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#### I. Publications in Journals

- 1. Jafari-Chermahini, M., Tavakol, H. 2023. Employing nano-SnFe2O4 in the Synthesis of Arylbenzimidazoles, the Computational Study of the Reaction Mechanism, and examining the Products as Putative Human Transmembrane Protein Activators. Research on Chemical Intermediates, accepted.
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- Darrudi, M., Tavakol, H., & Momeni, M. M. 2023. Electrochemical co-deposition of cobalt and graphene, produced from recycled polypropylene, on TiO2 nanotube as a new catalyst for photoelectrochemical water splitting. International Journal of Hydrogen Energy, 48(9), 3495-3510.
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- 10. Tavakol, H, Ganbari, A., 2022. Nitrogen-modified graphene as a metal-free carbocatalyst for

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- 12. Abtahi, B. and Tavakol, H., **2021**. CuI-catalyzed, one-pot synthesis of 3-aminobenzofurans in deep eutectic solvents. Applied organometallic chemistry, accepted
- 13. Haghshenas, H., Kaviani, B., Firouzeh, M. and Tavakol, H., **2021**. Developing a variation of 3D-QSAR/MD method in drug design. Journal of Computational Chemistry, 42, 917–929.
- Jafari-Chermahini, M.T. and Tavakol, H., 2021. One-Pot Synthesis of Hantzsch 1, 4-Dihydropyridines by a Series of Iron Oxide Nanoparticles: Putative Synthetic TRPV6 Calcium Channel Blockers. ChemistrySelect, 6, 2360-2365.
- Tavakol, H., Momeni, M.M. and Mohammadi, B., 2021. Low-temperature preparation and photoelectrochemical properties of TiO2 nanotubes-graphene-CNT hybrid structure. Environmental Progress & Sustainable Energy, p.e13613.
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  2020 AMBER Force Field Parameters for Cobalt-Containing Biological Systems: A Systematic Derivation Study. J. Phys. Chem. B 124, 777–787
- Nedasadat Hasheminejad, Hossein Tavakol and Willi Salvenmoser; 2020 Preparation of golddecorated simple and sulfur-doped carbon spheres for desulfurization of fuel. Journal of Cleaner production, 264, 121684
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- 29. H Tavakol, D Shahabi, F Keshavarzipour, F Hashemi 2020 Theoretical calculation of simple and doped CNTs with the potential adsorption of various ions for water desalination technologies Structural Chemistry, 31, 399–409
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- Tavakol, Hossein; Mahmoudi, Amir; Ranjbari, Mohammad-Amin 2019 Synthesis of di- and tri-substituted thiourea derivatives in water using choline chloride-urea catalyst. Journal of sulfur chemistry, 40(2), 113-123
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- 49. Tavakol, Hossein; 2017 Study of binding energies using DFT methods, vibrational frequencies and solvent effects in the interaction of silver ions with uracil tautomers. Arabian Journal of Chemistry, 10, S786–S799.
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- 51. Keshavarzipour, Fariba; Tavakol, Hossein; 2017 Zinc cation supported on carrageenan magnetic nanoparticles: A novel, green and efficient catalytic system for one-pot three component synthesis of quinoline derivatives. Applied Organometallic Chemistry, 31, e3682
- 52. Shahabi, Dana; Tavakol, Hossein; 2017 Synthesis of 14H-dibenzo xanthene derivatives using choline chloride/tin (II) chloride deep eutectic solvent and Fe3O4/λ-carrageenan/Zn (II) Journal of the Iranian Chemical Society, 14:135–142
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- 58. Dehghanian, Fariba; Haghshenas, Hamed; Kay, Maryam; Tavakol, Hossein; **2016** A molecular dynamics investigation on the interaction properties of AzrC and its cofactor. Journal of the Iranian Chemical Society, 13, 2143-2153.
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#### **II.** Other publications

#### a. Books

- Physical Organic Chemistry (in Persian), 2014, Publisher: IUT publications.
- The basics of polymers' chemistry (in Persian), April 2012, Publisher: Noavaran Sharif
- Translation (to Persian) for: "Basic one- and two dimentional NMR Spectroscopy", Horst Friebolin, Forth edition, April 2009, Publisher: Gostareshe olume paye (1<sup>st</sup> and 2<sup>nd</sup> print)

• Theory and experiments in organic chemistry laboratory (in Persian), June 2009, Publisher: Aras rayaneh

