

## Assoc. Prof. DİLARA ÖZBAKIR IŞIN

### Personal Information

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### International Researcher IDs

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Yoksis Researcher ID: 51286

### Education Information

Doctorate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 1996 - 2003

Postgraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 1994 - 1996

Undergraduate, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, Turkey 1989 - 1993

### Foreign Languages

English, B2 Upper Intermediate

### Dissertations

Doctorate, 2-Pirolidonun yapısal özellikleri ve dimer oluşumu üzerine bağlı grup etkisinin AB initio moleküler orbital yöntemleriyle incelenmesi, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2003

Postgraduate, Bazı organik bileşiklerin indirgenme tepkimeleri, Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 1996

### Research Areas

Natural Sciences

### Academic Titles / Tasks

Associate Professor, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2021 - Continues

Assistant Professor, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2004 - 2021

Research Assistant, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 1994 - 2004

### Academic and Administrative Experience

Deputy Head of Department, Sivas Cumhuriyet University, Fen Fakültesi, Kimya Bölümü, 2021 - Continues

Sivas Cumhuriyet Üniversitesi, Fen Fakültesi, Kimya Bölümü, 2009 - 2012

## Courses

Uzmanlık Alan Dersi, Doctorate, 2019 - 2020  
Organik Kimya - II, Undergraduate, 2018 - 2019  
Uzmanlık Alan Dersi, Postgraduate, 2018 - 2019  
Organik Kimya, Undergraduate, 2019 - 2020  
Tez Çalışması, Doctorate, 2018 - 2019  
Teorik Organik Kimyaya Giriş, Undergraduate, 2018 - 2019  
Tez Çalışması, Postgraduate, 2018 - 2019  
Organik Kimya, Undergraduate, 2019 - 2020  
UZMANLIK ALAN DERSİ, Postgraduate, 2017 - 2018, 2016 - 2017  
Organik Tepkime Mekanizmaları, Undergraduate, 2018 - 2019  
Organik Kimya, Undergraduate, 2017 - 2018  
Organik Tepkime Mekanizmaları, Undergraduate, 2018 - 2019  
ORGANİK KİMYANIN İLKELERİ, Doctorate, 2017 - 2018, 2016 - 2017  
ORGANİK KİMYA, Undergraduate, 2017 - 2018, 2016 - 2017  
Organik Kimya - I, Undergraduate, 2018 - 2019  
Organik Kimyanın İlkeleri, Doctorate, 2018 - 2019  
Uzmanlık Alan Dersi, Doctorate, 2017 - 2018  
ORGANİK KİMYA LAB., Undergraduate, 2017 - 2018  
TEORİK ORGANİK KİMYAYA GİRİŞ, Undergraduate, 2017 - 2018, 2016 - 2017  
ORGANİK TEPKİME MEKANİZMALARI, Undergraduate, 2017 - 2018  
ORGANİK KİMYA-II, Undergraduate, 2017 - 2018, 2016 - 2017  
ORGANİK KİMYA-I, Undergraduate, 2017 - 2018  
BİTİRME ÖDEVİ, Undergraduate, 2017 - 2018  
Bitirme Ödevi/Tezi, Undergraduate, 2017 - 2018  
Teorik Organik Kimyaya Giriş, Undergraduate, 2015 - 2016  
Organik Kimya II, Undergraduate, 2014 - 2015  
Seminer Dersi, Doctorate, 2015 - 2016  
Bitirme Ödevi/Tezi, Undergraduate, 2014 - 2015  
Seminer Dersi, Postgraduate, 2013 - 2014  
Organik Kimya I, Undergraduate, 2014 - 2015  
Organik Kimya I Lab., Undergraduate, 2012 - 2013  
Organik Kimya II Lab., Undergraduate, 2011 - 2012  
Genel Kimya I, Undergraduate, 2011 - 2012  
Genel Kimya, Undergraduate, 2010 - 2011  
Genel Kimya Laboratuvarı I, Undergraduate, 2010 - 2011  
Genel Kimya, Undergraduate, 2009 - 2010  
Organik Kimya Lab, Undergraduate, 2008 - 2009  
Genel Kimya Laboratuvarı I, Undergraduate, 2009 - 2010  
Genel Kimya II, Undergraduate, 2007 - 2008  
Genel Kimya II, Undergraduate, 2008 - 2009  
Genel Kimya Lab - II, Undergraduate, 2006 - 2007  
Organik Kimya, Undergraduate, 2006 - 2007  
Organik Kimya, Undergraduate, 2006 - 2007  
Kimya IV, Undergraduate, 2005 - 2006

