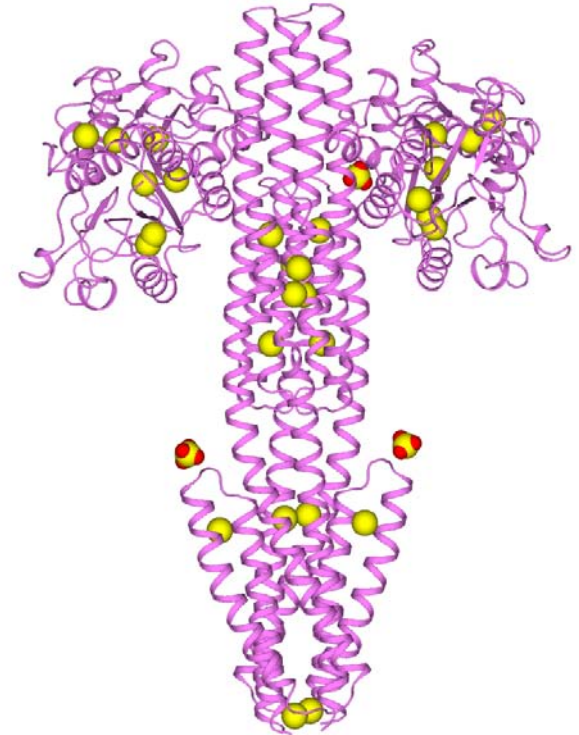


A New Approach for Solving Protein Structures

- Scientists from NSLS, the New York Structural Biology Center and Columbia University discovered a new synchrotron x-ray method to determine protein structures. Their method addresses the “phase problem,” the loss of information describing the x-rays’ relative positions, or “phase.” Without phase, the structure cannot be solved.
- One way to evaluate phase involves adding a heavy atom to the protein crystal, which absorbs and re-emits x-rays with a unique, strong resonance. From the absorption resonant diffraction data, scientists can determine the phase. When x-rays of one wavelength are used, this method is called single-wavelength anomalous diffraction (SAD).
- At NSLS beamline X4A, the group retrieved the phases without adding heavy atoms. They used the off-resonance scattering from the proteins’ own sulfur atoms (which is relatively weak but strong enough to be workable), and combined the SAD signals from multiple crystals.
- Averaging the data from many crystals dramatically reduces the signal-to-noise ratio, making phase determination significantly easier.



A native protein structure as determined using the multiple-crystal SAD method. The complex of four protein chains is shown as a ribbon diagram and is colored violet. The anomalously scattering substructure, containing 28 sulfur atoms and three sulfate ions, is represented as spheres (yellow for sulfur, yellow/red for sulfate).