同濟大學
TONGJI UNIVERSITY

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

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Outline

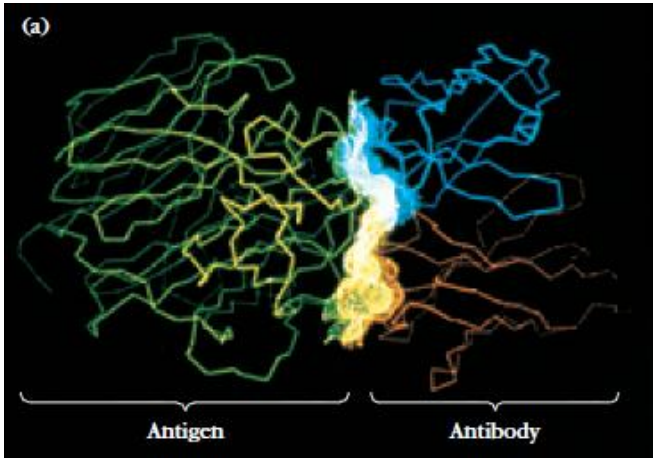
- **Introduction**

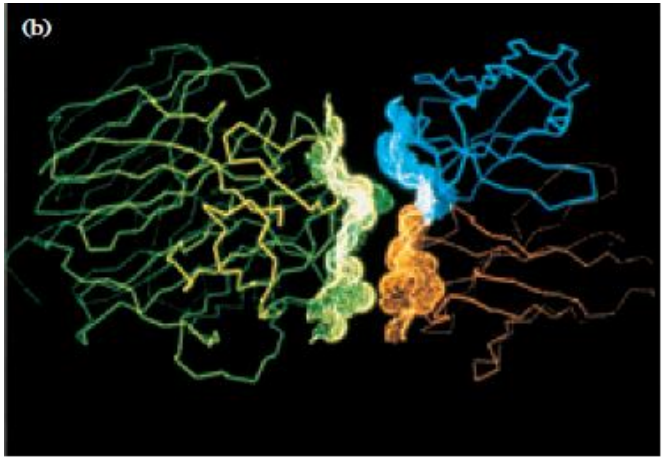
- Can we predict the conformational epitope?
  - Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro , SEPPA
  - B-Pred---a structure based B-cell epitopes prediction server (?)
  - Evaluation

- How to improve -- Future?

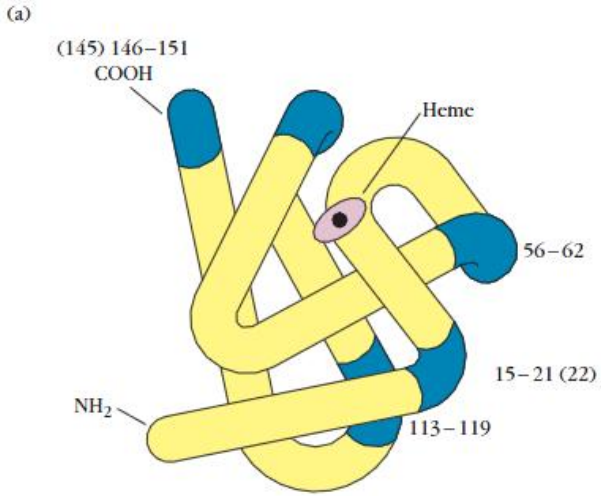
- Software Demo: SEPPA

- Antigen-antibody interaction

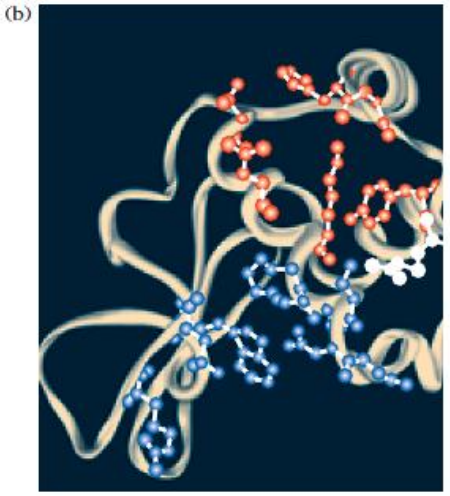




- B-cell epitope
  - Linear epitope
  - Conformational epitope



Sperm whale myoglobin



Hen egg-white lysozyme

Outline

- **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

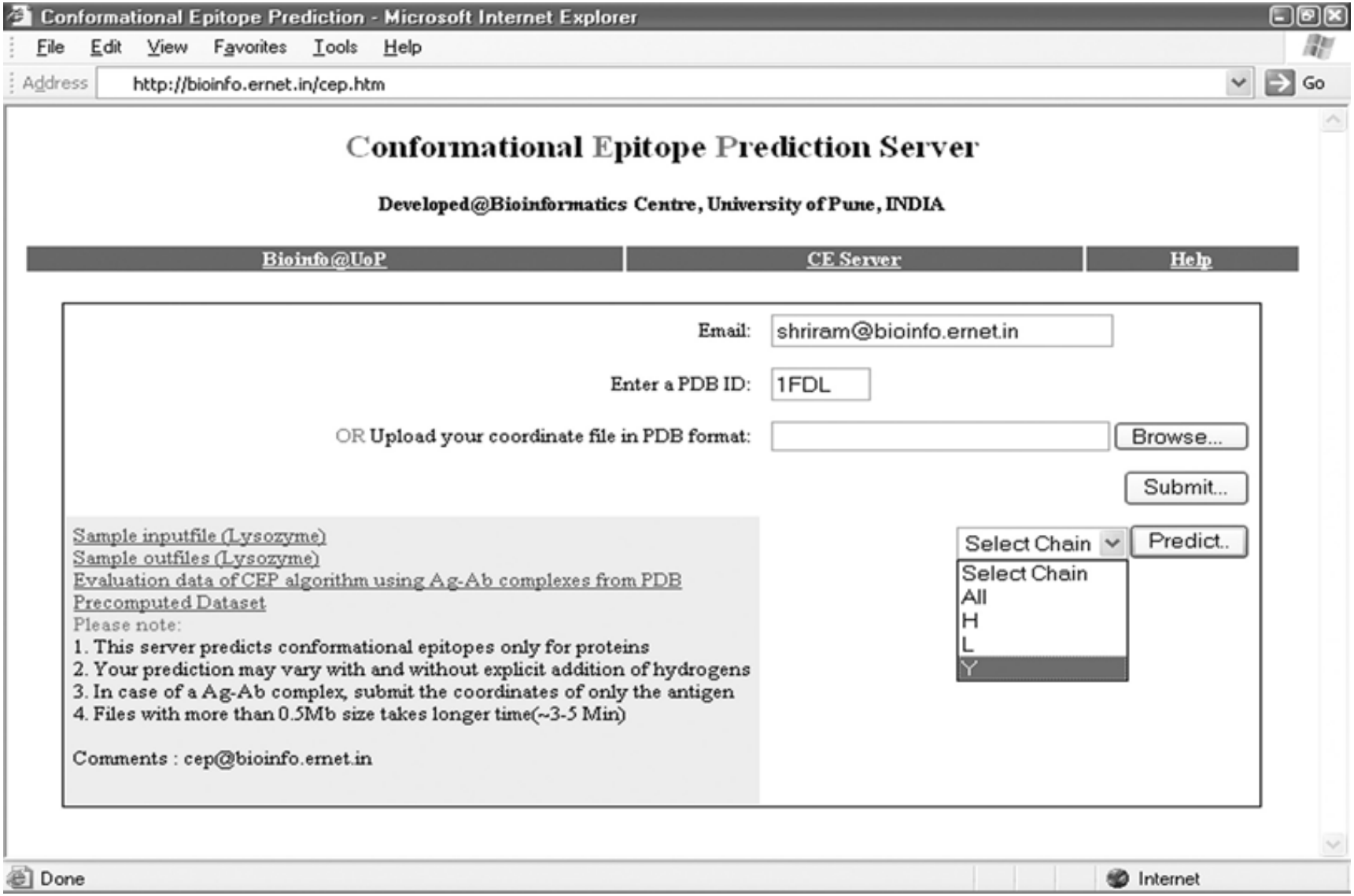
CEP (http://bioinfo.ernet.in/cep.htm)

a conformational epitope prediction server

Kulkarni-Kale U, et.al *Nucleic Acid Res*, 2005,33: W168-171

- Featured
  - Solvent accessibility of surface residues
  - Spatial distance cut-off

CEP


Conformational Epitope Prediction - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Address http://bioinfo.ernet.in/cep.htm
Go
Conformational Epitope Prediction Server
Developed@Bioinformatics Centre, University of Pune, INDIA
Bioinfo@UoP
CE Server
Help
Email: shriram@bioinfo.ernet.in
Enter a PDB ID: 1FDL
OR Upload your coordinate file in PDB format:
Browse...
Submit...
Sample inputfile (Lysozyme)
Sample outfiles (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
Select Chain
Predict..
Select Chain
All
H
L
Y
Done
Internet

2. DiscoTope

DiscoTope

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

Haste-Andersen P, et.al *Protein Sci,* 2006,15(11): 2558-2567

- Featured
  - Amino acid statistics-→propensity scale matrixes
  - Spatial information
  - Surface exposure