# b. National conferences (abstracts)

- H. Tavakol, F. Jahanimogadam, F. Noormoha-mmadian and I. Yavari, Reaction of 2-Acetylpyrole with Acetylenic Esters in Presence of Phosphorous Nucleophiles, 8<sup>th</sup> Iranian Seminar of Organic Chemistry, Tehran University, Tehran, Iran, September 1999
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- H. Tavakol and A. Heydari, One-Pot Synthesis of β- (N- Hydroxy Amino) Esters from Aldehydes 11<sup>th</sup> Iranian seminar of Organic Chemistry, Isfahan University of Technology, Isfahan, Iran, 3-6 February 2005
- H. Tavakol and A. Heydari, One-pot reduction of aldimines in LPDE 5M 12<sup>th</sup> Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
- H. Tavakol and A. Heydari, Preparation of various hydroxylamines in three component aminoreduction reaction 12<sup>th</sup> Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
- H. Tavakol and A. Heydari, Preparation of trisubstituted hydrazines from aldehydes 12<sup>th</sup> Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
- 9. H. Tavakol and S. Zakery, Diastreoselective addition to SAMP hydrazones 12<sup>th</sup> Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
- H. Tavakol and S. Zakery, Preparation of secondary amines from one-pot reduction of ketimines 13<sup>th</sup> Iranian seminar of Organic Chemistry, Bu-Ali Sina University, Hamedan, Iran, 6-8 September 2006.
- 11. H. Tavakol and S. Zakery, Synthesis of α-Cyanohydroxylamines from Aldehydes 13<sup>th</sup> Iranian seminar of Organic Chemistry, Bu-Ali Sina University, Hamedan, Iran, 6-8 September 2006.
- 12. A. Heydari, H. Hamadi and H. Tavakol, Direct conversion of epoxides to alpha substituted phosphonates and beta-hydroxy phosphonates in lithiumperchlorate/diethyl ether solution 13<sup>th</sup> Iranian seminar of Organic Chemistry, Bu-Ali Sina University, Hamedan, Iran, 6-8 September 2006.
- H. Tavakol, Preparation of hydrazones from one-pot reduction of ketohydrazones 3<sup>rd</sup> Iranian national congress on chemistry, Islamic azad university of varamin, Varamin, Iran. 16,17 May 2007, Oral presentation.

- H. Tavakol, Investigation of Tautomerism in Amidoximes by Theoretical Method 15<sup>th</sup> Iranian seminar of Organic Chemistry, Razi University of Kermanshah, Kermanshah, Iran, 3-5 September 2008.
- 15. G. Geimachy, S. Ghammamy, A. Mehrani, T. Banibairami and H. Tavakol, Ionic Liquids: Synthesis and Characterisation of Triphenylphosphonium pentachlorohalophosphate (C6H5)3PH+[PCl5X]-, (X=F, Cl, I), (TPPPCHP) 12<sup>th</sup> Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
- 16. G. Geimachy1, M. alihosseinzadhe, S. Ghammamy, T. Banibairami and H. Tavakol, Synthesis, characterization of two new phosphates ionic liquids 12<sup>th</sup> Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
- 17. K. Nozarian, M. Montazerozohori, H. Tavakol and S. Khani, Synthesis, spectral and theoretical studies of some new zinc and cadmium complexes of a bidentate ligand 12<sup>th</sup> Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
- M. Razzaghi, M. Montazerozohori, H. Tavakol, A. Hojjati, Synthesis, spectral and theoretical studies of some new complexes of Zinc halides 12<sup>th</sup> Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
- 19. M. Sedighipoor, M. Montazerozohori, H. Tavakol, M. H. Habibi, Synthesis, spectral, theoretical and electrochemical studies of some new complexes ofmercury and cadmium with a new asymmetric Schiff base ligand 12<sup>th</sup> Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
- 20. M. Sedighipoor, M. Montazerozohori, H. Tavakol, M. H. Habibi, Synthesis, spectroscopic, theoritical and electrochemical studies of some new Zn(II), Cu(I) complexes, 12<sup>th</sup> Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
- 21. H. Tavakol and S. Zakery, DFT study of rate and equilibrium constants in tautomerism of organic structures, 15<sup>th</sup> Iranian Chemistry Congress, Hamedan, Iran, September 2011
- 22. H. Tavakol and S. Zakery, Computational Study of dynamic properties and level crossing in 2-(pyridin-2-yl) furan-3-ol, 15<sup>th</sup> Iranian Chemistry Congress, Hamedan, Iran, September 2011
- 23. M. Montazerozohori, H. Tavakol, S. A. Musavi and S. Yadegari, Theoretical study of some recently synthesized mercury complexes with a Schiff base ligand, 15<sup>th</sup> Iranian Chemistry Congress, Hamedan, Iran, September 2011
- M. Montazerozohori, H. Tavakol, S. A. Musavi and M. Hosseinpour, Theoretical study of some recently synthesized mercury and cadmium complexes with N, N-bis (3-(2nitrophenyl)propenaldehydene)-1, 2-phenylenediamine, 15<sup>th</sup> Iranian Chemistry Congress, Hamedan, Iran, September 2011.
- 25. H. tavakol, Hammett equation in the rate and equilibrium constant of keto-enol tautomerism, 18<sup>th</sup> Iranian seminar of Organic Chemistry, Zahedan, Iran, February 2012, Oral presentation.
- 26. H. tavakol, Tautomery scheme in 4-acyl pyrazolone, 18<sup>th</sup> Iranian seminar of Organic Chemistry, Zahedan, Iran, February 2012.
- 27. F. Keshavarzipour and H. Tavakol, Green synthesis of coumarin by Knoevenagel condensation using deep eutectic solvent choline chloride.2ZnCl<sub>2</sub> . 22<sup>nd</sup> Iranian seminar of organic chemistry, Tabriz, Iran, August 2014, Oral presentation.
- c. National conferences (full papers)

