



A SEEDRUG Conference

NMR Applications in Life Sciences

Exploring Peptides & Proteins

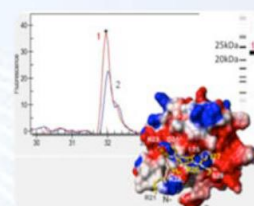
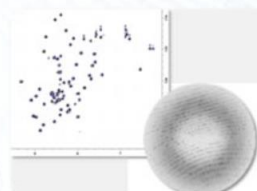
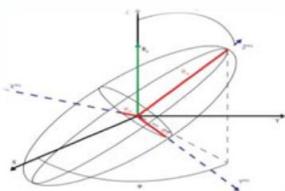
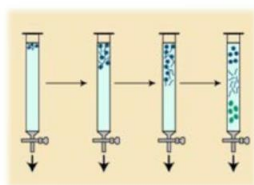
A multi-pronged approach to Structure-Function Linkages in Biomedicine



A Tribute to Paul Cordopatis

18-20 June 2015

Cultural and Conference Center, University of Patras, Greece



Opening Lecture: Kurt Wüthrich, Nobel Laureate 2002 (Chemistry)
(ETH, Zurich, CH & The SCRIPPS, La Jolla, USA)

Invited Speakers:

Umit Akbey (Berlin, DE)
Frederick Allain (Zurich, CH)
David Andreu (Barcelona, SP)
Kleomenis Barlos (Patras, GR)
Somer Bekiroglou (TUBITAK, TR)
Rolf Boelens (Utrecht, NL)
John Christodoulou (London, UK)
Isabella Felli (Florence, IT)
Ioannis Gerothanassis (Ioannina, GR)
Torsten Herrmann (Lyon, FR)
Ferenc Hudecz (Budapest, HU)
Babis Kalodimos (New Jersey, US)
Michael Kokkinidis (Heraklion, GR)
George Kokotos (Athens, GR)
Stamatios Liokatis (Berlin, DE)
Claudio Luchinat (Florence, IT)
Theodosia Maina (Athens, GR)

Jean Martinez (Montpellier, FR)
Minos Matsoukas (Patras, GR)
Evangelos Moudrianakis (Baltimore, US)
Hartmut Oschkinat (Berlin, DE)
Kyriacos Petratos (Heraklion, GR)
Janez Plavec (Ljubljana, SI)
Miquel Pons (Barcelona, ES)
Aikaterini Rousaki (Heraklion, GR)
Michael Sattler (Munich, DE)
Harald Schwalbe (Frankfurt, DE)
Nikolaos Sgourakis (California, US)
Georgios Skretas (Athens, GR)
Manfred Spraul (Karlsruhe, DE)
Kostas Tripsianes (Brno, CZ)
Giannis Vakonakis (Oxford, UK)
Maria Zervou (Athens, GR)

Organizing Committee:

George A. Spyroulias (Chairman), Stavros Topouzis (WP Leader), Manolis Foustieris, Fotini N. Lamari, Vassiliki Magafa, Nikos Moschonas, Sotirios Nikolaropoulos, George Pairas, Theodore Tselios

Further Information: <http://www.seedrug.upatras.gr/>

ANTIOXIDANT EFFECTS OF WINE EXTRACTS TREATED IN A CELL CULTURE AS PROBED BY COMET ASSAY AND NMR BASED METABOLOMICS

Paris Christodoulou^{1,2}, Katerina Kokkotou^{1,3}, Maria Liouni², Panagiotis Georgiadis^{1*},
Maria Zervou^{1*}

¹*Institute of Biology, Medicinal Chemistry and Biotechnology, National Hellenic Research Foundation, 48 Vas. Constantinou Ave., Athens 11635, Greece,*

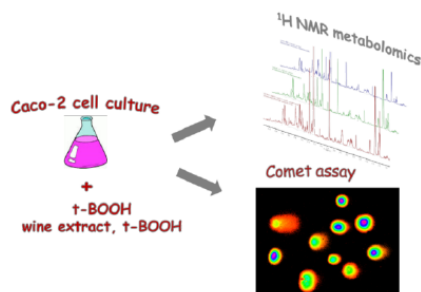
²*Department of Chemistry, University of Athens, Panepistimiopolis Zografou, Athens 15771, Greece,*

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This study applies the single-cell gel electrophoresis (comet assay) and NMR-based metabolomics to investigate the potential beneficial effect of wine extract (lyophilized) on a) cell viability and b) enhancement of cell antioxidant defenses, in Caco2 cells subjected to t-BOOH-induced oxidative stress. The Caco-2 cell line, an immortalized line of heterogeneous human epithelial colorectal adenocarcinoma cells, is a valuable *in vitro* tool for studies related to the analysis of specific types of DNA damage¹. The comet assay was exploited to measure DNA strand breaks as a measure of oxidative damage². In parallel, the extracellular footprint and intracellular fingerprint were assessed by ¹H NMR metabolomics in order to detect metabolic perturbations induced by t-BOOH treatment and addition of t-BOOH in a cell culture pretreated with wine extract.

Trypan blue exclusion test of cell viability determined that a 48 hour treatment of Caco2 with wine extract in concentration ranging from 0.5 to 5000 µg/ml did not cause any cytotoxic effects. Comet assay measurements (expressed as %DNA in tail) showed that the 48-hour wine extract-treatment of Caco2 cells at concentrations of 0.5, 5, 50, 500 and 5000 µg/ml could inhibit oxidative DNA damage induced by the addition of 250 µM t-BOOH for 1 hour, by 26.1%, 50.1%, 37.3%, 45.8% and 48.0%, respectively.

The workflow for cell extracts NMR-based metabolomics applied a dual methanol/chloroform extraction protocol as previously described³ and profiling of the aqueous phase. Preparations with no agent, with addition of t-BOOH and with wine-extract pretreatment followed by addition of t-BOOH have been studied. The identification of metabolites has been assisted by the use of 2D NMR spectroscopy, metabolomic databases as Chenomx NMR Suite and literature data³. Preliminary results on the comparative survey between the three substrates suggest a potential role of NMR metabolomics in the identification of novel biomarkers associated with the protective effects of wine against oxidative DNA-damage.



References:

¹ Rao, A. L.; Sankar, G. G. Caco-2 cells: An overview. *JPR HC*, 2009, 2, 260.

² Wenjuan, L.; Michael, A. M.; Wei-Guo Z. The comet assay: A sensitive method for detecting DNA damage in individual cells. *Methods*, 2009, 48, 46–53.