3. ELLiPro

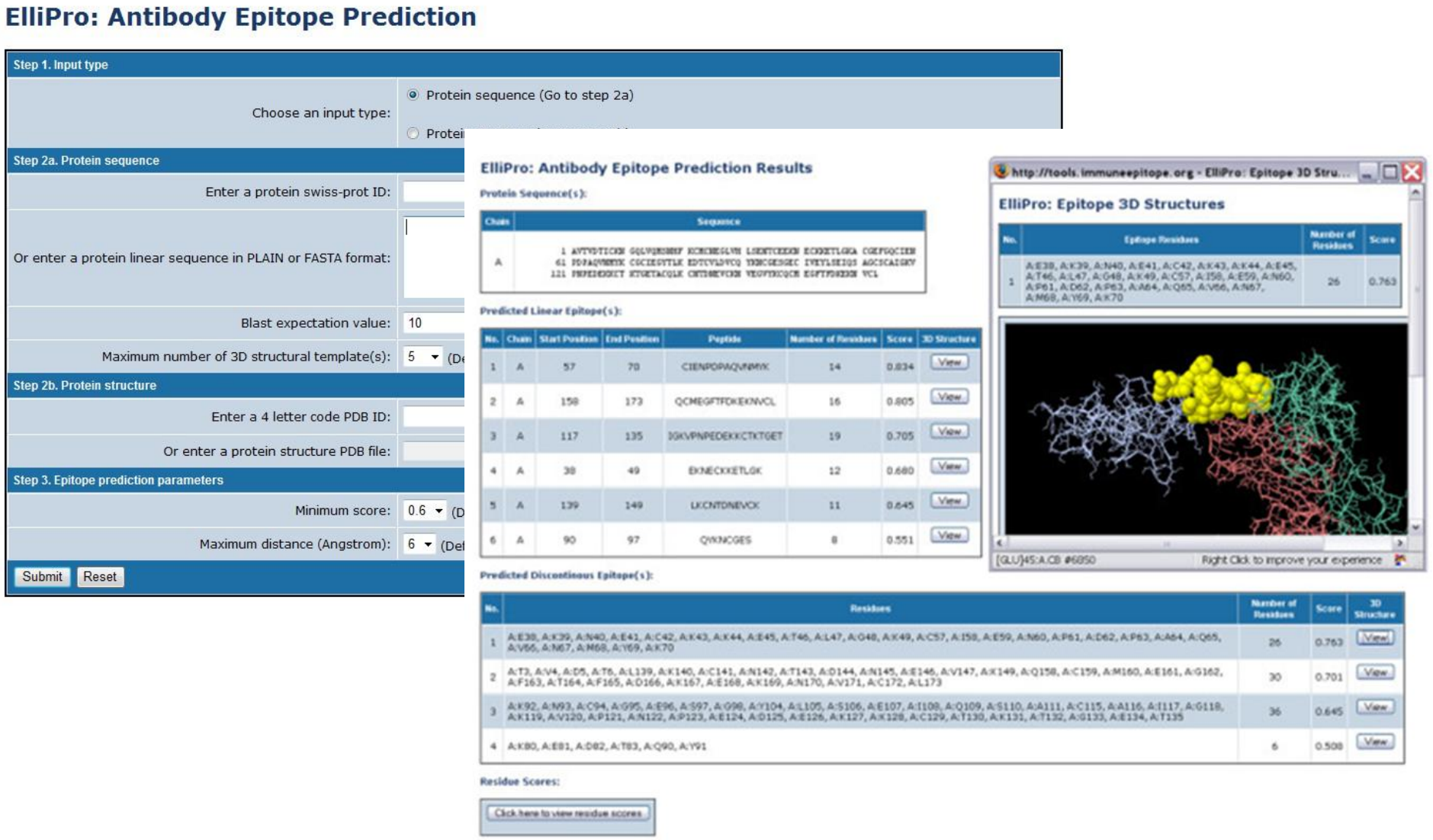
ElliPro (http://tools.immuneepitope.org/tools/ElliPro)

A now structure-based tool for the prediction of antibody epitopes

Ponomarenko J, et.al *BMC Bioinformatics*, 2008,9:514-522

- Featured
  - simplified the surface of protein antigens as an ellipsoid
  - Calculated the protruding index for surface residues.

ELLiPro


ElliPro: Antibody Epitope Prediction
Step 1. Input type
Choose an input type:
Protein sequence (Go to step 2a)
Step 2a. Protein sequence
Enter a protein swiss-prot ID:
Or enter a protein linear sequence in PLAIN or FASTA format:
Blast expectation value:
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
Submit
Reset
ElliPro: Antibody Epitope Prediction Results
Protein Sequence(s):
Chain
Sequence
Predicted Linear Epitope(s):
No.
Chain
Start Position
End Position
Peptide
Number of Residues
Score
3D Structure
Predicted Discontinous Epitope(s):
Residues
Residue Scores:
Click here to view residue scores
http://tools.immuneepitope.org - ElliPro: Epitope 3D Stru...
ElliPro: Epitope 3D Structures
Epitope Residues
Right Click to improve your experience

4. PEPOP

PEPOP

Computational design of immunogenic peptides

Moreau V, et.al *BMC Bioinformatics*, 2008,9:71-86

- 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

Sweredoski M J, *Bioinformatics*, 2008,24(12): 1459-1460

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

6. SEPPA

SEPPA

A computational server for **S**patial **E**pitope **P**rediction of **P**rotein **A**ntigens

- 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 HEXAMERIC HUMAN IL-6/IL-6 ALPHA RECEPTOR/GP130 COMPLEX

Change parameters and reload

Chain: A | Naccess 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 Jmol
- Solvent accessibility plot (naccess)
- Model quality plot (verify3D)

Full sequence overview

+/-

Aminoacids marked in red belong to an hotspot (naccess and V3D values above the setted 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 naccess or V3D value

Mouseover on any aminoacid for more information

```
  1 ELLDPCGYIS PESPVVQLHS NFTAVCVLKE KCMDYFHVNA NYIVWKTNHF TIPKEQYTII NRTASSVTFT DIASLNIQLT CNILTFGQLE QNVYGITIIS
101 GLPPEKPKNL SCIVNEGKKM RCEWDGGRET HLETNFTLKS EWATHKFADC KAKRDTPTSC TVDYSTVYFV NIEVWVEAEN ALGKVTSDHI NFDPVYKVKP
201 NPPHNLSVIN SEELSSILKL TWTNPSIKSV IILKYNIQYR TKDASTWSQI PPEDTASTRS SFTVQDLKPF TEYVFRIRCM KEDGKGYWSD WSEEASGIT
```

Peptide scan results summary for chain A of 1P9M.pdb

+/-

Aminoacids marked in red belong to an hotspot (naccess and V3D values above the setted thresholds)

Aminoacids marked with an underline belong to an interface

Copy | CSV | Excel | PDF | Print

Show 10 entries

Sequence start	Sequence End	Peptide sequence	Solvent exposure	Structure quality	Positive
1	20	ELLDPCGYISPESPVVQLHS	51.226	0.504	1
4	23	DPCGYISPESPVVQLHSNFT	44.860	0.510	1
7	26	GYISPESPVVQLHSNFTAVC	38.355	0.511	
10	29	SPESPVVQLHSNFTAVCVLK	39.270	0.498	
13	32	SPVVQLHSNFTAVCVLKEKC	39.405	0.509	
16	35	VQLHSNFTAVCVLKEKCMDY	42.800	0.524	1
19	38	HSNFTAVCVLKEKCMDYFHV	41.520	0.528	1
22	41	FTAVCVLKEKCMDYFHVNAN	39.985	0.529	
25	44	VCVLKEKCMDYFHVNANYIV	39.860	0.535	
28	47	LKEKCMDYFHVNANYIVWKT	38.865	0.550	

First | Previous | 1 | 2 | 3 | 4 | 5 | Next | Last

Outline

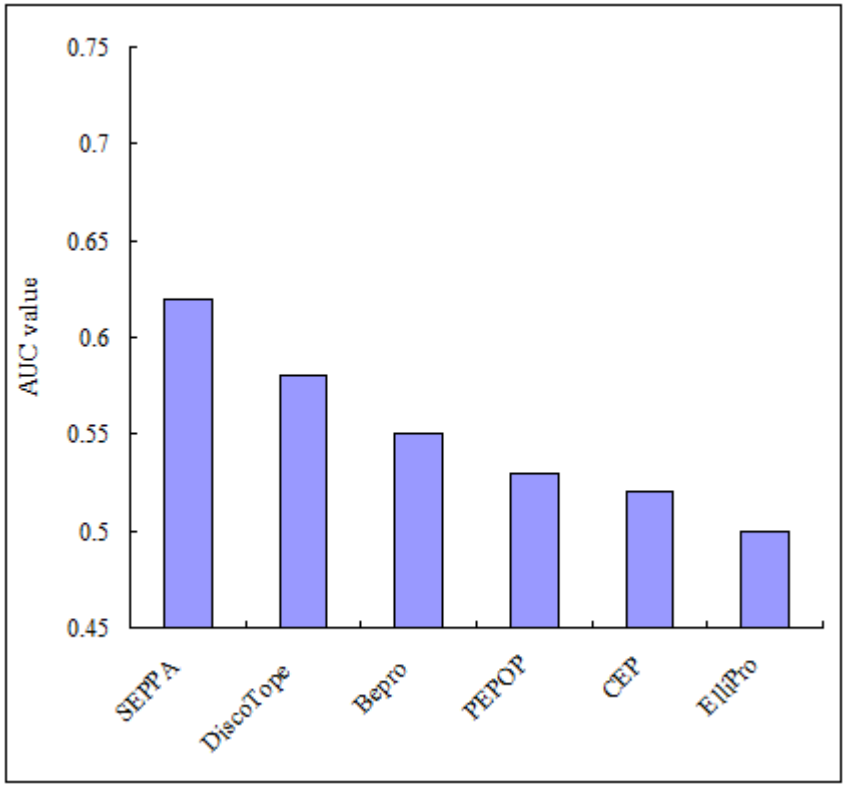
- **Can we predict the conformational epitope?**
  - Current tools---CEP, DiscoTope, ElliPro, PEPOP, BEpro
  - **Evaluation**
- Software Demo: SEPPA

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



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

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

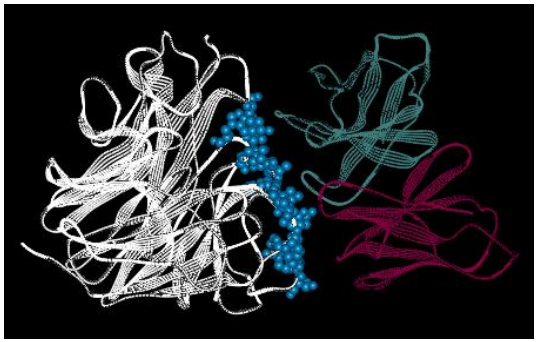
Future improvement

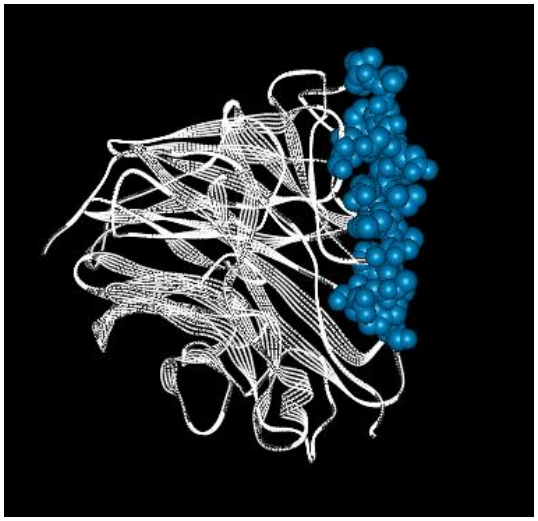
- Research status
  - Hydrophilic, accessibility, antigenicity, flexibility, charge distribution, secondary structure and etc.
  - The prediction accuracies of previous methods are underperformance
  - "…available prediction methods based on unidirectional analysis do not cope satisfactorily with the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

