





## Welcome

On behalf of the Local Organizing Committee, we are delighted to welcome you to the **9th International Conference on Multicomponent Reactions and Related Chemistry (MCR2026)**, held in Guangzhou, China, from January 13 to 16, 2026.

MCR2026 brings together **approximately 100 participants**, including **45 distinguished speakers from 11 countries**, reflecting the truly international and collaborative nature of the multicomponent reactions community. In close collaboration with the Scientific Advisory Board, the Organizing Committee has prepared a rich and stimulating scientific program that highlights current frontiers in multicomponent reactions, catalysis, and their applications in drug discovery and related fields. Particular emphasis is placed on the active participation, visibility, and development of young scientists.

We would like to express our sincere appreciation to senior researchers for their continued generosity, mentorship, and support, which play a vital role in fostering the next generation of scientists and advancing the field as a whole.

The conference is hosted at **Sun Yat-sen University**, one of China's leading research institutions, offering an inspiring academic setting that combines a strong scientific tradition with a dynamic and modern research environment in the vibrant city of Guangzhou.

We warmly invite you to share your exciting research, engage in in-depth scientific discussions, and enjoy the culture and hospitality of Guangzhou. We are confident that MCR2026 provides both an intellectually rewarding and personally enjoyable experience.

We wish you a productive and memorable conference and are very pleased to welcome you to MCR2026.

With best regards,

**Prof. Albert Chan Sun-Chi**

**Prof. Wenhao Hu**

Co-Chairs of the Local Organizing Committee  
MCR2026



## *Committee*

### **International Advisory Board**



Erik Van der Eycken, The University of Leuven, Belgium



Albert Chan Sun-Chi, Sun Yat-sen University, China



Wenhao Hu, Sun Yat-sen University, China

### **Organizing Committee**

Albert Chan Sun-Chi, Sun Yat-sen University, China

Wenhao Hu, Sun Yat-sen University, China

Wenjing Zhao, Sun Yat-sen University, China

Taoda Shi, Sun Yat-sen University, China

Yijia Yuan, Sun Yat-sen University, China

Dongying Xu, Sun Yat-sen University, China

Huanqian Mo, Sun Yat-sen University, China

Fang Yang, Sun Yat-sen University, China

Yunlin Liu, Guangzhou University, China

Shikun Jia, Zhengzhou University, China

Cheng Zhang, Guangzhou Medical University, China

Xiang Fu, Sun Yat-sen University, China

Feng Xiong, Sun Yat-sen University, China

## *Programme*



**Yifeng Chen**  
East China University of Science and  
Technology, Shanghai, PR China



**Lingling Chu**  
Donghua University, PR China



**Jia-Rong Chen**  
Central China Normal University, PR  
China



**Alexander Dömling**  
Czech Advanced Technology and  
Research Institute, Palacký University  
Olomouc, Czech Republic



**Xiu-Qin Dong**  
College of Chemistry and Molecular  
Sciences, Wuhan University, PR China



**Ouldouz Ghashghaei**  
University of Barcelona, Spain



**Hanmin Huang**  
University of Science and Technology  
of China, PR China



**Rongrong Hu**  
South China University of Technology,  
PR China



**Zhenghui Kang**  
Shanghai Institute of Material  
Medica/Zhongshan Institute for Drug  
Discovery, CAS



**Rodolfo Lavilla**  
University of Barcelona, Spain



**Aiwen Lei**  
College of Chemistry and Molecular  
Science, Wuhan University, Wuhan,  
PR China



**Junlong Li**  
College of Pharmacy, Chengdu  
University, PR China



**Zhong Lian**  
Sichuan University, Chengdu, PR  
China



**Xiaohua Liu**  
Sichuan University, PR China



**Xinyuan Liu**  
Southern University of Science and  
Technology, PR China



**Keiji Maruoka**  
Kyoto University, Japan and  
Guangdong University of Technology,  
PR China



**Thomas J. J. Müller**  
Heinrich Heine University Düsseldorf,  
Germany



**Romano V. A. Orru**  
Vrije Universiteit Amsterdam, The  
Netherlands



**Shiliang Shi**  
Shanghai Institute of Organic  
Chemistry, PR China



**Wei Shu**  
Southern University of Science and  
Technology, Shenzhen, Guangdong,  
PR China



**Leonid G. Voskressensky**  
Patrice Lumumba Peoples' Friendship  
University of Russia (RUDN  
University), Moscow, Russia



**Xiaoming Wang**  
Shanghai Institute of Organic  
Chemistry, Shanghai, PR China



**Ludger Wessjohann**  
Leibniz Institute of Plant Biochemistry  
(IPB), Germany



**Hua Wu**  
Shanghai Jiao Tong University,  
Shanghai, PR China



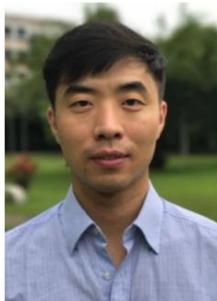
**Wanqing Wu**  
South China University of  
Technology, Guangzhou, PR  
China



**Xuesong Wu**  
Huazhong University of Science  
and Technology, Wuhan, PR China



**Zhenghu Xu**  
Shandong University, Jinan, PR  
China



**Junfeng Yang**  
Department of Chemistry, Fudan  
University, PR China



**Guoyin Yin**  
Wuhan University, Wuhan, Hubei,  
PR China



**Andrei K. Yudin**  
Department of Chemistry,  
University of Toronto, Canada



**Min Zhang**  
South China University of  
Technology, Guangzhou, PR  
China



**Wei Zhang**  
University of Massachusetts  
Boston, USA



**Xingang Zhang**  
University of Chinese Academy of  
Sciences, Chinese Academy of  
Sciences, Shanghai, PR China



**Guangfan Zheng**  
Northeast Normal University,  
Changchun, PR China



**Shifa Zhu**  
South China University of  
Technology, Guangzhou, PR  
China

### *Campus Map*



## Conference Agenda

| Lecture Location: Sun Yat-sen University, <b>Lingnan MBA Center MBA402</b> |   |                          |  |
|--|---|--------------------------|--|
| <b>2026-01-12 (Mon) 14: 00-21: 30 Registration</b>                         |   |                          |  |
| Location: Sun Yat-sen University, Sun Yat-sen Kaifeng Hotel                |   |                          |  |
| <b>2026-01-13 (Tue) Morning</b>  |   |                          |  |
| Time   | Event   | Host                     |  |
| 8:00-8:05  | Opening ceremony- <b>Wenhai Hu</b>  | <b>Wenhai Hu</b>         |  |
| 8:05-8:10  | Welcome from IAB Committee- <b>Erik Van der Eycken</b> , The University of Leuven, Belgium  |                          |  |
| 8:10-8:15  | Welcome from SYSU, Office of International Cooperation & Exchange office for Hongkong, Macao & Taiwan affaires-   |                          |  |
| 8:15-8:20  | Launch speech- <b>Albert Chan Sun-Chi</b>   |                          |  |
| 8:20-8:30  | Conference Photo Session  |                          |  |
| 8:30-9:10  | PS- <b>Alexander Dömling</b> (CATRI, PUO, Czech Republic): <i>Automation + Miniaturization = Acceleration</i>   | <b>Aiwen Lei</b>         |  |
| 9:10-9:35  | KS- <b>Xin-Yuan Liu</b> (SUST, China): <i>Cu/Chiral Anionic Ligand-Catalyzed Enantioselective Cross-Couplings</i>   |                          |  |
| 9:35-10:00   | KS- <b>Hanmin Huang</b> (USTC, China): <i>Aminoalkyl Cyclopalladated Complex: Discovery and Applications</i>  |                          |  |
| 10:00-10:25  | KS- <b>Xingang Zhang</b> (SIOC, CAS, China): <i>Metal Difluorocarbene Catalytic Couplings</i>   |                          |  |
| <b>10:25-11:05 Coffee Break &amp; Poster Session</b>                       |   |                          |  |
| 11:05-11:30  | KS- <b>Hua Wu</b> (SJTU, China): <i>Rearrangement Reactions-Driven N-Heterocycle Synthesis and Modification</i>   | <b>Xiaodan Zhao</b>      |  |
| 11:30-11:55  | KS- <b>Xiaoming Wang</b> (SIOC, CAS, China): <i>Biphosphine LigandEnabled Dirhodium-Catalyzed Carbene Difunctionalization</i>                                     |                          |  |
| 11:55-12:20  | KS- <b>Jia-Rong Chen</b> (CCNU, China): <i>Photoredox and Copper-Catalyzed Controlled Generation of Radical Anions and Multicomponent Radical Reaction Design</i> |                          |  |
| <b>12:20-14:00 Lunch break</b>   |   |                          |  |
| <b>2026-01-13 (Tue) Afternoon</b>  |   |                          |  |
| 14:00-14:40  | PS- <b>Keiji Maruoka</b> (Kyoto Univ., Japan): <i>Development of New Photoinduced Multi-Component Radical Relay Reactions</i>                                     | <b>Alexander Dömling</b> |  |
| 14:40-15:05  | KS- <b>Rongrong Hu</b> (SCU, China): <i>Elemental Chalcogen-Based Multicomponent Polymerizations</i>  |                          |  |
| 15:05-15:30  | KS- <b>Ouldouz Ghashghaei</b> (UB, Spain): <i>Reaction Space Charting of Multicomponent Processes</i>   |                          |  |
| <b>15:30-16:10 Coffee Break &amp; Poster Session</b>                       |   |                          |  |
| 16:10-16:35  | KS- <b>Xiuqin Dong</b> (WHU, China): <i>Efficient Construction of Chiral Molecules via Cooperative Catalysis</i>  | <b>Shanshui Meng</b>     |  |
| 16:35-17:00  | KS- <b>Min Zhang</b> (SCU, China): <i>Catalytic Reduction-Specified Tandem Reaction</i>   |                          |  |
| 17:00-17:05  | Sponsor Talk — <b>Guoyin Lai</b> (Guangzhou Flower Flavours & Fragrances Co., Ltd, China)   |                          |  |
| 17:05-17:15  | OP- <b>Maxim A. Mironov</b> (UFU, Russia) <i>Multicomponent Reactions with Biopolymers as a Powerful Tool for Preparation of 3-D Microstructures</i>              |                          |  |
| 17:15-17:25  | OP- <b>Dong Xing</b> (ECNU, China): <i>Asymmetric Three-Component Difunctionalization of Alkenes via Radical Relay</i>  |                          |  |

|  |  |                 |  |
|--|--|-----------------|--|
| 17:25-17:35  | OP— <b>Zhongqiu Xing</b> (NJU, China): <i>Synergistic Photobiocatalysis for Enantioselective Triple Radical Sorting</i>  |                 |  |
| 17:35-17:45  | OP— <b>Shenghan Teng</b> (FJU, China): <i>Modular Synthesis of Luminescent Boron-Containing Heterocycles From B-Alkynones Trifluoroborates, Amines and Arynes</i>                              |                 |  |
| <b>18:00-19:30 Dinner</b>                            |  |                 |  |
| <b>2026-01-14 (Wed) Morning</b>                      |  |                 |  |
| 8:00-8:40  | PS— <b>Aiwen Lei</b> (WHU, China): <i>Alternating Current (AC) Electrolysis toward Organic Syntheses</i>   | Keiji Maruoka   |  |
| 8:40-9:05  | KS— <b>Lingling Chu</b> (DHU, China): <i>Asymmetric Multicomponent Radical Cross-Couplings</i>   |                 |  |
| 9:05-9:30  | KS— <b>Wei Shu</b> (SUST, China): <i>Catalytic Asymmetric Cross-Hydrodimerization of Hydrocarbons</i>  |                 |  |
| 9:30-9:55  | KS— <b>Yifeng Chen</b> (ECUST, China): <i>Asymmetric Radical Addition Chemistry</i>  |                 |  |
| <b>09:55-10:35 Coffee Break &amp; Poster Session</b> |  |                 |  |
| 10:35-11:00  | KS— <b>Junfeng Yang</b> (FDU, China): <i>Pd-Catalyzed Asymmetric Three-Component Coupling of N-Sulfonylhydrazones</i>  | Liangbin Huang  |  |
| 11:00-11:25  | KS— <b>Guangfan Zheng</b> (NENU, China): <i>Multicomponent Radical Reactions Leveraging the Persistent Radical Effect</i>  |                 |  |
| 11:25-11:50  | KS— <b>Wanqing Wu</b> (SCUT, China): <i>Heteroatom-Promoted Sequential Conversions of Unsaturated Hydrocarbons</i>   |                 |  |
| <b>11:50-14:00 Lunch break</b>                       |  |                 |  |
| <b>2026-01-14 (Wed) Afternoon</b>                    |  |                 |  |
| 14:00-14:40  | PS— <b>Andrei K. Yudin</b> (UofT, Canada): <i>Isoreactivity in Chemistry</i>   | Rodolfo Lavilla |  |
| 14:40-15:05  | KS— <b>Romano V. A. Orru</b> (VU Amsterdam, Netherlands): <i>Isocyanides: Chemical Chameleons</i>  |                 |  |
| 15:05-15:30  | KS— <b>Zhong Lian</b> (SCU, China): <i>Mechanical Synthetic Chemistry</i>  |                 |  |
| 15:30-15:55  | KS— <b>Junlong Li</b> (CDU, China): <i>Remote Site-selective Arene C-H Functionalization Enabled by N-Heterocyclic Carbene Organocatalysis</i>   |                 |  |
| <b>15:55-16:35 Coffee Break &amp; Poster Session</b> |  |                 |  |
| 16:35-17:00  | KS— <b>Xiaohua Liu</b> (SCU, China): <i>Asymmetric Multicomponent Reaction Catalyzed by Chiral Metal Complexes</i>   | Jun Wang        |  |
| 17:00-17:25  | KS— <b>Zhenghu Xu</b> (SDU, China): <i>Tandem Metal Relay Catalysis to polycycles</i>  |                 |  |
| 17:25-17:30  | Sponsor Talk — <b>Yiming Li</b> 3S-TECH  |                 |  |
| 17:30-17:40  | OP— <b>Yu Qian</b> (SYSU, China): <i>Multicomponent Reactions with Rh Carbonynoids</i>   |                 |  |
| 17:40-17:50  | OP— <b>Georg Manolikakes</b> (RPTU, Germany): <i>Modular Synthesis of Sulfonamides and Sulfonates via Electrochemical Fixation of Sulfur Dioxide</i>   |                 |  |
| 17:50-18:00  | OP— <b>A. S. Golubenkova</b> (RU., Russia): <i>A Domino Route From Imidazolines and Electron-Deficientalkynes to Polysubstituted Pyrroles, Tetrahydropyrrolo[1,2-A]Pyrazines and Pyridines</i> |                 |  |
| <b>2026-01-15 (Thur) Morning</b>                     |  |                 |  |
| 8:40-9:05  | KS— <b>Guoyin Yin</b> (SCUT, China): <i>Nickel Chain-Walking Catalysis for Multicomponent Alkene Functionalization</i>   |                 |  |

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|--|---|------------------------|
| 9:05-9:30  | KS — <b>Wei Zhang</b> (UMB, USA): <i>Integrated One-Pot Stepwise Synthesis and Organocatalysis</i>  | <b>Andrei K. Yudin</b> |
| 9:30-9:55  | KS— <b>Leonid G. Voskressensky</b> (RU, Russia): <i>Electron-Deficient Alkynes – Universal Synthons for Producing Condensed Aza-Heterocyclic Systems</i>  |                        |
| 10:35-11:00  | KS— <b>Rodolfo Lavilla</b> (UB, Spain): <i>Heterocyclic Multicomponent Reactions. New Reactivity Trends and Biomed Applications (25 Years of MCR Research in Barcelona)</i>   | <b>Honggen Wang</b>    |
| <b>09:55-10:35 Coffee Break &amp; Poster Session</b> |   |                        |
| 11:00-11:25  | KS— <b>Shiliang Shi</b> (SIOC, CAS, China): <i>Asymmetric NHC–Metal Catalysis</i>   | <b>Honggen Wang</b>    |
| 11:25-11:50  | KS— <b>Xuesong Wu</b> (HUST, China): <i>Light-Driven Multicomponent Radical Reactions with Sulfur-Containing Small Molecules</i>  |                        |
| <b>11:50-14:00 Lunch break</b>                       |   |                        |
| 14:00-14:40  | KS— <b>Shifa Zhu</b> (ZSTU, China): <i>Catalytic Transformation of Acetylene</i>  | <b>Yunlin Liu</b>      |
| 14:40-15:05  | KS— <b>Ludger Wessjohann</b> (LIPB, Germany): <i>Tumor-targeting with MCR-derived drugs and conjugates</i>  |                        |
| 15:05-15:30  | KS— <b>Thomas J. J. Müller</b> (HHU Düsseldorf, Germany): <i>Sequentially Pd-Catalyzed Processes—Consecutive Multicomponent Synthesis of Functional Molecules in Catalyst Economic Fashion</i>                                  |                        |
| 15:30-15:55  | KS— <b>Zhenghui Kang</b> (SIMM, CAS, China): <i>Multicomponent Reactions Enabled by Metal Carbene Multifunctionalization</i>  |                        |
| <b>15:55-16:35 Coffee Break &amp; Poster Session</b> |   |                        |
| 16:35-16:45  | OP— <b>Minghui Wu</b> (AMIBM, Netherlands): <i>Non-Innocent Behaviour of Aromatic Isocyanides Under Visible Light: A Pathway to Thioformimidates and Dehydroalanine</i>   | <b>Zhongqiu Xing</b>   |
| 16:45-16:55  | OP— <b>M. I. D. Mardjan</b> (UGM, Indonesia): <i>Straightforward Access to Bioactive Quinazolinones Through One-Pot Reaction</i>  |                        |
| 16:55-17:05  | OP— <b>Ali O. Alqarni</b> (NU, Egypt): <i>Efficient Three-Step Synthesis of Novel Triazole-Hydrazone Hybrid Compounds: From Ethyl 5-Acetamido-1,2,4-Triazole-3-Carboxylate to Salicylaldehyde-Derived Fluorescent Molecules</i> |                        |
| 17:05-17:10  | Sponsor Talk — <b>Paul Wei</b> , (FLM, China)   | <b>Taoda Shi</b>       |
| 17:10-17:15  | Sponsor Talk — <b>Taoda Shi</b> , (MD, China)   |                        |
| 17:15-17:30  | Speaker & Poster Awards   |                        |
| 17:30-17:40  | Closing ceremony  | <b>Wenhao Hu</b>       |

### ***Cultural Excursion Program***

**2026-01-16 (Friday)**

**09:20:** Meet at the lobby of **Xue Ren Guan** (Scholars' Lodge) and depart

**09:30–10:50:** Visit to the **South Campus Museum**

**11:00–12:00:** Visit to the **University History Museum**

**12:00:** Lunch at **Xue Ren Guan** (Scholars' Lodge)

**13:00:** Meet at the lobby of **Xue Ren Guan** and depart

**13:45–14:45:** Visit to the **Chen Clan Ancestral Hall** (Chenjiaci)

**15:00–16:30:** Visit to **Shamian Island**

**16:30:** Return

**18:00:** Dinner at **Xue Ren Guan** (Scholars' Lodge)

**19:00:** **Pearl River Night Cruise**





### *Awards*

To encourage academic exchange and recognize outstanding scientific contributions, the conference will present awards for **Oral and Poster Presentations**.

