



**Silesian University
of Technology**

DISCIPLINE COUNCIL FOR CHEMICAL SCIENCES

mgr inż. Maria BZÓWKA

**ANALYSIS OF MOLECULAR ASPECTS OF PROTEINS REGULATION
CONSIDERING WATER MOLECULES AS A POTENTIAL MEDIATOR
IN INTERMOLECULAR INTERACTIONS**

**ATTACHMENT TO THE DOCTORAL THESIS:
CO-AUTHOR CONTRIBUTION STATEMENTS**

Supervisor: dr hab. Artur GÓRA, prof. PŚ

Gliwice, 2023

Co-Author Contribution Statements for Paper 1

[1] **Paper 1:** Mitusińska K., Raczyńska A., **Bzówka M.**, Bagrowska W., Góra A.
Applications of water molecules for analysis of macromolecule properties
Computational and Structural Biotechnology Journal (2020) 18, 355-365
<https://doi.org/10.1016/j.csbj.2020.02.001>



Doctoral School

Maria Bzówka MSc, BEng
PhD student

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K., Raczyńska A., Bzówka M., Bagrowska W., Góra A.

Applications of water molecules for analysis of macromolecule properties

Computational and Structural Biotechnology Journal (2020) 18, 355-365

<https://doi.org/10.1016/j.csbj.2020.02.001>

I declare the following contribution to this publication: 15%

I was involved in the literature search and data organisation (particularly regarding the applicability and functionality of software reviewed in the second and third part of the article). I was involved in writing the manuscript, reviewing and editing the final version and providing answers to the reviewers' comments.

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Dr
Karolina Mitusińska PhD
Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K., Raczyńska A., Bzówka M., Bagrowska W., Góra A.

Applications of water molecules for analysis of macromolecule properties

Computational and Structural Biotechnology Journal (2020) 18, 355-365

<https://doi.org/10.1016/j.csbj.2020.02.001>

I declare the following contribution to this publication: 40%

I was involved in the literature search and data organisation. I was involved in writing the manuscript and responding to the Reviewers' comments.

Yours sincerely,

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Agata Raczyńska
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CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

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<https://doi.org/10.1016/j.csbj.2020.02.001>

I declare the following contribution to this publication: 20%

I was involved in the literature search and data organisation. I was involved in writing the manuscript and preparation of figures.



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Gliwice, 17.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

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I declare the following contribution to this publication: 15%

I was involved in the literature search and data organisation. I was involved in writing the manuscript and preparation of figures.

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Artur Góra PhD, DSc
Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

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<https://doi.org/10.1016/j.csbj.2020.02.001>

I declare the following contribution to this publication: 10%

I conceived the project and contributed to its conceptualisation. I reviewed the manuscript and participated in responding to the reviewers' comments. I was responsible for project administration and supervision.

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Co-Author Contribution Statements for Paper 2

[2] **Paper 2:** Magdziarz T., Mitusińska K., **Bzówka M.**, Raczyńska A., Stańczak A., Banas M., Bagrowska W., Góra A.

AQUA-DUCT 1.0: structural and functional analysis of macromolecules from an intramolecular voids perspective

Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>



Doctoral School

Maria Bzówka MSc, BEng
PhD student

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Magdziarz T., Mitusińska K., Bzówka M., Raczyńska A., Stańczak A., Banas M., Bagrowska W., Góra A

AQUA-DUCT 1.0: structural and functional analysis of macromolecules from an intramolecular voids perspective

Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>

I declare the following contribution to this publication: 16,5%

I was involved in software development by testing new features that were added to drivers *valve* and *pond*. I was working with the main developer of the software on the optimisation of the *pond* driver for local-distribution analysis. I was testing different modes of analysis (*time-window* and *sandwich*). I was working on the following case studies: human soluble epoxide hydrolase, potato soluble epoxide hydrolase, and haloalkane dehalogenase LinB. I was involved in writing the manuscript, preparation of figures, reviewing and editing the final version and in providing answers to the reviewer's comments.

