

Asst. Prof. ANTOINE MARION

Personal Information

Office Phone: [+90 312 210](tel:+90312210) Extension: 5144

Email: amarion@metu.edu.tr

Web: <https://avesis.metu.edu.tr/amarion>

Address: Orta Doğu Teknik Üniversitesi Bilimsel Araştırma Kimya Bölümü Üniversiteler Mahallesi, Dumlupınar Bulvarı No:1
06800 Çankaya Ankara/TÜRKİYE

Education Information

Doctorate, Université Henri Poincaré: Nancy I, Sciences, Chemistry, France 2011 - 2014

Post Graduate, Université de Franche-Comté: Besançon, Chemistry, France 2009 - 2011

Under Graduate, Université de Franche-Comté: Besançon, Chemistry, France 2004 - 2009

Foreign Languages

German, B1 Intermediate

French, C2 Proficiency

Turkish, A1 Beginner

English, C2 Proficiency

Dissertations

Doctorate, Molecular dynamics using a semiempirical quantum force field : development and applications to systems of biological interest, Université Henri Poincaré: Nancy I, Sciences, Chemistry, 2015

Research Areas

Chemistry, Physical Chemistry, Computational Chemistry, Quantum Mechanics

Academic Titles / Tasks

Assistant Professor, Middle East Technical University, Faculty of Arts and Sciences, Department of Chemistry, 2018 -
Continues

