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50

Years of Annual Sessions
1971 – 2021

Golden Jubilee

The Tri Annual Publication of the Institute of Chemistry Ceylon

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The Tri-Annual Publication of the Institute of Chemistry Ceylon

Founded in 1971, Incorporated by Act of Parliament No. 15 of 1972

Successor to the Chemical Society of Ceylon, founded on 25th January 1941

Vol. 38 No. 2 **June 2021**

Guest Editorial

Student Corner

Theme for the year -

Sustainable Development through Chemical Sciences

Adamantane House, 341/22, Kotte Road, Welikada, Rajagiriya
Office ☎ : 2861231, 2861653, 4015230 📠 : 2870587
E mail : ichemc@sltnet.lk web page : www.ichemc.edu.lk

Outline of our Institute

The Institute of Chemistry Ceylon is a professional body and a learned society founded in 1971 and incorporated by act of Parliament No. 15 of 1972. It is the successor to the Chemical Society of Ceylon which was founded in 1941. Over 50 years of existence in Sri Lanka makes it the oldest scientific body in the country.

The Institute has been established for the general advancement of the science and practice of Chemistry and for the enhancement of the status of the profession of Chemistry in Sri Lanka. The Institute represents all branches of the profession and its membership is accepted by the government of Sri Lanka (by establishment circular 234 of 9-3-77) for purposes of recruitment and promotion of chemists.

Corporate Membership
Full membership is referred to as corporate membership and consists of two grades: **Fellow (F.I.Chem.C.)** and **Member (M.I.Chem.C.)**

Application for non-corporate membership is entertained for four grades: Associate (former Graduate) (A.I.Chem.C.), Licenciate (L.I.Chem.C.), Technician (Tech.I.Chem.C.) and Affiliate Member.

Revision of Membership Regulation
All Special Degree Chemists can now apply directly to obtain Associate (Graduate) Membership. Three year B. Sc. Graduates (with an acceptable standard of Chemistry) can
(i) directly become Licentiate
(ii) obtain corporate membership in a lesser number of years.

Tech.I.Chem.C.
Those who have passed the DLTC examination or LTCC examination or have obtained equivalent qualification and are engaged in the practice of Chemistry (or chemical sciences) acceptable to the Council are entitled to the designation Tech.I.Chem.C.
Members/Fellows with Membership for Life are entitled to the designation of **Chartered Chemist (C.Chem.)** on establishment of a high level of competence and professionalism in the practice of chemistry and showing their commitment to maintain their expertise.

All corporate members (Members / Fellows) are entitled to vote and become Council/ Committee members whether Chartered Chemists or not.

Membership Applications
Any application for admission to the appropriate class of membership or for transfer should be made on the prescribed form available from the Institute Office.

Current Subscription Rates
Fees should be payed on 1st of July every year and will be in respect of the year commencing from 1st July to 30th June

Fellow	Rs. 2000
Member	Rs. 2000
Associate	Rs. 1500
Licenciate	Rs. 1200
Technician	Rs. 750
Affiliate	Rs. 1200
Membership for Life	Rs. 15000

Entrance Fee

All the grades	Rs. 1000
Processing Fees*	Rs. 500
Processing Fee for Chartered Chemist designation	Rs. 5000
Institutional Members	Rs. 2500

*per application for admission/transfer to any grade

Headquarters Building
Adamantane House
341/22, Kotte Road, Welikada, Rajagiriya
Telephone : 2861653, 2861231, 4015230 Fax : 2870587
e-mail : ichemc@sltnet.lk web : www.ichemc.edu.lk

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Editorial and Publicity Committee

CHEMISTRY IN SRI LANKA

Chemistry in Sri Lanka is a tri-annual publication of the Institute of Chemistry Ceylon and is published in January, May and September of each year. It is circulated among the members of the Institute of Chemistry and students of the Graduateship/DLTC course and libraries. The publication has a wide circulation and more than 750 copies are published. Award winning lectures, abstracts of communications to be presented at the annual sessions, review papers, activities of the institute, membership news are some of the items included in the magazine.

The editor invites from the membership the following items for publication in the next issue of the Chemistry in Sri Lanka which is due to be released in September 2021.

- *Personal news of the members*
- *Brief articles of topical interests*
- *Forthcoming conferences, seminars and workshops*
- *Latest text books and monographs of interest to chemists*

All publications will be subjected to approval of the 'Editorial and Publicity Committee' and the Council of the Institute of Chemistry Ceylon.

Further, prospective career opportunities for chemists, could be advertised in Chemistry in Sri Lanka at a nominal payment. The editor welcomes suggestions from the members for improvement of the publication.

Guest Editorial

Celebrating Eighty Glorious Years of Excellence

Mr. Ranjith Dayananda
Former Senior Research Officer,
Industrial Technology Institute

The Institute of Chemistry Ceylon established in 1971 as one of the foremost professional organizations in Sri Lanka, is the successor to the Chemical Society of Ceylon founded in 1941. On the 25th of January 2021, the Institute celebrated its 80th anniversary and on the 27th of June, it will mark 50 glorious years of Annual Sessions.

Professor A Kandiah, the first President of the Chemical Society of Ceylon, who obtained support and corporation of all of his academic colleagues at the Department of Chemistry, University of Ceylon, successfully established this learned society for the benefit of discipline of Chemistry in the year 1941. The main objectives of the Chemical Society were to cultivate and promote the cause of chemical science by all practical means, raise the status and advance the interests of the profession of Chemistry in Ceylon. At this historic moment where we celebrate eighty years of excellence, it is worth mentioning the names of some eminent chemists who steered the Chemical Society of Ceylon, and they are Mr. D. H. Balfour, Dr. R. Child, Mr. D. A. Bruce, Mr. N. R. Chanmugam, Dr. E. L. Fonseka, Dr. A. W. R. Joachim, Dr. A. A. Hoover and Dr. N. G. Baptist. However, in the year 1971, the last president of the Chemical Society, Dr. R. O. B. Wijesekara's initiative led the Council to ably transform the society to Institute of Chemistry Ceylon as a fully-fledged professional body, which was recognized by a Parliament Act No 15 of 1972 on 28th April 1972. Since then during the past 50 years, 43 past Presidents and successive Councils have served with utmost dedication for the profession of chemistry and ably elevated the Institute as one of the most reputed professional organizations of Sri Lanka. This year, we proudly celebrate the 50th Anniversary of the Annual Sessions on the 27th of June, led by the current president Prof. Sagarika Ekanayake and the Council with immense satisfaction and glory. A commemorative stamp and a first day cover will be issued with the able support from the philatelic bureau on the 27th of June as practiced in the 25th Silver jubilee celebrations of the Institute, held in 1996.

When scrutinizing the past 50 years of the Institute, during the first decade *i.e.* 1970-1980, the temporary suspension of Entrance Fees with the introduction of Annual Membership Fee made it possible to attract more professionals and introduce useful professional programs for the enhancement of profession of Chemistry in all levels, chemical laboratories in particular. The Laboratory Technician Certificate course (LTCC) was initiated by Prof Senthishanguganathan, alongwith Dr E R Jansz and Prof R S Ramakrishana, in 1973 to cater middle level technicians, and was upgraded in 1999 to Diploma in Laboratory Technology in Chemistry (DLTC) which paved the foundation for the Graduateship in Chemistry programme. With new progressive steps made on the upliftment of LTCC course in 1999 to a Diploma in Laboratory Technology in Chemistry (DLTC), the coordinator, Mr. E. G. Somapala, a former Govt. Analyst for many decades, uninterruptedly achieved several milestones such as garnering popularity and recognition for the Course by getting accreditation and acceptance from the Medical Council, getting required training from main private hospitals in Sri Lanka and achieving recognition from National Vocational Qualification.

The Graduateship in Chemistry course initiated in 1979 led the foundation for the popularity of the Institute which paved the way not only to cater required professional chemists for Sri Lankan industries, but also in the academia. Majority of them are currently serving in many other countries as well. They have excelled themselves in gaining employment with the postgraduate qualifications they have achieved.

Even though the Establishment Circular No. 233 of 9.3.1977 gave due recognition for the qualifications offered by the Institute, some negative opinions arose from certain university academics stating that any educational qualifications offered by institutions other than state universities were not acceptable. The Institute took up the challenge in 1979, led by Prof. J. N. O. Fernando with the help and support of several others like Dr. E. R. Jansz, Prof. R. S. Ramakrishna and Dr. H. D. Gunawardena, who went forward and commenced the Graduateship Course in May 1979. This needs to be highlighted as the most significant milestone of the Institute in its fifty year history. Efforts led not only to produce 2000 more learned professionals but also the Institute ably generated an unprecedented amount of income which enabled it to have its five storey, two wing building named Adamantane House at a prime location in Sri Lanka in the year 2005. When going back to the period of 1981-2010, this decade seems to be the most fruitful exponentially grown era of the Institute. Currently, the Institute is proud to announce it consists of over 20 permanent academic staff with postgraduate qualifications and also over 40 non-academic staff for the smooth functioning of the Institute.

With the establishment of the College of Chemical Science (CCS) as an educational arm of the Institute of Chemistry Ceylon in 2002 by the then president Prof Tuley De Silva, the Institute became a well-organized academic institute apart from its professional educational activities. Due to the ever increasing demand, the College of Chemical Sciences (CCS) began conducting the GIC course in the newly owned Adamantane House from 2005 onwards, where the Institute named several halls and laboratories as a gratitude to several significant chemists who were well behind the success story of the Institute: Prof. P. P. G. L. Siriwardena Auditorium, Dr. R. O. B. Wijesekara Hall, Prof. J. N. O. Fernando Hall, Prof. H. D. Gunawardena Instrument Center and Prof. E. R. Jansz Laboratory. With the ever-increasing demand to accommodate the record number of students enrolled, classes were held during the whole week changing from its original weekend only, for the both DLTC and GIC courses for the first time from January 2011.

The first female President of the Institute Ms. Clodagh Nethsingha, left her ancestral home and the land of 30 perches in Dehiwala to the Institute by “Deed of Gift” in June 2010. Although we have two leased government lands, one at Welikada of 25 perches where we built Adamantane House, and the other at Malabe of 1 acre and 6 perches, which is the only property which belongs to the Institute, we pay our heartfelt gratitude to the Nethsingha family.

When 2011 was announced and declared by the Government of Sri Lanka as the International Year of Chemistry (IYC), UNESCO and IUPAC recognized the Institute of Chemistry Ceylon for its contribution to the enhancement of Sri Lankan life and society. Several IYC events were successfully organized by the committee chaired by one of its Graduate Chemists, Mr. N. M. S. Hettigedara. Among those were the exhibition CHEMEX 2011 and the issue of a stamp and first day cover with the images of world-renowned chemist, Madame Marie Curie to commemorate the centenary of her Nobel Prize for Chemistry, and of Prof. M. U. S. Sultanbawa, a distinguished Sri Lankan chemist.

In 2012, accreditation for the Graduateship Programme in Chemistry as a partial fulfillment for the award of Chartered Chemist status by the Royal Society of Chemistry (RSC), UK, was received and it further strengthened the professional qualification not only in Sri Lanka but internationally as well. With the increase in number of students and activities, the need for more space was strongly felt and a decision was taken to construct a five storied wing as an extension to the existing Adamantane House and in quick time the building was constructed and opened in 2014.

Prof. J. N. O. Fernando, the main architect of the present-day institute, the first ever Dean of the CCS and the Rector, who was the mastermind behind the Institute activities since its inception in 1971, prematurely departed on the 2nd of March 2015, just one month after his 72nd birthday, creating a huge vacuum in the Institute. Though we had several events organized during the last six years commemorating him and even having established a statue of his bust, which is the first statue built in the Institute history for a person, however we couldn’t yet completely fulfill all his ambitions. However, the Institute has so far ably coped up with planned activities and today we are in some relief that we are in a position to commemorate our Golden Jubilee with proud and profound manner, so that he is looking at us with some satisfaction as an architect of the present IChemC.

At the time the Institute celebrates her Golden Jubilee of Annual Sessions in 2021, it is a remarkable accomplishment that the Institute of Chemistry Ceylon was recognized as a Degree Awarding Institute in the year 2020 with a Government Gazette notification dated 2020.03.11. Even though it was believed from the beginning that though the Institute was well recognized by RSC as a degree awarding Institute, the Graduates produced by CCS may never be recognized in Sri Lanka by the authorities, now we have one more thing to be proud about.

Today, IChem is not only a professional body but also a fully-fledged educational entity no less than any other University in the island. Furthermore, in line with such a status, CCS is armed with a well-organized series of extracurricular activities for the students such as Rotaract, debating, and other sports and social activities organized by the academics for the benefit of students so no doubt that we are competitive with any other such institution in Sri Lanka at our Golden Jubilee year 2021.

With the planned new CCS Complex at Malabe already designed and about to commence its construction activities before end of the July 2021, the Institute will be an owner of another 8 storied new building which will cater the needs of Sri Lankan Chemistry loving students, professionals and whole lot who are benefitting from Chemical sciences.

Our vision for the next 25 years is to concentrate on getting due recognition for the profession of Chemists in the country as compared to other professions. We want to highlight the importance of the role that chemists play for the betterment of human life, and to make the Sri Lankan chemists not only a valuable asset to the country but for the whole world with skills to practice anywhere in the world and be competitive in the global scenario.

As we look back, the dedication shown towards their profession by former chemists, our past Presidents, early chemists need to be taken as an example by the present members, graduates and diplomates so far produced by the Institute in particular, especially at this commemorative celebration of the Golden Jubilee of Annual Sessions. At last we should remember them and also should follow what they have done for the Institute and as a whole for the benefit of the Sri Lankan Chemical science sector, a voluntary dedicated service to the Institute of Chemistry Ceylon during the past 80 years. Our ambition should be to see continuous nurturing in the form of innovation and opportunities for all the stakeholders of CCS; the students, lecturers, the staff and the administrators, who will then be able to work in collaboration to achieve the synergy of excellence and empowerment that are the hallmarks of any great institution.

Mr. Ranjith Dayananda *graduated from the College of Chemical Sciences, Institute of Chemistry Ceylon and obtained his MPhil from the University of Kelaniya. He has served at the Industrial Technology Institute and Silver Mill Group, and as a Past President of the Institute of Chemistry Ceylon.*

Cover Page

The Institute of Chemistry Ceylon, which was established in 1971 as the successor to the Chemical Society of Ceylon founded in 1941, is the oldest professional body in Sri Lanka. In keeping with its vision "to uplift the quality of life for a better world through the advancement of Chemical Sciences", the Institute of Chemistry Ceylon strives to enhance the profession of Chemistry, while catering to the advancement and application of chemical sciences in the country.

The Institute celebrated its 80th anniversary on the 25th of January 2021, and will be marking 50 glorious years of Annual Sessions on the 27th of June 2021. As it embarks on this historic milestone, the Institute of Chemistry Ceylon continues with its mission "to be the center of excellence in Chemical Sciences for the socio-economic development through education, research and innovation", while aspiring to brighten the horizons of the future of the chemical sciences in Sri Lanka.

INSTITUTE OF CHEMISTRY CEYLON
Golden Jubilee Annual Sessions and
80th Anniversary Celebrations 2021

Inauguration of the 50th Annual Sessions, Institute of Chemistry Ceylon

Sunday, June 27th 2021
at Adamantane House, Rajagiriya *via* ZOOM

Programme

8.30 am Registration of Participants

8.45 am National Anthem

8.50 am Welcome Address
Professor Sagarika Ekanayake
President, Institute of Chemistry Ceylon

9.00 am Presidential Address
"Sustainable Development through Chemical Sciences"
Professor Sagarika Ekanayake

9.30 am Issuance of the first day cover and stamp

9.45 am Address by the Chief Guest
Professor Kapila C. K. Perera
Secretary, Ministry of Education
Senior Professor, Department of Mechanical Engineering, Faculty of Engineering, University of Moratuwa

10.15 am Launching of the book, "Our Voyage through the Years"

10.30 am Presentation of Awards, Prizes and Certificates
Institute of Chemistry Ceylon Awards

- Distinguished Service Award : Mr K R Dayananda & Mr M R M Haniffa
- Dr C. L. De Silva Gold Medal : Prof U L B Jayasinghe
- Prof M U S Sultanbawa Award : Prof P B Ratnaweera
- CCS Research Award : Dr S R Gunatilake
- Long Service Award : Mr W R R Perera

Graduateship Examination in Chemistry

- Scholarships, Prizes and Awards
- J N Oleap Fernando Memorial Scholarship

11.30 am Dr C. L. De Silva Gold Medal Lecture
"Search for Bioactive Compounds from Sri Lankan Medicinal Plants and Endophytic Fungi"
Professor U L B Jayasinghe

12.10 pm Vote of Thanks
Professor Srianthie Deraniyagala
President Elect, Institute of Chemistry Ceylon

12.20 pm Close of Ceremony

12.30 pm Annual General Meeting – 2021 (for Corporate Members only)

Presidential Address

Sustainable Development through Chemical Sciences

Senior Professor Sagarika Ekanayake
BSc (Peradeniya), MPhil (Sri Jayewardenepura), PhD (Lund, Sweden), C.Chem., F.I.Chem.C.
President, Institute of Chemistry, Ceylon
Senior Professor of Chemistry, Department of Biochemistry, University of Sri Jayewardenepura

It has been an honour and a privilege to have been the 83rd President of the Institute of Chemistry Ceylon, the oldest of the basic scientific bodies in Sri Lanka during the period when the Institute is celebrating its 80th year in existence and celebrating the golden jubilee of annual sessions. The theme for the Council year 2020/21 was "Sustainable Development through Chemical Sciences".

Chemical Sciences encompasses a large array of sub-divisions of the five specific branches of chemistry and deliveries of which are required in order to produce knowledge, goods and services which are part and parcel of day to day life. Chemistry/Chemical Sciences also contributes significantly to find solutions to problems faced by the world today and to improve the conditions for the future. Consequently, chemical sciences have a remarkable effect on the economy and society, and work for the benefit of humanity and the environment by improving people's lives and ensuring the well-being of the planet thus have an essential role in achieving the Sustainable Development Goals (SDGs) identified by the United Nations in 2015.

Chemical sciences have been identified to play an essential role in seven priority SDGs and five additional SDGs. The main seven include Zero Hunger, Good Health & Well-being, Clean Water & Sanitation, Affordable & Clean Energy, Industries, Innovation & Infrastructure, Responsible Consumption & Production and Climate Action. I will very briefly elaborate the involvement of chemistry and the contribution the chemists have made or could make with few examples in achieving these seven priority goals. In addition to these seven goals, meeting the targets of nearly all of the SDGs will require an unparalleled amount of research and innovation related to chemical sciences.

The role chemists could play in achieving the "Zero Hunger" goal (SDG 2) is multifaceted. Chemistry will contribute in drought protection of food crops (eg: molecules [Opabactin] that help retain water in some plants), targeted crop protection (eg: pesticides which protect plants from pest infestations leading to higher yields) focusing more on using everyday substances (natural products), sustainable ammonia production (nitrification inhibitors to reduce nitrogen loss from denitrification, leaching, and greenhouse gas emission), phosphate recovery and reuse (utilizing filters, nanoparticles, electrochemistry), new approaches to fertilization (slow release using nanotechnology) to improve food production leading to high yields with reduced pollution, fortification of food to reduce malnutrition, increase the shelf life of food products through advanced packaging which will contribute to maintain food quality.

The next goal where chemists play an imperative role is Good Health & Well-Being (SDG 3). Starting with disease diagnosis and drug development leading to longer life expectancy with increased productivity is made possible through chemistry. Advances in chemistry provide an understanding of how human health is affected by disease and hazardous chemicals in our food, water and the environment. This is an area where in Sri Lanka the chemists need to work hand in hand with other researchers in fighting diseases like CKDu where the exact etiology is yet to be found after two decades. Research involving green synthesis routes for synthesis of essential materials, developing targeted drugs reducing environment pollution and using nanotechnology, are areas which have high potential to be developed and are currently being explored. Sri Lanka being a Biodiversity hotspot, research on abundant natural products from the terrestrial and marine flora and fauna to seek suitable products effective in controlling pathogenic and non pathogenic diseases is an area many of our chemists are working on. However, this needs to be taken beyond the laboratory level. Production of molecules/ingredients necessary for good health from abundant flora (eg: phytosterols, lycopene) using green chemistry has a high potential. Food chemistry research enlightens people on food selection for prevention or controlling various disease conditions, food preservation using natural ingredients for increasing shelf life and to reduce post-harvest losses etc. With the increase in non-communicable diseases in the world including our country, this is an area that has much research potential. This being one area that I dabble in research, the graduate chemists have proven foods that would be beneficial in controlling the blood sugar levels (eg: effect of processing and ingredients in controlling blood sugar levels) and achieving good health (eg: the importance of legumes, traditional Sri Lankan rice and parboiling and *kithul* treacle in controlling postprandial blood glucose levels) and in industry collaborative research in proving consumer safety of market products and their suitability for individuals needing to maintain blood glucose levels etc. My chemistry background helped me immensely in doing the research I am involved in which has contributed to some national guidelines and policy developments. The recent incidence in Sri Lanka where aflatoxins were reported in coconut oil is an area where the input of chemists to scientifically prove and to mitigate the effects is required.

Chemists could also contribute to ensuring availability and sustainable management of water and sanitation for all in several ways, the next sustainable development goal. Novel methods of water purification (P & G Purifier of Water [coagulant & disinfectant]) and economical desalination processes (we live in a tropical country, surrounded by sea – solar assisted desalination) are ways to contribute to providing access to safe and affordable drinking water to all. Indirectly, the water quality could be improved by using greener technologies and pollution prevention strategies which will also contribute to good health and well-being. Again related to the SDG 3 it is also necessary to develop new low-energy, high-efficiency separation methods for removal of various metals and micro-pollutants such as micro-plastics which is becoming a global problem. Minimizing water pollution due to the chemical industry by assisting in developing manufacturing practices that minimize water usage and practices for waste management will contribute to good health as well as reduce pollution (collaboration with Environmental Authority/industry). Research on novel methods for removal of heavy metals and other particulate matter are areas chemists have a major role. This is an area where more action and research are needed in our country as drinking water is taken from rivers where waste from many industries are released into the rivers without proper treatment. Collaborative research with industry and academia is the most suitable way to mitigate such effects. In this event not only chemists but contributions from other counterparts are required to achieve successful end results.

Chemical sciences could also contribute in helping to meet the Affordable and Clean Energy goal through the development of new materials for renewable energy, by being more energy efficient in the chemical processing industries, and by advancing cleaner fuel technologies. The development/use of abundant advanced materials available for renewable energy production, including photovoltaics, wind turbines, thermal energy, batteries and energy storage solutions are some areas the chemists could contribute by working with other disciplines. The chemical processing industries could contribute by improving the manufacturing efficiency through new catalysts, optimized process designs and new separation processes (drug, fertilizer, pesticide manufacturing). Renewable energy production is another area that chemists could contribute by finding alternatives for scarce or hazardous material used in solar and wind conversion from abundant, less toxic materials which again will reduce pollution and lead to less environment related health problems. Sri Lanka being a tropical country, research on materials abundant and less-toxic that could be utilized for generating solar power, will lessen our dependence on the monsoons for hydro-power. Sri Lanka is rich in mineral resources which could be utilized for development of novel strategies for clean energy generation.

The ninth Sustainable Development Goal (Industries, Innovation & Infrastructure) is also an area where chemists could contribute in many ways. To mention a few; upgrading infrastructure of chemical processing industries, design, synthesize and manufacture innovative advanced materials, coatings that make infrastructures more sustainable and durable and encouraging chemistry research that enhances innovation for commercial applications. Examples of this nature are few in our country even though this has been mentioned by the chemists in the 1980's where the collaborations of industry and universities to enhance sustainable development. However, the green building concept that is being applied in constructing new buildings is one step forward in our country which indirectly contributes to other SDGs. The new building of the Institute that is being built in Malabe has been designed adhering to the guidelines where many green aspects have been taken into consideration. Chemists using green chemistry practices could develop assessment methods that are efficient, generate minimal waste, and employ chemicals that are safe for humans and the environment. Bio-based chemicals derived from plants and other renewable agricultural, marine and forestry materials (waste) provide an alternative to conventional petroleum derived products. These could include a broad range of products such as lubricants, detergents, adhesives, inks, pesticides, fertilizers and bioplastics. In addition, the research into biofuels is an area of research where the focus can be with the abundance of natural products in our country substituting petroleum-derived counterparts. To cite two examples where the chemists working with other scientists have contributed to green synthesis - computer chips from chicken feathers (keratin), food containers from polylactic acid derived from corn starch by the action of microorganisms. In this context we have so much agricultural waste which could be used for such purposes where inputs from chemists are needed.

