

Immune Epitope Database Overview

www.iedb.org

Presented by: Alessandro Sette, IEDB Principal Investigator

Our goals for this user workshop

We want your input to make the IEDB better:

- Learn about real-life applications for the IEDB
- Identify and prioritize problems with the user interface, documentation, functionality etc.

We want to enable you to get the most out of the IEDB:

- The primary IEDB success metric is usage
- Best compliment for our program is if IEDB data & tools help in your research (citations)

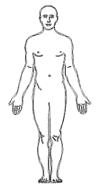
Immune Epitope Database

www.iedb.org

Database | Resource of experimentally-derived epitope information

- Allergens
- Infectious diseases
- Autoimmune diseases
- Transplantation / Alloantigens

... and more







Containing data on over **2.1 million unique structures** analyzed in over **6.4 million assays** from more than **23,200 curated references**.

Minimal Criteria for Epitope Inclusion

- Linear peptide <50 amino acids in length
- Tested as an immunogen or an antigen
- Discontinuous residues shown to be important in recognition
- Non-peptidic epitopes <5,000 Daltons
- Minimal information required (sequence, outcome, host, etc.)

Consistent data entry requires well defined data structure

Quantitation of CD8+ T Cell Responses to Newly Identified HLA-A*0201– restricted T Cell Epitopes Conserved Among Vaccinia and Variola (Smallpox) Viruses

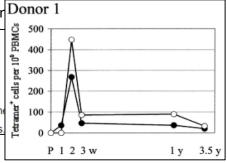
Masanori Terajima, John Cruz, Gregory Raines, Elizabeth D. Kilpatrick, Jeffrey S. Kenr

Francis A. Ennis

Materials And Methods

Donors.

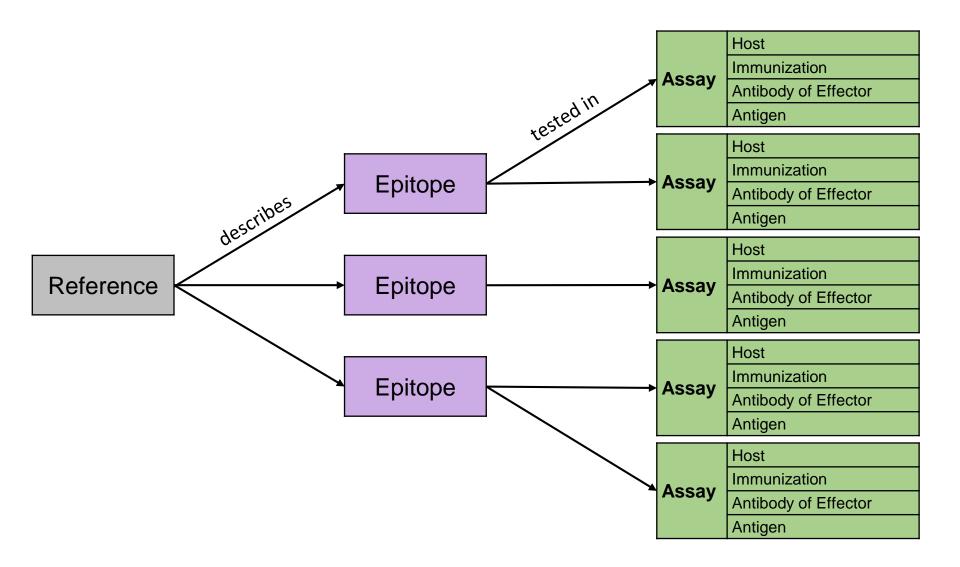
Donors in this study were three HLA-A*0201–positive laboratory workers received primary immunization by scarification with the licensed smallpox vaccine, Dryvax®, as recommended by the Centers for Disease Control and Prevention for laboratory per level working with vaccinia viruses.



			•
	Structure	Name	74A
		Chemical Type	Peptide / Protein
		Sequence	CLTEYILWV
		Domain / Region	Defined Epitope
Epitope		Species	Vaccina Virus Ankara
		Strain	Ankara (MVA)
	Source	Antigen	Putative 21.7k protein
		Antigen Accession	2772819
		Antigen Positions	79-87
Context	Immunization	Immunized Species	Homo sapiens
		Immunogen Type	Source species
		Administration	Scarification
	Assay	Antigen Type	Epitope
		Assay Type	ELISPOT
		Response Measured	Cytokine Release-IFN-g
		MHC Allele	HLA-A*0201
	· · · · · · · · · · · · · · · · · · ·	·	

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Data Structure: A Database of Experiments



Collaborations with Ontologies

- Provides standardized nomenclature, definitions, synonyms, and hierarchical relationships
- Makes curation easier → Finders
- Enhances user experience → Finders
- Ensures consistency and accuracy
- Finds errors
- Facilitates interoperability

