Curriculum Vitae

Name: Mehdi Sahihi
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h-index: 17 **i10-index:** 25 **Citations:** 700

Educations:

28.09.2007-28.09.2011	PhD of Physical chemistry, Isfahan University of Technology, Iran. **Thesis Title:** Thermodynamics stability and binding properties of β-lactoglobulin.
22.09.2004-19.02.2007	MSc of Physical chemistry, Isfahan University of Technology, Iran. **Thesis Title:** Solubility of fumaric acid in supercritical carbon dioxide and evaluation of available theoretical models.
23.09.1999-14.03.2004	BSc of chemistry, University of Isfahan, Iran.

Professional Experiences:

01.10.2021-Present	Marie Sklodowska-Curie Actions Individual Fellow, ICMAB-CSIC, Spain
01.11.2020-30.09.2020	Postdoctoral researcher, Université de technologie de Compiègne, France
01.06.2019-30.09.2020	Postdoctoral researcher, Université Gustave Eiffel, France
01.02.2019-31.05.2019	Postdoctoral researcher, Polish Academy of Sciences, Poland
01.06.2018-31.08.2018	Visiting researcher, Sabanci University, Turkey
09.04.2013-31.12.2018	Assistant Professor, University of Isfahan, Iran
01.05.2012-01.04.2013	Postdoctoral researcher, Isfahan University of Technology, Iran

CV Summary:

My primary research interest lies in studying structure and function of proteins and materials. I approach this research goal from an interdisciplinary perspective, using computational chemistry and experimental methods to answer physical chemistry questions. I have worked on molecular dynamics (MD) simulation of biomacromolecules, MD simulation and DFT calculations of materials, molecular docking, structure based drug design, homology modelling, QM/MM and TD-DFT calculations, HPC and GPU calculations, Moreover, I have a strong background in experimental biophysics to investigate the structure-function relationship of proteins. In the next phase of my career, I plan to focus on the major enterprise of using my computational skills to study the complex systems. My research has a clear impact; 45 ISI papers with 692 citations, h-index of 16, and i10-index of 25 (according to Google Scholar). My intense international activity includes over three years of working experience in four universities and research institutes in Poland, France and Spain. The international community, in turn, recognizes me as an established researcher in the field, trusting me for instance to act as reviewer for top journals. Throughout my career, I have shown independence in my research as well as strong leadership, team work, and coordinating skills, for instance by acting as the mentor of about 15 MSc and PhD theses.

Moreover, I have been PI of 2 national project grants and organizer of two national workshops. Since my PhD till now, I established an international collaboration with groups from the USA (William A Goddard III and Andres Jaramillo-Botero from California Institute of Technology; Xiaozhen Han and Bidisha Sengupta from Stephen F. Austin State University), Canada (Sabine Kuss, University of Manitoba), France (Michelle Salmain, Sorbonne University) and invitations to foreign research centers (for example, visiting researcher at Sabanci University in Turkey). Also, I have been selected for two international research mobility fellowships in Thailand and Finland. Finally, I have proven my ability to obtain competitive funding, including Marie Sklodowska-Curie Actions Individual Fellowship.

Technical Skills:

Computational

- Molecular Dynamics (MD) Simulation
- Advanced Sampling methods
- High Performance Computing (HPC)
- QM/MM Calculations
- Programming
- Molecular Docking
- DFT and TD-DFT Calculations
- GPU Computing
- Homology Modeling
- Structure Based Drug Design (SBDD)

Experimental

- UV-Vis spectroscopy
- CD Spectroscopy
- Dialysis
- Viscometry
- RT-PCR
- FT-IR Spectroscopy
- Fluorescence Spectroscopy
- Organic Solvent Precipitation
- Electrophoresis
- Enzyme Kinetics

Scientific Societies membership:

2010-Present Member, Iranian Biophysical Chemistry Society

2010-Present Member, Iranian Chemical Society

2009-Present Member, Iranian Chemical and Chemical Engineering Society

2009-Present Member, Iranian Biochemical Society

Reviewer in the international journals:

Journal of Biomolecular Structure and Dynamics, Ultrasonics: Sonochemistry, Journal of Analytical Chemistry, Journal of Luminescence, International Journal of Biological Macromolecules, The Protein Journal, Proteins: Structure, Function and Bioinformatics, Journal of Iranian Chemical society, Iranian Journal of Catalysis, Inorganica Chimica Acta, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Journal of Agriculture and Food Chemistry, Molecular Simulation, Journal of Molecular Structure, Computational Biology and Chemistry, Journal of Food Hydrocolloids, Computers in Biology and Medicine, Arabian Journal of Chemistry, ant *etc*.

