TopSpin

SD File Viewer

User Manual

Version 001

Innovation with Integrity

NMR

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1 Main User Interface Feature

The Multi-Structure Viewer is a viewer with several features to visualize Structure Data (SD) files:

- The possibility of visualizing all structures in SD files.
- Scroll through a large amount of data and zoom into desired one.
- Working with compressed files save disk space (e.g. .zip or .gz files downloaded from PubChem without decompression).

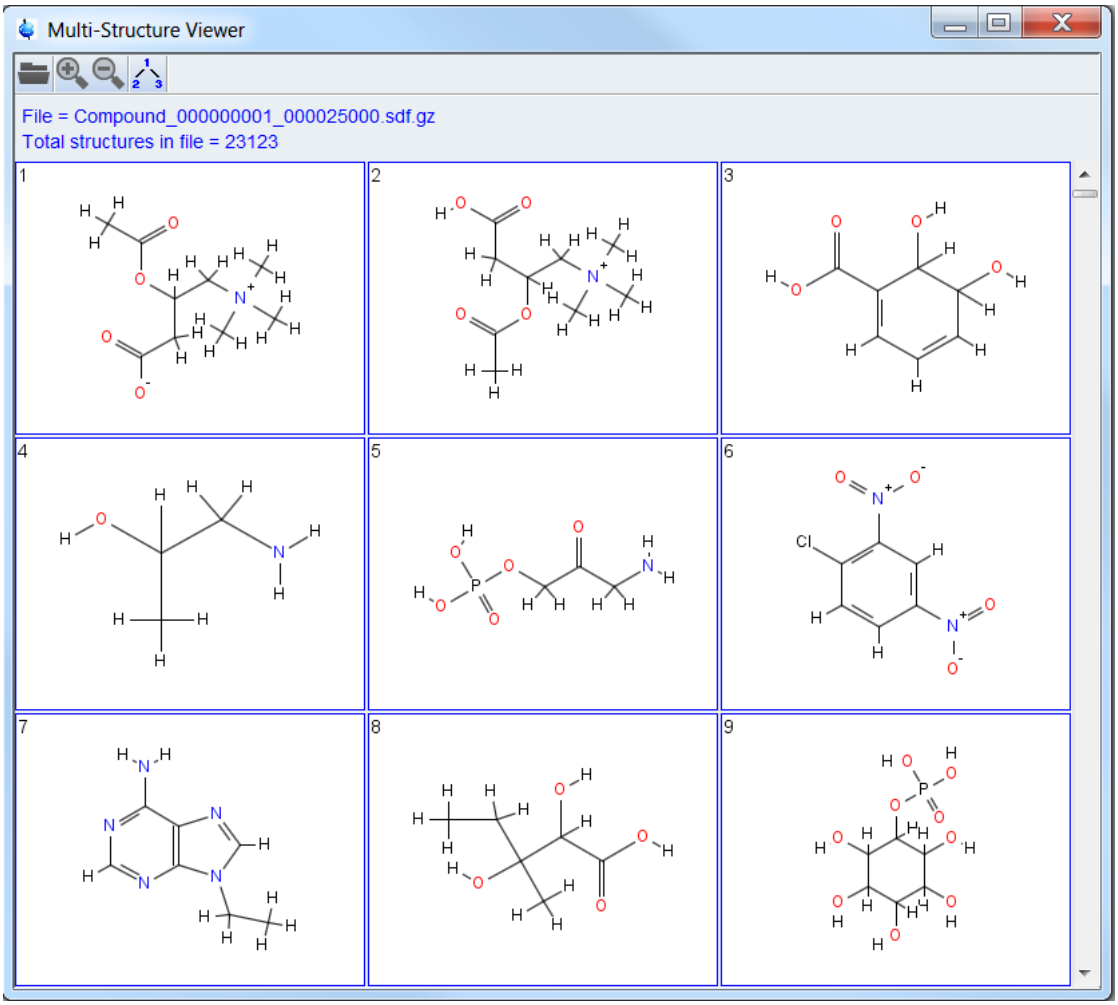

Figure 1.1: Multi-Structure Viewer

The editor provides a simple control with the following buttons:

- - Used to open a SD file.
- - Used to zoom in or zoom out to change the number of structures in the overview.
- - Used to toggle between atom numbers and single atoms.

1.1 Font and Format Conventions

Type of Information	Font	Examples
Shell Command, Commands, "All what you can enter"	Arial bold	Type or enter **fromjdx zg**
Button, Tab, Pane and Menu Names "All what you can click"	Arial bold, initial letters capitalized	Use the **Export To File** button. Click **OK**. Click **Processing**…
Windows, Dialog Windows, Pop-up Windows Names	Arial, initial letters capitalized	The Stacked Plot Edit dialog will be displayed.
Path, File, Dataset and Experiment Names **Data Path Variables** **Table Column Names** **Field Names (within Dialog Windows)**	Arial Italics	*$tshome/exp/stan/nmr/lists* *expno, procno,*
Parameters	Arial in Capital Letters	VCLIST

Program Code
Pulse and AU Program Names
Macros
Functions
Arguments
Variables
	Courier	`go=2`
		`au_zgte`
		`edmac`
		`CalcExpTime()`
		`XAU(prog, arg)`
		`disk2, user2`

AU Macro	Courier in Capital Letters	`REX` `PNO`

Table 1.1: Font and Format Conventions

2 Open Files

The viewer supported the following strcture file types: `.mol`, `.sdf`, `.sdf.gz`, `.sdf.zip`.

Start the editor in the TopSpin menu bar by clicking **Analyse | Structures | 2D Multi-Structure Viewer** or by using the **vstrucs** command.

As the editor opens the desired file has to be selected. Once the editor is open, it is possible to change the file by clicking the **Open**  button.

Open Files

3 Contact

Manufacturer

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