

# **Prof. Selçuk Gümüş**

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## **International Researcher IDs**

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## **Education Information**

Doctorate, Middle East Technical University, Fen Edebiyat Fakültesi, Kimya / Organik Kimya, Turkey 2002 - 2009  
Undergraduate, Middle East Technical University, Fen Edebiyat Fakültesi, Kimya Bölümü, Turkey 1995 - 2000

## **Foreign Languages**

English, C1 Advanced

## **Research Areas**

Chemistry, Organic Chemistry, Chemistry of Aromatic Compounds, Chemistry of Dyes and Pigments, Organic Reaction Mechanisms, Organic Spectroscopy, Organometallics, Natural Sciences

## **Academic Titles / Tasks**

Professor, Van Yüzüncü Yıl University, Fen Fakültesi, Kimya Bölümü, 2018 - Continues

Associate Professor, Van Yüzüncü Yıl University, Fen Fakültesi, Kimya Bölümü, 2013 - 2018

Assistant Professor, Van Yüzüncü Yıl University, Fen Fakültesi, Kimya Bölümü, 2010 - 2013

Research Assistant PhD, Van Yüzüncü Yıl University, Fen Fakültesi, Kimya Bölümü, 2010 - 2010

Research Assistant, Middle East Technical University, Fen Edebiyat Fakültesi, Kimya, 2000 - 2010

## **Academic and Administrative Experience**

Van Yüzüncü Yıl University, 2019 - Continues

Van Yüzüncü Yıl University, Araştırma-Geliştirme Alt Komisyonu Başkanı, 2019 - Continues

Van Yüzüncü Yıl University, Bilim Uygulama Ve Araştırma Merkezi Yönetim Kurulu Başkanı, 2018 - Continues

Van Yüzüncü Yıl University, 2018 - Continues

## **Advising Theses**

Gümüş S., YENİ MONO VE BİS-TRİAZOL TÜREVLERİNİN SENTEZİ VE HESAPSAL KİMYA UYGULAMALARI, Doctorate, N.Karakoyun(Student), 2018

Gümüş S., Mono ve Diazaantrasen Türevlerinin Aromatikliğinin İncelenmesi, Postgraduate, A.Köle(Student), 2018

Gümüş S., TRİ VE TETRAAZANAFTALİN TÜREVLERİNİN AROMATİKLİĞİNİN İNCELENMESİ, Postgraduate, M.AVCI(Student), 2016

Gümüş S., Çevre Dostu Enerjetik Materyallerin Dekompozisyon Mekanizmalarının Teorik Olarak İncelenmesi, Postgraduate, R.UYGUR(Student), 2016

Gümüş S., 1,3,5-TRİAZİN TABANLI ORGANİK ELEKTROLUMİNESANT MOLEKÜLLERİN ELEKTRONK ÖZELLİKLERİİNİN BELİRLENMESİ, Postgraduate, E.ARVAS(Student), 2014

Gümüş S., CLICK TPKİMESİ MEKANİZMASININ TEORİK OLARAK İNCELENMESİ, Doctorate, Z.Şilan(Student), 2014

