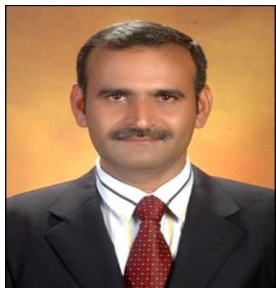


Curriculum Vitae



Prof. Lokanath N. K.

Director, Planning Monitoring Evaluation Board

Director, College Development Council

Professor

Department of Studies in Physics

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Current Positions

Director Planning Monitoring Evaluation Board, University of Mysore, Mysuru, India.

Director College Development Council, University of Mysore, Mysuru, India.

Coordinator DST-FIST program, DoS in Physics, University of Mysore, India.

Principal investigator National Single Crystal Diffractometer Facility, University of Mysore, Mysuru.

Nodal officer RUSA, University of Mysore, Manasagangotri, Mysuru, India.

Nodal officer NEP-2020 Implementation, University of Mysore, Manasagangotri, Mysuru, India.

Positions Held

Chairman Department of Studies in Physics, University of Mysore, Mysuru (2019-2021)

Coordinator CPEPA, University of Mysore, Mysuru, India. (2012-2018)

Coordinator UGC-SAP-II, DoS in Physics, University of Mysore, Mysuru, India. (2012-2018)

Education

1994-1998 **Ph.D.**, DoS in Physics, University of Mysore, Mysuru, India.

Research Experience

1999-2000 **Research Associate (CSIR)**, DoS in Physics, University of Mysore, Mysuru.

2000-2002 **Postdoctoral Fellow**, Samsung Biomedical Research Institute, Sungkyunkwan University School of Medicine, Suwon, South Korea.

2002-2007 **Scientist**, RIKEN Spring-8 Center, Harima Institute, Hyogo, Japan.

Jan-Feb 2008 **Visiting Professor**, Sungkyunkwan University, South Korea.

Research Contributions

- Published more than **409** research papers in reputed and high impact factor international journals.
- Delivered **47** invited lectures in the international conferences and other educational institutions in India and abroad.
- State of the art laboratory has been developed for collaborative research.

Contribution to CCDC and RCSB Protein Data Bank (PDB)

- More than 1000 crystal structure data have been deposited to CCDC.
- 70 protein structures (22 MAD, 33 MR and 15 complexes) have been deposited to PDB.

Awards and Honors

- Second Rank in M.Sc. University of Mysore, India.
- An article on ‘Dimeric core structure of modular stator subunit E of archaeal H⁺-ATPase’ appeared in the RIKEN Research Bulletin of May, Japan, 2007 (Vol. 2, No. 5).
- The research outcome of the structure of modular stator subunit E of archaeal H⁺-ATPase had been widely published in several Japanese newspapers on December 5, 2006.
- **Sir C. V. Raman Young Scientist’s** State Award (2012), Government of Karnataka.
- **Faculty Research** award by Career 360, New Delhi, 2018.

Research Interests

To understand the function of protein, it is necessary to determine its 3D-structure. The X-ray crystallography analysis is the most efficient method to determine protein 3D-structures at atomic level. The applications of protein structures are very useful for the benefit of society, development of advanced technology for structural biology and pharmaceuticals/industrial applications.

Combining macromolecular crystallography with small-molecule crystallography yields valuable information on any ligands which can help to address many of the challenges in generating small molecules for use in biological applications. Crystal structures of small molecules are a source of valuable structural information helpful in the process of drug design.

A small-molecule structure will give precise target values and reveal whether the conformation is the same as in the protein–ligand complex, giving information about the likely entropic components of binding and geometrical compromises made by the ligand. Finally, the interactions made by a small molecule when packing, including with solvent, can be compared with those made in a protein–ligand complex, suggesting where ligand modification may be considered. Future development in small molecule crystallography should also provide original solutions to complex problems related to polymorphism.

Research Projects

1. **DST-FIST II**, Department of Studies in Physics, University of Mysore.
2. **UGC-MRP**, Crystal Structure of ATP Binding Subunit of an ABC Transporter.
3. **IOE-UGC**, Structural biology of natural product enzymes.
4. **UPE-UGC**, Structure-function relation of the enzymes of propionate oxidation.
5. **CPEPA**, Processing characterization and applications of advanced functional nanomaterials.
6. **DST-PURSE**, Biologically important heterocyclic compounds.

