

Abdulaziz A Al-Saadi

List of Publications by Year in descending order

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138
papers

3,984
citations

109264

35
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149623

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138
all docs

138
docs citations

138
times ranked

3659
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 1 | Nitrogen-Enhanced Charge Transfer Efficacy on the Carbon Sheet: A Theoretical Insight Into the Adsorption of Anionic Dyes. <i>Arabian Journal for Science and Engineering</i> , 2022, 47, 419-427. | 1.7 | 7 |
| 2 | Structural and energetic effect of the intramolecular hydrogen bonding in 4,6-dihaloresorcinols: ab initio calculation, vibrational spectroscopy, and molecular docking studies. <i>Structural Chemistry</i> , 2022, 33, 57-69. | 1.0 | 3 |
| 3 | Evaluation of the inhibition performance of piperazine-based polyurea towards mild steel corrosion: The role of keto-enol tautomerization. <i>Journal of Molecular Structure</i> , 2022, 1248, 131485. | 1.8 | 5 |
| 4 | Surface-enhanced Raman scattering (SERS) spectroscopy for prostate cancer diagnosis: A review. <i>Photodiagnosis and Photodynamic Therapy</i> , 2022, 37, 102690. | 1.3 | 23 |
| 5 | Insights into end-capped modifications effect on the photovoltaic and optoelectronic properties of S-shaped fullerene-free acceptor molecules: A density functional theory computational study for organic solar cells. <i>Journal of Physical Organic Chemistry</i> , 2022, 35, . | 0.9 | 28 |
| 6 | A First-Principles Study on the Multilayer Graphene Nanosheets Anode Performance for Boron-Ion Battery. <i>Nanomaterials</i> , 2022, 12, 1280. | 1.9 | 11 |
| 7 | NMR evidence for hydrogen bonding stabilized anti conformation of 1-methoxy-1-methyl-3-phenylurea and the concentration detection by SERS. <i>Journal of Molecular Liquids</i> , 2022, 357, 119096. | 2.3 | 8 |
| 8 | SERS and EC-SERS detection of local anesthetic procaine using Pd loaded highly reduced graphene oxide nanocomposite substrate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 278, 121381. | 2.0 | 7 |
| 9 | Spectroanalytical SERS-based detection of trace-level procainamide using green-synthesized gold nanoparticles. <i>Surfaces and Interfaces</i> , 2022, 31, 102059. | 1.5 | 5 |
| 10 | SERS-Based Ultralow Concentration Detection of Anticancer Gemcitabine Using Size-Controlled Silver Nanoparticles. <i>Arabian Journal for Science and Engineering</i> , 2022, 47, 7197-7205. | 1.7 | 2 |
| 11 | Pilotyâ€™s acid and its hydrazide analogue: Insights from the density functional theory and vibrational spectroscopy on the conformational stability and chemical reactivity. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 249, 119317. | 2.0 | 1 |
| 12 | Molecular docking, spectroscopic, and quantum chemical studies on aromatic heterocycle tetrakis(4-pyridyl)cyclobutane regioisomers: potential membrane-permeable inhibitors. <i>Journal of Molecular Modeling</i> , 2021, 27, 94. | 0.8 | 4 |
| 13 | Comparative Exposure Assessment of Potential Health Risks through the Consumption of Vegetables Irrigated by Freshwater/Wastewater: Gujranwala, Pakistan. <i>Chemical Research in Toxicology</i> , 2021, 34, 1417-1429. | 1.7 | 8 |
| 14 | Porous Fluorocarbon from Rice Husk for the Efficient Separation of Gases. <i>Global Challenges</i> , 2021, 5, 2000124. | 1.8 | 1 |
| 15 | Electrochemically modulated SERS detection of procaine using FTO electrodes modified with silver-decorated carbon nanosphere. <i>Electrochimica Acta</i> , 2021, 387, 138463. | 2.6 | 33 |
| 16 | Conformational analysis and concentration detection of linuron: Spectroscopic NMR and SERS study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 263, 120223. | 2.0 | 5 |
| 17 | Fast and sensitive detection of Procainamide: Combined SERS and DFT modeling studies. <i>Journal of Molecular Liquids</i> , 2021, 343, 117633. | 2.3 | 23 |
| 18 | Blue- and white-light-emitting 2D-coordination polymers and their solid-state photodimerization reaction. <i>CrystEngComm</i> , 2021, 23, 7663-7670. | 1.3 | 1 |