#### **Conference Awards**

- **Best Oral Presentation**
  - 1st Prize: RMB 800
  - 2nd Prize: RMB 600
  - 3rd Prize: RMB 400
- **Best Poster Presentation**
  - 1st Prize: RMB 800
  - 2nd Prize: RMB 600
  - 3rd Prize: RMB 400

#### **Sponsored Awards**

In addition, *Molecular Diversity* will sponsor two special awards by providing **book vouchers** for:

- **Best Student Oral Presentation**
- **Best Student Poster Presentation**

Awardees will be selected by the conference evaluation committee based on scientific quality, originality, and presentation performance.



## Communication Index

### PLENARY SPEAKERS

PS-1. **Alexander Dömling.** *University of Groningen.* Netherlands

AUTOMATION + MINIATURIZATION = ACCELERATION

PS-2. **Aiwen Lei.** *Wuhan University.* China

ALTERNATING CURRENT (AC) ELECTROLYSIS TOWARD ORGANIC SYNTHESSES

PS-3. **Keiji Maruoka.** *Kyoto University.* Japan

DEVELOPMENT OF NEW PHOTOINDUCED MULTI-COMPONENT RADICAL RELAY REACTIONS

PS-4. **Andrei Yudin.** *University of Toronto.* Canada

ISOREACTIVITY IN CHEMISTRY

### KEYNOTE SPEAKERS

KS-1. **Yifeng Chen.** *East China University of Science and Technology.* China

ASYMMETRIC RADICAL ADDITION CHEMISTRY

KS-2. **Lingling Chu.** *Donghua University.* China

ASYMMETRIC MULTICOMPONENT RADICAL CROSS-COUPPLINGS

KS-3. **Jia-Rong Chen.** *Central China Normal University.* China

PHOTOREDOX AND COPPER-CATALYZED CONTROLLED GENERATION OF RADICAL ANIONS AND MULTICOMPONENT RADICAL REACTION DESIGN

KS-4. **Xiu-Qin Dong.** *Wuhan University.* China

EFFICIENT CONSTRUCTION OF CHIRAL MOLECULES VIA COOPERATIVE CATALYSIS

KS-5. **Ouldouz Ghashghaei.** *University of Barcelona.* Spain

REACTION SPACE CHARTING OF MULTICOMPONENT PROCESSES

KS-6. **Hanmin Huang.** *University of Science and Technology of China.* China

AMINOALKYL CYCLOPALLADATED COMPLEX: DISCOVERY AND SYNTHETIC APPLICATIONS

KS-7. **Rongrong Hu.** *South China University of Technology.* China

ELEMENTAL CHALCOGEN-BASED MULTICOMPONENT POLYMERIZATIONS

KS-8. **Zhenghui Kang.** *Shanghai Institute of Materia Medica.* China

Multicomponent Reactions Enabled by Metal Carbene Multifunctionalization



KS-9. **Rodolfo Lavilla.** *University of Barcelona.* Spain

HETEROCYCLIC MULTICOMPONENT REACTIONS. NEW REACTIVITY TRENDS AND BIOMED APPLICATIONS

KS-10. **Jun-Long Li.** *Chengdu University.* China

REMOTE SITE-SELECTIVE ARENE C-H FUNCTIONALIZATION ENABLED BY N-HETEROCYCLIC CARBENE ORGANOCATALYSIS

KS-11. **Zhong Lian.** *Sichuan University.* China

MECHANICAL SYNTHETIC CHEMISTRY

KS-12. **Xiaohua Liu.** *Sichuan University.* China

REMOTE SITE-SELECTIVE ARENE C-H FUNCTIONALIZATION ENABLED BY N-HETEROCYCLIC CARBENE ORGANOCATALYSIS

KS-13. **Xin-Yuan Liu.** *Southern University of Science and Technology.* China

Cu/CHIRAL ANIONIC LIGAND-CATALYZED ENANTIOSELECTIVE CROSS-COUPLEINGS

KS-14. **Thomas J. J. Müller.** *Heinrich Heine University Düsseldorf.* Germany

SEQUENTIALLY PD-CATALYZED PROCESSES-CONSECUTIVE MULTICOMPONENT SYNTHESIS OF FUNCTIONAL MOLECULES IN CATALYST ECONOMIC FASHION

KS-15. **Romano V.A. Orru.** *Maastricht University.* China

ISOCYANIDES: CHEMICAL CHAMELEONS

KS-16. **Shi-Liang Shi.** *Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences.* China

ASYMMETRIC NHC-METAL CATALYSIS

KS-17. **Wei Shu.** *Southern University of Science and Technology.* China

CATALYTIC ASYMMETRIC CROSS-HYDRODIMERIZATION OF HYDROCARBONS

KS-18. **Voskressensky L.G.** *Peoples' Friendship University of Russia.* Russia

ELECTRON-DEFICIENT ALKYNES-UNIVERSAL SYNTHONS FOR PRODUCING CONDENSED AZA-HETEROCYCLIC SYSTEMS

KS-19. **Xiaoming Wang.** *Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences.* China

BIPHOSPHINE LIGAND ENABLED DIRHODIUM-CATALYZED CARBENE DIFUNCTIONALIZATION

KS-20. **Ludger A. Wessjohann & team.** *Leibniz Institute of Plant Biochemistry.* Germany

TUMOR-TARGETING WITH MCR-DERIVED DRUGS AND CONJUGATES

KS-21. **Hua Wu.** *Shanghai Jiao Tong University.* China

REARRANGEMENT REACTIONS-DRIVEN N-HETEROCYCLE SYNTHESIS AND MODIFICATION

KS-22. **Wanqing Wu.** *South China University of Technology.* China



## HETEROATOM-PROMOTED SEQUENTIAL CONVERSIONS OF UNSATURATED HYDROCARBONS

KS-23. **Xuesong Wu.** *Huazhong University of Science and Technology.* China

LIGHT-DRIVEN MULTICOMPONENT RADICAL REACTIONS WITH SULFUR-CONTAINING SMALL MOLECULES

KS-24. **Zhenghu Xu.** *Shandong University.* China

ASYMMETRIC METAL RELAY CATALYSIS TO PLANAR CHIRAL [2.2]PARACYCLOPHANES

KS-25. **Junfeng Yang.** *Fudan University.* China

PD-CATALYZED ASYMMETRIC THREE-COMPONENT COUPLING OF N-SULFONYLHYDRAZONES

KS-26. **Guoyin Yin.** *South China University of Technology.* China

CATALYTIC REDUCTION-SPECIFIED TANDEM REACTION

KS-27. **Min Zhang.** *Sichuan University.* China

REMOTE SITE-SELECTIVE ARENE C-H FUNCTIONALIZATION ENABLED BY N-HETEROCYCLIC CARBENE ORGANOCATALYSIS

KS-28. **Wei Zhang.** *University of Massachusetts Boston.* USA

INTEGRATED ONE-POT STEPWISE SYNTHESIS AND ORGANOCATALYSIS

KS-29. **Xingang Zhang.** *Chinese Academy of Sciences.* China

METAL DIFLUOROCARBENE-INVOLVED CATALYTIC COUPLING

KS-30. **Guangfan Zheng.** *Northeast Normal University.* China

MULTICOMPONENT RADICAL REACTIONS LEVERAGING THE PERSISTENT RADICAL EFFECT

KS-31. **Shifa Zhu.** *Zhejiang Sci-Tech University.* China

CATALYTIC TRANSFORMATION OF ACETYLENE

## ORAL PRESENTATIONS

OP-1. **Ali O. Alqarni.** *Najran University.* Egypt

EFFICIENT THREE-STEP SYNTHESIS OF NOVEL TRIAZOLE-HYDRAZONE HYBRID COMPOUNDS: FROM ETHYL 5-ACETAMIDO-1,2,4-TRIAZOLE-3-CARBOXYLATE TO SALICYLALDEHYDE-DERIVED FLUORESCENT MOLECULES

OP-2. **Georg Manolikakes.** *RPTU Kaiserslautern-Landau.* Germany

MODULAR SYNTHESIS OF SULFONAMIDES AND SULFONATES VIA ELECTROCHEMICAL FIXATION OF SULFUR DIOXIDE



The 9<sup>th</sup> International Conference on  
Multicomponent Reactions and Related Chemistry  
13-16<sup>th</sup> Jan 2026



OP-3. **Muhammad Idham Darussalam Mardjan.** *Universitas Gadjah Mada. Indonesia*

STRAIGHTFORWARD ACCESS TO BIOACTIVE QUINAZOLINONES THROUGH ONE-POT  
REACTION

OP-4. **Maxim A. Mironov.** *Ural Federal University. China*

MULTICOMPONENT REACTIONS WITH BIOPOLYMERS AS A POWERFUL TOOL FOR  
PREPARATION OF 3-D MICROSTRUCTURES

OP-5. **Yu Qian.** *Sun Yat-sen University. China*

MULTICOMPONENT REACTIONS WITH RH CARBYNOIDS

OP-6. **Golubenkova A.S.** *Peoples' Friendship University of Russia. Russia*

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POLYSUBSTITUTED PYRROLES, TETRAHYDROPYRROLO[1,2-A]PYRAZINES AND  
PYRIDINES

OP-7. **Shenghan Teng.** *Fujian Normal University. China*

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OP-8. **Minghui Wu.** *Aachen-Maastricht Institute for Biobased Materials. Netherlands*

NON-INNOCENT BEHAVIOUR OF AROMATIC ISOCYANIDES UNDER VISIBLE LIGHT: A  
PATHWAY TO THIOFORMIMIDATES AND DEHYDROALANINE

OP-9. **Zhongqiu Xing.** *Nanjing University. China*

SYNERGISTIC PHOTOBIOCATALYSIS FOR ENANTIOSELECTIVE TRIPLE RADICAL  
SORTING



## PLENARY SPEAKERS

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Prof. Alexander Dömling is ERA Chair of the Innovative Chemistry Group at Palacký University Olomouc, where his research focuses on the design and discovery of bioactive compounds for difficult drug targets such as protein–protein interactions, transcription factors, and RNA. He received his PhD under Ivar Ugi at the Technical University of Munich and carried out postdoctoral studies with Nobel laureate Barry Sharpless at The Scripps Research Institute. At the University of Pittsburgh, where he became Full Professor, he co-developed the widely used web-based discovery tool **ANCHOR.QUERY**. From 2011 to 2022 he was Chair of Drug Design at the University of Groningen. He now leads the ERC Advanced Grant–funded **AMADEUS** platform, which introduces a novel paradigm for preclinical drug discovery by integrating nanoliter dispensing, high-throughput chemistry, purification, screening, and machine learning. With over 300 publications and more than 70 patents, he is also a serial entrepreneur translating innovation “from bench to bedside.”



## Automation + Miniaturization = Acceleration

“Boring is good,” some say, reflecting the steady reliability of traditional engineering, while “Data is the new oil” has become the mantra of modern innovation. Chemistry, long viewed as a conservative discipline, now stands at a transformative crossroads shaped by disruptive technologies. Artificial intelligence—through large language models (LLMs) and related tools—rapidly processes complex challenges, reshaping how we approach intellectual property, knowledge discovery, and molecular design. In parallel, highly miniaturized and automated synthesis platforms are redefining how molecules are created and optimized. In the Dömling laboratory, supported by the ERC Advanced Grant AMADEUS and the ERA Chair ACCELERATOR, we embrace the principle: Automation + Miniaturization = Acceleration. In 2019, we introduced acoustic droplet ejection (ADE) technology for small-molecule synthesis, enabling execution of thousands of reactions per day at nanoliter scale (ACS Cent. Sci. 2019, 5, 451-457). ADE combines unparalleled precision with high speed—2.5 nL droplets at up to 400 Hz into 1536-well plates—validated across dozens of transformations. Coupled with rapid MS analytics and miniaturized purification, this provides immediate feedback and compound availability. By integrating generative neural networks and property-driven selection, ADE generates “big data” for machine learning, advancing reactivity prediction and molecular optimization. Furthermore, coupling ADE with protein mass spectrometry accelerates discovery of covalent inhibitors against disease-relevant targets at unprecedented throughput. A new era is emerging in chemistry—defined by robust automation, data-rich experimentation, and the synergy of AI with miniaturized synthesis—redefining the discovery process itself.



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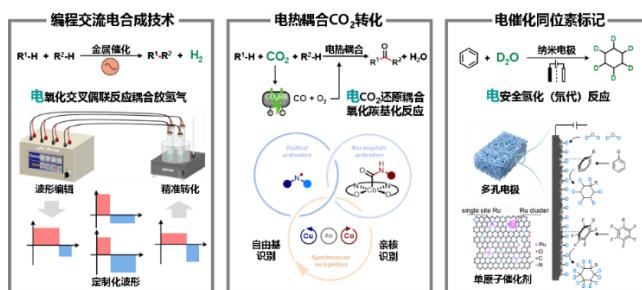
Lei Aiwen, a Second-Class Professor at Wuhan University, Vice Dean of the Advanced Institute of Wuhan University, and Associate Editor of the internationally authoritative journal Green Chemistry. He has received the 4th Yoshida Prize (2019), was named a Leading Talent in Scientific and Technological Innovation under the National "Ten Thousand Talents Program" (2017), a Chang Jiang Scholar Distinguished Professor (2014), a recipient of the National Science Fund for Distinguished Young Scholars (2010), the First Prize of the Outstanding Scientific Research Achievements (Science and Technology) of Institutions of Higher Education of the Ministry of Education (2017, first completer), and the First Prize of Natural Science of Hubei Province (2012, first completer). He serves as the Deputy Director of the Homogeneous Catalysis Professional Committee of the Catalysis Committee of the Chinese Chemical Society, a Member of the Organic Chemistry Disciplinary Committee of the Chinese Chemical Society, and a Member of the Physical Organic Chemistry Professional Committee of the Chinese Chemical Society.

## Alternating Current (AC) Electrolysis toward Organic Syntheses

Aiwen Lei

**Keywords:** *AC electrolysis, organic synthesis, metal-catalyzed electrolysis, reaction intermediates*

Electricity, as an important form of energy, has contributed to the rapid development of modern industry. The microscopic core of the precise control of electricity is the level of precise manipulation of electrons, which has been widely used in many fields and industries, such as electronic devices and intelligent control, mapping the progress of society, but the application in the synthesis of substances is still in the initial stage. Our team reports a programmable waveform alternating current (AC) synthesis technology that realizes two types of anodic oxidation-coupled cathodic hydrogen discharge reactions. By adjusting the parameters of frequency, current and duty cycle of the alternating current, customized current waveforms are generated, thus achieving precise control of transition metal catalytic species and breaking the dependence of traditional DC catalysis on diaphragm electrolytic cells. This study provides a new opportunity to introduce electronic precision control technology into the field of electrosynthesis. In addition, the team also reported the coupled oxidative carbonylation reaction mode of electroreduced carbon dioxide, in which CO, which is commonly used in industry, was replaced with inert and non-toxic carbon dioxide, and then asymmetric ureas, which are important for pharmaceutical and pesticide applications, were synthesized with high efficiency. In the study of nano-metal cathode-catalyzed reduction of deuterium substitution reaction, the team successfully synthesized high-value deuterium drugs, which are difficult to be achieved by traditional methods, by using cheap and easy-to-obtain deuterium water as deuterium source through the electrocatalytic strategy. The research results demonstrate the great potential of synthetic electrochemistry in drug development and practical applications.



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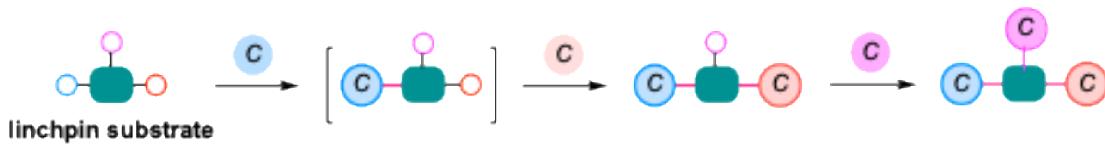
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Keiji Maruoka was born in Japan. He graduated from Kyoto University (1976) and received his Ph.D. (1980) from University of Hawaii (Thesis Director: Prof. H. Yamamoto). He became an assistant professor of Nagoya University (1980) and promoted to a lecturer (1985) and an associate professor (1990) there. He moved to Hokkaido University as a full professor (1995-2001), and then was a professor in the Graduate School of Science in Kyoto University (2000-2019). After formal retirement, he is now a specially-appointed professor in Kyoto University since 2019. He is also a chair professor of Guangdong University of Technology, China as a second-term Chang-Jiang Scholar. Recently, he was awarded the Chemical Society of Japan Award (2007), the Molecular Chirality Award (2007), Novartis Lectureship Award (2007/2008), Chunichi Cultural Prize (2010), Arthur C. Cope Scholar Awards (2011), Medal of Honor with Purple Ribbon (2011), Humboldt Research Award (2011), Torey Science & Technology Award (2012), Noyori Prize (2016), The Japan Academy Prize (2018), Fujiwara Award (2022), and 2023 Ryoji Noyori ACES award. He also serves as the President of the Chemical Society of Japan since 2024.

## Development of New Photoinduced Multi-Component Radical Relay Reactions

### Abstract

Rapid assembly of readily and widely available substrates into synthetically valuable molecules is of prime importance in modern organic synthesis. The use of small organic molecules that can be connected with multiple substrates by a sequential C–C bond-forming process has offered a multidirectional approach to increase molecular complexity with high modularity. Such multicomponent protocols utilizing linchpin compounds have enabled the expeditious construction of complex building blocks for natural products and biologically active compounds. However, their C–C bond-forming processes rely heavily on the use of organometallic reagents as strong nucleophiles, which narrows the scope of accessible products due to limited functional group compatibility. Moreover, complicated manipulations under cryogenic conditions with the strict prohibition of water are frequently required to control the reactivity of these reagents and intermediates. On the other hand, the chemistry of radical species can provide a complementary approach to that of ionic species for new bond formations. The recent advances in synthetic methodologies for the generation of radical species, such as photoredox catalysis and electrocatalysis, have made these conditions milder and more practical. Despite these breakthroughs, the linchpin coupling strategy based on radical-mediated C–C bond formations has been less explored. In this lecture, I would like to describe a metal-free, radical-mediated coupling approach using formyl- and carbonyl-stabilized phosphonium ylides as multifunctional linchpins under visible-light photoredox conditions. The stepwise and controllable generation of these radical intermediates allows sequential photocatalysis involving two mechanistically distinct radical additions, both of which are initiated by the same photocatalyst in one pot with a high functional-group tolerance.



