

CURRICULUM VITAE

LEENA SINHA

Nee LEENA BURMAN

PROFESSOR
Department of Physics
University of Lucknow
Lucknow



Education

Ph.D. (PHYSICS)- 1996
University of Lucknow

M. Sc. (PHYSICS)-1991
University of Lucknow

B. Sc. (PHYSICS)-1989
University of Lucknow

Positions held

Mahila P.G. College Lecturer in Physics	04/05/1996 - 04/05/2005
Reader in Physics University of Lucknow	04/05/2005 - 19/10/2006
Reader	19/10/2006 -19/10/2012
Professor	19/10/2012 -till date

Co-ordinator Physics Society. 26/08/2022 – till date
University of Lucknow

Research Credentials

Total number of publications: **91**
Total number of citations: **1970**
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h-Index: **23**
i10-Index: **50**
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Personal Details

DOB: 27th August 1970
Sex: Female
Nationality: Indian
Marital Status: Married

Teaching Experience

More than 29 years

Research Area

Quantum Chemistry
Molecular Docking
Molecular Dynamics Simulations
Sensors

Awards/Scholarships:

- ☐ 1992: Qualified U.G.C. NET J.R.F. examination.

Committee/Society Services at University of Lucknow:

- ☐ Co-ordinator Physics Society, Department of Physics, University of Lucknow, Lucknow.
- ☐ Member, Faculty Board of Science
- ☐ Member, Board of Studies, Department of Physics
- ☐ Member, Departmental Research Committee
- ☐ Member, various departmental committees.

Memberships and Affiliations:

- ☐ Life member of Materials research society of India (MRSI).
- ☐ Life member of Indian Science Congress.

Teaching undergraduate and postgraduate-level courses:

- ☐ Thermodynamics at the undergraduate level.
- ☐ Quantum mechanics and atomic spectra at the Postgraduate Level
- ☐ Supervision and mentoring of post-graduate students, guiding them in their master thesis projects.

Collaborations:

- ☐ Research Collaboration with **Prof. El-Emam**, Mansoura University, Faculty of Pharmacy Department of Medicinal Chemistry, **Egypt**. Collaboration involves joint discussions and exchange of scientific ideas, particularly in Chemical Synthesis and Computational Quantum Chemistry.
- ☐ Research Collaboration with **Prof. Salah Belaidi**, University of Biskra, **Algeria**, Group Head of Computational and Medicinal Chemistry.

Ph.D. Supervision:

Supervised six research students for their Ph.D. degree.

Research areas and Interest:

1. Quantum Chemistry
2. Chemical design of biomolecules in drug discovery and Drug design, Drug-likeness
3. QSAR modelling
4. Molecular docking and Molecular dynamics simulations
5. Sensors
6. Nanoclusters

