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# **Chemistry & Mass Spectrometry Congress**

October 18-19, 2017 Osaka, Japan

## **Scientific Tracks & Abstracts** **(Day 1)**



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### Syntheses of functional molecules via alkyne annulation

**Ruimao Hua**

Tsinghua University, China

Transition metal-catalyzed annulation of alkynes with high atom-utilization and economic steps, is one of the most important methods for construction of carbocyclic and heterocyclic compounds. In the presence of rhodium, palladium, copper or other transition metal complexes, we have studied the annulation of alkynes to develop the efficient synthetic methods for multi-substituted indoles and human 5-selective serotonin 2A receptor (h5-HT<sub>2A</sub>) antagonist, the natural product skeleton of cassiarin C; multi-substituted chrysenes as well as the fused cyclic quinolines.

### Biography

Ruimao Hua has received his Doctor of Philosophy degree in Environmental Chemistry and Engineering in 1996 from Tokyo Institute of Technology, Japan. He is currently a Professor of Chemistry in the Department of Chemistry, Tsinghua University. His research interests are on the development of organic synthetic methodology with the use of alkynes, the synthesis and applications of organic materials for displays (liquid crystal display and OLED display). He was authored and co-authored over 110 publications and authorized over 140 patents with another 55 patents pending.

ruimao@mail.tsinghua.edu.cn

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**A comprehensive insight into sampling and sample preparation steps for trace element determinations in plant material**

**Sabina Dołęgowska**

Jan Kochanowski University, Poland

Environmental monitoring is a process which consists of many interdependent steps. Each step ranging from selection of sampling sites through sampling of plant material to chemical analysis and data interpretation has to be thought over and all errors that come out of each stage should be identified because they can be a source of partial uncertainty. The quality of measurement describes total uncertainty that involves sampling, which is the main source of uncertainty (even up to 100%), sample preparation and to a lesser extent chemical analysis. Like sampling, sample preparation has also a notable impact on the measurement uncertainty. To provide further insight into the impact of sampling and sample preparation steps on the quality of measurement and the level of uncertainty chemical analysis of *Pleurozium schreberi* (Brid.) Mitt moss samples for selected trace elements (Cu, Fe, Mn, Zn) and rare earth elements (La-Lu) were done. All combined and duplicate samples were collected within three forested areas and prepared for analysis using two different treatment method, i.e., manually cleaning and triple rinsing with deionized water. The following statistical methods: ANOVA, RANOVA, modified RANOVA and range statistics were harnessed to calculate uncertainty of sampling, sample preparation and analysis. In all cases analytical uncertainty was below 3%. Sampling and sample preparation uncertainty varied from 3.8 to 12.8% and from 3.4 to 29.7%, respectively. The level of uncertainty was dependent on type of element, its intra- or extracellular distribution, specificity of sampling area and statistical method used for calculation.

**Biography**

Sabina Dołęgowska is an Assistant Professor at the Institute of Chemistry, Jan Kochanowski University in Kielce, Poland. She has graduated from the Institute of Chemistry in 2006, Jan Kochanowski University in Kielce and received her PhD degree from Gdańsk University of Technology in 2010. Her key interest is quality control of environmental studies, environmental chemistry and biogeochemistry, trace element and stable isotope geochemistry.

sabina.dolegowska@ujk.edu.pl

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### Biological active 1, 2, 4-triazole derivatives: Synthesis and biological studies

Zanariah Abdullah, Nafal Nazar Bahjat and Azhar Arifin  
University of Malaya, Malaysia

Ethyl 2-(ethylsulfanyl)benzoate was prepared by treating bromoethane with potassium carbonate and thioisocyclic acid. Ethyl 2-(ethylsulfanyl)benzoate was then converted to ethyl 2-(ethylsulfanyl)benzohydrazide. A series of 1-acythiosemicarbazides were then prepared from ethyl 2-(ethylsulfanyl)benzohydrazide, followed by cyclisation to form 1, 2, 4-triazole derivatives. The structures of intermediates and desired compounds were confirmed by spectroscopic analysis. *In vitro* DPPH radical scavenging activities of 1, 2, 4-triazole derivatives were studied and will be reported.

