1. Microarray Analysis of Gene Expression in Rat Mesenchymal Stem Cells

Akavia Uri David, Shur Irene and Benayahu Dafna

Dept of Cellular and Developmental Biology Sackler Faculty of Medicine, TAU

Microarray analysis of gene expression in mesenchymal stem cells cultured from young and old rats was analyzed to study their metabolic state. Overall 493 probes were identified as differentially expressed, which include defined genes and ESTs. The genes were clustered into 6 distinct groups using EXPANDER software.

2. The Multifaceted Receptors of the Human Nose

Tal Atarot[1], Ester Feldmesser[1], Miriam Khen[1], Tsviya Olender[1], Miriam Eisenstein[2] and Doron Lancet[1]

[1]Dept of Molecular Genetics, [2]Dept of Chemical Research Support, WIS

Olfactory receptors (ORs), the largest mammalian gene superfamily, were subjected to intra- and interspecies sequence comparisons. These afford a definition of sequence positions likely to underlie functional genetic variability as well as to mold the unique 3-dimensional structure of ORs. Transcriptomics revealed unusual OR expression patterns across normal human tissues.

3. Fine-Grain Matrix Graph Representation for Predicting Mutations Leading to Conformational Rearrangements in Small RNAs

Assaf Avihoo, Nir Dromi and Danny Barash

Dept of Computer Science, BGU

Previously, it was shown that predicting selective mutations leading to topological transitions in the secondary structure of RNAs can be achieved by a coarse-grain Laplacian matrix tree-graph representation. However, for small RNAs, such representations become ineffective. Fine-grain matrix representations are required.

4. ProTeus - An Archive of Functional Signatures in Protein Termini

Iris Bahir, Noam Kaplan and Michal Linial

Dept of Biological Chemistry, HUJI

Most methods that detect protein signatures rely on sequence similarity without considering any positional information. Herein we present a positional-based method for revealing short signatures in both termini among ~114,000 proteins from Swissport. Many of the signatures were previously overlooked. The results are presented as an interactive website - http://www.proteus.cs.huji.ac.il.

5. Insight into the Molecular Program of Meiosis, a DNA Microarray Analysis of the Murine System

Hiba Ben-Asher[1], Iris Shahar[2], Ramit Mehr[1] and Jeremy Don[1]

[1]Faculty of Life Sciences, BIU, [2]Functional Genomics Unit, Sheba Medical Center,

DNA microarrays were used to analyze gene expression during mouse meiosis. 790 sequences that showed expression change of 2 Log2 or more between meiotic stages, were clustered into 19 sub-groups. Bioinformatical programs were used to sort genes according to functional characteristics and to pinpoint potential key regulators.

6. Data Analysis for CGH Microarrays

Amir Ben-Dor, Doron Lipson, Anya Tsalenko, Alicia Scheffer, Michael Barrett, Elinor Dehan[1], Naftali Kaminski[1], Kristin Baird[2], Paul Meltzer[2], Steve Laderman, Laurakay Bruhn, and Zohar Yakhini

Agilent Technologies, Palo Alto, CA, [1]NHGRI, Bethesda, MD, [2]Sheba Medical Center, Tel Aviv

CGH performed on microarrays enables accurate measurement of changes in cancer genome DNA copy numbers. We present data analysis methods designed to accurately and robustly identify and characterize chromosomal aberrations in tumor cells as well as related expression characteristics. We show applications to colon cancer, lung cancer and breast cancer data.

7. An Autonomous Molecular Computer for Logical Control of Gene Expression

Yaakov Benenson[1,2], Binyamin Gil[2], Uri Ben-Dor[1], Rivka Adar[2] and Ehud Shapiro[1,2]

[1]Dept of Computer Science and Applied Mathematics, [2]Dept of Biological Chemistry, WIS

Early biomolecular computer research focused on laboratory-scale, human-operated computers for complex computational problems. Recently, simple molecular-scale autonomous programmable computers were demonstrated allowing both input and output information to be in molecular form. Here we describe an autonomous biomolecular computer that, at least in vitro, logically analyses the levels of messenger RNA species, and in response produces a molecule capable of affecting levels of gene expression.

8. Using Expression Data to Discover RNA and DNA Regulatory Sequence Motifs

Chaya Ben-Zilbersteun, Zohar Yakhini and Eleazar Eskin

A sequence motif is called rank-imbalanced (RIM), in the context of a ranked list of genes, if it occurs more in either ends of the list than is expected at random. We address methods and results related to RIMs in DNA/RNA sequences ranked by expression levels, degradation rates and other parameters

9. Searching for RNA Motifs Using Computational Geometry: The Structure to String (STR2) Method

O. Bergig, D. Barash and K. Kedem

Computer Science Dept, BGU

We present a novel approach for searching RNA motif structure in long genomes, with ideas taken from computational geometry. The method, called Structure to String (STR2), converts an RNA secondary structure into a shape representing string. We show examples of its applicability on aptamer domains that are functionally important

10. PROCEED: A Proteomic Experimental and Computational Methods for Identifying Plasma Membrane Proteins

Yaniv Bledi, Alex Inberg and Michal Linial

Dept of Biological Chemistry, Alexander Silverman Institute of Life Science, HUJI

Elucidating the profile of extracellular membrane proteins is vital for diagnostic and therapeutic development. We have devised a high-throughput MS-based platform to explore such proteins. The resulting shed peptides are analyzed by MS technology. A database of predicted membranous proteins serve to enhance protein identification success rate.