LIST OF PUBLICATIONS

1. Hydrazone-linked isatin-pyridine hybrids for EGFR inhibition: Insights from density functional and molecular docking analyses, Shilendra K. Pathak, Zohra Siddiqui, Anushree Maurya, Mamta Pal, Raj Shukla, Ruchi Srivastava, Vikas K. Shukla, Onkar Prasad, Leena Sinha, Journal of Molecular Structure, Volume 1356, 2026, 145130, ISSN 0022-2860, <https://doi.org/10.1016/j.molstruc.2025.145130>.
2. A Novel Pyridopyrimidine Derivative as a Potential Breast Cancer Agent: DFT, Docking, MD Simulation, and Cytotoxic Studies; Anushree Maurya, Lamya H. Al-Wahaibi, Mamta Pal, Raj Shukla, Zohra Siddiqui, Shilendra K. Pathak, Ruchi Srivastava, Vikas K. Shukla, Himani Kulshrestha, Mustafa Kurban, Ali A. El-Emam, Onkar Prasad, Leena Sinha*; Chemistry & Biodiversity (2025) Volume 22, Issue 12 e01955; <https://doi.org/10.1002/cbdv.202501955>.
3. A comparative study for polymer liquid mixture of poly(ethylene glycol) methyl ether methacrylate-475 with alkoxyethanol using thermoacoustical, simulations and spectroscopy tools. Hussain, A., Kumari, L., Shukla, S. et al. Eur. Phys. J. B 98, 161 (2025). <https://doi.org/10.1140/epjb/s10051-025-01012-2>.
4. Insights into Novel Isoniazide Encompassing triazolo[4,3-b][1,2,4]triazoles as Anti-TB, antioxidant and antidiabetic agents: A spectral analysis, DFT calculations, ADME, In vitro, and in silico molecular modeling studies, Parveen Rajesab, Basavarajaiah Suliphuldevara Mathada, Vidya Niranjana, Anushree Maurya, Anagha S. Setlur, Onkar Prasad, K. Chandrashekar, Leena Sinha, Journal of Molecular Structure, Volume 1334, 2025, 141876, ISSN 0022-2860, <https://doi.org/10.1016/j.molstruc.2025.141876>.
5. Unveiling a novel thiazolo[2,3-c][1,2,4]triazole scaffolds as a dual cyclooxygenase and cholinesterase inhibitors: Spectral analysis, DFT calculations, in vitro and in silico studies, Parveen Rajesab, Basavarajaiah Suliphuldevara Mathada, Vidya Niranjana, Leena Sinha, Anagha S. Setlur, Anushree Maurya, K. Chandrashekar, Onkar Prasad, Journal of Molecular Structure, Volume 1345, 2025, 143166, ISSN 0022-2860, <https://doi.org/10.1016/j.molstruc.2025.143166>.
6. In Silico and in Vitro Evaluation of (1H-indol-3-ylmethylene)-pyridin-3-yl-amine as a Potent Inhibitor for VEGFR2, EGFR and Progesterone Receptors. Siddiqui, Z., Maurya, A., Pal, M., Shukla, R., Pathak, S. K., Srivastava, R., Shukla, V. K., Prasad, O. and Sinha, L. (2025). Physical Chemistry Research, 13(2), 295-318. doi: 10.22036/pcr.2025.500025.2629.
7. Computational Study of Coumarin Compounds as Potential Inhibitors of Casein Kinase 2: DFT, 2D-QSAR, ADMET and Molecular Docking Investigations. Chennai, H. Y., Belaidi, S., Ouassaf, M., Sinha, L., Prasad, O., Serdaroğlu, G., & Chtita, S. (2025). Polycyclic Aromatic Compounds, 45(5), 843–862. <https://doi.org/10.1080/10406638.2024.2418408>
8. In silico insights into dual COX inhibition by fluoro-substituted indole derivative using DFT, molecular docking, and MD simulation studies. Mamta Pal, Raj Shukla, Anushree Maurya, Zohra Siddiqui, Ruchi Srivastava, Shilendra K. Pathak, Vikas K. Shukla, Onkar Prasad, Leena Sinha; Journal of the Chinese Chemical Society (2025) Volume 72, Issue 6 pp. 653-676; <https://doi.org/10.1002/jccs.70020>.

