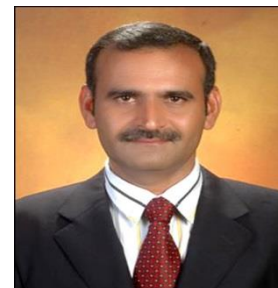


## Curriculum Vitae



**Prof. N. K. Lokanath**

**Director**

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**Professor**

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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.

### 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 **384** 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.

- Edge cutting laboratory has been developed for collaborative research

### Contribution to CCDC and RCSB Protein Data Bank (PDB)

- 1000 crystal structure data was deposited to CCDC and 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<sup>+</sup>-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<sup>+</sup>-ATPase had been widely published in much Japanese newspaper 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.

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## Seminars/Conferences Organised

- **Convenor**, International conference on nano materials and their application, University of Mysore, 1-2 March, 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.

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## 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.

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## 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. **Chetan 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.

## ➤ Present 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. **Chetan 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. **Niranjar S. N.** “Structural Investigation of Some Thiophene derivatives of Medicinal Interest”
8. **Vindya M. P.** “Structural Investigation of Some Pyroazole derivatives of Medicinal Interest”

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## Visits Abroad and 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-June 2 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 "Current Trends in Drug Discovery and Research"*, CDRI, Lucknow, India.
- 23-31 Aug 2005 *XX Congress of the International Union of Crystallography (IUCr)*, Firenze, Italy.
- 14-18 Apr 2004 *The First Pacific-Rim International Conference on Protein Science*, Pacifico Yokohama, Japan.

- 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 *9<sup>th</sup> International Conference on Biology and Synchrotron Radiation, Manchester, England.*
- 7-10 Sept 2009 *Participated in the Young Indian Scientists Colloquium, TIFR, Mumbai, India.*
- 8-11 Jan 2013 *International conference on Biomolecular forms and Functions, IISc, Bangalore.*
- 15-17 Mar 2012 *ICABS-2012, Kannur university, Kannur , Kerala, India.*
- 26-28 Nov 2011 *40<sup>th</sup> National Seminar on Crystallography, Osmania University, Hyderabad.*
- 16-17 Feb 2011 *International Symposium on Challenges in Drug Discovery, KSOU, Mysore.*
- 18-21 Jan 2010 *The Eighth Asia-Pacific Bioinformatics conference, IISc, Bangalore.*
- 4-7 Dec 2016 *14<sup>th</sup> Conference of the Asian Crystallographic Association, Hanoi-Vietnam.*
- 10-13 June 2016 *44<sup>th</sup> National Seminar on Crystallography, Pune, India.*
- 21-28 Aug 2017 *24<sup>th</sup> Congress of the International Union of Crstallography (IUCr), Hydrabad.*

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## Membership in Academic Bodies

1. Member, BOS in Physics, DoS in Physics, University of Mysore, 2007-
2. Member, BOE in Physics, DoS in Physics, University of Mysore, 2016-17
3. Member, BOS in PG-Physics, Mangalore University, mangalaganotrthri, Mangalore, 2015-18
4. BOS in Physics (PG), Govt. (Autonomous) College, Mandya, 2015-17
5. Member, BOS in Physics for UG, JSS College for Women (Autonomous), Mysuru, 2015-17.
6. AC Member, JSS College of Arts, Science and Commerce, Mysuru, 2015-17
7. AC Member, NIE Science College, Mysuru, 2015-17
8. AC Member, AVK College, Hassan, 2015-17
9. Member, BOS in Microbiology, Manasagangotri, Mysuru, 2007-10, 2014-17
10. Member, BOS in Physics, 2007-10, 2014-17
11. Member, BOS in PG-Physics Kuvempu University Shankaraghatta, 2014-17
12. Member, BOS in Physics, KSOU, 2014-17
13. Member, BOS in Material Sciences, Vignana Bhavan, Univeristy of Mysore, 2014-17
14. Member, BOE in Physics, Government College Mandya (Autonomous) 2013-14, 2014-15, 2015-16
15. Member, BOA in Physics, Kuvempu University Shankaraghatta, Shimoga, 2015-16

16. Member, Post-Graduate Sports Council, University of Mysore, 2015-16
17. G C Member N.I.E. First Grade College, Mysuru, 2015-16
18. BOE Chairman, Janapada Vishwavidyalaya for Traditional Science and Technology, 2014-15
19. Member PG Admission Committee, DoS in Physics, Manasagangotri, Mysuru, 2014-15, 2015-16
20. Member, BOS in Physics, Yuvaraja College of Mysore, Mysuru, 2014-15, 2016-18(UG)
21. Chairman, BOE in Physics, Material Sciences, Vignana Bhavan, University of Mysore, 2014-15
22. Member, K-SET Steering Committee, University of Mysore, 2015
23. Member, Governing Council, Sri Adichunchanagiri First Grade College, Channarayapatna, 2014-16
24. Chairman, BOE in Physics, DoS in Physics, 2013-14
25. BOE in Physics, Tumakur University, 2021
26. BOE in Physics, Magalore University, 2021
27. Member, Interdisciplanery Board for Guide Recognition under the Faculty of Science and Technology.

