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# Bioinformatics up to Date

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## Inside.....



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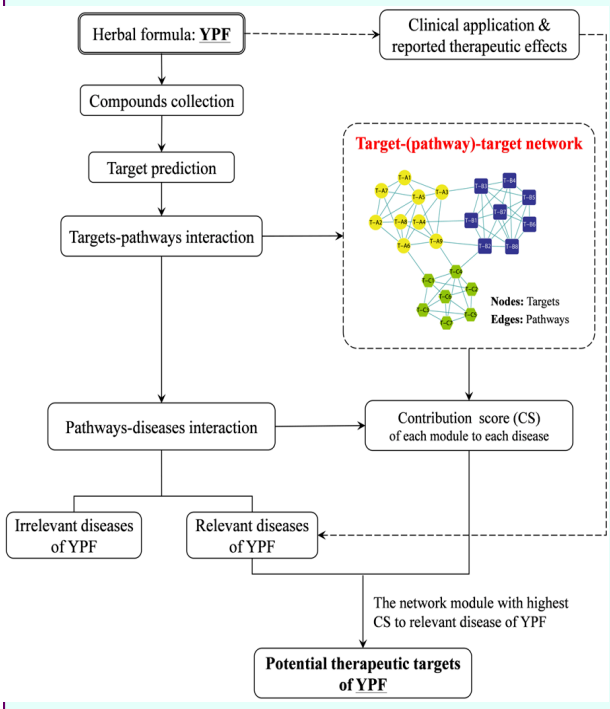
## About us

The Bioinformatics Infrastructure Facility (BIF) at Biotechnology division, CSIR NEIST, Jorhat runs under the Biotechnology Information System Network (BTISnet) programme of DBT, Ministry of Science & Technology, and Government of India. The Centre was established on 2nd February, 2008 to promote innovation in Biological research and education through Bioinformatics accomplishment. The main goal is to facilitate and expose students and researchers from different academic institutions of North East India in Bioinformatics. The center conduct training and workshops for enlightening the use of bioinformatics applications in biological research and development. The Centre has access to global information through 24 hour high speed internet facility, and also e-journal facilities with DeLCON, Science Direct etc. To date the Centre has profoundly extended support in R & D work with a great intensity to different biological discipline including medicinal chemistry, computer aided drug design, genomics and proteomic data analysis etc.

## A network pharmacology-based approach to analyse potential targets of traditional herbal formulas: An example of Yu Ping Feng decoction




Workflow of the novel NP-based method.

This study developed a novel network pharmacology based method to identify its potential therapeutic targets. By taking a classic herbal formula (Yu Ping Feng decoction, YPF) as an example. First, this study constructed a "targets–(pathways)–targets" (TPT) network in which targets of YPF were connected by relevant pathways; then, this network was decomposed into separate modules with strong internal connections; lastly, the propensity of each module toward different diseases was assessed by a contribution score. On the basis of a significant association between network modules and therapeutic diseases validated by chi-square test ($p$-value < 0.001), this study identified the network module with the strongest propensity toward therapeutic diseases of YPF. Further, the targets with the highest centrality in this module are recommended as YPF's potential therapeutic targets. By integrating the complicated "multi-targets–multi-pathways–multi-diseases" relationship of herbal formulas, the method promise for identifying its potential therapeutic targets, which could contribute to the modern scientific illustration of TCMs' traditional clinical applications.

*Source:* Huali Zuo ***et al.*** *Scientific Reports* (2018)