³ Insong, J.L.; Kellie, H.; Guoyun, B.; Michael, S.; NMR Metabolomic Analysis of Caco-2 Cell Differentiation. *J. Proteome Res.*, 2009, 8, 4104–4108

Chemical Biology

- P223** *Synthesis of Alkyl and Aryl Sulfonyl p-Pyridine Ethanone Oximes as Efficient DNA Photo-Cleavage Agents*
Andreou N.-P.¹, Dafnopoulos K.¹, Koumbis A. E.², Koffa M.¹, Psomas G.³, Fylaktakidou K. C.^{1*}
¹Laboratory of Organic, Bioorganic and Natural Product Chemistry, Molecular Biology and Genetics Department, DUTH, Alexandroupolis, Greece
²Laboratory of Organic Chemistry, Chemistry Department, AUTH, Thessaloniki, Greece
³Laboratory of Inorganic Chemistry, Chemistry Department, AUTH, Thessaloniki, Greece
 *e-mail: kfylakta@mbg.duth.gr
- P224** *DNA Photo-Cleavage Activity of Stable Sulfonyl Amidoximes: Structure Activity Relationship Studies*
Papastergiou A.¹, Koffa M.¹, Koumbis A. E.², Perontsis S.³, Psomas G.³, Fylaktakidou K. C.^{1*}
¹Laboratory of Organic, Bioorganic and Natural Product Chemistry, Molecular Biology and Genetics Department, DUTH, Alexandroupolis, Greece
²Laboratory of Organic Chemistry, Chemistry Department, AUTH, Thessaloniki, Greece
³Laboratory of Inorganic Chemistry, Chemistry Department, AUTH, Thessaloniki, Greece
 *e-mail: kfylakta@mbg.duth.gr
- P225** *Recently developed SMAC mimetics in synergy with oncogene inhibitors and apoptosis agents overcome resistance of cancer cells to apoptosis*
Philippos Perimenis, Alexandra Voulgari, Apostolos Galaris, Alexandros Pintzas
 Institute of Biology, Medicinal Chemistry and Biotechnology, National Hellenic Research Foundation, 48 Vas Constantinou Avenue, 116 35 Athens, Greece
- P226** *Epigenome-wide association study (EWAS) on the effects of Persistent Organic Pollutants*
Marios Gavriil¹, Ingvar A. Bergdahl², Domenico Palli³, Hannu Kiviranta⁴, Sotirios Kyrtopoulos¹, Paragiotis Georgiadis^{1*}
¹National Hellenic Research Foundation, Institute of Biology, Medical Chemistry and Biotechnology, Greece
²Department of Biobank Research, and Occupational and Environmental Medicine, Department of Public Health and Clinical Medicine, Umeå University, Sweden
³The Institute for Cancer Research and Prevention
⁴Chemical Exposure Unit, National Institute for Health and Welfare, Kuopio, Finland
 *email: panosg@eie.gr
- P227** *Dissociated Glucocorticoids: Development of novel compounds and evaluation of their activity*
Dimitra Siakouli, Athina Boulaka, Constantinos Potamitis, Konstantinos Papavasileiou, Marina Roussaki, Theodora Calogeropoulou, Manthos G. Papadopoulos, Panagiotis Zoumpoulakis, Maria Zervou, Michael N. Alexis, Dimitra J. Mitsiou*
 Institute of Biology, Medicinal Chemistry & Biotechnology, National Hellenic Research Foundation, Athens, Greece
 *e-mail: dmitsiou@eie.gr
- P228** *Enhancement of cell defence upon treatment with natural antioxidant matrices probed by comet assay and NMR-based metabolomics*
Paris Christodoulou^{1,2}, Katerina Kokkotou^{1,3}, Maria Liouni², Panagiotis Georgiadis^{1*}, Maria Zervou^{1*}
¹Institute of Biology, Medicinal Chemistry and Biotechnology, National Hellenic Research Foundation, 48 Vas. Constantinou Ave., Athens 11635, Greece,
²Department of Chemistry, University of Athens, Panepistimiopolis Zografou, Athens 15771, Greece
³Department of Pharmacognosy and Chemistry of Natural Products, School of Pharmacy, University of Athens, Panepistimiopolis Zografou, Athens 15771, Greece
 *e-mail: panosg@eie.gr; mzervou@eie.gr
- P229** *A screening of extracts from the Greek flora for the identification of skin protective agents*
Maria T. Angelopoulou¹, Ana Charalambides¹, Anastasios Kouroumalis¹, Adamantia Papadopoulou¹, Sotirios-Spyridon Vamvakas¹, Marianna Ralli², Nektarios Aligiannis³, Alexios-Leandros Skaltsounis³, Harris Pratsinis¹, Dimitris Kletsas^{1*}
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²Korres S.A. Natural Products, 57th klm. Athens-Lamia National Road, 32011, Inofyta, Greece
³Department of Pharmacognosy & Natural Products Chemistry, Faculty of Pharmacy, University of Athens, Zografou 15771, Greece,
 *e-mail: dkletsas@bio.democritos.gr
- P230** *Solubility enhancement of small molecules: From bioassays to crystallography – a TNF study*
Anthi Mettou^{1,2}, Polyxeni Alexiou³, Elias Couladouros³, Liepouri Fotini⁴, Maranti Anna⁴, Strongilos Alexandros⁴, Jean-Luc Ferrer⁵ and Kontopidis George^{1,2*}
¹Veterinary School, University of Thessaly, Karditsa, Greece
²Centre for Research and Technology of Thessaly (CERETETH), Volos, Greece
³Agricultural University of Athens, Athens, Greece
⁴Pro-ACTINA SA, Athens, Greece
⁵Institute de Biologie Structurale (IBS), Grenoble, France
 *email: gkontopidis@vet.uth.gr
- P231** *Virtual screening towards the selective inhibition of BRAFV600E oncoprotein*
 Constantinos Potamitis, Maria Goulielmaki, Alexander Pintzas, Panagiotis Zoumpoulakis, Maria Zervou
 National Hellenic Research Foundation, Institute of Biology, Medicinal Chemistry & Biotechnology
 Vassileos Constantinou 48, 11635 Athens, Greece
 e-mail: pzoump@eie.gr, mzervou@eie.gr