#### Biography

Zanariah Abdullah has involved in organic synthesis for more than 20 years. She continued her research in application of florescent molecules in surface chemistry, ionic liquids and biological activities studies. She is currently the Dean of Faculty of Science, University of Malaya, Kuala Lumpur, Malaysia.

zana@um.edu.my

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## Identification and origin of geochemical anomalies of trace elements in soils

**Agnieszka Galuszka**

Jan Kochanowski University, Poland

Natural variability of trace element distribution in the environment and substantial input of these elements from anthropogenic sources cause a large heterogeneity of geochemical data sets even on local scales. This is clearly visible in different post-industrial areas where the abundances of elements in soils can range over several orders of magnitude within very short distances. The term geochemical anomaly refers to an element concentration which is not typical for samples collected in a given area. In environmental geochemistry, the anomalous concentrations of elements can be estimated by comparison of the element concentration in the sample with that in a reference material, such as the post-Archean standard shale, the earth's crust (Clarke value) etc. This comparison can be used for calculation of many geochemical indices, for example Enrichment Factor (EF), Pollution Load Index (PLI), Geo-accumulation Index (GI). Geochemical anomalies can be separated from background values on the basis of statistical interpretation of results derived from environmental sample analyses. This study presents methodology of identification and interpretation of geochemical anomalies. Three datasets representing concentrations of As, Cd, Co, Cr, Cu, Ni, Pb and Zn in contaminated surface soils affected by multiple pollution sources were analyzed. The element concentration ranges were divided into background and anomalous populations with the use of the iterative  $2\sigma$  technique. The results showed that separation of geochemical anomalies from background concentrations can be helpful in selection of sites for detailed study on the origin of geochemical enrichments.

### Biography

Agnieszka Galuszka has been a Full Professor at the Institute of Chemistry, Jan Kochanowski University in Kielce since 2015. She has completed her PhD and DSc degrees at the Faculty of Earth Sciences and Environmental Management, University of Wrocław in 2002 and 2008, respectively. Her research interests are environmental geochemistry and biogeochemistry, stable isotope geochemistry, trace element geochemistry and green analytical chemistry. She has published 47 papers in scientific journals from the JCR database. She is an Associate Editor of the *International Journal of Environmental Science and Technology*.

agnieszka.galuszka@ujk.edu.pl

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**The use of stable isotope and Rare Earth Elements for solving environmental issues in acid mine drainage areas (south-central Poland)****Zdzisław M Migaszewski**  
Jan Kochanowski University, Poland

**W**isniowka Mt., located approx. 5 km north-east of Kielce (south-central Poland), belongs to the most interesting Acid Mine Drainage (AMD) areas throughout the world. It is built of upper Cambrian terrigenous rock formations with pyrite and hematite-goethite mineralization zones. The principal raw material is quartzite/quartzitic sandstone that have been extracted for over a century leaving abandoned quarries, tailings piles, mineral settling tanks and acid water bodies. The generation of AMD waters is initiated by oxidation of predominant As-rich gel-pyrite whose secondary products trigger subsequent reactions with metal- and REE-bearing minerals. The AMD lakes, ponds and pools are characterized by different geochemistry which patterns mineralogy and lithology of country rocks. Of the AMD water bodies, the Podwisniowka acid pit lake is highlighted by a low pH in the range of 2.2-2.4 and high concentrations of sulfates, Al, As, Co, Cr, Cu, Fe, Ni and REE. However, some strongly acidic seeps and pools contain even higher contents of trace elements, for instance as and REE up to 370 and 17.6 mg/l, respectively. It is noteworthy that two acid pit lakes show different NASC-normalized REE concentration patterns with positive medium REE (Podwisniowka) and heavy REE (Wisniowka) anomalies. Both S and O stable isotopes also display different delta values. These isotopes, REE, Y and some trace elements have been used as geochemical signatures for pinpointing localization of hotspots in the mining area as well as for determining a detrimental impact of acidic seeps and water bodies on neighboring rivers and farmer's wells.

**Biography**

Zdzisław M Migaszewski is currently a Full Professor at the Institute of Chemistry, Jan Kochanowski University in Kielce, Poland and a Chairman of the Scientific Board of the Polish Geological Institute in Warsaw. He has completed his graduation from the Faculty of Geology, University of Warsaw, Poland. He has completed his PhD and DSc degrees from the AGH University of Technology in Cracow and in 2009 was awarded a Professorship of Geology. His key interest is trace element and stable isotope geochemistry, mineralogy, sedimentary petrology and environmental analytical chemistry. He has conducted some projects in close collaboration with the US Geological Survey and University of New Mexico.

zmig@ujk.edu.pl

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### Kinetics and mechanism of oxidation of some amino acids by peroxodisulfate

**Abdelmahmod Saad**  
Red Sea University, Sudan

In this study two amino acids were chosen (DL alanine, DL serine) to determine their effect on dissociation of  $S_2O_8^{2-}$  ion. As the reaction was very slow,  $Ag^+$  ion was used as a catalyst. The kinetics measurement showed that the reactions in both cases were found in the first order with respect to  $S_2O_8^{2-}$ , half order with respect to  $Ag^+$  and zero order with respect to substrates. Mechanisms were proposed for these reactions according to the determined orders. The energy of activation (AE) was determined for each reaction and was found to be  $30.50 \text{ kJmol}^{-1}$  in case of DL serine and  $24.40 \text{ kJmol}^{-1}$  in case of DL alanine.

