

DR. SRINIVASA REDDY MUNNANGI

Ph.D. (Chemistry) • Vice Principal & Research Coordinator

Associate Professor in Chemistry, D.S. Government College for Women (A), Ongole, Andhra Pradesh, India – 523001

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Google Scholar: scholar.google.com/citations?user=CGPaLHMMAAAJ

EXECUTIVE PROFILE

Dr. Srinivasa Reddy Munnangi is an Associate Professor of Chemistry (Lecturer) with over three decades of combined research, teaching, and pharmaceutical industry experience. He holds a Ph.D. from Acharya Nagarjuna University, focusing on molecular interactions in imidazolium ionic liquids. His research spans chemical thermodynamics, computational chemistry, and machine learning for property prediction. He currently serves as Vice Principal and Research Coordinator at D.S. Government College for Women (A), Ongole, where he leads the institution's research centres and supervises doctoral candidates. He received the 2024 State Best Teacher Award in Chemistry (Government of Andhra Pradesh) and is an active peer reviewer for leading international chemistry journals.

As Vice Principal and Academic Secretary, he designed curriculum frameworks implementing Bloom's Taxonomy and monitored Programme and Course Outcomes. As Research Coordinator, he negotiated the establishment of research centres in Chemistry and Mathematics with Andhra Kesari University and AP state authorities, securing facilities for six Ph.D. students. As General Secretary of GCGTA, he advocated successfully for academic and service matters affecting government college faculty across Andhra Pradesh.



PROFESSIONAL APPOINTMENTS

Professor in Chemistry — D.S. Govt. College for Women (A), Ongole <i>Promotion deemed to be approved, pending administrative issuance.</i>	<i>31 May 2026 – present</i>
Vice Principal — D.S. Govt. College for Women (A), Ongole	<i>01 Jul 2025 – present</i>
Research Coordinator — D.S. Govt. College for Women (A), Ongole	<i>01 Jul 2023 – present</i>
Research Supervisor (Ph.D.) — Research Centre in Chemistry, Andhra Kesari University	<i>15 Dec 2025 – present</i>
Associate Professor in Chemistry — D.S. Govt. College for Women (A), Ongole	<i>Oct 2021 – present</i>
Assistant Professor in Chemistry — TRR Government Degree College, Kandukur	<i>Jun 2017 – Oct 2021</i>
Assistant Professor in Chemistry — KRK Government Degree College, Addanki	<i>Apr 2012 – May 2017</i>
Assistant Professor in Chemistry — Visvodaya Government Degree College, Venkatagiri	<i>Nov 2010 – Mar 2012</i>
Junior Lecturer in Chemistry — GJC, Payakarao Pet & GJC, Kandukur	<i>2004 – 2010</i>
Senior Chemist — Dr. Reddy's Research Foundation, Hyderabad	<i>Jun 1994 – Dec 1996</i>

LEADERSHIP & ADVOCACY

As General Secretary of GCGTA (2022–2024, re-elected 2024–2026), Dr. Munnangi negotiated directly with the Government of Andhra Pradesh and the State Higher Education Council on academic policies, service matters, and professional development for teaching staff, achieving substantive improvements in faculty working conditions and institutional support.

- ▶ **General Secretary, Government College Gazetted Teachers' Association (GCGTA)** — a service association recognised by the Govt. of A.P., serving 2022–2025, coordinating with the Commissionerate of Higher Education on teacher welfare and academic activities.
- ▶ Re-elected as General Secretary for a further term in 2025.

SCIENTIFIC INNOVATION

- ▶ **AI-driven antibacterial screening:** designed multi-assay virtual screening engines including a Virtual Antibiotic Screening Score (VASS) integrating predicted potency, drug-likeness and toxicity risk into a single ranking metric (Indian Patent Application 202641003372 A).
- ▶ **Thermodynamics-aware screening pipeline:** integrates adaptive molecular dynamics, MM/PBSA binding-free-energy decomposition and machine-learning pre-selection (Indian Patent Application 202541103130 A).
- ▶ **ML property prediction:** applied SVR, ensemble learning and neural networks to predict density, viscosity and refractive index of binary liquid and ionic-liquid mixtures with high accuracy.
- ▶ **Drug-discovery against SARS-CoV-2:** molecular-dynamics binding-energy calculations using the OPLS-AA force field.