## JALVIEW: a free program for multiple sequence alignment editing, visualisation and analysis.

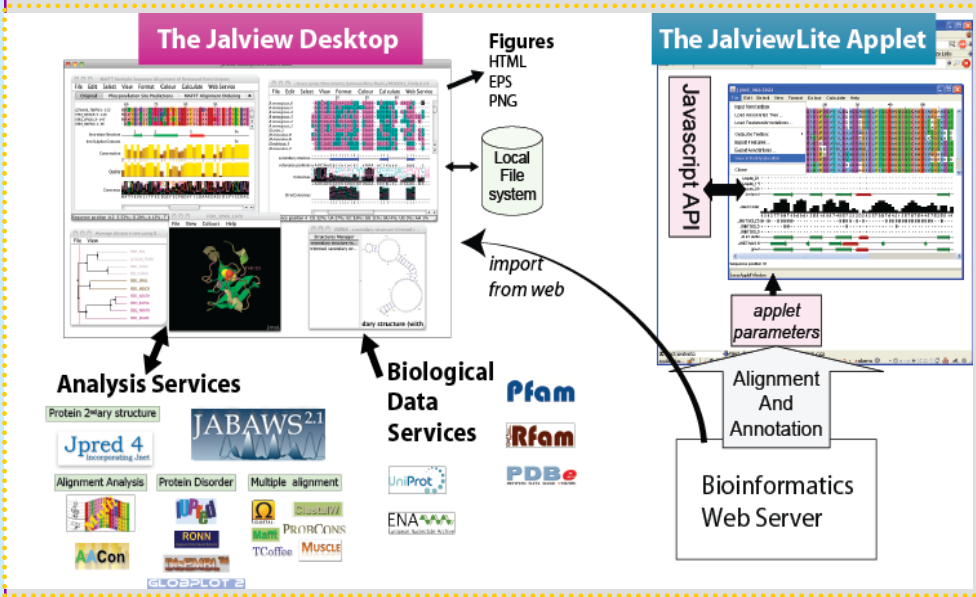



Fig: Overview of Jalview

Jalview is a tool written in Java to analyse the residue conservation patterns in a protein multiple alignment as well as being an interactive alignment editor. Unaligned sequences can be aligned either locally or remotely at the EBI with further analysis programs available remotely at the EBI. Access to the database entries for individual sequences is available through SRS. The sequence features can be extracted from the database entries and displayed graphically on the alignment. If three dimensional structures exist for any of the sequences then the structures can be displayed and coloured according to the colour scheme or conservation patterns in the multiple alignment.

**Availability of tool:** http://circinus.ebi.ac.uk:6543/jalview/ and http://www2.ebi.ac.uk/clustalw

*Source: http://www.jalview.org/*

## Altools: a user friendly NGS data analyser

Altools is fast, reliable and easy to use for the mining of NGS data. The software package also attempts to link identified polymorphisms and structural variants to their biological functions thus providing more valuable information than similar tools.

**Carried out at five different stimulated coverage levels**

| Coverage | 4x | 10x | 20x | 40x | 100x |
|---|---|---|---|---|---|
| dgwsim generated polymorphisms | 121,388 | 122,074 | 121,368 | 121,540 | 121,638 |
| dgwsim generated SNPs | 107,054 | 107,411 | 106,766 | 107,372 | 107,277 |
| dgwsim generated indels | 14,334 | 14,663 | 14,602 | 14,168 | 14,361 |
| Altools total called SNPs | 35,714 | 81,647 | 102,493 | 105,164 | 105,580 |
| Altools correctly called SNPs | 35,650 | 81,482 | 102,274 | 104,910 | 105,243 |
| Altools false positive SNPs | 64 | 165 | 219 | 254 | 337 |
| Altools total called indels | 3049 | 8307 | 11,134 | 11,542 | 11,657 |
| Altools correctly called indels | 3040 | 8280 | 11,112 | 11,503 | 11,621 |
| Altools false positive indels | 9 | 27 | 22 | 39 | 36 |
| PPV | | | | | |
| SNPs | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| Indels | 0.33 | 0.76 | 0.96 | 0.98 | 0.98 |
| Sensitivity | | | | | |
| SNPs | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| Indels | 0.21 | 0.56 | 0.76 | 0.81 | 0.81 |

Fig: Performance of the Altools platform (detection of polymorphisms). Statistical analysis of Altools polymorphism calling was carried out at five simulated coverage levels