**ΕΛΛΗΝΙΚΗ ΕΤΑΙΡΕΙΑ ΒΙΟΛΟΓΙΚΩΝ ΕΠΙΣΤΗΜΩΝ
HELLENIC SOCIETY FOR BIOLOGICAL SCIENCES**

**40^ο ΕΤΗΣΙΟ ΣΥΝΕΔΡΙΟ
40th ANNUAL CONFERENCE**

ΠΡΟΓΡΑΜΜΑ PROGRAMME

24-26 Μαΐου 2018

May 24-26, 2018

**BEROIA
VERIA**

**ΣΥΝΔΙΟΡΓΑΝΩΣΗ
ΔΗΜΟΣ ΒΕΡΟΙΑΣ**



92	ΜΙΑ ΝΕΑ ΜΕΘΟΔΟΣ ΓΙΑ ΤΟΝ ΕΝΤΟΠΙΣΜΟ ΚΑΙ ΤΗΝ ΚΑΤΗΓΟΡΙΟΠΟΙΗΣΗ ΥΠΟΔΟΧΕΩΝ ΜΕ ΕΝΕΡΓΟΤΗΤΑ ΤΥΡΟΣΙΝΙΚΗΣ ΚΙΝΑΣΗΣ (RTKs) ΜΕ ΤΗ ΧΡΗΣΗ PROFILE HIDDEN MARKOV MODELS
	Σπανογιάννης Γ., Μπαλτούμας Φ.Α., Λίτου Ζ.Ι., Χαμόδρακας Σ.Ι., Οικονομίδου, Β.Α. Εθνικό & Καποδιστριακό Πανεπιστήμιο Αθηνών, Τμήμα Βιολογίας, Τομέας Κυτταρικής Βιολογίας & Βιοφυσικής
93	ΕΥΡΕΙΑ ΑΝΑΛΥΣΗ ΕΠΙΓΟΝΙΔΙΩΜΑΤΟΣ (EWAS) ΣΕ ΑΙΜΑ ΟΜΦΑΛΙΟΥ ΛΩΡΟΥ ΤΗΣ ΜΗΤΕΡΑΣ ΤΗΣ ΣΤΑΤΙΣΤΙΚΗΣ ΟΜΑΔΑΣ ΠΛΗΘΥΣΜΟΥ RHEA. ΣΥΣΧΕΤΙΣΗ ΤΩΝ ΜΕΘΥΛΙΩΣΕΩΝ ΤΟΥ ΓΟΝΙΔΙΩΜΑΤΟΣ ΤΟΥ DNA ΜΕ ΤΟ ΜΗΤΡΙΚΟ/ΝΕΟΓΝΙΚΟ BMI ΚΑΙ ΤΟΥΣ ΟΡΓΑΝΙΚΟΥΣ ΡΥΠΑΝΤΕΣ
	Χριστοδούλου Πάρης, Λαδουκάκης Ευθύμιος, Βαφειάδη Μαρίνα, Χατζή Λύδα, Kiviranta Hannu, Rantakokko Ranu, Κυρτόπουλος Σωτήριος, Γεωργιάδης Παναγιώτης Τμήμα Βιοχημείας και Βιοτεχνολογίας, Πανεπιστήμιο Θεσσαλίας, Εθνικό Ίδρυμα Ερευνών Ινστιτούτο Βιολογίας Φαρμακευτικής Χημείας και Βιοτεχνολογίας, Εθνικό Μετσόβιο Πολυτεχνείο, Σχολή Χημικών Μηχανικών Εργαστήριο Βιοτεχνολογίας, Τομέας Κοινωνικής Ιατρικής Τμήμα Ιατρικής Πανεπιστήμιο Κρήτης, Department of Health Protection Chemicals and Health Unit National Institute for Health and Welfare Kuopio Finland
94	ΤΑΥΤΟΠΟΙΗΣΗ ΡΥΘΜΙΣΤΙΚΩΝ ΣΤΟΙΧΕΙΩΝ DNA ΑΠΑΡΑΙΤΗΤΩΝ ΓΙΑ ΤΗ ΣΤΟΧΑΣΤΙΚΗ ΕΚΦΡΑΣΗ ΓΟΝΙΔΙΩΝ ΚΑΤΑ ΤΟΝ ΚΥΤΤΑΡΙΚΟ ΕΠΑΝΑΠΡΟΓΡΑΜΜΑΤΙΣΜΟ
	Βαλάκος Δημήτριος, Κλάγκου Ελευθερία, Σιανίδης Γεώργιος, Παππαδοπούλου Μαρία Δέσποινα, Πολύζος Αλέξανδρος, Αγγελόπουλος Μάριος, Θάνος Δημήτριος Εργαστήριο Μοριακής Βιολογίας, Ίδρυμα Ιατροβιολογικών Ερευνών Ακαδημίας Αθηνών
Συνεδρία 19η Συντονιστής: Αναπλ. Καθηγητής Π. Λιάκος, Τμήμα Ιατρικής, Πανεπιστήμιο Θεσσαλίας	
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95	ΔΙΕΡΕΥΝΗΣΗ ΜΙΤΟΧΟΝΔΡΙΑΚΩΝ ΠΟΛΥΜΟΡΦΙΣΜΩΝ ΣΕ ΜΕΛΗ ΤΟΥ ΣΥΜΠΛΕΓΜΑΤΟΣ CERATITIS FAR (DIPTERA: TEPHRITIDAE)
	Μάρκου Αγγελική, Αυγουστίνος Αντώνιος, Μπούρτζης Κωνσταντίνος, Δροσοπούλου Ελένη Τομέας Γενετικής, Ανάπτυξης και Μοριακής Βιολογίας, Τμήμα Βιολογίας, Σχολή Θετικών Επιστημών, Αριστοτέλειο Πανεπιστήμιο Θεσσαλονίκης Insect Pest Control Laboratory, Joint FAO/IAEA Programme of Nuclear Techniques in Food and Agriculture, Seibersdorf, Vienna, Austria
96	ΕΚΦΡΑΣΗ ΤΟΥ ΓΟΝΙΔΙΟΥ TGM2 ΣΤΑ ΜΥΕΛΟΔΥΣΠΛΑΣΤΙΚΑ ΣΥΝΔΡΟΜΑ ΚΑΙ Ο ΡΟΛΟΣ ΤΗΣ ΑΥΤΟΦΑΓΙΑΣ ΣΤΗΝ ΠΑΘΟΓΕΝΕΙΑ ΤΗΣ ΝΟΣΟΥ
	Τσεκούρα Γ. ¹ , Σταυροπούλου Μ. ¹ , Κοντανδρεοπούλου Χ-Ν. ² , Πάργα Α. ¹ , Μπορονικόλα Γ. ¹ , Αλεπόρου Β. ¹ , Βύνιου Ν. ² , Παπασιδέρη Ι. ³ , Κόλλια Π. ¹ ¹ Τομέας Γενετικής και Βιοτεχνολογίας, Τμήμα Βιολογίας, Εθνικό & Καποδιστριακό Πανεπιστήμιο Αθηνών ² Α΄ Παθολογική Κλινική, Ιατρική Σχολή, Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών, Αθήνα, ³ Τομέας Βιολογίας Κυττάρου και Βιοφυσικής, Τμήμα Βιολογίας, Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών
97	Ο ΡΟΛΟΣ ΤΗΣ ΑΥΤΟΦΑΓΙΑΣ ΣΤΗΝ ΠΑΘΟΓΕΝΕΙΑ ΤΩΝ ΜΥΕΛΟΔΥΣΠΛΑΣΤΙΚΩΝ ΣΥΝΔΡΟΜΩΝ
	Τσεκούρα Γεωργία, Κοντανδρεοπούλου Χριστίνα Νεφέλη, Μπορονικόλα Γεωργία, Ταλιουράκη Αγγελική, Ρούσσου Σταματία, Διαμαντόπουλος Παναγιώτης, Βύνιου Νόρα, Αλεπόρου Βασίλική, Παπασιδέρη Ισιδώρα, Κόλλια Παναγούλα Τομέας Γενετικής και Βιοτεχνολογίας, Τμήμα Βιολογίας, Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών, Αθήνα, Α΄ Παθολογική Κλινική, Ιατρική Σχολή, Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών, Αθήνα, Τομέας Βιολογίας Κυττάρου και Βιοφυσικής, Τμήμα Βιολογίας, Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών



DNA damage/repair

P180

Antioxidant effects of wine extract in cell culture probed by comet assay and NMR-based metabolomics

Paris Christodoulou^{1,2}, Katerina Kokkotou^{1,3}, Maria Liouni², Panagiotis Georgiadis^{1*}, Maria Zervou^{1*}

¹Institute of Biology, Medicinal Chemistry and Biotechnology, National Hellenic Research Foundation, 48 Vas. Constantinou Ave., Athens 11635, Greece, ²Department of Chemistry, University of Athens, Panepistimiopolis Zografou, Athens 15771, Greece, ³Department of Pharmacognosy and Chemistry of Natural Products, School of Pharmacy, University of Athens, Panepistimiopolis Zografou, Athens 15771, Greece

This study applies the *in vitro* comet assay and NMR-based metabolomics to investigate the potential protective effect of wine extract (lyophilized) on cell viability as well as the antioxidant defenses activation in Caco2 cells submitted to t-BOOH-mediated oxidative stress. The Caco-2 cell line, an immortalized line of heterogeneous human epithelial colorectal adenocarcinoma cells, is a valuable *in vitro* tool for studies related to the analysis of specific types of DNA damage¹. The comet assay, was exploited to measure the DNA strand breaks in eukaryotic cells². In parallel, the extracellular footprint and intracellular fingerprint were assessed by ¹H NMR metabolomics in order to detect metabolic perturbations induced by t-BOOH treatment and addition of t-BOOH in a cell culture pretreated with wine extract.

Trypan blue exclusion test of cell viability determined that a 48 hour treatment of cells with wine extract in concentration ranging from 0.5 to 5000 µg/ml did not cause any cytotoxic or genotoxic effects. Moreover, comet assay measurements (expressed as %DNA in tail) showed that the 48-hour wine extract-treatment of cells at concentrations of 0.5, 5, 50, 500 and 5000 µg/ml could inhibit DNA damage induced by the addition of 250 µM t-BOOH for 1 hour, by 26.1%, 50.1%, 37.3%, 45.8% and 48.0%, respectively.

The workflow for cell extracts NMR-based metabolomics applied a dual methanol/chloroform extraction protocol as previously described³ and profiling of the aqueous phase. Preparations with no agent, with addition of t-BOOH and with wine-extract pretreatment followed by addition of t-BOOH have been studied. The identification of metabolites has been assisted by the use of 2D NMR spectroscopy, metabolomic databases as Chenomx NMR Suite and literature data³. Preliminary results on the comparative survey between the three substrates point to the potential of NMR metabolomics to target biomarkers associated with the protective effects of wine against DNA-damage.

¹ Rao, A. L.; Sankar, G. G. Caco-2 cells: An overview. *JPR HC*, 2009, 2, 260.

² Wenjuan, L.; Michael, A. M.; Wei-Guo Z. The comet assay: A sensitive method for detecting DNA damage in individual cells. *Methods*, 2009, 48, 46–53.

³ Insong, J.L.; Kellie, H.; Guoyun, B.; Michael, S.; NMR Metabolomic Analysis of Caco-2 Cell Differentiation. *J. Proteome Res.*, 2009, 8, 4104–4108

Πρόγραμμα Program



TIME	AUDITORIUM	CONFERENCE HALL
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Chairs: D. Stravopodis, R. Tenta

Chairs: D. Vlachakis, P. Makrythanasis

09:00-10:30

ORAL PRESENTATIONS 1

Molecular & Cellular Basis of Human Diseases I (O1-O6)

ORAL PRESENTATIONS 2

Systems Biology & Bioinformatics (O7-O12)

10:30-11:00

PLENARY LECTURE 1

What I cannot create, I do not understand:
dissecting insecticide resistance via genetic
manipulation and genome modification
in *Drosophila*

Speaker: Vassilis Douris
University of Ioannina

11:00-11:30

C o f f e e B r e a k

Chairs: R. Matsa, S. Taraviras

11:30-13:00

ORAL PRESENTATIONS 3

Stem Cells, Tissue Morphogenesis
& Regeneration (O13-O18)

13:00-13:30

PLENARY LECTURE 2

Gene regulation networks in neural
development

Speaker: Panagiotis Politis
BRFAA

13:30-14:00

PLENARY LECTURE 3

Linking adipose tissue gene regulation
to disease risk in the Greek population

Speaker: Antigoni Dimas
B.S.R.C. "Alexander Fleming"

Chair: K. Stathopoulos

*Lab Supplies
Scientific*

14:00-14:30

SPONSORED LECTURE 1

What is that? Can work with a small amount
of RNA, Is highly reactive, Has a very short
processing time, And leads to full length
clones

Speaker: Jürgen Lünzer
Managing Director Nippon Genetics

14:30-16:30

POSTER SESSION 1 (P1-P86)

