



Heidar Raissi

Professor

Faculty: Science

Department: Chemistry

Papers in Conferences

1. Quantum mechanical study of the interaction of DNA pyrimidine bases with Flutamide anticancer. حیدر رئیسی، کامل مائده، مرسلی علی ششمین کنفرانس بین المللی شیمی، پلیمر و مهندسی شیمی، شماره صفحات ۰۴۰۹ ۲۰۱۷، تهران، ۰۴۰۹ ۲۰۱۷.
2. The effect of substituted F and CH₃ on the structure and the HBS in the N-hydro-seleno-Nthioxoimidoformamide compound. حیدر رئیسی، زهرا کمالی، فریبا ملانیا دهمین همایش ملی شیمی دانشگاه پیام نور، شماره، ۱۰ ۱۰ ۲۰۱۲، کرمان، صفحات ۱۰ ۱۰ ۲۰۱۲.
3. Theoretical study of substitution effect on strength of the IHB in (Z)-N-(nitrosomethylene)selenohydroxylamine. حیدر رئیسی، سعیده سهیلی، فریبا ملانیا دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
4. Effect of substitution CH₃ and F on the intramolecular hydrogen bonding of ۳-Amino-propeneselenal DFT AIM and NBO studies. حیدر رئیسی، شهیرا اسلام دوست جامی، فریبا ملانیا دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
5. Investigation of stable conformers in (thioxosilyl) ethyleneselenol compound. حیدر رئیسی، زهرا کمالی، مهدی یوسفیان سقی دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
6. Theoretical study on intramolecular hydrogen bonding in ۳-Hydroxy-propeneselenal title compound. حیدر رئیسی، سعیده سهیلی، مهدی یوسفیان سقی دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
7. Theoretical Study the molecular structure and intramolecular hydrogen bond energies conformers of ۳-Amino-propeneselenal (APS) Energetic NBO and AIM analyses. حیدر رئیسی، شهیرا اسلام دوست جامی، مهدی یوسفیان سقی دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
8. Theoretical comparison of ۱۱ ۱-Trifluoro-۴-mercapto-but-۳-ene-۲-thione and ۴ ۴-Trifluoro-۳-thioxo-butanethial conformers. حیدر رئیسی، حکم آبادی لیلیا دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
9. Theoretical study of the intramolecular hydrogen bond strength in ۱-(thionitrosomethylene) hydrazine AIM and NBO studies. حیدر رئیسی، خانمحمدی آزاده دهمین همایش ملی شیمی دانشگاه پیام نور، شماره، ۱۰ ۱۰ ۲۰۱۲، کرمان، صفحات ۱۰ ۱۰ ۲۰۱۲.
10. S H . . . S intramolecular hydrogen bonds in (Z)-N-mercaptolithionitrosomethanimine The influence of external agents on -electron Delocalization. حیدر رئیسی، خانمحمدی آزاده دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
11. A theoretical study of the photochromic compound ۳-(۲ ۵-Dimethyl-thiophen-۳-ylmethylene)-۴-methylene-dihydro-furan-۲.۵-dione. حیدر رئیسی، حکم آبادی لیلیا دهمین همایش ملی شیمی دانشگاه پیام نور، شماره صفحات ۱۰ ۱۰ ۲۰۱۲، کرمان، ۱۰ ۱۰ ۲۰۱۲.
12. Theoretical study of substitution effect on strength of the intramolecular hydroge bond حیدر رئیسی

- دومین کنفرانس مهندسی صنایع، شماره صفحات ۱۸-۲۰۰۳، یزد، ۲۰۰۳، (Z)-N-18
13. The effect of substituted F and CH₃ on the structure and the strength of hydrogen bond in the N-hydro-seleno-Nthioxoimidofornamide compound, دومین کنفرانس مهندسی صنایع، شماره صفحات ۱۸-۲۰۰۳، یزد، ۲۰۰۳.
 14. Sensitivity mechanism of single-walled carbon nanotube as a drug delivery system toward the anticancer drug molecules, مشهد، 17 07 2018, pp. - بیستمین کنگره شیمی ایران.
 15. Mortazavi far Azam, A computational study on the electronic properties of single walled boron nitride nanotube as carrier for Carmustine molecule by DFT, مشهد، 2018, pp. - بیستمین کنگره شیمی ایران، 17 07.
 16. Theoretical study of adsorption behaviour of Thioguanine anticancer drug on the surface of fullerene C60 nanocage, مشهد، 17 07 2018, pp. - بیستمین کنگره شیمی ایران.
 17. Theoretical Study on Adsorption of methane molecule on nanostructured functionlized Graphene with hydroxyl and epoxide, مشهد، 17 07 2018, pp. - بیستمین کنگره شیمی ایران.
 18. Adsorption of Cr and Pd transition metal atoms on the pristine Zinc oxide nanotube a DFT approach, مشهد، 17 07 2018, pp. - بیستمین کنگره شیمی ایران.
 19. Single-Walled Boron Nitride Nanotubes as Effective Adsorbent for Separation and Adsorption CO₂ and CH₄ Monte Carlo Simulation, اولین کنگره بین المللی شیمی و نانو شیمی از پژوهش تا فناوری، تهران، 11 07 2018, pp. -
 20. Monte Carlo simulation of CH₄ and CO₂ Adsorption and Separation in Single-Walled Carbon Nanotubes, اولین کنگره بین المللی شیمی و نانو شیمی از پژوهش تا فناوری، تهران، 11 07 2018, pp. -
 21. Adsorption and Diffusion of CH₄ CO₂ N₂O and SO₂ gases on MOF-5 Molecular Dynamics study, تهران، 04 09 2017, pp. - ششمین کنفرانس بین المللی شیمی، پلیمر و مهندسی شیمی.
 22. Investigating the pi pi interaction between pyrazine and its different derivatives, تهران، 04 09 2017, pp. - بین المللی شیمی، پلیمر و مهندسی شیمی.
 23. Molecular Dynamics Simulation study of Adsorption and Diffusion of CH₄ and CO₂ gases on HUKST-1, تهران، 04 09 2017, pp. - ششمین کنفرانس بین المللی شیمی، پلیمر و مهندسی شیمی.
 24. Comprehensive Theoretical investigation of N₂O gas adsorption on the single- wall carbon nanotube, تهران، 04 09 2017, pp. - ششمین کنفرانس بین المللی شیمی، پلیمر و مهندسی شیمی.
 25. Study on the interaction of Single-Walled Carbon Nanotube with organometallic transition metal compounds, تهران، 04 09 2017, pp. - ششمین کنفرانس بین المللی شیمی، پلیمر و مهندسی شیمی.
 26. Insight into the Interaction between anticancer drug melphalan and functionalized carbon nanotube Density Functional Theory, تهران، 04 09 2017, pp. - ششمین کنفرانس بین المللی شیمی، پلیمر و مهندسی شیمی.
 27. Interaction of anticancer drug melphalan with carbone nanotube surface as a nanocarrier A Quantum Mechanical Approach, تهران، 2017, pp. - ششمین کنفرانس بین المللی شیمی، پلیمر و مهندسی شیمی، 04 09.
 28. Graphen oxide nanosheet A DFT study of NMR and NQR parameters, ششمین کنفرانس بین المللی، تهران، 04 09 2017, pp. - شیمی، پلیمر و مهندسی شیمی.
 29. Sulfur mustard gas adsorption on single-layer aluminum nitride nanostructures A DFT STUDY, تهران، 31 08 2017, pp. - پنجمین همایش بین المللی شیمی، مهندسی شیمی و نانو ایران.
 30. farzad farzaneh, Investigation the intermolecular hydrogen bonding between DNA thymine base dimer and its different derivatives, سومین کنفرانس بین المللی دستاوردهای نوین پژوهشی در شیمی و مهندسی، تهران، 23 09 2016, pp. - شیمی.
 31. farzad farzaneh, Investigation of the As Ga B and N-doped (6 0) aluminum phosphide nanotubes interactions with H₂S gas DFT study, سومین کنفرانس بین المللی دستاوردهای نوین پژوهشی در شیمی و مهندسی، تهران، 23 09 2016, pp. - مهندسی شیمی.
 32. First-principles investigation of armchair aluminum phosphide nanotube for sensing phosgene, سمنان، 30 08 2015, pp. - هجدهمین کنگره شیمی ایران.
 33. The HCN adsorption on the outer surface of aluminum phosphide nanotube, هجدهمین کنگره شیمی، سمنان، 30 08 2015, pp. - ایران.

