International Conference on

MASS SPECTROMETRY AND PROTEOMICS

June 25-27, 2018 | Dublin, Ireland

DAY 1

Keynote Forum

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Magnus S Magnusson
University of Iceland, Iceland

Biography

Magnus S Magnusson is a Research Professor. He did his PhD from University of Copenhagen. He is the author of the T-pattern model and detection algorithms implemented in THEMETM (PatternVision.com). He has focused on real-time organization of behavior, co-directed DNA analysis, published numerous papers and given invited talks and keynotes at international conferences in ethology, psychology, neuroscience, mathematical sciences, science of religion, proteomics and mass spectrometry, and at universities in Europe, USA and Japan. He is the Associate Professor and Deputy Director 1983-1988, Anthropology Laboratory, Museum of Mankind, National Museum of Natural History, Paris. Repeatedly invited Professor in Psychology and Ethology (the biology of behavior) at the University of Paris, V, VIII and XIII. Since 1991, Founder and Director of the Human Behavior Laboratory (hbl.hi.is), University of Iceland. Since 1995, he is in collaboration between 32 universities on Methodology for the Analysis of Social Interaction (MASI) initiated at the University Rene Descartes, Sorbonne, Paris based on Magnusson's analytical model.

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ONLY LARGE-BRAIN MASS-SOCIETIES AS BEST REFLECTIONS OF THOSE OF PROTEINS: T-PATTERNS, SELF-SIMILARITY AND STRING-CONTROL ACROSS MANY ORDERS OF MAGNITUDE IN TIME AND SPACE

This work goes back to the 1970's, inspired among other by the ethological (biology of behavior) work of Nico Tinbergen, Konrad Lorenz and von Frish, rewarded in 1973 by a shared Nobel Prize in Medicine or Physiology, for their study of insect, animal and human behavior. Inspired also by studies of primate social groups and E. O. Wilson's monumental research on social insect societies evolved over hundreds of millions of years. If a mass society is taken to mean a society of, for example, more than ten thousand individuals, these are very rare in nature and mostly found in insects and in humans, the only large-brained species where mass-societies exist, and only in modern humans, that is, evolving in cultural time (tens of thousands of years), essentially a biological eye blink. The smallest individuals were insects. None were parts of others and there was no mentioning of self-similarity. Fractals, A.I., computational pattern detection or nanoscience were barely mentioned. Access to computers with adequate software was rare. Comparisons of animal and human mass societies were mostly between those of insects and "modern" humans. Technological and scientific progress now facilitates cell biology research, where striking analogies have appeared between human mass-societies and the "Cell City" of proteins. The present work has to a large extent focused on the development of mathematical/statistical pattern types, the T-pattern and the T-system, which have allowed detection of self-similarity of various kinds from the temporal scales of human and neuronal interactions to the spatial nano scale of DNA and proteins, notably mobile and motor neurons bringing to light, essential similarities between protein and mass societies of modern humans, absent in all other mass societies. The time may thus have come for "nano-ethology" add a new focus to the study of molecules within the biological cell.

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Yong-Xi Li
Medpace Bioanalytical Laboratories, USA

Biography

Yong-Xi Li has completed his Postdoctoral trainings at Kansas State University, Cornell University, USA. Currently, he is Executive Director at Medpace Bioanalytical Laboratories after he served as vice presidents at XenoBiotic Labs and Ricerca Bioscience. His experiences are focusing on bioanalysis: TK, PK, ADA, NAB (and Cell base Nab), PD markers including method developments, validations, sample analysis for small molecule, protein and antibody therapies. He and his group developed many such applications by using LC-MS/MS and immunoassays (ELISA, ECL and Flow cytometry.....). He is author, co-author of more than 150 papers, book, presentations in reputed journals, and conferences. He is also serving as an organizing committee member for one of biotech conferences.

