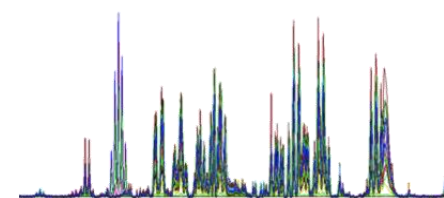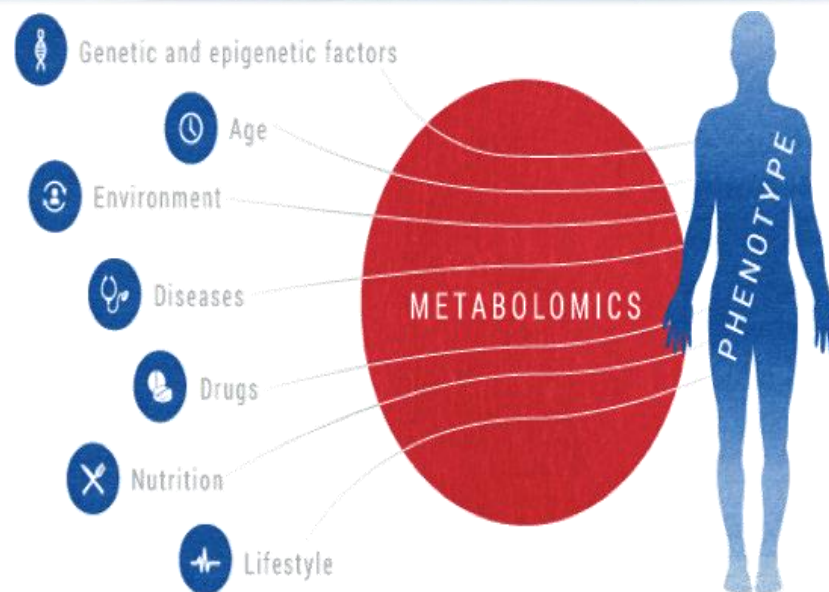26. **Understanding the effects of non-saccharomyces yeasts on sauvignon blanc aroma profiles using metabolomics and sensory analysis.** M. E. Beckner Whitener, J. Stanstrup, V. Panzeri, S. Carlin, B. Divol, M. Du Toit, U. Vrhovsek

27. **M-IOLITE: An Integrated suite for the streamlining metabolomic analysis.** C. Maga-Nteve, M.I.Klapa

28. **Metabolomics in brain research; a case study of adult onset hypothyroidism reveals brain regional variation and sex differentiation.** Vasilopoulou C.G., Margarity M., Klapa M.I.

29. **Studying the effects of combined high salinity and elevated CO_2 on tomato development using GC-MS and LC-MS metabolomic analysis** M.E. Papadimitropoulos, G.Tooulakou, I. Giannakos, C. Kittas, P. Kalaitzis, M. I. Klapa

30. **NMR and LC-HRMS based metabolomics for the discovery of novel bio-active small molecules from marine synbionts.** E.Baira, D. Benaki, E. Gikas, E. Mikros, N. Fokialakis

31. **A new data processing procedure of UPLC-ESI(-)-HRMS untargeted metabolomics employing spectral slicing and stitching** Baira E., Siapi E., Zoumpoulakis P ., Deligeorgis S-G., Skaltsounis A-L., Gikas E.

32. **XCMS optimization in high-throughput LC-MS**. C. Beirnaert, M.Cuykx, A.Covaci, K.Laukens.

33. **Exploitation of global microbial biodiversity for the Discovery of Novel Cosmeceuticals using LC-HRMS based metabolomics** C. Almeida, N. Lemonakis, Jose Perez del Palacio, N.Tsafantakis, V. González-Menéndez, I. González, F. Reyes E.Gikas, N. Fokialakis, O. Genilloud

34. **How do I analyze a double-blind crossover study? A nutri-metabolomics example.** N. Lemonaki., M. Halabalaki., V. Mougios., E. Mikros ., N. Bliziotis .,A.L. Skaltsounis E. Gikas .

