

## **Prof. SAFİYE ERDEM**

### **Personal Information**

**Email:** erdem@marmara.edu.tr

**Web:** <https://avesis.marmara.edu.tr/erdem>

### **International Researcher IDs**

ScholarID: RXgd40kAAAAJ

ORCID: 0000-0001-6043-4765

ScopusID: 24463261600

Yoksis Researcher ID: 3191

### **Education Information**

Postgraduate, Villanova University, College Of Liberal Arts And Sciences, Kimya Bölümü, United States Of America 1986 - 1988

Undergraduate, Bogazici University, Faculty Of Arts And Sciences, Department Of Chemistry, Turkey 1980 - 1985

### **Foreign Languages**

English, C1 Advanced

### **Dissertations**

Postgraduate, Dimerization of water soluble metalloporphyrins, Villanova University, 1988

### **Research Areas**

Natural Sciences

### **Academic Titles / Tasks**

Professor, Marmara University, Faculty of Arts and Sciences, Chemistry, 2008 - Continues

Associate Professor, Marmara University, Faculty of Arts and Sciences, Chemistry, 2002 - 2008

Assistant Professor, Marmara University, Faculty of Arts and Sciences, Chemistry, 1999 - 2002

Lecturer, Bogazici University, Faculty Of Arts And Sciences, Department Of Chemistry, 1997 - 1999

Research Assistant, Bogazici University, Faculty Of Arts And Sciences, Department Of Chemistry, 1992 - 1997

Research Assistant, Villanova University, College Of Liberal Arts And Sciences, Kimya, 1986 - 1988

### **Academic and Administrative Experience**

Marmara University, Faculty of Arts and Sciences, Chemistry, 2013 - Continues

Marmara University, Faculty of Arts and Sciences, 2013 - Continues

Marmara University, Faculty of Arts and Sciences, 2010 - Continues  
Marmara University, Faculty of Arts and Sciences, Chemistry, 2005 - 2015  
Marmara University, Faculty of Arts and Sciences, Chemistry, 2010 - 2013  
Marmara University, Faculty of Arts and Sciences, Chemistry, 2009 - 2010  
Marmara University, Institute for Graduate Studies in Pure and Applied Sciences, 2008 - 2010  
Marmara University, Faculty of Arts and Sciences, Chemistry, 2008 - 2009  
Marmara University, Faculty of Arts and Sciences, Chemistry, 1999 - 2001

## Advising Theses

Erdem S., Danış Ö., Arilkumarin türevlerinin beta-laktamaz ve karbapenemaz aktivitesi üzerine etkilerinin incelenmesi, Postgraduate, B.Hamur(Student), 2019  
ERDEM S., Computational and mechanistic studies on the formation of cyclic systems, Doctorate, Ö.SARI(Student), 2017  
ERDEM S., Flavoenzimlerdeki flavin oksidasyonu mekanizmasının hesapsal modellenmesi, Postgraduate, İ.Demir(Student), 2017  
ERDEM S., Flavin redoks tepkimesine süstitüent etkisinin modellenmesi, Postgraduate, A.Topal(Student), 2017  
ERDEM S., Monoamin oksidaz (mao) enzimlerinin hidrür transferi mekanizması tek basamaklı mı çok basamaklı mıdır?, Postgraduate, K.Çakır(Student), 2016  
ERDEM S., Asimetrik aldol tepkimeleri için yeni bir katalizör: Homoboroprolin'in asimetrik katalizör etkisinin modellenmesi, Postgraduate, H.DÜLGER(Student), 2016  
ERDEM S., Computational modelling of axial chirality of 2-arylimino-3- arylthiazolidine isomers, Postgraduate, G.Sabuncu(Student), 2014  
ERDEM S., Erdem S., Monoamin oksidaz (MAO)inhibitör etkili yeni pirazolin türevleri ile moleküler doking, Postgraduate, S.Türkkan(Student), 2013  
ERDEM S., Mao inhibitörleri ile akılcı ilaç tasarımına yönelik qsar analizi, Doctorate, M.Köktürk(Student), 2013  
ERDEM S., Hidrazon türevi mao inhibitörleri ile akılcı ilaç tasarımına yönelik qsar analizi, Postgraduate, O.Aydın(Student), 2011  
ERDEM S., Polihalojenlenmiş nitrobütadienlerin aromatik aminlerle verdiği reaksiyon mekanizmalarının hesapsal olarak modellenmesi, Postgraduate, Ö.Sarı(Student), 2011  
ERDEM S., erdem S., Experimental and computational studies of interactions between small molecules and DNA, Postgraduate, M.Biçen(Student), 2011  
ERDEM S., MAO A enziminin aktif bölgesinin ONIOM yöntemi ile modellenmesi, Doctorate, V.Enisoğlu(Student), 2010  
ERDEM S., Monoamin oksidaz enzimi için önerilen biradikal mekanizma ile ilgili yapı-aktiflik incelemeleri, Postgraduate, B.Büyükmenekşe(Student), 2009  
ERDEM S., Kliksalidon-n-oksitlerin senteziyle ilgili reaksiyon mekanizmalarının hesapsal modellenmesi, Doctorate, G.Altınbaş(Student), 2008  
ERDEM S., Monoamin oksidaz substratlarının enzimin aktif bölgesi içinde QM/MM yöntemi ile modellenmesi, Postgraduate, M.Ali(Student), 2007  
ERDEM S., Fulven türevlerinin aromatikliğinin nics yöntemi ile araştırılması, Postgraduate, R.Keleş(Student), 2007  
ERDEM S., Para-süstitüe benzilaminlerin monoamin oksidaz ile tepkimelerinde yapı-aktiflik ilişkisinin incelenmesi, Postgraduate, O.Can(Student), 2007  
ERDEM S., Mao enziminin oksazolidon ve benzeri heterosiklik bileşikler ile inhibisyonunun kimyasal modellenmesi, Postgraduate, Ü.Boz(Student), 2006  
ERDEM S., 2-Asetoksi-2,6,6-trimetilbisiklo [3.1.0] heksan'ın termal proliz mekanizmasının modellenmesi, Postgraduate, F.Uyar(Student), 2005  
ERDEM S., Monoamin oksidaz inhibisyonu ile ilişkili model amin bileşiklerinin koformasyonel analizi, Postgraduate, A.Kırsakal(Student), 2005  
ERDEM S., Application of the characteristic root index model to the estimation of physico-chemical and biological properties of selected endocrine disrupting chemicals, Postgraduate, M.ÖZKUL(Student), 2005  
ERDEM S., C=N bağıncı içeren bazı bileşiklerin singlet oksijen reaksiyonları ile önerilen mekanizmaların hesapsal

incelenmesi, Postgraduate, A.GENÇÇAKIR(Student), 2004

ERDEM S., Erdem S., Monoamin oksidaz (MAO) enziminin aminleri oksitleme mekanizmasının hesapsal yöntemlerle incelenmesi, Postgraduate, Ö.Karahan(Student), 2004

ERDEM S., 2-Süstitüe-Metiltiyoetilamin türevlerinin konformasyonel analizi, Postgraduate, M.Durmuş(Student), 2003

ERDEM S., Mono Amin Oksidaz (MAO) enziminin ekleme eliminasyon mekanizmasının hesapsal yöntemlerle incelenmesi, Postgraduate, İ.Yıldız(Student), 2003

ERDEM S., Fulven türevlerinin kararlılığı ve süstitüent etkisi, Postgraduate, S.Atalay(Student), 2002

