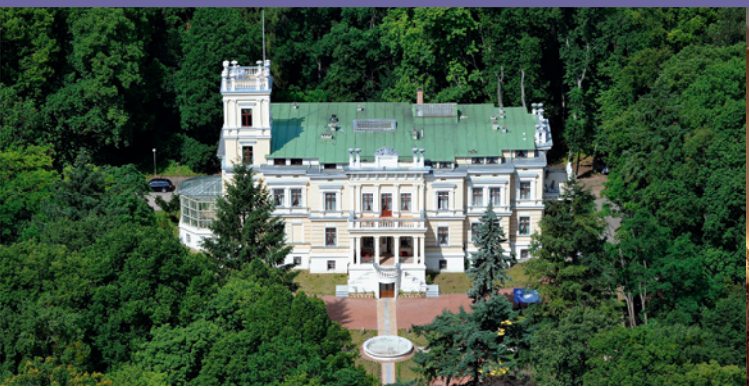
IV EURO WG

Conference on Operational Research
in Computational Biology, Bioinformatics and Medicine



Poznan – Biedrusko (Poland)
26-28 June, 2014

EURO
The Association of European
Operational Research Societies

POLITECHNIKA POZNAŃSKA
POZNAN UNIVERSITY OF TECHNOLOGY

Dear Participants,

Welcome to the 4th Conference of the EURO Working Group of Operational Research on Computational Biology, Bioinformatics and Medicine. EWG CBBM was established with numerous founding members at a satellite meeting of the EURO XXI 2006 Conference in Iceland, July 2-5, 2006. Soon after its foundation, the EWG CBBM organized and supported many events. One of the most important events that EWG CBBM organizes is the EWG CBBM conference. After successful completion of the first three conferences (Prague, Czech Republic, 8 July 2007; Rome, Italy, 15-17 September 2008, Nottingham, United Kingdom, 13-15 September 2012) we are happy to have you for another exciting conference in Poznan. The objective of EWG CBBM is to promote and to facilitate communication links among European (and other) researchers working in areas of operational research in computational biology, bioinformatics and medicine. Therefore, this conference is a keystone event that brings established researchers and leaders in the research community together with young researchers in an intellectually stimulating atmosphere. In addition to our distinguished invited speakers and contributed talks, the local organizing committee prepared an excellent social program.

On behalf of the Managing Board of EWG CBBM, I would like to express my sincere thanks to everyone who contributed to the success of 4th Conference of the EURO Working Group of Operational Research on Computational Biology, Bioinformatics and Medicine.

Metin Turkay
Chair, EWG CBBM

PROGRAM COMMITTEE

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Tomasz Żok	(PUT University, Poland)

CONTENTS

POZNAN UNIVERSITY OF TECHNOLOGY – technology in a positive climate

Poznan University of Technology (PUT) grew out of the State School of Mechanical Engineering which was established in 1919. Currently, it is one of the leading technical universities in Poland which has become one of the most recognized landmarks of the region and even the whole country. To a large extent this was possible due to the renowned pragmatism and reliability of the people of Poznan.

The autonomous state institution consisting of ten faculties provides teaching for about 21 thousand students. PUT offers Bachelor, Master and Doctorate courses in Polish and English, within many fields of science, most prestigious being Computer Science and Bioinformatics. Moreover there are postgraduate courses and workshops for people interested in updating their technical knowledge. 12 hundred academic staff members do research and run educational tasks. To work and study at such a prestigious university as PUT, one has to effectively combine conceptual impetus, the pragmatism of an engineer, as well as interpersonal skills.

We do not retreat from the world: technological development is accompanied by the greatest respect for human beings, protection of the natural environment and sustainable economic development. We have an open-minded approach to science. PUT plays an important role in international scientific life: we take an active part in scientific exchange and international projects and cooperate with many companies and research institutions both in Poland and abroad. We combine the development of the latest scientific disciplines with the transfer of this knowledge and technology into the practical dimension. We have close relationship with business. Our partners' encouragement and advice help us not only to adjust our educational programs so as to meet the requirements of the market, but primarily, to make our position among other universities stronger.

SCHEDULE OVERVIEW

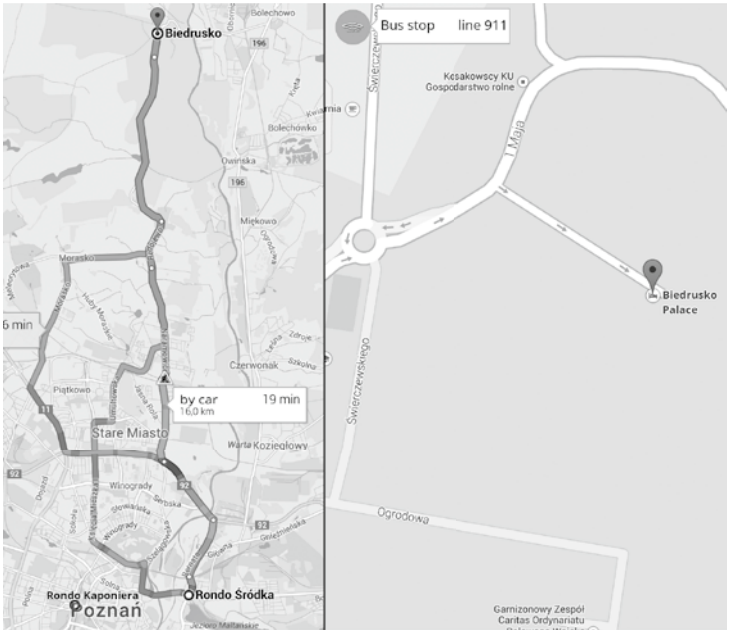
Wednesday June 25th, 2014	**19:00-21:00**	welcome reception
Thursday June 26th, 2014	**08:45-09:00**	opening
	09:00-10:40	session I (chair: J. Blazewicz)
	10:40-11:00	coffee break
	11:00-12:40	session II.A (chair: R.W. Adamiak) and II.B (chair: P. Formanowicz)
	12:40-14:00	lunch
	14:00-15:40	session III (chair: K. Ecker)
	15:40-16:00	coffee break
	16:00-17:15	session IV.A (chair: A. Swiercz) and IV.B (chair: P.Bertolazzi)
	19:00	dinner
Friday June 27th, 2014	**09:00-10:40**	session V (chair: G. Felici)
	10:40-11:00	coffee break
	11:00-12:15	session VI.A (chair: M. Szachniuk) and VI.B (chair: P. Lukasiak)
	12:15-14:00	lunch
	14:00-18:30	social event (trip)
	19:00	conference dinner
Saturday June 28th, 2014	**09:00-10:40**	session VII (chair: M. Turkay)
	10:40-11:00	coffee break
	11:00-12:40	session VIII.A (chair: P. Wojciechowski) and VIII.B (chair: C. Oguz)
	12:40-13:00	closing
	13:00-14:30	lunch

