

Immune Epitope Database NEWSLETTER

Volume 3, Issue 3

<http://www.immuneEPITOPE.org>

October 2006

B Cell Antibody Tools & Evaluation Meeting Summary

In a workshop sponsored by the National Institute for Allergy and Infectious Diseases (NIAID) on September 7 & 8, 2006 in Washington D.C., a panel of immunologists and bioinformaticians convened to discuss the current state and future directions for the B cell epitope prediction field. The specific goals of the workshop were to review currently available B cell epitope prediction tools, agree upon metrics to evaluate tool performance, identify a body of relevant training and test data, and develop recommendations for advertising and implementing these suggestions to the broader research community.

After a brief introduction to some of the issues involved in the field of B cell epitope prediction, participants presented their most current algorithms and datasets. Although clearly an improvement over previous methods, the performance gap between B cell epitope predictions and those for T cells remains large. The most commonly cited reason for this issue was the lack of high-quality datasets on which to train and test the methods. While additional positive epitope data is needed, the limited availability of negative data has proved to be a major hindrance to development.

With these issues in mind, the participants proposed a set of guidelines for the assembly of relevant datasets for tool development. Additionally, methods and metrics for tool evaluation were discussed. In order to facilitate collaboration and speed the development of new methods, it was agreed that the datasets and tools should share a common file format. This step will simplify the process of establishing metaservers for tool consolidation and automated evaluation.

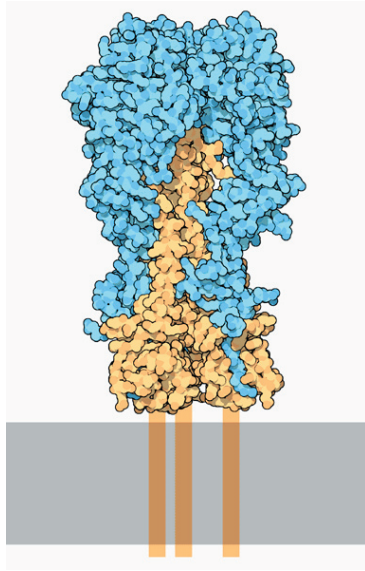
We anticipate that the implementation of the recommendations set forth at this workshop will greatly accelerate the de-

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velopment of B cell epitope prediction tools. A detailed meeting report is in the process of being prepared for publication. The ultimate measure of success for this workshop will be the the sharing of datasets and development of improved or novel B cell epitope prediction tools. It is hoped that such resources will lead to increased confidence in and widespread use of B cell epitope prediction tools by the greater community.

Featuring: *The Hemagglutinin Protein*



Hemagglutinin is composed of two different types of chains, shown in blue and orange. Blue for targeting mechanism and orange for initiating attack.

Hemagglutinin was a molecule on the Protein Databank's (PDB) **Molecule of the Month** column produced by Dr. David Goodsell. The PDB article focuses on the structural aspects of the protein, with many references to relevant protein structures in the PDB. It describes how hemagglutinin contributes to the pathogenesis of various Influenza strains and illustrates the changes that occur in the protein structure after it enters a cell. There is also a discussion and illustration of antibody interactions with the protein and potential biological consequences.

To read more about this protein and its structure on the PDB website, please visit:

http://www.pdb.org/pdb/static.do?p=education_discussion/molecule_of_the_month/pdb76_1.html

The European Bioinformatics Institute (EBI) also included the "Bird Flu"-Haemagglutinin in their **Protein of the Month** spotlight with an article by Jennifer McDowell. This article offers a bioinformatics perspective on haemagglutinin and discusses the different strains of flu and its ability to evolve. A companion article explores the ability of influenza to cross species barriers. Please visit the InterPro database and the Protein of the Month series:

http://www.ebi.ac.uk/interpro/potm/2006_4/Page1.htm

Recent Publications

A paper describing the IEDB curation process appeared in the July issue of BMC Bioinformatics:

Vita R, Vaughan K, Zarebski L, Salimi N, Fleri W, Grey H, Sathiamurthy M, Mokili J, Bui HH, Bourne PE, Ponomarenko J, de Castro R Jr, Chan RK, Sidney J, Wilson SS, Stewart S, Way S, Peters B, Sette A.

Curation of complex, context-dependent immunological data. BMC Bioinformatics. 2006 Jul 12;7:341. PMID: 16836764).

The article describes the methods used to identify and extract relevant data from the scientific literature in an efficient and accurate manner, and the processes developed for manual and semi-automated curation. The experiences described have applicability to other databases housing complex biological data and requiring a high level of curation expertise. The full text article is freely available from Pubmed Central and Biomed Central. [Click here](#) to link directly to the article.

Programming a Link to the IEDB



If you are interested in creating a HTML hyperlink on your website directly to the IEDB, there are various ways to do it. Below we have outlined each approach with samples. The red text in the sample links below indicates where you would add your values, based on your research needs.

For further information, please visit the homepage under Online Help/Resources/Linking to the IEDB. Registered users can log in to submit a Help Request for additional assistance. [Registration](#) is free, and only takes a few minutes.

