# Appendics

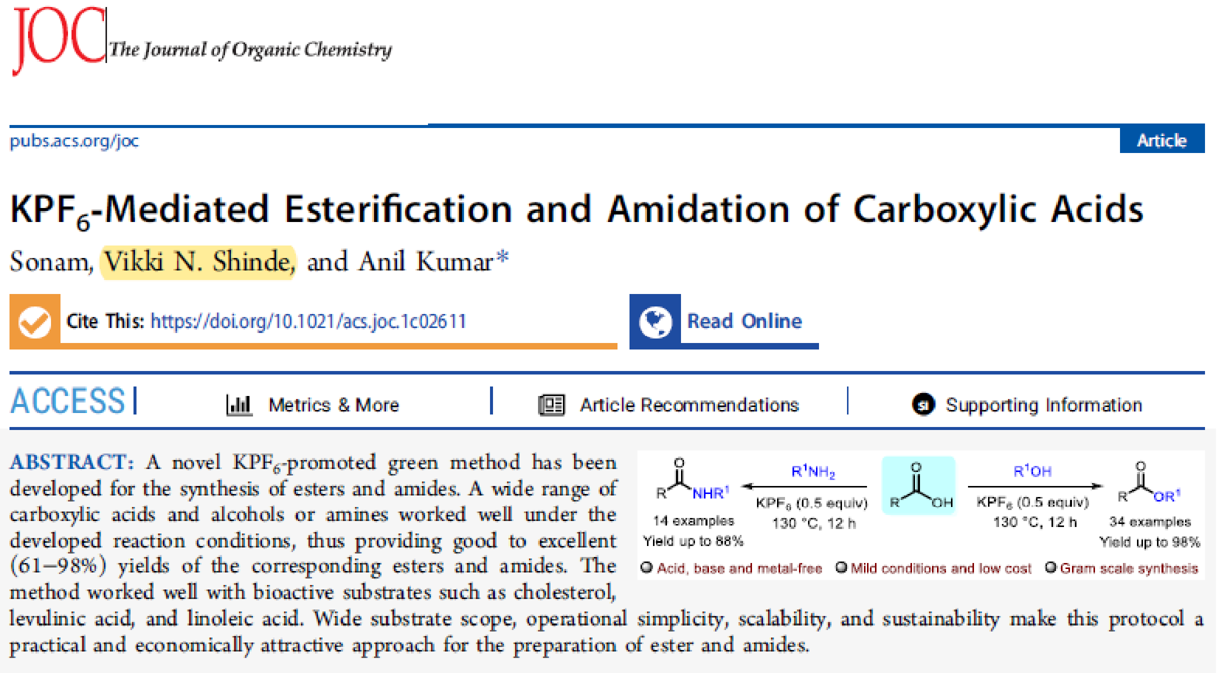
# List of Publications *[A-1]*

1. Nitesh K. Nandwana, **Vikki N. Shinde**, Hitesh K. Saini, Anil Kumar, Copper-catalyzed one-pot tandem reaction for the synthesis of imidaz[1,2-*a*][1,2,3]triazolo[1,5-*a*]quinazoline. *Eur. J. Org. Chem.* **2017**, 6445-6449.
2. **Vikki N. Shinde**, Shiv Dhiman, Krishnan Rangan, Dalip Kumar, Anil Kumar, Synthesis of imidazopyridine-fused indoles *via* one-pot sequential Knoevenagel condensation and cross-dehydrogenative coupling. *Org. Biomol, Chem.*, **2018**, 16, 6123-6132.
3. Om P. S. Patel, Shiv Dhiman, Shahid Khan, **Vikki N. Shinde**, Sonam Jaspal, Manu R. Srivathsa, Prabhat N. Jha, Anil Kumar, Straightforward TBHP-mediated synthesis of 2-amidobenzoic acids from 2-arylindoles and their antimicrobial activity. *Org. Biomol. Chem.*, **2019**, 17, 5962-5970.
4. **Vikki N. Shinde**, Nattamai Bhuvanesh, Anil Kumar, Hemant Joshi, Design and syntheses of palladium complexes of NNN/CNN pincer ligands: catalyst for cross-dehydrogenative coupling reaction of heteroarene. *Organometallics,* **2020**, 39, 324-333.
5. Nitesh K. Nandwana, Shiv Dhiman, **Vikki N. Shinde**, Uwe Beifuss, Anil Kumar, Synthesis of π-expanded azole-fused imidazo[1,2-*a*]pyridine derivatives and their photophysical properties. *Eur. J. Org. Chem.* **2020**, 2576-2582.
6. Om P. S. Patel, Sonam Jaspal, **Vikki N. Shinde**, Nitesh K. Nandwana, Krishnan Rangan, Anil Kumar, Phenyliodine(III) diacetate-mediated 1,2-ipso-migration in mannich bases of imidazo[1,2-*a*]pyridines: Preparation of *N*-acetoxymethyl/ alkoxymethyl-*N*-arylimidazo[1,2-*a*]pyridine-3-amine. *J. Org. Chem.* **2020**, 85, 7309-7321.
7. Neha Meena, Shobha Sharma, Ramprasad Bhatt, **Vikki N. Shinde**, Anurag Prakash Sunda, Nattamai Bhuvanesh, Anil Kumar, Hemant Joshi, A selenium-coordinated palladium(II) trans-dichloride molecular rotor as a catalyst for site-selective annulation of 2-arylimidazo[1,2-*a*]pyridine. *Chem. Commun.* **2020**, 56, 10223.
8. Khima Pandey, **Vikki N. Shinde**, Krishnan Rangan, Anil Kumar, KOH-mediated intramolecular amidation and sulfenylation: A direct approach to access 3-(arylthiol)imidazo[1,2-*a*]pyridine-2-ol. *Tetrahedron* **2020**, 76, 131499.
9. Sonam Jaspal, **Vikki N. Shinde**, Neha Meena, Dhanajay S. Nipate, Krishnan Rangan, Anil Kumar, Metal-free benzoylation of imidazoheterocycles by oxidative decarboxylation of arylglyoxylic acids. *Org. Biomol. Chem.*, **2020**, 18, 9072-9080.

10. **Vikki N. Shinde**, Tapta Kumar Roy, Sonam Jaspal, Dhanajay S. Nipate, Neha Meena, Krishnan Rangan, Anil Kumar, Rhodium(III)-catalyzed annulation of 2-arylimidazo[1,2-*a*]pyridines with maleimides: Synthesis of 1*H*-benzo[*e*]pyrido-[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-diones and their photophysical studies. *Adv. Synth. Catal.*, **2020**, *362*, 5751-5764.
11. **Vikki N. Shinde**, Krishnan Rangan, Dalip Kumar, Anil Kumar, Rhodium(III)-catalyzed dehydrogenative annulation and spirocyclization of 2-arylindoles and 2-(1*H*-pyrazol-1-yl)-1*H*-indoles with maleimides: A facile access to isogranulatimide alkaloids analogues. *J. Org. Chem*. **2021**, 86, 2328-2338.
12. Dhanajay S. Nipate, Sonam Jaspal, **Vikki N. Shinde**, Krishnan Rangan, Anil Kumar, TEMPO-mediated cross-dehydrogenative coupling of indoles and imidazo[1,2-*a*]pyridines with fluorinated alcohol. *Org. Lett*. **2021**, 23, 1373-1377.
13. **Vikki N. Shinde,** Dhanajay S. Nipate, Krishnan Rangan, Anil Kumar, Switchable regioselective hydroalkylation of 2-arylindoles with maleimides. *Org. Biomol. Chem.*, **2021**, 19, 4910-4921
14. **Vikki N. Shinde**, Krishnan Rangan, Dalip Kumar, Anil Kumar, Palladium-catalyzed weakly coordinating lactone directed C–H bond functionalization of 3-arylcoumarins: Synthesis of bioactive coumestan derivatives. *J. Org. Chem*. **2021**, 86, 9755−9770.
15. Nitesh K. Nandwana, Bhawani, **Vikki N. Shinde**, Krishnan Rangan, Anil Kumar, Copper-catalyzed tandem three-component synthesis of imidazo/benzimidazo[1,2-*c*]quinazolines, *ChemistrySelect* **2021**, *6*, 12205– 12208.
16. Dhanajay S. Nipate, Sonam, **Vikki N. Shinde**, Krishnan Rangan, Anil Kumar, TEMPO-Mediated synthesis of indolyl/imidazo[1,2-*a*]pyridinyl-substituted *para*-quinone methides from butylated hydroxytoluene, *J. Org. Chem*. **2021**, *86*, 17090–17100.
17. Neha Meena, Sunil Kumar, **Vikki N. Shinde**, Rajagopala S., Himanshi, Nattamai Bhuvanesh, Anil Kumar, Hemant Joshi, Synthesis of bulky selenium ligand stabilized palladium dichloride molecular rotors and their catalytic applications for silver-free regioselective decarboxylative coupling of coumarin-3-carboxylic Acids: experimental and computational insights. *Chem. Asian J.* **2021**, httpsdoi.org10.1002asia.202101199.
18. Sonam, **Vikki N. Shinde**, Anil Kumar, $KPF_6$-mediated esterification and amidation of carboxylic acids. *J. Org. Chem.* **2022**, *https://doi.org10.1021acs.joc.1c02611*.