11. The Correction of Essential Artifacts in Microarray Data

Brodsky L., Weining Song, A. Bolshoy, E. Trifonov and E. Nevo

Genome Diversity Center, Institute of Evolution, Haifa University

A technical factor might influence significant number of gene expression profiles, and its influence would be seen in profiles of one or several Principal Components. A geometrical nonuniformity on microarray template of PC-projections for gene-profiles gives an opportunity to correct data by eliminating an artifactual component of every gene-profile pattern.

12. Comparative Analysis Detects Dependencies Among the 5‘ Splice Site Positions

Ido Carmel, Saar Tal, Ida Vig and Gil Ast

Dept of Human Genetics, Sackler Faculty of Medicine, TAU

Human-mouse comparative genomics is an informative tool to assess sequence functionality as inferred from its conservation level. We used this approach to examine dependency between different positions of 5' splice site by analyzing the frequencies of changes between different positions of homologous human-mouse 5'ss pairs.

13. Construction of GPCR Transmembrane Domains by Using a Partial Rhodopsin Template and Applying Iterative Stochastic Elimination.

Sofia Chero-Schwartz and Amiram Goldblum

Dept of Medicinal Chemistry, School of Pharmacy, HUJI

The ISE algorithm was applied for conformational searching of the transmembrane domain of G-protein coupled receptors. The alternative TM conformations were found by randomizing the backbone dihedral angels of the endoplasmic half of the rhodopsin template structure. Finally, 100-200 clusters of conformations were obtained. Structures from these clusters form the basis for subsequent construction of GPCR models.

14. Unitary Pseudogenes in Bacterial Genomes: Lifestyle and Gene Loss

Tal Dagan[1] and Dan Graur[1,2]

[1]Dept of Zoology, George S. Wise Faculty of Life Sciences, TAU, [2]Dept of Biology and Biochemistry, University of Houston, TX USA

Patterns of gene loss can be inferred from studies of unitary pseudogenes, i.e., pseudogenes devoid of functional paralogs. In this study, we examine the effects of lifestyle on the frequency of unitary pseudogenes in 140 fully sequenced bacterial genomes. Expectedly, parasitic bacteria were found to have lost a considerable number of gene functions. In particular, genes encoding metabolic functions were found to be prone to pseudogenization. Friedman

15. Predicting the Structure of an Arrestin Dimer Using Structural Bioinformatic Methods

Hilda David and Joel Hirsch

Dept of Biochemistry, TAU

Arrestins play a key role in quenching signal transduction initiated by G protein coupled receptors. It has been suggested that arrestin activity is regulated by dimerization. By analyzing models of all possible dimers that appear in the crystalline lattices of different crystal forms, we predict the most likely dimeric permutations present in solution

16. Positive Selection at a Single Amino-Acid Site

Adi Doron, Adi Stern, Itay Mayrose, Ophir Cohen, Nimrod Rubinstein, Eran Bacharach and Tal Pupko

Dept. of Cell Research and Immunology, TAU

We developed a probabilistic-based approach which identifies site-specific instances of positive Darwinian selection at the amino acid level. Our algorithm estimates a non-synonymous/synonymous ratio score, incorporating an evolutionary codon-based substitution model. A web server then projects these scores onto the molecular surface of a protein with known 3D structure.

17. MASS: Multiple 3D Alignment by Secondary Structures

Oranit Dror, Hadar Benyamini, Ruth Nussinov and Haim Wolfson

Tel-Aviv University

MASS is a highly efficient method for aligning multiple protein structures. Using secondary structure information improves the accuracy of the alignments and achieves efficiency and robustness. The method is independent of the sequence of secondary structure elements; thus capable of detecting non-topological 3D motifs. Additionally, MASS is able to recognize motifs shared only by a subset of the input molecules.

18. Noisy Bootstrapping Improves the Robustness of Classification of Gene Expression Data

Niv Efron and Nathan Intrator

School of Computer Science, TAU

Noisy bootstrapping is shown to improve and robustify classification with an increased number of genes. We use LDA for feature selection and classification of microarray data. Results show our classifier is accurate and competitive to other published methods, although it is simple and enables considering larger sets of genes.

19. Gene Expression Analysis of Human Leukemia and Cell Differentiation

Uri Einav, Michal Mashich, Osnat Ravid, Dafna Tsafrir, Ilan Tsafrir and Eytan Domany

Dept of Physics of Complex Systems, WIS

Three different gene expression analysis studies related to leukemia and differentiation are shown. Analysis was preformed using various statistical, clustering (CTWC, SPC) and sorting (SPIN) methods.

20. Development and Application of Theoretical Tools for Predicting the Structures of Molecular Complexes

M. Eisenstein, E. Ben-Zeev, N. Kowalsman, D. Segal, A. Berchanski, A. Heifetz, B. Shapira, A. Ben-Shimon and E. Katzir

Dept of Chemical Research Support and Biological Chemistry, WIS

Docking techniques can be used to predict the multitude of interactions that sustain the living cell. Our docking algorithm (MolFit) tests geometric, electrostatic and hydrophobic surface complementarity, and allows incorporation of external data from biochemical and bioinformatics studies. MolFit successfully predicted most of the targets in the blind CAPRI experiment.

