HIV Database Immunology Workshop

https://www.hiv.lanl.gov/

immuno@lanl.gov
seq-info@lanl.gov

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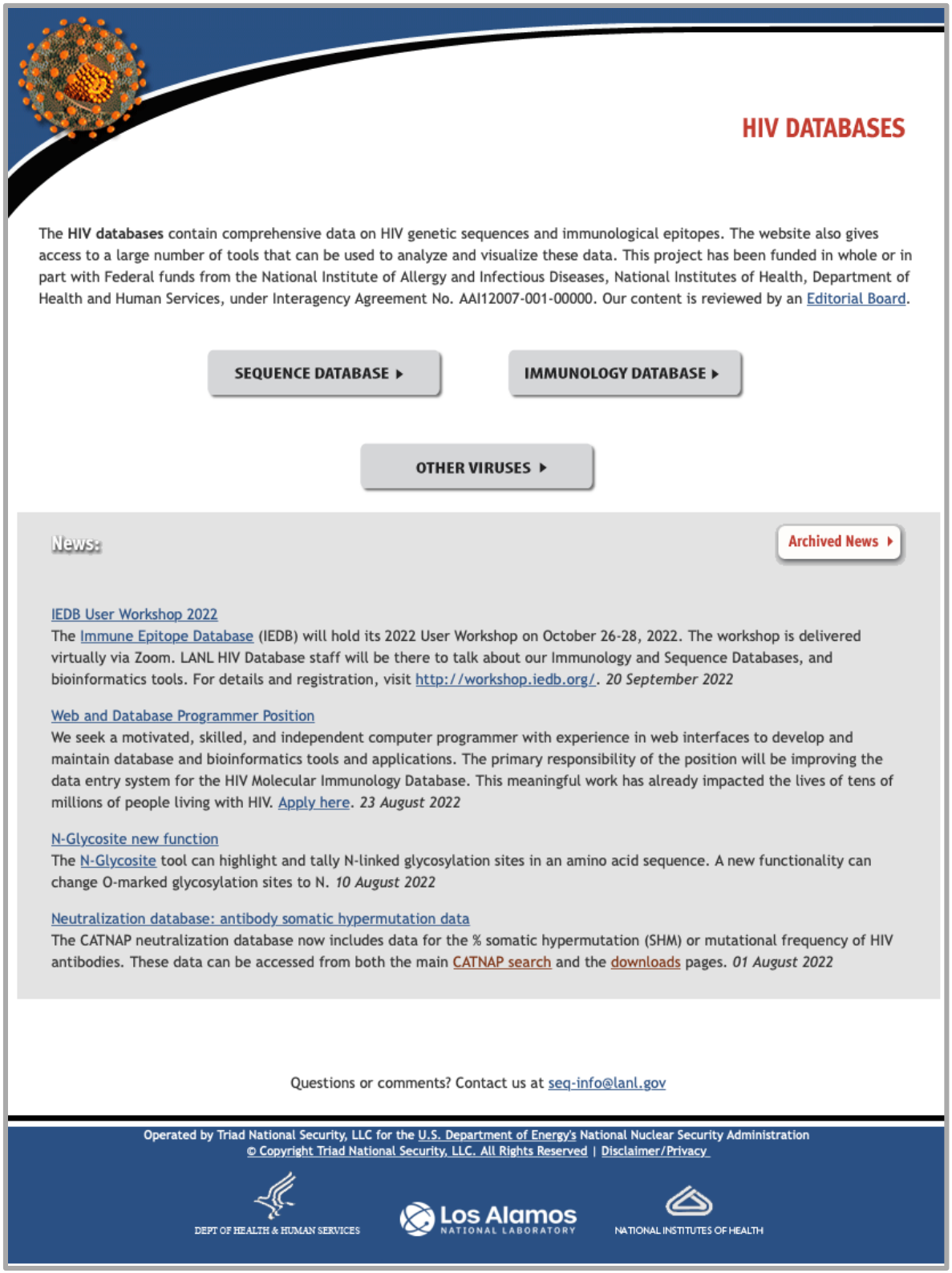
Contract Office Representative: Anjali Singh, NIAID, NIH

Theoretical Biology and Biophysics, T-6
Los Alamos National Laboratory

LA-UR-22-31269



HIV DATABASES

The **HIV databases** contain comprehensive data on HIV genetic sequences and immunological epitopes. The website also gives access to a large number of tools that can be used to analyze and visualize these data. This project has been funded in whole or in part with Federal funds from the National Institute of Allergy and Infectious Diseases, National Institutes of Health, Department of Health and Human Services, under Interagency Agreement No. AAI12007-001-00000. Our content is reviewed by an Editorial Board.

SEQUENCE DATABASE ▸

IMMUNOLOGY DATABASE ▸

OTHER VIRUSES ▸

News:

Archived News ▸

IEDB User Workshop 2022

The Immune Epitope Database (IEDB) will hold its 2022 User Workshop on October 26-28, 2022. The workshop is delivered virtually via Zoom. LANL HIV Database staff will be there to talk about our Immunology and Sequence Databases, and bioinformatics tools. For details and registration, visit http://workshop.iedb.org/. *20 September 2022*

Web and Database Programmer Position

We seek a motivated, skilled, and independent computer programmer with experience in web interfaces to develop and maintain database and bioinformatics tools and applications. The primary responsibility of the position will be improving the data entry system for the HIV Molecular Immunology Database. This meaningful work has already impacted the lives of tens of millions of people living with HIV. Apply here. *23 August 2022*

N-Glycosite new function

The N-Glycosite tool can highlight and tally N-linked glycosylation sites in an amino acid sequence. A new functionality can change O-marked glycosylation sites to N. *10 August 2022*

Neutralization database: antibody somatic hypermutation data

The CATNAP neutralization database now includes data for the % somatic hypermutation (SHM) or mutational frequency of HIV antibodies. These data can be accessed from both the main CATNAP search and the downloads pages. *01 August 2022*

Questions or comments? Contact us at seq-info@lanl.gov

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Data and Tools

Pathogen

- Sequence
- Structure
- Modifications
- Ab Epitopes (linear or discontinuous)

Host

- CTL/HTL Epitopes
- Presenting HLA
- Immune Response
- Antibodies
- Ab Neutralizations
- Ab Features/Contacts
- Patient Database

Many "HIV Immunology" tools are broadly applicable

- ***Tools list is color-coded by range of use***

HIV molecular immunology database

Databases | Search | Tools | Products | Publications | search site | Search Site

HIV Molecular Immunology Database: Tools & Links

Tools Produced by the Los Alamos HIV Databases

- CATNAP: Compile, Analyze and Tally NAb Panels Download or analyze neutralization data
- CombiNAber Predict the neutralization of combinations of antibodies
- HIV Genome Browser Display HIV genome and proteome
- QuickAlign Align amino acids or nucleotides against our alignments
- Analyze Align Show weblogos, calculate frequency by position, and find variants in an alignment
- Alignment Slicer Cut vertical slices from sequence alignments
- PeptGen Generate overlapping peptides for any protein
- PepMap Generate peptide maps in Fasta, HTML and PDF formats
- Motif Scan Scan alignments for HLA binding motifs
  - HLA genotype/serotype dictionary
  - HLA genotype/motif dictionary
  - HLA supertype dictionaries
- Hepitope Search for hopeful epitopes based on HLA enrichment
- HLA Frequency Analysis Tools Calculate HLA frequencies or HLA linkage disequilibrium in a population
- ELF Epitope location finder
- Sequence Locator Tool Find the location of any HIV/SIV sequence
- SeqPublish Produce pretty alignments for publication
- Heatmap Display a table of numbers using colors to represent the numerical values
- Epigraph Vaccine Suite Design and assess Epigraphs for vaccine design
- Mosaic Vaccine Suite Design and assess polyvalent protein sequences for T-cell vaccines
- N-Glycosite Find N-linked glycosylation sites
- Highlighter Highlight matches and mismatches in a set of aligned sequences
- Protein Feature Accent View 3D graphics of HIV proteins
- Variable Region Characteristics analyzes Env variable loops and reports length, glycosolations, and net charge

- Tools specific for HIV/SIV
- General use tools with some HIV/SIV-specific features
- General use tools

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HIV Immunology Database - 2022 Additions

Continuing Efforts

- Curated annotations
- Maintained and updated tools, maps and tables
- Updated Help pages
- Published annual compendium

Upgrades

- Expanded and searchable patient database, linked Seq and Immuno Patient Codes and Database IDs
- HLA nomenclature updated further, consistent with 2022 HLA update
- Somatic hypermutation data added to Neutralization DB (=CATNAP)
- API for JSON and CSV download capability expanded

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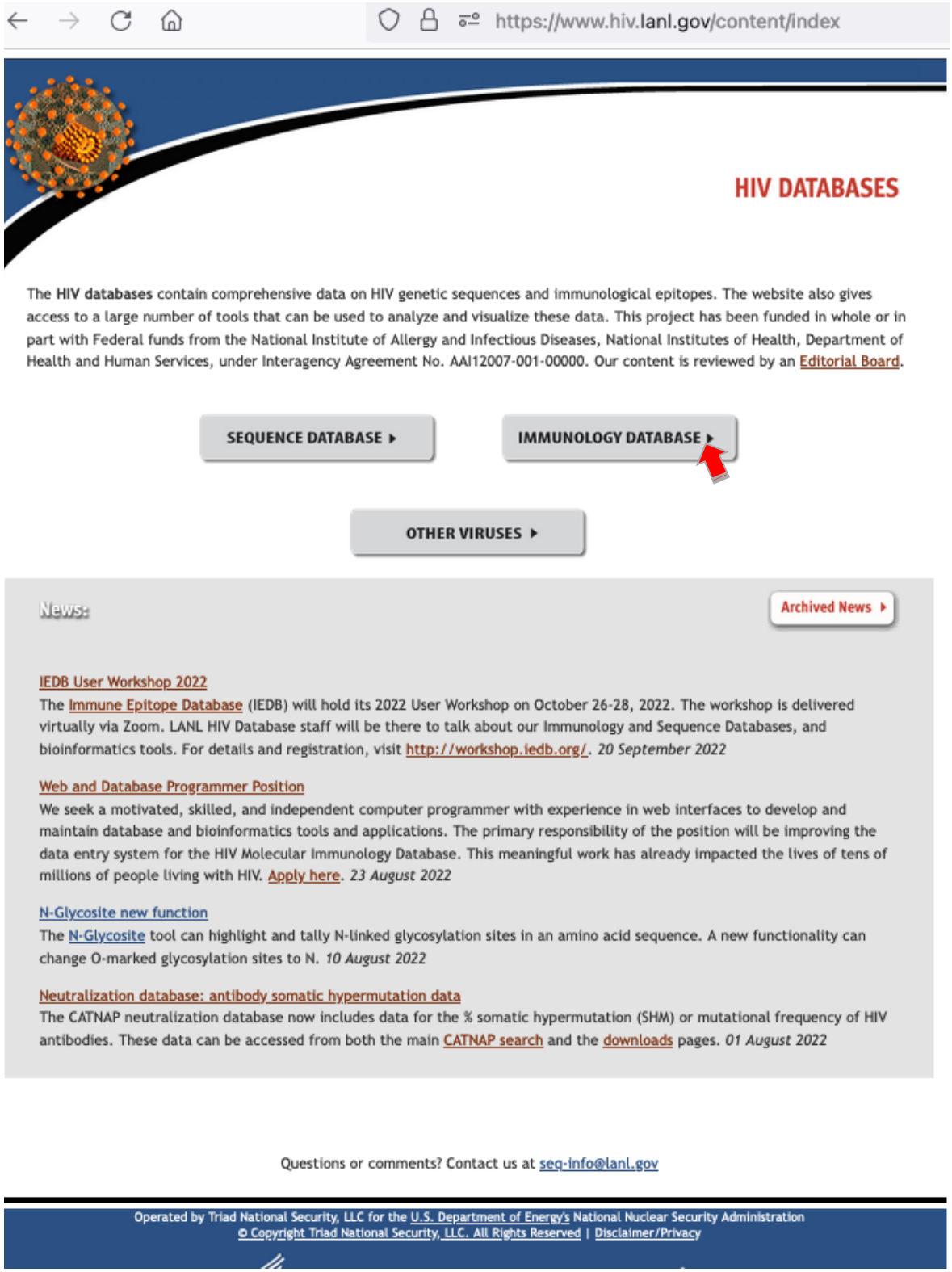

https://hiv.lanl.gov/

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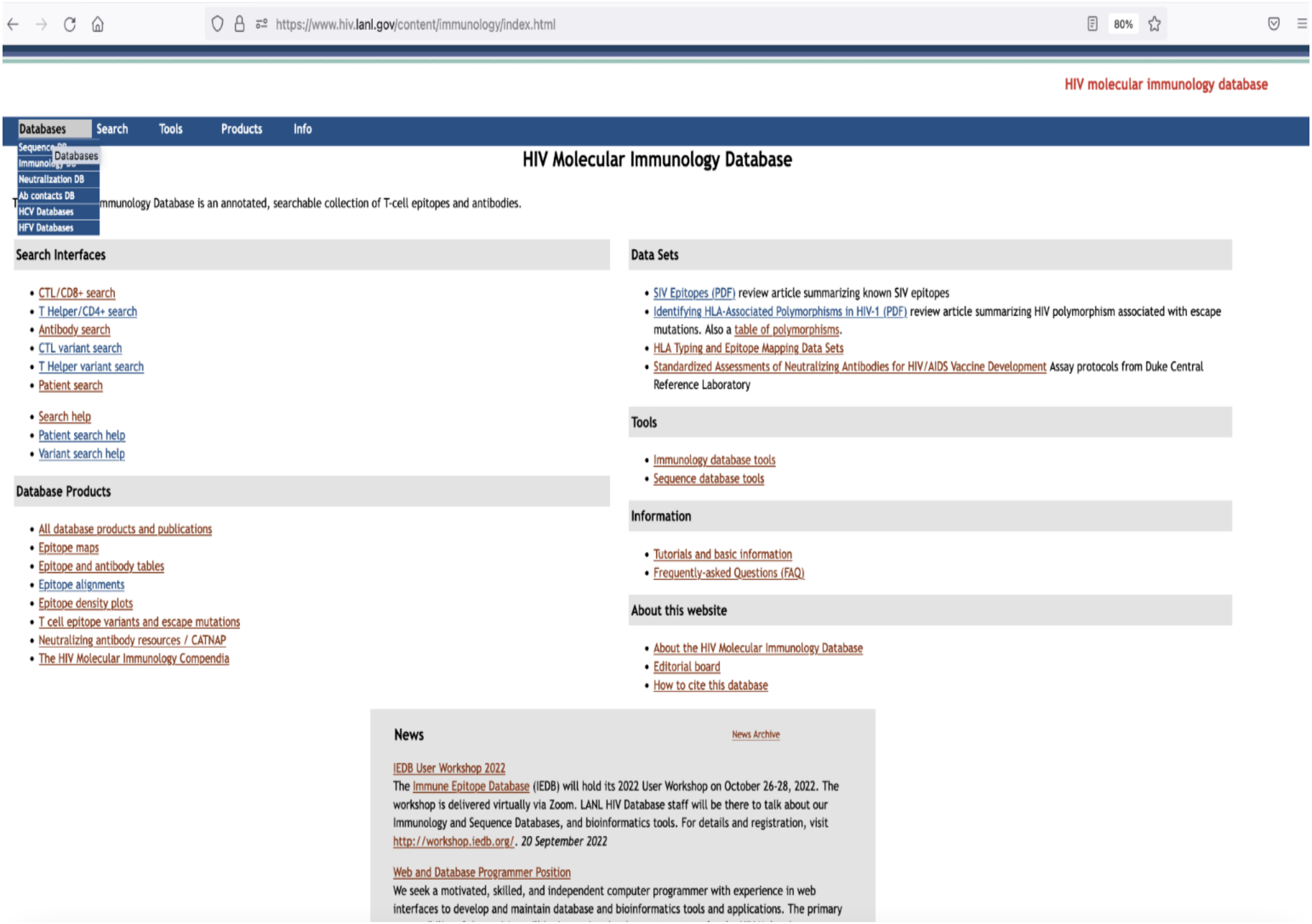

https://www.hiv.lanl.gov/content/immunology/index.html

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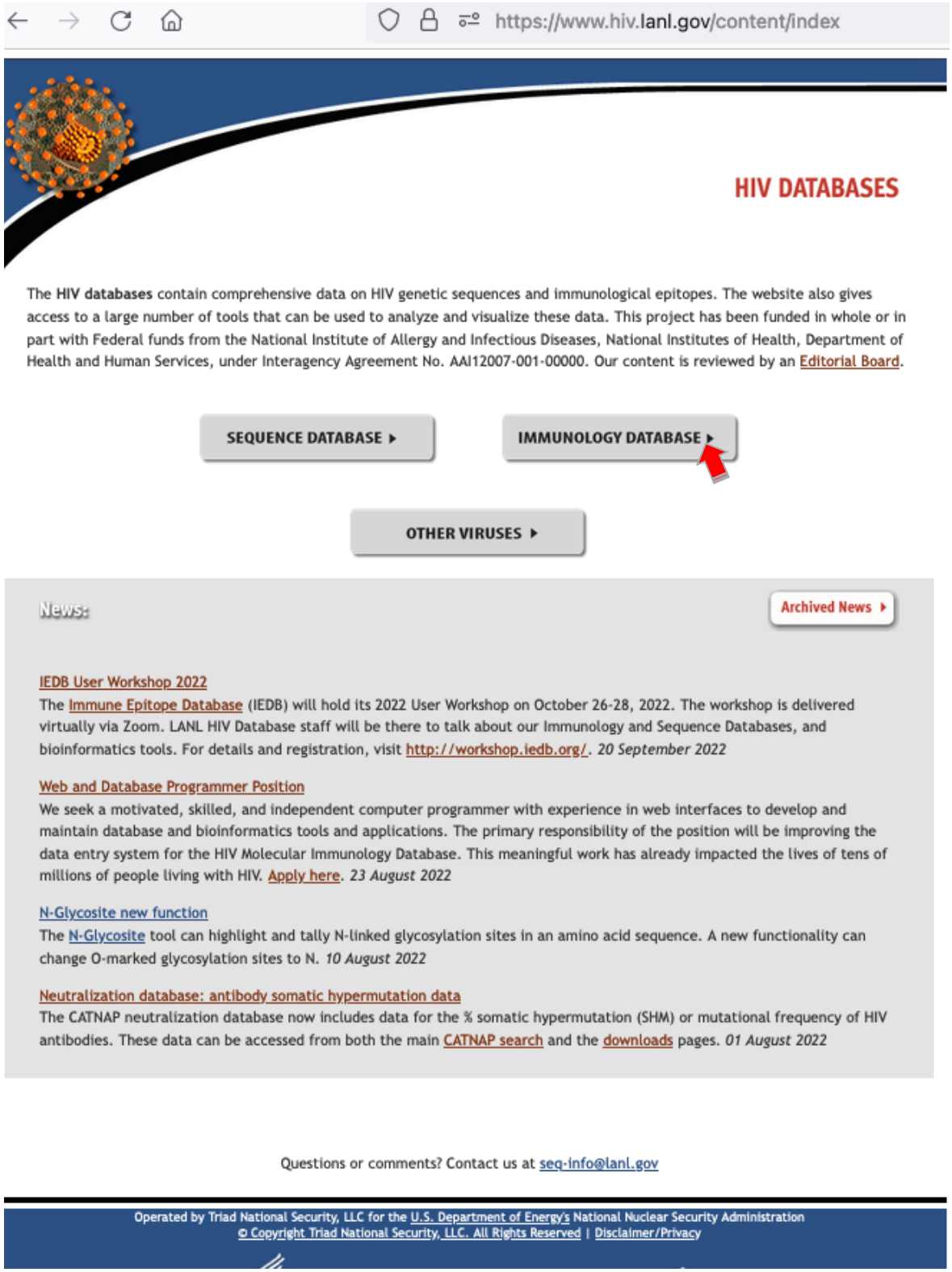
Rapid Epitope Searches - and Sequential