Responsible Consumption and Production, the 12th SDG is another key goal where chemists could contribute in abundance. According to UN the Sustainable consumption and production is about doing more and better with less by decoupling economic growth from environmental degradation, increasing resource efficiency and promoting sustainable lifestyles. This is mainly based on the use of the natural environment and resources by us, the humans. However, the uses of these resources have negative impacts on the planet endangering the systems on which our survival and the future depend. We ourselves are mainly responsible for this goal as each year, for example - an estimated one third of all food produce ends up as waste thrown away by consumers and retailers, or spoiled due to transportation difficulties and poor post-harvest practices. Improvement of post-harvest techniques by developing energy efficient techniques/methodologies (food packaging, natural additives to prevent food waste), innovative & efficient waste management, waste recycling by developing method to recover their original raw materials or use waste to generate valuable products and increase bio-based products (eg: tree trimmings to generate cellulose etc. by auto-hydrolysis, forest based-fabrics) are some ways in which the chemists have contributed to reduce the life cycle impacts of consumption.

In adding to achieving the Climate Action SDG, in addition to many other disciplines, Chemistry will play a critical role. Chemical research is crucial for lessening and adapting to climate change. A primary cause being the increasing concentrations of greenhouse gases and particulate matter in the atmosphere as the result of human activities. It is recorded that past decade was the warmest decade, with 2019 the second warmest year with carbon dioxide and other greenhouse gases reaching highest levels in 2019. In 2020, due to the COVID-19 pandemic, with a decline in human activities mostly due to reduction in ground travel, a 6.3% reduction in carbon emissions is recorded. It is imperative that we remember that the climate changes will affect the natural resources in turn affecting food and water availability and cause spread of vector borne diseases and epidemics. The chemists working with other scientists will need to find answers in increasing food production with limited water resources and methods to control vectors using more eco-friendly, naturally abundant materials and searching/developing novel drugs for controlling epidemics and in addressing other health problems that will be due to global warming. In limiting carbon emissions from fossil fuels, which is fast becoming a problem in our country as in other countries, research in to bio-fuels from waste or biomass or other energy efficient methods for industry, development of products that will enable other sectors to reduce their carbon footprints, using biodegradable resources in day to day requirements are research areas that we chemists could work on. The application of green and sustainable chemistry helps eliminate or reduce hazardous chemical pollution. In this the "Reagent Guide" which allows chemists to choose a 'greener' choice of reaction conditions, "Solvent Selection Guide" developed to rate solvents based on health, safety, and environmental criteria and many other such tools contribute to green chemistry and needs to be taken advantage of. The recent experience we had with the X-Press Pearl disaster affecting the environment, the livelihood of many, economy and a food source of Sri Lankans, need careful research studies on the numerous effects on the environment and to mitigate the effects. In this context, the Institute has taken steps in collaborating with NARA for studying the impacts and in addressing some problems.

The Institute of Chemistry Ceylon has been involved in producing Graduate Chemists for over 40 years and is the oldest non-state higher education institute in the country. The Institute plays a leading role in producing young Chemists who are equipped and are able to contribute to sustainable development in many different ways. In addition, the Institute takes a leading role in informing chemists and the society of current trends, developments, advancements in chemical sciences through many activities such as seminars, workshops etc., and contributes to deal with problems related to chemical sciences emerging in the country contributing to quality education (SDG 4) and gender equality (SDG 5).

Development of a younger generation with the knowledge, an aptitude for research, development and innovation is very much encouraged at the Institute of Chemistry. This is clearly shown by the number of graduands who have taken up higher studies after obtaining their Graduateship qualification. In numbers, from inception over 350 students have completed or are engaged in postgraduate research all over the world and many are contributing to development and innovations in many areas of chemistry. This is over 1/5th of all students who have completed studies at the Institute. If we consider the data of the last 40 years, it is evident the role the Institute has played in contributing chemists to the world, which in number, is over 1700.

In addition to these seven goals, meeting the targets of nearly all of the SDGs will require an unparalleled amount of research and innovation related to chemical sciences. However, it is clear that chemists alone are not able to achieve sustainable development. Thus, multidisciplinary research with different experts, subject specialists contributing as a team is essential and needs to be promoted in Sri Lanka.

During my presidency the activities initiated and accomplished were geared to further promote the educational programmes of the institute (BSc, GIC, DLT), strengthen collaboration between industry and the Institute and continue with the development projects that were already in progress. Due to the COVID-19, the educational activities were promoted mainly through social media and by updating the web page to an informative website and giving publicity to Institutes' own graduates who have achieved peaks in their career, and are contributing to sustainable development in many ways. Partly I believe these resulted in an unprecedented number of students registering for the courses this year. In addition, the curricula of the educational programmes were scrutinized and updated. An e-repository was established for storage and easy retrieval of Institute publications to disseminate knowledge and to increase the ranking of the Institute, which is now recognized by Google Scholar. This year we registered under the IFSL scheme of the MOE facilitating less advantaged students to follow the BSc in Chemical Sciences degree at our Institute contributing to CSR. We began to enroll foreign students for our educational programmes in 2021 and were in time to align with the Government policy of increasing foreign student intake to the universities which have been initiated by the Export Development Board. In obtaining professional recognition for Chartered Chemists, the legal actions are proceeding with Graduate Chemists working towards achieving this. However, recognition for Chartered Chemists was achieved through interactions with the Consumer Affairs Ministry where the Institute was recognized as the focal point of Chemists to obtain assistance in matters related to consumer products and with other institutes. Despite many lockdowns due to COVID-19 pandemic and the Institute closures, we were able to foster and strengthen partnering with industry to increase chances of research collaborations, innovations and employment opportunities for our graduates and also to generate funds and to increase membership by many seminars

(06) that we have conducted using online platforms. With the Council approval, many policy decisions, which will have a positive impact on the Institute's future and activities, were implemented. Building project at Malabe Campus, which was stagnated following laying of the Foundation stone due to COVID pandemic, was revived soon after the country opened and the UDA clearance for building construction was obtained in January 2021. The bids were called and submitted in June 2021 and the evaluation to select the contractor for the construction of the building is ongoing. Even though we are unable to celebrate the Golden Jubilee Annual Sessions as intended, a theme seminar where eminent scientists from five different countries will deliver talks on various aspects related to sustainable development through chemical sciences. A new technical session for graduate chemists, who are pursuing higher studies to elaborate on their contributions to sustainable development was introduced for the 50th Annual Sessions. In celebrating the 50th Annual Sessions, a first day cover and a stamp is designed to be launched. In addition, as a dedication to all who have contributed to the success of the Institute, the book "Our Journey through the Years" capturing the journey of 80 years of the Institute will be launched.

"*Alone we can do so little; together we can do so much*"
– Helen Keller

Finally, the not so easy journey of the past 10 months through a global pandemic was made easy due to the contribution of many individuals. First and foremost, my family for the unending moral support extended during this period. I take this opportunity to offer my heartfelt gratitude to my two secretaries Dr. U. Jayasundera, Dr. N. A. D. Wageesha, treasurer Dr. A. A. P. Keerthi, assistant treasurer Dr. T. Gunasekera, editor Dr. S. R. Gunathilaka and his team, secretary education, Dr. G. Thiripuranathar and assistant secretary Ms. S. Narasinghe without whose support it would not have been possible to reach the goals I set and more. I am extremely grateful to the Chairpersons of the Board of Trustees, Admission & Ethical Practices Committee and College of Past Presidents for the support extended in many ways. In addition, I thank the Council 2020/21 for helping to make many policy decisions for the betterment of the Institute, though sometimes convincing, some were not easy. I fail in my duty if I don't thank my writing team, Ms. P. Jayasinha, Dr. D. Udukala, Prof. R. Wijesekera and Ms. J. Liyanage for making "Our Voyage through the Years" a reality, and Mr. S. Jayasinghe for always responding to requests of photographs. Internal auditor, Mrs. C. Fonseka for working long hours to correct all the matters related to finances with the accounts team cannot be left out. I am very thankful to all the staff of Institute of Chemistry Ceylon, Dean, visiting professors and internal academics, registrar, administrative, laboratory, non-academic, security and cleaning staff, all of whom helped me immensely to achieve what I aspired to achieve during this period.

"*The future depends on what you do today*"
– Mahathma Ghandi

***Professor Sagarika Ekanayake** obtained her BSc in Chemistry from the University of Peradeniya and MPhil in Biochemistry from the University of Sri Jayewardenepura, Sri Lanka. She completed her PhD in Applied Nutrition & Food Chemistry at the University of Lund, Sweden. She currently serves as a Senior Professor at the Department of Biochemistry, Faculty of Medical Sciences, University of Sri Jayewardenepura and as a visiting professor at the College of Chemical Sciences.*

Chief Guest at the 50th Annual Sessions

Professor Kapila C. K. Perera

Chief Guest's Address

Professor Kapila C. K. Perera

Secretary, Ministry of Education

Senior Professor, Department of Mechanical Engineering, Faculty of Engineering, University of Moratuwa

A well grounded education provides meaning to a person's life and his mission, and one's mission that is devoted towards the betterment of one's nation and society, is a cause for kindled hope of a better tomorrow. We, at the Ministry of Education, consider it our mission to nurture a society of competent citizens capable of keeping with the global trends, through innovative and modern approaches to transformative education, which would in turn contribute to the sustainable, socio-economic development of Sri Lanka. I believe that the Institute of Chemistry Ceylon, which is celebrating its golden jubilee this year, is one of the 'catalysts' that keep driving this nation into the horizons of a better tomorrow.

Since its inception in 1941 as the Chemical Society of Ceylon, and following its succession and establishment in 1971, the Institute of Chemistry Ceylon has served as the professional body of chemists in Sri Lanka, dedicated to the advancement and application of chemical sciences in the country. Following its mission "to be the center of excellence in chemical sciences for the socio-economic development through education, research and innovation", the Institute continues to fulfill its legacy by addressing timely chemistry related-issues, popularizing the chemical sciences amongst the general public and uplifting chemical education in the country. I feel blessed to be gracing this occasion at the moment when this esteemed institution celebrates eighty years of excellence, as it continues in its mission of revolutionizing the chemical sciences in Sri Lanka.

We, at the Ministry of Education, strive to impart innovative and modern approaches to the national education system so as to enable the creation of life-long learners possessing the ability to thrive in a global environment. I firmly believe that the Institute of Chemistry Ceylon shares the vision we follow at the Ministry of Education: "to reach excellence in global society through competent citizens who share the Sri Lankan identity", as evident by the groundbreaking strides undertaken to contribute towards a society with good values by offering intellectual growth through education in chemical sciences. In keeping with this vision, the College of Chemical Sciences, the educational arm of the Institute of Chemistry Ceylon, has committed itself to imparting quality education in Chemistry, equipping its aspiring chemists not only with a high level of chemistry knowledge, but also with the necessary moral and cultural values and ethics, which has helped them fluorish as better professionals primed to contribute to the national wellbeing. What with the limited capacities of state universities, the College of Chemical Sciences renders an immeasurable service in catering to those who are deprived of a university education, to pursue their careers in Science. Furthermore, the Institute should be applauded for its dedication in promoting the popularization of Chemistry at a national level and encouraging students to understand its importance in today's world. The International Chemistry Olympiad 2020 saw the emergence of three bronze medallists and one honorable mention from Sri Lanka which was a remarkable feat as this was the first time in history that Sri Lanka participated at the IChO, which exemplifies the hidden potential of the local talent. The role played by the Chemistry Olympiad Sri Lanka (COSL) committee of the Institute of Chemistry Ceylon (IChemC) in selecting and training the Sri Lankan team should be duly commended.

In the recent past, the country has had to tackle certain issues such as waste management, aflatoxins in edible oil and the X-Press Pearl fire, which were promptly addressed by the Institute whose scientific body has been committed to sharing its expertise to provide sustainable solutions. Sri Lanka is blessed with a treasure trove of resources which are under-utilized and extremely crucial in transforming the national economy towards sustainability and improving the quality of life. Employing these resources and subsequent value addition requires the collateral development of chemical technology in the country. Over the years, the Institute of Chemistry Ceylon has devoted itself to conducting relevant and high-impact research to expand the boundaries of scientific knowledge and technological capacity of the country, and lending a voice to the innovators in the field. I hope that the Institute will continue in this task and focus on exploiting the treasure trove that the country has been opportunely bestowed with, by employing the vast knowledge base and skilled workforce that is being produced by your esteemed institution each year. I commend the initiatives taken by the Institute of Chemistry Ceylon in striving to bridge the gap between academia and industry, and shaping the careers of so many aspiring chemists, garnering them a kaleidoscope of opportunities to excel in the global environment.

I congratulate all the award winners on your outstanding achievements and wish you all the best in ascending to even greater heights in the future. I salute the Council of the Institute of Chemistry Ceylon for the year 2020/21 headed by Prof. Sagarika Ekanayake, for undertaking the mission to align this year’s objectives with a theme of such vital importance to our country as a whole; “Sustainable Development Through Chemical Sciences”. Moreover I applaud your undying commitment towards accomplishing your mission at a time the whole world is in the clutches of a global pandemic, which makes me reaffirm that the Institute of Chemistry Ceylon will undoubtedly continue to be a ‘catalyst’ propelling all of us into the horizons of a better tomorrow.

***Prof. Kapila Perera** obtained his BSc in Engineering from the University of Moratuwa, Sri Lanka, and was awarded his Masters and PhD in Mechanical Engineering from the University of California, USA. He has served as a Senior Professor, a Head of the Department of Mechanical Engineering and a Dean of the Faculty of Engineering. He currently serves as the Secretary to the Ministry of Education, Sri Lanka. He is also a former Vice Chancellor of the University of Moratuwa.*

Distinguished Service Awards – 2021

Mr. Ranjith Dayananda obtained his primary education at Huganthota Primary School, Bentota and Mahinda College, Galle, and secondary education at Ananda College Colombo. He obtained his LTCC qualification in 1979 and joined the first batch of GIC students and graduated as a professional graduate chemist from the College of Chemical Sciences, Institute of Chemistry Ceylon in 1984. Subsequently, he obtained his postgraduate Diploma at Uppsala University, Sweden and MPhil from University of Kelaniya in Analytical Chemistry.

He served in Grenada in 2004, as an expert technical advisor for spices & essential oils for FAO, and has undergone special training in essential oil, fragrances and perfumery, in France, Poland and India. He served as a Senior Research Officer at the Industrial Technology Institute (formerly known as Ceylon Institute of Scientific and Industrial Research) till his retirement in 2011 after 35 years of service, and has also served as Senior R&D Manager in Silver Mill Group. Throughout his career, Mr. Dayananda has been involved in the research and development surrounding spices, essential oils, distillation technologies and herbal product development, quality assurance of food and consultancy on control of aflatoxin contamination.

Mr. Dayananda's contribution to the development of the Institute of Chemistry Ceylon is immense. He has served as a member of the Council for over 35 years, having held many honorary positions. He was the first Graduate Chemist to be inducted as the President of the Institute of Chemistry Ceylon (2015/16) and currently serves as the Chairman of the Board of Trustees of the Institute. He is the immediate past Chairman of the College of Past Presidents and is the founder President of the Alumni Association of the College of Chemical Sciences. Mr. Dayananda has contributed immensely to the upliftment of the programmes and activities conducted by the College of Chemical Sciences, having served as a lecturer and examiner of the Graduateship programme, and was awarded the Yeoman Service Award of the Institute of Chemistry Ceylon in 2011.

In recognition of his outstanding contribution towards the betterment of the Institute, the Council of the Institute of Chemistry Ceylon has unanimously decided to award Mr. K. R. Dayananda the Distinguished Service Award at the 50th Annual Sessions of the Institute of Chemistry Ceylon in 2021.

Distinguished Service Awards – 2021

Mr. M. R. M. Haniffa completed his primary education at Beminiwatte Vidyalaya and his secondary education at Trinity College Kandy. Having represented Trinity College Kandy (TCK) and Sri Lanka Schools Hockey, he was awarded the TCK Hockey Lion in 1974. He went on to captain the Hockey Team of the University of Colombo, and also represented the University in cricket and basketball as an undergraduate. Mr. Haniffa graduated from the University of Colombo in 1979, obtaining a BSc Special Degree in Chemistry with Second Class (Upper Division) Honors. He completed his Masters degree in Chemistry at the University of Hawaii at Manoa (USA) in 1997, and joined the Open University of Sri Lanka as a Senior Lecturer in Chemistry. He has served as the Head of the Department of Chemistry, Faculty of Natural Sciences and as the Head of the Department of Basic Sciences, Faculty of Health Sciences at OUSL.

Mr. Haniffa has a long association with the Institute of Chemistry Ceylon and the College of Chemical Sciences, having been closely involved with its activities since 1998. Since 1999, Mr. Haniffa has been a visiting lecturer at the College of Chemical Sciences, Institute of Chemistry Ceylon. He has served the Institute in an exemplary manner, contributing to its betterment through the many key positions he has held including President of IChemC (2016/2017), Dean, College of Chemical Sciences (2015), and a recurring honorary member of the Council and the Academic Board of IChemC. Consequently, he was awarded the "Yeoman Service Award" in 2009 in recognition of his outstanding contribution towards the betterment of the Institute.

Through the years, Mr. Haniffa has played a significant and valuable role in the development of the Institute of Chemistry Ceylon. In recognition of the valuable and dedicated service rendered by him on behalf of the Institute, the Council of the Institute of Chemistry Ceylon has unanimously decided to award Mr. M. R. M. Haniffa the Distinguished Service Award at the 50th Annual Sessions of the Institute of Chemistry Ceylon in 2021.

Dr. C L de Silva Gold Medal Award

Awarded for an outstanding research contribution in any branch of Chemical Sciences and/ or the use of such research for National Development during the last five (5) years in Sri Lanka. Credit will be given for the utilization of local raw materials, and where the contribution has already resulted in (i) a publication in a Citation Indexed Journal or (ii) registering a Patent or (iii) where the contribution has already resulted in a positive impact in the development and innovation in the industry.

Dr. C. L. De Silva Gold Medal Award - 2021

Prof. Lalith Jayasinghe obtained his BSc. (Hons) in Chemistry in 1985 and PhD in Natural Products Chemistry in 1992, from the University of Peradeniya, and was awarded a Diploma in Natural Products Chemistry by the Tokyo Institute of Technology, Japan in 1994. He has served as a Visiting Scientist at the Tokyo Institute of Technology, Japan, University of Mississippi, USA, and University of Milan, Italy, and as a Visiting Professor at the Tokyo Institute of Technology and Meiji University, Japan. He was an Alexander von Humboldt Research Fellow at the University of Hohenheim, Stuttgart and Jacobs University Bremen, Germany, and has held the IPICS Fellowship at University of Karachi, Pakistan and UNESCO-Monbusho Research Fellowship.

Prof. Jayasinghe has 94 scientific publications to his name, alongwith 3 book chapters and 280 communications, and has an h-index of 23 with 1887 citations. His research interests include investigation of extracts from plant sources and, epiphytic and endophytic fungi, for use in agriculture and human health, chemistry and bioactivity of edible fruits, plant secondary metabolites and LC-MS profiling of bioactive extracts. He is the recipient of numerous awards including the Kandiah Memorial Award of the Institute of Chemistry Ceylon in 1992, TWAS-NARASA Young Scientist Award in 1992, SUSRED Award of NSF in 2017 and eight Presidential Awards for scientific publications.

He is currently serving as a Senior Research Professor at NIFS, Kandy, Sri Lanka.

Abstract of Dr. C L de Silva Gold Medal Award - 2021

Search for Bioactive Compounds from Sri Lankan Medicinal Plant and Endophytic Fungi

Lalith Jayasinghe

National Institute of Fundamental Studies, Kandy

Natural Products are compounds produced by living organisms found in nature. These can be used to improve the quality of human life. Over 3500 flowering plants, including ~800 endemics, are inhabiting Sri Lanka, of these only a relatively low number of plants have been chemically and biologically investigated. The country's native fungal flora is around 25,000 and a vast majority remains to be studied for bioactive metabolites. Our recent findings of natural products with biological active from medicinal plants and endophytic fungi are presented here.

Inhibition of pancreatic lipase is an attractive approach for treatment of diet-induced obesity. Activity-guided isolation of pancreatic lipase inhibitors from the methanol extract of *Trigonella foenum-graecum* seeds furnished vicenin-1 (**1**), isoschaftoside (**2**), schaftoside (**3**) and trigonelline (**4**). These compounds, at 250 µg/

ml, inhibited lipase activity at 60.3% (**1**), 33.8% (**2**) and 95.5% (**3**). This is the first report of lipase inhibitory active metabolites from *T. foenum-graecum*.

Biscogniauxia capnodes, an endophytic fungus isolated from the fruit of *Averrhoa carambola*, produced *in vitro* two isocoumarins, reticulol (**5**) and 6-O-methyl-reticulol (**6**), and two dihydroisocoumarins, 5-methylmellein (**7**) and 7-hydroxy-5-methylmellein (**8**). The compound 5 showed antioxidant activity. This is the first report of isolation of *B. capnodes* as an endophyte, as well as the compounds 5 - 8 from *B. capnodes*.

Metabolites of *Colletotrichum siamense*, isolated from *Piper nigrum*, furnished antifungal indole-3-acetic acid (IAA) (**9**) and uracil (**10**), while those of *Phialemonium curvatum* from the leaves of *Passiflora edulis* yielded 3-indole acetic acid (**9**), uracil (**10**), 4-hydroxybenzoic acid (**11**), solaniol (**12**), uridine (**13**) and glycerol (**14**). The absolute stereochemistry of solaniol (**12**) and the complete ^{13}CNMR were assigned. *Neofusicoccum parvum* was isolated as an endophyte from fruits of *Elaeocarpus serratus*. Chromatographic separation of the ethyl acetate extracts furnished (*R*)-7-hydroxymellein (**15**), (*3R,4R*)-4-hydroxymellein (**16**), (*3R,4S*)-4-hydroxymellein (**17**), (*R*)-5-hydroxymellein (**18**), (*R*)-mellein (**19**), (*3R,4R*)-4,7-dihydroxymellein (**20**), (*6R,7S*)-dia-asperlin (**21**), CJ-14445 (**22**) and 13,14,15,16-tetranorlabd-7-ene-19,6β:12,17-diolide (**23**). This is the first report of the isolation of an endophytic fungus from *E. serratus*, and the compounds **15**, **18**, **20**, **22** and **23** from *N. parvum*. It is important to note that **15** - **21** are smaller molecules with an oxygen heterocyclic ring system which is significant in organic synthesis.

Fermented culture filtrates of *Talaromyces purpurogenus* from *Pouteria campechiana*, upon chromatography, furnished a new furanone analogue of talaroconvolutin A, named talarofuranone (**24**), along with talaroconvolutin A (**25**), 4-hydroxyacetophenone (**26**), tyrosol (**27**) and ergosterol (**28**). Compound **25** responded positively to brine shrimp lethality assay and shoot and root growth assay for lettuce seeds. *Pestalotiopsis microspora* was isolated from *Manilkara zapota* and the EtOAc extract of its culture filtrate and the mycelium led to the isolation of a new azaphilonoid named pitholide E (**29**), in addition to previously identified pitholide B (**30**), pitholide D (**31**), pestalotin (LL-P880α) (**32**), PC-2 (**33**), LL-P880β (**34**), tyrosol (**27**) and 4-oxo-*4H*-pyran-3-acetic acid (**36**). Isolation of compounds, **29**-**33**, **35** and **36**, from *P. microspora* was reported for the first time. These results explain the potential of higher plants and endophytic fungi as excellent sources of bioactive compounds.

Keywords: Medicinal plants, Endophytic fungi, Bioactivity, Lipase inhibitor

Professor M. U. S. Sultanbawa Award for Research in Chemistry

Awarded for the best research paper presented at the Annual Sessions of the Institute of Chemistry Ceylon, for the unique, distinguished and significant contribution made to the cause of Science, Chemistry, Education and Research in Sri Lanka.

