

# Prof. Nurcan Tüzün

## Personal Information

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## Education Information

Doctorate, Boğaziçi Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (Dr), Turkey 1997 - 2002

Post Graduate, Boğaziçi Üniversitesi, Fen Bilimleri Enstitüsü, Kimya (Y) (Tezli), Turkey 1996 - 1997

Under Graduate, Boğaziçi Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, Turkey 1991 - 1996

## Foreign Languages

English

## Research Areas

Chemistry, Natural Sciences

## Academic Titles / Tasks

Professor, İstanbul Teknik Üniversitesi, Fen-Edebiyat, Kimya, 2017 - Continues

Associate Professor, İstanbul Teknik Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2009 - 2017

Assistant Professor, İstanbul Teknik Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2003 - 2009

Research Assistant, Boğaziçi Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, 1996 - 2003

## Professional Experience

Deputy Head of Department, İstanbul Teknik Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2015 - Continues

Erasmus Coordinator, İstanbul Teknik Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2003 - Continues

Vice Dean, İstanbul Teknik Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2010 - 2012

Deputy Head of Department, İstanbul Teknik Üniversitesi, Fen-Edebiyat Fakültesi, Kimya Bölümü, 2008 - 2009

## Articles Published in Journals That Entered SCI, SSCI and AHCI Indexes

- **Amberlyst-15-catalyzed Procedure for the Synthesis of Novel 2,4-Dihydroxybenzoyl-1,2,3-triazoles and Molecular Modelling Studies for Hsp-90 Inhibition**  
Gündüz H., Kumbaracı İ. V. , Özkılıç Y., Tüzün N., Talinli N.  
CHEMISTRYSELECT, vol.4, pp.7278-7283, 2019 (Journal Indexed in SCI)
- **Mechanism of Kynurenine 3-Monooxygenase-Catalyzed Hydroxylation Reaction: A Quantum Cluster Approach**  
Özkılıç Y., Tüzün N.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.123, pp.3149-3159, 2019 (Journal Indexed in SCI)
- **Superior Sensor for Be<sup>2+</sup> Ion Recognition via the Unprecedented Octahedral Crystal Structure of a One-Dimensional Coordination Polymer of Crown Fused Zinc Phthalocyanine**  
Yayuz O., Alçay Y., Kaya K., Sezen M., Atasın S. K. , Yıldırım M. S. , Özkılıç Y., Tüzün N., Yılmaz İ.

INORGANIC CHEMISTRY, vol.58, pp.909-923, 2019 (Journal Indexed in SCI)