Funding, prizes and awards:

2021 Marie-Sklodowska-Curie Actions individual fellowship, ICMAB, Spain (173000 Euro)
Project title: *Interaction of envelope Viruses with materials*.

2019 The research mobility program fellowship of ÅAU, Abo Academy University, Finland (7000 Euro).

2017 Interaction of curcumin and quercetin with beta-lactoglobulin: the effect of protein genetic variants and investigation of competitive ligand binding. Iran National Science Foundation, Iran. (PI; 150,000,000 IRR)

2015 Interaction of Saffron bio-active ligands and beta-lactoglobulin, Research Council of University of Isfahan, Isfahan, Iran. (PI; 40,000,000 IRR)

2012 FAOBMB YSP-Travel Fellowship to participate in the Young Scientist Program, Bangkok, Thailand (2000 USD).

Publications in peer-reviewed scientific journals:

1- H. Alipour, M. Asgari Bajgirani, M. Sahihi*, "Investigation of mechanical, thermal, electrical, and hydrogen diffusion properties in ternary V-Ti-X alloys: a density functional theory study", *The Journal of Physical Chemistry C*, 2022, 126 (3), 1672-1687. (Q1, IF=4.126)

2- J. Sanz Garcia, M. Gaschard, I. Navizet, M. Sahihi, … "Inhibition of cathepsin B by ferrocenyl indenes highlights a new pharmacological facet of ferrocifens", *European Journal of Inorganic Chemistry*, In Press. (Q2, IF=2.524)

3- M. Sahihi, A. Jaramillo-Botero, W.A. Goddard III, F. Bedoui*," Interfacial interactions investigation in a model composite material: insights into α→β Phase Transition of the Magnetite Reinforced Poly(Vinylidene Fluoride) systems by All-Atom Molecular Dynamics Simulation", *The Journal of Physical Chemistry C*, 2021, 125, 39, 21635–21644. (Q1, IF=4.126)

4- M. Sahihi*, F Gaci, I Navizet, "Identification of new alpha-synuclein fibrillogenesis inhibitor using in silico structure-based virtual screening", *Journal of Molecular Graphics and Modelling*, 2021, 108, 108010. (Q2, IF=2.518)

5- X. Han*, M. Sahihi, S. Whitfield, I. Jimenez, "Tuning Excited State of Bipyridyl Platinum (II) Complexes with Bio-active Flavonolate Ligand: Structures, Photoreactivity, and DFT Calculations", *Inorganica Chimica Acta*, 2020, 513, 119952. (Q2, IF=2.545)

6- M. Sahihi*, J. S. Garcia, I. Navizet*, "Bioluminescent NLuc-Furimamide complex: A theoretical study on different protonation states", *Journal of Physical Chemistry B*, 2020, 124, 13, 2539-2548. (Q1, IF=2.991, cited by 2)

7- S. G. Mansouri, H. Zali-Boeini*, K. Zomorodian, B. Khalvati, R. Helali Pargali, A. Dehshahri, H. Amiri Rudbari, M. Sahihi, Z. Chavoshpour "Synthesis of novel naphtho [1, 2-e][1, 3] oxazines bearing an arylsulfonamide moiety and their anticancer and antifungal activity evaluations". *Arabian Journal of Chemistry*, 2020, 13 (1), 1271-1282. (Q1, IF=5.165, cited by 5)

8- Z. Chavoshpour-Natanzi, M. Sahihi* "Encapsulation of quercetin-loaded β-lactoglobulin for drug delivery using modified anti-solvent method" *Food Hydrocolloids*, 2019, 96, 493-502. (Q1, IF=9.147, cited by 21)

