
Resume:

Avat (Arman) Taherpour - Ph.D
Professor of Organic Chemistry

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Invited part time co-worker: Medical Biology Research Center, Kermanshah University of Medical Sciences, Kermanshah, Iran.

Research Programs:

Visiting Academic: The University of Queensland, Reactive Intermediates and Unusual Molecules Group (Professor Curt Wentrup's Group, Chemistry Building, School of Molecular and Microbial Office, Brisbane, Qld 4072, Australia. 2006.

Research programs:

*The University of Queensland, Reactive Intermediates and Unusual Molecules Group (Professor Curt Wentrup's Group, Chemistry Building, School of Molecular and Microbial Office, Brisbane, Qld 4072, Australia. Under Supervision Professor Curt Wentrup FAA., 2006-2007.

*The University of Queensland (UQ), Reactive Intermediates and Unusual Molecules Group (Professor Curt Wentrup's Group, Chemistry Building, School of Molecular and Microbial Office, Brisbane, Qld 4072, Australia. Under Supervision Professor Curt Wentrup FAA. July-September 2008 and . July-September 2009.

*The University of New England (UNE), Chemistry Department, Science and Technology Faculty, UNE, Armidale, Australia (Professor S. Glover's Group) November 2011-Feruary 2012.

*The University of Melbourne, Chemistry Faculty, Melbourne, Australia (Professor Jonathan White's Group) 2016-2017.

Courses Taught (in accordance with the educational program of Iran in universities):

B. S.:

General Chemistry (I & II), Organic Chemistry (1,2 & 3), Spectroscopy in Organic Chemistry, Organometallic Chemistry, Systematic Identification of Organic Compounds, Fundamentals of Polymer Chemistry, Physical Organic Chemistry, Extraction of Essential Oils from Medicinal Herbs, Pharmaceutical Chemistry, Synthesis of Organic Compounds.

M. S.:

Advanced Organic Chemistry, Heterocyclic Chemistry, Pharmaceutical Chemistry, Fundamental of Molecular Spectroscopy, Special Topics, Physical Organic Chemistry, Synthesis of Organic Compounds, Theoretical Chemistry of Nanostructures, Computational Chemistry.

Ph.D.:

Advanced Organic Chemistry, Heterocyclic Chemistry, Synthesis of Organic Compounds, Reactive Intermediates, Asymmetric Synthesis, Stereochemistry, Molecular Spectroscopy, Computational Nano-Chemistry, Special Topics, Theoretical Chemistry of Nanostructures.

Managerial Positions:

- Head of Elites Foundation of Kermanshah Province, Kermanshah, Iran (2018-upto now).
- Chairman of the Scientific Council of “*Elites Foundation of Kermanshah Province*”, Kermanshah, Iran (2018-upto now).
- Manager of Relations with Industry and Entrepreneurship of Razi University, Kermanshah, Iran (2012-2014).
- Head of Nano-Chemistry Department of Razi University, Kermanshah, Iran (2014-2016).
- Member of Technology Council of Kermanshah University of Medical Sciences, Kermanshah University of Medical Sciences, Kermanshah, Iran (2018-upto now).
- Director of Relations with Industry of Arak Islamic Azad University, Arak, Iran (1996-97).
- Head of Chemistry Department of Arak Islamic Azad University, Arak, Iran (1999-2001)
- Dean of Graduate School of Arak Islamic Azad University, Arak, Iran (1998-1999).

Research Interests:

- 1) Computational Chemistry, Molecular Modeling and Theoretical Chemistry.
- 2) Organic Compounds Synthesis. Microwave Synthesis of Organic Compounds.
- 3) Physical Organic Studies.
- 4) Spectroscopic Studies of Organic Compounds (NMR, IR, UV).
- 5) Phytochemistry and Extraction of Essential Oil from Herbs.
- 6) Microwave Assisted Synthesis in Organic Chemistry, FVT and Photochemistry.
- 7) Nano-Chemistry and related sciences.

Number of Graduated M.Sc. and Ph.D.Under Supervision (up to 02/2016):

- Graduated M.Sc. students of Chemistry and Nano-Chemistry 134.
- Graduated Ph.D. students of Chemistry 7.
- Current M.Sc. Students of Chemistry 2. (In Razi University and other Universities in Iran).
- Current Ph.D. Students of Chemistry 3. (In Razi University and other Universities in Iran).
- Current Ph.D. Students of Nano-Chemistry 2. (In Razi University, Iran).
- Graduated Post-doc researcher under supervision at Razi University: 1 (2016-2018)
- Current Post-doc researcher under supervision at Razi University: 1 (2020)

Membership:

- Member of the Chemical Society of Iran (CSI).
-Member of the Central Committee of the Iranian Chemical Society (CCICS; 2010-2012).

List of Publications in Journals and Paper Presented:

- 1- S. Khaef, A. Rostami, V. Khakyzadeh, M. A. Zolfigol, **A. A. Taherpour**, M. Yarie, Regioselective Ortho-CH sulfenylation of free phenols catalyzed by Co(II)-immobilized on silica-coated magnetic nanoparticles, *Molecular Catalysis*, 2020, 484, 110772.
- 2- P. Ghasem, M. Yarie, MA. Zolfigol, **A.A. Taherpour**, M. Torabi, Ionically tagged magnetic nanoparticles with urea linker: Application for preparation of 2-aryl-quinoline-4-carboxylic acids via an anomeric based oxidation mechanism, *ACS Omega*, 2020, 5, 3207–3217.
- 3- M. Hashemi, **A.A. Taherpour**, Theoretical Kinetic and Thermodynamic Studies of the Strain Energies and Ring Size Effects of the 1,3-Dipolar Cycloaddition Reactions on Ethinamate Medicine Analogs, *Journal of Molecular Structure*, 2020, 1204, 127544.
- 4- M. Hashemi, **A.A. Taherpour**, Structural Assessment of Hydrogen Bonds on Methylpentynol-Azide Clusters To Achieve Regiochemical Outcome of 1,3-Dipolar Cycloaddition Reactions Using Density Functional Theory, *ACS Omega*, 2020, 5(11), 5964-5975.
- 5- N. Moradi, M. Shamsipur, **A.A. Taherpour**, A. Pashabadi, Impedimetric determination of Cs (I) using AuNPs@ PoPD-DB24C8: A targeted molecular-scale perturbation, *Analytica Chimica Acta*, 2020, 1108, 118-128.
- 6- M. Mahmoodi, A. Bamoniri1, A.A. Taherpour, One-pot synthesis of 2H-Indazolo[2,1-b]phthalazine-triones via nano γ -Al₂O₃/BF₃/Fe₃O₄ as an efficient catalyst and theoretical DFT study on them, *J. Heterocycl. Chem.*, 2020, Accepted for Publication.
- 7- M. Shamsipur, K. Molaei, F. Molaabasi, S. Hosseinkhani, **A. A. Taherpour**, M. Sarparast, S. Ebrahim Moosavifard, A. Barati, Aptamer-Based Fluorescent Biosensing of Adenosine Triphosphate and Cytochrome c via Aggregation-Induced Emission Enhancement on Novel Label Free DNA-Capped Silver Nanoclusters/Graphene Oxide Nanohybrids, *ACS Applied Materials & Interfaces*, 2019, 11, 49, 46077-46089.
- 8- M. Saeed Mirzaei, **Avat Arman Taherpour**, Saber Mirzaei, Proton shuttle efficiency of bicarbonate: A theoretical study on tautomerization and CO₂ hydration, *Tetrahedron*, 2019, 75(48), 130693.
- 9- Farimah Mousavi, **Avat Arman Taherpour**, A carbon nanotube-iron (III) oxide nanocomposite as a cathode in dye-sensitized solar cells: Computational modeling and electrochemical investigations, *Electrochimica Acta*, 2019, 318, 617-624.
- 10- F Mousavi, M Shamsipur, **A.A. Taherpour**, A Pashabadi, *Electrochimica Acta*, A rhodium-decorated carbon nanotube cathode material in the dye-sensitized solar cell: Conversion efficiency reached to 11%, *Electrochimica Acta*, 2019, 308, 373-383.
- 11- Elaheh Babaee, AliBarati, Mohammad Bagher Gholivand, **Avat (Arman) Taherpour**, Narges Zolfaghari, Mojtaba Shamsipur, Determination of Hg²⁺ and Cu²⁺ ions by dual-emissive Ag/Au nanocluster/carbon dots nanohybrids: Switching the selectivity by pH adjustment, *Journal of Hazardous Materials*, 2019, 367, 437-446.
- 12- Mojtaba Shamsipur, Saied Saeed Hosseiny Davarani, Davood Nematollahi, **Avat (Arman) Taherpour**, Sara Dehdashtian, Afshin Pashabadi, One-step electrochemically driven production of aza macrocycle-based pseudocryptand: An accessible route for creating of diverse cryptand-resembles compounds, *Electrochimica Acta*, 2019, 296, 102-111.

- 13- **A. A.Taherpour**, M. Zolfigol, Reply to the Comment on “A convenient method for preparation of 2-amino-4,6-diphenylnicotinonitrile using HBF₄ as an efficient catalyst via an anomeric based oxidation: A joint experimental and theoretical study” [J. Mol. Struct. 1137 (2017) 674-680], by S. Salehzadeh and F. Maleki, J. Mol. Struct. 1154 (2018) 587-589”, *Journal of Molecular Structure*, 2019, 1179, 719-724.
- 14- Mohsen Irandoost, Maryam Haghghi, **Avat Arman Taherpour**, Narges Zolfaghar, Electrochemical Sensing of 2-methyl-4, 6-dinitrophenol by Nanomagnetic Core Shell Linked to Carbon Nanotube Modified Glassy Carbon Electrode, *Materials Science & Engineering C*, 2019, 99, 211-221.
- 15- M Shamsipur, L Samandari, **AA Taherpour**, A Pashabadi, Sub-femtomolar detection of HIV-1 gene using DNA immobilized on composite platform reinforced by a conductive polymer sandwiched between two nanostructured layers: A solid signal-amplification strategy, 2019, *Analytica chimica acta* 1055, 7-16.
- 16- Morteza Sarparast, Fatemeh Molaabasi, Reza Ghazfar, Mona Maleka Ashtiani, Mohammad Balooch Qarai, **Avat Arman Taherpour**, Saeed Pourjafari Amyab, Mojtaba Shamsipur, Efficient ethanol oxidation by hemoglobin-capped gold nanoclusters: The critical role of Fe in the heme group as an oxophilic metal active site, *Electrochemistry Communications*, 2019, 103, 42-47.
- 17- **A. A. Taherpour**, N. Zolfaghar, M. Jamshidi, O. Rezaei, Z. Shahri, Structural Distortions of Fullerene C₆₀ⁿ (n=0 to -6) Under Jahn-Teller Effects; A First Principle DFT Study, *Journal of Molecular Structure*, 2019, 1184, 546-556.
- 18- Nahid Shahabadi, Sara Amiri, **Avat Arman Taherpour**, Human serum albumin binding studies of a new platinum (IV) complex containing the drug pregabalin: Experimental and computational methods, *Journal of Coordination Chemistry*, 2019, 72 (4), 600-618.
- 19- **A. A. Taherpour** and P Ghasemi, Bergman cyclization reactions in fused enediynes: a DFT study, *Journal of the Iranian Chemical Society*, 2019, 16(9), 1965–1976.
- 20- **A. A. Taherpour** and M. A. Zolfigol, Reply to the comment on “A convenient method for preparation of 2-amino-4,6-diphenylnicotinonitrile using HBF₄ as an efficient catalyst via an anomeric based oxidation, *Journal of Molecular Structure*, 2019, 1179, 719-724.
- 21- M Bayat, **AA Taherpour**, SM Elahi, Molecular interactions between PAMAM dendrimer and some medicines that suppress the growth of hepatitis virus (Adefovir, Entecavir, Telbivudine, Lamivudine, Tenofovir): a theoretical study, *International Nano Letters*, 2019, 9(3), 231–244.
- 22- E. Rajaian and **A. A. Taherpour**, Kinetic Study of reactions between Nitrile Oxides, Nitrile sulfides and Triazoles with simple cycloalkynes with DFT method, Nashrieh Shimi va Mohandes Shimi Iran (NSMSI), 2019, 38.
- 23- M Shamsipur, A Barati, **AA Taherpour**, M Jamshidi, Resolving the Multiple Emission Centers in Carbon Dots: From Fluorophore Molecular States to Aromatic Domain States and Carbon-Core States, *The Journal of Physical Chemistry Letters-ACS*, 2018, 9, 4189–4198.
- 24- M Shamsipur, **A.A. Taherpour**, A Pashabadi, Comprehensive facilitating of water oxidation reaction by ultrasonic attenuation of hydrogen-bonded structure of water, *Ultrasonics-Sonochemistry*, 42, 2018, 381–389.