- Linear Antibody Epitope Search
- Use of HIV Genome Browser Tool
- Find overlapping Helper/HTL Epitopes
- Overlapping CTL Epitope Search
- Discontinuous Antibody Epitope Searches



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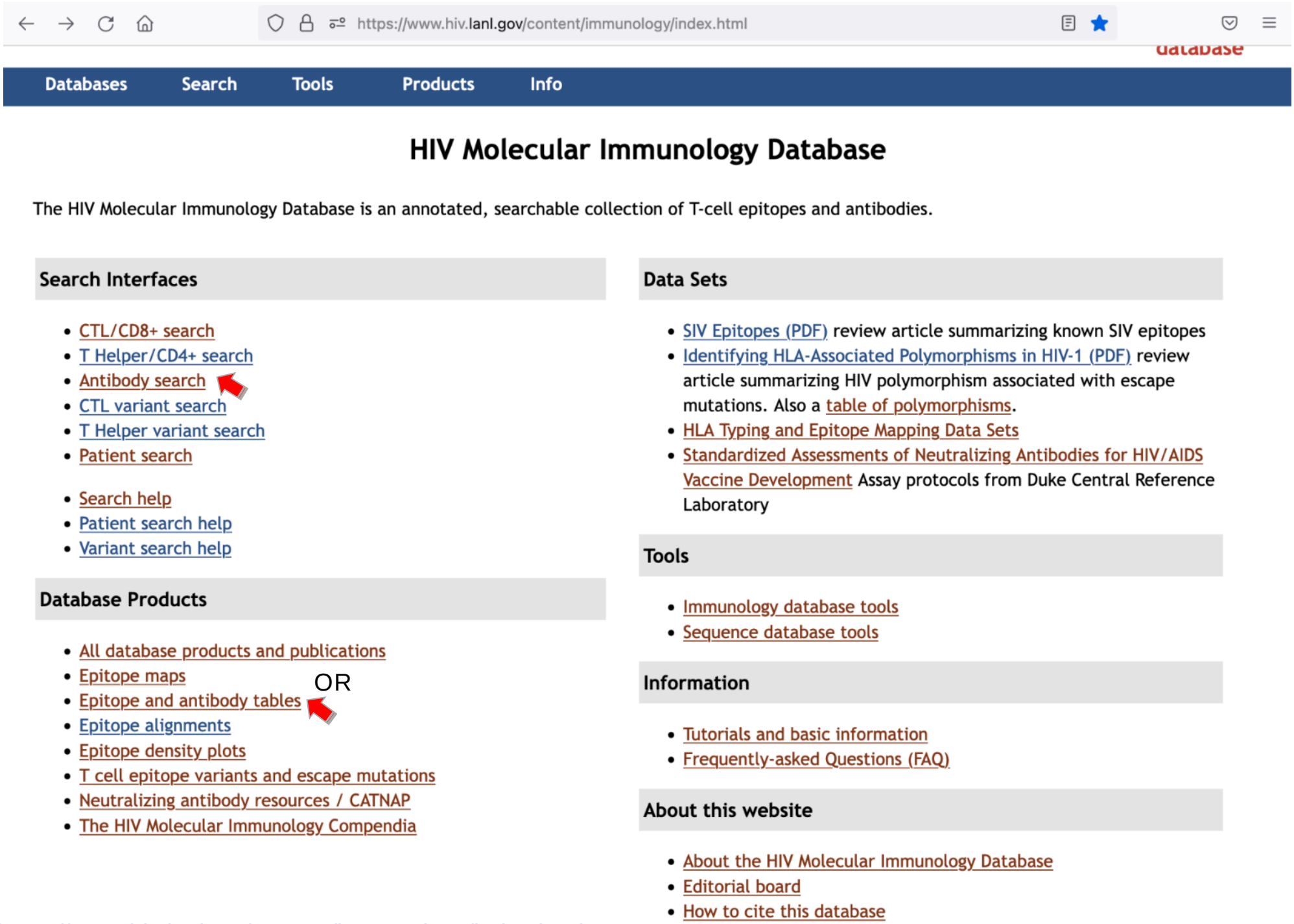
Linear Antibody Epitope Search



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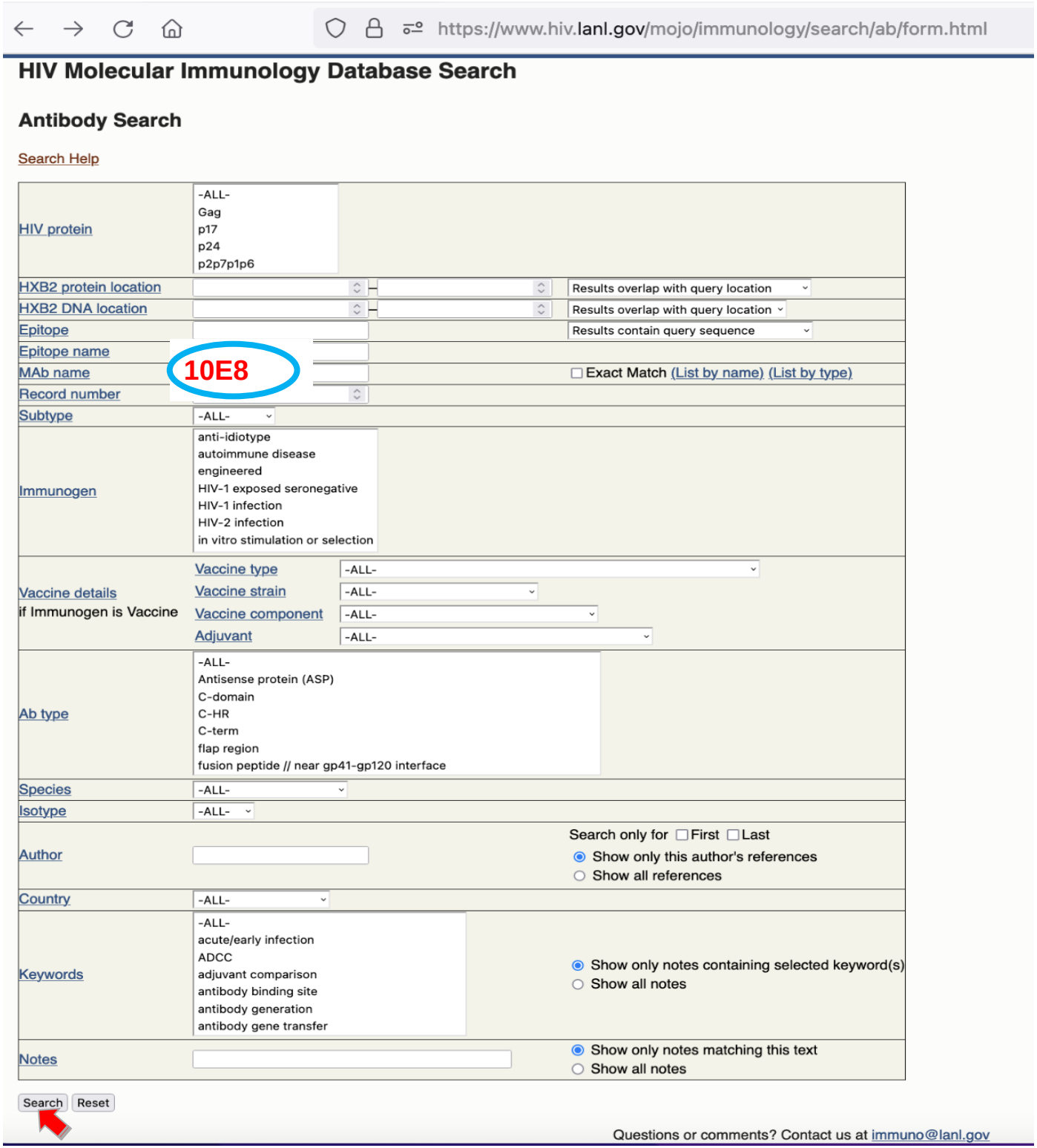

https://www.hiv.lanl.gov/mojo/immunology/search/ab/form.html

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Genbank Accession K03455.1

https://www.hiv.lanl.gov/mojo/immunology/search/ab/results?start=&end=&range_span=ove 80%

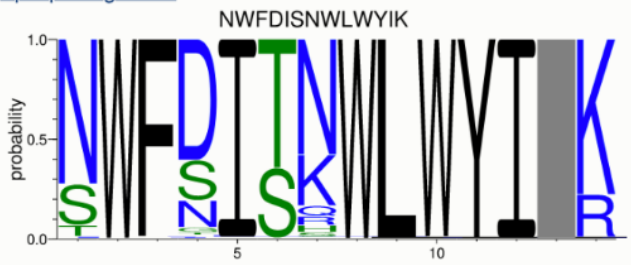
Displaying record number 2708

Download this epitope record as JSON. [Help]

MAb name	10E8
HXB2 location	gp160(671–683)
Author location	DNA(8235..8273)
Epitope	NWFDISNWLWYIK
Subtype	B
Ab type	gp41 MPER (membrane proximal external region)
Neutralizing	P (tier 2)
Contacts and Features	View contacts and features
Species (Isotype)	human(IgG3)
Immunogen	HIV-1 infection
Patient MHC/HLA	Donor N152:
Keywords	ADCC, antibody binding site, antibody generation, antibody interactions, assay or method development, autoantibody or autoimmunity, glycosylation, immunoprophylaxis, neutralization, vaccine antigen design, variant cross-reactivity, viral fitness and reversion, vaccine-induced immune responses, computational epitope prediction, acute/early infection, binding affinity, immunotherapy, mother-to-infant transmission, review, subtype comparisons, antibody sequence, structure, antibody gene transfer, antibody lineage, antibody polyreactivity, bispecific/trispecific, broad neutralizer, chimeric antibody, contact residues, transmission pair

gp160 Epitope Map

Epitope Alignment



View neutralization details

Notes

Showing 73 of 73 notes.

- 10E8: A novel antibody was isolated from donor CAP248, who first developed cross-neutralizing antibodies after about 1 year of infection. The neutralization breadth of CAP248-2B, isolated from a sample taken 3.5 years post-infection, largely recapitulates the donor's serum breadth, and was able to neutralize 22% of a panel of cross-clade viruses at IC_{20}. CAP248-2B was predicted to be derived from germline genes IGHV4-31*05, IGHD6-13*01, IGHJ3*01/02, IGLV2-14*01, and IGLJ1*01. The crystal structure suggested binding of the unusually long 19aa light chain of the paratope to both the C terminus of gp120 and to parts of gp41. The gp160 cleavage site was also the site of unusual escape mutations in the donor's viral

https://www.hiv.lanl.gov/mojo/immunology/search/ab/results?

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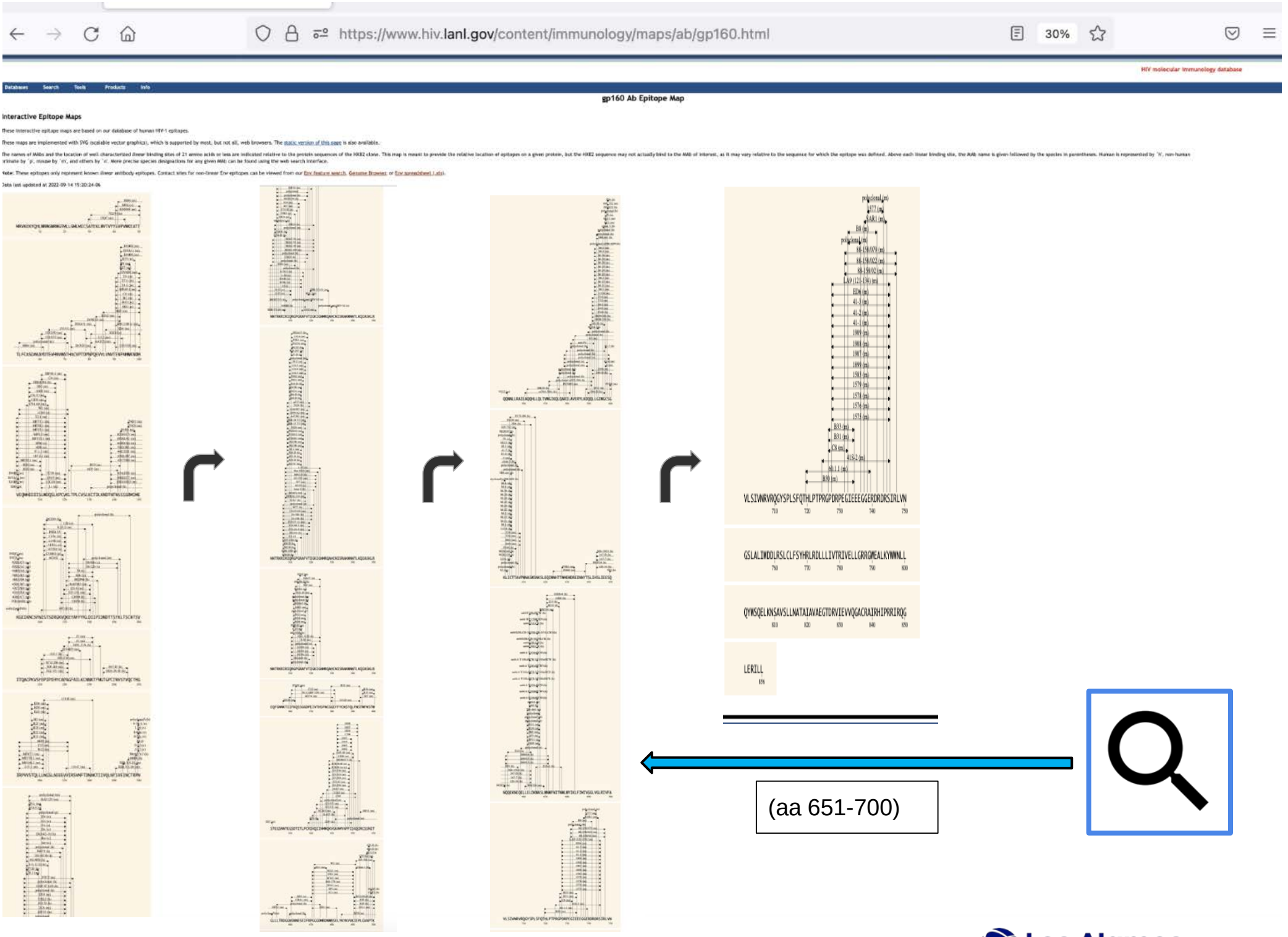

https://www.hiv.lanl.gov/content/immunology/maps/ab/gp160.html

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https://www.hiv.lanl.gov/content/immunology/maps/ab/gp160.html

gp160 Ab Epitope Map

Interactive Epitope Maps

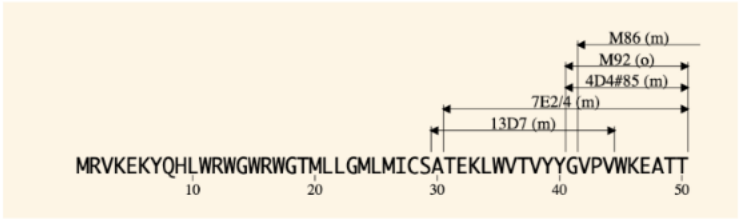
These interactive epitope maps are based on our database of human HIV-1 epitopes.

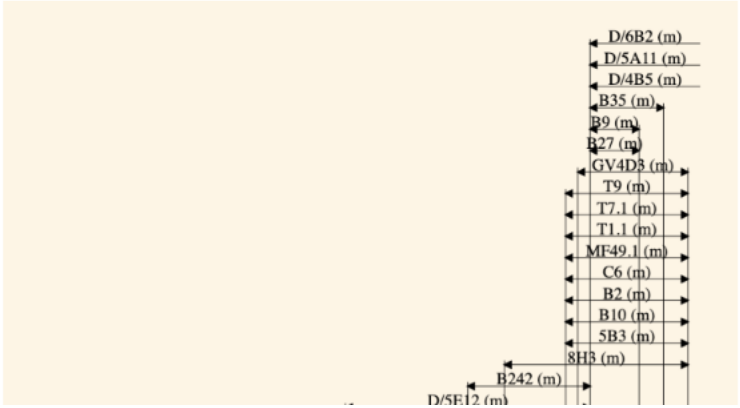
These maps are implemented with SVG (scalable vector graphics), which is supported by most, but not all, web browsers. The static version of this page is also available.

The names of MAbs and the location of well characterized *linear* binding sites of 21 amino acids or less are indicated relative to the protein sequences of the HXB2 clone. This map is meant to provide the relative location of epitopes on a given protein, but the HXB2 sequence may not actually bind to the MAb of interest, as it may vary relative to the sequence for which the epitope was defined. Above each linear binding site, the MAb name is given followed by the species in parentheses. Human is represented by `h', non-human primate by `p', mouse by `m', and others by `o'. More precise species designations for any given MAb can be found using the web search interface.

Note: These epitopes only represent known *linear* antibody epitopes. Contact sites for non-linear Env epitopes can be viewed from our Env feature search, Genome Browser, or Env spreadsheet (.xls).

Data last updated at 2022-09-14 15:20:24-06





From Linear Ab Epitope Search to HIV Genome Browser

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https://www.hiv.lanl.gov/content/immunology/maps/ab/gp160.html

https://www.hiv.lanl.gov/content/sequence/genome_browser/browser.html

HIV sequence database

DATABASES SEARCH ALIGNMENTS TOOLS PUBLICATIONS INFO

HIV GENOME BROWSER TOOL

HIV Genome Browser

Purpose: Interactive view of the HIV genome and proteome for juxtaposition and exploration of multiple types of data. Help.

Starting Views

NOTE: These are just starting points! Within the genome browser, you can move among any of these views. Please read the quick tips and Help file before you start!