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### **Membership in Advisory Committee**

1. Member, Technical review committee 103<sup>rd</sup> 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

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### **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. Mahesh, Pampa, K. J., Karthik, C. S., Hema, M. K., Mallu, P. and **Lokanath, N. K.**, Post-synthetic modification of supramolecular assemblies of  $\beta$ -diketonato Cu (II) complexes: comparing and contrasting the molecular topology by crystal structure and quantum computational studies. *Cryst. Eng. Comm.* 24, 4344-4369.
2. 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  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-Fe<sub>3</sub>O<sub>4</sub>/CeO<sub>2</sub> heterojunction catalyst enriched with oxygen vacancies. *J. Mol. Liq.* 335, 116186.
3. Alkanad, Khaled, Abdo Hezam, GC Sujay Shekar, Q. A. Drmosh, Murad QA AL-Gunaid, and **Lokanath, N. K.**, Magnetic recyclable  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>-Fe<sub>3</sub>O<sub>4</sub>/Co<sub>3</sub>O<sub>4</sub>-CoO nanocomposite with a dual Z-scheme charge transfer pathway for quick photo-Fenton degradation of organic pollutants. *Catal. Sci. Technol.* 11, 3084-3097.
4. 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.
5. Udaya Kumar, A. H., Kumara, K., Harohally, N. V., Pampa, K. J., and **Lokanath, N. K.** Square Planar trans-N<sub>2</sub>O<sub>2</sub> Cu (II) Complex: Synthesis, Crystal Structure, Hirshfeld Surface, DFT, Antimicrobial and Docking Studies. *Chem. Select*, 6(24), 6240-6255.
6. 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 a superlative antibacterial agent against MRSA: Synthesis, structural quantum-chemical and molecular docking studies. *J. Mol. Struct.*, 130774.
7. 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.
8. 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.
9. 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.

10. 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.
11. 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.
12. 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.
13. Thamotharan, 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.
14. 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.
15. 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.
16. 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.
17. 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.
18. 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.
19. Mahesha, Raveesha, T. C., Hema, M. K., Pampa, K. J., Chandrashekara, 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.



20. Kuthyala, S., Sheikh, S., Nagaraja, G. K., Kannika, B. R., Madan Kumar, S., Chandra Nayak, S. and **Lokanath, N. K.**, Towards the synthesis of imidazopyridine derivatives: characterization, single crystal XRD, Hirshfeld analysis, and biological evaluation. *Chem. Select.*, 6(4), 843-851.
21. Iqbal, S., Potharaju, R., Naveen, S., **Lokanath, N. K.**, Mohanakrishnan, A. K. and Gunasekaran, K., Design, crystal structure determination, molecular dynamic simulation and MMGBSA calculations of novel p38-alpha MAPK inhibitors for combating Alzheimer's disease. *Journal of Biomolecular Structure and Dynamics*, 1-14.
22. Mahesha, Raveesha, T. C., Hema, M. K., Pampa, K. J., Chandrashekara, 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.
23. Karthik, C. S., Kumara, K., Naveen, S., Mallesha, L., Mallu, P., Urs, M. D. and **Lokanath, N. K.**, Thermal, optical, etching, structural studies and theoretical calculations of [1-(2, 5-Dichloro-benzenesulfonyl)-piperidin-4-yl]-(2,4-difluoro-phenyl)-methanone oxime. *J. Mol. Struct.*, 1224, 129077.
24. Kotian, A., Kamat, V., Naik, K., Kokare, D. G., Kumara, K., **Lokanath, N. K.** and Revankar, V.K., 2021. Hydroxyacetone derived N4-methyl substituted thiosemicarbazone: Syntheses, crystal structures and spectroscopic characterization of later first-row transition metal complexes. *J. Mol. Struct.*, 1224, 129055.

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25. Al-Zaqri, N., Suleiman, M., Al-Ali, A., Alkanad, K., Kumara, K., **Lokanath, N. K.**, Zarrouk, A., Alsalmeh, A., Alharthi, F.A., Al-Taleb, A. and Alsyahi, A., Exo double left right arrow Endo Isomerism, MEP/DFT, XRD/HSA-Interactions of 2, 5-Dimethoxybenzaldehyde: Thermal, 1BNA-Docking, Optical, and TD-DFT Studies. *Molecules*, 25(24).
26. Manjunatha, N. K., Gayathri, B. H., **Lokanath, N. K.**, Swamy, M. T., Nayaka, S. C., Siddaraju, B. P., Ragini, N., Mohammed, A. G., Kannika, B. R. and Kumar, S. M., A solid-state analysis of metformin picrate salt. *Chem.Data Collect.*, 30, 100577.
27. Jyothi, K. L. and **Lokanath, N. K.**, Understanding the formation of novel hydrated gallic acid-creatinine molecular salt: crystal structure, Hirshfeld surface and DFT studies. *J. Chem. Crystallogr.*, 50(4), 410-421.
28. Kumar, S. M., Kumar, V., Al-Ghorbani, M., Holla, B. S., Poojary, B., Praveen, P., Nayak, S. C., Mohan, J. S., Thamotharan, S., Shamprasad, V. R. and **Lokanath, N. K.**, Theoretical and experimental solid-state studies of Ethyl 1-benzyl-2-(thiophen-3-yl)-1H-benzo [d] imidazole-5-carboxylate. *Z. Kristallogr. Cryst. Mater.*, 235(11), 569-579.
29. Hema, M. K., ArunRenganathan, R. R., Nanjundaswamy, S., Karthik, C. S., Mohammed, Y. H. I., Alghamdi, S., **Lokanath, N. K.**, Rai, V.R., Nagashree, S. and Mallu, P., N-(4-

