

SRI VENKATESWARA INTERNSHIP PROGRAM FOR RESEARCH IN ACADEMICS (SRI-VIPRA)



SRI-VIPRA

Project Report of 2024: SVP-2432

"Morita Baylis Hillman Reaction and its Synthetic Applications"

IQAC Sri Venkateswara College University of Delhi Benito Juarez Road, Dhaula Kuan, New Delhi New Delhi -110021

SRIVIPRA PROJECT 2024

Title : Morita Baylis Hillman Reaction and its Synthetic Applications

Name of Mentor: Prof. Sharda Pasricha Name of Department: Chemistry Designation: Professor



List of students under the SRIVIPRA Project

S.No	Photo	Name of the student	Roll number	Course	Signature
1		Kashish Mann	1523062	B.sc. (H) Chemistry	Hardin
2		Harsh Pahuja	1522080	B.sc. (H) Chemistry	larth

3		Nitesh Kushwaha	1522050	B.sc. (H) Chemistry	Nitesh Kushwaha
4		Pahi Talukdar	1523045	B.sc. (H) Chemistry	Pahi ^o Tauikolar.
5	Schoo	Harsh Pundir	1523027	B.sc. (H) Chemistry	Hansletundur
6		Priya Bharti	1523067	B.sc. (H) Chemistry	Riyerarti
7		Mhonyani L Ezung	1523008	B.sc. (H) Chemistry	Mhomysuni



Signature of Mentor

Certificate of Originality

This is to certify that the aforementioned students from Sri Venkateswara College have participated in the summer project SVP-2432 titled "**Morita Baylis Hillman Reaction and its Synthetic Applications**". The participants have carried out the research project work under my guidance and supervision from 1st July, 2024 to 30th September 2024. The work carried out is original and carried out in an online/offline/hybrid mode.

Signature of Mentor

Acknowledgements

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TABLE OF CONTENTS

S.No	Торіс	Page No.
1.	Introduction	5
2.	Our work-Use of ICT tools for research	6-7
3.	Our Work-Morita Baylis Hillmann reaction- An Introduction	8
4.	Synthetic and Biological Applications of Morita Baylis Hillmann Reaction	9
5.	Work done so far	10
6.	Future goals	10
7.	References	



Introduction:

A. While conducting a literature review, ICT tools are Scholar, Mendeley, Chemdraw, Scopus, Google Scholar, BioRender, and Adobe Illustrator are indispensable. Scopus and Google Scholar facilitate comprehensive literature searches, while Mendeley aids in reference management. Chemdraw helps in drawing the chemical structures, while BioRender and Adobe Illustrator enhance the visualization of scientific data, making complex concepts more accessible.

Finding the research papers on the relevant topic through Google Scholar and Scopus is the first step in writing a literature review. The students were trained on how to pose questions, how to improvise data and get most relevant papers for the topic of choice and finally how to export data in Excel format.

After the relevant data was obtained, the students were briefed on how to use Mendeley desktop to download relevant Pdfs and save in a folder.

Mendeley has become an indispensable resource for scholars, researchers, and students, providing an extensive feature aimed at optimizing the study process. As a reference management software, Mendeley allows users to efficiently organize and manage their references and citations. One of its primary applications is the ability to import references from a wide array of sources, including academic databases, websites, and PDF documents. This functionality helps researchers maintain a well-structured library, making it easier to keep track of important literature throughout the research process. Mendeley has capability to generate citations and bibliographies automatically in various formats, such as APA, MLA, and Chicago. This feature is particularly beneficial for those engaged in writing academic papers, as it saves time and ensures accuracy in referencing. Users can seamlessly insert citations while composing their documents, allowing for a more streamlined writing experience. Mendeley is particularly good at annotating PDFs; users may highlight text, make comments, and place bookmarks right on research pages. With the help of this interactive feature, scholars may read and comprehend the content more effectively and fully. The platform facilitates collaboration among research teams by enabling users to establish shared libraries and groups. By allowing users to instantly share references, notes, and comments, this tool improves teamwork and creates a more engaging study atmosphere. The social networking aspect of Mendeley also connects users with other researchers in their field, encouraging the exchange of ideas and the discovery of new research opportunities. Moreover, Mendeley provides access to a vast repository of academic papers, facilitating literature discovery based on users' interests and research topics. This feature is essential for keeping up with the latest developments in a particular field, as it allows researchers to explore relevant studies and broaden their understanding of the subject matter. The integration of Mendeley

with word processing software, such as Microsoft Word and LibreOffice, further enhances its utility. This integration allows users to manage citations and bibliographies directly within their writing environment, making it simpler to create polished, well-referenced documents. Reading and annotating a research article for relevant portion is a significant part of literature review. Students were introduced to the terms like abstract, introduction, results and discussion, experiment, conclusion and supplementary information. How to annotate relevant data, which portions to keep and which portions to ignore was the next part of training. Students were finally told how to store annotated PDF in Mendeley desktop.

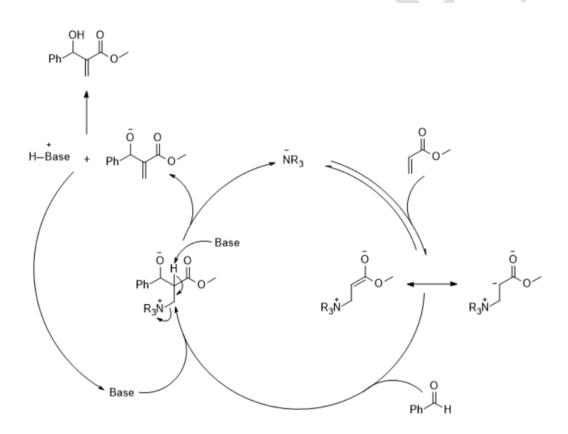
After annotating a document, the next step in the project was to update the reporting language and prepare a literature review. An important component of the reporting part is use of Chemdraw for drawing the chemical reactions and reporting the reaction parameters. The students were given sessions on use of Chemdraw and advanced chemdraw tools for chemical drawing.

Biorender is a Discovery Studio Visualizer (BIOVIA). After optimizing the molecule in chemdraw 3D, they can be exported in biorender to see its composition and the binding sites. It is also used for 2D diagram of the molecule. It may also adjust the visibility of the receptor and ligand while learning about the protein-ligand interaction, including bond kinds and distances. Students were taught how to investigate the H-bonding, charge, ionizability, aromatic, and hydrophobic properties of the protein and ligand. Students were given a training on use of biorender for enhancing the visualization of scientific data, making complex concepts more accessible. Biorender training was followed by training students on the use of Adobe illustrator.

Adobe Illustrator is commonly used for graphic designing and editing images and videos. It is a tool to design icons, logos, illustrations etc. It can be used to design the complex structures of the molecules and the reactions using number of drawing tools, customized brushes to make reactions attractive and more presentable.

The Morita-Baylis-Hillman (MBH) reaction is a carbon-carbon bond-forming reaction between an activated alkene and an aldehyde, catalyzed by a nucleophilic catalyst such as a tertiary amine or phosphine. Despite its utility, there is a significant knowledge gap in the possible use of MBH reaction for synthesis of value-added compounds. Current research is focused on reviewing the latest reports on optimized reaction conditions, developed new catalysts, % catalyst loading and used solvents, to improve yields and selectivity of MBH reactions reported in the last five years.

Morita-Baylis-Hillman, or MBH reaction is a carbon-carbon bond-forming reaction between an activated alkene and a carbon electrophile, typically an aldehyde or ketone in the presence of a nucleophilic catalyst, such as a tertiary amine or phosphine. This reaction is famous for its ability to create densely functionalized products under mild circumstances, making it a useful tool in organic synthesis. The reaction also introduces chiral centre, which is crucial for the synthesis of enantiomerically enriched compounds. It is named after Anthony B. Baylis and Melville E. D. Hillman, two of the chemists who developed the reaction at Celanese; and K. Morita, who published earlier work on the same. The MBH reaction generally proceeds through three main steps: Michael Addition, Electrophilic Quenching, Proton Transfer and **Elimination.** The DABCO (triethylenediamine), common catalysts include DMAP(4dimethylaminopyridine), DBU (diazabicyloundecene), and various phosphines. It offers several advantages in organic synthesis, but the reaction is extremely slow. Mechanism:



Morita–Baylis–Hillman (MBH) adducts are an important family of chemical synthesis intermediates that give chemists flexible tools to build intricate molecular structures.

MBH adducts are used as building blocks in the synthesise of natural and pharmaceutical compounds which is one of their main uses. The building of complex molecular framework is made possible by the additional transformation of these adducts into a range of functionalised molecules. Their versatility is demonstrated by the fact that they may undergo a range of reactions, including cyclization, reduction, and oxidation. In addition to their synthetic utility, MBH adducts are particularly valuable for their stereochemical outcomes. The capacity to produce stereochemically defined molecules is essential in medicinal chemistry, as the three-dimensional configuration of atoms can greatly affect a drug's efficacy and safety profile. Moreover, MBH adducts play a crucial role in diversity-oriented synthesis (DOS), a strategy that emphasizes the generation of a wide array of structurally diverse compounds from a common precursor. The reactions involving MBH adducts can yield multiple products through various downstream transformations, making them ideal for creating compound libraries that can be screened for biological activity. This approach is particularly advantageous in drug discovery, where identifying novel lead compounds is a primary goal. In summary, MBH adducts are essential intermediates in organic synthesis that have a variety of uses, including the synthesis of chiral centers and complicated compounds. Their importance in the creation of pharmaceuticals and the larger area of organic chemistry is highlighted by their capacity to go through a variety of transformation and support diversity-oriented synthesis. MBH adducts' importance in the synthesis of intricate, physiologically significant structures is anticipated to grow as more study is done on their reactivity and applications. This will further establish their status as essential components of the synthetic chemist's toolbox.

Work done so far:

Having identified the target area, all the relevant papers have been downloaded and saved in Mendley desktop. The students have categorised the data and arranged them in a logical manner. The writing work on literature review has begun and students are being trained to write the literature review in a logical and cohesive manner.

Future Goal:

To continue with the writing of the literature review and correspond it to a journal. The learnings from the review article will be used to design the synthesis of some value added products and the same shall be taken up in the lab.