19. Neha Meena, **Vikki N. Shinde**, Sonam, Krishnan Rangan, Anil Kumar, Synthesis of imidazofused isoquinolines *via* Ru(II)-catalyzed oxidative annulation of alkenyl azoles with maleimides. (Manuscript under preparation).
20. Sonam, Nitesh K. Nandwana, **Vikki N. Shinde,** Krishnan Rangan, Anil Kumar, Ruthenium(II)-catalyzed C–H activation and cascade annulation towards 6-hydroxy-6-phenylbenzo[4,5]imidazo[2,1-*a*]isoquinolin-5(6*H*)-ones. (Manuscript under preparation).
21. **Vikki N. Shinde**, Neha Meena, Sonam, Krishnan Rangan, Anil Kumar, Catalyst switchable regioselective oxidative annulation of 2-arylimidazo[1,2-*a*]pyridines with cinnamaldehydes. (Manuscript under preparation).
22. **Vikki N. Shinde**, Bhawani, Sonam, Krishnan Rangan, Anil Kumar, Mechanochemical Ruthenium-Catalyzed O*rtho*-Alkenylation of *N*-Heteroaryl Arenes with Alkynes under Ball-Milling Conditions (Manuscript under preparation).
23. **Vikki N. Shinde**, Bhawani, Dhanajay S. Nipate, Sonam, Neha Meena, Krishnan Rangan, Dalip Kumar, Anil Kumar, Manganese(I)-catalyzed *ortho*-hydroalkylation of aryl substituted *N*-heteroaromatic compound with maleimides. *J. Org. Chem.* **2021**, (Submitted)

# Abstract of Publications [A-2]



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## KPF$_6$-Mediated Esterification and Amidation of Carboxylic Acids

Sonam, Vikki N. Shinde, and Anil Kumar*

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**ABSTRACT:** A novel KPF$_6$-promoted green method has been developed for the synthesis of esters and amides. A wide range of carboxylic acids and alcohols or amines worked well under the developed reaction conditions, thus providing good to excellent (61−98%) yields of the corresponding esters and amides. The method worked well with bioactive substrates such as cholesterol, levulinic acid, and linoleic acid. Wide substrate scope, operational simplicity, scalability, and sustainability make this protocol a practical and economically attractive approach for the preparation of ester and amides.

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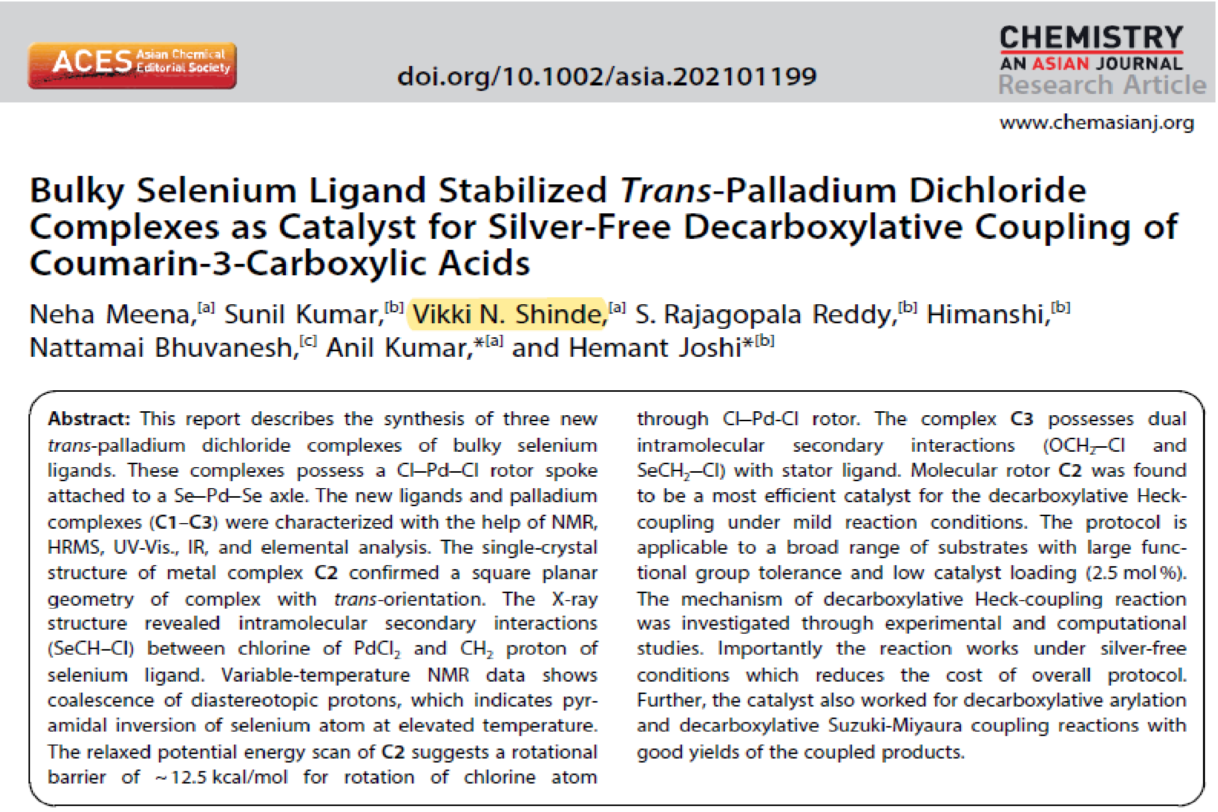

ACES Asian Chemical Editorial Society

doi.org/10.1002/asia.202101199

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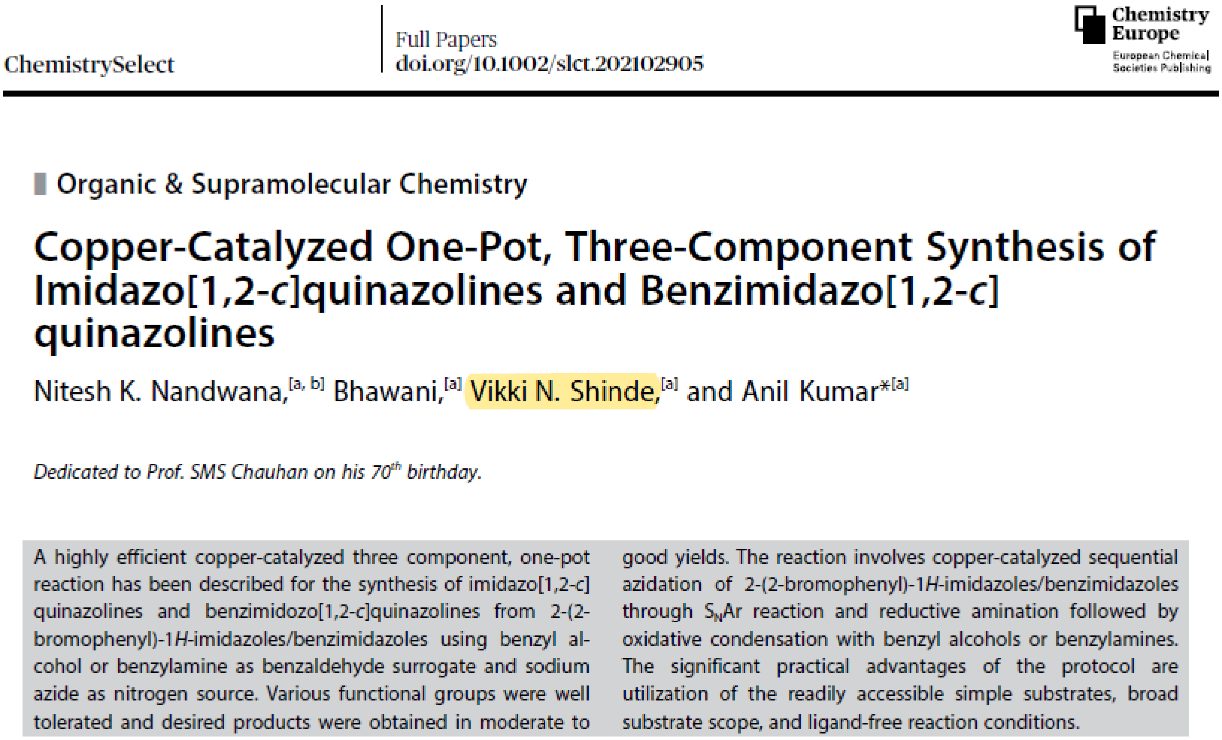
## Bulky Selenium Ligand Stabilized *Trans*-Palladium Dichloride Complexes as Catalyst for Silver-Free Decarboxylative Coupling of Coumarin-3-Carboxylic Acids