HIV-1 protein-level views:

▪ Env ▪ Gag ▪ Nef ▪ Pol ▪ Rev ▪ Tat ▪ Vif ▪ Vpr ▪ Vpu

HIV-1 protein-specific examples:

- Env with CTL epitopes + entropy
- Pol with drug resistance sites + entropy

Nucleotide-level views:

- HIV-1 gene map
- SIV Mac239 gene map
- HIV-1 5' LTR

Quick Tips

- Mouseovers! Look for mouseovers to guide you.
- Click and right-click! Features link to loads of information and analysis via click and right-click. If your mouse doesn't have right-click, use Ctrl-click.
- Zoom! There are several ways to zoom in/out. Some features can only be seen when zoomed-in or zoomed-out.
- For details about this interface, see HIV Genome Browser Help.
- Watch the screencast video on the JBrowse website.

References

- Skinner ME, Holmes IH. Setting up the JBrowse genome browser. Curr Protoc Bioinformatics. 2010 Dec;Chapter 9:Unit 9.13. PMID: 21154710
- Skinner ME, Uzilov AV, Stein LD, Mungall CJ, Holmes IH. JBrowse: a next-generation genome browser. Genome Res. 2009 Sep;19(9):1630-8. PMID: 19570905

https://www.hiv.lanl.gov/content/sequence/genome_browser/browser.html

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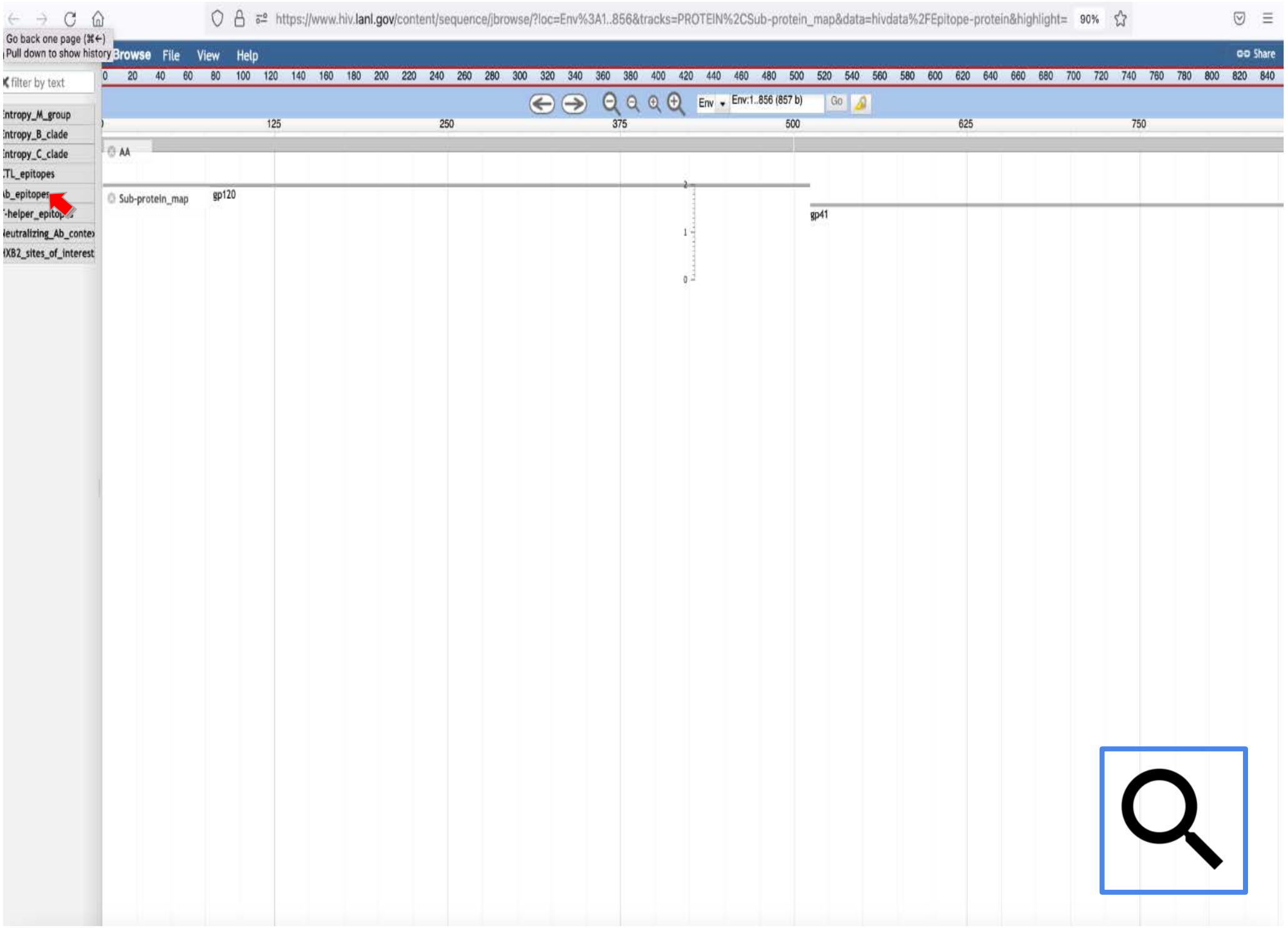

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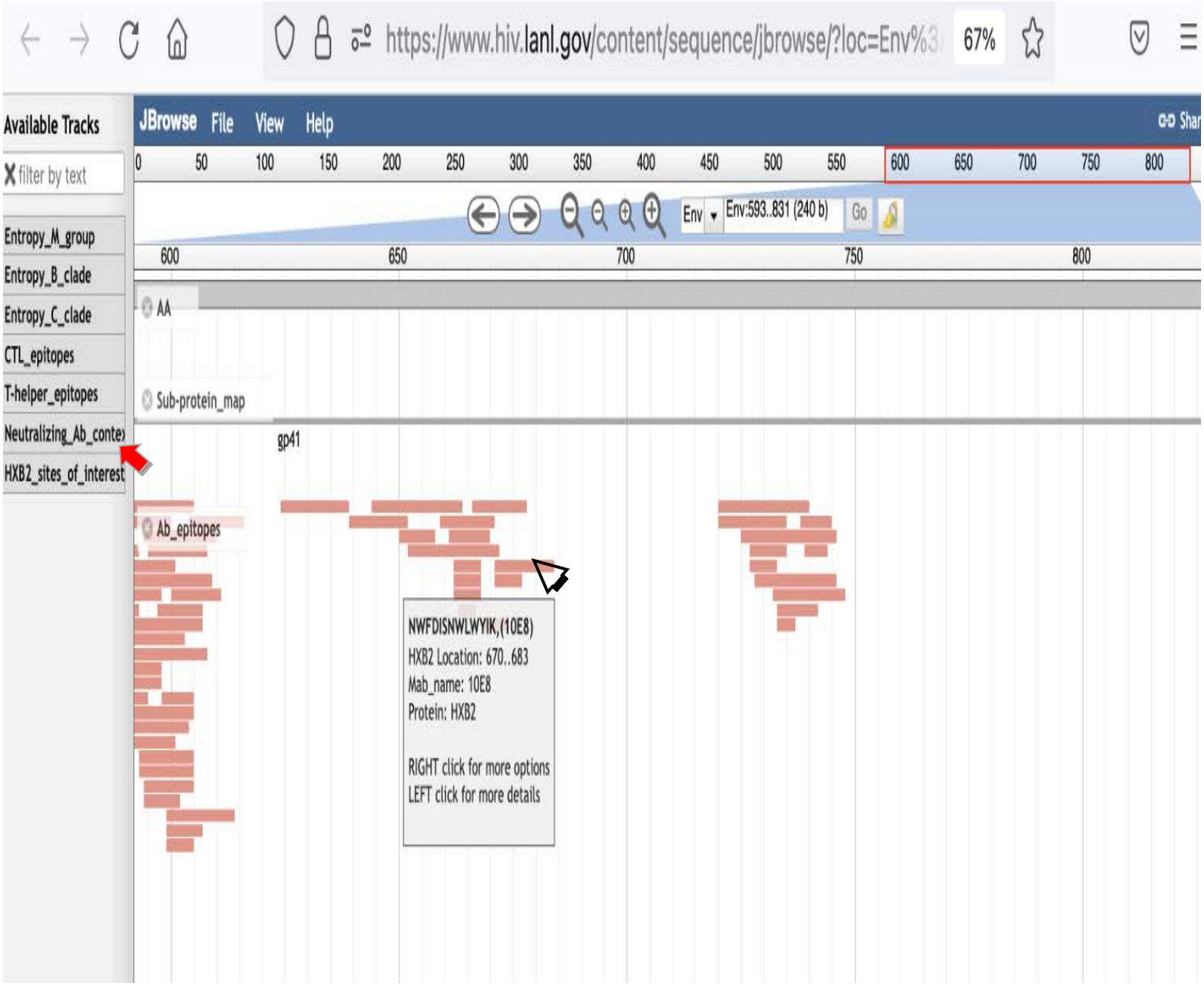

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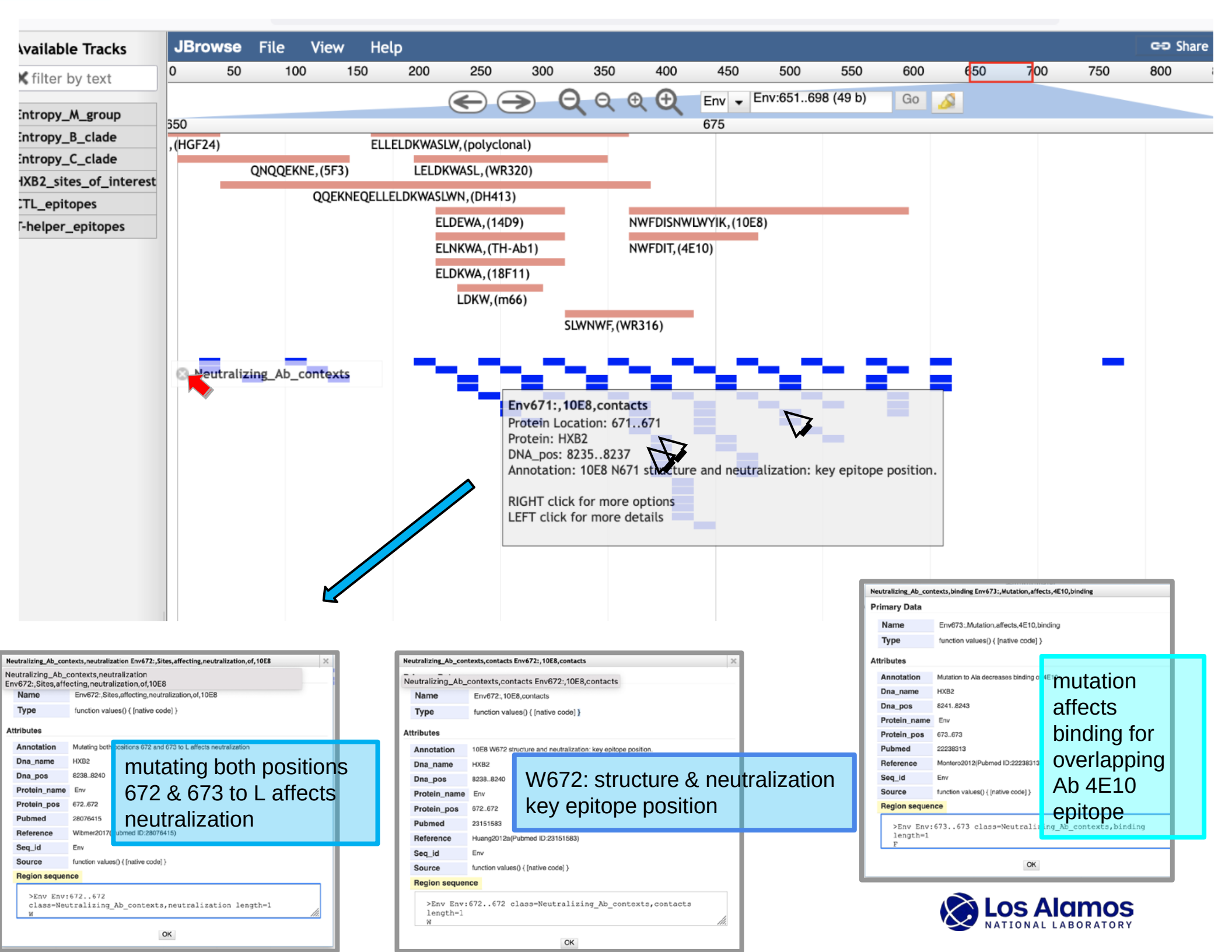
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Entropy_M_group
Entropy_B_clade
Entropy_C_clade
HXB2_sites_of_interest
CTL_epitopes
T-helper_epitopes
JBrowse
File
View
Help
Share
0
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
Env
Env:651..698 (49 b)
Go
650
675
,(HGF24)
ELLELDKWASLW,(polyclonal)
QNQQEKNE,(5F3)
LELDKWASL,(WR320)
QQEKNEQELLELDKWASLWN,(DH413)
ELDEWA,(14D9)
NWFDISNWLWYIK,(10E8)
ELNKWA,(TH-Ab1)
NWFDIT,(4E10)
ELDKWA,(18F11)
LDKW,(m66)
SLWNWF,(WR316)
Neutralizing_Ab_contexts
Env671:,10E8,contacts
Protein Location: 671..671
Protein: HXB2
DNA_pos: 8235..8237
Annotation: 10E8 N671 structure and neutralization: key epitope position.
RIGHT click for more options
LEFT click for more details
Neutralizing_Ab_contexts,neutralization Env672:,Sites,affecting,neutralization,of,10E8
Name
Env672:,Sites,affecting,neutralization,of,10E8
Type
function values() { [native code] }
Attributes
Annotation
Mutating both positions 672 and 673 to L affects neutralization
Dna_name
HXB2
Dna_pos
8238..8240
Protein_name
Env
Protein_pos
672..672
Pubmed
28076415
Reference
Wibmer2017(Pubmed ID:28076415)
Seq_id
Env
Source
function values() { [native code] }
Region sequence
>Env Env:672..672
class=Neutralizing_Ab_contexts,neutralization length=1
W
OK
mutating both positions 672 & 673 to L affects neutralization
Neutralizing_Ab_contexts,contacts Env672:,10E8,contacts
Name
Env672:,10E8,contacts
Type
function values() { [native code] }
Attributes
Annotation
10E8 W672 structure and neutralization: key epitope position.
Dna_name
HXB2
Dna_pos
8238..8240
Protein_name
Env
Protein_pos
672..672
Pubmed
23151583
Reference
Huang2012a(Pubmed ID:23151583)
Seq_id
Env
Source
function values() { [native code] }
Region sequence
>Env Env:672..672 class=Neutralizing_Ab_contexts,contacts
length=1
W
OK
W672: structure & neutralization key epitope position
Neutralizing_Ab_contexts,binding Env673:,Mutation,affects,4E10,binding
Primary Data
Name
Env673:,Mutation,affects,4E10,binding
Type
function values() { [native code] }
Attributes
Annotation
Mutation to Ala decreases binding
Dna_name
HXB2
Dna_pos
8241..8243
Protein_name
Env
Protein_pos
673..673
Pubmed
22238313
Reference
Montero2012(Pubmed ID:22238313
Seq_id
Env
Source
function values() { [native code] }
Region sequence
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OK
mutation affects binding for overlapping Ab 4E10 epitope
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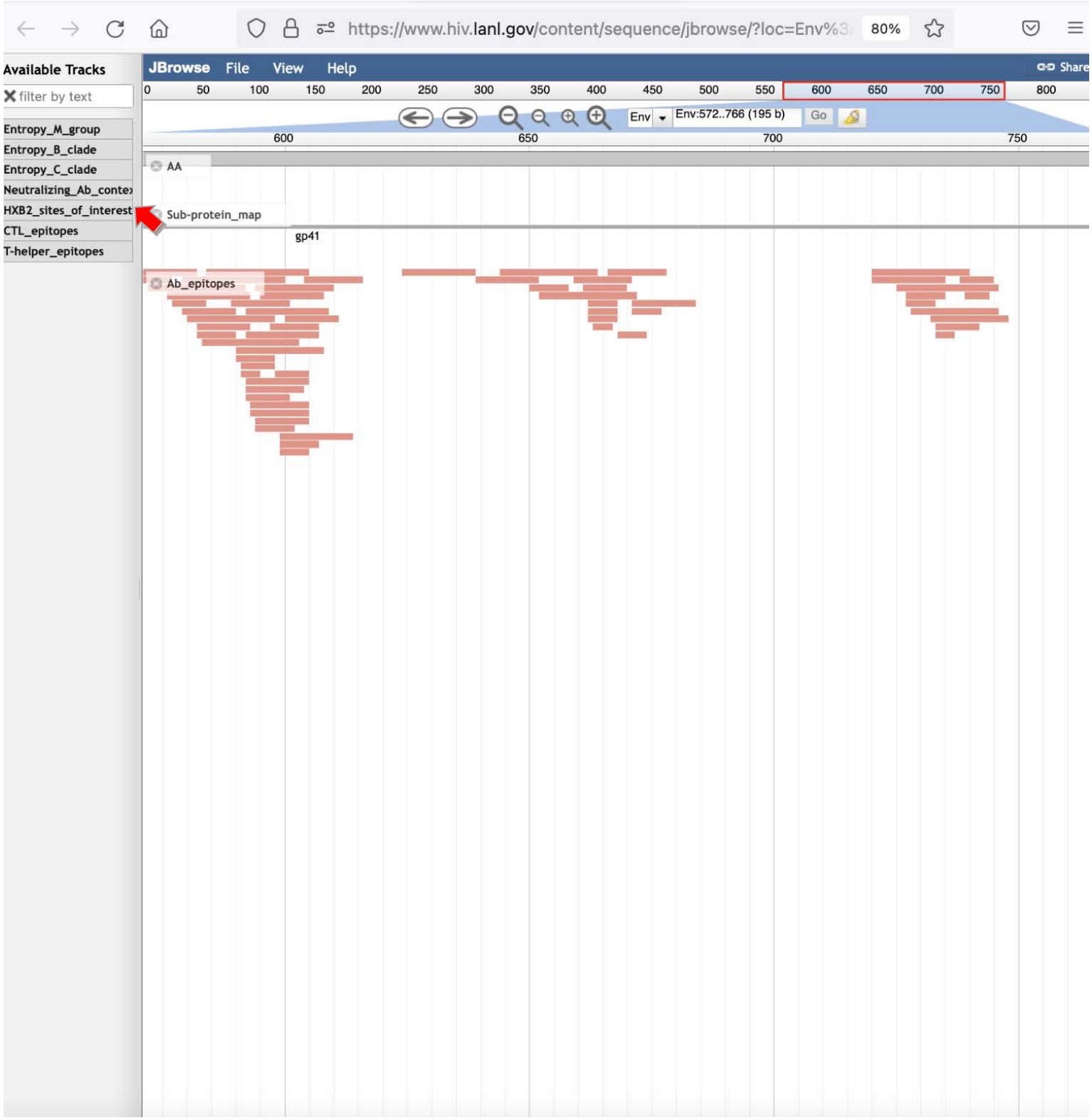

