MANGALORE UNIVERSITY

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www.mangaloreuniversity.ac.in

Government of India
Ministry of Human Resource Development

GIAN
GLOBAL INITIATIVE OF ACADEMIC NETWORKS

MHRD Scheme - Global Initiative on Academic Network (GIAN)

a six day course on

Enabling Technology for Organic Synthesis

17 – 22 September 2018

Organised by

Department of Postgraduate Studies and Research in Chemistry
Mangalore University, Mangalagangothri-574 199, Karnataka, India

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About Mangalore University

Mangalore University was established in 1980 to fulfil the aspirations of the people of undivided Dakshina Kannada and Kodagu districts of Karnataka. The campus of Mangalore University called Mangalagangothri is located about 20 km to the south east of the historic port city of Mangalore. The vision of the University is 'to evolve as a national centre of advanced studies and to cultivate quality human resource'. The mission of the University is to provide excellent academic, physical, administrative, infrastructural and moral ambience. In addition, it aims at excellence in teaching, learning and research and to contribute towards building a socially-sensitive, humane, inclusive society. The University is committed to fulfil the objectives stated in the mission, by providing good infrastructural facilities to develop the University as a national centre in all spheres - teaching, learning, research and governance.

Mangalore University has grown impressively since its inception. Mangalore University is the first University in the country to start Bachelor degree programs in Hotel Management, Fashion Design, Garment Design and Leather Design. It is also the first University to start post-graduate program in Human Consciousness and Yogic Science and one of the first in the country and the first one in the state to start a full-fledged Master's and Doctoral program in Materials Science. The University has taken steps to establish contacts through exchange of scholars with Universities in USA, UK, Finland, Japan, Korea, Taiwan, Norway, Germany and other countries.

Research performance of Mangalore University is evidenced in the award of Rs. 16.6 crores grant by the Department of Science and Technology (DST), under PURSE scheme. The Microtron Centre, developed with the Department of Atomic Energy (DAE) support, is a national facility. The Centre for Application of Radiation and Radioisotope Technologies (CARRT) and Centre for Advanced Research in Environmental Radioactivity (CARER) are research centres which collaborate with a large number of research institutions at regional and national levels. The Ocean and Atmospheric Science and Technology Cell (OASTC), set up in collaboration with Department of Ocean Development (DOD), acts as a nodal centre to promote research in ocean and atmospheric sciences. Ministry of Human Resource Development (MHRD) in the first phase has identified Mangalore University as one of the beneficiaries of RUSA Grant.

Various surveys and independent research studies have placed Mangalore University in very high positions. H-index of the University in 2018 has been 62 that show the excellent research progress. As per the week education survey the ranking of Mangalore University is 34 among multi-purpose Indian Universities and it secured 14th position among Southern Universities. University has been place at number 3 in Green matric ranking. Today, true to its vision and mission, Mangalore University stands poised to reach greater heights of excellence in the years to come.

About the Department

The Department of Chemistry was established in 1981 with an intake of 9 students in the Government College, Mangalore. In 1982, the department was shifted to university campus, Mangalagangotri and in 1986 to the present science faculty building. The department started M.Sc. course in Applied Chemistry in the year 1996 and M.Sc. Organic Chemistry course in the year 2007. Presently, the department is running three M.Sc. Courses in Chemistry, Applied Chemistry and Organic Chemistry with a combined intake of about 140 students and PhD programme in Chemistry. As on today the Department has produced over 1400 M.Sc. graduates, 50 M.Phil and over 225 Ph.D. graduates. Presently about 70 Research Scholars are working for their Doctoral Degree.

The Department has also contributed to science significantly by carrying out research and published over 2700 research papers in peer reviewed national and international journals of reputation and presented about 2000 research articles in national and international Conferences. The faculties have received several prestigious fellowships and awards in recognition of their research contributions. They include Alexander von Humbolt Research Fellowship of Germany, JSPS Research Fellowship of Japan, Commonwealth Research Fellowship of U.K., Post-Doctoral Research Fellowships from US Research foundations and Korean Federation of Science & Technology, 'Dr. Kalpana Chawla Young Women Scientist' State Award of Karnataka, 'Best teacher' award of Mangalore University etc.

The faculty members are actively engaged in research in Frontier Areas of Chemistry and Interdisciplinary Areas. Research Project Grants of about Rs. 2 Crores have been sanctioned to the department by UGC, DST, DAE, NPCIL, KSCST, BRNS etc. The department has also entered into MOU with Industries and R&D organizations such as Nuclear Power Corporation of India, Kaiga, Rallis Agrochemical Research Station, Bangalore and Strides Arcolab, Mangalore.

The department is Supported with UGC- SAP (I Phase- Rs. 37 Lakhs & II Phase- Rs. 75 Lakhs) and DST-FIST (I Phase -Rs. 42 Lakhs) Grants. The Department conducted 3 International Conferences, 10 workshops and several lecture series. The Department has revised / updated M. Sc. course contents 8 times, almost once in every four years and is recently updated in 2016. The students graduating from our department have been recognized for their academic excellence in industries, professional and academic institutions in India and Abroad. Several premier chemical industries and R & D centres recruit our students through campus Selection. Several students have cleared GATE/SLET/NET examinations. Several Alumni of the Department have occupied prestigious in industries and academic institutions. The Department has great potential for expansion, particularly because of large scale investment in Greater Mangalore on Chemical Industries like Petrochemical Company, Pharmaceutical and Speciality Chemical Industries, Thermal Plant, BASF etc.

Course Overview

Advances in method development for organic synthesis, in reaction control and in product analysis have significantly impacted the way in which synthetic chemistry is performed. This course describes currently available methods, which enable new strategies for synthesis. *Continuous flow chemistry* is one of the most widely used enabling technologies. With the help of many illustrative examples, the course will demonstrate that flow chemistry is not only changing the way about thinking and conducting chemistry, but also offering opportunities in terms of cost, efficiency and safety.

Course Objectives

On completion of the course a participant should be able to:

i) Appreciate the range of enabling technologies available in synthesis and be able to identify different reaction technology equipment and summarize key criteria to consider before using it.

ii) Know the strategies and protocols required to implement new routes within target-oriented syntheses.

iii) Identify key problems in both small-scale academic synthesis and large-scale industrial synthesis of important compounds.

iv) Understand main principles in the use of enabling technologies and related industrial issues together with application to target molecules.

v) Explain when alternative tools and techniques may offer significant benefit to a desired reaction outcome.

Teaching Faculty with allotment of Lectures and Tutorials

Prof. Thomas Wirth (TW)

Course details

This course is designed to teach enabling technology methods in organic synthesis to the senior undergraduate and graduate students of chemistry / medicinal chemistry / participants from relevant subjects. The course will be taught in English. The five units of the course are designed to provide a detailed overview on current developments and capabilities using enabling technologies in the research laboratory and in industry. The participant will get familiar with the batch / flow differences, with the capabilities and limitations of flow chemistry, their application for the safe use of hazardous compounds, the incorporation of photo- and electrochemistry and the potential for the unique generation and use of short-lived intermediates in synthesis. The possibility of incorporating online analysis in flow chemistry allows direct reaction monitoring and reaction control, which has been evolved into autonomous systems. These, and also industrial examples where enabling technologies are directly incorporated in medium and even large-scale synthesis, will be presented in the course with the help of many illustrative examples.

Participant evaluation is based on attendance and a final test.

Course Duration: 17th Sep 2018 to 22nd Sep 2018

Class	Date	Contents
1	Day 1 (2 hrs)	Enabling Technologies – An overview, Batch and flow reactions (properties). Flow Chemistry I: Mixing aspects
2	Day 2 (2 hrs)	Flow Chemistry II (Safe synthesis, hazardous compounds, reactive intermediates), Flow Chemistry III (Photochemistry)
3	Day 3 (2 hrs)	Flow Chemistry IV (Electrochemistry), Mechanochemistry
4	Day 4 (2 hrs)	Optimisation techniques (Design of Experiment, DoE), Modern analysis and integration in automated synthesis
5	Day 5 (2 hrs)	Application of enabling technologies: Synthesis of API's (advanced pharmaceutical intermediates), Industrial applications of enabling technologies (up scaling, production on scale)
6	Day 6 (2 hrs)	Tutorials: Research Seminar (Iodine Chemistry and Flow Synthesis) and Evaluation
Total	12 hours	

Lecture Schedule:

Day 1 (17th Sep 2018):

Lecture 1 & 2: 10.30am to 11.30am & 11.45am to 12.45pm (2 hrs): TW

Enabling Technologies – An overview, Batch and flow reactions (properties). Flow Chemistry I: Mixing aspects:

12 Principles of Green Chemistry, Microwave Chemistry – Equipment, Solvents, Examples, Microwave chemistry in flow.

Differences between Batch and Flow Chemistry, Batch vs. Flow Optimization, Flow Chemistry - Basics, Examples of Reactors, Materials, Pumps, Pressure, Advantages. Mixing: Volume-to-Surface Ratio / Mass transfer, Heat Transfer, Mixing in Batch, Flow Regimes, Biphasic mixing, Examples, Unusual mixing regimes: CCC, Separations after mixing.

Day 2: (18th Sep 2018):

Lecture 3 & 4: 10.30am to 11.30am & 11.45am to 12.45pm (2 hrs): TW

Flow Chemistry II (Safe synthesis, hazardous compounds, reactive intermediates), Flow Chemistry III (Photochemistry)

Safe Chemistry through flow synthesis 1. Azides 2. Aminations 3. Organometallic reagents 4. Lithiations 5. Supercritical fluids. Photochemistry: History, Introduction, Light sources, Photocycloadditions, Polymer functionalizations, Dangerous reagents, Singlet oxygen, Waste Water treatment, Photoredox chemistry.

Day 3: (19th Sep 2018):

Lecture 5 & 6: 10.30am to 11.30am & 11.45am to 12.45pm (2 hrs): TW

Flow Chemistry IV (Electrochemistry), Mechanochemistry

Electrochemistry: Introduction, General Aspects, Industrial Use, different cells, Batch vs. flow electrochemistry, medium/large scale synthesis, indirect electrolysis, divided cells, paired electrolysis, anodic oxidation, cathodic oxidation, mediators, cross coupling.

Mechanochemistry or: Solid - solid reactions, ball mills, solvent-free routes, C-C bonds in synthesis, liquid-assisted grinding, MOF's, X-ray analysis in situ.

Day 4: (20th Sep 2018):

Lecture 7 & 8: 10.30am to 11.30am & 11.45am to 12.45pm (2 hrs): TW

Optimisation Techniques (Design of Experiment, DoE), Modern analysis and Integration in Automated synthesis

DoE - Design of Experiments, Low Resolution Design, High Resolution Design, Which Type of Design, How to work with DoE, 4 case studies

Modern analysis and integration in automated synthesis: Flow IR, Flow NMR, Flow MS, feedback / automated control, 2 examples.

Day 5: (21st Sep 2018):

Lecture 9 & 10: 10.30am to 11.30am & 11.45am to 12.45pm (2 hrs): TW

Application of enabling technologies: Synthesis of API's (advanced pharmaceutical intermediates), Industrial applications of enabling technologies (up scaling, production on scale)

Detailed discussion: aliskiren hemifumarate, prexasertib monolactate monohydrate and other examples from recent literature.

Day 6: (22nd Sep 2018):

Lecture 11 & 12: 10.30am to 11.30am & 11.45am to 12.45pm (2 hrs): TW

Tutorials: Research Seminar (Iodine Chemistry and Flow Synthesis) and Evaluation

Who can attend?:

- *Executives, Scientists and Researchers from manufacturing, service and government organizations including R&D laboratories.*
- *Faculty, Guest faculties from reputed academic institutions and technical institutions.*
- *Student at all levels (MSc/MTech/PhD)*
- *International Participants*

Number of participants for the course will be limited to fifty.

Fees:

Executives, Scientists and Researchers from manufacturing, service and government organizations including R&D laboratories	*Rs. 2000/-*
Faculty, Guest faculties from reputed academic institutions and technical institutions	*Rs. 1500/-*
Student at all levels (MSc/MTech/PhD)	*Rs. 1000/-*
International participants	*250 USD*

Note: The participants will be provided with accommodation on payment basis.

Detailed CV of Experts:
Prof. Thomas Wirth

Thomas Wirth (born: 04. August 1964) obtained his Diplom (1989) from the University of Bonn/ Germany, and PhD (1992) on the use of 2-vinylindoles in synthesis from the Technical University of Berlin/Germany with Prof. S. Blechert. After a postdoctoral stay (1993) working on the memory of chirality with Prof. K. Fuji at Kyoto University/Japan as a JSPS fellow, he started his independent research at the University of Basel/Switzerland. In the group of Prof. B. Giese he obtained his habilitation on stereoselective oxidation reactions (1999) supported by various scholarships before taking up his current position at Cardiff University in 2000. He was invited as a visiting professor to a number of places, he received the Werner Prize from the New Swiss Chemical Society (2000), the Wolfson Research Merit award (2016, Royal Society) and the Bader award (2016, RSC). He was an associate Editor of *Synlett* (2002-2010) and chairman of the RSC local section (2005-2007). He currently serves on the Editorial Boards of *Molecules* (1998-), *Current Radiopharmaceuticals* (2007-), *Philosophic Nature* (2008-), *Synthesis/Synlett* (2011-), *ChemistryOpen* (2012-) and is editor of the *Journal of Flow Chemistry* (2011-).
Thomas Wirth is the author of 204 publications including several reviews and book chapters and has written/edited 6 books (*h*-index = 48, >6500 citations, Web of Science, Feb 2017, Researcher ID: http://www.researcherid.com/rid/C-4835-2011). During the last 20 years, Thomas Wirth has been very active in presenting research results and given 329 lectures including 11 plenary lectures and 28 invited lectures at conferences. 20 postdoctoral researchers, 34 PhD students, 20 Diploma and MChem students and 72 summer students have successfully completed their projects in the Wirth group. For further information see:http://www.cf.ac.uk/chemy/wirth.html

Dr. Mahagundappa R Maddani (Course Coordinator)

Mangalore University
Assistant Professor
Department of Chemistry
Mangalagangotri-574199 (INDIA)

Dr. Mahagundappa R. Maddani

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E-mail: mahagundappa@gmail.com

PERSONAL INFORMATION
Born: 1981; Indian

ACADEMIC POSITION

Assistant Professor at Department of Chemistry, March 2014 - Present
Mangalore University, Mangalagangotri-574199

EDUCATION

Ph.D. *Dept. of Organic Chemistry*, Indian Institute of Science, Bangalore INDIA 2010
M.Sc. *Dept. of Chemistry*, Karnatak University, Dharwad, INDIA 2003

Industrial Experience

Advinus Therapeutics Ltd., Bangalore Oct 2011 – Feb 2014
Designation: Principal Scientist

Aurigene (Accelerating discovery) Ltd., Bangalore, INDIA Jan 2005 – June 2005
Designation: Science Associate

CIPLA Ltd, Bangalore, India June 2003 – Dec 2004
Designation: Synthetic Organic Chemist

Postdoctoral research: June 2010 – May 2011
Research: "Stereoselective synthesis of enantiopure compounds for biological studies"
Institut de Chimie Moléculaire et des Matériaux d'Orsay, University of Paris Sud-XI, France

Advisor: Professor HENRI B. KAGAN

Ph.D Thesis**:** *"Chemistry of Molybdenum Xanthate ($MoO_2[Et_2NCS_2]_2$): Applications in Organic Synthesis"*
August 2005-June 2010
Department of Organic Chemistry, Indian Institute of Science, Bangalore, INDIA
Supervisors**:** Dr. K. R. PRABHU and Prof. S. CHANDRASEKARAN

AWARDS & FELLOWSHIPS

- **Lectureship award** from Council of Scientific & Industrial Research (CSIR) in 2009 National Eligibility Test (NET) required for Lectureship in India
- The **Guha Research Medal** (Best thesis award) 2009 – 2010 for the best research 2010 work during Ph.D programme in Organic Chemistry department, IISc. Bangalore

PUBLICATIONS – 7 ; BOOK – 1 Book Chapter ; PATENTS - 2

Prof. Boja Poojary (Course Co-coordinator)

Boja Poojary (born: 15. September 1968) obtained his MSc (1993) from the Mangalore University, and PhD (2000) on "Studies on some Cyclic Peptides and Heterocyclic derivatives of Amino Acids & Peptides" from Mangalore University, India with Dr. S. L. Belagali, Professor, Department of Environmental Chemistry, University of Mysore, Mysore and Dr. B. Shivarama Holla, Department of Chemistry, Mangalore University, Mangalgangothri. He qualified State Level Education Test-Eligibility for Lectureship in Universities and Colleges conducted by Government of Karnataka during 1994-1995. He started teaching profession at Department of Chemistry, Mangalore University, as senior lecturer (2000-2005), as reader (2005-2008), and as Associate Professor (2008-2011). He then promoted as Professor in the year 2011 and he is currently serving as Professor and Chairperson, department of Chemistry, Mangalore University.

Boja Poojary is the author of 116 publications (National and International) and 83 conference proceedings. He has involved actively in various administrative services as coordinator, BOE Chairman, Convener, Director. He also organized several conferences/Workshops/Seminars during last 20 years. He also completed successfully projects funded by UGC, National Agricultural Innovation Project (NAIP) & Indian Council of Agricultural Research (ICAR) under Basic & Strategic Research in the Frontier Areas of Agricultural Sciences, New Delhi.

His research area includes Bioorganic Chemistry and Medicinal Chemistry. His research area is very relevant for the modern days, as scientific community as a whole is thinking of developing good drugs, vaccines, antibodies for deadly diseases like AIDS, which are also showing their ugly head in our country well. The research activities include-Development of new methodologies for the preparation of biologically important Heterocyclic molecules, naturally occurring cyclic peptides and heterocyclics linked with peptides. The structural studies and evaluation of biological potency of the synthesized molecules for their varied activities.
The application of molecular design to the creation of new molecules which may have medical applications, which may exhibit novel reactivity or which may be of interest in the context of molecular electronics, e.g., by forming non-linear optical materials. Development of convergent synthetic pathways of MCRs (Multi Component Reactions-one pot synthesis) in the synthesis of biologically important Heterocyclic molecules as they show advantages over linear or divergent approaches with respect to speed, time, yield and reproducibility.

He has successfully guided 07 PhD candidates and 01 MPhil candidate till date. Currently, 06 candidates are pursuing their PhD degree under his supervision.