

Breakthrough in molecular control: New bioinspired double helix with switchable chirality

August 8 2024





The synthesized double-helical monometallofoldamers exhibiting controllable chirality switching can lead to the development of novel artificial supramolecular systems for molecular information processing. Credit: Hidetoshi Kawai from Tokyo University of Science



The deoxyribonucleic acid or DNA, the molecular system that carries the genetic information of living organisms, can transcribe and amplify information using its two helical strands. Creating such artificial molecular systems that match or surpass DNA in functionality is of great interest to scientists. Double-helical foldamers are one such molecular system.

Helical foldamers are a class of artificial molecules that fold into welldefined helical structures like helices found in proteins and nucleic acids. They have garnered considerable attention as stimuli-responsive switchable molecules, tuneable chiral materials, and cooperative supramolecular systems due to their chiral and conformational switching properties.

Double-helical foldamers exhibit not only even stronger chiral properties but also <u>unique properties</u>, such as the transcription of chiral information from one chiral strand to another without chiral properties, enabling potential applications in higher-order structural control related to replication, like nucleic acids.

However, the artificial control of the chiral switching properties of such artificial molecules remains challenging due to the difficulty in balancing the dynamic properties required for switching and stability. Although various helical molecules have been developed in the past, reversal of twist direction in double-helix molecules and supramolecules has rarely been reported.

In a breakthrough, a team of researchers from Tokyo University of Science, Japan, led by Professor Hidetoshi Kawai from the Department of Chemistry, Faculty of Science, and including Mr. Kotaro Matsumura from the Department of Chemistry, developed a novel mechanical motif, called double-helical monometallofoldamers with controllable chiral switching.



Prof. Kawai explains, "In this research, we succeeded in synthesizing a double helical mononuclear complex bridged with a single metal cation in the center of the helices to balance both stability and dynamic properties. These structures can undergo inversion switching by changing the left and right winding directions of both helix strands using different solvents."

Their study was published in the *Journal of the American Chemical Society* on July 19, 2024.



The synthesized double-helical monometallofoldamers feature a metal cation in the center bridging the two helical strands, offering both controllable helicity switching and chiral transfer and amplification. Credit: Hidetoshi Kawai from Tokyo University of Science

The researchers synthesized the double-helical monometallofoldamers from two bipyridine-type strands with L-shaped units, which after forming a complex with a zinc cation formed double-helical structures. X-ray crystallography revealed the double-helical structures with a metal cation in their center.

The researchers investigated the switchability of monometallofoldamers



in response to external stimuli and found that helix terminals of the double-helical form can unfold in solutions, resulting in the open form, favored at high temperatures, and refold to the double-helical form, favored at low temperatures.

Interestingly, the helicity of the double-helical monometallofoldamer with chiral chains can be controlled in response to achiral solvents. For example, in non-polar solvents (toluene, hexane, Et₂O), it becomes lefthanded or M-form, and in Lewis basic solvents (acetone, DMSO), it becomes right-handed or the P-form. The conformation of chiral chains introduced into the helix strands was found to be important for this M/P switching.

Furthermore, they found that when a helix strand with chiral chains is mixed with a strand without chiral chains, the winding direction of the helix is transmitted and amplified to the achiral strand without chiral chains, with the helicity inversion ability maintained.

Emphasizing the significance of this new molecule, Mr. Matsumura says, "Our synthesized double-helical monometallofoldamers has the potential to be applied to new switching chiral materials that output diverse chiral properties by small inputs and can be used to develop chiral sensors.

"In addition, we expect that this novel molecular structure will lead to facilitate the genesis of deracemized and organized supramolecular systems as those found in nature by transmitting and amplifying their superior chiral properties."

Overall, this study marks a significant step towards realizing artificial controllable double-helical structures, paving the way for novel high-order molecular systems and molecular information processing.

More information: Kotaro Matsumura et al, M/P Helicity Switching



and Chiral Amplification in Double-Helical Monometallofoldamers, Journal of the American Chemical Society (2024). DOI: <u>10.1021/jacs.4c06560</u>

Provided by Tokyo University of Science

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