## Advising Theses

Özbakır Işın D., Bazı flavonoidlerin antioksidan özelliklerinin yoğunluk fonksiyonel teorisi (DFT) ile incelenmesi,

Doctorate, Ş.ERDOĞAN(Student), 2022

Özbakır Işın D., 3-stirilkromon türevlerinin antioksidan etkinliklerinin kuantum mekaniksel incelenmesi, Postgraduate, E.ÇAKMAK(Student), 2019

ÖZBAKIR IŞIN D., Urazolün proton transfer tepkimelerinin ab initio moleküler orbital yöntemleri ile incelenmesi, Postgraduate, Ş.ERDOĞAN(Student), 2012

ÖZBAKIR IŞIN D., 3-hidroksitropolonun proton transfer tepkimesi üzerine bağlı grup ve çözücü etkilerinin ab initio moleküler orbital yöntemleri ile incelenmesi, Postgraduate, V.GÜL(Student), 2012

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

- I. **“Property Prediction from Structural Differences”: II. Application to the molar diamagnetic susceptibilities of amino acids**  
BATIR G. G., ÖZBAKIR IŞIN D.  
Journal of Molecular Liquids, vol.404, 2024 (SCI-Expanded)
- II. **Molecular docking and A DFT study on the antiradical activity of naringenin and hesperetin with nitric oxide, peroxy, and methoxy radicals**  
Erdoğan Ş., Özbakır Işın D.  
Journal of Physical Organic Chemistry, vol.36, no.4, 2023 (SCI-Expanded)
- III. **Molecular insights into the corrosion inhibition mechanism of omeprazole and tinidazole: a theoretical investigation**  
Kaya S., Lgaz H., Thakkur A., Kumar A., Özbakır Işın D., Karakuş N., Ben Ahmed S.  
Molecular Simulation, vol.49, no.17, pp.1632-1646, 2023 (SCI-Expanded)
- IV. **Kaya's composite descriptor and Maximum Composite Hardness Rule for chemical reactions**  
Kaya S., Özbakır Işın D., Karakuş N.  
JOURNAL OF THE INDIAN CHEMICAL SOCIETY, vol.99, no.3, 2022 (SCI-Expanded)
- V. **A DFT study on OH radical scavenging activities of eriodictyol, Isosakuranetin and pinocembrin**  
Erdogan S., ÖZBAKIR IŞIN D.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.40, no.21, pp.10802-10811, 2022 (SCI-Expanded)
- VI. **Theoretical insights about inhibition efficiencies of some 8-Hydroxyquinoline derivatives against the corrosion of mild steel**  
ÖZBAKIR IŞIN D., KARAKUŞ N., Lgaz H., KAYA S., Chung I.  
MOLECULAR SIMULATION, vol.46, no.17, pp.1398-1404, 2020 (SCI-Expanded)
- VII. **Spectral analysis and detailed quantum mechanical investigation of some acetanilide analogues and their self-assemblies with graphene and fullerene**  
Almuqrin A. H., Al-Otaibi J. S., Mary Y. S., Thomas R., KAYA S., ÖZBAKIR IŞIN D.  
JOURNAL OF MOLECULAR MODELING, vol.26, no.9, 2020 (SCI-Expanded)
- VIII. **A theoretical evaluation on free radical scavenging activity of 3-styrylchromone derivatives: the DFT study**  
Cakmak E., ÖZBAKIR IŞIN D.  
JOURNAL OF MOLECULAR MODELING, vol.26, no.5, 2020 (SCI-Expanded)
- IX. **A computational study on corrosion inhibition performances of novel quinoline derivatives against the corrosion of iron**  
ERDOĞAN Ş., Safi Z. S., KAYA S., ÖZBAKIR IŞIN D., Guo L., KAYA C.  
JOURNAL OF MOLECULAR STRUCTURE, vol.1134, pp.751-761, 2017 (SCI-Expanded)
- X. **Theoretical study on the investigation of antioxidant properties of some hydroxyanthraquinones**  
ÖZBAKIR IŞIN D.  
MOLECULAR PHYSICS, vol.114, no.24, pp.3578-3588, 2016 (SCI-Expanded)
- XI. **Quantum chemical study on the inhibition efficiencies of some sym-triazines as inhibitors for mild steel in acidic medium**  
ÖZBAKIR IŞIN D., KARAKUŞ N.

