Early Stage Researcher position as a PhD scholarship available at the Department of Chemistry, University of Milan (ITALY), in the framework of the EU-funded Marie Skłodowska-Curie ITN-EID training network TECHNOTRAIN "Enabling TECHNOlogies-driven chemistry: a tailored TRAINing research program for batch and flow synthesis of chiral amino derivatives".

#### The TECHNOTRAIN network

The main aim of TECHNOTRAIN is to create a training platform for young European researchers, based on the creativity, flexibility and accuracy characteristic of an academic working environment, but with an industrial focus.

"TECHNOTRAIN" consortium wants to enhance and encourage young European researchers providing them with a wide, pragmatic and dynamic overview of the scientific industrial domain. "TECHNOTRAIN" has as specific objective to develop stereoselective, catalytic synthetic methods applicable for industrial production of enantiomerically pure, functionalized amino derivatives featuring a quaternary stereocenter. Target molecules will be chiral pharmaceutically active ingredients, or immediate precursors, including nonproteogenic alfa-disubstituted-amino acids. More generally, the project research activity will focus on the preparation of other differently functionalised, quaternary chiral amines, with the aim both to successfully synthesize specific target molecules and to develop highly efficient, technology-driven methodologies. The combination of two modern, catalytic strategies (photocatalysis and organocatalysis) with safe and environmental friendly technologies is a key step towards the development of a more efficient, sustainable chemistry, in line with the Europe strategy. The "TECHNOTRAIN" approach of 'training through research' in emerging and interdisciplinary areas, is crucial for preparing the future generation of scientists able to transfer green, sustainable chemistry into industrial processes.

"TECHNOTRAIN" is a 1:1 industrial/academic twinning where <u>three PhD</u> research projects will be carried out in full collaboration between the private and the public research site, as witnessed by a 1:1 allocation of person months of each ESR between University of Milano and a German company in Dortmund. The research projects are of strong interest both from a scientific and an industrial point of view, and will necessitate frequent contacts of the partner units.

### Research group and general conditions

The PhD students will be placed at the Department of Chemistry, University of Milan, in the laboratory of Prof. Maurizio Benaglia, and under his supervision (group website: http://users2.unimi.it/Benagliagroup/index.html). The recruited PhD students will be enrolled in the PhD programme in "Industrial Chemistry", and will be covered under the social security scheme. They will receive a Monthly Living Allowance plus a Mobility Allowance compliant with the applicable EC Marie Skłodowska-Curie Actions-ITN general conditions.

The recruited PhD students will participate in the network's training activities and work placements at the laboratories of the participating academic and industrial partners. In addition, the training programme of the recruited ESRs will be supplemented by regular meetings and workshops.

#### The research project

## ESR1: In batch and in flow catalytic addition of C1 fragments to C=N bonds

ESR 1, associated to WP1, will develop new, "ad hoc" tailored catalysts for the enantioselective organocatalytic addition on differently functionalized ketoimines of cyanide anion, employing, among others, photochemical activation methodologies. ESR 1 will investigate the use of *ad hoc* modified chiral thiourea-based catalysts, but also of chiral phase transfer catalysts, to control the cyanide addition to unprotected ketimines. Innovative catalytic strategies for this type of reaction will be explored, based on the concept of chiral ion pair. Additionally, unprecedented stereoselective reactions of imines with CO<sub>2</sub> will be investigated. Finally, the use of micro-(meso)-reactors will be also considered.

#### ESR 2:Stereoselective reactions of nitroester promoted by different organocatalysts

ESR 2 will study unprecedented synthetic strategies for the synthesis of  $\alpha$ ,  $\alpha$ –disubstituted amino acids and, among others, of fluorinated chiral amino acid derivatives, employing newly designed

organocatalysts, especially a new generation of chiral phase transfer catalyst. Additionally, a second strategy will be explored, that starts from easily available ketones, converted to nitroolefins which will be organocatalytically reduced to afford enantiopure nitroalkanes, as highly functionalised starting materials for the alkylation step. Also for these challenging transformations, continuous flow processes will be considered, to perform a fast screening of the reaction conditions, and then, with the optimized conditions in hand, scale up the reaction.