34. Maasoumeh Jafarpour ,Structure and Properties of the Second and Third Generation Manganese-oxo Porphyrins in the Presence of Imidazole A Comparative DFT Study ,pp. 262-262 ,30 08 2015, سمنان.
35. Maasoumeh Jafarpour ,Quantum-Chemical study on the Stacking Interactions between High Valent oxo-Manganese Porphyrin Nanoparticles ,pp. 263-263 ,30 08 2015, سمنان.
36. ,Mola Adeleh ,investigation of pristine and Pd-Doped SWCNT as a Sensor for chemical sensing of formaldehyde ,pp. 819- ,2014, تهران , 21 10.
37. _ ,A computational assessment of molecular structure intramolecular hydrogen bond and HNMR of hydrogen- ethaneselenal ,pp. 959-960 ,29 10 2013, بابلسر.
38. _ ,DFT study of the rotation barrier electronic structure intramolecular hydrogen bond topological parameters and aromaticity indices in (Z)-(nitrosomethylene)hydrazine ,pp. 957-958 ,29 10 2013, بابلسر.
39. _ ,Theoretical study of intermolecular interaction between oxalic acid and H O NH NH CH ,pp. 1027-1027 ,07 09 2013, یزد.
40. Hossein Farsi ,Preparation and electrochemical capacitive behaviors of nanostructured molybdenum oxides ,pp. - ,03 09 2012, تهران.
41. Hossein Farsi ,The Electrochemical Studies of Sol Gel Prepared Nanostructured Nickel Titanate ,pp. - ,28 08 2012, تهران.
42. Hossein Farsi ,On the Effects of Electrolyte on the Capacitive Behavior of Nanostructured Molybdenum Oxides ,pp. 713-717 ,10 03 2010, کیش.
43. Hossein Farsi ,Electrodeposition of nanostructured molybdenum oxide and its capacitive behavior ,pp. - ,14 05 2008, زاهدان.

Papers in Journals

1. Seyed Yousef Mosavian, Meissam Noroozifar, Mohammad Ali Karimi Zarchi, Zeinab Hamidi, Najmeh Sabbaghi, Derivatives of [P4-VP] 2% DVB as corrosion inhibitors for St-37 in 1 M H₂SO₄: an experimental and theoretical investigations, Polymer bulletin, Vol. 1, No. 1, pp. 1-30, 2022, JCR, Scopus.
2. Mohammad Yahya Hanafi-Bojd, Milad Iranshahy, Asghar Zarban, The combination of polyphenols and phospholipids as an efficient platform for delivery of natural products, Scientific Reports, Vol. 1, No. 13, pp. 1-20, 2023, JCR, Scopus.
3. Significantly enhanced performance for phenol compounds removal by MOF-5 nano-composite via its surface modification. Npj clean water, شماره ۷, شماره صفحات ۱-۲۰۲۴, ISI, JCR, Scopus.
4. seyede leila Razavi Khoosfi, Efficient immobilization of horseradish peroxidase enzyme on transition metal carbides, Journal of Molecular Liquids, Vol. 1, No. 386, pp. 1-10, 2023, ISI, JCR, Scopus.
5. ameneh zabolli arbab din mohamad, Hassan Hashemzadeh, The state of art in the prediction of efficiency and modeling of the processes of Benzene removal from water environment, Journal of Molecular Liquids, Vol. 1, No. 378, pp. 1-35, 2023, ISI, JCR, Scopus.
6. Halimeh Mirsalari, Afsaneh Maleki, Azim Soltanabadi, The assessment of boron nitride nanotubes and functionalized carbon nanotubes as containers for anticancer drug delivery of dacarbazine and effect of urea on adsorption process by molecular dynamics, Structural Chemistry, Vol. 3, No. 33, pp. 871-882, 2022, JCR, Scopus.
7. Architectural design of 2D covalent organic frameworks (COFs) for pharmaceutical pollutant removal. Npj clean water, شماره ۷, شماره صفحات ۱-۱۵, ISI, JCR, Scopus.
8. Ionic liquids and Graphene: The ultimate combination for High-Performance supercapacitors. Journal of Molecular Liquids, شماره ۴۰۱, شماره صفحات ۱۲۴۵۲۳-۱۲۴۵۴۵, ISI, JCR, Scopus.

