Programme for ***25th Regional Conference of***
Orissa Chemical Society and National seminar
on
"FRONTIERS IN RECENT CHEMICAL RESEARCH"
Organized by
DEPARTMENT OF CHEMISTRY
KENDRAPARA AUTONOMOUS COLLEGE, KENDRAPARA
Dt. 13th and 14th March, 2022

Proposed Programme
13.03.2022 (Sunday)
Registration and High Tea : 9.00 am - 10.00 am

INAUGURAL SESSION : 10.00AM - 11.45AM

1.	Inauguration by lighting the lamp	:	10.00 am
2.	Opening song by the students of the College	:	10.05 am
3.	Welcome address by The Principal **Dr. R.P. Tripathy**	:	10.15 am
4.	Introduction to Guests - **Dr. P.K. Das** Reader in Chemistry & Organising Secretary of the Seminar	:	10.20 am
5.	Presentation of theme of the seminar- **Dr. D.N. Gochhayat** Asso. Prof. in Chemistry & Convenor of the Seminar	:	10.25 am
6.	Report of Orissa Chemical Society **Dr. Debashis Mohanty** Secretary, OCS	:	10.30 am
7.	Release of the Souvenir - **Prof. Ashok ku. Das** Hon'ble Vice chair person, Odisha State Higher Education Council, Bhubaneswar	:	10.35 am
8.	Address by Guest of Honour- **Prof. (Dr.) Satyaban Jena** Former Prof. and Head, P.G Dept. of Chemistry Utkal University, Vani Vihar, Bhubaneswar	:	10.40 am
9.	Address by Chief Guest- **Prof. Ashok Ku. Das** Hon'ble Vice chair person, Odisha State Higher Education Council, Bhubaneswar	:	10.50 am
10.	Address by the President of OCS – **Prof. Surendra Nath Mohanty**	:	11.10 am
11.	Felicitation to Chief Guest , Guest of Honour, **President OCS and Secretary OCS**	:	11.30 am
12.	Vote of Thanks - **Dr. Girija Prasad Mishra** Lecturer in Chemistry & Joint Organising Secretary of the Seminar	:	11.35 am

13.03.2022 (Sunday)

TECHNICAL SESSION - 1 (11.45 am - 1.00 pm)

Chair Person	:	**Prof. C.S Panda**, Former Prof. of Chemistry Berhampur University	
Coordinator	:	**Dr. A. Parija**, Reader in Chemistry Salipur Autonomous College, Salipur	
Key Note Speaker	:	**Prof. (Dr.) Ashoka kumar Mishra** Prof. and Dean, Academic Research IIT, Madras	: 11.45 - 12.25 pm
Invited Speaker	:	**Prof. (Dr.) C.S. Purohit** School of Chemical Sciences, NISER Bhubaneswar	: 12.25 - 1.00 pm

TECHNICAL SESSION - 2 (1.00 pm - 2.00 pm)

Chair Person	:	**Prof. Ashutosh Samantaray** Former Prof. of Chemistry OUAT, Bhubaneswar
Coordinator	:	**Dr. Sunasira Mishra** Asst. Prof., Khallikote Unitary University, Berhampur

Invited Speakers :

1. **Prof. (Dr.) Arun Kumar Padhy** : 1.00 - 1.30 pm
   Prof. and Head, Dept. of Chemistry
   Central University of Jharkhand
2. **Prof. Tirupati Barla** : 1.30 - 2.00 pm
   Asst. Prof., Dept. of Chemistry
   IISER, Berhampur

LUNCH : 2.00 pm - 3.00 pm

TECHNICAL SESSION - 3 (3.00 pm - 5.00 pm)

Chair Person	:	**Prof. Sarat Ch. Das** Former President, OCS
Coordinator	:	**Dr. Bibhuti Bhusan Parida** Asst. Prof., P.G Dept. of Chemistry, Berhampur University

Invited Speakers :

1. **Prof. (Dr.) Ajay Ku. Behera** : 3.00 - 3.25pm
   School of Chemistry, Sambalpur University
2. **Dr. Jaydev Dinda** : 3.25 - 3.50pm
   Associate Prof. of Chemistry
   Utkal University, Vani Vihar, Bhubaneswar
3. **Dr. Sitaram Mohapatra** : 3.50 - 4.15pm
   Asst. Prof. of Chemistry
   Ravenshaw university, Cuttack
4. **Dr. Satyanarayan Sahoo** : 4.15 -4.40pm
   Associate Prof., P.G. Dept. of Chemistry
   Berhampur University, Berhampur
5. **Ms. Smitabala Panda** : 4.40 - 5.00pm

14.03.2022 (Monday)

TECHNICAL SESSION - 4 (10.00am - 11.30 am)

(Augmenting Chemistry Teaching in Composite Degree Colleges of the State)

Chair Person : **Prof. S.N. Mohanty**
President, OCS

* Opening Remark
by the Session Chair : **Prof. S.N. Mohanty**

* Inviting opinions from the audience and discussions on the same.

TECHNICAL SESSION - 5 (11.30 am - 12.45pm)

Chair Person : **Dr. Bamakanta Garnaik**
Former Head, PG Dept. of Chemistry,
Berhampur University

Co-ordinator : **Dr. Pradyumna Choudhury**
Reader in Chemistry,
Salipur (Auto.) College, Salipur

Invited Speakers :

1. **Prof. Sarat Ku. Swain** : 11.30 - 11.55am
   Prof. of Chemistry, VSSUT, Burla
2. **Dr. Ganngam Phaomei** : 11.55 - 12.20pm
   Asso. Prof. of Chemistry, Berhampur University
3. **Dr. Bibhuti Bhusan Parida** : 12.20 - 12.45pm
   Asst. Prof., P.G Dept. of Chemistry, Berhampur University

TECHNICAL SESSION - 6 (12.45 pm - 1.45 pm)

Chair Person : **Prof. Sarat Ku. Swain**
Prof. of Chemistry, VSSUT, Burla

Co-ordinator : **Dr. Dushasana Parida**
Reader in Chemistry, Pattamundai College

Oral Presentations :

1. **Dr. Sunasira Mishra** : 12.45 - 1.05pm
   Asst. Prof., Khallikote Unitary University, Berhampur
2. **Dr. Debasmita Bharatia** : 1.05 - 1.25pm
   VSSUT, Burla
3. **Ms. Namrata Behera** : 1.25 - 1.45pm
   NISER, Bhubaneswar

LUNCH : 2.00 pm - 3.00 pm

VALEDICTORY SESSION (3.00 pm - 4.00 pm)

Invited Speaker

MONITORING DISSOLVED ORGANIC MATTER USING FLUORESCENCE

Prof. Ashok Kumar Mishra
Department of Chemistry,
Indian Institute of Technology Madras, Chennai 600036

Water in natural as well as man-made sources contain 'Dissolved Organic Matter' (DOM) to varying extents. DOM in water is often of natural as well as anthropogenic origin. Monitoring the nature and type of DOM is important as often a variety of DOM pose health hazard. Quite a few DOM components are fluorescent, which can enable their easy, sensitive and rapid monitoring. Miniaturization of measuring instruments and the fibre-optic compatibility of optical methods can make the monitoring process on-site/on-line.

This talk will present some of our research on the topic. We have developed new concepts and protocols towards understanding the complex fluorescence originating from DOM. A variety of instrumentation have also been developed in our laboratory that enables rapid and sensitive monitoring. Our noteworthy contribution to the monitoring of the presence of faecal matter in water will also be discussed in detail.

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IMIDAZOLE CHEMISTRY : SMALL MOLECULES DOING WONDERS

Prof. Arun Kumar Padhy
Department of Chemistry, Central University of Jharkhand, Ranchi, India

Abstract :

Imidazole is a five membered heterocyclic molecule. Its being the part of the nucleic bases it has a wide application. The most important ones being found in the anti-fungal agent. Recent advances have seen that molecule containing imidazole nucleus can also act as anti-tumor agents and other important biological activity. Leaving behind potential biological activity, imidazoles find its application in purification of gases in the form of ZIF. This talk will cover some of the important applications of imidazole chemistry.

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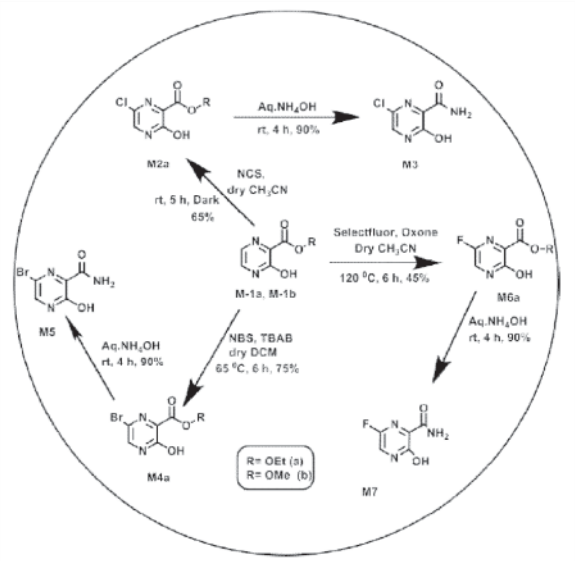
ELECTROPHILIC SUBSTITUTION IN PYRAZINE : A HIGH YIELDING SYNTHESIS OF FAVIPIRAVIR#

Dr. Chandra ShekharPurohit
NISER,Bhubaneswar

Pyrazine derivatives are used in human welfare. For example, Pyrazinamide is a well- known drug for tuberculosis.[1–3] Favipiravir is an essential antiviral drug molecule having notable performance against SARS-CoV-2. It is also a derivative of pyrazine. Pyrazines are p- electron-deficient molecules and therefore, electrophilic substitution is difficult. To perform such a reaction, an electron-donating group is essential. Considering resonance structures, one can expect the presence of the phenolic group in position-3 activates the 6th position for electrophilic substitution. Thus, this position may directly be halogenated with the suitable electrophilic reagent. Various groups have synthesized favipiravir in multiple steps (average 6-8 steps) with an overall yield (0.44 - 23%). This talk will elaborate a two-step synthesis with an improved overall product yield of 41%. Also the lactim–lactam tautomerization of favipiravir and its analogous molecules will be discussed.



A Schematic Representation of the Synthesis

References

1. M. Kim, V. Franke, B. Brandt, E. D. Lowenstein, V. Schöwel, S. Spuler, A. Akalin and C. Birchmeier, Nat. Commun., 2020, 11, 6375.

2 O. Zimhony, J. S. Cox, J. T. Welch, C. Vilchèze and W. R. Jacobs, Nat. Med., 2000, 6, 1043–1047. 3 A. Scorpio and Y. Zhang, Nat. Med., 1996, 2, 662–667.

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NONCOVALENT INTERACTIONS WITH SP^3-CARBON

Himansu S. Biswal

School of Chemical Sciences, National Institute of Science Education and Research (NISER), Bhubaneswar, India e-mail: himansu@niser.ac.in

The last decade has seen several discoveries of noncovalent supramolecular forces such as tetrel bonding, pnictogen bonding, chalcogen bonding, halogen bonding and aerogen bonding and last but not least, the hydrogen bonds with sulfur and selenium. These interactions are essential to understanding supramolecular chemistry and biomolecular structures. In this talk, I shall present recent developments and our contributions in this research area[1,2], explaining the existences and general consensus and counterintuition about carbon-bond (**C-bond**)[3], Carbon-centered hydrogen bond (**H-bond**) and most recent carbo-hydrogen bond ($\mathbf{C_H}$**-bond**)[4] in proteins and nucleic acids.

A genre of noncovalent interactions such as C5-hydrogen bond, halogen bond, and reciprocal carbonyl-carbonyl interactions involving carbonyl groups of proteins discovered in recent years is proved to be useful in de novo protein structure and function prediction. However, in proteins, the occurrence, strength, and importance of carbon bonds (C-bonds), the highly directional hydrophobic interactions between an electron-rich carbonyl-oxygen acceptor and an electron-deficient sp^3-hybridized carbon σ-hole donor through $n \rightarrow \sigma^*$ electron delocalization are yet to be perceived. With the help of careful protein structure analysis, quantum calculations, nuclear magnetic resonance and infrared spectroscopic methods, we discovered ubiquitous existences of C-bonds in proteins and determined C-bond energies precisely. We demonstrated the implications of C-bonds in explaining the photochemistry of oxygen-storage protein myoglobin and protein-DNA. It is highly anticipated that the inclusion of C-bonds in computational force fields would unravel many more implications of C-bonds in the structure, function and dynamics of proteins and protein-ligand/drug complexes.

Hydrogen bond (H-bond) without lone pair(s) of electrons and π-electrons is a concept developed two to three years ago. H-bonds involving less electronegative tetrahedral carbon are beyond the classical concepts on H-bonds. Careful protein structure analysis aided with several quantum chemical calculations suggests that these H-bonds are of moderate strength. These C-H···C H-bonds are blue-shifted and are dispersive in nature. We developed an empirical equation to estimate the C-H···C H-bond energy in proteins from the distances between the carbon and hydrogen atoms. In proteins, the binding energies range from -5.4 kJ/mol to -14.0 kJ/mol. The C-H···C H-bonds assist the substrate binding in proteins. We also explored the potential role of these carbon-cantered H-bonds

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Prof. Thirupathi Barla
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Phone: +91680 2227768.

Abstract:

*Without organic molecules such as medications, crop-protections, nutrition's, fragrances and flavours, human life would be impossible. These compounds are very important for medical practices because 25% of medications in use today are derived from natural products. So, our research program directed towards total synthesis of biologically active natural products or model compounds having potential bioactivities. As part of ongoing research, we have achieved total synthesis of the proposed elgonene C (Figure 1), its (4R,5R)-diastereomer by second-generation oxazoborolidinium ion catalysed Diels-Alder reaction, Sharpless asymmetric dihydroxylation, Ni-catalysed redox-active ester cross-carboxy coupling reaction as key steps.1 We also also work the development of new methodologies with high levels of selectivity and purity. Accordingly, we have prepared highly functionalized dibenzobicyclo[3.2.1]octadienone scaffold, which has been found in naphthocyclinones, engelharquinones, rubialatin A, etc., under mild t*ransition metal-free conditions by aryne insertion reaction with 2-keto-1,3-indandiones. The application of this methodology has been demonstrated to the synthesis of the 6/6/5/6/6 scaffold of rubialatin A (Scheme 1). 1HNMR experimental studies confirm that the reaction proceeds through the formation of benzocyclobutane followed by a 7-member carbocycle ring.2

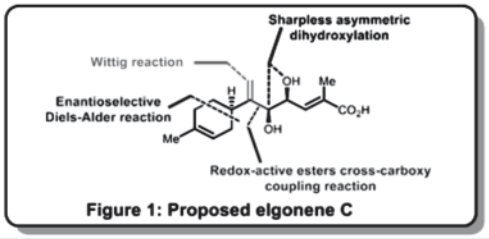
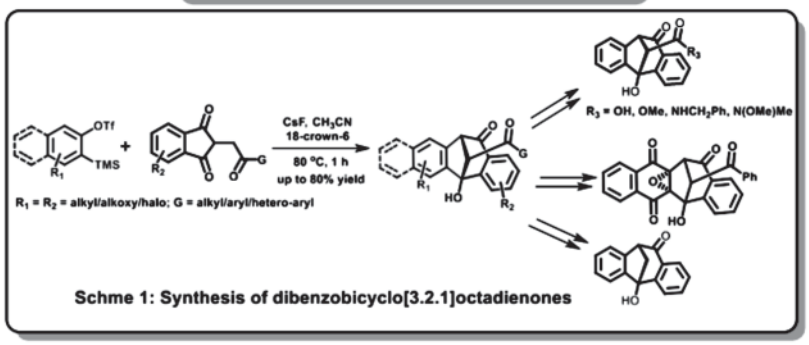


Figure 1: Proposed elgonene C



Schme 1: Synthesis of dibenzobicyclo[3.2.1]octadienones

References

1.Sudip, M.; Thirupathi, B. *Org. Biomol. Chem.*, **2022**, Accepted Manuscript, DOI: 10.1039/D2OB00094F

2.Hazra, G.; Mishra, G.; Dandela, R.; Thirupathi, B. *J. Org. Chem.* **2022** (Under review)

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Fascinating Dimedone Chemistry : A Journey from Spiro to Condensed Heterocycles

Prof. Ajaya Kumar Behera.
Organic Synthesis Laboratory
School of Chemistry, Sambalpur University, Jyoti Vihar, Burla
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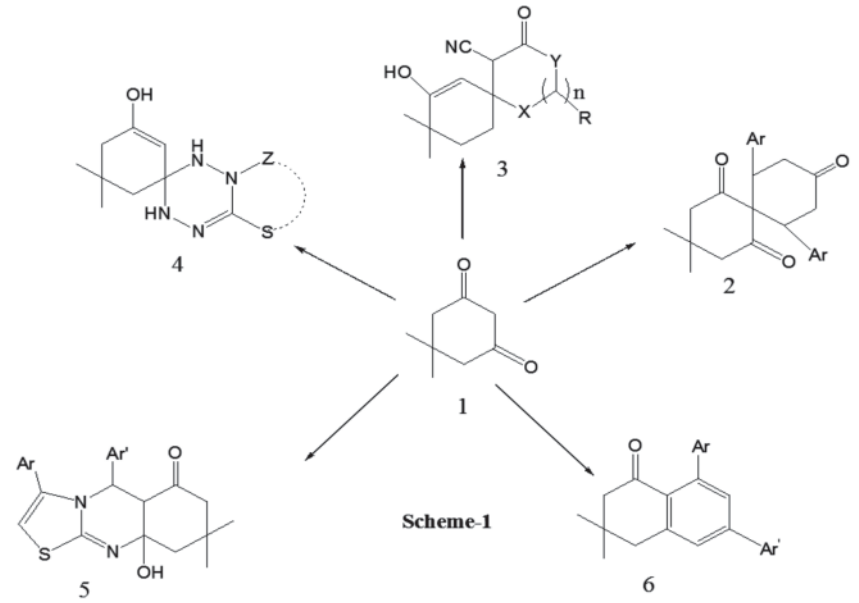
Dimedone is an interesting motif in most organic transformations. This cyclic diketone and its derivatives possess many biological properties such as anticarcinogenic, antioxidant, antihistaminic and anticoagulant. The tautomeric enol form of dimedone and its active methylene scaffold have been exploited to explore diverse spiro and condensed heterocyclic derivatives as depicted in the Scheme-1.



Scheme-1

2:Ar = C_6H_5, *p*-$MeOC_6H_4$, *p*-ClC_6H_4 ; **3**: n= 0,1;X= S, CH-CN, NH; Y= NR_2,=N,= O /S

5: Ar = C_6H_5, *p*-$MeOC_6H_4$, *p*-ClC_6H_4, *p*-BrC_6H_4, *p*-HOC_6H_4

Ar' = C_6H_5, *p*-$MeOC_6H_4$, *p*-MeC_6H_4 *p*-ClC_6H_4, *p*-BrC_6H_4, *p*-HOC_6H_4,*p*-$NO_2C_6H_4$

6: Ar = Ar' = C_6H_5, *p*-$MeOC_6H_4$, *p*-ClC_6H_4, *p*-BrC_6H_4, *p*-$NO_2C_6H_4$

The microbial activities, fluorescence and sensing behavior towards ionic species of some of the novel synthesized compounds have been studied.

References:

1. **A.K.Behera**, R. K.Behera, P.P Mahanta, P. Majumdar, *Synth. Commun*. **2013,** 43, 899–914.
2. **A. K. Behera**, R.K. Behera , A. Pati, P. Majumdar, *JOHC* , **2013,** 50, 703-712.
3. P.Majumdar, P. P. Mohanta, S. Sahu **A.K.Behera**, *Synth. Commun.*, **2018,** 48, 14, 1747–1754.
4. P. P. Mohanta, S. Sahu, P. Majumdar, A. K. **Behera**, *Synth. Commun.* ***2019****, 49, 21, 2941–2951.*
5. Prajna Parimita Mohanta, Hari Pati & **Ajaya Kumar Behera**, **2020**, *RSC Advance 10,15354.*
6. P.P.Mohanta, Aparna P.Devi, B.P.Bag, H.N.Pati & **A.K.Behera,** *RSC Advance***, 2021**,**11**,2021.

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