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Maths4Life Programme - 2024 Call

TERMS & CONDITIONS

The Articles of Association of the *Fundació Institut de Recerca Biomèdica (IRB Barcelona)* (hereafter referred to as IRB Barcelona or the Institute) establish that this institution will promote activities that address collaboration and knowledge transfer and also make calls for fellowship (herein referred to as grant) applications and subsequent awards of the same.

The grants are assigned to students enrolled in a BSc or MSc programme who undertake a research internship under the supervision of group leaders at IRB Barcelona.

I. Objective

These Terms and Conditions serve to regulate the summer internship grants for the 2024 Maths4Life call.

II. Grant Call

The tenth edition of the “Maths4Life” initiative is aimed at outstanding and highly motivated BSc and MSc students from the national and international¹ community with a strong interest in mathematics and statistics.

Five grants are offered to undertake an internship at IRB Barcelona from July to September 2024. The grant stipends included in this call will be covered by IRB Barcelona structural funds for a maximum of 3 months from the start of the internship.

A total of 250 h of research work (minimum of 20 h/week) will be distributed from July to September 2024 upon agreement with the project supervisor at IRB Barcelona.

Awardees will be hired by IRB Barcelona and will receive a gross amount of €1200 for the training period.

¹ Only students from the European Union are eligible.



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Awardees will be offered the opportunity to participate in in-house institutional activities.

Awardees will be supervised by a group leader at IRB Barcelona (or the designated senior researcher) previously assigned and agreed with the awardee before signature of the contract. This group leader will oversee that the duties assigned to the awardee are fulfilled and will notify IRB Barcelona's Academic Office of issues affecting the undertaking of these duties or other pertinent circumstances, so that corrective measures can be taken and/or proceedings to withdraw the grant can be started.

III. Requirements and Selection Criteria

1.- The Maths4Life Programme has been designed to encourage and further the training of young emerging researchers in biomedical research topics.

- Addressed to students who have completed at least 120 ECTS of a BSc degree in Mathematics, Physics, Statistics, Informatics, and related areas by June 2024 and MSc students in the same fields.
- Sound knowledge of statistics or programming for the field of biology, chemistry or medicine.
- Good knowledge of English.

2.- Candidates will be selected exclusively on merit, on the basis of academic records, motivation letter, as well as other criteria, such as internationalisation, previous research experience, and letter of reference. No selection criteria for positive or negative discrimination will be applied.

IV. Application Procedure

Applicants should send the documents listed below to phd@irbbarcelona.org , indicating "Maths4Life candidacy" in the subject box before 9 May 2024.

- CV
- A scanned copy of the student's certified Academic Record. These documents must show the grades attained in exam periods.
- Additional certificates, prizes, and recognitions
- Motivation letter



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- A letter of reference from university lecturers or scientists with whom the student has studied or worked. Only letters with an official letterhead and signature will be accepted.

Applicants should indicate up to two research groups in which they would like to work, in order of preference. Moreover, if they are interested in a particular research group, they should make reference to it in the motivation letter. More information on the research activities of each group can be found on the IRB Barcelona web pages.

Referees must send their letters directly to IRB Barcelona at: phd@irbbarcelona.org. Only letters with an official letterhead and signature will be accepted. Applicants are responsible for ensuring that their referees send the letter. Applications not accompanied by this letter will not be eligible.

Applicants should submit information wherever possible in English (CV, motivation letter, summary of work experience). If the certified academic record is not in Catalan, Spanish or English a translation into one of these languages should be provided.

V. Selection

After the application deadline:

1. A Review Board comprising IRB Barcelona group leaders and members of the IRB Barcelona PhD Advisory Committee will draw up a preliminary list of candidates.
2. Group leaders may interview the invited candidates and will make a final selection.
3. Applicants can follow the status of their application upon request to the email phd@irbbarcelona.org
4. Applicants who have not been successful but have received a positive evaluation will be put on a waiting list to cover possible renunciations and future positions.



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VI. Calendar

4 April 2024 - Call opening

9 May 2024 - Call deadline and preselection of candidates

31 May 2024 - Notification sent to successful candidates

Summer internships start as of 1st July 2024.

At the end of the internship, each student must prepare a summary report and send it to the IRB Barcelona Academic Office at phd@irbbarcelona.org, as well as to the project supervisor.

VII. Communication of Grant Award

1. Selected candidates will be informed of the grant award via email. After acceptance of the grant, awardees will receive detailed information. Students will also present their research work undertaken during the internship in an open seminar organised for the IRB Barcelona community.