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**The 9<sup>th</sup> International Conference on  
Multicomponent Reactions and Related Chemistry  
13-16<sup>th</sup> Jan 2026**



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Andrei Yudin is the Tier I Canada Research Chair in Medicine by Design and Professor of Chemistry at the University of Toronto. He received his undergraduate degree from Moscow State University in 1992 and earned his Ph.D. in 1996 at the University of Southern California under the supervision of G. K. S. Prakash and Nobel Laureate George A. Olah. He then pursued postdoctoral studies with Nobel Laureate K. Barry Sharpless at The Scripps Research Institute before beginning his independent career at the University of Toronto in 1998. He was promoted to Associate Professor in 2002 and to Full Professor in 2007. Professor Yudin's research has pioneered new concepts in chemical reactivity, macrocycle synthesis, and peptide modification, with broad impact on drug discovery and fundamental chemical reactivity. His contributions have been recognized with numerous honors, including the 2025 Liebig Fellowship (University of Giessen, Germany), the 2024 Arthur C. Cope Scholar Award (American Chemical Society), the 2024 IOCF Zen-ichi Yoshida Lectureship (Kyoto University), the 2022 Konrad Adenauer Award from the Humboldt Foundation (Germany), and the 2023 Organic Reactions Lectureship at the University of California–Irvine. In the past 3 years he has also served as a Visiting Professor at Sorbonne University, Hokkaido University, and the Australian National University. He is currently an Associate Editor for *Chemical Science* (Royal Society of Chemistry).

## ISOREACTIVITY IN CHEMISTRY

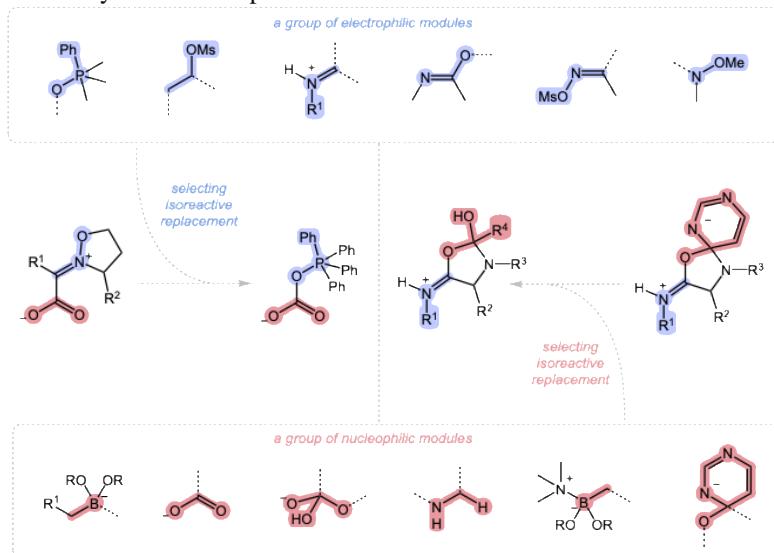
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**Keywords:** *isoreactivity, synthetic half-reactions, reaction discovery*

The concept of isoreactivity seeks to reveal parallels in chemical behavior by comparing the functional roles of structural modules within reaction mechanisms. This framework enables systematic analysis of diverse transformations through the replacement of structural modules that preserve reaction viability, even when the underlying mechanism diverges. Isoreactive module replacement is expected to modify intrinsic barriers and thermodynamic contributions to activation profiles while maintaining the overall feasibility of the forward reaction pathway. Isoreactive relationships extend traditional isoelectronic and isolobal analogies by addressing cases where comparable reactivity cannot be adequately captured by existing conventions. The language of functional modules highlights mechanistic relationships that elude the peripheral modifications encoded by typical substituent changes. By illuminating the mechanistic roles of deep-seated, structurally distinct subunits that enable viable reaction trajectories, isoreactivity establishes a practical and inclusive vocabulary for describing chemical reactivity in multicomponent reactions.





## KEYNOTE SPEAKERS

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## Asymmetric Radical Addition Chemistry

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**Keywords:** *asymmetric catalysis, radical chemistry, cobalt, carbonyl addition*

The catalytic asymmetric addition of carbonyls with organometallic reagents represents a well-established method for chiral amine and alcohol synthesis. Nevertheless, these approaches are dominated by the use of moisture- and air-sensitive organometallic reagents. Moreover, the most reliable organometallic nucleophiles, including organolithium, Grignard reagent and a small number of dialkylzinc reagents, are less functionality-group tolerable. Herein we report a catalytic asymmetric radical addition protocol with various unactivated alkyl halides, including alkyl iodides, alkyl bromides and alkyl chlorides, enabling the formation of chiral  $\alpha$ -amino esters, alcohols, amides and sulfonamide with a high level of enantioselectivity and excellent functional group tolerance.

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In 2016, she joined Donghua University as a Professor and established her independent research group. Her research interests lie in the areas of transition metal catalysis and radical chemistry. She has authored over 50 publications as a corresponding author in top-tier journals such as Chemical Society Reviews, Journal of the American Chemical Society, Nature Communications, and Angewandte Chemie International Edition, etc.

Dr. Chu is a recipient of the National High-Level Talent Program and the Excellent Youth Program of the National Natural Science Foundation of China. Her scientific contributions have been recognized with several prestigious awards, including the Second Prize of the National Natural Science Award (second rank), the First Prize of Natural Science of Shanghai Municipality (second rank), the Shanghai Women's Innovation Award, and the Thieme Chemistry Journals Award.



## "Asymmetric Multicomponent Radical Cross-Couplings"

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The development of efficient catalytic multicomponent reactions (MCRs) is highly sought-after in chemical synthesis. Particularly, catalytic radical MCRs represent a powerful technology for rapidly constructing molecular complexity from readily available starting materials with complementary reactivity and selectivity. However, due to the exceptionally high reactivity of open-shell radical species, catalytic asymmetric radical MCRs remain largely under-developed. One of the research interests in the Chu group at Donghua University is developing enantioselective radical MCR reactions via nickel catalysis. This talk will present enantioselective radical three-component difunctionalization reactions of alkenes via nickel catalysis based on chelation and sensitization strategies. Computational and experimental mechanistic studies will be briefly discussed.



**The 9<sup>th</sup> International Conference on  
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## Photoredox and Copper-Catalyzed Controlled Generation of Radical Anions and Multicomponent Radical Reaction Design

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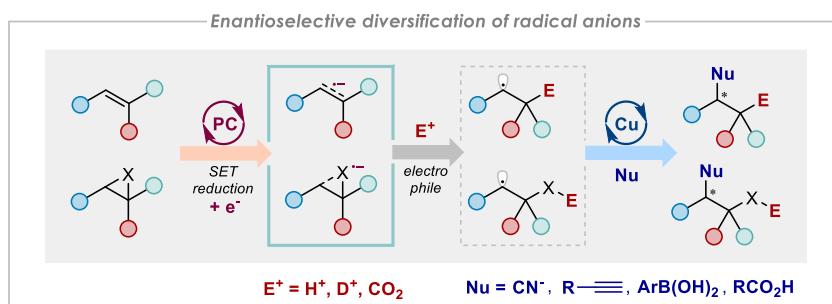
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**Keywords:** multicomponent radical reaction, photoredox catalysis, copper catalysis, radical anions

Radical anions, which possess both the properties of radicals and anions, are an important type of intermediate in organic synthesis transformations.<sup>1</sup> However, the common methods for generating such reactive intermediates often require relatively harsh conditions, leading to difficulties in controlling the reactivity and limited functional group compatibility. In recent years, with the development of photoredox catalysis and transition metal catalysis,<sup>2</sup> the chemistry of radical anions has ushered in new opportunities. Building on our previous work in photocatalysis and copper catalysis,<sup>3</sup> we have developed a synergistic mode of photoredox and copper catalysis for controllable generation and efficient transformations of radical anions, including asymmetric cynanofunctionalization of alkenes, hydroalkynylation and hydroarylation of alkenes, and hydrofunctionalization of epoxides.<sup>4</sup>



**Fig. 1** Enantioselective diversification of radical anions

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## Efficient Construction of Chiral Molecules *via* Cooperative Catalysis

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**Keywords:** cooperative catalysis, non-covalent interactions, asymmetric catalytic reactions ...

Based on cooperative catalysis strategy, our research group focuses on the development of novel chiral phosphine ligands and efficient asymmetric catalytic systems for the efficient synthesis of chiral molecules. Our research work mainly focused on the following two aspects: (1) Developing new chiral bisphosphine ligands based on non-covalent ion-pair and hydrogen-bond cooperative catalysis strategies. By introducing non-covalent interactions into the ligands, the interaction between the ligands and reaction substrates is enhanced, which could provide favorable chiral induction environment and improve reaction reactivity. These ligands have been applied to a series of asymmetric hydrogenation reactions, efficiently synthesizing a variety of structurally diverse chiral molecules with excellent reaction results;<sup>1-2</sup> (2) Efficiently constructing multifunctionalized chiral molecules based on a synergistic catalytic system combining organocatalysis and photocatalysis.<sup>3</sup> Additionally, we realized stereodivergent synthesis of structurally important chiral molecules bearing multiple stereocenters using bimetallic synergistic catalytic system.<sup>4</sup> We made an effort to the precise assembly of diverse chiral scaffolds, mechanistic investigations, and applying these methodologies to develop new synthetic routes for important chiral pharmaceuticals and bioactive molecules.



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Ouldouz received her BSc. in Chemistry and her first MSc. Polymer Sciences from Sharif University of Technology (Iran). Moving to Barcelona, she received a second MSc. and her PhD in Experimental and Industrial Organic Chemistry from the University of Barcelona (UB). She was appointed as the adjunct professor of Organic Chemistry and Medicinal Chemistry at the Faculty of Pharmacy (UB) in 2021 and joined IDIBELL as a research collaborator in 2025. She has co-authored 25 scientific publications and has participated in various collaborative projects with public and private partners. Her research focuses on developing chemical tools for biomedical research by facilitating synthetic approaches.

## REACTION SPACE CHARTING OF MULTICOMPONENT PROCESSES

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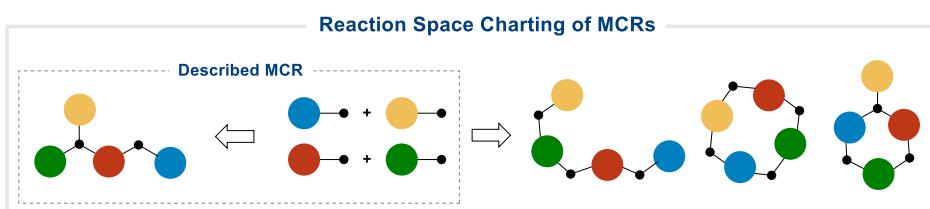
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**Keywords:** *Multicomponent Reactions, Reaction Discovery, Chemical Diversity, Drug Discovery*

Reaction space charting aims to explore and describe a chemical transformation to fully understand the processes involved. In this way, the studied system can be exploited to extend its reach or develop new applications. Charting is particularly appealing in reaction discovery, as it enables the discovery of previously unknown reaction pathways and the development of new processes.<sup>[1]</sup>

In this context, multicomponent reactions (MCRs), which combine three or more reactants to generate a unified adduct, epitomize the need for reaction space charting due to their inherent complexity (number of reactants, reactive intermediates, potential reaction pathways, etc.). Our group has applied the charting approach to address the multiparametric nature of MCRs with the aim of expanding their synthetic reach, gaining further mechanistic insights, and eventually developing meaningful applications in drug discovery and biomedicine.<sup>[2]</sup>

As a representative example, a thorough mapping of the interactions among carbonyls, amines, and isocyanoacetates led to the discovery of new multicomponent processes through novel reaction pathways, thereby achieving vast chemical diversity from simple, off-the-shelf reagents. The heterocyclic nature of the generated scaffolds renders them well-suited for biomedical applications, and the streamlined synthetic access enables rapid construction of chemical libraries, which are critical in medicinal chemistry research.<sup>[3]</sup> Ongoing collaborations with biological research groups focus on studying these applications.



### Acknowledgements

Funding from Ministerio de Ciencia e Innovación (Spain) and the European Regional Development Fund (EDFR) (PID2022-139180OB-I00), as well as AGAUR (Government of Catalonia) (2024 PROD 00106, 2025 INNOV 00017: to Concepcio Soler), is acknowledged.

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## Aminoalkyl Cyclopalladated Complex: Discovery and Synthetic Applications

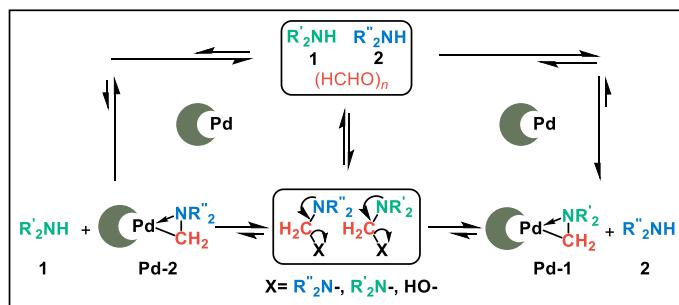
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**Keywords:** *cyclopalladated complex, aminoalkylation, C–N bond metathesis, adaptive DKR*

The rapid development of transition metal catalysis has drastically expanded chemists' capability to construct chemical bonds, enabling a broad range of efficient carbon–carbon and carbon–heteroatom coupling protocols that are highly desirable for synthetic organic chemistry. Such remarkable success can be largely attributed to the discovery and identification of new reactive organometallic intermediates and insights into the fundamental chemistry of these well-defined “leading complexes”. In this context, it is recognized that the discoveries, preparations, and detailed reactivity investigations of these well-defined organometallic “leading complexes” are vitally important to the development of new and effective catalytic transformations, and to tackling the challenges in synthetic chemistry in general. In past ten years, we have developed a “nitrogen-containing C-bound complex” as the key intermediate for new catalytic aminoalkylation reactions, in which the ligand moiety was C-bound instead of N-bound to the late transition metal center.<sup>[1]</sup> The complex could introduce an electron-donating amine group from metal–aminoalkyl species into the target product through C–C bond formation instead of through C–N bond construction via late transition metal-amido species. With these general concepts in mind, our group designed and prepared a Pd–aminoalkyl complex, which has exhibited unique and versatile reactivities in various types of aminomethylation reactions. In this talk, we will present our recent progress in this project.<sup>[2]</sup>



**Scheme 1**

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## ELEMENTAL CHALCOGEN-BASED MULTICOMPONENT POLYMERIZATIONS

Rongrong Hu<sup>a</sup>

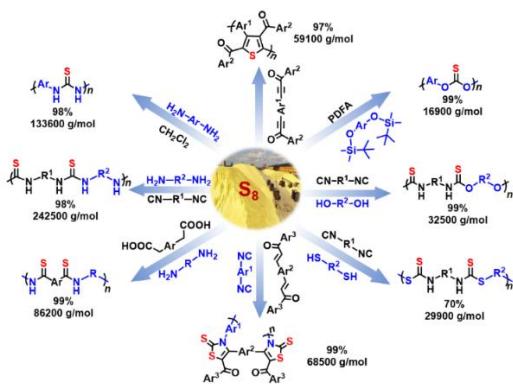
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**Keywords:** *multicomponent polymerization, elemental sulfur, selenium, sulfur-containing functional polymer*

Chalcogen-containing polymers have attracted increasing attention, owing to their fascinating properties such as high refractive indices, metal coordination ability, self-healing capability, optoelectronic property, and so on. Currently, the lack of economic monomers and efficient synthetic approaches are the main challenges for the development of chalcogen-containing polymers. Elemental sulfur with large surplus from worldwide petroleum industry, and elemental selenium as byproduct from metal refinery industry, are hence idea sources for the preparation of chalcogen-containing polymers, despite of the challenges of poor solubility of sulfur/selenium in organic solvents and their toxicity to transition metal catalysts.

In this talk, a series of elemental sulfur-based multicomponent polymerizations (MCPs) will be introduced to directly convert elemental sulfur to sulfur-containing polymers such as polythioamides, polythioureas, polythiocarbonates, and polythiophenes with well-defined structures, good solubility, high yields, and high molecular weights ( $M_w$ ) in one step. For example, a KF-assisted MCP of sulfur,  $\text{CH}_2\text{Cl}_2$ , and aromatic diamines has enabled efficient and economic synthesis of various aromatic polythioureas.<sup>[1]</sup> Moreover, through the efficient room temperature polymerization of elemental sulfur/selenium and alkynone, non-emissive poly(1,4-dithiin)s/poly(1,4-diselenin)s could be afforded, which could be completely transformed to emissive polythiophenes/polyselenophenes upon heating or oxidation.<sup>[2,3]</sup> These polymers could exhibit tunable thermal properties, mechanical properties,<sup>[4]</sup> optical characteristics, and degradability, making them promising candidates for applications including precious metal enrichment and recovery, high-refractive-index materials, and solid-state electrolytes. These MCPs are economic, efficient, and convenient tools for the direct conversion from elemental chalcogen to profitable chalcogen-containing functional polymers, which could accelerate the development of chalcogen-containing polymers with diversified structures and functionalities, demonstrating their great potential in sustainable polymer materials.



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**The 9<sup>th</sup> International Conference on  
Multicomponent Reactions and Related Chemistry  
13-16<sup>th</sup> Jan 2026**



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Zhenghui Kang, Associate Researcher, Young Principal Investigator, Shanghai Institute of Materia Medica/Zhongshan Institute for Drug Discovery, CAS.

Dr. Zhenghui Kang earned the Ph.D. in Organic Chemistry from East China Normal University in 2018, under the supervision of Professor Wenhao Hu. From July 2018 to January 2022, he conducted postdoctoral research at the School of Pharmaceutical Sciences, Sun Yat-sen University, under the joint guidance of Professor Wenhao Hu. In March 2022, he joined the Shanghai Institute of Materia Medica/Zhongshan Institute for Drug Discovery, Chinese Academy of Sciences, where he serves as an Associate Researcher and Young Principal Investigator. His current research primarily focuses on medicinal chemistry, asymmetric catalysis, and organic synthetic chemistry.