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

Reitmaier R, **Review of immunoinformatic approaches to in-silico B-cell epitope prediction**. *Nature Precedings*, 2007

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





PDB: 1A14:N

- Research procedure

Dataset

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

Methods

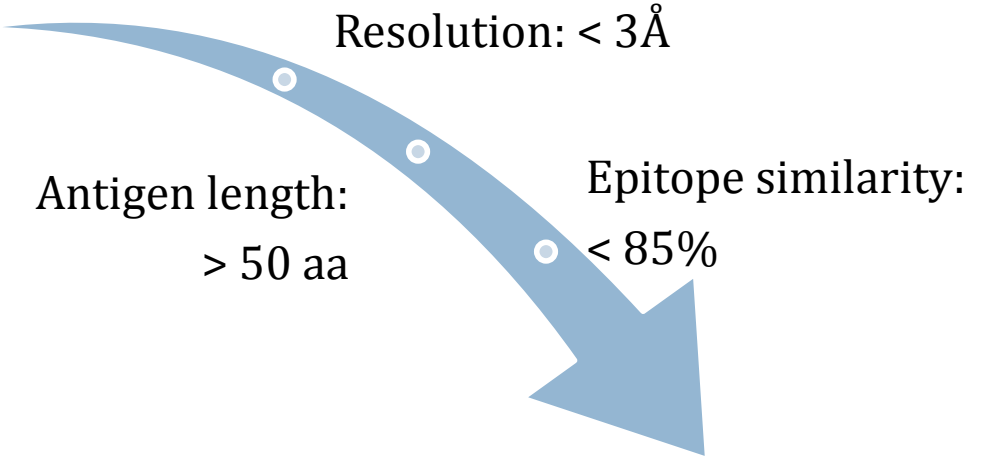
- Physical-chemical features
- Sequence feature
- Regional 3-D structural features

Dataset

- PDB (dated April 28th, 2011)

Keyword search:

antibody | antigen | Fab | Fv | Fc | IgG | immu* etc.



161 PDB structures of immunoglobulin complex

166 B-cell epitopes

Results

Epitope size

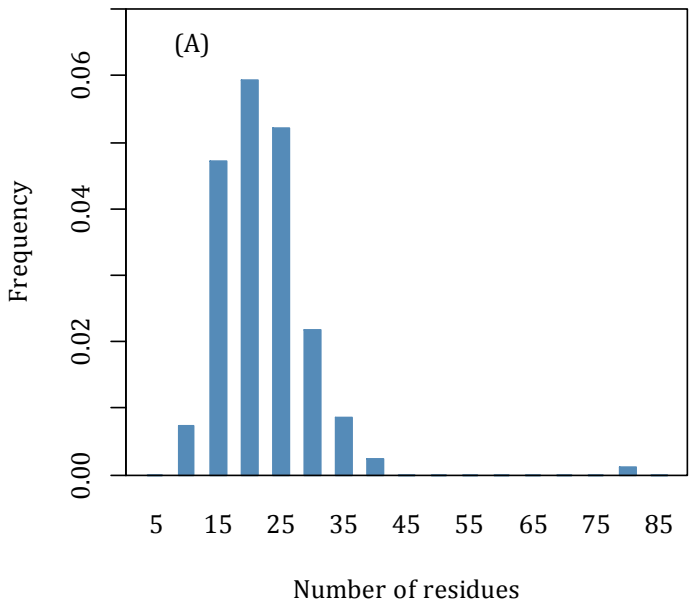
1. **The number of residue Fig. (A)**
2. The sum of ASA
3. Distances among epitope residues

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

- Conclusion

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

Distribution of epitope residue number



- Result

Range: 15 ~ 30 AA
Average(μ): 22.18±7.53 AA

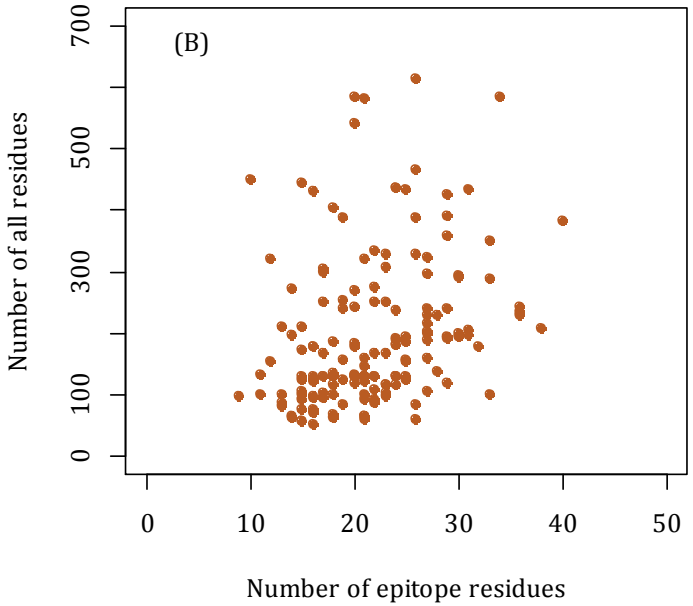
Outlier data 1BGX:T 80 AA

Average(μ): 21.83±6.04 AA

The Coefficient of Variance of epitope and protein residue numbers(CV = σ/μ)

$CV_{epitope}$ = 0.36
$CV_{protein}$ = 0.74

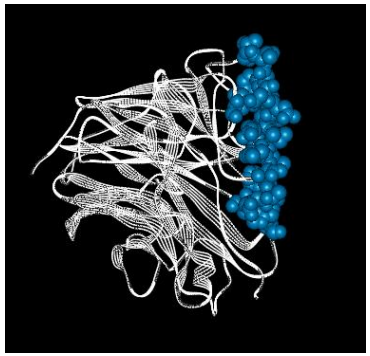
Comparison of residue numbers



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**



PDB ID: 1A14:N

- 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

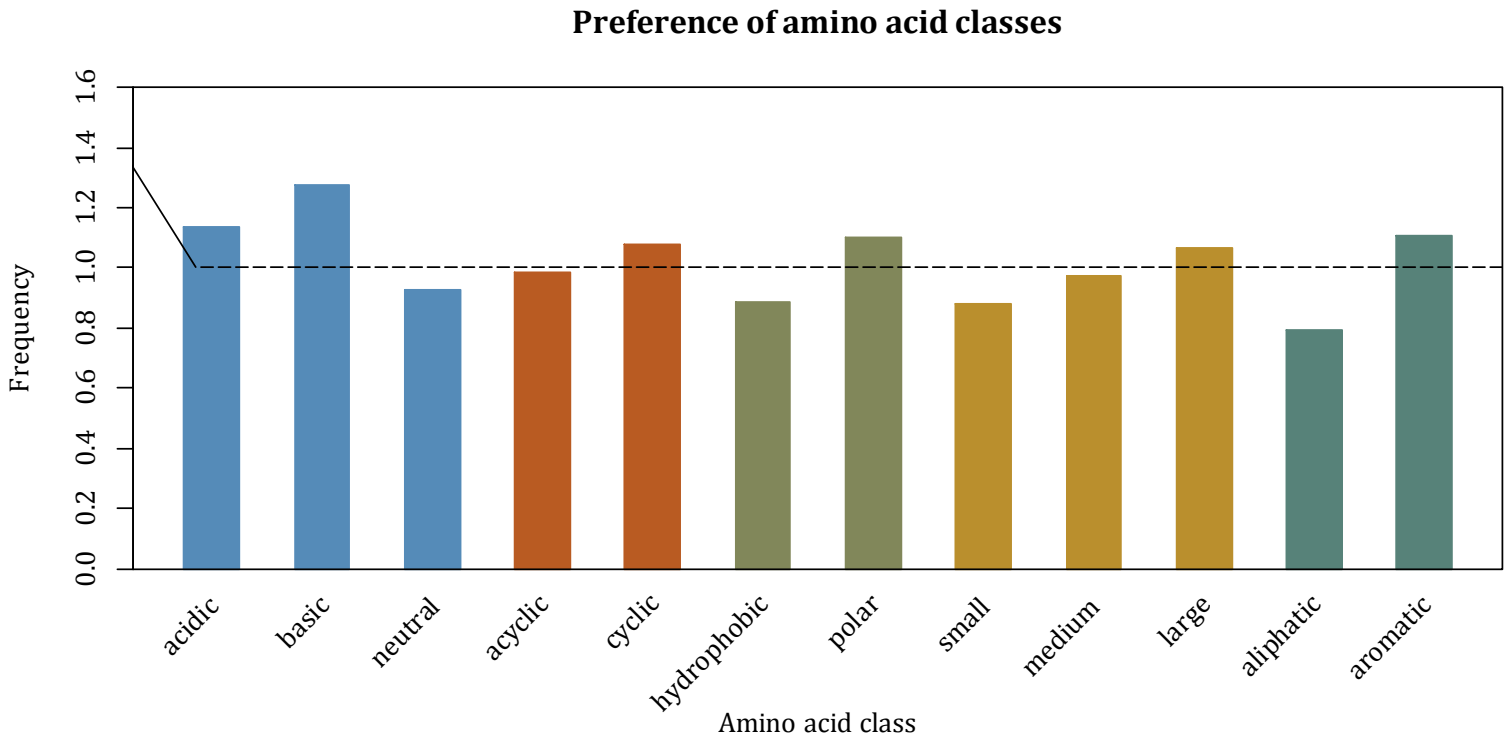
- Hypothesis
  - Interaction residues tend to have higher accessible surface area (ASA)
- Relative ASA

$$relASA = \frac{ASA}{index_i}$$ ($index_i$: the ASA of amino acid X in tri-peptide *ALA-X-ALA*)

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

Chothia C, **The nature of the accessible and buried surfaces in proteins**. *J Mol Biol*, 1976. **105**(1): p. 1-12.