External Resources and Ontologies

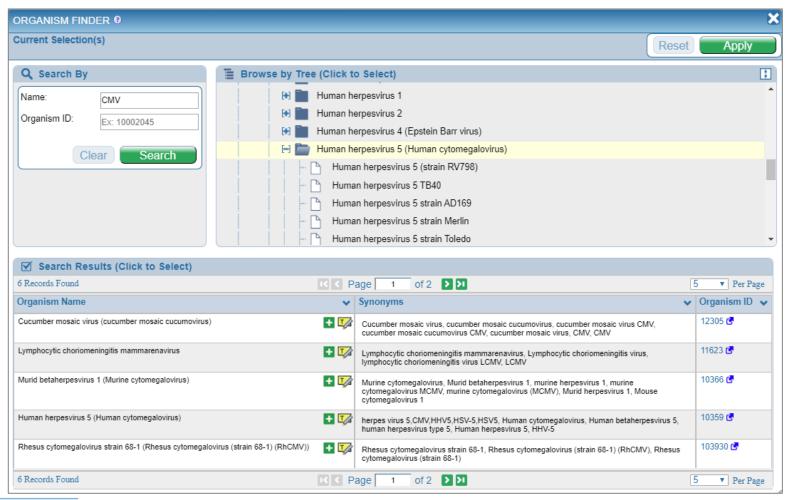
Peptidic Epitope

Amino acid sequence
Protein source
Organism source

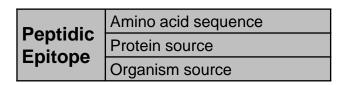


Human herpesvirus 5 (HHV-5) NCBI

taxon:10359

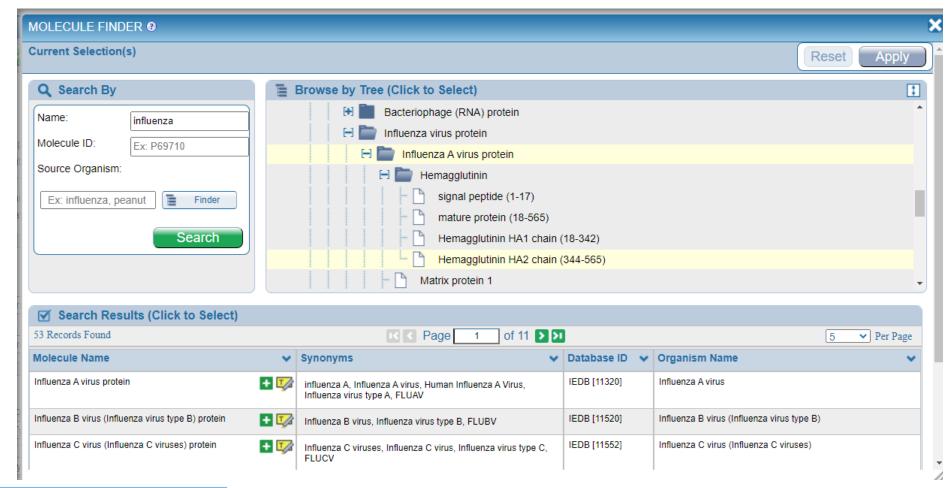


External Resources and Ontologies





PKYVKQNTLKLAT hemagglutinin HA1 GenBank/UniProt GI:AAL62329.1—UniProt:Q8V285



Literature Curation

PubMed / PDB

- Complex query
- Bi-weekly

240K retrieved

Classifier

- Content based categories
- Retrained annually

151K epitope related

Abstract Review

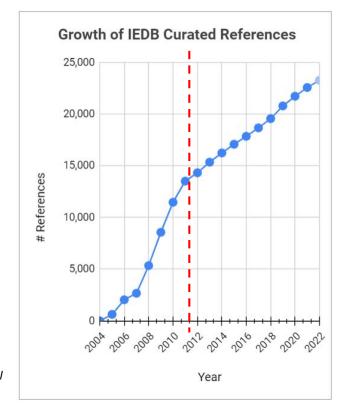
- Manual scan
- Confirmation of classification

44K likely curatable

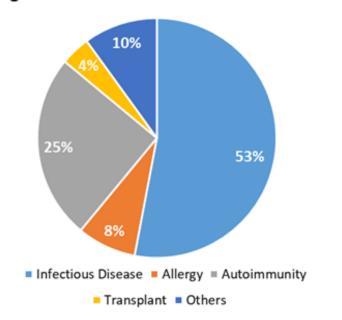
Manual Curation

- Assigned to curators
- Peer review

23K curated



Categorical Breakdown of Curated References



Note: 2022 data is based on Q1-3. Red line indicates historical curation completed.

Consistency and Quality Control Measures

- Manually curated by a team of PhD-level scientists with specific expertise
- Formal curation guidelines and peer review
 <u>Curation Manual</u>: http://curationwiki.iedb.org/wiki/index.php/Main_Page
- External immunological experts
- Built in validation in the curation application

Data Submissions

- Primarily sourced through NIAID Epitope Discovery contracts
- Data deposition is open to the general research community on a case-by-case basis

As of October, 2022:

- Data from 340 submissions is publicly available & 80 submissions are in process or on-hold
- Submitted data comprises ~20% of epitopes available in the IEDB

Inquire by contacting: nblazeska@lji.org or submissionsupport@iedb.org!

