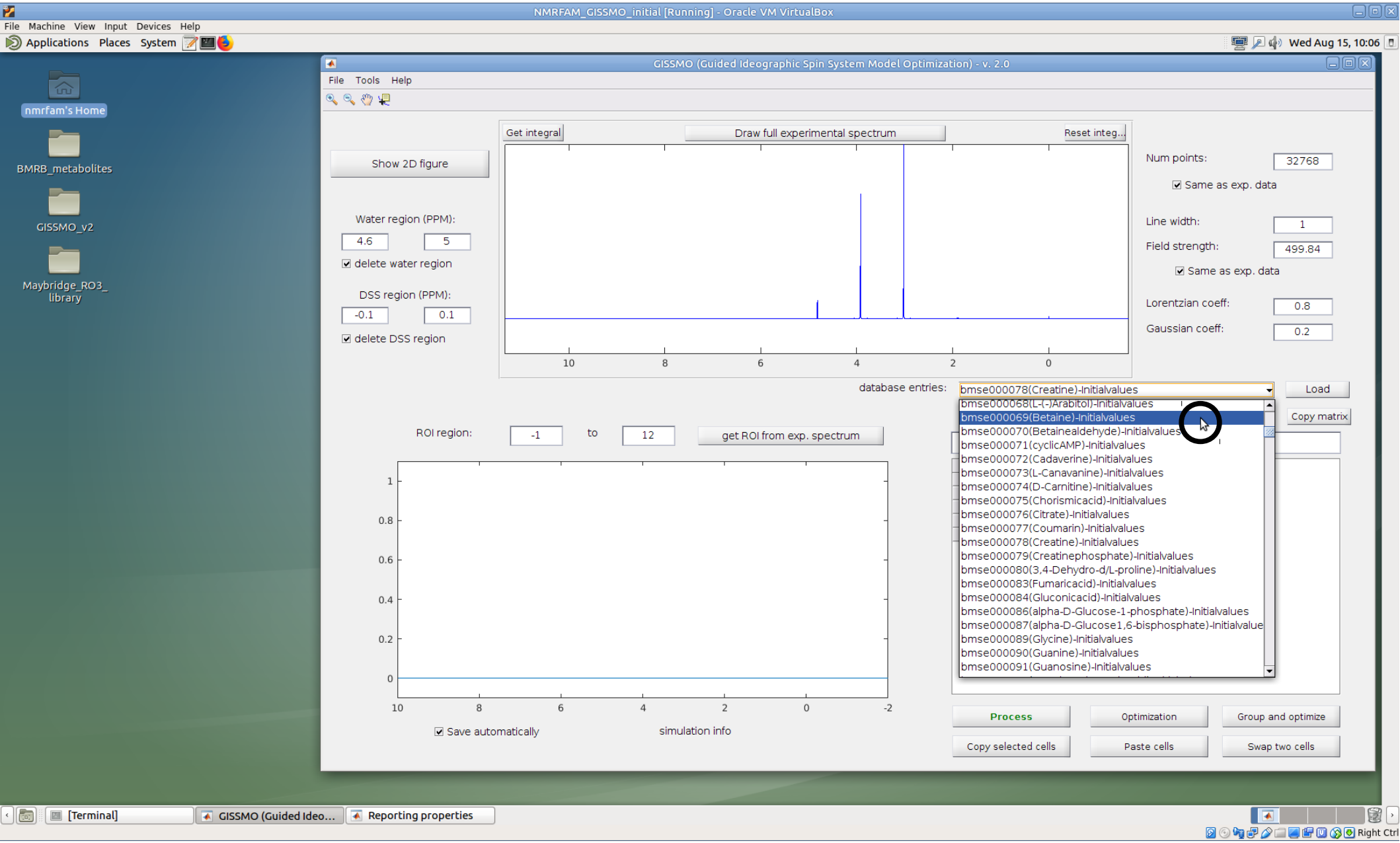
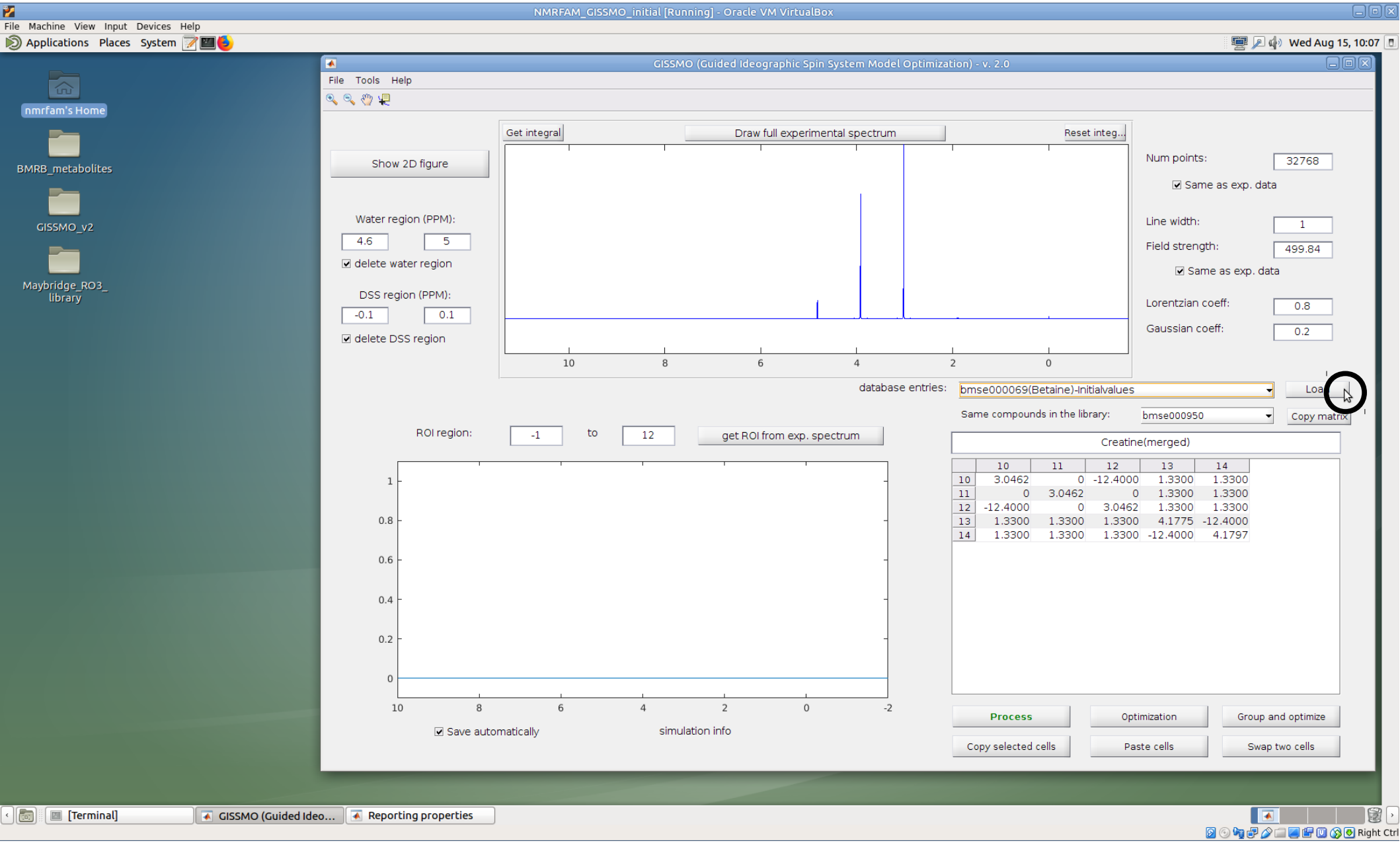
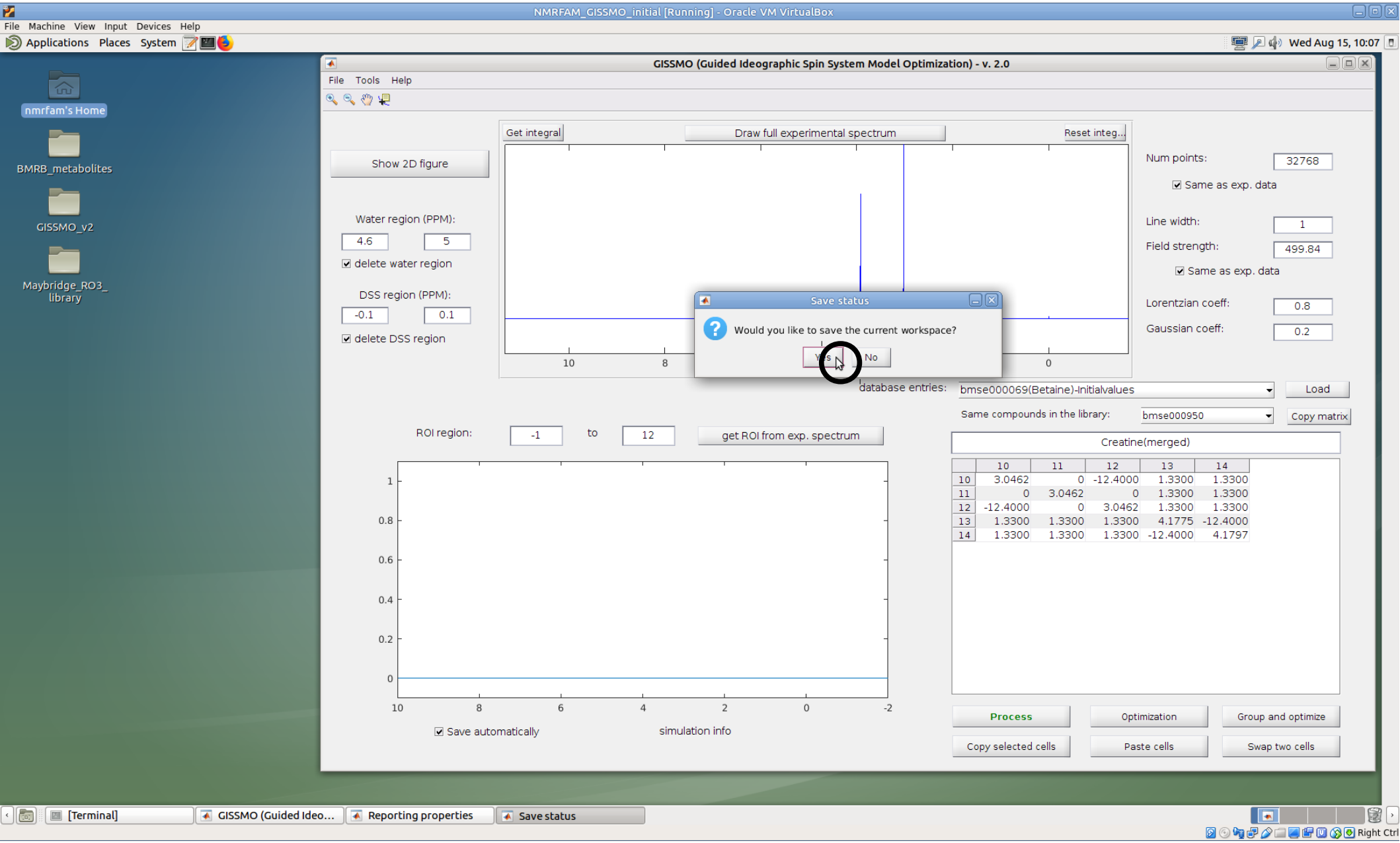
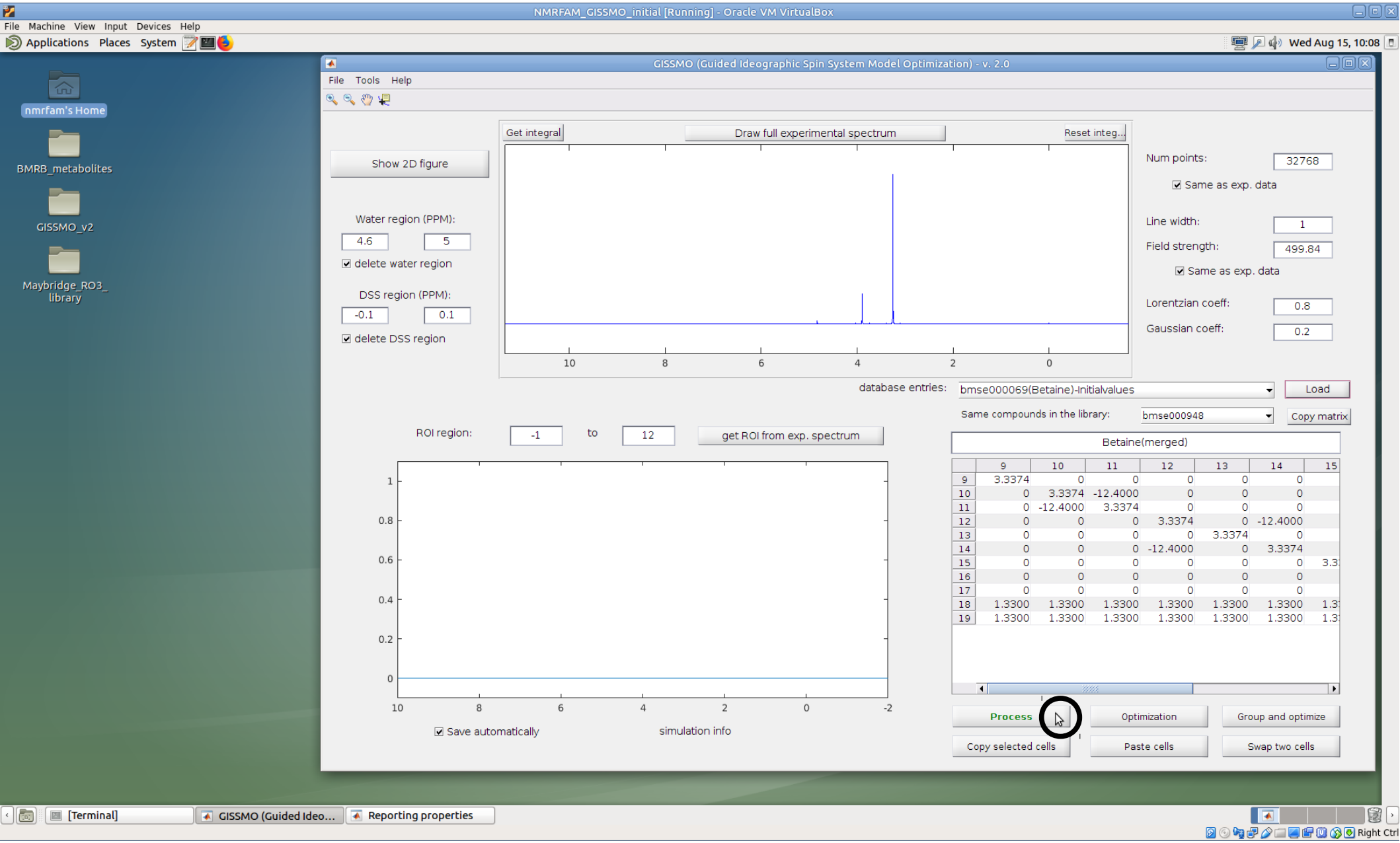

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:06
nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000078(Creatine)-Initialvalues
Load
Copy matrix
bmse000068(L-(-)Arabitol)-Initialvalues
bmse000069(Betaine)-Initialvalues
bmse000070(Betainealdehyde)-Initialvalues
bmse000071(cyclicAMP)-Initialvalues
bmse000072(Cadaverine)-Initialvalues
bmse000073(L-Canavanine)-Initialvalues
bmse000074(D-Carnitine)-Initialvalues
bmse000075(Chorismicacid)-Initialvalues
bmse000076(Citrate)-Initialvalues
bmse000077(Coumarin)-Initialvalues
bmse000078(Creatine)-Initialvalues
bmse000079(Creatinephosphate)-Initialvalues
bmse000080(3,4-Dehydro-d/L-proline)-Initialvalues
bmse000083(Fumaricacid)-Initialvalues
bmse000084(Gluconicacid)-Initialvalues
bmse000086(alpha-D-Glucose-1-phosphate)-Initialvalues
bmse000087(alpha-D-Glucose1,6-bisphosphate)-Initialvalue
bmse000089(Glycine)-Initialvalues
bmse000090(Guanine)-Initialvalues
bmse000091(Guanosine)-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
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Right Ctrl

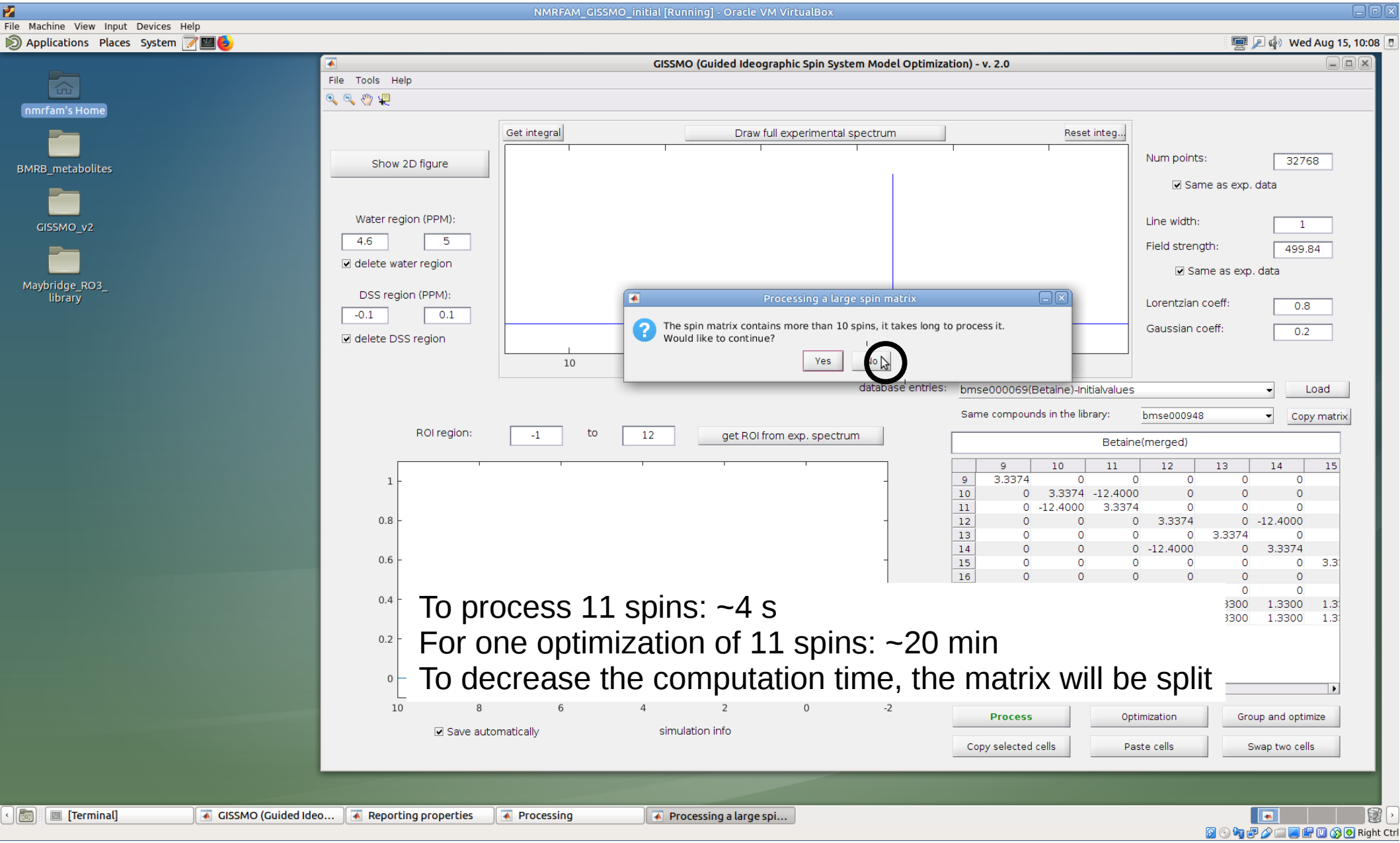



| | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|
| 10 | 3.0462 | 0 | -12.4000 | 1.3300 | 1.3300 |
| 11 | 0 | 3.0462 | 0 | 1.3300 | 1.3300 |
| 12 | -12.4000 | 0 | 3.0462 | 1.3300 | 1.3300 |
| 13 | 1.3300 | 1.3300 | 1.3300 | 4.1775 | -12.4000 |
| 14 | 1.3300 | 1.3300 | 1.3300 | -12.4000 | 4.1797 |

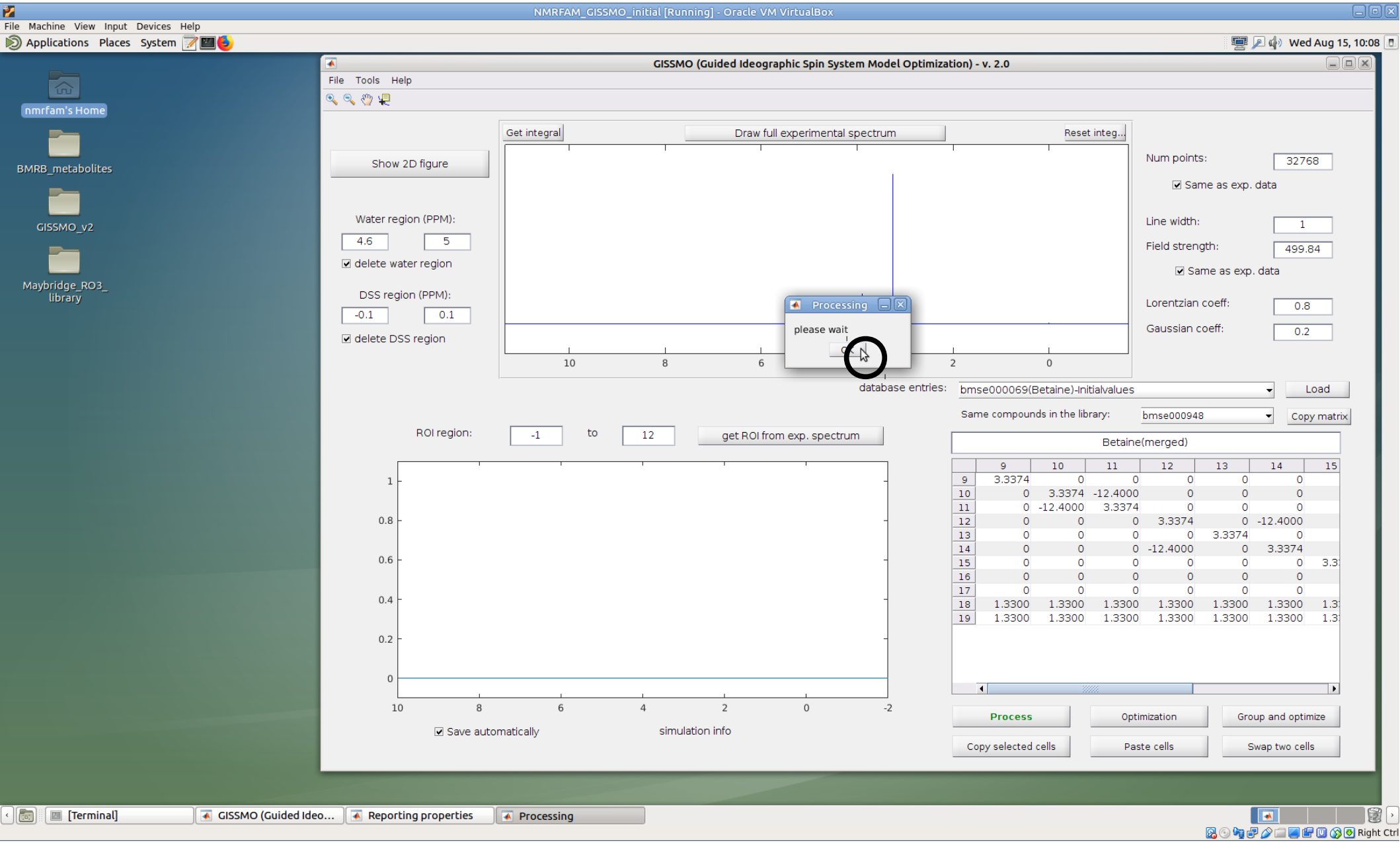

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:07
nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000950
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Creatine(merged)
10 11 12 13 14
10 3.0462 0 -12.4000 1.3300 1.3300
11 0 3.0462 0 1.3300 1.3300
12 -12.4000 0 3.0462 1.3300 1.3300
13 1.3300 1.3300 1.3300 4.1775 -12.4000
14 1.3300 1.3300 1.3300 -12.4000 4.1797
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Save status
Right Ctrl