LOCATION AND TRANSPORTATION

CONFERENCE VENUE

The Conference will be held at the 130-year-old neo-renaissance Biedrusko Palace.

Biedrusko Palace (Zamek Biedrusko)
1 Maja 82
62-003 Biedrusko (near Poznan), Poland
Phone: Piotr (+48 500 188 120), Marta (+48 512 313 361)
Website: www.zamekbiedrusko.pl



HOW TO REACH THE VENUE BY PUBLIC TRANSPORT

from Poznan Airport

Take bus L from the Airport to Rondo Kaponiera
Take bus 63 from Rondo Kaponiera to Dworzec Śródka (bus station)
Take bus 911 from Dworzec Śródka to Biedrusko/Park

from Poznan Train Station

Take tram 6 from Most Dworcowy to Rondo Śródka
Take bus 911 from Dworzec Śródka (bus station) to Biedrusko/Park

from any place in Poznan

First one should reach Dworzec Śródka (bus station).
From Dworzec Śródka take bus 911 to Biedrusko/Park.
The schedule for bus 911 from Poznan/Dworzec Śródka is avaiable here:
http://www.mpk.poznan.pl/component/transport/911SRDW22/#MpkBoard

The other possibility is to take a taxi which is more convenient and faster but more expensive.

By car from Rondo Śródka, Poznan

See map on page 8

Conference transport

Conference organizers can organize transport from Poznan Airport or Poznan Train Station directly to Biedrusko Palace for groups only.

REGISTRATION

Conference materials will be provided upon check-in at our registration desk. You can check in to the conference at the reception on Wednesday and at the conference venue on Thursday and Friday. The registration desk working hours:
Wednesday: 17:00-21:00
Thursday: 8:30-18:00
Friday: 8:30-13:00
Saturday: 8:30-13:00
Last-minute changes to the conference program will be posted at the registration desk. If you need help with anything please also report to the registration desk.

Poznan

There is no way to not love Poznan. Everyone who once came here to study, see monuments, taste Poznan lifestyle and cuisine will be under the spell of the city. Because Poznan, the cultural and economic capital of the Greater Poland is the dream city for resourceful, active, full of passion, and wanting to live intensively people. Beautiful and full of green areas, the city magnetizes both students and tourists.

Capital of the Greater Poland is famous for historic Old Town with perfectly renovated houses, numerous restaurants, cafes where the social life flourishes till the late evening hours. Doing sightseeing, students and tourists shouldn't omit such places like: the Town Hall, Basilica of Our Lady of Perpetual Help and St. Mary Magdalene in Poznan (called also Poznan fara), Ostrów Tumski, or the Imperial Castle. Around the city there is the rail trail composed of 7 rail trails that meet in the city center.

A great prestige has the International Theater Festival of Malta, which attracts representatives from many countries of the world. On the Malta Regatta Course the World Cup, European and World Championship in rowing and canoeing are held frequently. Poznan is also famous for its International Fair. Stary Browar is an interesting shopping, art and business centre. It was elected by ICSC as the one of the most beautiful shopping centres in the world.

Poznan has got an international airport Ławica. Near Poznan there are also: a military airport Poznan-Krzesiny (where F16 fighters are stationed) as well as two sport airdromes. Tourists and students spend their free time in places like: Malta Lake, Botanical Garden, the new zoo, Wilson park, Sołacki park, Citadel, Morasko, and in numerous pubs, music clubs, cafes, or discoes.

Biedrusko

Biedrusko is a village near Poznan in the administrative district of Gmina Suchy Las. It lies on the Warta river bank. The first information about Biedrusko comes from the 14th century. It is the centre of a large military training area, which was set up by the German Army at the beginning of the 20th century, and taken over by the Polish army after World War I.
Biedrusko Palace was built in the years 1877-1880 in the neoclassical style. It was built by architect Louis Hunh for Otto Albrecht von Treskow. For many years housed the garrison club (casino). The palace has very interesting location in the nature park on a hill near Warta river.

SOCIAL PROGRAM

Wednesday, June 25th, 2014 at 19:00

Welcome Reception in the cellars of Biedrusko Palace

We are looking forward to seeing you in Poznan-Biedrusko! Our welcome reception on June 25th will take place in the atmospheric cellars of Biedrusko Palace – former military casino that remembers Albrecht von Treskov, first owner of the palace, with his gambling affairs, a place that witnessed military councils and heard countless stories of Polish and Prussian soldiers.

Thursday, June 26th, 2014 at 14:00

Guided Tour of the Polish State beginnings

On Thursday afternoon, we will meet in front of Biedrusko Palace and take a bus tour to Lednica. The tour will give a chance to discover the historic origins of Poland. We will visit the Museum of the First Piasts, located on the island with relics of residential and sacral stone architecture from the times of Mieszko I – the first ruler of the Polish state (10th century) and Boleslaw Chrobry (Boleslaus the Valiant) – the first king of Poland (10th/11th century). We will see a reconstruction of the typical Wielkopolska village with diverse architectural structures from the 17th to 20th centuries. At 16:30 we will enjoy traditional Polish drinks and snacks.

Friday, June 27th, 2014 at 19:00

Conference dinner at Biedrusko Palace restaurant

On Friday at 19:00, we will start our conference dinner at Biedrusko Palace restaurant, greeted by the Folk Dance Ensemble Chludowianie. Next, we will enjoy an evening with a taste of Polish summer and live music completing an atmosphere of the palace feast. Food and drinks are included in the conference fee.

