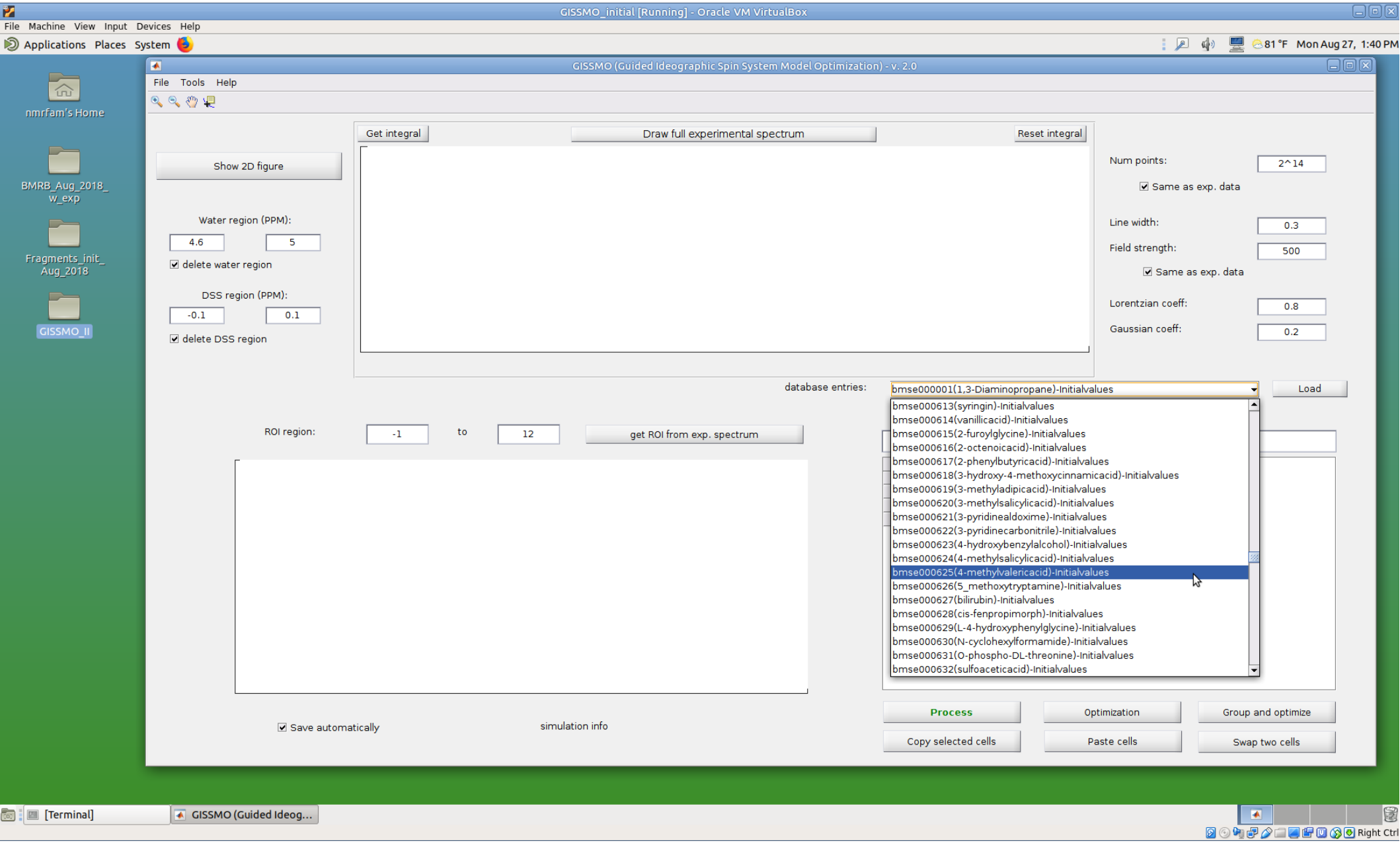
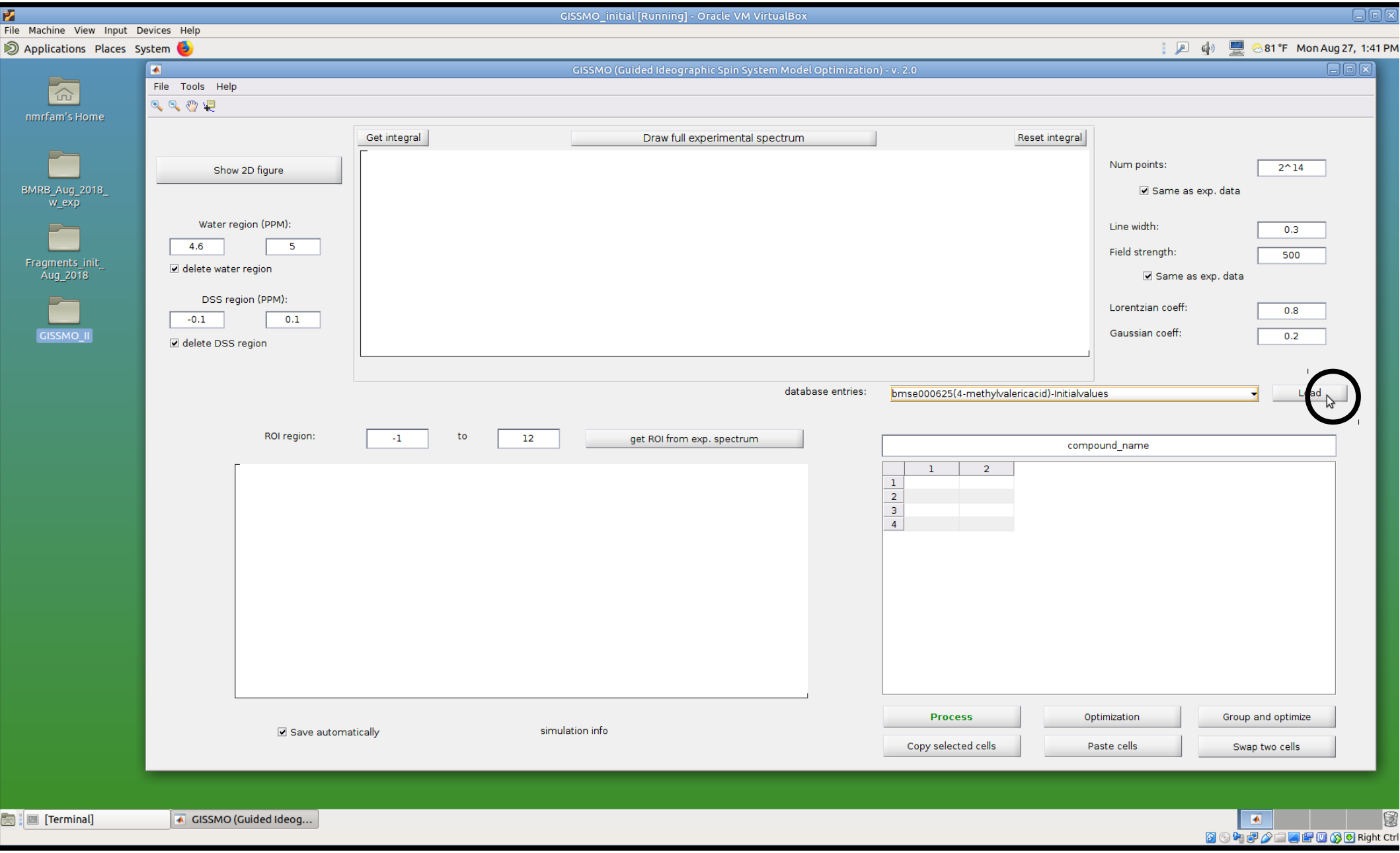
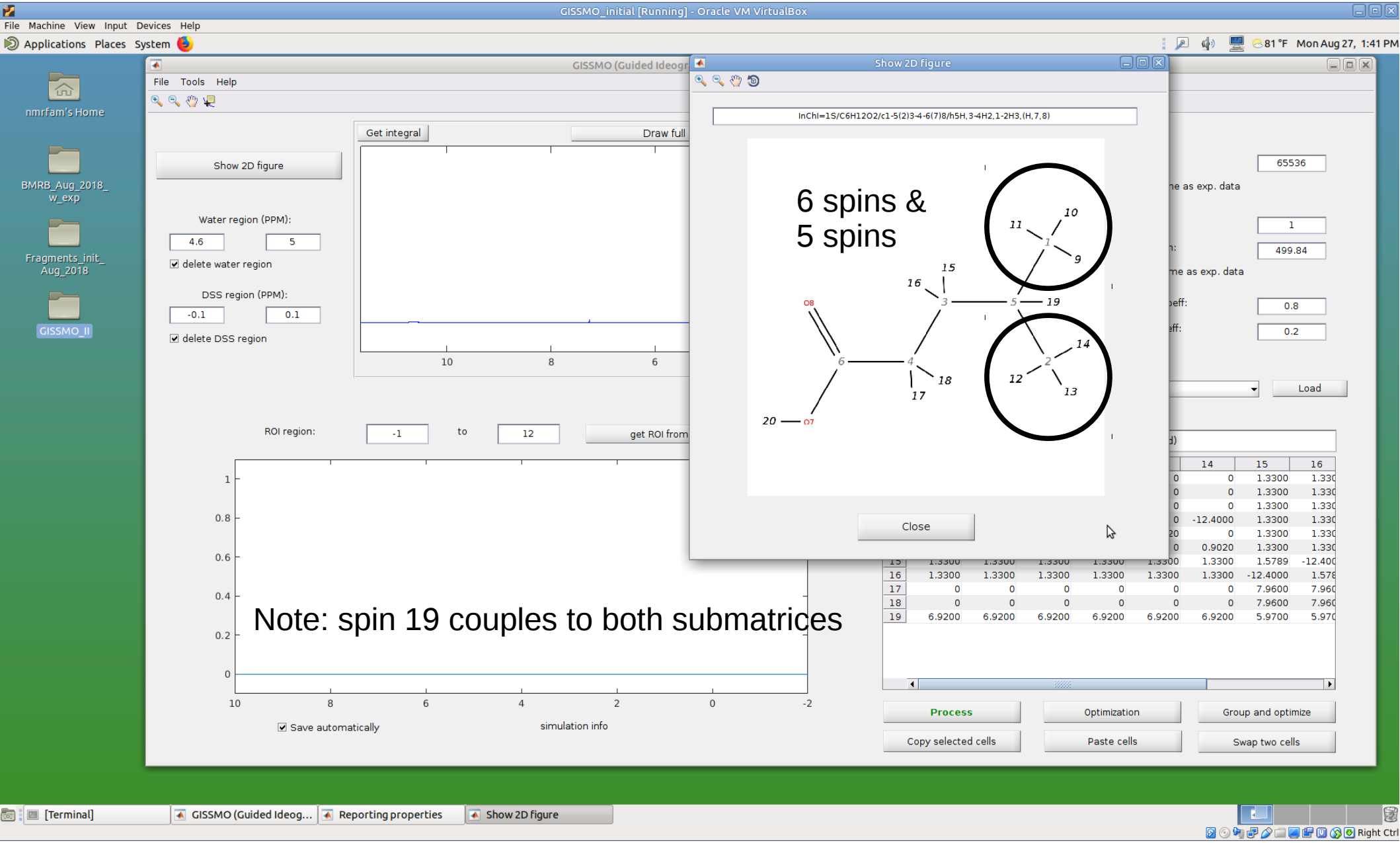
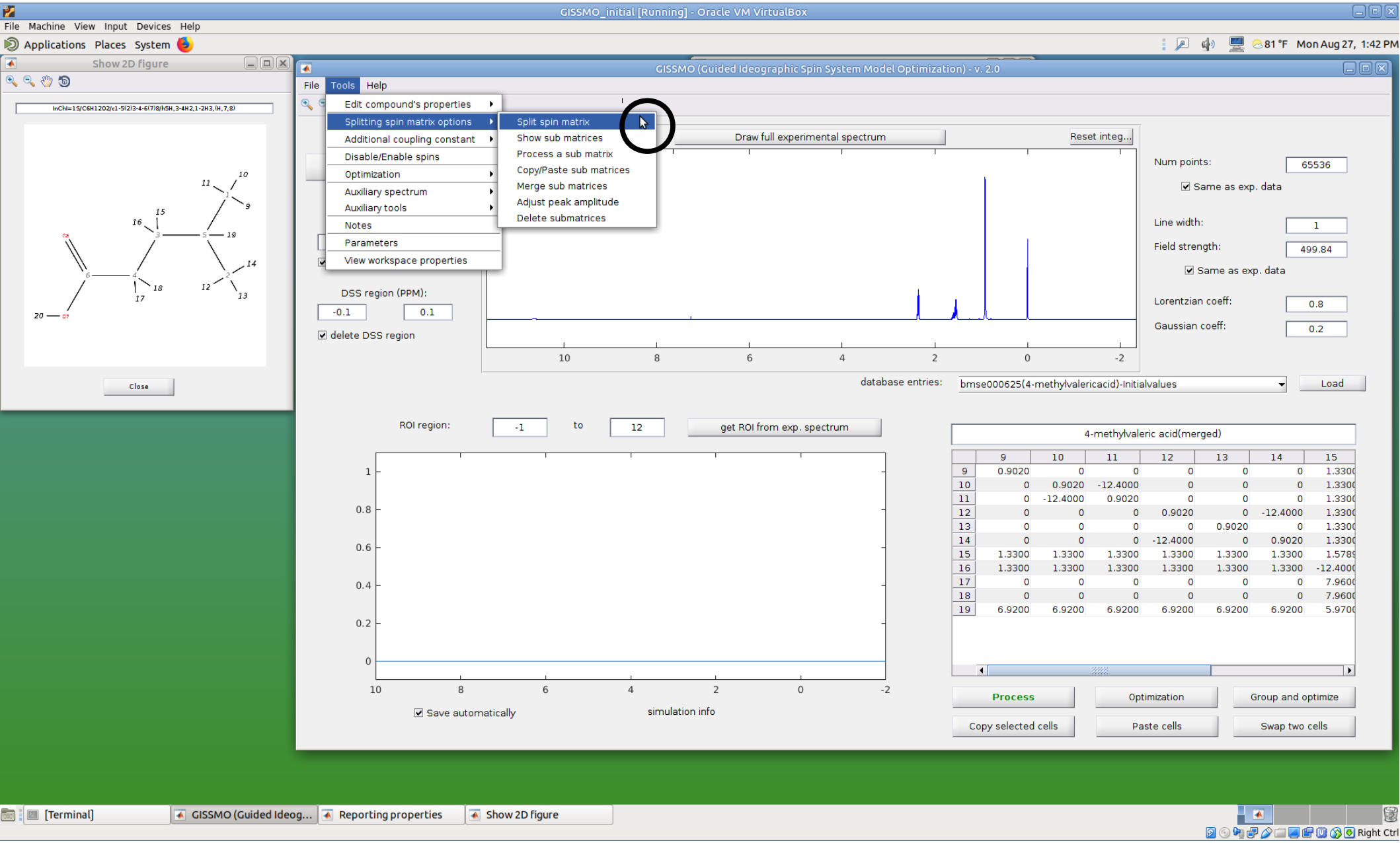

GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:40 PM
nmrfam's Home
BMRB_Aug_2018_w_exp
Fragments_init_Aug_2018
GISSMO_II
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
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:
bmse000001(1,3-Diaminopropane)-Initialvalues
Load
bmse000613(syringin)-Initialvalues
bmse000614(vanillicacid)-Initialvalues
bmse000615(2-furoylglycine)-Initialvalues
bmse000616(2-octenoicacid)-Initialvalues
bmse000617(2-phenylbutyricacid)-Initialvalues
bmse000618(3-hydroxy-4-methoxycinnamicacid)-Initialvalues
bmse000619(3-methyladipicacid)-Initialvalues
bmse000620(3-methylsalicylicacid)-Initialvalues
bmse000621(3-pyridinealdoxime)-Initialvalues
bmse000622(3-pyridinecarbonitrile)-Initialvalues
bmse000623(4-hydroxybenzylalcohol)-Initialvalues
bmse000624(4-methylsalicylicacid)-Initialvalues
bmse000625(4-methylvalericacid)-Initialvalues
bmse000626(5_methoxytryptamine)-Initialvalues
bmse000627(bilirubin)-Initialvalues
bmse000628(cis-fenpropimorph)-Initialvalues
bmse000629(L-4-hydroxyphenylglycine)-Initialvalues
bmse000630(N-cyclohexylformamide)-Initialvalues
bmse000631(O-phospho-DL-threonine)-Initialvalues
bmse000632(sulfoaceticacid)-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 Ideog...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:41 PM
nmrfam's Home
BMRB_Aug_2018_w_exp
Fragments_init_Aug_2018
GISSMO_II
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:
bmse000625(4-methylvalericacid)-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
[Terminal]
GISSMO (Guided Ideog...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:41 PM
nmrfam's Home
BMRB_Aug_2018_w_exp
Fragments_init_Aug_2018
GISSMO_II
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Show 2D figur
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
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:
bmse000625(4-methylvalericacid)-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
11 spins
Need to split matrix
4-methylvaleric acid(merged)
9 10 11 12 13 14 15 16
9 0.9020 0 0 0 0 0 1.3300 1.330
10 0 0.9020 -12.4000 0 0 0 1.3300 1.330
11 0 -12.4000 0.9020 0 0 0 1.3300 1.330
12 0 0 0 0.9020 0 -12.4000 1.3300 1.330
13 0 0 0 0 0.9020 0 1.3300 1.330
14 0 0 0 -12.4000 0 0.9020 1.3300 1.330
15 1.3300 1.3300 1.3300 1.3300 1.3300 1.3300 1.5789 -12.400
16 1.3300 1.3300 1.3300 1.3300 1.3300 1.3300 -12.4000 1.578
17 0 0 0 0 0 0 7.9600 7.960
18 0 0 0 0 0 0 7.9600 7.960
19 6.9200 6.9200 6.9200 6.9200 6.9200 6.9200 5.9700 5.970
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Right Ctrl



Note: spin 19 couples to both submatrices


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:42 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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:
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
-1
to
12
get ROI from exp. spectrum
4-methylvaleric acid(merged)
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

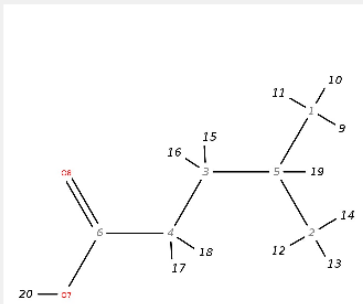
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:42 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

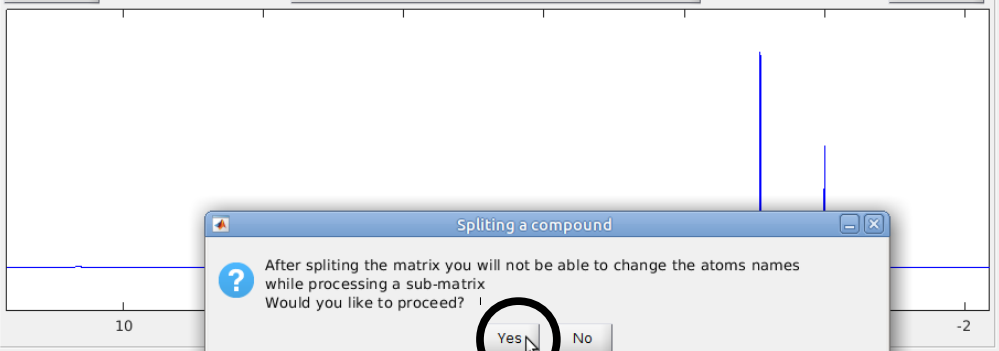
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

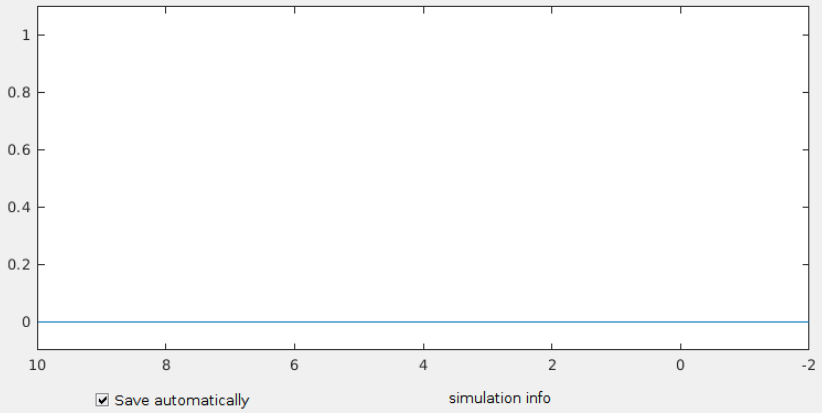
Spliting a compound

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

valericacid)-Initialvalues Load

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



Save automatically

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9020	0	0	0	0	0	1.3300
10	0	0.9020	-12.4000	0	0	0	1.3300
11	0	-12.4000	0.9020	0	0	0	1.3300
12	0	0	0	0.9020	0	-12.4000	1.3300
13	0	0	0	0	0.9020	0	1.3300
14	0	0	0	-12.4000	0	0.9020	1.3300
15	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	1.5789
16	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	-12.4000
17	0	0	0	0	0	0	7.9600
18	0	0	0	0	0	0	7.9600
19	6.9200	6.9200	6.9200	6.9200	6.9200	6.9200	5.9700

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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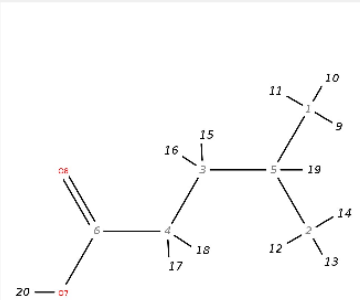
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

GISSMO (Guided Ideation) - v. 2.0

File Tools Help

Number of subMatrices

Number of sub-matrices 2

ok Cancel

Show 2D figure

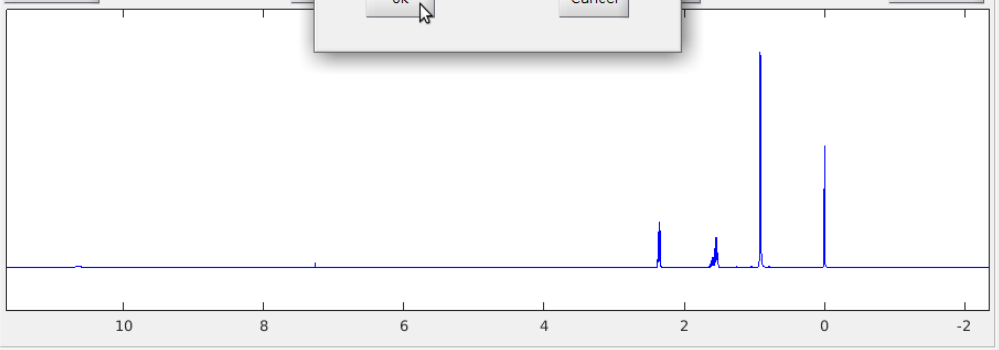
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Get integral Reset integ...



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

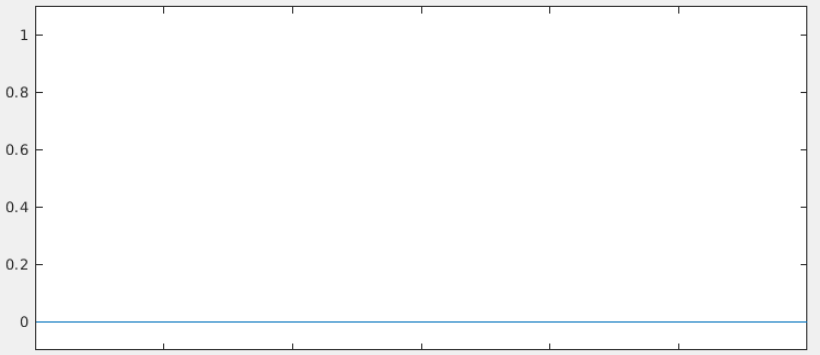
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues Load

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



Save automatically

simulation info

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9020	0	0	0	0	0	1.3300
10	0	0.9020	-12.4000	0	0	0	1.3300
11	0	-12.4000	0.9020	0	0	0	1.3300
12	0	0	0	0.9020	0	-12.4000	1.3300
13	0	0	0	0	0.9020	0	1.3300
14	0	0	0	-12.4000	0	0.9020	1.3300
15	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	1.5789
16	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	-12.4000
17	0	0	0	0	0	0	7.9600
18	0	0	0	0	0	0	7.9600
19	6.9200	6.9200	6.9200	6.9200	6.9200	6.9200	5.9700

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Number of subMatrices

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:43 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

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	choose
16	choose
17	subMatrix(1)
18	subMatrix(2)
19	choose

Split

Cancel

Reset integ...

