

# Smart Designing of Organic Molecules and How to Publish Research Findings in Reputed Journals



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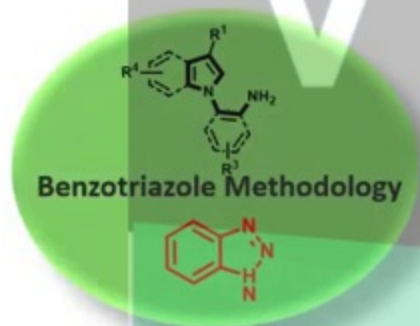
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# Start of Journey : Indolo/Pyrrolo/Imidazo fused Heterocycles



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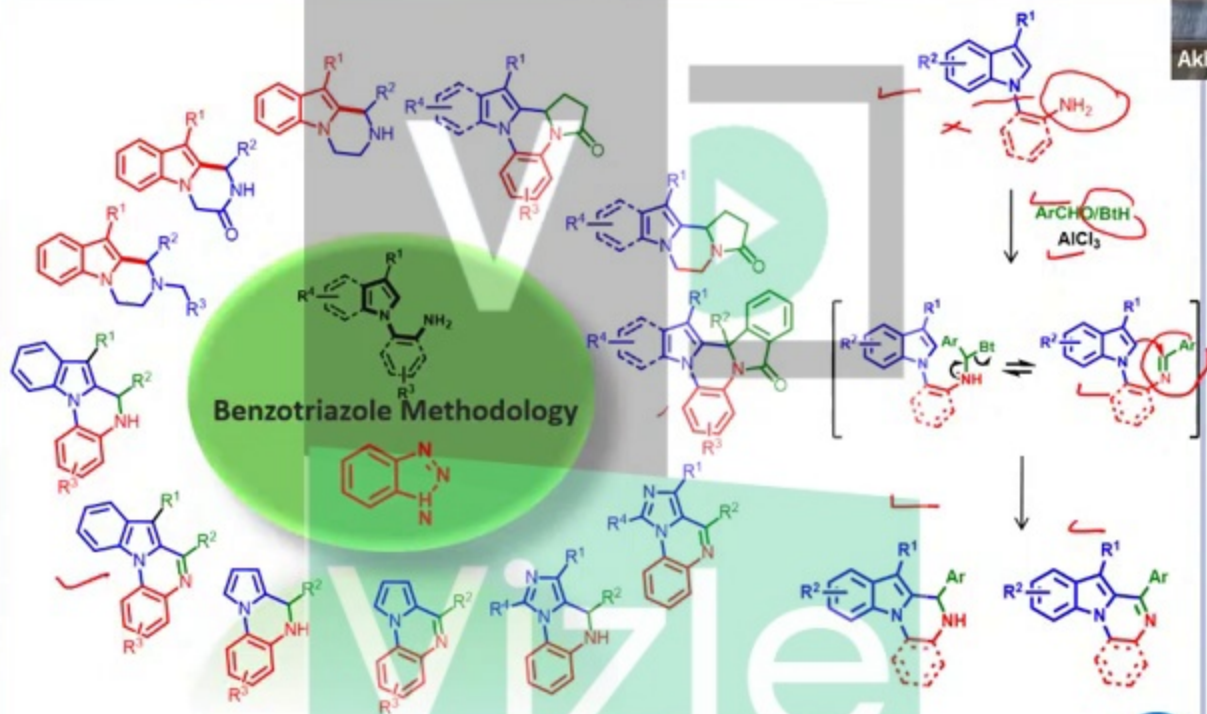


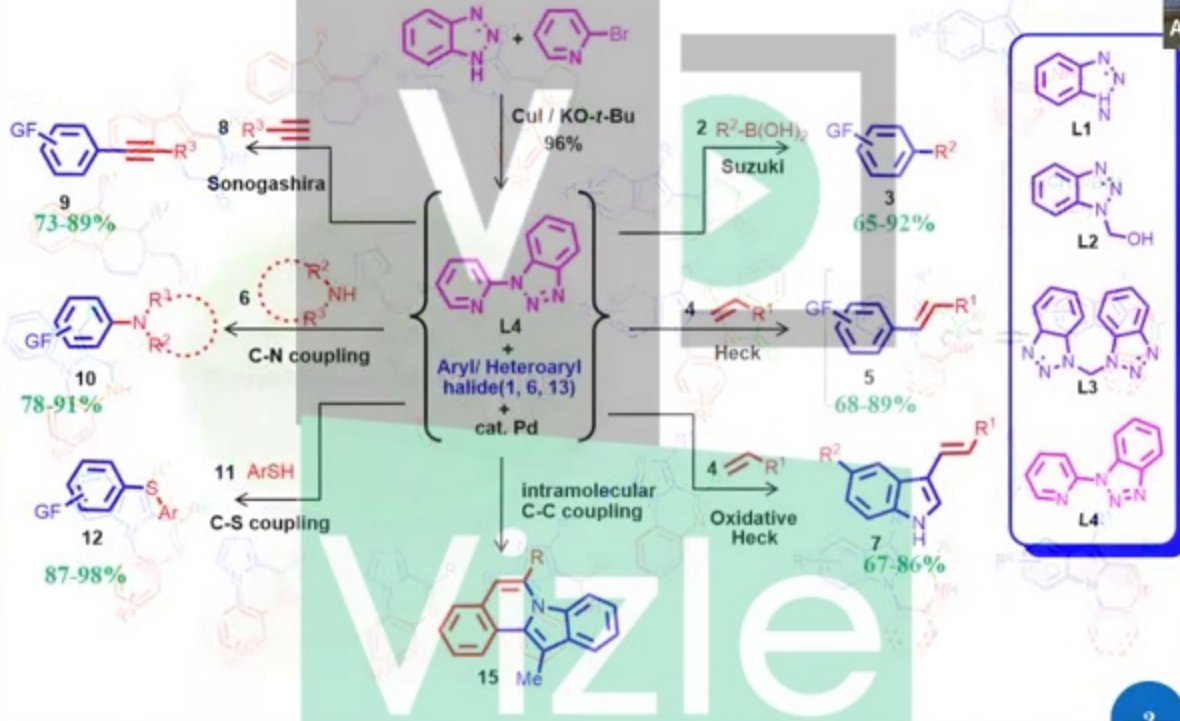
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*J. Org. Chem.* **2003**, *68*, 4938; *Tetrahedron*, **2005**, *61*, 9513; *Bioorg. Med. Chem.* **2006**, *14*, 2747;  
*Bioorg. Med. Chem. Lett.* **2006**, *16*, 413, *Eur. J. Org. Chem.* **2011**, *76*, 6998

