

## Asst. Prof. ANTOINE MARION

### Personal Information

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### Education Information

Doctorate, Université Henri Poincaré: Nancy I, Sciences, Chemistry, France 2011 - 2015

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

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

### Foreign Languages

German, B1 Intermediate

French, C2 Mastery

Turkish, A1 Beginner

English, C2 Mastery

### 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, Postgraduate, 2018 - 2019

General Chemistry, Undergraduate, 2018 - 2019

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

- I. **Peptide stapling by late-stage Suzuki-Miyaura cross-coupling**  
Gruss H., Feiner R. C., Mseya R., Schroeder D. C., Jewginski M., Mueller K. M., Latajka R., MARION A., Sewald N.  
BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY, vol.18, 2022 (Journal Indexed in SCI)
- II. **The Q41R mutation in the HCV-protease enhances the reactivity towards MAVS by suppressing non-reactive pathways**  
Zheng C., Schneider M., MARION A., Antes I.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.24, no.4, pp.2126-2138, 2022 (Journal Indexed in SCI)
- III. **Fullerene-Based Mimics of Biocatalysts Show Remarkable Activity and Modularity.**  
Gülseren G., Saylam A., Marion A., Özçubukçu S.  
ACS applied materials & interfaces, vol.13, no.38, pp.45854-45863, 2021 (Journal Indexed in SCI)
- IV. **Peptidotriazolamers Inhibit A $\beta$ (1-42) Oligomerization and Cross a Blood-Brain-Barrier Model.**  
Tonali N., Hericks L., Schroeder D. C., Kracker O., Krzemieniecki R., Kaffy J., Le Joncour V., Laakkonen P., MARION A., Onger S, et al.  
ChemPlusChem, vol.86, pp.840-851, 2021 (Journal Indexed in SCI Expanded)
- V. **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)
- VI. **Extended interaction networks with HCV protease NS3-4A substrates explain the lack of adaptive capability against protease inhibitors**  
Dultz G., Shimakami T., Schneider M., Murai K., Yamane D., MARION A., Zeitler T. M., Stross C., Grimm C., Richter R. M., et al.  
JOURNAL OF BIOLOGICAL CHEMISTRY, vol.295, no.40, pp.13862-13874, 2020 (Journal Indexed in SCI)
- VII. **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)
- VIII. **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)
- IX. **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)
- X. **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)
- XI. **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)
- XII. **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)
- XIII. **Ca<sup>2+</sup> 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)
- XIV. **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)
- XV. **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)
- XVI. **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)
- XVII. **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)
- XVIII. **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)
- XIX. **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)
- XX. **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)
- XXI. **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)
- XXII. **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)

## Articles Published in Other Journals

- I. **Activity-Based Photosensitizers with Optimized Triplet State Characteristics Toward Cancer Cell Selective and Image Guided Photodynamic Therapy**  
Kilic E., ELMAZOĞLU Z., Almammadov T., KEPİL D., Etienne T., MARION A., GÜNBAŞ E. G., Kolemen S.  
ACS Applied Bio Materials, 2022 (Journal Indexed in ESCI)

## Refereed Congress / Symposium Publications in Proceedings

- I. **L-Tyr(tBu)-OH: An Outstanding Low Molecular Weight Organogelator**  
AYKENT G., ZEYTUN C., Marion A., ÖZÇUBUKÇU S.  
4th Organic Chemistry Congress with Int. Participation, 4 - 07 October 2018

## **Citations**

Total Citations (WOS):208

h-index (WOS):9

## **Awards**

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