ECO Summer School 2012

June 11-15, 2012
Verona (Italy)

QSAR/QSPR modelling
Chemoinformatics
Molecular descriptors

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Hosted by:
University of Milano-Bicocca
Milano Chemometrics and QSAR Research Group

Organization:
R. Todeschini, D. Ballabio, V. Consonni, A. Mauri

Program of the ECO Summer School 2012, in Verona, Italy , 11 - 15 June 2012

SUNDAY, 10 JUNE		
Arrivals		Hotel Marco Polo (Hall)
18:00 - 20:00	Registration	
MONDAY, 11 JUNE		
09:00 - 09:30	**Welcome and Introduction by the Organizer**	Hotel Marco Polo (Floor -1)
Practical Lessons		
09:30 - 13:00	**QSAR: from molecular structure to models**	
	Andrea Mauri, Davide Ballabio, University of Milano Bicocca, Italy	
	Alberto Manganaro, KODE Srl, Pisa, Italy	
09:30 - 10:30	Preparation of toxicological data	
10:30 - 11:00	**Coffee break**	
11:00 - 12:00	Molecular representation: formats and matching	
12:00 - 13:00	Retrieval of experimental toxicological data	
13:00 - 14:30	**Lunch break** (Restaurant at Hotel Mastino)	
Practical Lessons		Hotel Marco Polo (Floor -1)
14:30 - 18:30	**How to build a QSAR model**	
14:30 - 15:00	Introduction to molecular descriptors	
	Roberto Todeschini and Viviana Consonni, University of Milano Bicocca, Italy	
15:00 - 16.00	Calculation and screening of molecular descriptors by means of Dragon software	
	Andrea Mauri, University of Milano Bicocca, Italy	
16:00 - 16:30	**Coffee break**	
16:30 - 17:30	QSAR Modelling: how to build a predictive model	
	Davide Ballabio, University of Milano Bicocca, Italy	
17:30 - 18:30	Applying existing QSAR models: practical examples on VEGA platform	
	Alberto Manganaro, KODE Srl, Pisa, Italy	
TUESDAY, 12 JUNE		
Practical Lessons		Hotel Marco Polo (Floor -1)
09:00 - 12:45	**The QSAR toolbox**	
	Emiel Rorije, Dutch National Institute for Public Health and the Environment, The Netherlands	
09:00 - 09:45	Introduction to the OECD QSAR Toolbox, Read Across and Category approaches	
09:45 - 10:30	Demonstration of two examples of using the QSAR Toolbox (acute fish toxicity and BCF)	
10:30 - 11:00	**Coffee break**	
11:00 - 12:45	Interactive session using the toolbox	
13:00 - 14:00	**Lunch break** (Restaurant at Hotel Mastino)	
14:00 - 15:20	**Fellows presentations** (10 min each) - *Chair: Karl-Werner Schramm*	otel Marco Polo (Floor -1)
	Valentina Zingarelli, Helmholtz-Zentrum München	
	Katarzyna Odziomek, Linneuniversitetet	
	Matteo Cassotti, Helmholtz-Zentrum München	
	Chris Eckstein, Universiteit Leiden	
	Jacques Ehret, Universiteit Leiden	
	Evanthia Giagloglou, Università degli Studi di Milano Bicocca	
	Tine Ringsted, Università degli Studi di Milano Bicocca	
15:20 - 15:50	**Coffee break**	
15:50 - 17:00	**Fellows presentations** (10 min each) - *Chair: Willie Peijnenburg*	
	Martina Perisa, Hochschule Fresenius	

	Pantelis Sopasakis, Helmholtz-Zentrum München	H
	Ioana Oprisiu, Helmholtz-Zentrum München	
	Inge van Driezum, Hochschule Fresenius	
	Swapnil Chavan, Linneuniversitetet	
	Ian Ken Dimzon, Hochschule Fresenius	
17:15 - 19:00	**General Assembly** *only for ECO project leaders and manager*	
19:30 - 20:30	**Cocktail Party** (Restaurant at Hotel Mastino)	
WEDNESDAY, 13 JUNE		
09:00 - 09:40	**Fellows presentations** (10 min each) - *Chair: Josè Maria Navas*	Hotel Marco Polo (Floor -1)
	Lan Song, Universiteit Leiden	
	Oleksandra Ieromina, Universiteit Leiden	
	Isabel O'Connor, Radboud Universiteit Nijmegen	
Scientific Excursion		
09:45 - 12:30	**Visit to APTUIT Medicine Research Center**	
09:45	Departure in front of Hotel Mastino	
09:45 - 10:00	Bus ride	
10:00 - 10:15	Introduction to Aptuit Research Center, *Dr. Alfonso Pozzan*	
	Note: all of the participants must have their identity card / passport	
10:15 - 10:30	Visit to biological laboratories	
10:40 - 12:00	Visit to chemical laboratories, *Dr. Alfonso Pozzan*	
	- Chemical development lab, kilo-lab, pilot plant, *Dr. P.Westerduin*	
	- Pharmaceutical development lab, *Dr. M. Galvan*	
12:30 - 22:00	**Scientific trip to Venice lagoon**	
12:30	Departure from Aptuit Medicine Research Center	
12:30 - 14:30	**Light meal during the bus ride**	
14:30	Estimated arrival in Venezia (Tronchetto)	
14:30 - 19:30	Free time for Venice tour	
20:00	Departure from Tronchetto	
20:30	Stop for dinner at Autogrill near Padova	
22:00	Arrival in Verona	
THURSDAY, 14 JUNE		
09:00 - 09:30	**Welcome by the President of IAMC (R. Todeschini) and the Coordinator of the ECO project (I. Tetko)**	Palazzo Castelvecchio Conference Hall
Theoretical Lessons		
09:30 - 13:00	**Chemoinformatics and mathematical methods for modelling** - *Chair: Roberto Todeschini*	
09:30 - 10:15	Sparse statistical methods: theory, applications, software	
	Peter Filzmoser, Vienna University of Technology, Austria	
10:15 - 10:45	Combining chemo-bio-informatics and experimental methods in transmembrane protein structure resolution	
	Marjana Novic, University of Ljubljana, Slovenia	
10:45 - 11:15	**Coffee break**	
11:15 - 12:15	New artificial adaptive systems for intelligent data mining	
	Massimo Buscema, SEMEION (Italy) and University of Colorado (CO)	
12:15- 13:00	Evaluation of empirical models for calibration and classification	
	Kurt Varmuza, Vienna University of Technology , Austria	
13:00 - 14:00	**Lunch break** (Palazzo Castelvecchio - Giardino del Pozzo)	
Theoretical Lessons		
14:00 - 17:10	**Chemoinformatics and mathematical methods for modelling** - *Chair: Edward Kirby*	
14.00 - 14:30	Computer classification, design and search of organic reactions	
	Nikolay Zefirov, Moscow State University, Russia	
14.30 - 15:00	An integral equation approach to chemical and photophysical kinetics	
	Mario Nuno Berberan-Santos, Technical University of Lisbon, Portugal	
15:00 - 15:30	Graphical Bioinformatics	

	Milan Randic, Drake University (IA) and University of Ljubljana, Slovenia	Palazzo Castelvecchio Conference Hall
15:30 - 16:00	**Coffee break**	
16:00 - 16:25	AutoGraphiX-3: a new computer environment for studying graph theory	
	Gilles Caporossi, HEC Montreal, Quebec, Canada	
16:25 - 16:50	Bounds and relations involving betweenness centrality in some families of graphs	
	Snjezana Majstorovic, University of Osijek, Croatia	
16:50 - 17:10	Polybenzenes and relared nanostructures	
	Mircea Diudea, "Babes-Bolyai" University, Cluj, Romania	
17:10 - 18:30	**Fellows' presentations (10 min each)** - *Chair: Igor Tetko*	
	Alessandra Pirovano, Radboud Universiteit Nijmegen	
	Ahmed Abdelaziz, Helmholtz Zentrum München	
	Rajesh Rathore, Helmholtz Zentrum München	
	Mona Connolly, Instituto Nacional de Investigacion y Tecnologia Agraria y Alimentaria	
	Tobias Lammel, Instituto Nacional de Investigacion y Tecnologia Agraria y Alimentaria	
	Kamel Mansouri, Università degli Studi di Milano Bicocca	
	Faizan Sahigara, Università degli Studi di Milano Bicocca	
21:00	**Gala Dinner** (Palazzo Castelvecchio restaurant)	
FRIDAY, 15 JUNE		
Theoretical Lessons		Palazzo Castelvecchio Conference Hall
09:00 - 12:45	**Graph theory and topological indices** - *Chair: Milan Randic*	
09:00 - 09:45	The Topological Index Deluge	
	Ivan Gutman, University of Kragujevac, Serbia	
09:45 - 10:15	On DNA Graph and its application to DNA fragment assembly	
	Ali Iranmanesh, Tarbiat Modares University, Tehran, Iran	
10:15 - 10:35	Recent results on bipartite edge and vertex frustration of molecular graphs	
	Ali Reza Ashrafi, University of Kashan, Iran	
10:35 - 11:00	**Coffee break**	
11:00 - 11:30	Prediction of stability constants of coordination compounds from their connectivity indices	
	Nenad Raos, Institute for Medical Research and Occupational Health, Zagreb, Croatia	
11:30 - 12:00	Interpolation method and topological indices	
	Sandi Klavzar, University of Ljubljana and University of Maribor, Slovenia	
12:00 - 12:45	Molecules in silico	
	Adalbert Kerber, University of Bayreuth, Germany	
13:00 - 14:00	**Lunch break** (Palazzo Castelvecchio - Giardino del Pozzo)	
Theoretical Lessons		Palazzo Castelvecchio Conference Hall
14:00 - 15:30	**Graph theory and topological indices** - *Chair: Nikolay Zefirov*	
14.00 - 14:30	Some new applications of graph eigenvalues and spectral moments	
	Jorge Galvez, University of Valencia, Spain	
14:30 - 14:50	Integral eigenvalues of Cayley graphs	
	Bojan Mohar, University of Ljubljana, Slovenia	
14.50 - 15:10	Graphs and thermodynamics	
	Lionello Pogliani, University of Calabria, Italy	
15:10 - 15:30	Design of bivalent ligands as neuroprotective and anti-cancer compounds	
	Vladimir Palyulin, Lomonosov Moscow State University, Russia	
15:30	Closure	

MONDAY, 11 JUNE

9:00 – 9:30

Molecular descriptors, QSAR strategies and chemometrics

The discovery of relationships among different concepts, in particular concepts provided by different scientific fields, represents the most important way to develop new scientific knowledge and transform isolated information into a deeper theoretical knowledge.
The concepts of molecular structure, its representation by theoretical molecular descriptors and its relationship with experimental properties of molecules are an inter-disciplinary network, where a lot of theories, knowledge, and methodologies and their interrelationships are present, leading to a new scientific research field with a relevant follow-up in several practical applications.
Molecular descriptors are numerical indices encoding some information related to the molecular structure. They can be both experimental physico-chemical properties of molecules and theoretical indices calculated by mathematical formulas or computational algorithms.
Molecular descriptors, tightly connected to the molecular structure, play a fundamental role in scientific research, being the theoretical core of a complex network of knowledge, as it is shown in Figure 1. Indeed, molecular descriptors are based on several different theories, such as quantum chemistry, information theory, organic chemistry, graph theory, etc., and are used to model several different properties of chemicals in scientific fields such as toxicology, analytical chemistry, physical chemistry, medicinal, pharmaceutical, and environmental chemistry.

