

(Organic Chemistry)  
Oral Abstract

*Title: Isomerism due to Mechanical Bonding: Radial [5]catenanes of Isomeric Sequences of Peripheral Interlocked Macrocycles*

Antony Wing Hung Ng and Ho Yu Au-Yeung\*

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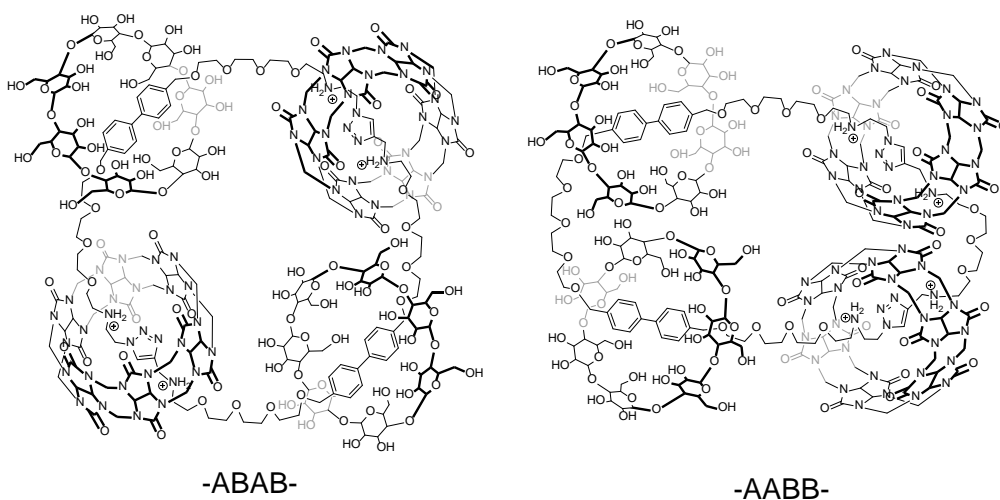
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Abstract:

Similar to encoding genetic information by sequences of nucleotides in DNA, arranging macrocycles in specific sequences by mechanical bond is important to the realization of new generation information-embedded molecular machines. Synthesis of hetero[n]catenane with multiple numbers and types of interlocked macrocycles is however very challenging due to the difficulty in the precise control of macrocycle interlocking process.<sup>1</sup>

In this presentation, the first example of a pair of hetero[5]catenane having specific isomeric sequences of interlocked  $\beta$ -cyclodextrin ( $\beta$ -CD) and cucurbit[6]uril (CB[6]) is reported.<sup>2</sup> Cucurbit[6]uril-mediated azide-alkyne cycloaddition (CBAAC) was employed to synthesize the isomers from strategically-designed building blocks with good efficiency. A pair of [5]catenane isomers with either a cyclic –ABAB– or –AABB– sequences of the interlocked  $\beta$ -CD and CB[6] was obtained in high yields (>80%). Due to the different binding strength of the macrocycles, sequence-dependent dynamics and fragmentation behaviour of the [5]catenane isomers were observed from variable-temperature NMR and tandem mass spectrometry. By enhancing or weakening the solution ionic strength, the translocation kinetics of the  $\beta$ -CD in the –ABAB– [5]catenane isomer could be tuned accordingly. This work deepens our understanding on the macrocycle dynamics and implicates the potential of mechanically-interlocked molecules (MIMs) in information-embedded functional materials.

