



Dipartimento di Fisica

CALL FOR RESEARCH FELLOWSHIP N. 13/2025 – REP.303 /2025 July 8, 2025

Title: *“Development of a computational protocol within the project “Take the (bi)cycle: a new computational pipeline for transformative screening and design of (bi)cyclic peptides..” - Scientific Manager: prof. Attilio Vittorio Vargiu*

THE DIRECTOR

Having considered Law nr. 240, December 30, 2010, assessing “Regulations for the organization of the Universities, of the academic staff and their recruitment and delegating to the Government the enhancement of quality and efficiency of the University system”, and the art. 18, co.5, lett. f;

Having considered Law nr. 35, April 4, 2012, which converted into law the Decree Law nr. 5, February 9, 2012, with amendments, containing urgent provisions on the simplification and development, in particular the art. 49, comma 1, lett. h, which amended the Art. nr. 18, co.5, lett. F, Law nr. 240, December 30, 2010;

Having considered D.lgs. nr. 196, June 30, 2003, “Personal Data Protection Code”, as modified by d.lgs. nr.101, August 10, 2018, establishing procedures to adapt the national law provisions for the adaptation of national law to the General Data Protection Regulation (EU) 2016/679 (GDPR), on data protection and privacy

Having considered D.L. nr. 45, April 7, 2025, converted with amendments by L. 5 June 2025, n. 79 (and in particular paragraph 4 of art. 1-bis);

Having considered D.lgs. nr. 82, March 7, 2005, “Digital Administration Code“, as amended;

Having considered D.lgs. nr. 198, April 11, 2006, "Code of equal opportunities between men and women" as amended;

Having regard to D.P.R. nr. 189, July 30, 2009, in particular the Art.2, "Recognition of foreign qualifications for access to public competitions";

Having considered the University Statute issued by D.R. nr. 339, March 27, 2012, lastly amended by D.R. nr. 305, March 28, 2022;

Having considered the University Regulation about research grants, last amended by D.R. no. 432, June 13, 2018;

Having considered the research project “Two-year research projects at the University of Cagliari – Year 2023” – CUP: F23C25000160007, Principal Investigator prof. Attilio Vittorio Vargiu;

Having considered Prof. Vargiu’s request of a selection procedure for the assignment of nr. 1 research grant, with a duration of 12 (twelve) months, and a gross amount of the perceiver of € 19.367,00, (nineteen thousand, three hundred and sixty seven euros) entitled “Development of a

computational protocol within the project “Take the (bi)cycle: a new computational pipeline for transformative screening and design of (bi)cyclic peptides.” –



scientific manager Attilio Vittorio Vargiu, funded by Fondazione di Sardegna – CUP F23C25000160007,

principal investigator prof. Attilio Vittorio Vargiu;

Having considered the D.D. 292/2025 – July 4, 2025, which approved the request made by prof. Vargiu;

Having considered D.lgs. nr. 33, March 14, 2013, "Reorganization of the regulations concerning the obligations of publicity, transparency and dissemination of information by the Public Administrations" as amended;

Ascertained the availability of funds to cover the fellowships on the project RICALTRO_CTC_FDS_2023_VARGIU

HEREBY DECREES

ARTICLE ONE

(Characteristics of the project programme)

A selection, based on qualifications and interview, has been published to assign the fellowship with the following characteristics:

Funding Authority: Fondazione di Sardegna

Project deadline: June 16, 2027

Place for the implementation of the research: Department of Physics – University of Cagliari

Scientific Manager: Attilio Vittorio Vargiu

Fellowship number: 1

Fellowship duration: 12 months

Annual gross amount: € 19.367,00

Title of the project (Italian): “Sviluppo di un protocollo computazionale all’interno del progetto “Take the (bi)cycle: a new computational pipeline for transformative screening and design of (bi)cyclic peptides.”

Brief description of the project (Italian):

Gli obiettivi del progetto di ricerca riguardano lo sviluppo di: i) un protocollo computazionale basato su metodi di campionamento avanzato delle configurazioni di proteine, per migliorare la predizione delle strutture di complessi formati tra proteine e molecole generiche; ii) un protocollo computazionale basato su metodi di campionamento avanzato e machine-learning al fine di generare migliaia di diverse conformazioni di peptidi, in particolare ciclici e bicicli. Il fine principale dell’attività di ricerca sarà quello di migliorare l’accuratezza delle predizioni computazionali di strutture di complessi formati tra proteine e tali peptidi. Il titolare dell’assegno si occuperà di sviluppare entrambi i punti. È



richiesta familiarità con la teoria e i programmi di docking molecolare e dinamica molecolare, lo scripting nei linguaggi bash, tcl, python..

Title of the project (English): “Development of a computational protocol within the project “Take the (bi)cycle: a new computational pipeline for transformative screening and design of (bi)cyclic peptides.”