## Published journal articles indexed by 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. **In vitro and in silico investigation of inhibitory activities of 3-arylcoumarins and 3-phenylazo-4-hydroxycoumarin on MAO isoenzymes**  
Yuce-Dursun B., Daniş Ö., Ozalp L., Sahin E., Demir S., Erdem S., Ogan A.  
STRUCTURAL CHEMISTRY, vol.34, no.5, pp.1715-1729, 2023 (SCI-Expanded)
- III. **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)
- IV. **Cheminformatics and Machine Learning Approaches to Assess Aquatic Toxicity Profiles of Fullerene Derivatives**  
Fjodorova N., Novič M., Venko K., Rasulev B., Türker Saçan M., Tugcu G., Sağ Erdem S., Toropova A. P., Toropov A. A.  
International Journal of Molecular Sciences, vol.24, no.18, 2023 (SCI-Expanded)
- V. **Identification of some novel amide conjugates as potent and gastric sparing anti-inflammatory agents: In vitro, in vivo, in silico studies and drug safety evaluation**  
KULABAŞ N., Set İ., Aktay G., GÜRSOY Ş., DANIŞ Ö., OGAN A., Sağ Erdem S., Erzincan P., Helvacioğlu S., Hamitoğlu M., et al.  
Journal of Molecular Structure, vol.1285, 2023 (SCI-Expanded)
- VI. **Stable hemiaminals from axially chiral pyridine compounds**  
Tuncel S. T., Demir I., ERDEM S., Dogan I.  
Chirality, vol.35, no.6, pp.365-375, 2023 (SCI-Expanded)
- VII. **A QSAR study to predict the survival motor neuron promoter activity of candidate diaminoquinazoline derivatives for the potential treatment of spinal muscular atrophy**  
Sabuncu Gürses G., ERDEM S., Saçan M.  
SAR and QSAR in environmental research, vol.34, no.3, pp.247-266, 2023 (SCI-Expanded)
- VIII. **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)
- IX. **Newly synthesized piperazine derivatives as tyrosinase inhibitors: in vitro and in silico studies**  
DOKUZPARMAK Ç., ÖZ TUNCAY F., Ozdemir S. B., Kurnaz B., Demir I., ÇOLAK A., ERDEM S., YILDIRIM N.  
JOURNAL OF THE IRANIAN CHEMICAL SOCIETY, vol.19, no.7, pp.2739-2748, 2022 (SCI-Expanded)
- X. **How fullerene derivatives (FDs) act on therapeutically important targets associated with diabetic diseases**  
Fjodorova N., Novic M., Venko K., Drgan V., Rasulev B., SAÇAN M., ERDEM S., Tugcu G., Toropova A. P., Toropov A. A.  
COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL, vol.20, pp.913-924, 2022 (SCI-Expanded)

- XI. **A Bifunctional B,N-Based Asymmetric Catalytic Nitrostyrene-Michael Addition Acting through a 10-Membered Ring Cyclic Transition State**  
Du Y., Sari O., ERDEM S., Whiting A.  
HELVETICA CHIMICA ACTA, vol.104, no.12, 2021 (SCI-Expanded)
- XII. **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)
- XIII. **Synthesis of hydrazine containing piperazine or benzimidazole derivatives and their potential as  $\alpha$ -amylase inhibitors by molecular docking, inhibition kinetics and in vitro cytotoxicity activity studies**  
Cakmak U., ÖZ TUNCA Y., Basoglu-Ozdemir S., AYAZOĞLU DEMİR E., Demir I., ÇOLAK A., ÇELİK UZUNER S., ERDEM S., YILDIRIM N.  
MEDICINAL CHEMISTRY RESEARCH, vol.30, no.10, pp.1886-1904, 2021 (SCI-Expanded)
- XIV. **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)
- XV. **Synthesis of Benzoxazole-2-carboxylate Derivatives: Electronic- and Position-effect of Functional Groups and Computational Modeling of the Selectivity for Oxazole Ring**  
Kuzu B., SARI Ö., ERDEM S., ALGÜL Ö., Mengeş N.  
CHEMISTRYSELECT, vol.6, no.10, pp.2529-2538, 2021 (SCI-Expanded)
- XVI. **One-pot synthesis of oxazolidinones and five-membered cyclic carbonates from epoxides and chlorosulfonyl isocyanate: theoretical evidence for an asynchronous concerted pathway**  
Demir E., SARI Ö., ÇETİNKAYA Y., ATMACA U., ERDEM S., ÇELİK M.  
BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY, vol.16, pp.1805-1819, 2020 (SCI-Expanded)

## Refereed Congress / Symposium Publications in Proceedings

- I. **ANTIOXIDANT AND ANTI-COLLAGENASE ACTIVITY OF ST. JOHN'S WORT (HYPERICUM PERFORATUM L.)**  
YILDIZ İ., Özalp L., ERDEM S., MOUTSİNGA E. G. B. K., DANIŞ Ö., OGAN A.  
3. INTERNATIONAL MARMARA SCIENTIFIC RESEARCH AND INNOVATION CONGRESS 19-20 NOVEMBER 2022 İSTANBUL/ TURKE, İstanbul, Turkey, 19 November 2022, vol.1
- II. **Etakrinik Asit Oksidazol Türevlerinin Glutatiyon S-transferaz İnhibisyonu Üzerine Moleküler Doking Çalışması**  
FINDIK V., ERDEM S.  
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018
- III. **Tiyol-en Tepkimelerinin Bölgeseci Halkalaşma Reaksiyonuna Hesapsal Bir Yaklaşım**  
SİNEK Ö., FINDIK V., ERDEM S.  
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018
- IV. **Tiyol-in Reaksiyon Mekanizmalarının Teorik Olarak İncelenmesi**  
VARINCA B. T., FINDIK V., ERDEM S.  
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018
- V. **Tiyil Radikali ve Alkenler Arasında Gerçekleşen Bölgeseci Halkalaşma Reaksiyonuna Hesapsal Yaklaşım**  
SERT E. M., FINDIK V., ERDEM S.  
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018
- VI. **Monoamin Oksidaz Kataliz Mekanizmasının Kuantum Öbeği ve ONIOM Yöntemleri İle Bütünleşik Modellenmesi**  
ERDEM S., ÇAKIR K., ENGİN H.  
30. ULUSAL KİMYA KONGRESİ, Turkey, 5 - 08 November 2018