*Radial hetero[5]catenane*



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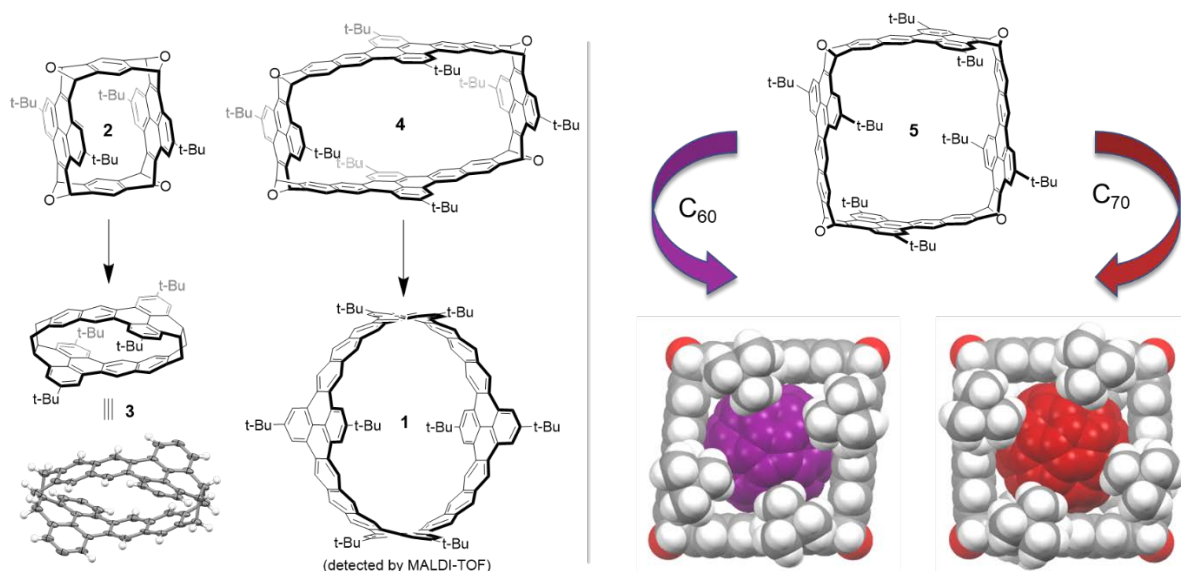
# (Organic Chemistry) Oral Abstract

## From Carbon Nanoboxes to Zigzag Carbon Nanobelts: Synthesis and Host-Guest Chemistry

Han Chen, Zeming Xia, Qian Miao \*

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Zigzag carbon nanobelts are a long-standing challenging target for organic synthesis. This study presents the synthesis of box-shaped tetraepoxy carbon nanobelts, which were synthetic precursor of zigzag carbon nanobelts. The successful synthesis of them involved iterative Diels–Alder reactions as a key step to form macrocycles. The synthetic study of carbon nanobox **2** toward fully conjugated zigzag carbon nanobelts resulted in a hydrogenated zigzag carbon nanobelt **3**, which was identified with single-crystal X-ray crystallography.<sup>1</sup> Octabenzocyclo[20]cyclacene **1**, an undocumented zigzag carbon nanobelt, was synthesized from carbon nanobox **4** and detected by MALDI-TOF. Furthermore, the study of their application in host-guest chemistry revealed the formation of supramolecular complexes between carbon nanobox **5** and fullerenes. The UV/Vis absorption and fluorescence spectra, and theoretical studies showed their interesting ball-in-box structures.



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2. Chen H.; Xia Z.; Miao Q. to be submitted

**(Organic Chemistry)**  
**Oral Abstract**

**Biosynthetic study of fungal tetrahydroxanthones**

City U - Wei Xingxing

Xanthones are a widespread and representative class of natural products that display various potent biological activities. However, the molecular basis for the xanthone biosynthesis, particularly the mechanism of xanthone skeleton generation, remains poorly understood. Here, *in vivo* and *in vitro* reconstitution of the biosynthesis of fungal tetrahydroxanthones (THXs), blennolides A and C, led to the identification and characterization of the key enzymes for THX biosynthesis and diversification. We have not only provided an in-depth model of the THX biosynthesis but also achieved the total biosynthesis of fungal THXs in a heterologous host for the first time.