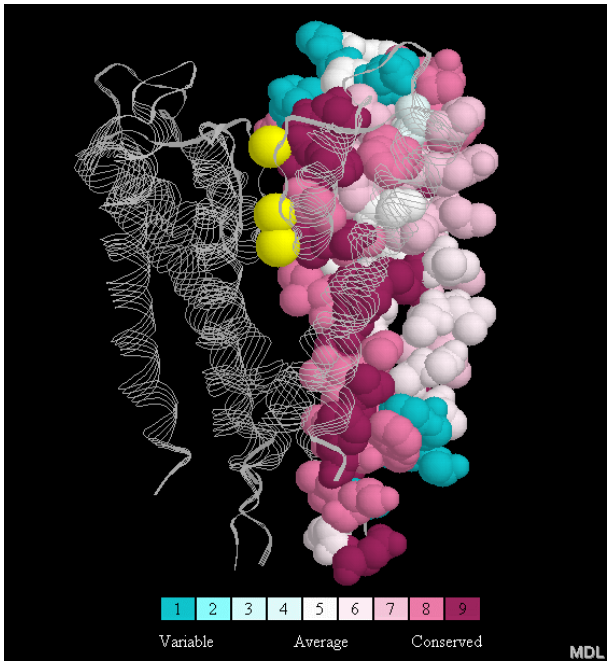
Epitope preference of residue



- 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

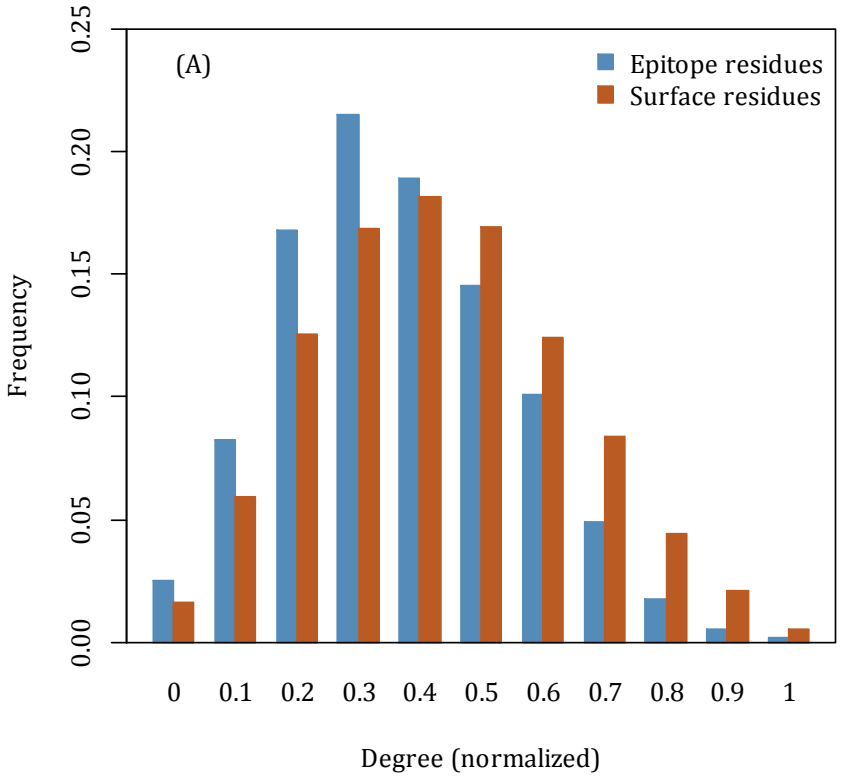


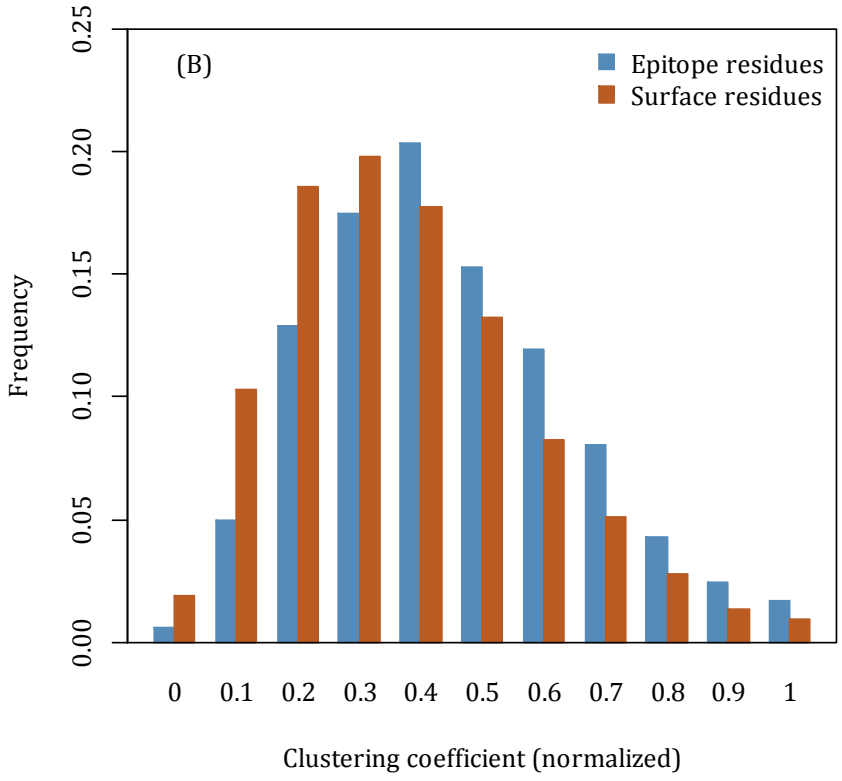
ConSurf

Server for the Identification of Functional Regions in Proteins

Ashkenazy H, Erez E, Martz E, Pupko T, and Ben-Tal N, **ConSurf 2010: calculating evolutionary conservation in sequence and structure of proteins and nucleic acids**. *Nucleic Acids Res*, 2010. **38**(Web Server issue): p. W529-33.

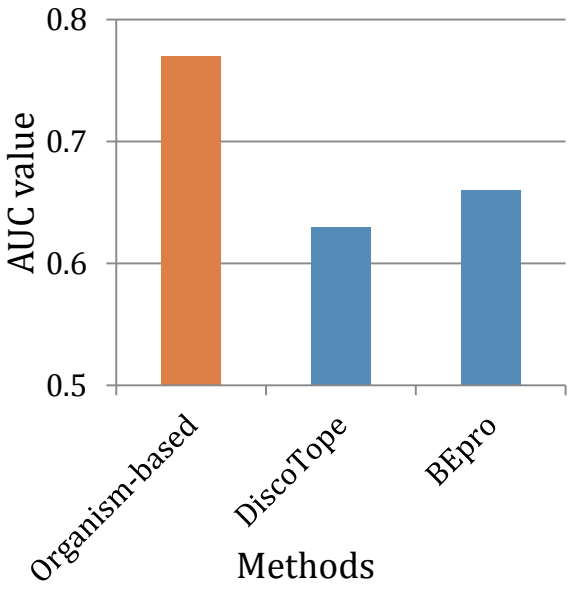
- Result
  - Epitope residues are surrounded with less neighboring residues
  - The neighboring residues of epitope residues are more compact





- Prediction performance and comparison

PDB_chain	Antibody organism	AUC	
		Organism-independent	Organism-based
3QWO_C	Mus musculus	0.65	0.74
3AY4_C	Homo sapiens	0.88	0.94
3SE9_G	Homo sapiens	0.76	0.75
3SE8_G	Homo sapiens	0.82	0.81
3SDY_B	Homo sapiens	0.58	0.71
3NPS_A	Homo sapiens	0.78	0.86
3RKD_A	Mus musculus	0.39	0.47
3SKJ_E	Homo sapiens	0.52	0.51
3R1G_B	Homo sapiens	0.78	0.93
3SGJ_C	Homo sapiens	0.89	0.89
3SGK_C	Homo sapiens	0.92	0.90
Average		0.72	0.77



t-test: $p<0.01$

General characteristics	B-cell epitope size(the number of residues, ASA and regional distances)
	B-cell epitope sequence continuity
Physical chemical features	**Accessibility**
	Epitope preference (residue, residue-pair and residue-triangle)
	AAindex amino acid indices (544 indices)
Sequence features	**Sequence conservation**
Regional structural epitope	**Topological parameters(degree and clustering coefficient)**
	Gaussian curvature
	Protruding index
	Planarity index
Epitope-paratope interaction pattern	Epitope-paratope residues interaction preference

Thank You !

reference

1. **Sun J**, Xu TL, Wang SN, Li GQ, Wu D, and Cao ZW, Does difference exist between epitope and non-epitope residues? Analysis of the physicochemical and structural properties on conformational epitopes from B-cell protein antigens. *Immunome Res, 2011. 7(3): p. 11.*

2. Xu XL, **Sun J**, Liu Q, Wang XJ, Xu TL, Zhu RX, Wu D, and Cao ZW, Evaluation of spatial epitope computational tools based on experimentally-confirmed dataset for protein antigens*. Chinese Science Bulletin, 2010. 55(20): p. 2169-2174.*

3. Wu D, **Sun J**, Xu TL, Wang SN, Li GQ, Li YX, and Cao ZW, Stacking and energetic contribution of aromatic islands at the binding interface of antibody proteins*. Immunome Res, 2010. 6 Suppl 1: p. S1.*

4. Wu D, Xu TL, **Sun J**, Dai JX, Ding GH, He Y, Zhou ZF, Xiong H, Dong H, and Jin WR, Structure modeling and spatial epitope analysis for HA protein of the novel H1N1 influenza virus*. Chinese Science Bulletin, 2009. 54(13): p. 2171-2173.*

5. **Sun J**, Wu D, Xu TL, Wang XJ, Xu XL, Tao L, Li YX, and Cao ZW, SEPPA: a computational server for spatial epitope prediction of protein antigens*. Nucleic Acids Res, 2009. 37(Web Server issue): p. W612-6.*

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

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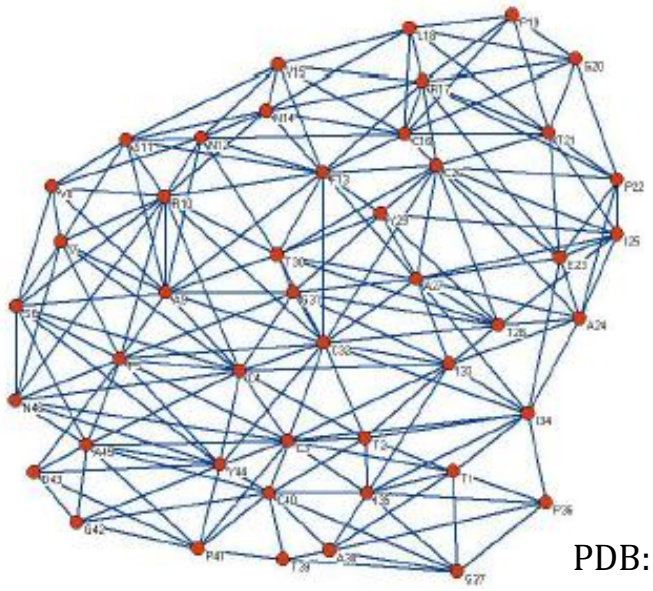
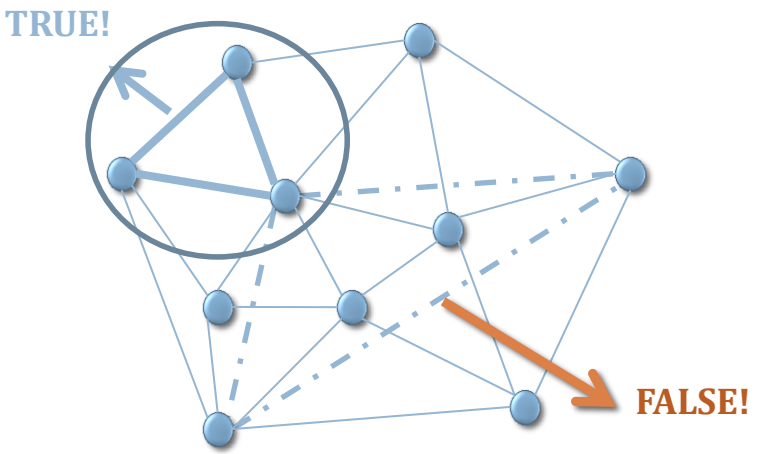
- **Software Demo: SEPPA**