21. Modeling Side Chain Conformations Using Surface Areas

Eran Eyal, Rafael Najmanovich, Brendan J. McConkey, Marvin Edelman and Vladimir Sobolev

Weizmann Institute of Science

Contact and accessible surfaces are used as the core of a scoring function to simultaneously predict conformations of protein side-chains. Our publicly available program exhibits good combination of accuracy and speed. Most atoms prefer intra-molecular contact over solvent contacts. This might correspond to the driving force for maximizing packing

22. A Bayesian LOD Score for Linkage Analysis of Complex Diseases

Ma'ayan Fishelson, Dmitry Rusakov, and Dan Geiger

Technion, I.I.T.

We propose a Bayesian averaging approach, called MBLOD, for analyzing complex diseases. According to MBLOD, the LOD-score is computed under two inheritance models, recessive and dominant. We commit to the inheritance model producing the higher score, and subtract 0.3 from the maximum LOD-score to correct for two tests.

23. Closed Loops of TIM Barrel Protein Fold

Frenkel, Z.M., I.N. Berezovsky and E.N. Trifonov

Genome Diversity Center, Institute of Evolution, University of Haifa

RMSD comparisons and presentation of protein sequences in binary code show, that TIM-barrel proteins consist from descendants of several types of basic closed loop prototypes. Comparison of these prototypes point to very likely common prototype - closed loop of 28 aa, containing one alpha-helix, characterized by specific binary consensus sequence.

24. Studying Protein Cavities - How Empty Voids Influence Protein Dynamics

Ran Friedman, Esther Nachliel and Menachem Gutman

Tel Aviv University

Due to the Van der Waals repulsion, the structures of proteins contain many cavities. We have suggested a new computational approach for studying the dynamics of proteins, based on an analysis of their cavities' inventory. The approach will be demonstrated in the proton pumping protein Bacteriorhodopsin.

25. Supervised Partitioning of the Protein Space: An Information - Theoretic Approach

Menachem Fromer[1], Moriah Friedlich[1], Noam Kaplan[2], Nathan Linial[1] and Michal Linial[2]

[1]School of Computer Science and Engineering, [2]Dept of Biological Chemistry, HUJI

The BF (Best Front) technique uses an information-theoretic defined distance to automatically determine the optimal level in a hierarchical tree of proteins, relative to a given annotation set. This novel method was tested on the ProtoNet hierarchy using Pfam annotations. The quality of this BF is assessed at http://www.protonet.cs.huji.ac.il/bestFront/.

26. Modeling and Analysis of Heterogeneous Regulation in Biological Networks

Irit Gat-Viks, Amos Tanay and Ron Shamir

School of computer science, TAU

We propose a computational framework for the representation, analysis and learning of biological networks from data. Our methodology builds on prior biological knowledge, handles heterogeneous regulatory mechanisms (transcriptional, translational and metabolic) and allows realistic, loopy, network topology. We demonstrate our methods on the yeast lysine biosynthetic pathway and infer lysine enzymes regulation.

27. Gene Expression Profile of Human Embryonic Stem Cells, Tissue Progenitors and Differentiated Cells

Michal Golan-Mashiach, Jean-Eudes Dazard, Sharon Gerecht, Nir, Ninette Amariglio, Tamar Fisher, Jasmine Jacob-Hirsch, Bella Bielorai, Sivan Osenberg, Omer Barad, Gad Getz, Amos Toren, Gideon Rechavi, Joseph Eldor-Itskovitz, Eytan Domany and David Givol

WIS, Rambam Medical Shatsky Center, Chaim Sheba Medical Center

We compared the transcription profile of human embryonic stem cells (ESC) with that of progenitor/stem cells of human hematopoietic and keratinocytic origins, along with their mature differentiated cells. We propose that ESC use a novel “just in case” design principle to achieve pluripotency by expressing more genes than adult cells.

28. Iterative Stochastic Elimination Algorithm for Studying Protein-Ligand Interactions

Boris Gorelik, Efrat Noy and Amiram Golbdlum

Dept of Medicinal Chemistry, School of Pharmacy, HUJI

Introducing flexibility into computations of Protein-ligand interactions is important for correctly considering the roles of multiple binding modes, and are essential for drug design. Iterative Stochastic Elimination (ISE) Algorithm has been successfully employed previously for protein flexibility. In this poster, we present our initial attempts to implement ISE for rigid and flexible ligand docking to proteins

29. High Density Linkage Disequilibrium Mapping Using Models of Haplotype Block Variation

Gideon Greenspan and Dan Geiger

Computer Science, Technion

We have developed a high density LD mapping technique which takes account of haplotype blocks and works directly with both phased and unphased SNP data. Our method significantly outperforms mapping by individual SNPs and a competing haplotype-based approach. HaploBlock is available at: http://bioinfo.cs.technion.ac.il/haploblock/.

30. Rarity of Conservation in Highly Regulated Operons

Einat Hazkani-Covo and Dan Graur

Dept of Zoology, TAU, Dept of Biology and Biochemistry, University of Houston, Texas

Evolutionary conservation of a single protein is associated with its number of protein-protein interactions. In analogy, we hypothesized that the same is true for operons - complex genetic elements. We tested whether operons controlled by many transcription factors will be evolutionary more conserved than operons under the control of a single transcription factor. We found no such relation

31. Signal Deconvolution for Microarray Gene Expression Data

Moshe Havilio

Compugen LTD, Tel Aviv

A new algorithm for expression detection and background adjustment in microarray experiments is presented. The algorithm relies on the deconvoluted experimental signal distribution for evaluating the expression probability and adjusting the background for each probe. It does not depend on the presence or reliability of negative or positive controls in the experiment. The algorithm's applicability is demonstrated in a diverse set of expression experiments, and its performance is compared with methods that use negative controls.

