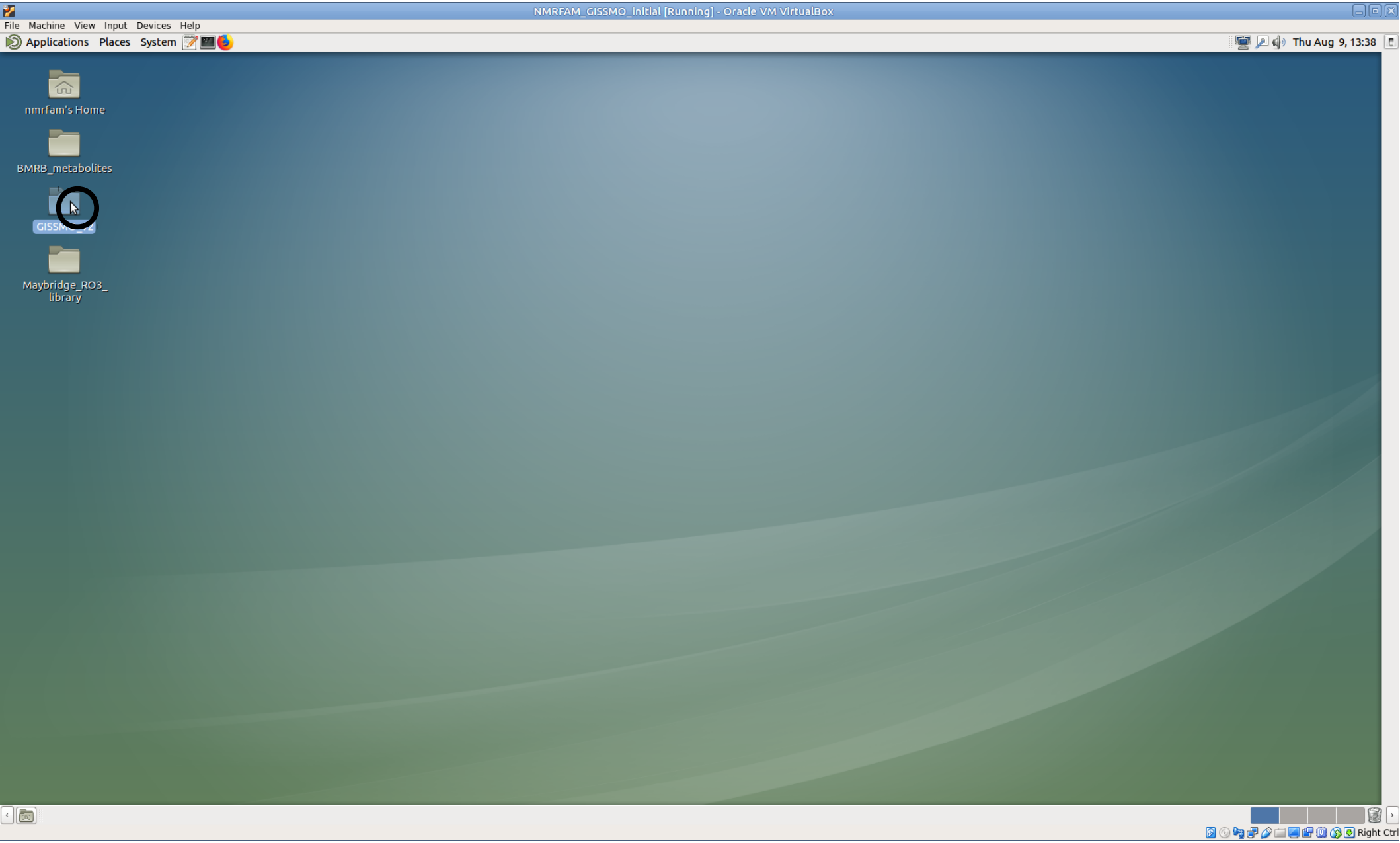
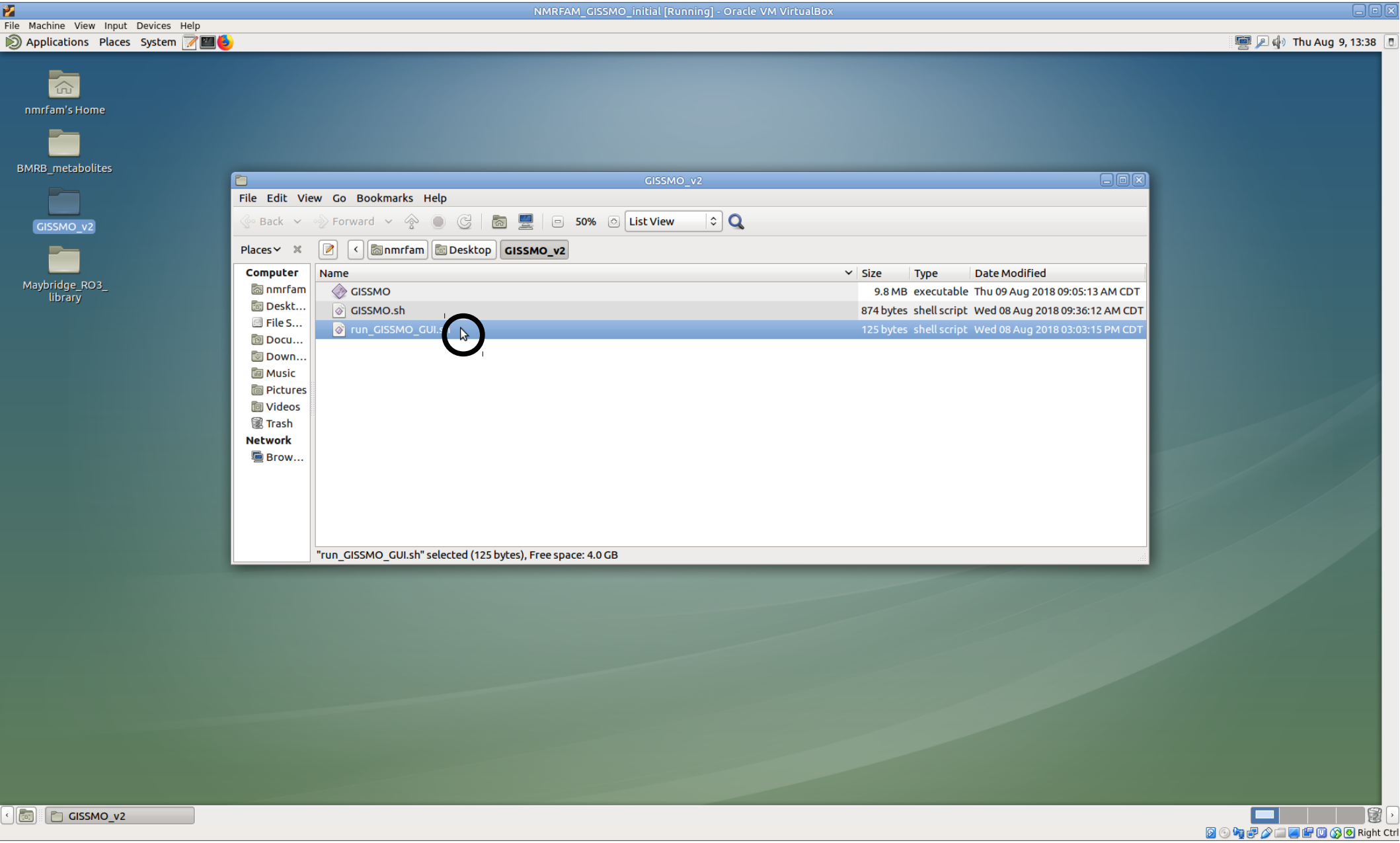
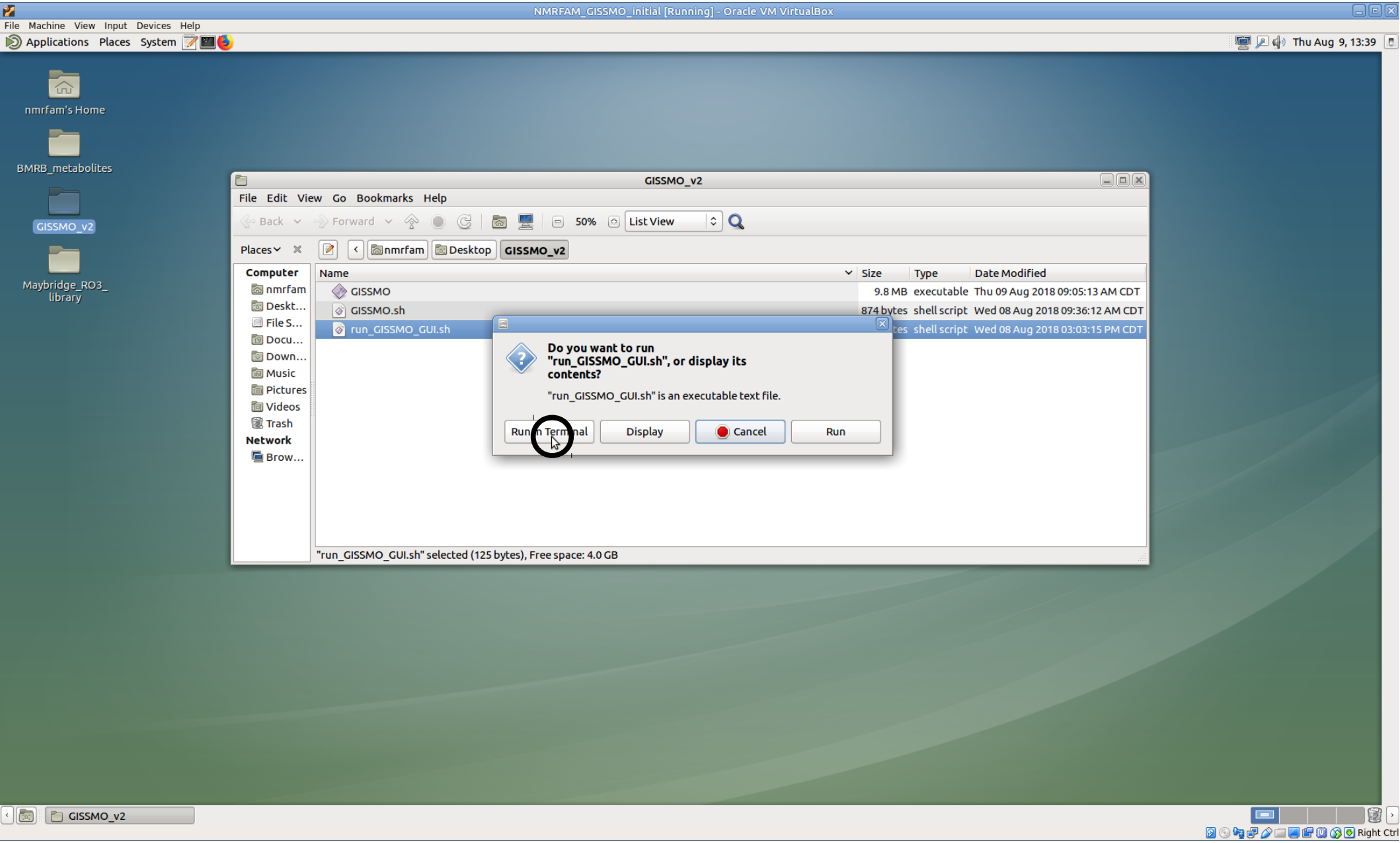
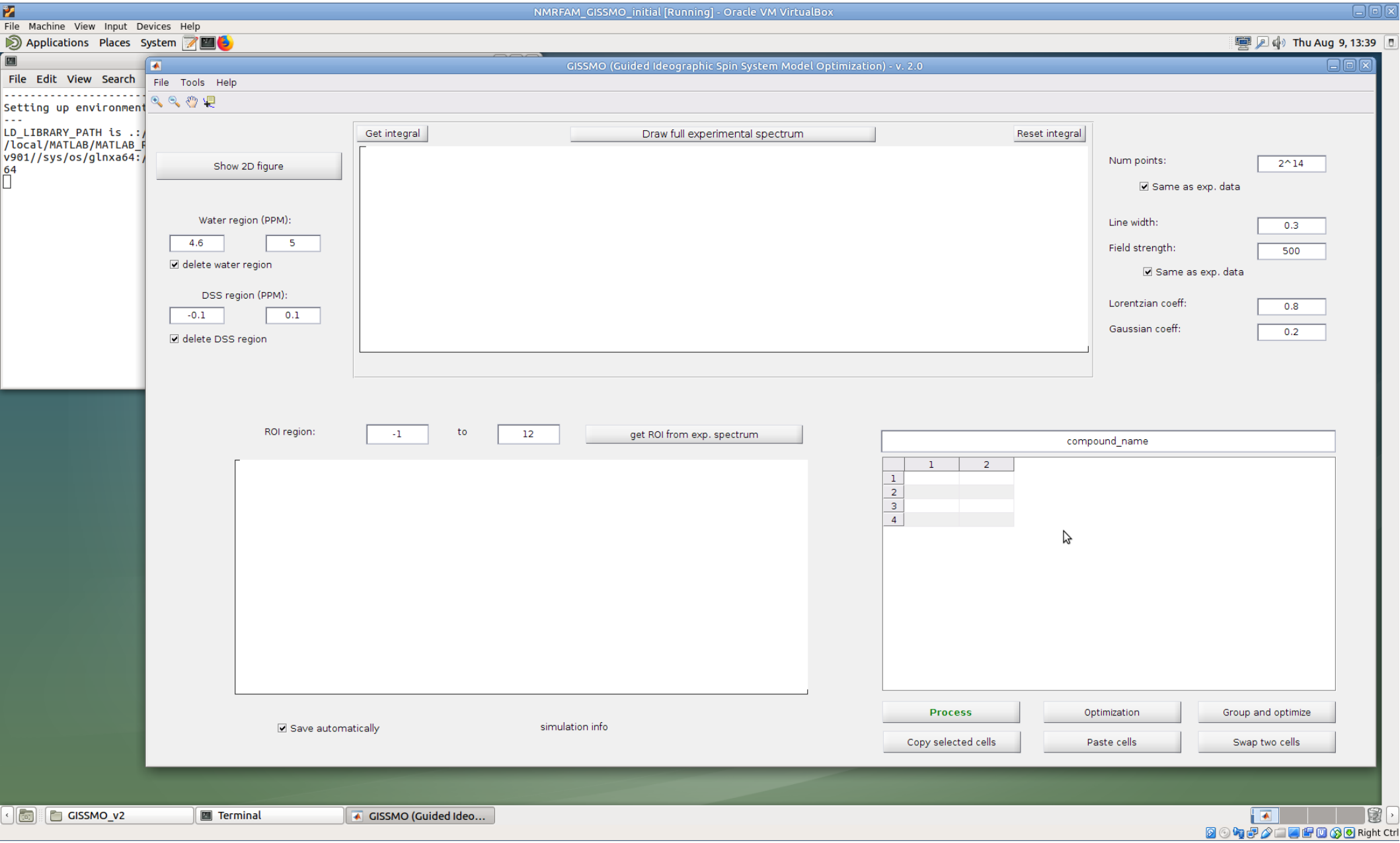
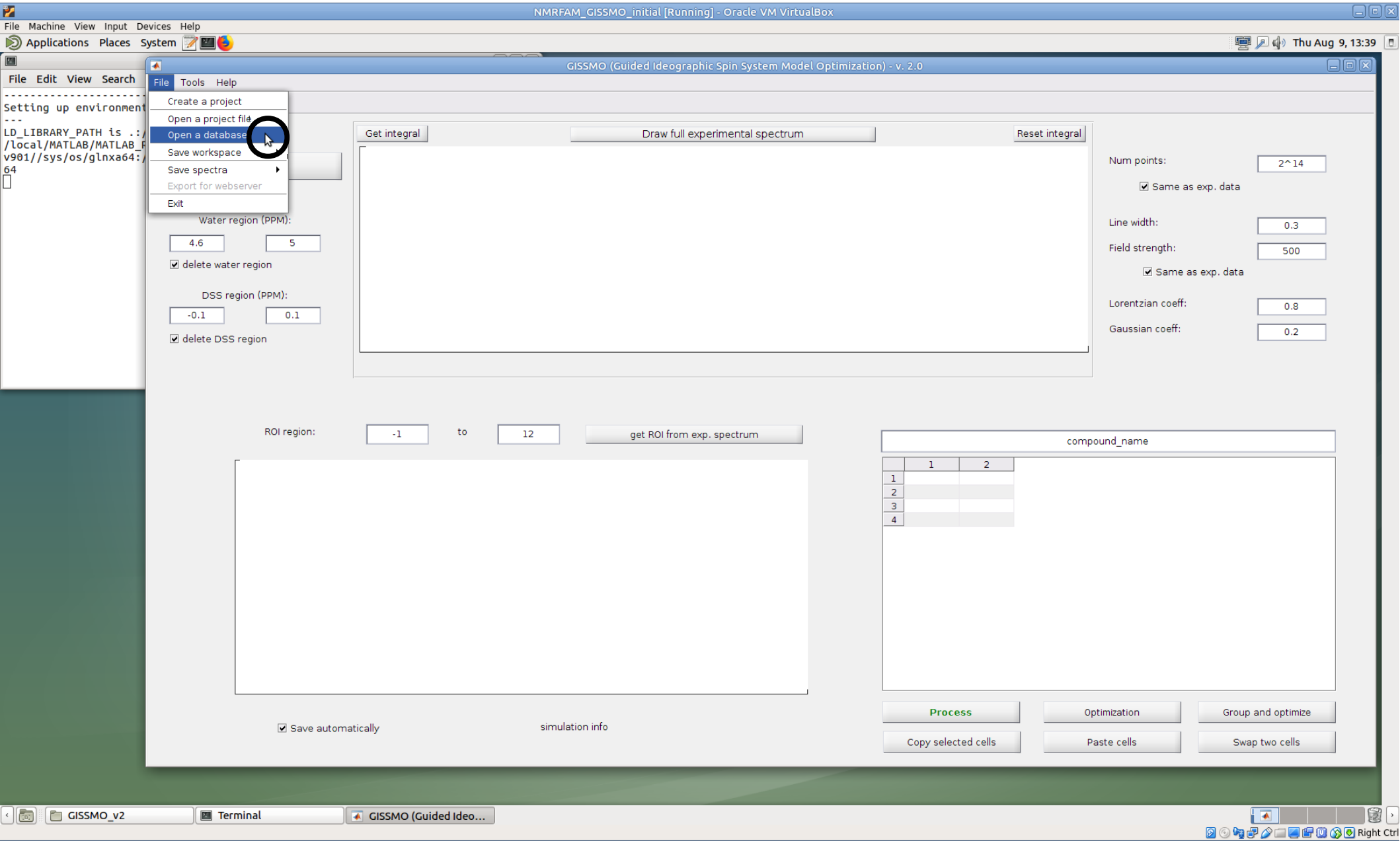
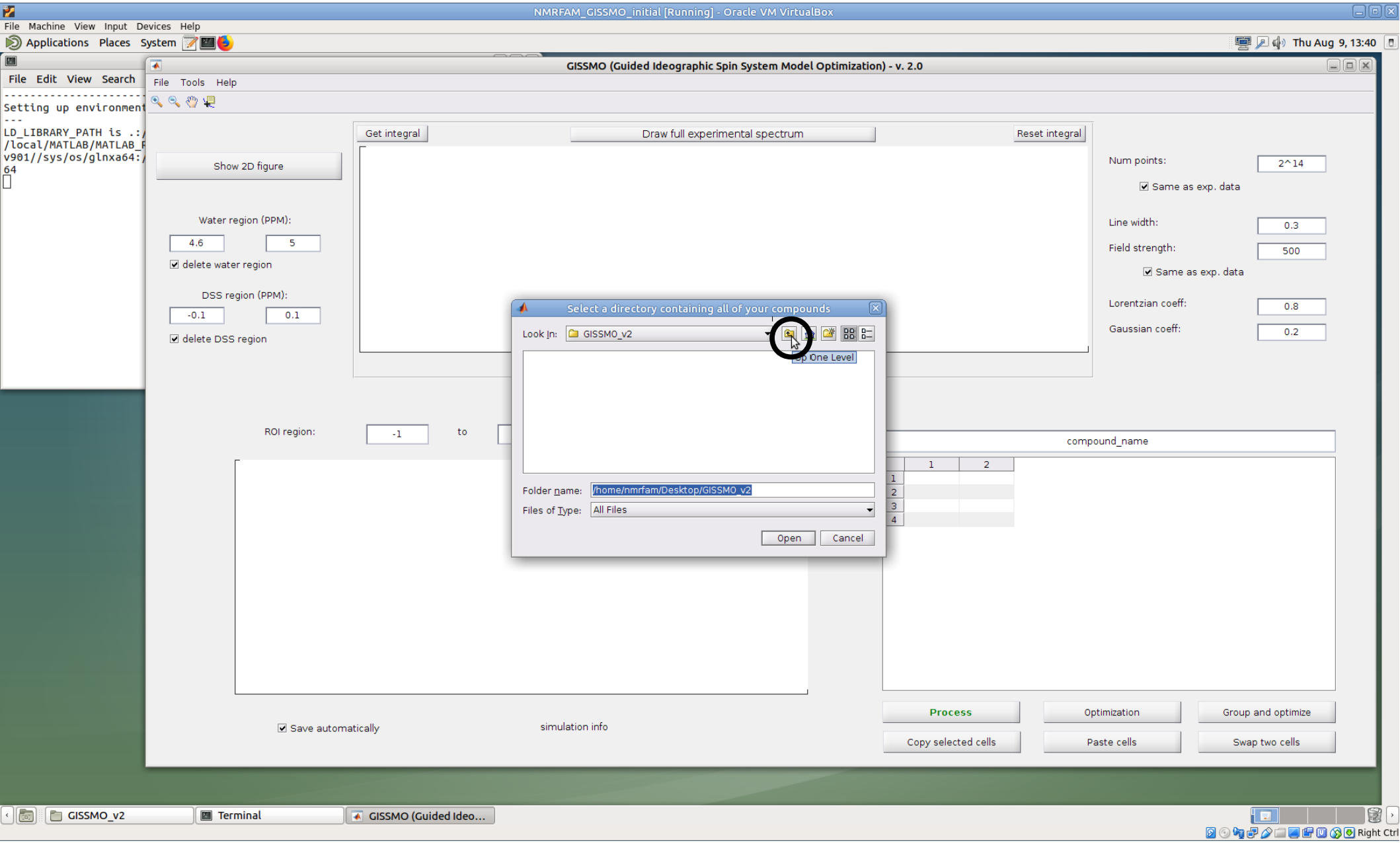

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:38
nmrfam's Home
BMRB_metabolites
Maybridge_RO3_ library
Right Ctrl

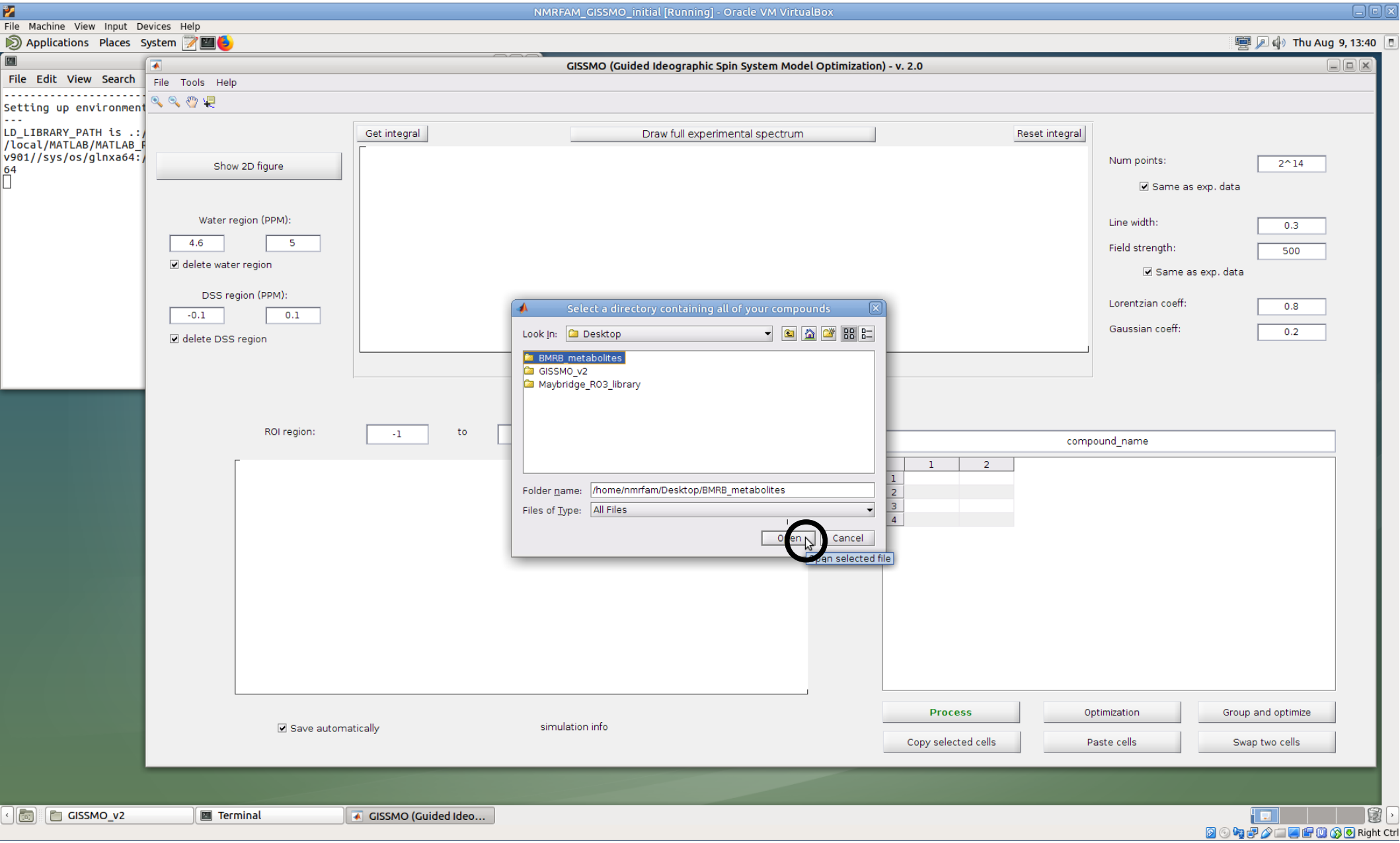

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:38
nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO_v2
File Edit View Go Bookmarks Help
Back Forward 50% List View
Places nmrfam Desktop GISSMO_v2
Computer
nmrfam
Deskt...
File S...
Docu...
Down...
Music
Pictures
Videos
Trash
Network
Brow...
Name Size Type Date Modified
GISSMO 9.8 MB executable Thu 09 Aug 2018 09:05:13 AM CDT
GISSMO.sh 874 bytes shell script Wed 08 Aug 2018 09:36:12 AM CDT
run_GISSMO_GUI.s 125 bytes shell script Wed 08 Aug 2018 03:03:15 PM CDT
"run_GISSMO_GUI.sh" selected (125 bytes), Free space: 4.0 GB
GISSMO_v2
Right Ctrl