## Multicomponent Reactions Enabled by Metal Carbene Multifunctionalization

**Zhenghui Kang,<sup>a</sup> Baofan Wang<sup>a</sup> and Wenhao Hu<sup>b</sup>**

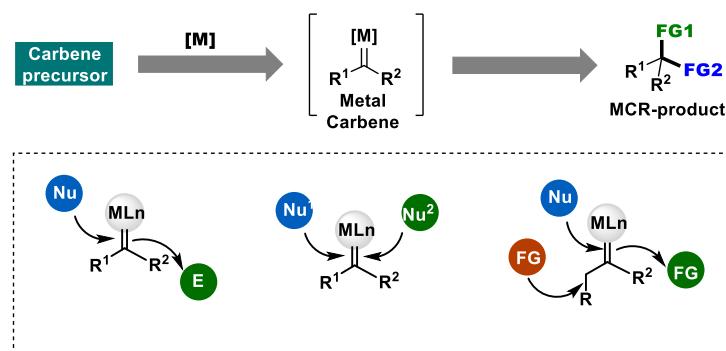
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**Keywords:** Metal carbenes, Multicomponent reaction, Interception of two active intermediates

Metal carbenes represent a pivotal class of reactive intermediates in organic synthesis. Capitalizing on the ambiphilic character of the carbene carbon, the direct multifunctionalization of this reactive center enables a versatile platform and a powerful strategy for the development of novel multicomponent reactions, wherein carbene species act as C<sub>1</sub> synthons that couple with two partners via interception of reactive intermediates to afford one-carbon-extended products. Herein, we present three distinct multicomponent reaction (MCR) platforms enabled by the multifunctionalization of metal carbenes. These encompass: (i) sequential electrophilic/nucleophilic carbene carbon functionalization; (ii) transformations initiated by electrophilic capture of the carbene followed by a secondary nucleophilic addition; and (iii) a four-component coupling strategy that achieves triple functionalization of metal carbene intermediates. The applications of this methodology in the synthesis of natural products and pharmaceuticals, as well as the reaction mechanism—particularly the nature of the reactive intermediates and the structure of the metal carbene—will be discussed.



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Rodolfo Lavilla studied Pharmacy at the University of Barcelona, and later he obtained an M.S. in Medicinal Chemistry and a Ph.D. in Organic Chemistry there. After a postdoctoral stage at the University of California, San Diego, he entered faculty at the University of Barcelona where he is now full Professor of Organic & Medicinal Chemistry. His research interests deal with heterocyclic chemistry, multicomponent reactions, functional probes, medicinal chemistry and selective peptide modifications. He has published over 150 research articles, reviews, book chapters and patents, and holds collaborations with pharma companies and research groups in medicinal and biological chemistry.

## HETEROCYCLIC MULTICOMPONENT REACTIONS. NEW REACTIVITY TRENDS AND BIOMED APPLICATIONS (25 years of MCR Research in Barcelona)

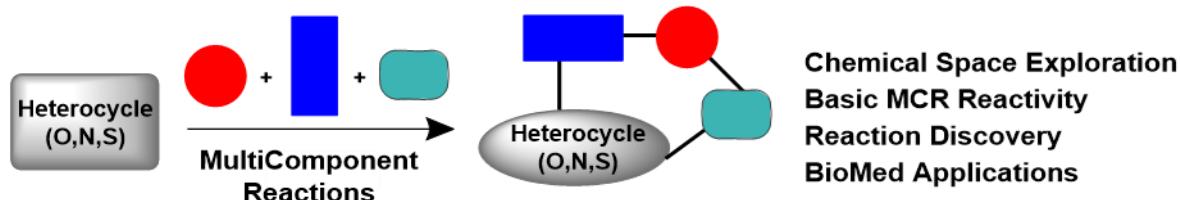
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**Keywords:** *Azines, Azoles, Heterocycles, Isocyanides, Reaction Discovery, BioMed Applications*

Heterocycles are privileged scaffolds in multicomponent reactions (MCRs), offering unique advantages that set them apart in synthetic chemistry. Their intrinsic reactivity enables the rapid generation of unparalleled structural diversity, provides a fertile platform for reaction discovery, and serves as a powerful tool for the combinatorial synthesis of chemical libraries. Over the past 25 years, our research in Barcelona has explored and expanded the scope of heterocycle-based MCRs, leading to the development of novel methodologies and reaction trends.<sup>[1]</sup> Given that the majority of approved drugs contain heterocyclic frameworks, the scaffolds obtained through these processes are inherently well-suited for medicinal chemistry and drug discovery. Our approach facilitates the efficient exploration of the MCR-related chemical space, a critical step in establishing robust structure–activity relationships (SAR).<sup>[2]</sup> In this presentation, we will highlight representative examples, illustrating how heterocyclic MCRs can accelerate the identification of bioactive compounds and open new avenues in biomedical research.



**Figure 1.** Heterocycle-based MCRs.

### Acknowledgements

Funding from Ministerio de Ciencia e Innovación (Spain) and the European Regional Development Fund (EDFR) (PID2022-139180OB-I00), and Generalitat de Catalunya (SGR 2021, 00357) are acknowledged.

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Jun-Long Li is a distinguished professor serving as the Vice Dean of the College of Pharmacy at Chengdu University and Deputy Director of the Sichuan Institute of Industrial Drug Discovery. He earned his Ph.D. from Sichuan University in 2013 and was subsequently a German Humboldt Scholar (2013-2015).

His primary research focuses on asymmetric catalysis and the synthesis of chiral drugs. Professor Li is a recipient of numerous prestigious accolades, including the National Young Chang Jiang Scholar award, and high-level provincial talent titles such as the Sichuan Emei Plan and Sichuan Outstanding Young Scholar. As a principal investigator, he has led three national research projects, including grants from the National Natural Science Foundation of China. His scientific contributions have been recognized with several awards, including the First Prize of Sichuan Science and Technology Progress Award and the international Thieme Chemistry Journals Award.

He has authored over 60 influential publications in leading international journals, including *Nature Catalysis*, *Science Advances*, *Chemical Society Reviews*, *Journal of the American Chemical Society*, and *Angewandte Chemie International Edition*.

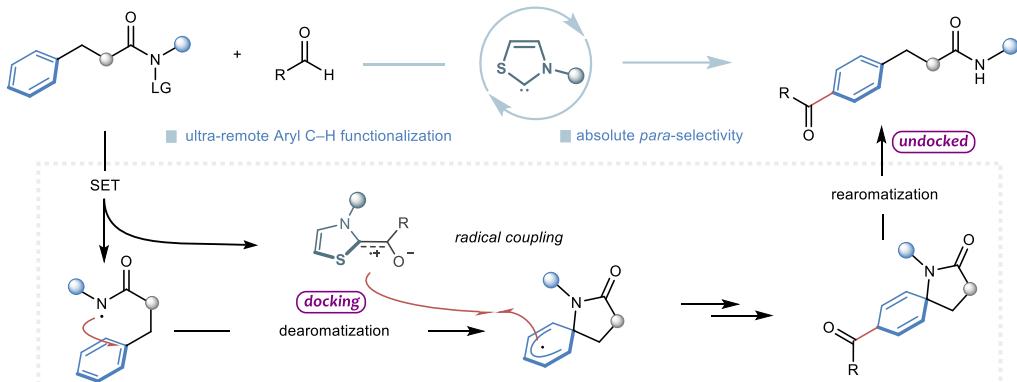
## Remote Site-selective Arene C–H Functionalization Enabled by N-Heterocyclic Carbene Organocatalysis

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Catalytic site-selective functionalization of distal C–H bonds represents a formidable challenge in organic synthesis. Particularly, the precise functionalization of distal aromatic C(sp<sup>2</sup>)–H bonds remain largely unexplored. Here we present a highly para-selective acylation strategy to target ultra remote aryl C(sp<sup>2</sup>)–H bonds, eight chemical bonds away from an activated functionality, through radical N-heterocyclic carbene organocatalysis. This method is developed on the basis of a unique single-electron pathway involving the site-selective activation of aryl C–H bonds by a nitrogen-centered radical generated in situ. Importantly, this organocatalytic approach shows potential for the functionalization of drugs, amino acids and peptides, thus highlighting its importance for medicinal chemistry. Our investigation encompassed meticulous mechanistic studies, including control experiments and density functional theory calculations, to unravel the intricacies behind the observed site selectivity and shed light on the mechanism of radical N-heterocyclic carbene organocatalysis.



**Scheme 1.** *N*-radical-directed para-selective acylation of ultraremote arene C–H bonds.



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Zhong Lian, a professor at Sichuan University, has been selected for the Youth Program of the Thousand Talents Plan by the Central Organization Department, the Thousand Talents Plan of Sichuan Province, and has been recognized as an academic leader by the Sichuan Provincial Health Commission. He obtained his bachelor's degree in 2009 from East China Normal University, under the supervision of Prof. Hong Ran (Shanghai Institute of Organic Chemistry); in 2012, he earned his master's degree from the Shanghai Institute of Organic Chemistry, under the guidance of Prof. Shi Min; and in 2015, he completed his PhD at Aarhus University in Denmark, under the supervision of Prof. Troels Skrydstrup. From 2016 to 2018, he conducted postdoctoral research in the Prof. Bill Morandi's research group at the Max Planck Institute for Coal Research in Germany. Since May 2018, he has been a full professor at Sichuan University. His main research focuses on mechanical synthetic chemistry.

## Mechanical Synthetic Chemistry

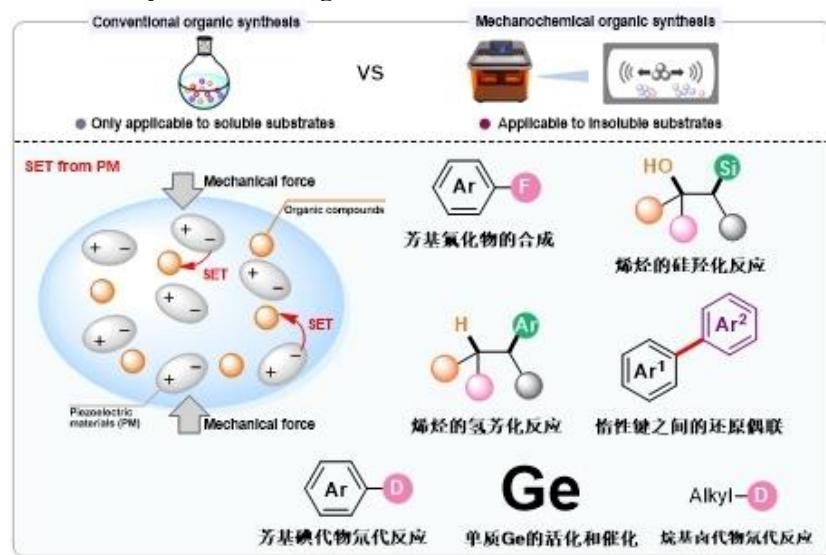
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**Keywords:** Mechanochemistry, Piezoelectric catalysis

Mechanochemistry, a green and sustainable approach to chemical synthesis conducted under solvent-free or solvent-minimized conditions, has had a profound impact on synthetic chemistry. The piezoelectric effect describes how certain crystalline materials, when subjected to mechanical stress, undergo changes in their internal charge distribution that generate an electric field or voltage. Under mechanical force, polarized piezoelectric materials facilitate single-electron transfer reactions, opening new avenues for radical-based solid-state synthesis. Leveraging this principle, we have achieved the Balz–Schiemann reaction and the hydroxysilylation of alkenes under mild conditions. We have also developed a novel piezo-catalytic pathway—continuous mechanical force–induced electron transfer (ConMET)—enabling dehalogenative deuteration of aryl and alkyl halides and the hydroarylation of alkenes. In addition, we have utilized mechanical force to activate and catalyze elemental germanium and to promote reductive coupling reactions between aryl fluorides and aryl ethers, among other transformations.



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## Asymmetric multicomponent reaction catalyzed by chiral metal complexes

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Asymmetric multicomponent reactions demonstrate an efficient access to complex chiral molecules from simple materials. This one pot strategy features simple operation, step economy, and environmental friendliness, which has been widely applied in modular synthesis and drug discovery. Nevertheless, this approach faces competition from two-component reactions and challenges in stereocontrol over highly reactive intermediates. In the past few years, our group developed several asymmetric multicomponent reactions mediated by chiral metal complexes, including copper(I)-catalyzed asymmetric C–H insertion/1,3-copper shift/nucleophilic addition for synthesis of chiral tetrasubstituted allenoates, asymmetric azide-alkyne cycloaddition/[2+2] cascade reaction for synthesis of chiral spiroazetidinimine oxindoles, asymmetric hydrocyanation/Michael reaction for synthesis of chiral cyanide-containing pyrrolidine-2,5-diones, asymmetric photoinduced asymmetric cyanoalkylalkynylation for synthesis of chiral alkyne-bearing nitriles, iron(II) or ytterbium(III)-catalyzed enantioselective difunctionalization of  $\alpha,\beta$ -unsaturated carbonyl compounds, such as haloazidation, carboazidation, diazidation, and *anti*-dihalogenation, enabling synthesis of chiral azides and dihaloalkanes, as well as organocatalyst/palladium(0) synergistically catalyzed 1,4-addition/arylation tandem reaction for synthesis of chiral tetrasubstituted allenes. In these reactions, detailed mechanisms were studied to elucidate the reaction process and enantioinduction.



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Prof. Dr. Xin-Yuan Liu, Chair Professor and Department Head of Chemistry at SUSTech. As the corresponding author, he has published over 110 papers on "Asymmetric Catalytic Radical Chemistry" in top-tier journals such as Science (1), Nature (1), Nat. Chem. (5), Nat. Catal. (3), Nat. Synth. (2), Chem (2), JACS (13), Angew. Chem. (21), etc. He has obtained many honors and awards, such as XPLOTER prize, The First-Class Prize of the Natural Science Award of Guangdong Province, Boehringer Ingelheim Lectureship (Boston College), The National Science Fund for Distinguished Young Scholars, The National Science Fund for Excellent Young Scholar, The Scholar Program-Youth Project (Ministry of Education, China), CCS-BASF Innovation Prize, CCS Youth Chirality Award, The Distinguished Lectureship Award (Chemical Society of Japan), CAPA Distinguished Faculty Award (CAPA), ACP Lectureship Awards (Taiwan District, Japan and Korea), etc.

## Cu/Chiral Anionic Ligand-Catalyzed Enantioselective Cross-Couplings

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### Keywords: Radical, Chiral Anionic

Radical reactions have emerged as one of the most powerful and efficient tools for the construction of carbon–carbon and carbon–heteroatom bonds in organic synthesis. However, the development of catalytic asymmetric radical reactions to realize the stereochemical control of open-shell intermediates still remains a formidable challenge owing to the high reactivity of such free radical species. To solve this problem, our group has developed copper(I)/chiral anionic ligand catalyst to achieve a number of enantioselective radical transformations: such as the C–H functionalization, alkene difunctionalization and cross–coupling of alkyl halides, etc. The role of chiral anionic ligand is dual: it not only tunes the reducing capability of copper for the reaction initiation but also provides excellent stereocontrol induction of the reactive radical species through multiple models.

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Thomas J. J. Müller, born in Würzburg, Germany, in 1964, studied chemistry (1984-1989) at the University of München (LMU) (diploma 1989; Ph.D. 1992). After a post-doctoral stay at Stanford University (1993/1994) as a Feodor Lynen fellow (Alexander von Humboldt foundation), he developed his independent research at Technical University Darmstadt and LMU (1994-1999; habilitation 2000) (as recipient of the Liebig fellowship of the Funds of Chemical Industry and the habilitation scholarship of DFG). After a professorship at the University of Heidelberg (2002-2006) he is a chaired full professor at the University of Düsseldorf since 2006, and since 2019 the spokesman of the Research Training Group 2482 funded by the German Science Foundation (DFG). In 2013 he was awarded with First Prize of Evonik Call for Research Proposals (ECRP). He was a member of the board of Liebig Society of Organic Chemistry for two election periods (2016-2023). Since 2021 he is a foreign member of the National Academy of Sciences of Ukraine. He was elected in 2023 as a member of the DFG decision panel on funding of projects in chemistry. He is member of board of several foundations and selection committees. His research interests encompass synthetic and physical-organic chemistry of functional chromophores, and the design of novel one-pot reactions, documented in more than 350 publications.

