



Waterford Institute of Technology  
INSTITIÚID TEICNEOLAÍOCHTA PHORT LAIRGE

## Postgraduate Scholarship Information Sheet

<b>Scholarship title</b>	Enantioselective synthesis of biologically relevant molecules using catalysis in continuous flow
<b>Reference number</b>	WD_2017_PhD_026w
<b>Supervisor(s)</b>	Dr Mike Kinsella, Dr Claire Lennon, Dr Joe O'Mahony
<b>Research Group</b>	Pharmaceutical and Molecular Biotechnology Research Centre
<b>Department / School</b>	Dept of Science, School of Science and Computing
<b>Duration</b>	4 years
<b>Status: Full-time / part-time</b>	Full-time
<b>Funding information</b>	Funding agency: Waterford Institute of Technology Funding programme: WIT PhD Scholarship
<b>Value of the scholarship (per annum)</b>	Stipend: €10,000 Fees: €4,500 Research costs: €2,000
<b>Teaching requirement (if any)</b>	Two hours of academic development activities per week during the academic year in line with scholarship requirements
<b>Closing date and time</b>	Monday 24 <sup>th</sup> April 2017 at 5pm GMT
<b>Commencement date</b>	1 <sup>st</sup> September 2017

### Post summary

Applications are invited from suitably qualified candidates seeking to pursue a PhD in the area of organic and analytical chemistry with an interest in engineering on a recently funded research project within the Pharmaceutical and Molecular Biotechnology Research Centre (PMBRC) at WIT. This project will include aspects of reactor design and manufacture, organic synthesis, analytical method development and characterisation for the purpose of design, synthesis and evaluation of novel organic catalysts for enantioselective synthetic organic reactions. The project will also include evaluation of biocatalysts for organic reactions generating a researcher with a broad set of skills highly relevant to the Pharmaceutical Industry.

We have previously completed and published studies applying organocatalysis in batch mode and are currently working in this area. Our novel prolinamide catalysts have been applied to the aldol reaction giving high enantiomeric excesses and yield using standard laboratory conditions and glassware. We would now like to extend this work to convert these successful batch enantioselective organocatalysts into flow processes, serving as a proof-of-concept that organocatalysts in batch conditions can be applied to continuous processes, via homogeneous and/or heterogeneous catalysis conditions.

In a second strand of work, we have successfully screened a library of bacterial isolates and discovered a novel whole cell catalyst, which was found to efficiently catalyse nitrile hydrolysis with remarkably high enantioselectivity. This isolate was subsequently tested with 33 related nitriles. We would also like to adapt this biocatalytic nitrile hydrolysis to flow conditions. The advantages of microbes/enzymes as catalysts when applied in continuous flow reactors are also significant. Residence times are shorter, the reactor can

give increased productivity and handling of substrates of low solubility is improved. The consistent, reproducible reaction conditions can lead to purer product.

The project objectives are as follows:

- To design and engineer a laboratory scale flow reactor with appropriate process control and sensing and evaluate in-house catalysts in the synthesis of oxindoles, assessing the product yield, residence time and enantiomeric excess.
- To adapt a microbial isolate for application to the flow reactor for the synthesis of  $\beta$ -hydroxy acids and amides from nitriles.
- To significantly broaden the reaction scope of the most efficient flow system by applying it to both homogeneous and heterogeneous conditions and train the student to expert level in this area.
- To investigate alternative reactions catalysed in continuous flow such as Mannich and Michael reactions.
- To enhance existing, and create new collaborations with academic and industrial partners to strengthen the research portfolio and international visibility and dissemination of work carried out in the PMBRC

The student will gain experience in several complementary disciplines, including organic chemistry, analytical chemistry and engineering. The student will work within the PMBRC, with a wide range of equipment and expertise available.

### **Standard duties and responsibilities of the scholarship**

With regard to the duties for the academic development of the scholarship student, the following are some examples of these duties but not restricted to:

- Teaching
- Tutorials and outreach programmes
- Laboratory supervision
- Undergraduate mentoring
- Student retention
- Promotional activities and open day events
- Conference and networking organisation

### **Person specification**

#### **Qualifications**

##### Essential

- Applicants should hold or expect to attain, as a minimum, a 2.1 Honours degree<sup>1</sup>, or equivalent, by the 1<sup>st</sup> of August 2017, in Chemistry, Pharmaceutical Science, Biotechnology, Molecular Biology, Analytical Chemistry, Chemical Engineering, Organic Chemistry, Pharmaceutical Chemistry, Synthetic Chemistry or related chemistry discipline, however preference will be given to those with a 1H or Masters in Chemistry/Pharmaceutical Science. Organic and analytical chemistry should be a core theme of the degree.

##### Desirable

- Knowledge of pharmaceutical science, synthesis of pharmaceutical drugs and experience in analytical characterisation techniques.

<sup>1</sup> If undergraduate examination results are not known at the time of application, WIT may make a provisional offer of a scholarship on condition that the applicant's bachelor's degree results is a first class or upper second-class honours.

## Knowledge & Experience

### Essential

- Applicants must have experience in the synthesis, characterisation and purification of organic compounds including multi-step chemical synthesis.
- The applicant must be competent in the interpretation of NMR, MS, IR and UV spectra along with preparing samples and where appropriate running experiments to generate spectra. In addition knowledge of the use of HPLC and instrumental software to run such analytical characterisation instrumentation is required.
- Applicants should have an interest in green chemical synthesis and use of new more environmentally friendly methods to synthesise pharmaceutical intermediates as well an interest in reactor design and engineering
- A good level of generic skills such as literature review skills, use of on-line databases, report writing would also be required.

### Desirable

- The candidate has completed an undergraduate project or equivalent in synthetic chemistry or has gained relevant synthetic experience within the pharmaceutical industry.
- Experience of method development for HPLC, GC, LC-MS or GC-MS.
- Experience in the operation of analytical instrumentation such as HPLC, GC, GC-MS, LC-MS, NMR and the use of control software for such instrumentation.

## Skills & Competencies

### Essential

- Applicants whose first language is not English must submit evidence of competency in English, please see [WIT's English Language Requirements](#) for details.
- The applicant must have a high level of self-motivation, be able to think and work independently.
- Good communication skills, motivation to learn, both from peers and independently.
- Good IT skills, including Microsoft office is essential. Knowledge of statistical techniques would be an advantage.

### Desirable

- Knowledge of scientific Database searching, literature review writing and good scientific writing skills.
- Experience on the use of chemical drawing software packages, reference management software

## Further information

For any informal queries, please contact Mike Kinsella at [mkinsella@wit.ie](mailto:mkinsella@wit.ie)

For queries relating to the application and admission process please contact the Postgraduate Admissions Office via email [pgadmissions@wit.ie](mailto:pgadmissions@wit.ie) or telephone +353 (0)51 302883.

Website: [www.wit.ie](http://www.wit.ie)

## Application procedure

Please download the Research Postgraduate Application Form from the WIT Website.

Any queries relating to the application process should be emailed to [pgadmissions@wit.ie](mailto:pgadmissions@wit.ie).

**The Institute may decide to interview only those applicants who appear from the information available, to be the most suitable, in terms of experience, qualifications and other requirements of the post.**

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