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

bmse000625(4-methylvalericacid)-Initialvalues

Load

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

Spins 9-14 → group 1
Spins 15-19 → group 2

Save automatically

simulation info

4-methylvaleric acid(merged)

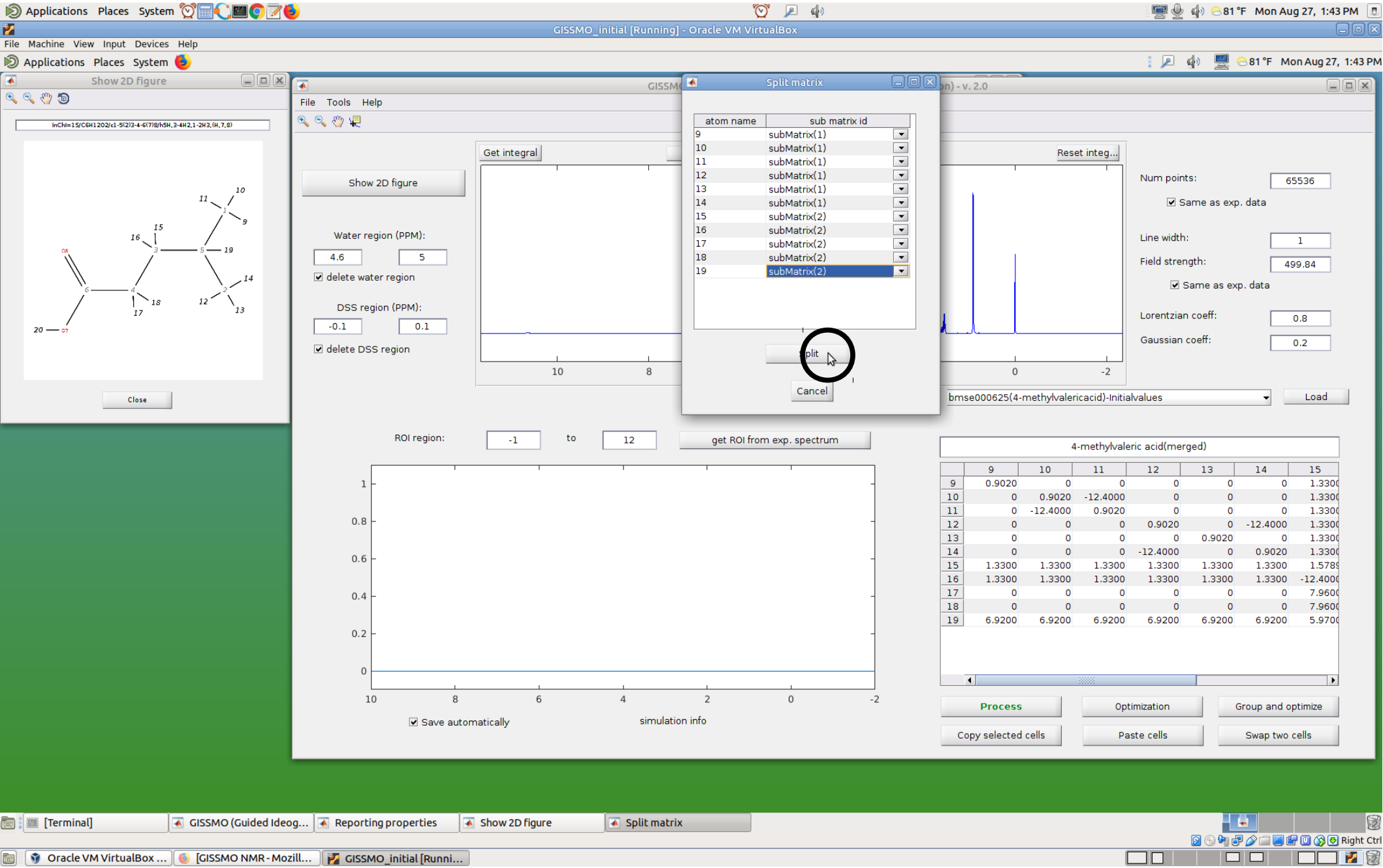
	9	10	11	12	13	14	15
9	0.9020	0	0	0	0	0	1.3300
10	0	0.9020	-12.4000	0	0	0	1.3300
11	0	-12.4000	0.9020	0	0	0	1.3300
12	0	0	0	0.9020	0	-12.4000	1.3300
13	0	0	0	0	0.9020	0	1.3300
14	0	0	0	-12.4000	0	0.9020	1.3300
15	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	1.5789
16	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	-12.4000
17	0	0	0	0	0	0	7.9600
18	0	0	0	0	0	0	7.9600
19	6.9200	6.9200	6.9200	6.9200	6.9200	6.9200	5.9700

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Split matrix

Right Ctrl


Applications Places System
81 °F Mon Aug 27, 1:43 PM
GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Show 2D figure
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(2)
16 subMatrix(2)
17 subMatrix(2)
18 subMatrix(2)
19 subMatrix(2)
Split
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
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
-1
to
12
get ROI from exp. spectrum
Save automatically
simulation info
4-methylvaleric acid(merged)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Split matrix
Oracle VM VirtualBox ...
[GISSMO NMR - Mozill...
GISSMO_initial [Runni...

GISSMO_initial [Running] - Oracle VM VirtualBox

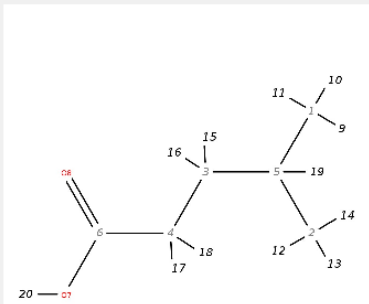
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:43 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

GISSMO (Guided Ideation) - v. 2.0

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

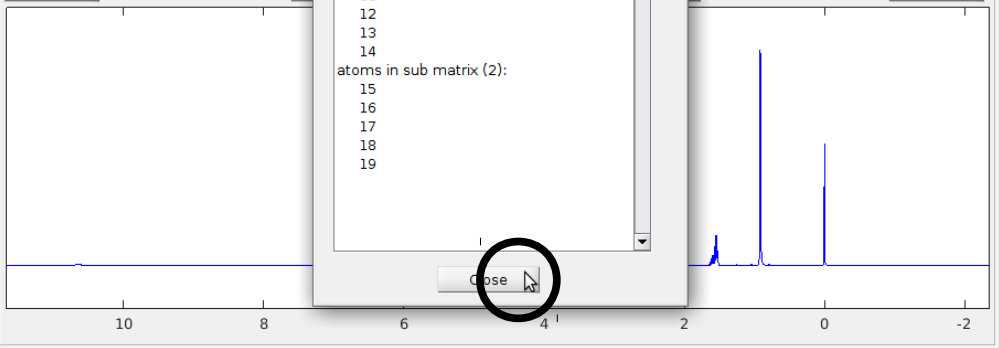
DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset integ...



Show sub-matrices

Sub matrices:

atoms in sub matrix (1):
9
10
11
12
13
14
atoms in sub matrix (2):
15
16
17
18
19

Close

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

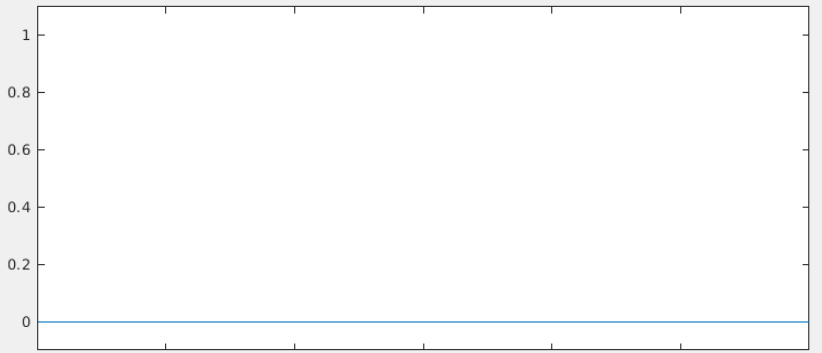
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues

Load

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



Save automatically

simulation info

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9020	0	0	0	0	0	1.3300
10	0	0.9020	-12.4000	0	0	0	1.3300
11	0	-12.4000	0.9020	0	0	0	1.3300
12	0	0	0	0.9020	0	-12.4000	1.3300
13	0	0	0	0	0.9020	0	1.3300
14	0	0	0	-12.4000	0	0.9020	1.3300
15	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	1.5789
16	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	-12.4000
17	0	0	0	0	0	0	7.9600
18	0	0	0	0	0	0	7.9600
19	6.9200	6.9200	6.9200	6.9200	6.9200	6.9200	5.9700

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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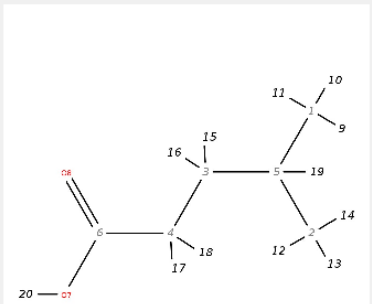
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



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

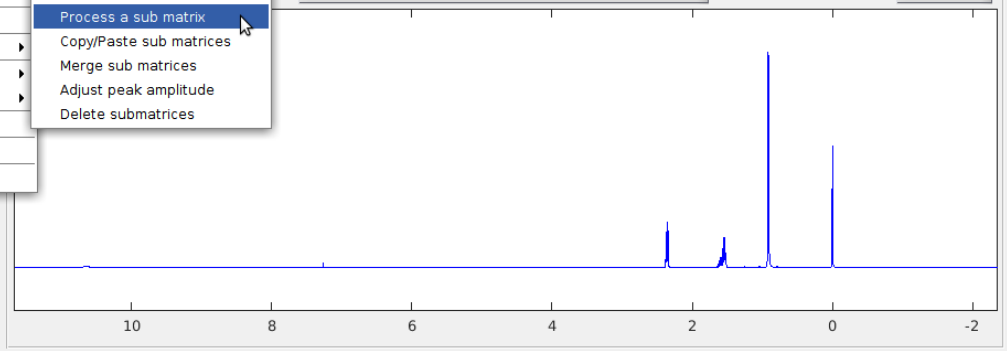
Merge sub matrices

Adjust peak amplitude

Delete submatrices

Draw full experimental spectrum

Reset integ...



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

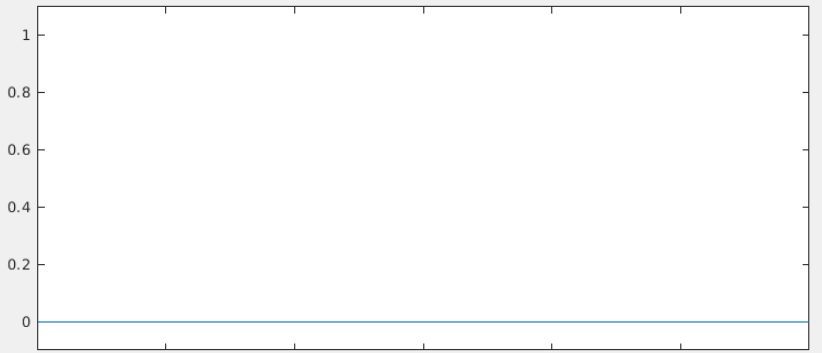
DSS region (PPM):

-0.1 0.1

delete DSS region

database entries: bmse000625(4-methylvalericacid)-Initialvalues Load

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



Save automatically

simulation info

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9020	0	0	0	0	0	1.3300
10	0	0.9020	-12.4000	0	0	0	1.3300
11	0	-12.4000	0.9020	0	0	0	1.3300
12	0	0	0	0.9020	0	-12.4000	1.3300
13	0	0	0	0	0.9020	0	1.3300
14	0	0	0	-12.4000	0	0.9020	1.3300
15	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	1.5789
16	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	-12.4000
17	0	0	0	0	0	0	7.9600
18	0	0	0	0	0	0	7.9600
19	6.9200	6.9200	6.9200	6.9200	6.9200	6.9200	5.9700

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

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Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

Close

GISSMO (Guided Ideization) - v. 2.0

File Tools Help

Choose a submatrix to process

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

Choose Cancel

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...

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: bmse000625(4-methylvalericacid)-Initialvalues Load

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

Save automatically

simulation info

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9020	0	0	0	0	0	1.3300
10	0	0.9020	-12.4000	0	0	0	1.3300
11	0	-12.4000	0.9020	0	0	0	1.3300
12	0	0	0	0.9020	0	-12.4000	1.3300
13	0	0	0	0	0.9020	0	1.3300
14	0	0	0	-12.4000	0	0.9020	1.3300
15	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	1.5789
16	1.3300	1.3300	1.3300	1.3300	1.3300	1.3300	-12.4000
17	0	0	0	0	0	0	7.9600
18	0	0	0	0	0	0	7.9600
19	6.9200	6.9200	6.9200	6.9200	6.9200	6.9200	5.9700

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

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File Machine View Input Devices Help

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

Expand around methyls

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

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

Save automatically

simulation info

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9020	0	0	0	0	0
10	0	0.9020	-12.4000	0	0	0
11	0	-12.4000	0.9020	0	0	0
12	0	0	0	0.9020	0	-12.4000
13	0	0	0	0	0.9020	0
14	0	0	0	-12.4000	0	0.9020

Methyl spins

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

1.05 1 0.95 0.9 0.85 0.8 0.75

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: bmse000625(4-methylvalericacid)-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

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9020	0	0	0	0	0
10	0	0.9020	-12.4000	0	0	0
11	0	-12.4000	0.9020	0	0	0
12	0	0	0	0.9020	0	-12.4000
13	0	0	0	0	0.9020	0
14	0	0	0	-12.4000	0	0.9020

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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File Machine View Input Devices Help

Applications Places System

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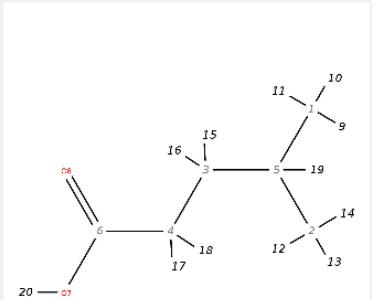
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

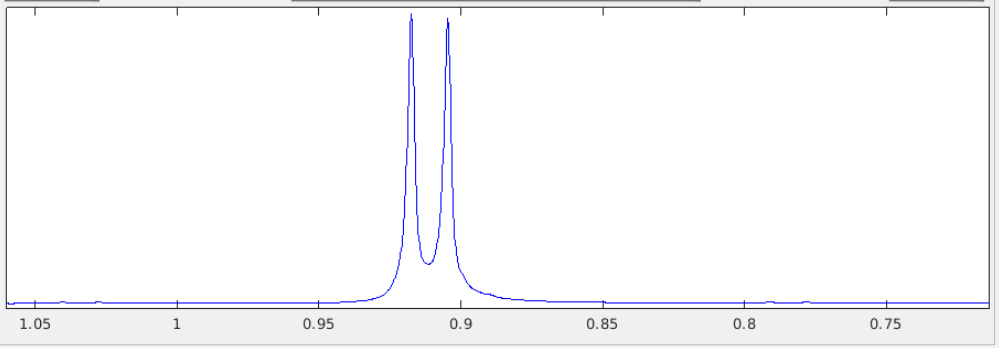
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

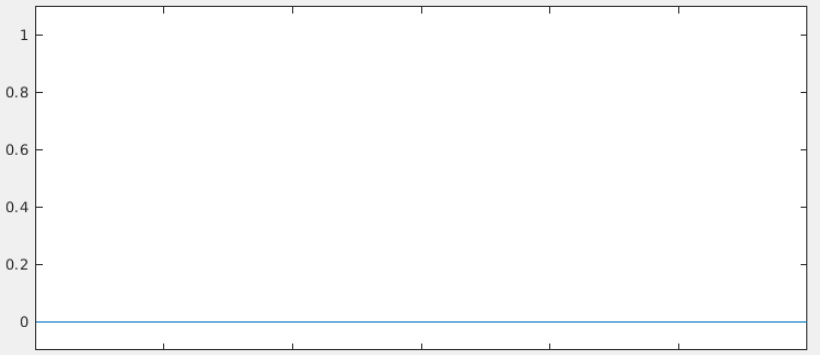
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum



Save automatically

simulation info

4-methylvaleric acid(sub_matrix_1)

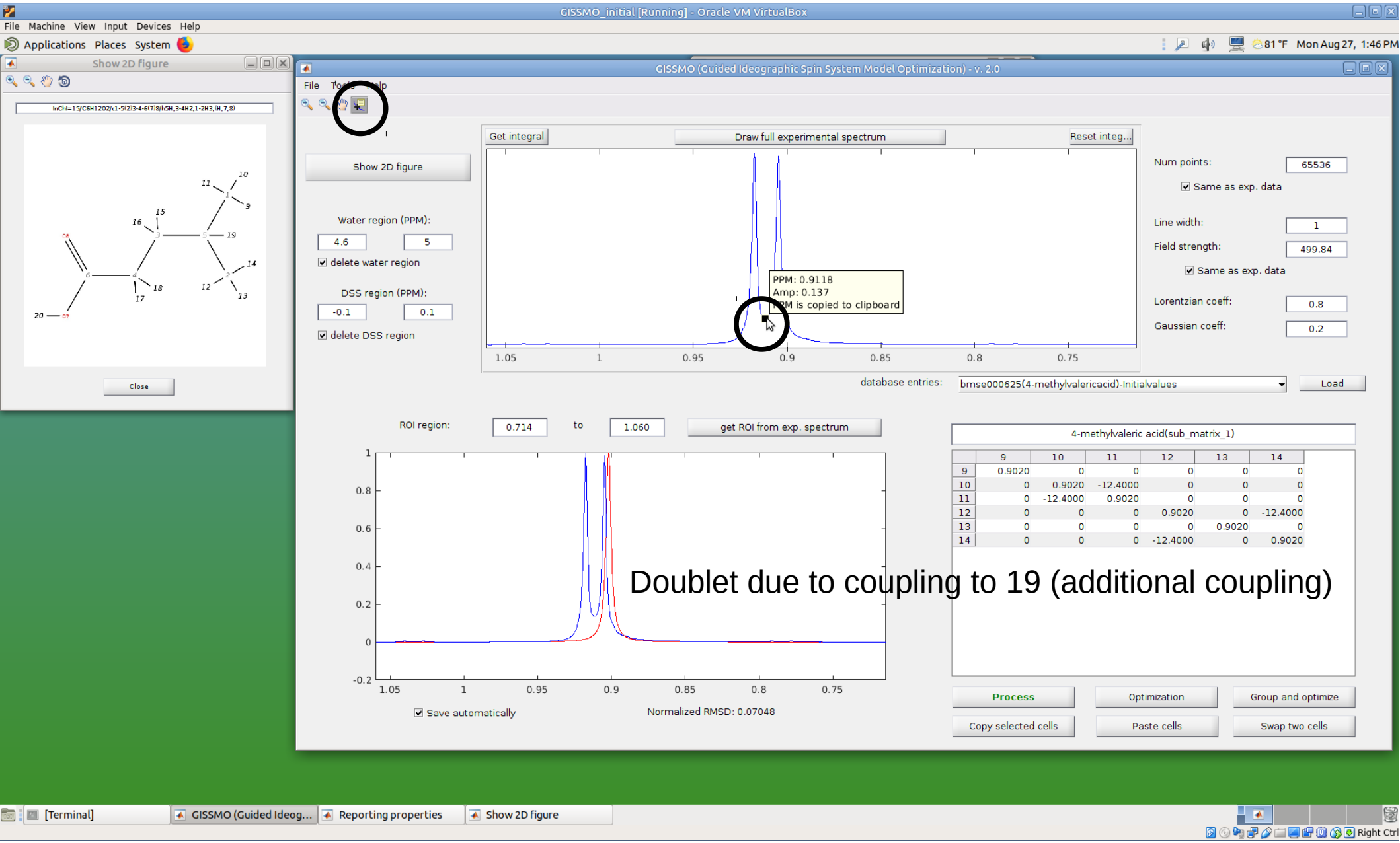
	9	10	11	12	13	14
9	0.9020	0	0	0	0	0
10	0	0.9020	-12.4000	0	0	0
11	0	-12.4000	0.9020	0	0	0
12	0	0	0	0.9020	0	-12.4000
13	0	0	0	0	0.9020	0
14	0	0	0	-12.4000	0	0.9020

Proces | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
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Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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...
PPM: 0.9118
Amp: 0.137
PPM is copied to clipboard
1.05 1 0.95 0.9 0.85 0.8 0.75
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
0.714
to
1.060
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.07048
4-methylvaleric acid(sub_matrix_1)
9 10 11 12 13 14
9 0.9020 0 0 0 0 0
10 0 0.9020 -12.4000 0 0 0
11 0 -12.4000 0.9020 0 0 0
12 0 0 0 0.9020 0 -12.4000
13 0 0 0 0 0.9020 0
14 0 0 0 -12.4000 0 0.9020
Doublet due to coupling to 19 (additional coupling)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

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File Machine View Input Devices Help

Applications Places System

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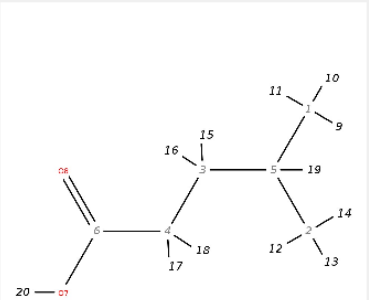
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

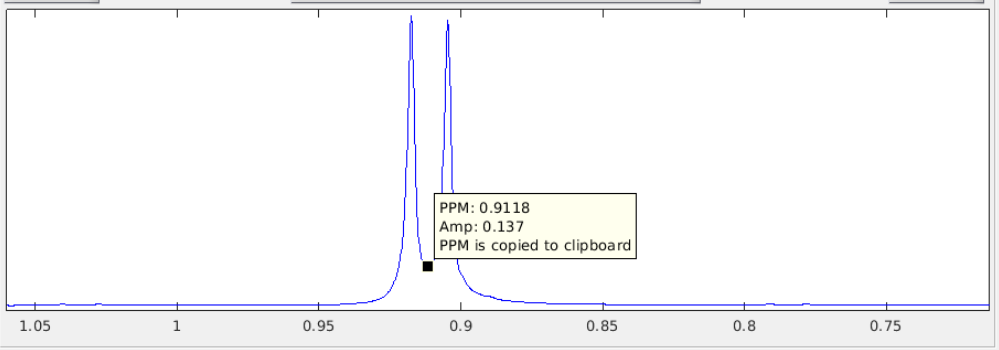
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

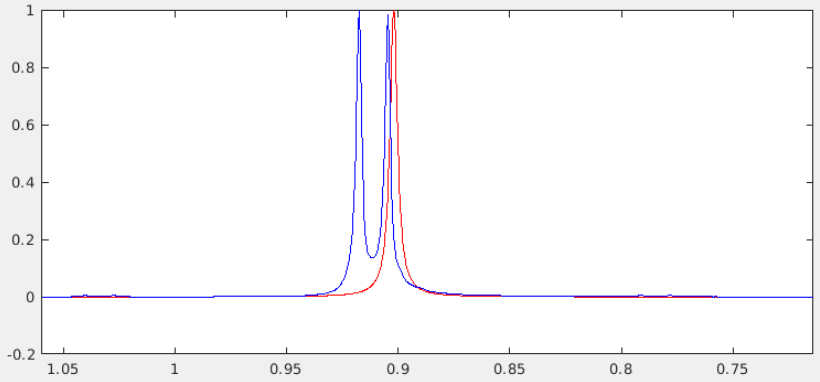
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07048

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9020	-12.4000	0	0	0
11	0	-12.4000	0.9020	0	0	0
12	0	0	0	0.9020	0	-12.4000
13	0	0	0	0	0.9020	0
14	0	0	0	-12.4000	0	0.9020