Neha Meena,[a] Sunil Kumar,[b] Vikki N. Shinde,[a] S. Rajagopala Reddy,[b] Himanshi,[b] Nattamai Bhuvanesh,[c] Anil Kumar,*[a] and Hemant Joshi*[b]

**Abstract:** This report describes the synthesis of three new *trans*-palladium dichloride complexes of bulky selenium ligands. These complexes possess a Cl–Pd–Cl rotor spoke attached to a Se–Pd–Se axle. The new ligands and palladium complexes (**C1**–**C3**) were characterized with the help of NMR, HRMS, UV-Vis., IR, and elemental analysis. The single-crystal structure of metal complex **C2** confirmed a square planar geometry of complex with *trans*-orientation. The X-ray structure revealed intramolecular secondary interactions (SeCH–Cl) between chlorine of PdCl$_2$ and CH$_2$ proton of selenium ligand. Variable-temperature NMR data shows coalescence of diastereotopic protons, which indicates pyramidal inversion of selenium atom at elevated temperature. The relaxed potential energy scan of **C2** suggests a rotational barrier of ~12.5 kcal/mol for rotation of chlorine atom through Cl–Pd-Cl rotor. The complex **C3** possesses dual intramolecular secondary interactions (OCH$_2$–Cl and SeCH$_2$–Cl) with stator ligand. Molecular rotor **C2** was found to be a most efficient catalyst for the decarboxylative Heck-coupling under mild reaction conditions. The protocol is applicable to a broad range of substrates with large functional group tolerance and low catalyst loading (2.5 mol%). The mechanism of decarboxylative Heck-coupling reaction was investigated through experimental and computational studies. Importantly the reaction works under silver-free conditions which reduces the cost of overall protocol. Further, the catalyst also worked for decarboxylative arylation and decarboxylative Suzuki-Miyaura coupling reactions with good yields of the coupled products.



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Organic & Supramolecular Chemistry

## Copper-Catalyzed One-Pot, Three-Component Synthesis of Imidazo[1,2-*c*]quinazolines and Benzimidazo[1,2-*c*]quinazolines

Nitesh K. Nandwana,[a, b] Bhawani,[a] Vikki N. Shinde,[a] and Anil Kumar*[a]

*Dedicated to Prof. SMS Chauhan on his 70th birthday.*

A highly efficient copper-catalyzed three component, one-pot reaction has been described for the synthesis of imidazo[1,2-*c*]quinazolines and benzimidozo[1,2-*c*]quinazolines from 2-(2-bromophenyl)-1*H*-imidazoles/benzimidazoles using benzyl alcohol or benzylamine as benzaldehyde surrogate and sodium azide as nitrogen source. Various functional groups were well tolerated and desired products were obtained in moderate to good yields. The reaction involves copper-catalyzed sequential azidation of 2-(2-bromophenyl)-1*H*-imidazoles/benzimidazoles through $S_N$Ar reaction and reductive amination followed by oxidative condensation with benzyl alcohols or benzylamines. The significant practical advantages of the protocol are utilization of the readily accessible simple substrates, broad substrate scope, and ligand-free reaction conditions.

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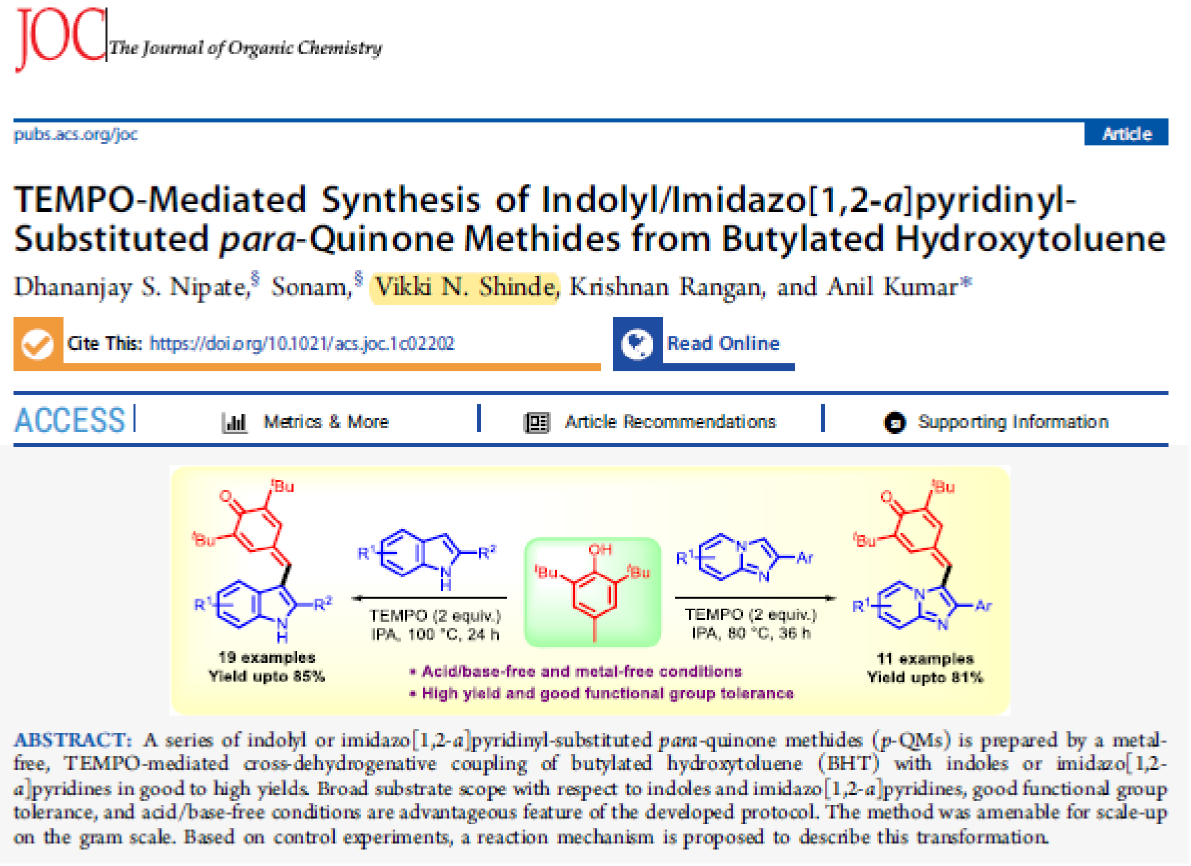

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## TEMPO-Mediated Synthesis of Indolyl/Imidazo[1,2-*a*]pyridinyl-Substituted *para*-Quinone Methides from Butylated Hydroxytoluene

Dhananjay S. Nipate,§ Sonam,§ Vikki N. Shinde, Krishnan Rangan, and Anil Kumar*

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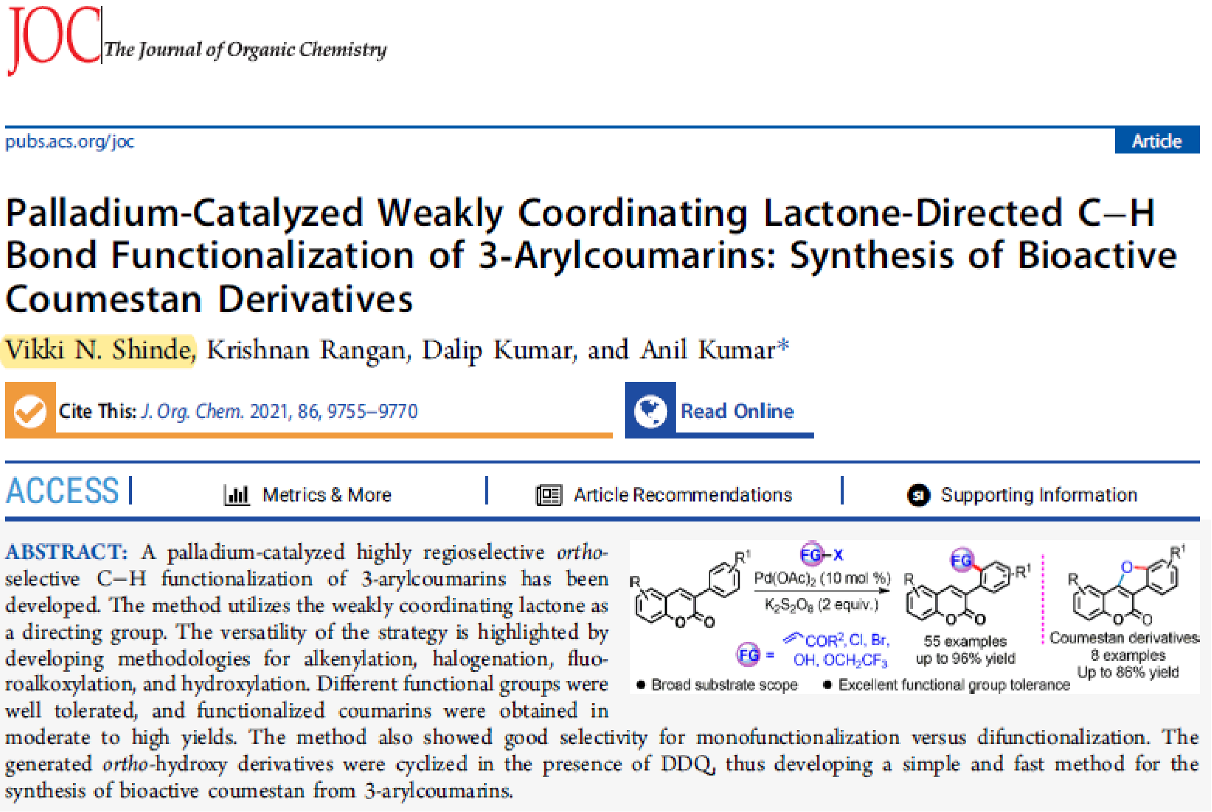
**ABSTRACT:** A series of indolyl or imidazo[1,2-*a*]pyridinyl-substituted *para*-quinone methides (*p*-QMs) is prepared by a metal-free, TEMPO-mediated cross-dehydrogenative coupling of butylated hydroxytoluene (BHT) with indoles or imidazo[1,2-*a*]pyridines in good to high yields. Broad substrate scope with respect to indoles and imidazo[1,2-*a*]pyridines, good functional group tolerance, and acid/base-free conditions are advantageous feature of the developed protocol. The method was amenable for scale-up on the gram scale. Based on control experiments, a reaction mechanism is proposed to describe this transformation.