#### Biography

Abdelmahmod Saad has completed his PhD from Al Neelain University. He is currently the Dean of Faculty of Applied Sciences, Red Sea University in Sudan. He has published more than 10 papers in reputed journals.

mahmodsaad000@yahoo.com

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### The kinetics and mechanism of alcohol oxidation in alkaline 12-tungstocobaltate (III)

Latona Dayo Felix  
Osun State University, Nigeria

The kinetics of the oxidation of alcohol by 12-tungstocobaltate (III) in alkaline medium as a function of oxidant, alcohol, OH<sup>-</sup>, ionic strength and temperature were studied spectrophotometrically at  $\lambda_{\max}$  624 nm under pseudo first order conditions. The kinetic study showed first order dependence on  $[\text{Co}^{\text{III}}\text{W}_{12}]$ ,  $[\text{Alcohol}]$  and  $[\text{OH}^-]$ . Ionic strength effect on the reaction showed that the charges on the ions at the rate determining step are opposite and the reaction between alcohols and 12-tungstocobaltate (III) in alkaline medium exhibits 1:1 stoichiometry. The oxidative products were identified by FTIR spectroscopy. Salt effect was investigated by using  $\text{NaNO}_3$  and  $\text{KCl}$ . Michaelis-Menten plot showed the presence of an intermediate complex. Thermodynamic parameters were evaluated and a mechanism related to this reaction is proposed.

d1latona@yahoo.com  
dayo.latona@uniosun.edu.ng

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# **Chemistry & Mass Spectrometry Congress**

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## **Scientific Tracks & Abstracts** **(Day 2)**



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### Applications of laser-based ionization mass spectrometer in molecular photodissociation

King-Chuen Lin

National Taiwan University, Taiwan

By using the time-of-flight mass spectrometer, we have provided insight into interrelation of the ionization and fragmentation mechanism of ketene. When a Resonance-Enhanced Multiphoton Ionization (REMPI) technique is applied via the Rydberg state, the (2+1) REMPI process leads to a direct photoionization of ketene under low ionizing laser energy. When the (2+2) REMPI process dominates, the ketene ion is produced by the rovibrational autoionization of a superexcited state. The second application is to investigate competitive bond dissociation mechanisms for bromoacetyl chloride, 2- and 3-bromopropionyl chlorides following the transition  $1 [n(O) \rightarrow \pi^* (C=O)]$  at 234-235 nm. The branching ratios of C-Br/C-Cl bond fission were evaluated to be 0.47, 0.24 and 0.098, respectively, by using (2+1) REMPI technique equipped with velocity ion imaging. The mechanisms for C-Cl and C-Br bond fission are discussed. We will report photodissociation dynamics of methyl formate  $HCOOCH_3$  at photolysis wavelengths from 225 to 255 nm. Ion imaging of CO and H are acquired. The translational energy distributions of CO comprise three channels of triple fragmentation, roaming and Transition State (TS) processes, as photolysis wavelength is  $>248$  nm.

#### Biography

King-Chuen Lin is a Distinguished Professor of the Department of Chemistry at National Taiwan University and a Distinguished Research Fellow of National Science Council, Taiwan. He has received his BS degree in Chemistry from National Taiwan University, Taiwan, PhD in Chemistry from Michigan State University, USA and Postdoctoral career at Cornell University, USA. His research interests are photodissociation and reaction dynamics in gas and condensed phases, atmospheric chemistry and single molecule spectroscopy. He has published more than 172 related papers.

kclin@ntu.edu.tw

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**The application of mass spectrometry technology in clinical medicine and traditional Chinese medicine**

**Lin Zhang**

Dalian Medical University, China

LC-MS as a technological mean has been widely used in the field of clinical medicine and traditional Chinese medicine, including quality control and pharmacokinetics study, take Zibu Piyin Recipe, Shuanghua Baihe tablets, Chaiqin Qingning capsule as example; metabonomics and proteomics study, take Diabetes-Associated Cognitive Decline as example.