Method

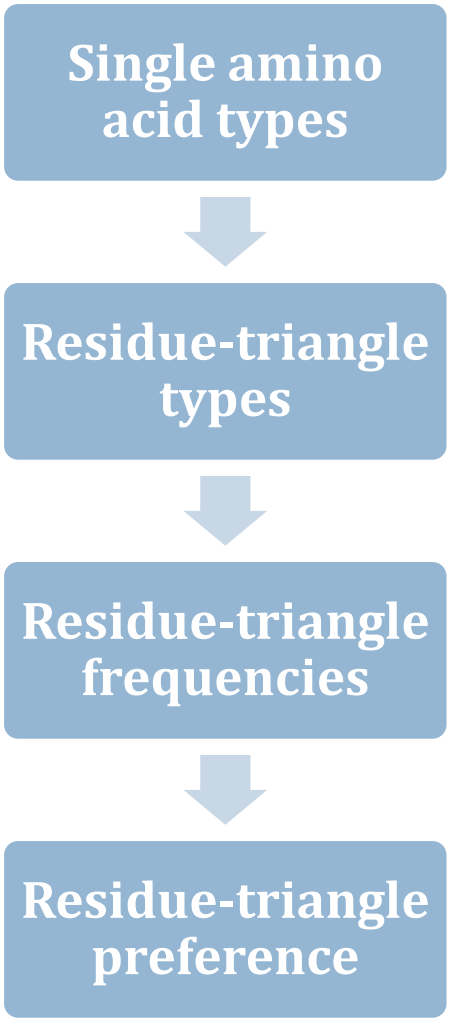
- The definition of unit patch of residue-triangle
  - Three surface residues, the least distances between any two among the three
  - Cutoff: 4Å
  - Epitope/non-epitope surface residue-triangle
- Why the definition?
  - Different epitope preference of different types of residue-triangle
  - All epitope residues function as a whole



PDB: 1CRN



- The generation of residue-triangle preference (training part)



r_i: A, R, N, D, C, Q…

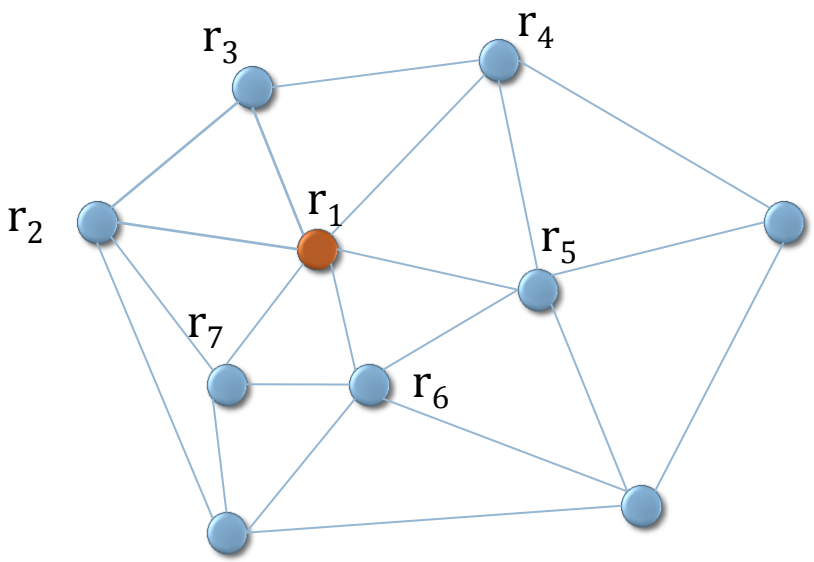
t_m: (A, A, R), (R, D, Q), (N, C, Q)…

Ot_m

$Rt_m = (Ot_m)_{epitope} / (Ot_m)_{non\text{-}epitope}$

- The scoring of residue-triangle preference (prediction part)

For any surface residue r_1:



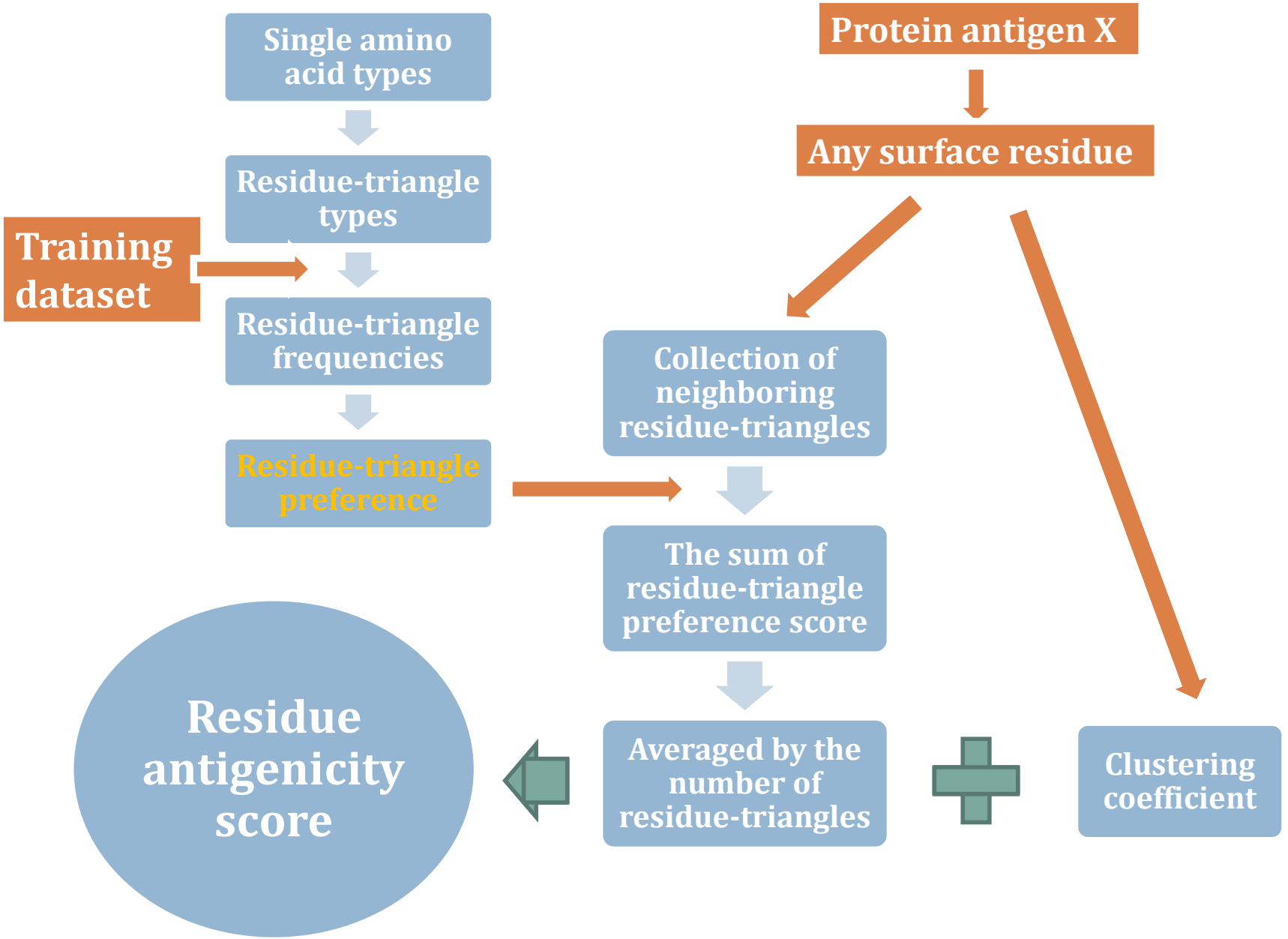
Collection of neighboring residue-triangles

↓

The sum of residue-triangle preference score

↓

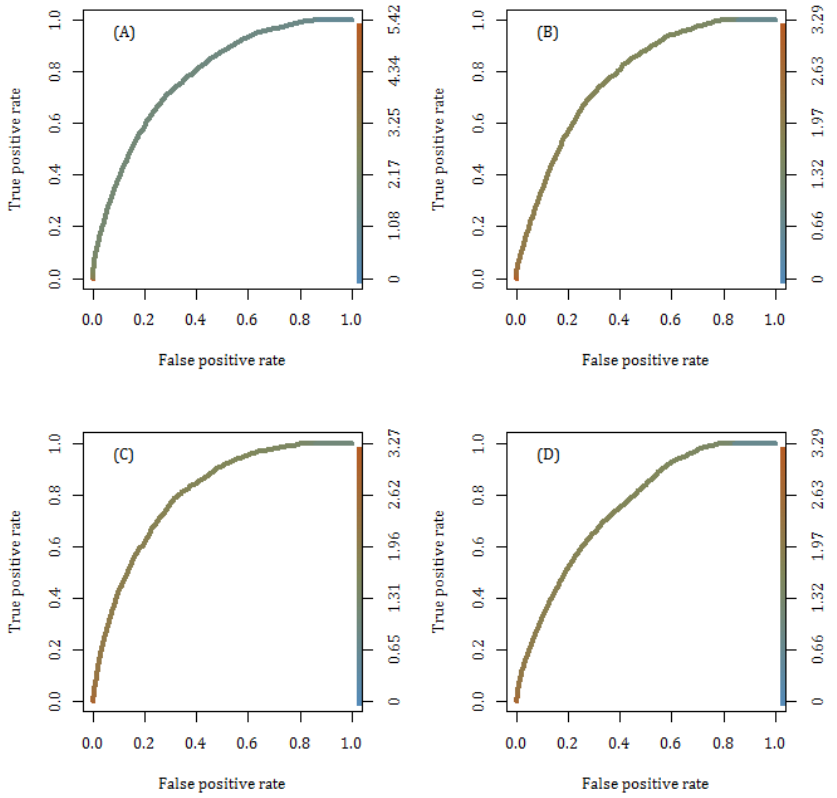
Averaged by the number of residue-triangles


