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I. Publications in Journals

1. Sadegh, F., Tavakol, H. **2022**. Eco-friendly synthesis of a noble trimetallic magnetic aerogel, Ag/CoFe₂O₄, and employing it as a catalyst in the reduction of nitroaromatics. *Results in Chemistry*, 4, 100592.
2. Darrudi, M., Tavakol, H., Momeni, M. **2022**. 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*, accepted.
3. Tavakol, H., Firouzi, M. **2022**. Synthesis of 14H-dibenzoxanthenes in a green media using Sn (II)/nano silica as an efficient catalyst. *Frontiers in Chemistry*, accepted.
4. Tavakol, H., Abedi, B. **2022**. Phosphorous-modified Porous Carbon Supported Nickel Nanoparticles as a Catalyst for the Reduction of Nitroaromatics in Water. *ChemistrySelect*, 7(36), e202200391.
5. Tavakol, H., Ganbari, A., **2022**. Nitrogen-modified graphene as a metal-free carbocatalyst for the solvent-free oxidative homo- and heterocoupling of amines. *J. Iran. Chem. Soc. Journal of the Iranian Chemical Society* 19 (5), 2041-2051.
6. Ranjbari, M.A. and Tavakol, H., **2021**. Catalyst-Free Synthesis of Benzofuran Derivatives from Cascade Reactions between Nitroepoxides and Salicylaldehydes. *The Journal of Organic Chemistry*, 86, 4756–4762.
7. Abtahi, B. and Tavakol, H., **2021**. CuI-catalyzed, one-pot synthesis of 3-aminobenzofurans in deep eutectic solvents. *Applied organometallic chemistry*, accepted
8. 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.
9. 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.
10. 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.
11. Ranjbari, M.A., Tavakol, H. and Manoukian, M., **2021**. Regioselective and solvent-free arylation of β -nitrostyrenes with mono- and dialkyl anilines. *Research on Chemical Intermediates*, 47, 709–721
12. Tavakol, H., Haghshenas, H. **2021**. A DFT study on the interaction of doped carbon nanotubes

- with H₂S, SO₂ and thiophene. *Quantum Reports*, 3(3), 366-375.
13. Tavakol, H., Salimpour, S. and Salvenmoser, W., **2020**. The synthesis of sulfur-doped carbon nanofibers using chemical vapor deposition on the nickel-ferrite catalyst and the gold decoration of the product for morphine sensing. *SN Applied Sciences*, 2, 2018.
 14. Abtahi, B. and Tavakol, H., **2020**. Conversion of β -Nitrostyrenes to Naphthofurans via a Cascade Reaction with α - and β -Naphthols. *ChemistrySelect*, 5, 12582-12585.
 15. Abtahi, B. and Tavakol, H., **2020**. Choline chloride-urea deep eutectic solvent as an efficient media for the synthesis of propargylamines via organocuprate intermediate. *Applied Organometallic Chemistry*, 34, p.e5895.
 16. Hamed Haghshenas, Hossein Tavakol, Bitra Kaviani, and Gholamhossein Mohammadnezhad; **2020** AMBER Force Field Parameters for Cobalt-Containing Biological Systems: A Systematic Derivation Study. *J. Phys. Chem. B* 124, 777–787
 17. Nedasadat Hasheminejad, Hossein Tavakol and Willi Salvenmoser; **2020** Preparation of gold-decorated simple and sulfur-doped carbon spheres for desulfurization of fuel. *Journal of Cleaner production*, 264, 121684
 18. Sara Kamali, Mohammad Zhiani, Hossein Tavakol; **2020** Synergism effect of first row transition metals in experimental and theoretical activity of NiM/rGO alloys at hydrogen evolution reaction in alkaline electrolyzer. *Renewable Energy*, 154, 1122-1131
 19. Hossein Tavakol, Fahaimah Hassan, Dana Shahabi; **2020** Using ONIOM calculations to investigate the abilities of simple and N, B, S-doped carbon nanotubes in sensing of carbon monoxide. *Int J Quantum Chem.* 120, e26214.
 20. Mohammad Taqi Jafari-Chermahini and Hossein Tavakol; **2020** Sulfur-doped Graphene as an Efficient Metal-free Carbocatalyst for the Synthesis of 1,5-Benzodiazepines Derivatives, *ChemistrySelect*, 5, 968-978
 21. Mohammad A. Ranjbari and Hossein Tavakol; **2020** Synthesis of α -cyano hydroxylamine via three-component reactions and Computational mechanistic study. *Reaction Kinetics, Mechanisms and Catalysis*, 129, 349–369
 22. Hossein Tavakol, Mohammad Zhiani and Fereshteh Shareifyan-ghahfarokhi; **2020** Gold-decorated sulfur-doped carbon nanotubes as electrocatalyst in hydrogen evolution reaction. *Gold Bulletin*, 53, 63-76.
 23. Bakhshi, Pourya; Tavakol, H; **2020** Oil removal from water using highly hydrophobic, ultralight carbon microspheres. *International Journal of Environmental Science and Technology*, 17, 1649–1656
 24. 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
 25. F Hassani, H Tavakol **2020** Sulfur doped carbon porous as an efficient catalyst for sustainable energy processes. *Environmental progress & sustainable Energy*, 39, 1, 13299
 26. Tavakol, H; Ranjbari, MA; Jafari-Chermahini MT; **2019** Mechanistic details for the reaction of methyl acrylate radical anion: a DFT study. *Reaction Kinetics, Mechanisms and Catalysis*, 128:629–643
 27. MT Jafari Chermahini, H Tavakol **2019** Immobilized Gelatin- λ -Carrageenan on Magnetite Nanoparticles as an Efficient Organocatalyst for Enantioselective Biginelli Reaction *ChemistrySelect* 4 (6), 1895-1902

