

## Asst. Prof. ANTOINE MARION

### Personal Information

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### International Researcher IDs

ScholarID: [fwtWHu8AAAAJ](https://orcid.org/0000-0002-8266-8957)

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Publons / Web Of Science ResearcherID: AAC-4712-2019

ScopusID: 56288351300

Yoksis Researcher ID: 278083

### 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

## Advising Theses

MARION A., Towards a general descriptor for the prediction of PKA, Postgraduate, A.GÖÇER(Student), 2022

MARION A., New protocol for scanning minor and major grooves along DNA to find best interaction mode with drug molecules, Postgraduate, A.GÜLKAYA(Student), 2022

## Published journal articles indexed by SCI, SSCI, and AHCI

- I. **Tetraphenyl-1,4-dioxin and Tetraphenyl-pyrane-4-one: Old Molecules, New Insights**  
SOYDAN M., Okyar B., ZORLU Y., MARION A., ÖZÇUBUKÇU S.  
ACS OMEGA, vol.8, no.22, pp.19656-19662, 2023 (SCI-Expanded)
- 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 (SCI-Expanded)
- III. **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 (SCI-Expanded)
- IV. **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 (SCI-Expanded)
- V. **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 (SCI-Expanded)
- VI. **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 (SCI-Expanded)
- VII. **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 (SCI-Expanded)
- VIII. **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 (SCI-Expanded)
- IX. **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 (SCI-Expanded)
- X. **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 (SCI-Expanded)
- XI. **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 (SCI-Expanded)
- XII. **Simple Tyrosine Derivatives Act as Low Molecular Weight Organogelators**  
Aykent G., Zeytun C., Marion A., Ozcubukcu S.  
SCIENTIFIC REPORTS, vol.9, 2019 (SCI-Expanded)
- XIII. **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 (SCI-Expanded)
- XIV. **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 (SCI-Expanded)
- XV. **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 (SCI-Expanded)
- XVI. **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 (SCI-Expanded)
- XVII. **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 (SCI-Expanded)
- XVIII. **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 (SCI-Expanded)
- XIX. **Glutathione Biosynthesis: Structure, Mechanism, and Metal Promiscuity of Carboxypeptidase GII**  
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 (SCI-Expanded)
- XX. **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 (SCI-Expanded)
- XXI. **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 (SCI-Expanded)
- XXII. **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 (SCI-Expanded)
- XXIII. **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 (SCI-Expanded)

## 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, vol.5, no.6, pp.2754-2767, 2022 (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

**Metrics**

Publication: 25

Citation (WoS): 280

Citation (Scopus): 279

H-Index (WoS): 9

H-Index (Scopus): 10

**Awards**

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