- P50 The effect of dendrimers and magnetic nanoparticles on human blood lymphocytes**
Maria-Anthi Kakavoulia^{1,2*}, Maria Karakota¹, Martha Kaloyianni-Dimitriadi², Eleftherios Halevas³, Marina Sagnou³, Georgios Koliakos¹
¹Laboratory of Biological Chemistry, Medical School, Aristotle University of Thessaloniki, Greece
²Laboratory of Animal Physiology, School of Biology, University of Thessaloniki, Greece
³Institute of Biosciences and Applications, National Centre for Scientific Research, "Demokritos", Athens, Greece
 *email: mariaantk@bio.auth.gr
- P51 Development of New Selective Glucocorticoid Receptor Agonists: hit-to-lead optimization**
Dimitra Siakouli, Eftichia Kritsi, Alia-Christina Tenchiu, Nikiforos Travlos, Georgios Panagiotou, Athina Boulaka, Katerina Nasaj, Constantinos Potamitis, Olga Kirkilessi, Andromachi Tzani, Theodora Calogeropoulou, Cécile Arbez-Gindre, Michael N. Alexis, Ioannis D. Kostas, Maria Zervou, Dimitra J. Mitsiou*
 Institute of Chemical Biology, National Hellenic Research Foundation, Athens, Greece
 *e-mail: dmitsiou@eie.gr
- P52 Biological Evaluation of a 2-(4'-Aminophenyl)benzothiazole Diagnostic Agent for Breast Cancer**
Barbara Mavroidi¹, Marina Sagnou¹, Antonio Shegani², Maria Paravatou-Petsotas², Ioannis Pirmettis², Minas Papadopoulos², Maria Pelecanou^{1*}
¹Institute Biosciences and Applications, National Centre for Scientific Research "Demokritos", Athens, Greece
²Institute of Nuclear & Radiological Sciences & Technology, Energy & Safety, National Center for Scientific Research "Demokritos", Athens, Greece
 *e-mail: pelmar@bio.demokritos.gr
- P53 Identification and biochemical characterization of a poly-ADP-ribose polymerase like enzyme in *Thermus thermophilus* HB8**
Papi Rigini, Tsianiou Athanasia, Velali Ekaterini, Pantazaki Anastasia*
 Lab of Biochemistry, Dep of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, 54124, Greece
- P54 Anti-inflammatory and antioxidant effect of cannabidiol on adult male mice with induction of inflammation**
Konstantinos Mesiakaris¹, Marilena Kaperoni¹, Korina Atsopardi^{1,2*}, Marigoula Margarity², Konstantinos Poulas¹
¹Laboratory of Molecular Biology and Immunology, Department of Pharmacy, University of Patras, Greece
²Laboratory of Human and Animal Physiology, Department of Biology, University of Patras, Greece
- P55 Evaluation of anxiety behavior and acetylcholinesterase's isoforms activity of adult mice after cigarette smoke exposure**
Korina Atsopardi^{1,2*}, Konstantinos Kanellopoulos Kotsonis², Vasileios Kafantogias², Theofanis Tsiliras², Konstantinos Poulas¹, Marigoula Margarity²
¹Laboratory of Molecular Biology and Immunology, Department of Pharmacy, University of Patras, Rio 26504, Greece
²Laboratory of Human and Animal Physiology, Department of Biology, University of Patras, 26504, Rio, Greece
- P56 Effect of N-acetylcysteine on anxiety-like behavior and acetylcholinesterase's isoforms activity in specific brain regions of pentylenetetrazol-treated mice**
Despina Matsentidou¹, Eleni Makarouni¹, Korina Atsopardi^{1,2*}, Maria Anesti³, Marigoula Margarity¹, Nikolaos T. Panagopoulos¹
¹Laboratory of Human and Animal Physiology, Department of Biology, University of Patras, Rio 26504, Greece
²Laboratory of Molecular Biology and Immunology, Department of Pharmacy, University of Patras, Rio 26504, Greece
³Laboratory of Developmental Biology, Department of Biology, University of Patras, Rio 26504, Greece
- P57 In vitro fermentation of edible Greek mushrooms of high β -glucan content by human Gut Microbiota: cytotoxic, genotoxic and metabolic profiling of the products**
Athina Boulaka^{1*}, Paraschos Christodoulou^{1*}, Marigoula Vlassopoulou^{1,3}, Georgios I. Zervakis², Adamantini Kyriacou³, Maria Zervou¹, V. Pletsas¹, Panagiotis Georgiadis¹
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³Harokopio University, Department of Nutrition and Dietetics, 17676 Kalithea, Greece
 *Athina Boulaka and Paraschos Christodoulou equally contributed to this work

Cell Communication & Signaling

- P58 Flavone quercetin inhibits IL-1 β -induced inflammation in human osteoarthritis chondrocytes**
Aliki-Ioanna Apostolou^{*}, Maria-Elpida Christopoulou, Alexios J. Aletras
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ΑΝΑΡΤΗΜΕΝΕΣ ΑΝΑΚΟΙΝΩΣΕΙΣ (POSTERS)

POSTER 05

NMR metabolic profiling of Greek Pistacia lentiscus leaves and fruit extracts for the identification of biomarkers with skin beneficial effects

Cheilari Antigoni¹, Papalexis Patroklos¹, Vontzalidou Argyro¹, Dina Evanthia¹, Smyrnioudis Ilias², Aligiannis Nektarios¹

¹Department of Pharmacognosy and Natural Products Chemistry, Faculty of Pharmacy, National and Kapodistrian University of Athens, ²Chios Mastic Gum Growers Association

POSTER 06

Έλεγχος επουλωτικής δράσης in vivo αιθερίων ελαίων από φυτά του γένους Hypericum L., που φύονται στον ελλαδικό χώρο

Γραφάκου Μαρία-Ελένη¹, Διαμαντή Αγγελική¹, Σημηριώτη Ελευθερία², Τερεζάκη Ασημίνα², Μπάρδα Χριστίνα¹, Σφηνιαδάκης Ιωάννης³, Ράλλης Μιχαήλ², Σκαλτσά Ελένη¹

¹Τομέας Φαρμακογνωσίας και Χημείας Φυσικών Προϊόντων, Τμήμα Φαρμακευτικής, Σχολή Επιστημών Υγείας, Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών, ²Τομέας Φαρμακευτικής Τεχνολογίας, Εργαστήριο Δερματοφαρμακολογίας, Τμήμα Φαρμακευτικής, Σχολή Επιστημών Υγείας, Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών, ³Παθολογοανατομικό Εργαστήριο, Ναυτικό Νοσοκομείο Αθηνών

POSTER 07

In vitro ζύμωση Βασιδιομυκήτων από το εντερικό μικροβίωμα του ανθρώπου: Κυτταροτοξική, γονοτοξική και μεταβολομική ανάλυση των προϊόντων

Μπούλακα Αθηνά¹, Χριστοδούλου Παράσχος¹, Λιανού Ελένη^{1,3}, Μήτσου Ευδοκία², Βλασσοπούλου Μαριγούλα¹, Ζερβάκης Γεώργιος⁴, Καραγκούννη-Κύρτσου Αμαλία³, Κυριακού Αδαμαντίνη², Ζερβού Μαρία¹, Γεωργιάδης Παναγιώτης¹, Πλέτσα Βασιλική¹

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ABSTRACTS of the 55th Congress of the European Societies of Toxicology (EUROTOX 2019)
TOXICOLOGY – SCIENCE PROVIDING SOLUTIONS
Helsinki, Finland, 8th–11th of September, 2019

different species was developed. To this end, anaerobic incubations with fecal samples from rat, pig and human were optimized to define the reaction kinetics for the formation of α -ZEL and β -ZEL from ZEN. In all species tested, α -ZEL was formed to a higher extent than β -ZEL; the ratios of these metabolites were 2:1 in rats and pigs and 6:1 in humans. To facilitate interspecies comparison, the *in vitro* catalytic efficiencies (K_{cat}) for α -ZEL and β -ZEL were scaled up to relevant *in vivo* K_{cat} values, considering species differences in fecal production. Pigs had the highest *in vivo* K_{cat} for α - and β -ZEL formation of 234 and 157 mL/h, respectively, and rats the lowest K_{cat} of 0.6 and 0.16 mL/h respectively. The *in vivo* K_{cat} for α -ZEL and β -ZEL in humans were 51 and 7 mL/h, showing the highest relative preference for conversion to α -ZEL. A comparison to liver K_{cat} based on published data for pigs and rats indicates that in these species the K_{cat} of the microbiome is comparable to that of the liver, underlining the important role of the microbiome in toxicology. The developed model is an indispensable tool to study intestinal microbial metabolism of xenobiotics, and can be applied to derive rates of metabolism in different species.

