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Coupling of N-Aryl Tetrahydroisoquinoline and Indole Derivatives Catalyzed By Catenane-Coordinated Copper(I)

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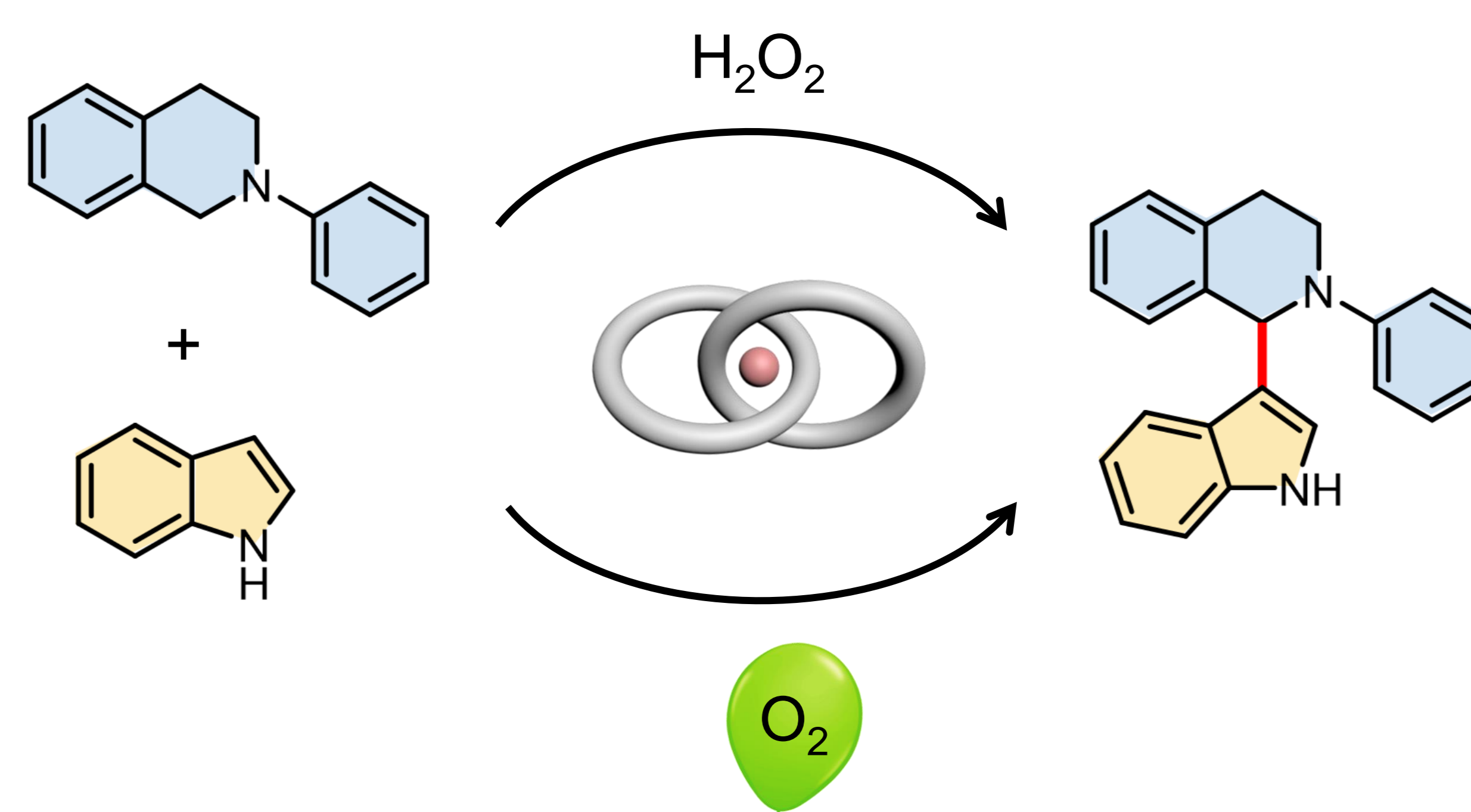
Background

Reported Works:

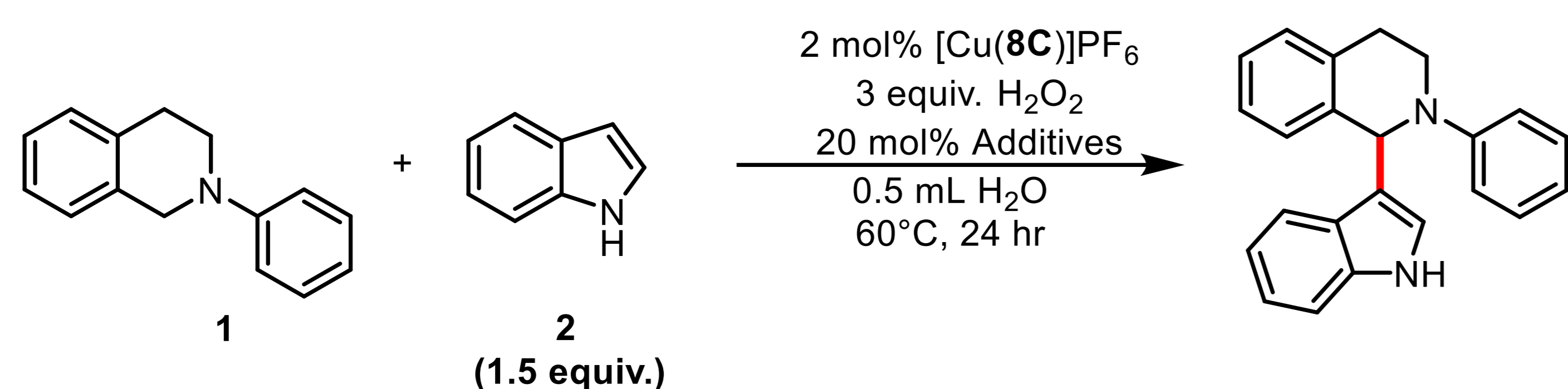
- Use of Fe/Cu-based catalysts
- Organic solvent
- Use of bulky peroxides

This Work:

- [2]Catenane as catalyst, where the mechanically interlocked ligands provide stabilization and a responsive coordination geometry on Cu(I).¹
- Aqueous reaction medium.
- Two different oxidants.
- Water as by-product.



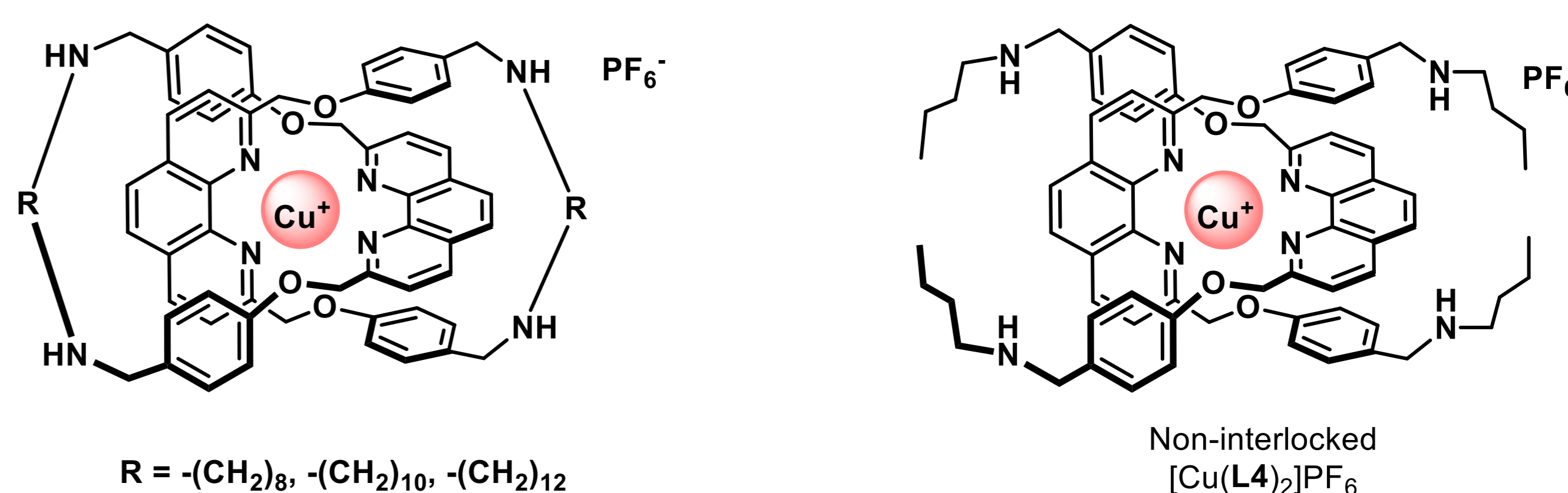
Condition Optimization



Entry	Solvent	Additives	Yield (%)
1	MeCN	-	29
2	H ₂ O	-	55
3	H ₂ O	Benzoic acid	37
4	H ₂ O	2,5-Dimethylbenzoic acid (DMBA)	77
5	H ₂ O	Potassium Carbonate	43