## Jury Memberships

Doctorate, Doktora tez savunması, Atatürk Üniversitesi, September, 2018

Post Graduate, Tez Savunma, Van Yüzüncü Yıl Üniversitesi, December, 2017

Post Graduate, Tez Savunma Jürisi, YÜZÜNCÜ YIL ÜNİVERSİTESİ, May, 2016

Post Graduate, Tez Savunma Jürisi, ATATÜRK ÜNİVERSİTESİ, May, 2015

Post Graduate, Tez Savunma Jürisi, YÜZÜNCÜ YIL ÜNİVERSİTESİ, January, 2014

Post Graduate, Tez Savunma Jürisi, YÜZÜNCÜ YIL ÜNİVERSİTESİ, April, 2013

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

- I. **Supramolecular Arrangement and DFT analysis of Zinc(II) Schiff Bases: An Insight towards the Influence of Compartmental Ligands on Binding Interaction with Protein**  
Chowdhury M. S., Gumus S., Dasgupta S., Majumder I., Bhattacharya A., Das D., Mukhopadhyay J., Bose D., Dasgupta S., Akinay Y., et al.  
CHEMISTRYOPEN, vol.11, no.6, pp.1-11, 2022 (SCI-Expanded)
- II. **Effects of asymmetric acceptor and donor positioning in deep blue pyridyl-sulfonyl based TADF emitters**  
Haykır G., Aydemir M., Danos A., Gümüş S., Hızal G., Monkman A. P., Türksoy F.  
DYES AND PIGMENTS, vol.194, pp.109579-109594, 2021 (SCI-Expanded)
- III. **Synthesis, biological evaluation of antioxidant-antibacterial activities and computational studies of novel anthracene- and pyrene-based Schiff base derivatives**  
GÜMÜŞ A., OKUMUŞ V., GÜMÜŞ S.  
Turkish Journal Of Chemistry, vol.44, pp.1200-1215, 2020 (SCI-Expanded)
- IV. **NOVEL PYRAZOLE-CENTERED DERIVATIVES HAVING MONO/DI CHIRAL CENTERED GROUP AS ORGANOCATALYST FOR HENRY REACTION**  
Cetin A., Bildirici İ., Gümüş S.  
MACEDONIAN JOURNAL OF CHEMISTRY AND CHEMICAL ENGINEERING, vol.39, no.1, pp.17-30, 2020 (SCI-Expanded)
- V. **INVESTIGATION OF TADF PROPERTIES OF NOVEL DONOR-ACCEPTOR TYPE PYRAZINE DERIVATIVES**  
İRAK Z. Ş. T., Gümüş A., Gümüş S.  
JOURNAL OF THE CHILEAN CHEMICAL SOCIETY, vol.64, no.1, pp.4303-4309, 2019 (SCI-Expanded)
- VI. **The solvatochromism and electronic structure of (E)-2-(2-hydroxystyryl)quinolin-8-ol**  
Gümüş A., Gulseven Sidir Y., SIDIR İ., Gümüş S.  
TURKISH JOURNAL OF CHEMISTRY, vol.43, no.6, pp.1503-1521, 2019 (SCI-Expanded)
- VII. **Synthesis, Characterization, DFT Studies, and Photodiode Application of Azo-azomethine-Based Ligand and Its Transition-Metal Complexes**  
Tombak A., İmer A. G., Syan R. H. B., Gülcancı M., Gümüş S., OCAK Y. S.

- JOURNAL OF ELECTRONIC MATERIALS, vol.47, no.12, pp.7240-7250, 2018 (SCI-Expanded)
- VIII. **SYNTHESIS, SOLVATOCHROMISM, ELECTRONIC STRUCTURE AND NONLINEAR OPTIC PROPERTIES OF QUINOLIN-8-YL-2-HYDROXYBENZOATE**  
Gümüş A., Gülseven Sidir Y., Sidir İ., Gümüş S.  
MACEDONIAN JOURNAL OF CHEMISTRY AND CHEMICAL ENGINEERING, vol.37, no.2, pp.145-158, 2018 (SCI-Expanded)
- IX. **The investigation of sky-blue emitting anthracene-carbazole derivatives: Synthesis, photophysics and OLED applications**  
Haykir G., AYDEMİR M., Han S. H., Gümüş S., Hızal G., Lee J. Y., Turksoy F.  
ORGANIC ELECTRONICS, vol.59, pp.319-329, 2018 (SCI-Expanded)
- X. **SYNTHESIS, SOLVATOCHROMISM, ELECTRONIC STRUCTURE AND NONLINEAR OPTIC PROPERTIES OF QUINOLIN-8-YL 2-HYDROXYBENZOATE**  
Gümüş A., SIDIR Y. G., SIDIR İ., Gümüş S.  
MACEDONIAN JOURNAL OF CHEMISTRY AND CHEMICAL ENGINEERING, vol.37, no.2, pp.145-158, 2018 (SCI-Expanded)
- XI. **Synthesis of bis(thiosemicarbazone) derivatives: Definition, crystal structure, biological potential and computational analysis**  
Ates D., Gulcan M., Gumus S., Sekerci M., Ozdemir S., Sahin E., Colak N.  
PHOSPHORUS SULFUR AND SILICON AND THE RELATED ELEMENTS, vol.193, no.1, pp.14-22, 2018 (SCI-Expanded)
- XII. **Synthesis of 2-substituted 8-propargyloxyquinoline derivatives and determination of their antioxidant, antibacterial, and DNA binding activities**  
Gümüş A., OKUMUŞ V., Gümüş S.  
TURKISH JOURNAL OF CHEMISTRY, vol.42, no.5, pp.1358-1369, 2018 (SCI-Expanded)
- XIII. **Synthesis and antioxidant, aggregation, and electronic properties of 6-tert-butyl-1,4-benzodioxine substituted phthalocyanines**  
Ağırtaş M. S., Cabir B., Gümüş S., Ozdemir S., Dundar A.  
TURKISH JOURNAL OF CHEMISTRY, vol.42, no.1, pp.100-111, 2018 (SCI-Expanded)
- XIV. **SYNTHESIS AND COMPUTATIONAL CALCULATIONS OF NOVEL CHIRAL BIS-1,2,3-TRIAZOLE DERIVATIVES**  
Gümüş A., Gümüş S.  
MAEJO INTERNATIONAL JOURNAL OF SCIENCE AND TECHNOLOGY, vol.3, no.2, pp.165-176, 2017 (SCI-Expanded)
- XV. **INVESTIGATION OF AROMATICITY OF TRI AND TETRAAZANAPHTHALENE DERIVATIVES**  
Gümüş S., Gümüş A., Avcı M.  
MAEJO INTERNATIONAL JOURNAL OF SCIENCE AND TECHNOLOGY, vol.3, no.2, pp.177-192, 2017 (SCI-Expanded)
- XVI. **SYNTHESIS AND COMPUTATIONAL CALCULATIONS OF NOVEL CHIRAL BIS-1,2,3-TRIAZOLE DERIVATIVES**  
Gümüş A., Gümüş S.  
MAEJO INTERNATIONAL JOURNAL OF SCIENCE AND TECHNOLOGY, vol.3, no.2, pp.165-176, 2017 (SCI-Expanded)
- XVII. **Design, stereoselective synthesis and computational calculations of novel hybrid compounds via Pauson-Khand reactions**  
Gümüş S., Aslan N., Buyukadali N. N., Gümüş A.  
TETRAHEDRON-ASYMMETRY, vol.28, no.3, pp.479-484, 2017 (SCI-Expanded)
- XVIII. **A COMPUTATIONAL STUDY ON A SERIES OF PHENANTHRENE AND PHENANTHROLINE BASED POTENTIAL ORGANIC PHOTOVOLTAICS**  
Gümüş A., Gümüş S.  
MACEDONIAN JOURNAL OF CHEMISTRY AND CHEMICAL ENGINEERING, vol.36, no.2, pp.239-249, 2017 (SCI-Expanded)
- XIX. **Stereoselective synthesis of benzofuran and benzothiophene substituted dihydropyran derivatives via ring closing metathesis**  
Buyukadali N. N., Aslan N., Gümüş S., Gümüş A.