9- M. Anjomshoa, M. Torkzadeh-Mahani, M. Sahihi, … "Tris-chelated complexes of nickel(II) with bipyridine derivatives: DNA binding and cleavage, BSA binding, molecular docking, and cytotoxicity" *Journal of Biomolecular Structure and Dynamics*, 2019, 37 (15), 3887-3904. (Q3, IF=3.392, cited by 11)

10- Z. Kazemi, H. Amiri Rudbari*, M. Sahihi*, … "New homochiral and heterochiral Mo(VI) complex from racemic ligand: Synthesis, X-ray structure, diastereomers separation and biological activities" *Polyhedron*, 2019, 170, 70-85. (Q2, IF=3.052, cited by 5)

11- H. Molaee, M. Sahihi*, … "A combined computational/experimental study on HSA binding of two water soluble Schiff base ligands derived from pyridine derivative and ethylendiamine" *Journal of Biomolecular Structure and Dynamics*, 2019, 37(3), 641-648. (Q3, IF=3.392, cited by 3)

12- M. Dehkhodaei, M. Sahihi*, H. Amiri Rudbari "Spectroscopic and molecular docking studies on the interaction of Pd(II) & Co(II) Schiff base complexes with β-lactoglobulin as a carrier protein". *Journal of Biomolecular Structure and Dynamics*, 2018, 36(12), 3130-3136. (Q3, IF=3.392, cited by 8)

13- Z. Adibipour, N. Fani, A.K. Bordbar*, M. Sahihi "Exploring the Interaction Mechanism of Coumarin with Bovine β-Casein: Spectrofluorometric and Molecular Modeling Studies". *Physical Chemistry Research*, 2018, 6, 627-638. (cited by 1)

14- M. Dehkhodaei, M. Sahihi*, … "Multi experimental and computational studies for DNA and HSA interaction of new nano-scale ultrasound-assisted synthesized Pd (II) complex as a potent anticancer drug". *Journal of Molecular Liquids*, 2018, 253, 61-71.264, 386-397. (Q1, IF=6.165, cited by 7)

15- M. Ariyaeifar, H. Amiri Rudbari*, M. Sahihi*, … "Chiral halogenated Schiff base compounds: green synthesis, anticancer activity and DNA-binding study" *Journal of Molecular Structure*, 2018, 1161,497- 511. (Q2, IF=3.196, cited by 14)

16- A. Jamshidvand, M. Sahihi*, … "Studies on DNA binding properties of new Schiff base ligands using spectroscopic, electrochemical and computational methods: Influence of substitutions on DNA-binding". *Journal of Molecular Liquids*, 2018, 253, 61-71. (Q1, IF=6.165, cited by 32)

17- M. Dehkhodaei, M. Sahihi*, H. Amiri Rudbari*, F Momenbeik "DNA and HSA interaction of Vanadium (IV), Copper (II), and Zinc (II) complexes derived from an asymmetric bidentate Schiff-base ligand: multi spectroscopic, viscosity measurements, molecular docking, and ONIOM studies". *Journal of Biological Inorganic Chemistry*, 2018, 23 (2), 181-192. (Q1, IF=3.358, cited by 26)

18- Z. Chavoshpour-Natanzi, M. Sahihi*, S. Gharaghani "Structural stability of β-lactoglobulin in the presence of cetylpyridinum bromide: spectroscopic and molecular docking studies". *Journal of Biomolecular Structure and Dynamics*, 2018, 36(3), 753-760. (Q3, IF=3.392, cited by 4)

19- H. Abolhassani, A. K. Bordbar*, N. Fani, Z. Adibipour, M. Sahihi, … "Spectroscopic and molecular modeling probing of biophysical influence of β-casein nano-protein on adrenaline and arachidonoyl adrenaline". *Monatshefte für Chemie-Chemical Monthly*, 2018, 149 (1), 185-196. (Q3, IF=1.451, cited by 1)

20- M. Dehkhodaei, M. Sahihi*, … "Studies of DNA- and HSA-binding properties of new nano-scale green synthesized Ni (II) complex as anticancer agent using spectroscopic methods, viscosity measurement, molecular docking, MD simulation and QM/MM". *Journal of Molecular Liquids*, 2017, 248, 24–35. (Q1, IF=6.165, cited by 18)