*Source:* DOI:10.1186/s13062-016-0110-0

**Bioinfo. Animation** (Source :Anna Bauer-Mehren *et al.* PLoS ONE , vol. 6, iss. p )

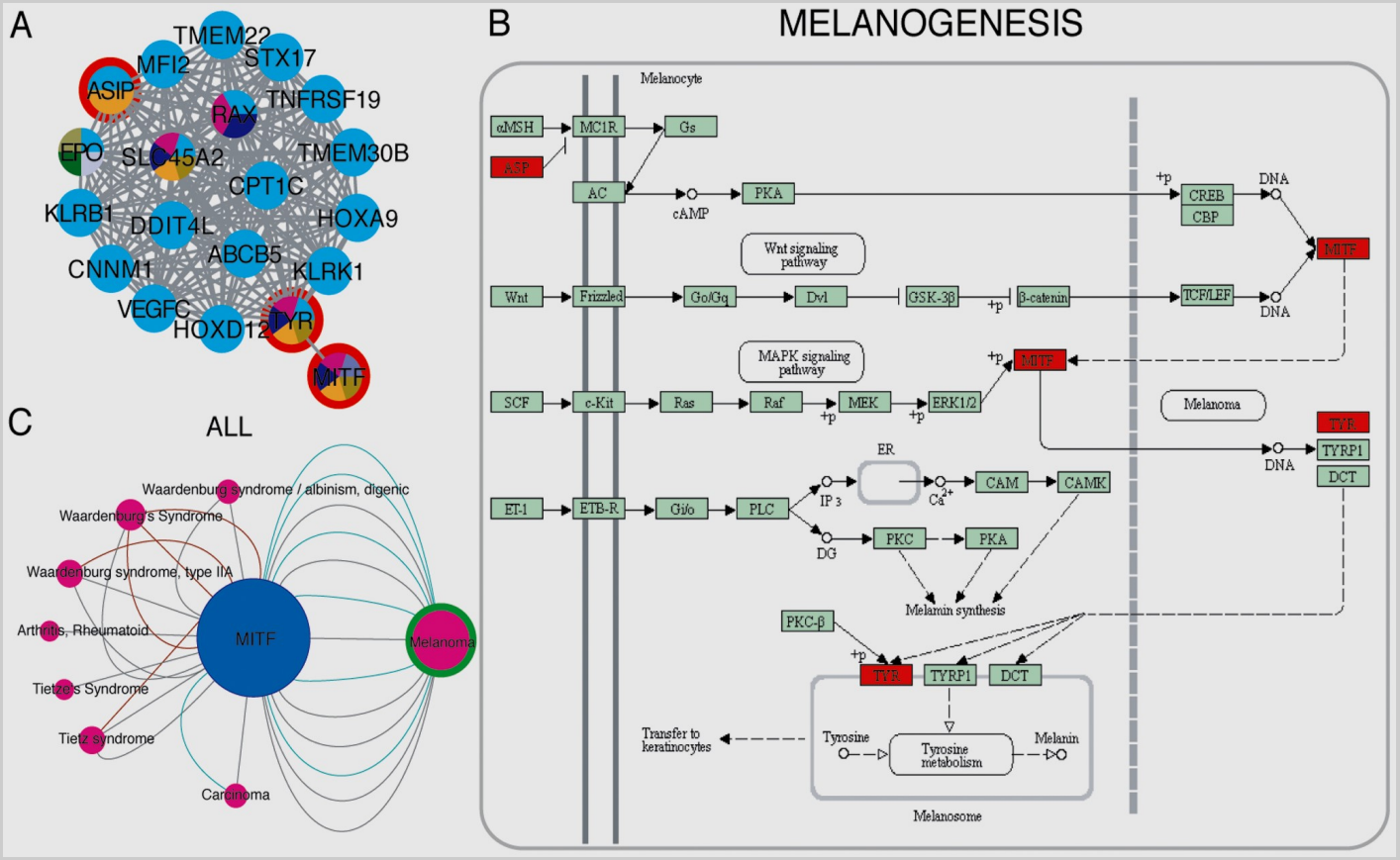
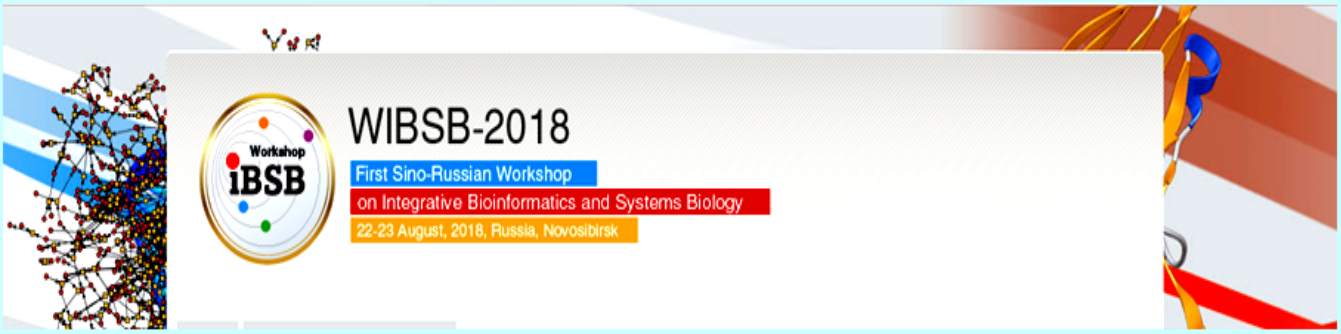



Fig:Gene-Disease-Network-Analysis-Reveals-Functional-Modules-in-Mendelian-Complex .

