

CURRICULUM VITAE

Tumula Nagaraju

Lecturer in Chemistry,
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Objective

To be associated with a progressive organization that gives scope to apply my knowledge and skills, and to be a part of a team that dynamically works towards the growth of the organization.

Education and Research Experience

- **Ph.D.** in Organic Chemistry, Department of Organic Synthesis and Process Chemistry, CSIR-Indian Institute of Chemical Technology, Hyderabad, India (2015-2020). Secured First Class with Distinction 84.2%.
- **Research Title:** “**Metal-Free Oxidative Strategies for the Construction of Heterocyclic Compounds: Synthesis of 1,2,4-Thiadiazoles, 2-Aminobenzo[d]thiazoles and 1,2,4-Triazolo[1,5-a]pyridines**”.
- **Research Supervisor:** **Dr. P. Radha Krishna**, Chief Scientist, Department of Organic Synthesis and Process Chemistry, CSIR-Indian Institute of Chemical Technology, Hyderabad, India.
- **M.Sc.** (Master of Science) in Organic Chemistry, Department of Chemistry, Andhra University, Visakhapatnam, Andhra Pradesh, India (2011-13). Secured First Class with Distinction 85.8%.
- **B.Sc.** (Bachelor of Science) in Chemistry, Andhra University, Visakhapatnam, Andhra Pradesh, India (2008-11). Secured First Class with 80.8%.
- **B.Ed.** (Bachelor of Education) in Physical Science, Andhra University, Visakhapatnam, Andhra Pradesh, India (2013-14). Secured Second Class with 72.8%.

Fellowships and Awards

- Junior Research Fellow (CSIR, based on National Aptitude Screening) for the period of 2 years in Indian Institute of Chemical Technology, Hyderabad. June 2015 to June 2017.
- Senior Research Fellow (CSIR, based on National Aptitude Screening) for the period of June 2017 to 2020 in Indian Institute of Chemical Technology, Hyderabad.
- **Certificate of merit for University first in M.Sc. Organic Chemistry.**

Achievements

- A novel and expeditious approach for the synthesis of ***N*-fused and 3,4-disubstituted 5-imino-1,2,4-thiadiazole derivatives** has been achieved through the molecular iodine-catalyzed oxidative cyclization.
- A convenient approach for the synthesis of **3,4-disubstituted 5-imino-1,2,4-thiadiazoles and 2-aminobenzo[*d*]thiazoles** has been developed using phenyliodine diacetate (PIDA).
- An effective and expeditious approach for the construction of biologically important **5-guanidino-1,2,4-thiadiazole and 1,2,4-triazolo[1,5-*a*]pyridine derivatives** has been developed. This new protocol involves the phenyliodine(III) diacetate (PhI(OAc)₂)-mediated oxidative cyclization of thioureas/2-aminopyridines and imidates *via* N-S and N-N bond formation at ambient temperature.
- An effective and new approach succeeded for the making of regioselective **3*H*-1,2,4-dithiazol-3-imines** through S-S and C-N bond formation for the first time from benzothioamides and isothiocyanates under transition-metal-free conditions.
- An environmentally benign and convenient strategy for the synthesis of **4,5-disubstituted/*N*-fused 3-amino-1,2,4-triazoles and 3-substituted 5-amino-1,2,4-thiadiazoles** from isothiocyanates has been developed.
- Synthesized proposed structures of novel antimalarial pyranone **Cryptorigidifoliol E**.

Expertise

- Development of Metal-free protocols for the efficient synthesis of biologically active heterocyclic compounds.

- Asymmetric and multi-step synthesis of biologically important natural products.
- Skilled in designing the total synthesis of pyranones.
- Interpretation of the structure of organic compounds using ^1H NMR, ^{13}C NMR, IR, MASS spectroscopic data and 2D-NMR (1D-NOE & 2D-NOSEY) experiments.
- Profound efficiency in handling of hygroscopic air sensitive reagents and reactions.
- Highly conversant with the experimental techniques such as HPLC, IR, Thin layer chromatography and Column chromatography.
- Capable of performing collaborative and independent work, skilled in synthesis of mg-kg Scale.
- Literature search through Reaxys and Scifinder to solve the chemistry related problems.

Research Interests

- Development of new methodologies for the biologically active scaffolds.
- Medicinal Chemistry and Chemical biology.
- Development of parallel synthesis to provide compound libraries to explore SAR.
- Total synthesis of natural products.