- 25- **A.A. Taherpour**, Z Shahri, O Rezaei, M Jamshidi, T Fellowes, Adsorption, intercalation and sensing of helium on yttrium functionalized open edge boron nitride: A first principle DFT and TDDFT study, *Chemical Physics Letters*, 2018, 691, 231-237.
- 26- M. Shamsipur, **A.A. Taherpour**, H. Sharghi, V. Lippolis, A. Pashabadi, A low-overpotential nature-inspired molecular chromium water oxidation catalyst, *Electrochimica Acta*, 2018, 265, 316-325.
- 27- **A.A. Taherpour**, M. Jamshidi, O. Rezaei, A.R. Belverdi, Photoinduced electron transfer process on emission spectrum of *N,N'*-bis(salicylidene)-1,2-phenylenediamine as a Mg²⁺ cation chemosensor: A first principle DFT and TDDFT study, *Journal of Molecular Structure*, 1161, 2018, 339–344.
- 28- M Irandoust, M Haghghi, **A.A. Taherpour**, M Jafarzadeh, Electrochemical sensing of trifluralin in water by fluconazole-immobilized Fe₃O₄/SiO₂ nanomagnetic core–shell linked to carbon nanotube modified glassy carbon electrode; an experimental and theoretical modeling, *Journal of the Iranian Chemical Society*, 15(3), 2018, 719-732.
- 29- M. Bayat, **A.A. Taherpour**, S.M. Elahi, T Fellowes, Separation of anticancer medicines carmustine, lomustine, semustine and melphalan by PAMAM dendrimer: a theoretical study, *Journal of the Iranian Chemical Society*, 2018, 691, 231-237.
- 30- M. S. Mirzaei, **A.A. Taherpour**, Tautomeric Preferences of the cis- and trans- Isomers of Axitinib, *Chemical Physics*, 2018, 507, 10-18.
- 31- **A.A. Taherpour**, P. Gholami, M. Jamshidi, S. Hatami, N. Zolfaghar, Theoretical Studies on Photo-Induced Electron Transfer Process on [Thioridazine].C₆₀ Nano-Complex; A First Principle DFT and TD-DFT, *Journal of Photochemistry and Photobiology A: Chemistry*, 2018, accepted for publication.
- 32- S. Mirzaei, **A.A. Taherpour**, M.H. Kalilian, Importance of Azo-Hydrazo Tautomerization in the Oxidative Degradation of Procarbazine by Cytochrome P450: Computational Insights, *ChemistrySelect*, 2018, 3(22), 6028-6173.
- 33- AR Belverdi, MB Jamshidi, **AA Taherpour**, M Jamshidi, O Rezaei, Novel donor-acceptor non-fullerene metal-organic solar cells: A first DFT and TD-DFT study *Physica B: Condensed Matter*, 2018, 542, 37-43.
- 34- M Shamsipur, **AA Taherpour**, H Sharghi, A Pashabadi, Transduction of interaction between trace tryptophan and surface-confined chromium salen using impedance spectroscopy. A sensing device that works based on highly selective inhibition of mediator's Faradaic process, *Analytica Chimica Acta*, 2018, 1030, 70-76.
- 35- **AA Taherpour**, F Mousavi, Carbon nanomaterials for electroanalysis in pharmaceutical applications, Fullerenes, Graphenes and Nanotubes, Book Chapter; Chapter 6 from book “Fullerenes, Graphenes and Nanotubes: A Pharmaceutical Approach”, 1th Ed., Elsevier Publisher, 2018, 169-225; ISBN: 978-0-12-813691-1.
- 36- F Shiri, M Norouzibazaz, A Yari, **A.A. Taherpour**, A DFT study of both the hydrolytic degradation and protonation of semustine in variation conditions of pH and also interaction of drug with DNA nucleobases, *Structural Chemistry*, 2018, 29, 1465–1474.

