

## Asst. Prof. VOLKAN FINDIK

### Personal Information

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### International Researcher IDs

ScholarID: volkan

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### Education

Post Doctorate, Modélisation et Simulation Multi Echelle MSME , Chimie Théorique, France 2023 - Continues

Doctorate, Laboratoire de Physique et Chimie Théoriques, Chimie Théorique, France 2019 - 2022

Doctorate, Marmara University, Institute for Graduate Studies in Pure and Applied Sciences, Department of Chemistry, Turkey 2018 - 2022

Postgraduate, Bogazici University, Institute Of Science, Kimya Anabilim Dalı, Turkey 2015 - 2018

Undergraduate, Bogazici University, Faculty Of Education, Department Of Mathematics And Science Teaching, Turkey 2009 - 2015

### Foreign Languages

English, C2 Mastery

### Dissertations

Doctorate, Atomistic simulations of the amine acetylation reaction and the covalent inhibition of the enzyme phosphoinositide 3-kinase (pi3k), Marmara University, Faculty of Sciences, Department of Chemistry, 2022

Postgraduate, Theoretical investigation of Thiol-ene Click reactions: A DFT perspective, Bogazici University, Institute Of Science, 2018

### Research Areas

Chemistry, Computational Chemistry

### Academic Positions

Research Assistant, Marmara University, Faculty of Arts and Sciences, Chemistry, 2017 - Continues

### Journal articles indexed in SCI, SSCI, and AHCI

- I. **Novel methoxyphenylthio-substituted phthalocyanines: synthesis, characterization, proton-transfer, and acid-sensing properties**  
Ağcaabat R., Seslikaya C., FINDIK V., ERDEM S., ODABAŞ Z.  
New Journal of Chemistry, vol.48, no.4, pp.1623-1633, 2024 (SCI-Expanded)
- II. **New Horizon in Phospha-Michael Reaction: Ultrafast Double Addition of P-H Bond-Bearing Nucleophiles to Electron-Deficient Triple Bonds and Its Use for Functional Monomer Synthesis and Polymer Modification**  
Sagdic G., Daglar O., ÇAKMAKÇI E., FINDIK V., ERDEM S., Tunca Ü., Günay U. S., Durmaz H.  
Macromolecules, vol.56, no.17, pp.7006-7022, 2023 (SCI-Expanded)
- III. **Mechanistic Investigation of Lysine-Targeted Covalent Inhibition of PI3K delta via ONIOM QM:QM Computations**  
FINDIK V., Gercik B. T. V., Sinek O., ERDEM S., Ruiz-Lopez M. F.  
JOURNAL OF CHEMICAL INFORMATION AND MODELING, vol.62, no.24, pp.6775-6787, 2022 (SCI-Expanded)
- IV. **Theoretical Investigation of the Biogenetic Pathway for Formation of Antibacterial Indole Alkaloids from Voacanga africana**  
Soysal E. N., Findik V., Dedeoglu B., AVIYENTE V., Tantillo D. J.  
ACS OMEGA, vol.7, no.35, pp.31591-31596, 2022 (SCI-Expanded)
- V. **Influence of ionic liquids on the electronic environment of atomically dispersed Ir on (MgO)(100)**  
Akgul D., Kurtoglu-oztulum S. F., Zhao Y., FINDIK V., Monari A., Uzun A., AVIYENTE V.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.24, no.18, pp.11305-11314, 2022 (SCI-Expanded)
- VI. **Origins of the photoinitiation capacity of aromatic thiols as photoinitiators: a computational study**  
FINDIK V., Findik B. K., AVIYENTE V., Monari A.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.23, no.42, pp.24377-24385, 2021 (SCI-Expanded)
- VII. **Mechanistic insights into lysine-targeting covalent inhibition through a theoretical study of ester aminolysis**  
FINDIK V., Ruiz-Lopez M. F., ERDEM S.  
ORGANIC & BIOMOLECULAR CHEMISTRY, vol.19, no.45, pp.9996-10004, 2021 (SCI-Expanded)
- VIII. **Insight into the Thiol-yne Kinetics via a Computational Approach**  
FINDIK V., Varınca B. T., DEĞİRMENCİ İ., ERDEM S.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.125, no.17, pp.3556-3568, 2021 (SCI-Expanded)
- IX. **Solvent Effects on Thiol-Ene Kinetics and Reactivity of Carbon and Sulfur Radicals**  
Munar I., FINDIK V., Degirmenci I., Aviyente V.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.124, no.13, pp.2580-2590, 2020 (SCI-Expanded)
- X. **Theoretical investigation of thiol-ene click reactions: A DFT perspective**  
Findik V., Degirmenci I., Catak S., Aviyente V.  
EUROPEAN POLYMER JOURNAL, vol.110, pp.211-220, 2019 (SCI-Expanded)

