Postdoctoral Research Associate position

The Laboratory of Metalloprotein Biology, located at the Institute of Biochemistry and Biophysics Polish Academy of Sciences and headed by dr. hab. Kevin Waldron, seeks a productive, creative, and highly motivated Postdoctoral Research Associate. The successful candidate will join a collaborative, interdisciplinary team studying the structure, function and evolution of proteins from the family of iron- or manganese-dependent superoxide dismutase (SOD) enzymes and their role at the host-pathogen interface (Garcia *et al., PLoS Pathog.* 2017). This position is funded by the National Institutes of Health (R01 AI155611), and is in collaboration with the laboratory of microbiologist Dr Thomas Kehl-Fie, University of Illinois Urbana-Champaign, USA.

Our lab studies the structure and function of metalloproteins. It's estimated that approximately one-third of all proteins, and nearly half of all enzymes, require an essential metal ion to function (Waldron *et al., Nature* 2009). Most metalloenzymes are assumed to be specific for their cognate metal cofactor, showing reduced activity with other metal ions *in vitro* and *in vivo*. Our work aims to determine what molecular properties determine this specificity (Barwinska-Sendra *et al., Nat. Comms.* 2020), and how such specificity evolves (Sendra *et al., Nat. Ecol. Evol.* 2023). We are exploiting the SODs as a remarkable model system, as some SOD isozymes absolutely require manganese (Mn), others absolutely require iron (Fe), whereas other SODs can utilise either of these metals as cofactor, termed cambialistic enzymes, despite all forms sharing essentially identical structures.

Building on our recent biochemical, microbiological and evolutionary studies of these ubiquitous metalloenzymes, which play a crucial role in cellular defence against oxidative stress, we are using biochemistry, biophysics and structural biology approaches to determine how a unique pair of SOD enzymes from *Staphylococcus aureus* function at the atomic level, including the first extensive study of the structural dynamics of these proteins. We are now seeking a postdoctoral researcher with a strong computational research background, experience in quantum/molecular mechanical modelling methods as applied to transition metal complexes and expertise with FORTRAN programming for high performance computing applications, to assist in these projects.

Job description:

The successful applicant will be responsible for executing computer-based research within the project. They will use innovative modelling approaches to simulate the catalysis by SOD enzymes, the dynamics of the active site structure, and study possible routes of substrate entry and product release. This computational work will build on our extensive structural and biochemical data on this family of enzymes, and will aim to generate structural hypotheses that can be tested by biochemists in the laboratory. The project will involve collaborating closely with existing team members applying biochemical and biophysical analyses to SOD enzymes, as well as with collaborating international research groups to develop novel bioinformatic methods for studying these ubiquitous metalloenzymes.

Requirements for the candidate:

• A PhD in bioinformatics or a related subject. There is no limit of years post PhD completion.

• A proven track record in publishing high quality research, and a demonstrable passion for science.

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• Ability to work both independently (under appropriate supervision) and as part of a collaborative and interdisciplinary team, including training junior researchers in computational methods and collaborating in achieving team goals.

• Demonstrable hands-on experience in computational methods for *in silico* statistical mechanics applied to the study of enzyme kinetics.

• Experience with quantum mechanics/molecular mechanics hybrid simulations of enzyme catalysis, ideally using CP2K, and quantum chemical calculations applied to transition metal complexes.

• Experience in FORTRAN programming for high performance computing applications.

• Proficiency in spoken and written English.

We offer:

• A full-time employment contract for 5 months, starting from 1st August 2024 or as soon as possible thereafter.

• Gross salary of about 9,300 PLN/month. Net salary depends on individual circumstances influencing tax.

• A position with 100% focus on research (no teaching obligations) in a leading laboratory group and within a dynamic and interdisciplinary team.

• Opportunities for training, including interactions with collaborating laboratories of leading experts in diverse fields.

Informal inquiries:

Informal inquiries are very welcome. Please send an email to kwaldron@ibb.waw.pl including any questions, a brief description of your motivation and other relevant information.

How to apply:

The application, in English, should be sent to Dr. Kevin Waldron (kwaldron@ibb.waw.pl). Please include the subject heading "NIH Postdoc application" in your email. Applications must be written in English, and should contain a scientific CV (no more than 5 pages), a cover letter with a description of the applicant's key achievements and motivation (up to 2 pages), and contact details for 2 potential academic referees, including your PhD supervisor. All documents should be merged in a single pdf file.

Selected candidates will be invited for an interview (possibly on-line). Applications submitted after the deadline will be still considered if the position is not filled.

Please include the following statement in your application: "I hereby give my consent for the processing of my personal data by the Institute of Biochemistry and Biophysics PAS with its seat in Warsaw Pawińskiego 5a, 02-106 hereinafter referred to as the Institute for the purpose of the recruitment process and for future recruitment processes conducted by the Institute under Art. 23 ust 1 pkt 1 of the Personal Data Protection Act dated on 29 August 1997, consolidated text: Journal of Laws 2016, item 922 with further amendments and

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under Art. 6 ust.1 lit. a of 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 GDPR (Dz. U. UE. L. z 2016 r. Nr 119)".

Closing date: July 16th, 2024

The evaluation process will start immediately upon receipt of the applications. Selected candidates will be invited for interview. The competition may be extended until the finding of a suitable candidate.

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