9. Synthesis, Structural, DFT studies, Biological Effectiveness, and Molecular Docking Aspects of Multitarget Novel N-(4-Phenylthiazol-2-yl)hydrazine carboxamide Hybrids as COX inhibitors, Anti-TB, and Anti-oxidant activity, Basavaraj Hiremath, Anushree Maurya, Nagesh GY, Onkar Prasad, Prashantha Karunakar, Leena Sinha, Mukhtar Ahmed, Basavarajaiah SM, Journal of Molecular Structure, Volume 1321, Part 4, 2025, 140081, ISSN 0022-2860, <https://doi.org/10.1016/j.molstruc.2024.140081>.
10. Drug delivery potential of γ -graphyne, 6,6,12-graphyne and γ -graphdiyne for 5-Fluorouracil: insights from DFT calculations. Maurya, A., Mishra, A. N., Srivastava, J., Mishra, S., Pal, M., Shukla, R., Sinha, L. (2025). Composite Interfaces, 32(8), 1193–1213. <https://doi.org/10.1080/09276440.2025.2460350>.
11. A comprehensive analysis of the spectroscopic and drug-like properties of dimethyl 5-hydroxybenzene-1,3-dicarboxylate: insights from DFT and MD simulations. Pal, M., Maurya, A., Shukla, R., Siddiqui, Z., Pathak, S. K., Srivastava, R., Sinha, L. (2024). Molecular Simulation, 50(15), 1246–1261. <https://doi.org/10.1080/08927022.2024.2397463>.
12. A Thermoacoustical and DFT Exploration of Physio-chemical Properties for N,N-dimethylacetamide (DMA) with Water; Laxmi Kumari, Ajaz Hussain, Harshit Agarwal, Abhishek Mishra, Ratindra Gautam, Rahul Singh, Yashveer Gautam, Monal Singh, Leena Sinha, Onkar Prasad And Manisha Gupta* ORIENTAL JOURNAL OF CHEMISTRY; ISSN: 0970-020 X CODEN: OJCHEG 2024, Vol. 40, No.(2).
13. Identification of novel curcumin derivatives against pancreatic cancer: a comprehensive approach integrating 3D-QSAR pharmacophore modeling, virtual screening, and molecular dynamics simulations. N Chahbaoui, S Khamouli, M Alaqrbeh, S Belaidi, L Sinha, S Chtita, M. Bouachrine; J Biomol Struct Dyn.(2024), 42(22), 12021–12039. <https://doi.org/10.1080/07391102.2023.2266502>.
14. Experimental and theoretical quantum chemical studies of 2-(2-acetamidophenyl)-2-oxo-N-(pyridin-2-ylmethyl)acetamide and its copper(II) complex: molecular docking simulation of the designed coordinated ligand with insulin-like growth factor-1 receptor (IGF-1R). El-Sayed, D.S., Sinha, L. & Soayed, A.A. BMC Chemistry 18, 112 (2024). <https://doi.org/10.1186/s13065-024-01217-z>.
15. Synthesis, spectroscopic analysis, molecular docking, molecular dynamics simulation of 5-(adamantan-1-yl)-4-(3-chlorophenyl)-2,4-dihydro-3H-1,2,4-triazole-3-thione, a potential anti-proliferative agent. Alaa S. Abdelrazeq, Hazem A. Ghabbour, Lamya H. Al-Wahaibi, Mohammed S. M. Abdelbaky, Santiago Garcia-Granda, Ali A. El-Emam, Shilendra K. Pathak, Ruchi Srivastavae, Anushree Mauryae, Vikas K. Shuklaf, Onkar Prasade and Leena Sinha. Polycyclic Aromatic Compounds. <https://doi.org/10.1080/10406638.2023.2219362>.
16. DFT Study of the Adsorption Behavior of Adenine on the Nano-SiO₂ Cluster; Meftah, N., Keressa, A., Belaidi, S. *et al.* Silicon (2023). <https://doi.org/10.1007/s12633-023-02292-y>.
17. Spectroscopic, electronic structure, molecular docking, and molecular dynamics simulation study of 7-Trifluoromethyl-1H-indole-2-carboxylic acid as an aromatase inhibitor. Isha Singh, Ruchi Srivastava, Vikas K Shukla, Shilendra K Pathak, Tanay Burman, Aamal A Al-Mutairi, Ali A El-Emam, Onkar Prasad, Leena Sinha; Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy; Volume 280, 2022, 121530.

