFKFEDVESALHLFKTTVNSLISDQ
LLMRNHLRDLMGVPCNYKFWYLEHAKTGETSVPKCWLVTNGSYLNETHFSDQIEQEA
DNMITEMLRKDYIKRQGSTPLALMDLLMFSTAYLVSIFLHLVKIPTRHRIKGGSCPKP
HRLTNKGICSCGAFKVPGVKTVWKR
```

Or select file containing sequence(s) No file chosen

Choose a Prediction Method

Prediction Method [?] Show all the method versions: **NetMHCpan 4.1 EL (recommended epitope predictor-2023.09)** [Help on prediction method selections](#)

Specify what to make binding predictions for

MHC source species: **human**

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

Allele	Length
<input type="text"/>	<input type="text"/>

[Upload allele file](#) [?]

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

Specify Output

Sort peptides by: **Predicted Score (descend)**

Output format: **XHTML table**

Email address (optional): [?]

Prediction method

Allele & length

Email ID

MHC I Binding Prediction - Result

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[Download](#)
[Contact](#)

tools.iedb.org/mhci/

MHC-I Binding Prediction Results

Input Sequences

#	Name	Sequence
1	LCMV Armstrong Protein GP	MGQIVTMFEALPHIIDEVINIVIIVLIVITGIKAVYNFATCGIFALISFLLLAGRSCGMVGLKGPDIYKG VYQFKSVEFDMSHLNLTMPNACSAANNSHHYISMGTSGLELFTTNDISIHNFCNLTSAFNKKTF DHTLMSIVSSLHLSIRGNSNYKAVSCDFNNGITIQYNLTFSDAQSAQSQCRTRFRGRVDMFRFA FGGKYMRSGWGWGTGSDGKTTWCSQTSYQYLIQNRWENHCTYAGPFGMSRILLSQEKTKF FTRRLAGTFTWTLSDSSGVENPGGYCLTKWMILAAELKCFGNTAVAKCNVNHDAEFCMDMLRLI DYNKAAALSFKEDVESALHLFKTTVNSLISDQLLMRNHLRDLMGVPCNYSKFWYLEHAKTGE TSVPKCWLVTNGSYLNETHFSDQIEQEADNMITEMLRKDYIKRQGSTPLALMDLLMFSTSAYLV SIFLHLVKIPTHRIKGGSCPKPHRLTNKGICSCGAFKVPGVKTVWVRR

NetMHCpan allele distance [?](#)

Input Allele	Closest Allele	Distance
HLA-A*02:01	HLA-A*02:01	0.000

Prediction method: NetMHCpan EL 4.1 **High Score = good binder**

* The 'IEDB recommended' method was updated in September 2020 to NetMHCpan EL 4.1 More information is available on the [help](#) page.

[Download result](#)

Citations

Allele	#	Start	End	Length	Peptide	Core	Icore	Score	Percentile Rank
HLA-A*02:01	1	6	14	9	TMFEALPHI	TMFEALPHI	TMFEALPHI	0.942547	0.03
HLA-A*02:01	1	10	18	9	ALPHIIDEV	ALPHIIDEV	ALPHIIDEV	0.920331	0.03
HLA-A*02:01	1	137	145	9	TLMSIVSSL	TLMSIVSSL	TLMSIVSSL	0.882391	0.04
HLA-A*02:01	1	447	455	9	YLVSIPLHL	YLVSIPLHL	YLVSIPLHL	0.855633	0.06
HLA-A*02:01	1	14	22	9	IIDEVINIV	IIDEVINIV	IIDEVINIV	0.807736	0.08
HLA-A*02:01	1	13	21	9	HIIDEVINI	HIIDEVINI	HIIDEVINI	0.779939	0.09
HLA-A*02:01	1	339	347	9	ALHLFKTTV	ALHLFKTTV	ALHLFKTTV	0.565798	0.22
HLA-A*02:01	1	450	458	9	SIFLHLVKI	SIFLHLVKI	SIFLHLVKI	0.530163	0.24
HLA-A*02:01	1	45	53	9	ALISFLLLA	ALISFLLLA	ALISFLLLA	0.525738	0.25
HLA-A*02:01	1	349	357	9	SLISDQLLM	SLISDQLLM	SLISDQLLM	0.510305	0.26
HLA-A*02:01	1	440	448	9	LMFSTSAYL	LMFSTSAYL	LMFSTSAYL	0.483579	0.27
HLA-A*02:01	1	320	328	9	RLIDYNKAA	RLIDYNKAA	RLIDYNKAA	0.438929	0.32
HLA-A*02:01	1	435	443	9	ALMDLLMFS	ALMDLLMFS	ALMDLLMFS	0.386032	0.39
HLA-A*02:01	1	27	35	9	IVITGIKAV	IVITGIKAV	IVITGIKAV	0.36266	0.42
HLA-A*02:01	1	42	50	9	GIFALISFL	GIFALISFL	GIFALISFL	0.285315	0.57

MHC II Binding Prediction

tools.iedb.org/mhcii/

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MHC-II Binding Predictions

Specify Sequence(s)

Enter protein sequence(s) in FASTA format

