B-CELL CONFORMATIONAL EPITOPE PREDICTION: CURRENT STATUS AND FUTURE DIRECTION

Dr. zhiwei cao

Tongji University, shanghai China
Outline

Introduction

Can we predict the conformational epitope?
- Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro, SEPPA
- B-Pred---a structure based B-cell epitopes prediction server (?)
- Evaluation

How to improve -- Future?

Software Demo: SEPPA
• Antigen-antibody interaction

• B-cell epitope
  • Linear epitope
  • Conformational epitope

Sperm whale myoglobin

Hen egg-white lysozyme
Can we predict the conformational epitope?

Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro

- SEPPA Version 1.0---Spatial Epitope Prediction of Protein Antigens
- B-Pred---a structure based B-cell epitopes prediction serve

Software Demo: SEPPA
1. CEP

CEP (http://bioinfo.ernet.in/cep.htm)
a conformational epitope prediction server


- **Featured**
  - Solvent accessibility of surface residues
  - Spatial distance cut-off
Conformational Epitope Prediction Server

Developed at Bioinformatics Centre, University of Pune, INDIA

Bioinfo@UoP | CE Server | Help

Email: shriam@bioinfo.ernet.in

Enter a PDB ID: 1FDL

OR Upload your coordinate file in PDB format:

Sample inputfile (Lysozyme)
Sample outputfile (Lysozyme)
Evaluation data of CEP algorithm using Ag-Ab complexes from PDB
Precomputed Dataset

Please note:
1. This server predicts conformational epitopes only for proteins
2. Your prediction may vary with and without explicit addition of hydrogens
3. In case of a Ag-Ab complex, submit the coordinates of only the antigen
4. Files with more than 0.5Mb size takes longer time (~3-5 Min)

Comments: cep@bioinfo.ernet.in
2. DiscoTope

Prediction of residues in discontinuous B-cell epitopes using protein 3D structures.


• Featured
  • Amino acid statistics-\(\rightarrow\) propensity scale matrixes
  • Spatial information
  • Surface exposure
3. ELLiPro

ELLiPro (http://tools.immuneepitope.org/tools/ELLiPro) is a novel structure-based tool for the prediction of antibody epitopes.


- Featured
  - simplified the surface of protein antigens as an ellipsoid
  - Calculated the *protruding index* for surface residues.
ELLiPro: Antibody Epitope Prediction

Step 1. Input type
Choose an input type:
- Protein sequence (Go to step 2a)
- Protein structure

Step 2a. Protein sequence
Enter a protein swiss-prot ID:
Or enter a protein linear sequence in PLAIN or FASTA format:
Blast expectation values: 10
Maximum number of 3D structural template(s): 5

Step 2b. Protein structure
Enter a 4 letter code PDB ID:
Or enter a protein structure PDB file:

Step 3. Epitope prediction parameters
Minimum score: 0.6
Maximum distance (Angstrom): 6

ELLiPro: Antibody Epitope Prediction Results

Predicted Linear Epitope(s):

Predicted Discontinuous Epitope(s):

Residue Scores:
4. PEPOP

PEPOP
Computational design of immunogenic peptides


- Featured
  - Similar to CEP
  - Solvent accessible surface *cluster*
  - Conformational character
5. BEpro

Bepro
Improved discontinuous B-cell epitope prediction using multiple distance thresholds and half sphere exposure


- Featured
- improved DiscoTope
  - Spatial attribute of half sphere exposure
  - Solvent accessibility of surface residues
6. SEPPA

SEPPA
A computational server for Spatial Epitope Prediction of Protein Antigens

• Key question
  • An effective method for B-cell epitope prediction

• Featured
  • Propensity index of Unit patch of residue-triangle
  • Topological parameter---clustering coefficient
7. B-pred

- B-pred (http://immuno.bio.uniroma2.it/bpred)
- a structure based B-cell epitopes prediction server

Luciano Giaco, et.al *Advances and Applications in Bioinformatics and Chemistry* 2012:5 11–21