9. afsaneh ghahari, Design of a hydroxy channel based on the selectivity of water permeation via ions exclusion, *Npj clean water*, Vol. 1, No. 6, pp. 1-9, 2023, JCR.
10. Molecular mechanism of drug transport and release through zeolitic imidazole framework nanospheres for versatile drug delivery applications, *Journal of Molecular Liquids*, Vol. 1, No. 371, pp. 120822-120829, 2023, JCR, Scopus.
11. seyede leila Razavi Khoosfi, Validation of an MD simulation approach for electrical field responsive micelles and their application in drug delivery, *Scientific Reports*, Vol. 1, No. 13, pp. 1-12, 2023, JCR, Scopus.
12. ameneh zaboli arbab din mohamad, Graphene Oxide Hosting a pH-Sensitive Prodrug: An In Silico Investigation of Graphene Oxide-Based Nanovehicle toward Cancer Therapy, *ACS Applied Bio Materials*, Vol. 1, No. 1, pp. 1-11, 2023, Scopus.
13. Gholamreza Jafari, Ali Saberinasab, Phosphatidylcholine in the tear film of the eye: enhanced topical delivery of fluorometholone to the eye, *Inorganic Chemistry Communications*, Vol. 1, No. 150, pp. 110506-110511, 2023, JCR, Scopus.
14. ameneh zaboli arbab din mohamad, Faezeh Fallahi, Cation-pi interaction: A strategy for enhancing the performance of graphene-based drug delivery systems, *Inorganic Chemistry Communications*, Vol. 1, No. 141, pp. 109542-109550, 2022, JCR, Scopus.
15. ameneh zaboli arbab din mohamad, roghayeh yaghoubi, Assessment of two-dimensional materials on the biological membrane permeability of Epirubicin anti-cancer drug, *Applied Surface Science*, Vol. 1, No. 610, pp. 155557-155563, 2022, JCR, Scopus.
16. Abdul Raqib Haqyar, Hassan Hashemzadeh, A strategy toward therapeutic improvement of electric field-sensitive gemcitabine prodrugs in 2D metal-organic frameworks in view of their structure and interactions, *Inorganic Chemistry Communications*, Vol. 14, No. 135, pp. 109281-109288, 2022, JCR, Scopus.
17. seyede leila Razavi Khoosfi, Strategy to improve Cu-BTC metal-organic frameworks performance in removal of Rhodamine B: MD and WT-MtD simulations assessment, *Npj clean water*, Vol. 1, No. 5, pp. 1-8, 2022, JCR.
18. afsaneh ghahari, Proposing two-dimensional covalent organic frameworks material for the capture of phenol molecules from wastewaters, *Npj clean water*, Vol. 1, No. 5, pp. 1-7, 2022, JCR.
19. A new insight into the transfer and delivery of anti- SARS-CoV-2 drug Carmofur with the assistance of graphene oxide quantum dot as a highly efficient nanovector toward COVID-19 by molecular dynamics simulation†, *RSC Advances*, Vol. 22, No. 12, pp. 14167-14174, 2022, ISI, JCR, Scopus.
20. Ahmad Haghi, On the role of alkanethiol Au complex in the formation of gold deposits; an in-silico approach, *Chemical Geology*, Vol. 1, No. 610, pp. 121101-121112, 2022, JCR, Scopus.
21. حیدر رئیسی, سمانه پاسبان موشکی, New insights into Hexakis macrocycles as a novel nano-carrier for highly potent anti-cancer treatment: A new challenge in drug delivery, *Colloids and Surfaces B: Biointerfaces*, ۸, ۲۰۲۱-۱, شماره صفحات ۲۰۲, شماره ۱۹۷, مجلد ۱۹۷, شماره ۲۰۲, JCR, Scopus.
22. حیدر رئیسی, حلیمه میرسالاری, افسانه مالکی, عظیم سلطان ابادی, Investigation of the Pristine and Functionalized Carbon Nanotubes as a Delivery System for the Anticancer Drug Dacarbazine: Drug Encapsulation, *Journal of Pharmaceutical Sciences*, ۲۰, شماره صفحات ۲۰۰۵, شماره ۲, مجلد ۲, شماره ۲۰, ISI, JCR, Scopus.
23. حیدر رئیسی, رابعه خرم پور, حسین شکی, علی مرسلی, حسن هاشم زاده, The scrutinised DFT and MD studies on the adsorption of D-penicillamine drug on α -Fe₂O₃ nanoparticle as a highly efficient carrier, *MOLECULAR SIMULATION*, ۱۱, ۲۰۲۰-۱, شماره صفحات ۴۶, شماره ۱۶, مجلد ۱۶, شماره ۱۶, JCR.
24. حیدر رئیسی, علی عرب, نجمه داستانی, DFT computational study towards investigating Cladribine anticancer drug adsorption on the graphene and functionalized graphene, *Structural Chemistry*, ۳۱, شماره ۳۱, شماره صفحات ۱۷۰۵, ۲۰۲۰-۱۶۹۱, JCR, Scopus.
25. حیدر رئیسی, حیدر مرادنیا, مهناز شهابی چشمه موسی, The performance of the single-walled carbon nanotube covalently modified with polyethylene glycol to delivery of Gemcitabine anticancer drug in the aqueous environment, *Journal of Biomolecular Structure and Dynamics*, ۱, شماره ۳۴, شماره صفحات ۱, مجلد ۱, شماره ۱, JCR.

۹،۲۰۲۰،ISI،JCR،Scopus.