28. 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
29. Hosseini-Kharat, Mahboubeh; Tavakol, Hossein; Mohammadi, Tecush **2019** Antiproliferative activity of morpholine-based compounds on MCF-7 breast cancer, colon carcinoma C26 and normal fibroblast NIH-3T3 cell lines and study of their binding affinity to calfthymus-DNA and bovine serum albumin. *Journal of Biomolecular Structure and Dynamics*, 37(14), 3788-3802.
30. P Bakhshi, H Tavakol **2019** Synthesis of Si-Doped CNT and Its Catalytic Ability in Hydrogen Evolution Reaction *ChemistrySelect* 4 (2), 521-526
31. M Manoukian, H Fashandi, H Tavakol **2019** Polysulfone-highly uniform activated carbon sphere mixed-matrix membrane intended for efficient purification of dye wastewater. *Materials Research Express* 6 (5), 055313
32. H Tavakol, MA Ranjbari, A Mahmoudi **2019** DFT study on the mechanistic details of the hydrolysis of dicyan using acetaldehyde as the first organocatalyst. *Computational and Theoretical Chemistry* 1154, 37-43
33. Manoukian, Meghmik; Tavakol, Hossein; Fashandi, Hossein; **2018** Synthesis of highly uniform sulfur-doped carbon spheres and its application for cationic dye removal in comparison with non-doped carbon spheres. *Journal of Environmental Chemical Engineering*, 6, 6904–6915.
34. Jafari-Chermahini, Mohammad; Tavakol, H; **2018** Adsorption of CO₂ on sodium iodide (NaI) *n* (*n* ≤ 10) clusters: A density functional theory investigation. *Computational and Theoretical Chemistry* 1145, 37–43.
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36. Hassani, Fahimeh, and Hossein Tavakol **2018** Synthesis of sulfur-doped carbon nanotubes from sulfur powder using chemical vapor deposition. *Fullerenes, Nanotubes and Carbon Nanostructures* 26(8), 479-486.
37. Mohammadi, Fatemeh; Tavakol, Hossein; **2018** Synthesis of phosphorus doped carbon nanotubes using chemical vapor deposition. *Fullerenes, Nanotubes and Carbon Nanostructures*, 26(4), 218-225.
38. Shahabi, Dana, Tavakol, Hossein; **2018** High Catalytic Ability of Fe₃O₄/EDTA Magnetic Nanocatalyst in Comparison with Various Deep Eutectic Solvents for One-Pot Synthesis of 4H-Pyrans. *Journal of Nanoanalysis*, 5(1), 49-57.
39. Ranjbari, Mohammad-Amin; Tavakol, Hossein **2018** Theoretical study of the possible mechanisms for the synthesis of dialkyl thiourea from dithiocarbamate *Heteroatom Chemistry*, 29 (3), p1-9, e21421.
40. Shahabi, Dana, Tavakol, Hossein; **2018**. A DFT study on the catalytic ability of aluminum doped graphene for the initial steps of the conversion of methanol to gasoline. *Computational and Theoretical Chemistry*, 1127, 8-15.
41. Shafieyoon, Parvaneh; Mehdipour, Ebrahim; Tavakol, Hosein; **2018** Polystyrene bis[N-(2-pyridyl) sulfonamide] palladium(II): Synthesis, characterization as a catalyst for coupling reactions. *Phosphorus, Sulfur, and Silicon and the Related Elements*, 193(5), pp. 324-328.