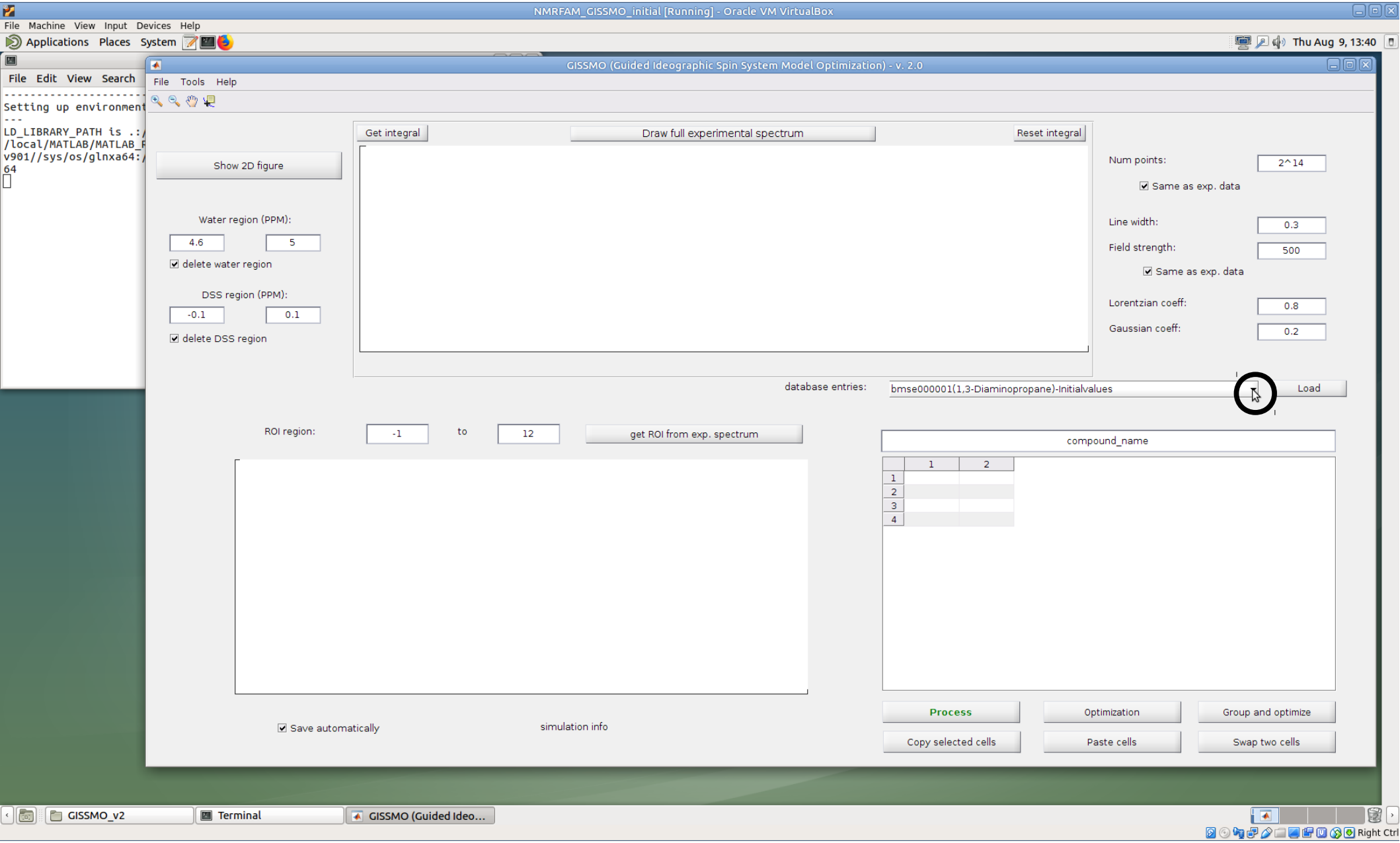

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:39
nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO_v2
File Edit View Go Bookmarks Help
Back Forward 50% List View
Places nmrfam Desktop GISSMO_v2
Computer
nmrfam
Deskt...
File S...
Docu...
Down...
Music
Pictures
Videos
Trash
Network
Brow...
Name Size Type Date Modified
GISSMO 9.8 MB executable Thu 09 Aug 2018 09:05:13 AM CDT
GISSMO.sh 874 bytes shell script Wed 08 Aug 2018 09:36:12 AM CDT
run_GISSMO_GUI.sh shell script Wed 08 Aug 2018 03:03:15 PM CDT
Do you want to run "run_GISSMO_GUI.sh", or display its contents?
"run_GISSMO_GUI.sh" is an executable text file.
Run in Terminal
Display
Cancel
Run
"run_GISSMO_GUI.sh" selected (125 bytes), Free space: 4.0 GB
GISSMO_v2
Right Ctrl

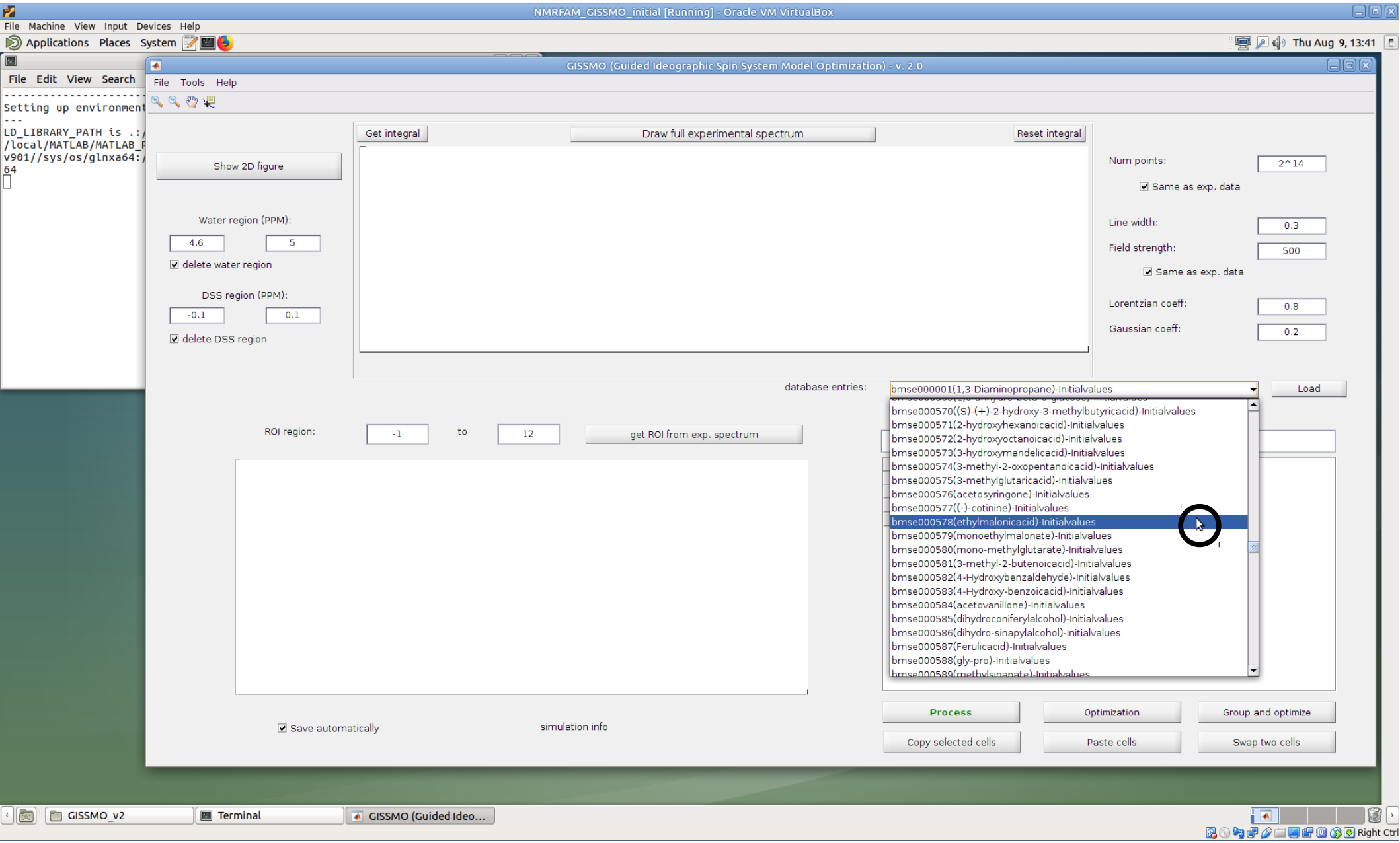

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:39
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integral
Show 2D figure
Num points:
2^14
Same as exp. data
Water region (PPM):
4.6
5
delete water region
Line width:
0.3
Field strength:
500
Same as exp. data
DSS region (PPM):
-0.1
0.1
delete DSS region
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
ROI region:
-1
to
12
get ROI from exp. spectrum
compound_name
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 Ideo...
Right Ctrl

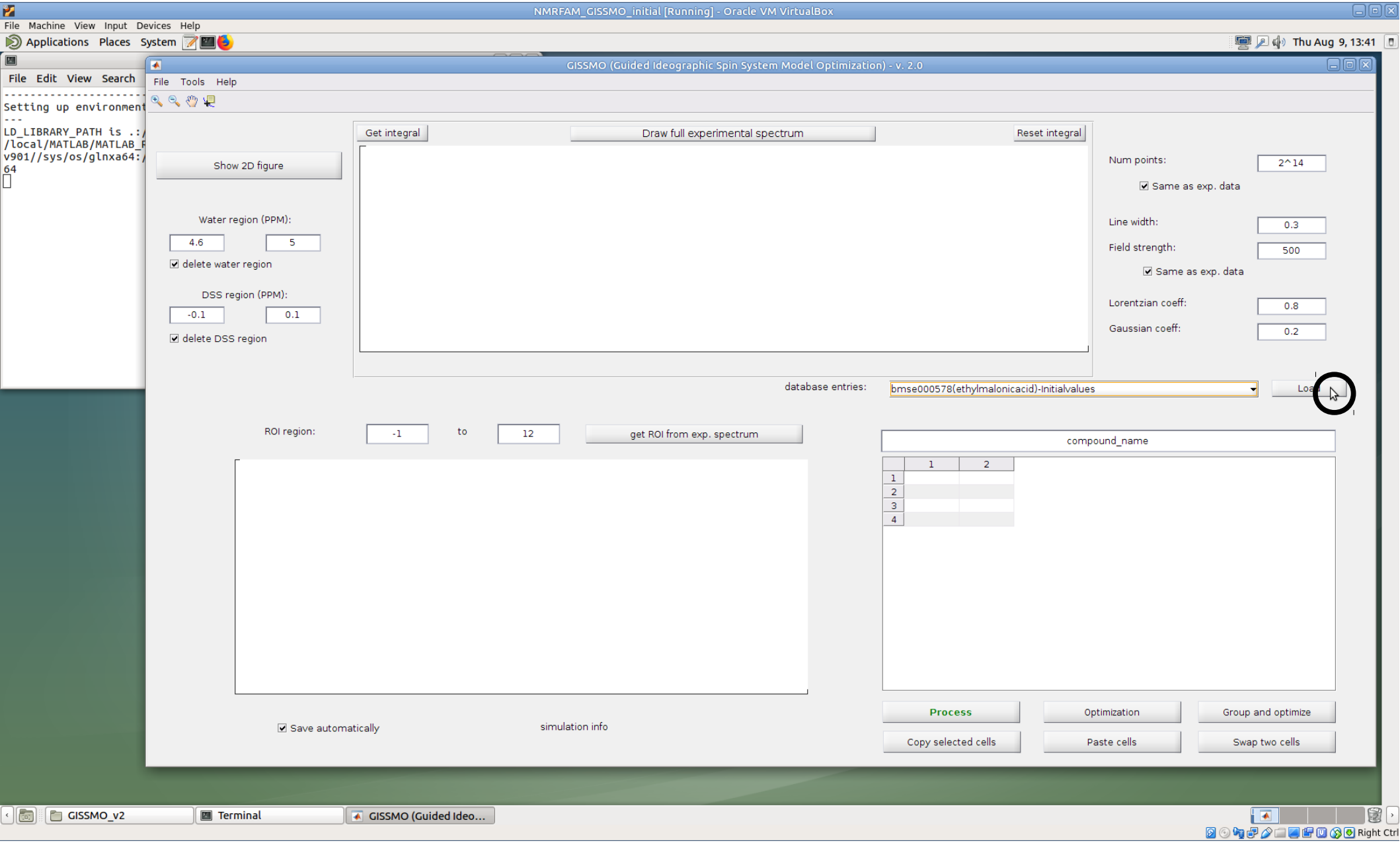

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:39
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Create a project
Open a project file
Open a database
Save workspace
Save spectra
Export for webserver
Exit
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Get integral
Draw full experimental spectrum
Reset integral
Num points:
2^14
Same as exp. data
Line width:
0.3
Field strength:
500
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
ROI region:
-1
to
12
get ROI from exp. spectrum
compound_name
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 Ideo...
Right Ctrl

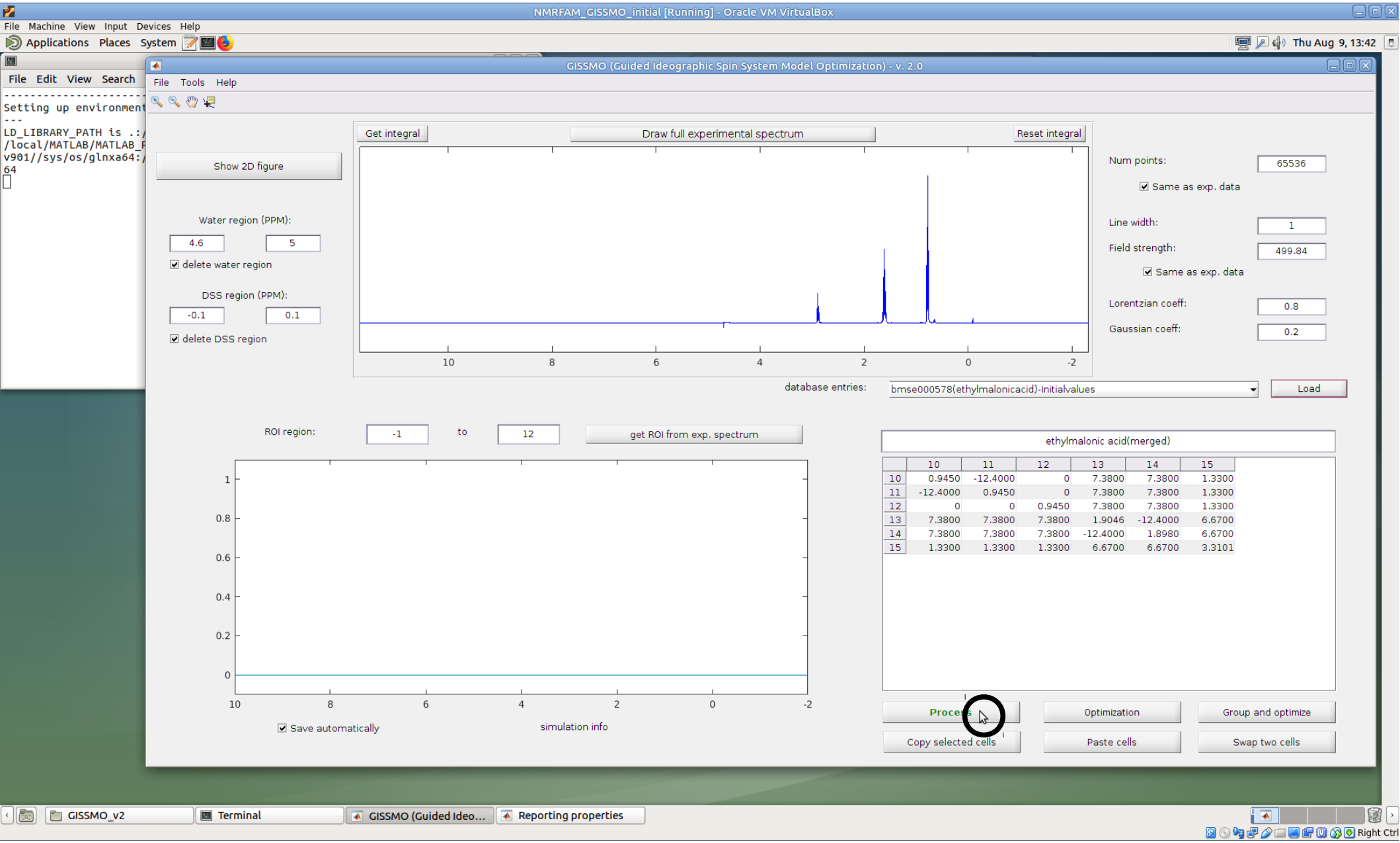

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:40
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
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
Field strength:
500
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
Select a directory containing all of your compounds
Look In:
GISSMO_v2
Up One Level
Folder name:
/home/nmrfam/Desktop/GISSMO_v2
Files of Type:
All Files
Open
Cancel
ROI region:
-1
to
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 Ideo...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:40
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
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
Field strength:
500
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
ROI region:
-1
to
Select a directory containing all of your compounds
Look In:
Desktop
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_library
Folder name:
/home/nmrfam/Desktop/BMRB_metabolites
Files of Type:
All Files
Open
Cancel
Open selected file
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 Ideo...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:40
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
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
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
3
4
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


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:41
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
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
Field strength:
500
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000001(1,3-Diaminopropane)-Initialvalues
Load
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
ROI region:
-1
to
12
get ROI from exp. spectrum
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


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:41
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integral
Show 2D figure
Num points:
2^14
Same as exp. data
Water region (PPM):
4.6
5
delete water region
Line width:
0.3
Field strength:
500
Same as exp. data
DSS region (PPM):
-0.1
0.1
delete DSS region
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
ROI region:
-1
to
12
get ROI from exp. spectrum
compound_name
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 Ideo...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:42
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
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
10 8 6 4 2 0 -2
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
-1
to
12
get ROI from exp. spectrum
1 0.8 0.6 0.4 0.2 0
10 8 6 4 2 0 -2
Save automatically
simulation info
ethylmalonic acid(merged)
10 11 12 13 14 15
10 0.9450 -12.4000 0 7.3800 7.3800 1.3300
11 -12.4000 0.9450 0 7.3800 7.3800 1.3300
12 0 0 0.9450 7.3800 7.3800 1.3300
13 7.3800 7.3800 7.3800 1.9046 -12.4000 6.6700
14 7.3800 7.3800 7.3800 -12.4000 1.8980 6.6700
15 1.3300 1.3300 1.3300 6.6700 6.6700 3.3101
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
GISSMO_v2
Terminal
GISSMO (Guided Ideo...
Reporting properties
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:46

File Edit View Search

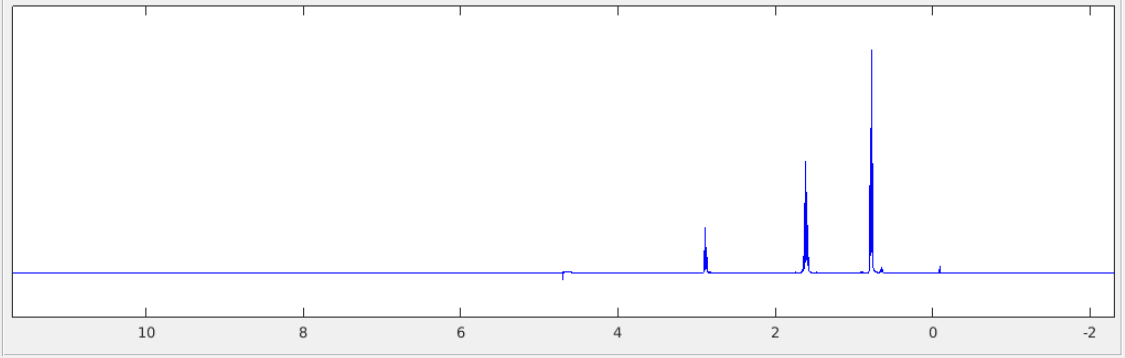
```
Setting up environment
---
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
Warning: Setting the '
 mode is active.
> In matlab.uitools.in
  In matlab.uitools.in
s)) (line 86)
  In GISSMO>Draw_exper
  In GISSMO>Draw_full_
  In gui_mainfcn (line
  In GISSMO (line 16)
  In matlab.graphics.i
raw_full_exp_spectrum_
```

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset integral

Show 2D figure



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

Water region (PPM): 4.6 5

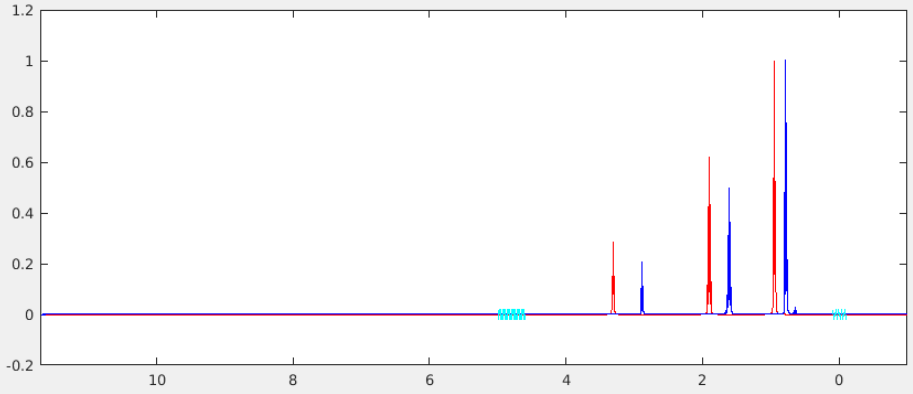
delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

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



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

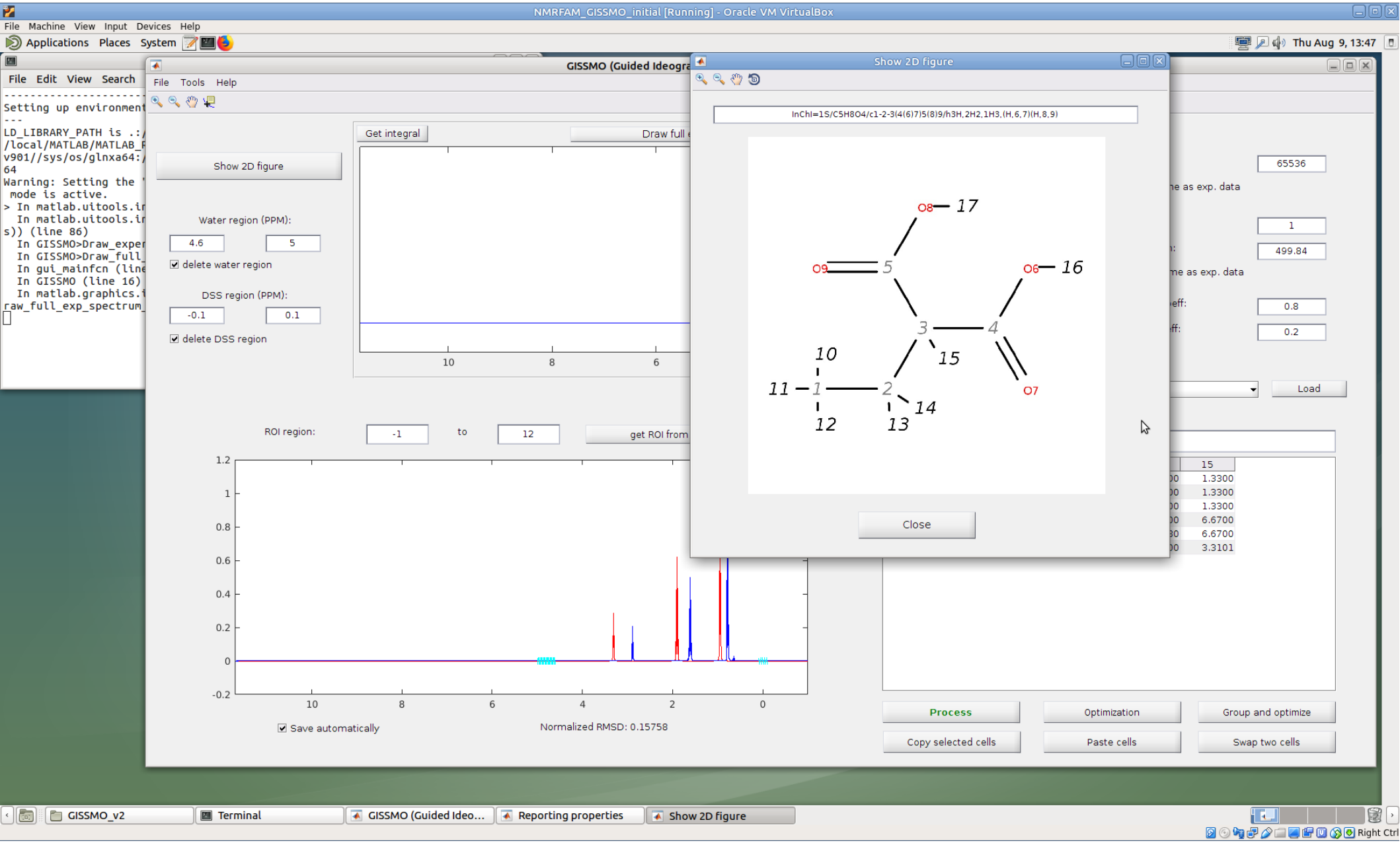
	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	3.3101

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

GISSMO_v2 | Terminal | GISSMO (Guided Ideo... | Reporting properties

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:47
File Edit View Search
Setting up environment
LD_LIBRARY_PATH is .:/
/local/MATLAB/MATLAB_R
v901//sys/os/glnxa64:/
64
Warning: Setting the '
mode is active.
> In matlab.uitools.in
In matlab.uitools.in
s)) (line 86)
In GISSMO>Draw_exper
In GISSMO>Draw_full_
In gui_mainfcn (line
In GISSMO (line 16)
In matlab.graphics.i
raw_full_exp_spectrum_
GISSMO (Guided Ideogra
File Tools Help
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Get integral
Draw full
10
8
6
ROI region:
-1
to
12
get ROI from
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
10
8
6
4
2
0
Save automatically
Normalized RMSD: 0.15758
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
O8 17
O9
5
O6 16
3
4
10
15
11
1
2
O7
14
12
13
Close
65536
1
499.84
0.8
0.2
Load
15
1.3300
1.3300
1.3300
6.6700
6.6700
3.3101
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
GISSMO_v2
Terminal
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

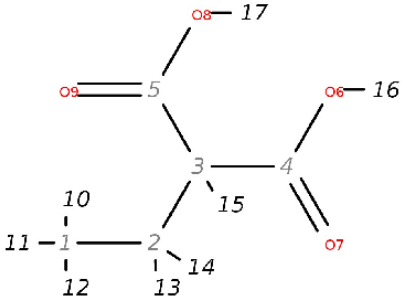
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:48

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Zoom In

Show 2D figure

Water region (PPM):

4.6 5

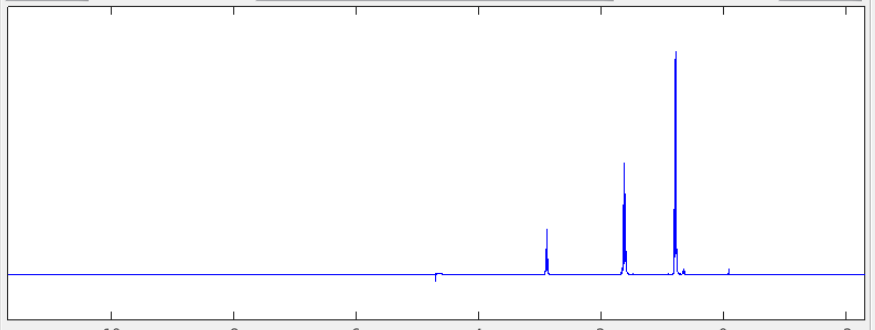
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral | Draw full experimental spectrum | Reset inte...