- **New ferrocenyl naphthoquinone fused crown ether chemosensors: Highly selective, kinetically and regio controlled colorimetric, beryllium ion recognition**  
Alçay Y., Yavuz Ö., Gelir A., ATASEN S. K. , KARAOĞLU K., Yücel B., TUZUN N., Yılmaz İ.  
Journal of Organometallic Chemistry, vol.868, pp.131-143, 2018 (Journal Indexed in SCI Expanded)
- **Computational investigation of the control of the thermodynamics and microkinetics of the reductive amination reaction by solvent coordination and a co-catalyst**  
Boz E., Tüzün N., Stein M.  
RSC ADVANCES, vol.8, pp.36662-36674, 2018 (Journal Indexed in SCI)
- **A DFT study on the mechanism of Rh-catalyzed competitive 1,2-versus 1,3-acyloxy migration followed by [5+1] and [4+1] cycloadditions of 1,4-enynes with CO**  
COSKUN D., Tüzün N.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, vol.851, pp.97-103, 2017 (Journal Indexed in SCI)
- **Structural investigation of vesnarinone at the pore domains of open and open-inactivated states of hERG1 K<sup>+</sup> channel**  
Kayık G., Tüzün N., Durdagi S.  
JOURNAL OF MOLECULAR GRAPHICS & MODELLING, vol.77, pp.399-412, 2017 (Journal Indexed in SCI)
- **Mechanism of CuAAC reaction: In acetic acid and aprotic conditions**  
Ozen C., Tuzun N.  
JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL, vol.426, pp.150-157, 2017 (Journal Indexed in SCI)
- **Investigation of PDE5/PDE6 and PDE5/PDE11 selective potent tadalafil-like PDE5 inhibitors using combination of molecular modeling approaches, molecular fingerprint-based virtual screening protocols and structure-based pharmacophore development**  
Kayık G., Tüzün N., Durdagi S.  
JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY, vol.32, pp.311-330, 2017 (Journal Indexed in SCI)
- **In silico design of novel hERG-neutral sildenafil-like PDE5 inhibitors**  
Kayık G., Tüzün N., Durdagi S.  
JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS, vol.35, pp.2830-2852, 2017 (Journal Indexed in SCI)
- **A DFT Study on the Binuclear CuAAC Reaction: Mechanism in Light of New Experiments**  
Özkılıç Y., Tüzün N.  
ORGANOMETALLICS, vol.35, pp.2589-2599, 2016 (Journal Indexed in SCI)
- **Ag-catalyzed azide alkyne cycloaddition: a DFT approach**  
Boz E., Tüzün N.  
DALTON TRANSACTIONS, vol.45, pp.5752-5764, 2016 (Journal Indexed in SCI)
- **Synthesis, reactions and DFT study of tropolone N,N-dimethylthiocarbamate**  
Zaim O., Tüzün N., Cevik B., Ozcan H., BOZ E.  
TETRAHEDRON, vol.71, pp.5391-5398, 2015 (Journal Indexed in SCI)
- **A Quantum Mechanical Study on the Propagation Kinetics of N-methylacrylamide: Comparison With N,N-Dimethylacrylamide in Free Radical Polymerization**  
Kayık G., Tüzün N.  
MACROMOLECULAR THEORY AND SIMULATIONS, vol.24, pp.218-231, 2015 (Journal Indexed in SCI)
- **A Theoretical Study On Rh(I) Catalyzed Enantioselective Conjugate Addition Reactions of Fluoroalkylated Olefins**  
Boz E., HASLAK Z. P. , Tüzün N., KONUKLAR F. A. S.  
ORGANOMETALLICS, vol.33, pp.5111-5119, 2014 (Journal Indexed in SCI)
- **Stereoselective propagation in free radical polymerization of acrylamides: A DFT study**  
Kayık G., Tüzün N.  
JOURNAL OF MOLECULAR GRAPHICS & MODELLING, vol.49, pp.55-67, 2014 (Journal Indexed in SCI)
- **Prediction of the H-1 NMR spectra of epoxy-fused cyclopentane derivatives by calculations of chemical shifts and spin-spin coupling constants**  
Ozen C., Yıldırım A., Tüzün N., Haslak P., Dogan E., Acar E., Aviyente V.

MOLECULAR PHYSICS, vol.111, pp.3147-3155, 2013 (Journal Indexed in SCI)

