

POSTERS

Abstracts



8th Edition of International Conference on
Chemistry Education and Research

August 27-28, 2018 | Zurich, Switzerland

August 27-28, 2018
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DOI: 10.21767/2472-1123-C5-015

ORGANIC CHEMISTRY: THEORY, REACTIVITY, MECHANISMS IN MODERN SYNTHESIS

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Modern synthesis including asymmetric synthesis, have made fantastic progress during the last 40 years, especially by developing and applying new catalytic reactions. This contributes to render modern technologies more and more sustainable. Synthetic chemists, biochemists and chemical engineers must be able to predict whether a given equilibrium under given conditions will be exergonic or not. For that, thermochemical calculations and statistical thermodynamics are extremely simple, accurate and valuable tools to answer this question. In the same time one needs to be able to predict the rate of the reactions that will lead to the above equilibrium. Knowledge of reaction mechanisms (how nature transforms matter) and theories of reactivity are the most useful tools to help the molecular scientists. The Vogel-Houk textbook has been written to help engineers of molecules to approach satisfying answers to the above questions and help scientists to understand the dynamics of molecules. It complements other textbooks of organic chemistry and physical organic chemistry. It also gives a lot of data the molecular scientists will find useful for

the invention of new reactions and processes. It presents the most important concepts of the reactivity of organic and organometallic compounds. The book present 8 chapters that are: equilibria and thermochemistry; additivity rules for thermodynamic parameters and deviations; the rates of chemical reactions; molecular orbital theories; pericyclic reactions; organic photochemistry; catalytic reactions and; transition metal-catalyzed C-C bond forming reactions. A companion workbook gives the literature references and answers to problems.

Biography

Pierre Vogel, PhD degree from the University of Lausanne, 1969 (Prof. H. Prinzbach). After post-doctoral stays at Yale University, New Haven, USA (Prof. Martin Saunders) and at Syntex, Mexico-City (Prof. Pierre Crabbé) he return to Lausanne and become Full Professor of chemistry in 1977, first at the University of Lausanne, then (2001) at the EPFL. He has authored and co-authored more than 525 scientific publications and collected more than 12'100 citations.

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DOI: 10.21767/2472-1123-C5-015

CADMIUM IONS ADSORPTION BEHAVIOR ONTO SHELLFISH FOSSIL

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As a result of having examined cadmium ion adsorption using a shellfish fossil for the purpose of removing metal in the soil and metal ions, Ability for remarkable adsorption was recognized about a shellfish fossil. The similar findings are reported in the naturally derived inorganic matters such as oyster shell. However, there is hardly a study example about the detailed behavior of the ability for high adsorption. In this study, we made the adsorption isotherm from a water solution of cadmium about two kinds of shellfish fossils for the purpose of clarifying this. We make the mechanics of sorption of the shellfish fossil clear more and will study the practical development of this adsorption materials in future.

Biography

Dr Atsuko Fukuyama has completed her PhD in Environmental science by department of Earth and Environmental Sciences Graduate School of Natural Science and Technology Kanazawa University. She has worked as cooperation researcher of the oil contaminated soil by bioremediation at Kanazawa University. She has published more than 27 papers in journals and conference, and am working as a visiting associate professor at University of Fukui. The Society Prize, the Japanese Society of Geo-Pollution Science, Medical Geology and Urban Geology (2017).

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August 27-28, 2018
Zurich, SwitzerlandElena Atrazheva et al., J Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

GRAVSTOICH: AN INTERACTIVE TOOL FOR PRACTICE AND ENHANCEMENT IN STOICHIOMETRIC CALCULATIONS

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Stoichiometric calculations are both basic and the most important calculations covered in introductory chemistry. However, it is also one of the most challenging concepts taught in both high school and college/university level chemistry. Students coming from high school usually struggle to understand stoichiometric calculations; particular when dimensional analysis is applied. An interactive tool is designed for gravimetric stoichiometric calculations (GravStoich). GravStoich is designed to assist the students and guide them through stoichiometric calculations, as well as to reinforce the balancing of chemical equations and use of significant figures. GravStoich is adaptive according to students' improvement in solving the stoichiometric problems. GravStoich guides the students through the solution of the problem using three levels of assistance. Level 1 - Students are given a blank flowchart to assist in solving the gravimetric questions. Use of flowcharts helps the students to understand the logic behind the calculations involved in stoichiometric problems. Level 2 - Students are given a blank dimensional analysis set-up to assist in solving a gravimetric problem. Level 3 - Students are only provided a blank area to input the final answer to the problem. Regardless of the level of assistance, GravStoich provides a full feedback on how

the problem is solved using dimensional analysis. GravStoich has the potential to be customized to any kind of chemical problems involving stoichiometric calculations: electrochemistry, gas and solution stoichiometry. GravStoich can be used on any computer platform using Adobe Flash. We believe GravStoich is an excellent interactive tool that helps to fill the gap between high school chemistry and college/university introductory chemistry courses with this challenging concept.

Biography

Elena Atrazheva has completed her PhD in Organic Chemistry from Engelhardt Institute of Molecular Biology (Moscow, Russia) and Postdoctoral studies from the Faculty of Chemistry and the Faculty of Pharmacy and Pharmaceutical studies at the University of Alberta, Edmonton, Canada. Her main research focus was on the synthesis of nucleotides and nucleosides. She has worked as a Research Scientist for several pharmaceutical companies in Canada. In 2005 she started her teaching career at the Mount Royal University as an Instructor for Organic Chemistry courses. Since 2007, she has joined the Northern Alberta Institute of Technology (NAIT) as a full-time Instructor. She is teaching introductory level courses for Organic and General Chemistry.

