66 **Ulla Tørnæs:** Danish science minister Ulla Tørnæs outlines the merits of the social sciences and humanities

168 **Clayton Hamilton:** The WHO's Clayton Hamilton considers the potential of e-health and its impact in Europe

242 **Jeffrey D Sachs:** PEN speaks to Professor Jeffrey Sachs on sustainable agriculture, climate change and public health

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VICENTE MARTÍ-CENTELLES TELLS PEN ABOUT THE DEVELOPMENT OF A PIONEERING METHOD IN THE EVALUATION OF NITRATE POLLUTION

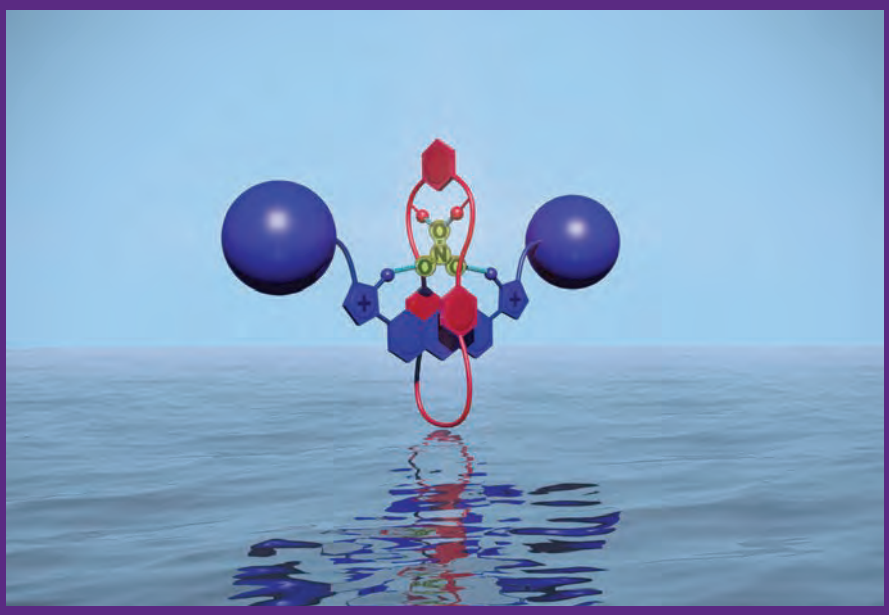
Selective recognition

Among the many different chemical species, the nitrate anion plays a significant role in our lives. By regulating a crucial part of the functions of living organisms, as well as in the environment where some anions can have a harmful effect, it is a pollutant molecule found in fertilisers, the water we drink, and in rivers. As such, anions have inspired chemists to develop efficient anionic receptors. These receptors operate by means of supramolecular interactions to efficiently identify the guest molecule in the recognition cavity. The geometry of these receptors can be as simple as an acyclic receptor, or can involve a more pre-organised macrocyclic or cage receptor and, finally, it can be as sophisticated as a rotaxane or a catenane chemical structure.

Vicente Martí-Centelles

A postdoctoral researcher at the Universitat Jaume I, Castellón de la Plana, Spain, has recently designed an innovative model for the selective recognition of nitrates, which is big news for the prevention of environmental pollution. The idea, developed by Vicente Martí-Centelles during a postdoctoral research stay at the University of Oxford, UK, paves the way for nitrate detection in water samples in different contexts, environmental or medical, to check for high levels and take preventive measures where necessary. It is a groundbreaking model with a purpose-designed chemical structure that homes in on this pollutant.

Speaking to Pan European Networks, Martí-Centelles explained that the blanket use of fertilisers in agriculture and the subsequent abundance of the nitrate anion has caused the alteration of the natural aquatic ecosystem. He said: "Fertilisers are used for improving the growth of plants by providing them with essential nutrients. The increase in the world population has increased the demand for food and, as such, the use of fertilisers in agriculture is essential to accomplish these requirements. Not all the amount of the nutrients offered by these fertilisers can be absorbed by the plants, however, and their excessive use in agriculture causes high levels of nutrients to remain the environment, resulting in the alteration of the natural aquatic ecosystem.



