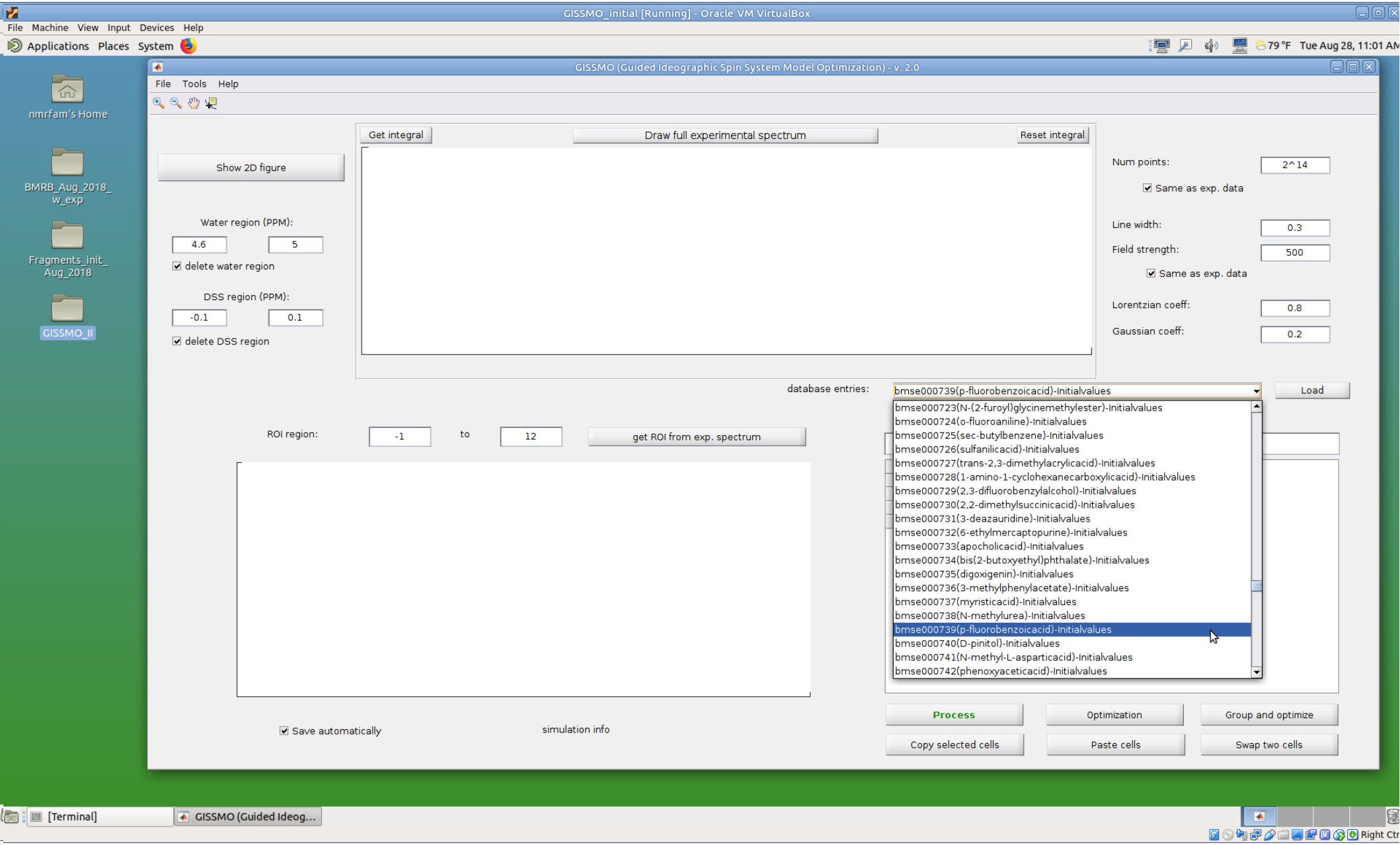
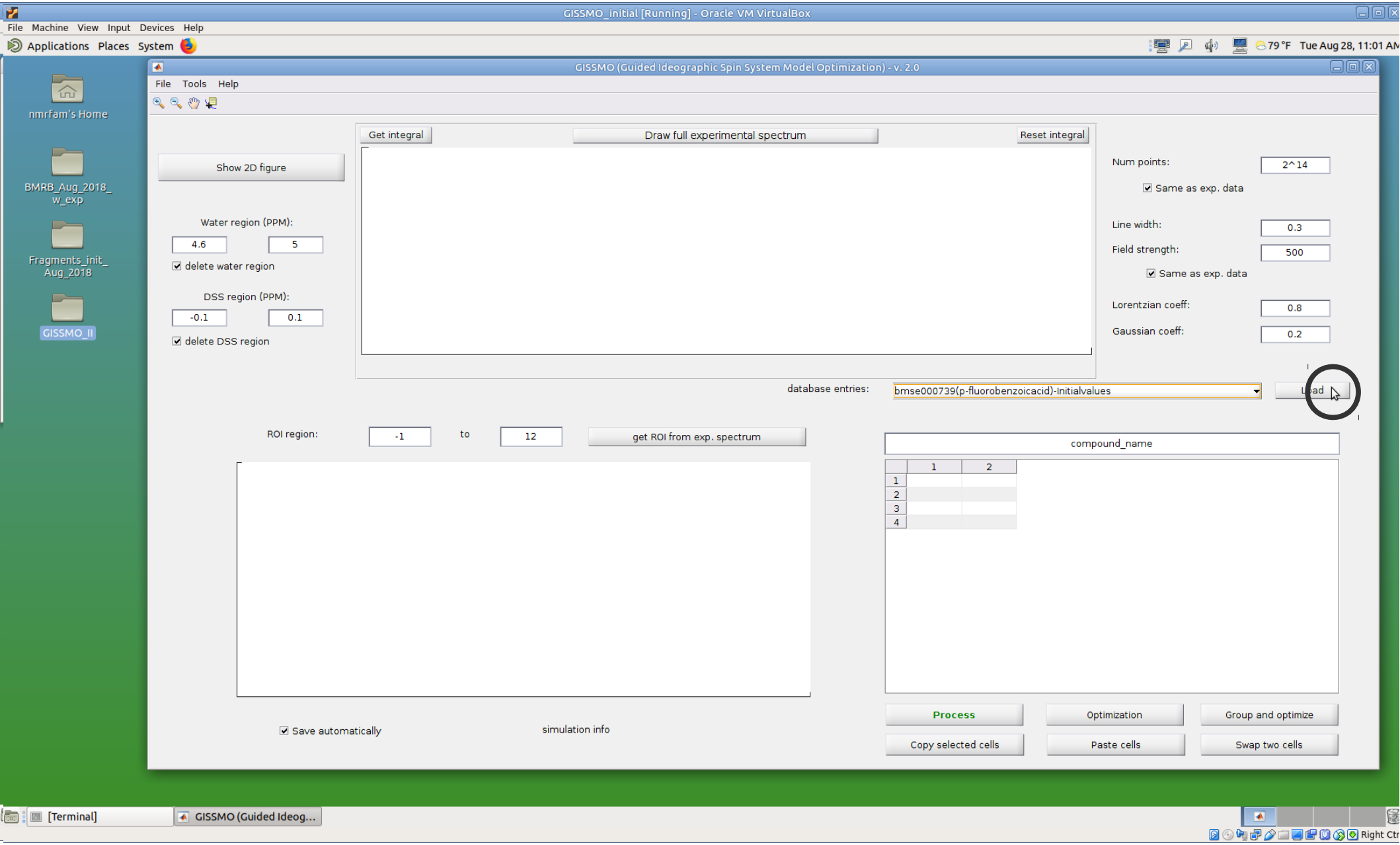
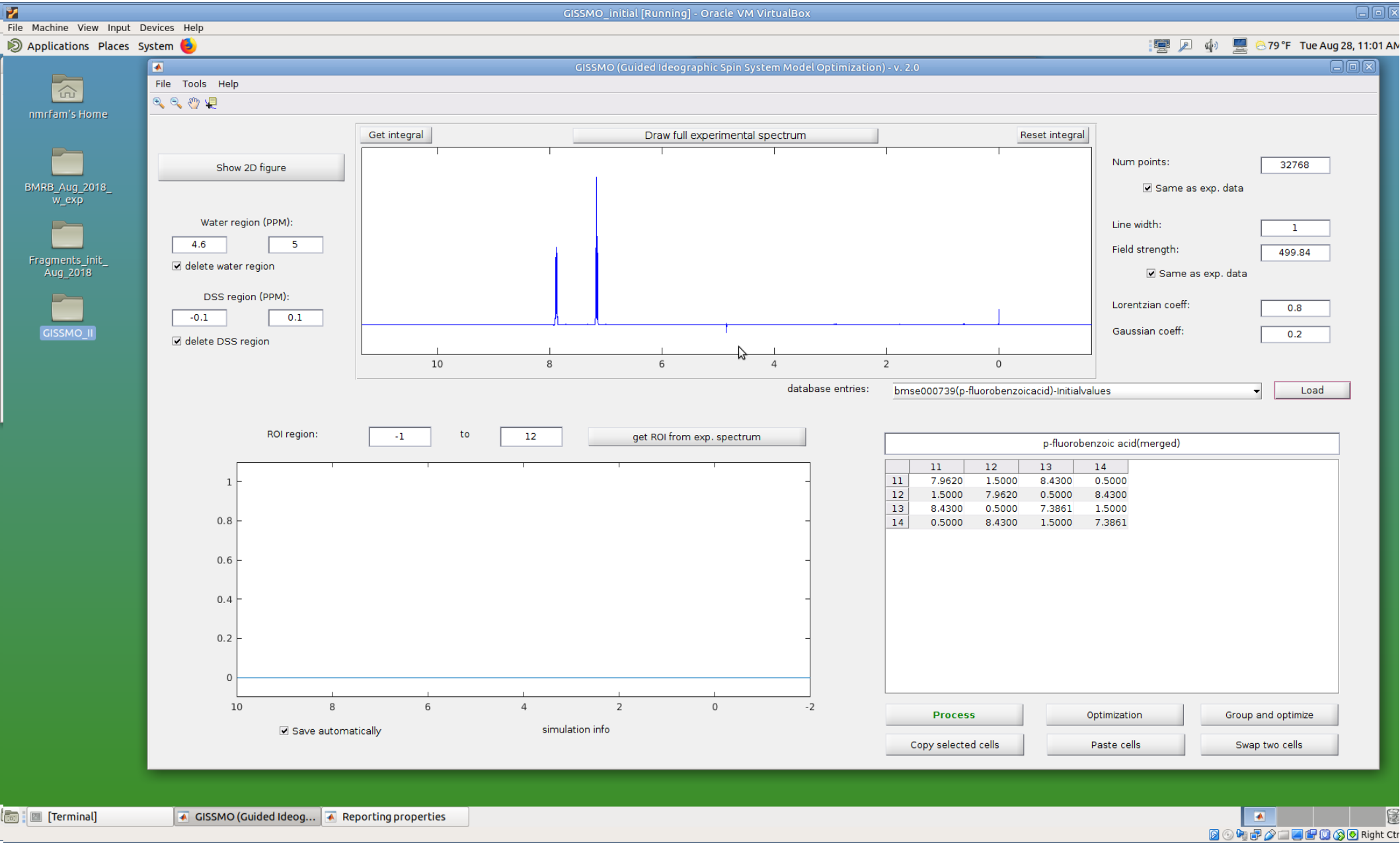
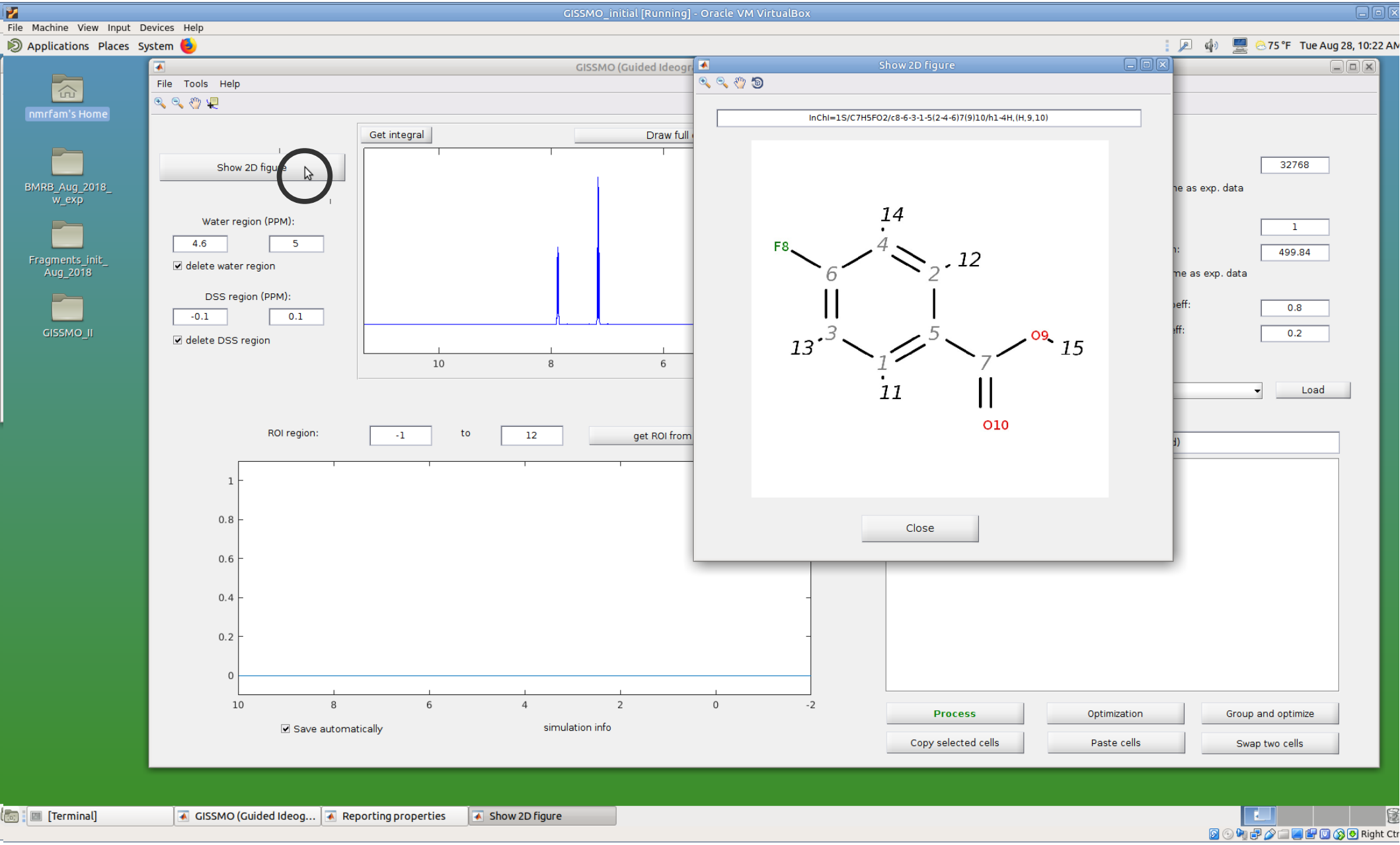

GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
79 °F Tue Aug 28, 11:01 AM
nmrfam's Home
BMRB_Aug_2018_w_exp
Fragments_init_Aug_2018
GISSMO_II
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset integral
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
2^14
Same as exp. data
Line width:
0.3
Field strength:
500
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
bmse000723(N-(2-furoyl)glycinemethylester)-Initialvalues
bmse000724(o-fluoroaniline)-Initialvalues
bmse000725(sec-butylbenzene)-Initialvalues
bmse000726(sulfanilicacid)-Initialvalues
bmse000727(trans-2,3-dimethylacrylicacid)-Initialvalues
bmse000728(1-amino-1-cyclohexanecarboxylicacid)-Initialvalues
bmse000729(2,3-difluorobenzylalcohol)-Initialvalues
bmse000730(2,2-dimethylsuccinicacid)-Initialvalues
bmse000731(3-deazauridine)-Initialvalues
bmse000732(6-ethylmercaptopurine)-Initialvalues
bmse000733(apocholicacid)-Initialvalues
bmse000734(bis(2-butoxyethyl)phthalate)-Initialvalues
bmse000735(digoxigenin)-Initialvalues
bmse000736(3-methylphenylacetate)-Initialvalues
bmse000737(myristicacid)-Initialvalues
bmse000738(N-methylurea)-Initialvalues
bmse000739(p-fluorobenzoicacid)-Initialvalues
bmse000740(D-pinitol)-Initialvalues
bmse000741(N-methyl-L-asparticacid)-Initialvalues
bmse000742(phenoxyaceticacid)-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 Ctr


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
79 °F Tue Aug 28, 11:01 AM
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:
bmse000739(p-fluorobenzoicacid)-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 Ctr


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
79 °F Tue Aug 28, 11:01 AM
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:
32768
Same as exp. data
Water region (PPM):
4.6
5
delete water region
Line width:
1
Field strength:
499.84
Same as exp. data
DSS region (PPM):
-0.1
0.1
delete DSS region
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
10 8 6 4 2 0
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
-1
to
12
get ROI from exp. spectrum
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.9620 1.5000 8.4300 0.5000
12 1.5000 7.9620 0.5000 8.4300
13 8.4300 0.5000 7.3861 1.5000
14 0.5000 8.4300 1.5000 7.3861
1 0.8 0.6 0.4 0.2 0
10 8 6 4 2 0 -2
Save automatically
simulation info
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Right Ctr


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
75 °F Tue Aug 28, 10:22 AM
nmrfam's Home
BMRB_Aug_2018_w_exp
Fragments_init_Aug_2018
GISSMO_II
GISSMO (Guided Ideogr
File Tools Help
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Get integral
Draw full
10
8
6
ROI region:
-1
to
12
get ROI from
1
0.8
0.6
0.4
0.2
0
10
8
6
4
2
0
-2
Save automatically
simulation info
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
12
2
6
3
13
5
O9
15
1
7
11
O10
Close
32768
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
Right Ctr

GISSMO_initial [Running] - Oracle VM VirtualBox

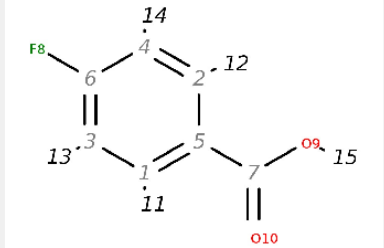
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:25 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

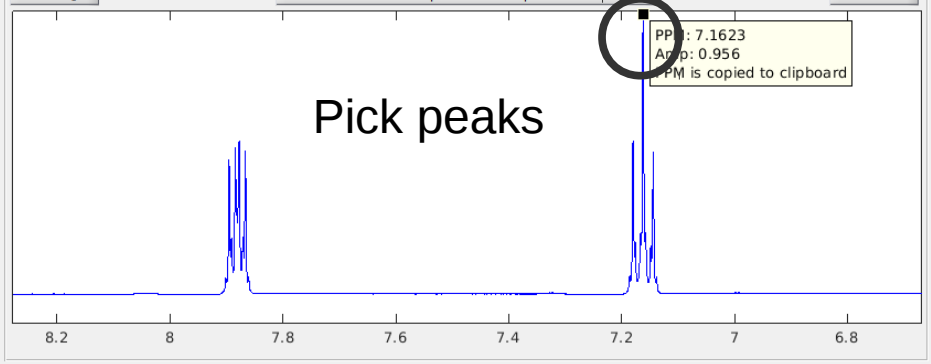
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

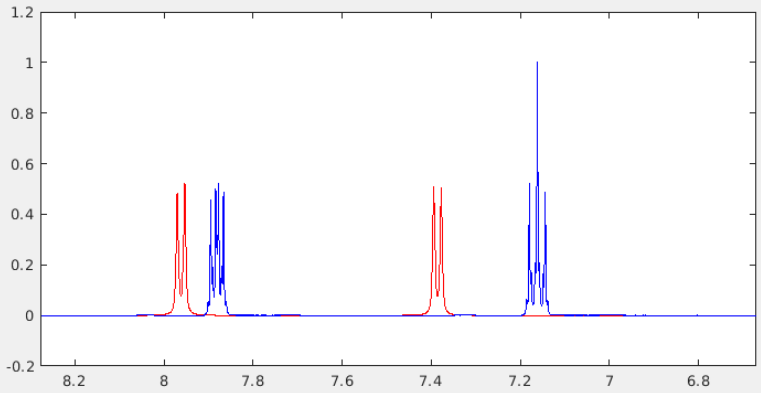
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 6.670 to 8.278 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.13933

p-fluorobenzoic acid(merged)

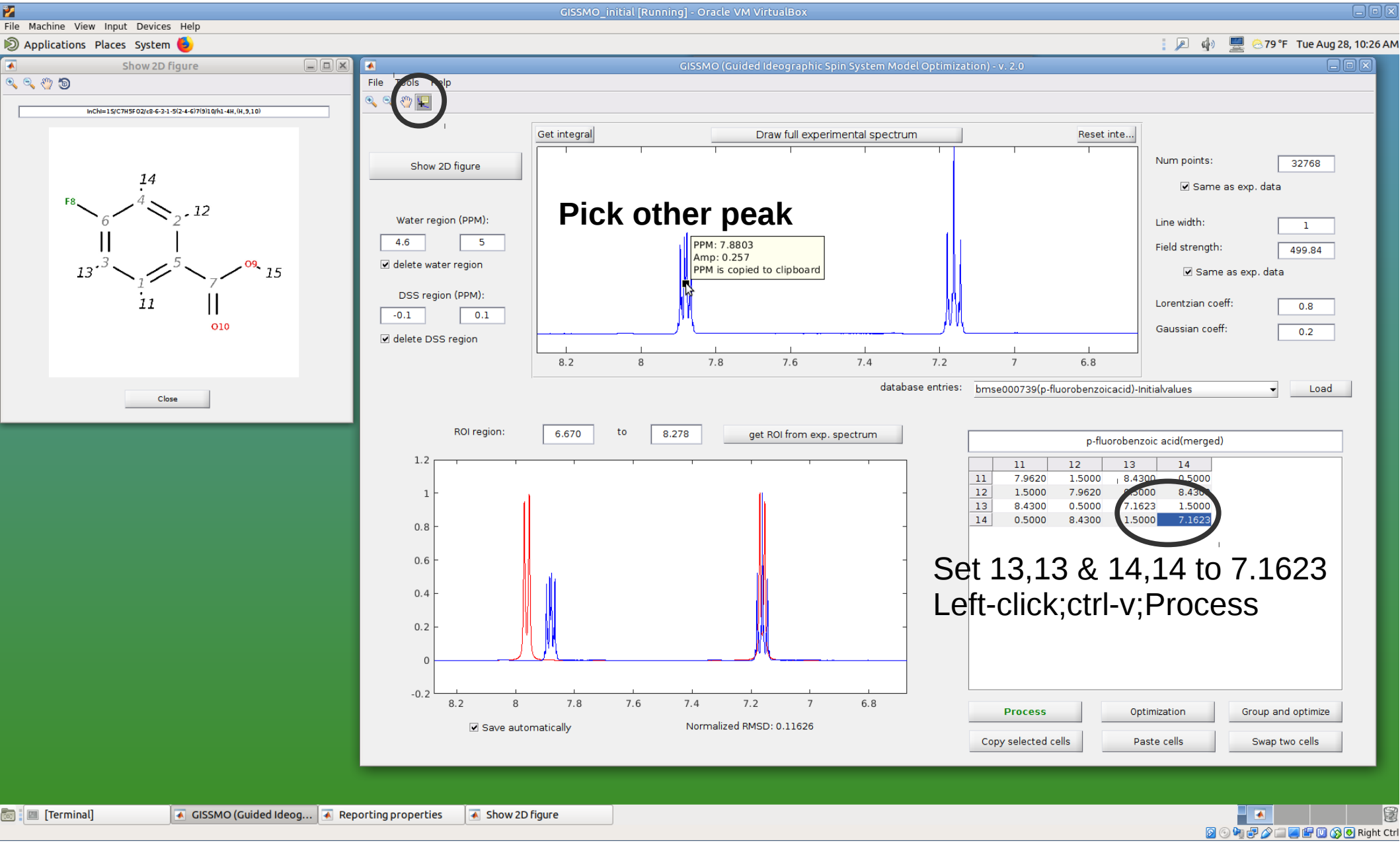
	11	12	13	14
11	7.9620	1.5000	8.4300	0.5000
12	1.5000	7.9620	0.5000	8.4300
13	8.4300	0.5000	7.1623	1.5000
14	0.5000	8.4300	1.5000	7.1623