```
>West Nile virus envelope glycoprotein
FNCLGMSNRDFLEGVSGATWVDLVLEGDSVCVTIMSKDKPTIDVKMMNMEANLAEVRSYCYLATVSDLT
KAACPTMGEAHNDKRAPFVCRQGVVDRGWGNGCGLFGKGSIDTCAKFACTKAIGRTILKENIKYEVA
IFVHGPTTVESHGNYSTQVGATQAGRFSITPAAPSYTLKLGVEYGEVTVDCPRSGIDTNAYYVMTVGTKT
FLVHREWFMDLNLPPWSSAGSTVWRNRETLMEFEEPHATKQSVIALGSQEGALHQAALAGAIPEFSSNTVK
LTSGLHKCRVKMEKQLQKGTTYGVCSKAFKFLGTPADTGHGTVVLELQYTGTDGPKVPISSVASLNDLT
PVGRILVTNPFVSVATANAKVLIELEPPFGDSYIVVGRGEQQINHHWHKSGSIGKAFTTLKGAQLAA
LGDTAWDFGVSQVFTSVGKAVHQVFGGAFRSLFGGMSWITQGLLALLWGINARDRSIALTFLAVGG
VLLFLSVNVHA
```

Or select file containing sequence(s) No file chosen

Choose a Prediction Method

Prediction Method [?] Show all the method versions: NetMHCIIpan 4.1 EL (recommended epitope predictor-2023.09) [Help on prediction method selections](#)

Specify what to make binding predictions for

Select species/locus: Human, HLA-DR

Select MHC allele(s)
Select α & β chains separately if applicable: [?] Allele
[Select full HLA reference set:](#) [?] [Upload allele file:](#) [?]

Select 7-allele HLA reference set: [?]

Select length(s) [?]

<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Specify Output

Sort peptides by: Percentile Rank

Output format: XHTML table

Email address (optional): [?]

MHC II Binding Prediction Methods - Benchmarking

http://tools.iedb.org/auto_bench/mhcii/weekly/

MHC II Automated Server Benchmarks

This is a [live](#) ranking of MHC II servers based on performance, which continues to be reevaluated over time. The weekly IEDB releases are automatically checked for datasets large enough to add to the benchmarks. The benchmark metrics in the table below will only be updated on releases where such new data is becoming available.

Accumulated overall ranking scores

[Ranking scores](#) based on data sets submitted to the IEDB for the last at least 5 references.

Server	2023-09-01	2023-07-28	2023-04-21	2023-03-03	2023-01-27	2022-10-28	2022-09-16	2022-09-02	2022-06-17	2022-06-10	2022-04-08	2022-04-01	2021-12-10	2021-11-05	2021-10-29	2021-07-23	2021-04-23	2021-04-16	2021-02-19	2021-01-22	2020-12-18	2020-10-30	2020-10-23	2020-08-07	2020-06-26	2020-05-01	2020-03-27	2020-03-16	2020-01-03	2019-07-02	2019-05-24	2019-03-22	2018-11-23	
NetMHCIIpan-4.1 BA	85	82	70	71	70	70	76	65	65	65	65	65	67	66	65	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NetMHCIIpan-4.0 BA	76	78	68	70	68	68	70	65	66	66	63	63	63	62	61	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NetMHCIIpan-3.2	67	67	64	65	64	63	52	51	51	50	61	63	69	70	77	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NN-align 2.3	56	59	51	49	49	48	45	63	64	67	67	67	65	67	67	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NetMHCIIpan-3.1	53	54	66	56	54	55	41	47	47	41	46	46	48	50	54	58	57	58	55	58	46	49	60	61	60	64	55	64	65	65	71	84	79	
Consensus IEDB method	50	58	58	59	59	61	57	66	66	68	65	66	63	62	63	66	66	71	73	69	73	76	62	60	60	58	58	61	64	66	64	64	64	64
NetMHCIIpan-4.1 EL	45	39	51	54	57	57	54	32	32	33	36	36	38	36	38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
SMM-align	43	42	50	50	47	48	42	55	56	52	50	47	50	51	53	49	51	43	43	43	57	61	57	57	54	56	38	41	43	39	43	49	35	
NN-align	38	42	44	43	43	42	43	58	58	57	57	59	55	56	57	68	64	73	73	75	59	60	73	74	78	79	88	75	71	71	66	54	63	
NetMHCIIpan-4.0 EL	27	24	47	47	50	51	48	31	31	29	34	33	37	34	38	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Tepitope (Sturmli)	26	30	39	39	41	41	37	31	27	41	36	37	41	39	29	21	24	17	18	14	21	29	27	25	27	26	33	28	26	26	29	21	47	
Comlib matrices	20	14	7	4	4	4	13	17	17	15	18	16	16	16	17	10	11	8	8	7	30	38	25	25	21	10	0	0	5	5	5	10	4	

- Similar to the MHC Class I benchmark set-up

Andreatta et al, Bioinformatics, 2017

TepiTool – MHC I and II Binding Prediction

tools.iedb.org/tepitool/

Home	Help	Reference	Download	Contact
----------------------	----------------------	---------------------------	--------------------------	-------------------------

TepiTool

Steps **1** 2 3 4 5 6

SEQUENCE - Provide sequence data:

Enter sequence(s) in FASTA or PLAIN format.

```
>LCMV Armstrong, Protein GP
MGQIVTMFEALPHIIDVINIVIVLIVITGIKAVYNFATCGIFALISF
```

FASTA format detected.

Or upload file containing sequence(s) No file chosen

TepiTool – MHC I and II Binding Prediction

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TepiTool

[Steps](#)[1](#)[2](#)[3](#)[4](#)[5](#)[6](#)

REVIEW: Review selections, enter job details & submit data:

Summary:

No. of sequences	1
Host species	Human
Allele class	Class II
Alleles	1.DRB1*01:01
Duplicate peptides	Removed
Peptide lengths selected	15mers (Only one length for class II)
Approx no. of peptides included	8
Peptide overlap	10 AA residues
Conservancy analysis	Peptides conserved in at least % sequences
Prediction method	IEDB recommended
Peptide selection criterion	Based on predicted consensus percentile rank (Cutoff selected = 10)

Job details:

Job name (optional)	<input type="text" value="Job 1"/>
Email (optional - will notify when job is finished)	<input type="text" value="bpeters@lji.org"/>

[Start Over](#)[Back](#)[Submit](#)

(Please note that you will not be able to make any more changes once submitted. You will have to start again if you want to do so.)

tools.iedb.org/tepitool/



TepiTool – MHC I and II Binding Prediction

TepiTool

Prediction results - concise ([Download table](#) )

Seq #	Peptide start	Peptide end	Peptide sequence	Consensus percentile rank	Allele
1	23	37	IIVLIVITGIKAVYN	0.2644	HLA-DRB1*01:01
1	4	18	IVTMFEALPHIIDEV	0.1227	HLA-DRB1*01:01
1	28	42	VITGIKAVYNFATCG	0.0354	HLA-DRB1*01:01
1	11	25	LPHIIDEVINIVIV	0.0053	HLA-DRB1*01:01
1	33	47	KAVYNFATCGIFALI	0.0024	HLA-DRB1*01:01
1	16	30	DEVINIVIVLIVIT	0.0016	HLA-DRB1*01:01

Download results details:

Non-redundant results 	Prediction results with redundant peptides within each sequence removed - Includes positives and negatives
Complete results 	Prediction results of all peptides

Citation information:

If you use these predictions in a manuscript, please include the following in the method section:

For complete list of references please click here: [References](#)

Input sequences:

Seq #	Seq title	Sequence
1	LCMV Armstrong, Protein GP	MGQIVTMFEALPHIIDEVINIVIVLIVITGIKAVYNFATCGIFALISF

Other input parameters:

Input summary:	
No. of sequences	1
Host species	Human
Allele class	Class II
Alleles	DRB1*01:01
Duplicate peptides	Removed
Peptide lengths selected	15mers (Only one length for class II)
Peptide overlap	10 AA residues
Conservancy analysis	No
Prediction method	IEDB recommended
Peptide selection criterion	Predicted percentile rank
Cutoff for peptide selection criterion	10
Job name	Job 1
Email	nblazeska@lji.org

tools.iedb.org/tepitool/

B Cell Tools

IEDB Analysis Resource

[Overview](#) [T Cell Tools](#) **[B Cell Tools](#)** [Analysis Tools](#) [Tools-API](#) [Usage](#) [Download](#) [Datasets](#) [Contribute Tools](#) [References](#)

B Cell Epitope Prediction Tools

B Cell Epitope Prediction

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

A collection of methods to predict linear B cell epitopes based on sequence characteristics of the antigen using amino acid scales and HMMs.

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

This method incorporates solvent-accessible surface area calculations, as well as contact distances into its prediction of B cell 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 of antibody and protein 3D structures.

Structure Tools



[LYRA \(Lymphocyte Receptor Automated Modelling\):](#)

The LYRA server predicts structures for either T-Cell Receptors (TCR) or B-Cell Receptors (BCR) using homology modelling. Framework templates are selected based on BLOSUM score, and complementary determining regions (CDR) are then selected if 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 on the immune receptor features for receptor-specific epitope predictions. This tool extracts weekly updated 3D complexes of antibody-antigen, TCR-pMHC and MHC-ligand from the Immune Epitope Database (IEDB) and clusters them based on antigens, receptors and epitopes to generate benchmark datasets. Users can customize structural quality and clustering parameters (e.g. resolution, R free factors, antigen or epitope sequence identity) to generate these datasets based on their need.



: Tools under AR Labs which are experimental and are not quite ready for production yet. They are intended for further research, updates and testing.



B Cell Epitope Prediction – Sequence Based

Home Help Example Reference Download Contact

Antibody Epitope Prediction

Specify Input

Enter a Swiss-Prot ID (example: P02185)

Or enter a protein sequence in plain format (50000 residues maximum, 250 residues for Bepipred 2.0):

