1st INTERNATIONAL COMPUTATIONAL BIOLOGY WORKSHOP

12 to 14 December, 2017

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Computational Biology Research Center

More Info.

www.bioinformatics.aut.ac.ir/workshop/

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Computational Biology Research Center

First International Computational Biology (ICOBI) Workshop

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Section 1. Introduction

Computational biology workshops are advanced and specialized international events in which renowned researchers discuss and argue about their latest research and scientific achievements among other scholars.

The first course of this workshop will be held at the Computational Biology Research Center (CBRC), Faculty of Mathematics and Computer Science, at Amirkabir University of Technology on December 12st, this year. The audiences of this workshop are professors, researchers and students throughout the country, who are eager to participate in scientific workshops and discussions. The workshop has a computational approach for new topics both in biological systems (networks) and molecular biology. More information is available at the event's website:

http://bioinformatics.aut.ac.ir/workshop

The following contents of this document include: objectives of the workshop, a brief description of the activities and research carried out at the CBRC, the scientific and research background of the workshop's scientific committee and secretary, as well as a brief description of the workshop's scientific subjects.

Section 2. The Objectives

The technology and science advancements in the field of molecular biology in the last decade have made it possible for researchers to spend little time and money on collecting valuable data from living creatures.

The current speed at which novel high-throughput technologies are developing and large-scale biological data are produced offers tremendous opportunities for enhancing our molecular understanding of biological systems. The purpose of the International computational biology workshop at Amirkabir University is to bring together researchers and scholars from around the world, who are interested in the application of computational systems, algorithmic concepts and information technologies to address challenging problems in Bioinformatics research, with a particular focus on the genome, protein and RNA.

The objectives of this educational/research course are:

- Acquainting with knowledge boundaries in the field of bioinformatics;
- Establishing research groups and conducting research related to the course fields;
- Collaboration of researchers from different countries;
- Linking research centers and researchers interested in related industries;
- Establishing a dynamic scientific/research relationship among researchers and research centers.

Nowadays, the support of industry and its participation in universities' research activities is common. This fact not only contributes to the development of academic activities, but also establishes a proper link between the academic community and industry. We hope that by holding this event, we will take a small step, in accomplishing the bigger goal which is enhancing the university-industry collaboration in our beloved Iran.

Section 3. A review of the center's activities

The Computational Biology Research Center (CBRC) was founded in 2010 by Dr. Fatemeh Zare-Mirakabad, a faculty member of the Amirkabir University of Technology. Its purpose is to be a place for students and scholars who are interested in computational topics of bioinformatics. This center has played a significant role in promoting the scientific level of students and researchers by creating a relaxed and friendly environment. CBRC lab currently consists of a group of motivated highly qualified personnel, including 14 undergraduate students, 55 Master's students and 11 PhD. students, as well as 4 researchers, gathered to work and exchange state-of-the-art ideas in bioinformatics field.

Here are some research fields this center is focused on:

1. Genome reconstruction
2. DNA repair
3. Single-nucleotide polymorphism
4. Single-nucleotide variations
5. producing gene regulator networks
6. Reverse prediction of the second protein structure
7. Reverse prediction of the third protein structure (Protein Design)
8. Predicting the Interaction of Two Proteins
9. Protein networks alignment
10. Finding complex in protein networks
11. RNA secondary structure prediction
12. RNA secondary structure prediction including pseudoknots
13. Analysis of SHAPE data in RNA
14. Predicting the second structure of RNA using SHAPE data
15. Reverse predicting of the second structure of RNA (RNA Design)
16. Comparison of the third structure of the two RNAs
17. Predicting the Interaction of Two RNAs
18. Haplotype and genotype prediction
19. Destruction of Metabolic Networks
20. Destruction of bio-networks (finding important nodes in bio-networks)

3.1. Previous Activities

Since 2013, the Computational Biology Research Center (CBRC) of the Amirkabir University of Technology in cooperation with the Faculty of Computer Science and Statistics of the University of Tehran, has held weekly seminars in various fields of the latest bioinformatics topics. These seminars were held with the presence of professors Dr. Fatemeh Zare, Dr. Mohamad Ganj Tabesh, Dr. Abbas Nozari, Dr. Zarineh and Master's students of Amirkabir University, Tehran University and Tarbiat Modares University. Students discussed and exchanged ideas at the seminars in a friendly and scientific atmosphere.

Following these research activities, the center also held a conference named "BioDay" in 2015, in which the three topics of protein engineering, RNA design with SHAPE data and Reverse prediction of the second protein structure were discussed. In this event Dr. Hasan Pezashki from UC Berkeley and two researchers from the center, Marzieh Movahedi and Mohadese Lotfi, presented their latest scientific achievements.

Currently, research groups on various subjects such as f RNA, protein, DNA, gene network and protein network are working under the supervision of Dr. Fatemeh Zare. These motivated students are gathered several times a week to exchange and discuss ideas of their topic of interest.

The group of RNA has 6 researchers working on subjects such as Predicting the second structure of RNA using SHAPE data, Predicting the Interaction of Two RNAs, RNA design by taking different structures at different temperatures and comparing the third structure of two RNAs. Three researchers are working on topics such as protein design, Investigation of Protein-Lipid-Nanoparticle Coronas, identifying the location of interaction of two proteins, working with protein databases and tools designed for protein analysis. In another research group, students discuss topics on DNA, such as genome reconstruction, DNA restoration and Single-nucleotide variations. Other groups focus on networks. One is working on gene network, specifically Gene regulating networks, producing genetic networks and comparing centralized networks. Other focuses on protein networks, investigating topics like protein networks alignment and finding complexes in protein networks.

Section 4 Academic background of the secretary and scientific committee

Dr. Fatemeh Zare-Mirakabad

Assistant Professor in Department of Mathematics and Computer Science, Amirkabir University of Technology (Polytechnic Tehran), Tehran, Iran.

Telephone: +98-21-64545674
Fax: +98-21-66497930
E-mail address: f.zare@aut.ac.ir

Education:

Amirkabir University of Technology 1992-1996 B.Sc. in Applied Mathematics

Sharif University of Technology 2000-2003 M.Sc. in Computer Science

Thesis: Use of Markov Chains in Solving Counting Problems

Tehran University 2006-2009 Ph.D. in Bioinformatics

Thesis: Algorithms for Pattern Finding in Biological Sequences

Research Interests:

- Bioinformatics
- Nanotechnology
- Biotechnology
- Genetic
- Artificial intelligence
- Algorithm.

Recent Papers:

- Lotfi, M., Zare-Mirakabad, F., and Montaseri, S. (2017) RNA design using simulated SHAPE data. Genes & Genetic Systems, 16-00067.

- Montaseri, S., Ganjtabesh, M., and Zare-Mirakabad, F. (2016) Evolutionary algorithm for RNA secondary structure prediction based on simulated SHAPE data. PloS one **11**, e0166965.
- Seyfari, Y., Didehvar, F., Banaee, H., and Zare-Mirakabad, F. (2016b) Evaluating the Accuracy of Splice Site Prediction based on Integrating Jensen-Shannon Divergence and a Polynomial Equation of Order 2. Genome **151**.
- MOLLALO, M., and ZARE, M.F. (2016) MOTIF FINDING IN UPSTREAM REGULATORY REGIONS OF CO-EXPRESSED GENES USING CUCKOO OPTIMIZATION ALGORITHM AND SIMULATED ANNEALING.
- Movahedi, M., Zare-Mirakabad, F., and Arab, S.S. (2016) Evaluating the accuracy of protein design using native secondary sub-structures. BMC bioinformatics **17**, 353.
- Kouhsar, M., Zare-Mirakabad, F., and Jamali, Y. (2015) WCOACH: Protein complex prediction in weighted PPI networks. Genes & genetic systems **90**, 317-324.
- Lotfi, M., Zare-Mirakabad, F., and Montaseri, S. (2015) RNA secondary structure prediction based on SHAPE data in helix regions. Journal of theoretical biology **380**, 178-182.
- Soheila Montaseri , Nasrollah Mogadam Chakeri, FATEMEH ZARE MIRAKABAD (2015) RNA secondary structure prediction based on genetic algorithm. IRANIAN JOURNAL OF BIOLOGY **27**, 428 _ 437.
- Ganjtabesh, M., Montaseri, S., and Zare-Mirakabad, F. (2015) Using temperature effects to predict the interactions between two RNAs. Journal of theoretical biology **364**, 98-102.
- Montaseri, S., Zare-Mirakabad, F., and Moghadam-Charkari, N. (2014) RNA-RNA interaction prediction using genetic algorithm. Algorithms for Molecular Biology **9**, 17.
- Talebzadeh, M., and Zare-Mirakabad, F. (2014) Transcription factor binding sites prediction based on modified nucleosomes. PloS one **9**, e89226.
- Ganjtabesh, M., Zare-Mirakabad, F., and Nowzari-Dalini, A. (2013) Inverse RNA folding solution based on multi-objective genetic algorithm and Gibbs sampling method. EXCLI journal **12**, 546.
- Torabi Dashti, H., Zare-Mirakabad, F., Aghaeepour, N., Ahrabian, H., and Nowzari-Dalini, A. (2013) PreRkTAG: Prediction of RNA Knotted

Structures Using Tree Adjoining Grammars. Iranian Journal of Biotechnology **11**, 3-13.