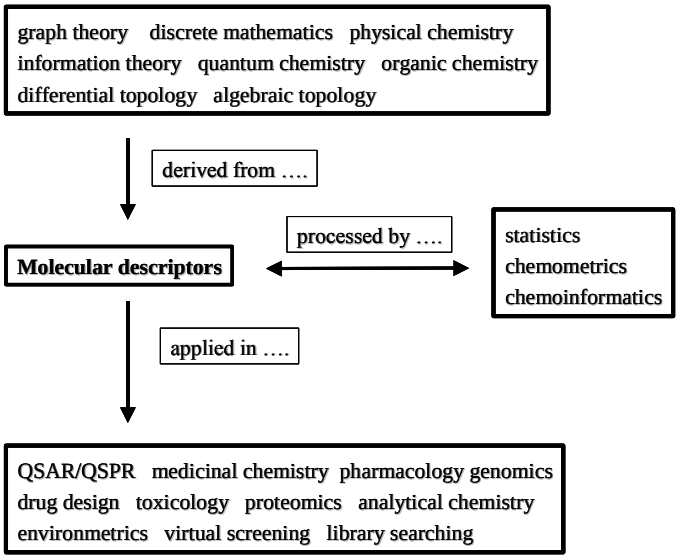

Figure 1. General scheme of the relationships among molecular structure, molecular descriptors, chemometrics and QSAR/QSPR.

Moreover, in order to obtain reliable estimates of molecular properties, data elucidation, and data mining, molecular descriptors are processed by several methods provided by statistics, chemometrics, and chemoinformatics. In particular, chemometrics for about 30 years has been developing classification and regression methods able to provide – although not always - reliable models, for both reproducing the known experimental data and predicting the unknown data. The modeling process usually has not only explanatory purposes, but also predictive purposes. The interest in predictive models able to give effective reliable estimates has been largely growing in the last few years as they are more and more considered useful and safer tools for predicting data on chemicals.

Quantitative Structure–Activity Relationships (QSARs) are the final result of the process which starts with a suitable description of molecular structures and ends with some inference, hypothesis, prediction on the behaviour of molecules in environmental, biological, and physico-chemical systems in analysis (Figure 2).

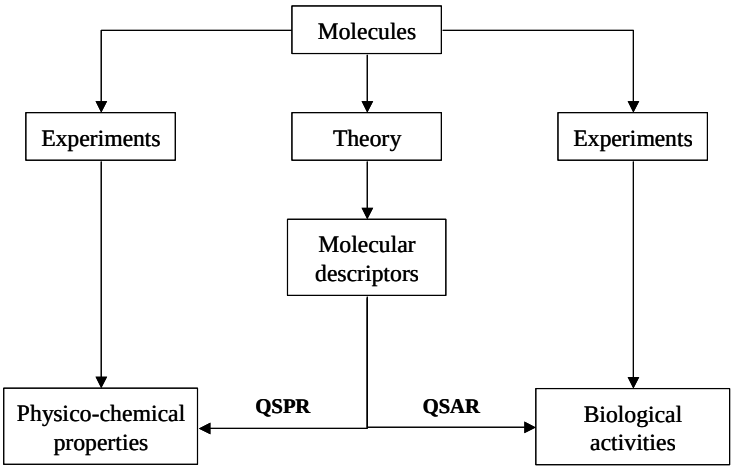

Figure 2. General scheme of the QSAR/QSPR philosophy.

QSARs are based on the assumption that the structure of a molecule (for example, its geometric, steric and electronic properties) must contain the features responsible for its physical, chemical, and biological properties and on the ability to capture these features into one or more numerical descriptors. By QSAR models, the biological activity (or property, reactivity, etc.) of a new designed or untested chemical can be inferred from the molecular structure of similar compounds whose activities (properties, reactivities, etc.) have already been assessed.

Behind the well-known approach called Quantitative Structure-Activity Relationships (QSAR), other specific approaches aimed at relating the molecular structure to some experimental (or calculated) properties are Quantitative Structure-Reactivity Relationships (QSRR), Quantitative Shape-Activity Relationships (QShAR), the molecular shape being considered as a component of the molecular structure, Quantitative Structure-Chromatographic Relationships (QSCR), Quantitative Structure-Toxicity Relationships (QSTR), Quantitative Structure-Biodegradability Relationships (QSBR), Quantitative Similarity-Activity Relationships (QSiAR), Quantitative Structure-Enantioselective Retention Relationships (QSERR), and so on. Generally speaking, the QSPR (Quantitative Structure–Property Relationship) acronymous is used when any property different from biological activity is modeled.

It has been nearly 45 years since the QSAR modeling firstly was used into the practice of agrochemistry, drug design, toxicology, industrial and environmental chemistry. Its growing power in the following years may be mainly attributed to the rapid and extensive development in methodologies and computational techniques that have allowed to delineate and refine the many variables and approaches used to model molecular properties. Furthermore, the interest in QSAR is more and more growing because nowadays these tools are not only used for research purposes but also to produce data on chemicals in the interest of time and cost effectiveness.

Chemometrics is largely applied in QSAR research, both from a methodological and a technical point of view. Indeed, it provides tools and ideas to describe molecular structures and model their properties with a continuous attention to the basic chemometric philosophy, based on model validation, information synthesis by new indices, and graphical representation of data information.

From R. Todeschini, V. Consonni and P. Gramatica: *Chemometrics in QSAR*, in Comprehensive Chemometrics, Elsevier, 2009, vol. 4, Chap. 5.

MONDAY, 11 - MORNING SESSION : 09:30 – 13:00

QSAR: from molecular structure to models

Preparation of toxicological data

The relevance of the preparation of suitable and reliable sets of molecules for QSAR modeling will be highlighted, as an introduction for the following lessons.

Molecular representation: formats and matching

The main issues related to molecular representation will be faced: how to represent molecules in digital formats, details about the most common formats (SMILED, SD File, Inchi), most common problems related to ambiguous representations.
Exercises proposed in the practical session: drawing a molecular structure from a SMILES string; building a SMILES string from a molecular structure.

Retrieval of experimental toxicological data

The main steps for retrieving useful set of molecules will be faced, together with the most common problems related to possibly unreliable sources. Tools for converting and checking molecule formats, in order to understand and fix them, will be presented.
Exercises proposed in the practical session: use of on-line tools in order to retrieve and check molecules.

MONDAY, 11 - AFTERNOON SESSION : 14:30 – 18:30

How to build a QSAR model

Introduction to molecular descriptors

Theoretical introduction to molecular descriptors: main types of descriptors and their characteristic for representing molecular structural features.

Calculation and screening of molecular descriptors by means of Dragon software

The main steps for the calculation of molecular descriptors by means of Dragon software will be presented together with an initial screening analysis: correlation between descriptors, principal component analysis and correlation with a given experimental toxicological response. A practical section of descriptor calculation will be carried out on a real QSAR dataset.
Exercises proposed in the practical session: calculation and analysis of resulting descriptor on a test dataset.

QSAR Modelling: how to build a predictive model

Main keys to build a QSAR predictive model will be highlighted: methods for descriptors selection, tools for model validation and main mathematical approaches for both QSAR qualitative and quantitative models will be introduced.

Applying existing QSAR models: practical examples on VEGA platform

An actual open-source QSAR software platform will be presented (VEGA), and an end point of particular interest such as BCF will be used to show how to use the software and how to interpret the results of the QSAR model. Exercises proposed in the practical session: prediction of the BCF value for a compound with VEGA and analysis of the resulting output.

DAVIDE BALLABIO

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Davide Ballabio graduated in Environmental Sciences in 2002 and since then he has been working in chemometrics applied to food science and Quantitative Structure Activity Relationship (QSAR). In 2006 he discussed his PhD thesis (Università degli Studi di Milano, Italia).
He is author of thirty-four peer reviewed papers published on international scientific journals of analytical and environmental chemistry, chemometrics and chemoinformatics, and food chemistry, and referee for several international scientific journals. His main research interests are chemometric methods for characterization and analysis of food and environmental data, QSAR/QSPR modelling, artificial neural networks, pattern recognition and variable selection algorithms.
He is author of several MATLAB toolboxes for the calculation of multivariate models.

VIVIANA CONSONNI

Dept. Environmental Sciences, University of Milano Bicocca
P.za della Scienza 1, 20126 Milano, Italy

Viviana Consonni received her PhD in chemical sciences from the University of Milano in 2000 and is now full researcher of chemometrics and chemoinformatics at the Department of Environmental Sciences of the University of Milano-Bicocca (Milano, Italy). She is a member of the Milano Chemometrics and QSAR Research Group and has more than 10 years experience in multivariate analysis, QSAR, molecular descriptors, multicriteria decision making, and software development. She is author of more than 40 publications in peer-reviewed journals and of the books ‘‘Handbook of Molecular Descriptors’’ (2000) and “Molecular Descriptors for Chemoinformatics” (2009) by R. Todeschini and V. Consonni, Wiley-VCH. In 2006, she obtained the International Academy of Mathematical Chemistry Award for distinguished young investigators and, in June 2009, was elected Member of the Academy.

