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International Researcher IDs

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Publons / Web Of Science ResearcherID: GRS-8669-2022

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Education Information

Postgraduate, Ankara University, Fen Bilimleri Enstitüsü, Chemistry, Turkey 2021 - Continues

Undergraduate, Ankara University, Fen Fakültesi, Kimya Bölümü, Turkey 2016 - 2021

Research Areas

Bioinformatics, Chemistry, Physical Chemistry, Computational Chemistry, Chemistry of Dyes and Pigments, Natural Sciences

Academic Titles / Tasks

Research Assistant, Ankara University, Fen Fakültesi, Kimya Bölümü, 2023 - Continues

Published journal articles indexed by SCI, SSCI, and AHCI

- Computational insights into bis-N,N-dimethylaniline based D- π -A photosensitizers bearing divergent-type of π -linkers for DSSCs**
Nalçakan H., Kurtay G., Sarıkavak K., Şen N., Sevin Düz F.
Journal of Molecular Graphics and Modelling, vol.122, 2023 (SCI-Expanded)

Articles Published in Other Journals

- Targeting LIMK1 in Alzheimer's Disease: A Multifaceted Computational Investigation Involving ADMET, Virtual Screening, Molecular Docking, and Molecular Dynamics**
Eşkin D., NALÇAKAN H., KURTAY G., Akkan Y., TÜRK M., Uras B.
Journal of the Turkish Chemical Society, Section A: Chemistry, vol.11, no.4, pp.1425-1440, 2024 (Scopus)
- AN IN SILICO PHARMACOKINETIC INVESTIGATION OF ORGANIC LUMINOGENS: UNDERSTANDING THE NIR AIEGENS AND THEIR INTERACTIONS WITH SERUM ALBUMINS**

Nalçakan H., Kurtay G., Özdil D. T., Yılmaz Z.

ANKARA UNIVERSİTESİ ECZACILIK FAKULTESİ DERGİSİ, vol.48, no.1, pp.1-19, 2023 (Scopus)

III. **Bridging Molecular Docking to Molecular Dynamics to Enlighten Recognition Processes of Tailored D-A/D-A-D Types' AIEgens with HSA/BSA**

Nalçakan H., Kurtay G.

Journal of advanced research in natural and applied sciences (Online), vol.9, no.3, pp.670-687, 2023 (Peer-Reviewed Journal)

Refereed Congress / Symposium Publications in Proceedings

I. **Alzheimer's Alchemy: Unveiling the Dual-Inhibitory Potential of Tacrine-Donepezil Hybrids**

NALÇAKAN H., TÜRK M., KURTAY G.

6th International Eurasian Conference on Biological and Chemical Sciences, Ankara, Turkey, 11 - 13 October 2023

II. **Computational Modeling of Novel Filgotinib Derivatives as Potent Janus Kinase (JAK1/JAK2)**

Inhibitors: A Detailed Molecular Docking and in-silico ADMET Analysis

NALÇAKAN H., ÜNALAN A. T., KURTAY G., SEVİN DÜZ F.

11. International Drug Chemistry Conference, Antalya, Turkey, 10 - 12 March 2023

III. **Molecular Docking and in-silico ADMET Studies of Newly Designed Pyrrolo[2,3-d]pyrimidine Derivatives to Inhibit Janus Kinases (JAK1/JAK2)**

ÜNALAN A. T., NALÇAKAN H., KURTAY G., SEVİN DÜZ F.

11. International Drug Chemistry Conference, Antalya, Turkey, 09 March 2023

IV. **Molecular Docking, in silico ADMET Analyses and Computational Approach of Novel Fedratinib Derivatives as Potent JAK2 Inhibitors to Reveal Binding Potentials for Myelofibrosis (MF) Treatment**

NALÇAKAN H., KURTAY G., GÜNGÖR T.

8th International BAU Drug Design Congress - Bahçeşehir University, İstanbul, Turkey, 15 - 17 December 2022

V. **Computational Modelling of Abrocitinib Derivatives/Metabolites and Unveiling their Janus Kinase (JAK) Inhibitory Activities using Molecular Docking and in silico ADMET Studies**

NALÇAKAN H., KURTAY G., GÜNGÖR T.

5th International Eurasian Conference on Biological and Chemical Sciences, İstanbul, Turkey, 23 - 25 November 2022

VI. **Boyaya Duyarlı Güneş Hücrelerine Yönelik Yeni D- π -A Tipi Organik Boyarmaddelerin Teorik Olarak Modellenmesi ve Fotoanot Bileşen Performanslarının İncelenmesi**

NALÇAKAN H., KURTAY G.

34. Ulusal Kimya Kongresi - Yalova Üniversitesi, Yalova, Turkey, 1 - 06 September 2022

VII. **Molecular Docking Approach to Enlighten Photodynamic Therapy Applicability of the Tailored D-A or D-A-D Types' AIEgens**

NALÇAKAN H., KURTAY G.

2. Computer-Aided Drug Design Symposium and Workshop - Linking Design, Biology, Chemistry and Medicine, İstanbul, Turkey, 11 - 12 May 2022

VIII. **Molecular Design and Theoretical Investigation of bis-N,N-dimethylaniline-based Novel D- π -a Photosensitizers Possessing Divergent π -linkers for Dssc Application**

NALÇAKAN H., Sarıkavak K., KURTAY G.

5th International Organic Chemistry Congress, Malatya, Turkey, 14 October 2021 - 17 October 2023

Supported Projects

Önal M., Kurtay G., Yanardağ T., Nalçakan H., Project Supported by Higher Education Institutions, Stereolitografi/Eriyik Yiğma Modellemesi ile Baskılanmış Elektrokimyasal Hücrelerde Grafen Katkılı Baskı Elektrotların Korozyon Dayanımının İncelenmesi ve Endokrin Bozucu Nitro-Polisiklik Aromatik Hidrokarbonların Amperometrik Tayininde Kullanımı, 2024 -

