Call for the selection of 2 research contracts

The University of Pisa announces public selection procedures for the award of 2 research contracts in accordance with Article 22 of Law 240/2010 as set out in Annex A) to this call, in which the information sheets indicating the reference structure, the description of the research project, the specific responsibility within the project and the functions to be performed, as well as the scientific disciplinary area and information on the interview, are provided.

Deadline for submitting the application: 22 August 2025 at 1.00 p.m.

Contract duration: 24 months

All-inclusive annual administrative gross amount: €54.000,00

Admission requirements:

• A PhD or medical specialisation degree.
Students enrolled in the third year of a PhD programme or in the final year of a postgraduate medical specialisation programme are also eligible to apply, provided they obtain their degree within six months from the publication date of the selection notice. Failure to meet this requirement candidates will lose the right to be awarded the research contract.

Documents to be attached:

The application must include:

a)   A research development project related to the research project specified for the selection in Annex A);

b)   A comprehensive scientific-professional curriculum containing all the necessary elements for assessing prior research activities and any relevant work experiences, in connection with the content of the research project under consideration (specifically indicating: date/duration, place of completion, etc.);

c)   For individuals with a foreign doctoral degree, an equivalence decree or determination; if the candidate already holds one, a copy of the foreign doctoral degree or a suitable certification issued by the foreign institution, confirming the components, duration, and activities of the doctoral programme undertaken to achieve the doctoral degree;

d)   Additional documents that the candidate deems useful for the selection purposes;

e)   Publications that the candidate considers relevant for the selection, considering the maximum number set for the selection, as indicated in Annex A), with a list signed by the candidate;

f)   Photocopies of the tax code and a current valid identification document.

Candidates must submit the publications they intend to present exclusively in PDF format through the dedicated section of the online procedure.

Each publication shall not exceed 30 megabytes.

Publications not enclosed with the application will not be considered by the Selection Board. Lists with links to texts are not allowed as a replacement for publications.

Applications

Applications must be submitted online only, using the following link: https://pica.cineca.it/unipi/

or shall be invalid. An e-mail inbox is required to login and complete the application.

Candidates can login into PICA platform using the digital identifier SPID (Sistema Pubblico d'Identità Digitale - Public Digital Identity System), selecting the University of Pisa among the available Institutions.

If candidates have no SPID, they can request it according to the procedures set forth on the website www.spid.gov.it.

Candidates can also login with the credentials issued directly by PICA platform (please note: in order to apply online, the system requires an e-mail inbox for self-registration), with their LOGINMIUR, REPRISE or REFEREES account.

Applicants should provide all the required data and upload all documents in PDF format.

The system allows saving an application draft within the application deadline, recording the online application's date and sending a receipt with an automatic reply. After the deadline, the system will not allow login nor application submission.

Each application will be assigned a unique identification number to be referred to in all subsequent communications, along with the selection code provided by the application form.

Under penalty of exclusion, the application shall be valid only if including all the required data, the copy of a valid ID and:

 – if submitted without accessing with digital identifier SPID, the applicant's signature is compulsorily required;

- If submitted by accessing with digital identifier SPID, the application will be automatically processed by the system and the applicant's signature is not required.

Applicants undertake to promptly communicate in writing any variations of what declared in the application form.

The communication shall be edited in PDF format, signed and forwarded to the Rector of the University of Pisa by the Italian certified e-mail system address (P.E.C. Posta Elettronica Certificata): protocollo@pec.unipi.it or emailed to concorsi_contratti@unipi.it , within the application's submission deadline.

An applicant's valid identification document shall be annexed.

For further information on application submission, please refer to concorsi_contratti@unipi.it.

For technical problems support only, please click on the bottom link available at https://pica.cineca.it/unipi.

Selection procedure:

For the selection under Annex A) the Director of the Department appoints a Selection Board consisting of the head of the research project and two other members.

Candidates are assessed comparatively on the basis of the following elements:

a) Quality, originality and innovativeness of the research development project, with reference to the research project under consideration;

b) Relevance and significance of the research activities previously carried out, as well as any work experience, in relation to the contents of the research project subject to the selection, in addition to documented qualifications (such as, for example, grade point average, postgraduate diplomas, any contracts, scholarships, conference presentations, and other documented qualifications);

c) Quality, originality and innovativeness of the attached publications, as well as their relevance to the research project under consideration;

d) An interview aimed at assessing the knowledge of the basic subjects of the scientific disciplinary sector to which the subject of the research project belongs, the suitability for carrying out the research activity under the contract and for the implementation of the research project, as well as the evaluation of knowledge of the English language and/or other languages relevant to the research (as reported in the Annex A). During the interview, the Selection Board also assesses the knowledge of the Italian language for foreign candidates.

The Selection Board has 100 points available for the comparative evaluation of the candidates: 60 points can be allocated for the criteria mentioned above under a), b) and c), and 40 points for the interview.

The Selection Board may stipulate a minimum score below which eligibility cannot be awarded.

Candidates are summoned for the interview on the day and time specified in the Annex A) for the procedure.