- 37- Ghasemhezaveh, MM Khodaei, DFT study of 1,3-dipolar cycloaddition reaction of 2-(4-azidophenyl) benzo[d]thiazole with acetylene derivatives, *Indian Journal of Chemistry-B*, 2018, 57, 858-869.
- 38- M Shamsipur, A Pashabadi, **A.A. Taherpour**, K Bahrami, H Sharghi, Manganese mediated oxidation of progesterone in alkaline medium: Mechanism study and quantitative determination, *Electrochimica Acta*, 2017, 225, 292-302.
- 39- **A.A. Taherpour**, F Ghasemhezaveh, A Yari, MM Khodaei, N2 elimination thermolysis reactions of 9-(4- and 5-substituted-1,2,3-triazol-1-yl)acridines to produce 1H-pyrido-[4,3,2-kl] derivatives – A theoretical study, *Chemical Physics Letters* 676, 154–168, 2017.
- 40- MB Gholivand, H Peyman, K Gholivand, H Roshanfekr, **A.A. Taherpour**, R Yaghobi, Theoretical and Instrumental Studies of the Competitive Interaction Between Aromatic α -Aminobisphosphonates with DNA Using Binding Probes, *Applied Biochemistry and Biotechnology*, 2017, 182(3), 925–943.
- 41- **A.A. Taherpour**, A Yari, F Ghasemhezaveh, MA Zolfigol, The First Principle Computational Study for the Competitive Mechanisms of Oxidative Aromatization of 2-Substituted Imidazolines using KMnO₄/SiO₂, *Journal of the Iranian Chemical Society (JICS)*, 2017, 41(12), 2485–2493.
- 42- MA Zolfigol, M Kiafar, M Yarie, **A.A. Taherpour**, T Fellowes, AN Hancok, T. Fellows, A. Yari, A convenient method for preparation of 2-amino-4, 6-diphenylnicotinonitrile using HBF 4 as an efficient catalyst via an anomeric based oxidation: A joint experimental and theoretical study, *Journal of Molecular Structure-Elsevier*, 2017, 1137, 674-680.
- 43- MB Gholivand, H Peyman, K Gholivand, H Roshanfekr, **AA Taherpour**, R. Yaghobi, Experimental and theoretical studies of interaction of aliphatic chain α -aminobisphosphonates with DNA, *Journal of Photochemistry and Photobiology A: Chemistry*, 2017, 338, 183-191.
- 44- **AA Taherpour**, M Jamshidi, O Rezaei, Recognition of switching on or off fluorescence emission spectrum on the Schiff-bases as a Mg²⁺ chemosensor: A first principle DFT and TD-DFT study, *Journal of Molecular Structure*, 2017, 1147, 815-820.
- 45- N Shahabadi, B Bazvandi, **AA Taherpour**, Synthesis, structural determination and HSA interaction studies of a new water soluble Cu(II) complex derived from 1,10-phenanthroline and ranitidine drug, *Journal of Coordination Chemistry*, 2017, 70(18), 3186-3198.
- 46- **A. A. Taherpour**, Theoretical Studies of the Free Energies of Electron Transfer and Electron Transfer Kinetics in Nanostructure Supramolecular Complexes of Cis-Unsaturated Thiocrown Ethers and Ce and Gd Endohedral Metallofullerenes [X-UT-Y][M@C₈₂] (M=Ce,Gd), *Arab. J. Chem.*, 2017, 10, S609–S616.
- 47- R Aliveisi, **AA Taherpour**, I Yavari, A DFT Study of Electronic Structures and Relative Stabilities of Isomeric n,m-Diazaphenanthrines, *J. Polycyclic Aromatic Compounds*, 2017, 10.1080/10406638.2017.1343195.
- 48- N Shahabadi, M Mahdavian, **AA Taherpour**, F Ghasemhezaveh, Synthesis, characterization and in vitro DNA binding studies of a new copper(II) complex containing antioxidant ferulic acid, *Journal of Coordination Chemistry*, 2017, 70(15), 2589-2605.