21- M. Sahihi*, G. Borhan "The effects of single-walled carbon nanotubes (SWCNTs) on the structure and function of human serum albumin (HSA): Molecular docking and molecular dynamics simulation studies". *Structural Chemistry*, 2017, 28, 1815-1822. (Q3, IF=1.887, cited by 7)

22- I. Khosravi*, M. Sahihi, H. Amiri Rudbari, G. Borhan, Z. Chavoshpour-Natanzi "The interaction of a new Schiff base ligand with human serum albumin: molecular docking and molecular dynamics simulation studies". *Journal of Macromolecular Science Part B: Physics*, 2017, 56(9), 636-643. (Q3, IF=1.504, cited by 3)

23- I. Khosravi*, M. Sahihi*, M. Dashtbani, H. Amiri Rudbari, G. Borhan "Deoxyribonucleic acid and bovine serum albumin interaction with the asymmetric Schiff base ligand and its molybdenum (VI) complex: multi spectroscopic and molecular docking studies". *Journal of Macromolecular Science Part B: Physics*, 2017, 56(9), 655-669. (Q3, IF=1.504, cited by 2)

24- M. Dehkhodaei, M. Khorshidifard, H. Amiri Rudbari*, M. Sahihi*, … "Synthesis, characterization, crystal structure and DNA, HSA-binding studies of four Schiff base complexes derived from salicylaldehyde and isopropylamine". *Inorganica Chimica Acta*, 2017, 466, 48-60. (Q2, IF=2.545, cited by 23)

25- Z. Kazemi, H. Amiri Rudbari*, V. Mirkhani*, M. Sahihi, … "Self-recognition of the racemic ligand in the formation of homochiral dinuclear V(V) complex: In vitro anticancer activity, DNA and HSA interaction". *European Journal of Medicinal Chemistry*, 2017, 135, 230–240. (Q1, IF=6.514, cited by 23)

26- B. Sengupta*, M. Sahihi, M. Dehkhodaei, D. Kelly, I. Arany "Differential roles of 3-Hydroxyflavone and 7- Hydroxyflavone against nicotine-induced oxidative stress in rat renal proximal tubule cells". *PloS One*, 2017, 12(6), e0179777. (Q1, IF=3.240, cited by 14)

27- M. Anjomshoa*, M. Torkzadeh-Mahani, J. Janczak, C. Rizzoli, M. Sahihi, F. Ataei, M. Dehkhodaei "Synthesis, crystal structure and Hirshfeld surface analysis of copper(II) complexes: DNA- and BSA binding, molecular modeling, cell imaging and cytotoxicity". *Polyhedron*, 2016, 119, 23–38. (Q2, IF=3.052, cited by 20)

28- Z. Kazemi, H. Amiri Rudbari*, M. Sahihi*, … "Synthesis, characterization and separation of chiral and achiral diastereomers of Schiff base Pd(II) complex: A comparative study of their DNA- and HSA binding". *Journal of Photochemistry and Photobiology B: Biology*, 2016, 163, 246–260. (Q1, IF=6.252, cited by 25)

29- M. Khalesi*, R. Jahanbani, D. Riveros-Galan, V. Sheikh-Hassani, M. Sheikh-Zeinoddin, M. Sahihi, … "Antioxidant activity and ACE-inhibitory of Class II hydrophobin fromwild strain Trichoderma reesei". *International Journal of Biological Macromolecules*, 2016, 91, 174-179. (Q1, IF=6.953, cited by 16)

30- I. Khosravi, F. Hosseini, M. Khorshidifard, M. Sahihi*, H. Amiri Rudbari* "Synthesis, characterization, crystal structure and HSA binding of two new N,O,O-donor Schiff-base ligands derived from dihydroxybenzaldehyde and tert-butylamine". *Journal of Molecular Structure*, 2016, 1119, 373-384. (Q2, IF=3.196, cited by 32)

31- Z. Kazemi, H. Amiri Rudbari*, M. Sahihi*, … "Synthesis, characterization and biological application of four novel metal-Schiff base complexes derived from allylamine and their interactions with human serum albumin: Experimental, molecular docking and ONIOM

computational study". *Journal of Photochemistry and Photobiology B: Biology*, 2016, 162, 448-462. (Q1, IF=6.252, cited by 52)