## (Organic Chemistry) Oral Abstract

**Structure engineering of porphyrin-based hole transporting materials for perovskite solar cells** [Chen Jiabang](#) Zhu xunjin\* [xjzhu@hkbu.edu.hk](mailto:xjzhu@hkbu.edu.hk)

### Abstract

Perovskite solar cells (PSCs) are a new type of organic-inorganic thin-film solar cells developed from dyesensitized solar cells. Due to its high efficiency, low cost and easy preparation characteristics, perovskite solar cells have attracted the research interest of a huge number of scientific researchers and have achieved very significant achievements. From 2009 to the present, its light conversion efficiency has increased from 3.8%<sup>[1]</sup> Increased to 25.2%<sup>[2]</sup>. However, hole transport materials like Spiro-OMeTAD which was used mostly in perovskite solar cell often needed doping to increase its mobility, and this would decrease its stability, which was unfavorable for its scalable application.

Herein, four porphyrin-based hole transport materials (HTM) were designed, synthesized, and used in perovskite solar cell. Compared with traditional HTM Spiro-OMeTAD, they were more convenient to synthesize and non-doped. They got a comparable power conversion efficiency of 18.12%, which is just slightly lower than Spiro-based device (19.71%). At the same time, the device of based on these four new HTM could remain at least 80% of their efficiency after 31 days under ambient environment, while Spirobased device degraded to 54% of its original efficiency.

### References

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2. NREL Best Research Cell Efficiencies, <https://www.nrel.gov/pv/assets/pdfs/best-research-cellefficiencies.pdf> (accessed: April2020).

### Zoom to ask the author:

<https://hkbu.zoom.us/j/3248229158?pwd=Q21HZELjVFBNT2NVcmpzTnhvNWFYQT09>  
(Meeting ID: 324 822 9158 )

# (Organic Chemistry) Oral Abstract

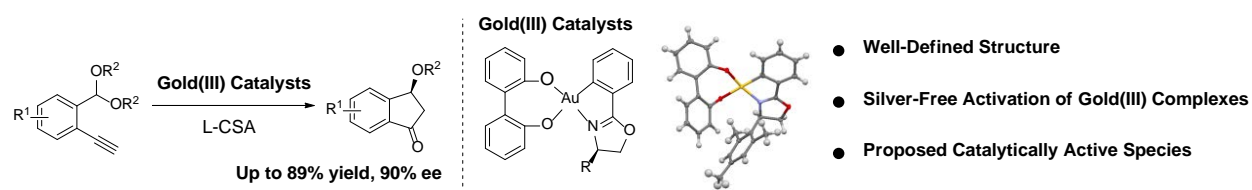
## Chiral Cyclometallated Oxazoline Gold(III) Complex-Catalyzed Asymmetric Carboalkoxylation of Alkynes

Jia-Jun Jiang, Jian-Fang Cui, Bin Yang, Yulu Ning, Nathanael Chun-Him Lai, and Man-Kin Wong\*  
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### Abstract

Although the reactivity of gold in homogeneous catalysis has been underestimated in the last century, the past decade has witnessed significant progress in gold catalysis. Gold catalysts present distinguished reactivity, excellent selectivity and high functional group compatibility in diverse organic transformations. Gold(I)-catalyzed organic reactions with good stereoselectivity are well demonstrated; yet, asymmetric gold(III) catalysis remains largely unexplored.

Herein, we demonstrate asymmetric catalysis using novel chiral O,O'-chelated 4,4'-biphenol cyclometallated oxazoline gold(III) complexes. High yields (up to 89%) and enantioselectivities (up to 90% ee) were achieved in asymmetric carboalkoxylation of alkynes. Enantioselectivity could be significantly improved from 19% to 90% ee by increasing the steric size of the substituent on the chiral oxazoline ligand. Catalytically active gold(III) species and the origin of chiral induction were studied and proposed.



### References

Jiang, J.-J.; Cui, J.-F.; Yang, B.; Ning, Y.; Lai, N. C.-H.; Wong, M.-K. *Organic Letters*, **2019**, *21*, 6289–6294.