Seminars/Conferences Organised

- **Nodal Officer**, Association of Indian Universities, *96th Annual general meet and national seminar on realizing SDGs through HEIs*, Vice Chancellors' Meet, University of Mysore, March 23-25, 2022.
- **Convenor**, International conference on nano materials and their application, University of Mysore, March 1-2, 2018.
- **Convenor**, International symposium on chemical biology approach to metabolism, chemical genomics and epigenomics and second annual meeting of chemical biology society, India, Feb 18-19, 2015.
- **Convenor**, National symposium on X-ray crystallography, DoS in Physics, November 29, 2014.

Service on Editorial Board

- Reviewer, Journal of Molecular Structure, MCLC, Journal of Crystallography, Acta Cryst. Sections, B, C, D, E and F, Polyhedron, Journal of chemical crystallography.

Research Guidance

➤ Awarded Ph.D. Students

1. **Manjunath B. C.** “Study of Crystal and Molecular Structure of Biologically Important Heterocyclic Compounds”, 2014.
2. **Prabuswamy M.** “Crystal and Molecular Structure Studies of Biologically active Quinoline Derivatives”, 2014.
3. **Manjula M.** “Crystal Structure of ATP Binding Subunit of an ABC Transporter”, 2015.
4. **Madan Kumar S.** “X-ray Diffraction Studies and Structure-Function Relationship of NAD/NADP Dependent Dehydrogenase”, 2015.
5. **Amrutha Kala A. L.** “Synthesis, Characterization and Crystal Structure of Schiff Base Derivative”, 2018.
6. **Karthik Kumara** “Structural Investigation of Some Heterocyclic Compounds of Biological Interest”, 2018.
7. **Chethan Prathap K. N.** “Crystal and Molecular Studies of Medicinally Important Heterocyclic Compounds”, 2018.
8. **Nagaraja K. P.** “Growth and Characterisation of mixed oxalate crystals”, 2020
9. **Jyothi K. L.** “Structural Studies of Some Biologically Important Piperidine Derivatives”, 2020.
10. **Hema M. K.** “Synthesis and Structural Investigation of Some Metal Complexes of Biological Interest”, 2020.
11. **Pramodh B.** “Spectroscopic Analysis and Structural Studies of Some Molecules of Biological interest”, 2021.

➤ Current Ph.D. Students

1. **Khalid Mohammad Abdo.** “Structural and characterization of some semiconductor nanoheterostructures for photocatalytic applications”.
2. **Mahesha** “Synthesis, structural and quantum computational studies of biologically active ligand metal complexes”.
3. **Chethan B. S.** “Synthesis, structural analysis and computational studies of metal-organic complexes”.
4. **Uday Kumar A. H.** “Structural and quantum computational studies on metal complexes of biological interest”.
5. **Sujay Shekar G. C.** “Design and investigation of some hybrid organic-inorganic nanocomposites for photocatalytic applications”.
6. **Vinay Kumar D. C.** “Synthesis and study of heterogeneous nanomaterials”.
7. **Niranjana S. V.** “Structural Investigation of Some Thiophene derivatives of Medicinal Interest”.
8. **Vindya M. P.** “Structural Investigation of Some Pyrozole derivatives of Medicinal Interest”.
9. **Akhila A.** “Structural and characterization of some semiconductor nanoheterostructures for photocatalytic applications”

Participation in Conferences

- 18-21 Nov 2001 *The Fourth Asian Crystallography Association*, Bangalore, India.
- 26-27 July 2002 *Annual Meeting of Structural-Biological Whole Cell Project of Thermus thermophilus HB8*, SPring-8, Japan.
- 28 May-2 June 2003 *International symposium on Diffraction Structural Biology*, Tsukuba, Japan.
- 19-20 Mar 2003 *The Eighth Harima International Forum of Structural Biology of Biological Machinery*, SPring-8, Japan.
- 11-12 Sept 2003 *RIKEN/BBSRC Symposium of Japan-UK Protein Structural Biology*, Japan.
- 1-3 Aug 2003 *Annual Meeting of Structural-Biological Whole Cell Project of Thermus thermophilus HB8*, SPring-8, Japan.
- 17-21 Nov 2004 *The Third International Conference on Structural Genomics*, Washington, USA.
- 7-11 Sept 2004 *The Eighth Conference on Biology and Synchrotron Radiation*, Himeji, Japan.
- 30 July-1 Aug 2004 *Annual Meeting of Structural-Biological Whole Cell Project of Thermus thermophilus HB8*, SPring-8, Japan.
- 17-20 Feb 2004 *Second International Symposium on Current Trends in Drug Discovery and Research*, CDRI, Lucknow, India.
- 14-18 Apr 2004 *The First Pacific-Rim International Conference on Protein Science*, Pacifico Yokohama, Japan.