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# Palladium-Catalyzed Weakly Coordinating Lactone-Directed C−H Bond Functionalization of 3-Arylcoumarins: Synthesis of Bioactive Coumestan Derivatives

Vikki N. Shinde, Krishnan Rangan, Dalip Kumar, and Anil Kumar*

Cite This: *J. Org. Chem.* 2021, 86, 9755−9770 Read Online

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**ABSTRACT:** A palladium-catalyzed highly regioselective *ortho*-selective C−H functionalization of 3-arylcoumarins has been developed. The method utilizes the weakly coordinating lactone as a directing group. The versatility of the strategy is highlighted by developing methodologies for alkenylation, halogenation, fluoroalkoxylation, and hydroxylation. Different functional groups were well tolerated, and functionalized coumarins were obtained in moderate to high yields. The method also showed good selectivity for monofunctionalization versus difunctionalization. The generated *ortho*-hydroxy derivatives were cyclized in the presence of DDQ, thus developing a simple and fast method for the synthesis of bioactive coumestan from 3-arylcoumarins.

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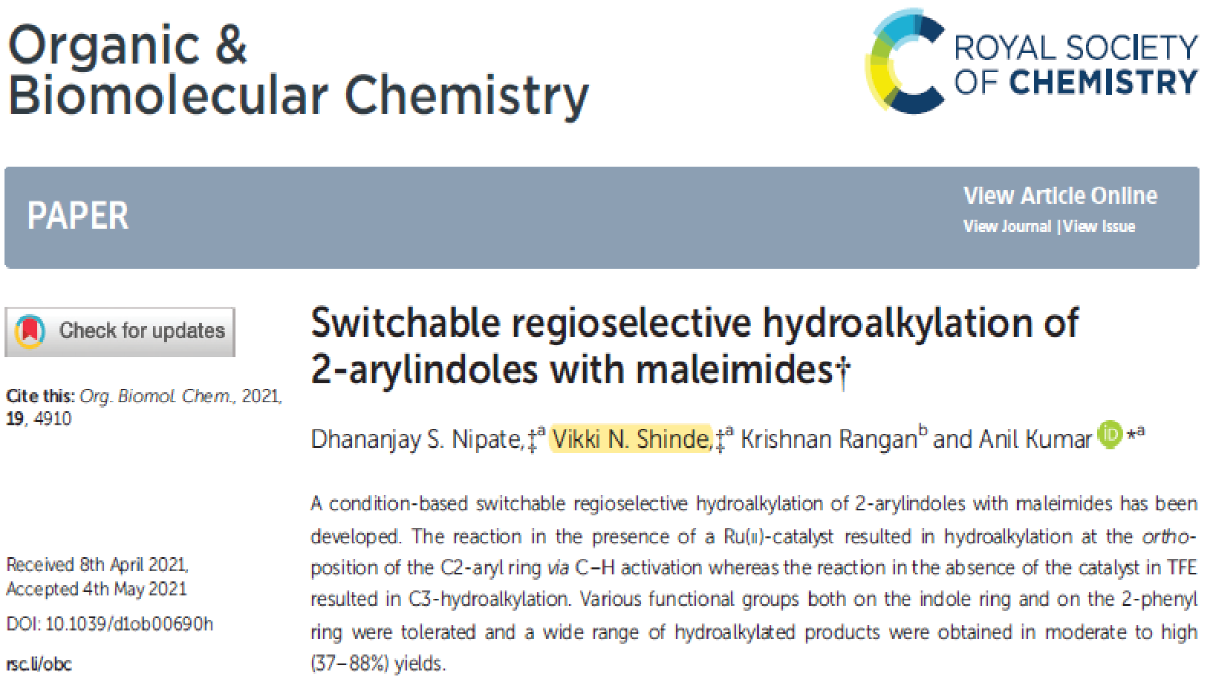

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# Switchable regioselective hydroalkylation of 2-arylindoles with maleimides†

Dhananjay S. Nipate,‡[a] Vikki N. Shinde,‡[a] Krishnan Rangan[b] and Anil Kumar *[a]

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Accepted 4th May 2021

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rsc.li/obc

A condition-based switchable regioselective hydroalkylation of 2-arylindoles with maleimides has been developed. The reaction in the presence of a Ru(II)-catalyst resulted in hydroalkylation at the *ortho*-position of the C2-aryl ring *via* C−H activation whereas the reaction in the absence of the catalyst in TFE resulted in C3-hydroalkylation. Various functional groups both on the indole ring and on the 2-phenyl ring were tolerated and a wide range of hydroalkylated products were obtained in moderate to high (37–88%) yields.

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# TEMPO-Mediated Cross-Dehydrogenative Coupling of Indoles and Imidazo[1,2-*a*]pyridines with Fluorinated Alcohols

Dhananjay S. Nipate,[§] Sonam Jaspal,[§] Vikki N. Shinde, Krishnan Rangan, and Anil Kumar*

**Cite This:** *Org. Lett.* 2021, 23, 1373−1377 **Read Online**

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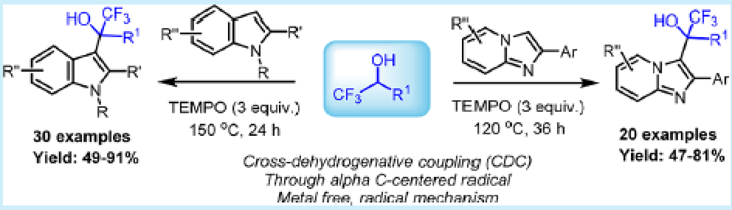

**ABSTRACT:** A simple and highly efficient metal-free method has been developed for hydroxyfluoroalkylation of indoles and imidazo[1,2-*a*]pyridines via TEMPO-mediated C($sp^3$)−H and C($sp^2$)−H bond cross-dehydrogenative coupling of fluorinated alcohols and indoles. The protocol showed broad substrate scope, afforded good yields of hydroxyfluoroalkylated products, and was amenable for scale-up. Mechanistic investigation indicated involvement of the radical pathway.