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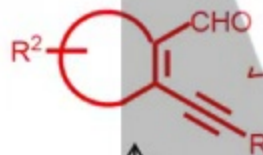




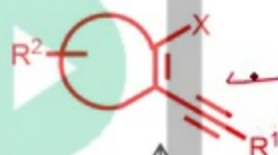
# BUILDING BLOCKS



O-Alkynyl Aldehydes



O-Halo Arylalkynes



SONOGASHIRA COUPLING



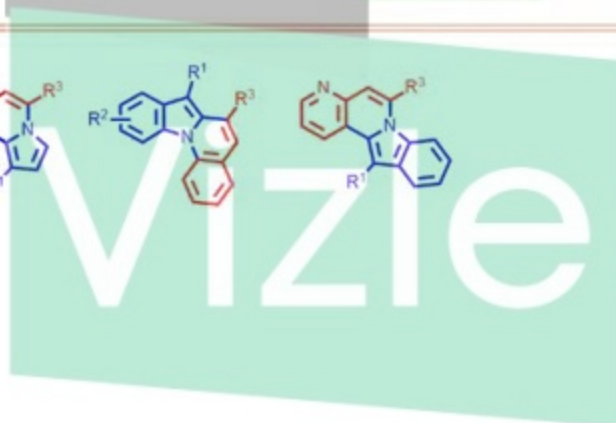
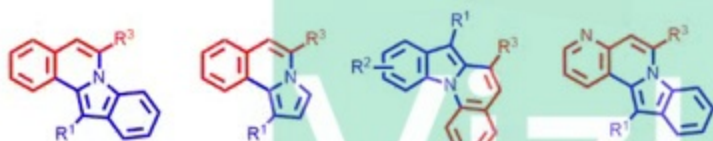
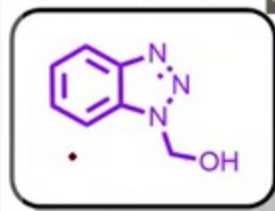
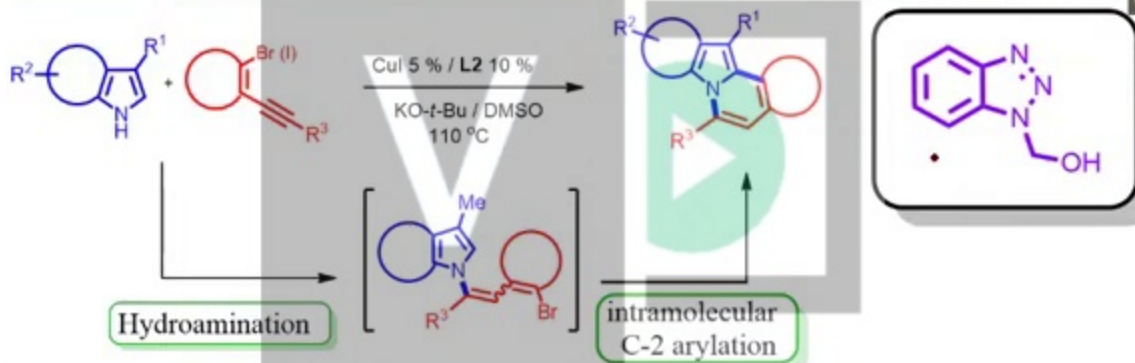
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## Part I: Hydroamination of Alkynes

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# Regio- and Stereoselective Preferential Hydroamination of Haloaryalkynes over *N*-Arylation of Aryl Halides



