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Education Information

Doctorate, Ondokuz Mayıs University, Lisansüstü Eğitim Enstitüsü, Kimya Anabilim Dalı, Turkey 2014 - 2019

Postgraduate, Ondokuz Mayıs University, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), Turkey 2011 - 2014

Undergraduate, Suleyman Demirel University, Fen-Edebiyat Fakültesi, Kimya Bölümü, Turkey 2006 - 2010

Dissertations

Doctorate, Synthesis and Characterization of a Series of Macrogol Bonded Symmetric and Asymmetric Structured Phthalocyanine Compounds , Ondokuz Mayıs University, Kimya (Dr), 2019

Postgraduate, Synthesis and Characterization of Macromolecular Network Polymeric Phthalocyanine Compounds, Ondokuz Mayıs University, 2014

Research Areas

Natural Sciences

Academic Titles / Tasks

Research Assistant PhD, Ondokuz Mayıs University, Fen Fakültesi, Kimya Bölümü, 2011 - Continues

Published journal articles indexed by SCI, SSCI, and AHCI

- I. **A Schiff Base with Polymorphic Structure ($Z'=2$): Investigations with Computational Techniques and in Silico Predictions**
Şahin S., Can N. N.
POLYCYCLIC AROMATIC COMPOUNDS, vol.43, no.10, pp.9269-9294, 2023 (SCI-Expanded)
- II. **A New Molecular Structure and Computational Analyses: DFT Studies, NLO Properties, ADMET**

Predictions, Biological Targets, and Docking Experiments

Şahin S.

Polycyclic Aromatic Compounds, 2023 (SCI-Expanded)

- III. **A single-molecule with multiple investigations: Synthesis, characterization, computational methods, inhibitory activity against Alzheimer's disease, toxicity, and ADME studies**
Şahin S.
COMPUTERS IN BIOLOGY AND MEDICINE, vol.146, 2022 (SCI-Expanded)
- IV. **(E)-N-(3-chlorophenyl)-1-(5-nitro-2-(piperidin-1-yl)phenyl)methanimine: X-Ray, DFT, ADMET, Boiled-Egg Model, Druggability, Bioavailability, and Human Cyclophilin D (CypD) Inhibitory Activity**
Şahin S., DEGE N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1250, 2022 (SCI-Expanded)
- V. **Synthesis, characterization, computational analyses, in silico ADMET studies, and inhibitory action against SARS-CoV-2 main protease (Mpro) of a Schiff base**
Şahin S., DEGE N.
TURKISH JOURNAL OF CHEMISTRY, vol.46, no.5, pp.1548-1572, 2022 (SCI-Expanded)
- VI. **Synthesis, characterization, X-ray, HOMO-LUMO, MEP, FT-IR, NLO, Hirshfeld surface, ADMET, boiled-egg model properties and molecular docking studies with human cyclophilin D (CypD) of a Schiff base compound: (E)-1-(5-nitro-2-(piperidin-1-yl)phenyl)-N-(3-nitrophenyl) methanimine**
Şahin S., DEGE N.
POLYHEDRON, vol.205, 2021 (SCI-Expanded)
- VII. **A newly synthesized small molecule: the evaluation against Alzheimer's Disease by in silico drug design and computational structure analysis methods**
Şahin S., DEGE N.
JOURNAL OF MOLECULAR STRUCTURE, vol.1236, 2021 (SCI-Expanded)
- VIII. **A3B type unsymmetrical and amphiphilic phthalocyanines: Synthesis, characterization, thermal stability and aggregation studies**
Şahin S., Ağar E.
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.227, 2020 (SCI-Expanded)
- IX. **Synthesis, spectroscopic properties, thermal properties and aggregation behaviors of macrogol-substituted phthalocyanines**
Şahin S., Ağar E.
JOURNAL OF MOLECULAR STRUCTURE, vol.1187, pp.121-131, 2019 (SCI-Expanded)
- X. **The Crystallographic, Spectroscopic and Theoretical Studies on (E)-2-(((4-fluorophenyl)imino)methyl)-4-nitrophenol and (E)-2-(((3-fluorophenyl)imino)methyl)-4-nitrophenol Compounds**
Demirtas G., DEGE N., Ağar E., Şahin S.
IRANIAN JOURNAL OF CHEMISTRY & CHEMICAL ENGINEERING-INTERNATIONAL ENGLISH EDITION, vol.37, no.5, pp.55-65, 2018 (SCI-Expanded)
- XI. **Crystal Structure of 2-((E)-(5-Bromo-2-hydroxybenzylidene)hydrazono)-1,2-diphenylethanone(1)**
Kaynar N. K., Yavuz M., TANAK H., Şahin S., Buyukgungor O., Ağar E.
CRYSTALLOGRAPHY REPORTS, vol.63, no.3, pp.375-378, 2018 (SCI-Expanded)
- XII. **Molecular and Crystal Structure of 2-((E)-[(5-Chloro-2-methoxyphenyl)imino]methyl)-4-nitrophenol(1)**
Kaynar N. K., Ağar E., TANAK H., Şahin S., Buyukgungor O., Yavuz M.
CRYSTALLOGRAPHY REPORTS, vol.63, no.3, pp.372-374, 2018 (SCI-Expanded)
- XIII. **Crystal structure of (E)-4-nitro-2-((2-phenoxy-phenylimino)methyl)phenol, C₁₉H₁₄N₂O₄**
Köysal Y., Bülbül H., Kantar E. N., Coskun E., Şahin S., DEGE N.
ZEITSCHRIFT FÜR KRISTALLOGRAPHIE-NEW CRYSTAL STRUCTURES, vol.232, no.1, pp.9-10, 2017 (SCI-Expanded)
- XIV. **Molecular and crystal structure of 2-((E)-[(4-Methylphenyl)imino]methyl)-4-nitrophenol: A redetermination**