- Sadeghi, M.-R., Zare-Mirakabad, F., Tahmasebi, M., and Sadeghi, M. (2012) EPWM: An Extended Position Weight Matrix for Motif Representation in Biological Sequences.
- Montaseri, S., Moghadam-Charkari, N., and Zare-Mirakabad, F. (2012) A heuristic approach to RNA–RNA interaction prediction. Journal of theoretical biology **300**, 206-211.
- Zare-Mirakabad, F., Ahrabian, H., Sadeghi, M., Hashemifar, S., Nowzari-Dalini, A., and Goliaei, B. (2009) Genetic algorithm for dyad pattern finding in DNA sequences. Genes & genetic systems **84**, 81-93.
- Ahrabian, H., Nowzari-Dalini, A., and Zare-Mirakabad, F. (2009) A Constant Time Algorithm for DNA Add. International Journal of Foundations of Computer Science **20**, 549-558.
- Zare-Mirakabada, F., Davoodib, P., Ahrabiana, H., Nowzari-Dalinia, A., Sadeghic, M., and Goliaeia, B. (2009) Finding motifs based on suffix tree. Avanced Modeling and Optimization **11**.
- Zare-Mirakabad, F., Sadeghi, M., Ahrabian, H., and Nowzari-Dalini, A. (2009b) RNAComp: A new method for RNA secondary structure alignment. Match **61**, 789.
- Zare-Mirakabad, F., Ahrabian, H., Sadeghi, M., Nowzari-Dalini, A., and Goliaei, B. (2009b) New scoring schema for finding motifs in DNA Sequences. BMC bioinformatics **10**, 93.
- Ahrabian H, Nowzari-Dalini A., Razaghi M, Zare-Mirakabad F (2007) Parallel generation of the biological trees. The Electronic International Journal Advanced Modeling and Optimization **9**, 1-14.

Presented Papers in International and National Conferences:

- Identification of transcription factors binding sites on the human genome using artificial neural network, 25th Iranian Conference on Electrical Engineering (ICEE 2017).
- Time pattern clustering for gene expression of yeast microarray data using data mining methods, 23rd Iranian Conference on Biomedical Engineering (ICBME 2016)
- Predicting protein complexes in protein weighted networks by COACH and Semantic Similarity methods, the 5th Bioinformatics Conference of Iran, 2015.

- Analyzing SHAPE data on the RNA secondary structure, The 5th Bioinformatics Conference of Iran, 2015.
- A new method for Haplotype inference based on Maximum parsimony, The 4th Bioinformatics Conference of Iran, 2013.
- Genome structural variation discovery by Genetic algorithm, The 4th Bioinformatics Conference of Iran, 2013.
- A ranking method to predict the position of protein binding based on entropy, Moscow Conference on Computational Molecular Biology (MCCMB13).
- A PSO Inspired Harmony Search Algorithm, Third International Conference on Contemporary Issues in Computer and Information Sciences (CICIS 2012).
- MSSRNA: Make a sequence for a given RNA secondary structure based on genetic algorithm and Gibbs sampling, International Conference on Operations Research & Optimization, 2011.
- Predict the RNA-RNA interaction based on a heuristic method, The 42nd Annual Iranian Mathematics Conference, 2011.
- Gene Expression Similarity with Polygonal Chain Alignment, 2nd International Conference on Contemporary Issues in Computer and Information Sciences (CICIS 2011)

Thesis Supervised:

- Haplotype assembly,
- RNA-RNA interaction prediction,
- Genome assembly,
- Finding Patterns in Protein-Protein Interaction Networks,
- Building gene expression networks using microarrays data,
- Building phylogenetic trees from frequent clustering,
- Finding the Relationship between Drugs and Diseases Using Learning Algorithms,
- Prediction of transplantation sites of transcription factors on the human genome using deep neural network,

- Predict the risk of stroke based on the degree of fatty liver using neural network,
- Protein-protein interaction prediction based on geometric properties,
- Estimating the basic parameters in cancer Simulation,
- Inverse protein folding Based on polymers in PDB,
- Detection of non-sexual mutations in tumor–normal sequencing,
- Detection cancer cells in a blood test using image processing techniques,
- Construction of gene regulatory networks using multiple data sets,
- Genome assembly and read mapping using reference in the next generation technologies,
- Modeling DNA double-strand breaks repair in the cell cycle,
- Identification of genes and gene products necessary in the destruction of biological networks,
- RNA secondary structure prediction based on ant colony,
- A computational approach to drug discovery using data integration approaches,
- Detection of causality from nonlinear dynamics of short-term micro-array time series data,
- Pairwise alignment of RNA 3D structures using geometric methods,
- Global alignment of protein–protein interaction networks,
- Study and modeling gene-gene interactions in the gene network,
- Complex detection in protein networks based on network topology,
- Prediction of consensus folding in a set of unaligned RNA sequences
- Comparison of RNA structures based on image processing methods,
- Discovering Controllability in Bio Networks,
- Determining the Computational Complexity of Boolean satisfiability problem with the Special condition and its Applications,
- Classification and clustering high dimensional data by resampling approach,
- Determining the type and boundary of structural Variation in human genome by geometric algorithms,
- Presentation of a new model for motif representation based on coding theory,

- Identification of splicing positions in DNA sequences,
- Detection of Single Nucleotide Polymorphism in the genome sequence,
- Identifying the parameters and structure of large-scale systems with intelligent optimization methods,
- Inverse folding predictions of protein structure,
- Object recognition by the mechanism of the brain's visual system,
- Phylogenetic tree regeneration for a set of haplotypes,
- Finding relation between Regulation of gene expressions and histone acetylation changes,
- Investigating gene dependency based on synergy,
- Modeling the process of Repairing Double-Strand DNA Breaks during the cell cycle,
- RNA inverse structure folding prediction based on SHAPE-Directed,
- Face Recognition with Processing steps in the visual system approach,
- A method for predicting human reaction times to different visual stimulus,
- Haplotype assembly from genotype data based on parsimony method,
- Using DNA computing methods to solve some of the MAP problems,
- Motif finding based on PSO algorithm,
- Multi-strand protein alignment by exploratory algorithms,
- Simulations of cancer tumor growth,
- Structural equilibrium of RNA molecules with pseudocode,
- Motif finding in biological sequences based on Huffman codes,
- Predicting linked sites in proteins by geometric algorithms,
- Analysis of the relation between epigenetic Modifications and gene transcription,
- Evolutionary Modeling of Tumor Growth Using Cellular Automata,
- Reconstruction of evolutionary relation between creations based on Triad rooted,
- Study of gene expressions regions in Arabidobis genome,
- Finding structural variations in the genome,
- Haplotype inference from genotype data,
- Dyad Motif finding in biological sequences,

- Study of finding Motif algorithms in Biological Sequences,
- Gene prediction algorithms,
- Using Biometric Facial Recognition to identify individuals,
- Detection of folding in protein structure by learning models,
- Classification of Gene Expression Data by Geometric Algorithms,
- Study of coding models on biological sequences,
- Reconstruction of the phylogenetic networks of rooted triplets or unrooted quadruplets.

Educational Experience:

Courses in Amirkabir University of Technology:

Bioinformatics, Theory of Computer Science, Data Structures & Algorithms, Introduction to the Theory of Computation, Design & Analysis of Algorithms, Topics in Mathematics & Its Applications, Special Topics (Biological Databases), Compiler, Theory of Automata & Languages, C Programming.

Courses in Sharif University:

Graph theory, Discrete mathematics.

Courses in Shahid Beheshti University:

Discrete mathematics,Design & Analysis of Algorithms, Compiler, Theory of Automata & Languages, Principles of Computer & Programming, Advanced Programming, Theory of Computation.

Courses in Shahid Rajaee University:

Principles of Computer & Programming

Seminars and Workshops:

Introduction to Concepts of Computer Science and its Applications, Iranian Bioinformatics Society (IBIS).

Speaking in the scientific community:

Bioinformatics Conference of Iran,
2nd International and 10th National Biotechnology,
Institute for Research in Fundamental Sciences (IPM).

Research projects:
Predict RNA-RNA interaction, School of Biological Sciences, IPM - Institute for Research in Fundamental Sciences'.

Mathematical modeling of the process of double strand DNA break repair in the cell cycle, School of Biological Sciences, IPM - Institute for Research in Fundamental Sciences.

Awards and honors:

- 1st rank in Ph.D.
- Ranked second among Amirkabir University students.
- Top Student in Bachelor.