Improved product yield with addition of acidic additive

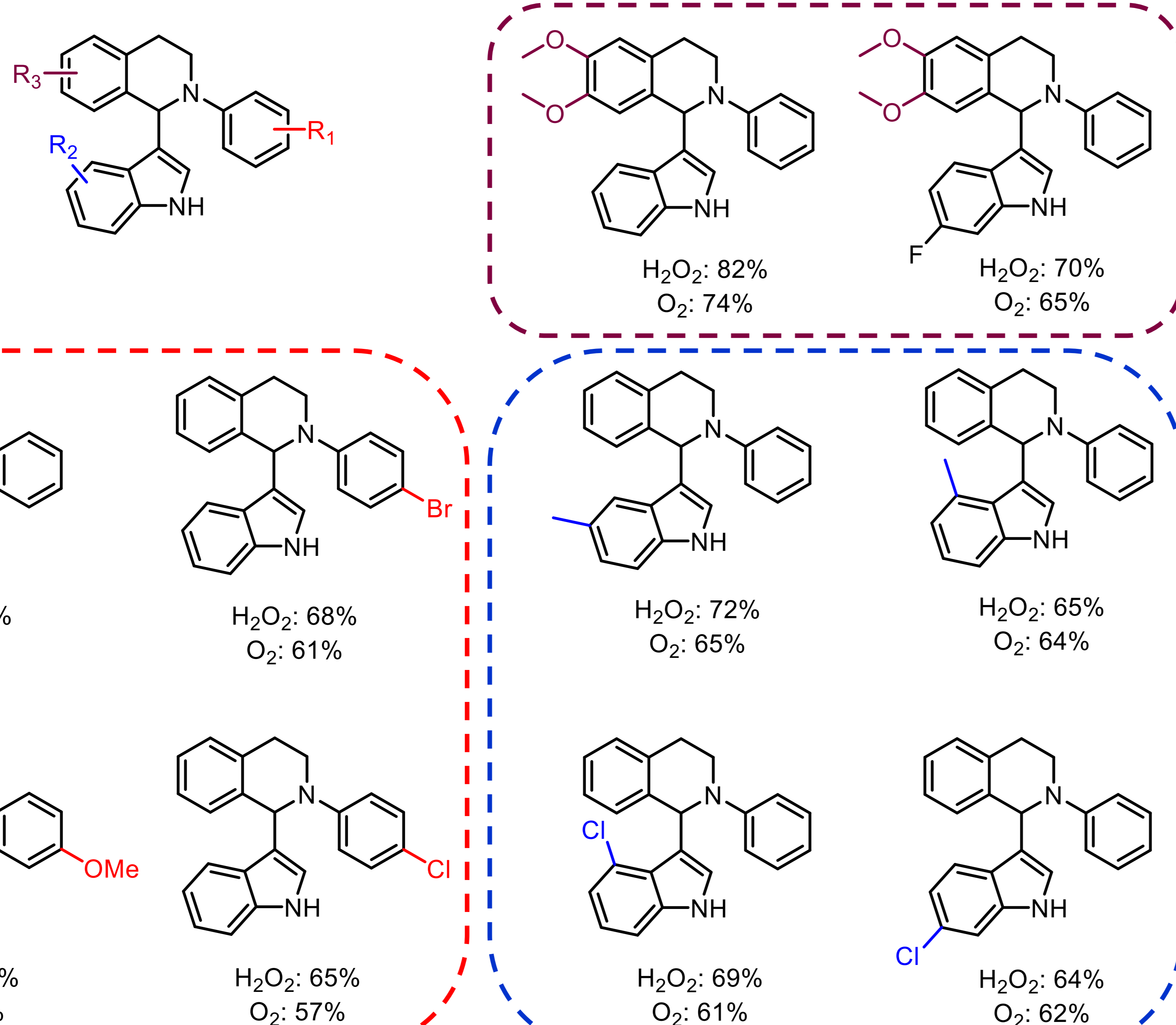
Interlocked vs Non-interlocked Catalysts



Entry	Cu Species	Yield (%)
1	[Cu(L4)]PF ₆	32
2	[Cu(8C)]PF ₆	77
3	[Cu(10C)]PF ₆	68
4	[Cu(12C)]PF ₆	35

Catalyst activity affected by the tightness of mechanical bond

Substrate Scope



Future Works

1. Post functionalization of the [2]catenane to investigate new properties and improve efficiency.
2. Develop a [2]rotaxane with similar Cu(I) coordinated phenanthroline core for catalysis.

Reference

1. Zhu L., Li J., Yang J. and Au-Yeung H. Y., Cross dehydrogenative C–O coupling catalysed by a catenane-coordinated copper(I). *Chem. Sci.* **2020**, *11*, 13008-13014.

Acknowledgements

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