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

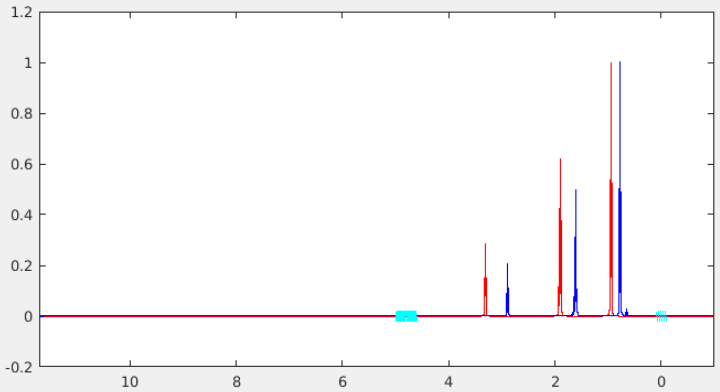
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

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



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	3.3101

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

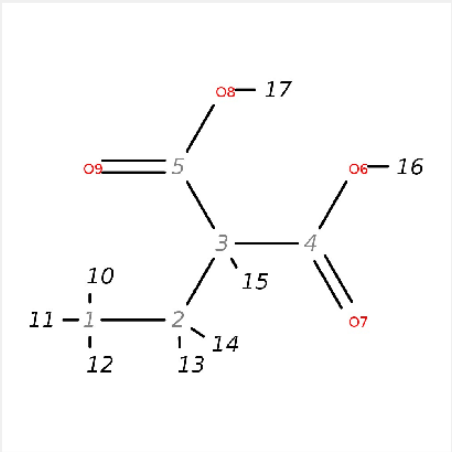
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:48

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

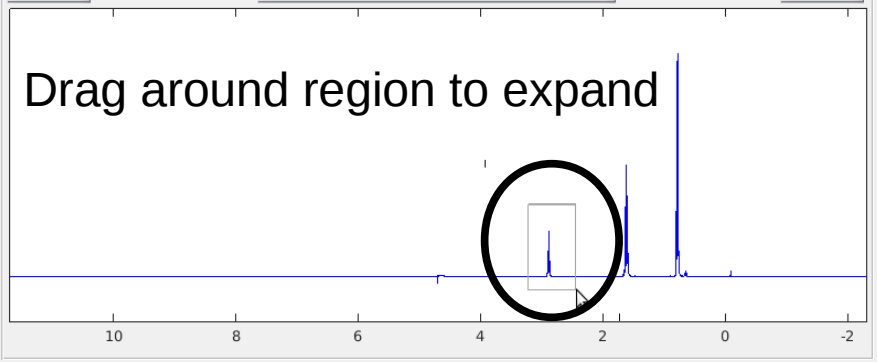
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

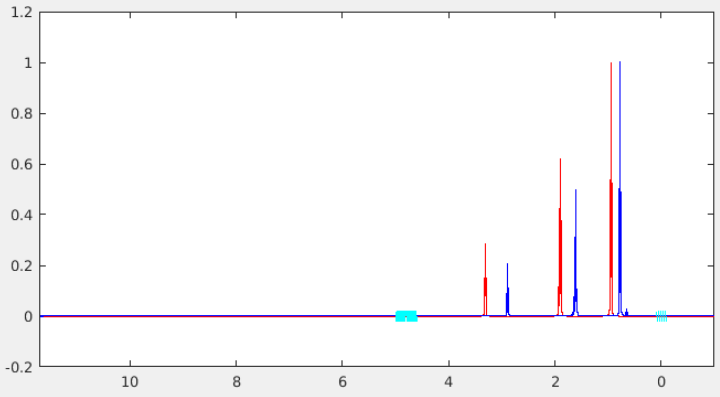
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

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



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	3.3101

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

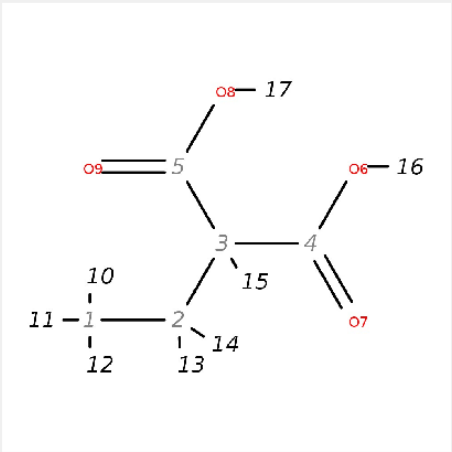
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:49

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

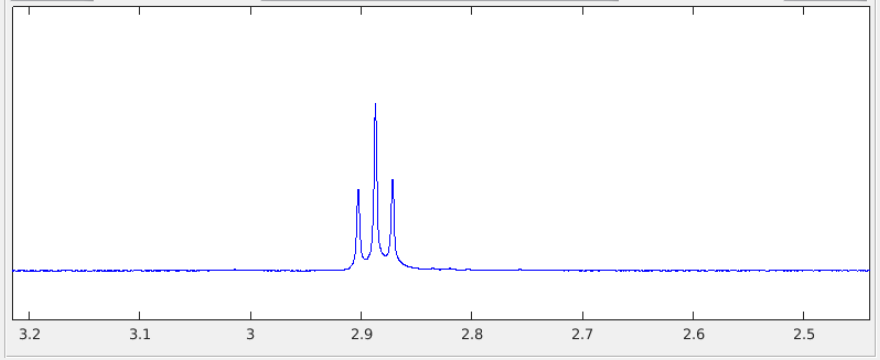
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

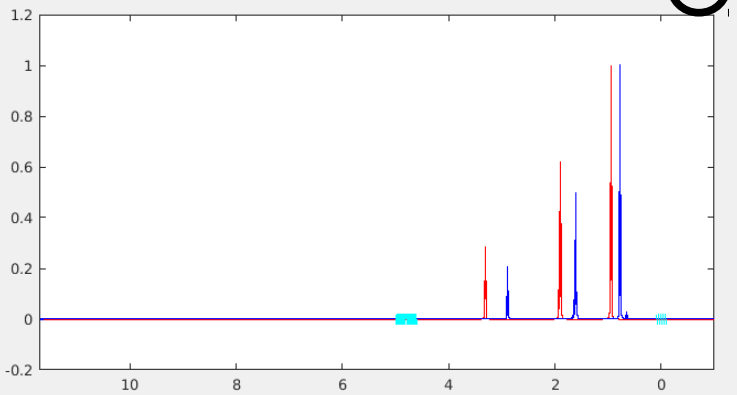
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

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



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	3.3101

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

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NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

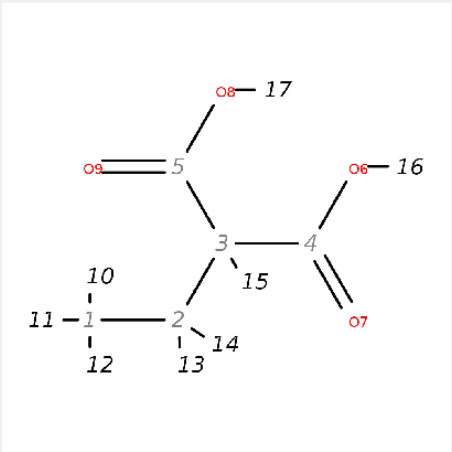
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:50

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Select a point on spectra

Get integral | Draw full experimental spectrum | Reset inte...

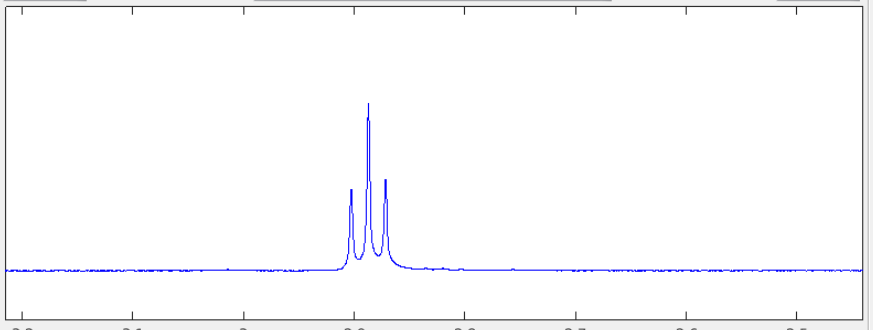
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

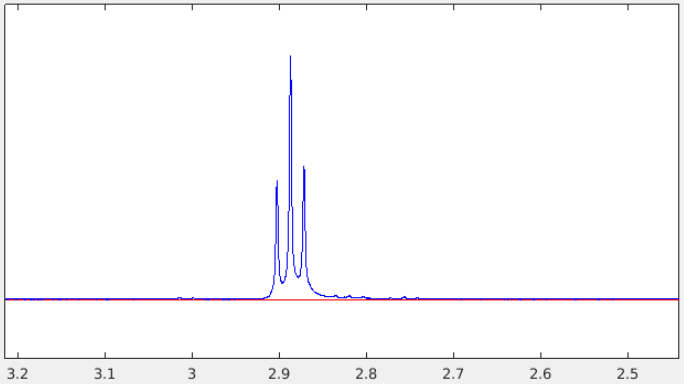
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 2.441 to 3.215 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	3.3101

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

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NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

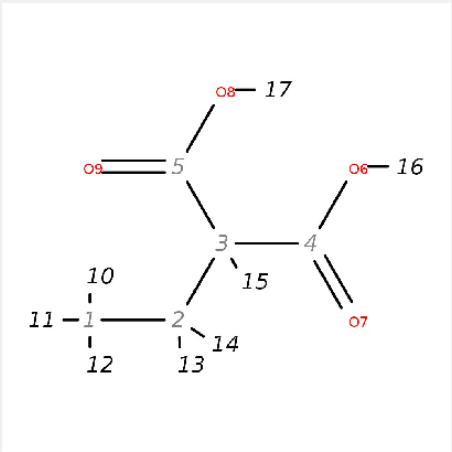
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:50

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

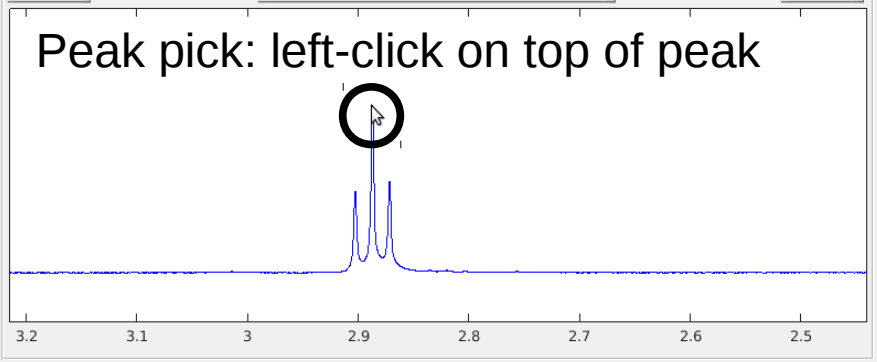
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

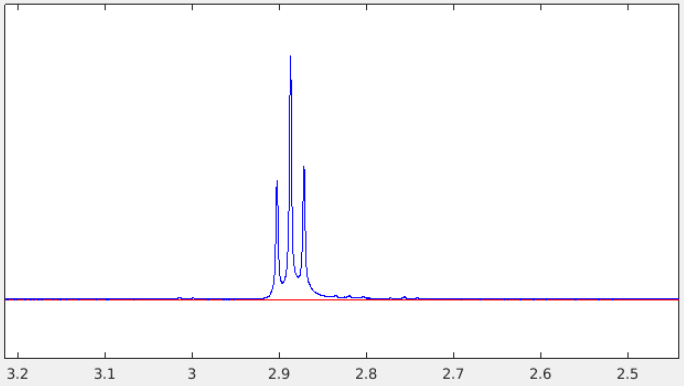
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 2.441 to 3.215 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

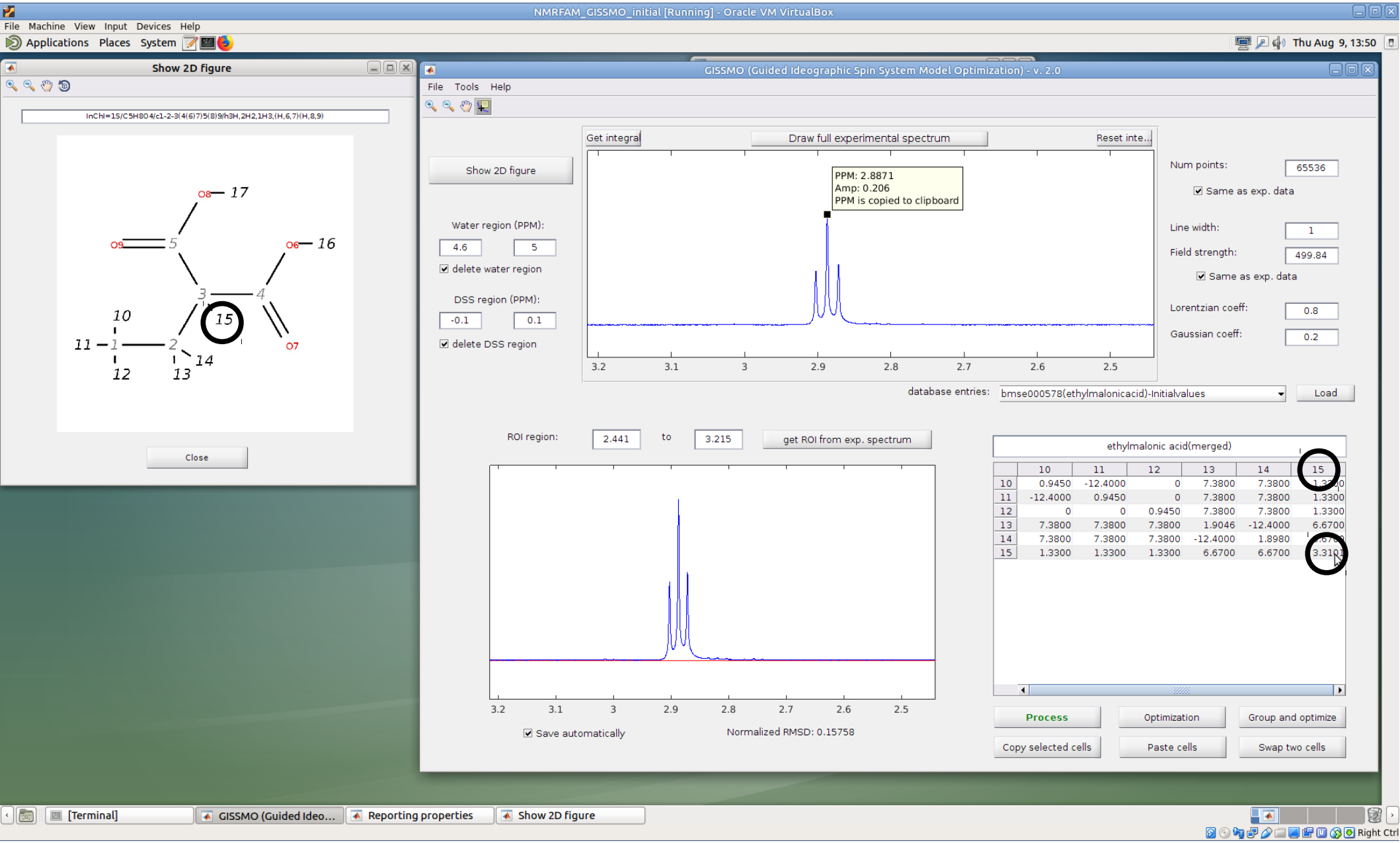
	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	3.3101

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:50
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 2.8871
Amp: 0.206
PPM is copied to clipboard
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
2.441
to
3.215
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.15758
ethylmalonic acid(merged)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

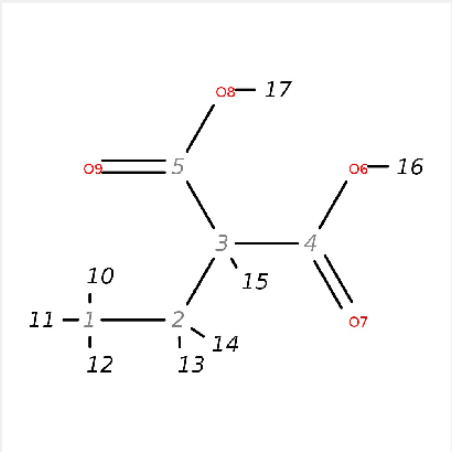
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:52

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

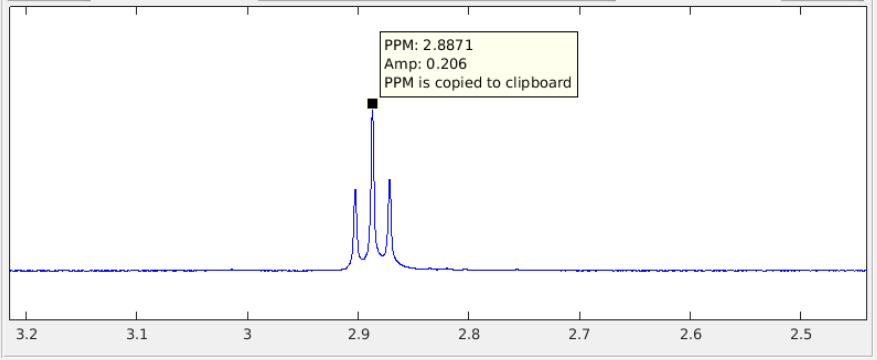
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

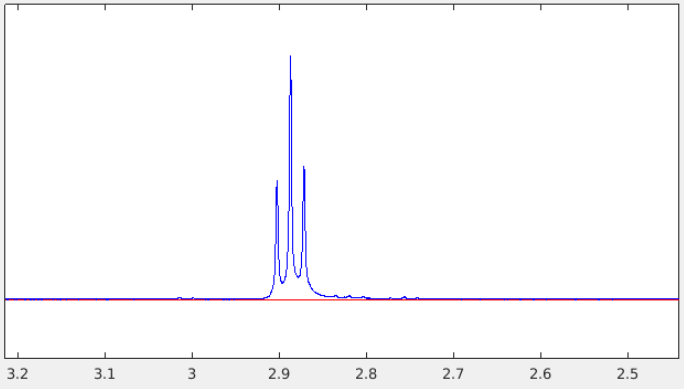
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 2.441 to 3.215 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	3.3101

Left-Click
To highlight

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

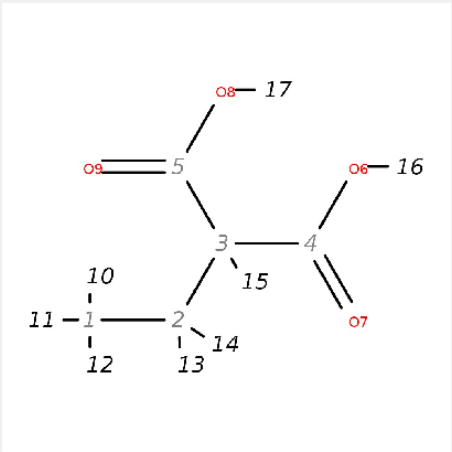
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:53

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

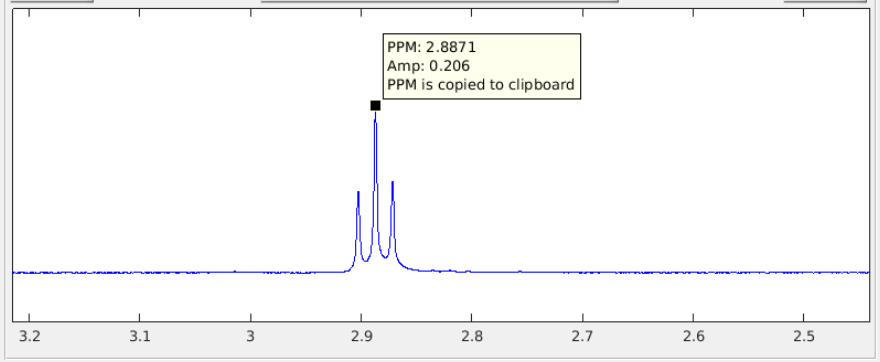
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

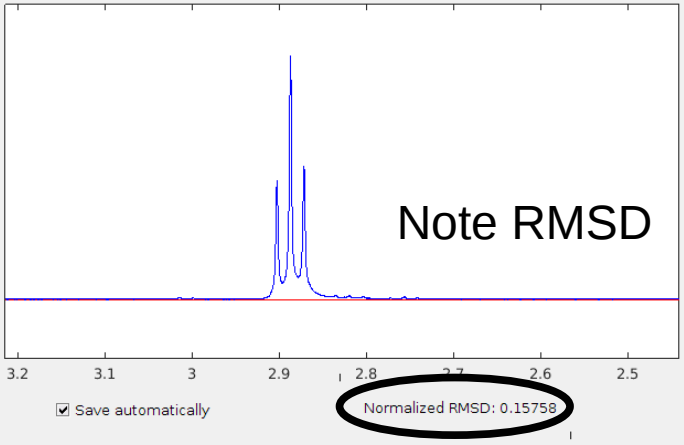
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 2.441 to 3.215 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.15758

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.7000	6.6700	2.8871

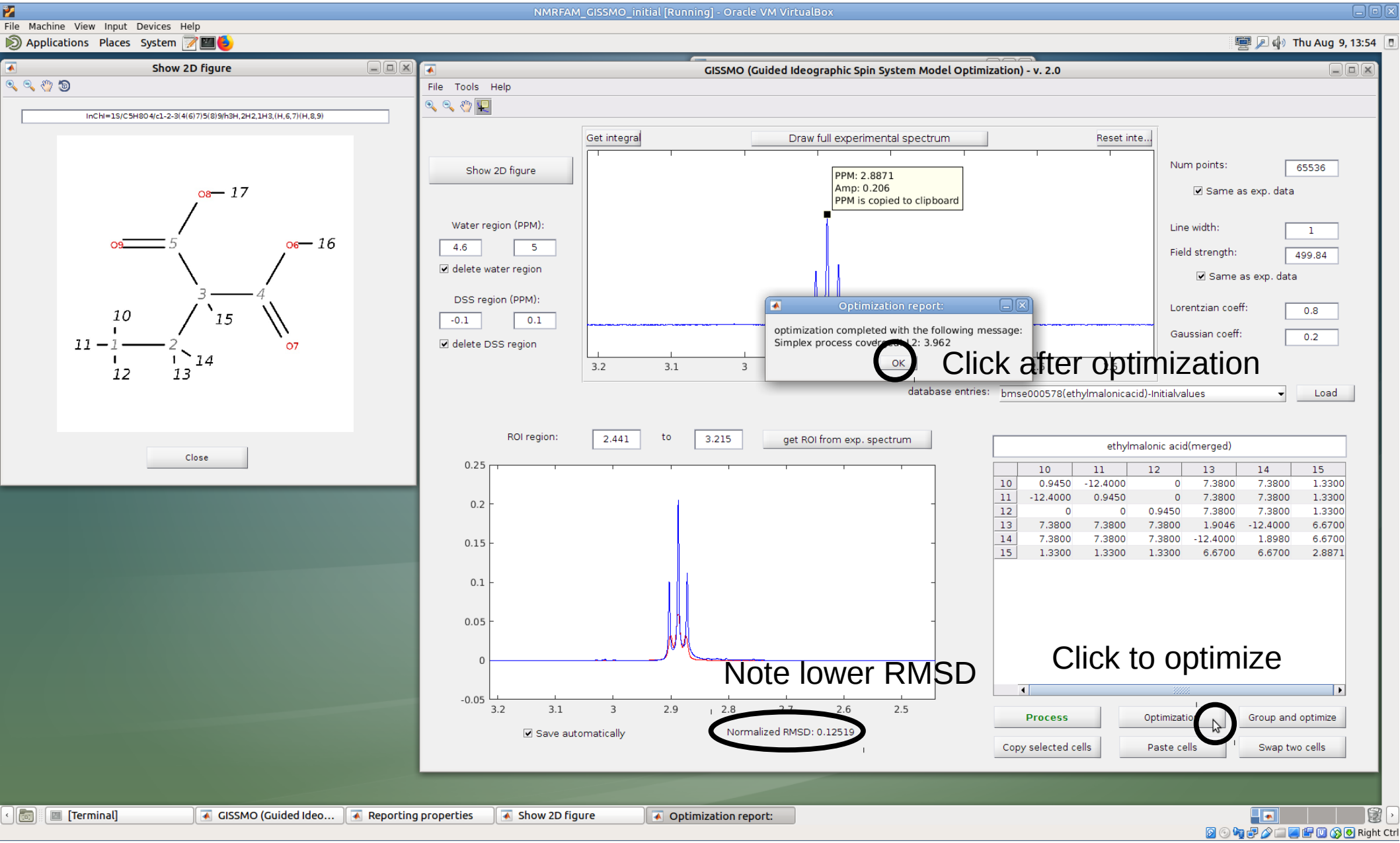
Ctrl-v
To copy from clipboard

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl



	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	2.8871

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

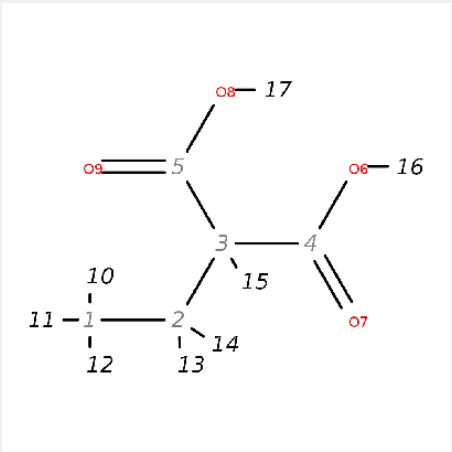
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:54