Professor M. U. S. Sultanbawa Award for Research in Chemistry - 2021

Prof. Pamoda B. Ratnaweera obtained her BSc Special Degree in Zoology with first-class honours having topped the batch at the University of Colombo in 2007, and obtained her PhD in Natural Products Chemistry also from the University of Colombo, in 2015. Prof. Ratnaweera has served as a faculty member for over twelve years at the Faculty of Applied Sciences, Uva Wellassa University, Sri Lanka. She also served as a Visiting Scientist at the Department of Chemistry, University of British Columbia, Canada, in 2012, 2014 and 2016. Prof. Ratnaweera possesses over 17 research publications in peer-reviewed indexed journals and two patents to her credit. Her research was funded by the National Science Foundation Sri Lanka and through a University research grant. She has also won the Royal Society Commonwealth Grant, UK in 2016 to work on a collaborative research project in a biosynthetic enzyme laboratory at the University of British Columbia, Canada. Prof. Ratnaweeera was the recipient of the prestigious General Research Committee Postgraduate Research Award of the Sri Lanka Association for the Advancement of Science (SLAAS) in 2016, Vice Chancellor’s Award of the Uva Wellassa University for the most outstanding young researcher of the year 2017, and Chandrasena Memorial Award of the Institute of Chemistry, Ceylon in 2019. She received Presidential Awards for her high-quality natural product research publications presented in some prestigious journals. She currently serves as a Professor in Natural Products Chemistry attached to the Department of Science and Technology at the Uva Wellassa University of Sri Lanka.

Prof. Ratnaweera will be awarded the Professor M. U. S. Sultanbawa Award for Research in Chemistry for the presentation of her research on “Antibacterial activities of peptaibols, trichocellin A-I and B-II, isolated from the endophytic fungus Trichoderma reesei” in 2020.

CCS Research Award

Awarded annually to a full time internal academic of the College of Chemical Sciences, Institute of Chemistry Ceylon, for the most outstanding contributions to scientific research in the course of a particular year. The criteria for the evaluation of the awardee includes peer-reviewed scientific publications, including research articles, review articles, and book chapters, conference presentations and Web of Science citations garnered throughout the course of the year.

CCS Research Award - 2021

Dr. Sameera Ranmal Gunatilake obtained the Graduateship in Chemistry qualification with a first class honors from the College of Chemical Sciences, Institute of Chemistry Ceylon in 2007 and obtained his PhD in Analytical Chemistry from the Mississippi State University, USA. His research interests include developing novel analytical methods to determine trace level organic and inorganic analytes from various environmental matrices, producing engineered, biomass derived, carbonaceous materials for water remediation and agricultural applications, and developing chemical education concepts and incorporating theories of education philosophy into classroom teaching, learning and evaluation. Currently, Dr. Gunatilake has seventeen publications to his name, with over 450 Web of Science citations and an h-index of 11. His publications include four review articles, four book chapters, and eleven original research articles. Dr. Gunatilake was the humble recipient of the Presidential Award for Scientific Publications, Sri Lanka in 2017, and the Ramakrishna Memorial award of the Institute of Chemistry Ceylon in 2020. Dr. Gunatilake currently serves as a Senior Lecturer at the College of Chemical Sciences, and is also the Honorary Editor of the Institute of Chemistry Ceylon.

Long Service Award - 2021

Mr. W. R. R. Perera joined the Institute of Chemistry Ceylon in 2006, and was promoted to the post of laboratory attendant in 2009. Since 2017, he has been serving as a laboratory assistant at the Institute, in which he continues his duties with diligence and discipline. Based on its unanimous decision to recognize him for his fifteen years of exemplary service, the Institute of Chemistry Ceylon will be felicitating Mr. Perera with a Long Service Award at the 50th Annual Sessions in 2021.

Theme Seminar on

Sustainable development through Chemical Sciences

Date : 28.06.2021 **Venue : Adamantane House**

Programme

8.45 a.m.	Registration and Refreshments
9.15 a.m.	Welcome Address **Prof. Sagarika Ekanayake** *President, Institute of Chemistry Ceylon*
9.30 a.m.	Keynote Address Humankind faces a bright future, and so chemistry **Prof. Ehud Keinan** *President, the Israel Chemical Society*
10.40 a.m.	The Role of Geochemistry and Mineral Chemistry in Sustainable Development **Dr. Bernard Prame** *Deputy Director at Geological Survey of Sri Lanka*
11.20 a.m.	Biochar-based water treatment - a Sustainable Technology for Clean Water in Developing Countries **Prof. Dinesh Mohan** *School of Environmental Sciences,Jawaharlal Nehru University, New Delhi*
12. 00 p.m.	Sustainable development through application of scientific research output **Prof. Gamini Rajapaksha** *Senior Professor, University of Peradeniya*
12.40 p. m	Lunch
1.40 p.m.	Natural Products - A Sustainable Source of Therapeutic and Nutraceuticals **Prof. Iqbal Choudhary** *Director ICCBS, and Coordinator General COMSTECH*
2.20 p.m.	Closing the nutrient loop: Phosphorus management in protein farming **Prof. Nanthi Bolan** *University of Newcastle, Australia*
3.00 p.m.	Panel discussion
3.55 p.m.	Vote of Thanks

Theme Seminar - "Sustainable development through Chemical Sciences"

Theme Seminar

Humankind Faces a Bright Future, and so Chemistry

Ehud Keinan

The Schulich Faculty of Chemistry, Technion - Israel Institute of Technology

As a result of the population growth, mankind faces severe global challenges, including limited availability of energy, raw materials, food, fresh water, air quality, and health problems, which seem daunting because they cannot be solved on the basis of our current technologies. Since the times of Thomas Malthus (1800) till these days, ignorant prophets and cynical politicians have always come up with apocalyptic predictions for the future of humanity. In contrast, I predict that the humankind will survive on this planet for many years to come, that the above-listed challenges will be met by yet unknown technologies, and chemistry will play a central role in any solution. The future of humankind seems brighter than ever for 5 main reasons:

1. The explosion of human knowledge outgrows the explosion of population.
2. Science is totally unpredictable.
3. Social networking grows exponentially.
4. Personal liberty propagates worldwide.
5. Human dignity propagates worldwide.

Our real problems are not those listed above, but rather the increasing gaps between the advanced societies and those who are left behind in the darkness of scientific and technological ignorance, in misconception and poverty. It is our responsibility as scientists to help closing these gaps.

An obvious trend in the world economy is a dramatic shift of wealth from the traditional West to East Asia. These trends reflect fundamental differences between Western and Eastern Heritage and culture, including social values, business culture, religious heritage and basic philosophy of life.

Since we live in artificial environments on products of human imagination and creativity, and since the human imagination and creativity have no limits, the effective area of planet Earth keeps expanding and our future seems brighter than ever.

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Prof. Keinan *obtained his PhD in Chemistry from the Weizmann Institute of Science, Israel and conducted his postdoctoral research at the University of Wisconsin, USA. He was Dean of the Schulich Faculty of Chemistry, Technion - Israel Institute of Technology, Adjunct Professor at the Scripps Research Institute in California, founder and first Head of the Institute of Catalysis Science and Technology, Technion, Pro-Vice-Chancellor and Dean of Sciences, GTIIT, Guangdong, China, and a Distinguished Visiting Chair at the Academia Sinica, Taiwan. His research interests include biocatalysis with antibodies and synthetic enzymes, organic synthesis, molecular-computing, supra-molecular chemistry, improvised explosives, and drug discovery. He has published nearly 200 research papers, 22 patents, and four books and is the recipient of numerous awards having been recognized for academic excellence and scientific innovation. Prof. Keinan has served as Editor-in-Chief of the Israel Journal of Chemistry (Wiley-VCH) since 2009, President of the Israel Chemical Society since 2009, Member of the Executive Committee and Director of Communications at the Federation of Asian Chemical Societies (FACS), Editor-in-Chief of the AsiaChem magazine, founder and first Editor of the ICE magazine, member of the IUPAC Bureau (2016-2023), and member of IUPAC Evaluation Committee. He currently holds the Benno Gitter & Ilana Ben-Ami Professor of Chemistry at the Schulich Faculty of Chemistry, Technion - Israel Institute of Technology.*

The Role of Geochemistry and Mineral Chemistry in Sustainable Development

Bernard Prame

Geological Survey and Mines Bureau

The chemical sciences have a broad reach into the fields of technology, economy, and human health, and there are already diverse ways chemists are contributing to support global sustainable development. American Chemical Society (ACS) has identified United Nations' seven priority Sustainable Development Goals (SDG) that are foundational to the work of the chemistry community. These are: (1) Zero Hunger, (2) Good Health & well Being, (3) Clean Water & Sanitation, (4) Affordable & Clean Energy, (5) Industries, Innovations & Infrastructure, (6) Responsible consumption & Production and (7) Climate Action. Geochemistry or Mineral chemistry has an important role to play in achieving each of the above goals.

The prosperity of our societies and standards of living are directly related to the ability to find, exploit, and manage metal and mineral resources. Metal and mineral deposits are, in fact, geochemical anomalies and, as such, applied geochemistry plays a critical role throughout the mineral resources value chain, from early-stage exploration to mine closure including rehabilitation. The fundamentals of element mobility (i.e., transport and fixation) in the near-surface environment are used by geochemists to detect mineral deposits at depth, reveal element distributions in and around deposits, assess the total geochemical environment, and decide on effective and environment-friendly extraction and waste disposal techniques. Both pure and applied research ventures play fundamental roles in providing the techniques to manage metal resources and thereby benefit society. During mine operations and mine-closure activities, the oxidative dissolution of sulfidic minerals releases extremely acidic leachate, sulphate and potentially toxic elements such as As, Ag, Cd, Cr, Cu, Hg, Ni, Pb, Sb, Th, U, Zn from different mine tailings and waste dumps. For the sustainable rehabilitation and disposal of mining waste, the sources and mechanisms of contaminant generation, fate and transport of contaminants have to be clearly understood.

With projections of population growth to nearly 9 billion people by 2050, the world needs adequate supplies of mineral raw materials for industry and fertilizer to fulfill the aspirations of the growing population. Recycling and substitution will play an important role in supply but cannot eliminate the demand for primary resources in the coming decades. This is largely because mineral stocks are locked in durable infrastructure that cannot be recycled immediately. Recycling of discarded material originally extracted from minerals will be a challenge for the scientists. Researchers including metallurgists and geochemists are currently collaborating under the theme of "Wealth from Waste" to invent new recycling technologies in this field. This group focuses on 'Mining above Ground Resources', which are the metals contained in collections of discarded manufactured products and consumer goods.

Geochemistry has contributed significantly to the understanding of ground-water systems over the last 50 years. Historic advances include development of the hydrochemical facies concept, application of equilibrium theory, investigation of redox processes, and radiocarbon dating. Hydrochemical and isotopic information can be used to interpret the origin and mode of ground-water recharge. Geochemical techniques are the key tools to assess ground water quality, identify toxicity and recommend permissible (safe) levels as well as remediation processes. Hydrogeochemical and soil geochemical mapping are extremely useful tools in mineral exploration, land-use planning, environmental monitoring, understanding geo-medical issues and soil nutritional/toxicity properties (i.e. Se deficiency, As-Cd toxicity, Skeletal-Dental Fluorosis, Chronic Kidney Decease). Sri Lanka has made some progress in producing these geochemical data sets but limited spatial coverage and poor sample density impair their applications.

Climatologists have found that global greenhouse gas emissions need to reach zero by around 2050 to avert the worst effects of climate change. Many of the world's leading economies have set goals to eliminate pollution from fossil fuels in the next few decades. Both generation and storage of clean energy require increased quantities of minerals like silica, graphite and cobalt-nickel ore. For example, an electric vehicle requires six times more mineral material than a car that runs on fossil fuels. According to International Energy Agency the world isn't mining enough minerals to reach a future that runs on clean energy (IEA). In fact, mineral ores containing chemical elements such as Li, Co and Ni are the building blocks for clean energy economies. Countries can't meet their new climate goals without sufficient quantities of these minerals. Thus, exploration geochemists will have a heightened responsibility to explore suitable deposits containing these materials. Another growing area that contributes to the sustainability of mineral raw material is nanotechnology. Development of nanomaterial-based batteries with higher storage capacities will boost the industry that produce clean energy. Research is also advancing towards replacing rather inefficient silica cells with nano particles. Applications of graphene technology in sustainable development efforts are highly promising, yet to be fully evaluated. Sri Lanka has the advantage of having world's purest graphite deposits with C>99.5% in developing and promoting natural graphite-based graphene products. Geological carbon-sequestration is promising greenhouse gas mitigation technology. It is estimated that at least 2000 Gt of CO2 can be accommodated underground globally. Geochemistry plays a significant role in many aspects of geologic carbon sequestration, from dissolution and precipitation of minerals in the reservoir and seal rocks, to modification of the properties of mineral surfaces and their effects on fluid flow and capillary trapping. This abstract has attempted to summarize and highlight some of the key areas where our geochemical and mineral chemical understating is essential in the global sustainable development efforts. In this context the important role played by geochemists and mineral chemists can't be overemphasized.

***Dr. Prame** graduated from University of Peradeniya in 1980 with a Special (Hon) degree in Geology. He obtained his Ph. D. from University of Bonn, Federal Republic of Germany, specializing in Petrochemistry and petrology of Precambrian metamorphic rocks of Sri Lanka. His entire professional career of 35 years has been with the Geological Survey Department and its successor institution, the Geological Survey and Mines Bureau. There, he has held positions such as Assistant Director and Deputy Director before appointed as the Director General of the Geological Survey and Mines Bureau in 2014. He has carried out a number of important research studies in petrology, petrochemistry and geochemistry at prestigious institutions such as University of Chicago (USA), University of Bonn (Germany) and National Polar Research Institution, Tokyo (Japan). Dr. Prame has authored or co-authored more than 15 full papers in peer reviewed journals and over 50 abstracts at various geoscientific conferences. He was elected as President of the Geological Society of Sri Lanka in 2002 and was awarded the 'Ananda Coomaraswamy Medal' in recognition of his scientific contributions to geology of Sri Lanka and services to the geological community of the country. He is also a recipient of the Presidential Award for scientific publication.*

Biochar-based water treatment- a Sustainable Technology for Clean Water in Developing Countries

Dinesh Mohan

School of Environmental Sciences, Jawaharlal Nehru University, New Delhi, India

The 17 Goals were adopted by all UN Member States in 2015, as part of the 2030 Agenda for Sustainable Development which set out a 15-year plan to achieve the Goals. Action is needed on a number of fronts, including harnessing and maximizing the potential of technological innovation. Such technologies include carbon capture and storage systems, more efficient irrigation methods, essential medicines, household water purification devices, and manufacturing processes that minimize waste and pollution. There are similarities between the Vedas and SDGs. In the ancient scriptures, Earth is treated as a mother and the well-being of Mother Earth is critical for Environment and Life preservation. Similarities are expected from the SDGs by considering the biodiversity importance and ecological balance. SDG 14 outlines the need for conservation and sustainable use of oceans and rivers to maintain marine biodiversity while SDG 15 addresses conservation of forests, protection of animals, land biodiversity and goal to prevent degradation and desertification. In other words, the 17 UN SDGs and Ancient Indian scriptures are propagating the same sustainability principles. In Vedas, especially in Atharv Veda, references to water quality are available. A water treatment method was also suggested to improve the drinking water quality as explained in the following shloks:

अज्जनमुस्तोशीरैः शराजकोशातकामलकचूर्णैः।
कतकफलसमायुक्तैर्योगः कूपे प्रदातव्यः।। Vr.S.54.121 ।।

कलुषं कटुकं लवणं विरसं सलिलं यदि वाशुभगन्धि भवेत।
तदनेन भवत्यमलं सुरसं सुसुगन्धि गणैरपरैश्च युतम।। Vr.S.54.122 ।।

Similarities between the Vedas and SDGs will be discussed. How the sustainability was executed in the ancient times and how this got diluted over time will be overviewed. Some sustainable water treatment technologies developed by our group will also be discussed to revive our ancient practices to achieve the UN sustainable goals.

***Dr. Mohan** obtained his PhD in Chemistry from the Indian Institute of Technology, Roorkee, India. He has served as a visiting scholar at the University of Southern Queensland, Australia, Institute of Fundamental Studies, Kandy, Sri Lanka, Kangwon National University, Korea, Universidad Autónoma San Luis, México and Indian Institute of Technology (Indian School of Mines), Dhanbad, India. His research interests involve wastewater monitoring, assessment, modeling and remediation, climate change mitigation, biorefining and carbon cycling, development of low cost adsorbents, including biochar, and their applications in water and soil remediation. Dr. Mohan has over 150 publications to his name, with over 36,000 citations and a h-index of 71. He is currently serving as a Professor in the School of Environmental Sciences at Jawaharlal Nehru University, New Delhi and also as an adjunct professor at Department of Chemistry, Mississippi State University, USA.*

Sustainable Development through Application of Scientific Research Output

R. M. G. Rajapakse

Department of Chemistry, University of Peradeniya, Sri Lanka

The progress of humankind and the society depends mainly on application of scientific research outputs for their benefit. The sustainable development of a society or a country, in particular, or the entire world, in general, thus relies on the development of eco-friendly products for the use of humankind and the biota. As such, the researchers involved in developing new inventions should mandatorily consider further stepping forward to convert the invention into a marketable product. However, almost all inventions made in Sri Lanka are finally ending up as documents in the respective higher degree theses and as publications in various journals. Every effort should, therefore, be taken to increase the number of commercial products generated from scientific discoveries.

It is impossible to demarcate basic research and applied research. One may consider the greatest discoveries made by distinguished scientists such as Robert Hooke, Sir Isaac Newton, Albert Einstein and such other scientists are mostly theoretical. However, these discoveries have applications ranging from developing toilet tissues, taking a catch in the cricket tournament, developing motor vehicle engines, jet propulsion, gravitational lens, nuclear energy, GPS system, quantum computing and also in predicting stock market trends. Therefore, the theoretical equations put forward by the above scientists are now in use in almost all areas of human needs. In this lecture, it is expected to demonstrate the sustainable development through harnessing scientific research outputs in seven distinct steps. The first step reveals how to make ground-breaking discoveries. To do so, one has to follow and learn from legends. It is expected to take five distinct examples from the set of legends and to reveal how their scientific outputs came into real world applications. The discussion will then be directed to cutting edge technologies such as nanotechnology and its benefits to a country like Sri Lanka. Scientific research is mandatorily multidisciplinary in nature. Therefore, in the step 2, it is hoped to advise the young and emerging researchers to be involved in multi-disciplinary research in the form of a team work. This point will be highlighted from the research activities carried out in my research group in order to stress the importance of research collaborations. The step 3 is the contributions to the national development. Scientists should get together with industries to help develop industrial products suitable for the future global market. In order to do so, a knowledge in future market trends is required and the R&D activities could then be fine-tuned to suit to develop such requirements since the sustainable retention of products in the global market depends on how the products are modified to suit customers. The step 4 is to contribute to international development and establish career as a distinguished scientist in the global context. Step 5 would be to let the recognition come to you rather than you going behind asking for the recognition. That recognition gained would be of high importance in persuading industries to contribute to the process of converting new developments to a product in the consumer market. As the step 7, the researcher should have a knowledge in market strategies and ways and means of getting the recognition for the products developed. It is always convenient to tie up with the existing state and/or private sector organizations and the respective bodies such as relevant ministries and to work in harmony towards achieving the ultimate goal. Obtaining the state sector sponsorship and finding suitable and trustable commercial partners are useful for the conversion of the research output to a product in the consumer market. The product should comply with all the requirements and the certificates of the tests carried out from an accredited laboratory should be provided. A product would not sustain in the market if it has adverse consequences on the biota, ecosystem and the environment. As such, prime consideration should be devoted to developing eco-friendly, bio-degradable products so as not to give a burden to the environment when the product is eventually discarded to the environment. Step 8 is the self-satisfaction gained by the positive contribution made to the benefit of the humankind.

***Prof. Rajapakse** graduated from the University of Peradeniya obtaining a B.Sc. Special Degree in Chemistry with First Class (Honours). He completed his PhD in 1988 at the Department of Chemistry, Imperial College of Science, Technology and Medicine, University of London. He has worked as a Postdoctoral Research Scientist at Imperial College, UMIST, University of Bath, University of Central Lancashire and University of Liverpool, UK and The Max Planck Institute for Polymer Research, Germany. He was a Visiting Senior Scientist at the University of Texas at Arlington and the University of Mississippi, USA, and a Regular Visiting Professor at the Research Institute of Electronics, Shizuoka University, Japan and a JSPS Fellow at the Faculty of Engineering, Shizuoka University, Japan. His research interests include electronically conducting polymers, photodynamic therapy, environmental pollution abatement, gas sensors, conversion of local minerals to value added nanomaterials, custom-made prostheses for orthopaedic transplants, solar cells, fuel cells, supercapacitors, lithium ion batteries and flow batteries, targeted delivery of anticancer drugs, photon up-conversion based hydrogen generation from water photo-splitting, mosquito larvae control, advanced and intelligent textiles. Prof. Rajapakse has over 125 indexed publications and over 200 journal publications in total, together with over 200 conference proceedings and 10 Patent Local Applications and 1 World Patent Application. He has won over 20 awards including the CVCD Award for Best Research in Physical Science and Presidential Awards for Research Publications. Since 1990, he has been attached to the Department of Chemistry, University of Peradeniya, and currently serves as a Senior Professor in Chemistry.*

Theme Seminar

Natural Products – A Sustainable Source of Therapeutics and Nutraceuticals

M. Iqbal Choudhary and Atta-ur-Rahman

International Center for Chemical and Biological Sciences

(H. E. J. Research Institute of Chemistry, Dr. Panjwani Center for Molecular Medicine and Drug Research),

University of Karachi, Pakistan

Sciences at the interface of chemistry and biology have led to increased opportunities for the identification of lead molecules against various therapeutic targets. For centuries, natural products have served as key sources of therapeutic agents, and still many of current drugs are derived from medicinal plants. However, synthesis of natural products is still a challenging task due to various reasons, including structural and stereochemical complexities. These problems can circumvent with the help of biocatalysis and combinatorial biosynthesis, as enzymes have high selectivity and specificity and they can work under mild conditions in both organic and aqueous media.

During the last four decades, our research has been focused on the discovery of chemical constituents from medicinal plants used in traditional medicines, as well as identifying new biotransformed products with therapeutic potential. This has resulted in the identification of several novel lead molecules against various therapeutic targets. Emphasis has been on the discovery of natural products and their analogs against chronic disorders, including, cardiovascular, cancer, diabetes, inflammatory Alzheimer's and Parkinson's diseases.

Novel analogues of existing drugs such as tibolones (postmenopausal osteoporosis), exemestane (anti-cancer drug), medrysone (anti-inflammatory agent) and many others were synthesized using biotransformation tools. Thus, potent anti-inflammatory, and anti-cancer agents were identified as lead molecules. Furthermore, inhibitors of key enzymes related to several diseases were also identified.

Diabetes is a chronic disease that occurs when pancreatic beta-cells do not produce enough insulin (Type 1), or when the body cannot effectively use the insulin it produces (Type 2). Loss of β-cell mass and function underlies much of the pathology of diabetes. Current treatments for diabetes are unable to halt the decline in functional β-cell mass. Therefore, strategies to prevent β-cell apoptosis are urgently required. Over 1,500 fully characterized synthetic and natural compounds were evaluated for their ability to increase β-cell mass and function in the presence of cytokines (IL-1β, TNF-α, and IFN-γ). The most promising natural compounds, include silymarin, bergenin, cinnamic acid, vanillin, and kaempferol. These compounds were found to suppress increased cytokines and cellular ATP levels, decreased caspase-3 activity, decreased cellular nitrite production, and increased glucose-stimulated insulin secretion (GSIS).

During this presentation, some recent examples of our studies highlighting the translational potential of bioactive natural products, and biotransformation against non-communicable chronic diseases will be presented.

