Informatics Expertise to Support Life and Health Sciences Research and Industry

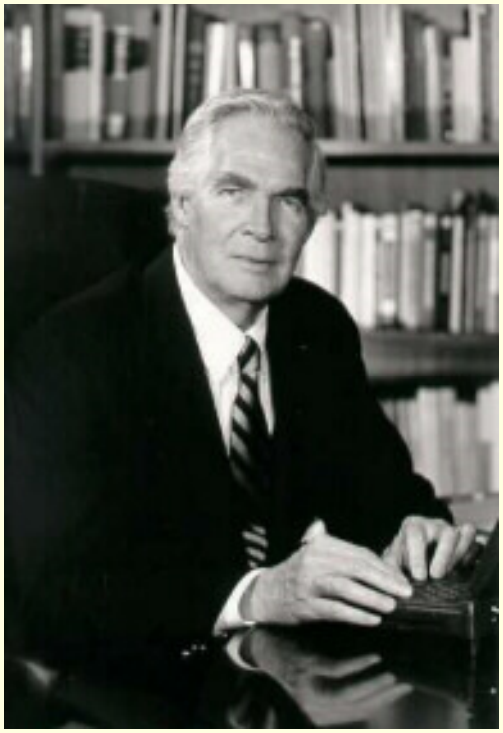
Chi-Ren Shyu, Ph.D.
shyuc@missouri.edu

Director, Informatics Institute
University of Missouri – Columbia

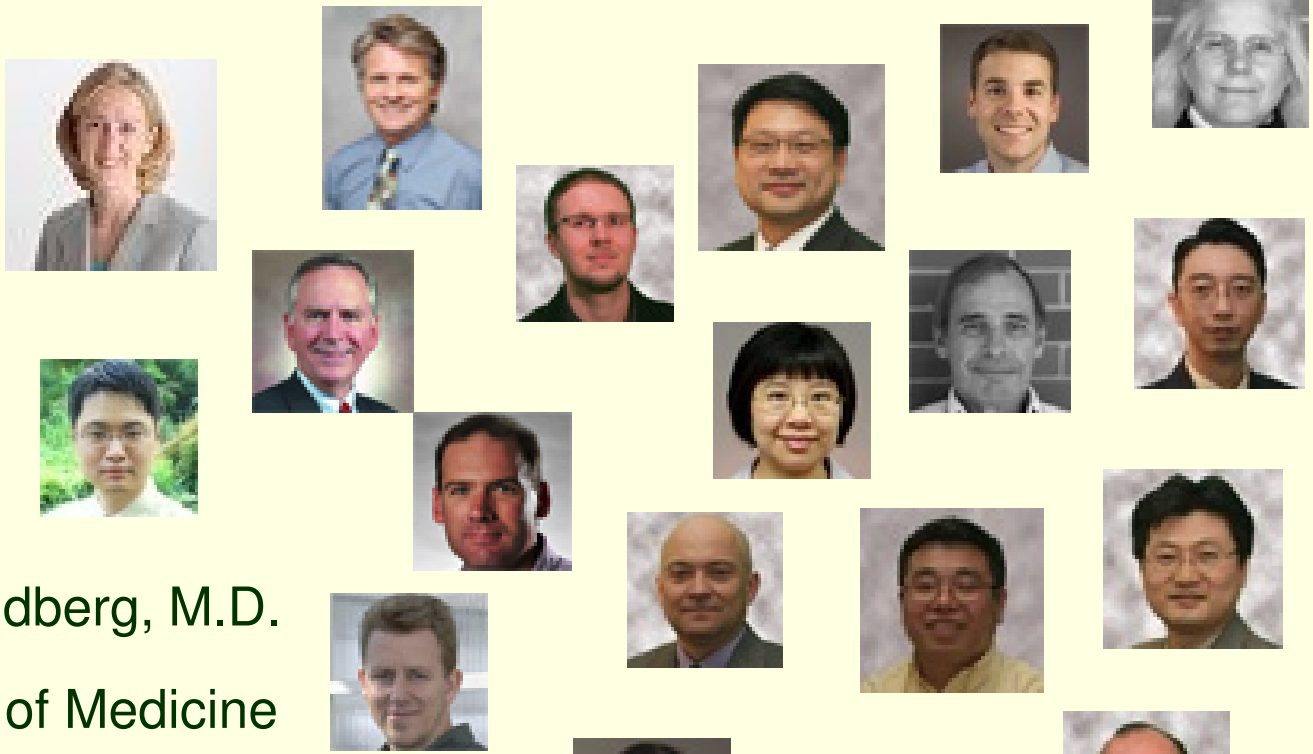
http://MUII.missouri.edu

Informatics Research Expertise

Informatics at MU



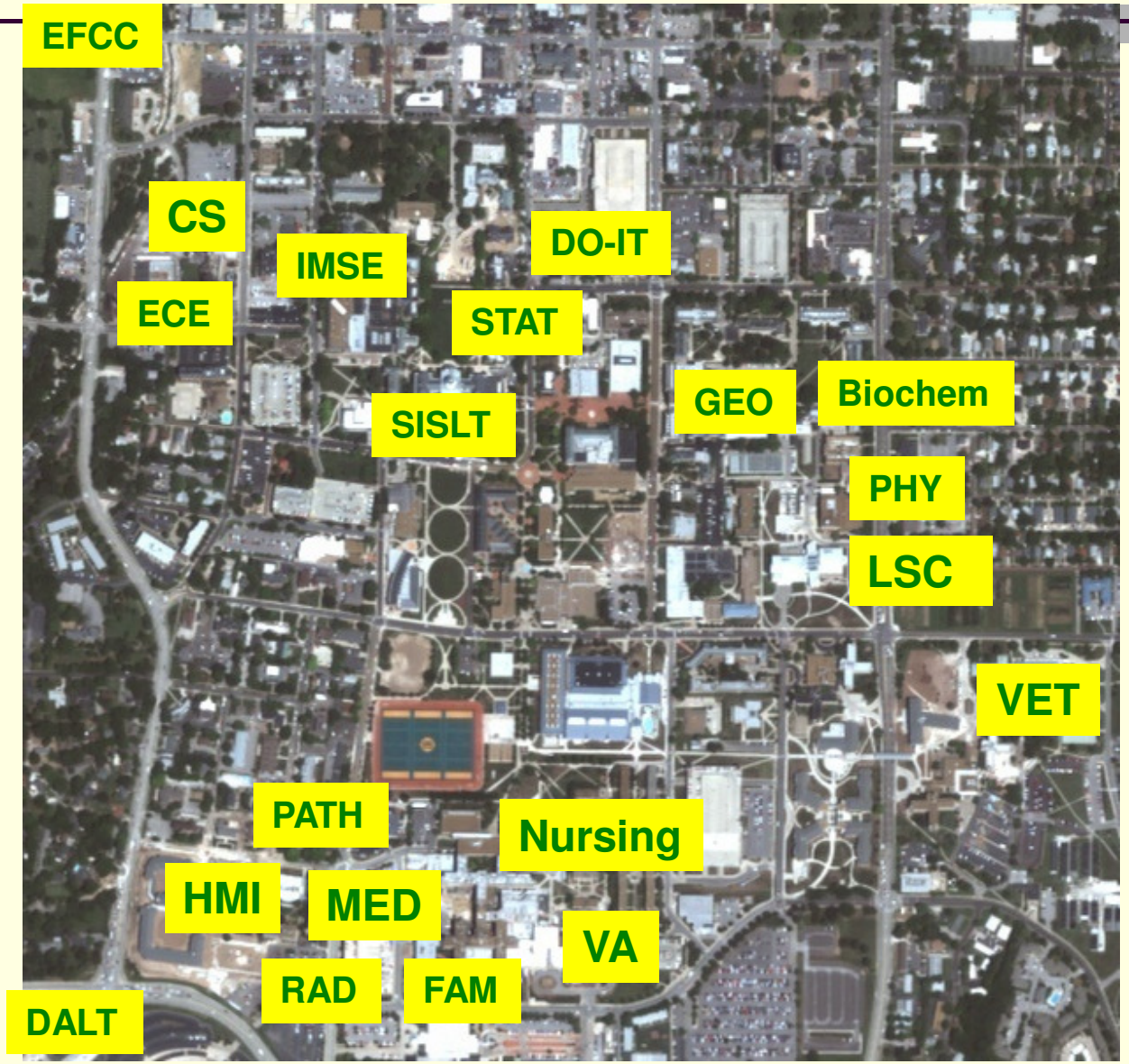
In 2010, MU Informatics Institute (**MUII**) has **30** core faculty members, **25** doctoral students, **$8M** ongoing informatics related research and training programs.



60's— 80's Donald A.B. Lindberg, M.D.

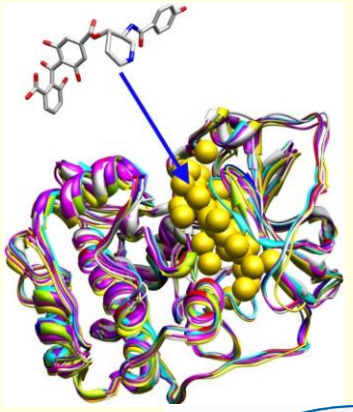
Director of the National Library of Medicine has pioneered in applying computer technology to health care beginning in 1960 at MU