VIII. Rights of Awardees

1. To be provided with the necessary assistance to perform their studies and research activities. They will have a tutor who will provide assistance during their internship at IRB Barcelona.
2. To have their intellectual and industrial property rights regulated by the employment contract with IRB Barcelona.
3. To have employment and Social Security rights derived from the formal employment contract with IRB Barcelona.
4. To exercise intellectual property rights derived from their training activity in accordance with their contribution, as established in the Intellectual Property Law, Royal Decree 1/1996, 12 April. These rights will be independent, compatible and accumulative with other rights that may arise from the research developed, without negatively affecting the rights of the joint effort when the awardees participate in or are associated with a joint research project.
5. To have possible industrial property rights regulated by Patent Law 24/2015, 24 July, and Royal Decree 55/2002, 18 January, governing the exploitation and license of



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rights on discoveries made in public research organisations. Said rights will not be linked to the grant.

IX. Responsibilities of Awardees

1. To fulfil the terms and conditions established in this call.
2. To perform their research activity under the supervision of a project supervisor at IRB Barcelona while the grant is effective. In addition, they must perform the activities foreseen in the research training and specialisation programmes of the Institute, as well as satisfactorily fulfil the objectives of the training programme.
3. To comply with the internal regulations of IRB Barcelona, particularly regarding working conditions and the prevention of occupational risks.
4. To inform IRB Barcelona in advance of articles carrying their names that are published in scientific journals.
5. To undertake the duties that correspond to them as a result of being hired by IRB Barcelona, as well as those associated with inclusion in the Social Security System.
6. To inform IRB Barcelona if they receive other grants or funding.

X. Termination of Grants

The grants will be revoked if the awardee has withheld or falsified information. The grant will also be terminated if the awardee does not fulfil the responsibilities described in point IX.

XI. Incompatibility

Awardees will be devoted exclusively to the research or technical training and specialisation activities defined in this call. The grants included in this call are not compatible with any other type of grant or fellowship from other public or private organisations.



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XII. Data Protection

In accordance with Regulation (EU) 2016/679 (General Data Protection Regulation), Organic Law 3/2018 of December 5, and other applicable regulations governing personal data protection, any personal data provided by applicants will be incorporated into the Academic file of IRB Barcelona, for which the Institute is the data processor. The purpose of keeping such data is to manage our relationship with applicants. Applicants may exercise the rights of access, rectification deletion, opposition, transfer and expiry, as well as limitation in data processing of said information by contacting the Institute at the following e-mail address: dataprotection@irbbarcelona.org, or by writing to the following postal address: C/ Baldiri Reixac, 10, 08028, Barcelona.

XIII. Dissemination

Any information regarding this grant will be placed on the announcement board on the IRB Barcelona web site.

XIV. Clarification

The Head of Human Resources and Academic Affairs Department of IRB Barcelona or designated representative will be responsible for clarifying queries regarding these terms and conditions.

Barcelona, 4 April 2024

Maribel Labrid,
Head of Human Resources and Academic Affairs.



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ANNEX 1. IRB Barcelona Research groups participating in the 2024 Maths4Life call

Research group	Group Leader	Description of the project
<u>Molecular Modelling and Bioinformatics</u>	Modesto Orozco	<p>Anticipating molecular trajectories from AI approaches.</p> <p>Supervisors: Milosz Wieczor / Modesto Orozco</p> <p>Development of physics-based coarse grained models for nucleic acids simulations.</p> <p>Supervisors: David Ferrer / Modesto Orozco</p>
<u>Structural Bioinformatics and Network Biology</u>	Patrick Aloy	<p>Data Science to expand the bioactive chemical space</p> <p>Biological data is accumulating at an unprecedented rate, escalating the role of data-driven methods in computational drug discovery. The urge to couple biological data to cutting-edge machine learning has spurred developments in data integration and knowledge representation, especially in the form of heterogeneous, multiplex and semantically-rich biological networks. Today, thanks to the propitious rise in knowledge embedding techniques, these large and complex biological networks can be converted to a vector format that suits the majority of machine learning implementations. Indeed, we have generated biological embeddings, or bio-prints, that capture complex relationships between small molecules and other biological entities such as targets or diseases (Duran-Frigola et al. 2020 Nat Biotechnol; Bertoni et al. 2021 Nat Commun). However, only a tiny fraction of the possible chemical space has been so far explored, meaning that most compounds able to modulate biological activities (i.e. drugs) are yet to be discovered. Accordingly, the main objective of this project is to couple our bio-prints to inverse design algorithms to generate new chemical</p>

