DEPARTMENT OF CHEMISTRY, RESEARCH GRANTS

Individual Research Grants received from different agencies:

S.No	Title of the Project and Sanction Letter No	Funding Agency	Sanctioned Amount (in Lakhs)	Duration of the Project	Supervisor/Principal investigator/Co-investigator	No. of Research Fellows/Man power	Objectives	Out comes
1	Computational Analysis of Mutational Effects on HIV-1 Antiretroviral Therapy and Target Oriented Synthesis of Potential Lead molecules	SERB	4200000	4 Years 2019-2023	Principal Investigators Prof M Vijjullatha	2	A Comprehensive study on the sensitivity/resistance profile and failure of antiretroviral therapy (ART) due to regular mutations causing drug resistance will be computationally analyzed. High level reduced susceptibility for ATV with mutations on PI like I50L, I84V, and N88S; for LPV are I47A, V82 A/F/T/S and I84V. Reduced susceptibility for ATV being G48V/M, L90M; for	The docking results for the newly designed molecules provide additional hydrogen bond interactions with residues Val 27, Val 59 and Gly 60 along with His 62, Phe 32. The higher binding affinities of designed molecules N1, N2, N9 and N10 may be attributed to the additional hydrophobic interaction. 3D-QSAR studies, PHASE pharmacophore points, CoMFA and CoMSIA, field distribution are in good conformity with the structural

							DRV V32I, I50V, I54L/M, L76V and I84V; for LPV V32I, I50V, I54V/T/A/L/M, L76V and I84V will be checked by Computer Aided Drug Design (CADD) techniques. Analysis of all mutational effects of HIV-1 RT on the FDA approved drugs will be carried out. Major NRTI resistance observed for 3TC and FTC for mutation at M184V/I in the region of non-thymidine analog mutations (TAMs); K65R being TDF and ABC; L74V/I for ABC and Y115F for ABC. High level reduced susceptibility observed in NNRTI resistance mutations L100I for EFV, ETR and RPV; K101E/P for NVP, EFV, ETR and RPV; K103N/S for NVP/EFV;	requirements of the active site of capsid assembly inhibitors that allows conception of a plausible template for designing novel potent inhibitors. Therefore, the CoMFA and CoMSIA model together with the application of valuable clues from pharmacophore variants are expected to be fast and convenient tools to design new potential inhibitors against HIV-1 capsid assembly. The comprehensive study on the sensitivity/resistance profiles of HIV-1 mutations has assisted in understanding how the mutations are reducing the drug affinity towards the proteins. The effects of each HIV protease mutation on the binding affinity of PIs were studied by

							V106A/M for NVP, EFV; Y181C/I/V for NVP, ETR, RPV; Y188L/C/H for NVP; Y188L/C for EFV; Y188L for RPV; G190A/S/E/Q for NVP, EVP and M230L for NVP, EFV/RPV will be analyzed for the effect of mutations on approved drugs based on protein-ligand interactions. The target-oriented synthesis of new lead molecules that have shown better interactions with HIV-1 PR and Hybrid Pyrimidine analogs that were designed based on the essential characteristic features that could possibly act on all three targets such as HIV-1 PR, RT and HIV-1 CA proteins will be synthesized.	performing *insilico* analysis using docking technique. The correlation between the computational & experimental data reveals that the computational protocol followed in this study might be valuable to predict drug resistivity profile associated with amino acid mutations. Based on the overall docking studies, mutants showed high sensitivity to saquinavir and indinavir and high resistivity to fosamprenavir and tipranavir among 8 FDA approved drugs. These results suggest the usage of these particular drugs towards mutants providing a personalized treatment. This study helps the physician to prescribe selective drug strategy for the patients who are infected with HIV

								containing mutated HIV protease. Among the 25 synthesized compounds except the compounds 2I, 2V and 2Y all compounds exhibit less concentration i.e., better activity than the Standard AZT (Zidovudine), hence *insilico* design and synthesis paved the way for optimization of nearly potent molecules toward HIV-1.

1. Title of the project proposal: **Layered Perovskites and Hollandites as visible light driven photocatalysts for degradation of**

organic pollutants and water splitting

2. Funding Agency: **CSIR, New Delhi**

3. Sanctioned amount (in Lakhs): **Rs.45.82**

4. Duration of the Project: **3 years and 3 months**

5. Principal Investigator: **Dr. M. Vithal, Department of Chemistry, O.U., Hyderabad – 500 007**

Co-Iinvestigator(s) (i). Dr. G. Prasad, Department of Physics, O. U., Hyderabad – 500 007
(ii). Dr. N.R. Munirathnam, Scientist F, Center for Materials for Electronics and Technology (CMET), Hyderabad-500 051

6. Number research fellows/man power: **One**

7. Objectives/Questions to be answered:

The objectives of the project are

(i) To synthesize layered perovskites and hollandites with (a) homogeneous size distribution and optimum particle size for catalytic applications and (b) high chemical stability and tunable bandgap energy

(ii) To synthesize cation/anion doped perovskites and hollandites to enhance the visible light photocatalytic activity and water splitting efficiency.

(iii). To study the photodegradation of dye pollutants

8. Outcomes

(a). One student got training in dye degradation and water splitting studies.

(b). Publications:

1. Hydrothermal synthesis of C-doped $K_2Al_2Ti_6O_{16}$ as a visible light–activated photocatalyst in the degradation of organic dyes

Gundeboina Ravi, P. Venkataswamy, **M. Vithal**

Journal of Australian Ceramic Society, 56 (2020), 1351-1358 **Impact Factor: 1.741**

2. Enhancement of photocatalytic activity of sodium bismuth titanate by doping with copper, silver and tin ions

Sreenu K, P. Venkataswamy, G. Ravi, CH. Sudhakar Reddy, B. Jaganmohan Reddy, and **M. Vithal**

ZeitschriftfüranorganischeundallgemeineChemie, 2019, 645, 529–536

Impact Factor: 1.414

3.Ion exchange synthesis of Ag^+ incorporated $LiAlO_2$ and its application in photodegradation of organic dyes.

Gundeboina Ravi and **M. Vithal** SN Applied Sciences, 2019, 1, 164

Impact Factor: 2.8

4. Layered $Na_2W_4O_{13}$ and its Cation/anion doped analogues for the treatment of polluted water. Gundeboina Ravi, Srinivas Mamidi, Sreenu K, Pandiri Manjula, Kammara Vaishnavi, **M**.**Vithal,** Flat Chem., 2019, 13, 1–7

Impact Factor: 5.829

5. Synthesis, characterization, luminescence and photocatalytic studies of layered perovskites $NaMMgWO_6$ (M = La, Pr, Sm). Sreenu K, Gundeboina Ravi, CH Sudhakar Reddy, Ravinder Guje &**M. Vithal**. Indian Journal of Chemistry, 2018,57A, 435

Impact Factor -0.412

6. Aurivillius family of layered perovskites, $BiREWO_6$ (RE = La, Pr, Gd and Dy): Synthesis, characterization and photocatalytic studies. Srinivas Mamidi, Gundeboina Ravi, Sreenu K, RadhaVelchuri and **M. Vithal**ComptesRendus Chimie, 2018, 21, 547-552

Impact Factor: 3.117

List of publications (2016-2023)
2023:

66. *Electrocatalytic Hydrogen Evolution by a Uranium(VI) Polyoxometalate: an Environmental Toxin for Sustainable Energy Generation*
M. Sateesh, S. Asha, A. Ravi, P. Saha, A. Vinod Kumar, B. Sathyanarayana, **Muga Vithal**, and S. K. Das. Inorg. Chem. 2023, 62, 19664−19676. https://doi.org/10.1021/acs.inorgchem.3c03018. **Impact Factor: 4.6**

65. *Synthesis, characterization and photocatalytic studies of visible light responsive $K_3MTe_3O_{12}$ (M = Cr, Fe and Ga)*
Gaddameedi Hima Bindu, Kadari Ramaswamy, Puppala Veerasomaiah, **Muga Vithal**
Chemical papers 77 (2023) 7603-7614. **Impact Factor: 2.2**

64. *Synthesis, characterization and photocatalytic studies of Ag^+, Cu^{2+} and Sn^{2+} doped layered $Li_2Cd(PO_3)_4$*
Pallati Srilekha, Kammara Vaishnavi, Gaddameedi Hima Bindu, AmarapuriTrinadh&**M. Vithal,** Inorganic and Nano-Metal Chemistry, 53 (2023)
DOI: 10.1080/24701556.2023.2213226
Impact Factor: 1.7