Zoom to ask the author: <https://polyu.zoom.us/j/4884529612> (Meeting ID: 4884529612)

(Organic Chemistry)  
Oral Abstract

Total Synthesis of Lepadine Alkaloids

HKUST – Ma Fong

**Abstract**

Lepadine alkaloids are a family of decahydroquinoline alkaloids isolated from marine natural sources; these compounds have shown significant cytotoxicity against human cancer cell lines or antimalarial activity. Here a new approach has been developed, in which aza-Achmatowicz rearrangement and a mild intermolecular [3+2] cycloaddition were used to construct the central decahydroquinoline skeleton.

**References**

1. (a) Kubanek, J.; Williams, D. E.; De Silva, E. D.; Allen, T.; Andersen, R. J. *Tetrahedron Lett*, **1995**, *36*, 6189–6192. (b) Wright, A. D.; Goclik, E.; Konig, G. M.; Kaminsky, R. *J. Med. Chem.*, **2002**, *45*, 3067–3072. (c) Davis, R. A.; Carroll, A. R.; Quinn, R. J. *J. Nat. Prod.*, **2002**, *65*, 454–457. (d) Ómarsdóttir, S.; Wang, X.; Liu, H.-B.; Duggan, B. M.; Molinski, T. F. *J. Org. Chem.*, **2018**, *83*, 13670-13677.

## (Organic Chemistry) Oral Abstract

### Total Synthesis of Malacidin A by $\beta$ -Hydroxyaspartic Acid Ligation Mediated Cyclization and Absolute Structure Establishment

Zhenquan Sun, Xuechen Li\*

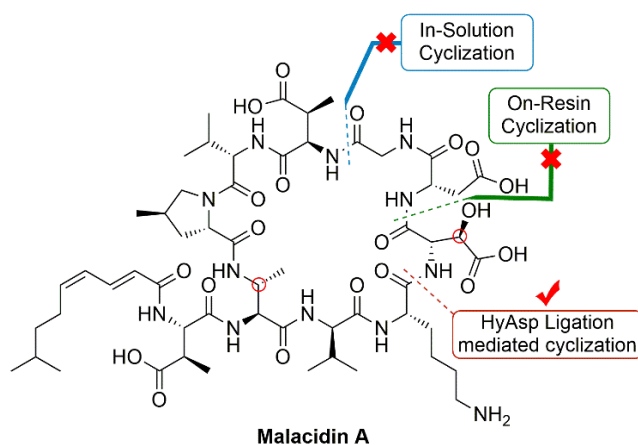
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#### Abstract

Developing new antibiotics is still an urgent need to fight against the increasing drug-resistant pathogens. Malacidin A is a new member of Calcium-Dependent Antibiotics (CDAs) discovered recently with excellent activity against antibiotic-resistant pathogens. Also, its action of mode is distinct from classical CDAs', which needs further investigation. However, stereochemistry of it is still not fully comprehensive. Herein, the total syntheses of Malacidin A and its analogues are presented by combination of Fmoc-based Solid-Phase Peptide Synthesis (SPPS) and  $\beta$ -HydroxyAspartic acid ligation mediated cyclization. Suitable protecting groups for non-proteinogenic amino acids are developed therefore, especially the HyAsp. Utilizing this strategy, different analogues can be synthesized in convenient way which provides opportunity for further Structure-Activity Relationship (SAR) study. Finally, the exact chemical structure of Malacidin A is confirmed by detailed comparison of 1D- and 2D-NMR spectrum between native compound's and four synthetic analogues', which is further supported by complementary Marfey's analysis.



#### Reference

1. Hover, B. M., et al. *Nat. microbiol.*, **2018**, 3, 415-422.
2. Sun, Z., et al. *Angew. Chem. Int. Ed.*, **2020**, 59, 1-6.

