

Computational Chemistry Tools and Workflows Foundation Course

AGILE LEADERS
Training Center

AGILE LEADERS
Training Center

Computational Chemistry Tools and Workflows Foundation Course

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

AGILE LEADERS
Training Center

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.

AGILE LEADERS
Training Center

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.

AGILE LEADERS
Training Center

Training Course Categories

- Agile PM and Project Management Training Courses
- Agribusiness & Food Security Training Courses
- Aviation Management and Operations Training Courses
- Certified Courses By International Bodies
- Communication and Public Relations Training Courses
- Crisis Management and Business Continuity Training Courses
- Data Analytics Training and Data Science Courses
- Digital Government & Public Service Training Courses
- Education and Learning Development Training Courses
- Environment & Sustainability Training Courses
- Facilities and Real Estate Training Courses
- Finance and Accounting Training Courses
- Governance, Risk and Compliance Training Courses
- Healthcare Management Training Courses
- Heritage Conservation and Museum Management Training Courses
- Hospitality and Tourism Training Courses
- Human Resources Training and Development Courses
- IT Security Training & IT Training Courses
- Leadership and Management Training Courses
- Legal Training, Procurement and Contracting Courses
- Maintenance Training and Engineering Training Courses
- Marketing, Customer Relations, and Sales Courses
- NGO, Humanitarian and Development Management Training Courses
- Occupational Health, Safety and Security Training Courses
- Oil & Gas Training and Other Technical Courses
- Personal & Self-Development Training Courses

AGILE LEADERS
Training Center

Training Course Categories

- Quality and Operations Management Training Courses
- Secretarial and Administration Training Courses
- Shipping, Maritime and Ports Training Courses

AGILE LEADERS
Training Center

Training Cities

Abu Dhabi UAE	**Accra** Ghana	**Addis Ababa** Ethiopia
Amman Jordan	**Amsterdam** Netherlands	**Athens** Greece
Baku Azerbaijan	**Bali** Indonesia	**Bangkok** Thailand
Barcelona Spain	**Berlin** Germany	**Cairo** Egypt
Cape town South Africa	**Casablanca** Morocco	**Chicago** USA
Doha Qatar	**Dubai** UAE	**Frankfurt** Germany
Geneva Switzerland	**Istanbul** Turkey	**Jakarta** Indonesia
Johannesburg South Africa	**Kuala Lumpur** Malaysia	**Kuwait** Kuwait
Lagos Nigeria	**Langkawi** Malaysia	**Lisbon** Portugal
London UK	**Madrid** Spain	**Manama** Bahrain
Marbella Spain	**Milan** Italy	**Montreux** Switzerland
Munich Germany	**Muscat** Oman	**Nairobi** Kenya

AGILE LEADERS
Training Center

Training Cities

New York USA	**Nice** France	**Paris** France
Phuket Thailand	**Port Louis** Mauritius	**Porto** Portugal
Prague Czech Republic	**Rome** Italy	**San Diego** USA
Seoul South Korea	**Sharm El-Sheikh** Egypt	**Singapore** Singapore
Tashkent Uzbekistan	**Tbilisi** Georgia	**Tokyo** Japan
Toronto Canada	**Trabzon** Turkey	**Vienna** Austria
Zanzibar Tanzania	**Zoom** Online Training	**Zurich** Switzerland