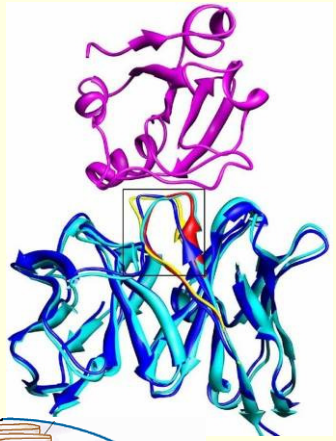
MUII is currently a campus-wide hub for informatics research, education, and services

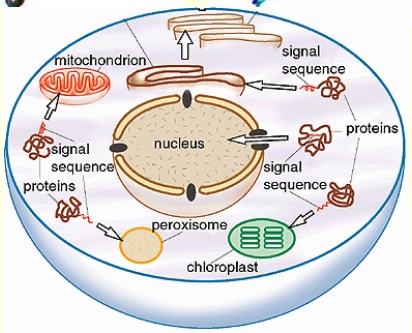


Bioinformatics

High throughput sequencing, structure biology, cancer research, neural sciences, animal sciences, translational bioinformatics, etc.



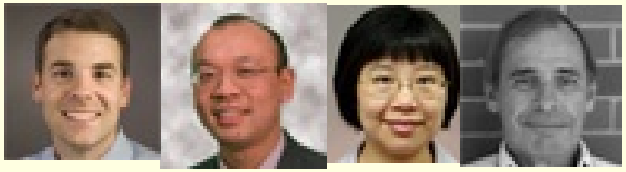


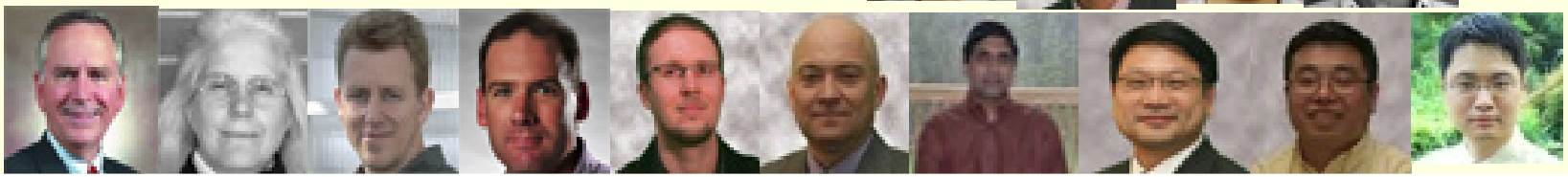


Highlights:

MULTICOM methods were ranked among best in six categories during the 8th Critical Assessment of Techniques for Protein Structure Prediction (CASP8), 2008.

ProteinDBS is the first real-time protein 3D structure retrieval engine.