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A SENSITIVE METHOD FOR QUANTITATIVE ANALYSIS OF OLIGONUCLEOTIDE THERAPEUTIC DRUG IN HUMAN PLASMA BY LC-MS/MS METHODOLOGY

Synthetic and polymeric oligonucleotides (RNA, DNA and their analogs) have been developed in recent many years as therapeutic drugs against a wide range of diseases conditions. During the studies, a challenge step is bioanalytical analysis. Although Scientists have used many technologies, for example gels, capillary electrophoresis, high-resolution ion exchange chromatography and MALDI etc. for the analysis in biofluids since 1970s, successful bioanalytical technologies have been eventually focused on ELISA and LC-MS/MS methodologies. However the ELISA assay cannot distinguish, in the most cases, full length parent oligonucleotides from shortened species of their metabolites or other endogenous molecules, thus preventing it from being widely utilized in metabolism studies, especially for quantitation analysis. In our laboratories, we have developed or validated LC-MS/MS Methods for 13-mer to 20-mer oligonucleotides (and analogs) which are more accurately and specifically than ELISA methods developed at our laboratories in biological matrixes, e.g. plasma, urine, and tumor samples. In this presentation, our specified extraction procedures of oligonucleotides from plasma: liquid-liquid, solid phase SPE, and immunoprecipitation extractions will be discussed. Meanwhile LC-MS/MS conditions, ion pair reagents in UPLC and multi-charge species situation in mass spectrometer will be presented. Under our optimized conditions, 10-20 ng/mL of LLOQ were reached which is the one of most sensitive method. Methods are used for pre-clinical and clinical sample analysis in our laboratories.

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Alon Savidor, J Syst Biol Proteome Res 2018, Volume 2

Alon Savidor

Weizmann Institute of Science, Israel

Biography

Alon Savidor completed his PhD at 2008 from the University of Tennessee and The Oak Ridge National Laboratory at Tennessee, USA. He completed his post-doctorate fellowship at the Tel Aviv University, Israel, at 2013, and since then he is a staff scientist at the Nancy and Stephen Grand Israel National Center for Personalized Medicine, Weizmann Institute of Science, Israel.

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DATABASE INDEPENDENT PROTEIN SEQUENCING (DIPS) ENABLES FULL-LENGTH DE-NOVO PROTEIN AND ANTIBODY SEQUENCE DETERMINATION

De-novo, full-length sequencing of unknown proteins such as antibodies or constituents of metaproteomes remains a challenging problem. Traditional 'bottom-up' proteomics approaches use proteolytic digestion, LC-MS/MS and database searching to elucidate peptide identities and their parent proteins. Protein sequences absent from the database cannot be identified, and even if present in the database, complete sequence coverage is rarely achieved even for the most abundant proteins in the sample. To this aim we have developed Database Independent Protein Sequencing (DiPS), a novel method for unambiguous, rapid, database independent, full-length protein sequencing. The method is based on non-enzymatic, semi-random cleavage of the protein by microwave assisted acid hydrolysis (MAAH), LC-MS/MS analysis, peptide de novo sequencing, extraction of peptide tags, and their assembly into a consensus sequence using a novel algorithm named Peptide Tag Assembler (pTA). The method, which was recently published, now also allows for differentiation between the isobaric leucine and isoleucine residues, and was successfully applied to a variety of proteins and clinically relevant antibodies.

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Jelena T
Vilnius University, Lithuania

Biography

Jelena T has completed her PhD in 2000 at the Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania. She is a senior research fellow at the Vilnius University, Lithuania. She has more than 150 publications that have been cited over 200 times, and her publication H-index is 7.

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ELECTRON-IMPACT FRAGMENTATION OF THE GLUTAMINE AMINO ACID MOLECULE: EXPERIMENTAL AND THEORETIC STUDIES

The results on the mass-spectrometric studies of the glutamine molecule ($C_5H_{10}N_2O_3$) fragmentation are presented to show the simplest theoretical approach to predict the products of the fragmentation reactions under the low (<150 eV) energy electron impact. This approach allowed us to identify the chemical composition of the most abundant glutamine molecule fragments, evaluate their absolute appearance energies E_{ap} and find the most probable pathways of their formation. For example, among a series of ionic fragments identified, the absolute appearance energy E_{ap} of the m/z=41 a.m.u. fragment was found by us for the first time both experimentally and theoretically. The experimental appearance energy E_{ap} obtained using the Marquardt-Levenberg fitting procedure was found to be 12.2 eV. Our theoretical DFT-calculation for different conformers of the $C_2H_3N_+$ and C_2HO^+ ions having the above mass has shown that in the near-threshold electron energy region the most probable is production of the CHCHNH$^+$ (i.e. $C_2H_3N^+$) ion with the appearance energy E_{ap} of 10.34 eV, when this fragment is directly formed from the parent glutamine molecule. The details of the approach and the results of the quantum-chemical analysis of the possible ion production pathways for glutamine will be presented at the Conference. This study is closely related to the 'Mass Spectrometry in Metabolomics' and 'Mass Spectrometry in Drug Discovery' research programmes.