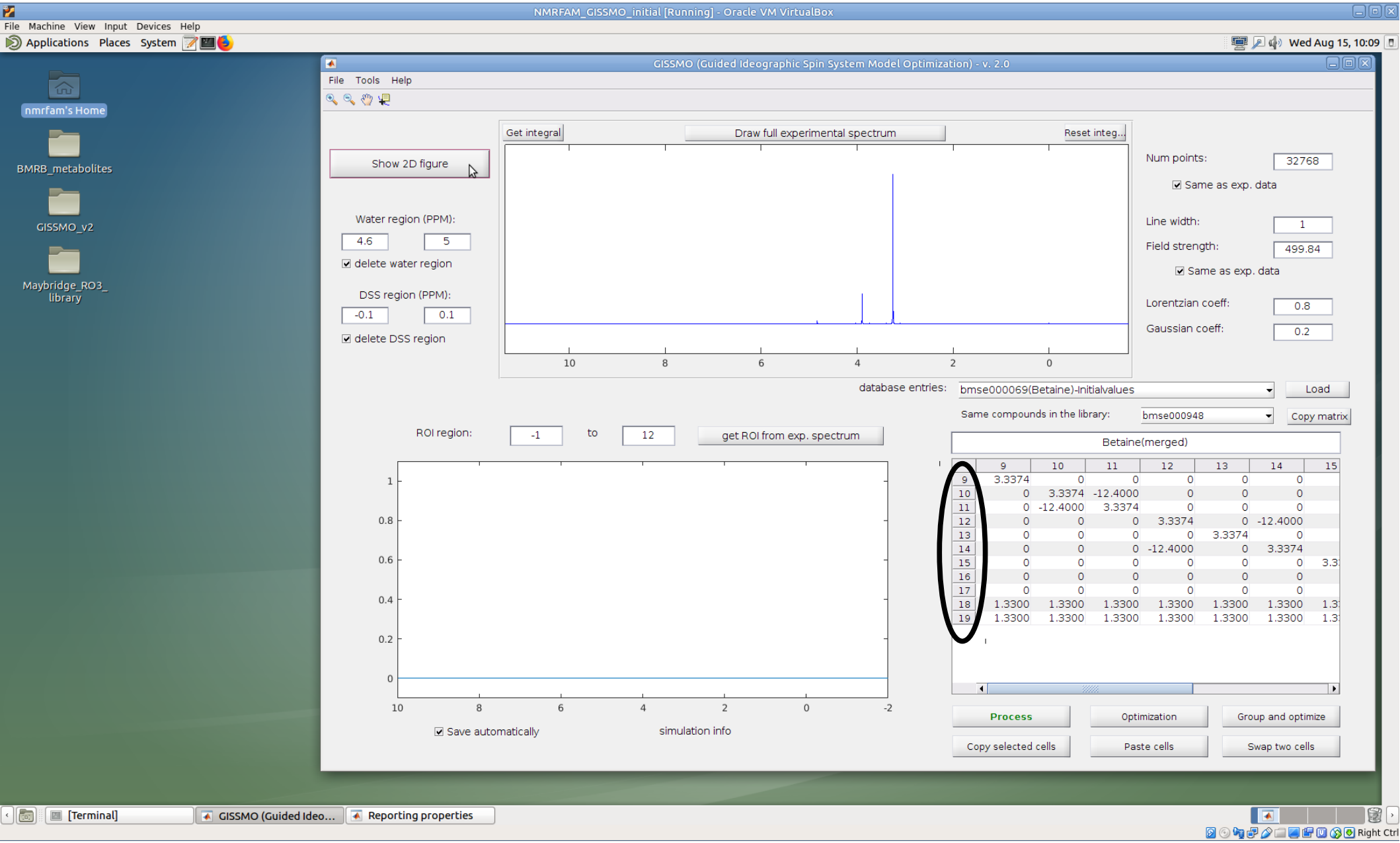



| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.3374 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.3374 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.3374 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.3374 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.3374 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.3374 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.3 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |
| 19 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |

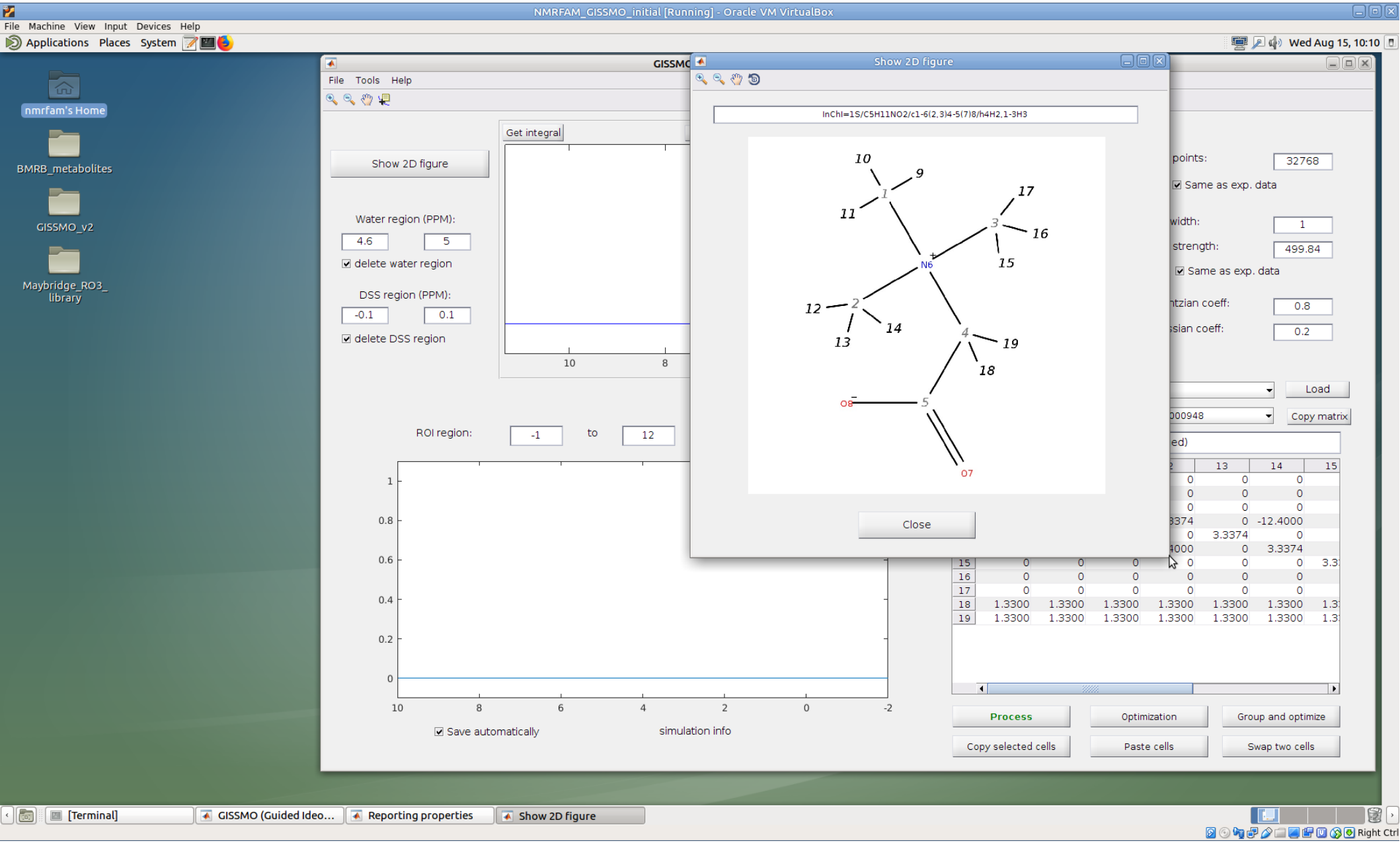


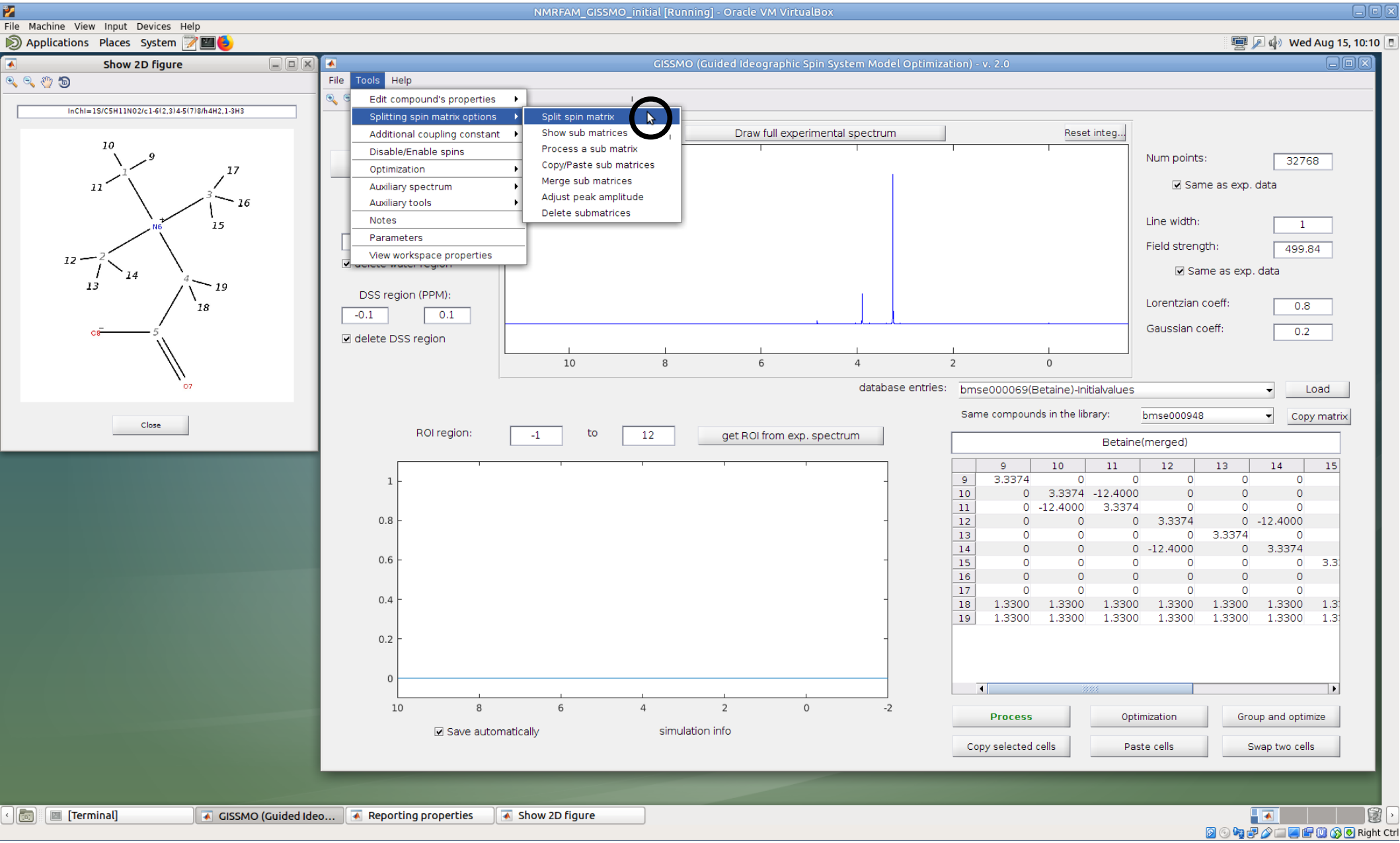

To process 11 spins: ~4 s
For one optimization of 11 spins: ~20 min
To decrease the computation time, the matrix will be split


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:08
nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Processing
please wait
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(merged)
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Processing
Right Ctrl




| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.3374 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.3374 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.3374 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.3374 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.3374 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.3374 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.3 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |
| 19 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:10
nmrfam's Home
BMRB_metabolites
GISSMO_v2
Maybridge_RO3_ library
GISSMO
File Tools Help
Show 2D figure
Get integral
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
ROI region:
-1
to
12
Save automatically
simulation info
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
points:
32768
Same as exp. data
width:
1
strength:
499.84
Same as exp. data
0.8
0.2
Load
Copy matrix
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
Wed Aug 15, 10:10
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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
Split spin matrix
Show sub matrices
Process a sub matrix
Copy/Paste sub matrices
Merge sub matrices
Adjust peak amplitude
Delete submatrices
Draw full experimental spectrum
Reset integ...
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(merged)
Save automatically
simulation info
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

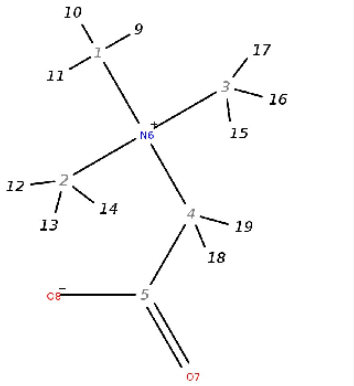
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:11

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

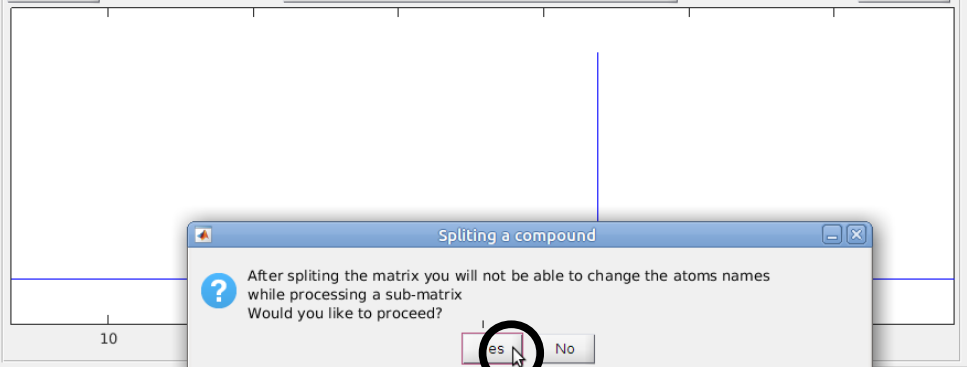
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

### Spliting a compound

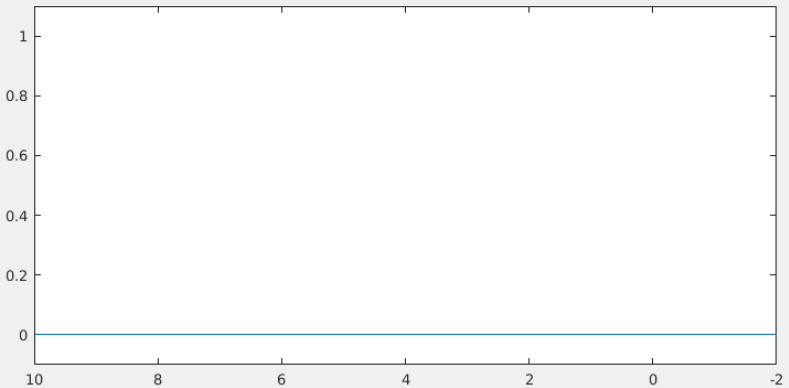
After spliting the matrix you will not be able to change the atoms names while processing a sub-matrix
Would you like to proceed?

Yes No

-Initialvalues Load

Same compounds in the library: bmse000948 Copy matrix

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




Save automatically simulation info

Betaine(merged)

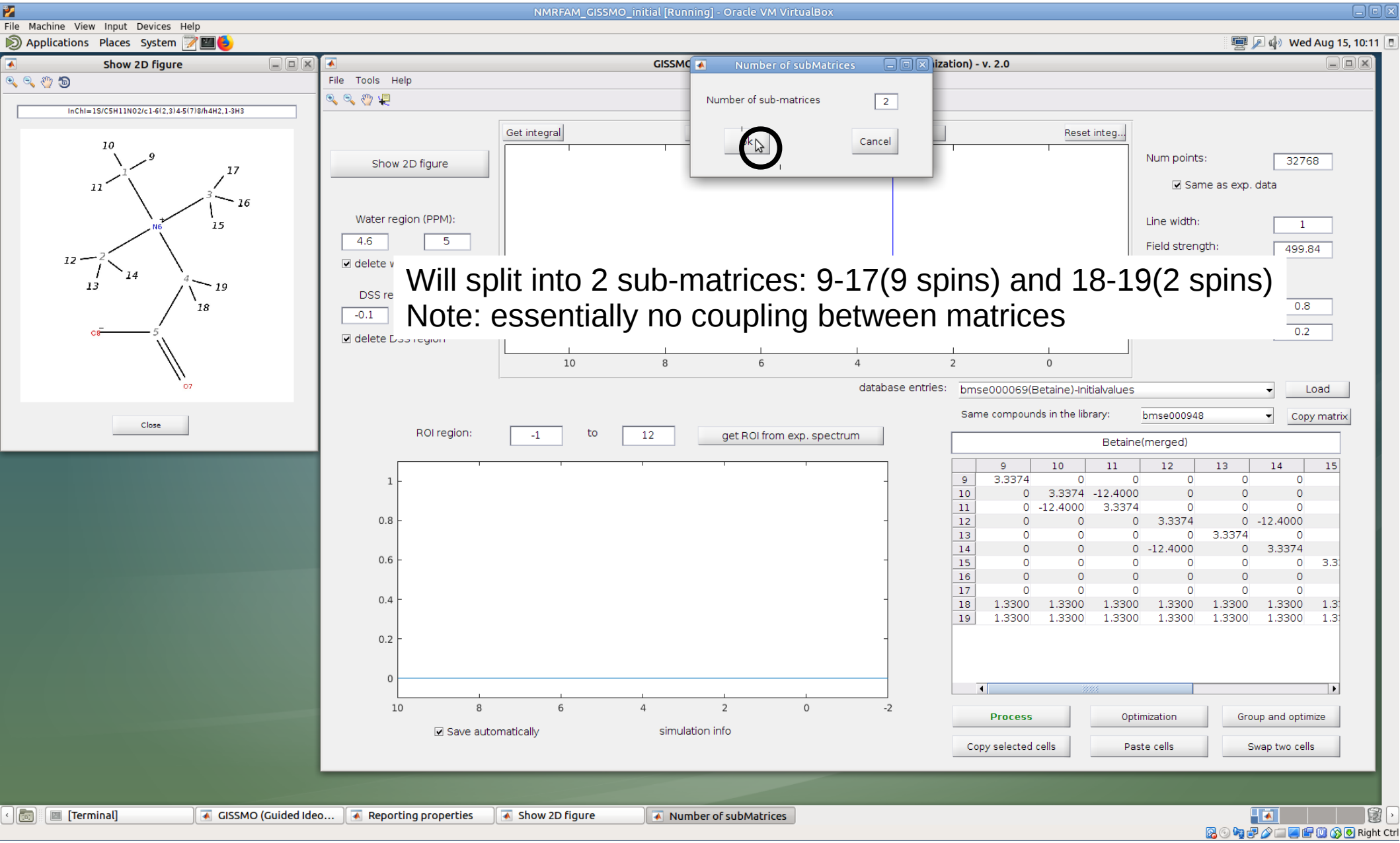
| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.3374 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.3374 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.3374 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.3374 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.3374 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.3374 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.3 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |
| 19 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |

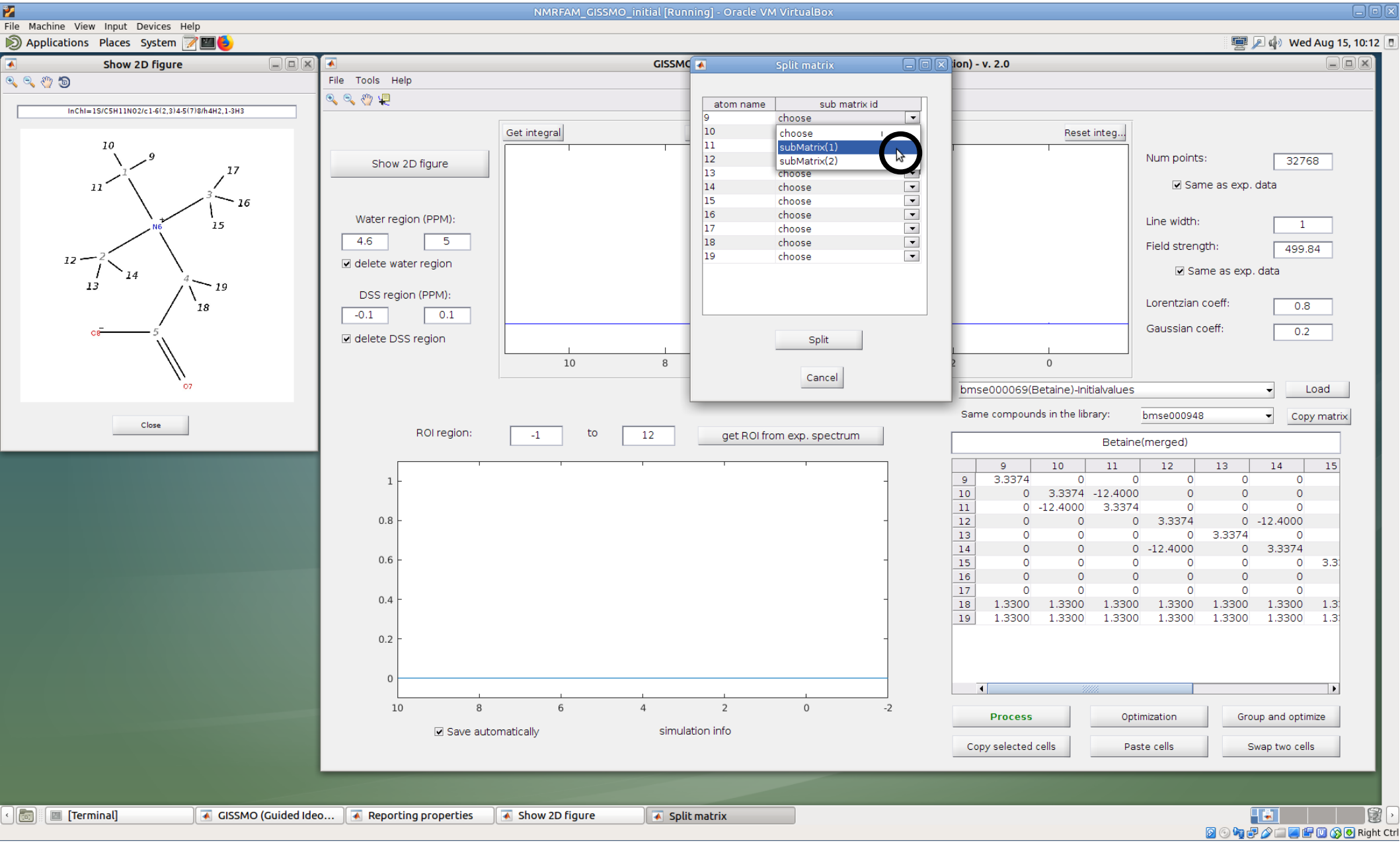
Process | Optimization | Group and optimize