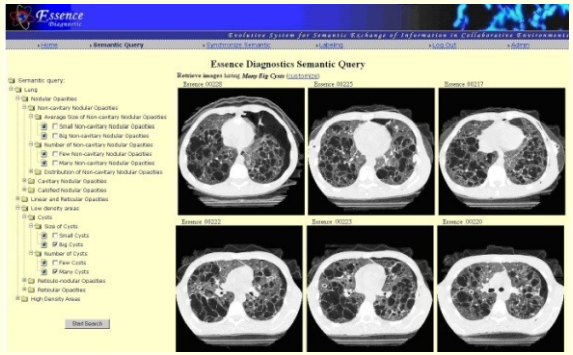


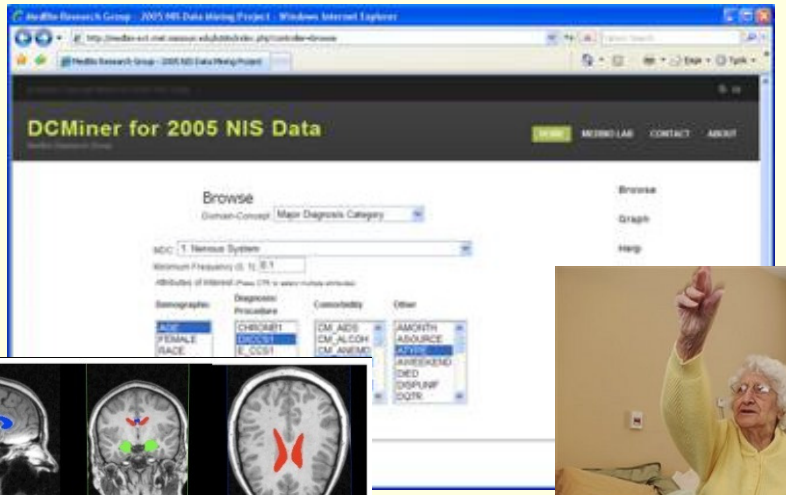


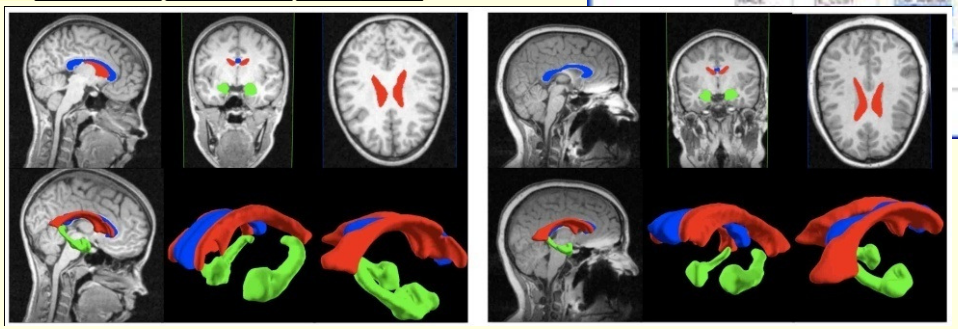
Informatics Research Expertise

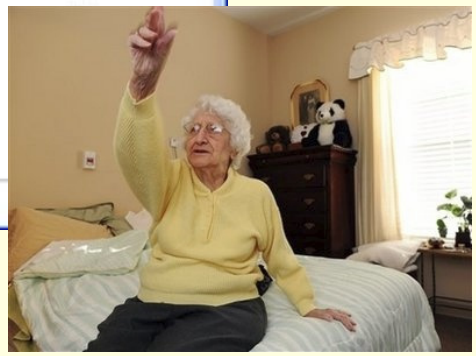
Medical/Health Informatics

EMR/EHR, Imaging Informatics, Healthcare Quality, Texting Mining, Human Computer Interaction, Nursing Informatics, Elder Care, Autism, etc.





