Interactive Vaccine Designer

A portlet for the interactive design of individualized vaccines

Getting Started

The Interactive Vaccine Designer is avaiable as a portlet of [QPortal](#).

How-to

Data preperation

Upload file

1. Press the *Directory*-Button
2. Select the structure of your input data
   - Each allele in a row or the alleles as individual columns

3. Enter the column names as they are named in your input file.
   - Immunogenicity is always required
   - Method is required if the input includes data from several methods
   - TAA column is needed if the type of antigen is given (TAA/TSA), otherwise all input is handled as TSA

4. Specify the alleles and allele expressions
   - Make sure the alleles fit to your input file, this is not done automatically yet.

5. Choose a file from your directory and press the *Upload*-Button

⬆ Data Preperation

> ℹ Welcome to the **Interactive Vaccine Designer**. The functionality is based on [EpitopeSelector](#), a software package for RNA-Seq based neo-epitope selection. You can either **upload** your epitope prediction results from your computer or select one from our **database**.

[🖥 Directory]   [🗄 Database]

▸ Epitope Pre-Selection

⇄ Parameter Adjustment

◔ Results Overview

[⊗ Reset] [⊕ Next]

⬆ Data Preperation

> ℹ Your epitope prediction file has to be in one of the **following structures**. Choose the fitting structure.

Each allele in a row

...	...	...	HLA	...	...	...
ADEDSAGD	...	...	A*01:01	...	...	...
ADEDSAGD	...	...	A*02:02	...	...	...
ADEDSAGD	...	...	B*01:01	...	...	...
ADEDSAGD	...	...	B*02:02	...	...	...
ADEDSAGD	...	...	C*01:01	...	...	...
ADEDSAGD	...	...	C*02:02	...	...	...
...	...	...	...	...	...	...

Alleles as columns

...	A*01:01	A*02:02	B*01:01	B*02:02	C*01:01	C*02:02
ADEDSAGD	...	...	...	...	...	...
AGDLSDSE	...	...	...	...	...	...
ALSRTSQS	...	...	...	...	...	...
DSAGDLSD	...	...	...	...	...	...
GEWTVAPT	...	...	...	...	...	...
GKKVKGAQ	...	...	...	...	...	...
...	...	...	...	...	...	...

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▸ Epitope Pre-Selection

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◔ Results Overview

[⊗ Reset] [⊕ Next]

⬆ Data Preperation

> ℹ Specify the **column names** of your epitope prediction file. If the columns do not exist leave them empty.

Immunogenicity Column *

    prediction_score

Method Column

    method

Transcript Expression Column

    transcript_expression

TAA Column

Distance Column

Uncertainty Column

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▸ Epitope Pre-Selection

⇄ Parameter Adjustment

◔ Results Overview

⊗ Reset   ⊕ Next

⬆ Data Preperation

> ℹ Specify the corresponding **HLA alleles** and the **allele expressions** as FPKM values.

HLA-A alleles

HLA-A*03:01   *

HLA-A*68:01   *

HLA-B alleles

HLA-B*15:01   *

HLA-B*40:01   *

HLA-C alleles

HLA-C*03:03   *

HLA-C*03:04   *

HLA-A expression *	HLA-B expression *	HLA-C expression *
10	10	10

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↗ Epitope Pre-Selection

⇌ Parameter Adjustment

◕ Results Overview

⊗ Reset   ⊕ Next

Choose file from database

1. Press the *Database*-Button
2. Select if you want to choose an allele file from the database or manually enter the allele information (in this example the allele file is chosen from the database, too)
3. Select the structure of your input data
   - Each allele in a row or the alleles as individual columns

4. Enter the column names as they are named in your input file.
   - Immunogenicity is always required
   - Method is required if the input includes data from several methods
   - TAA column is needed if the type of antigen is given (TAA/TSA), otherwise all input is handled as TSA

5. Specify allele expressions
6. Choose a project from your space and the epitope prediction file of your choice. Also choose an allele file.
   - Make sure the allele-file fits to your input file, this is not done automatically yet.

⬆ Data Preperation

> ⓘ You can now decide wether you want to **upload** an allele file or choose one from our **database**. The allele file has to contain the alleles for which the epitope prediction has been performed.

⌨ Manual   🗄 Database

⬅

▶ Epitope Pre-Selection

⇄ Parameter Adjustment

◔ Results Overview

⊗ Reset   ⊕ Next

Epitope Pre-Selection

1. Select a method to view its peptides and corresponding information in the table.
2. Peptides you want to have in your final set can be marked as included.
3. Peptides you do not want to have in your final set can be marked as excluded, so they are ignored during the computation
4. Click on the *Next*-Button to continue.

Data Preperation

Epitope Pre-Selection

> ℹ Select the **peptide sequences** you would like to exclude or include in your final solution. Double click on the corresponding peptide and check one of the boxes. Click next to continue with the parameter settings.

Select a Method *

netmhcpan-3.0

Selection				
✅	❌	Neopeptide	Length	Mutation
☑	☐	**DLVTYQNHNKT**	**11**	**X_153135642**
☐	☑	ASPDLRDI	8	7_117874809
☐	☐	DELLVRLGE	9	20_34053635
☐	☐	HYVRCTRQVT	10	6_44241190
☐	☐	GSPGEKGALQS	11	10_102777991
☐	☐	GSKDDGKF	8	14_97327021
☐	☐	VIVPIVTA	8	13_33258074
☐	☐	APKTLPKAA	9	3_123383038
☐	☐	EMAAESLPFSF	11	12_57911177
☐	☐	DQRMCHPRC	9	5_167553854

Parameter Adjustment

Results Overview

⊗ Reset   ⊕ Next

Parameter Adjustment

1. Set the parameter values as needed, but be aware that for some parameter combinations the interavtive vaccine designer cannot compute a solution. Choose the parameters wisely.
2. Press the *Run*-Button to start the computation. Is the computation takes to much time it can be easily canceled by pressing the *Cancel*-Button. If the computation is not successfull a corresponding notification shows up and you should try to check if your parameters do make sense or if you falsely

described your epitope prediction or allele file.