18. Study of molecular association in binary mixtures of poly(vinyl pyrrolidone) (PVP) with ethanol, 1-propanol and 1-butanol through thermo-acoustical, FT-IR, UV–Vis spectroscopy and DFT studies. Laxmi Kumari, Leena Sinha, Onkar Prasad & Manisha Gupta; *Eur. Phys. J. D* **75**, 296 (2021).
19. Surface modification and characterization of h-BN-doped PVP thin film and its application as humidity sensor with theoretical DFT calculations. Laxmi Kumari, Utkarsh Kumar, Leena Sinha, Onkar Prasad, B. C. Yadav & Manisha Gupta, *Chemical Papers* volume 75, pages 4055–4068 (2021).
20. Thermoacoustic and DFT Analysis of N, N-Dimethylacetamide (DMA) with 1-Propanol and Methanol at 293.15, 303.15, and 313.15 K. H Agarwal, L Kumari, L Sinha, O Prasad, M Gupta - *Brazilian Journal of Physics*, 51(3) 515-526 (2021).
21. DFT study on the electronic properties, spectroscopic profile, and biological activity of 2-Amino-5-trifluoromethyl-1, 3, 4-thiadiazole with anticancer properties, Isha Singh, Lamya H Al-Wahaibi, Ruchi Srivastava, Onkar Prasad, Shilendra K Pathak, Saurabh Kumar, Shama Parveen, Monisha Banerjee, Ali A El-Emam, Leena Sinha, *ACS omega*, 5(46) 30073-30087 (2020).
22. Thermodynamic, spectroscopic and DFT studies of binary mixtures of poly(vinylpyrrolidone)(PVP) with ethanol, 1-propanol and 1-butanol. L Kumari, S Gupta, I Singh, O Prasad, L Sinha, M Gupta, *Journal of Molecular Liquids* 299, 112237 (2020).
23. Virtual screening in drug-likeness and structure/activity relationship of pyridazine derivatives as Anti-Alzheimer drugs. A Zerroug, S Belaidi, I BenBrahim, L Sinha, S Chtita. *Journal of King Saud University-Science* 31 (4), 595-601 (2019).
24. Experimental and theoretical DFT (B3LYP, X3LYP, CAM-B3LYP and M06-2X) study on electronic structure, spectral features, hydrogen bonding and solvent effects of 4-methylthiadiazole-5-carboxylic acid. I Singh, AA El-Emam, SK Pathak, R Srivastava, VK Shukla, O Prasad, and Leena Sinha, *Molecular Simulation* 45 (13), 1029-1043 (2019).
25. First principle study of a potential bioactive molecule with tetrahydroisoquinoline, carbothiomide and adamantane scaffolds. MM Al-Shehri, ARA Al-Majed, HI Aljohar, AA El-Emam, SK Pathak, Alok K.Sachan, OnkarPrasad, LeenaSinha, *Journal of Molecular Structure* 1143, 204-216 (2017).
26. A combined experimental and theoretical DFT (B3LYP, CAM-B3LYP and M06-2X) study on electronic structure, hydrogen bonding, solvent effects and spectral features of methyl 1H-indol-5-carboxylate. R Srivastava, FAM Al-Omary, AA El-Emam, SK Pathak, M Karabacak, Vijay Narayan, Satish Chand, Onkar Prasad, Leena Sinha, *Journal of Molecular Structure* 1137, 725-741 (2017).
27. Structural and Spectroscopic Analysis of Indole-3-Carbinol by First Principle Calculations, SK Pathaka, O Prasada, L Sinha, *Int J Chem Sci* 15 (4), 212 (2017).
28. Spectroscopic and electronic structure calculation of a potential antibacterial agent incorporating pyrido-dipyrimidine-dione moiety using first principles. S Fatma, A Bishnoi, V Singh, FAM Al-Omary, AA El-Emam, S Pathak, Ruchi Srivastava, Onkar Prasad, Leena Sinha. *Journal of Molecular Structure* 1110, 128-137 (2016).
29. Conformational search, spectral analysis and electronic properties of 5-(4-Pyridinyl)-1, 3, 4-thiadiazol-2-amine. VK Shukla, MA Al-Alshaikh, AA El-Emam,