# (Organic Chemistry) Oral Abstract

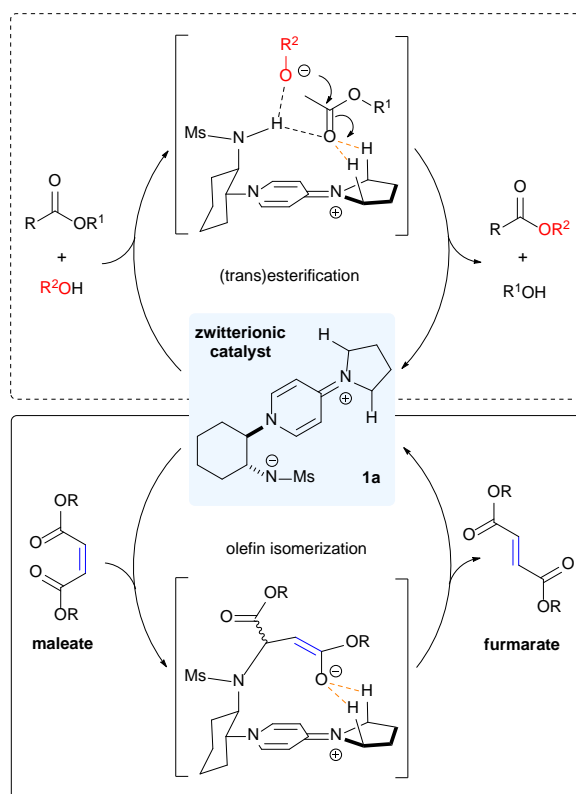
## Amide/Iminium Zwitterionic Catalysts for (Trans)esterification and Isomerization of Maleic Acid Diesters to Fumaric Acid Diesters

Ying-Pong Lam

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### Abstract

A class of zwitterionic organocatalysts based on an amide anion/iminium cation charge pair has been developed. They are catalytically applicable to transesterifications, dehydrative esterifications and isomerization of maleic acid diesters to fumaric acid diesters. Mechanistic studies reveal that the amide anion and iminium cation work synergistically in activating the reaction partners, with the iminium cationic moiety interacting with the carbonyl substrates through nonclassical hydrogen bonding. The reaction can be applied to large-scale synthesis of biodiesel under mild conditions.



### References

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Zoom to ask the author: <https://cuhk.zoom.us/j/5075489287> (Meeting ID: 507-548-9287)



**(Organic Chemistry)**  
**Oral Abstract**

Systematic study of the structure-property relationship of a series of near-infrared absorbing push-pull heptamethine chromophores for electro-optics

Di Zhang,<sup>1</sup> Jie Zou,<sup>1</sup> Taili Liu,<sup>1,2</sup> Sai Wing Tsang<sup>2</sup> and Jingdong Luo<sup>1\*</sup>

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**Abstract:** High performance organic and polymeric electro-optic (EO) materials and devices are of intense interest to meet the challenge by encoding electrical signals into the optical domain for future communications and ultrafast signal processing systems.<sup>1</sup> One challenge which remains to be addressed in organic EO materials chemistry is whether donor–pi–bridge–acceptor (D–pi–A) chromophores exhibiting large molecular hyperpolarizabilities (*beta* values) can be synthesized with high efficacy, processed and integrated reliably to construct electric field poled thin films with high EO coefficients and good stability.<sup>2,3</sup> In this presentation, we will report our recent research progress in concise synthesis and systematic study of the structure-property relationship of a series of near-infrared absorbing push-pull heptamethine chromophores for electro-optics. This series of tricyanodihydrofuran-based dipolar heptamethines contains different electron donors of indoline, benzo[e]indoline, benz[cd]indoline, and Michler’s base derivatives. They can be synthesized in high yields by direct condensation reactions with donor and acceptor moieties under the same or similar reaction conditions, and can be further modified by efficient nucleophilic substitution reactions. This series of dipolar chromophores exhibit high near-infrared absorption, tunable bond-length alternation (BLA), excellent chemical stability and large molecular hyperpolarizabilities. Poled polymers containing these dipolar heptamethines give high poled-induced noncentrosymmetric order, and excellent modulation efficiency at both band edge (900 nm to 1100 nm) and off-resonance telecom wavelength range (1300 nm to 1550 nm). Our studies suggest that concise synthesis and molecular design of push-pull polymethines can be well guided by the tabulation of their linear and NLO properties in bulk materials, and streamline future development of high performance organic EO materials for photonic applications.

**References:**

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- [2] (a) Luo, J.; Lin, F.; Li, Z. A.; Li, M.; Kim, T.-D.; Jang, S. H. and Jen, A. K. Y. *J. Mater. Chem. C*, **2017**, 5, 2230-2234; (b) Bentoumi, W.; Mulatier, J.-C.; Bouit, P. A.; Maury, O.;

**(Organic Chemistry)**  
**Oral Abstract**

Barsella, A.; Vola, J. P.; Chastaing, E.; Divay, L.; Soyer, F.; Barny, P. L.; Bretonnière, Y. and Andraud, C. *Chem. Eur. J.*, **2014**, *20*, 8909-8913; (c) Pascal, S.; Getmanenko, Y. A.; Zhang, Y.; Davydenko, I.; Ngo, M. H.; Pilet, G.; Redon, S.; Bretonnière, Y.; Maury, O.; Ledoux-Rak, I.; Barlow, S.; Marder, S. R. and Andraud, C. *Chem. Mater.*, **2018**, *30*, 3410-3418.

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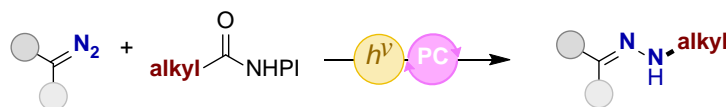
(Organic Chemistry)  
Oral Abstract

Photoredox Decarboxylative C(sp<sup>3</sup>)-N Coupling of  $\alpha$ -Diazoacetates  
with Alkyl *N*-Hydroxyphthalimide Esters  
for Diversified Synthesis of Functionalized *N*-Alkyl Hydrazones

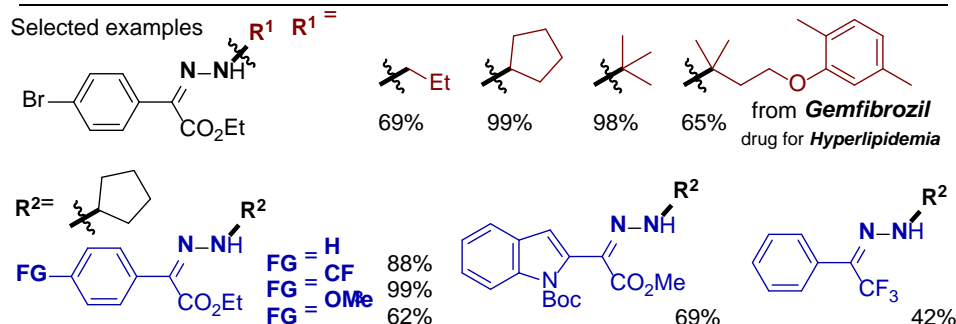
Yip-Chi Chow and Wing-Yiu Yu\*

State Key Laboratory of Chemical Biology and Drug Discovery, Department of Applied  
Biology and Chemical Technology, The Hong Kong Polytechnic University

Abstract



- metal-free
- scalable
- mild conditions
- >60 examples, up to 99% yields



Herein we report a metal-free photocatalytic coupling reaction for the synthesis of structurally and functionally diverse *N*-alkyl hydrazones from  $\alpha$ -diazoacetates and *N*-alkyl hydroxyphthalimide esters. By employing Rose Bengal as a photocatalyst with yellow LEDs irradiation, over 60 *N*-alkyl hydrazones were synthesized. Fluorescence quenching analysis and deuterium incorporation experiments reveal that Hantzsch ester serves as both an electron donor and proton source for the reaction. This strategy offers a simple retrosynthetic disconnection for conventionally inaccessible C(sp<sup>3</sup>)-rich *N*-alkyl hydrazones.

