

Prof. SAFİYE ERDEM

Personal Information

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International Researcher IDs

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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, 2013 - Continues

Marmara University, Faculty of Arts and Sciences, Chemistry, 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

Supervised Theses

Erdem S., Danış Ö., Arilkumarin türevlerinin beta-laktamaz ve karbapenemaz aktivitesi üzerine etkilerinin incelenmesi, Postgraduate, B.Hamur(Student), 2019
ERDEM S., Flavoenzimlerdeki flavin oksidasyonu mekanizmasının hesapsal modellenmesi, Postgraduate, İ.Demir(Student), 2017
ERDEM S., Flavin redoks tepkimesine sübtitüent etkisinin modellenmesi, Postgraduate, A.Topal(Student), 2017
ERDEM S., Computational and mechanistic studies on the formation of cyclic systems, Doctorate, Ö.SARI(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., Fulven türevlerinin aromatikliğinin nics yöntemi ile araştırılması, Postgraduate, R.Keleş(Student), 2007
ERDEM S., Para-sübtitüe benzilaminlerin monoamin oksidaz ile tepkimelerinde yapı-aktiflik ilişkisinin incelenmesi, Postgraduate, O.Can(Student), 2007
ERDEM S., Monoamin oksidaz substratlarının enzimin aktif bölgesi içinde QM/MM yöntemi ile modellenmesi, Postgraduate, M.Ali(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., Mono Amin Oksidaz (MAO) enziminin ekleme eliminasyon mekanizmasının hesapsal yöntemlerle incelenmesi, Postgraduate, İ.Yıldız(Student), 2003

ERDEM S., 2-Süstitüe-Metiltyoetilamin türevlerinin konformasyonel analizi, Postgraduate, M.Durmuş(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 α -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)

Papers Published in Refereed Scientific Meetings

- 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

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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.

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

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

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

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

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

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

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- LXIV. **Nörotransmitter Aminlerin MAO Enzimi ile Oksitlenme Mekanizmasının PM6 Yöntemiyle Modellenmesi**
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- LXV. **Monoamin Oksidaz Enziminin Nörotransmitter Aminleri Oksitleme Mekanizmasına Elektron çekici Grupların Etkisinin İncelenmesi**
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- LXVI. **Alzheimer Tedavisine Yönelik Akılcı İlaç Tasarımı Asetilkolinesteraz ve Monoamin Oksidaz İnhibitörleri İle QSAR Analizi**
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- LXVII. **Pirolotriazepin Türevlerinin Sentezi ve Reaksiyon Mekanizmasının DFT Yöntemi ile Modellenmesi**
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- LXIX. **7 Azaindolizin Türevlerinin Sentezi ve Reaksiyon Mekanizmasının DFT Metodu ile Modellenmesi**
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- LXX. **Molecular Docking of New Coumarin Derivatives As Selective Inhibitors of Monoamine Oxidase A and B**
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- LXXVI. **2 o metoksifenil imino 3 o metoksifenil 4 hidroksitiazolidin izomerlerinin aksiyel kiralitesinin hesapsal modellenmesi**

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- LXXVII. **Monoamin oksidaz enziminin amin oksidasyonu için alternatif bir mekanizma**
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- LXXVIII. **Monoamin oksidaz enziminin amin oksitleme mekanizmasının hesapsal yöntemler kullanarak karşılaştırılması**

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- LXXIX. **Monoamin oksidaz enziminin aktif bölgesinde p süstitüe benzilaminlerin yapı aktiflik ilişkilerinin incelenmesi**

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- LXXX. **A DFT Study of Modelling Cellulose**

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- LXXXI. **Density Functional Theory Investigation on Structural and Electronic Properties of Metallophthalocyanines Zn and Ni**

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- LXXXII. **Modelling the Reaction Mechanism for the Formation of Triazepine Derivatives A Computational DFT Study**

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- LXXXIII. **Insights into the Binding Mode of New N substituted Pyrazoline Derivatives to MAO**

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- LXXXIV. **Computational Modeling of the Direct Hydride Transfer Mechanism for the MAO**

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- LXXXV. **QSAR modeling on the monoamine oxidase inhibitory activity of hydrazone derivatives**

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- LXXXVI. **QSAR study of pyrazole derivatives as monoamine oxidase inhibitors**

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- LXXXVIII. **Hidrazon Türevi MAO İnhibitörleri ile Akılcı İlaç Tasarımına Yönelik Kantitatif Yapı Aktivite İlişkisi Oluşturulması**