Single amino acid types
Residue-triangle types
Training dataset
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
Residue antigenicity score

Results

The prediction performance of SEPPA

Testing dataset	AUC
(a) SEPPA training dataset	0.77
(b) IEDB dataset	0.76
(c) DiscoTope training dataset	0.80
(d) Epitome dataset	0.75



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

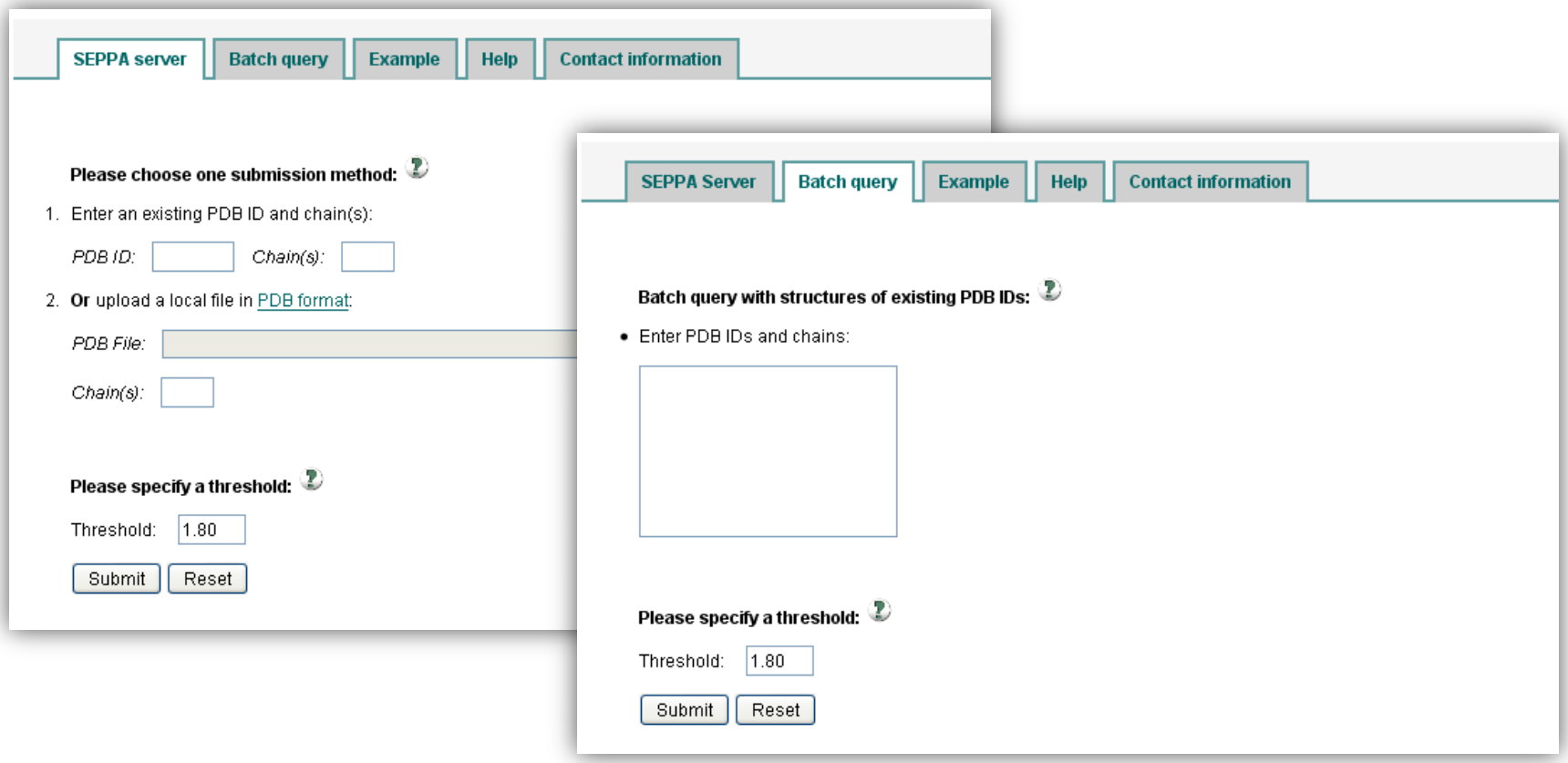
Comparison of prediction performance

Methods	Average AUC	Successful pick-up rate
SEPPA (1.80)	**0.64**	**96.64%**
CEP	0.52	NA
DiscoTope (-7.70)	0.60	89.08%
BEpro (1.30)	0.56	90.76%

SEPPA --- Spatial Epitope Prediction of Protein Antigens

SEPPA

http://lifecenter.sgst.cn/seppa



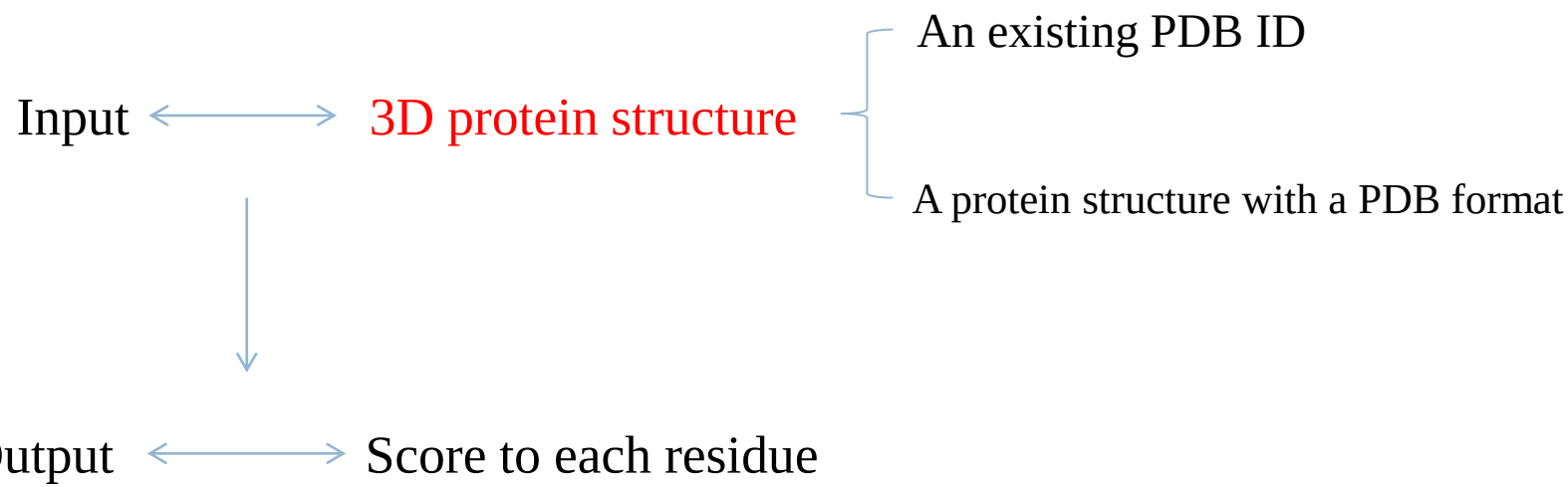
Paper published--- Sun J, Wu D, Xu TL, Wang XJ, Xu XL, Tao L, Li YX, and Cao ZW, **SEPPA: a computational server for spatial epitope prediction of protein antigens**. *Nucleic Acids Res*, 2009. **37**(Web Server issue): p. W612-6.

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

SEPPA

For conformational B-cell epitope prediction



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

SEPPA Homepage

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

SEPPA server | Batch query | Example | Help | Contact information

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

07490

http://bio.shmtu.org

Demo Data--------1NCA

Refined crystal structure of the influenza virus N9 neuraminidase-NC41 Fab complex

Molecular Description (from PDB)

Molecular Description

Classification: Hydrolase(o Glycosyl)
Structure Weight: 92741.77

Molecule: INFLUENZA A SUBTYPE N9 NEURAMINIDASE
Polymer: 1 **Type:** protein **Length:** 389
Chains: N
EC#: 3.2.1.18
Organism Influenza A virus (A/tern/Australia/G70C/1975(H11N9))
UniProtKB: P03472

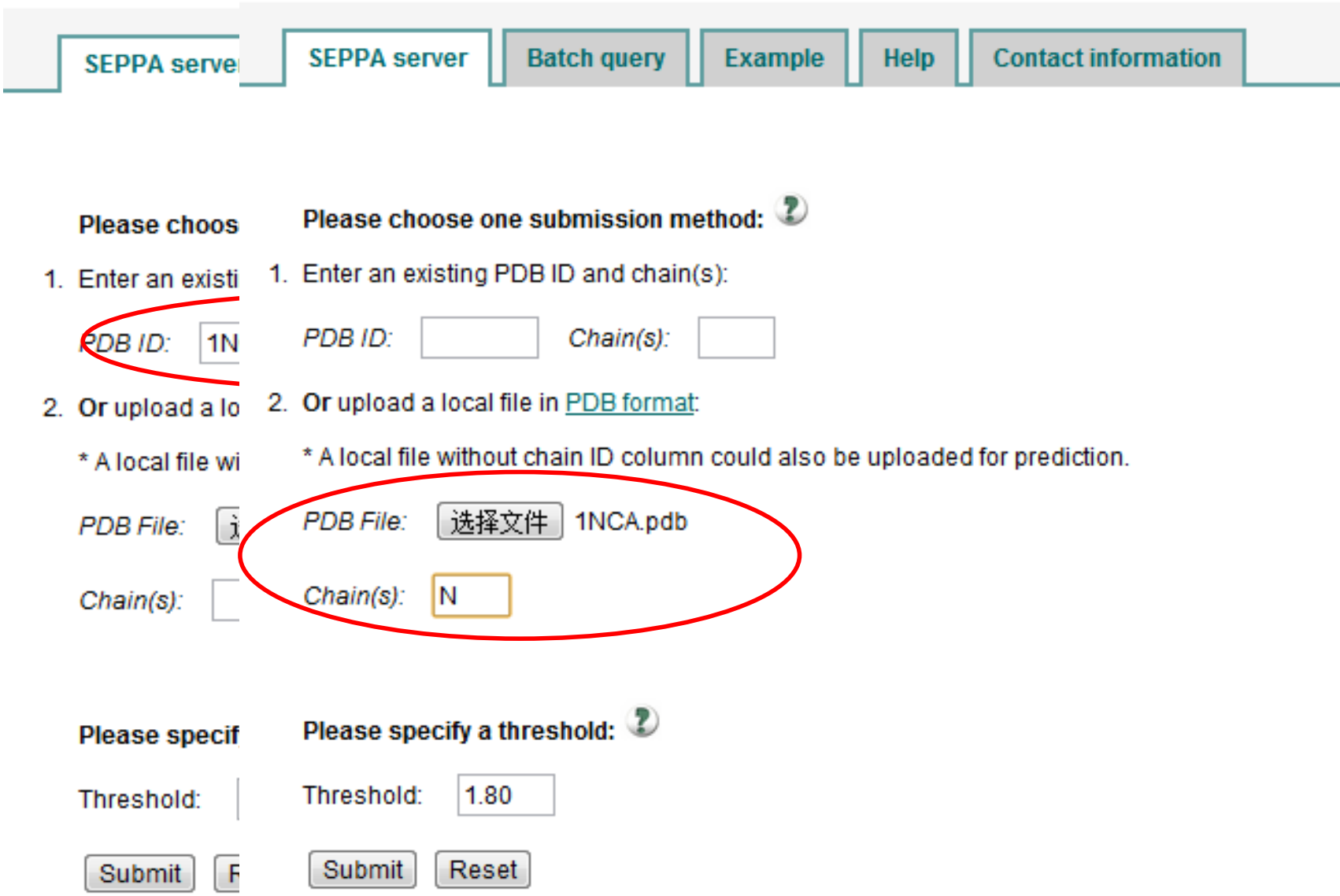
Molecule: IGG2A-KAPPA NC41 FAB (LIGHT CHAIN)
Polymer: 2 **Type:** protein **Length:** 214
Chains: L
Organism Mus musculus