Direct Submission Process

Submission

 Investigators submit files via IEDB data submission tool



Review

 Automated validation and manual curator review check data consistency

Submitter confirms final approval



Release

Public release date set by submitter



IEDB.org: Homepage & Cumulative Data



Home

Specialized Searches Analysis Resource

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Welcome

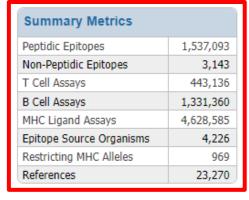
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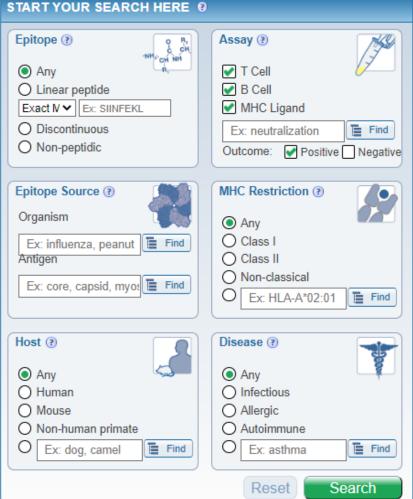
Learn More

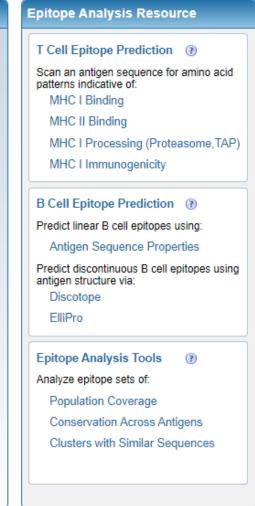
Upcoming Events & News

AAI Exhibitor Booth May 6-10 FOCIS Exhibitor Booth June 21-24 Oct 26-28 Virtual User Workshop * register here

IEDB SARS-CoV-2 Epitope Analysis Videos







IEDB.org: Homepage & Search Interface



Home Specialized Searches Analysis Resource

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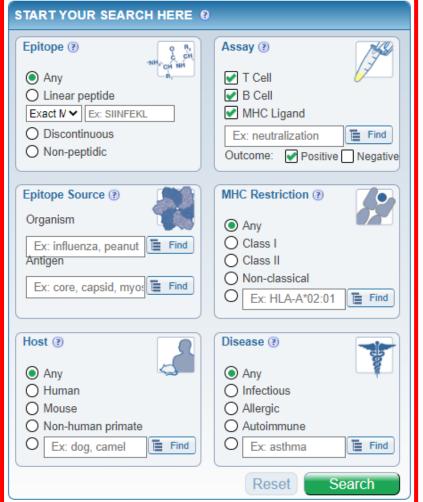
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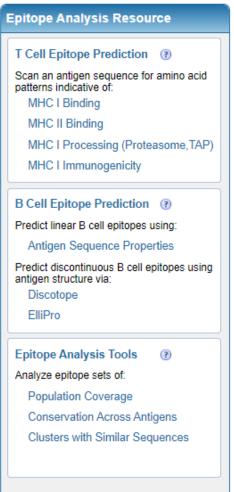
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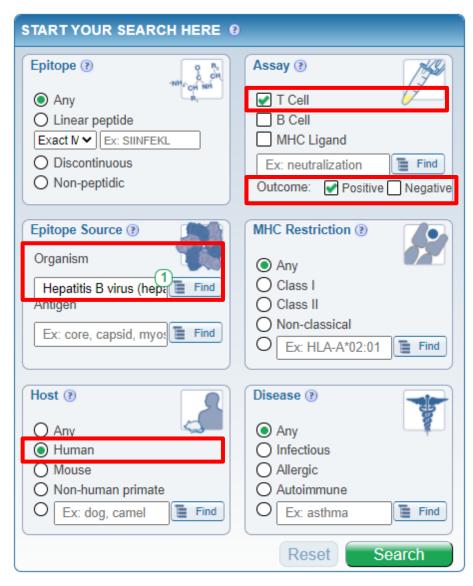
Summary Metrics	
Peptidic Epitopes	1,537,093
Non-Peptidic Epitopes	3,143
T Cell Assays	443,136
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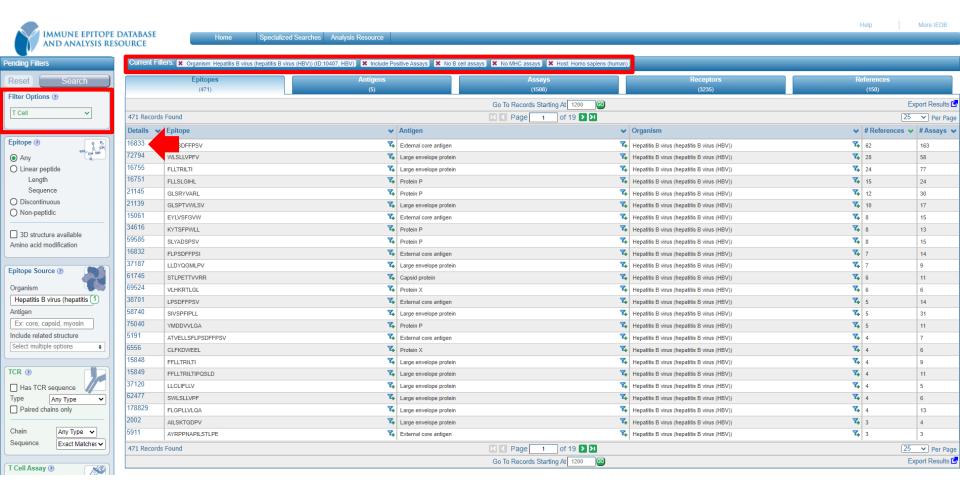