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
79 °F Tue Aug 28, 10:26 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Get integral
Draw full experimental spectrum
Reset inte...
Pick other peak
PPM: 7.8803
Amp: 0.257
PPM is copied to clipboard
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
6.670
to
8.278
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.11626
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.9620 1.5000 8.4300 0.5000
12 1.5000 7.9620 0.5000 8.4300
13 8.4300 0.5000 7.1623 1.5000
14 0.5000 8.4300 1.5000 7.1623
Set 13,13 & 14,14 to 7.1623
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

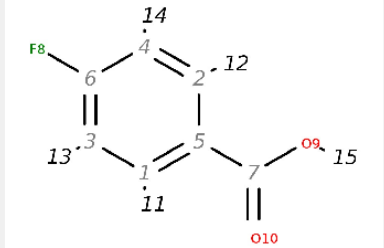
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:26 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

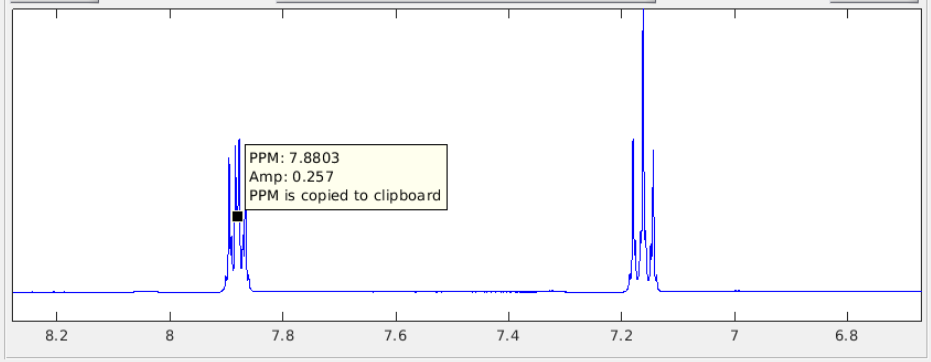
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

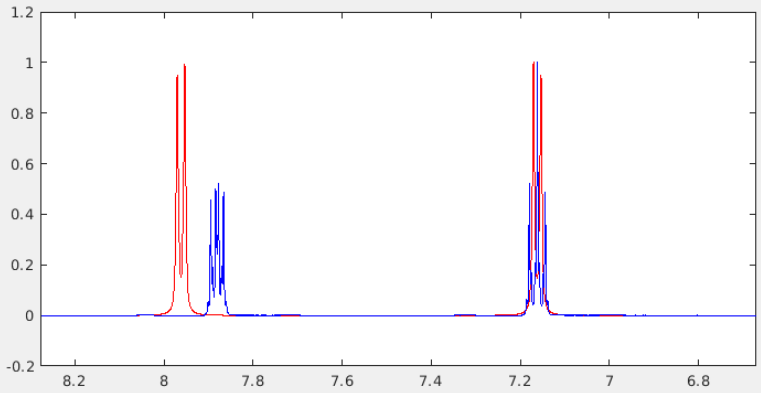
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 6.670 to 8.278 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.11626

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	1.5000	8.4300	0.5000
12	1.5000	7.8803	0.5000	8.4300
13	8.4300	0.5000	7.1623	1.5000
14	0.5000	8.4300	1.5000	7.1623

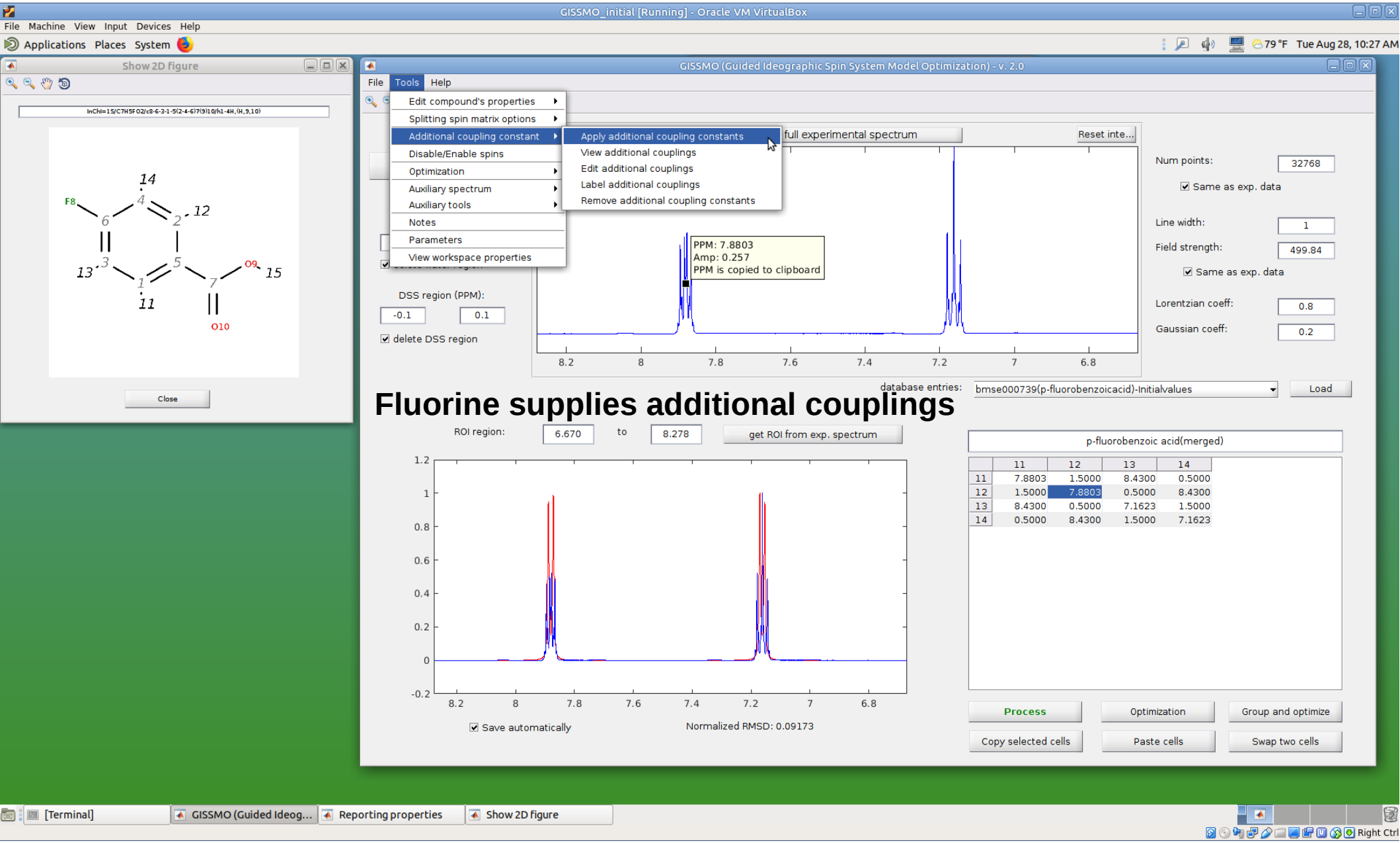
Set 11,11 & 12,12 to 7.8803
Left-click;ctrl-v;Process

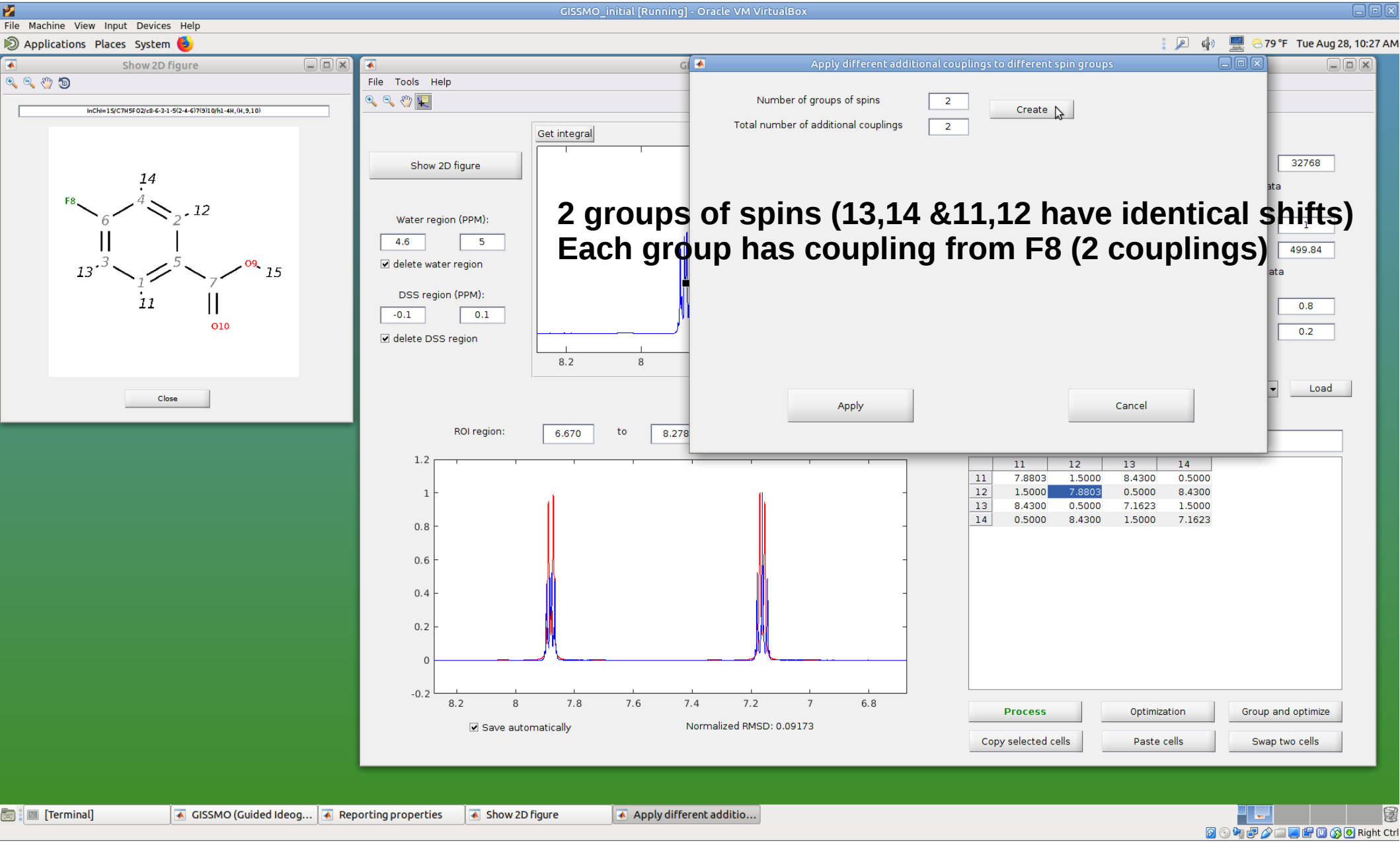
Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

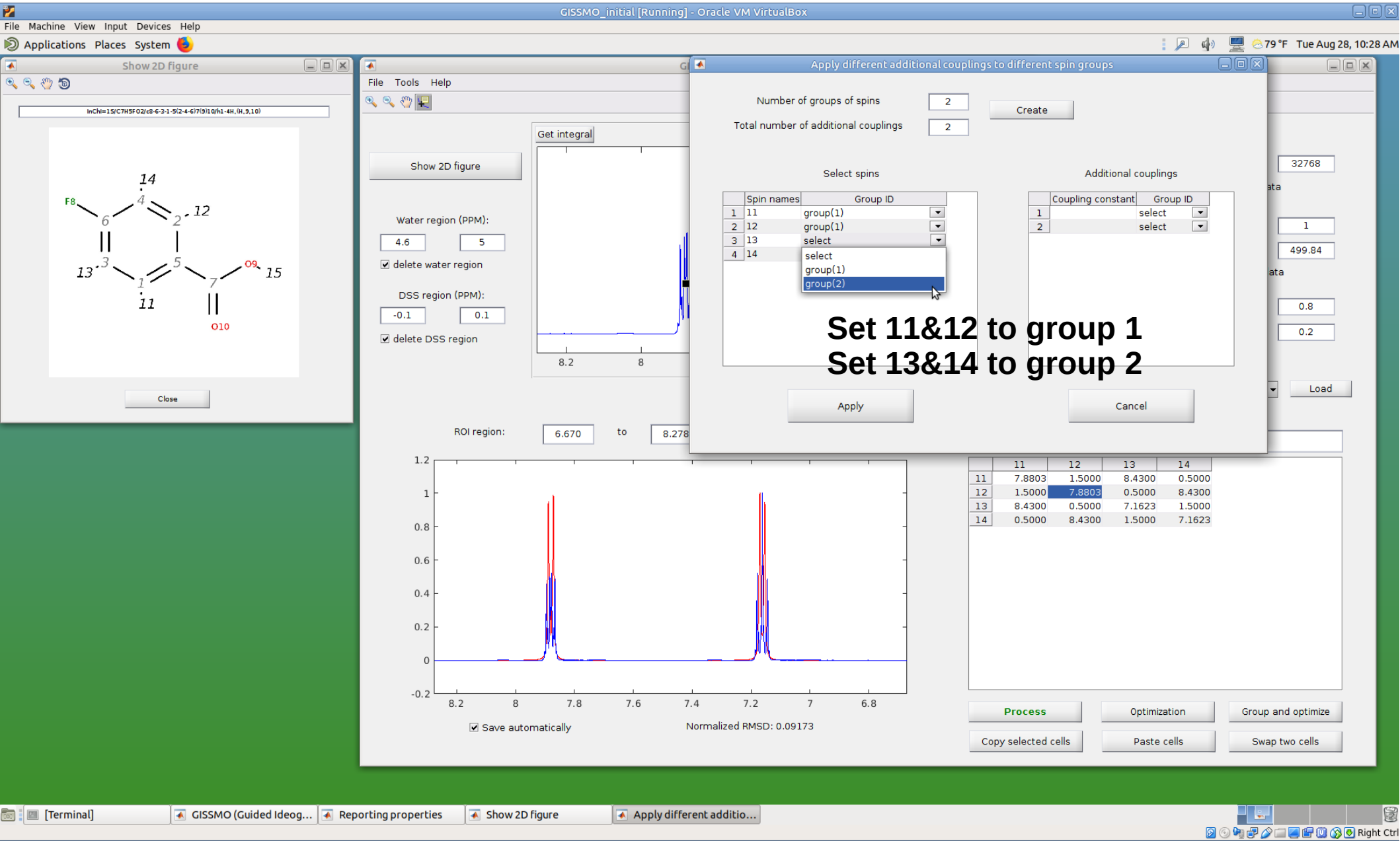
[Terminal] | GISSMO (Guided Ideog... | Reporting properties | Show 2D figure

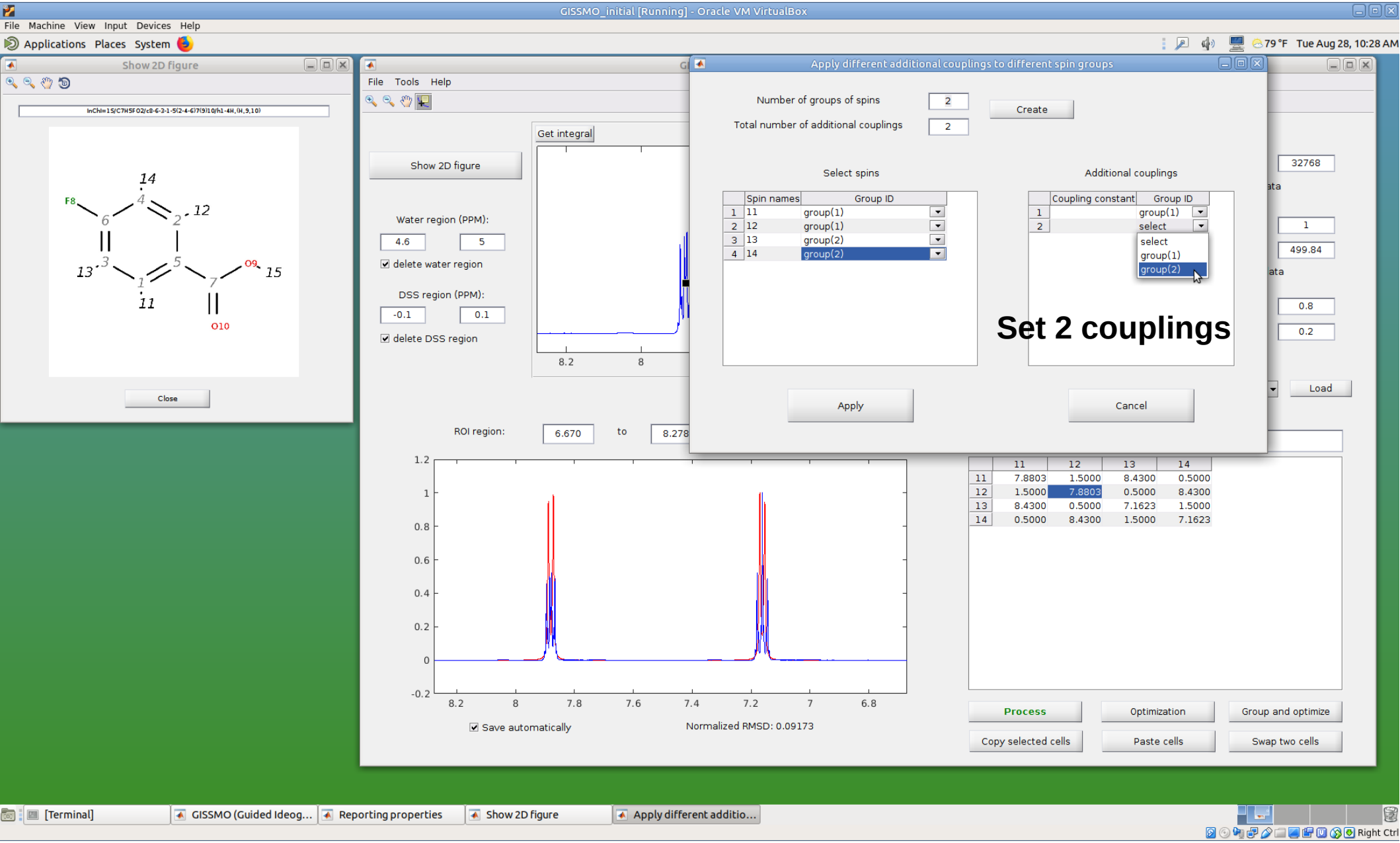
Right Ctrl

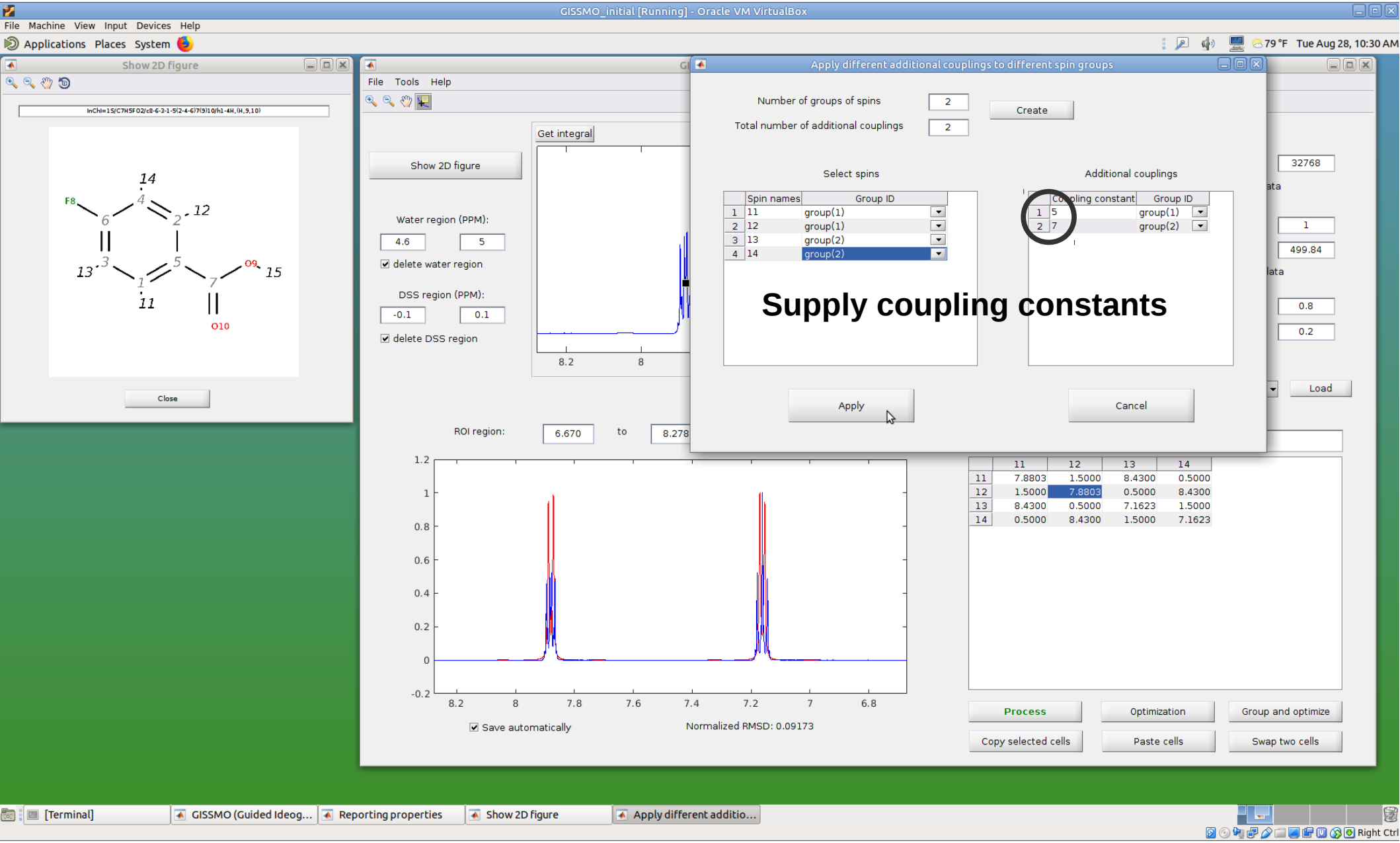

GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
79 °F Tue Aug 28, 10:27 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - 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
full experimental spectrum
Reset inte...
PPM: 7.8803
Amp: 0.257
PPM is copied to clipboard
8.2 8 7.8 7.6 7.4 7.2 7 6.8
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
Fluorine supplies additional couplings
ROI region:
6.670
to
8.278
get ROI from exp. spectrum
1.2 1 0.8 0.6 0.4 0.2 0 -0.2
8.2 8 7.8 7.6 7.4 7.2 7 6.8
Save automatically
Normalized RMSD: 0.09173
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 1.5000 8.4300 0.5000
12 1.5000 7.8803 0.5000 8.4300
13 8.4300 0.5000 7.1623 1.5000
14 0.5000 8.4300 1.5000 7.1623
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Right Ctrl