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- LXXXIX. **Modeling The Mechanism Of The Reaction Between Polyhalogenated Nitrobutadienes And Electron Deficient Anilines**
ERDEM S.
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- XC. **ONIOM calculations in the active site of monoamine oxidase B First computational evidence for the direct hydride transfer mechanism**
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- XCI. **A comparative computational investigation on the proton and hydride transfer mechanisms of monoamine oxidase using model molecules**
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- XCII. **Molecular docking of new MAO A selective pyrazoline derivatives**
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- XCIII. **Computational investigation on the structure activity relationship of the proposed biradical mechanism for monoamine oxidase**
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- 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**
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- XCVI. **QSAR STUDY OF PHENYLALKYLAMINE DERIVATIVES AS MONOAMINE OXIDASE INHIBITORS**
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- XCVII. **QSAR study on xanthone derivatives as monoamine oxidase inhibitors**
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- XCVIII. **Effect of Tyr407 and Tyr444 Mutations on Substrate Nucleophilicity in Monoamine Oxidase A**
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- CI. **Amine Oxidation Mechanism Of Monoamine Oxidase Revisited Structure Activity Relationships On Direct Hydride Transfer Mechanism**
ERDEM S.
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- CII. **ONIOM Calculations On The Active Site Of Human MAO A And Its Tyrosine 444 Mutant Enzymes**
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- CIII. **Computational Modeling Of The Single Electron Transfer Mechanism For Monoamine Oxidase**
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- CIV. **Computational Studies on The Active Site of Monoamine Oxidases**
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- CV. **Model studies on the aromatic ring amine hydrogen bonding interactions Performance of ONIOM methodology**
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- CVI. **ONIOM Calculations on the active site of human monoamine oxidase B and its Tyr435 mutants Function of the aromatic cage**
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- CVIII. **Theoretical investigation on the reaction mechanism of quinoxalinone N oxide synthesis A DFT study**
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- CIX. **A plausible pathway for nucleophilic addition of trichloronitroethylene to aniline through cis trans isomerization**
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- CX. **Stereoelectronic Effects on the Conformational Barrier of Model Amine Compounds Related with the Inhibition of Monoamine Oxidase**
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- CXI. **Modelling the Effect of Heteroatom on the Inhibition of Monoamine Oxidase by Oxazolidinone and Related Heterocycles**
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- CXII. **Assessment and Modelling of the Toxicity of Substituted Aromatic Compounds to Five Aquatic Species**
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- CXIII. **Thermal rearrangement of 2 acetoxy 2 6 6 trimethylbicyclo 3 1 0 hexane Theoretical elucidation of the mechanism**
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- CXIV. **Principal Component Analysis on Aromaticity of Substituted Fulvenes**
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- CXV. **2 Asetoksi 2 6 6 Trimetilbisiklo 3 1 0 Hekzan ın Termal Pirolyzi İçin Önerilen Biradikal Mekanizmaların Modellenmesi**
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- CXVII. **MAO B Enziminin Oksozolidinon ve Benzeri Heterosiklik Bileşikler ile İnhibisyonunun Teorik**

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KELEŞ R., ÖZPINAR G., ERDEM S.

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

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- CXXXI. **Mono Amin Oksidaz MAO İnhibisyonu ile İlişkili Model Amin Bileşiklerinin Konformasyonel Analizi**
KIRSAKAL A., ERDEM S.
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- CXXXII. **DFT Calculations For the Determination of Aromaticity of 1 3 4 Thiodiazole 2 Thione and Its Oxygen Analogs**
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- CXXXIII. **QSPR Study on the Bioconcentration Factors of Nonionic Organic Compounds in Fish by Characteristic Root Index and Semi empirical Molecular Descriptors**
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- CXXXVI. **Modeling of Monoamine Oxidase B inactivation The Role Of Non Bonded Interactions and Stereoelectronic Effects in Enzyme Adducts**
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- CXXXVIII. **Modeling of Monoamine Oxidase B Inactivation The Role of None Bonded Iteractions and StereoElectronic Effects in Enzyme Adducts**
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- CXLIII. **Bis 4 4 İsoşyanatofenil Fenil Fosfinoksitten Çıkılarak Hazırlanan İzosiyanat Sonlu Prepolimerlerde Reaktivitenin Teorik İncelenmesi**
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- CXLV. **Heteroatom İçeren Heptilamin Türevlerinin Sentezi ve MAO B İnaktivasyonuna Etkileri**
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