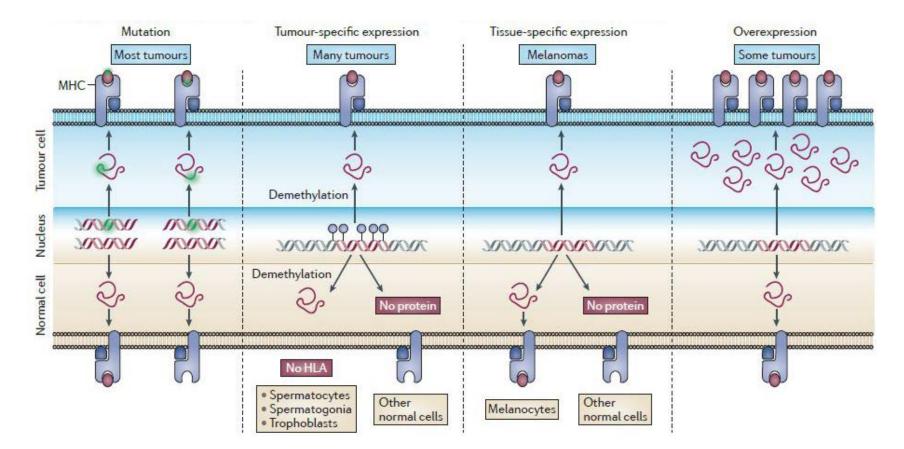


Cancer Epitope Database and Analysis Resource (CEDAR)

Presented by: Zeynep Koşaloğlu-Yalçin, Instructor Cancer Bioinformatics

²⁰²³ IEDB User Workshop

Cancer Epitopes are Derived from Cancer Antigens



Coulie et al, Nat Rev Cancer. 2014 Feb

Motivation for the CEDAR Project

- IEDB hosts epitope data for
 - Allergy
 - Infectious diseases
 - Autoimmune diseases
 - Transplantation / Alloantigens
 - But <u>NOT</u> Cancer

We received funding from the **National Cancer Institute** to develop a resource for cancer epitopes



Cancer Epitope Database and Analysis Resource (CEDAR)



Database



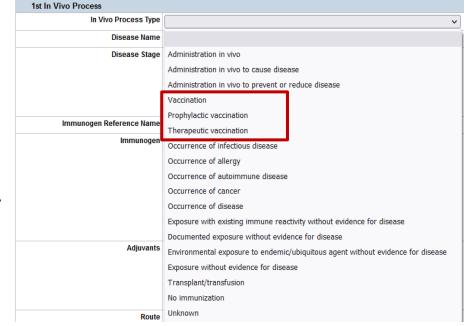


Comprehensively cataloging all cancer epitope-related data linked to the biological, immunological, and clinical contexts Computational epitope prediction and analysis tools providing researchers access to predictive strategies and objective evaluations of their performance

4

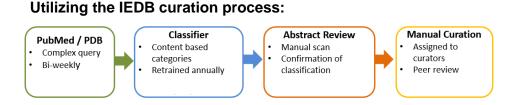
CEDAR Database Design Process

- <u>Reached Out to Experts</u>: Interviewed cancer experts to identify important search fields for cancer research
- **<u>Prototyped User Interfaces:</u>** Designed database query interface wireframes
- Introduced Cancer Curation Rules, for example:
 - i. Captured cancer types in more detail
 - ii. Distinguished vaccination types (prophylactic / therapeutic)
 - iii. Distinguished between allo- and xeno-adoptive transfer.