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|----|--|-----|-----------|
| 19 | UV-absorbing benzamide-based dendrimer precursors: synthesis, theoretical calculation, and spectroscopic characterization. <i>New Journal of Chemistry</i> , 2021, 46, 75-85. | 1.4 | 3 |
| 20 | Understanding the Influence of Electron-Donating and Electron-Withdrawing Substituents on the Anticorrosive Properties of Imidazole: A Quantum-Chemical Approach. <i>Arabian Journal for Science and Engineering</i> , 2020, 45, 153-166. | 1.7 | 5 |
| 21 | Sensitive SERS detection and characterization of procaine in aqueous media by reduced gold nanoparticles. <i>Sensors and Actuators B: Chemical</i> , 2020, 304, 127057. | 4.0 | 44 |
| 22 | Synthesis and Characterization of Fluorocarbon from Rice Husk and its Application as an Efficient Sorbent for Micro-Solid-Phase Extraction of N-Nitrosamines in Desalinated Water Samples. <i>Chromatographia</i> , 2020, 83, 95-105. | 0.7 | 4 |
| 23 | New imidazole-based dimers as potential inhibitors for mild steel corrosion in acidic media: Electrochemical and DFT evaluation. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2020, 71, 292-299. | 0.8 | 13 |
| 24 | Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuron. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117580. | 2.0 | 26 |
| 25 | Inhibition of mild steel corrosion in CO ₂ and H ₂ S saturated acidic media by a new polyurea-based material. <i>Materials and Corrosion - Werkstoffe Und Korrosion</i> , 2020, 71, 646-662. | 0.8 | 13 |
| 26 | In Silico Modeling of New α -Series-Based Near-Infrared Sensitive Non-Fullerene Acceptors for Efficient Organic Solar Cells. <i>ACS Omega</i> , 2020, 5, 24125-24137. | 1.6 | 103 |
| 27 | Computational study of SERS effects in some aliphatic and cyclic carboxylic acids with silver nanomaterials. <i>Journal of Physics: Conference Series</i> , 2020, 1564, 012008. | 0.3 | 2 |
| 28 | DFT evaluation of the effects of OH, NH ₂ and Br substituents on the properties of 2,2'-bipyridine derivatives. <i>Journal of Taibah University for Science</i> , 2020, 14, 1527-1537. | 1.1 | 8 |
| 29 | SERS-based trace-level quantification of sulindac: Spectroscopic and molecular modeling evaluation. <i>Journal of Molecular Liquids</i> , 2020, 312, 113402. | 2.3 | 21 |
| 30 | Impact of Degree of Hydrophilicity of Pyridinium Bromide Derivatives on HCl Pickling of X-60 Mild Steel: Experimental and Theoretical Evaluations. <i>Coatings</i> , 2020, 10, 185. | 1.2 | 14 |
| 31 | Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione. <i>Journal of Molecular Structure</i> , 2019, 1175, 269-279. | 1.8 | 16 |
| 32 | Spectroscopic, DFT and trace detection study of procaine using surface-enhanced Raman scattering technique. <i>Chemical Physics Letters</i> , 2019, 730, 617-622. | 1.2 | 24 |
| 33 | Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide 1,1-dimethyl-3-phenylurea. <i>Heliyon</i> , 2019, 5, e01987. | 1.4 | 46 |
| 34 | Impact of electron-withdrawing and electron-donating substituents on the corrosion inhibitive properties of benzimidazole derivatives: A quantum chemical study. <i>Journal of Molecular Structure</i> , 2019, 1196, 348-355. | 1.8 | 55 |
| 35 | Droplet flow-assisted heterogeneous electro-Fenton reactor for degradation of beta-blockers: response surface optimization, and mechanism elucidation. <i>Environmental Science and Pollution Research</i> , 2019, 26, 14313-14327. | 2.7 | 9 |
| 36 | Principal components analysis of Raman spectral data for screening of Hepatitis C infection. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2019, 221, 117173. | 2.0 | 36 |