P24-008

A comparative study on risk characterization methods for combined inhalation exposures to biocide mixtures in consumer products

*S. Shin, Y. Lim, H. Kim, J. Kim

Korea Research Institute of Chemical Technology, Chemical Safety Research Center, Daejeon, Republic of Korea

Biocides have been broadly developed and used in different sectors, manufacturing, construction, and service industries. Consumer products can include one or more biocides for maintaining the function of original products without any biological contamination. Many scientific studies have shown that mixture toxicity can be caused by cocktail effects (also known as joint effect or combined effect) among mixture components even at their no observed effect concentrations (NOECs).

Global biocidal product regulations (BPRs), e.g., European Union BPR, and Korean 'Consumer Chemical Products and Biocides Safety Act (also known as K-BPR)', have been newly adopted and updated for improving the authorization process of biocides. The mixture toxicity is taken into consideration in the risk assessment of biocidal products under those BPRs. In general, chemical risk assessment can be determined by considering both hazard and exposure data concerning target chemical products. Risk characterization is a final step in the risk assessment to assess if risks are adequately controlled by estimating the risk characterization ratio (RCR) indicating the ratio of the estimated exposure and the derived no-effect levels (e.g. DNELs). If the RCR does not exceed one, it can be considered that the risk is properly controlled within given exposure conditions. However, studies on estimating the RCR of combined exposures to different mixture components are still lack for developing a reliable mixture risk assessment despite a need for developing appropriate risk assessment methods for mixtures.

Therefore, the objectives of this study were i) to conduct a comparative case study on different risk characterization methods for combined inhalation exposures to different biocide mixtures; and ii) to examine possible deviations between RCRs calculated by different methods so that future challenges in the mixture risk assessment could be derived.

P24-009

In vitro fermentation of *pleurotus ostreatus* and *ganoderma lucidum* by human gut microbiota: cytotoxic, genotoxic and metabolomic analysis of the products

*P. Georgiadis¹, P. Christodoulou¹, E. Lianou^{1,2}, A. Boulaka¹, E. Mitsou², M. Vlassopoulou¹, G. I. Zervakis⁴, A. D. Karagouni³, A. Kyriacou², M. Zervou¹, V. Pletsas¹

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Edible basidiomycetes are known for their health-promoting properties. Growing evidence supports that their immune-modulating and anti-cancer effects are mediated by their prebiotic capacity. β -glucans, a group of β -D-glucose polysaccharides abundant in the fungal cell walls, are considered responsible for their potential prebiotic effects. The use of indigenous fungal genetic resources to develop nutraceuticals is, thus, of great importance.

In the present study, the prebiotic activity of *Pleurotus ostreatus* and *Ganoderma lucidum* cultivated mushrooms deriving from Greek habitats with high β -glucan content and the **cytotoxic, genotoxic and metabolomic analysis of their fermentation products** is being investigated. Hence, the whole fungus as well as β -glucan enriched extracts were tested for their ability to alter the composition of the intestinal microbe following their *in vitro* fermentation by fecal slurry of healthy volunteers. Lyophilized fungal substrates and inulin, an established prebiotic, at appropriate concentrations, were *in vitro* fermented for 24 hours. *In vitro* fermentation without any additional carbon source was in parallel carried out to be used as reference.

The fermentation products were found to be cytotoxic in hematopoietic U937, colorectal CaCo2 cell lines as well as Peripheral Blood MonoCytes (PBMCs) cells in a dose-dependent manner. The global metabolic profiling of fermented products was assessed by the use of ¹H NMR spectroscopy, and metabolites resonances were assigned guided by Chenomx NMR Suite and literature data. Preliminary results revealed variations in the profile of the products as a result of the *in vitro* fermentation of *P.ostreatus* and *G.lucidum* derived substrates. A comparative survey between the above substrates, using chemometrics in combination with 2D NMR spectroscopy will be further applied and discussed, in order to identify biomarkers associated with the health promoting effects and the biological activities of *P. ostreatus* and *G. lucidum*.

Acknowledgments: This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH – CREATE – INNOVATE (project code: T1EDK-03404).

Paraschos Christodoulou and Eleni Lianou equally contributing first authors, Maria Zervou, Vassiliki Pletsas and Panagiotis Georgiadis equally contributing corresponding authors

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ABSTRACT BOOK

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OP_36

IN VITRO FERMENTATION OF PLEUROTUS ERYNGII MUSHROOMS BY HUMAN GUT MICROBIOTA: META-TAXONOMIC ANALYSIS, ANTI-GENOTOXIC AND METABOLOMIC PROFILING OF THE FERMENTATION PRODUCTS

Christodouloy P^{1,6}, Boulaka A¹, Vlassopoulou M^{1,2}, Christodoulou P³, Kerezoudi E², Saxami G², Mitsou E², Koutrotsios G⁴, Zervakis G⁴, Kyriacou A², Moulos P⁵, Zervou M¹, Pletsas V¹, Georgiadis P¹

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Edible mushrooms are known for their health-promoting properties since ancient years. They contain a variety of bioactive compounds, including β -glucans, that possess immunomodulatory and anti-cancer activities. Their non-digestible dietary fibers content has been shown to have a beneficial effect on intestinal well-being, acting as substrate for growth and function of intestinal bacterial populations.

Mushrooms produced by a *Pleurotus eryngii* strain of Greek origin were fermented in vitro by fecal slurry of asymptomatic volunteers aged >60 years old (three male, two female), for 24 hours. In parallel, fermentations without any additional carbon source were carried out and used as negative controls. Fermentation supernatants (FSs) were collected, and their anti-genotoxic properties were investigated in human whole blood cells, obtained from non-smoking volunteers (two male, two female), using Lymphocyte Cytokinesis - block Micronucleus Assay. The global metabolic profile of FSs was assessed using ¹H NMR spectroscopy and metabolites resonances were

assigned employing the Chenomx NMR Suite, 2D NMR spectroscopy, Metabominer platform and literature data. Finally, we established a meta-taxonomic approach to examine the in vitro fermentation-induced changes in gut microbiota communities. Amplicon-based Next Generation Sequencing of the DNA which correspond to the hypervariable regions of 16S ribosomal RNA was applied.