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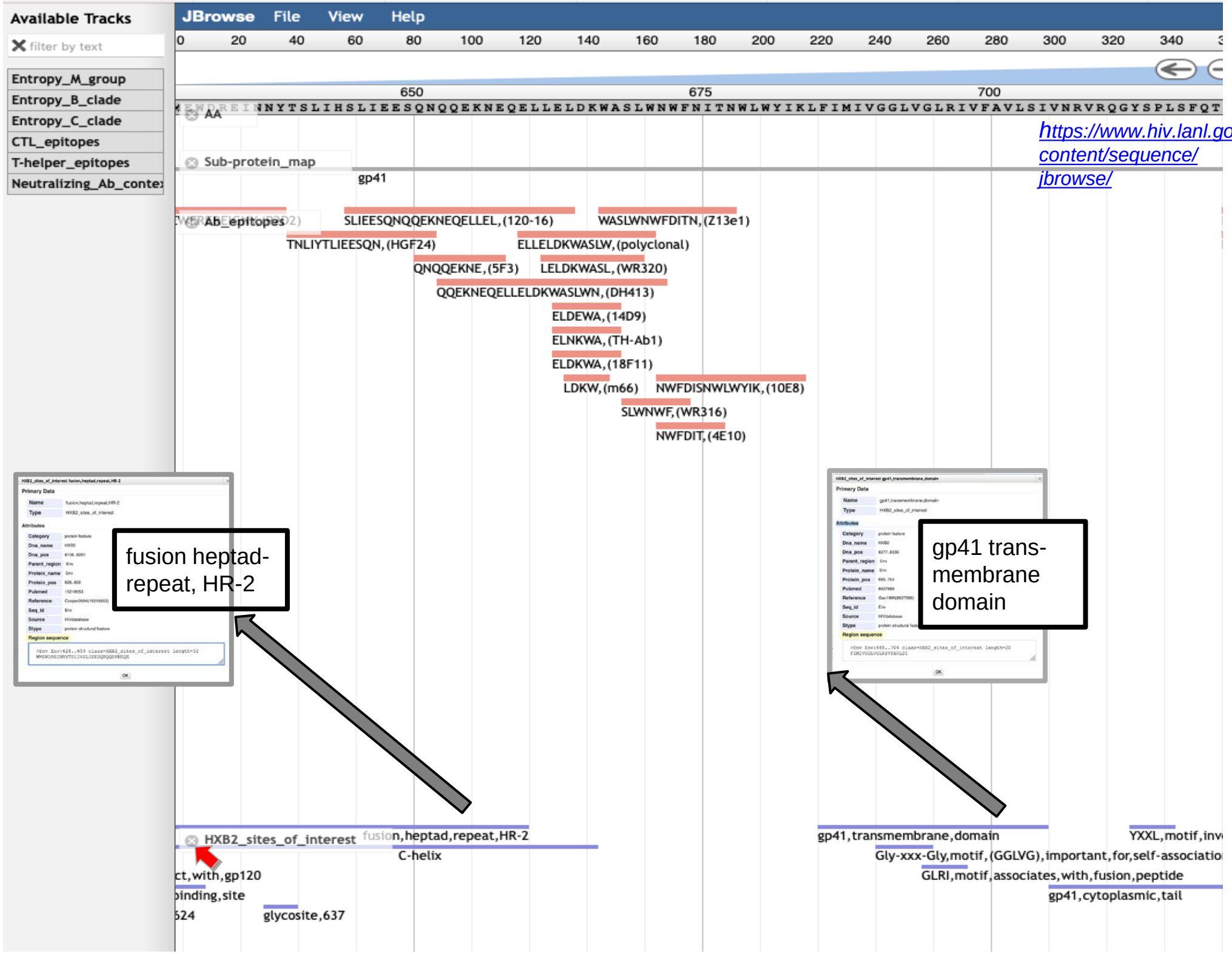
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Entropy_M_group
Entropy_B_clade
Entropy_C_clade
CTL_epitopes
T-helper_epitopes
Neutralizing_Ab_contex
JBrowse
File
View
Help
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AA
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gp41
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ELNKWA, (TH-Ab1)
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LDKW, (m66)
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SLWNWF, (WR316)
NWFDIT, (4E10)
https://www.hiv.lanl.gov/content/sequence/jbrowse/
fusion heptad-repeat, HR-2
gp41 trans-membrane domain
HXB2_sites_of_interest
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C-helix
gp41,transmembrane,domain
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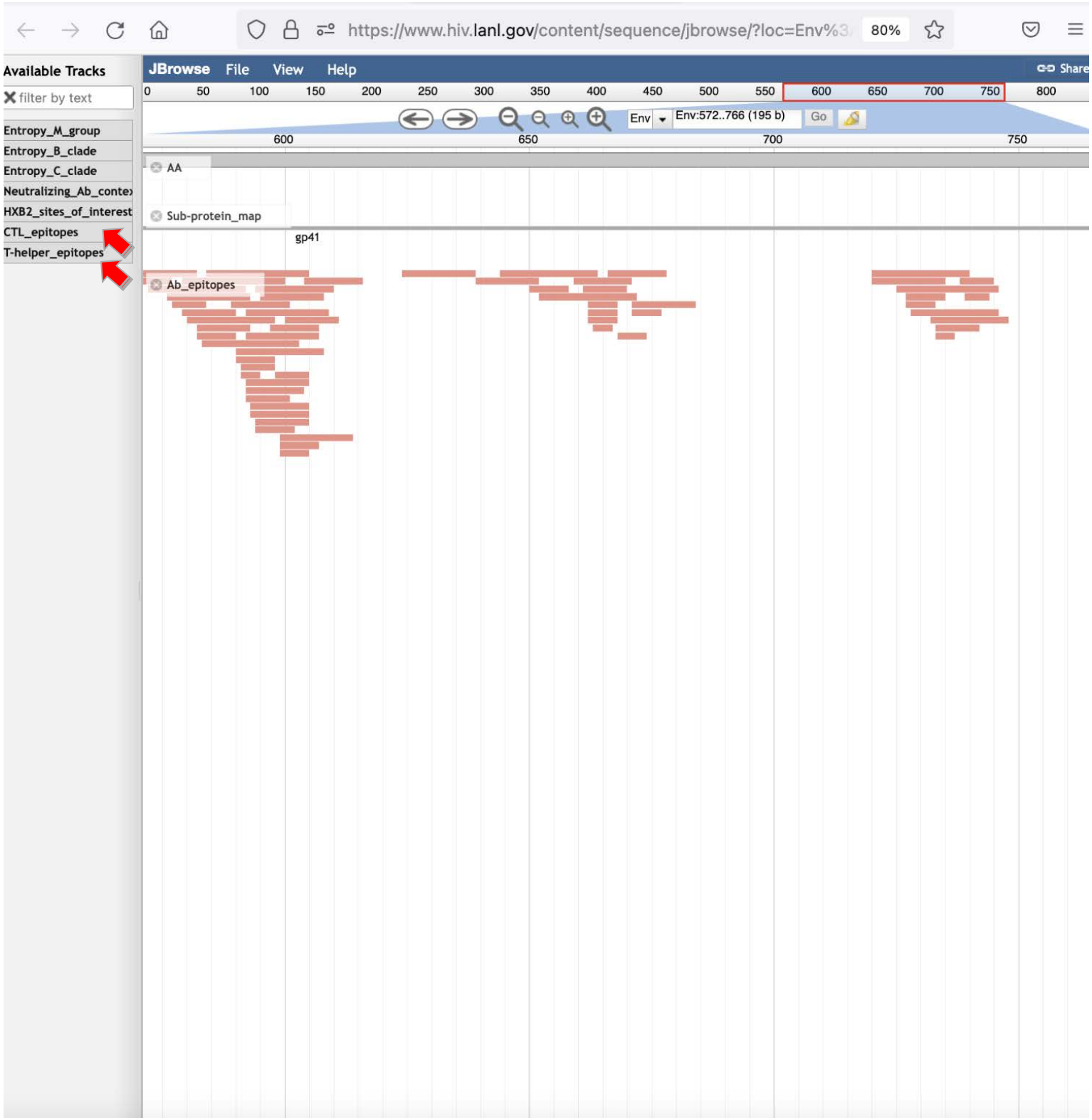

Overlapping HTL and CTL Epitopes ??

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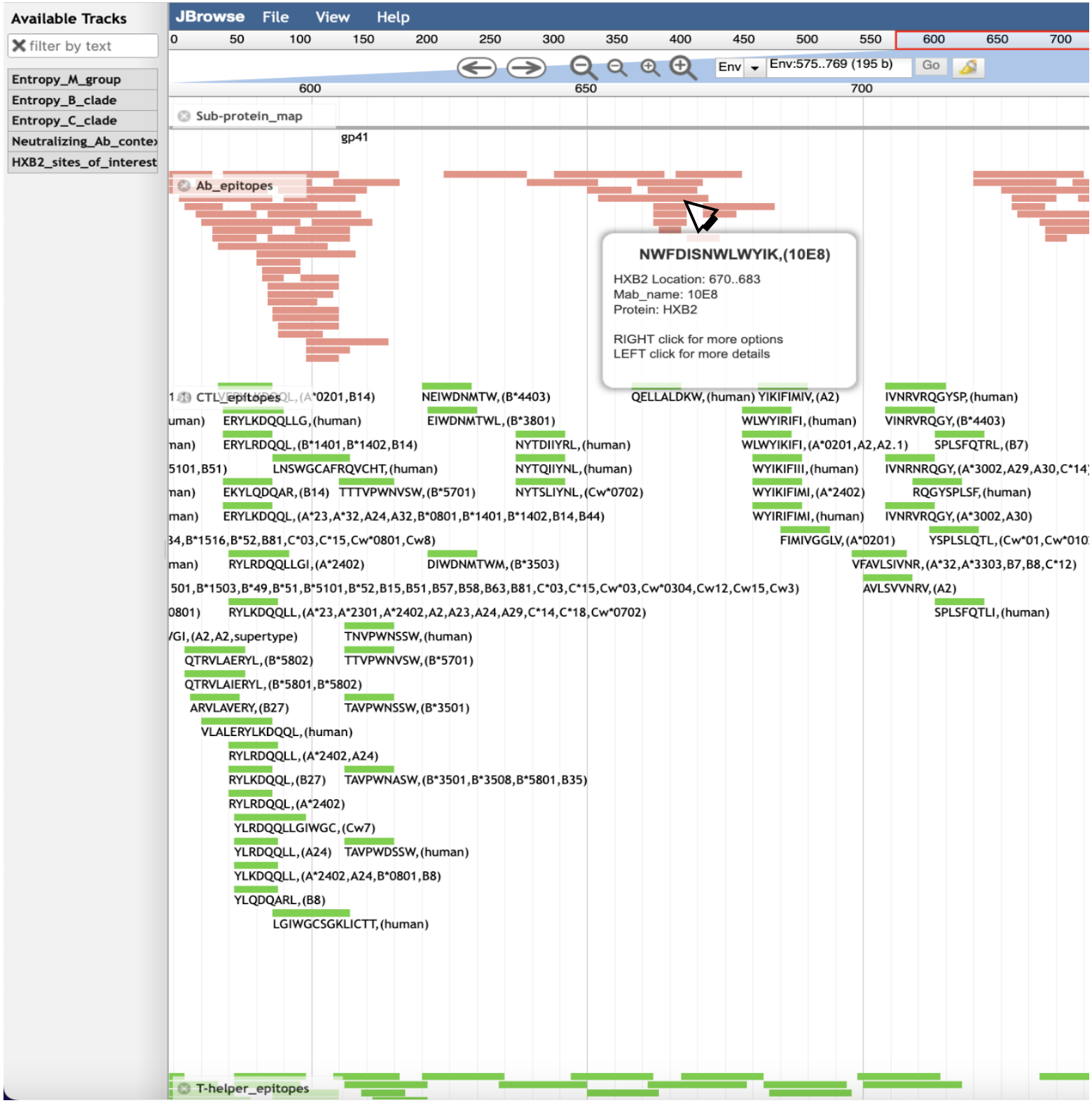

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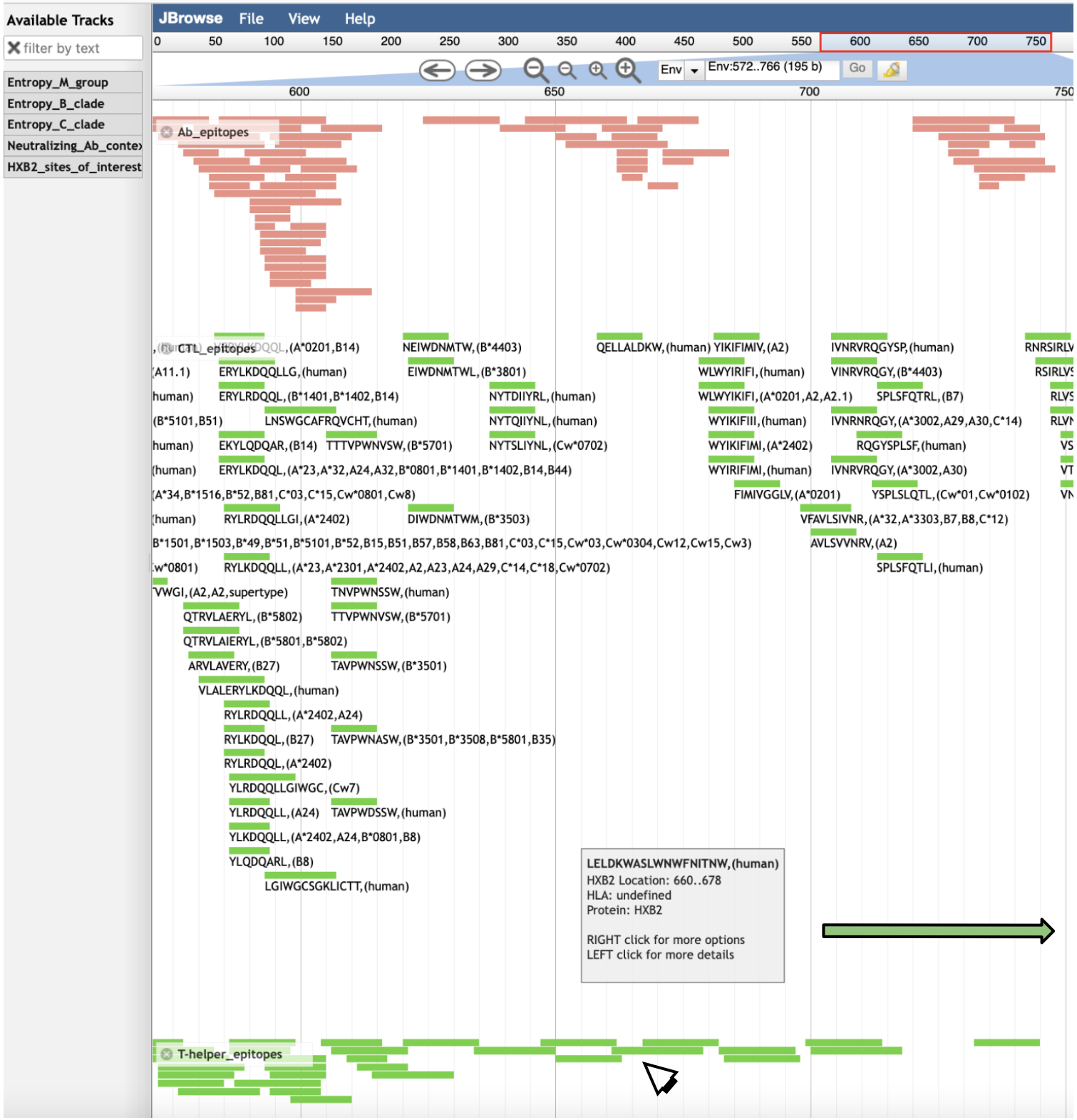
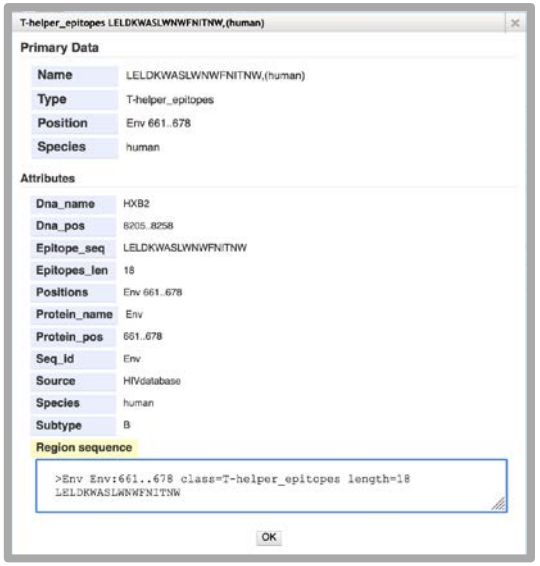


Overlapping HTL Epitope



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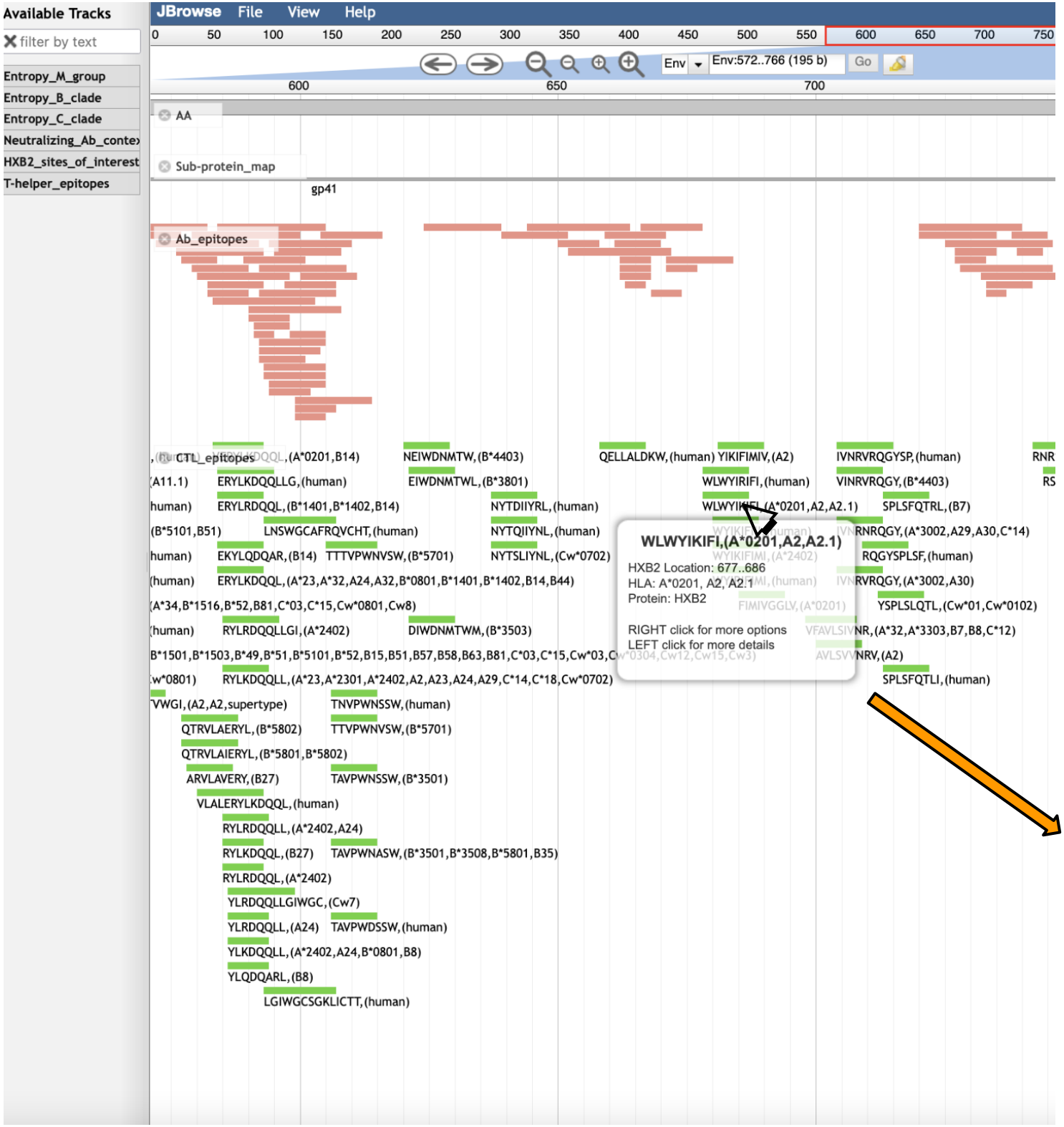
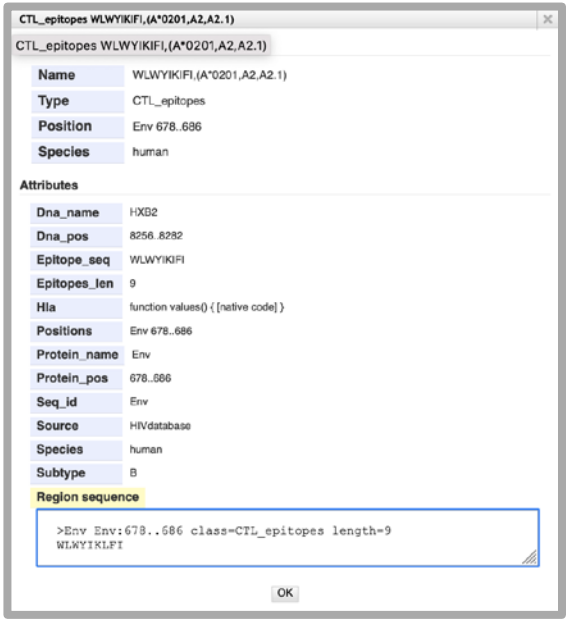