63. *Photocatalytic degradation studies of carbon and sulfur-doped K2Ta2O6*
Rani Angineni, Perala Venkataswamy, Naveen Kumar Veldurthi, Kadari Ramaswamy,Mannepalli Sudheera, and **Muga Vithal**, J Mater Sci: Mater Electron (2023) 34:633. https://doi.org/10.1007/s10854-023-09973-9
Impact Factor: 2.801

62. *Fabrication of Ag/AgBr/LaAl0.5Cr0.5O3 composite with enhanced photocatalytic performance for the degradation of methylene blue and 4-chlorophenol*
Gaddameedi Hima Bindu, Kadari Ramaswamy, AmarapuriTrinadh, Puppala Veerasomaiah, and **Muga Vithal,** J. Australian Ceramic society, 2023 https://doi.org/10.1007/s41779-023-00842-6 **I**
mpact Factor: 1.9

61. *Synthesis and photoluminescence studies of Na323xLnxSbO (PO4)2 (Ln = Eu, Sm and Tb, and $0 \leq x \leq 0.1$ mol%) phosphors for white light emitting diodes*
AmarapuriTrinadh, Koneti Srikanth, Kunja Laxminarayana, Pallati Srilekha, **Muga Vithal**, and Mudavat Srinivas, J Mater Sci: Mater Electron (2023) 34:83

https://doi.org/10.1007/s10854-022-09463-4
Impact Factor: 2.801

2022

60.*Preparation, characterization and photocatalytic studies of $LaAl_{0.5}Fe_{0.5}O_3$, $LaAl_{0.5}Cr_{0.5}O_3$ and $LaCr_{0.5}Fe_{0.5}O_3$.*
Gaddameedi Hima Bindu, Vaishnavi Kammara, Pallati Srilekha, K.Swetha, Y. KalyanaLaxmi, P.Veerasomaiah and **Muga Vithal**, J. Mol. Structure, 2022, 134220
https://doi.org/10.1016/j.molstruc.2022.134220.
Impact Factor: 3.801

59. *A Novel Approach for Generation of Oxygen Vacancies in Trirutile MnSb2O6 and Their Impact on Photocatalytic Degradation of MO Dye*
Manasa Sunku, Perala Venkataswamy, Gaddameedi Hima Bindu, Pallati Srilekha, M. Srinivas, and **M. Vithal,** European J of Inorganic chemistry, 2022, e202200550
https://doi.org/10.1002/ejic.202200550
Impact Factor: 2.3

58. *Effect of Ag^{+}, Cu^{2+} and Sn^{2+} Doping on Structural, Optical and Photocatalytic Properties of $KGe_{0.5}Te_{1.5}O_6$ with Defect Pyrochlore Structure*
Gaddameedi Hima Bindu, Manasa Sunku, Kadari Ramaswamy, Pallati Srilekha, Puppala Veerasomaiah and **Muga Vithal**, Chemistry Select, 7 (2022) e202202780, https://doi.org/10.1002/slct.202202780.
Impact Factor: 2.307

57.*Emission (Gd^{3+} and Sm^{3+}) and ESR (Gd^{3+}) studies of $La_{1-x}Ln_xB_3O_6$ ($Ln = Gd, Sm; 0 \le x \le 0.2$ for Gd; $0 \le x \le 0.1$ for Sm) phosphors*
Kunja Laxminarayana, Koneti Srikanth, AmarapuriTrinadh, Pallati Srilekha, Muga Vithal, Mudavat Srinivas
J. Mater. Sci.: Mater. Electron. (2022). https://doi.org/10.1007/s10854-022-08786-6
Impact factor: 2.779

56.*Preparation, Characterization and Photocatalytic Activity studies of Ag^{+}, Cu^{2+} and Sn^{2+}-doped Li_2GeTeO_6 under Visible Light Irradiation*
Vaishnavi Kammara, Perala Venkataswamy, Manasa Sunku, Kadari Ramaswamy, Gaddameedi Hima Bindu, Sudhakar Reddy Chandiri, **M. Vithal**

Adv. Mater. Lett. 13 (2022) 031703.
Impact factor: NA

55. *Preparation, characterization and photocatalytic studies of parent and ion-doped Li_2TiTeO_6*
Kammara Vaishnavi, Perala Venkataswamy, Kadari Ramaswamy, Pallati Srilekha, **Muga Vithal**
Materials Science in Semiconductor Processing 148 (2022) 106805
https://doi.org/10.1016/j.mssp.2022.106805.
Impact factor 4.644

54. *Preparation, characterization and visible light photocatalytic studies of $Ag/AgBr/Li_2ZrO_3$ composite*.
Vaishnavi Kammara, Perala Venkataswamy, G.Ravi, K. Ramaswamy, Manasa Sunku, **M. Vithal**
Inorganic Chemistry Communications 141 (2022) 109504, https://doi.org/10.1016/j.inoche.2022.109504
Impact Factor: 3.428

53. *Facile ion-exchange synthesis of Gd-doped $K_2Ta_2O_6$ photocatalysts with enhanced visible light activity.*
Rani Angineni, Venkataswamy Perala, Ramaswamy Kadari, Srilekha Pallati, Sreenu Kurra, **M. Vithal .**Journal of the Indian Chemical Society 99 (2022) 100495
Impact Factor: 0.243

52. *Preparation, characterization and photocatalytic activity studies of transition metal ion doped $K_2Ta_2O_6$.*
Rani Angineni, Perala Venkataswamy, Kadari Ramaswamy, Shiv Raj, Naveen Kumar Veldurthi, **M. Vithal** . Polyhedron 214 (2022) 115620
Impact Factor (IF) – 2.975https://doi.org/10.1016/j.poly.2021.115620

51. *$Ag_2VO_2PO_4$ Nanorods: Synthesis, Characterization, Photoactivity & Antibacterial activity.*
Vaishnavi Kammara, Perala Venkataswamy, Rani Angineni, G. Hima Bindu, Suresh Velpula, Karuna Rupula, **M. Vithal**
Zeitschrift für anorganische und allgemeineChemie 648 (2022) e202100264
https://doi.org/10.1002/zaac.202100264
Impact Factor: 1.414

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50. *Preparation, Characterization and Photocatalytic activity studies of C- and N-doped $CoSb_2O_6$.*

Manasa Sunku, Ravi Gundeboina, CH. Shilpa Chakra, Vimala Kaniki Reddy, **M. Vithal**
Inorganic Chemistry Communications 134 (2021) 109064
Impact Factor: 3.428
https://doi.org/10.1016/j.inoche.2021.109064

49. *Optical characteristics of europium and terbium doped strontium orthogermanate phosphors.*
Koneti Srikanth, LavudiNarsihma, Kunja Laxminarayana, **M. Vithal**, Mudavat Srinivas
Journal of Indian Chemical Society 98 (2021) 100237
Impact Factor: 0.243

48. *Photocatalytic degradation of methylene blue over N-doped $MnWO_4$ under visible light irradiation.* K. Sravan Kumar, Kammara Vaishnavi, Perala Venkataswamy, Gundeboina Ravi, Kadari Ramaswamy, **M. Vithal,** J. Ind. Chem. Soc. 98 (2021) 100140 **Impact Factor: 0.243**

47. *Facile Ion Exchange Synthesis of Ag, Cu, and Sn Incorporated Defect Pyrochlore $K_2Ta_2O_6$ towards Visible-Light-Responsive Photocatalytic Activity.*
Rani Angineni, Jyothsna Angineni, Naveen Kumar Veldurthi, Perala Venkataswamy, **M. Vithal**
Chemistry Select 6 (2021) 8306-8314
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46. *Transition metal ion (Ni^{2+}, Cu^{2+} and Zn^{2+}) doped defect pyrochlore, $KTaTeO_6$: Synthesis, characterization and photocatalytic studies*
M. Sudheera, P. Venkataswamy, K. Ramaswamy, G. Ravi, N. Chittibabu, **M. Vithal**
Indian Journal of Chemistry -Section A (IJC-A), (2021),
Impact Factor: 0.412
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45. *Synthesis of Nitrogen-doped $KTaTeO_6$ with Enhanced Visible Light Photocatalytic Degradation of Methylene Blue*
M. Sudheera, P. Venkataswamy, G. Ravi, K. Ramaswamy, N. Chitti Babu, **M. Vithal**
Advanced Materials Letters 12 (2020) 21041621 (1-10)

44. *Synthesis, characterization and photocatalytic dye degradation studies of novel defect pyrochlore, $KHf_{0.5}Te_{1.5}O_6$,* M. Sudheera, G. Ravinder, G. Ravi, P. Venkataswamy, K. Vaishnavi, N. Chittibabu, **M. Vithal**