32. Chromosomal Organization Is Shaped by the Transcription Regulatory Network

Ruth Hershberg, Esti Yeger-Lotem and Hanah Margalit

Hadassah medical school, HUJI and The Technion

We study the relationship between transcription regulation and chromosomal organization using methods borrowed from network analysis. Integrated networks representing both types of data are created and searched for network motifs that recur more than expected at random. Motifs found demonstrate that transcription regulation shaped chromosomal organization in pro- and eukaryotes

33. RNAMAT - A Visualization Tool and a Clustering Algorithm

Yair Horesh and Ron Unger
Dept of Computer Science and Faculty of Life Science, BIU

The discovery of novel RNA molecules is a major computational challenge. RNAMAT is based on a 2D-representation of the potential structure of candidate RNA molecules. Summation of matrices reveals common features. RNAMAT displays all potential base-pairings including pseudoknots. A clustering algorithm is used to reveal unknown subclasses of RNA.

34. Meshi - A New Object Oriented Package for Molecular Simulations

Nir Kalisman, Ami Levi, Sharon Zafriri, Ram Jenovski and Chen Keasar

Ben Gurion University

We present a new object oriented package for molecular modeling which was designed to accelerate the development of novel energy functions and optimization procedures. The new package includes classes for molecular elements (e.g. atoms,), geometry (e.g. torsion angles), energy functions (e.g. atomEnvironment) and optimization algorithms (e.g. LBFGS).

35. Continuous Treatment of the Backbone and Sidechain Torsion Space

Nir Kalisman and Chen Keasar

We developed a practical method for the generation of continuous functions describing 2D torsion scatter-plots (Ramachandran, CHI1-CHI2, etc.). The functions are constructed by dense sampling of the scatter-plot densities, followed by cubic spline fitting. The resulting functions capture almost the exact form of the original plot and show superior properties to discontinuous treatments.

36. PANDORA: Keyword-Based Analysis of Protein Sets by Integration of Annotation

Sources

Noam Kaplan and Michal Linial

Institute of Life Sciences, HUJI

PANDORA is a web-based tool that provides automatic graphical representation of the biological knowledge associated with any set of proteins. PANDORA uses a unique approach of keyword-based graph analysis that focuses on detecting subsets of proteins that share unique biological properties and the intersections of such sets. Available at: http://www.pandora.cs.huji.ac.il

37. Genome-Wide de novo Prediction of Transcription Factor Binding

Tommy Kaplan[1], Nir Friedman[1] and Hanah Margalit[2]

[1]Dept of Computer Science and Engineering [2]Dept of Molecular Genetics and Biotechnology, Faculty of Medicine, HUJI

Our approach combines sequence and structure to learn context-specific DNA-recognition preferences and to predict binding sites of novel transcription factors. We apply it to the Cys2His2 zinc finger family, and predict targets in Drosophila in a genome-wide manner. We infer the factors' function and activity using their targets' annotations and expression.

38. Making Sense Out of Multi-Knockout Experiments: The Rad6 Example

Alon Kaufman[1], Martin Kupiec[2] and Eytan Ruppin[3]
[1]ICNC, HUJI, [2]Dept of Molecular Microbiology and Biotechnology, TAU, [3]Schools of Computer Science and Medicine, TAU

This work presents the first study applying Multi-perturbation Shapley value Analysis (MSA) to genetic multi-knockout data. The MSA identifies the importance of genes in the Rad6 DNA repair pathway of the yeast, quantifying their contributions and characterizing their functional interactions as well as providing a new functional description of the Rad6 pathway.

39. Viral Piracy and Mammal Divergence

Eddo Kim and Yossef Kliger

Faculty of Life Sciences, BIU and Compugen LTD, Tel Aviv

Large dsDNA viruses acquire host proteins to evade host defense. Identifying such proteins is important for basic research and biotechnological applications, but is often difficult because of low sequence similarity. We report that human proteins, which were subject to recent viral piracy, are less conserved than other human proteins.

40. GERBIL: A New Algorithm for Resolving and Block Partitioning of Genotypes Using Maximum Likelihood

Gad Kimmel and Ron Shamir

School of Computer Science, TAU

We have developed a new algorithm and software for the simultaneous phasing and block partitioning of a population of genotypes. Our algorithm is based on a novel stochastic model. On two large-scale real genotype data sets, our algorithm outperformed three state-of-the-art phasing algorithms. It also revealed stronger association in two case/control studies

41. Curvature Distribution in Prokaryotic Genomes

Limor Kozobay-Avraham, Sergey Hosid and Alexander Bolshoy

Genome Diversity Center, Institute of Evolution, University, Haifa

We analyzed all available complete prokaryotic genomes using the software CURVATURE to predict whether promoter region of certain prokaryotes characterized by higher intrinsic DNA curvature located within or upstream to these region. The results confirm our former hypothesis that DNA curvature has a functional adaptive significance determined by temperature selection

42. Down-Regulation of the Catalytic Activity of the EGF Receptor via Direct Contact between the Kinase and C-Terminal Domains

Meytal Landau, Sarel J. Fleishman and Nir Ben-Tal

Dept of Biochemistry, George S. Wise Faculty of Life Sciences, TAU

The ErbBs are unique among RTKs, as their catalytic elements are constitutively ready for phospho-transfer. The absence of conformational regulation raises a fundamental dilemma: namely, by what mechanism is spurious activation avoided? Our studies, using various computational tools suggest a novel molecular regulation mechanism.