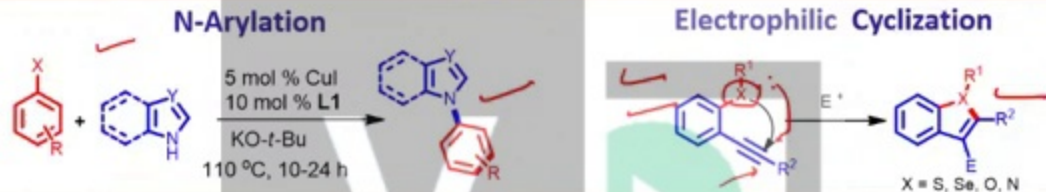


# Hypothesis

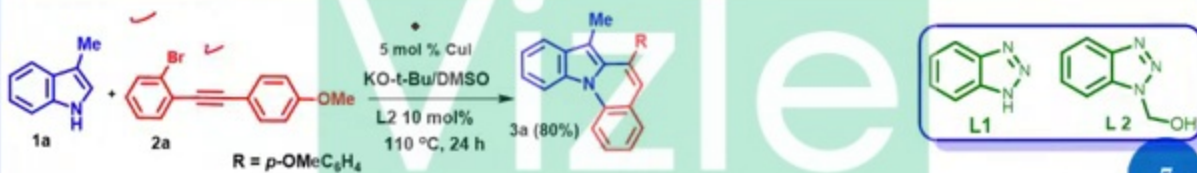


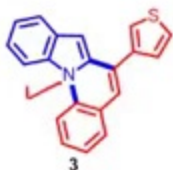
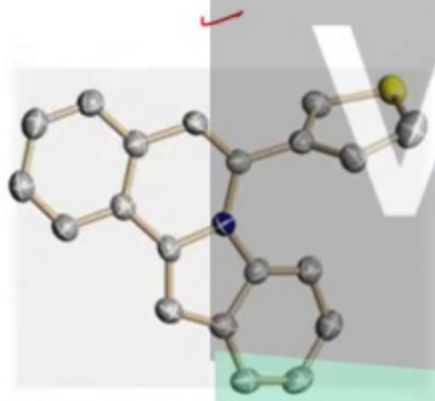
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# Hypothesis



Scheme 1



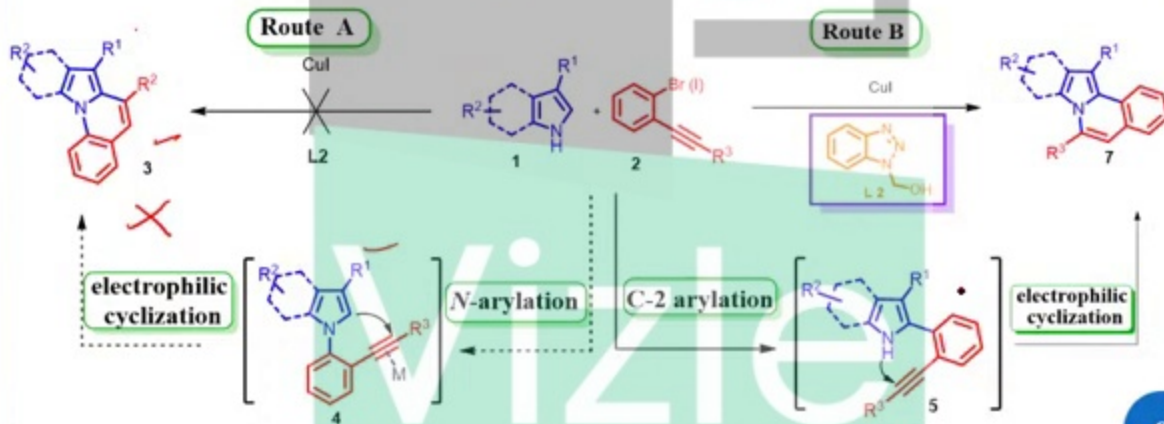




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**The X-ray results:**

- rule out the formation of [1,2-a]quinolines **3** by route A.
- Product **7** may arise via initial C-2 arylation, and intramolecular electrophilic cyclization (Scheme 2, route B).

**Scheme 2**

**1<sup>ST</sup> Control experiment :**

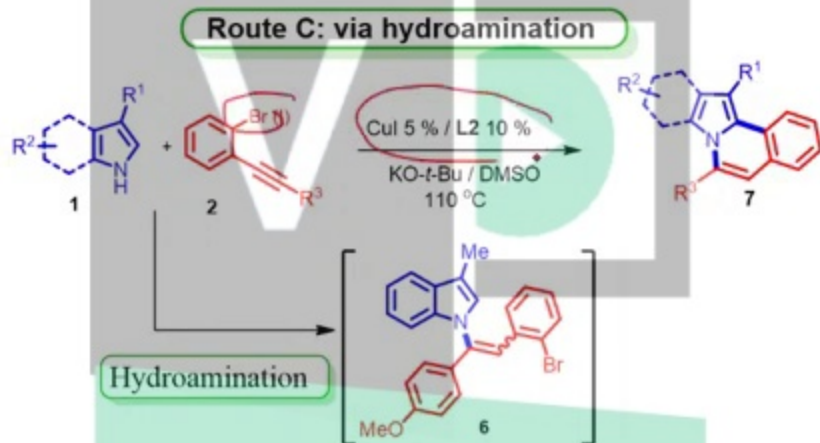
- coupling of 4-bromoanisole **8** with indole and pyrrole in identical reaction condition (Scheme 3).