Molecule: IGG2A-KAPPA NC41 FAB (HEAVY CHAIN)
Polymer: 3 **Type:** protein **Length:** 221
Chains: H
Organism Mus musculus
UniProtKB: P01865

More information

http://www.rcsb.org/pdb/explore/explore.do?structureId=1NCA

Data input


SEPPA server
Batch query
Example
Help
Contact information
Please choos
Please choose one submission method:
1. Enter an existi
1. Enter an existing PDB ID and chain(s):
PDB ID:
1N
PDB ID:
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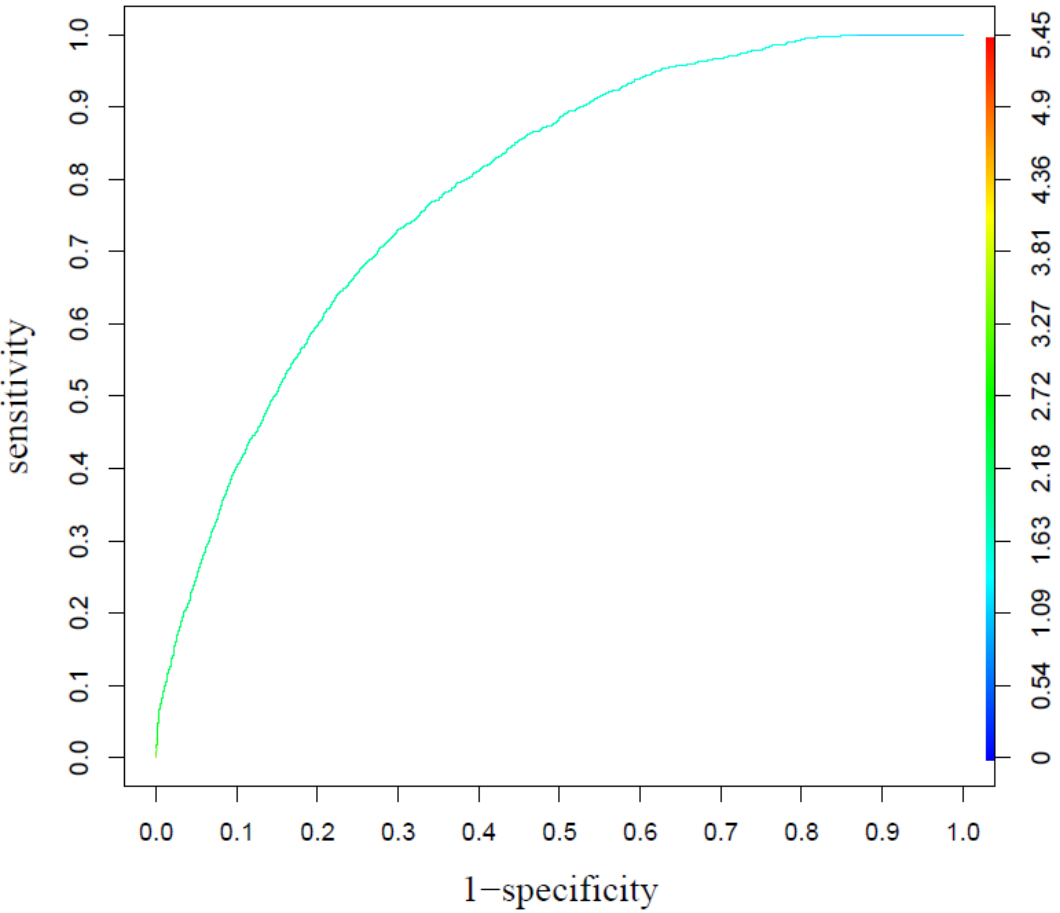
2. Or upload a lo
2. Or upload a local file in PDB format:
* A local file wi
* A local file without chain ID column could also be uploaded for prediction.
PDB File:
选择文件
1NCA.pdb
Chain(s):
Chain(s):
N
Please specif
Please specify a threshold:
Threshold:
Threshold:
1.80
Submit
Submit
Reset

Parameter Threshold

The default value of THRESHOLD is set at 1.80.

lower threshold ⟶ more residues will be included as predicted epitope residues



Threshold	Sensitivity	Specificity	Accuracy
1.55	0.959	0.259	0.377
1.60	0.927	0.345	0.448
1.65	0.859	0.452	0.531
1.70	0.778	0.558	0.612
1.75	0.672	0.658	0.684
1.80	0.568	0.740	0.739
1.85	0.459	0.810	0.782
1.90	0.363	0.860	0.809
1.95	0.278	0.900	0.829
2.00	0.217	0.927	0.844

Output Page

Summary for the prediction result

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

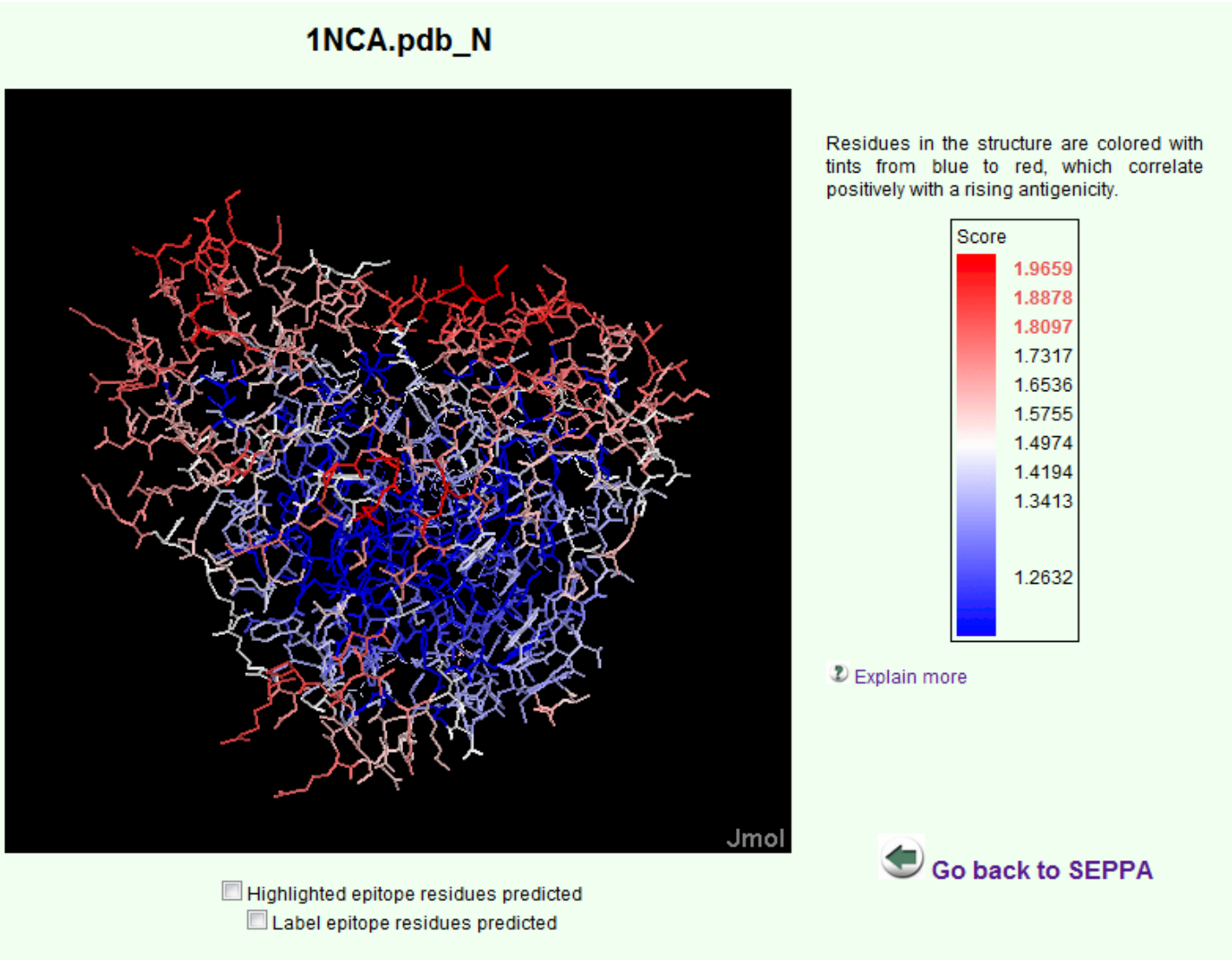
1-50	IRDFNNLTKG LCTiNSWHIY GKDNAvRIgE DSDVLvTREp YvsCDPDECR
51-100	fyaLSQGTTI RGKHSNGTIH DRSQYRAlIs WPLSSPPTVY NSRVECIGWS
101-150	stsCHDgKTR MSiciSGPNN NaSaViWYNR RPVTEINTWA RNIlRTQEsE
151-200	CVCHNgVCPv VfTdGSATGP AETRiYyfKE gKILKWEPLA GTAKHIEECS
201-250	CYgERAEITc tcRdNWQGsN RpViRIDPVA MTHTSQyICS pVLTdNPRPN
251-300	DPTVGKCNDP YPGNNNNgVK GFSyLDGVNT wlGRTISIAS RSgYEmLKvP
301-350	NaLTDDKSKP TQGQTivLNT DWsGYSgSfm DYWAEGECYR aCfYvelIRG
351-400	RPKEDKVWWT SNsIvsMCSS TEFLGQWDWP DGAKIEYFL