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43. Shahabi, Dana; Tavakol, Hossein; **2017** DFT, NBO and molecular docking studies of the adsorption of fluoxetine into and on the surface of simple and sulfur-doped carbon nanotubes. *Applied Surface Science* 420, 267–275
44. 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.
45. Tavakol, Hossein; Hashemi, Fateme; Molavian, Mohammad-Reza; **2017** Theoretical investigation on the performance of simple and doped graphenes for the surface adsorption of various ions and water desalination. *Structural Chemistry*, 28, 1687-1695
46. 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
47. 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
48. Hassani, Fahimeh; Tavakol, Hossein; Keshavarzipour, Fariba; Javaheri, Amin; **2016** A simple synthesis of sulfur-doped graphene using sulfur powder by chemical vapor deposition. *RSC Advances*, 6, 27158-27163
49. Shahabi, Dana; Tavakol, Hossein; **2016** One-pot synthesis of quinoline derivatives using choline chloride/tin (II) chloride deep eutectic solvent as a green catalyst. *Journal of Molecular Liquids* 220, 324-328
50. Saadat, Kayvan; Tavakol, Hossein; **2016** Study of noncovalent interactions of end-capped sulfur-doped carbon nanotubes using DFT, QTAIM, NBO and NCI calculations. *Structural Chemistry*, 27, 739-751.
51. Tavakol, Hossein; Keshavarzipour, Fariba; **2016** The substituent effect on the energy profiles of inter and intramolecular proton transfers between Phosphine Oxide-Phosphinous Acid Tautomers. *Heteroatom Chemistry*, 27, 210-220
52. Haghshenas, Hamed; Kay, Maryam; Dehghanian, Fariba; Tavakol, Hossein; **2016** Molecular dynamics study of biodegradation of azo dyes via their interactions with AzrC azoreductase *Journal of Biomolecular Structure and Dynamics*. 34, 453-462
53. 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.
54. Tavakol, Hossein; Keshavarzipour, Fariba; **2016** sulfur doped carbon nanotube as a potential catalyst for the oxygen reduction reaction. *RSC Advances* 6, 63084-63090
55. Keshavarzipour, Fariba; Tavakol, Hossein; **2016** The synthesis of coumarin derivatives using choline chloride/zinc chloride as a deep eutectic solvent. *Journal of the Iranian Chemical Society* 13, 149-153
56. Tavakol, Hossein; Khedri, Neda; **2015**, DFT Study of the effects of counter ions on bonding, molecular and spectral properties of pentafluorophenyl xenonium difluoride cation *Journal of Chemical Sciences* 127, 1675-1685