- 49- M Torkashvand, MB Gholivand, **AA Taherpour**, A Boochani, A Akhtar, Introduction of a carbon paste electrode based on nickel carbide forinvestigation of interaction between warfarin and vitamin K1, *Journal of Pharmaceutical and Biomedical Analysis*, 2017, 139, 156-164.
- 50- M Motiei, S Kashanian, **AA Taherpour**, Hydrophobic amino acids grafted onto chitosan: a novel amphiphilic chitosan nanocarrier for hydrophobic drugs, *Drug Development and Industrial Pharmacy*, 2017, 43(1), 1-11.
- 51- **A.A.Taherpour**, M. Jamshidi, DFT and TD-DFT Theoretical Studies on Photo-induced Electron Transfer Process on [Cefamandole].C₆₀ Nano-Complex, *Journal of Molecular Graphics and Modelling*, 2017, 75, 42-48.
- 52- Mohammad Ali Zolfigol, Maliheh Safaiee, Bahar Ebrahimghasri, Saeed Baghery, Saied Alaie, Mahya Kiafar, **Avat(Arman) Taherpour**, Yadollah Bayat, Asiye Asgari Application of novel nanostructured dinitro pyrazine molten salt catalyst for the synthesis of sulfanylpyridines via anomeric based of oxidation, *J Iran Chem Soc, JICS*, 2017, 14 (9), 1839–1852.
- 53- MB Gholivand, H. Payman, K. Gholivand, A.A. Taherpour, Experimental and computational evidence on the interaction of cycloalkyl α -aminobisphosphonates with calf thymus DNA" for DNA and Cell Biology, *DNA and Cell Biology*, 2017, 36(7), 541–551.
- 54- N Shahabadi, M Pourfolad, **A.A. Taherpour**, Synthesis, characterization and in vitro DNA binding studies of a new copper(II) complex containing an antiviral drug, valganciclovir, *Journal of Coordination Chemistry*, 2017, 70(2), 201-222.
- 55- **Avat(Arman)Taherpour**, Mohammad Ali Zolfigol, Replay to the Comments on “Experimental and theoretical studies of thenanostructuredFe₃O₄@SiO₂@(CH₂)₃Im}C(CN)₃catalyst for 2-amino-3-cyanopyridine preparation via an anomeric based oxidation”, *RSC Adv.*, 2016, 6, 50100-50111, and “The first computational study for the oxidative aromatization of pyrazolines and 1,4-dihydropyridines using 1,2,4-triazolinediones: an anomeric-based oxidation”, *RSC Adv.*, 2016, 6, 102280-102291, *RSC-Advances*, 2017, 7, 53617-53621.
- 56- **A.A. Taherpour**, M. Mahmoodi, M. Khodaei, N. Tamasoki, A First Principle DFT Study of Solvent Effects on Metiamide Tautomers and Imaginary Interactions with H₂-Receptors, *J Iran Chem Soc, JICS*, 2017, 14, 1613–1632.
- 57- R Aliveisi, **AA Taherpour**, I Yavari, A DFT Study of Structures and Stabilities of Isomeric Furo-, Thieno-, and Selenophenopyridines, *Phosphorus, Sulfur, and Silicon and the Related Elements*, 2017, 192(4), 422-426.
- 58- S. Taban, **AA Taherpour**, Theoretical Study of 1,3-Dipolar Reactions of Myrcene and Trimethylsilylazide, *Letters in Organic Chemistry*, 2017, 14 (3), 159 – 171.
- 59- **A.A. Taherpour**, S. Khaef, A. Yari, S. Nikeafshar, etal, Chemical Composition Analysis of the Essential Oil of Mentha piperita L. from Kermanshah-Iran by Hydrodistillation and HS/SPME Methods, *Journal of Analytical Science and Technology*, 2017, 8(11), 10.1186/s40543-017-0122-0.
- 60- **AA Taherpour**, A Taherpour, N Zolfaghari-Kerahroudi, Study of electron transfer process between fullerenes and membrane cells of Escherichia coli in the presence of dinitrophenol and dicyclohexylcarbodiimide, *Arabian Journal of Chemistry*, 2017, 10 (2), S2363–S2371.

- 61-E Rajaeian, **AA Taherpour**, Kinetic Study of Reaction between Allyl Compounds of Mg and Ethylene: Computational Investigation, *Iran. J. Chem. Chem. Eng.*, 2017, 36 (2), 7-15.
- 62-**AA Taherpour**, A Yari, F Ghasemhezaveh, MM Khodaei, DFT study of 1,3-dipolar cycloaddition reaction of 2-(4-azidophenyl) benzo[d]thiazole with acetylene derivatives, *Ind. J. Chem. Sec.-B*, 2017, (accepted for publication).
- 63-**AA Taherpour**, MM Khodaei, BAH Ameen, M Ghaitouli, N Mahdizadeh, H. Amjadian, Chemical composition analysis of the essential oil of Solanum nigrum L. by HS/SPME method and calculation of the biochemical coefficients of the components, *Arabian Journal of Chemistry* 2017, 10(2), S2372–S2375.
- 64-**AA Taherpour**, F Jahanian, Theoretical Study of Diffusion Flow of Neurotransmitters Through Single-Wall Armchair(10,10) and Zigzag(18,0) Carbon Nanotubes, *Iranian Journal of Science and Technology, Transactions A: Science*, 2017, 41(3), 787-808.
- 65-M. Irandoust, M. haghghi, **A.A. Taherpour**, Electrochemical Determination of Antinonin by Cefazolin-Immobilized Fe₃O₄/SiO₂ Nanomagnetic core shell Linked to Carbon Nanotube Modified Glassy Carbon Electrode; an Experimental and Theoretical modeling, *Electrochemistry -The Electrochemical Society of Japan (ECSJ)*, 2017, (Accepted for Publication), DOI:.
- 66-E Rajaeian, E Mirzaei, **AA Taherpour**, Theoretical Calculation of Thermodynamic and Kinetic Quantities for 1,3 Dipolar Cycloaddition Reactions Between Nitrile Sulfides R-CNS (R = H, CH₃, Ph and Ph(CH₃)₃) with 7–10 Membered Simple Cycloalkynes, *Iranian Journal of Science and Technology, Transaction A, Science*, 2017, 41, 1139-1148.
- 67-M. Shamsipur, **A.A. Taherpour** and A. Pashabadi, Interrupting the flux of delocalized electrons on a dibenzo-18-crown-6-embedded graphite sheet and its relative counteraction in the presence of potassium ions, *Analyst*, 2016, 141, 4227-4234.
- 68-MH Khalilian, S Mirzaei, **AA Taherpour**, The simulation of UV spectroscopy and electronic analysis of temozolomide and dacarbazine chemical decomposition to their metabolites, *Journal of Molecular Modeling*, 22(11), 2016, 270.
- 69-S Mirzaei, **AA Taherpour**, S Mohamadi, Mechanistic study of allopurinol oxidation using aldehyde oxidase, xanthine oxidase and cytochrome P450 enzymes, *RSC Advances*, 2016, 6, 109672-109680.
- 70-M. Shamsipur, L Allahyari, J Fasihi, **AA Taherpour**, Z. Asfari, A. Valinejad, Study of complexation between two 1,3-alternate calix[4]crown derivatives and alkali metal ions by electrospray ionization mass spectrometry and density functional theory calculations, *Journal of Molecular Structure*, 1108, 15, 2016, 16–24.
- 71-M Shamsipura, A Pashabadia, **AA Taherpour**, B Hemmateenejad, Synthesis and characterization of glucose-capped CdSe quantum dots. Electrochemical and computational studies of corresponding carbon-ionic liquid electrode for quantitative determination of minoxidil, *Journal of Electroanalytical Chemistry*, 2016.