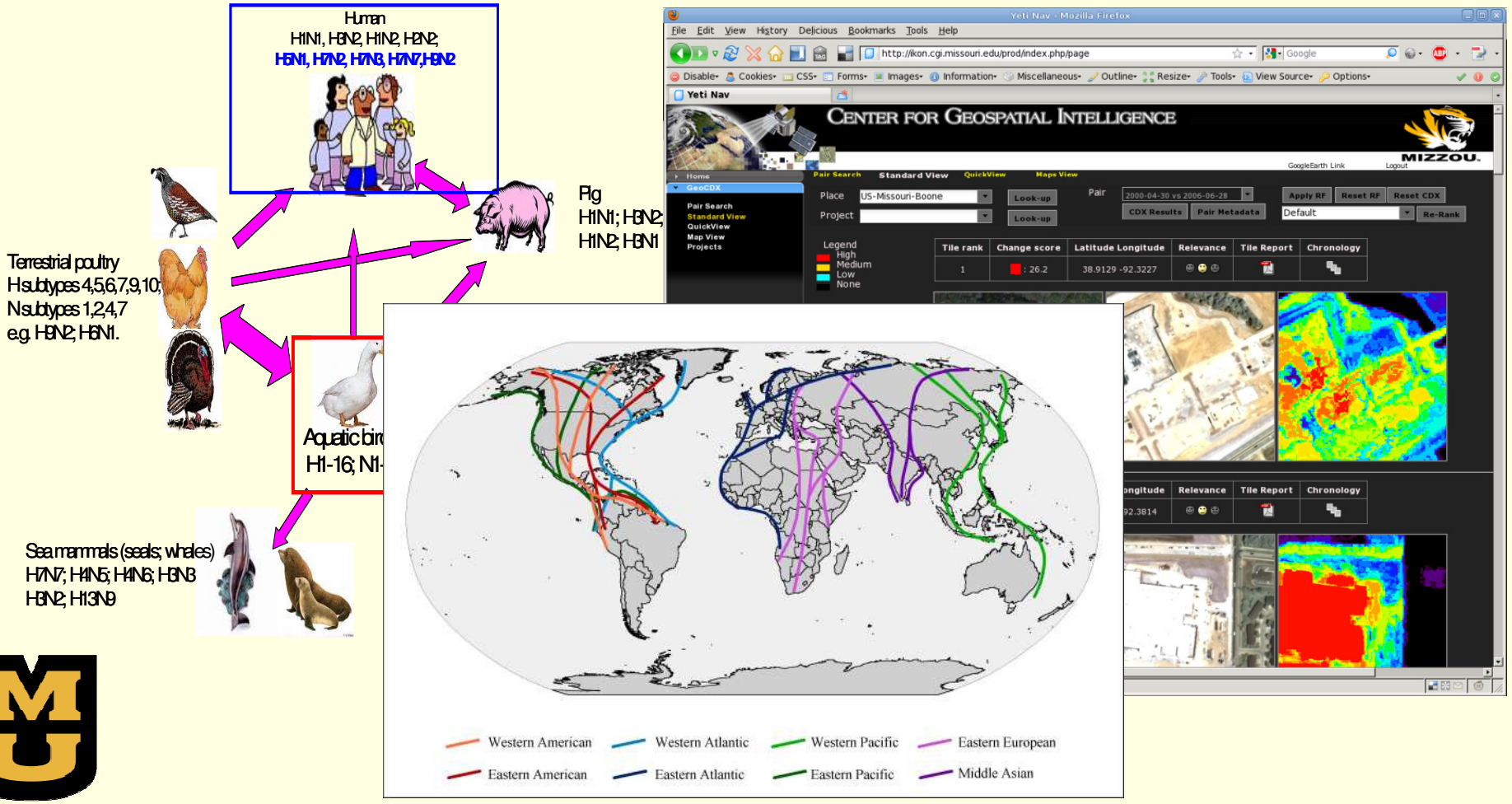




Informatics Research Expertise

Geospatial Informatics

Epidemiology, intelligence applications, agriculture applications, crime analysis, environmental studies, etc.



Scenario –Personalized Medicine/Healthcare

Personalized Genomics – Bioinformatics tools to analyze individual genomes from SNP, partial/full genome sequence, etc.

Structural Bioinformatics – Rational drug design, host-pathogen interaction, etc.

Human Factors Studies, Data Mining from Omics Databases and EMR – Patient safety, Next generation search engine for medical multimedia data, etc.

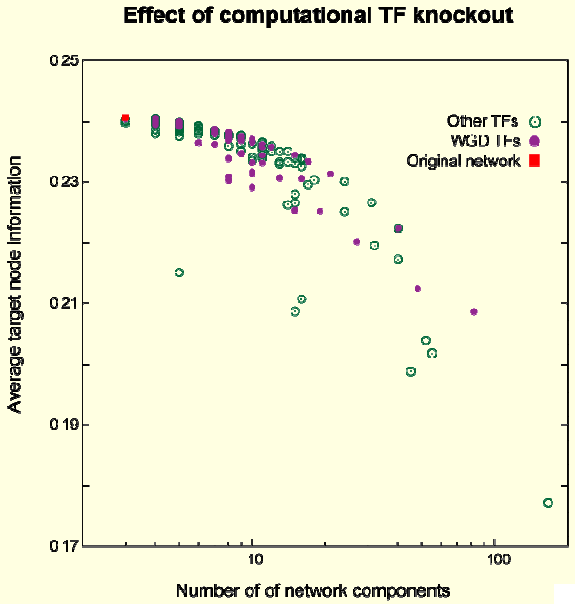
Informatics Research Expertise

Gavin Conant

conantg@missouri.edu

Division of Animal Sciences and
Informatics Institute
University of Missouri
Web: web.missouri.edu/~conantg

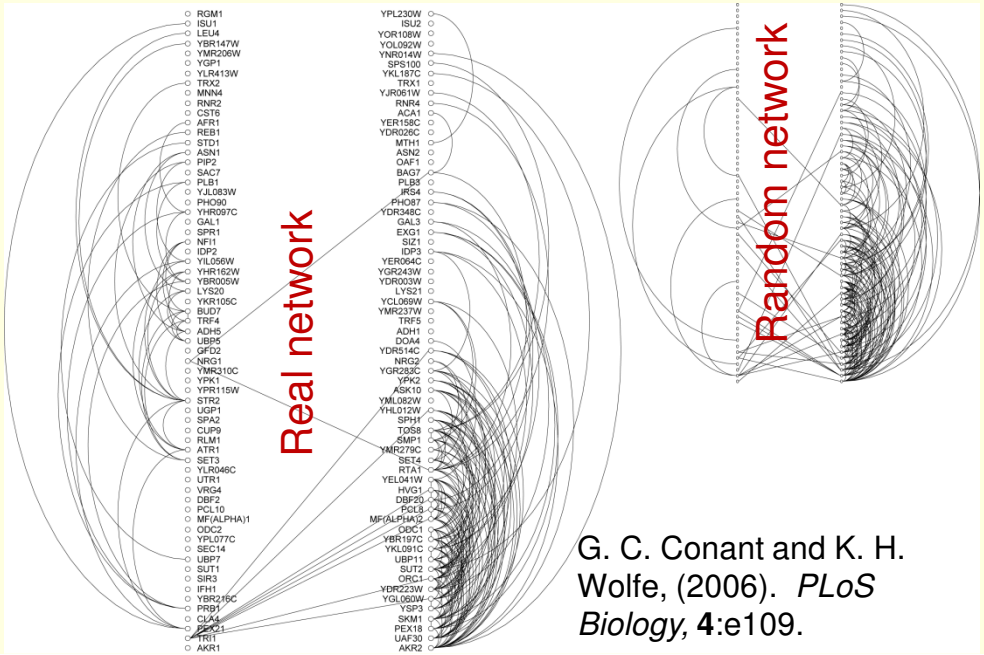
Development of regulatory complexity through genome duplication



Transcription factors with surviving duplicates from a genome duplication in yeast are more central in the regulatory network

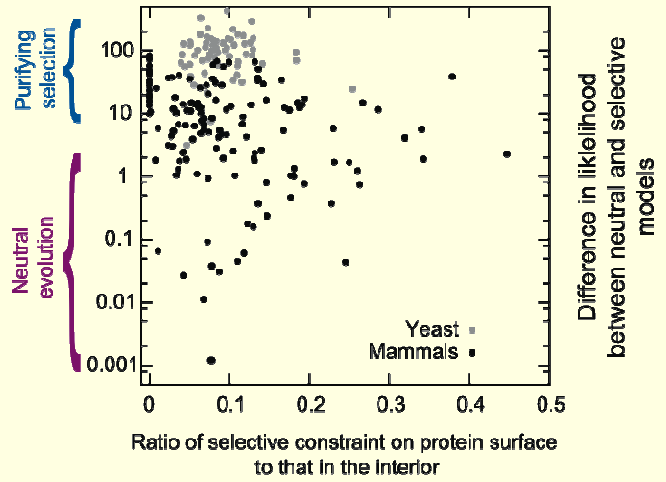
G. C. Conant, (2010) *Proceedings of the Royal Society, Biological Sciences,* **277**: 869.