57. Saadat, Kayvan; Tavakol, Hossein; **2015** An exceptional functionalization of doped fullerene observed via theoretical studies on the interactions of sulfur-doped fullerenes with halogens and halides. *RSC Advances*, 5, 55227-55237
58. Karami, Kazem; Haghghat Naeini, Nasrin; Eigner, Vaclav; Dusek, Michal; Lipkowski, Janusz; Hervesd, Pablo; Tavakol, Hossein; **2015** Palladium complexes with 3-phenylpropylamine ligands: synthesis, structures, theoretical studies and application in the aerobic oxidation of alcohols as heterogeneous catalysts. *RSC Advances* 5, 102424-102435
59. Tavakol, Hossein; Hassani, Fahimeh; **2015** Adsorption of molecular iodine on the surface of sulfur-doped carbon nanotubes: theoretical study on their interactions, sensor properties, and other applications. *Structural Chemistry*, 26, 151-158
60. Chiniforoshan, Hossein; Radani, Zahra Sadeghian; Tabrizi, Leila; Tavakol, Hossein; Sabzalian, Mohammad R; Mohammadnezhad, Gholamhossein; Görls, Helmar; Plass, Winfried; **2015** Pyrazinamide drug interacting with Co (III) and Zn (II) metal ions based on 2, 2'-bipyridine and 1, 10-phenanthroline ligands: Synthesis, studies and crystal structure, DFT calculations and antibacterial assays. *Journal of Molecular Structure*, 1081, 237-243
61. Keshavarzipour, Fariba; Tavakol, Hossein; **2015** Deep Eutectic Solvent as a Recyclable Catalyst for Three-Component Synthesis of β -Amino Carbonyls. *Catalysis Letters*, 145, 1062-1066
62. Tabrizi, Leila; Chiniforoshan, Hossein; Tavakol, Hossein; **2015** New mixed ligand palladium (II) complexes based on the antiepileptic drug sodium valproate and bioactive nitrogen-donor ligands: Synthesis, structural characterization, binding interactions with DNA and BSA, in vitro cytotoxicity studies and DFT calculations. *Spectrochimica Acta A*, 141, 16-26
63. Tavakol, Hossein; Keshavarzipour, Fariba; **2015** A DFT study of inter-and intramolecular proton transfer in 2-selenobarbituric acid tautomers, *Structural Chemistry*, 26, 1049-1057
64. Tavakol, Hossein; Shahabi, Dana; **2015** DFT, QTAIM, and NBO Study of Adsorption of Rare Gases into and on the Surface of Sulfur-Doped, Single-Wall Carbon Nanotubes. *The Journal of Physical Chemistry C*, 119, 6502-6510
65. Tavakol, Hossein; Mollaei-Renani, Akram; **2014** Coupled cluster, MP2, and DFT study of structures, stabilities, vibrations, and bonding properties of $XXeOH$ (X= F, Cl, Br, and I) *Structural Chemistry* 25, 1013-1022
66. Tabrizi, Leila; Chiniforoshan, Hossein; McArdle, Patrick; Tavakol, Hossein; Rezaei, Behzad; Dehcheshmeh, Mohammad Mohammadi; **2014** Selective gas sorption and electrochemical properties of a dicyanamide coordination polymer: Insight from experimental and theoretical study *Polyhedron* 69, 84-89
67. Karami, Kazem; Hosseini-Kharat, Mahboubeh; Rizzoli, Corrado; Tavakol, Hossein; Lipkowski, Janusz; **2014** Structural and theoretical studies of mono and di-insertion of symmetric alkynes into the Pd-C σ bond of cyclopalladated secondary (tert-butyl and ethyl) benzylamines *Journal of Organometallic Chemistry* 752, 152-160
68. Abdolmaleki, Amir; Tavakol, Hossein; Molavian, Mohammad Reza; Firouz, Koorosh; **2014** Synthesis, FT-IR, NMR and DFT analysis of a new salophen based on diaminophenazine moiety. *Journal of Molecular Structure*, 1062, 44-47