```
VLSEGEWQLVLHVWAKVEADVAGHGQDILIRLFKSHPETLEKDFRKFHLKTEAEMKASEDLKKHGVTVL  
ALGAILKKKGHHEAELKPLAQSHATKHKIPIKYLEFISEAIIHVLHSRHPGNFGADAGGAMNKALELFRKDIA  
AKYKELGYQG
```

Choose a method:

- [Bepipred Linear Epitope Prediction 2.0](#)
- [Bepipred Linear Epitope Prediction](#)
- [Chou & Fasman Beta-Turn Prediction](#)
- [Emini Surface Accessibility Prediction](#)
- [Karpplus & Schulz Flexibility Prediction](#)
- [Kolaskar & Tongaonkar Antigenicity](#)
- [Parker Hydrophilicity Prediction](#)

Submit Reset

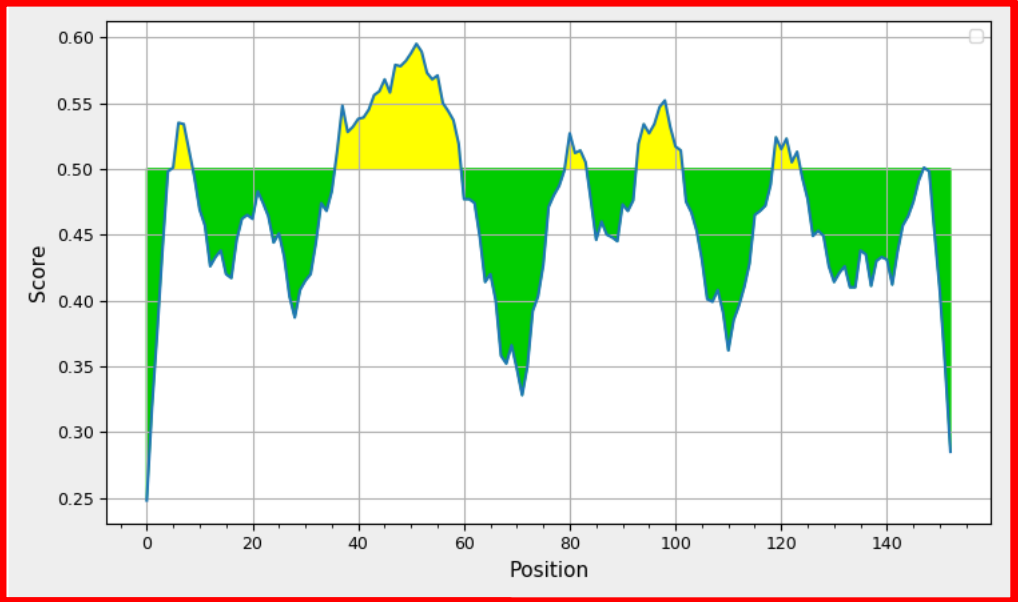
tools.iedb.org/bcell/

Bepipred Linear Epitope Prediction 2.0 Results

Input Sequences

1 VLSEGENQLV LHVWAKVEAD VAGHGQDILI RLFKSHPETL EKDFRFKHLK TEAEMKASED
 61 LKKHGVTULT ALGAILKKGK HHEAELKPLA QSHATKHKIP IKYLEFISEA IIHVLHSRHP
 121 GNFGADAGGA MNKALELFRK DIAAKYKELG YQG

Center position: 4 Threshold: 0.500



Average: 0.466 Minimum: 0.248 Maximum: 0.595

Predicted peptides:

No.	Start	End	Peptide	Length
1	6	9	ENQL	4
2	37	60	PETLEKDFRFKHLKTEAEMKASED	24
3	81	84	HHEA	4
4	94	102	ATKHKIPIK	9
5	120	124	PGNFG	5
6	148	148	E	1

Predicted residue scores:

Position	Residue	Score	Assignment
0	V	0.248	.
1	L	0.319	.
2	S	0.377	.
3	E	0.440	.
4	G	0.498	.
5	E	0.501	E

B Cell Epitope Prediction – Sequence Based

tools.iedb.org/bcell/

B Cell Epitope Prediction – Structure Based

tools.iedb.org/discotope/

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DiscoTope: Structure-based Antibody Prediction

Step 1: Please enter the 4-letter PDB ID
Or upload a PDB file

1z40 (example: 1z40)

Browse... No file selected.

Step 2: Please enter PDB Chain ID

A

Step 3: Select version

1.1

RCSB PDB 155587 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education
PROTEIN DATA BANK

Search by PDB ID, author, macromolecule, sequence, or ligands Go

Advanced Search | Browse by Annotations

PDB-101 EMBL Data Resource WorldWide Protein Data Bank Foundation

Structure Summary 3D View Annotations Sequence Sequence Similarity Structure Similarity Experiment

Biological Assembly 1

1Z40

AMA1 from Plasmodium falciparum

DOI: 10.2210/pdb1Z40/pdb

Classification: [UNKNOWN FUNCTION](#)

Organism(s): [Plasmodium falciparum \(isolate 3D7\)](#)

Expression System: [Escherichia coli BL21\(DE3\)](#)

Deposited: 2005-03-14 Released: 2005-08-16

Deposition Author(s): [Bai, T.](#), [Becker, M.](#), [Gupta, A.](#), [Strike, P.](#), [Murphy, V.J.](#), [Anders, R.F.](#), [Batchelor, A.H.](#)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.901 Å

R-Value Free: 0.236

R-Value Work: 0.192

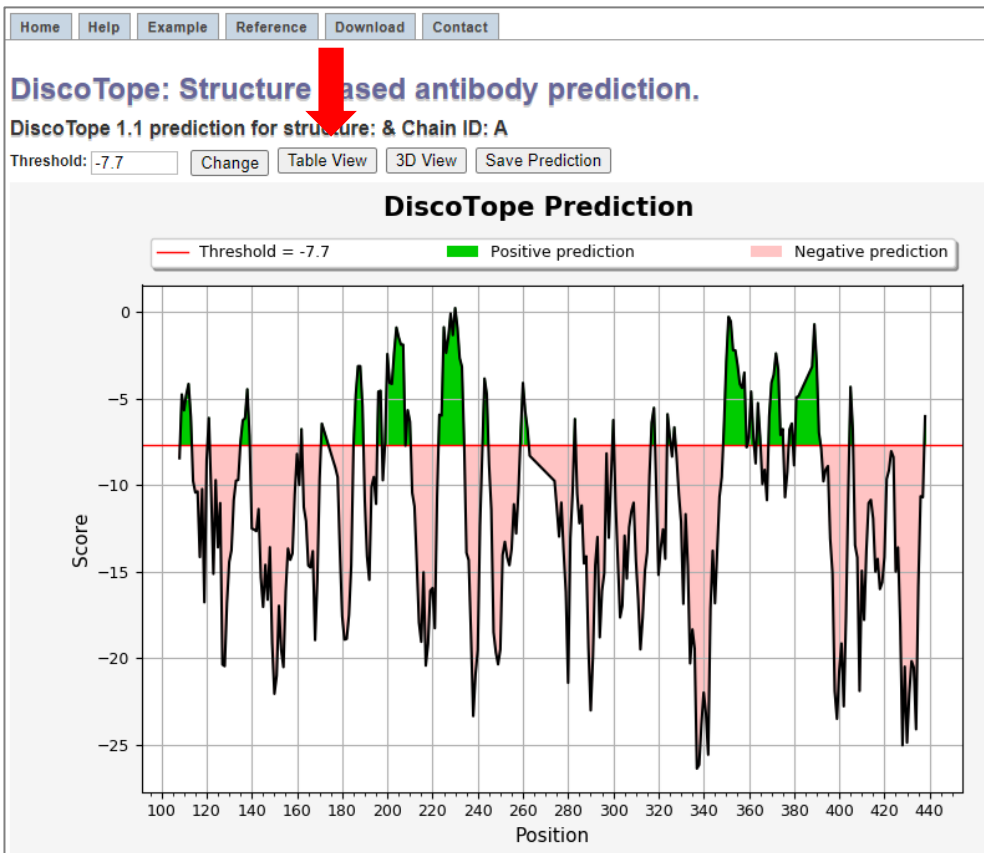
wwPDB Validation

Metric	Percentile Ranks	Value
Rfree		0.234
Clashscore		5
Ramachandran outliers		1.0%
Sidechain outliers		3.2%
RSRZ outliers		16.2%

3D View: Structure | Electron Density | Ligand Interaction