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August 27-28, 2018
Zurich, SwitzerlandMarzieh Sohrabi et al., J Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

A NOVEL CHEMOSENSOR ACTING AS A FLUORESCENT "OFF-ON" ZN²⁺ SENSOR: EXPERIMENTAL, LOGIC GATE BEHAVIOR AND TD-DFT CALCULATIONS

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There is a huge scope for the exploration of the role of zinc in biological systems. Therefore, it is highly desired to develop a sensitive method for its detection. Unlike other metal ions such as Mn²⁺, Fe²⁺, or Cu²⁺, the Zn²⁺ in biological systems cannot be detected by spectroscopic methods, thus the fluorescence stands out as a method of choice. The Hqpzc, N-(quinoline-8-yl)pyrazine-2-carboxamide, as a small fluorogenic molecule with a selective "Off-On" switching behavior for detection of Zn²⁺ and a colorimetric sensor for Cu²⁺, comprises of quinoline as the fluorophore and pyrazine-2-carboxamide as the chelating group. This chemosensor exhibits a remarkable fluorescence response with a detection limit of 1.11×10^{-6} M when investigated in acetonitrile and the fluorescence intensity enhances significantly upon addition of one equivalent of Zn²⁺. The selectivity of Hqpzc for Zn²⁺ is based on the chelation-enhanced fluorescence (CHEF) mechanism. The binding mode of the Hqpzc with Zn²⁺ was investigated through Job's plot experiment, the fluorescence and UV-vis titration, ESI-MS, and density functional theory calculations. These results revealed that the binding stoichiometric ratio between Hqpzc and Zn²⁺ in acetonitrile is 1:1. The limit of detection (LOD) for Cu²⁺ is 1.48×10^{-5} M in acetonitrile solvent and the association constant (K_a) for Hqpzc-Zn²⁺ and Hqpzc-Cu²⁺ complexes are 3.837×10^4 and

7.352×10^7 M⁻¹, respectively. Other interfering ions such as Na⁺, K⁺, Ca²⁺, Mg²⁺, Fe²⁺, Co²⁺, Ni²⁺, Cu²⁺, Cd²⁺, Hg²⁺, Mn²⁺, Cr³⁺ and Al³⁺, show either no or slight change in the fluorescence intensity of Hqpzc in the presence of Zn²⁺. Notably, in the presence of Zn²⁺, the Hqpzc fluorescence exhibits reversibility with SCN⁻, and the fluorescent signals of Hqpzc are utilized to construct an INHIBIT type logic gate at the molecular level. Theoretical calculations, carried out with TD-DFT method, support the experimental observations.

Biography

Marzieh Sohrabi is a PhD student in Inorganic Chemistry, Isfahan University of Technology, Isfahan, Iran. Bsc. Azad University of Shahr-e-Rey, Tehran, Iran, 2003; MSc. Azad University of Shahr-e-Rey, Tehran, Iran, 2008. Research interest: Synthesis and characterization of emissive ligands and their metal complexes with their application as sensors for detection of biologically important ions such as Co²⁺, Cu²⁺, Zn²⁺. Construction of molecular probes for application in live cell imaging. Construction of molecular logic gates from chemical light switches based on emission properties of small molecules. Synthesis and characterization of emissive organometallic complexes and their application in biology as anticancer drugs, and computational chemistry.

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8th Edition of International Conference on
Chemistry Education and Research

August 27-28, 2018 | Zurich, Switzerland

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Zurich, SwitzerlandJiménez Martínez et al., J Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

LEARNING THE NOMENCLATURE AND FORMULATION OF INORGANIC COMPOUNDS WITH JIGSAW COOPERATIVE LEARNING METHOD

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It is well-known that students tend to find problems when learning the formulation and nomenclature of inorganic chemical compounds. They assume their study as the memorization of a set of particular rules, which will vary according to the type of nomenclature and the family studied; instead of approaching this task as a global study with a certain number of particularities. As a result, students presumably end up memorizing an endless number of concretions, in very few cases reasoning. The search for a solution to this issue would be appropriate, since the negative predisposition of students to the study of the formulation and nomenclature of inorganic chemical compounds could be changed, making it more attractive, interesting and motivating. Likewise, creating a relaxed and calm environment in the classroom would foster that students fearlessly express their difficulties. In this vein, implementing the use of cooperative structures would facilitate other competences acquisition. Therefore, this didactic approach is based on cooperative learning, since the Jigsaw technique is used. Students will assume the role of members of the IUPAC (International Union of Pure and Applied Chemistry). Then, this proposal also falls within the scope of contextualized collaborative learning, since students can somehow connect with their daily experiences and assume a role during the teaching-learning process, in which the teacher

would be the promoter of the teaching while students set the pace. In conclusion, the main aim of the present paper is to find a way to revert the sometimes tedious process of memorizing the formulation and nomenclature of inorganic chemical compounds and make their study more interesting for students through a methodology that enables them to play an active role in the process and learn from each other.