More IEDB

Example Query: HBV T Cell Epitopes in Humans



Results Summarized in Tables



Detail Pages Summarize Relevant Information

Details Pages:

- Epitope Summary
- Compiled Data
 - MHC Ligand Assay(s)
 - B Cell Assay(s)
 - T Cell Assay(s)
- External Resources

Also available for:

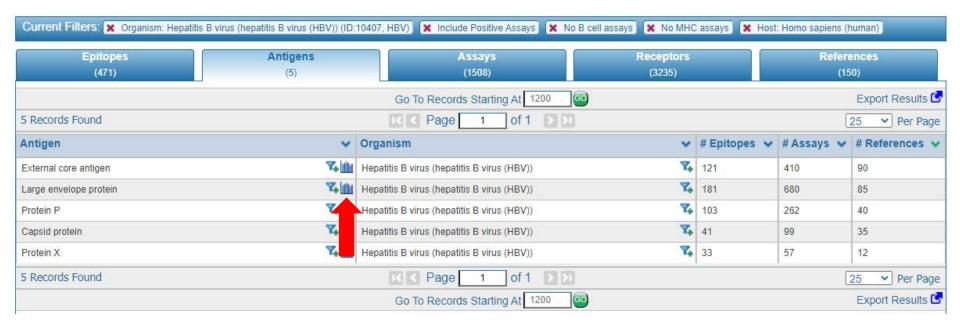
- Assays
- Receptors
- References

EPITOPE SUMMARY

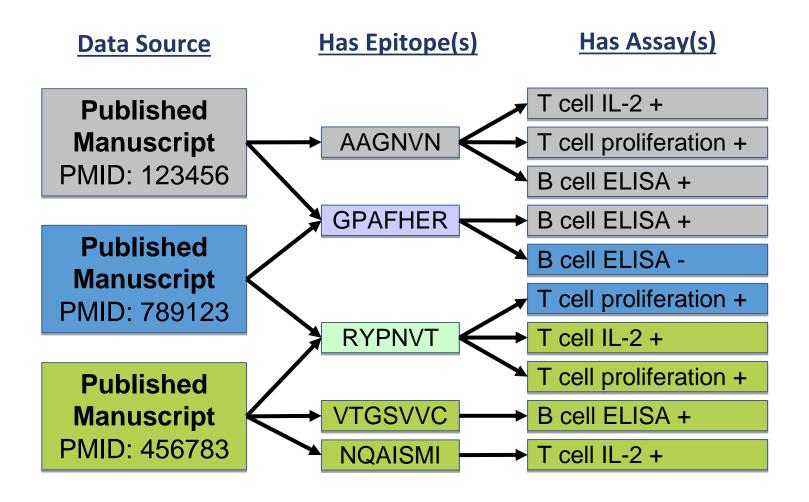
FLPSDFFPSV is a linear peptidic epitope (epitope ID 16833) studied as part of External core antigen from Hepatitis B virus (hepatitis B virus (HBV)) and Capsid protein from Hepatitis B virus (hepatitis B virus (HBV)). This epitope has been studied for immune reactivity in 100 publication(s), tested in 215 T cell assays, 8 B cell assays, 88 MHC ligand assays and has 3D structure(s) 30XR, 30XS, 1HHH and 30XB

COMPUED DATA			
COMPILED DATA			
MHC Ligand Assay(s) 88	0	Positive / All	
MHC molecule HLA-A*02:01		35/35	
HLA-A*02:03		8/8	
HLA-A*02:06		8/8	
HLA-A*02:06 HLA-A*02:02		6/6	
HLA-A*02:07		4/4	
HLA-A*68:02		4/4	
HLA-A*03:01		0/3	
HLA-A*11:01		0/3	
HLA-A*02:05		2/2	
HLA-A*01:01		0/2	
HLA-B*07:02		0/2	
HLA-B*15:02		0/2	
HLA-A*02:04		1/1	
HLA-A*02:11		1/1	
HLA-A2		1/1	
HLA-B44		1/1	
H2-Kd		0/1	
HLA-A*24:02		0/1	
HLA-A*31:01		0/1	
HLA-A*68:01		0/1	
Mamu-A1*001:		0/1	
B Cell Assay(s) 8		•	
Assay Type		Positive / All	
qualitative bindi	ng	7/7	
dissociation constant KD		1/1	
T Cell Assay(s) 215			
Assay Type		Positive / All	
cytotoxicity		63/74	
IFNg release		65/66	
qualitative bindi	ng	45/50	
TNFa release		7/8	
IL-2 release		4/4	
proliferation		4/4	
IL-4 release		2/2	
TNF release		2/2	
activation 1/1			
EXTERNAL RESOURCES			
Resource	Link		
ANALYSIS TOOLS IEDB.ORG IEDB-AR: MHC-I Processing	Predict MHC class I proces	sing 🗹	
ANALYSIS TOOLS IEDB-AR: MHC-I	Predict MHC class I binding affinity ☑		
ANALYSIS TOOLS IEDB.ORG IEDB-AR; B cell scales	Predict B cell epitopes Predict B cell epitopes Predict B cell epitopes Predict B cell		

