Curriculum Vitae

M.Sc. Krzysztof Kamil Bojarski

Principal Investigator at Laboratory of Molecular Modeling,
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Personal information:

Date of birth: 07.10.1993
Birth place: Lębork, Poland
Citizenship: Poland

Research experience and academic degrees:

2019 – present Principal Investigator at the Laboratory of Molecular Modeling, Department of Theoretical Chemistry, Faculty of Chemistry, University of Gdańsk in Preludium 16 Grant Project: 'Computational insights into procathepsin maturation mediated by glycosaminoglycans'.

2019 Project Assistant at the Laboratory of Molecular Modeling, Department of Theoretical Chemistry, Faculty of Chemistry, University of Gdańsk in Sonata Bis 8 Grant Project: 'Modeling of glycosaminoglycan-induced formation of protein structure and enhancement of biologically relevant protein-ligand interactions'.

2017 – 2019 Project Assistant at the Laboratory of Molecular Modeling, Department of Theoretical Chemistry, Faculty of Chemistry, University of Gdańsk in Polonez 2 Grant Project: 'Computational approaches to study protein-glycosaminoglycan interactions'.

2017 Master Degree in Chemistry, Department of Theoretical Chemistry, Faculty of Chemistry, University of Gdańsk, Poland Master Thesis: 'Effect of restraint type and strength on the quality of protein models obtained with homology-restrained UNRES simulations'.

2015 Bachelor Degree in Chemistry, Department of Biophysics, Faculty of Department of Organic Chemistry, Faculty of Chemistry, University of Gdańsk, Poland.

Research interest:

Protein-glycosaminoglycans interactions, glycosaminoglycans conformational analysis, molecular dynamics, molecular docking, coarse-grained modeling.

Computer Programs/Skills:

- AMBER, VMD, Chimera UCSF, Pymol, Avogadro
- R statistical package, bash scripting, gnuplot

List of scientific publications, abstracts and proceedings of the meetings:

A. Publications:

1. **Bojarski K.K.,** Karczyńska A.S., Samsonov S.A. Role of Glycosaminoglycans in Procathepsin B Maturation: Molecular Mechanism Elucidated by a Computational Study. J Chem Inf Model. 2020, 60(4):2247-2256

2. Lecaille F., Chazeirat T., **Bojarski K.K.,** Renault J., Saidi A., Prasad V.G.N.V., Samsonov S.A., Lalmanach G. Rat cathepsin K: enzymatic specificity and regulation of its collagenolytic activity. Biochim Biophys Acta – Proteins Proteom. 2020, 1868(2):1-11

3. Potthoff J[†]., **Bojarski K.K.,**[†] Kohut G., Lipska A.G., Liwo A., Kessler E., Ricard-Blum S., Samsonov S.A. Analysis of procollagen C-proteinase enhancer-1/glycosaminoglycan binding sites and of the potential role of calcium ions in the interaction. Int J Mol Sci. 2019, 20(20):1-24

[†] - equal contribution

4. Samsonov S.A., Lubecka E. A., **Bojarski K. K.,** Ganzynkowicz R., Liwo A. Local and Long Range Potentials for Heparin-Protein Systems for Coarse-Grained Simulations. Biopolymers. 2019, 110(8):1-12

5. **Bojarski K.K.,** Becher J., Riemer T., Lemmnitzer K., Möller S., Schiller J., Schnabelrauch M., Samsonov S.A. Synthesis and in silico characterization of artificially phosphorylated glycosaminoglycans. J Mol Struct, 2019, 1197:401-416

6. **Bojarski K.K.,** Sieradzan A.K., Samsonov S.A., Molecular Dynamics Insights into Protein-Glycosaminoglycan Systems from Microsecond-Scale Simulations. Biopolymers, 2019, 110(7):1-15

7. Uciechowska-Kaczmarzyk U., Babik S., Zsila F., **Bojarski K.K.,** Beke-Somfai T., Samsonov S.A. Molecular Dynamics-Based Model of VEGF-A and Its Heparin Interactions. J Mol Graph Mod. 2018, 82:157-166

8. **Bojarski K. K.,** Samsonov S. A. Glycosaminoglycans mediate the function of cathepsin proteases. Review. 'VII All Polish Conference: Young Scientists in Poland – Research and Development'. Wydawnictwo Młodzi Naukowcy. 2017. Epub.

9. Karczyńska A., Mozolewska M. A., Krupa P., Giełdoń A., **Bojarski K. K.,** Zaborowski ., Liwo A., Ślusarz R., Ślusarz M., Lee J., Joo K., Czaplewski C. Use of the UNRES force field in template-assisted prediction of protein structures and the refinement of server models: Test with CASP12 targets. J Mol Graph Mod. 2018, 83:92-99

B. Oral and poster presentations:

1. **Bojarski K.K.,** Samsonov S.A. Challenges in modeling protein-glycosaminoglycan systems, 34th Molecular Modeling Workshop 2020, 17-19.02.2020 Erlangen, Germany, *Oral presentation.*

2. **Bojarski K.K.,** Samsonov S.A. (Pro)cathepsins and glycosaminoglycans – the significance of their complexes in biological systems, 5th Korean-Polish Conference on „Protein Folding: Theoretical and Experimental Approaches", 16-18.09.2019, Seoul, South Korea, *Oral presentation.*