Prof. Burkhard Morgenstern

Professor of Bioinformatics in Göttingen University

Member of Institute for Microbiology and Genetics Dept. of Bioinformatics

Education:
1993 Diploma (Mathematics), LMU München
1996 PhD (Dr. Math.), Bielefeld University
1997 - 1998 Visiting Scientist, North Carolina State University, Raleigh, NC, USA
1998 - 2000 RPR/Aventis, Dagenham, Essex, UK
2000 - 2001 MIPS, MPI für Biochemie, Martinsried and GSF, Neuherberg
2001 - 2002 Group leader and faculty member at International Graduate School in Bioinformatics and Genome Research, Bielefeld University

Research Interests:

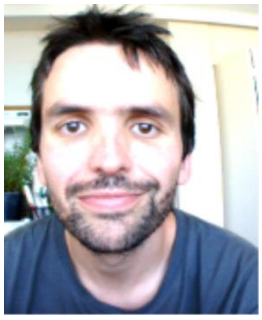
- Sequence alignment, alignment-free sequence comparison
- Sequence analysis, Phylogenic algorithms, metabolomics algorithms
- Spectroscopy data analysis
- Phylogeny reconstruction, metagenomics, motif discovery and remote homology detection using machine learning methods
- Reconstruction and classification of genome and HIV virus using the Qualzent's theory

Recent Papers:

- Leimeister, C.-A., Dencker, T., and Morgenstern, B. (2017) Anchor points for genome alignment based on Filtered Spaced Word Matches. arXiv preprint arXiv:1703.08792.
- Leimeister, C.-A., Sohrabi-Jahromi, S., and Morgenstern, B. (2017b) Fast and accurate phylogeny reconstruction using filtered spaced-word matches. Bioinformatics 33, 971-979.

- Leimeister, C.-A., Hahn, L., and Morgenstern, B. (2016) Fast alignment-free phylogeny reconstruction using spaced words. Invited talk, SeqBio 2016, Nantes.
- Hahn, L., Leimeister, C.-A., Ounit, R., Lonardi, S., and Morgenstern, B. (2016) RasBhari: optimizing spaced seeds for database searching, read mapping and alignment-free sequence comparison. PLoS computational biology 12, e1005107.
- Leimeister, C.-A., and Morgenstern, B. (2014) Kmacs: the k-mismatch average common substring approach to alignment-free sequence comparison. Bioinformatics 30, 2000-2008.
- Leimeister, C.-A., Boden, M., Horwege, S., Lindner, S., and Morgenstern, B. (2014) Fast alignment-free sequence comparison using spaced-word frequencies. Bioinformatics 30, 1991-1999.
- Al Ait, L., Yamak, Z., and Morgenstern, B. (2013) DIALIGN at GOBICS—multiple sequence alignment using various sources of external information. Nucleic acids research 41, W3-W7.
- Corel, E., Pitschi, F., and Morgenstern, B. (2010) A min-cut algorithm for the consistency problem in multiple sequence alignment. Bioinformatics 26, 1015-1021.
- Meinicke, P., Lingner, T., Kaever, A., Feussner, K., Göbel, C., Feussner, I., Karlovsky, P., and Morgenstern, B. (2008) Metabolite-based clustering and visualization of mass spectrometry data using one-dimensional self-organizing maps. Algorithms for Molecular Biology 3, 9.
- Subramanian, A.R., Kaufmann, M., and Morgenstern, B. (2008) DIALIGN-TX: greedy and progressive approaches for segment-based multiple sequence alignment. Algorithms for Molecular Biology 3, 6.

Dr. Yann Ponty



Faculty member of the Bioinformatics group
Computer Science department (LIX) of École Polytechnique
Member of the INRIA/LIX AMIB team

Education:
University of Paris-Sud 1997, B.C. in computer science

University of Paris-Sud 2001, master in computer science

University of Paris-Sud 2003, PHD in computer science

Boston College 2006, Post-doctoral in Computational Molecular Biology

Pierre-and-Marie-Curie University 2008

Simon Fraser University 2013, Visiting Scientist

Research interests:

- RNA structure prediction, RNA design
- RNA/RNA, RNA/Proteins, and Proteins/Proteins interactions
- Random generation and enumerative combinatory
- Discrete Algorithms (Dynamic programming)
  RNA visualization

Recent Papers:

- Duchemin, W., Anselmetti, Y., Patterson, M., Ponty, Y., Bérard, S., Chauve, C., Scornavacca, C., Daubin, V., and Tannier, E. (2017) DeCoSTAR: Reconstructing the ancestral organization of genes or genomes using reconciled phylogenies. Genome biology and evolution **9**, 1312-1319.
- Churkin, A., Retwitzer, M.D., Reinharz, V., Ponty, Y., Waldispühl, J., and Barash, D. (2017) Design of RNAs: comparing programs for inverse RNA folding. Briefings in bioinformatics, bbw120.
- Haleš, J., Héliou, A., Maňuch, J., Ponty, Y., and Stacho, L. (2016) Combinatorial RNA Design: Designability and Structure-Approximating Algorithm in Watson–Crick and Nussinov–Jacobson Energy Models. Algorithmica, 1-22.

- Drory Retwitzer, M., Reinharz, V., Ponty, Y., Waldispühl, J., and Barash, D. (2016) incaRNAfbinv: a web server for the fragment-based design of RNA sequences. Nucleic acids research **44**, W308-W314.
- Reinharz, V., Ponty, Y., and Waldispühl, J. (2016) Combining structure probing data on RNA mutants with evolutionary information reveals RNA-binding interfaces. Nucleic acids research **44**, e104-e104.
- Zhang, Y., Ponty, Y., Blanchette, M., Lécuyer, E., and Waldispühl, J. (2013) SPARCS: a web server to analyze (un) structured regions in coding RNA sequences. Nucleic acids research **41**, W480-W485.
- Reinharz, V., Ponty, Y., and Waldispühl, J. (2013) Using structural and evolutionary information to detect and correct pyrosequencing errors in noncoding RNAs. Journal of Computational Biology **20**, 905-919.

Dr. Abbas Zare Mirkabad

Member of the Scientific Board of Razi Vaccine and Serum Research Institute

Education:

BS in Microbiology at Shivaji University of India

Master of Biochemistry, University of Mumbai, India

PhD in Biochemistry (Toxicology), University of Bombay, India

PhD in Toxicology, University of Mumbai, India

4934 Senior Researcher - 4911 ICMR, India

1373 1371 Fellow of the School of Animal Disease - RVSRI

1385 1373 Head of the Faculty of Biochemistry – RVSRI

2731 Head of the School of Poisonous Animals and Production of Antidotes

Research interests:

- Molecular Biology
- Biotechnology and Biochemistry
- toxicology
- Cancer and its treatment
- Biological purification
- Isolation of anti-cancer peptides from poison
- Investigating the Effects of Scorpion Venom in Animals

Recent Papers:

- Angaji, S., Houshmandi, A., and Zare Mirakabadi, A. (2016) Acute Effects of the Iranian Snake (Naja Naja Oxiana) Venom on Heart. Biomacromolecular Journal **2**, 97-101.
- Ebrahim, K., Shirazi, F.H., Mirakabadi, A.Z., and Vatanpour, H. (2015) Cobra venom cytotoxins; apoptotic or necrotic agents? Toxicon **108**, 134-140.

- Ebrahim, K., Vatanpour, H., Zare, A., Shirazi, F.H., and Nakhjavani, M. (2016) Anticancer activity a of Caspian cobra (Naja Naja oxiana) snake venom in human cancer cell lines via induction of apoptosis. Iranian journal of pharmaceutical research: IJPR **15**, 101.
- Esmaeili Jahromi, H., Zare Mirakabadi, A., and Kamalzadeh, M. (2016) Evaluation of Iranian snake 'Macrovipera lebetina'venom cytotoxicity in kidney cell line HEK-293. Asia Pacific Journal of Medical Toxicology **5**, 49-54.
- Koohi, M.K., Zare Mirakabadi, A., Moharrami, M., and Hablolvarid, M.H. (2009) Anti-cancer effect of ICD-85 (venom derived peptides) on MDA-MB231 cell line (in vitro) and experimental mice with breast cancer (in vivo). Iranian Journal of Veterinary Medicine **3**.
- Mirakabadi, A.Z., Khatoonabadi, S.M., and Teimoorzadeh, S. (2011) Antivenom injection time related effects of Hemiscorpius lepturus scorpion envenomation in rabbits. Archives of Razi Institute **66**, 139-145.
- Moradhaseli, S., Mirakabadi, A.Z., Sarzaeem, A., Dounighi, N.M., Soheily, S., and Borumand, M.R. (2013) Preparation and characterization of sodium alginate nanoparticles containing ICD-85 (venom derived peptides).
- Pipelzadeh, M.H., Jalali, A., Taraz, M., Pourabbas, R., and Zaremirakabadi, A. (2007) An epidemiological and a clinical study on scorpionism by the Iranian scorpion Hemiscorpius lepturus. Toxicon **50**, 984-992.
- Valikhanfard-Zanjani, E., Zare-Mirakabadi, A., Oryan, S., Goodarzi, H.R., and Rajabi, M. (2016) Specific antivenom ability in neutralizing hepatic and renal changes 24 hours after Latrodectus dahli envenomation. Journal of arthropod-borne diseases **10**, 237.
- Valikhanfard-Zanjani, E., Zare-Mirakabadi, A., and Zayerzadeh, E. (2017) Antivenom Efficacy in Neutralizing Histopathological Complications Following Latrodectus dahli Envenomation. Journal of Arthropod-Borne Diseases **11**, 42-49.
- Zare-Mirakabadi, A., Sarzaeem, A., Moradhaseli, S., Sayad, A., and Negahdary, M. (2012) Necrotic effect versus apoptotic nature of Camptothecin in human cervical cancer cells. Iranian journal of cancer prevention **5**, 109.
- Zokaee, F., Kaghazchi, T., and Zare, A. (1999) Cell harvesting by microfiltration in a deadend system. Process biochemistry **34**, 803-810.

