

Computer Basics

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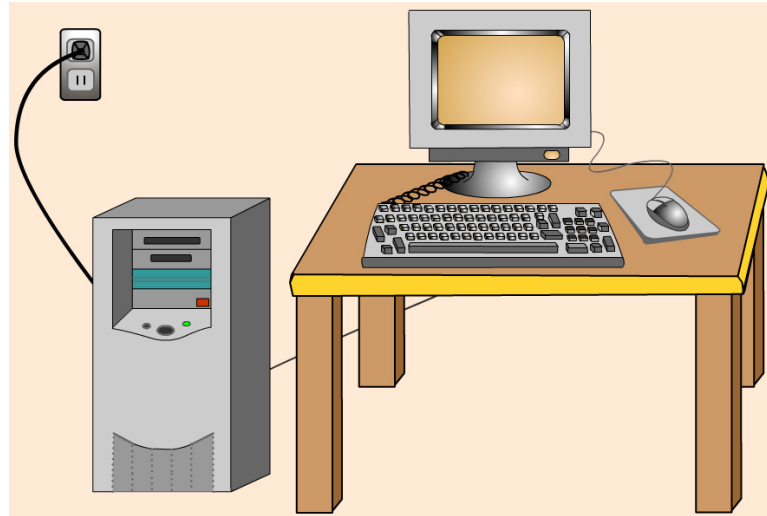


Computer lab policy

- Sign and return them.

What is a computer?

- An programmable device (**hardware**) that can store, retrieve and process data. It is a machine that executes commands (**software**) to perform mathematical and logical operations.



What is a computer?

- Hardware
 - “The stuff that you can build”.
 - CPU
 - Memory (RAM)
 - Storage (hard drive)
 - Monitor, keyboard, mouse, cables, etc.
- Software
 - “The stuff that you can write.”
 - The abstract components of the computer that controls the hardware by executing commands and processing data.
 - Software are stored physical media (such as hard drive).

What is a computer?

- Customize a DELL computer on its website.
- Customize a Gateway computer on its website.

Software

- System software
 - Manages and controls hardware.
 - Examples: operating systems like Windows, Linux, and Mac OSX.
- Application software
 - Programs are supposed to help human to do their jobs.
 - Examples: Microsoft Word, Powerpoint, Excel, Firefox.

Programming Languages

- An artificial language to control the behavior of a machine.
- It has own syntax and semantic rules, just like human languages.
- Different languages for different kind of tasks
 - PERL for text management.
 - R, S-PLUS, SAS, or Matlab for math/statistics.
 - C++, JAVA, C# for software engineering.

Bioinformatics research and open-source software

- Proprietary software
Windows – consumer oriented.
- Open-source software
Linux – research oriented.



Open-source software

- Most bioinformatics software are open-source, including many that are considered to be the best ones.
- The open source definition
 - <http://www.opensource.org/docs/osd>
- Open-source vs. free software

Problems related to computers

- Computer security problems
 - Computer viruses and other malicious software
 - Always back your data.
 - Counter with antivirus software.
 - Spyware.
 - Counter with spyware scanners.
 - Intrusions
 - Counter with firewalls.
- Occupational hazard
 - Carpal tunnel syndrome.
 - Counter with ergonomic solutions.
 - Lower back pain.
 - Proper posture.
 - Dry eyes.
 - Compulsive email checking.

When software goes wrong, it can be a monumental blunder.

LETTERS

edited by Etta Kavanagh

Retraction

WE WISH TO RETRACT OUR RESEARCH ARTICLE "STRUCTURE OF MsbA FROM *E. coli*: A homolog of the multidrug resistance ATP binding cassette (ABC) transporters" and both of our Reports "Structure of the ABC transporter MsbA in complex with ADP•vanadate and lipopolysaccharide" and "X-ray structure of the EmrE multidrug transporter in complex with a substrate" (1–3).

The recently reported structure of Sav1866 (4) indicated that our MsbA structures (1, 2, 5) were incorrect in both the hand of the structure and the topology. Thus, our biological interpretations based on these inverted models for MsbA are invalid.

An in-house data reduction program introduced a change in sign for anomalous differences. This program, which was not part of a conventional data processing package, converted the anomalous pairs (I+ and I–) to (F– and F+), thereby introducing a sign change. As the diffraction data collected for each set of MsbA crystals and for the EmrE crystals were processed with the same program, the structures reported in (1–3, 5, 6) had the wrong hand.

The error in the topology of the original MsbA structure was a consequence of the low resolution of the data as well as breaks in the elec-

tron density for the connecting loop regions. Unfortunately, the use of the multicopy refinement procedure still allowed us to obtain reasonable refinement values for the wrong structures.

The Protein Data Bank (PDB) files 1JSQ, 1PF4, and 1Z2R for MsbA and 1S7B and 2F2M for EmrE have been moved to the archive of obsolete PDB entries. The MsbA and EmrE structures will be recalculated from the original data using the proper sign for the anomalous differences, and the new C α coordinates and structure factors will be deposited.

We very sincerely regret the confusion that these papers have caused and, in particular, subsequent research efforts that were unproductive as a result of our original findings.

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Files

- Test Files and Binary Files are mis-leading names.
 - See “Text File” in Wikipedia.
 - All data in computer are stored in binary codes (0,1)
- Text Files
 - Files contain only characters (often in ASCII format)
 - ASCII, American Standard Code for Information Interchange
 - Commonly used in bioinformatics. For example, sequence files are often stored in FASTA format in text files.
 - Can be edited by text editors
- Binary Files
 - Files contain data that cannot be interpreted as text.
 - For example, *.doc *.exe

View text file under Linux

- View text files:
 - “cat”
 - “more”
 - “less”
 - “head”
 - “tail”
- Edit text files:
 - “nano”

FASTA sequence file

>This is a fasta header

ATGCGTTGCAAAATTTNATG

Test text files under cygwin

- Optional

Test your ID and password

Test some software

- Swiss PDB Viewer
- MEGA 4