**Biography**

Lin Zhang has completed her PhD from Shenyang Pharmaceutical University, China. She has worked in Meiji Pharmaceutical University for one year and three months during her Doctoral studies. She is the Associated Professor in College (Institute) of Integrative Medicine. She has published more than 20 papers in reputed journals and has been serving as a Committee Member of many branches of World Federation of Chinese Medicine Societies.

zhl8247@163.com

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**Chemical constituents from the rhizomes of *Curcuma zedoaria* and assessment of their biological activities****Omer Abdalla Ahmed Hamdi**  
Al-Neelain University, Sudan

Phytochemical investigation of *C. zedoaria* resulted in the isolation of 21 compounds. Isolated compounds include 18 sesquiterpenes and three labdane diterpenes. Various chromatographic techniques were used for the detection and isolation of the compounds. Extensive spectroscopic methods including NMR, IR, UV, GC-MS, LC-MS were used for the identification of the isolated compounds. Isolated compounds were subjected to cytotoxicity, anti-oxidant and neuroprotective assays. Curcumenol and dehydrocurdione showed the highest protection (100%) against hydrogen peroxide induced oxidative stress in NG108-15 cells at the concentrations of 4 and 8  $\mu\text{M}$ , respectively. In the oxygen radical antioxidant capacity assay, zerumbone epoxide showed the highest antioxidant activity with a Trolox Equivalent (TE) of 35.41  $\mu\text{M}$  per 100  $\mu\text{g}$  of sample. In the MTT based cytotoxicity assay against four cancer cell lines (Ca 41 Ski, MCF-7, PC-3 and HT-29), curcumenone and curcumenol displayed strong anti-proliferative activity ( $\text{IC}_{50}$  8.3 and 9.3  $\mu\text{g}/\text{ml}$ , respectively). A quantum chemical study was performed to investigate their relationship with cytotoxic activity and revealed that the dipole moment ( $\mu$ ), molecular volume (V), molecular area (A), polarizability ( $\alpha$ ) and hydrophobicity (log P) are the most important descriptors that influence the cytotoxic activity of the compounds under investigation. The two most active compounds; curcumenol and curcumenone were investigated for their binding to Human Serum Albumin (HSA). The spectrofluorometric analysis, in conjunction with molecular docking study suggested that both curcumenol and curcumenone could bind to binding sites I and II of HSA with intermediate affinity while site I was the preferred binding site for both molecules.

**Biography**

Omer Abdalla Ahmed Hamdi has completed his PhD from University Malaya in Malaysia. He is the Director of Center of Natural Product Research and Drug Discovery. He has published more than 12 papers in reputed journals.

omerhamdi2001@hotmail.com

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## CHEMISTRY &amp; MASS SPECTROMETRY CONGRESS

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**Hydrophilic interaction liquid chromatographic determination of anti-diabetic drug, Glimepiride, in pharmaceutical formulations**Yuegang Zuo<sup>1</sup>, Si Zhou<sup>1</sup>, Pengxiao Zuo<sup>1</sup> and Yiwei Deng<sup>2</sup><sup>1</sup>University of Massachusetts Dartmouth, USA<sup>2</sup>University of Michigan, USA

Glimepiride is one of the most widely prescribed anti-diabetic drugs and contains both hydrophobic and hydrophilic functional groups in its molecules and thus could be analyzed by either reversed-phase High Performance Liquid Chromatography (HPLC) or Hydrophilic Interaction Liquid Chromatography (HILIC). In the literature, however, only reversed-phase HPLC has been reported. In this study, a simple, rapid and accurate hydrophilic interaction liquid chromatographic method was developed for the determination of glimepiride in pharmaceutical formulations. The analytical method comprised a fast ultrasound-assisted extraction with acetonitrile as a solvent followed by HILIC separation and quantification. The effects of various HILIC parameters on the separation and determination will be discussed in details at the presentation. The developed method has been successfully applied to determine the glimepiride contents in pharmaceutical formulations and human fluids.

**Biography**

Yuegang Zuo is currently a Full Professor in Analytical and Environmental Chemistry and Director of Graduate Programs at Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth. He has completed his BS degree in Chemistry from Wuhan University in 1982, MS degree in Environmental Chemistry from the Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences in 1984 and PhD in Environmental Science from Swiss Federal Institute of Technology, Zurich in 1992. His recent researches focused on separation, identification and quantification of pharmaceuticals and personal care products (PPCPs) and phenolic antioxidants in plants, pharmaceuticals, foods and the related environments and examine their occurrence, sources, distribution, transportation and fate in the bio-chemosphere. He has published over 70 peer-reviewed papers in prestigious international scientific journals such as *Science and Environmental Science and Technology*.

yzuo@umassd.edu

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