SESSION OVERVIEW

Thursday, 26th June, 2014

Stream	Session	Time	Speaker	Title
		chair:	**Jacek Blazewicz**	
	I	09:00-09:50	**Eric Westhof**	Constraints and Limits Due to Base Tautomerism in Ribosome Decoding Fidelity
	I	09:50-10:15	**Michal Startek**	TRANScendence: a Web-Based Transposon Mining and Activity Chronology Reconstruction Tool
	I	10:15-10:40	**Eva Lee**	Strategies for Predicting the Immunity of Vaccines
		chair:	**Ryszard W. Adamiak**	
A	II	11:00-11:25	**Kamil Kwarciak**	Tabu Search Algorithm for Classical and Isothermic DNA Sequencing by Hybridization with Partial Information about Repetitions
A	II	11:25-11:50	**Klaus Ecker**	Graphlet Method for Improving the Prediction of Functionally Related Genes
A	II	11:50-12:15	**Liana Amaya Moreno**	Exploring Genetic Networks with Time-Discrete Dynamics
A	II	12:15-12:40	**Marcin Radom**	APetri Net Based Model of Interleukin-18 Involvement in Atherosclerosis
		chair:	**Piotr Formanowicz**	
B	II	11:00-11:25	**Giulia Fiscon**	A New Greedy Randomized Procedure for the Feature Selection Problem
B	II	11:25-11:50	**Michal Kierzynka**	Graph Construction for the Whole Genome Assembly Problem
B	II	11:50-12:15	**Wojciech Frohmberg**	New Approach to De Novo Assembly of a Long Genome
B	II	12:15-12:40	**Marek Chlopkowski**	High-Order Statistical Compressor for Long-Term Storage of DNA Sequencing Reads
		chair:	**Klaus Ecker**	
	III	14:00-14:50	**Katarzyna J. Purzycka**	RNAComposer. Challenges in Modelling Three-Dimensional Structures of Large RNAs
	III	14:50-15:15	**Tomasz Ratajczak**	RNAlyzer - a Web Server for Computational Quality Evaluation of RNAs
	III	15:15-15:40	**Tomasz Zok**	An Algorithm to Extract RNA Secondary Topology from the 3D Structure

Thursday, 26th June, 2014

Stream	Session	Time	Speaker	Title
		chair:	**Aleksandra Swiercz**	
A	IV	16:00-16:25	**Anna Gogolinska**	Petri Nets Formalism Facilitates Analysis of Complex Structural Data
A	IV	16:25-16:50	**Shabbar Naqvi**	Modelling Classification of Breast Cancer Grading with Type-ll Fuzzy Sets and Spectral Data
A	IV	16:50-17:15	**Adam Kozak**	A Role of Hemojuvelin in Iron Metabolism Modeled and Analyzed by Petri Net Approach
		chair:	**Paola Bertolazzi**	
B	IV	16:00-16:25	**Agnieszka Mickiewicz**	AmiRNA Designer - a New Method of Artificial miRNA Design
B	IV	16:25-16:50	**Natalia Szostak**	Sorting Signals Targeting mRNA into Hepatic Extracellular Vesicles
B	IV	16:50-17:15	**Celia Cintas**	Automatic Landmarking App for Bioanthropology

Friday, 27th June, 2014

Stream	Session	Time	Speaker	Title
		chair:	**Giovanni Felici**	
	V	09:00-09:50	**Giuseppe Lancia**	20 Years of Haplotyping: an Overview
	V	09:50-10:15	**Luigi De Giovanni**	A Column Generation Approach for Pure Parsimony Haplotyping
	V	10:15-10:40	**Emanuel Weitschek**	Rule Based Analysis of Genomic Sequences: a Viral Case Study
		chair:	**Marta Szachniuk**	
A	VI	11:00-11:25	**Maria C. De Cola**	Orderly Colored Paths for the RNA Assignment Problem in 3D NMR Spectra
A	VI	11:25-11:50	**Mehmet S. Apaydin**	Automating the Usage of Unambiguous NOEs in Nuclear Vector Replacement for NMR Protein Structure-Based Assignments
A	VI	11:50-12:15	**Rupak Pal**	Modeling Conformational Preferences of Modified Uridines with Polarizable Force Fields
		chair:	**Piotr Lukasiak**	
B	VI	11:00-11:25	**Rafal Jakubowski**	Towards Efficient Docking of Chemical Compounds into Protein Cavities
B	VI	11:25-11:50	**Mehmet Tardu**	Structure Based Drug Design for SIRT6
B	VI	11:50-12:15	**Seref Gul**	Designing Small Organic Molecules to Regulate Circadian Clock in Mammals

Saturday, 28th June, 2014

Stream	Session	Time	Speaker	Title
		chair:	**Metin Turkay**	
	VII	09:00-09:50	**Marek Figlerowicz**	Copy Number Variations in Plant Genomes
	VII	09:50-10:15	**Giovanni Felici**	Optimal Discretization of Continuous Features for Mining Gene Expression Data
	VII	10:15-10:40	**Valentina Fustaino**	Integrated Analysis of DNA Copy Number and Gene Expression Data in Lung Cancer Models of Resistance to Targeted Therapy
		chair:	**Pawel Wojciechowski**	
A	VIII	11:00-11:25	**Tomasz Prejzendanc**	ModeLang - Controlled Natural Language for Describing Viral Infection Models
A	VIII	11:25-11:50	**Marta Kulik**	Structure and Electrostatics Based Analysis of Ribosomal RNA Complexes with Aminoglycosides
A	VIII	11:50-12:15	**Malgorzata Szelag**	In Silico Comparative Modeling of STAT Proteins as a Novel Approach in Finding Specific Compounds of Functional Inhibition
A	VIII	12:15-12:40	**Gerhard- Wilhelm Weber**	Reconstruction of Gene-Environment Networks Under Uncertainty
		chair:	**Ceyda Oguz**	
B	VIII	11:00-11:25	**Daniele Soria**	Breast Cancer Classification: from Consensus Clustering to Fuzzy Logic
B	VIII	11:25-11:50	**Martin Riedel**	Classification of Salmonella Serovars Based on Laser-Diffuse-Light-Images Using Learning Vector Quantizers
B	VIII	11:50-12:15	**Weronika Wronowska**	Computational Modeling of Sphingolipid Metabolism in Cancer and Neurodegeneration
B	VIII	12:15-12:40	**Piotr Gawron**	A Tool for Visualization and Analysis of Molecular Networks on the Example of Parkinson's Disease

