

## Assoc. Prof. AYHAN ÜNGÖRDÜ

### Personal Information

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### International Researcher IDs

ScholarID: OzftQ3gAAAAJ

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Yoksis Researcher ID: 56502

### Education Information

Undergraduate, Sivas Cumhuriyet University, Mühendislik Fakültesi, Bilgisayar Mühendisliği Bölümü, Turkey 2014 - Continues

Doctorate, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Kimya (Dr), Turkey 2009 - 2017

Postgraduate, Sivas Cumhuriyet University, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), Turkey 2004 - 2007

Undergraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 2000 - 2004

### Foreign Languages

English, B2 Upper Intermediate

### Dissertations

Doctorate, BAZI DNA BAZ ÇİFTLERİ İLE GEÇİŞ METAL KOMPLEKSLERİNİN DFT YÖNTEMİYLE İLETKENLİK HESAPLAMALARI, Sivas Cumhuriyet Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (Dr), 2017

Postgraduate, Fe<sub>2</sub>(CO)<sub>4</sub>(?<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub> kompleksinin <sup>13</sup>C-izotopomerlerinin karbonil gerilme bölgesindeki titreşim spektrumlarının analizi, Sivas Cumhuriyet Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (YI) (Tezli), 2007

### Research Areas

Organic Chemistry

### Academic Titles / Tasks

Associate Professor, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2022 - Continues

Research Assistant, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2009 - 2022

### Academic and Administrative Experience

Erasmus Program Institutional Coordinator, Sivas Cumhuriyet University, 2022 - Continues

## Courses

Organik Kimya, Undergraduate, 2022 - 2023  
Bitirme Ödevi/Tezi, Undergraduate, 2022 - 2023  
İleri Organik Kimya I, Postgraduate, 2022 - 2023  
Genel Kimya, Undergraduate, 2022 - 2023  
Organik Kimya Laboratuvarı, Undergraduate, 2022 - 2023  
Genel Kimya, Undergraduate, 2022 - 2023  
Seminer Dersi, Postgraduate, 2022 - 2023  
Genel Kimya, Undergraduate, 2021 - 2022  
Organik Kimya, Undergraduate, 2021 - 2022  
Uzmanlık Alan Dersi, Postgraduate, 2022 - 2023, 2021 - 2022  
Organik Kimya , Undergraduate, 2021 - 2022  
Genel Kimya, Undergraduate, 2017 - 2018  
Genel Kimya, Undergraduate, 2017 - 2018

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

- I. **The detailed investigation on OLED features of some purely organic TADF materials**  
ÜNGÖRDÜ A.  
Materials Today Communications, vol.39, 2024 (SCI-Expanded)
- II. **Organic light-emitting diode behaviors of some synthesized platinum(II)-based complexes**  
ÜNGÖRDÜ A.  
International Journal of Quantum Chemistry, vol.123, no.21, 2023 (SCI-Expanded)
- III. **The design of push-pull substituted coronene molecules for optoelectronic applications**  
Demir C., ÜNGÖRDÜ A.  
Materials Chemistry and Physics, vol.301, 2023 (SCI-Expanded)
- IV. **Optoelectronic and electric properties of 8-Hydroxyquinoline-Based complexes with divalent metal ions**  
ÜNGÖRDÜ A.  
Materials Chemistry and Physics, vol.281, 2022 (SCI-Expanded)
- V. **Antioxidant activities of Alyssum virgatum plant and its main components**  
KOÇ E., ÜNGÖRDÜ A., CANDAN F.  
STRUCTURAL CHEMISTRY, vol.33, no.1, pp.267-279, 2022 (SCI-Expanded)
- VI. **The performance of Cu-mediated metal-DNA parts for nanowires: DFT and NEGF-DFT studies**  
Üngördü A.  
MATERIALS TODAY COMMUNICATIONS, vol.24, 2020 (SCI-Expanded)
- VII. **Electronic Properties of Artificial Metal-DNA Base Pair Complexes Formed from Hydroxypyridone Base**  
ÜNGÖRDÜ A., TEZER N.  
CHEMISTRYSELECT, vol.5, no.24, pp.7267-7276, 2020 (SCI-Expanded)
- VIII. **Electronic, optical, and charge transfer properties of porphyrin and metallated porphyrins in different media**  
ÜNGÖRDÜ A.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.120, no.6, 2020 (SCI-Expanded)
- IX. **Antioxidant properties of methanolic extract of 'Veronica multifida' and DFT and HF analyses of its the major flavonoid component**  
Koç E., Üngördü A., Candan F.  
Journal of Molecular Structure, vol.1197, pp.436-442, 2019 (SCI-Expanded)
- X. **Charge transfer properties of Gaq3 and its derivatives: An OLED study**  
ÜNGÖRDÜ A.