PATENTS

Three patent applications (first applicant and inventor on all three) published in the Official Journal of the Indian Patent Office under Section 11A of the Patents Act, 1970. Applications are at the publication stage (not yet granted).

Application No.	Title	Status	Claims
202641003372 A	Virtual Antibiotic Screening Engine and Multi-Assay Virtual Antibiotic Screening Score (VASS)	Published 30/01/2026 (filed 13/01/2026)	14
202541103130 A	Thermodynamics-Aware Molecular Screening with Adaptive MD/MM-PBSA and Machine-Learning Preselection	Published 28/11/2025 (filed 27/10/2025)	8
202641003237 A	A Deterministic Quantum-Chemically Derived Method and System for Predicting Liquid-Phase Thermophysical and Thermodynamic Properties of Binary Liquid Mixtures	Published 30/01/2026 (filed 12/01/2026)	6

INSTITUTIONAL SERVICE

- ▶ **Academic audits & accreditation:** manages internal and external audits including IQAC/NAAC documentation; as additional NAAC Coordinator, achieved the highest score of 3.35/4.00 among all affiliated colleges in the state.
- ▶ **NIRF rankings:** coordinates the college's NIRF submissions across teaching, research and outreach for three years.
- ▶ **Board of Studies:** Chairman or member for UG & PG Chemistry programmes at Acharya Nagarjuna University and Andhra Kesari University, responsible for curriculum design and examination standards.
- ▶ **Committee membership:** IQAC, NAAC, and Research and Academic Council; contributes to admissions, examinations and continuous quality improvement.

OUTREACH & COMMUNICATION (Most Recent)

- ▶ **National Webinar — “Tiny Wonders, Big Future: Making and Understanding Nanomaterials”** (Physics & Chemistry with IQAC), 3 April 2024; 68 participants. Coordinator.
- ▶ **National Webinar — “Innovative Materials for Sustainable Energy”** (Chemistry & Physics), 29 August 2022; 195 participants. Organising Secretary.
- ▶ **Conference paper — “Computational Chemistry in Drug Discovery”**, National Seminar ACAS-2021, Acharya Nagarjuna University, March 2021.
- ▶ **Conference paper — “Artificial Intelligence in Drug Design and Biomolecular Research”**, International Conference RACPABS-2020, March 2020.
- ▶ **Session Chair — IMCEST-2025 International Conference**, QIS College of Engineering and Technology, 26 November 2025.

PEER REVIEW SERVICE

Active reviewer for international chemistry and chemical engineering journals published by Elsevier, Wiley, and Springer Nature. Reviewer recognition certificates issued by The Journal of Chemical Thermodynamics (4), Results in Optics (2), Chemical Papers (2), Scientific Reports (2), Microbial Risk Analysis (2), and others.