Conferences and Symposia

- Actively participated and presented poster in International Conference “**Sustainable Chemistry for Health, Environment and Materials (Su-Chem 2018)**” held at CSIR-Indian Institute of Chemical Technology, Hyderabad, India, during 05-08 August, 2018.
- Actively participated and gave an oral presentation in “**XIV JNOST-2018**” Conference for Research Scholars held at CSIR-Indian Institute of Chemical Technology, Hyderabad, India, during 28th November to 01st December, 2018.
- Actively participated in “**CRSI-ACS National Symposium**” held at CSIR-Indian Institute of Chemical Technology, Hyderabad, India, on 13 July, 2017.
- Actively participated and presented poster in National Conference “**CRSI-National Symposium**” held at CSIR-Indian Institute of Chemical Technology, Hyderabad, India, during 14-16 July, 2017.

- Actively participated in International Conference “**Nature Inspired Initiatives in Chemical Trends (NIICT)**” held at CSIR-Indian Institute of Chemical Technology, Hyderabad, India, during 19-20 September, 2016.

List of Publications

1. I₂-Catalyzed Oxidative N-S Bond Formation: Metal-Free Regiospecific Synthesis of *N*-Fused and 3,4-Disubstituted 5-Imino-1,2,4-Thiadiazoles. **Nagaraju, T.**; Nagesh, J.; Radha Krishna, P.; Mangarao, N. *J. Org. Chem.* **2017**, *82*, 5310-5316.
2. Hypervalent Iodine(III)-Mediated Solvent-Free, Regioselective Synthesis of 3,4-Disubstituted 5-Imino-1,2,4-thiadiazoles and 2-Aminobenzo[*a*]thiazoles. **Nagaraju, T.**; Radha Krishna, P.; Mangarao, N. *Adv. Synth. Catal.* **2018**, *360*, 2806-2812.
3. PhI(OAc)₂-Mediated Regioselective Synthesis of 5-Guanidino-1,2,4-thiadiazoles and 1,2,4-Triazolo[1,5-*a*]pyridines *via* Oxidative N-S and N-N Bond Formation. **Nagaraju, T.**; Radha Krishna, P.; Mangarao, N. *Synthesis* **2019**, *51*, 3600-3610.
4. Transition-Metal-Free PhI(OAc)₂-Mediated Oxidative S-S and C-N Bond Formation: Regioselective Synthesis of 3*H*-1,2,4-Dithiazol-3-imines. **Nagaraju, T.**; Radha Krishna, P. *Tetrahedron Lett.* **2019**, DOI: 10.1016/j.tetlet.2019.151424.
5. I₂-Mediated Oxidative C-N and N-S Bond Formation in Water: A Metal-Free Synthesis of 4,5-Disubstituted/*N*-Fused 3-Amino-1,2,4-triazoles and 3-Substituted 5-Amino-1,2,4-thiadiazoles. Nagesh, J.; **Nagaraju, T.**; Radha Krishna, P.; Mangarao, N. *J. Org. Chem.* **2018**, *83*, 5715-5723.
6. Total Synthesis of the Proposed Structures of Novel Antimalarial Pyranone Cryptorigidifoliol E. Manikanta, G.; **Nagaraju, T.**; Radha Krishna, P. *Synthesis* **2016**, *48*, 4213-4220.

Personal Details

Name	:	TUMULA NAGARAJU
Father Name	:	BANGARRAJU
Date of Birth	:	19 JULY, 1991
Sex	:	Male
Marital Status	:	Married
Nationality	:	Indian

Religion : Hindu
Languages Known : English, Telugu and Hindi
Hobbies : Playing Cricket, Listening Music

Place: Hyderabad

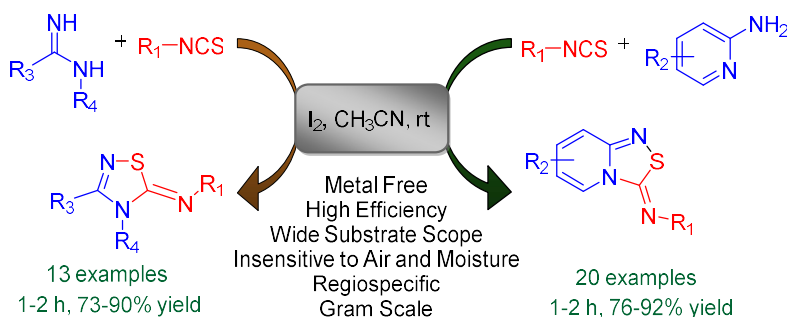
Date: (T. NAGARAJU)

RESEARCH SUMMARY

I₂-Catalyzed Oxidative N-S Bond Formation: Metal-Free Regiospecific Synthesis of N-Fused and 3,4-Disubstituted 5-Imino-1,2,4-thiadiazoles

(J. Org. Chem. 2017, 82, 5310-5316)