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70. Chiniforoshan, Hossein; Pourrahim, Nasimeh; Tabrizi, Leila; Tavakol, Hossein; Sabzalian, Mohammad R; Notash, Behrouz; **2014** Syntheses, studies and crystal structure of new coordination polymers of mercury (II) with phenylcyanamide derivative ligands *Inorganica Chimica Acta*, 416, 85-92
71. Montazerzohori, Morteza; Tavakol, Hossein; Kheiri, S; Musavi, SA; Joohari, S; **2014** Synthesis, spectral characterization and theoretical investigation of some new mercury four coordinated complexes. *Bulgarian Chemical Communications*, 46, 96-103
72. Shakeri, Jamaladin; Hadadzadeh, Hassan; Tavakol, Hossein; **2014** Photocatalytic reduction of CO₂ to CO by a dinuclear carbonyl polypyridyl rhenium (I) complex *Polyhedron*, 78, 112-122
73. Tavakol, Hossein; Mollaei-Renani, Akram; **2014** DFT, AIM, and NBO study of the interaction of simple and sulfur-doped graphenes with molecular halogens, CH₃OH, CH₃SH, H₂O, and H₂S. *Structural Chemistry*, 25, 1659-1667
74. Tavakol, Hossein; Hassani, Fahimeh; Mollaei-Renani, Akram; **2014** A theoretical study of stabilities, reactivities and bonding properties of XKrOH (X= F, Cl, Br and I) as potential new krypton compounds using coupled cluster, MP2 and DFT calculations *RSC Advances*, 4, 47540-47548
75. Shamohamadi, Shayan; Bustanian, Mohammad; Tavakol, Hossein; **2013** Removing Cd²⁺ from water and wastewater by blowy sand; the effects of total hardness and pH *Desalination and Water Treatment*, 51, 3463-3471
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77. H. Tavakol, H. Mohammadi, S.A. Aslanzadeh; **2013** DFT Study of Kinetic and Thermodynamic Parameters of Tautomerism in 4-acyl Pyrazolone. *Iranian Journal of mathematical chemistry*, 4, 185-199
78. Karami, Kazem; Salimian, Mina; Hosseini-Kharat, Mahboubeh; Bruno, Giuseppe; Rudbari, Hadi Amiri; Tavakol, Hossein; **2013** Synthesis, structural and theoretical studies of Pd (II) complexes containing an orthometallated C, C-chelating phosphorus ylide. *Polyhedron*, 61, 143-150
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84. Tavakol, Hossein; Esfandyari, Maryam; Taheri, Salman; Heydari, Akbar; **2011** Investigation of structure, vibrational and NMR spectra of oxycodone and naltrexone: A combined experimental and theoretical study, *Spectrochimica Acta Part A*, 79, 574-582
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86. Tavakol, Hossein; **2011** Free energy relationships via tautomerism in para-acetophenone derivatives. *Computational and Theoretical Chemistry*, 976, 88-93
87. Tavakol, Hossein; Sabzyan, Hassan; **2011** Possibility of non-adiabatic level crossing by DFT study of tautomerism and potential energy surfaces in of 3-hydroxy-5-(pyrimidin-2-yl)-2H-pyrrol-2-one and its tautomer. *Journal of Physical Organic Chemistry*, 24, 414-422
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94. Tavakol, Hossein; Arshadi, Sattar; **2009** Theoretical investigation of tautomerism in N-hydroxy amidines. *Journal of molecular modeling*, 15, 807-816
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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 dimensional NMR Spectroscopy", Horst Friebolin, Forth edition, April 2009, Publisher: Gostareshe olume paye (1st and 2nd print)
- Theory and experiments in organic chemistry laboratory (in Persian), June 2009, Publisher: Aras rayaneh

