INTERNATIONAL WORKSHOP ON MOLECULAR SPECTROSCOPY AND BIOLOGICAL APPLICATIONS

JUNE 17-18 2019, ISTANBUL, TURKEY

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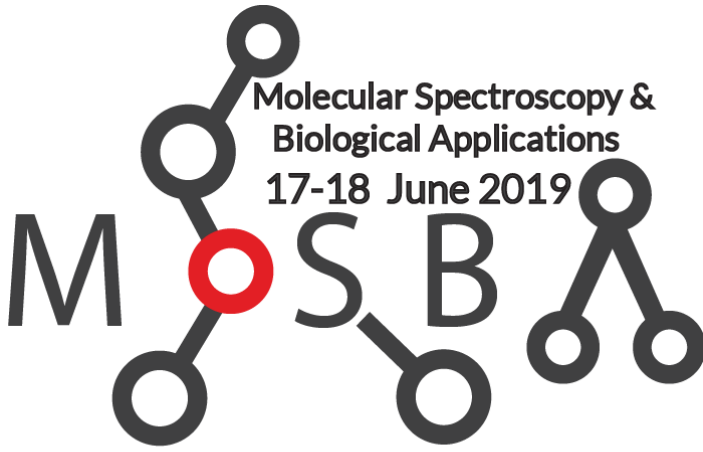
ERDAL İNÖNÜ CONFERENCE HALL

BOOK OF ABSTRACT

ISTANBUL TURKEY

JUNE 17-18

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Molecular Spectroscopy &
Biological Applications
17-18 June 2019

Istanbul Kultur University, Istanbul, Turkey

WELCOME TO MOSBA

DEAR COLLEAUGES,

We cordially invite you to attend the Molecular Spectroscopy and Biological Applications Workshop (MOSBA 2019), to be held in Istanbul Kultur University, Erdal İnönü Conference Hall, 17-18 June 2019.

The scope of the workshop is to encourage the exchange of idea among people interested in molecular spectroscopy and molecular biology.

Gülce ÖĞRÜÇ ILDIZ
Chair, MOSBA-2019

Topics

The congress will include the scientific topics below:

1. Raman Spectroscopy

2. IR Spectroscopy

3. Multivariate Analysis

4. Spectroscopy of Biological Systems

5. Spectroscopy and Food Chemistry

6. Plant Biotechnology

7. Molecular Diagnostics

The scientific program of the workshop will include invited talks and flash talks and posters.

Organizing Committee:

Gulce Ogruc Ildiz
(Istanbul Kultur University, Turkey)
Gizem Yavuz
(Istanbul University, Turkey)
Gokhan Halimoglu
(Istanbul University, Turkey)
Hayrunnisa Nur Kabuk
(Istanbul Kultur University, Turkey)
Ahmet Karadag
(Istanbul Kultur University, Turkey)

Scientific Committee:

Sevgi Bayari
(Hacettepe University, Turkey)
Rui Fausto
(Coimbra University, Portugal)
Gulce Ogruc Ildiz
(Istanbul Kultur University, Turkey)
Olcay Bolukbasi Yalcinkaya
(Istanbul University, Turkey)
Ayberk Yilmaz
(Istanbul University, Turkey)

Speakers:

Sevgi Bayari
(Hacettepe University, Turkey)
Rui Fausto
(Coimbra University, Portugal)
Olcay Bolukbasi Yalcinkaya
(Istanbul University, Turkey)
Ayberk Yilmaz
(Istanbul University, Turkey)
Oyku Irigul Sonmez
(Biruni University, Turkey)
Ozge Celik
(Istanbul Kultur University, Turkey)
Alp Ayan
(Istanbul Kultur University, Turkey)
Gizem Yavuz
(Istanbul University, Turkey)
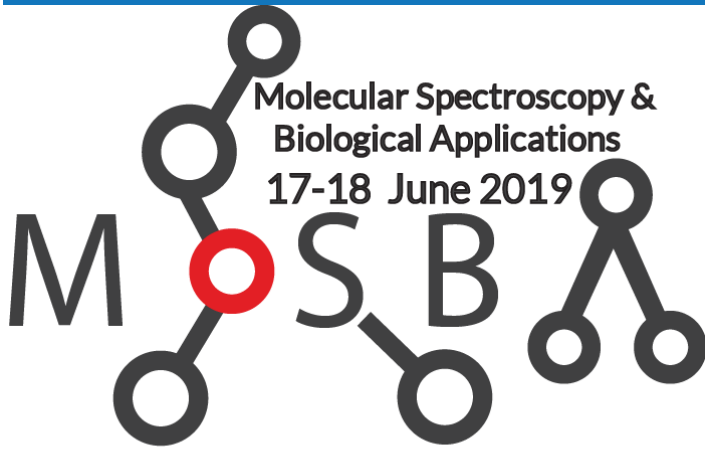**Gokhan Halimoglu**
(Istanbul University, Turkey)
Hayrunnisa Nur Kabuk
(Istanbul Kultur University, Turkey)
Ahmet Karadag
(Istanbul Kultur University, Turkey)
**Alize Yilmazlar**
(Biruni University, Turkey)

Molecular Spectroscopy &
Biological Applications
17-18 June 2019

MoSBA

Istanbul Kultur University, Istanbul, Turkey

Scientific Program

09:00-09:30	Registration
09:30-10:30	*Sevgi Bayari* *Applications of Vibrational Spectroscopy and Imaging*
10:30-11:30	*Rui Fausto* *Strategies for Identifying Samples Through Spectroscopy and Chemometrics: A Case Study Focusing on Body Fluids*
11:30-12:30	*Oyku Irigul Sonmez* *A Novel Molecular Diagnostics Approach to Determine Susceptibility to Cardiovascular Diseases*
12:30-13:30	**LUNCH BREAK**
13:30-14:30	*Olcay Bolukbasi Yalcinkaya* *Solvent Effect on Infrared Spectra of Anti-hypertension Drug Molecules*
14:30-15:30	*Ozge Celik* *Applications of Spectrophotometric Techniques in Plant Biotechnology*
15:30-16:00	**COFFEE BREAK**
16:00-17:00	*Ayberk Yilmaz* *Global Optimization and Vibrational Frequencies of a Lennard-Jones Cluster Containing 7 Atoms*
17:00-18:00	*Alp Ayan* *Improving Salinity Tolerance of Local Rice Varieties by Gamma Radiation*

09:30-10:00	**Gizem Yavuz** *Vibrational Spectroscopy and Chemometrics in the Diagnosis of Schizophrenia (SZ) and Bipolar Disorder (BP)*
10:00-10:30	**Alize Yilmazlar** *The Effect of Polymorphisms in TAS2R38 Gene on the Perception of Bitterness*
10:30-11:00	**Hayrunnisa Nur Kabuk** *Raman Spectroscopic and Chemometric Study on Yellow Dent and Purple Flint Maize Kernel*
11:00-11:30	**COFFEE BREAK**
11:30-12:00	**Gökhan Halimoglu** *Attention Deficit / Hyperactivity Disorder in Adults: A Biomarker Study*
12:00-12:30	**Ahmet Karadag** *X-ray Powder Diffraction (XRD) Study of a Fulgurite*
12:30-13:00	**Closing Ceremony**
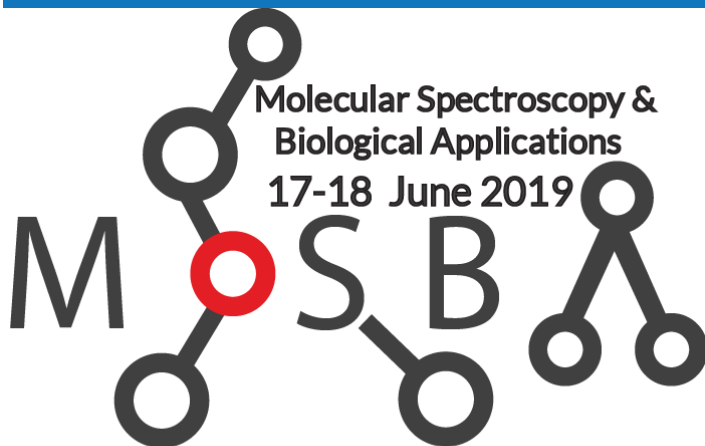
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SPEAKERS TEXTS

