

BIOVIA is a software developed by Dassault Systèmes' of France. Its power lies in the integration of the diversity of science, experimental processes and information requirements in the fields of research, development, quality improvement and manufacturing.

### BIOVIA helps:

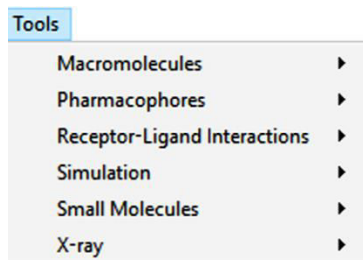
1. to reduce the time of development of a product
2. to reduce the cost involved in research
3. to create new products

### BIOVIA has three modules:

1. **Discovery Studio**: for research on bio-materials, drug design, biosensors etc.
2. **Material Studio**: for research on polymers, nano-technology and new materials
3. **Pipeline Pilot**: for research on machine learning and artificial intelligence

### Screenshots of some menu to show the major fields of application

#### Discovery studio



#### Macromolecules

- Build and Edit Nucleic Acid
- Build and Edit Protein
- Query Online Databases
- Protein Report and Analysis
- Prepare Protein
- Search Sequences by Similarity
- Align Sequences and Structures
- Analyze Sequences
- Analyze Protein Conservation Pattern
- Superimpose Proteins
- Create Homology Models
- Search Side-Chain Rotamers
- Minimize and Refine Protein
- Model Antibody
- Dock and Analyze Protein Complexes
- Design Protein
- Predict Protein Formulation Properties
- Analyze Transmembrane Proteins

#### Pharmacophores

- Create Pharmacophore Automatically
- Create Pharmacophore Manually
- Edit and Cluster Features
- Search, Screen and Profile
- Build Databases
- Compare Pharmacophores
- Customize Pharmacophore Features

#### Receptor-Ligand Interactions

- View Interactions
- Define and Edit Binding Site
- Dock Ligands
- Fragment Based Design
- Lead Optimization

#### Simulation

- Run Simulations
- Run Free Energy Simulations
- Setup Constraints
- Change Forcefield
- Analyze Trajectory

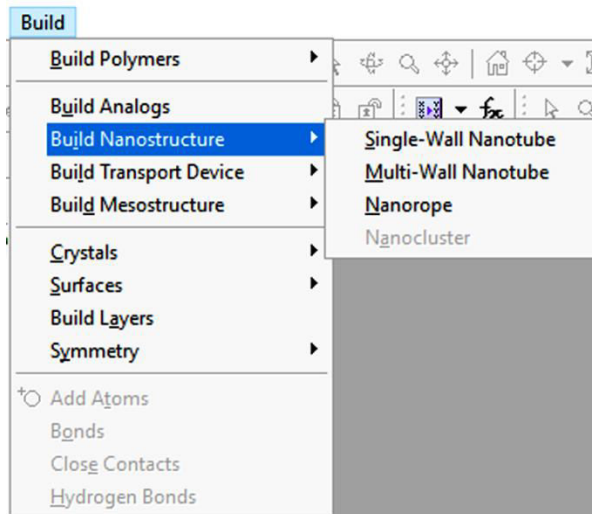
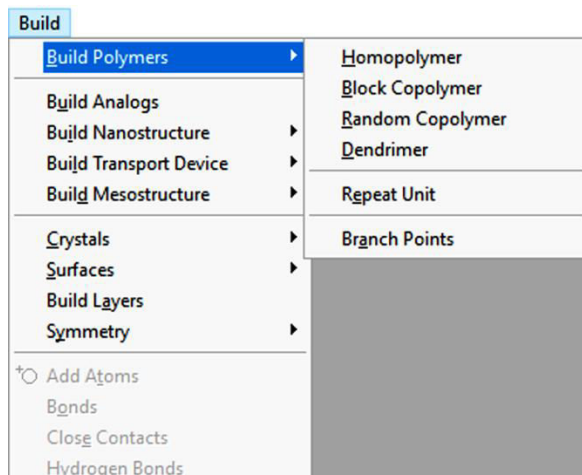
#### Small Molecules

- Sketch Molecules
- Build Fragment
- Prepare or Filter Ligands
- Search Small Molecule Conformations
- Minimize Ligands
- Align Small Molecules
- Calculate Molecular Properties
- Create QSAR Model
- Study SAR
- Design and Analyze Libraries
- Select Subset Libraries
- Molecule Browser

#### X-ray

- Build and Refine X-ray Structure
- Place and Refine X-ray Ligand
- Edit X-ray Structure
- Navigate and Label 3D Structure
- Validate Protein Structure

## Material Studio



| Modules                    |  |
|----------------------------|--|
| <b>A</b> dsorption Locator | ▶ to simulate a substrate loaded with an adsorbate or an adsorbate mixture of a fixed composition              |
| <b>A</b> morphous Cell     | ▶ to construct three-dimensional periodic structures of molecular liquids and polymeric systems                |
| <b>B</b> lends             | ▶ to predict phase diagrams, interaction parameter, mixing energy, free energy etc. of polymer blends          |
| <b>C</b> antera            | ▶ to predict the outcome of a reaction in terms of the composition of the product mixture                      |
| <b>C</b> ASTEP             | ▶ to perform quantum mechanics calculations that explore the properties of crystals and surfaces               |
| <b>C</b> CDC               | ▶ to query Cambridge Structural Database (CSD) instances   |
| <b>C</b> onformers         | ▶ to identify the low energy conformation of a molecule  |
| <b>D</b> FTB+              | ▶ to apply Kohn-Sham energy in Density Functional Theory with respect to charge density fluctuations           |
| <b>D</b> Mol3              | ▶ to model the electronic structure and energetics of molecules, solids, and surfaces                          |
| <b>F</b> orcite            | ▶ a collection of molecular mechanics tools based on high level quantum mechanical calculations                |
| <b>G</b> aussian           | ▶ to predict the structure, energies, thermodynamic properties, NMR and vibrational spectra of molecules       |
| <b>G</b> ULP               | ▶ to perform simulations on 3D periodic solids, gas phase clusters, and isolated defects in bulk materials     |
| <b>K</b> inetix            | ▶ to simulate chemical and physical processes at crystal surfaces using kinetic Monte Carlo methods            |
| <b>M</b> esoDyn            | ▶ to analyze morphologies of materials in the range of 10-100 nm, both quantitatively and qualitatively        |
| <b>M</b> esoSite           | ▶ to do mesoscale simulations with classical molecular mechanics by Martini or Shinoda2007 forcefield          |
| <b>M</b> orphology         | ▶ to study particle shape and effects of altering the growth rate of particular faces on crystal morphology    |
| <b>O</b> NETEP             | ▶ to employ density functional theory in the density matrix formulation for insulators etc.                    |
| <b>P</b> olymorph          | ▶ to predict potential stable or metastable crystal structures directly from the molecular structure           |
| <b>Q</b> MERA              | ▶ to handle data for quantum mechanical (QM) and molecular mechanics (MM) forcefield calculations              |
| <b>R</b> eflex             | ▶ to simulate and analyze X-ray, electron, and neutron diffraction data  |
| <b>S</b> orption           | ▶ to predict adsorption isotherms, binding sites, binding energies, sorption selectivities, solubilities, etc. |
| <b>S</b> ynthia            | ▶ to make rapid estimates of polymer properties using empirical and semi-empirical methods                     |
| <b>V</b> AMP               | ▶ to predict geometries, heats of formation and electrostatic properties of molecules                          |

## *Pipeline Pilot*

