

## Prof. FATMA SEVİN DÜZ

### Personal Information

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### International Researcher IDs

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Publons / Web Of Science ResearcherID: G-9254-2013

Yoksis Researcher ID: 10901

### Education Information

Doctorate, Hacettepe University, Fen Fakültesi, Kimya, Turkey 1990 - 1995

Postgraduate, Hacettepe University, Fen Bilimleri Enstitüsü, Kimya A.B.D., Turkey 1986 - 1989

Undergraduate, Hacettepe University, Fen Fakültesi, Kimya Bölümü, Turkey 1982 - 1986

### Research Areas

Carbon Chemistry, Photochemistry of Organics, Organic Reaction Mechanisms, Organometallics

### Academic Titles / Tasks

Professor, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2004 - Continues

Professor, Hacettepe University, Fen Bilimleri Enstitüsü, 2012 - 2016

Associate Professor, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 1998 - 2004

Assistant Professor, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 1996 - 1998

### Academic and Administrative Experience

Head of Department, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2020 - Continues

University Executive Board Member, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2013 - 2016

Hacettepe Üniversitesi, Fen Bilimleri Enstitüsü, 2012 - 2016

Fakülte Akademik Kurul Üyesi, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2009 - 2012

Deputy Head of Department, Hacettepe University, Fen Fakültesi, Kimya Bölümü, 2002 - 2005

### Advising Theses

Sevin Düz F., HgY ve AgY zeolitlerine adenin ve timin bazlarının adsorpsiyonunun teorik çalışması, Postgraduate, Ö.KINIK(Student), 2018

Sevin Düz F., Metal iyonlarına duyarlı yeni tasarlanmış ferrosenil tiyazol benzimidazol sensörün teorik olarak

incelenmesi, Postgraduate, M.ALŞAN(Student), 2018

Sevin Düz F., Yeni tasarlanmış ferrosenil üre benzimidazol sensörlerinin metal, redoks ve fotokimyasal özelliklerinin DFT metodu ile incelenmesi, Postgraduate, F.ŞİMŞEK(Student), 2018

SEVİN DÜZ F., Yeni tasarlanan benzimidazol temelli metal-aracılı DNA-baz çiftlerinin floresans özelliklerinden yararlanarak mantık kapılarının dft yöntemi ile teorik incelenmesi, Doctorate, M.ASGHARI(Student), 2016

SEVİN DÜZ F., Theoretical investigation of structural and electronic properties of some transition metal ansa complexes, Doctorate, D.YÜKSEL(Student), 2013

SEVİN DÜZ F., HfCl<sub>4</sub> ile atomik karbon reaksiyonlarının deneysel ve teorik incelenmesi, Postgraduate, H.DİBEK(Student), 2012

SEVİN DÜZ F., Computer aided drug design study of cyclin dependent kinase 2 (CDK2) inhibitors, Doctorate, A.ECE(Student), 2011

SEVİN DÜZ F., Molecular modelling studies of TRPV1 receptor antagonists, Doctorate, T.TAŞKIN(Student), 2010

SEVİN DÜZ F., Karbon ark yöntemi ile tungsten metalofulleren ve türevlerinin deneysel ve teorik incelenmesi, Postgraduate, E.DÜĞME(Student), 2010

SEVİN DÜZ F., An experimental investigation on heavy metal adsorption onto dye-loaded zeolite Y, Doctorate, M.ABDUL(Student), 2009

SEVİN DÜZ F., DÜZ B., Catalytic activity of metal carbenes, synthesized with atomic carbon and tungsten hexachloride (WCl<sub>6</sub>), in olefin metathesis reactions, Postgraduate, D.YÜKSEL(Student), 2007

SEVİN DÜZ F., A theoretical investigation on the adsorption of heavy metals on dye containing zeolite, Doctorate, T.TÜĞSÜZ(Student), 2007

Sevin Düz F., Theoretical investigations of atomic carbon reactions with substituted cyclopentene compounds, Postgraduate, R.YILMAZ(Student), 2005

Sevin Düz F., An experimental and computational investigation of the reaction of atomic carbon generated in carbon arc reactor with aniline, Postgraduate, A.ECE(Student), 2005

Sevin Düz F., Zeolite catalyzed photooxidation of cyclohexane, Postgraduate, İ.SÖKMEN(Student), 2000