- TETRAHEDRON-ASYMMETRY, vol.27, no.19, pp.954-959, 2016 (SCI-Expanded)
- XX. **Hydroxyl group effect in novel NNN type pyridine based ruthenium (II) complex for the transfer hydrogenation of ketones**  
Sahin I., Emir S., İSPİR E., Karakaya I., Gümüş S., Ulusoy M., KARABUĞA Ş.  
CATALYSIS COMMUNICATIONS, vol.85, pp.30-33, 2016 (SCI-Expanded)
- XXI. **Synthesis of metallophthalocyanines with four oxy-2,2-diphenylacetic acid substituents and their structural and electronic properties**  
Abdalrazaq S. M., Cabir B., Gümüş S., Ağırtaş M. S.  
HETEROCYCLIC COMMUNICATIONS, vol.22, no.5, pp.275-280, 2016 (SCI-Expanded)
- XXII. **Isoquinoline-substituted triazole and pyran derivatives: synthesis and computational studies**  
Yenidede D., Gümüş S., Gümüş A.  
TURKISH JOURNAL OF CHEMISTRY, vol.40, no.4, pp.655-666, 2016 (SCI-Expanded)
- XXIII. **Synthesis, Aggregation Behavior, and Electronic Properties of some Metallophthalocyanines with 2-Isopropyl-5-methylphenoxy Substituents**  
Ağırtaş M. S., KARATAS C., Gümüş S.  
ZEITSCHRIFT FÜR ANORGANISCHE UND ALLGEMEINE CHEMIE, vol.641, no.7, pp.1334-1339, 2015 (SCI-Expanded)
- XXIV. **Synthesis of Some Novel Phthalocyanines with Methyl 2-(oxy)-2,2-diphenylacetate Substituents, Evaluation of Their Antioxidant- Antibacterial Activities and Electronic Properties**  
Ağırtaş M. S., KARATAS C., Gümüş S., Okumus V.  
ZEITSCHRIFT FÜR ANORGANISCHE UND ALLGEMEINE CHEMIE, vol.641, no.2, pp.442-447, 2015 (SCI-Expanded)
- XXV. **Efficient transfer hydrogenation reactions with quinazoline-based ruthenium complexes**  
Karabuga S., Bars S., Karakaya I., Gümüş S.  
TETRAHEDRON LETTERS, vol.56, no.1, pp.101-104, 2015 (SCI-Expanded)
- XXVI. **Synthesis and investigation of intra-molecular charge transfer state properties of novel donor-acceptor-donor pyridine derivatives: the effects of temperature and environment on molecular configurations and the origin of delayed fluorescence**  
Aydemir M., HAYKIR G., TURKSOY F., Gümüş S., Dias F. B., Monkman A. P.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS, vol.17, no.38, pp.25572-25582, 2015 (SCI-Expanded)
- XXVII. **Metallo and metal free phthalocyanines bearing (4-(1(4-phenoxyphenyl)-1-phenylethyl)phenol substituents: Synthesis, characterization, aggregation behavior, electronic, antioxidant and antibacterial properties**  
Ağırtaş M. S., GUVEN M. E., Gümüş S., Ozdemir S., Dundar A.  
SYNTHETIC METALS, vol.195, pp.177-184, 2014 (SCI-Expanded)
- XXVIII. **Metallo Phthalocyanines bearing 2-Isopropyl-6-methylpyrimidin-4-yloxy Substituents: Synthesis, Characterization, Aggregation Behavior, Antioxidant and Antibacterial Activity, and Electronic Properties**  
Ağırtaş M. S., DEDE E., Gümüş S., Dundar A., Okumus V.  
ZEITSCHRIFT FÜR ANORGANISCHE UND ALLGEMEINE CHEMIE, vol.640, no.10, pp.1953-1959, 2014 (SCI-Expanded)
- XXIX. **TG Index, its Graphical Matrix Representation and Application on Polyenes**  
Gümüş S., Turker L.  
BULLETIN OF THE KOREAN CHEMICAL SOCIETY, vol.35, no.5, pp.1413-1416, 2014 (SCI-Expanded)
- XXX. **New water soluble phenoxy phenyl diazenyl benzoic acid substituted phthalocyanine derivatives: Synthesis, antioxidant activities, atypical aggregation behavior and electronic properties**  
Ağırtaş M. S., Çelebi M., Gümüş S., Ozdemir S., Okumus V.  
DYES AND PIGMENTS, vol.99, no.2, pp.423-431, 2013 (SCI-Expanded)
- XXXI. **A Computational Study on Substituted and Unsubstituted Mono and Diazaanthracenes**  
Gümüş S., AKBAY M.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.33, no.5, pp.519-532, 2013 (SCI-Expanded)
- XXXII. **A computational study on azaazulenes**