## SEQUENTIALLY PD-CATALYZED PROCESSES – CONSECUTIVE MULTICOMPONENT SYNTHESIS OF FUNCTIONAL MOLECULES IN CATALYST ECONOMIC FASHION

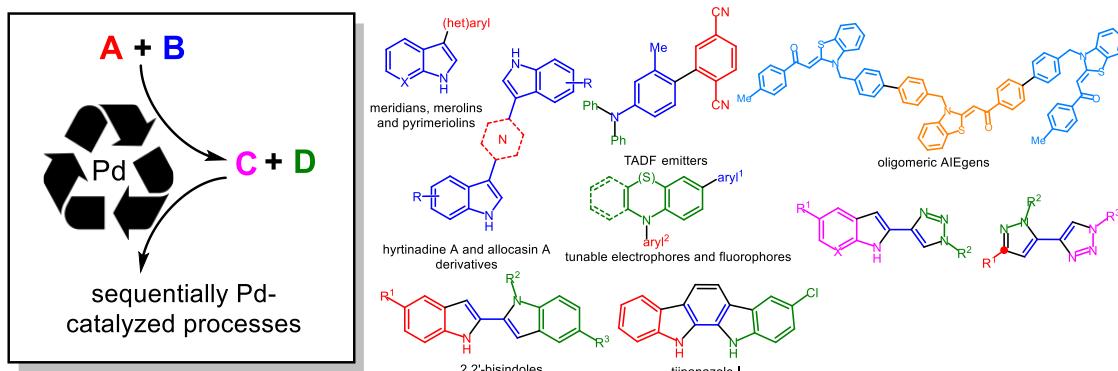
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**Keywords:** anti-infectiva, apoptosis inducers, catalysis, consecutive reactions, functional chromophores, multicomponent reactions, palladium

One-pot reactions – in a consecutive, sequential or domino fashion – are highly efficient and efficacious routes to functional molecules in life and materials sciences. Heterocyclic systems cover a vast spectrum of applications and are therefore highly interesting. Transition metal catalyzed multi-component sequences have raised considerable attention since they enable transformations with high tolerance of functional groups.<sup>[1]</sup> Likewise, sequentially Pd-catalyzed processes have opened new avenues to one-pot syntheses of numerous classes of heterocyclic frameworks.<sup>[2-4]</sup> This one-pot methodological concept, in particular the Masuda-Suzuki sequence,<sup>[5]</sup> is most elegantly applied to the syntheses of various classes of functional heterocycles, ranging from functional chromophores to the key steps in very concise syntheses of marine alkaloids,<sup>[6,7]</sup> kinase inhibitors,<sup>[8]</sup> and anti-infectiva.<sup>[9,10]</sup>



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Romano Orru completed his PhD in organic chemistry at the Agricultural University of Wageningen, The Netherlands. From 1996 to 2000 he worked at the Technical as well as at the Karl-Franzens University of Graz, Austria on synthetic applications of bio-transformations. In 2000, he returned to the Netherlands, and was appointed Assistant Professor and later Associate Professor (2003) of Synthetic & Bioorganic Chemistry at Vrije Universiteit Amsterdam, where he was appointed chair in 2007. End of 2019 he moved to the AachenMaastricht Institute for Biobased Materials of Maastricht University as a professor of Organic Chemistry. Early 2022 he became the Scientific Director of AMIBM. His research focuses on the utilisation of one-pot cascade reactions and multi-component reactions to improve the efficiency, sustainability and precision of organic compound synthesis, with emphasis on applications in the field of pharmaceutical science. For that, he develops novel MCRs and employs them in combination with biocatalysts in one-pot processes to access targeted molecules in a stereoselective fashion. In another research line he develops isocyanides as versatile C1 building blocks in (transition) metal-catalyzed insertion reactions towards privileged heterocyclic scaffolds. He is considered a leader in his field and has contributed much to this emerging area



## ISOCYANIDES: CHEMICAL CHAMELEONS

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**Keywords:** isocyanides, spirocyclizations, photochemistry, alkaloids, peptoids,

In the past 15 years we worked on a number of Tandem- and Multi Component Reaction strategies that involve isocyanides. We discovered many interesting new reactions that were applied in a range of chemistry fields, covering medicinal and combinatorial chemistry, catalysis, biotransformations, fotochemistry and natural product synthesis. We have explored classical MCR approaches where isocyanides can act as both electrophiles as well as nucleophiles, biocatalytic asymmetric Ugi-type transformations, but also both transition-metal as well as base-metal mediated and catalyzed insertion chemistry. Recently, we embarked on radical-type chemistry involving isocyanides discovering remarkable charge-transfer behavior in (auto) photocatalysis. In this presentation I will highlight the fascinating chameleonic behaviour of isocyanides and show their remarkable value as C1-building blocks in synthetic organic method development.

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Shi-Liang Shi received his Ph.D. in organic chemistry from the University of Tokyo in 2011 under the supervision of Prof. Masakatsu Shibasaki and Motomu Kanai. After one year of postdoctoral research with Prof. Motomu Kanai as a JSPS fellow, he joined the group of Prof. Stephen Buchwald at MIT as a postdoctoral fellow. In the summer of 2016, he started his independent research as a professor at the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences. His research interests focus on the design of chiral NHC ligands and their application to challenging enantioselective catalytic transformations from readily available starting materials.

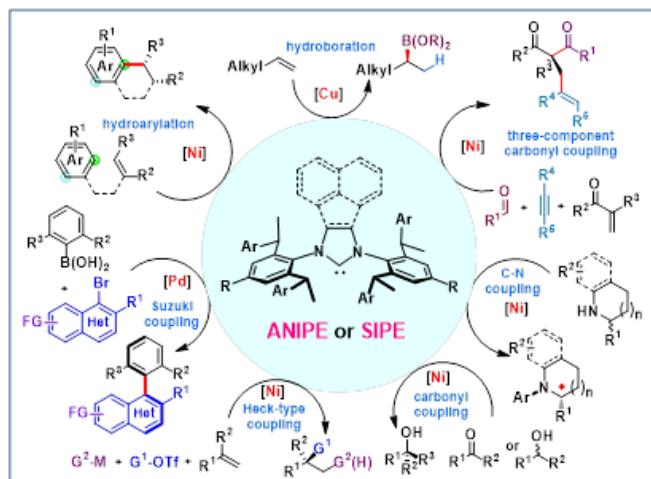
## Asymmetric NHC-Metal Catalysis

Shi-Liang Shi

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**Keywords:** chiral NHCs, asymmetric catalysis, C-H activation, cross-coupling, carbonyl addition

The elaboration of multi-components in a single chemical transformation permits a highly simplified organic synthesis with excellent step-economy and atom-economy; however, controlling the chemo-, regio- and enantio-selectivity in these multicomponent reactions is challenging. Thus, the development of suitable chiral ligands for asymmetric multicomponent transformation is highly demanding. Among all the chiral ligands, N-heterocyclic carbene (NHC) ligands, with their distinctive electronic and steric properties, enable the activation of a range of inert substrates. This holds significant promise for metal-catalyzed synthesis. However, designing chiral NHC ligands with high chiral induction ability is challenging due to their mono-coordination and flexible conformation. The privileged chiral NHC ligand is especially rare, which hampers the advancement of chiral NHC-metal catalysis. This report details the development of novel, induced-fit  $C_2$ -symmetric chiral NHC ligands, named ANIPE and SIPE, and their application in various challenging enantioselective transition-metal-catalyzed transformations, including alkene functionalization, C-H activation, cross-coupling, and carbonyl addition reactions<sup>[1-12]</sup>.



**Figure 1.** Induced-fit chiral NHC for asymmetric metal catalysis

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## Catalytic Asymmetric Cross-Hydrodimerization of Hydrocarbons

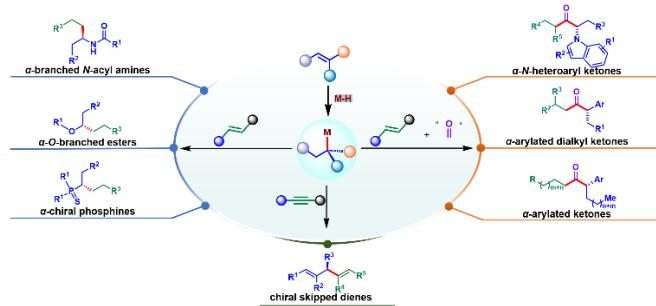
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**Keywords:** Earth-Abundant-Metal-Catalysis, Asymmetric Cross-Hydrodimerization, Unsaturated Hydrocarbons

Saturated stereogenic carbon centers comprise majority of the framework of organic molecules.<sup>[1]</sup> However, flexible configuration as well as increased steric hindrance of  $sp^3$  hybridized centers impose challenges for direct constructing such stereogenic centers. Traditional cross-coupling heavily relies on the use of stoichiometric preformed alkyl nucleophiles or/and alkyl electrophiles, which significantly limited the scope and application. Therefore, to develop new cross-coupling reaction modes to build saturated stereogenic carbon centers with the control of regio- and stereochemistry is highly demanding yet challenging.<sup>[1]</sup> Our interests lie in the development of earth-abundant-metal-catalyzed asymmetric  $sp^3$ -cross-coupling reactions, with an emphasis on developing new reaction modes without using stoichiometric alkyl nucleophiles or alkyl electrophiles (Scheme 1).<sup>[3]</sup>



**Scheme 1.** Catalytic asymmetric cross-hydrodimerization of unsaturated hydrocarbons

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## ELECTRON-DEFICIENT ALKYNES – UNIVERSAL SYNTHONS FOR PRODUCING CONDENSED AZA-HETEROCYCLIC SYSTEMS

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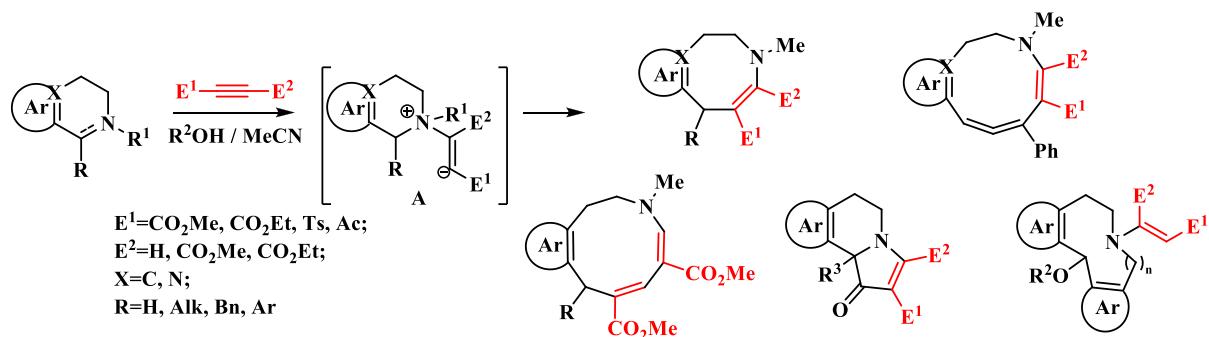
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**Keywords:** domino reaction, aza-heterocycle, electron-deficient alkynes

In the synthesis of heterocyclic compounds, electron-deficient alkynes hold a prominent position as key reagents. Activated alkynes, due to their ability to undergo a variety of transformations, have found extensive application in reactions involving nitrogen-containing heterocycles.

We have developed methods for synthesizing annelated nitrogen-containing rings of medium size, specifically 5- and 6-membered rings, which incorporate pharmacophore groups [1-4]. These methods utilize electron-deficient alkynes and alkenes and are based on domino and multicomponent reactions. Many of the resulting compounds demonstrate significant bioactivity.



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**The 9<sup>th</sup> International Conference on  
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## Biphosphine Ligand Enabled Dirhodium-Catalyzed Carbene Difunctionalization

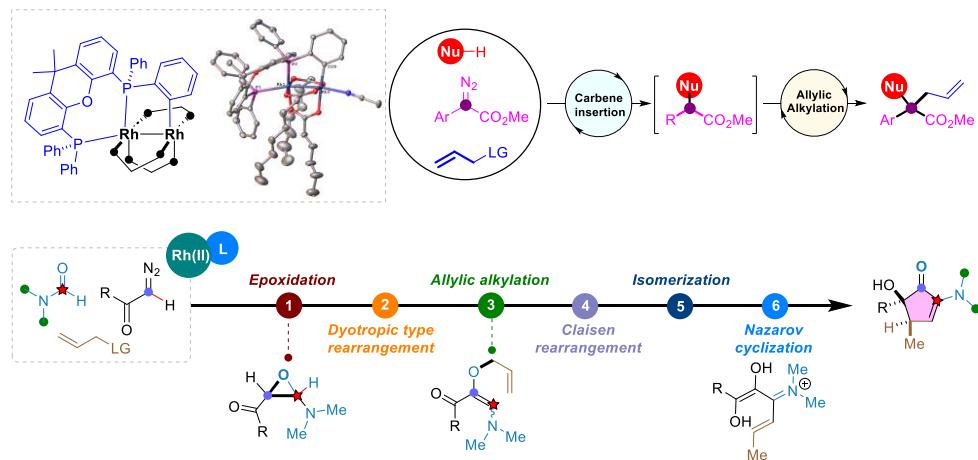
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**Keywords:** *dirhodium, difunctionalization of carbene; three-component reactions, bimetallic catalysis*

Dirhodium complexes represent a prominent class of dinuclear metal catalysts, widely recognized for their exceptional efficiency in carbene transfer reactions. However, their catalytic versatility has been constrained by the limited ability of dirhodium(II) species to undergo two-electron oxidative addition. To overcome this limitation, we introduced biphosphine ligands to modulate the electronic and catalytic properties of dirhodium centers. This strategic modification facilitates oxidative addition and expands the reactivity profile of dirhodium beyond classical carbene-mediated transformations. Leveraging this approach, we developed a series of efficient and novel diazo difunctionalization reactions. Notably, a three-component coupling of amines, diazo compounds, and allylic substrates was achieved under dirhodium(II)/Xantphos catalysis, affording  $\alpha$ -quaternary  $\alpha$ -amino acid derivatives with high atom and step economy. Mechanistic studies support a relay process involving dirhodium-catalyzed carbene insertion followed by allylic alkylation, wherein ligand coordination critically enhances catalytic activity in the allylic alkylation step. Furthermore, with dimethylformamide (DMF) as solvent, the system enabled an unprecedented six-step domino process involving C=O bond cleavage and skeletal reorganization. This transformation catalyzed by dirhodium/Xantphos, formally inserts a carbonic carbon into the C=O bond of formamide, with concurrent migration of the  $\alpha$ -substituent, yielding cyclopentenone derivatives. Key steps include epoxidation, dyotropic type rearrangement, allylic alkylation, Claisen rearrangement, isomerization, and Nazarov cyclization.



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Professor Wessjohann studied organic chemistry in Hamburg (Germany), Southampton (UK) and Oslo (Norway). As Postdoc he worked on the total synthesis of Taxol with Paul Wender at Stanford U. (USA). He is an expert in the chemistry of natural products and their applications. His research spans from analytical via synthetic chemistry to mode of action studies of bioactive compounds, and their application in organisms. For data analyses also proprietary algorithms and informatics tools are developed. The knowledge generated is channelled into applications, e.g. for new drug leads, flavor compounds, or plant protectants. He received numerous scholarships, prizes and honors, e.g. the Microsoft IT Founders Award, or membership in the Brazilian Academy of Science. His research is published in some 600 publications and 30 patent families. h-index >75.

He is a founding PI of the GLACIER world health centre ([www.glacieronehealth.org](http://www.glacieronehealth.org)), the German Centre for integrative Biodiversity Research (iDiv), the Leibniz science campus “plant based bioeconomy”, “DiP - digitalization of plant-based value chains”, and other consortia to promote the sustainable use of plant and fungal chemistry in agriculture and health. He founded seven start-up companies and is advisor to science organizations, companies and governments.



## Tumor-targeting with MCR-derived drugs and conjugates

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Although finding new bioactive principles is and will remain a cornerstone of drug development, it commonly is not the activity of a compound that poses an application problem, but bioavailability and specificity to a certain tissue, e.g. cancerous vs. healthy cells. Thus, modifications that improve selectivity and ADME-properties (absorption, distribution, metabolism, excretion) are often more relevant topics than increasing potency, including so called targeting strategies with PDCs/ADCs (peptide/antibody drug conjugates).

MCR technology is ideal to bring various functions in a molecule together in a defined combination. It therefore allows us to not only synthesize the bioactive war head but, ideally in one step, it can introduce linkers, membrane ankers, fluorescent dyes or other functions, or directly link targeting moieties at the same time. Especially useful is the Ugi reaction, as it is insensitive to water and allows us to generate and link peptides. I will present some of our recent works to improve and target bioactive molecules with the support of MCR chemistry in the fields of anticancer, antiinfective, and immunomodulatory applications in human and plant disease.



**The 9<sup>th</sup> International Conference on  
Multicomponent Reactions and Related Chemistry  
13-16<sup>th</sup> Jan 2026**



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## Rearrangement Reactions-Driven *N*-Heterocycle Synthesis and Modification

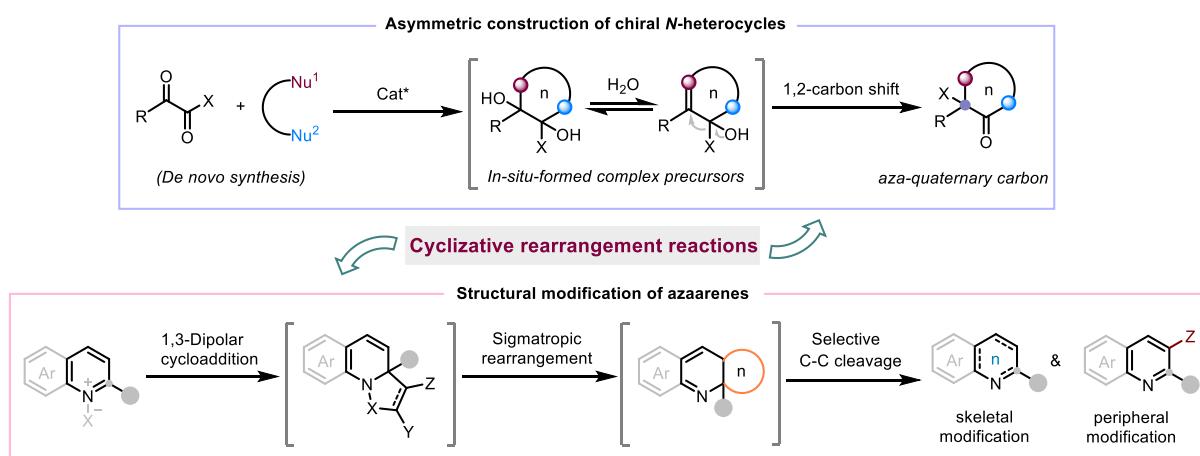
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**Keywords:** rearrangement reactions, *N*-heterocycle synthesis, structural modification, organocatalysis

To address the challenges of selective synthesis and precise modification of *N*-heterocycles, we focus on rearrangement chemistry as the core and propose an "intermolecular cyclizative rearrangement strategy". Through the strategic integration of cyclization and rearrangement events, we



have devised two-component and multi-component reaction systems that in situ generate transient, highly reactive cyclic intermediates. These species then engage in either directed 1,2-rearrangement or concerted rearrangement pathways, thereby enabling both the streamlined synthesis of *N*-heterocyclic scaffolds and the precise structural modification of azaarenes.

The main research content involves the following two aspects: (1) Based on the cyclizative 1,2-rearrangement strategy of ambielectrophilic-ambinucleophilic reagents, the stereoselective construction of chiral *N*-heterocycles is realized;<sup>[1-5]</sup> (2) Based on the 1,3-dipolar cycloaddition/concerted rearrangement strategy, the precise skeleton modification and direct C-H functionalization of azaarenes are achieved.<sup>[6-8]</sup> This strategy combines the advantages of two reaction types, avoids tedious substrate synthesis, drives interdisciplinary innovation in rearrangement and heterocyclic chemistry.

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Wanqing Wu received her Bachelor's degree from Hunan University in 2005 and her Ph.D. from Peking University in 2010. She then conducted postdoctoral research at South China University of Technology from 2010 to 2013, after which she joined the faculty. She was promoted to Professor in 2014. Her research focuses on the efficient conversion and high-value utilization of unsaturated compounds. To date, she has published over 100 papers in journals such as *Acc. Chem. Res.*, *J. Am. Chem. Soc.*, and *Angew. Chem. Int. Ed.*, and has been granted more than 10 patents. She also received the First Prize of the Natural Science Award from the Ministry of Education (as the third contributor). Her honors include selection for the National Youth Talent Program, the Guangdong Outstanding Young Scientist, the Guangdong Excellent Youth Team, the ChemComm Emerging Investigators, and the Thieme Chemistry Journals Award.