- Zokaee, F., Kaghazchi, T., Zare, A., and Soleimani, M. (2002) Isomerization of lactose to lactulose—study and comparison of three catalytic systems. Process Biochemistry **37**, 629-635.

Dr. Mehdi Sadeghi

Head of the School of Biological Sciences, IPM - Institute for Research in Fundamental Sciences.

Faculty member of the medical genetics group, National Institute of Genetics and Biotechnology

Research interests:

- Bioinformatics
- Structural Biology
- Systems Biology
- Game theory

Recent Papers:

- Malekpour, S.A., Pezeshk, H., and Sadeghi, M. (2016) PSE-HMM: genome-wide CNV detection from NGS data using an HMM with Position-Specific Emission probabilities. BMC bioinformatics 18, 30.
- Jafari, R., Sadeghi, M., and Mirzaie, M. (2016) Investigating the importance of Delaunay-based definition of atomic interactions in scoring of protein–protein docking results. Journal of Molecular Graphics and Modelling 66, 108-114.
- Malekpour, S.A., Pezeshk, H., and Sadeghi, M. (2016a) PSE-HMM: genome-wide CNV detection from NGS data using an HMM with Position-Specific Emission probabilities. BMC bioinformatics 18, 30.
- Ejlali, N., Pezeshk, H., and Sadeghi, M., (2015) A Note on the Parrondo's Paradox, The 10th Seminar on Probability and Stochastic Processes, 140.
- Khosravi, P., Gazestani, V.H., Pirhaji, L., Law, B., Sadeghi, M., Goliaei, B., and Bader, G.D. (2015) Inferring interaction type in gene regulatory networks using co-expression data. Algorithms for Molecular Biology 10, 23.
- Sharifi-Zarchi, A., Totonchi, M., Khaloughi, K., Karamzadeh, R., Araúzo-Bravo, M.J., Baharvand, H., Tusserkani, R., Pezeshk, H., Chitsaz, H., and Sadeghi, M. (2015) Increased robustness of early embryogenesis

through collective decision-making by key transcription factors. BMC systems biology 9, 23.

- Khosravi, P., Gazestani, V.H., Pirhaji, L., Law, B., Sadeghi, M., Goliaei, B., and Bader, G.D. (2015) Inferring interaction type in gene regulatory networks using co-expression data. Algorithms for Molecular Biology 10, 23.
- Anaraki, M.P., and Sadeghi, M. (2014) Efficient fast heuristic algorithms for minimum error correction haplotyping from SNP fragments. International journal of computational biology and drug design 7, 358-368.
- Khosravi, P., Gazestani, V.H., Akbarzadeh, M., Mirkhalaf, S., Sadeghi, M., and Goliaei, B. (2015) Comparative analysis of prostate cancer gene regulatory networks via hub type variation. Avicenna journal of medical biotechnology 7, 8.

Dr. Ali Sharifi Zarchi

Faculty member of Computer Engineering at the Sharif University of Technology

Education:
Sharif university of technology Education 2000, B.C Computer engineering

Sharif university of technology Education 2004, Master Computer engineering

Institute Of Biochemistry And Biophysics 2007, Ph.D. Bioinformatics

Research Interests:

- Embryonic stem cells
- Data Structures & Algorithms
- Bioinformatics

Recent Papers:

- Al-Husini, N., Sharifi, A., Mousavi, S.A., Chitsaz, H., and Ansari, A. (2017) Genomewide Analysis of Clp1 Function in Transcription in Budding Yeast. Scientific Reports 7.
- Dorri, F., Mahini, H., Sharifi-Zarchi, A., Totonchi, M., Tusserkani, R., Pezeshk, H., and Sadeghi, M. (2014) Natural biased coin encoded in the genome determines cell strategy. PloS one 9, e103569.
- Fonoudi, H., Ansari, H., Abbasalizadeh, S., Larijani, M.R., Kiani, S., Hashemizadeh, S., Zarchi, A.S., Bosman, A., Blue, G.M., and Pahlavan, S. (2015) A universal and robust integrated platform for the scalable production of human cardiomyocytes from pluripotent stem cells. Stem cells translational medicine 4, 1482-1494.
- Gholami, M., Arbabi, A., Sharifi-Zarchi, A., Chitsaz, H., and Sadeghi, M. (2014) ARYANA: Aligning Reads by Yet Another Approach. BMC bioinformatics 15, S12.
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- Taleahmad, S., Mirzaei, M., Parker, L.M., Hassani, S.-N., Mollamohammadi, S., Sharifi-Zarchi, A., Haynes, P.A., Baharvand, H., and Salekdeh, G.H. (2015) Proteome analysis of ground state pluripotency. Scientific reports 5.

Prof. Hamid Pezeshk

Full Professor at the Department of Mathematics, Statistics and Computer Science, Tehran University.

Member of International Society for Clinical Biostatisticians.

Member of the Council of the Iranian Statistical.

Member of the Editorial Board of the News Letter and the Notices of the Iranian Mathematical.

Member of Iranian Statistical Society fellow of the Royal Statistical Society.

Member of Iranian Mathematical Society.

Research interests:

- Bayesian statistic and probability
- Bioinformatics
- *Bayesian sample size* methods

Recent Papers:

- Malekpour, S.A., Pezeshk, H., and Sadeghi, M. (2016) PSE-HMM: genome-wide CNV detection from NGS data using an HMM with Position-Specific Emission probabilities. BMC bioinformatics **18**, 30.
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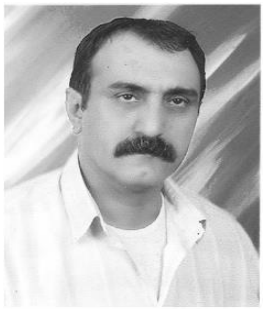
through collective decision-making by key transcription factors. BMC systems biology **9**, 23.

- Kazemi-Pour, A., Goliaei, B., and Pezeshk, H. (2015) Protein complex discovery by interaction filtering from protein interaction networks using mutual rank coexpression and sequence similarity. BioMed research international 2015.
- Dorri, F., Mahini, H., Sharifi-Zarchi, A., Totonchi, M., Tusserkani, R., Pezeshk, H., and Sadeghi, M. (2014) Natural biased coin encoded in the genome determines cell strategy. PloS one **9**, e103569.

Dr. Abbas Nowzari Dalini



Associate Professor in Department of Mathematics, Statistics and Computer Science, Tehran University.

Research interests:

- Bioinformatics
- Analysis of algorithm
- Machine learning
- Artificial Neural Network
- Data Structures

Recent Papers:

- Bidkhori, G., Narimani, Z., Ashtiani, S.H., Moeini, A., Nowzari-Dalini, A., and Masoudi-Nejad, A. (2013) Reconstruction of an integrated genome-scale co-expression network reveals key modules involved in lung adenocarcinoma. PloS one 8, e67552.
- Ahrabian, H., Ganjtabesh, M., Nowzari-Dalini, A., and Razaghi-Moghadam-Kashani, Z. (2013) Genetic algorithm solution for partial digest problem. International journal of bioinformatics research and applications 9, 584-594.
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- Kheradpisheh, S.R., Sharifizadeh, F., Nowzari-Dalini, A., Ganjtabesh, M., and Ebrahimpour, R. (2014) Mixture of feature specified experts. Information Fusion 20, 242-251.
- Mohammadzadeh, J., Ganjtabesh, M., and Nowzari-Dalini, A. (2014) Topological properties of RNA variation networks over the space of RNA shapes. MATCH Commun. Math. Comput. Chem 72, 501-518.
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protein interaction networks. Computational and mathematical methods in medicine 2014.

- Mohammadzadeh, J., Ganjtabesh, M., and Nowzari-Dalini, A. (2014) Topological properties of RNA variation networks over the space of RNA shapes. MATCH Commun. Math. Comput. Chem 72, 501-518.
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Prof. Changiz Eslahchi

Professor of Algorithms in Bioinformatics in Shahid Beheshti University.

Member of Iranian Mathematical Society.

Member of Iranian Bioinformatics Society.

Member of International Society for Computational Biology.

Research interests:

- Finding cancer marker by graph-based analysis.
- Phylogenetic networks construction.
- Finding modules and decomposing metabolic networks.
- Protein complex prediction in PPI networks.
- Drug-target interaction prediction problem.
- Protein localization prediction problem.