Standalone Viewers

B Cell Epitope Prediction – Structure Based



DiscoTope - Result

DiscoTope 1.1 prediction for structure: & Chain ID: A

The positive predictions are displayed in green.

Chain ID	Residue ID	Residue Name	Contact Number	Propensity Score	DiscoTope Score
A	108	ASN	14	-1.459	-8.459
A	109	PRO	11	0.724	-4.776
A	110	TRP	13	0.804	-5.696
A	111	THR	12	1.211	-4.789
A	112	GLU	11	1.331	-4.169
A	113	TYR	14	0.929	-6.071
A	114	MET	18	-0.779	-9.779
A	115	ALA	20	-0.444	-10.444
A	116	LYS	21	0.122	-10.378
A	117	TYR	24	-2.172	-14.172
A	118	ASP	21	0.257	-10.243
A	119	ILE	32	-0.783	-16.783
A	120	GLU	21	1.954	-8.546
A	121	GLU	15	1.366	-6.134
A	122	VAL	20	-0.374	-10.374
A	123	HIS	28	-1.144	-15.144
A	124	GLY	22	1.274	-9.726
A	125	SER	29	0.887	-13.613
A	126	GLY	28	2.951	-11.049
A	127	ILE	35	-2.881	-20.381
A	128	ARG	29	-5.973	-20.473
A	129	VAL	30	-1.817	-16.817
A	130	ASP	31	1.048	-14.452
A	131	LEU	31	1.727	-13.773
A	132	GLY	25	1.617	-10.883
A	133	GLU	19	-0.26	-9.76
A	134	ASP	18	-0.714	-9.714
A	135	ALA	15	-0.017	-7.517
A	136	GLU	15	1.225	-6.275
A	137	VAL	22	4.846	-6.154
A	138	ALA	15	3.024	-4.476
A	139	GLY	12	-1.166	-7.166
A	140	THR	18	-3.524	-12.524
A	141	GLN	20	-2.583	-12.583
A	142	TYR	24	-0.673	-12.673
A	143	ARG	24	0.606	-11.394

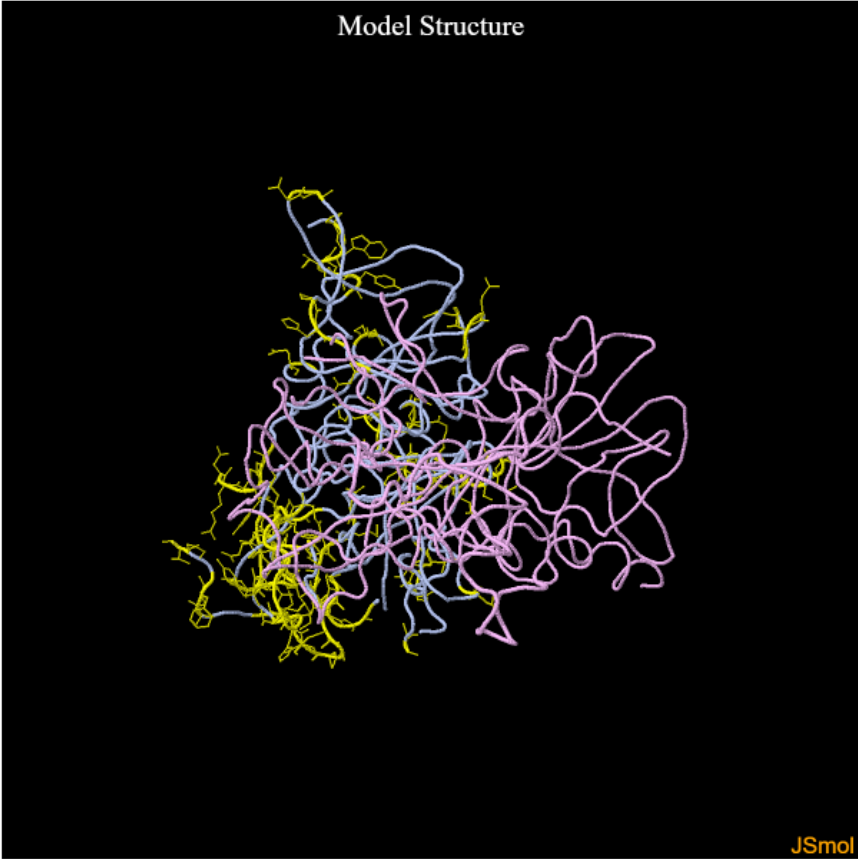
B Cell Epitope Prediction – Structure Based

Home Help Example Reference Download Contact

JSmol-Rendered PDB Structure

Chart View Table View Save Prediction

Model Structure



JSmol

Chain ID	Residue ID	Residue Name	Contact Number	Propensity Score	Discoptoe Score	View
A	109	PRO	11	0.724	-4.776	CPK
A	110	TRP	13	0.804	-5.696	CPK
A	111	THR	12	1.211	-4.789	CPK
A	112	GLU	11	1.331	-4.169	CPK
A	113	TYR	14	0.929	-6.071	CPK
A	121	GLU	15	1.366	-6.134	CPK
A	135	ALA	15	-0.017	-7.517	CPK
A	136	GLU	15	1.225	-6.275	CPK
A	137	VAL	22	4.846	-6.154	CPK
A	138	ALA	15	3.024	-4.476	CPK
A	139	GLY	12	-1.166	-7.166	CPK
A	162	ASN	11	-1.279	-6.779	CPK
A	171	THR	9	-1.963	-6.463	CPK
A	186	THR	10	0.194	-4.806	CPK
A	187	GLU	7	0.361	-3.139	CPK
A	188	PRO	7	0.361	-3.139	CPK
A	189	LEU	11	0.049	-5.451	CPK
A	196	ASP	12	1.384	-4.616	CPK
A	197	GLU	15	2.938	-4.562	CPK
A	199	ARG	20	2.492	-7.508	CPK
A	200	HIS	13	4.057	-2.443	CPK
A	201	PHE	16	3.888	-4.112	CPK

Standalone (Local) Version

tools.iedb.org/main/download/

IEDB Analysis Resource



IEDB Tools Downloads

Complete Download: IEDB Analysis Resource Virtual Machine Image

For users that would like to run the entire analysis resource locally, a virtual machine image file is available with a paid commercial license. The image is kept in sync with the current version of the IEDB Analysis Resource and is updated on a six month cycle. Please [contact us](#) for details on licensing options.

Standalone Downloads