- VII. **In vitro and In silico Investigation of Tyrosinase Inhibition By Some Novel Triazole Derivative Compounds Containing Fluoroquinolone Skeleton**  
KURNAZ B., ÇOLAK A., ÖZDEMİR S. B., DEMİRBAŞ N., DEMİR İ., ERDEM S.  
1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018
- VIII. **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
- IX. **In Silico Investigation on Anti-Depression Effects of Hypericum Perforatum Flavanoids: Molecular Docking with Monoamin Oxidases**  
YILDIZ İ., ERDEM S., OGAN A.  
1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018
- X. **Molecular Docking of New Hybrid Triazole Derivatives into Tyrosinase Enzyme**  
DEMİR İ., ERDEM S., ÇOLAK A., DEMİRBAŞ N.  
1.Euroasia Biochemical Approaches Technologies Congress, 27 - 30 October 2018
- XI. **The effect of substituents on Phthalocyanine-DNA binding: molecular dynamics and docking studies**  
ÖZALP L., ERDEM S., ÖZBİL M.  
International conference on applied mathematics, modeling and Life Sciences, 3 - 05 October 2018
- XII. **In silico modelling on fish toxicity of Pharmaceuticals**  
EMİNOĞLU E. M., SAÇAN M., ERDEM S.  
International conference on applied mathematics, modeling and Life Sciences, 3 - 05 October 2018
- XIII. **Modelling the catalytic and inhibition mechanisms of monoamine oxidase: A combined ONIOM and quantum cluster approach**  
ERDEM S.  
International conference on applied mathematics, modeling and life Sciences, 3 - 05 October 2018
- XIV. **Nontarget binding of cannabinoids in central nervous system: molecular docking with monoamine oxidases**  
DERVİŞOĞLU C., ERDEM S.  
International conference on applied mathematics, modeling and life Sciences, 3 - 05 October 2018
- XV. **Revisiting Fish Toxicity of Active Pharmaceutical Ingredients: Mechanistic Insights from Integrated Ligand-/Structure-based Assessments on Acetylcholinesterase**  
SAÇAN M., Minovski N., Eminoğlu E. M., ERDEM S., Novic M.  
18th International Conference on QSAR in Environmental and Health Sciences, 11 - 15 June 2018
- XVI. **Molecular dynamics and docking studies on the interactions of DNA with quaternary metallo phthalocyanines**  
ÖZALP L., ERDEM S., ÖZBİL M.  
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017
- XVII. **Synthesis of stable tetrahedral intermediates (hemiaminals) and kinetics of their conversion to thiazol-2-imines**  
GÜNAL Ş. E., GÜRSES G. S., ERDEM S., DOĞAN H. İ.  
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017
- XVIII. **Mechanistic dft study on the function of homoboroprolines asymmetric catalyst in enantioselective aldol reactions**  
ERDEM S., DÜLGER H., DEMİREL N.  
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017
- XIX. **Mechanistic DFT study on one-pot synthesis of heterocyclic compounds**  
atbakar m., ERDEM S., ÖCAL SUNGUROĞLU Z. N., erden i.  
International Symposium on Chemistry V A Computation Applications on Molecular Nanoscience, 30 October 2017
- XX. **Molecular docking of arylcoumarins to carbapenemase enzyme**  
ERDEM S., HAMUR B., DANIŞ Ö.  
International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 October 2017
- XXI. **A combined experimental and theoretical study for the formation of indolizine,**

**pyrrolo[1,2,a]pyrazine, pyrrolo[1,2-a]pyrazinone**

SARI Ö., MENGEŞ N., ERDEM S., BALCI M.

Chemistry Via Computation – International Symposium on Chemistry Via Computation Applications on Molecular Nanoscience, 30 - 31 October 2017

- XXII. **Synthesis of stable tetrahedral intermediates (hemiaminals) and kinetics of their conversion to thiazol-2-imines**  
EROL GÜNAL Ş., SABUNCU GÜRSER G., ERDEM S., DOĞAN H. İ.  
International Symposium on Chemistry via Computation applications on Molecular Nanoscience, 30 October 2017
- XXIII. **Novel Chiral Monoamine Oxidase Inhibitors: Molecular Docking Studies on N-aryloxazolidinediones**  
YÜCE DURSUN B., ERDEM S., GÖKHAN KELEKÇİ N., DOĞAN H. İ., EROL Ş.  
5th International BAU Drug Design Congress, 19 October 2017 - 21 January 2018
- XXIV. **Novel Chiral Monoamine Oxidase Inhibitors: Molecular Docking Studies on N-Aryloxazolidinediones**  
YÜCE DURSUN B., ERDEM S., GÖKHAN KELEKÇİ N., DOĞAN H. İ., EROL GÜNAL Ş.  
5th International BAU Drug Design Congress, 19 - 21 October 2017
- XXV. **Potansiyel Karbapenemaz İnhibitörü Aril Kumarin Türevleri ile Moleküler Doking Hesapları**  
HAMUR B., ERDEM S.  
3. Hesaplamalı Kimya Kongresi, Turkey, 12 - 14 October 2017
- XXVI. **Flavinin re-Yüzünden Oksidasyon Mekanizmasının Hesapsal Modellenmesi**  
DEMİR İ., ERDEM S.  
3. Hesaplamalı Kimya Kongresi, 12 - 14 October 2017
- XXVII. **DFT computations on the mechanism of flavinoxidative half-reaction**  
ERDEM S., DEMİR İ.  
11th European Conference on Theoretical and Computational Chemistry, 4 - 07 September 2017
- XXVIII. **Substituent effect on the reduction tendency and conformation of flavin ring: a DFT study**  
ERDEM S., TOPAL A.  
11th European Conference on Theoretical and Computational Chemistry, 4 - 07 September 2017
- XXIX. **Enzim Kataliz Mekanizmaları ile Rasyonel İlaç Tasarımı: Monoamin Oksidaz Enziminin Kovalent Geri-dönüşümlü İnhibisyonu**  
ERDEM S.  
5. İlaç Kimyası: İlaç Etkin Maddesi Tasarımı, Sentezi, Üretimi ve Standardizasyonu Kongresi, 30 March - 02 April 2017
- XXX. **Flavinin si-Yüzünden Oksidasyon Mekanizmasının Hesapsal Modellenmesi**  
DEMİR İ., ERDEM S.  
5. İlaç Kimyası: İlaç Etkin Maddesi Tasarımı, Sentezi, Üretimi ve Standardizasyonu Kongresi, 30 March - 02 April 2017
- XXXI. **In Silico Modelling of DNA Quaternized Metallophthalocyanine Binding M Zn Ni Cu**  
Özalp L., ERDEM S., YÜCE DURSUN B.  
4. BAU DRUG DESIGN Congress, İstanbul, Turkey, 13 - 15 October 2016
- XXXII. **A Hybrid Proton and Hydride Transfer Mechanism for the Serotonin Oxidation of Monoamine Oxidase A**  
ÇAKIR K., ERDEM S., ENİSOĞLU ATALAY V., DÜLGER H.  
4. BAU DRUG DESIGN Congress, 13 - 15 October 2016
- XXXIII. **Synthesis anti inflammatory activity and molecular modeling studies on cox 1 and cox 2 inhibition of novel amide conjugates of some NSAIDs**  
KULABAŞ N., GÜRSOY Ş., ERZİNCAN P., YÜCE DURSUN B., AKTAY G., ERDEM S., OGAN A., KÜÇÜKGÜZEL İ.  
17th Tetrahedron Symposium, 28 Haziran-1 Temmuz 2016, Barselona, Spain, 28 June - 01 July 2016
- XXXIV. **Synthesis anti inflammatory activity and molecular modeling studies on cox 1 and cox 2 inhibition of novel amide conjugates of some NSAIDs**  
KULABAŞ N., GÜRSOY Ş., ERZİNCAN P., YÜCE DURSUN B., AKTAY G., ERDEM S., OGAN A., KÜÇÜKGÜZEL İ.  
17th TETRAHEDRON SYMPOSIUM : Challenges in Biological, Bioorganic & Medicinal Chemistry, Sitges, Spain, 28 June - 01 July 2016