Applications of Vibrational Spectroscopy and Imaging

Sevgi Bayari

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Vibrational spectroscopy encompasses four complementary techniques: near-infrared (NIR), mid-infrared (MIR), terahertz (or far-infrared; FIR), and Raman spectroscopies. All these techniques are popular, rapid, sensitive, non-destructive and non-invasive methods. In the last decade, the different variants of infrared (IR) spectroscopy as well as Raman spectroscopy have also emerged as promising methods for medical diagnosis, when used in combination with imaging accessories and chemometric procedures.

Vibrational spectroscopy provides information on vibrational movements of atoms that are related with the chemical composition and structural arrangement of the atoms of the studied sample. The vibrational spectrum of a sample (either infrared or Raman) is unique, like a fingerprint, and can be used for identification, structure elucidation, reaction monitoring, quality control, and investigation of interactions within a given sample. In particular, the vibrational spectra of a patient's bio-specimen (e.g., a body fluid) represent fingerprint-like signatures of his biochemical standing, which may be correlated with his health status. Relatively to other methods currently used for this purpose, vibrational spectroscopy techniques have the advantage that no additional markers or labelling are required.

The primary aim of this talk is to present the fundamentals of IR and Raman spectroscopies, and to provide some illustrative examples of the use of these techniques in various scientific disciplines, ranging from Chemistry and Physics to Biosciences. In particular, the power of vibrational spectroscopy to probe subtle compositional changes in tissues and body fluids (especially blood components) that accompany diseases' biochemistry will be shown.

Strategies for Identifying Samples Through Spectroscopy and Chemometrics: A Case Study Focusing on Body Fluids

Rui Fausto

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In this seminar, I will focus on the use of spectroscopy, together with simple chemometric methods, for identification/classification of samples. Possible strategies to successfully use this methodology will be addressed using a practical approach where illustrative examples will be presented and discussed with the audience. Though the described methodology has a rather broad domain of application, taking into account the ongoing research interests at the IKU Molecular Spectroscopy Laboratory, I will center on identification/classification of body fluids (BFs).

A brief overview of the chosen body fluids main chemical constituents and a general description of their infrared spectra will be first presented, which will be followed by the presentation of some simple statistics-based classification methods [Principal Component Analysis (PCA), Cluster Analysis, Partial Least Squares (PLS) and Q-statistics Analysis]. The application of the method to the identification/classification of body fluids will take into account the possible variability of the samples, in particular along the time. A discrimination scheme based on a dichotomous classification tree with hierarchical clustering will be presented for this purpose.

The talk will follow closely the article by Takamura, Watanabe, Akutsu and Ozawa [1], to whom the credits for the described experiments shall be given.
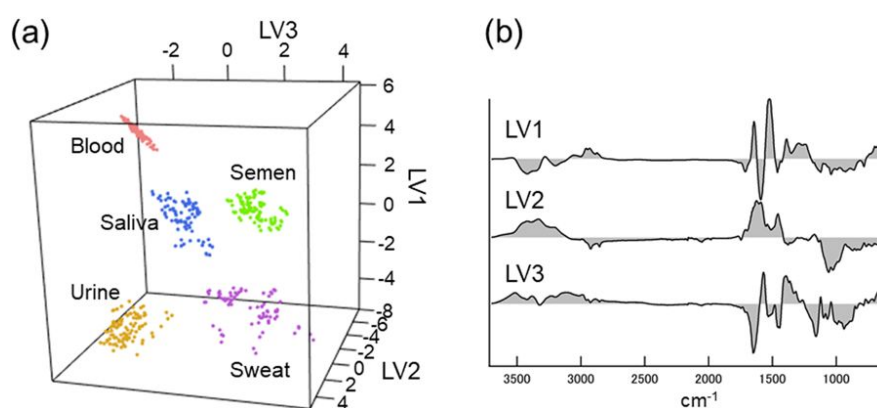

Figure. (a) 3-Dimensional dot plot of the PLS scores for the FTIR spectra of five BF types calculated by a five-class PLS model for fresh BFs. (b) Weight loading vectors corresponding to the first three latent variables (LVs) in the developed five-class PLS model.