A cartoon representation of the chemical structure of the nitrate anion receptor

"In this regard, the three main macronutrients used in fertilisers are nitrogen, phosphorus and potassium. Nitrogen is widely used as ammonium nitrate (NH_4NO_3) in fertilisers. Therefore the nitrate anion is a pollutant present in the water – high levels of which are harmful to health and the environment. For example, the disease methaemoglobinaemia, also known as 'blue baby syndrome', in infants is caused by exposure to high levels of nitrate; symptoms include an abnormal accumulation of haemoglobin."

Pioneering model

The pioneering model developed by Martí-Centelles includes the design of a chemical structure that allows tailored selective recognition of this pollutant. In this regard, the work shows that it is possible to selectively prepare receptors by carefully designing the geometry of the recognition cavity of the receptor.

Martí-Centelles explained: "In particular, the receptor we have developed provides a strong interaction with the nitrate anion allowing its strong recognition. This has been achieved by a three-dimensional cavity which was specially designed with convergent hydrogen bond donor groups arranged in an appropriate geometry to tightly allocate the nitrate anion (trigonal shape) by hydrogen bonding supramolecular interactions. This therefore allows its selective recognition over other anions such as phosphates (tetrahedral shape)."

Challenge

According to Martí-Centelles, the biggest challenge he encountered when designing the specific chemical structure that will hone in on this pollutant was the relatively poor tendency for it to participate in hydrogen bonds, which are the key supramolecular interactions needed to form a host-guest complex.

"Therefore," he said, "we created a complex rotaxane structure with a tailormade three-dimensional structure which has been a key factor for the efficient and selective recognition of the nitrate anion. The synthesis of this interlocked structure has also been challenging. The rotaxane consists of an isophthalamide-containing macrocycle interlocked in an axle composed of an acridine and two triazolium moieties with a stopper in each side."

The preparation of a resin containing the nitrate selective receptor would allow contaminated water to pass through a filter which would capture the nitrate, resulting in drinkable, nitrate-free water

Future applications

Moving forwards, Martí-Centelles told PEN that the development of appropriate sensors that work by a simple change of colour would provide valuable information about the content of nutrients in the ground, which would enable farmers to choose the appropriate composition and amount of the required fertiliser, a significant step in reducing the amount of fertilisers being used and thus the amount of pollutants leaching into the ground and into the water table.

He continued: "This will also save farmers money, while the detection of nitrate in water samples in different contexts, such as environmental or medical, could also allow necessary preventive measures in the case of high levels of nitrate to be taken in a timely manner."

Other potential applications of nitrate selective receptors include water purification systems similar to those with resins that exist to remove calcium from water. "In this regard," Martí-Centelles said, "the preparation of a resin containing the nitrate selective receptor would allow contaminated water to pass through a filter which would capture the nitrate, resulting in drinkable, nitrate-free water.

"Additionally," he concluded, "in the near future there is a very real possibility that the development of new receptors could allow the selective and efficient recognition of a series of important anions, making possible their detection and even removal from contaminated water."

Given that the population is indeed continuing to grow, and with it the pressures on natural resources, the development of new and innovative tools that will not only help in remediation processes, but also stand to have a significant impact on the behaviours behind some of the harmful processes, are to be welcomed. What is more, at the individual level, that this model was developed by Martí-Centelles at such an early stage in his career is a significant achievement and hints at his potential to impact on this area in the future.

The research was conducted during a postdoctoral stay at the University of Oxford, supervised by Professor Paul D Beer, within the programme of the Generalitat Valenciana VALi+d.

Martí-Centelles' project has been endorsed by a professor of organic chemistry at the UJI, Santiago Luis Lafuente. The various steps were performed at the Universitat Jaume I and the University of Oxford, and by a research stay in Biótica, part of the Scientific, Technologic and Business Park of Jaume I, Espaitec.

After finishing the VALi+d postdoctoral research project funded by Generalitat Valenciana, Martí-Centelles, of La Pobla Tornesa, Spain, joined the School of Chemistry at the University of Edinburgh as a postdoctoral researcher in the Paul Lusby Research Group.

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