43. Construction of Conformational Ensembles by the Iterative Stochastic Elimination Algorithm – ISE

Tal Lavy and Amiram Goldblum

Dept of Medicinal Chemistry, School of Pharmacy, HUJI

We compare the effects of ISE on the conformational search of a ligand (Disoxaril, WIN51711) known to adopt alternate conformations in different environments, to a full exhaustive search with limited combinatorial space. Various parameters of ISE have been tested in order to find the optimal combinations for the sampling of conformations and for discarding values that contribute consistently to high-energy conformations. We present in this poster various tests for making decisions in this particular problem.

44. Longest Order-Preserving Subsets (LOPS): Algorithms and Applications to Genomic Data

Doron Lipson and Zohar Yakhin

CS Dept, Technion, Agilent Labs, CA

An order-preserving subset (OPS), in a set of k-dimensional vectors, is a subset that can be ordered so that every element is smaller than its successor, in all k coordinates. A longest OPS (LOPS) is one of maximal cardinality. In k=2 LOPS can be computed in O(nlogn) time. We present an O((n^1.6)logn) extension for k>2 and applications to gene expression and DNA copy number microarray data.

45. McRate: Site-Specific Evolutionary Rate Inference over the Whole Tree Space

Itay Mayrose, Amir Mitchell and Tal Pupko

Dept of Cell Research and Immunology, George S. Wise Faculty of Life Sciences, TAU

We describe a Bayesian method that uses Markov chain Monte Carlo to calculate site-specific conservation scores in protein sequences. Our novel algorithm takes into account all possible evolutionary relationships among the sequences under study. We show that this approach is superior over existing methods that assume only a single phylogeny.

46. Exploring the Exocytotic Process by a Chemical Kinetic Approach

Aviv Mezer[1], Esther Nachliel[1], Menachem Gutman[1] and Uri Ashery[2]

[1]The Laser Laboratory, Dept of Biochemistry, [2]Dept of Neurobiochemistry, TAU

We have created a comprehensive kinetic model describing exocytosis as a dynamic interaction between synaptic proteins. The interactions between key synaptic proteins were transformed into differential rate equations to reconstruct the process of exocytosis. This method provides a platform to predict and quantify the effects of protein and manipulations on exocytosis.

47. Enhanced Statistics for Local Alignment of Multiple Alignments Improves Protein Function and Structure Prediction

Milana Morgenstern and Shmuel Pietrokovski

Dept of Molecular Genetics, WIS

We present an enhanced score significance estimation procedure for LAMA, a method for ungapped profile-to-profile comparison. It is based on column-to-column score probabilities combined using Fisher's Chi-Square method. The improved LAMA was found most sensitive in a large-scale comparison with other profile-to-profile comparison methods using various parameters.

48. Searching for Human Insulators

Yael Mutsafi, Ran Blekhman, Itay Mayrose, Tal Pupko and Eran Bacharach

Dept of Cell Research and Immunology, George S. Wise Faculty of Life Sciences, TAU

Insulators are DNA elements separating independently regulated gene domains. CTCF is a multivalent insulator binding protein, which blocks improper enhancer-promoter interaction. A genomic search for CTCF-insulator sequences in several human gene loci suggests novel CTCF insulator sites in the gene regions of Rb1, Top1, LMO2, polR2A, KHK and MHC.

49. A Stochastic Approach to Interactions of Protein-DNA

Ilanit Mymoni and Amiram Goldblum

Dept of Medicinal Chemistry and Natural Products, School of Pharmacy, HUJI

In the poster we present our approach to the construction of a Force Field for non-bonding interactions between proteins and DNA. The atomic type values will be randomly picked from a range of discrete values and ISE will be used to find the best “tables of values” for the atomic parameters

50. Dipeptide Frequencies in Structural and Sequence Databases

Efrat Noy, Anwar Rayan and Amiram Goldblum

Dept of Medicinal Chemistry and Natural Products, School of Pharmacy, HUJI

Dipeptide databases in non-redundant proteins have been constructed for predicting loop conformations. In such a database we noticed a considerable difference between the frequency of some dipeptides in one and in the opposite direction (XZ vs. ZX). Structural explanations for such preferences have not been found yet, and we examine the dipeptide preferences in longer peptide sequences.

51. Structural Stability Prediction of Short Beta-Hairpin Peptides by Molecular Dynamics and Knowledge Based Potentials

Karin Noy, Nir Kalisman and Chen Keasar

Dept of Computer Sciences and Dept of Life Sciences, BGU

We present a computational approach for structural stability prediction of short peptides by using two orthogonal computational techniques: Molecular Dynamics and knowledge based potentials. The major observation is a clear correlation between the experimental and computed both stabilities. The prediction scheme implied by this correlation can help the design of efficient combinatorial peptide libraries.

52. Exploiting the Exploiters: Identification of Pathogen-Host Peptide, Mimicry as a Source for Modules of Functional Significance

Amir Orlev and Eyal Akiva, Shmuel A. Ben-Sasson

Dept of Experimental Medicine and Cancer Research, HUJI

Peptide mimicry refers to the existence of pathogenic and host proteins sharing a similar short amino-acid sequence with equivalent functionality. The pathogen might use this determinant to manipulate host cellular activities. The software peptideHunter, http://peptidehunter.md.huji.ac.il was developed to efficiently identify peptide mimicry. Such peptides demonstrated selective biological effect, experimentally.