Recent Papers:

- Sadeghi, M., Khosrowabadi, R., Bakouie, F., Mahdavi, H., Eslahchi, C., and Pouretemad, H. (2017) Screening of autism based on task-free fMRI using graph theoretical approach. Psychiatry Research: Neuroimaging 263, 48-56.
- Movahedi, F., Eslahchi, C., Pourbarat, M., and Shahrokhi-Dehkordi, M. (2015) ANALYSIS OF DYNAMICAL SYSTEM TO TRANSITION PROBABILITIES IN THE BIRTH-DEATH MARKOV PROCESS IN THE EPIDEMIC MODEL. Far East Journal of Dynamical Systems 26, 61.
- Aghdam, R., Alijanpour, M., Azadi, M., Ebrahimi, A., Eslahchi, C., and Rezvan, A. (2016) Inferring gene regulatory networks by PCA-CMI using Hill climbing algorithm based on MIT score and SORDER method. International Journal of Biomathematics 9, 1650040.
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- Hassanzadeh, R., Eslahchi, C., and Sung, W.-K. (2014) Do triplets have enough information to construct the multi-labeled phylogenetic tree? PloS one 9, e103622.

Dr. Zahra Razaghi Moghadam

Assistant Professor of Systems Biology, Tehran University.

Research interests:

- Systems Biology and Bioinformatics
- Network Analysis
  Network Medicine

Recent Papers:

- Kashani, Razaghi-Moghadam-Kashani, Z., Ahrabian, H., Elahi, E., Nowzari-Dalini, A., Ansari, E.S., Asadi, S., Mohammadi, S., Schreiber, F., and Masoudi-Nejad, A. (2009) Kavosh: a new algorithm for finding network motifs. BMC bioinformatics 10, 318.
- Ganjtabesh, M., Ahrabian, H., Nowzari-Dalini, A., and Moghadam, Razaghi-Moghadam-Kashani, Z. (2012) Genetic algorithm solution for double digest problem. Bioinformation 8, 453.
- Gholami Rudi, A., Shahrivari, S., Jalili, S., and Razaghi Moghadam Kashani, Z. (2013) RANGI: a fast list-colored graph motif finding algorithm. IEEE/ACM Transactions on Computational Biology and Bioinformatics (TCBB) 10, 504-513.
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knowledge to prioritize cancer candidate genes. Journal of biomedical informatics 64, 139-146.

Dr. Seyed Shahriar Arab

Assistant Professor of School of Biological Sciences, Tarbiat Modares University.

Member of Institute for Research in Fundamental Sciences (IPM) · Computer Sciences · Bioinformatics.

Research interests:

- Bioinformatics and Computational Biology
- Protein Structure
- Genomics
- Bioinformatics
- Protein Folding

Recent Papers:

- Jabbari, S., Dabirmanesh, B., Arab, S.S., Amanlou, M., Daneshjou, S., Gholami, S., and Khajeh, K. (2017) A novel enzyme based SPR-biosensor to detect bromocriptine as an ergoline derivative drug. Sensors and Actuators B: Chemical 240, 519-527.
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- Azimi, A., Ghaffari, S.M., Riazi, G.H., Arab, S.S., Tavakol, M.M., and Pooyan, S. (2016) α-Cyperone of Cyperus rotundus is an effective candidate for reduction of inflammation by destabilization of microtubule fibers in brain. Journal of ethnopharmacology 194, 219-227.
- Rahimzadeh, M., Sadeghizadeh, M., Najafi, F., Arab, S., and Mobasheri, H. (2016) Impact of heat shock step on bacterial transformation efficiency. Molecular Biology Research Communications 5, 257.
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- Jabbari, S., Dabirmanesh, B., Arab, S.S., Amanlou, M., Daneshjou, S., Gholami, S., and Khajeh, K. (2017) A novel enzyme based SPR-biosensor to detect bromocriptine as an ergoline derivative drug. Sensors and Actuators B: Chemical 240, 519-527.

Dr. Mohammad Ganjtabesh

Faculty member of Department of Mathematics Computer Science, Tehran University

Education:
Tabriz university 2001, B.C in Pure mathematics

Tehran university 2003, Master in Computer science

Tehran university 2008, Ph.D. in Computer science

École Polytechnique, Ph.D. in computer science

Research Interests:

- Bioinformatics Algorithms (RNA structure)
- Computational neuroscience

Recent papers:

- Ahrabian, H., Ganjtabesh, M., Nowzari-Dalini, A., and Razaghi-Moghadam-Kashani, Z. (2013) Genetic algorithm solution for partial digest problem. International journal of bioinformatics research and applications 9, 584-594.
- Esmaili-Taheri, A., and Ganjtabesh, M. (2015) ERD: a fast and reliable tool for RNA design including constraints. BMC bioinformatics 16, 20.
- Esmaili-Taheri, A., Ganjtabesh, M., and Mohammad-Noori, M. (2014) Evolutionary solution for the RNA design problem. Bioinformatics 30, 1250-1258.
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- Ganjtabesh, M., Zare-Mirakabad, F., and Nowzari-Dalini, A. (2013) Inverse RNA folding solution based on multi-objective genetic algorithm and Gibbs sampling method. EXCLI journal 12, 546.
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- Kheradpisheh, S.R., Ghodrati, M., Ganjtabesh, M., and Masquelier, T. (2016b) Deep networks can resemble human feed-forward vision in invariant object recognition. Scientific reports 6, 32672.
- Kheradpisheh, S.R., Ghodrati, M., Ganjtabesh, M., and Masquelier, T. (2016c) Humans and deep networks largely agree on which kinds of variation make object recognition harder. Frontiers in computational neuroscience 10.
- Kheradpisheh, S.R., Nowzari-Dalini, A., Ebrahimpour, R., and Ganjtabesh, M. (2014a) An evidence-based combining classifier for brain signal analysis. PloS one 9, e84341.
- Kheradpisheh, S.R., Sharifizadeh, F., Nowzari-Dalini, A., Ganjtabesh, M., and Ebrahimpour, R. (2014b) Mixture of feature specified experts. Information Fusion 20, 242-251.
- Mohammadzadeh, J., Ganjtabesh, M., and Nowzari-Dalini, A. (2014) Topological properties of RNA variation networks over the space of RNA shapes. MATCH Commun. Math. Comput. Chem 72, 501-518.
- - (2016) An Analytical RNA Secondary Structure Benchmark for the RNA Inverse Folding Problem. Current Bioinformatics 11, 571-577.
- Montaseri, S., Ganjtabesh, M., and Zare-Mirakabad, F. (2016) Evolutionary algorithm for RNA secondary structure prediction based on simulated SHAPE data. PloS one 11, e0166965.
- Taghipour, S., Zarrineh, P., Ganjtabesh, M., and Nowzari-Dalini, A. (2017) Improving protein complex prediction by reconstructing a high-confidence protein-protein interaction network of Escherichia coli from different physical interaction data sources. BMC bioinformatics 18, 10.

Dr. Sajjad Gharaghani

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Education:
Shahrood University of Technology 2004, B.C in General chemistry

Mazandaran University 2008, Master in Analytical chemistry

Isfahan University of Technology 2012, PHD in Analytical chemistry

Research Interests:

- Bioinformatics
- Computational neuroscience
- Biological networks
- Pharmacology Systems
- Computational methods for drug design
- Chemometrics
- Cheminformatics
- Quantitative structure–activity relationship
- Machine learning methods in drug identification

Recent papers:

- Amini, Z., Fatemi, M.H., and Gharaghani, S. (2016) Hybrid docking-QSAR studies of DPP-IV inhibition activities of a series of aminomethyl-piperidones. Computational biology and chemistry 64, 335-345.
- Benvidi, A., Abbasi, S., Gharaghani, S., Tezerjani, M.D., and Masoum, S. (2017) Spectrophotometric determination of synthetic colorants using PSO–GA-ANN. Food chemistry 220, 377-384.
- Chavoshpour-Natanzi, Z., Sahihi, M., and Gharaghani, S. (2017) Structural stability of β-lactoglobulin in the presence of cetylpyridinum bromide: spectroscopic and molecular docking studies. Journal of Biomolecular Structure and Dynamics, 1-8.
- Ebrahimi, M., Mani-Varnosfaderani, A., Khayamian, T., and Gharaghani, S. (2016) An in silico approach to design peptide mimetics based on

docking and molecular dynamics simulation of EGFR–matuzumab complex. Journal of the Iranian Chemical Society 13, 1805-1817.