- AK Sachan, R Srivastava, OnkarPrasad, Leena Sinha. *Journal of Molecular Structure* 1108, 112-125 (2016).
30. Investigations on Molecular Structure, Electronic Properties, NLO Properties and Comparison of Drug-Likeness of Triazolothiadiazole Derivatives by Quantum Methods and QSAR Analysis, A Kerassa, S Belaidi, D Harkati, T Lanez, O Prasad, L Sinha, *Reviews in Theoretical Science* 4 (1), 85-96 (2016).
 31. Prediction of molecular properties and spectroscopic profile of Riluzole with different functionals (B3LYP, M06-2X, MPWLYP): A combined theoretical and experimental study, VK Shukla, AK Sachan, SK Pathak, R Srivastava, O Prasad, L Sinha, *Journal of Molecular Structure* 1106, 265-276 (2016).
 32. Spectroscopic and electronic structure calculation of a potential chemotherapeutic agent 5-propyl-6-(p-tolylsulfanyl) pyrimidine-2, 4 (1H, 3H)-dione using first principles. MA Al-Alshaikh, OA Al-Deeb, NZ Alzoman, AA El-Emam, R Srivastava, Alok K. Sachan, Onkar Prasad, Leena Sinha, *Journal of Molecular Structure* 1100, 225-236 (2015).
 33. Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid, M Karabacak, L Sinha, O Prasad, S Bilgili, AK Sachan, AM A siri, A Atac, *Journal of Molecular Structure* 1095, 100-111 (2015).
 34. Structure activity relationship and quantitative structure-activity relationships modeling of antitrypanosomal activities of alkyl diamine cryptolepine derivatives. S Belaidi, T Salah, N Melkemi, L Sinha, O Prasad. *Journal of Computational and Theoretical Nanoscience* 12 (9), 2421-2427 (2015).
 35. Study on molecular structure, spectroscopic behavior, NBO, and NLO analysis of 3-methylbezothiazole-2-thione. S Chand, FAM Al-Omary, AA El-Emam, VK Shukla, O Prasad, L Sinha. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 146, 129- 141 (2015).
 36. Exploring QSARs of some benzenesulfonamides incorporating cyanoacrylamide moieties as a carbonic anhydrase inhibitors (specifically against tumor-associated isoforms IX and XII). AM Alafeefy, HA Abdel-Aziz, F Carta, CT Supuran, SK Pathak, O Prasad, and Leena Sinha, *Journal of enzyme inhibition and medicinal chemistry* 30 (4), 519-523 (2015).
 37. A Combined theoretical and experimental study of conformational and spectroscopic profile of 2-acetamido-5-aminopyridine. SK Pathak, R Srivastava, AK Sachan, O Prasad, L Sinha. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 143, 147-157 (2015).
 38. Conformational and spectroscopic behaviors of 2, 4-xylyl isothiocyanate. M Cinar, M Karabacak, S Chand, VK Shukla, L Sinha, O Prasad, *Journal of Molecular Structure* 1087, 113-120 (2015).
 39. FT-IR and FT-Raman spectroscopic signatures, vibrational assignments, NBO, NLO analysis and molecular docking study of 2-{[5-(adamantan-1-yl)-4-methyl-4H-1, 2, 4-triazol-3-yl]sulfanyl}-N,N-dimethylethanamine. MS Almutairi, AM Alanazi, ES Al-Abdullah, AA El-Emam, SK Pathak et. al. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 140, 1- 14(2015).
 40. Development of certain novel N-(2-(2-(2-oxoindolin-3-ylidene) hydrazinecarbonyl) phenyl)-benzamides and 3-(2-oxoindolin-3-ylideneamino)-2-substituted quinazolin-4 (3H)-ones as CFM-1 analogs: Design, synthesis, QSAR