Upcoming event

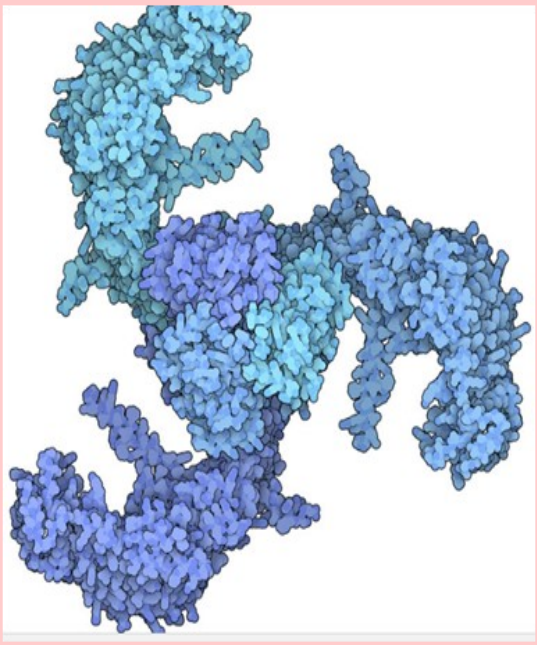




1.http://conf.bionet.nsc.ru/srw2018/en/
2. http://www.sgrfconferences.org/2018/NGBT/#

# Piezo1 Mechanosensitive Channel

Our senses rely on molecular machines that monitor the environment and generate a signal when something interesting happens. For things like taste, this is fairly straight-forward: taste sensors just need to recognize characteristic molecules that we eat, like sour acids or sweet sugars. Touch, however, is much trickier. For that, the sensor needs to monitor the shape of a cell surface. Several recent structures are revealing how this is accomplished in cells.



## Under A Microscope:

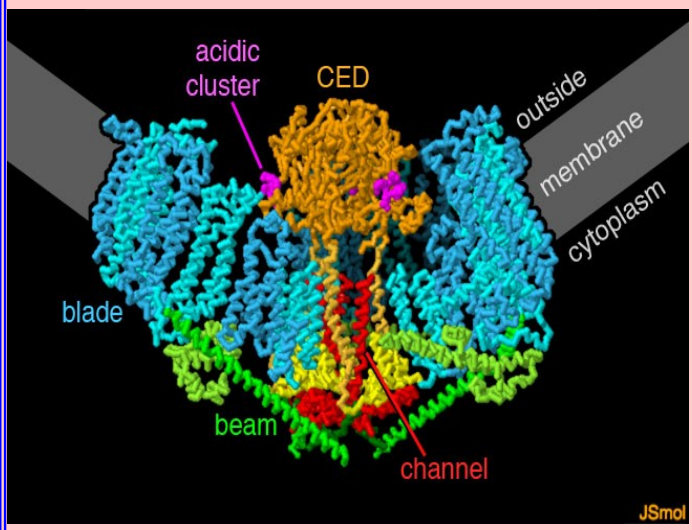
Structures have recently been determined for Piezo1 using cryoelectron microscopy: a low-resolution structure was determined in 2015 (PDB entry 3jac) and three more detailed structures have just been released (PDB entries 6b3r, 6bpz, 5z10). They all reveal a complex molecular machine composed of three identical protein subunits. The subunits come together in the center to form a membrane-spanning ion channel, and three curving blades extend away from the channel. The blades are thought to probe the state of the surrounding membrane, opening the channel when the membrane is distorted.

## Putting Pressure on Piezos

Two similar Piezo proteins give our cells a sense of touch. Piezo2 is found in sensory neurons, where it controls gentle touch sensations. Piezo1, on the other hand, is found in non-sensory tissues, where it helps cells sense local changes in fluid pressure. This is important, for example, in processes like blood flow, and also helps give us our ongoing feeling for how all our limbs are positioned. Changes in the tension of membranes cause these Piezo proteins to open up and allow positively-charged ions like calcium to enter the cell. This change in ion concentration triggers the sensory response of the cell.

## Exploring the Structure

The Piezo1 structures reveal many functional domains within the long protein chains. The blades (blue) are composed of a series of similar domains that are embedded in the membrane. As you can see in the structure, the blades are not flat, but instead bend the membrane into a cup shape. A cluster of acidic amino acids (magenta) in the CED domain (orange) is though to help manage access of calcium ions to the central channel, which is surrounded by three helices (red). A beam (green) connects the blades and the channel, presumably linking changes in the shapes of the blades to opening of the channel. To explore this structure in more detail, click on the image for an interative JSmol.




Source: http://pdb101.rcsb.org/motm/223

**Kindly send us your feedback to**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