Biography

Jiménez-Martínez has completed her PhD in Food Technology in the University of Murcia. She earned her chemistry degree from the University of Valencia. Additionally, she received her master's degree on industry and chemical research, having specialized in analytical chemistry, from the University of Santiago de Compostela. She has also worked as a chemist in two research projects: one of them on neonatal screening and the other on ultrasound technology for winemaking. She is currently studying a master's degree in teacher training at the Catholic University of Murcia. Santiago López-Miranda has 14 years of teaching experience at the UCAM Universidad Católica de Murcia, as a professor of mathematics and physics. Besides, he has 6-year experience in the master's degree in teacher training. He has also participate in numerous teaching innovation activities, especially related to online teaching.

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August 27-28, 2018
Zurich, SwitzerlandRonojoy Sen Gupta et al., J Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

INVESTIGATION OF THE ANTIBACTERIAL ACTIVITY OF MODIFIED REDUCED GRAPHENE OXIDE (MRGO) NANOSHEETS AGAINST *S. AUREUS*

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Carbon-based nanotechnology is a promising field of research for its potential application in the fields of bio-sensors, health care and biomedical sciences. Graphene nanosheets due to their one atom thickness are the ideal candidate for trapping the bacteria for transmission and scanning electron microscopy imaging. In this paper, we report on the antibacterial activity of reduced graphene oxide nanosheets synthesized by modified Hummer's method. MRGO nanosheets were characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM) and atomic force microscopy (AFM) along with disc diffusion technique, which was employed to evaluate anti-bacterial activity of nanosheets using *S. aureus* as model microorganism. The cell viability of *S. aureus* decreased significantly when it was exposed to MRGO nanosheets as revealed in the spectrophotometric study of bacterial growth. A clear zone of inhibition was also observed in the cultured plates treated with MRGO, revealing its antibacterial property. AFM study revealed that structural defects of MRGO were probably responsible for membrane integrity disruption leading to bacterial cell death. To elucidate the bactericidal activity, SEM and TEM studies were

carried out. Studies showed that the defects formed in the MRGO synthesis is the main factor for the effective antibacterial activity. Further molecular studies are required to completely reveal the antibacterial property of MRGO nanosheets.

Biography

Ronojoy Sen Gupta, has completely his PhD degree in Physiology from the Department of Physiology, University of Calcutta, Kolkata, India. He has worked as Postdoctoral fellow in Molecular Endocrinology laboratory, Hormone Research Center, Chonnam National University and Department of Life Sciences, Gwangju Institute of Science and Technology, Gwangju, South Korea. He has worked as faculty in Department of Biotechnology and Bioinformatics, SMMTR, Sikkim Manipal University, India. At present he is working as Director, Genobiotek, Kolkata, India. Alok Chattopadhyay, has completed his PhD degree in Physiology from the Department of Physiology, University of Calcutta, Kolkata, India. He is now working as Assistant Professor, Department of Physiology, Harimohan Ghosh College, University of Calcutta, India.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

THREE DIMENSIONAL SOLAR CELLS

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Solar cells that are flexible and three dimensionally structured to absorb light from any incident angle would serve a wide range of applications in the domestic, commercial, and military sectors, and can be readily incorporated into fabric-based systems. We report the fabrication of novel dye sensitized solar cells incorporating functional centers, CdS and CdSe quantum dot sensitizers, an efficient P3HT/PCBM bulk hetero junction layer, and well structure nano and micro porous TiO₂ oxide layers. The prepared cells were morphologically characterized using AFM and SEM, and were electrically tested over a range of cell lengths

and in series/parallel configurations. Efficiencies of up to 7% were observed, and the cells performed well in series and parallel configurations, suggesting that cells with this configuration are well suited for deployment in multi-cell systems. Therefore, solid state power wires have great prospects to develop multifunctional structural composites with inherent light sensing capabilities for structural or aerospace safety and e-textiles by weaving our optoelectronic wires into reinforcing fabrics.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

EXPLORING THE FLIPPED CHEMISTRY CLASSROOM: A QUALITATIVE STUDY TO CHARACTERIZE THE ELEMENTS USED IN SUPPORTING A FLIPPED LEARNING ENVIRONMENT

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This qualitative study is part of a larger project to better understand the impacts of flipped learning on a diverse set of courses and students. Current studies of flipped learning in higher education Science, Technology, Engineering, and Mathematics (STEM) disciplines have mainly focused on single-courses and outcomes such as attendance, enjoyment of the learning environment, course grades, and course completion rates. Review of these studies show mixed results regarding the effectiveness of flipping. This split may be the result of differences in adoption or adaptation of the flipped method or differences in the assessment practices used to gauge effectiveness. Therefore, this multi-course multi-institution study, utilizing a coordinated set of assessment instruments, and accounting for adoption practices, is novel in scope and its potential for transforming the understanding of this learning environment. To better understand what it means to 'flip' a chemistry class, we interviewed instructors about their adoption practices, conducted classroom observations, analyzed classroom artifacts, and

conducted student focus groups. Data collection took place in six introductory/general chemistry courses at four universities in the United States. The instructor-reported elements of all six courses were nearly identical, that is, all courses required students to 1) watch videos to acquire content knowledge outside of class, 2) complete pre-class assessments of knowledge, 3) build applications of knowledge through in-class activities, and 4) further assess knowledge through online homework. However, the way in which some elements were structured within a course were very different and could be responsible for varied course outcomes. For example, we observed that poor alignment of video content with the pre-class assessment and/or in-class activity reduced students' use of and perceived value in the videos. In addition, we found broad levels of engagement during in-class activities. An overview of similarities and differences, including their potential impacts will be presented.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

