















NMRFAM\_GISSMO\_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0

Thu Aug 9, 13:40

Setting up environment

```
LD_LIBRARY_PATH is :/local/MATLAB/MATLAB_F  
v901//sys/os/glnxa64:  
64
```

Get integral Draw full experimental spectrum Reset integral

Show 2D figure

Water region (PPM): 4.6 5  delete water region

DSS region (PPM): -0.1 0.1  delete DSS region

Num points:  $2^{14}$   Same as exp. data

Line width: 0.3  Same as exp. data

Field strength: 500  Same as exp. data

Lorentzian coeff: 0.8  Gaussian coeff: 0.2

database entries: bmse000001(1,3-Diaminopropane)-Initialvalues Load

ROI region: -1 to 12 get ROI from exp. spectrum

compound\_name

	1	2
1		
2		
3		
4		

Save automatically simulation info

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

GISSMO\_v2 Terminal GISSMO (Guided Ide... Right Ctrl

The screenshot shows the GISSMO software interface running in a Linux desktop environment. The main window title is "GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0". The interface includes a toolbar at the top with "File", "Edit", "View", "Search", "File", "Tools", and "Help" menus. On the left, there's a terminal window showing system environment variables like LD\_LIBRARY\_PATH and a file browser window titled "GISSMO\_v2". The main workspace contains several input fields and buttons: "Get integral", "Draw full experimental spectrum", "Reset integral", "Show 2D figure", "Water region (PPM)" (4.6, 5), "delete water region" checkbox, "DSS region (PPM)" (-0.1, 0.1), "delete DSS region" checkbox, "Num points" (2^14), "Line width" (0.3), "Field strength" (500), "Lorentzian coeff" (0.8), "Gaussian coeff" (0.2), "database entries" (bmse000001(1,3-Diaminopropane)-Initialvalues), and a "Load" button. A large central area is a blank white space. Below it, there's a "ROI region" selector (-1 to 12) and a "get ROI from exp. spectrum" button. At the bottom, there are buttons for "Process", "Optimization", "Group and optimize", "Copy selected cells", "Paste cells", and "Swap two cells". A "simulation info" section is also present. A table titled "compound\_name" is shown with four rows labeled 1 through 4, each having columns for 1 and 2. A circled cursor is over the "Load" button.

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Thu Aug 9, 13:41

Setting up environment

```
LD_LIBRARY_PATH is :/local/MATLAB/MATLAB_F  
v901//sys/os/glnxa64:  
64
```

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Show 2D figure

Water region (PPM): 4.6 5  delete water region

DSS region (PPM): -0.1 0.1  delete DSS region

ROI region: -1 to 12 get ROI from exp. spectrum

database entries:

- bmse000001(1,3-Diaminopropane)-Initialvalues
- bmse000570((S)-(+)2-hydroxy-3-methylbutyricacid)-Initialvalues
- bmse000571(2-hydroxyhexanoicacid)-Initialvalues
- bmse000572(2-hydroxyoctanoicacid)-Initialvalues
- bmse000573(3-hydroxymandelicacid)-Initialvalues
- bmse000574(3-methyl-2-oxopentanoicacid)-Initialvalues
- bmse000575(3-methylglutaricacid)-Initialvalues
- bmse000576(acetosyringone)-Initialvalues
- bmse000577((-)-cotinine)-Initialvalues
- bmse000578(ethylmalonicacid)-Initialvalues
- bmse000579(monoethylmalonate)-Initialvalues
- bmse000580(mono-methylglutarate)-Initialvalues
- bmse000581(3-methyl-2-butenoicacid)-Initialvalues
- bmse000582(4-Hydroxybenzaldehyde)-Initialvalues
- bmse000583(4-Hydroxy-benzoicacid)-Initialvalues
- bmse000584(acetovanillone)-Initialvalues
- bmse000585(dihydroconiferylalcohol)-Initialvalues
- bmse000586(dihydro-sinapylalcohol)-Initialvalues
- bmse000587(ferulicacid)-Initialvalues
- bmse000588(gly-pro)-Initialvalues
- bmse000589(methylsinanate)-Initialvalues

Load

Save automatically

simulation info

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

GISSMO\_v2 Terminal GISSMO (Guided Ideo...)

Right Ctrl

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File Machine View Input Devices Help

Applications Places System

GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0

Thu Aug 9, 13:41

Setting up environment

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LD_LIBRARY_PATH is ./  
/local/MATLAB/MATLAB_F  
v901//sys/os/glnxa64:  
64
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Get integral Draw full experimental spectrum Reset integral

Show 2D figure

Water region (PPM): 4.6 5  delete water region

DSS region (PPM): -0.1 0.1  delete DSS region

Num points:  $2^{14}$   Same as exp. data

Line width: 0.3  Same as exp. data

Field strength: 500  Same as exp. data

Lorentzian coeff: 0.8  Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-initialvalues

ROI region: -1 to 12

compound\_name

	1	2
1		
2		
3		
4		

Save automatically

simulation info

GISSMO\_v2 Terminal GISSMO (Guided Ideo...)

Right Ctrl















































































































