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Kişisel Bilgiler

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No:1 06800 Çankaya Ankara/TÜRKİYE

Eğitim Bilgileri

Bütünleşik Doktora, Université Henri Poincaré: Nancy I, Sciences, Chemistry, Fransa 2011 - 2015

Yüksek Lisans, Université de Franche-Comté: Besançon, Chemistry, Fransa 2009 - 2011

Lisans, Université de Franche-Comté: Besançon, Chemistry, Fransa 2004 - 2009

Yabancı Diller

Almanca, B1 Orta

Fransızca, C2 Ustalık

Türkçe, A1 Başlangıç

İngilizce, C2 Ustalık

Yaptığı Tezler

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

Araştırma Alanları

Kimya, Fizikokimya, Hesapsal Kimya, Kuantum Mekanik

Akademik Unvanlar / Görevler

Dr.Öğr.Üyesi, Orta Doğu Teknik Üniversitesi, Fen Edebiyat Fakültesi, Kimya Bölümü, 2018 - Devam Ediyor

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

Verdiği Dersler

advanced topics in physical chemistry, Yüksek Lisans, 2018 - 2019

General Chemistry, Lisans, 2018 - 2019

SCI, SSCI ve AHCI İndekslerine Giren Dergilerde Yayınlanan Makaleler

- 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, cilt.18, 2022 (SCI İndekslerine Giren Dergi)
- 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, cilt.24, sa.4, ss.2126-2138, 2022 (SCI İndekslerine Giren Dergi)
- III. **Fullerene-Based Mimics of Biocatalysts Show Remarkable Activity and Modularity.**
Gülseren G., Saylam A., Marion A., Özçubukçu S.
ACS applied materials & interfaces, cilt.13, sa.38, ss.45854-45863, 2021 (SCI İndekslerine Giren Dergi)
- IV. **Peptidotriazolamers Inhibit A β (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, cilt.86, ss.840-851, 2021 (SCI Expanded İndekslerine Giren Dergi)
- 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, cilt.64, sa.1, ss.586-601, 2021 (SCI İndekslerine Giren Dergi)
- 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, cilt.295, sa.40, ss.13862-13874, 2020 (SCI İndekslerine Giren Dergi)
- 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, cilt.62, sa.16, ss.7417-7430, 2019 (SCI İndekslerine Giren Dergi)
- 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, cilt.9, 2019 (SCI İndekslerine Giren Dergi)
- 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, cilt.25, sa.7, 2019 (SCI İndekslerine Giren Dergi)
- 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, cilt.7, 2019 (SCI İndekslerine Giren Dergi)
- XI. **Simple Tyrosine Derivatives Act as Low Molecular Weight Organogelators**
Aykent G., Zeytun C., Marion A., Ozcubukcu S.
SCIENTIFIC REPORTS, cilt.9, 2019 (SCI İndekslerine Giren Dergi)
- 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, cilt.59, sa.1, ss.206-214, 2019 (SCI İndekslerine Giren Dergi)
- XIII. **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, cilt.13, sa.10, 2018 (SCI İndekslerine Giren Dergi)
- 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, cilt.1859, sa.5, ss.342-356, 2018 (SCI İndekslerine Giren Dergi)
- 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, cilt.57, sa.9, ss.1542-1551, 2018 (SCI İndekslerine Giren Dergi)
- 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, cilt.24, sa.4, ss.953-961, 2018 (SCI İndekslerine Giren Dergi)
- 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, cilt.58, sa.1, ss.90-110, 2018 (SCI İndekslerine Giren Dergi)
- XVIII. **Gliotoxin Biosynthesis: Structure, Mechanism, and Metal Promiscuity of Carboxypeptidase GIIJ**
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, cilt.12, sa.7, ss.1874-1882, 2017 (SCI İndekslerine Giren Dergi)
- 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, cilt.17, 2017 (SCI İndekslerine Giren Dergi)
- 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, cilt.54, sa.6, ss.1429-1439, 2015 (SCI İndekslerine Giren Dergi)
- 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, cilt.54, sa.8, ss.2200-2213, 2014 (SCI İndekslerine Giren Dergi)
- 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, cilt.141, sa.3, 2014 (SCI İndekslerine Giren Dergi)

Diğer Dergilerde Yayınlanan Makaleler

- 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 (ESCI İndekslerine Giren Dergi)

Hakemli Kongre / Sempozyum Bildiri Kitaplarında Yer Alan Yayınlar

- 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 Ekim 2018

Atıflar

Toplam Atıf Sayısı (WOS):208

h-indeksi (WOS):9

Ödüller

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