Journal	Scope of Review	Year
Chemical Engineering Journal Advances (Elsevier)	Chemical Thermodynamics/ Machine Learning	2025
ChemistrySelect (Wiley)	ML pipeline for predicting molecular refractive index.	2026
Chemical Papers (Springer Nature)	ML prediction of bio-based oxygenated fuel additives' properties.	2026
Chemical Papers (Springer Nature)	Robust ML modeling of biodiesel's pure fatty acid methyl esters' viscosity.	2026
Chemical Physics Impact (Elsevier)	MD-derived potential of mean force probing hydrophobic coupling.	2026
Discover Chemistry (Springer Nature)	MD study of dialkyl imidazolium ionic liquids with POPC membranes.	2025
The Journal of Chemical Thermodynamics (Elsevier)	Crown-ether, ionic-liquid, anisole system for Li-isotope separation.	2026
The Journal of Chemical Thermodynamics (Elsevier)	C9 aromatic-isomer binary mixtures analyzed by RK, GN, and Eyring.	2026
Microbial Risk Analysis (Elsevier)	Atom-counting and Patel–Erickson–Battley modelling of Gibbs energy.	2025
Malaysian Journal of Chemistry	Thiourea derivative as a non-ionic surfactant.	2026
Results in Optics (Elsevier)	CatBoost/AdaBoost/RF (CSA-tuned) predicts RI over 3,185 measurements.	2026
Results in Optics (Elsevier)	MLP-ANN, LSSVM, RF models of LiBr/H ₂ O refractive index over 2,240 points.	2025

Journal	Scope of Review	Year
Scientific Reports (Springer Nature)	Ivermectin solubilization in hydrophilic and hydrophobic DES.	2026
Scientific Reports (Springer Nature)	Physicochemical characterisation of sulfolane and DES mixtures.	2026
Science Journal of Chemistry (SciencePG)	Excess properties of cumene + aromatic-hydrocarbon systems at 298.15 K.	2026
Science Journal of Chemistry (SciencePG)	Experimental and theoretical ultrasonic study of binary liquid mixtures.	2025

RESEARCH FUNDING

Project / Title	Agency	Amount	Role / Year
Minor Research Project — Synthesis, Characterization and Cis-Trans Isomerization of Azobenzene-Porphyrins / Metalloporphyrins	UGC (SERO), Hyderabad	Rs. 1,40,000	Principal Investigator, 2015–16
Financial Assistance for Conference — “Recent Trends in Chemistry”, KRK Govt. Degree College, Addanki	UGC (SERO), Hyderabad	Rs. 1,41,649	Organiser, 2014–15

AWARDS & HONOURS

- ▶ **State Best Teacher Award in Chemistry** — Government of Andhra Pradesh, 2024 (G.O.Rt.No.163, HE(MC) Dept., 08.11.2024).
- ▶ **Exemplary Performance Award** — presented by the District Collector & Magistrate on behalf of the Government of Andhra Pradesh for exemplary performance in the department.

EDUCATION

Degree	Institution	Year
Ph.D., Chemistry	Acharya Nagarjuna University	2016
M.Phil., Chemistry	Acharya Nagarjuna University	2012
M.Sc., Chemistry	Andhra University	1993
B.Sc., Chemistry (First Class)	Acharya Nagarjuna University	1989

CONTINUOUS LEARNING & RESEARCH TRANSLATION

Dr. Munnangi continually updates his technical skill set and translates new training directly into published research. He completed an 8-week NPTEL-AICTE Faculty Development Programme in “Computational Chemistry and Classical Molecular Dynamics” (September 2018), then shifted his output toward molecular dynamics simulations, modelling SARS-CoV-2 binding energies with the OPLS-AA force field in 2020.

He completed the SWAYAM Plus “AI for Chemistry” course through IITM Pravartak (August 2025); his 2025–2026 patents and papers focus on AI-driven virtual screening and ML-based prediction of thermophysical properties. Consolidated scores for the AI and MD courses were 68% and 66% respectively.

AUTHORED BOOKS

- ▶ Chemistry in Daily Life: Exploring the Everyday Wonders (Amazon KDP; ISBN 979-8867456122)
- ▶ The Secret Life of Tea: A Mugful of Chemistry (Amazon KDP; ISBN 979-8867660291)
- ▶ Chemical Enigmas: Exploring the Unknown in Chemistry (Amazon KDP; ISBN 979-8867685850)
- ▶ Chemical Paradigms: From Heresy to Breakthrough (Amazon KDP; ISBN 979-8867693640)
- ▶ Eureka Moments: Pioneering Innovations that Shaped Our World (Amazon KDP; ISBN 979-8867787929)

PUBLICATIONS

38 peer-reviewed publications (first author: 9; corresponding author: 13 recent publications); 460 citations, h-index 12, i10-index 17 (Google Scholar). Corresponding-author papers are marked with an asterisk (*).