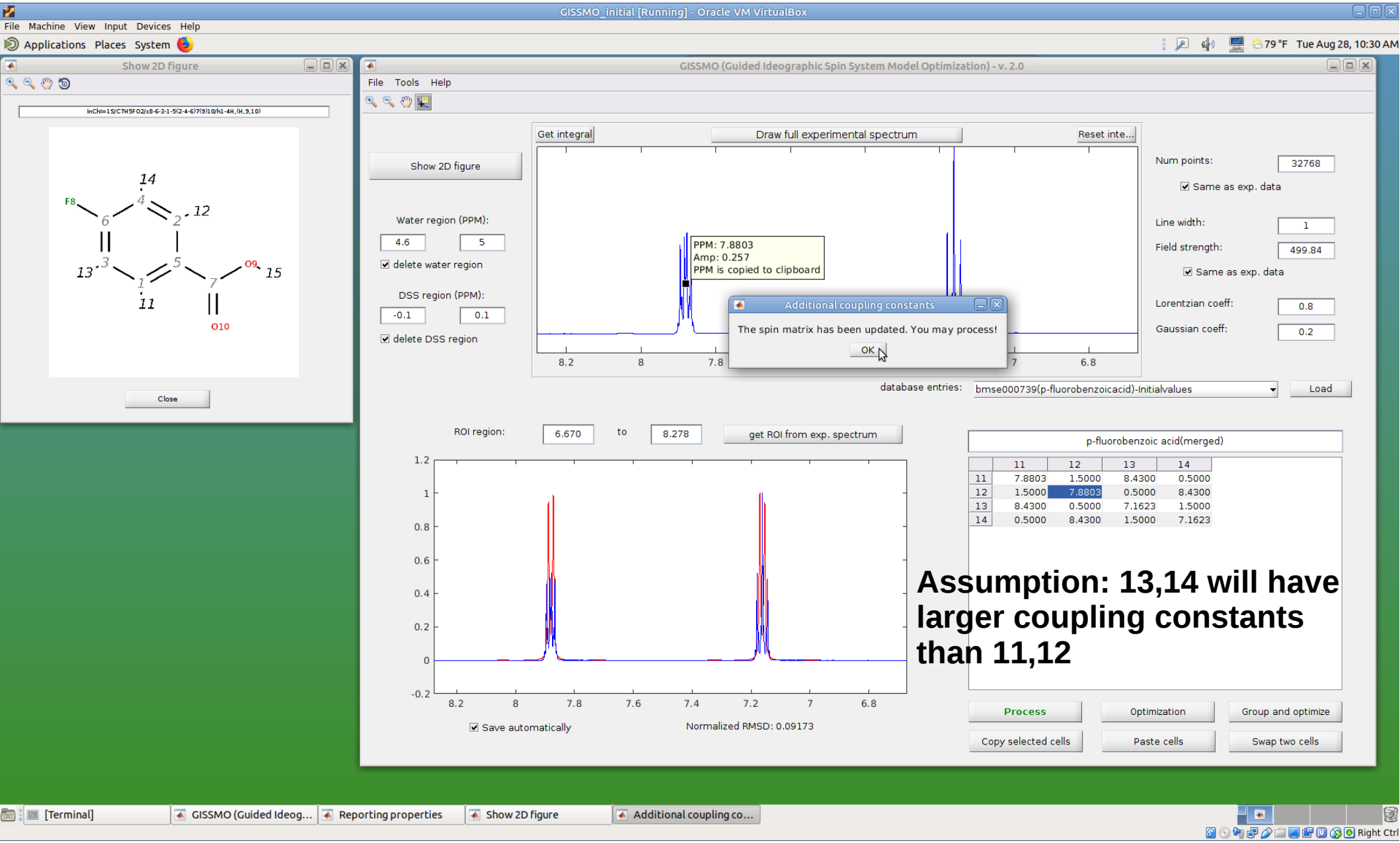


	11	12	13	14
11	7.8803	1.5000	8.4300	0.5000
12	1.5000	7.8803	0.5000	8.4300
13	8.4300	0.5000	7.1623	1.5000
14	0.5000	8.4300	1.5000	7.1623


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
79 °F Tue Aug 28, 10:28 AM
Show 2D figure
Close
File Tools Help
Get integral
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
ROI region:
6.670
to
8.278
Save automatically
Normalized RMSD: 0.09173
Apply different additional couplings to different spin groups
Number of groups of spins
2
Total number of additional couplings
2
Create
Select spins
Additional couplings
Spin names
Group ID
Coupling constant
select
group(1)
group(2)
Set 11&12 to group 1
Set 13&14 to group 2
Apply
Cancel
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
Load
[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
79 °F Tue Aug 28, 10:28 AM
Show 2D figure
Close
File Tools Help
Show 2D figure
Get integral
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
ROI region:
6.670
to
8.278
Save automatically
Normalized RMSD: 0.09173
Apply different additional couplings to different spin groups
Number of groups of spins
2
Total number of additional couplings
2
Create
Select spins
Spin names
Group ID
11 group(1)
12 group(1)
13 group(2)
14 group(2)
Additional couplings
Coupling constant
Group ID
select
group(1)
group(2)
Set 2 couplings
Apply
Cancel
32768
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
79 °F Tue Aug 28, 10:30 AM
Show 2D figure
Close
File Tools Help
Get integral
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
ROI region:
6.670
to
8.278
Save automatically
Normalized RMSD: 0.09173
Apply different additional couplings to different spin groups
Number of groups of spins
2
Total number of additional couplings
2
Create
Select spins
Spin names
Group ID
11 group(1)
12 group(1)
13 group(2)
14 group(2)
Additional couplings
Coupling constant
Group ID
5 group(1)
7 group(2)
Supply coupling constants
Apply
Cancel
32768
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
79 °F Tue Aug 28, 10:30 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 7.8803
Amp: 0.257
PPM is copied to clipboard
8.2
8
7.8
7
6.8
Additional coupling constants
The spin matrix has been updated. You may process!
OK
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
6.670
to
8.278
get ROI from exp. spectrum
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
8.2
8
7.8
7.6
7.4
7.2
7
6.8
Save automatically
Normalized RMSD: 0.09173
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 1.5000 8.4300 0.5000
12 1.5000 7.8803 0.5000 8.4300
13 8.4300 0.5000 7.1623 1.5000
14 0.5000 8.4300 1.5000 7.1623
Assumption: 13,14 will have larger coupling constants than 11,12
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

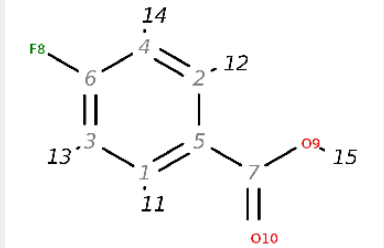
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:30 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

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

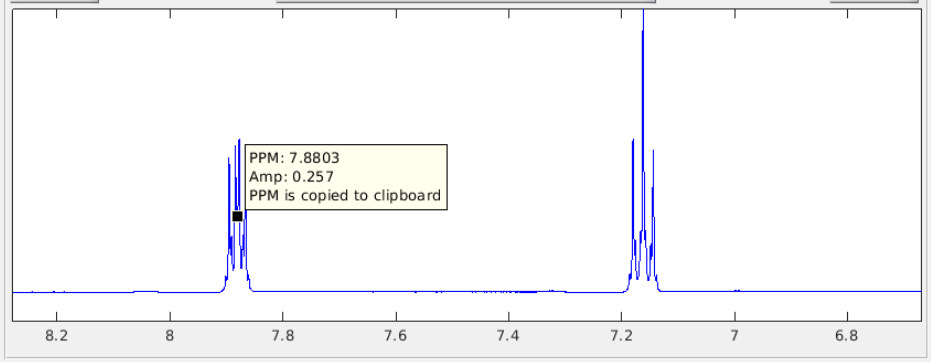
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

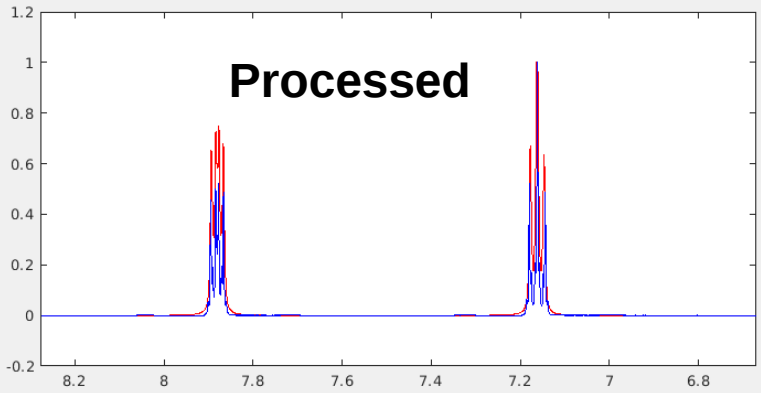
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 6.670 to 8.278 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.05852

p-fluorobenzoic acid(merged)

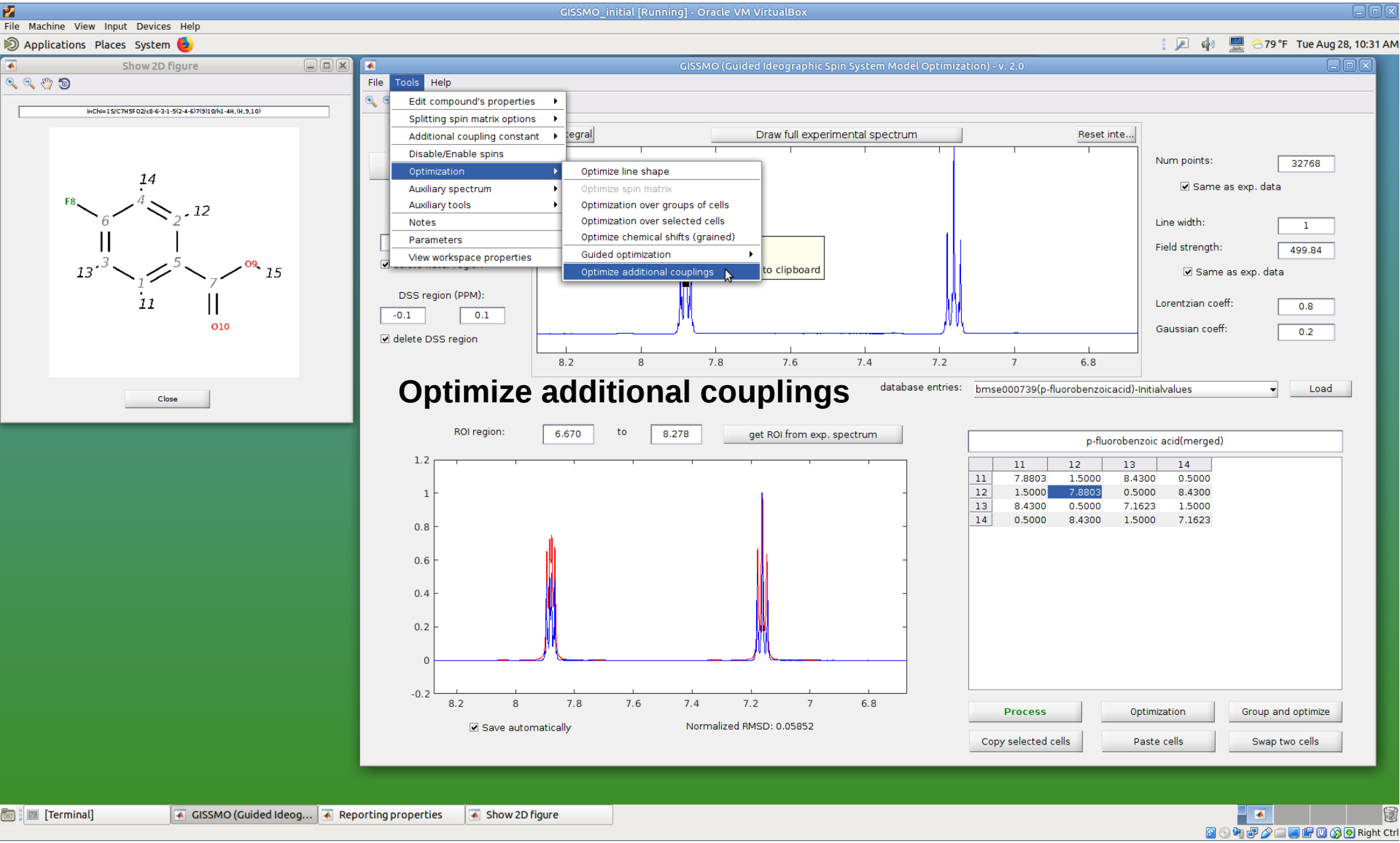
	11	12	13	14
11	7.8803	1.5000	8.4300	0.5000
12	1.5000	7.8803	0.5000	8.4300
13	8.4300	0.5000	7.1623	1.5000
14	0.5000	8.4300	1.5000	7.1623

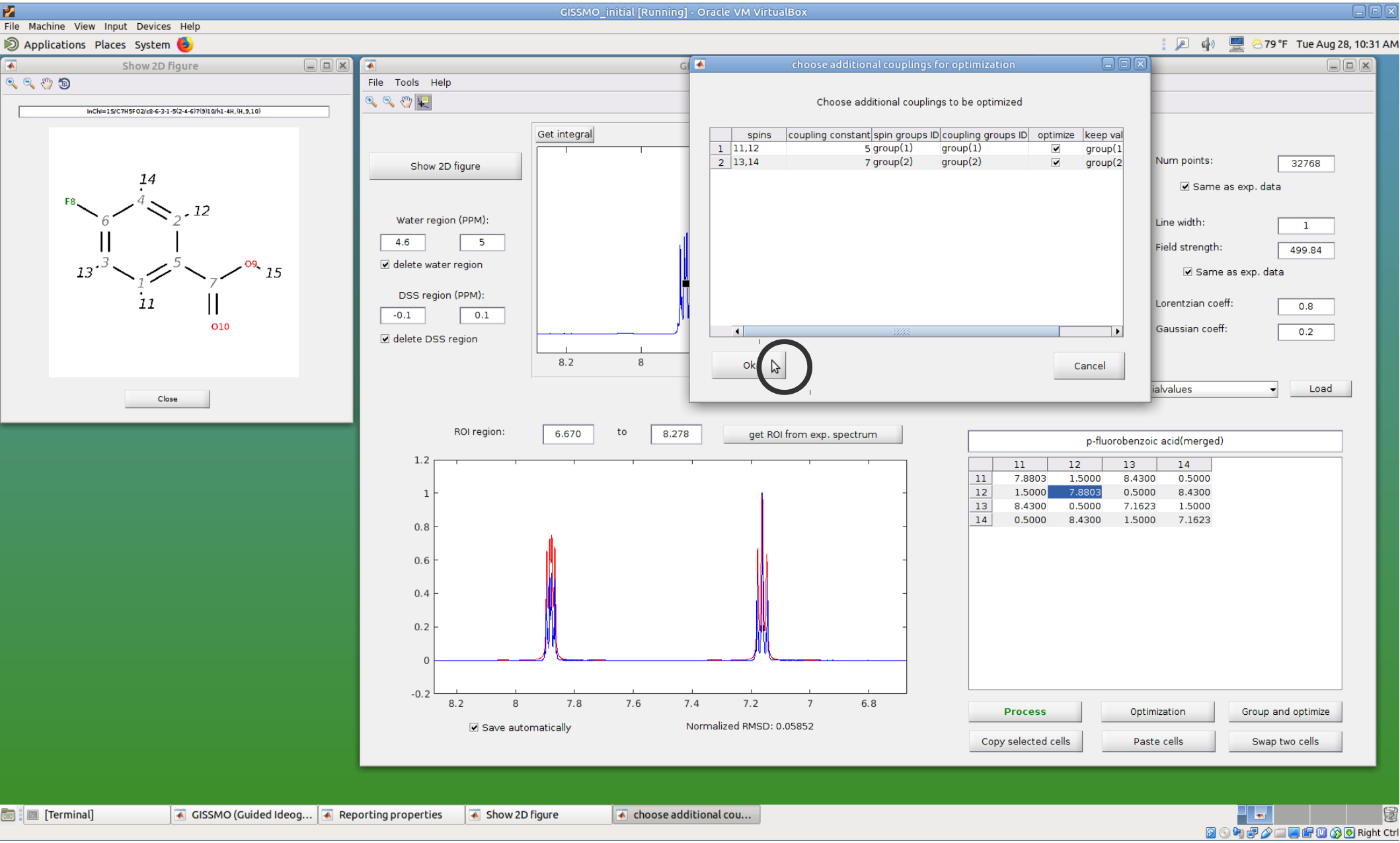
Process | Optimization | Group and optimize

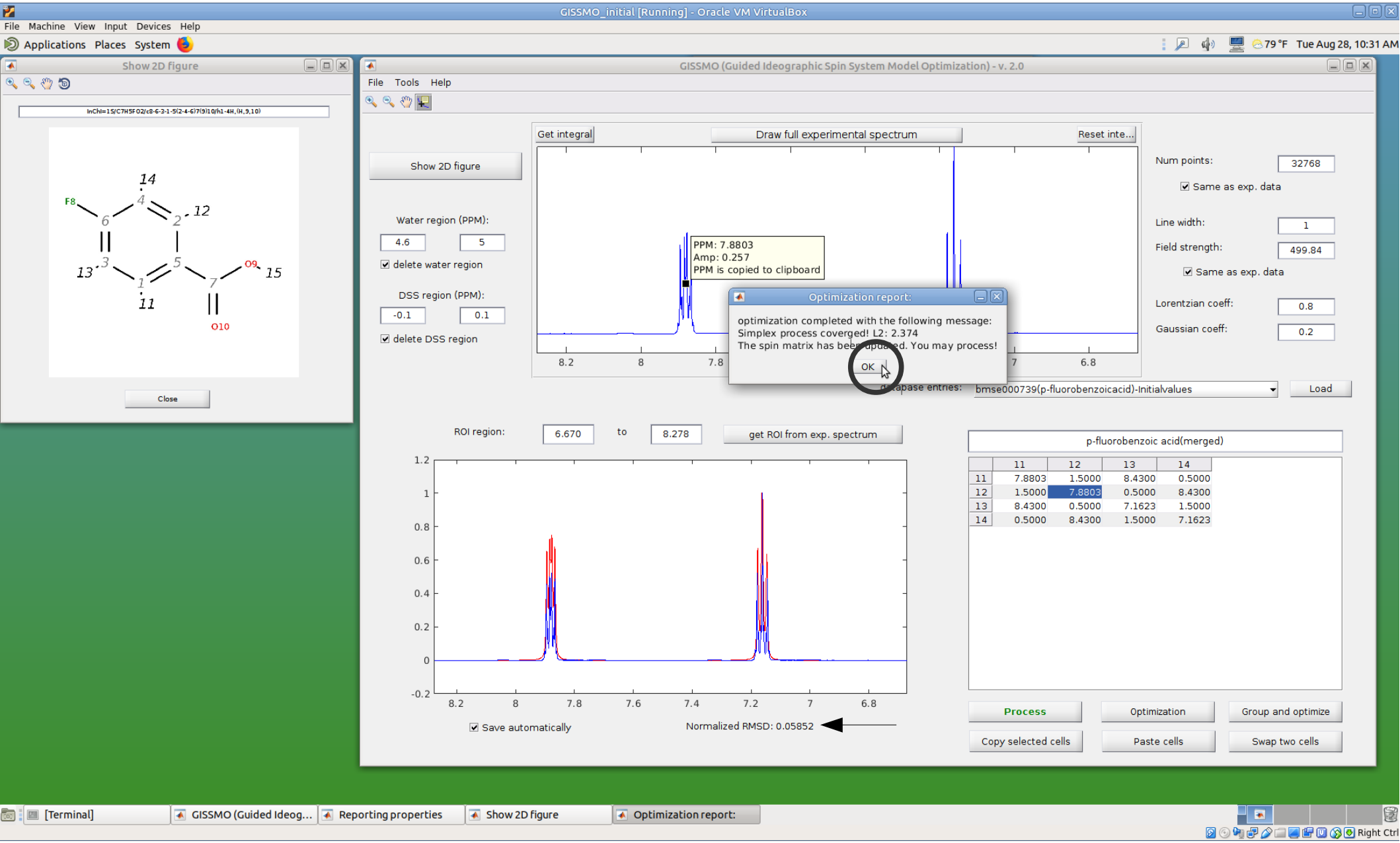
Copy selected cells | Paste cells | Swap two cells

[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
79 °F Tue Aug 28, 10:31 AM
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 inte...
to clipboard
Num points: 32768
Same as exp. data
Line width: 1
Field strength: 499.84
Same as exp. data
Lorentzian coeff: 0.8
Gaussian coeff: 0.2
DSS region (PPM):
-0.1
0.1
delete DSS region
Optimize additional couplings
database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region: 6.670 to 8.278
get ROI from exp. spectrum
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 1.5000 8.4300 0.5000
12 1.5000 7.8803 0.5000 8.4300
13 8.4300 0.5000 7.1623 1.5000
14 0.5000 8.4300 1.5000 7.1623
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
Save automatically
Normalized RMSD: 0.05852
[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
79 °F Tue Aug 28, 10:31 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
File Tools Help
Get integral
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
8.2
8
choose additional couplings for optimization
Choose additional couplings to be optimized
spins
coupling constant
spin groups ID
coupling groups ID
optimize
keep val
1 11,12 5 group(1) group(1) group(1
2 13,14 7 group(2) group(2) group(2
Ok
Cancel
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
ialvalues
Load
ROI region:
6.670
to
8.278
get ROI from exp. spectrum
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
8.2
8
7.8
7.6
7.4
7.2
7
6.8
Save automatically
Normalized RMSD: 0.05852
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 1.5000 8.4300 0.5000
12 1.5000 7.8803 0.5000 8.4300
13 8.4300 0.5000 7.1623 1.5000
14 0.5000 8.4300 1.5000 7.1623
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
79 °F Tue Aug 28, 10:31 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
PPM: 7.8803
Amp: 0.257
PPM is copied to clipboard
8.2
8
7.8
7
6.8
Optimization report:
optimization completed with the following message:
Simplex process coverged! L2: 2.374
The spin matrix has been updated. You may process!
OK
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
6.670
to
8.278
get ROI from exp. spectrum
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
8.2
8
7.8
7.6
7.4
7.2
7
6.8
Save automatically
Normalized RMSD: 0.05852
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 1.5000 8.4300 0.5000
12 1.5000 7.8803 0.5000 8.4300
13 8.4300 0.5000 7.1623 1.5000
14 0.5000 8.4300 1.5000 7.1623
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

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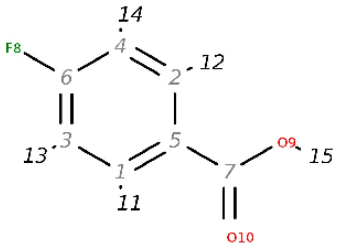
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

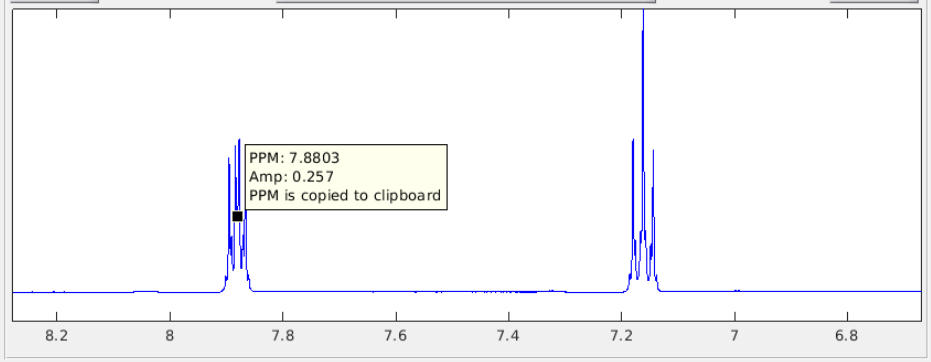
Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

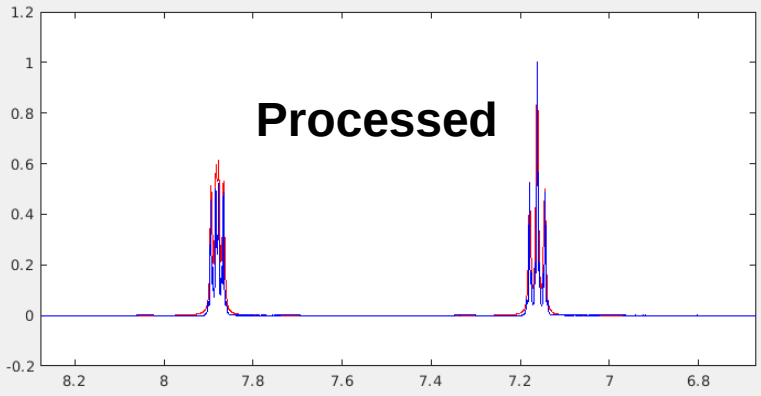
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 6.670 to 8.278 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04130

p-fluorobenzoic acid(merged)