[1]   A. Takamura, K. Watanabe, T. Akutsu, T. Ozawa, *Scientific Reports*, 8 (2018) Art. Nº 8459.

A Novel Molecular Diagnostics Approach to Determine Susceptibility to Cardiovascular Diseases

Oyku Irigul Sonmez

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Cardiovascular diseases are the most common cause of death worlwide and thrombosis shows itself as one of the most serious signs of these diseases (CVDs). CVDs are caused by the interaction of genetic and environmental risk factors and moreover, endothelial dysfunction, fever, abnormal lipoprotein and homocysteine metabolism, dysfunctional caogulation and fibrinolysis play a key role in their pathogenesis. The susceptibility to CVD is associated with polymorphisms carried on a variety of genes. Hence, the aim of this particular study was to identify 12 polymorphisms that cause thrombosis and atherosclerosis. These polymorphisms are associated with coagulation (F2, F5, F13A1, FGB), fibrinolytic system (SERPINE1), platelet adhesion (ITGB3), homocysteine metabolism (MTHFR), reninangiotensin system (ACE) and lipid metabolism (APOE). As a result, these 12 polymorphisms that directly cause thrombosis and atherosclerosis were determined using a novel molecular diagnostic method. This methodology has let us make a sensitive, reliable and accurate diagnosis on CVD susceptibility.

Solvent Effect on Infrared Spectra of Anti-hypertension Drug Molecules

Olcay Bolukbasi and *Ayberk Yilmaz*

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Furosemide, bumetanid and indapamide are important drug molecules used in the treatment of hypertension. The aim of this study was to investigate soluble-solvent interactions of anti-hypertension drug molecules in four different solvents (ethanol, methanol, DMSO and THF) using FT-IR spectroscopy and DFT calculations. The optimized geometry and vibrational wavenumbers of the molecules in different solvent media were investigated by DFT/B3LYP and the Conductive Polarized Continuity Model (CPCM) with the 6-31G(d,p) basis set. Solvent effects on the vibrational spectra are discussed.
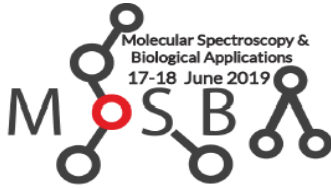
Applications of Spectrophotometric Techniques in Plant Biotechnology

Ozge Celik

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Plant biotechnology is a set of techniques used to adapt plants for specific needs or opportunities. The main aim is to develop new varieties and traits *via* several molecular techniques.

Radiation treatment is one of the most widely used methods to induce recombinations among plant genome. It gives the opportunity to increase the frequency of the mutations that happen spontaneously, to generate desired mutants with desirable traits to be bred with other cultivars.

Molecular analysis in selection studies has recently been gaining increased importance. Especially for improvements of seeds, complementary analysis methods became effective to discriminate molecular differences from mother seeds. The elemental and molecular structural alterations underwent by gamma-induced mutants of seeds give information about protein, lipid and carbohydrate structure of the mutants, whoch can then be compared with those of control groups. IR and energy dispersive X-ray fluorescence (EDXRF) spectrometric methods are effectively used in plant biotechnology applications.
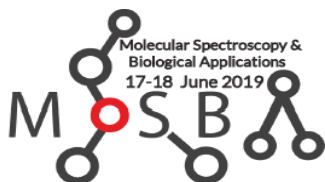
Global Optimization and Vibrational Frequencies of a Lennard-Jones Cluster Containing 7 Atoms

