IITB-Monash Research Academy

Indian Institute of Technology Bombay | MONASH University

An Indian-Australian research partnership

Project Title:	**Synthesis of biologically relevant heterocycles via Aliphatic C-H Activation**	
Project Number	**IMURA0695**	
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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****,*
3	***Catalysis****, Reaction Eng*
4	*Math, CFD, Modelling, Manufacturing*
5	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*
6	*Earth Sciences and Civil Engineering (Geo, Water, Climate)*
7	*Bio, Stem Cells, Bio Chem, Pharma, Food*
8	*Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng* *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	*Advanced computational engineering, simulation and manufacture*
2	*Infrastructure Engineering*
3	***Clean Energy***
4	*Water*
5	*Nanotechnology*
6	*Biotechnology and Stem Cell Research*

The research problem

Importance of heterocycles is widely known in biological chemistry as they shows excellent diverse biological activities, but to reach them in a sustainable, atom economical way is itself a challenging because of tediousness in synthetic of methodologies used. Selective catalytic transformations using transition metal catalysis offers a powerful method for synthesis of pharmaceuticals and bioactive natural products. Functionalization at carbon centres has immensely emerged in synthetic chemistry over the past decades owing to omnipresence of C–H bond in almost every organic molecule. To enhance the bioactive nature of non-polar molecules present in biological system, nature has routinely been extraditing efficient and selective functionalization by catalytic activity of enzymes. But due to high bond dissociation energy of aliphatic C–H bond than aromatic C–H bond, directing functionalization is a great challenge in synthetic chemistry. These concerned problems demand their unambiguous attention in fields of drug design and diversification. In this proposal, we express our accord to develop and comprehend some unique and unexplored areas of metal mediated selective aliphatic C-H functionalization.

Project aims

In our project we aim to employ the inexpensive transition metals for development of chelation assisted methodology for aliphatic C-H activation of alkanes by using a) Monodentate chelation model b)Bi/multidentate chelation model for selective functionalization γ, ɗ, ε C-H bond of aliphatic systems.

Expected outcomes

a) Methodologies will be optimized and scope will be evaluated
b) Results will be published in peer-reviewed journals.
c) Effective catalysts may be patented following the guidelines.
d) Application of catalyst in industrial and academic settings.
e) Further evaluation of existing methodology in the context of our findings.

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

Selective functionalization at carbon centers is an extremely important topic in present day as it utilizes the most abundant material hydrocarbons/alkanes as a molecular tool for synthetic manipulations. Employing directing group (**DG**) in performing the desired functionalization at carbon centres has served as a ubiquitous strategy in addressing such a challenge. We strive to overrule requirements of pre-functionalized coupling partners or acidic hydrogen for performing **directing group** assisted functionalization onto the aliphatic C-H bond. A conceptually reaching remote carbon locations bonds for selective functionalization of aliphatic molecules however, remained a great problem. Meticulous design & studies of various directing groups will enable the relatively unreactive C–H bonds as potent candidates in the realm of transition metal catalysis. We propose to expand and discover new modes transformations for distal aliphatic sp^3 (γ, ɗ, ε etc.) thereby unravelling some rigorous and enthralling experiences of this unreported solution. We expect to reveal the invention of a powerful synthetic tool box that will be synthetically parallel to biological systems in predicting selectivity with excellent efficiency of biological active molecules.

Capabilities and Degrees Required

B. Sc. (Chemistry)
M. Sc. (Chemistry)

Potential Collaborators

Prof. David W. Lupton

Select up to **(4)** keywords from the Academy's approved keyword list **(available at www.iitbmonash.org)** relating to this project to make it easier for the students to apply.

Aliphatic C-H activation, Transition metal catalysis, directing group assisted, distal C-H activation