

## Assoc. Prof. AYHAN ÜNGÖRDÜ

### Personal Information

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### 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>( $\eta^5$ -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

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

### Courses

Genel Kimya II, Undergraduate, 2017 - 2018

Genel Kimya, Undergraduate, 2017 - 2018

Genel Kimya 2, Undergraduate, 2017 - 2018

Genel Kimya, Undergraduate, 2017 - 2018

Genel Kimya, Undergraduate, 2017 - 2018

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

- I. **Optoelectronic and electric properties of 8-Hydroxyquinoline-Based complexes with divalent metal ions**  
ÜNGÖRDÜ A.  
Materials Chemistry and Physics, vol.281, 2022 (Journal Indexed in SCI)
- II. **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 (Journal Indexed in SCI)
- III. **The performance of Cu-mediated metal-DNA parts for nanowires: DFT and NEGF-DFT studies**  
Üngördü A.  
MATERIALS TODAY COMMUNICATIONS, vol.24, 2020 (Journal Indexed in SCI)
- IV. **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 (Journal Indexed in SCI)
- V. **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 (Journal Indexed in SCI)
- VI. **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 (Journal Indexed in SCI)
- VII. **Charge transfer properties of Gaq3 and its derivatives: An OLED study**  
ÜNGÖRDÜ A.  
CHEMICAL PHYSICS LETTERS, vol.733, 2019 (Journal Indexed in SCI)
- VIII. **Quantum chemical calculations on sparfloxacin and boron complexes**  
ÜNGÖRDÜ A., SAYIN K.  
CHEMICAL PHYSICS LETTERS, vol.733, 2019 (Journal Indexed in SCI)
- IX. **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 (Journal Indexed in SCI)
- X. **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 (Journal Indexed in SCI)
- XI. **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 (Journal Indexed in SCI)
- XII. **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 (Journal Indexed in SCI)
- XIII. **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 (Journal Indexed in SCI)

## 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 (Other Refereed National Journals)
- II. **Investigation of NLO Properties of Pyridine Benzimidazole Derivatives: Ab-Initio Approach**  
ÜNGÖRDÜ A.  
Cumhuriyet Science Journal, pp.105-117, 2018 (Other Refereed National Journals)
- 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 (Refereed Journals of Other Institutions)
- 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 (Refereed Journals of Other Institutions)

## Refereed Congress / Symposium Publications in Proceedings

- I. **Benzen ve Çok Halkalı Aromatik Bileşiklerin Optoelektronik Özelliklerinin Tahmini**  
ÜNGÖRDÜ A.  
32. Ulusal Kimya Kongresi, Turkey, 17 - 19 September 2020, pp.150
- II. **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
- III. **Oled Behaviours of  $\alpha$ ,  $\beta$ -Substituted Naphthalene Compounds**  
ÜNGÖRDÜ A.  
2nd International Conference on Physical Chemistry and Functional Materials, 25 - 27 June 2019
- IV. **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
- V. **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
- VI. **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
- VII. **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
- VIII. **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
- IX. **Anticancer effect of proton pump inhibitor on hepatocellular carcinoma**  
SAYIN K., ÜNGÖRDÜ A., ATASEVEN H.  
APASL Single Topic Conference, 27 - 29 September 2018
- X. **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

- XI. **Theoretical Study on Electrical Conductivity of Metal-DNA Base Pairs Formed From Artificial Mercaptopyridone Base**  
ÜNGÖRDÜ A.  
13th Nanoscience and Nanotechnology Conference (NANOTR13), Antalya, Turkey, 22 - 25 October 2017
- XII. **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
- XIII. **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
- XIV. **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
- XV. **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
- XVI. **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
- XVII. **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

## Supported Projects

Üngördü A., Project Supported by Higher Education Institutions, Platin bazlı komplekslerin optoelektronik özelliklerinin belirlenmesi: Bir OLED çalışması, 2020 - 2021

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

SAYIN K., ÜNGÖRDÜ A., Project Supported by Higher Education Institutions, Flavonoid Baisalin ve Oksovanadyum(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

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

## Citations

Total Citations (WOS):157

h-index (WOS):7