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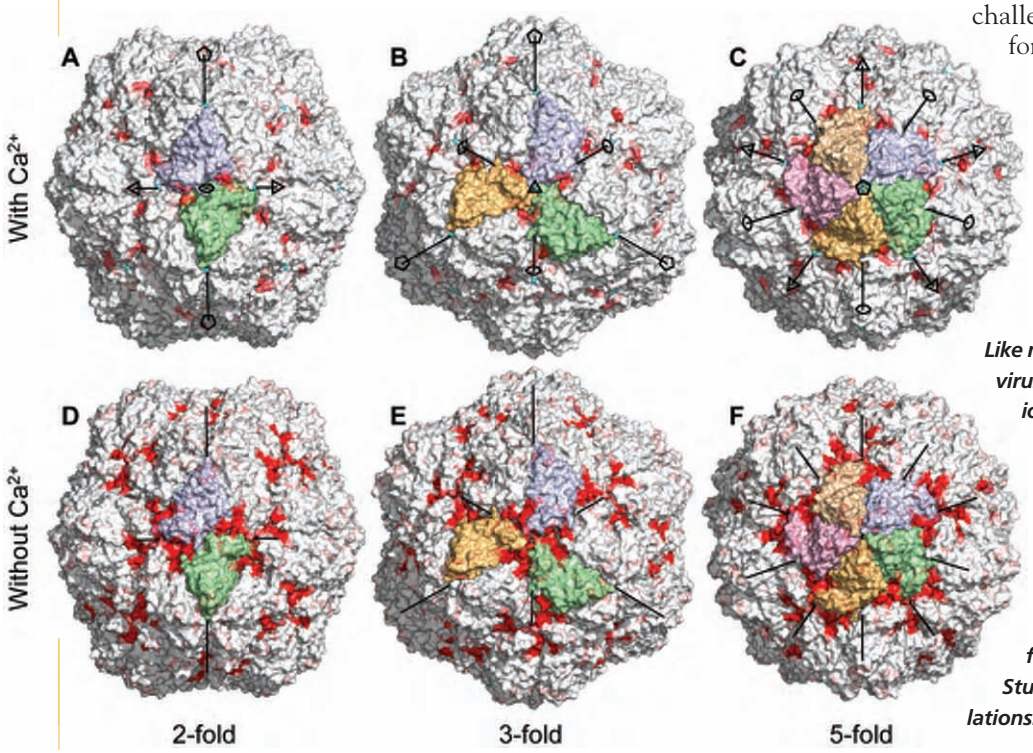
Dissolving a Viral Capsid

After a satellite tobacco necrosis virus particle infects a cell, it sheds the calcium ions that hold the capsid proteins together. Next, the proteins start to repel each other, the capsid swells and water begins to enter. It's a process that hasn't been observed directly, but can now be seen in the longest and biggest virus simulation to date—a one-microsecond long, full-atom, molecular dynamics simulation by **David van der Spoel, PhD**, professor of biology in the department of cell and molecular biology at Uppsala University, Uppsala, Sweden and his graduate student, **Daniel Larsson**.

"We are seeing the beginning of the infection process as the capsid starts to open up," van der Spoel says. Next, his lab plans to add the genome to the simulation—a challenge because there is no structure for the genome.

"Even though it's not a virus that attacks humans, most viruses have a similar protein shell that protects the genome," van der Spoel notes. "If you can tinker with the shell, then you can use it as an additional route to combat viruses." □



Like many virus particles, the satellite tobacco necrosis virus (the smallest known virus) has multiple lines of icosahedral symmetry—two-fold (A,D), three-fold (B,E) and five-fold (C,F). Larsson and van der Spoel's simulation reveals areas where water can permeate the capsid (red) with (A,B,C) and without (D,E,F) bound calcium ions. The nearly symmetrical water-permeable zones suggest where the capsid is least stable and most likely to open up to release the genome. Reprinted from Larsson DSD, et al., Virus Capsid Dissolution Studied by Microsecond Molecular Dynamics Simulations.* PLoS Comput Biol *8(5) (2012).