- Featured
  - Sliding window
  - Average solvent exposure
B-pred

Job summary
Job password: WMnsFg
pdb file: 1P9M.pdb
Structure name: CRYSTAL STRUCTURE OF THE HEMAMERIC HUMAN IL-6/IL-6 ALPHA RECEPTOR/GP130 COMPLEX

Change parameters and reload
Chain: A, Naaccess threshold: 40.98, Verify3D threshold: 0.2, Peptides length: 20, Sliding offset: 3, Analyse 1P9M.pdb

Output options
- Full sequence overview
- Full peptide results summary
- Local peaks/hotspots report
- Quick view in 3mol
- Solvent accessibility plot (naaccess)
- Model quality plot (verify3D)

Full sequence overview
Aminoacids marked in red belong to an hotspot (naaccess and V3D values above the settled thresholds)
Aminoacids marked with an underline belong to an interface
Aminoacids in LIGHT GREY are not present in the structure file and do not have an associated naaccess or V3D value
Mouseover on any aminoacid for more information

Peptide scan results summary for chain A of 1P9M.pdb
Aminoacids marked in red belong to an hotspot (naaccess and V3D values above the settled thresholds)
Aminoacids marked with an underline belong to an interface

<table>
<thead>
<tr>
<th>Sequence start</th>
<th>Sequence End</th>
<th>Peptide sequence</th>
<th>Solvent exposure</th>
<th>Structure quality</th>
<th>Positive</th>
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<tbody>
<tr>
<td>1</td>
<td>20</td>
<td>LLDPCGYISP EPSPVPVQLHSNFT</td>
<td>51.226</td>
<td>0.504</td>
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<tr>
<td>4</td>
<td>23</td>
<td>DPCGYISP EPSPVPVQLHSNFT</td>
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<td>0.510</td>
<td>1</td>
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<tr>
<td>7</td>
<td>26</td>
<td>GYISPE PVCPSVPVQLHSNFTAVC</td>
<td>38.355</td>
<td>0.511</td>
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<tr>
<td>10</td>
<td>29</td>
<td>SPESPVPVQLHSNFTAVCGLK</td>
<td>39.270</td>
<td>0.498</td>
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<tr>
<td>13</td>
<td>32</td>
<td>SPVQLHSNFTAVCGLKKEK</td>
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<td>0.509</td>
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<tr>
<td>16</td>
<td>35</td>
<td>VQLHSNFTAVCGLKKEK</td>
<td>42.800</td>
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<tr>
<td>19</td>
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<td>HSNFTAVCGLKKEKMDYFHV</td>
<td>41.520</td>
<td>0.528</td>
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<td>22</td>
<td>41</td>
<td>FTAVCGLKKEKMDYFHVNAN</td>
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<td>0.529</td>
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<tr>
<td>25</td>
<td>44</td>
<td>VVLKERKMDYFHVNANAYIV</td>
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<tr>
<td>28</td>
<td>47</td>
<td>LKERKMDYFHVNANYIVYR</td>
<td>38.865</td>
<td>0.550</td>
<td></td>
</tr>
</tbody>
</table>
Can we predict the conformational epitope?

- Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro

Evaluation

Software Demo: SEPPA
Evaluation of spatial epitope computational tools

- **Dataset**
- **IEDB & CED:**
  - 110 antigen-antibody complexes crystal structure (antigen sequences > 50 amino acids)

- **Parameters**
  - Sensitivity, positive predictive value, successful pick-up rate and Area under receiver operating characteristic curve (AUC)
**Results of evaluation**

<table>
<thead>
<tr>
<th>Methods</th>
<th>Sensitivity</th>
<th>Positive predictive value</th>
<th>The successful pick-up rate (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SEPPA</td>
<td>0.4914</td>
<td>0.2650</td>
<td>55.50</td>
</tr>
<tr>
<td>DiscoTope</td>
<td>0.3565</td>
<td>0.2116</td>
<td>40.00</td>
</tr>
<tr>
<td>BEpro</td>
<td>0.1789</td>
<td>0.2205</td>
<td>28.20</td>
</tr>
<tr>
<td>CEP</td>
<td>0.1774</td>
<td>0.1720</td>
<td>8.18</td>
</tr>
<tr>
<td>PEPOP</td>
<td>0.1973</td>
<td>0.1946</td>
<td>2.73</td>
</tr>
<tr>
<td>ElliPro</td>
<td>0.0676</td>
<td>0.1580</td>
<td>3.64</td>
</tr>
</tbody>
</table>