THE EFFECT OF ACTIVE LEARNING VIDEOS ON ORGANIC CHEMISTRY LEARNING

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A challenge that many students face when learning organic chemistry involves balancing concept learning and concept application in problem-solving. Too often, students lean towards rote memorization and binge learning to learn organic chemistry without understanding the concepts behind them. This leads to lower retention of information and limited ability of the students to efficiently progress further in their organic chemistry education. In this project, we offer supplemental video resources as a tool for students to learn and apply organic chemistry one concept at a time. The videos differ from simple concept review in that they integrate active learning exercises. Video length generally ranges from three to ten minutes and follow a basic template of concept introduction, connection to previously learned topics, followed by a concept check where students are asked to pause the video and solve the displayed problem based off of previous and newly acquired knowledge. The videos continue the pattern of concept coverage followed by application exercises, allowing students to

interact with and use the concepts instead of passively absorbing material. After each problem, a short explanation is given where concept utilization is emphasized. The goal is to increase student knowledge retention and learning by supplying additional online resources that allow the student to actively engage in the material. Student participation in the study was selected on a voluntary basis from the Organic Chemistry II course. Participation involved watching a set number of videos per week as per course schedule, followed by an online survey. Short written assignments addressed students' conceptual and practical understanding from the videos. Small groups met periodically to discuss content progress and the effects of video utilization during the semester-long course, with discussion centered around the student's ability to connect concepts, as well as inquiry into the video's role in student learning.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

INCORPORATING ACTIVE LEARNING COMPONENT IN TEACHING ORGANIC CHEMISTRY COURSES

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Studying organic chemistry is complicated and stressful for the majority of students. Teaching faculties are trying to implement different tools and techniques to help students learn the material and also reduce the anxiety associated with the learning process. It is well-known fact that using active learning principals in teaching helps students master their knowledge in this subject. For example: creatively designed homework problem sets and clicker questions during lecture, thoughtfully created extra credit activities, organized discussion sessions and course assignments. Implementation of these activities for the second and third year undergraduate Organic and Bio-Organic Chemistry courses will be discussed. Students can be actively involved in these activities not only as learners but, also as mentors. Mentors can participate in preparation and conducting discussion

sessions, preparing sets of clicker or review questions, share their experience during lab preparation sessions or even help with creation of new laboratory experiments. Our mentors are students who have recently successfully completed the course and come from work study or volunteering positions. Different learning activities such as: extra credit projects, discussion sessions, laboratory skills seminars, literature searching assignments, etc. are used in these courses. This talk will focus on the students' experience as learners and mentors for our organic chemistry courses at the University of Toronto Scarborough. Also discussed will be the feedback from mentors and mentees as well as methods of assessment and the advantages of each approach.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

CHEMISTRY EDUCATION FOR UNDERGRADUATE AND HIGH SCHOOL STUDENTS: USING BIOFUEL ANALYSIS TO LEARN THEORY FROM EXPERIMENTAL

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UNESCO recommended introduction of Education for Sustainable Development, at high school and undergraduate levels. Consequently, educators introduced new syllabi and innovative teaching through a problem oriented approach. The latter dwells on current, socio economically important themes, especially those related to green chemistry and sustainability. Increasingly, educators are shifting to student centered active learning teaching where the students work in groups to solve relevant problems. Active learning should be extended to high school students. On all levels, we should link the experimental results to theory. We used active learning to present diverse topics to high school and undergraduate students. Examples are experiments on chemical kinetics to teach reaction mechanism; dyeing and SEM microscopy to explain the reason for consumer

preference for natural fibers, and different methods of analysis of bioethanol and biodiesel and their blends with petroleum based fuels (gasoline and diesel oil). Methods for the latter analysis include the use of natural or synthetic dyes that show solvatochromism (UV Vis) and simple instrumental analysis, e.g., to measure the densities and refractive indices of fuel blends. Qualitative and quantitative analysis of fuel composition was done using simple gas chromatography–flame ionization detector (GC/FID) and advanced equipment, gas chromatography–mass spectrometry (GC/MS). The positive answer of the students to our approach is stimulating; the contact between high school and the university is both demanding and rewarding.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

VISIBLE LIGHT PHOTOINITIATORS OF POLYMERIZATION: TOWARDS HIGH EFFICIENCY, LOW COST AND NON-TOXIC INITIATORS

Frédéric Dumur

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Considering the serious environmental pollution and energy crisis resulted from human activities, light-activated chemical reactions are of critical importance for the sustainable development of mankind. In this regard, photocatalysis has attracted great interest and researchers from academia, industry, and government research laboratories have made remarkable progress in this field, including solar fuels (CO₂ capture, water splitting, etc.), pollutants degradation, and chemical synthesis. Recently, the concept of visible-light photoredox catalysis has been successfully adopted in polymer synthesis upon soft conditions. Organometallic compounds with excellent photochemical properties (e.g. strong visible light absorption, long excited state lifetimes) have a great potential as photoinitiators for free-radical initiated [(meth)acrylates] and cation initiated (epoxides or vinyl ethers) polymerizations. Over the years, a series of ruthenium-, iridium- or zinc- complexes have been successfully

developed and applied as photoinitiators. However, the search for photocatalysts based on low-cost and non-toxic metals and allowing efficient polymerization reactions at low concentrations in the photocurable formulation remains today highly interesting and challenging. Parallel to this, a new family of photoinitiators has emerged in 2018, i.e. the TADF photoinitiators that are specially designed to exhibit long-living excited states and that can clearly compete with the traditional metal-based photoinitiators. In this presentation, recent advances in the design of metal-based and metal-free photoinitiators will be presented. The recent results obtained with these new families of photoinitiators pave the way towards the development of a new generation of highly efficient, low cost and non-toxic photoinitiators operating under visible light and soft irradiation conditions, what is cruelly missing in industries at present.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

