PRESENTED BY:
BDG LIFESCIENCES

COMPUTER AIDED DRUG DESIGN

10 DAY PROGRAM

EVERY DAY 90 MIN LIVE SESSION

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INTRODUCTION

How are new medicines discovered before they ever enter a laboratory?
Today, many drugs are first designed and tested on computers using advanced simulation tools. This field is called Computer-Aided Drug Designing (CADD) — and it is one of the most exciting intersections of biology, chemistry, physics, and artificial intelligence.
This 10-Day Program in Computer-Aided Drug Designing introduces high school students to the same computational techniques used by pharmaceutical scientists and researchers worldwide. Students will learn how potential drug molecules are:

- Designed
- Tested virtually against disease targets
- Simulated for stability
- Screened for safety and effectiveness

This program is ideal for students interested in:

- Pre-med and biomedical careers
- Biotechnology and pharmaceutical sciences
- Drug discovery research
- Science fair computational projects
- AI in medicine

TRAINERS

The training programs at BDG Lifesciences are conducted by highly experienced resource persons with strong academic and research backgrounds in bioinformatics, computational biology, drug discovery, molecular modeling, genomics, and artificial intelligence applications in life sciences. Our trainers include research professionals and subject-matter experts who have worked on real-world research projects, guided students for science fairs and publications, and delivered advanced workshops internationally. With over a decade of experience mentoring students—from high school to postgraduate levels—our team focuses on building strong conceptual foundations while providing hands-on exposure to industry-standard tools and research methodologies. The teaching approach emphasizes clarity, structured progression, practical application, and personalized guidance to ensure students not only understand the concepts but also gain confidence in applying them independently.

OVERVIEW

This program is structured into three major stages of modern drug discovery:

STAGE 1: MOLECULAR DOCKING (VIRTUAL DRUG BINDING STUDIES)

Students begin with the theoretical foundations of:

- Computer-Aided Drug Designing
- Ligand-based drug design
- Structure-based drug design

They then move into hands-on molecular docking using professional software tools such as:

- AutoDock Tools
- AutoDock Vina
- PyRx
- Chimera
- PyMOL
- Discovery Studio Visualizer

Students will learn to:

- Install and configure scientific software
- Prepare protein and ligand files
- Define active sites (grid box preparation)
- Perform docking simulations
- Conduct multi-ligand docking
- Predict binding interactions
- Generate publication-quality visualizations
- Interpret docking scores and binding energy results

They will also explore active site prediction and analyze docking results using real protein-ligand examples.

STAGE 2: MOLECULAR DYNAMICS SIMULATION (MD SIMULATION)

In this stage, students simulate how proteins and drug molecules behave over time under realistic biological conditions using:

- GROMACS
- VirtualBox environment
- VMD
- QTGrace / Xmgrace

Students perform:

- Protein topology preparation
- Ligand topology preparation
- Complex formation
- Solvation and ionization
- Energy minimization
- Equilibration phases (NPT and NVT)
- Production MD run

They then analyze simulation data using universal structural analysis parameters such as:

- RMSD
- RMSF
- Hydrogen bonds
- Energy profiles
- Radius of gyration

Students will also learn trajectory visualization and even generate simulation movies.
This stage provides exposure to real computational biophysics techniques used in pharmaceutical research.

STAGE 3: ADMET SCREENING & DRUG SAFETY EVALUATION

The final stage focuses on evaluating whether a potential drug molecule is safe and viable using:

- SwissADME
- Protox-III
- SwissTargetPrediction

Students perform:

- ADMET screening (Absorption, Distribution, Metabolism, Excretion, Toxicity)
- Toxicity prediction
- Target prediction

This helps students understand that drug discovery is not just about binding — it is also about safety and biological compatibility.

FEE- $ 226 US

Just in this fee, this program offers hands-on exposure to real pharmaceutical research tools and simulation techniques that professionals use in drug discovery. The value of the skills, research experience, and career clarity students gain far exceeds the cost, making it a powerful early investment in their future in medicine, biotech, or computational science.

NOTE-

- All live sessions will be conducted via Zoom.
- A concise summary of each session will be provided to participants for revision and reinforcement.
- The recording of each session will be shared for future reference and review.
- A Certificate of Completion will be awarded by BDG Lifesciences upon successful completion of the program.

BENEFITS OF THIS COURSE

REAL PHARMACEUTICAL RESEARCH EXPOSURE

Students use authentic computational tools used in biotech and pharma industries.

STRONG INTERDISCIPLINARY FOUNDATION

Students gain understanding in:

- Structural biology
- Biophysics
- Computational chemistry
- Systems biology

This is excellent preparation for pre-med, biotechnology, and biomedical engineering pathways.

SCIENCE FAIR & RESEARCH ADVANTAGE

Students can apply these techniques to:

- Computational drug discovery projects
- Target-protein studies
- Disease-focused in silico research

These are highly impressive at science fairs and competitive research programs.

COLLEGE APPLICATION DIFFERENTIATION

Demonstrates:

- Exposure to advanced biomedical technology
- Initiative beyond high school curriculum
- Experience in real computational research workflows

STUDENTS UNDERSTAND HOW AI AND COMPUTATIONAL TOOLS ARE ACCELERATING MEDICINE DEVELOPMENT GLOBALLY.

THIS 10-DAY PROGRAM SERVES AS A FOUNDATION FOR DEEPER MENTORED RESEARCH PROJECTS, PREPARATION FOR EXTENDED 3–5 MONTH COMPUTATIONAL DRUG DISCOVERY PROGRAMS & A STEPPING STONE TOWARD BIOTECH INTERNSHIPS