P. eryngii FSs were found to protect lymphocytes against the damage induced by Mitomycin C, a known genotoxic agent. In addition, the metabolomic and metataxonomic profiles showed significant variations as a result of mushroom's in vitro fermentation. Multiple regression analysis was employed for the assignment of anti-genotoxicity to specific constituents of the multi-component mixture of the metabolome. The identified metabolites, associated with the anti-genotoxic effects of the fermentation, will be further evaluated as for their correlation with changes of gut composition at family, genus or even species level.

This research has been co-financed by the European Union and Greek national funds through the Operational Program Competitiveness, Entrepreneurship and Innovation, under the call RESEARCH – CREATE – INNOVATE (project code: T1EDK-03404).



PP_121

IN VIVO GENOPROTECTIVE PROPERTIES OF PLEUROTUS ERYNGII HOT WATER EXTRACT

Boulaka A¹, Mantellou P^{1,3}, Vlassopoulou M^{1,4}, Christodoulou P¹, Koutrotsios G², Zervakis G², Kyriacou A⁴, Pletsas V¹, Georgiadis P¹

¹National Hellenic Research Foundation, Institute of Chemical Biology, ²Agricultural University of Athens, Laboratory of General and Agricultural Microbiology, ³University of Ioannina, Department of Biological Applications and Technology, ⁴Harokopio University, Department of Nutrition and Dietetics

The exploitation of natural bioactive ingredients is a current trend in cancer and other multifactorial diseases prevention. Edible mushrooms are known for their beneficial biological properties, and many studies indicate that at least some of these activities are due to their prebiotic effect which alters the gut microbiome and consequently, affect the immune-responses and various metabolic pathways.

In the present study, the anti-genotoxic effect of *Pleurotus eryngii*, an edible mushroom from Greek habitats of the Greek flora, was investigated in vivo. Young (8-9 weeks old) and aged (17-18 months old) CD-1 mice were treated orally (gavage), once daily, with mushroom's hot-water extract at different dosing regimen for 14 days. At the end of the treatment period, the genotoxic agent cyclophosphamide was administered intraperitoneally. The genoprotective properties of the mushroom extract were assessed in whole blood cells and bone marrow cells, against the

damage caused by cyclophosphamide, by the micronucleus assay. Furthermore, the ability of the extract to regulate the antioxidant and inflammation mechanisms of the cell were studied by quantifying the mRNA expression levels of Nrf2 and Nfκβ genes in gut and liver tissues, using qRT-PCR.

According to our results, the *P. eryngii* extract exerts significant genoprotective activity mainly in the bone marrow cells of both young and aged animals. After the administration of the mushroom extract, Nrf2 expression levels were increased in liver whereas, Nfκβ levels were increased in gut. These results are indicative of alterations in antioxidant defense, inflammation and gut homeostasis signaling pathways. However, further studies are needed in order to elucidate the *P. eryngii* health promoting properties and its beneficial for the organism mode of action.

This research was co-funded by the EU and Greek national funds, through the Operational Program Competitiveness, Entrepreneurship and Innovation under the call RESEARCH-CREATE-INNOVATE (T1EDK-03404).



**10th International Conference of the
Hellenic Crystallographic Association**



**Hellenic Crystallographic
Association (HeCrA)**

**October 15 - 17, 2021
Congress Center, NCSR Demokritos, Athens, Greece**

**10th International Conference of the
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10th International Conference of the Hellenic Crystallographic Association

Congress Center, NCSR Demokritos, Athens, Greece

October 15 - 17, 2021

The 10th International Conference of the Hellenic Crystallographic Association (HeCrA) follows the biennial successful series of meetings organized by HeCrA. This year the conference is taking place at the Congress Center of the National Centre for Scientific Research "Demokritos" in Agia Paraskevi, Athens, Greece.

The aim of this meeting is to promote and support research and education in the fields of **molecular structure**. Plenaries and workshops are accompanying the scientific sessions of the conference. In addition to X-ray crystallography for the study of biological macromolecules, small molecules and inorganic materials, conference sessions are dedicated to other biophysical methods (CryoEM, X-FEL, NMR, XAFS, spectroscopic methods and other related techniques) and structural bioinformatics emphasizing the progress of structural sciences in recent years. Attendees will also have the opportunity to be introduced to the state-of-the-art methodology of cryo-electron microscopy.

The conference is taking place mainly in an in-person format. An online attendance is also possible. Due to the emergency measures aiming to confine the SARS-CoV2 spread, the in-person participation is permitted to persons who are fully vaccinated or have recovered from COVID-19 in the previous 6 months (see ΦΕΚ-B' 4577/03.10.2021, pages 60832 - 60839). Thus, every participant on arrival must present one of the following documents in digital or print form.

A limited number of IUCr-funded bursaries for travel, accommodation and subsistence expenses, will be granted to eligible young students who have traveled to Athens from abroad or from other Greek cities. The successful format of the previous conferences is retained. The speakers' list includes keynote and invited speakers together with speakers (including younger researchers) selected from abstract submissions, in order to capture the latest research findings in the field. Also, two poster sessions with posters on display throughout the conference have been scheduled.

We are thankful to the members of the Scientific Committee of this conference for their advice and assistance for the selection of speakers. We are also thankful to the organizers of the previous meetings for their invaluable advice throughout the conference preparations. We would like to express our gratitude to Assoc. Prof. Bernhard Lohkamp and Dr. Paul Emsley for the preparation of a COOT workshop.