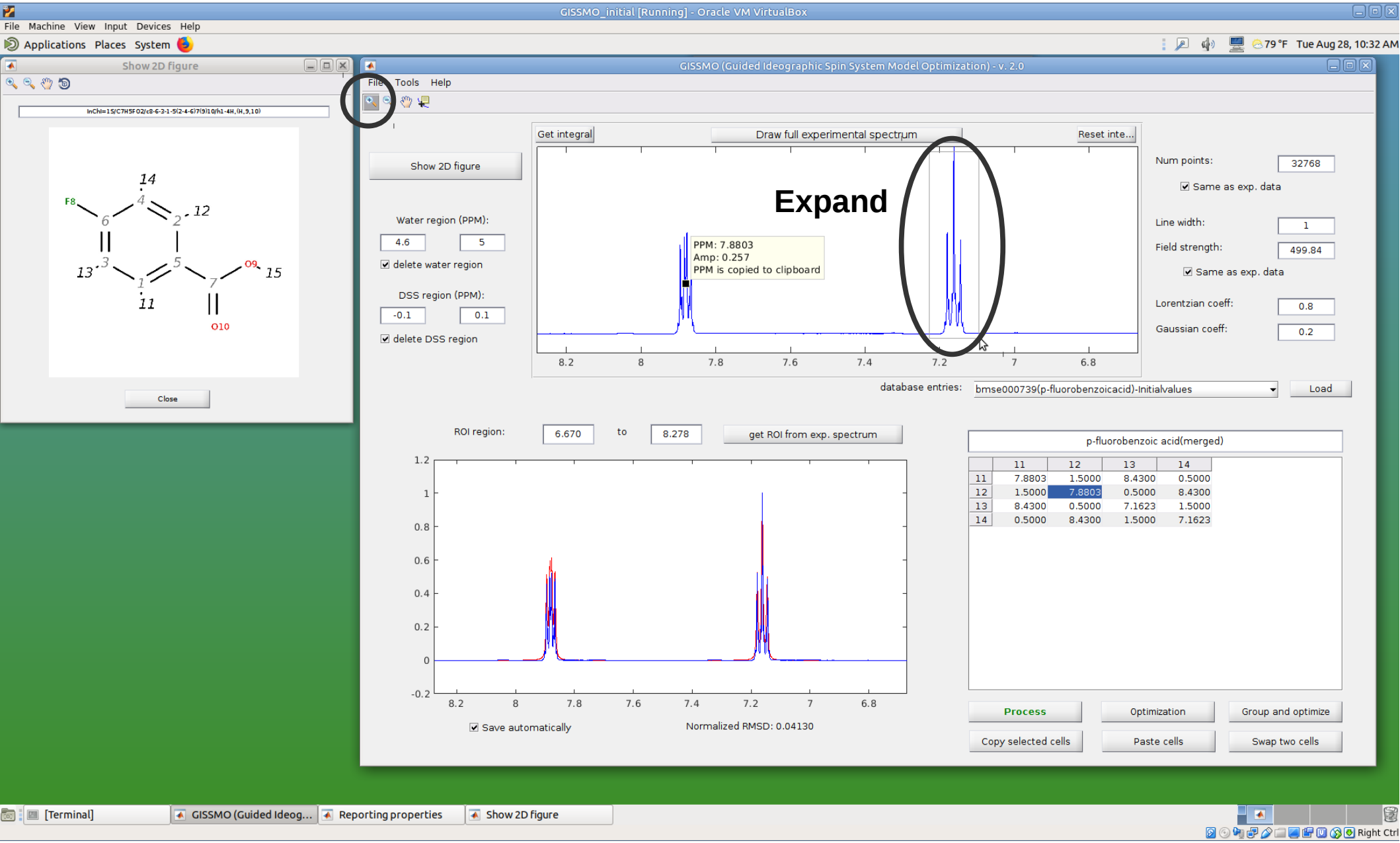
	11	12	13	14
11	7.8803	1.5000	8.4300	0.5000
12	1.5000	7.8803	0.5000	8.4300
13	8.4300	0.5000	7.1623	1.5000
14	0.5000	8.4300	1.5000	7.1623

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
79 °F Tue Aug 28, 10:32 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Get integral
Draw full experimental spectrum
Reset inte...
Expand
PPM: 7.8803
Amp: 0.257
PPM is copied to clipboard
8.2
8
7.8
7.6
7.4
7.2
7
6.8
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
6.670
to
8.278
get ROI from exp. spectrum
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
8.2
8
7.8
7.6
7.4
7.2
7
6.8
Save automatically
Normalized RMSD: 0.04130
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 1.5000 8.4300 0.5000
12 1.5000 7.8803 0.5000 8.4300
13 8.4300 0.5000 7.1623 1.5000
14 0.5000 8.4300 1.5000 7.1623
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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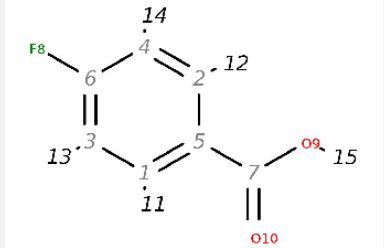
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)

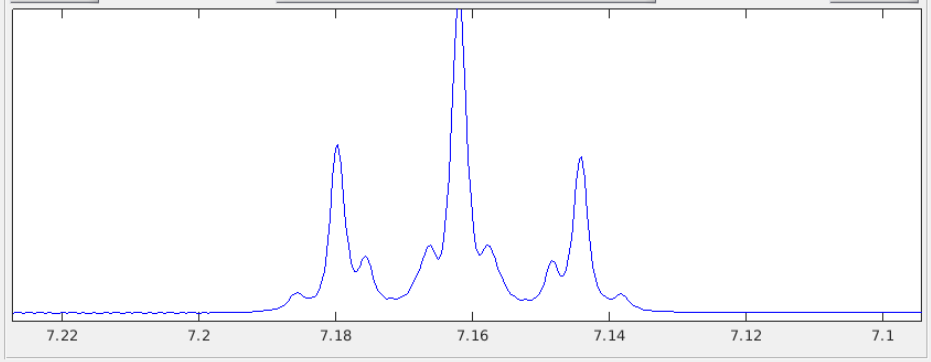


Close

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

File Tools Help

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



Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region

Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

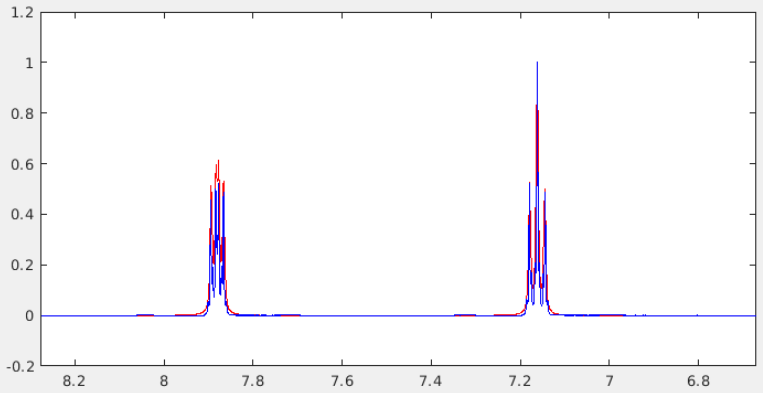
Lorentzian coeff: 0.8

Gaussian coeff: 0.2

Get ROI ...;Process

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 6.670 to 8.278 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04130

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	1.5000	8.4300	0.5000
12	1.5000	7.8803	0.5000	8.4300
13	8.4300	0.5000	7.1623	1.5000
14	0.5000	8.4300	1.5000	7.1623

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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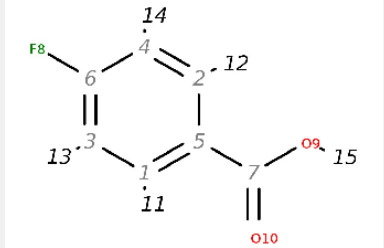
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

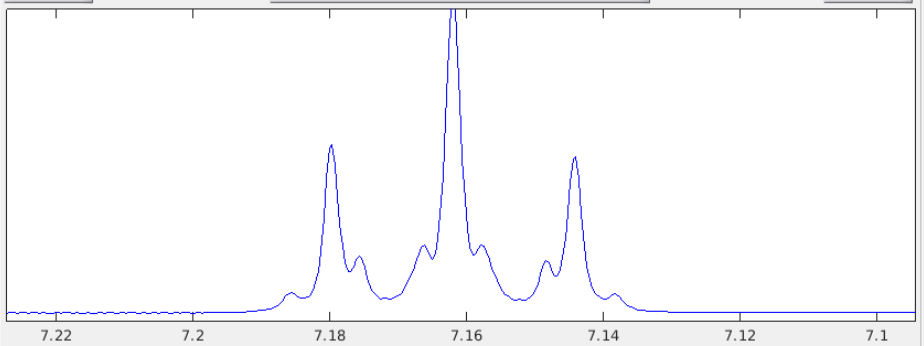
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

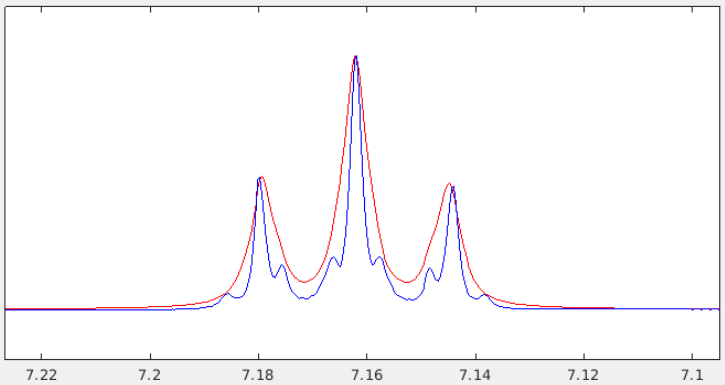
Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04130

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	1.5000	8.4300	0.5000
12	1.5000	7.8803	0.5000	8.4300
13	8.4300	0.5000	7.1623	1.5000
14	0.5000	8.4300	1.5000	7.1623

Linewidths look broad

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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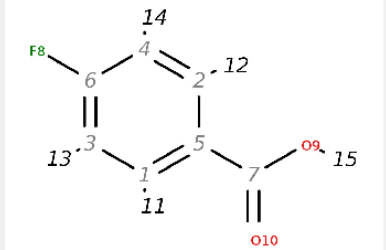
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

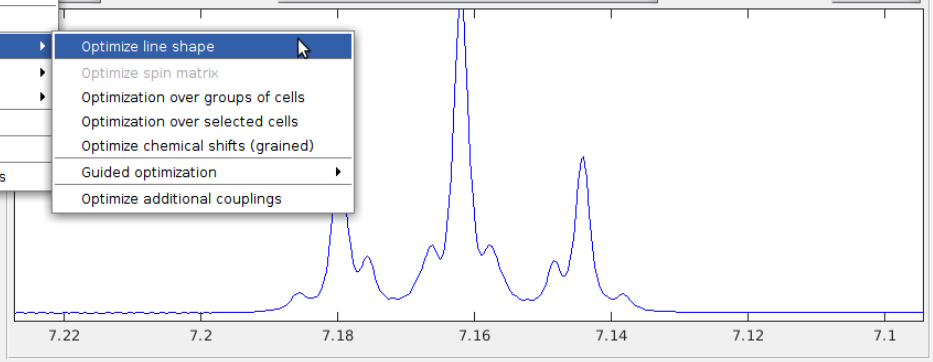
Edit compound's properties
Splitting spin matrix options
Additional coupling constant
Disable/Enable spins
Optimization
Auxiliary spectrum
Auxiliary tools
Notes
Parameters
View workspace properties

Optimize line shape
Optimize spin matrix
Optimization over groups of cells
Optimization over selected cells
Optimize chemical shifts (grained)
Guided optimization
Optimize additional couplings

egral

Draw full experimental spectrum

Reset inte...



Num points: 32768

Same as exp. data

Line width: 1

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.8

Gaussian coeff: 0.2

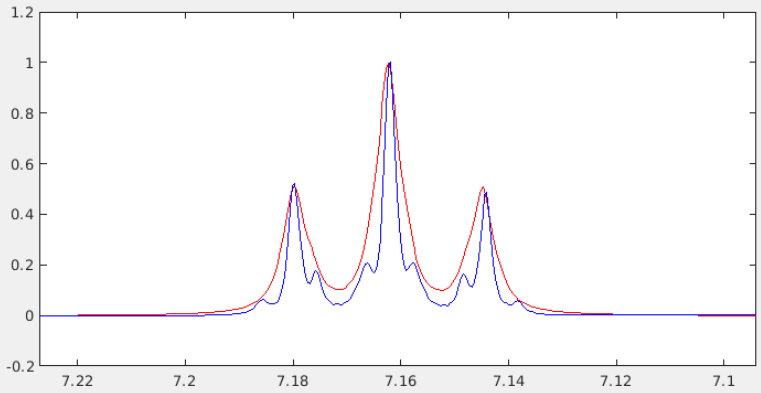
DSS region (PPM):

-0.1 0.1

delete DSS region

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04420

p-fluorobenzoic acid(merged)

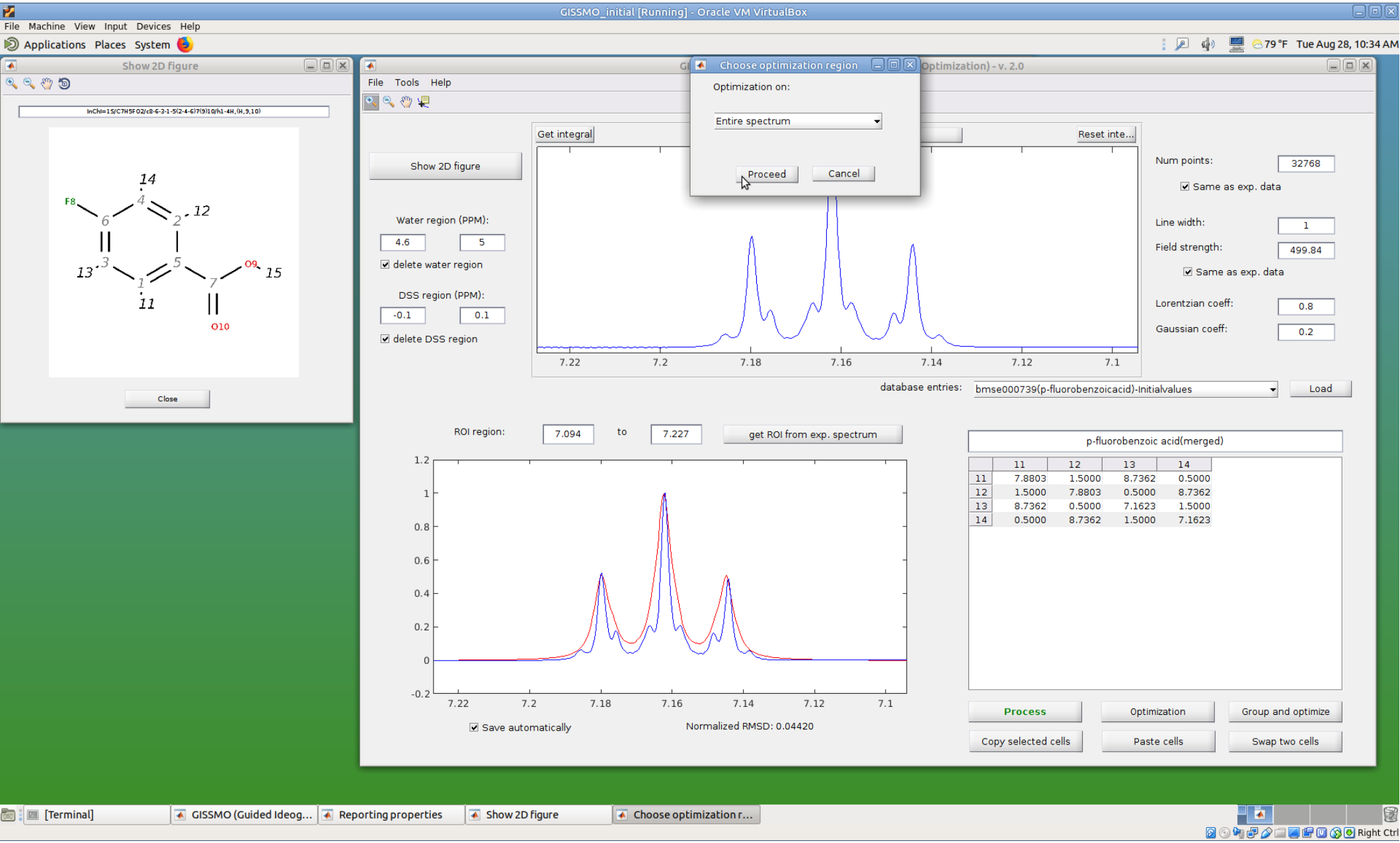
	11	12	13	14
11	7.8803	1.5000	8.7362	0.5000
12	1.5000	7.8803	0.5000	8.7362
13	8.7362	0.5000	7.1623	1.5000
14	0.5000	8.7362	1.5000	7.1623

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
79 °F Tue Aug 28, 10:34 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
Choose optimization region
Optimization on:
Entire spectrum
Proceed
Cancel
File Tools Help
Optimization) - v. 2.0
Get integral
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
7.22
7.2
7.18
7.16
7.14
7.12
7.1
Num points:
32768
Same as exp. data
Line width:
1
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.8
Gaussian coeff:
0.2
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
7.094
to
7.227
get ROI from exp. spectrum
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
Save automatically
Normalized RMSD: 0.04420
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 1.5000 8.7362 0.5000
12 1.5000 7.8803 0.5000 8.7362
13 8.7362 0.5000 7.1623 1.5000
14 0.5000 8.7362 1.5000 7.1623
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Choose optimization r...
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

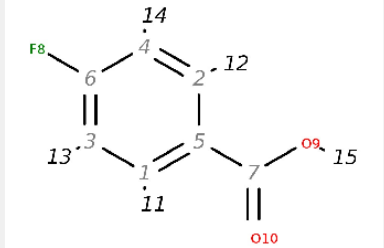
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:34 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

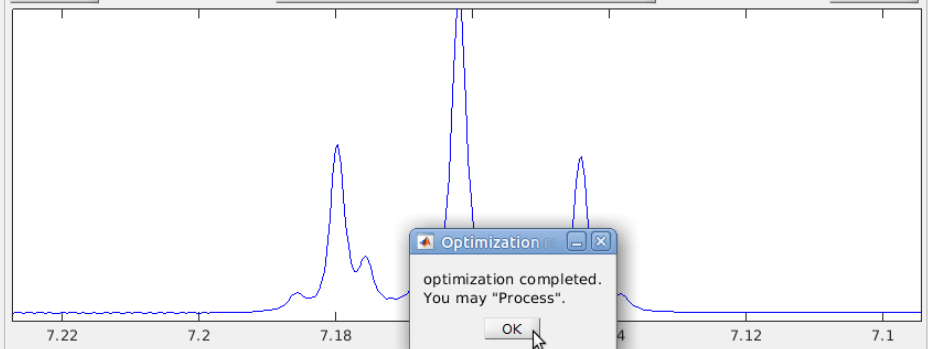
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Optimization

optimization completed.
You may "Process".

OK

Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

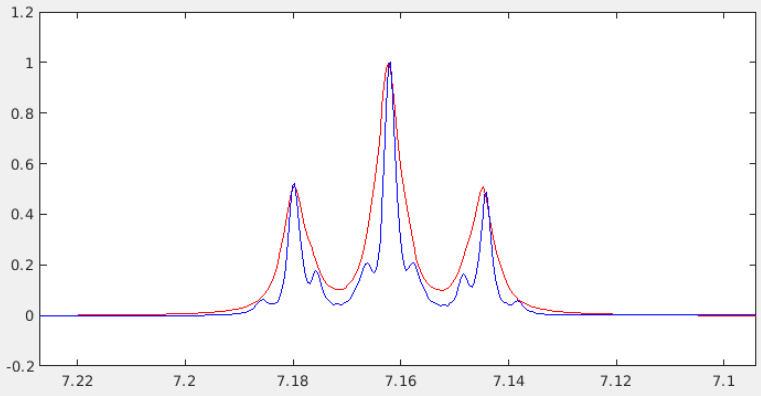
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.04420

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	1.5000	8.7362	0.5000
12	1.5000	7.8803	0.5000	8.7362
13	8.7362	0.5000	7.1623	1.5000
14	0.5000	8.7362	1.5000	7.1623

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

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File Machine View Input Devices Help

Applications Places System

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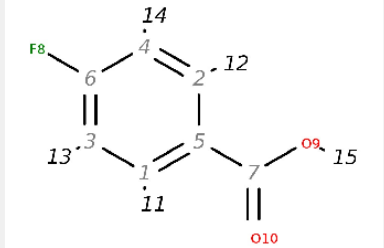
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

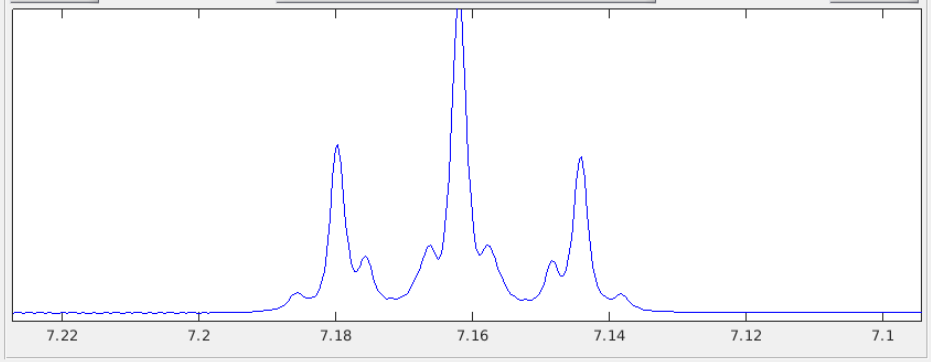
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

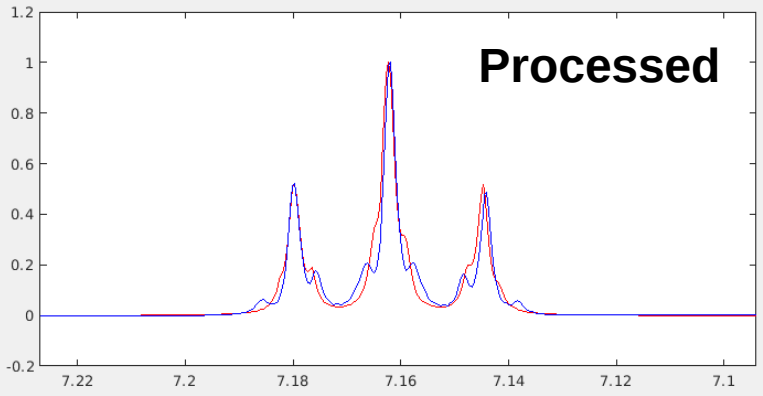
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.02289

p-fluorobenzoic acid(merged)

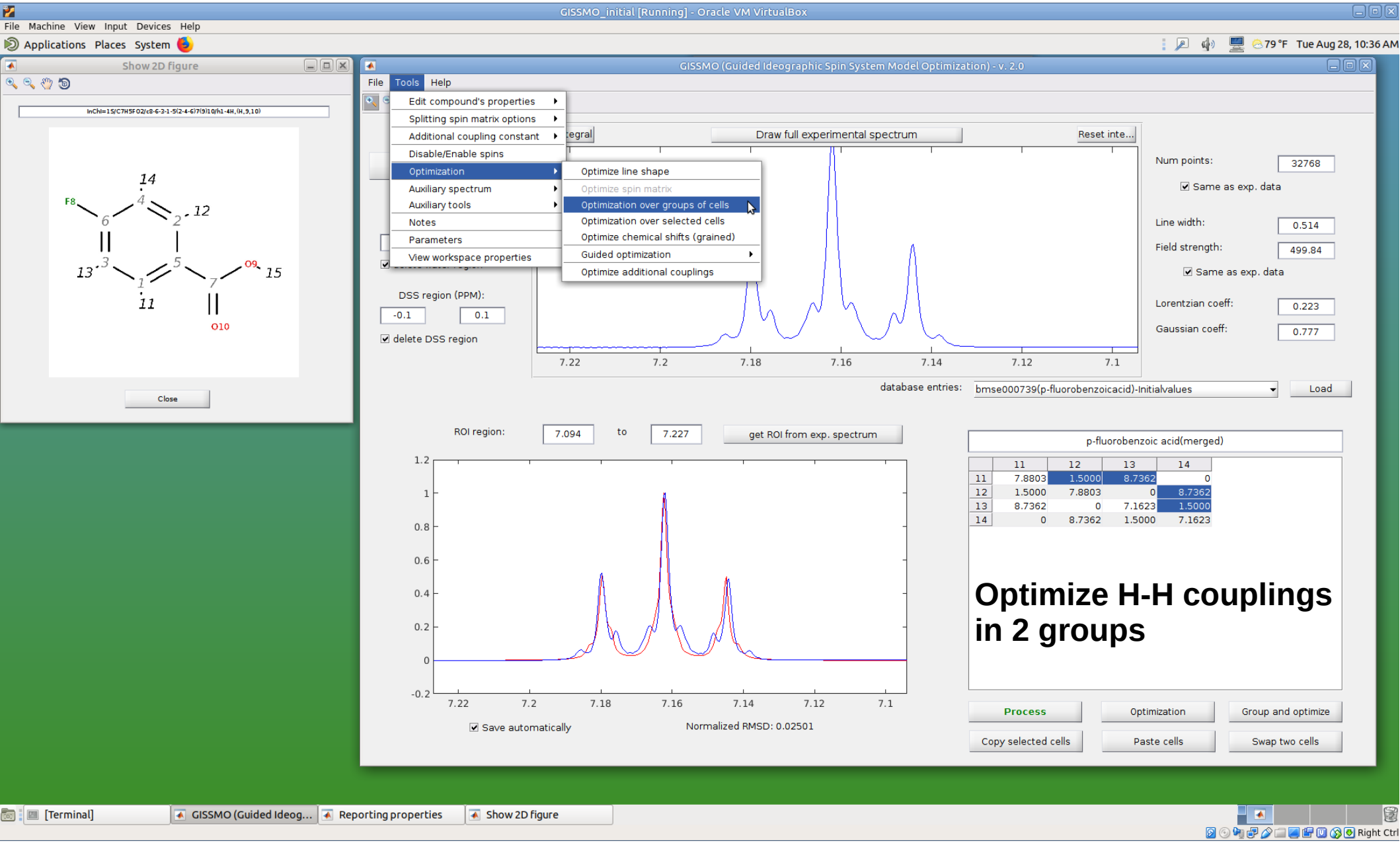
	11	12	13	14
11	7.8803	1.5000	8.7362	0
12	1.5000	7.8803	0	8.7362
13	8.7362	0.5000	7.1623	1.5000
14	0	8.7362	1.5000	7.1623

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
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 inte...
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
Same as exp. data
Line width:
0.514
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.223
Gaussian coeff:
0.777
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
7.094
to
7.227
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.02501
p-fluorobenzoic acid(merged)
Optimize H-H couplings in 2 groups
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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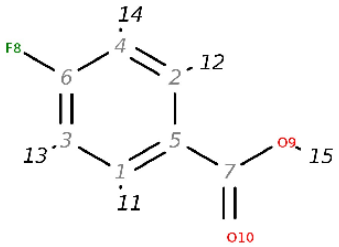
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset inte...