b. National conferences (abstracts)

1. H. Tavakol, F. Jahanimogadam, F. Noormoha-mmadian and I. Yavari, Reaction of 2-Acetylpyrole with Acetylenic Esters in Presence of Phosphorous Nucleophiles, 8th Iranian Seminar of Organic Chemistry, Tehran University, Tehran, Iran, September 1999
2. M. Kassaie and H. Tavakol, Study of Substituent Effects in Phenyl Carbene and Rearrangement Products Via Ab-initio Calculations, Third Islamic Azad University Conference, Islamic Azad University, Tehran, Iran, April 2002
3. H. Tavakol and I. Yavari, Regioselectivity in Addition to Alkylpropionates, 10th Iranian Seminar of Organic Chemistry, Guilan University, Rasht, Iran, September 2002
4. H. Tavakol and A. Heydari, Addition of Allyl Tributyl Stananne to Oxime Ethers: Synthesis of Homoallylic Hydroxylamines
5. H. Tavakol and A. Heydari, One-Pot Synthesis of β - (N- Hydroxy Amino) Esters from Aldehydes 11th Iranian seminar of Organic Chemistry, Isfahan University of Technology, Isfahan, Iran, 3-6 February 2005

6. H. Tavakol and A. Heydari, One-pot reduction of aldimines in LPDE 5M 12th Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
7. H. Tavakol and A. Heydari, Preparation of various hydroxylamines in three component aminoreduction reaction 12th Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
8. H. Tavakol and A. Heydari, Preparation of trisubstituted hydrazines from aldehydes 12th Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
9. H. Tavakol and S. Zakery, Diastereoselective addition to SAMP hydrazones 12th Iranian seminar of Organic Chemistry, Ahwaz jundi shapour university of medical science, Ahwaz, Iran, 7-9 March 2006.
10. H. Tavakol and S. Zakery, Preparation of secondary amines from one-pot reduction of ketimines 13th 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 13th 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 13th Iranian seminar of Organic Chemistry, Bu-Ali Sina University, Hamedan, Iran, 6-8 September 2006.
13. H. Tavakol, Preparation of hydrazones from one-pot reduction of ketohydrazones 3rd Iranian national congress on chemistry, Islamic azad university of varamin, Varamin, Iran. 16,17 May 2007, Oral presentation.
14. H. Tavakol, Investigation of Tautomerism in Amidoximes by Theoretical Method 15th 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) 12th 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 12th Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
17. K. Nozarian, M. Montazerzohori, H. Tavakol and S. Khani, Synthesis, spectral and theoretical studies of some new zinc and cadmium complexes of a bidentate ligand 12th Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
18. M. Razzaghi, M. Montazerzohori, H. Tavakol, A. Hojjati, Synthesis, spectral and theoretical studies of some new complexes of Zinc halides 12th Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.
19. M. Sedighipoor, M. Montazerzohori, H. Tavakol, M. H. Habibi, Synthesis, spectral, theoretical and electrochemical studies of some new complexes of mercury and cadmium with a new asymmetric Schiff base ligand 12th Iranian Inorganic Chemistry Seminar, Rasht, Iran, September 2010.

20. M. Sedighipoor, M. Montazerzohori, H. Tavakol, M. H. Habibi, Synthesis, spectroscopic, theoretical and electrochemical studies of some new Zn(II), Cu(I) complexes, 12th 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, 15th 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, 15th Iranian Chemistry Congress, Hamedan, Iran, September 2011
23. M. Montazerzohori, H. Tavakol, S. A. Musavi and S. Yadegari, Theoretical study of some recently synthesized mercury complexes with a Schiff base ligand, 15th Iranian Chemistry Congress, Hamedan, Iran, September 2011
24. M. Montazerzohori, H. Tavakol, S. A. Musavi and M. Hosseinpour, Theoretical study of some recently synthesized mercury and cadmium complexes with N, N-bis (3-(2nitrophenyl)propenaldehyde)-1, 2-phenylenediamine, 15th Iranian Chemistry Congress, Hamedan, Iran, September 2011.
25. H. tavakol, Hammett equation in the rate and equilibrium constant of keto-enol tautomerism, 18th Iranian seminar of Organic Chemistry, Zahedan, Iran, February 2012, Oral presentation.
26. H. tavakol, Tautomery scheme in 4-acyl pyrazolone, 18th 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.2ZnCl₂ . 22nd 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 2nd Internatnal conference on mathematical chemistry, Kashan, Iran, April 2009, Oral presentation.
2. M. Montazerzohori, H. Tavakol, A. Hojati and A. Rahiminia, Synthesis, identification and theoretical study of some mercuric halide complexes 8th national Payam-e-noor conference in chemistry, Qazvin, Iran, September 2010.
3. M. Montazerzohori, H. Tavakol, A. Hojati and J. Hasanalyan, Synthesis, and identification of some mercuric azide and thiocyanate complexes 8th national Payam-e-noor conference in chemistry, Qazvin, Iran, September 2010.
4. M. Montazerzohori, H. Tavakol, A. Hojati and A. Rahiminia, Synthesis, identification and theoretical study of some cadmium azides and thiocyanate complexes 8th national Payam-e-noor conference in chemistry, Qazvin, Iran, September 2010.
5. H. Tavakol, T. Hadad, The Effect of Water on the Equilibrium and Rate Constant of Tautomerism in Hydroxamic Acids, 14th Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.
6. H. Tavakol, S. Amiraslanzadeh, Study of Isomery Scheme in Acetyl Hydrazides by DFT Calculations, 14th Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.
7. M. Montazerzohori , H. Tavakol ,A. Hojjati and K. Nozarian, Theoretical studies of some new synthesized four coordinated cadmium complexes, 14th Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.

8. 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), 14th Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.
9. 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, 14th Iranian Physical Chemistry Conference, Kish Iceland, Kish, February 2011.

d. International conferences

1. 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
2. H. Tavakol and S. Zakery, In Situ Addition of Organometallic Reagents to Oxime Ethers, 40th IUPAC congress, Beijing, china, 14-19 August 2005, Oral presentation.
3. H. Tavakol and S. Zakery, Multicomponent Additions to C=N Double Bond in Lithium Perchlorate 3rd 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 Organometallic 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
- 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-September 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 of 14th 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