#	Title	Authors	Year	Journal / Publisher	IF
1	AI-assisted, theory-guided electrolyte screening using DFT frontier descriptors and the Rational Discovery Toolkit	Munnangi A.S.M., Munnangi V., Nayeem S.M., Shaik S., Arhan S.M.R., Munnangi S.R.*	2026	Next Materials (Elsevier)	1.9
2	Experimental Measurements, MD Simulations and ML Predictions for the γ -Butyrolactone–N,N-Dimethylacetamide Binary System	Munnangi A.S.M., Koppolu H.K.R., Nayeem S.M., Polineni I., Munnangi S.R.*	2025	ChemistrySelect (Wiley)	2.0
3	Exploring molecular interactions through thermophysical properties and MD simulations in [Emim][NTf2] and 2-EE mixtures	Etukuri N.B., Aangothu S.R., Prathipati S., Munnangi S.R., Khandapu B.M.K., Chintala J.N.P.K., Bollikolla H.B.*	2025	J. Chem. Thermodynamics (Elsevier)	2.2
4	Molecular Interactions and IR Spectral Insights in [Emim][Triflate] and 2-Alkoxyethanol Mixtures: Refractive Index Predictions	Munnangi A.S.M., Aangothu S.R., Krishnan V.B.R.K., Ravulapalli L.T., Munnangi S.R.*	2025	J. Chem. & Eng. Data (ACS)	2.1
5	Characterising molecular interactions of [Emim][triflate] with 2-methoxyethanol and 1-methyl-2-pyrrolidone	Aangothu S.R., Prathipati S., Krishnan V.B.R., Ghanta S.R., Munnangi S.R.*	2025	Physics and Chemistry of Liquids (T&F)	1.1
6	Experimental and MD study of molecular interactions in γ -butyrolactone – dimethyl formamide systems with ML density predictions	Munnangi A.S.M., Nayeem S.M., Koppolu P., Munnangi S.R.*	2025	J. Chem. Thermodynamics (Elsevier)	2.2
7	Integrating experimental data, MD and ML for physicochemical insights into γ -butyrolactone and isopropyl acetate binary system	Munnangi A.S.M., Nayeem S.M., Prathipati S., Munnangi S.R.*	2025	J. Molecular Liquids (Elsevier)	5.2
8	Fusion of Experimental and ML: Predicting Refractive Index and Molecular Interactions in [Bmim][Triflate] with 1-Butanol and 1-Pentanol	Koppolu H.K.R. et al.	2025	Jordan Journal of Chemistry (Scopus)	0.5
9	Exploring molecular interactions of dorzolamide hydrochloride in aqueous solutions: thermophysical techniques and molecular simulations	Rayinuthala Y., Medepalli D.R., Munnangi S.R.*, Nayeem S.M., Ravulapalli L.T.	2024	Canadian J. Chemistry (Scopus)	1.0
10	Thermodynamic insights into moxifloxacin hydrochloride interactions in aqueous solutions	Rayinuthala Y., David Raju M., Munnangi S.R.*, Nayeem S.M., Polineni I.	2024	Chemical Papers (Springer)	2.2
11	Intermolecular interactions in [Bmim][PF6] + 1-octyl-2-pyrrolidone binary mixtures	Prathipati S., Srinivasa Rao V., Munnangi S.R., Gopiseti R.S., Alam M.M., Bollikolla H.B.*	2023	J. Chem. Thermodynamics (Elsevier)	2.2
12	Molecular interactions of memantine hydrochloride in aqueous solutions by thermophysical methods and MD simulations	Rayinuthala Y., David Raju, Munnangi S.R.*, Nayeem S.M., Rameez Arhan S.M.	2023	J. Indian Chemical Society (Elsevier)	3.4
13	Target SARS-CoV-2: binding energies with dexamethasone/umifenovir by MD using OPLS-AA force field	Nayeem S.M.*, Sohail E.M., Ridhima G., Munnangi S.R.	2022	Research on Biomedical Engineering (Springer)	2.0
14	Target SARS-CoV-2: theoretical exploration on clinical suitability of certain drugs	Nayeem S.M.*, Sohail E.M., Srihari N.V., Indira P., Munnangi S.R.	2021	J. Biomolecular Structure & Dynamics (T&F)	2.4
15	A molecular interactions study between [Bmim][PF6] and N-methylpyrrolidone	Prathipati S., Vipparla S.R., Munnangi S.R., Nayeem S.M., Bollikolla H.B.*	2021	J. Chem. Thermodynamics (Elsevier)	2.2
16	Computational exploration for clinical suitability of Remdesivir to SARS-CoV-2	Nayeem S.M.*, Sohail E.M., Sudhir G.P., Munnangi S.R.	2020	European J. Pharmacology (Elsevier)	4.7
17	Volumetric, Ultrasonic, Spectroscopic and MD Studies of [Emim][NTf2] with 2-Propoxyethanol (298.15–318.15 K)	Prathipati S., Aangothu S.R., Munnangi S.R., Khandapu B.M.K., Bollikolla H.B.*	2020	J. Chem. & Eng. Data (ACS)	2.1