NEW SOLUTIONS AND PEDAGOGICAL INNOVATIONS FOR CHEMISTRY EDUCATION THROUGH COLLABORATIVE LUMA-ECOSYSTEM

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Some examples of the successful LUMA activities are presented, and the use of design-based research method as a tool for new solutions pedagogical innovations, especially in chemistry education. The aim of LUMA Centre Finland (abbreviated from "luonnontieteet", the Finnish word for natural sciences, and "mathematics") is to inspire and motivate 3-19 years old children and youth into science through the latest methods and activities

of science and technology education. In addition, the aim is also to support the life-long learning of teachers working on levels of education from early childhood to universities, and strengthen the development of research-based teaching. LUMA Centre Finland is an umbrella organization for the collaboration of schools, 12 Finnish universities and the business sector.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

MAGNETOELECTROPOLISHING AND HIGH-VOLTAGE ELECTROPOLISHING OF METALS AND ALLOYS

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Electropolishing of metals and alloys has been developed for many decades now, with its ascents in recently patented magnetoelectropolishing (MEP) process. Most of electropolishing processes proved its usability for a variety of metallic materials, beginning specifically from austenitic stainless steels, through titanium, nickel, cobalt, copper, and their alloys, including many other metals, such as aluminum and its alloys, intermetallic compounds (nitinol), as well as niobium and tantalum. During MEP the stirring is self-imposed by Lorentz force as a result of interaction of electric and magnetic fields. The influence of magnetic field on electrochemical process in MEP can be divided into three main categories: (1) the effect of magnetic field on the mass transfer, (2) effect on kinetics of the electrode reaction, and (3) effects relating to morphology and chemistry of the surface after electrodisolution. The additional external magnetic field applied in the MEP process results in effective modifying the metal surface properties of treated parts in comparison with the properties obtained after a standard electropolishing (EP). During

MEP, beneficial modification of oxide layer of treated metals and alloys is obtained. After MEP the protective oxide formed on the surface differs significantly in morphology, homogeneousness, thickness, kind and quantity of foreign species incorporated in it. Concerning the last matter – we found the non-standard conditions of high-voltage electropolishing (HVEP) process (up to 450 V) result in incorporation of some interesting elements from the electrolyte into the surface film. Our studies revealed the copper enrichment of stainless steel, with simultaneous reduction of chromium in the surface layer. Under magnetoelectropolishing of metallic biomaterials, the corrosion resistance, biocompatibility, osseointegration, endothelialization, cleanability, anti-galling and anti-seizing properties are achieved. Some other advantages of MEP are de-hydrogenation of surface layer and a high increase in fatigue resistance, the effects especially valuable in the parts of small diameters or cross-sections.

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August 27-28, 2018
Zurich, Switzerland

J Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

STUDY OF CHANGES IN THE HYDROCHEMICAL REGIME OF DRINKING WATER SOURCE - GEGHAROT RIVER, ARMENIA

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Changes in freshwater resources availability, quality, stream flow and in river ecosystems are the major expected impacts of anthropogenic pressure and climate change in watersheds. Freshwater reduction deteriorates water supply and increases water demand. Thus, a long-term study of the quality and quantity of freshwater sources is urgently required, as well as identification and prediction of expected hydrochemical changes are needed. In current work, the determination of changes in concentrations of over 22 metals in the source of the Gegharot River was done for 2007-2016. The Gegharot River is main drinking water source of the relatively large villages (about 1700-3000 person) of Aragats Mountain region in Armenia. The runoffs of snow-melt water at 2200 m down top of the mountain are the parts of Gegharot River's streams system and they flow through the manganin and iron ores.

The anthropogenic and climate change impacts on the river water quality were studied and estimated. It was shown, that in the result of the changes of climate conditions, natural acid springs were started to mix with the Gegharot source, which leads the decrease in pH value until 3-4, as well as 10-100 increase in concentrations of Mn, Fe, Ni and other metals in water during one-two months in summer and autumn. Due to the deterioration of environmental flow in mid-flow of the river, as a result of small HPPs operation, the hydrochemical changes in the Gegharot source was observed longer and more frequently. Thus, the Gegharot drinking water source is being violated by the anthropogenic impact and is strongly required to be protected.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

COMPUTATIONAL MATERIALS DESIGN FOR ENERGY AND ENVIRONMENTAL APPLICATIONS

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The world's dependence on fossil fuels has led to the need for alternate sources of energy as supplies dwindle, as well as a growing need to remove harmful compounds from the air. Hydrogen energy and lithium-ion batteries are promising candidates for supplanting fossil fuels for automobile applications while novel adsorbents like metal-organic frameworks (MOFs) are promising materials for removing harmful gases. To date, the author's researches have been concerned with both aspects of the fossil fuel problem. Regarding hydrogen energy, his researches are focused on understanding the thermodynamics of metal hydride reactions for hydrogen storage applications. Specifically, the goal is to screen thermodynamically promising metal hydride reactions from a full database of metal hydride mixtures using first-principles calculations. The large-scale screening approach

ultimately provides a number of promising single-step or multi-step metal hydride reactions. On the other hand, his research focus in the field of the lithium-ion batteries is on fundamentally understanding the thermodynamics and redox properties of promising electrode materials which would directly affect the battery capacity. The author's researches on MOFs are related to investigating promising MOFs for the removal and separation of harmful gases. Quantum mechanical methods are used to screen and assess functional groups that would be incorporated into MOF ligands to preferentially adsorb harmful gases under humid conditions. In conclusion, his research goal is to contribute to the community for the transition to environmentally friendly ecosystems.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