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## Scheme 4



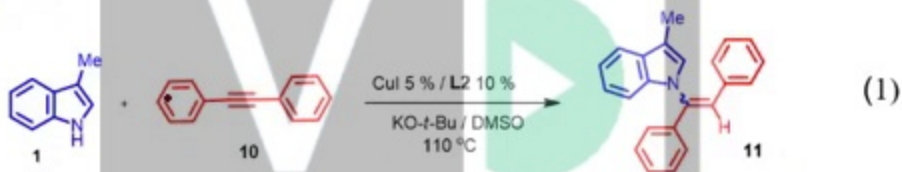
➤ The formation of the products 7 by N-C (regioselective hydroamination)





## 2<sup>nd</sup> Control Experiment

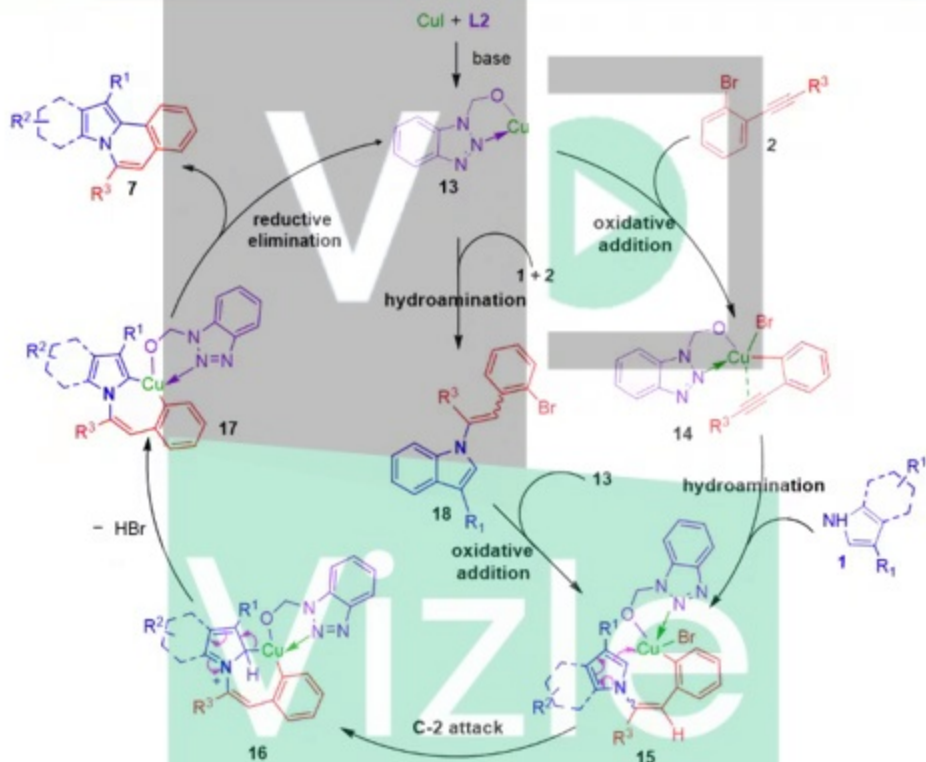
Scheme 5



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# Proposed Mechanism





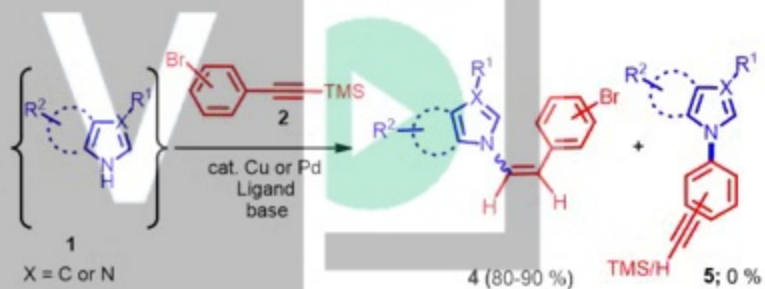
## Support for the Proposed Mechanism



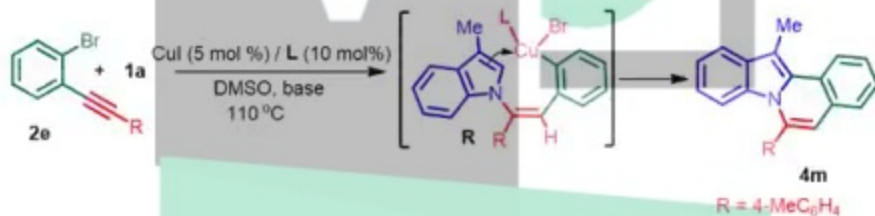


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### Regioselective Preferential Nucleophilic Addition of N-Heterocycles onto Haloaryl-alkynes over N-Arylation of Aryl Halides