35. **Alteration in the liver metabolome of rats with metabolic syndrome after treatment with hydroxytyrosol. An MS and NMR based metabolomics study .** I.V.Dagla, N. Lemonakis, H. Poudyal, L. Brown, D. Benaki, Al. Skaltsounis, E. Mikros, E. Gikas

36. **A metabolomics study for the discovery of multiply sclerosis biomarkers in cerebrospinal Fluid by HRMS and NMR** C. Tsiagkas, D. Benaki, N. Lemonakis, A. Ioannidis' S. Chatzipanagiotou, C. Nikolaou, M. Anagnostouli, E. Mikros, E. Gikas

37. **Could Pharmacometabolomics uncover the resistance to clopidogrel?** A.I. Milioni, D. Benaki, M.E. Tsoumani, N. Lemonakis, E. Gikas, A.D. Tselepis, E. Mikros

4th Workshop
on Holistic Analytical Methods
for Systems Biology Studies
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Aristotle University Thessaloniki, Greece
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14. **QSRR modeling for metabolite standards analyzed by two different chromatographic columns and by using multiple linear regression (MLR).** Ch. Zisi, I. Sampsonidis, A. Pappa-Louisi, P. Nikitas, M. Witting, H. Gika, S. Kalogiannis, G. Theodoridis

15. **NMR-driven identification of biomarkers related with blood neoplastic diseases –Analysis of data acquired in two different magnetic fields (600&700MHz).** S.A. Chasapi, L. Tenori, A. Karela, S.E. Bariamis, K. D. Marousis, A. Spyridonidis, C.Luchinat, G A. Spyroulias

16. **Comprehensive two-dimensional gas chromatography coupled with ToF-MS, a powerful tool for analysis of the volatomes of grapes and wines.** S. Carlin, K. Suklje, F. Mattivi, U. Vrhovsek

17. **"Continuous or Interval Aerobic Training" A comparative H[1] –NMR metabonomics study on athletes.** C.A. Chatziioannou, A. Zafeiridis, H. Sarivasiliou, K. Dipla, I. S. Vrabas, P. Zoumpoulakis, C. Baskakis, A. Pechlivanis, G.Theodoridis

18. **Retention index determination of 94 metabolites with LC-MS/MS: Preliminary Data** O. Begou, H. G. Gika, G. Theodoridis, M. Witting, M. Quilliam.

19. **Assessing validation parameters in multitargeted LC-MS/MS method for metabolite profiling application** E. Tsakelidou, C. Virgiliou, H. Gika, N. Raikos, G. Theodoridis

20. **Untargeted and targeted metabolomics of rat caecum extracts for the discovery of exercise biomarkers.** O. Deda, T. Panagoulis, H. Gika, I. Taitzoglou, V. Mougios, G. Theodoridis

21. **Study of derivatization reactions prior to GC-MS metabolomics analysis. Preliminary Results** G. Moros, A.C Chatziioannou, H. Gika, N. Raikos, G.Theodoridis

22. **Development of a Multi–Analyte hydrophilic interaction Liquid Chromatography-Mass Spectrometry (HILIC-UPLC-MS/MS) method for the quantitation of polar metabolites in Bee products** Pina A., Theodorou H., Begou O., Kalogiannis S., Tananaki C., Thrasyvoulou A., Zotou A., Gika H., Theodoridis G.

23. **Application of HILIC-UPLC-MS/MS method for the analysis of polar metabolites in honey and crude royal jelly** Theodorou H., Pina A., Begou O., Kanelis D., Dimou M., Kalogiannis S., Tananaki C., Thrasyvoulou A., Zotou A., Gika H., Theodoridis G.

24. **Differences in metabolomics profile of three exercise modes in individuals with metabolic syndrome** Siopi, A., Deda, O., Manou, V., Kellis, S., Theodoridis, G., Christoulas, K., Mougios, V

25. **Urinary Metabolomics profile of newborns of the western Greece region through high-definition NMR analysis.** S. E. Bariamis, I. Georgakopoulou, S.A. Chasapi, K. Marousis, S. Fouzas, A. Tsidoni, M. Spraul, H. Schäfer, C. Luchinat, A. Varvarigou, G.A. Spyroulias

POSTERS

1. **A novel platform for automated GC-MS based metabolomics.** Opekarová I., Moos M., Řimnáčová L., Zahradníčková H., Hušek P., Šimek P.