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

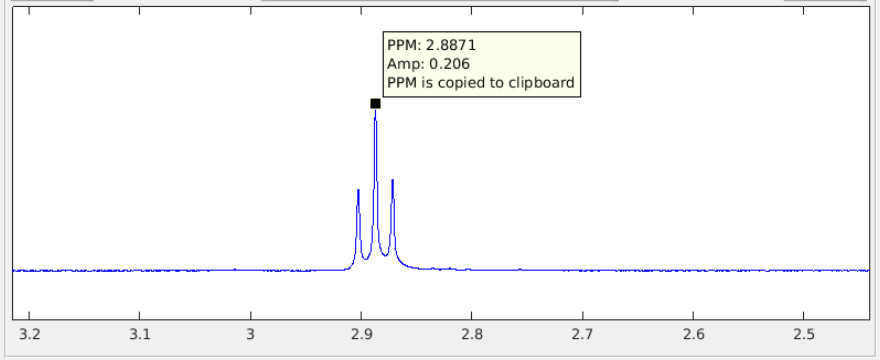
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

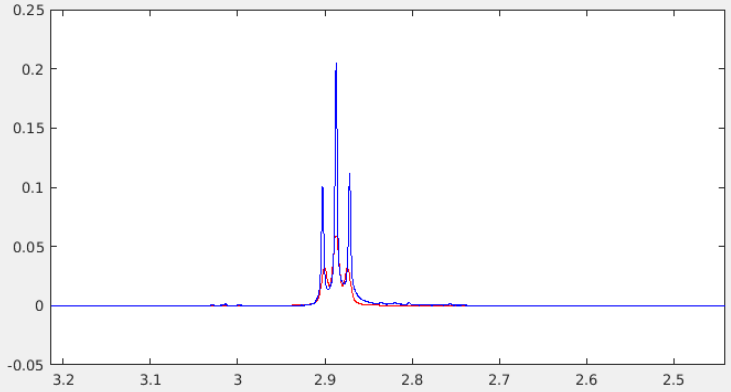
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 2.441 to 3.215 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12519

ethylmalonic acid(merged)

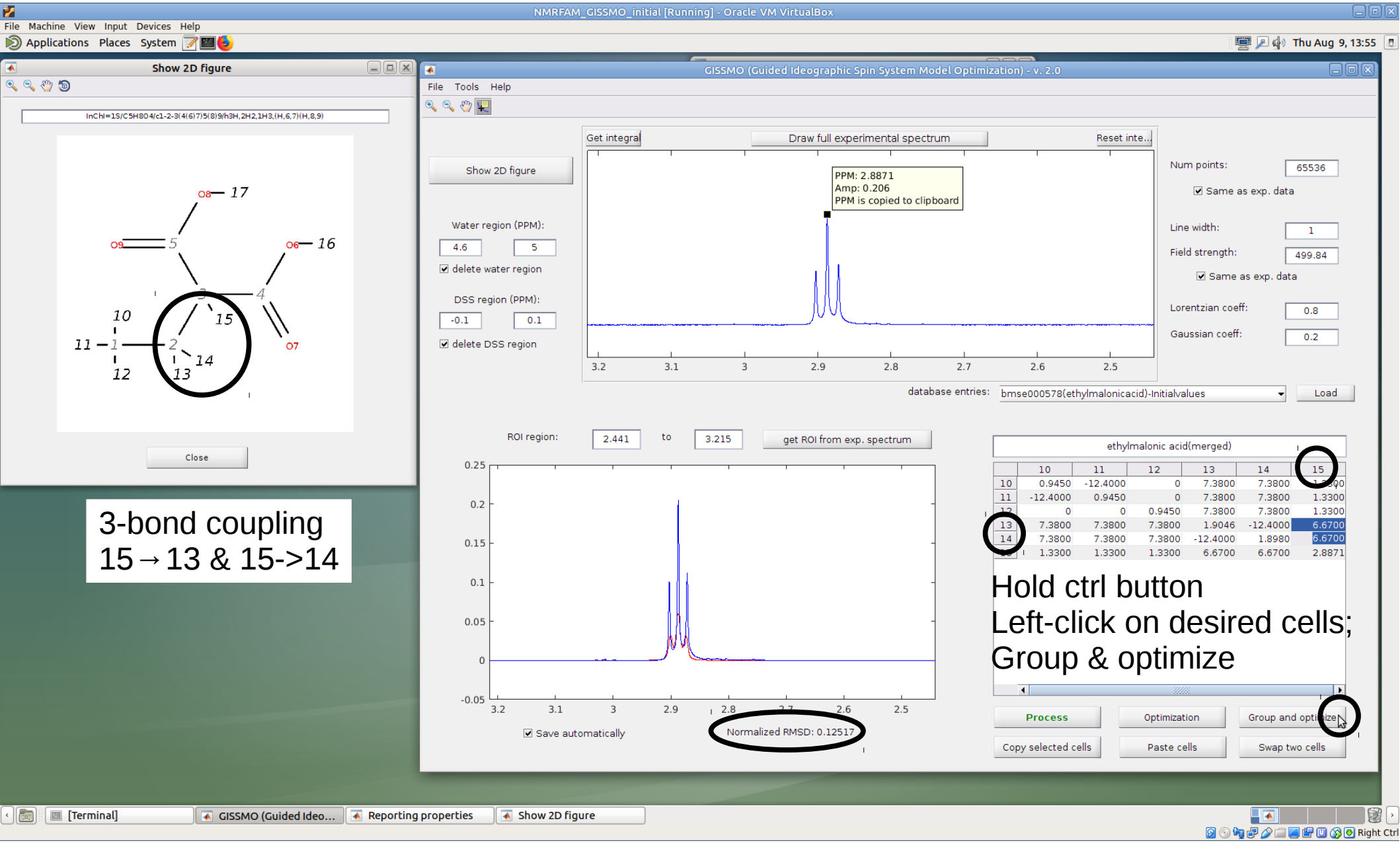
	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl



	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	6.6700
14	7.3800	7.3800	7.3800	-12.4000	1.8980	6.6700
15	1.3300	1.3300	1.3300	6.6700	6.6700	2.8871

3-bond coupling
15→13 & 15->14

Hold ctrl button
Left-click on desired cells;
Group & optimize

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

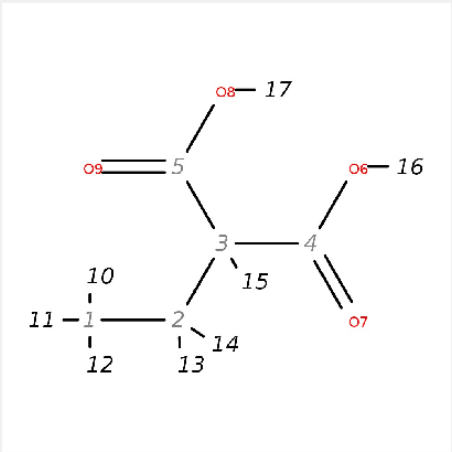
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:55

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

PPM: 2.8871
Amp: 0.206
PPM is copied to clipboard

3.2 3.1 3 2.6 2.5

Optimization report:

optimization completed with the following message:
Simplex process covergedL2: 6.097

OK

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

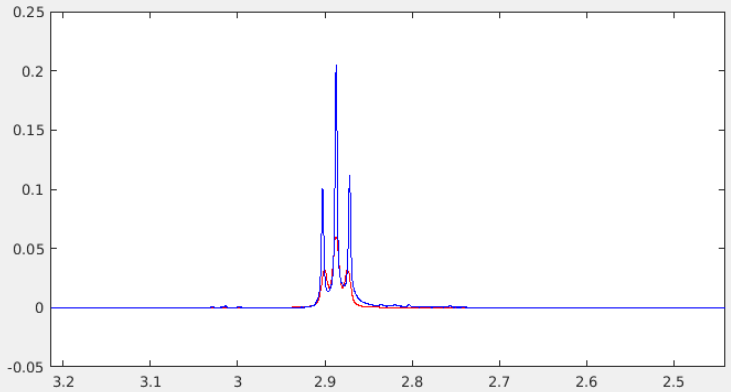
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 2.441 to 3.215 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12517

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	1.3300	1.3300	1.3300	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Optimization report:

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

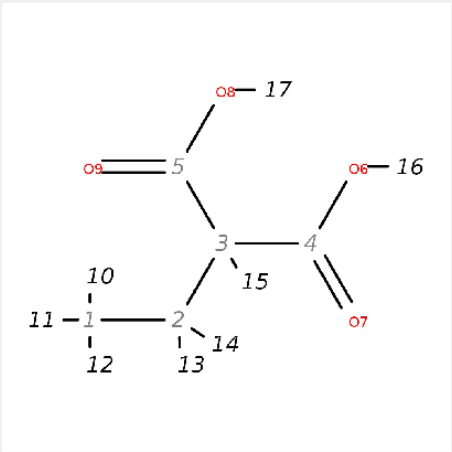
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:55

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

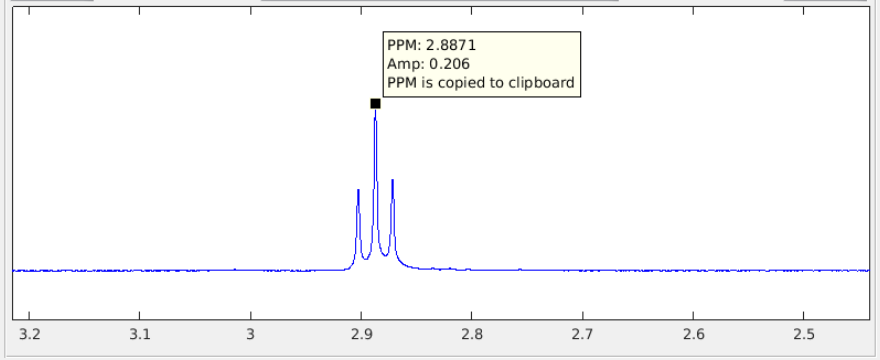
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

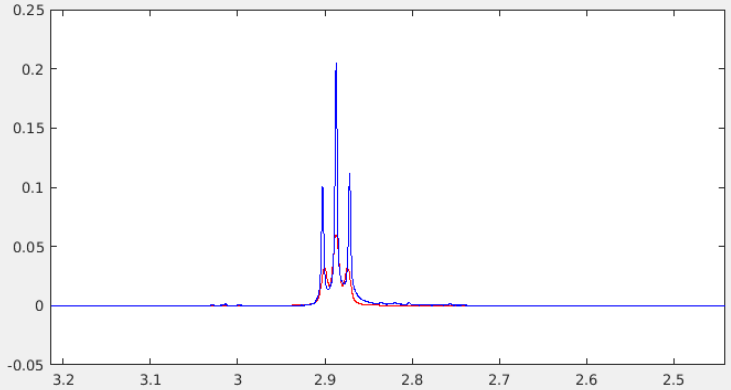
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 2.441 to 3.215 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12517

ethylmalonic acid(merged)

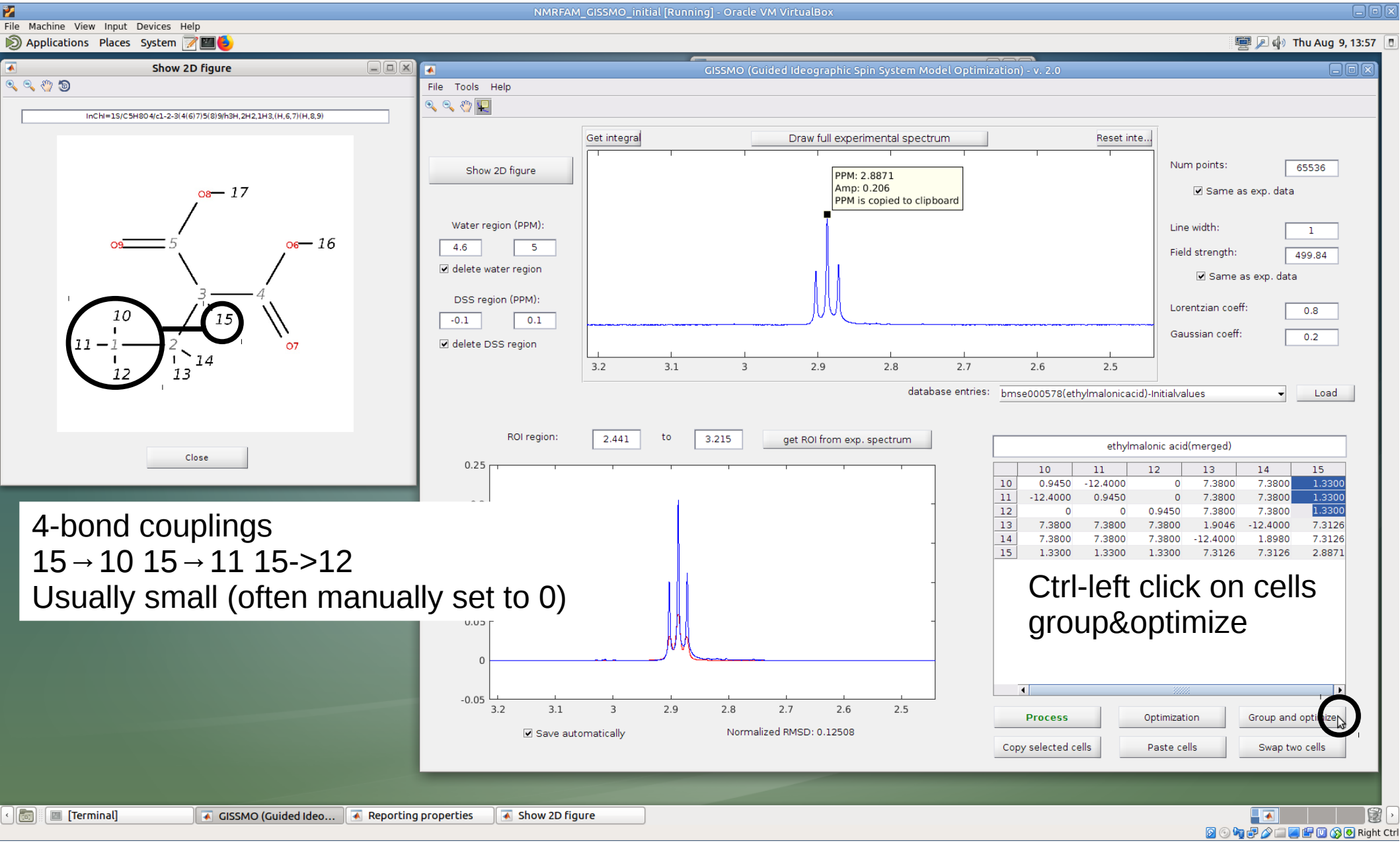
	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	1.3300	1.3300	1.3300	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl



	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	1.3300
11	-12.4000	0.9450	0	7.3800	7.3800	1.3300
12	0	0	0.9450	7.3800	7.3800	1.3300
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	1.3300	1.3300	1.3300	7.3126	7.3126	2.8871

4-bond couplings
15→10 15→11 15->12
Usually small (often manually set to 0)

Ctrl-left click on cells
group&optimize

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

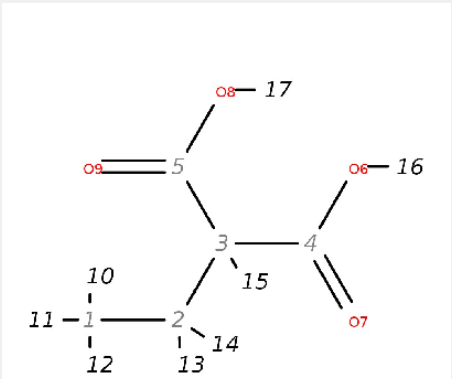
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:57

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

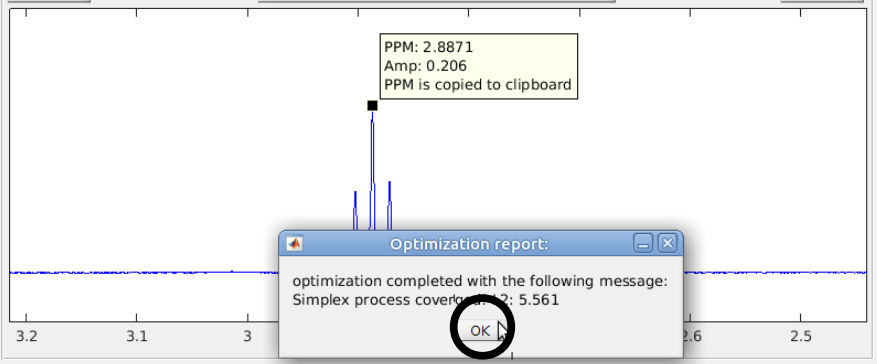
File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

Show 2D figure

Water region (PPM): 4.6 5 delete water region

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



Optimization report:

optimization completed with the following message:
Simplex process covering ... 2: 5.561

OK

Num points: 65536 Same as exp. data

Line width: 1

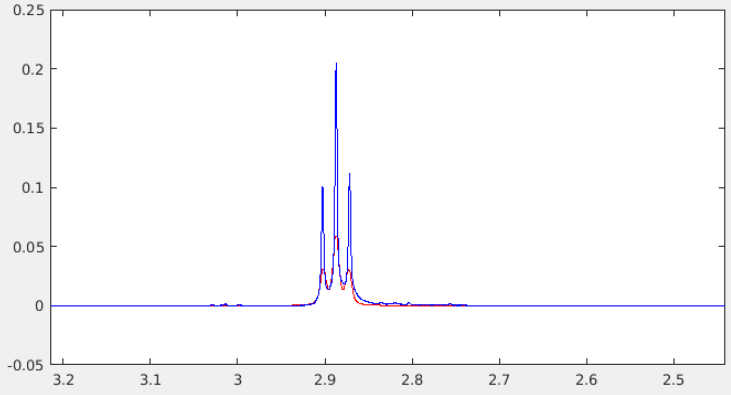
Field strength: 499.84 Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 2.441 to 3.215 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12508

ethylmalonic acid(merged)

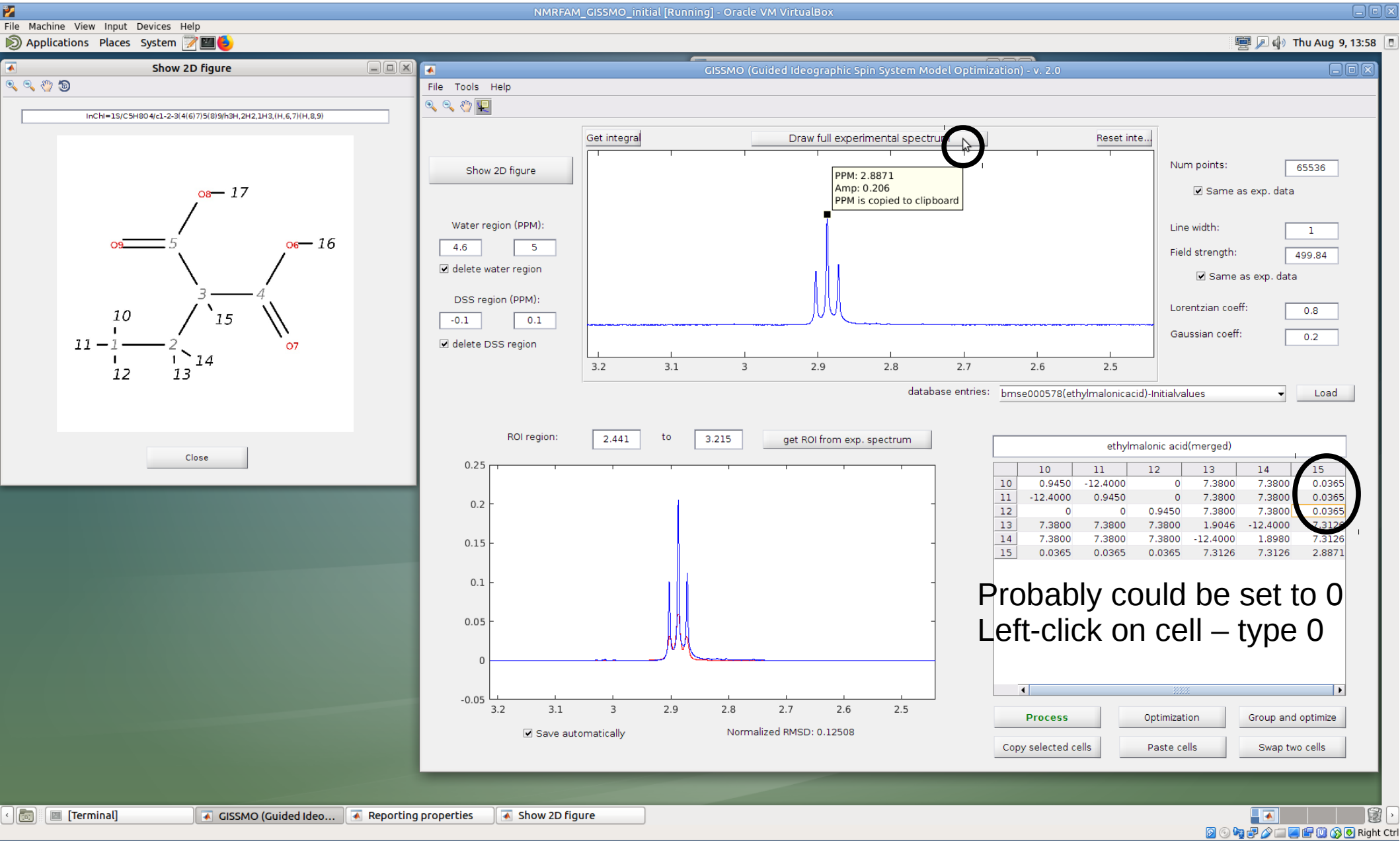
	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.9450	0	7.3800	7.3800	0.0365
12	0	0	0.9450	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Optimization report:

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 13:58
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 2.8871
Amp: 0.206
PPM is copied to clipboard
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
2.441
to
3.215
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.12508
ethylmalonic acid(merged)
Probably could be set to 0
Left-click on cell – type 0
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

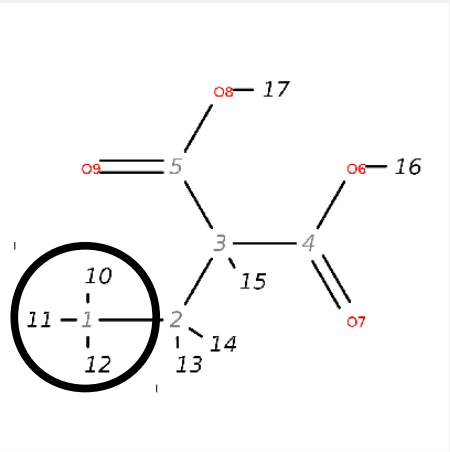
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:58

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

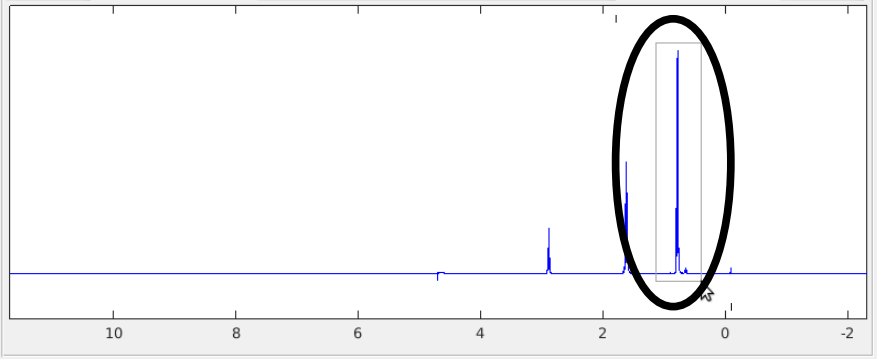
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