- 23-31 Aug 2005 *XX Congress of the International Union of Crystallography (IUCr)*, Firenze, Italy.
- 12-16 Nov 2006 *Fifth East Asian Biophysics Symposium and Forty-Fourth Annual Meeting of the Biophysical Society of Japan (EABS and BSJ)*, Okinawa, Japan.
- 22-27 July 2006 *American Crystallographic Association (ACA)*, Honolulu, Hawaii, USA.
- 7-8 Mar 2006 *The fourth international workshop on X-ray damage to biological crystalline samples*, Spring-8, Japan.
- 13-17 Aug 2007 *9th International Conference on Biology and Synchrotron Radiation*, Manchester, England.
- 7-10 Sept 2009 *Participated in the Young Indian Scientists Colloquium*, TIFR, Mumbai, India.
- 18-21 Jan 2010 *The Eighth Asia-Pacific Bioinformatics conference*, IISc, Bangalore.
- 26-28 Nov 2011 *40th National Seminar on Crystallography*, Osmania University, Hyderabad.
- 16-17 Feb 2011 *International Symposium on Challenges in Drug Discovery*, KSOU, Mysore.
- 15-17 Mar 2012 *ICABS-2012*, Kannur university, Kannur, Kerala, India.
- 8-11 Jan 2013 *International conference on Biomolecular forms and Functions*, IISc, Bangalore.
- 4-7 Dec 2016 *14th Conference of the Asian Crystallographic Association*, Hanoi-Vietnam.
- 10-13 June 2016 *44th National Seminar on Crystallography*, Pune, India.
- 21-28 Aug 2017 *24th Congress of the International Union of Crystallography (IUCr)*, Hyderabad.
- 20-24 Feb, 2019 *11th International Workshop on Advanced Materials: IWAM*, Ras Al Khaimah, Dubai.

Membership in Academic Bodies

1. Member, BOS in Physics, DoS in Physics, University of Mysore, 2007- till date.
2. Member, Interdisciplinary Board for Guide Recognition under the Faculty of Science and Technology, 2021- till date.
3. Chairman, BOS in Physics, KSOU, Mysuru, 2014- till date.
4. Member, BOE in Physics, Tumkur University, 2021- till date.
5. Member, BOE in Physics, Mangalore University, 2021- till date.
6. Member, BOE in Physics, DoS in Physics, University of Mysore, 2016-17.
7. Member, BOS in PG-Physics, Mangalore University, Mangalagangothri, Mangaluru, 2015-18.
8. Member, BOS in Physics (PG), Govt. (Autonomous) College, Mandya, 2015-17.
9. Member, BOS in Physics for UG, JSS College for Women (Autonomous), Mysuru, 2015-17.
10. Member, Academic Council, JSS College of Arts, Science and Commerce, Mysuru, 2015-17.
11. Member, Academic Council, NIE Science College, Mysuru, 2015-17.
12. Member, Academic Council, AVK College, Hassan, 2015-17.
13. Member, BOS in Microbiology, Manasagangothri, Mysuru, 2007-10, 2014-17.