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

Download the score file

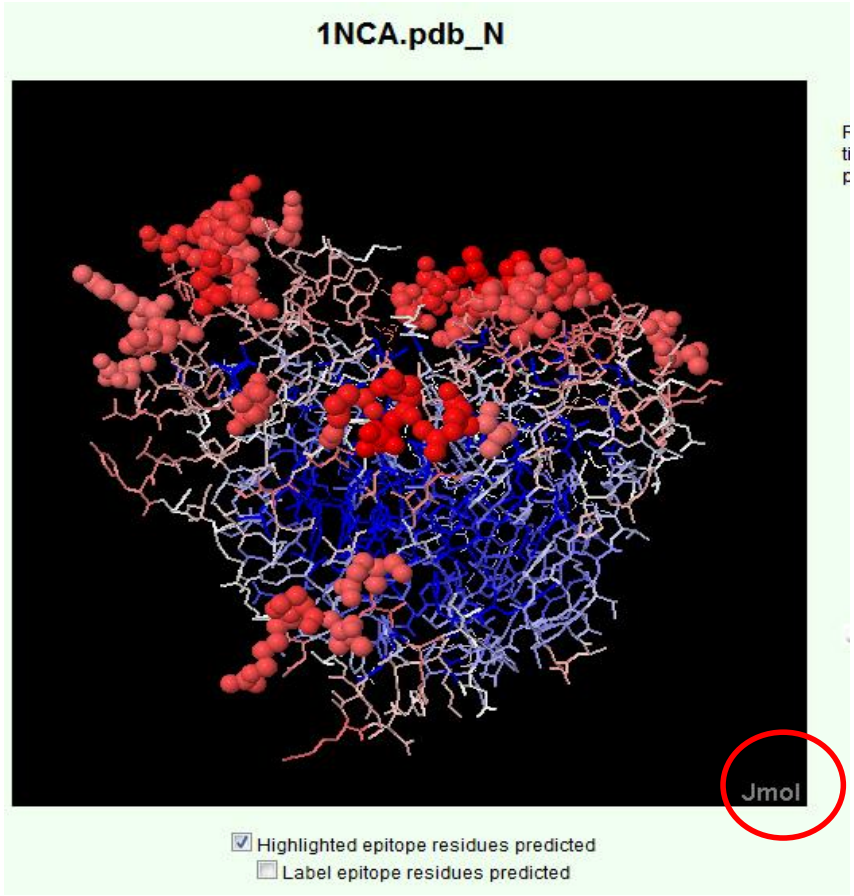
Explain the result

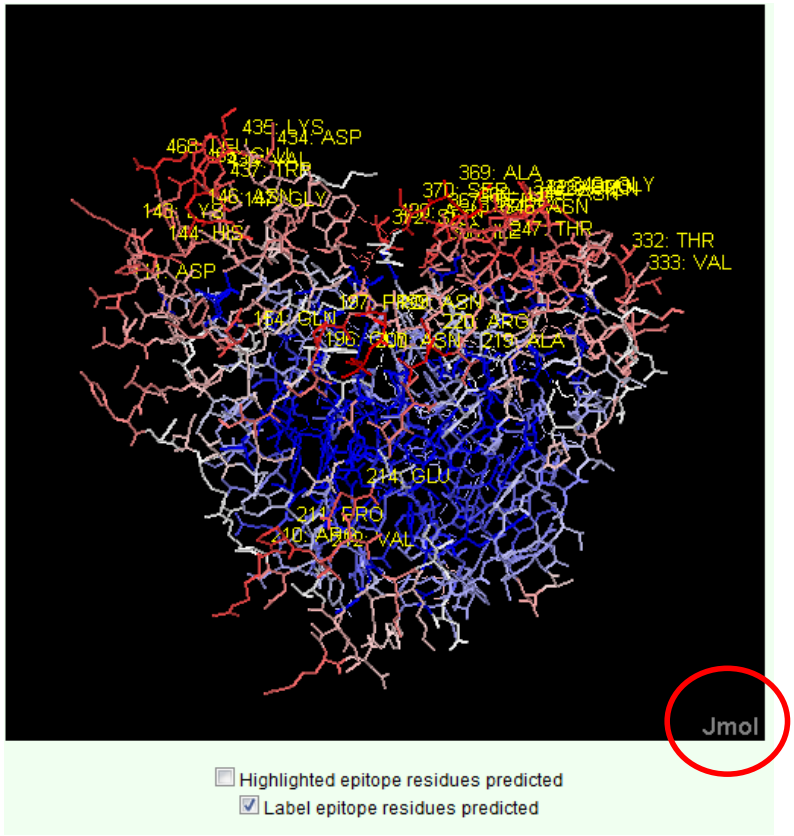
View 3D structure in Jmol



Tints from blue to red represent a rising antigenicity

View 3D structure in Jmol

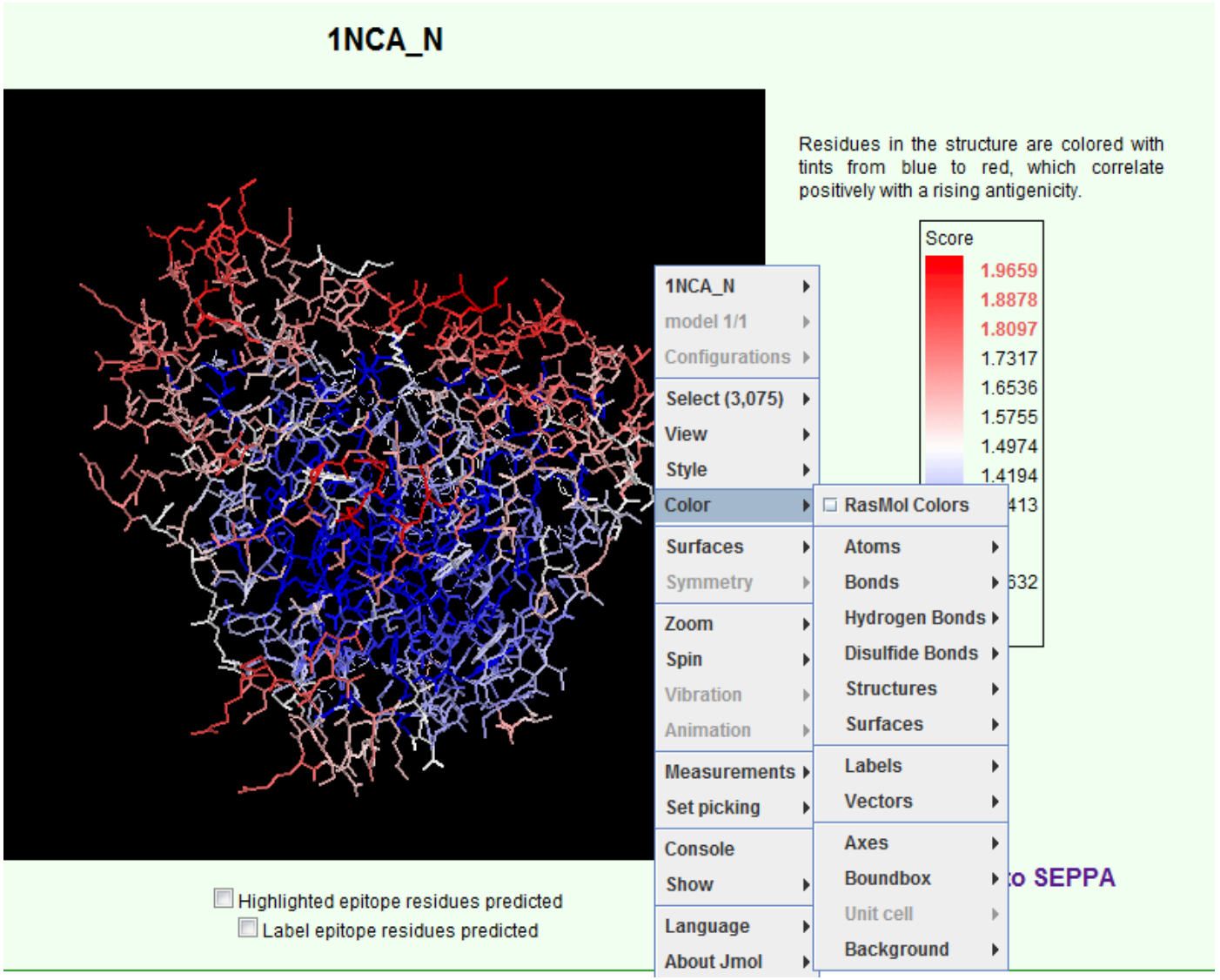




Selecting the "Highlighted epitope residues predicted" checkbox

Selecting the "Label epitope residues predicted" checkbox

View 3D structure in Jmol



A glance of the prediction result

1-50	IRDFNNLTKG LCTiNSWHIY GKDNAvRIgE DSDVLvTREp YvsCDPDECR
51-100	fyaLSQGTTI RGKHSNGTIH DRSQYRAlIs WPLSSPPTVY NSRVECIGWS
101-150	stsCHDgKTR MSiciSGPNN NaSaViWYNR RPVTEINTWA RNIlRTQEsE
151-200	CVCHNgVCPv VfTdGSATGP AETRiYyfKE gKILKWEPLA GTAKHIEECS
201-250	CYgERAEITc tcRdNWQGsN RpViRIDPVA MTHTSQyICS pVLTdNPRPN
251-300	DPTVGKCNDP YPGNNNNgVK GFSyLDGVNT wlGRTISIAS RSgYEmLKvP
301-350	NaLTDDKSKP TQGQTivLNT DWsGYSgSfm DYWAEGECYR aCfYvelIRG
351-400	RPKEDKVWWT SNsIvsMCSS TEFLGQWDWP DGAKIEYFL

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

The complete score file

```
SEPPA(Spatial Epitope Prediction of Protein Antigens)
[Designed for B-cell Conformational Epitope Prediction]

Thu Oct 11 01:53:13 2012


----SEPPA Prediction Result-----

Antigenic Prediction for 1NCA.pdb:

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

chainID resSeq  resName score

N    81   ILE 1.69
N    82   ARG 1.79
N    83   ASP 1.66
N    84   PHE 1.65
N    85   ASN 1.50
N    86   ASN 1.53
N    87   LEU 1.43
N    88   THR 1.54
N    89   LYS 1.50
N    90   GLY 1.47
N    91   LEU 1.39
```

Summary Information

Predicted score for each residue

Multiple PDB ID entries

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