Identification of partitioned cellular subnetworks created by genome duplication in yeast



G. C. Conant and K. H. Wolfe, (2006). *PLoS Biology,* **4**:e109.

Demonstration of *neutral* evolution on the surface of mammalian proteins



G. C. Conant (2009). *Trends in Genetics,* **25**: 377

Informatics Research Expertise

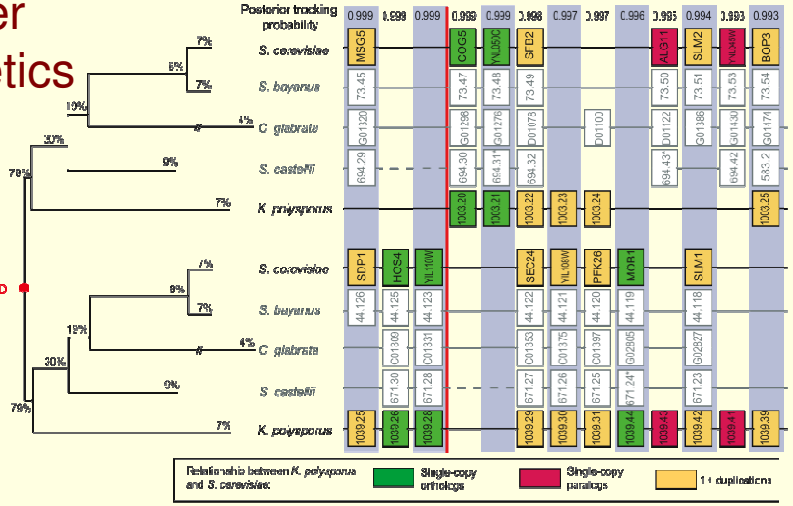
Gavin Conant

conantg@missouri.edu

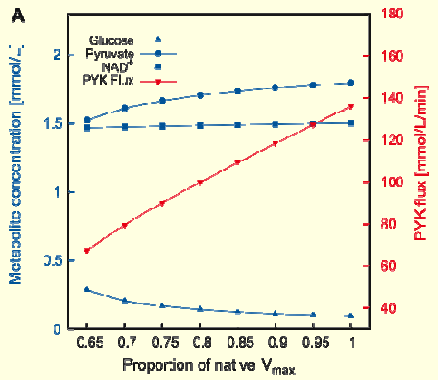
Division of Animal Sciences and
Informatics Institute
University of Missouri
Web: web.missouri.edu/~conantg

Gene order phylogenetics

G. C. Conant and K. H. Wolfe (2008) *Genetics*, **179**: 1681



Adaptation of yeasts to glucose-rich environments by genome duplication

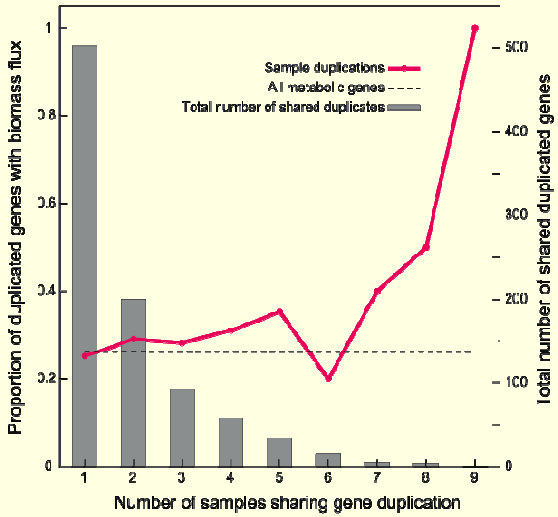


Pyruvate up after WGD

This favors fermentation

G. C. Conant and K. H. Wolfe (2007) *Molecular Systems Biology*, **3**: 129.

Effects of gene duplication on cancer-cell metabolism



As the number of tumor samples sharing a duplication increases left to right, the proportion of duplicated metabolic genes present in reactions involved in producing biomass increases (pink line).

Unpublished data

1. Genome duplication led to an increased concentration of glycolytic enzymes
2. Differential scaling of respiration and fermentation means an increased importance of fermentation
3. A polyploid yeast was at a selective advantage because it used glucose rapidly

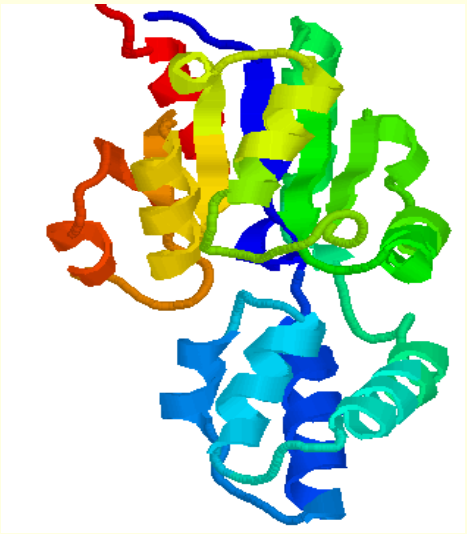
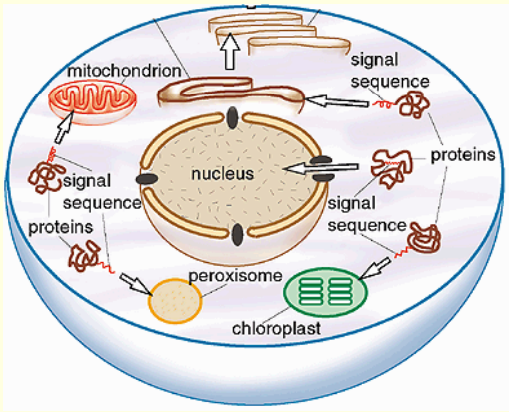
Informatics Research Expertise

Jianlin Jack Cheng

chengj@missouri.edu

Computer Science and
Informatics Institute
University of Missouri

Prediction of Protein Structure, Function, and Interaction

AGCWY… →  → 

Sequence **Structure** **Interaction & Function**

Rational drug design: A known protein structure may provide a guide to design a drug that modulates the protein's function for curing a disease.