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|----|--|-----|-----------|
| 37 | Preparation and Characterization of Biomass Carbon-Based Solid Acid Catalysts for the Esterification of Marine Algae for Biodiesel Production. <i>Bioenergy Research</i> , 2019, 12, 433-442. | 2.2 | 17 |
| 38 | Quantum chemical designing of indolo[3,2,1-jk]carbazole-based dyes for highly efficient nonlinear optical properties. <i>Chemical Physics Letters</i> , 2019, 719, 59-66. | 1.2 | 108 |
| 39 | First theoretical probe for efficient enhancement of nonlinear optical properties of quinacridone based compounds through various modifications. <i>Chemical Physics Letters</i> , 2019, 715, 222-230. | 1.2 | 125 |
| 40 | Characterization of valeric acid using substrate of silver nanoparticles with SERS. <i>Journal of Molecular Liquids</i> , 2019, 273, 536-542. | 2.3 | 57 |
| 41 | Mechanistic studies of the influence of halogen substituents on the corrosion inhibitive efficiency of selected imidazole molecules: A synergistic computational and experimental approach. <i>Applied Surface Science</i> , 2019, 471, 494-505. | 3.1 | 51 |
| 42 | Synthesis, spectroscopic characterization and in vitro cytotoxic as well as docking studies of cis-diammine platinum(II) complexes of thiones. <i>Inorganica Chimica Acta</i> , 2019, 484, 347-351. | 1.2 | 5 |
| 43 | Structural, spectroscopic and docking properties of resorcinol, its -OD isotopomer and dianion derivative: a comparative study. <i>Structural Chemistry</i> , 2018, 29, 403-414. | 1.0 | 11 |
| 44 | Synthesis, X-ray structure and cytotoxicity evaluation of carbene-based gold(I) complexes of selenones. <i>Inorganica Chimica Acta</i> , 2018, 476, 46-53. | 1.2 | 15 |
| 45 | First Theoretical Framework of Triphenylamine-Dicyanovinylene-Based Nonlinear Optical Dyes: Structural Modification of π -Linkers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4009-4018. | 1.5 | 193 |
| 46 | Silver loaded graphene as a substrate for sensing 2-thiouracil using surface-enhanced Raman scattering. <i>Sensors and Actuators B: Chemical</i> , 2018, 254, 1110-1117. | 4.0 | 100 |
| 47 | A selective detection approach for copper(II) ions using a hydrazone-based colorimetric sensor: spectroscopic and DFT study. <i>RSC Advances</i> , 2018, 8, 39983-39991. | 1.7 | 26 |
| 48 | Selective colorimetric sensing of nickel (II) ions using 2-hydroxy-5-nitrobenzaldehyde-4-hydroxybenzoylhydrazone ligand: Spectroscopic and DFT insights. <i>Journal of Molecular Liquids</i> , 2018, 264, 58-65. | 2.3 | 7 |
| 49 | Spectroscopic and DFT assessment of bridging ligand effect on the structural and electronic properties of dinuclear iridium- and rhodium-based complexes. <i>Inorganica Chimica Acta</i> , 2018, 482, 299-306. | 1.2 | 5 |
| 50 | Silver-loaded graphene as an effective SERS substrate for clotrimazole detection: DFT and spectroscopic studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 201, 354-361. | 2.0 | 59 |
| 51 | Synthesis and characterization of functionalized polythiophene for polymer-sensitized solar cell. <i>Dyes and Pigments</i> , 2017, 141, 406-412. | 2.0 | 17 |
| 52 | Synthesis, characterization and in vitro cytotoxicity of platinum(II) complexes of selenones [Pt(selenone) ₂ Cl ₂]. <i>Journal of Coordination Chemistry</i> , 2017, 70, 1020-1031. | 0.8 | 12 |
| 53 | Silver nanoparticles for detection of methimazole by surface-enhanced Raman spectroscopy. <i>Materials Research Bulletin</i> , 2017, 91, 173-178. | 2.7 | 65 |
| 54 | Ultra-trace detection of methimazole by surface-enhanced Raman spectroscopy using gold substrate. <i>Vibrational Spectroscopy</i> , 2017, 90, 96-103. | 1.2 | 40 |