14. Member, BOS in Physics, 2007-10, 2014-17.
15. Member, BOS in PG-Physics, Kuvempu University, Shivamogga, 2014-17.
16. Member, BOS in Material Sciences, Vijnana Bhavan, Univeristy of Mysore, Mysuru, 2014-17.
17. Member, BOE in Physics, Government College (Autonomous), Mandya, 2013-14, 2014-15, 2015-16.
18. Member, BOA in Physics, Kuvempu University, Shankaraghatta, Shivamogga, 2015-16.
19. Member, Post-Graduate Sports Council, University of Mysore, Mysuru, 2015-16.
20. Member, Governing Council, N.I.E. First Grade College, Mysuru, 2015-16.
21. Chairman, BOE, Janapada Vishwavidyalaya for Traditional Science and Technology, 2014-15.
22. Member PG Admission Committee, DoS in Physics, Manasagangotri, Mysuru, 2014-15, 2015-16.
23. Member, BOS in Physics, Yuvaraja College of Mysore, Mysuru, 2014-15, 2016-18(UG).
24. Chairman, BOE in Phycis, Material Sciences, Vignana Bhavan, Univeristy of Mysore, 2014-15.
25. Member, K-SET Steering Committee, University of Mysore, Mysuru, 2015.
26. Member, Governing Council, Sri Adichunchanagiri First Grade College, Channarayapatna, 2014-16.
27. Chairman, BOE in Physics, DoS in Physics, Univeristy of Mysore, Mysuru, 2013-14.

Membership in Advisory Committee

1. Member, Technical review committee, 103rd Indian Science Congress, 2016.
2. Member, Local Organizing Committee, Two-day National Seminar on Biological Products for crop, animal and human health problems and aspects, 21-22 Aug 2015.
4. Member, Cultural Committee for Centenary Celebration, University of Mysore, 2015.
5. Member, Reception Committee for Centenary Celebration, University of Mysore, 2015.

Membership in scientific societies

- American Crystallography Association
- Indian Crystallography Association
- International Union of Biochemistry and Molecular Biology
- International Union of Crystallography
- Asian Crystallography Association
- Japanese Biochemical Society
- Korean Crystallography Association

1. Alnaggar G., Khaled A., Sujay Shekar G. C., Bajiri M. A., Drmosh Q. A. Q., **Lokanath N. K.**, and Ananda S., Rational design of 2D TiO₂-MoO₃ Step-scheme heterostructure for boosted photocatalytic overall water splitting. *New J. Chem.* *46*, 9629-9640.
2. Sujay Shekar G. C., Khaled A., Alnaggar G., Zaqri N. A., Bajiri M. A., Thejaswini B., and **Lokanath N. K.**, Surface defect engineered CeO_{2-x} by ultrasound treatment for superior photocatalytic H₂ production and water treatment. *Catal. Sci. Technol.*, *12*, 2071-2083.
3. Khaled A., Ali O., Sujay Shekar G. C., Hezam A., Bajiri M. A., and **Lokanath N. K.**, Highly Efficient Degradation of Organic Compounds via β-Bi₂O₃ Semiconductor Under Visible Illumination, *IOP Conf. Ser.: Mater. Sci. Eng.* *1221*, 012040.
4. Lohith T. N., Hema M. K., Karthik C. S., Sandeep S., Mallesha L., Alsaiari N. S., **Lokanath N. K.** and Kumaraswamy S. R., Persistent prevalence of non-covalent interaction in pyrimidine containing sulfonamide derivative: A quantum computational analysis. *J. Mol. Struct.*, *1252*, 133378.
5. Lohith T. N., Shamanth S., Sridhar M. A., Mantelingu K., and **Lokanath N. K.**, Synthesis, molecular structure, Hirshfeld surface, energy framework and DFT studies of 1, 3, 4 oxadiazole derivative. *J. Mol. Struct.*, *1252*, 132203.
6. Jayashankar J., Hema M. K., Karthik C. S., Suma D., Kumaraswamy S. R., **Lokanath N. K.**, Mallu P., Nethaji M. and Lu, N. (2022). Enchant OH...O interactions in hydrated 6-amino-2-methoxypyrimidin-4 (3H) one resembles as water flow in the channel: Crystallographic and theoretical investigations. *J. Mol. Struct.*, *1263*, 133098.
7. Hegde P. L., Bhat S. S., Revankar V. K., Shaikh S. A., Kumara K., and **Lokanath N. K.** (2022). Syntheses, structural characterization and evaluation of the anti-tubercular activity of copper (II) complexes containing 3-methoxysalicylaldehyde-4-methylthiosemicarbazone. *J. Mol. Struct.*, *1257*, 132589.
8. Arunagiri C., Selvakumar S., and **Lokanath N. K.** (2022). Structural, Optical, Spectral, Thermal and Third-order NLO Behaviour of 4-Chlorobenzhydrazide Trichloro Acetate Single Crystal. *Braz. J. Phys.*, *52*(3), 1-16.
9. Akhileshwari P., Sharanya K., Sallam H. H., Sridhar M. A., and **Lokanath N. K.** (2022). Crystal structure elucidation and DFT studies of imidazopyridine-pyrazoline derivative. *J. Mol. Struct.*, *1251*, 132063.