8th Critical Assessment of Techniques for Protein Structure Prediction (CASP8), 2008

MU Ranked among best in seven categories:

- Template-free modeling
- Template-based modeling
- High-accuracy modeling
- Contact map prediction
- Disorder prediction
- Protein domain prediction
- Protein model quality prediction

Informatics Research Expertise

Dmitry Korkin

korkined@missouri.edu

Computer Science and
Informatics Institute
University of Missouri

Bioinformatics pipeline to study host-pathogen interactions (HPIs)

Gather HPI data

Identify HPI key players

Characterize HPIs

Study phenomena

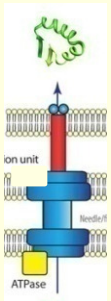
Apply to specific systems

Literature mining

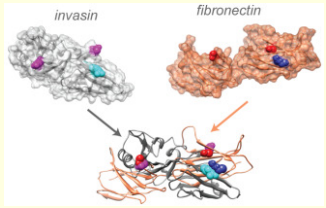
Community HPI data portal

PHI2WEB

Prediction of effector proteins

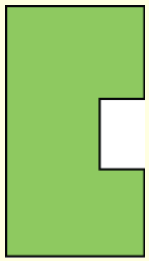


Molecular mimicry detection

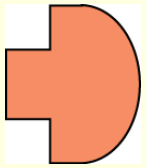


Our collaborations

Virulent mimicry in host-pathogen interactions



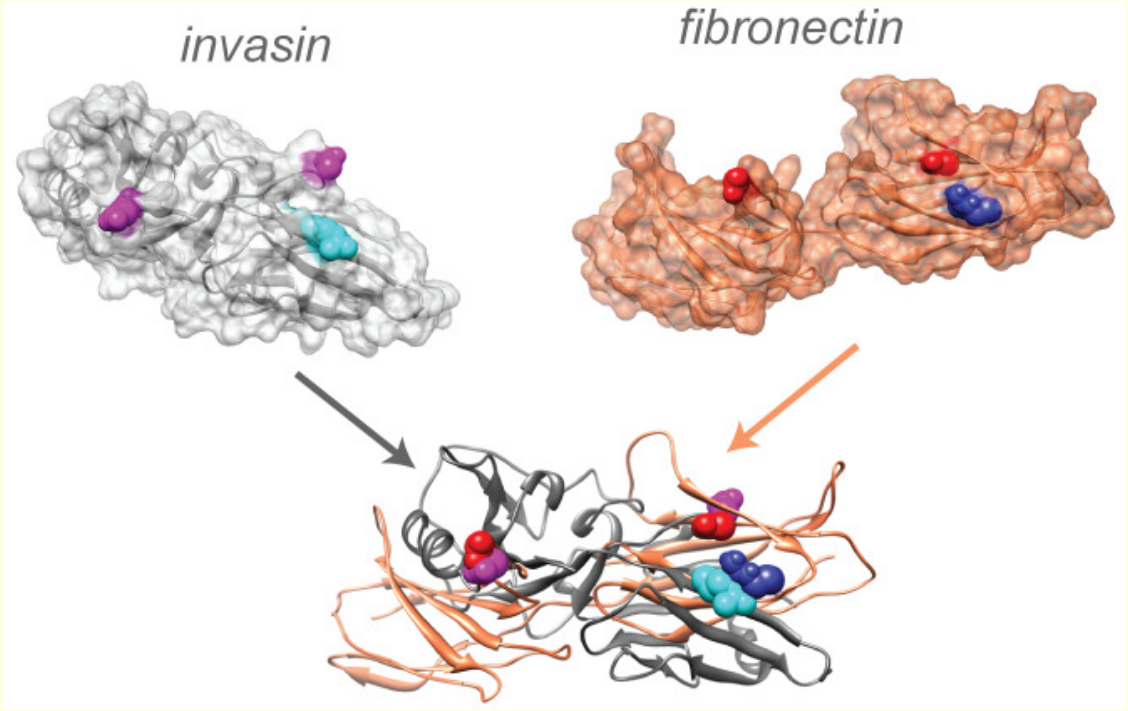
Host integrin



Host fibronectin

Yersinia

invasin



Currently, no computational methods available!

Informatics Research Expertise

Xiaoqin Zou

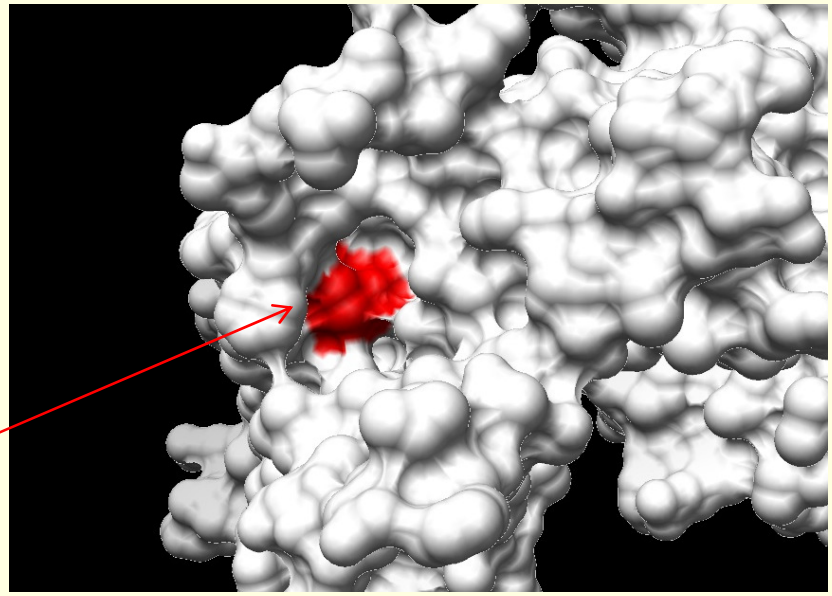
zoux@missouri.edu

Physics and
Informatics Institute
University of Missouri

Rational drug design against a potassium channel that is responsible for the long-QT syndrome (a genetic heart problem) and sudden death.