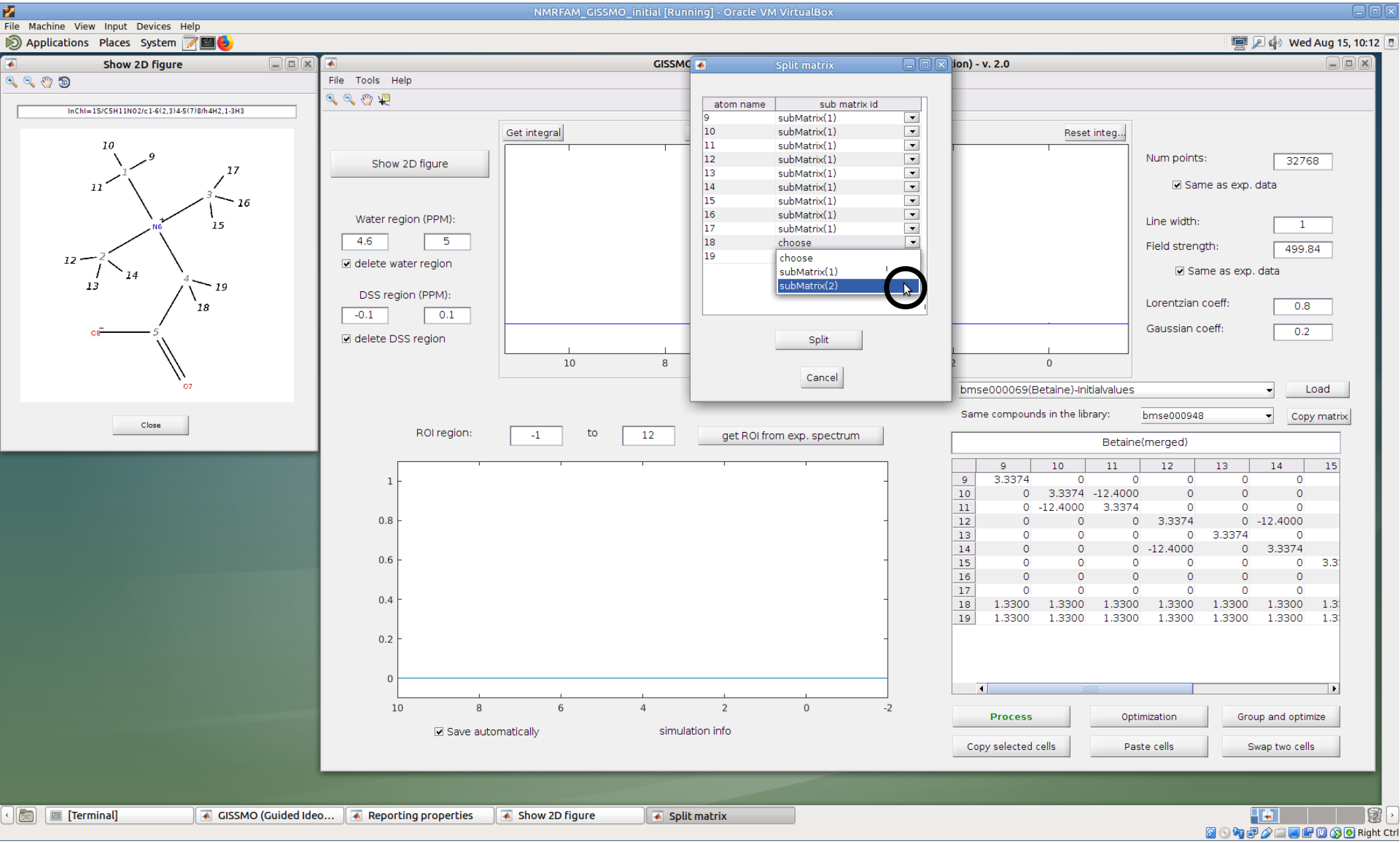
Copy selected cells | Paste cells | Swap two cells

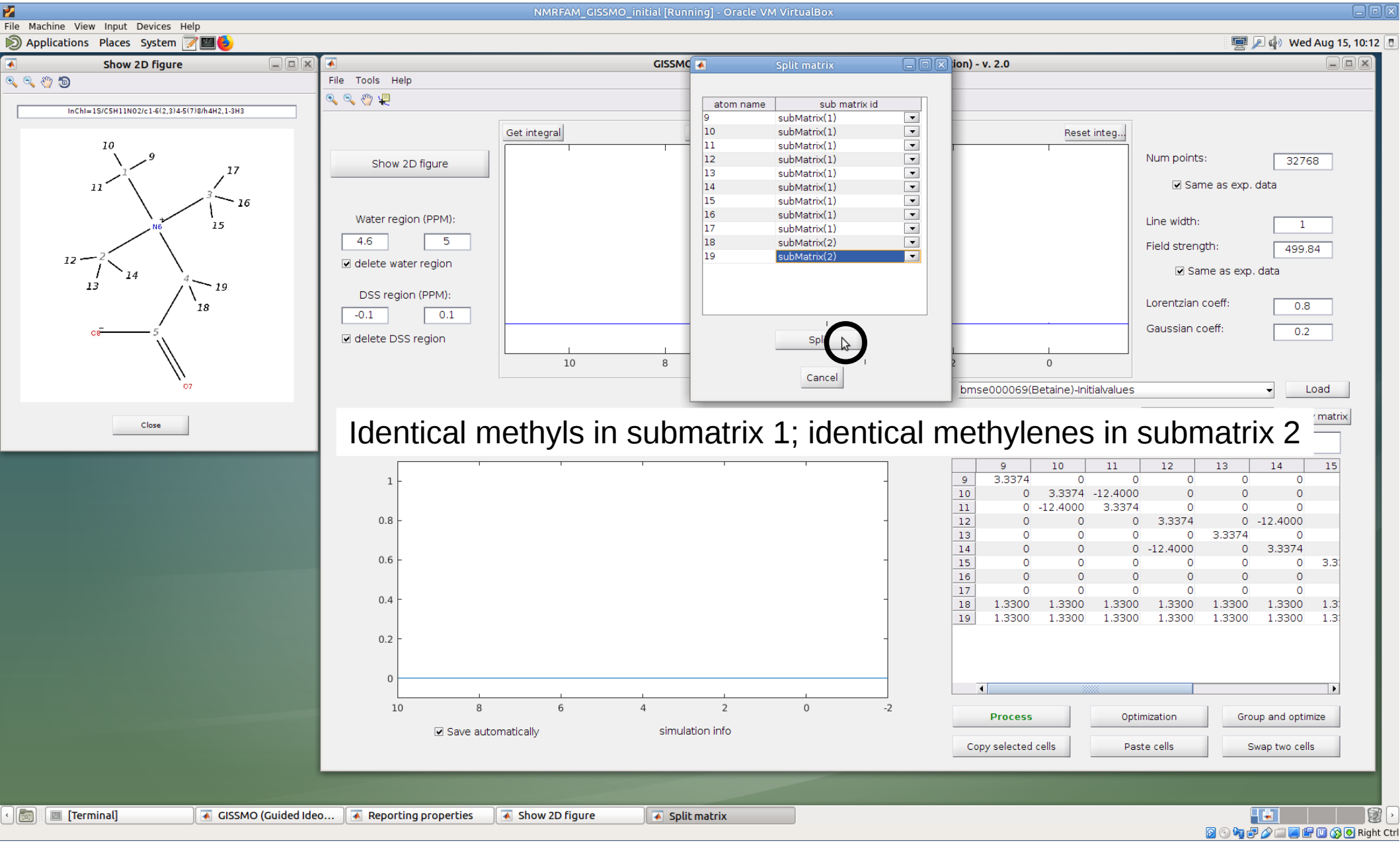
[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Spliting a compound

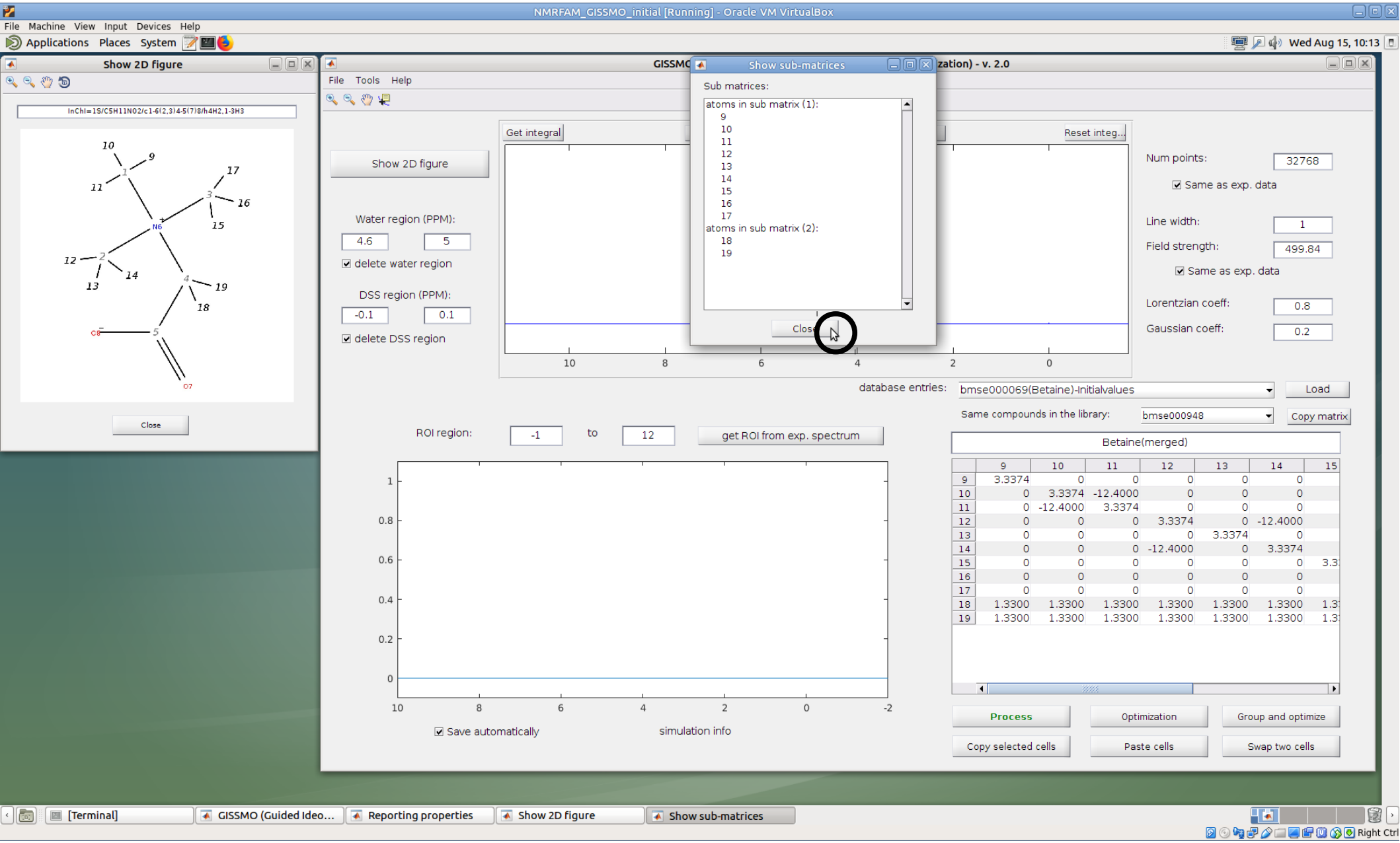
Right Ctrl

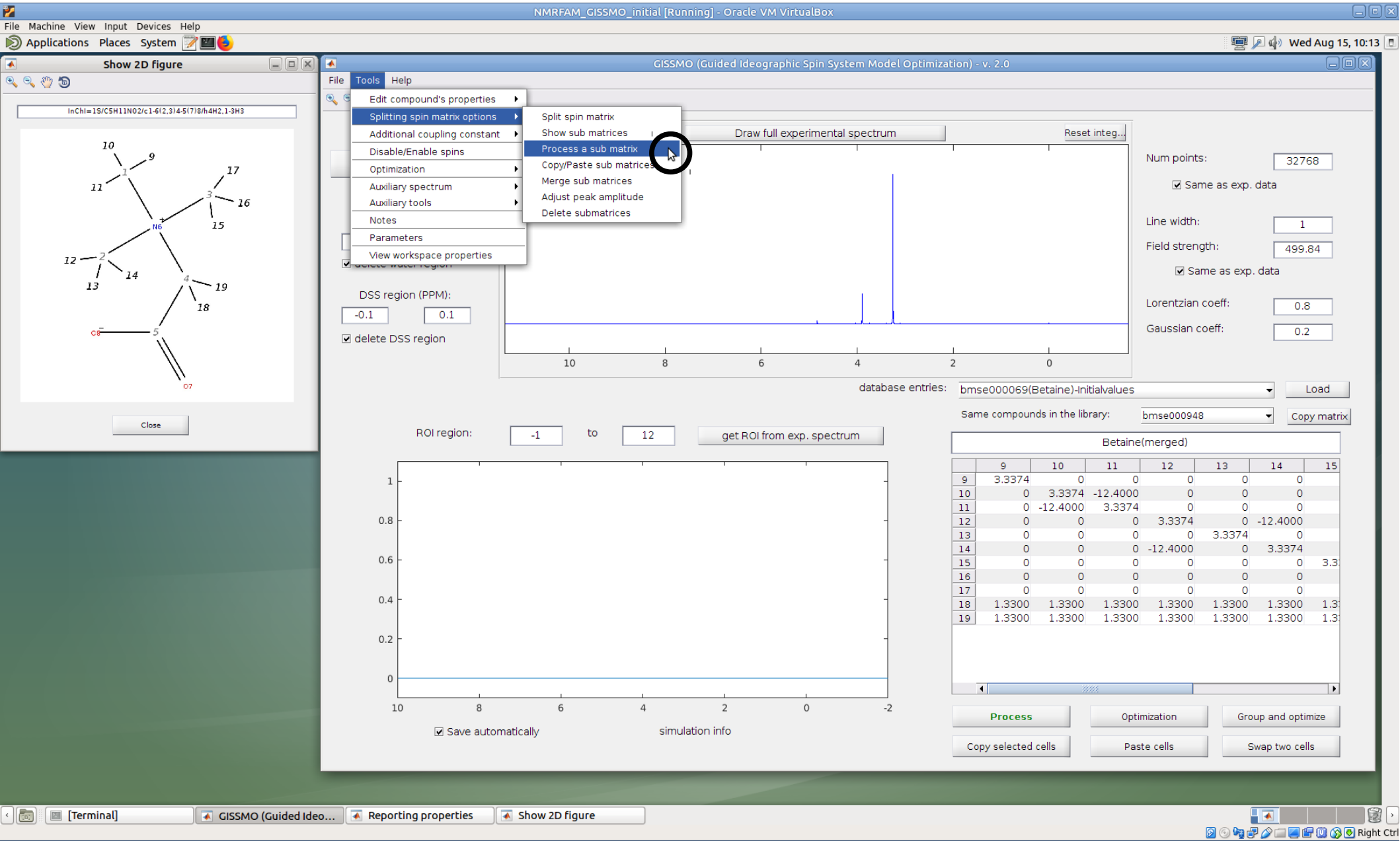

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:11
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
File Tools Help
Number of subMatrices
Number of sub-matrices
2
OK
Cancel
Get integral
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete w
DSS re
-0.1
delete DSS region
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
0.8
0.2
Will split into 2 sub-matrices: 9-17(9 spins) and 18-19(2 spins)
Note: essentially no coupling between matrices
database entries:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(merged)
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Number of subMatrices
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:12
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
File Tools Help
Split matrix
atom name
sub matrix id
choose
subMatrix(1)
subMatrix(2)
Split
Cancel
Show 2D figure
Get integral
Reset integ...
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(merged)
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Split matrix
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:12
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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 integ...
Split matrix
atom name
sub matrix id
9 subMatrix(1)
10 subMatrix(1)
11 subMatrix(1)
12 subMatrix(1)
13 subMatrix(1)
14 subMatrix(1)
15 subMatrix(1)
16 subMatrix(1)
17 subMatrix(1)
18 choose
19
choose
subMatrix(1)
subMatrix(2)
Split
Cancel
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(merged)
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Split matrix
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:12
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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 integ...
Split matrix
atom name
sub matrix id
9 subMatrix(1)
10 subMatrix(1)
11 subMatrix(1)
12 subMatrix(1)
13 subMatrix(1)
14 subMatrix(1)
15 subMatrix(1)
16 subMatrix(1)
17 subMatrix(1)
18 subMatrix(2)
19 subMatrix(2)
Cancel
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
bmse000069(Betaine)-Initialvalues
Load
Identical methyls in submatrix 1; identical methylenes in submatrix 2
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Split matrix
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:13
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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 integ...
Show sub-matrices
Sub matrices:
atoms in sub matrix (1):
9
10
11
12
13
14
15
16
17
atoms in sub matrix (2):
18
19
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(merged)
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Show sub-matrices
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:13
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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
Split spin matrix
Show sub matrices
Process a sub matrix
Copy/Paste sub matrices
Merge sub matrices
Adjust peak amplitude
Delete submatrices
Draw full experimental spectrum
Reset integ...
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(merged)
Save automatically
simulation info
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

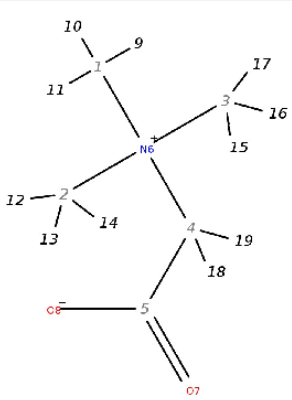
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:14

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

## GISSMO (Guided Ideo... mization) - v. 2.0

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

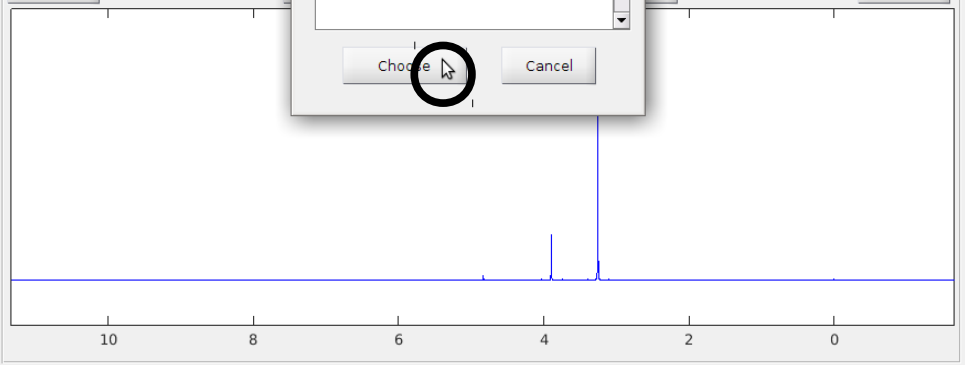
DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset integ...