53. Contact Potentials for Protein Design by Iterative Stochastic Elimination

Regina Politi, Masha Mikhlin and Amiram Goldblum

Dept of Medicinal Chemistry and Natural Products, School of Pharmacy, HUJI

We search for the best sequences that stabilize a 3D structure. Two major issues are the scoring function and searching the huge sequence space. In this poster, we test the ability to construct residue-residue contact potentials by applying our Iterative Stochastic Elimination (ISE) Algorithm. The scores are based on comparison to calorimetric results for protein unfolding of protein mutants, in staphylococcal nuclease

54. Interface Cores in Sandwich-Like Proteins

Vladimir Potapov[1], Vladimir Sobolev[1], Marvin Edelman[1], Alexander Kister[2,3] and Israel Gelfand[3]

[1]Dept of Plant Sciences, WIS, [2]Dept of Health Informatics, University of Medicine and Dentistry, NJ [3]Dept of Mathematics, Rutgers University, NJ

We define protein-protein interface and domain cores for immunoglobulins containing about half the residues and surface areas of the full interfaces. Residues of the two cores are structurally connected, imparting rigidity at the interface core. The rule of positional connectivity extends generally to sandwich-like proteins interacting in a sheet-sheet fashion.

55. HMMERHEAD - Accelerating HMM Searches on Large Databases

Elon Portugaly and Matan Ninio

School of Computer Science and Engineering, HUJI

HMMs are powerful tools for remote homology detection. However, searching a sequence database using an HMM is a computationally expensive process. We provide HMMER Hashing Enabled Acceleration Device (HMMERHEAD) - a heuristic acceleration of the HMMER package search software. Experiments show a15-fold acceleration, while retaining 99% of the results.

56. Distinguishing between Databases Using the ISE Algorithm - A Novel Approach to Discriminate Between Drugs and Non-Drugs

Anwar Rayan, Andrea Scaiewicz, Inbal Geva-Dotan, Dinorah Barasch and Amiram Goldblum

Dept of Medicinal Chemistry and the David R. Bloom Center for Pharmacy, HUJI

Distinguishing between drug-like and non drug-like molecules is becoming a central issue and an alternative to predicting pharmacokinetic properties of molecules. We have developed a new approach to discriminate between drugs and non-drugs using the Iterative Stochastic Elimination (ISE) algorithm originally devised in our lab.

57. The Made-In-Israel Bioinformatics Portal

Yossi Rosenberg, Ron Unger and Meir Edelman

The national Center Of Knowledge for Bioinformatics Infrastructure

The Made-In-Israel Bioinformatics portal is an initiative of COBI (national Center Of Knowledge for Bioinformatics Infrastructure) whose mission is to promote the use of Israeli bioinformatics tools and development of additional tools. The portal offers links to Israeli bioinformatic online servers and software downloading sites and host applications that need heavy resources.

58. Dynamic Annotation of Genes, Using Medline Literature and Custom Terms

Ran Rubinstein[1,2], Itamar Simon[1]

[1]Dept. of Molecular Biology and [2]COBI, Faculty of Medicine, HUJI

Genomic experiments often result in long lists of affected genes. While static annotations for genes are provided by online databases, they are often irrelevant to the scientific question the researcher is pursuing. We provide a tool for creating dynamic annotations for genes, based on automatic Medline searches with the researcher's custom terms.

59. Centrality of Weak Interhelical H-Bonds in Membrane Protein Functional Assembly and Conformational Gating

Ilan Samish, Eran Goldberg and Avigdor Scherz

Weizmann Institute of Science

Membrane protein functional assembly and conformational gating involve weak, backbone-mediated inter-helical hydrogen bonds. These bonds cluster in the conserved, buried protein core and correlate with the residue packing scale. Different conformational gating examples are discussed. The results provide parameters for structure and function prediction.

60. PatchDock: Efficient Algorithm for Unbound Docking of Rigid Molecules

D. Schneidman-Duhovny, R. Nussinov and H.J. Wolfson.

Tel Aviv University

PatchDock is an algorithm for unbound (real life) docking of molecules. The algorithm carries out rigid docking, with surface variability/flexibility implicitly addressed through liberal intermolecular penetration. PatchDock succeeds in docking of large proteins (antibody with antigen) and small drug molecules. The running times of the algorithm are of the order of several minutes. The webserver running PatchDock is available from http://bioinfo3d.cs.tau.ac.il/PatchDock.

61. Screening of Alternative Models for Transitional B Cell Maturation

G Shahaf, M. Cancro, D. Allman and R. Mehr.

Faculty of Life Sciences, BIU

Our aim is to elucidate the B cell maturation in the spleen using several optional mathematical models that we have constructed. We wrote a computer program that numerically simulates B cell population dynamics in the spleen, and we used it to fit the various alternative models to the experimental data, in order to find out which model fits the data best.

62. Flexible Pairwise Alignment with Hinge Detection and Multiple Structural Alignment of Proteins

Maxim Shatsky, Ruth Nussinov and Haim Wolfson

Tel-Aviv University

Two methods are presented. FlexProt carries out flexible structural comparisons of hinge-bent proteins without prior knowledge of the flexible hinge regions. MultiProt carries out multiple structure comparisons of proteins, and finds common geometric cores for all possible number of molecules from the input. Both methods are highly efficient. http://bioinfo3d.cs.tau.ac.il/

63. Structural Analysis of Residue Interaction Graphs

Arye Shemesh, Gil Amitai, Einat Sitbon, Maxim Shklar, Dvir Netanely, Ilya Venger and Shmuel Pietrokovski.