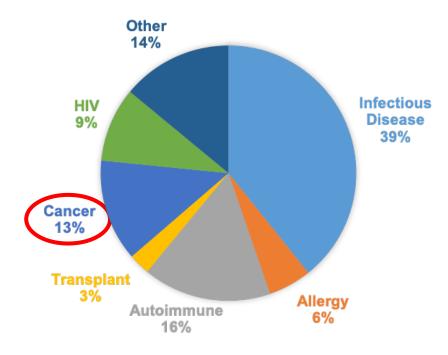
²⁰²³ IEDB User Workshop

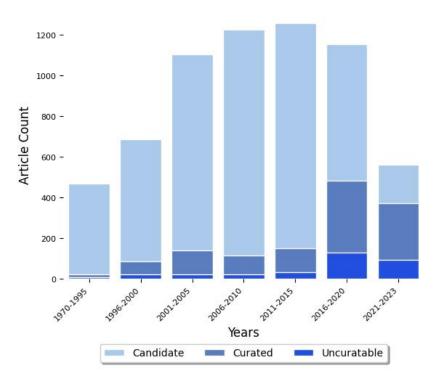
Curation of Cancer-related Epitope Data



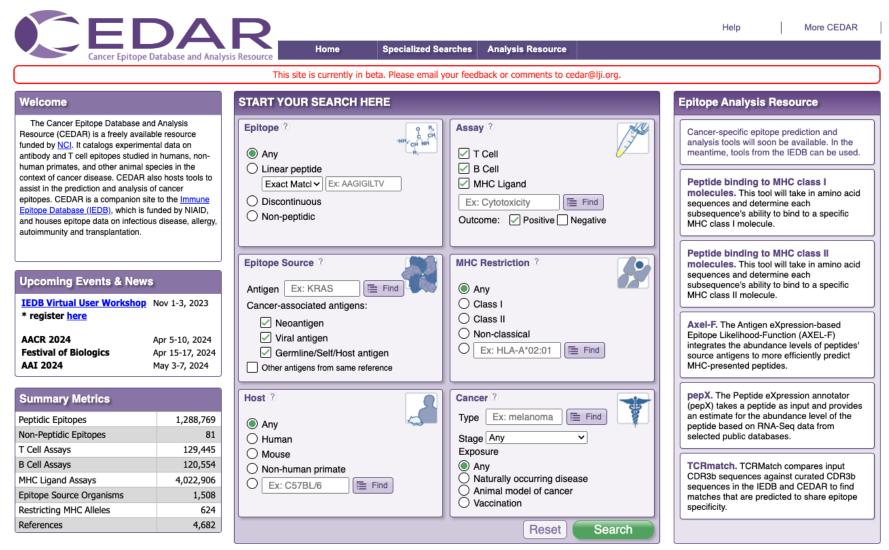
Cancer Curated Category	% Complete	No. of Papers
Prostate Cancer	99%	235
Neoepitope category	96%	450
Published papers in 2023	85%	57
Published papers in 2022	97%	110
Published papers in 2021	97%	83
Published papers in 2020	95%	109
Published papers in 2019	83%	92

Breakdown of Classified and Curatable References





cedar.iedb.org



Provide Feedback | Help Request | Solutions Center | Tool Licensing Information

Supported by a grant from the National Cancer Institute, a component of the National Institutes of Health.

Last Updated: September 06, 2023

Data in CEDAR

- 77,557 T cell Assays
 - 37,056 unique epitopes from 10,941 antigens
- 46,321 B Cell Assays
 - 19,815 unique epitopes from 862 antigens
- 705,286 Ligand Elution Assays
 - 214,905 unique epitopes from 3,651 antigens

T Cell Data in CEDAR

Most epitopes are from common cancer types

Disease Type	# epitopes
melanoma	8,172
healthy	7,084
colorectal cancer	6,577
lung non-small cell carcinoma	2,445
hepatocellular carcinoma	1,071
bile duct cancer	876
skin melanoma	788
pancreatic ductal adenocarcinoma	668
glioblastoma	611
pancreatic cancer	431