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Tomasz Magdziarz, PhD

Email address: tomasz.magdziarz@gmail.com

Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Magdziarz T., Mitusińska K., Bzówka M., Raczyńska A., Stańczak A., Banas M.,
Bagrowska W., Góra A.

AQUA-DUCT 1.0: structural and functional analysis of macromolecules from an
intramolecular voids perspective

Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>

I declare the following contribution to this publication: 20%

I contributed to the conceptualisation of the project. I was the main developer of the computer code for AQUA-DUCT software. I was involved in writing the manuscript and responding to the Reviewers' comments.

Signature





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Dr
Karolina Mitusińska PhD
Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Magdziarz T., Mitusińska K., Bzówka M., Raczyńska A., Stańczak A., Banas M., Bagrowska W., Góra A

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Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>

I declare the following contribution to this publication: 18,5%

I was involved in the software development by running small-molecule tracking analysis for several different systems. I was involved in running benchmarking section. I was involved in writing the manuscript and responding to the Reviewers' comments.

Yours sincerely,

Karolina Mitusińska

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Agata Raczyńska
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20.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

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Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>

I declare the following contribution to this publication: 7,5%

I prepared various tutorials, e.g. for clustering, trimming paths, and smoothing paths. I was involved in writing the documentation and figures preparation.



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Prague, 15.11.2023

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Faculty of Science, Charles University, Czech Republic

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Magdziarz T., Mitusińska K., Bzówka M., Raczyńska A., Stańczak A., Banas M.,
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intramolecular voids perspective

Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>

I declare the following contribution to this publication: 5 %

I performed the MD simulation of the haloalkane dehalogenase LinB with different substrates
for consolidator mode usage (rare events analysis).



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Michał Banas, BEng

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Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Magdziarz T., Mitusińska K., Bzówka M., Raczyńska A., Stańczak A., Banas M.,
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Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>

I declare the following contribution to this publication: 7,5%

I was the developer of the Graphical User Interface (GUI) version for AQUA-DUCT 1.0 and
Kraken module for data visualisation.



Signature

Gliwice, 17.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Magdziarz T., Mitusińska K., Bzówka M., Raczyńska A., Stańczak A., Banas M., Bagrowska W., Góra A.

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Bioinformatics (2020) 36 (8), 2599-2601

<https://doi.org/10.1093/bioinformatics/btz946>

I declare the following contribution to this publication: 5%

I was testing different functionalities of the AQUA-DUCT 1.0 software.

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Artur Góra PhD, DSc
Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

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Magdziarz T., Mitusińska K., Bzówka M., Raczyńska A., Stańczak A., Banas M., Bagrowska W., Góra A

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I declare the following contribution to this publication: 20%

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Co-Author Contribution Statements for Paper 3

[3] **Paper 3: Bzówka M.***, Mitusińska K.*, Raczyńska A., Samol A., Tuszyński J.A., Góra A.
Structural and Evolutionary Analysis Indicate That the SARS-CoV-2 Mpro Is a Challenging
Target for Small-Molecule Inhibitor Design

International Journal of Molecular Sciences (2020) 21, 1-17

<https://doi.org/10.3390/ijms21093099>

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M. *, Mitusińska K. *, Raczyńska A., Samol A., Tuszyński J.A., Góra A.

Structural and Evolutionary Analysis Indicate That the SARS-CoV-2 Mpro Is a Challenging Target for Small-Molecule Inhibitor Design

International Journal of Molecular Sciences (2020) 21, 1-17

<https://doi.org/10.3390/ijms21093099>

I declare the following contribution to this publication: 30%

I was responsible for running all mixed-solvent molecular dynamics simulations and their further analysis with AQUA-DUCT software, including the analysis of the intramolecular voids and hot-spots. Also, I was involved in conducting the same analysis with AQUA-DUCT software for classical MD simulations. I was involved in comparison of crystal structures of main proteases from SARS-CoV-2 and SARS-CoV and the analysis of the plasticity of their binding cavities. I was also involved in the analysis of the potential mutability of SARS-CoV-2. I was involved in writing the manuscript, preparation of figures, reviewing and editing the final version and in providing answers to the reviewers' comments.