CHEMICAL PHYSICS LETTERS, vol.733, 2019 (SCI-Expanded)

- XI. **Quantum chemical calculations on sparfloxacin and boron complexes**  
ÜNGÖRDÜ A., SAYIN K.  
CHEMICAL PHYSICS LETTERS, vol.733, 2019 (SCI-Expanded)
- XII. **Investigations of structural, spectral and electronic properties of enrofloxacin and boron complexes via quantumchemical calculation and molecular docking**  
SAYIN K., ÜNGÖRDÜ A.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.220, 2019 (SCI-Expanded)
- XIII. **Investigation of anticancer properties of caffeinated complexes via computational chemistry methods**  
SAYIN K., ÜNGÖRDÜ A.  
SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, vol.193, pp.147-155, 2018 (SCI-Expanded)
- XIV. **Effect on frontier molecular orbitals of substituents in 5-position of uracil base pairs in vacuum and water**  
ÜNGÖRDÜ A., TEZER N.  
JOURNAL OF THEORETICAL & COMPUTATIONAL CHEMISTRY, vol.16, no.7, 2017 (SCI-Expanded)
- XV. **DFT study on metal-mediated uracil base pair complexes**  
ÜNGÖRDÜ A., TEZER N.  
JOURNAL OF SAUDI CHEMICAL SOCIETY, vol.21, no.7, pp.837-844, 2017 (SCI-Expanded)
- XVI. **The solvent (water) and metal effects on HOMO-LUMO gaps of guanine base pair: A computational study**  
ÜNGÖRDÜ A., TEZER N.  
JOURNAL OF MOLECULAR GRAPHICS & MODELLING, vol.74, pp.265-272, 2017 (SCI-Expanded)

## Articles Published in Other Journals

- I. **Structural, Spectral, Biological and Antioxidant Analyses of Baicalin and Its Vanadium Complexes: A DFT Study**  
SAYIN K., ÜNGÖRDÜ A.  
Cumhuriyet Science Journal, vol.41, no.1, pp.11-21, 2020 (Peer-Reviewed Journal)
- II. **Investigation of NLO Properties of Pyridine Benzimidazole Derivatives: Ab-Initio Approach**  
ÜNGÖRDÜ A.  
Cumhuriyet Science Journal, pp.105-117, 2018 (Peer-Reviewed Journal)
- III. **Metal-mediated thymine base pair complexes: A DFT study**  
ÜNGÖRDÜ A., TEZER N.  
Turkish Computational and Theoretical Chemistry, vol.1, no.1, pp.35-41, 2017 (Scopus)
- IV. **EFFECT OF SOME ELECTRON DONOR AND ELECTRON ACCEPTOR GROUPS ON STABILITY OF COMPLEXES ACCORDING TO THE PRINCIPLE OF HSAB**  
KAYA S., KAYA C., ERKAN KARİPER S., ÜNGÖRDÜ A.  
JOURNAL OF NEW RESULTS IN SCIENCE, pp.82-89, 2014 (Peer-Reviewed Journal)

## Books & Book Chapters

- I. **Sadeleştirilmiş Anlatımıyla Temel Üniversite Kimyası**  
Kanberoğlu G., Çaylak O., Saygı K. Ö., Sivrikaya Özak S., Güngör Ö., Polat Ü., Gürbüz A., Seven Erdemir Ü., Gündoğdu A., Çalmlı M. H., et al.  
Akademisyen Kitabevi, Ankara, 2023

