

Computational Chemistry Tools and Workflows Foundation Course

25 – 29 October 2027
Zoom

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Ref: 1864_239260 **Date:** 25 – 29 October 2027 **Location:** Zoom **Fees:** 3000 Euro

Overview

Computational Chemistry Tools and Workflows Foundation Course is a one-week programme for chemistry, materials, pharmaceutical and R&D professionals who leave with a Reproducible Molecular Modelling Workbook. Participants prepare molecular structures, select force-field or quantum approaches, optimize geometries, examine conformations, calculate properties, represent solvation, run introductory molecular dynamics and evaluate results. The course is vendor-neutral and emphasizes assumptions, validation and reproducibility. Agile Leaders Training Center develops practical computational-chemistry literacy.

Who Should Attend

- Chemists beginning computational modelling work
- Materials scientists evaluating molecular structures and properties
- Pharmaceutical researchers supporting molecular investigations
- Laboratory scientists extending experimental work with calculations
- Chemical engineers and R&D professionals reviewing simulation results

Participants should understand basic molecular structure and chemistry. Programming experience is helpful but not required; advanced method development and high-performance computing administration are outside scope.

Departments and Industries

The course supports molecular-level investigation across research and product-development environments.

- Chemical and materials research
- Pharmaceutical and biotechnology development
- Energy, catalysis and process research
- Academic and contract laboratories
- Product development and technical services

Learning Objectives

By the end of this course, participants will be able to:

- Prepare molecular structures and record modelling assumptions
- Distinguish molecular mechanics, quantum chemistry and hybrid approaches
- Set up geometry optimization and conformational investigations
- Calculate and interpret selected molecular properties
- Build an introductory molecular-dynamics workflow
- Validate, document and reproduce computational results

Course Agenda

Day 1: Structures, Models and Reproducible Setup

- Molecular Representation, Protonation and Charge Checklist
- Coordinate, Connectivity and Structure-Quality Review
- Computational Question, Assumption and Boundary Worksheet
- Input, Output, Version and Metadata Record
- Reproducible Molecular Modelling Workbook Structure

Day 2: Molecular Mechanics and Conformational Analysis

- Force-Field Terms, Parameters and Applicability Map
- Energy Minimization and Convergence Review
- Bonded and Non-Bonded Interaction Interpretation
- Conformer Generation and Relative-Energy Table
- Constraint, Restraint and Sensitivity Check

Day 3: Quantum Chemistry and Molecular Properties

- Electronic-Structure Method and Basis-Set Decision Guide
- Geometry Optimization and Frequency Check Workflow
- Charge, Dipole and Orbital Property Review
- Solvation Model and Environment Assumption Record
- Method, Cost and Accuracy Comparison Matrix

Day 4: Molecular Dynamics, Validation and Interpretation

- System Preparation, Force Field and Initial Configuration
- Energy Minimization, Equilibration and Production Sequence
- Time Step, Ensemble and Trajectory-Control Checklist
- Structural, Energetic and Sampling Analysis
- Benchmark, Experimental Comparison and Uncertainty Log

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Day 5: Integrated Computational Chemistry Workflow

- Exercise: Prepare and Quality-Check a Molecular Structure
- Exercise: Compare Conformers and Optimization Evidence
- Exercise: Select a Method for a Molecular Property
- Exercise: Review a Molecular-Dynamics Trajectory
- Capstone Exercise: Complete a Reproducible Molecular Modelling Workbook

Practical Exercises

The course uses suggested activities that connect computational settings with chemically defensible interpretation.

- Suggested activity: document structure preparation and modelling assumptions
- Suggested activity: compare force-field and quantum-method purposes
- Suggested activity: inspect convergence, conformers and calculated properties
- Suggested activity: reproduce a workflow from its input and metadata record

FAQs

Is prior programming experience required?

No. The course explains workflow logic and records first; participants may use graphical or scripted examples according to the available environment.

Which software does the course teach?

The course is vendor-neutral. Examples illustrate transferable setup, validation, visualization and interpretation practices rather than one commercial interface.

How do molecular mechanics and quantum chemistry differ?

Molecular mechanics uses parameterized force fields to describe structures and interactions, while quantum chemistry treats electronic structure for properties and reactions requiring that detail.

What makes a computational result reproducible?

Reproducibility requires saved structures, methods, parameters, software versions, inputs, random seeds where relevant, outputs and a clear analysis procedure.

What practical output is completed?

Participants complete a Reproducible Molecular Modelling Workbook linking the scientific question, model setup, calculations, checks, results and interpretation.

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Conclusion

Participants leave with a disciplined method for moving from a chemical question to a documented computational result. The workbook makes choices, limitations, validation evidence and interpretation visible. It supports collaboration between experimental and computational teams while providing a foundation for more specialized modelling study.