Indian Journal of Chemistry -A (IJC-A), 59 (2020), 1092-1099,
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43. *Hydrothermal synthesis of C-doped $K_2Al_2Ti_6O_{16}$ as a visible light–activated photocatalyst in the degradation of organic dyes*
Gundeboina Ravi, P. Venkataswamy, **M. Vithal**
Journal of Australian Ceramic Society, 56 (2020), 1351-1358,
Impact Factor : 1.741

42. *Biosynthesis of CMC-Guar gum-Ag nanocomposites for inactivation of food pathogenic microbes and its effect on the shelf life of strawberries*
Vimala Kanikireddy, KokkarachedуVaraprasad, M. Sandhya Rani, P. Venkataswamy, Boggu Jaganmohan Reddy, **M. Vithal**
Carbohydrate Polymers 236 (2020) 116053
Impact Factor : 10.723
https://doi.org/10.1016/j.carbpol.2020.116053

41. *A New Ag/AgBr/$LaAlO_3$ Plasmonic Composite: Synthesis, Characterization, and Visible-light Driven Photocatalytic Activity*
P. Venkataswamy, M. Sudheera, K. Vaishnavi, K. Ramaswamy, G. Ravi, **M. Vithal**
Journal of Electronic Materials 49 (2020) 2358–2370
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40. *Cr-doped CeO_2 Nanorods for CO Oxidation: Insights into Promotional Effect of Cr on Structure and Catalytic Performance*
P. Venkataswamy, D. Devaiah, D. Jampaiah, D. Mukherjee,**M. Vithal**, B. M. Reddy,
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Impact Factor : 2.936

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39. *Synthesis and Impedance studies of potassium bismuth tri phosphate electrolyte*
C. Shankaraiah, V. Gangadhar, **M. Vithal**, G. Prasad
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Impact Factor (IF) – NA

38. *Effect of ion (Ag^+, N^{3-}) doping on the photocatalytic activity of Ruddlesden-Popper type layered perovskite $K_2Nd_2Ti_3O_{10}$*

K. Ramaswamy, G. Ravi, P. Venkataswamy, V. Radha, N.R. Muniratnam, **M. Vithal**
ComptesRendus Chimie, 2019, 22, 667-677.
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37. *Carbon nanospheres supported visible-light-driven ZnSb2O6: Synthesis, Characterization and photocatalytic degradation studies*
S. Manasa, G. Ravi, P. Venkataswamy, K. Vaishnavi and **M. Vithal**
SN applied Sciences, 1 (2019) 1046-1057
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36. *Enhancement of photocatalytic degradation of an organic pollutant by WO_3 nanopowders: carbon doping,* Vasanthi Pillay, Gundeboina Ravi and**Vithal Muga,**
Indian Journal of Chemistry, 58A (2019) 763-771
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35**.** *Fabrication of Novel Ag/AgBr/$Cs_2Nb_4O_{11}$ Ternary Composite for Visible-Light Driven Photocatalysis*
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34.*Potassium Zirconium Oxalate: A novel precursor for the preparation of perovskite, pyrochlore and Nasicon type materials*
M. Malathi, Kammara Vaishnavi, G. Ravi, Manasa Sunku and **M. Vithal**
Journal of Solid State Chemistry2019, 276, 133-138
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33. *Enhancement of photocatalytic activity of sodium bismuth titanate by doping with copper, silver and tin ions*
Sreenu K, P. Venkataswamy, G. Ravi, CH. Sudhakar Reddy, B. Jaganmohan Reddy, and **M. Vithal**
Zeitschriftfüranorganische und allgemeineChemie, 2019, 645, 529–536
IF : 1.414

32.*Ion exchange synthesis of Ag^+ incorporated $LiAlO_2$ and its application in photodegradation of organic dyes.* GundeboinaRaviand**M. Vithal**
SN Applied Sciences, 2019, 1, 164

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31. *Layered $Na_2W_4O_{13}$ and its Cation/anion doped analogues for the treatment ofpollutedwater.*Gundeboina Ravi, Srinivas Mamidi, Sreenu K, PandiriManjula, KammaraVaishnavi,**M**.
Vithal, Flat Chem., 2019, 13, 1–7
IF : 5.829

30. *Development of alginate – gum acacia - Ag^0 nanocomposites via green process for inactivation of foodborne bacteria and impact on shelf life of black grapes* (*Vitisvinifera*)
VimalaKanikireddy, K.Kanny, Y.Padma, RadhaVelchri, Gundeboina Ravi, B. Jagan Mohan Reddy, and **Muga Vithal,** J. Appl. Polym. Sci. 2019, 136, 47331

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29. *ZnO-Nanoparticles Decorated On CeO_2 Nanorods: An Efficient Catalyst For The Co Oxidation*. Perala Venkataswamy, Damma Devaiah, Deboshree Mukherjee, **Muga Vithal**, Benjaram M. Reddy
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IF – Not Available

28. *Nanocrystalline Mn-doped and Mn/Fe co-doped Ceria Solid Solutions for Low Temperature CO Oxidation.* Perala Venkataswamy, Deboshree Mukherjee, Damma Devaiah, **M. Vithal**, B. M. Reddy. Current Nanomaterials 2018, 3, 103-113
IF – Not Available

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Journal of the Australian Ceramic Society, 2018, 54, 671-678
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25. *Synthesis, characterization, luminescence and photocatalytic studies of layered perovskites $NaMMgWO_6$ (M = La, Pr, Sm).* Sreenu K, Gundeboina Ravi, CH Sudhakar Reddy, Ravinder Guje &**M. Vithal**. Indian Journal of Chemistry, 2018, 57A, 435
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24. *Nanostructured $KTaTeO_6$ and Ag-doped $KTaTeO_6$ defect pyrochlores: Promising photocatalysts for dye degradation and water splitting*. Perala Venkataswamy, CH. Sudhakar Reddy, Ravi Gundeboina, GullapelliSadanandam, Naveen Kumar Veldurthi, **M. Vithal**
Electronic Materials Letters, 2018, 14, 446-460
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PeralaVenkataswamy, DeshettiJampaiah , Ahmad EsmaielzadehKandjani , Ylias M. Sabri , Benjaram M. Reddy, and **M. Vithal**.
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Catal.Lett.2017, 147, 2028-2044
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19. *Low temperature synthesis of fluorite – type Ce based oxides of composition Ln2Ce2O7 (ln = Pr, Nd and Eu): Photodegradation and luminescence studies.* Malathi, M.; Sreenu, K.;Ravi, Gundeboina; Vijaya Kumar,P.; Sudhakar Reddy,CH.;

Ravinder, Guje;Radha, Velchuri; **Vithal, M.** Journal of Chemical Sciences 2017, 129, 1193-1203.
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14. *Synthesis, characterization and photocatalytic activity studies of tellurium containing defect pyrochlores, $MSn_{0.5}Te_{1.5}O_6$ (M = K, Ag, $Cu_{0.5}$ and $Sn_{0.5}$).* Ravinder Guje; Ravi Gundeboina; Ramaswamy Kadari; Sreenu K; Sudhakar Reddy,CH.;Malathi,M.;RadhaVelchuri;**Muga Vithal.** Indian Journal of Chemistry, 2016, 55A, 1174. **IF - 0.412**

13. *Degradation of organic pollutants by Ag, Cu and Sn doped Waste Printed Circuit Boards.* Kadari Ramaswamy; VelchuriRadha; M. Malathi; MunirathnamNagegownivari;**Muga Vithal**. Waste Management 2016, 60, 629. **IF : 8.816**

12. *Synthesis, Characterization and tin/copper – nitrogen substitutional effect on Photocatalytic activity of honeycomb ordered P2-*

$Na_2Ni_2TeO_6$. Kadari, Ramaswamy; Velchuri Radha; Sreenu K; Ravi Gundeboina; MunirathnamNagegownivari; **Muga Vithal**. Materials Research Express 2016, 3,115902.
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11. *Fabrication and Visible-light induced Photocatalytic Activity of $NaNbO_3$ Oriented Composite Photocatalyst Coupled with N-$NaNbO_3$ and V-$NaNbO_3$*. Naveen Kumar, V.; Reddy, J.R.; Ravi, G.; Ravinder, G.;Radha, V.; Venkata Swamy, P.; **Vithal, M**. Chemistry Select 2016, 1, 2783. **IF : 2.307**

10. *Facile room temperature ion exchange synthesis of H^+ doped $KM_{0.33}Te_{1.67}O_6$ (M = Al, Cr and Fe) and their photocatalytic and conductivity studies.* Ravinder G.; Reddy, J.R.; Sudhakar Reddy, CH.; Sreenu, K.; Ravi, G.; **Vithal, M.** Advanced Materials Letters 2016,7, 536
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9. *Degradation of Methylene blue and Rhodamine B using a new visible light responsive photocatalyst, $KSb_2PO_{8-x}N_y$.*Ravi, G.; Sudhakar Reddy, CH.; Sreenu, K.; Ravinder G.; Radha, V.; **Vithal, M.**ActaMetallurgica Sinica (English Letters) 2016, 29, 235.