### Choose a submatrix to process

choose a sub matrix
subMatrix(1)
subMatrix(2)

Choose Cancel

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

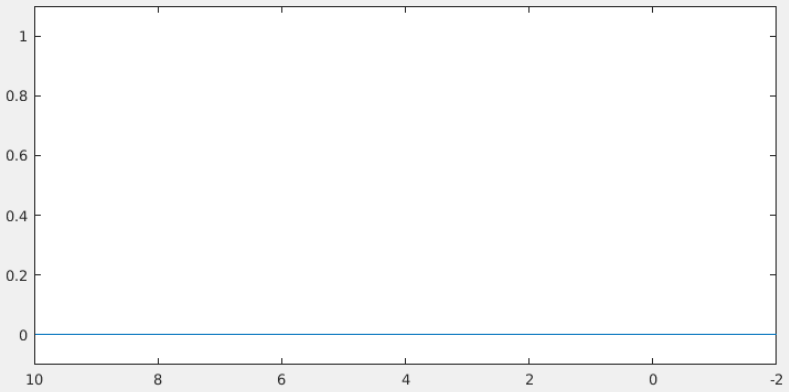
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues Load

Same compounds in the library: bmse000948 Copy matrix

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




Save automatically simulation info

Betaine(merged)

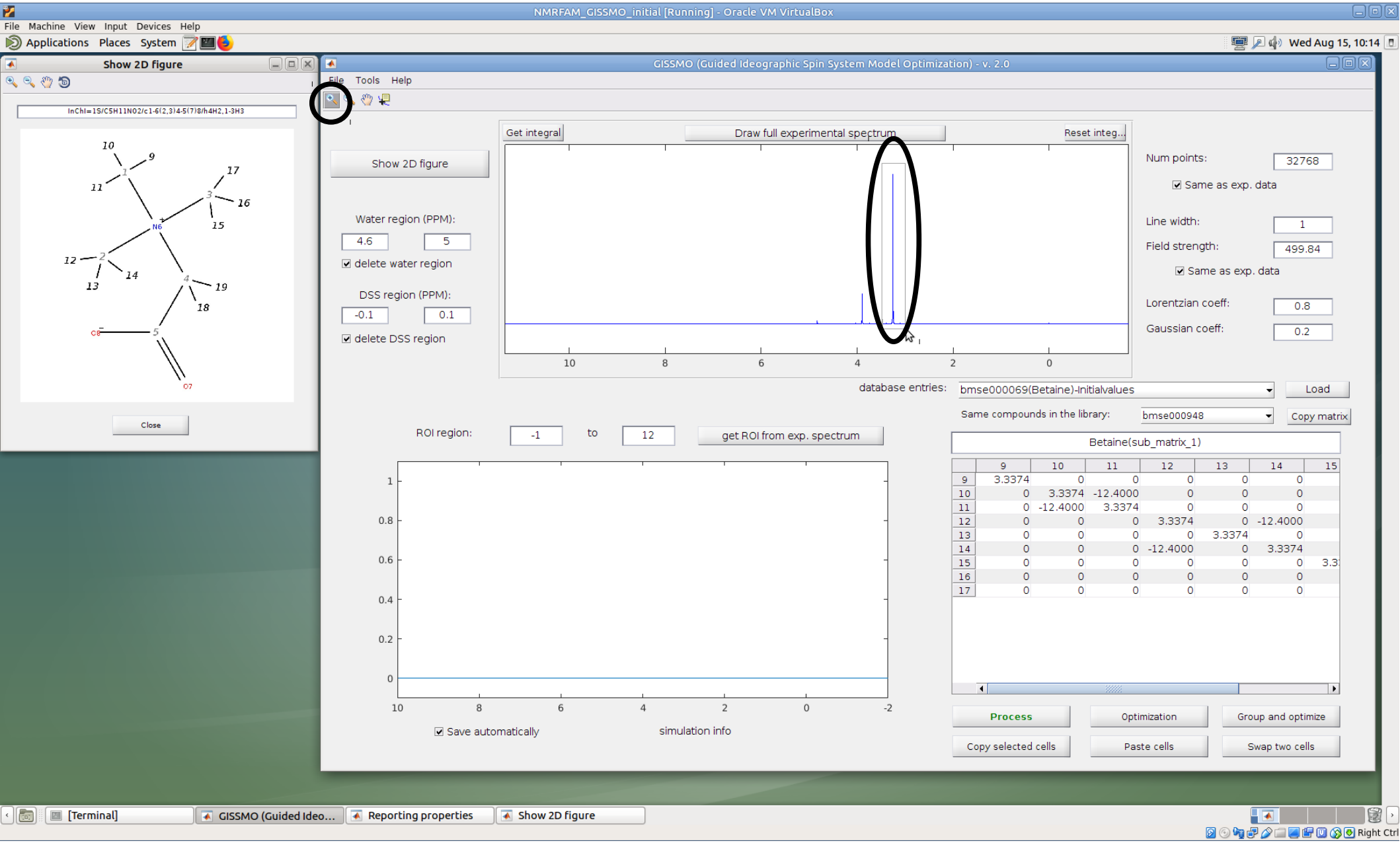
| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.3374 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.3374 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.3374 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.3374 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.3374 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.3374 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.3 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |
| 19 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |

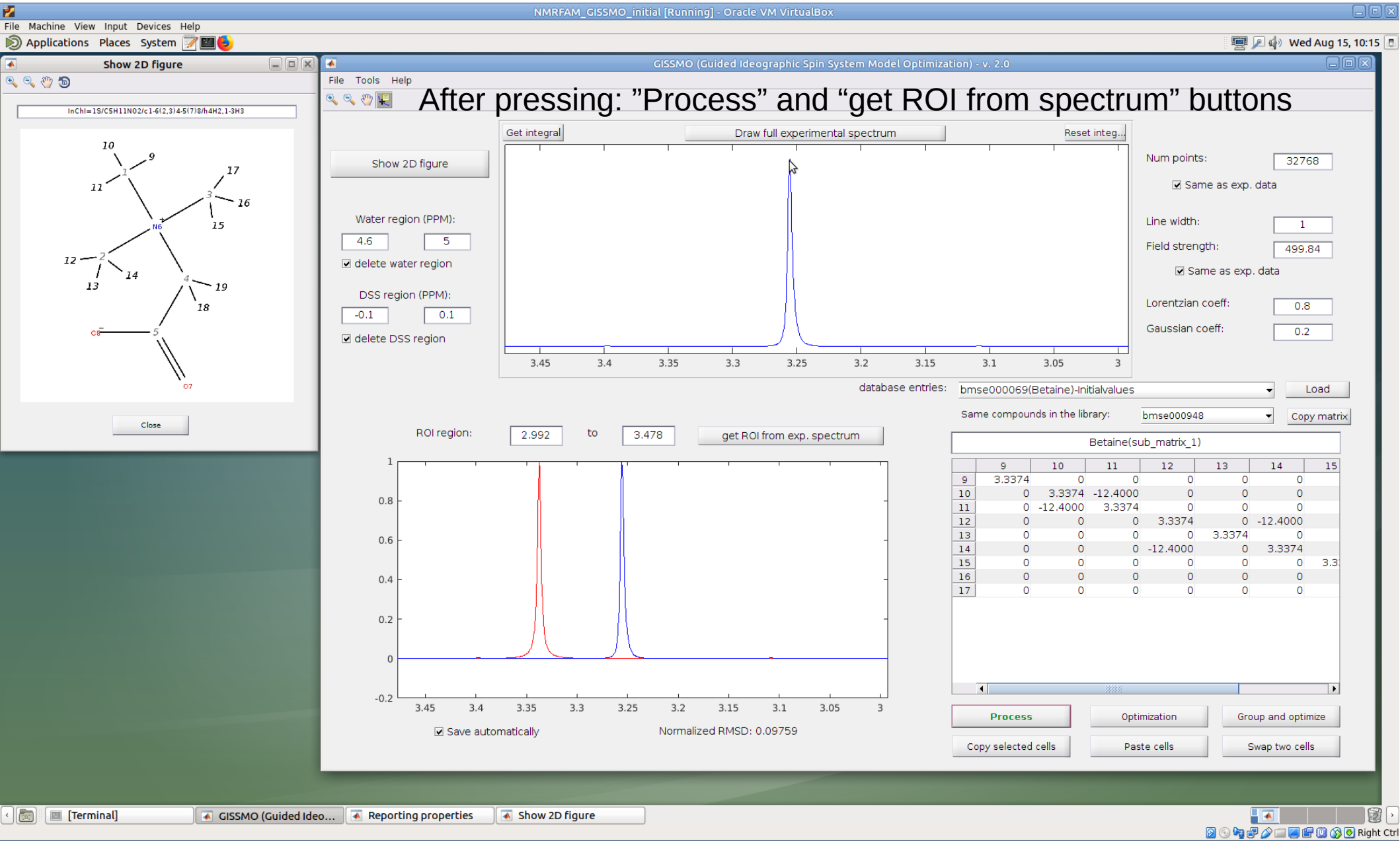
Process Optimization Group and optimize

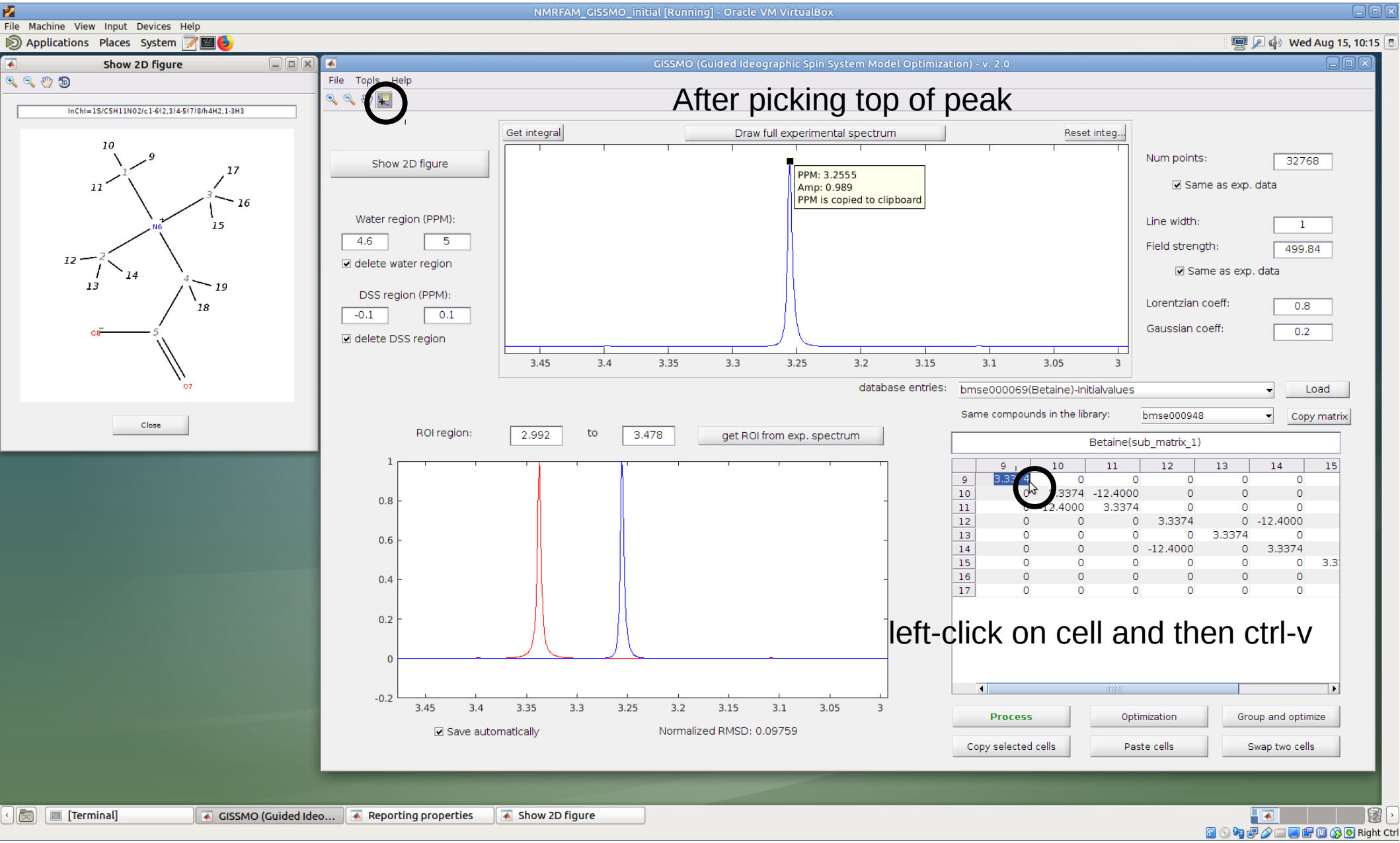
Copy selected cells Paste cells Swap two cells

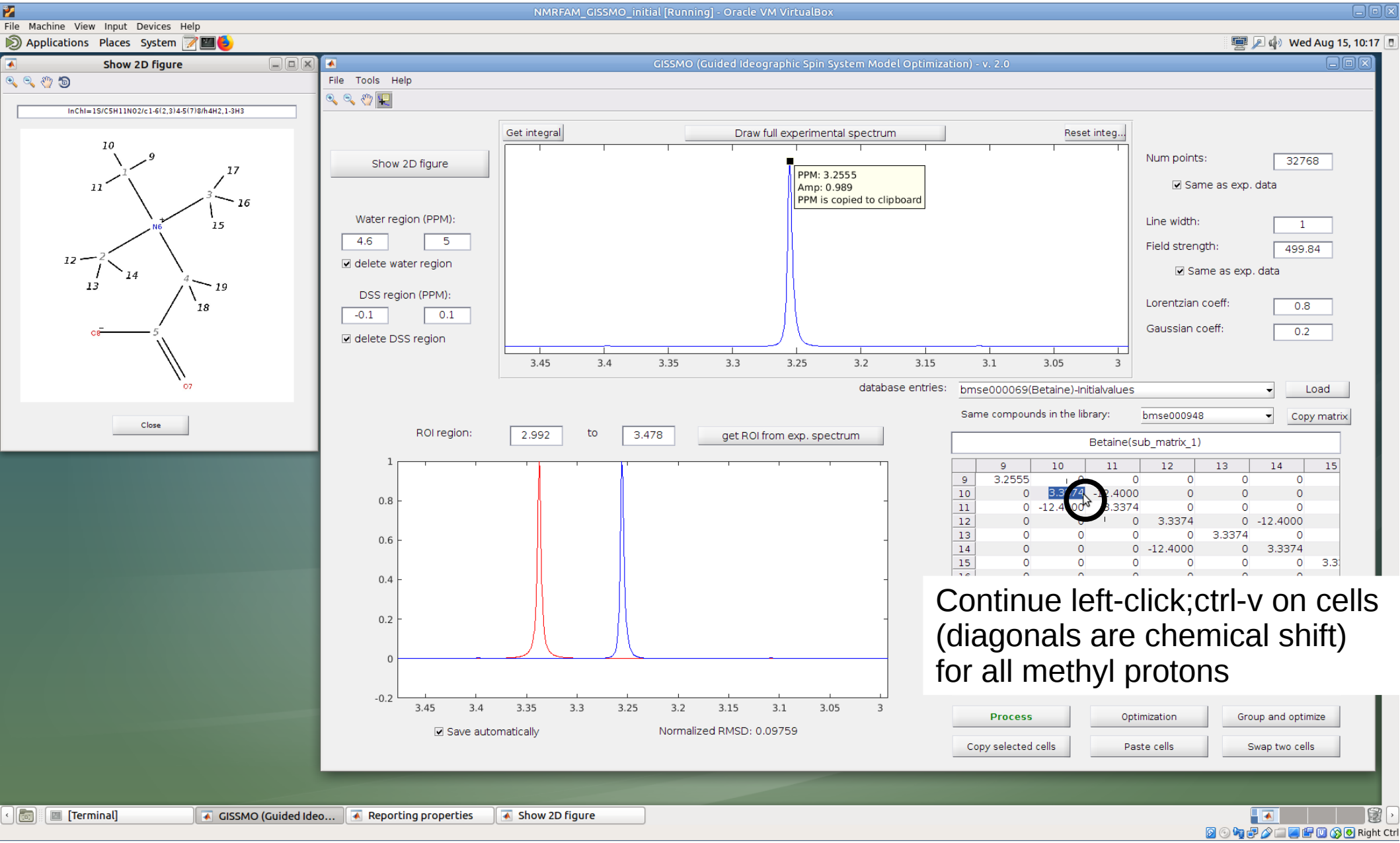
[Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure Choose a submatrix t...

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:14
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1
to
12
get ROI from exp. spectrum
Betaine(sub_matrix_1)
Save automatically
simulation info
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
Wed Aug 15, 10:15
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
After pressing: ”Process” and “get ROI from spectrum” buttons
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_1)
Save automatically
Normalized RMSD: 0.09759
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
Wed Aug 15, 10:15
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
After picking top of peak
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
PPM: 3.2555
Amp: 0.989
PPM is copied to clipboard
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_1)
left-click on cell and then ctrl-v
Save automatically
Normalized RMSD: 0.09759
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
Wed Aug 15, 10:17
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 3.2555
Amp: 0.989
PPM is copied to clipboard
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_1)
Save automatically
Normalized RMSD: 0.09759
Continue left-click;ctrl-v on cells
(diagonals are chemical shift)
for all methyl protons
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

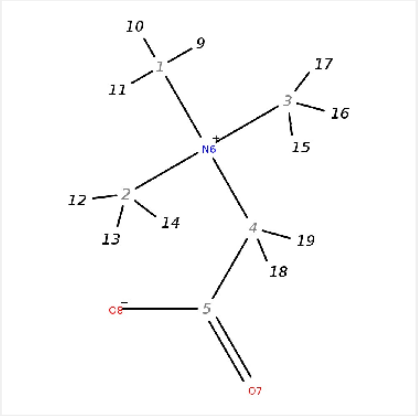
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:17

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

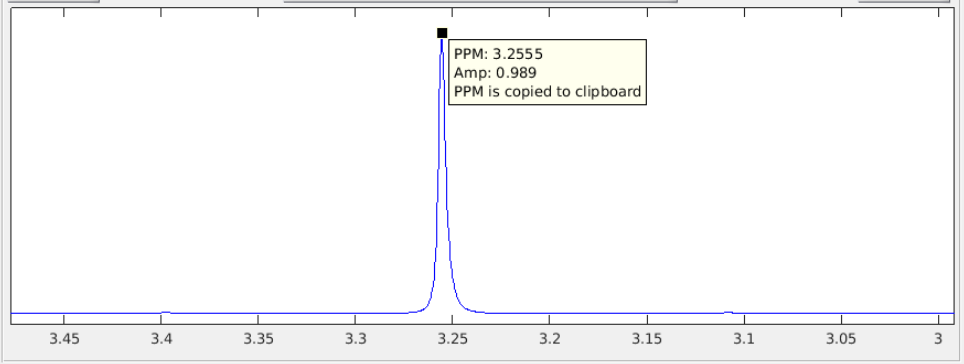
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

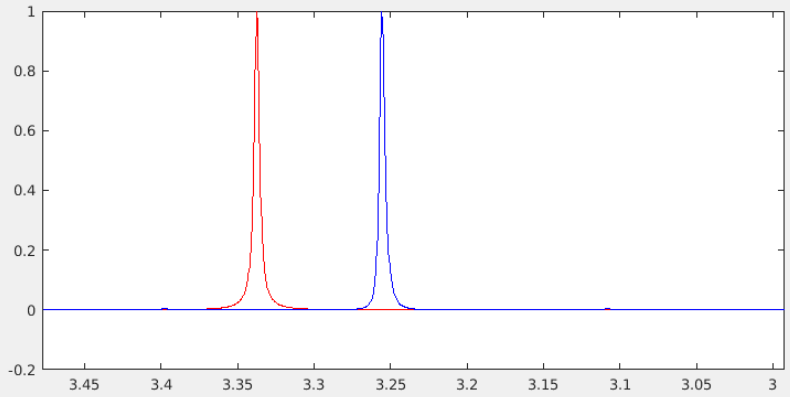
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 2.992 to 3.478 get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.09759

Betaine(sub_matrix_1)

| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.2555 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.2555 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.3374 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.3374 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.3374 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.3374 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.3 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 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

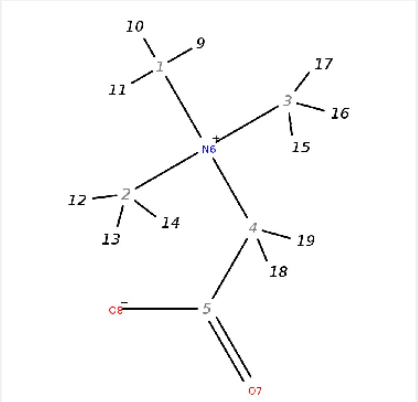
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:18

Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

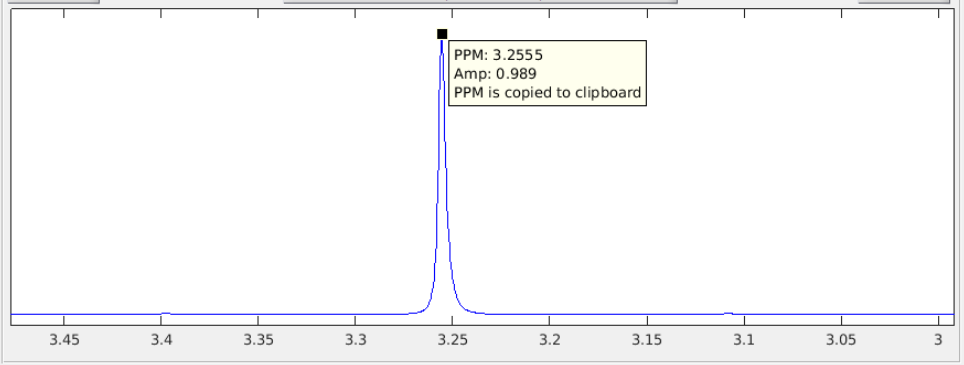
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

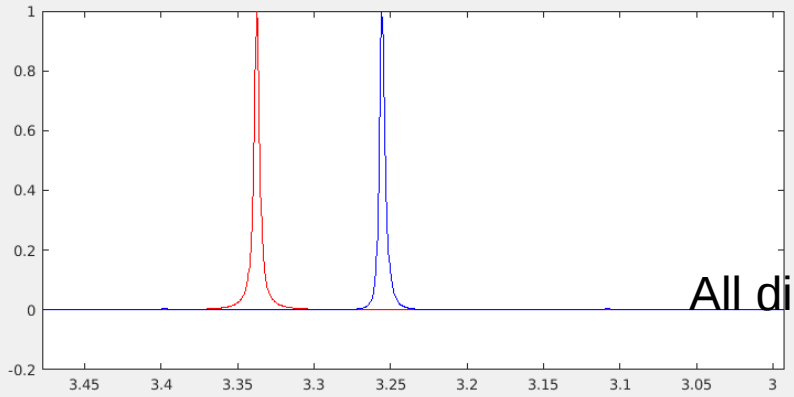
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 2.992 to 3.478 get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.09759

Betaine(sub_matrix_1)

| | 11 | 12 | 13 | 14 | 15 | 16 | 17 |
|---|---|---|---|---|---|---|---|
| 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 2.4000 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 3.2555 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 0 | 3.2555 | 0 | -12.4000 | 0 | 0 | 0 |
| 13 | 0 | 0 | 3.2555 | 0 | 0 | 0 | 0 |
| 14 | 0 | -12.4000 | 0 | 3.2555 | 0 | 0 | 0 |
| 15 | 0 | 0 | 0 | 0 | 3.2555 | 0 | 0 |
| 16 | 0 | 0 | 0 | 0 | 0 | 3.2555 | -12.4000 |
| 17 | 0 | 0 | 0 | 0 | 0 | -12.4000 | 3.2555 |

All diagonal cells set to same value

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

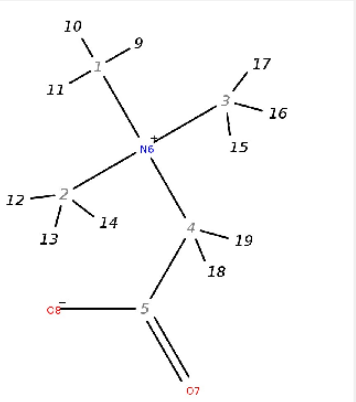
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:19

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

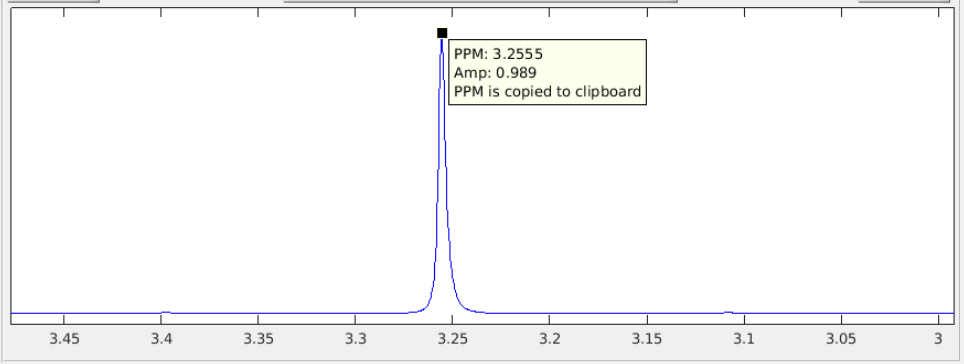
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

