

**Name:- Dr. Rohitkumar Gulabrao Gore**

**Address(Optional):-**

**Personal Details:-**

<b>Name</b>	<b>GORE</b>	<b>ROHITKUMAR</b>	<b>GULABRAO</b>
	<i>SURNAME</i>	<i>FIRST NAME</i>	<i>MIDDLE NAME</i>
<b>Department</b>	<b>Chemistry</b>		
<b>Designation</b>	<b>Assistant Professor</b>		
<b>Qualification(s)</b>	<b>M. Sc., Ph. D.</b>		
<b>Certification(s)/Professional Courses/Exams</b>	<b>-</b>		
<b>Email-Id</b>	<b>@fergusson.edu</b>		
	<b>rohitggore@gmail.com</b>		
<b>Office Contact No:-</b>	<b>020 30866148</b>		
<b>Mobile No(Optional):-</b>			

**Member Of:-**

<b>College Committees</b>	<b>Other Committees</b>
	<b>NACC Criteria 4</b>

**Research Done:**

**\* PhD: "Novel Low Antimicrobial Toxicity Imidazolium Ionic Liquids: Design, Synthesis and Their Applications in Organic Synthesis"**

Molten salts which are ionic (i.e. a mixture of cation and anion) in nature and have a melting point below 100 °C are termed as Ionic liquids (ILs). ILs have received more attention in the last couple of decades due to their unique properties such as low vapour pressure, high thermal stability, non-flammability, control over the product distribution and recyclability. Due to the control over fugative emission; ionic liquids can be a possible replacement for

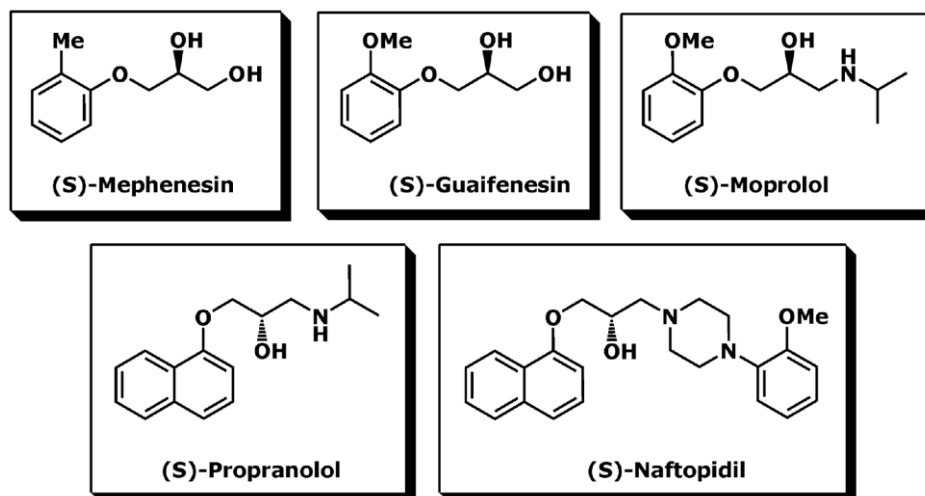
volatile organic compounds (VOCs), which are commonly used as solvents in organic processes. Ionic liquids have already been found useful in different fields of chemistry, such as organic chemistry, electrochemistry, analytical chemistry and biochemistry.

The thesis is focused on the application of ionic liquids in the context of Green Chemistry principles in Organic synthesis. A library of novel imidazolium ionic liquids was designed and synthesised in efforts to find molecules which had reduced anti-microbial toxicity and increased aerobic biodegradation. Synthesis of novel ionic liquids has been carried with efficient and easy methods to achieve atom economy, reduced number of steps and high yields. Ionic liquids synthesized in the lab have been tested either as a catalyst in acetalization reactions, or as a solvent in the Baylis-Hillman and asymmetric Carbonyl-Ene reactions. These studies have given excellent results and clearly demonstrated the potential and applicability of ionic liquids in organic synthesis. Working with our collaborators, biocompatibility of these ionic liquids has been studied. Preliminary studies of the toxicity of all ionic liquids were performed against a panel of 12 fungi and 8 bacterial strains. Antifungal and antibacterial toxicity studies demonstrated that most of these ionic liquids did not inhibit the growth of any organism screened at concentrations of 2.0 mM. Biodegradation studies of the novel ionic liquids have also been performed and have given valuable information on the next step in rational design towards readily biodegradable ionic liquids.