Many of the tools hosted on the IEDB-AR are available as command-line tools. They are freely available to academic users through an open source license. Please [contact us](#) to inquire about a commercial license or if you have any questions in general. For a complete list of standalone tools, including previous versions, please click [here](#).

Linear B cell epitope predictor

This allows for scoring of amino acid residues using the 6 scale-based methods of the linear B cell epitope prediction tool.

- [Linear B cell epitope predictor](#)

MHC class I & II epitope predictors

For users with batch processing needs, the MHC class I and II binding prediction tools are available as standalone scripts for download. These command line tools are kept in sync with the web tools and should therefore produce the same results as clicking through the web interface.

- [MHC Class I](#)
- [MHC Class II](#)

EIIIPro

This will produce the same output as the web version of the tool but does not include the initial template finding functionality. It accepts either a PDB ID or a path to a PDB file as input. Usage instructions are printed by calling the program without any parameters.

- [EIIIPro](#)

Class I Immunogenicity

This tool uses amino acid properties as well as their position within the peptide to predict the immunogenicity of a peptide MHC (pMHC) complex.

- [Class I Immunogenicity](#)

Proteasomal Cleavage Prediction

The distributions 'IEDB_NetChop-1.0.tar.gz' contains methods for NetChop, NetCTL and NetCTLpan. NetChop is a predictor of proteasomal processing based upon a neural network. NetCTL is a predictor of T cell epitopes along a protein sequence. It also employs a neural network architecture. NetCTLpan is an update to the original NetCTL server that allows for prediction of CTL epitope with restriction to any MHC molecules of known protein sequence.

- [Proteasomal Cleavage Prediction](#)

Population Coverage

This tool calculates the fraction of individuals predicted to respond to a given epitope set on the basis of HLA genotypic frequencies and on the basis of MHC binding and/or T cell restriction data. HLA allele genotypic frequencies were obtained from [Allele Frequency database](#).

- [Population Coverage](#)

TCRMatch

TCRMatch compares input CDR3b sequences against curated CDR3b sequences in the IEDB to find matches that are predicted to share epitope specificity. Matches are determined by sequence similarity, which is scored using a comprehensive k-mer comparison.

- [TCRMatch](#)

- Run programs on your local machine
- Advantages:
 - No internet needed
 - Very helpful in case of large data sets
 - Free for non-profit & academia
 - Available for industry at a nominal fee
- license@iedb.org

Standalone (Local) Version