- Gumus S.  
HETEROCYCLIC COMMUNICATIONS, vol.19, no.5, pp.369-373, 2013 (SCI-Expanded)
- XXXIII. **Synthesis, Characterization, and Theoretical Studies on Some Metallophthalocyanines With Octakis Phenoxyacetamide Substituents**  
Ağırtaş M. S., Gümüş S.  
SYNTHESIS AND REACTIVITY IN INORGANIC METAL-ORGANIC AND NANO-METAL CHEMISTRY, vol.43, no.5, pp.628-634, 2013 (SCI-Expanded)
- XXXIV. **Computational Study on All Possible Diamino-Dinitropyrimidines and Their Mono- and Dioxide Derivatives**  
Gumus S., ATALAR T.  
JOURNAL OF ENERGETIC MATERIALS, vol.30, no.4, pp.335-357, 2012 (SCI-Expanded)
- XXXV. **Substituent effect on the aromaticity of 1,3-azole systems**  
Gümüş S., Turker L.  
HETEROCYCLIC COMMUNICATIONS, vol.18, no.1, pp.11-16, 2012 (SCI-Expanded)
- XXXVI. **OH Radical Reactions with Nitroimidazole and Nitrotriazole Derivatives**  
Gumus S.  
JOURNAL OF ENERGETIC MATERIALS, vol.30, no.2, pp.156-168, 2012 (SCI-Expanded)
- XXXVII. **Isomeric Structures of Furoxan-Fused [2,2]paracyclophane-A DFT Study**  
Turker L., Gümüş S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.32, no.4, pp.487-502, 2012 (SCI-Expanded)
- XXXVIII. **A novel molecular descriptor, TG index, for calculating the detonation properties of explosives**  
Turker L., Gümüş S.  
INDIAN JOURNAL OF CHEMISTRY SECTION A-INORGANIC BIO-INORGANIC PHYSICAL THEORETICAL & ANALYTICAL CHEMISTRY, vol.50, no.2, pp.141-148, 2011 (SCI-Expanded)
- XXXIX. **The aromaticity of substituted diazanaphthalenes**  
Gumus S.  
COMPUTATIONAL AND THEORETICAL CHEMISTRY, vol.963, pp.263-267, 2011 (SCI-Expanded)
- XL. **A computational study on substituted diazabenzenes**  
Gumus S.  
TURKISH JOURNAL OF CHEMISTRY, vol.35, no.5, pp.803-808, 2011 (SCI-Expanded)
- XLI. **Synthesis of Some Novel Pyrimidine Derivatives and Investigation of their Electrochemical Behavior**  
Akbaş E., Levent A., Gümüş S., SUMER M. R., AKYAZI I.  
BULLETIN OF THE KOREAN CHEMICAL SOCIETY, vol.31, no.12, pp.3632-3638, 2010 (SCI-Expanded)
- XLII. **Studies on the Different Reaction Pathways between 3-Acetyl-5-benzoyl-6-methyl-2-phenyl-4H-pyran-4-one and Alkylamines**  
Genç H., Tan M., Gümüş S., Menges N., Bildirici İ., ŞENER A.  
BULLETIN OF THE KOREAN CHEMICAL SOCIETY, vol.31, no.9, pp.2633-2636, 2010 (SCI-Expanded)
- XLIII. **Structural and Molecular Orbital Studies of Si-Phenyl Silaanthracenes**  
Turker L., Gumus S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.30, no.2, pp.61-74, 2010 (SCI-Expanded)
- XLIV. **A DFT Study on Nitro Derivatives of Pyridine**  
Turker L., Gumus S., Atalar T.  
JOURNAL OF ENERGETIC MATERIALS, vol.28, no.2, pp.139-171, 2010 (SCI-Expanded)
- XLV. **Biocatalytic carboxylation**  
GLUECK S. M., Guemues S., FABIAN W. M. F., FABER K.  
CHEMICAL SOCIETY REVIEWS, vol.39, no.1, pp.313-328, 2010 (SCI-Expanded)
- XLVI. **Structural and Molecular Orbital Properties of Some Boroxine Derivatives-A Theoretical Study**  
Türker L., Gümüş S., Atalar T.  
BULLETIN OF THE KOREAN CHEMICAL SOCIETY, vol.30, no.10, pp.2233-2239, 2009 (SCI-Expanded)
- XLVII. **A DFT study on nitrotriazines**  
Turker L., Atalar T., Gumus S., Camur Y.