Group cells for optimization

Group all cells in one group

cell spin nam...	group id
11-12	Group(1)
11-13	Group(2)
12-14	Group(2)
13-14	choose

choose
Group(1)
Group(2)
Group(3)
Group(4)

Setup 2 groups

OK Cancel

Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

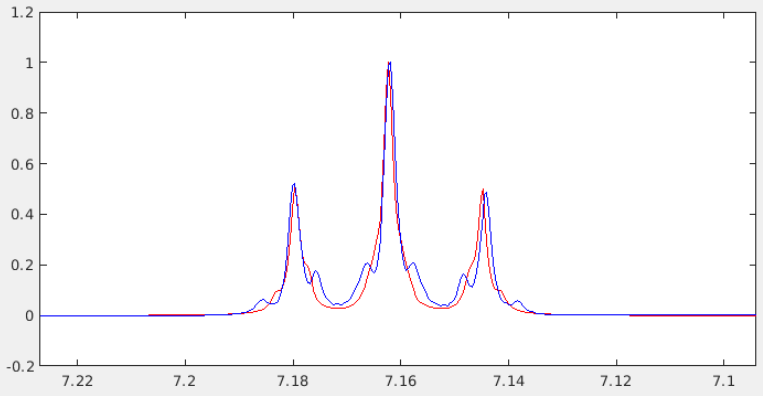
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.02501

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	1.5000	8.7362	0
12	1.5000	7.8803	0	8.7362
13	8.7362	0	7.1623	1.5000
14	0	8.7362	1.5000	7.1623

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Group cells for optimiz...

Right Ctrl

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File Machine View Input Devices Help

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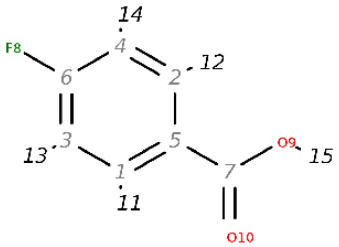
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral

Reset inte...

Group cells for optimization

Group all cells in one group

cell spin nam...	group id
11-12	Group(1)
11-13	Group(2)
12-14	Group(2)
13-14	Group(1)

OK Cancel

Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

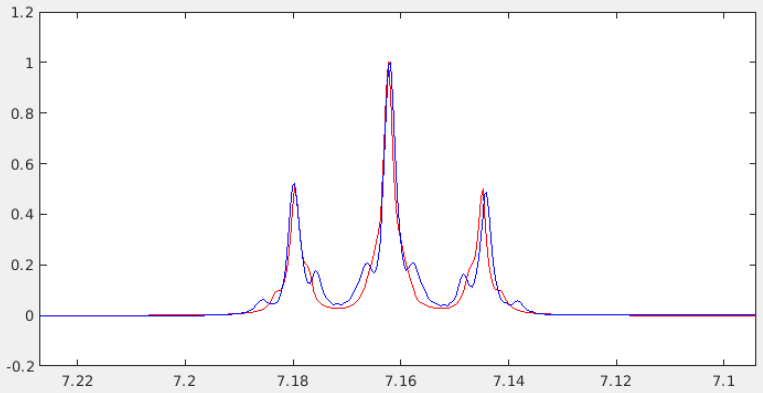
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.02501

p-fluorobenzoic acid(merged)

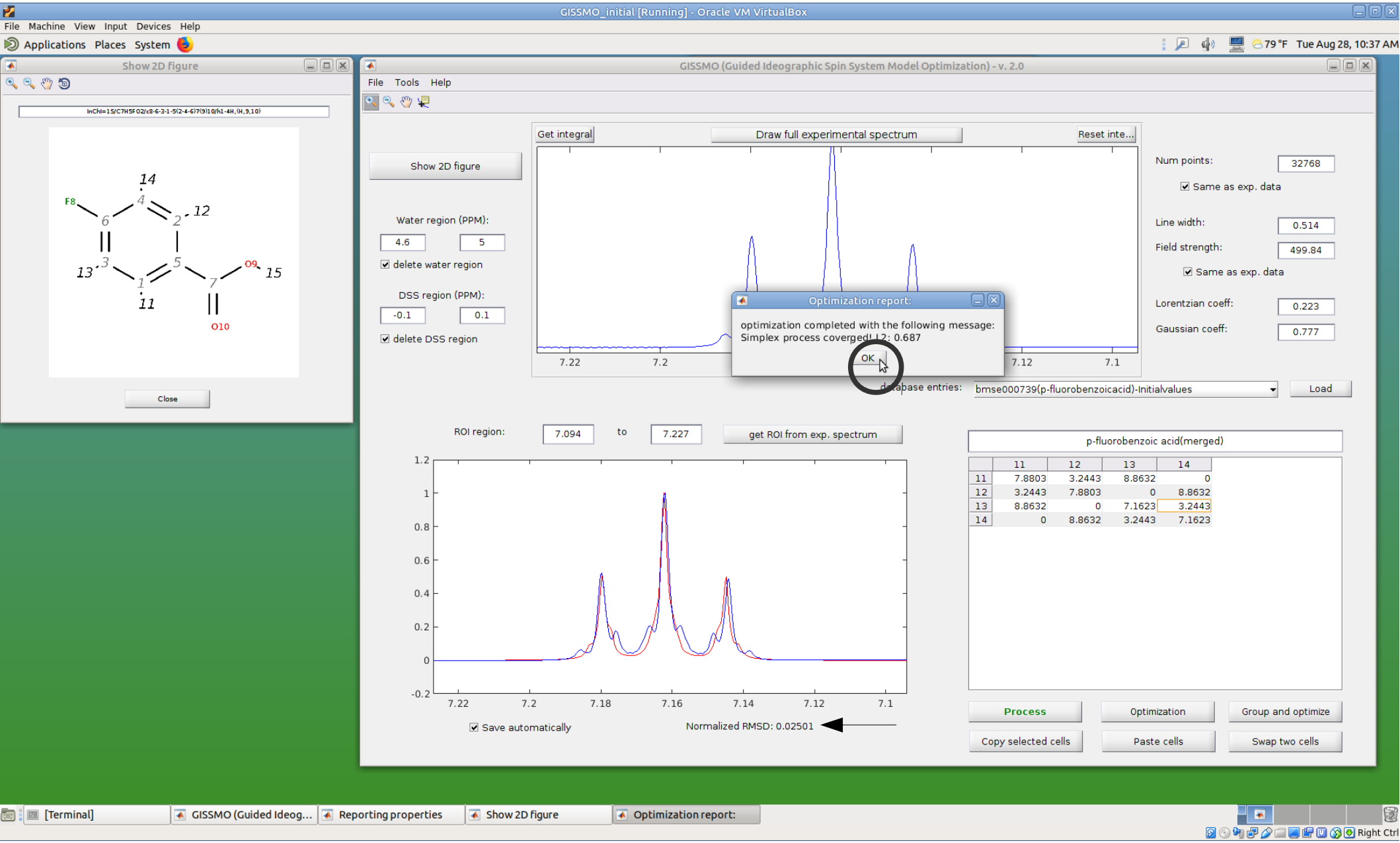
	11	12	13	14
11	7.8803	1.5000	8.7362	0
12	1.5000	7.8803	0	8.7362
13	8.7362	0	7.1623	1.5000
14	0	8.7362	1.5000	7.1623

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Group cells for optimiz...

Right Ctrl



	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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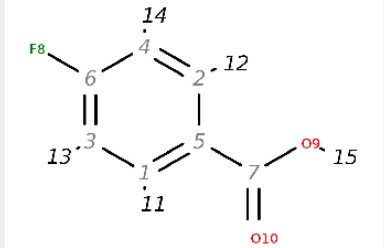
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

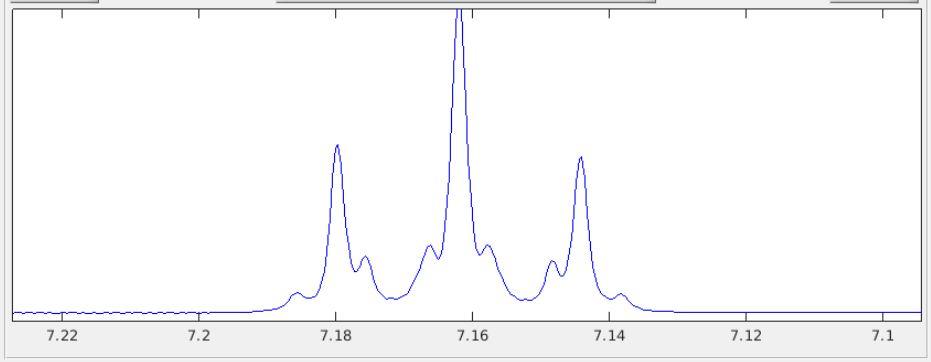
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

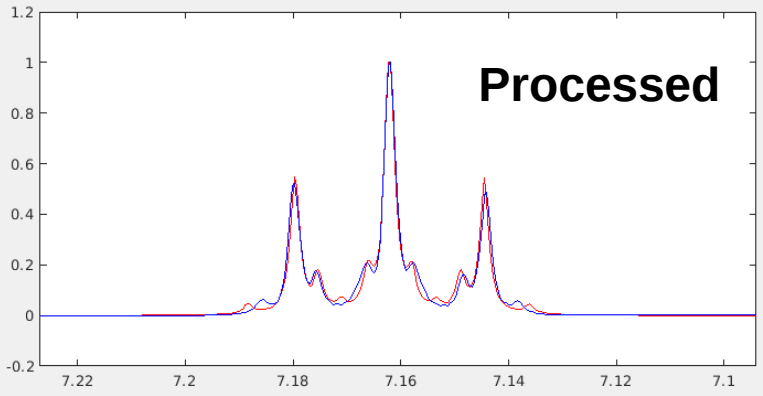
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01596

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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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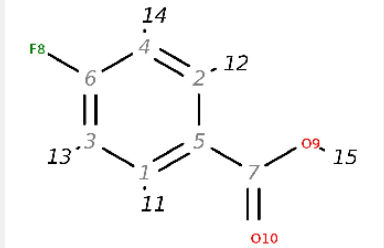
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

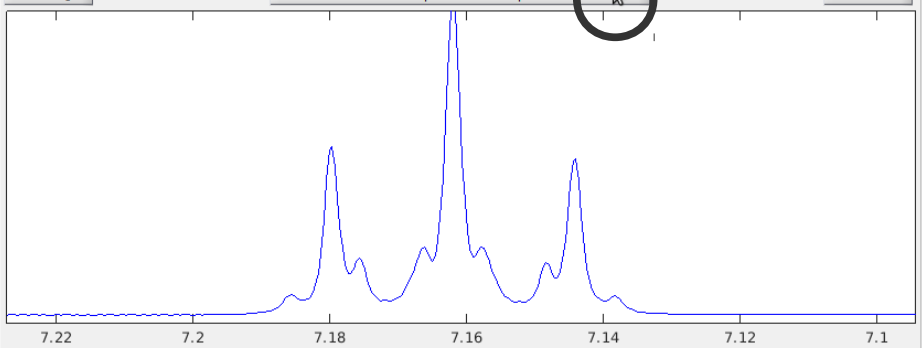
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

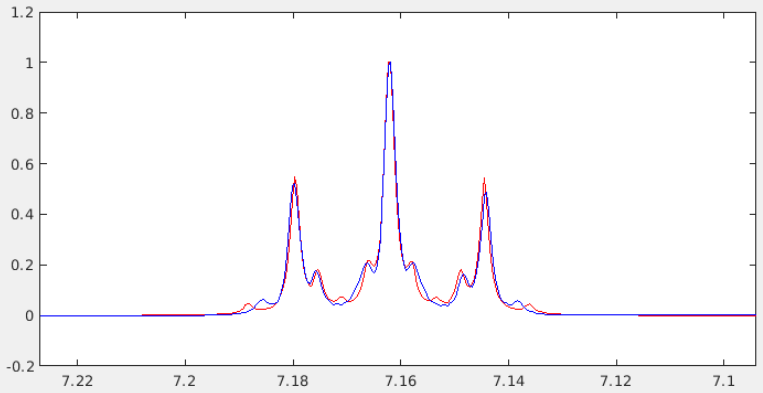
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01596

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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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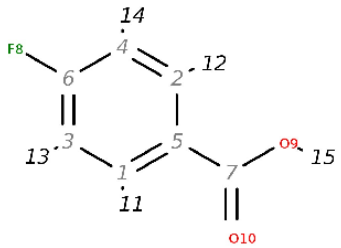
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

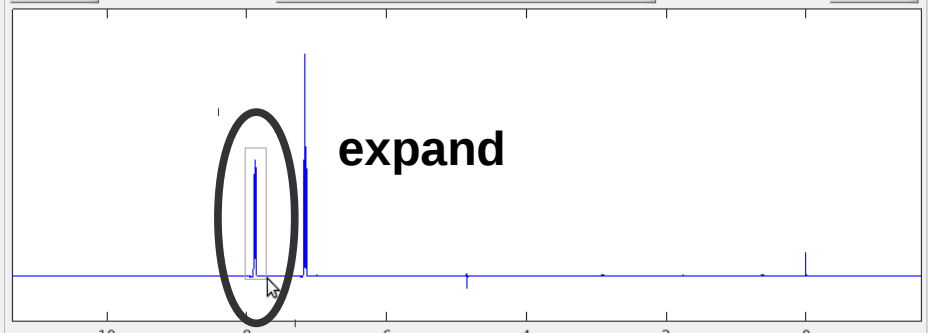
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

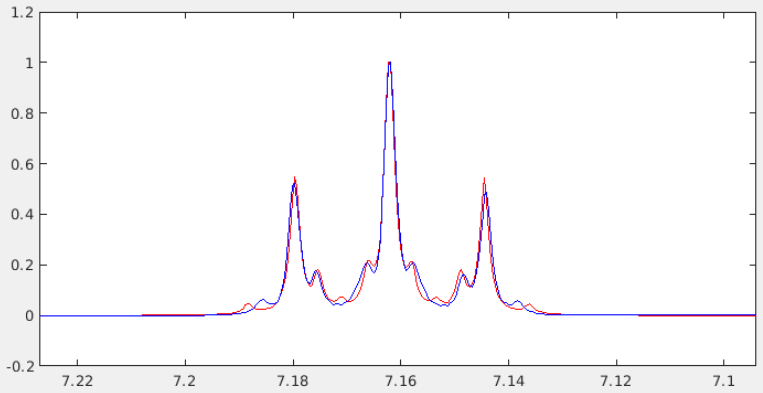
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.094 to 7.227 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01596

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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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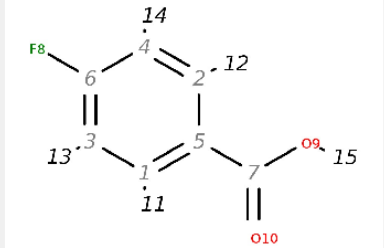
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

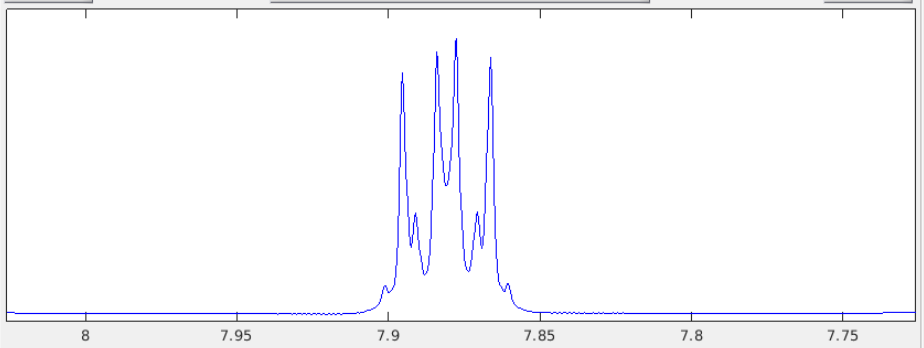
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

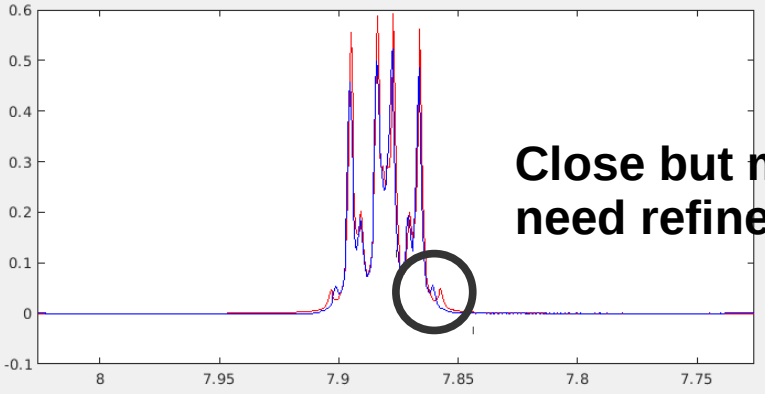
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.726 to 8.026 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01596

Close but may need refinement

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

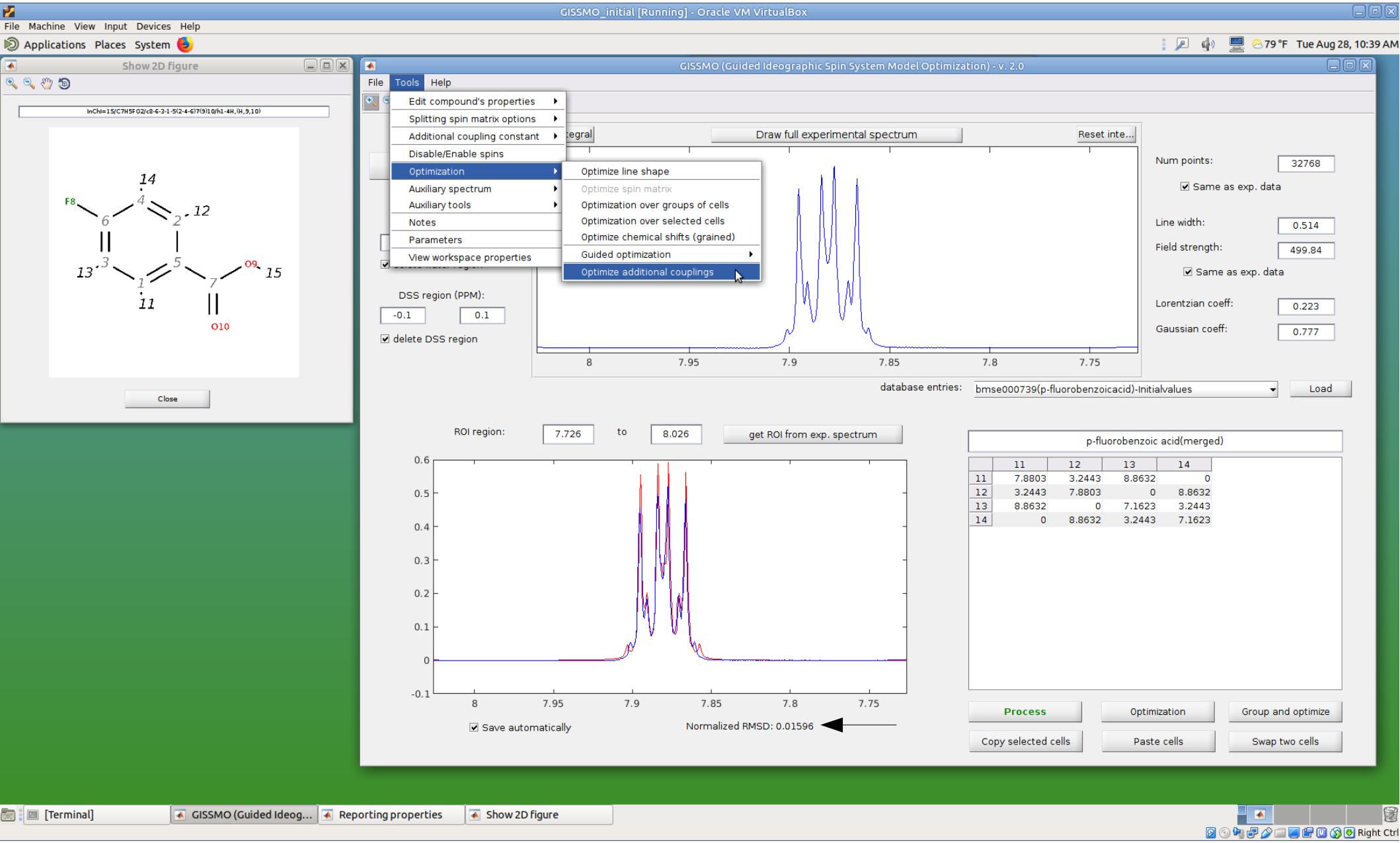
Next 15 slides show attempts to refine. Watch RMSD

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/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
O9
O10
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 inte...
Num points: 32768
Same as exp. data
Line width: 0.514
Field strength: 499.84
Same as exp. data
Lorentzian coeff: 0.223
Gaussian coeff: 0.777
DSS region (PPM):
-0.1
0.1
delete DSS region
database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region: 7.726 to 8.026 get ROI from exp. spectrum
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 3.2443 8.8632 0
12 3.2443 7.8803 0 8.8632
13 8.8632 0 7.1623 3.2443
14 0 8.8632 3.2443 7.1623
Save automatically
Normalized RMSD: 0.01596
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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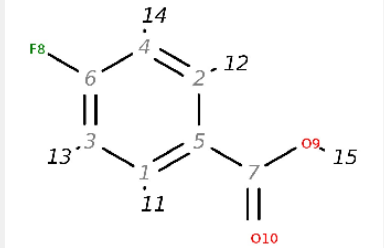
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

File Tools Help

Get integral

Show 2D figure

Water region (PPM):

4.6 5

delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

8 7.9

choose additional couplings for optimization

Choose additional couplings to be optimized

	spins	coupling constant	spin groups ID	coupling groups ID	optimize	keep va
1	11,12	5.5185	group(1)	group(1)	☑	group(1
2	13,14	8.6364	group(2)	group(2)	☑	group(2

Ok Cancel

Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

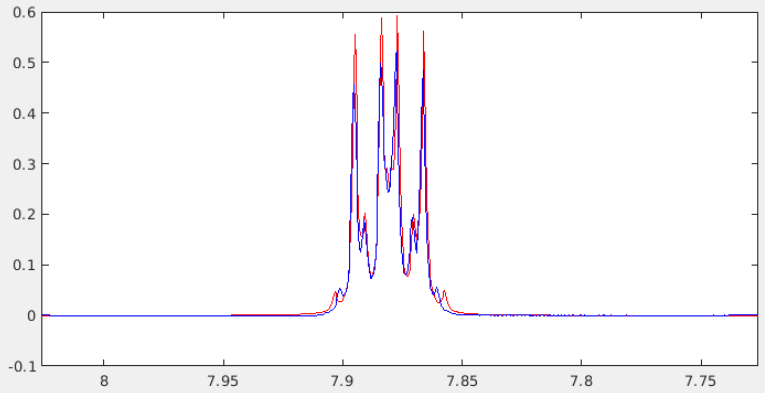
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

ialvalues Load

ROI region: 7.726 to 8.026 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01596

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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

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File Machine View Input Devices Help

Applications Places System

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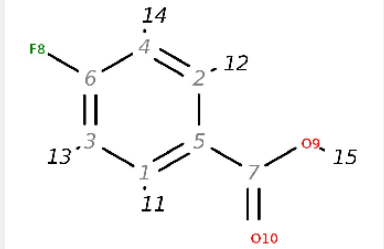
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

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

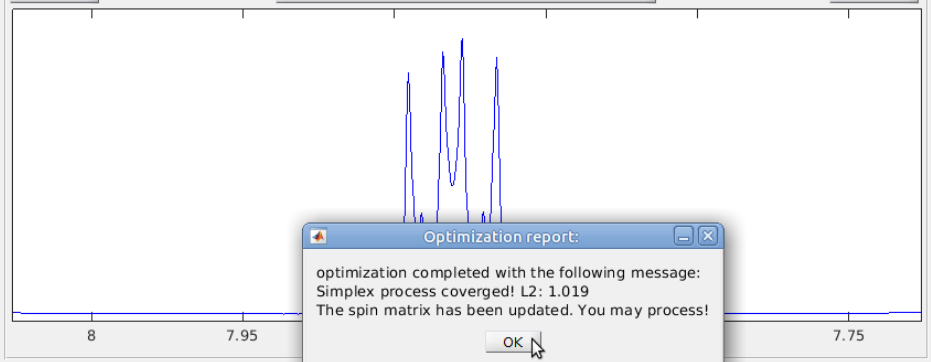
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

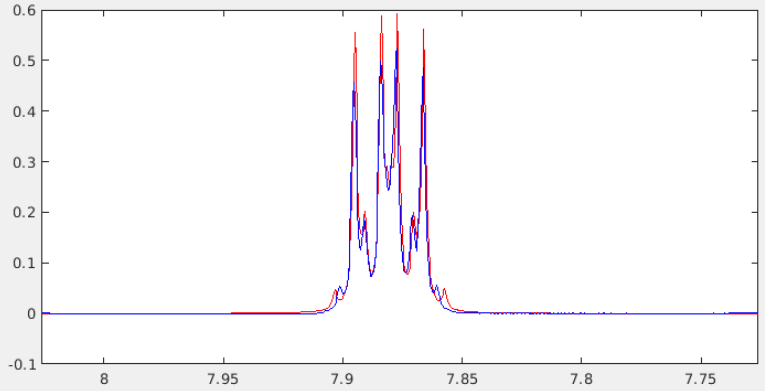
Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 1.019
The spin matrix has been updated. You may process!