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8. *Preparation, characterization and photocatalytic studies of Cu^{2+}, Sn^{2+} and N^{3-} substituted $K_5Sb_5P_2O_{20}$*. Sudhakar Reddy, CH.; Sreenu, K.; Reddy, J.R.; Hari Padmasri, A; Ravi, G.; **Vithal, M**. Journal of Chemical Sciences 2016, 128, 663.

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7. *A series of novel double perovskite oxides $NaMTi_2O_6$ (M = Eu, Sm, and Gd): Preparation, characterization and photocatalytic studies under visible and solarlightirradiation.*Sreenu, K.; Naveen Kumar, V; Reddy, J.R.; Sudhakar Reddy, CH.; **Vithal, M.**Journal of Materials Science: Materials in Electronics 2016, 27, 4194
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6. *Enhanced photoactivity of Antimony Phosphates by substitution of H^+, Cu^{2+} and N^{3-} in the $K_3Sb_3P_2O_{14}.xH_2O$ crystal lattice*. Sreenu, K.; Sudhakar Reddy, CH.; Reddy, J.R.; Radha, V: Suresh, P.; **Vithal, M.** Research on Chemical Intermediates 42, 2016, 5765. **IF : 3.134**

5. *Photocatalytic degradation of Methylene blue and Methyl violet using cation doped (Sn^{2+} and Ag^{+}) barium tellurite phosphate, $Ba_2TeO(PO_4)_2$.*Sudhakar Reddy, CH.;, Sreenu, K.; Reddy, J. R.; Ravi, G.; Ravinder, G.; Malathi, M.; **Vithal, M.** Indian Journal of Chemistry 2016, 55A, 9.

IF- 0.412

4. *Synthesis, characterization and photocatalytic activity of $Ag^{+}$and Sn^{2+} doped $KTi_{0.5}Te_{1.5}O_6$*. Ravinder, G.;Ravi, G.;Reddy, J. R.; Naveen Kumar, V.; Sreenu, K.; **Vithal, M.** Photochem. Photobiol. 2016, 92, 223. **IF : 3.521**

3. *Synthesis, characterization, luminescence and electrical conductivity of the metal ions (M) doped $KAl_{0.33}W_{1.67}O_6$*. Ravi, G.; Sravan Kumar, K.; Ravinder, G.; Sreenu, K.; Prasad, G.; **Vithal, M.** Journal of Solid State Chemistry 2016, 233, 342.
IF- 3.656

2. *Preparation and characterization of nitrogen doped K2M2Ti6O16 (M = Cr and Fe) with enhanced photocatalytic activity.* Ramakrishna, S.; Mahender, N.; Reddy, J. R.;, Sreenu, K.; Nagabhushan, N.; **Vithal, M.** Indian Journal of Chemistry 2016, 54A, 1026.
IF-0.412

1. *Enhanced visible light photocatalytic activity of Sn doped Bi_2WO_6 nanocrystals*
B.Vijayakumar, Muvva D Prasad,**M.Vithal,** Materials Letters, 152, 2015,200-202
IF : 3.574

Prof. SHIVARAJ(UGC-BSR Faculty Fellow),

Department of chemistry,

Osmania University.

Research project sanctioned and in progress from 2018 onwards:

S.No	Title of the project and Sanctioned Letter No.	Funding Agency	Sanctioned amount in (lakhs)	Duration of the project	Supervisor / Principal Investigator/ Co-investigator	No of research fellows/ manpower	Objectives	Outcomes
1.	"Studies on crystal structure, DNA interactions, cytotoxic and antibacterial activity of 5-cyclohexyl-2-methixybenzenamine Schiff Bases and their bivalent metal Complexes" & 26-13/ 2020 (BSR)	UGC-BSR faculty fellowship	15,00,000/-	3 years	**Dr. Shivaraj**	**SWATHI M** joined as a project fellow on 07-02-2022 .She has been **awarded** on 29-6-2024.	1. Preparation of Schiff bases by condensation of 5-cyclohexyl-2-methoxybenzenamine with substituted salicylaldehydes and their bivalent (M(II) where M= Co, Ni, Cu, Zn and Ruetc) transition	**4**were published and **1** paper has been accepted for publication from the project

							metal complexes. 2. Characterization of the above Schiff bases and their metal complexes by elemental analysis elemental analysis, UV, IR, NMR, ESR, TGA, Mass, magnetic susceptibilities and single crystal XRD analysis. 3. Testing the schiff bases and their metal complexes for biological activity such as antifungal, antibacterial, antioxidant,	

							antimalarial, antituberculosis, anti-diabetic and cytotoxic activity. 4. DNA binding and cleavage studies of Schiff bases and their metal complexes.	
2.	"Synthesis, Characterization, Antimicrobial activity, DNA cleavage and Crystal studies of mixed ligand Copper (II) Complexes of Isoxazole Schiff Base and heterocyclic compounds" & 002/OU/UPE/FAR/CO/2013	UGC-UPE-FAR	23,57,046 /-	5 years	**Dr.Shivaraj**	1. Student **G. Nirmala** was joined as a project fellow on 01-01-2014 .She has	1. Preparation of Schiff bases by condensation of 5-amino-3,4 dimethyl isoxazole with heterocyclic aldehydes / substituted salicylaldehydes and their Cu(II) complexes.	**4** papers were published from the project.

						been **awarded** on 16-6-2020.	2. Preparation of Binary and ternary metal complexes. 3. Single crystal development of the above ligands and their metal complexes by various single crystal development methods.. 4. Characterization of the above ligands and their metal complexes by elemental analysis, TG, DTA, IR, NMR, ESR, Mass, Electronic Spectroscopic	

							methods, magnetic susceptibilities and XRD studies . 5. Testing the ligands and their metal complexes for antimicrobial activity such as antifungal, antibacterial activity. 6. DNA binding and cleavage studies by absorption titration, viscometric titration and Gel electrophoresis methods.	

3.	"Synthesis, structural antimicrobial,cytotoxic and DNA interaction studies of bivalent transition metal mixed ligand complexes with bioactive benzothiozole Schiff bases and other ligands" & DST-SERB SB/EMEQ-(141/2014)	DST-SERB	33,69,200	5 years	Dr.Shivaraj	1 Student **Daravath Sreenu** was joined as a project fellow on 01-01-2014.He has been **awarded** on 16-6-2020.	1. Preparation of Schiff bases by condensation of 5-amino-3,4 dimethyl isoxazole with heterocyclic aldehydes / substituted salicylaldehydes and their Cu(II) complexes. 2. Preparation of Binary and ternary metal complexes. 3. Single crystal development of the above ligands and their metal complexes by various single crystal development	**4** papers were published from the project.

							methods.. 4. Characterization of the above ligands and their metal complexes by elemental analysis, TG, DTA, IR, NMR, ESR, Mass, Electronic Spectroscopic methods, magnetic susceptibilities and XRD studies . 5. Testing the ligands and their metal complexes for antimicrobial activity such as antifungal, antibacterial	

							activity. 6. DNA binding and cleavage studies by absorption titration, viscometric titration and Gel electrophoresis methods.	

