

Bioinformatics up to Date

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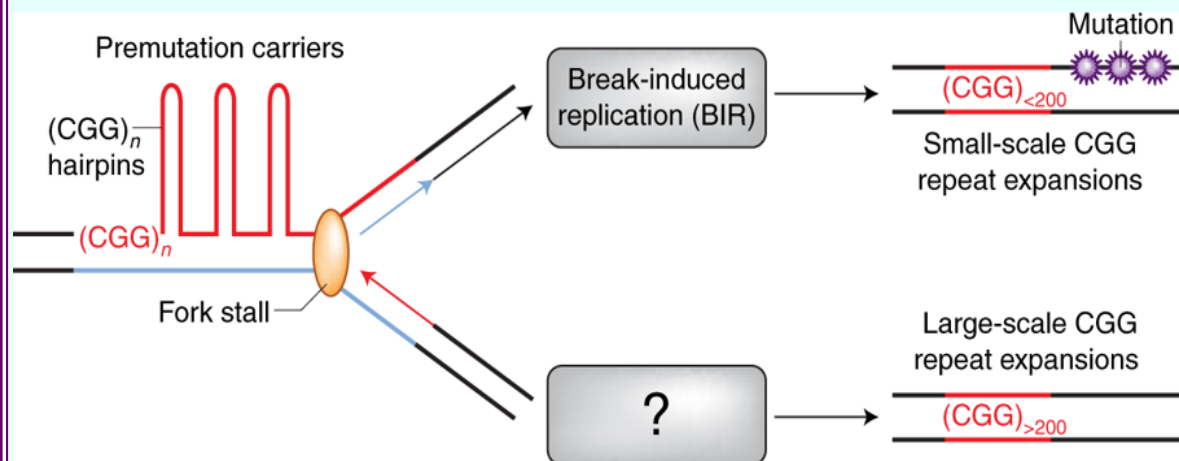
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About us

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.

Break-induced replication sparks CGG-repeat instability

The mechanism underlying CGG-repeat expansions of a CGG repeat located in the 5' untranslated region (UTR) of the *FMR1* gene on X Chromosome in patients with fragile X premutation are responsible for various disorders, including fragile X syndrome (FXS), Friedreich's ataxia (FRDA), myotonic dystrophy type 1 (DM1)



Model for CGG-repeat instability in patients with fragile X premutation.

and Huntington's disease (HD). Using a new experimental system in mammalian cells, a study in this issue reports that break-induced replication has a role in CGG-repeat instability. Replication forks stall at DNA secondary structures formed by the CGG repeats. If a replication fork is not rescued and collapses, the resulting DNA damage is repaired via break-induced replication (BIR). This results in instability of small-scale repeats and mutations at adjacent DNA segments. The mechanism responsible for large-scale CGG-repeat expansions to be determined.

Source: *Nature Structural & Molecular Biology* volume 25, pages643–644 (2018)

PyPhi: A toolbox for integrated information theory

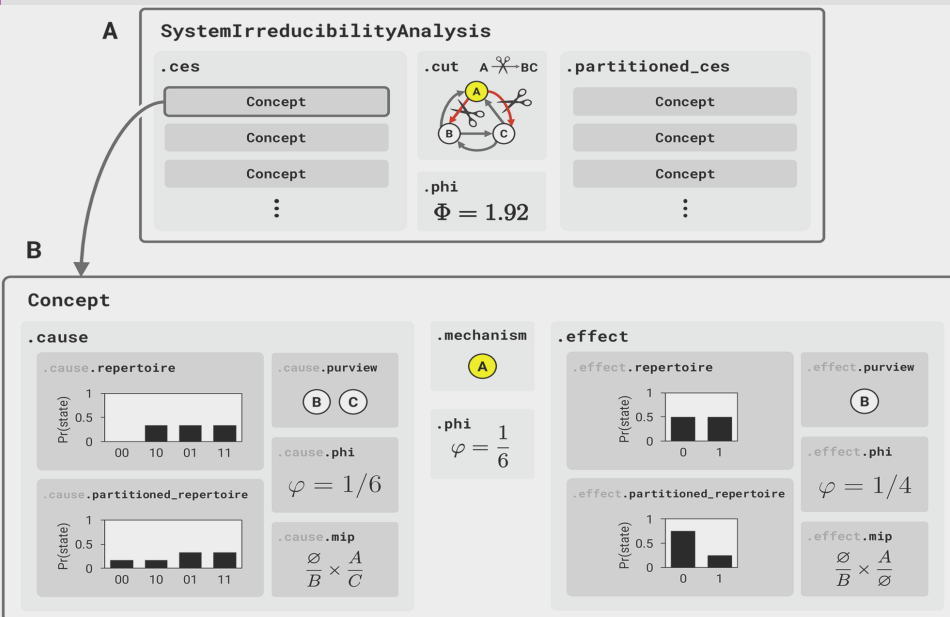


Fig: Output result of this software with both cause and effect data.

and demonstrate PyPhi's functionality in the course of analyzing an example system, and then describe details of the algorithm's design and implementation.