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

- I. **Computational insights into bis-N,N-dimethylaniline based D- $\pi$ -A photosensitizers bearing divergent-type of  $\pi$ -linkers for DSSCs**  
NALÇAKAN H., KURTAY G., Sarıkavak K., Şen N., SEVİN DÜZ F.  
Journal of Molecular Graphics and Modelling, vol.122, 2023 (SCI-Expanded)
- II. **Comparative cation sensing properties of a newly designed urea linked ferrocene-benzimidazole dyad: a DFT study**  
Sarıkavak K., Kurtay G., Sevin F.  
JOURNAL OF MOLECULAR MODELING, vol.26, 2020 (SCI-Expanded)
- III. **The discovery of potential cyclin A/CDK2 inhibitors: a combination of 3D QSAR pharmacophore modeling, virtual screening, and molecular docking studies**  
Ece A., Sevin F.  
MEDICINAL CHEMISTRY RESEARCH, vol.22, no.12, pp.5832-5843, 2013 (SCI-Expanded)
- IV. **QSAR and docking studies of inhibition activity of 5,6-dihydro 11-alkylbenzo[alpha]carbazole derivatives against estrogen receptor**  
Taskin T., Sevin F.  
TURKISH JOURNAL OF CHEMISTRY, vol.35, no.3, pp.481-498, 2011 (SCI-Expanded)
- V. **Exploring QSAR on 4-cyclohexylmethoxyppyrimidines as antitumor agents for their inhibitory activity of CDK2**  
Ece A., Sevin F.  
Letters in Drug Design and Discovery, vol.7, no.9, pp.625-631, 2010 (SCI-Expanded)
- VI. **Diastereoselective control through hydrogen bonding in the aziridination of the chiral allylic alcohols by acetoxyaminoquinazolinone**

ÇAKICI M., Karabuga S., KILIÇ H., Ulukanli S., ŞAHİN E., Sevin F.

Journal of Organic Chemistry, vol.74, no.24, pp.9452-9459, 2009 (SCI-Expanded)

- VII. **QSAR approach to correlate TRPV1 antagonist activity for a series of heteroaromatic urea**  
Taskin T., Sevin F.  
QSAR and Combinatorial Science, vol.28, no.10, pp.1098-1111, 2009 (SCI-Expanded)
- VIII. **Reaction of atomic carbon with isomeric cresols**  
Sökmen I., Ece A., DÜZ B., Sevin F.  
Letters in Organic Chemistry, vol.6, no.8, pp.650-653, 2009 (SCI-Expanded)
- IX. **Application of carbon arc-generated Mo and W-based catalyst systems to the ROMP of norbornene**  
DÜZ B., Elbistan C. K., Ece A., Sevin F.  
Applied Organometallic Chemistry, vol.23, no.9, pp.359-364, 2009 (SCI-Expanded)
- X. **DFT study of the 1-octene metathesis reaction mechanism with WC16/C catalytic system**  
YÜKSEL D., DÜZ B., SEVIN F.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.112, no.20, pp.4636-4643, 2008 (SCI-Expanded)
- XI. **Theoretical investigation on chemical and biochemical activities of 5,6-dihydro-11H-benzo[α]carbazole and its derivatives**  
Taskin T., Sevin F.  
Journal of Molecular Structure: THEOCHEM, vol.803, pp.61-66, 2007 (SCI-Expanded)
- XII. **A DFT study on the structures and absorption spectra of the M-1-nitroso-2-naphthol complexes (M = Ni, Cu, Cr, Cd, Pb)**  
Tüğsüz T., Sevin F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.775, pp.29-37, 2006 (SCI-Expanded)
- XIII. **The first example of tungsten-based carbene generation from WC1(6) and atomic carbon and its use in olefin metathesis**  
Duz B., Yuksel D., Ece A., Sevin F.  
TETRAHEDRON LETTERS, vol.47, no.29, pp.5167-5170, 2006 (SCI-Expanded)
- XIV. **A theoretical study on the location of Ni2+, Cu2+, Cr2+, Cd2+ and Pb2+ in zeolite Y**  
Tüğsüz T., Doğan M., Sevin F.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.728, pp.103-109, 2005 (SCI-Expanded)
- XV. **A Computational Investigation of the Reactions of Methylene, Chlorocarbene, and Dichlorocarbene with Cyclopropane**  
Sevin F., McKee M. L., Shevlin P. B.  
Journal of Organic Chemistry, vol.69, no.2, pp.382-386, 2004 (SCI-Expanded)
- XVI. **Theoretical investigation of intramolecular trapping of strain allene: Endo-bicyclo[3.2.1]octa-2,3-dien-6-ol**  
Sevin F., Doğan M.  
Journal of Molecular Structure, pp.265-270, 2003 (SCI-Expanded)
- XVII. **Oxidation of cyclohexane catalyzed by metal-ion-exchanged zeolites**  
Sökmen I., Sevin F.  
Journal of Colloid and Interface Science, vol.264, no.1, pp.208-211, 2003 (SCI-Expanded)
- XVIII. **The effect of the proton on electropolymerization of the thiophene**  
Can M., Sevin F., Yildiz A.  
Applied Surface Science, vol.210, pp.338-345, 2003 (SCI-Expanded)
- XIX. **Trapping of a cycloheptatetraene in the reaction of atomic carbon with phenol**  
Sevin F., Sökmen I., DÜZ B., Shevlin P. B.  
Tetrahedron Letters, vol.44, no.16, pp.3405-3407, 2003 (SCI-Expanded)
- XX. **Reactions of 1,3-cyclohexadiene with singlet oxygen. A theoretical study**  
Sevin F., McKee M.  
Journal of the American Chemical Society, vol.123, no.19, pp.4591-4600, 2001 (SCI-Expanded)
- XXI. **Density functional calculations of methyl lithium, t-butyl lithium, and phenyllithium oligomers: Effect of hyperconjugation on conformation**

