# Hydrodealkenylative C(Sp3)–C(Sp2) Bond Scission

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## SUMMARY

UCLA researchers in the Department of Chemistry and Biochemistry have developed a new chemical reaction that combines ozone, an iron salt, and a hydrogen atom donor to enable hydrodealkenylative cleavage of $C(sp^3)$–$C(sp^2)$ bonds in a widely applicable manner.

## BACKGROUND

The commercial accessibility of complex molecules very often relies on starting material cost. There is a limit to the natural products, drugs and agrochemicals available for research and commercialization due to the complexity and cost of synthesizing chiral molecules. Traditionally, the assembly of complex molecules from simple precursors, is accompanied, more often than not, by the need to install carbon centers with precisely defined stereochemical arrangements. Despite the bevy of methods available to accomplish such goals, sometimes it can be more efficient and cost-effective to reorganize starting materials already containing the required complexity and/or stereochemistry into the desired molecular structures. Such, deconstructive strategies can provide access to challenging, or otherwise inaccessible, molecular structures. While there are some examples of $C(sp^2)$–$C(sp^2)$ bond scissions and $C(sp^3)$–$C(sp^3)$ bond fragmentations, general methods for the functionalization of $C(sp^3)$–$C(sp^2)$ bonds remain elusive. Given the profuse number of organic molecules containing these linkages, activation of such bonds in a controllable manner would be extremely useful.

## INNOVATION

UCLA researchers targeted the less common deconstructive strategy toward complexity—particularly one involving C–C bond scission. The hydrodealkenylative cleavage of $C(sp^3)$– $C(sp^2)$ bonds, performed using oxygen, an iron salt, and a hydrogen atom donor. These reactions are simple to operate and reach completion within 30 minutes, delivering their products in high yields—even on decagram scales. Researchers have used this transformation to produce desirable synthetic intermediates and applied it in the total syntheses of complex molecules. With broad substrate scope and high functional group compatibility, this methodological advance lays new paths for the syntheses of organic molecules with utility in chemistry, biology, and medicine.

## APPLICATIONS

- Cost-effective synthesis of chiral building blocks
- Medicinal chemistry methodology

## ADVANTAGES

- Mild conditions
- High yielding
- Scalable method
- Broad substrate scope
- High functional group compatibility

## STATE OF DEVELOPMENT

The developed methodology has been applied in the synthesis of desirable synthetic intermediates in high yields and up to decagram scale.

Expensive chiral building blocks have been prepared from up to $10^4$-fold cheaper starting materials.

## PATENT STATUS

### CONTACT

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### INVENTORS

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### OTHER INFORMATION

KEYWORDS

bond fragmentation, C(sp3)– C(sp2) bonds, C-C bond scission, organic synthesis, agrochemicals, drugs, hydrodealkenylation

CATEGORIZED AS

- **Materials & Chemicals**
  - Agricultural
  - Biological
  - Chemicals
- **Medical**
  - Research Tools
- **Research Tools**
  - Reagents
- **Agriculture & Animal Science**
  - Chemicals

RELATED CASES

2019-603-0

| Country | Type | Number | Dated | Case |
|---|---|---|---|---|
| United States Of America | Issued Patent | 12,122,730 | 10/22/2024 | 2019-603 |
| European Patent Office | Published Application | 3944739 | 02/02/2022 | 2019-603 |

## RELATED MATERIALS

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- Smaligo, A. J.; Swain, M.; Quintana, J. C.; Tan, M. F.; Kim, D. A.; Kwon, O. “Hydrodealkenylative C(sp3)-C(sp2) bond fragmentation” Science, 2019, 364, 681–685.

## ADDITIONAL TECHNOLOGIES BY THESE INVENTORS

- Novel Non-Peptidomimetic Prenyltransferase Inhibitors
- Small Molecule Agonists of VDAC2 to Treat Cardiac Arrhythmias and Heart Failure
- Compound Library Made Through Phosphine-Catalyzed Annulation/Tebbe/Diels-Alder Reaction



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