## SCHOLARSHIP OFFER

Position in the project:	PhD Student in Cheminformatics
Scientific discipline:	Computer Science / Technical Computer Science / Computational Chemistry
Job type (employment contract/scholarship):	Scholarship
Number of job offers:	1
Renumeration:	5000 PLN net per month
Position starts on:	Not earlier than 1 <sup>st</sup> January 2025
Maximum period of contract/scholarship agreement:	4 years
Institution:	Jagiellonian University, Cracow
Project leader:	Bartosz Zieliński
Project title:	Interpretable and Interactive Multimodal Retrieval in the Drug Discovery Process
	<i>Project is being carried out within the First Team FENG programme of the Foundation for Polish Science</i>
Project description:	The drug discovery process is complex, requiring substantial financial investment and many years of work to bring a new drug to market. One way to shorten the time and reduce the costs of this process is through artificial intelligence. This approach can reduce the number of failures in clinical trials and facilitate the exploration of the chemical compound space. In this project, we propose utilizing tools based on knowledge retrieval and interactive,



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	interpretable machine learning to increase the efficiency of the drug discovery process. The developed tool will be able to analyze images of cellular events, such as those obtained in the CellPainting (CP) protocol, and identify potential small-molecule drugs that can induce specific cellular events. It will make drug discovery, such as hit identification, virtual screening, and drug repurposing, faster and more cost-effective. We will collaborate with Matthias Zeppelzaur, an expert in knowledge retrieval, and Ardigen SA, a global leader in Al-based services for pharmaceutical companies. Ardigen also develops phenAID software, which enables advanced analysis of images obtained using the CP protocol.
Key responsibilities include:	<ol> <li>Planning and conducting computational experiments on deep learning models for small molecules;</li> <li>Implementing novel training techniques and interpretable models;</li> <li>Searching public databases for compound annotations;</li> <li>Analyzing and visualizing results;</li> <li>Preparing manuscripts;</li> <li>Presenting scientific data at international conferences.</li> </ol>
Profile of candidates/requirements:	<ol> <li>MSc degree in Computer Science, Computational Chemistry, or a related field;</li> <li>PhD student status required during the contract period;</li> <li>Experience in cheminformatics modeling or deep learning for graphs;</li> <li>Practical experience in the analysis of scientific data;</li> <li>Proficiency in programming with Python;</li> <li>Familiarity with the drug discovery process;</li> <li>Ability to work on interdisciplinary projects;</li> <li>Fluency in both written and spoken English.</li> </ol>
Required documents:	<ol> <li>Motivation letter;</li> <li>Curriculum vitae;</li> <li>Documents verifying experience and background;</li> <li>Recommendation from a scientific supervisor.</li> </ol>
We offer:	<ol> <li>A 48-month scholarship, subject to periodic evaluation;</li> <li>Scientific and organizational support;</li> <li>Opportunities to work within an interdisciplinary research team publishing in top-tier conferences and journals (see <u>https://gmum.net/</u>).</li> </ol>
Please submit the documents to:	dorota.ramotowska@uj.edu.pl



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Application deadline:	16 December 2024
General rules of the recruitment process:	<ol> <li>Candidates may apply simultaneously for all positions offered by the project, but it must be indicated on the application form.</li> <li>The decision will be made by the Recruitment Committee of the Faculty of Mathematics and Computer Science at the Jagiellonian University.</li> <li>The Recruitment Committee reserves the right to invite only selected candidates for an interview, which take place on December 17, 2024.</li> <li>The Recruitment Committee also reserves the right to close the competition without selecting a candidate.</li> <li>The results of the competition will be announced before December 31, 2024.</li> </ol>
For more details about the position please visit:	xaipaint.matinf.uj.edu.pl
Euraxess job/scholarship offer:	PhD Student (EURAXESS Scholarship Offer id: https://www.euraxess.pl/jobs/293935)



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## Personal data processing information for job applicants

According to Article 13 of the Regulation (EU) 2016/679 of the European Parliament and of the Council of 27 April 2016 on the protection of natural persons with regard to the processing of personal data and on the free movement of such data, and repealing Directive 95/46/EC (General Data Protection Regulation – hereinafter GDPR), the Jagiellonian University informs that:

- 1. The Administrator of your personal data is the Jagiellonian University with its registered office in Gołębia 24, 31-007 Kraków, respresented by the Rector of UJ.
- 2. The Jagiellonian University appointed the Data Protection Officer www.iod.uj.edu.pl, Gołębia 24, 30-007 Kraków. The Officer can be contacted by email: iod@uj.edu.pl or at the telephone number 12 663 12 25.
- 3. Your personal data will be processed in order to:

a. conduct recruitment process for the position specified in the advertisement - as part of the legal obligation of the Administrator pursuant to Art. 6 (1) lit c of the GDPR in connection with the Polish Labour Code;

b. conduct recruitment process for the position specified in the advertisement based on your consent pursuant to Art. 6 (1) lit a of the GDPR – your consent is granted by the clear action of submitting your CV with the Administrator. The consent to the processing of personal data concerns data that you voluntarily provide as part of your CV, which do not result from Polish Labour Code.

- 4. The obligation to provide your personal data results from the law (it applies to personal data processed under Article 6 (1) lit c of the GDPR). Failure to provide you personal data will result in your inability to take part in the recruitment process. Submission of personal data processed on the basis of consent (Article 6 (1) lit a of the GDPR) is voluntary.
- 5. Your data will be processed during the recruitment period. In the event of not concluding the contract with you, your data will be deleted after the recruitment process.
- 6. You have the right of access to the content of your personal data, as well as the right to correct, delete, restrict processing, transfer, object to processing on the terms and conditions set out in the GDPR.
- 7. If the processing is based on consent, you have the right to withdraw the consent at any time, which shall not affect the lawfulness of processing based on the consent given before the withdrawal. Withdrawal of consent to the processing of personal data can be sent by e-mail to: dorota.ramotowska@uj.edu.pl or by post to the following address: Wydział Matematyki i Informatyki UJ, ul. Prof. S. Łojasiewicza 6, 30-348 Kraków, Poland, or you can withdraw your consent in person at Faculty of Mathematics and Computer Science of the JU, ul. Prof. S. Łojasiewicza 6, 30-348 Kraków, Poland.
- 8. Your personal data will not be subject to automated decision making or profiling.
- 9. You have the right to lodge a complaint with the Inspector General for the Protection of Personal Data, if you feel that the processing of your personal data violates the GDPR regulations.



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