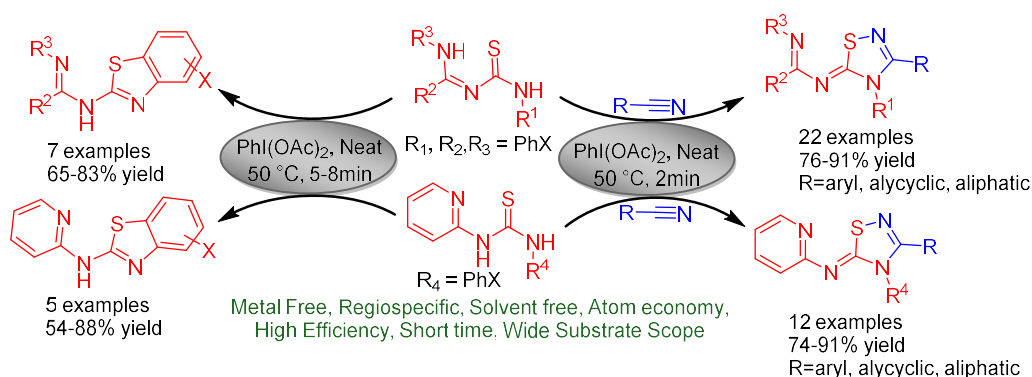
A novel and expeditious approach for the synthesis of N-fused and 3,4-disubstituted 5-imino-1,2,4-thiadiazole derivatives has been achieved through the molecular iodine-catalyzed oxidative cyclization of 2-aminopyridine/amidine and isothiocyanate via N-S bond formation at ambient temperature. The present one-pot transition-metal-free protocol provides the facile and highly efficient regiospecific synthesis of various 1,2,4-thiadiazole derivatives in a scaled-up manner with good to excellent yields using inexpensive I₂ as a catalyst.



Hypervalent Iodine(III)-Mediated Solvent-Free, Regioselective Synthesis of 3,4-Disubstituted 5-Imino-1,2,4-thiadiazoles and 2-Aminobenzo[d]thiazoles

(Adv. Synth. Catal. 2018, 360, 2806-2812)

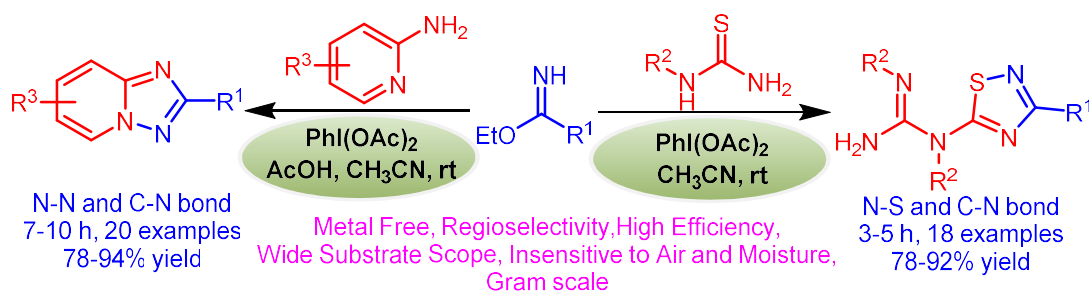
A convenient approach for the synthesis of 3,4-disubstituted 5-imino-1,2,4-thiadiazoles and 2-aminobenzo[*d*]thiazoles has been developed using phenyliodine diacetate (PIDA). This approach involves a metal-free oxidative C-N, N-S and C-S bond formations under neat conditions. High regioselectivity, solvent-free conditions, short reaction time and broad functional group compatibility are the notable features of this report.



PhI(OAc)₂-Mediated Regioselective Synthesis of 5-Guanidino-1,2,4-thiadiazoles and 1,2,4-Triazolo[1,5-*a*]pyridines *via* Oxidative N-S and N-N Bond Formation

(*Synthesis*, 2019, 51, 3600-3610)

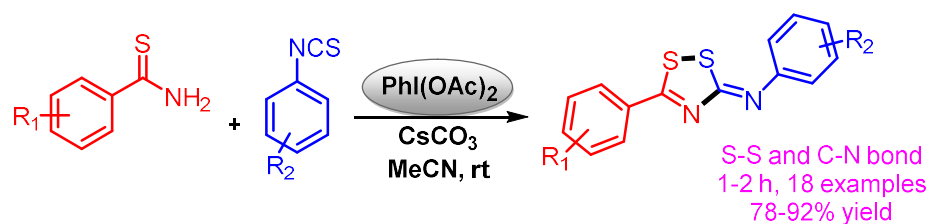
An effective and expeditious approach for the construction of biologically important 5-guanidino-1,2,4-thiadiazole and 1,2,4-triazolo[1,5-*a*]pyridine derivatives has been developed. This new protocol involves the phenyliodine(III) diacetate (PhI(OAc)₂)-mediated oxidative cyclization of thioureas/2-aminopyridines and imidates *via* N-S and N-N bond formation at ambient temperature. This method furnishes the versatile 5-guanidino-1,2,4-thiadiazoles and 1,2,4-triazolo[1,5-*a*]pyridines in a scalable manner with high efficiency and excellent regioselectivity.