Prof. Choudhary *earned his B. Sc. Degree in Chemistry, Biochemistry and Botany in 1980, and his M. Sc. Degree in Organic Chemistry in 1983, from the University of Karachi, Pakistan. He completed his PhD in Organic Chemistry at the H. E. J. Research Institute of Chemistry, University of Karachi in 1987 and was awarded a D.Sc. by Al-Farabi Kazakh National University, Kazakhstan in 2019. He has served as a visiting professor in universities worldwide including the University of Rhode Island, USA, the School of Healthcare Sciences at Manchester Metropolitan University, UK, and University Kebangsaan Malaysia (UKM). Prof. Choudhary has, since 1990, been among the world leaders in the field of natural product chemistry, and has made pioneering contributions in the discovery of novel natural products, which have been recognized by prestigious national and international awards and honors, and fellowships of several academies of science. He is the recipient of 3 civil awards awarded by the President of Pakistan. He has 1,154 publications (citations 29,850, h index 70) in the fields of organic and bioorganic chemistry, along with 74 international patents (56 US Patents), 87 books and 40 book chapters. Prof. Choudhary is currently serving as the Director and Professor of Bioorganic and Natural Product Chemistry at the International Center for Chemical and Biological Sciences (H. E. J. Research Institute of Chemistry and Dr. Panjwani Center for Molecular Medicine and Drug Research), University of Karachi and Coordinator General COMSTECH (Organization of Islamic Cooperation Standing Committee on Scientific and Technological Cooperation).*

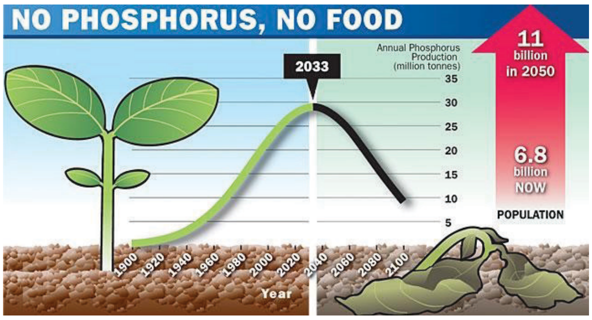
Prof. Rahman *received his B.Sc (Hons.) in Chemistry in 1963, followed by M.Sc in Organic Chemistry from the University of Karachi, Pakistan. He obtained his Ph.D. in Organic Chemistry from the University of Cambridge, UK in 1968. He was subsequently awarded a Doctorate of Science by University of Cambridge in 1987, a Doctorate of Education by Coventry University in 2007, a Doctorate of Science by Bradford University in 2010, and a Doctor of Philosophy by Asian Institute of Technology, Thailand in 2010. His research interests include isolation and structure elucidation of bioactive substances from medicinal plants as well as marine plants and animals, development of novel methods for structure elucidation and synthetic transformations of biologically and biosynthetically interesting compounds. He is the author of 1232 publications in several fields of organic chemistry, including 771 research publications, 45 international patents, 70 chapters in books, and 341 books published largely by major US and European presses. He is the Editor-in-Chief of eight European Chemistry journals. Prof. Rahman is one of the most decorated scientists of Pakistan having being honored and recognized globally for his scientific contributions. He currently serves as the Patron-in-Chief of the International Center for Chemical and Biological Sciences (H. E. J. Research Institute of Chemistry and Dr. Panjwani Center for Molecular Medicine and Drug Research), University of Karachi.*

Closing the nutrient loop: Phosphorus management in protein farming

Nanthi Bolan

University of Newcastle, Australia

When nutrients are applied in excess of food and fodder crops' requirements, they can escape from fields to surrounding soils, air, and waterways, thereby leading to environmental degradation and economic loss. Moreover, the portion of the nutrients harvested in food and fodder crops, and subsequently consumed by human and farm animals is generally concentrated in the locations where humans and animals reside, with the majority of the nutrients excreted along with wastes. Thus, there is an uncoupling of the site of nutrient inputs to soil to meet crop demands and the site of recovery of nutrients exported from farms. Closing the nutrient loop includes strategies to recover nutrients from sources in which nutrients tend to concentrate that include wastewater treatment plants, livestock production facilities, compost operations, and food processing plants, and recycle these nutrients back to cropping systems. By recovering nutrients from these sources, we can increase the amount of nutrients recycled for food and fodder production, thereby creating a more 'closed' system and achieving food security.



Poultry meat and egg are the major sources of protein consumption by the human population in most countries. The poultry industry is one of the largest and fastest growing agro-based industries in the world. This can be attributed to an increasing demand for poultry-based protein products including meat and egg. However, a major problem facing the poultry industry is the large-scale accumulation of wastes including manure and litter, which may pose disposal and pollution problems unless environmentally and economically sustainable management technologies are evolved. Poultry litter and manure are rich in nutrients, especially nitrogen and phosphorus, and most of the litter produced by the poultry industry is currently applied to agricultural land as a source of nutrients and soil amendment. However, environmental pollution, resulting from nutrient and contaminant leaching, can occur when poultry litter is applied under soil and climatic conditions that do not favour an effective agronomic utilisation of the manure-borne nutrients by food and fodder crops.

This presentation examines the poultry feed, manure, soil and nutrient management practices to improve the phosphorus use efficiency in poultry farming. Phosphorus is a major nutrient in food production, but we have only a finite supply of P ('P Peak'). Large-scale application of poultry manure results in the accumulation and loss of P in soils. Efficient management of P in the poultry industry is essential to achieve economic and environmental sustainability. Manure management practices include efficient feed use, P recovery from manure, and soil and crop management.

It is important to note that poultry manure may also contain contaminants such as heavy metals (*e.g.*, arsenic) and antibiotics which can be toxic to soil microorganisms and plants. Therefore, it is imperative to devise integrated management practices to manage nutrients and contaminants in poultry farming, thereby improving the nutrient use efficiency and farm productivity.

***Prof. Bolan** has been a visiting scientist at the University of Newcastle upon Tyne (United Kingdom), University of Georgia (USA), Federal Agricultural Research Centre (Germany), University of LaFrontera (Chile), and Jinju National University (Korea). He has served as the Professor of Soil Science at Massey University, New Zealand, and also as the Chair in Environmental Science at the University of South Australia (UniSA), the Dean of Graduate Studies of UniSA and as a Program Leader of the Co-operative Research Center for Contaminant Assessment and remediation of the Environment. He is currently serving as a Professor of Environmental Chemistry at the University of Newcastle, Australia while serving as a Program Leader of the Co-operative Research Center for High Performance Soils. He is one of the Chief Investigators of the Australian Centre for Cannabinoid Clinical and Research Excellence undertaking research on the distribution and bioavailability of contaminants in cannabis. Prof. Bolan's teaching and research interests include agronomic value of manures, fertilisers and soil amendments, soil acidification, nutrient and carbon cycling, pesticide and metal pollutants interactions in soils, greenhouse gas emission, soil remediation, mine site revegetation, and waste and wastewater management. He has supervised more than 60 postgraduate students, and was awarded the Massey University Research Medal for excellence in postgraduate students' supervision. He has published more than 400 book chapters and journal papers, and was awarded the M.L. Leamy Award in recognition of the most meritorious contribution to soil science. Prof. Bolan has achieved more than 32,000 citations with an H index of 84 (Google Scholar), and is one of the Web of Science's Globally Highly Cited Researchers for 2018, 2019 and 2020.*

50th Annual Sessions of Institute of Chemistry Ceylon
Technical Sessions

Time: 8.30 am – 3.00 pm **Date: 29th June 2021**

CCS Alumni Postgraduate Symposia

Chair - Prof. Nilwala Kottegoda

Time	Title	Presenting Author	Corresponding Author	Reference No.
8.30 a.m. - 8.45 a.m.	Development of a natural product library with potent activity against the Human Parasite *Trichomonas vaginalis*	Thilini Peramuna	Thilini Peramuna	PG24
8.45 a.m. - 9.00 a.m.	Optimization of Proteomics-based Substrate Trapping with Histone Deacetylase 1	Kavinda E. Herath	Mary Kay H. Pflum	PG25
9.00 a.m. - 9.15 a.m.	Highly Efficient Hydrogen Evolution and Hydrazine Oxidation of Platinum *via* Tuning the Interfacial Dissolved-Gas Concentration	Ruchiranga Ranaweera		PG26

Presentations of Prof. M. U. S. Sultanbawa Award for Research in Chemistry

Session Chair - Prof. Namal Priyantha Heenkenda

Time	Title	Presenting Author	Corresponding Author	Reference No.
9.15 a.m. - 9.30 a.m.	Synthesis of Precursors of Cycloparaphenylenes using Ullmann Coupling	L. G. Edirisinghe	I. R. Fernando	SB1
9.30 a.m. - 9.45 a.m.	Synthesis and characterization of platinum complexes with ethylenediamine and diethylenetriamine sulphonamide ligands towards biological applications	I. L. Hettige	N. T. Perera	SB3
9.45 a.m. - 10.00 a.m.	Invasive plant-derived biochar for sorptive removal of hexavalent chromium in aqueous media	Anusha Ekanayake	Meththika Vithanage	SB16
10.00 a.m. - 10.15 a.m.	Characterization of some selected compost samples for the presence of microplastics and heavy metals associated with them	Thilakshani Atugoda	Meththika Vithanage	SB17

Technical Sessions – 1

Session Chair - Dr. Gobika Thiripuranathar / Dr. A. A. P. Keerthi

Time	Title	Presenting Author	Corresponding Author	Reference No.
10.45 a.m. - 11.00 a.m.	Bio-assay Guided Screening of Antioxidant Activity and Acetylcholinesterase Inhibitory Activity of fruit pulp of Musa balbisiana ABB	L. A. M. Fernando	Isurika R. Fernando	TO2
11.00 a.m. - 11.15 a.m.	Effect of Cooking on Antioxidant Properties of Selected Traditional Rice Varieties	B. A. Lishana C. Wimalarathne	Sagarika Ekanayake	TO4
11.15 a.m. - 11.30 a.m.	Antioxidant properties of selected *Hela Suwaya* herbal porridges	Bismi T. Randiligama	Sagarika Ekanayake	TO5
11.30 a.m. - 11.45 a.m.	CHANGES of the quality of palmyrah fruit pulp (PFP) exposed to open-air and the antimicrobial effect of herbal extracts on common microbes in spoiled (PFP)	S.Srivijeindran	S.Srivijeindran	TO6
11.45 a.m. - 12.00 p.m.	Proximate Composition of TetraPacked Fresh Milk in Sri Lankan Market	Harshika N. Disanayaka	Sagarika Ekanayaka	TO9
12.00 p.m. - 12.15 p.m.	Investigation of Antityrosinase and Antioxidant Activity of Polyscias balfouriana L.H.Bailey (Koppa Plant)	E. G. Divyanjalee Suraweera	Kushan C. Weerasiri	TO12
12.15 p.m. - 12.30 p.m.	potential hypoglycemic activity of Kaempferol rhamnoside isolated from Olax zeylanica (Malla) leaves	N.G.D.Anuradha	M. G. A. N. Perera	TO18

Technical Sessions – 2

Session Chair - Dr. Sisira Weliwegamage

Time	Title	Presenting Author	Corresponding Author	Reference No.
1.30 p.m. - 1.45 p.m.	Biosynthesis, Characterization, Photocatalytic and Fluorescence quenching activity of Zinc Oxide nanoparticles	K. Kaleem	G. Thiripuranathar	TI7

1.45 p.m. - 2.00 p.m.	Morphological and photocatalytic properties of zinc oxide nanoparticles synthesized from agricultural wastes of *Nephelium lappaceum* L. and *Garcinia mangostan* L.	K. M. K. G. Perera	G. Thiripuranathar	TI8
2.00 p.m. - 2.15 p.m.	*In silico* identification of natural product inhibitors of HMG-CoA reductase	Archchana Ganeshalingam	Chinthaka N. Ratnaweera	TI10
2.15 p.m. - 2.30 p.m.	A Computational Study of Cyclindependent Kinases 1 (CDK1) butyrolactone I complex and the Role of Mg Ion in the Active Site	Chanikya D. Jayawardana	Chinthaka N. Ratnaweera	TI11
2.30 p.m. - 2.45 p.m.	A study on complexation, stoichiometry and binding of selected anionic organic pollutants and protonated polyaza macrocycles	Danushka M. Kumarasinghe	Isurika R. Fernando	TI23

Technical Sessions – 3

Session Chair - Dr. Udaya K. Jayasundara

Time	Title	Presenting Author	Corresponding Author	Reference No.
1.30 p.m. - 1.45 p.m.	Removal of Selected Textile Dyes from Effluent Water Using Mineral Adsorbents and Activated Carbon	Y. K. G. D. Sanaree	U. S. K. Weliwegamage	TA13
1.45 p.m. - 2.00 p.m.	Effect of biochar application on plant uptake of sulfamethoxazole in soil	S. Keerthanan	Meththika Vithanage	TA14
2.00 p.m. - 2.15 p.m.	Evaluation and correlation of the influence of production parameters on biochar characteristics and its influence on the adsorption of three industrial dyes.	Dineth Saumya	Sameera R. Gunatilake	TA19
2.15 p.m. - 2.30 p.m.	Correlation and the Impact of Feedstock Type and Production Conditions on Heavy Metal Adsorption by Biochar: A Comprehensive Meta-Analysis	Vindya Samarakoon	Sameera R. Gunatilake	TA20

2.30 p.m. - 2.45 p.m.	Influence of feedstock and production conditions on characteristics of biochar and its correlation for the adsorption of oxyanions: A Comprehensive metaanalysis	Lilogini Sutherson	Sameera R. Gunatilake	TA21
2.45 p.m. - 3.00 p.m.	A chemometric study on the effect of feedstock choice and pyrolysis conditions on biochar production and its influence on the remediation of pharmaceuticals from aqueous solutions.	Sachin Fernando	Sameera R. Gunatilake	TA22

Abstracts of Research Papers to be presented at the 50th Annual Sessions 2021

Abstract No: PG 24

Semisynthetic derivatization studies of the fungal metabolite phomasetin with activity against the human parasite *Trichomonas vaginalis*

Thilini Peramuna*
University of Oklahoma, Norman, OK 73019, USA
**Corresponding author: peramunu.g.peramuna-1@ou.edu*

Trichomonasis is the most prevalent sexually transmitted parasitic disease (STD) in the United States and is caused by *Trichomonas vaginalis*. The tetramate-containing natural product, phomasetin, has been identified as a promising candidate with good activity (EC_{50} = 0.35 μM) against this genitourinary tract parasite. A structure-activity study was undertaken to develop semi-synthetic derivatives of phomasetin with many of the derivatives containing modifications to the tetramate moiety using 'click' chemistry. The analogues containing triazole-linked phenol groups showed the most pronounced improvements in activity compared to the other structural modifications. The semisynthetic analogues of phomasetin hold promise to improve treatment options against *T. vaginalis* through the creation of compounds that exhibit improved activity and selectivity against the parasite.

Keywords: tetramic acid, fungi, natural products, *Trichomonas vaginalis*

Abstract No: PG 25

Optimization of Proteomics-based Substrate Trapping with Histone Deacetylase 1

Kavinda E. Herath and Mary Kay H. Pflum*
Department of Chemistry, Wayne State University, Detroit, MI 48202, USA
**Corresponding author: pflum@wayne.edu*

Histone writers and erasures – the proteins that add or remove histone post translational modifications – are key drivers of epigenetic transcriptional events inside the cell. Many enzymes that control epigenetic modifications are dysregulated in human diseases. For example, overexpression of the erasure histone deacetylase (HDAC) enzymes can lead to epigenetic changes in transcription and ultimately disease, such as cancer. We recently pioneered a simple method called substrate trapping to isolate HDAC1 substrates using an inactive HDAC1 mutant. Our recent publication documented that different HDAC1 mutants preferentially bound different substrates, suggesting that three mutants (H141A, F150A, C151A) should be used for efficient trapping. Based on this observation, we performed a proteomics-based trapping study of HDAC1 using all three optimal mutants simultaneously. In this study, using trapping with three mutants, 12 potential HDAC1 substrates were identified that were not observed when only a single mutant was used. Although trapping with three mutants identified novel substrates of HDAC1, the throughput of the experiment was low compared to trapping with a single mutant. Therefore, this study confirms that trapping with a single mutant is simple and effective, although three mutants may be desirable when high efficiency or a large number of substrates is necessary.

Keywords: Epigenetic, HDAC1, Trapping

Abstract No: PG 26

Highly Efficient Hydrogen Evolution and Hydrazine Oxidation of Platinum *via* Tuning the Interfacial Dissolved-Gas Concentration

Ruchiranga Ranaweera*
Department of Chemistry, Wayne State University, Detroit, MI 48202, USA
**Corresponding author: trranaweera@wayne.edu*

Regulating the dissolved-gas concentration at the electrode solution interface represents a promising universal strategy to achieve high efficiency towards gas evolution reactions. Here, we present a facile flurosurfactant modulation strategy to control the dissolved-gas concentration at the electrode/gas/electrolyte interface for enhanced hydrogen evolution reaction (HER) and hydrazine oxidation reaction (HzOR). With the flurosurfactant modulation, lowered dissolved gas concentrations at the catalytic interface and sufficient surface-active area exposure can be achieved. For HER, we used perfluorooctanesulfonate (PFOS), and for HzOR we used cationic fluorinated pyridinium sulfonate (CFPS). The low concentration of dissolved hydrogen near the electrode/electrolyte interface can significantly decrease overpotential at the interface and thus elevated hydrogen evolution current. Therefore, it is meaningful and fundamentally essential to control the dissolved-gas concentration at electrode/gas/electrolyte interface for HER. Herein, by using platinum as the platform, we present a facile and straightforward strategy to tune the dissolved-gas concentration at electrode/gas/electrolyte catalytic interface via potassium perfluorooctanesulfonate (PFOS) modulation for dramatically enhanced HER. The addition of PFOS was demonstrated to lower the dissolved-H_2 concentration at the reaction interface. When surfactant concentration increases, the solution surface tension decreases resulting in a lower nucleation energy barrier. Consequently, a lower supersaturation concentration is required for gas

nanobubble. Moreover, the desorption of PFOS from the electrode during HER facilitate sufficient exposure of the surface-active area. Benefiting from the lowered dissolved-gas concentration and sufficient exposure of surface area at the interface, the PFOS-modulated Pt exhibited a excelent electrocatalytic performance towards HER. Relative to pure Pt, the PFOS-modulated Pt yielded a much lower overpotential of 27 mV at a cathodic current density of 10 mA cm^{-2}. Moreover, the PFOS-modulated Pt showed a current density of 27 mA cm^{-2} at the overpotential of 40 mV, which was 2.4-fold higher than that of pure Pt. All the measurements are obtained by running the three independent experiments and getting the average value. Guided by the previous work, we developed a new facile cationic fluorosurfactant-modulation strategy to achieve enhanced HzOR activity. We synthesized a fluorinated pyridinium sulfonate surfactant (CFPS). Owing to the high surface activity of CFPS, the activation energy for N_2 bubble nucleation is reduced, leading to a decreased dissolved-gas concentration at the HzOR interface. The positive charge of CFPS also ensures the effective exposure of active sites during hydrazine oxidation. Benefited from both effects, the CFPS-modulated Pt showed a boosted catalytic activity towards HzOR. The CFPS modulated Pt exhibited a current density of 10 mA cm^{-2} at 562 mV *vs.* RHE, which was 2.1 times higher than that of pure Pt under the same potential. In summary, we develop PFOS and CFPS modulation strategy with precisely managed dissolved-gas concentration at electrode/gas/electrolyte interface for highly efficient hydrogen evolution and hydrazine oxidation, respectively. This work provides a systematic understanding of the gas-involved catalytic process and a convenient approach to realize high-performance electrocatalysis based on precisely controlling the dissolved-gas concentration at the catalytic interface.

Keywords: Electro catalyst, surfactant modulation, efficient hydrogen evolution and hydrazine oxidation

Abstract No: SB 1

Synthesis of Precursors of Cycloparaphenylenes Using Ullmann Coupling

Lashan G. Edirisinghe, Isurika R. Fernando*
Department of Chemistry, Faculty of Applied Sciences,
University of Sri Jayewardenepura, Nugegoda,10250, Sri Lanka
**Corresponding author: isurika.fernando@sjp.ac.lk*

[n]Cycloparaphenylenes ([n]CPPs) are carbon and hydrogen containing macrocycles which constitute of ‘n’ number of para-phenylene groups connected via 1,4-biphenyl -C-C- linkages. The chemical, photochemical and electrochemical properties of [n]CPPs make them potential candidates for a broad range of applications. Although [n]CPPs have aesthetically appealing chemical structures, their high energy geometries make them a synthetically challenging class of molecules. Synthesis of [n]CPPs reported thus far associated with expensive catalysts, starting materials and sophisticated reaction conditions. Therefore, this research project was focused on the synthesis of a series of precursors of [n]CPPs; dimer, trimer, tetramer and other oligomeric precursors of 1,4-chlorobenzene using Ullmann coupling with the eventual intention of cyclizing those precursors to obtain a series of [n]CPPs which is feasible in the Sri Lankan context. A number of synthetic attempts followed by the reaction condition optimization attempts were made using 1,4-chlorobenzene as the starting material and activated copper as the catalyst in various solvents at various temperatures to synthesize the [n]CPP precursors. Dimerization of 1,4-chlorobenzene was carried out using activated copper as the catalyst in N-methyl-2-pyrollidone (NMP) solvent at 140 °C. The crude mixture was subjected to column chromatography to obtain clear light yellow color liquid which was characterized using UV-visible, fluorescence and NMR spectroscopy. UV-visible spectra of the obtained product in chloroform exhibited a characteristic absorption peak for the $\pi \rightarrow \pi^*$ transition of the conjugated biphenyl rings which shows λ_{max} at 272 nm. The fluorescence spectra of the obtained product demonstrated a significant enhancement of the fluorescence activity compared to the starting material. The two doublets appeared in between chemical shift values of 7.00 - 8.00 ppm in the ^1H NMR

spectrum of product in $CDCl_3$ evidenced the formation of the dimer of 1,4-dicholorbenzene, 4,4'-dichlorobiphenyl. In summary, dimerization of 1,4-dichlorobenzene was carried out using Ullmann coupling. Reaction condition optimization and characterization of trimer, tetramer and other oligomers of 1,4-dichlorobenzene are currently underway.

Keywords: [n]Cycloparaphenylenes, Ullmann coupling, 1,4-dicholorbenzene, 4,4'- dichlorobiphenyl

Abstract No: SB 3

Synthesis and characterization of platinum complexes with ethylenediamine and diethylenetriamine sulphonamide ligands towards biological applications

I. L. Hettige[1], I. C. Perera[2] and N. T. Perera[1]*

[1] *Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda, 10250, Sri Lanka*

[2] *Department of Zoology and Environment Studies, University of Colombo, Colombo 00700, Sri Lanka*

** Corresponding author: theshi@sjp.ac.lk*

Diethylenetriamine and ethylenediamine are renowned tridentate and bidentate chelating ligands, and have been utilized to synthesize sulfonamide derivatized platinum complexes. The sulphonamide ligands were synthesized with the use of sulfonyl chlorides and the relevant amine in dioxane, while the platinum complexes were formulated by treating *cis*-$[Pt(DMSO)_2Cl_2]$ with the synthesized ligand. Synthesis of novel platinum-ethylenediamine sulphonamide complexes (C1=$[PtCl_2(N(SO_2$ biphenyl) ethylenediamine)], C2=$[PtCl_2(N(SO_2$azobenzene) ethylenediamine)]) was accomplished using synthesized ethylenediamine sulphonamide ligands, (L1=N(SO_2biphenyl)ethylenediamine, L2=N(SO_2azobenzene)ethylenediamine) while that of novel platinum-diethylenetriamine sulphonamide complexes (C3=$[PtCl_2(N(SO_2$azobenzene) diethylenetriamine)], C4=$[PtCl_2(N(SO_2$quinoline) diethylenetriamine)]) was carried out with the use of synthesized diethylenetriamine sulphonamide ligands (L3=N(SO_2azobenzene) diethylenetriamine), L4= N(SO_2quinoline)diethylenetriamine]. In this study, amphiphilic ligand systems were considered as an ideal approach to enhance uptake of coordination complexes by target cells. This was executed by employing the hydrophilicity of ethylenediamine and diethylenetriamine and the lipophilicity of the aromatic bulky sulphonamide fragment bound to its terminal amine group. The ligands and complexes were synthesized in good yield (66%-96%) and characterization of these synthesized compounds was conducted using UV-Visible spectroscopy, FTIR spectroscopy and NMR spectroscopy. UV-Visible spectra of the ligands indicate clear changes from starting material along with the presence of intra-ligand $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, giving rise to absorption peaks around 200-600 nm. Shifts of these peaks can be observed in the UV-Visible spectra of the complexes. The strong S-N band signifying the formation of the sulphonamide bond, was detected in the FTIR spectra of the ligand and was found to shift to higher wavenumbers in the ethylenediamine complexes as well as in the diethylenetriamine complexes. The shift could possibly be due to the donation of the nitrogen lone pair to form the platinum coordination complex. The peaks relevant to stretching vibration frequency of $-NH_2$ were found in the 3300-3500 cm^{-1} region of the FTIR spectra of the ethylenediamine ligands and could be seen shifting to lower wavenumbers in the complex due to coordination with platinum. ^1H NMR spectra were acquired for the ligands and complexes, where the noteworthy regions include the aromatic protons found in the range of 6.76-9.00 ppm and the methylene protons of the amine group in the ethylenediamine and diethylenetriamine backbone of the ligands, appearing at 2.80-3.00 ppm. Complexes display slightly higher fluorescence intensities in comparison to that of the ligands. Structural data was obtained from single crystal X-ray diffraction of L2 and C1 which validated the formation of the ligand and complex and provided distinct evidence of the deprotonation of the amine group in ethylenediamine upon coordination to metal in complex C1. Results of the *in silico* analysis of physico-chemical and pharmokinetic parameters as well as drug-likeliness of the ethylenediamine sulphonamide ligands show that they obey Lipinski's rule of five along with having lead-likeliness. Swiss TargetPrediction was used to identify several probable biological targets, suggesting that the novel compounds may act as lead compounds for novel anti-cancer drugs.

