

# Bioinformatics up to Date

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**Protein Data Bank**

**As of Tuesday**

**Jul 29, 2014 at**

**5 PM PDT there**

**are**

**102158 Structures**

## Stress-Tolerant Tomato Relative Sequenced

The genome of *Solanum pennellii*, a wild relative of the domestic tomato, has been published by an international group of researchers including the labs headed by Professors Neelima Sinha and Julin Maloof at the UC Davis Department of Plant Biology.



The new genome information may help breeders produce tastier, more stress-tolerant tomatoes. The work, published July 27 in the journal *Nature Genetics* [<http://www.nature.com/ng/journal/vaop/ncurrent/full/ng.3046.html>] was lead by Björn Usadel and colleagues at Aachen University in Germany. The UC Davis labs carried out work on the transcriptome of *S. pennellii* — the RNA molecules that are transcribed from DNA and then translated into protein messages written from DNA and taken to other parts of the cell to tell it what to do. Analyzing the RNA transcriptome shows which genes are active under different circumstances. The UC Davis team published a paper last year comparing the RNA transcripts of domestic tomato and three wild relatives, including *S. pennellii*.

Using the new genome data, the researchers found genes related to dehydration resistance, fruit development and fruit ripening. They also found genes that contribute to volatile compounds related to fruit scent and flavour.

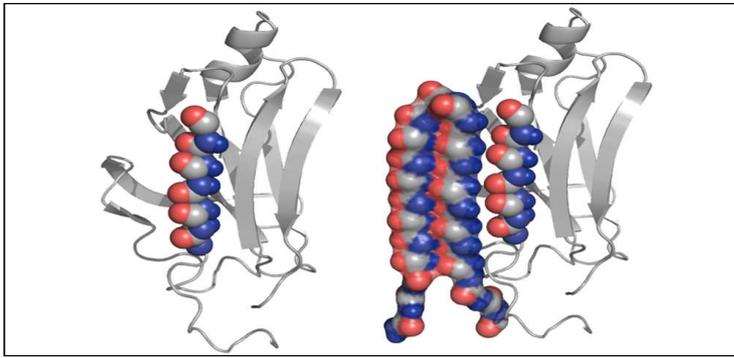
## Codon Optimization OnLine (COOL): a Web-based platform for Synthetic Gene Design

Codon optimization has been widely used for designing synthetic genes to improve their expression in heterologous host organisms. However, most of the existing codon optimization tools consider a single design criterion and/or implement a rather rigid user interface to yield only one optimal sequence, which may not be the best solution. The Codon Optimization OnLine (COOL), which is the first web tool developed that provides the multi-objective codon optimization functionality to aid systematic synthetic gene design. COOL supports a simple and flexible interface for customizing various codon optimization parameters such as codon adaptation index, individual codon usage and codon pairing. In addition, users can visualize and compare the optimal synthetic sequences with respect to various fitness measures. User-defined DNA sequences can also be compared against the COOL optimized sequences to show the extent by which the user's sequences can be further improved.

COOL is free to academic and non-commercial users and licensed to others for a fee by the National University of Singapore. Accessible at <http://bioinfo.bti.a-star.edu.sg/COOL/>.

## New Protein Structure Could Help Treat Alzheimer's, Related Diseases

University of Washington bioengineers have designed a peptide structure that can stop the harmful changes of the body's normal proteins into a state that's linked to widespread diseases such as Alzheimer's, Parkinson's, heart disease, Type 2 diabetes and Lou Gehrig's disease. The synthetic molecule blocks these proteins as they shift from their normal state into an abnormally folded form by targeting a toxic intermediate phase.



The discovery of a protein blocker could lead to ways to diagnose and even treat a large swath of diseases that are hard to pin down and rarely have a cure. The molecular structure of an amyloid protein can be only slightly different from a normal protein and can transform to a toxic state fairly easily, which is why amyloid diseases are so prevalent. The researchers built a protein structure, called "alpha sheet," that complements the toxic structure of amyloid proteins that they discovered in computer simulations. The alpha sheet effectively attacks the toxic middle state the protein goes through as it transitions from normal to abnormal. The findings were published online this month in the journal eLife. [<http://elifesciences.org/content/3/e01681>]

The researchers hope their designed compounds could be used as diagnostics for amyloid diseases and as drugs to treat the diseases or at least slow progression.