## Papers Presented at Peer-Reviewed Scientific Conferences

- I. **Theoretical Study on Lysine-Targeting Covalent Inhibition Mechanism in Water and PI3Kd Enzyme**  
Findik V., Erdem S., F. Ruiz-Lopez M.  
Congress on Electronic Structure Principles and Applications, Vigo, Spain, 21 - 24 June 2022, (Summary Text)
- II. **Advanced Atomistic Simulations on Amine Acetylation Reaction in Aqueous Medium**  
Findik V., Erdem S., F. Ruiz-Lopez M.  
LatinXchem, 07 September 2020, pp.1, (Summary Text)
- III. **Tiyil Radikali ve Alkenler Arasında Gerçekleşen Bölgeleşici Halkalaşma Reaksiyonuna Hesapsal Yaklaşım**  
SERT E. M., FINDIK V., ERDEM S.  
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018, (Summary Text)
- IV. **Etakrinik Asit Oksidazol Türevlerinin Glutatifon S-transferaz İnhibisyonu Üzerine Moleküler Doking**

## **Çalışması**

FINDIK V., ERDEM S.

30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018, (Summary Text)

V. **Tiyol-en Tepkimelerinin Bölgeseçici Halkalaşma Reaksiyonuna Hesapsal Bir Yaklaşım**

SİNEK Ö., FINDIK V., ERDEM S.

30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018, (Summary Text)

VI. **Tiyol-in Reaksiyon Mekanizmalarının Teorik Olarak İncelenmesi**

VARINCA B. T., FINDIK V., ERDEM S.

30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018, (Summary Text)

VII. **Molecular Dynamics and Docking Simulations on the Formate Dehydrogenase Enzymes**

FINDIK V., ÇAKAR M. M., ERDEM S., BİNAY B.

1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018, (Summary Text)

VIII. **Theoretical investigation of thiol-ene click reactions: a DFT perspective**

Fındık V., Değirmenci İ., Çatak Ş., Aviyente V.

CHEMISTRY VIA COMPUTATION "Applications on Molecular Nanoscience", İstanbul, Turkey, 30 October 2018, pp.64, (Summary Text)

IX. **Novel Tetrakis 4-(1-(pyridin-4-yl)ethoxyl) Substituted Phthalocyanine Derivatives: Synthesis and DFT/TD-DFT Calculations**

Fındık V., Erdem S., Çavuş A., Özdemir B., Akbal T., Özer M.

11th Congress on Electronic Structure Principles and Applications, Toledo, Spain, 17 - 19 July 2018, pp.1-2, (Summary Text)

X. **Tiyol-Alken Tepkimelerine Hesapsal Bir Yaklaşım**

Fındık V., Değirmenci İ., Çatak Ş., Aviyente V.

29. Ulusal Kimya Kongresi, Ankara, Turkey, 10 - 14 September 2018, pp.1, (Summary Text)

## **Metrics**

Publication: 20

Citation (WoS): 35

Citation (Scopus): 66

H-Index (WoS): 3

H-Index (Scopus): 4

## **Scholarships**

Ortak Denetimli Tez Bursları, Official Institutions of Foreign Countries, 2019 - 2022

Doktora Araştırma Bursu, Official Institutions of Foreign Countries, 2019 - 2019

## **Non Academic Experience**

GlaxoSmithKline, Finans