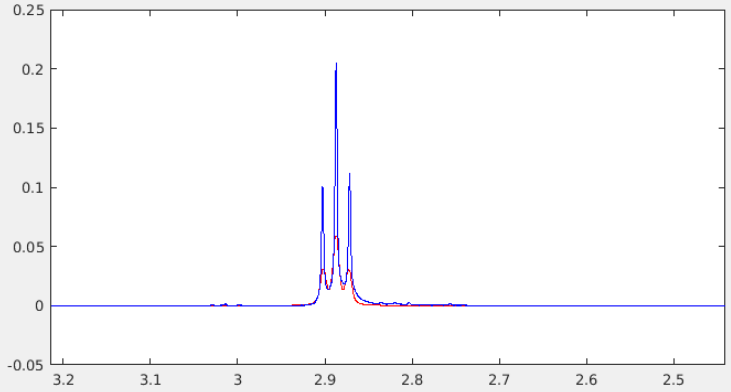
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 2.441 to 3.215 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12508

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.9450	0	7.3800	7.3800	0.0365
12	0	0	0.9450	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

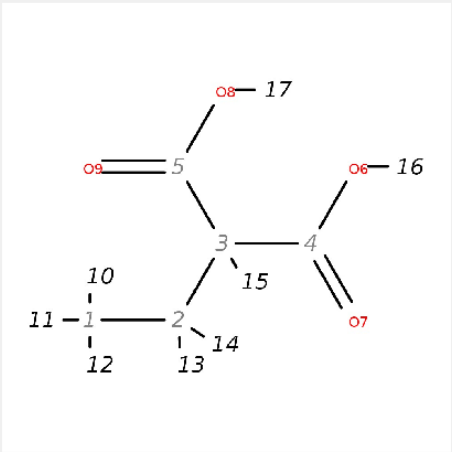
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:59

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

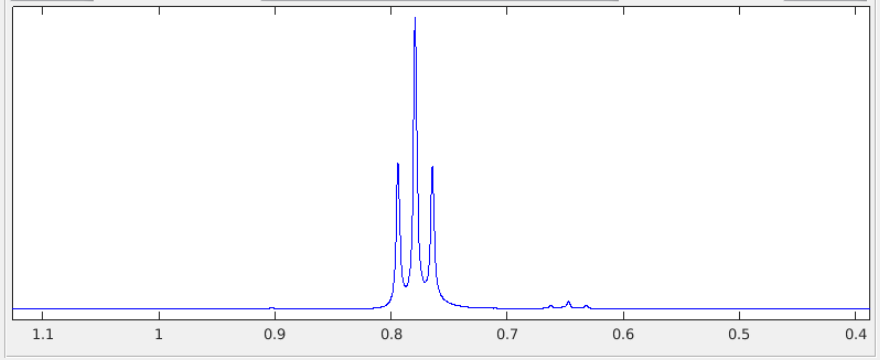
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

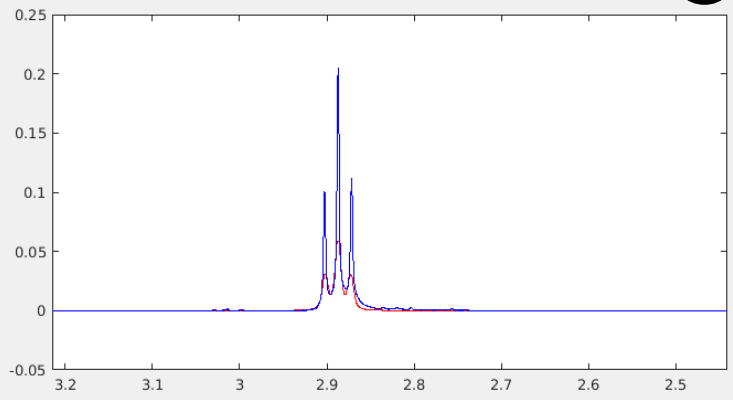
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 2.441 to 3.215 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12508

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.9450	0	7.3800	7.3800	0.0365
12	0	0	0.9450	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

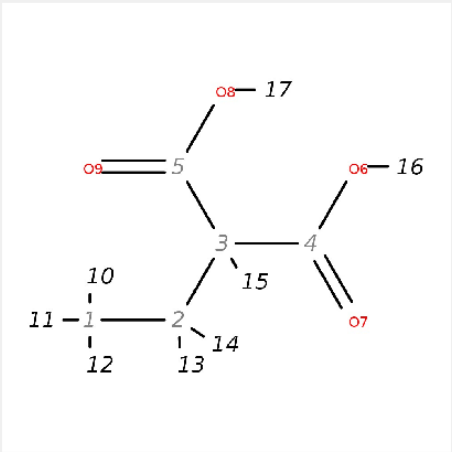
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 13:59

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

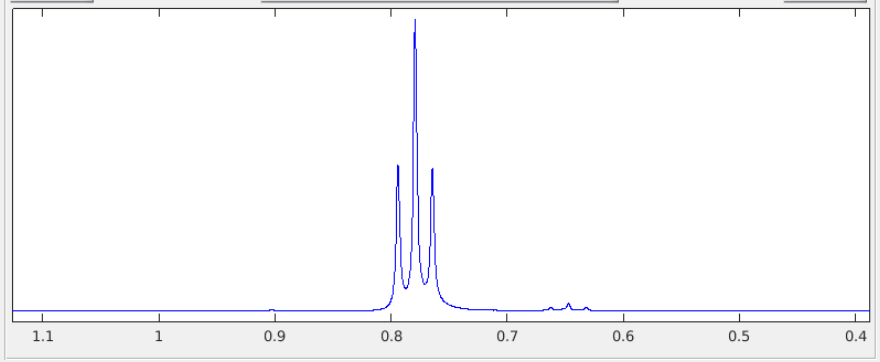
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

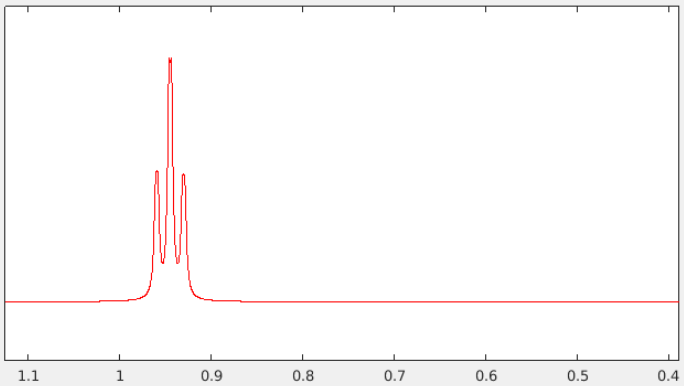
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 0.388 to 1.127 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.12508

ethylmalonic acid(merged)

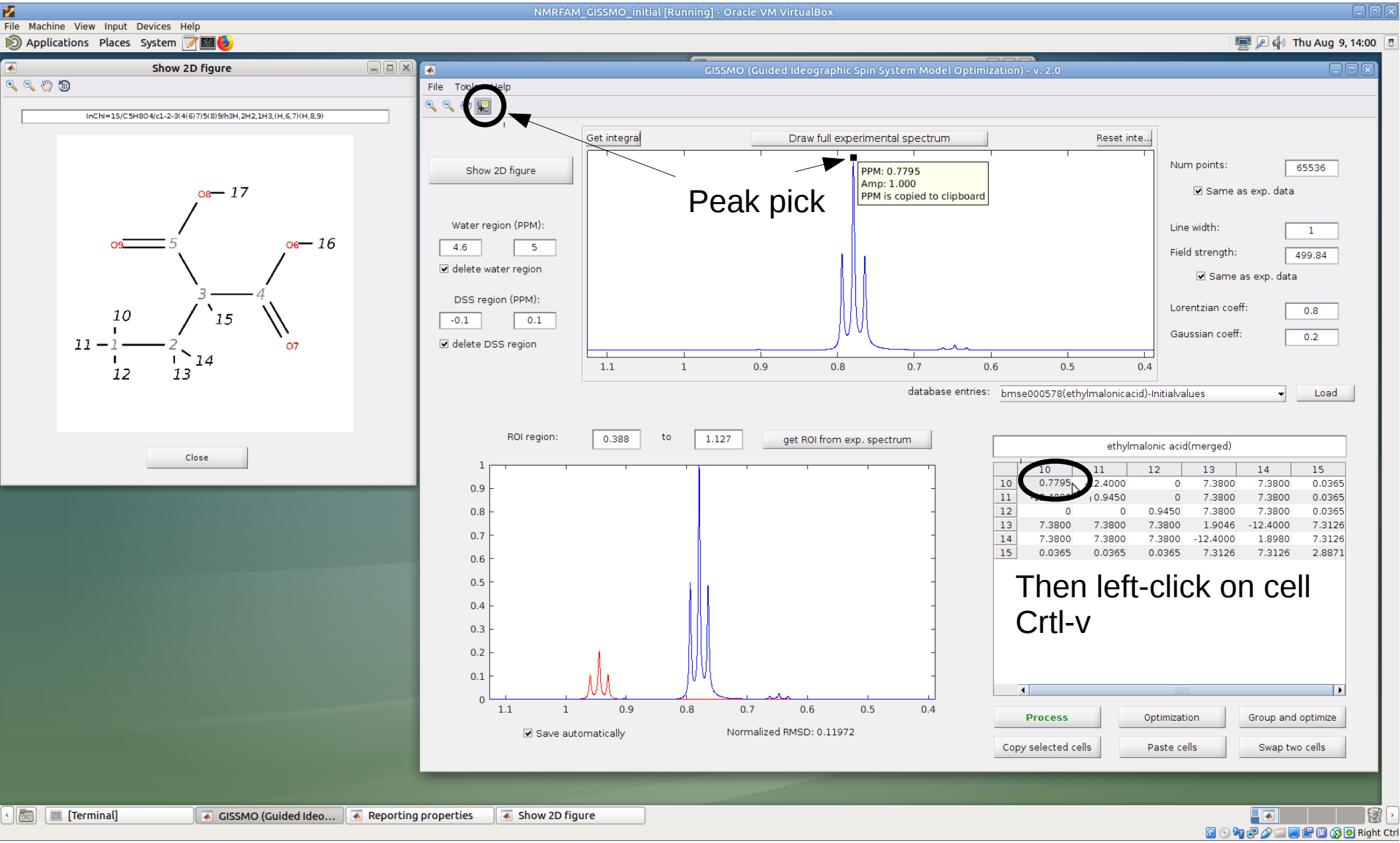
	10	11	12	13	14	15
10	0.9450	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.9450	0	7.3800	7.3800	0.0365
12	0	0	0.9450	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:00
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
O8 17
O9 5
O6 16
3 4
10
11 1 2 15
O7
12 13 14
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Peak pick
PPM: 0.7795
Amp: 1.000
PPM is copied to clipboard
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
0.388
to
1.127
get ROI from exp. spectrum
ethylmalonic acid(merged)
10 11 12 13 14 15
10 0.7795 2.4000 0 7.3800 7.3800 0.0365
11 0.9450 0 7.3800 7.3800 0.0365
12 0 0 0.9450 7.3800 7.3800 0.0365
13 7.3800 7.3800 7.3800 1.9046 -12.4000 7.3126
14 7.3800 7.3800 7.3800 -12.4000 1.8980 7.3126
15 0.0365 0.0365 0.0365 7.3126 7.3126 2.8871
Then left-click on cell
Crtl-v
Save automatically
Normalized RMSD: 0.11972
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

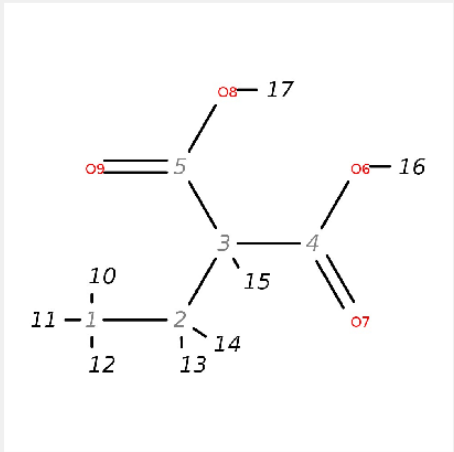
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:01

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

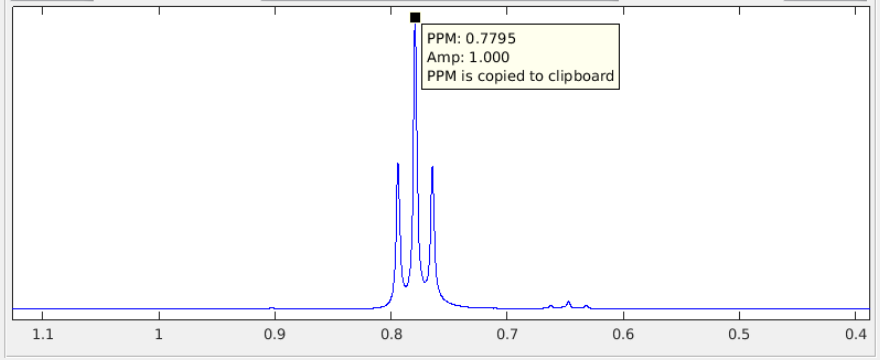
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

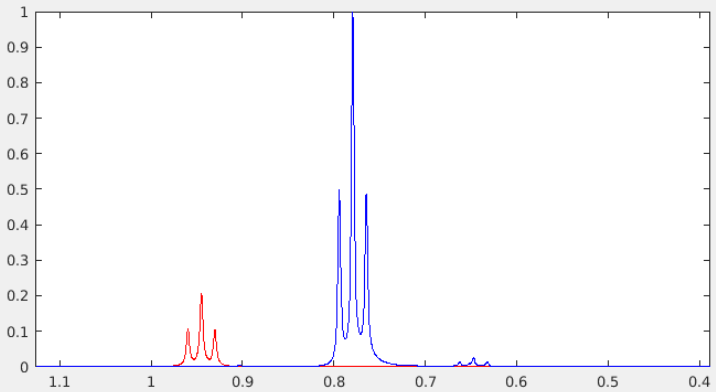
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 0.388 to 1.127 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.11972

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7795	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.7795	0	7.3800	7.3800	0.0365
12	0	0	0.9450	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Left-click on cell
Crtl-v

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

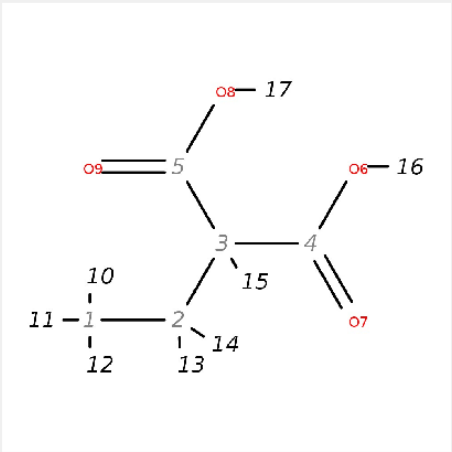
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:01

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

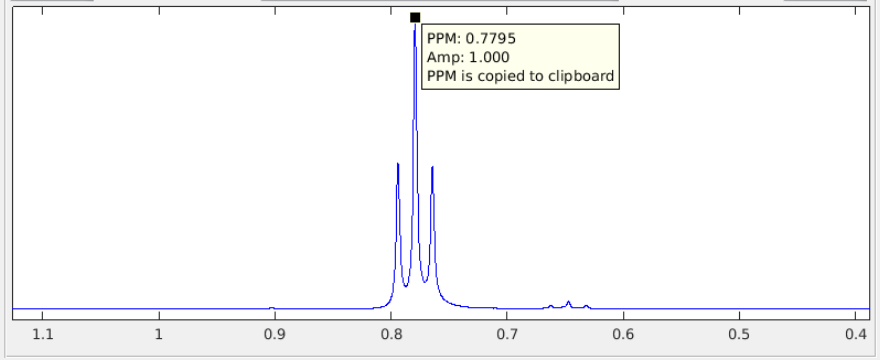
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

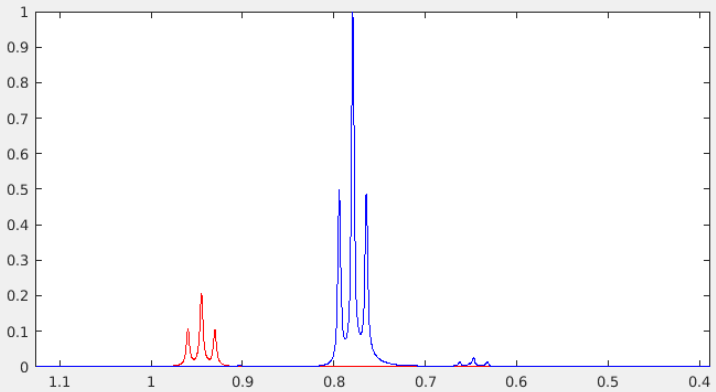
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 0.388 to 1.127 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.11972

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7795	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.7795	0	7.3800	7.3800	0.0365
12	0	0	0.9450	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Left-Clicked
Now ctrl-v

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

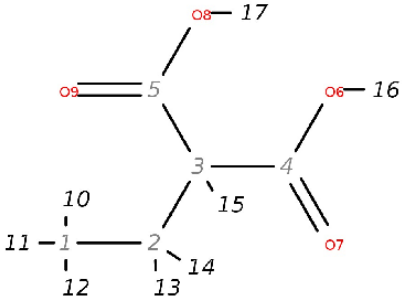
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:02

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

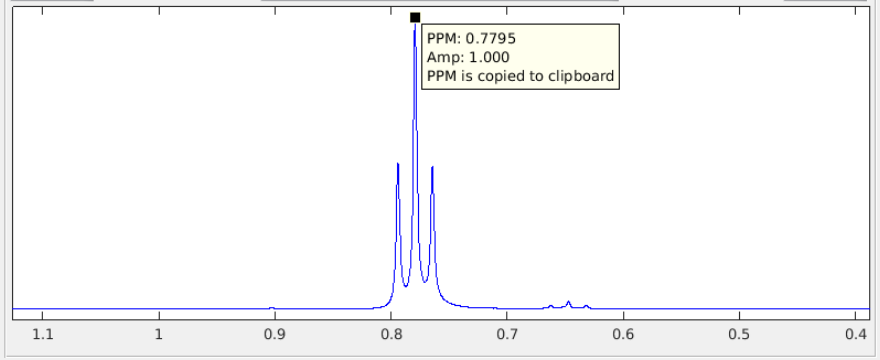
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

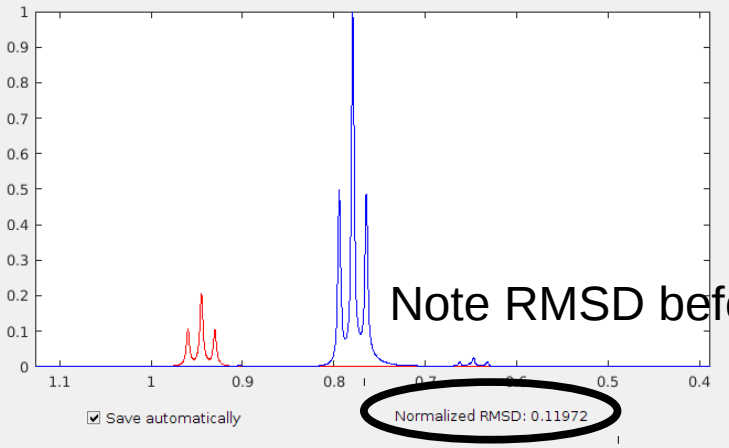
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 0.388 to 1.127 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.11972

Note RMSD before Processing

ethylmalonic acid(merged)

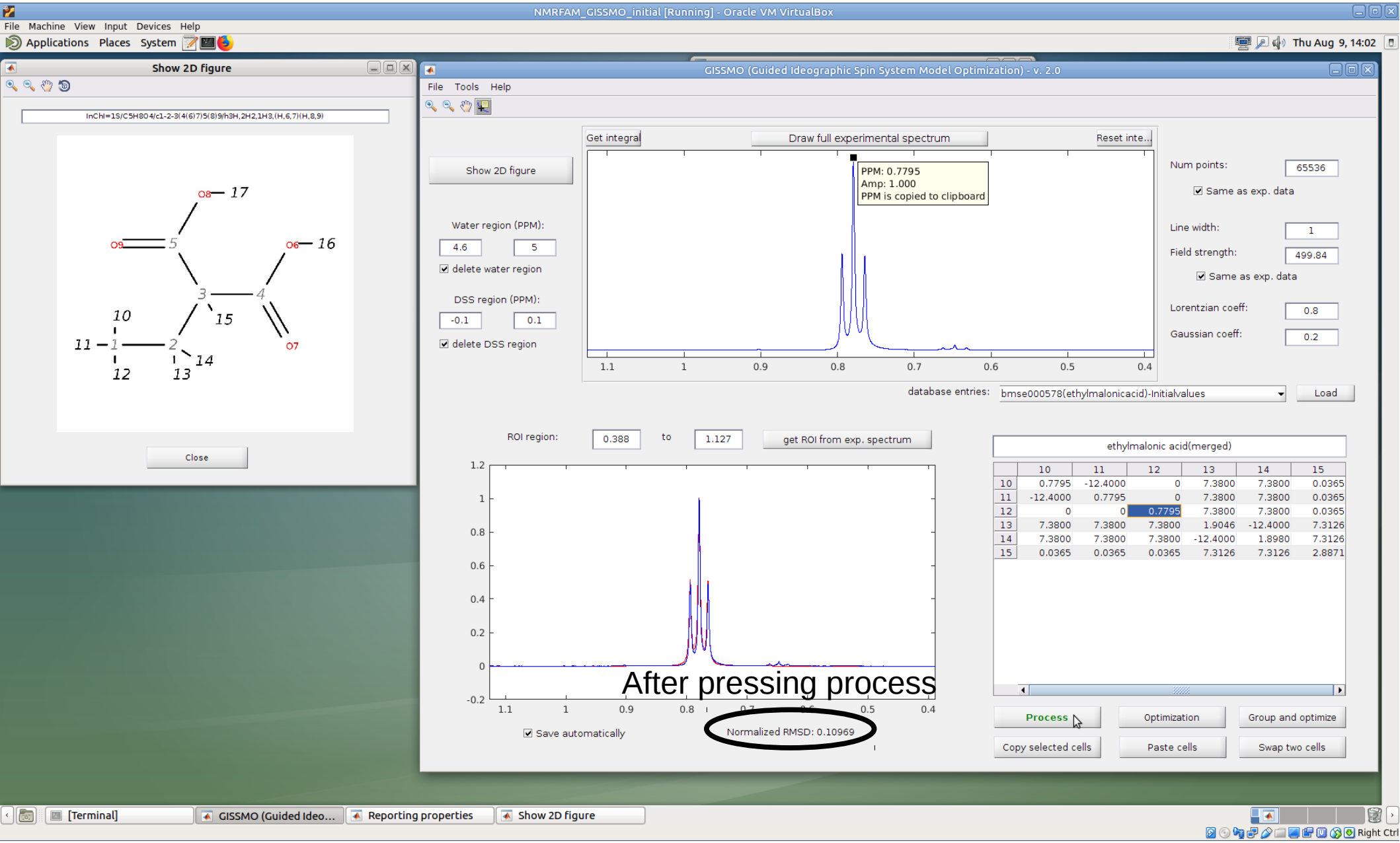
	10	11	12	13	14	15
10	0.7795	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.7795	0	7.3800	7.3800	0.0365
12	0	0	0.7795	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:02
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 0.7795
Amp: 1.000
PPM is copied to clipboard
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
0.388
to
1.127
get ROI from exp. spectrum
After pressing process
Save automatically
Normalized RMSD: 0.10969
ethylmalonic acid(merged)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

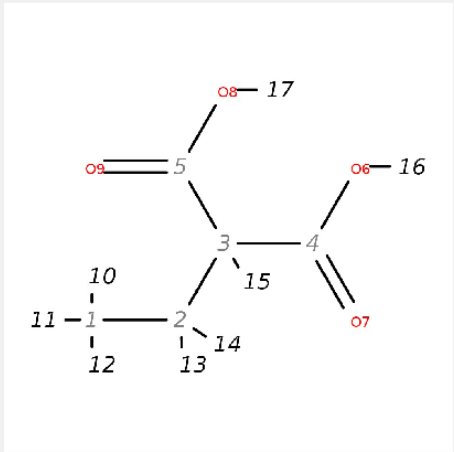
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:02

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

Show 2D figure

PPM: 0.7795
Amp: 1.000
PPM is copied to clipboard

Water region (PPM): 4.6 5 delete water region

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

Num points: 65536 Same as exp. data

Line width: 1

Field strength: 499.84 Same as exp. data

Lorentzian coeff: 0.8

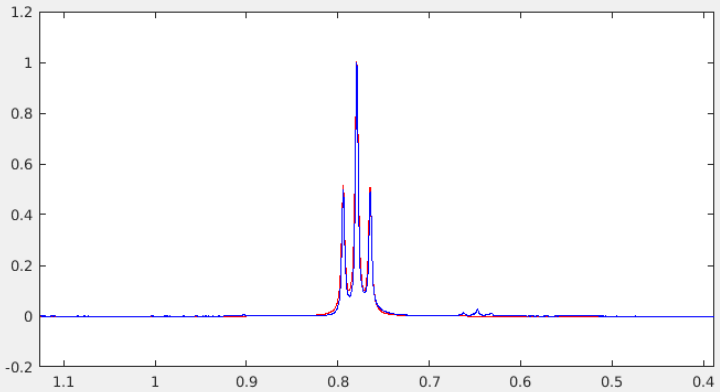
Gaussian coeff: 0.2

0.6 0.5 0.4

The 3 methyl protons
are always identical
due to chemical shift
averaging through rotation

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 0.388 to 1.127 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10969

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7795	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.7795	0	7.3800	7.3800	0.0365
12	0	0	0.7795	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Hold ctrl key
Left-click on cells
Group & optimize

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

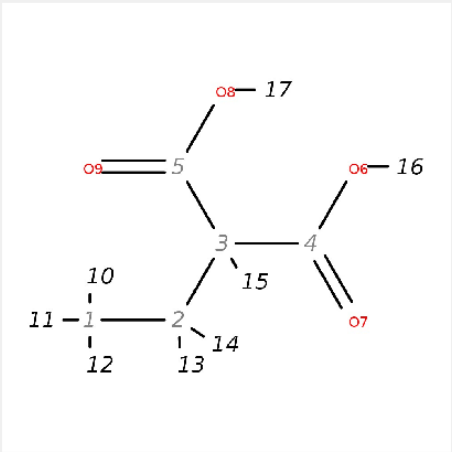
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:03