Kwon O., Sevin F., McKee M. L.

Journal of Physical Chemistry A, vol.105, no.5, pp.913-922, 2001 (SCI-Expanded)

- XXII. **A comparative semiempirical, ab initio and DFT study of decarbonylation of cyclic ketones part 1: Thermal fragmentation of cyclopropanone**

Balcioglu N., Sevin F.

JOURNAL OF MOLECULAR MODELING, vol.6, no.2, pp.48-54, 2000 (SCI-Expanded)

- XXIII. **Reaction mechanism of copper(I) catalysed head-to-head dimerization of 1-alkynes: An experimental and theoretical study**

Balcioglu N., Uraz I., Bozkurt C., Sevin F.

Polyhedron, vol.16, no.2, pp.327-334, 1997 (SCI-Expanded)

- XXIV. **Effect of alkyl groups on carbanion stability Part I. Interaction of small rings with adjacent carbanion centers**

Baleioglu N., Sevin F., Evin O. O., Peynircioglu N.

Berichte der Bunsengesellschaft/Physical Chemistry Chemical Physics, vol.96, no.2, pp.139-142, 1992 (SCI-Expanded)

## Articles Published in Other Journals

- I. **The Effect of Alkyl Groups on Carbanion Stability Part II. Analysis of  $\alpha$ -  $\beta$ -Alkyl Substitution on Experimental and Theoretical Acidities**

Balcioglu N., Sevin F., Evin Ö., Bekir Peynircioglu N.

Berichte der Bunsengesellschaft/Physical Chemistry Chemical Physics, vol.100, no.10, pp.1723-1728, 1996 (Scopus)

## Books & Book Chapters

- I. **KİMYA 2. CİLT (7. basımdan çeviri)**

GÜVEN A., YUSUFOĞLU A., UYANIK C., SEVİN DÜZ F., ARTOK L., KÖSE M., GÜLLÜ M., CANER N., YILDIRIM K., KÖKEN N., et al.

LİTERATÜR YAYINLARI, İstanbul, 2020

- II. **KİMYA 1. CİLT (7. basımdan çeviri)**

GÜVEN A., YUSUFOĞLU A., UYANIK C., SEVİN DÜZ F., ARTOK L., KÖSE M., GÜLLÜ M., CANER N., YILDIRIM K., KÖKEN N., et al.

LİTERATÜR YAYINLARI, İstanbul, 2017

- III. **Kovalent Bağ veElektron-NoktaYapıları**

SEVİN DÜZ F., GÜVEN A., ARTOK L., CANER N., GÜLLÜ M., KARAGÖLGE Z., KÖKEN N., KÖSE M., UYANIK C., YILDIRIM K., et al.

in: Kimya : Cilt-1, prof.dr. Cavit Uyanık, Editor, literatür yayıncılık, İstanbul, pp.1-32, 2017

- IV. **Organik Kimya**

SEVİN DÜZ F., UYANIK C., YUSUFOĞLU A. S., TÜLÜ M., ÖCAL SUNGURUĞLU Z. N., NEBİOĞLU M., GÜVEN A., GÜLLÜ M., DEMİRCAN A., bilgiç s., et al.

Literatür, İstanbul, 2016

- V. **ORGANİK KİMYA, YAPI VE İŞLEV, ÇALIŞMA VE PROBLEM ÇÖZÜMLERİ EL KİTABI**

SEVİN DÜZ F., UYAR T.