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Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Samol A., Tuszyński J.A., Góra A.

Structural and Evolutionary Analysis Indicate That the SARS-CoV-2 Mpro Is a Challenging Target for Small-Molecule Inhibitor Design

International Journal of Molecular Sciences (2020) 21, 1-17

<https://doi.org/10.1016/j.csbj.2020.02.001>

I declare the following contribution to this publication: 30%

I was involved in conducting a set of classical molecular dynamics simulations and analysing them. I was involved in writing the manuscript and responding to the Reviewers' comments.

Yours sincerely,

Karolina Mitusińska

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MSc, BEng

20.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Samol A., Tuszyński J.A., Góra A.

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International Journal of Molecular Sciences (2020) 21, 1-17

<https://doi.org/10.3390/ijms21093099>

I declare the following contribution to this publication: 10%

I performed the analysis of the energetic effect of amino acid substitutions.



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Aleksandra Samol, MSc
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Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Samol A., Tuszyński J.A., Góra A.

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Target for Small-Molecule Inhibitor Design
International Journal of Molecular Sciences (2020) 21, 1-17
<https://doi.org/10.3390/ijms21093099>

I declare the following contribution to this publication: 5%
I was involved in conducting the evolutionary analysis.



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Professor Jack A. Tuszyński
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University of Alberta
Email address: jacek.tuszynski@polito.it ; jackt@ualberta.ca

Co-Author contribution statement

Hereby, I certify that I am the Co-Author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Samol A., Tuszyński J.A., Góra A.

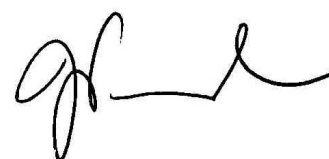
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International Journal of Molecular Sciences (2020) 21, 1-17

<https://doi.org/10.3390/ijms21093099>

I declare the following contribution to this publication: 5%

I contributed to the project's conceptualization. I was also involved in the reviewing and editing of the manuscript.



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Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Samol A., Tuszyński J.A., Góra A.

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<https://doi.org/10.3390/ijms21093099>

I declare the following contribution to this publication: 20%

I conceived the project and contributed to its conceptualisation. I reviewed the manuscript and participated in responding to the reviewers' comments. I was responsible for project administration and supervision.

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Co-Author Contribution Statements for Paper 4

[4] **Paper 4:** Fischer A.* , Sellner M.* , Mitusińska K.* , **Bzówka M.***, Lill M.A., Góra A., Smieško M.

Computational selectivity assessment of protease inhibitors against SARS-CoV-2

International Journal of Molecular Sciences (2021) 22 (4), 1-17

<https://doi.org/10.3390/ijms22042065>



Doctoral School

Maria Bzówka MSc, BEng
PhD student

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Fischer A. *, Sellner M. *, Mitusińska K. *, Bzówka M. *, Lill M.A., Góra A., Smieško M.

Computational selectivity assessment of protease inhibitors against SARS-CoV-2

International Journal of Molecular Sciences (2021) 22 (4), 1-17

<https://doi.org/10.3390/ijms22042065>

I declare the following contribution to this publication: 20%

I was involved in the analysis of the similarity of the selected panel of proteases. I was involved in performing classical molecular dynamics simulations with the water molecules tracking and hydration sites identification of the selected panel of proteases. I was also involved in the analysis of the co-solvent sites. I was involved in writing the manuscript, preparation of figures, reviewing and editing the final version and in providing answers to the reviewers' comments. I was responsible for coordinating the cooperation with international partners.

