IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Development of Photo-Asymmetric Desymmetrization Reactions via C-H Functionalization**	
Project Number	**IMURA1071**	
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IITB Department:	Chemistry	

Research Clusters:

Highlight which of the Academy's CLUSTERS this project will address?
(Please nominate JUST ***one.*** *For more information, see www.iitbmonash.org)*

1	*Material Science/Engineering (including Nano, Metallurgy)*
2	***Energy, Green Chem, Chemistry, Catalysis, Reaction Eng***
3	*Math, CFD, Modelling, Manufacturing*
4	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*
5	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*
6	*Bio, Stem Cells, Bio Chem, Pharma, Food*
7	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng*
8	*HSS, Design, Management*

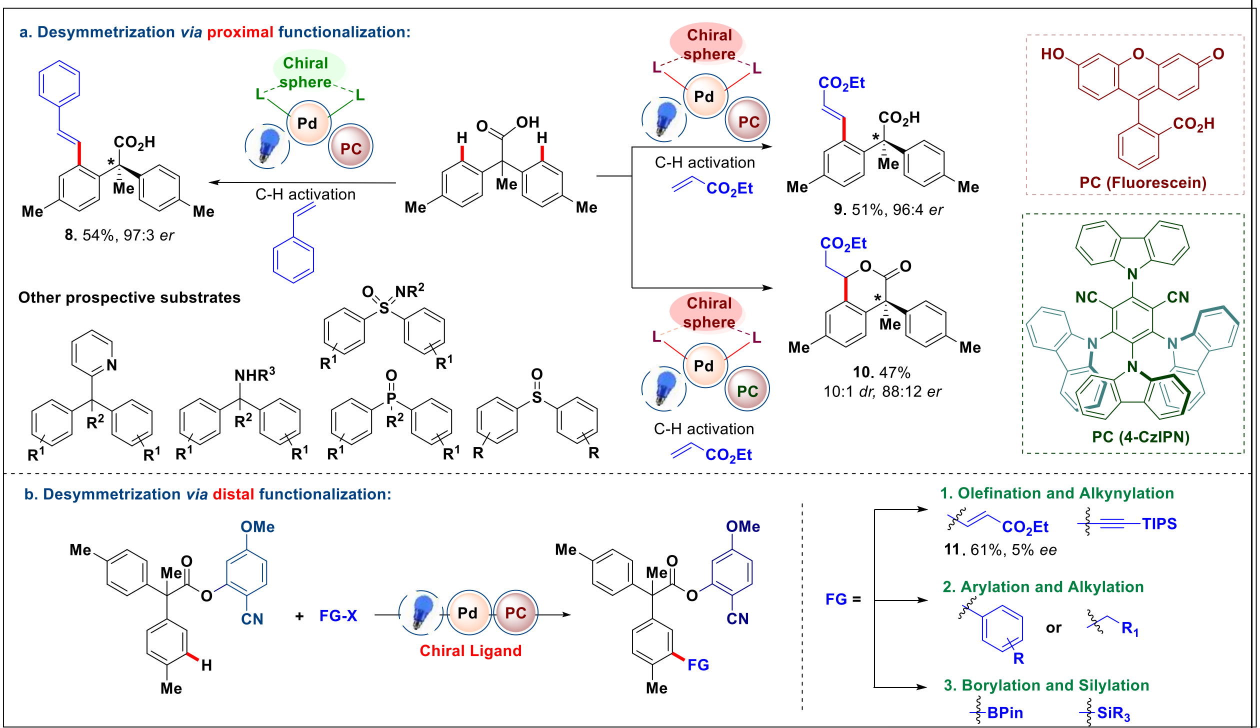
Research Themes:

Highlight which of the Academy's Theme(s) this project will address?
(Feel free to nominate more than one. For more information, see www.iitbmonash.org)

1	*Artificial Intelligence and Advanced Computational Modelling*
2	*Circular Economy*
3	***Clean Energy***
4	*Health Sciences*
5	*Smart Materials*
6	*Sustainable Societies*
7	*Infrastructure*

The research problem

Desymmetrization of molecules containing a mirror plane of symmetry is a simple and efficient pathway to creating chiral material. With the assistance of chiral auxiliaries like chiral MPAAs, an asymmetric transition state could lead to preferential functionalization taking place on only one of the mirroring aryl rings, leading to a chiral product.This is important for two perspectives. First, the generation of two chiral centers from an achiral starting material in a single step is synthetically constructive and efficient, given that control over the two chiral centers is possible. Second, the photocatalyst identity is not typically considered a factor in determining chemoselectivity in transition metal catalyzed C−H functionalization since its primary role in such processes is often the oxidative regeneration of the active transition metal catalyst. The project can also involved in developing additional types of functionalization such as alkynylation, arylation, alkylation, borylation and silylation.



Scheme: Palladium Photocatalyzed Desymmetrization of Diarylacetic Acids *via* C-H Olefination.

Project aims

The aim of this project is to enrich the field of asymmetric palladium catalyzed C−H functionalization specifically *via* photocatalysis. This project introduces chirality by utilizing prochiral symmetrical compounds which could be transformed into chiral molecules in a single step *via* the selective installation of a functional group onto one of the symmetrical sides.

What is expected of the student when at IITB and when at Monash?

The student is expected to learn how to set up optimisation reactions under photo conditions, designing new asymmetric ligands and photocatalysts, acquire and analyse HPLC data on a regular basis.

Expected outcomes

1. Succeeding in the proposed projects would establish palladium photocatalysis as an effective tool in synthesizing an array of chiral material *via* a range of transformative techniques.

2. Development of palladium photocatalysis and utilizing it in enantioselective functionalization

3. Utilization of palladium catalysis in introducing and controlling complex stereochemistry in single step transformations.

4. The proposed will positively impact many fields of research, industry, and medicine since the design and synthesis of chiral small organic molecules is an objective shared across the spectrum of scientific disciplines.

5. Results will be published in peer-reviewed journals

6. Effective catalysts may be patented following the guidelines

How will the project address the Goals of the above Themes?

To accomplish the proposed objective, we begin by exploring light catalysis as a green catalytic mode that eliminates the need for thermal energy and operates in the absence of harmful and expensive silver salts. Relying on light as the energy source of the proposed photocatalytic processes means reactions will be run at ambient temperatures. We expect that lowering the temperature will allow enhanced regio- as well as stereoselectivity in the reactions proposed.

Potential RPCs from IITB and Monash

Provide names of the potential research progress committee members (RPCs) and describe why they are most suited for the proposed project

Capabilities and Degrees Required

B. Sc. (Chemistry)
M. Sc. (Chemistry) with a good knowledge of organic and organometallic chemistry.

Necessary Courses

1. Organometallic chemistry
2. Organic Spectroscopy
3. Physical Organic chemistry

Potential Collaborators

Prof. David W. Lupton(Monash University)

Select up to **(4)** keywords from the Academy's approved keyword list **(available at http://www.iitbmonash.org/becoming-a-research-supervisor/)** relating to this project to make it easier for the students to apply.

C-H activation, Photocatalysis, Asymmetry C-H activation, Organometallic Chemistry, Transition metal catalysis.