ALBERTO MANGANARO

KODE S.r.l., Pisa, Italy

Degree in computer science. Expert in chemoinformatics, chemometrics and QSAR. Member of the Milano Chemometrics and QSAR Workgroup at Università di Milano-Bicocca, and of the Laboratorio di Chimica e Tossicologia dell'Ambiente at Istituto di Ricerche Farmacologiche Mario Negri. Co-founder of the scientific consultancy society Kode srl.

ANDREA MAURI

Dept. Environmental Sciences, University of Milano Bicocca
P.za della Scienza 1, 20126 Milano, Italy

Andrea Mauri received MSc degree in Environmental Sciences in 2000 from the Milano-Bicocca University and since April 2002 he has an on-going collaboration with the Milano QSAR and Chemometrics Research Group at the same University. In November 2007 he received the PhD in Chemistry at the Milano-Bicocca University with a thesis whose title is: "Protein and peptide multivariate characterisation using a molecular descriptor based approach". During his thesis, he spent six months in the Chemometrics Group at The National Institute of Chemistry, Ljubljana, Slovenia. His main research interests are quantitative structure-activity relationships (QSAR), molecular descriptors, multivariate analysis and software development. At present he has more than 20 publications on international peer-reviewed journals.

ROBERTO TODESCHINI

Dept. Environmental Sciences, University of Milano Bicocca
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Roberto Todeschini is full professor of chemometrics at the Department of Environmental Sciences of the University of Milano-Bicocca (Milano, Italy), where he constituted the Milano Chemometrics and QSAR Research Group. His main research activities concern chemometrics in all its aspects, QSAR, molecular descriptors, multicriteria decision making, and software development. President of the International Academy of Mathematical Chemistry, president of the Italian Chemometric Society, and "ad honorem" professor of the University of Azuay (Cuenca, Ecuador), he is author of more than 170 publications in international journals and of the books ''The Data Analysis Handbook'' by I.E. Frank and R. Todeschini, 1994, ''Handbook of Molecular Descriptors'' by R. Todeschini and V. Consonni, 2000 (almost 2000 citations), and "Molecular Descriptors for Chemoinformatics" by R. Todeschini and V. Consonni, 2009.

TUESDAY, 12 JUNE

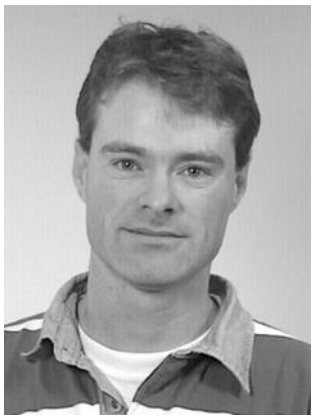
MORNING SESSION : 09:00 – 12:45

The QSAR toolbox

9:00 –9:45
Introduction to the OECD QSAR Toolbox and the concepts of Read Across and Category approaches. The main features and the line of thinking behind the QSAR Toolbox will be explained.

9:45 –10:30
Demonstration of two examples of using the QSAR Toolbox for the endpoints of acute fish toxicity and bioconcentration and introduction of two assignments to start interactive working with the toolbox.

11:00-12:45
Interactive session using the toolbox for the assignments and if time allows demonstration of some more advanced features (mixtures, metabolism, auto-oxidation etc.) that will be incorporated in the final version which is released in october (version 3.0).



EMIEL RORIJE
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Emiel Rorije graduated in (theoretical) chemistry (1992), has been working on (toxicological) QSAR evaluation and development since; in academia (University of Utrecht), government (RIVM) as well as industry (BASF). Ecotoxicology, prediction of (bio)degradation and microbial metabolism were the main topics at BASF, whereas his current work (2005-, RIVM) now focuses more on the application and development of human toxicological structure-activity models (skin irritation, skin and respiratory sensitization, reproductive and developmental toxicity), as well as ecotoxicological model development (PBT analysis, development of a priority scoring function for PBT and Long Range Transport Potential). Apart from daily work in REACH related substance evaluations he was recently involved in the EU 6th FW project “OSIRIS” (2008-2011) with a strong focus on development of Integrated Testing Strategies / Weight of Evicence procedures for Skin Sensitization; the coordination and execution of a retrospective evaluation of the multigeneration reproductive toxicity testing protocol and the introduction of the Extended One Generation Reproductive Toxicity study (EOGRTs) protocol for the OECD working group; and part of the OECD QSAR Toolbox Management group.

WEDNESDAY, 13 JUNE

MORNING SESSION : 10:00 – 12:30

Visit to APTUIT Medicine Research Center

Introduction to Aptuit Research Center, Dr. Alfonso Pozzan
Visit to biological laboratories
Visit to chemical laboratories, Dr. Alfonso Pozzan
- Chemical development lab, kilo-lab, pilot plant, Dr. P.Westerduin
- Pharmaceutical development lab, Dr. M. Galvan

ALFONSO POZZAN

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alfonso.pozzan@aptuit.com

Alfonso Pozzan is a senior principal investigator at Aptuit Verona, Computational Chemistry with accountability for chemoinformatics activities as well as providing computational chemistry support to integrated contract research lead identification and lead optimization projects and currently working on projects related to the AI and CNS therapeutic area. Prior to joining Aptuit in 2010 Dr Pozzan was senior principal investigator and manager within the GSK computational chemistry department Europe with accountability for supporting one Discovery Performance Unit (~25 medicinal chemists), leading scientific teams responsible for developing and implementing new computational methods, coordinate the resources required to keep the Computer Aided Drug Design infrastructure (CADD) up and running, liaising with external business partners. During his career within the Glaxo, GlaxoWellcome and GSK he supported more than 15 lead discovery and lead optimisation programs and directly contribute to discover one Macrolide antibacterial clinical candidates using 2D array design (WO2002050091, WO2002032917) one AMPA modulators clinical candidate using 3D structure based array design (WO2008113795, WO2002032917), one V1b antagonists and one Ghrelin antagonists clinical candidate using shape/pharmacophoric methods (WO2009130231, WO2009130232, WO2008148854, WO2008148853). Dr Pozzan led an international team that contributed to improve the GSK screening collection by knowledge based compound acquisitions, reagent design and acquisitions as well coordinate the efforts leading to the design and synthesis of many chemical libraries using external chemistry resources. For this efforts received from GSK an "Exceptional Science" award in 2004. Dr. Pozzan earned his Ph.D at the University of Padova working both in Italy and the US in the field of molecular dynamics simulations of DNA/RNA antitumor drug complexes.
Alfonso Pozzan is author/co-author of more than 30 peer review publications, co-inventor on 9 patents, and he as currently submitted 2 more patent applications.

The list of the latest 5 publications is here provided:

- Gabriella Gentile, Giancarlo Merlo, Alfonso Pozzan, Giovanni Bernasconi, Benjamin Bax, Paul Bamborough, Angela Bridges, Paul Carter, Margarete Neu, Gang Yao, Caroline Brough, Geoffrey Cutler c, Aaron Coffin c, Svetlana Belyanskaya,: 5-Aryl-4-carboxamide-

1,3-oxazoles: Potent and selective GSK-3 inhibitors, Bioorganic & Medicinal Chemistry Letters 22 (2012) 1989–1994.

- Fabio Maria Sabbatini, Romano Di Fabio, Sergio Melotto, Giovanni Bernasconi, Steve M. Bromidge, Lucilla D'Adamo, Marilisa Rinaldi, Chiara Savoia, Claudia Mundi, Carla Di Francesco, Laura Zonzini, Vivian J. A. Costantini, Benedetta Perini, Enzo Valerio, Alfonso Pozzan, Elisabetta Perdona', Filippo Visentini, Mauro Corsi: Azabicyclo[3.1.0]hexane-1-carbo hydrazides as as potent and selective GHSR1a ligands presenting a specific in vivo behaviour, Chem. Med.Chem (2011) 6, 1981-1985.

- Gabriella Gentile, Giovanni Bernasconi, Alfonso Pozzan, Giancarlo Merlo, Paola Marzorati, Paul Bamborough, Benjamin Bax, Angela Bridges, Caroline Brough, Paul Carter, Geoffrey Cutler, Margarete Neu, Mia Takada,: Identification of 2-(4-pyridyl)thienopyridinones as GSK-3β inhibitors , Bioorganic & Medicinal Chemistry Letters (2011), 21, 4823-4827.

- Profeta, Spada, Nalin, Andreotti, Pozzan, Miserazzi,: Reaction of 2-alkyl pyridine N-Oxide derivatives with Mosher's acyl chloride: first example of stereoselective Boekelheide rearrangement, Tetrahedron Letters (2010) 51, 6526-6530.

- Micheli, F., Antolini, M., Fabio, R.D., Pellacani, A., Pozzan, A., 2-Methyl-3-furanyl-4H-1,2,4-triazol-3-ylthioamides: a new class of selective Orexin 2 antagonists, Bioorganic & Medicinal Chemistry Letters (2010), 20, 6405-6407.

THURSDAY, 14 JUNE

09:00 - 09:30

Welcome by the President of IAMC and the coordinator of the ECO project

International Academy of Mathematical Chemistry

One of the reasons for initiating Academy that is concerned with various aspects of use of Discrete Mathematics and non-traditional Theoretical Chemistry disciplines is because several of this novel and not so novel applications of Mathematics in Chemistry have not been well received in some circles. It is not only that Chemical Graph Theory has been focus of unprecedented hostile campaigns in certain chemistry circles, but also it is known that difficulties accompanied early developments of the Density Functional as well as Artificial Neural Networks. The Journal of Chemical Physics, which grew because of a lack of appreciation of Quantum Chemistry by the chemical Establishment in 1930s became in 1970s part of the Establishment that has been excluding novelties inspired by application of Graph Theory in Chemistry. Lack of appreciation of the role of non-traditional mathematics in chemistry and misperception of significance of such work continues to hinder support for selected research projects in chemistry, which continue not to qualify for necessary research grants. It is possible that Academy, if it succeeds in attracting the best in the field and if it earns support of outstanding scientist of chemistry, may facilitate in full recognition of Mathematical Chemistry as a branch of chemistry equal to other chemical disciplines, not necessarily in importance but as a forum for discussing problems of chemistry. On the other hand Chemical Graph Theory and other mentioned areas had complete support in other circles of chemists. Journals like the Journal of Chemical Information and Computer Science among others has been very beneficial in publishing diverse contributions from Mathematical Chemistry over the past dozen years. Important journals are also The Journal of Mathematical Chemistry and MATCH Commun Math Comput Chem.
In like mode, chemometrics and its mathematical applications in chemistry had full support in journals such as Chemometrics and Intelligent Laboratory Systems and Journal of Chemometrics.
With the current growth of interest among mathematical chemists in complex biochemical systems it seems that for years to come we will be even more busy than ever in helping to characterize and contribute to understanding of ever more complex bio-systems and the interactions of molecules and bio-molecules involved if the mysterious world of living proteins.