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Andre Fischer, PhD
Scientist, dsm-firmenich
Email address: andre_fischer1994@hotmail.com

Co-Author contribution statement

Hereby, I certify that I am the co-author of the following publication:

Fischer A. *, Sellner M. *, Mitusińska K. *, Bzówka M. *, Lill M.A., Góra A., Smieško M.

Computational selectivity assessment of protease inhibitors against SARS-CoV-2

International Journal of Molecular Sciences (2021) 22 (4), 1-17

<https://doi.org/10.3390/ijms22042065>

I declare the following contribution to this publication: 20%

I contributed to the project's conceptualisation. I was involved in conducting cosolvent MD simulations, molecular docking, MD and MM/GBSA post-processing, and toxicity profiling. I was involved in writing the manuscript and responding to the reviewers' comments.

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Basel, 15.11.2023

Manuel Sellner, Assistant / PhD candidate
Computational Pharmacy
Department of Pharmaceutical Sciences
University of Basel, Switzerland
Email address: manuel.sellner@unibas.ch

Co-Author contribution statement

Hereby, I certify that I am the co-author of the following publication:

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I declare the following contribution to this publication: 20%

I was involved in molecular docking, MD and MM/GBSA post-processing, and toxicity profiling. I was involved in writing the manuscript.



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Dr
Karolina Mitusińska PhD
Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Fischer A.*, Sellner M.*, Mitusińska K.*, Bzówka M.*, Lill M.A., Góra A., Smieško M.

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<https://doi.org/10.3390/ijms22042065>

I declare the following contribution to this publication: 20%

I was involved in conducting a set of classical molecular dynamics simulations and analysing them. Also, I was involved in the analysis of the similarity of the selected proteins. I was involved in writing the manuscript..

Yours sincerely,

Karolina Mitusińska

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TU  ELING GROUP



THE EXCELLENCE IN RESEARCH

Basel, 15.11.2023

Markus A. Lill, Prof. Dr.
Computational Pharmacy
Department of Pharmaceutical Sciences
University of Basel, Switzerland
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Co-Author contribution statement

Hereby, I certify that I am the co-author of the following publication:

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<https://doi.org/10.3390/ijms22042065>

I declare the following contribution to this publication: 6,67%

I was involved in reviewing and editing the manuscript. I supervised the project.

A handwritten signature in black ink, appearing to read 'M A Lill', written in a cursive style.

Signature



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University
of Technology



RESEARCH
UNIVERSITY
EXCELLENCE INITIATIVE

Biotechnology Centre

Artur Góra PhD, DSc
Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

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HR EXCELLENCE IN RESEARCH



TU ELING GROUP

Basel, 15.11.2023

Martin Smieško, Prof. Dr.
Computational Pharmacy
Department of Pharmaceutical Sciences
University of Basel, Switzerland
Email address: martin.smiesko@unibas.ch

Co-Author contribution statement

Hereby, I certify that I am the co-author of the following publication:

Fischer A.*, Sellner M.*, Mitusińska K.*, Bzówka M.*, Lill M.A., Góra A., Smieško M.

Computational selectivity assessment of protease inhibitors against SARS-CoV-2
International Journal of Molecular Sciences (2021) 22 (4), 1-17
<https://doi.org/10.3390/ijms22042065>

I declare the following contribution to this publication: 6,67%

I was involved in reviewing and editing the manuscript. I supervised the project.



Signature

Co-Author Contribution Statements for Paper 5

[5] **Paper 5: Bzówka M.**, Mitusińska K., Hopko K., Góra A.

Computational insights into the known inhibitors of human soluble epoxide hydrolase

Drug Discovery Today (2021) 26 (8), 1914-1921

<https://doi.org/10.1016/j.drudis.2021.05.017>



Doctoral School

Maria Bzówka MSc, BEng
PhD student

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M., Mitusińska K., Hopko K., Góra A.