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10:00 – 10:30	<p style="text-align: center;"><u>Invited Lecture</u></p> <p>Marios Zouridakis, Dept. of Neurobiology, Hellenic Pasteur Institute, Athens, Greece</p> <p><i>“Co-crystal structures of the extracellular domain of human ACE2 receptor with the SARS-CoV2 receptor binding domain of Wuhan and three other variants of concern”</i></p>
10:30 – 10:45	<p style="text-align: center;"><i>Short talk</i></p> <p>Eftichia Kritsi, Institute of Chemical Biology, National Hellenic Research Foundation, Athens, Greece</p> <p><i>“Discovery of novel epigenetic inhibitors: A computational approach”</i></p>
10:45 – 11:00	<p style="text-align: center;"><i>Short talk</i></p> <p>Emmanuel Saridakis, Institute of Nanoscience and Nanotechnology, National Center for Scientific Research “Demokritos”, Athens, Greece</p> <p><i>“A novel, four subunit, “dimer-within-a-dimer” γ-cyclodextrin self-assembly”</i></p>
11:00 – 11:15	<p style="text-align: center;"><u>Presentation Sponsored by Anelis & RIGAKU</u></p> <p>Felix Hennersdorf, Rigaku Corporation</p> <p><i>“The latest range of Rigaku Oxford Diffraction instrument configurations for structural biology - example applications”</i></p>
11:15 – 11:45	COFFEE BREAK – POSTER SESSION I
4 th Session	<p><i>Characterization of materials (small molecules / inorganics) - structure and properties</i></p> <p>Chaipersons: Vassilis Psycharis, Catherine Raptopoulou</p>
11:45 – 12:30	<p style="text-align: center;"><u>Keynote Lecture</u></p> <p>George Christou, Dept. of Chemistry, University of Florida, USA</p> <p><i>“Molecular Nanoparticles: A Molecular Route to Ultra-small Nanoparticles of Important Metal Oxides”</i></p>
12:30 – 13:00	<p style="text-align: center;"><u>Invited Lecture</u></p> <p>Spyros Perlepes, Dept. of Chemistry, University of Patras, Greece</p> <p><i>“Single-Crystal X-Ray Crystallography of Small Inorganic Molecules: Quo Vadis?”</i></p>
13:00 – 13:30	<p style="text-align: center;"><u>Invited Lecture</u></p> <p>Panayotis Kyritsis, Dept. of Chemistry, National and Kapodistrian University of Athens, Greece</p>

POSTER074

A COMPUTATIONAL APPROACH FOR THE DISCOVERY OF NOVEL DNMT1 EPIGENETIC INHIBITORS

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In the past 20 years, the explosion of knowledge in epigenetics has revealed new pathways towards the treatment of multifactorial diseases rendering **the key players of the epigenetic machinery the focus of today's pharmaceutical landscape**. Among them, **DNA methyltransferases (DNMTs)** are responsible for DNA methylation to carbon five (C5) of cytosine in CpG dinucleotide sequences and consequently alter neighbouring gene expression. It has been proven that alterations in the function of DNMTs is causally linked with adverse health outcomes. This fact brings DNMTs in the limelight as an attractive and promising target for discovering novel **epigenetic inhibitors**, which can be used as starting points for further development of novel anticancer and other diseases drugs.¹

Even though this cutting-edge field incites researchers' interest and several inhibitors of key epigenetic players have been tested, **only seven epigenetic drugs** ("Epi-drugs") have been approved for human use by FDA up to date with limited usage mainly against haematological cancers. Application of epigenetic drugs in chronic diseases, as metabolic and neuropsychiatric disorders, remains mostly unexplored. The low specificity, the acute toxicity, the poor bioavailability and stability of "Epi-drugs" underscore the urgent need to design novel and target specific epigenetic agents with entirely different chemical scaffolds from known "Epi-drugs" which will eliminate these shortcomings.²

This study aims at the discovery of novel inhibitors of **natural origin** against DNMT1 isoform using a combination of structure and ligand-based computational approaches. A series of commercially available natural compounds chemo-libraries (e.g. Indofine, Analyticon Discovery, PhyProof, Nubbe, Specs, Enamine, MolPort, Ambinter etc) were virtually screened against our generated pharmacophore hypotheses and the retrieved compounds were further subjected to *in silico* docking studies and molecular dynamics simulations in order to establish an accurate and robust selection methodology. Our screening protocol prioritized a series of natural compounds, bearing completely diverse chemical scaffolds from known "Epi-drugs". The biological evaluation of the selected compounds inhibitory activity against DNMT1 is still in progress.

References:

1. O. Castillo-Aguilera *et al.*, Biomolecules, 7, 1-21, 2017.
2. V. Prachayasittikul *et al.*, Expert Opin. Drug Discov., 12, 345-362, 2017.

Acknowledgments:

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Abstracts for The Biochemistry Global Summit

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Title: In vitro fermentation of *Pleurotus eryngii* mushrooms by human Gut Microbiota: meta-taxonomic analysis and metabolomic profiling of the products

Author/s: P. Georajadis, P. Christodoulou, M. Vlassopoulou, S. Kaila, M. Bekyrou, M. Zervou, G.I.

In vitro fermentation of *Pleurotus eryngii* mushrooms by human Gut Microbiota: meta-taxonomic analysis and metabolomic profiling of the products

LB-02.5-01

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Current research has identified many of the health-promoting properties of edible mushrooms, ranging from antioxidant, antimicrobial and anticancer activities to immune enhancement and prebiotic action. They are a rich source of polysaccharides, mainly beta-glucans, peptidoglucans and contain a plethora of bioactive components, including chitins, unsaturated fatty acids, vitamins, triterpenic acids, lectins, statins, alkaloids, and polyphenols. Several mushroom bioactive compounds have been shown to exert their health-promoting properties through alterations in gut microbiota composition and the subsequently formed metabolites.

Lyophilized *Pleurotus eryngii* (PE) mushrooms of Greek habitats, selected due to their strong lactogenic effect and anti-genotoxic, immunomodulating properties, underwent in vitro static batch fermentation for 24 hours by fecal microbiota from eight elderly asymptomatic volunteers (>60 years old). Fermentations without any additional carbon source were carried out as negative controls. The fermentation-induced changes in fecal microbiota communities were examined using Next Generation Sequencing of the hypervariable regions of the 16S rRNA gene. Primary processing and analysis was conducted using the Ion Reporter Suite. Changes in the global metabolic profile were assessed by ¹H NMR spectroscopy, and metabolites were assigned by 2D NMR spectroscopy and Metabominer platform.

PLS-DA analysis of both metataxonomic and metabolomic data showed a significant cluster separation of PE fermented samples relative to controls. DEseq2 analysis showed that the abundance of families such as Lactobacillaceae, Ruminococcaceae and Ruminococcaceae were increased while others such as Clostridiales were decreased in PE samples. On the other hand, more than 20 metabolites, including several short-chain fatty acids, discriminate PE samples from the respective controls. Multi-omics analysis is currently underway to further elucidate these findings.

* The authors marked with an asterisk equally contributed to the work.

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P30	Screening of olive mill wastes and by-products from the region of Lakonia as sources of antioxidants for food and feed applications <u>I. Pyrka</u> ¹ , C. Koutra ² , S. Vassilios ² , F. T. Mantzouridou ¹ , P. Stathopoulos ² , A. L. Skaltsounis ² , N. Nenadis ¹ ¹ Laboratory of Food Chemistry and Technology, School of Chemistry, Aristotle University of Thessaloniki (AUTH), 54124 Thessaloniki, Greece ² Division of Pharmacognosy and Natural Products Chemistry, Department of Pharmacy, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens, Greece
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² *Processes and Products Quality Control Horizontal Laboratory, Zografou Campus, School of Chemical Engineering, National Technical University of Athens*

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