Protein Structures without Crystals

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Many proteins are inherently difficult to crystallize, due to various physical properties, e.g. membrane proteins, due to their large hydrophobic area, or amyloid-forming peptides and proteins due to very strong hydrogen bond networks in combination with hydrophobic interactions. Novel light sources (X-ray free electron lasers) may enable us to obtain structural information from small non-crystalline samples if we are able to gather enough scattering data before radiation damage destroys the sample. On the other end of the spectrum computer simulations of molecular dynamics may be able to predict structures of small proteins based on force fields within the near future. In the current presentation I give an overview of our work in both areas and how they are connected.

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