Overlapping CTL Epitope



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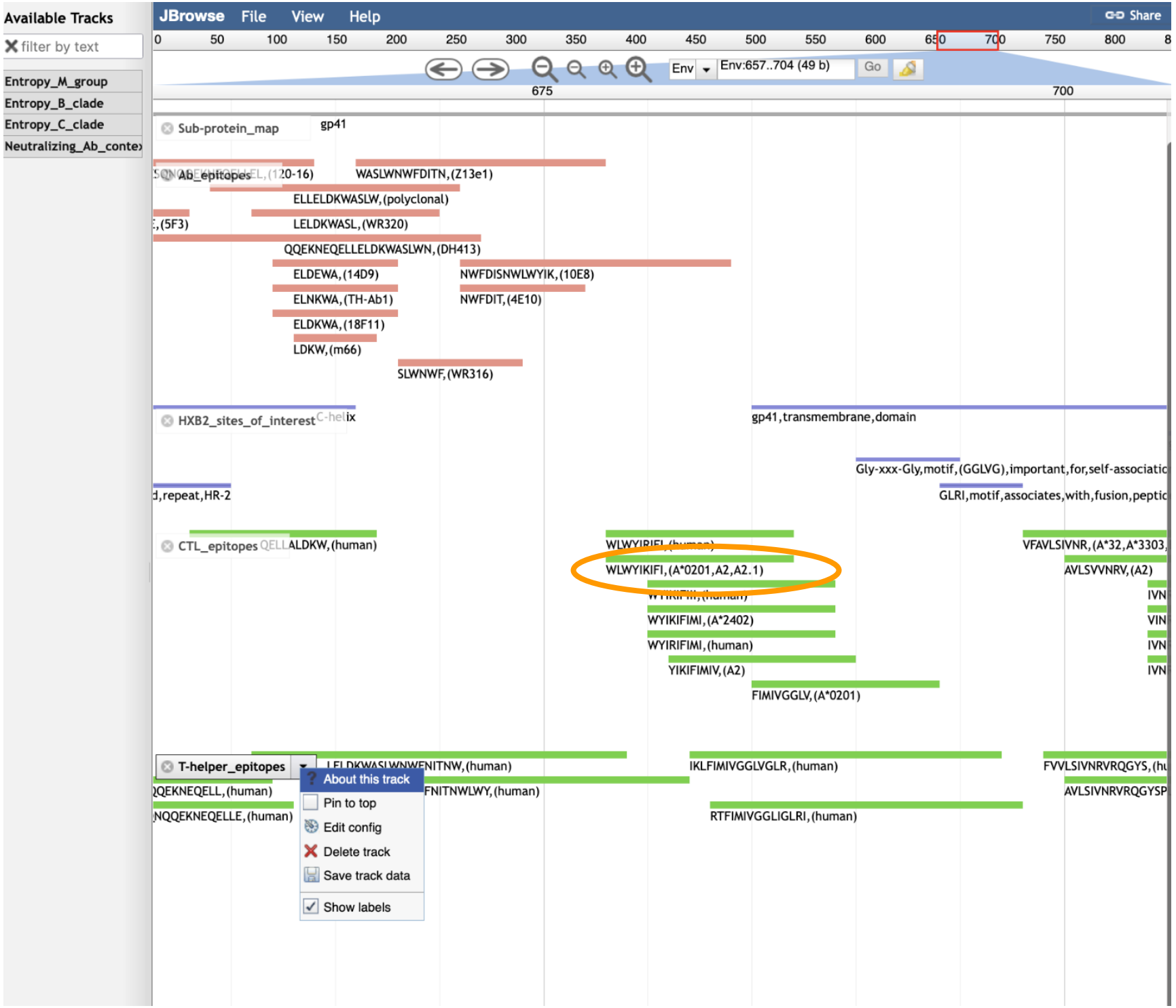
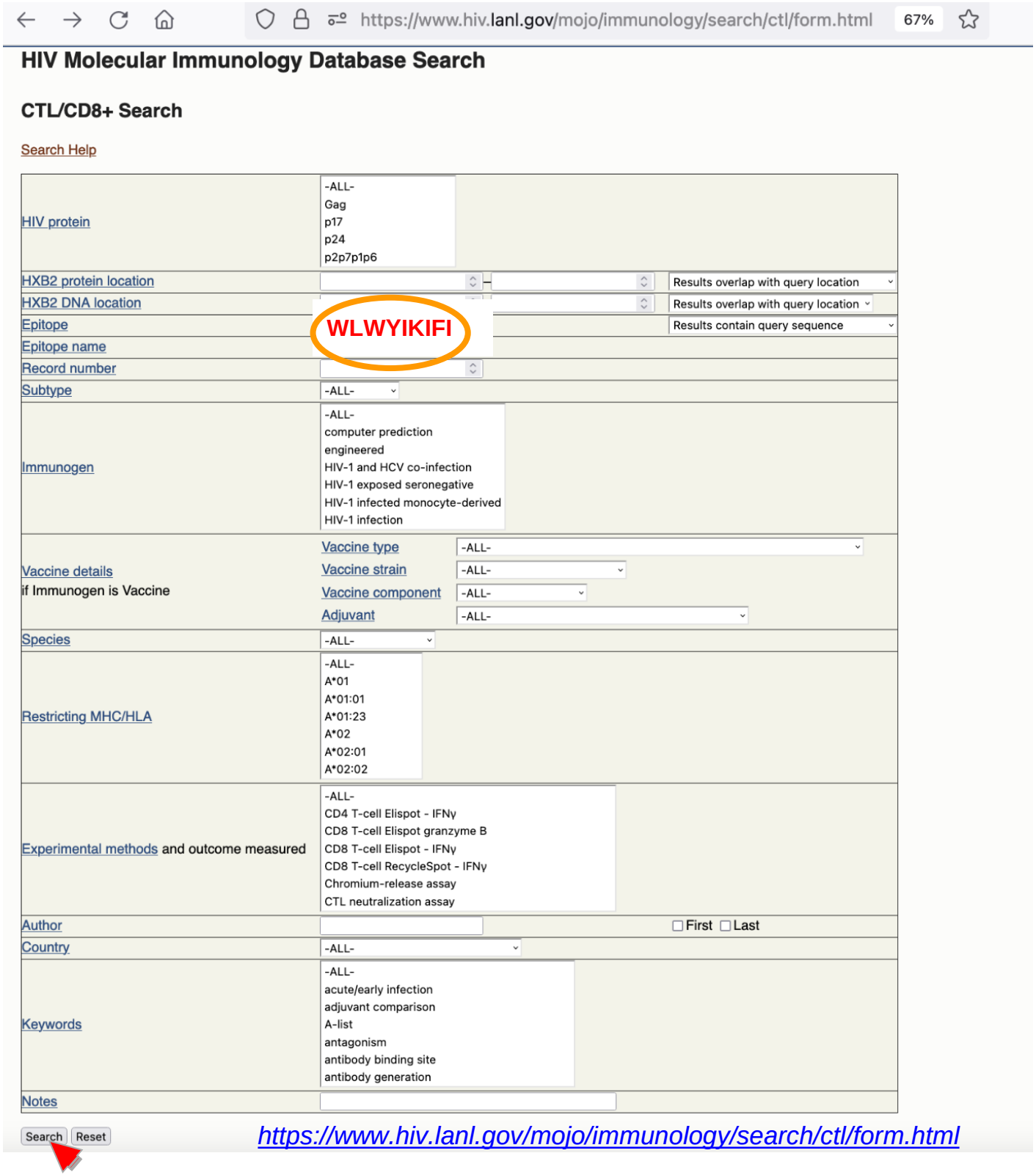


Los Alamos NATIONAL LABORATORY



Search for CTL Epitope

https://www.hiv.lanl.gov/mojo/immunology/search/ctl/form.html

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https://www.hiv.lanl.gov/mojo/immunology/search/ctl/results 80%

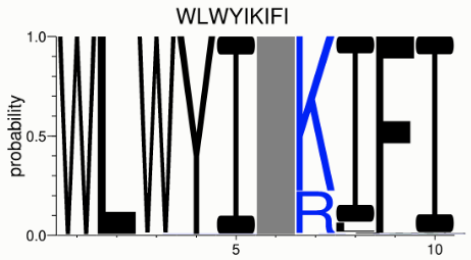
Displaying record number 55295

Download this epitope record as JSON. [Help]

HXB2 location	gp160(678–686) gp41(167–175) DNA(8256..8282)
Author location	Env
Epitope	WLWYIKIFI
Variants	WLWYIrIFI observed variant
Subtype	B
Species (Restricting MHC/HLA)	human(A*02:01)
Immunogen	HIV-1 infection
Patient MHC/HLA	A1, A19, B*35:01, B44, C*16, Cw7; A*02:01, A19, B14, B44, C*16, Cw8
Country	United States
Experimental methods	CD8 T-cell Elispot - IFNγ
Keywords	co-receptor, escape, HAART, ART, HLA associated polymorphism, mother-to-infant transmission, mutation acquisition, rate of progression

gp160 Epitope Map

Epitope Alignment



Show epitope variants

Notes

- HIV-1 mother-to-child transmission is studied for LTNPs by comparing entire genomes from 2 mother (M1, M2) and 2 daughter (D1, D2) RNA samples of a mother-child pair over 11 years. Genetic distance was 94% between subjects' strains. Divergence in sequences was attributed to distinct HLA selection pressures as ds/dn was larger for intra- rather than inter-person sequences. 10 new mutations in D2 were found related to unique daughter HLA alleles.
- Functional ELISpot studies using D2 and Nef peptides reveal strong associations between CTL responses and escape variants, contributing to delayed progression.
- LTNP status was not related to defective virus since all viral genes were intact and CTL response did not effectively control viral load. It is supposed that genetic HLA background and HIV-1 epitope-immune response interaction account for nonprogression of disease.
- All isolates contained R77Q in Vpr, a variation associated with reduction of cellular apoptosis.
- Epitope WLWYIKIFI was the only one mutated, to WLWYIrIFI in the mother M2 isolate. WLWYIKIFI was designated as being restricted to A2.1, a known alias for HLA-A*0201 which is expressed by daughter.

References

Reinis2007 Milan Reinis, Barbara Weiser, Carla Kuiken, Tao Dong, Dorothy Lang, Sharon Nachman, Yonghong Zhang, Sarah Rowland-Jones, and

Notes on CTL Epitope

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Discontinuous Antibody Epitope Search 1

Antibody Search

Search Help

HIV protein	-ALL- Gag p17 p24 p2p7p1p6	
HXB2 protein location		Results overlap with query location
HXB2 DNA location		Results overlap with query location
Epitope		Results contain query sequence
Epitope name		
MAb name	32/5.8.42	☐ Exact Match (List by name) (List by type)
Record number		
Subtype	-ALL-	
Immunogen	-ALL- anti-idiotype autoimmune disease engineered HIV-1 exposed seronegative HIV-1 infection HIV-2 infection	
Vaccine details if Immunogen is Vaccine	Vaccine type: -ALL- Vaccine strain: -ALL- Vaccine component: -ALL- Adjuvant: -ALL-	
Ab type	-ALL- Antisense protein (ASP) C-domain C-HR C-term flap region fusion peptide // near gp41-gp120 interface	
Species	-ALL-	
Isotype	-ALL-	
Author		Search only for ☐ First ☐ Last ◉ Show only this author's references ○ Show all references
Country	-ALL-	
Keywords	-ALL- acute/early infection ADCC adjuvant comparison antibody binding site antibody generation antibody gene transfer	◉ Show only notes containing selected keyword(s) ○ Show all notes
Notes		◉ Show only notes matching this text ○ Show all notes

Search Reset

https://www.hiv.lanl.gov/mojo/immunology/search/ab/form.html

Databases Search Tools Products Publications

HIV Molecular Immunology Database Search

Antibody Search

Search Help

Found 1 matching record:

Download these results as CSV or download as JSON [Help]

Displaying record number 1

Download this epitope record as JSON. [Help]

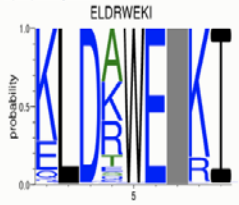
MAb name 32/5.8.42

HXB2 location Gag(12–19 + 100–105)
DNA(823..846,1087..1104)

Gag Epitope Map

Author location p17(12–19 IIIB)

Epitope Alignment



Epitope ELDRWEKI + ALDKIE (Discontinuous epitope)

Ab type

Neutralizing

Species (Isotype) mouse(IgG)

Immunogen vaccine

Keywords

Vaccine Details

Vaccine type viral lysate

Vaccine strain

Vaccine component

Adjuvant

Notes

Showing 1 of 1 note.

- 32/5.8.42: Binds to two discontinuous regions, positions 12-19 and 100-105, peptides ELDRWEKI and ALDKIE -- inhibited infectivity of cell free virus. *Papsidero1989*

References

Showing 1 of 1 reference.

Papsidero1989 L. D. Papsidero, M. Sheu, and F. W. Ruscetti. Human immunodefciency virus type 1-neutralizing monoclonal antibodies which react with p17 core protein:

https://www.hiv.lanl.gov/mojo/immunology/search/ab/results

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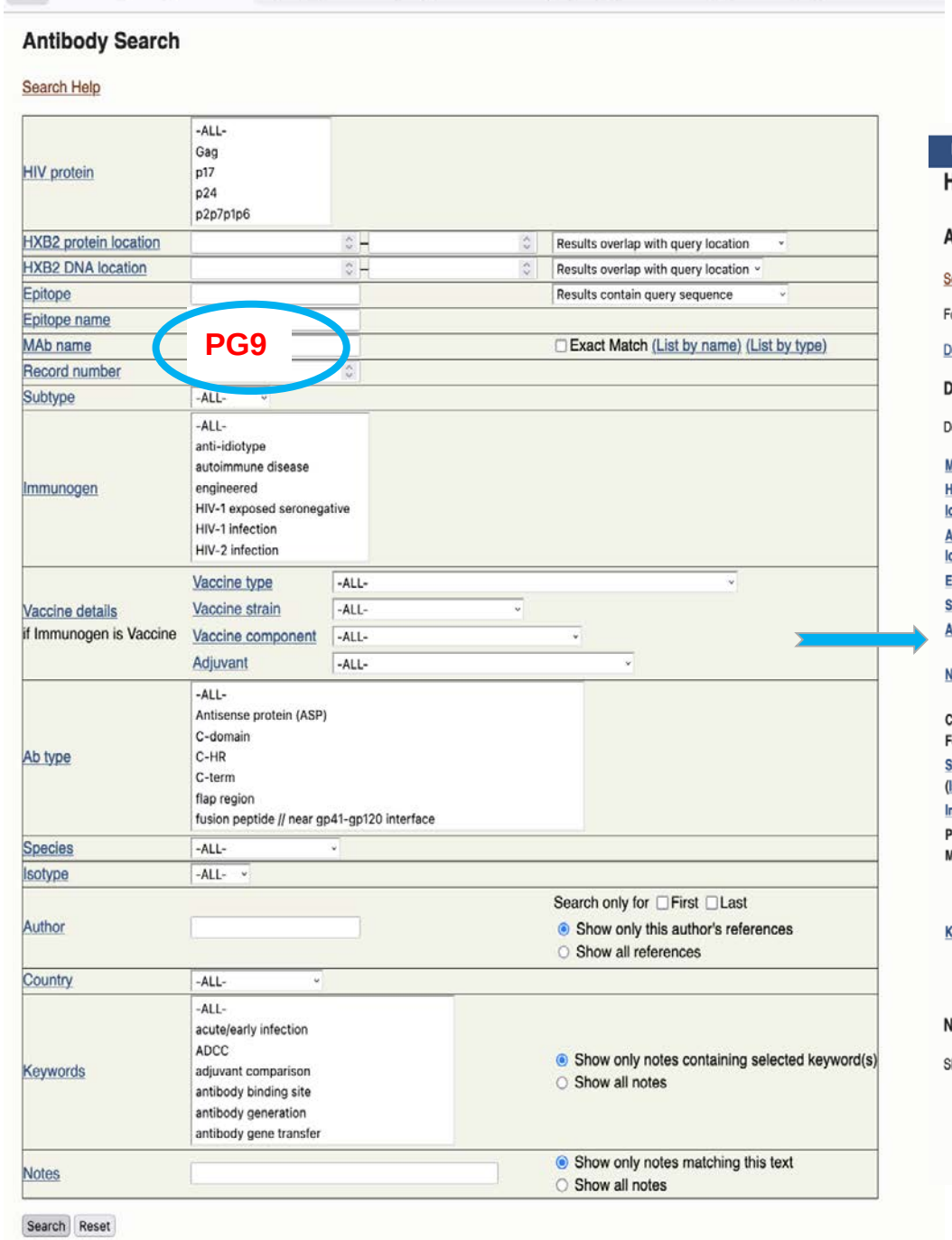
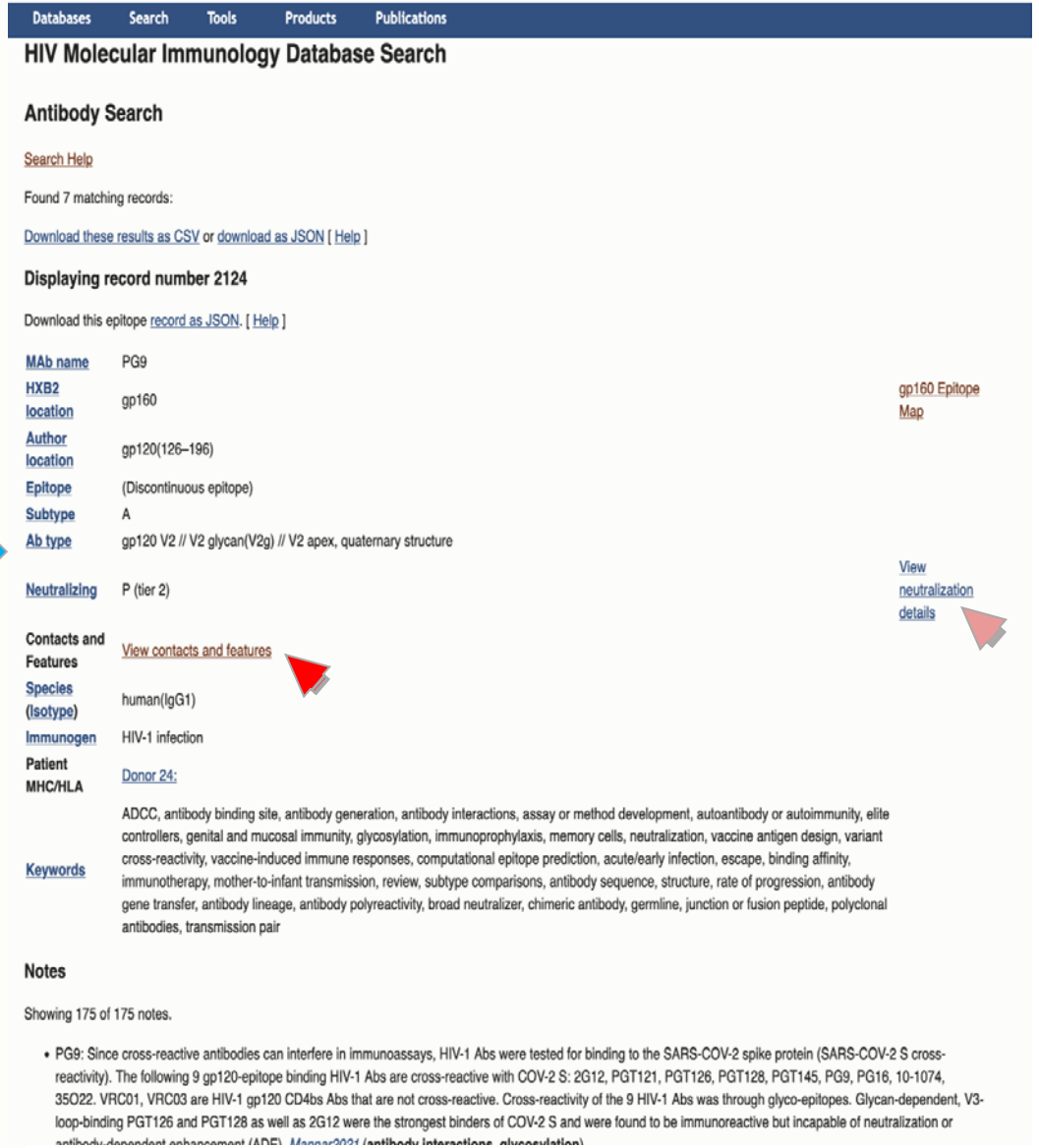
Discontinuous Antibody Epitope Search 2



https://www.hiv.lanl.gov/mojo/immunology/search/ab/form.html



https://www.hiv.lanl.gov/mojo/immunology/search/ab/results

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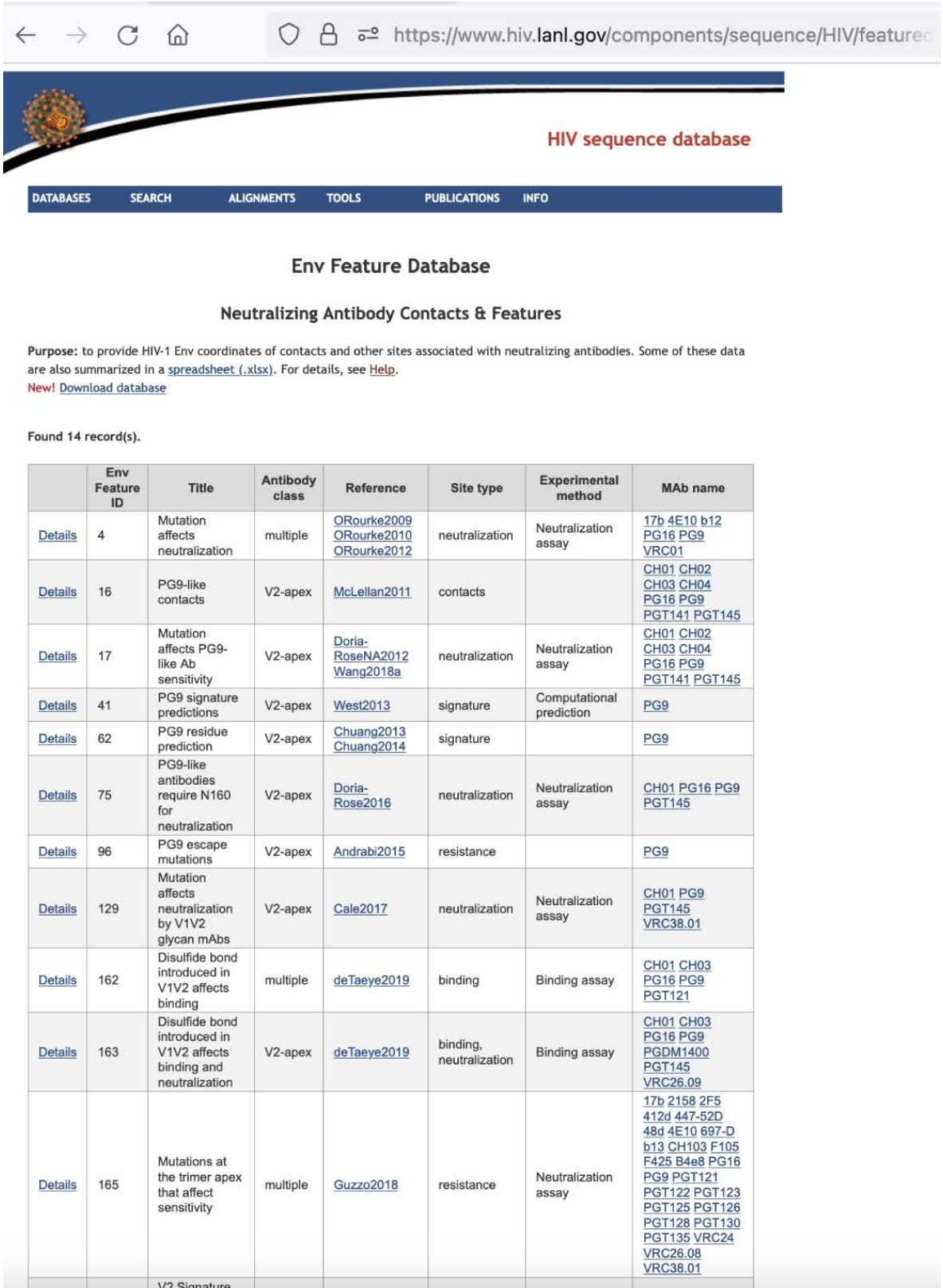
https://www.hiv.lanl.gov/components/sequence/HIV/feature

HIV sequence database

DATABASES SEARCH ALIGNMENTS TOOLS PUBLICATIONS INFO

Env Feature Database

Neutralizing Antibody Contacts & Features

Purpose: to provide HIV-1 Env coordinates of contacts and other sites associated with neutralizing antibodies. Some of these data are also summarized in a spreadsheet (.xlsx). For details, see Help.
New! Download database

Found 14 record(s).

	Env Feature ID	Title	Antibody class	Reference	Site type	Experimental method	MAb name
Details	4	Mutation affects neutralization	multiple	ORourke2009 ORourke2010 ORourke2012	neutralization	Neutralization assay	17b 4E10 b12 PG16 PG9 VRC01
Details	16	PG9-like contacts	V2-apex	McLellan2011	contacts		CH01 CH02 CH03 CH04 PG16 PG9 PGT141 PGT145
Details	17	Mutation affects PG9-like Ab sensitivity	V2-apex	Doria-RoseNA2012 Wang2018a	neutralization	Neutralization assay	CH01 CH02 CH03 CH04 PG16 PG9 PGT141 PGT145
Details	41	PG9 signature predictions	V2-apex	West2013	signature	Computational prediction	PG9
Details	62	PG9 residue prediction	V2-apex	Chuang2013 Chuang2014	signature		PG9
Details	75	PG9-like antibodies require N160 for neutralization	V2-apex	Doria-Rose2016	neutralization	Neutralization assay	CH01 PG16 PG9 PGT145
Details	96	PG9 escape mutations	V2-apex	Andrabi2015	resistance		PG9
Details	129	Mutation affects neutralization by V1V2 glycan mAbs	V2-apex	Cale2017	neutralization	Neutralization assay	CH01 PG9 PGT145 VRC38.01
Details	162	Disulfide bond introduced in V1V2 affects binding	multiple	deTaeye2019	binding	Binding assay	CH01 CH03 PG16 PG9 PGT121
Details	163	Disulfide bond introduced in V1V2 affects binding and neutralization	V2-apex	deTaeye2019	binding, neutralization	Binding assay	CH01 CH03 PG16 PG9 PGDM1400 PGT145 VRC26.09
Details	165	Mutations at the trimer apex that affect sensitivity	multiple	Guzzo2018	resistance	Neutralization assay	17b 2158 2F5 412d 447-52D 48d 4E10 697-D b13 CH103 F105 F425 B4e8 PG16 PG9 PGT121 PGT122 PGT123 PGT125 PGT126 PGT128 PGT130 PGT135 VRC24 VRC26.08 VRC38.01
Details		V2 Signature					