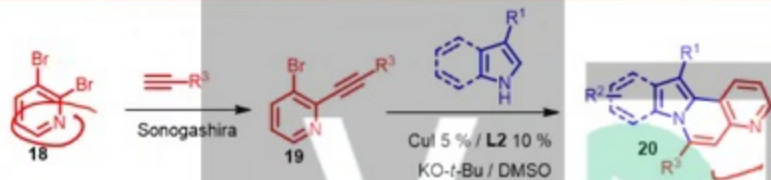


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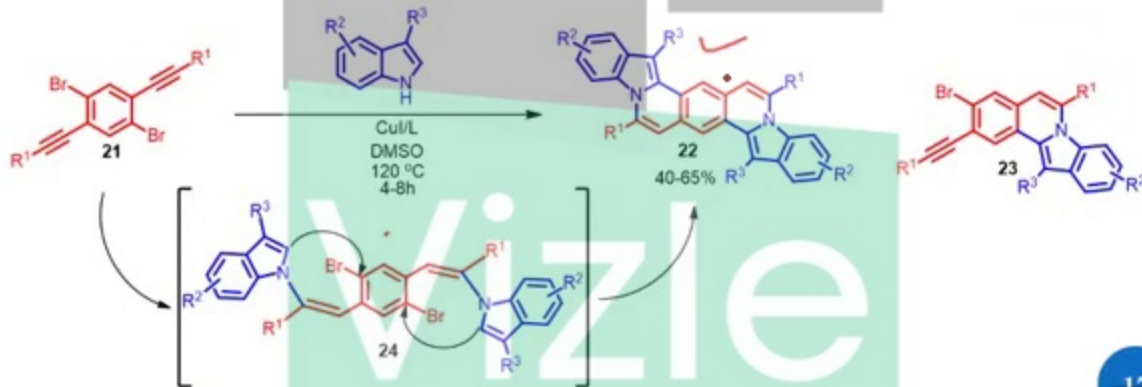
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## Scope 2: Tandem Synthesis of Naphthyridines



32 Examples  
69-87%

## Tandem Synthesis of Bisindoloisoquinolines

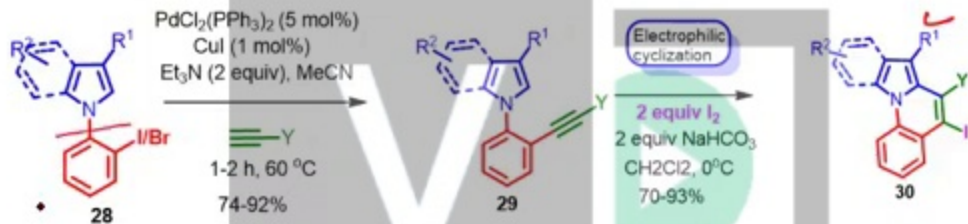




# Iodocyclization approach to Inolo[1,2-a]quinoline



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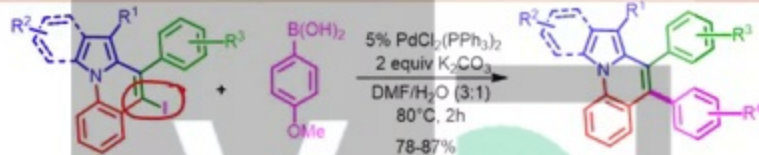
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# Diversification By Coupling Reactions

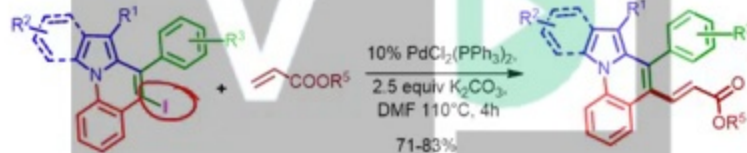


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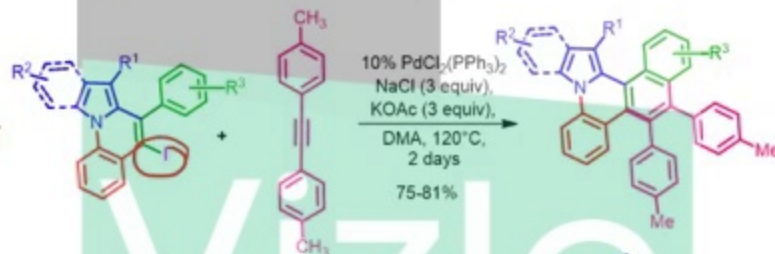
## SUZUKI COUPLING