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# Rhodium(III)-Catalyzed Dehydrogenative Annulation and Spirocyclization of 2-Arylindoles and 2-(1*H*-Pyrazol-1-yl)-1*H*-indoles with Maleimides: A Facile Access to Isogranulatimide Alkaloid Analogues

Vikki N. Shinde, Krishnan Rangan, Dalip Kumar, and Anil Kumar*

**Cite This:** *J. Org. Chem.* 2021, 86, 2328−2338 **Read Online**

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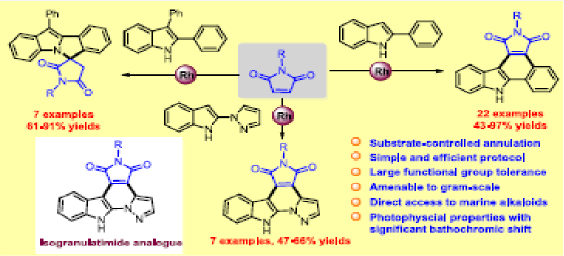
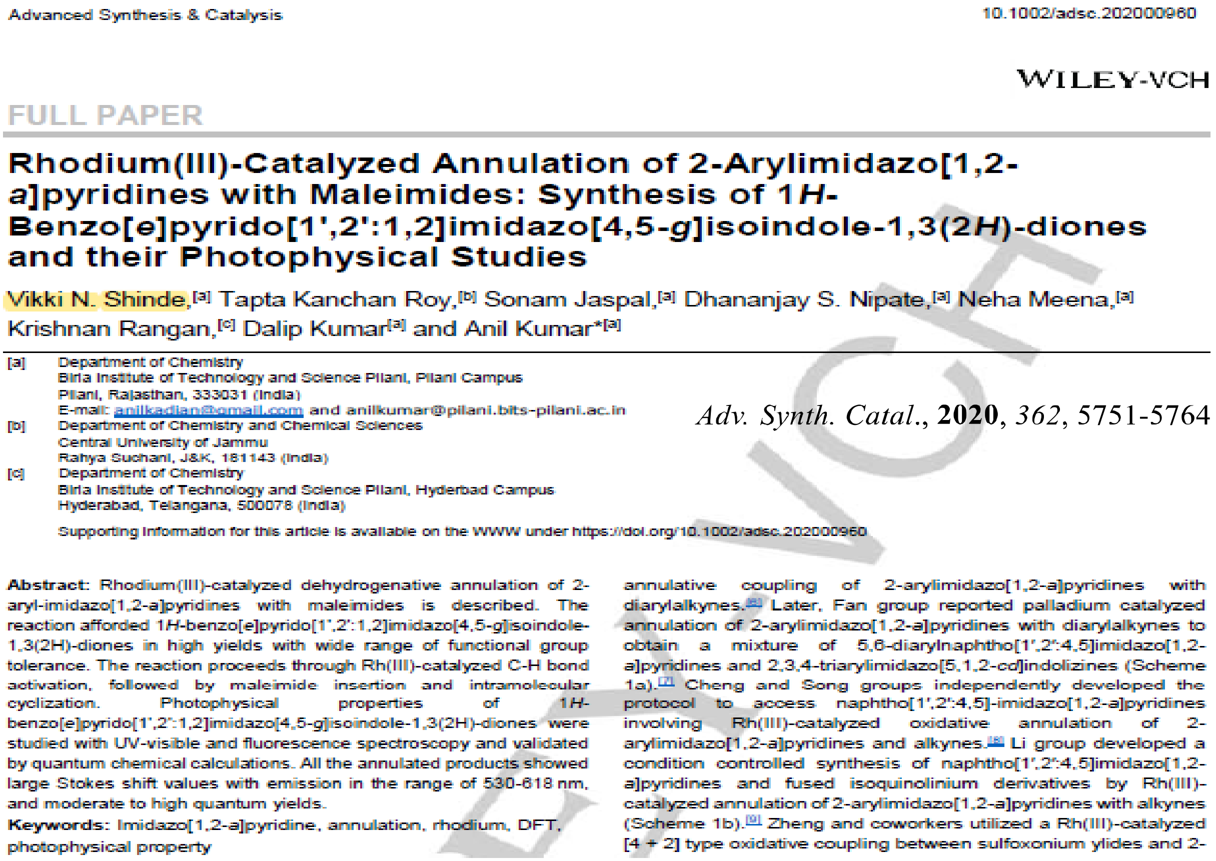
**ABSTRACT:** A Rh(III)-catalyzed dehydrogenative annulation and spirocyclization of 2-arylindoles and 2-(1*H*-pyrazol-1-yl)-1*H*-indole with maleimides is described. The cascade protocol provided highly functionalized benzo[*a*]pyrrolo[3,4-*c*]carbazole-1,3(2*H*,8*H*)-diones and spiro[isoindolo[2,1-*a*]indole-6,3′-pyrrolidine]-2′,5′-diones in good to excellent. The developed reaction methodology exhibited broad substrate scope with good functional group tolerance and is operationally simple and scalable. Photophysical properties of the annulated products were investigated. The annulated product of 2-(1*H*-pyrazol-1-yl)-1*H*-indole showed high absorption and emission values with a large red-shift as compared to that of 2-phenylindole.





Advanced Synthesis & Catalysis 10.1002/adsc.202000960

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FULL PAPER

# Rhodium(III)-Catalyzed Annulation of 2-Arylimidazo[1,2-*a*]pyridines with Maleimides: Synthesis of 1*H*-Benzo[*e*]pyrido[1',2':1,2]imidazo[4,5-*g*]isoindole-1,3(2*H*)-diones and their Photophysical Studies

Vikki N. Shinde,[a] Tapta Kanchan Roy,[b] Sonam Jaspal,[a] Dhananjay S. Nipate,[a] Neha Meena,[a] Krishnan Rangan,[c] Dalip Kumar[a] and Anil Kumar*[a]

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*Adv. Synth. Catal.*, **2020**, *362*, 5751-5764

Supporting information for this article is available on the WWW under https://doi.org/10.1002/adsc.202000960

**Abstract:** Rhodium(III)-catalyzed dehydrogenative annulation of 2-aryl-imidazo[1,2-a]pyridines with maleimides is described. The reaction afforded 1*H*-benzo[e]pyrido[1',2':1,2]imidazo[4,5-g]isoindole-1,3(2H)-diones in high yields with wide range of functional group tolerance. The reaction proceeds through Rh(III)-catalyzed C-H bond activation, followed by maleimide insertion and intramolecular cyclization. Photophysical properties of 1*H*-benzo[e]pyrido[1',2':1,2]imidazo[4,5-g]isoindole-1,3(2H)-diones were studied with UV-visible and fluorescence spectroscopy and validated by quantum chemical calculations. All the annulated products showed large Stokes shift values with emission in the range of 530-618 nm, and moderate to high quantum yields.

**Keywords:** Imidazo[1,2-a]pyridine, annulation, rhodium, DFT, photophysical property

annulative coupling of 2-arylimidazo[1,2-a]pyridines with diarylalkynes.[6] Later, Fan group reported palladium catalyzed annulation of 2-arylimidazo[1,2-a]pyridines with diarylalkynes to obtain a mixture of 5,6-diarylnaphtho[1',2':4,5]imidazo[1,2-a]pyridines and 2,3,4-triarylimidazo[5,1,2-*cd*]indolizines (Scheme 1a).[7] Cheng and Song groups independently developed the protocol to access naphtho[1',2':4,5]-imidazo[1,2-a]pyridines involving Rh(III)-catalyzed oxidative annulation of 2-arylimidazo[1,2-a]pyridines and alkynes.[8] Li group developed a condition controlled synthesis of naphtho[1',2':4,5]imidazo[1,2-a]pyridines and fused isoquinolinium derivatives by Rh(III)-catalyzed annulation of 2-arylimidazo[1,2-a]pyridines with alkynes (Scheme 1b).[9] Zheng and coworkers utilized a Rh(III)-catalyzed [4 + 2] type oxidative coupling between sulfoxonium ylides and 2-

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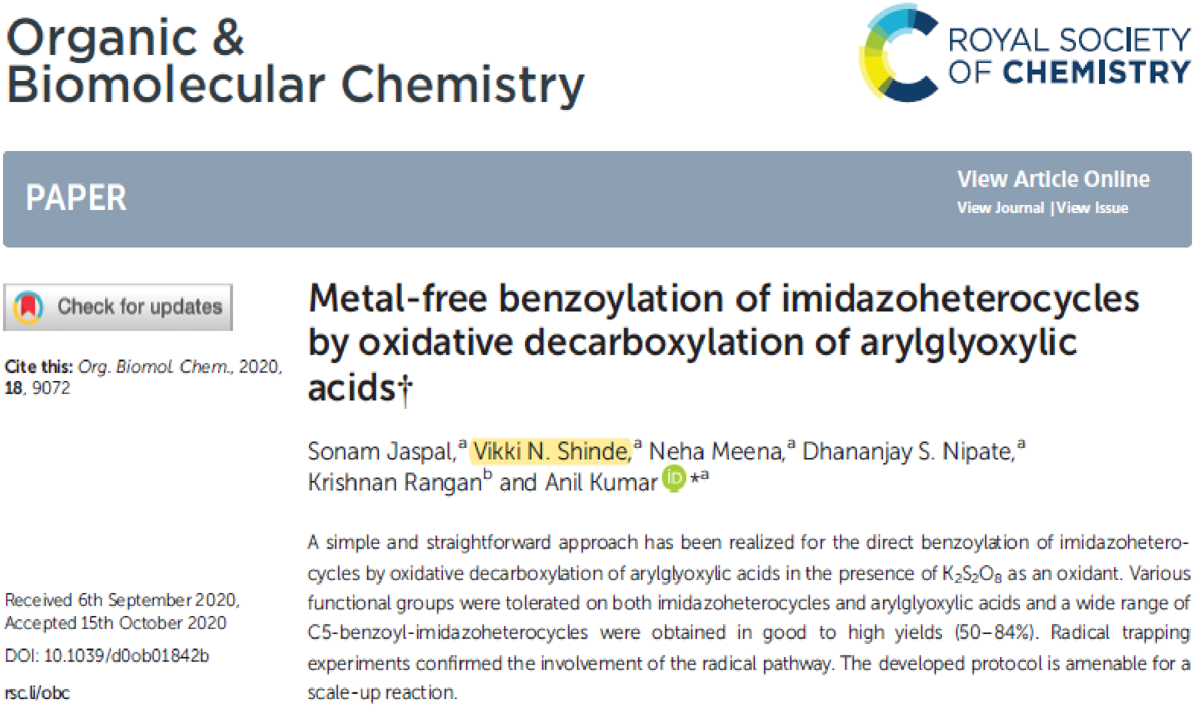