- Kazemi, Z., Rudbari, H.A., Sahihi, M., Mirkhani, V., Moghadam, M., Tangestaninejad, S., Mohammadpoor-Baltork, I., Azimi, G., Gharaghani, S., and Kajani, A.A. (2016) Synthesis, characterization and separation of chiral and achiral diastereomers of Schiff base Pd (II) complex: A comparative study of their DNA-and HSA-binding. Journal of Photochemistry and Photobiology B: Biology 163, 246-260.
- Kazemi, Z., Rudbari, H.A., Sahihi, M., Mirkhani, V., Moghadam, M., Tangestaninejad, S., Mohammadpoor-Baltork, I., and Gharaghani, S. (2016) Synthesis, characterization and biological application of four novel metal-Schiff base complexes derived from allylamine and their interactions with human serum albumin: Experimental, molecular docking and ONIOM computational study. Journal of Photochemistry and Photobiology B: Biology 162, 448-462.
- Malekpoor, M., Gharaghani, S., Sharifzadeh, A., Mirsattari, S.N., and Massah, A.R. (2015) Synthesis and antibacterial evaluation of novel xanthone sulfonamides. Journal of Chemical Research 39, 433-437.
- Massah, A.R., Gharaghani, S., Lordejani, H.A., and Asakere, N. (2016) New and mild method for the synthesis of alprazolam and diazepam and computational study of their binding mode to GABAA receptor. Medicinal Chemistry Research 25, 1538-1550.
- Moghadam, H., Rahgozar, M., and Gharaghani, S. (2016) Scoring multiple features to predict drug disease associations using information fusion and aggregation. SAR and QSAR in Environmental Research 27, 609-628.
- MotieGhader, H., Gharaghani, S., Masoudi-Sobhanzadeh, Y., and Masoudi-Nejad, A. (2017) Sequential and Mixed Genetic Algorithm and Learning Automata (SGALA, MGALA) for Feature Selection in QSAR. Iranian Journal of Pharmaceutical Research 16, 533-553.
- Nazarshodeh, E., and Gharaghani, S. (2017) Toward a hierarchical virtual screening and toxicity risk analysis for identifying novel CA XII inhibitors. Biosystems.
- Sheikhpour, R., Sarram, M.A., and Gharaghani, S. (2017) Constraint score for semi-supervised feature selection in ligand-and receptor-based QSAR on serine/threonine-protein kinase PLK3 inhibitors. Chemometrics and Intelligent Laboratory Systems 163, 31-40.

- Sheikhpour, R., Sarram, M.A., Gharaghani, S., and Chahooki, M.A.Z. (2017) Feature selection based on graph Laplacian by using compounds with known and unknown activities. Journal of Chemometrics.
- Sheikhpour, R., Sarram, M.A., Gharaghani, S., and Chahooki, M.A.Z. (2017) A Survey on semi-supervised feature selection methods. Pattern Recognition 64, 141-158.

Dr. Seyded Amir Marashi

University of Tehran , Tehran · Department of Biotechnology

Education:
Tehran University 1999, B.C in Biotechnology

Tehran University 2003, Master in Biotechnology

Freie Universitaet Berlin 2007 Ph.D. in Bioinformatics

Research Interests:

- Metabolic networks
- Gene regulation networks
- Analysis of gene
- Bioinformatics
- Protein structure

Recent papers:

- Ahmadi, M., Jafari, R., Marashi, S., and Farazmand, A. (2015) Indirect role of microRNAs and transcription factors in the regulation of important cancer genes: A network biology approach. Cellular and Molecular Biology 61, 100-107.
- Arabzadeh, M., Zamani, M.S., Sedighi, M., and Marashi, S.-A. (2017) A Graph-Based Approach to Analyze Flux-Balanced Pathways in Metabolic Networks. arXiv preprint arXiv:1703.06496.
- Asghari, A., Marashi, S.-A., and Ansari-Pour, N. (2017) A sperm-specific proteome-scale metabolic network model identifies non-glycolytic genes for energy deficiency in asthenozoospermia. Systems biology in reproductive medicine 63, 100-112.
- Babaei, P., Marashi, S.-A., and Asad, S. (2015) Genome-scale reconstruction of the metabolic network in Pseudomonas stutzeri A1501. Molecular BioSystems 11, 3022-3032.
- Bahramali, G., Goliaei, B., Minuchehr, Z., and Marashi, S.-A. (2017) A network biology approach to understanding the importance of chameleon proteins in human physiology and pathology. Amino acids 49, 303-315.

- Fouladiha, H., and Marashi, S.-A. (2017) Biomedical applications of cell- and tissue-specific metabolic network models. Journal of Biomedical Informatics.
- Fouladiha, H., Marashi, S.A., and Shokrgozar, M. (2015) Reconstruction and validation of a constraint-based metabolic network model for bone marrow-derived mesenchymal stem cells. Cell proliferation 48, 475-485.
- Ghadiri, M., Heidari, M., Marashi, S.-A., and Mousavi, S.H. (2017) A multiscale agent-based framework integrated with a constraint-based metabolic network model of cancer for simulating avascular tumor growth. Molecular BioSystems 13, 1888-1897.
- Hosseini, Z., and Marashi, S.-A. (2017) Discovering missing reactions of metabolic networks by using gene co-expression data. Scientific Reports 7.
- Jalili, S., and Marashi, S.-A. (2015) CAMWI: Detecting protein complexes using weighted clustering coefficient and weighted density. Computational biology and chemistry 58, 231-240.
- Khayer, N., Marashi, S.-A., Mirzaie, M., and Goshadrou, F. (2017) Three-way interaction model to trace the mechanisms involved in Alzheimer's disease transgenic mice. PloS one 12, e0184697.
- Lakizadeh, A., Jalili, S., and Marashi, S.-A. (2015) PCD-GED: Protein complex detection considering PPI Dynamics based on time series gene expression data. Journal of theoretical biology 378, 31-38.
- Mirfazeli, E.S., Marashi, S.-A., and Kalantari, S. (2016) In silico prediction of specific pathways that regulate mesangial cell proliferation in IgA nephropathy. Medical hypotheses 97, 38-45.
- Sohrabi-Jahromi, S., Marashi, S.-A., and Kalantari, S. (2016) A kidney-specific genome-scale metabolic network model for analyzing focal segmental glomerulosclerosis. Mammalian genome 27, 158-167.

Section 5. Scientific topics

In this section, we will briefly explain important topics and problems that are the focus of the workshop.

5.1. Genome

A genome is an organism's complete set of DNA, including all of its genes. Each genome contains all of the information needed to build and maintain that organism. In humans, a copy of the entire genome—more than 3 billion DNA base pairs—is contained in all cells that have a nucleus.

5.1.1. Genome assembly

Genome assembly algorithms are sets of well-defined procedures for reconstructing DNA sequences from large numbers of shorter DNA sequence fragments. Fragments are aligned against one another and overlapping sections are identified and merged.

Genome assembly is a challenging problem that requires time, resources and expertise. Before engaging in a genome sequencing project, it should thus be carefully considered whether a genome reference sequence is strictly necessary for the purpose in question. Genome sequences are merely a resource and in many cases will contribute very little per se to a problem in conservation biology. In case a genome draft is judged to be of significant value to address the problem at hand, it needs to be considered whether sufficient financial and computational resources are available to produce a genome of satisfactory quality. If funding is not available to obtain the appropriate read depth, it is advisable to utilize alternative approaches where possible (such as genotyping-by-sequencing or transcriptome sequencing), rather than settle for low-coverage whole-genome sequencing data. The latter would be a waste of funding, effort and time.

One important limitation of the current shotgun genome sequencing approaches that may be of particular importance in conservation biology is the fact that core genes with high conservation relevance, like immune genes of the MHC or olfactory receptor (OR) genes, are highly polymorphic and have many paralogs, which makes them particularly difficult to assemble. More generally, rapidly evolving genes or members of large gene families are often poorly represented in the final assembly and annotated gene set. Such regions and genes constitute a challenge even for very large sequencing projects of model

organisms. If the project is not carefully planned from the start, there is a risk that the regions of highest interest to conservation biology will not be correctly represented in the final draft of the genome. Manual annotation and use of additional data, such as targeted sequencing of bacterial artificial chromosome (BAC) clones, will often be necessary to include such genomic regions in the assembly. If information on such pre-identified candidate genes is the main aim of the study, it might even be more efficient to focus only on those regions rather than trying to sequence and assemble the whole-genome.

5.1.2. Single-nucleotide polymorphism

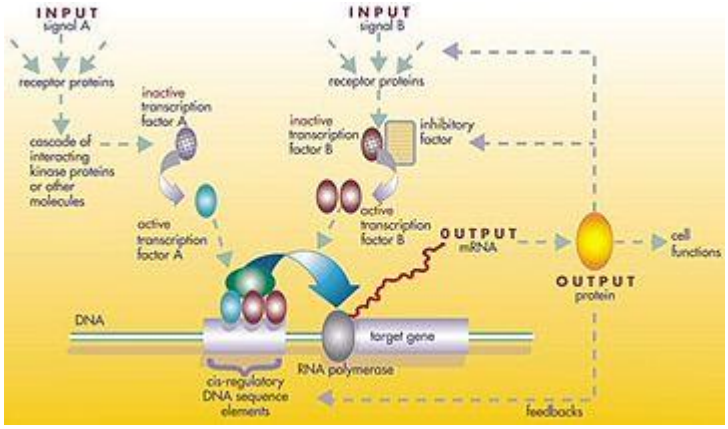
Single nucleotide polymorphisms, frequently called SNPs (pronounced "snips"), are the most common type of genetic variation among people. Each SNP represents a difference in a single DNA building block, called a nucleotide. For example, a SNP may replace the nucleotide cytosine (C) with the nucleotide thymine (T) in a certain stretch of DNA.

SNPs occur normally throughout a person's DNA. They occur once in every 300 nucleotides on average, which means there are roughly 10 million SNPs in the human genome. Most commonly, these variations are found in the DNA between genes. They can act as biological markers, helping scientists locate genes that are associated with disease. When SNPs occur within a gene or in a regulatory region near a gene, they may play a more direct role in disease by affecting the gene's function.