Antigens: Identifying Protein Source of Epitopes



Data Aggregation



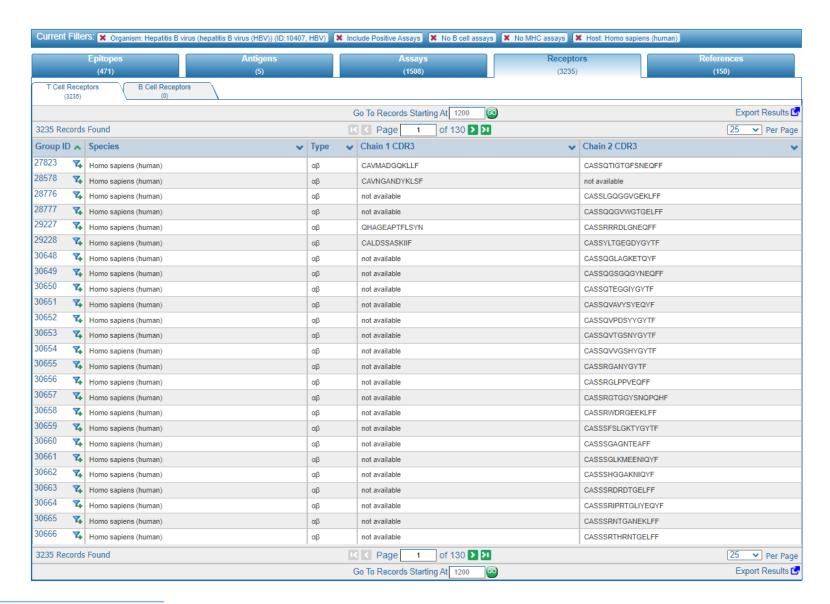
ImmunomeBrowser: Visualization on Reference Proteins



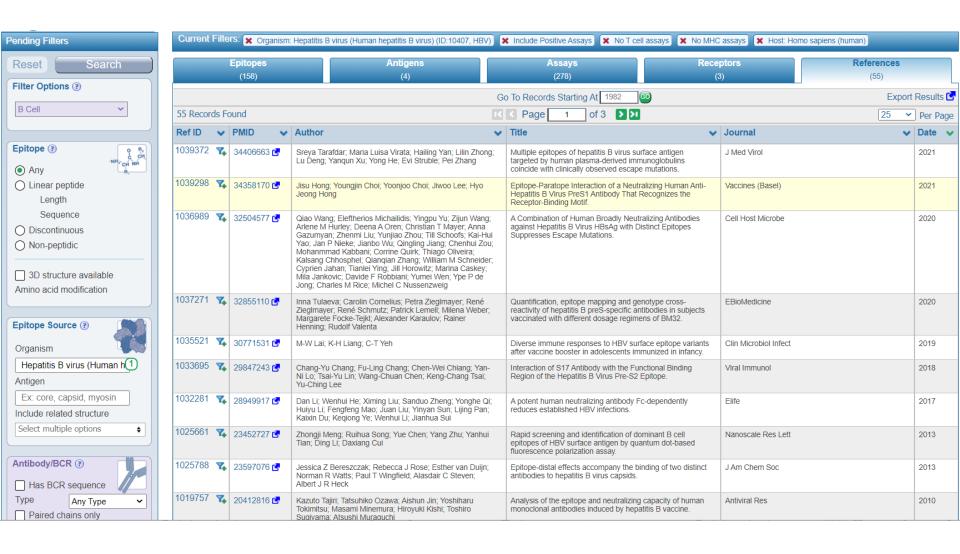
Assays: Experiments in which epitopes were tested



