# Nurcan S Tuzun

## List of Publications by Citations



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|---|---|---|---|
| 40 papers | 481 citations | 12 h-index | 20 g-index |
| 43 ext. papers | 534 ext. citations | 3.9 avg, IF | 3.88 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 40 | Spirodiporphyrins--as binuclear metal complexes. *Angewandte Chemie - International Edition*, **2003**, 42, 2857-62 | 16.4 | 78 |
| 39 | A DFT Study on the Binuclear CuAAC Reaction: Mechanism in Light of New Experiments. *Organometallics*, **2016**, 35, 2589-2599 | 3.8 | 39 |
| 38 | Reaction mechanism of ruthenium-catalyzed azide□alkyne cycloaddition reaction: A DFT study. *Journal of Organometallic Chemistry*, **2013**, 724, 167-176 | 2.3 | 31 |
| 37 | Cyclopolymerization reactions of diallyl monomers: exploring electronic and steric effects using DFT reactivity indices. *Journal of Physical Chemistry A*, **2009**, 113, 8704-11 | 2.8 | 30 |
| 36 | Modeling the free radical polymerization of acrylates. *International Journal of Quantum Chemistry*, **2005**, 103, 176-189 | 2.1 | 27 |
| 35 | A DFT Study on the Mechanism of Cyclopropanation via Cu(acac)2-Catalyzed Diazo Ester Decomposition. *Organometallics*, **2008**, 27, 4600-4610 | 3.8 | 23 |
| 34 | Metal-Catalyzed Cyclization Reactions of Carbonyl Ylides: Synthesis and DFT Study of Mechanisms. *Organometallics*, **2007**, 26, 2978-2985 | 3.8 | 22 |
| 33 | 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. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 311-330 | 5.6 | 20 |
| 32 | Theoretical study of factors controlling rates of cyclization of radical intermediates from diallylamine and diallylammonium monomers in radical polymerizations. *Journal of Organic Chemistry*, **2002**, 67, 5068-75 | 4.2 | 19 |
| 31 | The mechanism of copper-catalyzed azide-alkyne cycloaddition reaction: a quantum mechanical investigation. *Journal of Molecular Graphics and Modelling*, **2012**, 34, 101-7 | 2.8 | 18 |
| 30 | Ag-catalyzed azide alkyne cycloaddition: a DFT approach. *Dalton Transactions*, **2016**, 45, 5752-64 | 4.3 | 15 |
| 29 | A theoretical study on the mechanism of the cyclopolymerization of diallyl monomers. *Journal of Organic Chemistry*, **2003**, 68, 6369-74 | 4.2 | 14 |
| 28 | Modeling the effect of substitution on the Pb(OAc)4 mediated oxidative cleavage of steroidal 1,2-diols. *Journal of Organic Chemistry*, **2005**, 70, 7080-6 | 4.2 | 12 |
| 27 | A Computational Study on the Substituent Effect of Diallylamine Monomers in Their Cyclopolymerization Reactions. *Journal of Physical Chemistry A*, **2002**, 106, 8184-8190 | 2.8 | 12 |
| 26 | Superior Sensor for Be Ion Recognition via the Unprecedented Octahedral Crystal Structure of a One-Dimensional Coordination Polymer of Crown Fused Zinc Phthalocyanine. *Inorganic Chemistry*, **2019**, 58, 909-923 | 5.1 | 11 |
| 25 | Mechanistic Study on [3+2] Cycloaddition and Cyclopropanation Reactions of 1,3-Dioxepine Derivatives in the Presence of Copper(I) Catalyst. *Organometallics*, **2009**, 28, 4964-4973 | 3.8 | 10 |
| 24 | Modeling the cyclopolymerization of diallyl ether and methyl □[(allyloxy)methyl]acrylate. *International Journal of Quantum Chemistry*, **2007**, 107, 894-906 | 2.1 | 9 |