- JOURNAL OF HAZARDOUS MATERIALS, vol.167, pp.440-448, 2009 (SCI-Expanded)
- XLVIII. **A theoretical study on vomitoxin and its tautomers**  
Turker L., Guemues S.  
JOURNAL OF HAZARDOUS MATERIALS, vol.163, no.1, pp.285-294, 2009 (SCI-Expanded)
- XLIX. **1,3-Dipolar Cycloaddition Reactions of 1-Methyl-3-Oxidopyridinium Betaine with C-70-A Theoretical Study**  
Turker L., Gumus S.  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE, vol.6, no.4, pp.873-879, 2009 (SCI-Expanded)
- L. **ELECTROLUMINESCENT PROPERTIES OF CERTAIN POLYAROMATIC COMPOUNDS: PART 1-CHARACTERISTICS OF OLED DEVICES BASED ON FLUORESCENT POLYAROMATIC DOPANTS**  
Turker L., Tapan A., Gumus S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.29, no.3, pp.123-138, 2009 (SCI-Expanded)
- LI. **ELECTROLUMINESCENT PROPERTIES OF CERTAIN POLYAROMATIC COMPOUNDS: PART 2-ORGANIC EMITTERS**  
Turker L., Tapan A., Gumus S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.29, no.3, pp.139-159, 2009 (SCI-Expanded)
- LII. **DFT Studies on eta(6)-Coronene-Cr(CO)(3) Complexes**  
Turker L., Guemues S.  
ACTA CHIMICA SLOVENICA, vol.56, no.1, pp.246-253, 2009 (SCI-Expanded)
- LIII. **COMPUTATIONAL STUDIES ON NOVEL ENERGETIC MATERIALS: TETRANITRO-[2,2]PARACYCLOPHANES**  
Turker L., Atalar T., Guemues S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.29, no.5, pp.289-314, 2009 (SCI-Expanded)
- LIV. **A THEORETICAL STUDY ON SOME (1,4)CYCLOPHANES**  
Turker L., Gumus S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.29, no.2, pp.103-122, 2009 (SCI-Expanded)
- LV. **Biohydrogen production: molecular aspects**  
Turker L., Gumus S., Tapan A.  
JOURNAL OF SCIENTIFIC & INDUSTRIAL RESEARCH, vol.67, no.11, pp.994-1016, 2008 (SCI-Expanded)
- LVI. **Quantum chemical treatment of nivalenol and its tautomers**  
Turker L., Gumus S.  
JOURNAL OF HAZARDOUS MATERIALS, vol.153, pp.329-339, 2008 (SCI-Expanded)
- LVII. **Positional effect of nitrogen substitution on a certain perylene chromophore - A semiempirical treatment**  
Turker L., Gumus S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.28, no.1, pp.4-14, 2008 (SCI-Expanded)
- LVIII. **Ab initio and dft studies on certain eta(6)-Anthraquinone-Cr(CO)(3) complexes**  
Turker L., Gumus S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.28, no.3, pp.181-192, 2008 (SCI-Expanded)
- LIX. **A theoretical study on nitrourea and its tautomers**  
Turker L., Gumus S., Atalar T., Atlanel S.  
JOURNAL OF ENERGETIC MATERIALS, vol.26, no.3, pp.181-195, 2008 (SCI-Expanded)
- LX. **Molecular orbital treatment of some endohedrally doped C-60 systems**  
Türker L., Gumus S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.26, no.2, pp.145-162, 2006 (SCI-Expanded)
- LXI. **AM1, MNDO and MINDO/3 treatments of Huckel type cyclacenes**  
Turker L., Guemues S.  
POLYCYCLIC AROMATIC COMPOUNDS, vol.26, no.5, pp.367-384, 2006 (SCI-Expanded)
- LXII. **Hydrogen storage capacity of Mg@C-120 system**  
Türker L., Gumus S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.719, pp.103-107, 2005 (SCI-Expanded)