Dept of Molecular Genetics, WIS

We present a graph theory approach for studying protein structures. Structures were transformed to residue interaction graphs (RIGs), where nodes are residues and edges connect interacting residues. Centrality measures of RIG nodes identify various protein functional sites. Our method can analyze single structures, is independent of sequence conservation, and does not rely on prior training.

64. A Sequence Signature with a Role in Pore-Formation Common to Diverse Beta-Pore-Forming Toxins

Daniel Sher[1], Yelena Fishman[1], Mingliang Zhang[1], Jose-Miguel Mancheño[2] and Eliahu Zlotkin[1]

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beta-PFTs are a diverse group of proteins which create transmembrane pores. We have characterized the amino acids responsible for the difference in activity between two isoforms of one such toxin, Hydralysin. We combine these experimental data with alignments based on PSI-BLAST to suggest a “sequence signature” common to beta-PFTs.

65. GeneTide: Terra Incognita Discovery Endeavor - Comprehensive EST Assignment with Elucidation of de-novo GeneCards® Genes

Maxim Shklar, Orit Shmueli, Liora Strichman-Almashanu, Michael Shmoish, Tsippi Iny-Stein, Marilyn Safran and Doron Lancet

Dept of Molecular Genetics and Biological Services, WIS

Constructing a complete gene index for the >5 million human ESTs is intricate and elusive. GeneTide is a new automated system for associating EST sets with GeneCards genes. We find >15,000 sets that appear to define de-novo genes not currently present in GeneCards, constituting Terra Incognita candidates for future scrutiny.

66. GeneNote: A Bird's-Eye View of Gene Expression in Human Tissues

Orit Shmueli[1], Itai Yanai[1], Hila Benjamin-Rodrig[1], Micael Shmoish[1], Maxim Shklar[1], Alexandra Sirota[1], Asaf Madi[1], Arren Bar-Even[1], Shirley Horn-Saban[2], Ron Ophir[2], Liora Strichman-Almashano[1], Naomi Rosen[1], Marilyn Safran[2] Eytan Domani[3] and Doron Lancet[1]

[1]Dept of Molecular Genetics, [2]Biological Services and [3]Physics of Complex Systems, WIS

We carried out a genome-wide microarray expression profile analysis for 12 normal human tissues. These results are compared to electronic Northern and Serial Analysis of Gene Expression (SAGE) data for every gene (http://genecards.weizmann.ac.il/genenote/). Our results highlight the significance of midrange expression profiles as compared to housekeeping or single-tissue specific patterns.

67. SiteEngine: Functional Sites Structural Search Engine

Alexandra Shulman-Peleg, Ruth Nussinov, Haim J. Wolfson

Tel Aviv University

We present a novel method, SiteEngine, for recognition of regions on the surface of one protein that resemble a specific binding site of another. The method is based on physico-chemical properties and assumes no sequence or fold similarities. It is efficient and can search the entire PDB to recognize proteins that may bind similar binding partners and perform similar functions.

68. Evolution of Primate-Specific Alternative Alu Exons

Rotem Sorek[1,2,5], Galit Lev-Maor[1,5], Mika Reznik[1], Noam Shomron[1], Tal Dagan[3], Frida Belinky[3], Dan Graur[4] and Gil Ast[1]

[1]Dept of Human Genetics and Molecular Medicine, Sackler Faculty of Medicine, TAU [2]Compugen, Tel Aviv [3]Dept of Zoology, George S. Wise Faculty of Life Sciences, TAU [4]Dept of Biology and Biochemistry, University of Houston, Texas

Alu elements are short, primate specific retrotransposons that appear more than one million times in the human genome. We show that these elements can evolve to be new exons, and demonstrate that only small number of changes in their sequence is required for this process. This process can either cause genetic disorders or create new, primate-specific, exons.

69. Modeling of Antisense Overlaps for Gene Finding in Prokaryotic and Bacteriophage Genomes

Israel Steinfeld, Noa Chorev and Eyal Privman

School of Computer Science, TAU

We present a novel Hidden Marcov Model for prokaryotic and bacteriophage genomes, allowing same and opposite strand overlaps between genes. This gives the model a significant advantage in the dense genomes of bacteriophages. The model predicts up to 91% of the known genes of members of the Siphoviridae family.

70. GeneCards 2004: From High Quality Data Integration to Functional Genomics

Liora Strichman-Almashanu, Marilyn Safran, Naomi Rosen, Orit Shmueli, Maxim Shklar, Michael Shmoish, and Doron Lancet

Weizmann Institute of Science

The GeneCards compendium of human genes sifts, integrates and highlights information from diverse worldwide resources. With newly added features including pathways, classifications, EST analyses, and semi-automated quality assurance tools, the GeneCards suite of databases provides researchers with a powerful platform for profound understanding of gene function, expression and mutual interactions.

71. Identification of Transcriptional Programs along Defined Stages of Human Carcinogenesis

Tabach Yuval, Milyavsky Michael1, Zuk Or, Domany Eytan, Rotter Varda and Pilpel Yitzhak

Dept of Molecular Cell Biology, Dept of Physics of Complex Systems and Dept of Molecular Genetics, WIS

To understand tumorigenesis, we developed a stepwise model which combines spontaneous alterations with introduced modifications. Normal cells were cultured for 600 days and eventually gave rise to tumors. GenChip-analysis at defined points along this process, coupled with promoter study, revealed unexpected links between expression patterns, transcription factors and cancer development.