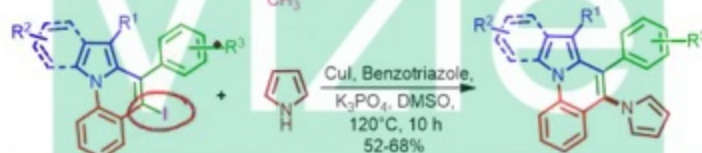
## HECK COUPLING

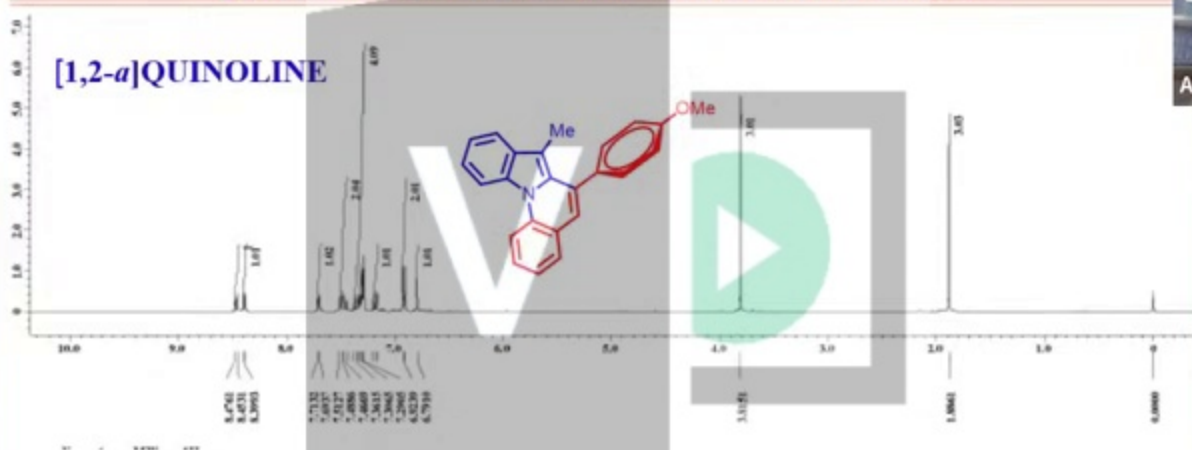


## ALKYNE ANNULATION



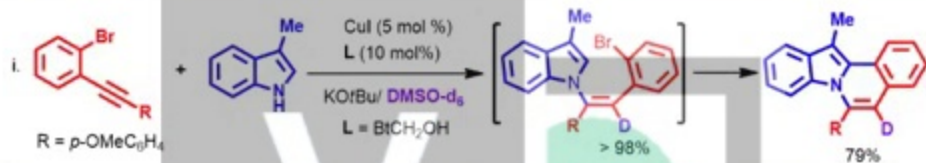
## G-N COUPLING





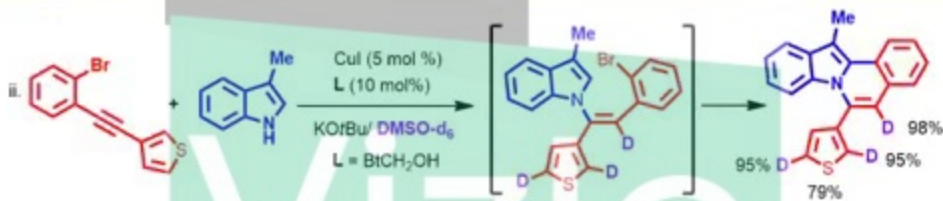
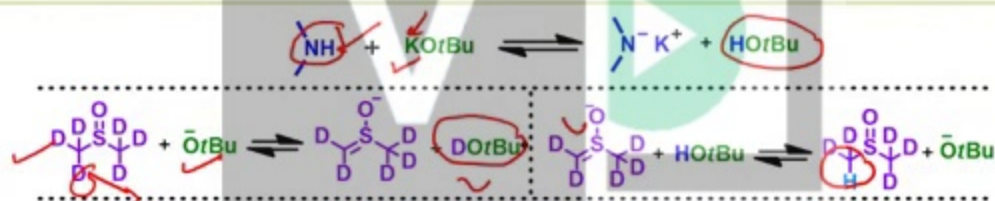
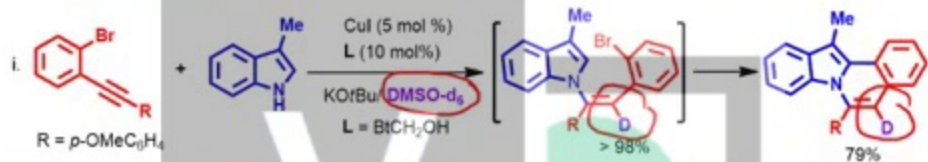
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# New Observation: Hydroamination of Alkynes Using DMSO-d<sub>6</sub>



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# New Observation: Hydroamination of Alkynes Using DMSO-d<sub>6</sub>



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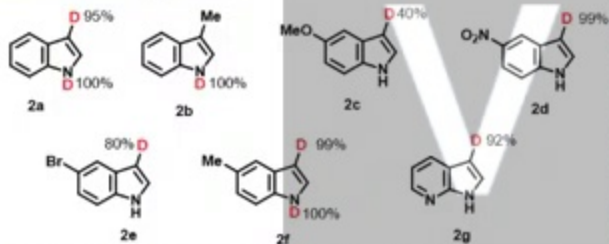
# Scope of Developed Protocol



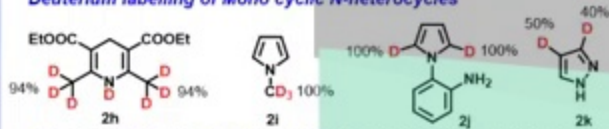
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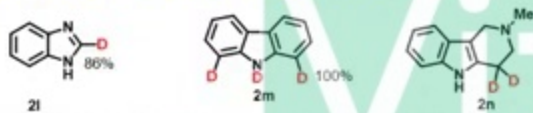
## Deuterium labelling of Indoles



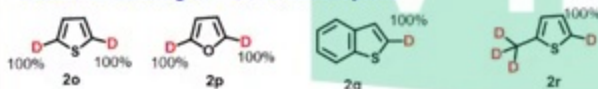
## Deuterium labelling of Mono cyclic N-heterocycles