- **Reaction mechanism of ruthenium-catalyzed azide-alkyne cycloaddition reaction: A DFT study**  
Boz E., Tüzün N.  
JOURNAL OF ORGANOMETALLIC CHEMISTRY, vol.724, pp.167-176, 2013 (Journal Indexed in SCI)
- **The mechanism of copper-catalyzed azide-alkyne cycloaddition reaction: A quantum mechanical investigation**  
Ozen C., Tüzün N.  
JOURNAL OF MOLECULAR GRAPHICS & MODELLING, vol.34, pp.101-107, 2012 (Journal Indexed in SCI)
- **A QSPR Study on the Physical Properties of Substituted Polypyrroles and Poly(paraphenylenes)**  
Yildirim E., AKSOY D., TUZUN N., Yurtsever M.  
DESIGNED MONOMERS AND POLYMERS, vol.14, pp.79-93, 2011 (Journal Indexed in SCI)
- **Mechanistic Study on [3+2] Cycloaddition and Cyclopropanation Reactions of 1,3-Dioxepine Derivatives in the Presence of Copper(I) Catalyst**  
Ozen C., KONUKLAR F. A. S. , Tüzün N.  
ORGANOMETALLICS, vol.28, pp.4964-4973, 2009 (Journal Indexed in SCI)
- **Cyclopolymerization Reactions of Diallyl Monomers: Exploring Electronic and Steric Effects Using DFT Reactivity Indices**  
Ugur I., De Vleeschouwer F., Tüzün N., Aviyente V., Geerlings P., Liu S., Ayers P. W. , De Proft F.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.113, pp.8704-8711, 2009 (Journal Indexed in SCI)
- **A DFT study on the mechanism of cyclopropanation via Cu(acac)(2)-catalyzed diazo ester decomposition**  
Oezen C., TUEZUEN N. S.  
ORGANOMETALLICS, vol.27, pp.4600-4610, 2008 (Journal Indexed in SCI)
- **An experimental and quantum mechanical study on electrochemical properties of N-substituted pyrroles**  
Tüzün N., BAYATA F., SARAC A. S.  
JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM, vol.857, pp.95-104, 2008 (Journal Indexed in SCI)
- **Metal-catalyzed cyclization reactions of carbonyl ylides: Synthesis and DFT study of mechanisms**  
Celik M. A. , YURTSEVER M., TUEZUEN N., GUENGOER F. S. , SEZER O., Anac O.  
ORGANOMETALLICS, vol.26, pp.2978-2985, 2007 (Journal Indexed in SCI)
- **Modeling the cyclopolymerization of diallyl ether and methyl alpha-[(allyloxy)methyl]acrylate**  
Tuzun N., AVIYENTE V.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.107, pp.894-906, 2007 (Journal Indexed in SCI)
- **Modeling the effect of substitution on the Pb(OAc)(4) mediated oxidative cleavage of steroidal 1,2-diols**  
Ozturk C., TOPAL K., Aviyente V., Tuzun N., FERNANDEZ E., ARSENIYADIS S.  
JOURNAL OF ORGANIC CHEMISTRY, vol.70, pp.7080-7086, 2005 (Journal Indexed in SCI)
- **Modeling the free radical polymerization of acrylates**  
Gunaydin H. M. , SALMAN S. Y. , Tuzun N., AVCI D., Aviyente V.  
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, vol.103, pp.176-189, 2005 (Journal Indexed in SCI)
- **A theoretical study on the mechanism of the cyclopolymerization of diallyl monomers**  
Tuzun N., Aviyente V., HOUK K.  
JOURNAL OF ORGANIC CHEMISTRY, vol.68, pp.6369-6374, 2003 (Journal Indexed in SCI)
- **Spirodiporphyrins - As binuclear metal complexes**  
Vogel E., MICHELS M., ZANDER L., LEX J., Tuzun N., HOUK K.  
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, vol.42, pp.2857-2862, 2003 (Journal Indexed in SCI)
- **A computational study on the substituent effect of diallylamine monomers in their cyclopolymerization reactions**  
Tuzun N., Aviyente V.  
JOURNAL OF PHYSICAL CHEMISTRY A, vol.106, pp.8184-8190, 2002 (Journal Indexed in SCI)
- **Theoretical study of factors controlling rates of cyclization of radical intermediates from diallylamine and diallylammonium monomers in radical polymerizations**  
Tuzun N., Aviyente V., HOUK K.  
JOURNAL OF ORGANIC CHEMISTRY, vol.67, pp.5068-5075, 2002 (Journal Indexed in SCI)
- **A computational approach to the polymerizabilities of diallylamines**

Tüzün N., AVİYENTE V., AVCI SEMİZ D., İNCE H. N.