Left click on cell; ctrl-v

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideog... | 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/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 0.9118
Amp: 0.137
PPM is copied to clipboard

1.05 1 0.95 0.9 0.85 0.8 0.75

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

1 0.8 0.6 0.4 0.2 0 -0.2

1.05 1 0.95 0.9 0.85 0.8 0.75

Save automatically

Normalized RMSD: 0.07048

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

All methyl spins
have same chemical shift

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 0.9118
Amp: 0.137
PPM is copied to clipboard

1.05 1 0.95 0.9 0.85 0.8 0.75

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

1 0.8 0.6 0.4 0.2 0 -0.2

1.05 1 0.95 0.9 0.85 0.8 0.75

Save automatically

Normalized RMSD: 0.07048

4-methylvaleric acid(sub_matrix_1)

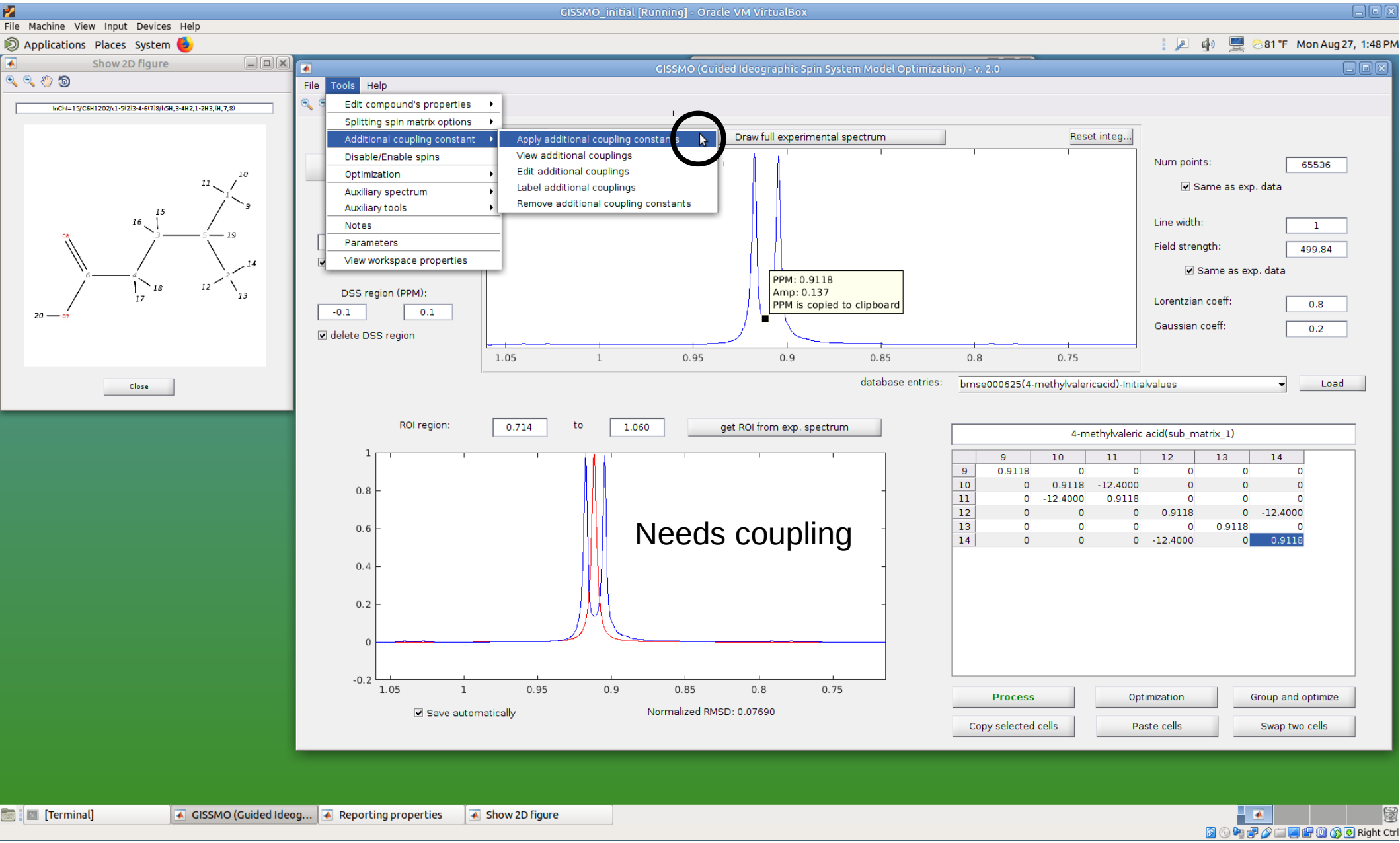
	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
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Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
Apply additional coupling constants
View additional couplings
Edit additional couplings
Label additional couplings
Remove additional coupling constants
Draw full experimental spectrum
Reset integ...
PPM: 0.9118
Amp: 0.137
PPM is copied to clipboard
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
0.714
to
1.060
get ROI from exp. spectrum
Needs coupling
Save automatically
Normalized RMSD: 0.07690
4-methylvaleric acid(sub_matrix_1)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

ROI region: 0.714 to 1.060

Save automatically

Normalized RMSD: 0.07690

Apply different additional couplings to different spin groups

Number of groups of spins 2

Total number of additional couplings 2

Create

Apply

Cancel

65536

1

499.84

0.8

0.2

Load

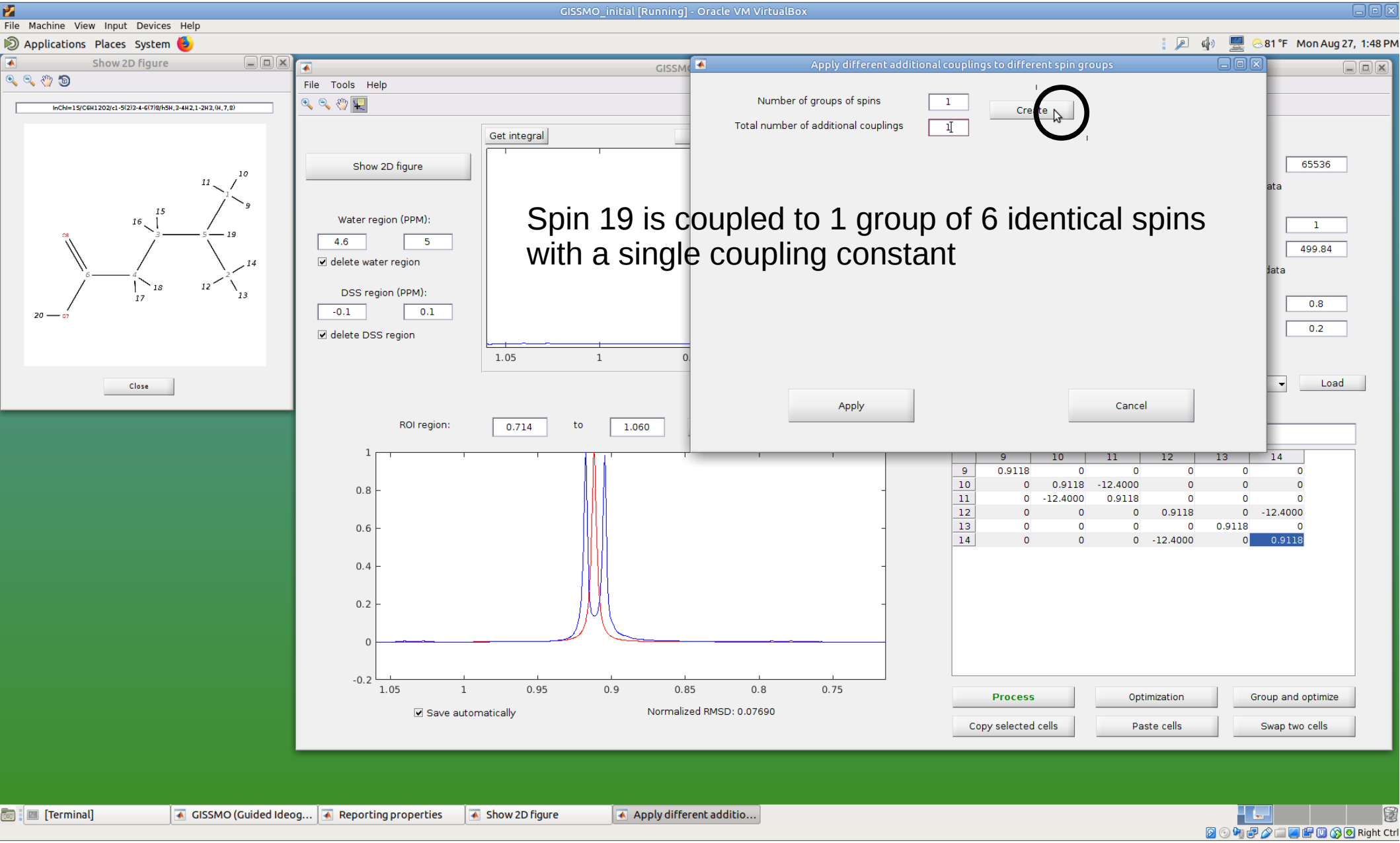
	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Apply different additio...

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:48 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
1.05
1
ROI region:
0.714
to
1.060
Save automatically
Normalized RMSD: 0.07690
Apply different additional couplings to different spin groups
Number of groups of spins
1
Total number of additional couplings
1
Create
Apply
Cancel
Spin 19 is coupled to 1 group of 6 identical spins
with a single coupling constant
65536
1
499.84
0.8
0.2
Load
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Apply different additio...
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:49 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

1.05 1

ROI region: 0.714 to 1.060

Save automatically

Normalized RMSD: 0.07690

Apply different additional couplings to different spin groups

Number of groups of spins 1

Total number of additional couplings 1

Create

Select spins

	Spin names	Group ID
1	9	select
2	10	select
3	11	group(1)
4	12	select
5	13	select
6	14	select

Additional couplings

	Coupling constant	Group ID
1		select

Apply

Cancel

65536

1

499.84

0.8

0.2

Load

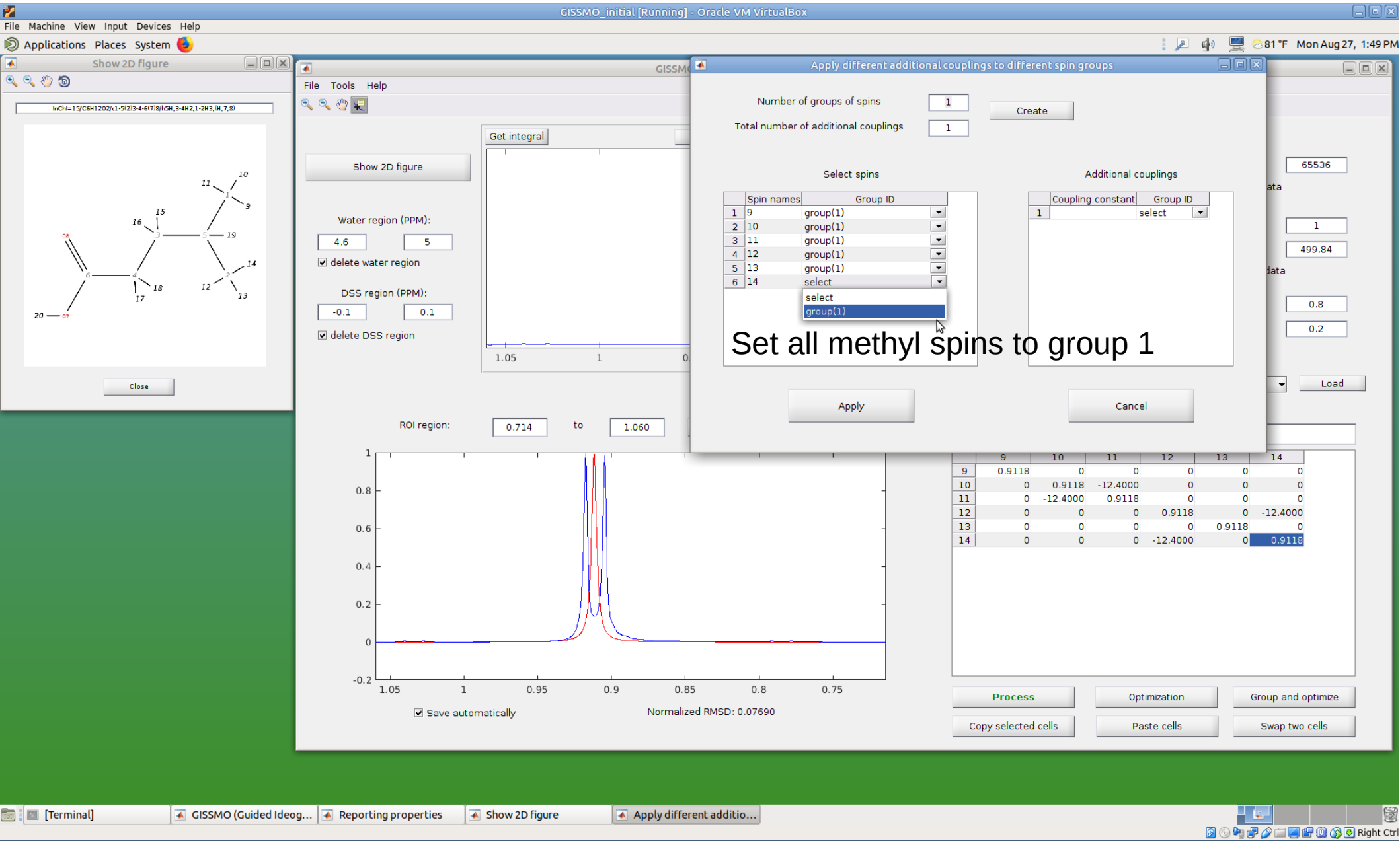
	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

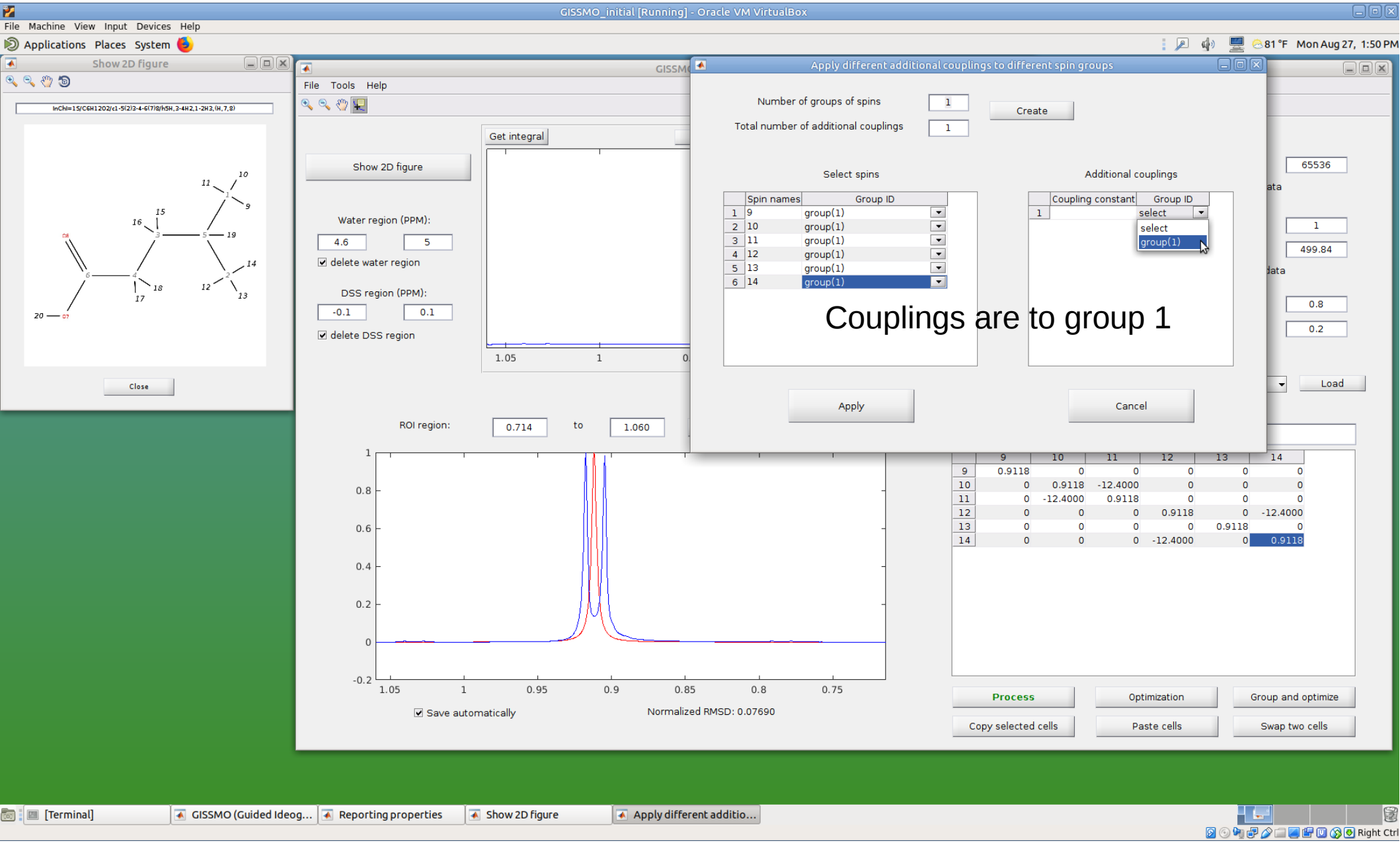
Process Optimization Group and optimize

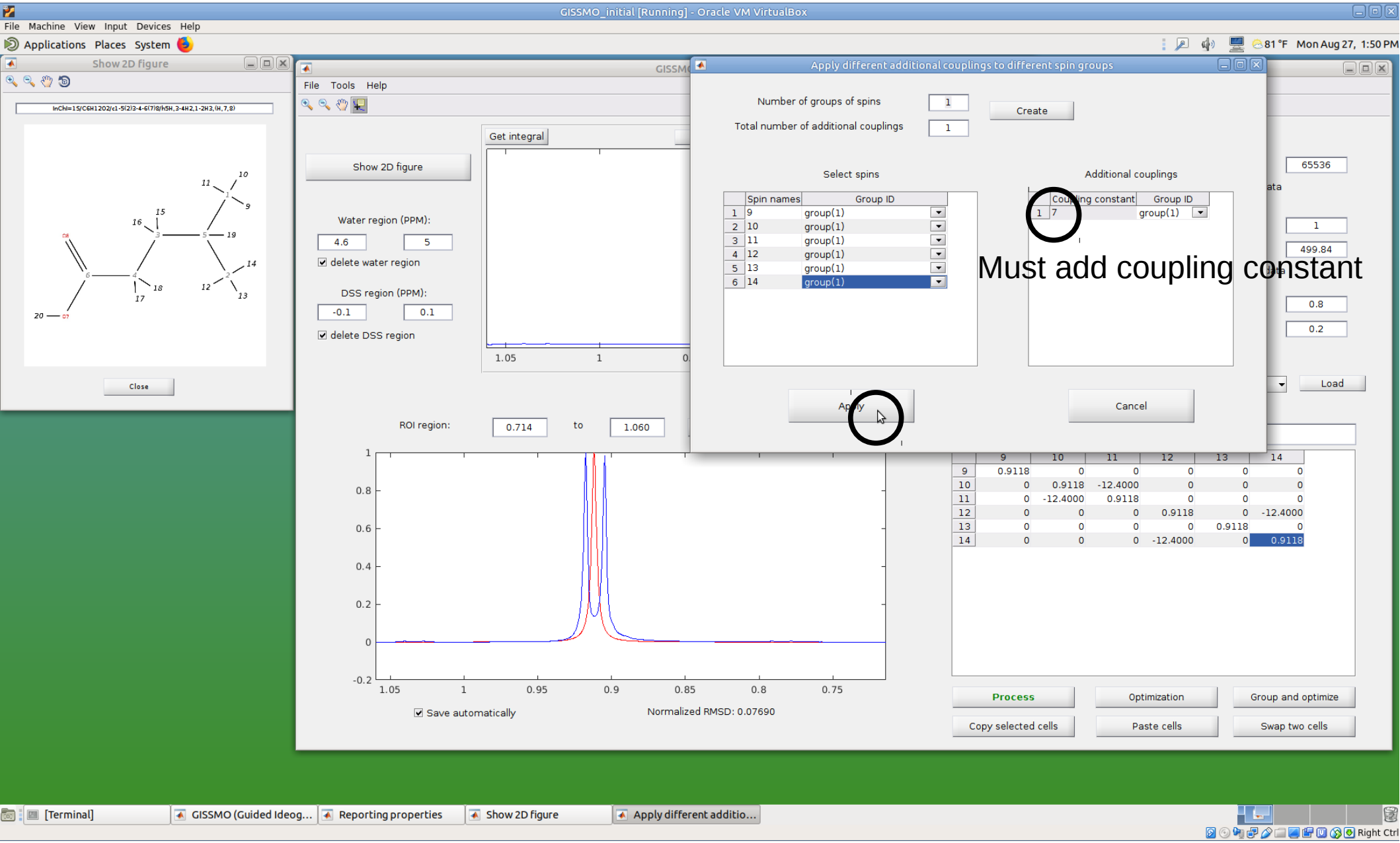
Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Apply different additio...

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:49 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
1.05
1
ROI region:
0.714
to
1.060
Save automatically
Normalized RMSD: 0.07690
Apply different additional couplings to different spin groups
Number of groups of spins
1
Total number of additional couplings
1
Create
Select spins
Spin names
Group ID
9 group(1)
10 group(1)
11 group(1)
12 group(1)
13 group(1)
14 select
select
group(1)
Additional couplings
Coupling constant
Group ID
select
Set all methyl spins to group 1
Apply
Cancel
65536
1
499.84
0.8
0.2
Load
9 10 11 12 13 14
9 0.9118 0 0 0 0 0
10 0 0.9118 -12.4000 0 0 0
11 0 -12.4000 0.9118 0 0 0
12 0 0 0 0.9118 0 -12.4000
13 0 0 0 0 0.9118 0
14 0 0 0 -12.4000 0 0.9118
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Apply different additio...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:50 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
1.05
1
ROI region:
0.714
to
1.060
Save automatically
Normalized RMSD: 0.07690
Apply different additional couplings to different spin groups
Number of groups of spins
1
Total number of additional couplings
1
Create
Select spins
Spin names
Group ID
9 group(1)
10 group(1)
11 group(1)
12 group(1)
13 group(1)
14 group(1)
Additional couplings
Coupling constant
Group ID
select
group(1)
Couplings are to group 1
Apply
Cancel
65536
1
499.84
0.8
0.2
Load
9 10 11 12 13 14
9 0.9118 0 0 0 0 0
10 0 0.9118 -12.4000 0 0 0
11 0 -12.4000 0.9118 0 0 0
12 0 0 0 0.9118 0 -12.4000
13 0 0 0 0 0.9118 0
14 0 0 0 -12.4000 0 0.9118
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Apply different additio...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:50 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
1.05
1
ROI region:
0.714
to
1.060
Save automatically
Normalized RMSD: 0.07690
Apply different additional couplings to different spin groups
Number of groups of spins
1
Total number of additional couplings
1
Create
Select spins
Spin names
Group ID
9 group(1)
10 group(1)
11 group(1)
12 group(1)
13 group(1)
14 group(1)
Additional couplings
Coupling constant
Group ID
7 group(1)
Must add coupling constant
Apply
Cancel
65536
1
499.84
0.8
0.2
Load
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Apply different additio...
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:50 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 0.9118

1.05 1 0.95 0.75

Additional coupling constants

The spin matrix has been updated. You may process!

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: bmse000625(4-methylvalericacid)-Initialvalues Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

1 0.8 0.6 0.4 0.2 0 -0.2

1.05 1 0.95 0.9 0.85 0.8 0.75

Save automatically

Normalized RMSD: 0.07690

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideog... | Reporting properties | Show 2D figure | Additional coupling co...