Epitope-specific B Cell and T Cell Receptors



References: Source of Information

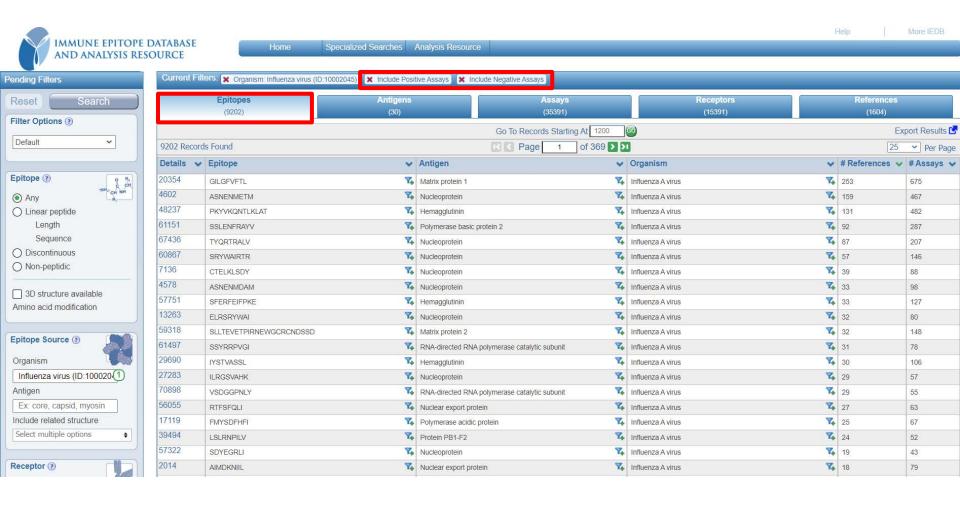


Example Query II: Influenza Virus Epitopes



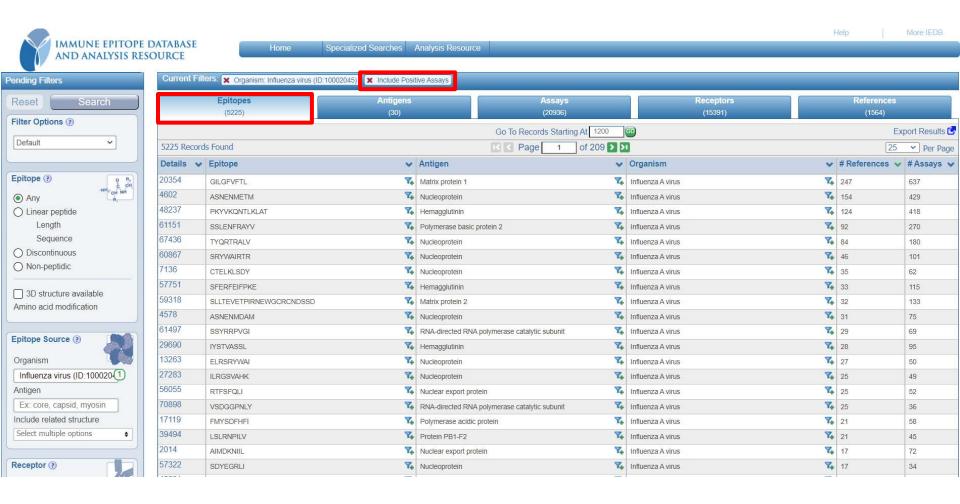
Results: All influenza virus epitopes

Both positive and negative assay outcomes



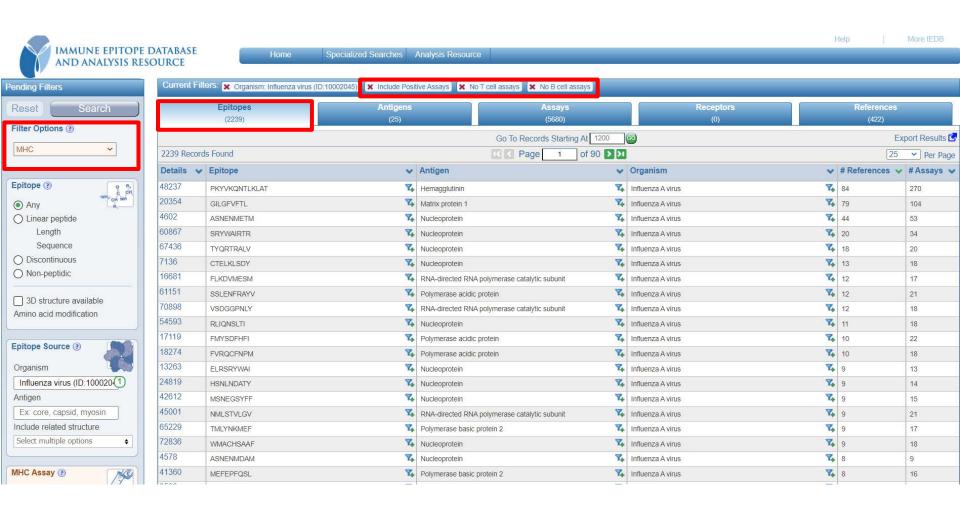
Results: Positive influenza virus epitopes

Positive assay outcomes



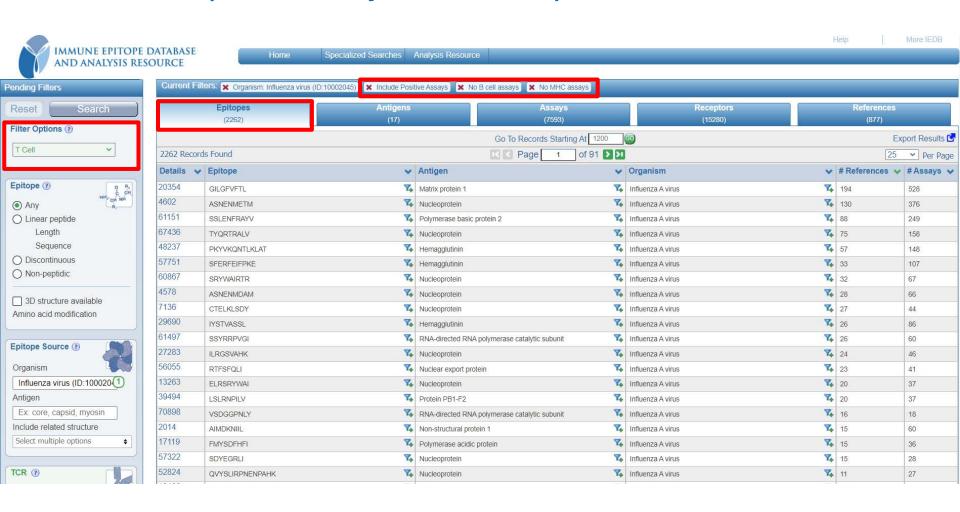
Results: Influenza virus epitopes that bind