OK

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 7.726 to 8.026 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01596

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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

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File Machine View Input Devices Help

Applications Places System

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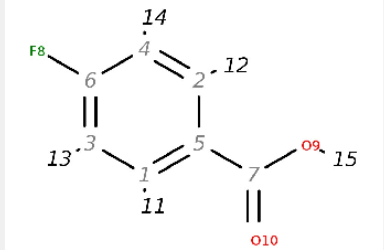
Show 2D figure

InChi=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

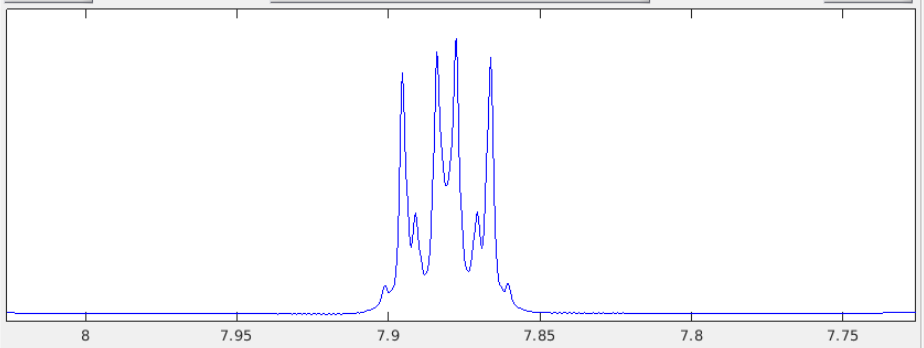
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

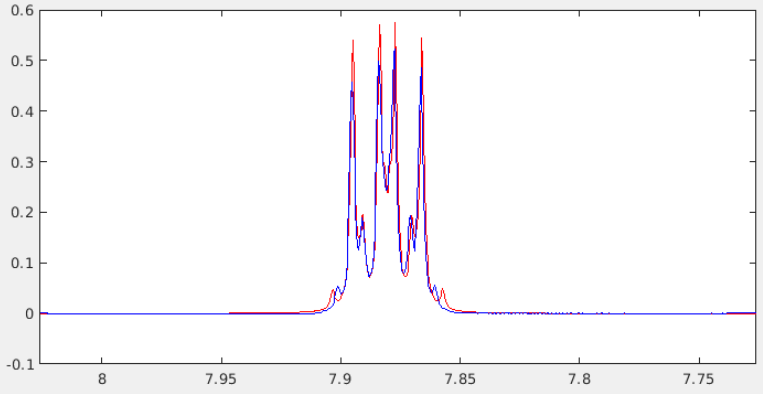
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.726 to 8.026 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01553

p-fluorobenzoic acid(merged)

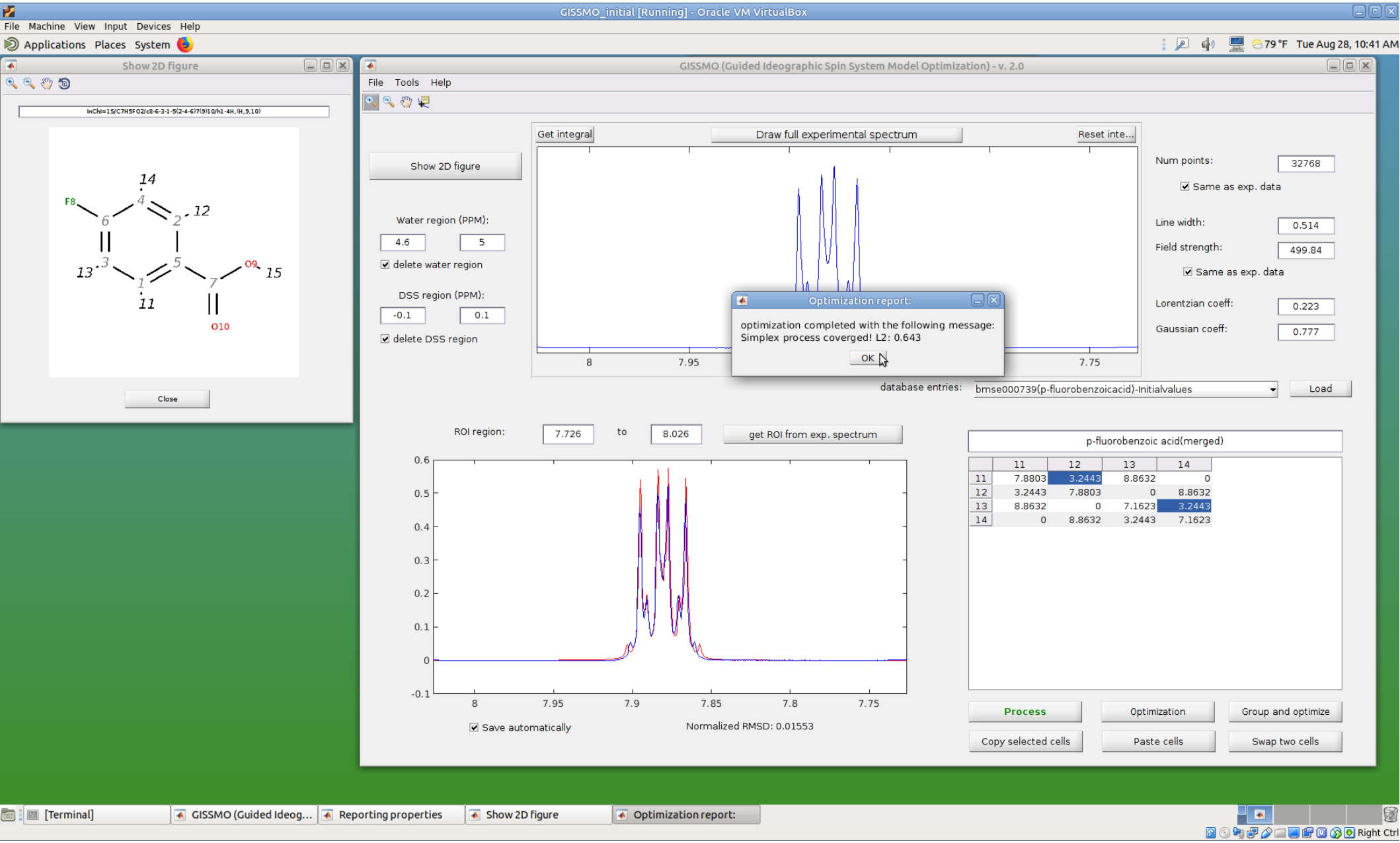
	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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
79 °F Tue Aug 28, 10:41 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
8
7.95
7.75
Optimization report:
optimization completed with the following message:
Simplex process coverged! L2: 0.643
OK
Num points:
32768
Same as exp. data
Line width:
0.514
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.223
Gaussian coeff:
0.777
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
7.726
to
8.026
get ROI from exp. spectrum
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
8
7.95
7.9
7.85
7.8
7.75
Save automatically
Normalized RMSD: 0.01553
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8803 3.2443 8.8632 0
12 3.2443 7.8803 0 8.8632
13 8.8632 0 7.1623 3.2443
14 0 8.8632 3.2443 7.1623
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

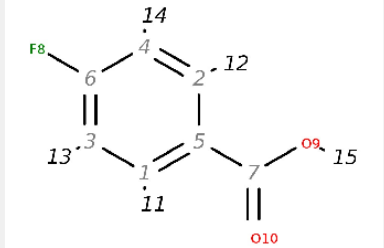
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:41 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

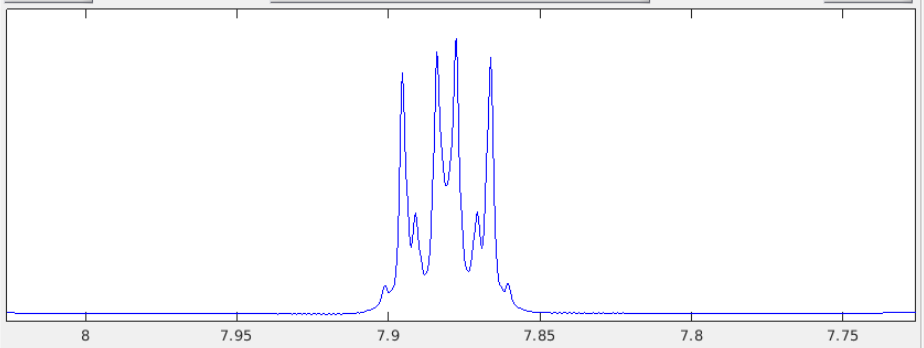
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

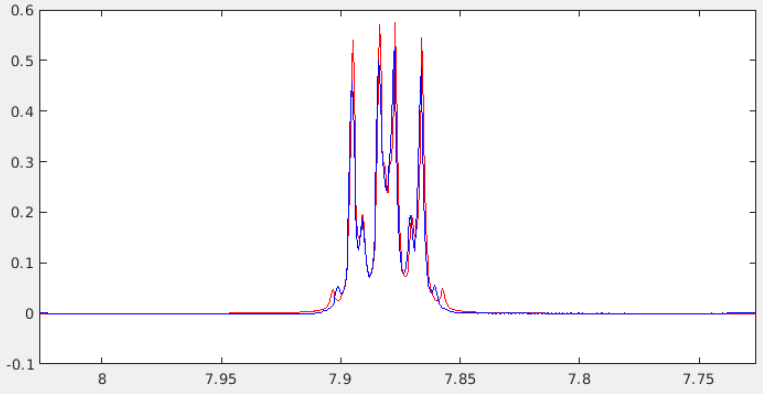
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.726 to 8.026 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01553

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8632	0
12	3.2443	7.8803	0	8.8632
13	8.8632	0	7.1623	3.2443
14	0	8.8632	3.2443	7.1623

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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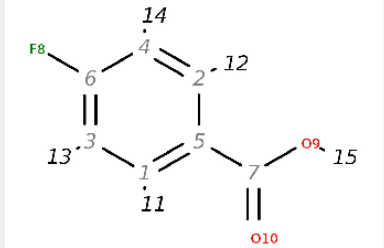
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

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

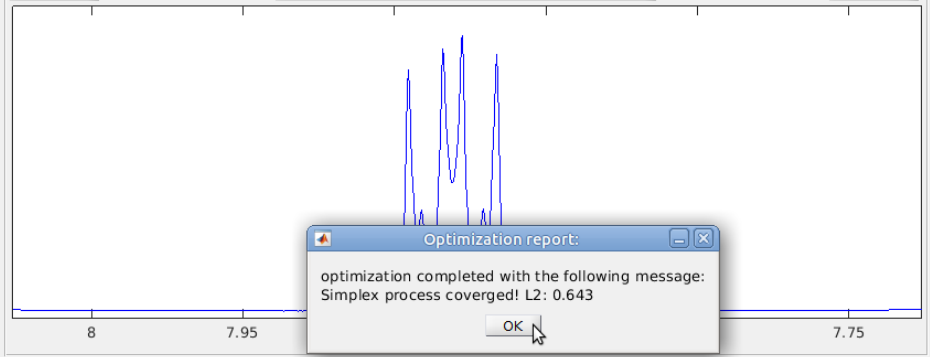
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Optimization report:

optimization completed with the following message:
Simplex process coverged! L2: 0.643

OK

Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

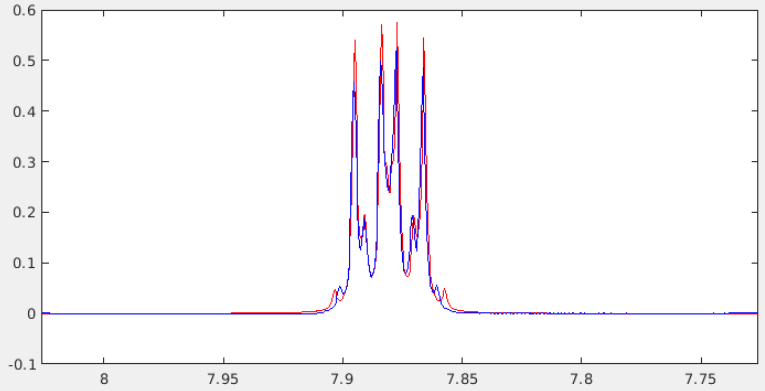
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues Load

ROI region: 7.726 to 8.026 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01553

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8803	3.2443	8.8630	0
12	3.2443	7.8803	0	8.8630
13	8.8630	0	7.1623	3.2443
14	0	8.8630	3.2443	7.1623

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

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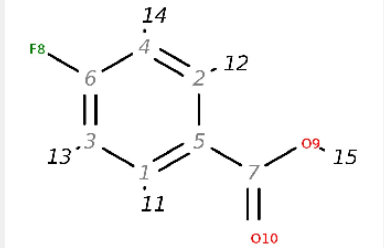
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

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

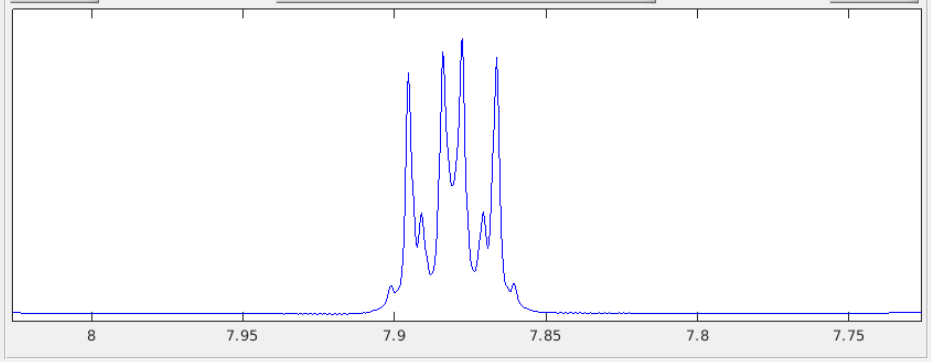
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

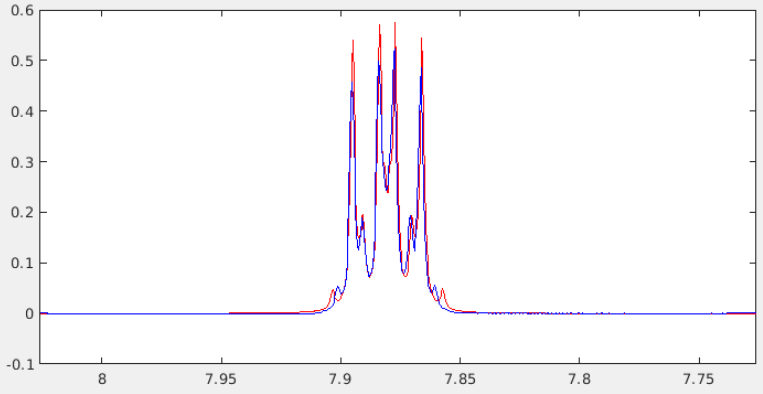
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.726 to 8.026 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.01553

p-fluorobenzoic acid(merged)

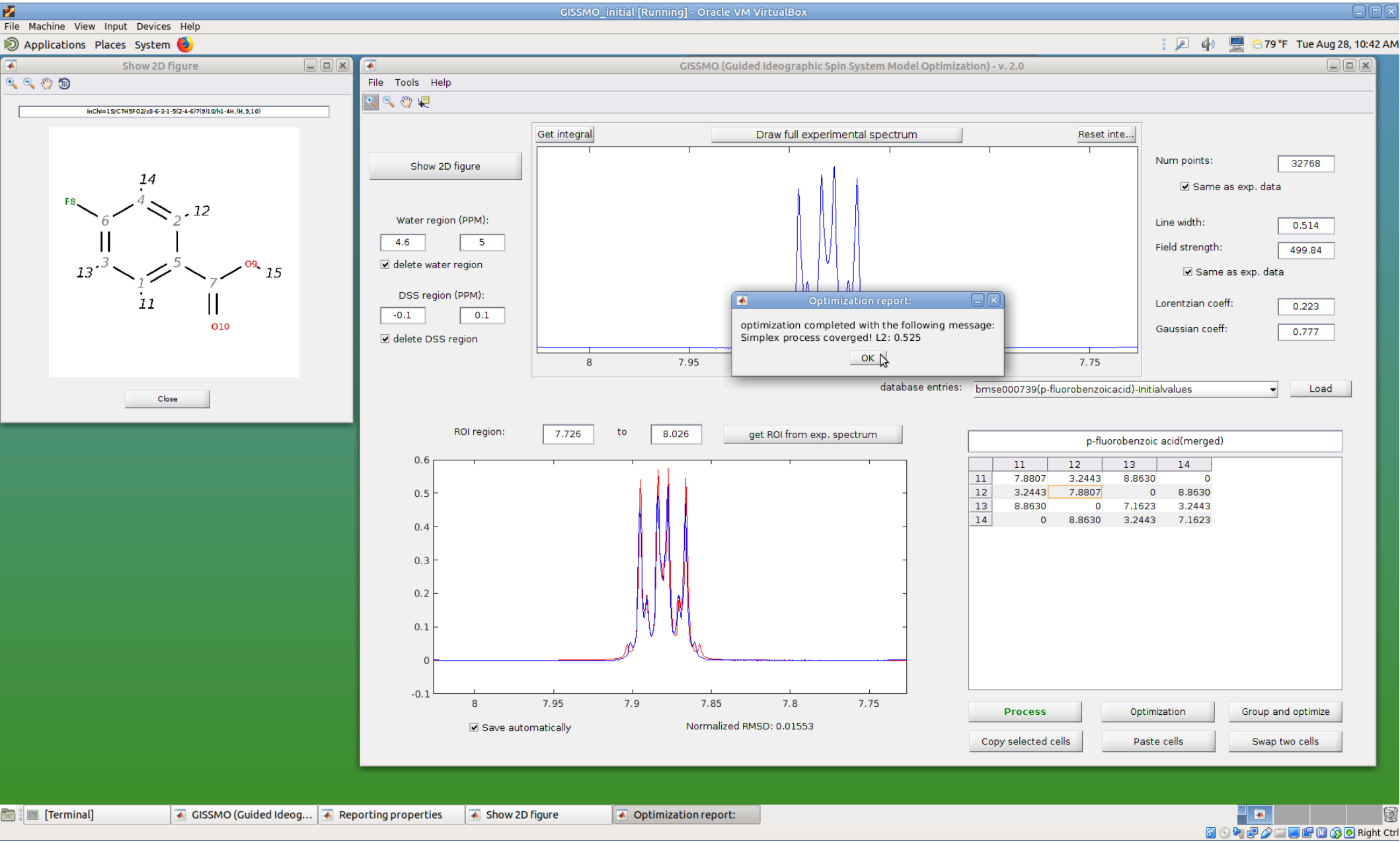
	11	12	13	14
11	7.8803	3.2443	8.8630	0
12	3.2443	7.8803	0	8.8630
13	8.8630	0	7.1623	3.2443
14	0	8.8630	3.2443	7.1623

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
79 °F Tue Aug 28, 10:42 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
8
7.95
7.75
Optimization report:
optimization completed with the following message:
Simplex process coverged! L2: 0.525
OK
Num points:
32768
Same as exp. data
Line width:
0.514
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.223
Gaussian coeff:
0.777
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
7.726
to
8.026
get ROI from exp. spectrum
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
8
7.95
7.9
7.85
7.8
7.75
Save automatically
Normalized RMSD: 0.01553
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8807 3.2443 8.8630 0
12 3.2443 7.8807 0 8.8630
13 8.8630 0 7.1623 3.2443
14 0 8.8630 3.2443 7.1623
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

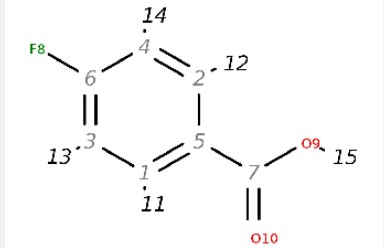
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:43 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