# **ESR 3**: Development of supported, recyclable chiral catalysts, of 3d-printed in wall functionalized mesoreactors and of catalytic reactors for flow chemistry processes

ESR 3 associated to WP3 will explore alternative immobilization strategies on different materials, in order to develop efficient recyclable chiral catalysts and to open new avenues towards more sustainable processes. The ESR will deal also with the preparation of catalytic reactors, to be used in continuous flow operations, and with the very challenging and unmet goal to realize in-wall functionalized reactors, taking advantage also of 3D-printing technologies.

All the ESRs will be involved in a final WP, devoted to the application of the selected methodologies to the preparation, in batch or flow mode, of chiral building blocks and intermediates of special interest, according the company indication.

Planned secondments: all ESR3 will spend 18 months in Milano and 18 months in Dortmund, with one possible short secondment (2-3 months) in another Institute ( to be defined).

Starting date of the PhD programme: May 1st 2019.

## Admission criteria for doctoral education at the University of Milan

In order to apply for a place in the PhD programme, students must have a second-level degree, an equivalent qualification, or an equivalent qualification by study level (Master's Degree) from a foreign University. In addition, English language skills at B2 level (minimum) is required to cover the position. The suitability of the foreign academic qualifications in terms of content is appraised by the Examining Board constituted for admission to each PhD programme, in compliance with the regulations in force in Italy and in the country in which the academic qualification was issued, and the international treaties or agreements pertaining to the conferment of qualifications for the continuation of studies.

#### Other specific requirements

## - Master degree in Chemistry or equivalent

- A suitable background for the open positions includes synthesis and structural characterization of chiral molecules;
- A basic background in catalysis will be also appreciated;
- Experience in performing laboratory work independently;
- Good collaborative and social skills and an open-minded mind-set;
- Good proficiency in written and spoken English (minimum B2 level).

## Mobility eligibility requirement

The fellow must not have resided in the country where the research training activities will take place for more than 12 months in the 3 years immediately prior to the recruitment date (and not have carried out their main activity (work, studies, etc.) in that country).

## **Experience eligibility requirement**

Eligible applicants must have less than 4 years research experience (Early Stage Researcher) at the signature of the contract (measured from the time the Master's degree has been obtained). Eligible applicants must not have a PhD yet.

#### **Application procedure**

The applicant must send the following documents (<u>included in a single PDF file</u>) to Prof. Maurizio Benaglia (Maurizio.benaglia@unimi.it) <u>within February 28 2019</u>, clearly indicating in the subject "Application for ESR position Technotrain":

- 1. Personal statement/motivation letter (up to 1 page) about the applicants' experience and interests
- 2. A complete CV (personal details academic/education history, research experience experimental skills, publications, English level etc.);
- 3. At least 2 reference letters (in English), at least one of them from one former supervisor and/or lecturer:
- 4. The scan of the degree (usually the Master Degree) which would formally entitle him/her to embark on a doctorate (in case the degree has not been obtained yet, it is necessary to send a declaration of the university stating that the degree will be obtained before the expected starting date) and an official list of grades obtained during the applicant's bachelor and master studies; this document is mandatory for applicants who do not have yet obtained the degree.
- 5. A summary of the Master Degree thesis or a brief description of the past scientific activity (max 2 pag.).

**IMPORTANT NOTE**: The applicants must assure their availability to start the PhD programme non later than **May 1**<sup>st</sup> **2019**.

#### Assessment criteria

Applications must be in English and will be evaluated against the following criteria:

- Educational record;
- scientific quality of the applicant's CV;
- previous experience in the subject of TECHONTRAIN research programme.

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