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OMICS Group International is an amalgamation of Open Access publications and worldwide international science conferences and events. Established in the year 2007 with the sole aim of making the information on Sciences and technology 'Open Access', OMICS Group publishes 400 online open access scholarly journals in all aspects of Science, Engineering, Management and Technology journals. OMICS Group has been instrumental in taking the knowledge on Science & technology to the doorsteps of ordinary men and women. Research Scholars, Students, Libraries, Educational Institutions, Research centers and the industry are main stakeholders that benefitted greatly from this knowledge dissemination. OMICS Group also organizes 300 International conferences annually across the globe, where knowledge transfer takes place through debates, round table discussions, poster presentations, workshops, symposia and exhibitions.

#### **About OMICS Group Conferences**

OMICS Group International is a pioneer and leading science event organizer, which publishes around 400 open access journals and conducts over 300 Medical, Clinical, Engineering, Life Sciences, Pharma scientific conferences all over the globe annually with the support of more than 1000 scientific associations and 30,000 editorial board members and 3.5 million followers to its credit.

OMICS Group has organized 500 conferences, workshops and national symposiums across the major cities including San Francisco, Las Vegas, San Antonio, Omaha, Orlando, Raleigh, Santa Clara, Chicago, Philadelphia, Baltimore, United Kingdom, Valencia, Dubai, Beijing, Hyderabad, Bengaluru and Mumbai.

# Frontiers of Metabolomics in Biomedical research.

Vladimir Tolstikov, PhD

#### **Metabolomics**



PubMed shows an exponential growth in the number of publications

# **Systems Biology**



# **NMR for Metabolomics**



The high reproducibility of NMR-based techniques gives this method a number of advantages over other analytical techniques in large-scale and long-term metabolomic studies, such as epidemiological studies.

High-Resolution NMR Spectrometers: 300 MHz (7Tesla)-900 MHz (21Tesla). Cryo-probe, flow through sampling.

In vivo MRI/MRS Scanners: 1.5 Tesla (80 MHz) – 7 Tesla (300 MHz) 4.7 Tesla (200 MHz) – 14 Tesla (600MHz)

What are NMR limitations? SENSITIVITY!!!! -NMR detects only high-abundant metabolites (micromole to millimole range); -NMR suffers from signal overlap between individual metabolites;

#### **Mass Spectrometry For Metabolomics**

- GC-MS GC-EI/CI-HRMS < 1ppm</li>
- CE-MS CE-HRMS < 5ppm

Inductive ionization (no contact)

- LC-MS > LC-HRMS < 5ppm
- LC-MS/MS systems \_\_\_\_\_\_\_ 10-50 folds more sensitive.
- HPLC >>> UPLC and HILIC.
- Lipidomics infusion-shotgun
- LC-MS-NMR
  LC-HRMS-HRNMR

What are MS limitations? - A great deal of information.

# Metabolomics Data

- Preprocessing: normalization, transformation, missing values and filtering
- Statistical analysis: unsupervised techniques, supervised techniques
- Metabolic biomarkers
- Metabolic biomarkers performance tests
- Pathway enrichment analysis
- Integration into omics data

### **Quality Assurance**

We have to distinguish between quality assurance as best scientific practice for withinlaboratory use and the regulatory use, which will typically require formal validation and acceptance of the method and a formal quality regime such as Good Laboratory Practice. Quality systems (QS) were developed originally for industrial production but they were increasingly introduced in many other sectors and organizations to establish a formal structure for establishing quality criteria.

Quality control procedures also include the estimation of the stability of the analytical procedure, the use of standards, error estimation of data reproducibility and criteria for data inclusion (and exclusion).

M. Bouhifd, et al. Review: Toxicometabolomics, J. Appl. Toxicol. 2013

### **Translational Medicine**

 Metabolomics technology is being utilized across the spectrum of drug discovery and development; from the assessment of unanticipated biochemical sequel of target engagement in transgenic models to monitoring media content to improve the efficiency of the manufacture of biologics, the impact of the technology is expanding dramatically. Applications critical for the pharmaceutical industry include translational medicine, biomarker discovery, and patient stratification. Technological innovation and cultural acceptance will be necessary to optimally use this powerful tool.

D. G. Robertson & U. Frevert, Metabolomics in Drug Discovery and Development. Clinical Pharmacology & Therapeutics (**2013**); 94 5, 559–561.

Human tissue samples are crucial in the early validation of one's genetically derived hypothesis, and validation requires precise biopsy methods and serial tissue sampling over the course of the disease. Potent new analytical tools for obtaining and analyzing human materials can facilitate corroboration of ideas: single-cell analyses; clinical-grade liquid chromatography–mass spectrometry; three-dimensional (3D) and 4D cultures; multiplex tissue-based assays and readout capabilities; and next-generation bioinformatic, metabolomics, and proteomics methods.

#### Citation:

E. A. Zerhouni, Turning the Titanic. *Sci. Transl. Med.* **6**, 221ed2 (2014). Elias A. Zerhouni is President of Global R&D, Sanofi, 75008 Paris, France, and former Director of the U.S. National Institutes of Health.

#### Metabolic Disease Type 2 diabetes

- ......This study—involving more than 8200 subjects—first examined whether established T2D risk factors previously identified from studies of European and Asian populations were also implicated in the Americas. At 82% of sites, the reported risk allele was the same across ancestries, with several sites also convincingly associated in the Americas. Next, they reported two new associations, one of which was tagged by a risk haplotype carrying four missense variants in the *SLC16A11* gene (which encodes a solute carrier) and was replicated in ~22,000 additional samples.
- Further expression studies of *SLC16A11* in HeLa cells (which do not normally express the gene) followed by metabolomics experiments revealed increases in triacylglycerol, a biomarker with previous reported association with T2D in prospective cohorts. In a final note of interest, the group also found that the risk haplotype matched a sequence from an unpublished genome of a Neanderthal from Denisova Cave, with identity extending a massive 73 kilobase in haplotype carriers.....

Benjamin F. Voight. Sci Transl Med 22 January **2014**: Vol. 6, Issue 220, p. 220ec16



# Conclusions

- Metabolomics evolved from routine phenotyping assay into advanced tool in biomedical research.
- Metabolomics is gaining confidence.
- Metabolomics needs advanced bioinformatics support.
- New developments and initiatives become available due to significant progress in analytical techniques and data handling methodologies.

#### Let Us Meet Again

#### We welcome you all to our future conferences of OMICS Group International

Please Visit: <u>www.omicsgroup.com</u> <u>www.conferenceseries.com</u> <u>www.pharmaceuticalconferences.com</u> <u>www.metabolomicsconference.com</u>