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Luis F Guido, J Syst Biol Proteome Res 2018, Volume 2

Luis Guido

University of Porto, Portugal

Biography

Luis Guido has completed his PhD in Analytical Chemistry from University of Porto (2004). He is Assistant Professor at the Faculty of Sciences, University of Porto, since 2004. He has published more than 40 papers in SCI indexed journals and 2 book chapters. He is reviewer for more than 10 peer-reviewed journals and editorial board member of several journals.

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USE OF GAS CHROMATOGRAPHY-MASS SPECTROMETRY FOR DETERMINATION OF CHEMICAL MARKERS OF BEER AGING

Beer stability is a major concern for the brewing industry, as beer characteristics may be subject to significant chemical changes during storage. A variety of flavors may arise, depending on the beer type and the storage conditions. This work aims at evaluating the impact of storage conditions, mainly the temperature and oxygen, on beer off-flavours development. The profile of some volatile compounds, such as phenylacetaldehyde, phenylethyl acetate and ethylphenyl acetate, responsible for the development of sweet and honey like flavors, has been monitored throughout natural (20ºC) and forced aging (37ºC). Beers maintained at 4ºC have been used as controls. The effect of the total oxygen content has also been investigated. The flavor stability of beers has been further evaluated by a well-trained sensory panel, and the sensory data was compared with the volatile compounds profile. Phenylethyl acetate proves to be a better chemical marker of temperature than phenylacetaldehyde. During storage at 20ºC, an increase up to 6-fold was observed for the phenylethyl acetate content. On the other hand, phenylacetaldehyde can be considered the best chemical marker of the presence of oxygen duting storage at 20ºC, as an increase up to 12-fold of the initial concentration was observed.

This work was funded by FCT/MEC through national fund and co-financed by FEDER (UID/QUI/50006/2013 – POCI/01/0145/FEDER/007265), under the Partnership Agreement PT2020.

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Yuichi Negishi, J Syst Biol Proteome Res 2018, Volume 2

Yuichi Negishi

Tokyo University of Science, Japanl

Biography

Yuichi Negishi received his Ph.D. degree in 2001 from Keio University, Japan. He is the professor of Tokyo University of Science, Japan. He has over 140 publications that have been cited over 7,200 times. In his publications, 10 papers are/were categorized to Top 1% Cited Papers. His publication H-index is 45. He has been awarded several prizes, including the PCCP Prize (2007), CSJ Award for Young Chemists (2008), Japan Society of Molecular Science Award for Young Chemists (2012), and Yagami Prize (2017).

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HIGH-PERFORMANCE LIQUID CHROMATOGRAPHY MASS SPECTROMETRY OF THIOLATE-PROTECTED METAL CLUSTERS

Small thiolate-protected gold clusters have attracted considerable attention as new functional nanomaterials because they have size-specific properties and functions that are not found for bulk gold. In particular, hydrophilic thiolate-protected gold clusters (hereinafter referred to as hydrophilic gold clusters) exhibit high biocompatibility and luminescence quantum yield in addition to pollution-free properties. Therefore, hydrophilic gold clusters are expected to be used in biomedical and environmental applications. Replacing some of the Au atoms in these clusters with different elements may impart them with even more useful functions. However, the synthesis of hydrophilic metal clusters has been less studied because of the complexity involved in evaluating the mass distributions of product mixtures. In this work, we found two hydrophilic interaction liquid chromatography (HILIC) columns for high-performance liquid chromatography (HPLC) suitable for the high-resolution separation of hydrophilic metal clusters. The mass distributions of the product mixtures of hydrophilic metal clusters were evaluated via HPLC mass spectrometry (LC/MS) using these HILIC columns. Consequently, we observed multiple clusters that had not been previously reported for glutathionate (SG)-protected gold clusters ($Au_n(SG)_m$). Additionally, we demonstrated that $Au_{n-x}M_x(SG)_m$ alloy clusters (M = Ag, Cu, or Pd) in which part of the Au in the $Au_n(SG)_m$ cluster is replaced by a heteroelement can be synthesized, similar to the case of hydrophobic alloy clusters. It is easy to evaluate the mass distributions of hydrophilic metal clusters using this method. Thus, remarkable progress in the synthesis techniques of hydrophilic metal clusters through the use of this method is anticipated, as is the situation for hydrophobic metal clusters.

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