- 1. H. Tavakol, Computational Study of Thiohydroxamic Acids Tautomers 2<sup>nd</sup> Internatnal conference on mathematical chemistry, Kashan, Iran, April 2009, Oral presentation.
- 2. M. Montazerozohuri, H. Tavakol, A. Hojati and A. Rahiminia, Synthesis, identification and theoretical study of some mercuric halide complexes 8<sup>th</sup> national Payam-e-noor conference in chemistry, Qazvin, Iran, September 2010.
- M. Montazerozohuri, H. Tavakol, A. Hojati and J. Hasanalyan, Synthesis, and identification of some mercuric azide and thiocyanate complexes 8<sup>th</sup> national Payam-e-noor conference in chemistry, Qazvin, Iran, September 2010.
- 4. M. Montazerozohuri, H. Tavakol, A. Hojati and A. Rahiminia, Synthesis, identification and theoretical study of some cadmium azides and thiocyanate complexes 8<sup>th</sup> national Payam-e-noor conference in chemistry, Qazvin, Iran, September 2010.
- H. Tavakol, T. Hadad, The Effect of Water on the Equilibrium and Rate Constant of Tautomerism in Hydroxamic Acids, 14<sup>th</sup> Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.
- 6. H. Tavakol, S. Amiraslanzadeh, Study of Isomery Scheme in Acetyl Hydrazides by DFT Calculations, 14<sup>th</sup> Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.
- M. Montazerozohori , H. Tavakol ,A. Hojjati and K. Nozarian, Theoretical studies of some new synthesized four coordinated cadmium complexes, 14<sup>th</sup> Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.
- S.Zabihi, A.Fayyazi, G.Geimachy, M.Fada, Sh.Ghammamy, H. Tavakol, A Theoretical Investigation Structure of Two Ionic Liquids (C6H5)3PH+[As2S3X]-, (X=Cl, I), 14<sup>th</sup> Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.
- T. Hadadi, H. Tavakol, H. Roohi, Z. Razmara, Quantum mechanical study of interaction between 1-methyl-2-thioxoimidazolidin-4-one and I2 in the gas phase, 14<sup>th</sup> Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.

# d. International conferences

- H. Tavakol and A. Heydari, One-Pot Synthesis of Substituted Hydroxylamines Using LPDE 5M, XVIIIth Turkish National Congress, Kafkas University, Kars, Turkey, 6-9 July 2004
- H. Tavakol and S. Zakery, In Situ Addition of Organomethalic Reagents to Oxime Ethers, 40<sup>th</sup> IUPAC congress, Beijing, china, 14-19 August 2005, Oral presentation.
- H. Tavakol and S. Zakery, Multicomponent Additions to C=N Double Bond in Lithium Perchlorate 3<sup>rd</sup> international conference on Multi-Component Reactions & Related chemistry Amsterdam, the Netherlands 9-13 July 2006, Oral presentation.
- 4. H. Tavakol, Synthesis of α-hydroxy amino phosphonates from aldehydes XVII EuCheMS Conference on Organometallic Chemistry, Sofia, Bulgaria, 1-6 September 2007.
- 5. H. Tavakol, Study of undergraduate chemistry education in Iran 9th European Conference on Research in Chemical Education, Istanbul, Turkey, 6-9 July 2008.
- 6. H. Tavakol and S. Zakery, Investigation of Hydroxamic Acid Tautomers by DFT Method 13th Intern. Conf. on the Applic. of Density Functional Theory in Chemistry and Physics, DFT09, Lyon, France, 31 August-4 September.
- 7. H. Tavakol, Study of tautomerism in azirine and related systems: DFT calculations in the gas phase and solvent, ICYC 2010, Penang, Malaysia, 23-25 June 2010.