No. of candidates awarded Ph.D degree from 2018 onwards: 16

S. No.	Name of the Candidate	Date of award
1.	Swathi M	29-06-2024

2	Tejaswi somapangu	19-06-2024
3.	Dasari Shiva Shankar	18-03-2023
4.	N. Jyothi	05-01-2023
5.	Kadasi Sandeep	01-11-2022
6.	Sreenu Daravath	3-11-2021
7.	Gurrala Sunitha	7th October 2021
8.	V. Sumalatha	11th June, 2021
9.	S. Sandhya Rani	17th April, 2021
10.	K. Venkateshwarlu	01 April, 2021
11.	Ganga Rajam	18th June 2020
12.	Nirmala Ganji	18th June 2020
13.	Gali Ramesh	13 Dec, 2019
14.	Sravanthi Siliveri	13 Dec, 2019
15.	Aveli Rambabu	25 May, 2018
16.	NarendulaVamshikrishana	23 Feb, 2018

No. of publications: 31

List of publications from the above mentioned projects

1. M. Swathi, Dasari Ayodhya, Shivaraj, Synthesis, characterization, investigation of DNA interactions and biological evaluation of Co(II), Ni(II), Cu(II) and Zn(II) complexes with newly synthesized 2-methoxy 5-trifluoromethyl benzenamine Schiff base, J.Flourec.(2024).(**accepted**)
2. M. Swathi, DasariAyodhya, Shivaraj, Design, structural characterization, DNA interaction studies, antibacterial,antioxidant, and cytotoxicity studies of Co(II), Ni(II), Cu((II), Zn(II) complexes containing 2-methoxy 5-trifluoromethyl benzenamine Schiff base, Res. Chem. 7 (2024) 101231.
3. N. Jyothi, Sreenu Daravath, M. Swathi, K Jagadeshbabu, NirmalaGanji, Shivaraj, Synthesis, geometry optimization and non-isothermal kinetic parameters ofcopper(II), nickel(II) and cobalt(II) complexes of 5-(trifluoromethyl)-2-methoxybenzenamine: DNA binding, cytotoxicity, cantioxidant and antimicrobial activity, J. Mol. Struct. 1295 (2024) 136529.
4. M. Swathi, D. Shiva Shankar, S. Daravath, N. Ganji, P.V.AnanthaLakshmi, Shivaraj, Computational studies, Cytotoxicity, DNA interactions of bioactive novel 2-methoxy 5-trifluoromethylbenzenamine Schiff base metal complexes, Inorganic Chemistry Communications 153(2023)110826.
5. K. JagadeshBabu, SreenuDaravath , M. Swathi , DasariAyodhya, Shivaraj, Synthesis, anticancer, antibacterial, antifungal, DNA interactions, ADMET, molecular docking, and antioxidant evaluation of novel Schiff base andtheir Co(II), Ni(II) and Cu(II) complexes Res. Chem. 6(2023)101121.
6. Exploration of DNA interaction, antimicrobial and antioxidant studies on binary transition metal complexes with isoxazole

Schiff bases: Preparation and spectral characterization, NirmalaGanji, SreenuDaravath, AveliRambabu, KadtalaVenkateswarlu, Dasari Shiva Shankar and Shivaraj*, *Inorganic Chemistry Communications,121 (2020) 108247.*

7. Structure elucidation of copper(II), cobalt(II) and nickel(II) complexes of benzothiazole derivatives: Investigation of DNA binding, nuclease efficacy, free radical scavenging and biocidal properties, Dasari Shiva Shankar, Nirmala Ganji, SreenuDaravath, KadtalaVenkateswarlu, **Shivaraj*,** Chemical Data Collections, ISSN: 2405-8300, (2020), 28, 100439,DOI: 10.1016/j.cdc.2020.100439 (Impact Factor- 2.063)
8. Structure elucidation of copper(II), cobalt(II) and nickel(II) complexes of benzothiazole derivatives: Investigation of DNA binding, nuclease efficacy, free radical scavenging and biocidal properties,SreenuDaravath , Aveli Rambabu , Dasari Shiva Shankar, **Shivaraj*,**Chemical Data Collections, ISSN: 2405-8300, (2019), 24, DOI: 10.1016/j.cdc.2019.100293, 100293, (Impact Factor-2.063) .
9. Synthesis, structural characterization, antioxidant, antimicrobial, DNA incision evaluation and binding investigation studies on copper(II) and cobalt(II) complexes of benzothiazole cored Schiff bases, SreenuDaravath, Aveli Rambabu, NarendrulaVamsikrishna, Nirmala Ganji and **Shivaraj*,** Journal of Coordination Chemistry, ISSN: 0095-8972, (2019), 72, 1973-1993, DOI: 10.1080/00958972.2019.1634263, (Impact Factor-1.9).
10. Copper(II) complexes with isoxazole Schiff bases: Synthesis, spectroscopic investigation, DNA binding and nuclease activities, antioxidant and antimicrobial studies. N. Ganji, A. Rambabu, N. Vamsikrishna, S. Daravath, Shivaraj*, J MolStruct, 1173 (2018) 173-182.
11. DNA incision evaluation, binding investigation and biocidal screening of Cu(II), Ni(II) and Co(II) complexes with isoxazole Schiff bases. N. Ganji, V.K. Chityala, M.P. Kumar, A. Rambabu, N. Vamsikrishna, S. Daravath, Shivaraj, J. Photochem. Photobiol. B Biol, 175 (2017) 132-140.
12. Crystal Structure, Spectral Characterization, Biological and DNA Binding Studies of Cu(II) Mixed Ligand Complexes of 5-Amino-3, 4-Dimethyl Isoxazole Schiff Bases and Heterocyclic Compounds. Ch. Vijay Kumar, M. Pradeep Kumar,

NirmalaGanji, D. Anil Kumar, S.S. Singh, P. Raghavaiah and Shivaraj***.** *Russian Journal of Coordination Chemistry.* 43 (5) (2017) 275-289.

13. Design, synthesis, spectral characterization, DNA interaction and biological activity studies of copper(II), cobalt(II) and nickel(II) complexes of -amino benzothiazole derivatives. Sreenu Dravath, Marri Pradeep Kumar, NarendrulaVamsikrishna, Nirmala Ganji, and **Shivaraj*.** Journal of Molecular Structure, ISSN: 0022-2860, (2017), 1144 (15) 47-158, DOI: 10.1016/j.molstruc.2017.05.022, (Impact Factor-3.8).

List of publications acknowledged the above mentioned projects

1. M. Swathi, Dasari Ayodhya, Shivaraj, Synthesis, characterization, investigation of DNA interactions and biological evaluation of Co(II), Ni(II), Cu(II) and Zn(II) complexes with newly synthesized 2-methoxy 5-trifluoromethyl benzenamine Schiff base, J.Flourec.(2024).(**accepted**)
2. M. Swathi, DasariAyodhya, Shivaraj, Design, structural characterization, DNA interaction studies, antibacterial,antioxidant, and cytotoxicity studies of Co(II), Ni(II), Cu((II), Zn(II) complexes containing 2-methoxy 5-trifluoromethyl benzenamine Schiff base, Res. Chem. 7 (2024) 101231.
3. N. Jyothi, Sreenu Daravath, M. Swathi, K Jagadeshbabu, NirmalaGanji, Shivaraj, Synthesis, geometry optimization and non-isothermal kinetic parameters ofcopper(II), nickel(II) and cobalt(II) complexes of 5-(trifluoromethyl)-2-methoxybenzenamine: DNA binding, cytotoxicity, cantioxidant and antimicrobial activity, J. Mol. Struct. 1295 (2024) 136529.
4. M. Swathi, D. Shiva Shankar, S. Daravath, N. Ganji, P.V.AnanthaLakshmi, Shivaraj, Computational studies, Cytotoxicity, DNA interactions of bioactive novel 2-methoxy 5-trifluoromethylbenzenamine Schiff base metal complexes, Inorganic Chemistry Communications 153(2023)110826.
5. Dasari Shiva Shankar, AveliRambabu, Swathi M, P. V. AnanthaLakshmi,andShivaraj, Copper(II) Complexes Derived

from Schiff Bases Containing4-Methylbenzylamine as a Core Unit: Cytotoxicity, pBR322-DNA Studies, Biological Assays, and Quantum Chem-ical Parameters, chem. Biodiversity 2023, e202300030

6. K. JagadeshBabu, SreenuDaravath , M. Swathi , DasariAyodhya, Shivaraj, Synthesis, anticancer, antibacterial, antifungal, DNA interactions, ADMET, molecular docking, and antioxidant evaluation of novel Schiff base andtheir Co(II), Ni(II) and Cu(II) complexes Res. Chem. 6(2023)101121.
7. K. Jagadesh Babu, DasariAyodhya, Shivaraj,Comprehensive investigation of Co(II), Ni(II) and Cu(II) complexes derived from a novel Schiff base: Synthesis, characterization, DNA interactions, ADME profiling, molecular docking, and in-vitro biological evaluation. Res. Chem. 6(2023)101110.
8. Exploration of DNA interaction, antimicrobial and antioxidant studies on binary transition metal complexes with isoxazole Schiff bases: Preparation and spectral characterization, NirmalaGanji, SreenuDaravath, AveliRambabu, KadtalaVenkateswarlu, Dasari Shiva Shankar and Shivaraj*, *Inorganic Chemistry Communications,121 (2020) 108247.*
9. Structure elucidation of copper(II), cobalt(II) and nickel(II) complexes of benzothiazole derivatives: Investigation of DNA binding, nuclease efficacy, free radical scavenging and biocidal properties, Dasari Shiva Shankar, Nirmala Ganji, SreenuDaravath, KadtalaVenkateswarlu, **Shivaraj*,** Chemical Data Collections, ISSN: 2405-8300, (2020), 28, 100439,DOI: 10.1016/j.cdc.2020.100439 (Impact Factor- 2.063)
10. Synthesis, structural characterization, DNA interaction, antibacterial and cytotoxicity studies of bivalent transition metal complexes of 6-aminobenzothiazole Schiff base. NarendrulaVamsikrishna, SreenuDaravath, NirmalaGanji, Nayeem Pasha, Shivaraj*. Inorganic ChemistryCommunications, 113 (2020) 107767.
11. Evaluation of DNA interaction, free radical scavenging and biologically active compounds of thermally stable p-tolylmethanamine Schiff bases and their binary Co(II) and Ni(II) complexes, Dasari Shiva Shankar, NirmalaGanji, SreenuDaravath, KadtalaVenkateswarlu and Shivaraj*, Chemical Data Collections 28 (2020) 100439.
12. Investigation on Co(II), Ni(II), Cu(II) and Zn(II) complexes derived from quadridentatesalen-type Schiff base: Structural

characterization, DNA interactions, antioxidant proficiencyand biological evaluation, Gali Ramesh, SreenuDaravath, M Swathi, V. Sumalatha, Dasari Shiva Shankar,Shivaraj∗, Chemical Data Collections, 28 (2020) 100434.

