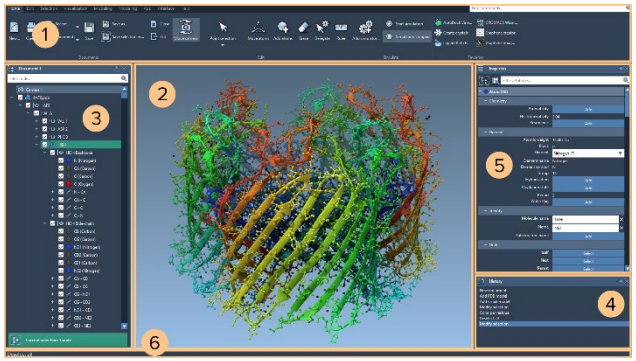
SAMSON Quick Start Guide



SAMSON's Graphical User Interface
(1) Menu bar. (2) Viewport. (3) Document view. (4) History. (5) Inspector. (6) Status bar

Thank you for your interest in SAMSON!

In this Quick Start Guide, you will find all the information you need to get up to speed with SAMSON.

Why did you start SAMSON?

To make it easier for people in nanoscience and nanotechnology to collaborate with each other and save the world.

We mean 'nanoscience and nanotechnology' in the widest possible sense: any science and technology performed at the atomic scale.

What is SAMSON?

SAMSON is an integrated **platform for molecular modeling,** with an open architecture that makes it suitable for drug design, life science, materials, physics, nanoscience, electronics, chemistry, education, and every combination.

SAMSON stands for:
'Software for Adaptive Modeling and Simulation Of Nanosystems'.

What are SAMSON Elements?

SAMSON Elements are **modules for SAMSON**, developed with the **SAMSON Software Development Kit.** SAMSON Elements may contain apps, editors, models, parsers, etc. for a wide variety of tasks. You can customize SAMSON by adding SAMSON Elements from SAMSON Connect. Free SAMSON Elements can be added in one click. Paid SAMSON Elements can be subscribed to and cancelled anytime.

You can also develop your own SAMSON Elements and distribute them on SAMSON Connect, for free or not.

Download SAMSON at https://www.samson-connect.net

How do I load and save molecules and files?

Use the **Home menu.** Opening and saving relies on **importers and exporters** provided in SAMSON Elements. Default importers and exporters support the PDB, xyz, mol2, sam (SAMSON) and samx (SAMSON XML) formats. Add more from SAMSON Connect.

How do I change the view?

Use the **Move camera** editor (active by default). When another editor is active, press and hold **Shift** to move the camera.

How do I use editors?

Editors **react to mouse and keyboard events**. Use editors to select, move, etc. nodes in the viewport. Select the active editor from the **Home menu** or the **Edit menu.** Default editors include:

Move camera (V): left mouse button to rotate the view, right mouse button to translate the view, double click on an atom or a bond to zoom to it, Shift + space to center on the selection, and mouse wheel to zoom in and out.

Point selection (S): left mouse button to select and move nodes, Ctrl / Cmd to add and remove nodes, right mouse button to show the context menu, mouse wheel to change the selection to parents or children.

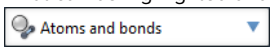
Rectangle selection (R): left mouse button outside selected nodes to draw a rectangle and select nodes, left mouse button on selected nodes to move them, Ctrl / Cmd to add nodes, Alt to remove nodes, right mouse button to show the context menu, mouse wheel to change the selection to parents or children.

Delegate (D): the Delegate editor transmits mouse and keyboard events to nodes, which may then respond in custom ways. Use this editor when nodes may have special functions (for example, drag the control points of the search domain in the AutoDock Vina app to resize it).

You can find more editors on SAMSON Connect.

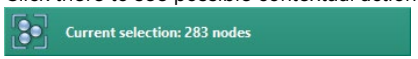
How do I select nodes?

Viewport: use a selection editor to select nodes in the viewport with the mouse. Use the selection filter in the **Selection menu** to control what can be highlighted and selected in the viewport.



Document view: click on nodes in the document view to select them and highlight them in the viewport. Use **Shift** and **Ctrl / Cmd** to perform complex selections. Filter nodes by entering a string or a Node Specification Language expression. Press enter to select.

The bottom part of the document view shows a **selection summary**. Click there to see possible contextual actions.



Find command: use the **Selection / Find... menu (Ctrl / Cmd + F)** to perform selections with the Node Specification Language.

How do I inspect nodes?

Use the **Inspector (Interface / Inspector, Ctrl / Cmd + I)** to view and edit the properties of selected nodes. Use the inspector controls to choose a) whether you inspect the descendants of the selected nodes as well, and b) whether you edit all selected nodes or only the last selected node. Use the filter to see matching attributes only.

How do I customize visualizations?

Add **visual models** to the document with the **Visualization / Add visual model... menu (Ctrl / Cmd + Shift + V)** or the **Add / Visual model... context menu**. Visual models are applied to the current selection (or the whole document if nothing is selected). Default visual models include Licorice, Lines, etc. Add more types of visual models from SAMSON Connect. Right click on nodes (or click on the **selection summary**) and use **Set color** from the context menu to apply color schemes to nodes. Use the **Interface / Preferences menu** for advanced rendering options. Use the checkbox next to each node in the document view to hide / show it in the viewport.

How do I perform interactive simulations?

Select the nodes you want to simulate (or nothing if you want to simulate everything) and use the **Home / Add simulator... menu (Ctrl / Cmd + Shift + M)** or the **Add / Simulator... context menu**. Choose an interaction model and state updater (see below).