## Deuterium labelling of Bi and Tri N-heterocycles



## Deuterium labelling of S and O-heterocycles

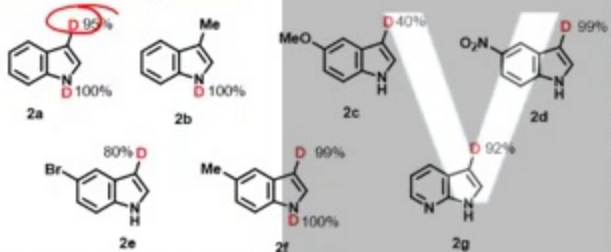




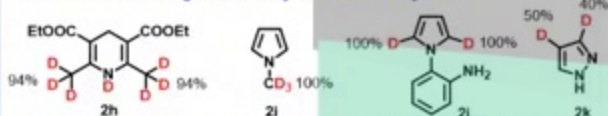
# Scope of Developed Protocol



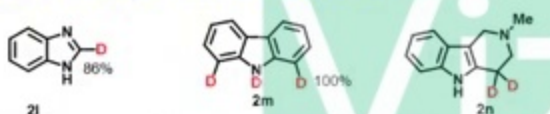
## Deuterium labeling of Indoles



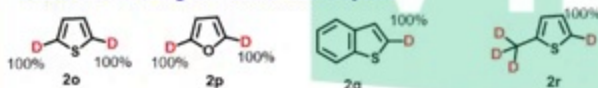
## Deuterium labeling of Mono cyclic N-heterocycles



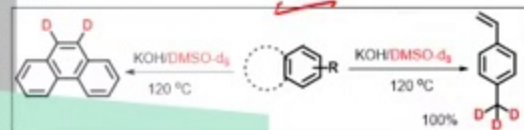
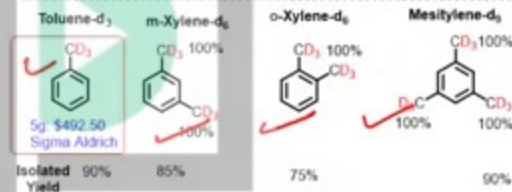
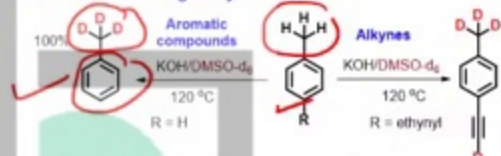
## Deuterium labeling of Bi and Tri N-heterocycles



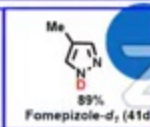
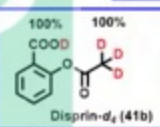
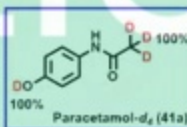
## Deuterium labeling of S and O-heterocycles



