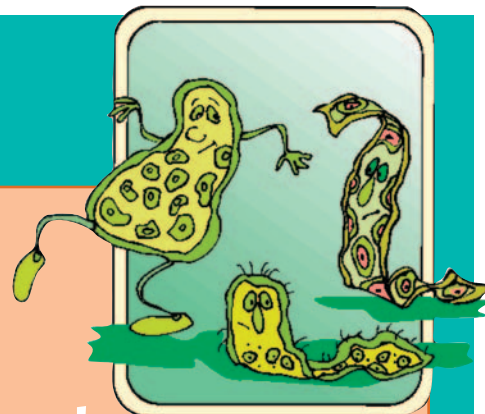


## Apply It.



# The Math behind X-Ray Crystallography...

## Some technical terms used:

Wave equations, Fourier transform, coordinate geometry, statistical analysis

## Uses and Applications:

Scientists use X-ray crystallography to “see” biologically important molecules that are too small for even the best light microscopes. A molecule’s structure can say a lot about how it functions to build your body, give you energy, keep you healthy, and more!

## How it works:

Biologists use recombinant DNA technology to trick cultured cells into making copies of the biological factor they want to study. It might be a protein that helps your muscles move, an enzyme that helps you digest your lunch, or a whole virus, like the one that makes you sick each winter. After they use purification techniques to separate the target molecule from everything else in the cell, biologists place it in solution and wait for the crystal to grow. It’s important that they be patient, check the progress of crystallization often, and keep very detailed notes about what they observe. Finally, when the crystal is large enough, biologists “shoot” it with a beam of X-rays. The X-rays interact with the crystal and are diffracted in different directions. The scattered X-rays are caught as spots on a detector, just like the one in a camera, but much larger.

Each spot represents one diffracted ray of X-ray photons that was produced by the crystalline molecule. Each is assigned coordinates to identify where it is on the detector, a process known as “indexing.” Each spot is also given an intensity value that describes how dark or light it is. Thousands of these spots are collected, and their summation, known as a Fourier transform, allows for calculation of the structure of the molecule. From there, computers are used to conduct iterative statistical analyses to help improve the accuracy of the molecular picture. Experiments are suggested to test what makes the molecule “work.” In the end, a large, detailed, and colorful diagram is available for scientists around the world to study. X-ray crystallography allows us to accurately model molecules down to the positions of every atom, even though no one has ever actually seen them!

## Interesting facts:

Dorothy Crowfoot Hodgkin was the sole winner of the Nobel Prize in Chemistry in 1964 for solving the structure of penicillin by X-ray crystallography. In 1969, after 35 years of work, Hodgkin was able to solve the structure of insulin using x-ray crystallography. In 1996, she was chosen to appear on British stamps celebrating “Women of Achievement.”

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<http://sci.sdsu.edu/sbp/index.html>

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