Keywords: platinum, ethylenediamine, diethylenetriamine

Abstract No: SB 16

Invasive plant-derived biochar for sorptive removal of hexavalent chromium in aqueous media

Anusha Ekanayake, Anushka U. Rajapaksha and Meththika Vithanage*
Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura,
Nugegoda, 10250, Sri Lanka
**Corresponding author: meththika@sjp.ac.lk*

Due to increased industrialization and urbanization, chromium (Cr) has been commonly used and released to the environment in a variety of industrial activities. Two primarily available valence states of chromium in the environment are trivalent chromium (Cr III) and hexavalent chromium (Cr VI). Cr(VI) is more soluble in water, causing health hazards to human beings and animals by all exposure roots. The rapid spread of invasive plants poses a severe threat to natural ecosystems. The present study aimed to investigate the effectiveness of biochars derived from the local invasive plant 'Giant Mimosa' (*Mimosa pigra*) in removing hexavalent chromium from contaminated water. In this study, plant species *Mimosa pigra* was subjected to slow pyrolysis at 350 °C within a 2-hour residence time to produce pristine *Mimosa pigra* biochar (MPBC). The physicochemical properties of MPBC were characterized by BET, SEM, XRD and FTIR analysis. The pH at point of zero charge (pHpzc) of MPBC was obtained as pH 7.874 by surface titrations at different $NaNO_3$ ionic strengths. Cr(VI) adsorption was studied as a function of pH with three different background electrolyte strengths. The highest Cr(VI) removal from solution occurred at pH 3 with an adsorption capacity of 3.10 mg g^{-1}, and adsorption decreased when the pH increased from 3 to 10. Results also indicated that the removal of Cr(VI) by the MPBC modified biochar depended on solution pH, and a low pH value was favorable for the Cr(VI) removal with all three ionic strengths. The results herein revealed that the *Mimosa pigra* derived biochar prepared in this study has a promising application in sorption and detoxification of Cr(VI) from an aqueous solution. Future studies will be carried out to investigate the sorption kinetic behaviors of MPBC and sorption parameters will also be calculated through batch isotherm experiments. Furthermore, pilot-scale testing will be conducted to investigate the applicability of the laboratory-tested material in the actual environment. The effectiveness of organo-functionalized biochars derived from *M. pigra* in removing hexavalent chromium from contaminated water will be assessed in future studies.

Keywords: Adsorption, Remediation, Invasive plants, *Mimosa pigra*

Abstract No: SB 17

Characterization of some selected compost samples for the presence of microplastics and heavy metals associated with them

Thilakshani Atugoda, Hansika Piyumalia and Meththika Vithanage*

Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura, Nugegoda, 10250, Sri Lanka

**Corresponding author: meththika@sjp.ac.lk*

Microplastics are ubiquitous in terrestrial environments as land-based sources mainly contribute to their origin. Mismanagement of solid waste can contribute to heavy loads of microplastics, which is of serious concern in Sri Lanka. The current study focuses on assessing the abundance and characteristics of microplastics from urban compost as an entry route for microplastics into the soil. Compost samples were taken from Karadiyana, Muthurajawela, and Kalutara municipal solid waste dumpsites. Microplastics were extracted in triplicates from 100 g of compost using saturated NaCl solution and sieved from 1 mm mesh size and wet peroxide digestion was carried out to remove organic matter. Microplastics were characterized based on shape, size, color, and the polymer identified using Fourier Transformation Infrared spectroscopy (FTIR). Associated trace metals were analyzed using Microwave plasma atomic emission spectrometer (MP-AES), subsequent to acid digestion procedures. The most abundant microplastics fraction in compost was polyethylene fragments in size range of 2-5 mm formed due to the breakdown of plastic materials present in the municipal solid waste. The abundance of microplastics in compost was 400, 360 and 410 particles kg^{-1} in Karadiyana, Kalutara, and Muthurajawela, respectively. Compared to other locations, Muthurajawela microplastics had significantly higher levels of heavy metal at concentrations of 1856, 238, 194, 406, 24 and 60 $\mu g\ g^{-1}$ for Zn, Cd, Cu, Ni, Pb and Cr, respectively. Heavy metal concentration of microplastics in Karadiyana compost samples were in the range of 32, 20, 4 $\mu g\ g^{-1}$ for Zn, Cu, Pb and Cr and for Kalutara samples 17, 4 and 8 $\mu g\ g^{-1}$ for Cu, Pb and Cr respectively. Muthurajawela soil is acidic due to the saline peat bog and therefore heavy metal leaching is very high. Municipal solid waste compost is vulnerable to terrestrial and aquatic -microplastics upon their application in agricultural purposes. The associated heavy metals in microplastics pose a greater risk as vectors for transferring trace elements along the food chain and bioaccumulating them in higher trophic levels.

Keywords: Plastic, Marine pollution, Solid waste management, Landfill, Leach

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Abstract No: TO 2

Bio-assay Guided Screening of Antioxidant Activity and Acetylcholinesterase Inhibitory Activity of fruit pulp of *Musa balbisiana* ABB

Aravindani M. Fernando[1], Anoja P. Attanayake[2] and Isurika R. Fernando[1]*

[1] Department of Chemistry, Faculty of Applied Sciences,
University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka.
[2] Department of Biochemistry, Faculty of Medicine, University of Ruhuna, Galle 80000, Sri Lanka.
** Corresponding author: isurika.fernando@sjp.ac.lk*

A non-communicable disease, Alzheimer's disease (AD) is the most prevailing progressive and irreversible neurological brain disorder among the elderly community. Although the precise cause for AD is still uncertain, acetylcholinesterase (AChE) inhibitors and antioxidants have been used to treat Alzheimer's patients. A recent study on evaluation of antioxidant activity and AChE inhibitory activity of aqueous, ethanol, ethyl acetate and hexane extracts of nearly three month old fruit pulps of three most abundant banana species commonly name as sour banana, sugar banana and 'anamalu' grown in Sri Lanka demonstrated that the ethanol extract of sour banana, *Musa balbisiana* ABB (Family: Musaceae) had the highest AChE inhibitory activity. Therefore, this study was focused on the bio-assay guided screening of potent antioxidants and AChE inhibitors from the ethanol extract of the fruit pulp of *Musa balbisiana* ABB with the intension to eventually isolate potential antioxidants and AChE inhibitors. Nearly three month old chopped fruit pulp of *Musa balbisiana* ABB were subjected to Soxhlet extraction using methanol as a solvent. Excess solvent was distilled off and the resulted ethanol extract was subjected to flash column chromatography using silica as the stationary phase with wet loading and a 1:1 mixture of ethyl acetate and methanol as the mobile phase. After carrying out thin layer chromatographic analysis for each eluate, fractions with similar retention factor was combined to obtain seven samples. The antioxidant activities and AChE inhibitory activities of seven major fractions and the crude ethanol extract were evaluated using 2, 2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay and Ellman's colorimetric assay, respectively. Ascorbic acid and donepezil were used as the standard compounds in DPPH assay and Ellman's assay, respectively. Among the seven combined fractions analysed, the fourth fraction exhibits the lowest IC_{50} value of 176.90 ± 0.66 mg L^{-1} representing the highest antioxidant activity for DPPH assay and the fifth fraction demonstrates the lowest IC_{50} value of 26.53 ± 0.59 mg L^{-1} signifying the highest AChE inhibitory activity for Ellman's assay. The highest IC_{50} values that demonstrates the lowest activities belongs to the first fraction and the fourth fraction for DPPH assay and Ellman's assay, respectively. In conclusion, the ethanol extract of *Musa balbisiana* ABB constitutes of potential AChE inhibitors as well as antioxidants. Therefore, *Musa balbisiana* ABB can be used as an edible source of promising antioxidants and AChE inhibitors. Bio-assay guided isolation of potential natural AChE inhibitors and antioxidants is currently underway with an intension of developing a nutraceutical/pharmaceutical agent targeting the management of AD.

Keywords: Bio-assay guided screening, Antioxidant activity, Acetylcholinesterase inhibitory activity, *Musa balbisiana* ABB

Abstract No: TO 4

Effect of Cooking on Antioxidant Properties of Selected Traditional Rice Varieties

B. A. Lishana C. Wimalarathne[1,2] and Sagarika Ekanayake[2]*
[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*
[2] *Department of Biochemistry, Faculty of Medical Sciences, University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka*
**Corresponding author: sagarikae@hotmail.com*

Rice (*Oryza sativa* L.) is the staple food for Sri Lankans. Currently over 300 different Sri Lankan traditional rice varieties are grown under all agro-climatic conditions in Yala and Maha seasons. Recent researches conducted have shown that traditional rice varieties contain naturally occurring antioxidant compounds. Present study evaluates the antioxidant properties of selected raw and cooked traditional rice varieties namely Suduheenati, Masuran, Rathdel and Kahawanu and the effect of cooking on the antioxidant properties of rice. Total phenolic content (TPC) was determined by the Folin-Ciocalteu method using gallic acid as the standard. The antioxidant potential was evaluated using 1,1-diphenyl-2-picryl-hydrazyl (DPPH) radical scavenging and ferric reducing antioxidant power (FRAP) assays using ascorbic acid as the standard. Mean TPC, DPPH and FRAP of raw rice flour were in the range of 3.9-6.8 mg Gallic Acid Equivalents (GAE) /g, 4.7-6.9 mg Ascorbic acid Equivalents (AE) /100g and 11.3-13.3 mg AE /100g respectively. Mean TPC, DPPH and FRAP of cooked rice flour were in the range of 3.3-6.3 mg GAE /g, 4.5-6.7 mg AE /100g and 10.9-12.9 mg AE /100g respectively. Mean TPC, DPPH and FRAP of freshly cooked rice were in the range of 1.1- 2.0

mg GAE /g, 1.4-2.2 mg AE /100g and 3.5-4.2 mg AE /100g respectively. The mean TPC and DPPH radical scavenging activities for both raw and cooked rice flour were in the order of *Suduheenati* > *Masuran* > *Rathdel* > *Kahawanu*. The order of FRAP for both raw and cooked rice flour were in the order of *Suduheenati* > *Masuran* > *Kahawanu* > *Rathdel*. Among raw and cooked rice flour, red rice (*Suduheenati, Masuran*) had significantly ($P \leq 0.05$) high antioxidant properties compared to white rice (*Rathdel, Kahawanu*). Cooking has reduced the TPC of red rice flour significantly ($P \leq 0.05$) whereas the reduction was not significant ($P \geq 0.05$) in white rice flour, DPPH scavenging activity and antioxidant power of FRAP have also reduced but not significantly ($P \geq 0.05$) for rice flour of the selected varieties. A positive significant correlation ($P \leq 0.01$) was observed between mean TPC contents and DPPH radical scavenging activity (r =0.919) and FRAP (r =0.910) for cooked rice flour with four samples, indicating that phenolic compounds present in rice provide the antioxidant activity by both the radical scavenging mechanism and reduction of oxidized intermediates in the chain reaction. The selected rice varieties exhibited high FRAP activity compared to DPPH radical scavenging activity indicating that reduction of oxidized intermediates in the chain reaction occurs more predominantly.

Keywords: Antioxidant properties, Traditional rice, Red and white rice, Raw and cooked rice

Abstract No: TO 5

Antioxidant Properties of Selected *Hela Suwaya* Herbal Porridge

Bismi Thisaruka Randiligama[1,2] and Sagarika Ekanayake[2*]

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *Department of Biochemistry, Faculty of Medical Sciences, University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka*

**Corresponding author: sagarikae@hotmail.com*

Herbal porridges that contain high amounts of plant materials are rich sources of antioxidants. These are made by incorporating rice, different leaf extracts and coconut milk. Commercial availability of easy to prepare porridges is currently a trend due to the lifestyle changes of people. No research has been done previously to study the antioxidant potential of commercially available herbal porridges. Thus in the present study the antioxidant potentials and total phenolic content of commercially available four *Hela Suwaya* herbal porridges were determined. Preparation of four (white, green, blue and yellow) porridges was done according to the written instructions provided with the specific pack, by using rice/flour mixture and the pre-prepared packet of spices supplied within the pack separately. It requires few ingredients including coconut milk to be added fresh as instructed. Folin-Ciocalteu method was used to determine the total phenolic content (TPC), whilst 2, 2-diphenyl-1-picrylhydrazyl (DPPH) and potassium ferric reducing antioxidant power (PFRAP) assays were performed to measure the antioxidant activities of porridges. Gallic acid (GA) and ascorbic acid (AA) was used as the standards. All the selected herbal porridges exhibited high antioxidant capacity as well as high amount of total phenolic compounds. The total phenolic contents of porridges were found to vary from 50.7 – 113.2 mg Gallic Acid Equivalents (GAE)/100 mL. Antioxidant potentials of porridges ranged from 5.7 – 9.5 mg Ascorbic acid Equivalents (AAE)/100 mL and 6.7 – 20.2 mg AAE/100 mL in DPPH assay and FRAP assay respectively. The Green porridge that was made incorporating rice, spices and mainly gotukola had the highest TPC and antioxidant potential. Types of rice and spices used are almost similar in all other porridges as well. The white porridge that was made using the least amount of herbs showed the least TPC and antioxidant potential. Results obtained indicated that the antioxidant potential varied significantly ($P \leq 0.05$) from porridge to porridge. There was a positive significant ($P \leq 0.01$) correlation between antioxidant activities and total phenolic content for the DPPH assay (r = 0.95) and for the FRAP assay (r = 0.87) even with four samples analyzed. These findings show that commercially available *Hela Suwaya* herbal porridges are a good source

of antioxidants and antioxidant potentials are mainly due to the phenolic compounds present

Keywords: antioxidant potential, herbal porridges, Folin Ciocalteu assay, DPPH assay, FRAP assay

Abstract No: TO 6

Changes of the quality of palmyrah fruit pulp (pfp) exposed to open-air and the antimicrobial effect of herbal extracts on common microbes in spoiled pfp

S. SriVijeindran[1,2*], Champa D. Jayaweera[1], S. Mohanadas[2] and A. Kirushanthi[2]

[1] Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura,
Nugegoda, 10250, Sri Lanka
[2] Palmyrah Research Institute, Kandy Road, Kaithady, Jaffna 40000, Sri Lanka
**Corresponding author: srthyln@yahoo.com*

Palmyrah (B*orassus flabellifer* L.) Fruit Pulp (PFP) has more health benefits. Spoiled PFP is mainly caused by acid-producing microbes like *A. aceti* and alcohol-producing microbes like *S. cerevisiae*. Chemically preserved PFP partially losses its natural characteristics during its storage for a long time. Edible natural preservatives which are harmless to human might be used to preserve the PFP effectively. The aim of this work is to analyze the changes in the quality of PFP when it is exposed to the open-air environment and also to compare the antimicrobial activity of the extracts from specific parts of edible herbal plants against prominent microbes present in the spoiled PFP. Initially, PFP was exposed to an open-air environment for three days for spoilage. Quality parameters such as Total Soluble Solids (TSS), pH , acidity, sugar (total and reducing), and Total Phenolic Content (TPC) of both fresh and spoiled PFP samples were determined using refractometric, potentiometric, titrimetric, Lane & Eynon, and Folin–Ciocalteu methods respectively. Screening of antimicrobial activity was done with reference to the organisms, *A. aceti*, *S. cerevisiae*, *S. aureus* and *E. coli* using agar well diffusion technique where chloramphenicol was used as a positive control. Broth dilution method was employed to determine the Minimum Inhibitory Concentration (MIC) of extracts. Parts of six different herbs; seeds of *Myristica fragrans* and *Syzygium cumini*, barks of *Cinnamomum verum* and *Vateria copallifera* and root of *Acorus calamus* and *Curcuma longa* were selected and their ethanolic (aq) extracts were obtained using both Soxhlet and maceration along with the ultra-sonication method. TSS of fresh PFP declined from 23.64±1.19 to 12.20±0 31in spoiled PFP. The reduction might be due to the conversion of sugars to organic acids by microbial activity. Percentage of both total and reducing sugars dropped from 16.71±0.52, 4.84±0.29 to 10.18±0.62, 3.49±0.17 respectively. The pH of fresh PFP declined from 5.12±0.10 to 3.25±0.28 in spoiled PFP and acidity (%) of fresh PFP raised from 0.40±0.05 to 1.54±0.03 in spoiled PFP. TPC (mg GAE/g) of fresh PFP was decreased to 0.619±0.14 from 9.289±0.15 when it was spoiled. It was found that TPC of *V. copallifera* extract from both maceration and Soxhlet treatment (431.14±4.78 and 475.44±4.80 mg GAE/g of crude extract respectively) was higher than other plant extracts. Antimicrobial effectiveness of plant extracts were tested against microbes at concentrations of 10 mg/ml extract from both maceration and Soxhlet treatment. The highest antimicrobial effect was observed in the *V. copallifera* extracts from maceration treatment, against the microbes, *A. aceti*, *S. cerevisiae*, *S. aureus* and *E. coli* with zone of inhibition of 23, 18, 19 and 19 mm, respectively. *V. copallifera* extracts showed considerable inhibitory effect when compared with chloramphenicol (0.1mg/ml). MIC of *M. fragrans*, *C. verum*, *V. copallifera* and *A. calamus* showed higher value (< 0.2 mg/ml) against *A. aceti* and *S. aureus* compared to other plant extracts. The results indicated that these plant extracts that demonstrated effectiveness against the particular microbes could be used as natural preservatives to control the spoilage of PFP.

Keywords: Antimicrobial activity, Herbal extracts, Palmyrah fruit pulp

Abstract No: TO 9

Proximate composition of tetra-packed fresh milk in Sri Lankan Market

H. N. Disanayaka[1, 2], Sagarika Ekanayake[2*] and A. A. P. Keerthi[1]

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *Department of Biochemistry, Faculty of Medical Sciences, University of Sri Jayewardenepura, Nugegoda 10250, Sri Lanka*

**Corresponding author: sagarikae@hotmail.com*

Fresh milk is well-known for its nutritional value and is considered as a healthy food product. In Sri Lanka, fresh milk is marketed as different types and by different manufactures. The objectives of this study were to proximate the composition of different local brands of tetra-packed fresh milk in Sri Lankan market, compare and legitimate the composition as suitable to digest as per the standards. In the study high selling three different local brands (A, B, C) were selected after a market survey. The moisture content, total solid content, ash content, total carbohydrate content, fat content, titratable acidity, total solid not fat (SNF) content and pH were determined (nx5). All the methods used for analyses were either AOAC methods or standard methods. All the values were expressed as mean of five replicates on fresh weight basis and significances were calculated at 95% confidence interval. The average values for moisture and total solid content were 87.82%, 88.37%, 88.03% and 12.18%, 11.63% and 11.97% respectively for A, B and C brands. The average values for ash content were 0.65%, 0.68% and 0.61% respectively for A, B and C brands. Slight variations with respect to the manufacturers were observed for carbohydrate contents (5.50%, 5.53% and 4.01%) and fat contents (3.8%, 3.8% and 4.1%) of A, B and C brands respectively. Titratable acidity which is a measurement of lactic acid in the milk was 0.16%, 0.15% and 0.15% for A, B and C respectively. The samples had a pH of 6.40 and SNF content of 8.4%, 7.8% and 7.9% for A, B and C respectively. Among the parameters studied three brands were not significantly different from each other except for the carbohydrate content. Difference in carbohydrate level may be due to the breed of the cow or due to addition of sugar as flavor enhancers. The moisture content of Sri Lankan fresh milk products was slightly higher than most of other published values. The titratable acidity was within the range of SLSI recommendation. However, the fat content of all three brands was higher than the SLSI value with brand C having the highest fat content. Since SLSI regulations for moisture, ash and carbohydrate content are non-existent these parameters were compared with the literature values and were within the accepted level. Thus, it could be recommended to introduce regulations for these parameters for Sri Lankan milk and milk products for betterment of the fresh milk industry and for the benefit of consumers.

Keywords: Tetra-packed, fresh milk, composition

Abstract No: TO 12

Investigation of Antityrosinase and Antioxidant Activity of *Polyscias balfouriana* L. H. Bailey (Koppa Plant)

E. G. Divyanjalee Suraweera[1] and Kushan C. Weerasiri[2*]

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *The Open University of Sri Lanka, Nawala, Nugegoda 11222, Sri Lanka*

**Corresponding author: kush.weerasiri@gmail.com*

Tyrosinase is a copper-containing enzyme that catalyses different reactions in melanin synthesis. It is a key enzyme in melanin biosynthesis, involve in determining the colour of mammalian skin and hair. Hence it has gained an important role in the fields of cosmetic, food and pharmaceuticals. *Polyscias balfouriana* L. H. Bailey is a species in the family Araliaceae and native to Australia (Queensland) and Papua New Guinea and commonly cultivated in South-eastern Asia and pacific region tropical islands. The leaves of this plant were extracted using hexane, ethanol, methanol and ethyl acetate. The obtained extracts were used to determine the antityrosinase activity and the antioxidant activities. Inhibitory activity of the mushroom tyrosinase method was used to determine the antityrosinase activity. All the three samples (ethanol, methanol and ethyl acetate) showed some antityrosinase activity. The most effective activity (48% inhibition) was observed for the ethanol extract with the concentration of 0.25 mg/mL. The standard (kojic acid) showed only 22% inhibition at the same concentration. However, when the ethanol extract concentration was raised the antityrosinase activity declined. This observation was opposite to the behaviour of standard and the other methanol and ethyl acetate extracts followed a similar trend to that of ethanol. In DPPH radical scavenging activity, the highest percentage scavenging activity was shown by the ethyl acetate extract (IC_{50} = 0.895 mg/mL) compared to the other two extracts ethanol and methanol. In comparison, the standards' (BHT) activity was higher the level of the sample extracts (IC50 = 0.739 mg/mL). The reducing capacity was showed by all the sample extracts, (ethanol, methanol and ethyl acetate). Among that ethyl acetate extract showed the best reducing ability. However their reducing power was below the level of standard, ascorbic acid. So, when comparing the three extracts ethanol, methanol and ethyl acetate; ethanol showed the most effective inhibition activity at 0.25 mg/mL concentration which was greater than the standards' inhibition activity at the same concentration. The DPPH scavenging activity was shown by two extracts except the methanol extract. From that ethyl acetate extract showed the highest scavenging activity. The reducing capacity was shown by all the sample extracts and among those also ethyl acetate showed the best reducing activity. But their reducing power was below the level of the standard. Therefore, according to the results *Polyscias balfouriana* L.H.Bailey leaves show some positive antityrosinase and antioxidant activity.

Keywords: Tyrosinase, enzyme, melanin, inhibition, *Polyscias balfouriana* L.H.Bailey, antityrosinase, antioxidant

Abstract No: TO 18

Potential hypoglycemic activity of *Kaempferol rhamnoside* isolated from *Olax zeylanica* (Malla) leaves

N. G. D. Anuradha[1], S. M. D. S. Gayathri[1], Gayani Imanthika Dias[1], Thilini Chathurangi Kananke[1], Kapila Tharanga Rathnayaka[1], Rasangi Sabaragamuwa[1], R. M. U. S. K. Rathnayaka[1], Merita Nirmali Wickramaratne[2] and M. G. A. N. Perera[1]*
[1] *Faculty of Applied Sciences, Sabaragamuwa University of Sri Lanka, Belihuloya 70140, Sri Lanka*
[2] *Faculty of Medicine, Sabaragamuwa University of Sri Lanka, Rathnapura 70000, Sri Lanka,*
**Corresponding author: namalperera@appsc.sab.ac.lk*

Olax zeylanica (Olacaceae) is a green leafy vegetable endemic to Sri Lanka. The unmatured leaves have been extensively used as a vegetable by the rural population of Sri Lanka and known to have good hypoglycemic properties. However, the plant has received very little scientific attention on its medicinal values. As a part of a program to identify hypoglycemic natural products from Sri Lankan edible plants, we report herein the isolation of a kaempferol-3,7-O-alpha-L-dirhamnoside from the methanol extract of Olax zeylanica leaves and its alpha glucosidase and alpha amylase inhibitory activities. Air dried leaf powder (150 g) was sequentially extracted at room temperature with Hexane, Dichloromethane and Methanol. Crude extracts were subjected to alpha amylase (Dinitro salicylic acid method) and alpha glucosidase inhibitory (p-nitrophenyl glucopyranoside method) activities. Crude methanol extract showed significant alpha amylase and alpha glucosidase inhibitory activities, hence subjected to further investigations. Methanol extract was diluted with water and partitioned with chloroform. Upon settling, the aqueous methanol layer gave a yellow precipitate which was recrystallized by hot methanol/water mixture to give a pale greenish yellow amorphous solid (300 mg) which showed characteristic UV absorption peaks at 252 nm and 347 nm indicated the presence of flavanol skeleton. ^{1}D NMR (1H-CD3OD) signals from δ 3.38 ppm to δ 5.6 ppm, in duplicates, and 13C-CD3OD signals from δ 70 ppm to δ 110 ppm, showed the presence of two hexose units. The presence of up field ^{1}H NMR signals at 0.96 ppm and δ 1.284 ppm (J=5.6-6 Hz), and two up field ^{13}C NMR signals around δ 15 ppm indicated the presence of two rhamnosyl methyl groups. Two anomeric H signals at δ 5.41 ppm and δ 5.57 ppm (coupling constants J =1.6 Hz), and two anomeric C signals at δ 102 ppm further confirmed the presence of two alpha rhamnosyl residues. The ^{1}H NMR signals at δ 7.80 (2H, d, J =8.7 Hz) and δ 6.95 ppm (2H, d, J =8.5 Hz) precisely matched with the 1H chemical shift values of B ring protons of flavanol structure (H-2′, H-6′ and H-3′, H-5′, respectively). Two meta-coupled doublets (J =2.1 Hz) at δ 6.46 and 6.72 ppm were attributed to the C-6 and C-8 protons of A ring protons of flavanol structure. 2D-NOESY and HSQC (CD3OD) spectral data indicated that the two alpha rhamnosyl residues were attached to the 3rd and 7th positions of the flavanol skeleton. These spectral data proved the structure of the isolated compound to be the kaempferol-3,7-O-alpha-L-dirhamnoside with the molecular formula $C_{27}H_{30}O_{14}$; Molecular Mass 578.16 (Experimental m/z 577.28 [M-H]). Isolated Kaempferol-3,7-O-alpha-L-dirhamnoside showed significant alpha glucosidase inhibitory activity and alpha amylase activity with IC50 values of 84.7 ± 1.7 µM and 5.9±0.37 µM respectively (n=3). For Acarbose positive control IC_{50} values were 74.0 ±2.0 µM and 3.1±0.08 µM respectively (n=3). Chemical structure of Kaempferol-3,7-O-alpha-L-dirhamnoside from Olax zeylanica and its antioxidant activity has been previously reported. Further the same compound has been identified in Bauhinia forficate which is a widely used antidiabetic herbal remedy in Brazil and from two Legume species, *Vicia faba* and *Lotus edulis*. The findings of this study provide some scientific evidence for the ethnomedicinal use of *Olax zeylanica* as a functional food against diabetes mellitus.

Keywords: *Olax zeylanica*, Hypoglycemic activity, Kaempferol rhamnoside

Abstract No: TI 7

Biosynthesis, Characterization, Photocatalytic and Fluorescence quenching activity of Zinc Oxide nanoparticles

Kazeema Kaleem and Gobika Thiripuranathar*
College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka
**Corresponding author: tgobika@ichemc.edu.lk*

Green synthesis of nanoparticles *via* biological entities has gained significant interest as an emerging technology due to the toxicity of nanoparticles (NPs) associated with conventional chemical synthesis processes. The present study focuses on the green synthesis of zinc oxide NPs using extracts of stems and leaves of *Sauropus androgynus* and *Oxalis corniculata* plants, which are used as biological capping and stabilizing agents from zinc acetate dihydrate (metal precursor). Semi-conducting zinc oxide NPs have gained great interest in the field of medicine, micro-electronics, and in water remediation. Zinc oxide NPs were synthesized by varying reaction conditions such as volume of plant extract (1 mL, 2 mL and 5 mL) and metal precursor concentration (0.01 mol dm^{-3} – 0.02 mol dm^{-3}) at a pH of 12. The synthesized NPs were collected by centrifuging and dried at a temperature of 60 °C for 14 hours. The formation of zinc oxide NPs in the reaction mixture was determined by Ultraviolet-Visible Spectroscopy and was characterized by Scanning Electron Microscopy, and Fourier Transform Infrared spectroscopy. The SEM images reported that the average size of zinc oxide NPs synthesized at optimum conditions was in the range of 79-89 nm with spherical, hexagonal and rod-shaped. Further the photocatalytic degradation and fluorescence quenching ability of zinc oxide NPs were studied. Photocatalytic degradation activity of zinc oxide NPs was determined by the degradation of 5 ppm solution of Methylene Blue dye under the illumination of sunlight for 3.30 hours. By triplicating the experimental readings, it was determined, NPs synthesized using *Oxalis corniculata* stem extract at a concentration of 5 mg/mL exhibited the highest percentage degradation of 60% where mean absorbance of methylene blue was reduced from 1.430 to 0.5720. Synthesized zinc oxide NPs quenched the fluorescence of Rhodamine B dye at 591 nm with increasing concentration. Intensity of Rhodamine B dye of concentration 5×10^{-4} mol/dm^{-3} (4160 a.u), decreased with increasing NPs concentration from 50 µg/mL to 1000 µg/mL. The highest fluorescence quenching of 71% was shown by Zinc oxide NPs synthesized with extracts of Sauropus androgyus leaves where intensity of Rhodamine B dye was reduced from 4160 a.u. to 1194 a.u. Hence synthesis of zinc oxide nanoparticles using biological entities is a novel and potential alternative to chemically synthesized nanoparticles.

Keywords: ZnO NPs, fluorescence resonance energy transfer, photocatalytic, Green synthesis

Abstract No: TI 8

Morphological and photocatalytic properties of zinc oxide nanoparticles synthesized from agricultural wastes of *Nephelium lappaceum* L. and *Garcinia mangostan* L.

K. A. S. S. Kuruppu, K. M. K. G. Perera, A. M. R. Chamara and G. Thiripuranathar*
College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka
**Corresponding author: tgobika@ichemc.edu.lk*

A facile, innovative and ecofriendly approach of biofabrication of zinc oxide nanoparticles (ZnO–NPs) using agricultural wastes (seed and peel) of N*ephelium lappaceum* L. and *Garcinia mangostana* L. have been demonstrated in this study. Characterizations of ZnO–NPs were carried out using Ultraviolet-Visible (UV–vis) spectrophotometry, Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Energy Dispersive spectroscopy (EDX), and Fourier Transform Infrared spectroscopy (FTIR). The formation of ZnO-NPs was preliminary confirmed by the UV–vis spectroscopy, by the appearance of peaks between 362–368 nm. The SEM and TEM images show flower and rod-like arrangements of nanocrystals. As per the TEM images, all the synthesized ZnO-NPs showed the particle size ranging from 29-334 nm. FTIR spectral analysis demonstrated peaks at 3269–3500 cm^{-1}, 2308–2361 cm^{-1}, 2103–2110 cm^{-1} and 1630–1640 cm^{-1}, 586–632 cm^{-1} for the plant extracts, whereas an additional peak appeared within the range of 458–499 cm^{-1} in synthesized ZnO–NPs. The degradation efficiency of ZnO–NPs was measured by the study of photo degradation of Methylene Blue and the results of ZnO–NPs synthesized via seed extract of *N. lappaceum* demonstrated the highest activity among all the synthesized NPs with a half-life of 78 min with 97% degradation efficiency at 150 min time frame.

Keywords: ZnO-NPs, biofabrication, degradation

Abstract No: TI 10

In silico identification of natural product inhibitors of HMG-CoA reductase

Archchana Ganeshalingam[1] and Chinthaka N. Ratnaweera[2*]

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *Department of Chemistry, Faculty of Science, University of Ruhuna, Matara 81000, Sri Lanka*

**Corresponding author: nadun@chem.ruh.ac.lk*

Coronary heart diseases such as hypercholesterolemia along with cancer and AIDS are the most studied diseases in the world. Inhibition of 3-hydroxy-3-methylglutaryl-coenzyme A reductase (HMG CoA reductase) which is the rate determining enzyme in the cholesterol synthesizing mevalonate pathway has been proven to control serum cholesterol levels. At present, statins have been extensively used as a medication to lower the serum cholesterol level. They have HMG CoA like moiety hence act as competitive reversible inhibitors. It has been found that the use of statins results in certain side effects. Since hypercholesterolemia is a chronic condition needing lifelong therapy, the use of natural product-based drugs can be more beneficial. Therefore, in this study, natural product compounds isolated from various plants that are used as drugs for hypercholesterolemia in ayurvedic medicine have been investigated for their inhibitor activity against the enzyme applying molecular docking and molecular dynamics. HMG CoA reductase is a tightly associated tetramer with a bipartite active site. The crystal structure of HMG CoA reductase (PDB ID: 3CCZ) was retrieved from the RCSB PDB database. For the initial model, only chains A and B were retained while the remaining chains and all other non-standard residues were removed using Chimera. The stability of the model was investigated through a 100 ns molecular dynamic simulation. Subsequently, selected compounds were docked to the enzyme using the Autodock Vina algorithm in PyRx software. Several commercially available statins were considered as references. The complex with the highest negative binding affinity was studied with a 100 ns molecular dynamic simulation. Results revealed that reference molecules showed binding affinities ranging from -6.4 to -8.2 kcal/mol. Several natural product ligands show comparable binding affinities (>7.0 kcal/mol) to the references and show drug likeliness. Coclaurine emerge as a promising candidate for further studies making a stable complex, stabilized after 25 ns from the start of the simulation with the highest negative binding affinity of -7.6 kcal/mol with two significant hydrogen bonds and showing drug likeliness.

Keywords: Hypercholesterolemia, Natural product inhibitors, *in-silico* study

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Abstract No: TI 11

A Computational Study of Cyclin-dependent Kinases 1 (CDK1) butyrolactone I complex and the Role of Mg Ion in the Active Site

Chanikya D. Jayawardana[1] and Chinthaka N. Ratnaweera[2*]

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *Department of Chemistry, Faculty of Science, University of Ruhuna, Matara 81000, Sri Lanka*

**Corresponding author: nadun@chem.ruh.ac.lk*

Cyclin-dependent kinases (CDK) 1, 2, 4, and 6 are the protein kinases that play a pivotal role in the cell cycle regulating of all eukaryotic organisms by phosphorylating proteins needed during the cell division cycle. Phosphorylation of protein kinase requires the assistance of a divalent metal ion, usually Mg^{2+} ion to facilitate the transfer of a phosphate group onto a particular residue (serine, threonine, or tyrosine) in a substrate. However, only CDK1 is required for the successful completion of the M-phase of the cell cycle. Therefore, inhibition of CDK1 is emerging as a drugable target for diseases caused by unregulated cell proliferation. Butyrolactone I is a

natural product with certain bioactivities that have been isolated from the endophytic fungus *Aspergillus terreus*. Experimental studies have revealed that butyrolactone I inhibits the activities of both CDK1 and CDK2. However, its inhibitory mechanism and the role of Mg^{2+} ion remain uninvestigated. In this study, the effect of butyrolactone I on the CDK1-cyclin B complex in the presence and absence of Mg^{2+} ion in the active site was evaluated by applying a computational methodology. The currently available CDK1 crystal structures do not contain any Mg^{2+} ion, therefore, our first step was to position the Mg^{2+} ion in the CDK1 crystal structure (PDB ID:5HQ0) based on the structural information of CDK2 (PDB ID:1HCK). The stability of the two models (with Mg^{2+}and without Mg^{2+}) were investigated by conducting a 200 ns molecular dynamics simulation. The root mean square deviation (RMSD) of the structures with respective to the starting structures were almost stable during the last 100 ns. Subsequently, butyrolactone I was docked into the active site of both models using Autodock Vina, and further molecular dynamic simulation of 200 ns was conducted for the best docking poses of each complex. Stable RMSD values indicated the stability of protein-ligand complex. MM-GBSA binding free energy calculations were conducted to further assess the stability of the complexes. Accordingly, the butyrolactone I CDK1 complex was more favorable in the absence of Mg^{2+} ion (ΔG = -25.50 kcal/mol) than its presence (ΔG = -19.2 kcal/mol).

Keywords: CDK1, Mg^{2+} ion, Butyrolactone I, Computational chemistry

Abstract No: TI 23

A study on complexation, stoichiometry and binding of selected anionic organic pollutants and protonated polyaza macrocycles

Danushka M. Kumarasinghe and Isurika R. Fernando*
Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura,
Nugegoda 10250, Sri Lanka
**Corresponding author: isurika.fernando@sjp.ac.lk*

Anionic organic pollutants (AOPs) generated by industrial and laboratory processors are accumulated in the environment while causing health problems for human beings. Therefore, this research project is focused on a fundamental study of the removal of three selected AOPs, namely dianions of hydroquinone, catechol and resorcinol from the environment using a supramolecular approach. Two electron deficient, PPAMs, namely PPAM1 and PPAM2 with different cavity sizes and shapes were synthesized by using a 1:1 molar mixture of diethylenetriamine along with a dialdehyde, terephthalaldehyde and isophthalaldehyde separately as starting materials by carrying out an imine metathesis, a reduction with sodium borohydride followed by a protonation with perchloric acid in order to obtain aqueous medium soluble macrocycle. After characterization of the PPAM1 and PPAM2 using spectroscopic techniques, the complexation is driven by ionic interactions between hexa-cationic PPAMs and dianionic AOPs in an aqueous solution was characterized by UV-visible spectroscopy and fluorescence spectroscopy. Stoichiometry and the binding constant between each PPAM with dianions of hydroquinone, resorcinol and catechol were determined using fluorescence spectroscopy by employing the Job's plot method and dilution method, respectively. The Job's plots of each PPAM and AOP used in this study demonstrated 1:2 stoichiometry between the PPAM and AOP indicating a partial displacement of the counter ion of the macrocycles. Binding constants between PPAMs and AOPs were calculated using the Benesi – Hildebrand equation. Among the three AOPs used in this study, dianions of hydroquinone exhibited the highest binding constants of 2.85×10^{6} mol^{-2}dm^{6} and 2.58×10^{6} mol^{-2}dm^{6} with PPAM1 and with PPAM2, respectively. The dianions of resorcinol exhibited the lowest binding constant of 8.21×10^{5} mol^{-2}dm^{6} and 8.12×10^{5} mol^{-2}dm^{6} for PPAM1 and PPAM2, respectively. In conclusion, fluorescence spectroscopy evidenced the complexation between PPAMs and AOPs. The cavity size and shape of the PPAM as well as the position of the dianions in AOPs

determined the binding constant.

Keywords: Anionic organic pollutants, Protonated polyaza macrocycles, Job's plot, Binding Constant, Benesi – Hildebrand method

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Abstract No: TA 13

Removal of Selected Textile Dyes from Effluent Water Using Mineral Adsorbents and Activated Carbon

Y. K. G. D. Sanaree, S. Nishadya, G. W. C. S. Perera and U. S. K. Weliwegamage*
College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka
**Corresponding author: weliwegama@yahoo.com*

Removal ability of the textile dyes, Methylene Blue, Rodamine B and Congo Red from water was investigated in this study. Static experiments were conducted using each dye with selected adsorbents, Kabok, Brick Clay, Granite Chips and activated carbon. In each experiment, 1.00 g of adsorbent was treated with 25.00 cm^3 of 2.6 x 10^{-5} mol dm^{-3} dye solutions. Absorbances of each solution were measured at their respective λ_{max} values at a time duration of 0 - 240 min and their average values are reported. The continuous flow experiments were carried out with best adsorbent for each dye identified by static experiments, using 2.6 x 10^{-5} mol dm^{-3} dye solutions. The flow rate of the column was kept as 10 mL/min. The experiment was conducted for 120 minutes.According to the static experiment results, the natural adsorbents, Kabok and Brick Clay showed the best percentage removal of Methylene Blue with 98.8% and 95.7% which was better compared with activated carbon, 83.3%. In contrast, Rodamine B was best removed by activated carbon with percentage removal of 82.5%. Among the inorganic mineral adsorbents, Brick Clay showed a percent removal of 64.1% for Rodamine B. Congo red was best removed by Brick Clay with 96.6% efficiency compared to 43.4% removal of activated carbon.The breakthrough curves of the continuous flow experiments show the potential of removing congo red and methylene blue using Brick Clay and Kabok respectively.

Keywords: Mineral adsorbents, wastewater, methylene blue, absorption

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Abstract No: TA 14

Effect of biochar application on plant uptake of sulfamethoxazole in soil

Y. S. Keerthanan and Meththika Vithanage*
Department of Chemistry, Faculty of Applied Sciences, University of Sri Jayewardenepura,
Nugegoda, 10250, Sri Lanka
**Corresponding author: meththika@sjp.ac.lk*

The purpose of this study was to assess the effect of cinnamon wood biochar (CWBC) in minimizing the plant uptake of sulfamethoxazole (SUL) from the contaminated soil. For this purpose, *Ipomoea aquatica* was grown in soil and 2.5% w/w CWBC amendment contaminated with 50 mg/kg of SUL for 4 weeks. The results suggest that the root uptake of SUL relatively higher than by shoot. The plant uptake of SUL was significantly reduced by 60% when 2.5% w/w of CWBC was added to the soil. The bioaccumulation factor of SUL in *Ipomoea aquatica* grown in soil was 158.38. This was decreased by 76% with the addition of 2.5% of CWBC to the soil. In contrast to the controlled experiment, the retention of SUL in CWBC amendment was increased by 65%. The present study suggested that the application of CWBC to the agricultural soil effectively decreased the plant uptake while increased SUL retention in soil. Thus, the application of biochar to the soil limits human exposure of SUL *via* food crops.

Keywords: Pharmaceutical and personal care products, biochar, immobilization, plant uptake

Abstract No: TA 19

Evaluation and correlation of the influence of production parameters on biochar characteristics and its influence on the adsorption of three industrial dyes

Dineth Saumya[1], Chathuri Peiris[1], Sachith P. Abeysundara[2] and Sameera R. Gunatilake[1]*

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *Department of Statistics and Computer Science, Faculty of Science, University of Peradeniya, Peradeniya 20400, Sri Lanka.*

**Corresponding author: ranmal@ichemc.edu.lk*

Remediation of waste water containing hazardous dyes using biochar (BC), as an adsorption technique, is a cost effective and efficient method. As a statistical approach, this study was focused on how feedstocks, pyrolysis temperature, production method and modification affect to the physiochemical properties of BC and how these properties affect to the adsorption of methylene blue (MB), crystal violet (CV) and rhodamine B (RB) from aqueous medium. Since there was no studies have been conducted to evaluate and correlate its specific impact on the adsorption of these cationic dyes, utilized approximately 151 peer-reviewed articles with 240 entries from years 2015 to 2020, to predict reasonably the influence of these physiochemical properties quantitatively to dye adsorption with the aid of statistical correlation and regression meta-analysis using the R programming language in RStudio, to help to understand the factors and characteristics used to produce BC commercially fulfilling the necessity of industrial applications. Pore volume and surface area of BC produced by plant-based materials had significant ($p \leq 0.05$) positive correlations, $r = 0.22$ and $r = 0.17$ with pyrolysis temperature respectively whereas, at low temperatures (250-450 °C), they were enhanced by basic modifications. The stability was seen to be greater in basic modified wood-based BCs, pyrolyzed at medium to high temperature which was confirmed by the statistically specified regions of Van-Krevelen diagrams. Maximum adsorption capacity of BC in MB adsorption had a higher variability on plant-based materials which were modified by acids and metal salts produced at high temperatures whereas CV had a higher variability on animal-based materials. In RB adsorption, BC made up by plant-based materials which modified mostly using bases, at low pyrolysis temperatures (250 °C - 450 °C) had a higher variability. Pseudo-second-order kinetics and Langmuir isotherm models were fitted for the adsorption of these three dyes. MB and CV were most adsorptive at neutral to high pHs (6-10) whereas RB it was low to neutral (1-9), Therefore, this data collected could be used to improve the effectiveness of cationic dye removal from wastewater, considering pyrolysis conditions and useful physiochemical properties of specific BC types.

Keywords: Biochar, Methylene blue, Crystal violet, Rhodamine B, Modifications, Van-Krevelen diagrams, meta- analysis

Abstract No: TA 20

Correlation and the Impact of Feedstock Type and Production Conditions on Heavy Metal Adsorption by Biochar: A Comprehensive Meta-Analysis

Vindya Samarakoon[1], Chathuri Peiris[1], Sachith P. Abeysundara[2] and Sameera R. Gunatilake[1]*
[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*
[2] *Department of Statistics and Computer Science, Faculty of Science, University of Peradeniya, Peradeniya 20400, Sri Lanka.*
**Corresponding author: ranmal@ichemc.edu.lk*

Biochar (BC) is a ubiquitous, porous, carbonaceous solid produced by the pyrolysis of biomass under anaerobic conditions, which can be used as a fuel as well as an adsorbent. Although the potential use of biochar in aqueous systems to adsorb heavy metals has gained attention recently, no studies have been conducted to evaluate and correlate its specific impact on the adsorption of Cu^{2+}, Cd^{2+} and Pb^{2+} metal cations. In this study, the correlation between pyrolysis temperature, pyrolysis method, feedstock type, modifications applied, and physiochemical properties of BC and their statistical significances were evaluated considering the adsorption of Cu^{2+}, Cd^{2+} and Pb^{2+} metal cations. For the statistical analysis, over 500 individual data entries were extracted from 172 peer-reviewed articles that were published in the years 2014 to 2018, and the correlation studies were done using the R programming language in RStudio. Biochar used in the adsorption of Cu^{2+}, Cd^{2+} and Pb^{2+} exhibited moderate positive correlations with specific surface area and pyrolysis temperature ($r_{Cu}= 0.47$, $r_{Cd} = 0.37$ and $r_{Pb} = 0.49$) whereas pore size and ash content exhibited negative or negligible correlations. Both aromaticity ($r_{Cu}= -0.48$, $r_{Cd} = -0.53$ and $r_{Pb} = -0.34$) and polarity ($r_{Cu}= -0.33$, $r_{Cd} = -0.37$ and $r_{Pb} = -0.51$) were negatively correlated with pyrolysis temperature for all three metal cations. The maximum sorption capacity (MSC) and pyrolysis temperature showed a statistically significant, weak positive correlation ($r=0.26$, $p \leq 0.05$) for Cu^{2+} adsorption, whereas for both Cd^{2+} and Pb^{2+} it was found to be negligible ($r_{Cd} = -0.02$, $r_{Pb} = 0.08$). Pyrolysis method did not show any statistically significant relationship for MSC with Cu^{2+} and Cd^{2+} ($p \geq 0.05$) but it was statistically significant for MSC with Pb^{2+} ($p=0.01$). Sludge based BC showed the highest variability for MSC with Cu^{2+} and Pb^{2+} whereas fungi based BC exhibited the highest variability for MSC with Cd^{2+}. Magnetized, oxidized and base modified BC showed the highest variability for MSC with Cu^{2+}, Cd^{2+} and Pb^{2+} respectively. Therefore, an insight was gained on what factors should be considered when selecting pyrolysis conditions and feedstock types, in order to produce BC with useful physiochemical properties that will specifically aid in the adsorption of Cu^{2+}, Cd^{2+} and Pb^{2+} metal cations from aqueous systems.

Keywords: Biochar, Heavy metals, Pyrolysis conditions, Feedstock type, Meta-analysis, Physiochemical properties

Abstract No: TA 21

Influence of feedstock and production conditions on characteristics of biochar and its correlation for the adsorption of oxyanions: A Comprehensive meta-analysis

Lilogini Sutherson[1], Chathuri Peiris[1], Sachith P. Abeysundara[2] and Sameera R. Gunatilake[1]*

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *Department of Statistics and Computer Science, Faculty of Science, University of Peradeniya, Peradeniya 20400, Sri Lanka.*

**Corresponding author: ranmal@ichemc.edu.lk*

Water contamination by oxyanions can be considered as a major environment problem. Biochar (BC) is a carbon rich porous material produced *via* biomass pyrolysis under limited oxygen condition. Biochar has been widely used in remediating both inorganic and organic compounds including anionic compounds. Much research has been carried out to study the effects of feedstock type (FT), modification type (MT) and pyrolysis temperature (PT) on the properties of biochar. However, correlation to BC characteristic in the removal of specific anionic adsorbates are lacking. Thus, this work helps researchers to get a quantitative approach to predict the relationship between BC precreation parameters and the final BC properties to specifically remove anionic contaminants such as nitrate (NO_3^-), phosphate (PO_4^{3-}), chromate ($Cr_2O_7^{2-}$), and arsenate (AsO_4^{3-}). 283 individual data points from 129 peer reviewed articles were extracted. Data were characterized, FT as algae, plant, animal, sludge and wood, MT as acid, base, magnetic and metal impregnation, PT ranges were categorized in to 5 main ranges to perform the meta-analysis using R-Statistical software. Based on the analysis, with increasing PT, specific surface area (SSA), biochar pH, ash content increase whereas O%, H%, N%, H/C and O/C decrease. Wood based BC generally showed a greater carbon content. Pyrolysis temperature range between 451-650 °C and wood-based BC gave a high stabilize BC. Generally metal impregnation modification results a better sorption ability to adsorb anionic contaminants. Higher SSA of BC might facilitate the adsorption ability. Optimum SSA observed for NO_3^-, PO_4^{3-}, $Cr_2O_7^{2-}$, AsO_4^{3-} respectively for plant, algae, sludge, and wood type biochar. Finding of this study will help future researchers to choose the better FT and production conditions to remove specific anionic compounds from aqueous medium.

Keywords: Biochar, Meta-analysis, Anionic contaminants, Adsorption.

Abstract No: TA 22

A chemometric study on the effect of feedstock choice and pyrolysis conditions on biochar production and its influence on the remediation of pharmaceuticals from aqueous solutions

Sachin Fernando[1], Chathuri Peiris[1], Sachith P. Abeysundara[2] and Sameera R. Gunatilake[1]*

[1] *College of Chemical Sciences, Institute of Chemistry Ceylon, Rajagiriya 10107, Sri Lanka*

[2] *Department of Statistics and Computer Science, Faculty of Science, University of Peradeniya, Peradeniya 20400, Sri Lanka.*

**Corresponding author: ranmal@ichemc.edu.lk*

Removal of antibiotics and non-steroidal anti-inflammatory drugs (NSAIDs) from aqueous ecosystem is a serious concern due to their extensive usage and resulting the adverse effects on human and ecological health. Biochar (BC) is a ubiquitous carbonaceous adsorbent which is an excellent promising adsorbent for removal of antibiotics and NSAIDs such as tetracycline (TC), sulfonamides (SA), ibuprofen (IBP), and diclofenac (DF) due to their unique surface functionality and porosity. Discriminant analysis of approximately 380 data sets based on 151 peer-reviewed articles, in this study we elucidated the choice of feedstock category, pyrolysis temperature, and modification type that influence the physiochemical properties of BC. Through meta-analysis, it was found that with increasing pyrolysis temperature, the BC physiochemical properties such as specific surface area (SSA), carbon (C) content, aromaticity and BC stability increased, whereas hydrogen content, oxygen content, and polarity decreased. Additionally, wood-based feedstock and pyrolysis temperature of 651-850 ^{o}C, was found to be the optimum conditions to obtain a BC with greater SSA, C content, and stability. Furthermore, with increasing SSA and pore volume of biochar led to greater adsorption capacities of TC, SA, IBP, and DF. It appears that highest maximum adsorption capacity shows by animal & algae-based BC, and acid modified BC for TC; wood-based BC and magnetized BC for SA; sludge-based BC and base modified BC for IBP; sludge-based BC and magnetized BC for DF. Overall, 651-850 ^{o}C TR has the highest maximum adsorption capacity for all four antibiotics and NSAIDs. These predicted relationships can link biochar production to help make more well-developed biochar choices to enhance performance in remediation of given antibiotics and NSAIDs or similar molecules.

Keywords: biochar; meta-analysis; feedstock; antibiotics; physiochemical properties.

WCC Session at the 50th Annual sessions

Date: 29th June 2021 Time: 3.00 – 5.00 pm

Theme: Gender Equity and Women Empowerment

3.00 – 3.15 pm	Welcome Address **Prof. Priyani Paranagama** *Chair of Chemistry, University of Kelaniya and* *Director, Institute of Indigenous Medicine, University of Colombo & Chairperson, WCC*
3.15 - 3.20 pm	Introduction of Dr.Vicki Gardiner, President of the Federation of Commonwealth Chemistry **Prof. Chayanika Padumadasa** *Senior Professor, Department of Chemistry, University of Sri Jayewardenepura*
3.20 – 3.40 pm	Plenary Speech Empowering diversity in science through gender equality **Dr. Vicki Gardiner** *President, Commonwealth Chemistry*
3.40 – 3.45 pm	Introduction of Dr. Irosha Nawarathne **Dr. Ireshika De Silva** *Senior Lecturer, Department of Chemistry, University of Colombo*
3.45-4.05 pm	Plenary Speech Actions Vs Words to Liberate Women Chemists **Dr. Irosha Nawarathne** *Associate Professor in Chemistry, Lyon College, Arkansas, USA*
4.05- 4.10 pm	Introduction of Prof. Ayanthi N. Navaratne **Dr. Gobika Thiripuranathar** *Head of Department, College of Chemical Sciences, Institute of Chemistry Ceylon*
4.10-4.30 pm	Plenary Speech Contributing factors for empowerment of women chemists in Sri Lanka **Prof. Ayanthi N. Navaratne** *Senior Professor, Department of Chemistry, University of Peradeniya*
4.30-4.35 pm	Introduction of Ms. Chamari Wickramathilake **Dr. Medha Gunaratna** *Senior Lecturer, Department of Chemistry, University of Kelaniya*
4.35-4.55 pm	Plenary Speech Achieving gender equality and empowerment of women chemists **Ms. Chamari Wickramathilake** *Head of Exports & Regulatory Affairs, Link Naturals (Pvt) Ltd*
4.55 – 5.00 pm	Vote of Thanks **Dr. Dinusha Udukala** *Senior Lecturer, College of Chemical Sciences, Institute of Chemistry Ceylon & Secretary, WCC*

WCC Session - " Gender Equity and Women Empowerment"

Plenary Speech

Empowering diversity in science through gender equality

Vicki Gardiner
Commonwealth Chemistry

I am the first generation of my family to attend higher education. I am the mother of twin girls who are about to finish high school and start their life long learning careers. I was trained as a chemist. And I am passionate about the importance of education as an enabler, and, in particular, the role and inclusion of women in science, industry and our community.

Women make up 51% of the population yet are under-represented in science, engineering, technology and mathematics workforces. In Australia, only 16% of the STEM skilled workforce are women. So why is this the case and what can be done? But how can we also address gender equality as a scientific community?

This presentation will explore second generation gender bias from a Western perspective – how do we address this bias as society, leaders, teachers and parent. It will also introduce Commonwealth Chemistry, which is the Federation of Commonwealth Chemical Sciences Societies, and the role it is playing in contributing to the UN Sustainable Development Goals, in particular reducing inequality within and among countries in chemistry.

The Commonwealth is a uniquely diverse group of nations with shared values and a powerful voice. It represents all corners of the globe with a population of 2.4 billion and includes both advanced economies and developing countries. It is also home to 12 per cent of the world's researchers. Bound together in the spirit of the Commonwealth, Commonwealth Chemistry champions equal opportunity for all, drives innovation and promotes excellence in the chemical sciences for the benefit of the Commonwealth nations and their people.

One community, one voice, catalysing equality for all.

***Dr. Gardiner** graduated with a BSc (Hons) in Chemistry from the University of New England, Australia and obtained her PhD in Synthetic Chemistry from Monash University, Australia. She also attained a Graduate Certificate in Management, specialising in Project Management, from the University of New England. She held Post-Doctoral positions at both the University of Southampton and University of New South Wales, and was an Australian Research Council (ARC) Post-Doctoral Fellow and lecturer at the University of Tasmania. She has also served at AusIndustry (Department of Innovation, Industry, Science and Research), Marinova, a biotechnology company, and Engineers Australia-Tasmania Division. Dr. Gardiner has served as the President of the Royal Australian Chemical Institute, and is currently serving as the President of Commonwealth Chemistry.*

Actions Vs Words to Liberate Women Chemists

Irosha N. Nawarathne

Natural Sciences Division, Lyon College, Arkansas, USA

Despite nationwide initiatives to improve the retention of women and minorities in the sciences and engineering, the percentage of female graduate students in chemistry is at 40.9% and the percentage of female postdoctoral fellows is at 25.5% in 2019; furthermore the percentage of female chemists employed by the federal government has decreased by 4% from 2008 to 2017 in the United States. The gender inequality in science is an urgent issue; therefore, making progress empowering women in science is opportune. As pandemic took over the world, the motherhood penalty on female professionals in the sciences including chemistry has become even more prominent issue due to new norm of working remotely while you take care of your young children. This seemingly impact gender equality in the field as the productivity gap between a mother and their male/childless peers become increasingly larger allowing pandemic to reverse advances and further deepen the gender gap in science.

What actions can be taken by any established female chemist to support a peer and/or an emerging female chemist with the ambition to overcome the gender inequality in the field? Several recent communications have discussed the impact of following actions to increase the diversity in the workforce in chemistry and engineering fields: actively promote, advocate for, intentionally hire, support, and mentor the female students, faculty, and co-workers; speak up and amplify the voice against discriminatory words and actions; educate yourself and co-workers on systematic and insidious bias in the science; promote hiring merely based on merit; purposefully act from the editorial level to improve the representation and highlight the accomplishments of female chemists in scientific journals. The immediate and long-term consequences of aforementioned actions will liberate women to achieve more while advancing the field of chemistry. Educators also have the immense opportunity and responsibility to create an inclusive classroom that accepts all levels of diversity will ensure the full learning experience for all types of students and also facilitate the retention of more women and minorities in the sciences and engineering. Even an educator in the physical sciences can find ways to introduce the importance of human diversity to the advancement of society using an obvious (natural) connection to the class material so that the students get a novel yet effective perspective of diversity, which in turn gradually creates an inclusive classroom that nurtures all gender types equally, as the members of the classroom identify the importance of classroom diversity to the advancement of their microcommunity. With these critical goals in mind, an inclusive environment was promoted in an organic chemistry classroom by identifying and utilizing a natural point of entry in organic chemistry to emphasize the concepts of diversity and inclusion with the interest of promoting women representation in the field of chemistry. One simple action to empower women in the field is worth a thousand words!

Dr. Nawarathne *earned her BSc in Chemistry with First Class Honors from University of Colombo, Sri Lanka and her PhD in bioorganic chemistry from Michigan State University, USA. She joined the College of Pharmacy at University of Michigan in Ann Arbor, USA as a research fellow, where her research focused on antibiotic development. Her research interests include development of efficacious therapeutics from large natural product scaffolds, with proven biomedical applications, through targeted synthesis. She currently serves as an Associate Professor in Chemistry at Lyon College, Arkansas, USA.*

Contributing factors for empowerment of women chemists in Sri Lanka

Ayanthi N. Navaratne

Department of Chemistry, Faculty of Science, University of Peradeniya

Prior to considering the empowerment of women chemists in Sri Lanka, it is essential to look back to the Sri Lankan education system. From the sixteenth to nineteenth century, Sri Lanka was under the colonial ruling, and hence, all the state affairs as well as the education was conducted in English, even after British ruling. Under the circumstances prevailing that time, learning in English was limited to the children of rich and educated parents. During the post-colonial, local government ruling, Dr. Kannangara, then the Minister of Education, had expressed his opinion about inequality of education, which dealt with education in relation to the fairness, equality and impartiality of its distribution at all levels of educational sectors. As a result of this concept, Dr. Kannangara wanted to narrow down the gap between the rich and the poor. Consequently, he put forward the concept of establishing Central Schools (Madya Maha Vidyalaya), and ultimately this led to the free education. In his educational reforms, a special attention was given in the "Girls" education. In a democratic society, the aim of education is to help every boy and girl to achieve the highest degree of physical, mental and moral development. This is the equity of education. It is particularly important that girls should receive a good education because they will be the mothers of the next generation. It is also necessary to ensure that the school influences the buildup of character, and development of culture of a girl which is to be blended with home environment.

Sri Lanka has a universal healthcare system that extends free healthcare to all citizens, and is a national priority. It scores higher than the regional (South Asia) average in healthcare having high life expectancy and a lower maternal and infant mortality than its neighbors. Contribution of the current education and healthcare system have paved the way toward empowerment of women in Sri Lanka in comparison to the other countries in the South Asia region.

The Institute of Chemistry Ceylon is the successor to the Chemical Society of Ceylon (1941), and was established in the year 1971 for the general advancement of the science and practice of chemistry. It is the oldest such body in any branch of the basic sciences in Sri Lanka and is responsible for the maintenance and development of the profession of Chemistry. It is generally accepted that Chemistry is one of the hardest subjects to learn as well as to teach, and it was thought initially that Chemistry was an academic discipline of men. However, with time it was changed and a fair number of women chemists have evolved and, in some places, women chemists outnumber men. While the free education with equity and equality gained through reforms of the father of free education, late Dr. Kannangara, factors like local and worldwide opportunities for chemistry field, availability of role models of female chemists, encouragement of women to enter into chemistry by various organizations are the other contributing factors.

Prof. Navaratne *obtained her B.Sc. (Hon) degree in Chemistry from the University of Peradeniya and pursued her graduate studies in Chemistry at the Department of Chemistry, University of Hawaii at Manoa, Honolulu, USA, where she obtained her MS degree in Inorganic Chemistry (Bioinorganic Chemistry) and PhD in Analytical Chemistry (Bioelectroanalytical Chemistry). She has served as a Senior Lecturer of the Department of Chemistry at University of Kelaniya, and University of Peradeniya where she also served as the Head of the Department and was instrumental in the establishment of the Department of Environmental and Industrial Sciences. Prof. Navaratne has about 50 research publications in peer reviewed journals and 100 communications to credit her research, and is the recipient of many prestigious awards. Her current research interests include pesticide analysis and their fate in the environment, biosensors and development of novel food products. She is currently serving as a Senior Professor in Chemistry at the Department of Chemistry, Faculty of Science, University of Peradeniya.*

Achieving gender equality and empowerment of women chemists

Chamari Wickramathilake
Link Natural Products (Pvt.) Ltd

Gender equity or fairness of treatment for women and men, according to their respective needs is vital for achieving gender equality which is a global priority today. Women and girls represent half of the world's population and they represent half of world's human potential. Therefore, the empowerment of women and girls is essential to achieve economic, social and environmental sustainability. Achieving gender equality is among the 17 Sustainable Development Goals of the United Nations that has been identified as essential for achieving a better and more sustainable future for all. The world's advancement and sustainability hinges on continuous development in science. Women's contribution to science will be a pivotal part of development and sustainability.

Globally as well as in Sri Lanka, there has been progress in women empowerment in chemical sciences over the last few decades. There has been a tremendous progress in female enrollment in Chemistry education is Sri Lanka. In many instances, the vast majority of chemistry graduates are female. However, women representation in senior positions in chemical sciences is still far below parity. Even the talented women who have chosen their careers in science are not progressing to senior positions. Therefore, the participation of women in high level decision and policy making is weak. The empowerment of women who are already in the field of chemical sciences is vital for Sri Lanka to achieve the real meaning of gender parity.

When I reflect on my 17-year career in the private sector, I experienced many challenges as a woman. However, I was able to face and overcome those challenges and progress in my career to a senior leadership position. In my opinion, many women have the knowledge and skills to become leaders in their field. What I see as lacking, is the mental resilience and the perseverance to cope with the external pressures they face. Biological and socio-cultural conditioning may play a role in focusing more on the soft and emotionally sensitive nature of women.

To achieve a remarkable progress in women empowerment, the whole of society should be conscious about socio-cultural aspects that hinder the progress of females in some way. Every member in the family and the society has a role to play in achieving gender equality. It is important to develop the ability to persevere and the personality and self-confidence of young girls within the family, which will lay a foundation for them to develop themselves in future as successful women.

Mental resilience will pave the way to overcome many barriers that exist for women to get equal opportunities. Females hold disproportionate responsibilities in parenting and caring. Globally women spent three time as many hours in unpaid domestic work and care giving as men. Time has come to hold shared responsibilities in parenting and caring within the family.

What I see as most relevant for Sri Lanka today is the need of developing women in chemistry into leadership positions within academia and the industry. This will surely need some strategic initiatives. Areas such as personality development in primary and secondary education, mentoring and coaching as part of career development programs and implementation of best practices would essentially benefit women, helping them to live upto their full potential.

Ms. Wickramathilake *obtained her B.Sc. in Pharmacy from the University of Colombo and completed her MBA at the Postgraduate Institute of Management, University of Sri Jayawardenepura. She currently serves as the Head of Exports & Regulatory Affairs at Link Natural Products (Pvt.) Ltd.*

Aromaticity and Reactions of Aromatic Molecules/Ions

K. Sarath D. Perera

Senior Professor in Chemistry, Department of Chemistry, The Open University of Sri Lanka

Fully conjugated (**FC**) and unsaturated ring systems are known as aromatic compounds. Aromaticity is a chemical property that determines the stability of **cyclic** molecules. Basically, there are three structural features that determine the aromaticity of a compound.

1. *The ring system should be* ***fully planar****.*

Fully planar (**FP**) cyclic compounds are those, in which all the atoms are *sp*^{2} hybridized and exhibit trigonal planar geometry around each atom.

2. *Ring system should be* ***fully conjugated****.*

A conjugated cyclic structure possesses a **delocalized** electron cloud formed due to the overlap of *p*-orbitals on each carbon atom in the carbocycle, which are perpendicular to the ring.

3. *Ring system should obey the* ***Hűckel rule****.*

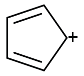
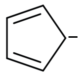
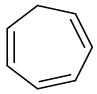
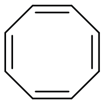
When a cyclic planar molecule has (**4n+2**) number of π-electrons, where n is an integer that compound is known to be aromatic. According to this rule, cyclic unsaturated planar systems with **2**, **6**, **10**, **14** or **18** π electrons are said to be aromatic.

Aromatic, anti-aromatic and non-aromatic molecules

A molecule is said to be **aromatic** (**A**) if it satisfies all three rules. An **anti-aromatic** (**AA**) molecule is a cyclic planar conjugated molecule that does not satisfy the Hűckel rule. Molecules which do not satisfy any of the three rules are called **non-aromatic** (**NA**).

Some examples for (**A**), (**AA**), and (**NA**) compounds are given below.

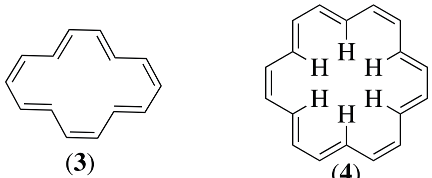
NP = Non-planar, **NC** = Non-conjugated

Compound	Property
 $(C_3H_3)^+$	FP, FC, A (2e)
 (C_4H_4)	FP, FC, AA (4e)
 $(C_5H_5)^+$	FP, FC, AA (4e)
 $(C_5H_5)^-$	FP, FC, A (6e)
Benzene (C_6H_6)	FP, FC, A (6e)
Naphthalene $(C_{10}H_8)$	FP, FC, A (10e)
Anthracene $(C_{14}H_{10})$	FP, FC, A (14e)
 (C_7H_8)	NP, NC, NA (6e)
 (C_8H_8)	NP, FC, NA (8e)

Completely conjugated monocyclic hydrocarbons are known as annulenes. The criteria to determine the aromaticity of higher **annulenes** are as same as mentioned above.

(1)
[10] annulene
NP, FC, NA(10e)

(2)
[12] annulene
FP, FC, AA(12e)



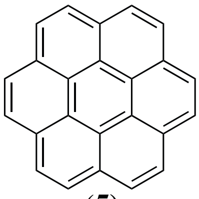
(3)
[14] annulene
FP, FC, A(14e)

(4)
[18] annulene
FP, FC, A(18e)

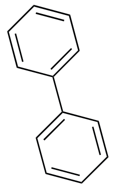
Fig.1 Some higher annulenes

As the number of carbons in annulenes increases the hydrogens placed outside and inside of the ring increase. [10]-Annulene tends to deviate from its planar geometry due to the steric influence of the inner hydrogens. Though [14]-annulene fulfills all features for aromaticity, the aromatic stability is only found at lower temperatures (30 °C). [18]-Annulene is the most stable higher aromatic annulene.

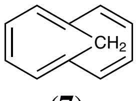
Exercise: *Determine the aromaticity of the following hydrocarbons: coronene (**5**), biphenyl (**6**) and bicyclo[4.4.1] undeca-1,3,5,7,9-pentaene (**7**).*



(**5**)



(**6**)

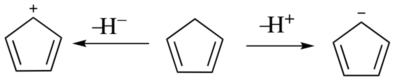


(**7**)

Electron filling of aromatic compounds

In an aromatic molecule, all bonding π orbitals are **filled** with paired electrons, while the presence of unpaired electrons in bonding, non-bonding or anti-bonding orbitals makes the molecule anti-aromatic.

Cyclopentadiene (Cp) (**9**) is not aromatic as it has a *sp*^{3}-hybridized carbon in the ring. Though its anion (**10**) and the cation (**8**) have planar structures and a similar number of π orbitals, their aromaticity differs as the numbers of delocalized π-electrons in the ring are 6e and 4e, respectively.

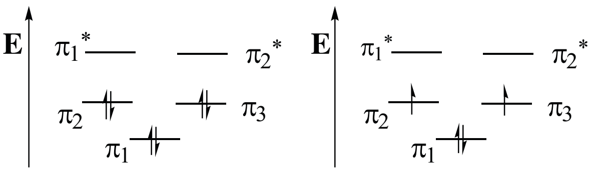


(**8**) (**9**) (**10**)

Fig. 2 Cation (**8**) and anion (**10**) derived from cyclopentadiene (**9**)

The anion (**10**) has (4n+2) π-electrons which are found as three sets of paired electrons in bonding π-orbitals (Fig. 3A), while the cation (**8**) has two unpaired electrons (Fig. 3B).

The aromaticity of a cyclic molecule gives extra stability to itself. The anti-aromatic state is less stable than the aromatic and non-aromatic states since anti-aromatic systems have the freedom to undergo conformational changes.



(**A**) (**B**)

Fig. 3 Filling of π-orbitals of Cp^- and Cp^+

Spherical aromaticity

Recently, scientists have discovered how to state the aromaticity of spherical structures, since the validity of the Hűckel rule limits only to planar structures.

A spherical structure such as a fullerene is said to be aromatic once its π-electron count satisfies $2(n+1)^2$ where n becomes an integer. The famous Buckminsterfullerene, C_{60} is nonaromatic as $n^2 = 29$.

Aromatic electrophilic substitution (AES)

Benzene ([6]-annulene) is the simplest aromatic annulene. Due to its high stability, it does not undergo typical reactions of alkenes. In an AES, ring hydrogen is substituted by an electrophilic reagent (E^+).

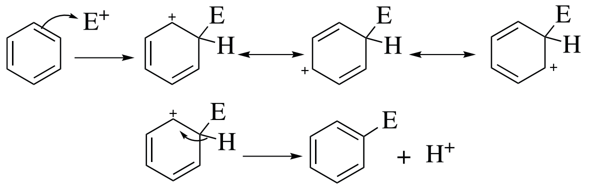
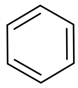


Fig. 4 Mechanism for AES reaction

Here the aromatic molecule acts as a nucleophile and the reaction mechanism involves three carbocations.

Halogenation, nitration, Friedel-Crafts alkylation and acylation, Gattermann-Koch formylation and sulfonation are some ES reactions of benzene (Table 1).

Table 1 Electrophilic substitution reactions of benzene (PhH); (X = Cl, Br)

Reactant	Conditions	Product(s)
	X_2/AlX_3	PhX
	conc. $HNO_3 + H_2SO_4$	$PhNO_2$
	$RX/AlCl_3$	PhR
	RCOX, $AlCl_3$	PhCOR
	SO_3, H_2SO_4	$PhSO_3H$
	$CO+HCl/CuCl/AlCl_3$	PhCHO

Ortho, meta and *para* directors

A mono-substituted benzene may undergo a substitution of a second hydrogen/group more easily than the benzene itself whilst some other substituted benzenes undergo reactions less easily due to deactivation of benzene ring. For example, aniline undergoes electrophilic substitution a million times faster than benzene does. On the other hand, at room temperature, nitrobenzene does not undergo electrophilic substitution.

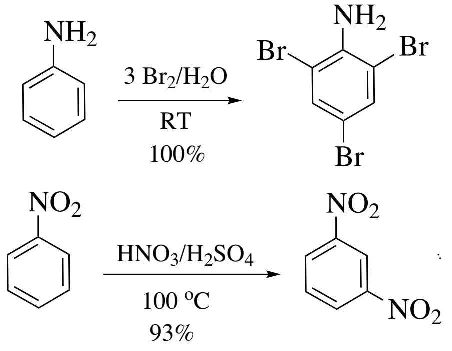
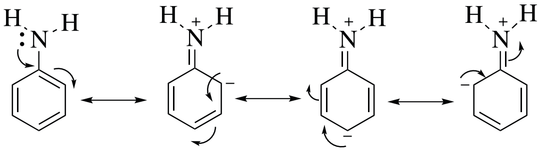
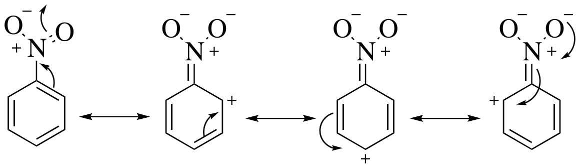


Fig. 5 AES reactions of $PhNH_2$ and $PhNO_2$

The NH_2 group of aniline is an **activating** group and its presence causes the ring to be more susceptible to further substitution. It is an ***ortho*** and ***para*** director and **resonance structures** of aniline are shown below.



The NO_2 group of nitrobenzene **deactivates** the benzene ring by withdrawing the electron density towards itself. Thus, it is a *meta* director (*meta*-carbons have more electron density); its resonance structures are shown below.

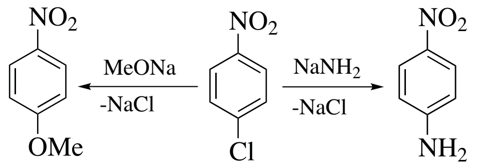


The following diagram gives the effect of the first substituent on the second substitution.

	ortho, para- **Directors**	***meta-*** **Directors**	
Increasing Activation ↑	$-NR_2$, R = H, alkyl	-COR	**Increasing Deactivation** ↓
	-OH	-COOR	
	-OR	$-SO_3H$	
	-NHCOR	-CHO	
	$-C_6H_5$ /aryl	-COOH	
	-R	-CN	
	-X (deactivating)	$-NO_2$	
		$-NR_3^+$	

Aromatic nucleophilic substitution (ANS)

Benzene, itself cannot undergo NS reactions easily. Benzene derivatives with electron withdrawing groups (EWGs) and benzylic halides can undergo ANS reactions. The chlorine in (**11**) can be replaced by nucleophiles such as MeO^- and H_2N^- to give (**12**) and (**13**).



(**12**) (**11**) (**13**)

Fig. 6 Examples for ANS reactions

ANS reaction needs a leaving group (LG) on the benzene ring and EWG/s at *meta* or/and *para* position/s to the LG. This is a two-step process with **addition** (nucleophile) and **elimination** (LG) reactions, thus it is called a $\mathbf{S_N(Ar)}$ reaction.

Note that ANS of chlorobenzene with $NaNH_2$ in liquid NH_3 proceeds *via* **benzyne mechanism**.

Addition reactions

Aromatic molecules can undergo some addition reactions: *e.g.* chlorination, catalytic hydrogenation, and Birch reduction.

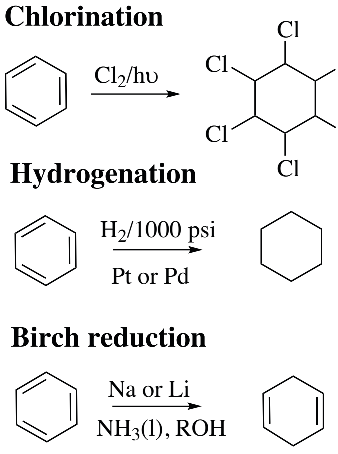


Fig. 7 Addition reactions of benzene

Complexes of aromatic molecules/ions

Aromatic molecules and ions can donate their π electron cloud to a metal centre to form **transitional metal complexes** such as [$(C_6H_6)Cr(CO)_3$], [$(C_6H_6)_2Cr$], [$FeCp_2$] and [$(C_6H_6)FeCp$]$^+$.

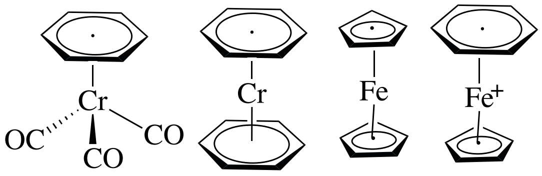


Fig. 8 Metal complexes of benzene & Cp^-

These arene and Cp complexes can be made easily by reacting benzene or CpH with metal salts. Upon coordination to a metal, benzene and Cp ligands become more susceptible towards **nucleophilic substitutions**.

NMR spectroscopy

NMR Spectroscopy serves as a useful tool in determining the aromaticity of a compound. The proton **chemical shift** (δ_H) of nonaromatic cyclooctatetraene (C_8H_8) appears around 5.78 ppm. In aromatic molecules, the protons attached to peripheral carbons are more **deshielded** or downfield shifted, and proton resonances appear above 7 ppm. In benzene, the six ring protons are chemically and magnetically equivalent and δ_H appear around 7.26 ppm in $CDCl_3$ due to **ring current**. Protons located inside the ring are **shielded** due to the induced magnetic field.

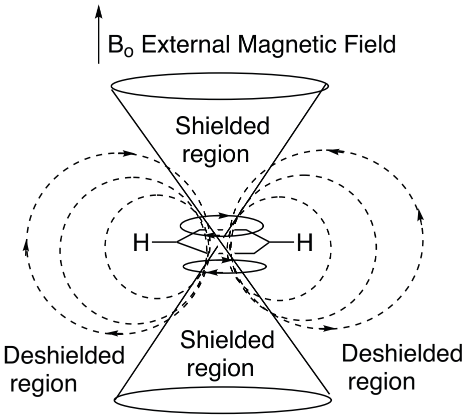


Fig. 9 Ring current of benzene in an applied magnetic field

[18]-Annulene (**4**) is an aromatic molecule and its six inner protons are **highly shielded** with a proton resonance at -**1.8** ppm. The twelve outer ring protons are highly **deshielded** with a proton resonance at **8.9** ppm. The δ_H of coronene (**5**) is also 8.9 ppm.

However, when one of the ring protons is substituted, the ring protons become magnetically inequivalent and show absorptions as a multiplet around the same areas. The carbon-13 resonances of aromatic carbons appear around 120-170 ppm.

Problems

1. Determine the aromaticity of the following: (i) pyrene, (ii) pyridine, (iii) thiophene and (iv) $C_7H_7^+$.
2. Write the major product/s formed during the following reactions.
   (i) PhH + $^nPrCl/AlCl_3$ →
   (ii) PhOH + $Br_2/FeBr_3$ →
   (iii) $PhCMe_3$ + $EtCl/AlCl_3$ →
   (iv) 2-Bromoanisole + $NaNH_2/NH_3$ →
   (v) 4-Chloronitrobenzene + NaOH/Δ→
   (vi) 2-Bromonitrobenzene + NaOMe →
3. Write the mechanism for the conversion of benzene into the following products.

(i) 4-Nitroaniline

(ii) 3-Iodosulphonic acid

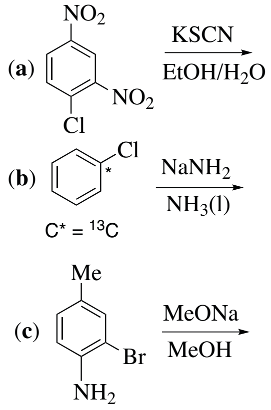
(iii) 4-Nitrocarboxylic acid

(iv) 3-Chloroaniline

4. Compare the proton chemical shifts of $[(C_6H_6)FeCp]^+$ with that of benzene.

5. Predict the number of peaks and their δ_H values for aza[18]annulene ($C_{17}H_{17}N$).

6. Determine the product(s) of the following substitution reactions.



Student Corner

Monsanto and Cativa processes of acetic acid synthesis

K. Sarath D. Perera

Senior Professor in Chemistry, Department of Chemistry, The Open University of Sri Lanka

In 1960, chemists at BASF developed the carbonylation of methanol into acetic acid.

$$CH_3OH + CO \xrightarrow{\text{catalyst}} CH_3COOH$$

Monsanto process

Monsanto Company introduced a new catalytic system in 1966. It is now known as the Monsanto acetic acid process, which operates at about 180 °C, under CO pressure of about 40 atm, using **rhodium catalyst**. Over six million tonnes of acetic acid are produced annually.

Catalyst

The catalyst system contains a **rhodium source** (*e.g.* $RhCl_3$, or $[RhCl(CO)(PPh_3)_2]$) and **iodide ions** (HI). The **active catalyst** is *cis*-$[Rh(CO)_2I_2]^-$.

Monsanto process consists of three coupled reactions/cycles. The cycles (i) and (iii) are **non-metallic** and (ii) is **organometallic**.

(i) Conversion of MeOH to MeI by HI.

$$MeOH + HI \longrightarrow MeI + H_2O \text{ -- (1)}$$

(ii) Catalytic carbonylation of MeI to MeCOI by the catalyst $[Rh(CO)_2I_2]^-$.

$$MeI + CO \longrightarrow MeCOI \text{ ------ (2)}$$

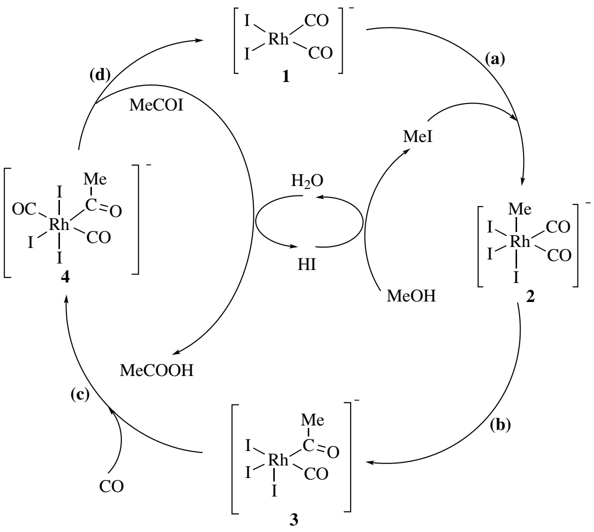
(iii) Hydrolysis of MeCOI to produce $MeCO_2H$ and HI.

$$MeCOI + H_2O \longrightarrow MeCO_2H + HI \text{ -- (3)}$$

The **overall reaction** is obtained by adding equations (1), (2) and (3), which gives

$$MeOH + CO \longrightarrow MeCO_2H$$

Let us look at the complete catalytic carbonylation process involving the active catalyst *cis*-$[Rh(CO)_2I_2]^-$. The proposed full catalytic cycle is given in scheme 1.



Scheme 1 Combined catalytic cycle for the Monsanto Process

(a) Oxidative addition of MeI to $[Rh(CO)_2I_2]^-$ **1** to give the octahedral methyl-complex ion *fac* -$[MeRh(CO)_2I_3]^-$ **2**; this is the rate determining step.

(b) Migration of Me on to a CO ligand gives the five-coordinate acetyl-complex ion $[(MeCO)Rh(CO)I_3]^-$ **3**.

(c) Coordination of another CO ligand to the complex ion **3** gives the octahedral complex ion $[(MeCO)Rh(CO)_2I_3]^-$ **4**; **4** can have either *fac*- or *mer*, *trans*-arrangement.

(d) Reductive elimination of MeCOI generates the active catalyst **1**. Finally, the hydrolysis of MeCOI produces $MeCO_2H$ and HI.

Higher alcohols can be carbonylated, but reactivity decreases in the following order.

$$\text{MeOH} > \text{EtOH} > \text{PrOH}$$

Cativa process

Cativa process was developed by BP Chemicals in 1996, and this process is based on a catalyst system containing **iridium** and **ruthenium**. The active catalyst is the anion *cis*-$[Ir(CO)_2I_2]^-$. Both Monsanto and Cativa processes are very similar, that they can use the same chemical plant. Initial studies by Monsanto had shown iridium to be less active than rhodium for the carbonylation of methanol to produce acetic acid. However, subsequent research showed that the iridium catalyst could be promoted by ruthenium, and this combination leads to a catalyst system that is superior to the rhodium-based systems. The proposed catalytic cycle is quite similar to the one shown in Scheme 1. Cativa process uses less water in the reaction mixture and decreases the formation of by-products, thus, it reduces the cost of production.

Synthesis of acetic anhydride

Industrially, acetic anhydride is produced by carbonylation of **methyl acetate** in a process that is very similar to Monsanto acetic acid synthesis.

$MeCO_2Me$ is used in place of methanol as a source of methyl iodide. **Rh(III) iodide** is the catalyst precursor. **LiI** is used instead of HI to generate MeI.

As acetic anhydride gets easily hydrolyzed, the whole process is conducted under anhydrous conditions in contrast to the Monsanto acetic acid synthesis.

Problems

1. EtBr oxidatively adds to $[RhBr_2(CO)_2]^-$ to give (**A**). (**A**) in the presence of CO, gives the acetyl complex (**B**). (**B**) reductively eliminates (**C**) to regenerate $[RhBr_2(CO)_2]^-$. Identify (**A**), (**B**) and (**C**).
2. Write the organometallic cycle for the conversion of ethanol into propionic acid using rhodium catalyst.
3. Comment on the rates of oxidative addition of MeI to the active catalyst with respect to Monsanto and Cativa processes.
4. Write balanced equations for the conversion of methyl acetate to acetic anhydride.

Mass Spectrometry

K. Sarath D. Perera

Senior Professor in Chemistry, Department of Chemistry, The Open University of Sri Lanka

Mass spectrometry is an analytical technique used to obtain information on the **structure** and **molecular weight/accurate mass** of a given compound. The main components of the mass spectrometer are the **ion source**, **mass analyzer** and **detector**. There are several methods for the ionization of the sample such as Electron Impact (EI), Chemical Ionization (CI), Fast Atom Bombardment (FAB), Electrospray Ionization and Matrix Assisted Laser Desorption Ionization (MALDI). The electron bombardment forms **radical cations** and **neutral fragments.** Those ions are sorted with respect to their mass/charge ratio (**m/z**), by the mass analyzer which operates under high vacuum conditions. Since most of the cations formed has a charge of +1, the peak position usually depends on the mass of the cation. The sorted ions are detected by the detector.

In a mass spectrum, each vertical line represents an ion or a molecular fragment while its height represents the **relative abundance**. Usually, the most intense peak is referred to as the **base peak** which is being given the 100% abundance while the peak with highest m/z ratio is referred to as the **molecular ion** peak. The molecular ion is a **radical cation** (*i.e.* a cation with an odd number of total electrons, *e.g.* $M^{+\cdot}$) which is formed when an **electron** from the given molecule is knocked away **once** when a high energy electron collides with it. This molecular ion eventually breaks down into other smaller radicals and cations with lower m/z values (Fig. 1).

Isotopes in mass spectra

Mass spectrometer can distinguish different masses of isotopes, e.g. ^{35}Cl & ^{37}Cl and ^{79}Br & ^{81}Br. The abundance of ^{35}Cl is 75.77% and that of ^{37}Cl is 24.23%. Thus, compounds containing one chlorine atom will show two molecular ion peaks corresponding to ^{35}Cl and ^{37}Cl. The $(M+2)^+$ peak will always be 1/3 of the peak of M^+. For example, the molecular ion peak of CH_3Cl is at m/z = 50 with 100% abundance and the (M+2) peak is at m/e = 52 with 33.3% relative abundance.

Similarly, compounds containing a bromine atom show two molecular ion peaks with same height corresponding to ^{79}Br and ^{81}Br as the abundance of each isotope is 50%.

Main types of fragmentations

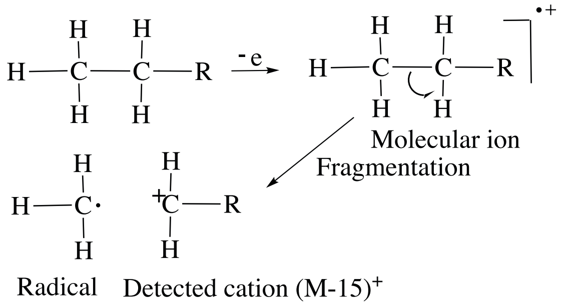


Fig. 1 Fragments of alkanes; $(M\text{-}R')^+$ ions

When an alkane is ionized an electron is removed forming the molecular radical cation ($M^{\cdot+}$) which is called the **parent peak** and is the mass of the compound. The fragmentation starts up from this radical molecular cation depending on its stability. Among those fragmentations, cleavages which lead to stable carbocations are much more favourable. The stability of carbocations (methyl, primary, secondary, tertiary, allyl, benzyl) increases as shown below (R = alkyl group).

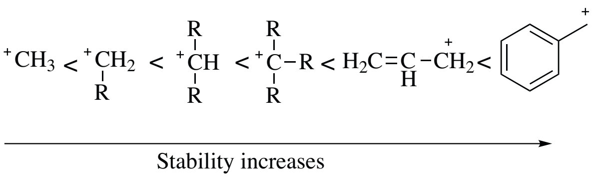


Fig. 2 Stability of carbocations

Alkenes and alkynes form their molecular radical ion ($M^{\cdot+}$) by losing a π-bonding electron, leaving the carbon skeleton of the compound undisturbed. The allylic cleavage occurring at terminal alkenes, always leads to a carbocation with m/z = 41.

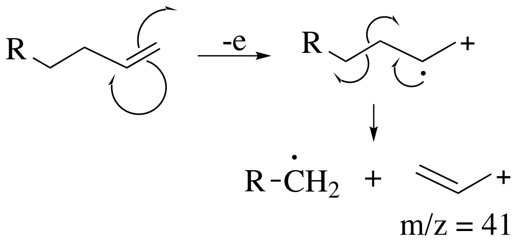


Fig. 3 Allylic cleavage of a terminal alkene

In alkynes, the loss of terminal hydrogen leads to a strong M-1 peak, and terminal alkyne favorably forms a propyl ion (m/z = 39; R = Me).

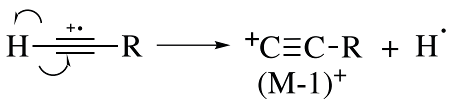


Fig. 4 Cleavage of a terminal alkyne

In aromatic compounds, fragmentation usually occurs at the benzylic position producing the benzylic ion which often rearranges to the **tropylium** ion (m/z = 91). The other prominent ion formed by fragmentation is the **phenyl** cation. The phenyl cation (m/z = 77) can further break down into smaller fragments such as acetylene and $C_4H_3^+$ (m/z = 51) and cyclopropenyl ion $C_3H_3^+$ (m/z = 39).

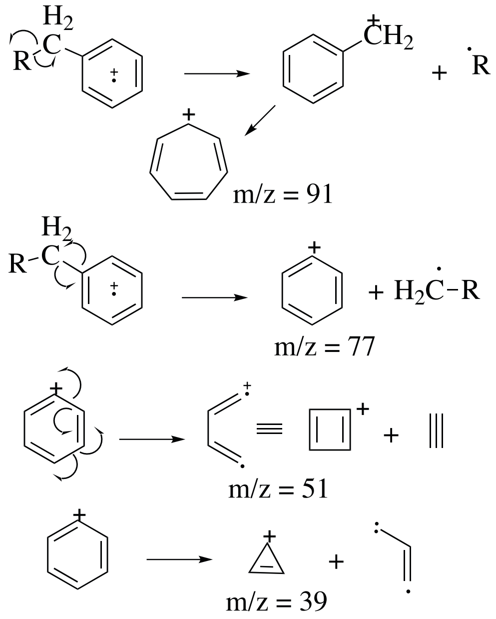


Fig. 5 Most prominent fragmentations of aromatic compounds

R-X type compounds where X = Cl, OH, NR_2 and OR show two prominent fragmentations: (a) C-X bond cleavage, (b) α-cleavage, where the α C cleaves from the carbon skeleton.

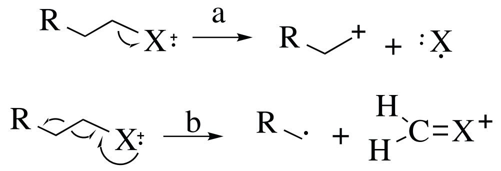
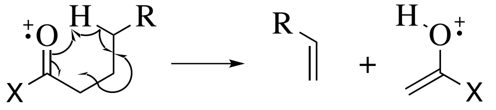


Fig. 6 (a) C-X bond cleavage (b) α-cleavage

McLafferty rearrangement

Compounds containing carbonyl groups show the **McLafferty rearrangement** apart from the usual α-cleavage and β-cleavage. It takes place in the presence of a γ-hydrogen, forming a **neutral olefin** and an **enol radical cation**.



Compound	X	m/z
Aldehyde	H	44
Methyl ketone	Me	58
Ethyl ketone	Et	72
Carboxylic acid	OH	60
Methyl ester	OMe	74
Ethyl ester	OEt	88
Amide	NH_2	59

Fig. 7 McLafferty rearrangements with m/z values for the formed enol radical cation

Nitriles and alkenes also undergo McLafferty rearrangement where the resulting fragments are $CH_2{=}C{=}NH^{\cdot+}$ (m/z = 41) and $CH_2{=}CHCH_3^{\cdot+}$ (m/z = 42), respectively.

Some common peaks observed in mass spectra are given below.

Cation	m/z	Cation	m/z
CH_3^+	15	CH_3CO^+	43
$CH_2=CH^+$	27	$C_3H_7^+$	43
$CH_3CH_2^+$	29	$O=C=NH_2^+$	44
$HC\equiv O^+$	29	$C_4H_7^+$	59
$CH_2=NH_2^+$	30	$C_6H_5^+$	77
CH_3O^+	31	$C_6H_7^+$	79
$CH_2=OH^+$	31	$C_7H_7^+$	91
$CH_2=CHCH_2^+$	41	$C_6H_5OH^+$	94

Molecular radical cation ($M^{\cdot+}$) can generate Me^+ and $(M-15)^+$ cations. Similarly, other peaks with the m/z value $(M-Y)^+$ can be observed due to the cleavage of a Y fragment.

For an example, the fragmentation products of hexanal are given below.

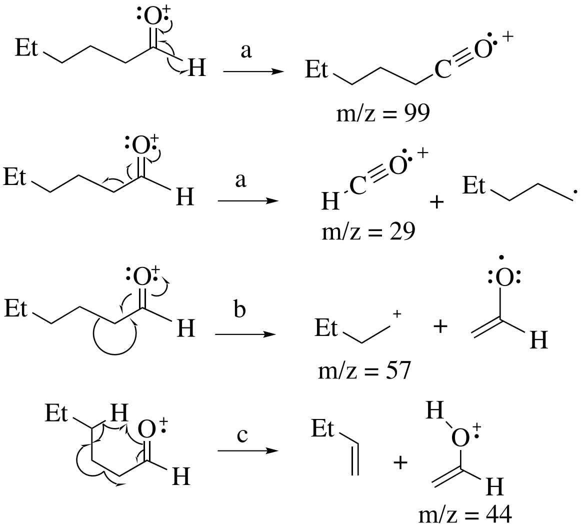


Fig. 8 Some fragmentation pathways of hexanal: (a) α cleavage, (b) β-cleavage and (c) McLafferty rearrangement

Most often, mass spectrometry is used with other analyzing techniques such as gas chromatography or liquid chromatography.

Problems

1. Estimate the relative intensities of isotope peaks of the molecular ion of 1,2-dichloro-4,5-dibromobenzene.
2. A compound with the composition $C_{10}H_{22}O$ shows mass peaks at m/e: 43, 55, 69, 73, 97, 115, 140 and 157. Deduce possible structural formulae.
3. A compound with the composition $C_9H_{18}O$ shows mass peaks at m/e: 43, 58, 71, 86, 99, 114 and 142. Deduce possible structural formulae.
4. $PhNO_2$ (m. wt. 123) shows peaks in its mass spectrum at m/e 107, 93, 77. Suggest structures for these ions.
5. Norbornene (C_7H_{10}) shows peaks in its mass spectrum at m/e 66, 39, 27. Suggest structures for these ions.
6. A compound with the composition $C_9H_{10}O_2$ shows mass peaks at m/e: 27, 29, 50, 77, 105, 122 and 135. Deduce possible structural formulae.

INSTITUTE OF CHEMISTRY CEYLON
Adamantane House, 341/22, Kotte Road,
Welikada Rajagiriya, Sri Lanka.
Tel: +94 11 286 1653, +94 11 401 5230
Fax: +94 11 287 0587
Email: ichemc@sltnet.lk
Web: www.ichemc.ac.lk