26. Molecular Insights into the Loading and Dynamics of Anticancer Drugs on Silicene and Folic acidconjugated Silicene nanosheets: DFT calculation and MD simulation،Journal of Biomolecular Structure and Dynamics،شماره ۳۸،شماره ۱،مجلد ۲۲،۲۰۲۰-۱،صفحات ۱-۲۲،ISI،JCR،Scopus.
27. Understanding dual delivery of doxorubicin and paclitaxel with boron nitride and phosphorene nanosheets as highly efficient drug delivery systems،Journal of Biomolecular Structure and Dynamics،شماره ۳۴،شماره ۱،مجلد ۱،ISI،JCR،Scopus.
28. Evaluation the synergistic antitumor effect of methotrexate–camptothecin codelivery prodrug from selfassembly process to acid-catalyzed both drugs release: A comprehensive theoretical study،JOURNAL OF COMPUTATIONAL CHEMISTRY،مجلد ۱۴۹۶،شماره ۱۶،شماره ۴۱،شماره ۱۴۸۶-۲۰۲۰،صفحات ۱۴۹۶،ISI،JCR،Scopus.
29. The transport of Idarubicin therapeutic agent using a novel graphene sheet as a drug delivery platform through a biomembrane،Journal of Molecular Liquids،مجلد ۶،۲۰۲۰-۱،شماره ۲۹۷،شماره ۱،JCR،Scopus.
30. Two dimensional porous frameworks of graphyne family as therapeutic delivery vehicles for Idarubicin biomolecule in silico: Density functional theory and molecular dynamics simulation،Journal of Molecular Liquids،شماره ۳۱۹،شماره ۱،صفحات ۱-۶،۲۰۲۰،JCR،Scopus.
31. Investigation of nanotubes as the smart carriers for targeted delivery of mercaptopurine anticancer drug،Journal of Biomolecular Structure and Dynamics،مجلد ۱۴،۲۰۲۰-۱،شماره ۳۹،شماره ۱،ISI،JCR،Scopus.
32. Predicting the efficiency of polyethylene glycol-functionalised graphene in delivery of temozolomide anticancer drug and investigating the effect of pH on the drug release process: DFT and free energy calculations،MOLECULAR SIMULATION،شماره ۱۸،شماره ۱۰،۲۰۲۰-۱،صفحات ۱-۴۶،JCR.
33. DFT study of Ni-doped graphene nanosheet as a drug carrier for multiple sclerosis drugs،Computational and Theoretical Chemistry،شماره ۱۱۹۶،شماره ۱۱۳۱۱۴،صفحات ۱۱۳۱۲۵،۲۰۲۰،JCR،Scopus.
34. Theoretical elucidation of the amino acid interaction with graphene and functionalized graphene nanosheets: insights from DFT calculation and MD simulation،Amino Acids،شماره ۵۲،شماره ۴،مجلد ۴،ISI،JCR،Scopus.
35. Probing the adsorption and release mechanisms of cytarabine anticancer drug on/from dopamine functionalized graphene oxide as a highly efficient drug delivery system،Journal of Molecular Liquids،شماره ۰،۲۰۲۰-۰،صفحات ۰-۰،JCR،Scopus.
36. Probing the adsorption and release mechanisms of cytarabine anticancer drug on/from dopamine functionalized graphene oxide as a highly efficient drug delivery system،Journal of Molecular Liquids،شماره ۱۱۲۴۵۸،شماره ۳۰۱،مجلد ۱،شماره ۱،۲۰۲۰-۱،صفحات ۱۱۲۴۷۰،JCR،Scopus.
37. Design of New Materials Based on Functionalization of Cu-BTC for Adsorption and Separation of CH₄ and CO₂: GCMC and MD Simulations Study،Russian Journal of Physical Chemistry A،شماره ۹۴،شماره ۷،مجلد ۷،JCR،Scopus.
38. Molecular dynamics simulation study of Glycine tip-functionalisation of single-walled carbon nanotubes as emerging nanovectors for the delivery of anticancer drugs،MOLECULAR SIMULATION،شماره ۱۲،شماره ۱،۲۰۱۹-۱،صفحات ۱-۱۲،JCR.
39. Development of the poly(L-histidine) grafted carbon nanotube as a possible smart drug delivery vehicle،Computers in Biology and Medicine،Vol. 11،No. 143،pp. 105336-105345،2022،JCR،Scopus.
40. PNIPAM/Hexakis as a thermosensitive drug delivery system for biomedical and pharmaceutical applications (vol 12، 14363، 2022)،Scientific Reports،Vol. 1،No. 12،pp. 1-12،2022،JCR،Scopus.
41. Ali Bina،Conjugation of a smart polymer to doxorubicin through a pH-responsive bond for targeted

- drug delivery and improving drug loading on graphene oxide†,RSC Advances,Vol. 1,No. 11,pp. 18809-18817,2021,ISI.JCR.Scopus.
42. „Design of new drug delivery platform based on surface functionalization of black phosphorus nanosheet with a smart polymer for enhancing the efficiency of doxorubicin in the treatment of cancer,Journal of Biomedical Materials Research Part A,Vol. 1,No. 109,pp. 1912-1921,2021,JCR.Scopus.
43. „Nanotechnology-based approaches for targeting and delivery of drugs via Hexakis (m-PE) macrocycles,Scientific Reports,Vol. 1,No. 11,pp. 8256-8263,2021,JCR.Scopus.
44. afsaneh ghahari,Design of a new drug delivery platform based on surface functionalization 2D covalent organic frameworks,Journal of the Taiwan Institute of Chemical Engineers,Vol. 1,No. 125,pp. 15-22,2021,JCR.Scopus.
45. seyede leila Razavi Khoosfi,Assessment of the effect of external and internal triggers on adsorption and release of paclitaxel from the PEI functionalized silicene nanosheet: A molecular dynamic simulation,Journal of Molecular Graphics and Modelling,Vol. 1,No. 106,pp. 107930-107938,2021,JCR.Scopus.
46. ameneh zaboli arbab din mohamad,Molecular interpretation of the carbon nitride performance as a template for the transport of anti-cancer drug into the biological membrane,Scientific Reports,Vol. 1,No. 11,pp. 18981-18993,2021,JCR.Scopus.
47. Mohammad Mehdi Firoozabadi,Influence of high-electronegativity atoms on the ^7Be decay rate,Physical Review C,Vol. 1,No. 102,pp. 14606-14606,2020,JCR.Scopus.
48. Torkzadeh , & Mahani Masoud,Zaboli Mahdiye,Stabilization of d-lactate dehydrogenase diagnostic enzyme via immobilization on pristine and carboxyl-functionalized carbon nanotubes, a combined experimental and molecular dynamics simulation study,ARCHIVES OF BIOCHEMISTRY AND BIOPHYSICS,Vol. 661,pp. 178-186,2019,JCR.
49. Mortazavifar Azam,Comparative prediction of binding affinity of Hydroxyurea anti-cancer to boron nitride and carbon nanotubes as smart targeted drug delivery vehicles,Journal of Biomolecular Structure and Dynamics,pp. 1-11,2019,ISI.JCR.Scopus.
50. „Understanding loading, diffusion and releasing of Doxorubicin and Paclitaxel dual delivery in graphene and graphene oxide carriers as highly efficient drug delivery systems,Applied Surface Science,No. 500,pp. 144220-0,2019,JCR.Scopus.
51. خرم پور, Molecular Insight into Adsorption Affinities of Carmustine Drug on Boron and Nitrogen Doped Functionalized Single-walled Carbon Nanotubes Using Density Functional Theory Including Dispersion Correction Calculations and Molecular Dynamics Simulation,Journal of Biomolecular Structure and Dynamics,Vol. 16,No. 38,pp. 4817-4826,2019,ISI.JCR.Scopus.
52. Mahnaz Shahabi,Molecular dynamics simulation study of Glycine tip-functionalisation of single-walled carbon nanotubes as emerging nanovectors for the delivery of anticancer drugs,MOLECULAR SIMULATION,pp. 0-0,2019,JCR.
53. „Assessment of dynamical properties of mercaptopurine on the peptide-based metal–organic framework in response to experience of external electrical fields: a molecular dynamics simulation,Journal of Molecular Modeling,Vol. 304,No. 25,pp. 0-0,2019,JCR.Scopus.
54. „Loading and release of anticancer drug from phosphorene as a template material with high efficient carrier: From vacuum to cell membrane,Journal of Molecular Liquids,Vol. 1,No. 291,pp. 111346-0,2019,JCR.Scopus.
55. „Enhance the efficiency of 5-fluorouracil targeted delivery by using a prodrug approach as a novel strategy for prolonged circulation time and improved permeation,International Journal of Pharmaceutics,No. 568,pp. 118491-0,2019,JCR.Scopus.
56. „A density functional theory-based analysis of the structural, topological and electronic properties of Gemcitabine drug adsorption on the pyrrolidine functionalized single-walled carbon nanotube,Journal of Biomolecular Structure and Dynamics,Vol. 10,No. 37,pp. 2477-2486,2019,ISI.JCR.Scopus.
57. „Theoretical investigation insights into the temperature triggered tegafur anticancer drug release