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 0.9118
Amp: 0.137
PPM is copied to clipboard

1.05 1 0.95 0.9 0.85 0.8 0.75

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

After “Process”

Save automatically

Normalized RMSD: 0.02970

4-methylvaleric acid(sub_matrix_1)

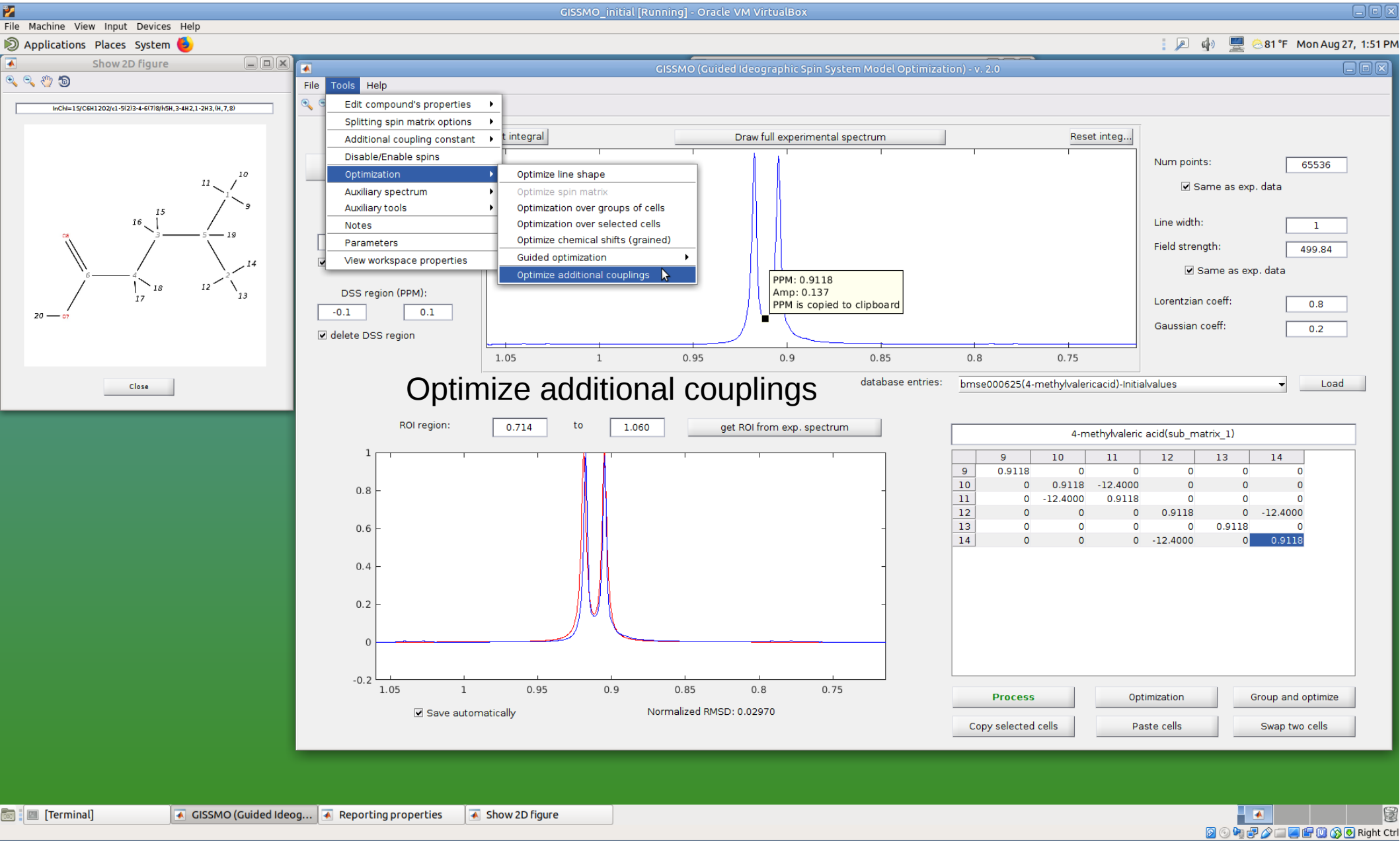
	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 1:51 PM
Show 2D figure
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
Optimize line shape
Optimize spin matrix
Optimization over groups of cells
Optimization over selected cells
Optimize chemical shifts (grained)
Guided optimization
Optimize additional couplings
Draw full experimental spectrum
Reset integ...
PPM: 0.9118
Amp: 0.137
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
DSS region (PPM):
-0.1
0.1
delete DSS region
Optimize additional couplings
database entries: bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region: 0.714 to 1.060
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.02970
4-methylvaleric acid(sub_matrix_1)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

choose additional couplings for optimization

Choose additional couplings to be optimized

	spins	coupling constant	spin groups ID	coupling groups ID	optimize	keep va
1	9,10,11,1...	7	group(1)	group(1)	☑	group(1

OK 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

values Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.02970

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure choose additional cou...

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 0.9118

1.05 1 0.95 0.75

Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 1.645
The spin matrix has be updated. You may process!

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

bmse000625(4-methylvalericacid)-Initialvalues

Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

1 0.8 0.6 0.4 0.2 0 -0.2

1.05 1 0.95 0.9 0.85 0.8 0.75

Save automatically

Normalized RMSD: 0.02970

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:52 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 0.9118
Amp: 0.137
PPM is copied to clipboard

1.05 1 0.95 0.9 0.85 0.8 0.75

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

1 0.8 0.6 0.4 0.2 0 -0.2

1.05 1 0.95 0.9 0.85 0.8 0.75

Save automatically

Normalized RMSD: 0.02534

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

Apply additional coupling constants
View additional couplings
Edit additional couplings
Label additional couplings
Remove additional coupling constants

Draw full experimental spectrum

Reset integ...

PPM: 0.9118
Amp: 0.137
PPM is copied to clipboard

1.05 1 0.95 0.9 0.85 0.8 0.75

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: bmse000625(4-methylvalericacid)-Initialvalues

Load

ROI region: 0.714 to 1.060

get ROI from exp. spectrum

1 0.8 0.6 0.4 0.2 0 -0.2

1.05 1 0.95 0.9 0.85 0.8 0.75

Save automatically

Normalized RMSD: 0.02534

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

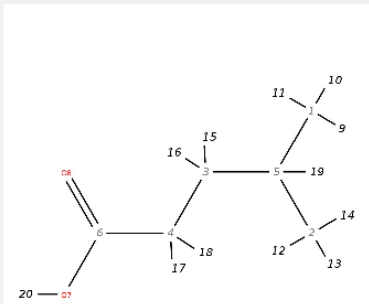
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:53 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

View additional coupling constants

	spin names	coupling	spins group ID	couplings group ID
1	9,10,11,1...	6.4194	group(1)	group(1)

Ok

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...

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

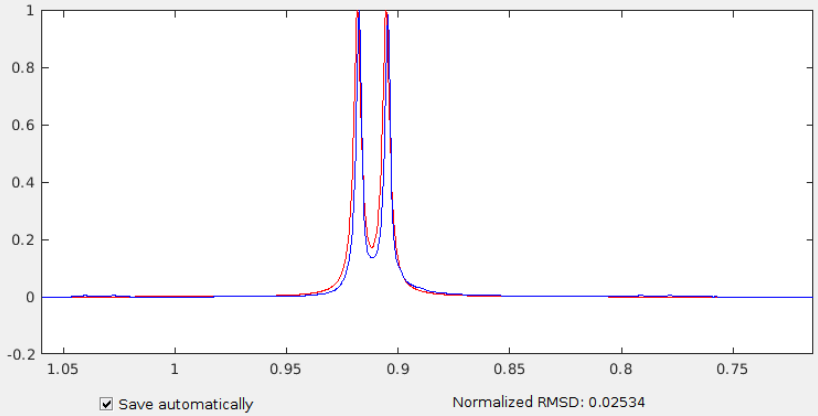
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

alericacid)-Initialvalues Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.02534

4-methylvaleric acid(sub_matrix_1)

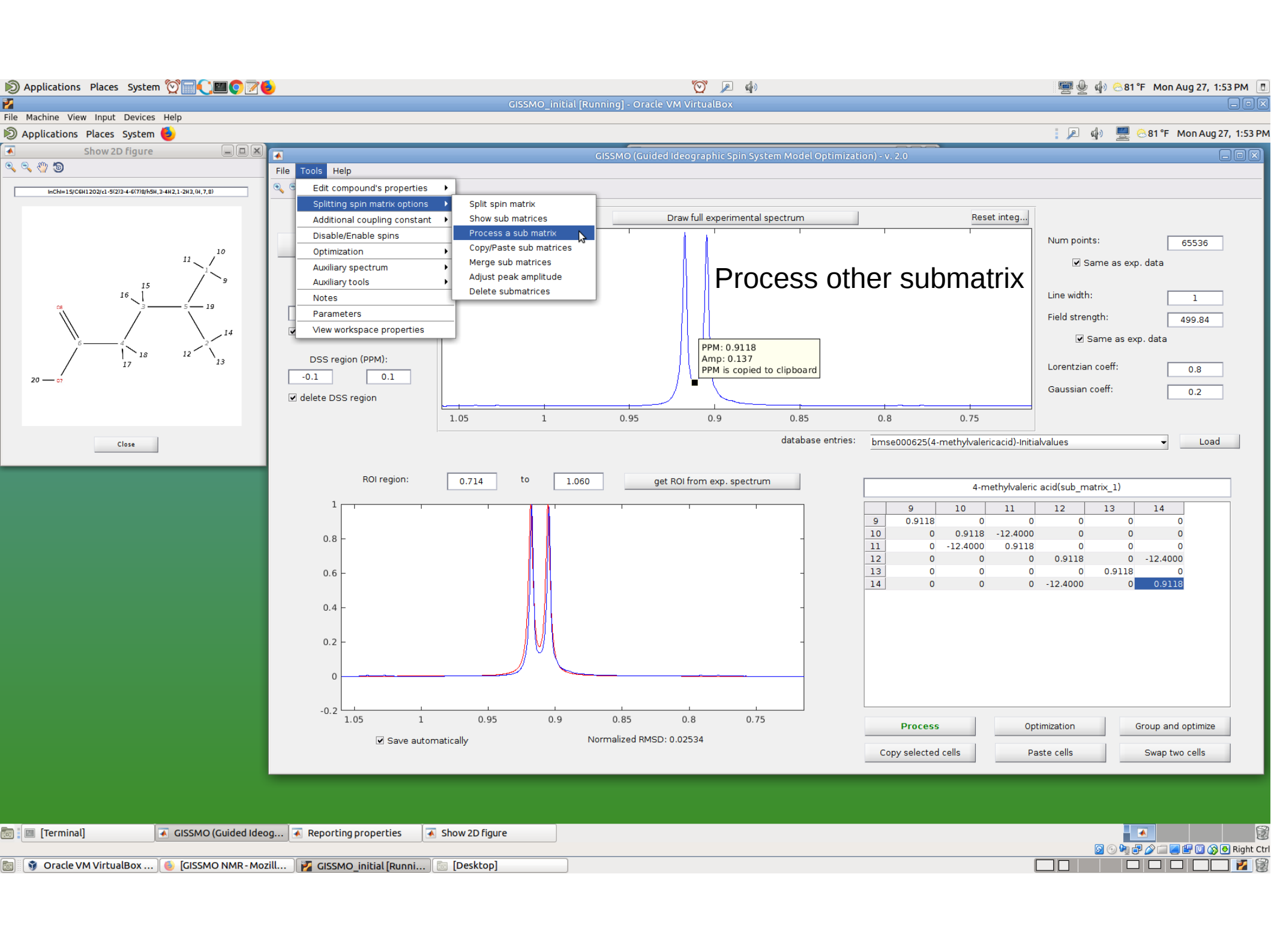
	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure View additional coupli...

Right Ctrl


Applications Places System
81 °F Mon Aug 27, 1:53 PM
GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Show 2D figure
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...
Process other submatrix
PPM: 0.9118
Amp: 0.137
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
DSS region (PPM):
-0.1
0.1
delete DSS region
database entries: bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region: 0.714 to 1.060
get ROI from exp. spectrum
4-methylvaleric acid(sub_matrix_1)
Save automatically
Normalized RMSD: 0.02534
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Oracle VM VirtualBox ...
[GISSMO NMR - Mozill...
GISSMO_initial [Runni...
[Desktop]

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:54 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

Close

GISSMO (Guided Ideization) - v. 2.0

File Tools Help

Choose a submatrix to process

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

Choose Cancel

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...

PPM: 0.9118
Amp: 0.137
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: bmse000625(4-methylvalericacid)-Initialvalues Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.02534

4-methylvaleric acid(sub_matrix_1)

	9	10	11	12	13	14
9	0.9118	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0
11	0	-12.4000	0.9118	0	0	0
12	0	0	0	0.9118	0	-12.4000
13	0	0	0	0	0.9118	0
14	0	0	0	-12.4000	0	0.9118

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:54 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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: 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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.02534

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3382	-12.4000	1.3300
18	7.9600	7.9600	-12.4000	2.3427	1.3300
19	5.9700	5.9700	1.3300	1.3300	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:54 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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: 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: bmse000625(4-methylvalericacid)-Initialvalues Load

Usually ignore this

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.02534

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3382	-12.4000	1.3300
18	7.9600	7.9600	-12.4000	2.3427	1.3300
19	5.9700	5.9700	1.3300	1.3300	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

Expand

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: bmse000625(4-methylvalericacid)-Initialvalues Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.08384

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3382	-12.4000	1.3300
18	7.9600	7.9600	-12.4000	2.3427	1.3300
19	5.9700	5.9700	1.3300	1.3300	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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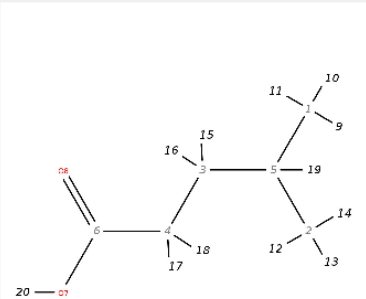
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

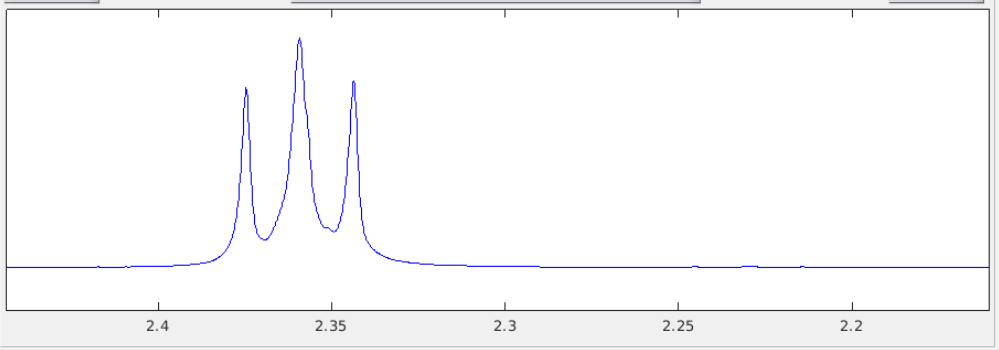
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

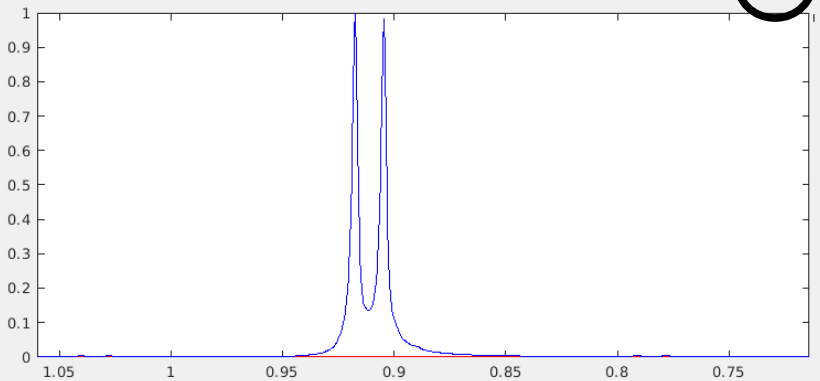
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 0.714 to 1.060 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.08384

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3382	-12.4000	1.3300
18	7.9600	7.9600	-12.4000	2.3427	1.3300
19	5.9700	5.9700	1.3300	1.3300	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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File Machine View Input Devices Help

Applications Places System

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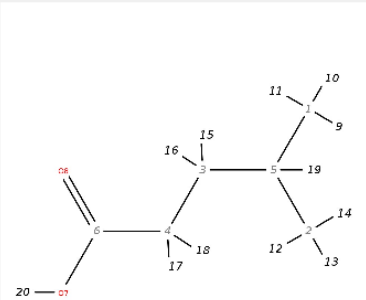
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

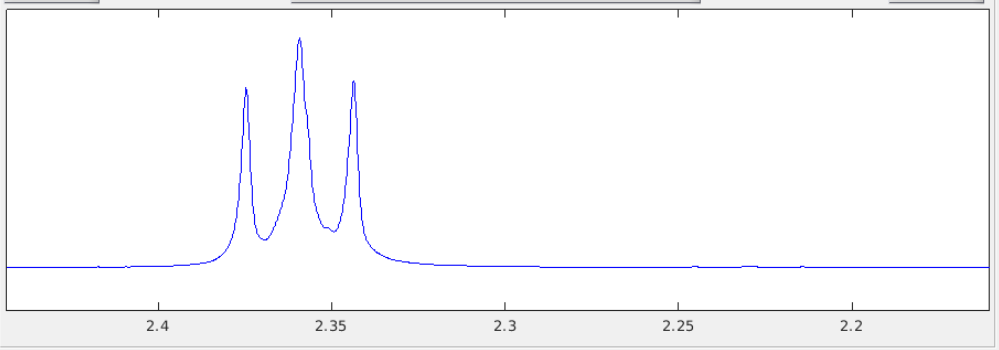
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

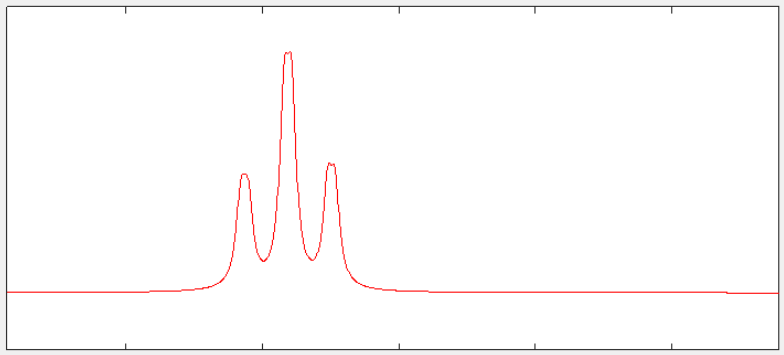
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.08384

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3382	-12.4000	1.3300
18	7.9600	7.9600	-12.4000	2.3427	1.3300
19	5.9700	5.9700	1.3300	1.3300	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

Pick peak

2.4 2.35 2.3 2.25 2.2

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: bmse000625(4-methylvalericacid)-Initialvalues Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum

0.25 0.2 0.15 0.1 0.05 0 -0.05

2.4 2.35 2.3 2.25 2.2

Save automatically

Normalized RMSD: 0.08384

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3382	-12.4000	1.3300
18	7.9600	7.9600	-12.4000	2.3427	1.3300
19	5.9700	5.9700	1.3300	1.3300	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 2.3594
Amp: 0.209
PPM is copied to clipboard

2.4 2.35 2.3 2.25 2.2

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum

0.25 0.2 0.15 0.1 0.05 0 -0.05

2.4 2.35 2.3 2.25 2.2

Save automatically

Normalized RMSD: 0.08384

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3382	-12.4000	1.3300
18	7.9600	7.9600	12.4000	2.3427	1.3300
19	5.9700	5.9700		1.3300	1.7328

Left-click;ctrl-v

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 2.3594
Amp: 0.209
PPM is copied to clipboard

2.4 2.35 2.3 2.25 2.2

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum

0.25 0.2 0.15 0.1 0.05 0 -0.05

2.4 2.35 2.3 2.25 2.2

Save automatically

Normalized RMSD: 0.08384

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	[illegible]	5.9700
17	7.9600	7.9600	2.3594	12.4000	1.3300
18	7.9600	7.9600	-12.4000	2.3594	1.3300
19	5.9700	5.9700	1.3300	1.3300	1.7328

Left-click;ctrl-v process

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 2.3594
Amp: 0.209
PPM is copied to clipboard

2.4 2.35 2.3 2.25 2.2

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

Long range couplings (4 bond) can be set to zero

ROI region: 2.161 to 2.444 get ROI from exp. spectrum

0.25 0.2 0.15 0.1 0.05 0 -0.05

2.4 2.35 2.3 2.25 2.2

Save automatically

Normalized RMSD: 0.07201

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3594	-12.4000	0
18	7.9600	7.9600	-12.4000	2.3594	1.3300
19	5.9700	5.9700	0	1.3300	1.7320

Left-click on cell; type 0

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 2.3594
Amp: 0.209
PPM is copied to clipboard

2.4 2.35 2.3 2.25 2.2

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum

0.25 0.2 0.15 0.1 0.05 0 -0.05

2.4 2.35 2.3 2.25 2.2

Save automatically

Normalized RMSD: 0.07201

4-methylvaleric acid(sub_matrix_2)

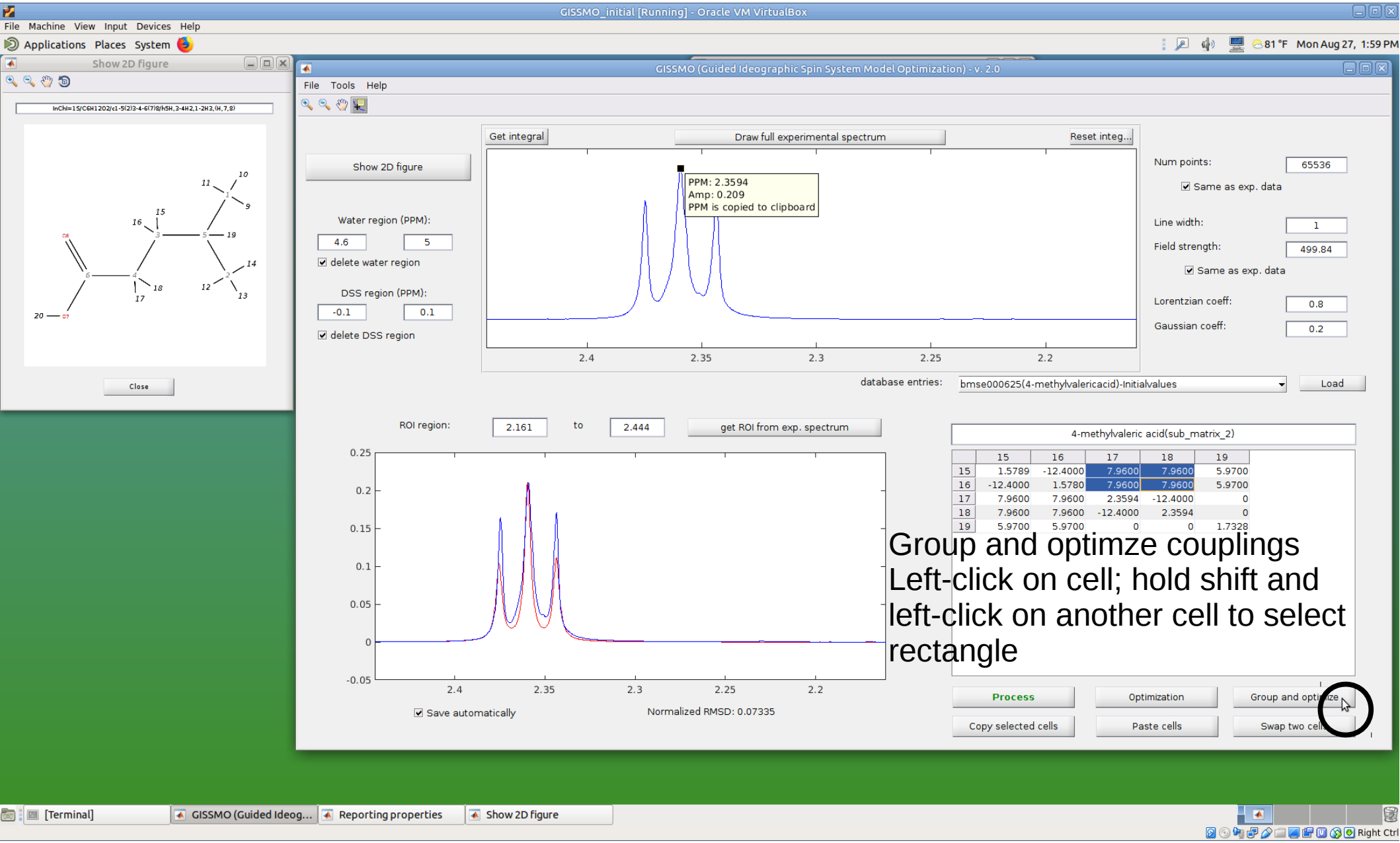
	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3594	-12.4000	0
18	7.9600	7.9600	-12.4000	2.3594	0
19	5.9700	5.9700	0	1.3300	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl



	15	16	17	18	19
15	1.5789	-12.4000	7.9600	7.9600	5.9700
16	-12.4000	1.5780	7.9600	7.9600	5.9700
17	7.9600	7.9600	2.3594	-12.4000	0
18	7.9600	7.9600	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

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File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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: 2.3594
Amp: 0.209
PPM is copied to clipboard

Optimization report:

optimization completed with the following message:
Simplex process coverged [illegible]

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.07335

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5780	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

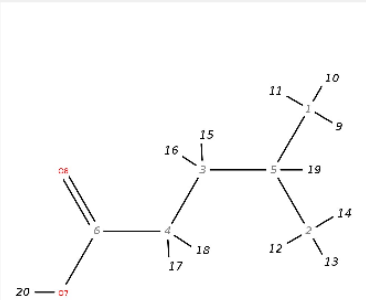
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 1:59 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

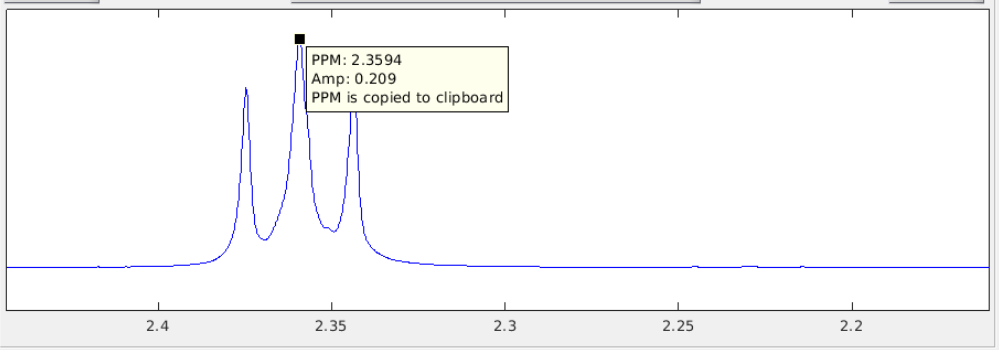
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

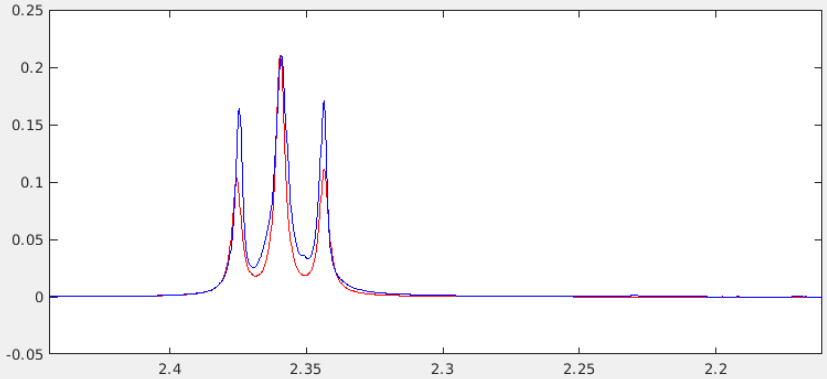
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07324

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5780	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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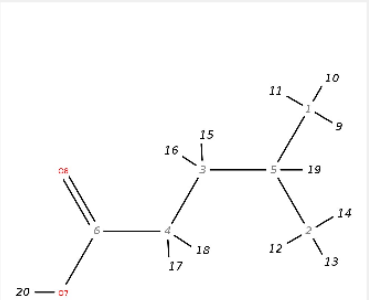
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

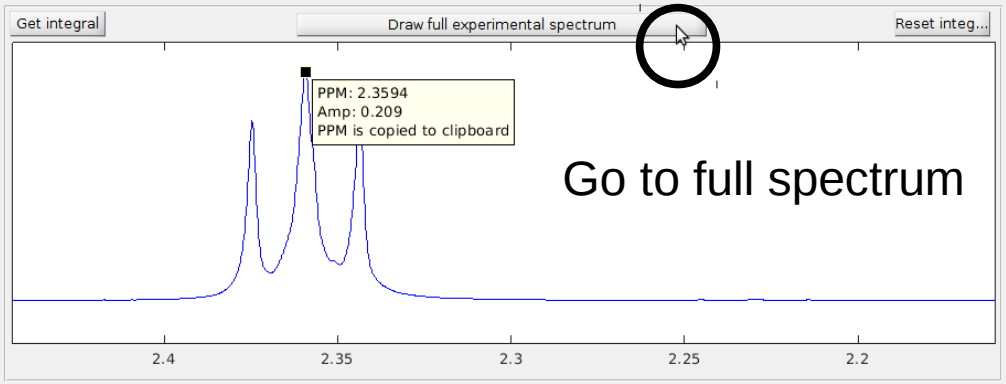
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

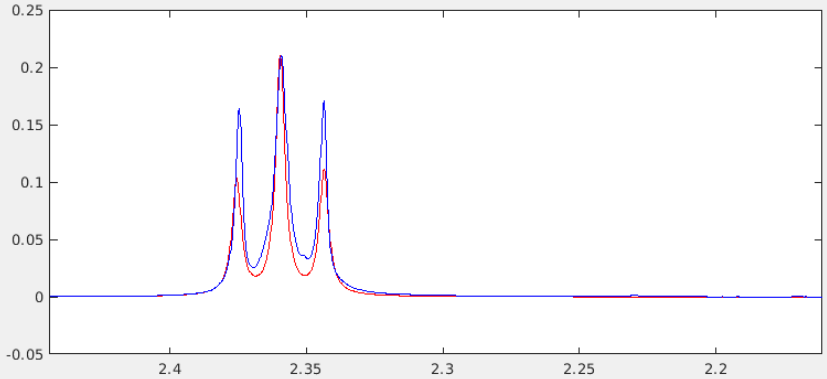
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.07324

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5780	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:00 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

expand

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 2.161 to 2.444 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.07324

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5780	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:01 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

Pick peak
15,16

PPM: 1.5405
Amp: 0.044
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 | get ROI from exp. spectrum

After process &
Go to ROI...

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

Save automatically

Normalized RMSD: 0.07324

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5789	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5780	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:01 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.5405
Amp: 0.044
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

Save automatically

Normalized RMSD: 0.07324

4-methylvaleric acid(sub_matrix_2)

			17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5780	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Left-click;ctrl-v on both 15,16 diagonals

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:02 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.5405
Amp: 0.044
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

After Process

Save automatically

Normalized RMSD: 0.04061

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:02 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

Pick 19

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

Save automatically

Normalized RMSD: 0.04061

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.7328

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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GISSMO_initial [Running] - Oracle VM VirtualBox

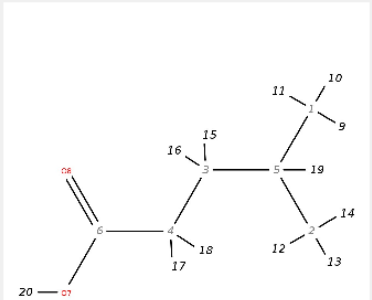
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:03 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

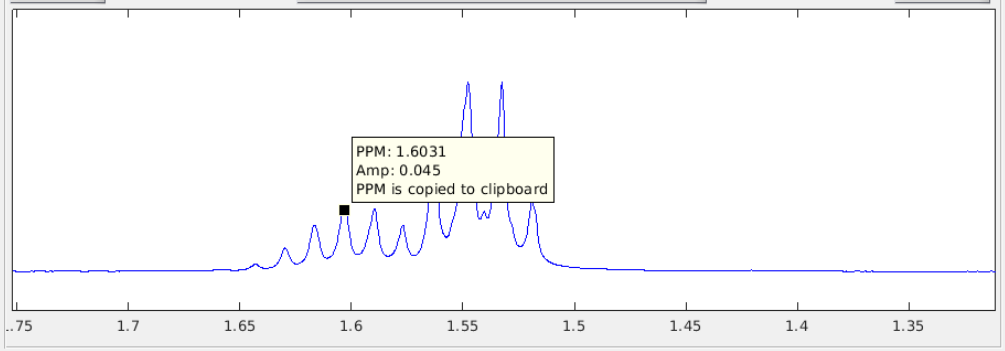
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

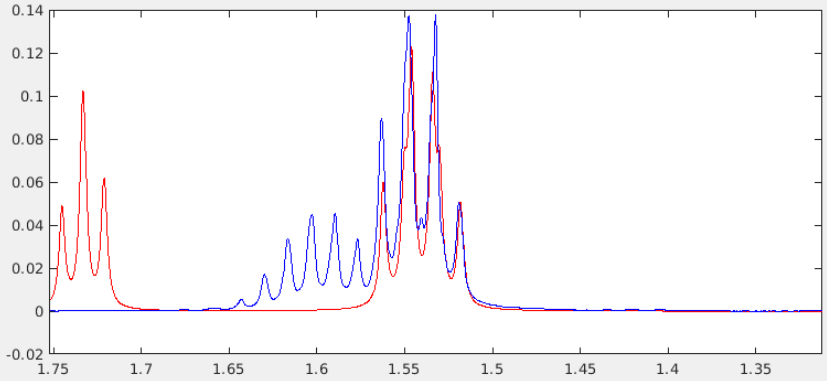
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04061

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.6031

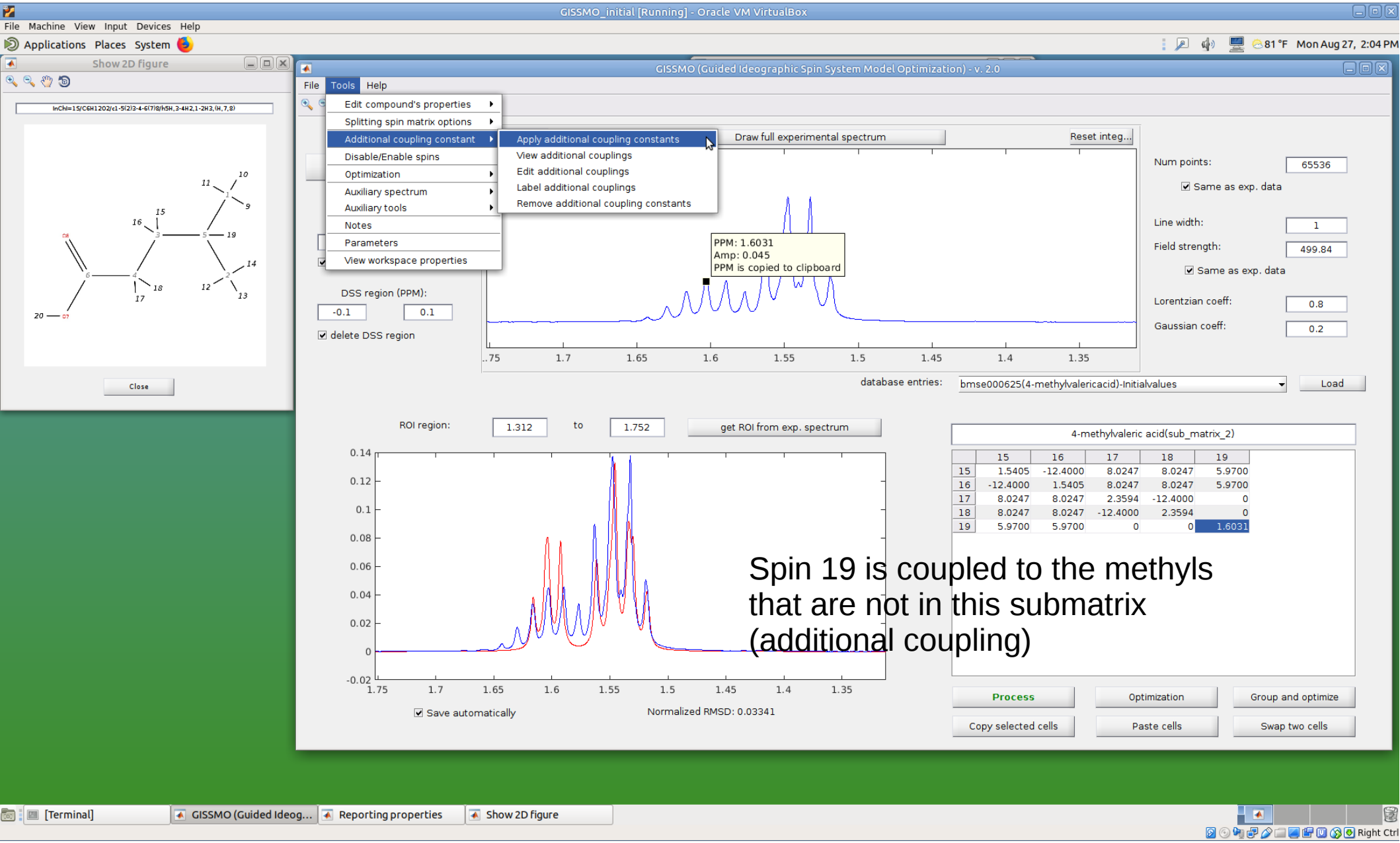
Left-click;ctrl-v
Then process

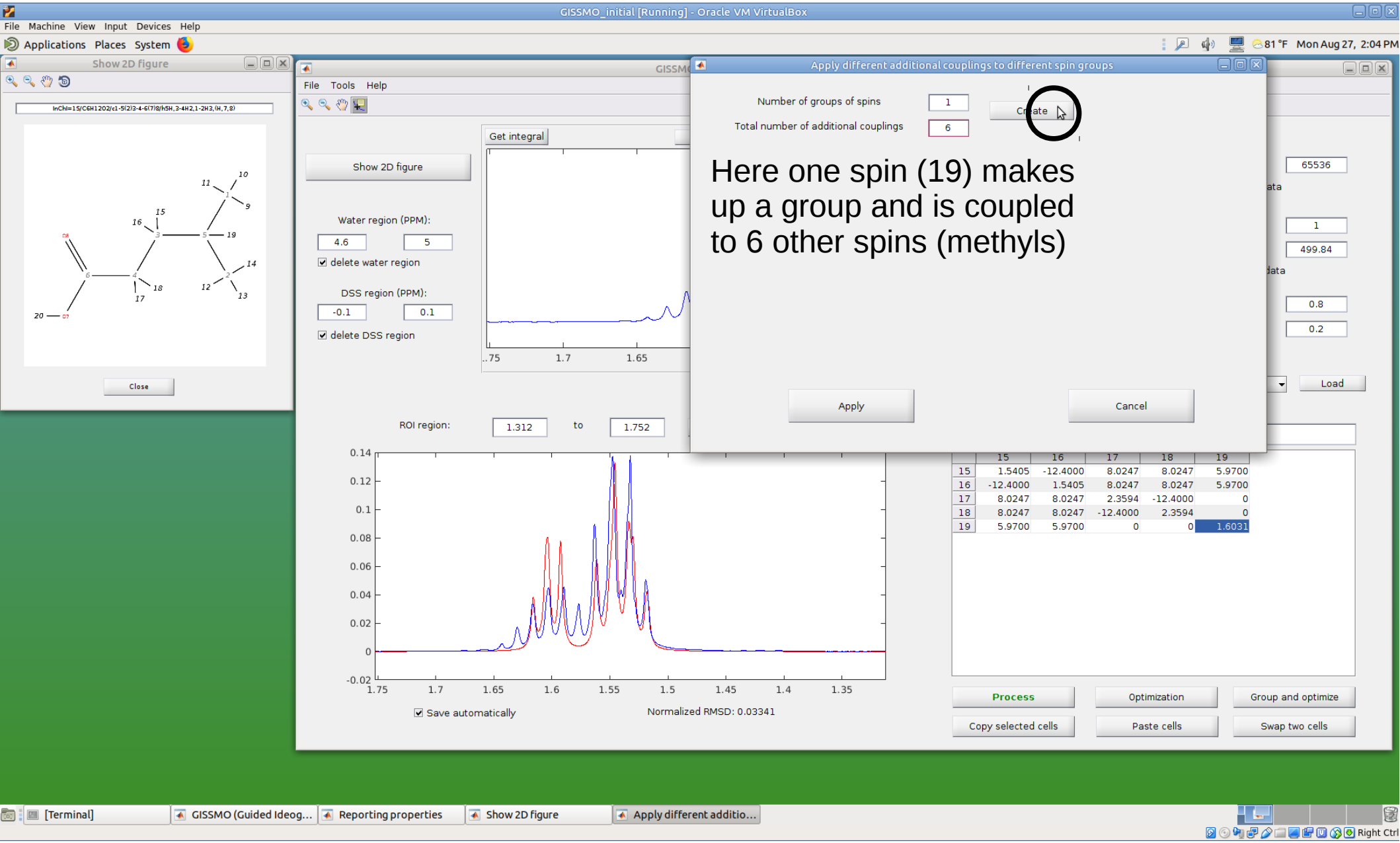
Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

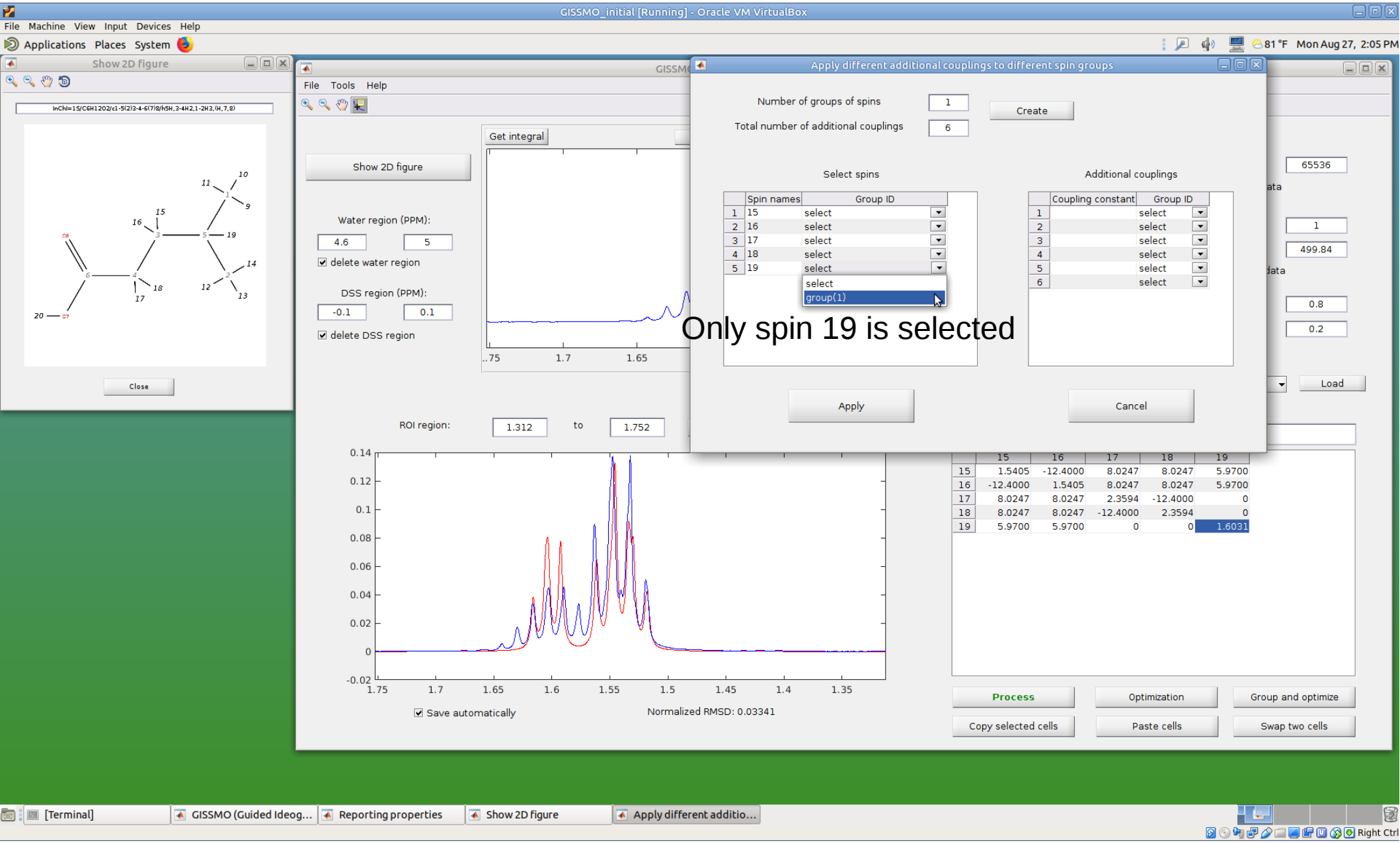
[Terminal] | GISSMO (Guided Ideog... | Reporting properties | Show 2D figure

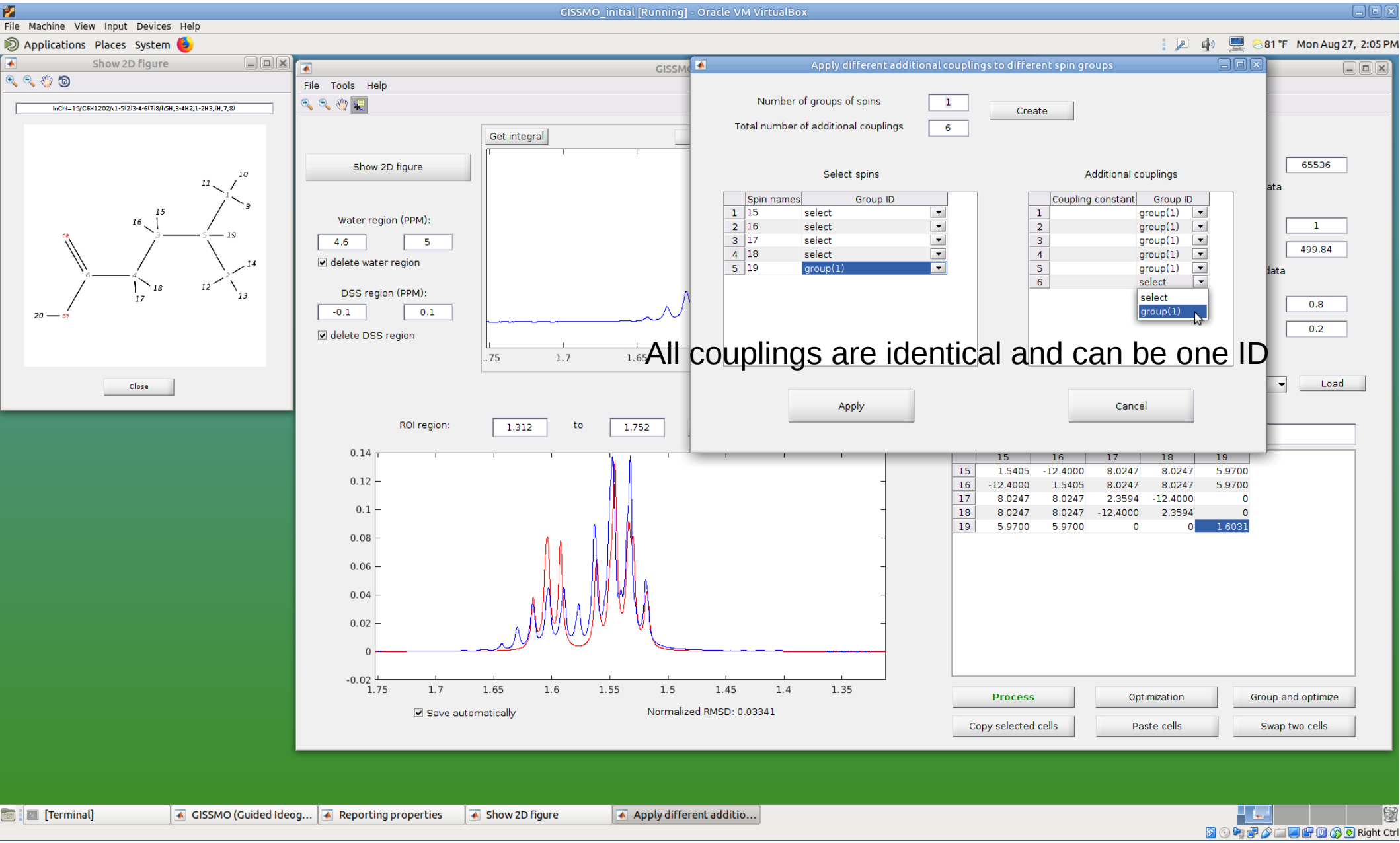
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:04 PM
Show 2D figure
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
Apply additional coupling constants
View additional couplings
Edit additional couplings
Label additional couplings
Remove additional coupling constants
Draw full experimental spectrum
Reset integ...
PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
1.312
to
1.752
get ROI from exp. spectrum
4-methylvaleric acid(sub_matrix_2)
15 16 17 18 19
15 1.5405 -12.4000 8.0247 8.0247 5.9700
16 -12.4000 1.5405 8.0247 8.0247 5.9700
17 8.0247 8.0247 2.3594 -12.4000 0
18 8.0247 8.0247 -12.4000 2.3594 0
19 5.9700 5.9700 0 0 1.6031
Spin 19 is coupled to the methyls that are not in this submatrix (additional coupling)
Save automatically
Normalized RMSD: 0.03341
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl



	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.6031


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:05 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
ROI region:
1.312
to
1.752
Save automatically
Normalized RMSD: 0.03341
Apply different additional couplings to different spin groups
Number of groups of spins
1
Total number of additional couplings
6
Create
Select spins
Spin names
Group ID
15
16
17
18
19
select
group(1)
Additional couplings
Coupling constant
Group ID
Only spin 19 is selected
Apply
Cancel
65536
1
499.84
0.8
0.2
Load
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Apply different additio...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:05 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
ROI region:
1.312
to
1.752
Save automatically
Normalized RMSD: 0.03341
Apply different additional couplings to different spin groups
Number of groups of spins
1
Total number of additional couplings
6
Create
Select spins
Spin names
Group ID
Additional couplings
Coupling constant
Group ID
select
group(1)
All couplings are identical and can be one ID
Apply
Cancel
65536
1
499.84
0.8
0.2
Load
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Apply different additio...
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:05 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

..75 1.7 1.65

ROI region: 1.312 to 1.752

Save automatically

Normalized RMSD: 0.03341

Apply different additional couplings to different spin groups

Number of groups of spins 1

Total number of additional couplings 6

Create

Select spins

	Spin names	Group ID
1	15	select
2	16	select
3	17	select
4	18	select
5	19	group(1)

Additional couplings

	Coupling constant	Group ID
1		group(1)
2		group(1)
3		group(1)
4		group(1)
5		group(1)
6		group(1)

Apply

Cancel

65536

1

499.84

0.8

0.2

Load

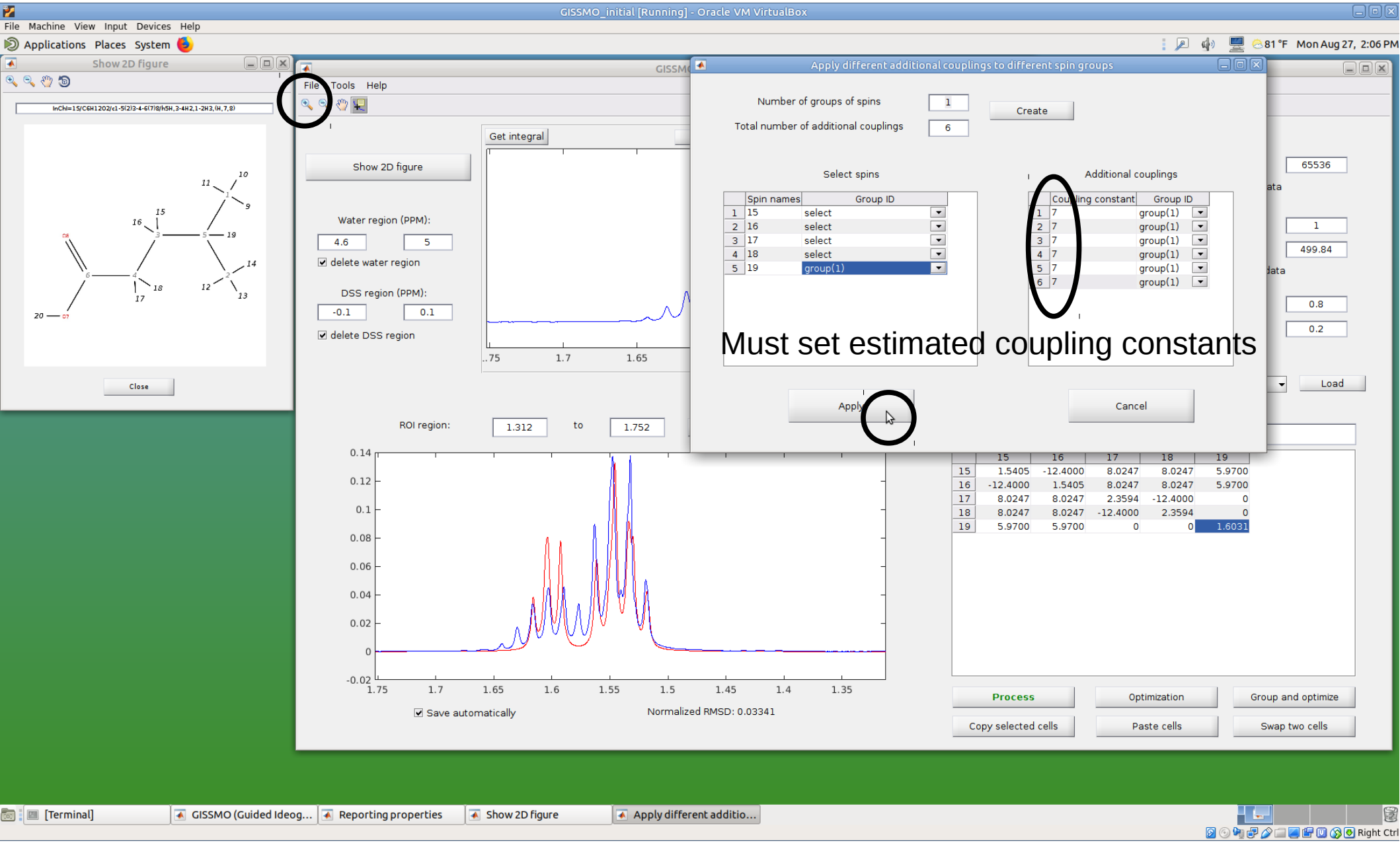
	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.6031

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Apply different additio...

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:06 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
ROI region:
1.312
to
1.752
Save automatically
Normalized RMSD: 0.03341
Apply different additional couplings to different spin groups
Number of groups of spins
1
Total number of additional couplings
6
Create
Select spins
Spin names
Group ID
15 select
16 select
17 select
18 select
19 group(1)
Additional couplings
Coupling constant
Group ID
7 group(1)
Must set estimated coupling constants
Apply
Cancel
65536
1
499.84
0.8
0.2
Load
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Apply different additio...
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:07 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

Additional coupling constants

The spin matrix has been updated. You may process!

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.03341

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.6031

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideog... | Reporting properties | Show 2D figure | Additional coupling co...

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:07 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

After Process

Save automatically

Normalized RMSD: 0.02681

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.6031

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideog... | 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/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

Save automatically

Normalized RMSD: 0.02681

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	5.9700
16	-12.4000	1.5405	8.0247	8.0247	5.9700
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	5.9700	5.9700	0	0	1.6031

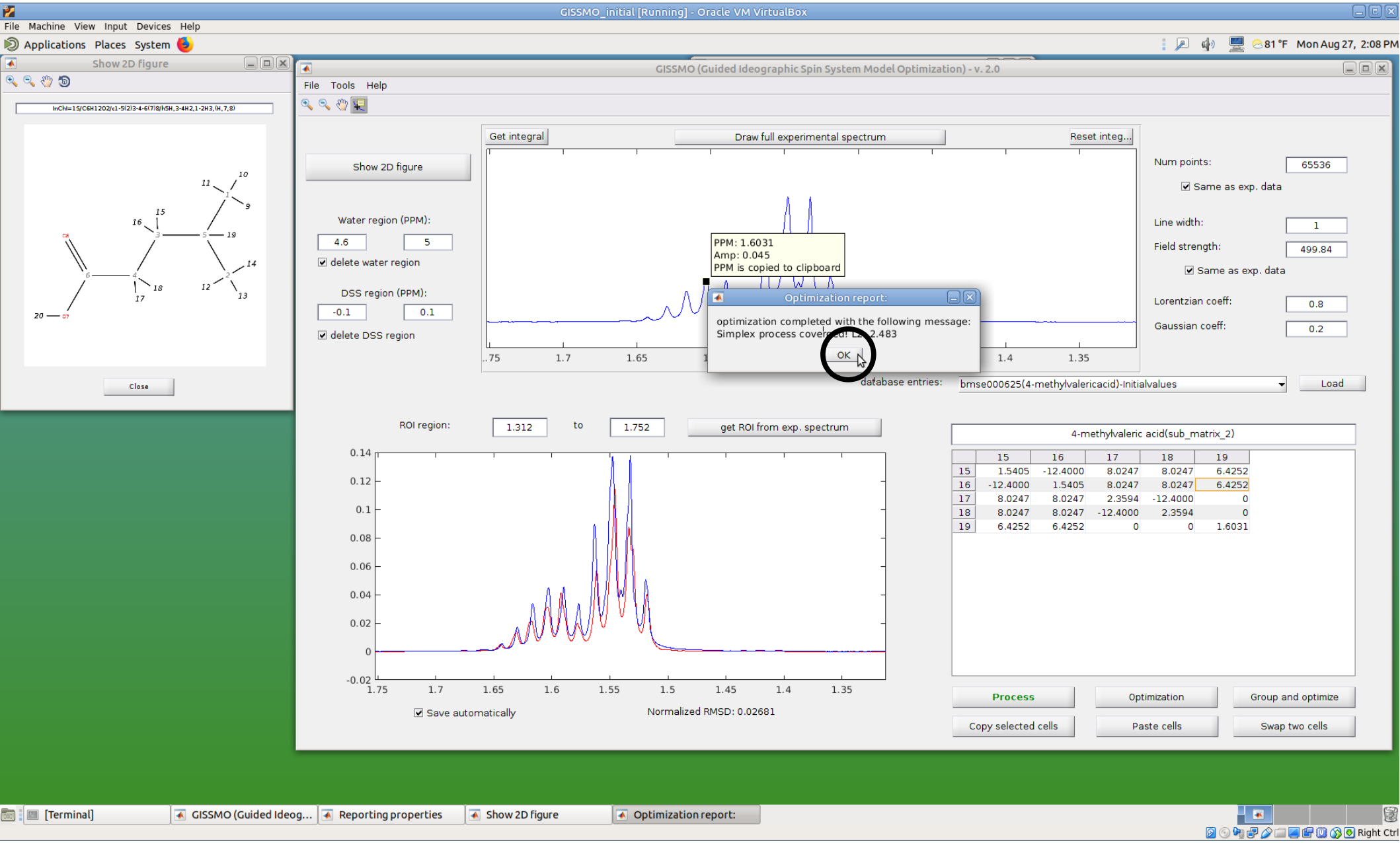
15,16 couplings to 19

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:08 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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: 1.6031
Amp: 0.045
PPM is copied to clipboard
Optimization report:
optimization completed with the following message:
Simplex process covered!
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
1.312
to
1.752
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.02681
4-methylvaleric acid(sub_matrix_2)
15 16 17 18 19
15 1.5405 -12.4000 8.0247 8.0247 6.4252
16 -12.4000 1.5405 8.0247 8.0247 6.4252
17 8.0247 8.0247 2.3594 -12.4000 0
18 8.0247 8.0247 -12.4000 2.3594 0
19 6.4252 6.4252 0 0 1.6031
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Optimization report:
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:08 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

Save automatically

Normalized RMSD: 0.02681

4-methylvaleric acid(sub_matrix_2)

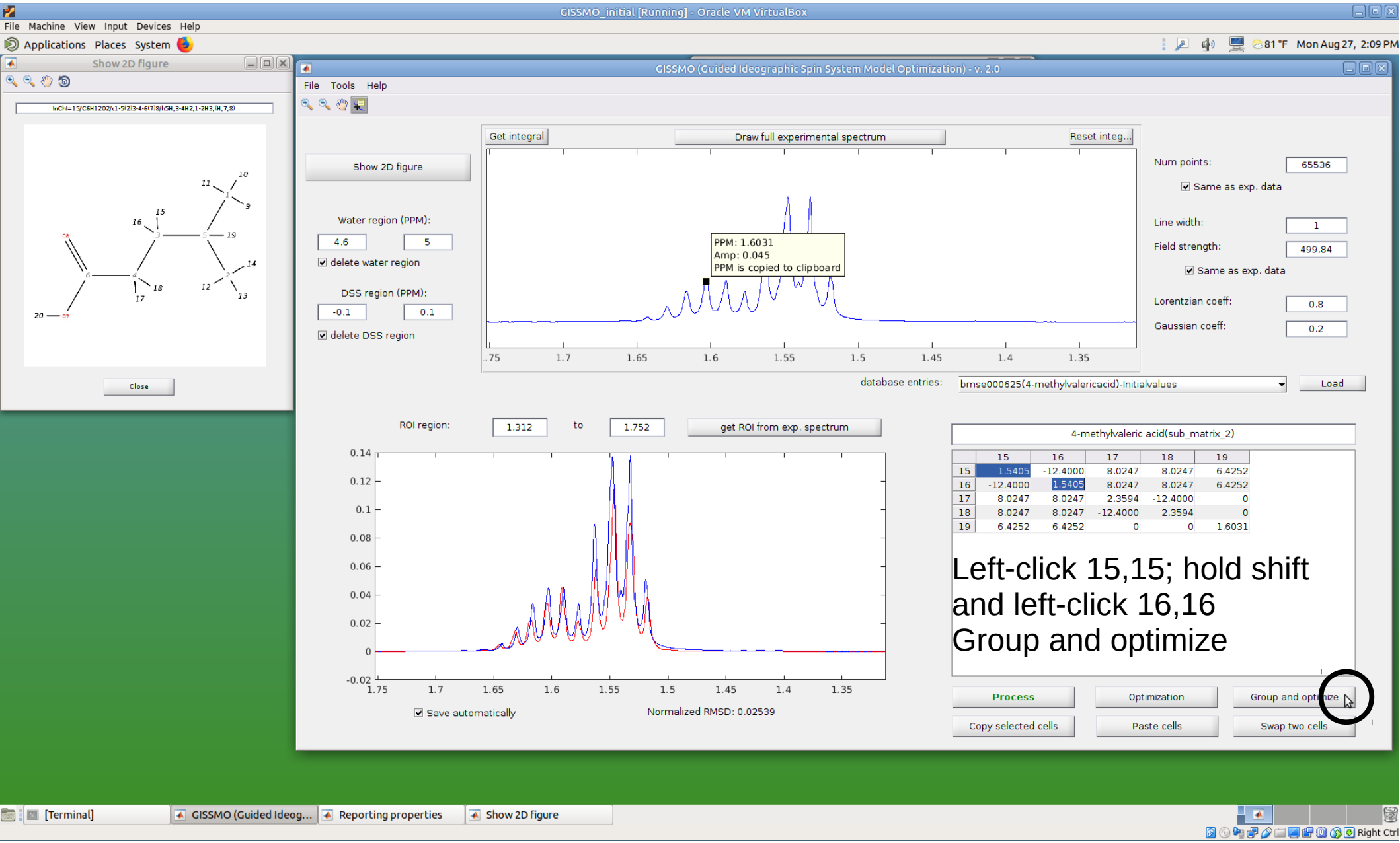
	15	16	17	18	19
15	1.5405	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5405	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6031

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
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Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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: 1.6031
Amp: 0.045
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
1.312
to
1.752
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.02539
4-methylvaleric acid(sub_matrix_2)
15 16 17 18 19
15 1.5405 -12.4000 8.0247 8.0247 6.4252
16 -12.4000 1.5405 8.0247 8.0247 6.4252
17 8.0247 8.0247 2.3594 -12.4000 0
18 8.0247 8.0247 -12.4000 2.3594 0
19 6.4252 6.4252 0 0 1.6031
Left-click 15,15; hold shift
and left-click 16,16
Group and optimize
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:09 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

Optimization report:

optimization completed with the following message:
Simplex process covered! L2: 1.448

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.02539

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6031

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

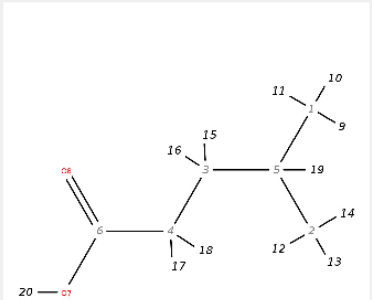
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:09 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

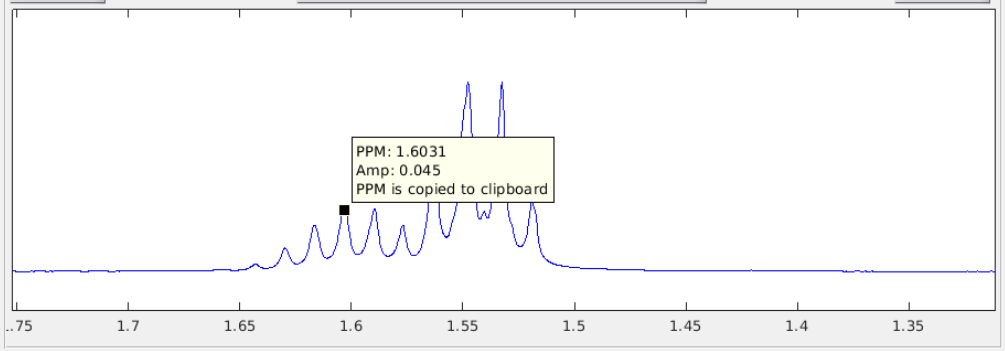
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

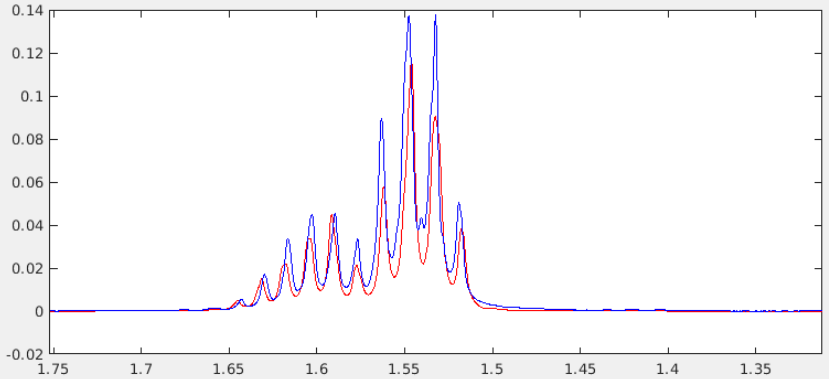
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.02539

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6031

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

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File Machine View Input Devices Help

Applications Places System

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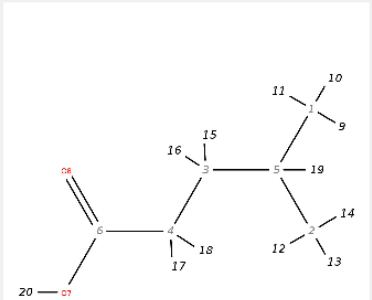
Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

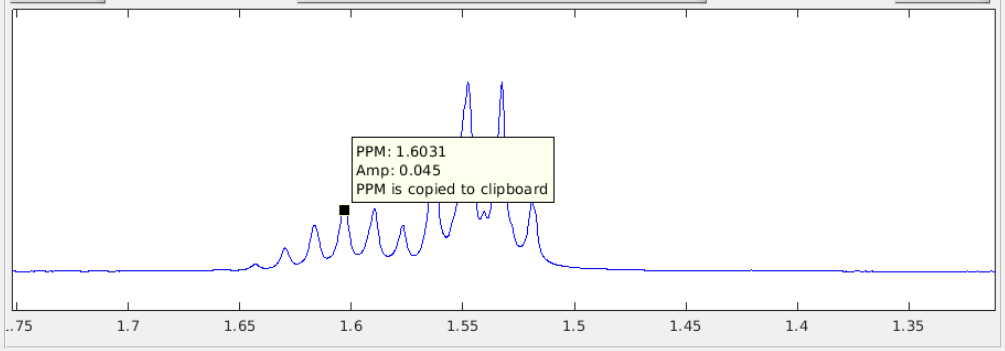
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

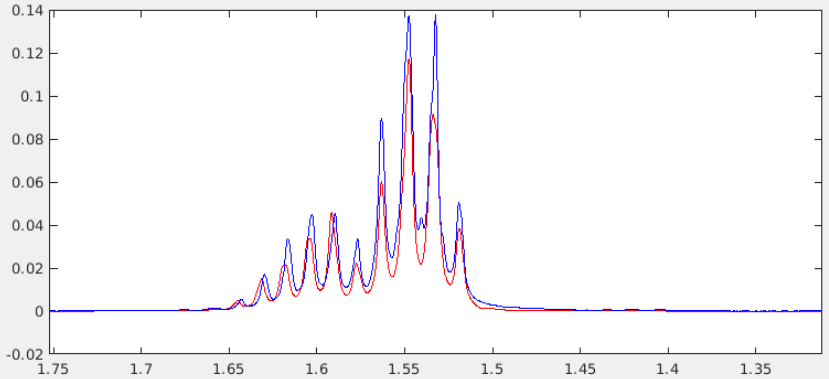
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01855

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6031

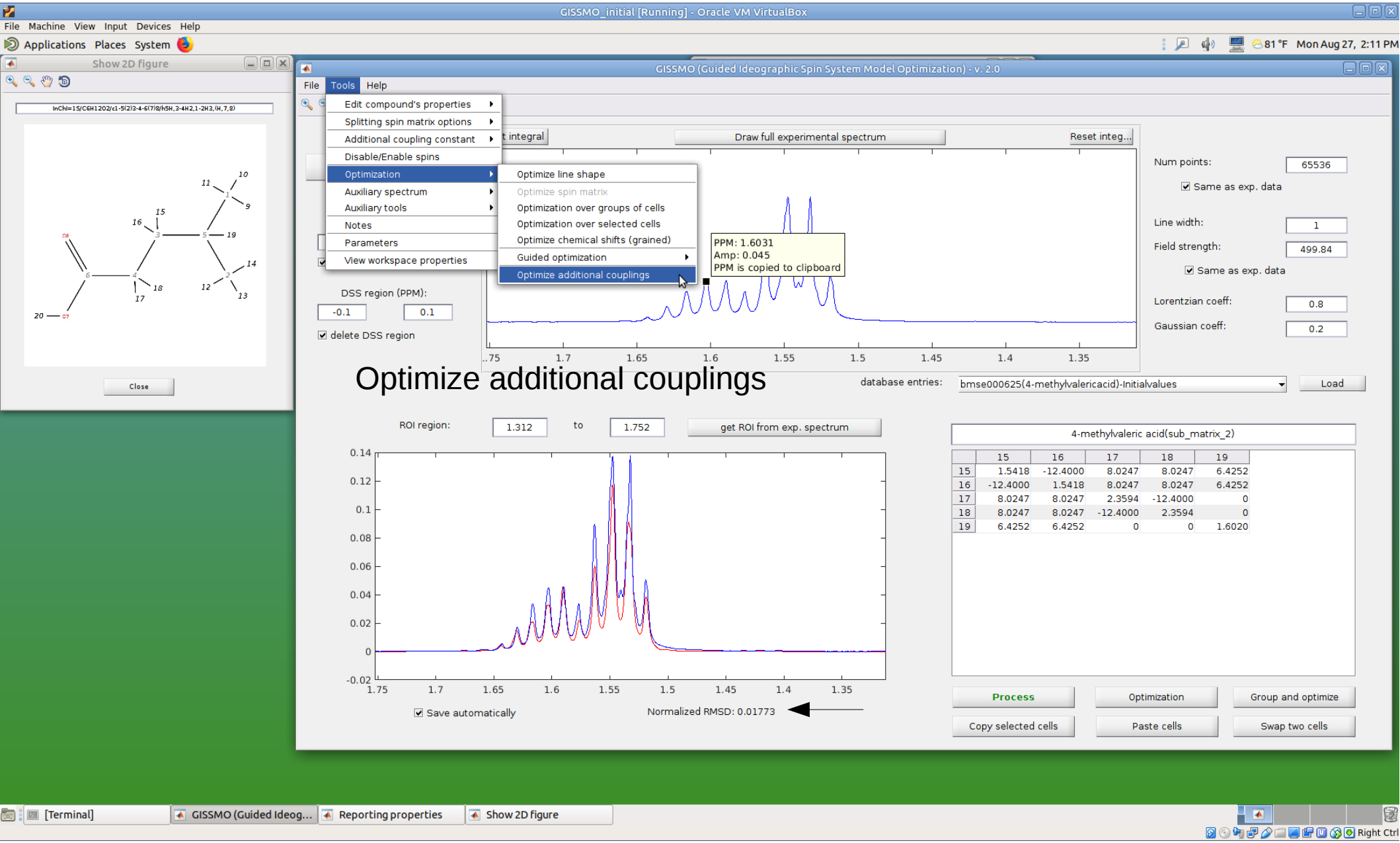
Optimize 19,19

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:11 PM
Show 2D figure
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
Optimize line shape
Optimize spin matrix
Optimization over groups of cells
Optimization over selected cells
Optimize chemical shifts (grained)
Guided optimization
Optimize additional couplings
Draw full experimental spectrum
Reset integ...
PPM: 1.6031
Amp: 0.045
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
DSS region (PPM):
-0.1
0.1
delete DSS region
Optimize additional couplings
database entries: bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region: 1.312 to 1.752
get ROI from exp. spectrum
4-methylvaleric acid(sub_matrix_2)
Save automatically
Normalized RMSD: 0.01773
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:11 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

choose additional couplings for optimization

Choose additional couplings to be optimized

	spins	coupling constant	spin groups ID	coupling groups ID	optimize	keep va
1	19	7	group(1)	group(1)	☑	group(1
2	19	7	group(1)	group(2)	☑	group(2
3	19	7	group(1)	group(3)	☑	group(3
4	19	7	group(1)	group(4)	☑	group(4
5	19	7	group(1)	group(5)	☑	group(5
6	19	7	group(1)	group(6)	☑	group(6