Brief description of the project (English):

The research performed by the fellow will be focused on: i) The development of a computational protocol based on advanced sampling methods for protein configurations to improve the prediction of the structures of complexes formed between proteins and generic molecules. ii) The development of a computational protocol based on advanced sampling methods and machine-learning tools to generate thousands of peptide configurations, particularly cyclic and bicyclic ones. The main aim of the research activity is to improve the accuracy of computational predictions of the structures of protein-peptide complexes. The researcher will be responsible for developing both objectives. Familiarity with molecular docking and molecular dynamics theory and programs, as well as scripting in bash, Tcl, and Python, is required.

ARTICLE TWO

(Admission requirements, incompatibility, and duration)

Admission to the selection is open to graduates, regardless of nationality, holding (ref. to the Italian university system):

A) A degree awarded according to the Italian Ministerial Decree nr. 270/2004 (laurea magistrale) in Physics, Chemistry, Electronic Engineering, Electrical Engineering, Computer Engineering, Chemistry, Pharmaceutical Chemistry and Technologies, Biotechnology, Computer Science

Validity and equivalence of degrees issued by foreign Universities must be assessed, in terms of duration, level of degree and fields of study in comparison to the degree listed above, and providing access to PhD education in the awarding country. The Selection Board will deliberate on its equivalence, in compliance with the current legislation in Italy and in the Country where it was issued, and within the framework of the international treaties or agreements concerning the recognition of qualifications for further studies for the sole purpose of the admission to the selection.

Additional evaluable qualifications (total score 60/100):

A) Phd in Physics, Chemistry, Electronic Engineering, Electrical Engineering, Computer Engineering, Chemistry, Pharmaceutical Chemistry and Technologies, Biotechnology, Computer Science up to a maximum 15/100;



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|---|-------------------------|
| B) Other academic qualifications | up to a maximum 10/100; |
| C) Scientific publications on related subject/methodologies | up to a maximum 20/100; |
| D) Work experience on relevant subject/methodologies | up to a maximum 15/100 |

The entry qualifications must be held by the deadline established for the submission of the applications to the selection.

Applicants will not be admitted to the selection if not awarding any of the entry qualifications mentioned above by the deadline given for the presentation of applications to the selection, and, additionally, if applicants fulfil one of the following criteria:

- Public permanent employees in universities, in institutions and public centres for research;
- Relatives by blood and marriage, within the fourth degree, with staff members of the proposing Department, or with the Rector, the General Manager, or with a member of the Board of Directors at the University (Art. 18, par. 1, lett. B and c, law 240/2010);
- if they have had any other relations with the University of Cagliari, or with other Universities, or with the authorities included in the art. 22, par. 1 of the law 240/2010, as researchers for fixed terms in accordance with the art. 24 of the L. 240/2010, and as grant holders according to the art. 22 of the law 240/2010, for more than twelve years, summing up the duration of the grant awarded in this call. The periods spent off work for pregnancy or for health problems will not be taken into account (par. 9, art. 22, law 240/2010).

The applicant is accepted to the selection conditionally; failing these qualifications, the Director can decide at any time, through a motivated decision, to reject the application.

The fellowship is not compatible with:

- Other fellowships awarded for any reason, with the exception of those granted by national or foreign institutions useful for integrating the research activity of the fellowship's holder during abroad periods;
 - The attendance to research doctorate courses with fellowship and medical specialization, in Italy and abroad;
 - Research grants;
 - Employment relationships, without prejudice to the possibility that the fellowships holder may be placed on unpaid leave;
 - Self-employment activity, even para-subordinate, with the exceptions listed in the following paragraph;
- 2 – The fellow may carry out occasional self-employment activities, even semi-subordinate, upon written communication to the Scientific Manager and on condition that:
- This activity is declared by the Scientific Manager compatible with the research activity presented in the Research Grant,
 - It does not involve a conflict of interest with the specific research activity carried out by the fellow



- c) Do not harm the University, in relation to the activities carried out.

ARTICLE THREE

(Applications)

Applications to the selection (form Annex A) and all the requested documentation, including the publications, must be submitted in PDF (portable document format) via certified mail (PEC) to protocollo@pec.unica.it within the 20th day starting from the day following the date of publication on the UNICA "Laureati" and "Department of Physics" websites. The subject must contain:

DIP. PHYSICS - Research grant N. 13/2025 - Scientific manager: prof. Attilio Vittorio Vargiu

The application form and the other documents that need to be signed will be signed by Digital Signature or handwritten signature.

The university administration will verify all the self-certifications according to T.U. 445/2000.

All communications between the office and the applicants will be forwarded only by PEC or e-mail. Applications and qualifications submitted after the deadline established for the presentation of applications to the selection will not be considered.

The university administration is not responsible for the lost of applications or related documents if this is due to incorrect contact details provided by the applicant or having failed or delayed in notifying any changes of the contact details, nor for any possible misdelivery or telegraph error.