- LXIII. **Peripherally B and N substituted cyclacenes**  
 Türker L., Gumus S.  
 JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.686, pp.91-95, 2004 (SCI-Expanded)
- LXIV. **Cyclacenes**  
 Türker L., Gumus S.  
 JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.685, pp.1-33, 2004 (SCI-Expanded)
- LXV. **A quire behavior of (Li+nH(2))@C-58 systems - an AM 1 treatment**  
 Türker L., Gumus S.  
 JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.684, pp.205-209, 2004 (SCI-Expanded)
- LXVI. **AM 1 treatment of endohedrally hydrogen doped C-56 systems, nH(2)@C-56**  
 Türker L., Gumus S.  
 JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.681, pp.21-25, 2004 (SCI-Expanded)
- LXVII. **Mono, B, N, Si, or Ge substituted cyclacenes. A theoretical study**  
 Türker L., Gumus S.  
 JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.679, no.3, pp.143-147, 2004 (SCI-Expanded)
- LXVIII. **An AM1 study on C-60@C-180 system**  
 Türker L., Gumus S.  
 JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.674, pp.15-18, 2004 (SCI-Expanded)
- LXIX. **Cyclacenes having mono boron or nitrogen atom in the backbone - a theoretical study**  
 Türker L., Gumus S.  
 JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.674, pp.185-189, 2004 (SCI-Expanded)

### Articles Published in Other Journals

- I. **Investigation of the aromaticity of mono, di, tri and tetraazaphenanthrene derivatives**  
 Ozturk E., İRAK Z. Ş. T., Karakoyun N., Gümüş A., Gümüş S.  
 Physical Sciences Reviews, vol.5, no.3, 2020 (ESCI)
- II. **(E)-2-((Fenilimino)metil) Fenol Molekülünün Teorik Olarak İncelenmesi**  
 Öztürk E., Turhan Irak Z., Gümüş S.  
 İĞDIR ÜNİVERSİTESİ FEN BİLİMLERİ ENSTİTÜSÜ DERGİSİ, vol.9, pp.407-414, 2019 (Peer-Reviewed Journal)
- III. **Potential thermally activated delayed fluorescence properties of a series of 2,3-dicyanopyrazine based compounds**  
 Gümüş A., Gümüş S.  
 PHYSICAL SCIENCES REVIEWS, vol.3, no.7, 2018 (ESCI)
- IV. **A Computational Study on Tri and Tetraazaanthracenes**  
 Köle A., Gümüş S.  
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## **YÖNTEMİYLE İNCELENMESİ**

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UMTEB 6. ULUSLARARASI MESLEKİ VE TEKNİK BİLİMLER KONGRESİ, İğdır, Turkey, 11 - 12 April 2019, pp.722-726

## **VI. FENANTREN TABANLI POTANSİYEL OLED YAPILARIN YAPISAL VE ELEKTRONİK ÖZELLİKLERİNİN İNCELENMESİ**

Öztürk E., Turhan Irak Z., Gümüş A., Gümüş S.

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Karakoyun N., Gümüş A., Gümüş S.

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## **VIII. MONOAZAPİRİDOKİNOLİZİN TÜREVLERİNİN AROMATİKLİK ÖZELLİKLERİNİN TEORİK OLARAK İNCELENMESİ**

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## **IX. Potential thermally activated delayed fluorescence properties of a series of 2,3-dicyanopyrazine based compounds**

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## **XI. 3,6-DIALKYLSULFANYLPHTHALONITRILES: COMPARATIVE MOLECULAR STRUCTURE, SPECTROSCOPIC AND DFT COMPUTATIONAL STUDIES**

Karakoyun N., Gümüş A., Gümüş S.

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## **XIII. DECOMPOSITION MECHANISMS OF NITROGEN RICH PYROTECHNICS**

Gümüş S., Gümüş A., Uygur R.

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## **XIV. POTENTIAL APPLICATION OF SOME PHENANTHRENE DERIVATES AS OLED COMPOUNDS**

Öztürk E., Turhan Irak Z., Gümüş A., Gümüş S.

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## **XV. Synthesis and Computational Studies on Anthracene Pyren Schiff Bases**

Gümüş A., Gümüş S.

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## **XVI. INVESTIGATION OF ELECTRONIC PROPERTIES OF SYNTHESIZED HETEROCYCLIC MANNICH BASES**

Turhan Irak Z., Beytur M., Manap S., Öztürk E., Gümüş S., Yüksek H.