- from the surface of graphene oxide nanosheet, *Journal of Biomolecular Structure and Dynamics*, pp. 0-0, 2019, ISI, JCR, Scopus.
58. „Predicting doxorubicin drug delivery by singlewalled carbon nanotube through cell membrane in the absence and presence of nicotine molecules: a molecular dynamics simulation study, *Journal of Biomolecular Structure and Dynamics*, pp. 0-0, 2019, ISI, JCR, Scopus.
59. „Carbon and boron nanotubes as a template material for adsorption of 6-Thioguanine chemotherapeutic: a molecular dynamics and density functional approach, *Journal of Biomolecular Structure and Dynamics*, pp. 0-0, 2019, ISI, JCR, Scopus.
60. „Density functional theory study towards investigating the adsorption properties of the γ -Fe₂O₃ nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug, *Adsorption*, pp. 1-15, 2019, JCR, Scopus.
61. „Understanding the role of hydrogen bonds in destruction of DNA by screening interactions of Flutamide anticancer drug with nucleotides bases: DFT perspective, MD simulation and free energy calculation, *Adsorption*, pp. 0-0, 2019, JCR, Scopus.
62. Ali Arab, Najme Dastani, „Adsorption of Ampyra anticancer drug on the graphene and functionalized graphene as template materials with high efficient carrier, *Adsorption*, Vol. 1, No. 26, pp. 879-893, 2019, JCR, Scopus.
63. Hossein Farsi, Shokufeh Moghiminia, Andrew Riley, Zhihai Li, The effects of electrolyte on the capacitive behavior of nanostructured molybdenum oxides, *JOURNAL OF CHEMICAL TECHNOLOGY AND BIOTECHNOLOGY*, Vol. 12, No. 94, pp. 3800-3805, 2019, ISI, JCR, Scopus.
64. „Using molecular dynamics simulation to explore the binding of the three potent anticancer drugs sorafenib, streptozotocin, and sunitinib to functionalized carbon nanotubes, *Journal of Molecular Modeling*, Vol. 159, No. 25, pp. 0-0, 2019, JCR, Scopus.
65. „A combined molecular dynamics simulation and quantum mechanics study on mercaptopurine interaction with the cucurbit 67 urils Analysis of electronic structure, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, Vol. 188, pp. 647-658, 2018, JCR, Scopus.
66. „Boosting BeONT Reactivity with HCN by Calcium and Magnesium Doping A DFT Investigation of Electronic Structure AIM NMR NQR and NBO Analysis, *Journal of Cluster Science*, Vol. 29, pp. 101-110, 2018, JCR, Scopus.
67. „Density functional theory calculations and molecular dynamics simulations of the adsorption of ellipticine anticancer drug on graphene oxide surface in aqueous medium as well as under controlled pH conditions, *Journal of Molecular Liquids*, Vol. 255, pp. 269-278, 2018, JCR, Scopus.
68. „Assessment of the chitosan-functionalized graphene oxide as a carrier for loading Thioguanine an antitumor drug and effect of urea on adsorption process Combination of DFT computational and Molecular Dynamics Simulation Studies, *Journal of Biomolecular Structure and Dynamics*, pp. 1-38, 2018, ISI, JCR, Scopus.
69. Kamel Maedeh, Morsali Ali, Assessment of the adsorption mechanism of Flutamide anticancer drug on the functionalized single-walled carbon nanotube surface as a drug delivery vehicle An alternative theoretical approach based on DFT and MD, *Applied Surface Science*, Vol. 434, pp. 492-503, 2018, JCR, Scopus.
70. Khorram Rabeeh, Morsali Ali, The computational study of the γ -Fe₂O₃ nanoparticle as Carmustine drug delivery system DFT approach, *Journal of Biomolecular Structure and Dynamics*, Vol. 2, No. 37, pp. 454-464, 2018, ISI, JCR, Scopus.
71. Mortazavifar Azam, Theoretical Prediction of Adsorption Properties of Carmustine Drug on Various Sites of the Outer Surface of the Single-Walled Boron Nitride Nanotube and Investigation of Urea Effect on Drug Delivery by DFT and MD, *Journal of Cluster Science*, Vol. 29, No. 1, pp. 93-99, 2018, JCR, Scopus.
72. „Comprehensive theoretical prediction of the dynamics and stability properties of Tegafur pharmaceutical agent on the Graphene based nanostructures in aqueous environment, *Applied Surface Science*, Vol. 455, pp. 32-36, 2018, JCR, Scopus.
73. „Covalent organic framework as smart and high efficient carrier for anticancer drug delivery a DFT