ABSTRACTS

CONSTRAINTS AND LIMITS DUE TO BASE TAUTOMERISM IN RIBOSOME DECODING FIDELITY

Eric Westhof
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The natural bases of nucleic acids can form a great variety of base pairs with at least two hydrogen bonds between them. They can be distributed in twelve main families, with the Watson-Crick family being one of them. The non-Watson-Crick base pairs can assemble into RNA modules that form recurrent, rather regular, building blocks of the tertiary architecture of folded RNAs. Some of the base pairs are isosteric between them, meaning that the distances between the C1' carbon atoms are very similar. The isostericity of Watson-Crick pairs forms the basis of RNA helices and of the resulting RNA secondary structure. The weak isostericity among non-Watson-Crick pairs leads to higher sequence conservation during evolution of homologous RNAs and, consequently, to greater difficulties in extracting 3D information from sequence analysis. Accurate recognition of Watson-Crick base pairs is a necessity during replication, transcription, and translational decoding. Polymerases and ribosomes exploit the isosteric geometries for recognition of Watson-Crick pairs on their minor groove edges. Although nucleic acids have a strong preference for one tautomer form, guaranteeing fidelity in their hydrogen bonding potential, base pairs observed in recent crystal structures of polymerases and ribosomes are best explained by an alternative base tautomer, leading to the formation of base pairs with Watson-Crick-like geometries. Several of these pairs with Watson-Crick-like geometries increase the number of isosteric pairs between complementary bases and cannot be distinguished from theminor groove edge. These observations set limits to geometric selection in molecular recognition of complementary Watson-Crick pairs for fidelity in replication and translation processes.

1 Fritsch, V., and Westhof, E. (2009). Molecular adaptation in RNA complexes. Structure 17, 784-786.
2 Demeshkina, N., Jenner, L., Westhof, E., Yusupov, M., and Yusupova, G. (2012). A new understanding of the decoding principle on the ribosome. Nature 484, 256-259.

TRANSCENDENCE: A WEB-BASED TRANSPOSON MINING AND ACTIVITY CHRONOLOGY RECONSTRUCTION TOOL

Michał Startek [1)], **Dariusz Grzebelus** [2)], **Anna Gambin** [3)]

[1)] Faculty of Mathematics, Informatics, and Mechanics, University of Warsaw, Poland

[2)] Agricultural University of Cracow, Poland

[3)] Institute of Informatics, Universty of Warsaw, Poland

ABSTRACT

In this talk we shall present TRANScendence: a web-based tool, based on the REPET software suitem enabling the analysis of genomes in search for transposons. The transposons are mined in a de-novo fashion, based on self-similarity of the analysed genome. The found transposons are clustered into families, and family activity chronology is reconstructed from the interruption graph, using a heuristics-based approach to find approximate solution to the NP-complete problem.

STRATEGIES FOR PREDICTING THE IMMUNITY OF VACCINES

Eva Lee
Center for Operations Research in Medicine and HealthCare,
Georgia Institute of Technology, USA

ABSTRACT

The ability to successfully predict the immunity and effectiveness of vaccines would facilitate the rapid evaluation of new and emerging vaccines, and the identification of individuals who are unlikely to be protected by a vaccine. In this talk we present a discrete support vector machine classification model and feature selection algorithm that are applied to the gene signatures to identify discriminatory sets and establish the classification rule that can classify the T cell response and the antibody response induced by the vaccine. This work is joint with Emory Vaccine Center.

TABU SEARCH ALGORITHM FOR CLASSICAL AND ISOTHERMIC DNA SEQUENCING BY HYBRIDIZATION WITH PARTIAL INFORMATION ABOUT REPETITIONS

Kamil Kwarciak [1], **Piotr Formanowicz** [2]

[1] Poznan University of Technology, Poland

[2] Institute of Computing Science, Poznan University of Technology, Poland

ABSTRACT

DNA sequencing by hybridization is one of the approaches to determine a sequence of nucleotides DNA consists of. It is comprised of two stages. The first one is a biochemical experiment. A combinatorial problem is solved in the second stage. The problem is intractable so a tabu search heuristic has been proposed. It solves the problem with positive and negative errors. Input data may come from classical or isothermic DNA chips. Moreover, a partial information about repetitions in an analysed DNA sequence is taken into account. Using this additional data leads to better sequence reconstruction.

GRAPHLET METHOD FOR IMPROVING THE PREDICTION OF FUNCTIONALLY RELATED GENES

Klaus Ecker [2], **Marek Blazewicz** [1]

[1] Institute of Computing Science, Poznan University of Technology, Poland

[2] Technische Universität Clausthal, Germany

ABSTRACT

The aim of the work was to create an algorithm capable of performing automatic identification and marking of functional modules of genes and proteins out of multiple datasets. Such approach allows minimizing the influence of the statistical noise in the results.

In order to determine the local network similarity, we have applied the idea of node graphlets, which measures the similarity of network topologies. We have proven the method to be effective for finding functionally related genes in biological networks with the use of the hypergeometrical statistical test.

EXPLORING GENETIC NETWORKS WITH TIME-DISCRETE DYNAMICS

Liana Amaya Moreno [1], **Ozlem Defterli** [2],
Armin Fügenschuh [1], **Gerhard-Wilhelm Weber** [3]
[1] Department of Mechanical Engineering,
Helmut Schmidt University, Germany
[2] Department of Mathematics and Computer Science, Cankaya
University, Ankara, Turkey
[3] Institute of Applied Mathematics,
Middle East Technical University, Turkey

ABSTRACT

We propose a new method to explore the characteristics of genetic networks whose dynamics are described by a linear discrete dynamical model. First we formulate and solve a parameter estimation problem in order to obtain the influence coefficients of the genes. We then use ideas from Vester's Sensitivity Model to understand the interactions among the genes and their role in the system. The method identifies prominent outliers. Numerical examples for different datasets containing mRNA transcript levels during the cell cycle of budding yeast are presented.

