1Å SAMSON 2023 R1 Quick Start Guide

SAMSON's Graphical User Interface
(1) Menu, (2) Viewport, (3) Document view, (4) History, (5) Inspector,
(6) Status bar, (7) Assets, (8) Animator

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.

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 design,** 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 Extensions?

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

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

How do I load and save molecules and files?

Use the **Home menu.** Opening and saving relies on **importers and exporters** provided in SAMSON Extensions. Default importers and exporters support the PDB, cif, mmtf, gro, mol2, sdf, sam (SAMSON), samx (SAMSON XML), and other formats. Add more from **SAMSON Connect**.

How do I change the view?

Hold right mouse button to rotate the view, hold mouse wheel (or right mouse button + **Ctrl / Cmd**) to translate it, mouse wheel to zoom in and out, use keyboard arrows (with and without **Ctrl / Cmd**, **Alt**), **Shift + Space** to center on the selection.

Activate the compass in the viewport and use it to easily orient the view.
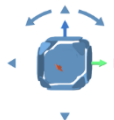
How do I use editors?

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

Select (R): left mouse button to select, left mouse button outside selected nodes to draw a rectangle and select nodes, **Ctrl / Cmd** to add nodes, **Alt** to remove nodes, right mouse button to show the context menu.

Move editors (D, M, K): displace, translate, and rotate selected nodes in global or local coordinates.

Add editor (A): add atoms, fragments, assemble assets to build molecules. See also: Bond editor, Charge editor.

Measure editor (Ctrl / Cmd + M): display distances and angles between atoms, click Enter to add a label.

You can find more editors on **SAMSON Connect**.
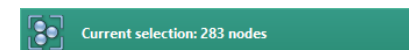
How do I select nodes?

Viewport: use a selection editor to select nodes in the viewport with the mouse, use the selection filter in the top-right corner of the viewport 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.

Current selection: 283 nodes

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

How do I inspect nodes?

Use the **Inspector** (**Interface > Inspector, Ctrl / Cmd + 2**) 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 > Visual model** menu (**Ctrl / Cmd + Shift + V**) or the toolbar 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**. To colorize, click on nodes (or click on the **selection summary**) and use **Material** from the toolbar menu to apply color schemes to nodes or use the **Visualization > Material** menu. 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.

Use default **Visual presets** (**Visualization > Visual model > Presets**) or create your own to visualize molecular systems.

How do I perform interactive simulations?

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

Use the **Home menu** 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**. Some Apps are provided by default with SAMSON. You can find and add more Apps on **SAMSON Connect > Marketplace**.

Open Apps from the **App menu** or from the **Find commands, apps**.

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

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How are SAMSON documents organized?

SAMSON documents are **hierarchies of SAMSON nodes**. A document hierarchy is visible in the **Document view**. Documents may contain folders, files, cameras, models (structural, visual, dynamical, interaction, property), simulators, labels, notes, conformations, paths, and node groups. Several node types are used to **organize, view, present, and annotate** a document:

Camera: used to produce 3D views in the **viewport**. Documents may contain multiple cameras. The **viewport** reflects the active one.

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

File: used to embed files. Embed files or folders with files by importing them in SAMSON via **Home** menu.

Script: a Python script to perform various tasks using the SAMSON Python API. Add a script using the **Edit > Script** menu.

Note: used to annotate documents, folders, results. Add a note using the **Edit > Note** menu. Use the **Inspector** to view and modify notes.

Node group: a node group is a saved selection. Use the **Select > Group** menu **(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 'Measure' editor), apps, etc. Customize the rendering of labels from the **Interface > Preferences** menu.

Presentation: used to create and store a presentation with animations. Use the **Animation** menu to create a presentation and add new animation effects. Use the **Animator** (**Ctrl / Cmd + 7**) to add and modify animations.

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 > File** 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 toolbar menu or the **Visualization > Visual model** menu **(Ctrl / Cmd + Shift + V)**. Visual models are applied to the current selection or to the whole document if nothing is selected. Default visual models include Licorice, Ribbons, etc. You can find more types of visual models on **SAMSON Connect**.

Dynamical model: used to describe the degrees of freedom in molecules. 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 model 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. Property models can be found in SAMSON Extensions on **SAMSON Connect**.

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

(G) 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.

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

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

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

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

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

(SC) 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), including coarse-grained atoms. In the Document view, atom icons are colored based on atom types.

Bond: used to represent bonds. The two atoms that a bond connects can be accessed via the **Inspector**.

Double-click on an atom or a bond to select and zoom on it.

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

Simulator: used to perform interactive or offline simulation. Add simulators to the document with the **Edit > 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 **Edit menu** to start and stop interactive simulation.

State updater: used to update simulations. State updaters are added to the 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 **Home > Store (S)** 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 context menu or the **Inspector** (**Interface > Inspector, Ctrl / Cmd + 2**) for more control.

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

Use the **Find everything** 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 **Favorite menu.**

How do I learn more?

Follow interactive tutorials in SAMSON: **Help > Tutorials** menu.

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