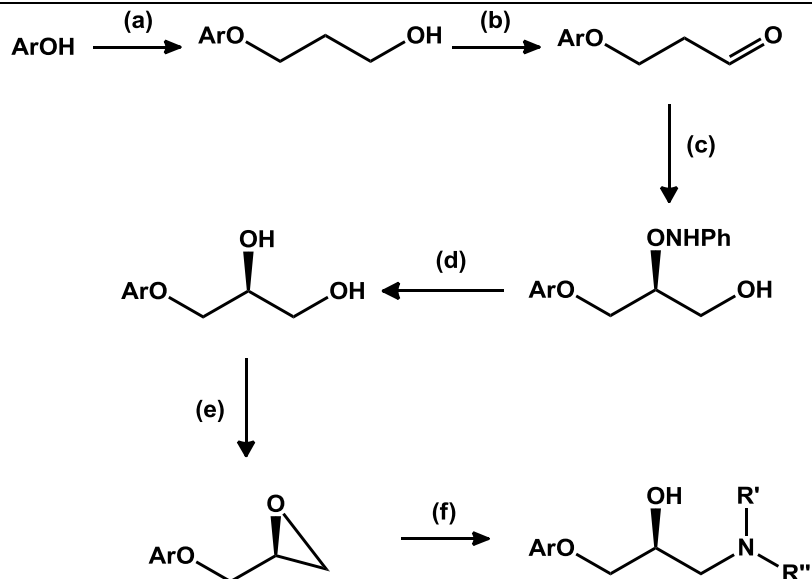
※ **"Proline catalyzed enantioselective synthesis of  $\beta$ -blockers"**

$\beta$ -Adrenergic blocking agents ( $\beta$ -blockers) are important drugs used for the treatment of hypertension and angina pectoris. Most of the  $\beta$ -blockers possess a general structure  $\text{Ar-O-CH}_2\text{CH(OH)CH}_2\text{NHCH(CH}_3)_2$  and have been used in the form of racemic mixtures. There are four types of receptors for these molecules ( $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$  and  $\beta_2$  adrenergic receptors). Blocking of the  $\beta$ -receptor system reduces the overall activity of the sympathetic nervous system.

Agents which are  $\beta$ -blockers are thus used to increase life expectancy after a heart attack. Although (*S*)-isomers are known to be much more effective (100-500 fold) than the (*R*)-isomer, these antihypertensive drugs are presently sold as racemic mixtures. To avoid unnecessary stress or in some cases the toxicity/side effect issues caused by the (*R*)-isomers, the administration of optically pure (*S*)-isomer is desirable.



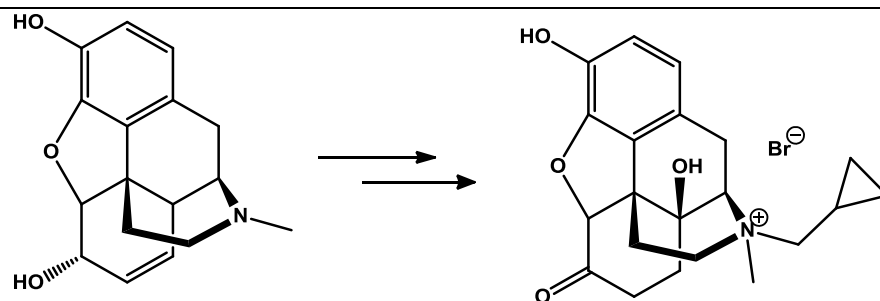
(*S*)-Propranolol, (*S*)-Moprolol are amongst the most widely used  $\beta$ -blockers, which possesses antihypertensive, antianginal, and sympatholytic properties. A number of molecules discussed above have been synthesized according to the generalized method:



**Reaction conditions:** (a) 3-Bromopropanol, 10% aq. NaOH, reflux, 6 h; (b) IBX, DMSO, rt, 2 h; (c) PhNO, L-Proline, Acetonitrile, -20 °C, 24 h then NaBH<sub>4</sub>, MeOH, -20 °C, 30 min; (d) 10% Pd/C, MeOH, H<sub>2</sub>, rt, 6h; (e) TsCl, NaH, THF, 0 °C, 30 min; (f) Amine, DCM, rt, 12h.

\* **"Novel synthesis and supply reference standards for the drug candidate identified by the client"**

This project was sponsored by Wyeth, USA. Our research focus was to design a synthetic route leading to a cost effective up scaling process for development of Naltrexone and derivatives thereof. In this project, my role was to carry out multi-step, small scale reactions such as protection & deprotection of alcohols, amines etc., oxidation (Swern, PCC, PDC, metal catalyzed in presence of oxygen etc.), reduction, selective hydrogenation and hydroxylation on the opiate scaffold. All compounds were purified by column chromatography and further characterised by different analytical techniques such as <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, GC-MS, HRMS and HPLC.



We have used *Morphine, Codeine and Thebaine* as a starting material, however due to the secrecy of the project I cannot give much information. In this project I have received more than 2 years research experience in the synthesis of opioid derivatives.