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|----|---|-----|-----------|
| 55 | Spherical silver nanoparticles as substrates in surface-enhanced Raman spectroscopy for enhanced characterization of ketoconazole. <i>Materials Science and Engineering C</i> , 2017, 76, 356-364. | 3.8 | 50 |
| 56 | Synthesis, X-ray structures and anticancer activity of gold(I)-carbene complexes with selenones as co-ligands and their molecular docking studies with thioredoxin reductase. <i>Journal of Organometallic Chemistry</i> , 2017, 848, 175-183. | 0.8 | 25 |
| 57 | Conformational, vibrational and DFT studies of a newly synthesized arylpiperazine-based drug and evaluation of its reactivity towards the human GABA receptor. <i>Journal of Molecular Structure</i> , 2017, 1147, 266-280. | 1.8 | 11 |
| 58 | Structural properties, vibrational spectra and surface-enhanced Raman scattering of 2,4,6-trichloro- and tribromoanilines: A comparative study. <i>Journal of Molecular Structure</i> , 2016, 1121, 7-15. | 1.8 | 38 |
| 59 | Spectroscopic (FT-IR, FT-Raman, UV, ¹ H and ¹³ C NMR) profiling and theoretical calculations of (2E)-2-[3-(1H-imidazol-1-yl)-1-phenylpropylidene]hydrazinecarboxamide: An anticonvulsant agent. <i>Journal of Molecular Structure</i> , 2016, 1118, 219-232. | 1.8 | 3 |
| 60 | Spectroscopic and theoretical evaluation of the metal-olefin interaction in di- η^4 -chlorobis (1,5-cyclooctadiene) complexes of Ir and Rh. <i>Vibrational Spectroscopy</i> , 2016, 86, 109-123. | 1.2 | 7 |
| 61 | Silver colloid and film substrates in surface-enhanced Raman scattering for 2-thiouracil detection. <i>RSC Advances</i> , 2016, 6, 75282-75292. | 1.7 | 77 |
| 62 | Density functional theory study of the substituent effect on the structure, conformation and vibrational spectra in halosubstituted anilines. <i>RSC Advances</i> , 2016, 6, 67794-67804. | 1.7 | 6 |
| 63 | Graphene Dendrimer-stabilized silver nanoparticles for detection of methimazole using Surface-enhanced Raman scattering with computational assignment. <i>Scientific Reports</i> , 2016, 6, 32185. | 1.6 | 181 |
| 64 | Dimethylphosphinate bridged binuclear Rh(i) catalysts for the alkoxy-carbonylation of aromatic C-H bonds. <i>Dalton Transactions</i> , 2016, 45, 16955-16965. | 1.6 | 6 |
| 65 | Conformational, NBO, NLO, HOMO-LUMO, NMR, electronic spectral study and molecular docking study of N,N-Dimethyl-3-(10H-phenothiazin-10-yl)-1-propanamine. <i>Journal of Molecular Structure</i> , 2016, 1122, 268-279. | 1.8 | 19 |
| 66 | Hydroxylamine reduced silver colloid for naphthalene and phenanthrene detection using surface-enhanced Raman spectroscopy. <i>Chemical Engineering Journal</i> , 2016, 304, 141-148. | 6.6 | 60 |
| 67 | Kinetic and computational evaluation of activated carbon produced from rubber tires toward the adsorption of nickel in aqueous solutions. <i>Desalination and Water Treatment</i> , 2016, 57, 17570-17578. | 1.0 | 11 |
| 68 | Collision induced dissociations of non- α -derivatized and trimethylsilyl- α -derivatized estradiols: similarities in fragmentation patterns. <i>Journal of Mass Spectrometry</i> , 2015, 50, 308-315. | 0.7 | 0 |
| 69 | Experimental and Theoretical Studies of the Vibrational and Electronic Properties of (2E)-2-[3-(1H-imidazol-1-yl)-1-phenyl-propylidene]-N-phenylhydrazinecarboxamide: An Anticonvulsant Agent. <i>Applied Sciences (Switzerland)</i> , 2015, 5, 955-972. | 1.3 | 9 |
| 70 | Molecular conformational analysis, vibrational spectra, NBO, NLO, HOMO-LUMO and molecular docking studies of ethyl 3-(E)-(anthracen-9-yl)prop-2-enoate based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 533-542. | 2.0 | 39 |
| 71 | Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-(phenylsulfanyl)-pyrimidine-5-carbonitrile, a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 413-424. | 2.0 | 17 |
| 72 | First principle calculations of the chemisorption of SO on doped carbon nanotubes and graphene. <i>Chemical Physics Letters</i> , 2015, 621, 65-70. | 1.2 | 9 |