Ayberk Yilmaz and *Olcay Bolukbasi*

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Basin-hopping algorithm is one of the most important methods designed for global optimization. In this talk, the Basin-Hopping Monte Carlo (BHMC) algorithm for global optimization and the lowest energy structures of a Lennar-Jones cluster containing 7 atoms will be presented. Then, the calculation of the second derivatives of total energies, which allow for the calculation of the fundamental vibrational frequencies, will be explained.
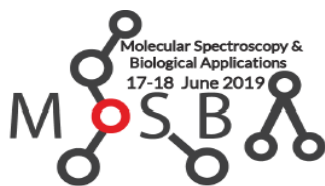
Improving Salinity Tolerance of Local Rice Varieties by Gamma Radiation

Alp Ayan

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It is aimed to obtain salinity tolerance on Osmancık-97 , which is widely planted rice variety in Turkey, and Mevlütbey, which is a rice variety improved in Black Sea region, by using gamma radiation. Rice seeds were irradiated by 0, 250, 300 ve 400 Gy dose of Cs-137 source. Irradiated seeds were planted in the experimental fields of Black Sea Agricultural Research Institute and physiological effects of radiation on

43 salt tolerant mutants belonging to Osmancık-97 variety were selected and planted to Trakya Agricultural Research Institute to obtain seeds. In vitro callus cultures were established in order to determine persistence of salt tolerance in M3 generation. In respect to the data obtained from in vitro studies, 250-2, 300-5, 400-2 and 400-5 mutants which presented better callus growth comparing to the untreated Osmancık-97 control calluses were selected for further molecular characterization studies.

Biochemical responses of selected salt tolerant mutants under salt treated and untreated conditions were evaluated by lipid peroxidation, proline content, photosynthetic pigment content, total protein content, enzyme activities of peroxidase, superoxide dismutase and catalase results.

Genetic distance between mutants and Osmancık-97 as their origin were determined by PCR reactions conducted with ISSR primers. Jaccard genetic similarity matrix was generated according to the band profiles and UPGMA dendrogram was drawn.

Two dimensional proteomic analysis of salt tolerant mutants were conducted. Evaluation of protein spot profiles of samples presented that 30 proteins were differed in expression.

As a result, four different salt tolerant rice mutants were obtained and it is the first time which presented that salt tolerant rice mutants can be induced by gamma radiation.
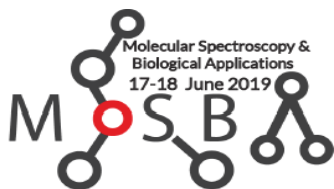
Vibrational Spectroscopy and Chemometrics in the Diagnosis of Schizophrenia (SZ) and Bipolar Disorder (BP)

Gizem Yavuz, Gulce Ogruc Ildız

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Schizophrenia (SZ) and bipolar disorder (BP) are severe neuropsychiatric syndromes that are characterized by an extensive spectrum of symptoms affecting approximately 2% of the world population; due to the heterogeneity of their symptoms, diagnosis of these disorders is complicated. Nowadays, diagnostic approaches for SZ and BP are based on patient interviews and subjective evaluations of clinical symptoms. However, there are still no molecular-based diagnostic tools to support clinical diagnosis.

This study intends to develop a screening methodology for the diagnosis of SZ and BP based on vibrational spectroscopy (e.g., Raman Spectroscopy) and chemometrics. Raman spectra of blood samples of SZ and BP patients will be investigated and compared with samples of healthy people, in order to identify spectral markers associated with SZ and BP. The analysis of the spectral data will be done with help of chemometric methods.

The Effect of Polymorphisms in TAS2R38 Gene on the Perception of Bitterness

Alize Yilmazlar

Molecular Biology and Genetics, Biruni University, Topkapi, Istanbul

Gustatory system in humans is composed of taste receptor cells (TCRs) that are believed to harbor taste ligands which can detect the stimuli that cannot cross the cell membrane. Products of TAS1R and TAS2R protein families that belong to G protein coupled receptor (GPCR) superfamily are involved in taste perception. There are several compounds which trigger taste perception. SNPs that are observed in Taste 2 Receptor Member 38 (TAS2R38) gene affect how phenylthiocarbamide (PTC) organic compound is perceived by TRCs. PTC is present in plants like cabbage, turnip, broccoli and Brussel sprouts that belong to Brassica species. In this study, the aim was to determine if there is a significant correlation between TAS2R38 polymorphisms and perception of other types of nutriments such as onion, garlic, chocolate, butter or coffee; and to see if there is a relation between the number of SNP occurrence and the sensitivity level towards bitterness. For this purpose, a questionnaire was prepared and volunteers were asked to fill it in order to determine what kind of nutriments they can consume. How often they can consume bitter tasting nutriments and how strong is the bitterness they can consume were among the questions asked. Following primer and prove designs, blood samples were collected, DNA was isolated and sequencing and qPCR methods were applied to detect the three SNPs that are generally observed in TAS2R38 gene.

