Dissecting the mechanism of protein unfolding by SDS

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Aleksei Aksimentiev, a professor of physics at the University of Illinois at Urbana-Champaign, directs the development of the software solutions for computer modeling in biotechnology. Credit: L. Brian Stauffer, University of Illinois at Urbana-Champaign.

Researchers at the University of Illinois at Urbana-Champaign have used

molecular dynamics simulations to understand how sodium dodecyl sulfate causes protein unfolding. SDS is commonly used in labs to separate proteins and determine their molecular weights. However, it is still unclear how SDS influences protein structure.

The paper "Protein unfolding by SDS: the microscopic mechanisms and the properties of the SDS protein assembly" was published in *Nanoscale*.

"Our study uncovered the microscopic details of how these interactions occur in several millionths of a second," said David Winogradoff, a postdoctoral research associate in the Aksimentiev group. "We were physically representing every single atom that was present in the system, and we did it at high temperatures to speed up the process of SDS binding to the protein as well as the unfolding."

The researchers used several supercomputers to create simulations of the SDS-protein interactions. "Using these different supercomputers we were able to complete our studies over the period of a week instead of a year," said Aleksei Aksimentiev, a professor of biological physics and a faculty member of the Beckman Institute for Advanced Science and Technology.

The simulations helped them to understand how SDS causes protein unfolding and to what extent the proteins unfold. "Our studies show that there are areas of proteins that are exposed and areas that are wrapped around SDS, like beads on a string," Aksimentiev said.

Although the simulations provide detailed insights into the interactions, they were too short to probe the balance between the SDS bound to the unfolded proteins and the SDS dissolved in the surrounding solution. "The molecular dynamics method allows us to provide fine molecular details that are inaccessible to other techniques," Winogradoff said.

"SDS has been used for a long time. Our study enables new applications of SDS as an unfolding agent to facilitate protein sequencing," Aksimentiev said. "We want to know how the SDS molecules are arranged on the proteins so that we can drive these chains through a nanopore and read the sequence."

More information: David Winogradoff et al, Protein unfolding by SDS: the microscopic mechanisms and the properties of the SDS-protein assembly, *Nanoscale* (2020). DOI: 10.1039/C9NR09135A

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