Computational insights into the known inhibitors of human soluble epoxide hydrolase

Drug Discovery Today (2021) 26 (8), 1914-1921

<https://doi.org/10.1016/j.drudis.2021.05.017>

I declare the following contribution to this publication: 60%

I contributed to the project's conceptualisation. I carried out all the analyses for known inhibitors co-crystallised with human soluble epoxide hydrolase. I performed the analysis of the interactions, including clustering of binding residues and inhibitors. I ran molecular dynamics simulations and further AQUA-DUCT analysis for the identification of tunnels and inner voids. I was involved in writing the manuscript, preparation of figures, reviewing and editing the final version and in providing answers to the reviewers' comments.

Maria Bzówka

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Dr
Karolina Mitusińska PhD
Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M., Mitusińska K., Hopko K., Góra A.

Computational insights into the known inhibitors of human soluble epoxide hydrolase

Drug Discovery Today (2021) 26 (8), 1914-1921

<https://doi.org/10.1016/j.drudis.2021.05.017>

I declare the following contribution to this publication: 20%

I was involved in helping in data organisation and editing the manuscript.

Yours sincerely,

Karolina Mitusińska

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Biotechnology Centre
MSc, BEng
Katarzyna Żurawska
(Hopko)

Gliwice, 20.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M., Mitusińska K., Hopko K., Góra A.

Computational insights into the known inhibitors of human soluble epoxide hydrolase

Drug Discovery Today (2021) 26 (8), 1914-1921

<https://doi.org/10.1016/j.drudis.2021.05.017>

I declare the following contribution to this publication: 5%

I did the general identification of chemical motives in inhibitors' structures.

Katarzyna Żurawska
(Hopko)

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Katarzyna.Zurawska@polsl.pl

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Biotechnology Centre

Artur Góra PhD, DSc
Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M., Mitusińska K., Hopko K., Góra A.

Computational insights into the known inhibitors of human soluble epoxide hydrolase

Drug Discovery Today (2021) 26 (8), 1914-1921

<https://doi.org/10.1016/j.drudis.2021.05.017>

I declare the following contribution to this publication: 15%

I conceived the project and contributed to its conceptualisation. I reviewed the manuscript and participated in responding to the reviewers' comments. I was responsible for project administration and supervision.

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Co-Author Contribution Statements for Paper 6

[6] **Paper 6:** Mitusińska K., Wojsa P., **Bzówka M.**, Raczyńska A., Bagrowska W., Samol A., Kapica P., Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P., Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 17,5%

I was involved in analyses of the flow of water molecules for all the analysed structures, particularly the determination of the appropriate parameters for detecting tunnels and their subsequent characteristics. I also participated in a general comparison of the soluble epoxide hydrolase members by analysing their structural features. I was involved in data organisation, reviewing the manuscript and responding to the reviewers' comments.

Maria Bzówka

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Dr
Karolina Mitusińska PhD
Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P., Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 30%

I was involved in conducting a set of classical molecular dynamics simulations, analysing them and organising data. I was involved in writing the manuscript and responding to the Reviewers' comments.

Yours sincerely,

Karolina Mitusińska

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17.11.2023

Piotr Wojsa, BEng

Email address: piotr.j.wojsa@gmail.com

Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P., Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 17,5%

I performed molecular dynamics simulation for *Vigna radiata* soluble epoxide hydrolase. I was involved in water path analysis for selected repetitions and figures preparation.

Signature

A handwritten signature in black ink, appearing to read 'Piotr Wojsa', written in a cursive style.



Doctoral School

Agata Raczyńska
MSc, BEng

20.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P., Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 5%

I conducted molecular dynamics simulation for human soluble epoxide hydrolase.



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Gliwice, 17.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P., Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 5%

I conducted molecular dynamics simulation for *Bacillus Megaterium* soluble epoxide hydrolase. I was involved in preparation of figures.