Website: http://www.iamc-online.org/index.htm

Environmental Chemoinformatics (ECO) Project

Environmental ChemOinformatic (ECO) Marie Curie Initial Training Network (ITN) is a collaborative action of 7 institutions from 5 EU countries (Germany, The Netherlands, Spain, Sweden, Italy). Project start and end dates: 01-10-2009 to 30-09-2013.
Objective: The implementation of the new EU legislation concerning the registration, evaluation, authorization and restriction of chemicals (REACH) requires demonstration of the safe manufacture of chemicals and their safe use throughout the supply chain.
REACH encourages development of new in vitro test methods and replacement of animal tests wherever possible by alternative methods. These goals are not achievable without well-trained

personnel with a broad expertise and knowledge in both experimental and computational areas of environmental sciences. The requirements for such scientists, however, are not limited to the REACH implementation itself.
Large companies and SMEs could be interested to employ such specialists to perform risk assessment and prioritization of molecules in the development stage. Therefore, the primary objective of this ITN is to contribute to the education of a new generation of scientists, environmental chemoinformaticans, who will receive advanced training in both environmental and computational methods.
To achieve this goal the ITN will train the fellows using expertise and knowledge of its partners in various complementary computational and experimental areas of environmental sciences. The additional training will also be offered by means of Winter and Summer Schools and will include both theoretical and practical courses.
The internships to the laboratories of associated partners will allow fellows to learn new methods and to broaden their knowledge in the field. A flexible system of Short Term Fellowships will offer additional targeted training to researchers originally not associated with the network.
Given the potentially great business impact of evaluating more than 120,000 industrial chemicals in the European market within the next decade, the fellows of this network may have a significant economic dimension with regard to the hazard evaluation of chemicals in Europe.

Website**:** http://www.eco-itn.eu

IGOR TETKO

Helmholtz Zentrum, Munich (Germany)

1989 MSc (summa cum laude) from Moscow Institute of Physics and Technology, USSR
1994 PhD in computational chemistry (Institute of Bioorganic and Petrochemistry, Kyiv, Ukraine)
1995-2001 Research scientist at the University of Lausanne
since 2001 Senior Research Scientist/Group leader at HMGU
2009-2013 coordinator of FP7 Marie Curie Initial Training Network "Environmental ChemOinformatics" (ECO)
2010 co-founder of eADMET GmbH company as a spin-off of HMGU

THURSDAY, 14 - MORNING SESSION : 09:30 – 13:00

Chemoinformatics and mathematical methods for modeling

Chair: Roberto Todeschini

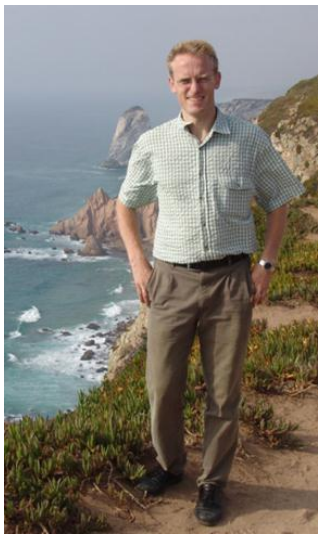
Thursday 14 June, 09:30 - 10:15

Sparse statistical methods: Theory, Applications, Software

Peter Filzmoser

High-dimensional data often contain many variables that are irrelevant for predicting a response or for an accurate group assignment. The inclusion of such variables in a regression or classification model leads to a loss in performance, even if the contribution of the variables to the model is small. Sparse methods for regression and classification are able to suppress these variables. This is possible by adding an appropriate penalty term to the objective function of the method.
An overview of recent sparse methods for regression and classification is provided (see, e.g., Filzmoser et al., 2012). The methods are applied to several high-dimensional data sets from chemometrics. A comparison with the non-sparse counterparts allows to getting an insight into their performance. Software based on the computing environment R will be presented.

References:
P. Filzmoser, M. Gschwandtner, and V. Todorov. Review of sparse methods in regression and classification with application to chemometrics. *Journal of Chemometrics*, Vol. 26, pp. 42-51, 2012.



PETER FILZMOSER
Statistics Department
Vienna University of Technology, Austria

Peter Filzmoser studied applied mathematics at the Vienna University of Technology, Austria, where he also wrote his doctoral thesis and habilitation devoted to the field of multivariate statistics. His research led him to the area of robust statistics, resulting in many international collaborations and various scientific papers in this area. His interest in applications of robust methods resulted in the development of R software packages. He was and is involved in the organization of several scientific events devoted to robust statistics. Since 2001, he has been a professor at the Statistics Department at Vienna University of Technology. He was visiting professor at the Universities of Vienna, Toulouse and Minsk.

Thursday 14, 10:15 - 10:45

Combining chemo-bio-informatics and experimental methods in transmembrane protein structure resolution

Marjana Novic

Biological membranes form the barrier through which both drugs and toxic molecules enter the organism. Despite the difficulties encountered in bio membrane research, membrane transport is the common step determining the effect of most drugs. For studying and analyzing membrane proteins, their transport activity for molecules of diverse chemical structure is of crucial importance. The aim of this work is to shed light onto the mechanism of transport and structural details of specific membrane proteins. The main target of interest will be bilitranslocase, the transporter of organic anions, such as bilirubin, from blood to liver cells [1]. We obtained experimental data on competitive inhibition of a number of structurally diverse molecules, including purines, pyrimidines (with their corresponding derivatives: nucleosides, nucleotides and congeners), anthocyanins and their mono- and di-glycosylated derivatives [2]. The lack of knowledge of the secondary structure of bilitranslocase makes any explanation of the transport mechanism challenging. For this reason we are attempting to resolve partially its 3D structure, starting with a prediction of transmembrane segments [3], continuing with 3D model of TM segments by NMR spectroscopy [4], and presently building the model of TM channel consisting of four TM domains of bilitranslocase.

1. On the mechanism of bilitranslocase transport inactivation by phenylmethylsulphonyl fluoride: Passamonti S, Battiston L, Sottocasa GL, Mol. Membr. Biol., 1999, 16, 167-172;
2. Experimental determination and prediction of bilitranslocase transport activity: Župerl Š, Fornasaro S, Novič M, Passamonti S, Anal. chim. acta; 2011, 705, 322-333;
3. Data-driven model for the prediction of protein transmembrane regions: Roy Choudhury A, Novič M, SAR QSAR environ. res., 2009, 20, 741-754.
4. Structural analysis of a peptide fragment of transmembrane transporter protein bilitranslocase: Perdih A, Roy Choudhury A, Župerl Š, Sikorska E, Zhukov I, Solmajer T, Novič M, PLoS ONE, 2012, In Press.

MARJANA NOVIC
Laboratory of Chemometrics
National Institute of Chemistry
Hajdrihova 19, SI-1000 Ljubljana, Slovenia

Born: 1955, July 19th in Ljubljana, Slovenia
married, two daughters

Education:
1974 Baccalaureat, High School in Ljubljana
1979 B. Sc. degree in Chemistry, University of Ljubljana
1983 M. Sc. degree in Computer Chemistry, University of Ljubljana
Master Degree Thesis: The Use of Fourier Transformation in

Chemical Information Systems Based on Infrared Spectroscopy

1985 Ph. D. in Chemistry, University of Ljubljana
Thesis: Hierarchical Clustering and Recognition of Chemical Structures and Structural Fragments on the Basis of 13C NMR spectra

Postdoctoral Education:

1986 University of Lausanne, Switzerland, with Professor G. Bodenhausen, 13 months. The field of research: the automated pattern recognition in 2-D NMR spectra.

1993 University of Tarragona, Spain, with Professor X. Rius, 1 month. The field of research: multivariate data analysis with application of neural networks.

1997 University of Cordoba, Spain, with professor M. Valcarcel, 3 months. The field of research: modelling in chemical kinetics research

2003 University of Tasmania, Australia, with professor Paul Haddad, 1 month. The research encompassed modelling in ion chromatography. Peak asymmetry was explained by a simple model of purely equilibrium processes in ion exchange chromatography. We started also the modelling with non-linear techniques in gradient elution chromatography.

Employment:

1979- National Institute of Chemistry, Laboratory for Chemometrics. Started research work under the supervision of Professor J. Zupan and D. Hadži, in the beginning in Infrared Spectroscopy, later as research associate in Laboratory for Chemometrics. The fields of research: Information Systems in Chemistry, Computer Supported Structure Elucidation, Pattern Recognition, Computer Simulation of Learning Process, Neural Networks, New Structure Representations and QSAR modelling.

Honours, membership:

1989 Boris Kidrič Fund Award for a significant contribution to the field of Computerized Automated Analysis of Spectroscopic Data.

2008 Member of International Academy of Mathematical Chemistry

Research interest:

(i) development and applications of standard and modern chemometrics techniques (clustering, classification, modelling, neural networks, genetic algorithms); (ii) handling of large amounts of multivariate data: transformations, projections, reductions, selection of variables and optimization of the data-representation for different modelling approaches; (iii) modelling using linear or non-linear methods – case studies in QSAR (modelling of biological properties) and in analytical chemistry, determination of 3D molecular structures, calculation of descriptors and structure representations; validation of QSAR models; (iv) in silico approach in the regulation of chemicals; (v) simulation of the detector signals for various analytical techniques including ion chromatography, flow injection analysis and infrared spectroscopy.

Author and co-author of over 100 scientific papers and 10 book chapters, Hirsch index 22 (web of sci.)

Thursday 14 June, 11:15 - 12:15

New artificial adaptive systems for intelligent data mining

Massimo Buscema

A theoretical overview about non Linear Artificial Adaptive Systems and Natural Computation will be presented. The new adaptive algorithms in evolutionary computation and Neural Networks developed at Semeion Institute will be compared with the more known patterns recognition systems. A new math of artificial adaptive systems, using ANNs and other complex algorithms as elementary operators, will be introduced.

MASSIMO BUSCEMA

SEMEION, Centro Ricerche di Scienze della Comunicazione,
via Sersale 117, 00128. Roma, Italy

Professor and Computer Scientist, expert in Neural Networks and Artificial Adaptive Systems.