PALME YAYINCILIK, 2014

- VI. **TERMOKİMYA**

Sevin Düz F.

in: GENEL KİMYA, İlkeler ve Modern Uygulamalar, CİLT 1, TAHSİN UYAR,SERPİL AKSOY,RECAİ İNAM, Editor, Palme Yayın Dağıtım, Ankara, pp.402-654, 2012

## VII. KİMYASAL KİNETİK

Sevin Düz F.

in: GENEL KİMYA, İlkeler ve Uygulamalar, Cilt 2, TAHSİN UYAR,SERPİL AKSOY,RECAİ İNAM, Editor, Palme Yayın Dağıtım, Ankara, pp.602-654, 2012

## VIII. ORGANİK KİMYA , YAPI VE İŞLEV

UYAR T., SEVİN DÜZ F.

Palme Yayıncılık, 2011

## Refereed Congress / Symposium Publications in Proceedings

- I. **Uranil İyonuna Duyarlı Yeni Tasarlanmış DO3A-Tabanlı Boronik Asit Türevlerinin Yapısal ve Spektral (IR ,NMR ve UV-vis) Özelliklerinin Teorik Olarak İncelenmesi**  
SEVİN DÜZ F., Sarıkavak K.  
3. Hesaplamalı Kimya Kongresi, Ankara, Turkey, 12 - 14 October 2017, vol.1, pp.1-53
- II. **Synthesis and Theoretical Study of Dihydrocarbazole and Its Derivatives**  
UZGÖREN BARAN A., ERGÜN M. Y., TAŞKIN TOK T., SEVİN DÜZ F., OKAY G.  
International Symposium on Medicinal Chemistry Research and Development 2005 (MCRD2005), KUŞADASI, Turkey, 28 September - 01 October 2005

## Supported Projects

SEVİN DÜZ F., KINIK Ö., SARIKAVAK K., Project Supported by Higher Education Institutions, HgY ve AgY Zeolitlerinin DNA Baz Çiftleri ile Etkileşimlerinin Teorik İncelenmesi, 2017 - 2017

Sevin Düz F., TUBITAK Project, URANİL İYONUNA DUYARLI RNA BAĞLANMIŞ DOTA-TEMELLİ PEPTİT BAĞ İÇEREN BORONİK ASİT TÜREVLERİNİN YAPISAL VE SPEKTROSKOPİK ÖZELLİKLERİNİN TEORİK OLARAK İNCELENMESİ, 2015 - 2017

Sevin Düz F., Project Supported by Higher Education Institutions, TORYUM IV KATYONU İLE DOTA KOMPLEKSLERİNİN SULU ORTAMDA DENGELİLİKLERİNİN VE SPEKTROSKOPİK ÖZELLİKLERİNİN HESAPSAL İNCELENMESİ, 2015 - 2016

SEVİN DÜZ F., TUBITAK Project, Yeni Tasarlanan Benzimidazol Temelli Metal Aracılı Dna Baz Çiftlerinin Floresans Özelliklerinden Yararlanarak Mantık Kapılarının Dft Yöntemi İle Teorik İncelenmesi, 2014 - 2016

SEVİN DÜZ F., Project Supported by Higher Education Institutions, 3D QSAR Farmakofor Modelleme Sanal Tarama ve Moleküler Yerleştirme Çalışmalarıyla Birlikte Potansiyel Siklin ACCK2 İnhibitorlerin Keşfi, 2015 - 2015

Sevin Düz F., TUBITAK Project, Karbon Ark Yöntemi İle Tungsten Metalofulleren Ve Türevlerinin Deneysel İncelenmesi, 2009 - 2009

Sevin Düz F., TUBITAK Project, TRPV1 Reseptör Antagonistlerinin Moleküler Modelleme Çalışmaları, 2007 - 2008

Sevin Düz F., TUBITAK Project, Karbon ARC reaktöründe oluşturulan atomik karbon ile anilin reaksiyonunun incelenmesi, 2004 - 2005

Sevin Düz F., TUBITAK Project, Atomik Karbonun Fenol ve Nanbornen ile Reaksiyonları, 2002 - 2004

Sevin Düz F., TUBITAK Project, Investigation of the Chemistry of Carbon Vapor, 2001 - 2002

Sevin Düz F., TUBITAK Project, Alkilliyum Agregatlarının Yapısı ve Sübstitüent Etkisi, 1996 - 1999

## Metrics

Publication: 35

Citation (WoS): 302

Citation (Scopus): 306

H-Index (WoS): 10

H-Index (Scopus): 10

### **Non Academic Experience**

Hacettepe Üniv. kimya böl.

Hacettepe Üniv. kimya böl.

Hacettepe Üniv. kimya böl.

Hacettepe Üniv. kimya böl.