- XXXV. **QSAR for Butyrylcholine Esterase BuChE Inhibition by Substituted Pyridylene hydrazone Derivatives**  
ERDEM S., SAÇAN M., ÇOMAK H.  
17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016), Miami, United States Of America, 13 - 17 June 2016
- XXXVI. **In Silico Approach to Monoamine Oxidase A Inhibitory Potential of New Coumarine Derivatives**  
ERZİNCAN P., ERDEM S., SAÇAN M., YÜCE DURSUN B., DANIŞ Ö., DEMİR S., OGAN A.  
. 17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016), Florida, United States Of America, 13 - 17 June 2016
- XXXVII. **QSAR Approach to Acetylcholine Esterase AChE Inhibitory Potential of Rasagiline and Selegiline Related Carbamate Derivatives**  
ERDEM S., SAÇAN M.  
17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016), Miami, United States Of America, 13 - 17 June 2016
- XXXVIII. **ZnII Ftalosiyanın Türevinin DNA Bağlanma Özelliklerinin in vitro ve in silico Yöntemlerle İncelenmesi**  
YÜCE DURSUN B., ÖZALP L., BAŞAK A. S., ERDEM S.  
2. Bilgisayar Destekli İlaç Tasarımı Uygulamalı Kursu, Turkey, 16 - 17 May 2016
- XXXIX. **Farmasötik Bileşiklerin Toksisitelerinin Torpedo californica AChE İnhibisyonu ile İlişkisi**  
EMİNOĞLU E. M., ERDEM S., SAÇAN M.  
2. Bilgisayar Destekli İlaç Tasarımı Uygulamalı Kursu, Turkey, 16 - 17 May 2016
- XL. **Yüksek Antioksidan Aktiviteye Sahip Yeni Kumarin Türevleri ile Kantitatif Yapı Aktivite İlişkileri ve Moleküler Doking**  
ERDEM S.  
4. İlaç Kimyası: İlaç Etkin Maddesi Tasarımı, Sentezi, Üretimi ve Standardizasyonu Kongresi, Turkey, 17 - 20 March 2016
- XLI. **In Silico Design of Potent Coumarin Derivatives for Treatment of Neurodegenerative Diseases**  
ERDEM S.  
COST Action CM1103 Final Meeting, 21 - 23 October 2015
- XLII. **Molecular Modeling Studies on COX 1 and COX 2 Inhibition of Novel Amide Conjugates of Some NSAIDs with Anti inflammatory Activity**  
KULABAŞ N., ERZİNCAN P., DANIŞ Ö., ERDEM S., OGAN A., KÜÇÜKGÜZEL İ.  
International Symposium on Drug Research & Development, Turkey, 15 - 17 October 2015
- XLIII. **Effect of active site residues and water molecules in amine oxidation mechanism of monoamine oxidase A quantum cluster approach**  
ERDEM S., ÇAKIR K., ENGİN H., ENİSOĞLU ATALAY V., DÜLGER H.  
10th European Conference on Computational Chemistry, 31 August - 03 September 2015
- XLIV. **3 Aril Kumarin Türevlerinin Sentezi Ve İnsan Monoamin Oksidaz A Ve B İnhibitörleri Olarak Etkilerinin İncelenmesi**  
YÜCE DURSUN B., ŞAHİN E., DANIŞ Ö., DEMİR S., OGAN A., ERDEM S.  
27. Ulusal Kimya Kongresi, Turkey, 23 - 28 August 2015
- XLV. **3 Aril kumarin türevlerinin sentezi ve insan monoamin oksidaz B ve B inhibitörleri olarak etkilerinin incelenmesi**  
YÜCE DURSUN B., ŞAHİN E., DANIŞ Ö., DEMİR S., OGAN A., ERDEM S.  
27. Ulusal Kimya Kongresi, Çanakkale, Turkey, 23 - 28 August 2015
- XLVI. **QSAR Models for Antioxidant Activity of New Coumarin Derivatives**  
ERZİNCAN P., SAÇAN M., YÜCE DURSUN B., DANIŞ Ö., DEMİR S., ERDEM S., OGAN A.  
8th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI-2015), 21 - 25 June 2015
- XLVII. **Monoamine Oksidaz Enzimindeki Flavin N5 Araürün Oluşumu Kataliz mi İnhibisyon mu**  
ÇAKIR K., DÜLGER H., ENİSOĞLU ATALAY V., ERDEM S.  
2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015
- XLVIII. **Pirolo Pirazin İndolizin Türevlerinin Sentezi ve Oluşum Mekanizmalarının Hesapsal Olarak**

## **Modellenmesi**

SARI Ö., MENGEŞ N., ERDEM S., BALCI M.

2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015

## **XLIX. Monoamin Oksidaz Enzimi Tarafından Katalizlenen Dopamin Oksidasyon Mekanizmasının Modellenmesi**

DÜLGER H., ÇAKIR K., ENİSOĞLU ATALAY V., ERDEM S.

2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015

## **L. Monoamine Oksidaz A ve B Enzimlerinin Nörotransmitter Aminleri Serotonin Dopamin Oksitlemesi Aynı Mekanizmayla mı Farklı Mekanizmalarla mı Gerçekleşir**

ÇAKIR K., ENİSOĞLU ATALAY V., AKYÜZ M. A., ERDEM S.

2. Ulusal Hesaplamalı Kimya Kongresi, Kars, Turkey, 2 - 05 June 2015

## **LI. Theoretical Modelling of Copolymerization reaction of cellulose units with methyl acrylate**

ABDURRAHMANOĞLU S., ERDEM S.

International Congress on Chemical Biological and Environmental Sciences ICCBES2015, 7 - 09 May 2015, pp.584-585

## **LII. Synthesis and biological evaluation of benzocoumarin derivatives as human monoamine oxidase A and B inhibitors**

DANIŞ Ö., YÜCE DURSUN B., DEMİR S., ALPARSLAN M. M., OGAN A., ERDEM S.

International Congress on Chemical Biological and Environmental Sciences (ICCBES2015), 7 - 09 May 2015

## **LIII. Monoamin Oksidaz A ve B inhibitörü olarak tasarlanan yeni kumarin türevleri ile moleküler doking**

ERZİNCAN P., YÜCE DURSUN B., DANIŞ Ö., DEMİR S., ERDEM S., OGAN A.

3. İlaç Kimyası: İlaç Etken Maddesi Tasarımı Sentezi, Üretimi ve Standardizasyonu Kongresi, Turkey, 20 - 23 March 2015

## **LIV. Monoamin Oksidaz A ve B İnhibitörü Olarak Tasarlanan Yeni kumarin Türevleri ile Moleküler Doking**

Erzincan P., Türker Saçan M., YÜCE DURSUN B., DANIŞ Ö., DEMİR S., ERDEM S., OGAN A.

3. Kimya İlaç Kongresi, Jenerik İlaçlar ve Kimyası, Turkey, 20 - 22 March 2015

## **LV. Monoamin Oksidaz A ve B İnhibitörü Olarak Tasarlanan Yeni Kumarin Türevleri İle Moleküler Doking**

ERDEM S., ERZİNCAN P., YÜCE DURSUN B., DANIŞ Ö., DEMİR S., OGAN A.

3. İlaç Kimyası Kongresi, Antalya, Turkey, 20 - 22 March 2015

## **LVI. Monoamin Oksidaz Enzimi Hidrür Mekanizmasının HOMO Moleküler Orbitaler ile Desteklenmesi**

ERDEM S., AKYÜZ M. A., HAZAL E., ÇAKIR K., ENİSOĞLU ATALAY V.

2. Ulusal Organik Kimya Kongresi, Ankara, Turkey, 24 - 26 September 2014

## **LVII. MONOAMİN OKSİDAZ MAO ENZİMİNDEKİ KOVALENT BAĞLI FLAVİNİN AMİN KATALİZLEME MEKANİZMASINA ETKİSİ**

ÇAKIR K., HAZAL E., ENİSOĞLU ATALAY V., ERDEM S.