- September 29, 2011.Decorated with the award of the Rotary Club of Rome for the Southeast Conference on "Mathematics and Artificial Intelligence together: the new goal for scientific research", Rome.
- September 28, 2011. Awarded the prize “150 years of the Unification of Italy Emigration: from the arms to the brain. Contribution of the Italian genius and the heart of scientific progress, economic and social development of the International Community”. Part of the "International Forum on Research and Treatment of Pain", Rome, Chamber of Deputies.
- From 2011 – today: Professor Adjoint at the Department of Mathematics and Statistics of the University of Colorado, Denver
- July 16, 2010. Awarded the "Meritorious Paper" for the paper "A New Meta-Classifier" presented in International Conference of the North American Fuzzy Information Processing Society (NAFIPS 2010). The award was presented by Ryerson University, Toronto, Ontario, Canada.
- In December 2010: winner of the National Award for Safety and Security (ONPS)
- In June 2010: winner of the International Ostia Award for Science
- From 2010 – today: Member of the Advisory Board . the Center for Computational and Mathematical Biology (CCMB) The CCMB is a center of the University of Denver, Colorado, USA.
- From 2009-today: Consultant of the italian “Presidenza del Consiglio dei Ministri”, Rome, Italy.
- From 2003- To 2007: Consultant of New Scotland Yard, London,UK.
- In 2003: Nominated “Grande Ufficiale al merito della Repubblica Italiana” by the President of Italian Republic.
- From 2000- To 2010: Consultant of Bracco Pharmaceutic Group, Milan, Italy.

- From 1985 – today: Founder and Director of Semeion – Research Centre of Science and Communication (a Scientific Organization Recognized by Italian Ministry of Research in 1991 and nominated “Special Institute” in 2005).
- From 1985-1986: Professor of “Computer Science and Linguistics” at the University of Perugia.
- From 1982-1985: Professor and Director of the Department of Science of Communications at the University of Charleston (West Virginia-USA).
- From 1979-1981: Assistant Professor in Science of Communications at American College of Rome - the University of Charleston (West Virginia-USA).
- 1978: Laurea in Letters and Philosophy (University of Rome, “La Sapienza”).

Director and Professor at Semeion, Research Center of Sciences of Communication, in Rome (Italy), via Sersale 117, 00128. www.semeion.it m.buscema@semeion.it .
Member on the Editorial Board of various international journals. He has designed, constructed developed new models and algorithms of Artificial Intelligence. Author of scientific publications on theoretical aspects of Natural Computation, with over 250 titles (scientific articles, essays, and books (23) on the same subject) and over 35 Software Systems used in many university and research Centres. Inventor of 20 international patents.
Scientific Director of research projects on the application of artificial intelligence systems in the biomedical field, homeland security and safety (quakes and slides down).

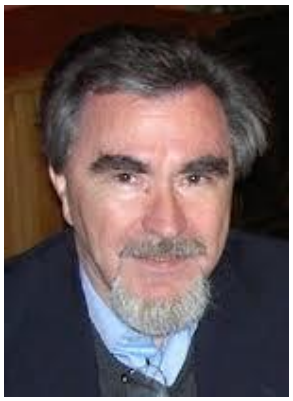
Thursday 14 June, 12:15 - 13:00

Evaluation of empirical models for calibration and classification

Kurt Varmuza

Relationships between data sets in chemistry are often too complicated to be understood sufficiently by theory. Furthermore, chemists often cannot directly measure what they want to determine. Examples of such problems are: recognition of the chemical structure from molecular spectral data, quantitative relationships between chemical structure data and substance properties or activities, quantitative analyses of complex mixtures, and determination of the origin of a sample. In these cases empirical models based on multivariate data analysis are useful. Typically, such models are developed from a calibration data set by regression methods, such as PLS (partial-least squares regression). Essential for empirical model are (1) an adequate complexity of the model (typical the optimum number of PLS components), and (2) a realistic estimation of the model performance when applied to new cases. These two aspects should be estimated separately. Furthermore, the variability of the used performance measure (e. g., standard error of prediction (SEP), or predictive ability) must be considered, as well as the variability of the optimum model complexity.
Because of the rather small number of samples in most data sets in chemistry, so called resampling techniques are necessary for the optimization of a model and the estimation of its performance. Besides various bootstrap methods the more strict strategy "repeated double cross validation" has found applications for calibration models (PLS) and several classification methods (DPLS, KNN). This strategy is easily applicable via free software in R for optimization of the model complexity, and for a separate and careful estimation of the model performance. Also the variabilities of the optimization parameter and of the performance measure are estimated - based on the results from differently composed random sets for calibration and test.

[1] K. Varmuza, P. Filzmoser: Introduction to multivariate statistical analysis in chemometrics, CRC Press, Boca Raton, FL, USA (2009). See www.lcm.tuwien.ac.at.
[2] P. Filzmoser, B. Liebmann, K. Varmuza: *J. Chemometrics,* **23** , 160 (2009).
[3] R. A language and environment for statistical computing. R Development Core Team, Vienna, Austria, 2012. www.r-project.org.



KURT VARMUZA
Vienna University of Technology, Austria

Kurt Varmuza studied chemistry at the Vienna University of Technology in Austria. Since 1992 he has been professor at this university (retired 2007). He is one of the pioneers in chemometrics and has a broad experimental background in mass spectrometry. His current research activities comprise chemometrics (empirical multivariate models, software development in R), chemoinformatics (QSPR, uniqueness of molecular descriptors), spectra-structure relationships, classification of materials in archaeometry and cosmo chemistry.

THURSDAY, 14 JUNE

AFTERNOON SESSION : 14:00 – 16:30

Chemoinformatics and mathematical methods for modeling

Chair: Edward C. Kirby

EDWARD C. KIRBY

36 Fishersview Court, Pitlochry, Scotland UK

Retired, but working as a freelance scientist, and chairman of the Resource Use Institute, Pitlochry. CV: Trained at St Andrews: BSc 1958, PhD 1961 (under David Reid on azulenes with electrophilic reagents): Post-Doc at Cambridge (England) 1961/62 under F.G. Mann, working on organo-phosphorus compounds: Industrial work with Laporte Industries (1962-1965), and then with British Oxygen chemicals (1965-1969), at which point I joined the Resource Use institute, working with R.H.S. Robertson and partners. I became interested in aromaticity, especially of non-benzenoids as a student at St Andrews. My fascination with the mathematical & graph theoretical aspects was triggered by a meeting organised by Nenad Trinajstić in Dubrovnik in 1979.

Thursday 14 June, 14.00 - 14:30

Computer classification, design and search of organic reactions

Nikolay Zefirov

Earlier Zefirov and Tratch have developed the "Formal-Logical Approach" as the basis for (1) classification of organic reactions, (2) exhaustive construction of symbolic equations, (3) search for novel reactions and reaction design, (4) non-empirical computer-assisted synthesis. This lecture briefly reviewed this approach for classification and description of organic reactions as well as demonstrates use of it to the search of novel reactions in the area of [2,3]-sigmatropic rearrangements, reactions with 6-centered linear-cyclic topology and application to heterocyclic chemistry for recyclization processe.

Selected Lit:

J.Org.Chem. Russ.,1975, *11*, 1785; 1976, *12*, 7; 1982, *18*, 1561; *Chemica Scripta*.,1980, *15*, 4; *Acc. Chem. Res*,1987, *20*, 237; *J. Chem. Inf. Comp. Sci.*,1988, *28*, 188; 1998, *38*, 331, 349; *J. Org.Chem. Russ.*,1989, *25*, 1585; *Analytica Chimica Acta*.,1990, *235*, 115; *MATCH*, 2002, *46*, 253, 275; *J.Phys.Org.Chem.*, 2003, *16*, 463; *Croat. Chim. Acta*.,2006, *79*, 339;

NIKOLAY S. ZEFIROV

Department of Chemistry
Lomonosov Moscow State University
Moscow 119991, Russia

Professor Nikolay S. Zefirov† graduated from Lomonosov Moscow State University (MSU) in 1958. For more than 50 years, he holds various positions at the Department of Chemistry of the MSU; since 1994, he is the head of Organic Chemistry Division. He received PhD and Dr. Sci. degrees in 1961 and 1966, respectively. Professor Zefirov was elected a corresponding member and a full member of the USSR Academy of Sciences in 1981 and 1987, respectively. Since 1987, he is the head of the Laboratory of Mathematical Chemistry and Computer-Assisted Synthesis at the N. D. Zelinsky Institute of Organic Chemistry of the Russian Academy of Sciences (RAS). In 1989–2006, he was the director of the Institute of Physiologically Active Compounds of the RAS; in 2006, he was appointed as a scientific supervisor at this institute. Professor Zefirov was awarded the Prize of the Government of the Soviet Union (1989) and Russia (2001). He received the Lomonosov Award (1983) and Butlerov Award (1994). Professor Zefirov is a member of the International Academy of Mathematical Chemistry. In 1974–1991, he headed the Division of Organic Chemistry at the D. I. Mendeleev USSR Chemical Society; currently, he is the president of the Medicinal Chemistry Section of D. I. Mendeleev Russian Chemical Society. His research interests cover theoretical and synthetic organic chemistry, medicinal chemistry, mathematical chemistry and computer-aided molecular design.

Thursday 14 June, 14.30 - 15:00

An integral equation approach to chemical and photophysical kinetics

Mario Berberan-Santos

Deterministic chemical and photophysical kinetics is based on systems of first-order differential equations (the rate equations) that once integrated, analytically or numerically, provide the time-evolution of the concentrations of all species of interest. An alternative formalism, based on integral equations, will be presented. Some applications illustrating its usefulness will also also discussed.

MARIO BERBERAN-SANTOS

Instituto Superior Tecnico
Technical University of Lisbon, Portugal

Mario Berberan-Santos is a Professor of Physical Chemistry at the Technical University of Lisbon. He has written over 180 research papers and book chapters, and two books, mostly on fluorescence spectroscopy and its applications. Out of all papers, about 60 are mathematical chemistry papers, or include significant mathematical chemistry aspects. He was co-author with Prof. Bernard Valeur of *Molecular Fluorescence*, 2nd ed., Wiley-VCH, 2012. He has held fellowships at the National Research Council of Canada (Ottawa), at Conservatoire National des Arts et Métiers (Paris, France), and at Laboratoire pour l'Utilisation du Rayonnement Electromagnétique (LURE, Univ. Paris-Sud, Orsay, France). He was Invited Full Professor at the École Normale Supérieure de Cachan (France). He is member of the Editorial Advisory Boards of *ChemPhysChem, A European Journal of Chemical Physics and Physical Chemistry* (since 2004), and of *MATCH: Communications in Mathematical and in Computer Chemistry* (since 2010). He is National Representative (since 2007) at the ChemPubSoc Europe publishing consortium. He was Secretary-General of the Portuguese Chemical Society (Sociedade Portuguesa de Química) in 2001-2004, and is President of the same society for the term 2010-2012. He is a Fellow of the Royal Society of Chemistry.