Results Overview

1. After a successful computation you are directly forwarded to the *Results Overview*. Here you can see each result of your current session in a tab. The computet epitopes can be filtered through by clicking the pie charts.
2. The *Reset*-Button let you start from the beginning and allows you to upload a new file
3. The *Re-run*-Button allows you run a new computation with different parameters. Just click on the Parameter Adjustment or Epitope-Preselection tab and make some changes and finally press the *Re-run*-Button
4. The *Save*-Button downloads all of the computed results in a Text-File to save it on a directory on your Computer.
5. Did you choose the database file upload there is an additional Button called *Register*. That button registers your current results to the corresponding project in the database.

ⓘ Here are the **results** of your current session. You have now the following options:

- **Reset** all settings and upload new files
- **Save** the current results locally on your computer
- **Register** the current results in our database
- **Change parameters** and **re-run** the epitope selection (adds another tab to your results)

Result 1

Epitopes	TAAs	Epitope Threshold	Distance Threshold	Antigen Constraint
10	0	0	0	0

Allele Constraint	Overlap Constraint	Distance2Self	Uncertainty
0	0	0	0

Covered HLAs	Covered Antigens	Immunogenicity	Risk
100 %	20 %	418.95	0

Type

Filter by Type

TSA

Genes

Filter by Gene

OR10A6
L1CAM
ZNF148
CLTC
ARHGAP30
TMEM63B
DDIT3,MARS
TGFB3
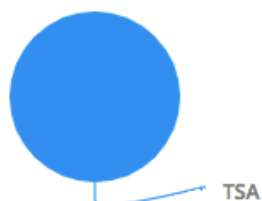
LAVDFMCFL	TSA	TMEM63B	6_44102460	0.059	0.205
FSSIDRQVY	TSA	ZNF148	3_124951627	0.083	0.234
AEMAAESLPF	TSA	DDIT3,MARS,MIR6758,MIR616	12_57911177	0.184	0.069
LSFDATDTV	TSA	TGFB3	14_76437504	0.058	0.174
HVVGAMQLY	TSA	CLTC	17_57725608	0.271	0.615
DLVTYQNHNKT	TSA	L1CAM	X_153135642	0.039	0.09

Alleles

Allele	log2(tumor_expression)
A*03:01	3.32
A*68:01	3.32
C*03:03	3.32
B*15:01	3.32
B*40:01	3.32
C*03:04	3.32

Genes

Gene	log2(tumor_expression)
ARHGAP30	6.91
TMEM63B	7.54
DDIT3,MARS,MIR6758,MIR616	6.69
TGFB3	7.16
CLTC	7
ZNF148	7.97
L1CAM	5.93
OR10A6	8.08
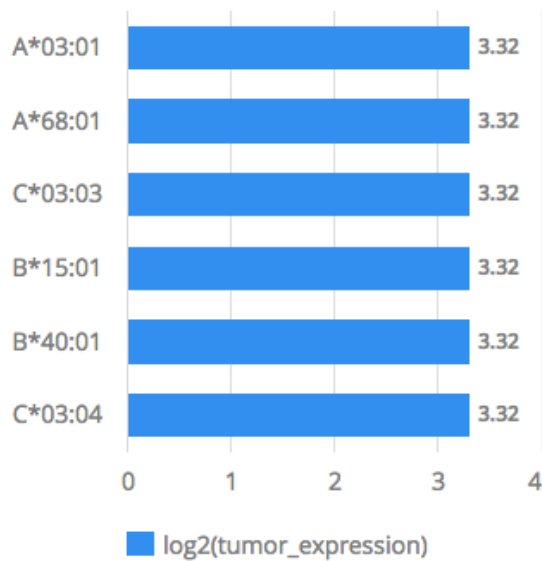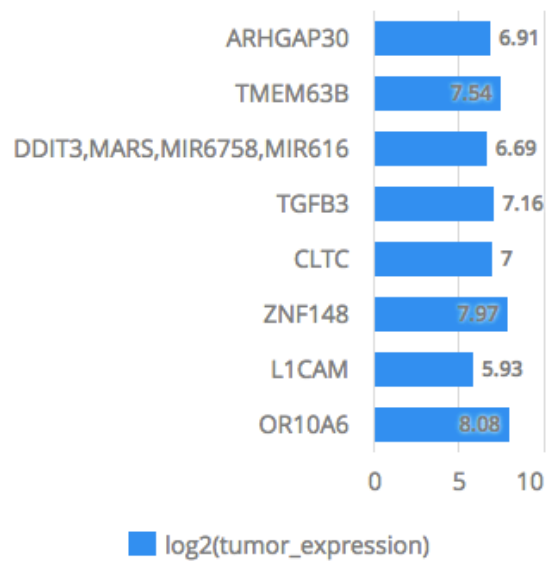
⊗ Reset   ⬇ Save   ⊙ Re-Run

Built With

- Vaadin - Java Web Framework
- Maven - Dependency Management
- EpitopeSelector - Software package for RNA-Seq based neo-epitope selection

Authors

- **Julian Späth** - *Initial work* - Quantitative Biology Center Tübingen

Problems

If you recognize any bugs or other problems please send an e-mail with the description of your problem directly to [Julian Späth](#).