- 72- **AA Taherpour**, R Rahimizadeh, Study of solvent effects on structural and conformational properties of cimetidine tautomers, *Medicinal Chemistry Research*, 2016, 25(9), 2042-2057.
- 73- MA Zolfigol, M Kiafar, M Yarie, **AA Taherpour**, M Saeidi-Rad, Experimental and theoretical studies of the nanostructured {Fe₃O₄@SiO₂-(CH₂)₃Im}C(CN)₃ catalyst for 2-amino-3-cyanopyridine preparation via an anomeric based oxidation, *RSC Advances*, 2016, 55(6), 50100-50111.
- 74- M Motiei, S Kashanian, **AA Taherpour**, Hydrophobic amino acids grafted onto chitosan: a novel amphiphilic chitosan nanocarrier for hydrophobic drugs, *Drug Development and Industrial Pharmacy*, 43, 2017, 1-11.
- 75- M Kiafar, MA Zolfigol, M Yarie, **AA Taherpour**, The first computational study for the oxidative aromatization of pyrazolines and 1, 4-dihdropyridines using 1, 2, 4-triazolinediones: an anomeric-based oxidation, *RSC Advances*, 2016, 6(104), 102280-102291.
- 76- M Shamsipur, L Allahyari, J Fasihi, **A. A. Taherpour**, Z Asfari, A Valinejad, Study of complexation between two 1, 3-alternate calix [4] crown derivatives and alkali metal ions by electrospray ionization mass spectrometry and density functional theory calculations, *Journal of Molecular Structure*, 2016, 1108, 16-24.
- 77- **A. A. Taherpour**, M. Rizebandi, F. Jahanian, E. Naghibi, N. Mahdizadeh, Theoretical Study of Electron Transfer Process Between Fullerenes and Neurotransmitters; Acetylcholine, Dopamine, Serotonin and Epinephrine in Nanostructures [Neurotransmitters].C_n Complexes, *Journal of Chemical Biology* (JOCB-Springer), 2016, 9 (1), 19-29.
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- 1- Ali Barati, Sara Karami; Mojtaba Shamsipur; Avat Arman Taherpour, Novel chromophore-doped carbon dots with multiple emission colors: Application in ratiometric sensing, cellular imaging, and wound healing, Submitted-2019.

- 2- A. A. Taherpour, M. Hashemi, Structural Assessing of the H-Bonding Arrays on the Methylpentynol-Azide Clusters to achieve the Regiochemical outcome of the 1,3-Dipolar Cycloaddition Reactions by DFT, Submitted-2019.
- 3- Avat Arman Taherpour, Parya Gholami keivanani, Morteza Jamshidi, Samira Hatami, Narges Zolfaghar, Theoretical Studies on Photo-Induced Electron Transfer Process on [Thioridazine].C60 Nano-Complex; A First Principle DFT and TD-DFT, Submitted-2019.

Seminars and Conferences:

Note: *Some of the National and International conference papers were not listed in the following series. The total numbers of the National and International conference papers presented (up to March 2018) were about 400.*

1-**A. A. Taherpour** and A. Jafari, Theoretical Study of Free Energies of Electrontransfer in the supramolecular complexes of Vitamin B12 with Fullerenes Cn Nanostructurs., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

2-**A. A. Taherpour** and H. Shafie and M. Harizi, Electronic Structural Studies of One Dimensional Fused Oligo-Selenophenes, Free Electron transfer, Activation Energies and Kinetic Properties in Nano Supramolecular Complexes of The Compounds with Fullerenes., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

3-**A.A. Taherpour** and H. Shafie and M. Harizi, Theoretical and Experimental Study of the poly fused selenophene (n) Electronic Spectra ., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

4-**A.A. Taherpour** and H. Shafie and M. Harizi, Quantitative Structural Relationship Study on Octanol-Water Partitioning Coefficients, Total Biodegradation, LC50 and Water solubility of One Dimensional Fused Oligo-Thiophenes ., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

5-**A.A. Taherpour** and B. Hormozi, Theoretical Study of Structural Relationships and Electrochemical Properties of NanoSupramolecular [Cytochromes]@Cn Complexes., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

6-**A.A. Taherpour** and N. Jahangiri , Free Activated Energies and Kinetic Properites of Electron Transfer Studies of [R].Cn (R=Cytochrome-c peroxidase, Cytochrome-c oxidase, Tyrosinase and Ascorbate oxidase) Nanostructur Complexes ., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

7-**A.A. Taherpour** and M. Rizehbandi , Theoritical Electrochemical Study and Free Energies of Electrontransfer of Dopamin (DA) with Fullerenes C60 Nanostructurs Complexes., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

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11-A.A. Taherpour . Theoretical and QSR Studies of Free Energies of Electron Transfer of Cis-Unsaturated Thiocrown Ethers and Their Nanostructures Complexes [X-UT-Y][M@C₈₂](M=Ce & Gd).,14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

12-A.A. Taherpour and L. Fathiyan, Electron Transfer Kinetic Theoretical and Quantitative Structural Relationship Studies of C_n@X-[HbA] (HbA=Hemoglobin A; X= α- and β-Fumarate Crosslinked Hemoglobins (αXL & βXL))Nanostructur Complexes., 14th conference of Iranian Physical Chemistry , Feb. 25-28, 2011, Tehran University campus Kish International, Kish-Iran.

