Highly charged molecules behave paradoxically

November 24 2017

Chemistry researchers have now discovered how certain small biomolecules attach to one another. The researchers' study also overturns the standard picture – particles with the same electrical charge appear to be drawn together and not vice versa. The results may be important for the development of new drugs.

A number of chemistry researchers from several institutions including Lund University in Sweden, have managed to identify a new mechanism that makes certain charged biomolecules attach to each other. The biomolecules in the present study serve as models for antibacterial peptides, that is, protein-like molecules that fulfil important functions in the body.

"Antibacterial peptides are important for our immune system. If we can figure out how they work, it may be of value in the development of new drugs", says Mikael Lund, chemistry researcher at Lund University.

The present study combines theoretical computer models with experiments. The researchers were very surprised when the data indicated that the small biomolecules were drawn to each other even though they had the same electrical charge. Nevertheless, the results were later confirmed by experiments.

"We were very surprised. These biomolecules have a high electrical charge, and the expectation was therefore that this would make them push each other away", says Mikael Lund.

Instead, the biomolecules in this study demonstrated apparently paradoxical behaviour. And the explanation for this lies at the atomic level. More specifically, it is about how certain atoms bind together at the ends of the molecular chain. The researchers' study can be described as atomic level detective work, which involves mapping the exact structure of all the atoms of the molecule.

The knowledge of how these biomolecules assemble themselves, and how their electrical charge works, is valuable in drug development contexts. The type of biomolecule concerned in this study is considered to be a promising candidate for transporting drugs into the cells of a patient, as the biomolecule has the ability to penetrate the cell casing. However, it is not yet entirely known how the biomolecule gets into the cells.

More information: Giulio Tesei et al. Self-association of a highly charged arginine-rich cell-penetrating peptide, *Proceedings of the National Academy of Sciences* (2017). DOI: 10.1073/pnas.1712078114

Provided by Lund University