13. Structure elucidation of copper(II), cobalt(II) and nickel(II) complexes of benzothiazole derivatives: Investigation of DNA binding, nuclease efficacy, free radical scavenging and biocidal properties,SreenuDaravath , AveliRambabu , Dasari Shiva Shankar, **Shivaraj*,***Chemical Data Collections*, 24 (2019) 100293.
14. Structure elucidation of copper(II), cobalt(II) and nickel(II) complexes of benzothiazole derivatives: Investigation of DNA binding, nuclease efficacy, free radical scavenging and biocidal properties,SreenuDaravath , Aveli Rambabu , Dasari Shiva Shankar, **Shivaraj*,**Chemical Data Collections, ISSN: 2405-8300, (2019), 24, DOI: 10.1016/j.cdc.2019.100293, 100293, (Impact Factor-2.063) .
15. Synthesis, structural characterization, antioxidant, antimicrobial, DNA incision evaluation and binding investigation studies on copper(II) and cobalt(II) complexes of benzothiazole cored Schiff bases, SreenuDaravath, Aveli Rambabu, NarendrulaVamsikrishna, Nirmala Ganji and **Shivaraj*,** Journal of Coordination Chemistry, ISSN: 0095-8972, (2019), 72, 1973-1993, DOI: 10.1080/00958972.2019.1634263, (Impact Factor-1.9).
16. Copper(II) complexes with isoxazole Schiff bases: Synthesis, spectroscopic investigation, DNA binding and nuclease activities, antioxidant and antimicrobial studies. N. Ganji, A. Rambabu, N. Vamsikrishna, S. Daravath, Shivaraj*, J MolStruct, 1173 (2018) 173-182.
17. Three mononuclear Cu(II) complexes based on p-tolylmethanamine Schiff bases: In-vitro cytotoxicity, DNA binding ability, Nuclease activity and antibacterial studies. D. Shiva Shankar, AveliRambabu, NarendrulaVamsikrishna, NirmalaGanji, SreenuDaravath and Shivaraj*, Inorganic Chemistry Communications, 98 (2018) 48-57. Impact Factor-1.79.
18. Synthesis, characterization, DNA binding ability, nuclease efficacy and biological evaluation studies of Co(II) , Ni(II) and Cu(II) complexes with benzothiazole Schiff base. SreenuDaravath, NarendrulaVamsikrishna, NirmalaGanji, KadtalaVenkateswarlu and Shivaraj*, Chemical Data Collectons, 17-18 (2018) 159-168.

19. Synthesis, Spectral Characterization, DNA Binding, Cleavage and Biological Evaluation on Co(II), Ni(II) and Cu(II) Complexes of Substituted Isoxazole Schiff Bases. Gali Ramesh, Marri Pradeep Kumar, AveliRambabu, NarendrulaVamsiKrishna, SreenuDaravath and Shivaraj*. Asian Journal of Chemical Sciences. 4 (3) (2018) 1-20. Impact Factor-3.6.
20. Crystal structure, DNA binding, cleavage, antioxidant and antibacterial studies of Cu(II), Ni(II) and Co(III) complexes with 2-((furan-2-yl) methylimino)methyl)-6-ethoxyphenol Schiff base: KadtalaVenkateswarlu, Marri Pradeep Kumar, AveliRambabu, NarendrulaVamsikrishn, SreenuDaravath, Krishnan Rangan, and Shivaraj*. Journal of Molecular Structure, 1160 (2018) 198-207. Impact Factor-2.12.
21. Mixed Ligand Complexes Derived from Semicarbazone Schiff Base and Heterocyclic Ligands:Structure and Antimicrobial Activity, K. Ganga Rajam, Marri Pradeep Kumar, K. JyothiKiran, and Shivaraj*, Russian Journal of General Chemistry, 88 (2018) 1000–1008.
22. DNA incision evaluation, binding investigation and biocidal screening of Cu(II), Ni(II) and Co(II) complexes with isoxazole Schiff bases. N. Ganji, V.K. Chityala, M.P. Kumar, A. Rambabu, N. Vamsikrishna, S. Daravath, Shivaraj, J. Photochem. Photobiol. B Biol, 175 (2017) 132-140.
23. Crystal Structure, Spectral Characterization, Biological and DNA Binding Studies of Cu(II) Mixed Ligand Complexes of 5-Amino-3, 4-Dimethyl Isoxazole Schiff Bases and Heterocyclic Compounds. Ch. Vijay Kumar, M. Pradeep Kumar, NirmalaGanji, D. Anil Kumar, S.S. Singh, P. Raghavaiah and Shivaraj**.** *Russian Journal of Coordination Chemistry.* 43 (5) (2017) 275-289.
24. Design, synthesis, spectral characterization, DNA interaction and biological activity studies of copper(II), cobalt(II) and nickel(II) complexes of -amino benzothiazole derivatives. Sreenu Dravath, Marri Pradeep Kumar, NarendrulaVamsikrishna, Nirmala Ganji, and **Shivaraj*.** Journal of Molecular Structure, ISSN: 0022-2860, (2017), 1144 (15) 47-158, DOI: 10.1016/j.molstruc.2017.05.022, (Impact Factor-3.8).

25. Design, synthesis, spectral characterization, DNA interaction and biological activity studies of copper(II), cobalt(II) and nickel(II) complexes of -amino benzothiazole derivatives. SreenuDravath, Marri Pradeep Kumar, NarendrulaVamsikrishna, NirmalaGanji, and Shivaraj*. Journal of Molecular Structure. 1144 (15) (2017) 47-158,. Impact Factor-2.12.
26. DNA interactions and biocidal activity of metal complexes of benzothiazole Schiff bases synthesis, characterization and validation. NarendrulaVamsikrishna, Marri Pradeep Kumar, Gali Ramesh, NirmalaGanji, SreenuDravath and Shivaraj*. Journal of Chemical Sciences. 129 (5) (2017) 609-622. Impact Factor-1.49.
27. Cu(II) complexes with 4-amino-3, 5-dimethyl isoxazole and substituted aromatic aldehyde Schiff bases: Synthesis, crystal structure, antimicrobial activity, DNA binding and cleavage studies. Marri Pradeep Kumar, NarendrulaVamsikrishna, Gali Ramesh, N.J.P. Subhashini and Shivaraj*. Journal of Coordination Chemistry. 70 (8) (2017) 1368-1388,. Impact Factor-1.68.
28. DNA interaction, antimicrobial studies of newly synthesized copper (II) complexes with 2-amino-6-(trifluoromethoxy) benzothiazole Schiff base ligands. AveliRambabu, Marri Pradeep Kumar, SomapanguTejaswi, NarendrulaVamsikrishna and Shivaraj*. Journal of Photochemistry & Photobiology, B: Biology 165 (2016) 147-156. Impact Factor-4.06.
29. Synthesis, Structural, DNA Binding and Cleavage Studies of Cu(II) Complexes Containing Benzothiazole Cored Schiff Bases,SomapanguTejaswi, Marri Pradeep Kumar, AveliRambabu, NarendrulaVamsikrishna and Shivaraj*. Journal of Fluorescence. 26 (6) (2016) 2151-2163. Impact Factor-1.91.
30. DNA Binding, Cleavage and Antibacterial Activity of Mononuclear Cu(II), Ni(II) and Co(II) Complexes Derived from Novel Benzothiazole Schiff Bases. N Vamsikrishna, M.P. Kumar, S. Tejaswi, A. Rambabu and Shivaraj*. Journal of Fluorescence. 26 (4) (2016) 1317-1329. Impact Factor-1.91.
31. Synthesis, crystal structure, DNA binding and cleavage studies of copper(II) complexes with isoxazole Schiff bases, Marri Pradeep Kumar, SomapanguTejaswi, AveliRambabu, Veerendra Kumar A. Kalalbandi and Shivaraj*. Polyhedron. 102 (2015) 111–120. Impact Factor-2.284.