- **Sensitivity**: The proportion of true positive tests out of the total number of tests that are positive.
- **Positive predictive value**: The proportion of positive tests that are true positives.
- **The successful pick-up rate (%)** indicates the successful rate of picking the target items.
Can we predict the conformational epitope?
- Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro, SEPPA
- B-Pred---a structure based B-cell epitopes prediction server (?)
- Evaluation

How to improve -- Future?

Software Demo: SEPPA
Future improvement

• Research status
  • Hydrophilic, accessibility, antigenicity, flexibility, charge distribution, secondary structure and etc.
  • The prediction accuracies of previous methods are underperformance
  • “...available prediction methods based on unidirectional analysis do not cope satisfactorily with the three dimensional reality of antigenic sites.”

• Key question
  • Does difference exist between B-cell epitope and non-epitope residues?
• Key question
  • Does difference exist between B-cell epitope and non-epitope residues?

Research procedure

Dataset

• Antigen-antibody immunoglobulin complex structure dataset
• B-cell epitope dataset

Methods

• Physical-chemical features
• Sequence feature
• Regional 3-D structural features

PDB: 1A14:N
Dataset

- PDB (dated April 28th, 2011)

Keyword search:
- antibody
- antigen
- Fab
- Fv
- Fc
- IgG
- immu*

Resolution: < 3 Å

Antigen length: > 50 aa

Epitope similarity: < 85%

161 PDB structures of immunoglobulin complex
166 B-cell epitopes
**Results**

**Epitope size**

1. The number of residue Fig. (A)
2. The sum of ASA
3. Distances among epitope residues

**Comparison between epitope and protein residue numbers** Fig. (B)

**Conclusion**

The relative constancy of epitope size is partially determined by the size of CDR

**Result**

Range: 15 ~ 30 AA  
Average(μ): 22.18±7.53 AA  
Outlier data 1BGX:T  80 AA  
Average(μ): 21.83±6.04 AA  

The Coefficient of Variance of epitope and protein residue numbers \(CV = \sigma/\mu\)  
\[CV_{\text{epitope}} = 0.36\]  
\[CV_{\text{protein}} = 0.74\]
Continuity

... 323 324 325 326 327 328 329 330 ... 339 340 341 ...
... THR ASP ASN PRO ARG PRO ASN ASP ... ASP PRO TYR ...

Core residue  Surface residue  Epitope residue

• Result
  • There are about 80% segments with a length less than 3 residues
  • There are at least one segment with a length more than 3 residues in most epitopes (165/166)
  • The longest segment in most epitopes (143/166) is more than 5 residues

• Conclusion
  • B-cell epitopes are defined spatially, but still comprised linear segments
Accessibility

• Hypothesis
  • Interaction residues tend to have higher accessible surface area (ASA)

• Relative ASA
  \[ \text{relASA} = \frac{ASA}{\text{index}_i} \]  
  \( (\text{index}_i: \) the ASA of amino acid X in tri-peptide ALA-X-ALA) \]

• Result
  • Epitope residues are with higher \text{relASA} than non-epitope surface residues
  • Significant differences have been observed in 82/166 (49.40%) data

Epitope preference of residue

Preference of amino acid classes

- Result
  - Residues with charged, polar, larger and aromatic R-groups tend to appear on epitope regions
Sequence conservation

• Result
  • Epitope residues are relatively less conservative comparing to non-epitope surface residues
  • Significant differences have been observed in 57/166 (34.34%) data

• Conclusion
  • Immune escape

ConSurf
Server for the Identification of Functional Regions in Proteins

• **Result**
  - Epitope residues are surrounded with less neighboring residues
  - The neighboring residues of epitope residues are more compact
- Prediction performance and comparison