A PETRI NET BASED MODEL OF INTERLEUKIN-18 INVOLVEMENT IN ATHEROSCLEROSIS

Marcin Radom [1)], **Dorota Formanowicz** [2)], **Piotr Formanowicz** [1)]
[1)] Institute of Computing Science, Poznan University of Technology, Poland
[2)] Poznan University of Medical Sciences, Poland

ABSTRACT

Interleukin-18, identified as co-stimulatory factor for interferon-gamma synthesis, acts in both acquired and innate immunity, making it a good inflammatory marker in atherosclerosis. It is produced mainly by monocytes/macrophages with potent activities on both macrophages and T-cells being involved in the development of atherosclerotic plaque and its complications.

The process of atherosclerosis with particular emphasis on the role of IL-18 has been modeled using Petri nets. Formal properties of the model have been analyzed, in particular t-invariants and MCT-sets.

A NEW GREEDY RANDOMIZED PROCEDURE FOR THE FEATURE SELECTION PROBLEM

Giulia Fiscon [1], **Emanuel Weitschek** [2], **Giovanni Felici** [3], **Paola Festa** [4]

[1] Department of Computer, Control, and Management Engineering Antonio Ruberti, Sapienza University of Rome and IASI of The National Research Council (CNR), Italy

[2] Department of Engineering, Roma Tre University, Italy

[3] Istituto di Analisi dei Sistemi ed Informatica, Consiglio Nazionale delle Ricerche, Italy

[4] Dept. of Mathematics and Applications, University of Napoli Federico II, Italy

ABSTRACT

Feature Selection (FS) arises in data analysis to reduce the dimension of large data. We focus on integer programs to model FS problems, describe a variant with its mathematical properties, and design a solution strategy whose performances are compared with those of well known FS methods. Our method is suitable for high-dimensional data where an exact solution approach results is unpractical. The experiments use randomly generated datasets and are designed to show the efficacy of the FS model and of the heuristics. Finally, our method has been successfully applied to real biological problems.

GRAPH CONSTRUCTION FOR THE WHOLE GENOME ASSEMBLY PROBLEM

Michal Kierzynka [1], **Wojciech Frohmberg** [1],
Pawel Wojciechowski [2], **Jacek Blazewicz** [1]
[1] Institute of Computing Science, Poznan University of Technology, Poland
[2] Poznan University of Technology, Poland

ABSTRACT

We propose a novel approach to the DNA de-novo assembly of big data sets coming from Next Generation Sequencing. The talk will cover the topic of detection so called promising pairs by employing the potential of alignment-free sequence comparison. The novelty of our solution lies in a special sorting technique that puts similar sequences close to each other. With such information the graph model is constructed with the use of an ultra fast sequence comparison on GPUs. The results of tests carried out on real data sets will be presented to demonstrate the accuracy of the algorithm.

NEW APPROACH TO DE NOVO ASSEMBLY OF A LONG GENOME

Wojciech Frohmberg
Institute of Computing Science, Poznan University of Technology, Poland

ABSTRACT

As next generation sequencing is becoming cheaper and more available more and more sequenced data need to be processed, in process of DNA assembly, as fast as only possible.
On the other hand, assembly still needs to be more accurate to be able to answer many biological questions and confirm medical hypothesies. To satisfy these demands we have implemented a method utilizing overlap-layout-consensus strategy in order to ensure high quality results and new technologies, in particular, GPU acceleration to produce these results efficiently.

HIGH-ORDER STATISTICAL COMPRESSOR FOR LONG-TERM STORAGE OF DNA SEQUENCING READS

Marek Chłopkowski, **Marta Kasprzak**
Institute of Computing Science, Poznan University of Technology, Poland

ABSTRACT

We present a specialized compressor designed for efficient data storage of FASTQ files produced by Illumina DNA sequencers. Since the method has been optimized for compression quality, it is especially suitable for long-term storage and for big research institutes producing data counted in petabytes. The compressor uses high-order statistical models for range encoding, similar to Markov models but with the whole input used to build the symbol context. Compression of reads is done in LZ-style with the use of 6-8th order model, while bases' scores are encoded with 3rd order model.

RNACOMPOSER. CHALLENGES IN MODELLING THREE-DIMENSIONAL STRUCTURES OF LARGE RNAS

Katarzyna J. Purzycka
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Z. Noskowskiego str. 12/14,61-704 Poznan, Poland
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Understanding the numerous functions that RNAs play in living cells depends critically on informative three-dimensional structures. However, it is difficult to assess 3D structures of RNAs experimentally. Structures determined by NMR spectroscopy and X-ray crystallography are limited by the size or structural flexibility of the RNA. We recently developed RNAComposer [1] – a machine translation-based method for automated prediction of RNA three-dimensional structure from a user-defined secondary structure model. The method was evaluated using a representative benchmark set of 40 RNAs with different complexities. We estimated the scope and quality of the predicted 3D models in terms of the secondary structure topology conservation, stereochemical properties, energy, precision and accuracy. The quality of the input 2D structure is critical to obtain an accurate 3D structure. The in silico prediction of the RNA secondary structure is advanced and can be strengthened by incorporating constraints from chemical probing. However, defining precise secondary structures for 3D structure prediction remains challenging. Namely, multiple RNA conformations, pseudoknots and long-range interactions are important to evaluate. Furthermore, even though RNAComposer can generate a large ensemble of tertiary structures within minutes, biologically relevant structures should be verified by independent analyses. During the presentation, I will introduce RNAComposer and discuss approaches we are taking to address difficulties arising from the prediction of 3D structures of large RNAs.

Adamiak and Blazewicz group was supported by 2012/06/A/ST6/00384 grant from National Science Centre, Poland.