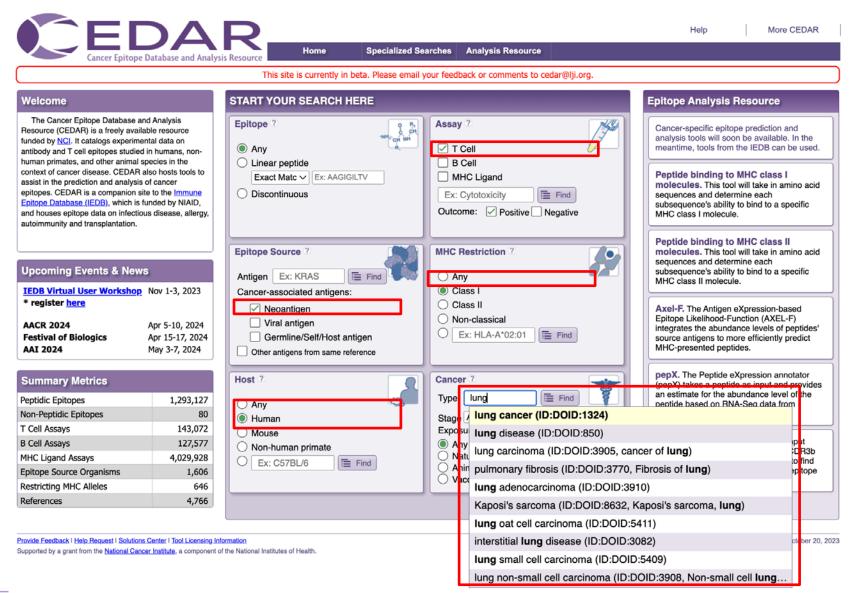
epitopes
173
149
70
65
60
53
53
45
31
23

Neoantigens in CEDAR

- 21,610 neoantigens with T cell assays currently in CEDAR
- 3,397 neoantigens with positive T cell assay outcomes
- → meta-analysis of these neoantigens ongoing

Example Query: Neoantigens in Lung Cancer

Positive data for Neoantigen T cell assay outcomes with MHC Class I restriction in human host

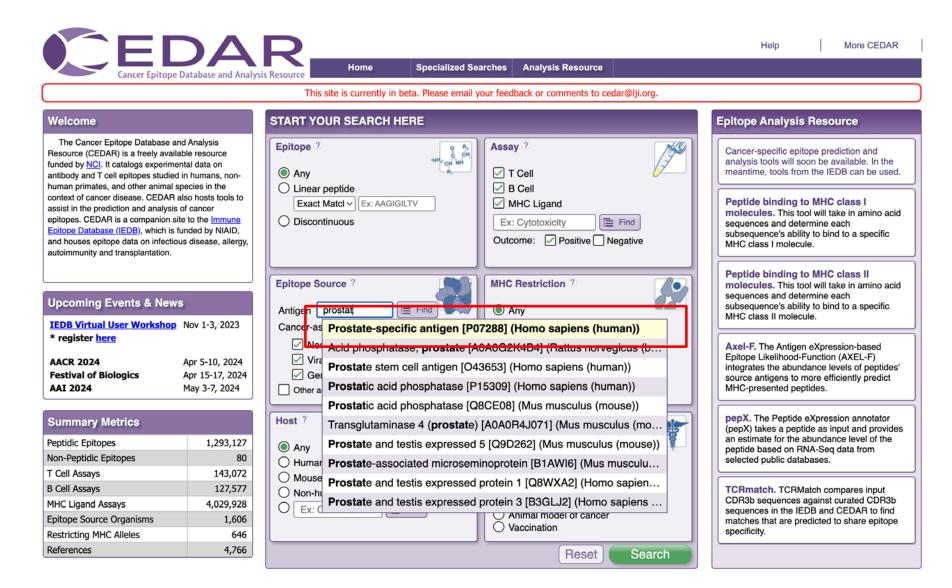


Example Results: Neoantigens in Lung Cancer

Positive data for Neoantigen T cell assay outcomes with MHC Class I restriction in human host