32- M. Sahihi* "In-Silico Study on the Interaction of Saffron Ligands and β-Lactoglobulin by Molecular Dynamics and Molecular Docking Approach". *Journal of Macromolecular Science Part B*, 2016, 55, 73-84. (Q3, IF=1.504, cited by 11)

33- Z. Kazemi, H. Amiri Rudbari*, V. Mirkhani*, M. Sahihi*, … "Synthesis, characterization, crystal structure, DNA- and HSA-binding studies of a dinuclear Schiff base Zn(II) complex derived from 2- hydroxynaphtaldehyde and 2-picolylamine". *Journal of Molecular Structure*, 2015, 1096, 110-120. (Q2, IF=3.196, cited by 46)

34- M. Khorshidifard, H. Amiri Rudbari*, B. Askari, M. Sahihi, … "Cobalt(II), copper(II), zinc(II) and palladium(II) Schiff base complexes: Synthesis, characterization and catalytic performance in selective oxidation of sulfides using hydrogen peroxide under solvent-free conditions". *Polyhedron*, 2015, 95, 1-13. (Q2, IF=3.052, cited by 75)

35- F. Mohammadi, M. Sahihi*, A. K. Bordbar* "Multispectroscopic and molecular modeling studies on the interaction of two curcuminoids with β-lactoglobulin". *Spectrochimica Acta Part A Molecular and Boimolecular Spectroscopy*, 2015, 140, 274-282. (Q2, IF=4.098, cited by 16)

36- M. Sahihi*, Y. Ghayeb "Binding of biguanides to β-lactoglobulin: molecular-docking and molecular dynamics simulation studies". *Chemical Papers*, 2014, 68, 1601-1607. (Q3, IF=2.097, cited by 12)

37- I. Khosravi, M. Sahihi* "Computational Studies on the Interaction of Arctiin and Liquiritin with β-lactoglobulin". *Journal of Macromolecular Science Part B*, 2014, 53, 1591-1600. (Q3, IF=1.504, cited by 5)

38- M. Sahihi*, Y. Ghayeb "An investigation of molecular dynamics simulation and molecular docking: Interaction of citrus flavonoids and bovine β-lactoglobulin in focus". *Computers in Biology and Medicine*, 2014, 51, 44-50. (Q1, IF=4.589, cited by 30)

39- M. Sahihi*, Y. Ghayeb, A. K. Bordbar "Interaction of β-Lactoglobulin with Resveratrol: Molecular Docking and Molecular Dynamics Simulation Studies", *Chemical and Biochemical Engineering Quarterly*, 2013, 27, 413-422. (Q3, IF=1.582, cited by 12)

40- M. Sahihi*, Z. Heidari-Koholi, A. K. Bordbar "The Interaction of Polyphenol Flavonoids with β-lactoglobulin: Molecular Docking and Molecular Dynamics Simulation Studies", *Journal of Macromolecular Science Part B*, 2012, 51, 2311-2323. (Q3, IF=1.504, cited by 41)

41- M. Sahihi, A. K. Bordbar*, Y. Ghayeb, N. Fani "Structure-Function Relationship of β-Lactoglobulin in the Presence of Sodium Dodecylbenzenesulfonate", *The Journal of chemical thermodynamics*. 2012, 52, 16- 23. (Q2, IF=3.178, cited by 9)

42- M. Sahihi, Y. Ghayeb, A. K. Bordbar* "Fluorescence Spectroscopic Study on Interaction of Retinol with β-lactoglobulinin the Presence of Cetylpyridinium Chloride", *Spectroscopy*, 2012, 27, 27-34. (Q3, IF=1.750, cited by 11)

43- M. Sahihi, A. K. Bordbar*, Y. Ghayeb "Thermodynamic stability and retinol binding property of β-lactoglobulin in the presence of cationic surfactants", *The Journal of chemical thermodynamics*. 2011, 43,1185-1191. (Q2, IF=3.178, cited by 10)

44- M. Sahihi, A. K. Bordbar*, Y. Ghayeb "Thermodynamic denaturation of β-lactoglobulin in the presence of cetylpyridinium chloride", *The Journal of chemical thermodynamics*. 2010, 42, 1423-1428. (Q2, IF=3.178, cited by 8)