Bagrowska Weronika

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Aleksandra Samol, MSc
Email address: 2aleksandrasamol@gmail.com

Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P.,
Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel
network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 5%

I performed molecular dynamics simulation for *Trichoderma reesei* soluble epoxide
hydrolase.


Signature

17.11.2023

Patryk Kapica, MSc

Email address: *kapica.patrick@gmail.com*

Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P.,
Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel
network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 5%

I did a literature review on substrate specificity.


Signature



Biotechnology Centre

Artur Góra PhD, DSc
Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K., Wojsa P., Bzówka M., Raczyńska A., Bagrowska W., Samol A., Kapica P., Góra A.

Structure-function relationship between soluble epoxide hydrolases structure and their tunnel network

Computational and Structural Biotechnology Journal (2022) 20, 193-205

<https://doi.org/10.1016/j.csbj.2021.10.042>

I declare the following contribution to this publication: 15%

I conceived the project and contributed to its conceptualisation. I was involved in writing and reviewing the manuscript. I participated in responding to the reviewers' comments. I was responsible for project administration and supervision.

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Co-Author Contribution Statements for Paper 7

[7] **Paper 7:** Mitusińska K.*, **Bzówka M.***, Magdziarz T., Góra A.

Geometry-Based versus Small-Molecule Tracking Method for Tunnel Identification: Benefits and Pitfalls

Journal of Chemical Information and Modeling (2022) 62 (24), 6803-6811

<https://doi.org/10.1021/acs.jcim.2c00985>



Doctoral School

Maria Bzówka MSc, BEng
PhD student

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K.*, Bzówka M.*, Magdziarz T., Góra A.

Geometry-Based versus Small-Molecule Tracking Method for Tunnel Identification: Benefits and Pitfalls

Journal of Chemical Information and Modeling (2022) 62 (24), 6803-6811

<https://doi.org/10.1021/acs.jcim.2c00985>

I declare the following contribution to this publication: 40%

I was involved in identifying tunnels in MD simulations using small-molecular tracking approach. I was partially involved in the identification of tunnels in crystal structures using a geometry-based approach. I was involved in refining the methods for comparing tunnels found in crystal structures with tunnels identified during MD simulations. I was involved in writing the manuscript, preparation of figures, reviewing and editing the final version and in providing answers to the reviewers' comments.

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Dr
Karolina Mitusińska PhD
Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K. *, Bzówka M. *, Magdziarz T., Góra A.

Geometry-Based versus Small-Molecule Tracking Method for Tunnel Identification: Benefits and Pitfalls

Journal of Chemical Information and Modeling (2022) 62 (24), 6803-6811

<https://doi.org/10.1021/acs.jcim.2c00985>

I declare the following contribution to this publication: 40%

I was involved in running geometry-based analysis for the set of the proteins. I was involved in writing the manuscript and responding to the Reviewers' comments.

Yours sincerely,

Karolina Mitusińska

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Tomasz Magdziarz, PhD

Email address: tomasz.magdziarz@gmail.com

Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Mitusińska K.*, Bzówka M.*, Magdziarz T., Góra A.

Geometry-Based versus Small-Molecule Tracking Method for Tunnel Identification: Benefits and Pitfalls

Journal of Chemical Information and Modeling (2022) 62 (24), 6803-6811

<https://doi.org/10.1021/acs.jcim.2c00985>

I declare the following contribution to this publication: 5%

I was involved in preparing scripts for the tunnel comparison.

Signature

A handwritten signature in blue ink that reads "Tomasz Magdziarz". The signature is written in a cursive style with a large initial 'T'.



Biotechnology Centre

Artur Góra PhD, DSc
Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Mitusińska K.*, Bzówka M.*, Magdziarz T., Góra A.

Geometry-Based versus Small-Molecule Tracking Method for Tunnel Identification: Benefits and Pitfalls

Journal of Chemical Information and Modeling (2022) 62 (24), 6803-6811

<https://doi.org/10.1021/acs.jcim.2c00985>

I declare the following contribution to this publication: 15%

I conceived the project and contributed to its conceptualisation I reviewed the manuscript and participated in responding to the reviewers' comments. I was responsible for project administration and supervision.