By IEDB ID:

The sample link below would link to the epitope record whose IEDB ID is 3172.

```
<a href="http://www.immuneepitope.org/httpQuery.do?dispatch=runquery&eid=3172">Your text goes here</a>
```

By PubMed ID:

The sample link below would link to the reference whose PubMed ID is 11425742.

```
<a href="http://www.immuneepitope.org/httpQuery.do?dispatch=runquery&pubmedId=1142572">Your text goes here</a>
```

By Sequence:

The sample link below would link to all epitope records whose linear sequence was AAKKAAAV.

```
<a href="http://www.immuneepitope.org/httpQuery.do?dispatch=runquery&elinseq=AAKKAAAV">Your text goes here</a>
```

By PDB ID:

The sample link below would return epitope records whose source had a PDB ID of 1wbx.

```
<a href="http://www.immuneepitope.org/httpQuery.do?dispatch=runquery&pdbId=1wbx">Your text goes here</a>
```

By NCBI Taxonomy ID:

The sample link below would return epitope records whose source species matched the NCBI Taxonomy ID 9606.

```
<a href="http://www.immuneepitope.org/httpQuery.do?dispatch=runquery&taxonomyId=9606">Your text goes here</a>
```

By NCBI Accession Number:

The sample link below would return epitope records whose source came from the NCBI accession number P06935.

```
<a href="http://www.immuneepitope.org/httpQuery.do?dispatch=runquery&es_accessionId=P06935">Your text goes here</a>
```

Science in the News

The Nobel Prize in Physiology or Medicine for 2006

Andrew Z. Fire and Craig C. Mello
for the discovery of

“RNA interference – gene silencing by double-stranded RNA”

Drs. Fire and Mello discovered a way to turn off genes, called RNA interference. This mechanism can be used to control gene expression, which is invaluable in treating a variety of diseases such as cancer, heart disease, and viral infections. It occurs naturally in plants, animals, and humans and is activated when RNA molecules occur as double-stranded pairs in the cell. These double-stranded pairs activate cellular machinery that eliminates all of the messenger RNA (mRNA) molecules that are identical to the double-stranded RNA. The disappearance of these mRNA molecules results in the silencing of the gene that is responsible for the specific mRNA production and subsequent protein expression. This method is already in use in basic science and may one day lead to promising clinical or agricultural applications in the future.

To read the press release of this event, please visit the Nobel Prize webpage, which is located [Here](#).

Summary Metrics as of October 6, 2006

Thanks to ongoing literature curation efforts and the direct submission of data, the number of epitopes in the IEDB grew by 25% in less than three months. As of 6 October 2006, the IEDB contained data from 2497 references and 45,785 records. A record is defined as a single molecular structure or entity within a single reference. The term “structure” is used because the IEDB collects data with both positive and negative values, in terms of binding to immune receptors (i.e., antibodies, MHC molecules, T cell Receptors). Only those structures that positively bind can truly be called “epitopes”. Structures can appear in multiple references, so the number of distinct structures (40,488) is always less than the number of records. When the structures with negative binding are disregarded, the number of distinct epitopes contained within the IEDB is 20,785.

Browsing Features in the IEDB

There are two different data browsing features in the IEDB. Both can be accessed via the Query pull-down menu or the Quick Links on the IEDB homepage.

Browse Records by Allele Name:

Once the “Browse Records by Allele Name” has been selected, a table of all the MHC alleles contained in the IEDB will be displayed. Each allele is listed in alphabetical order with the number of records associated with each allele shown under the Count column on the right hand side. Clicking on any of these numbers will display the records associated with the selected allele. Users have the option of exporting these data into an Excel spreadsheet via the link on the bottom of the table.

Browse Records by Species:

Likewise, users can find records associated with a specific epitope source species by selecting the “Browse Records by Species” option. A table similar to the one mentioned above will be displayed with all the epitope source species contained in the IEDB. The number of records associated with each species will also be shown as a link. Click on the corresponding number on the Count column to view the record list for a given species. Exporting the data into an Excel Spreadsheet is also an option.

Journals & Articles

Recommended Reading

AIDS

2004 Sep 3; 18(13):1819-26

PubMed ID: 15316343

Laney AS, Dollard SC, Jaffe HW, Offermann MK, Spira TJ, Gunthel CJ, Pellett PE, Cannon MJ

National Center for Infectious Diseases, Center for Disease Control & Prevention, Rollins School of Public Health, Atlanta, Georgia 30333, USA

Repeated measures study of human herpesvirus 8 (HHV-8) DNA and antibodies in men seropositive for both HHV-8 and HIV

Leora's Review: To study the natural history and pathogenesis of human herpes virus 8 (HHV-8) infection in HHV-8- and HIV-seropositive men, the authors examined blood samples from 87 patients. They found antibodies to two epitopes of HHV-8, and theorized that HHV-8 replication may be limited by high antibody titers, especially to one of the epitopes ORF65, or by other immune function for which antibodies are a marker. Although such an immune response may not stop Kaposi's sarcoma from occurring, it may inhibit the development of new lesions.

Infection and Immunity

2003 August; 71(8): 4633-4641

PubMed ID: 12874343

Weichhart T, Horky M, Sollner J, Gangl S, Henics T, Nagy E, Meinke A, von Gabain A, Fraser CM, Gill SR, Hafner M, von Ahsen U

Intercell AG, 1030 Vienna, Austria, 1 The Institute for Genomic Research, Rockville, Maryland 20850

Functional Selection of Vaccine Candidate Peptides from Staphylococcus aureus Whole-Genome Expression Libraries In Vitro

Huda's Review: The authors displayed all genomically-encoded peptides of the human pathogen Staphylococcus aureus. They then used human antibodies exhibiting a high titer against MRSA (Methicillin resistant Staphylococcus aureus) for screening the peptides. As a result, the authors were able to reveal new possible candidate peptides for vaccination against Staph aureus.

Contact Information

The Immune Epitope Database is supported by a contract from the National Institute of Allergy & Infectious Disease, NIH, DHHS (Contract #HHSN266200400006C). The newsletter is distributed four times a year. We welcome communication from the users of the IEDB database and invite suggestions for articles in future issues. Upon deployment of the database, we will actively solicit tool and epitope submissions. To subscribe to the IEDB newsletter or contact project staff, send your email information to the email address below.

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