- bromobenzylidene)-2, 3-dihydrobenzo [b][1, 4] dioxin-6-amine: Synthesis, crystal structure, docking and in-vitro inhibition of PLA2. *J. Mol. Struct.*, 1218, 128441.
30. Hema, M. K., Karthik, C. S., **Lokanath, N. K.**, Mallu, P., Zarrouk, A., Salih, K.S. and Warad, I., Synthesis of novel Cubane  $[\text{Ni}_4(\text{ONO})_4(\text{OCH}_3)_4(\text{OOH})_4]$  cluster: XRD/HSA-interactions, spectral, DNA-binding, docking and subsequent thermolysis to NiO nanocrystals. *J. Mol. Liq.*, 315, 113756.
  31. Prakash, M. S., Smitha, G., Somanatha, T. M., Suchetan, P. A., Swamy, G. K., Naveen, S. and **Lokanath, N. K.**, Novel tandem Knoevenagel-Michael condensation product of naphtho [2, 1-b] furan-2-carbaldehyde with dimedone: Synthesis, spectroscopic and crystal structure studies. *Chem. Data Collect.*, 28, 100458.
  32. Razak, N. S. A., Jamalis, J., Urs, M. D., Gowda, N. L., Reddy, K. R., **Lokanath, N. K.** and Naveen, S., Synthesis, characterization, crystal structure and theoretical simulation of novel ethyl 2-(7-hydroxy-4-methyl-2-oxo-2H-chromen-3-yl) acetate. *Chem. Data Collect.*, 28, 100425.
  33. Shaikh, N. A., Rathod, S. N., Bhat, S. S., Naveen, S., Shaikh, S., Revankar, V. and **Lokanath, N. K.**, Synthesis, Structural Characterization and Hirshfeld Surface Analysis of Mixed Ligand Copper (II) Complex. *Chem. Data Collect.*, 28, 00374.
  34. Kumar, C. P., Mohana, K. N., Raghu, M. S., Jagadeesha, M. B., Prashanth, M. K. and **Lokanath, N. K.**, Fluorine substituted thiomethyl pyrimidine derivatives as efficient inhibitors for mild steel corrosion in hydrochloric acid solution: Thermodynamic, electrochemical and DFT studies. *J. Mol. Liq.*, 311, 113311.
  35. Hema, M. K., Warad, I., Karthik, C. S., Zarrouk, A., Kumara, K., Pampa, K. J., Mallu, P. and **Lokanath, N. K.**, XRD/DFT/HSA-interactions in Cu (II) Cl/phen/ $\beta$ -diketonato complex: Physicochemical, solvatochromism, thermal and DNA-binding analysis. *J. Mol. Struct.*, 1210, 128000.
  36. Manjunatha, N., Kumar, S. M., Swamy, M., Siddaraju, B. and **Lokanath, N. K.**, Solid state and Computational studies of Ambroxol hydrochloride drug. *Chem. Data Collect.*, 27, 100377.
  37. Parol, V., Prabhu, A. N., Taher, M. A., Naraharisetty, S. R. G., **Lokanath, N. K.** and Upadhyaya, V., A third-order nonlinear optical single crystal of 3, 4-dimethoxy-substituted chalcone derivative with high laser damage threshold value: a potential material for optical power limiting. *J. Mater. Sci. Mater. Electron.*, 31(12), 9133-9150.
  38. Jyothi, K. L., Kumara, K., Hema, M. K., Gautam, R., Row, T. G. and **Lokanath, N. K.**, Structural elucidation, theoretical insights and thermal properties of three novel multicomponent molecular forms of gallic acid with hydroxypyridines. *J. Mol. Struct.*, 1207, 127828.
  39. Parol, V., Upadhyaya, V., Prabhu, A. N., **Lokanath, N. K.**, Taher, M. A. and Naraharisetty, S. R. G., A long-chain based bromo and methyl substituted chalcone derivatives; experimental and theoretical approach on nonlinear optical single crystals. *Mater. Res. Express*, 7(5), 055101.

40. Kumar, S. M., Hemraju, B. C., Anil, S. M., Manjunatha, N. K., Swamy, M. T., **Lokanath, N. K.**, Al-Ghorbani, M., Al-Zaqri, N. and Alsalmeh, A., Crystal structure, Hirshfeld surfaces, topology, energy frameworks and dielectric studies of 1-(2-chlorophenyl)-3, 3-bis (methylthio) prop-2-en-1-one. *Z. Kristallogr. Cryst. Mater.*, 235(3), 85-93.
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