AN ANALYSIS OF PRE-SERVICE CHEMISTRY TEACHERS MISCONCEPTIONS IN SYMBOLIC LEVEL OF STOICHIOMETRY

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In *situ* generated fluorescent gold nanoclusters (Au-NCs) are used for bio-imaging of three human cancer cells, namely, lung (A549), breast (MCF7), and colon (HCT116), by confocal microscopy. The amount of Au-NCs in non-cancer cells (WI38 and MCF10A) is 20–40 times less than those in the corresponding cancer cells. The presence of a larger amount of glutathione (GSH) capped Au-NCs in the cancer cell are ascribed to a higher glutathione level in cancer cells. The Au-NCs exhibit fluorescence maxima at 490–530 nm inside the cancer cells. The fluorescence maxima and matrix-assisted laser desorption ionization (MALDI) mass spectrometry suggest that the fluorescent Au-NCs consist This article surveys and investigates pre-service chemistry teachers' misconceptions in stoichiometry at the symbolic level, and possible solutions to address those misconceptions. Students and teachers broadly acknowledge the importance and difficulty of stoichiometry. Available research, meanwhile, also broadly acknowledges misconceptions at the symbolic level. In an effort to investigate associated misunderstandings, and to search for possible solutions, research was performed in Thai pre-service teachers. Fourteen Thai pre-service second year chemistry students participated. Three questions at the symbolic level of stoichiometry were presented asking students to solve

by written explanation. One-on-one interviews were conducted. 72% of pre-service chemistry teachers were not able to solve the problems because they had multiple misconceptions such as: misconceptions about the formula related to chemical bonding; misconceptions about the chemical equation and; misconceptions about the calculations and mathematics. The written testing and interviews revealed that art of the problem is that a strong foundation in mathematics and chemistry is important and related to solving the problem of stoichiometry at the symbolic level. At a deeper level, the misconceptions appear to relate to the abstractness of stoichiometry at the molecular level and symbolic level. To be effective, and meaningful, teachers should apply the so-called three levels of thinking carefully integrating and linking the macro, molecular and symbolic levels to teach students in the classroom. In the process, teachers must initially check the students' prior knowledge because students must be able to link prior knowledge such as how to write chemical formulas, how to balance chemical equations, and how to do stoichiometric calculations. In short, what is proposed is a holistic and integrative approach applying the multiple levels of chemistry with careful consideration of the students' prior knowledge.

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Chemistry Education and Research

August 27-28, 2018
Zurich, Switzerland

J Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

EVOLUTIONARY MODEL OF SUSTAINABLE CHEMISTRY

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According to the definition of sustainable development of the World Commission on Environment and Development, we should meet the needs of the present without compromising the ability of future generations to meet their own needs. The definition is ambiguous and provides very little accountability, as our prediction capabilities have had difficulties correctly forecasting scientific discoveries and technological developments, while our track record is even worse for predicting economic changes or societal transformations. Large amount of money was spent across the globe on projects, which have never addressed the real needs of future generations. More importantly, sustainability should be independent of economic and social aspects, as stake holders could have vested or even conflict

of interests in unsustainable developments. An alternative definition of sustainability was recently proposed, which was limited to resource replacement and waste remediation and disconnected from economic and societal issues. Resources, including energy, should be used at a rate at which they can be replaced naturally, and the generation of wastes cannot be faster than their remediation. It was used to evaluate the sustainability of basic chemicals and technologies. A new evolutionary model of sustainable chemistry will be also discussed, which provides a system for the combination of the intrinsic resource and waste management issues with economic and societal factors.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

SUSTAINABLE REUSE OF HIGH STRENGTH LEACHATE BY TREATMENT USING AEROBIC/ANOXIC PROCESSES

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Leachate originating from landfills poses a significant environmental threat to both the groundwater and surface water. In order to reuse it for irrigation, the leachate has to be collected and treated in a proper way. In this study, leachate samples were collected from a working landfill in Kuwait. Aerobic/anoxic (A/A) biological reactors were used to treat the collected leachate. The analysis of leachate show high solids content and high organic strength as expressed by its biochemical oxygen demand (BOD) and chemical oxygen demand (COD). The maximum COD concentration was 800 mg/l and the maximum

total dissolved solids (TDS) concentration was 24000 mg/l. The biological treatment of leachate was efficient for removal of organic compounds. The COD removal efficiency reached a value of 90% within a month. Nitrification rate was higher than denitrification processes. The nitrate concentration in the reactor decreased from a maximum value of 750 mg nitrate-N/L to a minimum of 300 mg nitrate-N/L in 20 days. In general the A/A treatment process has high efficiency in treatment of COD, solids, and ammonia concentrations.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