## Refereed Congress / Symposium Publications in Proceedings

- I. **OLED behaviors of some Pt-porphyrin and its derivatives**  
ÜNGÖRDÜ A.  
1st International Conference on Engineering, Natural and Social Sciences (ICENSOS 2022), Konya, Turkey, 20 December 2022
- II. **Modified TPD molecules as hole transfer materials**  
ÜNGÖRDÜ A.  
1st International Conference on Scientific and Academic Research (ISCAR 22), Konya, Turkey, 10 December 2022
- III. **Benzen ve Çok Halkalı Aromatik Bileşiklerin Optoelektronik Özelliklerinin Tahmini**  
ÜNGÖRDÜ A.  
32. Ulusal Kimya Kongresi, Turkey, 17 - 19 September 2020, pp.150
- IV. **Charge Transfer Rates of 8-Substituted Guanine Molecules in Different Media**  
ÜNGÖRDÜ A.  
2nd International Conference on Physical Chemistry and Functional Materials, Nevşehir, Turkey, 25 - 27 June 2019
- V. **Oled Behaviours of  $\alpha$ ,  $\beta$ -Substituted Naphthalene Compounds**  
ÜNGÖRDÜ A.  
2nd International Conference on Physical Chemistry and Functional Materials, 25 - 27 June 2019
- VI. **CHARGE TRANSFER PROPERTY OF TRIS(3-NITRO-8-HYDROXYQUINOLINATO)ALUMINIUM**  
ÜNGÖRDÜ A., SAYIN K.  
1. Uluslararası Battal Gazi Multidisipliner Çalışmalar Kongresi, Malatya, Turkey, 7 - 09 December 2018
- VII. **QUANTUM CHEMICAL CALCULATIONS ON FLAVONOİD BAICALIN IN WATER PHASE**  
SAYIN K., ÜNGÖRDÜ A.  
1. Uluslararası Battal Gazi Multidisipliner Çalışmalar Kongresi, Malatya, Turkey, 7 - 09 December 2018
- VIII. **REORGANIZATION ENERGY OF TRIS(3-AMINO-8-HYDROXYQUINOLINATO)ALUMINIUM COMPLEX**  
ÜNGÖRDÜ A., SAYIN K.  
1. Uluslararası Battal Gazi Multidisipliner Çalışmalar Kongresi, Malatya, Turkey, 7 - 09 December 2018
- IX. **DFT STUDIES OF HEAT SHOCK PROTEIN (HSP) INHIBITORS**  
SAYIN K., ÜNGÖRDÜ A.  
1. Uluslararası Battal Gazi Multidisipliner Çalışmalar Kongresi, Malatya, Turkey, 7 - 09 December 2018
- X. **Flavonoid Baisalin Bileşğinin Kuantum Kimyasal Hesaplamalar Yöntemleriyle İncelenmesi**  
SAYIN K., ÜNGÖRDÜ A., KARAKUŞ N.  
3rd International Mediterranean Science and Engineering Congress, Adana, Turkey, 24 - 26 October 2018
- XI. **Anticancer effect of proton pump inhibitor on hepatocellular carcinoma**  
SAYIN K., ÜNGÖRDÜ A., ATASEVEN H.  
APASL Single Topic Conference, 27 - 29 September 2018
- XII. **Mono-Azo Naftilamin Boyalarının İnhibisyon Mekanizmalarının Belirlenmesi: Hesaplamalı Korozyon Çalışması**  
SAYIN K., ÜNGÖRDÜ A., KARAKUŞ N.  
2nd international mediterranean science and engineering congress (IMSEC 2017), Adana, Turkey, 25 - 27 October 2017
- XIII. **Mono-Azo Naftilamin Boyalarının İnhibisyon Mekanizmasının Belirlenmesi: Hesaplamalı Korozyon Çalışması**  
SAYIN K., ÜNGÖRDÜ A., KARAKUŞ N.  
International Mediterranean Science and Engineering Congress (IMSEC 2017), 25 - 27 October 2017
- XIV. **Theoretical Study on Electrical Conductivity of Metal-DNA Base Pairs Formed From Artificial Mercaptopyrindone Base**  
ÜNGÖRDÜ A.  
13th Nanoscience and Nanotechnology Conference (NANOTR13), Antalya, Turkey, 22 - 25 October 2017
- XV. **NEGF Study On Metal-DNA Base Pairs Formed From Artificial Hydroxypyridone Base**  
ÜNGÖRDÜ A., TEZER N.

13th Nanoscience and Nanotechnology Conference (NANOTR13), Antalya, Turkey, 22 - 25 October 2017

