IITB-Monash Research Academy

An Indian-Australian research partnership

Project Title:	Studies on the chemistry and chemical engineering of the chemical modification of industrially relevant secondary alcohols	
Project Number	**IMURA0855**	
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IITB Department: Department of Chemistry/Dept of Chem Engg.

Research Clusters: **Research Themes:**

Highlight which of the Academy's CLUSTERS this project will address? *(Please nominate JUST **one.** For more information, see www.iitbmonash.org)*		**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	*Material Science/Engineering (including Nano, Metallurgy)*	***1***	*Advanced computational engineering, simulation and manufacture*
2	*Energy, **Green Chem, Chemistry**, **Catalysis**, Reaction Eng*	2	*Infrastructure Engineering*
3	*Math, CFD, Modelling,*	3	***Clean Energy***
4	*Manufacturing*	4	*Water*
5	*CSE, IT, Optimisation, Data, Sensors, Systems, Signal Processing, Control*	5	*Nanotechnology*
6	*Earth Sciences and Civil*	6	*Biotechnology and Stem Cell Research*
7	*Engineering (Geo, Water, Climate)*		
8	*Bio, Stem Cells, Bio Chem, Pharma, Food*		
	Semi-Conductors, Optics, Photonics, Networks, Telecomm, Power Eng		
	HSS, Design, Management		

The research problem

Many secondary alcohols (or other compounds with a sec-OH group) offer the possibility of value upgradation through manipulation of the sec-OH function. Dehydration (cyclohexanol to cyclohexene), oxidation (cyclohexanol to cyclohexanone, 2-butanol to methyl ethyl ketone), hydrogenolysis (glycerol to 1,3-propanediol) are examples. In many such cases, (for example, glycerol) the raw material with the sec-OH group is abundantly available, for example, as a byproduct of another process. However, one of the main challenges in such conversions is the selective removal/manipulation of the secondary alcohol, because of the easily oxidisable nature of the alcoholic group, steric factors, presence of other functional groups etc. Also, traditional methods for the oxidation of alcohols require stoichiometric amounts of oxidants such as hypochlorite, Cr-salts, Mn-salts, hypervalent iodine, oxygen with transition-metal catalysts, which have several drawbacks in terms of atom economy, economics, and environmental impact as most of the methods generate a huge amount of metal wastes or undesirable by-products. Selective catalytic transformations using transition metal catalysis offers one possible method for synthesis of pharmaceuticals and bioactive natural products. In this project we would like to develop economically attractive platform catalytic chemistries for the conversion of secondary alcohols to value added products, and carry out kinetic and reaction engineering studies to demonstrate scalability and process possibilities.

Project aims

In current project we aim to develop platform chemistries based on economically attractive

catalysts for the selective conversion of secondary alcohols, and demonstrate their process possibilities..

Expected outcomes

a) Methodologies will be optimized on carefully chosen candidate molecules and scope will be evaluated
b) Kinetics and reaction engineering studies will be carried out to establish reactor design methodologies.
c) Results will be published in peer-reviewed journals.
d) Effective catalysts may be patented following the guidelines.
e) Application of catalysts developed in industrial and academic settings.
f) Further evaluation of existing methodology in the context of our findings.

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

Selective removal of any functionality from organic molecule requires special set of critical and harsh reaction conditions but these methods always pose several problems because of other functional group present in molecule. Employing a suitable strategy, (e.g. directing group **DG**) in performing the desired functionalization/de-functionalization at carbon centres has served as a ubiquitous strategy in addressing such a challenge. Meticulous design & study of various directing groups under different catalytic system will allow us to bind C–OH secondary alcohols to directing group for easy and facile defunctionalisation. We propose to expand and discover new modes of these transformations for removal of secondary alcohols to make the method generalised and use abundant precursors to generate value added chemicals thereby unravelling some rigorous and enthralling experiences for this unreported solution. We expect to reveal this invention as a powerful synthetic tool box that will be synthetically parallel to industrial scale for unravelling new product line for billion dollar chemical industries.

Capabilities and Degrees Required

M. Sc. (Chemistry) with a good knowledge of reaction kinetics or M. Tech. (Chemical Engineering) with good familiarity with organic chemistry

Potential Collaborators

Prof. Alan Chaffee

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 and aromatic compounds, Removal of secondary alcohol from organic molecule, defunctionalisation, Transition metal catalysis, directing group.