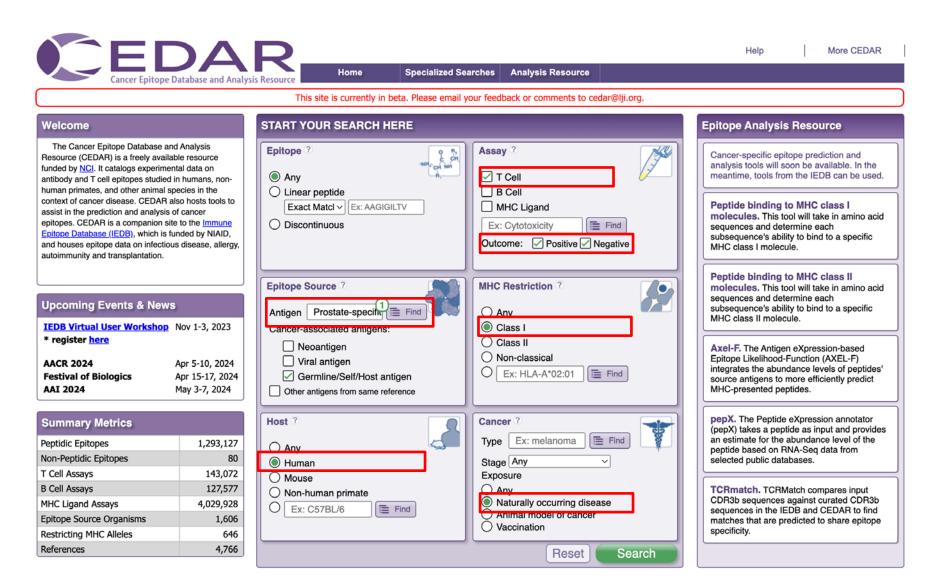
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Any Any	1101094	HVKITDFGRAK	Ϋ+	neoantigen: Epidermal gro	wth factor receptor	Homo sapiens (human)		2	2
Linear peptide	1104681	KITDFGRAK	Τ+	neoantigen: Epidermal gro	wth factor receptor	Homo sapiens (human)		2	6
Length	1312125	AIKTSPKANK	T+30	neoantigen: Epidermal gro	wth factor receptor	Homo sapiens (human)		2	2
Sequence	1312765	IPVAIKTSPK	T+3D	neoantigen: Epidermal gro	wth factor receptor	Homo sapiens (human)		2	2
Discontinuous	1334556	ATSPASASK	Τ+	neoantigen: Nuclear recep	or subfamily 4 group A member 1	Homo sapiens (human)		2	2
	1334611	MLICCCCTL	T+	neoantigen: Solute carrier	amily 12 member 4 (UniProt:Q9UP95)	Homo sapiens (human)		2	2
3D structure assays	1334628	SEHGFGPSL	T+	neoantigen: Mitochondrial	peptide methionine sulfoxide reductase	Homo sapiens (human)		2	2
nino acid modification	1334629	SEIISFKSL	T+	neoantigen: Fasciculation	and elongation protein zeta-1	Homo sapiens (human)		2	2
	1334647	VEWLGRCIL	Τ+	neoantigen: Chondroitin su	Ifate synthase 2	Homo sapiens (human)		2	2
itope Source ?	71668	VVGAVGVGK	Τ+	neoantigen: HRas proto-or	cogene, GTPase	Homo sapiens (human)		1	5
ganism 🛛 🚺	858771	ASNASSAAK	Τ+	neoantigen: Probable E3 u	biquitin-protein ligase HERC1	Homo sapiens (human)		1	5
Ex: influenza, peanut	858876	ETVSEQSNV	Τ+	neoantigen: Elongation fac	tor 2	Homo sapiens (human)		1	1
tigen	858895	FIASNGVKLV	Τ+	neoantigen: Alpha-actinin-		Homo sapiens (human)		1	7
Ex: core, capsid, myosin	858907	FLDEFMEGV		neoantigen: NADP-depend		Homo sapiens (human)		1	11
incer-associated antigens:	859210	MQLMPFGCLL		÷ .	in-tyrosine kinase (UniProt:Q504U8)	Homo sapiens (human)		1	1
Viral antigen	859309	QQITKTEV	Τ+		ription factor Y subunit gamma (Fragment)	Homo sapiens (human)		1	4
Germline/Self/Host antigen	1066141	LIMQLMPFGCL	T+30	neoantigen: Epidermal gro	wth factor receptor	Homo sapiens (human)	Τ+	+ 1	1
Other antigens from same reference	1087208	ETMQCSELYHM	Τ+	neoantigen: Kelch-like prot	ein 29	Homo sapiens (human)		1	1
	1087210	EVIVPLSGW	Τ+	neoantigen: ARVCF delta	atenin family member	Homo sapiens (human)		1	1
R ?	1087211	EVQQFLBY	T+	neoantigen: Xylosyl- and g	ucuronyltransferase LARGE1	Homo sapiens (human)		1	1
Has TCR sequence	1087238	QHQPNPFEV	Ϋ+	neoantigen: Inactive tyrosi	e-protein kinase PRAG1	Homo sapiens (human)		1	1
pe Any Type V	1087578	KLVVVGACGV		neoantigen: GTP-binding p		Homo sapiens (human)		1	1
Paired chains only	1113688	QPSGIILDY		neoantigen: Ephrin type-B		Homo sapiens (human)		1	1
	1114008	RAKLLGAEEK	T+80					1	1