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

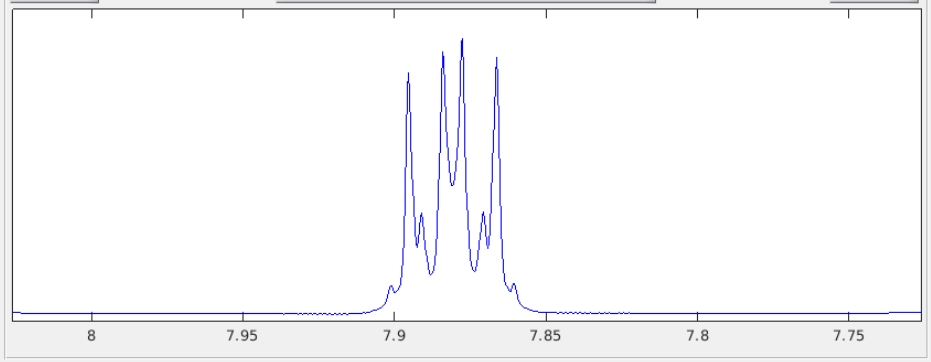
Show 2D figure

Water region (PPM): 4.6 5

delete water region

DSS region (PPM): -0.1 0.1

delete DSS region



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

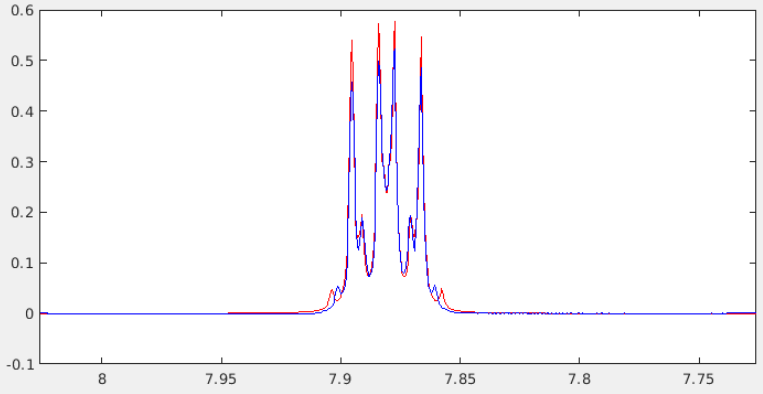
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.726 to 8.026 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.00903

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8807	3.2443	8.8630	0
12	3.2443	7.8807	0	8.8630
13	8.8630	0	7.1623	3.2443
14	0	8.8630	3.2443	7.1623

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

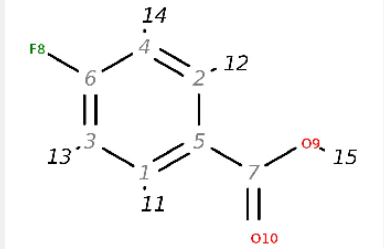
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:43 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

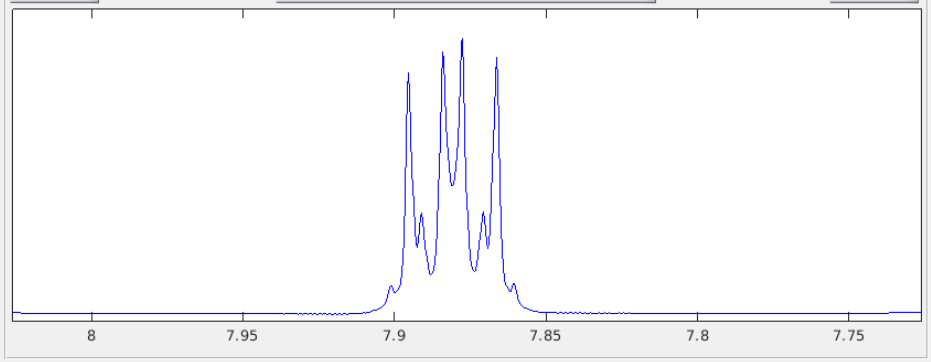
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

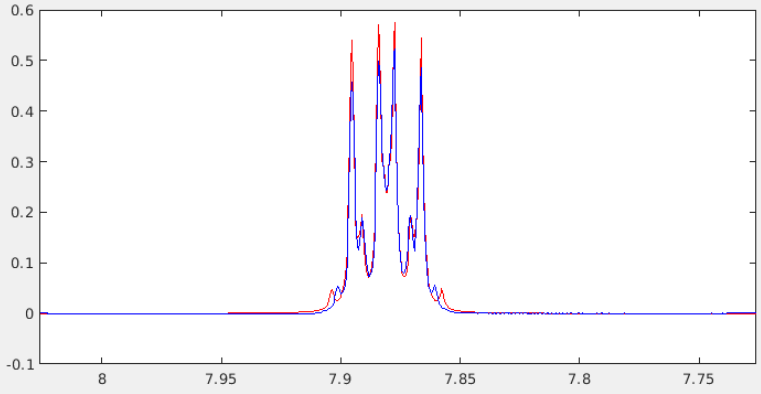
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.726 to 8.026 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.00895

p-fluorobenzoic acid(merged)

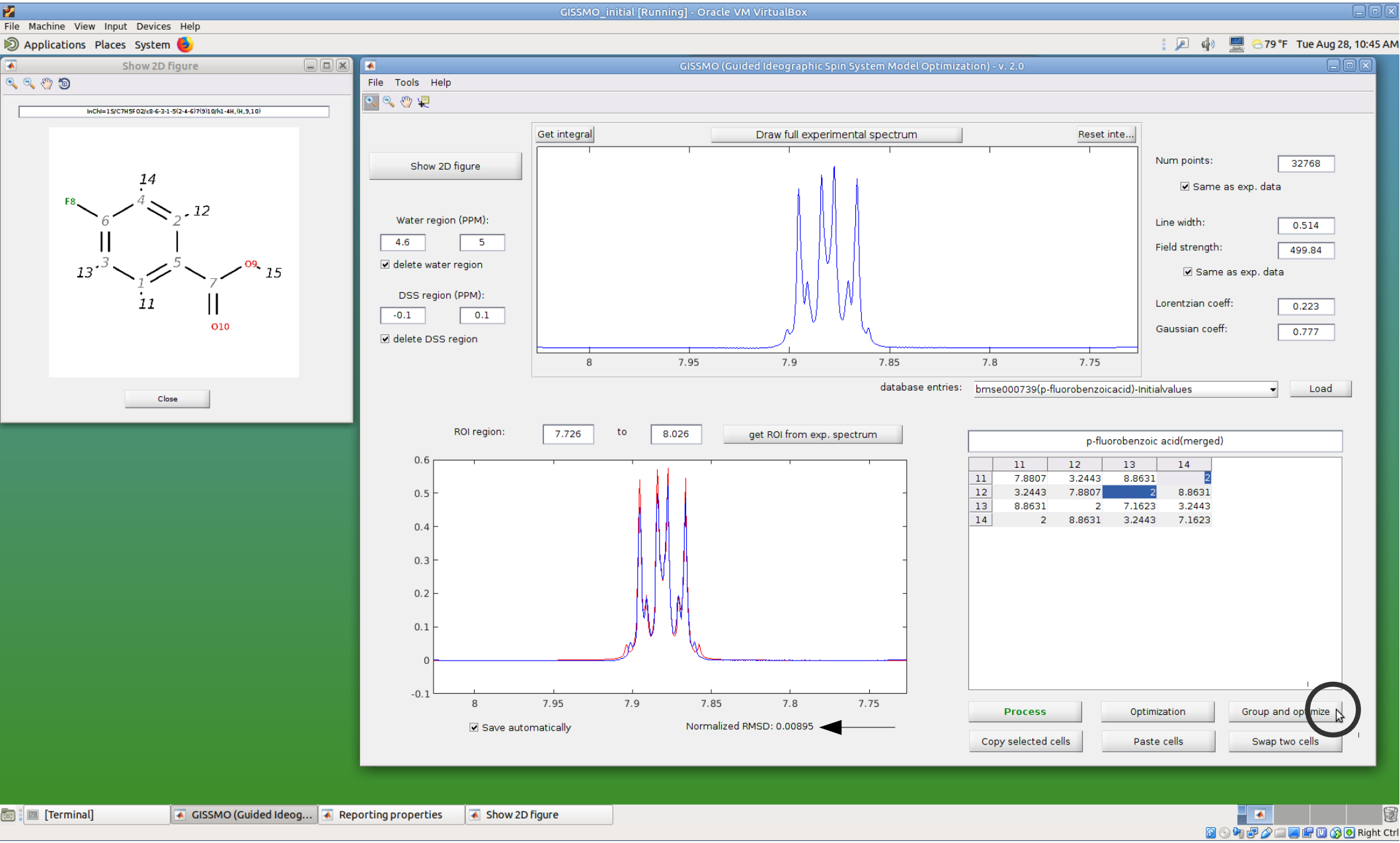
	11	12	13	14
11	7.8807	3.2443	8.8631	0
12	3.2443	7.8807	0	8.8631
13	8.8631	0	7.1623	3.2443
14	0	8.8631	3.2443	7.1623

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
79 °F Tue Aug 28, 10:45 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
Close
GISSMO (Guided Ideographic Spin System Model Optimization) - v. 2.0
File Tools Help
Get integral
Draw full experimental spectrum
Reset inte...
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
8
7.95
7.9
7.85
7.8
7.75
Num points:
32768
Same as exp. data
Line width:
0.514
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.223
Gaussian coeff:
0.777
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
7.726
to
8.026
get ROI from exp. spectrum
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
8
7.95
7.9
7.85
7.8
7.75
Save automatically
Normalized RMSD: 0.00895
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8807 3.2443 8.8631 2
12 3.2443 7.8807 2 8.8631
13 8.8631 2 7.1623 3.2443
14 2 8.8631 3.2443 7.1623
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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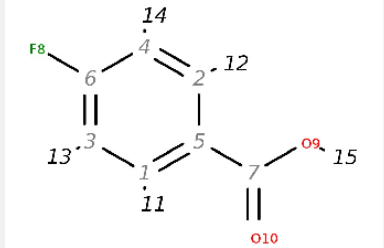
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

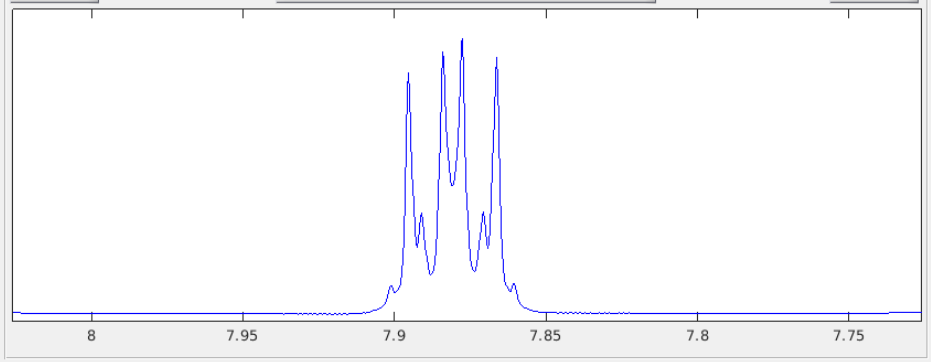
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

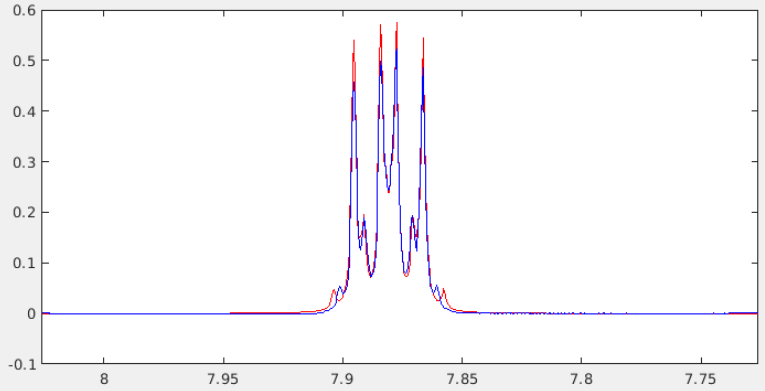
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues | Load

ROI region: 7.726 to 8.026 | get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.00895

p-fluorobenzoic acid(merged)

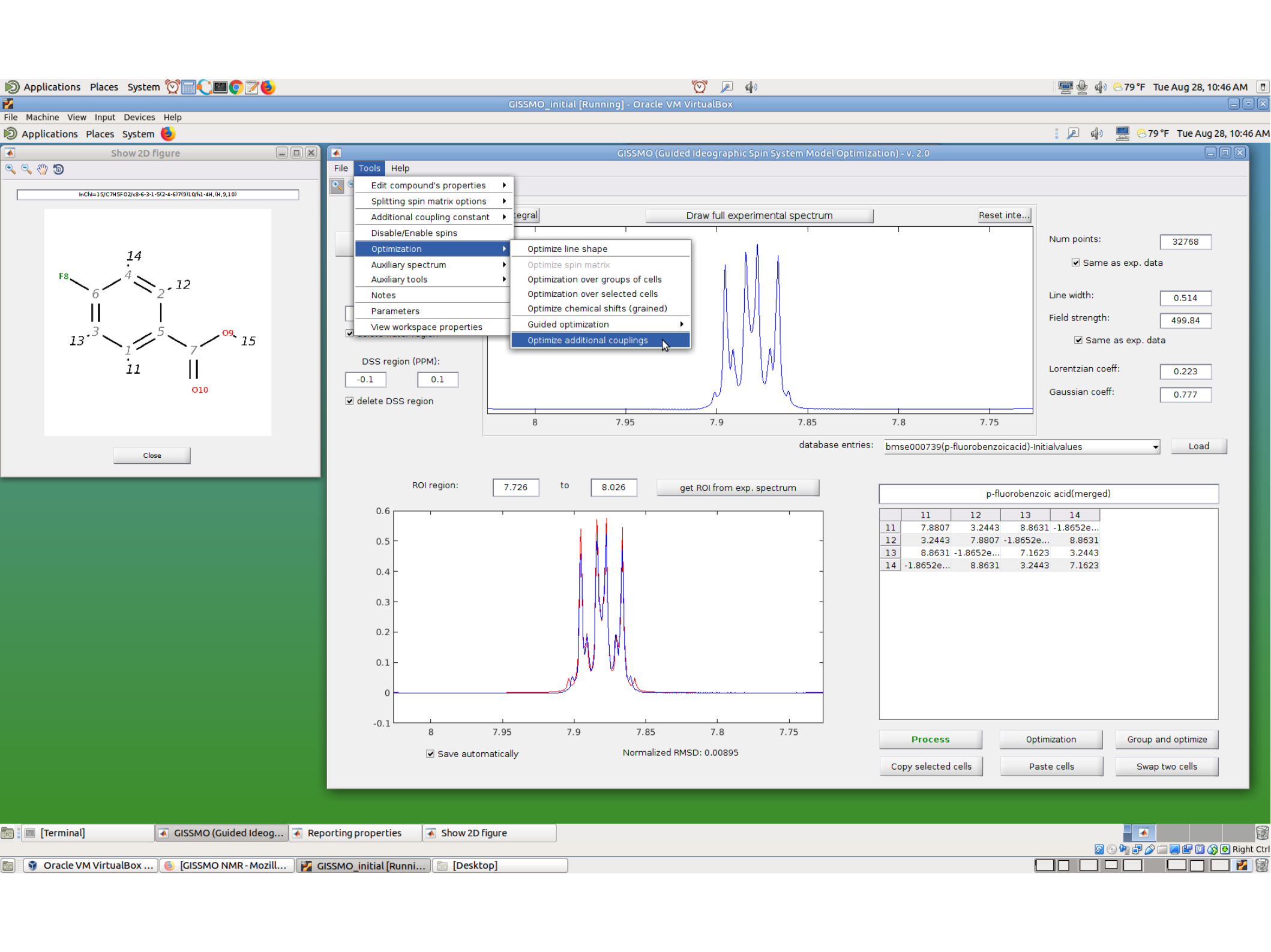
	11	12	13	14
11	7.8807	3.2443	8.8631	-1.8652e...
12	3.2443	7.8807	-1.8652e...	8.8631
13	8.8631	-1.8652e...	7.1623	3.2443
14	-1.8652e...	8.8631	3.2443	7.1623

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl


Applications Places System
79 °F Tue Aug 28, 10:46 AM
GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
79 °F Tue Aug 28, 10:46 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
14
4
6
2
12
13
3
5
1
7
O9
15
11
O10
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 inte...
Num points:
32768
Same as exp. data
Line width:
0.514
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.223
Gaussian coeff:
0.777
DSS region (PPM):
-0.1
0.1
delete DSS region
8
7.95
7.9
7.85
7.8
7.75
database entries:
bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region:
7.726
to
8.026
get ROI from exp. spectrum
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
8
7.95
7.9
7.85
7.8
7.75
Save automatically
Normalized RMSD: 0.00895
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8807 3.2443 8.8631 -1.8652e...
12 3.2443 7.8807 -1.8652e... 8.8631
13 8.8631 -1.8652e... 7.1623 3.2443
14 -1.8652e... 8.8631 3.2443 7.1623
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 ...
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[Desktop]
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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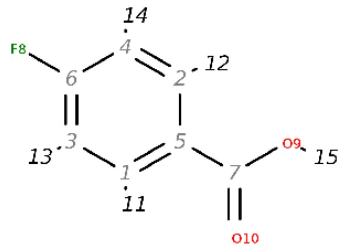
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

File Tools Help

Get integral

Show 2D figure

Water region (PPM):

4.6 5

delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

8 7.9

choose additional couplings for optimization

Choose additional couplings to be optimized

	spins	coupling constant	spin groups ID	coupling groups ID	optimize	keep va
1	11,12	5.6170	group(1)	group(1)	☑	group(1
2	13,14	8.7156	group(2)	group(2)	☑	group(2

OK Cancel

Num points: 32768

Same as exp. data

Line width: 0.514

Field strength: 499.84

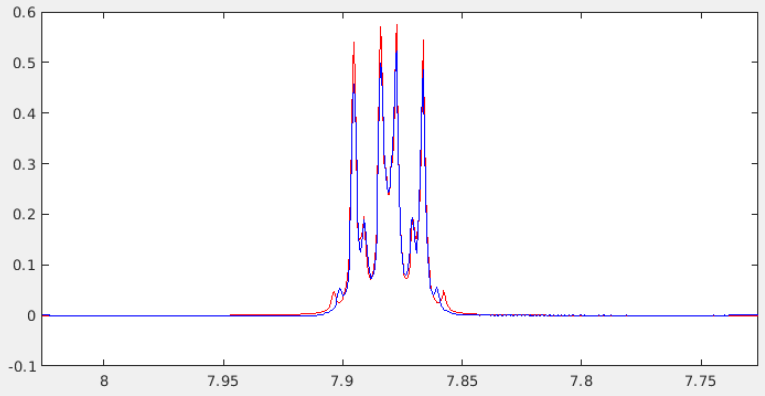
Same as exp. data

Lorentzian coeff: 0.223

Gaussian coeff: 0.777

ialvalues Load

ROI region: 7.726 to 8.026 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.00895

p-fluorobenzoic acid(merged)

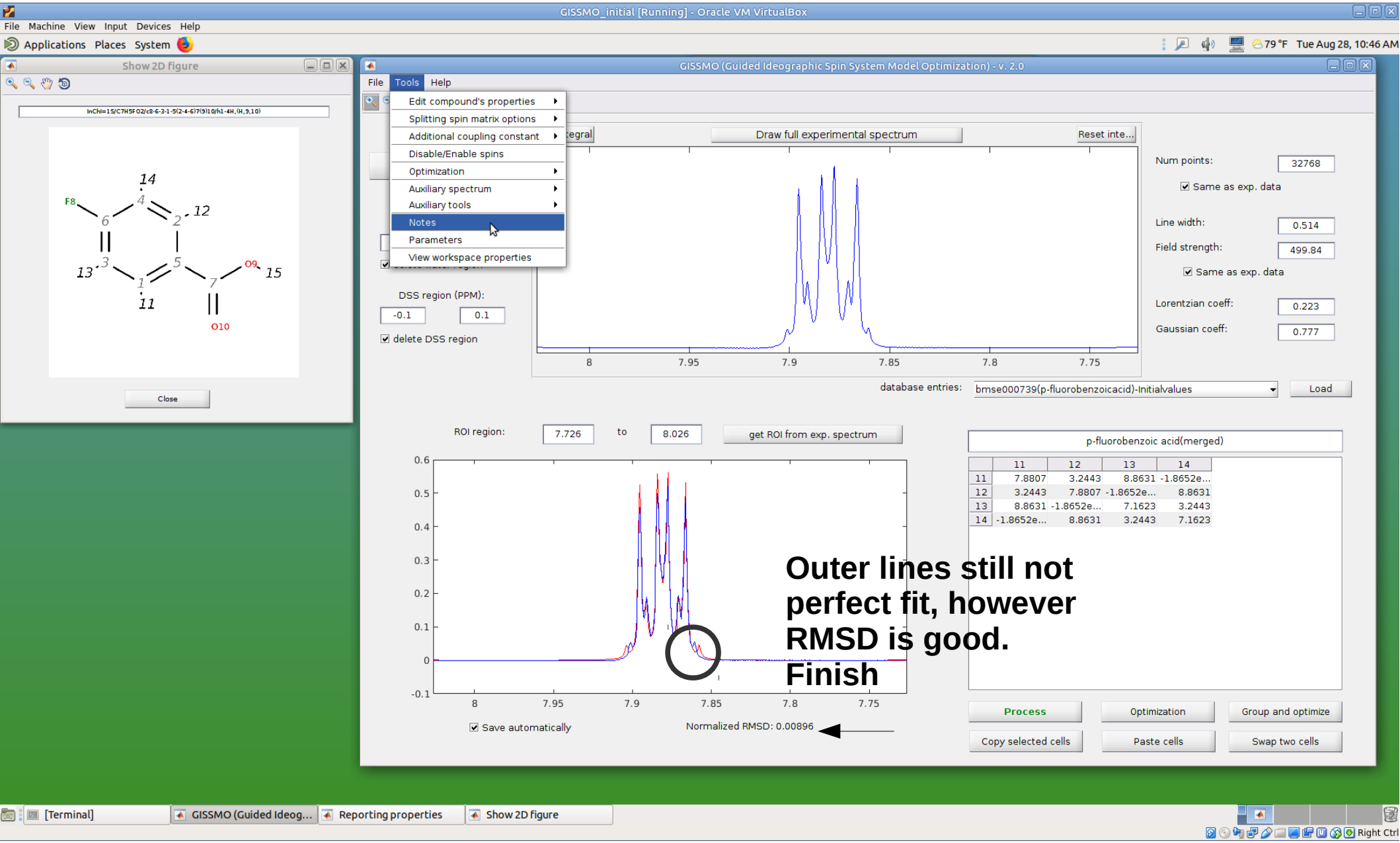
	11	12	13	14
11	7.8807	3.2443	8.8631	-1.8652e...
12	3.2443	7.8807	-1.8652e...	8.8631
13	8.8631	-1.8652e...	7.1623	3.2443
14	-1.8652e...	8.8631	3.2443	7.1623

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
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
Draw full experimental spectrum
Reset inte...
Num points: 32768
Same as exp. data
Line width: 0.514
Field strength: 499.84
Same as exp. data
Lorentzian coeff: 0.223
Gaussian coeff: 0.777
DSS region (PPM):
-0.1
0.1
delete DSS region
database entries: bmse000739(p-fluorobenzoicacid)-Initialvalues
Load
ROI region: 7.726 to 8.026
get ROI from exp. spectrum
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8807 3.2443 8.8631 -1.8652e...
12 3.2443 7.8807 -1.8652e... 8.8631
13 8.8631 -1.8652e... 7.1623 3.2443
14 -1.8652e... 8.8631 3.2443 7.1623
Outer lines still not perfect fit, however RMSD is good.
Finish
Save automatically
Normalized RMSD: 0.00896
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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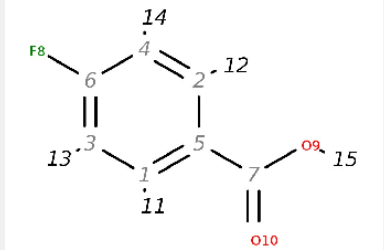
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

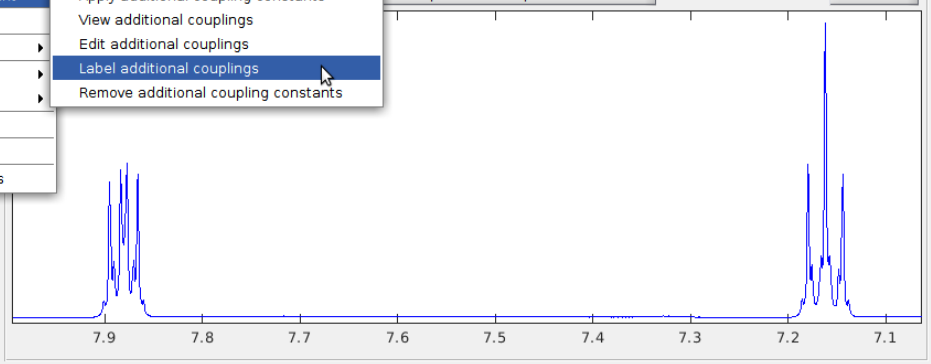
File Tools Help

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

full experimental spectrum

Reset inte...