10. Chethan B. S., and **Lokanath N. K.** Study of the crystal structure, H-bonding and noncovalent interactions of novel cocrystal by systematic computational search approach. *J. Mol. Struct.*, 1251, 131936.
11. Shaikh S. A., Bhat, S. S., Revankar V. K., Kulkarni B. D., Kumara K., **Lokanath N. K.**, and Butcher, R. J. Fluorophore Tagged Mixed Ligand Copper (II) Complexes: Synthesis, Structural Characterization, Protein Binding, DNA Cleavage and Anticancer Activity. *Chemistry Select*, 6(45), 12666-12676.
12. Nanjundaswamy S., Hema M. K., Karthik C. S., Rajabathar J. R., Arokiyaraj S., **Lokanath N. K.**, and Mallu P. Synthesis, crystal structure, in-silico ADMET, molecular docking and dynamics simulation studies of thiophene-cha¹³²⁵⁸⁹lcone analogues. *J. Mol. Struct.*, 1247, 131365.
13. Hegde, P. L., Naik, K., Bhat, S. S., Shaikh, S. A., Butcher, R. J., Lokanath, N. K., & Revankar, V. K. Syntheses and structural characterization of metal complexes of 4-(naphthalen-1-yl)-1-(quinolin-2-yl) methylene thiosemicarbazide: their in-vitro screening studies for antitubercular activity. *J. Co. Chem.*, 74(17-20), 3018-3030.
14. Akhileshwari P., Sharanya K., Sallam H. H., Sridhar M. A., and **Lokanath N. K.** Crystal structure elucidation and DFT studies of imidazopyridine-pyrazoline derivative. *J. Mol. Struct.*, 1251, 132063.
15. Swarup H. A., Chandrasekhar S., Jayanna B. K., Kumara K., **Lokanath N. K.**, Thimmaiah S. B., and Mantelingu K. Sulfuric acid-mediated synthesis of 2, 5-disubstituted 1, 3, 4-thiadiazole via intramolecular cyclization reaction from dithioesters: An approach to crystal structure prediction, DFT studies and Hirshfeld surface analysis. *J. Mol. Struct.*, 1251, 131970.
16. Vadavi R. S., Bhat S. S., Naveen S., Revankar V. K., Gudasi K. B., **Lokanath N. K.**, and Butcher, R. J. Synthesis, structural characterization and biological properties of cyclometalated iridium (III) complexes containing 2-methyl-3-[(E)-[(quinolin-2-yl) methylidene] amino} quinazolin-4 (3H)-one. *Inorganica Chimica Acta*, 531, 120735.
17. Majid A., Lakshmikanth M., **Lokanath N. K.**, and Priyadarshini, C. P. Generation, characterization and molecular binding mechanism of novel dipeptidyl peptidase-4 inhibitory peptides from sorghum bicolor seed protein. *Food Chemistry*, 369, 130888.
18. Chethan B. S., Chethan Prathap K. N. and **Lokanath N. K.** Design, synthesis, structural analysis and quantum chemical insight into the molecular structure of coumarin derivatives. *Mol. Syst. Des. Eng.*, 6, 1-26.
19. Somashekar M. N., Chetana P. R., Chethan B. S., Rajegowda H. R., Cooper M. A., Ziora Z. M., **Lokanath N. K.** and Srinatha B. S. Synthesis and characterization of Zinc (II) complex with ONO donor type new Phenylpropanehydrazide based ligand: Crystal Structure, Hirshfeld Surface Analysis, DFT, Energy Frameworks and Molecular Docking. *J. Mol. Struct.*, 132429.