<table>
<thead>
<tr>
<th>PDB_chain</th>
<th>Antibody organism</th>
<th>Organism-independent</th>
<th>Organism-based</th>
</tr>
</thead>
<tbody>
<tr>
<td>3QWO_C</td>
<td>Mus musculus</td>
<td>0.65</td>
<td>0.74</td>
</tr>
<tr>
<td>3AY4_C</td>
<td>Homo sapiens</td>
<td>0.88</td>
<td>0.94</td>
</tr>
<tr>
<td>3SE9_G</td>
<td>Homo sapiens</td>
<td>0.76</td>
<td>0.75</td>
</tr>
<tr>
<td>3SE8_G</td>
<td>Homo sapiens</td>
<td>0.82</td>
<td>0.81</td>
</tr>
<tr>
<td>3SDY_B</td>
<td>Homo sapiens</td>
<td>0.58</td>
<td>0.71</td>
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<tr>
<td>3NPS_A</td>
<td>Homo sapiens</td>
<td>0.78</td>
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<tr>
<td>3RKD_A</td>
<td>Mus musculus</td>
<td>0.39</td>
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<tr>
<td>3SKJ_E</td>
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<td>0.51</td>
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<td>0.78</td>
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<td>3SGJ_C</td>
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<td>3SGK_C</td>
<td>Homo sapiens</td>
<td>0.92</td>
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<tr>
<td>Average</td>
<td></td>
<td>0.72</td>
<td>0.77</td>
</tr>
</tbody>
</table>

**AUC value**

- **t-test:** p<0.01

**Methods**

- Antibody organism-based analysis and prediction
<table>
<thead>
<tr>
<th>Category</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>General characteristics</td>
<td>B-cell epitope size (the number of residues, ASA, and regional distances)</td>
</tr>
<tr>
<td></td>
<td>B-cell epitope sequence continuity</td>
</tr>
<tr>
<td>Physical chemical features</td>
<td><strong>Accessibility</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Epitope preference (residue, residue-pair, and residue-triangle)</strong></td>
</tr>
<tr>
<td></td>
<td>AAindex amino acid indices (544 indices)</td>
</tr>
<tr>
<td>Sequence features</td>
<td><strong>Sequence conservation</strong></td>
</tr>
<tr>
<td>Regional structural epitope</td>
<td><strong>Topological parameters (degree and clustering coefficient)</strong></td>
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<tr>
<td></td>
<td>Gaussian curvature</td>
</tr>
<tr>
<td></td>
<td><strong>Protruding index</strong></td>
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<tr>
<td></td>
<td><strong>Planarity index</strong></td>
</tr>
<tr>
<td>Epitope-paratope interaction pattern</td>
<td>Epitope-paratope residues interaction preference</td>
</tr>
</tbody>
</table>
Thank You!


Outline

- What area does antibody recognize?

- Can we predict the conformational epitope?
  - Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro
  - SEPPA Version 1.0---Spatial Epitope Prediction of Protein Antigens

- B-Pred---a structure based B-cell epitopes prediction serve

- Software Demo: SEPPA
Outline

- What area does antibody recognize?

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- Software Demo: SEPPA
Method

- The definition of unit patch of residue-triangle
  - Three surface residues, the least distances between any two among the three
  - Cutoff: 4Å
  - Epitope/non-epitope surface residue-triangle

- Why the definition?
  - Different epitope preference of different types of residue-triangle
  - All epitope residues function as a whole
- The generation of residue-triangle preference (training part)

Single amino acid types

Residue-triangle types

Residue-triangle frequencies

Residue-triangle preference

\( r_i \): A, R, N, D, C, Q...

\( t_m \): (A, A, R), (R, D, Q), (N, C, Q)...