- JOURNAL OF THE TAIWAN INSTITUTE OF CHEMICAL ENGINEERS, vol.50, pp.306-313, 2015 (SCI-Expanded)
- XII. **Theoretical Study on the Self- and Water-Assisted Proton Transfer Reaction of Urazole**  
Erdogan S., Isin D.  
CHEMISTRY OF HETEROCYCLIC COMPOUNDS, vol.50, no.7, pp.986-997, 2014 (SCI-Expanded)
- XIII. **Computational Investigation of the Substituent Effect on the Intramolecular Proton Transfer Reaction of 3-Hydroxytropolone**  
Gul V., ÖZBAKIR İŞİN D.  
CHINESE JOURNAL OF STRUCTURAL CHEMISTRY, vol.33, no.12, pp.1757-1767, 2014 (SCI-Expanded)
- XIV. **Computational study of the intramolecular proton transfer reactions of 3-hydroxytropolone (2,7-dihydroxycyclohepta-2,4,6-trien-1-one) and its dimers**  
ÖZBAKIR İŞİN D., KARAKUŞ N.  
JOURNAL OF MOLECULAR MODELING, vol.16, no.12, pp.1877-1882, 2010 (SCI-Expanded)
- XV. **A computational study on the self-association of -CN, -NH<sub>2</sub>, -CH<sub>3</sub> and -C(CH<sub>3</sub>)<sub>3</sub> derivatives of 2-pyrrolidinone**  
Isin D., Yekeler H.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.685, pp.117-126, 2004 (SCI-Expanded)
- XVI. **Concerning the solvent effect in the tautomerism of uracil, 5-fluorouracil, and thymine by density-functional theory and ab initio calculations**  
Yekeler H., Ozbakir D.  
JOURNAL OF MOLECULAR MODELING, vol.7, no.4, pp.103-111, 2001 (SCI-Expanded)

### Articles Published in Other Journals

- I. **DFT Study on Antioxidant Action Mechanisms of Naphthoquinone-Urazole Hybrids**  
ÖZBAKIR İŞİN D.  
Cumhuriyet Science Journal, vol.39, no.3, pp.734-744, 2018 (Peer-Reviewed Journal)
- II. **DENSITY FUNCTIONAL THEORY STUDY OF THE ANTIOXIDANTACTIVITY OF FORMLY CHROMONE SCHIFF BASES**  
ÖZBAKIR İŞİN D.  
Journal of the Turkish Chemical Society, Section A: Chemistry, vol.2, no.2, pp.78-80, 2015 (Peer-Reviewed Journal)
- III. **CORROSION INHIBITION EFFECT OF SOME AMINO SUBSTITUTEDTHIADIAZOLES ON COPPER QUANTUM CHEMICAL STUDY**  
KARAKUŞ N., ÖZBAKIR İŞİN D.  
Journal of the Turkish Chemical Society, Section A: Chemistry, vol.2, no.2, pp.62-66, 2015 (Peer-Reviewed Journal)