Most SNPs have no effect on health or development. Some of these genetic differences, however, have proven to be very important in the study of human health. Researchers have found SNPs that may help predict an individual's response to certain drugs, susceptibility to environmental factors such as toxins, and risk of developing particular diseases. SNPs can also be used to track the inheritance of disease genes within families. Future studies will work to identify SNPs associated with complex diseases such as heart disease, diabetes, and cancer.

5.1.3. Gene regulatory networks

A gene regulatory network is a set of genes, or parts of genes, that interact with each other to control a specific cell function. Gene regulatory networks are important in development, differentiation and responding to environmental cues.



In any given cell, thousands of genes are expressed and work in concert to ensure the cell's function, fitness, and survival. Each gene, in turn, must be expressed at the proper time and in the proper amounts to ensure the appropriate functional outcome. The regulation and expression of some genes are highly robust; their expression is controlled by invariable expression programs. For instance, developmental gene expression is extremely similar in a given cell type from one individual to another. The expression of other genes is more variable: Their levels are noisy and are different from cell to cell and from individual to individual. This can be highly beneficial in physiological responses to outside cues and stresses. Recent advances have enabled the analysis of differential gene expression at a systems level. Gene regulatory networks (GRNs) involving interactions between large numbers of genes and their regulators have been mapped onto graphic diagrams that are used to visualize the regulatory relationships. The further characterization of GRNs has already uncovered global principles of gene regulation. Together with synthetic network biology, such studies are starting to provide insights into the transcriptional mechanisms that cause robust versus stochastic gene expression and their relationships to phenotypic robustness and variability.

5.2. Protein

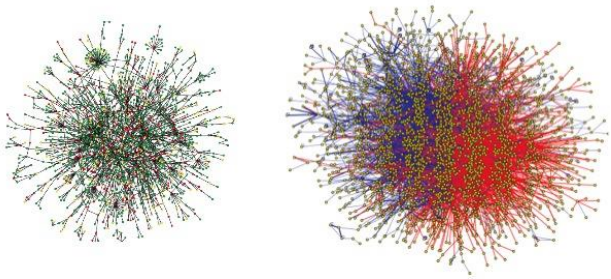
Proteins are large biomolecules, or macromolecules, consisting of one or more long chains of amino acid residues. Proteins perform a vast array of functions within organisms, including catalyzing metabolic reactions, DNA replication, responding to stimuli, and transporting molecules from one location to another. Proteins differ from one another primarily in their sequence of amino acids, which is dictated by the nucleotide sequence of their genes, and which usually results in protein folding into a specific three-dimensional structure that determines its activity.

5.2.2. Protein Networks

Protein–protein interactions (PPIs) are the physical contacts of high specificity established between two or more protein molecules as a result of biochemical events steered by electrostatic forces including the hydrophobic effect. Many are physical contacts with molecular associations between chains that occur in a cell or in a living organism in a specific biomolecular context.

Proteins rarely act alone as their functions tend to be regulated. Many molecular processes within a cell are carried out by molecular machines that are built from a large number of protein components organized by their PPIs. These interactions make up the so-called interactomics of the organism, while aberrant PPIs are the basis of multiple aggregation-related diseases, such as Creutzfeldt–Jakob, Alzheimer's disease, and may lead to cancer.

PPIs have been studied from different perspectives: biochemistry, quantum chemistry, molecular dynamics and signal transduction, among others. All this information enables the creation of large protein interaction networks – similar to metabolic or genetic/epigenetic networks – that empower the current knowledge on biochemical cascades and molecular etiology of disease, as well as the discovery of putative protein targets of therapeutic interest.



Two important topics in the Protein Networks are protein networks alignment and finding complexes in networks. A protein complex or multiprotein complex is a group of two or more associated polypeptide chains. Different polypeptide chains may have different functions. This is distinct from a multienzyme complex, in which multiple catalytic domains are found in a single polypeptide chain.

Protein complexes are a form of quaternary structure. Proteins in a protein complex are linked by non-covalent protein–protein interactions, and different protein complexes have different degrees of stability over time. These complexes are a cornerstone of many (if not most) biological processes and together they form various types of molecular machinery that perform a vast array of biological functions. The cell is seen to be composed of modular supramolecular complexes, each of which performs an independent, discrete biological function.

5.2.1. Prediction of interactions between proteins

Protein–protein interaction prediction is a field combining bioinformatics and structural biology in an attempt to identify and catalog physical interactions between pairs or groups of proteins. Understanding protein–protein interactions is important for the investigation of intracellular signaling pathways, modelling of protein complex structures and for gaining insights into various biochemical processes. Experimentally, physical interactions between pairs of proteins can be inferred from a variety of experimental techniques, including yeast two-hybrid systems, protein-fragment complementation assays (PCA), affinity purification/mass spectrometry, protein microarrays, fluorescence resonance energy transfer (FRET), and Microscale Thermophoresis (MST). Efforts to experimentally determine the interactome of numerous species are ongoing, and a number of computational methods for interaction prediction have been developed in recent years.

Proteins that interact are more likely to co-evolve, therefore, it is possible to make inferences about interactions between pairs of proteins based on their phylogenetic distances. It has also been observed in some cases that pairs of interacting proteins have fused orthologues in other organisms. In addition, a number of bound protein complexes have been structurally solved and can be

used to identify the residues that mediate the interaction so that similar motifs can be located in other organisms.

Computational methods in this field include the use of phylogenetic profiling, supervised learning methods, Bayes networks modelling, identification of structural patterns, and Domain-pair exclusion analysis. The most renowned algorithms in this area are GPS-Prot and BioPlex.

5.2.3. Protein design

Protein design (or protein engineering) is a technique by which proteins with enhanced or novel functional properties are created. Proteins can be engineered by rational design, which typically uses computational tools to identify useful mutations, or by directed evolution, which uses random mutagenesis coupled with a selection process to identify desired variants.

In other words, protein design is the rational design of new protein molecules to fold to a target protein structure, with the end goal of designing novel function and/or behavior. Proteins can be designed from scratch (de novo design) or by making calculated variants of a known protein structure and its sequence (termed protein redesign). Rational protein design approaches make protein-sequence predictions that will fold to specific structures. These predicted sequences can then be validated experimentally through methods such as peptide synthesis, site-directed mutagenesis, or artificial gene synthesis.

Rational protein design dates back to the mid-1970s, although initial protein design approaches were based mostly on sequence composition and did not account for specific interactions between side-chains at the atomic level. Recently, however, improvements in molecular force fields, protein design algorithms, and structural bioinformatics, such as libraries of amino acid conformations, have enabled the development of advanced computational protein design tools. These computational tools can make complex calculations on protein energetics and flexibility, and perform searches over vast configuration spaces, which would be unfeasible to perform manually. Due to the development of computational protein design programs, and important successes in the field, rational protein design has become one of the most important tools in protein engineering.

5.3. RNA

Ribonucleic acid (RNA) is a linear molecule composed of four types of smaller molecules called ribonucleotide bases: adenine (A), cytosine (C), guanine (G), and uracil (U). RNA is often compared to a copy from a reference book, or a template, because it carries the same information as its DNA template but is not used for long-term storage.

Each ribonucleotide base consists of a ribose sugar, a phosphate group, and a nitrogenous base. Adjacent ribose nucleotide bases are chemically attached to one another in a chain via chemical bonds called phosphodiester bonds. Unlike DNA, RNA is usually single-stranded. Additionally, RNA contains ribose sugars rather than deoxyribose sugars, which makes RNA more unstable and more prone to degradation.

RNA is synthesized from DNA by an enzyme known as RNA polymerase during a process called transcription. The new RNA sequences are complementary to their DNA template, rather than being identical copies of the template. RNA is then translated into proteins by structures called ribosomes. There are three types of RNA involved in the translation process: messenger RNA (mRNA), transfer RNA (tRNA), and ribosomal RNA (rRNA).

Although some RNA molecules are passive copies of DNA, many play crucial, active roles in the cell. For example, some RNA molecules are involved in switching genes on and off, and other RNA molecules make up the critical protein synthesis machinery in ribosomes.

5.3.1. RNA structure prediction

The structure of non-coding RNAs plays a key role to their function. Three types of structure define for RNAs. RNA primary structure consists of a linear sequence of nucleotides that are linked together by phosphodiester bonds including adenine (A), cytosine (C), guanine (G), or uracil (U). The secondary structure of RNA is the base pairing interactions. RNA tertiary structure is the three-dimensional shape of RNA. Classically, RNA structure determination has mostly been accomplished by X-Ray crystallography or Nuclear Magnetic Resonance approaches. These experimental methods are time consuming and expensive. Therefore, RNA tertiary structure predicts by using the

computational methods. Since, the secondary structure of RNA is base for RNA tertiary structure, RNA secondary structure prediction is one of important problems. The problem of RNA secondary structure prediction is, given an RNA sequence, to compute secondary structure with computational methods. Recently, the accuracy of RNA secondary structure prediction has been improved by adding SHAPE data as a pseudo-free energy.