- analysis and anticancer activity, AM Alafeefy, AE Ashour, O Prasad, L Sinha, S Pathak, FA Alasmari, *European Journal of Medicinal Chemistry* 92, 191-201 (2015).
41. Syntheses, structural elucidation, thermal properties, theoretical quantum chemical studies (DFT) and biological studies of barbituric-hydrazone complexes. AA Soayed, HM Refaat, L Sinha. *Journal of Saudi Chemical Society* 19 (2), 217-22 (2015).
 42. Spectral features, electric properties, NBO analysis and reactivity descriptors of 2-(2-Benzothiazolylthio)-Ethanol: Combined experimental and DFT studies. R Srivastava, L Sinha, M Karabacak, O Prasad, SK Pathak, AM Asiri, M.Cinar. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 136, 1205-1215 (2015).
 43. Experimental (FT-IR, FT-Raman, UV and NMR) and quantum chemical studies on molecular structure, spectroscopic analysis, NLO, NBO and reactivity descriptors of 3, 5-Difluoroaniline. SK Pathak, R Srivastava, AK Sachan, O Prasad, L Sinha, AM Asiri et. al. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 135, 283-295.
 44. Molecular structure, vibrational and electronic properties of 4-Phenyl-3H-1,3-thiazol-2-ol using density functional theory and comparison of drug efficacy of keto and enol forms by QSAR analysis, Alok K. Sachan, Shilendra K. Pathak, Satish Chand, Ruchi Srivastava, Onkar Prasad, Salah Belaidi, Leena Sinha. *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 132, 2014, 568-581. <https://doi.org/10.1016/j.saa.2014.05.01>.
 45. Structural and spectroscopic characterization of a novel potential anti-inflammatory agent 3-(adamantan-1-yl)-4-ethyl-1H-1,2,4-triazole-5(4H)thione by first principle calculations., *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* 124 (2014) 108–123.
 46. Structural, vibrational, and electronic properties of succinimide, N-hydroxy succinimide and N-methyl succinimide by density functional theory: a comparative study. AK Sachan, S Chand, R Srivastava, VK Shukla, SK Pathak, A Kumar, O Prasad, L Sinha, 2014, *J. Chem. Pharm. Res.* Volume 6, 211-227.
 47. Spectroscopic (FT-IR, FT-Raman, and UV–visible) and quantum chemical studies on molecular geometry, Frontier molecular orbitals, NBO, NLO and thermodynamic properties of 1-acetylindole, Vikas K. Shukla, Ebtehal S. Al-Abdullah, Ali A. El-Emam, Alok K. Sachan, Shilendra K. Pathak, Amarendra Kumar, Onkar Prasad, Abha Bishnoi, Leena Sinha, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 133, 2014, 626-638. <https://doi.org/10.1016/j.saa.2014.06.043>.
 48. FT-IR, FT-Raman and UV spectroscopic investigation, electronic properties, electric moments, and NBO analysis of anethole using quantum chemical calculations, L. Sinha, O. Prasad, S. Chand, A.K. Sachan, S.K. Pathak, V.K. Shukla, M. Karabacak, A.M. Asiri, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, Volume 133, 2014, 165-177, <https://doi.org/10.1016/j.saa.2014.05.034>.
 49. Quantum chemical study of molecular structure, non-linear optical and vibrational properties of pyridine and pentachloropyridine, Satish Chand, Shilendra K Pathak, Alok K Sachan, Ruchi Srivastava, Vikas K Shukla, V Narayan, A Kumar, Onkar

- Prasad, Leena Sinha, 2014, Journal of Chemical and Pharmaceutical Research, 6(3)1434-1444.
50. Theoretical Raman and FTIR vibrational analysis of 2-phenyl-1H-indene-1, 3 (2H)-dione by ab initio method, Jitendra Pathak, Vijay Narayan, Leena Sinha*, and Onkar Prasad, J. At. Mol. Sci. (2012) Vol. 3, No. 2, pp. 95-105 doi: 10.4208/jams.051111.063011a.
 51. A combined experimental and theoretical investigation of 2-Thienylboronic acid: Conformational search, molecular structure, NBO, NLO and FT-IR, FT-Raman, NMR and UV spectral analysis, A.K. Sachan, S.K. Pathak, L. Sinha, O. Prasad, M. Karabacak, A.M. Asiri, Journal of Molecular Structure, Volume 1076, 2014, 639-650, <https://doi.org/10.1016/j.molstruc.2014.08.011>.
 52. FT-IR, FT-Raman, NMR, UV and Quantum Chemical Studies on Monomeric and Dimeric Conformations of 3,5-dimethyl-4-methoxybenzoic acid. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 123 (2014) 352–362.
 53. Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 120 (2014) 126–136.
 54. An experimental and theoretical investigation of Acenaphthene-5-boronic acid: Conformational study, NBO and NLO analysis, molecular structure and FT-IR, FT-Raman, NMR and UV spectra. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 115 (2013) 753–766.
 55. Molecular structure, electronic properties, NLO, NBO analysis and spectroscopic characterization of Gabapentin with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 109 (2013) 298–307.
 56. The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMO–LUMO analysis of monomeric and dimeric structures of 4-chloro-3,5-dinitrobenzoic acid. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Volume 93 (2012) 33-46.
 57. Structural and spectroscopic characterization of a novel potential chemotherapeutic agent 3-(1-adamantyl)-1-[[4-(2-methoxyphenyl)piperazin-1-yl]methyl]-4-methyl-1H-1,2,4-triazole-5(4H)-thione by first principle calculations. Journal of Molecular Structure 1022 (2012) 49–60.
 58. Monomeric and dimeric structures, electronic properties and vibrational spectra of azelaic acid by HF and B3LYP methods. Journal of Molecular Structure 1022 (2012) 81–88.
 59. Theoretical Studies on the Isomers of Quinazolinone by first Principles. Research Journal of Recent Sciences, Vol. 1(3) (March 2012) 11-18.
 60. Vibrational, Structural and Electronic properties of 6-methyl nicotinic acid by Density Functional Theory. Journal of Chemical and Pharmaceutical Research, 4(6) (2012) 3287-3296.
 61. Electronic structure, electric moments and vibrational analysis of 5-nitro 2-furaldehydesemicarbazone: A D.F.T. study Computational and Theoretical Chemistry (Formerly Theochem). Vol. 973 (2011) 20-27.