FROM Epitope Search
TO Pathogen Attributes

- HIV protein maps
- HIV Genome Browser
- HIV sites of interest

~~~~~

FROM Epitope Search
TO Host Attributes

- Ab Contacts/Features
- Ab Neutralization

HOST-PATHOGEN
INTERACTION

- Vaccine Design

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~~~~~

https://hiv.lanl.gov/

We are happy to help with research questions on the use of our tools and database.

We appreciate ideas for further tool development!

Contact us:

immuno@lanl.gov or seq-info@lanl.gov

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HIV sequence database

DATABASES | SEARCH | ALIGNMENTS | TOOLS | PUBLICATIONS | INFO | search site | Search

- Search DB
- Advanced Search
- Intra-patient Search
- Next-gen Sequences
- Geography

HIV Sequence Database

Programs and Tools

Search Interface retrieves HIV and SIV sequences, which can then be aligned and used to build trees

Geography Search Interface retrieves HIV sequences based on geographical distribution

Genome Browser uses jBrowse to display diverse data about the HIV-1 genome and proteome

Tools for working with sequences lists all our online tools, organized by function

Alignments

HIV Premade Alignments includes Consensus and Ancestral Sequences, Subtype Reference Alignments, and Complete Alignments

Information

HIV Sequence Compendium print or order our annual publication

Tutorials and other information unpublished web-based content

Links to other HIV/AIDS tools and information

About this website

FAQ general information about this website

How to Cite this Database

Editorial Board

News: Archived News

HIV Molecular Immunology 2020

HIV Molecular Immunology 2020 is now available online. The PDF version is hypertext enabled and features clickable table-of-contents, indexes, references and links to external web sites. *27 January 2022*

2020 Alignments

The 2020 *Web*, *Filtered Web*, *Super Filtered Web*, and *Consensus* Alignments are now available online. The curated web alignments contain a full range of sequences available through the end of 2020. New consensus sequences are available, described by Linchangco et al. 2022. *24 January 2022*

last modified: Tue Sep 7 15:54 2021

Questions or comments? Contact us at seq-info@lanl.gov.

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Multiple paths to most tools

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HIV sequence database

DATABASES | SEARCH | ALIGNMENTS | TOOLS | PUBLICATIONS | INFO

HIV Database Tools

- Tools specific for HIV/SIV
- General use tools with some HIV/SIV-specific features
- General use tools

Analysis and Quality Control

- Entropy quantifies positional variation in an alignment using Shannon Entropy
- GenSig identifies genetic signatures. It can work on any phenotype file given in conjunction with a codon-aligned nucleotidealignment of a protein coding region
- Glycan Shield Mapping shows mapping absent hole-causing potential N-linked glycosylation sites (PNGS) on predicted glycan shields for an ENV sequence
- HIV BLAST finds sequences similar to yours in the HIV database
- Hypermut detects hypermutation
- jpHMM at GOBICS detects subtype recombination in HIV-1; hosted at GOBICS as a collaboration between the Department of Bioinformatics, University of Göttingen and the Los Alamos HIV Sequence Database
- N-Glycosite finds potential N-linked glycosylation sites
- PCOORD multidimensional analysis of sequence variation
- Quality Control runs several tools for quick troubleshooting of HIV-1 sequences; optional step prepares sequence submission for GenBank
- RAPR (Recombinant Analysis PRogram) uses the Wald-Wolfowitz Runs Test to check for recombination in every triplet in the alignment.
- RIP (Recombinant Identification Program) detects HIV-1 subtypes and recombination
- SNAP calculates synonymous/non-synonymous substitution rates
- SUDI Subtyping plots the distance of your sequence to established subtypes
- Variable Region Characteristics summarizes features of peptides from a protein alignment, reporting peptide characteristics such as length and N-linked glycosylation sites; particularly useful for characterizing variable regions of Env
- VESPA (Viral Epidemiology Signature Pattern Analysis) detects residues with different frequencies in two sequence sets

Alignment and sequence manipulation

- Align Multi-tool manipulates sequence alignments, including sorting, pruning, and renaming
- Alignment Slicer cuts vertical slices from sequence alignments
- Analyze Align shows weblogos, calculates frequency by position, and finds variants in an alignment
- Codon Alignment takes a nucleotide alignment and returns a codon alignment and translation
- Consensus Maker computes a customizable consensus
- ElimDupes compares the sequences within an alignment and eliminates any duplicates
- Gap Strip/Squeeze removes columns with more than a given % of gaps

Phylogenetics

- AnnotateTree creates a colored and weighted phylogenetic tree
- Branchlength calculates branch lengths between internal and end nodes; now included in the TreeRate tool
- FindModel finds which evolutionary model best fits your sequences
- IQ-TREE is a fast and effective stochastic algorithm for finding Maximum Likelihood trees, including site-specific rates of evolution at each alignment position
- PhyloPlace reports phylogenetic relatedness of an HIV-1 sequence with reference sequences
- PhyML generates much better trees than our simple TreeMaker tool
- Poisson-Fitter estimates time since MRCA and star-phylogeny. For use with acute (low diversity) samples
- Rainbow Tree Color code phylogenetic tree branches according to labels in the sequence names
- TreeMaker generates a Neighbor Joining phylogenetic tree
- TreeRate finds the phylogenetic root of a tree and calculates branch lengths and evolutionary rate

Immunology

- CATNAP (Compile, Analyze, Tally NAb Panels) provides meta-analysis of published neutralization panel data
- CombiNAber predicts and analyzes combination antibody neutralization scores using IC_{50} and/or IC_{80} for individual antibodies
- ELF (Epitope Location Finder) identifies known and potential epitopes within peptides
- Epigraph Tool Suite uses input of diverse sequences to generate Epigraph sequences for use in vaccine or reagent design
- Epilign (QuickAlign) aligns a protein sequence (e.g., epitope) to the appropriate protein alignment
- Heatmap displays a table of numbers by using colors to represent the numerical values
- Hepitope identifies potential epitopes based on HLA frequencies
- Neutralization Index computes a tier-like score for sera (using ID50 titers) or antibodies (using IC50 titers)
- Mosaic Vaccine Tool Suite designs and assesses polyvalent protein sequences for T-cell vaccines
- Motif Scan finds HLA anchor motifs in protein sequences for specified HLA serotypes, genotypes or supertypes
- PeptGen generates overlapping peptides from a protein sequence

Database search interfaces

- Advanced Search creates a custom search interface
- Antibodies search for HIV antibodies by protein, immunogen, AB type, isotype, author, keywords

HIV Tools:
>80% are
NOT
HIV-specific

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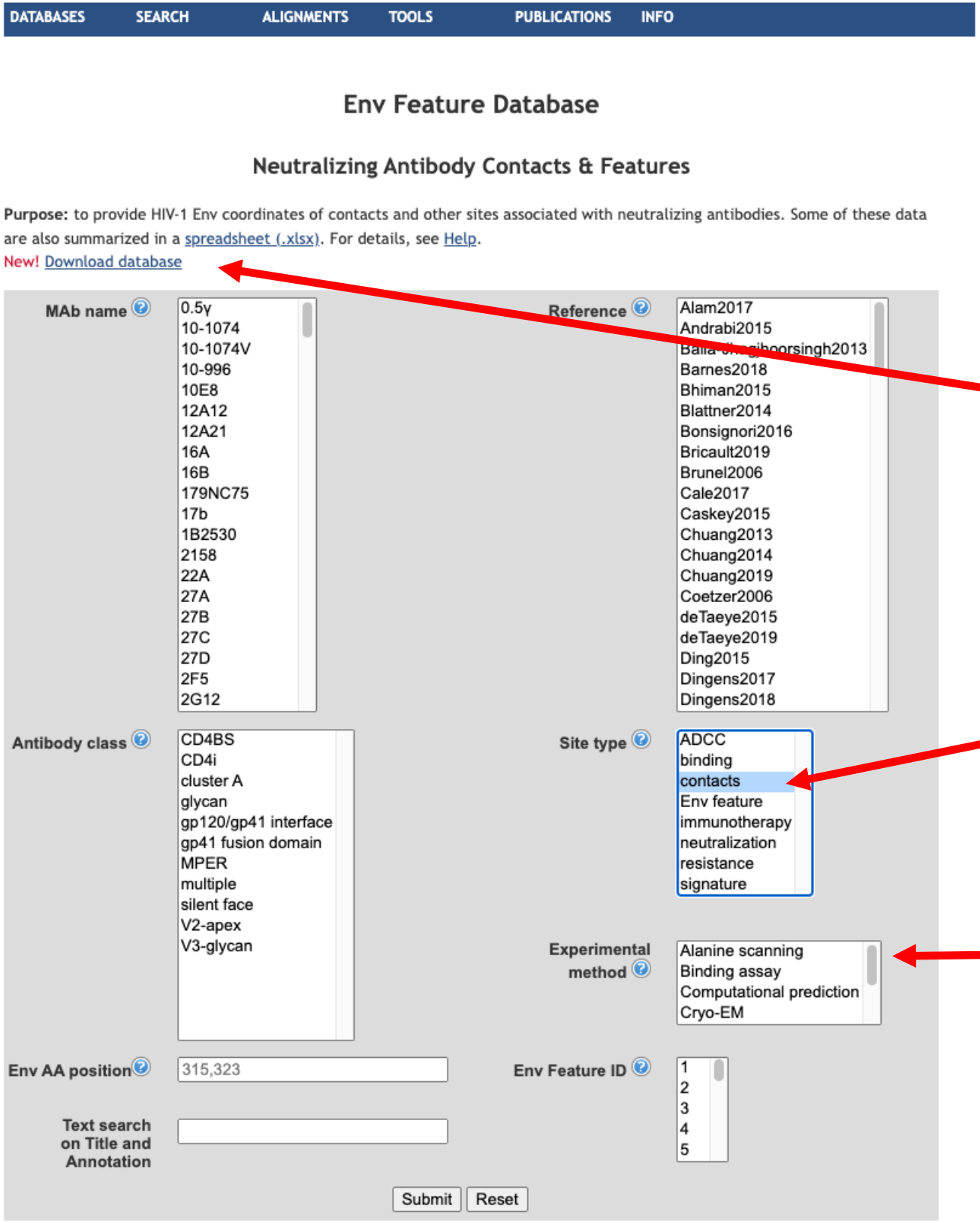
Feature and Contacts Database



Download all contact sites (and other features) in a single spreadsheet

Select “contacts” to get discontinuous antibody contacts

Almost all features are based on experimental data; any computational predictions are clearly delineated as such

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View Neutralizing Antibody Contacts & Features

Env Feature ID 8

Title VRC01 contacts

Antibody class CD4BS

Reference Wu2011 Zhou2010

Site type contacts

Experimental method

MAb name VRC01 (Immuno DB, CATNAP)

Links to VRC01 information and IC50 data

Env pos.	Feature	HXB2 AA	Entropy (0-3)			Annotation
			Group M	Subtype B	Subtype C	
97	gp120	K	0.433	0.421	0.511	VRC01 contact
			See Logo			
123	gp120	T	0.033	0.028	0.038	VRC01 contact
			See Logo			
128	gp120	S	0.188	0.339	0.088	VRC01 contact
			See Logo			
129	gp120	L	0.048	0.056	0.029	VRC01 contact
			See Logo			
276	gp120, Loop D	N	0.120	0.063	0.169	VRC01 contact
			See Logo			
278	gp120, Loop D	T	0.657	0.715	0.481	VRC01 contact
			See Logo			
279	gp120, Loop D	D	0.860	0.850	0.898	VRC01 contact
			See Logo			
280	gp120, Loop D	N	0.117	0.090	0.170	VRC01 contact
			See Logo			
281	gp120, Loop D	A	1.081	0.814	1.357	VRC01 contact
			See Logo			
282	gp120, Loop D	K	0.260	0.337	0.297	VRC01 contact
			See Logo			
283	gp120, Loop D	T	0.992	1.091	0.474	VRC01 contact
			See Logo			
365	gp120, CD4 binding loop	S	0.574	0.489	0.619	VRC01 contact
			See Logo			
366	gp120, CD4 binding loop	G	0.034	0.012	0.028	VRC01 contact
			See Logo			

Logo showing variability at this Env position

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Sequence Alignment Analysis Tool

AnalyzeAlign

Purpose: Show weblogos, calculate frequency by position, and find variants in an alignment. Explanation.

Input

Alignment [Sample Input]
- Paste or upload alignment
- Choose File HCV_ALL_2..._PRO.fasta
- Use LANL database alignment
  - Alignment type: Filtered web / Web / Subtype reference / Compendium
  - Organism: HIV-1/SIVcpz / HIV-2/SIVsmm / Other SIV
  - Region: Env
  - Subtypes: All / Major subtypes (A B C D F G CRF01 CRF02)

Sequence type: nucleotide / amino acid

Positions/range to analyze: 11-22
Total positions ≤ 200!

Range numbers refer to: alignment columns, including gaps / residues of 1st sequence / residues of HXB2

Group the sequences:
- Report results for all sequences as a single group
- Report separate results for subsets of sequences (email results)

Group sequences by:
- the characters in field 1 of names delimited by .
- first 1 character(s) in names
- paste or upload grouped sequence names (example)

Choose File No file chosen

- I am using a LANL alignment; group sequences by subtypes (the first field)

Logo options

Other options

Gap option: Delete gaps and shift alignment to C-terminus
- yes / no (for amino acid sequences only, useful for T-cell epitopes)

Frequency calculation: Cut-off for calculating frequency by position 95 %

Master sequence for finding variants:
- consensus of alignment / consensus of seq group
- 1st seq of alignment / 1st seq of seq group
- user-specified: Raw sequence; same length as range analyzed.

Output

Email results

Downloadable logo files: PDF EPS SVG

Combine logos for subsets into a page: Concatenate PDF or EPS logos as a x 1 matrix (row x column)
- Orientation: Portrait / Landscape
- Include logo of removed symbols, if option to remove symbols selected:

Submit Reset

Provide an alignment representing the variability of the organism (e.g., HCV E2 protein alignment)

Choose the positions to analyze; possibly the location of your favorite epitope(s).

Choose a master sequence as the basis of comparison

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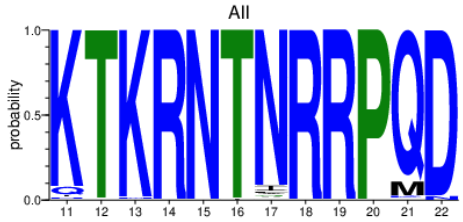
AnalyzeAlign example output

Logo



Download: PNG

A sequence logo showing the variability in the alignment.

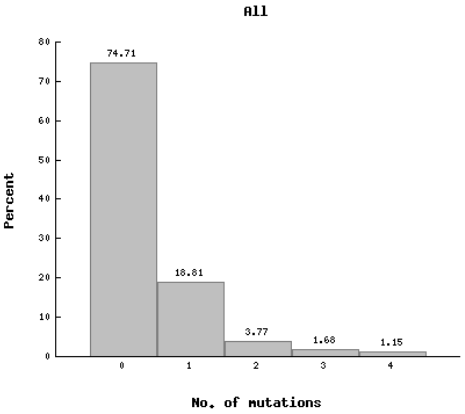
Frequency by position

See full raw counts — cutoff: 95%

	Percentage and raw count of non-gap	Non-gap/total (percentage)	Gap/total (percentage)
11	K: 92.08% (721) Q: 4.98% (39) other: 2.94% (23)	783/783 (100.00%)	0/783 (0.00%)
12	T: 98.72% (773) other: 1.28% (10)	783/783 (100.00%)	0/783 (0.00%)
13	K: 98.08% (768) other: 1.92% (15)	783/783 (100.00%)	0/783 (0.00%)
14	R: 99.62% (780) other: 0.38% (3)	783/783 (100.00%)	0/783 (0.00%)
15	N: 99.62% (780) other: 0.38% (3)	783/783 (100.00%)	0/783 (0.00%)
16	T: 98.98% (775) I: 1.02% (8)	783/783 (100.00%)	0/783 (0.00%)
17	N: 91.44% (716) I: 3.32% (26) Y: 1.15% (9) other: 4.09% (32)	783/783 (100.00%)	0/783 (0.00%)
18	R: 99.49% (779) other: 0.51% (4)	783/783 (100.00%)	0/783 (0.00%)
19	R: 99.87% (782) H: 0.13% (1)	783/783 (100.00%)	0/783 (0.00%)
20	P: 99.87% (782) R: 0.13% (1)	783/783 (100.00%)	0/783 (0.00%)
21	Q: 89.14% (698) M: 8.43% (66) other: 2.43% (19)	783/783 (100.00%)	0/783 (0.00%)
22	D: 97.32% (762) N: 2.68% (21)	783/783 (100.00%)	0/783 (0.00%)

A list of all variants present, relative to the selected master sequence.

Sequence variants



A histogram of the number of positions with mutations, relative to the master sequence.

Variant	Count	Pct.	No. of mutations
KTKRNTNRRPQD			
----------	585	74.71	0
----------M-	59	7.54	1
------I-----	24	3.07	1
Q----------	16	2.04	1
Q-----L---KN	8	1.02	4
R----------	7	0.89	1
--N---------	5	0.64	1
Q-----P----N	5	0.64	3
I----------	5	0.64	1
------Y-----	4	0.51	1
-I---------	3	0.38	1
------T-----	3	0.38	1
-----I------	3	0.38	1
I----I------	2	0.26	2
I-----Y-----	2	0.26	2
P---------K-	2	0.26	2

An alignment of all variants, relative to the master sequence chosen (including frequency of each).

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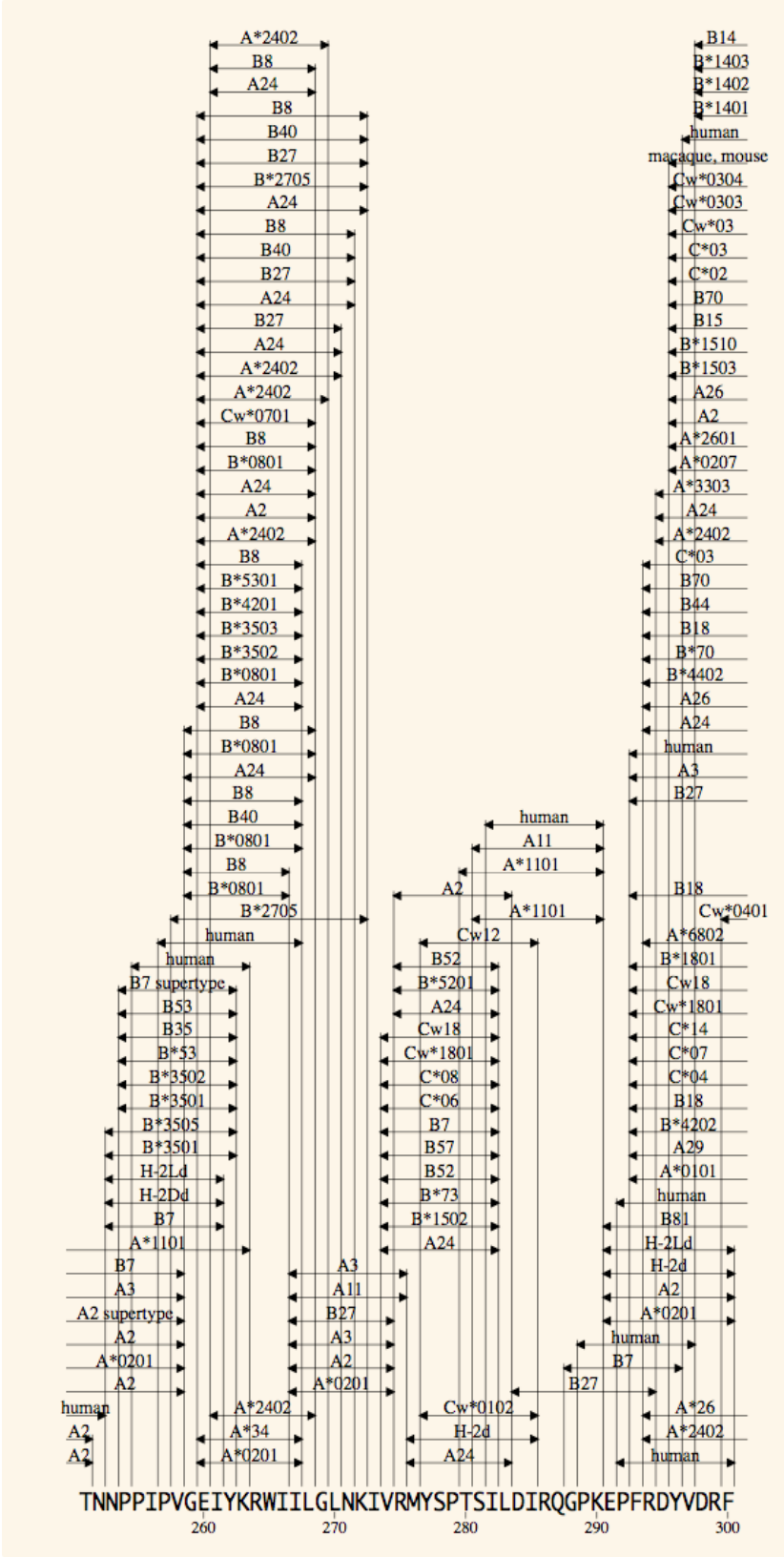
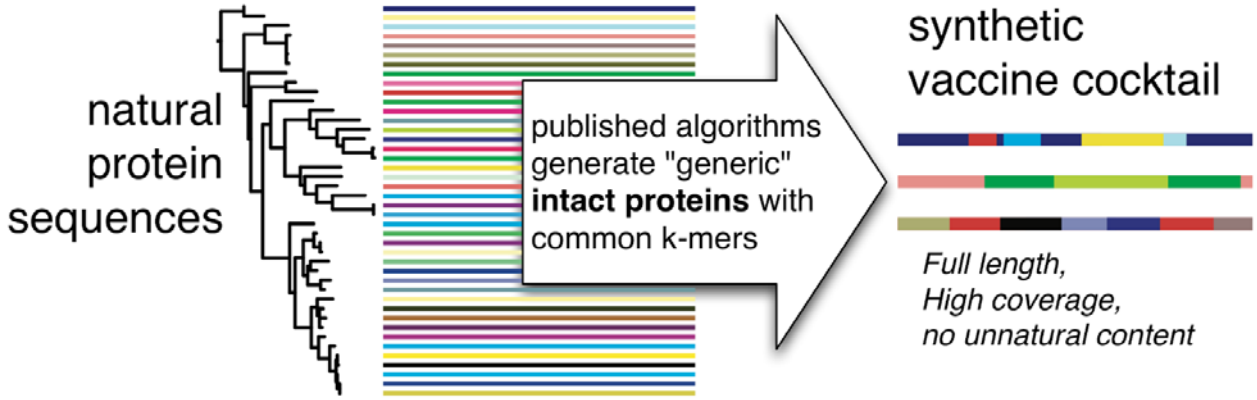
Vaccine Design Tools

HIV epitopes are densely packed at the population level

- Vaccinating a diverse population with individual epitopes is infeasible
- Escape forms for one HLA are frequently sensitive for a different HLA
- It may not be necessary to ***predict*** epitopes — but only to ***deliver*** them
- Optimized immunogen cocktails could deliver most epitopes likely to be present in infecting virus



Vaccine Design Tools: Mosaic/Epigraph



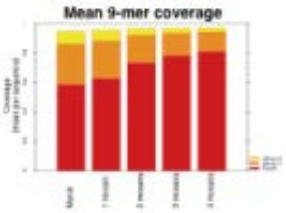
Design Tools

Generate candidate vaccine protein cocktails that optimize coverage of potential T-cell epitopes based on frequencies in sets of natural pathogen sequences

Mosaic Vaccine Designer — genetic algorithm (Fischer et al. 2007)

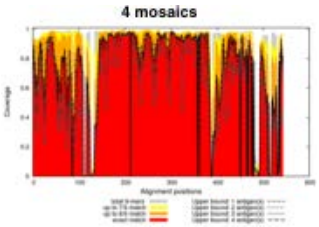
Epigraph — graph-theory approach (Theiler et al. 2016)

Evaluation tools



Epitope Coverage Assessment (EPICOVER)

Alignment-independent “k-mer” coverage by vaccines or peptides.



Positional Epitope Coverage Assessment (POSICOVER)

Alignment-based coverage by vaccines or peptides.

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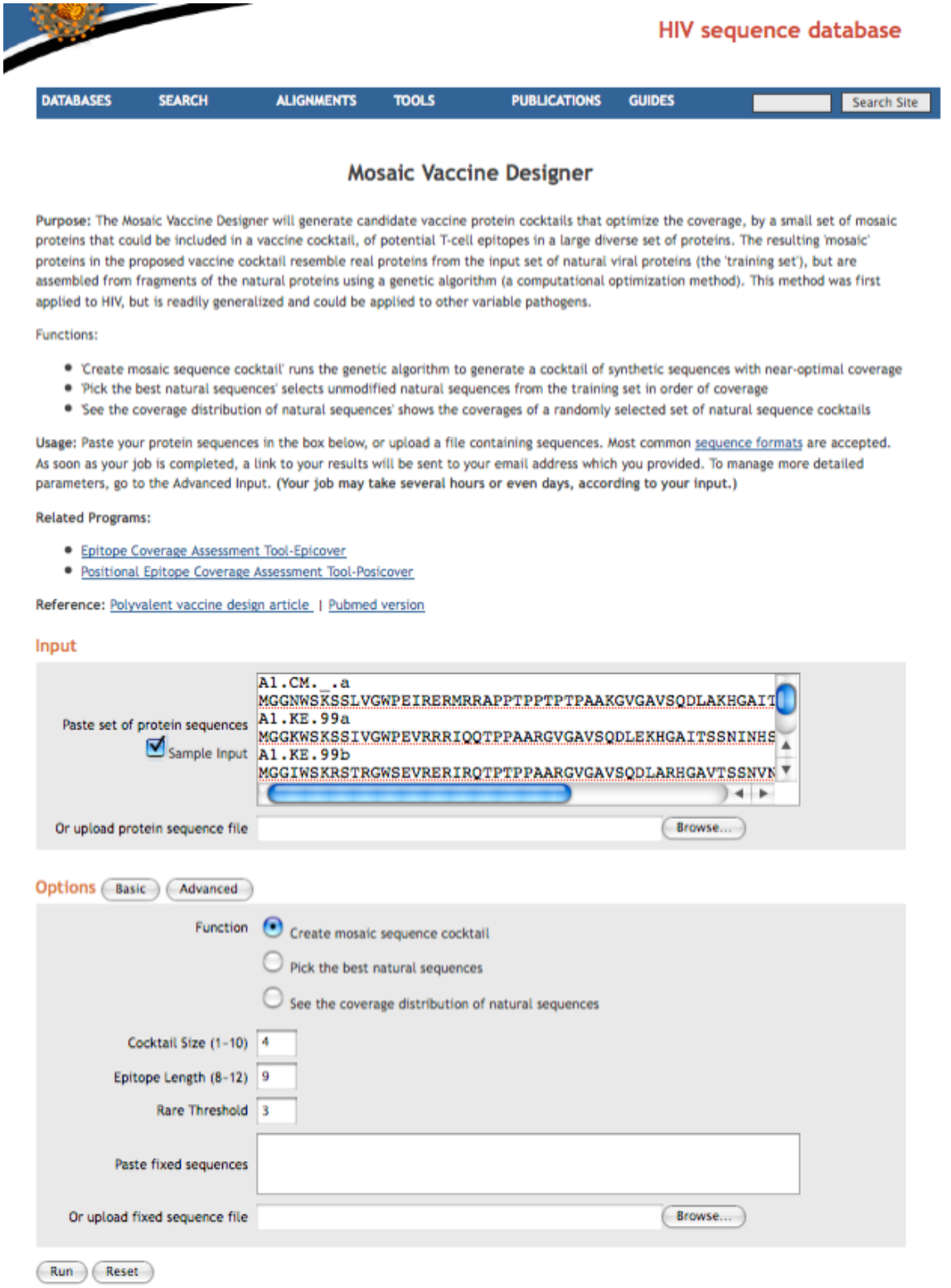
Mosaic Vaccine Designer

Method: genetic algorithm

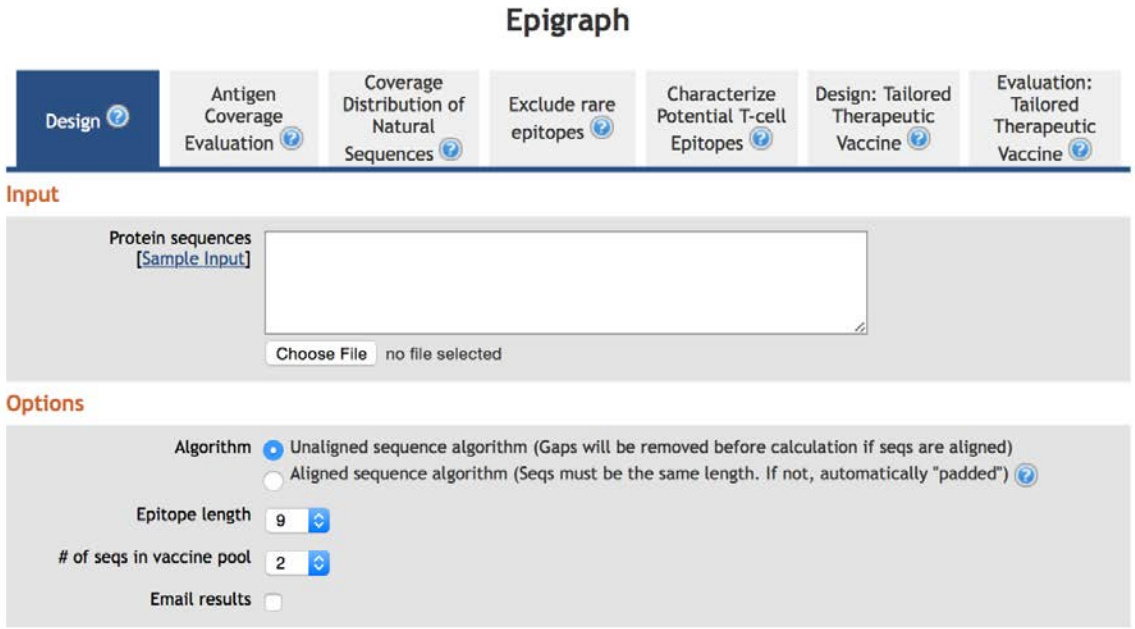
Target set: natural protein sequences from a diverse pathogen population

Cocktail size: how many mosaic protein sequences to generate

Epitope length: default is 9 amino-acids



EPIGRAPH



Method: evaluation of acyclic graph

Target set: natural protein sequences for the pathogen population

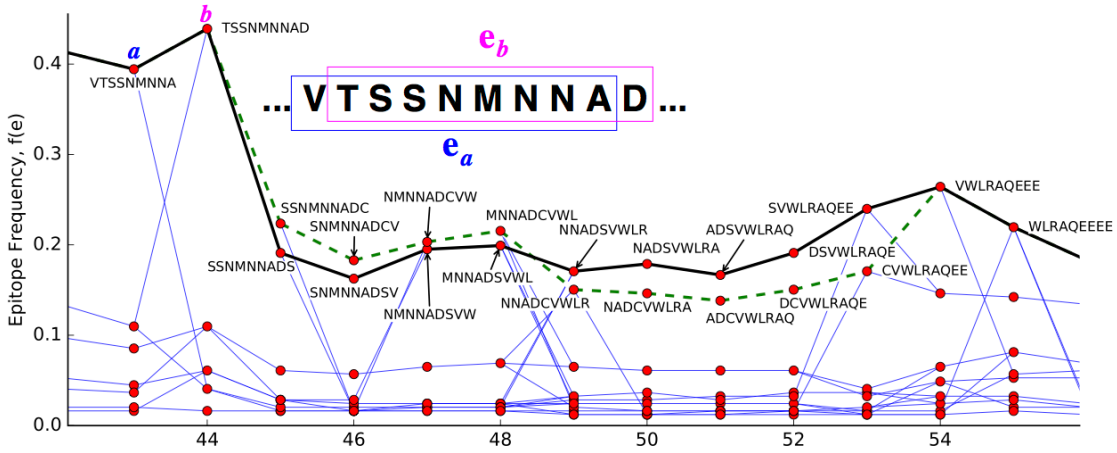
Cocktail size: how many mosaic proteins in the output set.

Epitope length: default is 9 amino-acids.

Advantages over Mosaic

Essentially optimal (fractionally better coverage)

Much faster: allows iteration and comparison of multiple input sets and alternate designs



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Vaccine Design Tools: Mosaic/Epigraph

Mosaic/Epigraph vaccine designs have been applied to many pathogens

Influenza Kingstad-Bakke *et al* Vaccine, 2019 37:5051, PMID: 31300285; Florik *et al*, PLoS One, 2017 Aug 3;12(8):e0181738; Kamlangdee *et al*, J Virol. 2016 Jul 11;90(15):6771-6783 and J Virol. 2014 Nov;88(22):13300-9, PMID:25210173

Dengue Hou *et al* Front Immunol. 2019 Jun 20;10:1429, PMID: 31281322

Rabies Stading *et al*, Plos Negl Trop Dis, 2017, PMID: 28976983

Pan-filoviruses Theiler *et al*, Sci Rep. 2016, PMID: 27703185, Rahim *et al*, PLoS Pathog. 2019 Feb 28;15(2):e1007564 PMID: 30817809

Chlamydia trachomatis Badamchi-Zadeh *et al*, Front Immunol, 2016, PMID: 27199987

Porcine Reproductive and Respiratory Syndrome Virus (PRRSV) Cui *et al*, PLoS One. 2019 Jan 31;14(1), PMID: 30794703

Dengue Fever Hou *et al*, Front Immunol. 2019 Jun 20;10:1429, PMID: 31281322

Hepatitis B Bruening E, Douglas J, Yusim K, *et al.*, being experimentally tested

Hepatitis C Yusim *et al.*, Clin Vaccine Immunol, 2013, PMID: 23221002

Lassa Virus Alex Bukreyev, https://apps.dtic.mil/sti/citations/AD1116972

HIV Chen *et al*. J Virol. 2022 96(7):e0216121, PMID: 35297660; Barouch *et al*. 2018 392(10143):232-243, PMID: 30047376

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CATNAP (Compile, Analyze and Tally NAb Panels)

What is CATNAP, *really*?

- A database of HIV antibody neutralization (IC50/80) data.
- A tool to analyze numerical data in association with variable sequences from any protein.

(Coming soon: a database of SARS-CoV-2 neutralization data)

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https://www.hiv.lanl.gov/components/sequence/HIV/neutralization/index.html

http://hiv.lanl.gov/catnap

CATNAP

Compile, Analyze and Tally NAb Panels

The CATNAP family of tools has been designed to facilitate the analysis of neutralizing antibodies (NAbs) through the identification of potential genetic signatures resulting from a NAb's interaction with a protein. While interactions between NAbs and HIV-1 Env are the emphasis, the Custom Input version can accomodate other types of data, including other proteins and organisms.

CATNAP

Purpose: Analyze our database of HIV-1 IC_{50} and IC_{80} neutralization data from publicly-available sources, in conjunction with HIV-1 Envelope sequences. Access our extensive databases of information about neutralizing antibodies and viruses used in published neutralization studies. Alignments of Env sequences for these viruses are also provided.

Help: CATNAP Help.

Download and analyze built-in HIV antibody IC50/80 data

CATNAP: Custom Input

Purpose: Find potential genetic signatures based on your own numerical data in association with protein sequences. In addition to neutralization data, this tool is flexible enough to accomodate almost any kind of data in conjunction with almost any protein sequence.

Help: Custom CATNAP Help.

Analysis of **your data** for any organism: numerical data linked to aligned sequences

CATNAP: Hybrid

Purpose: Compare and analyze your HIV-1 IC_{50} and IC_{80} neutralization data with published data. This tool will display your data side-by-side with data from our database of published HIV-1 neutralization data.

Help: Hybrid CATNAP Help.

Analysis of built-in IC50/80 data together with your own HIV antibody IC50/80 data

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CUSTOM CATNAP

SARS-COV-2 data from Wang et al. Nature 2022 Aug;608(7923):603-608

CATNAP: Custom Input

●≤0.01275(Q_1) ●≤0.321(Q_2) ●≤1.03175(Q_3) ●>1.03175 ○Undetected: UD

(A value occurring many times in the data set and ranging more than two color groups will take the most intense color which the value can be.)

More virus info in HIV Seq DB

Virus name	Tier	AA (NxST)	5-7	ADG-2	Brii-196	Brii-198	CAB-
Omicron_BA.1.1__EPI_ISL_10000001		N (+)	0.534	0.295	1.792	UD	0.01
Omicron_BA.1__EPI_ISL_10000028		N (+)	0.347	0.181	2.385	0.078	0.01
Omicron_BA.2.12.1__EPI_ISL_10783322		N	UD	UD	1.171	UD	0.02
Omicron_BA.2_L452M__EPI_ISL_10696425		N	UD	UD	0.907	UD	0.03
Omicron_BA.2_L452R__EPI_ISL_10242829		N	UD	UD	6.815	UD	0.04
Omicron_BA.2__EPI_ISL_10000005		N	UD	UD	1.346	0.782	0.03
Omicron_BA.4__EPI_ISL_11207535		N	UD	UD	0.978	UD	0.02
Geometric mean of detected			0.43046	0.23107	1.69815	0.24697	0.02
Geometric mean of detected & undetected*			21.0854	17.6517	1.69815	17.9905	0.02
% detected (detected/total)			29% (2/7)	29% (2/7)	100% (7/7)	29% (2/7)	100%

Rseq