Kaynar N. K., TANAK H., Şahin S., DEGE N., Ağar E., Yavuz M.

CRYSTALLOGRAPHY REPORTS, vol.61, no.2, pp.239-242, 2016 (SCI-Expanded)

- XV. **Crystal structure and spectroscopic characterization of (E)-2-(((4-bromo-2-(trifluoromethoxy)phenyl)imino)methyl)-4-nitrophenol: A combined experimental and computational study**

Tamer O., DEGE N., Demirtas G., AVCI D., ATALAY Y., Macit M., Şahin S.

JOURNAL OF MOLECULAR STRUCTURE, vol.1063, pp.295-306, 2014 (SCI-Expanded)

Articles Published in Other Journals

- I. **Crystal structure of 2-[[2-methoxy-5-(trifluoromethyl)phenyl]iminomethyl]-4-nitrophenol**

Karadayı N., Şahin S., Köysal Y., Coskun E., Buyukgungor O.

ACTA CRYSTALLOGRAPHICA SECTION E-CRYSTALLOGRAPHIC COMMUNICATIONS, vol.71, 2015 (ESCI)

- II. **2-[[3-Chloro-4-(4-chlorophenoxy)phenyl]iminomethyl]-4-nitrophenol**

Karadayı N., Köysal Y., Şahin S., Coskun E., Buyukgungor O.

ACTA CRYSTALLOGRAPHICA SECTION E-CRYSTALLOGRAPHIC COMMUNICATIONS, vol.69, 2013 (ESCI)

Refereed Congress / Symposium Publications in Proceedings

- I. **IN SILICO ASSESSMENT OF TYPE 2 DIABETES MELLITUS DRUGS AGAINST AMYLOID-B AND TAU AGGREGATION-FORMING SEGMENTS (KLVFFA, VQIVYK, GGVVIA, VQIINK) FOR ALZHEIMER'S DISEASE**

ŞAHİN S.

Materials, Method, and Technologies 2022, 24th International conference, 19-22 August, Burgas, BULGARIA, Burgas, Bulgaria, 19 - 22 August 2022, pp.351-362

- II. **Dual-targeting of β -amyloid and Tau Aggregation against Alzheimer's Disease with the Approved Trifluorinated Drugs**

ŞAHİN S.

Global Congress on Pharmaceutical Sciences and Clinical Research 2022, Japan, 20 - 22 July 2022, pp.117-125

- III. **Sentezlenen Schiff Bazı İçeren Bileşiğin Yapısal ve Spektroskopik Özelliklerinin Deneysel ve Teorik İncelenmesi**

KARAKURT T., AĞAR E., ŞAHİN S., YILDIZ Ş., PARLAK C.