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Gümüş S., Gümüş A.  
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- XIX. **QUANTUM CHEMICAL CALCULATIONS OF SOME 1,2,4-TRIAZOLE BASED COMPOUNDS**  
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- XX. **AROMATICITY OF MONOAZAPHENANTHERENE DERIVATIVES**  
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- XXI. **Substituent Effect on the Aromaticity of Diazanaphthalenes**  
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- XXII. **Investigation of Nonlinear Optical Properties of Donor-Acceptor Type Molecules**  
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- XXV. **Computational Investigation of Carbene and Cyclic Olefin Reaction Mechanism**  
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- XXIX. **Substituent Effect on the Aromaticity of Phosphazene**

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pp.1
- XXX. **Synthesis of Chiral Heteroaryl-Substituted Dihydropyran Derivatives via Ring Closing Enyne Metathesis Reaction**  
Gümüş A., Gümüş S., Büyükkadali N. N., Aslan N.  
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- XXXI. **Donör-Akseptör Bağlı Triazin Türevlerinin Doğrusal Olmayan Optik Özelliklerinin Dft Yöntemiyle İncelenmesi**  
Turhan İrak Z., Gümüş S.  
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- XXXII. **Determination of the Electronic Properties of Some Organic Electroluminescent Molecules with Density Function Theory**  
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- XXXV. **Kiral Benzofuran ve Benzotiyofen-Sübstitüe Dihidropiran Türevlerinin Kemoenzimatik Sentezi**  
Gümüş A., Büyükkadali N. N., Aslan N., Gümüş S.  
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- XXXVI. **Yeni Donor-Akseptör-Donör Tipi Piridin Türevlerinin Sentezi ve Molekül İçi Yük Transfer Özelliklerinin Araştırılması**  
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pp.39
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- XL. **Novel Azo-azomethine Based Dinuclear Metal(II) Complexes: Synthesis, Definitions, DFT Calculations and Biochemical Applications**  
BASHA SYAN R. H., Gülcen M., Karataş Y., Gümüş S., Özdemir S.  
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- XLI. **Isoquinoline-substituted hybrid compounds: Synthesis and computational studies**  
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- XLII. **A Theoretical Application of Click Reaction to Obtain Heterotricyclic Compounds**  
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- XLIII. **Siklik Alken Türevlerinin Karbenler ile Siklopropanasyon Tepkimelerinin Teorik Olarak İncelenmesi**  
Gümüş S., Olğun K.  
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- XLIV. **A Computational Study of Metallophthalocyanines with 2-Isopropyl-5-methylphenoxy Substituents**  
Gümüş S., Ağırtaş M. S.  
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- XLV. **1,3,5-Triazin Tabanlı Organik Elektroluminesant Moleküllerin Elektronik Özelliklerinin Belirlenmesi**  
Gümüş S., Arvas E.  
2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015, pp.78
- XLVI. **DHT Bileşığının Dekompozisyon Mekanizmasının Teorik Olarak İncelenmesi**  
Gümüş S., Uygur R.  
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- XLVII. **Click Tepkimesi Mekanizmasının Teorik Olarak İncelenmesi**  
Gümüş S., Turhan İrak Z. Ş.  
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- XLVIII. **1,10-Fenantrolin Tabanlı Organik Elektroluminesant Moleküllerin Elektronik Özelliklerinin Belirlenmesi**  
Gümüş S., Aydın K.  
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- XLIX. **Synthesis of a novel Acceptor-?- Anthracene-?- acceptor conjugated molecule and its electronic properties**  
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- L. **Design, Synthesis and Spectroscopic Studies of Anthracene-Based Small Organic Molecules**  
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- LI. **Synthesis of Some Novel Phthalocyanines with Methyl 2-(oxy)-2,2- diphenylacetate Substituents and their electronic Properties**  
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- Gümüş S., Project Supported by Higher Education Institutions, Metal Komplekslerin Spektroskopik Özelliklerinin Tayininde Uygun DFT Yönteminin Belirlenmesi, 2019 - 2021
- Gümüş S., Gümüş A., Project Supported by Higher Education Institutions, Benzofenon ve Triazofenon Temelli OLED Yapılarının Tasarlanması ve Kuantum Kimyasal Uygulamaları, 2018 - 2021
- Zahmakıran M., Gümüş S., Project Supported by Higher Education Institutions, Bilimsel ve Teknolojik Araştırma Projeleri Kapsamında Üniversite Alt Yapısının Güçlendirilmesi için Biyoluminans Kemiluminans ve Elektroluminans Ölçümleri için Spektroskopi Cihazı ve Donanımlarının Kurulması, 2019 - 2020
- Gümüş S., KELEŞ M. N., Project Supported by Higher Education Institutions, Yüksek Enerjili Yoğun Maddelerin Dekompozisyon Mekanizmalarının İncelenmesi, 2017 - 2020

Gümüş A., Gümüş S., Project Supported by Higher Education Institutions, Antrasen ve Piren Temelli Floresans Schiff Baz Türevlerinin Sentezi ve Elektronik Özelliklerinin Teorik Olarak İncelenmesi, 2018 - 2019