\( O_{t_m} \)

\( R_{t_m} = \frac{(O_{t_m})_{\text{epitope}}}{(O_{t_m})_{\text{non-epitope}}} \)
• The scoring of residue-triangle preference (prediction part)

For any surface residue $r_1$:

- Collection of neighboring residue-triangles
- The sum of residue-triangle preference score
- Averaged by the number of residue-triangles
Single amino acid types

Residue-triangle types

Residue-triangle frequencies

Residue-triangle preference

Protein antigen X

Any surface residue

Collection of neighboring residue-triangles

The sum of residue-triangle preference score

Averaged by the number of residue-triangles

Clustering coefficient

Training dataset

Residue antigenicity score

SEPPA --- Spatial Epitope Prediction of Protein Antigens
Results

<table>
<thead>
<tr>
<th>The prediction performance of SEPPA</th>
<th>Testing dataset</th>
<th>AUC</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) SEPPA training dataset</td>
<td>0.77</td>
<td></td>
</tr>
<tr>
<td>(b) IEDB dataset</td>
<td>0.76</td>
<td></td>
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<tr>
<td>(c) DiscoTope training dataset</td>
<td>0.80</td>
<td></td>
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<tr>
<td>(d) Epitome dataset</td>
<td>0.75</td>
<td></td>
</tr>
</tbody>
</table>

- Evaluation methods
  - ROC and AUC value
  - Successful pick-up rate

<table>
<thead>
<tr>
<th>Comparison of prediction performance</th>
<th>Methods</th>
<th>Average AUC</th>
<th>Successful pick-up rate</th>
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</thead>
<tbody>
<tr>
<td>SEPPA (1.80)</td>
<td>0.64</td>
<td>96.64%</td>
<td></td>
</tr>
<tr>
<td>CEP</td>
<td>0.52</td>
<td>NA</td>
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<tr>
<td>DiscoTope (-7.70)</td>
<td>0.60</td>
<td>89.08%</td>
<td></td>
</tr>
<tr>
<td>BEpro (1.30)</td>
<td>0.56</td>
<td>90.76%</td>
<td></td>
</tr>
</tbody>
</table>
Outline

- Can we predict the conformational epitope?
  - Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro, SEPPA
  - B-Pred---a structure based B-cell epitopes prediction server (?)
  - Evaluation

- How to improve -- Future?

- Software Demo: SEPPA
For conformational B-cell epitope prediction

Input $\rightarrow$ 3D protein structure

Output $\leftarrow$ Score to each residue

Higher score corresponds to higher probability the residue to be involved in an epitope

- An existing PDB ID
- A protein structure with a PDB format
SEPPA Homepage

http://lifecenter.sgst.cn/seppa/index.php

Please choose one submission method:

1. Enter an existing PDB ID and chain(s):
   PDB ID:    Chain(s):   

2. Or upload a local file in PDB format
   * A local file without chain ID column could also be uploaded for prediction.
   PDB File:  选择文件  未选择文件
   Chain(s):  

Please specify a threshold:

Threshold:  1.80

Submit  Reset
http://bio.shmtu.org
Refined crystal structure of the influenza virus N9 neuraminidase-NC41 Fab complex

Molecular Description (from PDB)

<table>
<thead>
<tr>
<th>Classification</th>
<th>Hydrolase (o Glycosyl)</th>
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<tr>
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<td>Molecule:</td>
<td>INFLUENZA A SUBTYPE N9 NEURAMINIDASE</td>
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<td>Polymer:</td>
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<td>Type:</td>
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<td>Length:</td>
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<td>EC#:</td>
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<td>Molecule:</td>
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<tr>
<td>Chains:</td>
<td>L</td>
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<tr>
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<tr>
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More information

http://www.rcsb.org/pdb/explore/explore.do?structureId=1NCA
Please choose one submission method:

1. Enter an existing PDB ID and chain(s):
   - PDB ID: [field]
   - Chain(s): [field]

2. Or upload a local file in PDB format:
   - A local file without chain ID column could also be uploaded for prediction.
   - PDB File: [field] 1NCA.pdb
   - Chain(s): [field] N

Please specify a threshold:

- Threshold: [field] 1.80

Submit [Button] Reset [Button]
Parameter Threshold

The default value of THRESHOLD is set at 1.80.

lower threshold \rightarrow more residues will be included as predicted epitope residues