Transition-Metal-Free $\text{PhI}(\text{OAc})_2$ -Mediated Oxidative S-S and C-N Bond Formation: Regioselective Synthesis of 3*H*-1,2,4-Dithiazol-3-imines

(*Tetrahedron Lett.* **2019**, DOI: 10.1016/j.tetlet.2019.151424)

An effective and new approach succeeded for the making of regioselective 3*H*-1,2,4-dithiazol-3-imines through S-S and C-N bond formation for the first time from benzothioamides and isothiocyanates under transition-metal-free conditions. This protocol proceeds by using hypervalent iodine(III) compound of phenyliodine diacetate ($\text{PhI}(\text{OAc})_2$) having additive cesium carbonate in acetonitrile solution at room temperature. Which provides facile access from readily available starting materials to synthesize 3*H*-1,2,4-dithiazol-3-imine derivatives with broad substrate scope, insensitive to air and moisture, atom economy and affluent up to gram scale.

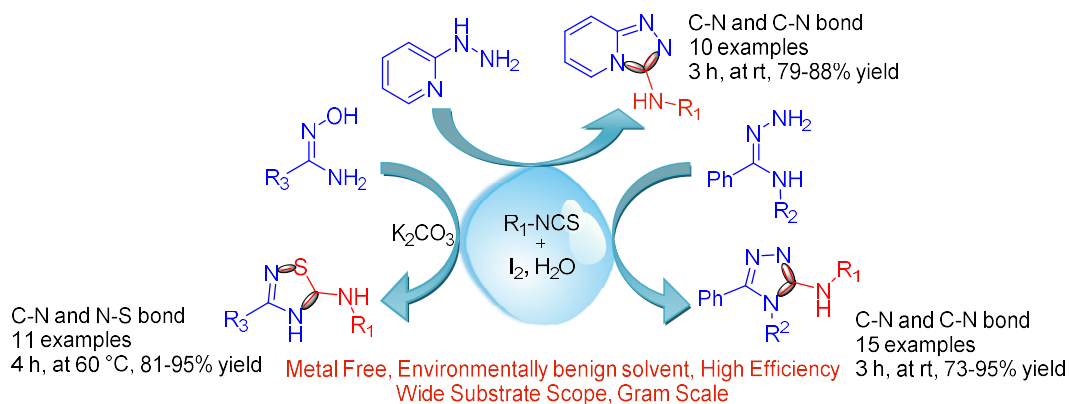


- Transition-metal-free
- Regioselectivity
- Atom economy
- High efficiency
- Wide substrate scope
- Gram-scale
- Insensitive to air and moisture

I_2 -Mediated Oxidative C-N and N-S Bond Formation in Water: A Metal-Free Synthesis of 4,5-Disubstituted/*N*-Fused 3-Amino-1,2,4-triazoles and 3-Substituted 5-Amino-1,2,4-thiadiazoles

(*J. Org. Chem.* **2018**, *83*, 5715-5723)

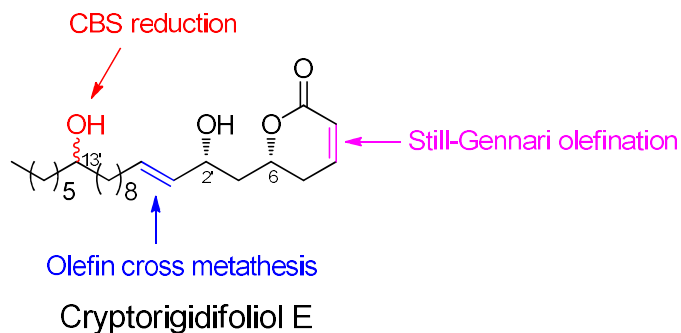
An environmentally benign and convenient strategy for the synthesis of 4,5-disubstituted/*N*-fused 3-amino-1,2,4-triazoles and 3-substituted 5-amino-1,2,4-thiadiazoles from isothiocyanates has been developed. This metal-free method involves I_2 -mediated oxidative C-N and N-S bond formations in water. Furthermore, this facile protocol exhibited excellent substrate tolerance in good to high yields and scalable fashion.



Total synthesis of the proposed structures of novel antimalarial pyranone Cryptorigidifoliol E

(*Synthesis* **2016**, *48*, 4213-4220)

Cryptorigidifoliol E was isolated from root wood of *Cryptocarya rigidifolia*. The synthetic sequence notably features Bartlett-Smith halocyclization to access chiral epoxide followed by its regioselective ring-opening reaction, Still-Gennari olefination, Corey-Bakshi-Shibata (CBS) ynone reduction, and olefin cross-metathesis as the key steps.



References

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