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UNIVERSITY**

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Medicinal and Pharmaceutical Chemistry**

The BOOK of
ABSTRACTS

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ORAL PRESENTATIONS			
P. No.	Name of Presenter	Affiliation	Title of Presentation
OP-1	Aakanksha Gurawa	Malaviya National Institute of Technology (MNIT), Jaipur	Photoinduced Radical Azidation of Olefins using λ^3 - Iodane Species
OP-2	Aashna Perwin	Jamia Millia Islamia, New Delhi	Synthesis of Aldehyde Monomers
OP-3	Aayushi Lodhi	Sardar Vallabhbhai National Institute of Technology (SVNIT), Surat	Green Synthesis of Quinazoline Based Heterocyclic Compounds Over Post Treated Zeolite H β
OP-4	Ajjur Rahaman	CSIR-Central Salt and Marine Chemicals Research Institute (CSMCRI), Bhavnagar	Catalytic N-Acylation of Cyclic Amines by Arylglyoxylic Acids through Radical-Radical Cross-Coupling
OP-5	Akhilesh Kumar	Banaras Hindu University, Varanasi	Conformational and Interactions Studies of Triazinone Derivative Linked with Pthalimido and Benzimidazole through Leonard Linker: Employing Theoretical Calculations
OP-6	Ankita Salunke	The Maharaja Sayajirao University of Baroda, Vadodra	Potential anti-osteoporotic effects of <i>Litsea glutinosa</i> on Saos-2 cells: A Molecular screening
OP-7	Debatrayee Dasgupta	The Maharaja Sayajirao University of Baroda, Vadodra	Controlled release of DOX from drug delivery system based on functionalized MCM-48: <i>in-vitro</i> , kinetics and <i>in-vivo</i> studies
OP-8	Bhagyashri Waghmare	M.S.G. Arts, Science and Commerce College, Malegaon, Nashik	Synthesis, Characterization and DFT Study Of (3Z)-3-(4-Chlorobenzylidene)-1-Methylpyrrolidin-2-one
OP-9	Hitesh P. Thumbar	R. K. University, Rajkot	Identification and Characterization of Some Process Related Substances and Degradation Products Using Advance Analytical Techniques
OP-10	Yashasvi Inaniyan	J.N.V. University, Jodhpur	Oxidative transformation of carbonyl compounds from oximes by using quinolinium dichromate (QDC)
OP-11	Aniket Gupta	CSIR-Central Salt and Marine Chemicals Research Institute (CSMCRI), Bhavnagar	Substrate-Ligand Cooperativity-Promoted α -Allylic Alkylation of Carbonyl Compounds with Unactivated Allylic Synthons
OP-12	Archana Ranjan	Amity University, Noida	Cu/Mn catalyzed C-N cross coupling reaction of Arylchlorides and Amines promoted by PAMAM dendrimer

Oral Presentation :08

OP8: Synthesis, Characterization and DFT Study of (3Z)-3-(4-Chlorobenzylidene)-1-Methylpyrrolidin-2-One

B.B. Waghmare^{1*}, B.S. Jagdale²

^{1*}*Department of Chemistry M.S.G. Arts, Science and Commerce College, Malegaon, Nashik Maharashtra, India*

²*Department of Chemistry, L.V.H. Arts, Science and Commerce College, Panchavati, Nashik Maharashtra India.*

**Corresponding Author - Tel-+91 9420343752, [Email: bhagyashri207@gmail.com](mailto:bhagyashri207@gmail.com)*

A Chalcone (3Z)-3-(4-chlorobenzylidene)-1-methylpyrrolidin-2-one (**I**), was synthesized. Compound **I** was characterized by proton and carbon-13 nuclear magnetic resonance (¹H- and ¹³C- NMR), Fourier transform infrared (FTIR) and mass (LC-MS) spectroscopic methods. Density Functional Theory (DFT) calculations for compound **I** were performed at B3LYP/6-311++G (d, p) level. Optimized geometry, frontier molecular orbital's (HOMO, LUMO), and IR and NMR parameters of compound **I** were obtained. The evaluations reveal that the calculation results support the experimental results.

Keywords: Chalcone, DFT, Optimized geometry, frontier molecular orbitals.