Thursday 14 June, 15:00 - 15:30

Graphical Bioinformatics

Milan Randic

A novel approach to the problem of protein alignments is described, which in comparison with existing approaches is visibly more efficient. This approach is based on superposition of amino acid adjacency matrices of a pair of proteins, which have been modified to record the sequential order of amino acids. As a result, one obtains simultaneously all segments of the two proteins which are shifted relative to one another by one or more positions in either directions, without need of aprior exhaustive search for an alignment that included unproductive directions and unknown displacement steps.

MILAN RANDIC

Drake University, Des Moines (IA) and University of Ljubljana, Slovenia

Milan Randić is native of Croatia and citizen of United States and Croatia, born in 1930. He studied Theoretical Physics at the University of Zagreb during 1949-1953 and studied for Ph. D degree at the University of Cambridge, England (1954-1958). From 1960 – 1970 he was at the Rudjer Bošković research institute in Zagreb, Croatia, where he founded the Theoretical Chemistry Group.
During 1971-1980 he was visiting various universities in USA including The John Hopkins, MIT, Harvard, Tufts, and Cornell. With 1973 his research oriented towards application of Discrete Mathematics and Graph Theory in particular to characterization of molecules and bio-molecules. During 1980 to 2000 he was distinguished professor in the Department of Mathematics and Computer Science at Drake University, Des Moines, Iowa. During the past 20 years he is spending three-four months each year at the National Institute of Chemistry, Ljubljana, Slovenia collaborating with scientists from its Laboratory for Chemometrics. He is member of the Croatian Academy of Sciences and Arts and founder of the International Academy of Mathematical Chemistry with the seat in Dubrovnik, the historic city on Adriatic coast. The Academy has about 70 members, including six Nobel Laureates as Honorary Fellows. With the year 2000 his research has been mostly shifted towards Bioinformatics, with particular emphasis on graphical representation and numerical characterization of DNA, RNA secondary structure, proteins and proteome, though his fascination with Kekulé valence structures and Aromaticity remains undiminished.
Among the 125 Most-Cited JACS Publications during its 125 years of publishing [1] Randić's paper on his connectivity index (*J. Am. Chem. Soc.* 1975**,** *97,* 6609-6615) is listed at position 94. This paper was also listed among 30 most cited publications in *J. Am. Chem. Soc*. since 1975 [2] – as of August 25, 2005). It recently passed 2000 citations.
Randić's last published paper (M.Randic, Very Efficient Search for Protein Alignment—VESPA, Journal of Computational Chemistry 2012, 33, 702–707) solved analytically over 40 years old problem on protein alignment, which during past 40 years has been approached (by trial-and-error approach, statistically, or using empirical parameters) by many computer scientists since 1970.
Milan Randić is Honorary Member of The Croatian Chemical Society, Honorary Member of The International Academy of Mathematical Chemistry and Honorary Member of The National Institute of Chemistry, Ljubljana, Slovenia.

Awards:

1966 Annual Science Award of the City of Zagreb, Croatia,
1988 Annual Award for Science of Republic of Slovenia (with B. Jerman-Blažič and I. Fabič)
1990 The Iowa Governor's Annual Science Achievement Award
1996 Herman Skolnik Award (Annual Award of the Division of Chemical Information of the American Chemical Society).
2011 Grand Pregl Award of the National Institute of Chemistry, Ljubljana, Slovenia.

In 2008 Randić is listed among 1% of most cited chemists total number of citations 12,028; and the Hirsch index h = 52.
His other interests include development of a universal pictographic language Nobel.

[1] "*JACS* at 125" highlighted select papers from among *JACS'* 125 most cited. *J. Am. Chem. Soc.*, 2003, *125*, 1-8.
[2] ISI Web of Science: Most cited papers from selected journals (Papers published since 1975)
[3] Essential Science Indicators, a new platform of ISI which provides information on selected (1% according to citation record) scientists, institutions, journals, etc) at # 1241.

Thursday 14 June, 16:00 - 16:25

AutoGraphiX-3: a new computer environment for studying graph theory

Gilles Caporossi

AutoGraphiX is a computer system that was developed at GERAD (Montreal, Canada) since 1997. The main goal of AGX is to search for extremal graph, graphs for which the value the invariant under study is maximized or minimized. The AGX system is now widely used and the main paper describing the system is now cited more than 90 times according to *Web of Knowledge.*
The last version of the system will be presented. It involves lots of important changes and improvements. Those improvements include the ability to handle multi-objective optimization, some new techniques to find conjectures, the capability to study vertex related values among others.

GILLES CAPOROSSI
GERAD and HEC Montréal, Montreal, Quebec, Canada
gilles.caporossi@gerad.ca

Gilles Caporossi is associate professor at HEC Montreal since 2003. He is member of the International Academy for Mathematical Chemistry, associate professor of the Data Mining Chair of HEC Montréal. His PhD thesis (2001 at École Polytechnique de Montréal) was dedicated to the development of the AutoGraphiX system for computer aided graph theory. He is co-author of 30 papers in pair reviewed journals and has 10 contributions in book chapters or pair reviewed conference proceedings.

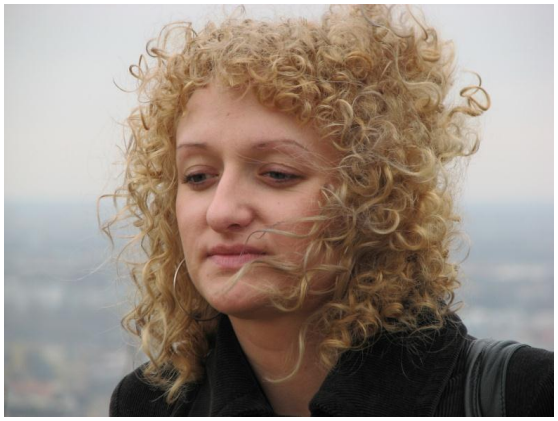
Thursday 14 June, 16:25 - 16:50

Bounds and relations involving betweenness centrality in some families of graphs

Snjezana Majstorovic

The problem of identification of the 'most important' vertices in a graph arises while confronting the analysis of network.
Among several important centrality measures such as Degree centrality, Centrality beyond nearest-neighbors, Closeness centrality and Information centrality, the Betweenness centrality deals with the relative importance of a vertex (or an edge) in the communication between other vertices in a graph.

A special type of such measure is the adjusted centrality of a vertex which is closely related to the Wiener index. This measure was studied on tree graphs. The results include some bounds for adjusted centrality of individual vertices of a tree as well as its relation to some other graph invariants.



SNJEŽANA MAJSTOROVIĆ
Department of Mathematics
University of Osijek, Croatia

Snježana Majstorović was born in Osijek in 1982. In June 2005. she graduated at Department of Mathematics, University of Osijek. In the same year she was employed as teaching assistant at the same institution and enroled the Postgraduate study in Mathematics at the Department of Mathematics, University of Zagreb. Her research interests are Combinatorics and Discrete mathematics. She has 6 published scientific papers. She participated at 4 international conferences.

Thursday 14 June, 16:50 - 17:10

Polybenzenes and relared nanostructures

Mircea Diudea

Polybenzene BTA_48 (Figure), designed by map operations, can dimerize either by identification of octagons R(8) to provide a diamond-like *fcc*-net or by identifying the “opening” rings R(12) when an “intercalated” dendrimer-dimer is formed, that can build a dendrimer. By growing, the dendrimer rather quickly superimpose over the diamond-like network. A third way is an “eclipsed” isomer, that can form multi-tori, negatively curved structures of various complexity. Multi-tori can evolve spherically or show a linear periodicity, in forming arrays as rods. The polybenzene armchair-opened BTA-multi-tori are compared to the zig-zag-opened BTZ-multi-tori. Their stability was evaluated by calculation of energetic parameters at Hartree-Foch and DFT level of theory.
A Graph-theoretical study has related the structure of multi tori to the genus of their embedding surface and established the lower and upper bound genus values. A description, in terms of Omega polynomial, of the two periodic linear BTX-networks is also presented.

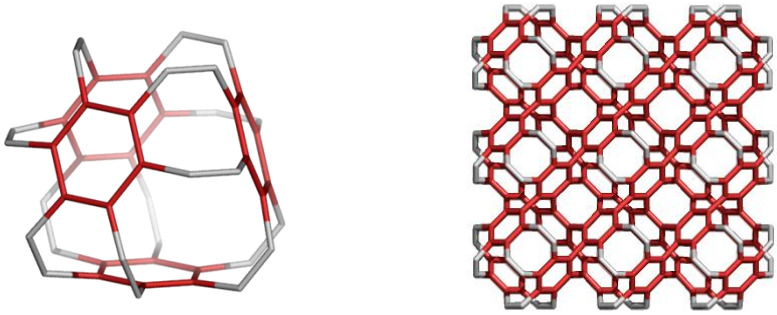


Figure. BTA_48 unit and the f_{cc} polybenzene network

References:
1. M. V. Diudea, A. Ilić, All-pentagonal face Multi Tori, *J Comput Theor Nanosci*, **2011**, *8*, 736-739.
2. M. V. Diudea, *Nanomolecules and Nanostructures - Polynomials and Indices*: **MCM** series, No. 10**,** Univ. Kragujevac, Serbia, **2010**.
3. M. V. Diudea, Cs. L. Nagy, *Periodic Nanostructures*, SPRINGER, 2007.
4. M. V. Diudea, Nanoporous carbon allotropes by septupling map operations. *J Chem Inf Model*. **2005**, *45*, 1002-9.