Raman Spectroscopic and Chemometric Study on Yellow Dent and Purple Flint Maize Kernel

Hayrunnisa Nur Kabuk, Gulce Ogruc Ildız

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In this study, the potential of micro-Raman spectroscopy coupled to a simple, standard chemometric method (principal component analysis, PCA), to investigate corn seed components (endosperm, germ and peel) was investigated. The two corn varieties most produced in Turkey (yellow dent and purple flint varieties) were investigated. Differences in the composition of the endosperm and germ of the two corn varieties were determined based on the analysis of the corresponding Raman spectra. The analyses were performed with help of chemometrics methods, specifically, principal component analysis, which allowed to discriminate well the two types of corn investigated, as illustrated in the Figure for the case of the germ.

The yellow dent type studied was found to have a relatively large protein content in the endosperm than the purple flint corn, as well as a higher amylopectin/amylose ratio. The germ of the two species differ mainly on the presence of slightly more starch in the case of the yellow dent corn, while the oil composition of both species is identical. The spectrum of corn shells revealed the presence of similar amounts of cellulose and lignin in the two investigated corn species.

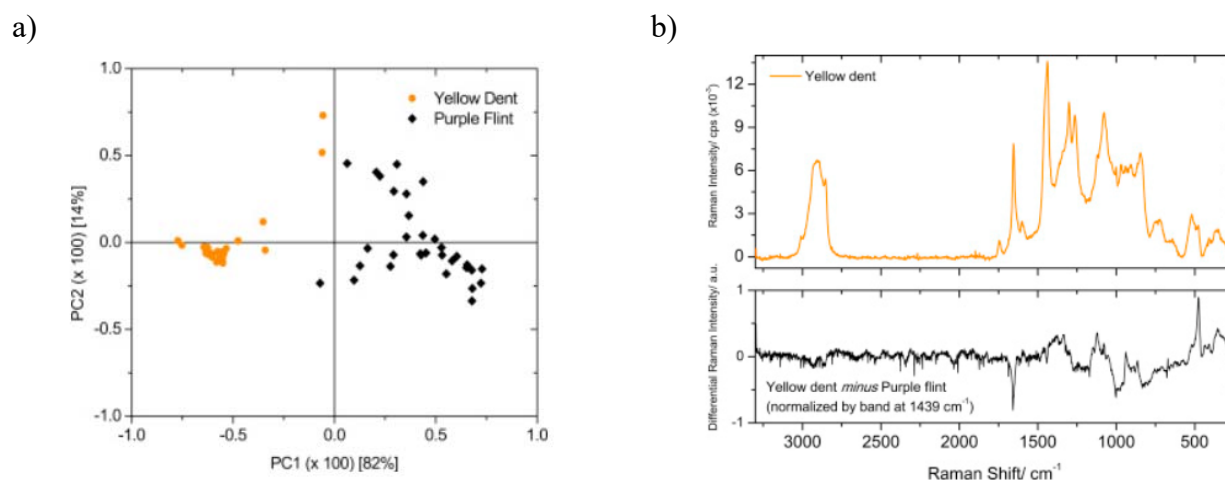This talk will follow closely the recently published article of Ogruc-Ildiz *et al.* [1].

a)   b)

Figure. (a) PCA scores plot of PC2 *vs.* PC1 principal components obtained from PCA of Raman spectra (3300-2700 and 1750-400 cm^{-1} spectral ranges) of the germ of the yellow dent and purple flint maize samples. Axes were normalized to unity. (b) Average Raman spectrum of the germ of the yellow dent maize (*top* panel), and the difference spectrum obtained by subtracting to this spectrum that of the purple flint germ (*bottom* panel). For spectral subtraction, the spectra were normalized by the peak intensity of the band at 1439 cm^{-1}.