<table>
<thead>
<tr>
<th>Threshold</th>
<th>Sensitivity</th>
<th>Specificity</th>
<th>Accuracy</th>
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</thead>
<tbody>
<tr>
<td>1.55</td>
<td>0.959</td>
<td>0.259</td>
<td>0.377</td>
</tr>
<tr>
<td>1.60</td>
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<td>1.65</td>
<td>0.859</td>
<td>0.452</td>
<td>0.531</td>
</tr>
<tr>
<td>1.70</td>
<td>0.778</td>
<td>0.558</td>
<td>0.612</td>
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<td>1.75</td>
<td>0.672</td>
<td>0.658</td>
<td>0.684</td>
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<tr>
<td>1.80</td>
<td>0.568</td>
<td>0.740</td>
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<td>1.85</td>
<td>0.459</td>
<td>0.810</td>
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</tbody>
</table>
Antigenic Prediction for 1NCA.pdb:

Chain: N
Threshold: 1.80
Number of total residues: 389
Number of predicted epitope residues: 39

View 3D structure in Jmol

Predicted result format: **EPITOPE RESIDUE** | NON-EPITOPE RESIDUE | core residue

Download the score file

Explain the result
Tints from blue to red represent a rising antigenicity.
Selecting the "Highlighted epitope residues predicted" checkbox

Selecting the "Label epitope residues predicted" checkbox
View 3D structure in Jmol

1NCA_N

Residues in the structure are colored with tints from blue to red, which correlate positively with a rising antigenicity.
A glance of the prediction result

<table>
<thead>
<tr>
<th>Residue Range</th>
<th>Sequence</th>
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</thead>
<tbody>
<tr>
<td>1-50</td>
<td>IRDFNNLTKG LCTiNSWHIY GKDNAvRIgE DSDVLvTREp YvsCDPDECR</td>
</tr>
<tr>
<td>51-100</td>
<td>fyaLSQGTITI RGKSNGTIH DRSQYRALIs WPLSSPPTVY NSRVECIGWS</td>
</tr>
<tr>
<td>101-150</td>
<td>stSCHDgKTR MSiciSGPN NaSaViWYNR RPVTENTwA RNIRlRTQEsE</td>
</tr>
<tr>
<td>151-200</td>
<td>CVCHNgVCPv VfTdGSAgTP AETriYyfKE gKILKEPLA GTAKHIEECS</td>
</tr>
<tr>
<td>201-250</td>
<td>CYgERAEITc tcRdNWqGsn RpViRlDPVA MTHTSQyICS pVLTdNPTEGR</td>
</tr>
<tr>
<td>251-300</td>
<td>DPTVGKCNDp YPGNNNgLVK gFSyLDGVNT w1GRTISIAS RsSyEmLKVp</td>
</tr>
<tr>
<td>301-350</td>
<td>NaLTDDKSkP TQGQTivLNT DwSiSYGsgSfm DYWAEGCYR aCfYvelIRG</td>
</tr>
<tr>
<td>351-400</td>
<td>RPKEDKvWWT SNsIvsMCSS TEFLGQQWDWP DGAKIEYFL</td>
</tr>
</tbody>
</table>

Notes:
Residues are listed sequentially.
The predicted epitope residues are highlighted in yellow.
The core residues are shown in lowercase.
### SEPPA Prediction Result

#### Antigenic Prediction for 1NCA.pdb:

- **Chain:** N
- **Threshold:** 1.80
- **Number of total residues:** 389
- **Number of predicted epitope residues:** 39

<table>
<thead>
<tr>
<th>chainID</th>
<th>resSeq</th>
<th>resName</th>
<th>score</th>
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</thead>
<tbody>
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<tr>
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<td>91</td>
<td>LEU</td>
<td>1.39</td>
</tr>
</tbody>
</table>
Multiple PDB ID entries

include PDB ID and chain ID(s), which are separated with space(s) in one line

Batch query with structures of existing PDB IDs:

- Enter PDB IDs and chains:

  1WCA  N
  1A14  N
  1NDM  C

Please specify a threshold:

Threshold: 1.80

Submit  Reset