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Co-Author Contribution Statements for Paper 8

[8] **Paper 8: Bzówka M***, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W., Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins - What can we learn from studying epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>



Doctoral School

Maria Bzówka MSc, BEng
PhD student

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M*, Mitusińska K.*, Raczynska A., Skalski T., Samol A., Bagrowska W., Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins-What can we learn from studying epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 25%

I performed the evolutionary analysis of the residues making up referential compartments and all tunnels in each of the selected member of soluble epoxide hydrolase subfamily. I participated in providing characteristic about the general evolutionary analysis of tunnels and a detailed analysis of the selected cases. I was involved in writing the manuscript, preparation of figures, reviewing and editing the final version and in providing answers to the reviewers' comments.

Maria Bzówka

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Dr
Karolina Mitusińska PhD
Research assistant

Gliwice, 10.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M*, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W., Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins-What can we learn from studying epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 25%

I was involved in conducting a set of classical molecular dynamics simulations. I was involved in writing the manuscript and responding to the Reviewers' comments.

Yours sincerely,

Karolina Mitusińska

Silesian University of Technology
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Doctoral School

Agata Raczyńska
MSc, BEng

20.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W., Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins - What can we learn from studying epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 15%

I participated in performing the variability analysis and characterisation of selected tunnels.



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Gliwice, 13.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W., Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins - What can we learn from studying epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 5%

I designed the statistical analysis workflow.



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Tomasz.Skalski@polsl.pl

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16.11.2023

Aleksandra Samol, MSc
Email address: 2aleksandrasamol@gmail.com

Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W.,
Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins - What can we learn from studying
epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 5%

I was involved in the preparation and adjusting of the Multiple Sequence Alignment.



Signature

Gliwice, 17.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W., Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins - What can we learn from studying epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 5%

I conducted molecular dynamics simulation for *Bacillus Megaterium* soluble epoxide hydrolase.

Weronika Bagrowska

Silesian University of Technology

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Weronika.Bagrowska@polsl.pl

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17.11.2023

Tomasz Magdziarz, PhD

Email address: tomasz.magdziarz@gmail.com

Co-author contribution statement

Hereby, I certify that I am the Co-author of the following publication:

Bzówka M.*, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W.,
Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins - What can we learn from studying
epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 5%

I was involved in preparing scripts for the tunnel comparison.

Signature





Biotechnology Centre

Artur Góra PhD, DSc
Head of Tunneling Group

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M*, Mitusińska K.*, Raczyńska A., Skalski T., Samol A., Bagrowska W., Magdziarz T., Góra A.

Evolution of tunnels in alpha/beta-hydrolase fold proteins-What can we learn from studying epoxide hydrolases?

PLoS Computational Biology (2022) 18 (5), 1-25

<https://doi.org/10.1371/journal.pcbi.1010119>

I declare the following contribution to this publication: 15%

I conceived the project and contributed to its conceptualisation I reviewed the manuscript and participated in responding to the reviewers' comments. I was responsible for project administration and supervision.

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Co-Author Contribution Statements for Paper 9

[9] **Paper 9: Bzówka M.**, Bagrowska W., Góra A.

Recent advances in studying Toll-like receptors with the use of computational methods

Journal of Chemical Information and Modeling (2023) 63 (12), 3669–3687

<https://doi.org/10.1021/acs.jcim.3c00419>



Doctoral School

Maria Bzówka MSc, BEng
PhD student

Gliwice, 09.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M., Bagrowska W., Góra A.