[1] M. Popenda, M. Szachniuk, M. Antczak, K. J. Purzycka, P. Lukasiak, N. Bartol, J. Blazewicz, and R. W. Adamiak. 2012 Automated 3D structure composition for large RNAs. Nucleic Acids Res, 40 (14):e112.

RNALYZER – WEB SERVER FOR COMPUTATIONAL QUALITY EVALUATION OF RNAS

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ABSTRACT

Demand for methods and tools to evaluate artificial models of RNA 3D structures is growing. Here we present RNAlyzer, a web server for comparative evaluation of RNA structures.

Idea behind RNAlyzer is to use well known quality measures such as RMSD or DI and apply them to evaluate models at different levels of precision defined by user. These levels of precision are achieved by comparing sets of atoms in a successively increasing range between models and reference structure. This approach allows identifying well and poorly predicted regions of the model in addition to its overall quality.

AN ALGORITHM TO EXTRACT RNA SECONDARY TOPOLOGY FROM THE 3D STRUCTURE

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ABSTRACT

Secondary structure plays an important role in RNA structural biology and bioinformatics. It is obtained through biochemical and chemical probing experiments or by means of extraction from the 3D structure. The latter approach is very fast and easy to use. In some cases – when the experimental validation is impossible – it is the only way to proceed, e.g. when the tertiary structure was predicted in silico. We present RNApdbee – a tool to extract RNA secondary structure from PDB files. It can process even very complex structures and provides the most clear textual and graphical outputs.

PETRI NETS FORMALISM FACILITATES ANALYSIS OF COMPLEX STRUCTURAL DATA

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ABSTRACT

Petri nets (PNs) are mathematical modeling languages. PN has a simple form of a bipartite graph with two types of nodes: places and transitions. Molecular Dynamics simulations (MD) are very time consuming calculations of time evolution of proteins. Unfortunately the MD output files are hard to analyze. In this work we create PNs based on a trajectory produced during MD simulation. Few algorithms were designed, one will be presented in detail. In the algorithm one place of PN corresponds to one amino acid from the MD. This PN approach may facilitate analysis of MD data.

MODELLING CLASSIFICATION OF BREAST CANCER GRADING WITH TYPE-II FUZZY SETS AND SPECTRAL DATA

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ABSTRACT

Breast cancer is one of the most commonly occurring cancers among women throughout the world including the U.K. After the diagnosis of the disease, classification of cancer grading is very important in estimating the long term survival. One of the widely accepted grading methods is the Nottingham Grading System (NGS) which is based on the microscopic evaluation of tumour cells by the histopathologists. In current work, we have used Type-II fuzzy logic in combination with FTIR spectral data to create a model that is useful in breast cancer grade classification.

A ROLE OF HEMOJUVELIN IN IRON METOBALISM MODELED AND ANALYZED BY PETRI NET APPROACH

Adam Kozak [1)], **Dorota Formanowicz** [2)], **Tomasz Głowacki** [1)], **Marcin Radom** [1)], **Piotr Formanowicz** [1)]

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ABSTRACT

Iron homeostasis mechanisms in human body depend on many factors. The most significant regulator is hepcidin which is a hormone produced in liver. It downregulates iron level by reduction of iron absorption from intestine. Hepcidin expression is affected by its coregulator hemojuvelin, inflammatory process, hypoxia, anemia and changes of iron. In this work a Petri net model of iron homeostasis regulation focused on the influence of hemojuvelin is presented. Structural analysis of the model and biological conclusions of this analysis are also presented.

AMIRNA DESIGNER – NEW METHOD OF ARTIFICIAL MIRNA DESIGN

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ABSTRACT

Artificial miRNA (amiRNA) are 21 nt RNA sequences that are absent in wild type plants. They can be introduced into the miRNA precursor-like structure and are able to influence the expression of selected genes. In this work, we present a new algorithm of amiRNA design. We have developed the new strategy to design both amiRNA and amiRNA* sequences based on the thermodynamic profiles. We have also prepared the off-target effect validation method. Our algorithm is able to generate amiRNA for organisms such as plants and animals.

SORTING SIGNALS TARGETING MRNA INTO HEPATIC EXTRACELLULAR VESICLES

Natalia Szostak [1)], **Agnieszka Rybarczyk** [1)],
Felix Royo [2)], **Marta Szachniuk** [3)], **Antonio del Sol** [4)],
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ABSTRACT

Intercellular communication mediated by extracellular vesicles has provedto play an important role in a growing number of biological processes. mRNA seems to be one of the most interesting content of these vesicles. mRNA localization depends on interactions between the cis-acting elements in the mRNA sequence and trans-acting factors, the RNA-binding proteins.

In this work, based on in silico bioinformatics tools, we have mapped a novel sequence, which may act as a zipcode for targeting mRNA into hepaticextracellular vesicles. Moreover, results of our analysis have been confirmed by a wet lab experiment.

AUTOMATIC LANDMARKING APP FOR BIOANTHROPOLOGY

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ABSTRACT

We introduce an app for automatic detection and acquisition of 2D and 3D facial landmarks, subsequent edition, data-export in several formats, and a plugin structure for adding diverse biometric algorithms such as age and sex estimation, eye color detection. This app allows solving practical data collection problems related to the handling of massive photographic databases.

Also it is aimed to improve the surveillance of external phenotypic information intended for Quantitative Genetic Analysis.

The software developed is based on open source tools and it is already available online.

20 YEARS OF HAPLOTYPING: AN OVERVIEW

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From the completion of the human genome project and from the huge amount of sequencing data nowadays available we have learned that the genetic makeup of humans is remarkably well-conserved. It is now clear that very small genomic regions that can vary from an individual to another must be responsible for the differences in the way we look. The smallest region consists of a single nucleotide and is called Single Nucleotide Polymorphism, or SNP (snip). SNPs are the predominant form of polymorphism, and they are fundamental in medical, drug-design and forensic applications.
Determining the values for a set of SNPs on the two copies of a chromosome is known as haplotyping. Haplotyping either an individual or an entire population gives rise to a set of nice and challenging combinatorial problems, which can be attacked by means of optimization techniques. These problems have been extensively studied by many researchers. In this talk, we will review the main results of this area in the past two decades, and present them in a unified setting. We will describe polynomial algorithms for some special cases, NP-hardness results for some others, and exponential (branch and bound) algorithms for still others.