```
spaul@ubuntu:~/tools/mhc_1$ ./src/predict_binding.py netmhcpan "HLA-A*02:01" 9 test_sequence.fasta
allele seq_num start end length peptide ic50 rank
HLA-A*02:01 1 6 14 9 TMFEALPHI 4.3 0.03
HLA-A*02:01 1 10 18 9 ALPHIIDEV 12.6 0.12
HLA-A*02:01 1 14 22 9 IIDEVINIV 43.3 0.47
HLA-A*02:01 1 38 46 9 FATCGIFAL 65.2 0.64
HLA-A*02:01 1 13 21 9 HIIDEVINI 97.3 0.87
HLA-A*02:01 1 2 10 9 GQIVTMFEA 245.5 1.8
HLA-A*02:01 1 27 35 9 IVITGIKAV 324.4 2.1
HLA-A*02:01 1 24 32 9 IVLIVITGI 651.0 3.0
HLA-A*02:01 1 17 25 9 EVINIVIIIV 3263.2 7.2
HLA-A*02:01 1 18 26 9 VINIVIIIVL 3491.7 7.5
HLA-A*02:01 1 3 11 9 QIVTMFEAL 3523.2 7.5
HLA-A*02:01 1 20 28 9 NIVIIIVLIV 4861.5 9.0
HLA-A*02:01 1 21 29 9 IVIIVLIVI 5959.9 12
HLA-A*02:01 1 31 39 9 GIKAVYNFA 6530.5 12
HLA-A*02:01 1 7 15 9 MFEALPHII 11337.5 17
HLA-A*02:01 1 37 45 9 NFATCGIFA 11579.5 17
HLA-A*02:01 1 26 34 9 LIVITGIKA 12185.2 18
HLA-A*02:01 1 33 41 9 KAVYNFATC 12713.3 18
HLA-A*02:01 1 22 30 9 VIIVLIVIT 13298.3 19
HLA-A*02:01 1 19 27 9 INIVIIVLI 14913.1 21
HLA-A*02:01 1 4 12 9 IVTMFEALP 15618.8 22
HLA-A*02:01 1 34 42 9 AVYNFATCG 18955.1 25
HLA-A*02:01 1 35 43 9 VYNFATCGI 19064.3 26
HLA-A*02:01 1 25 33 9 VLIVITGIK 19910.8 27
HLA-A*02:01 1 36 44 9 YNFATCGIF 21579.6 29
HLA-A*02:01 1 23 31 9 IIVLIVITG 22420.2 30
HLA-A*02:01 1 28 36 9 VITGIKAVY 28040.2 39
HLA-A*02:01 1 1 9 9 MGQIVTMFE 28618.9 40
HLA-A*02:01 1 32 40 9 IKAVYNFAT 28756.4 41
HLA-A*02:01 1 5 13 9 VTMFEALPH 28919.3 41
HLA-A*02:01 1 30 38 9 TGIKAVYNF 29272.8 42
HLA-A*02:01 1 11 19 9 LPHIIDEVI 29396.6 42
HLA-A*02:01 1 15 23 9 IDEVINIVI 32112.8 48
HLA-A*02:01 1 16 24 9 DEVINIVII 32893.9 50
HLA-A*02:01 1 9 17 9 EALPHIIDE 37902.4 66
HLA-A*02:01 1 29 37 9 ITGIKAVYN 38010.0 66
HLA-A*02:01 1 8 16 9 FEALPHIID 40600.3 76
HLA-A*02:01 1 12 20 9 PHIIDEVIN 48177.9 100
spaul@ubuntu:~/tools/mhc_1$ ./src/predict_binding.py netmhcpan "HLA-A*02:01" 9 test_s
spaul@ubuntu:~/tools/mhc_1$
```

prediction_results.txt x									
	allele	seq_num	start	end	length	peptide	ic50	rank	
1	HLA-A*02:01	1	6	14	9	TMFEALPHI	4.3	0.03	
2	HLA-A*02:01	1	10	18	9	ALPHIIDEV	12.6	0.12	
3	HLA-A*02:01	1	14	22	9	IIDEVINIV	43.3	0.47	
4	HLA-A*02:01	1	38	46	9	FATCGIFAL	65.2	0.64	
5	HLA-A*02:01	1	13	21	9	HIIDEVINI	97.3	0.87	
6	HLA-A*02:01	1	2	10	9	GQIVTMFEA	245.5	1.8	
7	HLA-A*02:01	1	27	35	9	IVITGIKAV	324.4	2.1	
8	HLA-A*02:01	1	24	32	9	IVLIVITGI	651.0	3.0	
9	HLA-A*02:01	1	17	25	9	EVINIVIIIV	3263.2	7.2	
10	HLA-A*02:01	1	18	26	9	VINIVIIIVL	3491.7	7.5	
11	HLA-A*02:01	1	3	11	9	QIVTMFEAL	3523.2	7.5	
12	HLA-A*02:01	1	20	28	9	NIVIIIVLIV	4861.5	9.0	
13	HLA-A*02:01	1	21	29	9	IVIIVLIVI	5959.9	12	
14	HLA-A*02:01	1	31	39	9	GIKAVYNFA	6530.5	12	
15	HLA-A*02:01	1	7	15	9	MFEALPHII	11337.5	17	
16	HLA-A*02:01	1	37	45	9	NFATCGIFA	11579.5	17	
17	HLA-A*02:01	1	26	34	9	LIVITGIKA	12185.2	18	
18	HLA-A*02:01	1	33	41	9	KAVYNFATC	12713.3	18	
19	HLA-A*02:01	1	22	30	9	VIIVLIVIT	13298.3	19	
20	HLA-A*02:01	1	19	27	9	INIVIIVLI	14913.1	21	
21	HLA-A*02:01	1	4	12	9	IVTMFEALP	15618.8	22	
22	HLA-A*02:01	1	34	42	9	AVYNFATCG	18955.1	25	
23	HLA-A*02:01	1	35	43	9	VYNFATCGI	19064.3	26	
24	HLA-A*02:01	1	25	33	9	VLIVITGIK	19910.8	27	
25	HLA-A*02:01	1	36	44	9	YNFATCGIF	21579.6	29	
26	HLA-A*02:01	1	23	31	9	IIVLIVITG	22420.2	30	
27	HLA-A*02:01	1	28	36	9	VITGIKAVY	28040.2	39	
28	HLA-A*02:01	1	1	9	9	MGQIVTMFE	28618.9	40	
29	HLA-A*02:01	1	32	40	9	IKAVYNFAT	28756.4	41	
30	HLA-A*02:01	1	5	13	9	VTMFEALPH	28919.3	41	
31	HLA-A*02:01	1	30	38	9	TGIKAVYNF	29272.8	42	
32	HLA-A*02:01	1	11	19	9	LPHIIDEVI	29396.6	42	
33	HLA-A*02:01	1	15	23	9	IDEVINIVI	32112.8	48	
34	HLA-A*02:01	1	16	24	9	DEVINIVII	32893.9	50	
35	HLA-A*02:01	1	9	17	9	EALPHIIDE	37902.4	66	
36	HLA-A*02:01	1	29	37	9	ITGIKAVYN	38010.0	66	
37	HLA-A*02:01	1	8	16	9	FEALPHIID	40600.3	76	
38	HLA-A*02:01	1	12	20	9	PHIIDEVIN	48177.9	100	
39	HLA-A*02:01	1	12	20	9	PHIIDEVIN	48177.9	100	

API Version (RESTful Interface)

tools.iedb.org/main/tools-api/

IEDB Analysis Resource

Overview | T Cell Tools | B Cell Tools | Analysis Tools | **Tools-API** | Usage | Download | Datasets | Contribute Tools | References

RESTful interface (IEDB-API):

Several IEDB Analysis tools can now be accessed via the RESTful (REpresentational State Transfer) Web Services. This service is currently only available for T-cell epitopes. The service sends POST request to the tools server, and relies on user supplied parameters. Below are some examples for requests to the server will work just as well (including a web browser). The full list of parameters and their values for MHC I and MHC II-binding, MHC I-processing and MHC-NP predictions are given in the table. In release 2.15, a new API system for the class I binding predictions was made public. For end users, it should result in faster prediction time for intensive methods such as NetMHCpan and PickPocket.
* If relevant services are missing, please [contact us](#).

Examples for Class-I binding prediction

1) To run a single allele and length combination:

```
$ curl --data "method=smm&sequence_text=SLYNTVATLYCVHQRIDV&allele=HLA-A*01:01&length=9" http://tools-cluster-interface.iedb.org
```

2) To specify a version for methods:

```
$ curl --data "method=netmhcpa-4.0&sequence_text=ARFTGIKTA&allele=HLA-A*01:01&length=9" http://tools-cluster-interface.iedb.org
```

A "-" is used to separate method name and method version. If the version is not specified, the default version will be chosen.

Available methods (and aliases)	Available versions (bold = default)
recommended	2023.09, 2020.09, 2020.04
ann	4.0
comblib_sidney2008	1.0
consensus	2.18
netmhcons	1.1
netmhcpa_ba (recommended_binding, netmhcpa)	4.1, 4.0
netmhcpa_el (recommended_epitope, recommended)	4.1, 4.0
netmhstabpan	1.0
pickpocket	1.1
smm	1.0
smmpmbec	1.0

3) To run multiple allele and length combinations:

```
$ curl --data "method=recommended&sequence_text=SLYNTVATLYCVHQRIDV&allele=HLA-A*01:01,HLA-A*02:01&length=8,9" http://tools-cluster-interface.iedb.org/tools_api/mhci/
```

4) To submit multiple sequences at a time, escape the special characters in a fasta-formatted sequence with URI codes.
E.g., we can predict for 2 sequences (with fasta names peptide1 and peptide2) with the following code:

```
$ curl --data "method=ann&sequence_text=%3Epeptide1%0AGHAKHVKFRLLKAAR%0A%3Epeptide2%0ALKAADASADADGSGSGSGS&allele=HLA-A*01:01,HLA-A*02:01&length=8,9" http://tools-cluster-interface.iedb.org/tools_api/mhci/
```

5) To receive the prediction result in your email address, input your email address with a parameter "email_address".
E.g., we can send the prediction result to the email address "youremail@example.com" (Don't forget to use your email address to replace it.) with the following code:

```
$ curl --data "method=recommended&sequence_text=SLYNTVATLYCVHQRIDV&allele=HLA-A*01:01,HLA-A*02:01&length=8,9&email_address=youremail@example.com" http://tools-cluster-interface.iedb.org/tools_api/mhci/
```

MHC-I binding command line parameters:

Parameter	Possible values	Default value	Required	Description
sequence_text			*	Input protein sequence.
method	recommended, netmhcpa_el (recommended_epitope), netmhcpa_ba (recommended_binding), consensus, ann, smmpmbec, smm, comblib_sidney2008, netmhcons, pickpocket, netmhstabpan	recommended		NetMHCpan 4.0 & 4.1 was trained on both binding affinity and eluted ligand data leveraging the information from both data types. We provide both Binding Affinity Prediction and Eluted Ligand Prediction option with method names as "netmhcpa_ba" and "netmhcpa_el", and "netmhcpa_ba" is the default method of netmhcpa 4.0 & 4.1. The "IEDB recommended" method was updated to use NetMHCpan 4.1 EL across all alleles as of Sep 2020. And two IEDB recommended methods were added on Sep 2023, one for the prediction of peptide binding and one for the prediction of epitopes. For more information, see the help page. To print the usage and list all available methods: <pre>\$ curl --data "" http://tools-cluster-interface.iedb.org/tools_api/mhci/</pre>

- Sends prediction request to the tools server at LJ
- No need to install tools on your machine
- Freely available to all users
- Can be incorporated in prediction pipelines
- Automatic update without reinstalling

API Version (RESTful Interface) – Example

	A	B
1	peptide	allele
2	EALPHIIDEVINI	HLA-B*58:01
3	AVAKCNVNHDAEFC	HLA-A*68:01
4	SKFKEDVESA	HLA-A*68:02
5	SHLNLTMPNA	HLA-A*01:01
6	LMRNHLRDLMGV	HLA-A*32:01
7	NPGGYCLTKWMILA	HLA-A*26:01
8	AQSAQSQCRT	HLA-A*01:01
9	LSIRGNSNYKAVSC	HLA-A*03:01
10	QCRTFRGRVDMF	HLA-B*53:01
11	GTSGLELFTND	HLA-A*11:01
12	NLTSAFNKK	HLA-A*23:01
13	CDMLRLIDYNKAA	HLA-B*53:01
14	YIKRQGSTPL	HLA-A*26:01
15	YMRSGWGWG	HLA-A*23:01
16	LVTNGSYLNETHF	HLA-B*58:01
17	TKFFTRRL	HLA-B*57:01
18	NVNHDAEFCMLRL	HLA-B*08:01
19	HIKGGSCPAPH	HLA-A*30:01
20	DGKTTWCSQTS	HLA-A*32:01
21	HFSQIEQEADNM	HLA-A*32:01
22	FSDQIEQEADNMI	HLA-B*57:01
23	CNYSKFWY	HLA-B*58:01
24	MSHLNLTMPNAC	HLA-A*02:01
25	SGVENPGGYC	HLA-B*44:03
26	VIIVLIVITGIK	H-2-Kb
27	FRGRVDMFR	HLA-B*51:01
28	HIKGGSCPAPHR	HLA-B*44:02
29	SIRGNSNYKAVS	H-2-Kb
30	IQYNLTFSDA	HLA-A*02:06
31	RTFRGRVL	HLA-B*15:01
32	DAQSAQSQCRTFRG	HLA-B*44:02
33	QNRTWENHCTYAGP	HLA-B*15:01
34	AFGGKYMRSWGWWT	HLA-B*07:02
35	SRILLSQEKTKFFT	HLA-A*31:01
36	SALHLFKTTVNSLI	H-2-Kb
37	RKDYIKRQGSTP	HLA-B*58:01
38	FKSVEFDMSHLNL	HLA-B*58:01