Num points: 32768

Same as exp. data

Line width: 0.542

Field strength: 499.84

Same as exp. data

Lorentzian coeff: 0.769

Gaussian coeff: 0.231

DSS region (PPM):

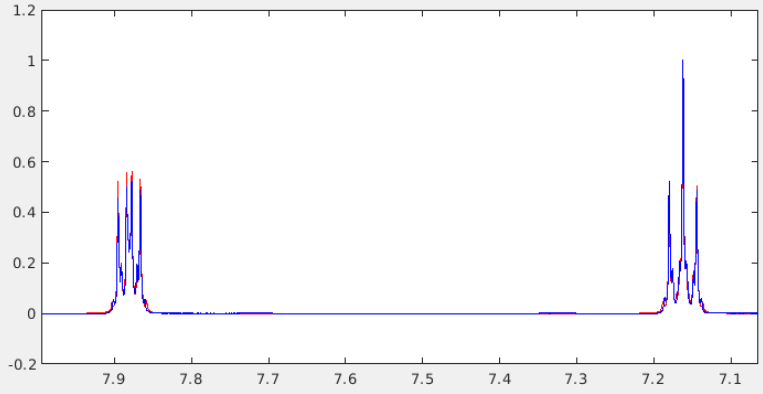
-0.1 0.1

delete DSS region

database entries: bmse000739(p-fluorobenzoic acid)-Initial values

Load

ROI region: 7.064 to 7.994 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.00724

p-fluorobenzoic acid(merged)

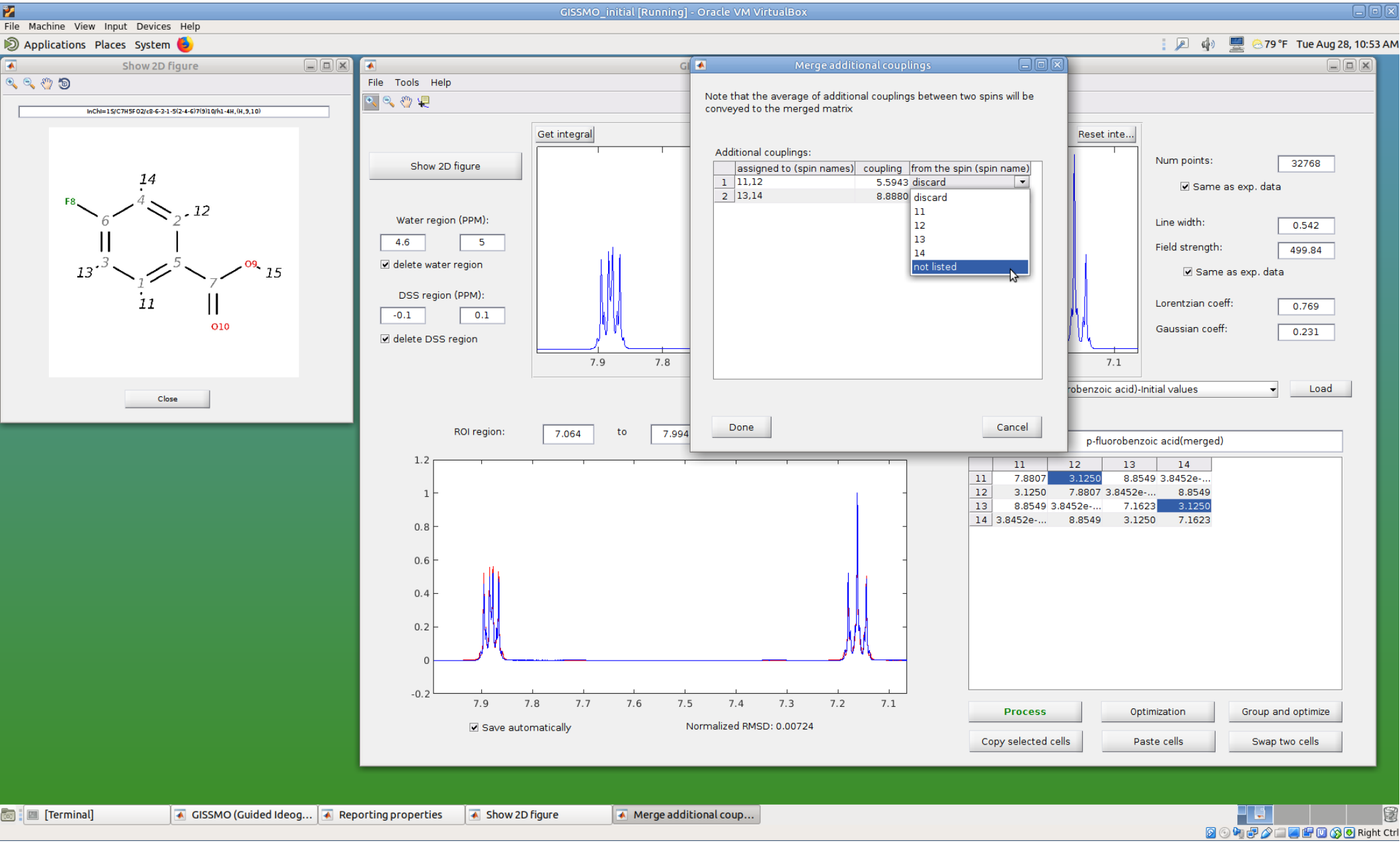
	11	12	13	14
11	7.8807	3.1250	8.8549	3.8452e-...
12	3.1250	7.8807	3.8452e-...	8.8549
13	8.8549	3.8452e-...	7.1623	3.1250
14	3.8452e-...	8.8549	3.1250	7.1623

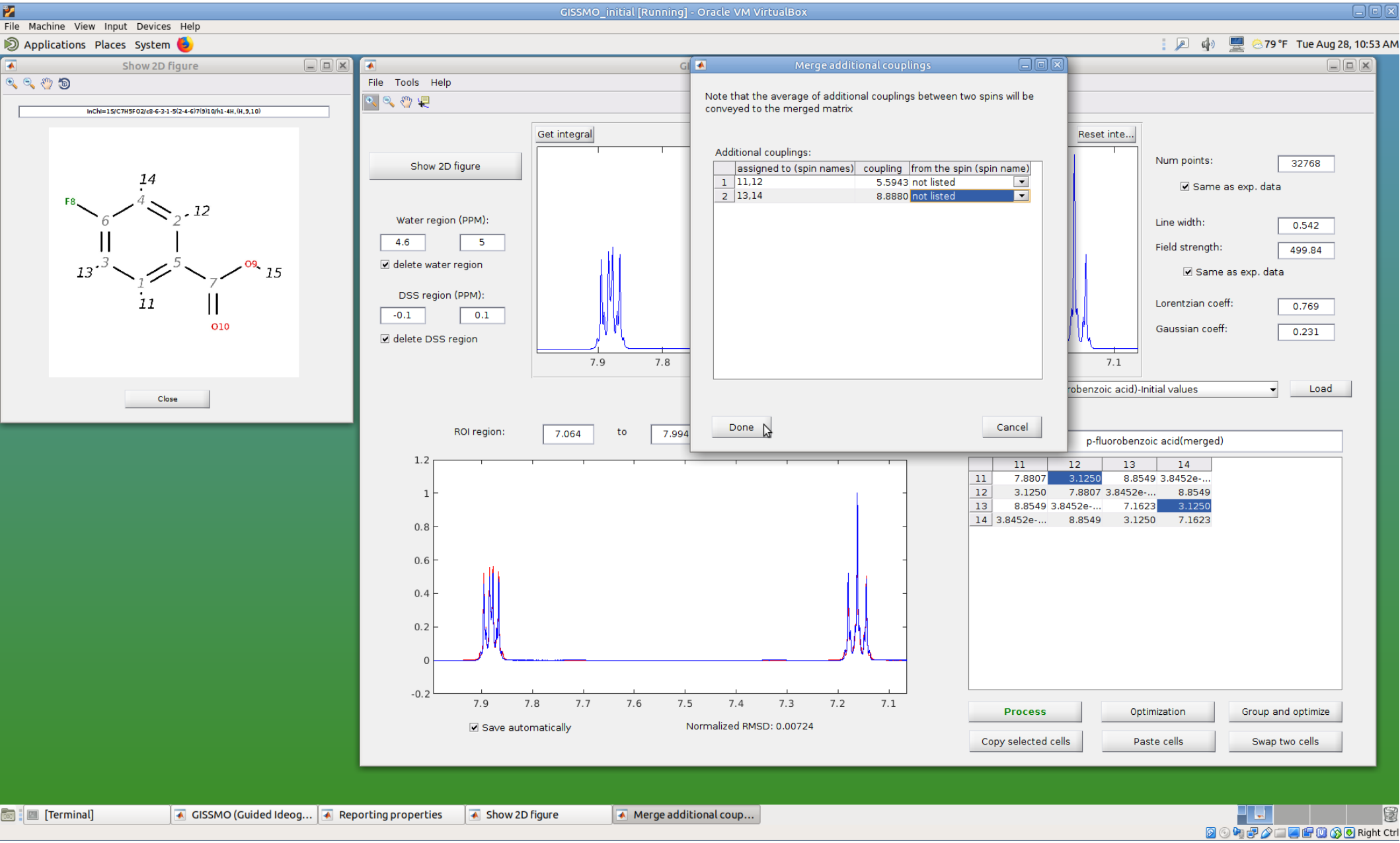
Process Optimization Group and optimize

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
79 °F Tue Aug 28, 10:53 AM
Show 2D figure
Close
File Tools Help
Show 2D figure
Get integral
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
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)
11,12
5.5943
13,14
8.8880
discard
11
12
13
14
not listed
Done
Cancel
Reset inte...
Num points:
32768
Same as exp. data
Line width:
0.542
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.769
Gaussian coeff:
0.231
Load
ROI region:
7.064
to
7.994
p-fluorobenzoic acid(merged)
Save automatically
Normalized RMSD: 0.00724
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Merge additional coup...


GISSMO_initial [Running] - Oracle VM VirtualBox
File Machine View Input Devices Help
Applications Places System
79 °F Tue Aug 28, 10:53 AM
Show 2D figure
Close
File Tools Help
Show 2D figure
Get integral
Reset inte...
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Num points:
32768
Same as exp. data
Line width:
0.542
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.769
Gaussian coeff:
0.231
Load
ROI region:
7.064
to
7.994
Save automatically
Normalized RMSD: 0.00724
p-fluorobenzoic acid(merged)
Process
Optimization
Group and optimize
Copy selected cells
Paste cells
Swap two cells
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)
11,12
5.5943
not listed
13,14
8.8880
not listed
Done
Cancel
[Terminal]
GISSMO (Guided Ideog...
Reporting properties
Show 2D figure
Merge additional coup...
Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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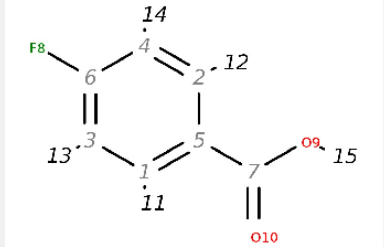
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

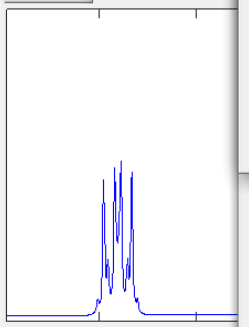
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral



Non hydrigen additional coupling

Add note for additional couplings on spins

11,12

with additional couplings of

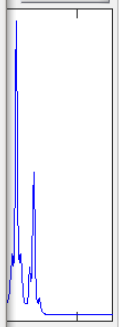
5.59427

F8

Done

Done Cancel

Reset inte...



Num points: 32768

Same as exp. data

Line width: 0.542

Field strength: 499.84

Same as exp. data

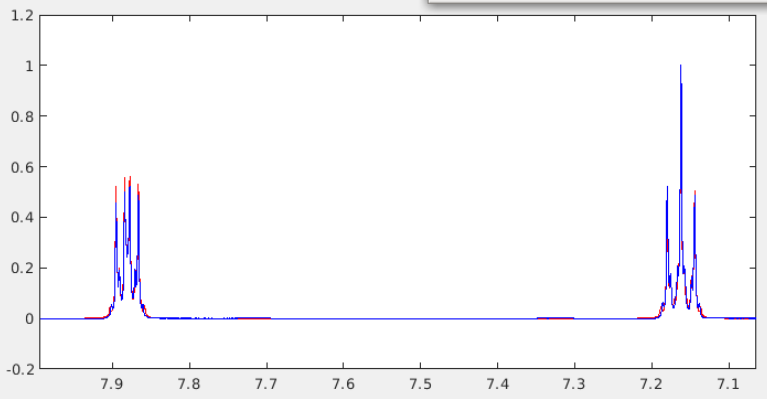
Lorentzian coeff: 0.769

Gaussian coeff: 0.231

robenzoic acid)-Initial values Load

ROI region: 7.064 to 7.994

p-fluorobenzoic acid(merged)



	11	12	13	14
11	7.8807	3.1250	8.8549	3.8452e-...
12	3.1250	7.8807	3.8452e-...	8.8549
13	8.8549	3.8452e-...	7.1623	3.1250
14	3.8452e-...	8.8549	3.1250	7.1623

Save automatically

Normalized RMSD: 0.00724

Process Optimization Group and optimize

Copy selected cells Paste cells Swap two cells

[Terminal] GISSMO (Guided Ideog... Reporting properties Show 2D figure Merge additional coup... Non hydrigen addition...

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

File Machine View Input Devices Help

Applications Places System

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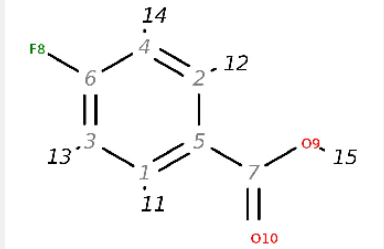
Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

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

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

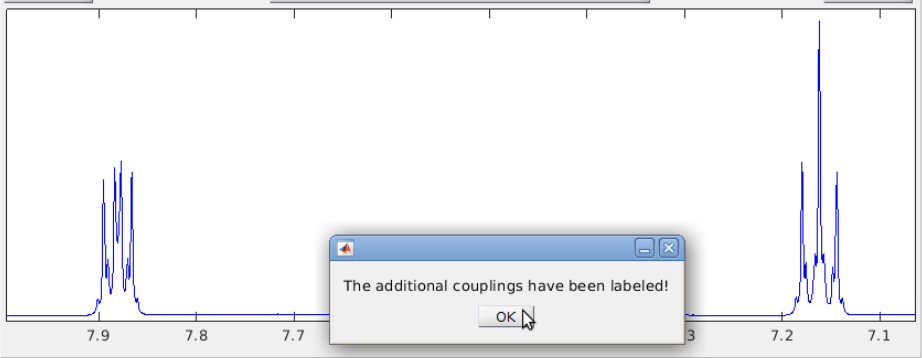
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

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



The additional couplings have been labeled!

OK

Num points: 32768

Same as exp. data

Line width: 0.542

Field strength: 499.84

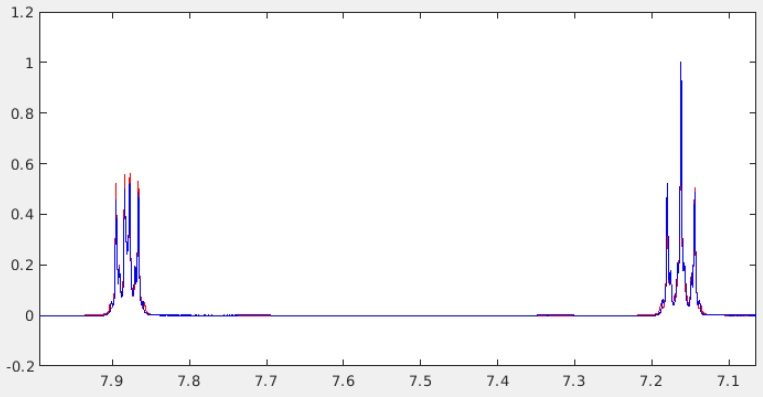
Same as exp. data

Lorentzian coeff: 0.769

Gaussian coeff: 0.231

database entries: bmse000739(p-fluorobenzoic acid)-Initial values | Load

ROI region: 7.064 to 7.994 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.00724

p-fluorobenzoic acid(merged)

	11	12	13	14
11	7.8807	3.1250	8.8549	3.8452e-...
12	3.1250	7.8807	3.8452e-...	8.8549
13	8.8549	3.8452e-...	7.1623	3.1250
14	3.8452e-...	8.8549	3.1250	7.1623

Process | Optimization | Group and optimize

Copy selected cells | Paste cells | Swap two cells

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

Right Ctrl

GISSMO_initial [Running] - Oracle VM VirtualBox

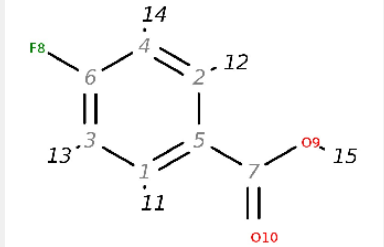
File Machine View Input Devices Help

Applications Places System

79 °F Tue Aug 28, 10:55 AM

Show 2D figure

InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)



Close

File Tools Help

Show 2D figure

Water region (PPM):

4.6 5

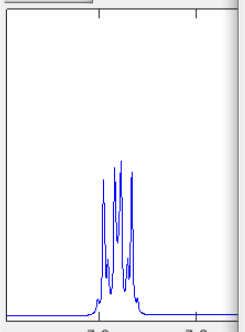
delete water region

DSS region (PPM):

-0.1 0.1

delete DSS region

Get integral



Notes

Status:

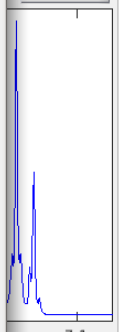
Initial values

Notes:

Non-hydrogen additional coupling;
spin name(s):"11,12", coupling of "5.594271" with "F8"
spin name(s):"13,14", coupling of "8.888026" with "F8"

Apply Cancel

Reset inte...



Num points: 32768

Same as exp. data

Line width: 0.542

Field strength: 499.84

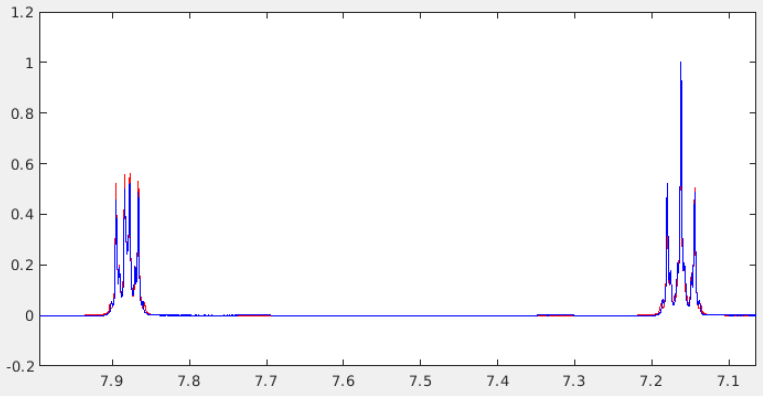
Same as exp. data

Lorentzian coeff: 0.769

Gaussian coeff: 0.231

database entries: bmse000739(p-fluorobenzoic acid)-Initial values Load

ROI region: 7.064 to 7.994 get ROI from exp. spectrum



Save automatically

Normalized RMSD: 0.00724

p-fluorobenzoic acid(merged)

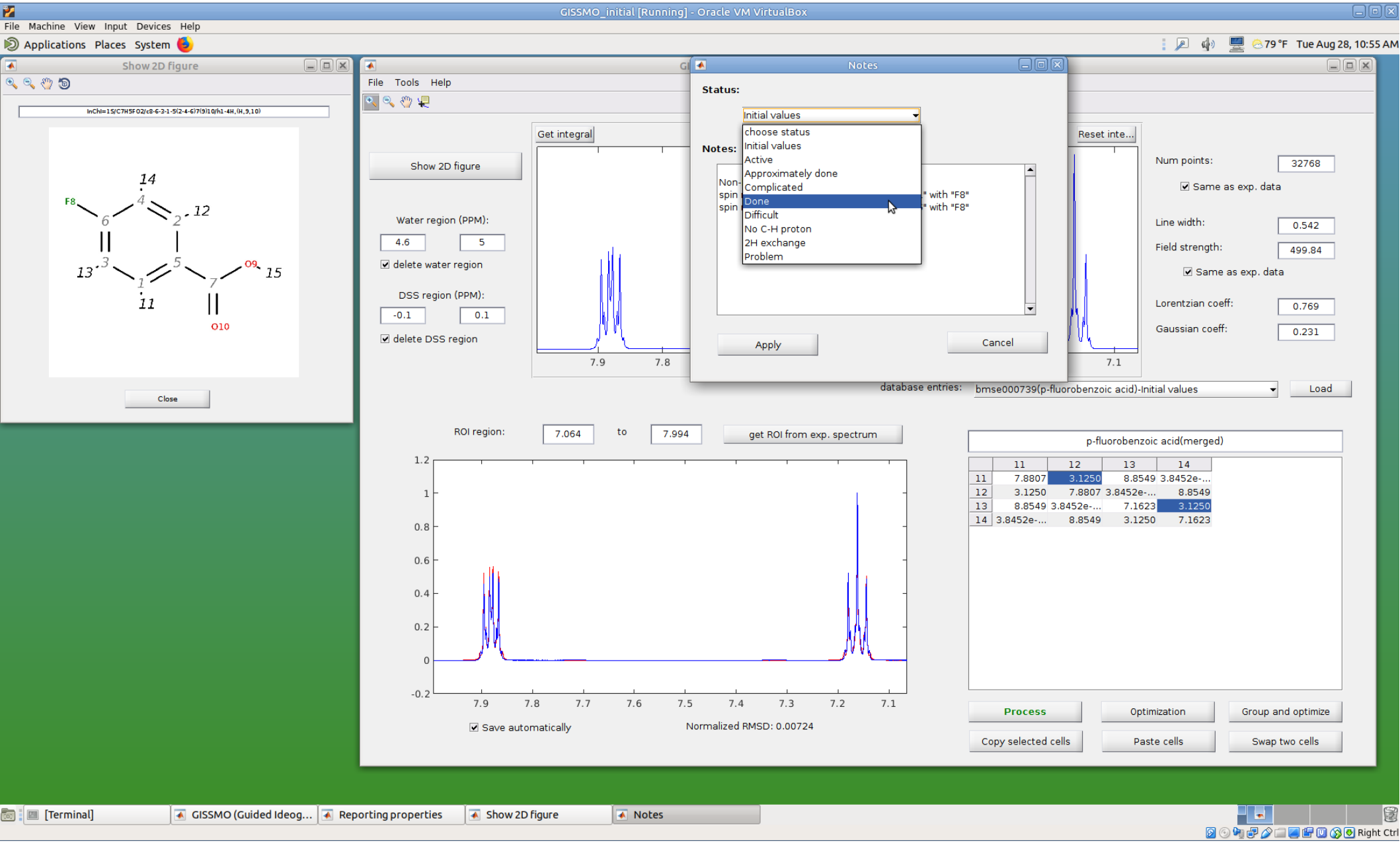
	11	12	13	14
11	7.8807	3.1250	8.8549	3.8452e-...
12	3.1250	7.8807	3.8452e-...	8.8549
13	8.8549	3.8452e-...	7.1623	3.1250
14	3.8452e-...	8.8549	3.1250	7.1623

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
79 °F Tue Aug 28, 10:55 AM
Show 2D figure
InChI=1S/C7H5FO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
F8
O9
O10
Close
File Tools Help
Show 2D figure
Water region (PPM):
4.6
5
delete water region
DSS region (PPM):
-0.1
0.1
delete DSS region
Get integral
Reset inte...
Notes
Status:
Initial values
choose status
Initial values
Active
Approximately done
Complicated
Done
Difficult
No C-H proton
2H exchange
Problem
Notes:
Apply
Cancel
Num points:
32768
Same as exp. data
Line width:
0.542
Field strength:
499.84
Same as exp. data
Lorentzian coeff:
0.769
Gaussian coeff:
0.231
database entries:
bmse000739(p-fluorobenzoic acid)-Initial values
Load
ROI region:
7.064
to
7.994
get ROI from exp. spectrum
Save automatically
Normalized RMSD: 0.00724
p-fluorobenzoic acid(merged)
11 12 13 14
11 7.8807 3.1250 8.8549 3.8452e-...
12 3.1250 7.8807 3.8452e-... 8.8549
13 8.8549 3.8452e-... 7.1623 3.1250
14 3.8452e-... 8.8549 3.1250 7.1623
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