Study of mobile protons in enzymes as revealed by subatomic x-ray and neutron diffraction experiments

Raul E. Cachau
Science Applications International Corporation (SAIC)-Frederick
National Cancer Institute, Frederick (USA)

We will present an analysis of proton dynamics in enzymes base on combined studies of the enzyme human aldose reductase (h-AR, 36 kDa) using single-crystal x-ray data (0.66 √Ö, 100K; 0.80 √Ö, 15K; 1.75 √Ö, 293K), neutron Laue data (2.2 √Ö, 293K), and quantum mechanical modeling. These complementary techniques unveil the internal organization and mobility of the hydrogen bond network that defines the properties of the catalytic engine, explaining how this promiscuous enzyme overcomes the simultaneous requirements of efficiency and promiscuity offering a general mechanistic view for this class of enzymes.