Availability of this tool: The tool is available on GitHub at <https://github.com/wmayner/pyphi>.

Source: <https://doi.org/10.1371/journal.pcbi.1006343>

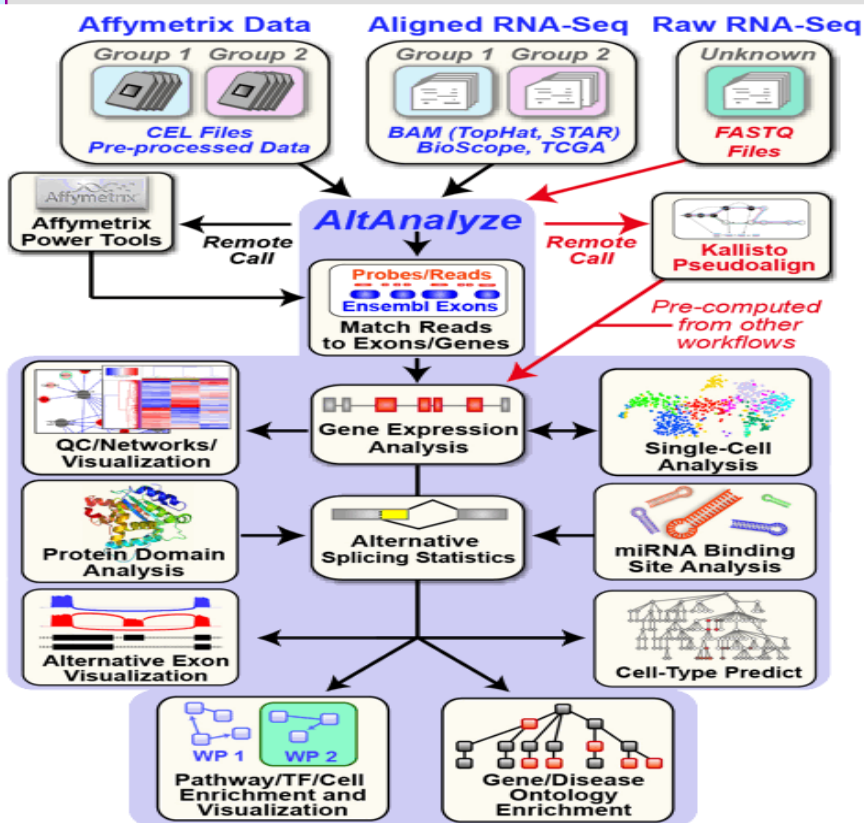


Fig: Performance and overview of AltAnalyze tool

Source: <https://altanalyze.readthedocs.io/en/latest/>

Integrated information theory provides a mathematical framework to fully characterize the cause-effect structure of a physical system. PyPhi, a Python software package that implements this framework for causal analysis and unfolds the full cause-effect structure of discrete dynamical systems of binary elements. The software allows users to easily study these structures, serves as an up-to-date reference implementation of the formalisms of integrated information theory, and has been applied in research on complexity, emergence, and certain biological questions. We first provide an overview of the main algorithm

Exploring the AltAnalyze: the new single-cell RNA-seq analysis tool

AltAnalyze is an extremely user-friendly and open-source analysis toolkit that can be used for a broad range of genomics analyses. These analyses include the direct processing of raw RNASeq or microarray data files, advanced methods for single-cell population discovery, differential expression analyses, analysis of alternative splicing/promoter/polyadenylation and advanced isoform function prediction analysis (protein, domain and microRNA targeting). Multiple advanced visualization tools is supported in AltAnalyze (e.g., network, pathway, splicing graph). AltAnalyze is compatible with various data inputs for RNASeq data (FASTQ, BAM, BED), microarray platforms (Gene 1.0, Exon 1.0, junction and 3' arrays). This software requires no advanced knowledge of bioinformatics programs or scripting or advanced computer hardware.

