

**ASSIGNMENT**

Course Title**: Introduction to Biology and Chemistry for Computation**

Course Code**:CSE 115**

Submitted By

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**1. Discuss the importance of computer in Biology.**

**Ans:** Computers can be used to simulate cellular growth, the human nervous system, motor control, disease transmission, and disease progression. All of these things are highly useful in biological and medical research. These are only a few of the many ways that computers can be used in life sciences.

Computers are widely applied in exploring the various aspects of biochemistry, another example is in its application in forensic DNA typing. Well appart from general management (publication finding, results keeping, organisation) the computer gets really usefull when computing biochemical systems by means of theoretical chemistry. Semi-empirical methods are now very efficient for the study of proteins and biochemical interactions in general. Biochemistry is also a wide field, going from the study of very small systems to the whole process going on in a living body. All those scalles are covered by modelisation methods and it is now quite common in biochemistry to use these modelisation to either compair the theoretical and the experimental (if the theoretical modelisation devised doesn't fit the experimental results it should mean that the studied system is not fully understood), either study the possibility of undergoing a given experiment. On that matter note that experiments in biochemistry tend to take a lot of time : you don't want to waist time and money on unsatisfying results, hence the use of the computers.

**Medical imaging** is the process of creating a picture of the inside of a human (or animal) body. An MRI scanner is a great example of this: it uses a gigantic magnet and our understanding of quantum mechanical physics to create an image of the inside of the body, including the brain. Computers can be used with MRI scanners, not only to create the image itself through the scanner's sensors, but also to analyze the image. A computer can classify the tissues shown in the image, guide neurosurgery, identify potential problems, measure the thickness of certain tissues, or even decode mental states. A computer can figure out the noun that a human being was thinking of through an MRI scan with high accuracy.

**Genomics** is a part of biology that focuses on understanding genomes, including their structure, function, evolution, and mapping. Genomes are the genetic material of an organism, including the rules that explain how to build the various cells in the body. Computer programs are vital to genomics these days. They can figure out the most likely evolutionary relationships between organisms by analyzing their genetics and can be used for gene and protein sequencing.

**Drug design and discovery** is about finding drugs that will help humans with particular diseases and problems. Computers can be used to figure out candidates far more quickly than any human could. This probably isn't surprising when you consider that humans contain 500,000 proteins, only a small percentage of which are well studied.

**Research-oriented computer programs** include software for the analysis of DNA sequences and of biochemical equilibria and kinetics. The programs act on real data from experiments, e.g. fitting experimental data to theoretically expected functions.

**Biotechnology** is the integration of natural sciences and Biotechnology, the use of living things to make products, is another field in which the biochemistry expert thrives. As well, the food industry attracts biochemists. In studies regarding food, biochemists might work in a number of practical ways, such as product development of foods that are least likely to cause weight gain, or developing foods that are have highly beneficial qualities. Most wineries and breweries use biochemistry frequently to evaluate yeasts and acids used to make alcohol.

Experts in biochemistry might also use their skills to make chemical products like herbicides or pesticides. Many work in small research labs that may study specific things or analyze materials for contaminants. For example testing water and food for live parasitic agents is a valued act of biochemistry.

Essentially, those specializing in biochemistry can use their knowledge in numerous ways in order to continue to improve the earth. They may learn to replace dangerous chemicals with safer ones, or find ways to improve health. They have a choice of fields that include applications in medicine, genetics, food science, biotechnology, and pharmaceuticals. Their work is of extraordinary value as we continue to discover the importance of chemical compounds that are the building blocks of all living things.

**2. Discuss the importance of computer in Chemistry.**

**Ans:** Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into computer programs, to calculate the structures and properties of molecules, groups of molecules, and solids. It is essential because, apart from relatively recent results concerning the hydrogen molecular ion (dihydrogen cation, see references therein for more details), the quantum many-body problem cannot be solved analytically, much less in closed form. While computational results normally complement the information obtained by chemical experiments, it can in some cases predict hitherto unobserved chemical phenomena. It is widely used in the design of new drugs and materials. When I took electronics engineering as my first degree, it was pointed out to me that my seriously bad grade at chemistry might be a problem with the material science part of the degree.

There is a term called Computational Chemistry, that is a branch of chemistry that uses computer simulation to assist in solving chemical problems. It uses methods of theoretical chemistry, incorporated into computer programs, to calculate the structures and properties of molecules, groups of molecules, and solids. It is essential because lot of problems in Chemistry, like the quantum many-body problem, cannot be solved analytically. While computational results normally complement the information obtained by chemical experiments, it can in some cases predict hitherto unobserved chemical phenomena.

A computer would be useful for data analysis, storage of information, for research and for simulation. Some chemical tests and results could be simulated. Computer-Aided Chemical Engineering is being done since 1950s to the present state in which virtually all chemical engineering is computer-aided. Computer-aids are used at every stage from deciding what chemical species to make, through the conceptual design of the processes, the detailed design, the on-line control, optimization and up to the decommissioning. Computer-aids are important for assessing and minimizing environmental impacts and hazards.

Chemists discovered a slick recurrence relation that converged very fast, making Bessel functions about as easy to evaluate as a square root. That technique is now in math libraries everywhere. If you look at the standard math library distributions for C, for example, you’ll find Bessel functions there… and those library routines use the methods that the chemists discovered.

DCS (Distributed Control System)

Petrochemical (oil) and refineries

Pulp and paper mills

Boiler controls and power plant systems

Nuclear power plants

Environmental control systems

Water management systems

Water treatment plants

Sewage treatment plants

Food and food processing

Agrochemical and fertilizer

Metal and mines

Automobile manufacturing

Metallurgical process plants

Pharmaceutical manufacturing

Sugar refining plants

Agriculture applications

The future of computational chemistry is extremely bright. With the rapid pace of increasing computer power and the widespread availability of cutting-edge electronic structure theory packages, researchers in academics and industry can study systems with ever-increasing complexity and make predictions of new materials and phenomena.

On-going developments in quantum Monte Carlo, orbital free density functional theory, and many body perturbation theory (e.g. random phase approximation or renormalized second order perturbation theory) hold the promise of more accurate calculations for realistic systems. Improvements in explicit/implicit solvent models will allow the modeling of reactions and protein folding more accurately in solution. Machine-learning in computational chemistry could aid the development of more accurate force-fields and in finding property descriptors and reaction coordinates.