Example Query: Prostate-specific Antigen



Example Query: Prostate-specific Antigen

Positive and negative data for T cell assay outcomes with MHC Class I restriction in human host



Example Results: Prostate-specific Antigen

Positive and negative data for T cell assays outcomes with MHC Class I restriction in human host

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	T+	1	1
	T+	. 1	1
Has TCR sequence	25 ~ F	Per Page Expo	ort Resu

Query can be refined further on the 'Results' page via our 'Filter Options'

Example Results: Prostate-specific Antigen

Epitope details page summarizes all assays and results for epitope



Specialized Searches Analysis Resource

EPITOPE SUMMARY

Home

KLQCVDLHV is a linear peptidic epitope (epitope ID 989936) studied as part of Prostate-specific antigen from Homo sapiens (human). This epitope has been studied for immune reactivity in 17 publication(s), tested in 67 T cell assays, 2 B cell assays and 10 MHC ligand assays.

MHC Ligand Assay(s) 10			
MHC molecule	Positive / All		
HLA-A2	5/5		
HLA-A*02:01	4/4		
HLA class I	1/1		
B Cell Assay(s) 2			
Assay Type	Positive / All		
qualitative binding	0/2		
T Cell Assay(s) 67			
Assay Type	Positive / All		
qualitative binding	13/13		
cytotoxicity	11/13		
IFNg release	7/12		
IL-4 release	3/5		
TNFa release	2/4		
IL-5 release	3/3		
proliferation	3/3		
type IV hypersensitivity (DTH)	3/3		
IL-10 release	1/3		
IL-13 release	2/2		
IL-2 release	2/2		
IL-12 release	0/2		
activation	1/1		
decreased disease	1/1		

EXTERNAL RESOURCES		
Resource	Link	
ANALYSIS TOOLS IEDB-AR: MHC-I Processing	Predict MHC class I processing &	
ANALYSIS TOOLS IEDB-AR: MHC-I	Predict MHC class I hinding affinity 🕼	

Additional Features Under Development (I)

Enable search for neoantigens derived from a specific amino acid mutation

Epitope S	Source (?		
Antigen	Ex: KRAS		
Cancer-a	ssociated antigens:		
🖌 Ne	eoantigen Mutation Ex. G12D		
Viral antigen			
Germline/Self/Host antigen			
Other antigens from same reference			

Additional Features Under Development (II)

Provide information about the mutation underlying the neoantigen

• Collaboration with external tools:

UCSC TransVar for mapping peptides to the genome (amino acid mutation vs DNA mutation)

OpenCRAVAT for retrieving information about the DNA mutation

Additional Features Under Development (II)

Provide information about the mutation underlying the neoantigen

EPITOPE SUMMARY		
MSAICQVY is a linear peptidic epitope (epitope ID 1	312368)., tested in 1 T cell assay	
COMPILED DATA		
Cell Assay(s) 1 Assay Type		Positive / All
activation		0/1
ARIANT INFORMATION		
Gene Symbol	1	MUC12
Protein Change		G121R
Uniprot Accession Number		Q9UKN1
Variant Type		Single Nucleotide Variant
Base Change		G>A
Chromosome		16
Position		16122155
dbSNP ID		rs750416230
1000 Genomes Allele Frequency		6.98*10 ⁻³
Damage Prediction		9/10 Damage Ratio
Clinical Relevance		
ClinVar Significance ClinVar Conditions		
Pathogenic (ID: 1	2584)	Non-small cell lung carcinoma; RASopathy
	OpenCRAV	AT Summary
EXTERNAL RESOURCES		
esource	Link	
ANALYSIS TOOLS IEDB-AR: MHC-I Processing	Predict MHC class I processing 🖉	
IEDB-AR: MHC-I	Predict MHC class I binding affinity	t
ANALYSIS TOOLS IEDB-AR: B cell scales	Predict B cell epitopes	