Failure to attend an interview by a candidate is considered an explicit indication of their intention to withdraw from the selection process.

Applicants for this selection are required to consult the University website at https://bandi.unipi.it/public/Bandi?type=COR (on the selection procedure page) during the two days preceding the date set for the interview.

On the University website (https://bandi.unipi.it/public/Bandi?type=COR), in the section dedicated to the procedure, the following will be published:

• **Assessment scores for criteria a), b) and c);**

• **The list of candidates admitted to the interview;**

• **Practical instructions for carrying out the interview and/or any details should the interview be rescheduled;**

• **The procedure approval decree and the merit ranking that takes into account the scores achieved by the candidates.**

The prospective doctoral or postgraduate student may only enter into a contract after obtaining a doctoral or postgraduate medical degree. In the event that the PhD candidate or postgraduate student fails to obtain the degree within six months from the publication date of the selection notice, they will lose the right to be awarded the research contract.

Please note that the English version is given as a matter of courtesy, for the only purpose of information. It cannot be legally used in the event of a dispute or a claim arising from the interpretation of this translation and concerning the contents, a possible uncertainty, contradiction, or discrepancy. Should this occur, the Italian version of the call should prevail as the only valid. For full Italian text see: https://bandi.unipi.it/public/Bandi?type=COR (on the selection procedure page).

Selection code - CDR_chim_2025_1_1

No. of positions 1

Department of Chemistry and Industrial Chemistry

GSD 03/CHEM-02 "Physical Chemistry"
SSD CHEM-02/A "Physical Chemistry"

CUP I53C24003150001

Head of the Research Project

Prof.ssa Benedetta Mennucci

Research Project:

A Deep learning from Nature to design novel photoEnzymes (DeepEn)

The emerging frontier of photobiocatalysis—a fusion of biocatalysis and photocatalysis—combines the selectivity of enzymes with the unique chemical transformations enabled by light-activated processes. In nature, photobiocatalysis is employed in photoenzymes, in which photosensitive cofactors drive catalytic reactions. Among the few natural photoenzymes identified so far, fatty acid photodecarboxylases (FAPs) represent a particularly interesting system. The mechanism of FAP enables the conversion of fatty acids into hydrocarbons and carbon dioxide through blue light, making it highly promising for applications in synthetic chemistry and beyond. An ambitious concept is to use FAP as a model for designing new photoenzymes, leveraging its efficient mechanism for generating radical species while enhancing its activity for synthetic applications, expanding substrate compatibility, and generating novel products.
The DeepEn project aims to address this challenge by combining the accuracy of multiscale modeling, grounded in quantum chemistry, with the capabilities of deep learning. The conceptual innovation lies in using multiscale modeling to guide the deep learning-based design of new photoenzymes. This will be achieved by identifying molecular descriptors that characterize the energetics and kinetics of the key stages in the photocatalytic cycle. These descriptors will serve as constraints to condition the sampling, via deep learning, of new protein sequences and structures.

Specific responsibilities within the project and functions to be performed:

The responsibility within the project will be to employ an integration of hybrid QM/MM techniques, along with adiabatic and nonadiabatic dynamics simulations, in order to model the electron transfer process that initiates the photocatalytic activity in fatty acid photodecarboxylases (FAPs). The goal is to identify specific molecular descriptors that govern this photoinduced process. These descriptors will include: specific protein residues that stabilize charge-transfer states; geometric arrangements of the active site that facilitate donor/acceptor encounter; and electric fields generated by the protein matrix at the reactive site.

Maximum number of publications that candidates may submit, including the doctoral thesis, if submitted: 8

Language skills:

English language

Date, time and mode of the interview:

8th September 2025 at 2 pm in telematic mode

Selection code - CDR_chim_2025_1_2

No. of positions 1

Department of Chemistry and Industrial Chemistry

GSD 03/CHEM-02 "Physical Chemistry"
SSD CHEM-02/A "Physical Chemistry"

CUP I53C24003150001

Head of the Research Project

Prof.ssa Benedetta Mennucci

Research Project:

A Deep learning from Nature to design novel photoEnzymes (DeepEn)

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Specific responsibilities within the project and functions to be performed:

The responsibility within the project will be to combine molecular dynamics simulations, aimed at sampling the conformational space of the photoenzyme, with polarizable hybrid QM/MM methods in order to model the reactive processes that follow the photoinduced event. In this context, it will be crucial to explore possible reaction pathways while accounting for the dynamic fluctuations of the protein. To this end, a novel integration of optimization techniques with QM/MM descriptions will be developed. The entire approach will be enhanced by machine learning techniques, with the goal of improving both efficiency and accuracy in the search for relevant geometries. The same strategy will also be applied in the absence of the substrate in the enzyme's active site, to investigate alternative phenomena such as the photoreduction of specific amino acid residues by the excited FAD. Understanding these mechanisms will be essential to limit the formation of undesired reactive pathways ("off-pathway") and enzyme inactivation.

Maximum number of publications that candidates may submit, including the doctoral thesis, if submitted: 8

Language skills:

English language

Date, time and mode of the interview:

8th September 2025 at 4 pm in telematic mode