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|----|--|-----|-----------|
| 73 | Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of 1-hydroxy-4,5,8-tris(4-methoxyphenyl) anthraquinone. <i>Journal of Physics and Chemistry of Solids</i> , 2015, 87, 110-121. | 1.9 | 20 |
| 74 | Iridium complexes as catalysts in the hydrogen transfer of isopropanol to acetophenone: Ligand effects and DFT studies. <i>Inorganica Chimica Acta</i> , 2015, 436, 146-151. | 1.2 | 14 |
| 75 | FT-IR, HOMOâ€“LUMO, NBO, MEP analysis and molecular docking study of 3-Methyl-4-[(E)-[4-(methylsulfanyl)-benzylidene]amino}1H-1,2,4-triazole-5(4H)-thione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 198-207. | 2.0 | 41 |
| 76 | Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis[(E)-anthranil-9-acrylic]anhydride based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 350-359. | 2.0 | 14 |
| 77 | Vibrational spectroscopic and molecular docking study of (2 E)- N-(4-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylprop-2-enamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 151, 335-349. | 2.0 | 15 |
| 78 | Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 150, 543-556. | 2.0 | 59 |
| 79 | Spectroscopic investigations, NBO, HOMOâ€“LUMO, NLO analysis and molecular docking of 5-(adamantan-1-yl)-3-anilinomethyl-2,3-dihydro-1,3,4-oxadiazole-2-thione, a potential bioactive agent. <i>Journal of Molecular Structure</i> , 2015, 1096, 1-14. | 1.8 | 50 |
| 80 | 1-Alkyl-1-methylpiperazine-1,4-dium salts: Synthetic, acidâ€“base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study. <i>Journal of Molecular Structure</i> , 2015, 1094, 210-236. | 1.8 | 15 |
| 81 | Spectroscopic investigation (FTIR spectrum), NBO, HOMOâ€“LUMO energies, NLO and thermodynamic properties of 8-Methyl-N-vanillyl-6-nonenamide by DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 146, 177-186. | 2.0 | 52 |
| 82 | Surface characterization and sorption efficacy of tireâ€“obtained carbon: experimental and semiempirical study of rhodamine B adsorption. <i>Surface and Interface Analysis</i> , 2015, 47, 785-792. | 0.8 | 58 |
| 83 | Synthesis, characterization and theoretical calculations of (1,2-diaminocyclohexane)(1,3-diaminopropane)gold(III) chloride complexes: in vitro cytotoxic evaluations against human cancer cell lines. <i>BioMetals</i> , 2015, 28, 827-844. | 1.8 | 16 |
| 84 | Normal co-ordinate analysis, molecular structural, non-linear optical, second order perturbation studies of Tizanidine by density functional theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 139, 189-199. | 2.0 | 2 |
| 85 | Infrared spectrum, structural and optical properties and molecular docking study of 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 529-538. | 2.0 | 36 |
| 86 | Spectroscopic investigation (FT-IR, FT-Raman), HOMOâ€“LUMO, NBO analysis and molecular docking study of a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 520-533. | 2.0 | 8 |
| 87 | Molecular structure, FT-IR, vibrational assignments, HOMOâ€“LUMO, MEP, NBO analysis and molecular docking study of ethyl-6-(4-chlorophenyl)-4-(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 138, 73-84. | 2.0 | 15 |
| 88 | Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO | | |

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|-----|---|-----|-----------|
| 91 | Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of 2-(Adamantan-1-yl)-5-(4-nitrophenyl)-1,3,4-oxadiazole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 973-983. | 2.0 | 37 |
| 92 | Vibrational spectroscopic studies and molecular docking of 10,10-Dimethylanthrone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 652-661. | 2.0 | 9 |
| 93 | FT-IR, molecular structure, first order hyperpolarizability, MEP, HOMO and LUMO analysis and NBO analysis of 4-[(3-acetylphenyl)amino]-2-methylidene-4-oxobutanoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 134, 63-72. | 2.0 | 36 |
| 94 | Visible light-induced photodegradation of rhodamine dyes over BiOCl, and the vital importance of the frontier orbital energy of the dye molecules in the reaction kinetics. <i>Research on Chemical Intermediates</i> , 2015, 41, 2753-2766. | 1.3 | 8 |
| 95 | Synthesis, structural and vibrational investigation on 2-phenyl-N-(pyrazin-2-yl)acetamide combining XRD diffraction, FT-IR and NMR spectroscopies with DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 608-616. | 2.0 | 30 |
| 96 | FT-IR, NBO, HOMOâ€“LUMO, MEP analysis and molecular docking study of 1-[3-(4-Fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl]ethanone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 483-493. | 2.0 | 65 |
| 97 | Molecular structure, FT-IR, vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 473-482. | 2.0 | 67 |
| 98 | Vibrational spectroscopic and molecular docking study of 2-Benzylsulfanyl-4-[(4-methylphenyl)-sulfanyl]-6-pentylpyrimidine-5-carbonitrile, a potential chemotherapeutic agent. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 569-580. | 2.0 | 21 |
| 99 | Spectroscopic investigation (FT-IR, FT-Raman and SERS), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of Opipramol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 547-559. | 2.0 | 32 |
| 100 | Synthesis, spectroscopic characterization, electrochemical behavior and computational analysis of mixed diamine ligand gold(III) complexes: antiproliferative and in vitro cytotoxic evaluations against human cancer cell lines. <i>BioMetals</i> , 2014, 27, 1115-1136. | 1.8 | 20 |
| 101 | Synthesis of g-C ₃ N ₄ /BiOClxBr ⁿ hybrid photocatalysts and the photoactivity enhancement driven by visible light. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2014, 461, 202-211. | 2.3 | 50 |
| 102 | Vibrational spectra of 3,5-diamino-6-chloro-N-(diaminomethylene) pyrazine-2-carboxamide: Combined experimental and theoretical studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 127, 157-167. | 2.0 | 15 |
| 103 | Carbonaceous adsorbent prepared from waste tires: Experimental and computational evaluations of organic dye methyl orange. <i>Journal of Molecular Liquids</i> , 2014, 191, 85-91. | 2.3 | 108 |
| 104 | Spectroscopic (FT-IR, FT-Raman) investigations and quantum chemical calculations of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-{3-[4-(3-methoxyphenyl)piperazin-1-yl]propyl}-4-azatricyclo[5.2.1.0 ^{2,6}]dec-8-ene-3,5-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 129, 438-450. | 2.0 | 15 |
| 105 | The vibrational assignments of the infrared and Raman spectra of the symmetrically substituted 2,3-diphenylquinoxaline and its N,Nâ€“dioxide: Experimental and computational study. <i>Journal of Molecular Structure</i> , 2014, 1058, 284-290. | 1.8 | 1 |
| 106 | Facile preparation of g-C ₃ N ₄ modified BiOCl hybrid photocatalyst and vital role of frontier orbital energy levels of model compounds in photoactivity enhancement. <i>Journal of Colloid and Interface Science</i> , 2014, 416, 212-219. | 5.0 | 113 |
| 107 | Intermolecular hydroamination versus stereoregular polymerization of phenylacetylene by rhodium catalysts based on Nâ€“O bidentate ligands. <i>Inorganic Chemistry Communication</i> , 2014, 40, 78-81. | 1.8 | 9 |
| 108 | Theoretical investigations on the molecular structure, vibrational spectra, HOMOâ€“LUMO analyses and NBO study of 1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 133, 639-650. | 2.0 | 26 |

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|-----|---|-----|-----------|
| 109 | Theoretical Studies on the Mechanism of Iridium-Catalyzed Alkene Hydrogenation by the Cationic Complex [IrH ₂ (NCMe) ₃ (P ⁱ) ₃] ⁺ . <i>Organometallics</i> , 2014, 33, 5156-5163. | 1.1 | 23 |
| 110 | Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-(3-chlorophenyl)prop-2-enoic anhydride based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 131, 471-483. | 2.0 | 32 |
| 111 | Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-phenylprop-2-enoic anhydride based on density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 638-646. | 2.0 | 27 |
| 112 | Theoretical investigations on the molecular structure, vibrational spectral, HOMO-LUMO and NBO analysis of 9-[3-(Dimethylamino)propyl]-2-trifluoro-methyl-9H-thioxanthen-9-ol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 491-501. | 2.0 | 42 |
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