GREEN SYNTHESIS AND CHARACTERIZATION OF METAL OXIDES/POLYMER NANOFIBERS FOR VARIOUS APPLICATIONS

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Green chemistry has been of great interest to researcher in the area of synthesis and fabrication of nanoparticles for waste water treatment and electrochemical sensors application. This research therefore report the green synthesis of metal and metal oxide nanoparticles for various application. The synthesized nanofibers were characterized by using spectroscopic, morphological and electrochemical techniques such as cyclic voltammetry and impedance spectroscopy. Further studies were conducted on the synthesized nanomaterials such as antimicrobial properties, toxicity studies, the electron transport

properties, stability and reproducibility of the nanomaterials. The purpose of the study is also to evaluate the electrochemical properties of nanoparticles synthesized via green plants extract and further applied towards the electrochemical detection of various biological and environmental molecules. The synthesized nanomaterials showed good applications in electrochemical sensors, waste water treatment and wound healing.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015**CANCER CELL IMAGING USING IN SITU GENERATED GOLD NANOCCLUSERS****Md Asif Amin¹ and Kankan Bhattacharyya²**¹Balurghat Mahila Mahavidyalaya, India²Indian Institute of Science Education and Research, India

In *situ* generated fluorescent gold nanoclusters (Au-NCs) are used for bio-imaging of three human cancer cells, namely, lung (A549), breast (MCF7), and colon (HCT116), by confocal microscopy. The amount of Au-NCs in non-cancer cells (WI38 and MCF10A) is 20–40 times less than those in the corresponding cancer cells. The presence of a larger amount of glutathione (GSH) capped Au-NCs in the cancer cell are ascribed to a higher glutathione level in cancer cells. The Au-NCs exhibit fluorescence maxima at 490–530 nm inside the cancer cells. The fluorescence maxima and matrix-assisted laser desorption ionization (MALDI) mass spectrometry suggest that the fluorescent Au-NCs consist

of GSH capped clusters with a core structure (Au₈₋₁₃). Time-resolved confocal microscopy indicates a nanosecond (1–3 ns) lifetime of the Au-NCs inside the cells. This rule out the formation of aggregated Au–thiolate complexes, which typically exhibit microsecond (.1000 ns) lifetimes. Fluorescence correlation spectroscopy (FCS) in live cells indicates that the size of the Au-NCs is .1–2 nm. For in situ generation, we used a conjugate consisting of a room-temperature ionic liquid (RTIL, [pmim][Br]) and HAuCl₄. Cytotoxicity studies indicate that the conjugate, [pmim][AuCl₄], is non-toxic for both cancer and non-cancer cells.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

NEW EXPLORATION IN BIOMINERAL PROCESSING OF LOW-GRADE ORES AND INDUSTRIAL WASTES

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The mineral processing industry is increasingly facing problems with processing of secondary resources like low grade ores and other industrial wastes for a green zero waste technology and sustainable economy. Failure of the conventional physico-chemical methods adopted for the metal recovery from such secondary resources in terms of economics and eco-friendly approach has doubled the problems in the mineral processing sector. Over the past few years, the advent and approach of microbial processing has seen a revolution in the mineral processing area. The main power of microorganisms is the ability to compensate the redox reaction within mineral matrix resulting in the easy dissolution of metals. However, the problem associated in the microbial processing is the metal toxicity towards microorganisms which has been solved by their adaptation to the higher concentration of heavy metals. It is now believed that these tiny bugs have the tremendous potential to recover metal values from such difficult to treat resources. With all the discussions available on the open literature, more and more information is being offered to understand the eco-physiology

of such microorganisms. The information on the diversity of oxidizers and reducers has enabled us to gather more and more data for their utilization in the mineral processing sector. Genetic manipulation is a powerful and unique tool which can bring drastic changes in the physical, chemical and biological properties in an organism. These changes bring about the extra ability to survive in the extreme environments that does not favour the natural species. Application of microalgae must be given top priorities in industries in solving environmental issues as well by means of remediation, biosorption and latest for energy production. Server directly predicts the key proteins involved in iron and/or sulphur oxidation by several groups of bioleaching bacteria that can be very helpful toward development of a novel microbial consortia. Hence, the applications of such bioinformatics predictions can help to shape the outlook of the bioleaching processing. It is believed that the coming years will see a more advanced and new designed reactors for the bioleaching process in the sustainable biotechnological industry.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

PURIFICATION OF SINGLE WALL CARBON NANOTUBE (SWNT) PRODUCED BY ARC-DISCHARGED METHOD BY SIMPLE AIR OXIDATION AND ACID REFLUX METHODS

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Arc discharge method is a suitable method for the mass production of single-walled nanotubes (SWNT). But this process also produces lots of impurity like amorphous carbon, graphite nanoparticles and metals particles (like Fe, Co, Ni or Y) along with this nanotube structure. A simple, cost effective but useful refinement technique for purification of SWNT produced by arc-discharged method is discussed in this report. This novel purification method is incorporated with air oxidation followed by nitric acid treatments to remove the unwanted particles. At the first stage of this purification, oxidation of SWNT in air at temperatures of 400°C for 4 h burns out the carbonaceous particles and in the next step nitric acid (HNO₃) reflux with for 8 h etches away the catalytic metal particles. The approach of a selective oxidative etching process is based on the fact that the burning temperature of amorphous carbons is faster than that of carbon nanotube

which involved at the first stage of purification here and in the second stage encrypted metal nano particles within SWNT can be melted into the acid by heat treatment. These two processes are complementary to each other to remove the carbonaceous particles and transition metals. This whole purification process provides a total yield of about 25-30 wt.% with the 77% purity which was confirmed by the thermogravimetric and NIR analysis respectively. The effects of each treatment in the purification process is also discussed by characterizing the intermediate products using thermogravimetric analysis, Raman spectroscopy, vis-NIR spectroscopy, scanning electron microscopy and transmission electron microscopy.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015

PHYTOCHEMICAL AND ANTIOXIDANT ASSESSMENTS OF THREE FRACTIONS FROM METHANOL EXTRACT OF SPATHODEA CAMPANULATA BEAUV. LEAVES

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Aims: To screen hexane, ethyl acetate and methanol fractions of the methanol extract of *Spathodea campanulata* leaves for secondary metabolites, to isolate and to characterize constituents of the ethyl acetate fraction using GC-MS and IR and to determine the antioxidant activities of the three fractions.