Ok

Slide right

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

values Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.01773

4-methylvaleric acid(sub_matrix_2)

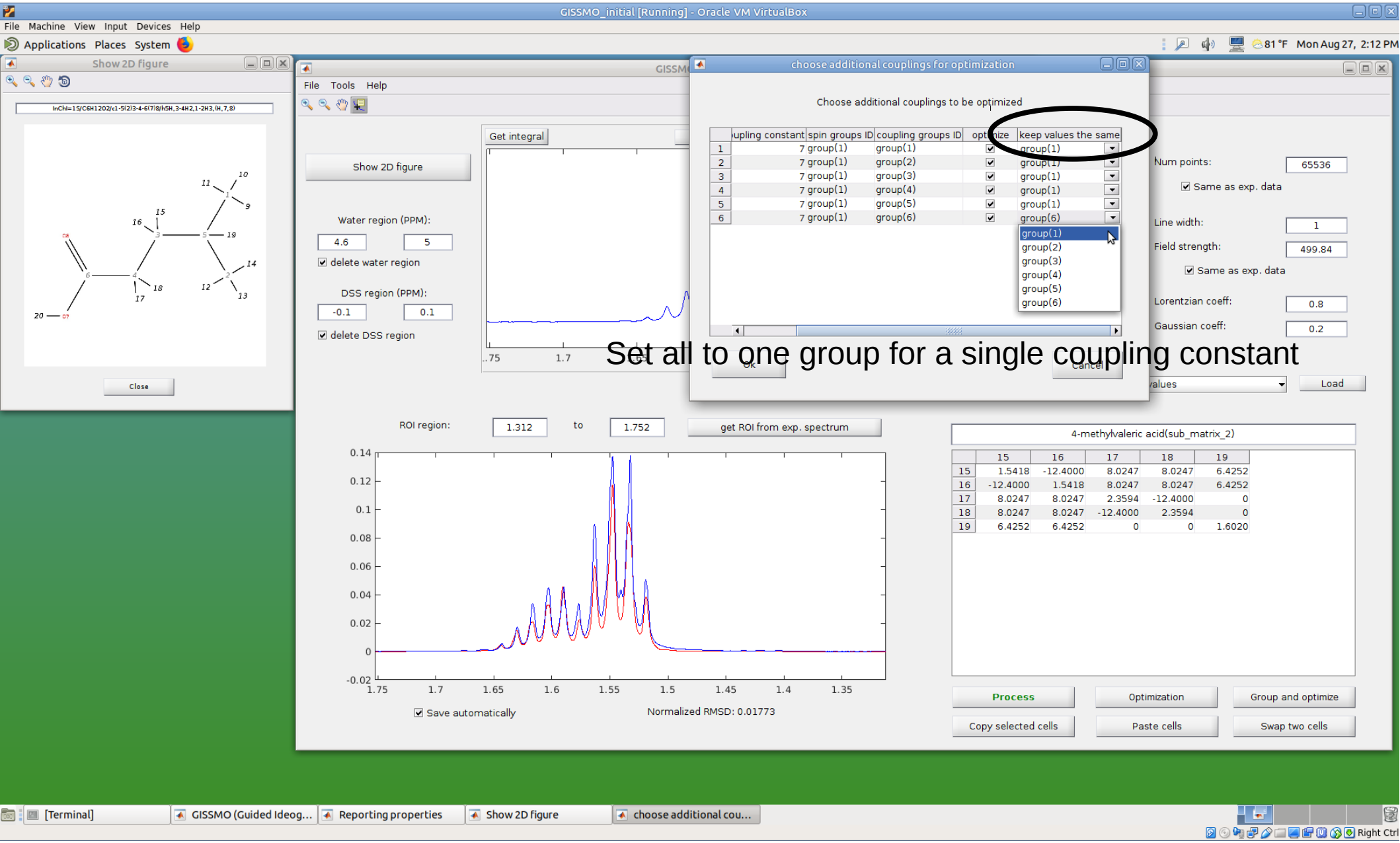
	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6020

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure choose additional cou...

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:12 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
choose additional couplings for optimization
Choose additional couplings to be optimized
upling constant
spin groups ID
coupling groups ID
optimize
keep values the same
1 7 group(1) group(1) group(1)
2 7 group(1) group(2) group(1)
3 7 group(1) group(3) group(1)
4 7 group(1) group(4) group(1)
5 7 group(1) group(5) group(1)
6 7 group(1) group(6) group(6)
group(1)
group(2)
group(3)
group(4)
group(5)
group(6)
Ok
Cancel
Set all to one group for a single coupling constant
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
Load
ROI region:
1.312
to
1.752
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.01773
4-methylvaleric acid(sub_matrix_2)
15 16 17 18 19
15 1.5418 -12.4000 8.0247 8.0247 6.4252
16 -12.4000 1.5418 8.0247 8.0247 6.4252
17 8.0247 8.0247 2.3594 -12.4000 0
18 8.0247 8.0247 -12.4000 2.3594 0
19 6.4252 6.4252 0 0 1.6020
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
choose additional cou...
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:12 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

choose additional couplings for optimization

Choose additional couplings to be optimized

	upling constant	spin groups ID	coupling groups ID	optimize	keep values the same
1	7	group(1)	group(1)	☑	group(1)
2	7	group(1)	group(2)	☑	group(1)
3	7	group(1)	group(3)	☑	group(1)
4	7	group(1)	group(4)	☑	group(1)
5	7	group(1)	group(5)	☑	group(1)
6	7	group(1)	group(6)	☑	group(1)

Ok

Cancel

Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

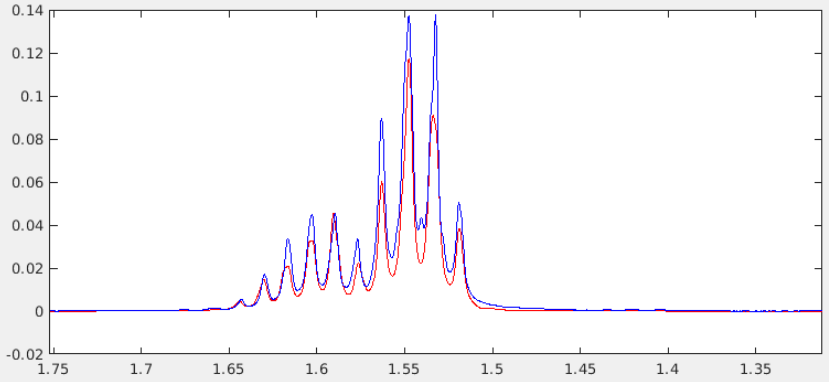
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

values Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01773

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6020

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure choose additional cou...

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:12 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 1.263
The spin matrix has bee updated. You may process!

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

bmse000625(4-methylvalericacid)-Initialvalues

Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.01773

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6020

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:13 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard

..75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

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: bmse000625(4-methylvalericacid)-Initialvalues | Load

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

0.14 0.12 0.1 0.08 0.06 0.04 0.02 0 -0.02

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

Save automatically

Normalized RMSD: 0.01745

4-methylvaleric acid(sub_matrix_2)

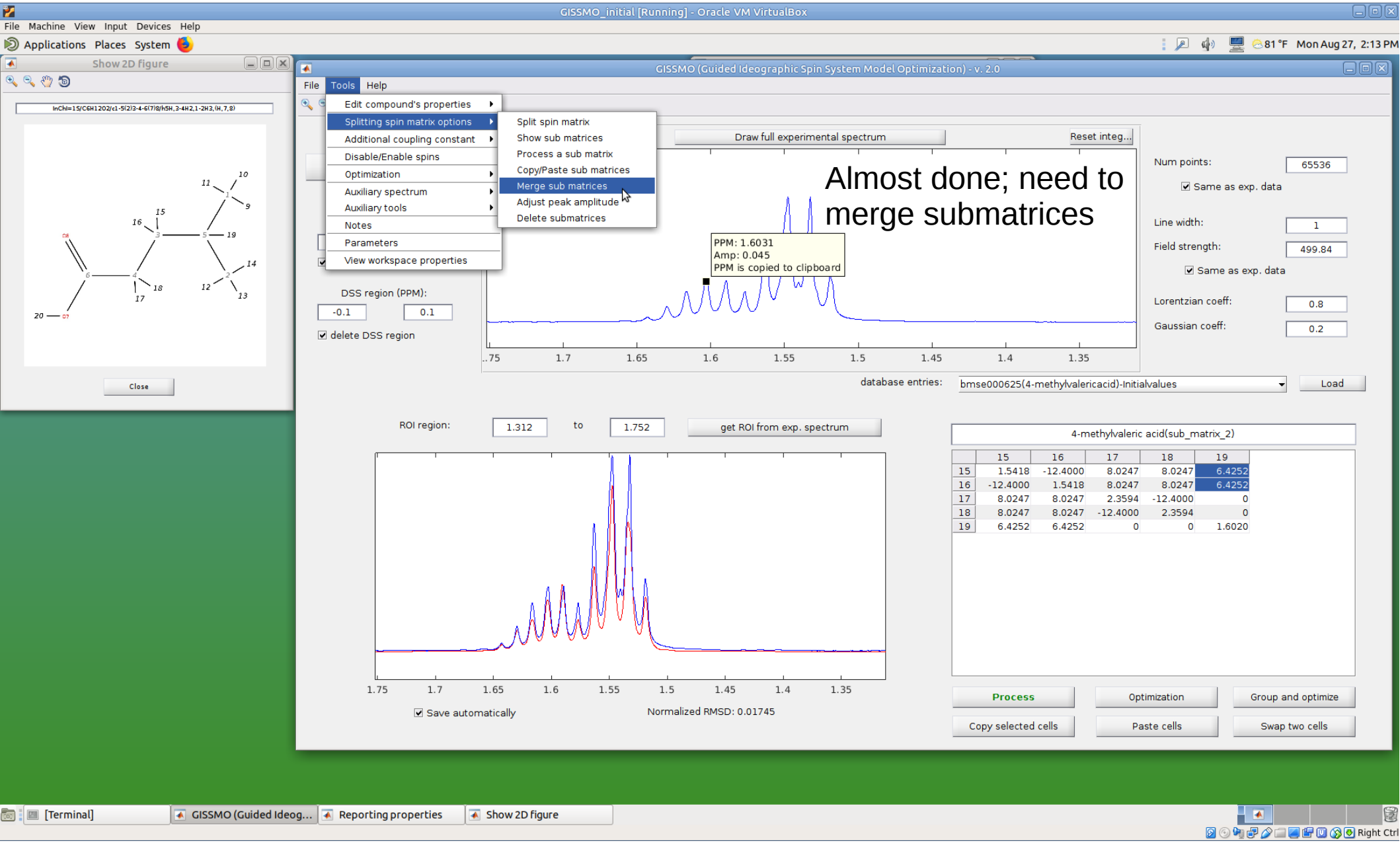
	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6020

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:13 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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...
Almost done; need to merge submatrices
PPM: 1.6031
Amp: 0.045
PPM is copied to clipboard
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
1.312
to
1.752
get ROI from exp. spectrum
4-methylvaleric acid(sub_matrix_2)
Save automatically
Normalized RMSD: 0.01745
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:14 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

..75 1.7 1.65

Scale sub-matrices

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

Preview

Done

ROI region: 1.312 to 1.752 get ROI from exp. spectrum

1.75 1.7 1.65 1.6 1.55 1.5 1.45 1.4 1.35

Save automatically

Normalized RMSD: 0.01745

4-methylvaleric acid(sub_matrix_2)

	15	16	17	18	19
15	1.5418	-12.4000	8.0247	8.0247	6.4252
16	-12.4000	1.5418	8.0247	8.0247	6.4252
17	8.0247	8.0247	2.3594	-12.4000	0
18	8.0247	8.0247	-12.4000	2.3594	0
19	6.4252	6.4252	0	0	1.6020

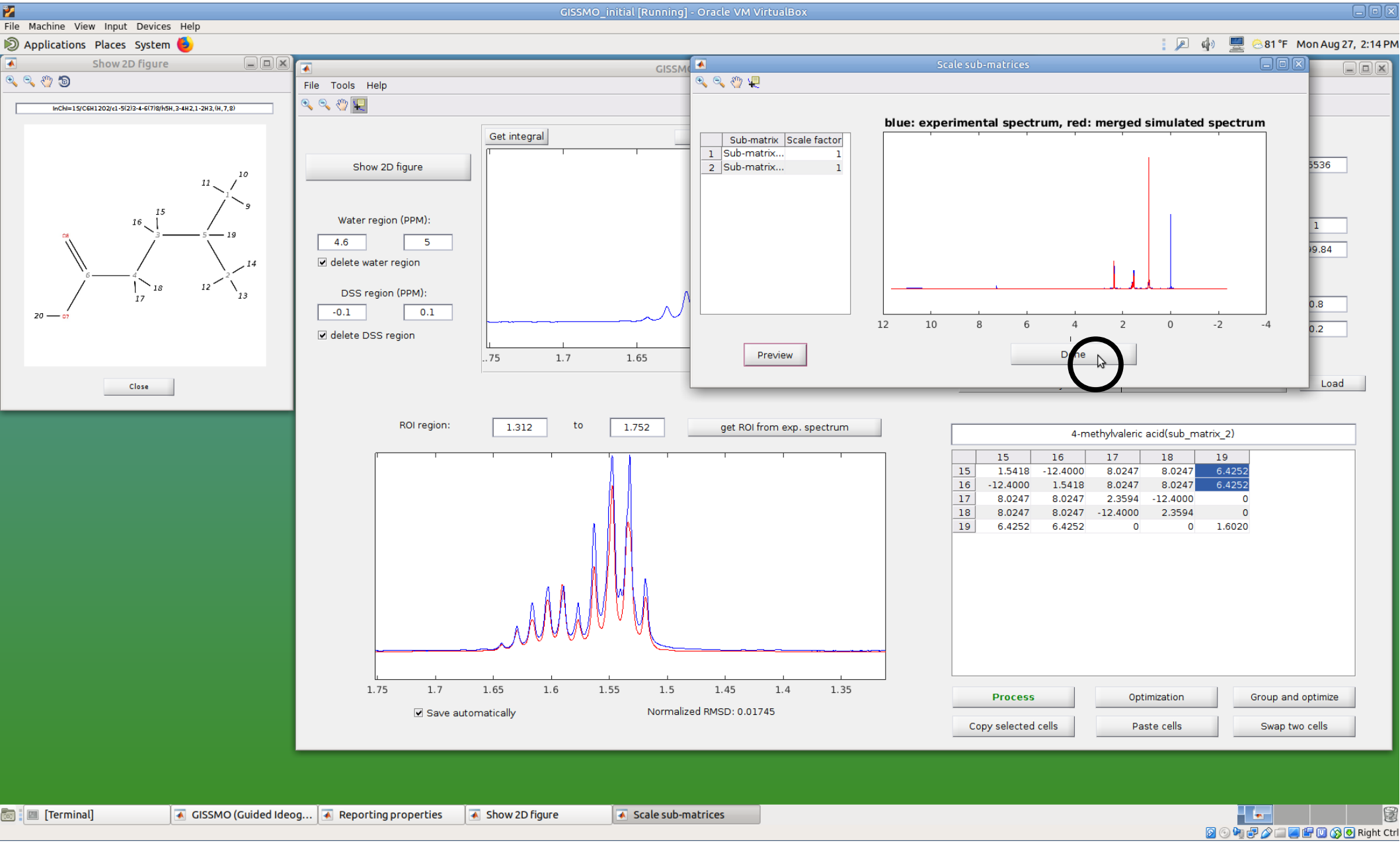
Load

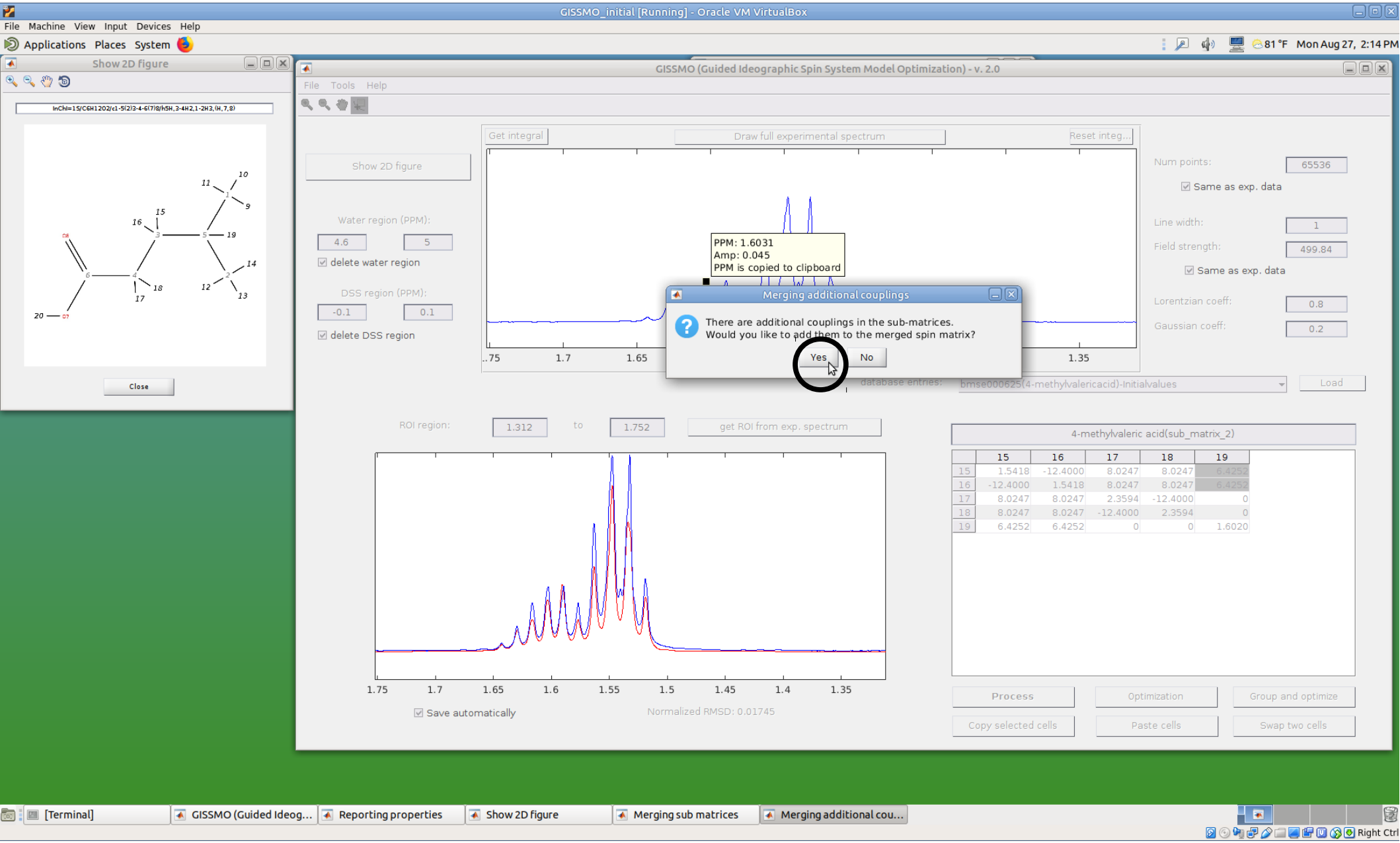
Process Optimization Group and optimize

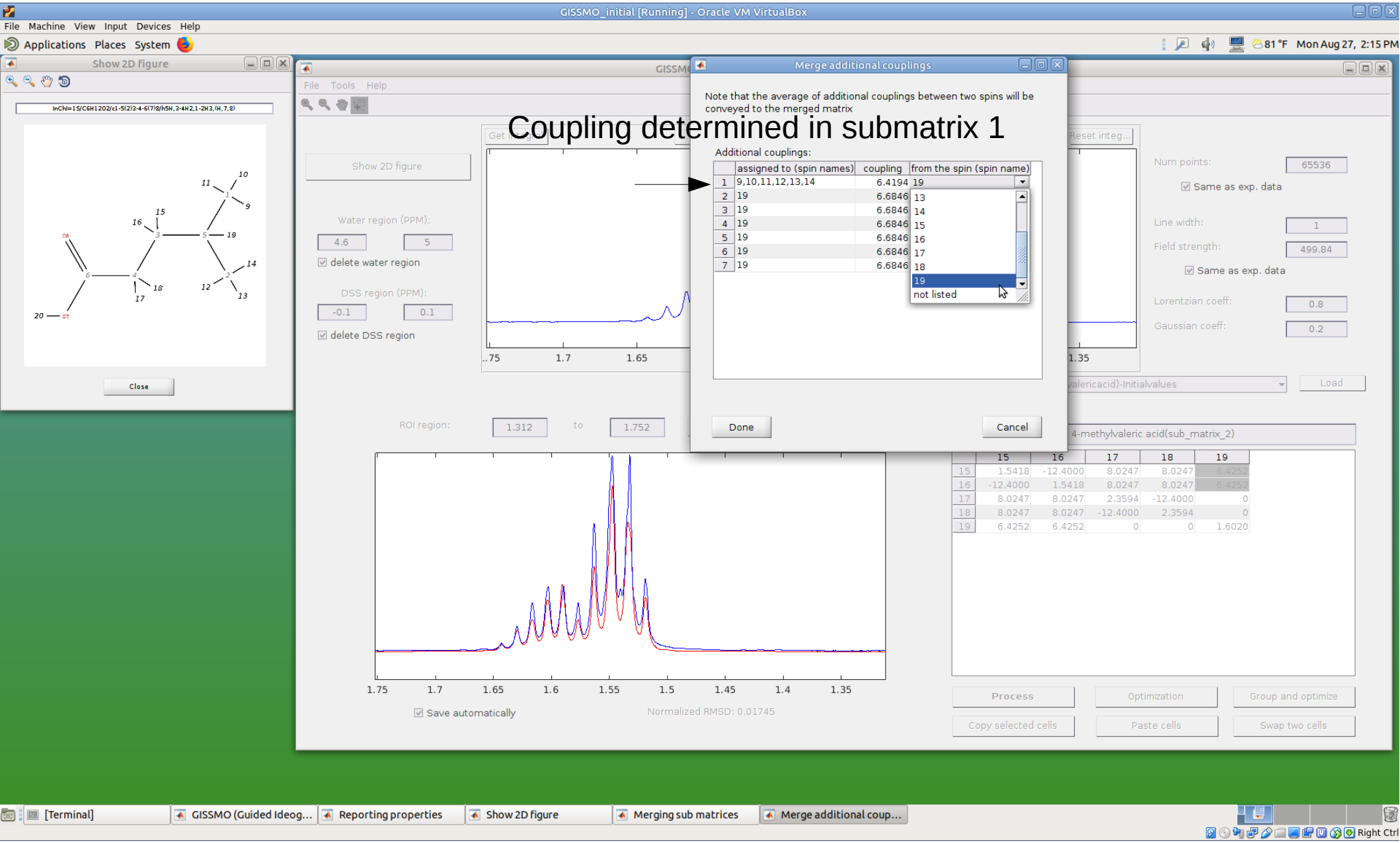
Copy selected cells Paste cells Swap two cells

