Geometric Computations in Molecular Biology : Introduction

Note Title 3/20/2007

1. Introductions
2. Where does this course fit
3. A primer on protein geometry & structure
   - atoms & bond geometry
   - hierarchy of protein structure
     - primary - sequence
     - secondary - helix & sheet
     - tertiary - folding

Exercise session: structure matching

Introduction http://www.ti.inf.ethz.ch/ew/courses/GCMB07/index.html

Instructor: Jack Snoeyink, prof of Computer Science at University of North Carolina at Chapell Hill

Assistant: Yves Brise, ETH Zurich

Bias: Computational Geometry & its Application

"Phenomenological" — the real models of molecules that we work with are those that are implemented in a computer.

Goals: Enable crossdisciplinary research & communication.

Sources: on-line modules from Lydia Kavraki, Patrice Koehl, books on reserve by Dill, Leach, others: Petsko & Ringe, Schlick, journal articles

Where does this course fit?

Central dogma of molecular biology [Crick '58]

genomics

DNA → RNA → protein

transcription translation

http://www.johnkyrk.com/DNAtranslation.html

this course

Central dogma of protein

folding proteomics

sequence → structure → function

This course is not: genomics, sequence-based bioinformatics, molecular dynamics, computational physics or chem.

What is a protein?

http://www.johnkyrk.com/aminoacid.html

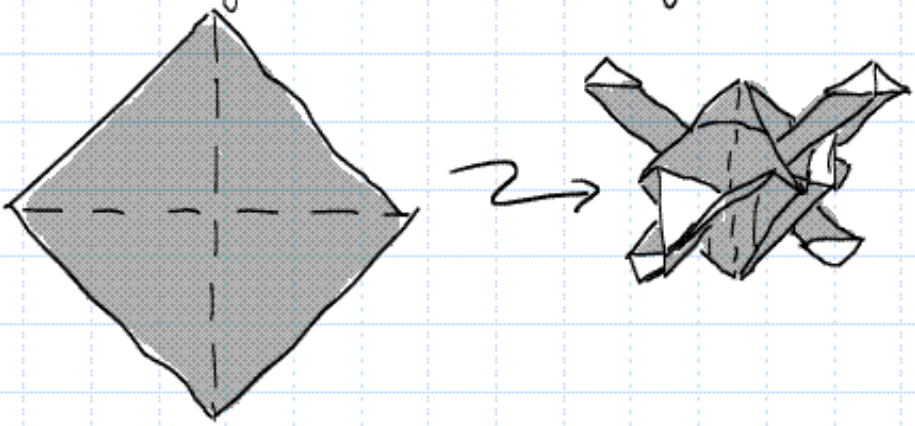
a building block for most of the structures & functions of life.

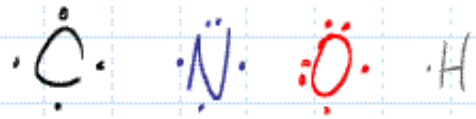
http://publications.nigms.nih.gov/structlife/chapter1.ht

a polymer of (mostly) Carbon, Nitrogen, Oxygen & Hydrogen atoms

Lewis symbols ·C· ·N· :O· ·H

actual 3-d arrangement – momotani's origami module.



Lewis symbols 

actual 3-d arrangement – momotani's origami module.

- Carbon makes four bonds in "tetrahedral conformation" (sp^3 hybridization, for those who've see quantum calculation of molecular orbitals.)

- Nitrogen's three bonds typically arranged as an equilateral triangle in the plane (sp^2 hybridization)

- Oxygen (+ two hydrogens) make water, whose interesting an vitally important geometry can also be shown with momotani's module.

http://www.johnkyrk.com/H2O.html