```

api_predictor.py x
import pandas as pd
import shlex, subprocess

peptide_data = pd.read_csv('peptides_to_predict.txt', sep='\t')
alleles = peptide_data['allele'].tolist()
peptides = peptide_data['peptide'].tolist()

def prediction(peptide, allele, length):
    command = 'curl --data "method=recommended&sequence_text=' + peptide + \
              '&allele=' + allele + \
              '&length=' + str(length) + \
              '" http://tools-cluster-interface.iedb.org/tools_api/mhci/'
    args = shlex.split(command)
    process = subprocess.Popen(args, stdout=subprocess.PIPE, stderr=subprocess.PIPE)
    output = process.communicate()
    consensus_percentile = output[0].decode('utf8').split('\t')[22]
    return consensus_percentile

output_file_name = 'prediction_results.txt'
output_file = open(output_file_name, 'w')
with open(output_file_name, 'a') as file to write:
    file to write.write('peptide\tallele\tlength\tpercentile_rank\n')
    for i in range(len(alleles)):
        peptide = peptides[i]
        allele = alleles[i]
        length = len(peptide)
        consensus_percentile = prediction(peptide, allele, length)
        write_line = peptide + '\t' + allele + '\t' + str(
            consensus_percentile)
        file to write.write(write_line)
output_file.close()
    
```

	peptide	allele	length	percentile_rank
1	EALPHIIDEVINI	HLA-B*58:01	13	53.0
2	AVAKCNVNHDAEFC	HLA-A*68:01	14	56.0
3	SKFKEDVESA	HLA-A*68:02	10	36.5
4	SHLNLTMPNA	HLA-A*01:01	10	46.5
5	LMRNHLRDLMGV	HLA-A*32:01	12	45.0
6	NPGGYCLTKWMILA	HLA-A*26:01	14	57.0
7	AQSAQSQCRT	HLA-A*01:01	10	28.5
8	LSIRGNSNYKAVSC	HLA-A*03:01	14	13.0
9	QCRTFRGRVDMF	HLA-B*53:01	13	41.0
10	GTSGLELFTND	HLA-A*11:01	12	46.0
11	NLTSAFNKK	HLA-A*23:01	9	28.5
12	CDMLRLIDYNKAA	HLA-B*53:01	13	53.0
13	YIKRQGSTPL	HLA-A*26:01	10	10.25
14	YMRSGWGWG	HLA-A*23:01	10	13.55

Versions of IEDB Analysis Resource tools

Web

<http://tools.iedb.org>

- Client uses browsers to submit data
- Predictions run on IEDB tools server
- Can be run on Windows/Mac/Linux
- Internet is needed
- May not be suitable for very large data sets
- Automatically updated

Standalone

<http://tools.iedb.org/main/download>

- Uses command line interface
- Downloaded from IEDB website
- Installed and run on local machine
- Runs on Linux only (can use virtual machines to run Linux on other OS)
- Internet not needed once installed
- Better for very large data sets
- Need to update for every release
- Free to academia/non-profit; License fee for industry

API

<http://tools.iedb.org/main/tools-api>

- Uses command line interface
- Predictions run on IEDB server
- Clients send parameters to IEDB server using commands or scripts
- Internet is needed
- Can be used to make custom scripts for use with large data sets
- Automatically updated
- Free to all

Points to Remember

- First stop is IEDB database
- Epitope prediction tools extrapolate from existing data to identify new candidate epitopes
 - ‘Machine learning’ approaches identify patterns
 - ROC curves / AUC values as preferred performance metrics
 - Prediction is a screening step, not confirmatory
 - Predicted peptides should be experimentally tested for verification
- Analysis tools help to examine existing sets of epitopes and gain new knowledge
 - No single metric of performance
 - Broad array of applications

IEDB Tools

Analysis Resource & Next-Generation Tools

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:

- T cell epitope prediction
- B cell epitope prediction
- Analysis tools

tools.iedb.org

Welcome to the Next-Generation IEDB Tools site!

As a companion site to the Immune Epitope Database (IEDB), this site provides a collection of tools for the prediction and analysis of immune epitopes.

New User? Learn to use the website here!

T Cell Prediction - Class I

MHC class I binding affinity, TAP processing, and Immunogenicity predictions

Type/paste/drag a sequence into this box or click 'Run' to use the example sequence:

>SARS2 spike glycoprotein

MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPFFSNVTWF

HAIHVSGTNGTKRFDNPVLPFNDGVYFASTKSNIRGWIFGTTLDLSDKQSLIVNINATNVIKVF

CEFQFCNDPFLGVYHKNKSWMESEFRVYSSANNCTFEYVSQPFLMDLEGKQGNFKNLREF

MHC
Allele(s)

Ex: HLA-A*02:01

0



Next-Generation Tools:

- Re-implementing existing tools with a focus on improving usability and function
- Launched in 2023
- More tools to be added

nextgen-tools.iedb.org

Test them out!