III. International Scientific and Vocational Studies Congress - Science and Health, Nevşehir, Turkey, 27 - 30 June 2019, pp.174-182

- IV. **Computational Investigations and Experimental of (E)-2-((2,4-dichlorophenylimino)methyl)-4-nitrophenol**

KARADAYI N., ŞAHİN S., AĞAR E., BÜYÜKGÜNGÖR O.

International Computational Science Congress(CSC2018), 26 - 28 October 2018

- V. **Computational and Experimental Investigations of (E)-2-((2,4-dichlorophenylimino)methyl)-4-nitrophenol**

KARADAYI N., ŞAHİN S., AĞAR E., BÜYÜKGÜNGÖR O.

CSC2018 - Computational Science Congress, Amasya, Turkey, 26 - 21 October 2018, pp.104-111

- VI. **An Investigation on Aggregation Status of Macrogol-Bound Zinc Phthalocyanine in Different Solvents**

ŞAHİN S., AĞAR E.

6th International BAU Drug Design Congress, 13 - 15 December 2018

- VII. **An Investigation about Aggregation Properties of Copper Phthalocyanine Bearing TEG**

ŞAHİN S., AĞAR E.

4 th Organic Chemistry Congress with International Participation, Antalya, Turkey, 4 - 07 October 2018

- VIII. **Investigating of Spectroscopic Properties and Synthesis of Phthalocyanines Substituted with 2,2'-xx-**

Methylenebis(4-chlorophenoxy)

ŞAHİN S., ERŞAHİN F., AĞAR E.

Tenth International Conference on Porphyrines and Phthalocyanines, Munich, Germany, 1 - 06 July 2018

IX. Investigating of Spectroscopic Properties and Synthesis of Phthalocyanine Containing Some Aza Group

ŞAHİN S., ERŞAHİN F., AĞAR E.

Tenth International Conference Porphyrines and Phthalocyanines, Munich, Germany, 1 - 06 July 2018

X. X-ray crystallographic and computational studies of (E)-2-(((4-bromophenyl)imino)methyl)-4,5-difluorophenol

ATALAY Ş., DURSUN M. E., BÜLBÜL H., AĞAR E., ŞAHİN S.

Turkish Physical Society 33rd International Physics Congress, BODRUM / MUĞLA, Turkey, 6 - 10 September 2017

XI. THE THEORETICAL AND CRYSTALLOGRAPHIC STUDIES ON (E)-2-(((4-BROMO-2-(TRIFLUOROMETHOXY)PHENYL)IMINO)METHYL)-4-NITROPHENOL

DEMİRTAŞ G., TAMER Ö., DEGE N., AVCI D., ATALAY Y., MACİT M., ŞAHİN S.

TURKISH PHYSICAL SOCIETY 33RD INTERNATIONAL PHYSICS CONGRESS, 6 - 10 September 2017

XII. Synthesis and Characterization of Some Polymeric Phthalocyanine Compounds

ŞAHİN S., Taşçı C., TOPCU Y., AĞAR E.

Eight International Conference on Porphyrins and Phthalocyanines ICPP-8, İstanbul, Turkey, 22 - 27 June 2014, pp.680

XIII. (E)-2-((4-Etilfenilimino)metil)-4-nitrofenol Bileşiğinin Deneysel ve Hesaplamalı Yöntemlerle İncelenmesi

ALPASLAN G., AĞAR E., ŞAHİN S., GÖKCE H., CEYLAN Ü., ÖZDEMİR N.

21. Yoğun Madde Fiziği Ankara Toplantısı, Ankara, Turkey, 25 December 2015, pp.19

XIV. Synthesis of Peripheral-Substituted Metal and Metal-Free Network Polymeric Phthalocyanine Compounds

ŞAHİN S., AĞAR E.

International Conference on Porphyrins and Phthalocyanines, 22 - 27 June 2014

XV. Synthesis and Characterization of Some Polymeric Phthalocyanine Compounds

ŞAHİN S., TAŞCI C., TOPCU Y., AĞAR E.

International Conference on Porphyrins and Phthalocyanines, 22 - 27 June 2014