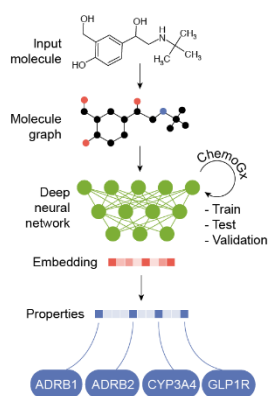


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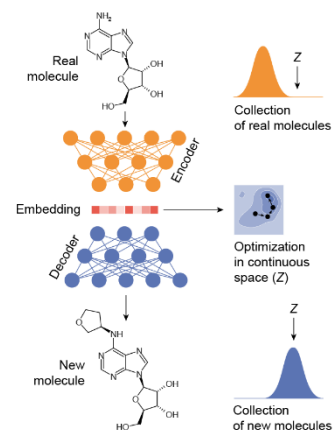


entities with a desired functionality. For instance, variational autoencoders or GANs are well suited to learn embeddings by simply reading the SMILES strings that are stored in large compound repositories and reversibly generate novel and valid SMILES strings, optimized for a certain property of interest, through the trained functions (Fernández-Torras et al. 2022 *Curr Opin Chem Biol*). All in all, the incorporation of machine learning methods, able to consider huge amounts of (individual) biological data, to the drug discovery process will trigger the development of thousands of novel compounds, finally enabling precision medicine.

A Property prediction
(e.g. multi-task learning)



B Small molecule generation
(e.g. variational autoencoder)



Deep learning in chemoinformatics. (A) A classical multi-target prediction exercise, based on chemogenomics (ChemoGx) data. Deep neural networks can read a molecule structure as a graph (e.g. convolutional graph networks), and be trained to optimally perform a multi-task classification. An inner (usually the last) layer of the network corresponds to the chemical embedding. (B) An autoencoder is a type of neural network that includes an encoder and a decoder, which compress and decompress the data, respectively. The encoder maps the input to a latent space (embedding), and the decoder maps the embedding back to the original representation. The embedding is a continuous vector that can be optimized for a certain property of interest 'Z'. The interpolated vectors can be then decoded to generate new molecules.



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<p><u>Laboratory of Molecular Biophysics</u></p>	<p>Xavier Salvatella</p>	<p>Prediction of the structural properties of polyglutamine sequences at the proteome level</p> <p>Polyglutamine sequences are frequent in intrinsically disordered domains of human proteins. Their lengths are not conserved and expansions beyond specific thresholds are associated with nine different neurodegenerative and neuromuscular disorders. We recently discovered that the polyglutamine tract in one such protein forms a metastable helix that gains stability upon expansion, suggesting that the helical conformation is involved in the onset of polyglutamine diseases. Very recently we have uncovered the rules that govern, for a given polyglutamine sequence, the stability of the helical conformation. The student will use the knowledge obtained in our laboratory to develop a predictor of such stability, and of how it is altered by expansion, which the student will also use to evaluate the hypothesis that the helical conformation of polyglutamine sequences is indeed involved in the onset of polyglutamine diseases. The work will involve the modification of existing codes, the optimization of parameters to agree with experiments, performing predictions at the proteome level and, if the student is interested, the development of a web-based graphical interface for the scientific community to use the newly developed predictor.</p> <ol style="list-style-type: none"> 1. Escobedo, A. et al. Side chain to main chain hydrogen bonds stabilize a polyglutamine helix in a transcription factor. Nat. Commun. 10, 2034 (2019). 2. Escobedo, A. et al. A glutamine-based single α-helix scaffold to target globular proteins. Nat. Commun. 13, 1-18 (2022).
<p><u>Gene Translation Laboratory</u></p>	<p>Lluís Ribas</p>	<p>Finding signs of the origin of life through big data analysis.</p> <p>This project in a collaboration with the Department of Biology of M.I.T., and will include traveling to Boston to discuss the results with our collaborators. The goal of the project is to explore the presence of ancient sequence signatures in the current datasets of transfer RNA (tRNA) sequences, looking for evidence of</p>





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		<p>ancestral complementary interactions between the precursors of modern tRNAs. These interactions probably played a role in the establishment of the Genetic Code and the origin of cellular life. Previous analyses searched these signatures using small sequence datasets (Rodin, Rodin, and Ohno, P.N.A.S. (1996)). Now we want to repeat these analyses with the current datasets of tRNA sequences, which will provide us with far stronger statistical power.</p> <p>We seek a talented student, with experience in statistical analysis and good communication skills in english, and willing to travel to Boston to present the results to our partners.</p>
<p>Biostatistics/Bioinformatics Core Facility</p>	<p>Camille Stephan-Otto</p>	<p>The candidate will investigate and implement current algorithms for analysis of spatial omics data.</p> <p>Their main tasks will be: explore literature to gather state of the art methodology in the field; implement selected software or algorithms to benchmark; apply all algorithms to existing pilot data; generate a report comparing the different methodologies.</p>



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