Positive assay outcomes for MHC assays



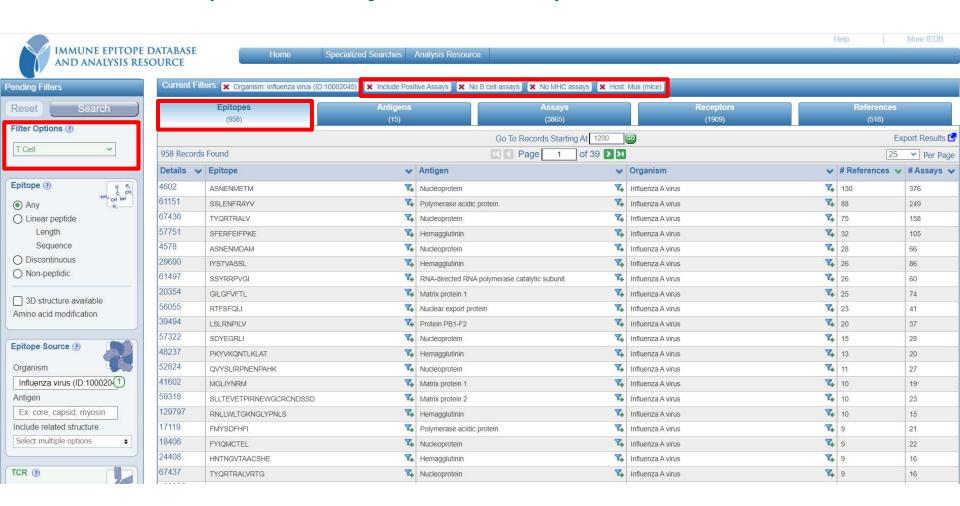
Results: Influenza virus epitopes that are immunogenic

Positive assay outcomes for T cell assays



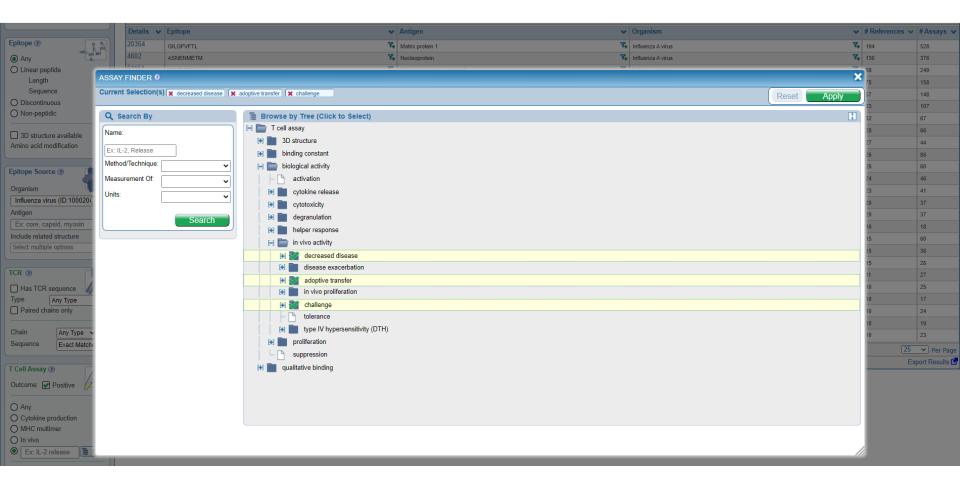
Results: Influenza virus mouse epitopes that are immunogenic

Positive assay outcomes for T cell assays in a mouse host



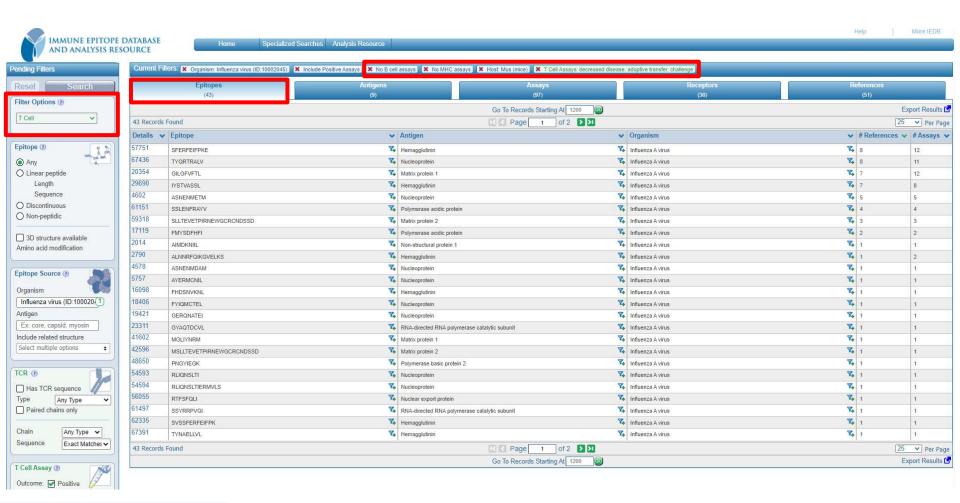
Results: Influenza virus epitopes that offer protection from disease

Positive assay outcomes for T cell assays (decreased disease, adoptive transfer, challenge) in a mouse host



Results: Influenza virus epitopes that offer protection from disease

Positive assay outcomes for T cell assays (decreased disease, adoptive transfer, challenge) in a mouse host