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

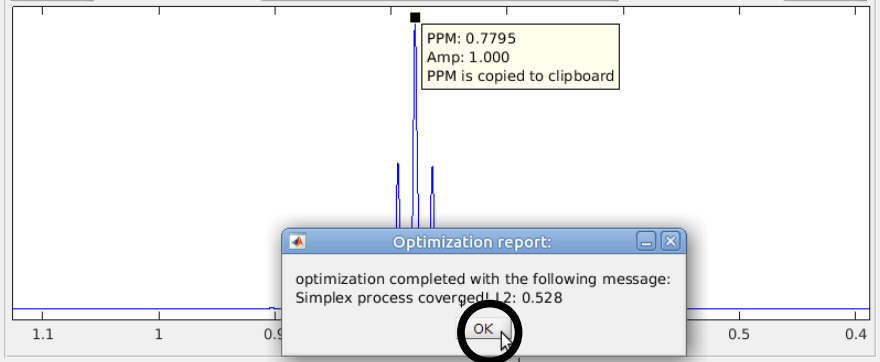
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Optimization report:

optimization completed with the following message:
Simplex process covered! L2: 0.528

OK

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

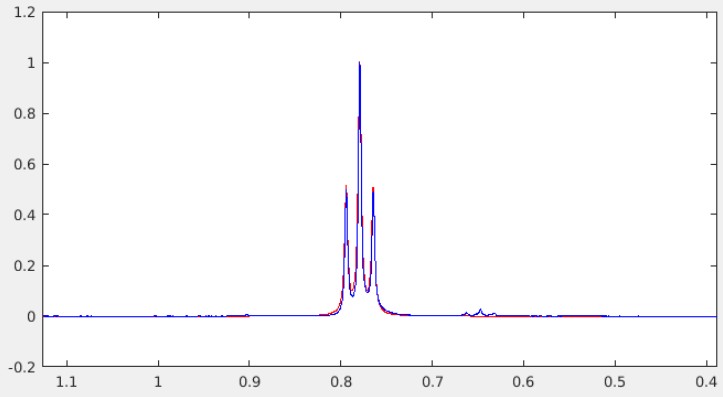
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 0.388 to 1.127 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10969

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.7794	0	7.3800	7.3800	0.0365
12	0	0	0.7794	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Optimization report:

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

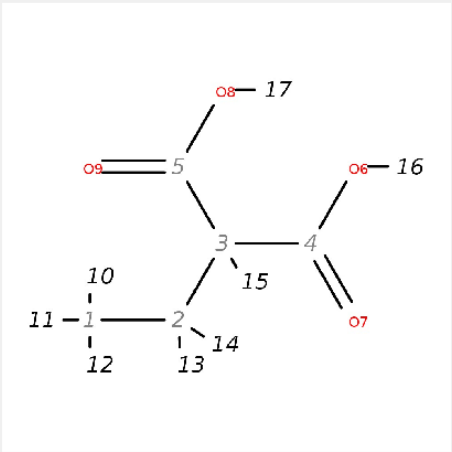
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:03

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

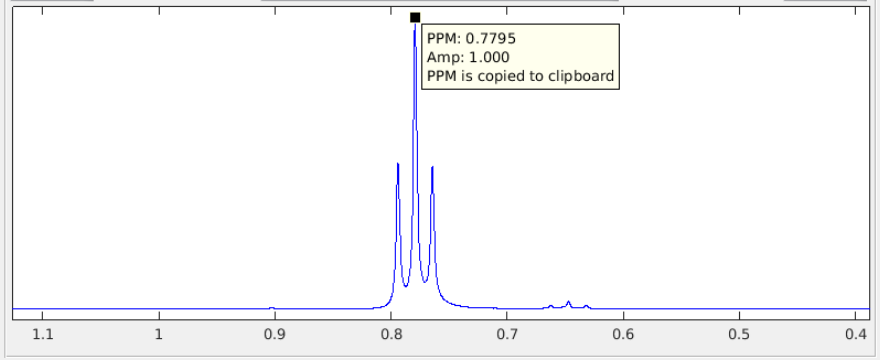
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

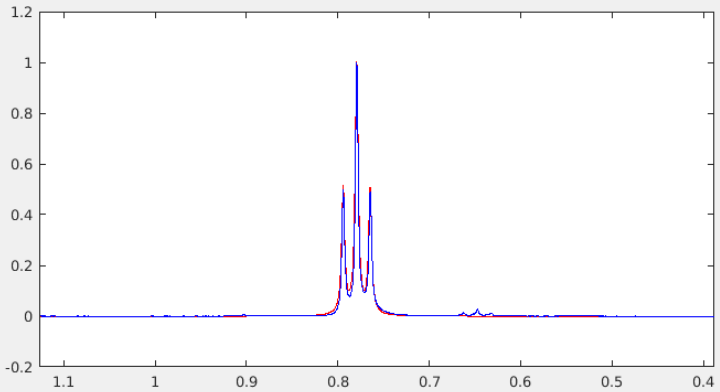
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 0.388 to 1.127 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10969

ethylmalonic acid(merged)

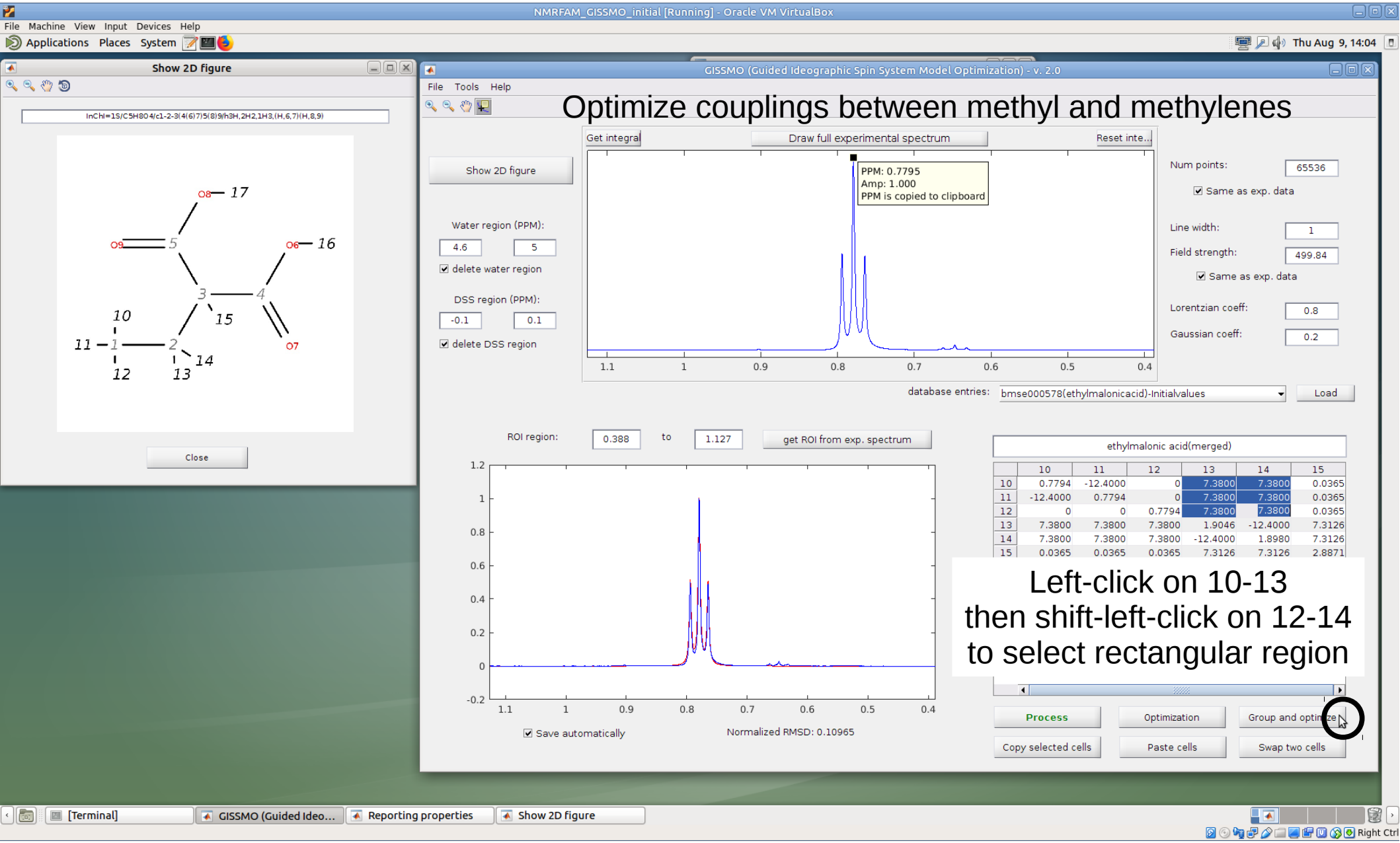
	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.3800	7.3800	0.0365
11	-12.4000	0.7794	0	7.3800	7.3800	0.0365
12	0	0	0.7794	7.3800	7.3800	0.0365
13	7.3800	7.3800	7.3800	1.9046	-12.4000	7.3126
14	7.3800	7.3800	7.3800	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

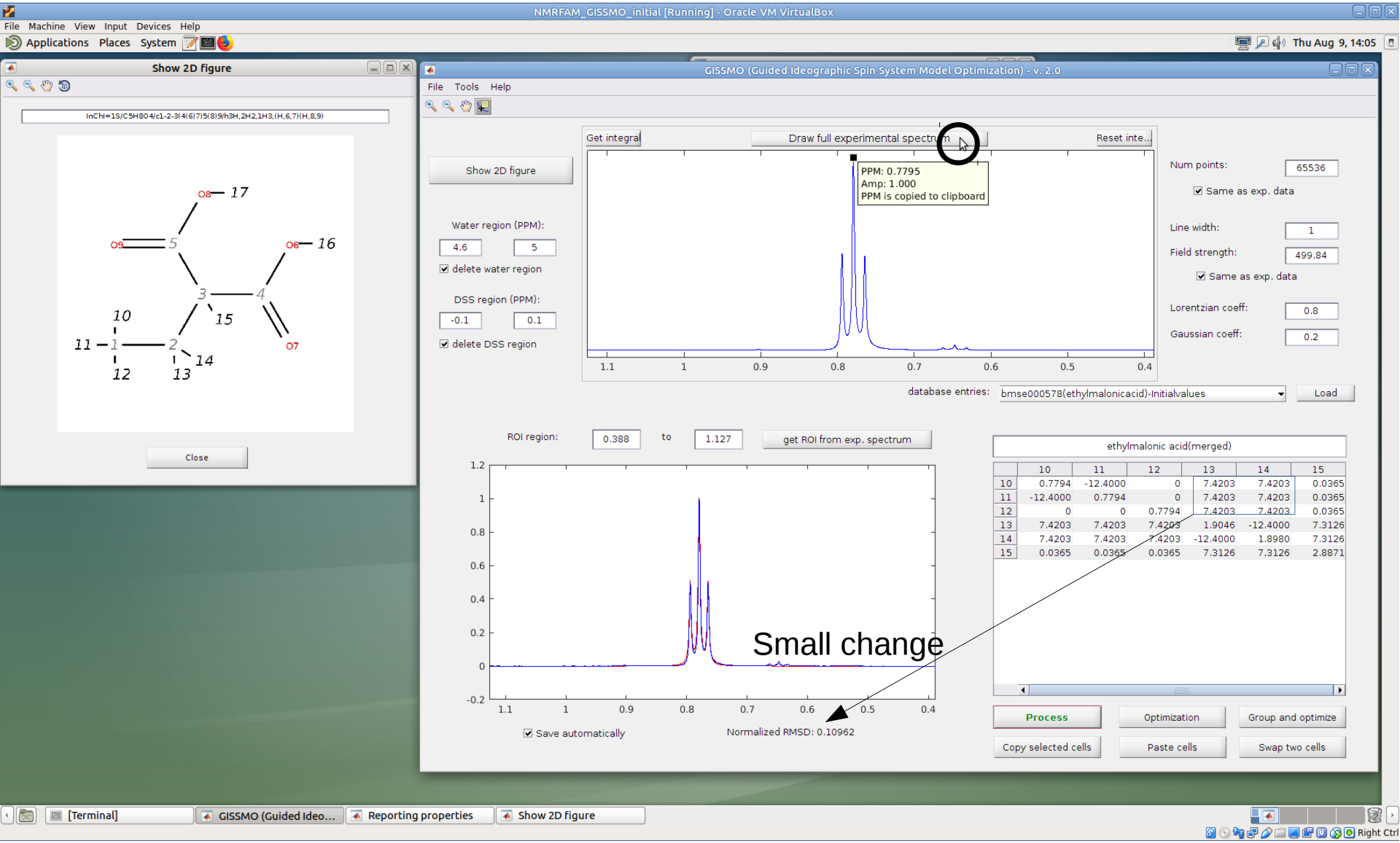
Proces | Optimization | Group and optimize

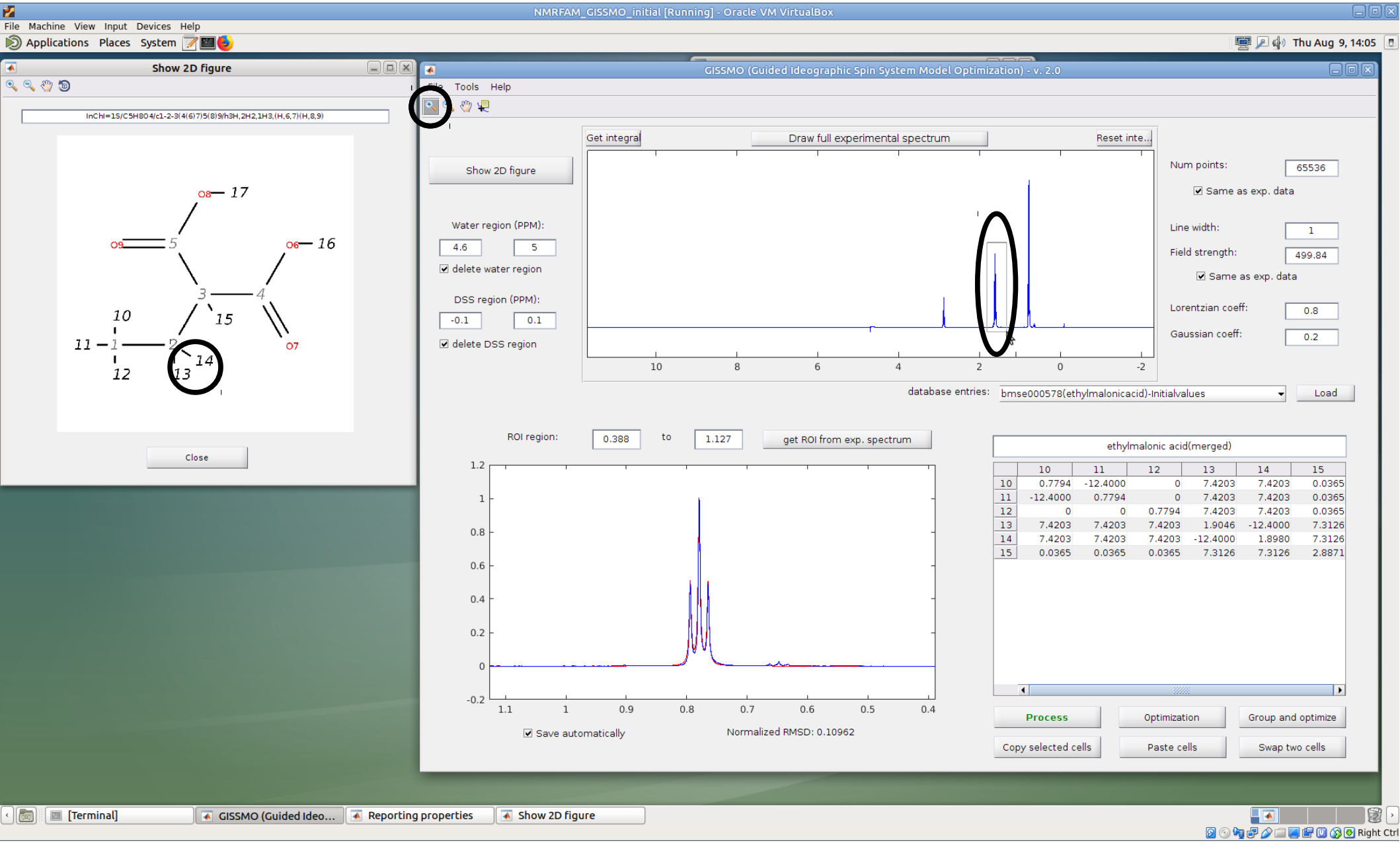
Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:04
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Optimize couplings between methyl and methylenes
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 0.7795
Amp: 1.000
PPM is copied to clipboard
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
0.388
to
1.127
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.10965
ethylmalonic acid(merged)
Left-click on 10-13
then shift-left-click on 12-14
to select rectangular region
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:05
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 0.7795
Amp: 1.000
PPM is copied to clipboard
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
0.388
to
1.127
get ROI from exp. spectrum
Small change
Save automatically
Normalized RMSD: 0.10962
ethylmalonic acid(merged)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl



	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.9046	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

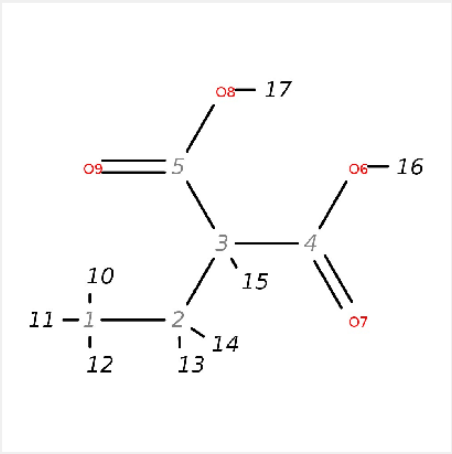
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:05

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

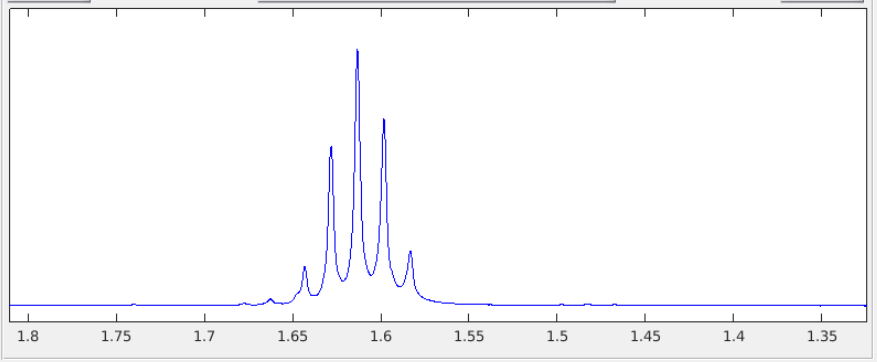
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

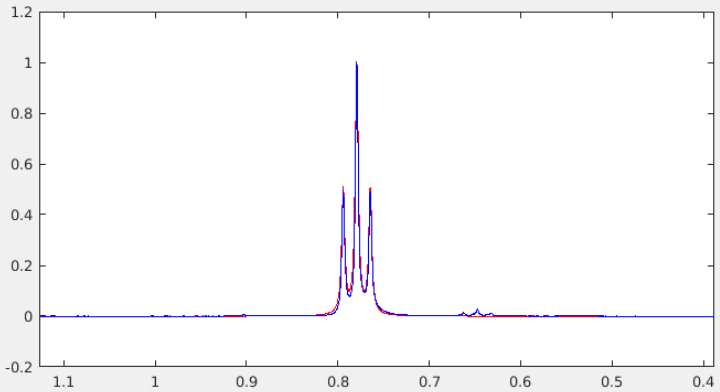
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 0.388 to 1.127 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10962

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.9046	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

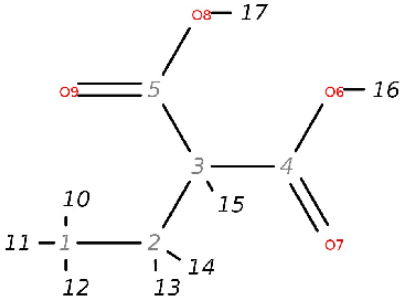
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:06

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

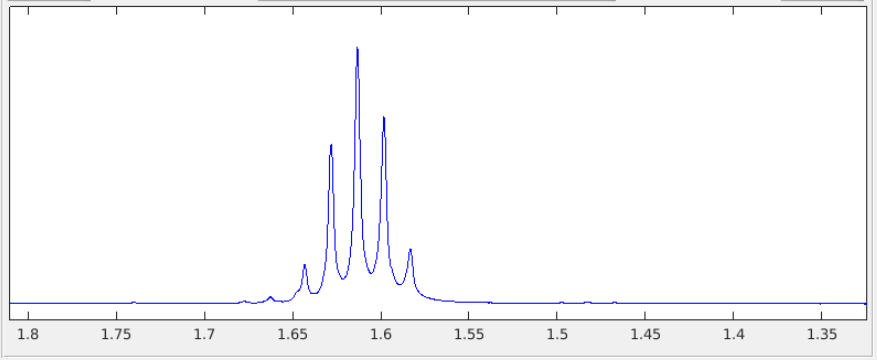
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

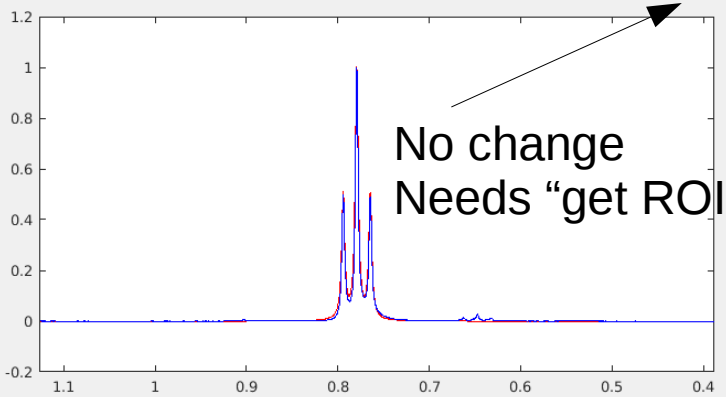
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 0.388 to 1.127 | get ROI from exp. spectrum



No change
Needs “get ROI ...”

Save automatically

Normalized RMSD: 0.10962

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.9046	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

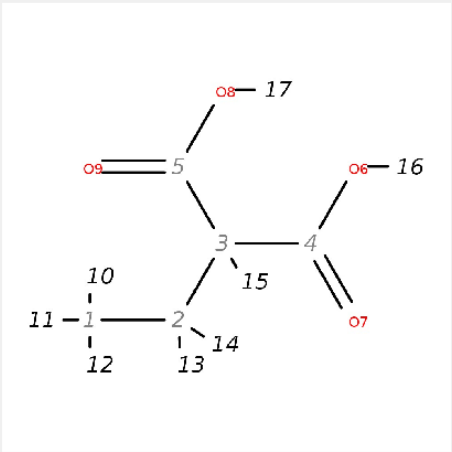
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:06

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

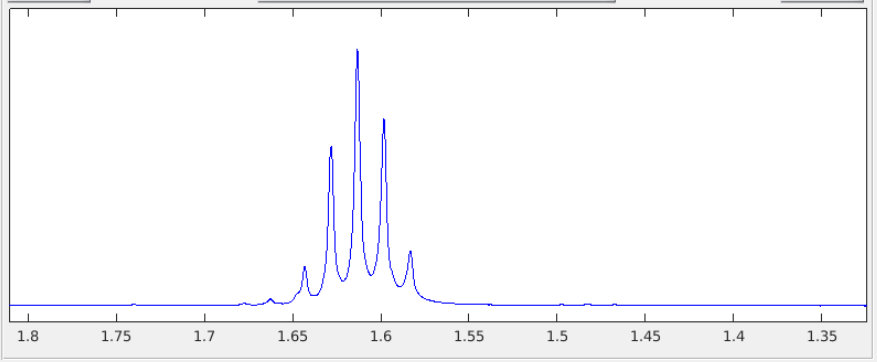
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

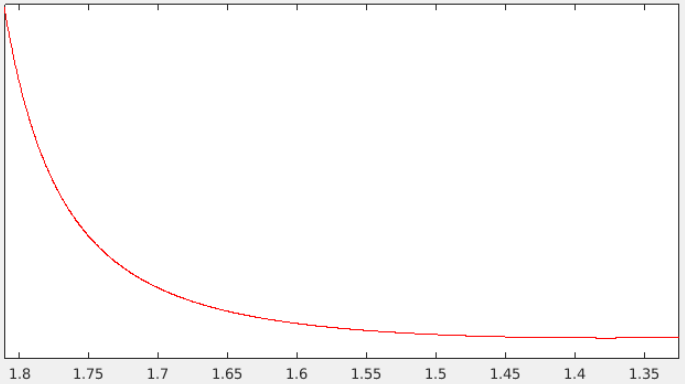
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 1.325 to 1.811 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10962

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.9046	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Then process

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

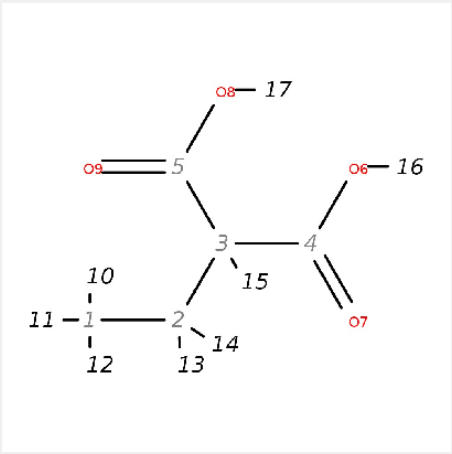
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:06

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

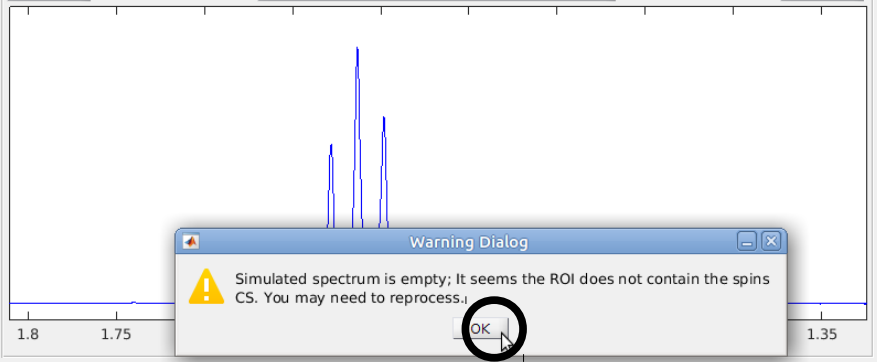
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

Warning Dialog

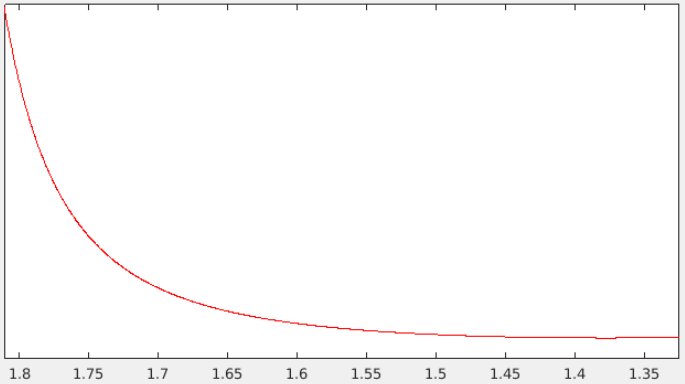
Simulated spectrum is empty; It seems the ROI does not contain the spins CS. You may need to reprocess.