2. Ulusal Organik Kimya Kongresi, Ankara, Turkey, 24 - 26 September 2014

## **LVIII. Asimetrik Aldol Tepkimeleri için Yeni Bir Katalizör Homoboroprolin in Asimetrik Katalizör Etkisinin Modellenmesi**

DÜLGER H., DEMİREL N., ERDEM S.

2. Ulusal Organik Kimya Kongresi, Ankara, Turkey, 24 - 26 September 2014

## **LIX. Nörotransmitter Aminlerin MAO Enzimi ile Oksitlenme Mekanizmasının M062X Yöntemiyle Modellenmesi Hidrür Transferi**

ENGİN H., ÇAKIR K., ENİSOĞLU ATALAY V., ERDEM S.

2. Ulusal Organik Kimya Kongresi, Ankara, Turkey, 24 - 26 September 2014

## **LX. Structure Activity Relationship on Monoamine Oxidase Catalyzed Oxidation of Substituted Benzylamines Competing Proton Hydride Transfer Mechanisms**

ERDEM S., AKYÜZ M. A., ENİSOĞLU ATALAY V.

4. International meeting on Pharmacy&Pharmaceutical Sciences, İstanbul, Turkey, 18 - 21 September 2014

## **LXI. COMPUTATIONAL MODELLING OF MONOAMINE OXIDASE CATALYSIS CONCERTED OR STEPWISE HYDRIDE TRANSFER MECHANISM**

ERDEM S., AKYÜZ M. A., ENİSOĞLU ATALAY V., ENGİN H., ÇAKIR K.



5th EuCheMS Chemistry Congress, İstanbul, Turkey, 31 August - 04 September 2014

- LXII. **QSAR Study on Glutathione S Transferase GST Inhibitory Activity of Ethacrynic Acid Oxadiazole Derivatives**  
OHANOĞLU L., SAÇAN M., ERDEM S.  
16th International Workshop on Quantitative Structure-Activity Relationship in Environmental and Health Sciences, Milan, Italy, 16 - 20 June 2014
- LXIII. **Monoamin Oksidaz Enzimlerinin Hidrür Mekanizmasının Dispersiyon Etkili DFT Yöntemleri İle Enzim Aktif Bölgesinde Modellenmesi**  
AKYÜZ M. A., ERDEM S.  
1.Ulusal Hesaplamalı Kimya Çalıştayı, Turkey, 29 - 31 May 2014
- LXIV. **Nörotransmitter Aminlerin MAO Enzimi ile Oksitlenme Mekanizmasının PM6 Yöntemiyle Modellenmesi**  
ÇAKIR K., ENGİN H., ENİSOĞLU ATALAY V., ERDEM S.  
1.Ulusal Hesaplamalı Kimya Çalıştayı, Turkey, 29 - 31 May 2014
- LXV. **Monoamin Oksidaz Enziminin Nörotransmitter Aminleri Oksitleme Mekanizmasına Elektron çekici Grupların Etkisinin İncelenmesi**  
ENGİN H., ÇAKIR K., ENİSOĞLU ATALAY V., ERDEM S.  
1.Ulusal Hesaplamalı Kimya Çalıştayı, Turkey, 29 - 31 May 2014
- LXVI. **Alzheimer Tedavisine Yönelik Akılcı İlaç Tasarımı Asetilkolinesteraz ve Monoamin Oksidaz İnhibitörleri İle QSAR Analizi**  
TÜRK H., SAÇAN M., ERDEM S.  
1.Ulusal Hesaplamalı Kimya Çalıştayı, Turkey, 29 - 31 May 2014
- LXVII. **Pirolotriazepin Türevlerinin Sentezi ve Reaksiyon Mekanizmasının DFT Yöntemi ile Modellenmesi**  
SARI Ö., MENGEŞ N., ABDULLAYEV Y., ERDEM S., BALCI M.  
1.Ulusal Hesaplamalı Kimya Çalıştayı, Turkey, 29 - 31 May 2014
- LXVIII. **P Süstitüe Benzilamin Türevlerinin Monoamin Oksidaz Enziminin Kataliz Mekanizmasına Etkilerinin İncelenmesi**  
ENİSOĞLU ATALAY V., ERDEM S.  
1.Ulusal Hesaplamalı Kimya Çalıştayı, Turkey, 29 - 31 May 2014
- LXIX. **7 Azaindolizin Türevlerinin Sentezi ve Reaksiyon Mekanizmasının DFT Metodu ile Modellenmesi**  
SARI Ö., MENGEŞ N., ERDEM S., BALCI M.  
1.Ulusal Hesaplamalı Kimya Çalıştayı, Turkey, 29 - 31 May 2014
- LXX. **Molecular Docking of New Coumarin Derivatives As Selective Inhibitors of Monoamine Oxidase A and B**  
ERZİNCAN P., DANIŞ Ö., YÜCE DURSUN B., GÜRBÜZ S., ERDEM S., OGAN A.  
2nd International BAU-Drug Design Symposium, 17 - 19 April 2014
- LXXI. **Effect of Tyr398 Mutations on Amine Oxidation Mechanism of MAO B Computational Investigation Using Model Structures**  
ENGİN H., ENİSOĞLU ATALAY V., ERDEM S.  
2nd International BAU-Drug Design Symposium, 17 - 19 April 2014
- LXXII. **Modeling Inhibition of Monoamine Oxidase by Xanthone Derivatives using Genetic Algorithm**  
KÖKTÜRK M., ERDEM S., TUĞCU G., SAÇAN M.  
2nd International BAU-Drug Design Symposium, 17 - 19 April 2014
- LXXIII. **The Effect of Tyr407 Mutations on Amine Oxidation Mechanism of MAO A Computational Investigation Using Model Structures**  
ENİSOĞLU ATALAY V., ERDEM S.  
2nd International BAU-Drug Design Symposium, 17 - 19 April 2014
- LXXIV. **Molecular Docking of New Coumarin Derivatives as Selective Inhibitors of Monoamine Oxidase A and B**  
PINAR E., DANIŞ Ö., YÜCE DURSUN B., DEMİR S., ERDEM S., OGAN A.  
2nd International BAU Drug Design Symposium, 17 - 19 April 2014
- LXXV. **AZAINDOLİZİN TÜREVLERİNİN SENTEZİ VE REAKSİYON MEKANİZMASININ DFT YÖNTEMİ İLE**

## MODELLENMESİ

ERDEM S.