62. Raman, FT-IR spectroscopic analysis and first-order hyperpolarizability of 3-benzoyl-5-chlorouracil by first principles. *Molecular Simulation*. Vol. 37, No. 2 (2011) 153–163.
63. Theoretical Raman and FTIR vibrational analysis of 2-phenyl-1H-indene-1,3(2H)dione by ab initio method. *Journal of At. Mol. Sci*. Vol. 3, No. 2 (May 2012) 95-105.
64. Electronic structure, electric moments and vibrational analysis of 3-(2-methoxyphenoxy) propane-1,2-diol by ab initio and density functional theory. *J. At. Mol. Sci*. Vol. 2, No. 3, (2011) 212-224.
65. Comparative study of frontier orbitals, molecular electrostatic potential surface of Oxygen Nano-clusters by first principles, *Chinese Journal of Physics*, Vol. 49 (2) (2011) 664-671.
66. Quantum Chemical study of Molecular structure, Non Linear Optical and Vibrational Properties of ortho and meta - Fluorobenzaldehyde. *Journal of Chemical and Pharmaceutical Research*, Vol. 3 Issue 5 (2011) 668-677.
67. Electronic structure, non-linear properties and vibrational analysis of Acenaphthene and its carbonyl derivative Acenaphthenequinone by density functional theory. *Journal of Molecular Structure: Theochem*, vol. 958, no. 1, (2010) 33-40.
68. Theoretical Raman and IR spectra of tegafur and comparison of molecular electrostatic potential surfaces, polarizability and hyperpolarizability of tegafur with 5-fluoro-uracil by density functional theory. *J. Atomic and Molecular Sciences*. Vol. 1, No. 3 (2010) 201-214.
69. Analysis of Vibrational, Structure, and Electronic properties of Rivastigmine by Density Functional Theory. *Journal of Applied Spectroscopy* Vol. 77, No. 4 (2010) 507-516.
70. Molecular structure and vibrational study on 2, 3-dihydro-1H-indene and its derivative 1H-indene-1,3(2H)-dione by density functional theory calculations. *Journal of Molecular Structure: Theochem*, 940, (2010) 82-86.
71. Theoretical study on effect of binding of Netropsin on thermal denaturation of synthetic oligo-nucleotides. *Der PharmaChemica*, 2(1), (2010) 224-235.
72. FTIR Spectra and Vibrational Spectroscopy of Lantadene A. *Der PharmaChemica*, 1(2), (2009) 162-169.
73. Quantum –Chemical Calculation on 5-Phenyl-2-(4-Pyridyl) Pyrimidine. *Journal of Applied Spectroscopy* Vol. 76, No. 5, (2009) 623-629.
74. Quantum chemical study and the effect of substitution of amino group on the reactivity of 4-Aminopyridine and 3,4-Diaminopyridine by Density Functional Theory. *Der PharmaChemica*, 1(2), (2009) 258-268.
75. Study of electrostatic potential surface and molecular orbitals of O4 nano cluster by first principles. *Der Pharma Chemica*, 1(2), (2009) 79-85.
76. Molecular structure and vibrational spectra of 2-formyl benzonitrile by density functional theory and ab initio Hartree–Fock calculations; N Misra, O Prasad, L Sinha, A Pandey. *Journal of Molecular Structure: THEOCHEM* 822 (1-3), 45-47 (2007).
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