```
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLH
----.----|----.----|----.----|----.----|----.----
--------10--------20--------30--------40--------5
```

```
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLH
MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLH
MFVFLVLLPLVSSQCVNLITRTQ---SYTNSFTRGVYYPDKVFRSSVLH
MFVFLVLLPLVSSQCVNLITRTQ---SYTNSFTRGVYYPDKVFRSSVLH
MFVFLVLLPLVSSQCVNLITRTQ---SYTNSFTRGVYYPDKVFRSSVLH
MFVFLVLLPLVSSQCVNLITRTQ---SYTNSFTRGVYYPDKVFRSSVLH
MFVFLVLLPLVSSQCVNLITRTQ---SYTNSFTRGVYYPDKVFRSSVLH
```

Spike sequence names

IC50 values UD=undetected

Spike sequence alignment; red N's have predicted glycosylation

* *Values are considered as undetected, if ($IC_{50/80}$)>cutoff or >100, ($ID_{50/80}$)<cutoff or <20. For the purpose of calculating means, each undetected sets to 100($IC_{50/80}$) or 20($ID_{50/80}$).*

# of antibodies or mixtures found: 21
# of viruses found: 7

Download neutralization data include ☑virus info ☐slice of alignment from position analysis

Position analysis

Analyze Rseq position 17 5-7

Position analysis of antibody 5-7 at position 17 of the alignment…

Analysis at position 17 for Ab 5-7

Amino Acid Counts

AA	Count	# for detected	# for undetected	Fisher test p-value	Odds ratio
N	7	2	5	1	0
Total	7	2	5		

N-linked Glycosylation Motif Counts

NxST	Count	# for detected	# for undetected	Fisher test p-value	Odds ratio
g+	2	2	0	0.04762	Inf
g-	5	0	5	0.04762	0
-	0	0	0	1	0
Total	7	2	5		

…shows a statistical difference in neutralization between glycosylated and non-glycosylated N.

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COVID-19 Viral Genome Analysis Pipeline

Enabled by data from GISAID

http://cov.lanl.gov

Home | Variants | Resources | Tools | search site | Search

This website provides analyses and tools for exploring accruing mutations in hCoV-19 (SARS-CoV-2) geographically and over time, with an emphasis on the Spike protein, using data from GISAID.

The SARS-CoV-2 sequence data used for these analyses was updated from GISAID on Sep 22, 2022.

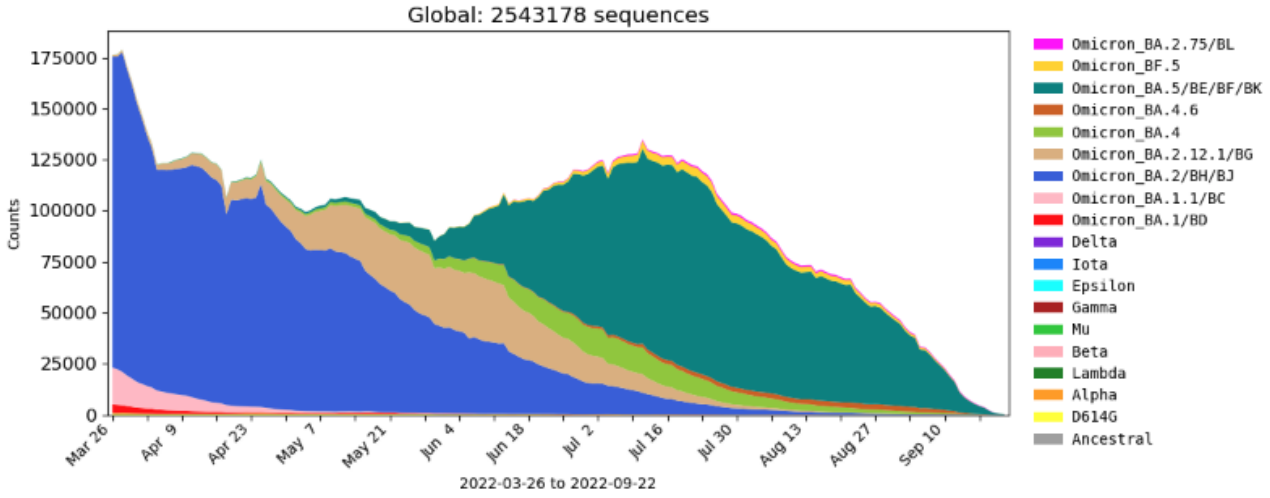
With the ever growing database of sequences in GISAID, sometimes the web connection times out before the analysis is complete. If you have this problem, please check "email results" and an email with a link will be sent to you when the job is complete.

News

Oct 3, 2022
We have released a new update to our listings of SARS-CoV-2 Spike Variants.

Aug 15, 2022
We have released a new update to our listings of SARS-CoV-2 Spike Variants.

See more



Embers plot, See data

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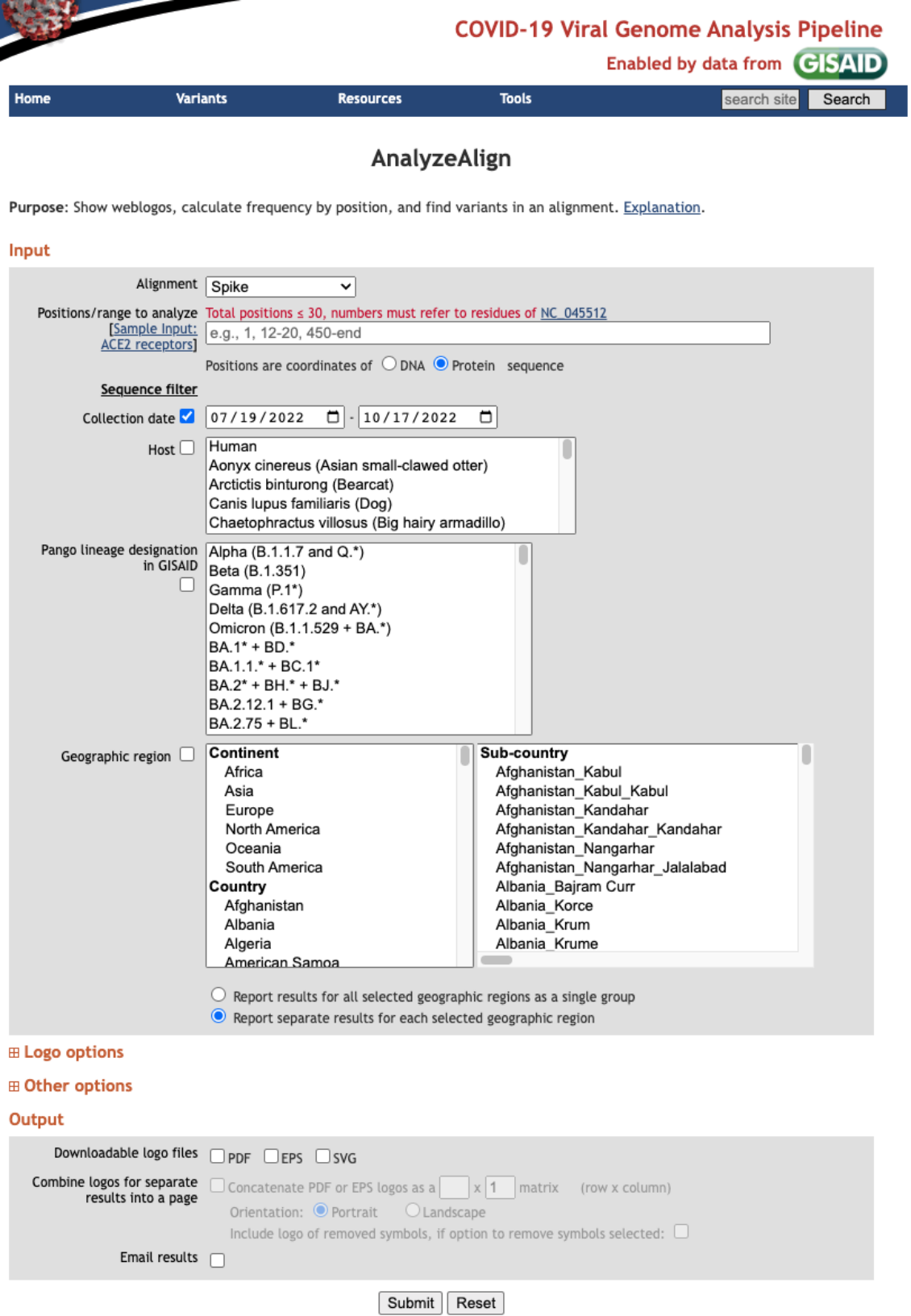

Same tool as AnalyzeAlign, with options specific to SARS-COV-2.

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Thank you for attending!

We are happy to help with research questions on the use of our tools and database.

We are thrilled to get ideas for further tool development!

Contact us:

seq-info@lanl.gov or immuno@lanl.gov