Key piece of puzzle sheds light on function of ribosomes

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(PhysOrg.com) -- When ribosomes produce protein in all living cells, they do so through a chemical reaction that happens so fast that scientists have been puzzled. Using large quantum mechanical calculations of the reaction center of the ribosome, researchers at Uppsala University in Sweden can now provide the first detailed picture of the reaction. The findings are published in the Web edition of *Proceedings of the National Academy of Sciences*, *PNAS*.

It was previously known how the chemical reaction goes about adding amino acids to the growing protein. Both computer simulations and x-ray crystallographic experiments have identified a hydrogen bonding network that appears to be the main explanation for the high speed of the reaction. What is especially remarkable is the presence of a couple of "trapped" water molecules seem to be the only parts of the ribosome that are in contact with the reacting chemical groups.

Doctoral candidate Göran Wallin and Professor Johan Ĺqvist at the Department of Cell and Molecular Biology at Uppsala University have carried out large-scale calculations of the ribosome reaction center, and this has enabled them to monitor the changes electronic structure during the reaction. With about a thousand quantum mechanical optimizations, they have succeeded in establishing exactly what the highest point of the energy surface looks like, the point that determines the speed of the reaction.

"Our calculations provide a detailed picture of the reaction and show that

the two water molecules play a central role in ribosome catalysis. One of the molecules participates directly in the reaction by 'shuffling' protons around, while the other one helps increase the speed of the reaction," explains Johan Ĺqvist.

The findings surprisingly show that it is just a few components in the ribosome's reaction center that induce the catalytic effect, whereas the surrounding structure mainly holds them in place.

"An exciting question for future research is whether these components are a vestige of a primordial and much simpler ribosome," says Johan Ĺqvist.

More information: www.pnas.org/content/early/201 … /0914192107.abstract

Provided by Uppsala University