Recent advances in studying Toll-like receptors with the use of computational methods

Journal of Chemical Information and Modeling (2023) 63 (12), 3669–3687

<https://doi.org/10.1021/acs.jcim.3c00419>

I declare the following contribution to this publication: 60%

I conceived the project and contributed to its conceptualisation. I performed the literature revision and organised all the data. I was involved in writing the manuscript, reviewing and editing the final version and in providing answers to the reviewers' comments. I was responsible for project administration and supervision.

Maria Bzówka

Silesian University of Technology



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Gliwice, 17.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following publication:

Bzówka M., Bagrowska W., Góra A.

Recent advances in studying Toll-like receptors with the use of computational methods

Journal of Chemical Information and Modeling (2023), 63 (12) 3669–3687

<https://doi.org/10.1021/acs.jcim.3c00419>

I declare the following contribution to this publication: 30%

I was involved in the literature search. I was involved in writing the manuscript and preparation of figures.

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Journal of Chemical Information and Modeling (2023) 63 (12), 3669–3687

<https://doi.org/10.1021/acs.jcim.3c00419>

I declare the following contribution to this publication: 10%

I contributed to the project's conceptualisation. I reviewed the manuscript.

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Co-Author Contribution Statements for Preprint 1

[10] **Preprint 1: Bzówka M., Szeleper K., Stańczak A., Borowski T., Góra A.**
The proteolytic cleavage of TLR8 Z-loop by furin protease - molecular recognition, reaction mechanism and role of water molecules

Research Square Preprint (2023)

<https://doi.org/10.21203/rs.3.rs-3590328/v1>



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Maria Bzówka MSc, BEng

PhD student

Gliwice, 15.11.2023

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Hereby, I certify that I am the co-author of the following publication:

Bzówka M., Szleper K., Stańczak A., Borowski T., Góra A.

Recent advances in studying Toll-like receptors with the use of computational methods

Preprint deposited in the Research Square repository

<https://doi.org/10.21203/rs.3.rs-3590328/v1>

I declare the following contribution to this preprint: 55%

I conceived the project and contributed to its conceptualisation. I performed analyses related to the prediction of the complex. I ran all molecular dynamics simulations for each reactions species. I did the analysis of the interaction network and the analysis of the reorganisation of water molecules using AQUA-DUCT software. I was involved in writing the manuscript, preparation of figures, ad data organisation. I was responsible for project administration and supervision.

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CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following preprint:

Bzówka M., Szleper K., Stańczak A., Borowski T., Góra A.,

The proteolytic cleavage of TLR8 Z-loop by furin protease - molecular recognition, reaction mechanism and role of water molecules

Preprint deposited in the Research Square repository
<https://doi.org/10.21203/rs.3.rs-3590328/v1>

I declare the following contribution to this preprint: 20%

I performed the QM/MM calculations and was involved in the parametrisation of non-standard residues for MD simulations. I was involved in data analysis, figures preparation and writing the manuscript.

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CO-AUTHOR CONTRIBUTION STATEMENT

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I declare the following contribution to this preprint: 15 %

I performed the QM-cluster calculations for the TLR8-furin complex, analysed and interpreted data.



Signature

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Co-Author contribution statement

Hereby, I certify that I am the co-author of the following preprint:

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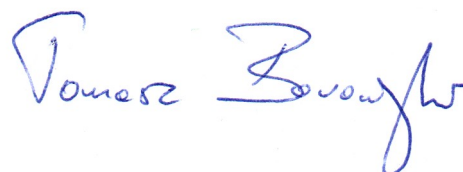
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Preprint deposited in the Research Square repository

<https://doi.org/10.21203/rs.3.rs-3590328/v1>

I declare the following contribution to this preprint: 5%

I provided the methodological support to QM and QM/MM calculations. I participated in reviewing the manuscript.



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Gliwice, 15.11.2023

CO-AUTHOR CONTRIBUTION STATEMENT

Hereby, I certify that I am the co-author of the following preprint:

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I declare the following contribution to this preprint: 5%

I contributed to the project's conceptualisation. I reviewed the manuscript.

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