MIRCEA V. DIUDEA
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EDUCATION
1957-1969 Primary, elementary and high school
1979 Faculty of Chemistry, University of Cluj
1980 - Ph. D., Institute of Chemistry, Cluj

EMPLOYMENT
1974-1980 Chemist at "Terapia" Drug Factory, Cluj
1980-1987 Researcher at Chemical-Pharmaceutical Research Institute, Cluj
1987-1990 Assistant Professor, Department of Chemistry, "Babes-Bolyai" University, Cluj
1990-1996 Associate Professor, Dept. of Organic Chemistry, "Babes-Bolyai" University, Cluj
1996 - Professor, Department of Organic Chemistry, "Babes-Bolyai" University, Cluj
Courses: 1. Biologically Active Compounds; 2. Molecular Topology. 3. Fullerenes and Nanostructures (Master)

FRIDAY, 15 JUNE

MORNING SESSION : 09:00 – 12:45

Graph theory and topological indices

Chair: Milan Randic

Friday 15 June, 09:00 - 09:30

The Topological Index Deluge

Ivan Gutman

In recent years, we are faced with an enormous increase of newly designed graph-based molecular structure descriptors (often referred to as "topological indices"). In the "old good times", such descriptors were invented in an attempt to properly describe some chemically relevant properties of the underlying compounds, and their usefulness was usually documented by appropriate examples. In "modern times", the new descriptors are often defined ad hoc, without any indication of their possible applicability, and are then used as a starting point for mathematical investigations. Practically in no case is there an attempt to show (and usually it could not be shown) that the new descriptor performs better than the already existing ones. For obvious scientific reasons, it would be desirable to stop or at least slow down this "topological index deluge". In the lecture, we point out some possible strategies how to achieve this goal.

09:30 - 09:45

Remarks on the Kekulè-Structure based theories of conjugated molecules

Ivan Gutman

In the 1970s and later, several theories were elaborated, by means of which the properties of polycyclic conjugated molecules, especially of benzenoid hydrocarbons, could be rationalized on the basis of their Kekulè structures. The most popular of these are the aromatic sextet theory (Clar), various approaches based on counting the Kekulè structures (Herndon, Hall, Cioslowski, Gutman, …), the theory of conjugated circuits (Randić), partition of π-electrons into rings (Randić & Balaban). We now show that in some ordinary, stable, strain-free benzenoid hydrocarbons the predictions of Kekulè-structure based theories are false. We provide convincing arguments for this falseness.

IVAN GUTMAN
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Born: September 2, 1947 in Sombor, Yugoslavia

1970: B.Sc. degree in chemistry
1973: M.Sc. degree in chemistry
1973: Ph.D. degree in chemistry (University of Zagreb)
1981: Ph.D. degree in mathematics (University of Belgrade)
1995: Habilitation (Attila Jozsef University, Szeged)
1971-1977: Institute "Rudjer Bošković", Zagreb, Croatia
1977-present: Faculty of Science, University of Kragujevac, Kragujevac, Serbia
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1988: member of the Serbian Academy of Science (full member since 1997)
2005: member of the International Academy of Mathematical Chemistry
2006: member of the Academy of Nonlinear Sciences (Moscow)

Published scientific papers:
>1170 (of that 43 in 2008, 43 in 2009, 47 in 2010, 39 in 2011, >16 in 2012)

Friday 15 June, 09:45 - 10:15

On DNA graph and its application to DNA fragment assembly

Ali Iranmanesh

DNA sequencing is one of important problems in molecular biology that proceeds in recognition of primary structure of DNA and determining the order of the nucleotide bases: adenine (A), guanine (G), cytosine (C), and thymine (T) in a molecule of DNA.
One of the new methods for DNA sequencing is DNA fragment assembly. DNA fragment assembly is a newly explored method of determining whether or not a reassembled strand of DNA, matches the original strand. One particular way to analyse this method is by using concepts from graph theory. In order to begin the graph theoretical phase, one needs a directed graph which is built from the spectrum (a set of some k-long oligonucleotides).
In this paper, by the concept of DNA graph, we will discuss about new approach to creating and analysing a DNA graph and its role in aiding DNA fragment assembly and determining the DNA structure. Graph theory and its concepts are used for application in many fields of study.

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Ali Iranmanesh (b. 1965 in Kerman) is the head of Faculty of Mathematical Sciences in Tarbiat Modares University. He obtained his Ph.D. in Mathematics. In 1995, he was appointed an Assistant Professor at the Department of Mathematics of the Tarbiat Modares University and Promoted to Professor in 2005.Now he has published more than 140 papers and compiled 3 volume of his collected papers. He is a recipient of several fellowships and awards. He was elected as the fourth Iranian Scientists in Nanoscience in 2008 and he was selected as a member of Academy of Mathematical Chemistry in 2010.He is an editor in chief of the Iranian Journal of Mathematical Sciences and Informatics .The main thrust of his research in the field nanoScience is studying applications of Topological indices in Chemistry, Nanocomputation, fullerenes and DNA sequencing.

Friday 15 June, 10:15 - 10:35

Recent results on bipartite edge and vertex frustration of molecular graphs

Ali Reza Ashrafi

A graph G with the vertex set V(G) is bipartite if V(G) can be partitioned into two subsets V_1 and V_2 such that all edges have one endpoint in V_1 and the other in V_2. The smallest number of edges that have to be deleted from a graph to obtain a bipartite spanning subgraph is called the ***bipartite edge frustration*** of *G* and denoted by φ(*G*). This topological index has important applications in computing stability of fullerenes. Fajtlowicz and and Larson [1] claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make fullerene graph bipartite. Then Došlić and his co-authors [2–4] considered mathematical properties of this new graph invariant into account. It is easy to see that φ(G) is a topological index and G is bipartite if and only if φ(G) = 0. It can be easily shown that φ(G) ≤ |E(G)|/2 and that the complete graph on n vertices has the maximum possible bipartite edge frustration among all graphs on n vertices. Because of this success it is natural to study its vertex version. The ***bipartite vertex frustration*** of G, ψ(G) is defined as the minimum number of vertices that have to be deleted from G to obtain a bipartite subgraph H of G [5]. In this talk we will report on our recent results about this topological inices.

1. S. Fajtlowicz, C.E. Larson, Graph-theoretic independence as a predictor of fullerene stability, Chem. Phys. Lett. **377** (2003) 485–494.
2. T. Došlić, Bipartivity of fullerene graphs and fullerene stability, Chem. Phys. Lett. **412** (2005) 336–340.

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Ali Reza Ashrafi received his M.Sc. from Shahid Beheshti University, and Ph.D. from the University of Tehran under direction of professor Mohammad Reza Darafsheh. He is currently a professor at the University of Kashan since 1994. His research interests are Chemical Graph Theory and Computational Group Theory. In 2007, 2008, 2009 and 2010 he elected as the best, second, third and third Iranian scientist in Nanoscience. Moreover, he elected as the best researcher of his country in basic science at 2009. He is now the editorial board member of MATCH and the Editor-in-Chief of the Bulletin of the Iranian Mathematical Society & Iranian Journal of Mathematical Chemistry.

Friday 15 June, 11:00 - 11:30

Prediction of stability constants of coordination compounds from their connectivity indices

Nenad Raos

There are many factors influencing the stability of coordination compounds, and therefore it is not surprissing that threre is yet no general model for prediction of stability constants. However, Dr. Miličević and me developed a number of QSPR models for the prediction of stability constants of coordination compounds based on connectivity index ${}^{3}\chi^{v}$. Recently, we developed models for simultaneous prediction of stability constants measured at different ionic strengths, temperature and in solutes of different compositions (*i.e.* water/organic mixtures).

NENAD RAOS

Institute for Medical Research and Occuptional Health, Zagreb, Croatia

Nenad Raos was born 1951 in Zagreb, Croatia. After graduating chemistry at Faculty of Sciences, Zagreb, he was permanently employed at the Institute for Medical Research and Occupational Health. In 1983 he finished his PhD thesis on the molecular-mechanics modelling of coordination compounds at the Zagreb University. He is autor and coautor of about 70 papers in theoretical and bioinorganic chemistry. In the last ten years he was developing QSPR models for the prediction of stability constants of coordination compounds.

Besides his scientific work, Dr. Raos is very profluent science writer. He is the autor of 12 books and seven exhibitions in popular science at the Technical Museum, Zagreb. Since 2006 Dr. Raos is editor-in-chief of *Priroda*, the oldest Croatian science magazine.

Friday 15 June, 11:30 - 12:00

Interpolation method and topological indices

Sandi Klavzar

Polynomial interpolation can be used to obtain closed formulas for topological indices of infinite series of molecular graphs. The method will be discussed on 1- and
2-parametric families of graphs. Its advantages and limitations will be pointed out. The method will be illustrated for 1- and 2-parametric families on fullerenes C_{12k+4} and on nanocones $CNC_k[n]$, respectively. The indices considered will be the Wiener index, the edge Wiener index, the eccentric connectivity index, the reverse Wiener index, and the Szeged index. This is a joint work with Yaser Alizadeh and in part also with Ali Iranmanesh.

SANDI KLAVZAR

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PERSONAL: *Born:* February 5, 1962, Ljubljana, SI; *Spoken languages*: Slovenian, English, German, Croatian and Serbian.

EDUCATION: Ph.D. in Mathematics, University of Ljubljana, SI; M.S. in Computer Science, University of Ljubljana, SI; B.S. in Technical Mathematics, University of Ljubljana, SI.

ACADEMIC EXPERIENCE: Professor of Discrete and Computational Mathematics, University of Maribor; Professor of Mathematics, University of Ljubljana; Advisor of 11 Ph.D. students in Mathematics; External member of several Ph.D. and Habilitation committees: Austria, France, India, Serbia. Longer research visits at Montanuniversität Leoben, Austria and Universität Bielefeld, Germany.

RESEARCH FIELDS: Discrete and Computational Mathematics, Combinatorics with Graph Theory, Applications of Discrete Mathematics in Chemistry, Tower of Hanoi Problems.

PROFESSIONAL EXPERIENCE/ LEADERSHIP: Chair of the Depatment of Mathematics, University of Maribor, SI, 1992 – 1994; Chair of the Department of Mathematics of Institute of Mathematics, Physics and Mechanics, SI, 2003 – 2007; Vice-president of the International Academy of Mathematical Chemistry 2011 – ; President of the The Society of Mathematicians, Physicists and Astronomers of Slovenia, 2010 – ; Permanent researcher and project leader of Institute of Mathematics, Physics and Mechanics, SI, 1990 –.