### Area of Interest in Research:

<b>Organic Synthesis</b>
<b>Asymmetric Catalysis &amp; Synthesis</b>

### Books Published:

Name of Book	Author(s)	ISBN No.	Year	Edition	Publisher
Ionic Liquids - New Aspects for the Future	Rohitkumar G. Gore, Nicholas Gathergood,	978-953-51-0937-2,	2013	1st	InTech

### Research publications:

1. Organocatalytic enantioselective synthesis of $\beta$ -blockers: (S)-Propranolol and (S)-Naftopidil, S. P. Panchgalle, R. G. Gore, S. P. Chavan and U. R. Kalkote, <i>Tetrahedron: Asymmetry</i> , <b>2009</b> , Vol. 20(15), pg. 1767-1770.
2. Highly recyclable, imidazolium derived ionic liquids of low antimicrobial and antifungal toxicity: A new strategy for acid catalysis, L. Myles, R. Gore, M. Spulak, N. Gathergood

and S. J. Connon, <i>Green Chemistry</i> , <b>2010</b> , Vol. 12, .1157-1162.
3. Tandem ionic liquid antimicrobial toxicity and asymmetric catalysis study: carbonyl-ene reactions with trifluoropyruvate, R. G. Gore, T.-K.-T. Truong, M. Spulak, L. Myles, S. Connon and N. Gathergood, <i>Green Chemistry</i> , <b>2013</b> , Vol. 15, pg. 2727-2739.
4. A new generation of aprotic yet Brønsted acidic imidazolium salts: low toxicity, high recyclability and greatly improved activity, L. Myles, R. G. Gore, N. Gathergood and S. J. Connon, <i>Green Chemistry</i> , <b>2013</b> , Vol. 15, pg. 2740–2746.
5. A new generation of aprotic yet Brønsted acidic imidazolium salts: effect of ester/amide groups in the C-2, C-4 and C-5 on antimicrobial toxicity and biodegradation, R. G. Gore, L. Myles, M. Spulak, Ian Beadham, M. T. Garcia, S. J. Connon and N. Gathergood, <i>Green Chemistry</i> , <b>2013</b> , Vol. 15, pg. 2747–2760.
6. “Low toxic” ionic liquids: greener and alternative solvent for asymmetric carbonyl-ene reaction of phenylglyoxal, R. G. Gore, T.-K.-T. Truong, M. Spulak, S. Connon and N. Gathergood, <b>2014</b> , Vol. 1, pg. 239-248

### Seminars and Workshops Attended:-

#### Oral Presentations:

1. Biodegradable Catalytic Asymmetric Methods - A study of solvents, organocatalysts and magnetic nanoparticle-supported catalysts, Conference: Green Chemistry in Ireland: including highlights of Environmental Technology projects funded by the EPA, DCU, Dublin, 15 April 2010.
2. Biodegradable, non-bactericidal Ionic liquids, Conference: 62nd Irish Universities Chemistry Research Colloquium, Queen’s University Belfast, 1-2 July 2010.
3. Green Catalysts for Organic Synthesis, Conference: 9th Annual Postgraduate Seminar, Dublin, 17 November 2011.
4. Greener Organocatalysis: Toxicity and biodegradation studies, Conference: Green Chemistry II: Sustainable Catalysis and Emerging Environmental Technologies, DCU, Dublin, 12 July 2012.

#### Poster Presentations:

1. Biodegradable, non-bactericidal Ionic liquids, R. G. Gore , S. Morrissey, B. Pegot, D. Coleman, I. Beadham, M. Gurbisz, M. Ghavre, M. T. Garcia, D. Ferguson, B. Quilty, N. Gathergood, Biodegradability and Toxicity of Ionic Liquids 2 (BATIL 2), 28-29 September 2009 in Frankfurt/Main, Germany.
2. Biodegradable, non-bactericidal Ionic liquids, R. G. Gore, L. Myles, D. Coleman, I. Beadham, M. Gurbisz, M. Ghavre, M. Spulak, M. Pour, B. Quilty, S. Connon and N. Gathergood, EPA National Research Conference, 23 June 2010, Croke Park, Dublin.
3. Highly recyclable, low antimicrobial and antifungal toxicity ionic liquids: A new strategy for Brønsted acid catalysed reaction, R. G. Gore, L. Myles, M. Spulak, M. Pour, S. Connon and N. Gathergood, Green Solvents Conference, 10-13 October 2010, Berchtesgaden, Germany.

### **Seminars and Workshops Organized:-**

--

### **Other Accomplishments:-**

Recipient of “ <b>Wesley Cocker Award</b> ” 2014, presented by Society of Chemical Industry (All Ireland Group, UK & Ireland) to recognise a young scientist – PhD student or undergraduate – in the Republic of Ireland who has made a major contribution in some aspect of chemistry relevant to Irish industry.
--