Computational epitope prediction and analysis tools providing researchers access to predictive strategies and objective evaluations of their performance

Overarching Analysis Resource Goals

- 1. Provide prediction tools <u>tailored to the needs of cancer</u> <u>immunologists</u>
- 2. Develop <u>novel prediction tools</u> for cancer epitopes
- 3. Provide web-implementations for published but hard to access cancer-epitope related tools in CEDAR
- 4. Use curated cancer epitope datasets to benchmark epitope prediction tools



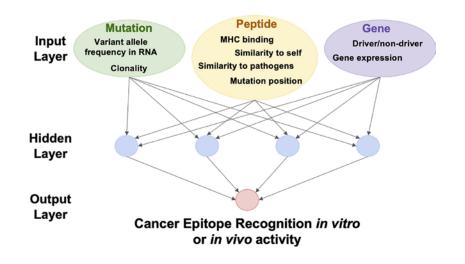
Develop <u>Novel Prediction Tools</u> for Cancer Epitopes

- 2 tools published recently
 - Axel-F: combined assessment of antigen expression and MHC binding
 - **pepX**: provides an estimate for the abundance level of the peptide based on RNA-Seq data from selected public databases such as TCGA, CCLE, etc



 include additional features when predicting epitopes

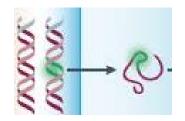




Provide prediction tools tailored to the needs of cancer immunologists (I)

• What neoepitopes are generated by a given DNA mutation?

DNA Protein Mutation Mutation



DNA Mutations in VCF format

##FORMAT = <id =="" dp<="" math="">, Number = 1, Type = Integer, Description = "Reference on the second se</id>						
##FORM	AT= <id=hq< td=""><td>,Number=2,T</td><td>ype=Ir</td><td>nteger,De</td><td>escrip</td><td>tion="Ha</td></id=hq<>	,Number=2,T	ype=Ir	nteger,De	escrip	tion="Ha
#CHROM	POS	ID	REF	ALT	QUAL	FILTER
20	14370	rs6054257	G	A	29	PASS
20	17330		т	A	3	q10
20	1110696	rs6040355	A	G,T	67	PASS
20	1230237		т		47	PASS
20	1234567	microsat1	GTC	G,GTCT	50	PASS

Mutated Peptides

IPDRAPGWTRNSCPAG KIPDRAPGWTRNSC RVKIPDRAPGWTR PDRAPGWTRNS

Provide prediction tools tailored to the needs of cancer immunologists (II)

• Side-by-side predictions for mutant and wild-type peptides

WT Peptide	MT Peptide	WT IC50	MTIC50	Δ IC50
IPDRAVGWTRNSCPAG	IPDRAPGWTRNSCPAG	30.63	278.54	247.91
KIPDRA <mark>V</mark> GWTRNSC	KIPDRA <mark>P</mark> GWTRNSC	4569.09	20.45	4548.64
RVKIPDRA <mark>V</mark> GWTR	RVKIPDRA <mark>P</mark> GWTR	789.43	3450.56	2661.13
PDRA <mark>V</mark> GWTRNS	PDRA <mark>P</mark> GWTRNS	7689.34	9870.23	2180.89

CEDAR & the Next-Generation Tools



Planned Releases

- <u>2.0</u> Target March 2024 Cancer-focused functionality
 - Peptide expression estimator (PepX)
 - Mutated peptide generation
 - Paired wild-type and mutant peptide predictions

IEDB Immune Epitope Database & Tools		Tools ▼ Help & Info ▼
Next-Generation IEDB Tools	immune epitopes.	
site released to public		New User? Learn to use the website here!
Appearances & Events	T Cell Prediction - Class MHC class I binding affinity, TA	L P processing, and Immunogenicity predictions
Virtuel 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	> SARS2 spike glycoprotein MFVFLVLLPLVSSQCVNLTTRT TEKSNIIRGWIFGTTLDSKTQSI	into this box or click 'Run' to use the example sequence:
Additional Resources	MHC Allele(s) Ex: HL	A-A*02:01
API	More tools coming soon.	
Downloads		https://nextgen-tools.iedb.org/