Methodology: Methanol extract of *Spathodea campanulata* leaves was obtained by cold extraction, and partitioned into hexane, ethyl acetate and methanol fractions. Phytochemical screenings of the fractions were carried out using standard procedures to identify the class of constituents present in each of them. Ethyl acetate fraction was subjected to column chromatographic separations by gradient elution, and isolates were TMS (trimethylsilyl) derivatized and characterized by GC-MS (gas chromatography-mass spectrometry). Antioxidant content was also evaluated on the three fractions using 2,2-diphenyl-picrylhydrazyl (DPPH) free radical scavenging method. Percentage of inhibition and IC₅₀ values were obtained for each fraction.

Results: Phytochemical screenings revealed presence of alkaloids, tannins, saponin, resins, phenol, cardiac glycosides,

steroids, flavonoids, anthraquinones and terpenoids in the three fractions in varying concentrations. Alkaloids, resins, phenol and cardiac glycosides were found to be intense in the three fractions while phlobatannins was found to be absent in all the three fractions. Three compounds isolated from the ethyl acetate fraction were characterized based on MS and IR spectral interpretations as palmitic acid, ethylamine and caffeic acid. Percentage of inhibition of the three fractions indicates that they have substantial antioxidant activity with the standards at high concentration of 250 to 1000 µg/mL. The hexane fraction has the highest antioxidant activity with an IC₅₀ of 178.46 µg/mL when compared to other fractions.

Conclusion: This paper reports phytochemical constituents and high antioxidant activity (at concentrations of 250 µg/ mL and above) of the African tulip tree (*Spathodea campanulata*) when compared to the standards. This has not been earlier reported in literature, our results support its wide ethno-medicinal applications.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015**PHYTOCHEMICAL STUDIES AND *IN VITRO* ANTIOXIDANT,
ANTIPROLIFERATIVE AND ANTIFUNGAL ACTIVITIES OF THE STEM BARK OF
BOSWELLIA DALZIELII HUTCH.****Yves S Kafuti¹ and Kalulu M Taba²**¹University of Kinshasa, DR Congo

B*Boswellia dalzielii* (*B. dalzielii*) Hutch. is from the genus *Boswellia* and the family of Burseraceae. It is a tree plant abundantly found in North-Western Nigeria and very common among the locals as a potent source of ethnomedicine. This work aims at evaluating the phytochemical, antioxidant, antiproliferative and antifungal activities of the stem bark of *Boswellia dalzielii*. The phytochemical screening of the stem bark of *B. dalzielii* indicated the presence of tannins, saponins, flavonoids, steroids, carbohydrate. The phenolic content was found to be highest in sub-fraction C (481.20±10.13 mg GAE/g) and flavonoid contents were found to be highest in methanolic extract (142.17±4.82 mg RE/g). *Boswellia dalzielii* stem bark extracts, fractions and sub-fractions B, C and D exhibited antioxidant capacity; and the highest antioxidant activities were recorded from aqueous fraction and

methanol extract for the DPPH; and aqueous fraction and sub-fraction D for the FRAP assay. Antiproliferative, sub-fractions C and D at the concentration of 125 µg/ml gave the highest percentage of inhibition (90%) followed by sub-fraction B (50%) at 250 µg/ml. The antifungal screening of the bark methanolic extract, fractions and sub-fractions showed activity against *Candida albicans*; ethyl acetate and aqueous fractions showed activity against *Penicillium notatum*, while there was no activity shown by methanolic extract, fractions and sub-fractions against *Aspergillus niger*. These results further showed that the stem bark of *Boswellia dalzielii* has high growth inhibitory activity on the seeds of *Guinea corn*; and therefore may possess anticancer component(s) which need(s) further investigation.

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August 27-28, 2018
Zurich, SwitzerlandJ Org Inorg Chem 2018, Volume 4
DOI: 10.21767/2472-1123-C5-015**ISOLATION, STRUCTURAL ELUCIDATION AND BIOACTIVITY STUDIES OF LEAF
EXTRACT OF *VERNONIA AMYGDALINA*****Muluye Melak Zenebe**

University of Gondar, Ethiopia

V*ernonia amygdalina* (VA) is a tropical African plant of the Asteraceae family and is occasionally cultivated for its medicinal uses, which include as a treatment for diarrhea, skin wounds, fever mastitis and warms infection. The aim of this study is to isolate and elucidate the structure of some of the chemical constituents from the leaf of *Vernonia amygdalina* and its bioactivities. Methanol extract of *Vernonia amygdalina*,

after repeated chromatography led to the isolation of a different compound, one of this compound (MM-4) is partially characterized based on the spectral data (IR, ¹H NMR, ¹³C NMR, and DEPT) and extracts from *Vernonia amygdalina* have been shown to have antimicrobial activity.

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