- XVI. **INVESTIGATION OF ANTICANCER PROPERTIES OF RU(II) AND OS(III) COMPLEXES: MOLECULAR DOCKING CALCULATIONS**  
SAYIN K., ÜNGÖRDÜ A.  
2nd International Gazi Pharma Symposium Series (GPSS-2017), Ankara, Turkey, 11 - 13 October 2017
- XVII. **THE ELECTRICAL CONDUCTIVITY OF METAL-DNA BASE PAIRS FORMED FROM NATURAL THYMINE BASE: A DFT STUDY**  
ÜNGÖRDÜ A., TEZER N.  
INTERNATIONAL CONGRESS ON SEMICONDUCTOR MATERIALS AND DEVICES (ICSMD-2017), Konya, Turkey, 17 - 19 August 2017
- XVIII. **DETERMINATION BY BAND THEORY OF ELECTRICAL CONDUCTIVITY OF METAL-DNA BASE PAIRS FORMED FROM ARTIFICIAL HYDROXYPYRIDONE BASE IN DIFFERENT FIELDS**  
ÜNGÖRDÜ A., TEZER N.  
INTERNATIONAL CONGRESS ON SEMICONDUCTOR MATERIALS AND DEVICES (ICSMD-2017), Konya, Turkey, 17 - 19 August 2017
- XIX. **THEORETICAL STUDY ON ELECTRICAL CONDUCTIVITY OF METAL-DNA BASE PAIRS FORMED FROM ARTIFICIAL HYDROXYPYRIDINETHIONE BASE**  
ÜNGÖRDÜ A., TEZER N.  
INTERNATIONAL CONGRESS ON SEMICONDUCTOR MATERIALS AND DEVICES (ICSMD-2017), Konya, Turkey, 17 - 19 August 2017
- XX. **NEGF STUDY ON METAL-MEDIATED THYMINE BASE PAIR COMPLEXES**  
ÜNGÖRDÜ A., TEZER N.  
INTERNATIONAL CONGRESS ON SEMICONDUCTOR MATERIALS AND DEVICES (ICSMD-2017), Konya, Turkey, 17 - 19 August 2017

## Supported Projects

Üngördü A., Project Supported by Higher Education Institutions, Koronen ve türevlerinin OLED davranışlarının belirlenmesi, 2022 - 2022

Üngördü A., Project Supported by Higher Education Institutions, Platin bazlı komplekslerin optoelektronik özelliklerinin belirlenmesi: Bir OLED çalışması, 2020 - 2022

Üngördü A., Project Supported by Higher Education Institutions, Grafenin Elektronik Özellikleri Üzerine Sübstitüent Etkisi: Hesaplamalı Çalışma, 2017 - 2021

Üngördü A., Sayın K., Project Supported by Higher Education Institutions, Flavonoid Baisalin ve Oksovanadyu(IV) Komplekslerinin Hesaplamalı Kimya Yöntemleriyle Yapısal, Spektral ve Biyolojik Özelliklerinin Araştırılması, 2018 - 2019

Üngördü A., Tezer N., Project Supported by Higher Education Institutions, Metal-merkezli sübstitüe 3-hidroksipiridin-4-tiyon (metal-DNA) komplekslerinin elektronik özelliklerinin belirlenmesi: Hesaplamalı kimya çalışması, 2017 - 2018

ÜNGÖRDÜ A., Project Supported by Higher Education Institutions, Yapay Merkaptopridon Bazından Elde Edilen Metal-DNA Baz Çiftlerinin Elektriksel İletkenliği Üzerine Teorik Çalışma, 2017 - 2017

Üngördü A., Tezer N., Project Supported by Higher Education Institutions, Yapay Hidroksipiridintiyon Bazından Elde Edilen Metal DNA'nın Elektriksel İletkenliği: DFT çalışması, 2016 - 2016

SAYIN K., KARAKUŞ N., ÜNGÖRDÜ A., Project Supported by Higher Education Institutions, Mono ve Bis Azo Naftilamin Boyalarının Hesaplamalı Kimya Yöntemleriyle Korozyon İnhibisyon Etkinliklerinin Belirlenmesi, 2016 - 2016

## Scientific Refereeing

CUMHURİYET SCIENCE JOURNAL, Other Indexed Journal, November 2022

Turkish Computational and Theoretical Chemistry, Other Indexed Journal, June 2022

CUMHURİYET SCIENCE JOURNAL, Other Indexed Journal, May 2022

Turkish Computational and Theoretical Chemistry, Other Indexed Journal, January 2022  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, November 2021  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, November 2021  
Naturengs, Other Indexed Journal, November 2021  
Ordu Üniversitesi Bilim ve Teknoloji Dergisi, Other Indexed Journal, August 2021  
Karaelmas Fen ve Mühendislik Dergisi, Other Indexed Journal, January 2021  
Türk Fen ve Sağlık Dergisi, National Scientific Refreed Journal, December 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, September 2020  
JOURNAL OF APPLIED PHYSICS, Journal Indexed in SCI-E, September 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, July 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, July 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, July 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, July 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, July 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, July 2020  
Turkish Computational and Theoretical Chemistry, Other Indexed Journal, July 2020  
JOURNAL OF COMPUTATIONAL BIOPHYSICS AND CHEMISTRY, Journal Indexed in SCI-E, March 2020

## **Metrics**

Publication: 41

Citation (WoS): 172

Citation (Scopus): 241

H-Index (WoS): 7

H-Index (Scopus): 9