20. Mahesha, Udaya Kumar, A. H., Vindya, K. G., Pampa, K. J., Rangappa, K. S., and **Lokanath, N. K.** Structure-Property Relationship in Thioxotriaza-spiro Derivative: Crystal structure and Molecular Docking Analysis against SARS-CoV-2 Main Protease. *J. Mol. Struct.*, 131746.
21. Zeghouan, O., Mahesha, Sellami, S., Kashi, I., Bouchameni, C., and **Lokanath, N. K.** Analysis of structural conformation and supramolecular self-assembly of novel oxalate-bridged tetranuclear Cu (II) complex by combined crystallographic and computational studies. *J. Mol. Struct.*, 131658.
22. Majid, A., Lakshmikanth, M., **Lokanath, N. K.**, and Priyadarshini, C. P. Generation, characterization and molecular binding mechanism of novel dipeptidyl peptidase-4 inhibitory peptides from sorghum bicolor seed protein. *Food Chemistry*, 369, 130888.
23. Nanjundaswamy, S., Hema, M. K., Karthik, C. S., Rajabathar, J. R., Arokiyaraj, S., **Lokanath, N. K.**, and Mallu, P. Synthesis, crystal structure, in-silico ADMET, molecular docking and dynamics simulation studies of thiophene-chalcone analogues. *J. Mol. Struct.*, 1247, 131365.

2021

24. Alkanad K., Hezam, A., Drmosh Q. A., Sujay Shekar G. C., AlObaid A. A., Warad I., and **Lokanath N. K.** Construction of Bi₂S₃/TiO₂/MoS₂ S-Scheme Heterostructure with a Switchable Charge Migration Pathway for Selective CO₂ Reduction. *Solar RRL*, 2100501.
25. Mahesh, Pampa K. J., Karthik C. S., Hema M. K., Mallu, P. and **Lokanath N. K.**, Post-synthetic modification of supramolecular assemblies of β -diketonato Cu (II) complexes: comparing and contrasting the molecular topology by crystal structure and quantum computational studies. *Cryst. Eng. Comm.* 24, 4344-4369.
26. Sujay Shekar G. C., Khaled Alkanad, Abdo Hezam, Ali Alsalmeh, Nabil Al-Zaqri, and **Lokanath, N. K.**, Enhanced photo-Fenton activity over a sunlight-driven ignition synthesized α -Fe₂O₃-Fe₃O₄/CeO₂ heterojunction catalyst enriched with oxygen vacancies. *J. Mol. Liq.* 335, 116186.
27. Khaled A., Abdo Hezam, Sujay Shekar G. C., Q. A. Drmosh, Murad QA AL-Gunaid, and **Lokanath, N. K.**, Magnetic recyclable α -Fe₂O₃-Fe₃O₄/Co₃O₄-CoO nanocomposite with a dual Z-scheme charge transfer pathway for quick photo-Fenton degradation of organic pollutants. *Catal. Sci. Technol.* 11, 3084-3097.
28. Kumara, K., Prabhudeva, M. G., Vagish, C. B., Vivek, H. K., Rai, K. M. L., **Lokanath, N. K.**, and Kumar, K. A. Design, synthesis, characterization, and antioxidant activity studies of novel thienyl-pyrazoles. *Heliyon*, 07592.
29. Udaya Kumar, A. H., Kumara, K., Harohally, N. V., Pampa, K. J., and **Lokanath, N. K.** Square Planar trans-N₂O₂ Cu (II) Complex: Synthesis, Crystal Structure, Hirshfeld Surface, DFT, Antimicrobial and Docking Studies. *Chem. Select*, 6(24), 6240-6255.
30. Hema, M. K., Karthik, C. S., Pampa, K. J., Mallu, P., & **Lokanath, N. K.**, 4, 4, 4-trifluoro-1-phenylbutane-1, 3-dione metal [Cu (II) and Ni (II)] complexes as an superlative antibacterial