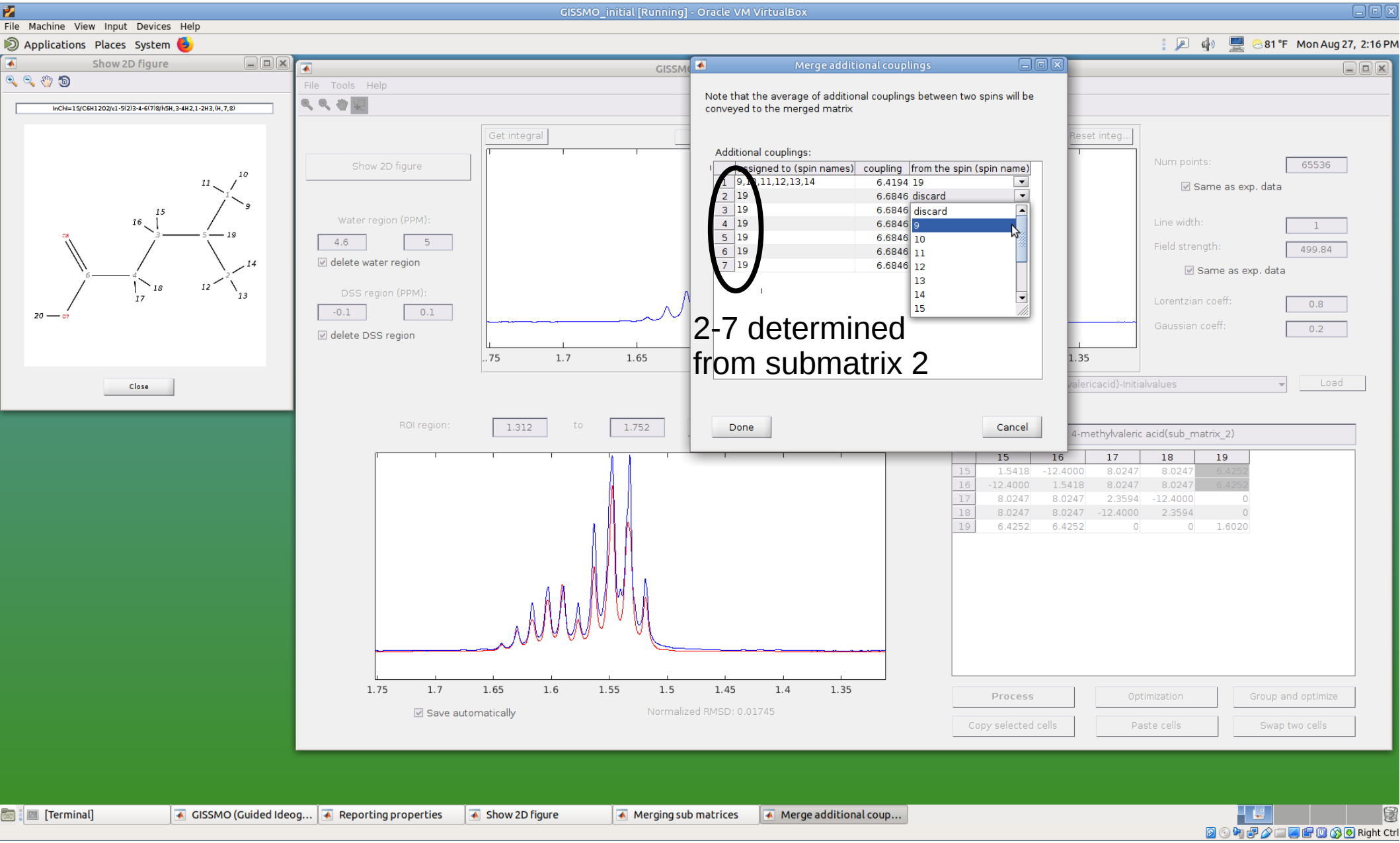
[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Scale sub-matrices

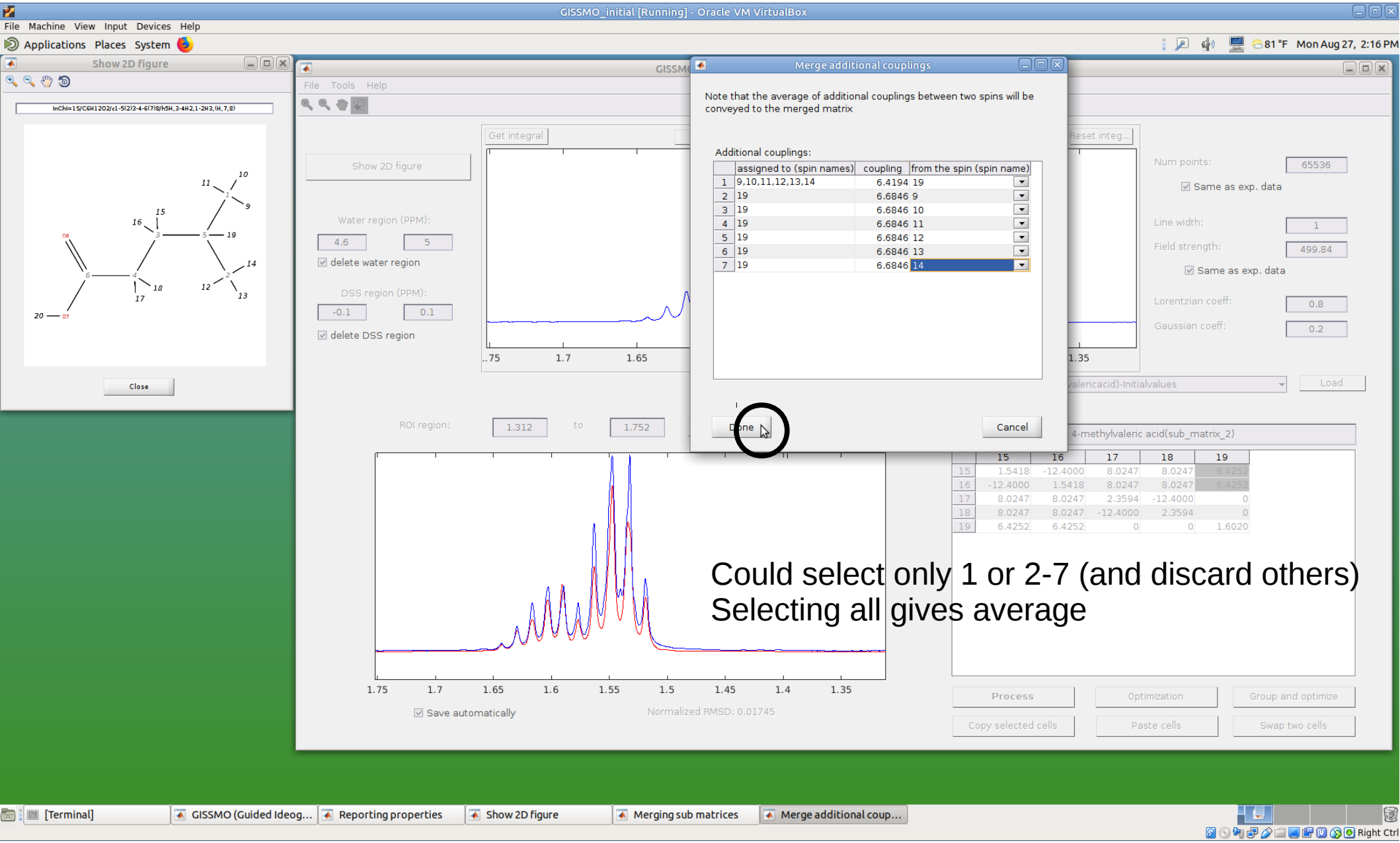
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:14 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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
Scale sub-matrices
Sub-matrix Scale factor
1 Sub-matrix... 1
2 Sub-matrix... 1
Preview
blue: experimental spectrum, red: merged simulated spectrum
Done
Load
ROI region:
1.312
to
1.752
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.01745
4-methylvaleric acid(sub_matrix_2)
15 16 17 18 19
15 1.5418 -12.4000 8.0247 8.0247 6.4252
16 -12.4000 1.5418 8.0247 8.0247 6.4252
17 8.0247 8.0247 2.3594 -12.4000 0
18 8.0247 8.0247 -12.4000 2.3594 0
19 6.4252 6.4252 0 0 1.6020
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Scale sub-matrices
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:14 PM
Show 2D figure
InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)
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: 1.6031
Amp: 0.045
PPM is copied to clipboard
Merging additional couplings
There are additional couplings in the sub-matrices.
Would you like to add them to the merged spin matrix?
Yes
No
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:
bmse000625(4-methylvalericacid)-Initialvalues
Load
ROI region:
1.312
to
1.752
get ROI from exp. spectrum
4-methylvaleric acid(sub_matrix_2)
15 16 17 18 19
15 1.5418 -12.4000 8.0247 8.0247 6.4252
16 -12.4000 1.5418 8.0247 8.0247 6.4252
17 8.0247 8.0247 2.3594 -12.4000 0
18 8.0247 8.0247 -12.4000 2.3594 0
19 6.4252 6.4252 0 0 1.6020
Save automatically
Normalized RMSD: 0.01745
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Merging sub matrices
Merging additional cou...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:15 PM
Show 2D figure
Close
Merge additional couplings
Note that the average of additional couplings between two spins will be conveyed to the merged matrix
Coupling determined in submatrix 1
Additional couplings:
assigned to (spin names)
coupling
from the spin (spin name)
9,10,11,12,13,14
6.4194
6.6846
not listed
Done
Cancel
Show 2D figure
Water region (PPM):
delete water region
DSS region (PPM):
delete DSS region
ROI region:
Save automatically
Normalized RMSD: 0.01745
Num points:
65536
Same as exp. data
Line width:
Field strength:
499.84
Lorentzian coeff:
Gaussian coeff:
Load
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Merging sub matrices
Merge additional coup...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
81 °F Mon Aug 27, 2:16 PM
Show 2D figure
Close
Merge additional couplings
Note that the average of additional couplings between two spins will be conveyed to the merged matrix
Additional couplings:
from the spin (spin name)
discard
2-7 determined from submatrix 2
Done
Cancel
Show 2D figure
Water region (PPM):
delete water region
DSS region (PPM):
delete DSS region
Get integral
Reset integ...
Num points:
65536
Same as exp. data
Line width:
Field strength:
499.84
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
Load
ROI region:
1.312
to
1.752
4-methylvaleric acid(sub_matrix_2)
Save automatically
Normalized RMSD: 0.01745
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Merging sub matrices
Merge additional coup...
Right Ctrl


GISSMO_initial [Running] - Oracle VM VirtualBox
Merge additional couplings
Note that the average of additional couplings between two spins will be conveyed to the merged matrix
Additional couplings:
assigned to (spin names)
coupling
from the spin (spin name)
Done
Cancel
Show 2D figure
Water region (PPM):
delete water region
DSS region (PPM):
delete DSS region
ROI region:
Save automatically
Normalized RMSD: 0.01745
Num points:
Same as exp. data
Line width:
Field strength:
Lorentzian coeff:
Gaussian coeff:
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
Could select only 1 or 2-7 (and discard others)
Selecting all gives average

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:19 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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

t integral

Draw full experimental spectrum

Reset integ...

Finished: mark Done

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: bmse000625(4-methylvalericacid)-Initialvalues

Load

ROI region: 0.730 to 2.664 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.01742

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9118	0	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0	0
11	0	-12.4000	0.9118	0	0	0	0
12	0	0	0	0.9118	0	-12.4000	0
13	0	0	0	0	0.9118	0	0
14	0	0	0	-12.4000	0	0.9118	0
15	0	0	0	0	0	0	1.5418
16	0	0	0	0	0	0	-12.4000
17	0	0	0	0	0	0	8.0247
18	0	0	0	0	0	0	8.0247
19	6.5520	6.5520	6.5520	6.5520	6.5520	6.5520	6.4252

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:19 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

bmse000625(4-methylvalericacid)-Initialvalues

Load

ROI region: 0.730 to 2.664 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.01742

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9118	0	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0	0
11	0	-12.4000	0.9118	0	0	0	0
12	0	0	0	0.9118	0	-12.4000	0
13	0	0	0	0	0.9118	0	0
14	0	0	0	-12.4000	0	0.9118	0
15	0	0	0	0	0	0	1.5418
16	0	0	0	0	0	0	-12.4000
17	0	0	0	0	0	0	8.0247
18	0	0	0	0	0	0	8.0247
19	6.5520	6.5520	6.5520	6.5520	6.5520	6.5520	6.4252

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

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GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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:

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

bmse000625(4-methylvalericacid)-Initialvalues

Load

ROI region: 0.730 to 2.664 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.01742

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9118	0	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0	0
11	0	-12.4000	0.9118	0	0	0	0
12	0	0	0	0.9118	0	-12.4000	0
13	0	0	0	0	0.9118	0	0
14	0	0	0	-12.4000	0	0.9118	0
15	0	0	0	0	0	0	1.5418
16	0	0	0	0	0	0	-12.4000
17	0	0	0	0	0	0	8.0247
18	0	0	0	0	0	0	8.0247
19	6.5520	6.5520	6.5520	6.5520	6.5520	6.5520	6.4252

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

Move on to next spectrum

2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8

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: bmse000625(4-methylvaleric acid)-Done | Load

bmse000613(syringin)-Initialvalues
bmse000614(vanillicacid)-Initialvalues
bmse000615(2-furoylglycine)-Initialvalues
bmse000616(2-octenoicacid)-Initialvalues
bmse000617(2-phenylbutyricacid)-Initialvalues
bmse000618(3-hydroxy-4-methoxycinnamicacid)-Initialvalues
bmse000619(3-methyladipicacid)-Initialvalues
bmse000620(3-methylsalicylicacid)-Initialvalues
bmse000621(3-pyridinealdoxime)-Initialvalues
bmse000622(3-pyridinecarbonitrile)-Initialvalues
bmse000623(4-hydroxybenzylalcohol)-Initialvalues
bmse000624(4-methylsalicylicacid)-Initialvalues
bmse000625(4-methylvaleric acid)-Done
bmse000626(5_methoxytryptamine)-Initialvalues
bmse000627(bilirubin)-Initialvalues
bmse000628(cis-fenpropimorph)-Initialvalues
bmse000629(L-4-hydroxyphenylglycine)-Initialvalues
bmse000630(N-cyclohexylformamide)-Initialvalues
bmse000631(O-phospho-DL-threonine)-Initialvalues
bmse000632(sulfoaceticacid)-Initialvalues

ROI region: 0.730 to 2.664 get ROI from exp. spectrum

1 0.8 0.6 0.4 0.2 0 -0.2

2.6 2.4 2.2 2 1.8 1.6 1.4 1.2 1 0.8

Save automatically

Normalized RMSD: 0.01742

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

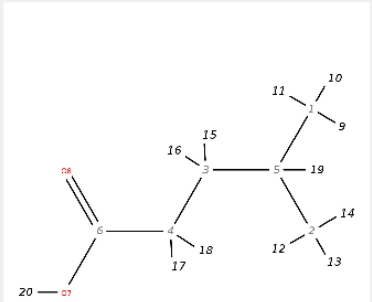
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:20 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

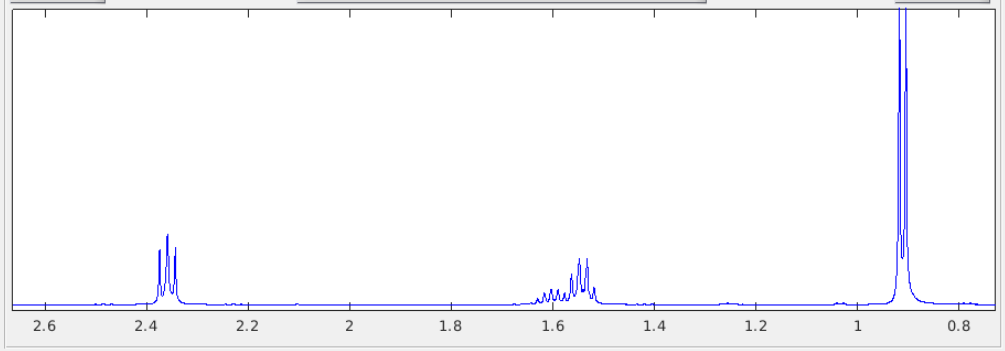
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

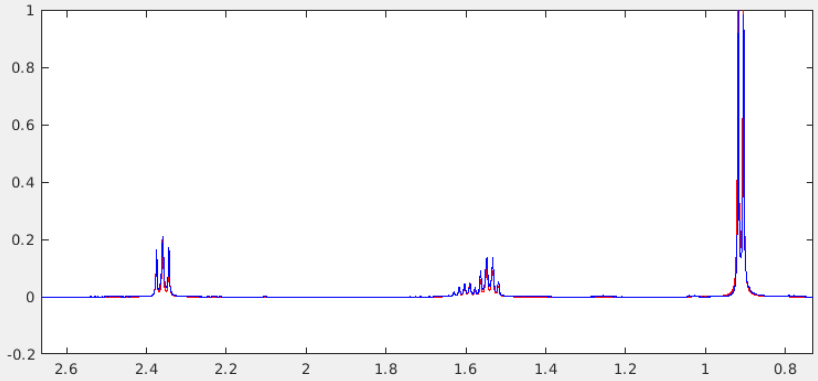
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

And load

database entries: bmse000626(5_methoxytryptamine)-Initialvalues | Load

ROI region: 0.730 to 2.664 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01742

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9118	0	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0	0
11	0	-12.4000	0.9118	0	0	0	0
12	0	0	0	0.9118	0	-12.4000	0
13	0	0	0	0	0.9118	0	0
14	0	0	0	-12.4000	0	0.9118	0
15	0	0	0	0	0	0	1.5418
16	0	0	0	0	0	0	-12.4000
17	0	0	0	0	0	0	8.0247
18	0	0	0	0	0	0	8.0247
19	6.5520	6.5520	6.5520	6.5520	6.5520	6.5520	6.4252

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:20 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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...

Don’t forget to save current workspace

Save status

Would you like to save the current workspace?

Yes No

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: bmse000626(5_methoxytryptamine)-Initialvalues Load

ROI region: 0.730 to 2.664 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.01742

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9118	0	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0	0
11	0	-12.4000	0.9118	0	0	0	0
12	0	0	0	0.9118	0	-12.4000	0
13	0	0	0	0	0.9118	0	0
14	0	0	0	-12.4000	0	0.9118	0
15	0	0	0	0	0	0	1.5418
16	0	0	0	0	0	0	-12.4000
17	0	0	0	0	0	0	8.0247
18	0	0	0	0	0	0	8.0247
19	6.5520	6.5520	6.5520	6.5520	6.5520	6.5520	6.4252

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

[Terminal] | GISSMO (Guided Ideog... | Reporting properties | Show 2D figure | Save status

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:21 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)

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: 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 completed!

The spin matrix is saved to
/home/nmrfam/Desktop/BMRB_Aug_2018_w_exp/bmse000625/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

hoxytryptamine)-Initialvalues Load

ROI region: 0.730 to 2.664 get ROI from exp. spectrum

Save automatically

Normalized RMSD: 0.01742

4-methylvaleric acid(merged)

	9	10	11	12	13	14	15
9	0.9118	0	0	0	0	0	0
10	0	0.9118	-12.4000	0	0	0	0
11	0	-12.4000	0.9118	0	0	0	0
12	0	0	0	0.9118	0	-12.4000	0
13	0	0	0	0	0.9118	0	0
14	0	0	0	-12.4000	0	0.9118	0
15	0	0	0	0	0	0	1.5418
16	0	0	0	0	0	0	-12.4000
17	0	0	0	0	0	0	8.0247
18	0	0	0	0	0	0	8.0247
19	6.5520	6.5520	6.5520	6.5520	6.5520	6.5520	6.4252

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

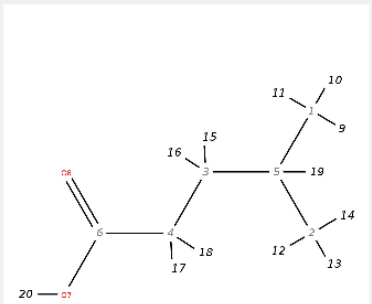
File Machine View Input Devices Help

Applications Places System

81 °F Mon Aug 27, 2:21 PM

Show 2D figure

InChI=1S/C6H12O2/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H,7,8)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

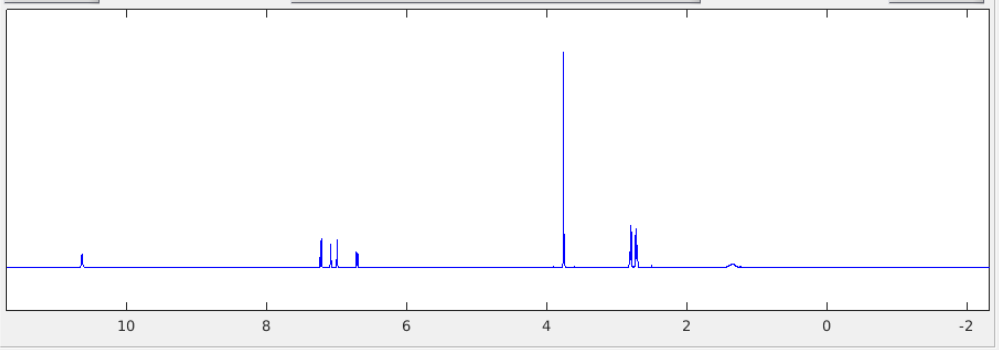
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 65536

Same as exp. data

Line width: 1

Field strength: 499.84

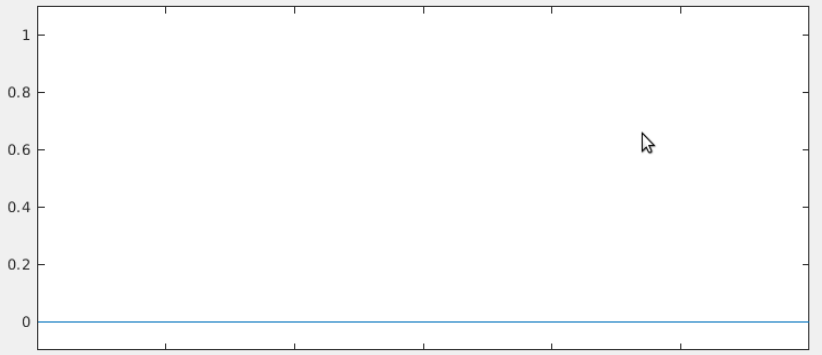
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000626(5_methoxytryptamine)-Initialvalues | Load

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



Save automatically

simulation info

5_methoxytryptamine(merged)

	15	16	17	18	19	20	21
15	3.8264	0	0	0	0	0	0
16	0	3.8264	-12.4000	0	0	0	0
17	0	-12.4000	3.8264	0	0	0	0
18	0	0	0	6.7301	8.4300	0	0
19	0	0	0	8.4300	7.2147	0	0
20	0	0	0	0	0	2.9464	-12.4000
21	0	0	0	0	0	-12.4000	2.9459
22	0	0	0	0	0	5.8000	5.8000
23	0	0	0	0	0	5.8000	5.8000
24	0	0	0	1.3300	0.5000	0	0
25	0	0	0	0	0	1.3300	1.3300

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl