

Report on National Webinar on "Facile synthesis of multifunctional thiazole-schiff base derivatives via multicomponent reaction and their anti-cancer evaluation and molecular docking studies "Held on 14thSeptember 2021

Date of Event	14.09.2021
Name and Type of Event	National Webinar on "Facile synthesis of multi-functional thiazole-schiff base derivatives via multicomponent reaction and their anti-cancer evaluation and molecular docking studies".
Conducted by	Mr. Ashwini Kumar, Dr.ChandraPrabha Sahu, Ms. D. Vally
Number of Participants	147

The Resource person **Dr. Archi Sharma** is Assistant Professor of the Department of Science and Technology, Mody University, Rajasthan.

She has completed her M.Sc. in Organic Chemistry from Guru Ghasidas (Central) University, Bilaspur, Chhattisgarh in the year 2012. Thereafter, she holds a **Phd** in synthetic orgaic chemistry from National Institute of Technology Raipur, she completed her Philosophy of Doctoral in the year 2018, she has rich experience of 7 years in academia and research. she has published **9** research paper including two review paper in well reputed international peer reviewed journals. Her research work recived 5 **H-index and 47 Citation** in a very short span of time, not only this, she has also co-authored **2 books**, Advances in structure and activity relationship of coumarin derivatives and Dehydroacetic Acid and Its Derivatives: Useful Synthons in Organic Synthesis under the renound Elsevier publication. Apart from her research work she is actively involved in teaching UG, PG and engineering students. Currently she is working as an assitant Professor in Mody womens' University of science and technology, Laxmangarh, Sikar, Rajasthan.

The speaker gave informative and illuminating lecture with valuable content. The session was valuable not only for students but for faculties, research scholars, industry persons and other participants. A series of multi-functional thiozole-schiff base derivatives have been synthesized via NBS mediated sequential, one-pot, three component reaction. All the synthesized compounds were characterized by analytical and spectral studies. The purity of the compounds was checked by TLC plates (E. Merck Mumbai, India). IR spectra (KBr) were recorded on Perkin Elmer 100 FTIR spectrophotometer. ¹H NMR and ¹³C NMR spectra were recorded on a Bruker AVANCE-1 (300 Hz and 75 Hz respectively) spectrometer in δ ppm using TMS as standard. Mass spectra (ESI-MS) were determined by Agilent 1290 infinity HPLC coupled with 6150B single quadruple LCMS spectrometer. The final compounds were screened against different cancer cell lines. Skin malignant melanoma (A375), epithelial cervix adenocarcinoma (HeLa) and human breast adenocarcinoma (MCF-7) cell lines were procured from National Centre for Cell Science (NCCS), Pune, India. At the onset of the treatment period, the cell viability was assessed by the 3-(4,5dimethylthiazol-2-yl)2,5-diphenyltetrazolium-bromide (MTT) assay (HiMedia, Mumbai, India). Among all the compounds 4b, 4c, 4f, 4g and 4h exhibited good anticancer activitiy against A375 cell line comparable to erlotinib. The same derivatives were also shown comparable inhibitory activities against MCF-7 cancer cell line. Compound 4h displayed comparable anticaner activity against three cancer cell lines A375, HeLa and MCF-7. Further all the newly synthesized compounds were estimated for its ADME analysis and docking profile for binding affinity towards Hsp90 proteins repectively.Based on sequence alignment and template structure, the predictive 3D structure model of Hsp90 was generated using homology modelling with prime application of Schrodinger. The in silico molecular docking studies for all the newly synthesized compounds were shown good to excellent binding affinity for Hsp90 proteins. To predict in silico ADME properties of ligands including absorption, distribution, metabolism and excretion using pre-calculated models, we used Ouikprop, (version 4.7, Schrödinger release, 2016-1) In ADME analysis, the best result for absorption and metabolism is shown by compound **4e**. While the parameter for excretion is found to be the best for compound 4h. The chemistry outlined here provides a facile, green multi-component reaction for the synthesis of multi-functional thiazole-schiff base derivatives. The present procedure offers advantages of commercially available starting materials, broad substrate scope, satisfactory yields and easy workup. In addition, final compounds have been found to possess good anti-proliferative activity against different cancerous cell lines.

Topic of National Webinar: - "Facile synthesis of multi-functional thiazole-schiff base derivatives via multicomponent reaction and their anti-cancer evaluation and molecular docking studies"

Date:-14th September 2021

Convener:-Mr. Ashwini Kumar

Co-Ordinator:-Dr. ChandraPrabha Sahu, Ms. D. Vally

Organizing Committee:-

Dr.AnupamKumari, Asst. Prof, Department of Engineering, ARKA JAIN University Miss Shatabhisa Sinha Asst. Prof., Department of Engineering, ARKA JAIN University Dr. Keerti Rai, Asst. Prof., Department of Engineering, ARKA JAIN University

About the Speaker:-

Dr. Archi Sharma is Assistant Professor of the Department of Science and Technolgy, Mody University, Rajasthan.She has completed her M.Sc. in Organic Chemistry from Guru Ghasidas (Central) University, Bilaspur, and Chhattisgarh in the year 2012. Thereafter, she holds a **Phd** in synthetic orgaic chemistry from National Institute of Technology Raipur, she completed her Philosophy of Doctoral in the year 2018, and she has rich experience of 7 years in academia and research. She has published **9** research paper including two review paper in well reputed international peer reviewed journals. Her research work recived 5 **Hindex and 47 Citation** in a very short span of time, not only this, she has also co-authored **2 books**, Advances in structure and activity relationship of coumarin derivatives and Dehydroacetic Acid and Its Derivatives: Useful Synthons in Organic Synthesis under the

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Venue and Participants:-

Webinar was conducted on Google Meet and also streaming online in you Tube. Total participants registered were 147 from different University/Institutes across India. Total numbers of attendees were 147.

Event Poster



Certificate Template:-



Screenshot :