- agent against MRSA: Synthesis, structural quantum-chemical and molecular docking studies. *J. Mol. Struct.*, 130774.
31. Naresh, P., Pramodh, B., Naveen, S., Ganguly, S., Panda, J., Sunitha, K., Maniukiewicz, W. and **Lokanath, N. K.**, *Cis* and *trans* isomers of 1-(5-bromothiophen-2-yl)-3-(10-chloroanthracen-9-yl) prop-2-en-1-one: Synthesis and characterization. *J. Mol. Struct.*, 1236, 130228.
 32. Kumar, A.D., Vivek, H.K., Srinivasan, B., Naveen, S., Kumara, K., **Lokanath, N. K.**, Byrappa, K. and Kumar, K.A., Design, synthesis, characterization, crystal structure, Hirshfeld surface analysis, DFT calculations, anticancer, angiogenic properties of new pyrazole carboxamide derivatives. *J. Mol. Struct.*, 1235, 130271.
 33. Arunagiri, C., Selvakumar, S., Kumar, M.S. and **Lokanath, N. K.**, Crystal structure, spectroscopic, quantum chemical and Hirshfeld surface analysis of [2-(3,4-Dimethoxy-phenyl)-ethyl]-(4-nitro-benzylidene)-amine: A combined experimental and theoretical study. *Chem. Data Collect.*, 33, 100679.
 34. Vagish, C. B., Kumara, K., Vivek, H. K., Bharath, S., **Lokanath, N. K.** and Kumar, K.A., Coumarin-triazole hybrids: Design, microwave-assisted synthesis, crystal and molecular structure, theoretical and computational studies and screening for their anticancer potentials against PC-3 and DU-145. *J. Mol. Struct.*, 1230, 129899.
 35. Pramodh, B., Prathap, K. C., Hema, M. K., Warad, I. and **Lokanath, N. K.**, Synthesis, structure, quantum computational and biological studies of novel thiophene derivatives. *J. Mol. Struct.*, 1229, 129587.
 36. Shruthi, C., Ravindrachary, V., Guruswamy, B., Prasad, D.J., Goveas, J., Kumara, K. and **Lokanath, N. K.**, Molecular structure, Hirshfeld surface and density functional theoretical analysis of a NLO active chalcone derivative single crystal A quantum chemical approach. *J. Mol. Struct.*, 1228, 129739.
 37. Thamocharan, S., Kumari, S.P., Ganesan, S. S., Kumar, S.M., Percino, M.J. and **Lokanath, N. K.**, 2021. Structural and energetics of weak non-covalent interactions in two chemically distinct classes of O/N-heterocycles: X-ray and theoretical exploration. *J. Mol. Struct.*, 1227, 129694.
 38. Madan, N., Sunil, K., Yamuna, I. K., Kumara, K. and Lokanath, **N. K.**, Synthesis, Characterization, Crystal Structure and Hirshfeld Surface Studies of Schiff Base Derivatives. *Eurasian J. Anal. Chem.*, 16(1), 11-23.
 39. Gurumallappa, Arun Renganathan, R. R., Hema, M. K., Karthik, C. S., Rani, S., Nethaji, M., Jayanth, H. S., Mallu, P., **Lokanath, N. K.** and Ravishankar Rai, V., 4-acetamido-3-nitrobenzoic acid-structural, quantum chemical studies, ADMET and molecular docking studies of SARS-CoV2. *J. Biomol. Struct. Dyn.*, 1-15.
 40. Pramodh, B., Naresh, P., Naveen, S., **Lokanath, N. K.**, Ganguly, S., Panda, J., Murugesan, S., Raghu, A.V. and Warad, I., Synthesis, spectral characterization, crystal structure and theoretical

investigation of (E)-3-(4-bromothiophen-2-yl)-1-(5-bromothiophen-2-yl) prop-2-en-1-one. *Chem. Data Collect.*, 31, 100587.

41. Naveen, S., Kumara, K., Kumar, A. D., Kumar, K. A., Zarrouk, A., Warad, I. and **Lokanath, N. K.**, Synthesis, characterization, crystal structure, Hirshfeld surface analysis, antioxidant properties and DFT calculations of a novel pyrazole derivative: Ethyl 1-(2, 4-dimethylphenyl)-3-methyl-5-phenyl-1H-pyrazole-4-carboxylate. *J. Mol. Struct.*, 1226, 129350.
42. Vagish, C. B., Kumar, A. D., Kumara, K., Vivek, H. K., Renuka, N., **Lokanath, N. K.** and Kumar, K. A., Environmentally benign synthesis of substituted pyrazoles as potent antioxidant agents, characterization and docking studies. *J. Iran. Chem. Soc.* 18(2), 479-493.
43. Mahesha, Raveesha, T. C., Hema, M. K., Pampa, K. J., Chandrashekhara, P. G., Mantelingu, K., Demappa, T. and **Lokanath, N. K.**, Analysis of supramolecular self-assembly of two chromene derivatives: Synthesis, crystal structure, Hirshfeld surface, quantum computational and molecular docking studies. *J. Mol. Struct.*, 1225, 129104.
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