#	Title	Authors	Year	Journal / Publisher	IF
18	Thermophysical, optical and spectroscopic study of Ethyl Lactate and Dimethyl Adipate (303.15–318.15 K)	Vani Latha S., Little Flower G., Munnangi S.R., Yugandhar Raju L., Nageswara Rao C.V., Ratnakar*	2019	Physics and Chemistry of Liquids (T&F)	1.1
19	Molecular interactions between [Emim][triflate] & 2-alkoxyethanols and theoretical comparison by PFP theory	Aangothu S.R., Munnangi S.R., Bollikolla H.B.*	2019	J. Chem. Thermodynamics (Elsevier)	2.2
20	Molecular interaction studies of 2-methoxyethanol and [Emim][NTf2]-based ionic liquid	Aangothu S.R., Munnangi S.R., Pushpa Raj G., Bollikolla H.B.*	2019	Physics and Chemistry of Liquids (T&F)	1.1
21	Molecular interactions between [Bmim][PF6] and N-vinyl-2-pyrrolidinone	Suneetha P., Krishna T.S., Gowrisankar M., Munnangi S.R., Ramachandran D.*	2018	J. Thermal Analysis & Calorimetry (Springer)	3.1
22	Volumetric, acoustic, optical and spectroscopic studies of [Bmim][NTf2] and diethyl carbonate	Srinivasa Rao V., Munnangi S.R., Aangothu S.R., Pushpa Raju G., Raju K.T.S., Bollikolla H.B.*	2018	Physics and Chemistry of Liquids (T&F)	1.1
23	Thermophysical investigations and prediction of calorimetric potentials in [Bmim][triflate] with 1-pentanol	Munnangi S.R., Srinivasa Rao G., Nayeem S.M., Raju K., Bollikolla H.B.*	2018	J. Thermal Analysis & Calorimetry (Springer)	3.1
24	Solute–Solvent Interactions in [Bmim][PF6] + 2-Pyrrolidone	Srinivasa Rao V., Munnangi S.R., Raju K.T.S.S., Rani B.L., Bollikolla H.B.*	2018	J. Solution Chemistry (Springer)	1.6
25	Molecular interactions between [Emim][triflate] with 2-methoxyethanol & N-methylpyrrolidone: Experimental and COSMO-RS	Aangothu S.R., Khan I., Munnangi S.R., Bollikolla H.B.*	2018	J. Molecular Liquids (Elsevier)	5.2
26	Intermolecular interactions in [Bmim][NTf2] and propylene carbonate using ultrasonic, optical and FT-IR studies	Srinivasa Rao V., Munnangi S.R., Raju K.T.S.S., Bollikolla H.B.*	2017	Karbala Int. J. Modern Science (Elsevier)	3.1
27	Solute-solvent interactions in [Bmim][NTf2] + dimethylcarbonate using physicochemical properties	Srinivasa Rao V., Munnangi S.R., Nayeem S.M., Raju K.T.S.S., Bala Murali Krishna K., Bollikolla H.B.*	2017	J. Chem. Thermodynamics (Elsevier)	2.2