Gümüş S., Project Supported by Higher Education Institutions, Antrasen-Piren Konjuge Schiff Bazın Sentezi ve Bilgisayarlı Hesaplamaları, 2018 - 2019

Gümüş S., Gümüş A., KARAKOYUN N., Karakoyun N., Project Supported by Higher Education Institutions, Yeni Mono ve Bis-Triazol Türevlerinin Sentezi ve Hesapsal Kimya Uygulamaları, 2017 - 2019

Gümüş S., KÖLE A., Project Supported by Higher Education Institutions, Mono ve Diazaantrasen Türevlerinin Aromatikliğinin İncelenmesi, 2018 - 2018

Gümüş S., Project Supported by Higher Education Institutions, Metal Yüklenmiş C60 Türevlerinin Hidrojen Depolama Kapasitelerinin Teorik Olarak İncelenmesi, 2017 - 2018

Gümüş A., Gümüş S., Project Supported by Higher Education Institutions, Kiral Benzofuran-sübstítüe Triazol Türevlerinin Sentezi, 2016 - 2017

Gümüş S., Gümüş A., Project Supported by Higher Education Institutions, İzokinolin Sübstítüe Triazol Türevlerinin Sentezi ve Bilgisayarlı Hesaplamaları, 2016 - 2017

Gümüş S., UYGUR R., Project Supported by Higher Education Institutions, Çevre dostu enerjetik materyallerin dekompozisyon mekanizmalarının teorik olarak incelenmesi, 2016 - 2017

Aktaş N., Çavuşoğlu Ş., Gümüş S., Project Supported by Higher Education Institutions, Merkezi Laboratuvar Akreditasyon ve Modernizasyon, 2015 - 2017

Gümüş A., YENİDEDE D., Gümüş S., Project Supported by Higher Education Institutions, Floresans Kemosensörlerin Tasarlanması, Sentezi ve Uygulamaları, 2015 - 2017

Gümüş S., TUBITAK Project, Azotça Zengin Ve Çevre Dostu (Yeşil) Piroteknikler, Daat, Dht, Diat Ve Cuat'In Dekompozisyon Mekanizmalarının Teorik Olarak İncelenmesi, 2015 - 2017

Gümüş S., Project Supported by Higher Education Institutions, Tri Ve Tetraazanaftalin Türevlerinin Aromatikliğinin İncelenmesi, 2015 - 2016

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Gümüş S., Project Supported by Higher Education Institutions, Metal Kompleks Katalizörlü Hidrojen Transfer Tepkimesinde Sübstítuent Etkisinin Teorik Olarak İncelenmesi, 2015 - 2015

Gümüş S., Project Supported by Higher Education Institutions, 1,3,5-Triazin Tabanlı Organik Elektroluminesant Moleküllerin Elektronik Özelliklerinin Belirlenmesi, 2015 - 2015

Gümüş S., Project Supported by Higher Education Institutions, Click Tepkimesi Mekanizmasının Teorik Olarak İncelenmesi, 2014 - 2015

Gümüş S., Project Supported by Higher Education Institutions, 1. Uluslararası Katılımlı Ulusal Hesaplamalı Kimya Çalıştayı, 2013 - 2014

Gümüş S., Project Supported by Higher Education Institutions, Yoğunluk Fonksiyon Teorisi Hesaplarını Kullanarak 1,2-dikarbonil Bileşiklerinin Çeşitli Nükleofiller İle Tepkimelerinin Mekanizmalarının Belirlenmesi, 2011 - 2014

## Activities in Scientific Journals

Computational Chemistry, Committee Member, 2018 - Continues  
Modern Organic Chemistry Research, Committee Member, 2018 - Continues

## Scientific Refereeing

International Journal of Hydrogen Energy, SCI Journal, December 2019  
Avrupa Bilim ve Teknoloji Dergisi , National Scientific Refreed Journal, December 2019  
Caucasian Journal of Science, National Scientific Refreed Journal, December 2019  
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Iğdır Üniversitesi Fen Bilimleri Enstitüsü Dergisi, National Scientific Refreed Journal, April 2019  
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International Journal of Chemical and Biomolecular Science, Other Indexed Journal, October 2016  
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Journal of the Turkish Chemical Society, Section A Chemistry, Other Indexed Journal, December 2015  
Chemistry International, Other Indexed Journal, December 2015  
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Zeitschrift für Anorganische und Allgemeine Chemie, SCI Journal, May 2014  
Zeitschrift für Anorganische und Allgemeine Chemie, SCI Journal, March 2014

## Scientific Consultations

Tubitak, Project Consultancy, Van Yüzüncü Yıl University, Fen Fakültesi, Kimya Bölümü, Turkey, 2014 - 2015

## Metrics

Publication: 137  
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H-Index (WoS): 12  
H-Index (Scopus): 13