3. **Bojarski K.K.,** Samsonov S.A. Cathepsins, glycosaminoglycans and biological role of their interactions, 19th International Scientific Conference „Sakharov Readings 2019: Environmental Problems of the XXI Century", 23-24.05.2019, Minsk, Belarus, *Oral presentation.*

4. **Bojarski K. K.** Computational insights into procathepsin maturation mediated by glycosaminoglycans, 33th Molecular Modeling Workshop 2019, 8-10.04.2018, Erlangen, Germany, *Oral presentation.*

5. **Bojarski K. K.** Microsecond scale MD study of a protein-heparin complex, Modeling and Design of Molecular Materials, 24-28.06.2018, Polanica Zdrój, Poland, *Oral presentation.*

6. Samsonov S. A., **Bojarski K. K.,** Uciechowska-Kaczmarzyk U. Computational insights into the glycosaminoglycan-mediated molecular mechanisms underlying cell signaling, 4th Polish-Korean Conference on Protein Folding: Theoretical and Experimental Approaches, 9-13.09.2018, Iława, Poland, *Oral presentation.*

7. **Bojarski K. K.,** Samsonov S. A. Impact of glycosaminoglycan chain polarity on the interaction with proteins, I Pomeranian Student Chemistry Symposium, 26-27.09.2020, On-line, *Poster presentation.*

8. **Bojarski K. K.,** Sieradzan A. K., Samsonov S. A. Microsecond scale MD study of a protein-heparin complex, Modeling and Design of Molecular Materials, 24-28.06.2018, Polanica Zdrój, Poland, *Poster presentation.*

9. **Bojarski K. K.,** Samsonov S. A. Computational Study on phosphorylated glycosaminoglycans, 4th Polish-Korean Conference on Protein Folding: Theoretical and Experimental Approaches, 9-13.09.2018, Iława, Poland, *Poster presentation.*

10. **Bojarski K. K.,** Sieradzan A. K., Samsonov S. A. Computational Analysis of FGF-Heparin system, Protein Formulation and Characterization; Characterization of Molecular Structure of Synthetic and Natural Polymers by Separation Techniques with Advanced Detectors, 23.05.2018, Warsaw, Poland, *Poster presentation.*

11. **Bojarski K. K.,** Karczyńska A., Czaplewski C., Liwo A. Effect of Dynamic Fragment Assembly pseudopotentials on the quality of protein models obtained with homology-restrained UNRES
simulations, CGW2017, 7.10.2017, Warsaw, Poland, *Poster presentation.*

12. **Bojarski K. K.** Modelowanie oddziaływań katepsyn z glikozaminoglikanami, VI Ogólnokrajowa Konferencja Naukowa Młodzi Naukowcy w Polsce – Badania i Rozwój, 27.11.2017, Gdańsk, Poland, *Oral presentation.*

Participation in scientific schools/workshops

26-27.09.2020	I Pomeranian Student Chemistry Symposium, On-line
17-19.02.2020	34th Molecular Modeling Workshop, Erlangen, Germany
16-18.09.2019	5th Korean-Polish Conference on „Protein Folding: Theoretical and Experimental Approaches", Seoul, South Korea
23-24.05.2019	19th International Scientific Conference „Sakharov Readings 2019: Environmental Problems of the XXI Century", Minsk, Belarus
8-10.04.2019	33th Molecular Modeling Workshop, Erlangen, Germany.
11-14.03.2019	School in molecular computational biochemistry, PAS, Kraków, Poland
9-13.09.2018	4th Polish-Korean Conference on Protein Folding: Theoretical and Experimental Approaches, 9-13.09.2018, Iława, Poland
24-28.06.2018	Modeling and Design of Molecular Materials, Polanica Zdrój, Poland.
23.05.2018	Protein Formulation and Characterization; Characterization of Molecular Structure of Synthetic and Natural Polymers by Separation Techniques with Advanced Detectors, Warsaw, Poland.
12-14.03.2018	32nd Molecular Modeling Workshop, Erlangen, Germany.
27.11.2017	VI Ogólnokrajowa Konferencja Naukowa Młodzi Naukowcy w Polsce - badania i rozwój, Gdańsk, Poland.
8.11.2017	SCIGRESS Workshop, Gdańsk, Poland.

7.10.2017	Coarse-graining Workshop, Warsaw, Poland.
5-9.02.2017	3rd Korean-Polish Conference on Protein Folding: Theoretical and Experimental Approaches, High-1 Resort, South Korea

Participation in short forms of training

12.2018	Study visit in laboratory of dr Fabiena Lecaille (Centre d'Etude des Pathologies Respiratoires, Inserm UMR 1100, University of Tours, Tours, France); during this visit an oral presentation was given which covered my current PhD's work.
9.2012	Study visit in laboratory of prof. Andersa Grubba (Institute of Laboratory Medicine, Department of Clinical Chemistry, University Hospital, Lund, Sweeden).

Teaching experience:

2019-2020	Teaching course of TI, two groups
2017-2020	Assistance at seminars in the course „Theoretical Chemistry”

Languages:

polish – native
english – fluent
german – basis
latin – advanced

Hobbies:

travelling, computer games, skiing