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**Cite this:** *Org. Biomol. Chem.*, 2020, **18**, 9072

# Metal-free benzoylation of imidazoheterocycles by oxidative decarboxylation of arylglyoxylic acids†

Sonam Jaspal,[a] Vikki N. Shinde,[a] Neha Meena,[a] Dhananjay S. Nipate,[a] Krishnan Rangan[b] and Anil Kumar *[a]

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Accepted 15th October 2020

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A simple and straightforward approach has been realized for the direct benzoylation of imidazoheterocycles by oxidative decarboxylation of arylglyoxylic acids in the presence of $K_2S_2O_8$ as an oxidant. Various functional groups were tolerated on both imidazoheterocycles and arylglyoxylic acids and a wide range of C5-benzoyl-imidazoheterocycles were obtained in good to high yields (50–84%). Radical trapping experiments confirmed the involvement of the radical pathway. The developed protocol is amenable for a scale-up reaction.

Tetrahedron 76 (2020) 131499

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# KOH-mediated intramolecular amidation and sulfenylation: A direct approach to access 3-(arylthio)imidazo[1,2-*a*]pyridin-2-ols

Khima Pandey [a], Vikki N. Shinde [a], Krishnan Rangan [b], Anil Kumar [a, *]

[a] *Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, 333031, India*
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Imidazo[1,2-*a*]pyridine
2-Aminopyridinium salt
Potassium hydroxide

## ABSTRACT

A simple and facile method for the synthesis of 3-(arylthio)imidazo[1,2-*a*]pyridin-2-ols has been developed by a KOH-mediated reaction of 2-aminopyridinium bromides with aryl thiols. The method afforded a wide range of 3-(arylthio)imidazo[1,2-*a*]pyridin-2-ols in moderate to excellent (56–95%) yields with excellent functional group tolerance. Synthetic utility of the protocol was demonstrated by gram-scale reaction and preparation of 2-aryl-3-(*p*-tolylthio)imidazo[1,2-*a*]pyridines from 3-(*p*-tolylthio)imidazo[1,2-*a*]pyridin-2-ol.

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rsc.li/chemcomm

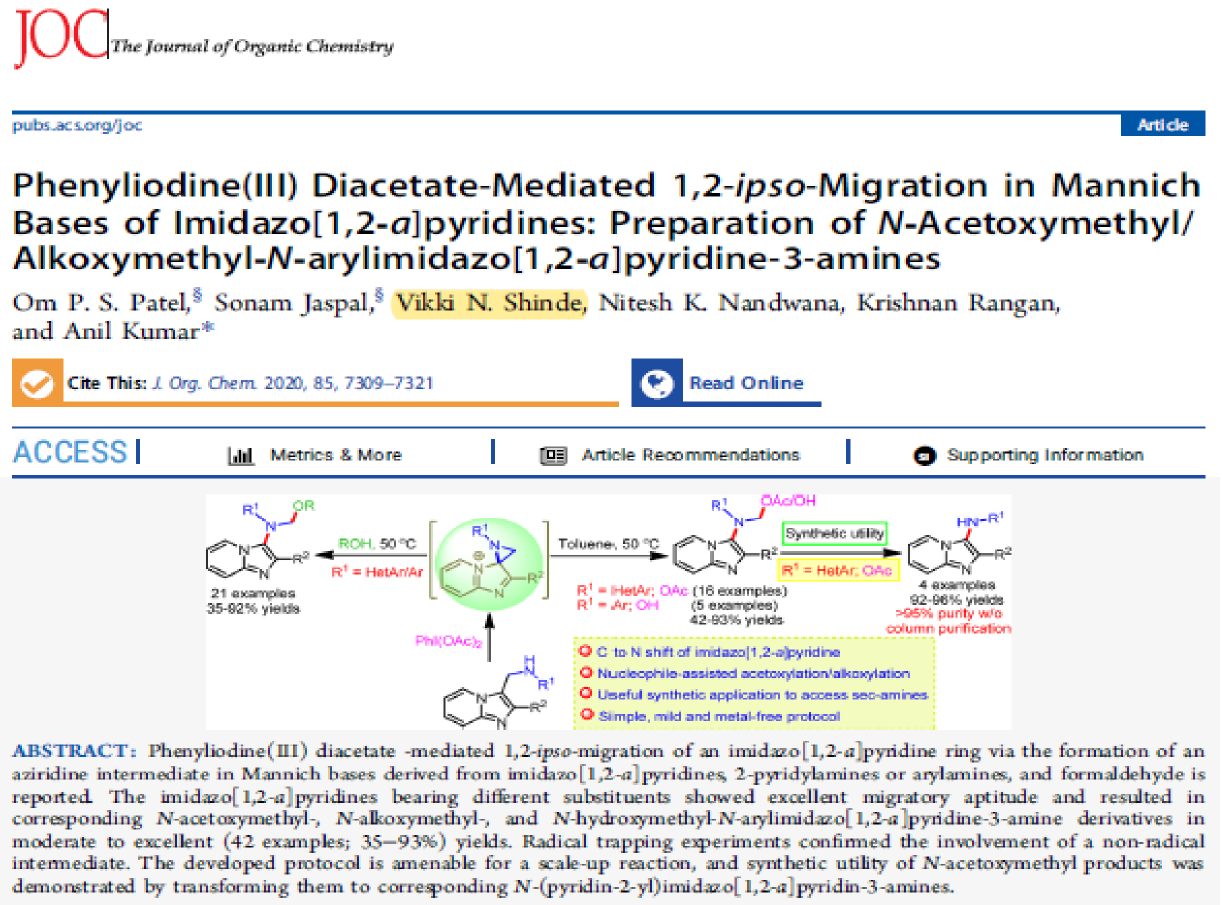
# A selenium-coordinated palladium(II) *trans*-dichloride molecular rotor as a catalyst for site-selective annulation of 2-arylimidazo[1,2-*a*]pyridines†

Neha Meena,[a] Shobha Sharma,[b] Ramprasad Bhatt,[a] Vikki N. Shinde,[a] Anurag Prakash Sunda,[c] Nattamai Bhuvanesh,[d] Anil Kumar *[a] and Hemant Joshi *[e]

**This report describes the synthesis of a new class of secondary interaction (SeCH···Cl)-controlled molecular rotor having a Cl–Pd–Cl rotor spoke attached onto a Se–Pd–Se axle. NMR data acquired at various temperatures established $\Delta G^{\ddagger}_{298K}/\Delta G^{\ddagger}_{350K}$ values of 15.5 and 17.2 kcal mol$^{-1}$ for a roughly 4.5 Å-long rotor. The molecular rotor showed excellent catalytic activity with reverse regioselectivity for annulation of 2-arylimidazo[1,2-a]pyridines (yields: ∼53–78%) with only 1.5 mol% catalyst loading.**

molecules.[1b] The Garcia-Garibay, Setaka, and Gladysz groups have explored molecular rotors in depth.

Triptycene rotors are among the very first extensively studied solution-state molecular rotors.[6] The shape, size and symmetry of the rotor unit significantly influence the rotor movement. Modern molecular machines have undergone careful design modifications to achieve rotor mobility in the solid state.[7] With respect to design, mostly all of the stator units are large organic



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# Phenyliodine(III) Diacetate-Mediated 1,2-*ipso*-Migration in Mannich Bases of Imidazo[1,2-*a*]pyridines: Preparation of *N*-Acetoxymethyl/Alkoxymethyl-*N*-arylimidazo[1,2-*a*]pyridine-3-amines

Om P. S. Patel,§ Sonam Jaspal,§ Vikki N. Shinde, Nitesh K. Nandwana, Krishnan Rangan, and Anil Kumar*

Cite This: *J. Org. Chem.* 2020, 85, 7309−7321 Read Online

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**ABSTRACT:** Phenyliodine(III) diacetate -mediated 1,2-*ipso*-migration of an imidazo[1,2-*a*]pyridine ring via the formation of an aziridine intermediate in Mannich bases derived from imidazo[1,2-*a*]pyridines, 2-pyridylamines or arylamines, and formaldehyde is reported. The imidazo[1,2-*a*]pyridines bearing different substituents showed excellent migratory aptitude and resulted in corresponding *N*-acetoxymethyl-, *N*-alkoxymethyl-, and *N*-hydroxymethyl-*N*-arylimidazo[1,2-*a*]pyridine-3-amine derivatives in moderate to excellent (42 examples; 35−93%) yields. Radical trapping experiments confirmed the involvement of a non-radical intermediate. The developed protocol is amenable for a scale-up reaction, and synthetic utility of *N*-acetoxymethyl products was demonstrated by transforming them to corresponding *N*-(pyridin-2-yl)imidazo[1,2-*a*]pyridin-3-amines.