2. İlaç Kimyası Kongresi, Antalya, Turkey, 21 - 23 March 2014

- LXXVI. **2 o metoksifenil imino 3 o metoksifenil 4 hidroksitiazolidin izomerlerinin aksiyel kiralitesinin hesapsal modellenmesi**  
SABUNCU GÜRSES G., ERDEM S., EROL Ş., DOĞAN İ.  
1.Ulusal Organik Kimya Kongresi, Sakarya, Turkey, 25 - 29 October 2013
- LXXVII. **Monoamin oksidaz enziminin amin oksidasyonu için alternatif bir mekanizma**  
ENİSOĞLU ATALAY V., ERDEM S.  
1.Ulusal Organik Kimya Kongresi, Turkey, 25 - 29 October 2013
- LXXVIII. **Monoamin oksidaz enziminin amin oksitleme mekanizmasının hesapsal yöntemler kullanarak karşılaştırılması**  
ENİSOĞLU ATALAY V., ERDEM S.  
1.Ulusal Organik Kimya Kongresi, Turkey, 25 - 29 October 2013
- LXXIX. **Monoamin oksidaz enziminin aktif bölgesinde p süstitüe benzilaminlerin yapı aktiflik ilişkilerinin incelenmesi**  
AKYÜZ M. A., ERDEM S.  
1.Ulusal Organik Kimya Kongresi, Turkey, 25 - 29 October 2013
- LXXX. **A DFT Study of Modelling Cellulose**  
ABDURRAHMANOĞLU S., ERDEM S.  
27th Molecular Modeling Workshop, 25 - 27 February 2013
- LXXXI. **Density Functional Theory Investigation on Structural and Electronic Properties of Metallophthalocyanines Zn and Ni**  
ERDEM S., SALMAN S., ÖZPINAR G., DURMUŞ M.  
Chemical Physics Congress-X (CPC-X), Ankara, Turkey, 10 - 12 October 2012
- LXXXII. **Modelling the Reaction Mechanism for the Formation of Triazepine Derivatives A Computational DFT Study**  
ERDEM S., SARI Ö., BALCI M., MENGEŞ N.  
Chemical Physics Congress-X (CPC-X), Ankara, Turkey, 10 - 12 October 2012
- LXXXIII. **Insights into the Binding Mode of New N substituted Pyrazoline Derivatives to MAO**  
ERDEM S., TÜRKKAN S., YELEKÇİ K., GÖKHAN KELEKÇİ N.  
15th Congress on Amine Oxidases 2012, 16 - 18 July 2012
- LXXXIV. **Computational Modeling of the Direct Hydride Transfer Mechanism for the MAO**  
AKYÜZ M. A., ERDEM S.  
15th Congress on Amine Oxidases 2012, 16 - 18 July 2012
- LXXXV. **QSAR modeling on the monoamine oxidase inhibitory activity of hydrazone derivatives**  
AYDIN O., SAÇAN M., ERDEM S., GÖKHAN KELEKÇİ N., GÖKŞEN U. S.  
6th International Symposium on Computational Methods in Toxicology and Pharmacy Integrating Internet Resources - CMTPI 2011, Maribor, Slovenia, 3 - 07 September 2011
- LXXXVI. **QSAR study of pyrazole derivatives as monoamine oxidase inhibitors**  
KÖKTÜRK M., ERDEM S., SAÇAN M., WRACKO M., NOVIC M., MINOVSKI N.  
6th International Symposium on Computational Methods in Toxicology and Pharmacy Integrating Internet Resources - CMTPI 2011, Maribor, Slovenia, 3 - 07 September 2011
- LXXXVII. **Polihalojenlenmiş nitrobutadienlerin elektronca eksik anilinlerle verdiği reaksiyon mekanizmasının DFT metodu ile modellenmesi**  
SARI Ö., ERDEM S., KAUFMANN D.  
25. Ulusal Kimya Kongresi, Erzurum, Turkey, 27 June - 02 July 2011
- LXXXVIII. **Hidrazon Türevi MAO İnhibitörleri ile Akılcı İlaç Tasarımına Yönelik Kantitatif Yapı Aktivite İlişkisi Oluşturulması**  
AYDIN O., ERDEM S., SAÇAN M., GÖKHAN KELEKÇİ N., GÖKŞEN U. S.  
25. Ulusal Kimya Kongresi, Erzurum, Turkey, 27 June - 02 July 2011

- LXXXIX. **Modeling The Mechanism Of The Reaction Between Polyhalogenated Nitrobutadienes And Electron Deficient Anilines**  
ERDEM S.  
9. Kimyasal Fizik Kongresi, Turkey, 14 - 16 October 2010
- XC. **ONIOM calculations in the active site of monoamine oxidase B First computational evidence for the direct hydride transfer mechanism**  
ERDEM S.  
The 14th International Amine Oxidase Workshop, 18 - 21 July 2010
- XCI. **A comparative computational investigation on the proton and hydride transfer mechanisms of monoamine oxidase using model molecules**  
ERDEM S.  
The 14th International Amine Oxidase Workshop, Canada, 18 - 21 July 2010
- XCII. **Molecular docking of new MAO A selective pyrazoline derivatives**  
ERDEM S.  
The 14th International Amine Oxidase Workshop, Canada, 18 - 21 July 2010
- XCIII. **Computational investigation on the structure activity relationship of the proposed biradical mechanism for monoamine oxidase**  
ERDEM S.  
The 14th International Amine Oxidase Workshop, Canada, 18 - 21 July 2010
- XCIV. **MAO A İçin Önerilen Polar Nükleofilik Mekanizma nın Modellenmesi Aromatik Aminoasitlerin Etkisi**  
ERDEM S.  
24. Ulusal Kimya Kongresi, Zonguldak, Turkey, 29 June - 02 July 2010
- XCV. **The Effect of Active Site Tyrosine Orientation on Binding Of New Pyrazoline Derivatives To MAO B Molecular Docking and Dynamic Simulations**  
ERDEM S.  
Third International Meeting on Pharmacy ve Pharmaceutical Sciences, İstanbul, Turkey, 9 - 12 June 2010
- XCVI. **QSAR STUDY OF PHENYLALKYLAMINE DERIVATIVES AS MONOAMINE OXIDASE INHIBITORS**  
ERDEM S.  
Third International Meeting on Pharmacy ve Pharmaceutical Sciences, İstanbul, Turkey, 9 - 12 June 2010
- XCVII. **QSAR study on xanthone derivatives as monoamine oxidase inhibitors**  
ERDEM S.  
QSAR 2010, Canada, 24 - 28 May 2010
- XCVIII. **Effect of Tyr407 and Tyr444 Mutations on Substrate Nucleophilicity in Monoamine Oxidase A**  
ENİSOĞLU ATALAY V., ERDEM S.  
PROTIST'10, İstanbul, Turkey, 24 - 25 April 2010
- XCIX. **Moleculer Docking of New Pyrazoline Derviatives To The Active Site Of Monoamine Oxidase**  
TÜRKKAN S., ERDEM S., YELEKÇİ K., GÖKHAN KELEKÇİ N., UMUT S G.  
5th International Symposium On Computational Methods In Toxicology And Pharmacology Intergrating Internet Resources (CMTPI-2009), 4 - 08 July 2009
- C. **MAO A nın Katalizleme Mekanizmasında Hangi Aminoasit Tyr407 Tyr444 Daha Etkin**  
ENİSOĞLU ATALAY V., ERDEM S., EDMONDSON D. E.  
23. Ulusal Kimya Kongresi, Sivas, Turkey, 16 - 20 June 2009
- CI. **Amine Oxidation Mechanism Of Monoamine Oxidase Revisited Structure Activity Relationships On Direct Hydride Transfer Mechanism**  
ERDEM S.  
13th International Amine Oxidase Meeting, PEKIN, China, 11 - 15 October 2008
- CII. **ONIOM Calculations On The Active Site Of Human MAO A And Its Tyrosine 444 Mutant Enzymes**  
ENİSOĞLU ATALAY V., ERDEM S., EDMONDSON D. E.  
13th International Amine Oxidase Meeting, 11 - 15 October 2008
- CIII. **Computational Modeling Of The Single Electron Transfer Mechanism For Monoamine Oxidase**  
ERDEM S., AKYÜZ M. A.