28	[TPA][Pro] Ionic Liquid as Efficient Reaction Medium for N-tert-Boc Protection of Amines	Durga T.V., Rambabu A., Munnangi S.R., Bollikolla H.B.*	2017	Asian J. Chemistry (Scopus)	0.5
29	Molecular interaction studies in [Emim][triflate] + 1-butanol from density, speed of sound and refractive index	Munnangi S.R., Raju K.T.S.S., Nayeem S.M., Bala Murali Krishna K., Bollikolla H.B.*	2017	Physics and Chemistry of Liquids (T&F)	1.1
30	Thermophysical properties of [Emim][ethylsulfate] and 2-propoxyethanol (298.15–328.15 K)	Munnangi S.R., Raju K.T.S.S., Aangothu S.R., Sharmila N., Bollikolla H.B.*	2016	J. Chem. Thermodynamics (Elsevier)	2.2
31	Molecular interactions in [Emim][triflate] + 1-pentanol from density, speed of sound and refractive index	Munnangi S.R., Khan I., Raju K.T.S.S., Suresh P., Bollikolla H.B.*	2016	J. Chem. Thermodynamics (Elsevier)	2.2
32	Solute–solvent interactions in [Emim][ethylsulfate] + 2-ethoxyethanol	Munnangi S.R., Nayeem S.M., Raju K.T.S.S., Srinivasa Rao V., Bollikolla H.B.*	2016	J. Molecular Liquids (Elsevier)	5.2
33	Excess Thermodynamic Properties of [Emim][ethyl sulfate] and 2-Methoxyethanol (298.15–328.15 K)	Munnangi S.R., Nayeem S.M., Raju K.T.S.S., Srinivasa Rao V., Bollikolla H.B.*	2016	J. Solution Chemistry (Springer)	1.6
34	Solute–solvent interactions in [Emim][BF4] + 2-ethoxyethanol	Munnangi S.R., Nayeem S.M., Raju K.T.S.S., Bollikolla H.B.*	2016	J. Thermal Analysis & Calorimetry (Springer)	3.1
35	Molecular interactions in [Emim][BF4] with 2-methoxyethanol using thermo-acoustic, volumetric and optical properties	Munnangi S.R., Nayeem S.M., Soumini C., Raju K.T.S.S., Bollikolla H.B.*	2016	Thermochimica Acta (Elsevier)	3.5
36	Thermoacoustic, volumetric and viscometric investigations of 1,4-dioxane with n-hexane/n-heptane/n-octane	Nayeem S.M., Kondaiah M., Sreekanth K., Munnangi S.R., Krishna Rao D.*	2016	J. Thermal Analysis & Calorimetry (Springer)	3.1
37	Determination of Lafutidine Through Oxidative Coupling Reaction in Bulk Sample and Dosage Forms	Munnangi S.R., Bollikolla H.B.*	2015	Int. J. Pharmaceutical Sciences & Research	—

#	Title	Authors	Year	Journal / Publisher	IF
38	Revolutionizing Healthcare: The Transformative Role of Machine Learning in Personalized Medicine	<i>Koppolu H.K.R., Munnangi A.S.M., Munnangi S.R., Ravulapalli L.T., Mukkamalla B.R.</i>	2025	J. Rare Cardiovascular Diseases (Scopus)	—