Samaneh Davoudi

Molecular Modeler

PERSONAL DATA

27th April 1987

Belgium (Ghent)

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Samaneh Davoudi

Samaneh-davoudi

SamanehDavoudi

https://samanehdavoudi.github.io/

SKILLS

Molecular Dynamics (MD)

Coarse-grained (CGMD)

Biased MD (Umbrella Sampling)

CG forcefield parametrization

High Performance Computing

Programming languages: C++, Python

Typesetting: Microsoft Word

Transferable: Presentation, Teamwork, Leadership, Problem-solving

Persian (Mother tongue)

English (Fluent)

Dutch (A2)

B

HONORS AND AWARDS

'Britton Chance Award' in ISOTT 2022 conference (click here)

Outstanding Bachelor's student, awarded "state-funded" studies for Master's without entrance exam

INTERESTS

Fitness with an experience as:

"Fitness coach", Tehran, Iran (2019)

REFERENCES

Professor An Ghysels
an.ghysels@ugent.be

Professor Siewert Jan Marrink
s.j.Marrink@rug.nl

Professor Sally Pias
sally.pias@nmt.edu

PERSONAL STATEMENT

Highly motivated and accomplished Researcher with expertise in molecular dynamics simulation. Seeking challenging research opportunities to contribute to advancements in biomedical science and technology. Open to exploring new realities and available for travel in Belgium and abroad.

INDUSTRIAL EXPERIENCE

Sales Expert, Saman Faraz Gheshm Co. (Petrochemical materials's export and import)
Tehran, Iran, 2013 – 2018

- developed a pro-active and dynamic approach spanning from both in technical and selling-related activities.

R&D expert, Science and Technology Park of of Tehran, Arian Setak Andish
Tehran, Iran, 2012 – 2013

- Collaborated with cross-functional teams, including engineers and scientists, to drive the development of novel products and solutions.

ACADEMIC EXPERIENCE

Researcher, IBiTech – Biommeda research group, Ghent University
Ghent, Belgium, Dec. 2019 – to date

- Simulated liposomes with varying sizes and compositions.
- Conducted biased molecular dynamics to calculate the pKa of fatty acids, contributing to a deeper understanding of their protonation states.
- Utilized Python programming to calculate permeability through curved membranes.
- Analyzed free energy and histogram profiles of permeants through curved membranes, providing insights into membrane permeation mechanisms.
- Investigated calcein permeation through liposomes using biased molecular dynamics, shedding light on drug delivery and encapsulation.
- Explored the role of caveolae in oxygen buffering, advancing knowledge of cellular oxygen homeostasis.
    - Parametrized a coarse-grained forcefield for oxygen molecules, facilitating efficient simulations of oxygen-protein interactions.
    - Calculated the partition coefficient of oxygen using Python, contributing to the understanding of oxygen solubility in biological environments.
- Presented research findings at various national and international conferences
- Published research work as the first author in several scientific articles (click here)
- Contributed in teaching "Modeling in medicine and biomedical engineering: case studies" course

Research visitor, Molecular Dynamics group, Groningen University
Groningen, The Netherlands, June 2023

- Coarse-grained oxygen forcefield parametrization under supervision of Prof. Siewert J. Marrink

Research Assistant, Molecular Simulation lab., AmirKabir University of Technology
Tehran, Iran, 2018-2019

- Assisted in molecular dynamics research projects.

EDUCATION

PhD student in Biomedical Engineering, Ghent University
Ghent, Belgium, Dec. 2019 – to date
Project title : Calculating the permeability of small drugs through PH-sensitive liposomes

Master's degree in Chemical Engineering (Nanotechnology), AmirKabir University of Technology, *Final grade: 16.55/20*
Tehran, Iran, Sep. 2009 – Jan. 2012
Project title : Molecular dynamics simulation of a membrane protein interacting with a lipid bilayer

- Evaluated interactions between PMCA membrane protein and DPPC bilayer using GROMACS, Utilizing both coarse-grained and all-atom molecular dynamics simulations.

Bachelor's degree in Chemical Engineering, AmirKabir University of Technology, *Final grade:* 17.25/20
Tehran, Iran, Sep. 2005 – May 2009