- calculations and molecular dynamics simulation study, *Journal of Physics D: Applied Physics*, Vol. 51, pp. 345401-, 2018, JCR.Scopus.
74. „Assessment of solvent effects on the inclusion behavior of pyrazinamide drug into cyclic peptide based nanotubes as novel drug delivery vehicles, *Journal of Molecular Liquids*, Vol. 268, pp. 326-334, 2018, JCR.Scopus.
75. Bakhtiari Akbar, Moradnia Heidar, A density functional theory-based analysis of the structural topological and electronic properties of Gemcitabine drug adsorption on the pyrrolidine functionalized single-walled carbon nanotube, *Journal of Biomolecular Structure and Dynamics*, Vol. 10, No. 37, pp. 2477-2486, 2018, ISI.JCR.Scopus.
76. Khorram Rabeeh, Analysis of the structures energetics and vibrational frequencies for the hydrogen-bonded interaction of nucleic acid bases with Carmustine pharmaceutical agent a detailed computational approach, *Structural Chemistry*, Vol. 29, pp. 1165-1174, 2018, JCR.Scopus.
77. Akbari Alireza, Mortazavifar Azam, DFT and MD investigations on the functionalized boron nitride nanotube as an effective drug delivery carrier for Carmustine anticancer drug, *Journal of Molecular Liquids*, Vol. 276, pp. 577-587, 2018, JCR.Scopus.
78. „Assessment of the chitosan-functionalized graphene oxide as a carrier for loading Thioguanine, an antitumor drug and effect of urea on adsorption process: Combination of DFT computational and Molecular Dynamics Simulation Studies, *Journal of Biomolecular Structure and Dynamics*, Vol. 10, No. 37, pp. 2487-2497, 2018, ISI.JCR.Scopus.
79. „The computational study of the α -Fe₂O₃ nanoparticle as Carmustine drug delivery system: DFT approach, *Journal of Biomolecular Structure and Dynamics*, pp. 0-0, 2018, ISI.JCR.Scopus.
80. Maasoumeh Jafarpour, Screening of different interactions in oxo-manganese porphyrin dimers containing axial N-donor ligands a theoretical study, *RSC Advances*, Vol. 8, pp. 9770-9774, 2018, ISI.JCR.Scopus.
81. „DFT Calculations and Molecular Dynamics Simulation Study on the Adsorption of 5-Fluorouracil Anticancer Drug on Graphene Oxide Nanosheet as a Drug Delivery Vehicle, *Journal of Inorganic and Organometallic Polymers and Materials*, Vol. 27, No. 3, pp. 805-817, 2017, JCR.Scopus.
82. „The functionalization of carbon nanotubes to enhance the efficacy of the anticancer drug paclitaxel a molecular dynamics simulation study, *Journal of Molecular Modeling*, Vol. 23, No. 8, pp. 222-232, 2017, JCR.Scopus.
83. „Solvent/co-solvent effects on the electronic properties and adsorption mechanism of anticancer drug Thioguanine on Graphene oxide surface as a nanocarrier Density functional theory investigation and a molecular dynamics, *Applied Surface Science*, Vol. 422, pp. 1030-1041, 2017, JCR.Scopus.
84. „Investigation of graphene-based nanomaterial as nanocarrier for adsorption of paclitaxel anticancer drug a molecular dynamics simulation study, *Journal of Molecular Modeling*, Vol. 23, pp. 36-43, 2017, JCR.Scopus.
85. „DFT and MD study of adsorption sensitivity of aluminium phosphide nanotube towards some air pollutant gas molecules, *MOLECULAR SIMULATION*, Vol. 43, No. 9, pp. 675-690, 2017, JCR.
86. „Evaluation of solvent and ion effects upon leflunomide adsorption characteristics on (60) zigzag single-walled carbon nanotube and immobilized dihydroorotate dehydrogenase activity A computational DFT and experimental study, *Journal of Molecular Liquids*, Vol. 231, pp. 528-541, 2017, JCR.Scopus.
87. „Assessment of DFT Calculations and Molecular Dynamics Simulation on the Application of Zinc Oxide Nanotube as Hydrogen Cyanide Gas Sensor, *Journal of Inorganic and Organometallic Polymers and Materials*, Vol. 1, pp. 1-8, 2017, JCR.Scopus.
88. „Screening of the structural topological and electronic properties of the functionalized Graphene nanosheets as potential Tegafur anticancer drug carriers using DFT method, *Journal of Biomolecular Structure and Dynamics*, Vol. 1, pp. 1-13, 2017, ISI.JCR.Scopus.
89. Khorram Rabeeh, Morsali Ali, Assessment of solvent effects on the interaction of Carmustine drug with the pristine and COOH-functionalized single-walled carbon nanotubes A DFT perspective, *Journal*

of Molecular Liquids, Vol. 240, pp. 87-97, 2017, JCR, Scopus.

90. Shaki Hosein, Morsali Ali, Hakimi Mohammad, Beyramabadi Ali, Mechanistic energetic and structural studies of single-walled carbon nanotubes functionalized with penicillamine, Journal of the Serbian Chemical Society, Vol. 82, No. 1, pp. 1-14, 2017, JCR, Scopus.
91. „Doped-SiCNT as a promising sensor for detection of CS₂ molecule, Journal of Sulfur Chemistry, Vol. 38, No. 4, pp. 372-383, 2017, JCR, Scopus.
92. Kamel Maedeh, Morsali Ali, Theoretical study of solvent and co-solvent effects on the interaction of Flutamide anticancer drug with Carbon nanotube as a drug delivery system, Journal of Molecular Liquids, Vol. 248, pp. 490-500, 2017, JCR, Scopus.
93. „Investigation of the molecular structure electronic properties AIM NBO NMR and NQR parameters for the interaction of Sc Ga and Mg-doped (6 0) aluminum nitride nanotubes with COCl₂ gas by DFT study, JOURNAL OF INCLUSION PHENOMENA AND MACROCYCLIC CHEMISTRY, Vol. 84, No. 1, pp. 99-114, 2016, JCR, Scopus.
94. „Solvent effects on the structural electronic properties and intramolecular N H O hydrogen bond strength of 5-aminomethylene-pyrimidine-2 4 6 trion with DFT calculations, Journal of Molecular Liquids, Vol. 215, pp. 77-87, 2016, JCR, Scopus.
95. „Solvent effects on the stability and the electronic properties of histidine/Pd-doped single-walled carbon nanotube biosensor, Journal of Molecular Liquids, Vol. 214, pp. 313-318, 2016, JCR, Scopus.
96. „Theoretical calculations of intramolecular hydrogen bond of the 2-Amino-2 4 6-cycloheptatrien-1-one in the gas phase and solution Substituent effects and their positions, Journal of Theoretical and Computational Chemistry, Vol. 15, No. 7, pp. 1650063-1650087, 2016, JCR, Scopus.
97. „Molecular dynamics simulation and quantum chemical studies on the investigation of aluminum nitride nanotube as phosgene gas sensor, JOURNAL OF INCLUSION PHENOMENA AND MACROCYCLIC CHEMISTRY, Vol. 86, No. 3, pp. 305-322, 2016, JCR, Scopus.
98. Farzad Farzaneh, DFT study of the adsorption of H₂S H₂Se and SO₂ gas molecules on the surface of Fullerene, International Journal of Advanced Biotechnology and Research, Vol. 7, No. 5, pp. 1227-1232, 2016, ISI.
99. Farzad Farzaneh, First-principles investigation of graphene sheet for sensing carbon dioxide, International Journal of Advanced Biotechnology and Research, Vol. 7, No. 5, pp. 1233-1238, 2016, ISI.
100. „The influence of nicotine on pioglitazone encapsulation into carbon nanotube the investigation of molecular dynamic and density functional theory, Journal of Biomolecular Structure and Dynamics, Vol. 7, pp. 1-15, 2016, ISI, JCR, Scopus.
101. „„„„A theoretical study on the structure of 2-amino-1 3 4-thiadiazole and its 5-substituted derivatives in the gas phase water THF and DMSO solutions, Journal of Molecular Liquids, Vol. 203, pp. 137-142, 2015, JCR, Scopus.
102. „Structural QTAIM thermodynamic properties bonding aromaticity and NMR analyses of cation interactions of mono and divalent metal cations (Li Na K Be₂), Journal of Theoretical and Computational Chemistry, Vol. 14, No. 6, pp. 1550044-1550076, 2015, JCR, Scopus.
103. „The analysis of electronic structures adsorption properties NBO QTAIM and NMR parameters of the adsorbed hydrogen sulfide on various sites of the outer surface of aluminum phosphide nanotube a DFT study, Structural Chemistry, Vol. 26, pp. 1059-1075, 2015, JCR, Scopus.
104. „Investigation of adsorption properties of CS₂ on interior and exterior surfaces of single-walled silicon-carbide nanotubes and effect of applied electric field electronic structure charge density and NMR studies, RSC Advances, Vol. 5, pp. 84022-84037, 2015, ISI, JCR, Scopus.
105. „Effects of the HCN adsorption on the structural and electronic parameters of the beryllium oxide nanotube, Structural Chemistry, Vol. 1, pp. 1-15, 2015, JCR, Scopus.
106. „Quantum chemical study on influence of the substitution effect on the structural and electronic properties and intramolecular hydrogen bonding of 2-nitrophenyl hydrosulfide in ground and electronic excited state, Structural Chemistry, Vol. 26, pp. 971-987, 2015, JCR, Scopus.