- 8. H. Tavakol, Computational study of inter and intramolecular proton transfer in amidrazones, Fourth International Symposium in Methods and Applications of Computational Chemistry, June 2011, Lviv, Ukraine.
- 9. A.R. Samzadeh, H. Tavakol, Theoretical study of inter and intramolecular proton transfer in N-hydroxy amidines, Fourth International Symposium in Methods and Applications of Computational Chemistry, June 2011, Lviv, Ukraine.

# III. HONORS, AWARDS AND FUNDS

- A visiting researcher award from Austrian Academy of Science (JESH program): 2015-2018
- Distinguished researcher in University of Zabol, 2010.
- Distinguished lecturer in University of Zabol, 2010.
- Distinguished researcher in University of Zabol, 2007.
- First class of honors in B.Sc., M.Sc., and Ph.D. educations
- First grade of young scientist in Tehran Province, 2001
- The sixth grade in Third Iranian Chemistry Olympics, 1998.

#### **IV. RESEARCH INTERESTS**

- Organic synthesis and catalyst
- Computational chemistry for the mechanism of chemical and biochemical processes

# V. EDUCATIONS

- Ph.D., Chemistry, Tarbiat Modares University, Tehran, Iran "Addition of Nucleophilic and Organomethalic Reagents to Oximes and Reduction of C=N Double Bonds with Boranes in Lithium Perchlorate/Diethyl Ether as a Solvent", Supervisor: Dr. Akbar Heydari, 17.70 from 20(%89), first class of honors, 2000-2004
- M.Sc., Organic Chemistry, Tarbiat Modares University, Tehran, Iran. "*Regioselective Addition of NH-Acids to Alkylpropionates in Presence of Triphenylphosphine*", Supervisor: Professor Issa Yavari, 17.94 from 20(%90), first class of honors, 1998 to 2000
- B.Sc., Applied Chemistry, University of Isfahan, Isfahan, Iran, 16.51 from 20(%83), first class of honors, 1994 to 1998

# VI. THOUGHT COURSES

- Undergraduate courses: Organic chemistry (fundamentals, 1, 2, 3), Physical organic chemistry, Separation and identification of organic molecules, Organic spectroscopy, Organic synthesis
- Graduate courses: Characterization of nanomaterials, Advanced organic spectroscopy, Advanced organic chemistry, Advanced physical organic chemistry, Supramolecular chemistry, Advanced NMR, Advanced computational chemistry, Advanced heterocyclic chemistry, Reactive intermediates

# VII. ADMINISTRATIVE BACKGROUNDS

- The head of organic chemistry division, Department of chemistry, Isfahan University of technology, 2016 to 2019 and 2021 to now
- A general secretary of "Equipment and material's committee" of Iranian chemical society, 2015 to 2018
- A member of scientific committee of organic chemistry's division of Iranian chemical society, 2010 to now
- The graduate school coordinator, Department of chemistry, Isfahan University of technology, 2012 to 2014
- Dean of faculty of science, university of Zabol, March 2008- September 2010.
- Head of chemistry department in university of Zabol, January 2006-September 2006 and September 2008 up to September 2009
- Vice-president of research office in university of Zabol, September 2006-March 2008
- A member of research council of university of Zabol, September 2006- September 2009
- A member of special research committee of university of Zabol, February 2005-September 2006
- A member of fellowship and employment council of university of Zabol, March 2008-Septebmber 2009
- A member of secretary of safety committee of university of Zabol, April 2007 up to now
- General secretary of laboratory equipment executive committee of university of Zabol, November 2008 up to now
- Chair and general secretary or 14<sup>th</sup> Iranian seminar of organic chemistry, 5-7 March 2008, university of Zabol, Zabol, Iran
- A member of executive committee of first national conference on Sistan honors, May 2008, university of Zabol, Zabol, Iran
- A member of executive committee of second international conference water crisis, March 2009, university of Zabol, Zabol, Iran