S.No	Title of the Project And sanction letter No.	Funding agency	Sanctioned Amount (Rs. Lakhs)	Year/Duration	Name of Supervisor	No. of Research Fellows/ Man Power	Objectives	Outcomes
19	Thiolation of heteroaromatics via C-H activation	UGC-BSR Startup Grant	6.0 lakhs	2015-2017	Dr. Raju J. Reddy		Objective-1: Cs2CO3-Mediated Vicinal Thiosulfonylation of 1,1-Dibromo-1-Alkenes with Thiosulfonates. Objective-2: Sequential One-Pot Approach for Thiolation of Imidazo[1,2-a]pyridines*via* C-H activation Under Transition-Metal Free Conditions	(i) We have successfully developed a novel Cs_2CO_3-mediated vicinal thiosulfonyl-ation of 1,1-dibromo-alkenes with thiosulfonates under mild reaction conditions. (ii) A simple and metal-free sequential one-pot protocol has been developed for the synthesis of varied C3-functionalized imidazo[1,2-*a*]pyridines.
20	Cascade C-H Functionalization for Synthesis of *N*,*S*-Heterocycles	DST-SERB/ECR	33.10 lakhs	2016-2019	Dr. Raju J. Reddy	1	The central theme of proposed project will cover the following key objectives: 1) To develop newer methodology for synthesis of functionalised phenothiazines in general via	(i) We have successfully developed a convenient protocol for the synthesis of allyl thiosulfonates. A range of aryl/heteroaryl/ aliphatic allyl bromides and sodium

							cascade C-H functionalization strategy. The scope further extended to synthesis of bioactive promazines and phenothiazine-proline derived oranocatalysts. 2) To determine for synthesis of the dibenzothiazepine derivatives via ortho-thiolation and intramolecular *N*-arylation. The substrate scope will explore and applicability for synthesis of trade marketed drugs, clotiapine and fumarate of quetiapine. 3) The construction N-fused type heterocycles can be prepared through cascade C-S and C-N bonds formation and readily extended to imidazo[2,1-*b*]thiazole moiety modification allow valuable	arylthiosulfonates were readily assembled to furnish allyl thiosulfonates. (ii) We have successfully developed a highly regioselective, iodine-mediated sulfonylation reaction of NH-1,2,3-triazoles using sodium sulfinates and thiosulfonates to provide N-sulfonylated triazoles in moderate to high yields. This protocol operationally simple and possesses a wide substrate scope, permitting the synthesis of a range of N2-sulfonyl triazoles which can be difficult to prepare by other methods. (iii) We have developed successfully azide-cycloaddition reaction of nitroallylic alcohols, acetates and sulfones were easily converted into a diverse NH-1,2,3-triazoles in good to high yields. This metal-free protocol is

							products. 4) To demonstrate the synthesis and utility of chiral N,S-heterocycles in asymmetric organocatalysis will be central to establish secondary amine derived multisite catalyst systems. 5) The diverse N,S-heterocycles will study of their pharmacological activities and depending on the biological data will be re-design and synthesize the modified structures to improve their activities.	straightforward, operationally simple and various functional groups were tolerated.
21	Oxidative Cross-Coupling for Divergent Synthesis of N-Heterocycles	CSIR (02(0340)	28.10 lakhs	2018- 2021	Dr. Raju J. Reddy	1	Objective 1 is to develop newer methodology for synthesis of functionalised indoles and pyrazine fused pyrroles via N-alkenylation and oxidative cyclization. Objective 2 is to determine for synthesis of the 1,2-dihydroisoquinoline derivatives by means	(i) We have successfully developed a metal-free synthesis of β-keto sulfones and β-keto thiosulfones using β-iodovinyl sulfones under mild reaction conditions. For the first time, β-iodovinyl sulfones served as indirect enolate in the presence of NaOAc.

							N-arylation and intramolecular oxidative C-C coupling. Objective 3 is the construction 1,4-benzodiazepines and fused imidazoles can be prepared through oxidative tandem C-N bond formation. Objective 4 is to develop an intramolecular oxidative cross-coupling for a facile construction of 2-benzazpine derivatives.	(ii) Palladium catalyzed synthesis of 3-sulfonylbenzofuranes from the β-iodovinyl sulfones with 2-bromophenols via a oxy-Michael addition and Heck-type reaction has been developed. A facile construction of 2,3-disubstituted benzofuranes has been achieved in a one-pot operation and a wide variety of 2,3-disubstituted benzofuranes were accessed in good to high yields. (iii) A unique phenylboronic acid-catalyzed dimerization–sulfonylation of S-benzyl thiosulfonates has been disclosed. A metal-free tandem construction of S–S and C–S bonds is an operationally simple method to access a wide range of benzyl disulfanylsulfone derivatives in high to excellent yields. Moreover, the robustness of this tandem

								transformation has been demonstrated
22	Design and Development of Atom Transfer Radical Cyclization (ATRC): Thiosulfonylation of Unactivated Carbon-Carbon Multiple Bonds	SERB-CRG	40.07 lakhs	2021 to 2024	Dr. Raju J. Reddy	1	Objective 1 is to develop 'O-propargyl benzylthiosulfonates' via vicinal thiosulfonylation by means of nickel and photoredoxcocatalysis to construct benzoxathiepines in general. Objective 2 is atom transfer radical cyclization (ATRC) extended to 'O-allyl benzylthiosulfonates' under the catalytic influence of nickel and organic dyes for the formation of benzoxathiepine derivatives. Objective 3 is to explore nickel-photoredoxcatalysed ATRC through exo-trig ring closure reaction of 'O-vinyl benzylthiosulfonates' to produce benzoxathines.	(i) The rationally designed propargylic alcohol-containing 1,6-enynes were prepared for the first time. A general and highly efficient sulfonyl radical-triggered cycloannulation of 1,6-enynols with sodium sulfinates was achieved for the tandem construction of C-S and C-C bonds in a single operation. (ii) Visible-light induced sulfonylative-cycloannaulation of 1,6-enynols with sulfinic acids using 4CZIPN as a photocatalyst was also established. An efficient sulfonyl radical-triggered cycloannulation of 1,6-enynols with sulfinic acids was achieved for the synthesis of 2,3-disubstituted benzofurans in moderate to high yields. Very recently,

								we have found an interesting reactivity of secondary acetate-derived 1,6-enynols under the same reaction conditions.

S. No	Title of the Project and Sanction Letter No.	Funding Agency	Sanctioned amount (in lakhs)	Duration of the Project	Supervisor/Principal Investigator/Co-investigator	No. of research fellows/man power	Objectives	Outcomes
1	**Green Synthesis of Nitrogen and Oxygen Contains Heterocyclic Compounds via Novel Methodologies and their Biological Evaluation** Sanction Letter No. ***SUR/2022/001828; dated 06 July 2023.***	**Science and Engineering Research Board(SERB)**	26,46,600/-	3 years	Prof. Yadagiri Bhongiri	01	**Objective-1**: To the development of more isoquinolone directed ortho C-H activation/annulation reactions for the synthesis of polycyclic isoquinolone derivatives is highly desirable. **Objective-2:** To develop the transitional metal mediated the new and one pot, an efficient synthetic methods for functionalized indole fused pyrano[3,2-c]chromen. **Objective-3:** To develop the transitional metal mediated the new and one pot, an efficient synthetic methods for functionalized fused indoles.	**Green** Synthesis of Nitrogen and Oxygen Contains Heterocyclic Compounds via Novel **Methodologies**and their Biological Evaluation. Here's a summary of the typical outcome: **Optimized Synthesis**:Heterocyclic compounds containing nitrogen and oxygen are important in pharmaceuticals, agrochemicals, and materials science. Green synthesis methods aim to create a wide range of these compounds efficiently. The use of template-assisted or cascade reactions can enable the rapid construction of complex heterocyclic structures with high specificity. **Biological Testing**:

								The biological activity of the synthesized heterocyclic compounds is crucial for their potential applications. Evaluation often includes testing for antimicrobial, antitumor, anti-inflammatory or other bioactive properties. Compounds with promising biological activities can be further optimized through structural modifications, guided by green synthetic principles.