13th International Amine Oxidase Meeting, 11 - 15 October 2008

- CIV. **Computational Studies on The Active Site of Monoamine Oxidases**  
ENİSOĞLU ATALAY V., AKYÜZ M. A., ERDEM S.  
2nd Workshop on Computer Aided Drug Design & Development Molecular Modelling, Ankara, Turkey, 26 - 29 June 2008
- CV. **Model studies on the aromatic ring amine hydrogen bonding interactions Performance of ONIOM methodology**  
AKYÜZ M. A., ERDEM S.  
Chemical Physics Conference VIII, 24 - 25 April 2008
- CVI. **ONIOM Calculations on the active site of human monoamine oxidase B and its Tyr435 mutants Function of the aromatic cage**  
ERDEM S., AKYÜZ M. A., EDMONDSON D. E.  
Chemical Physics Conference VIII, İstanbul, Turkey, 24 - 25 April 2008
- CVII. **ONIOM Calculations on the active site of human monoamine oxidase A Function of the aromatic cage**  
ENİSOĞLU ATALAY V., ERDEM S., EDMONDSON D. E.  
Chemical Physics Conference VIII, 24 - 25 April 2008
- CVIII. **Theoretical investigation on the reaction mechanism of quinoxalinone N oxide synthesis A DFT study**  
ÖZPINAR G., ERDEM S., KAUFMANN D.  
Chemical Physics Conference VIII, 24 - 25 April 2008
- CIX. **A plausible pathway for nucleophilic addition of trichloronitroethylene to aniline through cis trans isomerization**  
ÖZPINAR G., ERDEM S., MEYER C., KAUFMANN D. E.  
22. Darmstadter Molecular Modelling Workshop, 01 April 2008
- CX. **Stereoelectronic Effects on the Conformational Barrier of Model Amine Compounds Related with the Inhibition of Monoamine Oxidase**  
ERDEM S., ÇİĞİT A.  
5th International Symposium on Pharmaceutical Chemistry, 5 - 07 September 2007
- CXI. **Modelling the Effect of Heteroatom on the Inhibition of Monoamine Oxidase by Oxazolidinone and Related Heterocycles**  
ERDEM S., BOZ Ü.  
5th International Symposium on Pharmaceutical Chemistry, İstanbul, Turkey, 5 - 07 September 2007
- CXII. **Assessment and Modelling of the Toxicity of Substituted Aromatic Compounds to Five Aquatic Species**  
ERTÜRK D., SAÇAN M., ERDEM S.  
Fourth International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources, MOSKOW, 1 - 05 September 2007
- CXIII. **Thermal rearrangement of 2 acetoxy 2 6 6 trimethylbicyclo 3 1 0 hexane Theoretical elucidation of the mechanism**  
YELEKÇİ K., ERDEM S.  
234th ACS National Meeting, BOSTON, United States Of America, 19 - 23 August 2007
- CXIV. **Principal Component Analysis on Aromaticity of Substituted Fulvenes**  
ÖZPINAR G., ERDEM S.  
9th Euroasia Conference on Chemical Sciences, Antalya, Turkey, 9 - 13 September 2006
- CXV. **2 Asetoksi 2 6 6 Trimetilbisiklo 3 1 0 Hekzan ın Termal Pirolyzi İçin Önerilen Biradikal Mekanizmaların Modellenmesi**  
ERDEM S., YELEKÇİ K.  
XX. Ulusal Kimya Kongresi, Kayseri, Turkey, 4 - 08 September 2006
- CXVI. **Monoamin Oksidazın Amin Oksitleme Mekanizmasının Modellenmesi**  
AKYÜZ M. A., ERDEM S.  
XX. Ulusal Kimya Kongresi, Kayseri, Turkey, 4 - 08 September 2006
- CXVII. **MAO B Enziminin Oksozolidinon ve Benzeri Heterosiklik Bileşikler ile İnhibisyonunun Teorik**

## **Modellenmesi**

BOZ Ü., ERDEM S.

XX. Ulusal Kimya Kongresi, Turkey, 4 - 08 September 2006

### **CXVIII. Fulven Aromatikliğine Sübstitüent Etkisinin NICS Yöntemi İle Araştırılması**

KELEŞ R., ÖZPINAR G., ERDEM S.

XX. Ulusal Kimya Kongresi, Turkey, 4 - 08 September 2006

### **CXIX. The Aromatic Cage in the Active Site of Monoamine Oxidase B Effect on the Structural and Electronic Properties of Bound Benzilamine and p Nitrobenzylamine**

AKYÜZ M. A., ERDEM S., EDMONDSON D. E.

12th Amine Oxidase and Trace Amine Workshop, Rotterdam, Netherlands, 30 July - 03 August 2006

### **CXX. Mechanistic Investigation On the Preparation of Quinoxalinones Electrophilic Aromatic Substitution Mechanism**

ÖZPINAR G., ERDEM S., KAUFMANN D.

7th International Conference on Chemical Physics, Isparta, Turkey, 19 - 20 May 2006

### **CXXI. The Effect of Monoamine Oxidase B Active Site On the Structural and Electronic Properties of p Nitrobenzylamine**

AKYÜZ M. A., ERDEM S.

7th International Conference on Chemical Physics, Isparta, Turkey, 19 - 20 May 2006

### **CXXII. 2 Asetoksi 2 6 6 Trimetilbisiklo 3 1 0 Hekzanın 1 3 3 Trimetil 1 4 Sikloheksadien e Dönüşme Mekanizmasının Ab Initio ve DFT Hesaplamaları**

ERDEM S., YELEKÇİ K.

XIX. Ulusal Kimya Kongresi, Turkey, 30 September - 04 October 2005

### **CXXIII. QSAR Analysis of the Toxicity of Aromatic Compounds to the Alga Scenedesmus obliquus**

SAÇAN M., ERDEM S.

4th Indo-US Workshop on Mathematical Chemistry, Pune, India, 8 - 12 January 2005

### **CXXIV. Physico chemical properties of PCDD PCDFs and phthalate esters A QSPR study**

SAÇAN M., ERDEM S.

4th Indo-US Workshop on Mathematical Chemistry, Pune, India, 8 - 12 January 2005

### **CXXV. The Monoamine Oxidase Catalytic Pathway A Computational Study**

ERDEM S., KARAHAN Ö., YILDIZ İ., YELEKÇİ K.

Chemical PhysicsVI (The Sixth International Conference on Chemical Physics), İstanbul, Turkey, 15 - 17 October 2004

### **CXXVI. Substituent Effect on Fulvene Reactivity**

ÖZPINAR G., ERDEM S., ÖCAL SUNGURUĞLU Z. N.

Chemical PhysicsVI (The Sixth International Conference on Chemical Physics), İstanbul, Turkey, 15 - 17 October 2004

### **CXXVII. A Computational Study On The Amine Oxidation Mechanism of Monoamine Oxidase Polar Nucleophilic or Radical Mechanism**

ERDEM S., YILDIZ İ., KARAHAN Ö., YELEKÇİ K.

11th Amine Oxidase Workshop, 25 - 29 July 2004

### **CXXVIII. Mono Amin Oksidaz MAO Enziminin Aminleri Tek Elektron Transferi ile Oksitleme Mekanizmasının Hesapsal Yöntemlerle İncelenmesi**

ERDEM S., YELEKÇİ K., KARAHAN Ö.

XVIII. Ulusal Kimya Kongresi, Turkey, 5 - 09 July 2004

### **CXXIX. 1 3 4 Tiadiazol 2 Tion ve Oksijenli Türevlerinin Aromatikliklerinin Araştırılmasında DFT Hesaplamaları ve Temel Bileşen Analizi**

ERDEM S., ÖZPINAR G., SAÇAN M.

XVIII. Ulusal Kimya Kongresi, Turkey, 5 - 09 July 2004

### **CXXX. Organik Kirleticilerin Biyokonsantrasyon Faktörlerinin Karakteristik Kök İndeksi ve Kuantum Kimyasal Tanımlayıcılarla Modellenmesi**

SAÇAN M., ERDEM S., ÖZPINAR G., BALCIOĞLU A.