## Heteroatom-Promoted Sequential Conversions of Unsaturated Hydrocarbons

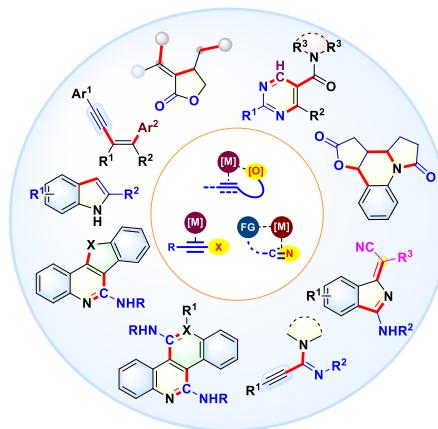
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**Keywords:** Heteroatom, Unsaturated Bonds, Sequential Conversion

Unsaturated bonds are important functional groups in organic chemistry. Many useful compounds can be synthesized by the sequential conversion of unsaturated bonds. However, due to the diversity of reaction sites and complex reaction modes of unsaturated bonds <sup>[1]</sup>, it is still a challenge to realize their selective conversions and high-value applications. In recent years, we have developed a series of unique strategies for unsaturated bond conversions involving the directing effect of heteroatoms. By introducing different oxygen-<sup>[2]</sup>, nitrogen-<sup>[3]</sup> and halogen-atoms <sup>[4]</sup> into the unsaturated bonds, the orderly coordination between the substrates and transition metals was promoted and precise control of reaction selectivity was realized. Moreover, some novel molecules with excellent biological reactivities and fluorescence performance have been constructed and applied.



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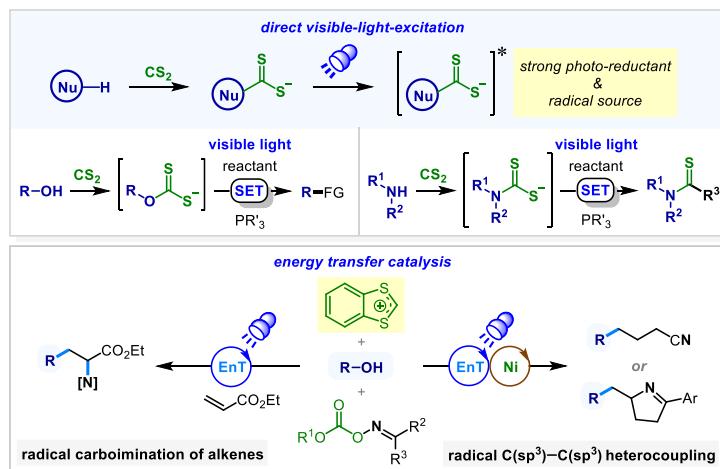
## Light-Driven Multicomponent Radical Reactions with Sulfur-Containing Small Molecules

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**Keywords:** radical deoxygenation, thiocarbamoylation, energy transfer, hydrogen atom transfer

Sulfur-containing organic structures frequently exhibit low redox potentials, low bond energies, and the capacity to stabilize adjacent carbocations and radicals. These characteristics contribute to the high reactivity of sulfur-containing groups and motifs. We have developed a strategy that utilizes sulfur-containing small molecules to convert relatively inert organic molecules into more reactive substances to participate in single electron transfer or hydrogen atom transfer processes. This strategy has been demonstrated to facilitate a series of novel light-driven multicomponent radical reactions, including: 1) Visible-light-promoted deoxygenative radical transformations of diverse primary, secondary, and tertiary alcohols<sup>[1]</sup> that were enabled by inexpensive carbon disulfide- and phosphine-assisted C–O bond activation via xanthate salt intermediates.<sup>[2]</sup> 2) Visible-light-driven multicomponent radical reactions of amines, carbon disulfide, and olefins in the presence of phosphines for mild, efficient, and versatile synthesis of acyclic thioamides, as well as  $\gamma$ -thiolactams.<sup>[3]</sup> 3) Photocatalytic energy transfer (EnT)-driven deoxygenative radical coupling reactions of alcohols with bifunctional oxime carbonates enabled by applying the 1,3-benzodithiolylium (BDT) cation as an efficient hydroxyl-activating reagent.<sup>[4]</sup>



**Acknowledgement:** We gratefully acknowledge the National Natural Science Foundation of China (22271109) for financial support.

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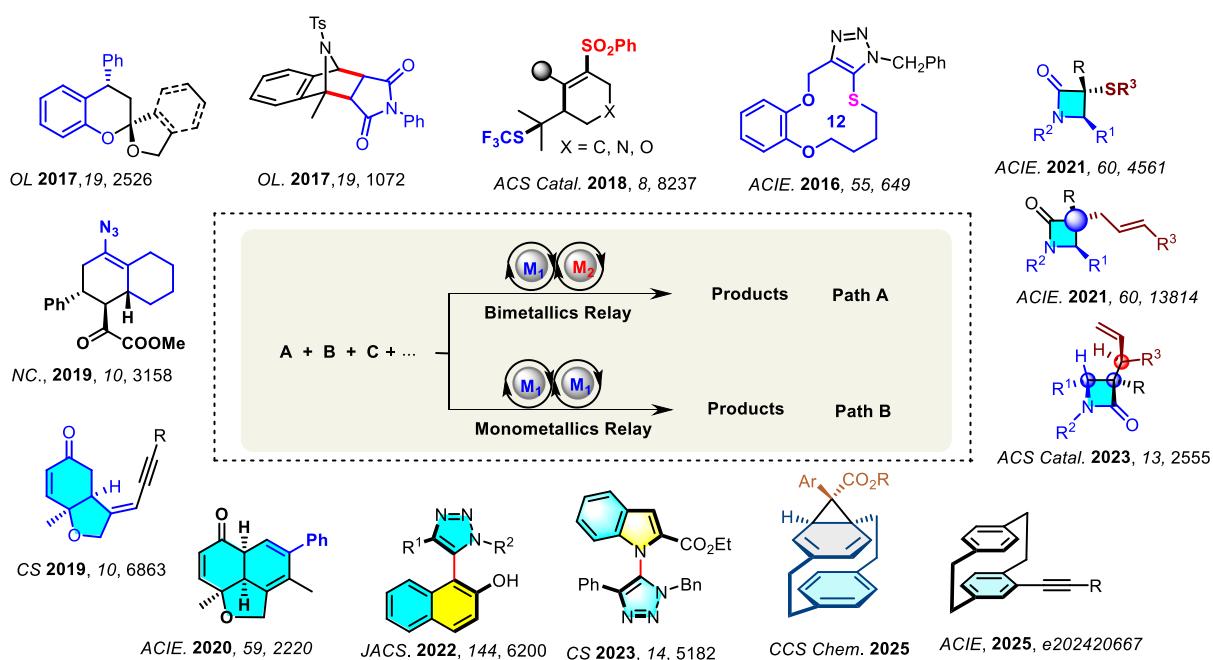
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**Research Summary:** Tandem Metal Relay Catalysis to polycycles



## Asymmetric Metal Relay Catalysis to Planar chiral [2,2]paracyclophanes

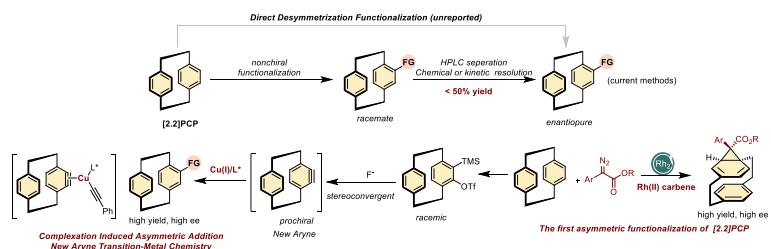
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**Keywords:** Asymmetric Catalysis, Relay, Planar chiral, paracyclophane

Planar chirality found tremendous use in many fields, such as chemistry, optics, and materials science. In particular, planar chiral [2,2]paracyclophanes (PCPs) are a type of structurally interesting and practically useful chiral compounds bearing unique electronic and photophysical properties and thus have been widely used in  $\pi$ -stacking polymers, organic luminescent materials, and as a valuable toolbox for developing chiral ligands or organocatalysts. However, the synthesis of chiral PCP derivatives remains a longstanding challenge. Current synthetic methods primarily rely on chiral preparative liquid chromatography separation or chemical and kinetic resolution reactions. Here, we report an enantioconvergent alkynylation of an in situ-formed dehydro-[2,2]-paracyclophane intermediate by asymmetric copper(I) catalysis. This approach enables the efficient synthesis of valuable planar chiral PCP building blocks and heterocycles with good yields and excellent enantioselectivity. The success of this reaction lies in the development of a practical route to access strained dehydro-[2,2]-paracyclophane intermediates, which can also be utilized in various strain-release nucleophilic or cycloaddition reactions to synthesize diverse functionalized PCPs. DFT calculations of this reaction suggest that the enantioselectivity is determined by the aryne complexation with chiral copper(I) acetylide and the subsequent insertion reaction. We anticipate that this new aryne system and its related synthetic applications will provide a new direction in traditional benzyne chemistry. This approach has the potential to serve as a general platform for constructing planar chiral PCPs and could open new avenues for the challenging construction of planar chirality.



**Figure 1.** Asymmetric Catalytic route to planar chiral [2,2]PCPs

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**The 9<sup>th</sup> International Conference on  
Multicomponent Reactions and Related Chemistry  
13-16<sup>th</sup> Jan 2026**



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## Pd-Catalyzed Asymmetric Three-Component Coupling of *N*-Sulfonylhydrazones

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**Keywords:** *Pd, carbene, N-Sulfonylhydrazones, Sadphos*

In recent years, the selective transformation of *N*-tosylhydrazones into functionalized molecular scaffolds has attracted significant attention; however, achieving enantiocontrol in these reactions remains a formidable challenge. By designing specialized sulfinamide–phosphine ('Sadphos') ligands, we have successfully harnessed the high reactivity of palladium carbenes, converting them into powerful tools for the precise construction of congested chiral centers via a modular enantioselective assembly strategy. This approach has enabled the development of a series of multicomponent reactions (MCRs) utilizing metal carbene intermediates.<sup>[1]</sup> Furthermore, DFT-based mechanistic investigations suggest that the enantio-determining step involves a concerted carbene formation and migratory insertion process, facilitated by the pronounced structural adaptability and flexible coordination behavior of the Sadphos ligands.

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## NICEKEL CHAIN-WALKING CATALYSIS FOR MULTICOMPONENT ALKENE FUNCTIONALIZATION

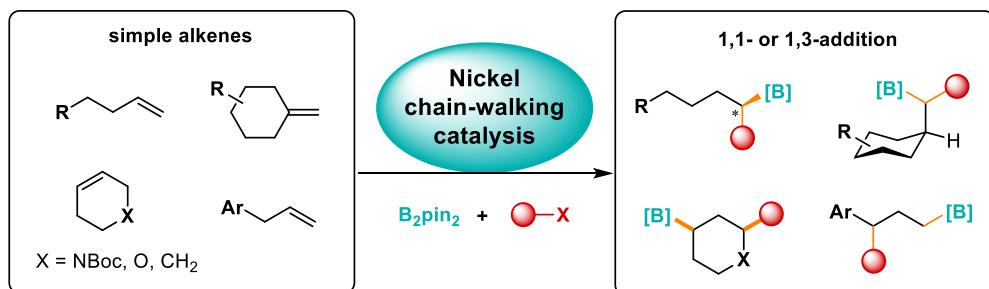
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**Keywords:** *Chain-walking catalysis, nickel, alkene functionalization, 1,n-addition( $n\neq 2$ )*

Chain-walking offers extensive opportunities for innovating synthetic methods that involve constructing chemical bonds at unconventional sites. This approach provides previously inaccessible retrosynthetic disconnections in organic synthesis. Through chain-walking, transition metal-catalyzed alkene difunctionalization reactions can take place in a 1, n-addition ( $n\neq 2$ ) mode. Unlike classical 1,2-regioselective difunctionalization reactions, there remains a scarcity of reports regarding migratory patterns. Moreover, the range of olefins utilized in these studies is quite limited. The Yin group focuses on developing valuable migratory difunctionalization reactions of alkenes through chain-walking. Our focus was on carboboration of alkenes utilizing nickel catalysis. The incorporation of a versatile boron group introduces a wealth of possibilities for subsequent diversifications, significantly enhancing the value of the resulting products and allowing for the creation of a broader range of valuable derivatives and applications.



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## Catalytic reduction-specified tandem reactions

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**Keywords:** Reductive tandem reactions, functional N-molecules, sustainable catalysis and synthesis

By employing unsaturated nitrogen-containing aromatics as the fundamental feedstocks, our group has been focusing on the utilization of their reductive intermediates to develop new tandem reactions in recent years (Fig. 1), and the developed synthetic methods were further applied for streamline synthesis of functional molecules such as biomedical, ligands, dyes, polymers, etc. By employing different strategies, the talk will present precise *in situ* interception of single reductive intermediates among multiple ones to develop tandem reactions involving both C–C and C–N bond formations. The contents will cover the following two sections: (1) Reductive functionalization of N-heteroarenes.<sup>[1]</sup> (2) Reductive tandem reactions for direct and diverse construction of functional N-containing molecules with abundantly available nitroarenes.<sup>[2]</sup>

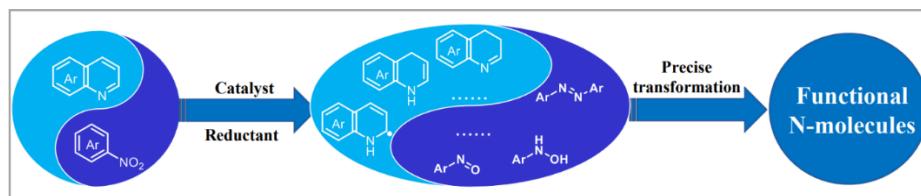


Figure 1. Reduction-specified tandem reactions

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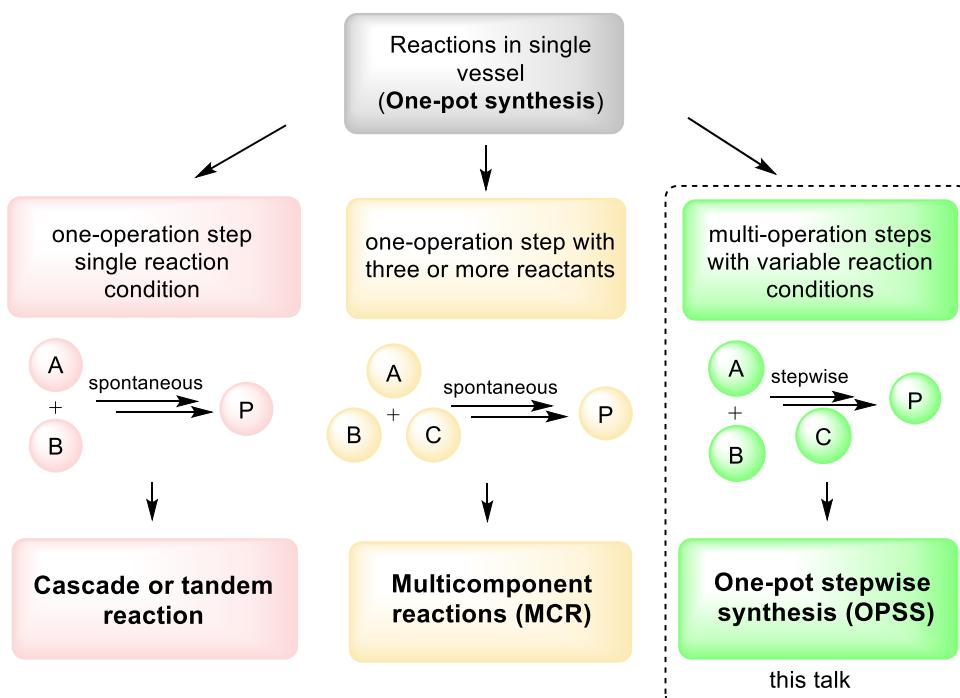
## INTEGRATED ONE-POT STEPWISE SYNTHESIS AND ORGANOCATALYSIS

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**Keywords:** One-pot synthesis, multicomponent reaction, cascade reaction, stepwise synthesis

One-pot synthesis is an active topic in organic chemistry due to its intrinsic advantages of simple operation, high mass efficiency, low cost, and less waste. Among three kinds of one-pot syntheses 1) cascade reactions, 2) multicomponent reactions (MCRs), and 3) one-pot stepwise synthesis (OPSS), OPSS could be more flexible and practical since it is carried out step wisely and have variable reaction conditions at different steps. This presentation highlights the recent development in our lab on the development of OPSS involving cyclization, cycloaddition, rearrangement, and organocatalysis for the synthesis of heterocyclic scaffolds, asymmetric molecules, and bioactive compounds.



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## Metal Difluorocarbene-Involved Catalytic Coupling

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**Keywords:** *organofluorine chemistry, metal difluorocarbene, catalytic coupling*

Difluorocarbene is a highly reactive intermediate with a singlet ground state and is widely used in the synthesis of fluoropolymers, such as Teflon. Owing to its ability to form two chemical bonds, compared with fluorine-containing carbocations, carbanions, and free radical intermediates, difluorocarbene is capable of expanding the chemical space and efficiently creating novel organofluorine molecules. However, the high reactivity of difluorocarbene limits its reaction types and makes it difficult to apply in controllable organic synthesis. Theoretically, coordination of transition metals with difluorocarbene would alter the electron density distribution of difluorocarbene, thereby providing a possibility for modulating its reactivity. However, the transition metal difluorocarbene complexes isolated so far lack catalytic reactivity, and catalytic reactions involving metal difluorocarbenes pose a long-standing challenge. In 2015, we discovered the first catalytic coupling reaction involving a metal difluorocarbene.<sup>[1]</sup> This presentation will mainly introduce the latest progress in palladium and copper difluorocarbene chemistry.<sup>[2-7]</sup>

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## Multicomponent Radical Reactions Leveraging the Persistent Radical Effect.