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- 69-**A. A. Taherpour**, et al., "Volatile Constituents of Stachys Lavandolifolia From Kurdistan of Iran", 14-ESOC, Helsinki-Finland, 4-8 July-2005, Poster presentation.
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- 83-**A. A. Taherpour** & S. Bigdeli-Kamal, "Oxidation of Barbituric Acid for Synthesis of Alloxane", 8th Iranian Seminar of Organic Chemistry, Kashan University, Kashan University-Iran, 16-18 May 2000.
- 84-**A. A. Taherpour** & H. Mansuri, "Oxidation of ε -Caprolactam by Using Microwave Irradiation", 8th Iranian Seminar of Organic Chemistry, Kashan University, Kashan University-Iran, 16-18 May 2000.
- 85-**A. A. Taherpour**, K. Izadi, "Semi-empirical Study of Structural Properties of Resorcin[4]arenes", 8th Iranian Seminar of Organic Chemistry, Kashan University, Kashan University-Iran, 16-18 May 2000.
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- 89-**A. A. Taherpour** & M. Solimani, "AM1 Study of Bergman Rearrangement of Z-C-,N-3imine-1,5-diyne and 3,4-diethynyl diamine", 13th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Modares University, Tehran, Iran, 16-18 Feb. 1999.
- 90-**A. A. Taherpour** & K. Nazari, "Semi-empirical Study of Transformation of PPIX-Zn-H₂O to PPIX-Zn-H₂O₂", 5th Iranian Seminar of Inorganic Chemistry, Esfahan University, Iran, 1-2 Sep. 1999.
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- 93-**A. A. Taherpour**, "Semi-empirical Study of the Structures of [(R)Calix^{TMS}₂]Al-H", The first Congress of Chemistry of I.A.University (Central Tehran Branch- Science & Louispasteur University), Tehran-Iran, 1-2 Dec. 1999.

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- 97-**A. A. Taherpour**, A. Jabari and I. Yavari, "Conformational Properties of diacetylene Carbocyclic Compounds", 2th International and 12th National Congress of Chemistry and Chemical Engineering, Shahid Bahonar, Kerman, Iran, 31 Sep.-2 Agu. 1997.
- 98-**A. A. Taherpour**, M. Dadgar and I. Yavari, "One-pot Synthesis of new Pyran Systems", 2th International and 12th National Congress of Chemistry and Chemical Engineering, Shahid Bahonar, Kerman, Iran, 31 Sep.-2 Agu. 1997.
- 99-**A. A. Taherpour**, A. Jabari and I. Yavari, "Theoretical Study & Comparison of Cyclononyne and 4,4,8,8-teramethylcyclononyne", 6th Iranian Seminar of Organic Chemistry, Tabriz University, Iran, 19-21 Agu. 1997.
- 100-**A. A. Taherpour** A. Shababi and I. Yavari, "Semi-empirical SCF-MO Study of Conformers of Thiocane", 4th Iranian Seminar of Organic Chemistry, Ferdowsi University, Mashhad, Iran, 12-14 Nov. 1996.
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- 102-**A. A. Taherpour**, "Coulomb Zero Centers Introducing and Application of them in Molecules", 4th Iranian Chemistry and Chemical Engineering Congress, Gillan University, Rasht, Iran, 4-6 Sep. 1996. [a hypothesis].
- 103-**A. A. Taherpour** & I. Yavari, "Conformational Properties of Z-Cyclodeca-3- ene-1,5-diyne & Z-Cycloundeca-3-ene-1,5-diyne", 3th Iranian Seminar of Organic Chemistry, Ferdowsi University, Mashhad, Iran, 17-19 Oct. 1995.
- 104-**A. A. Taherpour**, "Coulomb Zero Centers in Crown Ethers", 1th Iranian Seminar of Organic Chemistry, Shahid Beheshti University, Tehran, Iran, 16-18 Jan. 1991.

Books:

- 1) **A. A. Taherpour** and M. Talebi, "Modern IR-Spectroscopy", Published in Oct. **2001**, IRAN.
- 2) **A. A. Taherpour**, K. Zareh and H. Aghaie, "How to Use Chemical Literatures", Publisher: I.A.U.-IRAN, May. **2002**, Tehran-IRAN.
- 3) **A. A. Taherpour**, "Organic Chemistry (for B.S. Students)-1", Publisher: I.A.U.-IRAN, **2004**, Arak-IRAN.
- 4) **A. A. Taherpour**, "Organic Chemistry (for B.S. Students)-2", Publisher: I.A.U.-IRAN, **2005**, Arak-IRAN.

