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HERMES, THE FIRST COMMUNICATION SYSTEM FOR MOLECULES

It is the first artificial system in which remote parts of a molecule communicate by a dynamic mechanism. Nature uses an analogue strategy in the cellular respiration.

EMBARGO - 18 DECEMBER 21:00 CET

Bologna – The unprecedented case of two different remote parts of a synthetic molecule that can dynamically exchange chemical information is described. This strategy is employed to change in a controlled manner the acidity of a molecule that becomes 10 million times less acidic: the biggest change ever obtained with an artificial molecule. In our body the process that converts nutrients in energy exploits a similar mechanism, which is still partly unknown and was never mimicked before.

As reported today in the prestigious journal *PNAS*, the system – nicknamed *Hermes* – was designed, synthesized and operated by a research team based at the University of Bologna and National Research Council of Italy (CNR), led by professors Alberto Credi and Marco Lucarini.

Hermes

The key component of this communication system is a rotaxane, constituted by a ring-like molecule surrounding a thread-like molecule. The ring is free to shuttle along the thread, but it cannot escape because two "stoppers" prevent its dethreading. It is thanks to this shuttling ability that the ring enables the communication between the two extremities. One of these extremities is capable of receiving electric signals, whereas the other one is responsible for the acid/base properties. When an electron is caught by the first site, the ring transfers the information to the other extremity, causing a change of the acidity of the molecule. Therefore the ring acts as a messenger, from which the nickname *Hermes* (the messenger of the Greek Gods) derived. The absolute novelty of *Hermes* is that it can provide communication between two distant regions of a molecule that would otherwise be isolated in a rapid, efficient and selective manner. It represents an incredibly challenging task that Nature performs with highly sophisticated chemical structures. *Hermes* achieves the same result in a system of just a few atoms, easy to synthesize with common synthetic techniques. The rotaxane is one nanometer (a billionth of a meter) long.

An inexplicable experiment

Very similar systems were synthesized and investigated at the end of the 1990s in the area of molecular machines (a field awarded with the Nobel Prize in Chemistry last year), but nobody ever realized such a unique behavior. The discovery happened thanks to a surprising and initially inexplicable experiment: the only possibility to justify the experimental observations was that the molecule was able to put the two distal extremities in communication. "During the experiments I realized that the behavior of the rotaxane radically changed in the presence of different bases" – tells Giulio Ragazzon, the young researcher who participated in the work – "Thanks to the collaboration with the group of Prof. Lucarini, which studies the behavior of unpaired electrons with magnetic resonance techniques, it was possible to confirm our hypothesis, directly observing the ring position along the thread when the molecule receives an electron".

Relevance and future developments

Hermes deals with two fundamental subjects for molecular systems: long range communication and the coupling of electrical and chemical signals. The operation of most enzymes, natural molecules at the basis of life, relies on the former subject. The latter one lies at the foundation of key biological processes like photosynthesis and respiration, as well as of technological areas like fuel cells, sensors and catalysis. For this reason the discovery may have an impact well beyond the chemistry domain; indeed, the study is published in *PNAS* (*Proceedings of the National Academy of Sciences*), an important journal which covers all areas of Science, and not in a specialized chemistry journal as it usually happens.

With *Hermes* the researchers convert an electric signal into an acidity change; the same strategy, however, may be applied to process light signals or to release at will other molecules. Therefore this work could be relevant for the fields of energy conversion and drug delivery.

The project

Hermes is the result of a study in the framework of the activities of the ERC-funded project "LEAPS-Light effected autonomous molecular pumps", led by Prof. Alberto Credi, and realized at the Center for Light Activated Nanostructures (CLAN). CLAN is a joint research laboratory set up by the University of Bologna and the CNR, and it operates in the Institute for Organic Synthesis and Photoreactivity (ISOF) of the CNR Bologna Research Area. The CLAN mission is the development of nanoscale molecular systems and materials able to perform actions activated by light or related stimuli. This study is the result of collaboration between CLAN and the group of Chemistry of Free Radicals at the Chemistry Department "Ciamician" of the University of Bologna. The group of Prof. Credi, alumnus of Prof. Vincenzo Balzani, already attracted the media attention for fundamental contributions in the field of molecular machines, awarded with the Nobel Prize in Chemistry last year. The first molecular elevator (*Science*, 2004) and the first light-driven autonomous molecular pump (*Nature Nanotechnology*, 2015) were studied in this group.

The fundamental concept at the basis of this research is the mimicking in artificial systems of what Nature does to form structures, obtain mechanical movements and communicate using proteins and enzymes. In this specific case the focus is on the ability to communicate and convert a signal. In performing these studies, chemists operate like engineers and architects, however manipulating systems a billion times smaller, since their building blocks are molecules. The realization of artificial machines and motors of nanometer size is of great interest for the growth of nanotechnology, that is, a technology that allows the construction of highly miniaturized structures and devices. It is generally considered that nanotechnology will not only lead to lighter, tougher and smarter materials and to smaller and more powerful computer, but also revolutionize medicine and other areas of science and technology.

Reference to the original article

G. Ragazzon, C. Schäfer, P. Franchi, S. Silvi, B. Colasson, M. Lucarini, A. Credi: "Remote electrochemical modulation of pK_a in a rotaxane by co-conformational allostery" *Proc. Natl. Acad. Sci. U.S.A.*, in press.

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Web site of the ERC LEAPS project: https://site.unibo.it/leaps/en

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