**Ilke UGUR MARION**

**Address:** Meddenovo İlaç Araştırma ve Danışmanlık A.Ş.

 ODTÜ Teknokent, Ankara, TURKEY

**Phone:** +90 537 513 29 40

**Email address:** ilkeugur@meddenovo.com, ilkeugur@metu.edu.tr

**Field of expertise:** Drug design and computational innovation in pharmaceutical research.

Modelling reaction mechanisms and intermolecular interactions in organic, inorganic, bio-molecular, macro-molecular systems and their hybrids.

Drug design, molecular dynamics, quantum chemistry, free energy calculations, enzymatic catalysis for energy conversion.

**Work Experience**

**Co-founder & Managing Partner 2021- Current**

Meddenovo Drug Design and Consultancy Ltd.

**Postdoctoral Researcher**, Ankara, *Turkey* **2018 - Current**

*Development of computational protocols for therapeutics*

**Freelance Computational Chemist**, Ashwin-Ushas Corporation, *USA* **2017 - 2021**

*Modelling of dioxygen activation in nature*

**Postdoctoral Researcher**, TUM, *Germany* **2014 - 2017**

*Water splitting in nature, drug design*

**Visiting Researcher**, UCLA, *USA* **2012 August**

*Cycloaddition of metal-carbonyl complexes*

**Visiting Researcher**, Free University of Brussels, *Belgium* **2009 July**

*Cyclopolymerization reactions*

**Research Assistant**, Bogazici University, *Turkey* **2007 – 2011**

**Education**

Obtained joint PhD from:

Université de Lorraine, Theoretical Chemistry and Biochemistry, **France** **2009 - 2014**

Bogazici University, Chemistry Department, **Turkey**

***Thesis:*** *Implicit Investigation of the Deamidation Reaction in the Enzyme Triosephosphate Isomerase*

MSc, Bogazici University, Chemistry Department **2007 - 2009**

B.A., Bogazici University, Chemistry Department **2002 – 2007**

**Scientific Honors and Grants**

*TUBITAK* 1001 – Intellectual property owner **2022 – 2024**

A novel synthesis of the trientine molecule and the development of its derivatives

*TUBITAK* 1512 Entrepreneurship Support Program **2021**

*TUBITAK* 2218 **2020 - 2022**

Exploring the early stage fusion mechanism of the SARS-CoV-2 Spike protein and modelling of its inhibition

*TUBITAK* 2332 **2018 – 2020**

Development of a computational method to detect drug resistant mutations formed at the inhibitory binding sites of proteins

Joint PhD Grant by *TUBITAK*  **2012 – 2014**

Joint PhD Grant by *French Embassy*  **2011 – 2013**

**Institutional Duties**

Scientific consultant and board member **2018 – 2019**

*Sehir High School, Eskisehir, Turkey*

Principal Investigator of the Immunotherapy Project, **2016 – 2017**

*International Graduate School of Science and Engineering (IGSSE), TUM, Germany*

**Collaborators**

Roche GmbH, UCLA, Imperial College of London, French National Center for Scientific Research (CNRS), Michigan State University (MSU), Ludwig-Maximilians University (LMU)

**Computational Skills**

A great variety of computational chemistry and molecular modeling tools (MD, QM, QM/MM, MMGBSA) and related software (Gaussian, AMBER, AutoDock …)

Programming skills: bash, python

Graphical design

**Teaching and Supervision of Research**

Worked as a teaching assistant for the courses:  **2007 - 2015**

General, organic, inorganic, biochemistry, physical and computational chemistry at Bogazici University (Turkey) and TUM (Germany).

Supervised 4 theses at TUM **2015 – 2016**

Efficient calculation of protein-peptide binding affinities (master thesis)

Docking of small peptides into the sortase A binding pocket (master internship)

Conformational analysis of Miuraenamid A and D derivatives (bachelor thesis)

Ring closure of geranylgeranylpyrophosphate in cembrenol synthase (bachelor thesis)

**Publications**

19 scientific publications with 609 citations.

**Conference and Seminar Presentations**

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| 13. | High-Performance Computing Technologies in Drug Design Workshop (**2021**), Invited Speaker*High efficiency with high performance computing in drug design* |
| 12. | EuroCC Turkey Seminars (**2021**), Invited Speaker*Applying Efficient, High-Performance Computing in Drug Discovery* |
| 11. | 8. International Drug Chemistry Conference (**2020**) *Problem Specific Computational Chemistry Solutions in Drug Design* *(oral presentation)* |
| 10. | Bau Drug Design Congress, Turkey (**2017**)*Predicting the bioactive conformations of macrocycles (oral presentation)* |
| 9. | Molecular and Chemical Kinetics, Germany (**2015**)*Redox-coupled substrate water reorganization in the active site of Photosystem II (poster)* |
| 8. | 6th International Theoretical Biophysics Symposium, TheoBio, Sweeden (**2013**)*Detailed Analysis on the kinetics of the deamidation reaction in triosephosphate isomerase using microsecond MM molecular dynamics and QM/MM free energy samplings (oral presentation)* |
| 7. | 47th World Chemistry Congress, IUPAC, Turkey (**2013**)*Investigation of the deamidation reaction in triosephosphate isomerase by means of long range MD simulations (oral presentation)* |
| 6. | 10th Chemical Physics Congress, Turkey (**2012**)*Initiation of the reaction of deamidation in triosephosphate isomerase: investigations by means of MD simulations (oral presentation)* |
| 5. | 9th World Association of Theoretical and Computational Chemists, WATOC, Spain (**2011**) *Elucidation of the deamidation in triosophosphate isomerase with MD (poster)* |
| 4. | 9th Chemical Physics Congress, Turkey (**2010**)*Elucidation of the deamidation in triosophosphate isomerase with MD (poster)* |
| 3. | Faraday Discussion 145: Frontiers in Physical Organic Chemistry, UK (**2009**)*Modeling the chain transfer in the free radical polymerization of acrylamide (poster)* |
| 2. | Congress on Electronic Structure: Principles and Applications, ESPA, Spain (**2008**)*Intramolecular cyclization of diallyl monomers: DFT-based reactivity descriptors (poster)* |
| 1. | 8th Chemical Physics Congress, Turkey (**2008**)*Intramolecular cyclization of diallyl monomers: DFT-based reactivity descriptors (poster)*  |

**Language Skills**

Turkish - native, English – fluent, French – advanced, German - beginner

**Extracurricular Activities**

Performing arts, outdoor sports, creative writing.