## Deuterium labeling of Hydrocarbon



## Deuterated Drugs



# Base-Mediated Hydroamination of Alkynes



## Inter- and Intramolecular Hydroamination



*Acc. Chem. Res.* **2017**, *50*, 240-254

*J. Org. Chem.*, **2018**, *83*, 11686

*ACS Omega*, **2018**, *3*, 10612

*J. Org. Chem.*, **2017**, *82*, 10247

*A. J. Org. Chem.* **2016**, *5*, 213

*A. J. Org. Chem.* **2015**, *4*, 894

*Tet. Lett.* **2014**, *55*, 4724

*Chem. Commun.* **2014**, *50*, 8526

*J. Org. Chem.* **2014**, *79*, 172

*J. Org. Chem.* **2012**, *77*, 8191

*J. Org. Chem.* **2012**, *77*, 5633

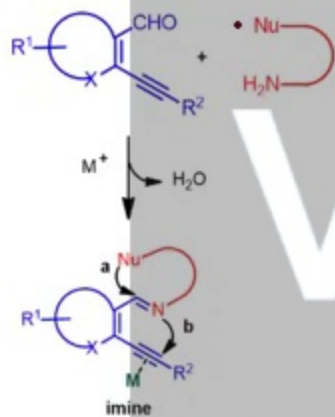
*Org. Lett.* **2011**, *13*, 1630

*Org. Lett.* **2012**, *14*, 1106

*Tetr. Lett.* **2014**, *55*, 1310

*Angew. Chem. Int. Ed.* **2009**, *48*, 1138-1143

# Designed Cascade Strategy

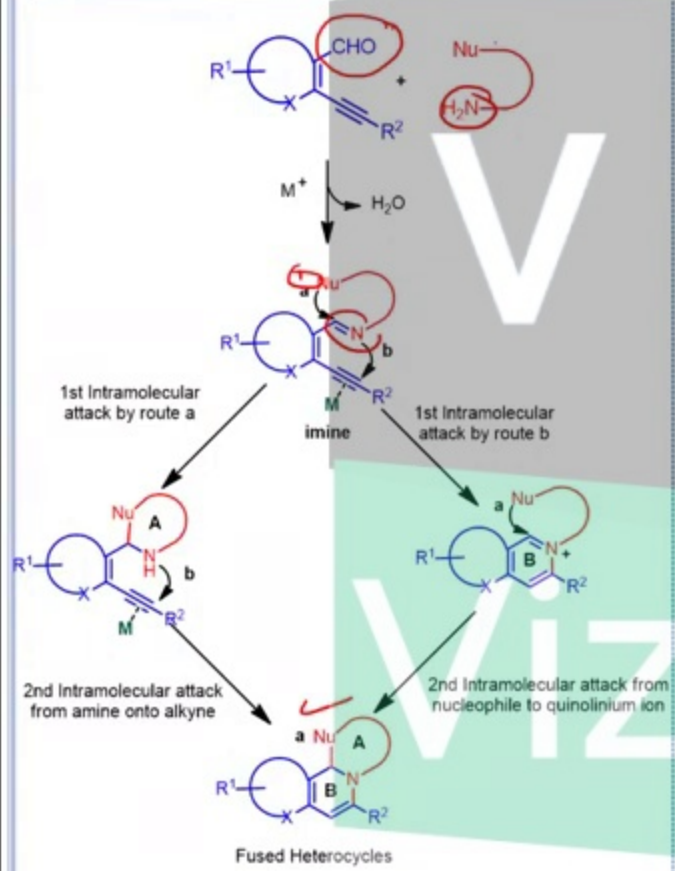


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1. *J. Org. Chem.*, **2018**, *83*, 6650
2. *J. Org. Chem.* **2016**, *81*, 9356–9371
3. *Green Chem.* **2016**, *18*, 6367–6372
4. *Org. Biomol. Chem.*, **2016**, *14*, 9063–9071
5. *Org. Biomol. Chem.* **2016**, *14*, 7639–7653
6. *J. Org. Chem.* **2015**, *80*, 10548–10560
7. *Tetrahedron Letters* **2014**, *55*, 2603–2608
8. *Tetrahedron Letters* **2014**, *55*, 610–615
9. *Org. Biomol. Chem.*, **2014**, *12*, 552–556
10. *J. Org. Chem.* **2013**, *78*, 6657–6669
10. *J. Org. Chem.* **2013**, *78*, 5372–5384
11. *J. Org. Chem.* **2013**, *78*, 4386–4401
12. *Eur. J. Org. Chem.* **2012**, 4590–4602
13. *Tetrahedron* **2012**, *68*, 9035–9044
14. *Org. Lett.* **2012**, *14*, 5184–5187
15. *J. Org. Chem.* **2012**, *77*, 8562–8573
16. *Green Chem.* **2011**, *13*, 1640–1643.
17. *J. Org. Chem.* **2011**, *76*, 5670–5684.
18. *ACS Comb. Sci.* **2011**, *13*, 530–536.
19. *Chem. Commun.* **2010**, *46*, 4064–4046
20. *J. Org. Chem.* **2010**, *75*, 7691–7703.

## Diversity Oriented Cascade Synthesis

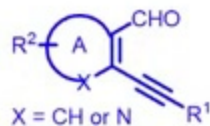


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One bullet more than 100 targets

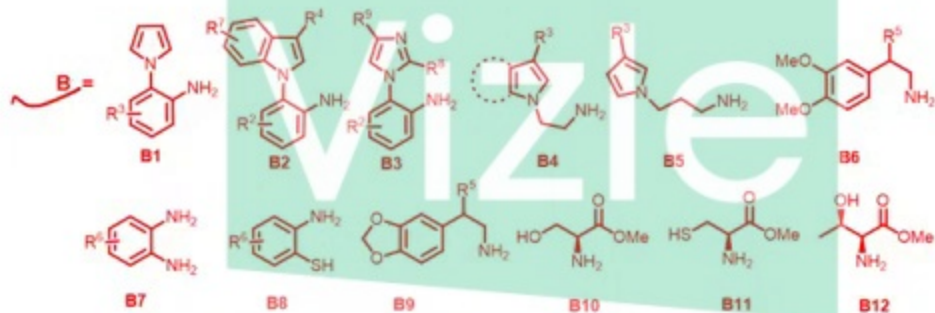
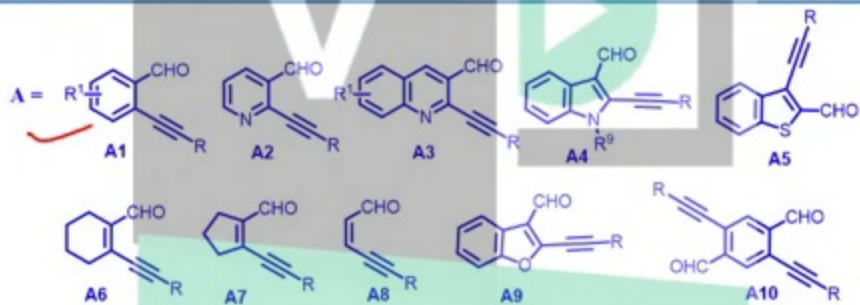
Designed scaffolds would be prepared by using two building blocks:

- i) *ortho*-aryl/alkynyl aldehydes
- ii) amine



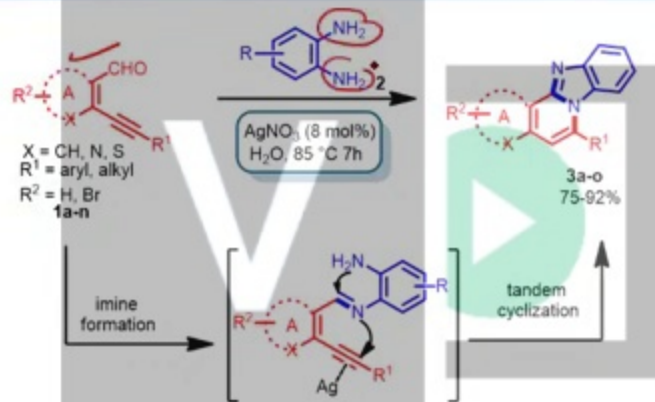
> 100 Scaffolds







# Synthesis of Fused Benzimidazoles



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