- XVIII. Ulusal Kimya Kongresi, Kars, Turkey, 5 - 09 July 2004
- CXXXI. **Mono Amin Oksidaz MAO İnhibisyonu ile İlişkili Model Amin Bileşiklerinin Konformasyonel Analizi**  
KIRSAKAL A., ERDEM S.  
XVIII. Ulusal Kimya Kongresi, Turkey, 5 - 09 July 2004
- CXXXII. **DFT Calculations For the Determination of Aromaticity of 1 3 4 Thiodiazole 2 Thione and Its Oxygen Analogs**  
ERDEM S., ÖZPINAR G., SAÇAN M.  
10th International Conference on The Applications of Density Functional Theory, Belgium, 7 - 12 September 2003
- CXXXIII. **QSPR Study on the Bioconcentration Factors of Nonionic Organic Compounds in Fish by Characteristic Root Index and Semi empirical Molecular Descriptors**  
SAÇAN M., ERDEM S., ÖZPINAR G., BALCIOĞLU A.  
Third-Indo Workshop on Mathematical Chemistry, United States Of America, 2 - 07 August 2003
- CXXXIV. **Computer Modelling of Addition Elimination Mechanism of Monoamine Oxidase**  
YILDIZ İ., ERDEM S., YELEKÇİ K.  
Chemical Physics V (The Fifth International Conference on Chemical Physics), İstanbul, Turkey, 31 October - 01 November 2002
- CXXXV. **Substituent Effect on the Stability of Mono and Di Substituted Fulvenes**  
ERDEM S., ÖCAL SUNGUROĞLU Z. N.  
Chemical Physics V (The Fifth International Conference on Chemical Physics), İstanbul, Turkey, 31 October - 01 November 2002
- CXXXVI. **Modeling of Monoamine Oxidase B inactivation The Role Of Non Bonded Interactions and Stereoelectronic Effects in Enzyme Adducts**  
ERDEM S., KAHRAMAN M. V., YELEKÇİ K.  
10th International Amine Oxidase Workshop , İstanbul, August 25-29, 2002, 25 - 29 August 2002
- CXXXVII. **Computer Modeling of MAO Inactivation Electronic Effects on the Stability of Enzyme Adduct Model Methylthio Ethylamine**  
ERDEM S.  
10 th International Amine Oxidase Workshop, İstanbul, Turkey, 25 - 29 August 2002
- CXXXVIII. **Modeling of Monoamine Oxidase B Inactivation The Role of None Bonded Iteractions and StereoElectronic Effects in Enzyme Adducts**  
ERDEM S., KAHRAMAN M. V., YELEKÇİ K.  
10 th International Amine Oxidase Workshop, İstanbul, Turkey, 25 - 29 August 2002
- CXXXIX. **Aromaticity of 1 3 4 Thiadiazole 2 Thione and Its Oxygen Analogous**  
ERDEM S., ÖZPINAR G.  
International Organic Chemistry Meeting, Hatay, Turkey, 25 - 28 March 2002
- CXL. **Metiltiyoetilaminin Konformasyonel Analizi**  
ERDEM S.  
XV. Ulusal Kimya Kongresi, İstanbul, Turkey, 4 - 07 September 2001
- CXLI. **2 Asetoksi 2 6 6 Trimetilbisiklo 3 1 0 Hekzanın Termal Proliz Mekanizmasının İncelenmesi**  
ERDEM S., YELEKÇİ K.  
XV. Ulusal Kimya Kongresi, Turkey, 4 - 07 September 2001
- CXLII. **Electronic Structure of New Aryl and Alkyl Substituted 1 3 4 Oxadiazole 2 thione Derivatives**  
ERDEM S., ÖCAL SUNGUROĞLU Z. N., AYDOĞAN F.  
The 12 th Europan Symposium on Organic Chemistry, Netherlands, 13 - 18 July 2001
- CXLIII. **Bis 4 4 İsoşyanatofenil Fenil Fosfinoksitten Çıkılarak Hazırlanan İzosiyanat Sonlu Prepolimerlerde Reaktivitenin Teorik İncelenmesi**  
ERDEM S.  
Chemical Physics IV, Eskişehir, Turkey, 28 - 29 September 2000
- CXLIV. **Monoamin Oksidaz Enziminin İnhibisyonunun Modellenmesi Aminoeterlerde İntramoleküler O H Etkileşimleri**  
ERDEM S., YELEKÇİ K.

Chemical Physics IV, Eskişehir, Turkey, 28 - 29 September 2000

- CXLV. **Heteroatom İçeren Heptilamin Türevlerinin Sentezi ve MAO B İnaktivasyonuna Etkileri**  
YELEKÇİ K., KAHRAMAN M. V., ERDEM S.  
XIV. Ulusal Kimya Kongresi, Turkey, 10 - 15 September 2000
- CXLVI. **Toluendiizosiyanttan Çıkılarak Hazırlanan İzosiyanat Sonlu Prepolimerlerde Reaktivitenin Teorik İncelenmesi**  
ERDEM S.  
XIV. Ulusal Kimya Kongresi, Diyarbakır, Turkey, 10 - 15 September 2000
- CXLVII. **Wallach Düzenleme Mekanizmasının Hesapsal Modellenmesi**  
ÖZEN A., ERDEM S., AVİYENTE V.  
XIV. Ulusal Kimya Kongresi, Diyarbakır, Turkey, 10 - 15 September 2000
- CXLVIII. **Inductive effect of a heteroatom containing heptylamine analogues on MAO B**  
YELEKÇİ K., SILVERMAN R., ERDEM S.  
9 th International Amine Oxidase Workshop, Barcelona, Spain, 9 - 12 July 2000
- CXLIX. **Porfirin Dimerlerinde Proton Transferinin Hesapsal Analizi**  
ERDEM S.  
XIII. Ulusal Kimya Kongresi, Samsun, Turkey, 4 - 09 September 1999
- CL. **A computational study of the reactivity of diethylnaphthalenes towards anionic polimerization**  
ERDEM S., AVİYENTE V.  
13th Canadian Symposium on Theoretical Chemistry, 2 - 07 August 1998
- CLI. **An Ab İnitio and PM3 study on conformational behaviour of 1 1 2 trihydroxyethane**  
ERDEM S., AVİYENTE V., RUÍZ LOPEZ M.  
NATO-ASI Symposium-Frontiers of Chemical Dynamics, Antalya, Turkey, 4 - 17 September 1994
- CLII. **2 Sübstitüe sikloheksanon propilen ketallerin konformasyonel dengesi üzerine çözücü etkileri**  
ERDEM S., AVİYENTE V., RUÍZ LOPEZ M.  
IX. Kimya ve Kimya Mühendisliği Sempozyumu, Trabzon, Turkey, 20 - 24 September 1993
- CLIII. **2 Metil ve 2 halo sikloheksanonun etilen ketallerinin konformasyonel dengeleri üzerine çözücü etkileri**  
ERDEM S., AVİYENTE V., RUÍZ LOPEZ M.  
VIII. Kimya Ve Kimya Mühendisliği Sempozyumu, İstanbul, Turkey, 7 - 11 September 1992

## Metrics

Publication: 209

Citation (WoS): 750

Citation (Scopus): 750

H-Index (WoS): 17

H-Index (Scopus): 16

## Non Academic Experience

Marmara Üniversitesi

Boğaziçi Üniversitesi

Boğaziçi Üniversitesi

Özel Ortadoğu Koleji

Özel Yükseliş Koleji

Villanova University

Boğaziçi Üniversitesi