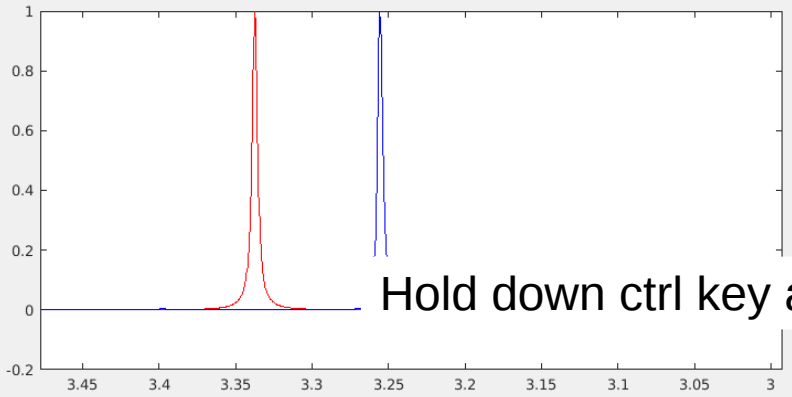
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 2.992 to 3.478 | get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.09759

Betaine(sub_matrix_1)

| | 11 | 12 | 13 | 14 | 15 | 16 | 17 |
|---|---|---|---|---|---|---|---|
| 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 2.4000 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 3.2555 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 0 | 3.2555 | 0 | -12.4000 | 0 | 0 | 0 |
| 13 | 0 | 0 | 3.2555 | 0 | 0 | 0 | 0 |
| 14 | 0 | -12.4000 | 0 | 3.2555 | 0 | 0 | 0 |
| 15 | 0 | 0 | 0 | 0 | 3.2555 | 0 | 0 |
| 16 | 0 | 0 | 0 | 0 | 0 | 3.2555 | -12.4000 |
| 17 | 0 | 0 | 0 | 0 | 0 | -12.4000 | 3.2555 |

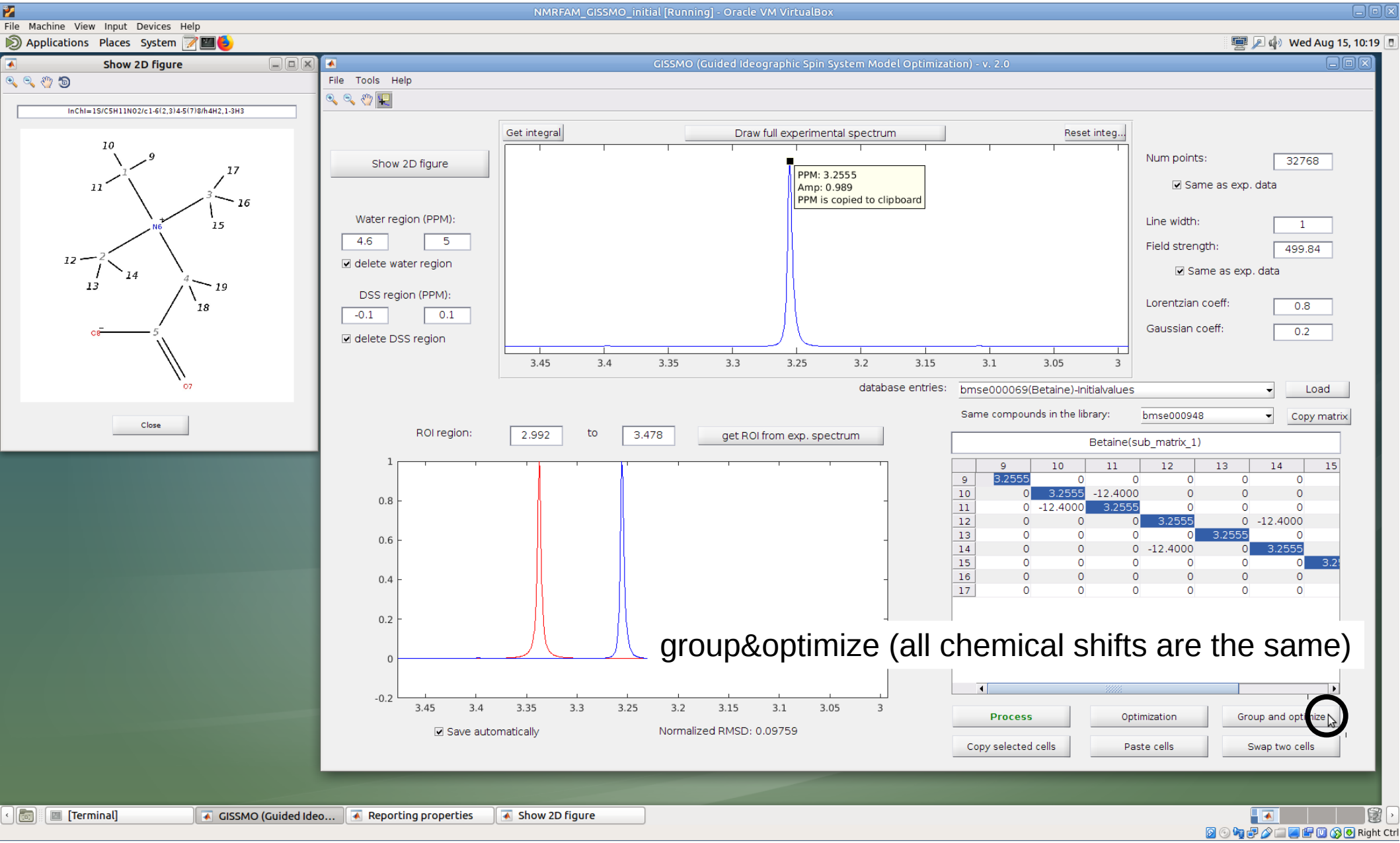
Hold down ctrl key and left-click on all diagonal cells

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
Wed Aug 15, 10:19
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 3.2555
Amp: 0.989
PPM is copied to clipboard
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_1)
Save automatically
Normalized RMSD: 0.09759
group&optimize (all chemical shifts are the same)
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

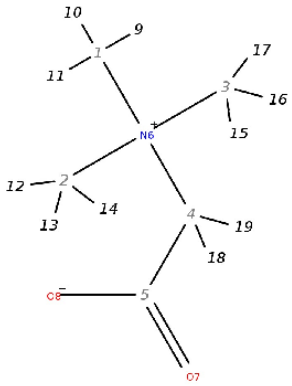
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:20

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

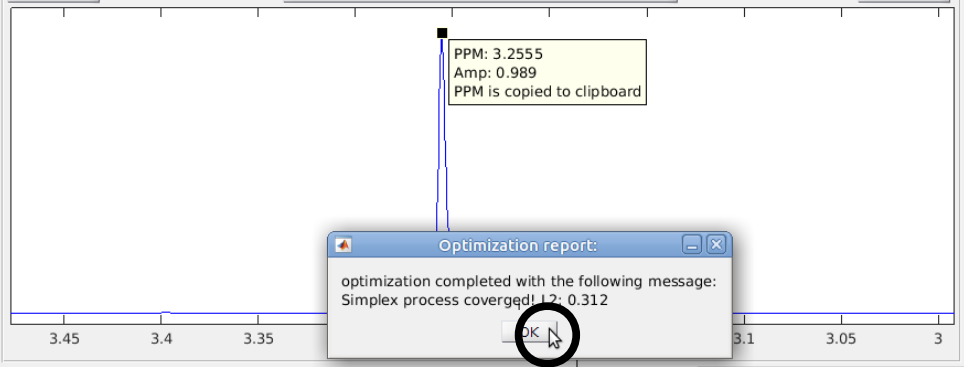
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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




Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 0.312

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

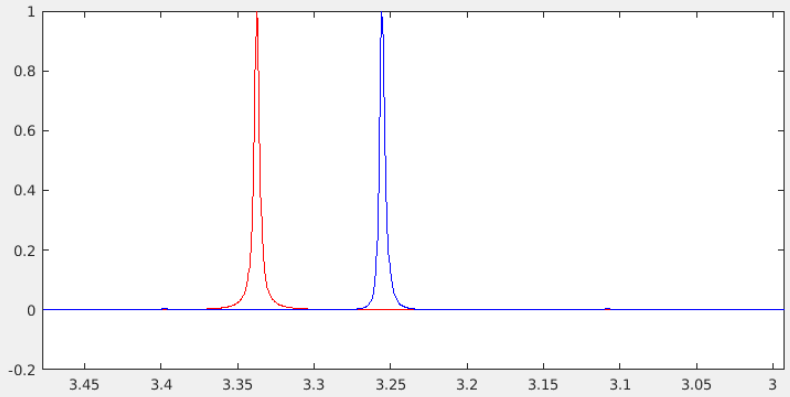
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 2.992 to 3.478 get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.09759

Betaine(sub_matrix_1)

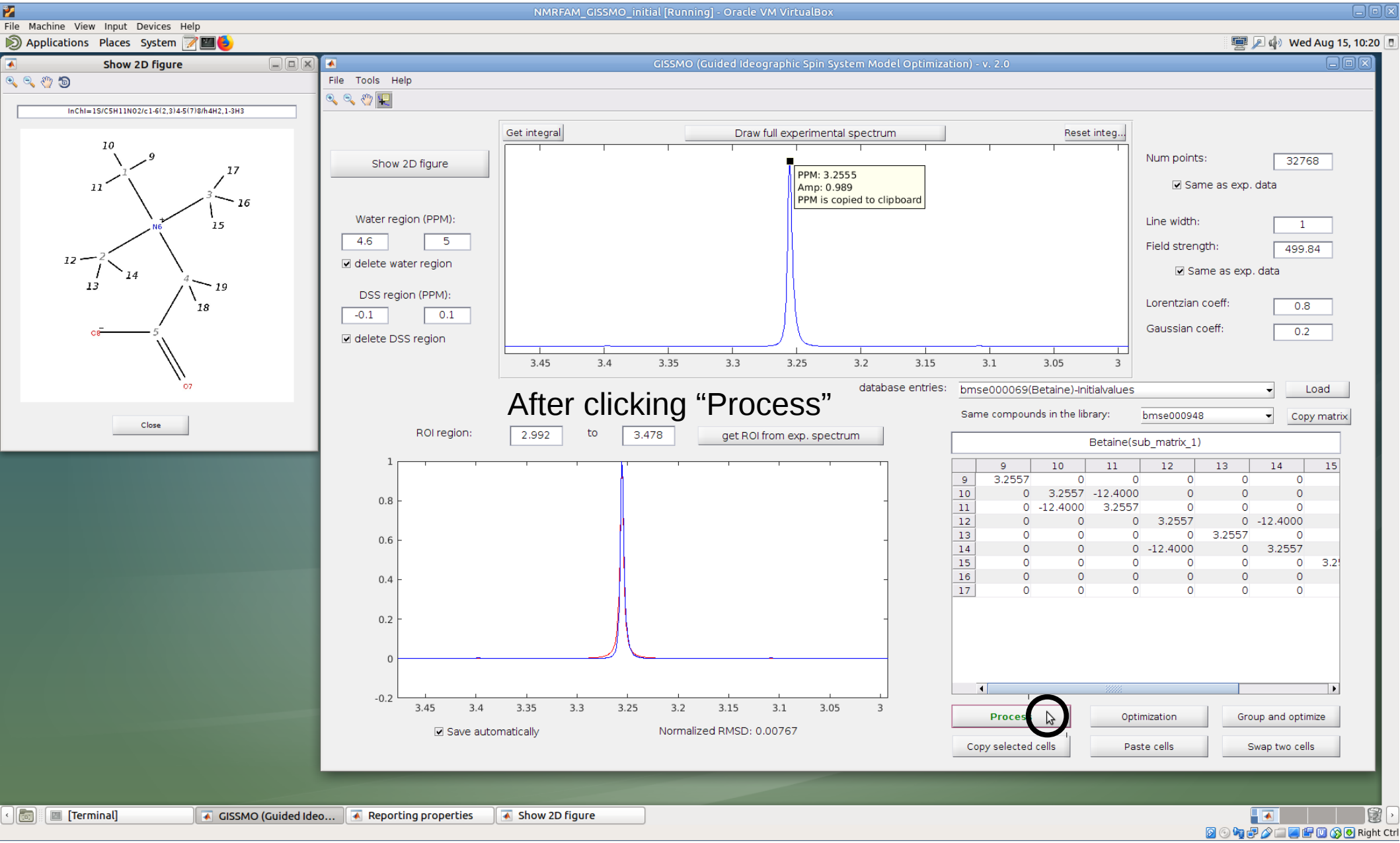
| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.2557 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.2557 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.2557 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.2557 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.2557 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.2557 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.2 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |

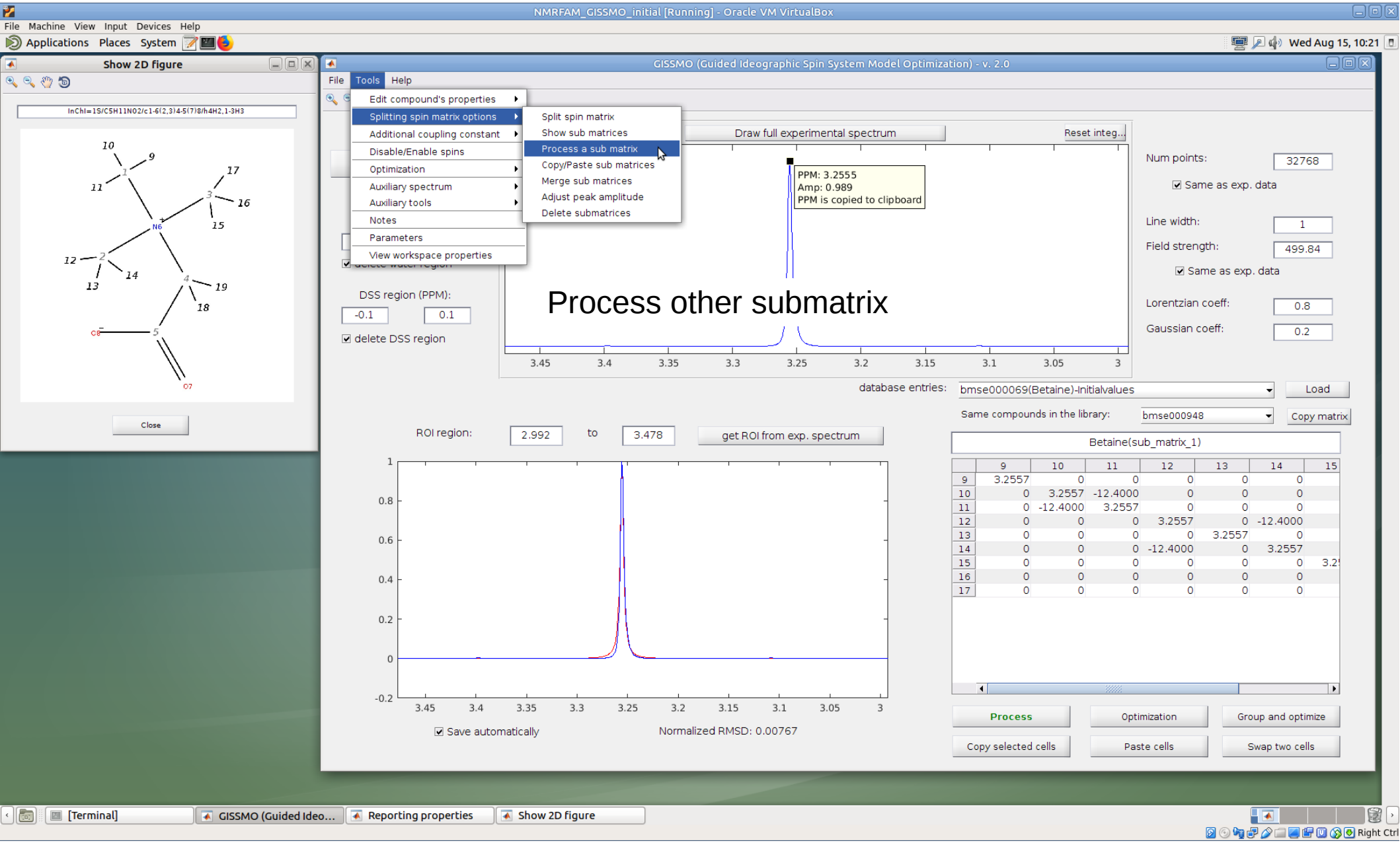
Process | Optimization | Group and optimize

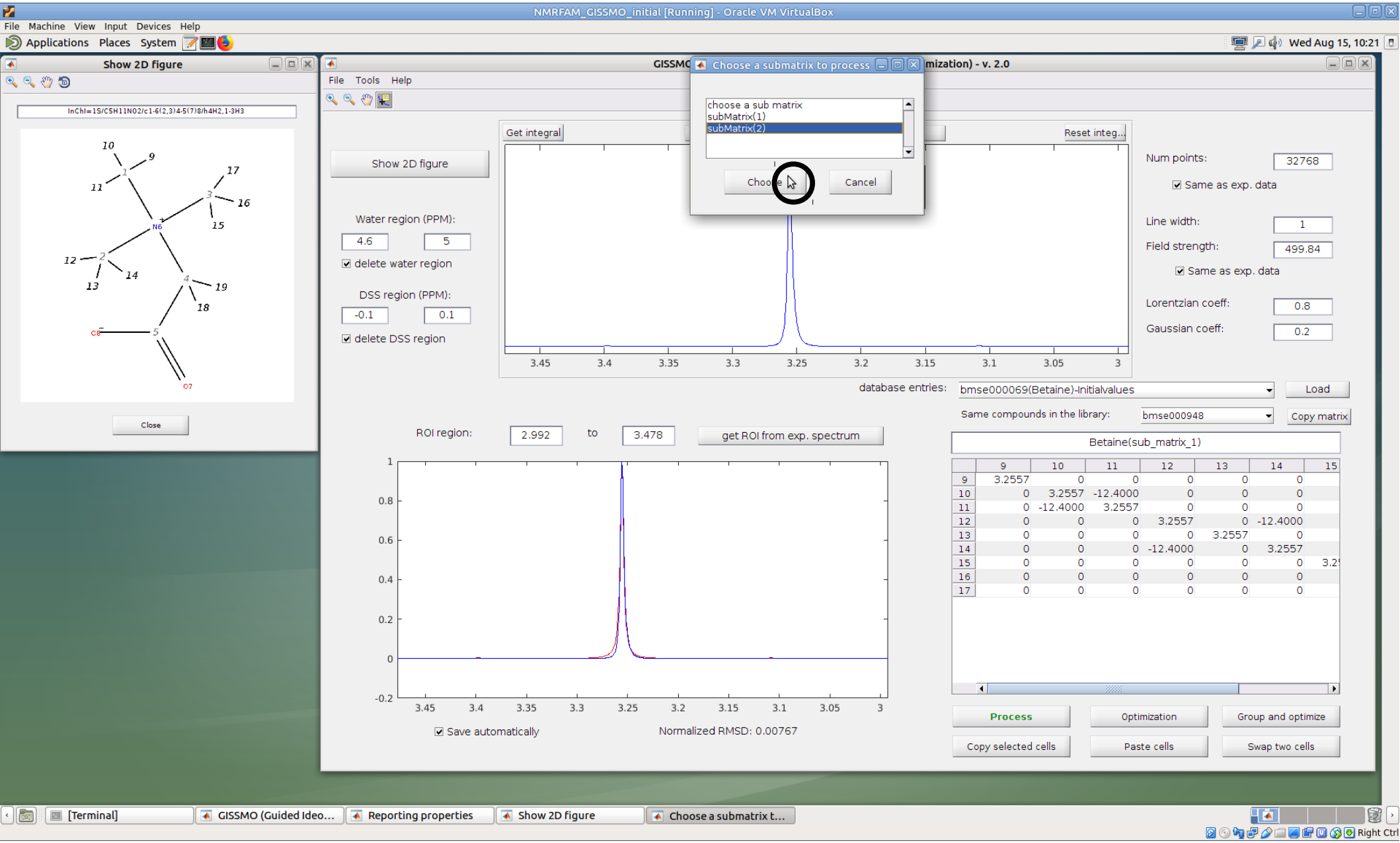
Copy selected cells | Paste cells | Swap two cells

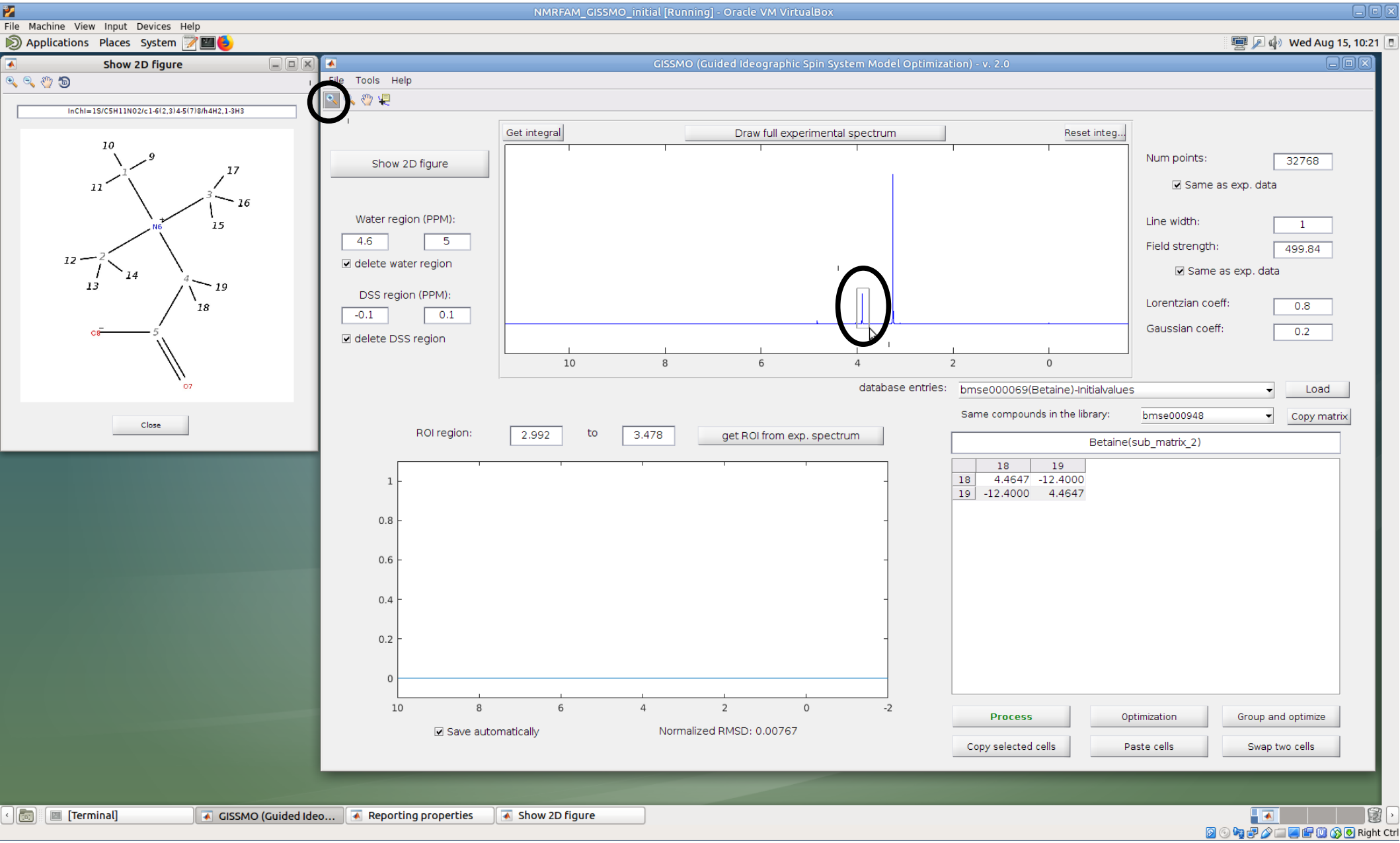
[Terminal] | GISSMO (Guided Ideo... | Reporting properties | Show 2D figure | Optimization report:

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:20
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 3.2555
Amp: 0.989
PPM is copied to clipboard
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
After clicking “Process”
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_1)
Save automatically
Normalized RMSD: 0.00767
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
Wed Aug 15, 10:21
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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
Split spin matrix
Show sub matrices
Process a sub matrix
Copy/Paste sub matrices
Merge sub matrices
Adjust peak amplitude
Delete submatrices
Draw full experimental spectrum
Reset integ...
PPM: 3.2555
Amp: 0.989
PPM is copied to clipboard
Process other submatrix
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_1)
Save automatically
Normalized RMSD: 0.00767
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
Wed Aug 15, 10:21
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
File Tools Help
Choose a submatrix to process
choose a sub matrix
subMatrix(1)
subMatrix(2)
Choose
Cancel
Get integral
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_1)
Save automatically
Normalized RMSD: 0.00767
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Choose a submatrix t...
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:21
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.992
to
3.478
get ROI from exp. spectrum
Betaine(sub_matrix_2)
18 19
18 4.4647 -12.4000
19 -12.4000 4.4647
Save automatically
Normalized RMSD: 0.00767
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
Wed Aug 15, 10:22
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Show 2D figure
Get integral
Draw full experimental spectrum
Reset integ...
Then peak pick
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
3.751
to
4.009
get ROI from exp. spectrum
Betaine(sub_matrix_2)
18 19
18 4.4647 -12.4000
19 -12.4000 4.4647
After clicking “get ROI ...” and “Process” keys
Save automatically
Normalized RMSD: 0.26467
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

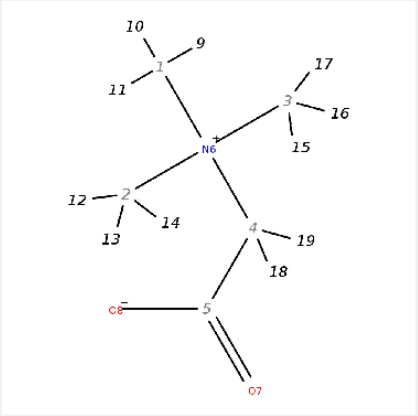
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:22

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

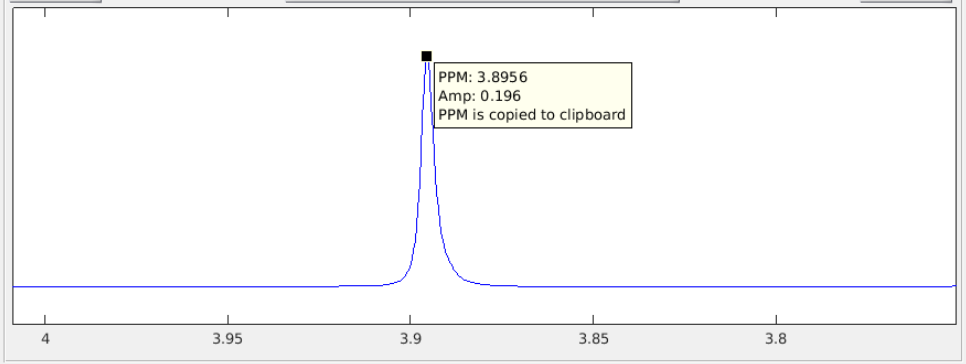
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

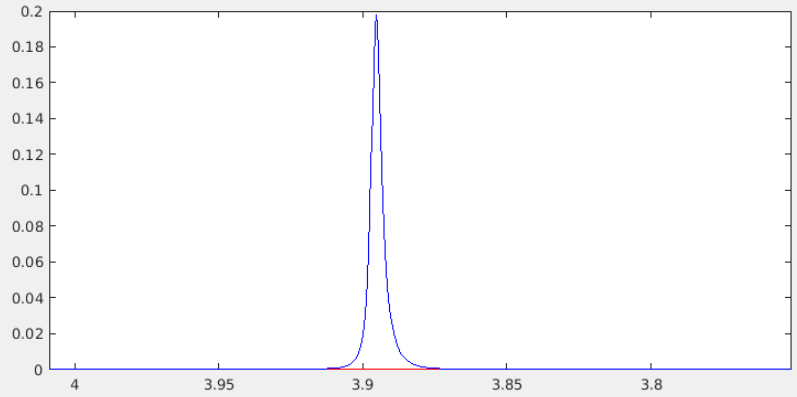
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 3.751 to 4.009 | get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.26467

Betaine(sub_matrix_2)

| | 18 | 19 |
|---|---|---|
| 18 | 4.4647 | -12.4000 |
| 19 | -12.4000 | 4.4647 |

Left-click cell and 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

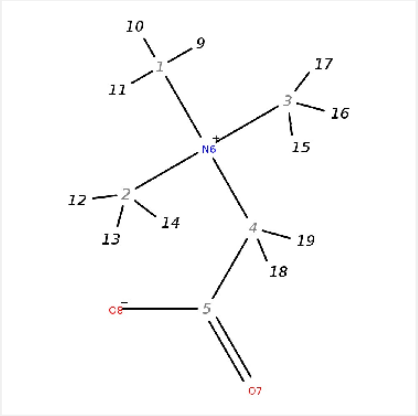
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:23

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

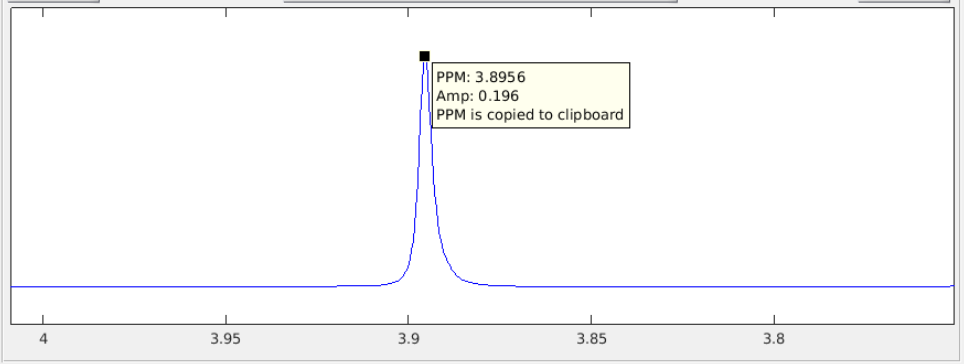
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

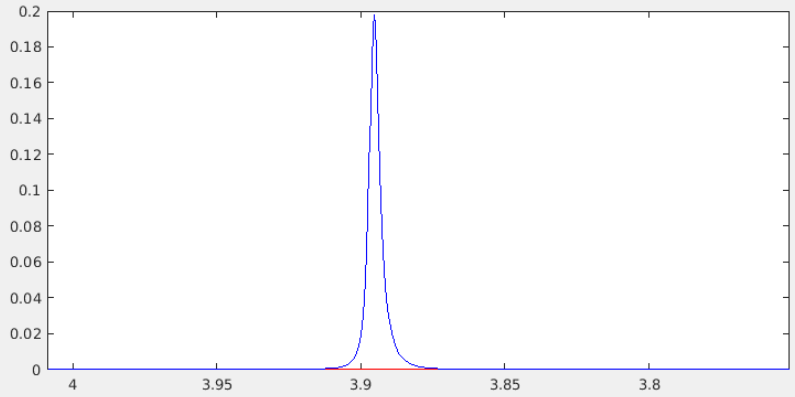
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 3.751 to 4.009 | get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.26467

Betaine(sub_matrix_2)

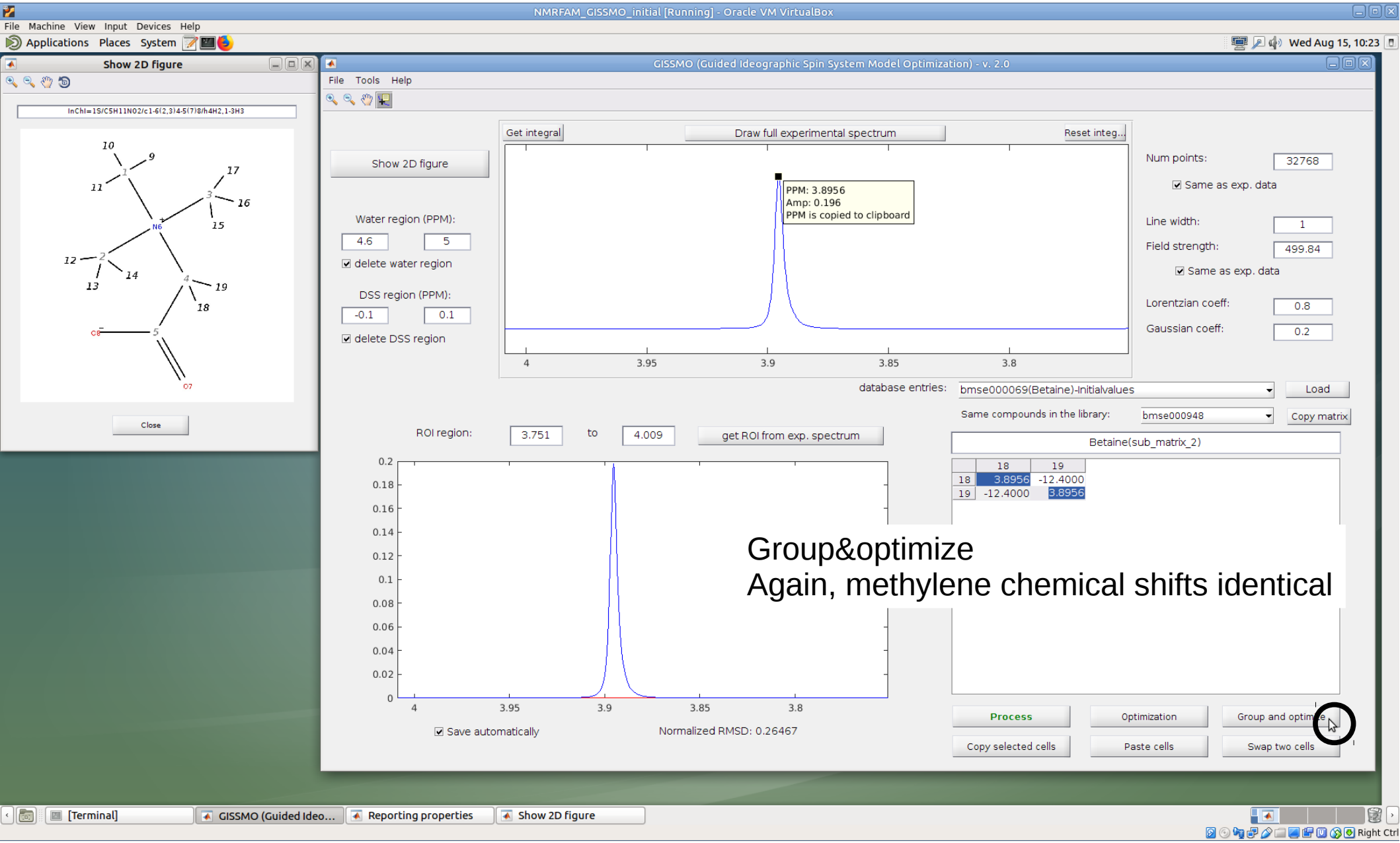
| | 18 | 19 |
|---|---|---|
| 18 | 3.8956 | -12.4000 |
| 19 | -12.4000 | 4.4647 |

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
Wed Aug 15, 10:23
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 3.8956
Amp: 0.196
PPM is copied to clipboard
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
3.751
to
4.009
get ROI from exp. spectrum
Betaine(sub_matrix_2)
18 19
18 3.8956 -12.4000
19 -12.4000 3.8956
Group&optimize
Again, methylene chemical shifts identical
Save automatically
Normalized RMSD: 0.26467
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

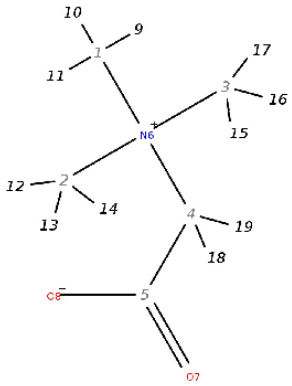
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:24

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

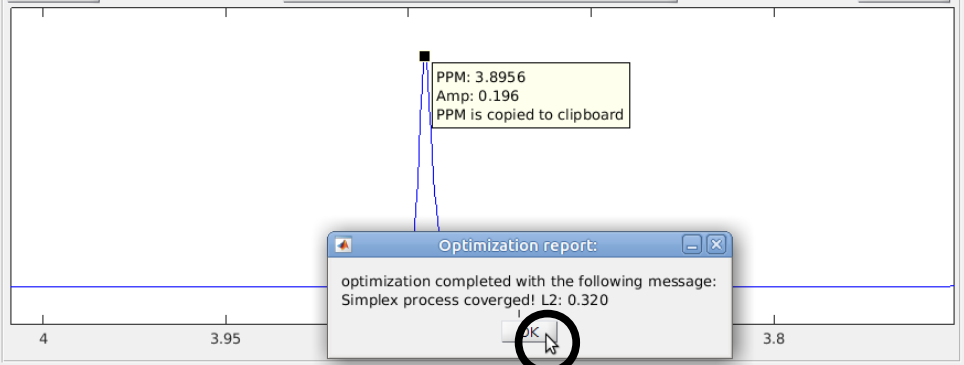
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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




Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 0.320

OK

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

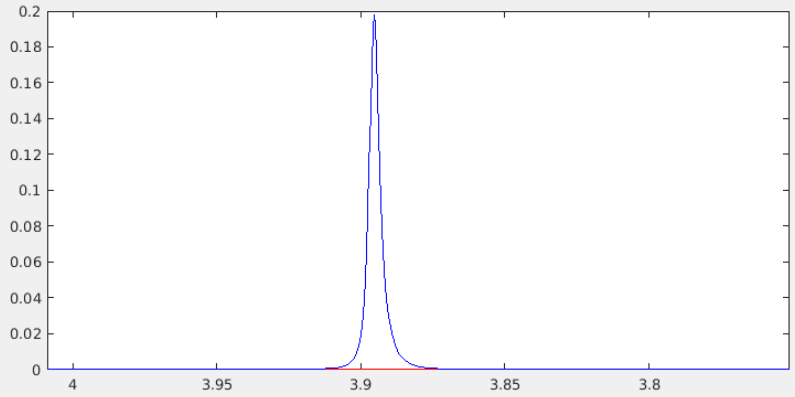
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 3.751 to 4.009 | get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.26467

Betaine(sub_matrix_2)

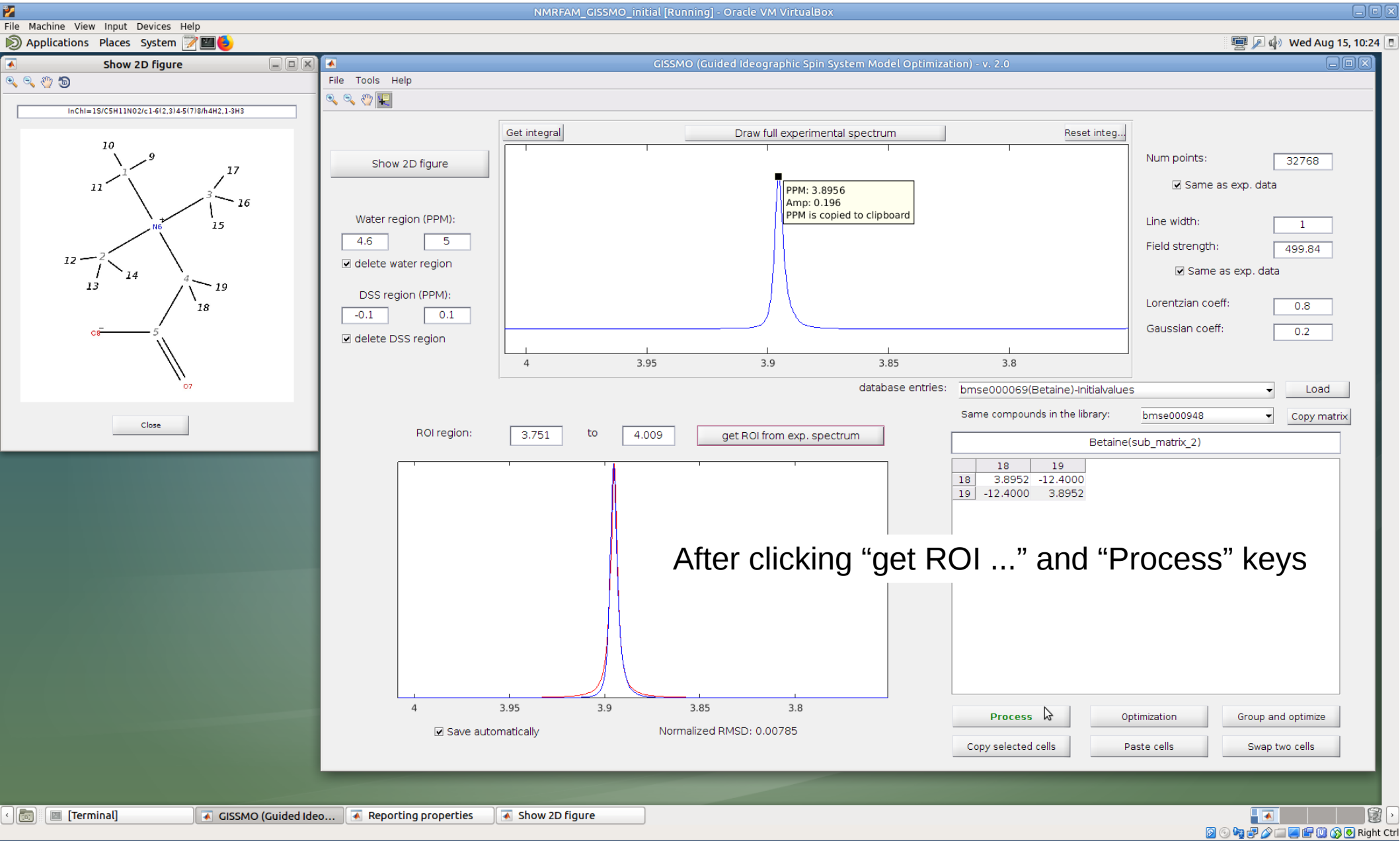
| | 18 | 19 |
|---|---|---|
| 18 | 3.8952 | -12.4000 |
| 19 | -12.4000 | 3.8952 |

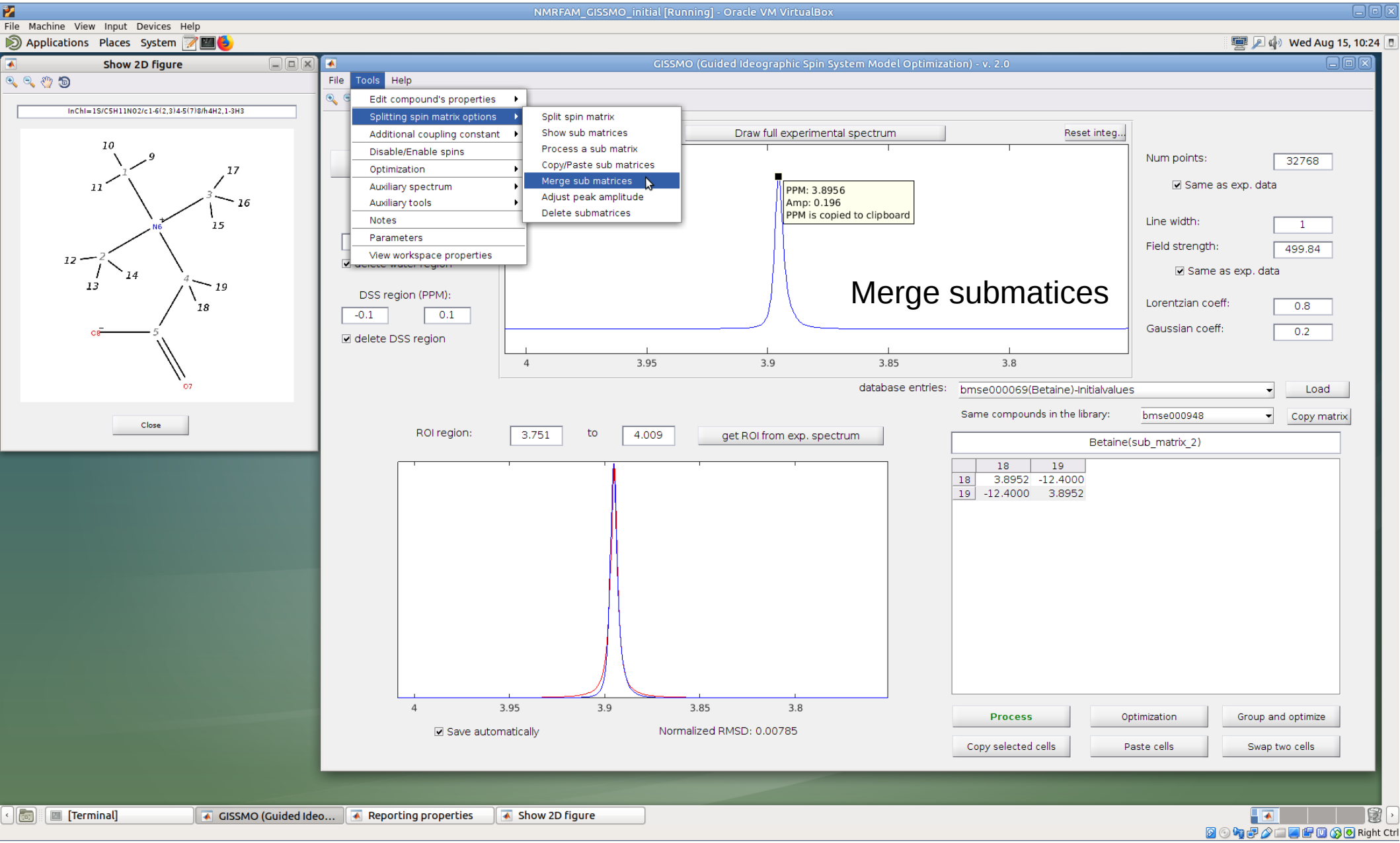
Process | Optimization | Group and optimize