The applicant must include in the application:

- a) substitutive declaration of certifications, issued pursuant to the D.P.R. 445 – 12.28.2000, relating to the candidate's educational, didactic, scientific, and professional curriculum (Annex B)
- b) substitutive declaration of certifications, issued pursuant to the D.P.R. 445 – 12.28.2000, relating to the possession of additional evaluable qualifications, certifications, and work experiences, detailed in English or in Italian, drawn up according to the format in Annex C
- d) publications with attached declaration certifying compliance with the original (Annex D), issued pursuant to the D.P.R. 445 – 12.28.2000;
- e) if the qualifications required for admission were obtained abroad, a copy of the statement of recognition attesting their validity in Italy. In the event that the recognition has not yet been made, the equivalence will be assessed, solely for the purpose of admitting the candidate to the selection, by the Selection Committee;
- f) remote interview request form (Annex E) filled with all the requested information;
- g) two-sided coloured scanned copy of a valid ID, with a clear photo
- h) list of the documents and qualifications presented as attachments to the application.



ARTICLE FOUR **(Selection Committee)**

The Selection Committee will be appointed by Director of Department's decree pursuant to the Art. nr. 5 of the University regulation and is composed of three experienced members, one of which acting as chairman, all chosen according to principles of equal opportunities, transparency and impartiality. The Committee is composed of:

- the Principal Investigator of the project
- two staff members from the same Macro-area Section or, if not available, from the same Area of the research project,

The Selection Committee can also be supplemented by one or more members designated by the funding entity as experts.

The selection ranking will be based on the qualifications and the interviews of the candidates, according to internationally recognized standards.

In the first session, the Selection Committee determines the evaluation criteria and the minimum score for being admitted to the interview; the applicants' ranking by the Committee will be in percent.

The Committee has 100 points totally, partitioned as follows:

- up to a maximum of 60/100 for the qualifications;
- up to a maximum of 40/100 for the interview.

The outcome of the assessment with its score, the possible admission to the interview, date and time of the interview, and the information on the procedures for carrying it out, will be published on the websites of Department of Physics and of University of Cagliari (unica.it) 15 days in advance.

The applicants will be included in the general ranked list on a decreasing order based on the total final score, obtained by adding qualification and interview scores. In case of further parity, the younger applicant will prevail.

ARTICLE FIVE **(Awarding of the research fellowship, start and end of the activity)**

After checking the selection documents and certifying the correctness of the Selection Committee's work, the general ranked list is approved by Director of Department's Decree and published on the University website.

The start of the activity will have to be certified providing a declaration of start research activity issued by the Principal Investigator to the Director of Department.

The fellow will carry out the project under the direct responsibility of the Principal Investigator of the project the fellowship has been awarded for. The fellow will be asked to



issue an activity report at the end of the research period, that will be evaluated by the Principal Investigator. The fellow will work on the project in the Department associated with the Principal Investigator, using any equipment and service available in it. Upon Principal Investigator's permission, the project can be carried out also in other research facilities of the University, in qualified structures and/or in Italian or foreign centres.

The fellow must comply with the obligation of confidentiality in relation to the information, news, documents and knowledge acquired during her/his activity.

The fellow must stipulate an adequate compulsory personal insurance policy both against the risk of accidents occurring during the period of presence in the University structures, or at external structures that can host the fellow upon Principal Investigator's agreement. The insurance policy should also cover civil liability towards third parties, possibly deriving from damage to persons or things. A copy of the policy must be delivered to the administration on the starting date of the research activities at the Department of reference.

The fellow's activity must be completed by the expiry date of the research project.

ARTICLE SIX (Tax and contribution framework)

The success of the research grant does not determine the establishment of an employment relationship, does not give rise to social security treatments, to evaluations for the purposes of legal and economic careers, nor to automatic recognitions for social security purposes.

The fellowship will be paid in monthly postponed instalments.

The emoluments of the research grant constitute income assimilated to that of an employee pursuant to art. 50, paragraph 1, letter c) of the Consolidated Law on Income Tax, Presidential Decree no. 917 of 22/12/1986, which must be subject to IRPEF taxation pursuant to art. 24 of Presidential Decree 600/1973 (Common provisions on the assessment of income taxes), in addition to being subject to IRAP with the related burden on the administration.

ARTICLE SEVEN (Personal data processing)

The University of Cagliari is responsible for the treatment of personal data according to the General Data Protection Regulation (GDPR) (EU) 2016/679, and the Personal Data Protection Code – Leg. Decree n. 196 of 30 June 2003, in respect of subjects' rights, fundamental freedoms and dignity. Privacy policy for the category of Citizens is published on the following website: https://www.unica.it/unica/it/utility_privacy.pag

According to Art. nr. 5 of the Law nr. 241, August 7, 1990, the management of the selection procedures related to this call is attributed to dr. Fernanda Marongiu, Administrative Manager of Department of Physics.

Candidates can exercise the right of access to the documents of the selection procedure according to the procedures set out in the D.P.R. 184 of 12.4.2006 (Regulation governing access to administrative documents).



ARTICLE EIGHT

(Advertising and safety regulations)

The current call will be published on the web site of the University, (https://www.unica.it/unica/it/laureati_s07_ss01.page).

For what not explicitly mentioned in this announcement the University shall act in compliance with the rules included in the Law nr.240/2010 and under the regulations of the awarding of research grants in this University.

The Director of Department of Physics
Prof. Michele Saba
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