45- M. Sahihi, H. S. Ghaziaskar*, M. Hajebrahimi "Solubility of maleic acid in supercritical carbon dioxide", *Journal of chemical engineering Data*. 2010, 55, 2596-2599. (Q1, IF=2.694, cited by 19)

Congresses (10 selected):

2022 The first international conference and the tenth national bioinformatics conference of Iran, Kish Island, Iran. *(Scientific committee member)*

2019 PHOTOBIOLOGIE SOUS LE SOLEIL, Sorbonne Université, France. *(M. Sahihi, I. Navizet, Oral presentation)*

2019 Biomolecules and Nanostructures 7, Polish Academy of Sciences, Poland. *(M. Sahihi, Poster presentation)*

2019 235th ECS meeting, Dallas, USA. *(S. Kuss, R.M. Islam, M. Sahihi, F. Schweizer, Oral presentation)*

2016 2nd international and 14th Iranian genetics congress, Sh. Beheshti University, Iran.

2016 2nd conference on protein and peptide sciences, University of Isfahan, Iran. *(Scientific committee member)*

2014 5th International Congress on nanoscience/nanotechnology, T. Modares University, Iran. *(M. Sahihi, G. Borhan, Poster presentation)*

2014 17th Iranian physical chemistry congress, K.N. Toosi University of Technology, Iran. *(M. Sahihi, G. Borhan, Poster presentation)*

2014 17th Iranian chemistry congress, V.A. University of Rafsanjan, Iran. *(M. Sahihi, Oral presentation)*

2013 16th Iranian physical chemistry congress, Babolsar University, Iran. *(M. Sahihi, Y. Ghayeb, Poster presentation)*

2011 15th Iranian Chemistry Congress, Bu-Ali Sina University, Iran. *(M. Sahihi, Poster presentation)*

2006 9th Iranian physical chemistry congress, Guilan University, Iran. *(M. Sahihi, Oral presentation)*

Supervising and mentoring activities:

1- F. Gaci (2020); **Internship Thesis:** Identification of new alpha-synuclein fibrillogenesis inhibitor using in silico structure-based virtual screening.

2- Z. Chavoshpour-Natanzi (2018); ***MSc Thesis:*** Encapsulation of quercetin as an antioxidant in β-lactoglobulin nanoparticles.

3- M. Dashtbani (2018); ***MSc Thesis:*** Interaction of carbon nanotube and DNA: a molecular dynamics simulation study.

4- H. Molaee (2018); ***PhD Thesis:*** Synthesis and characterization of novel chiral and achiral Schiff base ligands and their metal complexes and investigation of their biological activities.

5- Z. Fateminia (2017); ***MSc Thesis:*** Synthesis and characterization of some new ligands and complexes containing halogen and their interaction studies with HSA and DNA.

6- E. Sattarinejad (2016); ***PhD Thesis:*** Computational design of some piperine derivatives as novel survivin inhibitors.

7- M. Ariyaeifar (2016); ***MSc Thesis:*** Synthesis, characterization and x-ray crystal structure of some new metal-salen complexes and their interaction studies with HSA and DNA.

8- H. Abolhassani (2016); ***MSc Thesis:*** Binding assessment of adrenalin and arachidonic based synthetic derivative of adrenalin with nanoparticles of beta-casein: a chemometry and molecular modelling approach.

9- Z. Adibipour (2016); ***MSc Thesis:*** Binding and loading of beta-casein nanoparticles as drug carrier with coumarin.

10- F. Namazifar (2016); ***MSc Thesis:*** Comparison between the action of RNA-aptamer analogs of PSMA using molecular docking and MD simulation methods.

11- M. Atrian Afiyani (2016); ***MSc Thesis:*** Interaction of serotonin and arachidonoyl serotonin with casein nanoparticles: a chemometrics and molecular modeling approach.

12- F. Hosseini (2016); ***MSc Thesis:*** Interaction of curcumin and quercetin with beta-lactoglobulin: the effect of protein genetic variants and investigation of competitive ligand binding.

13- G. Borhan (2013); ***MSc Thesis:*** The effects of single-walled carbon nanotubes (SWCNTs) the structure and function of human serum albumin (HSA): Molecular docking and molecular dynamics simulation studies.