Use the **Home menu**, the **Modeling menu**, or press the **Space bar** to start and stop interactive simulation. Use selection editors to move atoms during simulation.

How do I use apps?

Apps **are generic tools with a Graphical User Interface**. One App you can get from SAMSON Connect, for example, is Protein Data Bank Downloader. You can find more Apps on SAMSON Connect.

Activate Apps from the **App menu**.

SAMSON Quick Start Guide

How are SAMSON documents organized?

SAMSON documents are **hierarchies of SAMSON nodes**. A document hierarchy is visible in the **Document view**.

Five node types are used to **organize, view and annotate**:

Document: the root node. Documents may contain folders, cameras, models (structural, visual, dynamical, interaction, property), simulators, labels, conformations, paths, and node groups.

Camera: used to produce three-dimensional views in the viewport. Documents may contain multiple cameras. The viewport reflects the active one.

Folder: used to organize nodes. Folders may contain other folders, cameras, models (structural, visual, dynamical, interaction, property), simulators, labels, conformations, paths, and node groups.

Node group: a node group is a saved selection. Use the **Selection / Create group (G)** to create a group from the current selection. Double click the group in the Document view to restore the saved selection. Right click for more options (add to selection, etc.).

Label: used to annotate nodes. Labels may be created by editors (for example the 'Ruler' editor), apps, etc. You can customize the rendering of labels from the **Interface / Preferences menu**.

Five node types represent the **five categories of models**:

Structural model: used to describe the geometry and topology of molecules. A structural model may only contain structural nodes. Create structural models by importing files with the **Home / Open... menu** (**Ctrl / Cmd + O**) or through editors and apps.

Visual model: used to provide custom visual representations of other nodes. Add visual models to the document with the **Visualization / Add visual model... menu (Ctrl / Cmd + Shift + V)** or the **Add / Visual model... context menu**.

Visual models are applied to the current selection or to the whole document if nothing is selected. Default visual models include Ball-and-stick, Licorice, Lines, etc. You can find more types of visual models on SAMSON Connect.

Dynamical model: used to describe the degrees of freedom in molecules. In SAMSON, dynamical models are **particle systems**: they associate one particle to each simulated atom, and each particle has three degrees of freedom (its x, y and z coordinates). Dynamical models are automatically added to the document when you add a simulator (see below).

Interaction model: used to describe energies and forces inside a dynamical model. Choose interaction models when you add simulators (see below). The default interaction models is the Universal force field. You can find more interaction models on SAMSON Connect.

Property model: used to describe properties outside the other four categories of models. Add property models to the document with the **Simulation / Add property model... menu (Ctrl / Cmd + Shift + P)** or the **Add / Property model... context menu**.

Property models are applied to the current selection or to the whole document if nothing is selected. Property models can be found in SAMSON Elements on SAMSON Connect.

Ten node types are used to **break down structural models into sub-structural components**:

Structural group: used to organize structural nodes. A structural group may contain atoms, backbones, bonds, chain, molecules, pseudo-atoms, residues, segments, side chains and structural groups.

Molecule: a molecule may contain structural groups, chains, segments, residues, atoms, pseudo-atoms, and bonds.

Chain: a chain may contain structural groups, segments, residues, atoms and bonds.

Segment: a segment may contain atoms, bonds, structural groups and residues.

Residue: used to represent an amino acid or a nucleic acid. A residue may contain a backbone and a side chain.

Backbone: used to represent an amino acid backbone or a nucleic acid backbone. A backbone may contain atoms and bonds.

Side chain: used to represent an amino acid side chain or a nucleic acid side chain. A side chain may contain atoms and bonds.

Atom: used to represent atoms (we are pretty sure you guessed). In the document view, atom icons are colored based on atom types.

Pseudo atom: used to represent pseudo atoms (for example for coarse graining).

Bond: used to represent bonds (something tells us you guessed this as well). The two atoms that a bond connects appear as children of the bond node in the document view. Double click these children to go to the actual atoms nodes.

Two node types are used for **simulation**:

Simulator: used to perform interactive or offline simulation. Add simulators to the document with the **Simulation / Add simulator... menu (Ctrl / Cmd + Shift + M)** or the **Add / Simulator... context menu**. Choose the interaction model and the state updater you want to use.

Simulators are applied to the current selection or to the whole document if nothing is selected.

Use the **Simulation menu** or press the **Space bar** to start and stop interactive simulation.

State updater: used to update simulations. State updaters are added to a document through simulators (see above).

Default state updaters include 'Interactive modeling', 'Steepest descent', 'Partitioned Euler', etc. Add more state updaters from SAMSON Connect.

Finally, two node types are used to **save conformations and paths**:

Conformation: used to store positions of atoms and pseudo atoms. Use the **Selection / Store conformation (C)** to create a stored conformation. Double click on the conformation in the document view to restore the saved positions.

Path: used to store positions, velocities, forces, energy and time along a path. Paths may be created by editors, apps, importers, etc. Double click on a path in the document view to start and stop animating it. Use the **Inspector** (**Interface / Inspector, Ctrl / Cmd + I**) for more control.

How do I find commands? How do I mark them as favorites?

Use the **Search box** on the top right part of the **Menu**. From there (and often directly from the menus themselves), you can mark commands, editors and apps as favorites and find them from the **Home menu**, the **Edit menu** and the **App menu.**

How do I learn more?

For documentation, tutorials, forums, etc., visit SAMSON Connect at https://www.samson-connect.net.