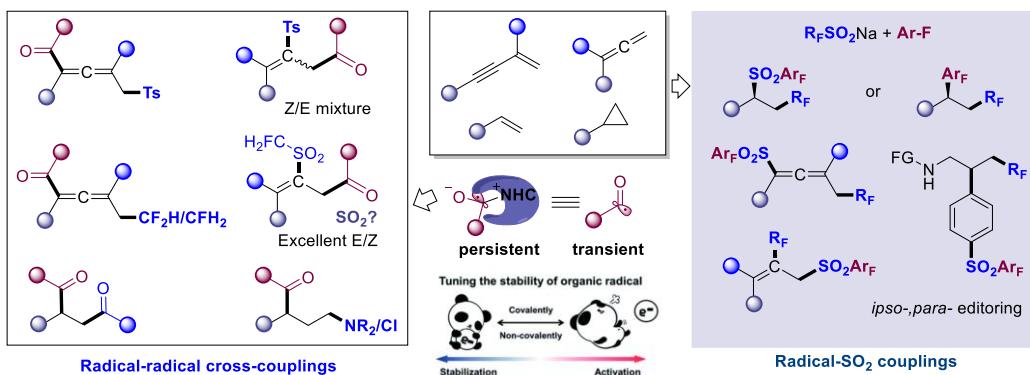
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**Keywords:** Radical Cross-Coupling, Photocatalysis, Multicomponent Reactions, Di-functionalization, Persistent Radical Effect

The “persistent radical effect” (PRE)<sup>[1]</sup> is a kinetic principle that explains the high selectivity often observed in cross-coupling reactions between radical species. This effect arises when two radicals with differing lifetimes are generated at equal rates: the more persistent radical accumulates, while the short-lived species remains at low concentration, leading to preferential cross-coupling. N-Heterocyclic carbenes (NHCs) facilitate the stabilization of acyl radicals, thereby paving the way for controlled radical acylation via radical–radical cross-coupling<sup>[2]</sup>. Inspired by seminal contributions from Ohmiya, Studer, Chi, and coworkers, we developed a visible-light-mediated dual catalytic system combining NHCs with photoredox catalysts (PCs) to achieve radical acylative difunctionalization of various unsaturated hydrocarbons, including olefins<sup>[3b]</sup>, 1,3-enynes<sup>[3c]</sup>, allenes, and cyclopropanes<sup>[3d,e]</sup>. Furthermore, by employing  $\text{CF}_2\text{SO}_2\text{Na}$  as a bifunctional reagent and harnessing the stabilized SOMO of sulfur dioxide, we accomplished controllable difluoromethylation–polyfluoroarylsulfonylation of unsaturated hydrocarbons<sup>[3f]</sup>, as well as ipso-/para-selective difluoromethylation–polyfluoroarylsulfonylation of aniline derivatives<sup>[3g]</sup>.



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## Catalytic Transformation of Acetylene

Shifa Zhu<sup>a,b</sup>

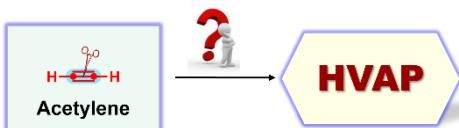
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**Keywords:** Acetylene, Transient Species

Acetylene is the simplest alkyne, which is one of the most important fundamental coal-based chemical feedstocks. However, research on the transformations of acetylene was mainly conducted before the 1960s. Furthermore, most of the research has focused on the low value-added fine chemicals. Due to the inherent unique structure, easily flammable and explosive properties of the acetylene molecule, there are very limited applicable methods for its transformation in literature. Recently, on the basis of achieving the diversity transformation of substituted alkynes, we turned our attention to the transformation of acetylene, with a focus on developing new catalytic systems suitable for acetylene. Following this interest, three different strategies of metal catalysis, photocatalysis and photoredox/metal dual catalysis has been developed to enable the efficient conversion of acetylene into high value-added chemicals under 1 atm through cleavage of carbon-carbon triple bond of acetylene molecule.<sup>[1-12]</sup>



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## ORAL PRESENTATIONS

## **Efficient Three-Step Synthesis of Novel Triazole-Hydrazone Hybrid Compounds: From Ethyl 5-Acetamido-1,2,4-triazole-3-carboxylate to Salicylaldehyde-Derived Fluorescent Molecules**

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**Keywords:** hydrazine, triazole, fluorescent, hydrazinolysis, salicylaldehyde, bibliographic.

This study reports the successful synthesis of a novel hydrazone-based fluorescent compound derived from triazole precursors through a systematic three-step synthetic approach. The synthetic pathway commenced with ethyl 5-acetamido-1,2,4-triazole-3-carboxylate as the starting material, which serves as a versatile scaffold for heterocyclic compound development. In the initial step, the ester functionality underwent hydrazinolysis reaction with hydrazine under controlled conditions to yield the corresponding hydrazide intermediate in good yield. The hydrazide product was thoroughly characterized and confirmed for structural integrity before proceeding to the subsequent transformation. The final step involved the condensation reaction between the hydrazide intermediate and salicylaldehyde under optimized reaction conditions, successfully affording the target hydrazone-based compound in excellent yield. The condensation reaction proceeded smoothly, demonstrating the compatibility and reactivity of the chosen synthetic components. Comprehensive structural characterization was performed using various spectroscopic techniques including NMR spectroscopy, mass spectrometry, and infrared spectroscopy to confirm the successful formation of the hydrazone linkage and overall molecular structure. The synthetic methodology developed in this work provides a reliable and efficient route for accessing triazole-hydrazone hybrid compounds, which represent an important class of heterocyclic structures with potential applications in medicinal chemistry and materials science. The high yields obtained throughout the synthetic sequence and the straightforward purification procedures make this approach attractive for further synthetic applications and structural modifications.



**The 9<sup>th</sup> International Conference on  
Multicomponent Reactions and Related Chemistry  
13-16<sup>th</sup> Jan 2026**



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## Modular Synthesis of Sulfonamides and Sulfonates Via Electrochemical Fixation of Sulfur Dioxide

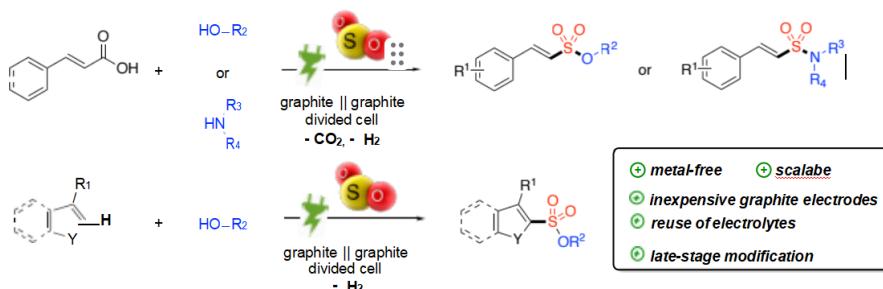
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**Keywords:** sulfonamides, sulfonates, sulfur dioxide, multicomponent reaction, electrosynthesis

Molecules containing a sulfonyl (-SO<sub>2</sub>-) functionality, such as sulfones, sulfonamides or sulfonates, play an important role in organic chemistry and have found widespread application, in particular in medicinal chemistry and material sciences. Therefore, the development of novel methods for a sustainable synthesis of these compounds is of great interest.<sup>[1]</sup> In the last years, the direct incorporation of sulfur dioxide (SO<sub>2</sub>) into organic molecules has emerged as versatile tool for a modular synthesis of sulfones and sulfonamides.<sup>[2]</sup> Furthermore, novel reagent-less activation procedures based on the photochemical or electrochemical fixation of SO<sub>2</sub> offer attractive opportunities for more sustainable syntheses of sulfur-containing organic molecules.<sup>[3]</sup> Herein, novel methods for the synthesis of sulfonates and sulfonamides via electrochemical fixation of sulfur dioxide as key building block are presented. These methods include two three-component reactions for the synthesis of alkyl alkenesulfonates<sup>[4]</sup> and alkene sulfonamides<sup>[5]</sup> from cinnamic acids, SO<sub>2</sub> and alkyl alcohols or amines in a decarboxylative transformation and a process for the synthesis of heteroaryl sulfonates via selective C(sp<sup>2</sup>)-H-functionalization.<sup>[6]</sup> All methods are metal-free and feature the use of inexpensive graphite electrodes in combination with simple-to-use SO<sub>2</sub> stock solutions. The applicability of these processes is demonstrated in scale-up and electrolyte reusability experiments as well as the late-stage modification of drug-like scaffolds.



Overall, these processes enable a highly modular construction of the sulfonyl functionality using sulfur dioxide as key building block using electricity as driving force. Both the direct decarboxylative transformation of cinnamic acids, as bio-based feedstocks and the direct functionalization of C-H-bonds provide intriguing opportunities for a more sustainable synthesis of medicinally relevant scaffolds.



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**Short biography :**

Dr. Muhammad Idham Darussalam Mardjan is an academic and researcher whose expertise lies in development of one-pot reactions to access bioactive heterocycles bearing nitrogen, oxygen and sulfur atoms. The library of heterocyclic compounds is then subjected to various biological assays, such as antiplasmodium, anticancer, antimicrobial and antidiabetic assays.

He completed his Undergraduate and Master education in Universitas Gadjah Mada, Indonesia, in the field of Organic Chemistry. He then pursued his Doctoral Degree (2013-2016) in Aix-Marseille Université, France, under the supervision of Prof. Laurent Commeiras and Dr. Jean-Luc Parrain. His doctoral thesis focused on the application of multicomponent reactions towards the synthesis of  $\gamma$ -hydroxybutyrolactams, polycyclic lactams, and spirolactams.

He has served as lecturer and researcher at Departement of Chemistry, Universitas Gadjah Mada, Indonesia, since 2014. In 2019-2022, he was a visiting scholar (supported by Fulbright Indonesia) in the laboratory of Prof. Gary Molander, University of Pennsylvania, United States. He continued to contribute to academic advancement as a visiting Scholar in the laboratory of Professor Laurent Commeiras in Aix-Marseille Université, France, in 2024.



## STRAIGHTFORWARD ACCESS TO BIOACTIVE QUINAZOLINONES THROUGH ONE-POT REACTION

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**Keywords:** quinazolinones, one-pot reaction, multicomponent reaction, antiplasmodium, anticancer

Quinazolinones represent an important class of heterocyclic compounds, known for their broad spectrum of biological activities. The construction of these scaffolds in effective and efficient manner has triggered considerable attention. This study reports a straightforward and general strategy for the synthesis of highly functionalized quinazolinones from readily available starting materials of isatoic anhydrides, primary amines and aldehydes or alcohols. In this context, we manage to employ one-pot reaction (multicomponent and sequential reactions) to create a library of diversely-substituted- quinazolines in good yields. it is also interesting to note that the synthesis of quinazolinones can be carried out in multigram scale. Moreover, the in vitro biological evaluation demonstrates that some derivatives exhibit potent activities against *Plasmodium falciparum* strains and cancer cell lines with minimal toxicity to the normal cells, making them good candidates for further development as antiplasmodium and anticancer agents.



**The 9<sup>th</sup> International Conference on  
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Maxim Mironov received his PhD in 1999 and has since participated in scientific and commercial projects related to combinatorial chemistry and biopolymers. He has worked intensively in the field of isocyanide-based multicomponent reactions. In 2009, he organized the MCR2009 conference in Yekaterinburg. In 2014, he accepted a full professorship at Ural Federal University, where his research interests focus on the synthesis of microgels and their practical applications in medicine, the food industry, and household chemicals. To implement his findings, he founded the company Biomicrogels in 2012, which is now successfully operating and developing. He is the author of many patents and scientific articles, and the winner of innovation competitions such as the Best Innovator of Moscow in 2021 and Innocentive.

## MULTICOMPONENT REACTIONS WITH BIOPOLYMERS AS A POWERFUL TOOL FOR PREPARATION OF 3-D MICROSTRUCTURES

Maxim A. Mironov, Yaroslava A. Menzorova, Mushtaq Hussain and Suleiman Bacha

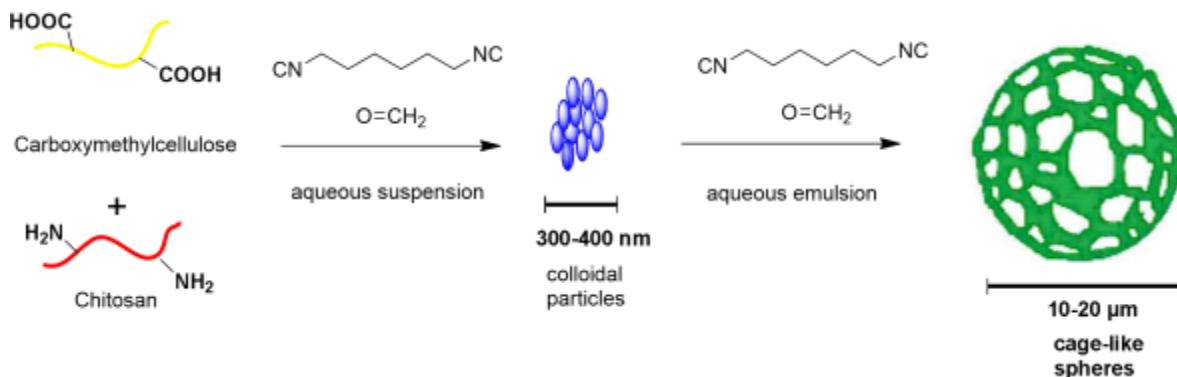
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**Keywords:** *Ugi, Passerini reactions, Polysaccharides, Colloidosomes, Cage-like microstructures*

Microstructures such as polymer capsules, porous colloidosomes, and cage-like microstructures in the form of spheres, tubes, and petals with sizes of 5–20  $\mu\text{m}$  are of interest as scaffolds for tissue engineering and 3-D bioprinting. Biopolymers are preferable over synthetic polymers for these purposes due to their biocompatibility with human tissues. However, traditional methods for producing 3-D microstructures based on biopolymers are a multi-step and labor-intensive process. Our group makes extensive use of multicomponent chemistry to achieve this in one or at most two steps. As a starting material we used polysaccharides such as: carboxymethyl cellulose, pectin, fucoidan, gum arabic and chitosan [1-4].



As an example, the figure shows the synthesis of cage-like microspheres based on carboxymethyl cellulose and chitosan. The cage-like structures were obtained in two steps by repeating the Ugi reaction. At the first stage, submicron colloidal particles based on carboxymethylcellulose and chitosan with a domain structure were obtained in an aqueous suspension. In the second stage, the Ugi reaction was carried out on the surface of Pickering emulsions with toluene. Removal of toluene and redissolution in water resulted in the microspheres with large holes on the surface. Varying the reaction conditions during this process made it possible to obtain structures with different porosity. The Ugi reaction in water is an ideal choice because it is characterized by high rates over a narrow pH range. This allows us to control the process of formation of cage-like structures. During the conference we will also present other examples of obtaining 3-D microstructures using multicomponent reactions. Particular attention will be paid to the study of the mechanism of this process, which occurs at the boundary of two phases under nonequilibrium conditions.



The practical use of the materials obtained during our research as carriers of biologically active substances and sorbents will also be demonstrated.

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## Multicomponent Reactions with Rh Carbonylids

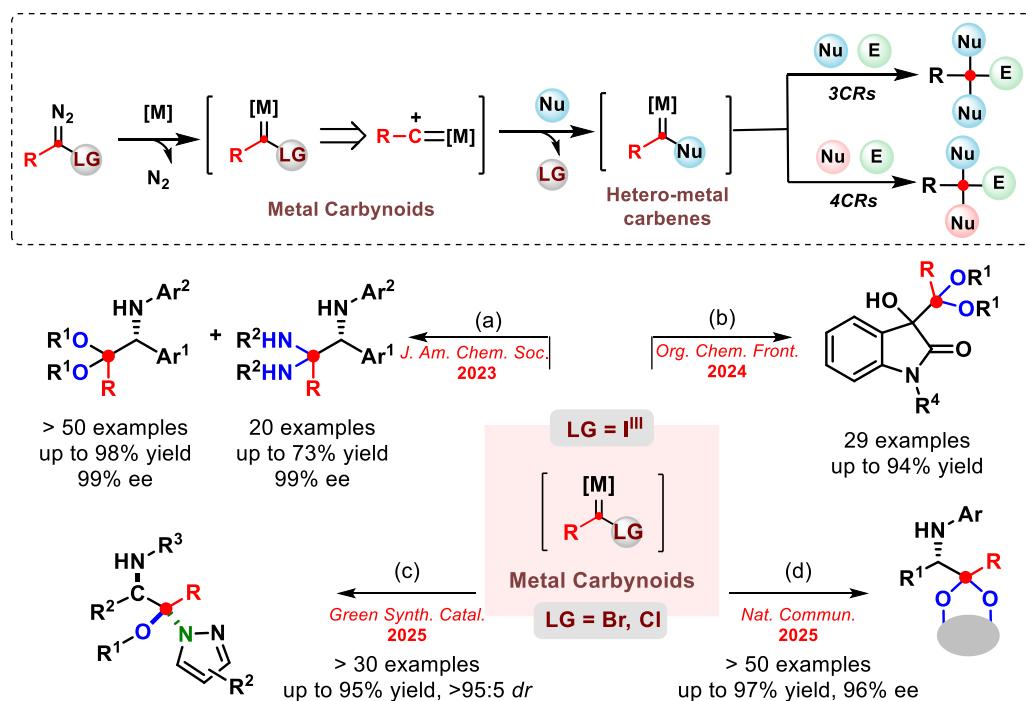
Yu Qian<sup>a</sup> and Wenhao Hu<sup>a</sup>

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**Keywords:** Rh Carbonylids; Reactive intermediates; Multicomponent reactions; Asymmetric synthesis

Multicomponent reactions involving reactive intermediates have become a powerful strategy for constructing structurally diverse and functionally complex molecules. In our research, we have developed a series of diazo compounds bearing leaving groups as precursors for metal Carbonylids, which serve as versatile reactive intermediates. Upon catalytic generation, these metal Carbonylids react with nucleophiles to form Fischer-type heteroatom-substituted metal carbenes, which then undergo a second nucleophilic attack to generate ylides, and are ultimately trapped by electrophiles. By employing cooperative catalysis or precisely controlling the formation rate of heteroatom-substituted metal carbenes, we achieve ordered reaction sequences with high stereochemical fidelity. This approach not only enables the efficient synthesis of structurally complex molecules but also provides a flexible platform for rapid assembly of diverse new chemical entities, which is valuable for drug discovery and functional molecule development.



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Alexandra Golubenkova received her master's degree in Organic Chemistry from PhD degree in Organic Chemistry from Peoples' Friendship University of Russia in 2020 and her PhD degree from the same university in 2023. The scientific interests mainly focus on heterocyclic chemistry, domino reactions methodology and new MCR reactions.

**A DOMINO ROUTE FROM IMIDAZOLINES AND ELECTRON-DEFICIENT  
ALKYNES TO POLYSUBSTITUTED PYRROLES,  
TETRAHYDROPYRROLO[1,2-A]PYRAZINES AND PYRIDINES**

Golubenkova A.S., Voskressensky L.G.