2. **A sample preparation approach for metabolic profiling of human saliva of smokers and nonsmokers by high performance liquid chromatography.** E. Barda, V.Sakkas, T. Albanis

3. **Assessment of a fast analytical methodology for urinary metabolomic biomarkers by liquid chromatography – mass spectrometry.** S. Vika, V. Sakkas, A.Makis, T. Palianopoulos, T. Albanis

4. **Boron nitrogen coumarin derivatives: Three metabolite building books blocks in one small molecule.** K. Theodoridis, H. G. Gika, E. Kotali, P.A. Harris, A. Kotali

5. **Analysis of the vector's bias in the spread of Malaria in the different incidence rates.** Sungchan Kim, Sungchan Kim, Il Hyo Jung

6. **Dynamical behavior of tumor viral therapy with immune response: Deterministic and stochastic analysis.** Kwang Su Kim, Sangil Kim and Il Hyo Jung

7. **The effect of electronic cigarettes smoking cessation: A mathematical modeling approach.** Jae Hun Jung, Il Hyo Jung

8. **Exploring the link between maternal dietary protein intake and the metabolic profile of second trimester amniotic fluid.** Fotiou M., Fotakis Ch., Tsakoumaki F., Kyrkou Ch., Athanasiadou E., Tsiaka T., Dimitropoulou A., Menexes G., Tarlatzis C.B., Biliaderis G. C., Athanasiadis P.A., Zoumpoulakis P., Michaelidou A.M.

9. **LC-MS/MS metabolic profiling study of shikonin's cytotoxicity on Huh-7 cell line.** E.D. Spyrelli, A. Nakas, C. Virgiliou, A.E. Koletti, H. Gika, G. Mossialos, V.P. Papageorgiou, A.N. Assimopoulou

10. **NMR Metabolomics-based study of DSS induced colitis in rats and effect of shikonin.** A. Nakas, O. Deda, I. Taitzoglou, T. Poutahidis, G. Theodoridis, V.P. Papageorgiou, A.N. Assimopoulou, H. Gika

11. **Metabolomics in epidemiologic studies of type II diabetes mellitus: Implications for the exposome.** Xanthi D. Andrianou, Stephanie Gaengler, Konstantinos C. Makris

12. **Determination of tungsten in plant and soil samples by inductively coupled plasma-mass spectrometry.** Ümran Seven Erdemir, Hülya Arslan, Gürcan Güleryuz, Seref Güçer

13. **ICP-MS as a holistic analytical method for the study of phytoaccumulation of heavy metal: A case study of erysimum pulchellum (wild) gay.** Ümran Seven Erdemir, Hülya Arslan, Gürcan Güleryuz, Seref Güçer

Sunday 17/4		Fundamentals Moderators: Kvalheim/Mougios/Wilson	Speaker	Institution
8:30	9:15	**Registration**		
9:15	9:30	Introduction and Overview	G. Theodoridis	Aristotle Univ.
9:30	10:05	The Path from Profile to Mechanistic Understanding	I.D. Wilson	Imperial College
10:05	10:35	Endogenous Metabolic Personalized Theranostics	T. Lundstedt	Uppsala Univ.
10:35	11:00	MultiOmics for Exposome Analysis	D. Sarigiannis	Aristotle Univ.
11:00	11:30	**Break**		
11:30	12:00	Analysis of Metabolomics Data	O. M. Kvalheim	Bergen Univ.
12:00	12:30	Metaboscape – A Metabolite Profiling Pipeline Driven by Automatic Compound Identification, or How to Link Hram QTOF Plant Metabolomics Data to Biology	A. Barsch	Bruker, Germany
12:30	13:00	A Novel Lipid Screening Platform Allowing a Complete Solution	D. Merkel	Sciex Europe
13:00	14:30	**Lunch/ Poster Session**		
14:30	15:00	The Importance of Human Volatilome	A. Agapiou	Univ. Cyprus
15:00	15:05	Introduction to Seminars	G. Theodoridis	Aristotle Univ.
15:05	16:10	**Seminar 1** Metabolite Identification	M. Witting	Helmholtz Inst. Munich
16:10	16:40	**Break**		
16:40	17:45	**Seminar 2** Data Treatment: Freeware and Commercial Software	P. Franceschi	FEM IASMA Trento
17:45	18:00	**Closure Wrap-Up**		