## Researchers Create Vaccine for Dust-Mite Allergies

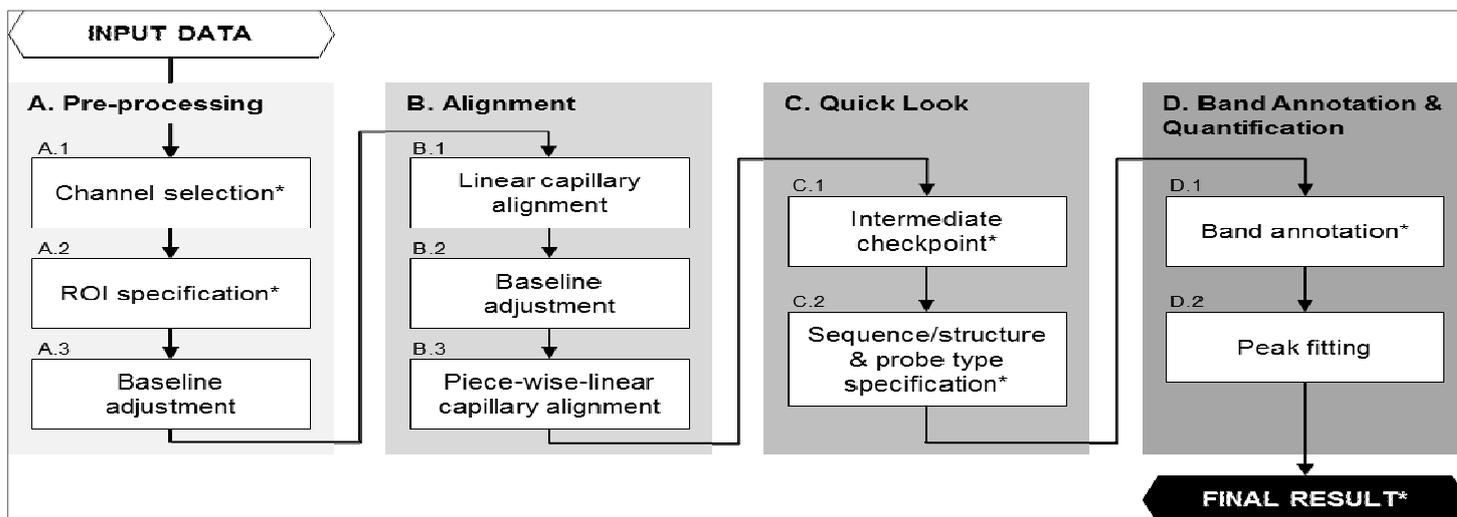
Researchers at the University of Iowa have developed a vaccine that can combat dust-mite allergies by naturally switching the body's immune response. In animal tests, the nano-sized vaccine package lowered lung inflammation by 83 percent despite repeated exposure to the allergens, according to the paper, published in the AAPS (American Association of Pharmaceutical Scientists) Journal. One big reason why it works, the researchers contend, is because the vaccine package contains a booster that alters the body's inflammatory response to dust-mite allergens.

Dust mites are ubiquitous, microscopic buggers who burrow in mattresses, sofas, and other homey spots. They are found in 84 percent of households in the United States, according to a published, national survey. Preying on skin cells on the body, the mites trigger allergies and breathing difficulties among 45 percent of those who suffer from asthma, according to some studies. Prolonged exposure can cause lung damage. Treatment is limited to getting temporary relief from inhalers or undergoing regular exposure to build up tolerance, which is long term and holds no guarantee of success. "Our research explores a novel approach to treating mite allergy in which specially-encapsulated miniscule particles are administered with sequences of bacterial DNA that direct the immune system to suppress allergic immune responses," says Peter Thorne, public health professor at the UI and a contributing author on the paper. "This work suggests a way forward to alleviate mite-induced asthma in allergy sufferers."

# HiTRACE

High-Throughput Robust Analysis  
for Capillary Electrophoresis

HiTRACE a suite of robust and efficient analysis of large-scale high-throughput CE data (Yoon et al., *Bioinformatics*, vol. 27, no. 13, pp. 17980- 1805, 2011). It has been intensively used for quantitating data for RNA and DNA based on the mutate-and-map methodology, chromatin footprinting, and other high-throughput structure mapping techniques. HiTRACE is based on command-line MATLAB scripts and requires nontrivial efforts to learn, use and extend.