White: Surface of part of the potassium channel;

Red: The region of interest for drug design



Research Highlights:

- 1 copyright (MDock software package);
- 1 patent filed (anticancer therapy);
- Third place in 4th CAPRI (an international competition on structure prediction of protein-protein complexes)

Informatics Research Expertise

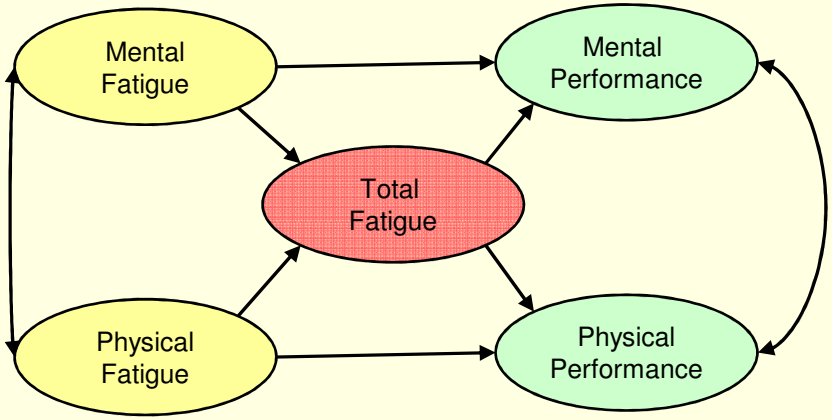
Linsey M. Barker

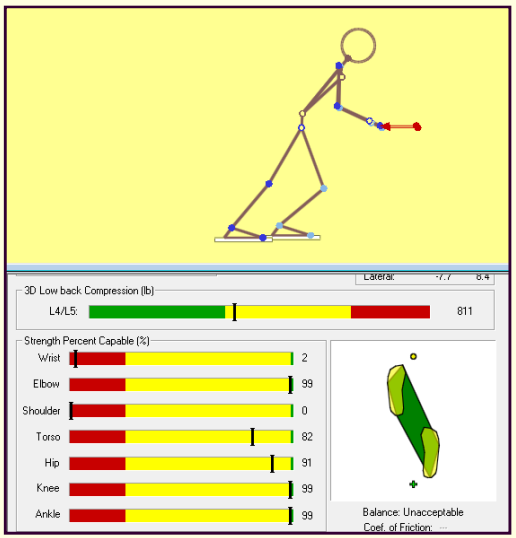
BarkerL@missouri.edu

IMSE Department and
Informatics Institute
University of Missouri

Human Factors in Healthcare Systems

- Application of modeling techniques to identify functional relationships between human constructs (e.g., fatigue, stress) and systems outcomes (e.g., performance, safety)
- Evaluation of medical technology design features to quantify physical and mental work demands for workers, reduce risk of worker injuries, and improve patient safety