14- S. Soroush (2013); ***MSc Thesis:*** Interaction of narcotic drugs and human serum albumin (HSA): Molecular docking and molecular dynamics simulation studies.

15- F. Jodairy (2013); ***MSc Thesis:*** Interaction of Aflatoxin M1 with milk proteins using molecular docking and molecular dynamics simulation methods.

Teaching experiences:

- *Principles of MD simulation* (two national workshops of computational chemistry for bio-molecules)
- *General Chemistry* (for bachelor students of chemistry, physics, biology and geology)
    - ✓ 7 semesters
    - ✓ **Some of the topics:** measurement and units, matter and energy, stoichiometry and chemical equations, thermochemistry, electronic structure of atoms, periodic trends,

molecular bonding and structure, gases, intermolecular forces, solution chemistry, equilibrium, oxidation-reduction reactions, and nuclear chemistry.

- *Biophysical chemistry methods* (for bachelor students of chemistry)
  - ✓ 4 semesters
  - ✓ **Some of the topics**: Intro: Structure Determination Methods & Light, Spectroscopy: Absorption and Fluorescence, NMR Spectroscopy: Spectra, Assignments & NOEs, Circular dichroism and proteins, singular value decomposition, IR Spectroscopy, Isothermal Titration Calorimetry, Differential Scanning Calorimetry, Chromatography and electrophoresis, Viscometry.
- *Biochemistry* (for bachelor students of chemistry)
  - ✓ 3 semesters
  - ✓ **Some of the topics**: The foundation of biochemistry, Water, Amino Acids, Peptides, and Proteins, The Three-Dimensional Structure of Proteins, Protein Function, Enzymes.
- *Advanced Thermodynamics* (for master students of physical chemistry)
  - ✓ 4 semesters
  - ✓ **Some of the topics**: Thermodynamic potentials, Maxwell relations, measurement of properties, Stability conditions, Phase equilibria, chemical potential, ideal mixtures, entropy and disorder, Osmosis and reverse osmosis, reversible and irreversible mixing, Gibbs phase rule, Raoult`s law, phase diagram, distillation, Activity and fugacity, Enthalpy and entropy constants, third law.
- *Principles of Biophysical Chemistry* (for master students of biophysical chemistry)
  - ✓ 3 semesters
  - ✓ **Some of the topics:** The structure of biological macromolecules, Statistical thermodynamics especially applied on biological systems, macromolecules in solution, conformational equilibria, membrane equilibria, ligand binding and cooperativity, Reaction kinetics with a specialization in precision in biosynthetic processes, Membrane structures, Methods to study equilibrium and speed for association-dissociation process, Membrane proteins and membrane transport, Processive enzymes, ligand binding with steric impediments in one and two dimensions, Physical

methods for studies of the interaction of biological macromolecules, Transport processes with relevance in biological systems and experimental biochemistry.

- *Computational Chemistry* (for master students of biophysical chemistry)
  - ✓ 3 semesters
  - ✓ **Some of the topics:** The Schrödinger equation, Born-Oppenheimer approximation, Hartree-Fock, spatial- and spin orbitals, electron correlation and an overview of electron correlation methods (MP2, CI and CC), atom-centred basis sets and plane waves, superposition error, density functional theory (DFT), M0lecular Dynamics simulation, Molecular docking.
- *Enzyme kinetics* (for PhD students of biophysical chemistry)
  - ✓ 3 semesters
  - ✓ **Some of the topics:** Enzymes and non-bonding interactions, Catalysis, Enzyme catalysis and energy diagrams, Experimental kinetics, Enzyme kinetics, Enzyme inhibition, Enzyme kinetics case studies.

Profiles:

- ORCID https://orcid.org/0000-0003-2923-1833
- Web of Science https://publons.com/researcher/AAY-1571-2020/
- Scopus http://www.scopus.com/authid/detail.url?authorId=36167134800
- Google Scholar https://scholar.google.com/citations?user=7pEcoNAAAAAJ&hl=en&oi=ao
- ResearchGate https://www.researchgate.net/profile/Mehdi_Sahihi
- LinkedIn https://www.linkedin.com/in/mehdi-sahihi/