Availability of this tool: The tool is available on <http://www.altanalyze.org/>

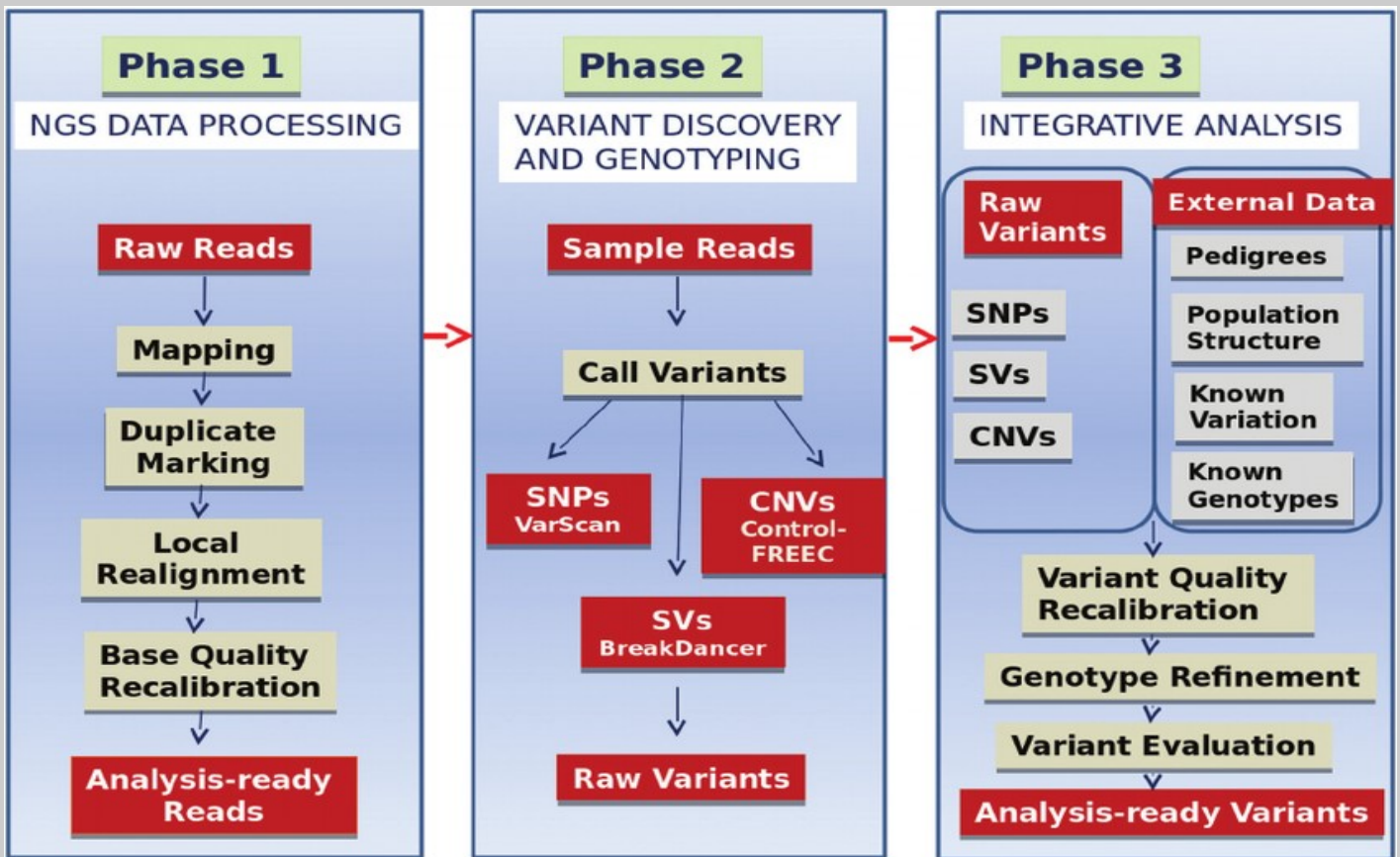


Fig: NGS Data Processing flowchart

Upcoming event

International Conference on
Computational Biology and Bioinformatics
 September 05-06 2018 Tokyo, Japan
 Theme: Computational Biology: Going into the future one click at a time

Buttons: Organizing Committee, Submit Abstract, Register Now, Program Schedule, Reader Base