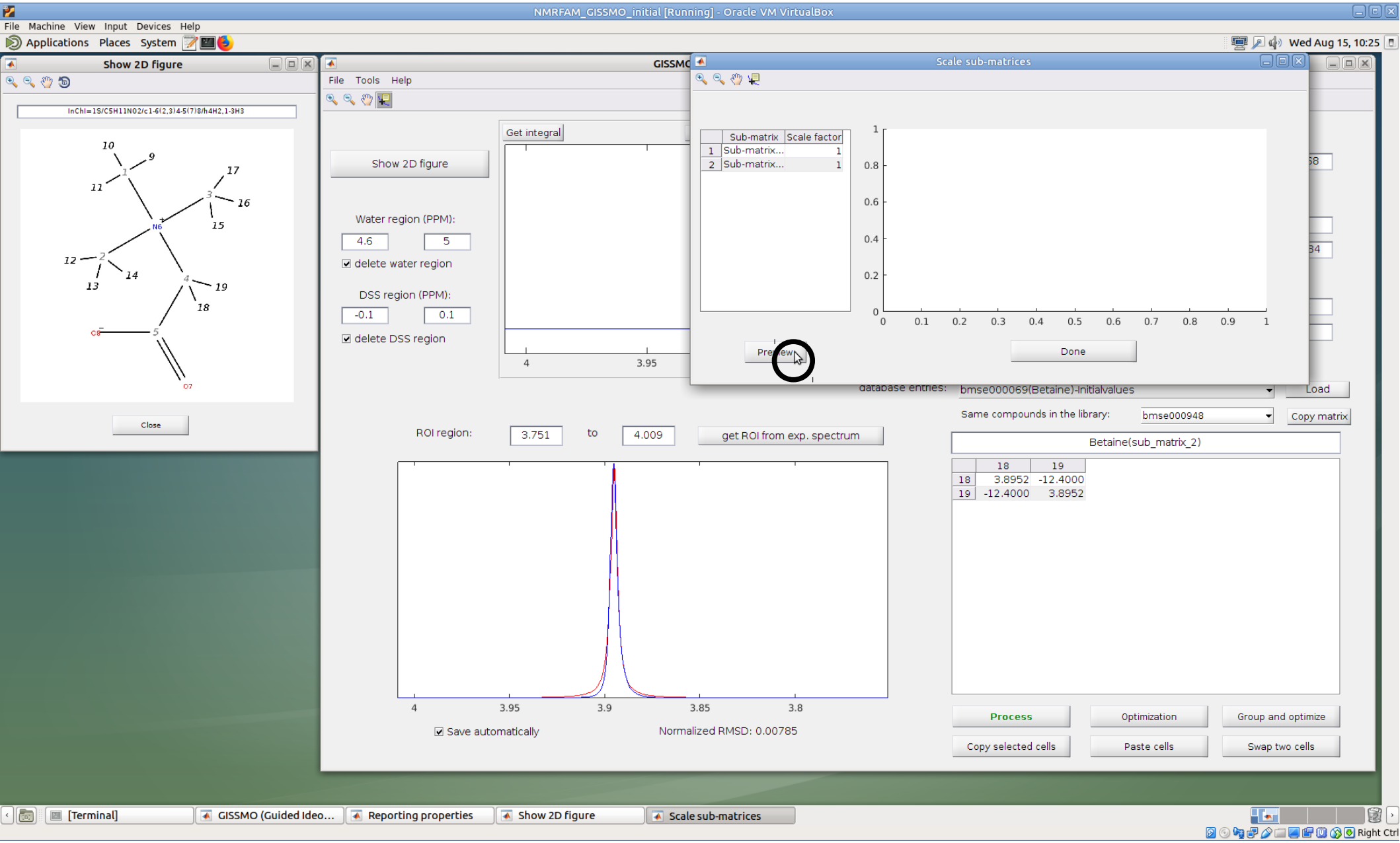
Copy selected cells | Paste cells | Swap two cells

[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
Wed Aug 15, 10:24
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 3.8956
Amp: 0.196
PPM is copied to clipboard
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
3.751
to
4.009
get ROI from exp. spectrum
Betaine(sub_matrix_2)
18 19
18 3.8952 -12.4000
19 -12.4000 3.8952
After clicking “get ROI ...” and “Process” keys
Save automatically
Normalized RMSD: 0.00785
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
Wed Aug 15, 10:24
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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
Split spin matrix
Show sub matrices
Process a sub matrix
Copy/Paste sub matrices
Merge sub matrices
Adjust peak amplitude
Delete submatrices
Draw full experimental spectrum
Reset integ...
PPM: 3.8956
Amp: 0.196
PPM is copied to clipboard
Merge submatices
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
3.751
to
4.009
get ROI from exp. spectrum
Betaine(sub_matrix_2)
18 19
18 3.8952 -12.4000
19 -12.4000 3.8952
Save automatically
Normalized RMSD: 0.00785
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
Wed Aug 15, 10:25
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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
4
3.95
Scale sub-matrices
Sub-matrix
Scale factor
1 Sub-matrix... 1
2 Sub-matrix... 1
Preview
Done
database entries:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
Betaine(sub_matrix_2)
18 19
18 3.8952 -12.4000
19 -12.4000 3.8952
ROI region:
3.751
to
4.009
get ROI from exp. spectrum
4
3.95
3.9
3.85
3.8
Save automatically
Normalized RMSD: 0.00785
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Scale sub-matrices
Right Ctrl

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:25

Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3

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

4 3.95

Scale sub-matrices

| | Sub-matrix | Scale factor |
|---|---|---|
| 1 | Sub-matrix... | 1 |
| 2 | Sub-matrix... | 1 |

blue: experimental spectrum, red: merged simulated spectrum

12 10 8 6 4 2 0 -2

Preview

Done

database entries: bmse000069(Betaine)-Initialvalues Load

Same compounds in the library: bmse000948 Copy matrix

ROI region: 3.751 to 4.009 get ROI from exp. spectrum

Betaine(sub_matrix_2)

| | 18 | 19 |
|---|---|---|
| 18 | 3.8952 | -12.4000 |
| 19 | -12.4000 | 3.8952 |

4 3.95 3.9 3.85 3.8

Save automatically

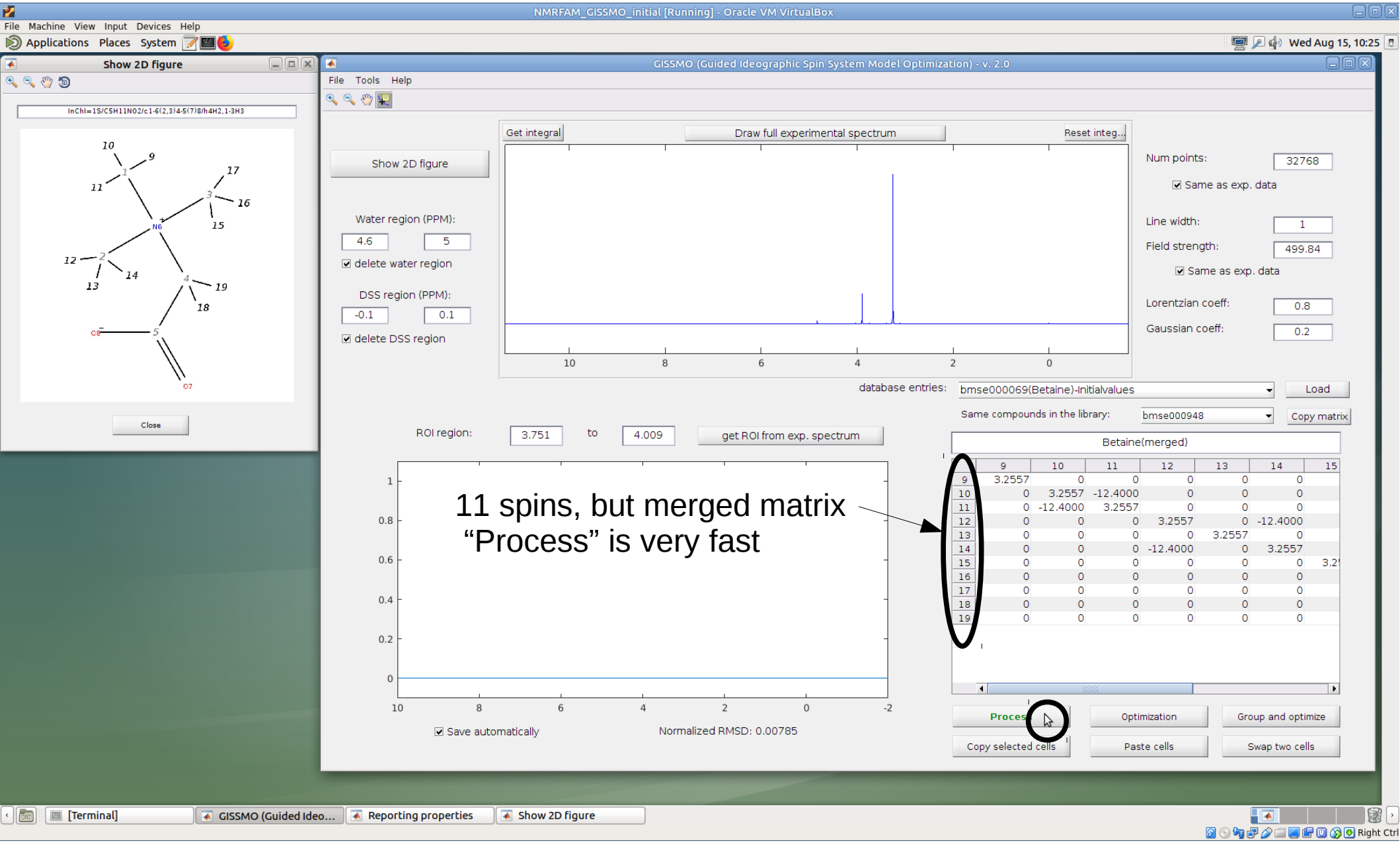
Normalized RMSD: 0.00785

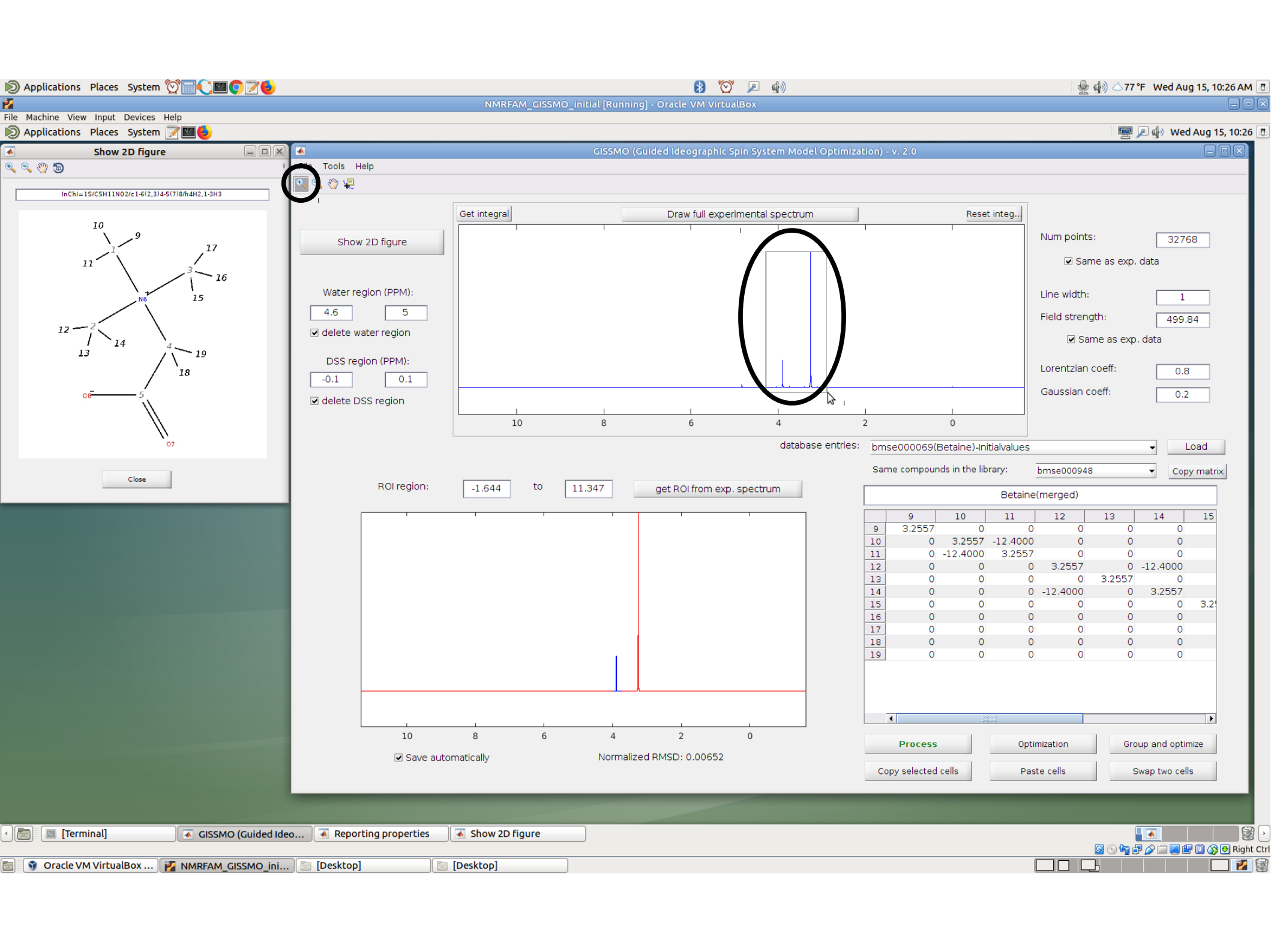
Process Optimization Group and optimize

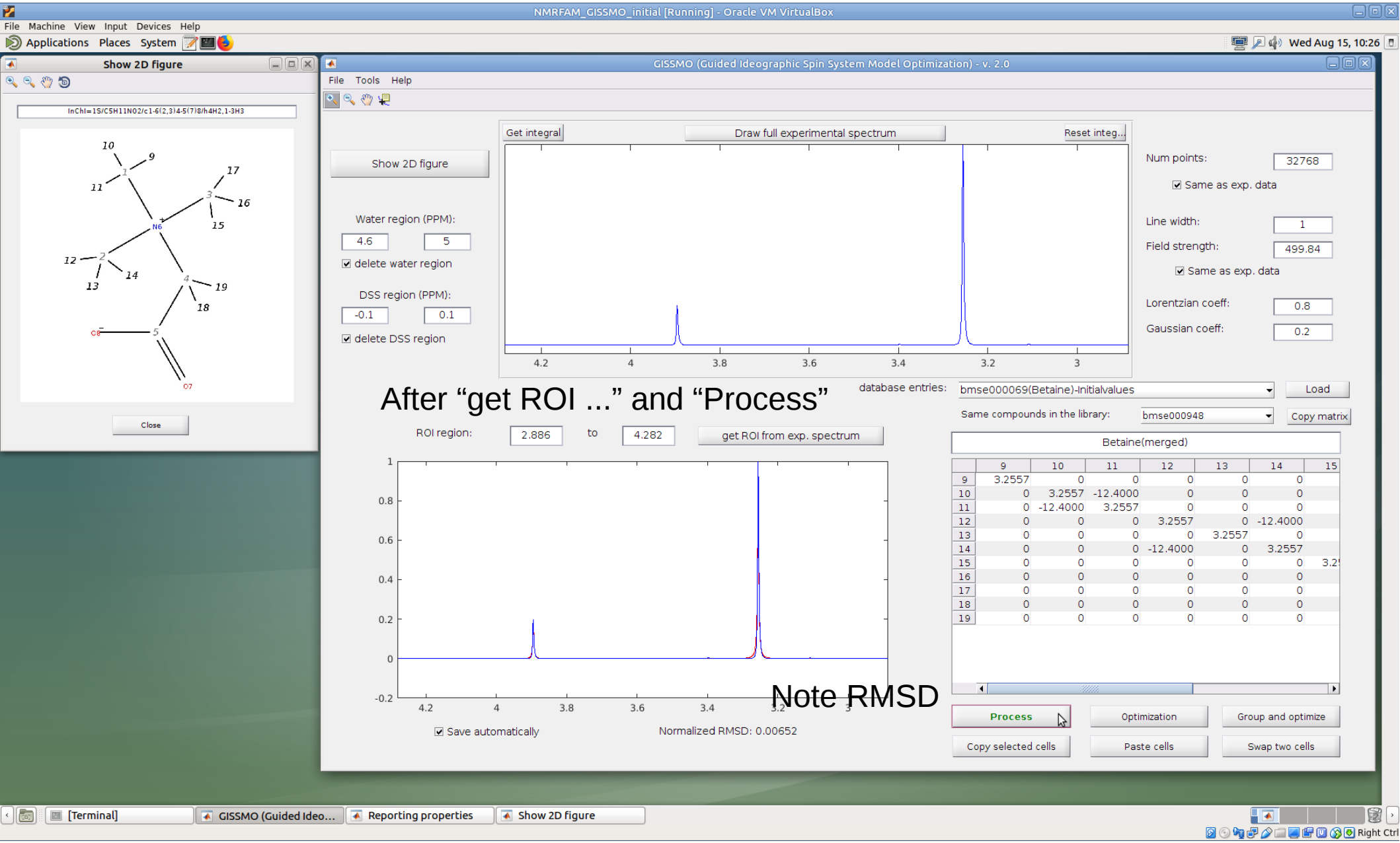
Copy selected cells Paste cells Swap two cells

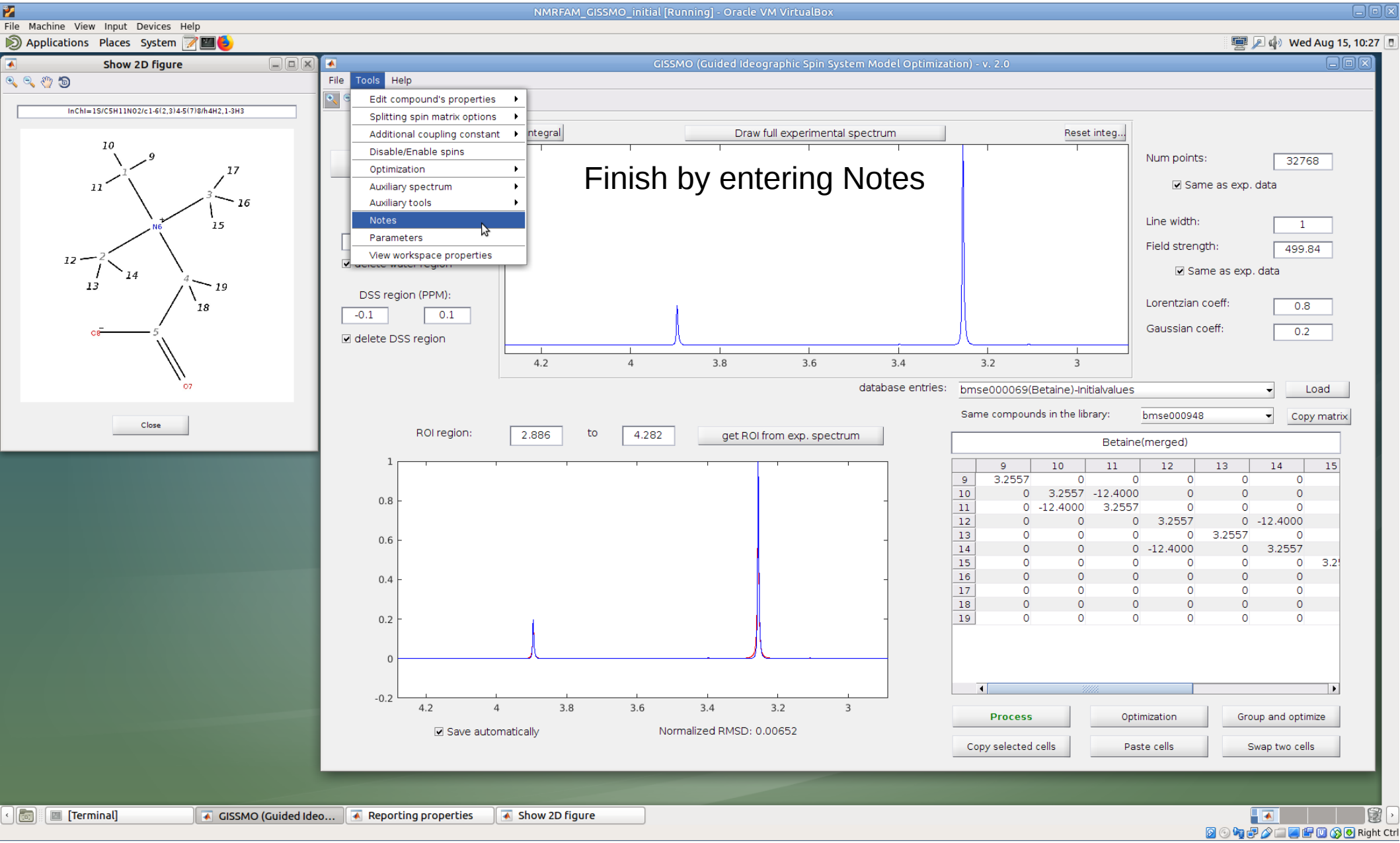
[Terminal] GISSMO (Guided Ideo... Reporting properties Show 2D figure Scale sub-matrices

Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:25
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
3.751
to
4.009
get ROI from exp. spectrum
11 spins, but merged matrix
"Process" is very fast
Betaine(merged)
Save automatically
Normalized RMSD: 0.00785
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Right Ctrl


Applications Places System
77 °F Wed Aug 15, 10:26 AM
NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:26
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
-1.644
to
11.347
get ROI from exp. spectrum
Betaine(merged)
Save automatically
Normalized RMSD: 0.00652
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideo...
Reporting properties
Show 2D figure
Oracle VM VirtualBox ...
NMRFAM_GISSMO_ini...
[Desktop]
[Desktop]
Right Ctrl


NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
Wed Aug 15, 10:26
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
After "get ROI ..." and "Process"
database entries:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.886
to
4.282
get ROI from exp. spectrum
Betaine(merged)
Note RMSD
Save automatically
Normalized RMSD: 0.00652
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
Wed Aug 15, 10:27
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
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 entering Notes
Draw full experimental spectrum
Reset integ...
Num points:
32768
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:
bmse000069(Betaine)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.886
to
4.282
get ROI from exp. spectrum
Betaine(merged)
Save automatically
Normalized RMSD: 0.00652
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

Wed Aug 15, 10:27

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3

Close

## GISSMO

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 integ...