S. No	Title of the Project and Sanction	Funding Agency	Sanctioned amount (in	Duration of the	Supervisor/Principal Investigator/ Co-	No. of research fellows/man power	Objectives	Outcomes

	Letter No.		lakhs)	Project	investigator			
1	**Design, and Synthesis of Nitrogen - Containing Heterocycles and In Vitro Studies of their Cytotoxic Activity.** Sanction Letter No. **SERB-SUR/2022/002286 Dated: 14 Nov 2023.**	**Science and Engineering Research Board (SERB)**	27,40,600/-	3 years	Prof Boda Sakram	01	**Objective-1**: To develop newer methodology for synthesis of novel 6-(3-bromo-2-fluoroaryl)-9-aryl-[1,2,4]triazolo[4,3-a][1,8] naphthyridines **Objective-2:** Synthesis of fused 6-(2-chloro-6-fluoroaryl)-9-aryl-imidazo[1,2- a][1,8]naphthyridine and 3-(6-(2-chloro-6-fluoroaryl)imidazo[1,2-a][1,8]naphthyridin-9-yl)-2Hchromen-2-onederivatives catalyzed by DABCO. **Objective-3:** Synthesis and characterization of novel 4-((3-aryl-1,8-naphthyridin-2-yl) amino)phenol derivatives. **Objective-4:** Synthesis of 6-aryl-8H-benzo[5,6][1,2,4]triazino[4,3-a][1,8]naphthyridin-11-oles and 7-aryl-5H-naphtho[2',1':5,6][1,2,4]triazino[4,3-a][1,8]naphthyridin-15-ol derivatives. **Objective-5:** Environmentally benign synthesis of 1,8-naphthyridinyl-4-thiazolidinone derivatives. **Objective-6:** Microwave-assisted synthesis of 1,8-naphthyridinyl-chromenyl-pyrazole carbaldehydes. **Objective-7:** to screen the newly synthesized compounds which are	The synthesis of 1,8-naphthyridines derivatives is an area of significant interest in medicinal chemistry due to their diverse biological activities. Here's a summary of the typical outcome: **Optimized Synthesis**: Improved methods for synthesizing 1,8-naphthyridines with higher yields, fewer steps, and more functional group compatibility are often key outcomes. **Biological Testing**: Comprehensive in vitro and in vivo testing to assess the efficacy, toxicity, and pharmacokinetic properties of new compounds. Successful candidates might progress to further preclinical or clinical development. Such as anti-tumour, anti-cancer, anti-psoriasis, anti-malarial and anti HIV and molecular docking studies. **Valuable insights into their potential as therapeutic agents, leading to further research and development in the field of medicinal** chemistry.

							mentioned in objectives 1-6 for their possible biological activities such as anti-tumour, anti-cancer, anti-psoriasis, anti-malarial and anti HIV and molecular docking studies.	

25	Design and synthesis of novel 2-aminochromone and 2-aminoquinolinone-containing 1,2,3 triazol, Isoxazole, 1,2,4-oxadiazol, and carboxamides: Biological evaluation for anti-HIV and anti-cancer activities	SERB-SURE	30.0 lakhs	2023-2026	Dr. T Gangadhar thalari	1	**Expected Output and Outcome of the proposal :** Functionalization of chromones and quinolines allows attaining chemical diversity suitable for either improving the pharmacological profile or discovering new biological studies. Carboxamides derivatives are widely used in the search for anti-asthmatic, anti-inflammatory, anticoagulant, anticancer, and antimicrobial activities. As a result, their application for neurodegenerative diseases, such as Parkinson was recently highlighted. Therefore, we would like to synthesize novel chromone and quinolines carboxamide derivatives with various amino acids bearing electron-donating and electron-withdrawing substituent's in different positions of the chromone and quinolines ring by using green chemistry mode. We will design novel heterocyclic analogues of 2-amino chromones and 2-aminoquinolinones using a computational tool based on synergistic/conjugate effect using triazoles, isooxazoles, oxadiazoles and carboxamides rings which would exhibit better selectivity against towards anticancer anti-HIV receptors. To understand the interaction and binding of the synthesized compounds, molecular docking will be performed by using Autodock Vina program. Molecular docking studies will reveal that all the synthesized compounds bind to the binding site of targeted sites, and it will give computational binding affinity. Data compilation: Results obtained from the various phases of work will be compiled and documented periodically, and the manuscript or patent will be published in due course.

1. Title of the project: **Synthesis of polycyclic aromatic hydrocarbons for organic field effect transistor applications**

2. Principal Investigator(s) and Co-Investigator(s): Dr. Someshwar Pola (PI)
Prof. M. Vithal
Dr. M. Sreenath Reddy

3. Implementing Institution(s) and other collaborating Institution(s): Department of Chemistry
UCS, Osmania University
Hyderabad-07

4. Date of commencement: 01-11-2015

5. Planned date of completion: 31-10-2018

6. Actual date of completion: 31-10-2018

Title of the Project: **Synthesis of polycyclic aromatic hydrocarbons for organic field effect transistor applications**

Objectives:

- Synthesis of new dibenzocoronenes, dithiophenecoronenes and tetrabenzo-diimidazocoronenes. Synthesis of new fluoro, chloro, methoxy and methyl substituted dibenzocoronenes, dithiophenecoronenes and tetrabenzodiimidazocoronenes.
- Characterization of the newly synthesized compounds by from spectral studies like NMR (1H and 13C), mass spectra, Cyclic Voltammetry, TGA, DSC, UV-visible, XRD and AFM.
- Comparison of transistor and structural properties new fluoro, chloro, methoxy and methyl substituted dibenzocoronenes,
- dithiophenecoronenes and tetrabenzo-diimidazocoronenes with their parent compounds
- Sublimation of final compounds to get pure materials and grow the crystals from gas flow technique. Fabrication of devices

by using these single crystals and collect the mobility.

- The results obtained from experimental to be compared with theoretical studies.

Outcomes:

- The synthesized coronenes, Tetraimidazocoronene (TIC), Tetraimidazobenzocoronene (TIBC), Tetraimidazodibenzocoronene (TIDBC), Tetrapyrazolocoronene (TPC), Tetrapyrazolobenzocoronene (TPBC), and Tetrapyrazolodibenzocoronene (TPDBC), have good physicochemical properties and are supported with DFT/TDDFT studies.
- On an ODTS-SiO_2 substrate at room temperature, the reported compounds were utilized to fabricate organic thin-film transistors (OTFTs) and shown hole mobilities from 0.16 to 0.44 cm^2/Vs and 0.39 to 0.71 cm^2/Vs respectively, with an on/off ratio of 10^2 to 10^6.
- Thin-film transistor based on TPDBC as the channel material displays a very high electron mobility of 1.94 cm^2/Vs and an on/off ratio of 10^2 respectively.
- These compounds are further supported by DFT/TD-DFT studies, providing insights into their structural and electronic properties.
- The development of an OFET sensor for glucose detection offers a promising approach for both invasive and non-invasive monitoring methods, with potential for high sensitivity and specific detection.
- OFETs can be manufactured at relatively low costs compared to conventional silicon-based sensors.

Consumable grants sanctioned for individual faculties under OUDST-PURSEprogramme

Name of PI	Grants allotted (Rs. in Lakhs @ 2017 - 21)
Prof. Shivaraj	**4.0**
Prof. M. Vijjulatha	**4.0**
Prof. P. Leelavathi	**4.0**
Dr. K. Shiva Kumar	**3.20**
Dr. Raju Jannapu Reddy	**3.87**
Prof. P. Veera Somaiah	**4.0**
Prof. A.K.Durga Bhavani	**4.0**
Prof. P.Vijay Kumar	**3.08**
Prof. Ch. Sarala Devi	**4.2**
Dr. D.A.Padmavathi	**3.04**
Prof. B. Satyanarayana	**4.0**
Prof. D. Ashok	**4.0**
Dr. N.J. PrameelaSubhashini	**4.0**
Dr. P.V. Anantha Lakshmi	**4.0**
Dr. A. Hari Padmasri	**4.0**
Prof. Ch. Arabham Lincoln	**3.0**
Prof.M. Vittal	**4.0**

Name of the project associates (PA) under sponsored projects

S. No.	Name of the PA	Supervisor	Fellowship awarding Agency
1	N. Praveen Kumar	Dr. K. Shiva Kumar	CSIR-EMR-II
2	Vemula Saiganesh	Dr. Raju Jannapu Reddy	CSIR-EMR-II
3	J. Jagadesh Kumar	Dr. Raju Jannapu Reddy	SERB-CRG
4	A. Haritha Kumari	Dr. Raju Jannapu Reddy	SERB-CRG
5	Barla Manohar	Prof. Yadagiri Bhongiri	SERB-SURE
6	Ergurala Naveen	Prof. Boda Sakram	SERB-SURE
7	Kolishik Shruthi	Dr. T Gangadhar thalari	SERB-SURE