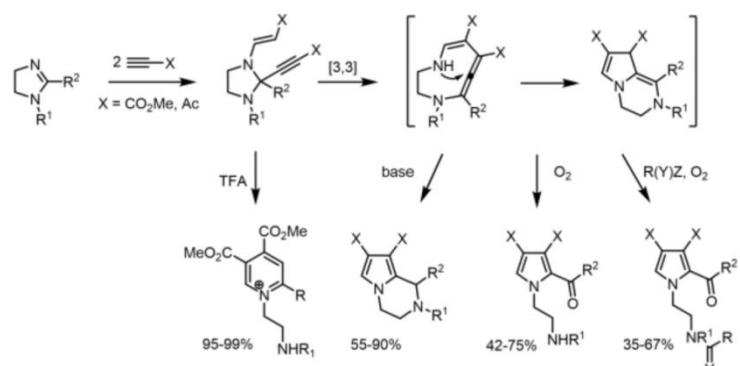
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**Keywords:** domino reaction, aza-heterocycle, electron-deficient alkynes

Nitrogen-containing compounds such as 1,2,3,4-tetrahydropyrrolo[1,2-a]pyrazines, N- substituted pyrroles, and pyridines are an important motifs due to their biological activities. In particular, polysubstituted pyrroles have anti-tumor activity and antibiotics while pyrrolo[1,2-a] pyrazine derivatives show neuropsychotropic properties. Thus, the synthesis of these widely exiting heterocyclic systems still attracts much attention of scientists.

The present work discloses our latest results, concerning three-component reaction of 2- imidazolines and electron-deficient terminal alkynes to form tetrasubstituted imidazolidines, which can undergo further transformations[1-3]. As a convenient starting material, we consider 2-imidazolines which can be easily obtained by new preparative methods discovered in recent times.



Obtained tetrasubstituted imidazolidines have an amino-ester fragment, cyclic aminal fragment and an electron-deficient triple bond, such a concentrated set of reaction centers allows us to expect a high synthetic potential of these compounds. It can be interesting as for investigation a mechanism of the proceeding reactions as for synthesis aimed at expanding molecular diversity.

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Prof. Shenghan Teng received his BS and MS degrees in Chemistry from East China Normal University under the guidance of Prof. Wenhao Hu. In 2016, he joined Prof. Jianrong Steve Zhou's group at Nanyang Technological University as a PhD student. After graduation, he carried out postdoctoral research with Prof. Teck-Peng Loh at NTU, working on green organic reactions in water. He joined Fujian Normal University in 2023 and was promoted to professor in December 2024. His research interests include asymmetric synthesis and organoboron chemistry.

## MODULAR SYNTHESIS OF LUMINESCENT BORON-CONTAINING HETEROCYCLES FROM $\beta$ -ALKYNONES TRIFLUOROBORATES, AMINES AND ARYNES

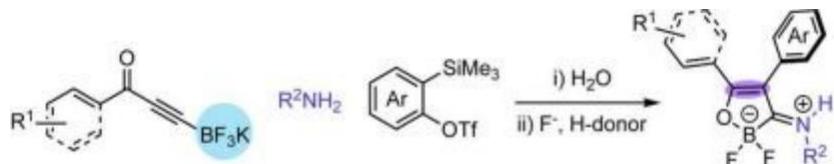
Shenghan Teng<sup>a</sup>\*, Lin Hu<sup>a</sup> and Peiyao Liang<sup>a</sup>

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**Keywords:** alkynes, aminoarylation, boron-containing heterocycles, one-pot methodologies, geometric selectivities, tunable emission

**Abstract[1]** : Selective aminoarylation of internal alkynes under transition metal-free conditions provides a sustainable route to fully substituted enamines that are useful in pharmaceuticals and organic electronics<sup>[2]</sup>. Incorporation of tetracoordinated boron further modulates photophysical properties, paving the way for advanced optoelectronic materials<sup>[3]</sup>. Yet existing aminoarylation strategies rely on ambiphilic reagents with limited functional-group compatibility and are inapplicable to boryl alkynes<sup>[4]</sup>. Recent work by Loh and coworkers revealed that benchtop-stable alkynone  $\beta$ -trifluoroborates react with diverse amines under physiological conditions to deliver stable oxaboracycles by forming covalent B–O bond<sup>[5]</sup>. Building on this amine-specific boron chemistry<sup>[6]</sup>, we report a streamlined intermolecular aminoarylation of alkynone  $\beta$ -trifluoroborates with amines and arynes via a sequential amine- click/aryne trapping process, affording *E*-selective oxaboracycles with high regio- and stereoselectivity under mild conditions<sup>[7]</sup>. Incorporation of tetracoordinated boron centers and aryl “rotors” not only induces aggregation-induced emission enhancement (AIEE) but also enables wavelength-tunable solid-state emission from violet to red. The resulting oxaboracyclic tetrasubstituted enamines exhibit key advantages as functional luminophores for biological applications, including large Stokes shifts, outstanding chemical and photostability, low cytotoxicity and excellent biocompatibility. Their potential utility is demonstrated by reliable performance as fluorescent probes for live-cell imaging.



- Elucidation the origin of *E*-selectivity and C-arylation
- Operational simplicity, broad scope and diverse elaboration
- Large Stokes shift, broadly tunable fluorescence and AIEE feature
- High biocompatibility and strong potential in living cell imaging

Figure 1. Streamlined synthesis of oxaboracyclic tetrasubstituted enamines via sequential amine-click/arylation process

See MCR2026 website for more details: <https://sps.sysu.edu.cn/mcr2026/>

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[ 1] We gratefully acknowledge the financial support from National Natural Science Foundation of China (NSFC 22401047), the Science and Technology Planning Project of Fujian Province (2024J01474), High-performance Computing Center of Fujian Normal University, Open Research Fund of Key Laboratory of the Ministry of

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Minghui Wu was born and raised in Sichuan, China. She finished her bachelor in Polymer science and engineering at Changzhou University in 2020. After that, she received The Dutch Orange Tulip Scholarship for the master and has gained the master's degree of Biobased Materials at Maastricht University in 2022. Since 2022, she has started the PhD journey under the supervision of Prof. Romano Orru, mainly focusing on isocyanide chemistry and photocatalysis. Till now, she has completed two projects and published them in Chemical Science and The Journal of Organic Chemistry.



## NON-INNOCENT BEHAVIOUR OF AROMATIC ISOCYANIDES UNDER VISIBLE LIGHT: A PATHWAY TO THIOFORMIMIDATES AND DEHYDROALANINE

Minghui Wu,<sup>a</sup> Jay Hanssen,<sup>a</sup> Camilla Russo,<sup>b</sup> Rajat Walia,<sup>c</sup> Mariateresa Giustiniano,<sup>b</sup> Ludovic Troian-Gautier,<sup>d</sup> Jordy M. Saya,<sup>a</sup> Romano Orru,<sup>a,\*</sup> Prabhat Ranjan <sup>a,d,\*</sup>

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**Keywords:** *Photochemistry, Visible light, Isocyanide cascade, Dehydroalanine (DHA) derivatives*

Thioformimidates play an important role in peptide modifications as the protection group<sup>1</sup>. The most common method for the synthesis of thioformimidates involves *S*-alkylation of thioformamides with aryl or alkyl halides. However, these processes often suffer from several limitations and purification problems due to the instability of thioformamides and limited substrate scope. Alternatively, thioformimidates can also be synthesized from isocyanides and thiols triggered by UV-light or AIBN initiator<sup>2</sup>. Generally, this reaction proceeds with the formation of a thiyl radical in the presence of UV-light or AIBN followed by thiyl radical addition on the isocyanide to generate an  $\alpha$ -thioimidoyl radical<sup>3</sup>. This radical can then undergo H-abstraction from thiols to form the final thioformimidates product. Despite the convenience of this method, less attention has been directed to this pathway due to the following reasons: a) the requirement of UV-light; b) poor reaction efficiency; c) the formation of unwanted side products such as 1,1-bisthiolation; d) C-S bond scission of the intermediate  $\alpha$ -thioimidoyl radical, leading to the generation of isothiocyanates.

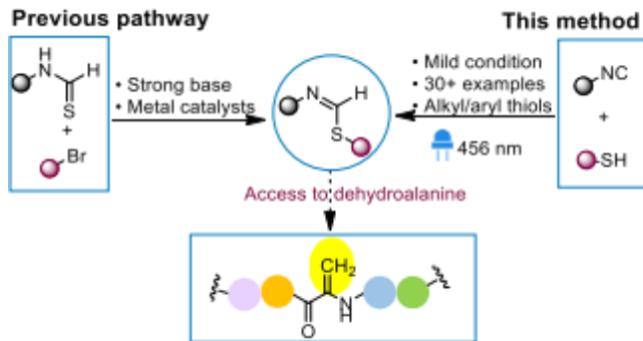


Figure 1. Visible light-mediated synthesis of thioformimidates and application to *dehydroalanine (DHA) derivatives*

Previously, we designed a photocatalyst-free pathway to spirocyclic scaffolds from tryptamine-derived isocyanides by employing blue light **4**. Given the significance of thioformimidates and the current limitations in versatile, sustainable synthetic methods, we focused on developing an innovative, photocatalyst-free, visible-light-driven approach for their synthesis. This study marks a significant advance in the field, as it not only improves existing methods for accessing thioformimidates but also reveals a previously camouflaged role of isocyanides in generation of thiyl radicals.

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Xing Zhongqiu was born and raised in Anhui, China. Now he is a Ph.D. candidate in Chemical Biology at Nanjing University, where he conducts interdisciplinary research at the intersection of synthetic biology and synthetic chemistry under the supervision of Researcher Huang Xiaoqiang. He is the first author of a *Nature* paper titled "Synergistic photobiocatalysis for enantioselective triple radical sorting." His work in the Huang Group contributes to the team's broader research portfolio—spanning biocatalysis, asymmetric photoelectrochemistry, artificial enzymes, and engineered microbial factories—which has been published in leading journals such as *Nature*, *Nature Catalysis*, *JACS*, and *Angewandte Chemie*.

## Synergistic photobiocatalysis for enantioselective triple radical sorting

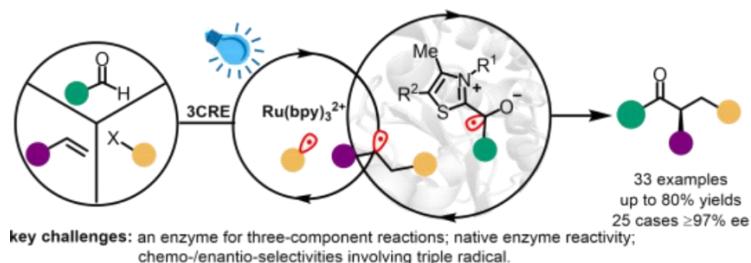
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Harnessing enzymes for non-natural asymmetric transformations, which are challenging for traditional chemocatalysis, holds great significance<sup>1-3</sup>. Despite the notable benefit of multicomponent reactions in broadening chemical space and enhancing molecular complexity<sup>4</sup>, achieving enzymatic conversion of three variable substrates into enantioenriched compounds via a single reaction has remained rare.<sup>5</sup> This limitation primarily arises because an enzyme's active site cannot concurrently tame multiple substrates or intermediates, especially in cases involving multiple radical intermediates<sup>6</sup>. Recently, chemocatalytic radical sorting has emerged as an enabling strategy for a variety of appealing reactions<sup>7,8</sup>. However, directing such processes in an enantioselective manner is highly challenging due to the inherent difficulty in the stereocontrol of radicals<sup>9</sup>. Herein, we repurpose a thiamine-dependent enzyme<sup>10,11</sup> through directed evolution and synergy with photoredox catalysis, to facilitate an unprecedented photobiocatalytic enantioselective three-component radical cross-coupling. Mechanistic investigations have provided crucial insights into how this dual photo-/enzyme system precisely directs the three distinct radicals involved in the transformation, unlocking new enzyme reactivity and enabling access to a variety of enantioenriched carbonyl compounds. Our approach has achieved exceptional stereoselectivity, with 25 out of 33 examples achieving  $\geq 97\%$  enantiomeric excess. This work not only expands the repertoire of biocatalysis but also provides a unique strategy for sorting multiple radicals complementing existing chemical tools.



**Figure** Artificial metalloenzymes result from anchoring an organometallic catalyst within a protein scaffold. The resulting hybrid catalyst can be optimized by combining both chemical and genetic strategies.

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| Chiral MC(2)                                 | Cellulose tris(phenylcarbamate)                      | Chiralcel OC     |
| Chiral MK(2)                                 | Cellulose tricinnamate                               | Chiralcel OK     |
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| Chiral MG(2)                                 | Cellulose tris(4-methylphenylcarbamate)              | Chiralcel OG     |
| Chiral MS(2)                                 | Cellulose tris((s)- $\alpha$ -methylbenzylcarbamate) |                  |
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|-------------------------------------|--|-----------------|
| Chiral ND(2)-RH                     | Amylose tris(3,5-dimethylphenylcarbamate)            | Chiraldak AD-RH |
| Chiral NY(2)-RH                     | Amylose tris(5-chloro-2-methylphenylcarbamate)       | Chiraldak AY-RH |
| Chiral NS(2)-RH                     | Amylose tris((s)- $\alpha$ -methylbenzylcarbamate)   | Chiraldak AS-RH |
| Chiral NZ(2)-RH                     | Amylose tris(3-chloro-4-methylphenylcarbamate)       |                 |
| Chiral NX(2)-RH                     | Amylose tris(4-chloro-3-methylphenylcarbamate)       |                 |
| Chiral NQ(2)-RH                     | Amylose tris(halogenated-methylphenylcarbamate)      |                 |
| Chiral NT(2)-RH                     | Amylose tris(3-chlorophenylcarbamate)                |                 |
| Chiral MD(2)-RH                     | Cellulose tris(3,5-dimethylphenylcarbamate)          | Chiralcel OD-RH |
| Chiral MZ(2)-RH                     | Cellulose tris(3-chloro-4-methylphenylcarbamate)     | Chiralcel OZ-RH |
| Chiral MJ(2)-RH                     | Cellulose tris(4-methylbenzoate)                     | Chiralcel OJ-RH |
| Chiral MX(2)-RH                     | Cellulose tris(4-chloro-3-methylphenylcarbamate)     | Chiralcel OX-RH |
| Chiral MQ(2)-RH                     | Cellulose tris(halogenated-methylphenylcarbamate)    |                 |
| Chiral MS(2)-RH                     | Cellulose tris((s)- $\alpha$ -methylbenzylcarbamate) |                 |
| Chiral MY(2)-RH                     | Cellulose tris(5-chloro-2-methylphenylcarbamate)     |                 |
| Chiral NJ(2)-RH                     | Amylose tris(4-methylbenzoate)                       |                 |
| Chiral NC(2)-RH                     | Amylose tris(phenylcarbamate)                        |                 |

| Chiral stational pahses for NP, SFC, PO and RP mode |   |                    |
|---|---|--------------------|
| Chiral INA  | Amylose tris(3,5-dimethylphenylcarbamate)immobilized          | Chiraldak IA       |
| Chiral INB  | Cellulose tris(3,5-dimethylphenylcarbamate)immobilized        | Chiraldak IB-N, IB |
| Chiral INC  | Cellulose tris(3,5-dichlorophenylcarbamate)immobilized        | Chiraldak IC       |
| Chiral IND  | Amylose tris(3,5-dimethylphenylcarbamate)immobilized          | Chiraldak ID       |
| Chiral INE  | Amylose tris(3,5-dimethylphenylcarbamate)immobilized          | Chiraldak IE       |
| Chiral INF  | Amylose tris(3-chloro-4-methylphenylcarbamate)immobilized     | Chiraldak IF       |
| Chiral ING  | Amylose tris(3-chloro-5-methylphenylcarbamate)immobilized     | Chiraldak IG       |
| Chiral INH  | Amylose tris((s)- $\alpha$ -methylbenzylcarbamate)immobilized | Chiraldak IH       |
| Chiral INK  | Cellulose tris(3-chloro-5-methylphenylcarbamate)immobilized   | Chiraldak IJ       |
| Chiral INJ  | Cellulose tris(4-methylbenzoate)immobilized                   | Chiraldak IK       |
| Chiral INM  | Cellulose tris(3-chloro-4-methylphenylcarbamate)immobilized   | Chiraldak IM       |
| Chiral INN  | Amylose tris(5-chloro-2-methylphenylcarbamate)immobilized     | Chiraldak IN       |
| Chiral INO  | Cellulose tris(4-chloro-3-methylphenylcarbamate)immobilized   |                    |





### 广州市普康慈善基金会简介 Guangzhou Pukang Foundation

Established in June 2017 and registered with the civil affairs department of Guangzhou, the PUKANG Foundation (abbreviated as PKF) is a non-profit organization with independent legal person status and qualifications for pre-tax deductions on charitable donations in China.

PKF adheres to a "people-centered" approach in supporting the development of the public health service system. It assists the government in enhancing the capacity and quality of public health services, strengthening the public health responsibilities of grassroots medical institutions, and promoting the improvement of prevention, diagnosis, treatment, and rehabilitation services within the primary healthcare system. The foundation focuses particularly on integrated healthcare and disease prevention initiatives, provides special funding for research on innovative technologies and their clinical application, and contributes to the advancement of public health, collectively striving toward the vision of a Healthy China.

PKF has assembled a professional team comprising clinical doctors, academic institutions, research organizations, enterprises, and nonprofit entities. With the support of government agencies, experts, scholars, entrepreneurs, and other partners, the foundation has launched a science education center grounded in health prevention and driven by social participation.

PKF has supported the scientific research and innovative applications of the Guangdong Clinical Research Center for Immune Diseases, providing concrete and effective data to facilitate the translation of research outcomes into clinical practice. It also assists the government in organizing health promotion campaigns and has actively promoted and implemented chronic disease prevention and control programs.

In addition, PKF has established a volunteer service team consisting of renowned clinical doctors. This dedicated team regularly conducts and participates in public health lectures and free medical consultation activities. By promoting the application of advanced medical technologies in clinical settings, the foundation remains committed to innovation and cutting-edge practices, utilizing scientific and technological achievements to benefit patients and contribute to the realization of a Healthy China.

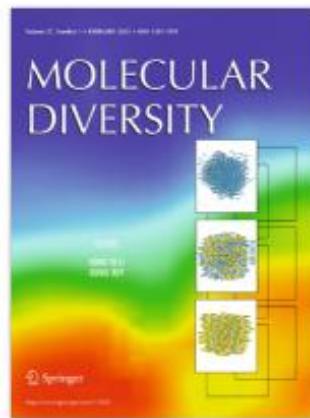


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