OK

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

Usually ignore this warning

ROI region: 1.325 to 1.811 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10962

ethylmalonic acid(merged)

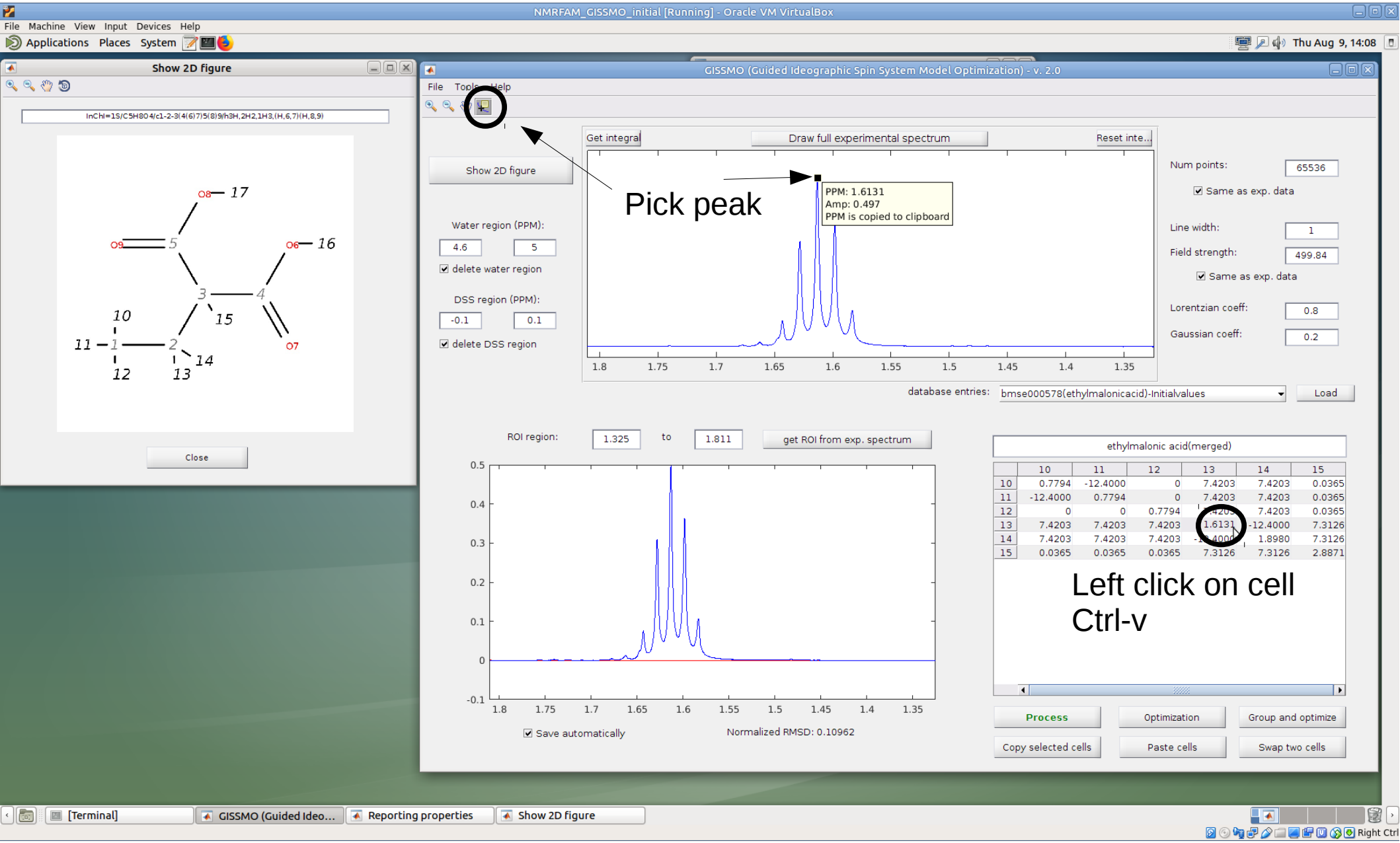
	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.9046	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Processing | Warning Dialog

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:08
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Pick peak
PPM: 1.6131
Amp: 0.497
PPM is copied to clipboard
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
1.325
to
1.811
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.10962
ethylmalonic acid(merged)
Left click on cell
Ctrl-v
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

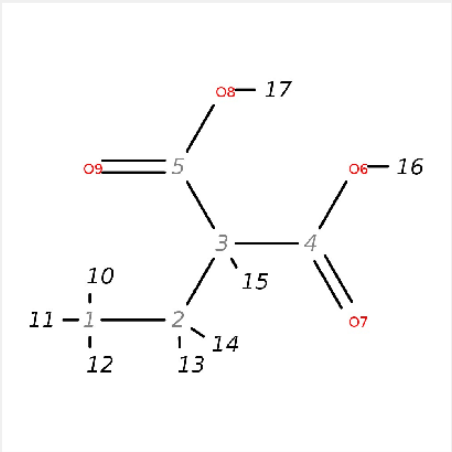
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:08

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

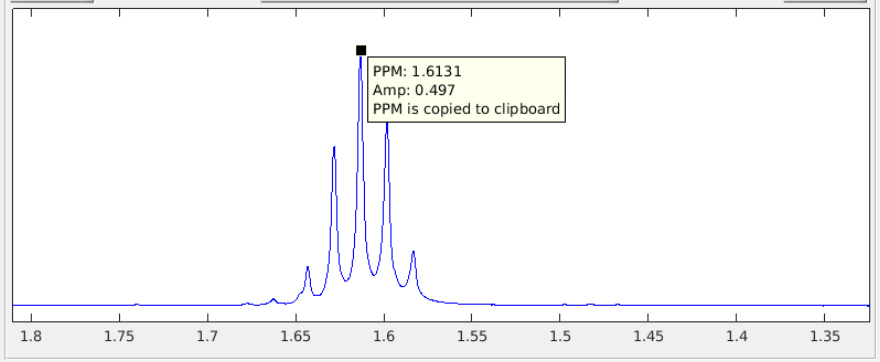
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

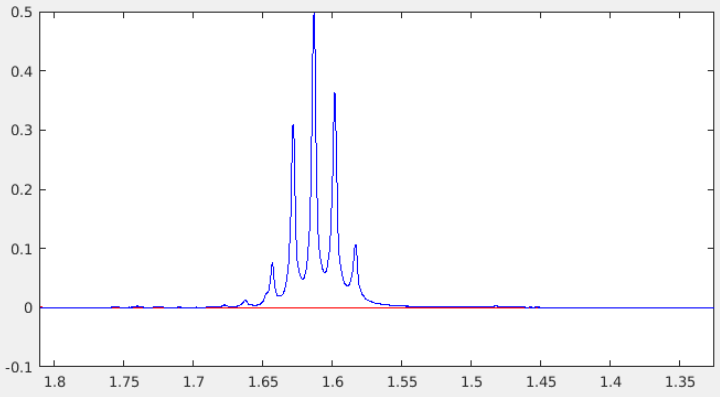
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 1.325 to 1.811 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10962

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.8980	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Left-click on cell
Ctrl-v

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

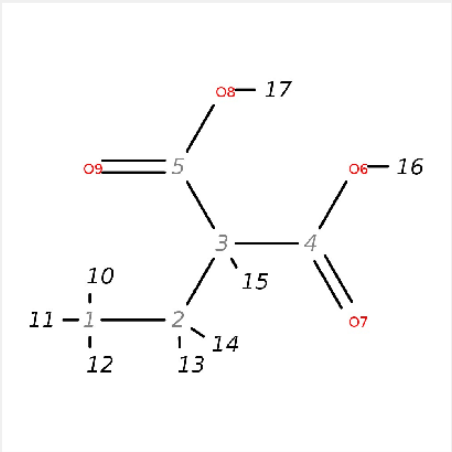
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:09

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Show 2D figure

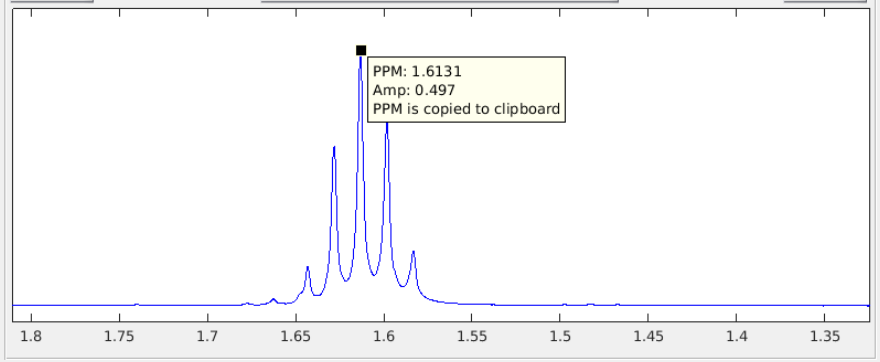
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Get integral | Draw full experimental spectrum | Reset inte...



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

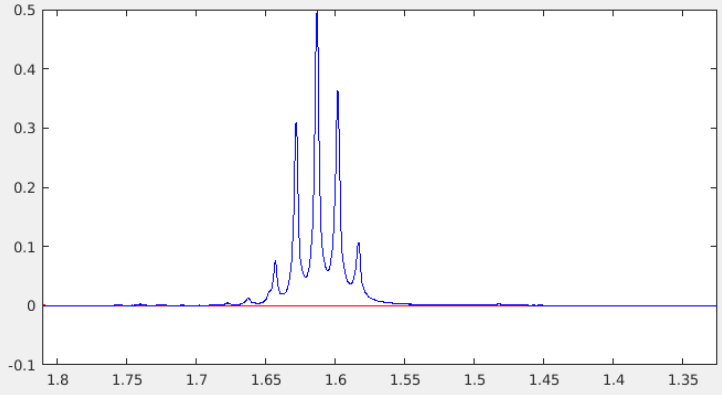
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 1.325 to 1.811 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.10962

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Proces | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

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File Machine View Input Devices Help

Applications Places System

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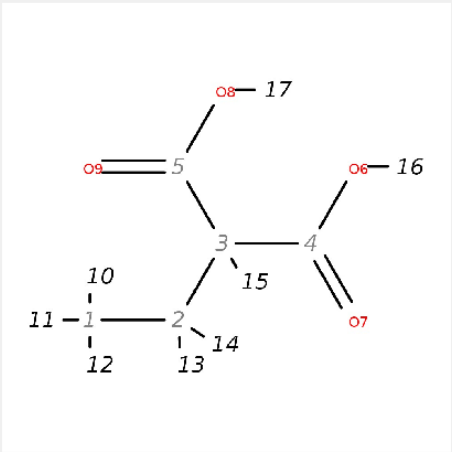
Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Show 2D figure

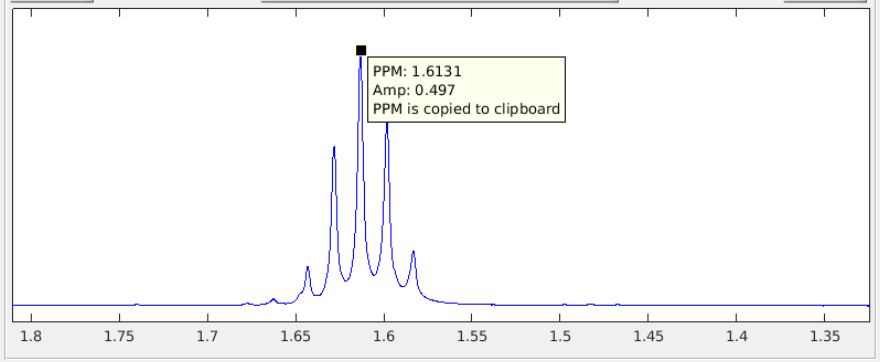
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Get integral | Draw full experimental spectrum | Reset inte...



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

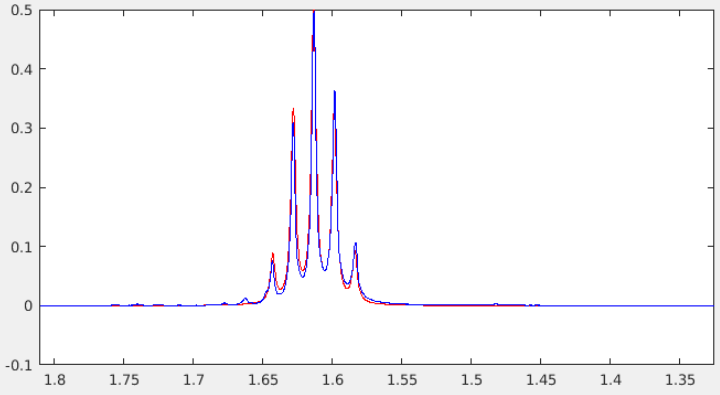
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 1.325 to 1.811 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01083

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Hold ctrl;left-click on cells
Group & optimize

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

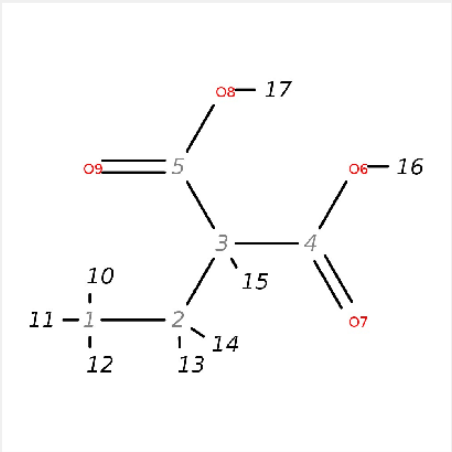
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:10

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

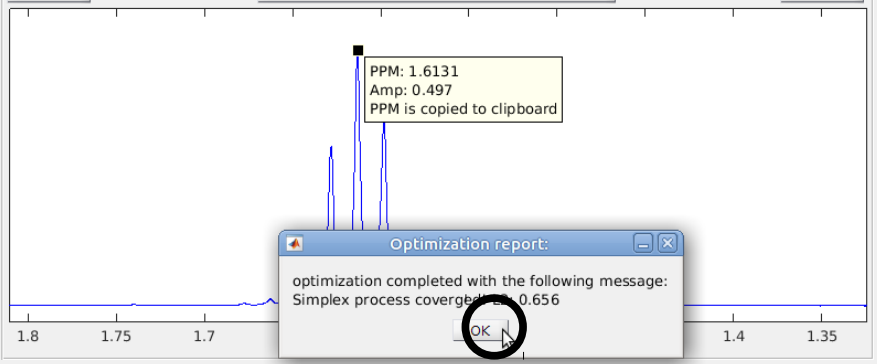
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Optimization report:

optimization completed with the following message:
Simplex process covergence: 0.656

OK

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

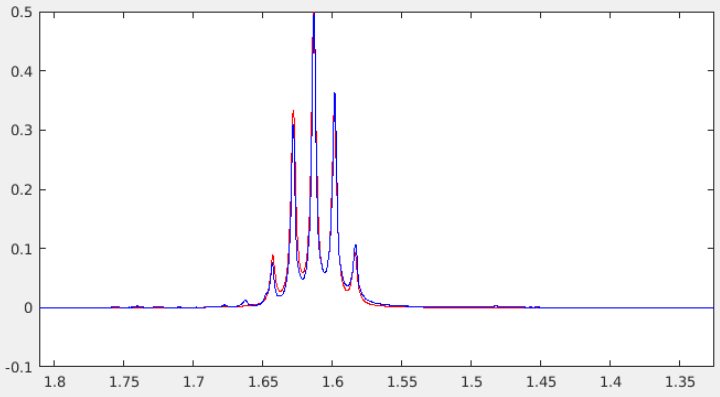
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 1.325 to 1.811 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01083

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Optimization report:

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

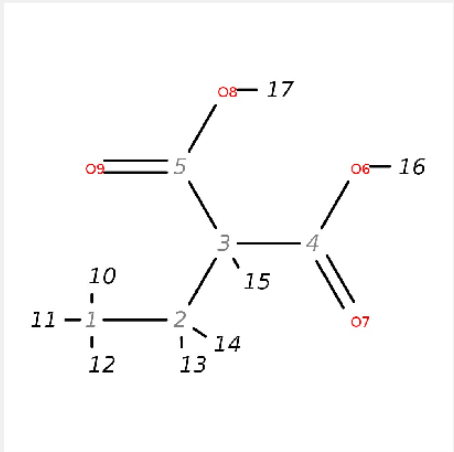
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:10

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Show 2D figure

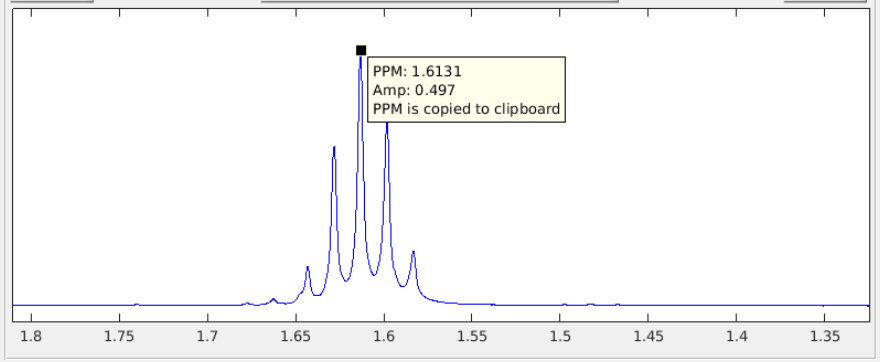
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Get integral | Draw full experimental spectrum | Reset inte...



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

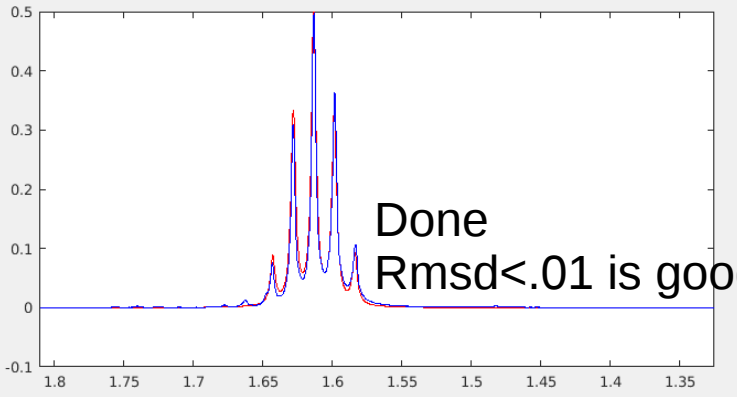
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues | Load

ROI region: 1.325 to 1.811 | get ROI from exp. spectrum



Done
Rmsd<.01 is good

Save automatically

Normalized RMSD: 0.01083

ethylmalonic acid(merged)

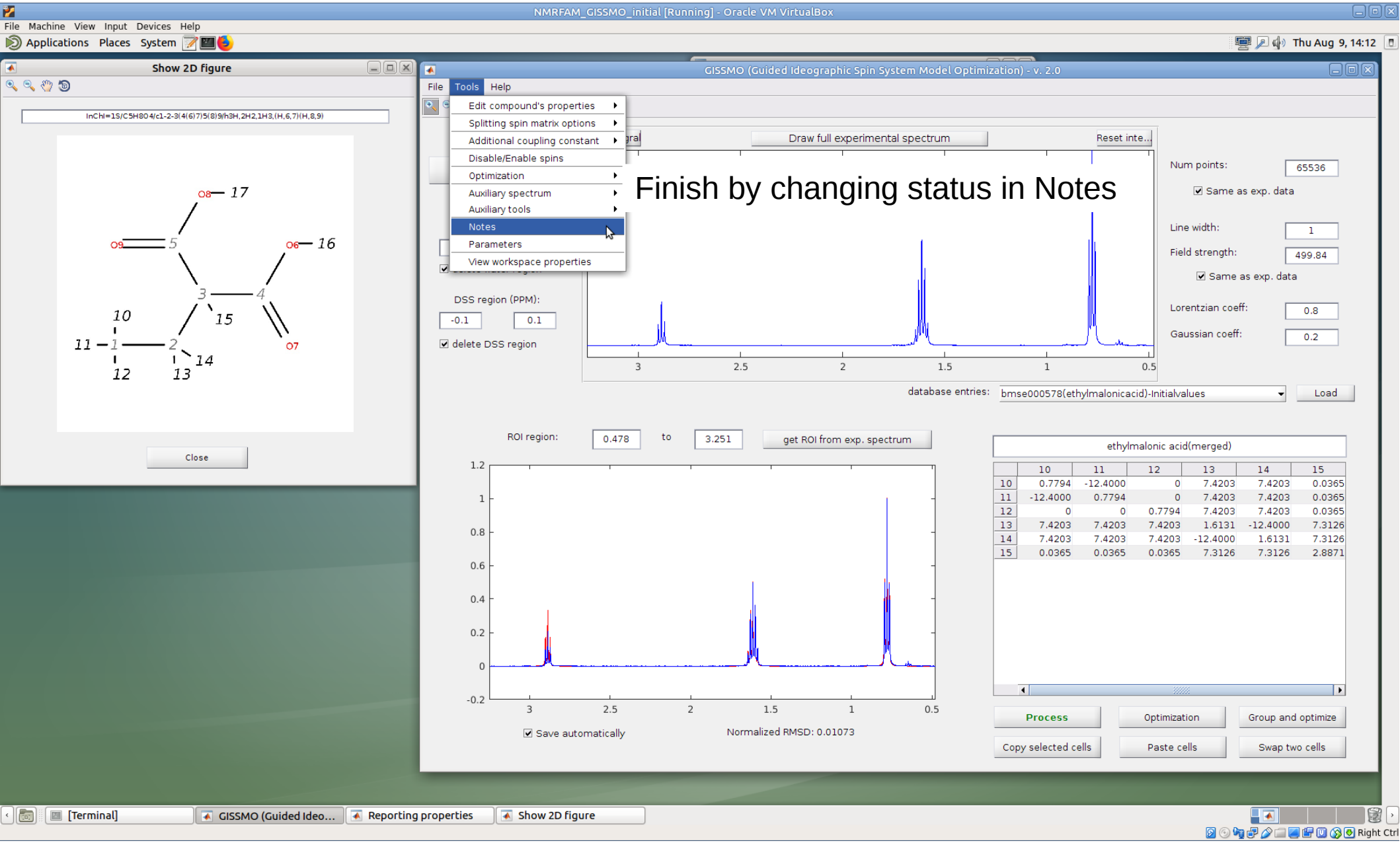
	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:12
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Edit compound's properties
Splitting spin matrix options
Additional coupling constant
Disable/Enable spins
Optimization
Auxiliary spectrum
Auxiliary tools
Notes
Parameters
View workspace properties
Finish by changing status in Notes
Draw full experimental spectrum
Reset inte...
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
DSS region (PPM):
-0.1
0.1
delete DSS region
database entries:
bmse000578(ethylmalonicacid)-Initialvalues
Load
ROI region:
0.478
to
3.251
get ROI from exp. spectrum
ethylmalonic acid(merged)
Save automatically
Normalized RMSD: 0.01073
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

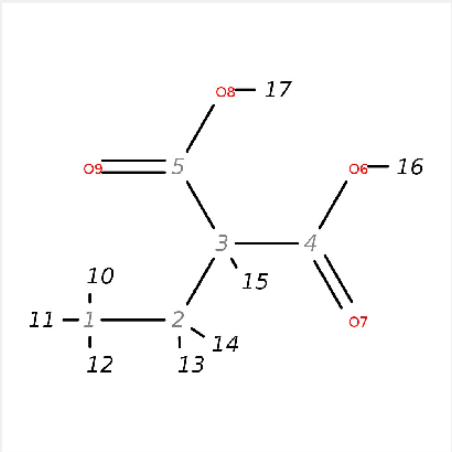
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:12

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset inte...

Notes

Status:

Initial values

choose status
Initial values
Active
Approximately done
Complicated
Done
Difficult
No C-H proton
2H exchange
Problem

Notes:

Apply Cancel

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

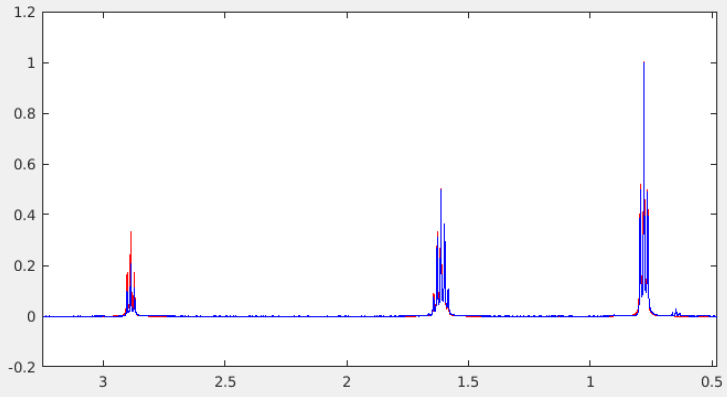
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

Good RMSD: status Done

ROI region: 0.478 to 3.251 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01073

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure Notes

Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

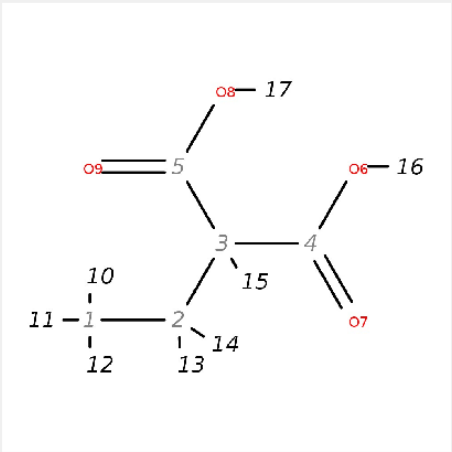
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:13

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset inte...