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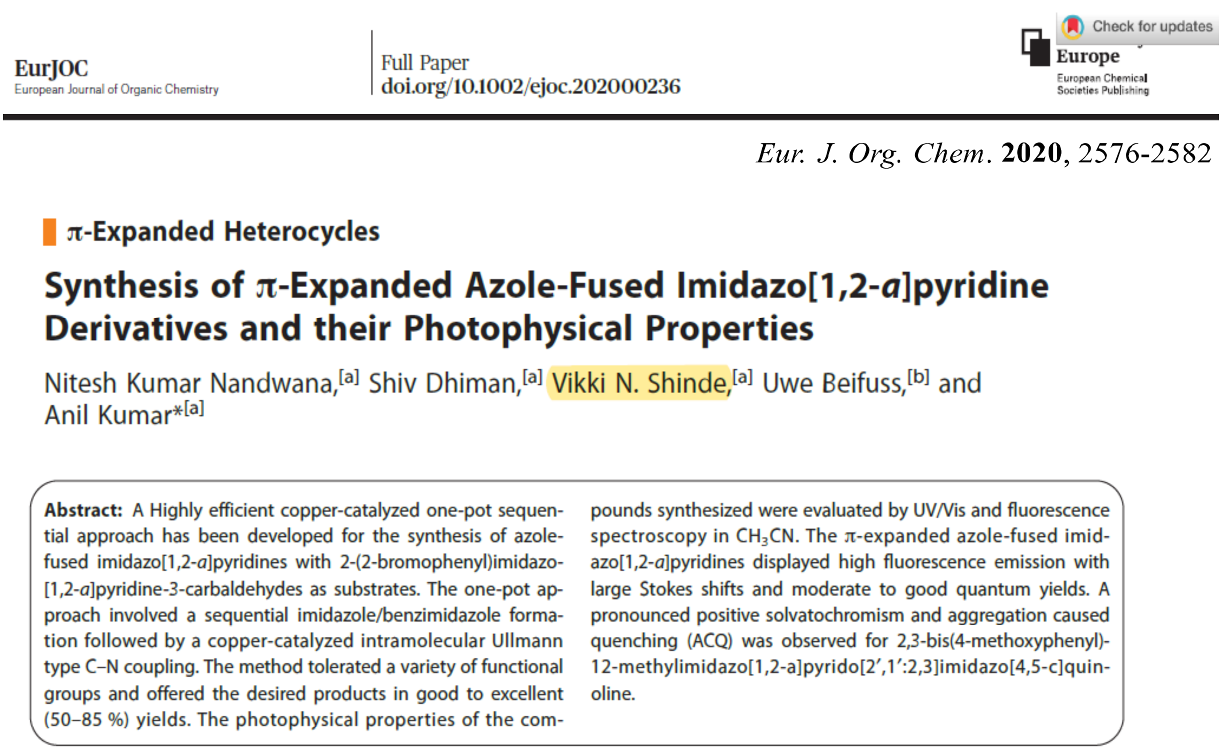

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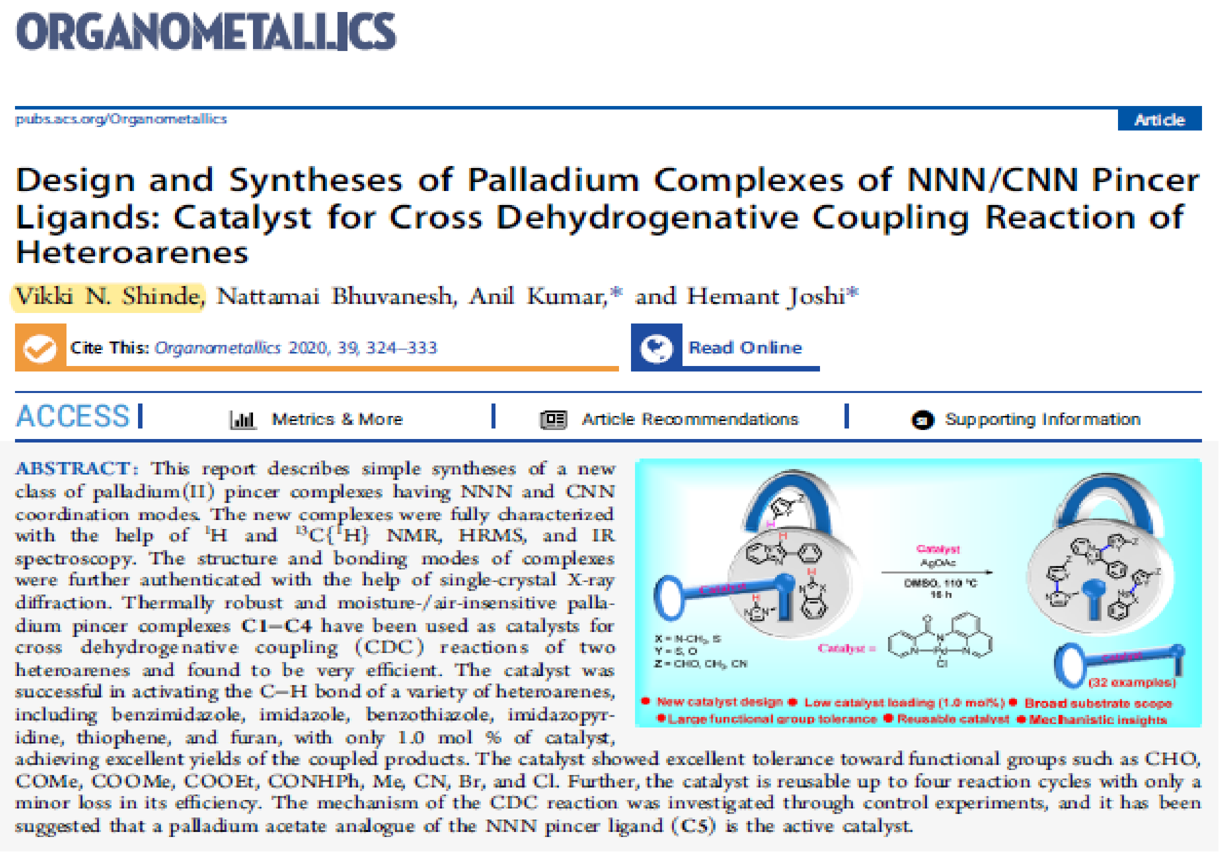
π-Expanded Heterocycles

# Synthesis of π-Expanded Azole-Fused Imidazo[1,2-*a*]pyridine Derivatives and their Photophysical Properties

Nitesh Kumar Nandwana,[a] Shiv Dhiman,[a] Vikki N. Shinde,[a] Uwe Beifuss,[b] and Anil Kumar*[a]

**Abstract:** A Highly efficient copper-catalyzed one-pot sequential approach has been developed for the synthesis of azole-fused imidazo[1,2-*a*]pyridines with 2-(2-bromophenyl)imidazo[1,2-*a*]pyridine-3-carbaldehydes as substrates. The one-pot approach involved a sequential imidazole/benzimidazole formation followed by a copper-catalyzed intramolecular Ullmann type C–N coupling. The method tolerated a variety of functional groups and offered the desired products in good to excellent (50–85 %) yields. The photophysical properties of the compounds synthesized were evaluated by UV/Vis and fluorescence spectroscopy in $CH_3CN$. The π-expanded azole-fused imidazo[1,2-*a*]pyridines displayed high fluorescence emission with large Stokes shifts and moderate to good quantum yields. A pronounced positive solvatochromism and aggregation caused quenching (ACQ) was observed for 2,3-bis(4-methoxyphenyl)-12-methylimidazo[1,2-a]pyrido[2′,1′:2,3]imidazo[4,5-c]quinoline.



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# Design and Syntheses of Palladium Complexes of NNN/CNN Pincer Ligands: Catalyst for Cross Dehydrogenative Coupling Reaction of Heteroarenes

Vikki N. Shinde, Nattamai Bhuvanesh, Anil Kumar,* and Hemant Joshi*

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**ABSTRACT:** This report describes simple syntheses of a new class of palladium(II) pincer complexes having NNN and CNN coordination modes. The new complexes were fully characterized with the help of $^1$H and $^{13}$C{$^1$H} NMR, HRMS, and IR spectroscopy. The structure and bonding modes of complexes were further authenticated with the help of single-crystal X-ray diffraction. Thermally robust and moisture-/air-insensitive palladium pincer complexes C1−C4 have been used as catalysts for cross dehydrogenative coupling (CDC) reactions of two heteroarenes and found to be very efficient. The catalyst was successful in activating the C−H bond of a variety of heteroarenes, including benzimidazole, imidazole, benzothiazole, imidazopyridine, thiophene, and furan, with only 1.0 mol % of catalyst, achieving excellent yields of the coupled products. The catalyst showed excellent tolerance toward functional groups such as CHO, COMe, COOMe, COOEt, CONHPh, Me, CN, Br, and Cl. Further, the catalyst is reusable up to four reaction cycles with only a minor loss in its efficiency. The mechanism of the CDC reaction was investigated through control experiments, and it has been suggested that a palladium acetate analogue of the NNN pincer ligand (C5) is the active catalyst.