107. „The hybrid of Pd and SWCNT (Pd loaded on SWCNT) as an efficient sensor for the formaldehyde molecule detection A DFT study,Sensors and Actuators B: Chemical,Vol. 212,pp. 55-62,2015,ISI,JCR.Scopus.
108. Maasoumeh Jafarpour,A DFT investigation of axial N-donor ligands effects on the high valent manganese-oxo meso-tetraphenyl porphyrin,Journal of Porphyrins and Phthalocyanines,Vol. 19,pp. 651-662,2015,JCR.Scopus.
109. Maasoumeh Jafarpour,Stereoelectronic effects of porphyrin ligand on the oxygen transfer efficiency of high valent manganese-oxo porphyrin species A DFT study,Journal of Porphyrins and Phthalocyanines,Vol. 19,pp. 1130-1139,2015,JCR.Scopus.
110. Maasoumeh Jafarpour,Significant hydrogen-bonding effect on the reactivity of high-valent manganese(V) oxo porphyrins in C H bond activation A DFT study,Journal of Porphyrins and Phthalocyanines,Vol. 19,pp. 1197-1203,2015,JCR.Scopus.
111. „Molecular structure and bonding character of mono and divalent metal cations (Li Na K Be₂ Mg₂ and Ca₂) with substituted benzene derivatives AIM NBO and NMR analyses,Structural Chemistry,Vol. 25,pp. 1327-1342,2014,JCR.Scopus.
112. Mohammad ali Nasser,Ali Allahresani,Grafting of a chiral Mn(III) complex on graphene oxide nanosheets and its catalytic activity for alkene epoxidation,RSC Advances,Vol. 4,pp. 26087-26094,2014,ISI,JCR.Scopus.
113. Mohammad ali Nasser,Ali Allahresani,Mild oxidation of alkenes catalyzed by Fe₃O₄/SiO₂ nanoparticles,Reaction Kinetics, Mechanisms and Catalysis,Vol. 112,pp. 397-408,2014,JCR.Scopus.
114. „Molecular structure conformational stability energetic and intramolecular hydrogen bonding in ground and electronic excited state of 3-mercapto propeneselenal,Structural Chemistry,Vol. 25,pp. 1153-1164,2014,JCR.Scopus.
115. „Theoretical study of substituents effects on characteristics of resonance-assisted hydrogen bond in (Z)-(thionitrosomethylene)hydrazine and its derivatives in ground and electronic excited state,Structural Chemistry,Vol. 25,pp. 1099-1109,2014,JCR.Scopus.
116. „Immunosuppressive agent leflunomide A SWNTs-immobilized dihydroorotate dehydrogenase inhibitory effect and computational study of its adsorption properties on zigzag single walled (6 0) carbon and boron nitride nanotubes as controlled drug delivery devices,European Journal of Pharmaceutical Sciences,Vol. 56,pp. 37-54,2014,JCR.Scopus.
117. „Comprehensive study of the structural and electronic properties of complexes formed by M z (Li Na K Be₂ Mg₂),Journal of Sulfur Chemistry,Vol. 36,pp. 48-66,2014,JCR.Scopus.
118. „Electronic structures intramolecular hydrogen bond interaction and aromaticity of substituted 4-amino-3-penten-2-one in ground and electronic excited state,Structural Chemistry,Vol. 25,No. 6,pp. 505-505,2014,JCR.Scopus.
119. Mohammad ali Nasser,Ali Allahresani,A new application of nano-graphene oxide as a heterogeneous catalyst in crossed,Iranian Journal of Catalysis,Vol. 4,No. 1,pp. 33-40,2014,isc.Scopus.
120. Hossein Farsi,Comparative optical and electrochemical studies of nanostructured NiTiO₃ and NiTiO₃-TiO₂ prepared by a low temperature modified Sol-Gel route,Electrochimica Acta,Vol. 132,pp. 512-523,2014,JCR.Scopus.
121. Hossein Farsi,Quantum chemical studies on molecular conformations, energetic and intramolecular hydrogen bonding in ground and electronic excited state of (thioxosilyl) ethyleneselenol,Journal of Sulfur Chemistry,Vol. 2,No. 35,pp. 152-163,2014,JCR.Scopus.
122. Khanmohammadi Azadeh,yoosefian mehdi,Ab initio and DFT studies on 1-(thionitrosomethylene) hydrazine conformers energies and intramolecular hydrogen-bond strength,Structural Chemistry,Vol. 24,No. 4,pp. 1123-1133,2013,JCR.Scopus.
123. „CONFORMATIONAL PROPERTIES AND INTRAMOLECULAR HYDROGEN BONDING OF 3-AMINO-PROPENESELENAL AN AB INITIO AND DENSITY FUNCTIONAL THEORY STUDIES,Journal of Theoretical and Computational Chemistry,Vol. 12,pp. 1350025-1350033,2013,JCR.Scopus.
124. Hossein Farsi,THEORETICAL INVESTIGATION OF SUBSTITUTION EFFECT IN 3-MERCAPTO-