More Exports



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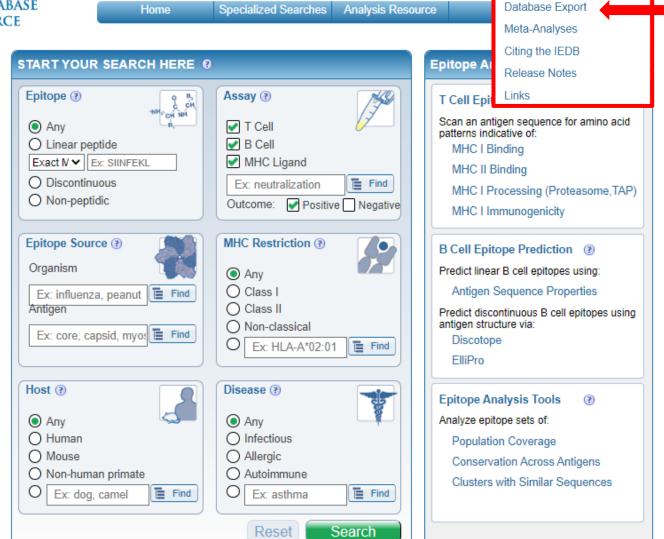
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Restricting MHC Alleles	969
References	23,270



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More IEDB

More Exports

http://www.iedb.org/database_export_v3

XML Database Export		
Complete Database Export	323MB	
<u>ledbAccessionList.zip</u>	49kB	
MhcAlleleNameList.zip	34kB	
<u>OrganismList.zip</u>	35MB	
<u>AssayTypeList zip</u>	5kB	
GeoLocList.zip	3kB	

IEDB Schema		
Curation.xsd (Primary IEDB schema)	48kB	
<u>CurationSimpleTypes.xsd</u>	303kB	
<u>IedbAccessionList.xsd</u>	909B	
MhcAlleleNameList.xsd	1kB	
<u>OrganismList.xsd</u>	751B	
<u>AssayTypeList.xsd</u>	771B	
GeoLocList.xsd	642B	

MySQL Database Export		
SQL Statement Export	379MB	
MyISAM Binary Export	819MB	

Physical Entity Relationship Diagram	
iedb public erd.pdf	31kB

CSV Metric Exports		
epitope full v3.zip	65MB	
antigen full v3.zip	2MB	
tcell full v3.zip	28MB	
bcell full v3.zip	36MB	
mhc_ligand_full (single_file.zip) (multi_file.zip)	168MB	
reference full v3.zip	12MB	
receptor full v3.zip	5MB	
iedb 3d full.zip	змв	

Stable ID Exports		
Linkout IDs Compact	21MB	
Linkout IDs Full	40MB	
ChEBI to Epitope ID Maps	158kB	
PDB to Epitope ID Maps	51kB	
Epitope ID to Linear Seg Maps	11MB	

Help integrated throughout the website



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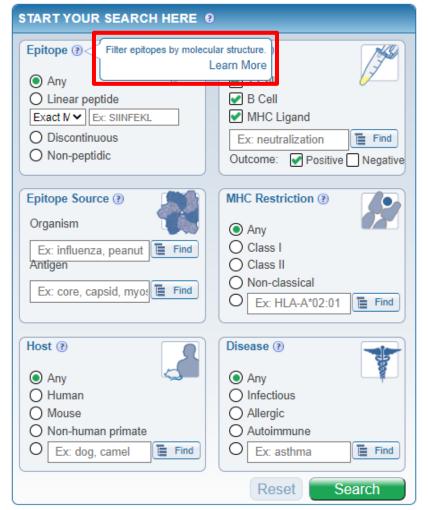
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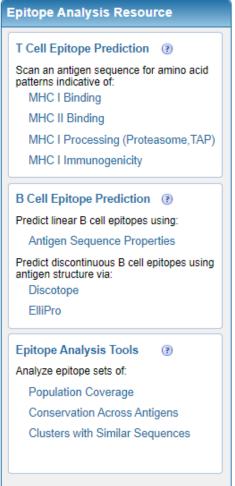
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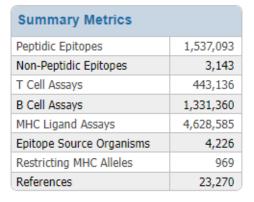
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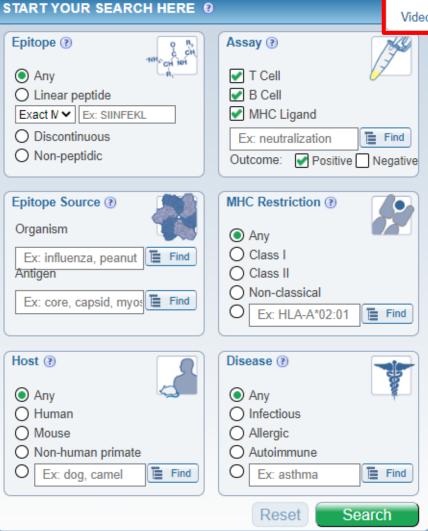
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T Cell Epitope Prediction Scan an antigen sequence for ami

Scan an antigen sequence for amino acid patterns indicative of:

MHC I Binding

Help

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

Solution Center: help.iedb.org

Accessible through header and footer on every page or submit via email to help@iedb.org



