

Chemists create new pathway to potential medicines

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Dartmouth researchers have discovered a new chemical reaction that has the potential to facilitate the search for pharmaceutical drugs.

The findings appear in the *Journal of the American Chemical Society*.

Organic synthesis is a scientific discipline central to the drug discovery process that is focused on building new carbon-based [molecules](#) that can affect biology—for example, targeting and destroying cancer cells. In the study, the authors describe a new chemical reaction that converts simple starting materials into architecturally complex molecules (a collection of atoms bonded to one another) called "decalins" in a single step. Decalins are carbon-based compounds containing two hexagon rings.

"The findings are noteworthy not only because this chemical reaction simplifies the laboratory preparation of such species, but also because our study reveals a unique mode of reactivity associated with metal-carbon bonds that are embedded in complex carbon-based structures. General species of the type studied here have previously been thought to be fleeting intermediates whose reactivity was difficult to control," says co-author Glenn Micalizio, a professor of chemistry. "An important part of this paper demonstrates our ability to reveal new reactivity patterns of these species, prompting them to engage in highly selective chemical transformations."

The findings, which are the latest to emerge from Micalizio's research

focusing on developing a class of [chemical reactivity](#) called "metallacycle-mediated cross-coupling," stand as among the most complex examples of this chemistry ever described. The term "metallacycle" refers to atoms bonded in a ring, with one of the atoms being a metal. The researchers have been aiming to control the assembly of organic structures that stepwise "encapsulate" a reactive metal center, followed by selective extrusion of the metal from the resulting organic structure. In the new study, the metal plays a central role in joining two molecules through a process that forges three carbon-carbon bonds in a highly selective fashion.

"This latest finding provides a concise and direct synthesis pathway that, due to the structure of the products delivered, will likely be quite valuable for the discovery and development of therapeutic agents," says Micalizio, whose work focuses on the design of organic chemical reaction methods and strategies to improve medicine and human health.

More information: Synthesis of Highly Functionalized Decalins via Metallacycle-Mediated Cross-Coupling, *J. Am. Chem. Soc.*, Just Accepted Manuscript. [DOI: 10.1021/jacs.5b02107](https://doi.org/10.1021/jacs.5b02107)

Provided by Dartmouth College

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