- 5) **A. A. Taherpour**, "Organic Chemistry (for B.S. Students)-3", Publisher: I.A.U.-IRAN, **2004**, Arak-IRAN.
- 6) **A. A. Taherpour**, "Organic Reaction Mechanisms", Publisher: I.A.U.-IRAN, **2004**, Arak-IRAN.
- 7) **A. A. Taherpour**, "The Rapid Interpretation of Spectral Data", Publisher: I.A.U.-IRAN, 1st Edition, **2007**, Arak-IRAN; 2nd Edition, **2010**.
- 8) **A. A. Taherpour** and M. Abdoli, "Medicinal Chemistry", Publisher: I.A.U.-IRAN, **2011**, Arak-IRAN. (*In press*).
- 9) **A. A. Taherpour** and M. Malekdar, "A Glance at Natural Products Synthesis", Publisher: I.A.U.-IRAN, **2011**, Arak-IRAN.
- 10) **A. A. Taherpour** and A. Taherpour; **Writing one chapter of the book entitled: "Urinary Tract Infectious"**, In Tech-Open Access Publisher, for **2011**. (Over 3000 downloaded Chaper, 2011-2015).
- 11) **A. A. Taherpour**, A. Taherpour, Z. Taherpour and O. Taherpour; **Writing one chapter of the book entitled: "Insomnia-Barbiturates"**, In Tech-Open Access Publisher, for **2011**. (Over 2000 downloaded Chaper, 2011-2015)
- 12) **A. A. Taherpour**, F. Mousavi, "Carbon Nano Materials for Electroanalysis in Pharmaceutical Applications", in Multi-Volume SET (I-XXVII) "Pharmaceutical Nanotechnology" section, **Elsevier Book Chapter, 2018**.

Registration Invention:

- 1) Registration Invention: "Making Salt Cells of IR-Spectrophotometers", as a Successful project in Iran, 2003. Registry Number: IRAN-1710803081-2003. (A. A. Taherpour & H. Hadadi).
- 2) Registration Invention: New One-pot Methods of Synthesis and Production of Mozobil and its 8-Hydrochloric Salt with High Efficiency (Rapid, Yield and Purity). Registry Number: IRAN-95150-2018.
- 3) Registration Invention: Water Circulator for Condensers, Registry Number: under process-2018.
- 4) Registration Invention: New One-pot Methods of Synthesis and Production of Edravone, Registry Number: under process-2018.

Number of Research Projects:

The numbers of individual terminated research projects are: 20.

Awards and Honours:

- 1) Outstanding Researcher, Islamic Azad University, 2002, Arak-Markazi, IRAN.
- 2) Outstanding Researcher, Islamic Azad University, 2002, Sanandaj-Kurdistan, IRAN.
- 3) Prize for book entitled: "*How to Use Chemical Literature*", Publisher: I.A.U.-IRAN, May. 2002, Tehran-IRAN.
- 4) Superior Researcher, Markazi Province of IRAN, 2003, Arak, IRAN.
- 5) Superior Researcher, Islamic Azad University, IRAN, 2003, Arak-Markazi Province, IRAN.
- 6) Superior Researcher, Islamic Azad University, IRAN, 2003, Sanandaj-Kurdistan Provence, IRAN.
- 7) Superior Researcher, Markazi Province of IRAN, 2005, Arak, IRAN.
- 8) Superior Researcher, Islamic Azad University, 2005, West Universities of Country, Sanandaj, Kurdistan Province-IRAN.
- 9) Superior Researcher, Markazi Province of IRAN, 2007, Arak, IRAN.
- 10) Superior Researcher, Zone-5 of Islamic Azad University, IRAN, 2007, Zone-5, IRAN.
- 11) Superior Researcher in IRAN in Islamic Azad Universities, 2007, IRAN.

- 12) Superior Researcher and Academic Member in Science and Technology, Markazi Province of IRAN, 2007, Arak, IRAN.
- 13) One of the 100 Superior Researcher Nano Technology Sciences, IRAN, 2008.
- 14) Superior Researcher and Academic Member in Science and Technology, Markazi Province of IRAN, 2008, Arak, IRAN.
- 15) Superior Researcher, Islamic Azad University, IRAN, 2008, Sanandaj-Kurdistan Province, IRAN.
- 16) Superior Researcher and Academic Member in Science and Technology, Kurdistan Province of IRAN, 2008, Sannandaj, IRAN.
- 17) Superior Researcher, Islamic Azad University, IRAN, 2009, Sanandaj-Kurdistan Province, IRAN.
- 18) One of the 100 Superior Researcher Nano-Technology Sciences, IRAN, 2009.
- 19) Superior Researcher, Islamic Azad University, 2009, IRAN.
- 20) Superior Researcher, Universities of IRAN, *Science, Research and Technology Ministry of Iran*, 2009, IRAN.
- 21) Superior Researcher, Markazi Province of IRAN, 2010, Arak, IRAN.
- 22) Superior researcher with more progress in nanotechnology research, 5th Nanotechnology Festival of IRAN, 2010, IRAN.
- 23) Selection of two (2) papers as 2 Top papers by "BioMedLib-The top 10 articles published", www.BioMedLib.com, 2011.
- 24) Superior Researcher, *1st Research, Scientific & Technological Festival of the Islamic Azad University*, Research and Technology Vice of I.A.U., 2011, Tehran-IRAN.
- 25) Honored by the National Endowment for the elite as one of the 30 Professor in Kermanshah-Iran, 2013.
- 26) Committee member for some of the industry-Iranian national standard, 2013-2014.
- 27) First place winners of the contest better idea in the Research week of 2015, Kermanshah University of Medical Sciences, Kermanshah-Iran.
- 28) Standard official expert in chemistry and chemical industry (Institute of Standards and Industrial Research of Iran).
- 29) Superior Researcher, Razi University, Kermanshah, IRAN, 2016 Research week, Kermanshah, Iran).
- 30) Superior Researcher, Razi University, Kermanshah, IRAN, 2018 Research week, Kermanshah, Iran).

Number of the Papers in Iranian (Persian language) Journals:

The number of papers in Persian (Farsi) language are 29.