A COLUMN GENERATION APPROACH FOR PURE PARSIMONY HAPLOTYPING

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ABSTRACT

We present two integer programming models for the Haplotype Inference by Pure Parsimony problem. The first model uses variables to decide the haplotype coordinates and the two haplotypes that explain each genotype, and contains quadratic constraints. By decomposition, we obtain a second linear model where all the possible haplotypes and genotype subsets are enumerated and each variable decides if a haplotype explains a genotype subset. Preliminary tests show that the linear relaxation, solved by column generation, is tight and often provides the optimal integer solution for small instances.

RULE BASED ANALYSIS OF GENOMIC SEQUENCES: A VIRAL CASE STUDY

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ABSTRACT

The analysis of genomic sequences is frequently adopted to perform automatic specimen to species assignments. Relevant results have been already obtained for animal species. Here we focus on families of viruses and present a method based on optimization algorithms to perform rule based classification of genomic sequences from these families. We present an extension designed to identify separation rules focusing on small regions of the sequences. The method is successfully applied to genomes and to gene regions of viruses and a collection of accurate classification rules are extracted.

ORDERLY COLORED PATHS FOR THE RNA ASSIGNMENT PROBLEM ON 3D NMR SPECTRA

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ABSTRACT

Starting from a 3D NMR spectrum, we build an edge-colored graph G such that a vertex is a cross-peak, and edges are colored according to the type of interaction occurred during the NMR experiment. Considering the sequence of iterations occurred as a sequence of colors to follow, we look for the orderly colored longest path (OCLP) on G. We describe two alternative IP formulations as flow problems with packing constraints, and evaluate the performance of an algorithm based on the solution of their relaxation combined with the separation of cycle inequalities in a Branch and Cut scheme.

AUTOMATING THE USAGE OF UNAMBIGUOUS NOES IN NUCLEAR VECTOR REPLACEMENT FOR NMR PROTEIN STRUCTURE-BASED ASSIGNMENTS

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ABSTRACT

Nuclear Magnetic Resonance (NMR) is one of the important experimental methods used to determine the protein structure. The bottleneck in NMR protein structure determination is assigning NMR peaks to corresponding nuclei, which is known as the assignment problem. The Structure Based Assignment (SBA) is an approach to solve the resonance assignment problem by using prior information about the protein that is obtained from a template structure. This assignment process is manually performed in many laboratories. In this work, we have developed methodologies and software to automate this process.

MODELING CONFORMATIONAL PREFERENCES OF MODIFIED URIDINES WITH POLARIZABLE FORCE FIELDS

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ABSTRACT

Reliable RNA modeling is hampered by the unavailability of accurate force field parameters for modifications in their sequence. We detected that the AMBER FF99 force field parameters proposed by Aduri et al. (JCTC,2007) and their combinations with recent revisions of the FF99 force field for RNA did not show satisfactory agreement with the experimental conformational characteristics for a set of modified uridines. We report the applicability of less extensively used but promising variants of the FF99 force field that add polarizable dipoles to atoms to simulate their conformational preferences.

TOWARDS EFFICIENT DOCKING OF CHEMICAL COMPOUNDS INTO PROTEIN CAVITIES

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ABSTRACT

Success of computer aided drug design depends on reliable parameters and data flow for new classes of prospective drugs. In our search for automated force field parameterization workflow, we have found relatively efficient way of verification of newly developed flavonoids models. A careful comparison of docking results, x-ray structures and controlled perturbations in classical minimization procedure allow us to determine "docking place convergence regions" in medically important proteins.

STRUCTURE BASED DRUG DESIGN FOR SIRT6

Mehmet Tardu, **Halil Kavakli**, **Metin Turkay**
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ABSTRACT

Mammalian Sirtuin6 (SIRT6) is a deacetylase of lysine 9 of histone H3. Recent evidence suggests SIRT6 as a key regulator of metabolism, ageing, apoptosis and DNA repair pathways. SIRT6 is thus considered an attractive therapeutic target for diseases such as cancer and neurodegenerative disorders. In this study, we performed virtual screening on a small molecule library (~7 million molecules) to find modulators of the SIRT6 enzyme activity by targeting its NAD+ substrate binding site. The compounds with minimum binding energies were selected and then analyzed according to important characteristics.

DESIGNING SMALL ORGANIC MOLECULES TO REGULATE CIRCADIAN CLOCK IN MAMMALS

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ABSTRACT

CRYptochrome is a core clock component controlling the circadian clock in mammals with 24h rhythmicity. Irregularity in the clock causes various diseases including Narcolepsy and cardiovascular diseases. In this work, we aim to find small molecules based on the 3D-structure of CRY to inhibit CRY- SCFFBXL3 interaction which induces CRY degradation, thus to control the clock rhythm and treat clock related diseases. We screened a large library (~7 million molecules) using docking. Compounds having the best binding energies were selected and analyzed according to the important characteristics.

COPY NUMBER VARIATION IN PLANT GENOMES

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Copy number variation (CNV) is a common type of polymorphism in the genomes of humans, animals and plants. CNV results from unbalanced DNA modifications, which trigger changes in the number of copies of a particular DNA sequence. Typically, copy number variants (CNVs) encompass relatively large DNA segments (from 1 kb to several Mb). In plants, the exploration of the extent and role of CNV is still just beginning. Initial genomic analyses indicate that CNV has greatly affected plant genome evolution. As in humans, also in plants multiple CNVs encompass protein coding genes, mainly the members of large families of functionally redundant genes.

OPTIMAL DISCRETIZATION OF CONTINUOUS FEATURES FOR MINING GENE EXPRESSION DATA

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ABSTRACT

In this work we consider a class of methods designed for classification and data analysis applied to the analysis of gene expression data obtained my microarray or NGS experiments. We focus on gene expression discretization, analyse the main issues related with this problem and propose an optimization model where the problem is to take into account the dependence between features and samples. An efficient solution algorithm for large problems is described, and comparisons with other discretization methods are provided. Practical results on microarray data conclude the presentation.