Monday 18/4		Life Sciences Moderators: Kaklamanos/Raikos/Franceschi	Speaker	Institution
9:00	9:30	Exercise Metabonomics	V. Mougios	Aristotle Univ.
9:30	9:55	Feature Selection Methods for Early Predictive Biomarker Discovery Using Untargeted Metabolomic Data	E. Pujos-Guillot	INRA, France
9:55	10:20	Utilizing an IMS-DIA-MS Workflow to Characterize and Quantify the Lipidome of a Patient Cohort Clinically Diagnosed with Obesity or Diabetes	I. Edwards	Waters UK
10:20	10:40	Mitochondria and Brain Disorders: A Systems Biology Approach	M. Filiou	Max Plank Psychiatry
10:40	11:00	Pharmacometabolomics-Guided Pharmacogenomics in Precision Medicine	T. Katsila	Univ. Patras
11:00	11:30	**Break**		
11:30	12:00	Metabolomics as Part of an Integrated Approach for the Identification of Predictive Markers of Type 2 Diabetes	B. Comte	INRA, France
12:00	12:30	Metabo-Auto, A Novel Platform for Automated Metabolomic GC-MS Profiling	P. Simek	Biology Centre, CZ
12:30	13:00	Metformin treated rats show alterations in the gut microbiome and plasma levels of bile acids, lipids and small molecules	P. Vorkas	Imperial College
13:00	14:30	**Lunch/ Poster Session**		
14:30	14:45	**St1:** Biomarker Discovery in Embryometabolomics Project	C. Virgiliou	Aristotle Univ.
14:45	15:00	**St2:** A Study of Exercise and Ageing Through Metabolomics-based Analysis	O. Deda	Aristotle Univ.
15:00	15:15	**St3:** Neonatal Sepsis Biomarker Discovery	C. Chatziioannou	Aristotle Univ.
15:15	16:15	**Seminar3** Untargeted / SemiTargeted LC-MS Metabolomics	P. Vorkas A. Pechlivanis	Imperial College
16:15	16:40	**Break**		
16:40	17:40	**Seminar 4** Targeted Metabolomics LC-MS/MS	F. Michopoulos C. Virgiliou	AZ UK/ Aristotle Univ.
17:40	17:55	**Closure Wrap-Up**		

Tuesday 19/4		Plant/Food/Nutrition Moderators: Simek/Kalogiannis/ /Klapa	Speaker	Institution
9:00	9:30	Fingerprinting the Salinity Effect on Large-Scale Hydroponic Tomato Cultures Using Integrated GC- and LC-MS Metabolomics	M. Klapa	FORTH Patras
9:30	10:00	Metabolomics in Systems Biology, Integrating Multiomics Data	K. Aliferis	Athens Agricult. Univ.
10:00	10:30	Challenges on analysing double-blind crossover experiments. A nutri-metabolomics example	N. Lemonakis	Athens Univ.
10:30	11:00	Food Analysis and Authentication Using NMR Based Metabolomics	A. Spyros	Univ. of Crete
11:00	11:30	**Break**		
11:30	11:55	Recent Developments in Food Screening by NMR	C. Napoli	Bruker, Italy
11:55	12:20	LC-MS Metabolomics Shows a Smart Way to Reduce Sulfites in Wine	P. Arapitsas	FEM IASMA Trento
12:20	12:40	Bioactive Properties, Mineral Contents, Phenolic Compounds and Fatty Acid Composition of Rose, Blackberry and Redberry Fruits Growing in Belarus	M. M. Özcan	Univ. Selcuk, Turkey
12:40	13:00	Advanced Metabolomics Study of Fungal Metabolism and its Regulation	I. Kalabokis	Athens Agricult. Univ.
13:00	14:30	**Lunch/ Poster Session**		
14:30	15:15	Round Table: Users Needs a Bottom Up Approach	Food Sciences and Regulation Scientists	
15:15	16:00	**Seminar 5:** NMR Based Metabolomics. Tips And Tricks	D. Benaki A. Pechlivanis	Athens Univ./ Imperial College
16:00	16:25	**Break**		
16:25	17:30	**Seminar 6:** GC-MS Metabolomics: Best Practice for Data Acquisition, Normalization and Analysis	G. Tooulakou C. Magka	FORTH Patras
17:30	17:45	**Closure Wrap-Up, Farewell**		