[1] Ildiz, G. O., Kabuk, H. N., Kaplan, E.S., Halimoglu, G. and Fausto, R., *'A Comparative Study of the Yellow Dent and Purple Flint Maize Kernel Components by Raman Spectroscopy and Chemometrics'*. J. Mol. Struct., **1184** (2019) 246. https://doi.org/10.1016/j.molstruc.2019.02.034.

Attention Deficit/Hiperactivity Disorder in Adults: a Biomarker Study

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Until recent years, Attention Deficit and Hyperactivity Disorder (ADHD) was thought to be limited only to childhood and thought to be absent in adults. Hovewer, recent studies have shown that ADHD lasts to adulthood at 70%, disrupting the social functioning of the affected person from education to work life.

Classical diagnostic methods for ADHD are long and, frequently, misleading. For these reasons, intense research have been made in the last years in order to better understand the neurobiology of the ADHD and find alternative approches to the classical diagnostic methods.

Spectroscopy has been emerging as a new tool for diagnosis in Medicine, especially for psychological disorders. In this study, we have been exploring the possibility of using Raman spectroscopy to identify biomarkers present in the blood serum that can be used for diagnosis of ADHD in adult patients.

X-ray Powder Diffraction (XRD) Study of a Fulgurite

Ahmet Karadag, Ersin Kaygısız, Namık Aysal, Abdullah Sinan Öngen,
Gulce Ogruc Ildız

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Fulgurites are vitrified or protocrystalline structures resulting from a lightning strike onto sandy soil, sand, rock or sediments. Frequently, fulgurites present a tubular form, though they may also appear as clumps or masses. In this investigation, X-Ray diffraction (XRD) studies are being undertaken in order to gather information on the mineralogical and chemical characteristics of desert fulgurites. First results will be presented.

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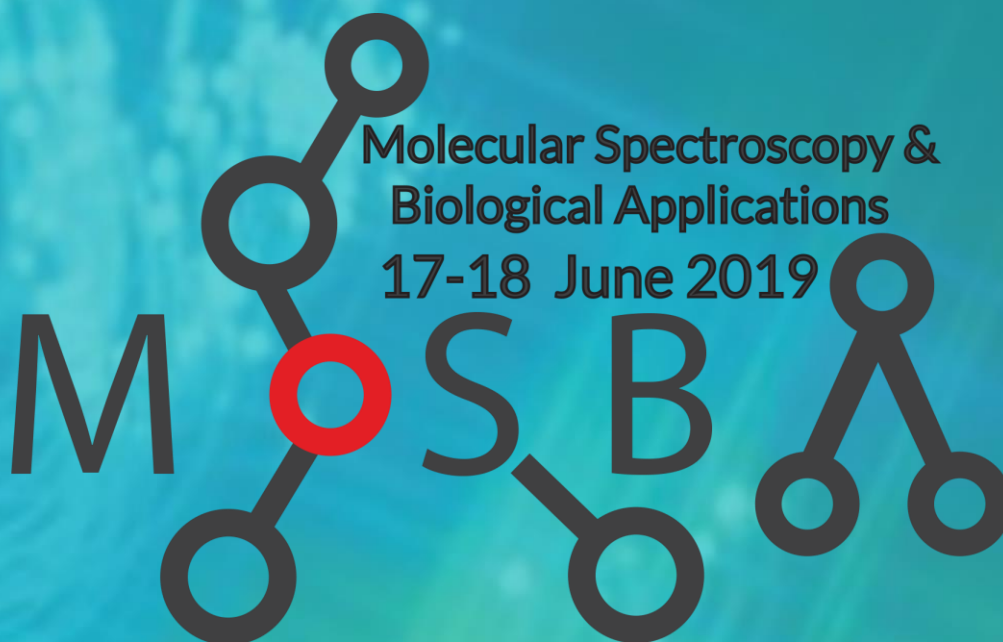
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