How do protein binding sites stay dry in water?

October 21 2011

In a report to be published soon in EPJE[1], researchers from the National University of the South in Bahía Blanca, Argentina studied the condition for model cavity and tunnel structures resembling the binding sites of proteins to stay dry without losing their ability to react, a prerequisite for proteins to establish stable interactions with other proteins in water.

E.P. Schulz and colleagues used models of nanometric-scale hydrophobic cavities and tunnels to understand the influence of geometry on the ability of those structures to stay dry in solution.

The authors studied the filling tendency of cavities and tunnels carved in a system referred to as an alkane-like monolayer, chosen for its hydrophobic properties, to ensure that no factors other than geometrical constraints determine their ability to stay dry.

They determined that the minimum size of hydrophobic cavities and tunnels that can be filled with water is on the order of a nanometer. Below that scale, these structures stay dry because they provide a geometric shield; if a water molecule were to penetrate the cavity it would pay the excessive energy cost of giving up its hydrogen bonds. By comparison, water fills carbon nanotubes that are twice as small (but slightly less hydrophobic) than the alkane monolayer, making them less prone to stay dry.

The authors also showed that the filling of nanometric cavities and tunnels with water is a dynamic process that goes from dry to wet over time. They believe that water molecules inside the cavities or tunnels are arranged in a network of strong cooperative hydrogen bonds. Their disruption by means of thermal fluctuations results in the temporary drying of the holes until new bonds are re-established.

One of the many potential applications is in biophysics, to study water-exclusion sites of proteins, and understand the physical phenomenon linked to the geometry of those sites, underpinning the widespread biological process of protein-protein associations.

More information: Schulz EP et al. (2011) Behavior of water in contact with model hydrophobic cavities, tunnels and carbon nanotubes. *European Physical Journal E.* 34: 114, DOI:10.1140/epje/i2011-11114-8

Provided by Springer