References

1. *Org. Lett.* **2019**, *21*, 8037–8043

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# (Organic Chemistry) Oral Abstract

## Catalytic Enantioselective Redox-A<sup>3</sup> Reaction of Tryptolines

Lixin LIANG, Rongbiao TONG

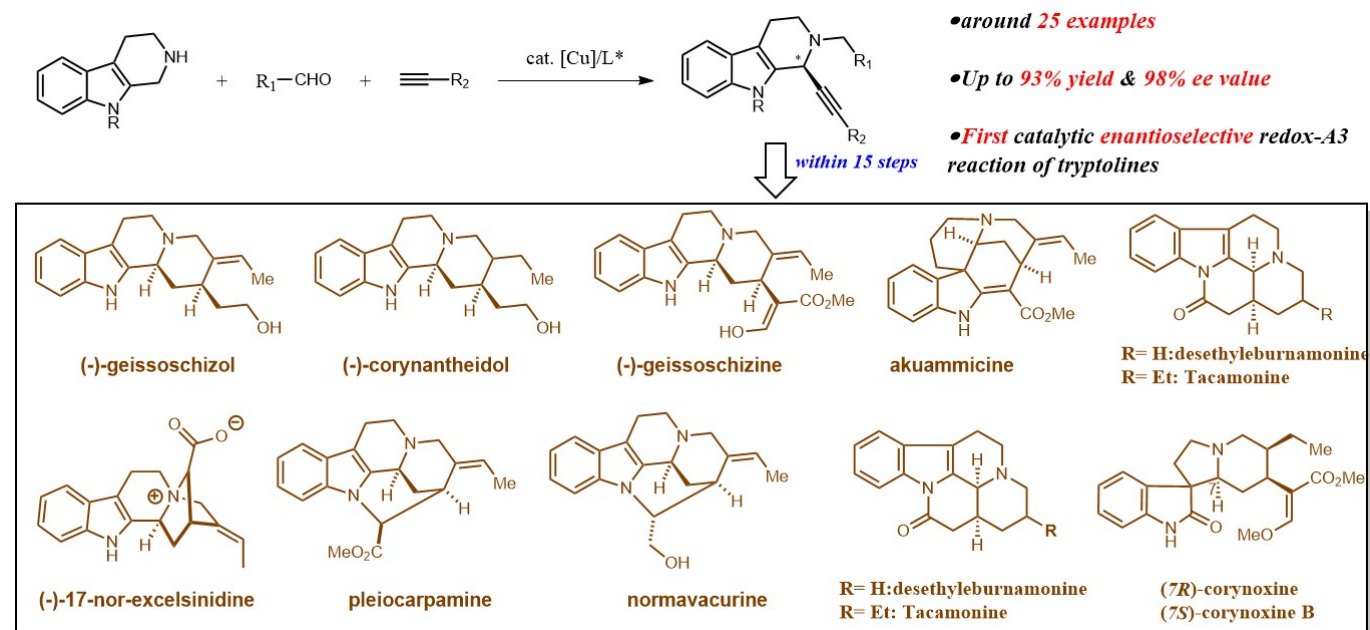
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### Abstract

Tryptolines (tetrahydro- $\beta$ -carbolines) are important building blocks for total synthesis of numerous natural products and bioactive molecules<sup>1</sup>. In this study, a new catalytic enantioselective redox-A<sup>3</sup> (amine, aldehyde and alkyne) reaction of tryptolines was developed, which achieves the first enantioselective synthesis of previously unattainable  $\alpha$ -alkynyl tryptolines in good yield and high enantioselectivity. The obtained  $\alpha$ -alkynyl tryptolines can approach to libraries of indole alkaloid natural products and analogues within 5 to 20 steps.



### References

1. Spindler, A.; Stefan, K.; Wiese, M. *J. Med. Chem.* **2016**, *59*, 6121-6135.