Prospective supervisor's form

Name of the supervisor: Marek Wojciechowski

Academic title: GUT Professor

Orcid ID number: https://orcid.org/0000- 0003-3003-8483

Faculty of Chemistry

Gdańsk University of Technology **Department of** Pharmaceutical Technology and Biochemistry

Phone: **+48** 347 1596

E-mail: marek.wojciechowski@pg.edu.pl

Personal web page: https://pg.edu.pl/

Discipline[i] chemical sciences [NCh] none

Optional

Key words (obligatory four key words describing research interests / expertise):

Computational chemistry

Computer aided drug design

Molecular dynamics

Docking

Bibliometric indicators

1. Number of journal publications in WoS/ Scopus: WoS:28/Scopus:29
2. Citations excluding self-citations: WoS 206 Scopus 218
3. Hirsch index: WoS 9 Scopus 9

1. The number of PhD students who have graduated under your supervision: 0
2. The number of PhD students currently supervised:
   a. within the current doctoral school: 0
   b. within doctoral studies (previous system): 0
3. Are you currently accepting new PhD students:
   a. Polish *Yes/No*: Yes
   b. Foreign *Yes/No*: No

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Research interests or topics offered for PhD research (no more than 2000 characters)[ii]

In the recent years, with the fast growing amount of experimental data in the structural databases like PDB, structure based drug design yet again attracts attention. Especially, since experimental high-throughput screening techniques, in the long run, turn out to be giving somewhat disappointing results.
Completely rational design of an active molecule, rooted in the knowledge of its molecular target as well as desired properties, though more tedious, gives much better results and is more rewarding, not only from the economical point of view.
Advancement of computational methods for rapid and accurate prediction of binding free energy allow not only to design new drug candidates but also, in the process of so called drug repurposing, radically shrinks time required to introduce an active molecule ready for treatment of more and more frequently emerging new diseases even of pandemic scale.
Research areas that PhD candidate can be involved in include computer aided drug design and molecular modeling of interactions between small molecules and their biological targets. Particularly, research topics may cover:
- design of new antifungal agents, mostly GlcN-6-P synthase inhibitors,
- studies on the structure and catalysis/inhibition mechanism of eukaryotic GlcN-6-P synthase
- development of tools and algorithms for studying interactions of small molecules with protein receptors

Funding or special equipment needed to carry out a PhD project[iii]:

1. Is funding available for experimental work: *Yes/No/not needed* — not needed
2. Is the equipment needed to complete a PhD project available in your lab/department: *Yes/No/not needed* — Yes

Most important publications – no more than 5 published after 1.01.2018

No	Authors/title/journal	Number of points according to the current list of the Ministry of Science and Higher Education	Publication year
1.	Wasilewski, T., Szulczyński, B., Wojciechowski, M., Kamysz, W., Gębicki, J. / Determination of long-chain aldehydes using a novel quartz crystal microbalance sensor based on a biomimetic peptide/ 2020 Microchemical Journal, 154,104509	70	2020
2.	Wasilewski, T., Szulczyński, B., Wojciechowski, M., Kamysz, W., Gębicki, J. A highly selective biosensor based on peptide directly derived from the harmOBP7 aldehyde binding site 2019 Sensors (Switzerland), 19(19),4284	100	2019

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3.	Kwiatkowska-Semrau, K., Wojciechowski, M., Gabriel, I., Crucho, S., Milewski, S. Modification of quaternary structure of Candida albicans GlcN-6-P synthase and its desensitization to inhibition by UDP-GlcNAc by site-directed mutagenesis	70	2018
4.			
5.			

Most recent externally funded projects you were involved in – no more than 3

No	Project title, the name of the Principal Investigator (PI) and the institution the project was carried out	Years	Role in the project [iv]
1.			PI
2.			PI
3.			PI

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Additional relevant information – (no more than 1600 characters)[v]

[i] You may select up to two disciplines out of 12 disciplines represented in the Doctoral School

[ii] Observe the limit of not more than 2000 characters

[iii] Leave only one answer

[iv] Select the role in the project: PI stands for principal investigator (refers to the holder of an independent grant and the lead researcher for the grant project), Co-I for co-investigator (Co-I assists the principal investigator in the management and leadership of the research project), R for researcher

[v] Add any other relevant information e.g. awards for PhD students whom you supervised (no more than 1600 characters)