Mechanistic view of biological function

A powerful tool for deciphering the underlying function based on dynamics of complex biomolecular systems is a combined use of neutron scattering methods and atomistic computer simulations. Using this approach we addressed the elastic properties of DNA that are necessary for this molecule to fold and unzip (**9**). The paper was highlighted in magazine Nature as a research highlight in biophysics. Interpretation of the low-frequency inelastic neutron spectra of fibril DNA by large scale phonon calculations revealed the frequency range of vibrational dynamics associated with the base-pair opening of the DNA molecule. We have also explained the softening of the protein DHFR dynamics upon ligand binding and managed to link this phenomenon with the observed increased value of compressibility of DHFR when complexed with the ligand methotrexate (**10**).

9. L. van Eijck, **F. Merzel**, M.R. Johnson, et al., *Direct Determination of the Base-Pair Force Constant of DNA from the Acoustic Phonon Dispersion of the Double Helix*, Phys. Rev. Lett. **107**, 088102 (2011)

10. E. Balog, D. Perahia, J.C. Smith, **F. Merzel**, *Vibrational Softening of a Protein on Ligand Binding*, J. Phys. Chem. B, **115**, 6811-6817 (2011)