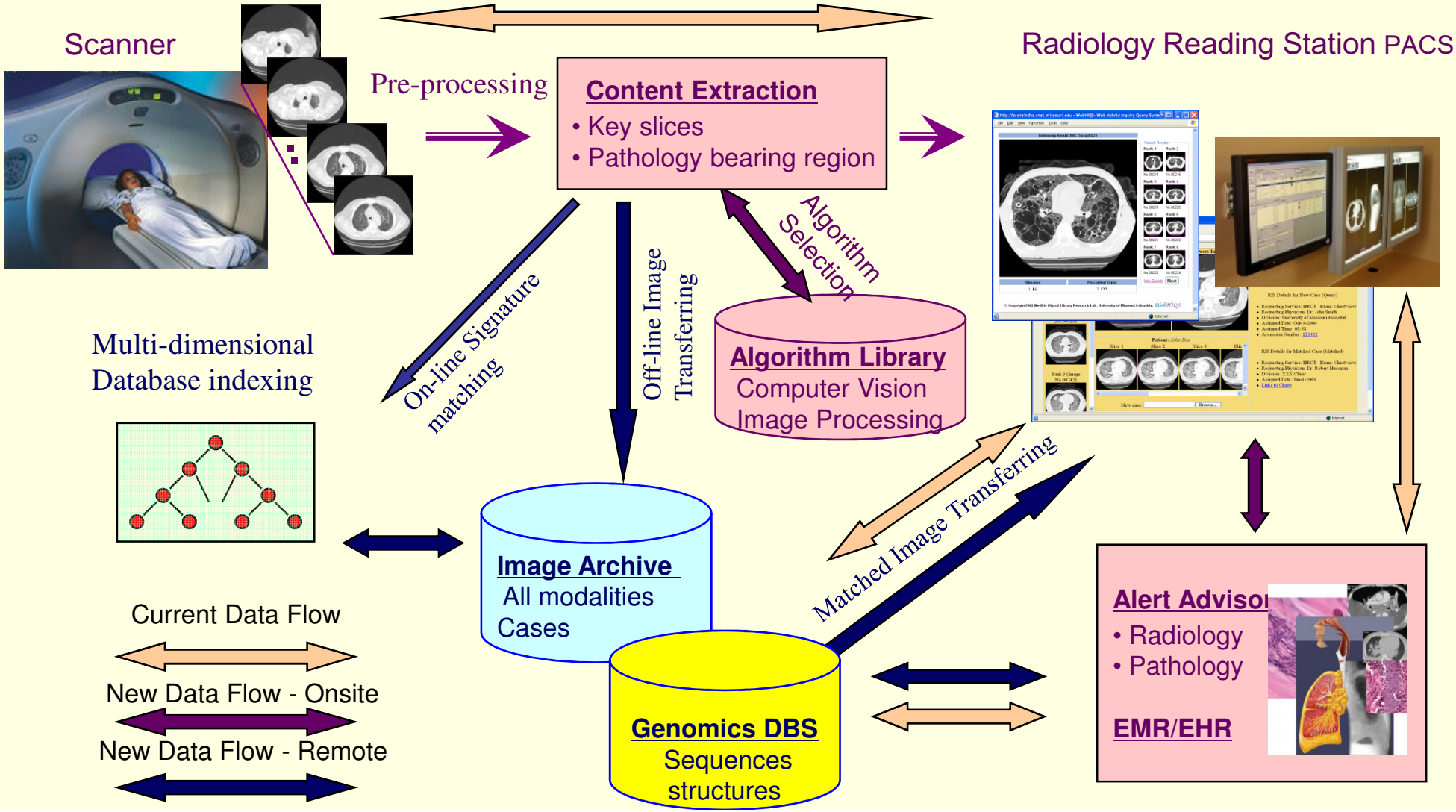
Informatics Research Expertise

Chi-Ren Shyu

ShyuC@missouri.edu

Computer Science and
Informatics Institute
University of Missouri

Next generation medical multimedia info system



Informatics Research Expertise

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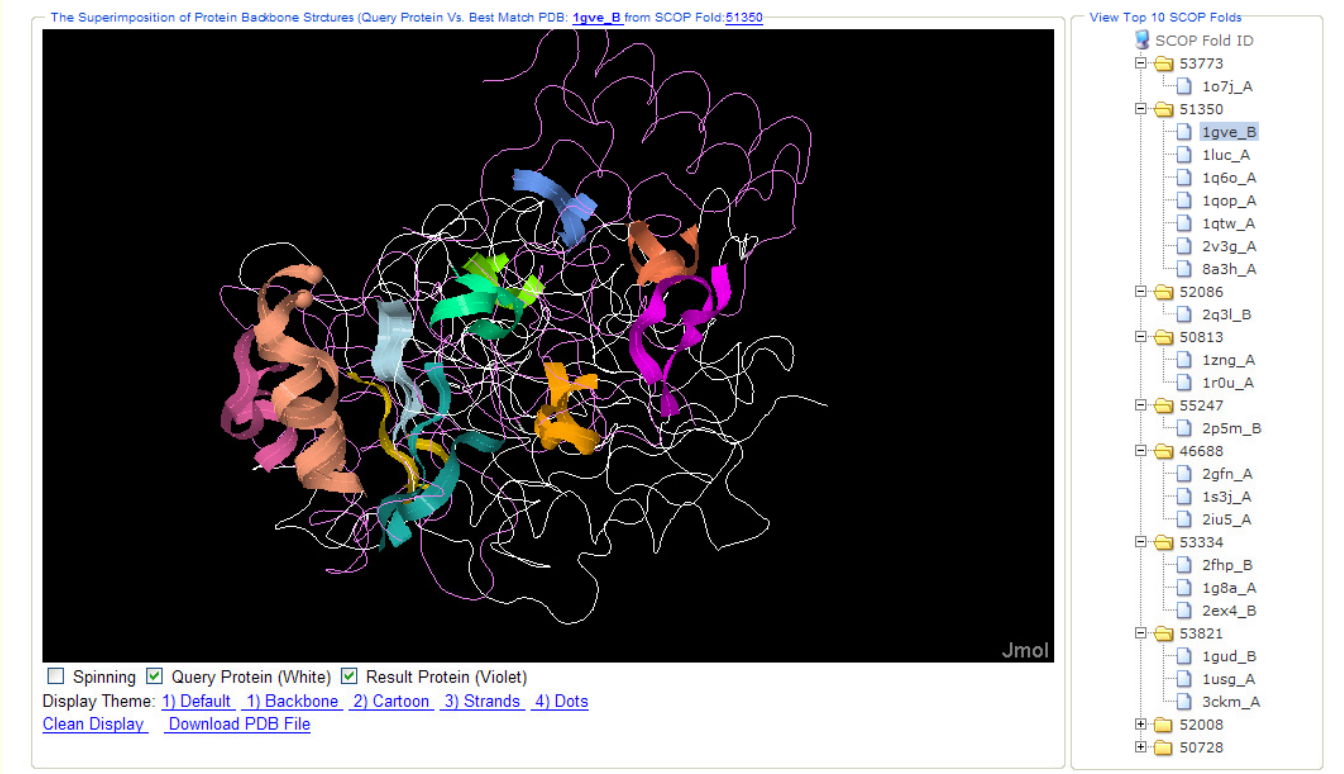
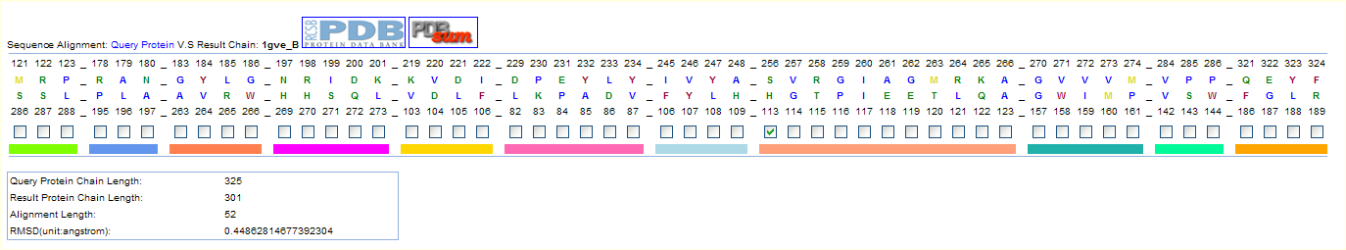
ShyuC@missouri.edu

Computer Science and
Informatics Institute
University of Missouri

Next generation search engines





Informatics Expertise – Maximizing Collaborators

- Teaming up with Kansas City area industry and research institutions
- Building a knowledge base that has up-to-date informatics expertise database in Missouri, Kansas, and surrounding states.
- Developing an incubation program to host start-ups, both physically and virtually, for commercialization of informatics software.