- PROPENETHIAL, Journal of Theoretical and Computational Chemistry, Vol. 12, pp. 1350045-1350078, 2013, JCR.Scopus.
125. „Molecular structure vibrational assignments conformational stability ground and excited state hydrogen-bonding analysis of 2-Nitroso vinyl amine, Journal of Theoretical and Computational Chemistry, Vol. 12, pp. 1350072-1350100, 2013, JCR.Scopus.
126. Hossein Farsi, Quantum chemical studies on molecular conformations energetic and intramolecular hydrogen bonding in ground and electronic excited state of (thioxosilyl) ethyleneselenol, Journal of Sulfur Chemistry, Vol. 35, pp. 152-163, 2013, JCR.Scopus.
127. „Substituent effect on the reaction mechanism of proton transfer in formamide, International Journal of Quantum Chemistry, Vol. 112, pp. 2378-2381, 2012, JCR.Scopus.
128. Hajiabadi H, Nowroozi A.R, Hasani M, Mohammadzadeh Jahani P, A comparative study of open-close and related rotamers methods to evaluate the intramolecular hydrogen bond energies in 3-imino-propen-1-ol and its derivatives, International Journal of Quantum Chemistry, Vol. 112, pp. 1384-1391, 2012, JCR.Scopus.
129. „The effect of substitution on structure intramolecular hydrogen bonding strength electron density and resonance in 3-amino 2-iminomethyl acryl aldehyde, Journal of Theoretical and Computational Chemistry, Vol. 11, No. 5, pp. 925-939, 2012, JCR.Scopus.
130. „Hydrogen bond studies in substituted imino-acetaldehyde oxime, Computational and Theoretical Chemistry, Vol. 996, pp. 68-75, 2012, JCR.Scopus.
131. „Comprehensive study of the interaction between hydrogen halides and methanol derivatives, International Journal of Quantum Chemistry, Vol. 112, pp. 2782-2786, 2012, JCR.Scopus.
132. „Theoretical study on α -aminoacrolein Density functional theory atoms in molecules theory and natural bond orbitals studies, Journal of Chemical Sciences, Vol. 124, No. 3, pp. 731-739, 2012, JCR.Scopus.
133. „Synthesis and theoretical study of intramolecular hydrogen bond at two possible positions in pyrazolo 1 2-b phthalazine, Chinese Journal of Chemistry, Vol. 30, pp. 779-784, 2012, JCR.Scopus.
134. „Conformational study of the (z)- (2-iminoethylidene)silyl amine at the MP2 DFT and G2MP2 levels, Computational and Theoretical Chemistry, Vol. 983, pp. 1-6, 2012, JCR.Scopus.
135. „Conformational study molecular structure and S..HN S..HN intramolecular hydrogen bond in thioformyl-3-aminoacrylaldehyde, Journal of Sulfur Chemistry, Vol. 33, No. 1, pp. 75-85, 2012, JCR.Scopus.
136. Nowroozi A., Evaluation of the origin of conformational and tautomeric preferences in N-formylformamide - A quantum chemical study, International Journal of Quantum Chemistry, Vol. 112, pp. 489-497, 2012, JCR.Scopus.
137. Hakimi Mohammad, Kukovec Boris, & Marko, Pouyanmehr Leila, Mohr Fabian, Esther Schuh, Solvent Free synthesis and crystal structure of s-cis and s-trans N N-bis (2-hydroxy cyclohexyl ethane-1 2-diamine), Structural Chemistry, Vol. 24, pp. 81-88, 2012, JCR.Scopus.
138. shakhs Imampour Jalal, Karimi Mohammad, Theoretical Description of Substituent Effects in 2 4-Pentanedione AIM NBO and NMR Study, Bulletin of the Chemical Society of Japan, Vol. 85, No. 1, pp. 87-92, 2012, JCR.Scopus.
139. „Theoretical study on α -aminoacrolein Density functional theory atoms in molecules theory and natural bond orbitals studies, Journal of Chemical Sciences, Vol. 124, No. 3, pp. 731-739, 2012, JCR.Scopus.
140. „„A comparative study in 3-imino-propen-1-ol and its derivatives, International Journal of Quantum Chemistry, Vol. 112, pp. 1384-1391, 2012, JCR.Scopus.
141. Maasoumeh Jafarpour, Stoeckli, & Evans Helen, Economical Oxygenation of Olefins and Sulfides Catalyzed by New Molybdenum(VI) Tridentate Schiff Base Complexes Synthesis and Crystal Structure, Zeitschrift für Anorganische und Allgemeine Chemie, Vol. 638, No. 6, pp. 1023-1030, 2012, JCR.Scopus.
142. „„Theoretical Description of Substituent Effects in 2,4-Pentanedione: AIM, NBO, and NMR Study, Bulletin of the Chemical Society of Japan, Vol. 1, No. 85, pp. 87-92, 2012, JCR.Scopus.

143. ,,Substituent effect on structure electron density and intramolecular hydrogen bonding in nitroso-oxime methane,International Journal of Quantum Chemistry,No. 111,pp. 3505-3516,2011,JCR.Scopus.
144. ,Hajiabadi H,Jahani P.M,Reinvestigation of intramolecular hydrogen bond in malonaldehyde derivatives An ab initio AIM and NBO study,International Journal of Quantum Chemistry,No. 111,pp. 3040-3047,2011,JCR.Scopus.
145. Nowroozi A.R, Roohi H, Poorsargol M,Jahani P.M,Hajiabadi H,N-H S and S-H N intramolecular hydrogen bond in -thioaminoacrolein A quantum chemical study,International Journal of Quantum Chemistry,No. 111,pp. 3008-3016,2011,JCR.Scopus.
146. Nowroozi A.R,Ab initio and DFT computational studies on molecular conformations and strength of the intramolecular hydrogen bond in different conformers of 3-amino-2-iminomethyl acryl aldehyde,Journal of Molecular Structure-theochem,No. 966,pp. 299-305,2011,ISI.JCR.
147. Nowroozi A.R, Roohi H,Hajiabadi H,Khalilinia E, Birgan M.N,O-H S intramolecular hydrogen bond in thiomalonaldehyde derivatives A quantum chemical study,Journal of Molecular Structure-theochem,No. 963,pp. 517-524,2011,ISI.JCR.
148. Hossein Farsi,,Theoretical study of the effects of substitution solvation and structure on the interaction between nitriles and methanol,International Journal of Quantum Chemistry,Vol. 112,pp. 1273-1284,2011,JCR.Scopus.
149. Maasoumeh Jafarpour,Factors affecting the reactivity and selectivity in the oxidation of sulfides with tetra-n-butylammonium peroxomonosulfate catalyzed by Mn (III) porphyrins Significant nitrogen donor effects,Polyhedron,Vol. 30,pp. 592-598,2011,JCR.Scopus.
150. Hossein Farsi,,On the pseudocapacitive behavior of nanostructured molybdenum oxide,JOURNAL OF SOLID STATE ELECTROCHEMISTRY,Vol. 14,pp. 643-650,2010,JCR.Scopus.
151. Hossein Farsi,gobal ferydoon,The pH effects on the capacitive behavior of nanostructured molybdenum oxide,JOURNAL OF SOLID STATE ELECTROCHEMISTRY,Vol. 14,pp. 681-686,2010,JCR.Scopus.
152. ,,The effects of substitutions on structure electron density resonance and intramolecular hydrogen bonding strength in a mercapto-propenethial,Journal of Molecular Structure-theochem,Vol. 960,pp. 1-9,2010,ISI.JCR.
153. Hossein Farsi,Intramolecular hydrogen bonding in 3-imino-propenylamine Theoretical investigations,International Journal of Quantum Chemistry,Vol. 109,pp. 1609-1616,2009,JCR.Scopus.
154. Flotation separation and electrothermal atomic absorption spectrometric determination of thallium in wastewater samples,Annali di Chimica,No. 96,pp. 17-23,2006,ISI.JCR.