Researcher, Technische Universität München, Life Sciences, 2015 - 2017

Courses

advanced topics in physical chemistry, Post Graduate, 2018 - 2019

General Chemistry, Under Graduate, 2018 - 2019

Articles Published in Journals That Entered SCI, SSCI and AHCI Indexes

- I. **Tuning the Biological Activity of RGD Peptides with Halotryptophan**
Kemker I., Schroeder D. C. , Feiner R. C. , Mueller K. M. , MARION A., Sewald N.
JOURNAL OF MEDICINAL CHEMISTRY, vol.64, no.1, pp.586-601, 2021 (Journal Indexed in SCI)
- II. **Cyclization of RGD Peptides by Suzuki-Miyaura Cross-Coupling**
Kemker I., Schnepel C., Schroeder D. C. , MARION A., Sewald N.
JOURNAL OF MEDICINAL CHEMISTRY, vol.62, no.16, pp.7417-7430, 2019 (Journal Indexed in SCI)
- III. **Actin stabilizing compounds show specific biological effects due to their binding mode**
Wang S., Crevenna A. H. , Ugur I., Marion A., Antes I., Kazmaier U., Hoyer M., Lamb D. C. , Gegenfurtner F., Kliesmetes Z., et al.
SCIENTIFIC REPORTS, vol.9, 2019 (Journal Indexed in SCI)
- IV. **Predicting the bioactive conformations of macrocycles: a molecular dynamics-based docking procedure with DynaDock**
Ugur I., Schroft M., Marion A., Glaser M., Antes I.
JOURNAL OF MOLECULAR MODELING, vol.25, no.7, 2019 (Journal Indexed in SCI)
- V. **1,4-Disubstituted 1H-1,2,3-Triazole Containing Peptidotriazolamers: A New Class of Peptidomimetics With Interesting Foldamer Properties**
Schroeder D. C. , Kracker O., Froehr T., Gora J., Jewginski M., Niess A., Antes I., Latajka R., Marion A., Sewald N.
FRONTIERS IN CHEMISTRY, vol.7, 2019 (Journal Indexed in SCI)
- VI. **Simple Tyrosine Derivatives Act as Low Molecular Weight Organogelators**
Aykent G., Zeytun C., Marion A., Ozcubukcu S.
SCIENTIFIC REPORTS, vol.9, 2019 (Journal Indexed in SCI)
- VII. **Semi-Empirical Born-Oppenheimer Molecular Dynamics (SEBOMD) within the Amber Biomolecular Package**
Marion A., Gokcan H., Monard G.
JOURNAL OF CHEMICAL INFORMATION AND MODELING, vol.59, no.1, pp.206-214, 2019 (Journal Indexed in SCI)
- VIII. **Ca²⁺ binding induced sequential allosteric activation of sortase A: An example for ion-triggered conformational selection**
Ugur I., Schatte M., Marion A., Glaser M., Boenitz-Dulat M., Antes I.
PLOS ONE, vol.13, no.10, 2018 (Journal Indexed in SCI)
- IX. **The low spin - high spin equilibrium in the S-2-state of the water oxidizing enzyme**
Boussac A., Ugur I., Marion A., Sugiura M., Kaila V. R. I. , Rutherford A. W.
BIOCHIMICA ET BIOPHYSICA ACTA-BIOENERGETICS, vol.1859, no.5, pp.342-356, 2018 (Journal Indexed in SCI)
- X. **Activity of Topotecan toward the DNA/Topoisomerase I Complex: A Theoretical Rationalization**
Bali S. K. , MARION A., Ugur I., Dikmenli A. K. , ÇATAK Ş., AVİYENTE V.
BIOCHEMISTRY, vol.57, no.9, pp.1542-1551, 2018 (Journal Indexed in SCI)
- XI. **1,5-Disubstituted 1,2,3-Triazole-Containing Peptidotriazolamers: Design Principles for a Class of Versatile Peptidomimetics**
Kracker O., Gora J., Krzciuk-Gula J., Marion A., Neumann B., Stammler H., Niess A., Antes I., Latajka R., Sewald N.
CHEMISTRY-A EUROPEAN JOURNAL, vol.24, no.4, pp.953-961, 2018 (Journal Indexed in SCI)
- XII. **Amber-Compatible Parametrization Procedure for Peptide-like Compounds: Application to 1,4-and 1,5-Substituted Triazole-Based Peptidomimetics**
Marion A., Gora J., Kracker O., Froehr T., Latajka R., Sewald N., Antes I.
JOURNAL OF CHEMICAL INFORMATION AND MODELING, vol.58, no.1, pp.90-110, 2018 (Journal Indexed in SCI)
- XIII. **Glitoxin Biosynthesis: Structure, Mechanism, and Metal Promiscuity of Carboxypeptidase Glij**
Marion A., Groll M., Scharf D. H. , Scherlach K., Glaser M., Sievers H., Schuster M., Hertweck C., Brakhage A. A. , Antes I., et al.
ACS CHEMICAL BIOLOGY, vol.12, no.7, pp.1874-1882, 2017 (Journal Indexed in SCI)
- XIV. **DynaDom: structure-based prediction of T cell receptor inter-domain and T cell receptor-peptide-MHC (class I) association angles**

Hoffmann T., Marion A., Antes I.

BMC STRUCTURAL BIOLOGY, vol.17, 2017 (Journal Indexed in SCI)

- XV. **Why Does Asn71 Deamidate Faster Than Asn15 in the Enzyme Triosephosphate Isomerase? Answers from Microsecond Molecular Dynamics Simulation and QM/MM Free Energy Calculations**

Ugur I., Marion A., Aviyente V., Monard G.

BIOCHEMISTRY, vol.54, no.6, pp.1429-1439, 2015 (Journal Indexed in SCI)

- XVI. **Rationalization of the pK(a) Values of Alcohols and Thiols Using Atomic Charge Descriptors and Its Application to the Prediction of Amino Acid pK(a)'s**

Ugur I., Marion A., Parant S., Jensen J. H. , Monard G.

JOURNAL OF CHEMICAL INFORMATION AND MODELING, vol.54, no.8, pp.2200-2213, 2014 (Journal Indexed in SCI)

- XVII. **Water interactions with hydrophobic groups: Assessment and recalibration of semiempirical molecular orbital methods**

Marion A., Monard G., Ruiz-Lopez M. F. , Ingrosso F.

JOURNAL OF CHEMICAL PHYSICS, vol.141, no.3, 2014 (Journal Indexed in SCI)

Citations

Total Citations (WOS):129

h-index (WOS):6

Awards

Marion A., Best PhD thesis award, Université De Lorraine (Université Henry Poincaré-Nancy I), September 2015