## Introduction

Have you ever seen those little pictures of a molecule of your prescribed medication? ...or a drawing of DNA showing two strands winding around each other?

Molecules are too small to be seen by normal microscopy.

X-ray crystallography is one of the few techniques that can visualize them and was used to determine the first molecular structures ever known.



Amoxicillin

Schematic picture of DNA

# X-rays & X-ray Crystallography

### How They Work

- X-ray beams are shot through a crystal composed of the material of interest and some of the X-rays diffract (veer off at different angles)
- We calculate how the diffracted X-rays would look, if they could be focused with a lens, to obtain the molecule's structure



This is an X-ray diffraction pattern from a protein crystal. Hundreds of these diffraction patterns are needed to determine a protein structure. The X-ray study can also reveal information about the drugs that bind to the proteins. The protein is chemically bound to a cancer-preventive nutrient. (Journal reference: Crichlow, Fan, Keeler, Hodsdon, and Lolis, Biochemistry. (2012) vol. 51, pag. 7506-7514)

### Where They Work

- X-rays, CAT scans, and Mammograms: Diagnostic imaging and treatment of diseases
- Insulin, Penicillin, and more: Development of medicine
- Airport Security: Scanning luggage and freight cargo
- DNA studies for Crime
  Investigation
- Understanding diseases: Sickle cell anemia, thyroid gland diseases, stomach ulcer, phobias, diabetes, hypertension, and more
- Identifying minerals in oil industry



The United Nations declares 2014 as the official International Year of Crystallography. It commemorates not only the centennial of X-ray diffraction, which allowed the detailed study of crystalline material, but also the 400th anniversary of Kepler's observation in 1611 of the symmetrical form of ice crystals, which began the wider study of the role of symmetry in matter.

Learn more at http://iycr2014.org

#### About IUCr

The International Union of Crystallography is a not-forprofit, scientific organization that aims to:

- promote international cooperation in crystallography
- contribute to all aspects of crystallography
- promote international publication of crystallographic research
- · facilitate standardization of methods, units, nomenclatures and symbols
- form a focus for the relations of crystallography to other sciences

The IUCr fulfils these objectives by publishing primary research journals and the International Tables for Crystallography series of reference volumes, distributing the quarterly IUCr Newsletter in print to nearly 600 libraries and various crystallographic meetings and electronically to more than 12,000 crystallographers and other interested individuals in 102 countries, maintaining the online World Directory of Crystallographers, and organizing the triennial Congress and General Assembly.

Visit www.iucr.org for more information

#### About ACA

The American Crystallographic Association Inc. is also non-profit, scientific organization of over 2,200 members in more than 60 countries, focused in North and South America. The organization aims to:

- promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution
- advance experimental and computational aspects of crystallography and diffraction

Visit www.amercrystalassn.org for more information

Brochure prepared by S. Narasinga Rao and designed by Vanessa Reitz (vjreitz.prosite.com)



# X-rays have in common?

# Crystallography!

- the science devoted to the study of the arrangement of atoms in matter

## We're Celebrating





ACA



Wilhelm Röntgen

1901

Discovery of X-rays



Alpha-helical structure of proteins, nature of

chemical bonds

1954

Linus Pauling

Francis Crick, James Watson & Maurice Wilkins Created DNA model: double-helical structure for biological information storage

1962



**Highlights of the Many Nobel Prizes** 

Herbert Hauptman & Jerome Karle Direct mathematical methods of determining crystallized materials

1985



Clifford Shull & Bertram Brockhouse Electron diffraction and neutron diffraction

1994

See a complete list of winners at iucr.org/people/nobel-prize



2009

Dan Shechtman Discovery of

2011

quasicrystals

1914 1915

Max von Laue Sir William H. & First demonstrated Sir William L. Bragg X-ray diffraction First atomic through crystals crystal structure



1962 1964 John Kendrew & Max Perutz Dorothy Hodgkin Hemoglobin: Transport Structures of protein, which led to cholesterol, the understanding of penicillin, vitamin Sickle Cell Anemia B12, and insulin

1976

William Lipscomb The structure of boranes, illuminating problems of

chemical bonding

Johann Deisenhofer, Robert Huber & Hartmut Michel First membrane protein that is essential to 1988 photosynthesis







Roger Kornberg Studies of the molecular basis of eukaryotic 2006 transcription

Martin Karplus, Michael Levitt & Arieh Warshel Development of sophisticated 2013 computer simulations for complex chemical processes





#### Additional Important Contributors to Crystallography



David Harker **Applied Patterson's** map to identify planes and sections on different axes in nolecular structures



MacKinnon Discoveries concerning channels in cell

2003

Peter Agre



The Patterson atoms





Arthur Patterson Function (equation) gives a map of the vectors between