5.3.2. RNA design

Generating artificial RNA sequences that would fold into a desired RNA structure is called the RNA design (RD) problem. This can be applied to ribozymes and riboswitches which could be used in medicine and drug design. In the last two decades, many algorithms and computational methods have been proposed for solving the RD problem; some of which are the INFO-RNA, ERD, MODENA and RNAifold methods.

5.3.3. Comparison of RNA structures

Knowing the 3-D structure of RNA is fundamental to understanding its biological function. Because of the fast evolutionary divergence of RNA molecules, which makes it difficult to produce structurally informative sequence alignments, multiple RNA structure alignment methods represent an important tool for functional annotation and evolutionary reconstruction of non-coding RNA.

The 3-D structure of a pair of RNA is given as input. The goal is to provide a one-to-one correspondence between the ribosome nucleotides of each of the two RNAs. As the number of RNA structures is increasing rapidly in databases, many methods have been proposed for RNA secondary structure comparison.

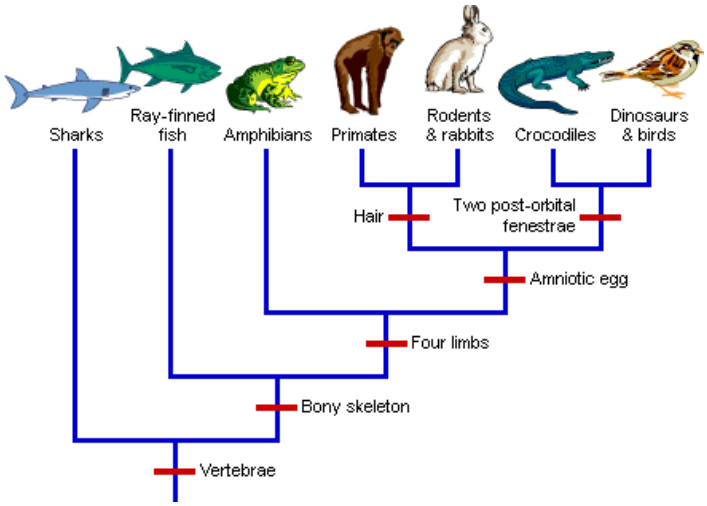
5.4 Phylogenetics

Biological evolution, simply put, is descent with modification. This definition encompasses small-scale evolution (changes in gene frequency in a population from one generation to the next) and large-scale evolution (the descent of different species from a common ancestor over many generations). Evolution helps us to understand the history of life.

Biological evolution is not simply a matter of change over time. Lots of things change over time: trees lose their leaves, mountain ranges rise and erode, but they aren't examples of biological evolution because they don't involve descent through genetic inheritance.

The central idea of biological evolution is that all life on Earth shares a common ancestor, just as you and your cousins share a common grandmother.

Through the process of descent with modification, the common ancestor of life on Earth gave rise to the fantastic diversity that we see documented in the fossil record and around us today. Evolution means that we're all distant cousins: humans and oak trees, hummingbirds and whales.



Computational phylogenetics is the application of computational algorithms, methods, and programs to phylogenetic analyses. The goal is to assemble a phylogenetic tree representing a hypothesis about the evolutionary ancestry of a set of genes, species, or other taxa. For example, these techniques have been used to explore the family tree of hominid species and the

relationships between specific genes shared by many types of organisms. Traditional phylogenetics relies on morphological data obtained by measuring and quantifying the phenotypic properties of representative organisms, while the more recent field of molecular phylogenetics uses nucleotide sequences encoding genes or amino acid sequences encoding proteins as the basis for classification. Many forms of molecular phylogenetics are closely related to and make extensive use of sequence alignment in constructing and refining phylogenetic trees, which are used to classify the evolutionary relationships between homologous genes represented in the genomes of divergent species. The phylogenetic trees constructed by computational methods are unlikely to perfectly reproduce the evolutionary tree that represents the historical relationships between the species being analyzed. The historical species tree may also differ from the historical tree of an individual homologous gene shared by those species.

5.5 Drug Discovery

Drug discovery is the therapeutic process of suggesting new candidate medications. This process takes a lot of time and money before a new drug is discovered. Furthermore, more than 90% of drugs fail during the development process. In order to address these problems, drug repositioning or repurposing applies known drugs to treat new diseases. By bypassing many early-stage clinical trials which the drug has already passed, the costs will be cut and so much time will be saved. This approach is especially effective in many fields of medicine where a wide variety of somewhat similar diseases have related underlying mechanisms and causes.

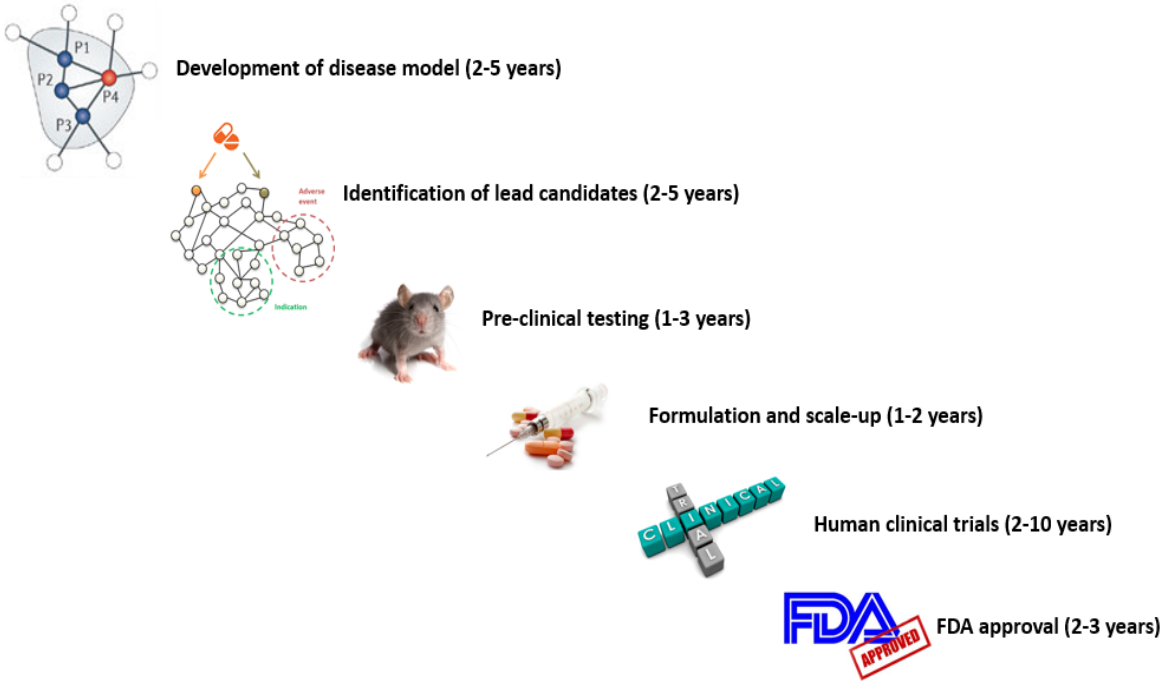


Figure1.1: The framework for drug discovery

As shown in Figure 1-1, the process of drug production, from the chemical formula to the laboratory stage, and ultimately to confirm its achievement, lasts about 20 years. With all the efforts made, we still see diseases that do not even respond to approved drugs and cause death.

Considering the leading issues in the world of pharmacy and medicine; Which we mentioned earlier, and the growing trend of diseases that have not yet been detected by effective drugs or diseases that have not responded positively to some drugs, Scientists are trying to replace better medicine.

Because they believe that the root of some diseases can be a single cause of the body, an idea that can help to increase the longevity or recovery of current patients, this is to use existing and approved drugs for the treatment of similar root diseases. By changing the drug's usage or changing the position of the drug or changing the target or destination of the drug, they can use the medicine in another way to treat another illness.

In general, the production of most drugs is initially discovered using either target-based or phenotypic analysis. The high incidence of treating untreatable or severe illnesses such as cancer, cardiovascular disease, diabetes and the like has created a major challenge for the pharmaceutical industry. In

addition, the emergence of drug resistance significantly reduces the effectiveness of drugs and makes it difficult to fight complex diseases.

Changing the position of the drug is the process of finding new applications for existing drugs for new prescriptions. Also, finding new uses for existing medications, recycling old medicines, and using defective drugs are known safety profiles. This safe information is the biggest advantage of changing the position of the drug, which highlights the reduction of costs and risks associated with the early stages, such as the toxicity of the drug in the early stages, and the shortening of the approval pathway for therapeutic prescriptions. For example, Gabapentin was initially developed for the treatment of epilepsy, but it is currently used for various uses, including pain relief, in particular pain with a neurological origin (such as headache and back pain). In another example, Rupirinol is prescribed to treat Parkinson's disease, which is used to treat restless leg syndrome. Given the benefits of changing the position of the drug, this approach is an alternative approach to discovery of the drug.

Given the number of existing diseases and the increasing trend, there are many medicines in the databases as well as the characteristics of each of the diseases and medications. So, doing any of the experiments experimentally and in a laboratory is not an optimal process, so the researchers are looking for a computational method that can use the computational tools to get the best drug suggestions at a less cost-effective time.