Discounts on Group Registrations

UK-INDIA CANCER BIOINFORMATICS WORKSHOP
 On
 Next-Generation Sequencing Data Analysis
 28th - 31st October, 2018 at ACTREC, Navi Mumbai, India

Logos: UNIVERSITY OF CALicut, KING'S College LONDON, ACTREC

Flowchart of NGS analysis: Tumor sample (DNA/RNA) → Exome sequencing / RNA-Seq → Read alignment → Variant calling / Transcript quantification → Copy ratio calculation / Copy number alterations → Somatic mutations / Differential expression → Integrated analysis

- [1. https://computational-biology.conferenceseries.com/](https://computational-biology.conferenceseries.com/)
- [2. https://indiabioscience.org/events/uk-india-cancer-bioinformatics-workshop](https://indiabioscience.org/events/uk-india-cancer-bioinformatics-workshop)

Legumain

Legumain has been given many names, reflecting its many different functions. In plants, it helps to process proteins in storage vacuoles, so it has been called vacuolar processing enzyme. In our cells, it processes proteins for the immune system, generating the short peptides displayed by MHC, and has been called asparaginyl endopeptidase (based on its preference for cleaving proteins after asparagine). It also acts as an enzyme that chews off amino acids at the end of protein chains, and was given another name for that function. Fortunately, the research world has settled down to the simpler name “legumain” to refer to the enzyme that performs all of these jobs.

Cutting and Pasting

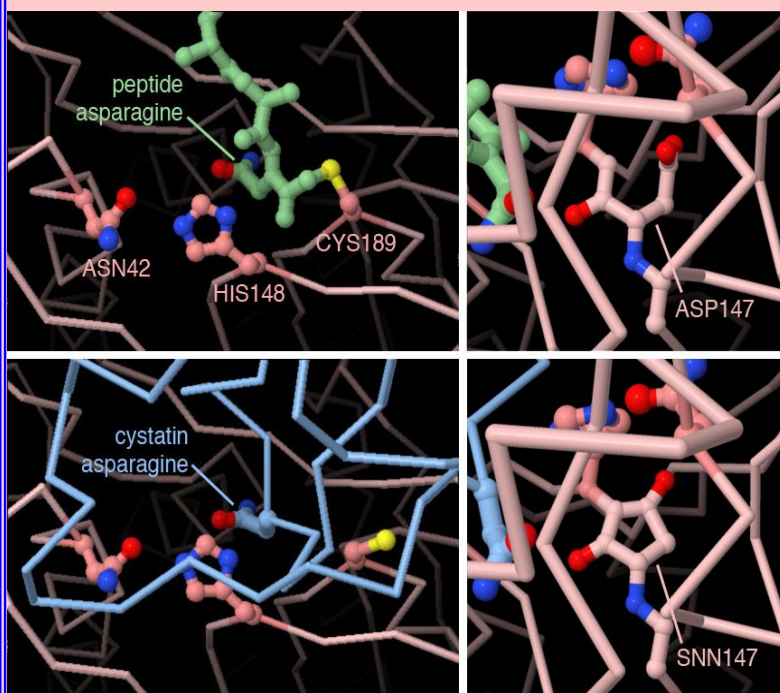
legumain revealed that it is also quite adept at reconnecting protein chains. For example, it is involved in the circular permutation of concanavalin A, and also assists with building of cyclic peptides that are used by plants for defense. This ligation reaction occurs in the same active site, but doesn't appear to use the cysteine amino acid. Instead, a nearby aspartate adopts an unusual chemical form (shown in the JSmol) and is thought to assist with the reaction.

Exploring the Structure

Legumain, with active site cysteine in yellow, histidine and asparagine in orange, and glycosylation in magenta.

PDB entry 4awb captures legumain in the middle of its reaction. At top left, a short peptide has been cleaved and half is left attached to the catalytic cysteine. Later, a water molecule will be used to release the attached peptide. PDB entry 4n60 shows legumain bound to the inhibitory protein cystatin.

As seen at bottom left, it also has an asparagine that fits into the specificity pocket, but it is cleaved very slowly, and when cleaved, it is also reconnected by legumain. The images on the right show an aspartate that adopts an unusual aminosuccinimide form that is thought to be important in the ligation reaction. Click on the image to explore the structure, and display the amino acids in the specificity pocket and the modified aspartate.



Source: <http://pdb101.rcsb.org/>

Kindly send us your feedback to

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