HiTRACE-Web analysis pipeline

## *iScreen*

iScreen a cloud-computing screening system for TCM (traditional Chinese medicine) intelligent based on TCM Database@Taiwan. iScreen is compacted web server for TCM docking and followed by customized de novo drug design. Here also implemented a protein preparation tool that both extract protein of interest from a raw input file and estimate the size of ligand

News and Updates	<b>TCM Docking &amp; Screening News</b>
Introduction	• 2011/06/22 iScreen has been accepted by <i>Journal of Computer-Aided Molecular Design (JCAMD)</i> ... (more)
Tutorial	• 2011/06/22 iScreen has been reported by <i>GenomeWeb Daily News</i> .
Protein Docking	• 2011/04/06 Add control ligand docking.
Browse Results	• 2010/11/29 Protein docking function online.
TCM Docking	
Tool	
About YC Lab	

bind site. In addition, iScreen is designed in user-friendly graphic interface for users who have less experience with the command line systems. For customized docking, multiple docking services, including standard, in-water, pH environment, and flexible docking modes are implemented. Users can download first 200 TCM compounds of best docking results. For TCM de novo drug design, iScreen provides multiple molecular descriptors for a user's interest. iScreen is the world's first web server that employs world's largest TCM database for virtual screening and de novo drug design.

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[<http://iscreen.cmu.edu.tw/intro.php>]

## CCBuilder: an interactive web-based tool

*for building, designing and assessing  
coiled-coil-protein assemblies*



### Patent News

## Integrated Bioinformatics Sensing Apparatus US 20140107452 A1

Publication number: US20140107452 A1

Publication date : Apr 17, 2014

Inventors : Min-Hsien Wu, Yi-Yuan Chiu, Hsin-Yao Wang,  
Song-Bin Huang

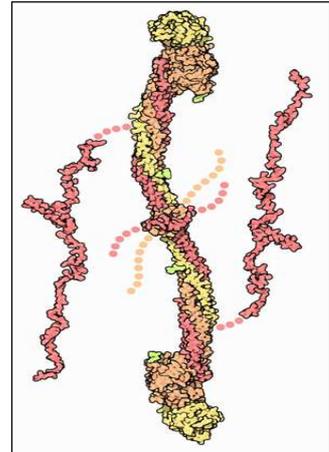
### ABSTRACT

An integrated bioinformatics sensing apparatus includes a piezoelectric sensing layer, an upper conductive layer, a bottom conductive layer and an information transmission controller. The piezoelectric sensing layer senses a physiological rhythm of a living organism to output a physiological rhythm signal, and the upper and bottom conductive layers sense a physiological electrical signal on a body surface of the living organism, and the information transmission controller receives and processes the physiological rhythm signal and the physiological electrical signal to generate and store the sensed bioinformatics, or transmit the signals to the external processing device to display the sensed bioinformatics. The simple-structured sensing apparatus can be attached onto the body surface of the living organism conveniently.

## Fibrin

Fibrin is normally present in an inactive form known as fibrinogen.

When given the signal, fibrinogen is converted to fibrin, which then assembles into an extended network of fibers. This changes normally-fluid blood into a jelly-like solid, which then dries to form a scab. Of course, it is very important to assemble fibrin networks only in the local area of the cut, and nowhere else, since the blood must continue flowing to other parts of the body. The fine-tuned control of blood clotting is controlled by a cascade of specialized proteins.



Fibrin is a large, flexible protein composed of six proteins chains. Since it has several flexible parts, it has been difficult to study, and many of the structures in the PDB contain only part of the molecule. Two PDB structures were

used to create this picture: 1m1j for the central core of the molecule, and 2baf for the two flexible arms at either side. The four little chains shown with dotted lines at the center, which unfortunately are not seen in the structure analyses, are the key to the activation of fibrin. The ends of these four chains are clipped by thrombin, changing inactive fibrinogen to active fibrin. These flexible chains then form the linkages that glue many fibrin chains into a fibril.

## Bioinformatics Carrier

1. Position for a Postdoctoral fellow in bioinformatics and genomics @ inStem, Institute for Stem Cell Biology and Regenerative Medicine, Bangalore <http://instem.res.in/open-positions>

2. Uni Delhi Gene regulation PhD Positions in Dr. Manu Agarwal's Laboratory @ Department of Botany, University of Delhi ; <http://helpbiotech.blogspot.in/2014/07/uni-delhi-gene-regulation-phd-positions.html>

3. <http://jobs.astrazeneca.com/jobs/details/11rRD1051> bioinformatics-scientist; Deadline for applications is 22nd of August

## Upcoming Events

### BioStatistics Workshop

29th to 30th September 2014  
ICSCCBPune, Maharashtra, India

**Website:** <http://www.icsccb.org/workshops/biostatistics-workshop/>

### 2014 BGI International Bioinformatics Workshop

15th to 18th September 2014  
Shenzhen, China

**Website:** [http://events.genomics.cn/en/training/show\\_training?id=121](http://events.genomics.cn/en/training/show_training?id=121)

Kindly send us your feedback to

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