PROFESSIONAL ACTIVITIES: Organizer or member of organizing committees of numerous international scientific meetings; Member of international professional societies AMS and ICA; Member of editorial boards of Ars Mathematicae Contemporanea, Asian-European Journal of Mathematics, Discrete Applied Mathematics, Discussiones Mathematicae Graph Theory, European Journal of Combinatorics, Iranian Journal of Mathematical Sciences and Informatics, MATCH Communications in Mathematical and in Computer Chemistry. Guest editor of several special issues of international journal (MATCH Comm. Math. Comput. Chem., Discrete Appl. Math., Discrete Math., Discuss. Math. Graph Theory, European J. Combin.); Active participant at numerous conferences and scientific meetings and invited speaker at conferences in Austria, Canada, China, Czech Republic, France, Germany, India, Iran, Japan, Poland, Romania, Slovenia, Spain, Taiwan.

HONORS AND GRANTS: Slovenian national award (Zoisovo priznanje) for important scientific achievements in the area of graph theory, 2000; Slovenian national award (Zoisova nagrada) for highest achievements in mathematics, 2007.

PUBLISHED WORK: Over 180 publications and 1000 citations in MathSciNet. Books:

1. W. Imrich, S. Klavžar, *Product Graphs : Structure and Reognition*, Wiley-Intersciences Series in Discrete Mathematics and Optimization, Wiley, New York, 2000, XV+358 pp.
2. W. Imrich, S. Klavžar, D.F. Rall, *Topics in Graph Theory*, A K Peters, Wellesley, Massachusetts, 2008., XIV+205 pp.
3. R. Hammack, W. Imrich, S. Klavžar, *Handbook* of *Product Graphs, Second Edition*, CRC Press, Boca Raton, 2011, XVIII+518 pp.

Friday 15 June, 12:00 - 12:45

Molecules in silico

Adalbert Kerber

The talk gives a brief description of the molecular structure generator MOLGEN, version 5.0, and its applications, in particular to the generation of molecular libraries, to molecular structure generation and to the generation of patent libraries in chemistry.

ADALBERT KERBER

Math. Department
University of Bayreuth, Germany

Born 29.06.1939 he studied mathematics and physics in Münster and Gießen, PhD in Gießen 1966 (on representation theory of symmetric groups), habilitation 1970, Prof. in Aachen from 1972 until 1979, when he moved to Bayreuth, where he run the chair Mathematik II at the Department of Mathematics until 2008, when he retired. He was one of the founders of MATCH in 1975 that he managed for several years as Editor-in-Chief. He ran several research projects on representation theory and on mathematical chemistry. One of the main results was MOLGEN, a molecular structure generator that exists in various versions and extensions like MOLGEN-MS, MOLGEN-COMB and MOLGEN-QSPR. He is the author of several books on representation theory, on finite group actions and on mathematics for economy. A joint book on Molecules in Silico is in preparation.

FRIDAY, 15 JUNE

AFTERNOON SESSION : 14:00 – 15:30

Graph theory and topological indices

Chair: Nikolay Zefirov

Friday 15 June, 14.00 - 14:30

Some new applications of graph eigenvalues and spectral moments

Jorge Galvez

Two cases are presented in which the use of certain graph-theoretical descriptors, namely eigenvalues and spectral moments of the edge adjacency matrix weighted by edge degrees, play a significant role.
The first case illustrates how the use of the eigenvalues enables a good discrimination between the scaffolds and frameworks of drug and non-drug compounds, what is of interest in drug design.
In the second case it is demonstrated that if the adequate graphs are properly assigned to each one of the twelve elementary particles of the Theoretical Physics' standard model, it can be predicted with an excellent accuracy the masses of these particles, using only spectral moments. It is shown thereby that the elementary particle's masses follow a very simple topological pattern, which is consistent with what stated in the perturbative string theory. This result opens a suggestive pathway to predict particle properties from graph-theoretical algorithms.

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Director of the Molecular Connectivity and Drug Design Unit. University of Valencia (Spain).
Author of over 140 scientific publications (some 100 in international journals) as well as 70 communications to congresses (44 of them international ones) and scientific meetings.
Author of several patents, national and international, on new lead compounds. Among them stand analgesics, anti-neoplastics, anti-malarials and anti-Alzheimer. Direction of First degree and Ph. D. theses, masters. Award-winner of two research prizes. Direction and partnership in national and internacional research projects. Lectures given in Spain, Italy, United Kingdom, Argentina , India, France, Croatia, Rumania and USA. Memberships: National Geographic Society (1976), Spanish Royal Society of Chemistry (1995), Group of Electrochemistry (1995), Academy of Medicine of Valencia (Spain) (1997), International Academy of Mathematical Chemistry,European Academy of Mathematical Chemistry (2007) and Spanish Society of Green Chemistry (2007). Scientific advisor of Medisyn Technologies (Minessota, USA) (since 2002).

Friday 15 June, 14:30 - 14:50

Integral eigenvalues of Cayley graphs

Bojan Mohar

A graph is called integral if all eigenvalues of its adjacency matrix are integers. Integral Cayley graphs of abelian groups have been classified Bridges and Mena (1982). In our work we obtain a new, character theoretic proof of their result and provide extension to hamiltonian groups in the the generalized setting of multigraphs. This is joint work with Roi Krakovski, Matt DeVos, and Azhvan Sheikh Ahmady.

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2. Speci_c Areas: Topological Graph Theory, Graph Coloring, Algebraic Graph Theory, Graphs and Matrices, In_nite Graphs, Algorithms and Complexity, Structural Graph Theory and Graph Minors.

Scientic Degrees
1. 1986, Ph. D. in Mathematics, University of Ljubljana, Slovenia.
2. 1984, M. Sc. in Mathematics, University of Ljubljana, Slovenia.
3. 1979, B. Sc. (Dipl. Ing.) in Mathematics, University of Ljubljana, Slovenia.

Scientic and Teaching Activity
1. 2004-present: Full Professor and Canada Research Chair, Simon Fraser University
2. October-November 2002, Visiting Researcher, McGill University, Montreal, Quebec, Canada
3. February 2002, Visiting Professor (Directeur d'études invité), École des Hautes Études en Sciences Sociales, Paris, France.
4. February 1998, Visiting Professor, Technische Universit□at Ilmenau, Germany
5. 1996-present Full Professor, University of Ljubljana
6. 1996/97 Visiting Professor, Georgia Institute of Technology, Atlanta, Georgia
7. 1991-1996 Associate Professor, University of Ljubljana
8. 1988-1991 Docent (Assistant Professor) of Discrete Mathematics and Computer Science, University of Ljubljana 1
9. 1988 Visiting Fulbright Scholar, Ohio State University, Columbus, Ohio
10. 1986/87 Postdoctoral Fellow, Simon Fraser University, Burnaby, B. C.
11. 1982{88 Assistant for Mathematics, University of Ljubljana

Friday 15 June, 14.50 - 15:10

Graphs and thermodynamics

Lionello Pogliani

Many equations of thermodynamics have an internal structure that goes well beyond their direct thermodynamic meaning. It is a structure that has to do in some way both with directed and simple graphs. In fact, the most important thermodynamic relationships, either centered on the energy or in the entropy concept, can be modeled by the aid of two types of directed graphs, the energy-digraph, or E-digraph, and the entropy digraph, or S-digraph. A set of meaningful symmetry operations done with simple graphs on the two previous digraphs allow to obtain, in automatic way, the most famous thermodynamic relationships, and allow also to solve thermodynamic problems.

LIONELLO POGLIANI
University of Calabria
Cosenza, Italy

Lionello Pogliani is a retired Professor in physical chemistry. He covered this position during the last twenty-two years at the University of Calabria, Cosenza, Italy. Up to next July his address will be: Chemistry Department, University of Calabria, 87036 Rende (CS), Italy, lionp@unical.it.
He graduated in Chemistry at the University of Firenze, Italy. He received his postdoctoral training at the department of Molecular Biology of the C. E. A. (Centre d'Etudes Atomiques) of Saclay, France, at the Physical Chemistry Institute of the Technical and Free University of Berlin, and at the Pharmaceutical Department of the University of California, San Francisco, CA. Here, he coauthored an experimental work, which was awarded with the GM Neural Trauma Research Award. He spent his sabbatical years at the Centro de Quimica-Fisica Molecular of the Technical University of Lisbon (Portugal) and at the Department of Physical Chemistry of the Faculty of Pharmacy of the University of Valencia-Burjassot (Spain). He contributed around 180 papers in experimental, theoretical, and didactical fields of physical chemistry, including chapters in specialized books, and made around 50 symposium presentations. He published a book on numbers 0, 1, 2, and 3 in the MCM (N° 2) series of MATCH. He is a member of the International Academy of Mathematical Chemistry (IAMC).

Friday 15 June, 15:10 - 15:30

Design of bivalent ligands as neuroprotective and anti-cancer compounds

Vladimir Palyulin

A series of new monovalent and bivalent positive AMPA receptor modulators have been designed using a number of techniques (QSAR, structure generation, analysis of binding sites, molecular docking and molecular dynamics, manual design of best fitting ligands using X-ray data for the dimer of the AMPA receptor glutamate binding domain). The best simultaneous fitting to the both binding sites of positive AMPA receptor modulators was found for a series of 3,7-diazabicyclo[3.3.1]nonane derivatives, though several other kinds of bivalent ligands with different spacers also fitted well into these sites. The bivalent modulators demonstrated the outstanding potency significantly exceeding the potency of monovalent liigands. *In vivo* studies of these compounds revealed the pronounced cognition-enhancing properties for them as well as the formation of stronger memory.
The potency of the designed bivalent ligands of tubulin (which is a target for anti-cancer drugs) also significantly exceeded the potency of monovalent ligands in *in vitro* experiments.

VLADIMIR PALYULIN
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Dr. Vladimir A. Palyulin graduated from Lomonosov Moscow State University in 1974. Since that time, he occupied research positions at the Department of Chemistry of the MSU; since 1998, he is a leading researcher. He received PhD degree in 1985 under the supervision of Professor Zefirov. Since 1988, he is the head of a research group. In 2008, he was elected a member of the International Academy of Mathematical Chemistry. He received the first prize of the D. I. Mendeleev USSR Chemical Society. His research interests include theoretical organic chemistry, mathematical chemistry, computer-aided molecular design of physiologically active compounds and medicinal chemistry.

Summer School 2012 of Marie Curie ITN Environmental ChemOinformatics, Verona 11-15 June 2012

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