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

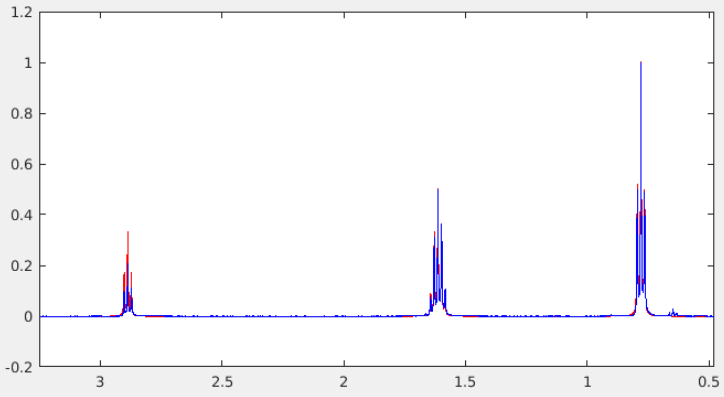
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000578(ethylmalonicacid)-Initialvalues Load

ROI region: 0.478 to 3.251 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01073

ethylmalonic acid(merged)

	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

Notes

Status:

Done

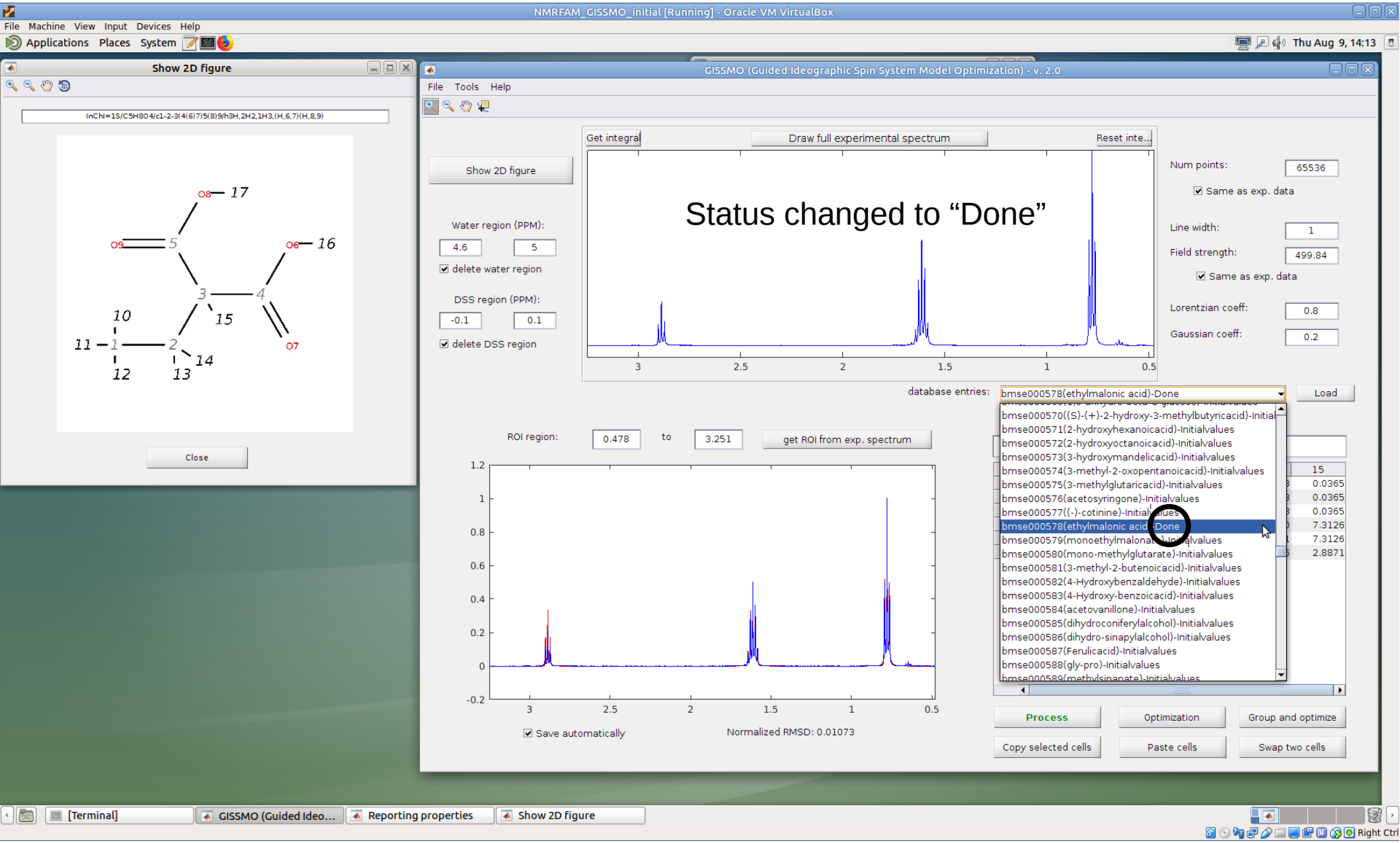
Notes:

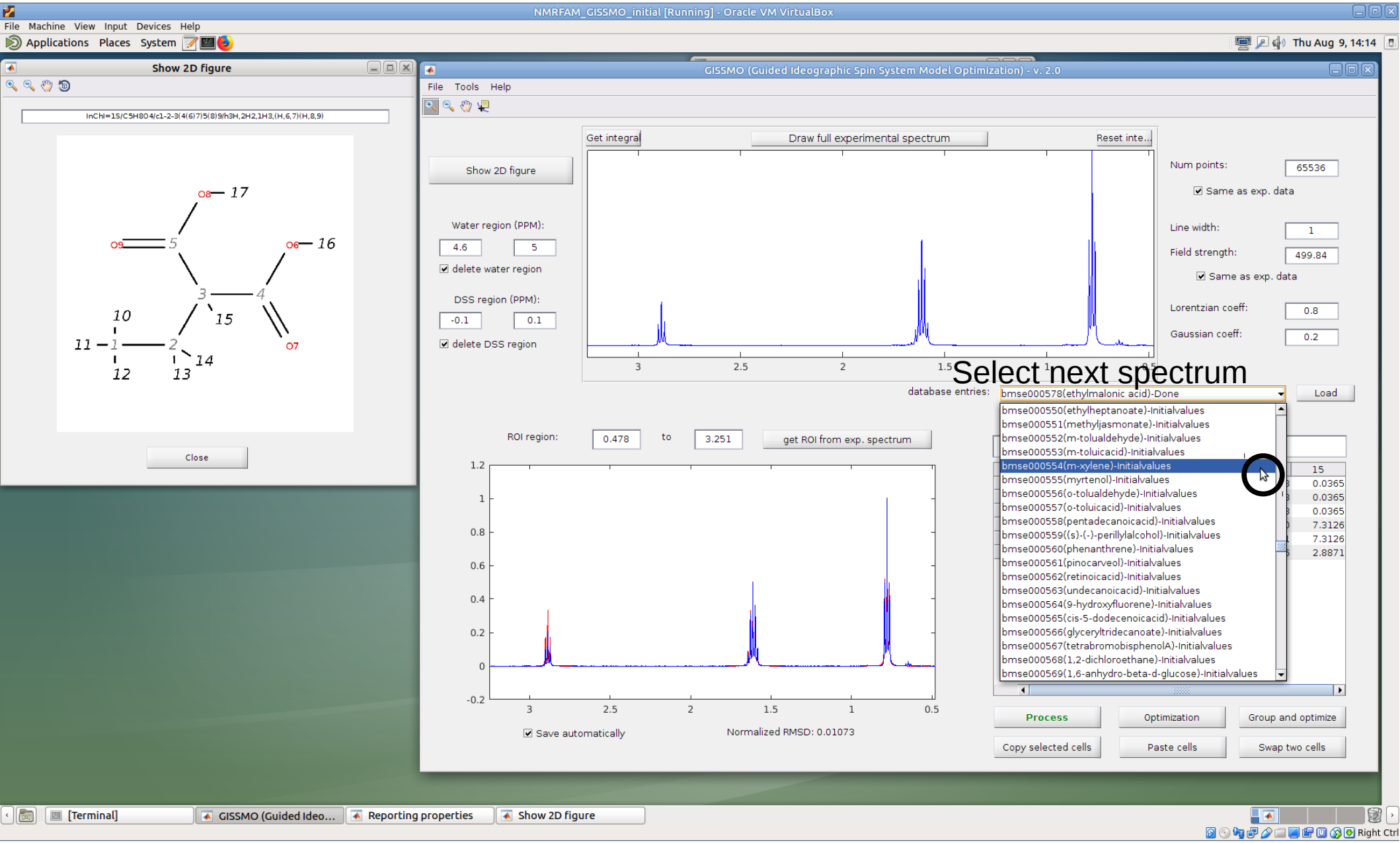
Add any comments here

Apply Cancel

[Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure Notes

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:13
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Status changed to “Done”
Num points:
65536
Same as exp. data
Water region (PPM):
4.6
5
delete water region
Line width:
1
Field strength:
499.84
Same as exp. data
DSS region (PPM):
-0.1
0.1
delete DSS region
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000578(ethylmalonic acid)-Done
Load
ROI region:
0.478
to
3.251
get ROI from exp. spectrum
bmse000570((S)-(+)-2-hydroxy-3-methylbutyricacid)-Initial
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(ethylmalonic acid)-Done
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(methylsinapate)-Initialvalues
15
0.0365
0.0365
0.0365
7.3126
7.3126
2.8871
Save automatically
Normalized RMSD: 0.01073
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:14
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
Select next spectrum
database entries:
bmse000578(ethylmalonic acid)-Done
Load
bmse000550(ethylheptanoate)-Initialvalues
bmse000551(methyljasmonate)-Initialvalues
bmse000552(m-tolualdehyde)-Initialvalues
bmse000553(m-toluicacid)-Initialvalues
bmse000554(m-xylene)-Initialvalues
bmse000555(myrtenol)-Initialvalues
bmse000556(o-tolualdehyde)-Initialvalues
bmse000557(o-toluicacid)-Initialvalues
bmse000558(pentadecanoicacid)-Initialvalues
bmse000559((s)-(-)-perillylalcohol)-Initialvalues
bmse000560(phenanthrene)-Initialvalues
bmse000561(pinocarveol)-Initialvalues
bmse000562(retinoicacid)-Initialvalues
bmse000563(undecanoicacid)-Initialvalues
bmse000564(9-hydroxyfluorene)-Initialvalues
bmse000565(cis-5-dodecenoicacid)-Initialvalues
bmse000566(glyceryltridecanoate)-Initialvalues
bmse000567(tetrabromobisphenolA)-Initialvalues
bmse000568(1,2-dichloroethane)-Initialvalues
bmse000569(1,6-anhydro-beta-d-glucose)-Initialvalues
ROI region:
0.478
to
3.251
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.01073
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

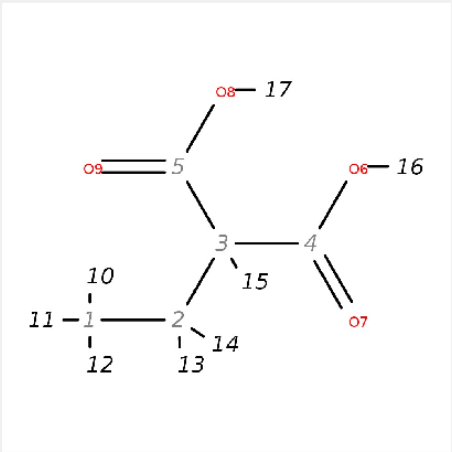
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:14

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

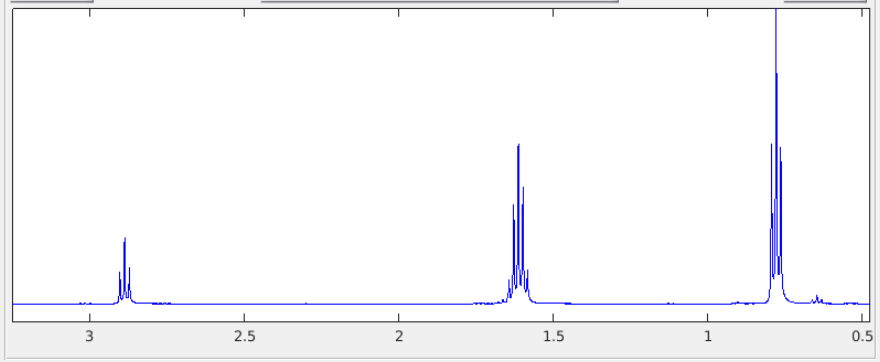
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

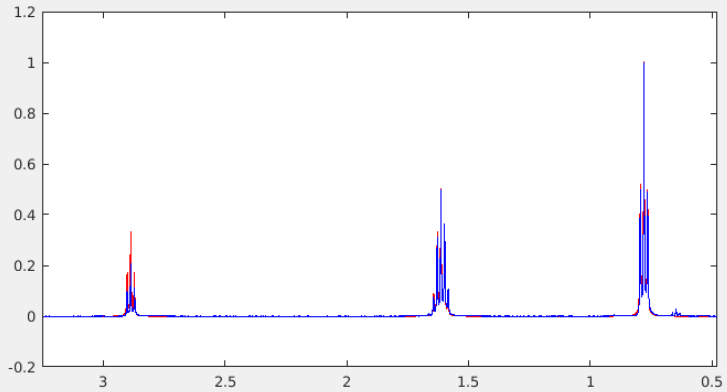
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000554(m-xylene)-Initialvalues | Load

ROI region: 0.478 to 3.251 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01073

ethylmalonic acid(merged)

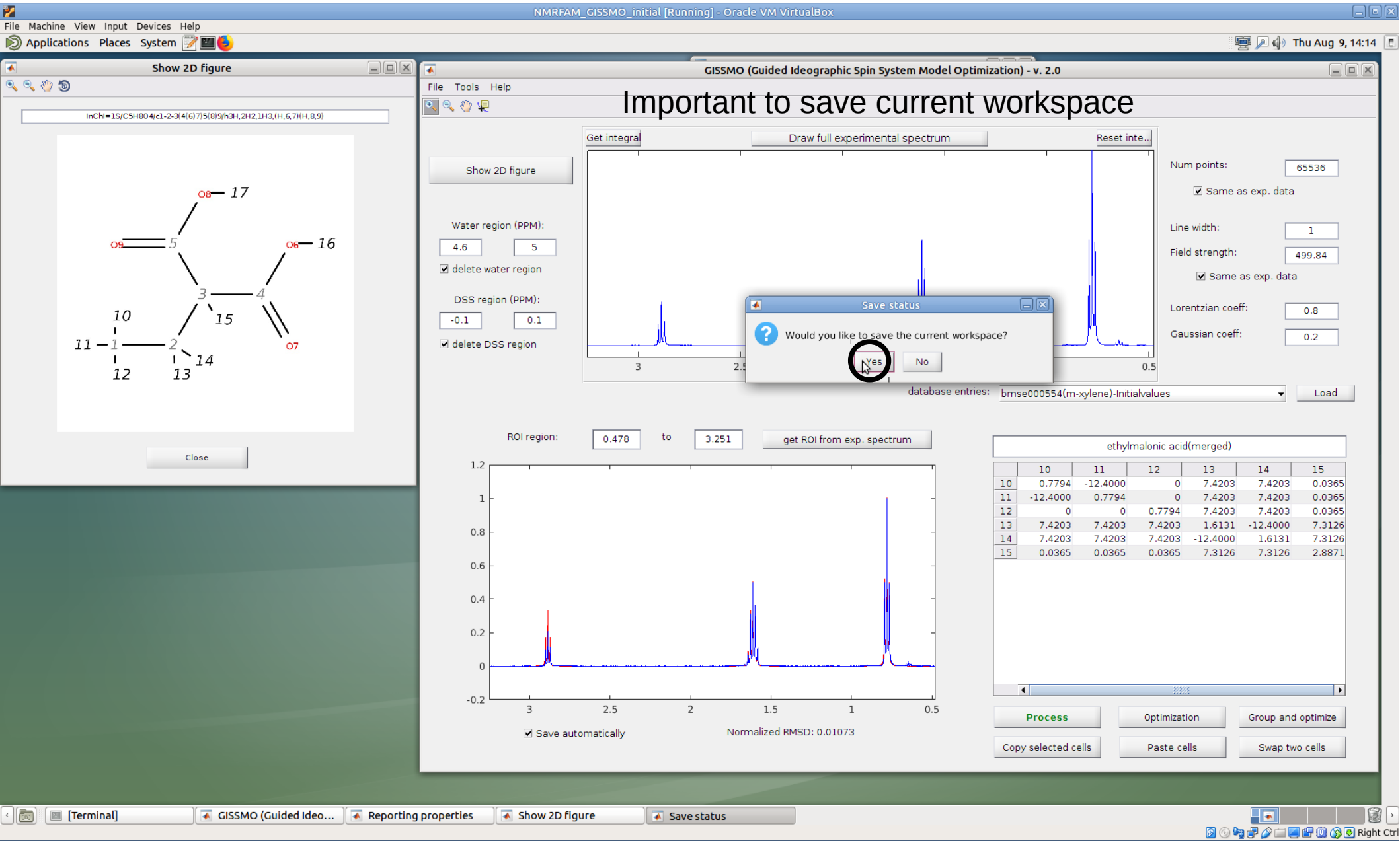
	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Thu Aug 9, 14:14
Show 2D figure
InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Important to save current workspace
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
65536
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
Save status
Would you like to save the current workspace?
Yes
No
database entries:
bmse000554(m-xylene)-Initialvalues
Load
ROI region:
0.478
to
3.251
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.01073
ethylmalonic acid(merged)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Save status
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

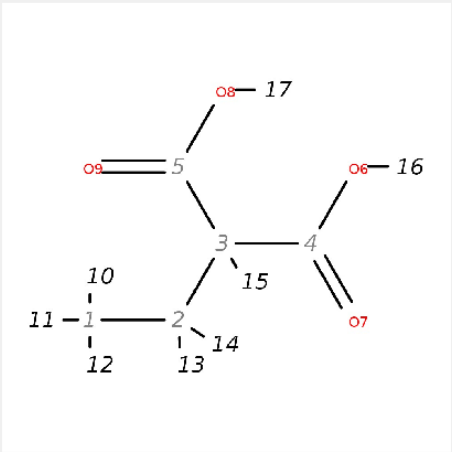
File Machine View Input Devices Help

Applications Places System

Thu Aug 9, 14:15

Show 2D figure

InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)



Close

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

File Tools Help

Get integral | Draw full experimental spectrum | Reset inte...

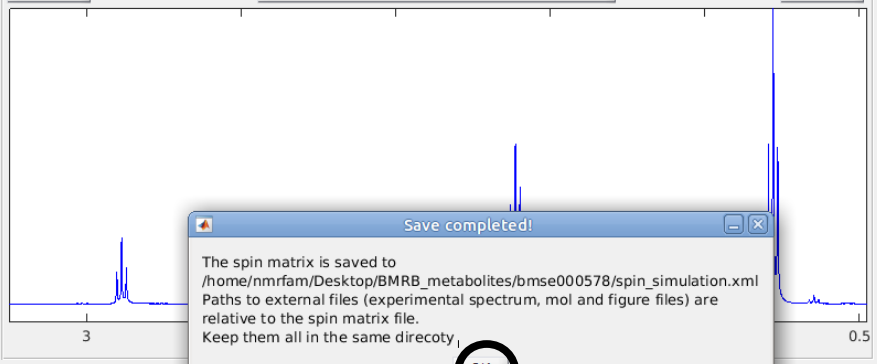
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

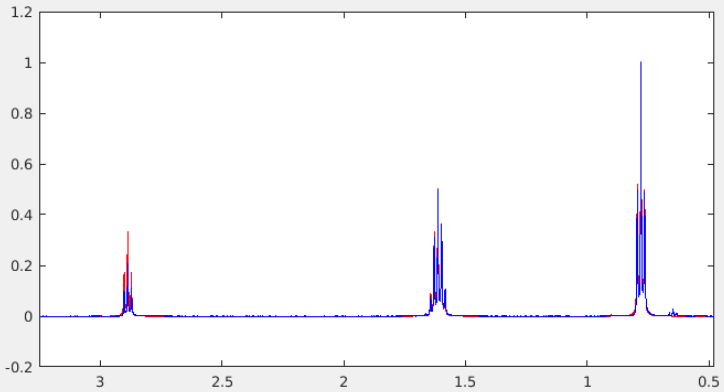
ene)-Initialvalues | Load

Save completed!

The spin matrix is saved to
/home/nmrfam/Desktop/BMRB_metabolites/bmse000578/spin_simulation.xml
Paths to external files (experimental spectrum, mol and figure files) are relative to the spin matrix file.
Keep them all in the same direcoty

OK

ROI region: 0.478 to 3.251 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01073

ethylmalonic acid(merged)

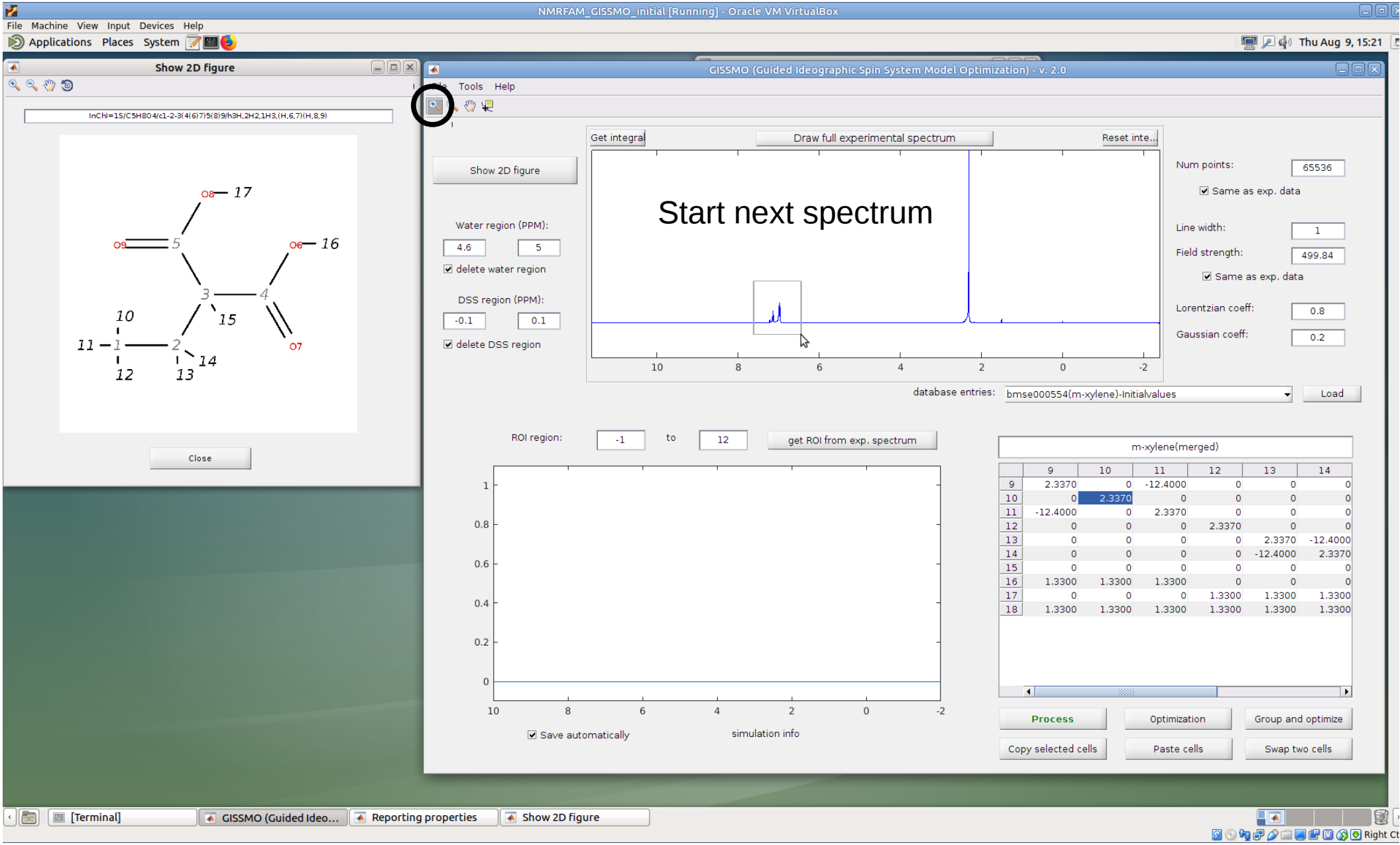
	10	11	12	13	14	15
10	0.7794	-12.4000	0	7.4203	7.4203	0.0365
11	-12.4000	0.7794	0	7.4203	7.4203	0.0365
12	0	0	0.7794	7.4203	7.4203	0.0365
13	7.4203	7.4203	7.4203	1.6131	-12.4000	7.3126
14	7.4203	7.4203	7.4203	-12.4000	1.6131	7.3126
15	0.0365	0.0365	0.0365	7.3126	7.3126	2.8871

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Save completed!

Right Ctrl



	9	10	11	12	13	14
9	2.3370	0	-12.4000	0	0	0
10	0	2.3370	0	0	0	0
11	-12.4000	0	2.3370	0	0	0
12	0	0	0	2.3370	0	0
13	0	0	0	0	2.3370	-12.4000
14	0	0	0	0	-12.4000	2.3370
15	0	0	0	0	0	0
16	1.3300	1.3300	1.3300	0	0	0
17	0	0	0	1.3300	1.3300	1.3300
18	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300