INTEGRATED ANALYSIS OF DNA COPY NUMBER AND GENE EXPRESSION DATA IN LUNG CANCER MODELS OF RESISTANCE TO TARGETED THERAPY

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ABSTRACT

Tyrosine Kinase iInhibitors (TKIs) constitute the most promising frontier of cancer treatment. However, the development of resistance mechanisms often makes the tumour insensitive to TKI-targeted therapy. The present work aims to identify genes and pathways involved in TKI-resistance. To this end, we developed cellular models of NSCLC and designed cellular, molecular and bioinformatics analyses. Preliminary functional enrichment analysis of genes, found consistently altered in resistant cell lines, indicates their involvement in key biological processes.

MODELANG – CONTROLLED NATURAL LANGUAGE FOR DESCRIBING VIRAL INFECTION MODELS

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ABSTRACT

Definition of computational models is often facing issues with mutual understanding when it requires a close cooperation between specialists of different scientific areas, like biologists and mathematicians. ModeLang is the language that is designed by us to make that cooperation much easier. As a Controlled Natural Language it is making specialists able to use slang that is common for their profession, allowing casual notes to become input data for the model. After parsing of the model it can be later used as a library for simulator, or it can be converted into some widely used formats.

STRUCTURE AND ELECTROSTATICS BASED ANALYSES OF RIBOSOMAL RNA COMPLEXES WITH AMINOGLYCOSIDES

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ABSTRACT

Aminoglycoside antibiotics bind to the ribosomal RNA (A site) and affect bacterial protein synthesis. Various modifications of these antibiotics have been tested to improve their affinity. However, many of these compounds were suggested and synthesized based on the trial-and-error method. We have analyzed various aminoglycosides and their targets using the multi-pole expansion approach to estimate the electrostatic interactions. A few repeatable patterns in which water molecules mediate the hydrogen bonds between the aminoglycoside and RNA were observed and used to suggest new A site binders.

IN SILICO COMPARATIVE MODELING OF STAT PROTEINS AS A NOVEL APPROACH IN FINDING SPECIFIC COMPOUNDS OF FUNCTIONAL INHIBITION

Małgorzata Szeląg [1)], **Anna Czerwoniec** [2)],
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ABSTRACT

Signal transducers and activators of transcription (STATs) facilitate action of cytokines, growth factors and pathogens. STAT activation is mediated by a highly conserved SH2 domain, which interacts with phosphotyrosine (pTyr) motifs for specific STAT-receptor contacts and STAT dimerization. Abnormal STAT activation is implicated in many diseases, making them attractive drug targets. By targeting the SH2-pTyr interaction, we developed a novel comparative virtual screening approach and identified STAT specific inhibitors that could serve as therapeutic strategies in cancer and inflammation.

RECONSTRUCTION OF GENE-ENVIRONMENT NETWORKS UNDER UNCERTAINTY

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ABSTRACT

The mathematical concept of gene-environment networks allows to reconstruct the functional relationships between genes and environmental factors like toxins and other cell factors. The identification of the inherent regulatory network mechanisms heavily depends on uncertain data. Two approaches are discussed:

a) ellipsoidal uncertainty as a set-theoretic regression approach and
b) polyhedral uncertainty by using robust optimization.

We present a simulation study for spline regression models of gene-environment networks and their robust versions under polyhedral uncertainty.

BREAST CANCER CLASSIFICATION: FROM CONSENSUS CLUSTERING TO FUZZY LOGIC

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[2] Computer Science & IT, University of Nottingham, UK
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ABSTRACT

Breast cancer is a heterogeneous disease, and different approaches have been used to define the diverse molecular classes. In this work, we introduce a framework to elucidate core classes in multi-dimensional biomedical data which has led to the discovery of new cancer subtypes. To improve and refine patients' classification, fuzzy logic and fuzzy rules have been utilised to create a new algorithm. The latest results have been used to develop a new tool (called Nottingham Prognostic Index Plus – NPI+) which will be helpful to predict outcome in the different molecular classes.

CLASSIFICATION OF SALMONELLA SEROVARS BASED ON LASER-DIFFUSE-LIGHT-IMAGES USING LEARNING VECTOR QUANTIZERS

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University of Applied Sciences Mittweida, Germany

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ABSTRACT

Classification of Salmonella serovars according to their specific properties and anti-gene behavior usually requires expansive biochemical measurements and costly equipment. In the setting proposed here, simple laser-diffuse-light-images of colonies were taken as data. After adaptive feature extraction, classification is done by a learning vector quantization approach.

COMPUTATIONAL MODELING OF SPHINGOLIPID METABOLISM IN CANCER AND NEURODEGENERATION

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[2)] Institute of Informatics, Universty of Warsaw, Poland

ABSTRACT

Here we report our research results on computational sphingolipidom study. For the first time we employ compartmentalization based on structure of nondifferentiated Human cell. We also analyzed the local sensitivity and variance decomposition of the model. Finally we utilized it to simulate molecular events, known to cause Alzheimer's disease and hepatocellular carcinoma. We assume that current model provides a comprehensive, functional integration of experimental data, and will have critical implications for understanding link between sphingolipid metabolism and cancer or Alzheimer's Disease.

A TOOL FOR VISUALIZATION AND ANALYSIS OF MOLECULAR NETWORKS ON THE EXAMPLE OF PARKINSON'S DISEASE

Piotr Gawron [1)], **Stephan Gebel** [1)], **Marek Ostaszewski** [1)], **Paul Antony** [1)], **Christophe Trefois** [1)], **Kazuhiro Fujita** [2)], **Sabine Mosch** [1)], **Rudi Balling** [1)]

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ABSTRACT

In the past years the knowledge on molecular mechanisms underlying various diseases has grown tremendously. This knowledge needs to be organized and easily explored to be efficiently utilized for hypothesis generation, drug discovery or experimental design. Various molecular mechanisms are usually represented as networks of a given type, like protein-protein interaction, gene regulatory or metabolic networks. We present a tool for visualization and analysis of complex molecular networks using web-based approach.

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