Provide web-implementations for published but hard to access cancer-epitope related tools in CEDAR

 Prioritize tools to implement in CEDAR based on cost-benefit analysis

Cell

Resource

Key Parameters of Tumor Epitope Immunogenicity Revealed Through a Consortium Approach Improve Neoantigen Prediction

Graphica	Abst	tract				
1.	Global	consortium to im	prove ne	oantigen pre	diction	
	LINCTEN	HLATyping	Sage →	Peptide Selection Along Falleries 90.4 Briston Almodiately 5.3	Byrthesis	
	1999 P	WES + RNA Sequencing		ATOREC_VENTINEY 6.8 ATOREC_VENTINEY 6.8	. .	ربر 🔘 مب

Authors

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LETTER

nature biotechnology ARTICLES

A large peptidome dataset improves HLA class I epitope prediction across most of the human population

Siranush Sarkizova^{1,2,13}, Susan Klaeger^{©,2,13}, Phuong M. Le³, Letitia W. Li³, Giacomo Oliveira³, Hasmik Keshishian², Christina R. Hartigan², Wandi Zhang³, David A. Braun^{2,3,4,5}, Keith L. Ligon^{2,4,6,7}, Pavan Bachireddy^{2,3,5}, Ioannis K. Zervantonakis[®]⁸, Jennifer M. Rosenbluth[®]⁸, Tamara Ouspenskaia², Travis Law^{®,2}, Sune Justesen⁹, Jonathan Stevens¹⁰, William J. Lane^{@,4,10}, Thomas Eisenhaure², Guang Lan Zhang^{3,4,11}, Karl R. Clauser², Nir Hacohen^{®,2,3,12*}, Steven A. Carr^{®,2*}, Catherine J. Wu^{®,2,3,4,5,11*}

doi:10.1038/nature24473

A neoantigen fitness model predicts tumour response to checkpoint blockade immunotherapy

Marta Luksza¹, Nadeem Riaz^{2,3}, Vladimir Makarov^{3,4}, Vinod P. Balachandran^{5,6,7}, Matthew D. Hellmann^{7,8,9}, Alexander Solovyov^{10,11,12,13}, Naiyer A. Rizvi¹⁴, Taha Merghoub^{7,15,16}, Arnold J. Levine¹, Timothy A. Chan^{2,3,4,7}, Jedd D. Wolchok^{7,8,15,16} & Benjamin D. Greenbaum^{10,11,12,13}

2023 IEDB User Workshop

Use curated cancer epitope datasets to benchmark epitope prediction tools

- Assemble comprehensive sets of cancer epitope data
- Make available in simple format for bioinformaticians for tool training and testing
- Conduct benchmarks of prediction tools on cancer epitope datasets
 - Manual compile and run benchmarks (initially)
 - Automated benchmarks of all tools implemented in CEDAR, using newly curated data

Examples of benchmark targets for prediction tools

- What peptides in a tumor sample are processed and presented on MHC
- What neo-epitopes are recognized by T cells from a cancer patient?

CEDAR at AACR 2024 – Booth 3753



Visit our booth!

Citing CEDAR in Research

JOURNAL ARTICLE

The Cancer Epitope Database and Analysis Resource (CEDAR) 👌

Zeynep Koşaloğlu-Yalçın ख़, Nina Blazeska, <u>Randi Vita</u>, Hannah Carter, Morten Nielsen, Stephen Schoenberger, Alessandro Sette, Bjoern Peters

Nucleic Acids Research, Volume 51, Issue D1, 6 January 2023, Pages D845–D852, https://doi.org/10.1093/nar/gkac902

Published: 17 October 2022 Article history •



CEDAR is an extension of the IEDB, containing cancer-related epitope data and tools





Literature curation is moving rapidly



Existing tools will be adapted to the needs of cancer researchers and novel cancer-specific tools will be developed. Cancer benchmark datasets are being assembled.



Community engagement has been initiated and will continually increase