IITB-Monash Research Academy

An Indian-Australian research partnership

Indian Institute of Technology Bombay | MONASH University

Project Title:	**Experimental and Computational approach to Squaramide based Foldamers**	
Project Number	**IMURA0340(A)** *(will be inserted by The Academy)*	
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Monash Co-supervisor(s) (Name, Email Id, Phone)	-NA-	
Monash Department:	School of Chemistry	
IITB Main Supervisor (Name, Email Id, Phone)	G. Naresh Patwari naresh@chem.iitb.ac.in	*Full name, Email*
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IITB Department:	Department of Chemistry	

Research Academy Themes:

Highlight which of the Academy's Theme(s) this project will address? 1

(*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

Define the problem

Understanding folding in hetero-polymers is a long standing issue which especially relates to the folding of biological macromolecules such as proteins, DNA and RNA. The free energy landscape of folding is quite rugged with the presence of multiple minima. In such cases understanding the folding pathways tends to become difficult as the chemical entities in the case of biopolymer are fixed which gives very little conformational flexibility to explore the free energy landscape. Squaramides, in this scenario offer an excellent the choice to understand the free energy landscape of the foldamers. The conformational flexibility is bought about the methylene linker groups $-(CH_2)_n-$ will be investigated. The role of substitutions on the preferential folding into helical and sheet like structures will be investigated. Further, the role of odd vs. even number of the methylene linker groups will also be investigated.

Project aims

Define the aims of the project

The aims of this project are to understand which fundamental components play an important role in the folding of the squaramide based foldamers. This will be achieved by combing experimental measurements along with both classical and *ab-initio* and molecular dynamics methods. The experimental methods will comprise of fluorescence spectroscopic techniques both in the energy and time domains. Additional methods such as fluorescence correlation spectroscopy and other structural techniques such as NMR and single-crystal XRD studies will also be used wherever necessary. First principles methods will include symmetry adapted perturbation theory (SAPT), effective fragment potential (EFP) and modifications of the SCS-MP2 method recently developed in Dr Pas's group to accurately calculate the free energy surface of the foldamers. The solvent effects will also be investigated through implicit solvent (polarisable continuum models) and explicit solvent (inclusion of actual solvent molecules as clusters) approaches. The computational results will be correlated with experimental data to establish a computer-aided design of the folding of this class of compounds.

Expected outcomes

Highlight the expected outcomes of the project

The outcomes of this project will be:

1. Role of conformational flexibility by introducing varying length of the linker groups connecting the on the squaramides.
2. Substitutions dependence on the substituents on switching from helical to sheet structures.
3. Role of odd vs. even number of methylene groups on the conformational flexibility of the squaramide foldamers.

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

Describe how the project will address the goals of one or more of the 6 Themes listed above.

High-level *ab initio*-based methods will be applied to predict energetics, structure and chemical reactivity of molecular aggregates of phenylacetylene and its substituted analogues, thus further advancing our understanding of how the structure and chemical reactivity of similar systems with weak intermolecular interactions can be tailored. The experiments will be carried out at IIT Bombay using fluorescence spectroscopic techniques along with some structural methods such as NMR and single-crystal XRD studies. The experimental results on these systems will be underpinned by computational results. This project will address the Advanced computational engineering, simulation and manufacture theme. *Ab initio*-based calculations will be conducted using the computational facilities available to Dr. Pas at Monash University.

Capabilities and Degrees Required

List the ideal set of capabilities that a student should have for this project. Feel free to be as specific or as general as you like. These capabilities will be input into the online application form and students who opt for this project will be required to show that they can demonstrate these capabilities.

A student should have MSc. in chemistry with basic understanding of quantum chemistry and physical chemistry and should have aptitude towards advanced experimental techniques.