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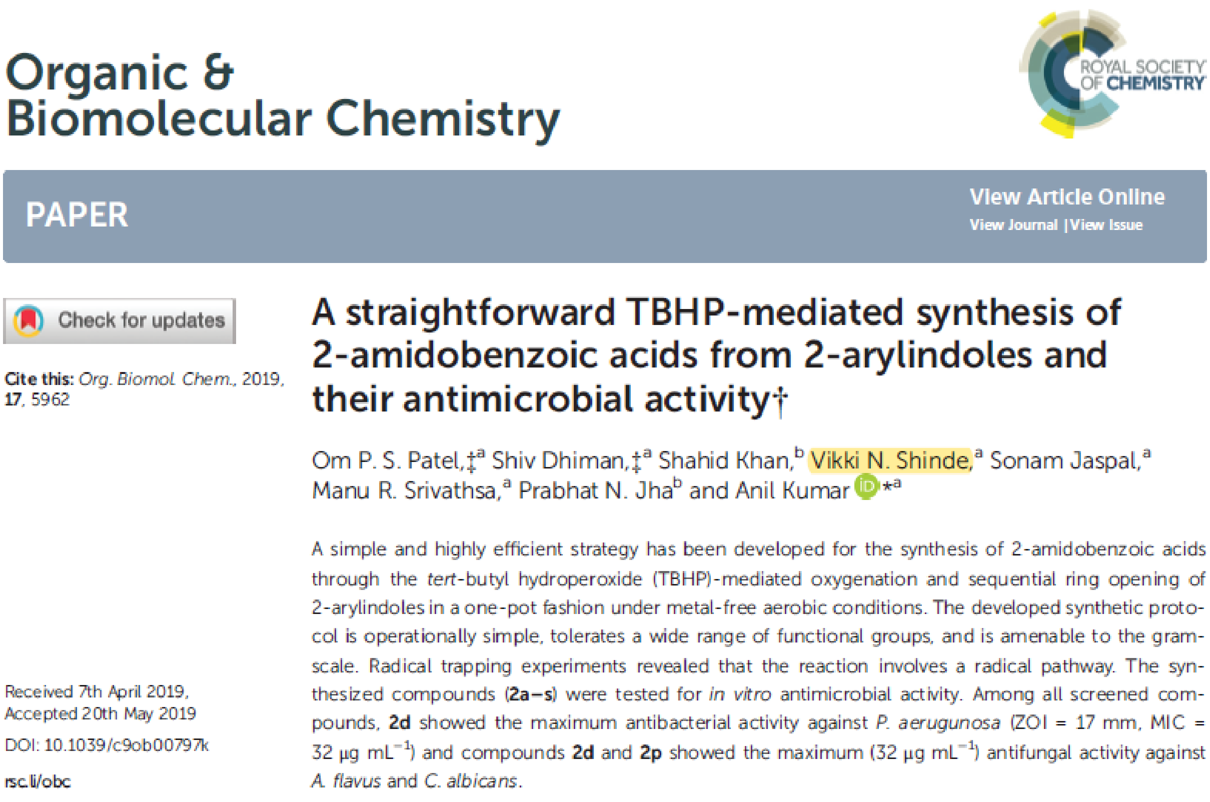

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# A straightforward TBHP-mediated synthesis of 2-amidobenzoic acids from 2-arylindoles and their antimicrobial activity†

Om P. S. Patel,‡[a] Shiv Dhiman,‡[a] Shahid Khan,[b] Vikki N. Shinde,[a] Sonam Jaspal,[a] Manu R. Srivathsa,[a] Prabhat N. Jha[b] and Anil Kumar *[a]

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A simple and highly efficient strategy has been developed for the synthesis of 2-amidobenzoic acids through the *tert*-butyl hydroperoxide (TBHP)-mediated oxygenation and sequential ring opening of 2-arylindoles in a one-pot fashion under metal-free aerobic conditions. The developed synthetic protocol is operationally simple, tolerates a wide range of functional groups, and is amenable to the gram-scale. Radical trapping experiments revealed that the reaction involves a radical pathway. The synthesized compounds (**2a–s**) were tested for *in vitro* antimicrobial activity. Among all screened compounds, **2d** showed the maximum antibacterial activity against *P. aerugunosa* (ZOI = 17 mm, MIC = 32 μg mL$^{-1}$) and compounds **2d** and **2p** showed the maximum (32 μg mL$^{-1}$) antifungal activity against *A. flavus* and *C. albicans*.

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**Cite this:** *Org. Biomol. Chem.*, 2018, **16**, 6123

# Synthesis of imidazopyridine-fused indoles *via* one-pot sequential Knoevenagel condensation and cross dehydrogenative coupling†

Vikki N. Shinde,‡[a] Shiv Dhiman,‡[a] Rangan Krishnan,[b] Dalip Kumar[a] and Anil Kumar*[a]

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A simple and efficient strategy for the synthesis of imidazopyridine-fused indoles has been developed that involves one-pot sequential Knoevenagel condensation of readily available active methylene azoles with *N*-substituted-1*H*-indole-3-carboxaldehydes or *N*-substituted-1*H*-indole-2-carboxaldehydes followed by palladium-catalyzed intramolecular cross dehydrogenative coupling reaction. A series of 36 derivatives was prepared by using this strategy. The products were obtained in moderate to excellent (32–94%) yields and showed broad substrate scope with tolerance of various functional groups and was amiable for gram scale preparation without problems.

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Communication

*Eur. J. Org. Chem.* **2017**, 6445-6449

## Domino Reactions

# Copper-Catalyzed One-Pot Tandem Reaction for the Synthesis of Imidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolines

Nitesh K. Nandwana,[a] Vikki N. Shinde,[a] Hitesh K. Saini,[a] and Anil Kumar*[a]

**Abstract:** A copper-catalyzed tandem reaction of 2-(2-bromoaryl)imidazoles/2-(2-bromoaryl)benzimidazoles, alkynes, and sodium azide was developed for the synthesis of imidazo[1,2-*c*][1,2,3]triazolo[1,5-*a*]quinazolines in moderate to excellent yields (50–85 %). The one-pot method involves copper-catalyzed azide–alkyne cycloaddition (CuAAC), intramolecular cross-dehydrogenative C–N bond formation, and Ullmann-type C–N coupling. This protocol involves the use of air as the oxidant under mild and ligand-free reaction conditions, and the reaction can be performed with a broad range of substrates with high efficiency.

# List of Presentations in Conferences *[A-3]*

1. **Vikki N. Shinde**, Pinku kaswan, Dalip Kumar, Anil Kumar, Copper-catalyzed deformylative coupling of cinnamaldehydes derivatives and naphthols, 23th ISCB International Conference on Interface of Chemical Biology in Drug Research, SRM University, Chennai, February 8-10, 2017.
2. **Vikki N. Shinde**, Shiv Dhiman, Dalip Kumar, Anil Kumar, One-pot sequential Knoevenagel condensation followed by Pd(II)-catalyzed intramolecular oxidative C(sp$^2$)–H/C(sp$^2$)–H cross coupling reactions: Direct access to annulated indole fused aza-heterocycles, 24th ISCB International Conference on Frontier Research in Chemistry & Biology Interface, Manipal University, Jaipur, January 11-13, 2018.
3. **Vikki N. Shinde**, Shiv Dhiman, Dalip Kumar, Anil Kumar, One-pot sequential Knoevenagel condensation and oxidative cross coupling reactions: Direct access of imidazopyridine fused indoles, 25th ISCB International Conference on Trends in Chemical and Biological Sciences: Impact on Health and Environment, Hotel Golden Tulip, Lucknow, January 12-14, 2019.
4. **Vikki N. Shinde**, Nattamai Bhuvanesh, Anil Kumar, Hemant Joshi, Design and syntheses of palladium complexes of NNN/CNN pincer ligands for catalytic dehydrogenative cross-coupling of heteroarenes, 26th ISCB International Conference on Integrating Chemical, Biological and Pharmaceutical Sciences for Innovations in Health Care, Nirma University, Gujrat, January 22-24, 2020.
5. **Vikki N. Shinde,** Dalip Kumar, Anil Kumar, "Palladium-Catalyzed C-H Bond Functionalization of 3-Arylcoumarins: Synthesis of Coumestan Derivatives" at JNOST 2022, School of Chemistry, University of Hyderabad, January 06 – 09, 2022.