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| 23 | An experimental and quantum mechanical study on electrochemical properties of N-substituted pyrroles. *Computational and Theoretical Chemistry*, **2008**, 857, 95-104 | | 9 |
| 22 | A computational approach to the polymerizabilities of diallylamines. *Journal of Molecular Modeling*, **2001**, 7, 257-264 | 2 | 9 |
| 21 | New ferrocenyl naphthoquinone fused crown ether chemosensors: Highly selective, kinetically and regio controlled colorimetric, beryllium ion recognition. *Journal of Organometallic Chemistry*, **2018**, 868, 131-143 | 2.3 | 9 |
| 20 | Synthesis and characterization of solution processable 6,11-dialkynyl substituted indeno[1,2-b]anthracenes. *Dyes and Pigments*, **2014**, 100, 104-117 | 4.6 | 8 |
| 19 | A Theoretical Study On Rh(I) Catalyzed Enantioselective Conjugate Addition Reactions of Fluoroalkylated Olefins. *Organometallics*, **2014**, 33, 5111-5119 | 3.8 | 7 |
| 18 | Stereoselective propagation in free radical polymerization of acrylamides: a DFT study. *Journal of Molecular Graphics and Modelling*, **2014**, 49, 55-67 | 2.8 | 7 |
| 17 | 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. *Journal of Organometallic Chemistry*, **2017**, 851, 97-103 | 2.3 | 7 |
| 16 | Mechanism of CuAAC reaction: In acetic acid and aprotic conditions. *Journal of Molecular Catalysis A* , **2017**, 426, 150-157 | | 6 |
| 15 | Computational investigation of the control of the thermodynamics and microkinetics of the reductive amination reaction by solvent coordination and a co-catalyst.. *RSC Advances*, **2018**, 8, 36662-36674 | 3.7 | 6 |
| 14 | Mechanism of Kynurenine 3-Monooxygenase-Catalyzed Hydroxylation Reaction: A Quantum Cluster Approach. *Journal of Physical Chemistry A*, **2019**, 123, 3149-3159 | 2.8 | 5 |
| 13 | Synthesis, reactions and DFT study of tropolone N,N-dimethylthiocarbamate. *Tetrahedron*, **2015**, 71, 5391-5398 | 2.4 | 5 |
| 12 | A new perspective on the beryllium sensor platform: Low symmetry phthalocyanine-based molecular design and ultra trace amount Be2+ ion recognition in aqueous media. *Sensors and Actuators B: Chemical*, **2021**, 329, 129002 | 8.5 | 4 |
| 11 | Structural investigation of vesnarinone at the pore domains of open and open-inactivated states of hERG1 K channel. *Journal of Molecular Graphics and Modelling*, **2017**, 77, 399-412 | 2.8 | 3 |
| 10 | Amberlyst-15-catalyzed Procedure for the Synthesis of Novel 2,4-Dihydroxybenzoyl-1,2,3-triazoles and Molecular Modelling Studies for Hsp-90 Inhibition. *ChemistrySelect*, **2019**, 4, 7278-7283 | 1.8 | 2 |
| 9 | A Quantum Mechanical Study on the Propagation Kinetics of N-methylacrylamide: Comparison With N,N-Dimethylacrylamide in Free Radical Polymerization. *Macromolecular Theory and Simulations*, **2015**, 24, 218-231 | 1.5 | 2 |
| 8 | In silico design of novel hERG-neutral sildenafil-like PDE5 inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2830-2852 | 3.6 | 1 |
| 7 | Prediction of the 1H NMR spectra of epoxy-fused cyclopentane derivatives by calculations of chemical shifts and spin–spin coupling constants. *Molecular Physics*, **2013**, 111, 3147-3155 | 1.7 | 0 |
| 6 | In silico methods predict new blood-brain barrier permeable structure for the inhibition of kynurenine 3-monooxygenase. *Journal of Molecular Graphics and Modelling*, **2020**, 100, 107701 | 2.8 | 0 |

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| 5 | A QSPR Study on the Physical Properties of Substituted Polypyrroles and Poly(paraphenylenes). *Designed Monomers and Polymers*, **2011**, 14, 79-93 | 3.1 |
| 4 | Cover Picture: Spirodiporphyrins As Binuclear Metal Complexes (Angew. Chem. Int. Ed. 25/2003). *Angewandte Chemie - International Edition*, **2003**, 42, 2805-2805 | 16.4 |
| 3 | Computational Survey of Recent Experimental Developments in the Hydroxylation Mechanism of Kynurenine 3-Monooxygenase. *Journal of Physical Chemistry A*, **2021**, 125, 9459-9477 | 2.8 |
| 2 | Non-peripherally substituted metallophthalocyanines catalyzed diastereoselective carbonyl-ylide reactions: Synthesis and DFT calculations. *Tetrahedron*, **2021**, 80, 131892 | 2.4 |
| 1 | Regioselectivity Patterns in Radical Cyclization of Diosphenol Derivatives with Different Ring Size: A Combined Experimental and DFT Study. *ChemistrySelect*, **2021**, 6, 1748-1755 | 1.8 |