JOURNAL OF MOLECULAR MODELING, vol.0, pp.257-264, 2001 (Journal Indexed in SCI Expanded)

- **A computational study of the conformational equilibria of alpha phenoxy alpha phenylthio alpha phenylseleno substituted cyclohexanones**

duran d., Tüzün N., AVİYENTE V.

JOURNAL OF CHEMICAL RESEARCH-S, vol.0, pp.411, 2000 (Journal Indexed in SCI Expanded)

- **Computational study of the anomeric effect in 2-[(4-substituted phenyl)seleno]-1,3-dithianes**

Senyurt N., Aviyente V.

JOURNAL OF THE CHEMICAL SOCIETY-PERKIN TRANSACTIONS 2, pp.1463-1470, 1998 (Journal Indexed in SCI)

## Expert Reports

- **Comparative density functional study of antioxidative activity of the hydroxybenzoic acids and their anions**

TÜZÜN N.

Turkish Journal Of Chemistry, 2015 (Journal Indexed in SCI Expanded)

## Supported Projects

Tüzün N., Project Supported by Higher Education Institutions, A DFT Study on the Stereoselective Propagation In Free Radical Polymerization of Acrylamides, 2016 - 2018

Tüzün N., Project Supported by Higher Education Institutions, Ag IN CLICK REACTION: A DFT STUDY, 2016 - 2018

Tüzün N., Project Supported by Higher Education Institutions, CuAAC MECHANİSM REVİSİTED: DİNUCLEAR INTERMEDIATES İN THE PRESENCE OF NHC LİGAND, 2015 - 2018

Tüzün N., Project Supported by Higher Education Institutions, RU VE CU KATALİZÖRÜ AZİT ALKİN KATILMA TEPKİMELERİ ÜZERİNE KUANTUM MEKANİK BİR ÇALIŞMA, 2010 - 2018

Tüzün N., Project Supported by Higher Education Institutions, ADFT STUDY ON THE MECHANİSM OF RUTHENİUM CATALYZED AZİDE-ALKYNE CYCLOADDİTION REACTION, 2009 - 2018

Tüzün N., Project Supported by Higher Education Institutions, Yapay Tatlandırıcı Moleküllerin Su ve Siklodekstrin Kompleksleri ile Etkileşimlerinin Yapı-Tat İlişkisi Açısından NMR Spektroskopisi ve Hesaplamalı Kimya Yöntemleri ile İncelenmesi, 2013 - 2014

Tüzün N., Project Supported by Higher Education Institutions, Bakır (I) Katalizörü 1,2,3-Triazol ve Fofuran Sentez Mekanizmalarına Teorik Bir Bakış, 2012 - 2014

Tüzün N., Project Supported by Higher Education Institutions, Rh (I) Katalizörlüğünde Floroalkili Olefinlerin Enantiyoseçici Konjuge Katılma Reaksiyonları Üzerine Hesapsal Bir Çalışma, 2012 - 2014

Tüzün N., Project Supported by Higher Education Institutions, N-Metilakrilamid Türevlerin Serbest Radikal Polimerizasyonunun Modellenmesi ve Taktisitelerinin İncelenmesi, 2010 - 2012

Tüzün N., Project Supported by Higher Education Institutions, Ru Katalizörlü Azid Alkin Siklolatılma Tepkime Mekanizmalarının Modellenmesi, 2010 - 2012

Tüzün N., Project Supported by Higher Education Institutions, Karbonil Yidlerin Halkalaşma Tepkimelerinde Regioselektivitenin Hesaplamalı Kimya Yöntemleri ile Modellenmesi a,b konjuge Ketonlar, 2005 - 2007

Tüzün N., Project Supported by Higher Education Institutions, a,b-Konjuge Keton, Aldehit ve Esterlerden Elde Edilen Karbonil Yidlerinin Mekanistik Davranışları: Hesapsal Bir Yaklaşım, 2003 - 2007

## Citations

Total Citations (WOS):341

h-index (WOS):11