### Refereed Congress / Symposium Publications in Proceedings

- I. **ÇİNKO, BAKIR VE DEMİRİN SULU ORTAMLARDA BAZI ORGANİK MADDELERLE KOROZYONUN İNCELENMESİ**  
ÖZBAKIR İŞİN D., ERDOĞAN Ş.  
1. ULUSLARARASI MALATYA UYGULAMALI BİLİMLER KONGRESİ, Malatya, Turkey, 20 - 22 December 2019, vol.2, pp.221-226
- II. **İHLAMUR (Tilia Cordata) BİTKİSİNDE BULUNAN NARİNGENİN BİLEŞİĞİNİN ANTİOKSİDAN ETKİ MEKANİZMASI VE AKTİOKSİDAN ÖZELLİKLERİNİN İNCELENMESİ**  
ERDOĞAN Ş., ÖZBAKIR İŞİN D.  
1. ULUSLARARASI MALATYA UYGULAMALI BİLİMLER KONGRESİ, Malatya, Turkey, 20 - 22 December 2019, vol.2, pp.227-233
- III. **The Theoretical Investigation on the Antioxidant Activity of Some Naphthoquinone-Urazole Hybrids**  
ÖZBAKIR İŞİN D.

20th International Conference on Advances in Chemistry and Applied Chemistry, 30 - 31 January 2018

- IV. **Investigation of antioxidant properties of some hydroxyanthraquinones A Density Functional Theory Study**  
ÖZBAKIR İŞİN D.  
28. Ulusal Kimya Kongresi, Mersin, Turkey, 15 - 21 August 2016
- V. **Density functional theory study of the antioxidant activity of formerly chromone schiff bases**  
ÖZBAKIR İŞİN D.  
XI. Chemical Physics Congress, 17 - 18 October 2014
- VI. **Quantum Chemical Study on the Inhibition Efficiencies of Some Sym triazines as Inhibitors for Mild Steel in Acidic Medium**  
ÖZBAKIR İŞİN D., KARAKUŞ N.  
XI. Chemical Physics Congress, 17 - 18 October 2014
- VII. **Corrosion Inhibition Effect of Some Amino Substituted Thiadiazoles on Copper Quantum Chemical Study**  
KARAKUŞ N., ÖZBAKIR İŞİN D.  
XI. Kimyasal Fizik Kongresi Piri Reis Üniversitesi, İstanbul, 17 - 18 October 2014
- VIII. **The investigation of the proton transfer reactions of urazole by ab initio molecular orbital theory**  
ERDOĞAN Ş., ÖZBAKIR İŞİN D.  
Chemical Physics X, 10 - 12 October 2012
- IX. **3 Hidroksitropolonun Proton Transfer Tepkimesi Üzerine Bağlı Grup Etkisinin DFT Yöntemiyle İncelenmesi**  
Gül V., ÖZBAKIR İŞİN D.  
XXV. Ulusal Kimya Kongresi, Turkey, 27 June - 02 July 2011
- X. **3 Hidroksitropolonun Proton Transfer Tepkimesi Üzerine Çözücü Etkisinin DFT Yöntemiyle İncelenmesi**  
ÖZBAKIR İŞİN D., KARAKUŞ N.  
24. Ulusal Kimya Kongresi, Zonguldak Karaelmas Üniversitesi, Turkey, 2 June - 02 July 2010
- XI. **A computational study on self association of CN and NH<sub>2</sub> of 2 pyrrolidinone**  
ÖZBAKIR İŞİN D., YEKELER H.  
Chemical Physics V, 31 October - 01 November 2002
- XII. **Investigation of solvent effect on the tautomerism of thymine by density functional theory and ab initio calculations**  
ÖZBAKIR D., YEKELER H.  
Chemical Physics IV, 28 - 29 October 2000
- XIII. **Bazı Organik Bileşiklerin İndirgenme Tepkimeleri**  
ÖZBAKIR D., ÖZKAN R.  
XIII. Ulusal Kimya Kongresi, Turkey, 31 August - 04 September 1999

## Metrics

Publication: 32

Citation (WoS): 240

Citation (Scopus): 319

H-Index (WoS): 6

H-Index (Scopus): 6