72. A Global View of the Selection Forces in the Evolution of Yeast Cis-regulation

Amos Tanay, Irit Gat-Viks and Ron Shamir

School of computer science, TAU

The interaction between transcription factors and their DNA binding sites is key to understanding gene regulation. By performing a genome-wide study of the evolutionary dynamics in yeast promoters, we provide a global view of the selection forces on transcription factor binding sites and obtain new insights about their functionality.

73. Electronic Micro-Dissection of Gene Expression in Cancer

D. Tsafrir[1], I. Tsafrir[1], M. Sheffer[1], T. Shay[1], D. Notterman[2] and E. Domany[1].

[1]Physics of complex systems, WIS, [2]RWJ Medical School

A problem in the analysis of microarray-based gene expression data is separating genes causally involved in a complex disease from innocent bystanders, whose expression levels appear altered due to secondary causes. We employ a novel exploratory analysis methodology to address this issue, using colon cancer as a model system.

74. Uncovering Structures by Self-Organization

Tsafrir, I., D. Tsafrir, L. Ein-Dor, O. Zuk and E. Domany

Dept of Physics of Complex Systems, WIS

Sorting Points Into Neighborhoods (SPIN) is a novel unsupervised method for data organization and visualization that imposes a linear ordering by iterative permutations. SPIN's intuitively color-coded image of a reordered distance matrix is shown to uncover elongated structures that can be interpreted as continuous variables in the data.

75. A Systematic Search for snoRNA Molecules in Trypanosomatids (GAS)

Shai Uliel, Xue-Hai Liang, Tirza Doniger, Shulamit Michaeli and Ron Unger

Faculty of Life Science, Bar-Ilan University, Ramat-Gan, Israel

A systematic search, based on three complementary approaches: Comparative genomics, tandem repeat finding, and specific motifs finding was conducted in order to identify snoRNA molecules in Trypanosome. About 120 C/D and H/ACA RNA molecules, organized in 19 clusters, were detected. Further developments are ongoing in order to identify novel ncRNA.

76. Two-Step Quantum Clustering Algorithm and its Application to Gene Expression Data of Prenatal Stressed Rats

Roy Varshavsky[1], Yoel Bogoch[1], Marta Weinstock-Rosin[2], Michal Linial[1] and David Horn[3]

[1]Dept of Biological Chemistry, HUJI, [2]School of Pharmacology, HUJI, [3]School of Physics and Astronomy, TAU

We applied a two-step clustering algorithm on microarray dataset that was taken from controlled and prenatal stressed rats. The algorithm first reduces the dataset size by the SVD method and then clusters similar entities (samples or genes) together. We succeeded to (1) classify the two major groups of the experiment and (2) identify groups of 'influential' genes.

77. ATRHunter: A Tool for Finding Approximate Tandem Repeats

Ydo Wexler, Zohar Yakhini, Yehezkel Kashi and Dan Geiger

Technion

We present an efficient tool for detecting approximate tandem repeats in genomic sequences. The algorithm is based on a flexible statistical model which allows a wide range of definitions of approximate tandem repeats. The ideas and methods underlying the algorithm are described and its effectiveness on genomic data is demonstrated.

78. Network Motifs in Integrated Cellular Networks of Transcription Regulation and Protein-Protein Interaction

Esti Yeger-Lotem[1,2] , Shmuel Sattath[1], Nadav Kashtan[3], Shalev Itzkovitz[3], Ron Milo[3], Ron Y. Pinter[2], Uri Alon[3], and Hanah Margalit[1]

[1]Dept of Molecular Genetics and Biotechnology, Faculty of Medicine, HUJI [2]Dept of Computer Science, Technion, [3]Dept of Molecular Cell Biology and Physics of Complex Systems, WIS

Genes and proteins generate complex molecular circuitry that enables the cell to process information and respond to stimuli.
We search this network of interactions for composite network motifs – characteristic network patterns consisting of both transcription regulation and protein-protein interactions that recur significantly more often than in random networks.

79. Prediction of Multi-Molecular Assemblies and Protein Structures by Multiple Combinatorial Docking

Inbar Yuval, Ruth Nussinov and Haim J. Wolfson

Tel Aviv University

We have developed an algorithm that extends the application of pairwise docking to multi-molecular assemblies. We apply it to predict both quaternary structures of oligomers and multi-proteins complexes. Moreover, adapting the algorithm to consider backbone connectivity, we also show that it may be useful in the prediction of protein tertiary structures. This application was widely tested showing highly accurate predictions and robustness for structural distortion of the input subunits.

80. Bioinformatic, In-Vitro Expression and Proteomic Analyses of the B. Anthracis Genome for Identification of Novel Vaccine Candidates

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Dept of Biochemistry and Molecular Genetics, Israel Institute for Biological Research, Ness-Ziona

In-silico analysis of the B. anthracis draft genome, aimed at identification of potential vaccine candidates and virulence- related genes, was carried out. Preliminary annotation, cellular location predictions, and comparative genomics resulted in identification of ~240 putative candidates; which were verified through functional genomic studies comprising of high- throughput in-vitro ORF expression and proteomic analysis of B. anthracis membrane proteins.