## 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: 32768

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: bmse000069(Betaine)-Initialvalues Load

Same compounds in the library: bmse000948 Copy matrix

ROI region: 2.886 to 4.282 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.00652

Betaine(merged)

| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.2557 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.2557 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.2557 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.2557 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.2557 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.2557 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.2 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 19 | 0 | 0 | 0 | 0 | 0 | 0 | |

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

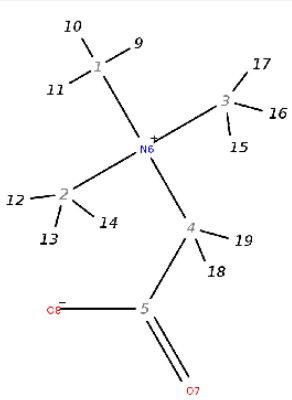
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:28

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

## GISSMO

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

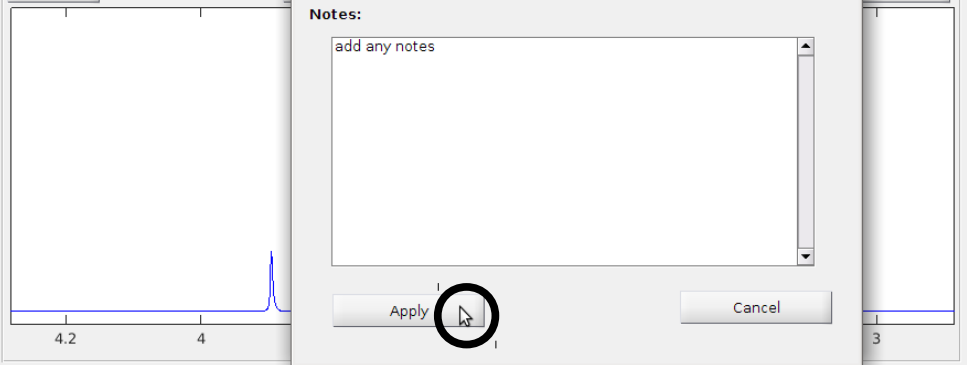
DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset integ...




## Notes

Status:

Done

Notes:

add any notes

Apply

Cancel

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

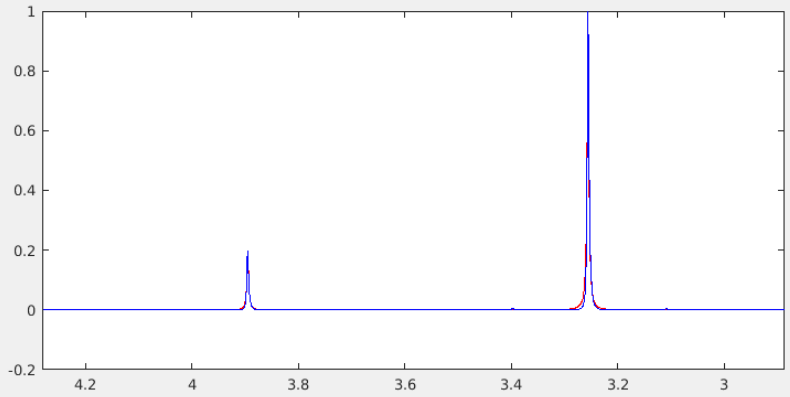
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000069(Betaine)-Initialvalues Load

Same compounds in the library: bmse000948 Copy matrix

ROI region: 2.886 to 4.282 get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.00652

Betaine(merged)

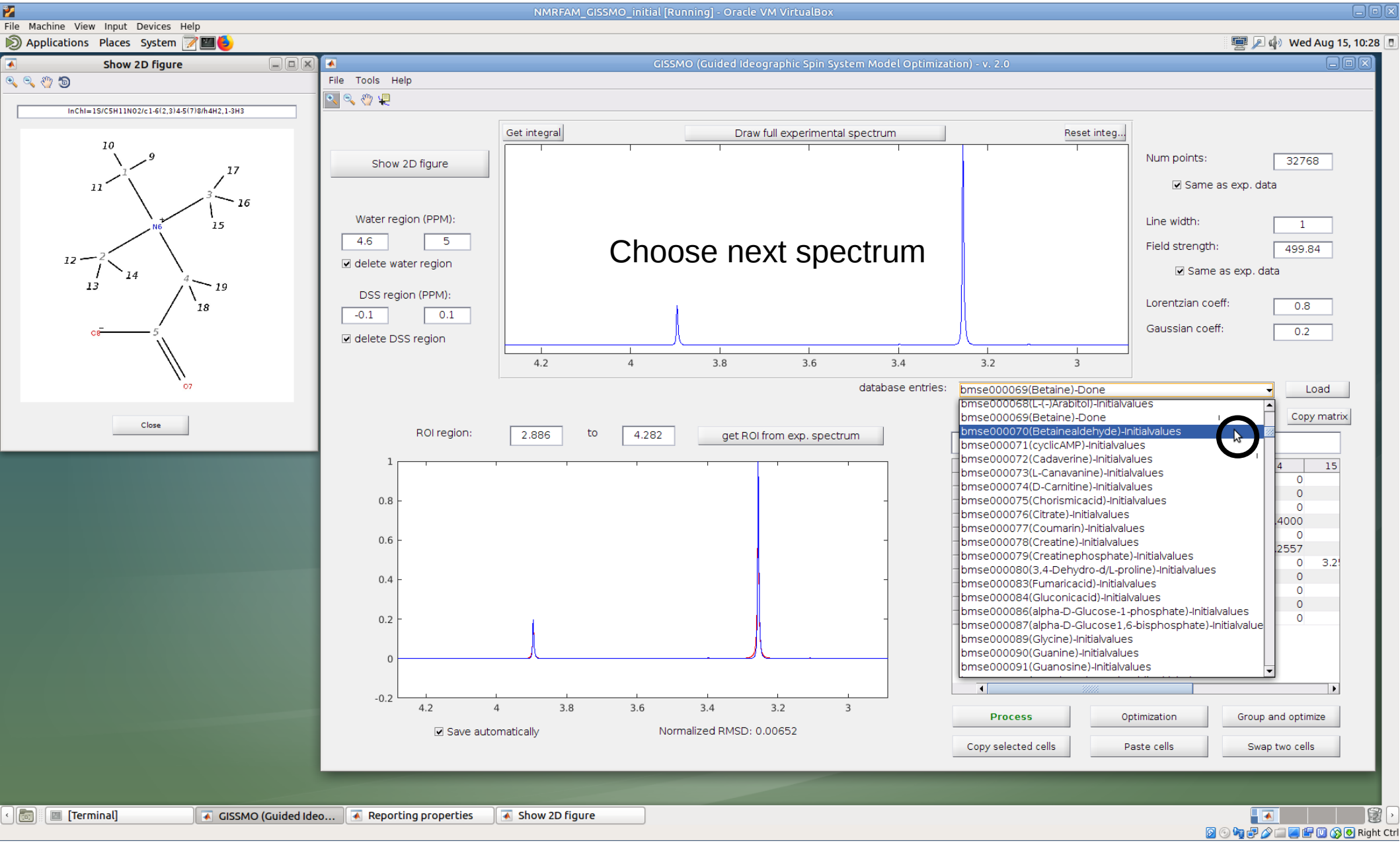
| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.2557 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.2557 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.2557 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.2557 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.2557 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.2557 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.2 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 19 | 0 | 0 | 0 | 0 | 0 | 0 | |

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
Wed Aug 15, 10:28
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Choose next spectrum
Num points:
32768
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:
bmse000069(Betaine)-Done
Load
Copy matrix
bmse000068(L-(-)Arabitol)-Initialvalues
bmse000069(Betaine)-Done
bmse000070(Betainealdehyde)-Initialvalues
bmse000071(cyclicAMP)-Initialvalues
bmse000072(Cadaverine)-Initialvalues
bmse000073(L-Canavanine)-Initialvalues
bmse000074(D-Carnitine)-Initialvalues
bmse000075(Chorismicacid)-Initialvalues
bmse000076(Citrate)-Initialvalues
bmse000077(Coumarin)-Initialvalues
bmse000078(Creatine)-Initialvalues
bmse000079(Creatinephosphate)-Initialvalues
bmse000080(3,4-Dehydro-d/L-proline)-Initialvalues
bmse000083(Fumaricacid)-Initialvalues
bmse000084(Gluconicacid)-Initialvalues
bmse000086(alpha-D-Glucose-1-phosphate)-Initialvalues
bmse000087(alpha-D-Glucose1,6-bisphosphate)-Initialvalue
bmse000089(Glycine)-Initialvalues
bmse000090(Guanine)-Initialvalues
bmse000091(Guanosine)-Initialvalues
ROI region:
2.886
to
4.282
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.00652
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

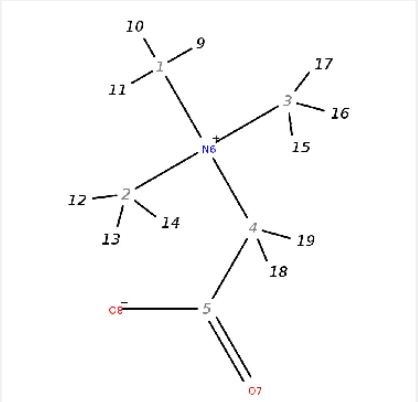
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:28

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

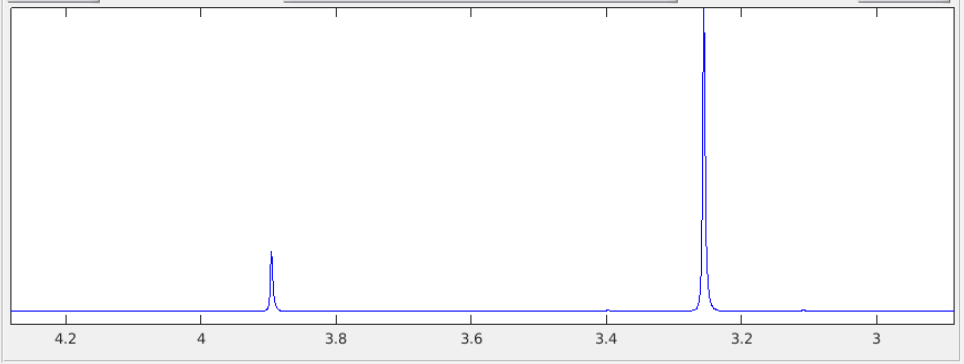
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

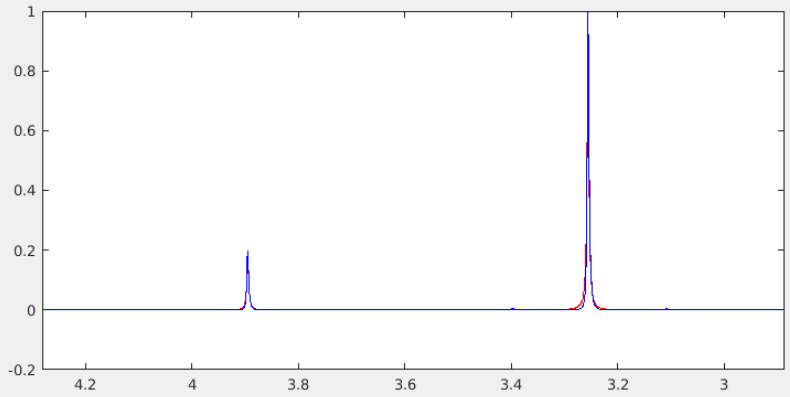
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000070(Betainealdehyde)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy m...

ROI region: 2.886 to 4.282 get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.00652

Betaine(merged)

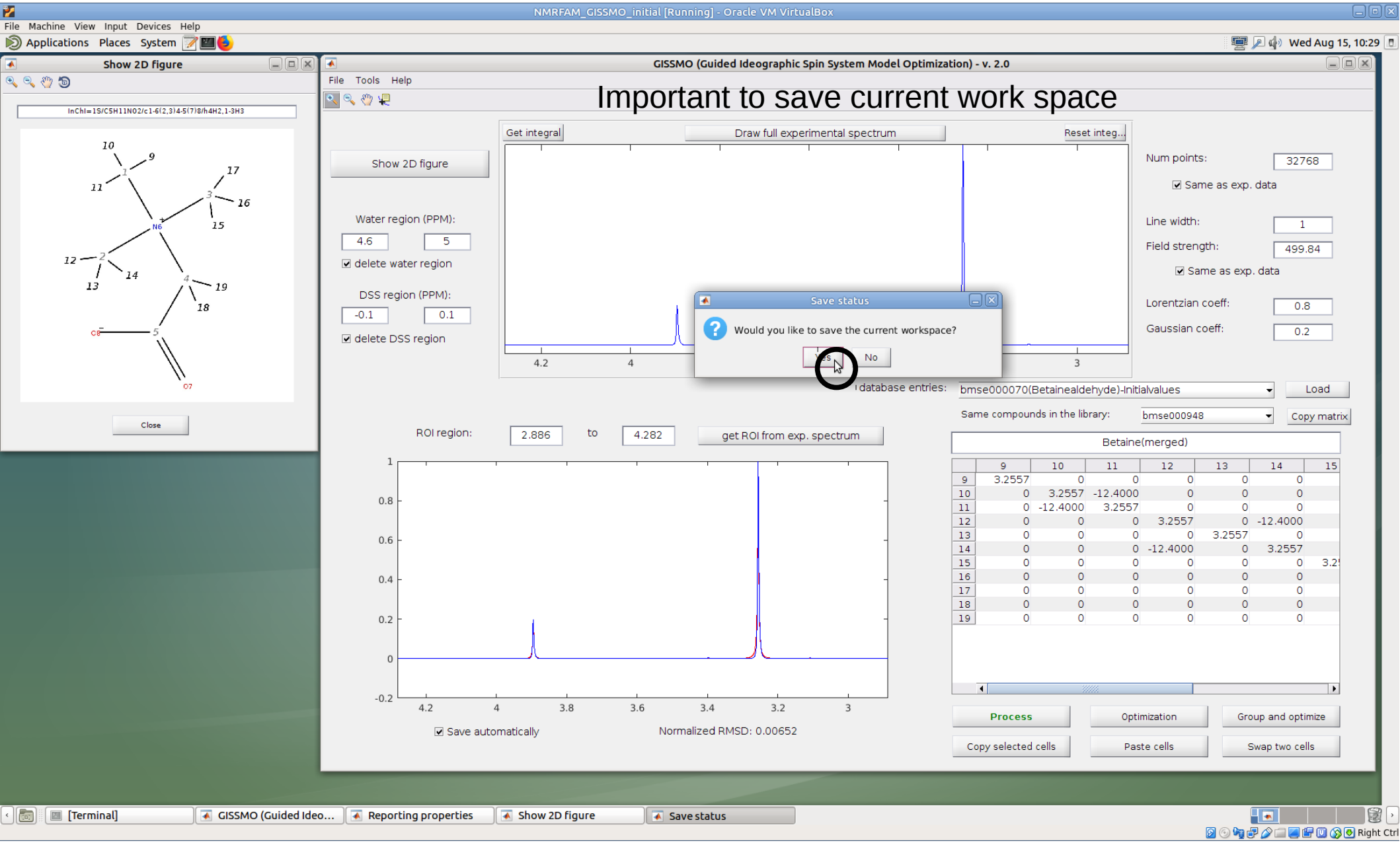
| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.2557 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.2557 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.2557 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.2557 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.2557 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.2557 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.2 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 19 | 0 | 0 | 0 | 0 | 0 | 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
Wed Aug 15, 10:29
Show 2D figure
InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Important to save current work space
Get integral
Draw full experimental spectrum
Reset integ...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
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:
bmse000070(Betainealdehyde)-Initialvalues
Load
Same compounds in the library:
bmse000948
Copy matrix
ROI region:
2.886
to
4.282
get ROI from exp. spectrum
Betaine(merged)
Save automatically
Normalized RMSD: 0.00652
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

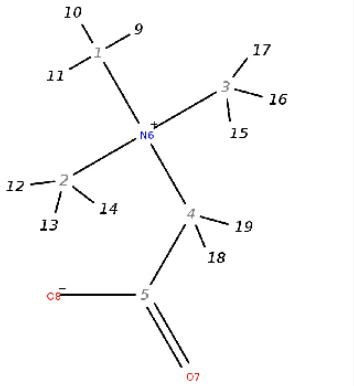
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:29

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

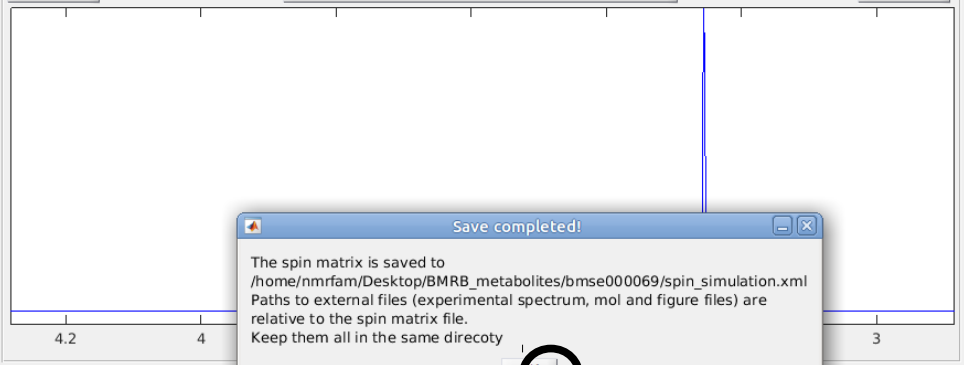
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

### Save completed!

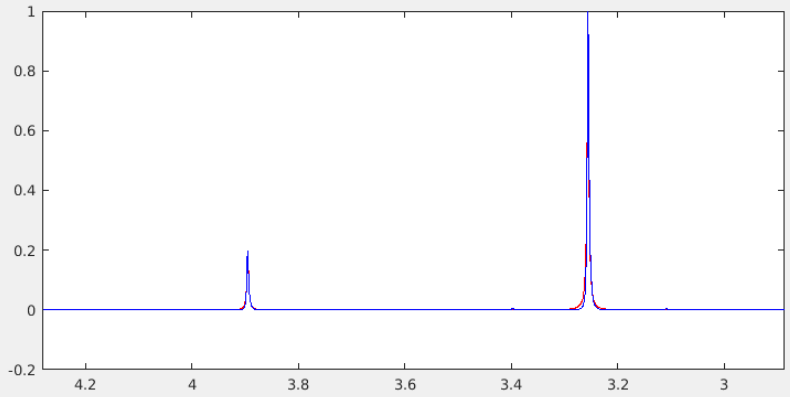
The spin matrix is saved to
/home/nmrfam/Desktop/BMRB_metabolites/bmse000069/spin_simulation.xml
Paths to external files (experimental spectrum, mol and figure files) are relative to the spin matrix file.
Keep them all in the same direcoty

OK

etainealdehyde)-Initialvalues | Load

Same compounds in the library: bmse000948 | Copy matrix

ROI region: 2.886 to 4.282 | get ROI from exp. spectrum




Save automatically

Normalized RMSD: 0.00652

Betaine(merged)

| | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|
| 9 | 3.2557 | 0 | 0 | 0 | 0 | 0 | |
| 10 | 0 | 3.2557 | -12.4000 | 0 | 0 | 0 | |
| 11 | 0 | -12.4000 | 3.2557 | 0 | 0 | 0 | |
| 12 | 0 | 0 | 0 | 3.2557 | 0 | -12.4000 | |
| 13 | 0 | 0 | 0 | 0 | 3.2557 | 0 | |
| 14 | 0 | 0 | 0 | -12.4000 | 0 | 3.2557 | |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | 3.2 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 18 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 19 | 0 | 0 | 0 | 0 | 0 | 0 | |

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

NMRFAM_GISSMO_initial [Running] - Oracle VM VirtualBox

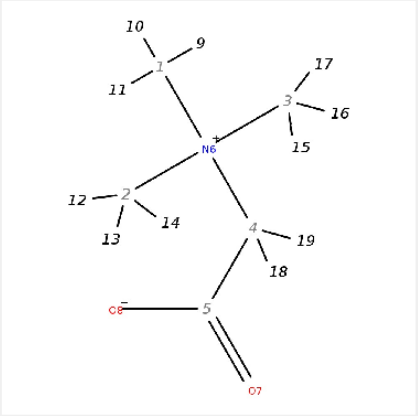
File Machine View Input Devices Help

Applications Places System

Wed Aug 15, 10:29

## Show 2D figure

InChI=1S/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3




Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

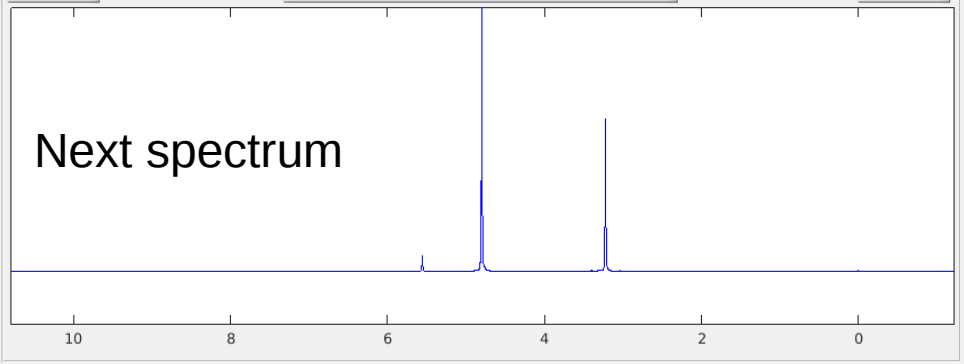
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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




Num points: 32768

Same as exp. data

Line width: 1

Field strength: 400.13

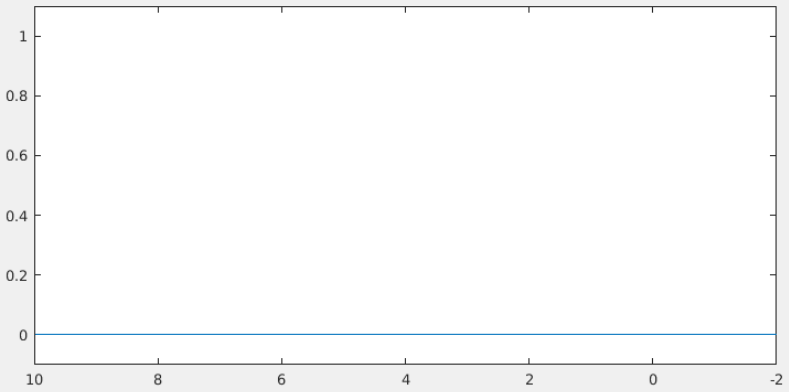
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000070(Betainealdehyde)-Initialvalues | Load

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




Save automatically

simulation info

Betaine aldehyde(merged)

| | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|---|---|
| 8 | 3.3077 | 0 | -12.4000 | 0 | 0 | 0 | |
| 9 | 0 | 3.3077 | 0 | 0 | 0 | 0 | |
| 10 | -12.4000 | 0 | 3.3077 | 0 | 0 | 0 | |
| 11 | 0 | 0 | 0 | 3.3077 | -12.4000 | 0 | |
| 12 | 0 | 0 | 0 | -12.4000 | 3.3077 | 0 | |
| 13 | 0 | 0 | 0 | 0 | 0 | 3.3077 | |
| 14 | 0 | 0 | 0 | 0 | 0 | 0 | 3.3 |
| 15 | 0 | 0 | 0 | 0 | 0 | 0 | -12.4 |
| 16 | 0 | 0 | 0 | 0 | 0 | 0 | |
| 17 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |
| 18 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3300 | 1.3 |
| 19 | 0 | 0 | 0 | 0 | 0 | 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